



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 20, 2021 – 10:32 PM JST

PDB ID : 7CJI  
Title : Photosystem II structure in the S1 state  
Authors : Li, H.; Shen, J.-R.; Suga, M.  
Deposited on : 2020-07-11  
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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

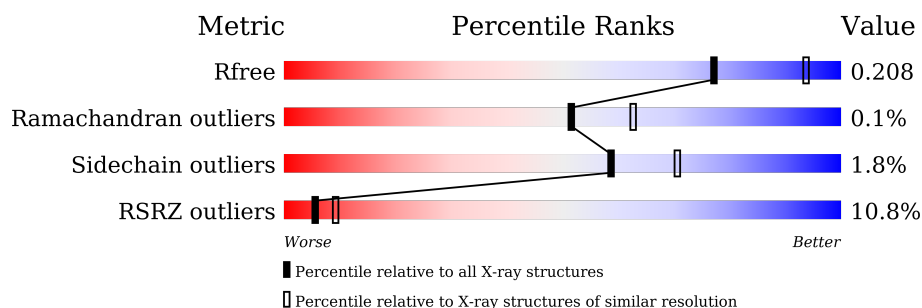
# 1 Overall quality at a glance

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 of 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>6%</div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div>8%</div> <div>96%</div> <div>..</div> </div>
2	B	505	<div> <div>6%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>12%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>8%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>10%</div> <div>99%</div> <div>.</div> </div>
4	D	342	<div> <div>6%</div> <div>99%</div> <div>.</div> </div>

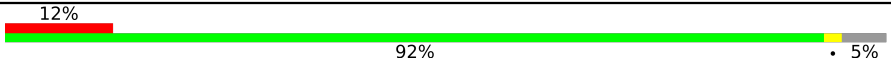
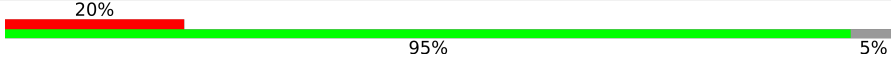
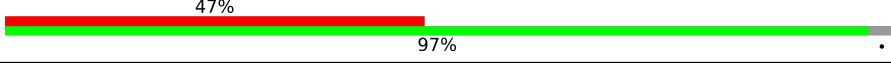
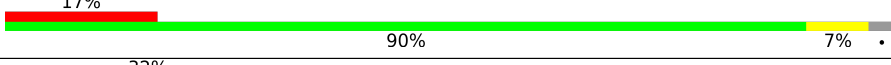
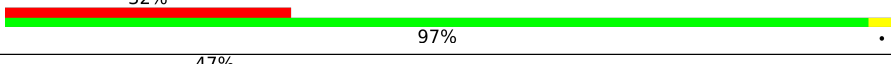
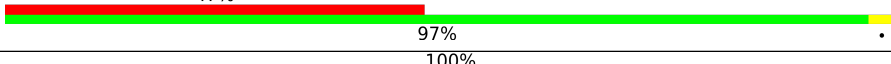

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16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

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Mol	Chain	Length	Quality of chain
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
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
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
27	SQD	f	102	-	-	-	X
30	UNL	A	414	-	-	-	X
30	UNL	j	101	-	-	-	X
31	LMG	C	521	-	-	-	X
33	HTG	B	622	-	-	-	X
33	HTG	b	622	-	-	-	X
34	LMT	C	525	-	-	-	X
34	LMT	a	412	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	e	101	-	-	-	X
34	LMT	m	103	-	-	-	X

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53071 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	2	0
			2634	1725	433	461	15			
1	a	334	Total	C	N	O	S	0	3	0
			2642	1731	434	462	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
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	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
			3513	2295	588	617	13			
3	c	455	Total	C	N	O	S	0	2	0
			3534	2311	591	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

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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	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	1	0
			668	435	108	125				
5	e	79	Total	C	N	O		0	0	0
			648	424	105	119				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

- Molecule 10 is a protein called Photosystem II 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	36	Total	C	N	O	0	1	0
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

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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	3	0
			1886	1177	318	386	5			
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O		0	0	0
			765	486	128	151				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

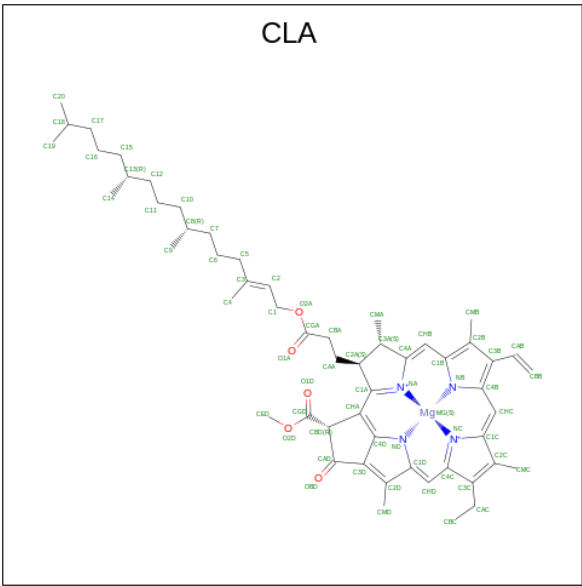
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



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

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

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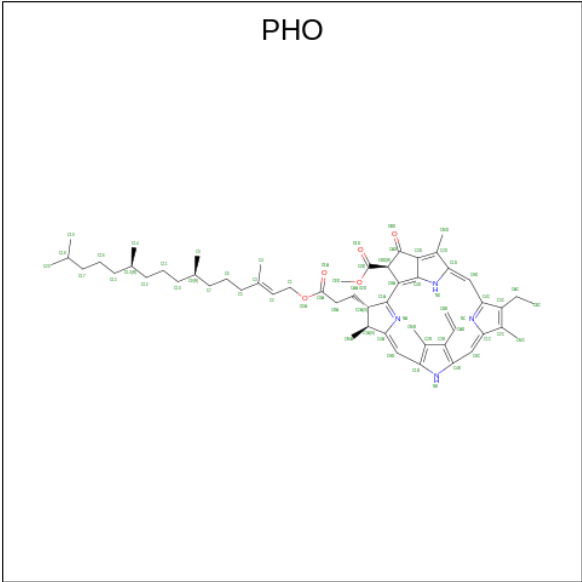
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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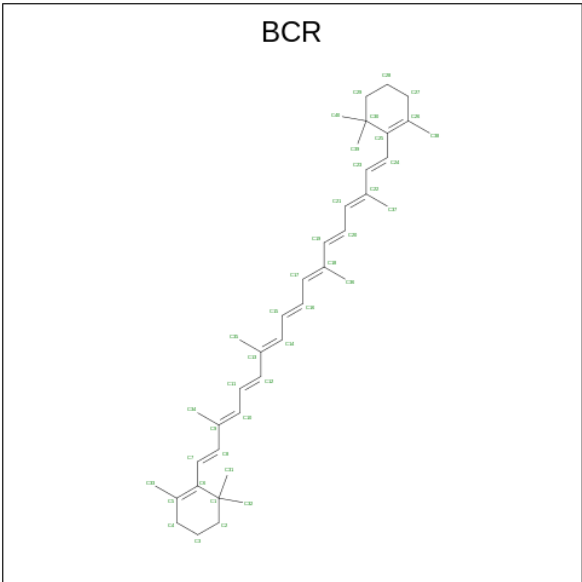
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

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



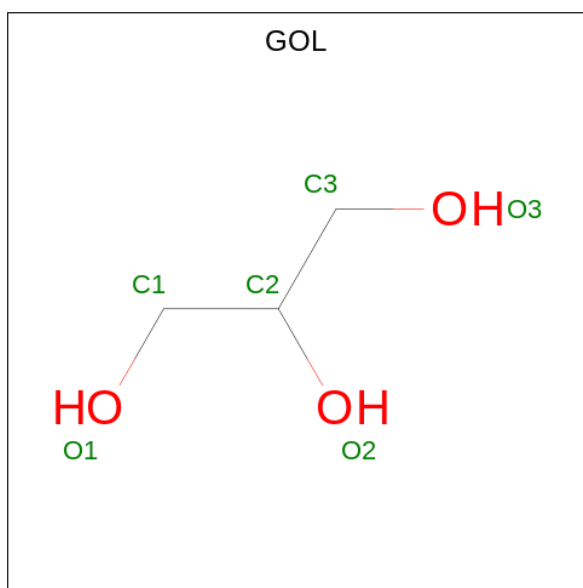
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

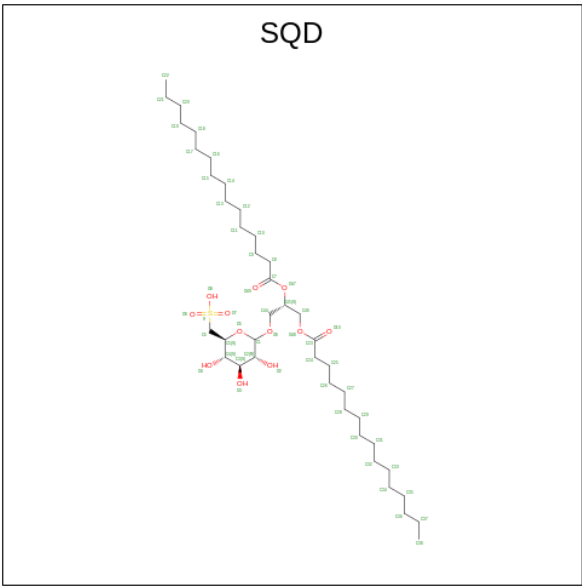
- Molecule 26 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

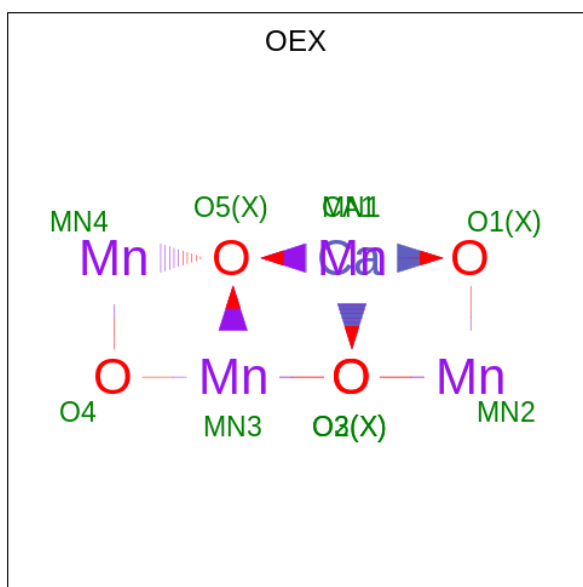
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



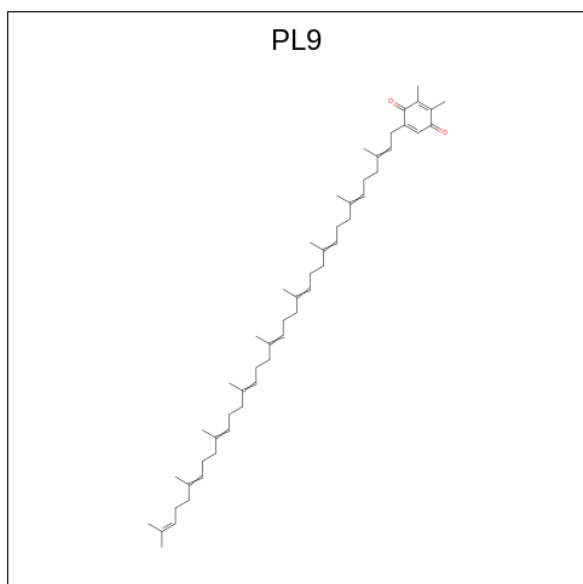
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	C	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0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

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn<sub>4</sub>O<sub>5</sub>).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



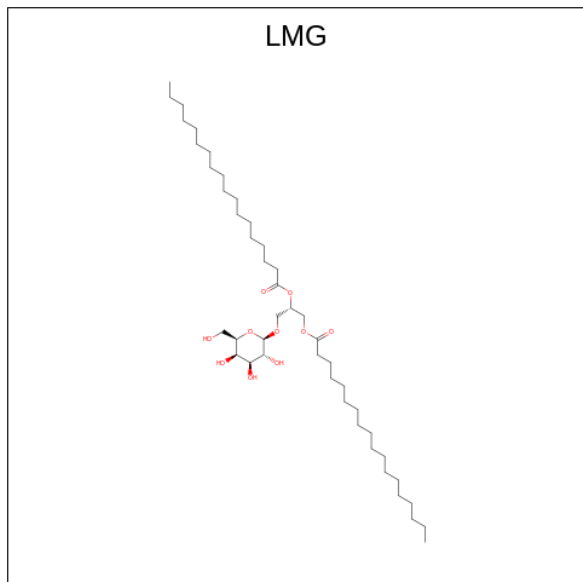


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

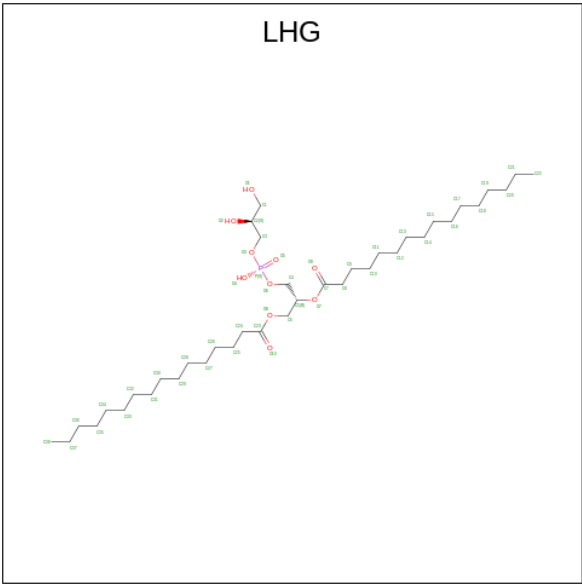
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	C	1	Total	C	O	0	0
			34	29	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



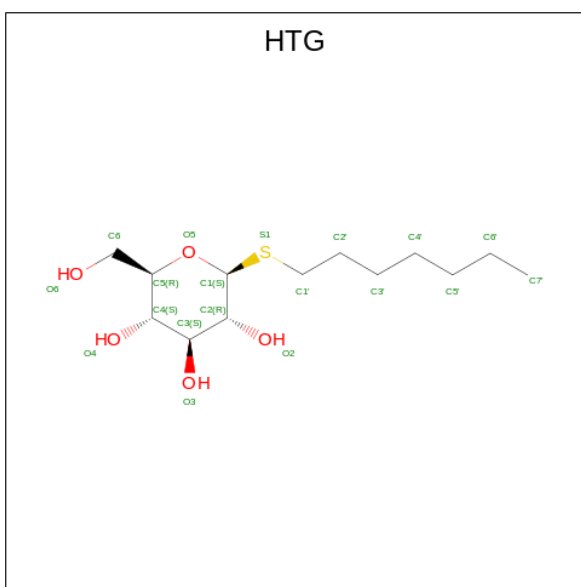
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			51	41	10		
31	C	1	Total	C	O	0	0
			51	41	10		
31	C	1	Total	C	O	0	0
			51	41	10		
31	D	1	Total	C	O	0	0
			51	41	10		
31	M	1	Total	C	O	0	0
			51	41	10		
31	Z	1	Total	C	O	0	0
			37	27	10		
31	a	1	Total	C	O	0	0
			51	41	10		
31	c	1	Total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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



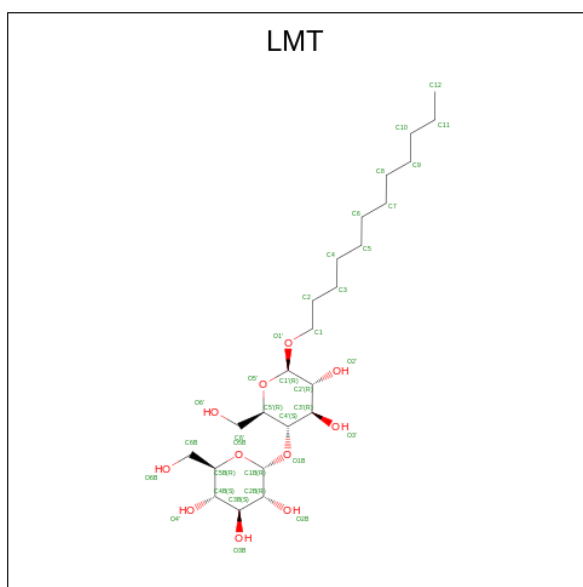
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	a	1	Total	C	O	P	0	0
			42	31	10	1		
32	b	1	Total	C	O	P	0	0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

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



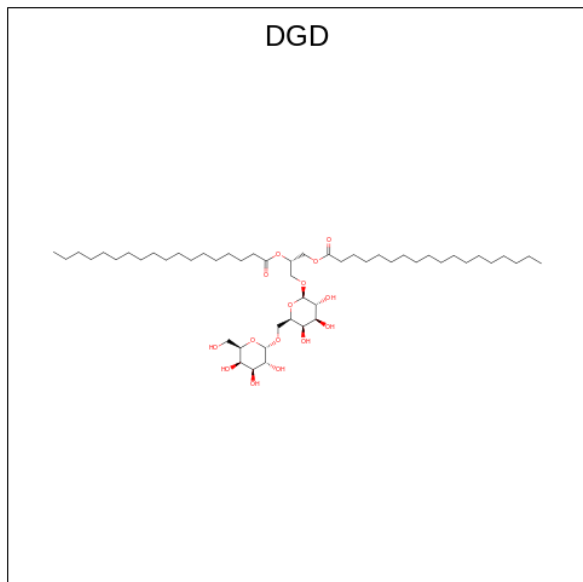
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			16	10	5	1		
33	V	1	Total	C	O		0	0
			11	6	5			
33	b	1	Total	C	O	S	0	0
			19	13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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



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

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



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

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

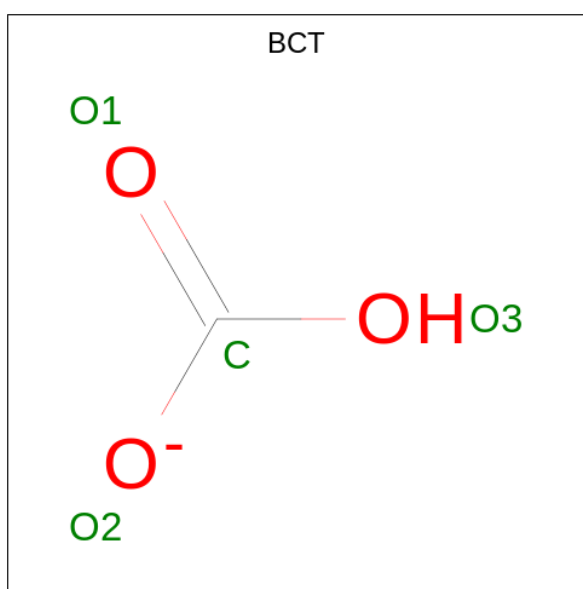
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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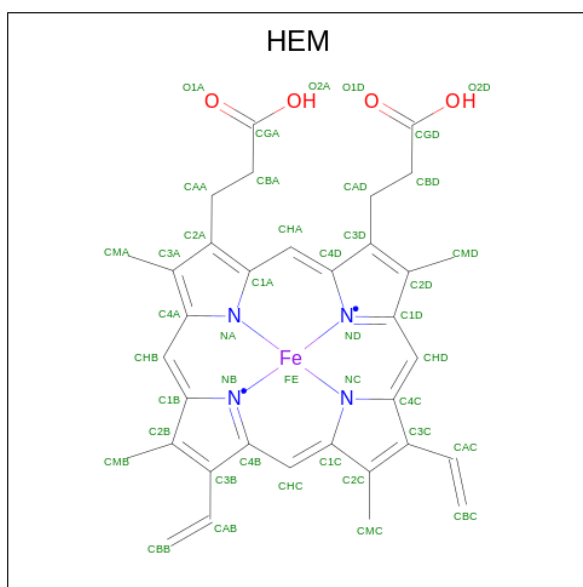
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	o	1	Total	Ca	0	0
			1	1		
36	v	1	Total	Ca	0	0
			1	1		

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



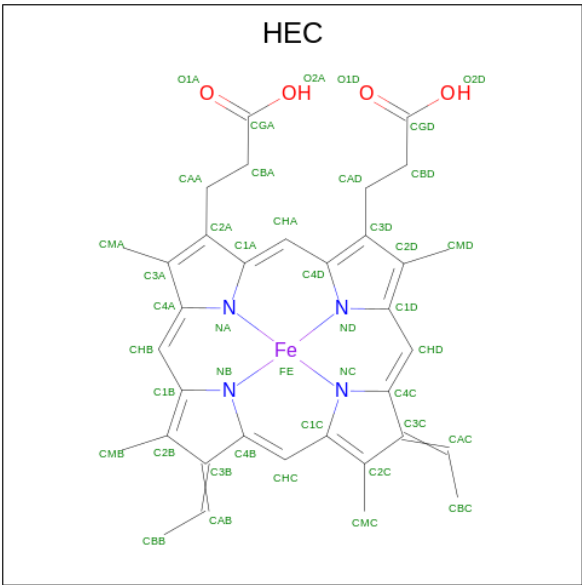
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 40 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).





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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	147	Total	O	0	0
			147	147		
41	B	207	Total	O	0	0
			207	207		
41	C	186	Total	O	0	0
			186	186		
41	D	132	Total	O	0	0
			132	132		
41	E	24	Total	O	0	0
			24	24		
41	F	8	Total	O	0	0
			8	8		
41	H	30	Total	O	0	0
			30	30		
41	I	3	Total	O	0	0
			3	3		
41	J	6	Total	O	0	0
			6	6		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	8	Total 8	O 8	0	0
41	M	16	Total 16	O 16	0	0
41	O	122	Total 122	O 122	0	0
41	T	15	Total 15	O 15	0	0
41	U	58	Total 58	O 58	0	0
41	V	93	Total 93	O 93	0	0
41	X	10	Total 10	O 10	0	0
41	Y	1	Total 1	O 1	0	0
41	R	1	Total 1	O 1	0	0
41	a	144	Total 144	O 144	0	0
41	b	222	Total 222	O 222	0	0
41	c	166	Total 166	O 166	0	0
41	d	127	Total 127	O 127	0	0
41	e	13	Total 13	O 13	0	0
41	f	5	Total 5	O 5	0	0
41	h	24	Total 24	O 24	0	0
41	i	2	Total 2	O 2	0	0
41	j	3	Total 3	O 3	0	0
41	k	5	Total 5	O 5	0	0
41	l	7	Total 7	O 7	0	0
41	m	11	Total 11	O 11	0	0

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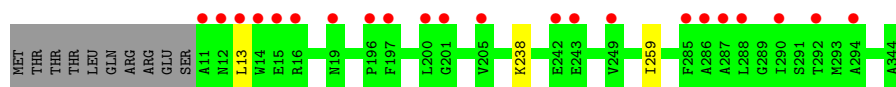
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	102	Total 102	O 102	0	0
41	t	11	Total 11	O 11	0	0
41	u	67	Total 67	O 67	0	0
41	v	56	Total 56	O 56	0	0
41	x	10	Total 10	O 10	0	0
41	y	3	Total 3	O 3	0	0

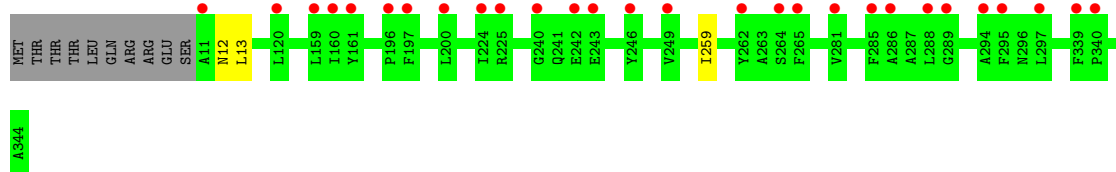
### 3 Residue-property plots [i](#)

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.

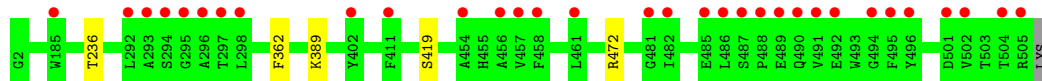
- Molecule 1: Photosystem II protein D1



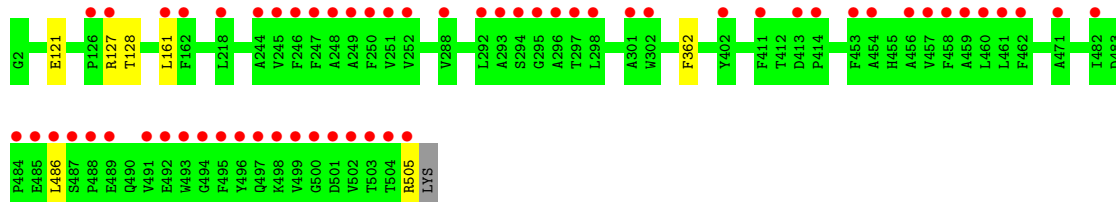
- Molecule 1: Photosystem II protein D1



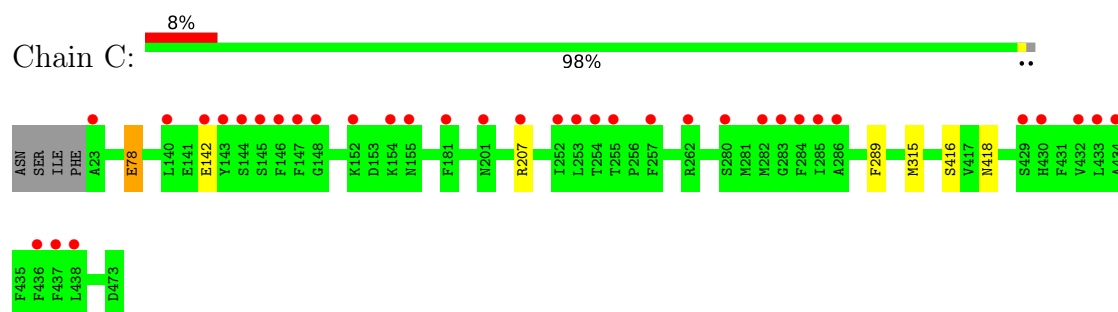
- Molecule 2: Photosystem II CP47 reaction center protein



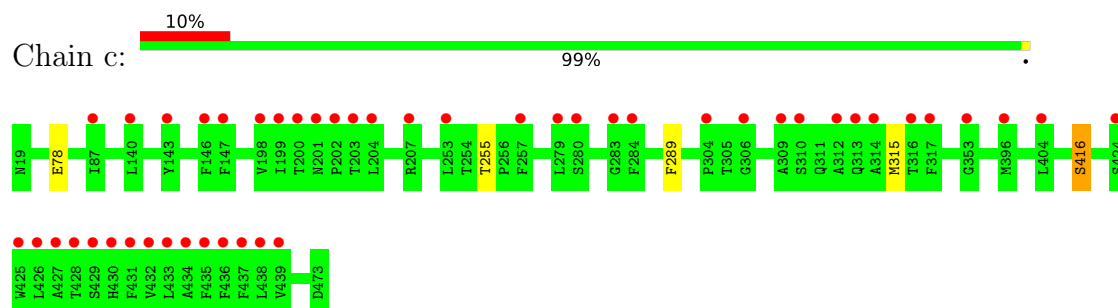
- Molecule 2: Photosystem II CP47 reaction center protein



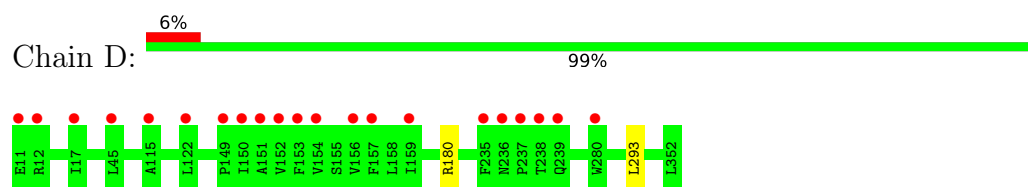
- Molecule 3: Photosystem II CP43 reaction center protein



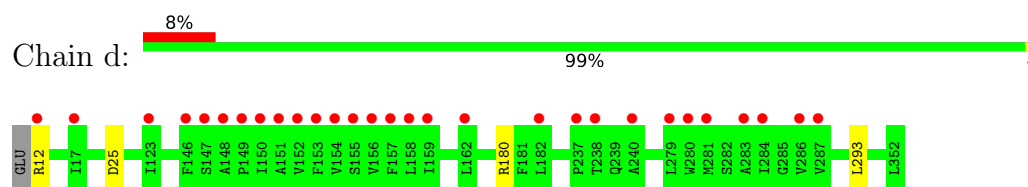
- Molecule 3: Photosystem II CP43 reaction center protein



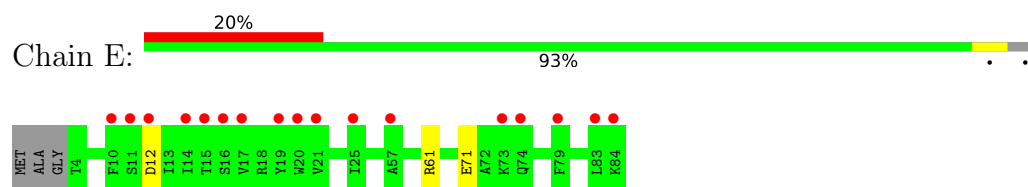
- Molecule 4: Photosystem II D2 protein



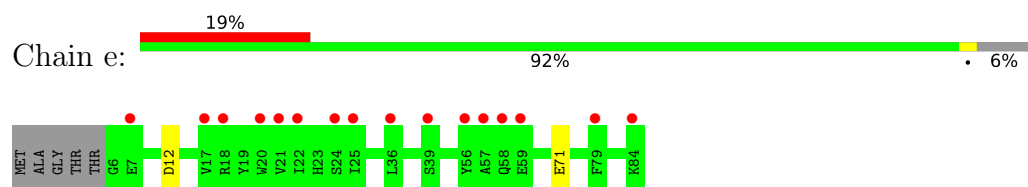
- Molecule 4: Photosystem II D2 protein



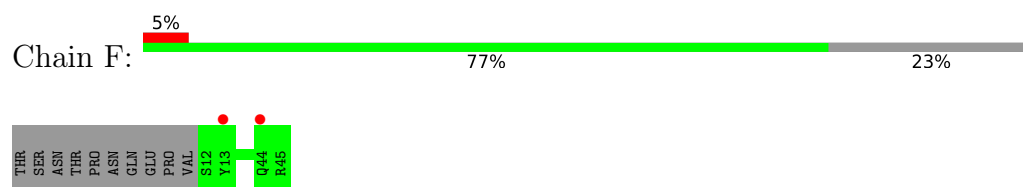
- Molecule 5: Cytochrome b559 subunit alpha



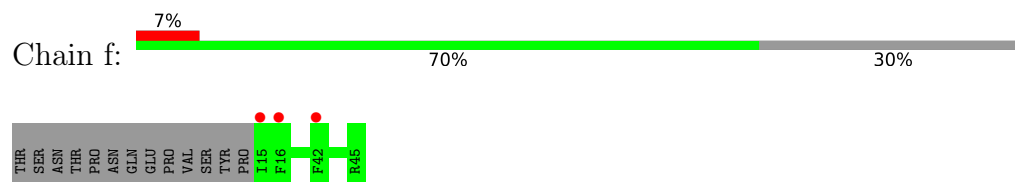
- Molecule 5: Cytochrome b559 subunit alpha



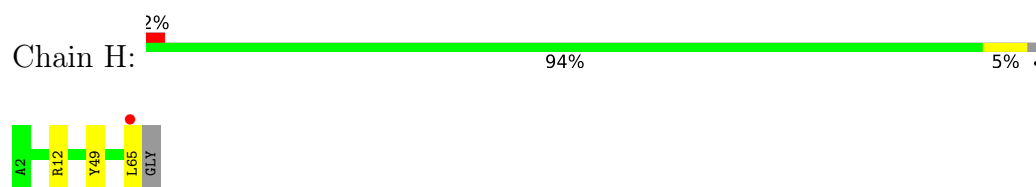
- Molecule 6: Cytochrome b559 subunit beta



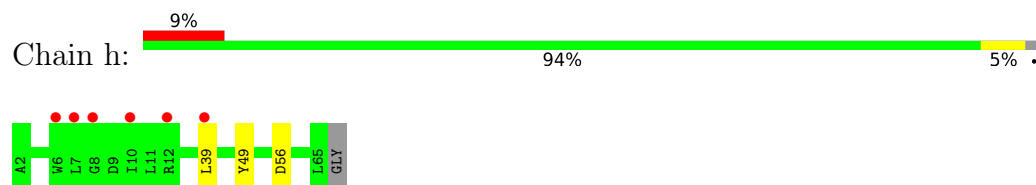
- Molecule 6: Cytochrome b559 subunit beta



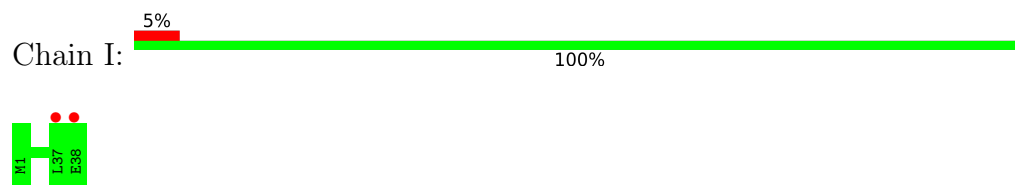
- Molecule 7: Photosystem II reaction center protein H



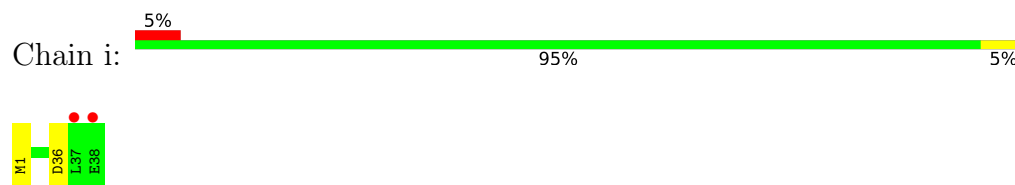
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

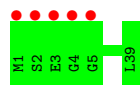


- Molecule 9: Photosystem II reaction center protein J





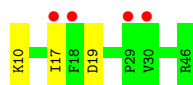
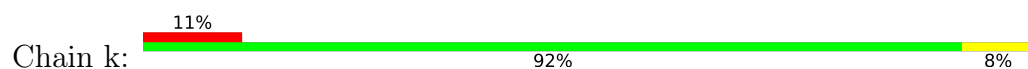
- Molecule 9: Photosystem II reaction center protein J



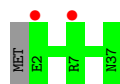
- Molecule 10: Photosystem II reaction center protein K



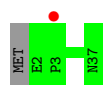
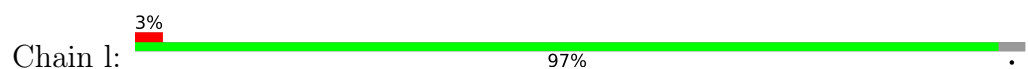
- Molecule 10: Photosystem II reaction center protein K



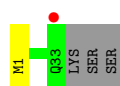
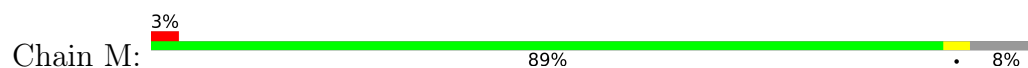
- Molecule 11: Photosystem II reaction center protein L



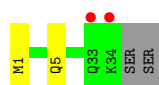
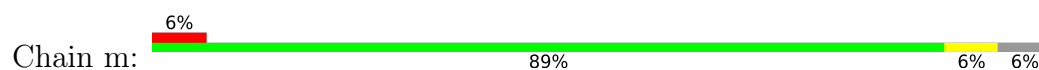
- Molecule 11: Photosystem II reaction center protein L



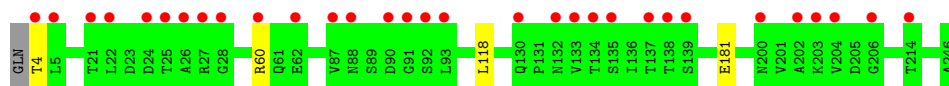
- Molecule 12: Photosystem II reaction center protein M



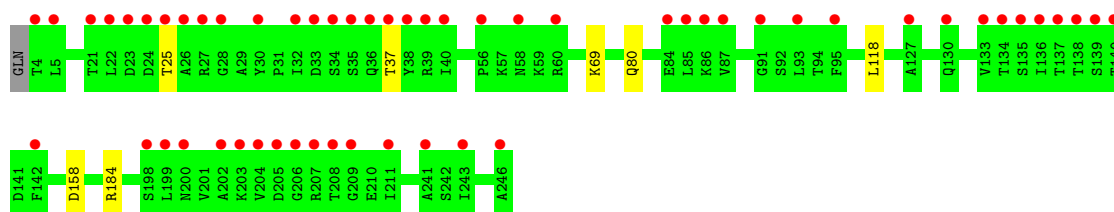
- Molecule 12: Photosystem II reaction center protein M



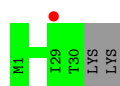
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



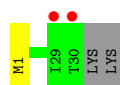
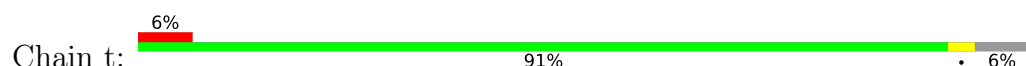
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



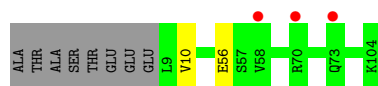
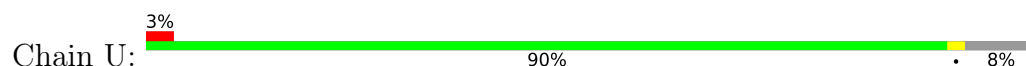
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T



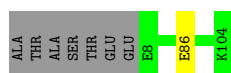
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



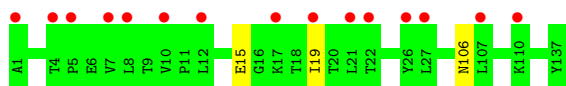




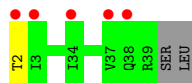
- Molecule 16: Cytochrome c-550



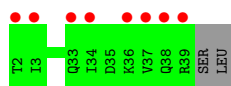
- Molecule 16: Cytochrome c-550



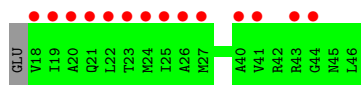
- Molecule 17: Photosystem II reaction center protein X



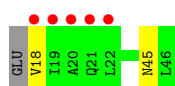
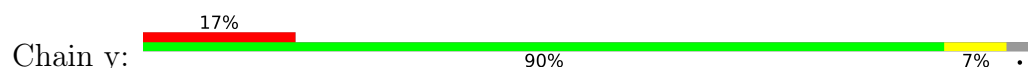
- Molecule 17: Photosystem II reaction center protein X



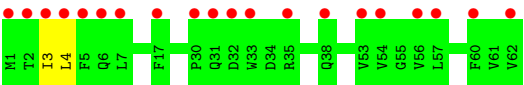
- Molecule 18: Photosystem II reaction center protein Ycf12



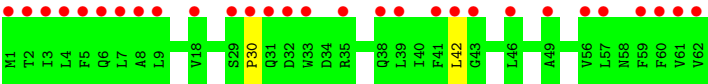
- Molecule 18: Photosystem II reaction center protein Ycf12



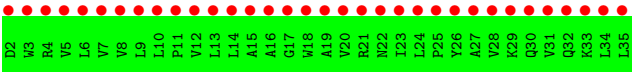
- Molecule 19: Photosystem II reaction center protein Z



• 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, $\alpha$ , $\beta$ , $\gamma$	126.02Å 231.70Å 288.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 2.35 52.70 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.93-2.35) 84.6 (52.70-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.160 , 0.208 0.162 , 0.208	Depositor DCC
$R_{free}$ test set	17532 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 77.1	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	53071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: LMT, CL, FE2, UNL, MG, HTG, BCT, HEC, SQD, BCR, LMG, GOL, LHG, PL9, DGD, OEX, CLA, FME, PHO, HEM, CA

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	0.42	0/2719	0.55	0/3708
1	a	0.40	0/2727	0.53	0/3719
2	B	0.42	0/4190	0.54	0/5708
2	b	0.40	0/4138	0.52	0/5640
3	C	0.39	1/3626 (0.0%)	0.51	0/4936
3	c	0.35	0/3648	0.49	0/4966
4	D	0.43	0/2821	0.56	0/3844
4	d	0.41	0/2812	0.53	0/3832
5	E	0.35	0/687	0.48	0/936
5	e	0.35	0/667	0.47	0/908
6	F	0.35	0/284	0.45	0/387
6	f	0.31	0/257	0.47	0/349
7	H	0.36	0/530	0.54	0/723
7	h	0.34	0/519	0.54	0/708
8	I	0.35	0/311	0.50	0/419
8	i	0.33	0/311	0.47	0/419
9	J	0.32	0/278	0.49	0/376
9	j	0.33	0/283	0.49	0/383
10	K	0.35	0/303	0.49	0/416
10	k	0.34	0/303	0.51	0/416
11	L	0.46	0/311	0.49	0/423
11	l	0.38	0/311	0.49	0/423
12	M	0.41	0/261	0.55	0/357
12	m	0.39	0/262	0.51	0/357
13	O	0.38	0/1917	0.58	0/2599
13	o	0.37	0/1910	0.58	1/2589 (0.0%)
14	T	0.47	0/257	0.50	0/349
14	t	0.45	0/257	0.45	0/349
15	U	0.38	0/776	0.54	0/1052
15	u	0.36	0/785	0.59	0/1064
16	V	0.35	0/1085	0.53	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.35	0/1085	0.51	0/1473
17	X	0.31	0/284	0.48	0/384
17	x	0.29	0/284	0.44	0/384
18	Y	0.29	0/216	0.43	0/289
18	y	0.27	0/216	0.43	0/289
19	Z	0.30	0/490	0.38	0/669
19	z	0.28	0/490	0.39	0/669
20	R	0.27	0/279	0.42	0/383
All	All	0.39	1/42890 (0.0%)	0.52	1/58368 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	78	GLU	C-N	5.08	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.39	123.16	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	41 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	41	47
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	34	38
3	c	455/455 (100%)	446 (98%)	8 (2%)	1 (0%)	47	56
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	329 (97%)	10 (3%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	31 (86%)	4 (11%)	1 (3%)	5	2
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	244/244 (100%)	237 (97%)	7 (3%)	0	100	100
13	o	243/244 (100%)	236 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	7
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5246/5384 (97%)	5124 (98%)	115 (2%)	7 (0%)	51	63

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
1	a	259	ILE
19	z	30	PRO

### 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	271/279 (97%)	269 (99%)	2 (1%)	84	91
1	a	272/279 (98%)	270 (99%)	2 (1%)	84	91
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	82
2	b	406/403 (101%)	399 (98%)	7 (2%)	60	72
3	C	356/356 (100%)	350 (98%)	6 (2%)	60	72
3	c	358/356 (101%)	353 (99%)	5 (1%)	67	78
4	D	277/277 (100%)	275 (99%)	2 (1%)	84	91
4	d	276/277 (100%)	272 (99%)	4 (1%)	67	78
5	E	73/73 (100%)	70 (96%)	3 (4%)	30	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	70/73 (96%)	68 (97%)	2 (3%)	42	52
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	51 (93%)	4 (7%)	14	14
7	h	54/54 (100%)	51 (94%)	3 (6%)	21	23
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	52
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	6
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	6
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	46
13	O	209/207 (101%)	205 (98%)	4 (2%)	57	68
13	o	208/207 (100%)	202 (97%)	6 (3%)	42	52
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	59
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	82
16	V	117/117 (100%)	115 (98%)	2 (2%)	60	72
16	v	117/117 (100%)	114 (97%)	3 (3%)	46	56
17	X	31/33 (94%)	30 (97%)	1 (3%)	39	47
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	8
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	41
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	68
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4352/4403 (99%)	4275 (98%)	77 (2%)	59	70



5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	49	TYR
16	v	15	GLU
8	i	36	ASP
13	o	37	THR
18	y	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	$\# Z  > 2$
12	FME	m	1	12	8,9,10	0.60	0	7,9,11	1.29	1 (14%)
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	0.97	0
8	FME	i	1	8	8,9,10	0.57	0	7,9,11	1.09	1 (14%)
14	FME	t	1	14	8,9,10	0.63	0	7,9,11	1.91	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.65	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	1/7/9/11	-

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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.48	117.47	122.82
12	M	1	FME	CA-N-CN	-2.93	118.32	122.82
14	t	1	FME	O-C-CA	-2.39	118.52	124.78
12	M	1	FME	O-C-CA	-2.26	118.87	124.78
12	m	1	FME	O-C-CA	-2.16	119.12	124.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 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
25	BCR	B	618	-	41,41,41	0.90	1 (2%)	56,56,56	1.53	12 (21%)
27	SQD	a	409	-	53,54,54	0.98	3 (5%)	62,65,65	1.66	11 (17%)
26	GOL	A	410	-	5,5,5	1.11	0	5,5,5	0.74	0
31	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.13	3 (5%)
35	DGD	c	517	-	63,63,67	0.91	2 (3%)	77,77,81	1.02	3 (3%)
23	CLA	d	404	-	59,73,73	2.02	12 (20%)	67,113,113	2.23	23 (34%)
25	BCR	A	409	-	41,41,41	1.00	1 (2%)	56,56,56	1.41	8 (14%)
28	OEX	A	412	41,1,3	0,15,15	0.00	-	-	-	-
23	CLA	c	507	-	59,73,73	2.01	14 (23%)	67,113,113	2.22	25 (37%)
26	GOL	c	526	-	5,5,5	0.80	0	5,5,5	1.05	0
23	CLA	B	611	-	59,73,73	1.99	12 (20%)	67,113,113	2.27	22 (32%)
23	CLA	d	403	-	59,73,73	1.94	13 (22%)	67,113,113	2.26	26 (38%)
23	CLA	C	512	3	59,73,73	2.05	16 (27%)	67,113,113	2.11	23 (34%)
27	SQD	a	411	-	53,54,54	1.02	3 (5%)	62,65,65	1.31	8 (12%)
23	CLA	c	505	41	59,73,73	2.09	14 (23%)	67,113,113	2.21	27 (40%)
33	HTG	B	622	-	19,19,19	0.84	1 (5%)	23,24,24	1.45	1 (4%)
23	CLA	C	502	-	59,73,73	1.95	13 (22%)	67,113,113	2.29	21 (31%)
26	GOL	b	623	-	5,5,5	0.97	0	5,5,5	1.09	0
33	HTG	D	413	-	16,16,19	1.11	2 (12%)	20,21,24	1.33	1 (5%)
23	CLA	C	503	-	59,73,73	2.01	13 (22%)	67,113,113	2.07	22 (32%)
25	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.60	11 (19%)
27	SQD	f	102	-	42,43,54	1.16	3 (7%)	51,54,65	1.29	6 (11%)
34	LMT	M	104	-	36,36,36	0.50	0	47,47,47	1.16	3 (6%)
27	SQD	B	620	-	53,54,54	1.02	3 (5%)	62,65,65	1.55	11 (17%)
23	CLA	B	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.13	22 (32%)
23	CLA	B	610	41	59,73,73	2.04	14 (23%)	67,113,113	2.19	22 (32%)
29	PL9	d	406	-	55,55,55	0.71	2 (3%)	68,69,69	1.65	18 (26%)
33	HTG	B	621	-	19,19,19	0.97	1 (5%)	23,24,24	1.55	4 (17%)
23	CLA	C	511	-	59,73,73	2.02	14 (23%)	67,113,113	2.24	22 (32%)
38	HEM	f	101	6,5	27,50,50	0.88	1 (3%)	17,82,82	2.15	3 (17%)
26	GOL	B	626	-	5,5,5	0.83	0	5,5,5	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	1.10	7 (9%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	d	402	41	59,73,73	2.00	13 (22%)	67,113,113	2.23	26 (38%)
23	CLA	c	509	-	59,73,73	2.10	13 (22%)	67,113,113	2.28	22 (32%)
23	CLA	D	405	-	59,73,73	1.99	13 (22%)	67,113,113	2.34	24 (35%)
31	LMG	D	414	39	51,51,55	0.85	3 (5%)	59,59,63	0.98	3 (5%)
26	GOL	B	627	-	5,5,5	1.04	0	5,5,5	0.87	0
23	CLA	c	508	41	59,73,73	2.02	12 (20%)	67,113,113	2.20	20 (29%)
34	LMT	e	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.86	1 (2%)
23	CLA	b	609	-	59,73,73	2.05	14 (23%)	67,113,113	2.16	23 (34%)
23	CLA	c	511	-	59,73,73	1.92	13 (22%)	67,113,113	2.22	23 (34%)
33	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.45	5 (21%)
29	PL9	a	414	-	55,55,55	0.64	1 (1%)	68,69,69	2.01	21 (30%)
34	LMT	b	620	-	25,25,36	0.51	0	30,30,47	0.62	0
23	CLA	D	406	-	59,73,73	2.00	13 (22%)	67,113,113	2.16	23 (34%)
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.12	1 (6%)
23	CLA	B	613	-	59,73,73	2.01	14 (23%)	67,113,113	2.18	20 (29%)
33	HTG	h	101	-	16,16,19	1.14	2 (12%)	20,21,24	2.13	7 (35%)
23	CLA	B	612	-	59,73,73	1.95	13 (22%)	67,113,113	2.39	23 (34%)
23	CLA	C	514	-	59,73,73	1.97	13 (22%)	67,113,113	2.21	23 (34%)
25	BCR	b	617	-	41,41,41	1.12	1 (2%)	56,56,56	1.43	6 (10%)
23	CLA	b	603	-	59,73,73	2.05	13 (22%)	67,113,113	2.35	22 (32%)
25	BCR	a	408	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	10 (17%)
34	LMT	t	101	-	26,26,36	0.50	0	31,31,47	1.03	2 (6%)
23	CLA	c	514	-	59,73,73	2.01	13 (22%)	67,113,113	2.16	25 (37%)
35	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	4 (5%)
23	CLA	B	605	-	59,73,73	1.98	14 (23%)	67,113,113	2.25	21 (31%)
23	CLA	B	606	-	59,73,73	1.94	14 (23%)	67,113,113	2.30	23 (34%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.54	9 (16%)
31	LMG	c	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	4 (6%)
26	GOL	c	501	-	5,5,5	1.02	0	5,5,5	0.88	0
34	LMT	a	418	-	36,36,36	0.50	1 (2%)	47,47,47	0.93	2 (4%)
31	LMG	C	521	-	51,51,55	1.02	3 (5%)	59,59,63	1.35	7 (11%)
23	CLA	A	404	-	59,73,73	2.01	14 (23%)	67,113,113	2.29	28 (41%)
25	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.52	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LMT	b	626	-	25,25,36	0.56	1 (4%)	30,30,47	1.25	3 (10%)
23	CLA	C	508	41	59,73,73	2.00	13 (22%)	67,113,113	2.17	23 (34%)
23	CLA	b	605	-	59,73,73	1.96	13 (22%)	67,113,113	2.28	22 (32%)
25	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	a	404	-	59,73,73	2.02	12 (20%)	67,113,113	2.40	27 (40%)
23	CLA	b	602	-	59,73,73	2.06	13 (22%)	67,113,113	2.35	25 (37%)
27	SQD	L	102	-	53,54,54	1.02	3 (5%)	62,65,65	1.62	10 (16%)
32	LHG	b	628	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
34	LMT	D	403	-	36,36,36	0.52	1 (2%)	47,47,47	0.81	2 (4%)
26	GOL	a	410	-	5,5,5	0.83	0	5,5,5	1.00	0
31	LMG	M	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.22	7 (11%)
34	LMT	C	525	-	36,36,36	0.53	1 (2%)	47,47,47	1.14	3 (6%)
23	CLA	b	606	-	59,73,73	1.94	13 (22%)	67,113,113	2.34	25 (37%)
23	CLA	c	513	-	59,73,73	2.00	13 (22%)	67,113,113	2.25	24 (35%)
32	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
25	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.69	12 (21%)
23	CLA	a	407	-	59,73,73	1.97	12 (20%)	67,113,113	2.24	22 (32%)
23	CLA	B	603	-	59,73,73	2.06	14 (23%)	67,113,113	2.30	20 (29%)
23	CLA	b	616	-	59,73,73	1.96	12 (20%)	67,113,113	2.37	23 (34%)
25	BCR	B	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.27	9 (16%)
27	SQD	D	415	-	42,43,54	1.15	3 (7%)	51,54,65	1.84	10 (19%)
32	LHG	d	409	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	3 (5%)
25	BCR	Y	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.85	16 (28%)
25	BCR	K	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	10 (17%)
33	HTG	b	621	-	19,19,19	0.99	1 (5%)	23,24,24	1.38	2 (8%)
32	LHG	D	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.03	4 (7%)
25	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.24	5 (8%)
31	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
33	HTG	C	522	-	19,19,19	0.91	1 (5%)	23,24,24	1.36	1 (4%)
23	CLA	C	513	-	59,73,73	2.07	13 (22%)	67,113,113	2.31	26 (38%)
32	LHG	A	416	-	48,48,48	0.89	2 (4%)	51,54,54	1.21	5 (9%)
26	GOL	O	302	-	5,5,5	0.85	0	5,5,5	1.02	0
23	CLA	A	408	-	59,73,73	2.00	13 (22%)	67,113,113	2.16	24 (35%)
32	LHG	D	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	c	503	-	59,73,73	1.98	12 (20%)	67,113,113	2.15	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PHO	A	407	-	67,69,69	2.10	18 (26%)	85,99,99	2.00	23 (27%)
23	CLA	C	504	-	59,73,73	2.00	13 (22%)	67,113,113	2.15	20 (29%)
35	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	1.15	6 (7%)
23	CLA	C	506	-	59,73,73	1.96	14 (23%)	67,113,113	2.11	19 (28%)
23	CLA	b	608	-	59,73,73	2.02	13 (22%)	67,113,113	2.22	23 (34%)
31	LMG	C	520	-	51,51,55	0.99	2 (3%)	59,59,63	0.99	4 (6%)
35	DGD	C	517	-	63,63,67	0.86	2 (3%)	77,77,81	1.18	6 (7%)
26	GOL	B	623	-	5,5,5	0.98	0	5,5,5	1.10	0
26	GOL	C	523	-	5,5,5	1.16	0	5,5,5	0.93	0
23	CLA	b	615	-	59,73,73	1.96	12 (20%)	67,113,113	2.15	19 (28%)
37	BCT	d	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	C	507	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	23 (34%)
31	LMG	A	415	-	51,51,55	0.92	2 (3%)	59,59,63	1.12	5 (8%)
25	BCR	b	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.36	10 (17%)
29	PL9	A	413	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
35	DGD	c	519	-	63,63,67	0.87	3 (4%)	77,77,81	0.98	4 (5%)
26	GOL	b	627	-	5,5,5	0.97	0	5,5,5	1.03	0
23	CLA	B	615	-	59,73,73	1.95	12 (20%)	67,113,113	2.23	22 (32%)
23	CLA	A	405	41	59,73,73	2.00	14 (23%)	67,113,113	2.24	25 (37%)
25	BCR	d	405	-	41,41,41	1.14	1 (2%)	56,56,56	1.82	13 (23%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.44	9 (16%)
35	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.02	3 (3%)
23	CLA	B	616	-	59,73,73	1.95	12 (20%)	67,113,113	2.28	21 (31%)
34	LMT	m	103	-	36,36,36	0.44	0	47,47,47	1.02	3 (6%)
23	CLA	B	604	-	59,73,73	1.98	13 (22%)	67,113,113	2.30	24 (35%)
23	CLA	B	602	-	59,73,73	2.01	13 (22%)	67,113,113	2.27	23 (34%)
23	CLA	b	612	-	59,73,73	2.02	15 (25%)	67,113,113	2.38	22 (32%)
25	BCR	k	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.61	12 (21%)
31	LMG	d	412	39	51,51,55	0.92	2 (3%)	59,59,63	0.90	3 (5%)
33	HTG	b	622	-	19,19,19	1.00	1 (5%)	23,24,24	1.69	3 (13%)
23	CLA	b	614	-	59,73,73	2.00	12 (20%)	67,113,113	2.26	24 (35%)
23	CLA	c	510	-	59,73,73	2.06	14 (23%)	67,113,113	2.23	21 (31%)
23	CLA	C	505	41	59,73,73	2.01	14 (23%)	67,113,113	2.22	24 (35%)
33	HTG	b	624	-	19,19,19	1.05	2 (10%)	23,24,24	1.38	2 (8%)
34	LMT	D	404	-	36,36,36	0.43	0	47,47,47	1.11	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PHO	D	402	-	67,69,69	2.12	16 (23%)	85,99,99	2.03	21 (24%)
23	CLA	b	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.19	20 (29%)
40	HEC	V	201	16	26,50,50	2.19	4 (15%)	18,82,82	2.29	7 (38%)
23	CLA	b	607	41	59,73,73	1.92	15 (25%)	67,113,113	2.21	21 (31%)
28	OEX	a	413	41,1,3	0,15,15	0.00	-	-	-	-
29	PL9	D	408	-	55,55,55	0.66	2 (3%)	68,69,69	1.72	19 (27%)
23	CLA	C	509	-	59,73,73	2.07	12 (20%)	67,113,113	2.33	21 (31%)
32	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.05	2 (4%)
37	BCT	D	401	21	0,3,3	0.00	-	0,3,3	0.00	-
40	HEC	v	203	16	26,50,50	2.23	4 (15%)	18,82,82	1.92	6 (33%)
23	CLA	B	608	-	59,73,73	1.95	13 (22%)	67,113,113	2.18	24 (35%)
34	LMT	B	628	-	25,25,36	0.46	0	30,30,47	1.01	2 (6%)
32	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.14	4 (7%)
23	CLA	A	406	41	59,73,73	1.97	13 (22%)	67,113,113	2.10	20 (29%)
31	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	7 (11%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.68	12 (21%)
27	SQD	C	501	-	53,54,54	0.97	3 (5%)	62,65,65	1.98	11 (17%)
23	CLA	C	510	-	59,73,73	2.10	13 (22%)	67,113,113	2.21	20 (29%)
24	PHO	a	416	-	67,69,69	2.12	18 (26%)	85,99,99	2.06	23 (27%)
34	LMT	a	412	-	36,36,36	0.63	1 (2%)	47,47,47	1.24	3 (6%)
27	SQD	A	411	-	53,54,54	1.06	3 (5%)	62,65,65	1.33	8 (12%)
34	LMT	E	102	-	36,36,36	0.55	1 (2%)	47,47,47	1.09	4 (8%)
32	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.10	5 (9%)
23	CLA	a	405	41	59,73,73	1.96	12 (20%)	67,113,113	2.09	22 (32%)
23	CLA	B	614	-	59,73,73	1.90	13 (22%)	67,113,113	2.32	24 (35%)
23	CLA	c	512	3	59,73,73	2.02	13 (22%)	67,113,113	2.13	23 (34%)
23	CLA	c	506	-	59,73,73	1.98	13 (22%)	67,113,113	2.17	19 (28%)
33	HTG	c	522	-	19,19,19	0.99	2 (10%)	23,24,24	1.39	1 (4%)
25	BCR	h	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	7 (12%)
23	CLA	b	604	-	59,73,73	1.93	13 (22%)	67,113,113	2.22	22 (32%)
25	BCR	c	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.49	11 (19%)
32	LHG	a	419	-	41,41,48	1.04	2 (4%)	44,47,54	0.97	2 (4%)
25	BCR	D	407	-	41,41,41	1.02	1 (2%)	56,56,56	1.78	14 (25%)
23	CLA	c	502	-	59,73,73	1.94	14 (23%)	67,113,113	2.12	23 (34%)
34	LMT	M	102	-	36,36,36	0.47	0	47,47,47	0.92	3 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	GOL	v	202	-	5,5,5	0.98	0	5,5,5	0.92	0
24	PHO	a	406	-	67,69,69	2.08	16 (23%)	85,99,99	2.02	24 (28%)
31	LMG	c	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.20	6 (10%)
23	CLA	B	609	-	59,73,73	1.92	13 (22%)	67,113,113	2.09	18 (26%)
31	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.51	7 (15%)
23	CLA	b	613	-	59,73,73	2.08	13 (22%)	67,113,113	2.21	22 (32%)
23	CLA	b	610	41	59,73,73	1.99	15 (25%)	67,113,113	2.35	23 (34%)
23	CLA	B	607	41	59,73,73	1.92	14 (23%)	67,113,113	2.15	22 (32%)
38	HEM	E	103	6,5	27,50,50	0.83	1 (3%)	17,82,82	2.30	4 (23%)
23	CLA	b	611	-	59,73,73	1.95	13 (22%)	67,113,113	2.21	21 (31%)
25	BCR	b	619	-	41,41,41	1.13	1 (2%)	56,56,56	1.55	12 (21%)
23	CLA	c	504	-	59,73,73	1.93	13 (22%)	67,113,113	2.22	21 (31%)

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
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	SQD	a	409	-	-	13/49/69/69	0/1/1/1
26	GOL	A	410	-	-	3/4/4/4	-
31	LMG	m	101	-	-	11/46/66/70	0/1/1/1
35	DGD	c	517	-	-	17/51/91/95	0/2/2/2
23	CLA	d	404	-	3/3/20/25	7/37/135/135	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	c	507	-	3/3/20/25	11/37/135/135	-
26	GOL	c	526	-	-	0/4/4/4	-
23	CLA	B	611	-	2/2/20/25	4/37/135/135	-
23	CLA	d	403	-	1/1/20/25	6/37/135/135	-
23	CLA	C	512	3	3/3/20/25	3/37/135/135	-
27	SQD	a	411	-	-	16/49/69/69	0/1/1/1
23	CLA	c	505	41	3/3/20/25	4/37/135/135	-
33	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	C	502	-	3/3/20/25	4/37/135/135	-
26	GOL	b	623	-	-	2/4/4/4	-
33	HTG	D	413	-	-	1/7/27/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	503	-	1/1/20/25	8/37/135/135	-
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
34	LMT	M	104	-	-	8/21/61/61	0/2/2/2
27	SQD	B	620	-	-	16/49/69/69	0/1/1/1
23	CLA	B	601	41	3/3/20/25	11/37/135/135	-
23	CLA	B	610	41	3/3/20/25	7/37/135/135	-
29	PL9	d	406	-	-	6/53/73/73	0/1/1/1
33	HTG	B	621	-	-	4/10/30/30	0/1/1/1
23	CLA	C	511	-	3/3/20/25	10/37/135/135	-
38	HEM	f	101	6,5	-	0/6/54/54	-
26	GOL	B	626	-	-	2/4/4/4	-
35	DGD	H	102	-	-	17/51/91/95	0/2/2/2
35	DGD	h	103	-	-	12/51/91/95	0/2/2/2
23	CLA	d	402	41	3/3/20/25	10/37/135/135	-
23	CLA	c	509	-	3/3/20/25	8/37/135/135	-
23	CLA	D	405	-	1/1/20/25	4/37/135/135	-
31	LMG	D	414	39	-	9/46/66/70	0/1/1/1
26	GOL	B	627	-	-	0/4/4/4	-
23	CLA	c	508	41	3/3/20/25	9/37/135/135	-
34	LMT	e	101	-	-	10/21/61/61	0/2/2/2
23	CLA	b	609	-	3/3/20/25	7/37/135/135	-
23	CLA	c	511	-	3/3/20/25	7/37/135/135	-
33	HTG	B	624	-	-	4/10/30/30	0/1/1/1
29	PL9	a	414	-	-	18/53/73/73	0/1/1/1
34	LMT	b	620	-	-	7/17/37/61	0/1/1/2
23	CLA	D	406	-	3/3/20/25	8/37/135/135	-
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1
23	CLA	B	613	-	3/3/20/25	8/37/135/135	-
33	HTG	h	101	-	-	2/7/27/30	0/1/1/1
23	CLA	B	612	-	3/3/20/25	4/37/135/135	-
23	CLA	C	514	-	3/3/20/25	10/37/135/135	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	b	603	-	2/2/20/25	7/37/135/135	-
25	BCR	a	408	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
23	CLA	c	514	-	3/3/20/25	11/37/135/135	-
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2
23	CLA	B	605	-	3/3/20/25	7/37/135/135	-
23	CLA	B	606	-	3/3/20/25	13/37/135/135	-
25	BCR	c	515	-	-	3/29/63/63	0/2/2/2
31	LMG	c	520	-	-	10/46/66/70	0/1/1/1
26	GOL	c	501	-	-	1/4/4/4	-
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
31	LMG	C	521	-	-	14/46/66/70	0/1/1/1
23	CLA	A	404	-	3/3/20/25	2/37/135/135	-
25	BCR	t	102	-	-	6/29/63/63	0/2/2/2
34	LMT	b	626	-	-	9/17/37/61	0/1/1/2
23	CLA	C	508	41	3/3/20/25	6/37/135/135	-
23	CLA	b	605	-	3/3/20/25	8/37/135/135	-
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
23	CLA	a	404	-	2/2/20/25	6/37/135/135	-
23	CLA	b	602	-	2/2/20/25	3/37/135/135	-
27	SQD	L	102	-	-	19/49/69/69	0/1/1/1
32	LHG	b	628	-	-	17/53/53/53	-
34	LMT	D	403	-	-	8/21/61/61	0/2/2/2
26	GOL	a	410	-	-	4/4/4/4	-
31	LMG	M	101	-	-	10/46/66/70	0/1/1/1
34	LMT	C	525	-	-	9/21/61/61	0/2/2/2
23	CLA	b	606	-	3/3/20/25	8/37/135/135	-
23	CLA	c	513	-	3/3/20/25	11/37/135/135	-
32	LHG	d	408	-	-	20/53/53/53	-
25	BCR	k	102	-	-	6/29/63/63	0/2/2/2
23	CLA	a	407	-	3/3/20/25	9/37/135/135	-
23	CLA	B	603	-	2/2/20/25	8/37/135/135	-
23	CLA	b	616	-	3/3/20/25	10/37/135/135	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	D	415	-	-	14/38/58/69	0/1/1/1
32	LHG	d	409	-	-	10/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
33	HTG	b	621	-	-	4/10/30/30	0/1/1/1
32	LHG	D	409	-	-	16/53/53/53	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
31	LMG	z	101	-	-	8/30/54/70	-
23	CLA	C	513	-	3/3/20/25	13/37/135/135	-
32	LHG	A	416	-	-	15/53/53/53	-
26	GOL	O	302	-	-	4/4/4/4	-
23	CLA	A	408	-	3/3/20/25	10/37/135/135	-
32	LHG	D	410	-	-	14/53/53/53	-
23	CLA	c	503	-	3/3/20/25	2/37/135/135	-
24	PHO	A	407	-	-	3/53/103/103	0/5/6/6
23	CLA	C	504	-	2/2/20/25	5/37/135/135	-
35	DGD	C	518	-	-	17/51/91/95	0/2/2/2
23	CLA	C	506	-	1/1/20/25	7/37/135/135	-
23	CLA	b	608	-	2/2/20/25	3/37/135/135	-
31	LMG	C	520	-	-	13/46/66/70	0/1/1/1
35	DGD	C	517	-	-	14/51/91/95	0/2/2/2
26	GOL	B	623	-	-	2/4/4/4	-
26	GOL	C	523	-	-	0/4/4/4	-
23	CLA	b	615	-	3/3/20/25	11/37/135/135	-
23	CLA	C	507	-	3/3/20/25	13/37/135/135	-
31	LMG	A	415	-	-	24/46/66/70	0/1/1/1
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
29	PL9	A	413	-	-	17/53/73/73	0/1/1/1
35	DGD	c	519	-	-	8/51/91/95	0/2/2/2
26	GOL	b	627	-	-	0/4/4/4	-
23	CLA	B	615	-	3/3/20/25	8/37/135/135	-
23	CLA	A	405	41	3/3/20/25	3/37/135/135	-
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
35	DGD	C	519	-	-	9/51/91/95	0/2/2/2
23	CLA	B	616	-	3/3/20/25	7/37/135/135	-
34	LMT	m	103	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	604	-	3/3/20/25	8/37/135/135	-
23	CLA	B	602	-	3/3/20/25	10/37/135/135	-
23	CLA	b	612	-	3/3/20/25	4/37/135/135	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LMG	d	412	39	-	8/46/66/70	0/1/1/1
33	HTG	b	622	-	-	3/10/30/30	0/1/1/1
23	CLA	b	614	-	3/3/20/25	12/37/135/135	-
23	CLA	c	510	-	3/3/20/25	10/37/135/135	-
23	CLA	C	505	41	3/3/20/25	6/37/135/135	-
33	HTG	b	624	-	-	2/10/30/30	0/1/1/1
34	LMT	D	404	-	-	9/21/61/61	0/2/2/2
24	PHO	D	402	-	-	1/53/103/103	0/5/6/6
23	CLA	b	601	41	3/3/20/25	13/37/135/135	-
40	HEC	V	201	16	-	0/6/54/54	-
23	CLA	b	607	41	3/3/20/25	2/37/135/135	-
29	PL9	D	408	-	-	9/53/73/73	0/1/1/1
23	CLA	C	509	-	3/3/20/25	7/37/135/135	-
32	LHG	E	101	-	-	16/46/46/53	-
40	HEC	v	203	16	-	0/6/54/54	-
23	CLA	B	608	-	2/2/20/25	2/37/135/135	-
34	LMT	B	628	-	-	2/17/37/61	0/1/1/2
32	LHG	L	101	-	-	12/53/53/53	-
23	CLA	A	406	41	2/2/20/25	6/37/135/135	-
31	LMG	a	417	-	-	13/46/66/70	0/1/1/1
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
27	SQD	C	501	-	-	13/49/69/69	0/1/1/1
23	CLA	C	510	-	3/3/20/25	4/37/135/135	-
24	PHO	a	416	-	-	7/53/103/103	0/5/6/6
34	LMT	a	412	-	-	7/21/61/61	0/2/2/2
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1
34	LMT	E	102	-	-	6/21/61/61	0/2/2/2
32	LHG	d	407	-	-	17/53/53/53	-
23	CLA	a	405	41	2/2/20/25	7/37/135/135	-
23	CLA	B	614	-	3/3/20/25	11/37/135/135	-
23	CLA	c	512	3	3/3/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	-	1/1/20/25	5/37/135/135	-
33	HTG	c	522	-	-	3/10/30/30	0/1/1/1
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	b	604	-	3/3/20/25	8/37/135/135	-
25	BCR	c	516	-	-	2/29/63/63	0/2/2/2
32	LHG	a	419	-	-	15/46/46/53	-
25	BCR	D	407	-	-	8/29/63/63	0/2/2/2
23	CLA	c	502	-	3/3/20/25	4/37/135/135	-
34	LMT	M	102	-	-	5/21/61/61	0/2/2/2
26	GOL	v	202	-	-	2/4/4/4	-
24	PHO	a	406	-	-	4/53/103/103	0/5/6/6
31	LMG	c	521	-	-	9/46/66/70	0/1/1/1
23	CLA	B	609	-	2/2/20/25	6/37/135/135	-
31	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
23	CLA	b	613	-	3/3/20/25	7/37/135/135	-
23	CLA	b	610	41	3/3/20/25	9/37/135/135	-
23	CLA	B	607	41	3/3/20/25	4/37/135/135	-
38	HEM	E	103	6,5	-	0/6/54/54	-
23	CLA	b	611	-	3/3/20/25	5/37/135/135	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	c	504	-	3/3/20/25	1/37/135/135	-

The worst 5 of 1142 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C3B-C2B	7.16	1.50	1.40
23	C	509	CLA	C3B-C2B	6.67	1.49	1.40
23	A	404	CLA	C3B-C2B	6.65	1.49	1.40
23	C	510	CLA	C3B-C2B	6.64	1.49	1.40
23	c	509	CLA	C3B-C2B	6.63	1.49	1.40

The worst 5 of 2271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	C4A-NA-C1A	-8.06	103.08	106.71
24	D	402	PHO	CMD-C2D-C1D	7.58	136.74	125.06
23	B	602	CLA	C4A-NA-C1A	-7.43	103.37	106.71
23	b	606	CLA	C4A-NA-C1A	-7.39	103.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CHD-C4C-C3C	-7.32	114.07	124.84

5 of 189 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	NA
23	A	404	CLA	ND
23	A	404	CLA	NC
23	A	405	CLA	NA
23	A	405	CLA	ND

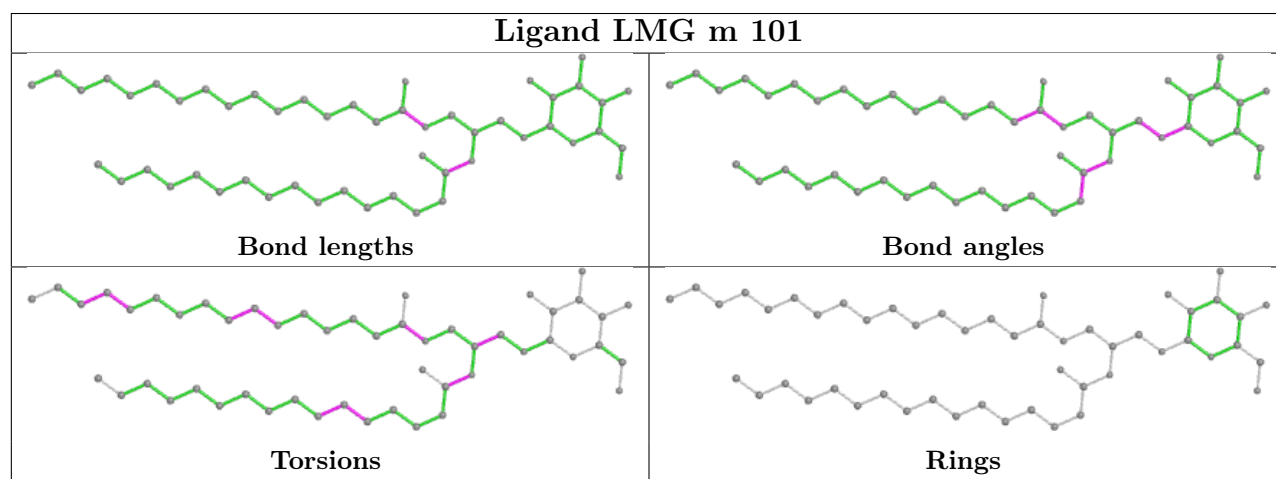
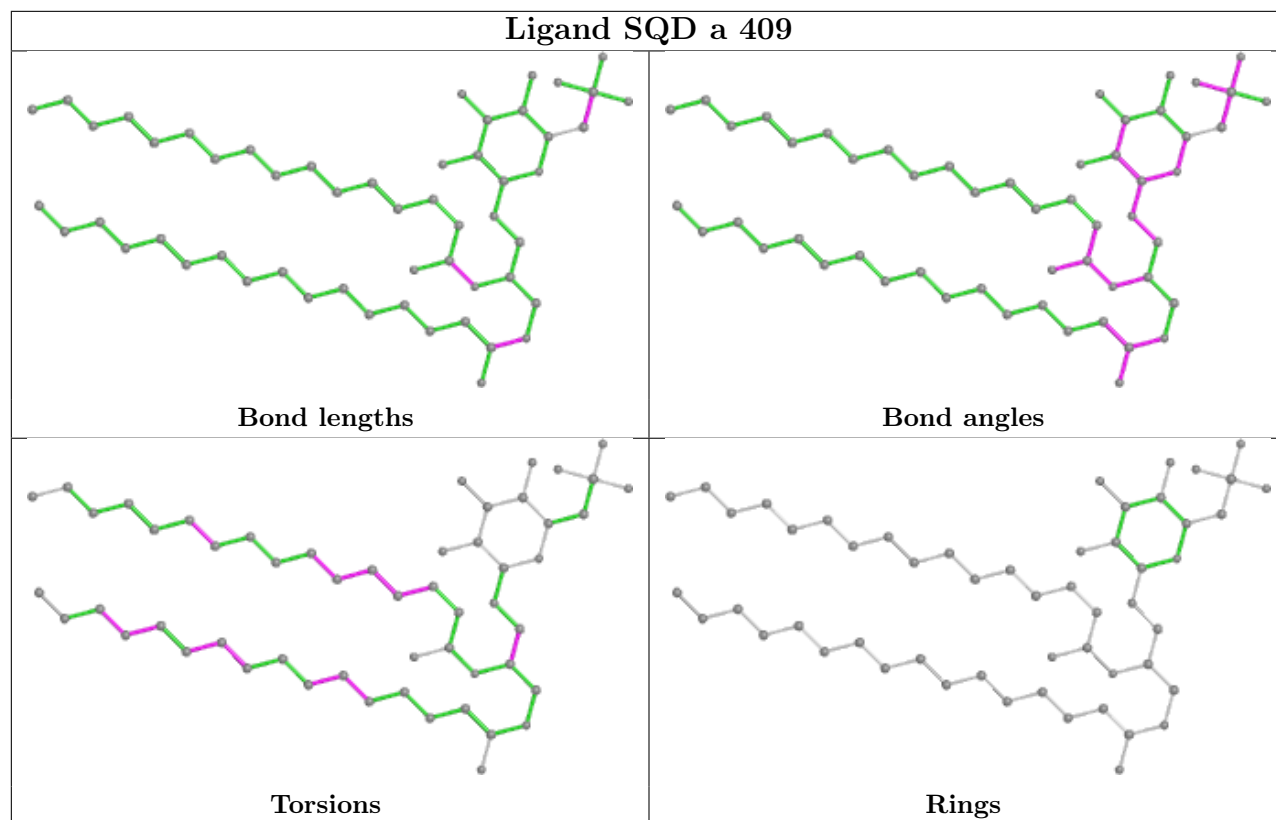
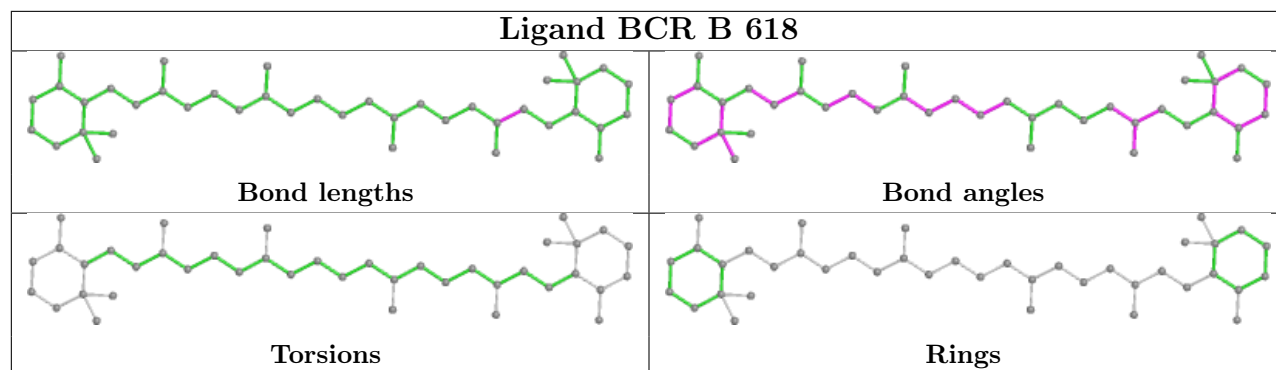
5 of 1279 torsion outliers are listed below:

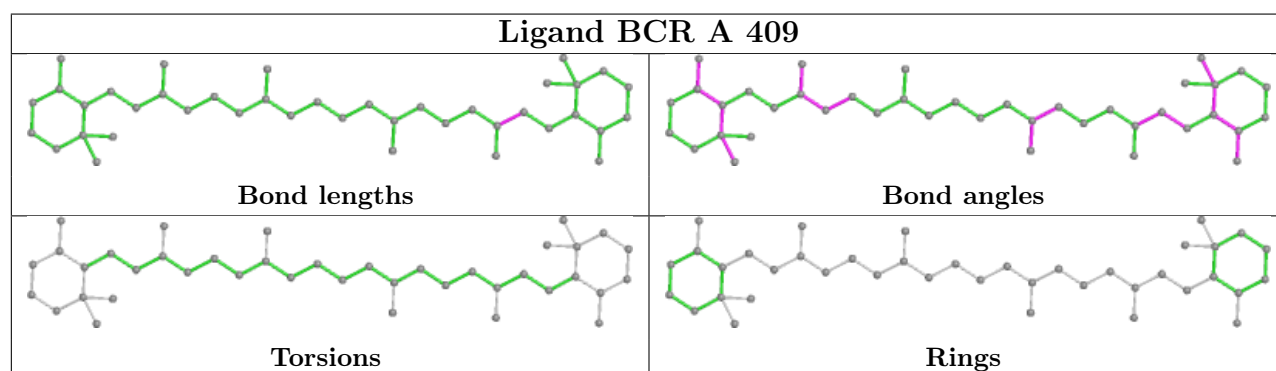
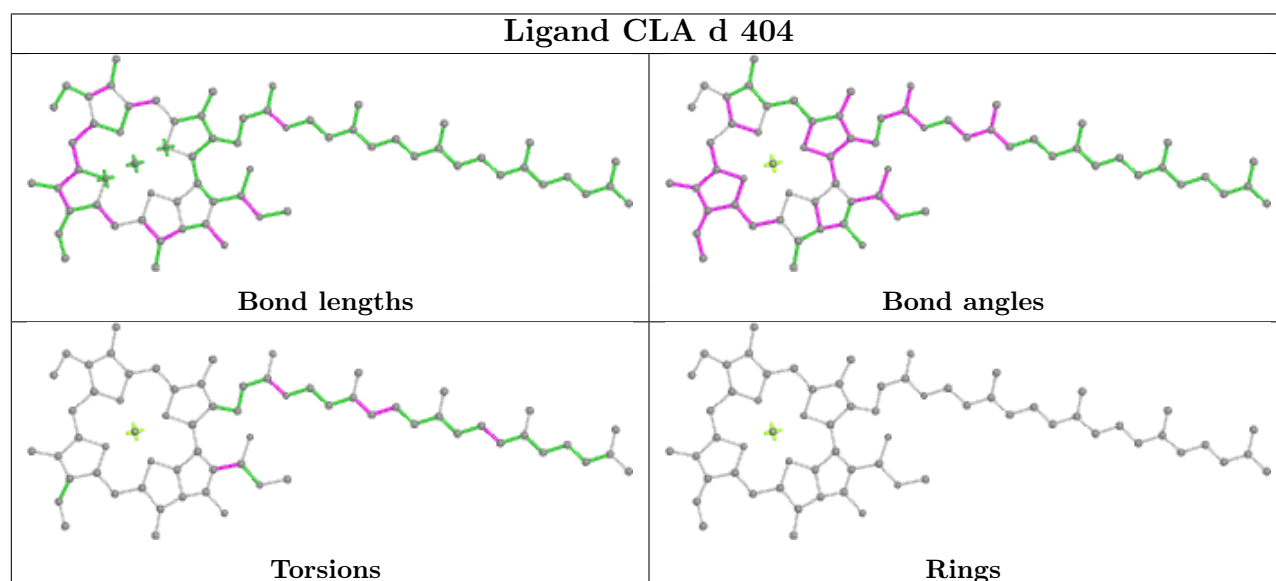
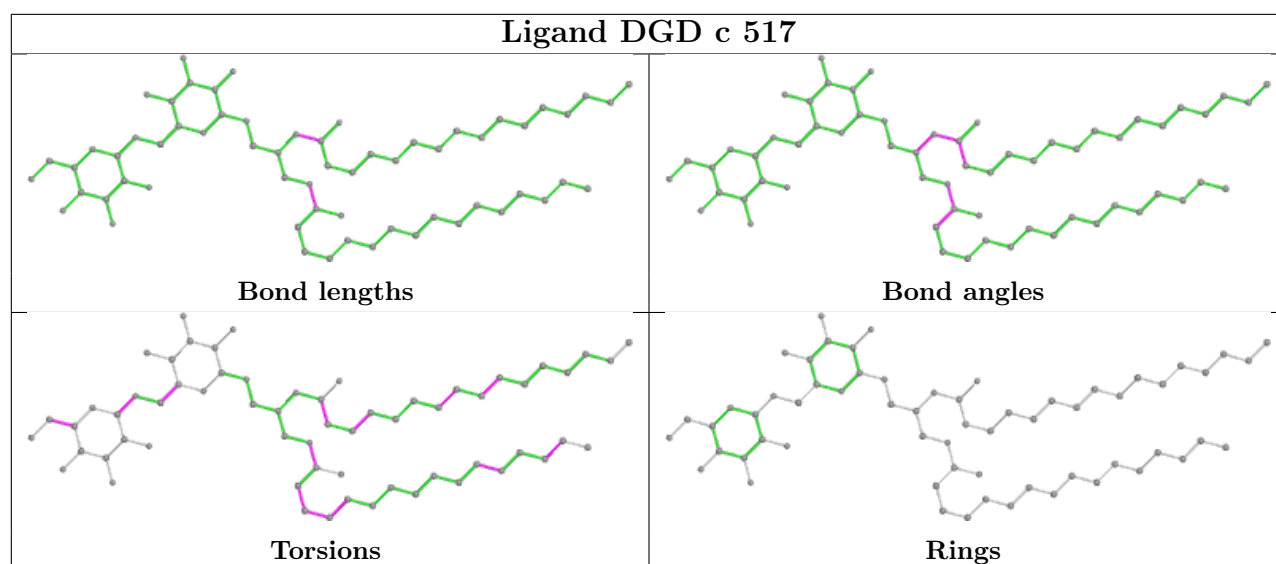
Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

No monomer is involved in short contacts.

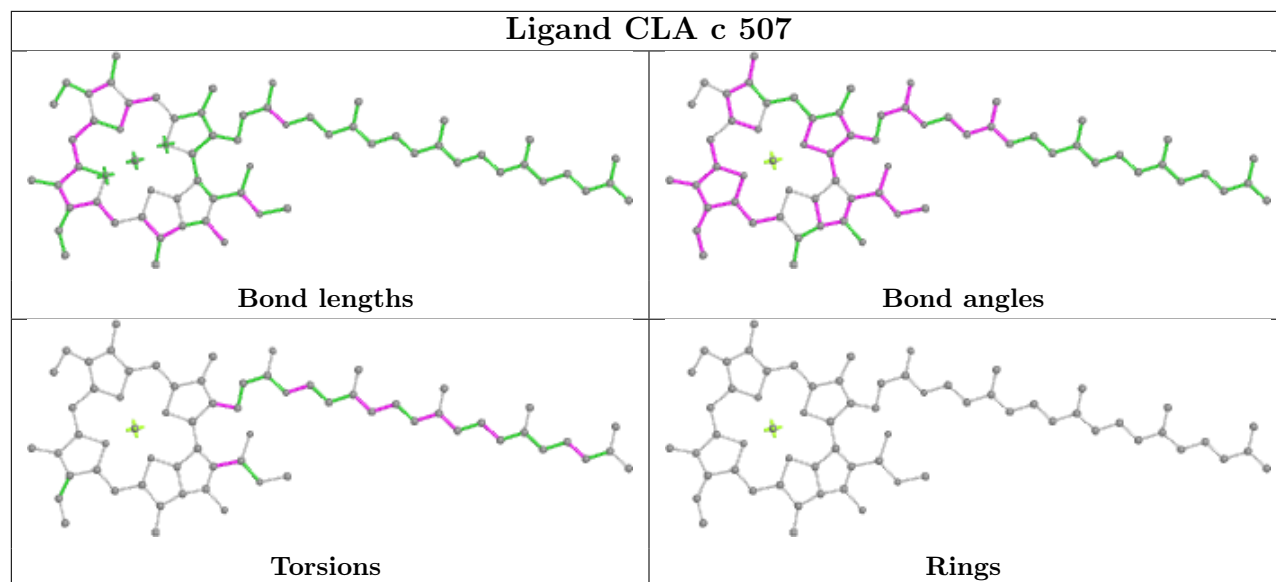
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



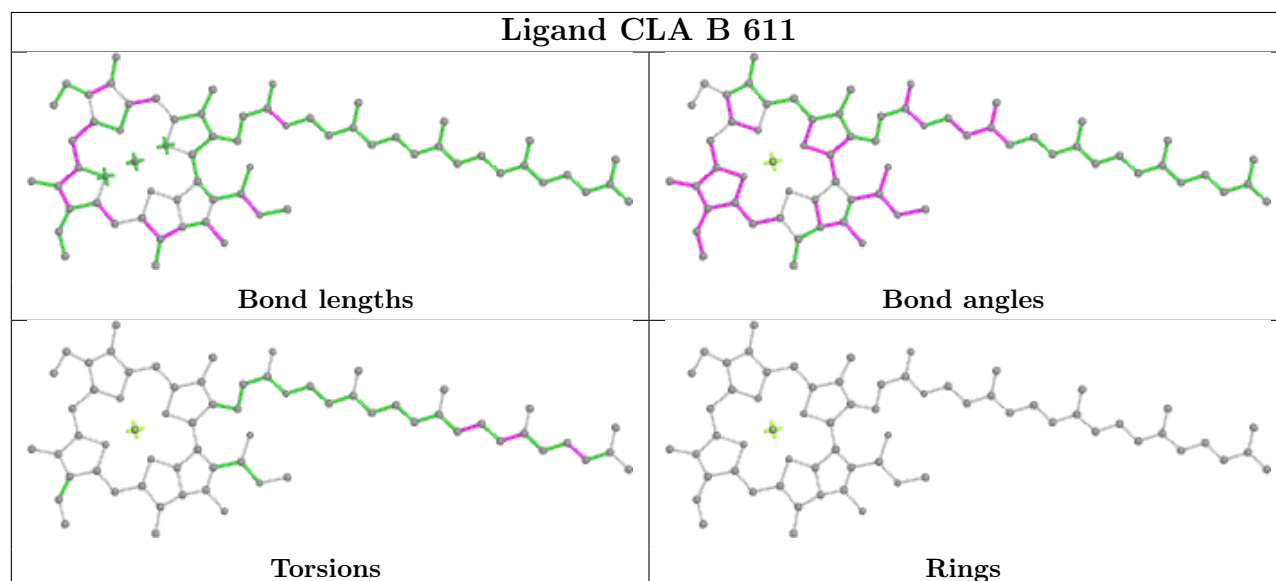




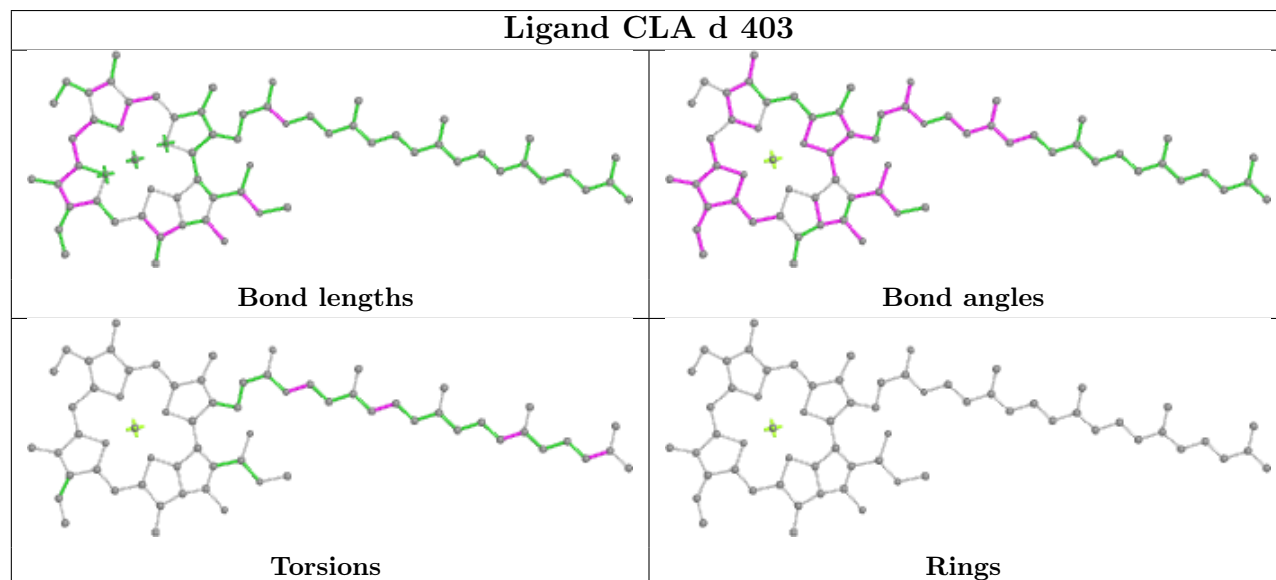
## Ligand CLA c 507



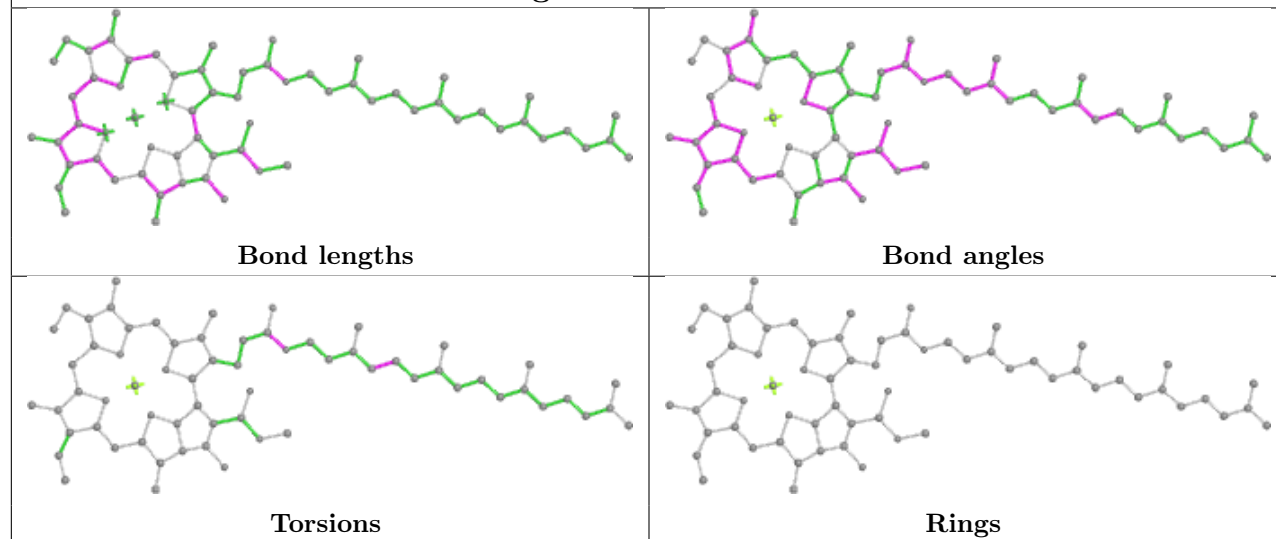
## Ligand CLA B 611



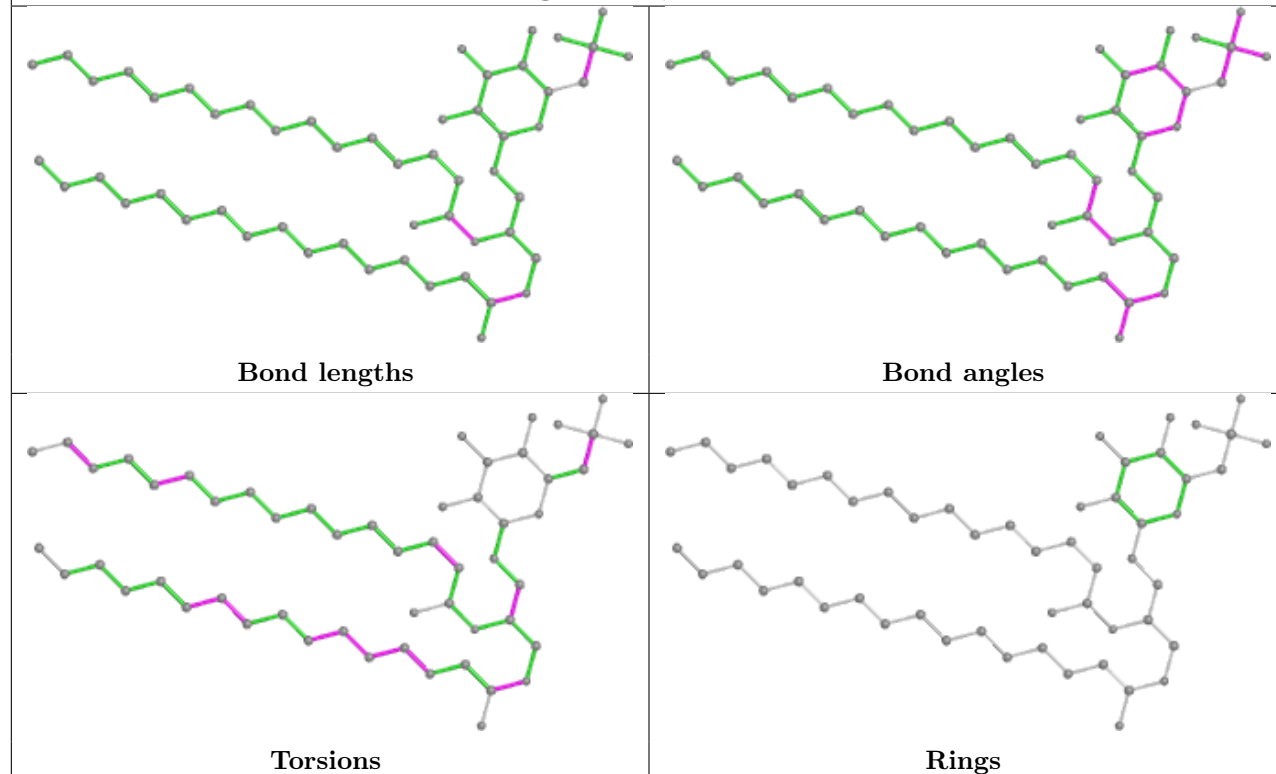
## Ligand CLA d 403



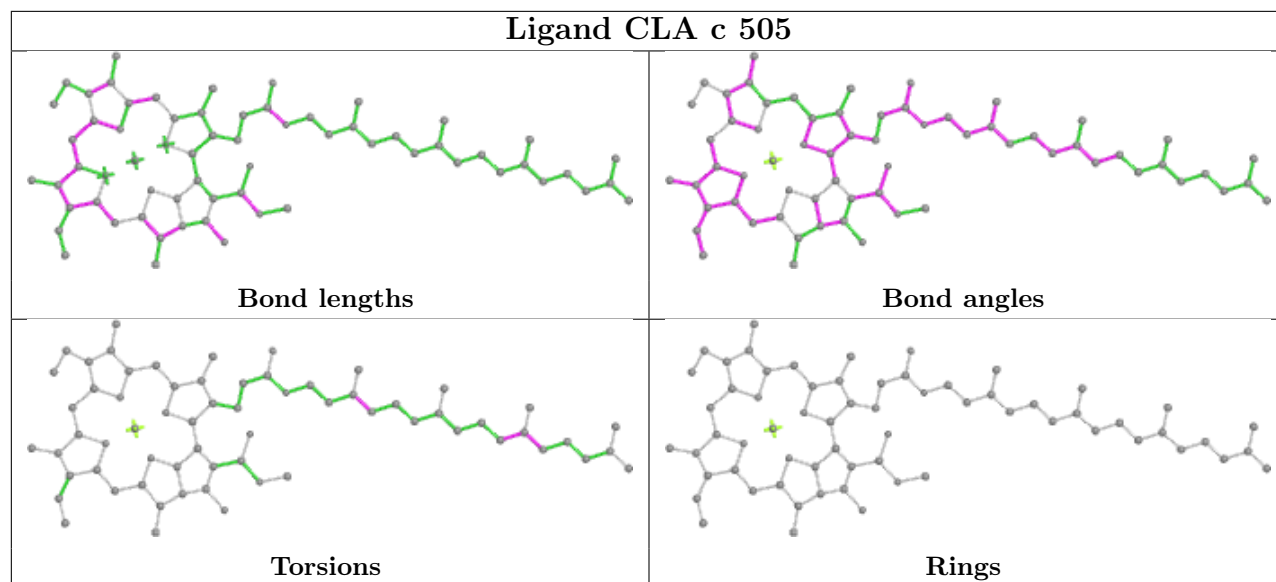
## Ligand CLA C 512



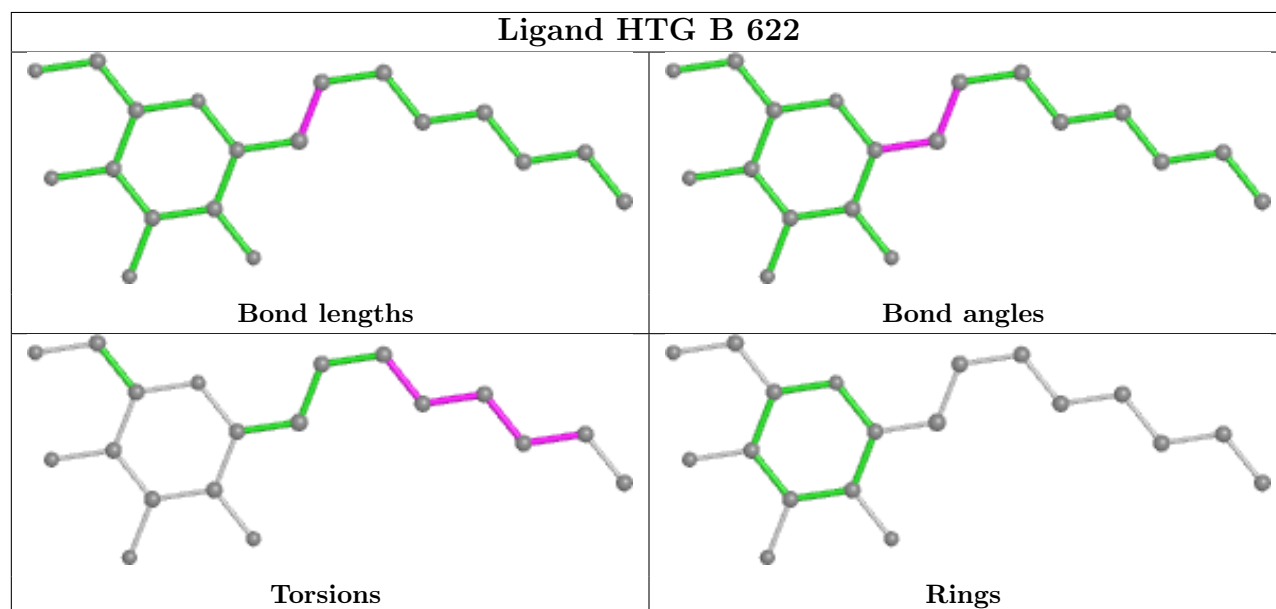
## Ligand SQD a 411



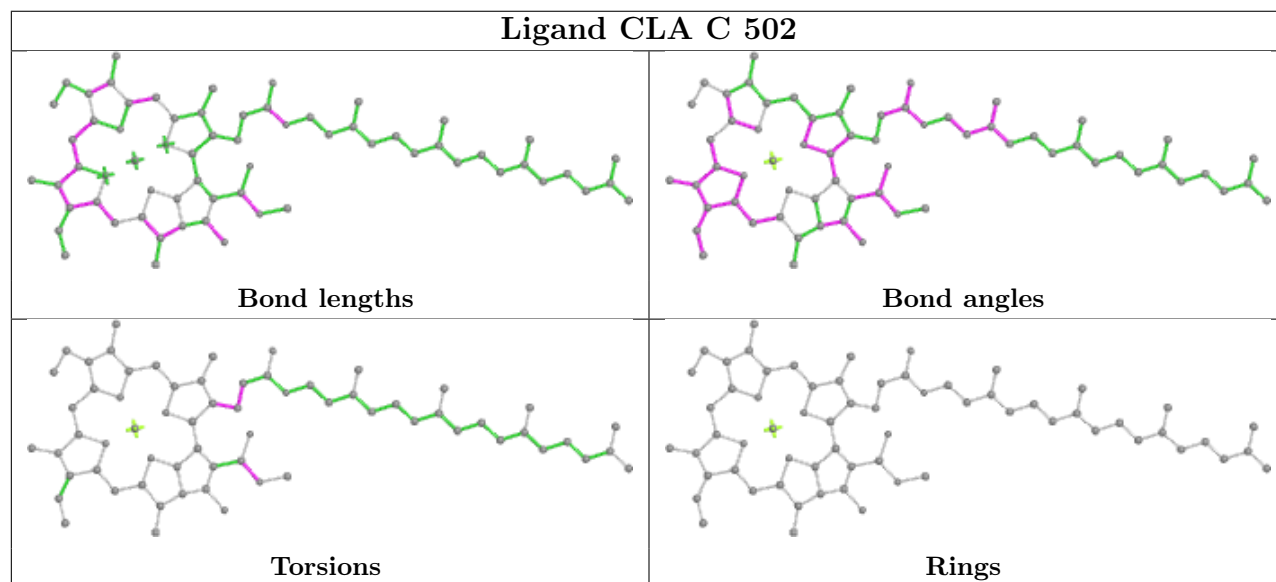
## Ligand CLA c 505

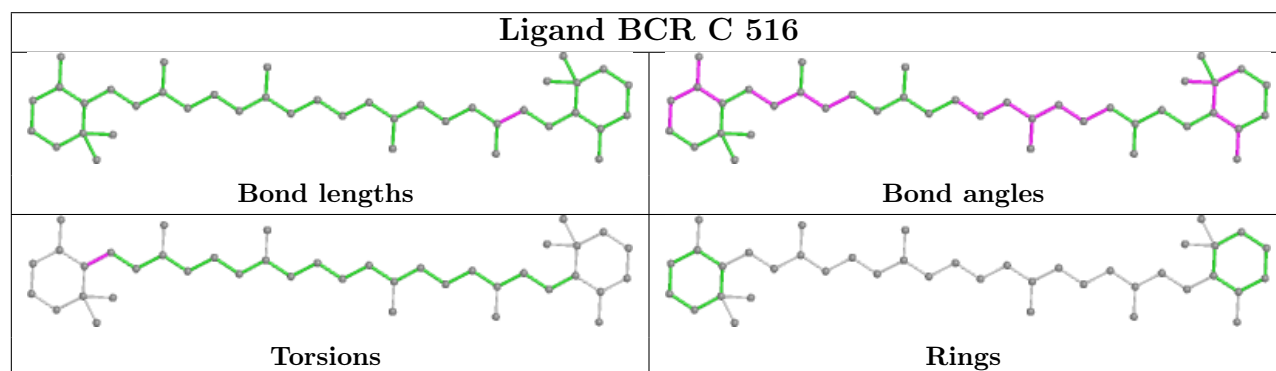
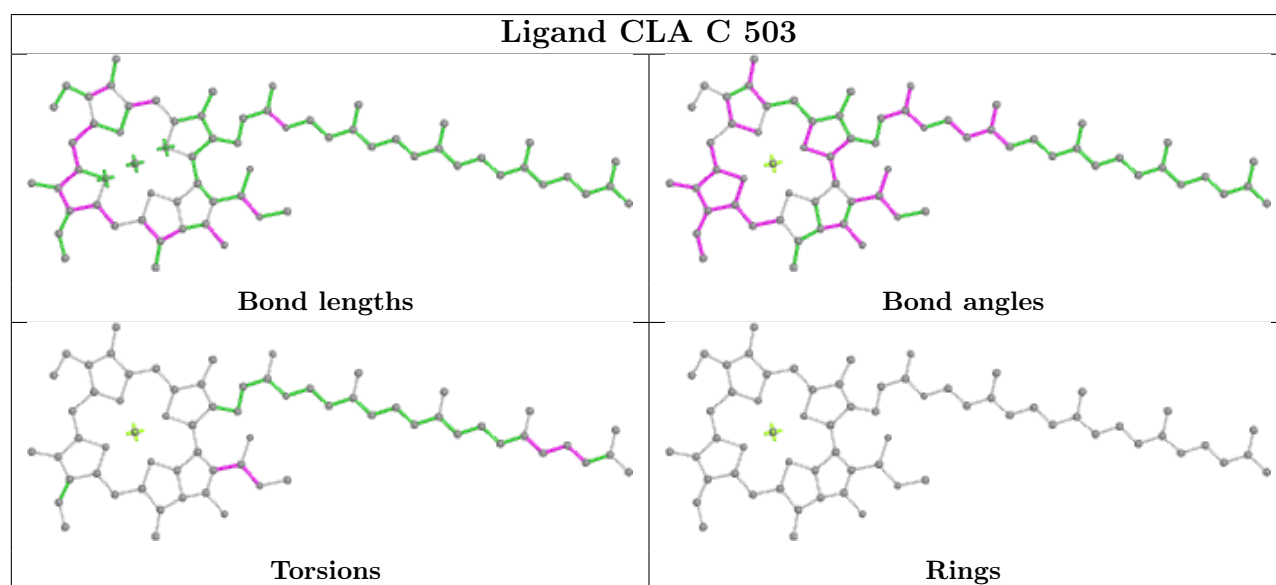
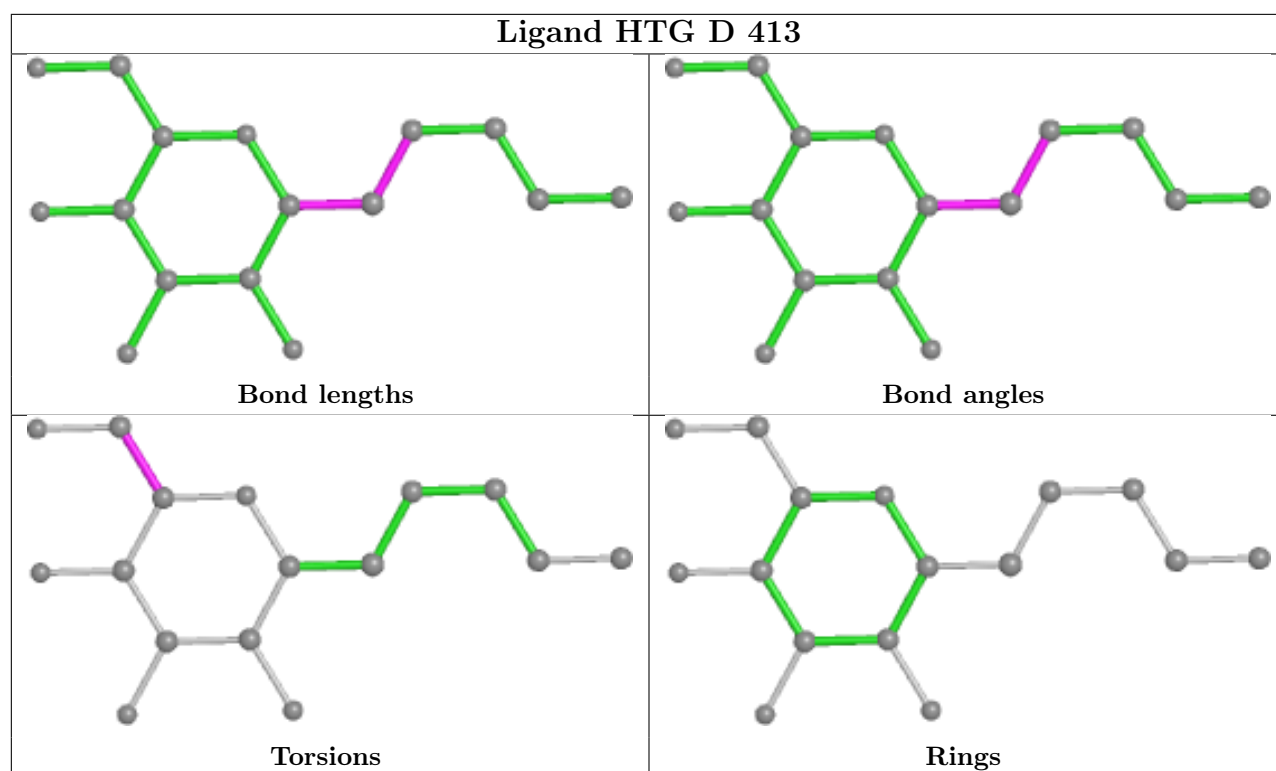


## Ligand HTG B 622

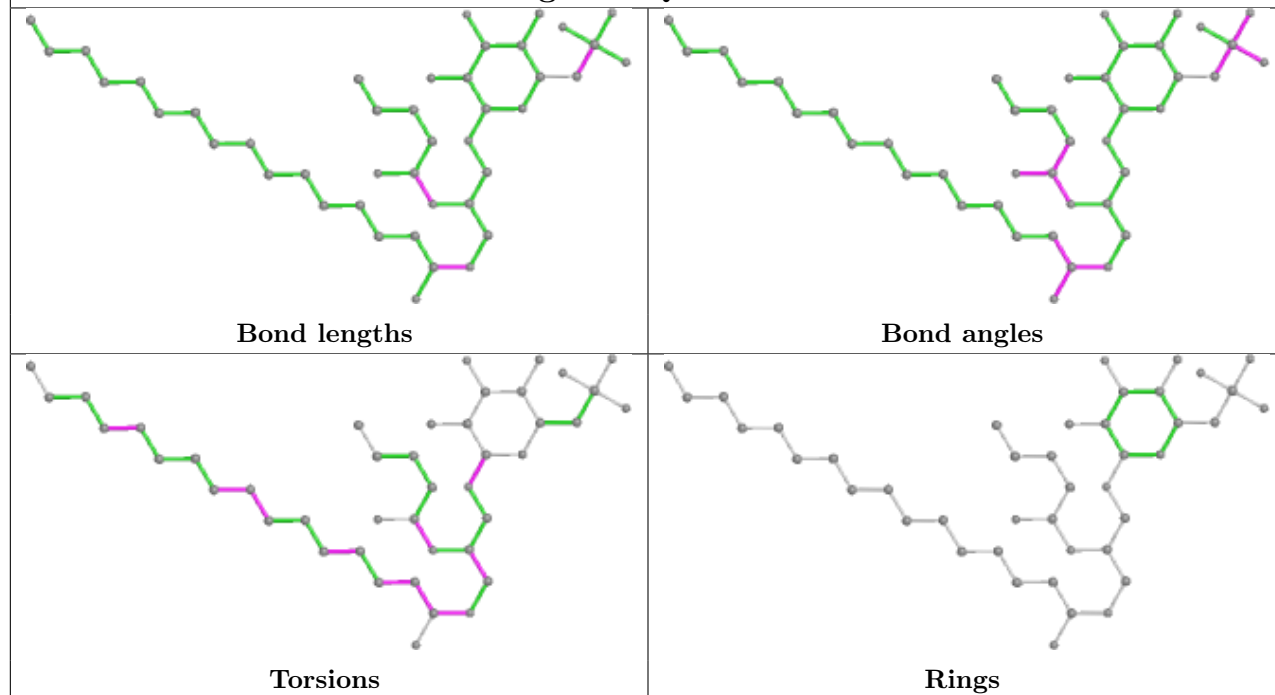


## Ligand CLA C 502

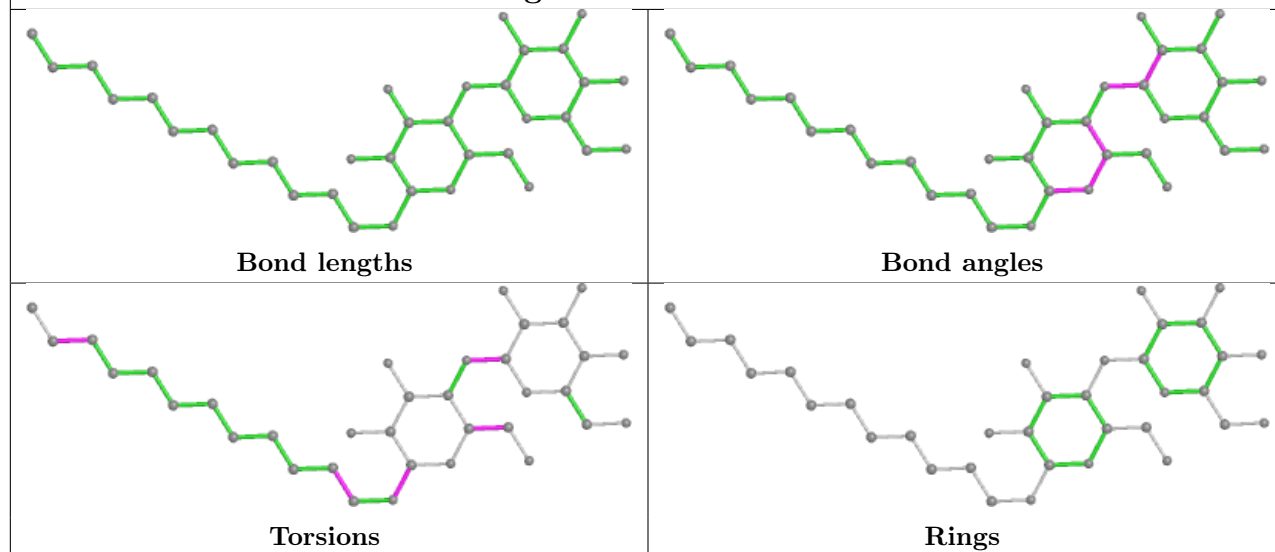


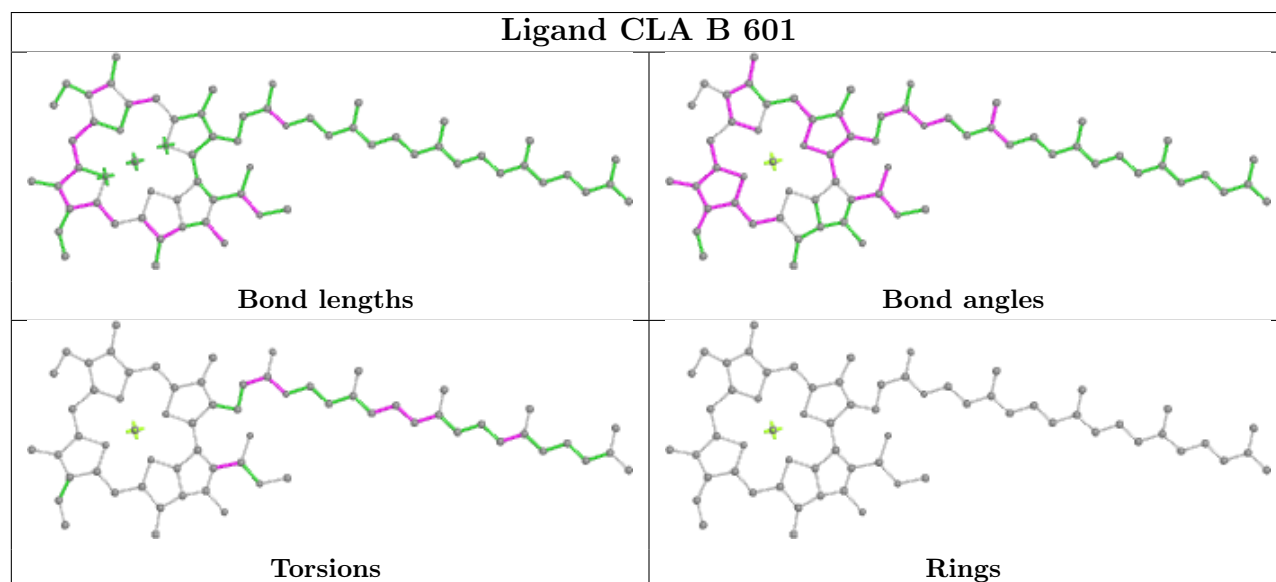
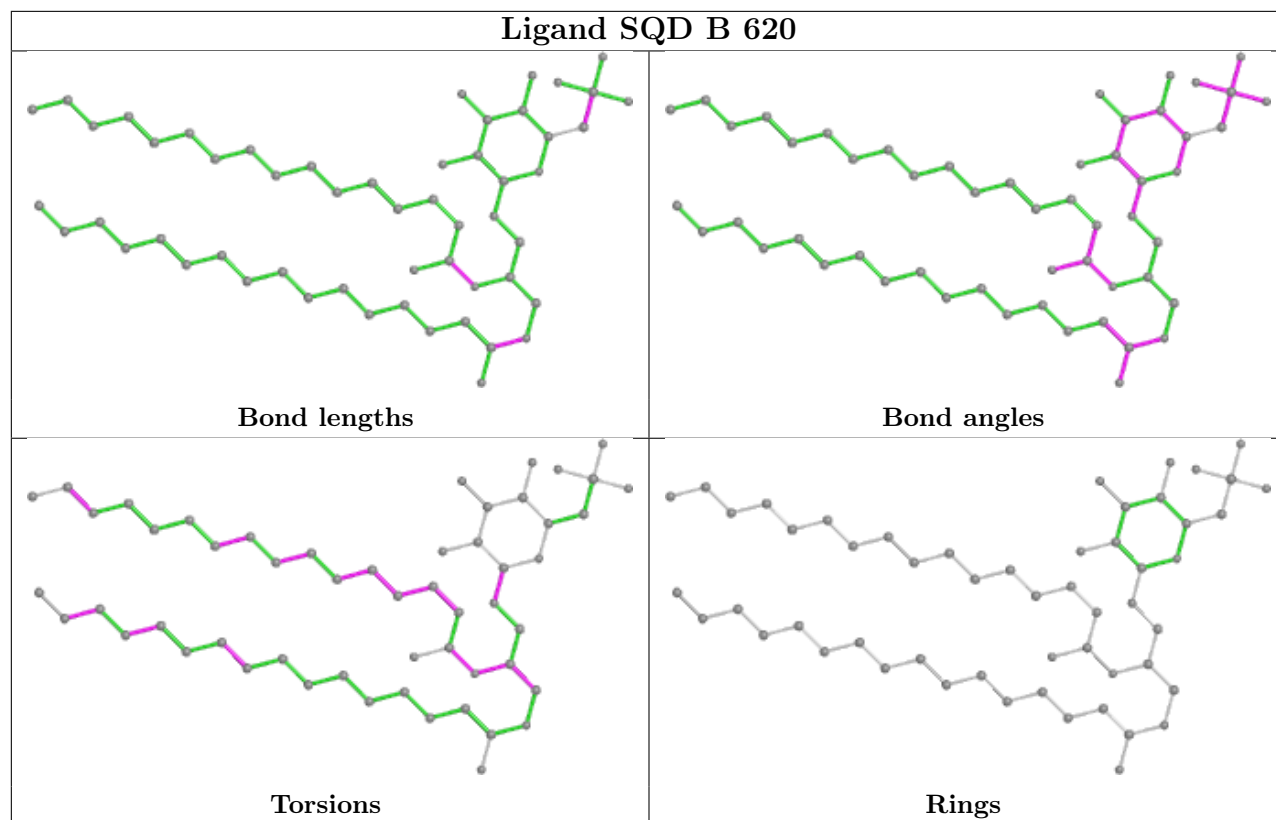


## Ligand SQD f 102

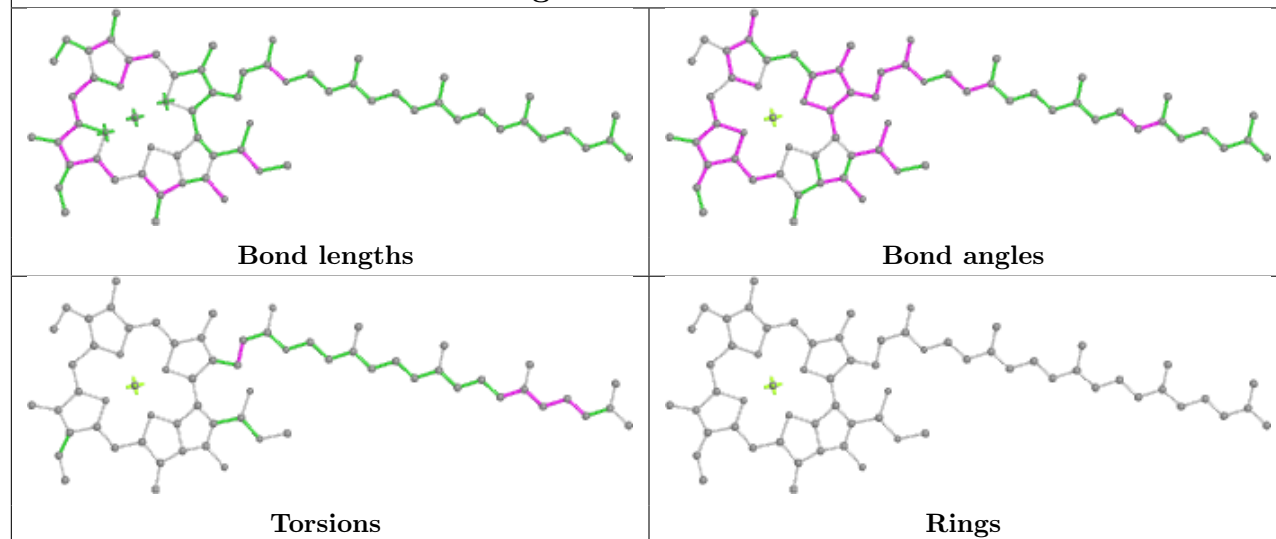


## Ligand LMT M 104

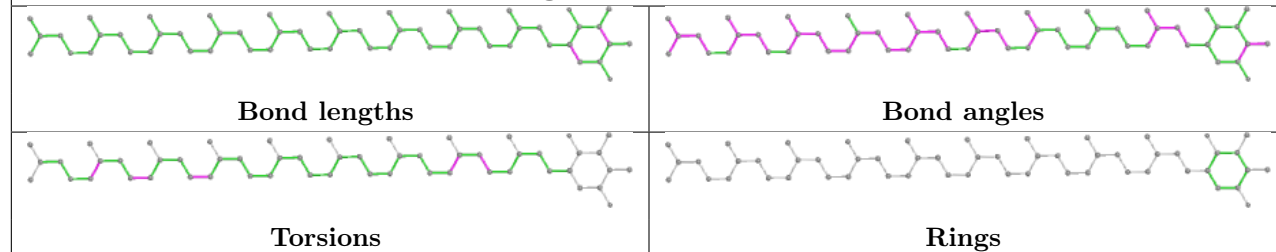




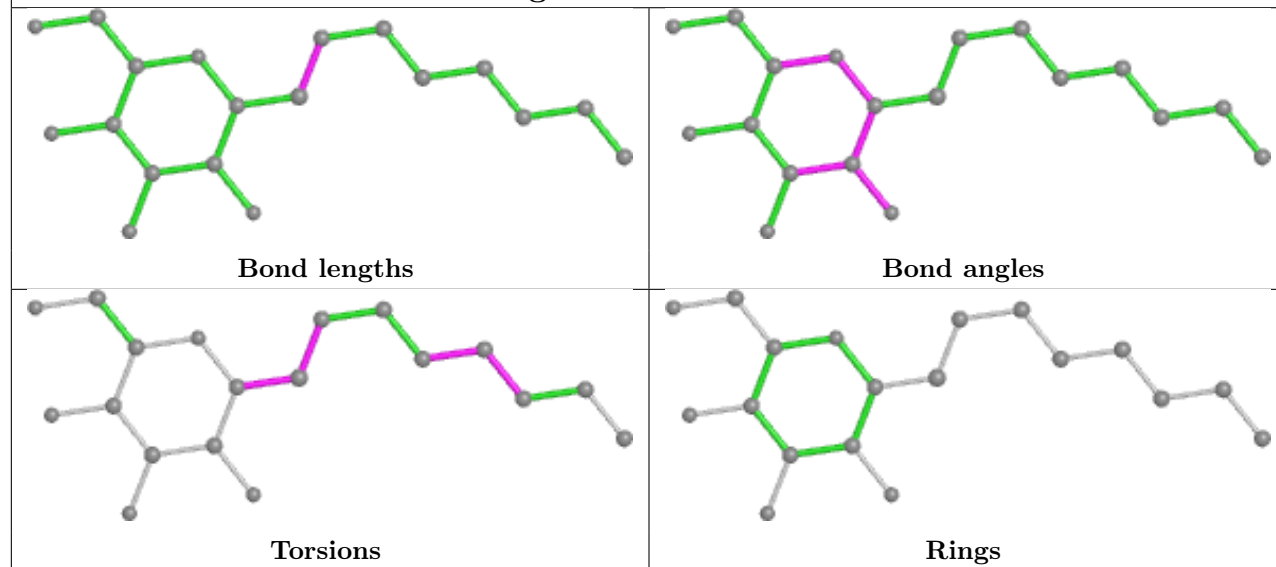
## Ligand CLA B 610



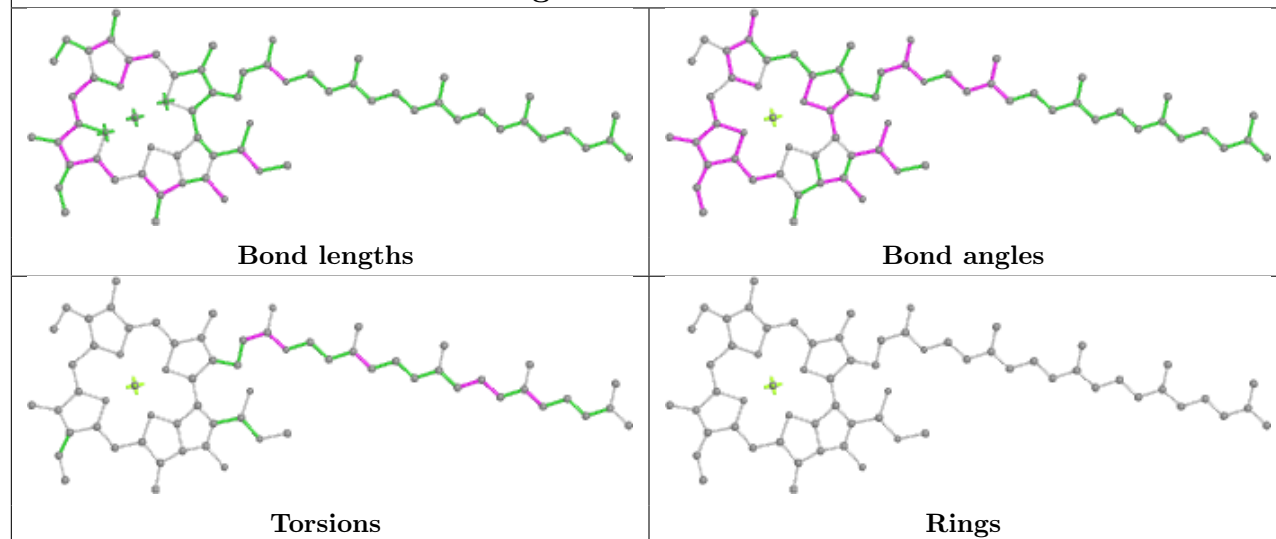
## Ligand PL9 d 406



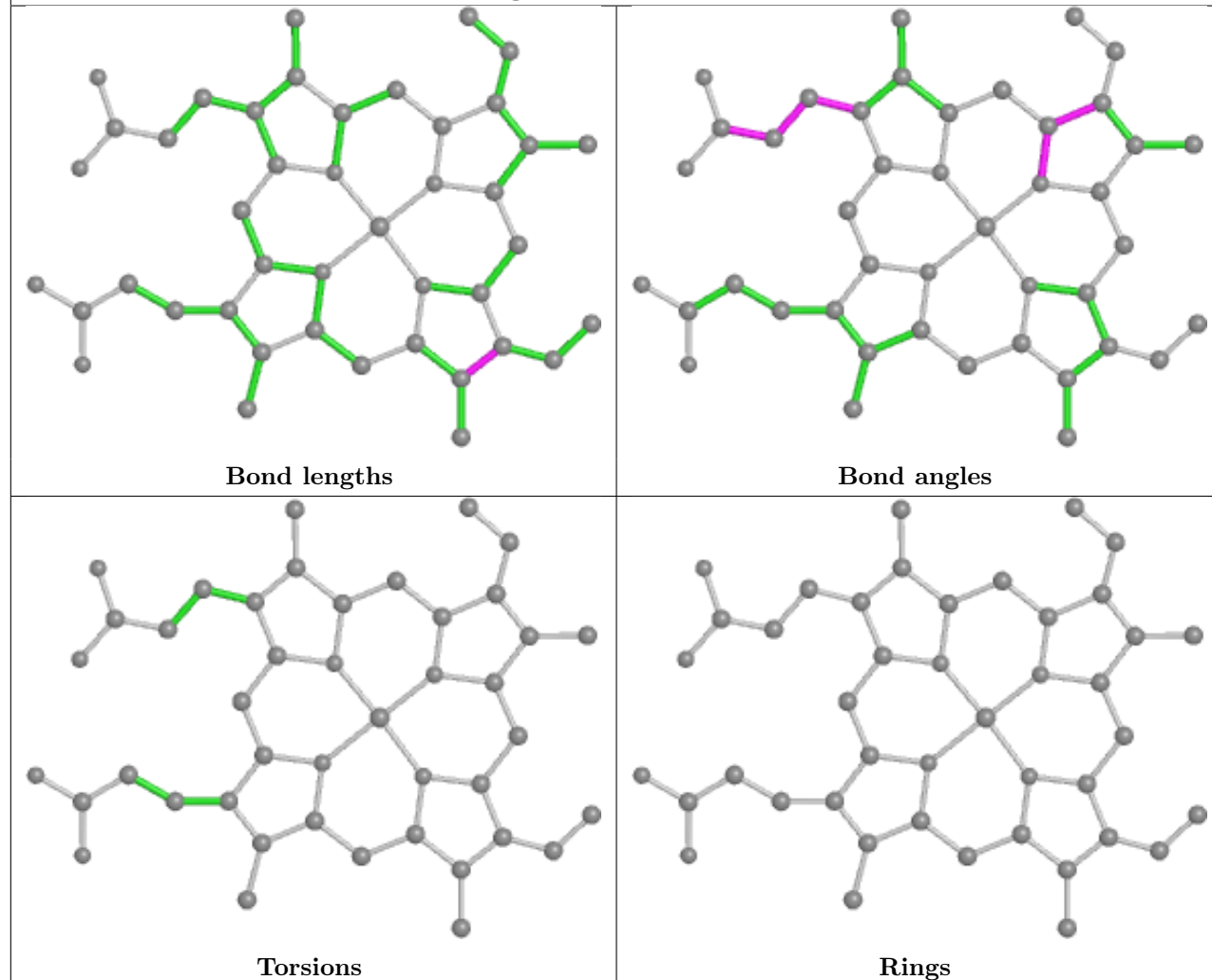
## Ligand HTG B 621



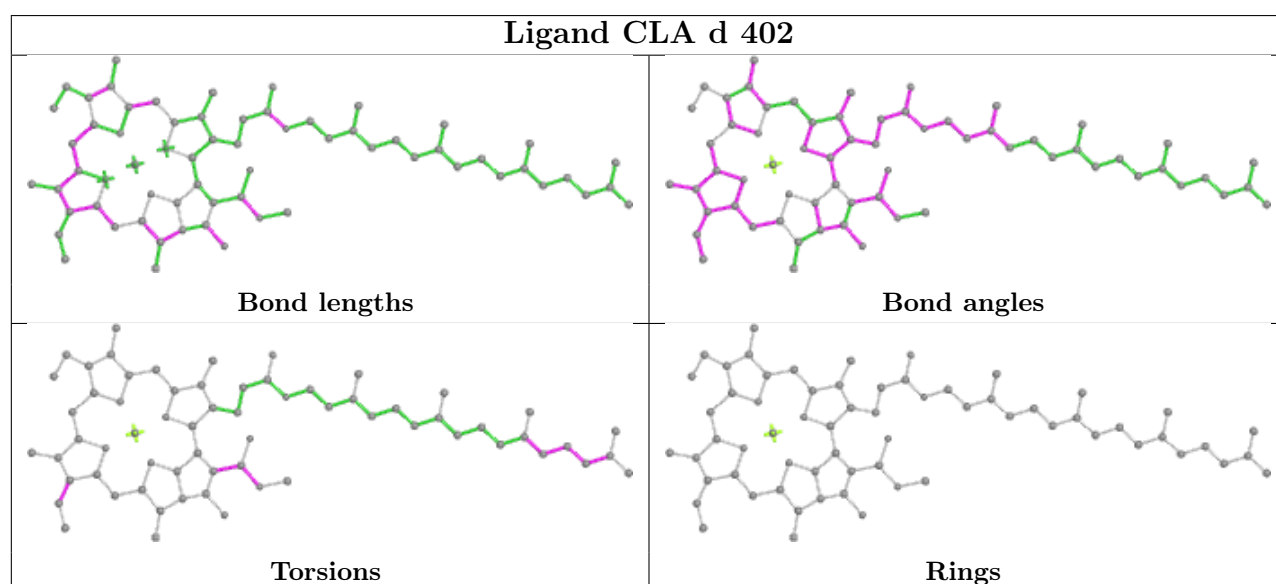
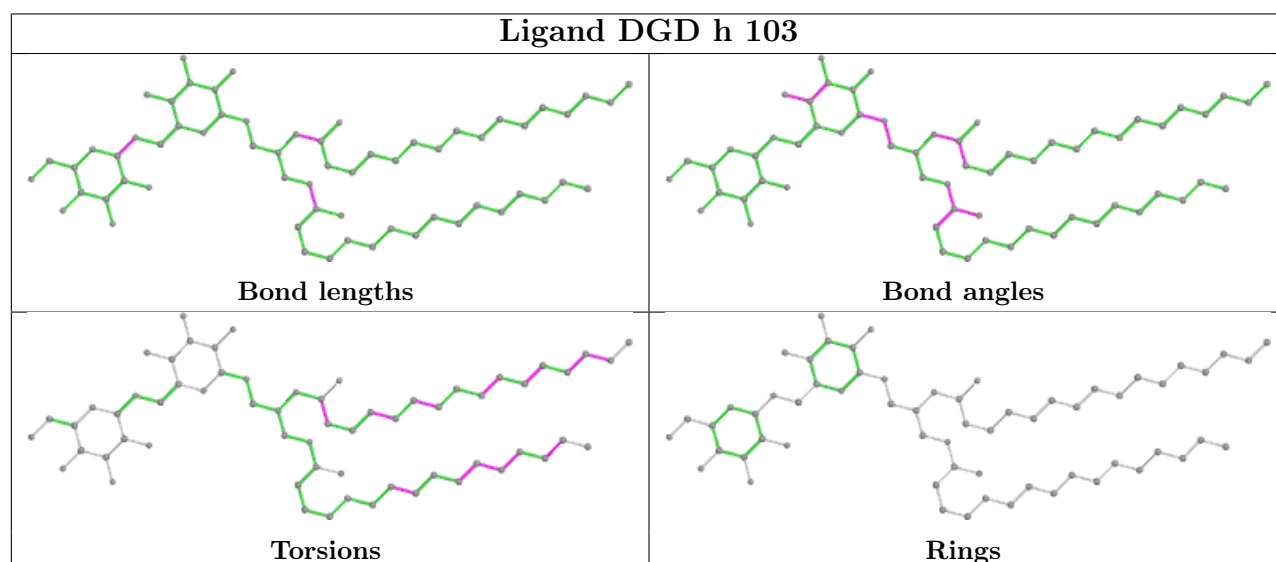
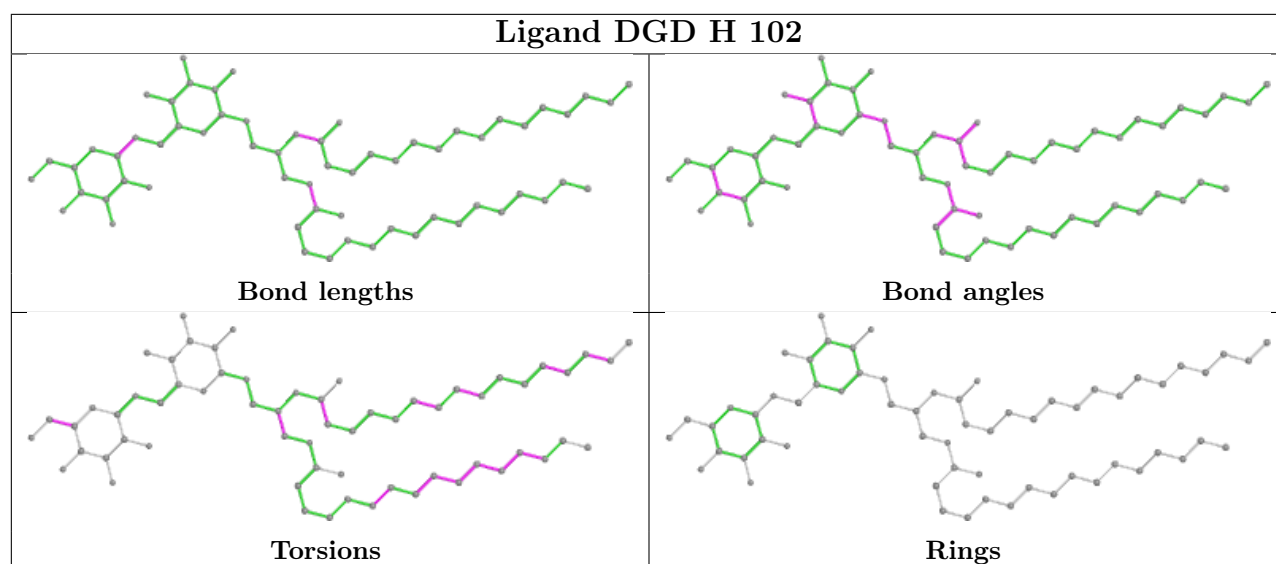
## Ligand CLA C 511



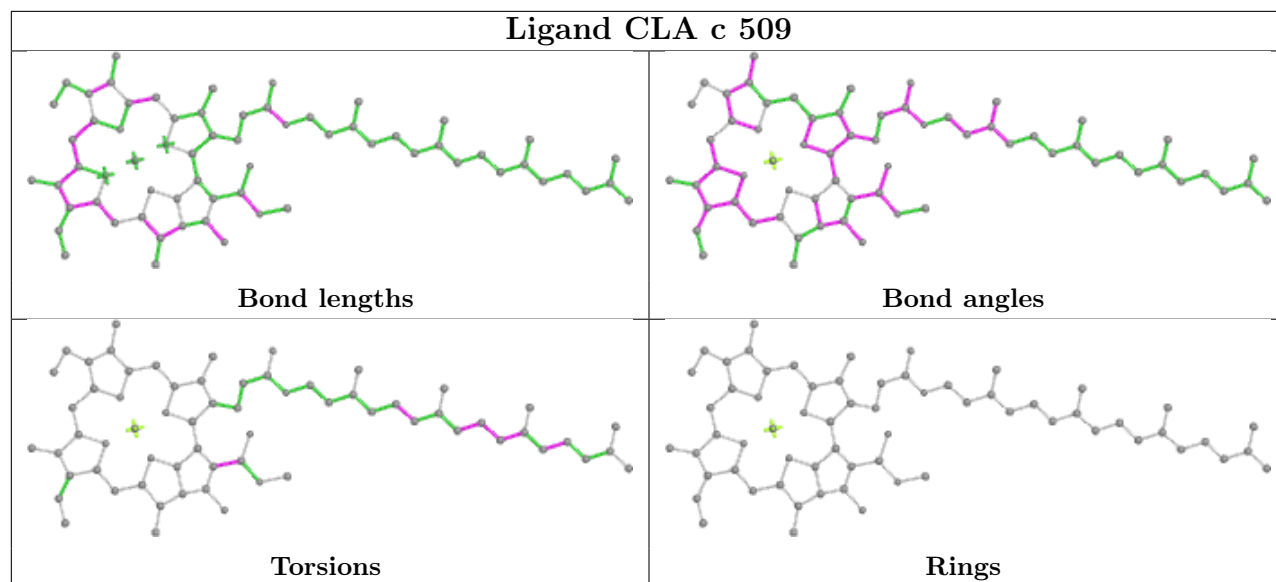
## Ligand HEM f 101



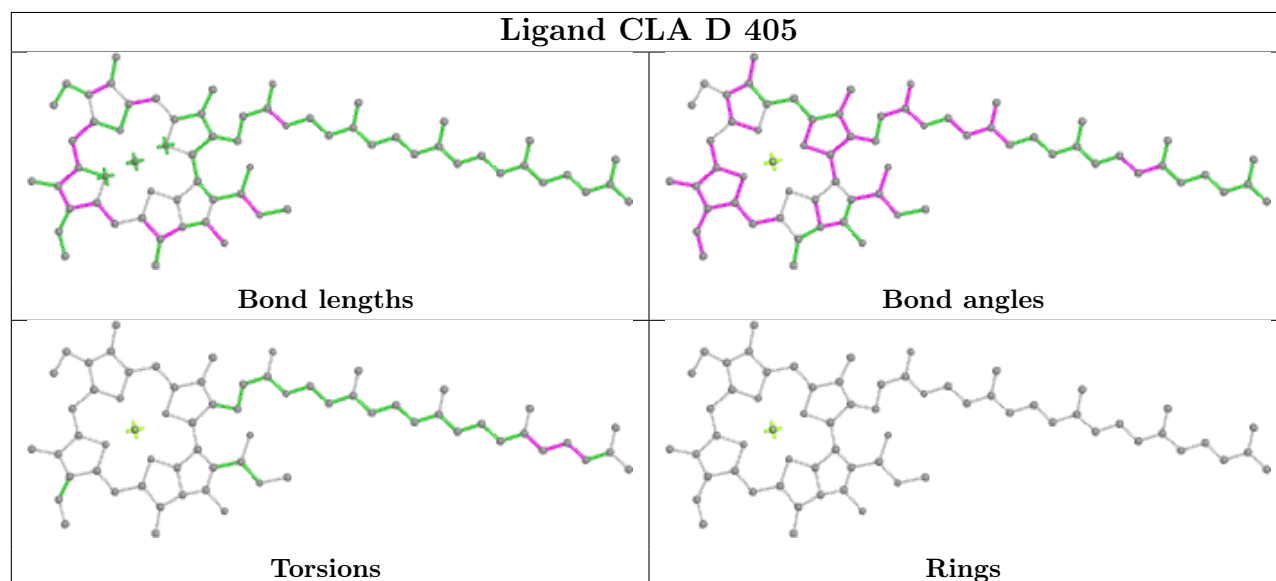




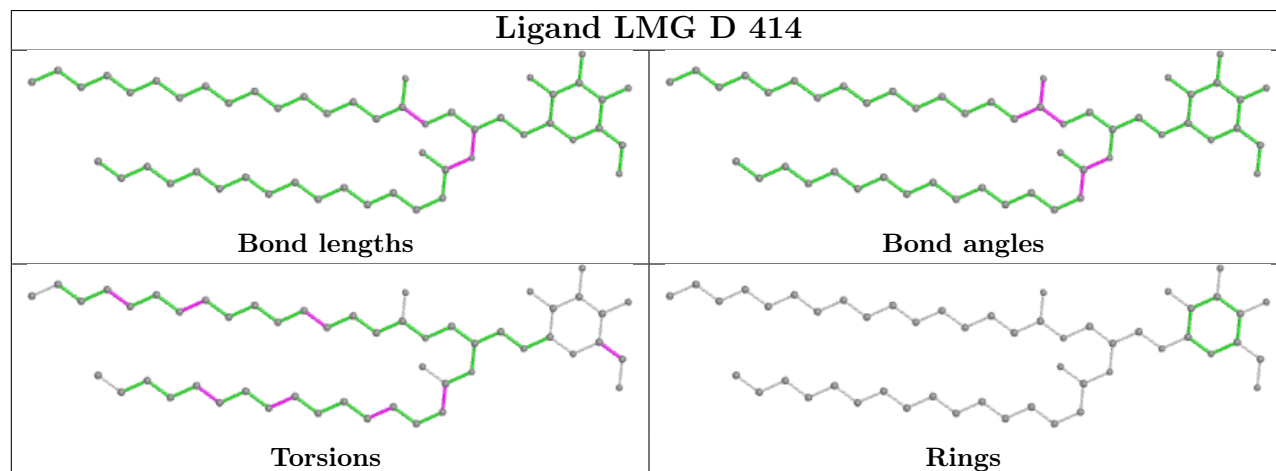
## Ligand CLA c 509



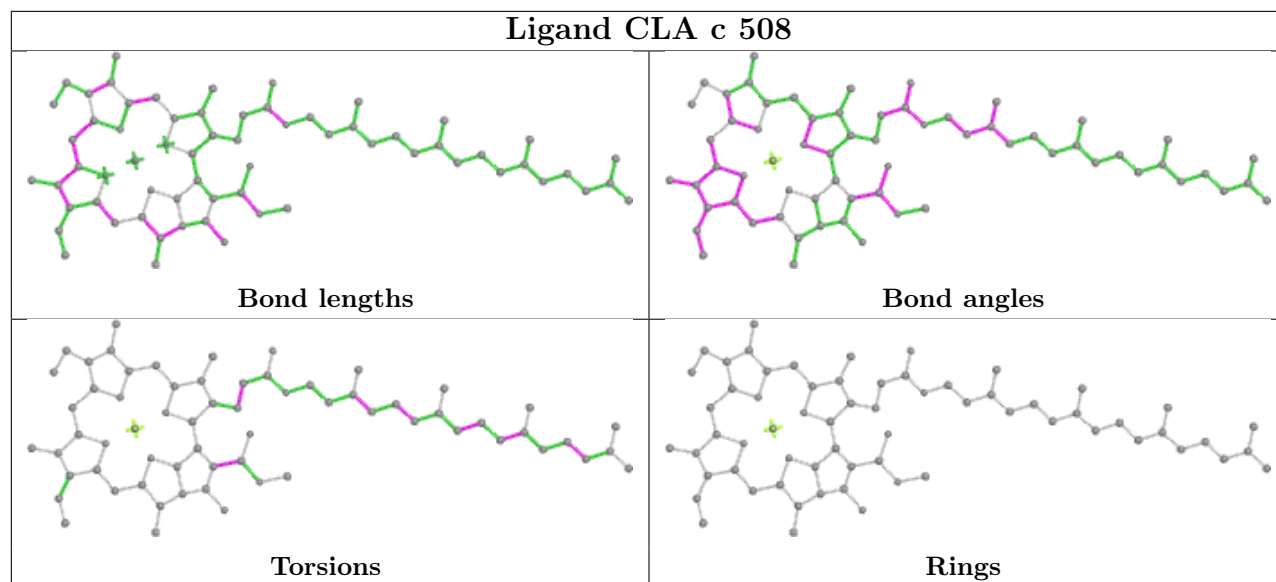
## Ligand CLA D 405



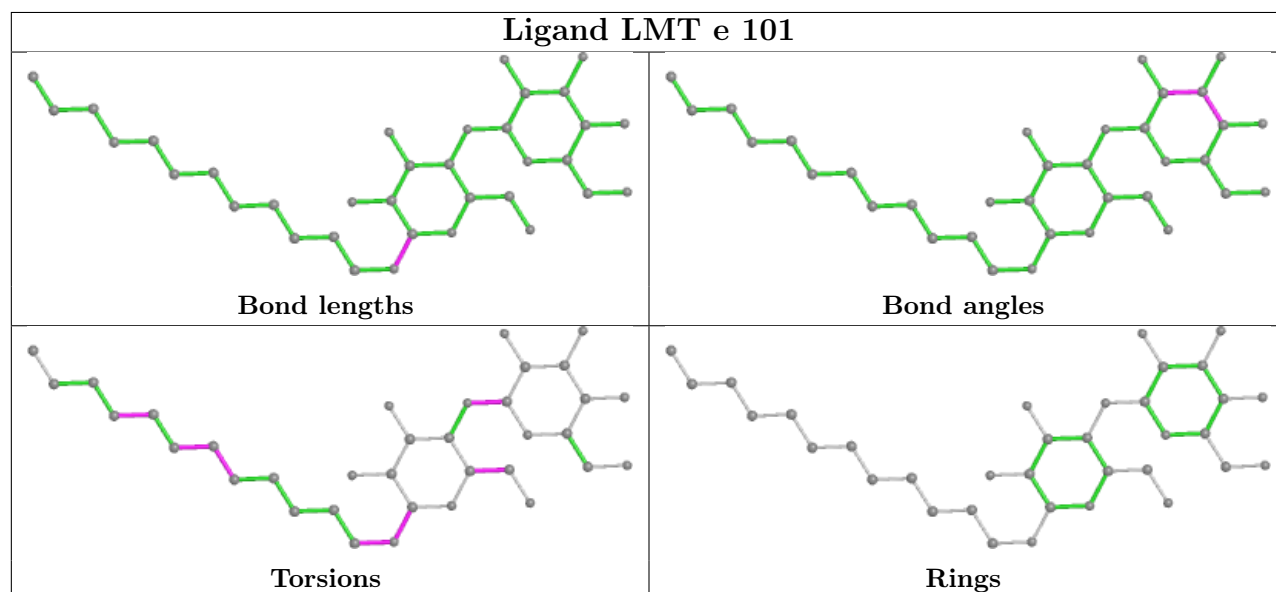
## Ligand LMG D 414



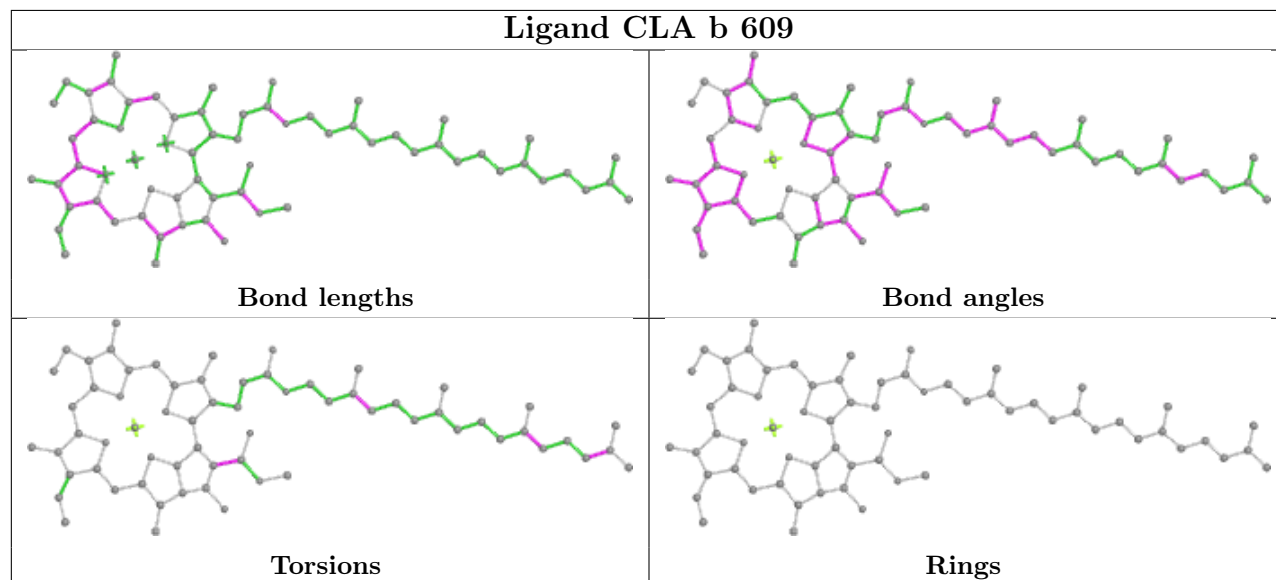
## Ligand CLA c 508



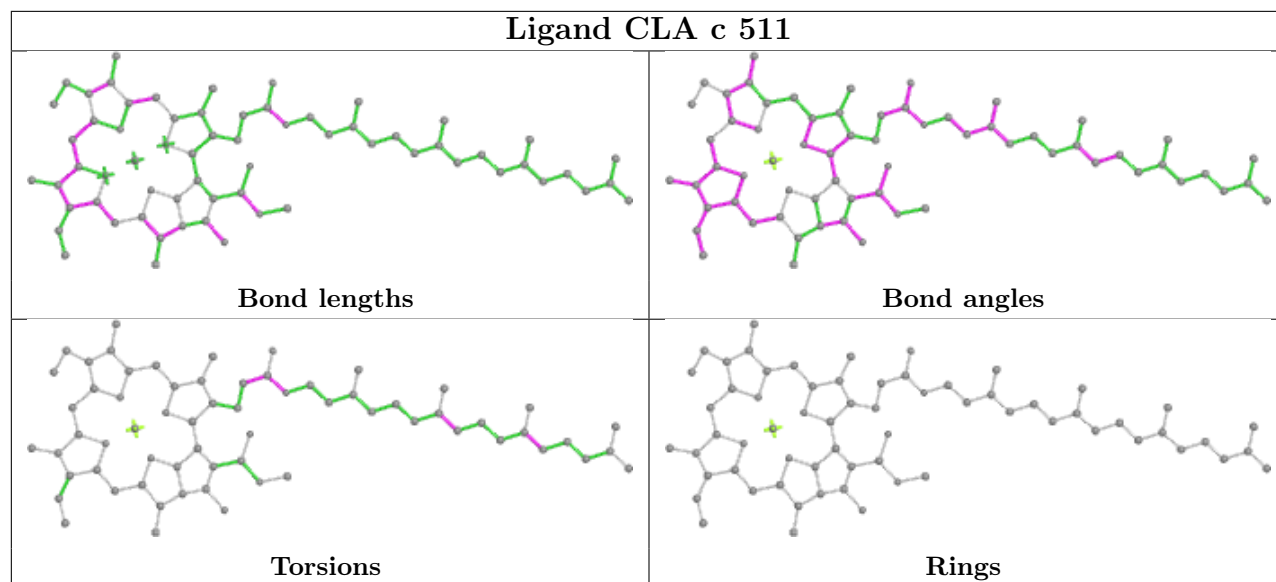
## Ligand LMT e 101



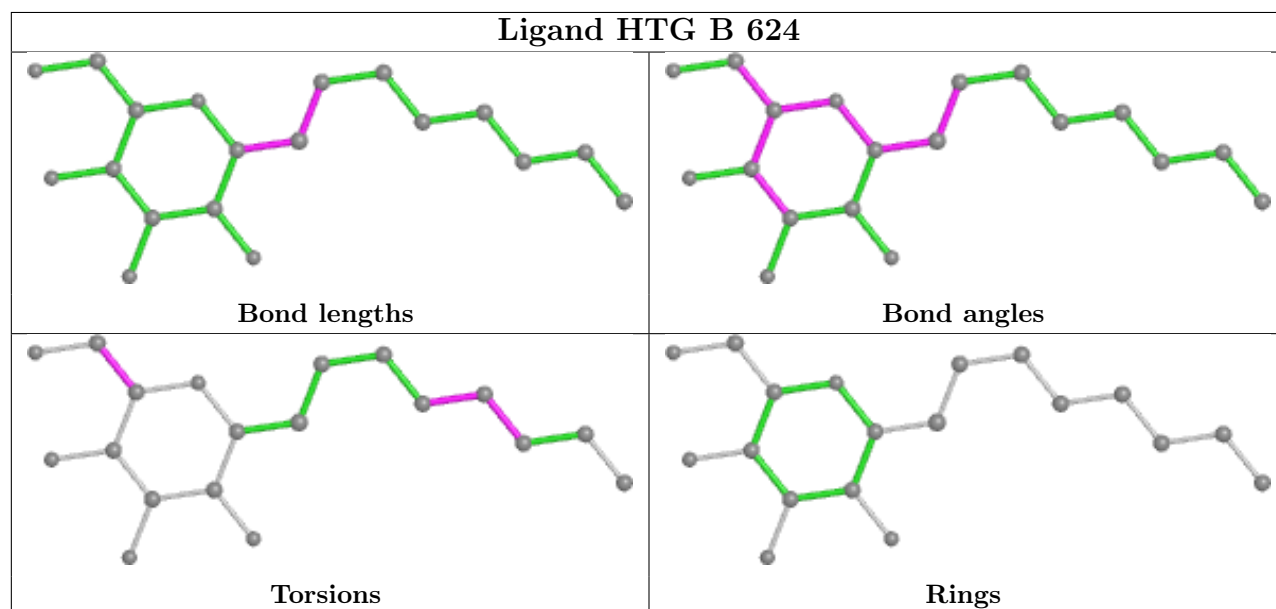
## Ligand CLA b 609



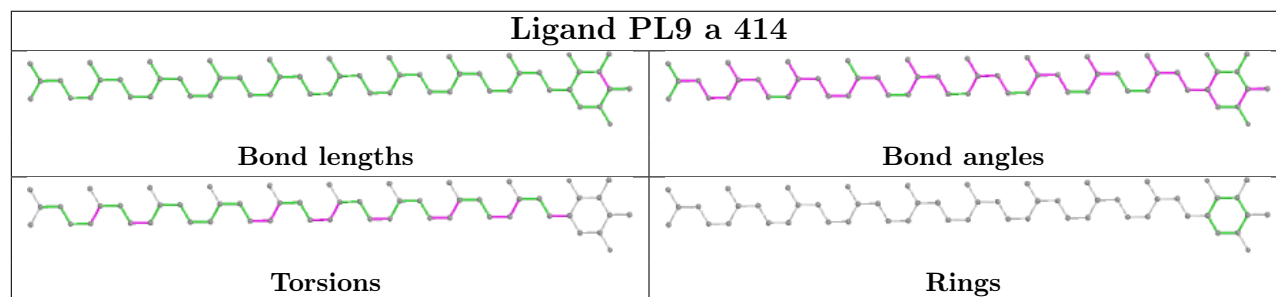
## Ligand CLA c 511

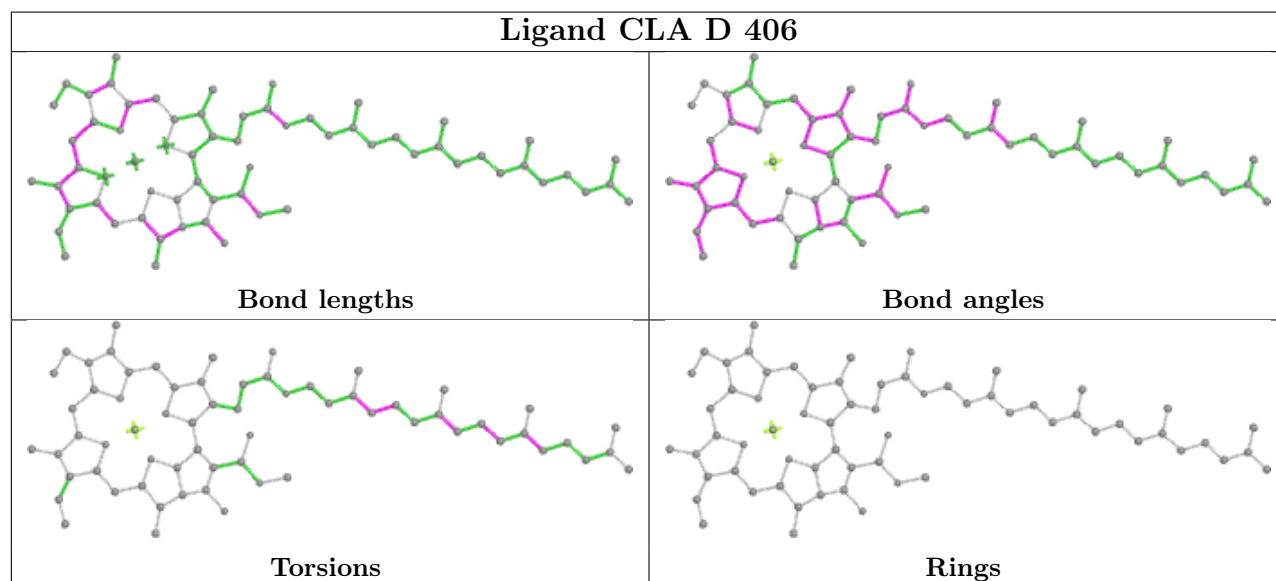
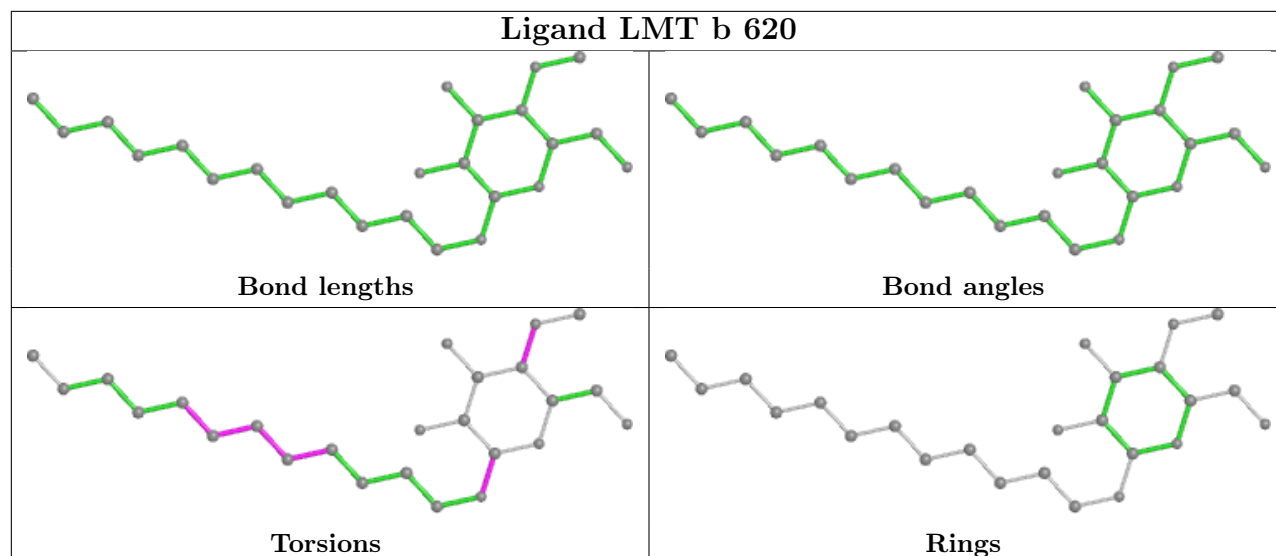


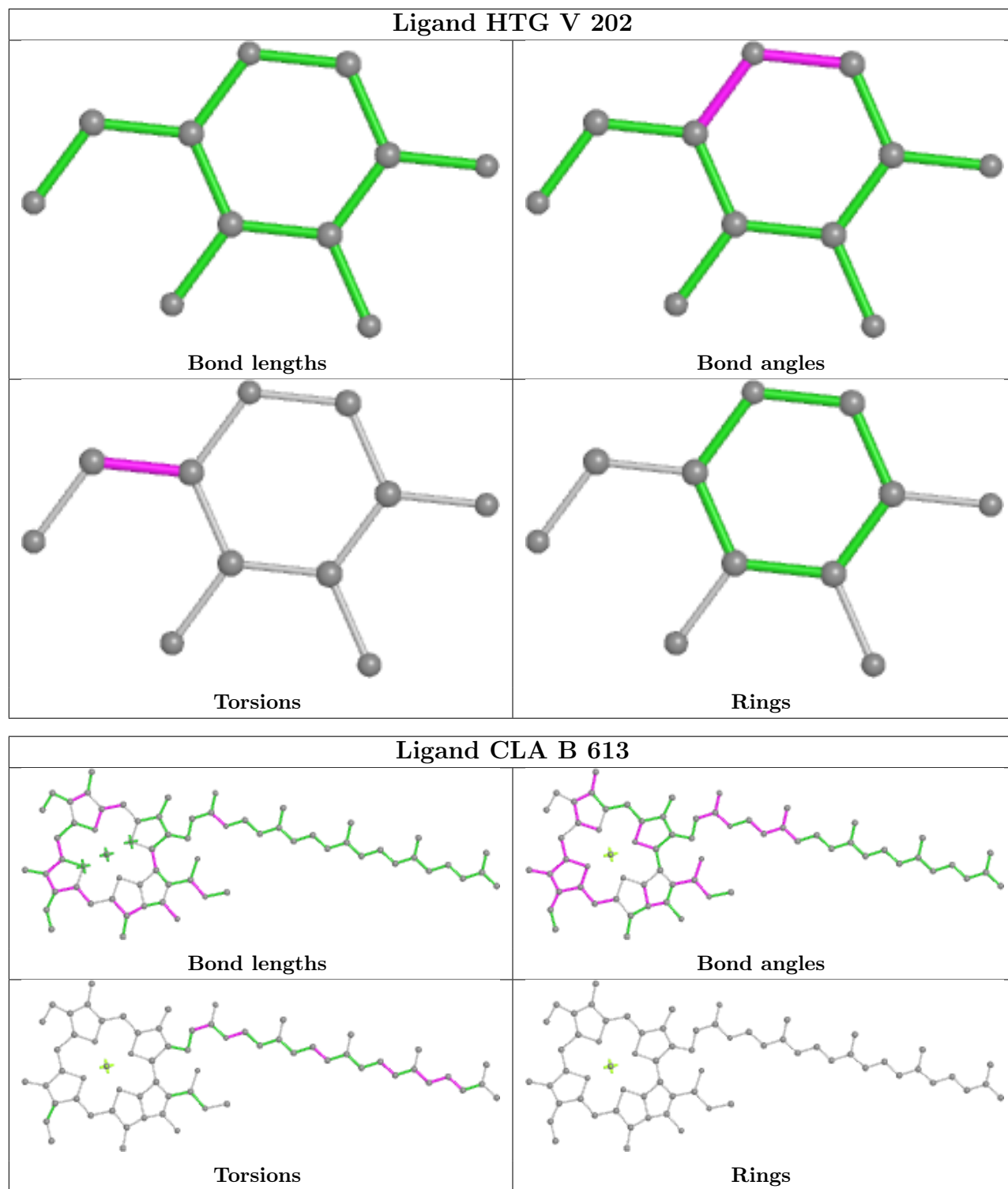
## Ligand HTG B 624

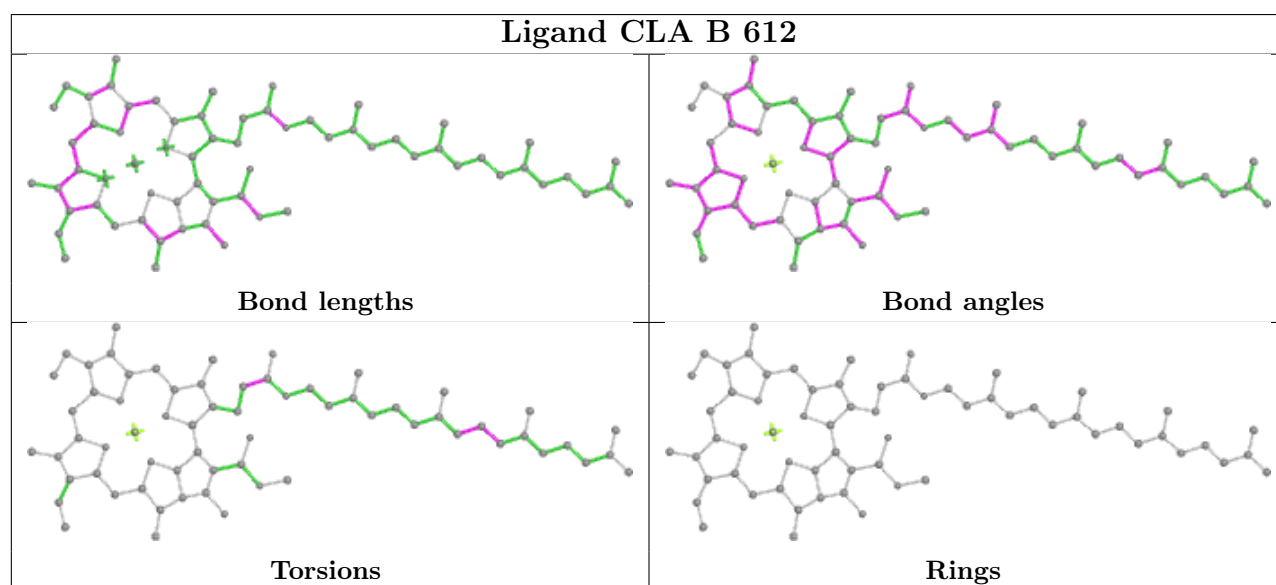
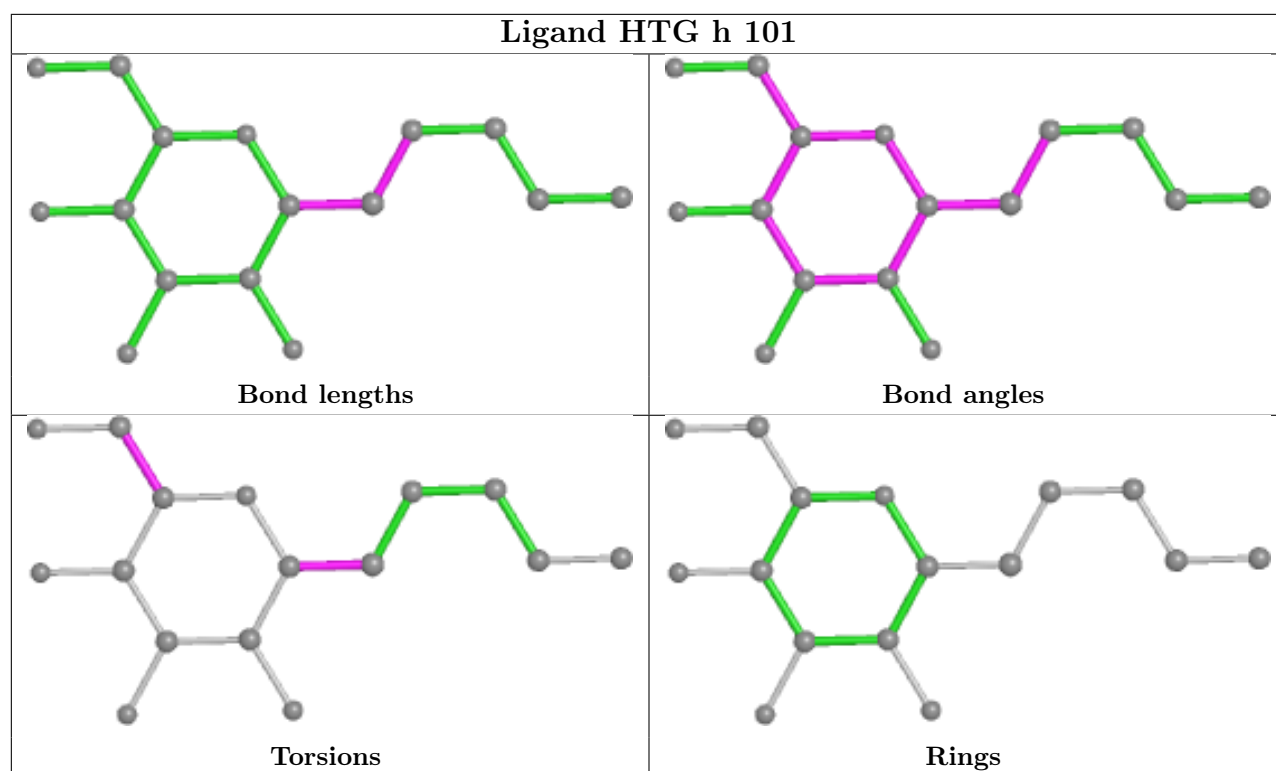


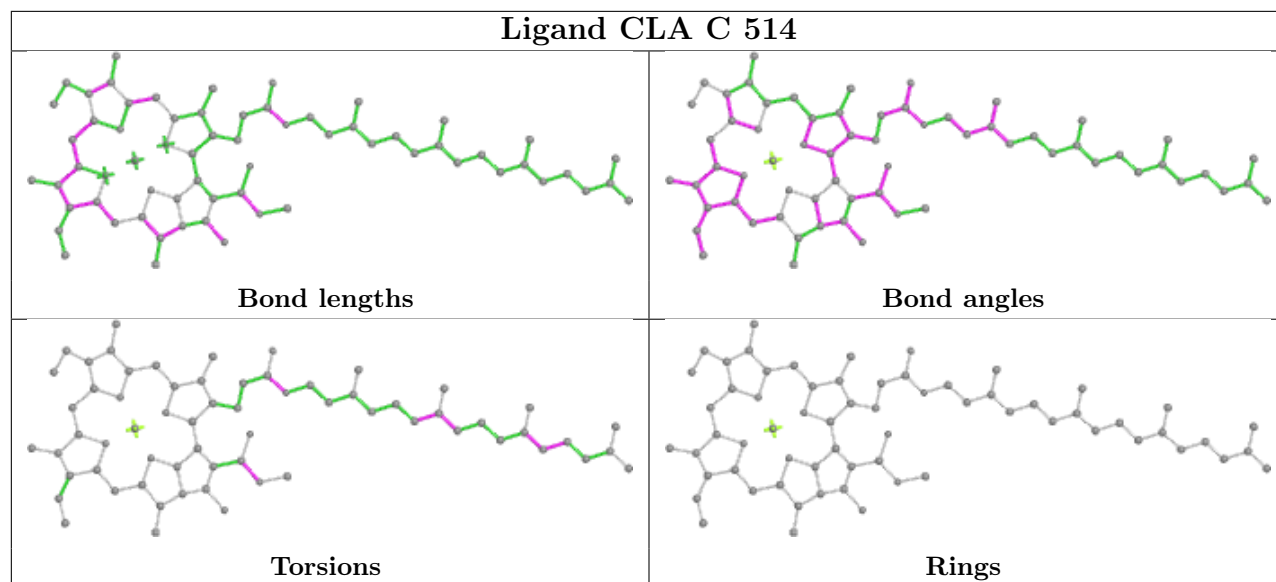
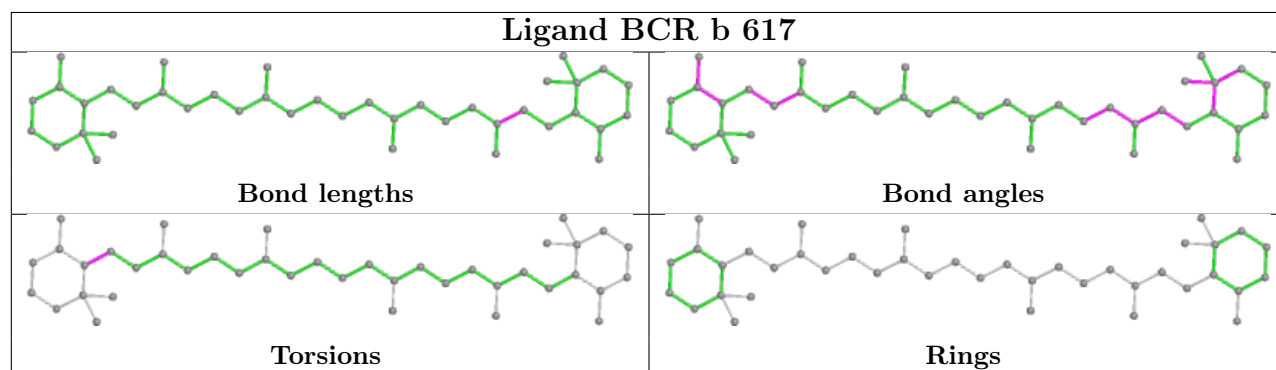
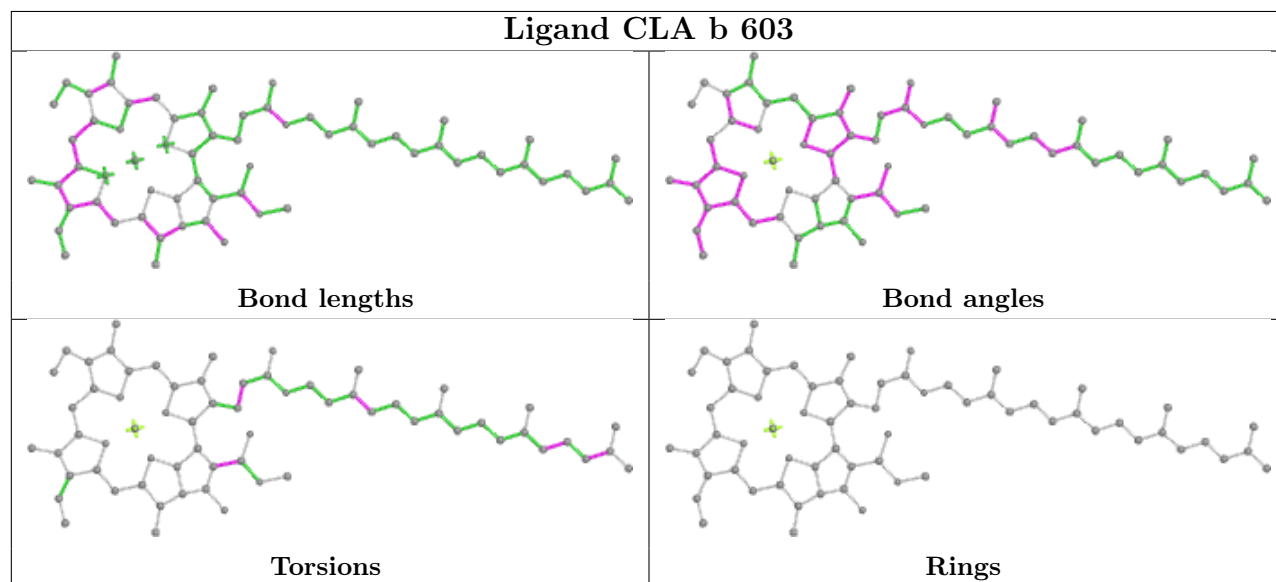
## Ligand PL9 a 414



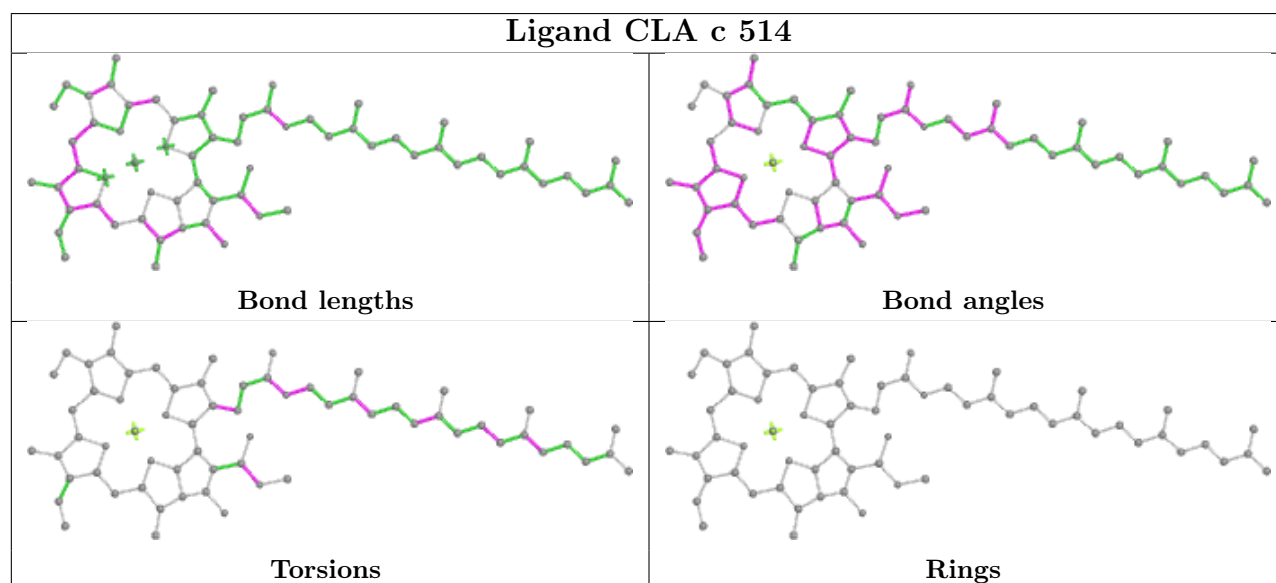
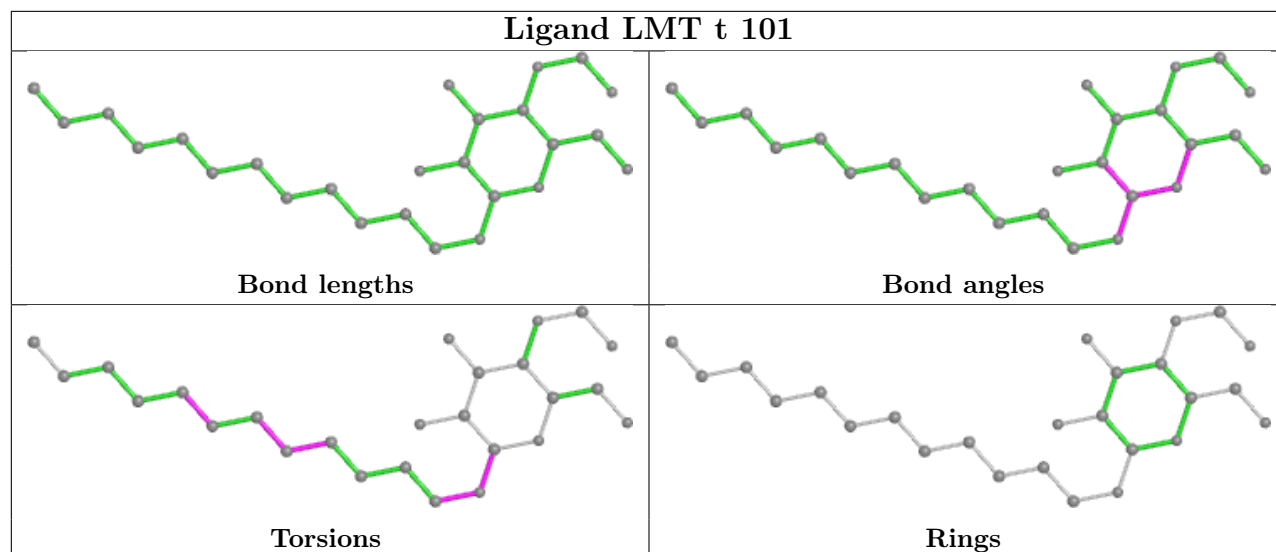
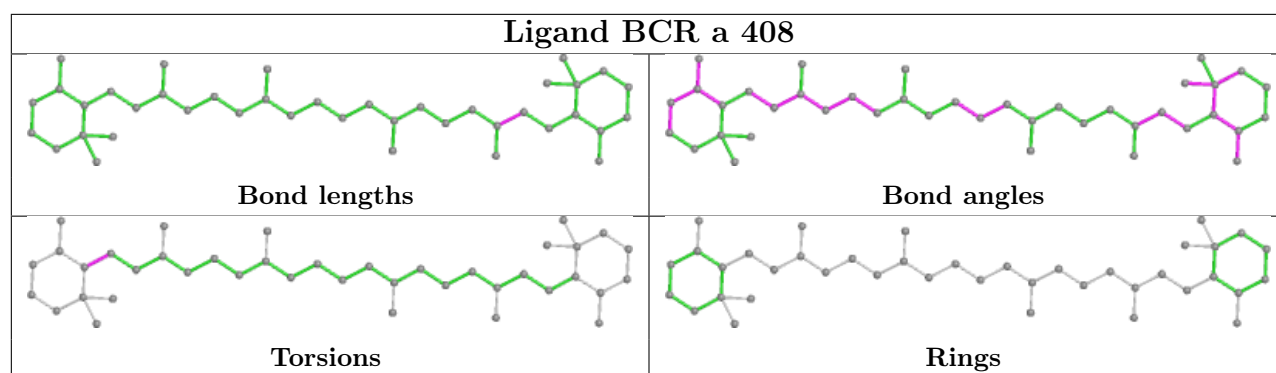


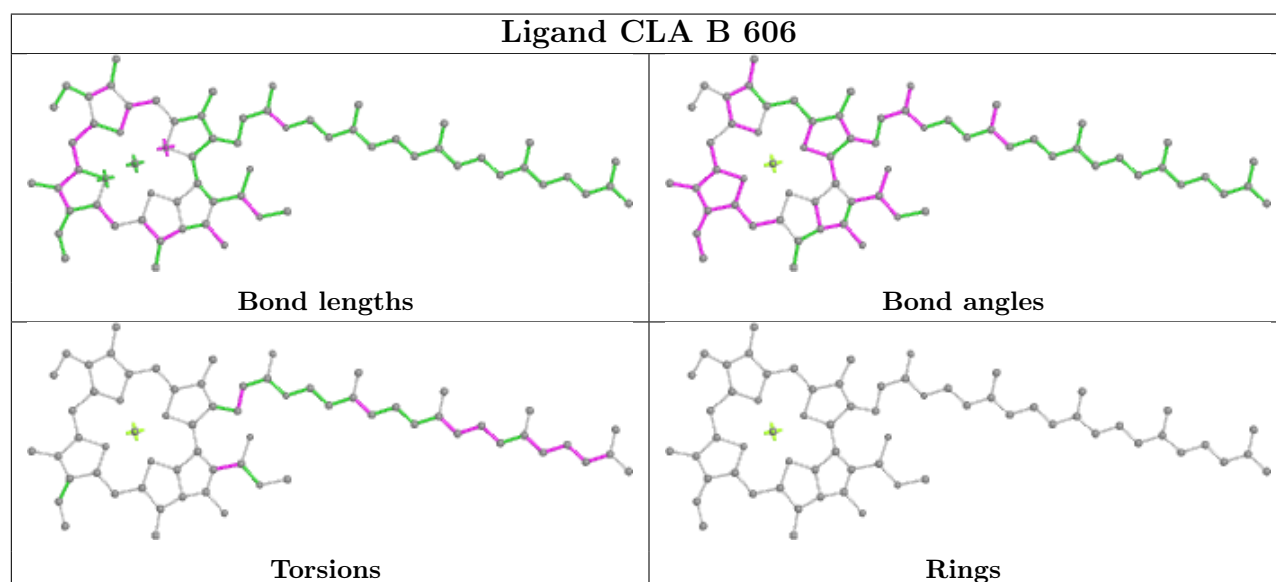
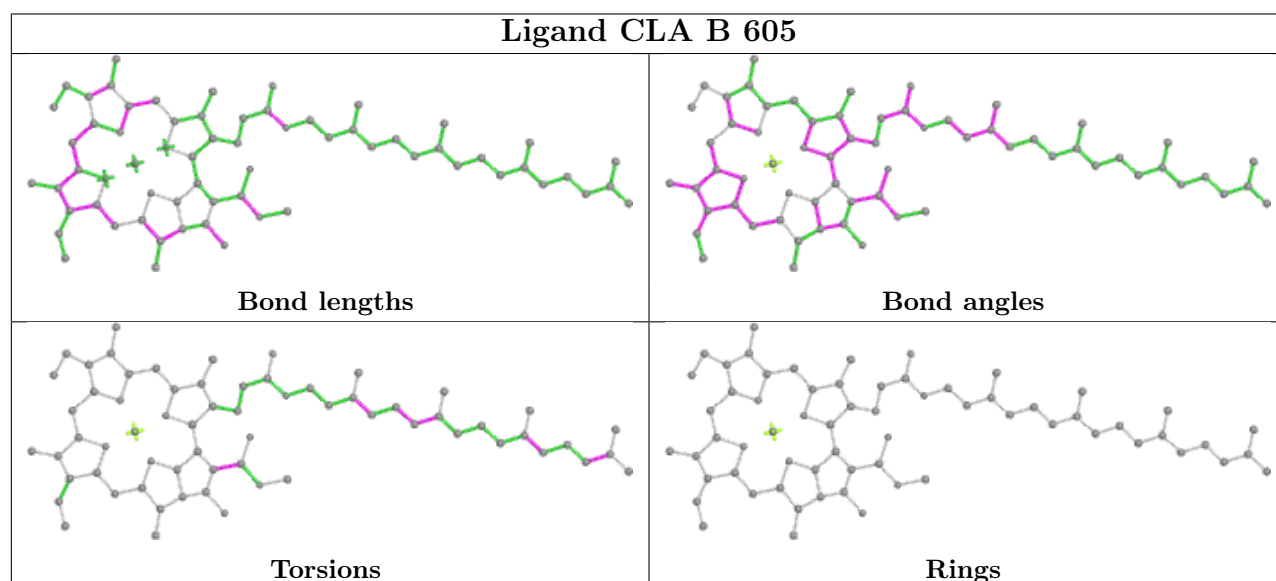
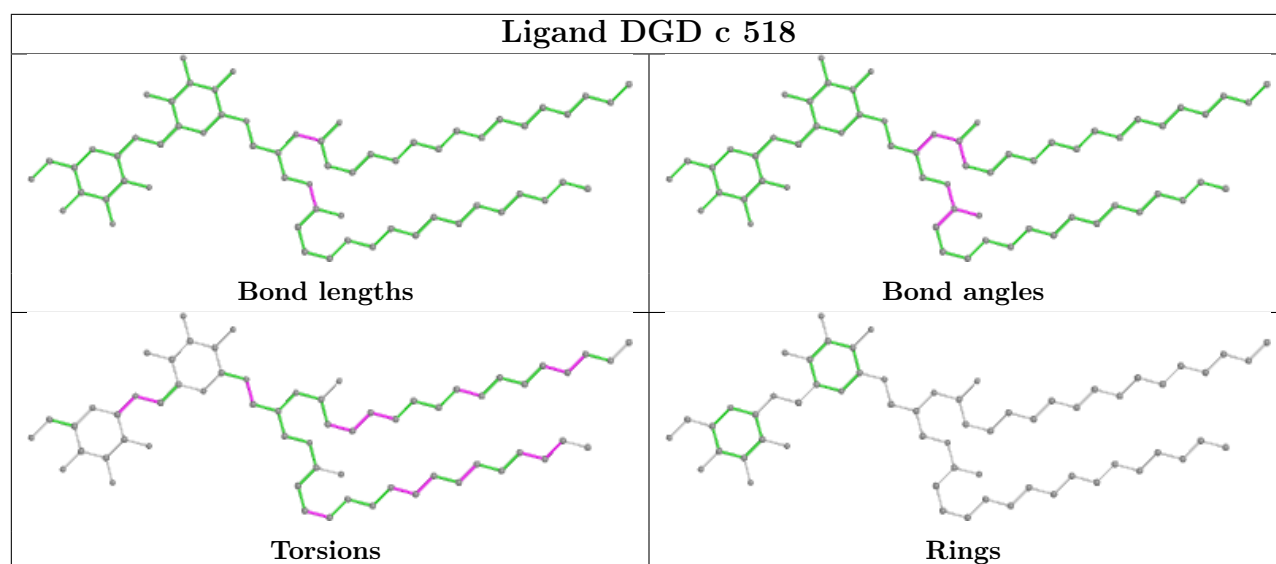


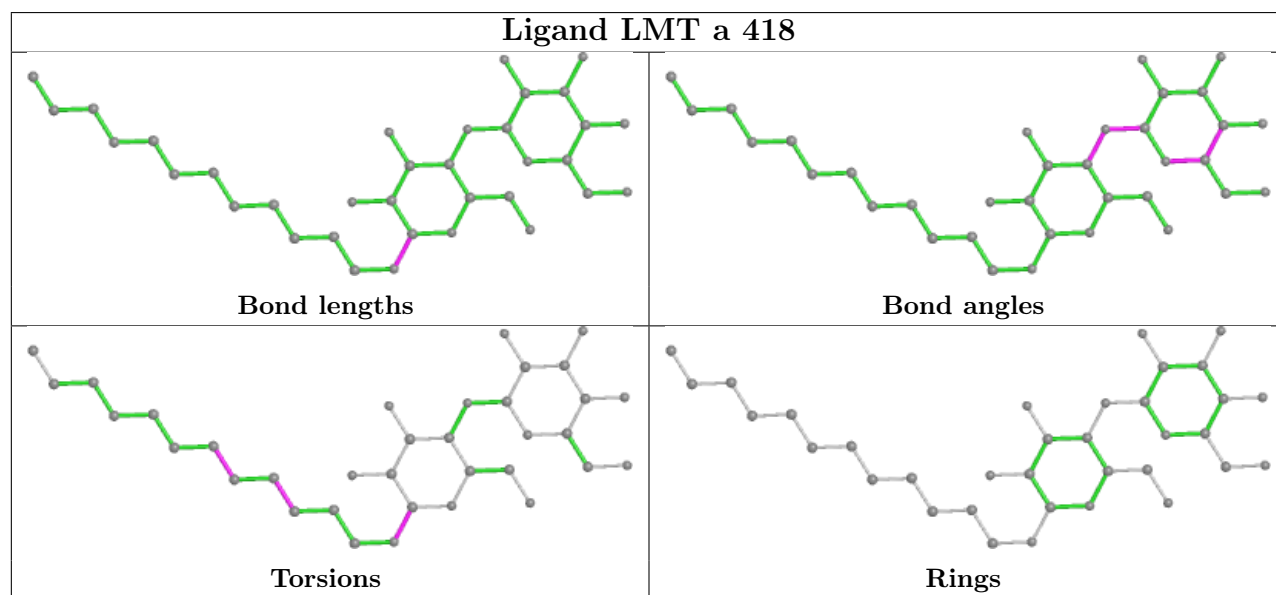
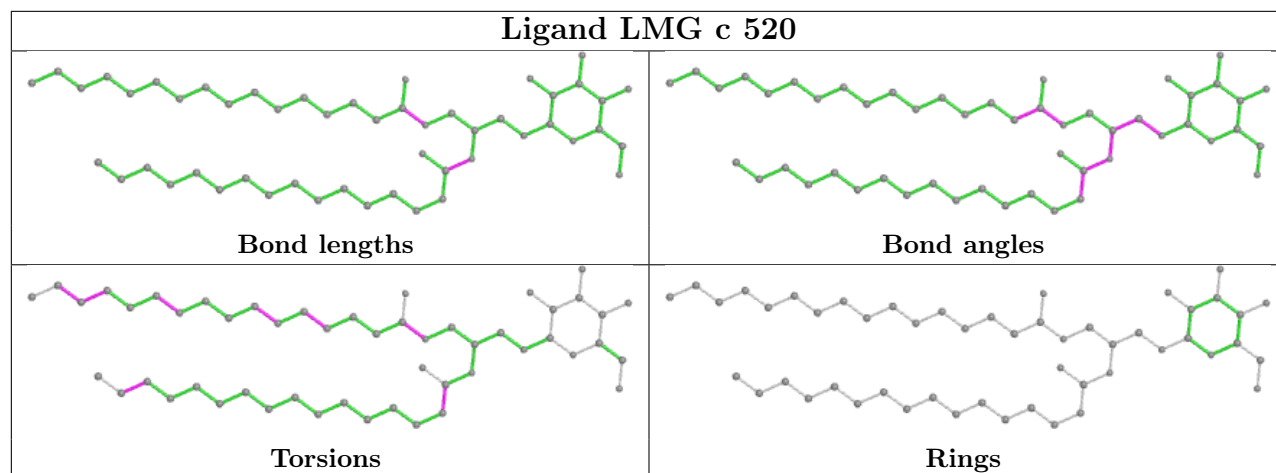
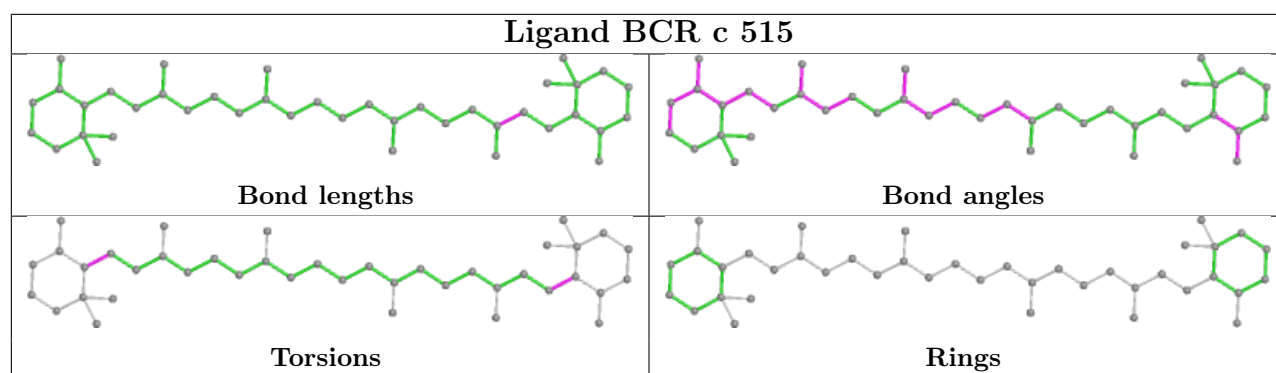


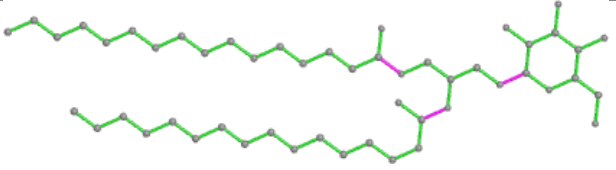
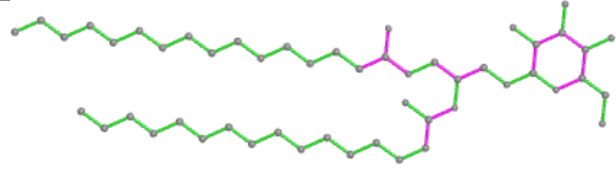
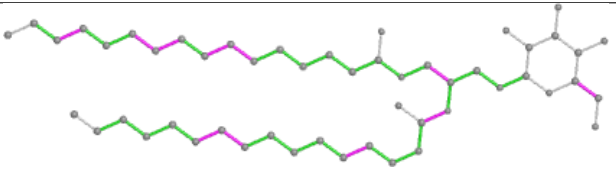
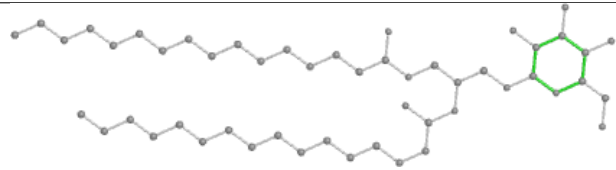
**Ligand CLA C 514****Ligand BCR b 617****Ligand CLA b 603**

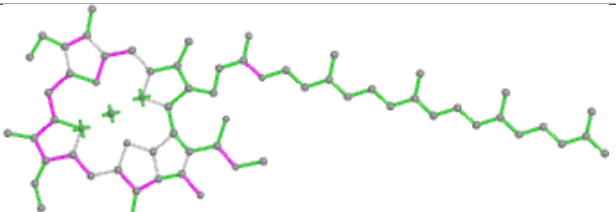
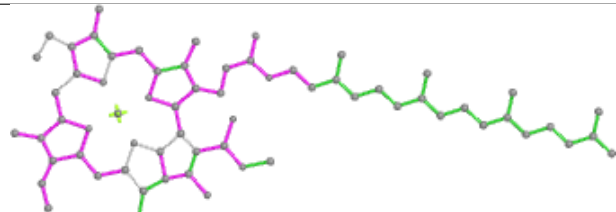
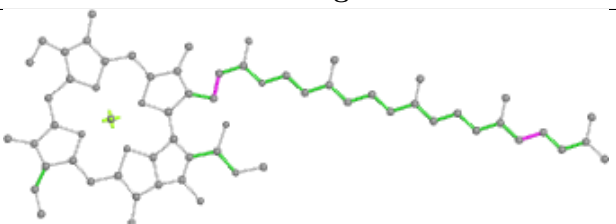
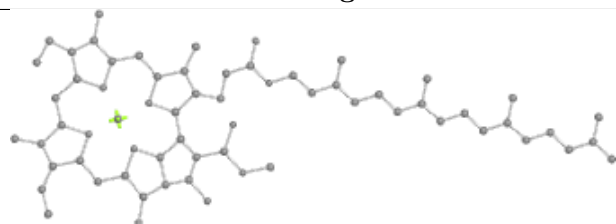



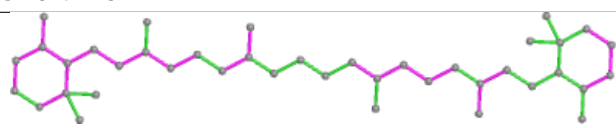
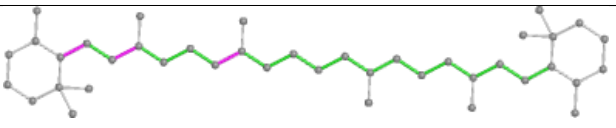
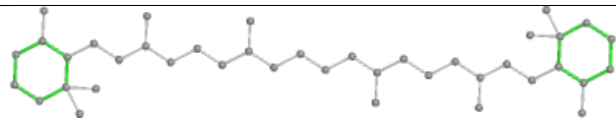


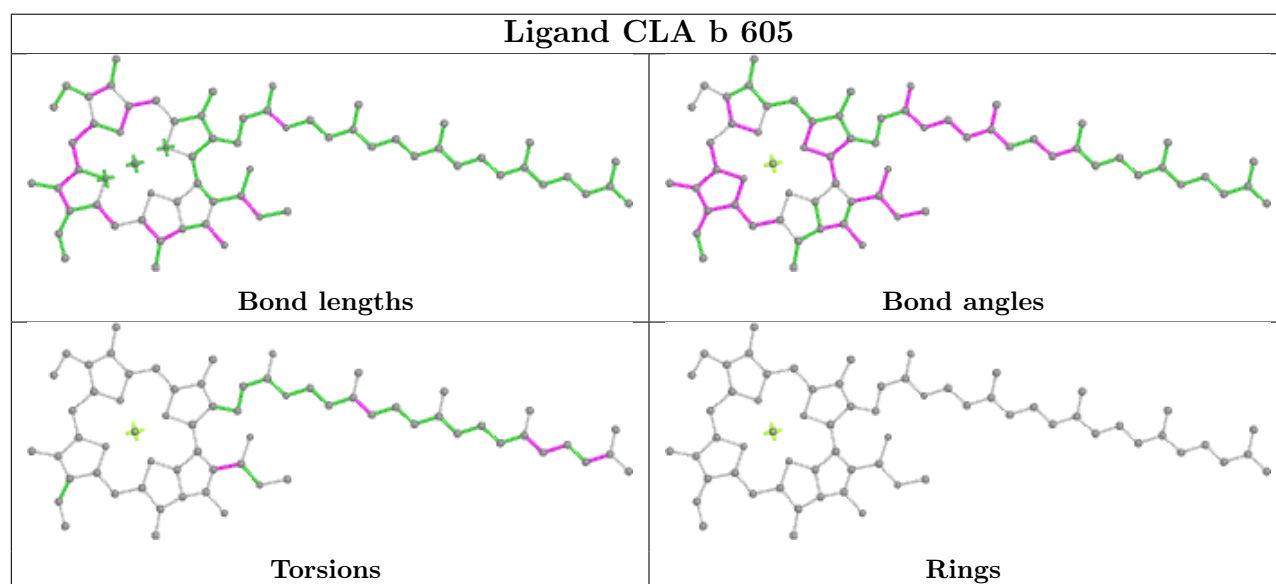
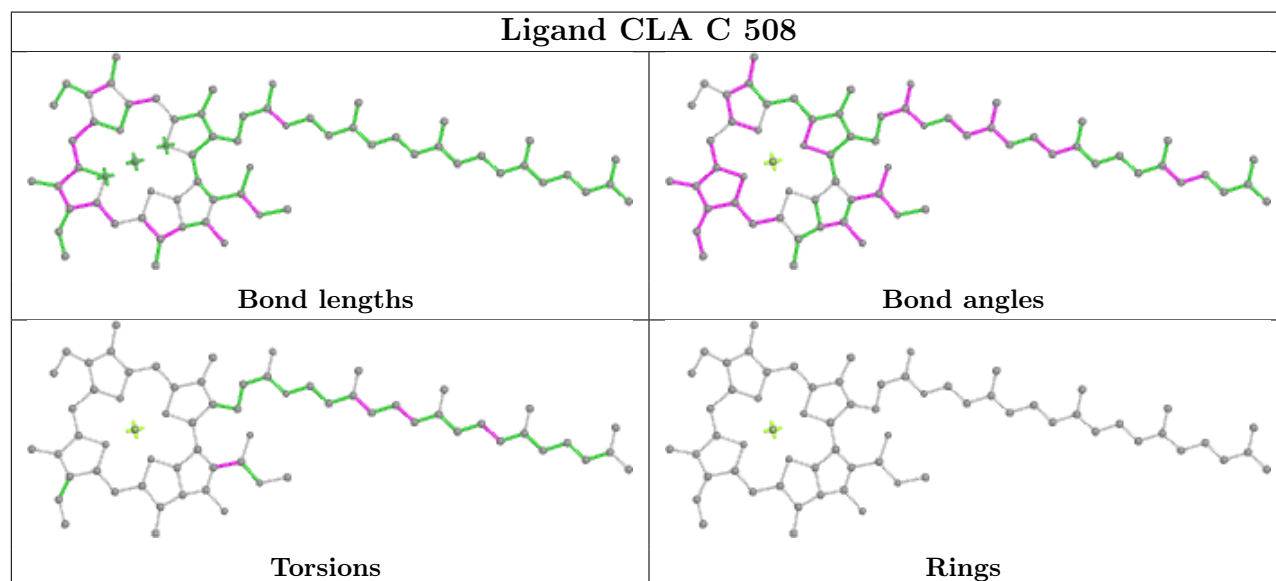
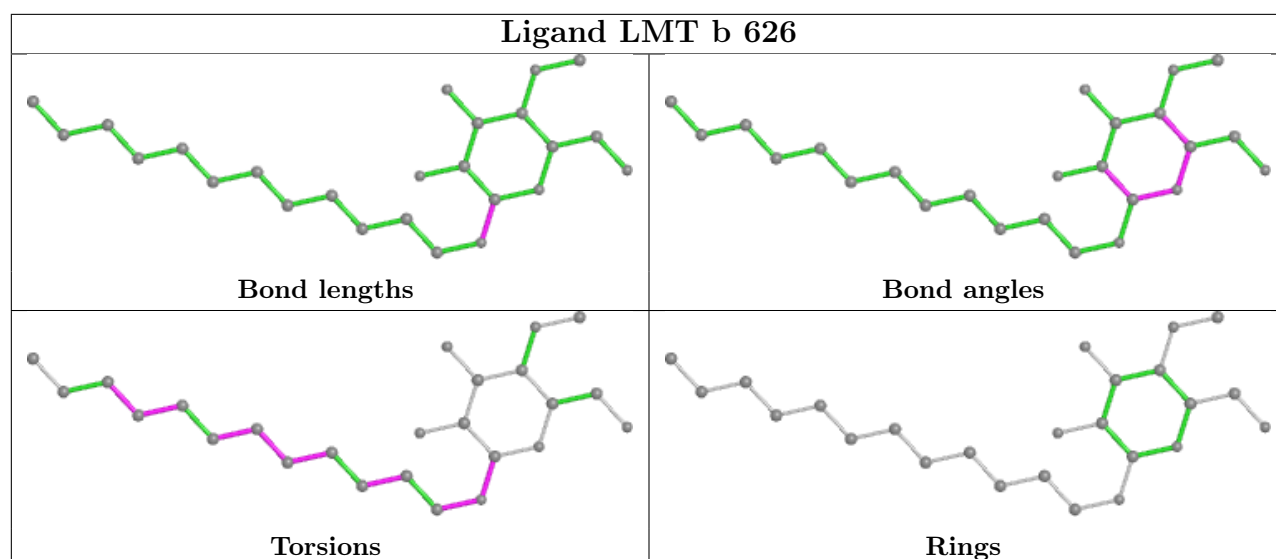


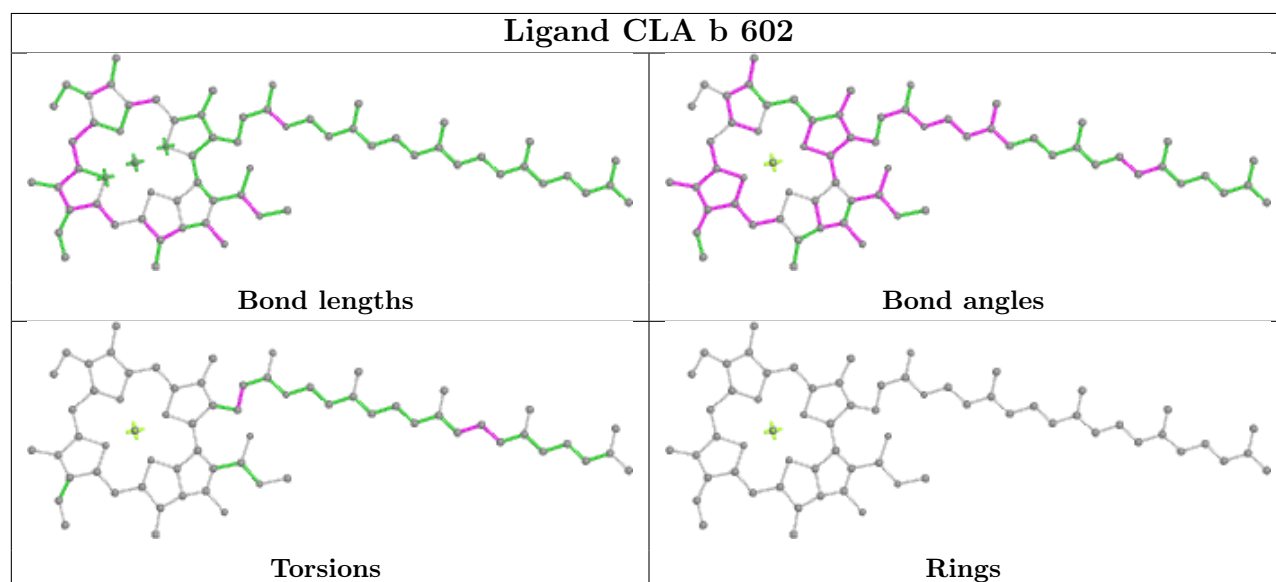
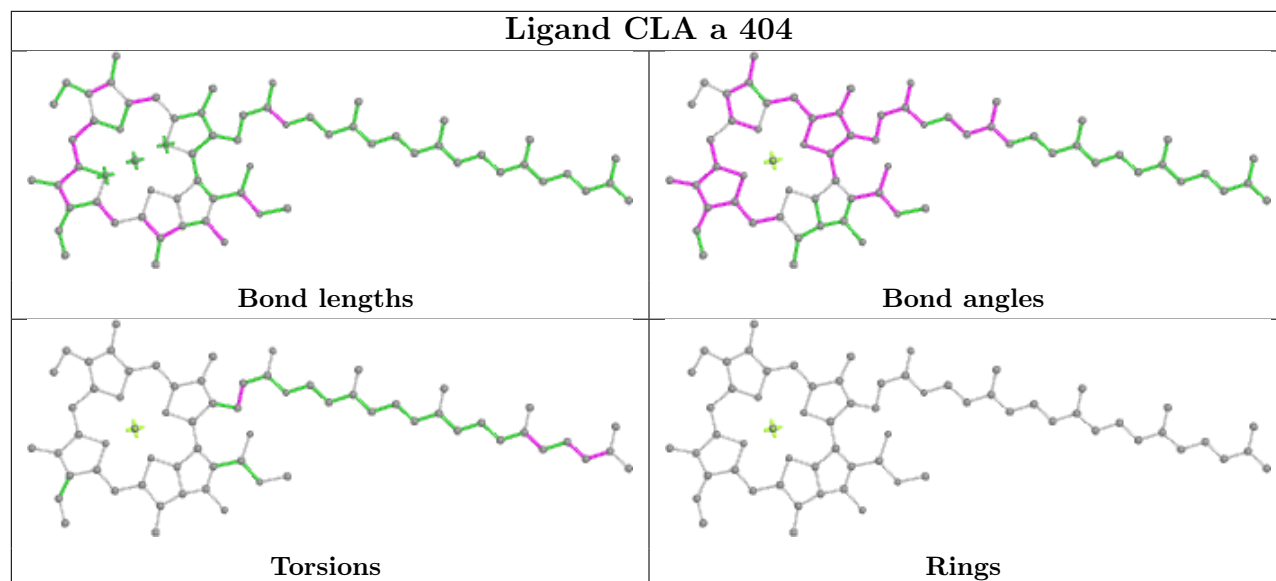
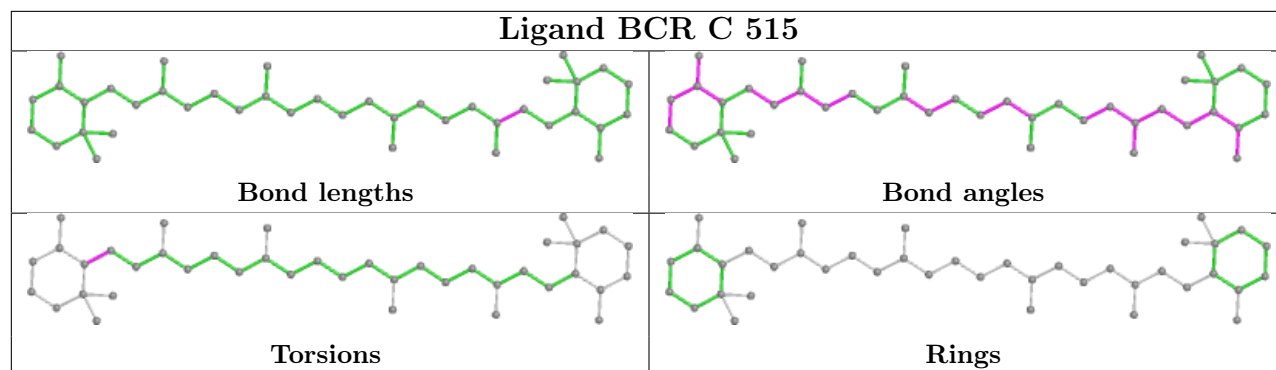


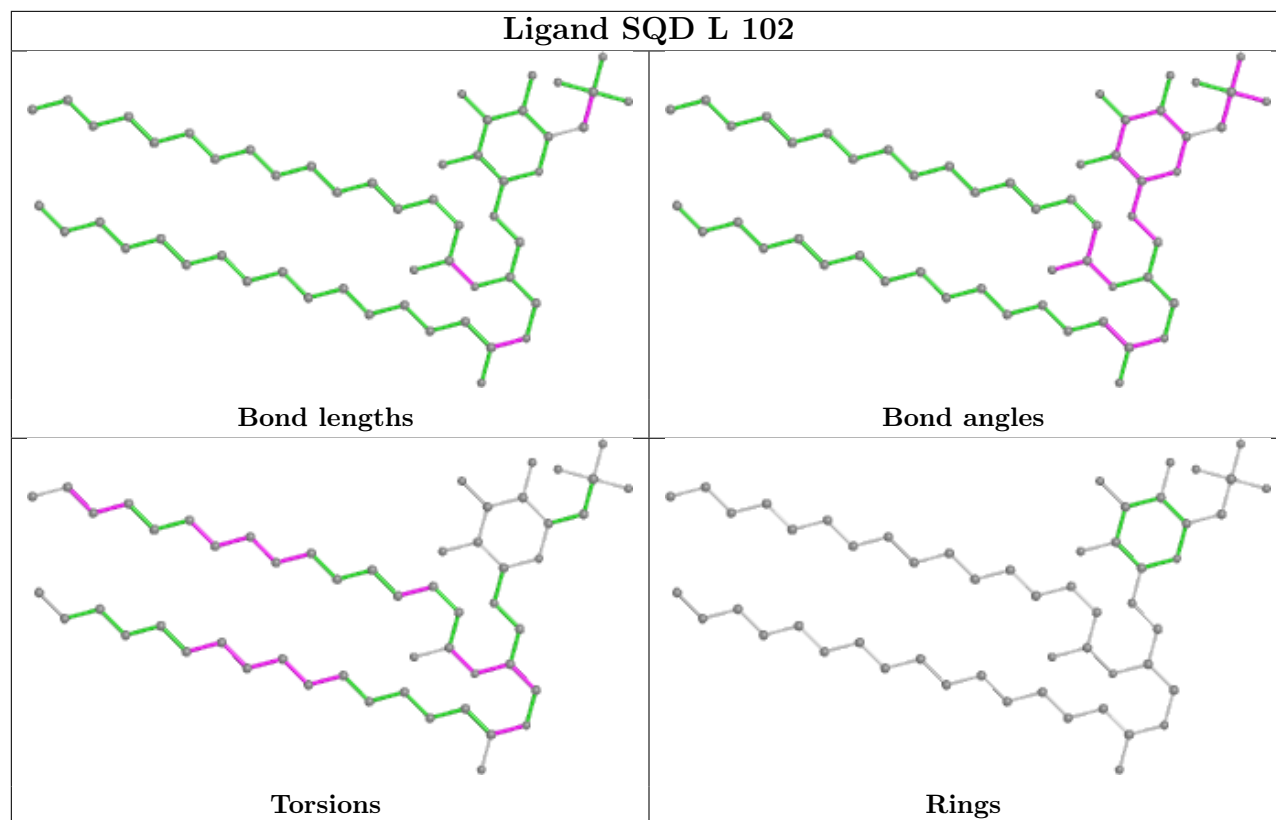
Ligand LMG C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

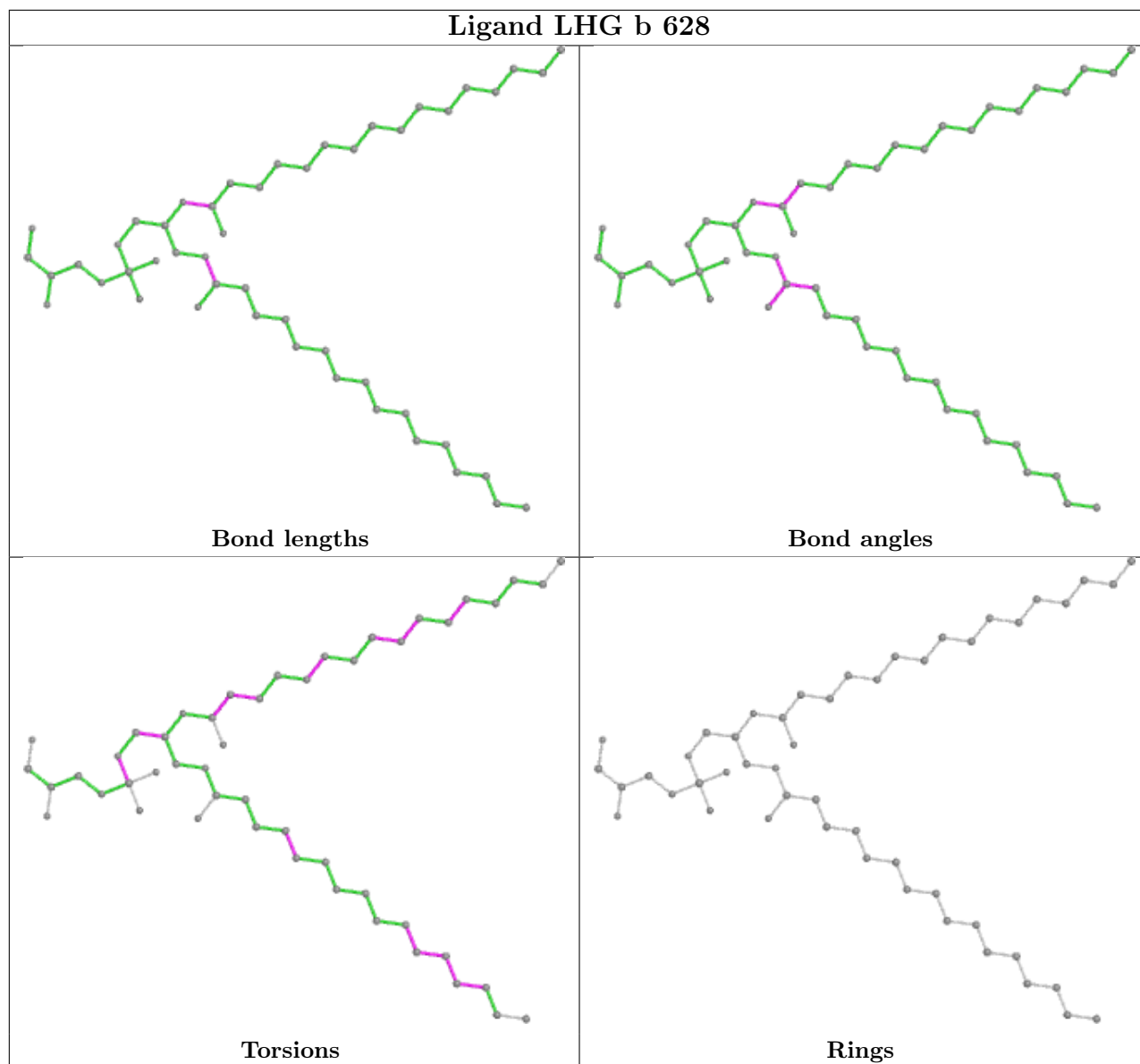
Ligand BCR t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



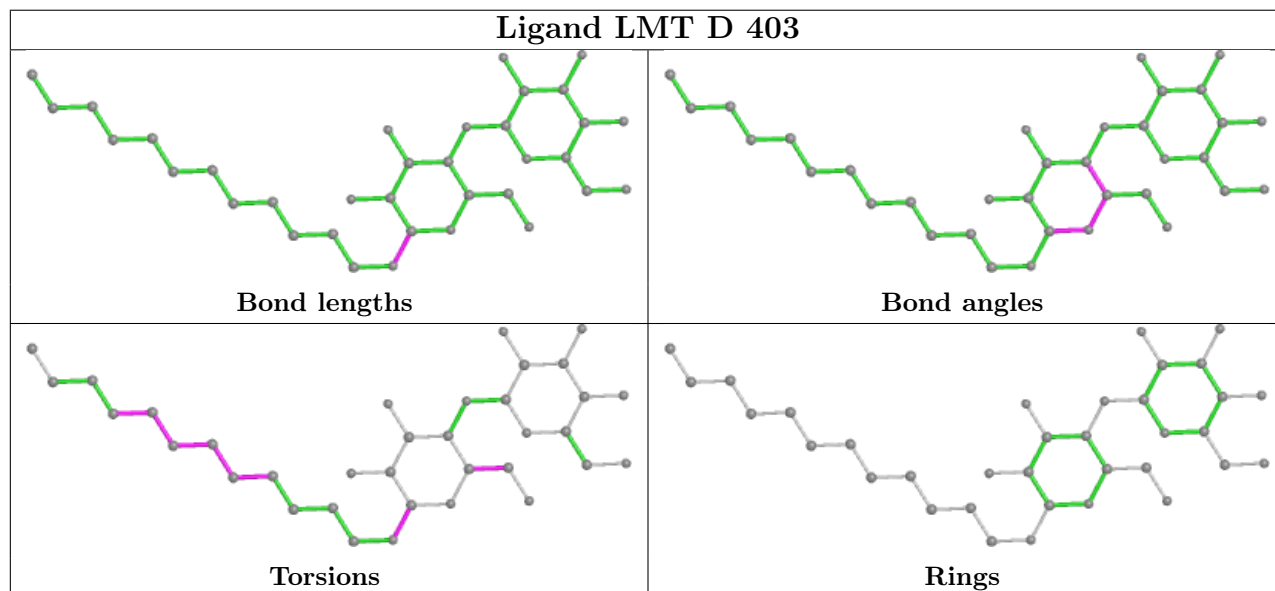




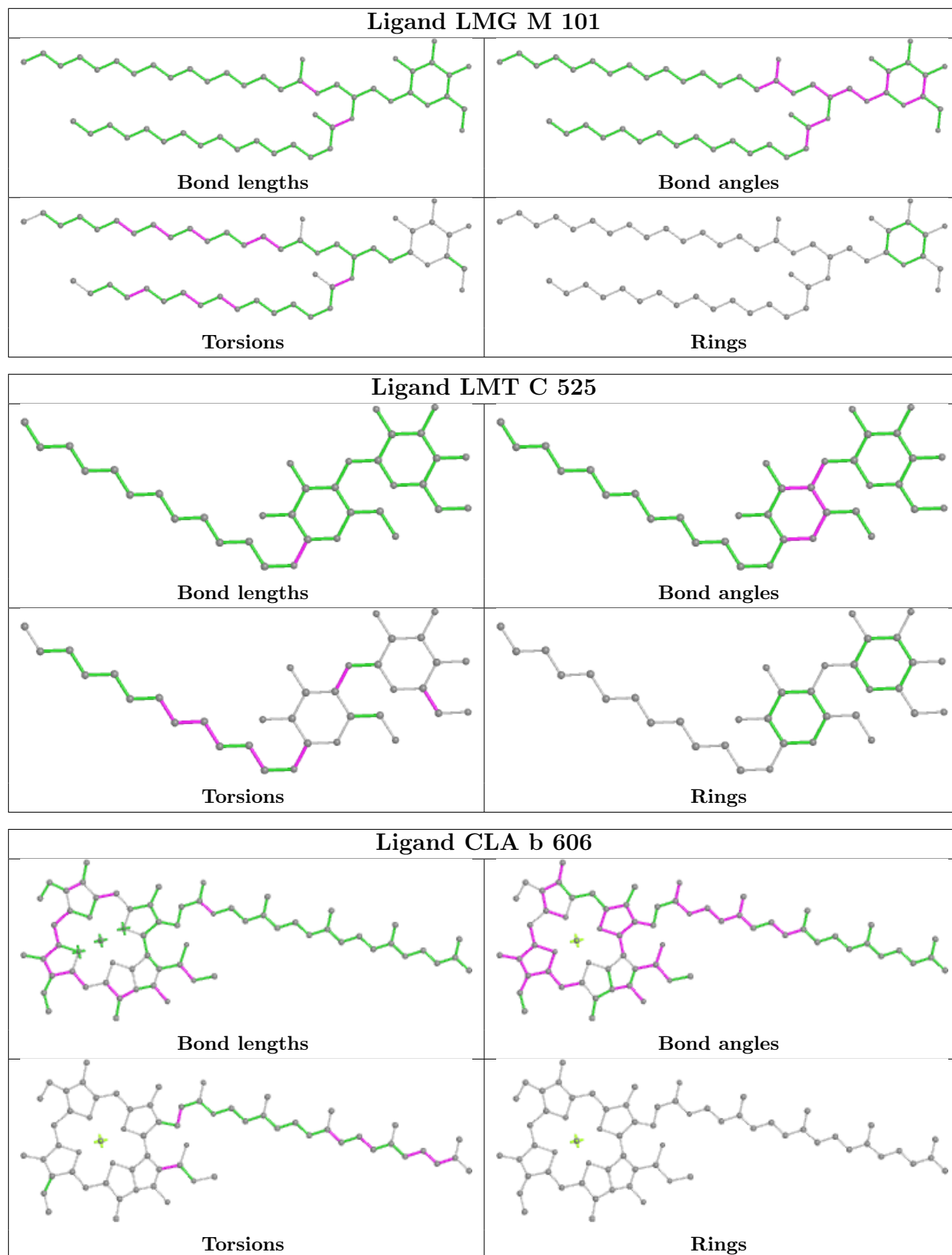
## Ligand LHG b 628



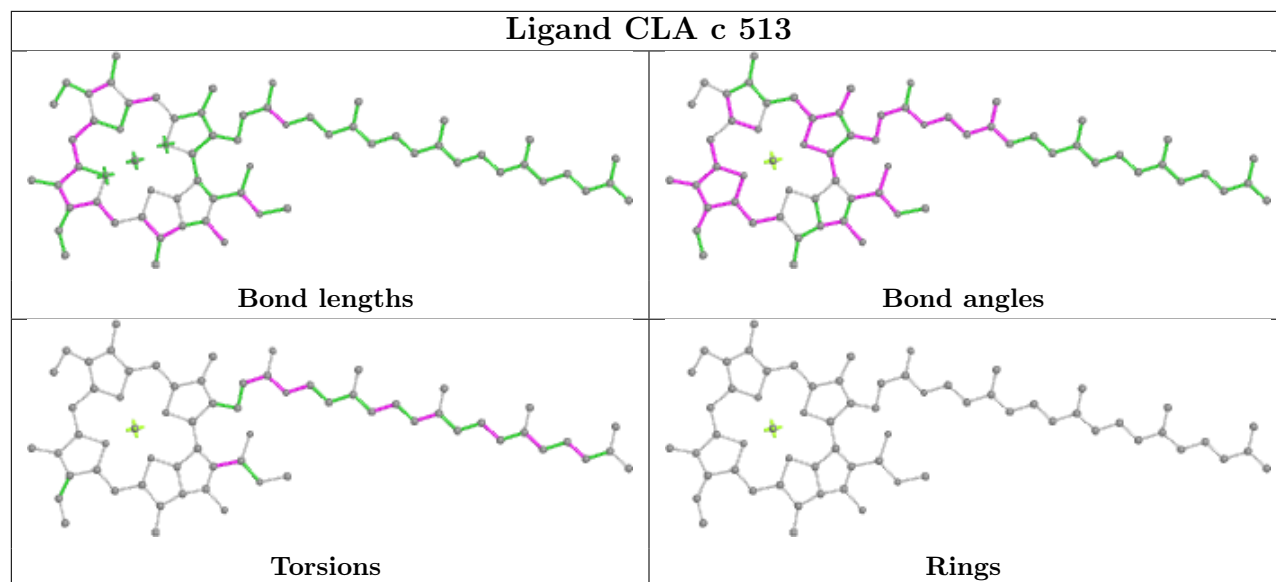
## Ligand LMT D 403



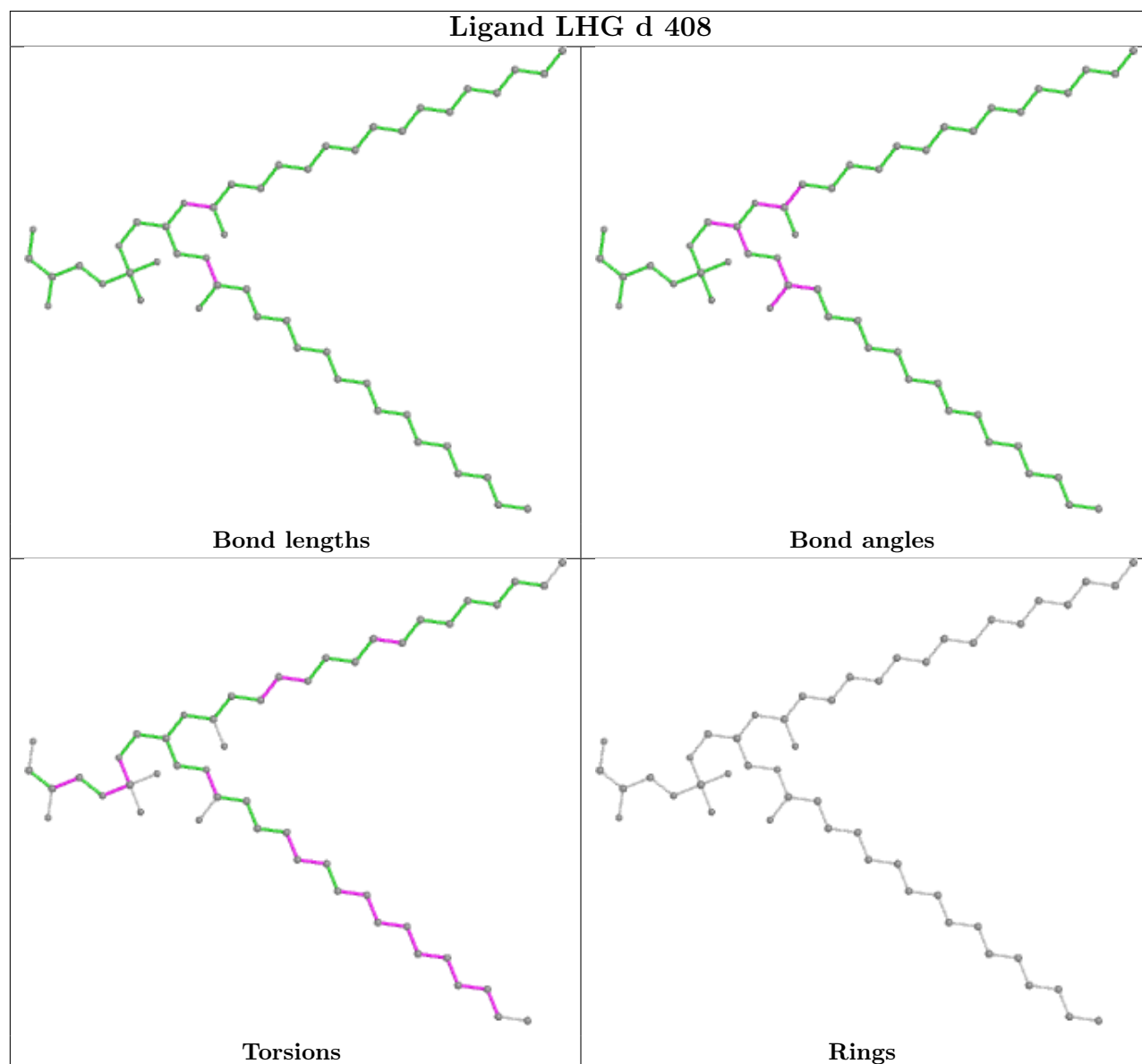


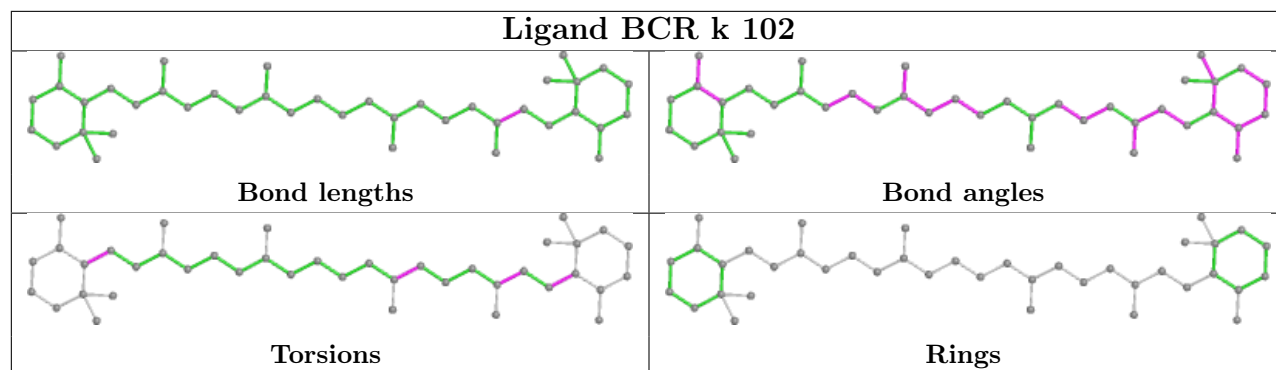
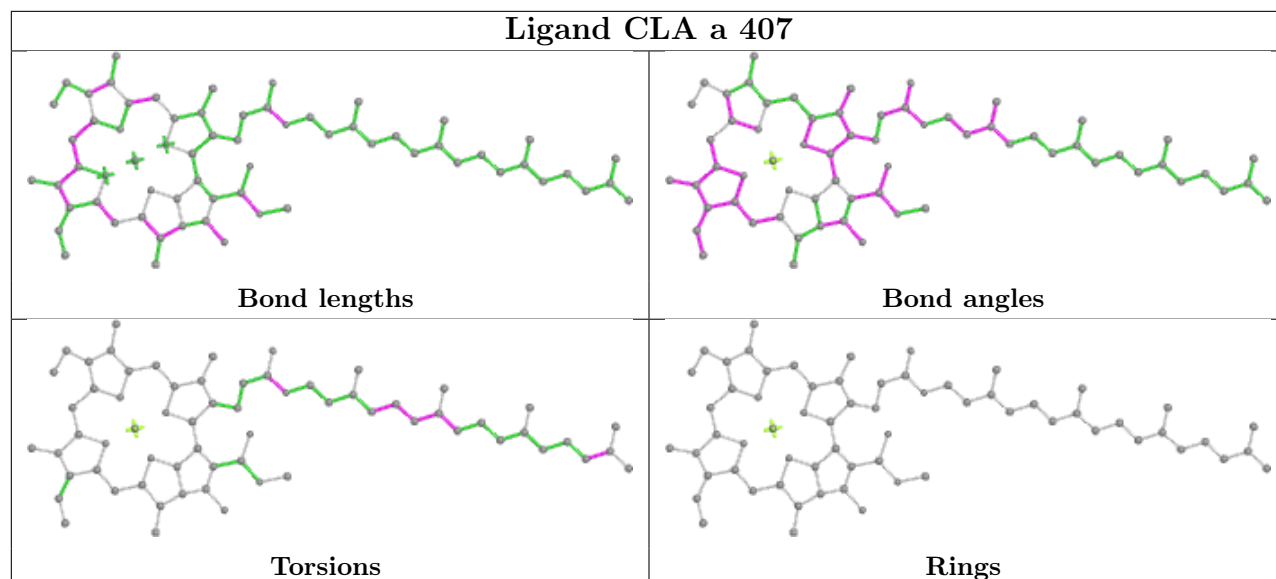
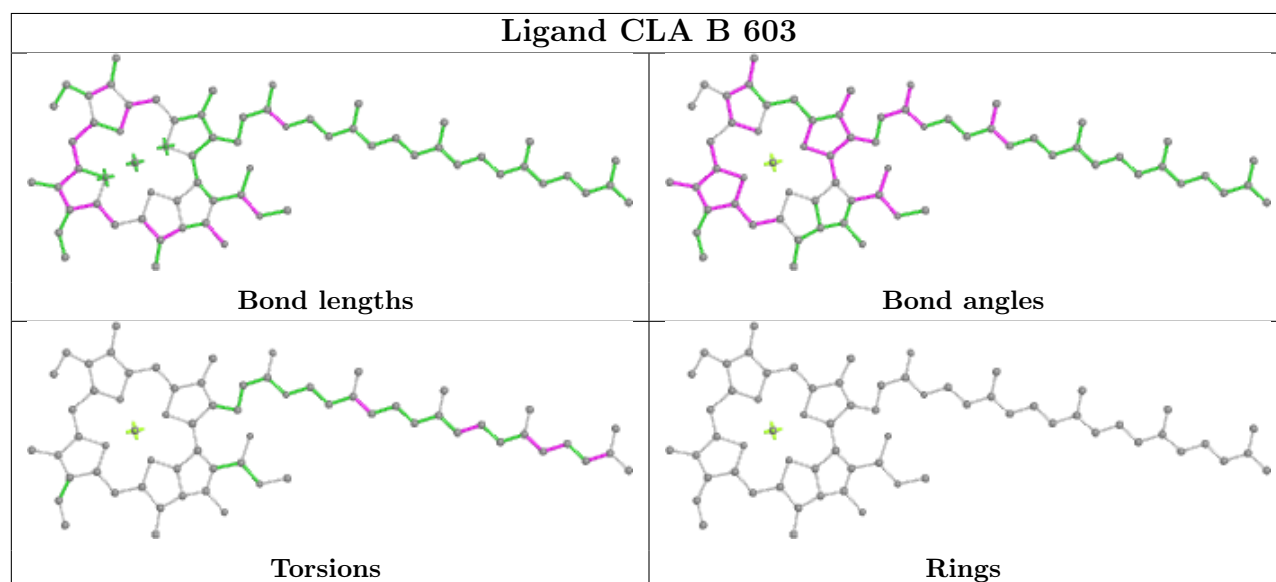


## Ligand CLA c 513

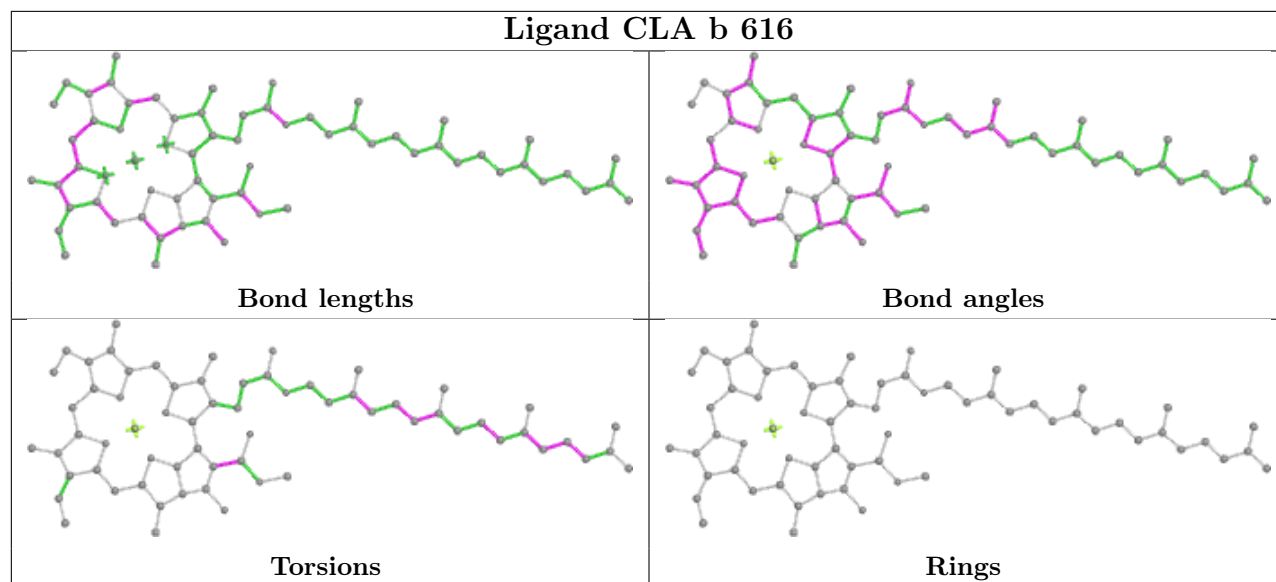


## Ligand LHG d 408

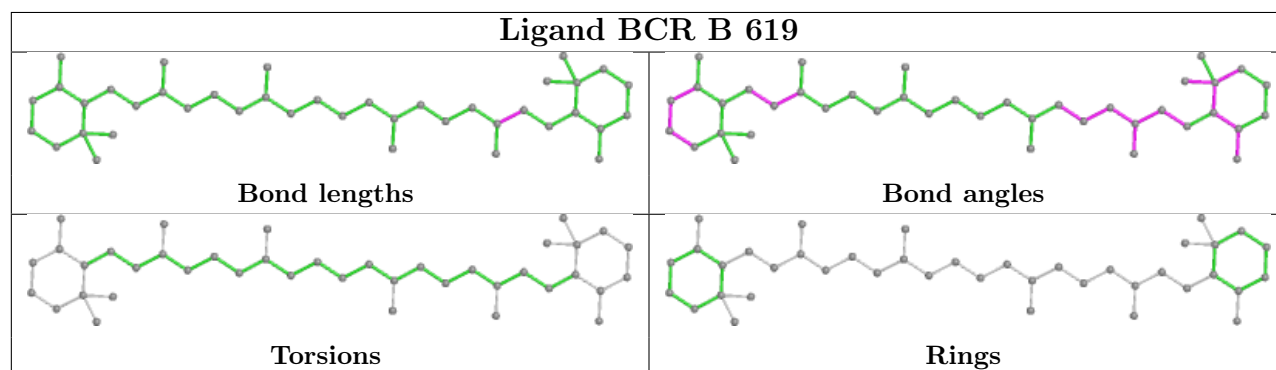


**Ligand BCR k 102****Ligand CLA a 407****Ligand CLA B 603**

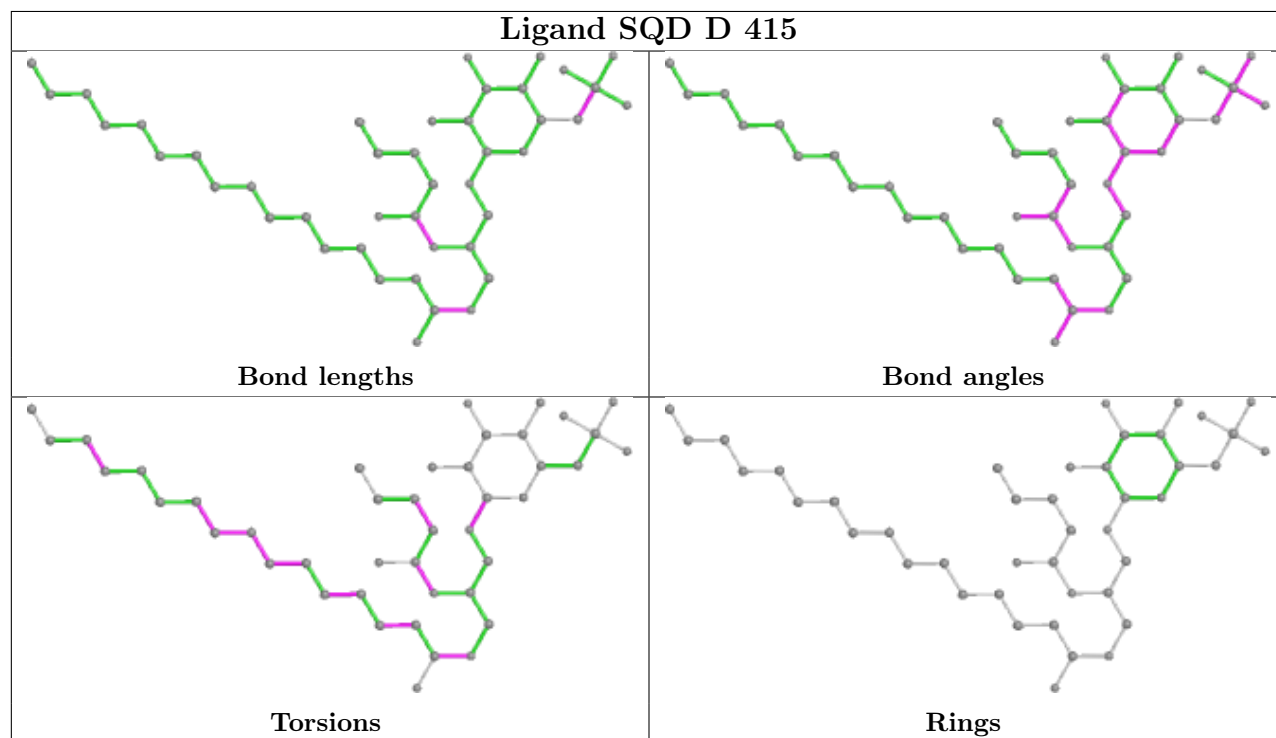
## Ligand CLA b 616



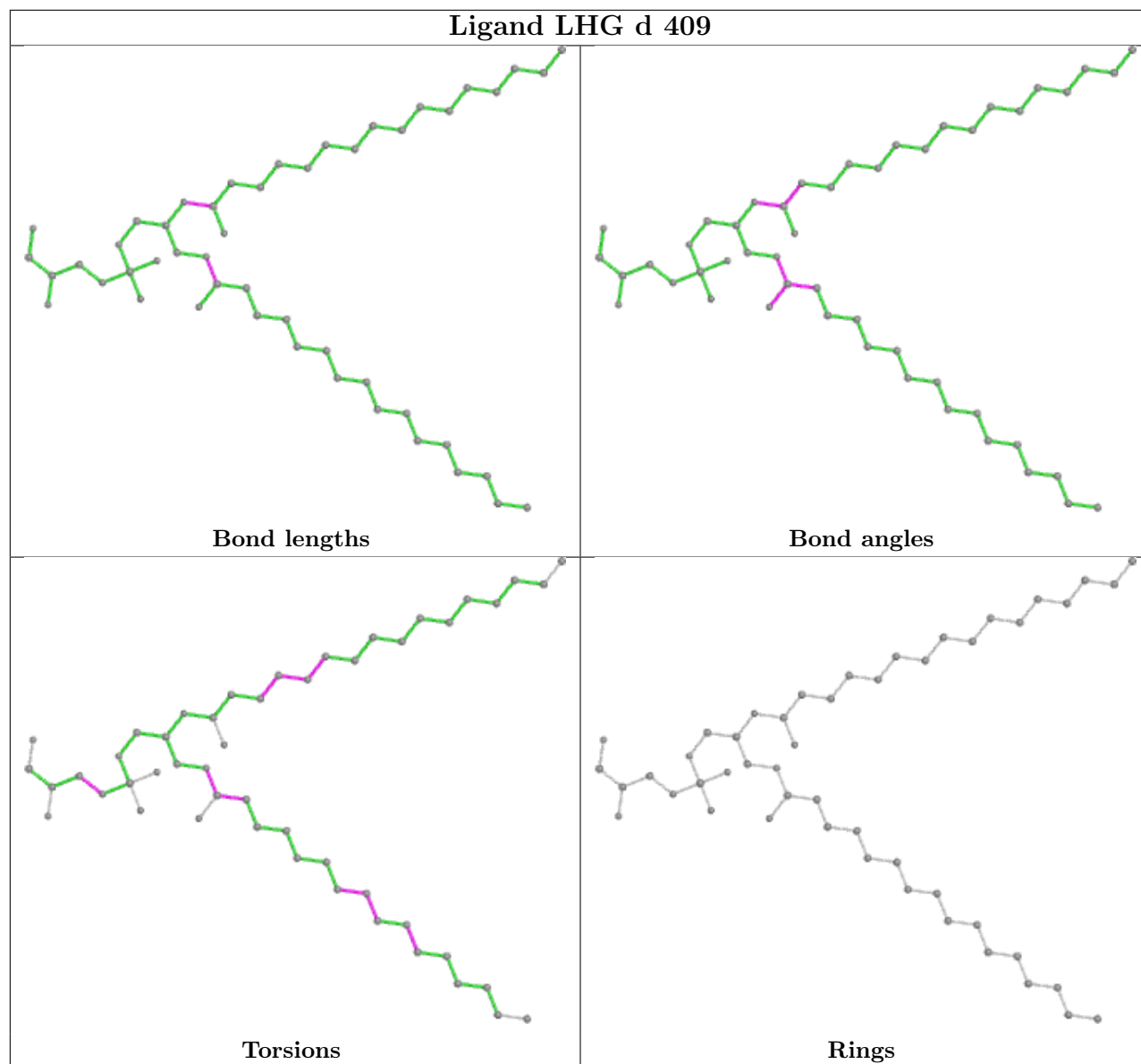
## Ligand BCR B 619



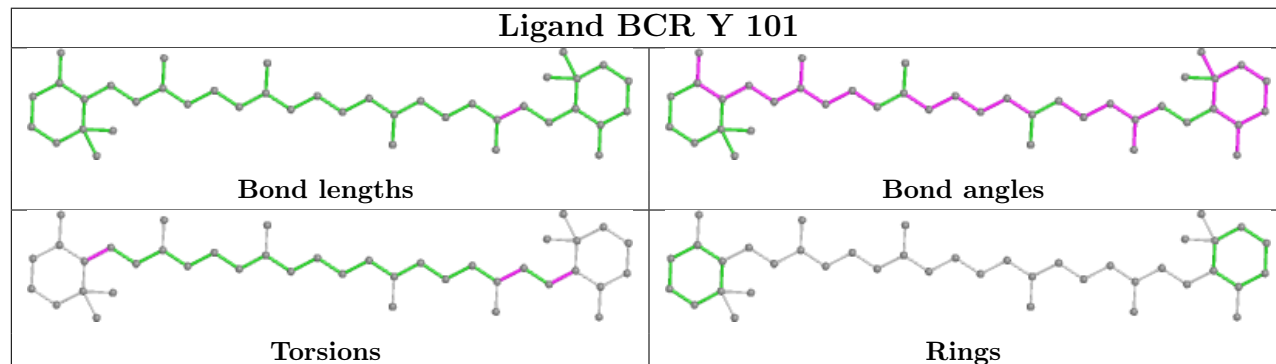
## Ligand SQD D 415

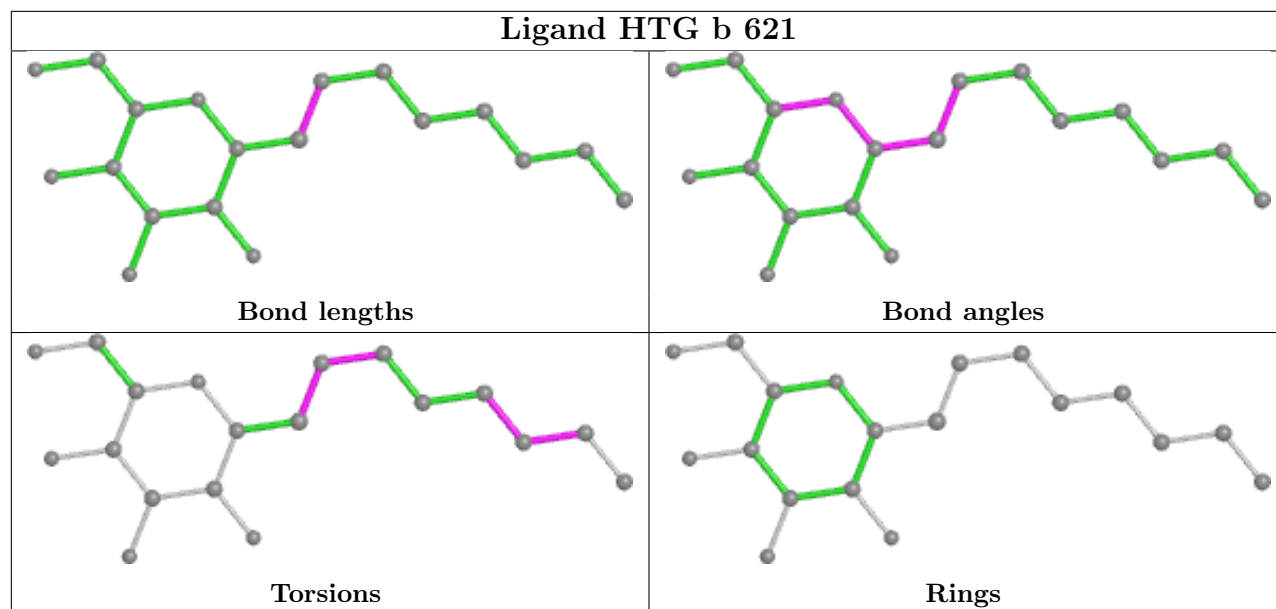
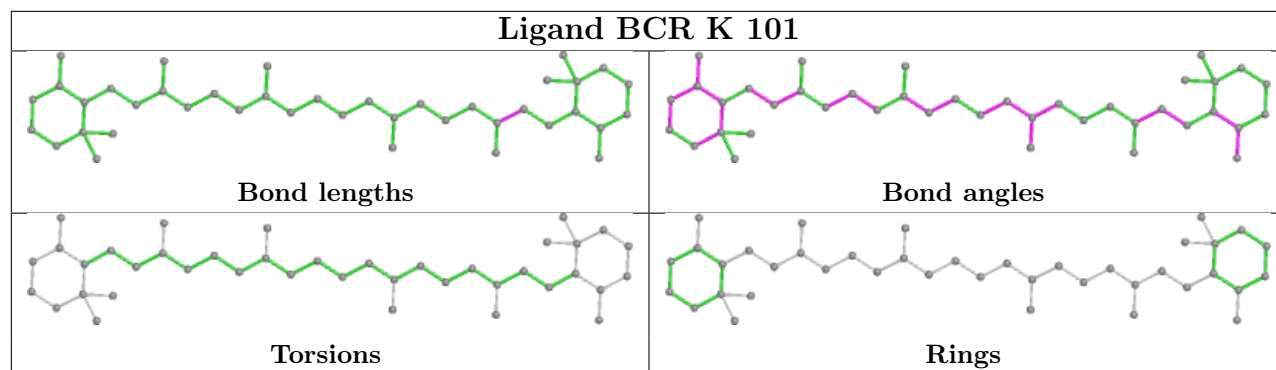


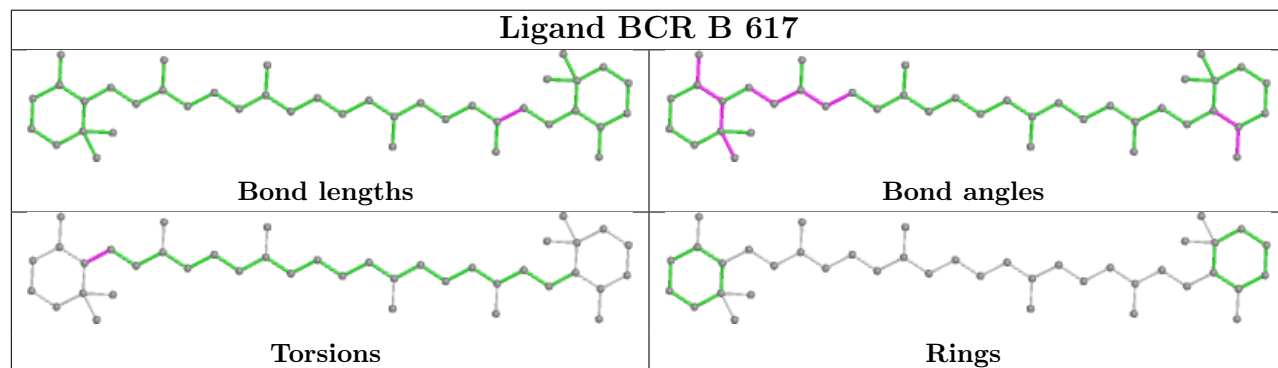
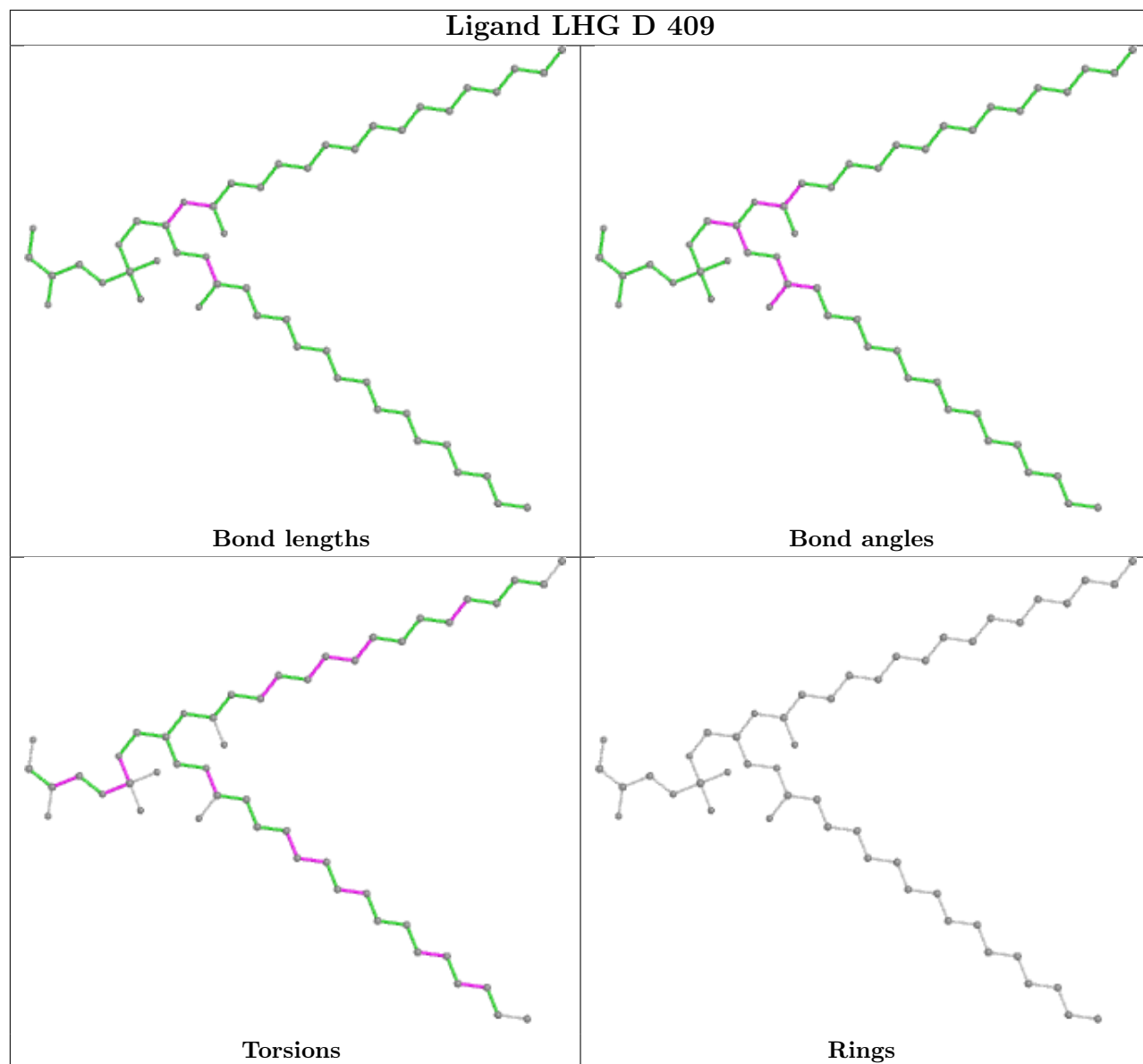
## Ligand LHG d 409

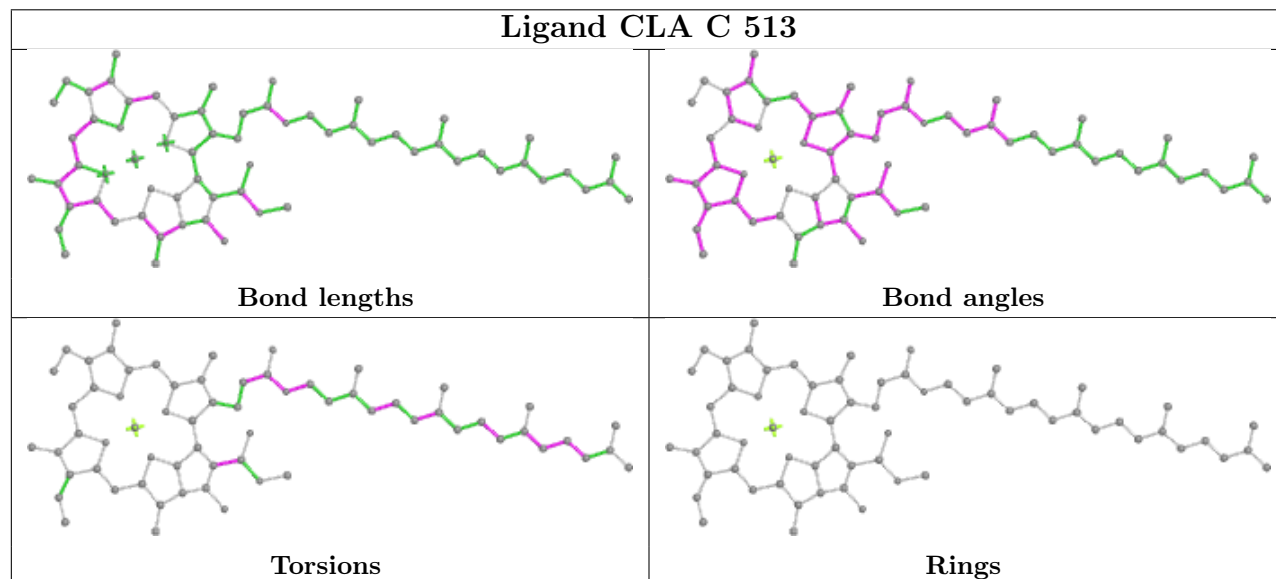
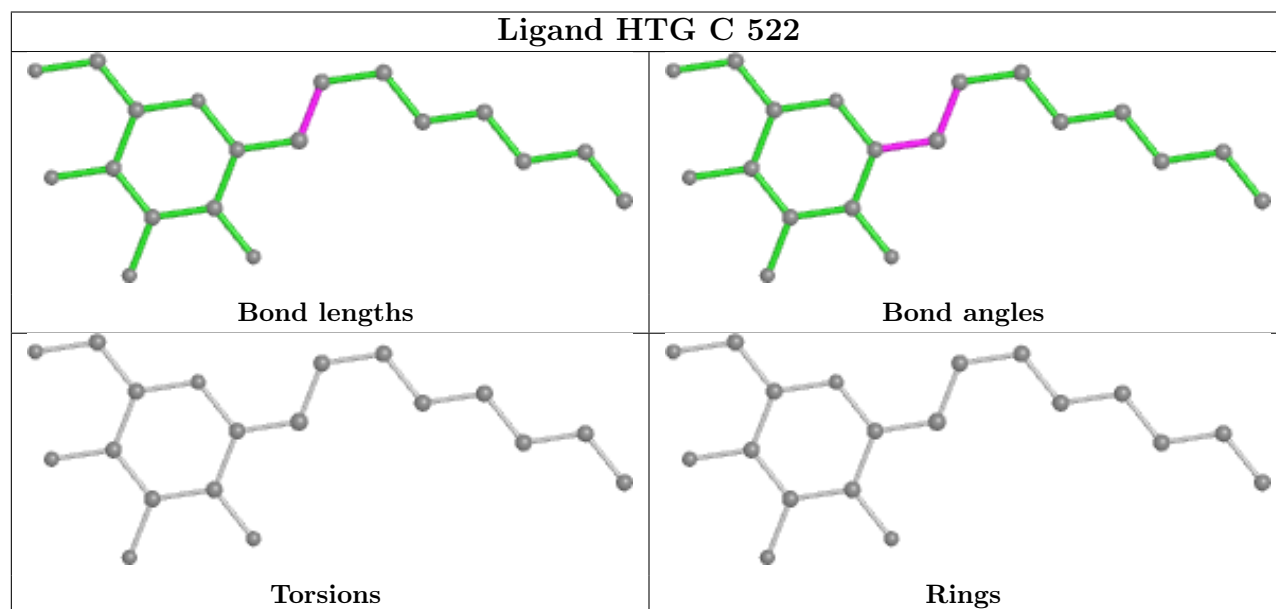
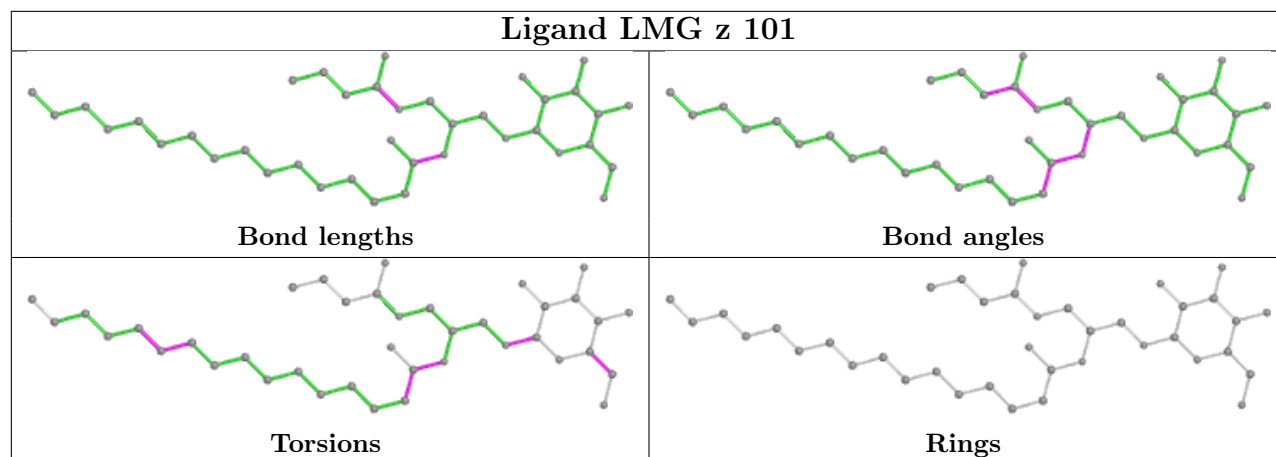


## Ligand BCR Y 101

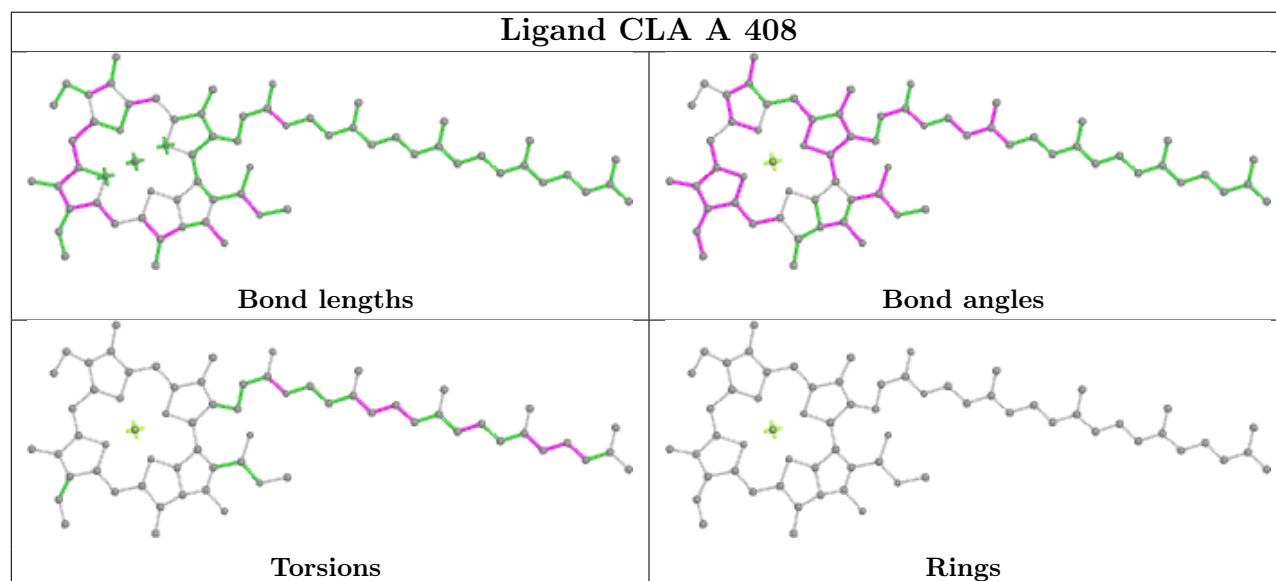
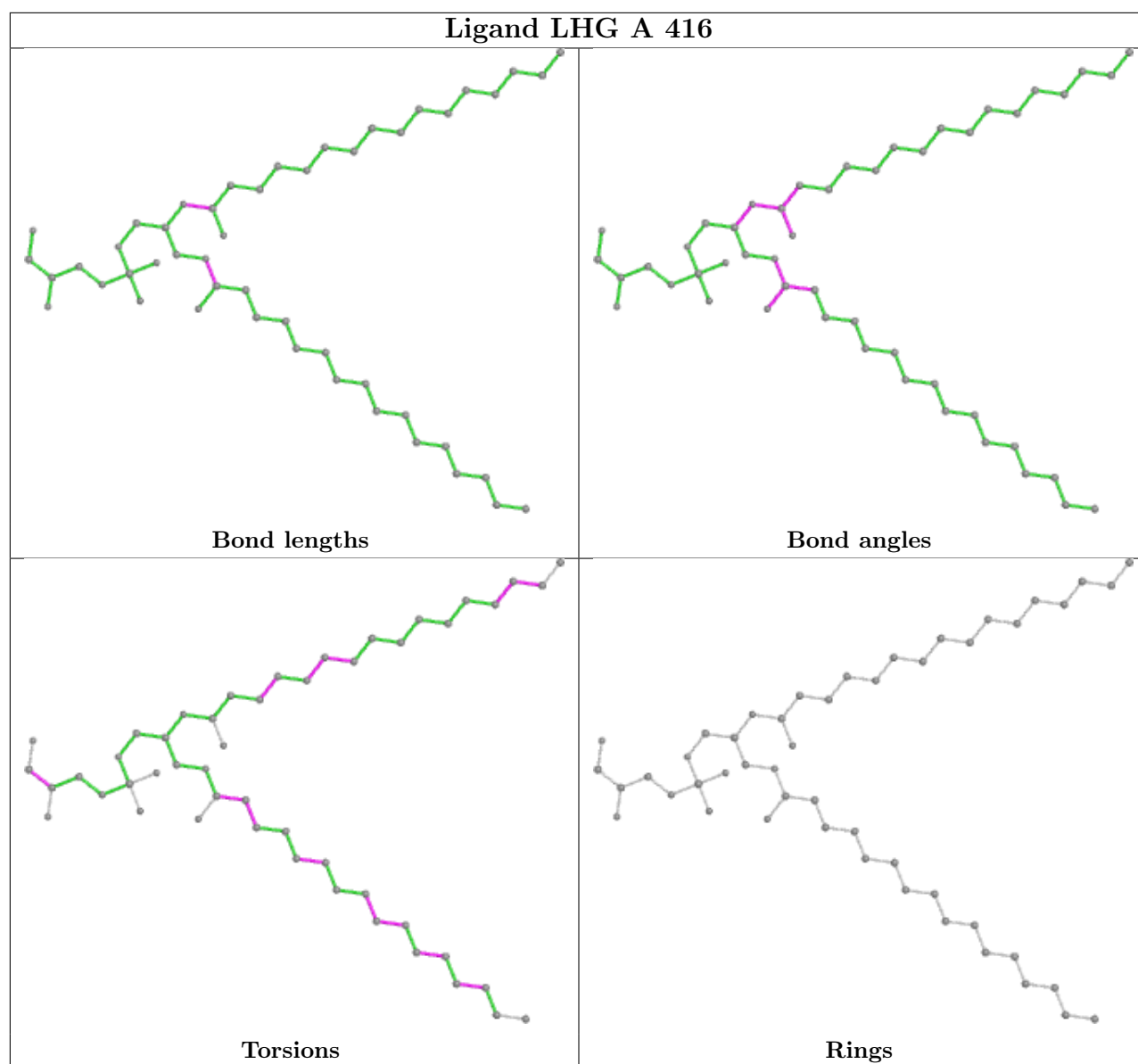


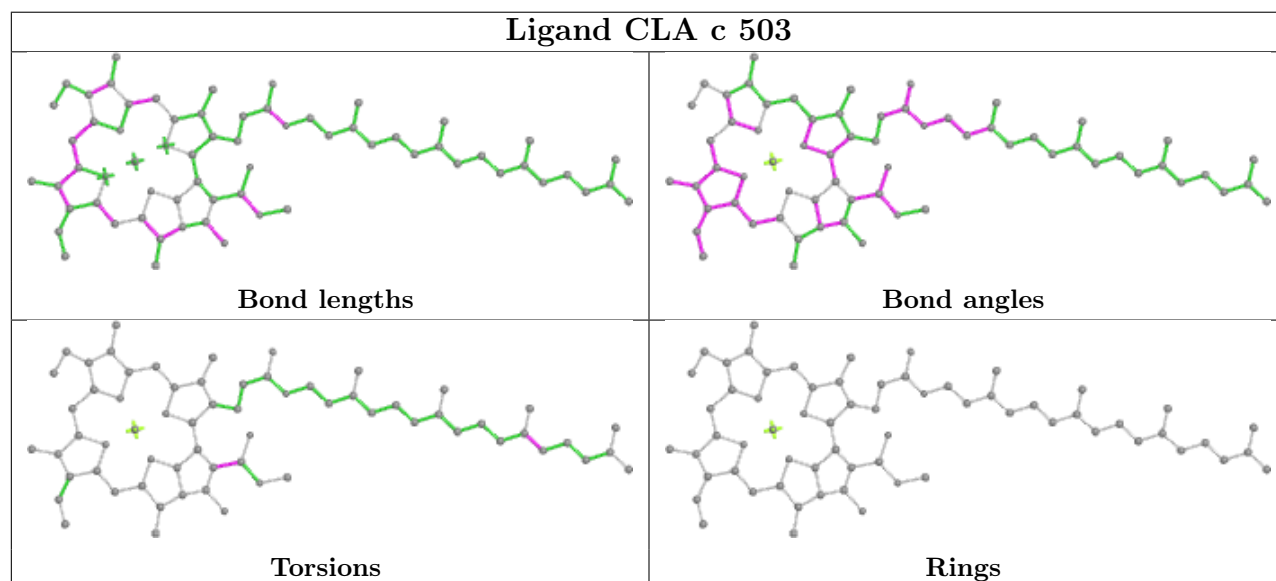
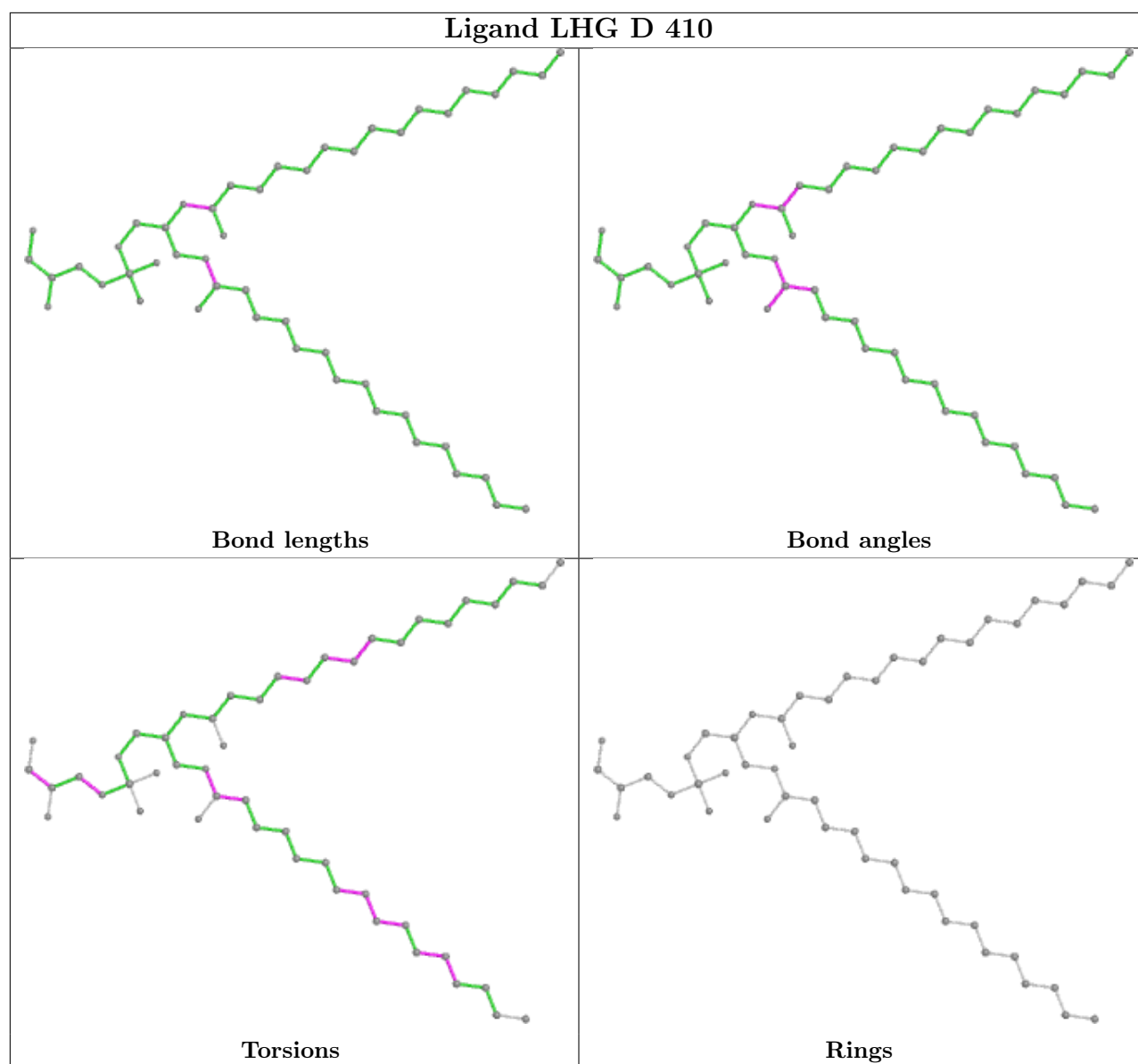


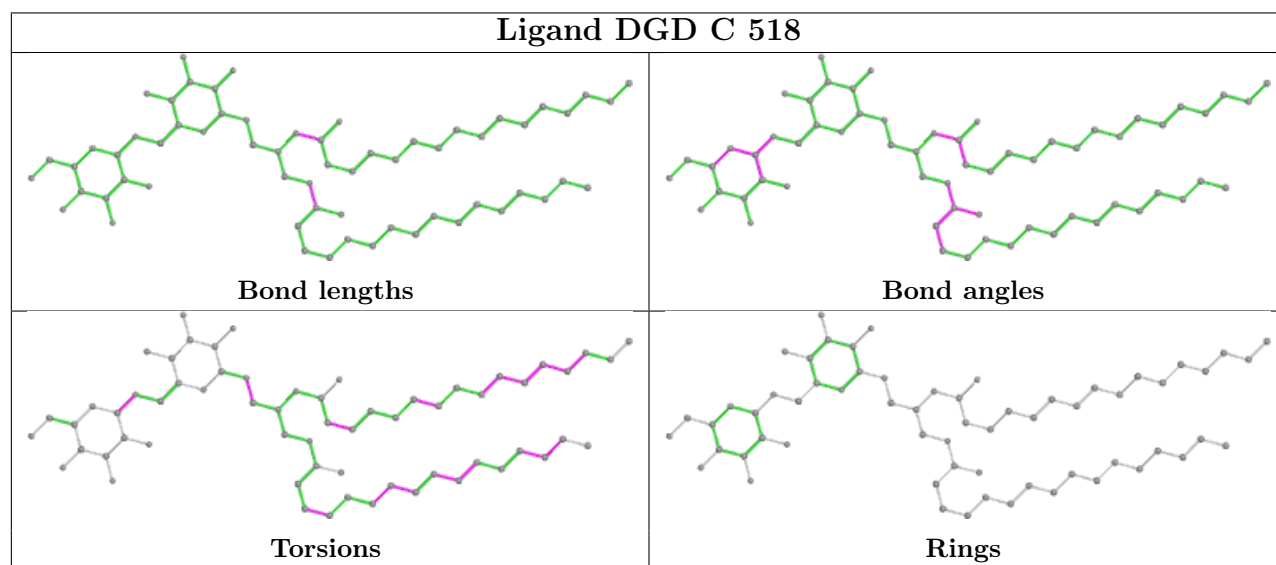
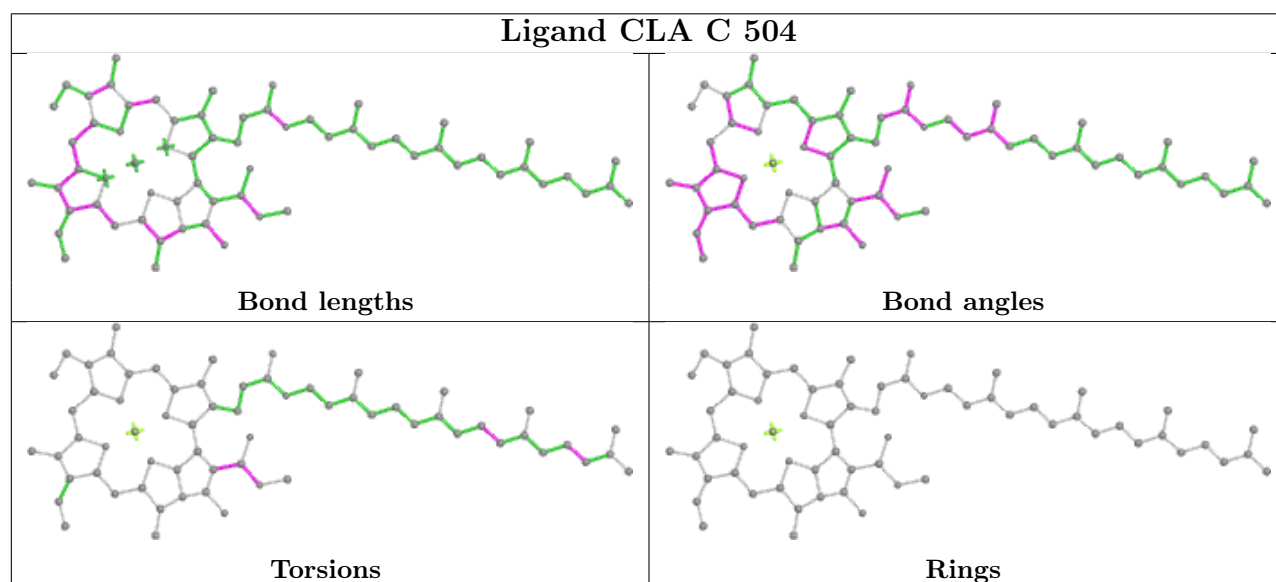
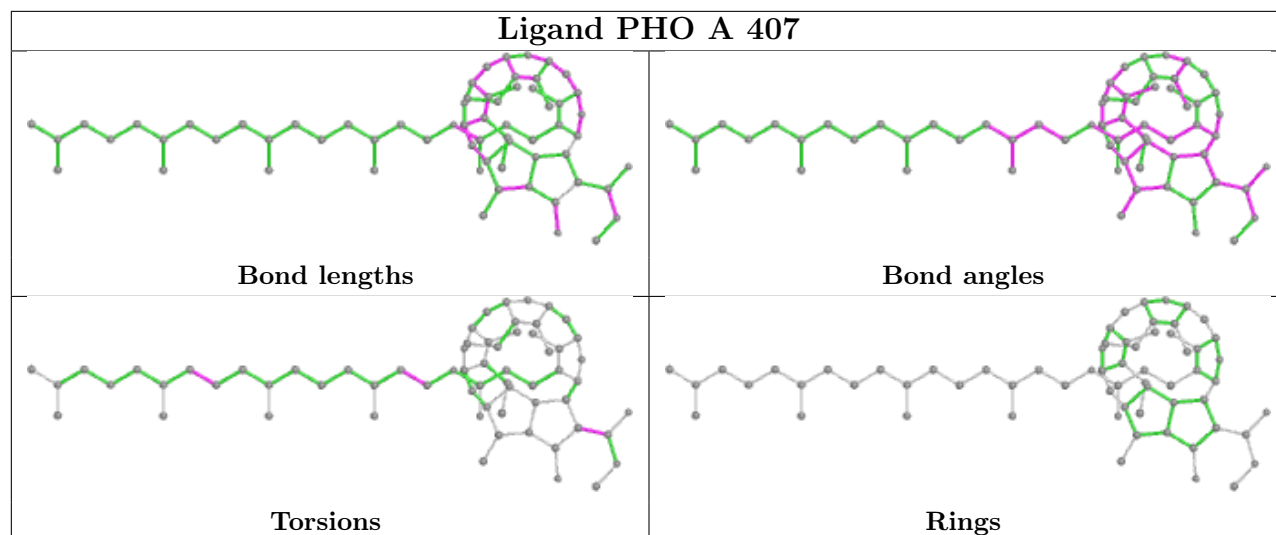


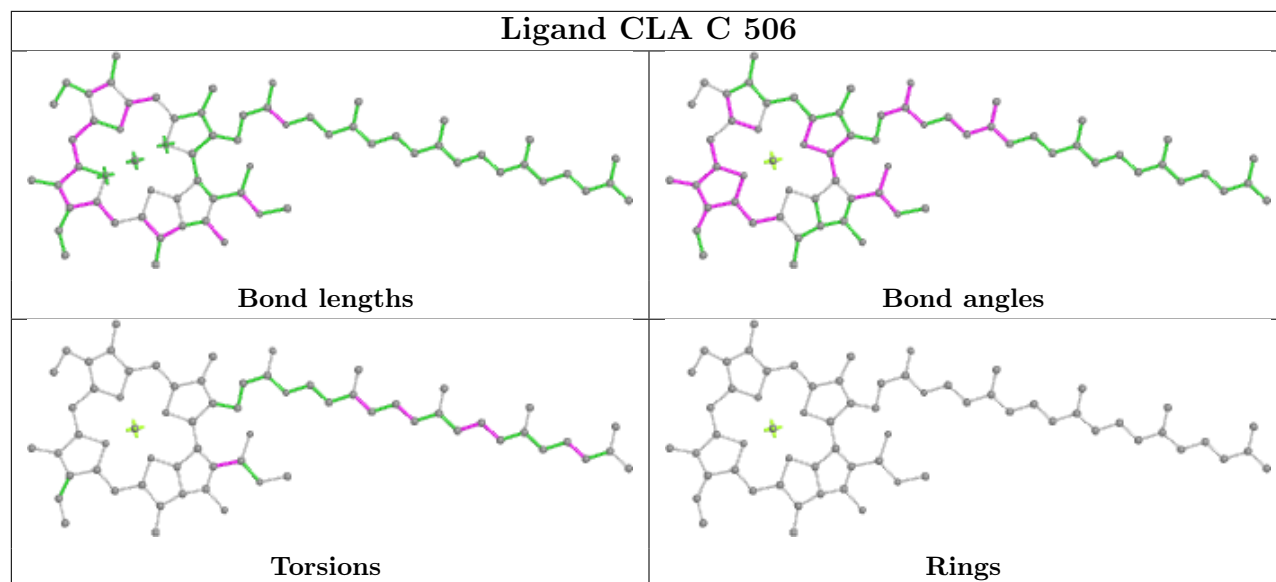
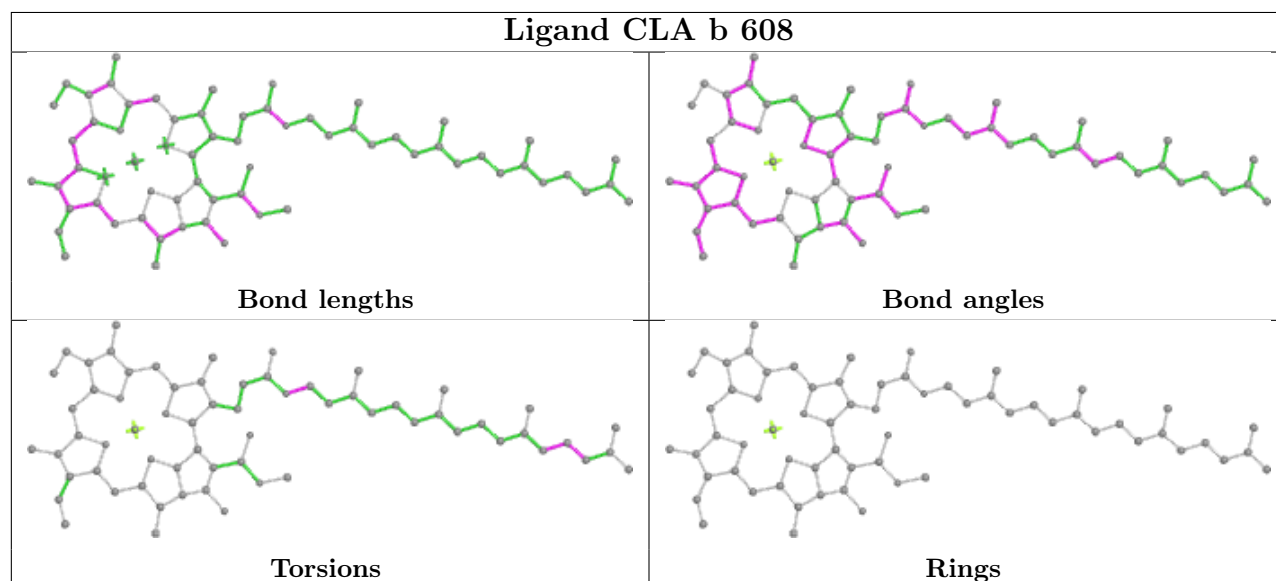
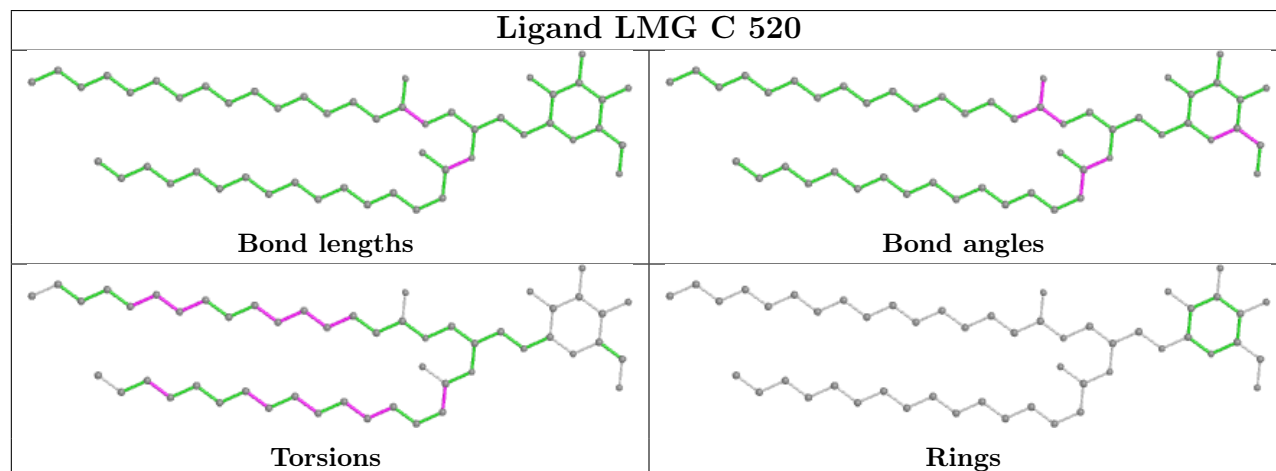


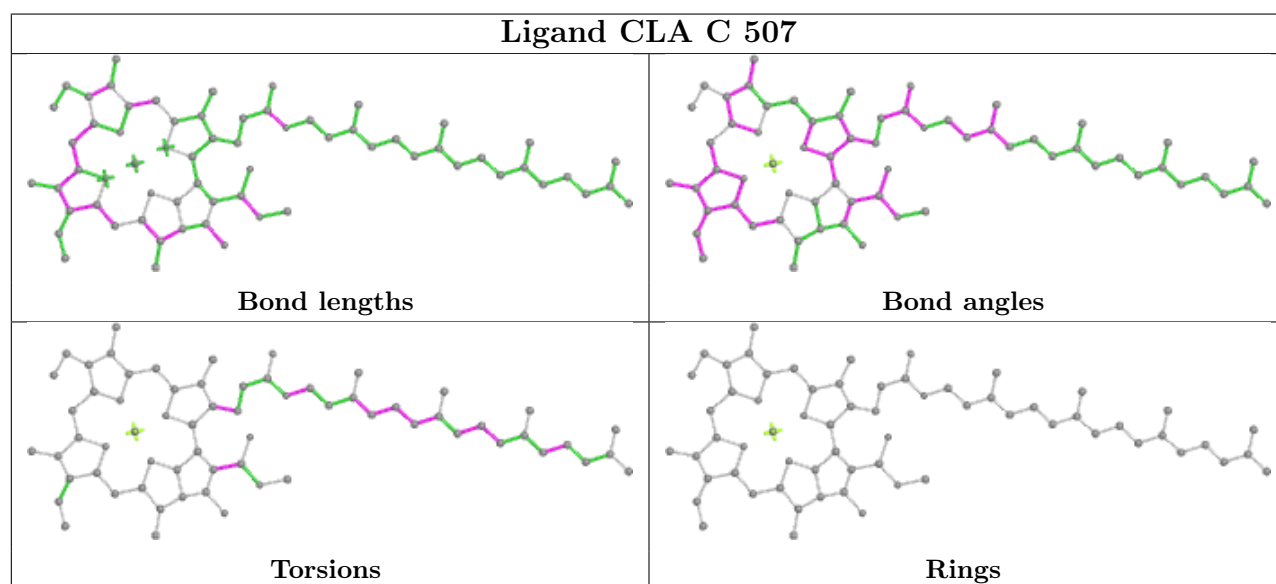
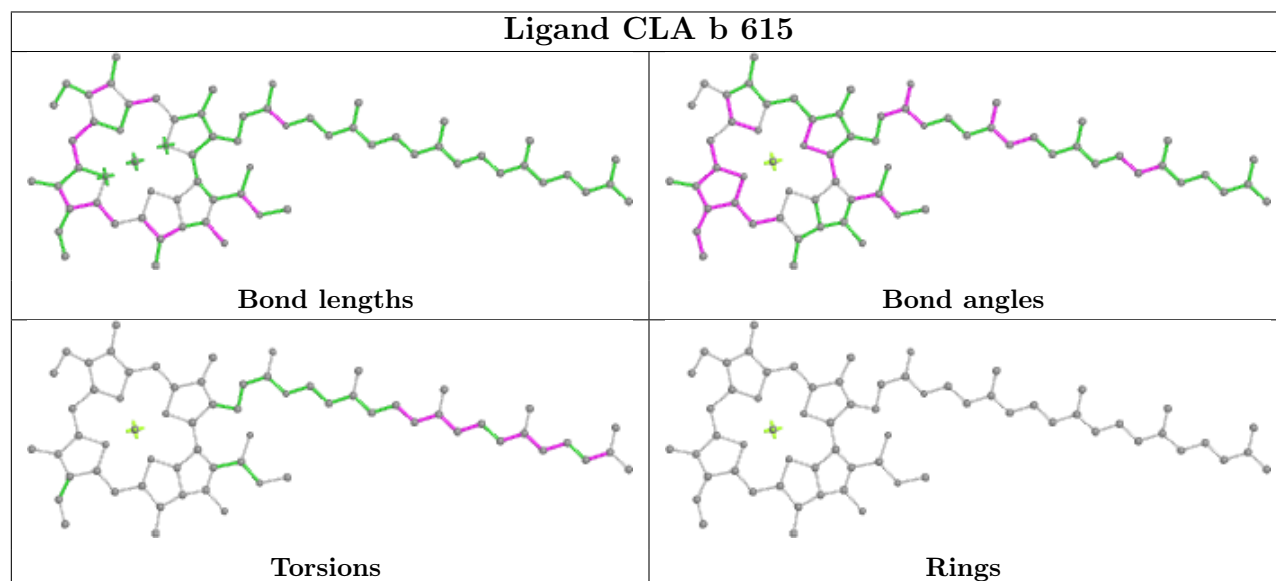
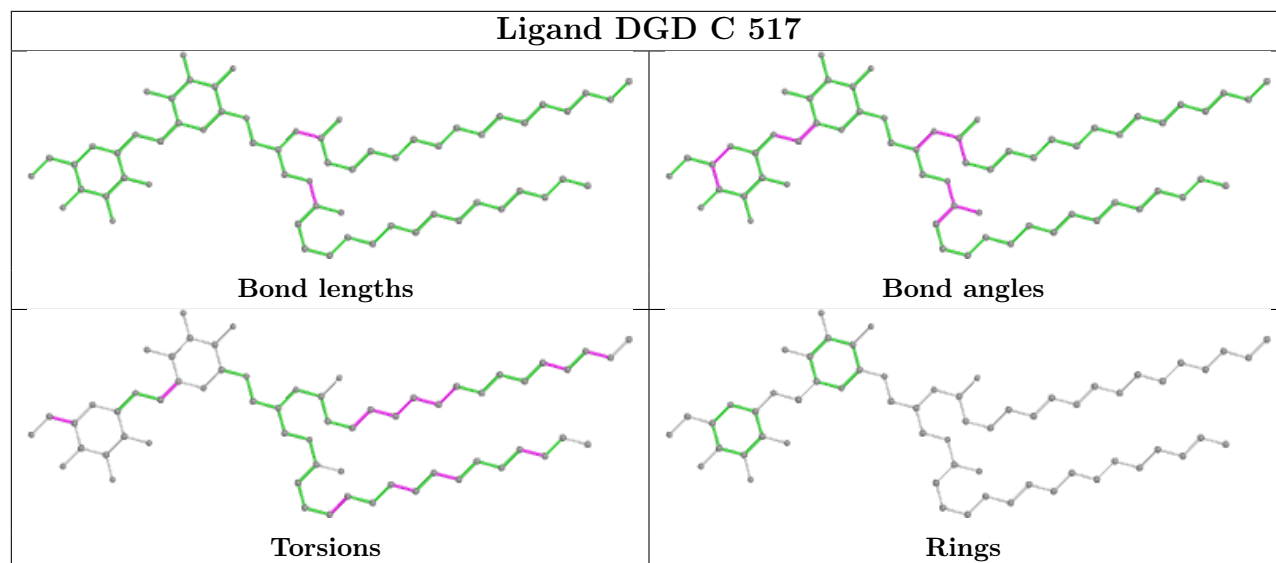


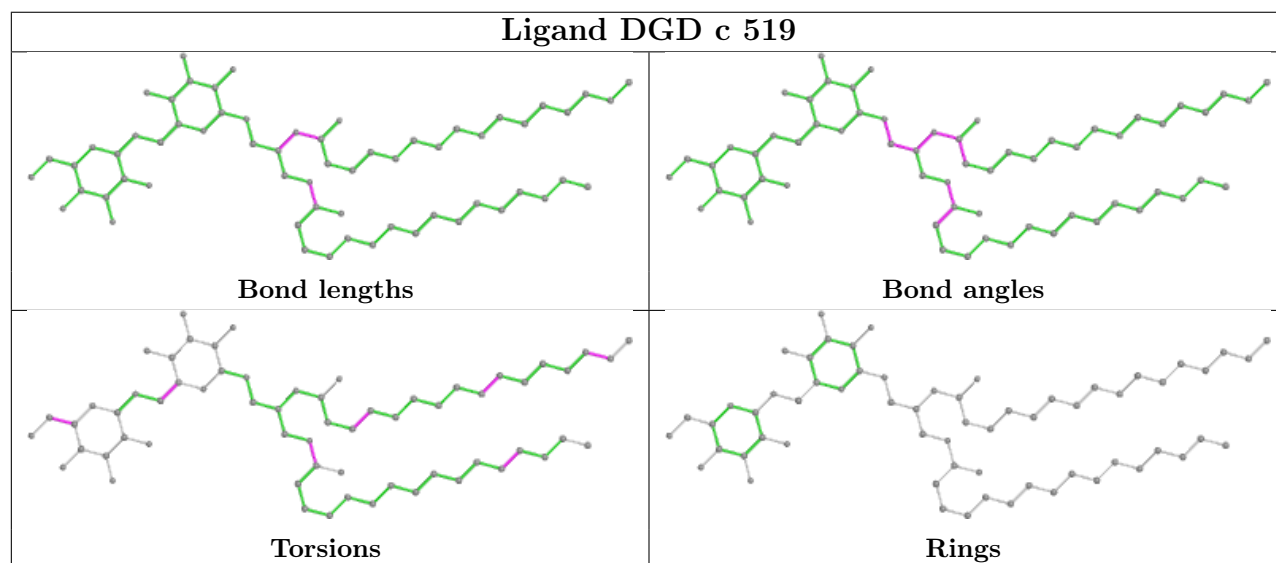
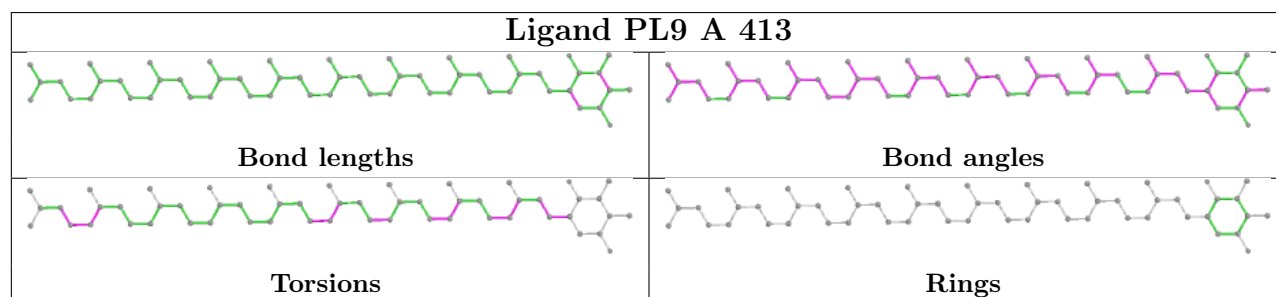
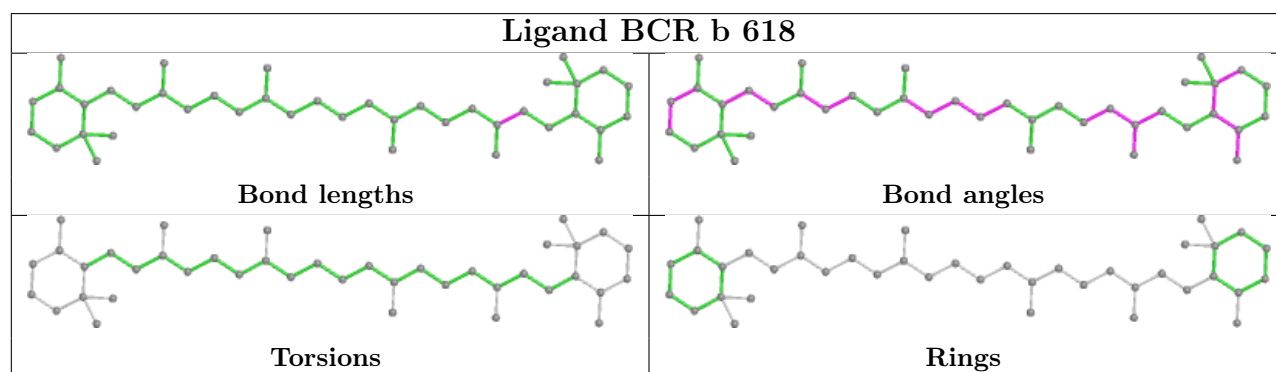
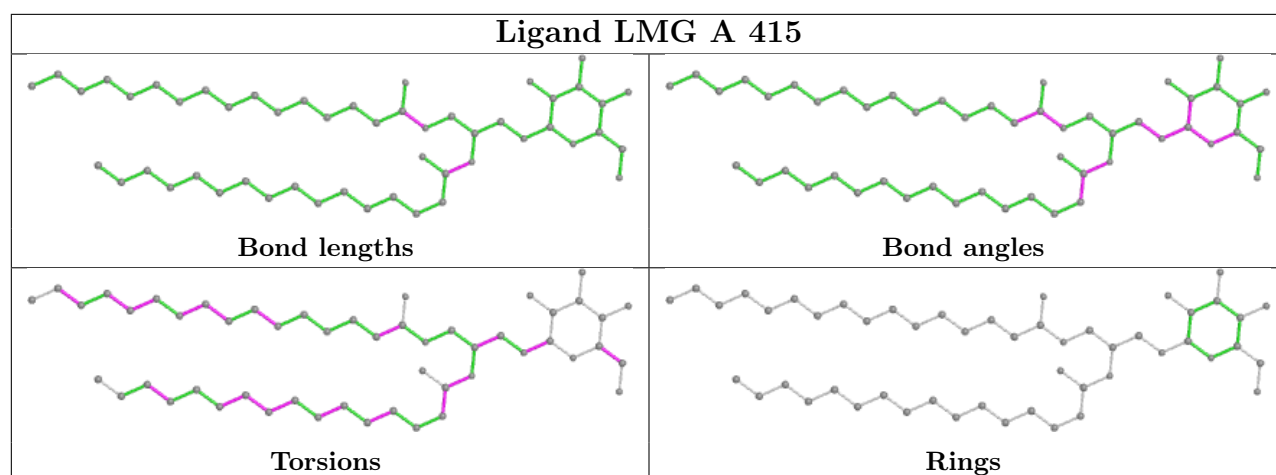


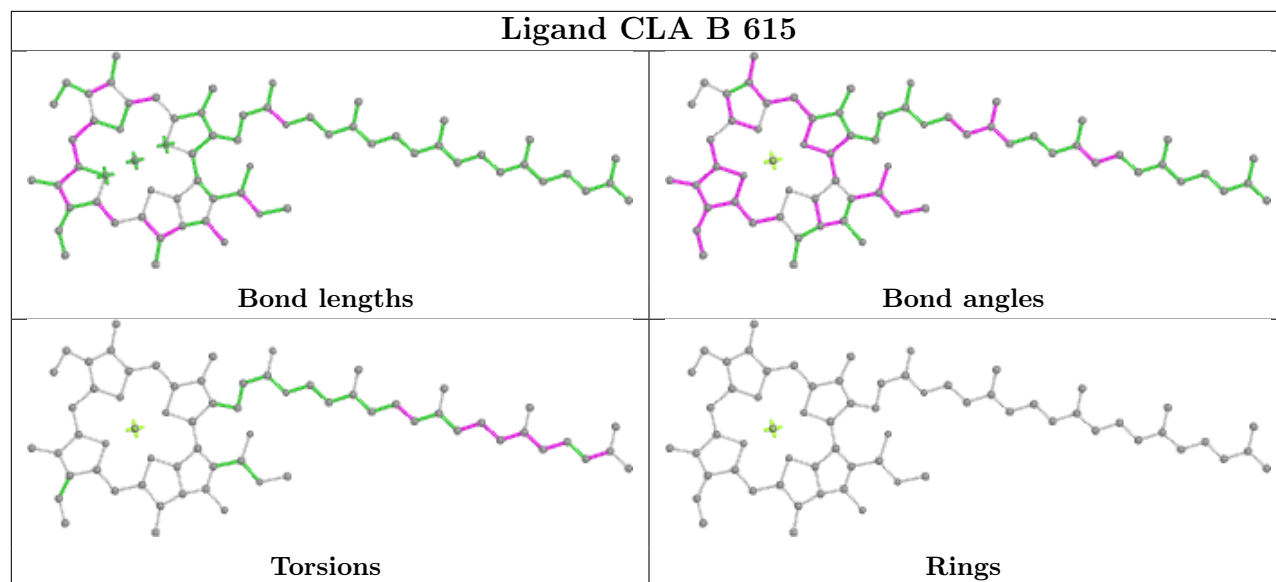
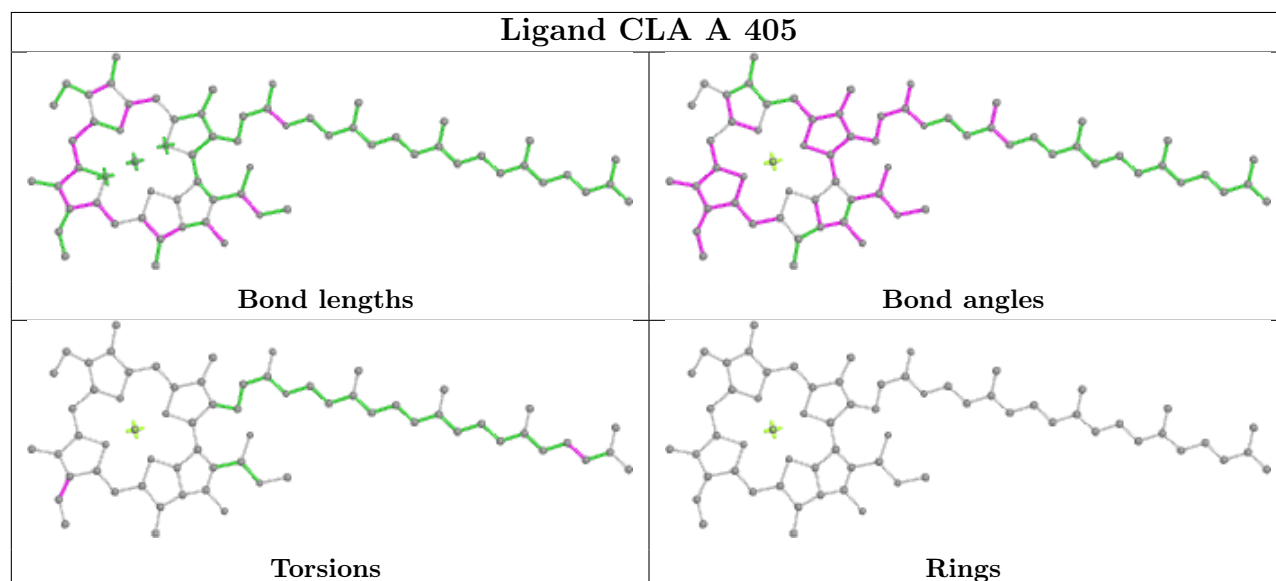
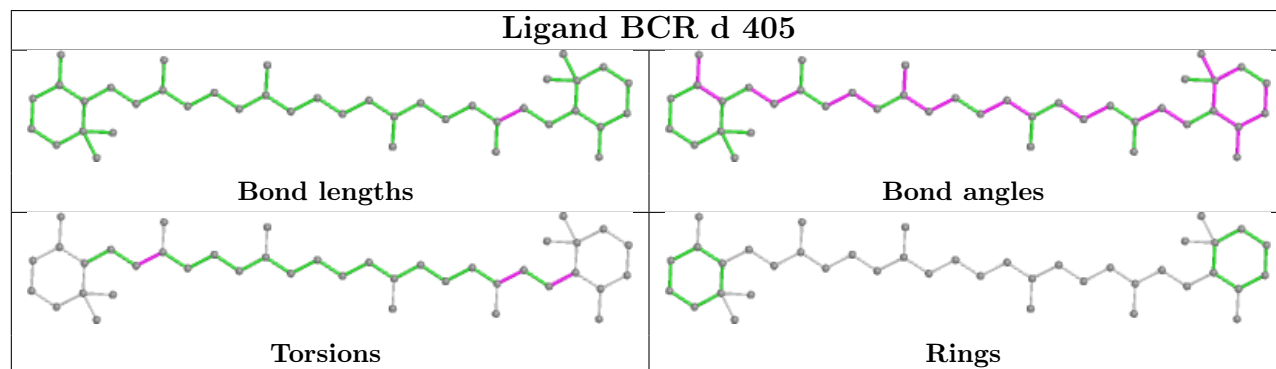


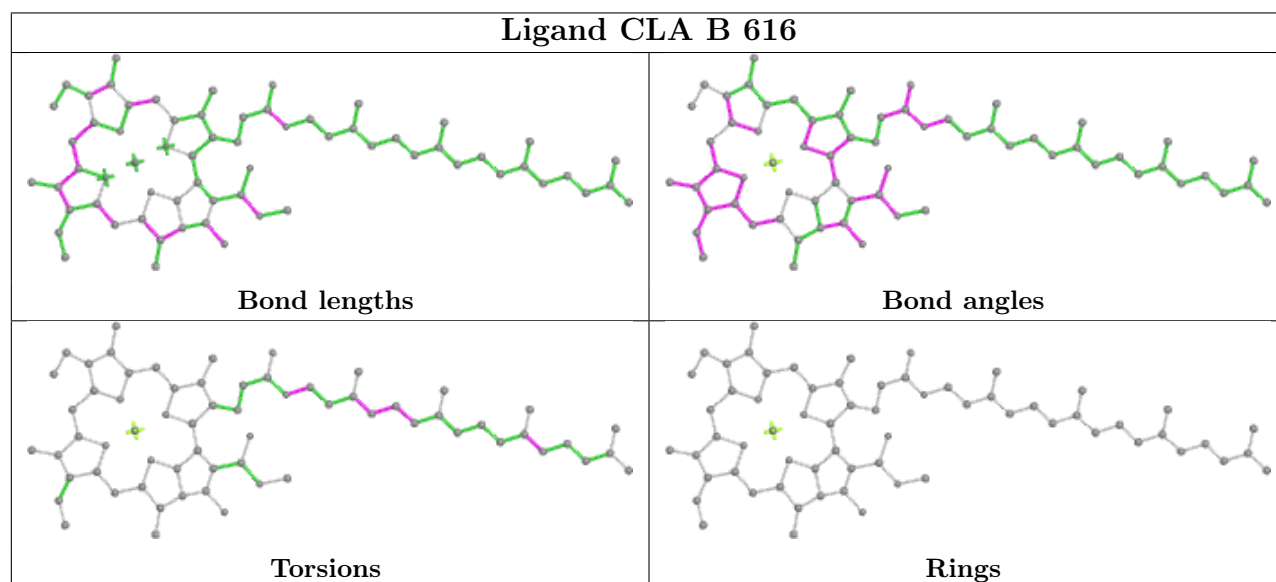
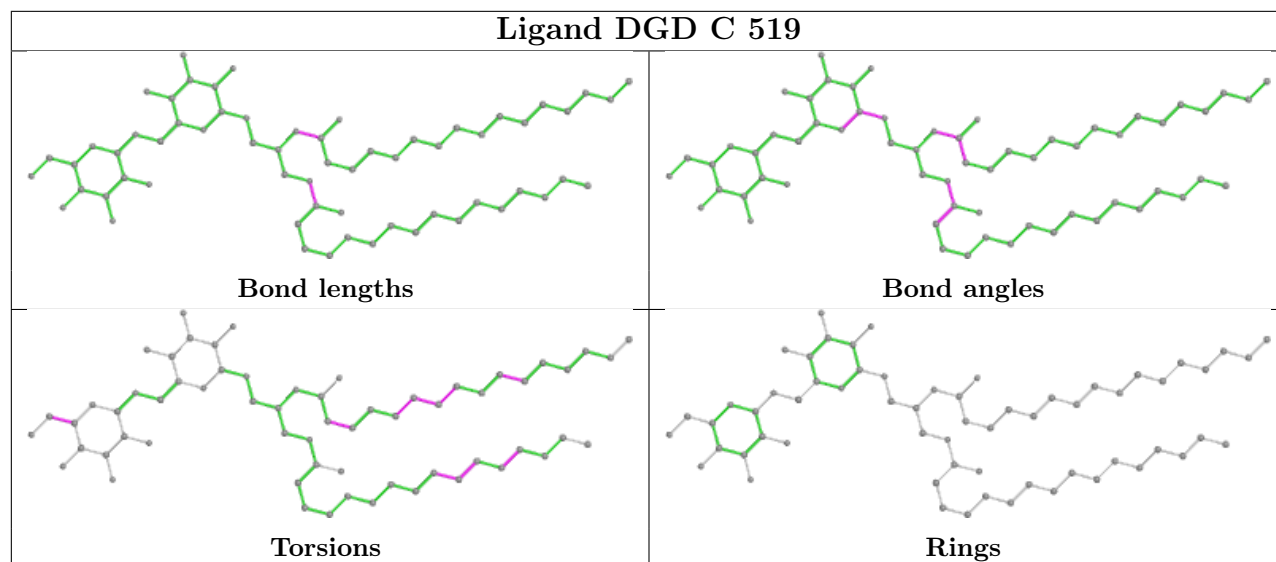
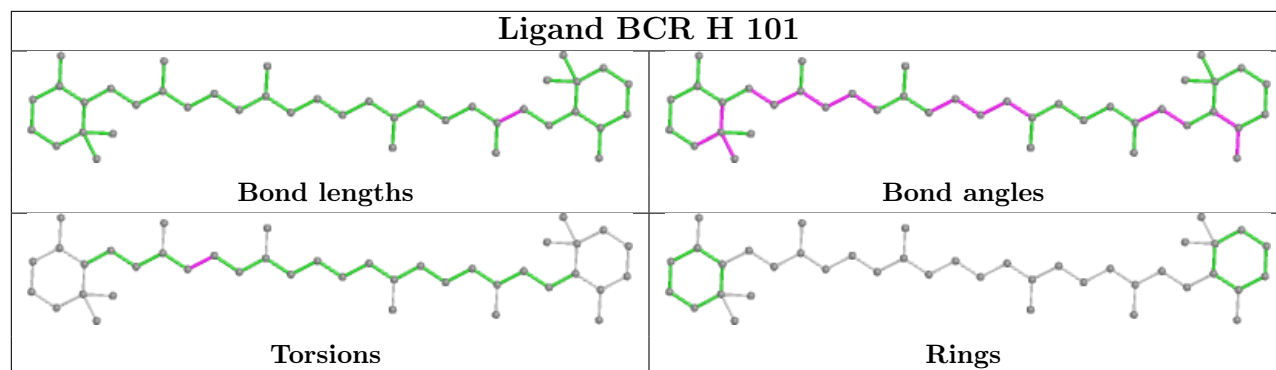


**Ligand CLA C 506****Ligand CLA b 608****Ligand LMG C 520**

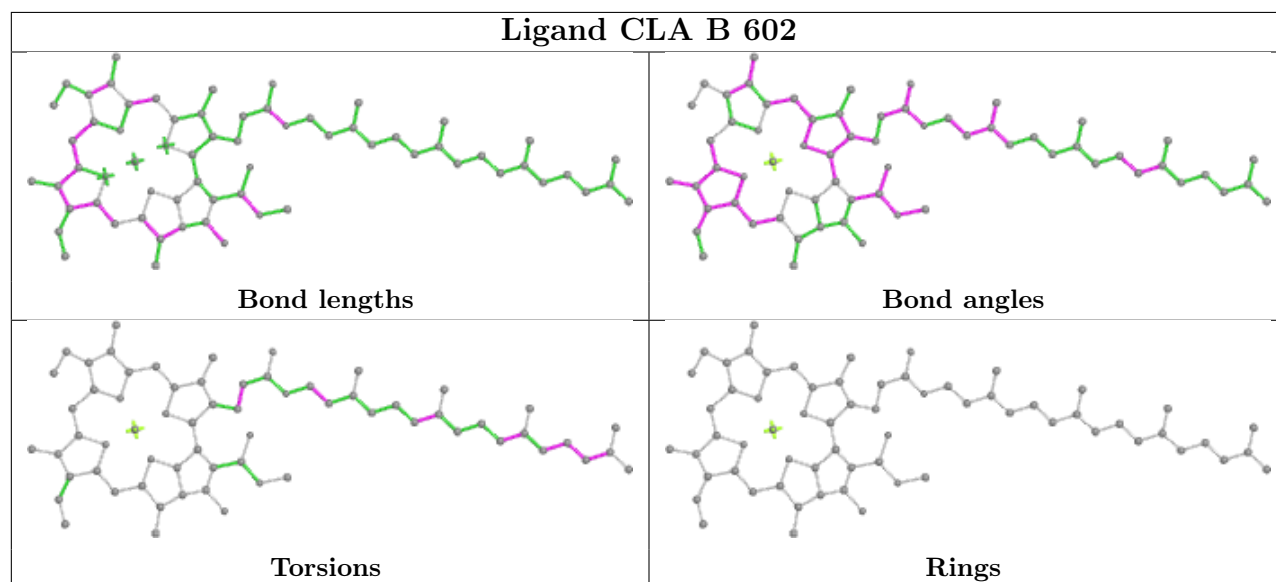
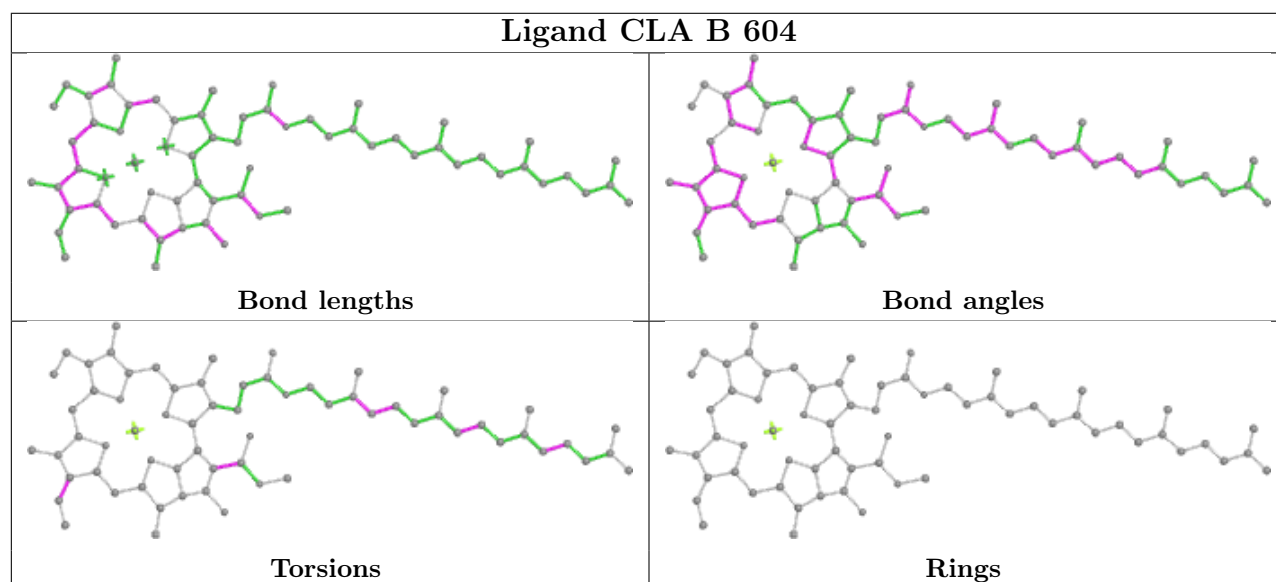
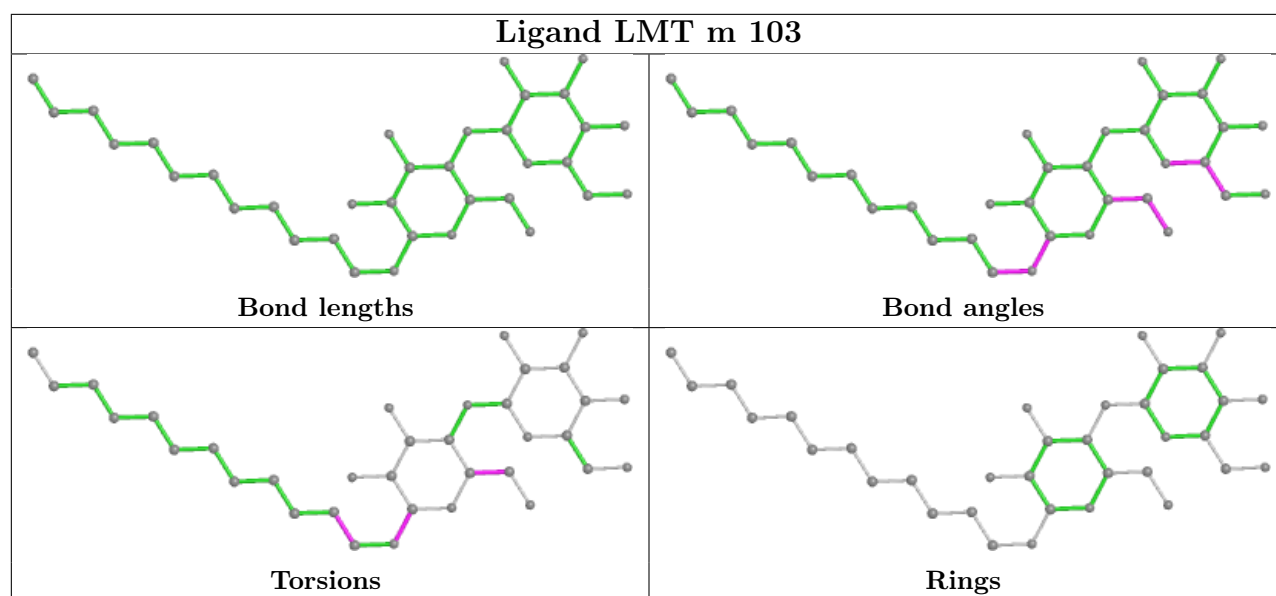


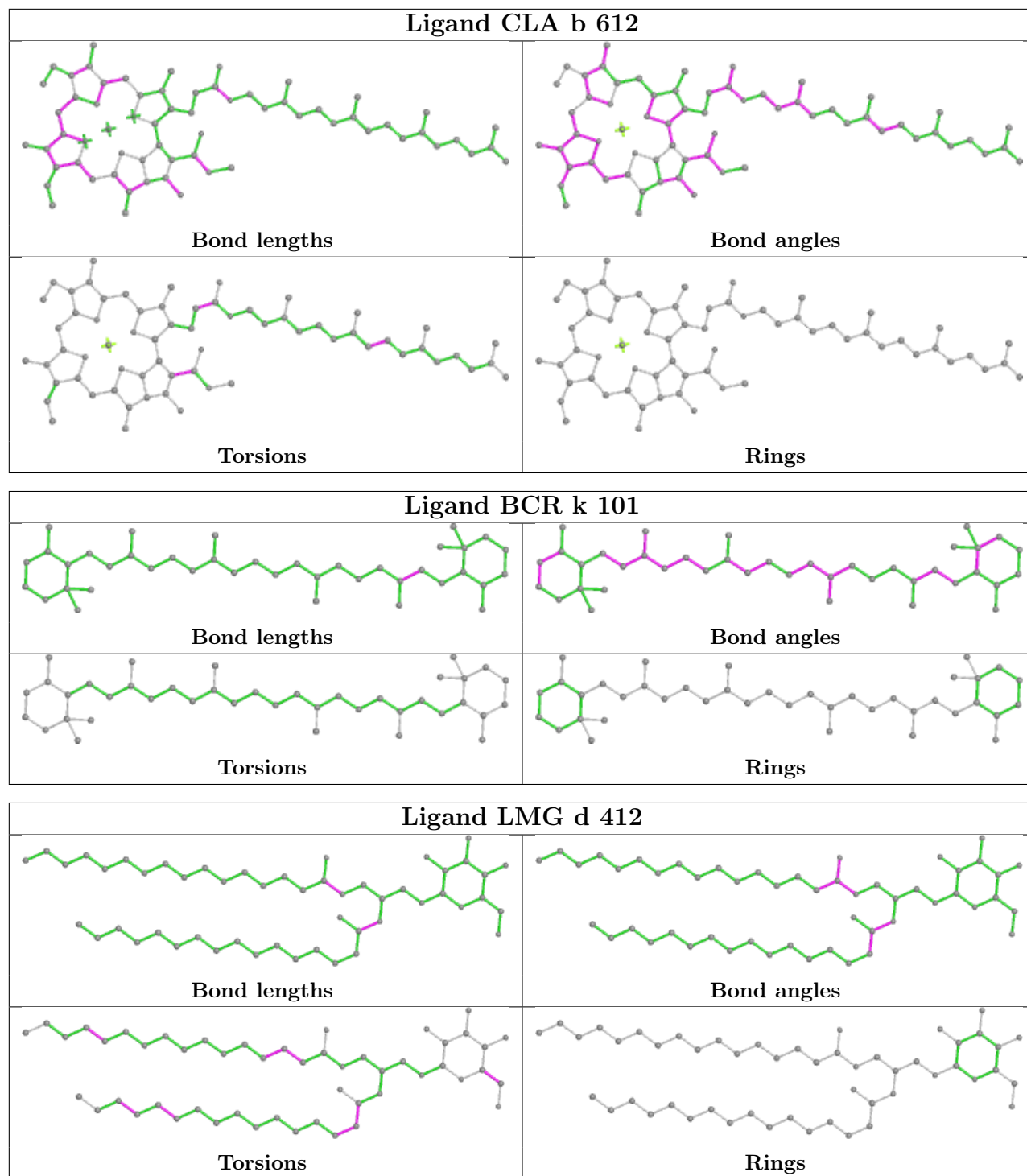


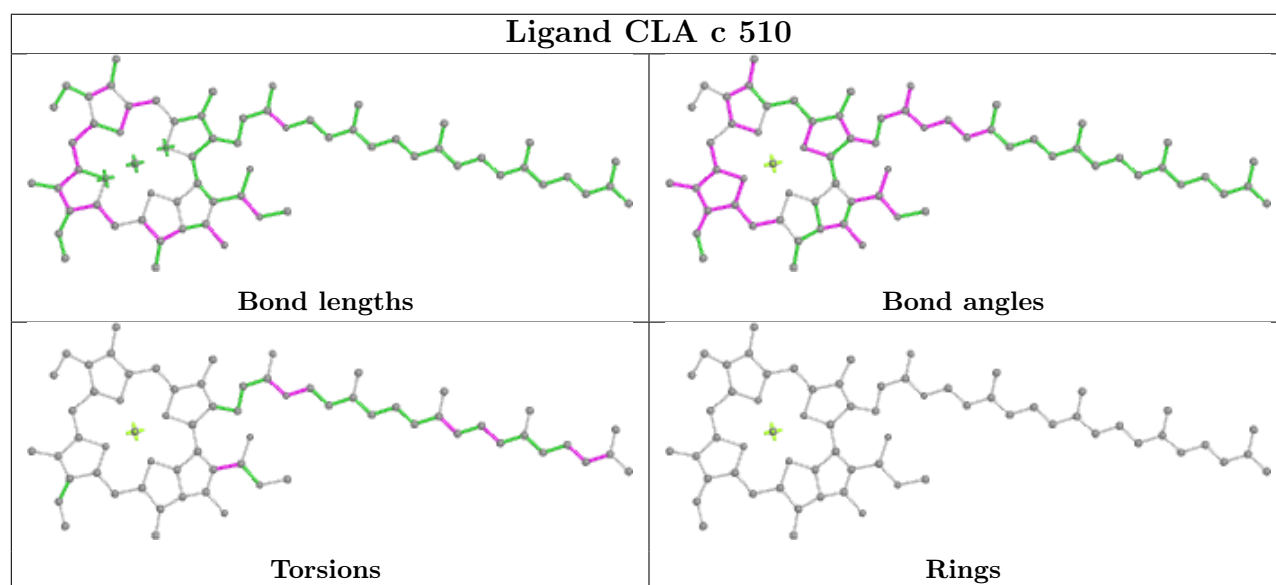
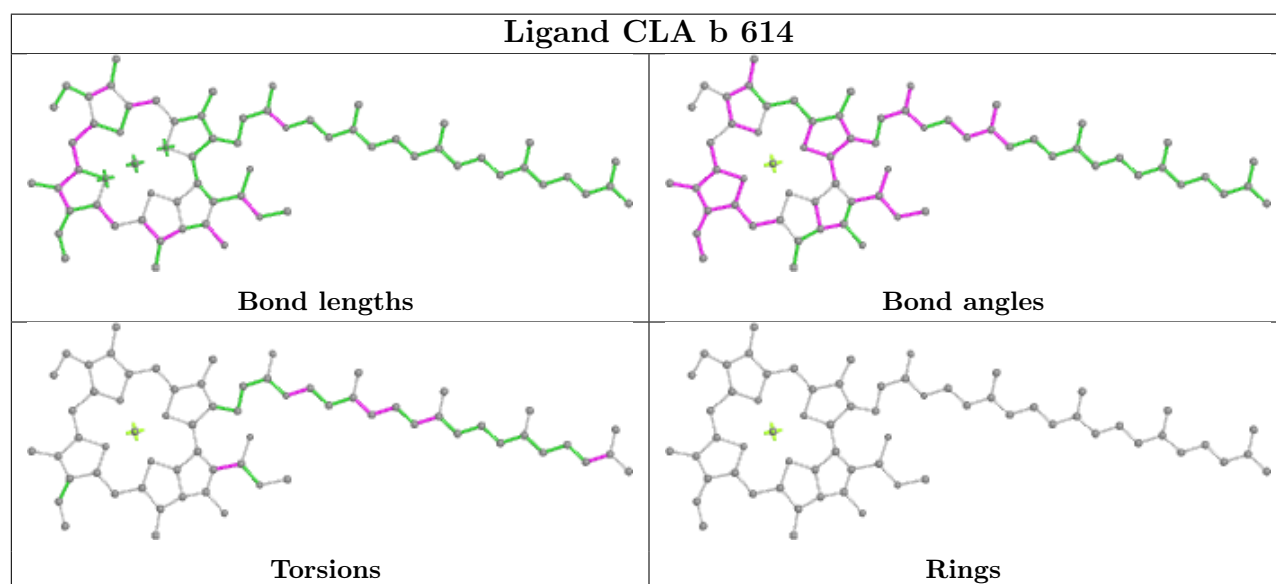
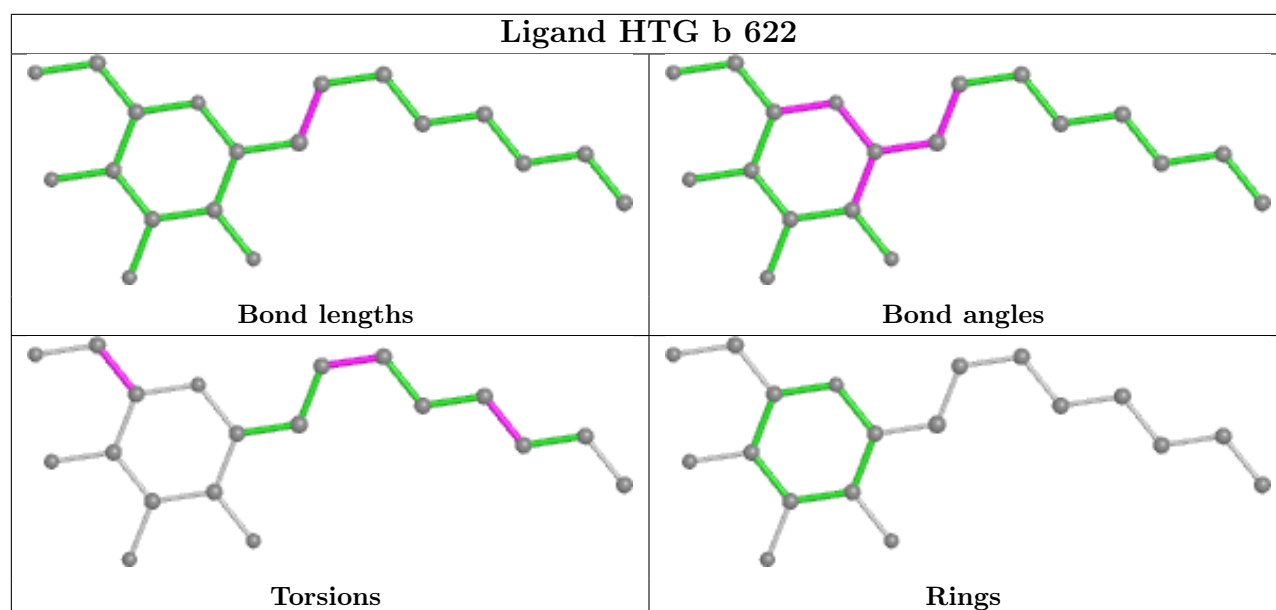
**Ligand CLA B 615****Ligand CLA A 405****Ligand BCR d 405**



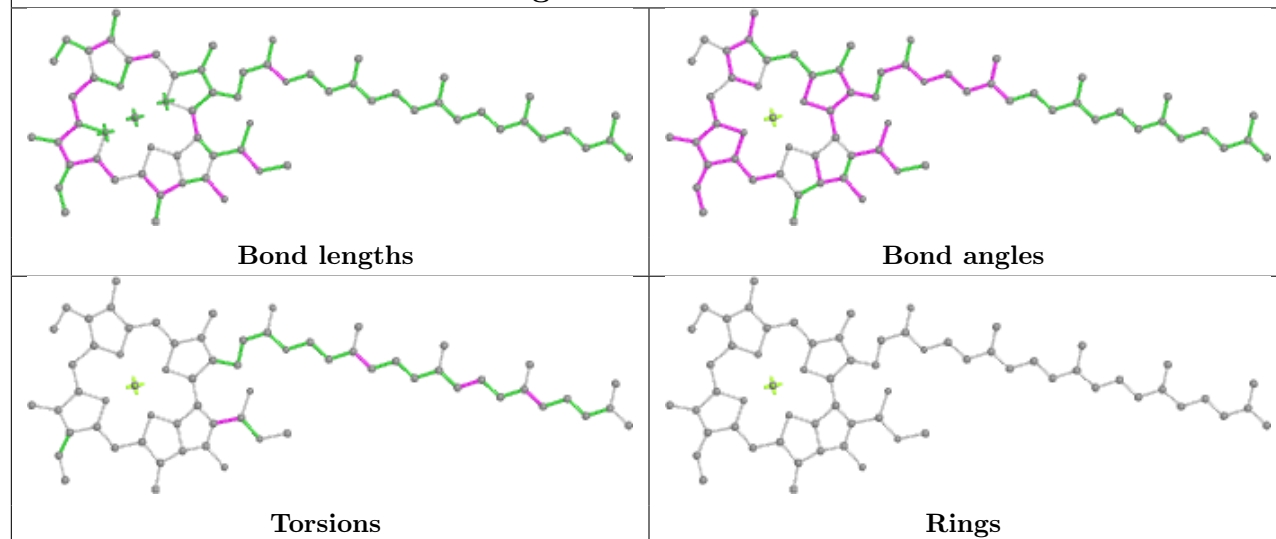




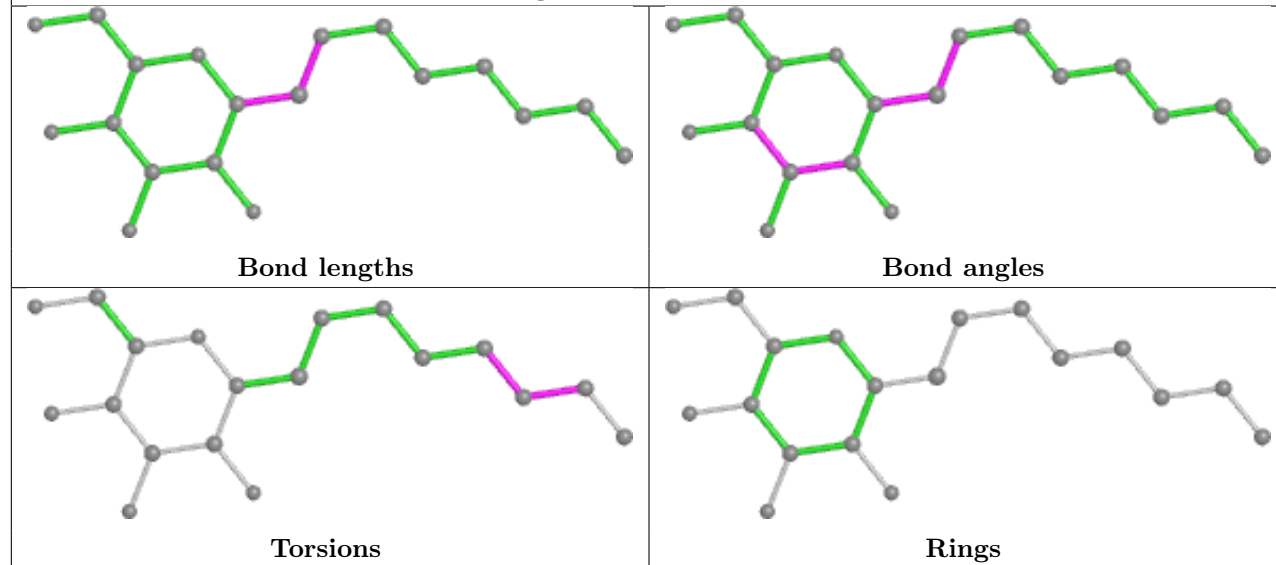




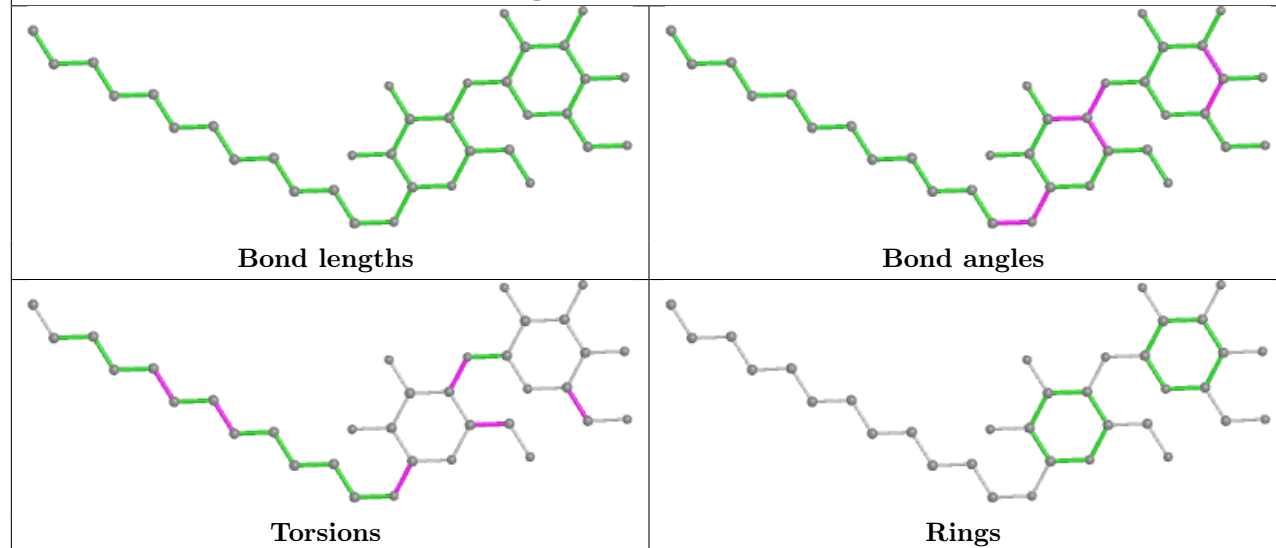
## Ligand CLA C 505

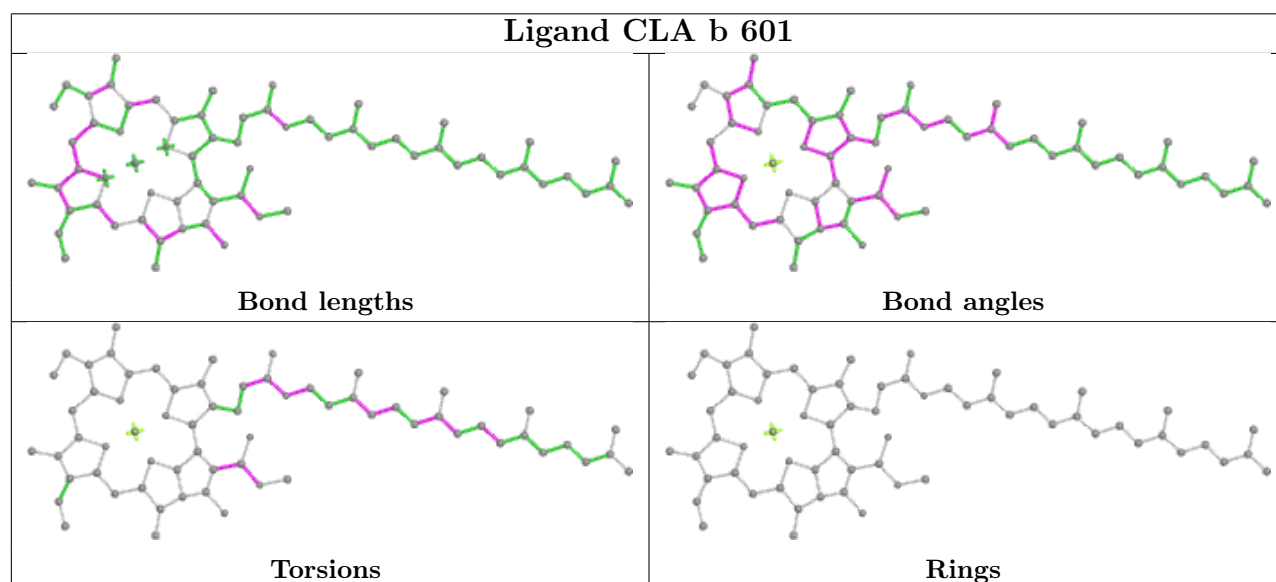
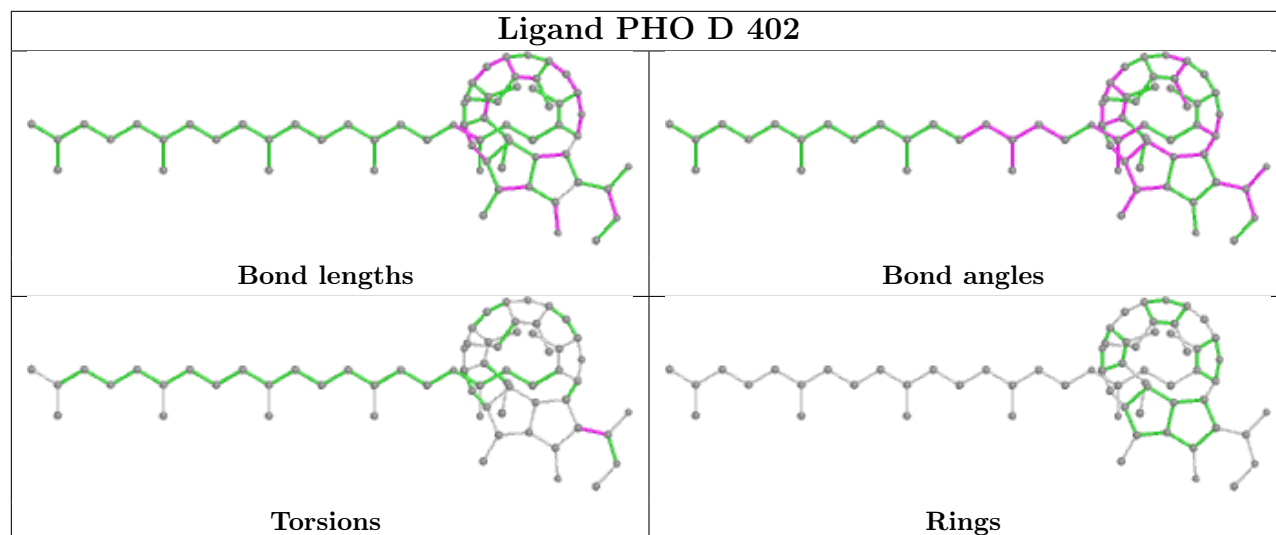


## Ligand HTG b 624

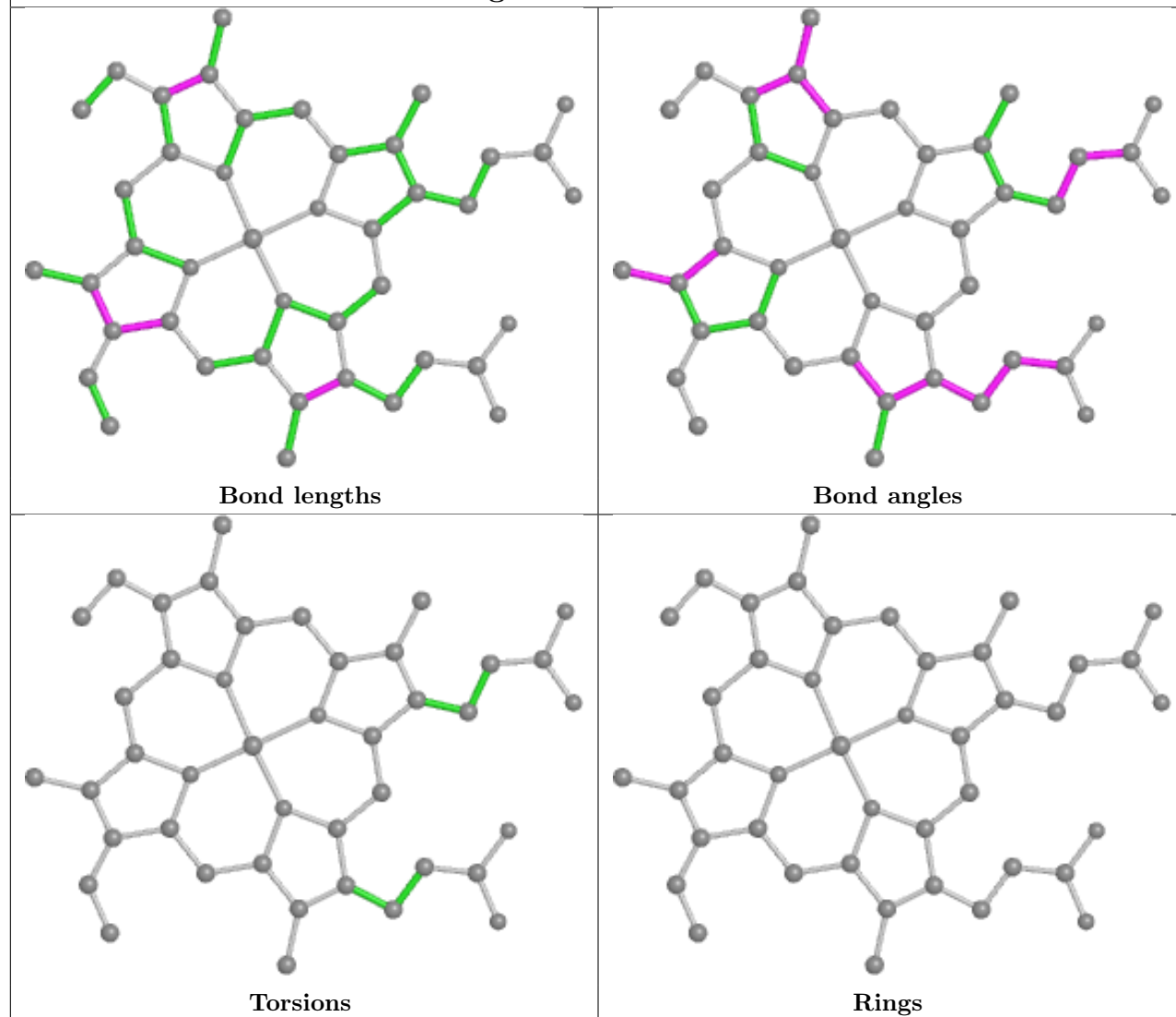


## Ligand LMT D 404

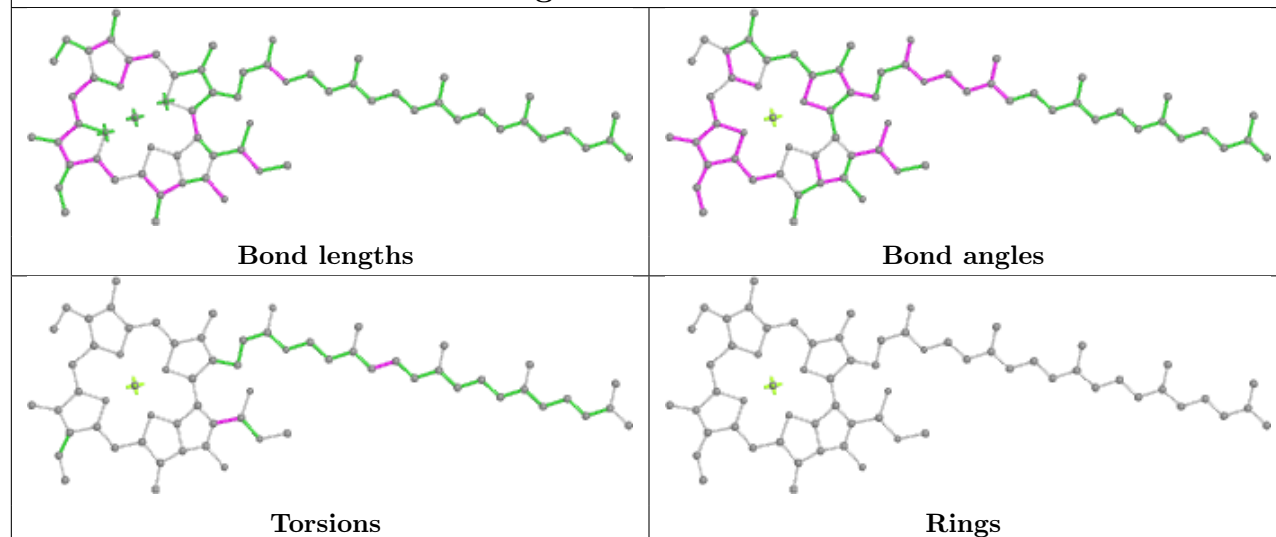


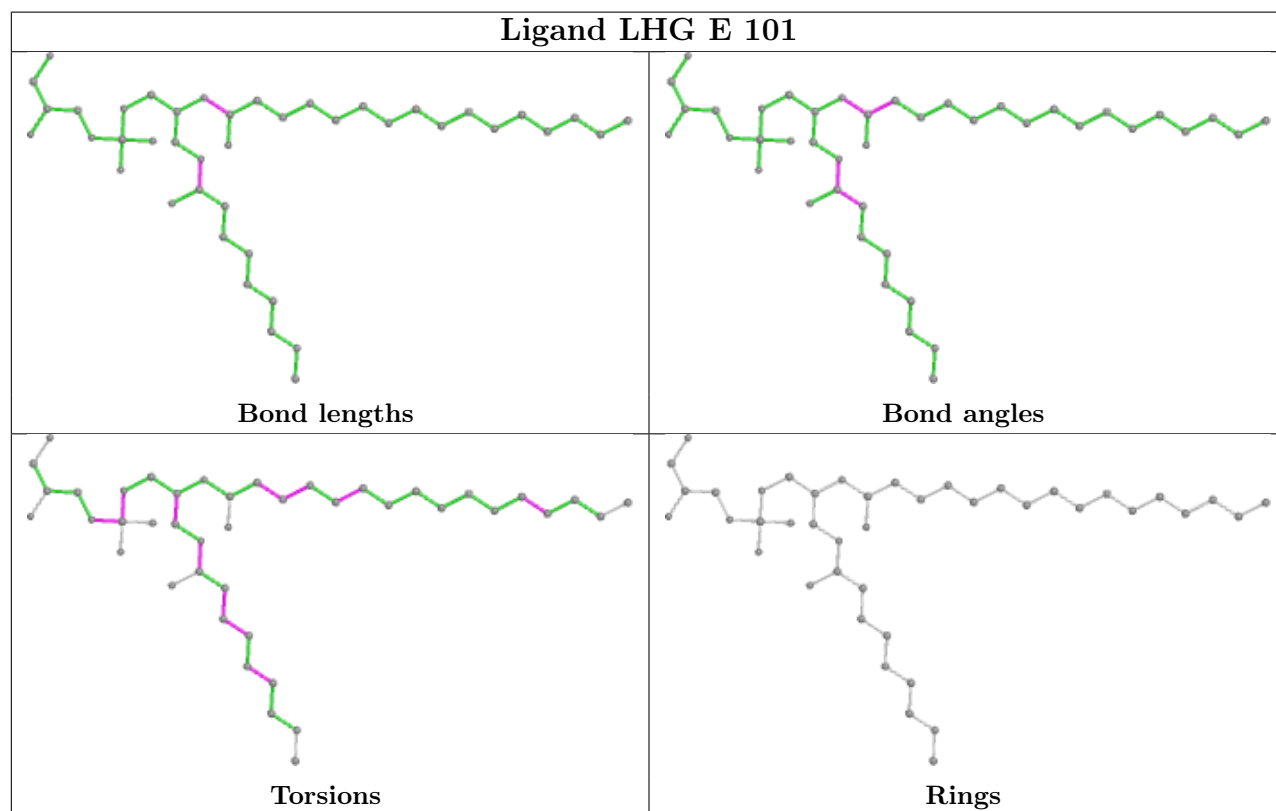
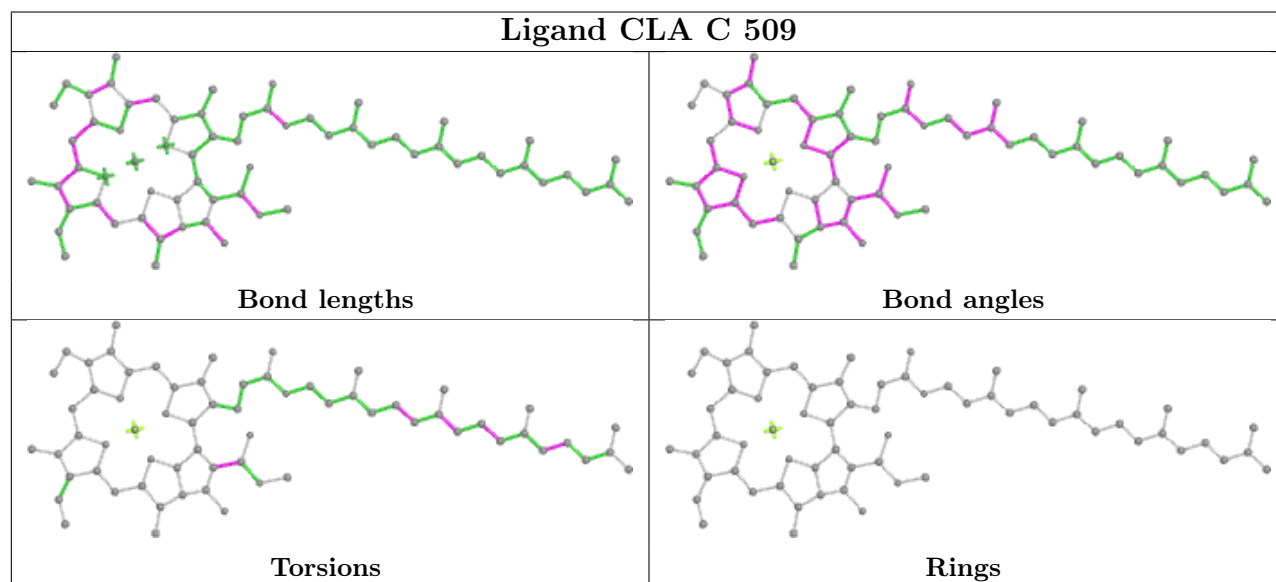
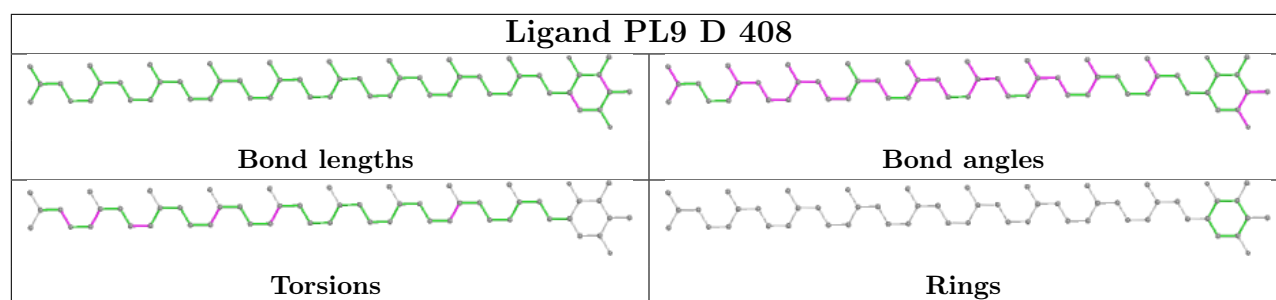


## Ligand HEC V 201

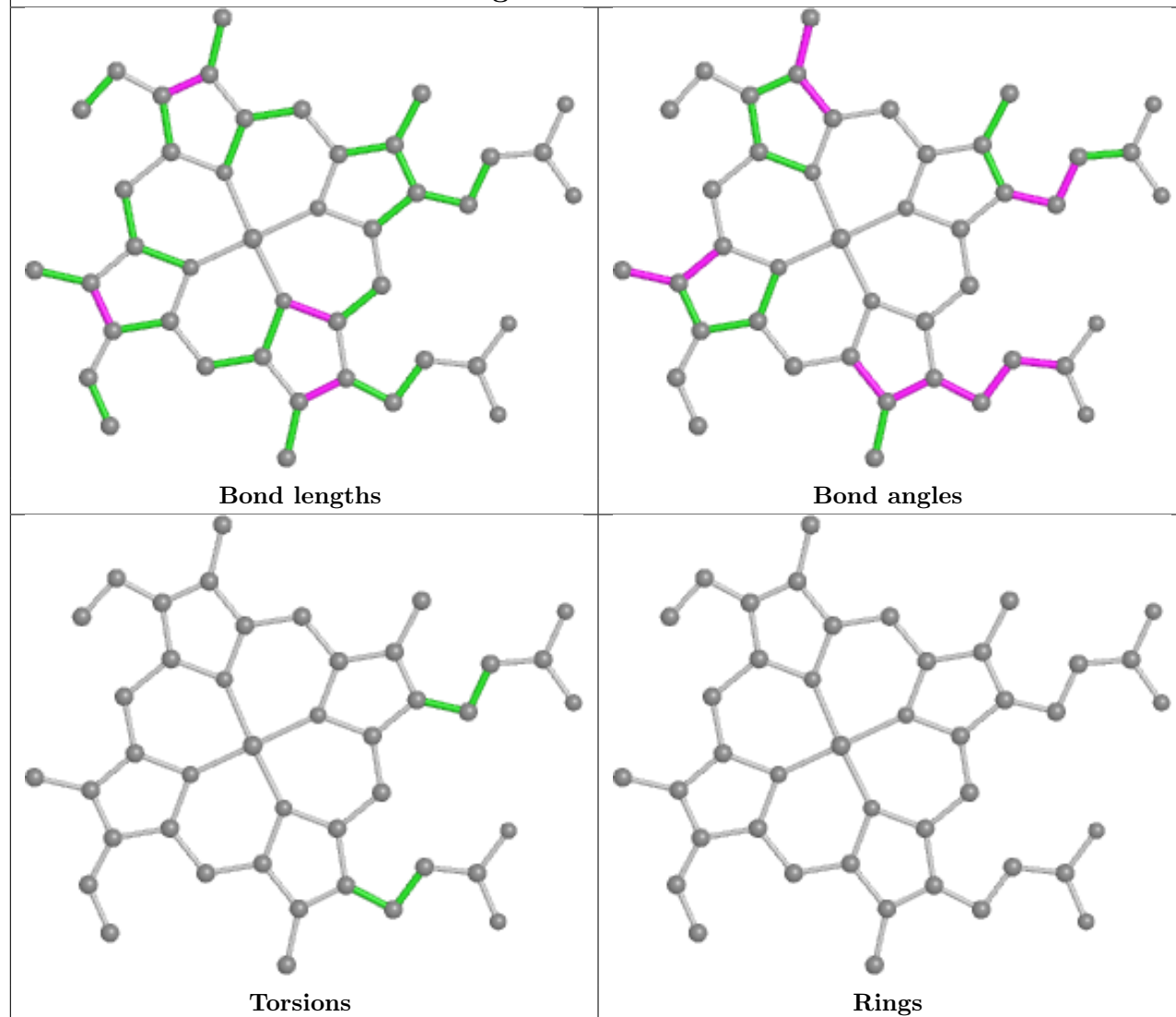


## Ligand CLA b 607

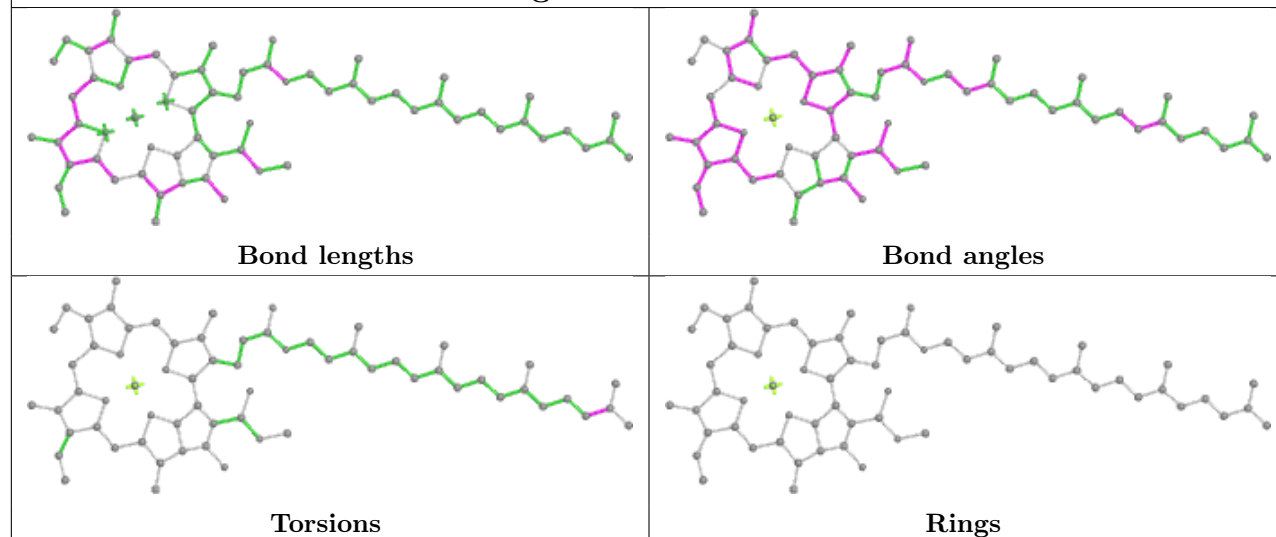




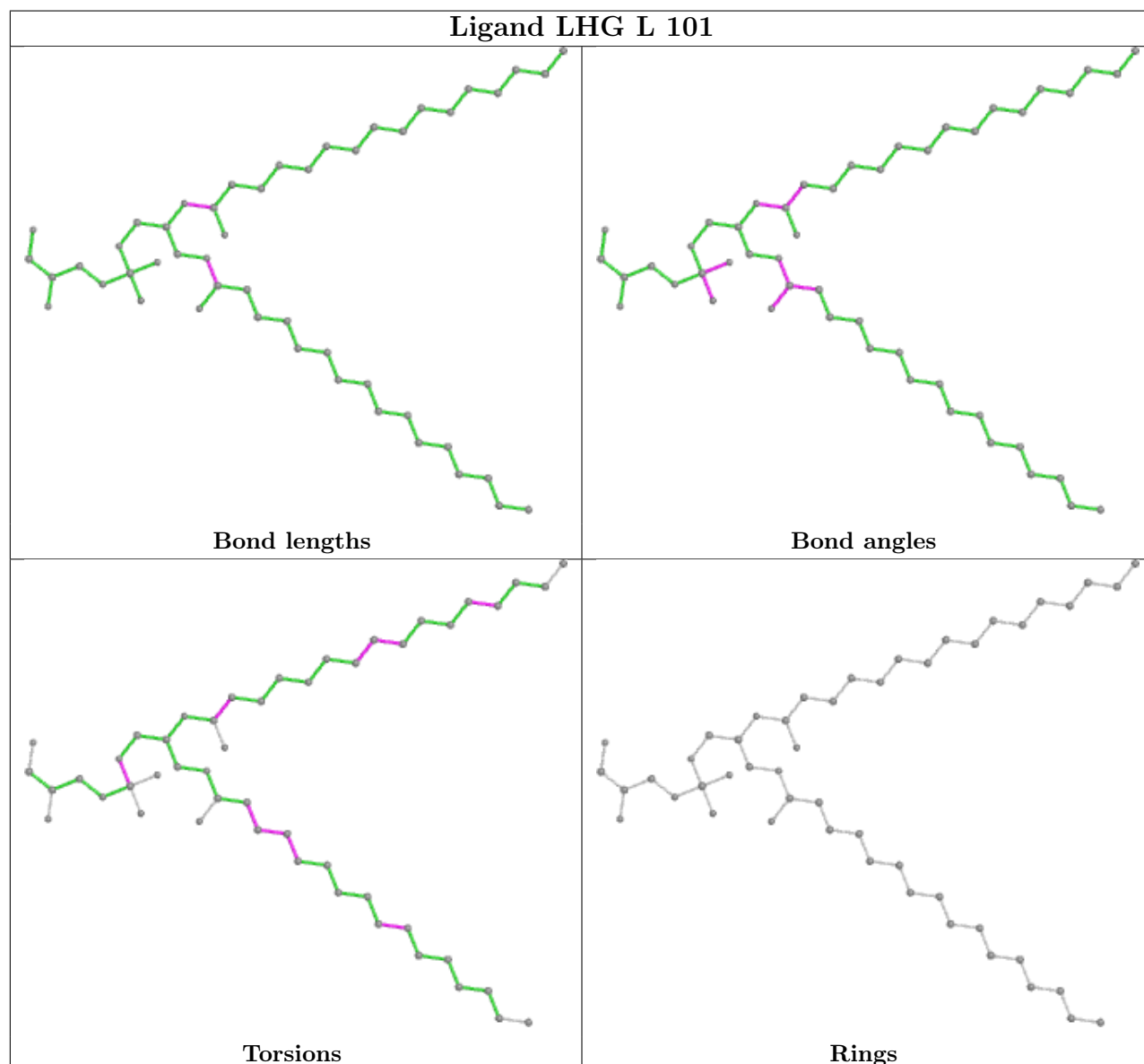
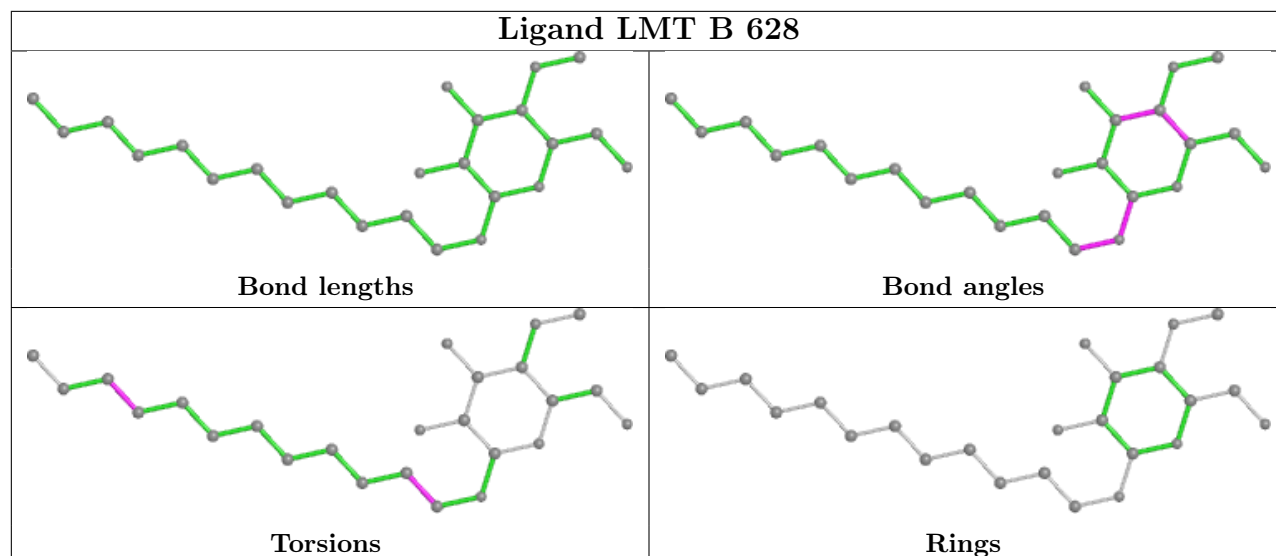
## Ligand HEC v 203



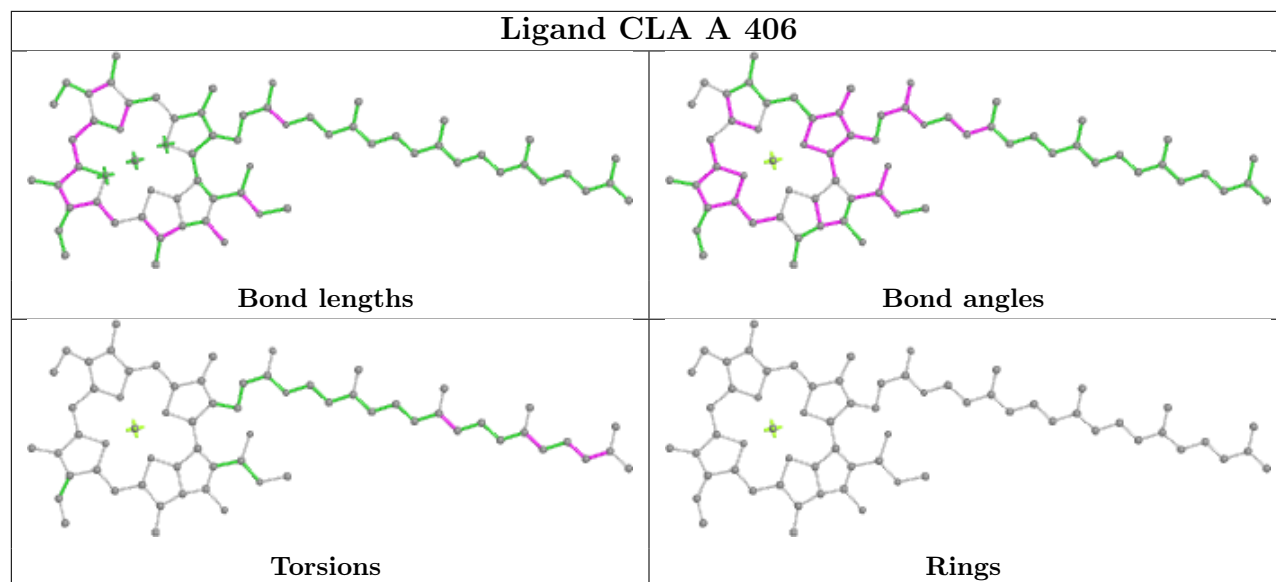
## Ligand CLA B 608



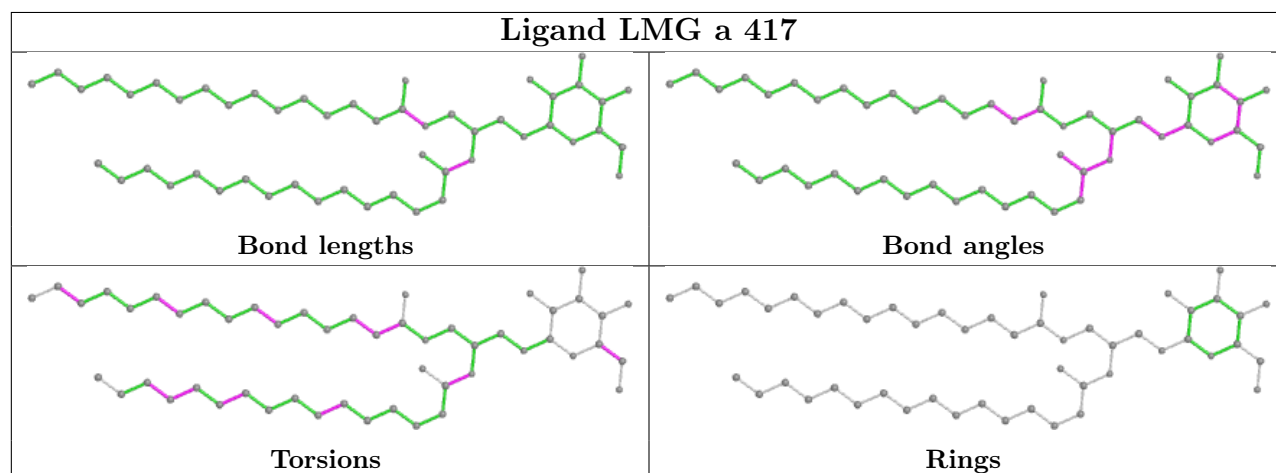




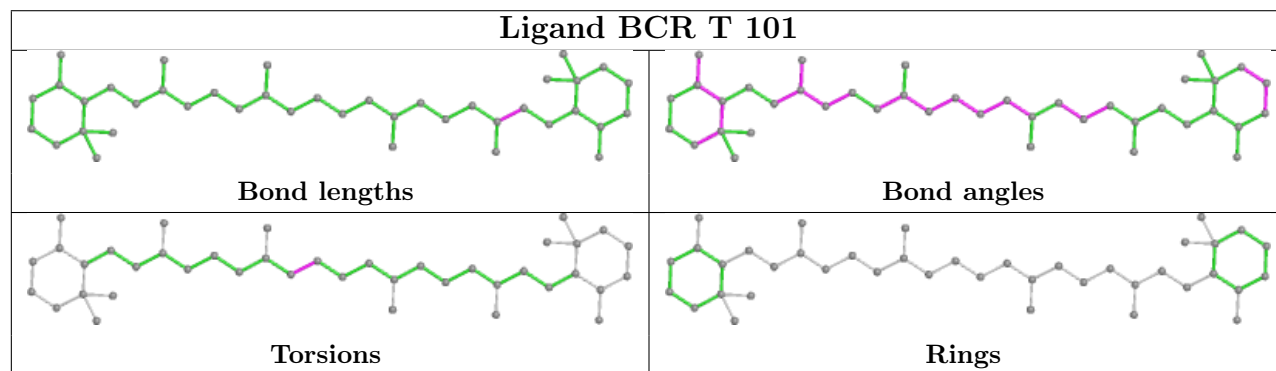
## Ligand CLA A 406

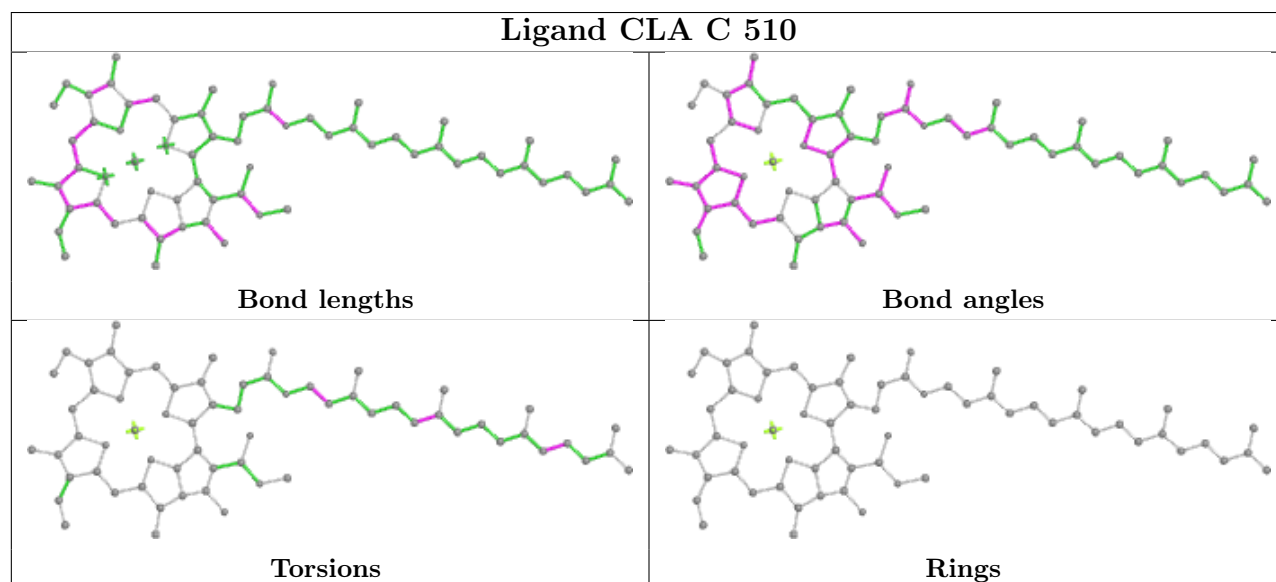
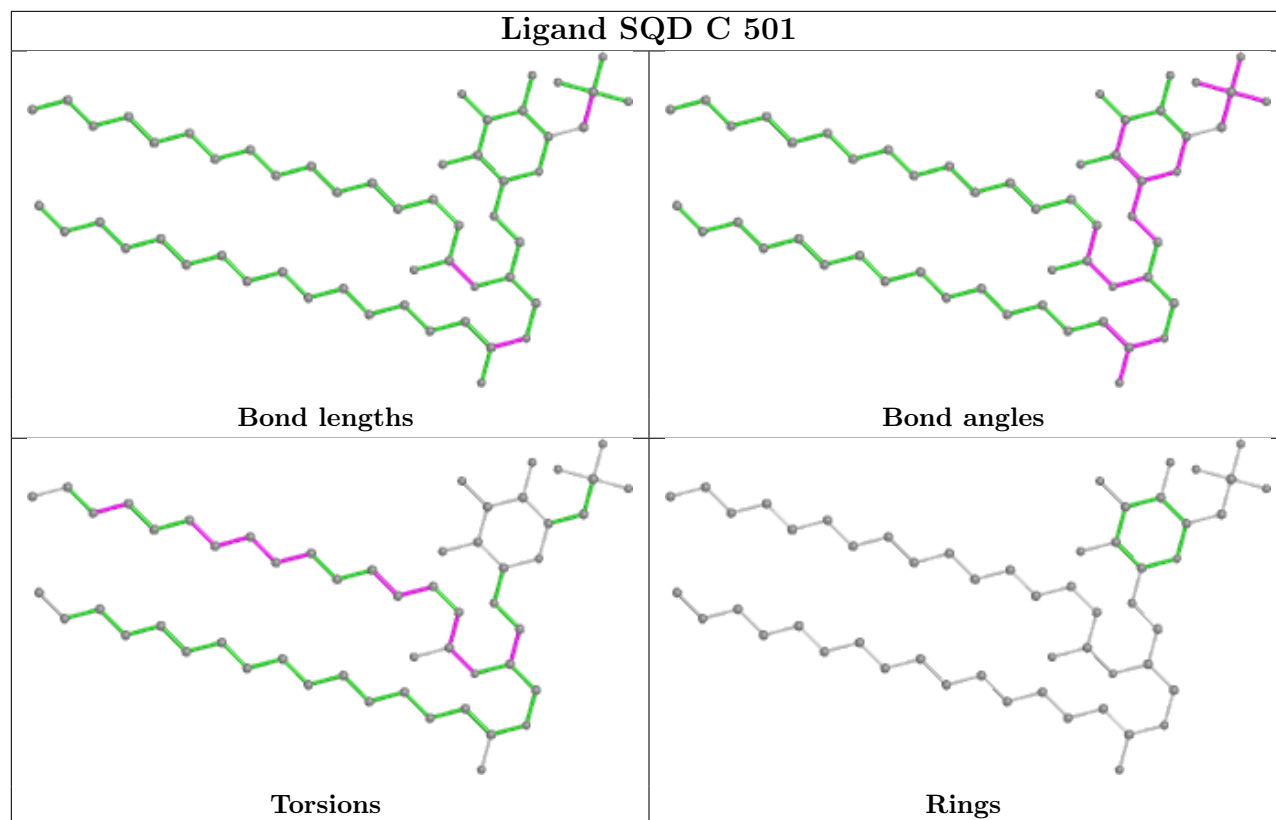


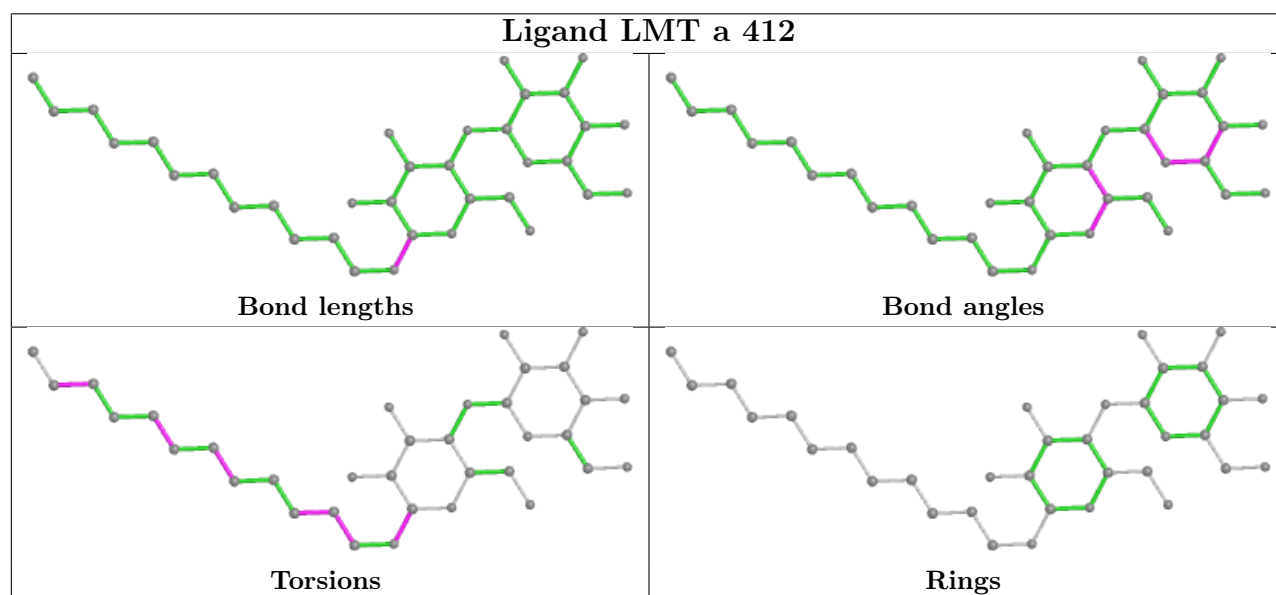
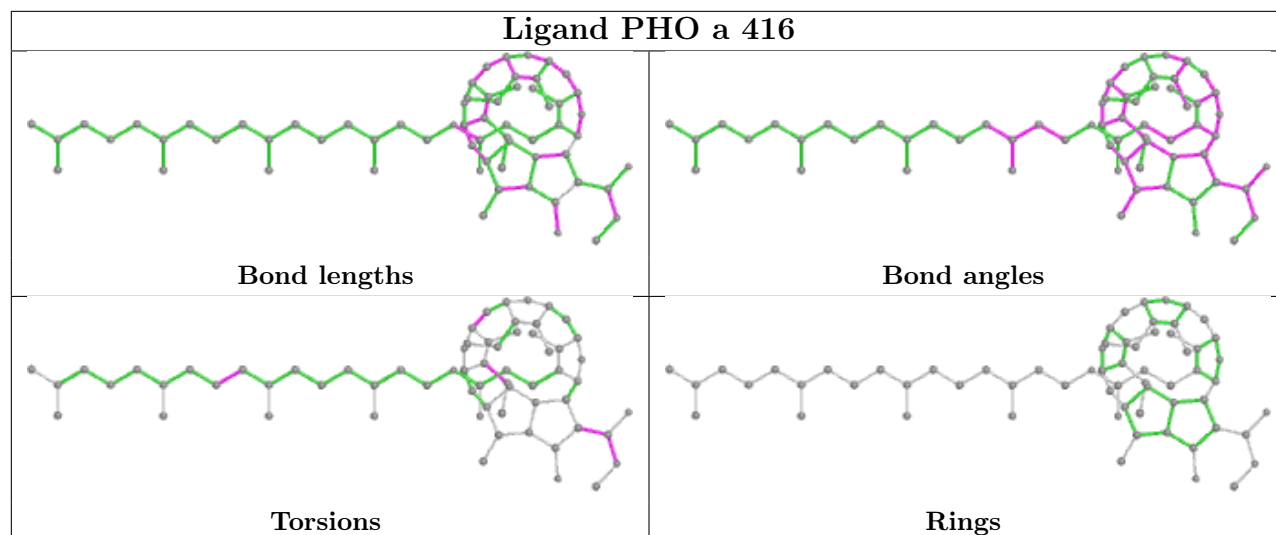
## Ligand LMG a 417

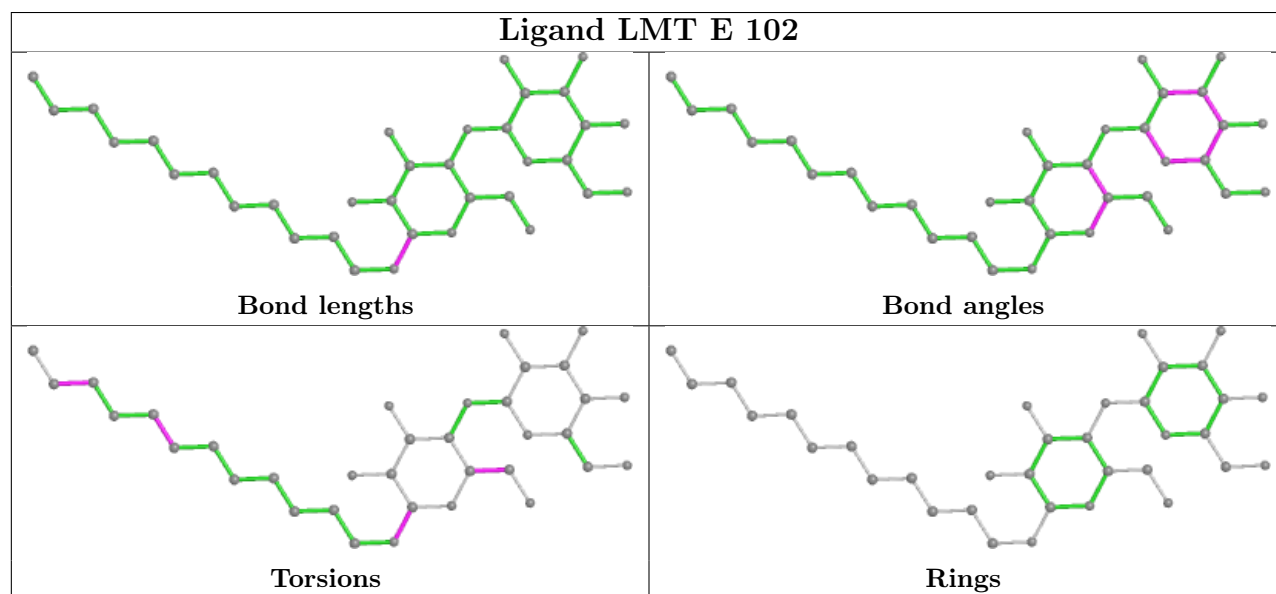
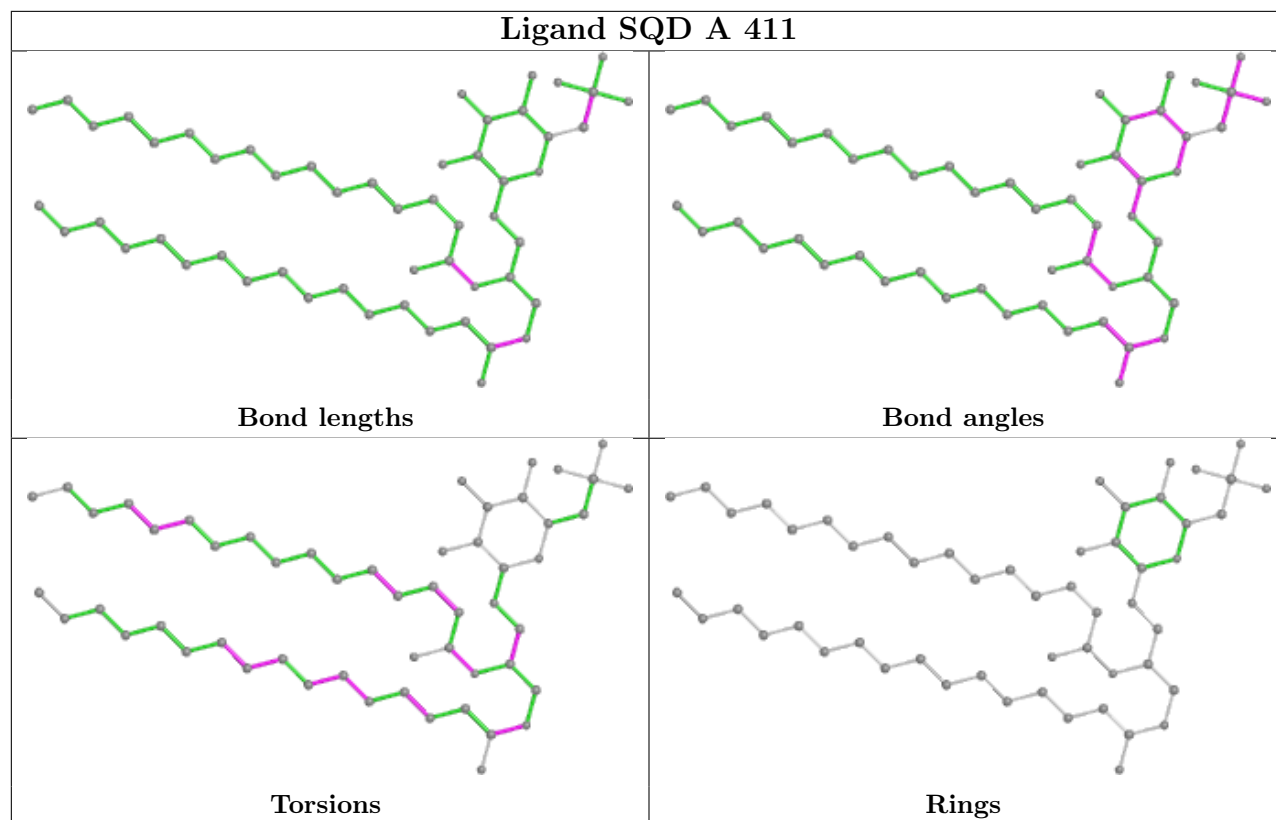


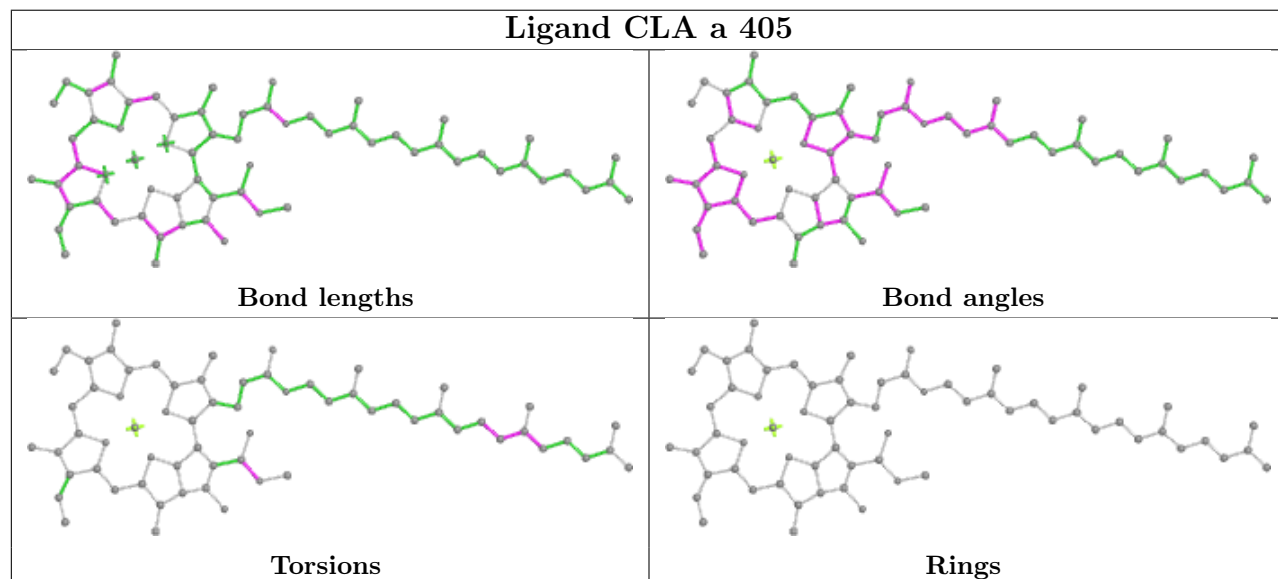
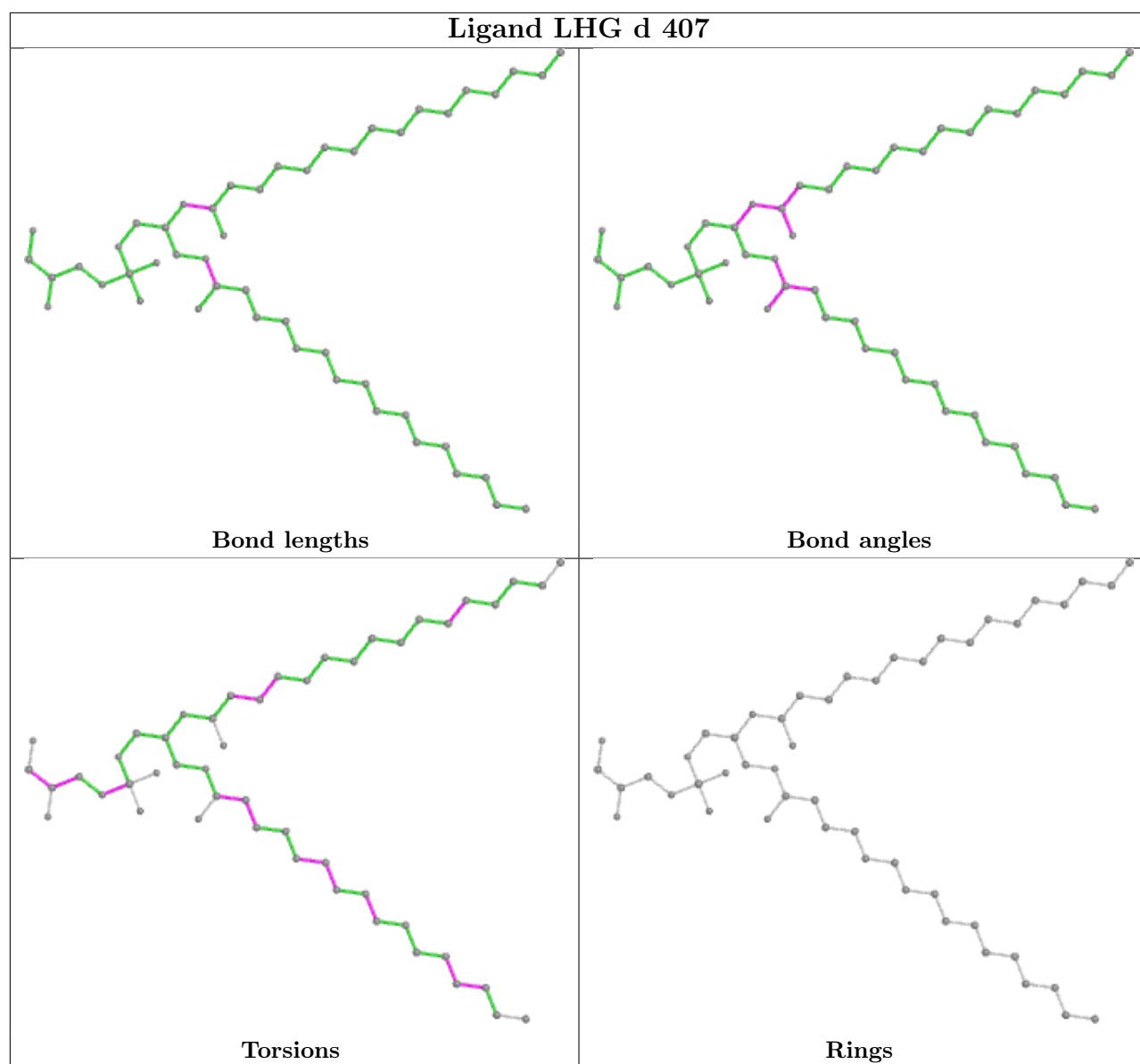
## Ligand BCR T 101



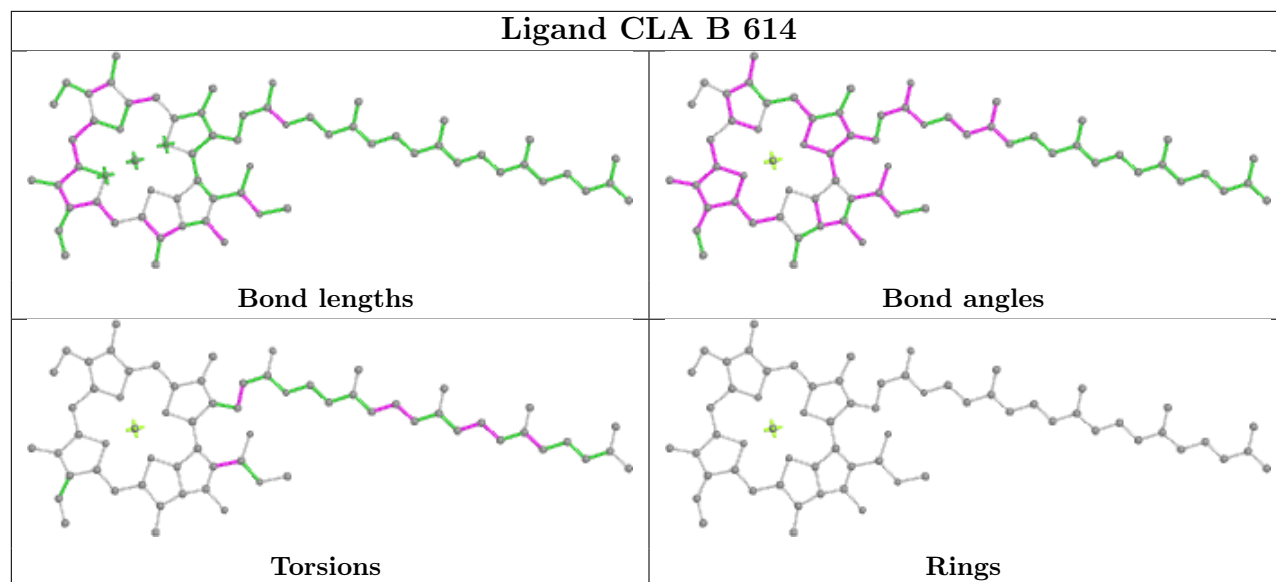




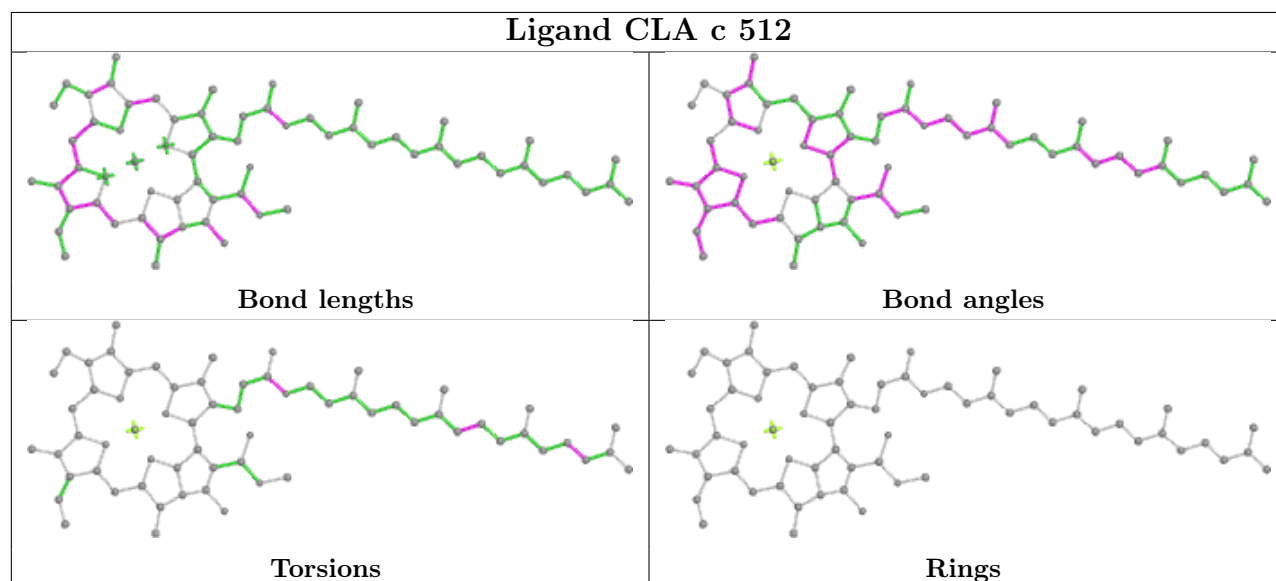




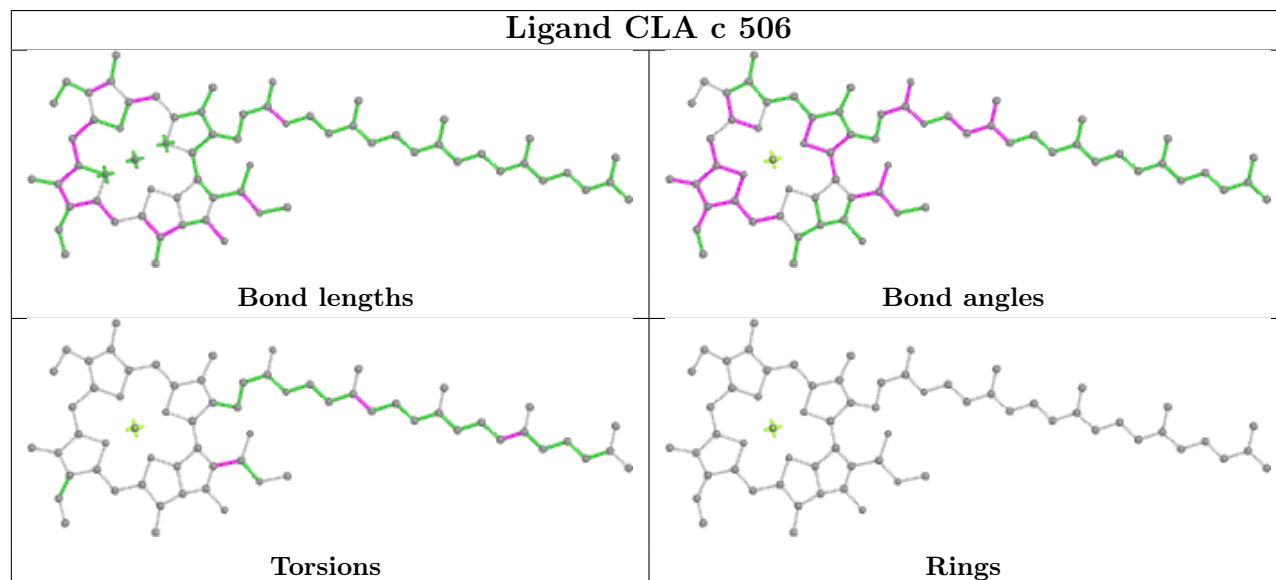
## Ligand CLA B 614

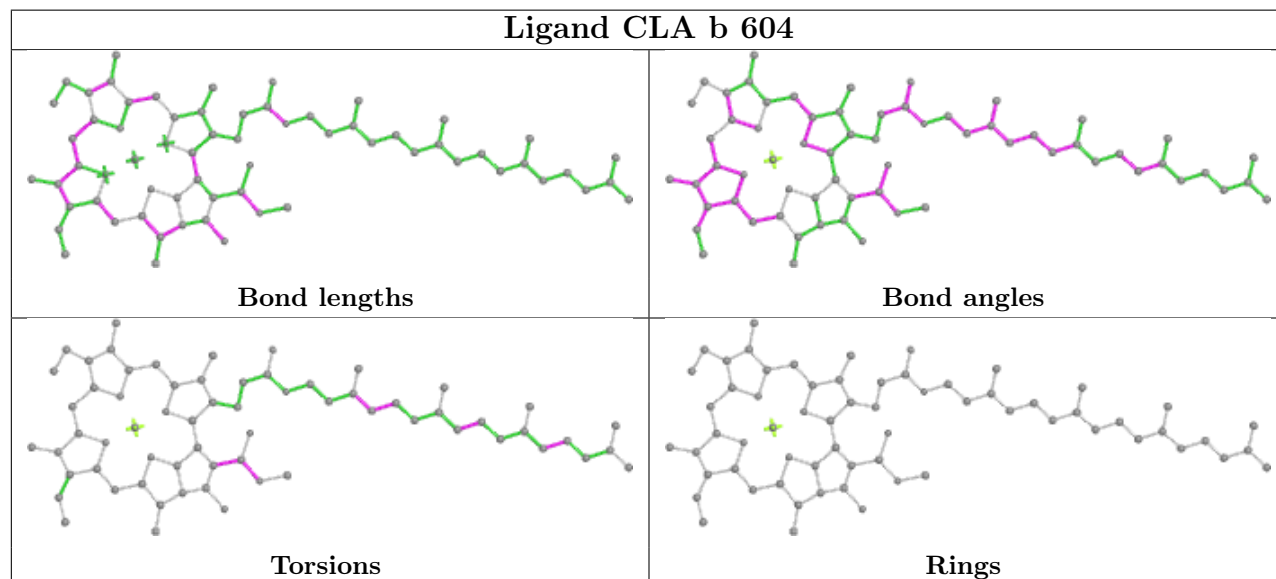
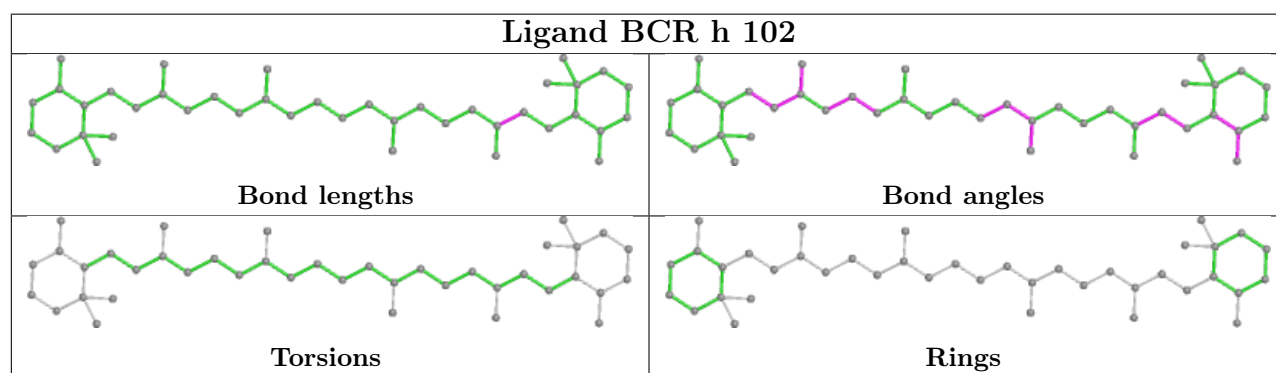
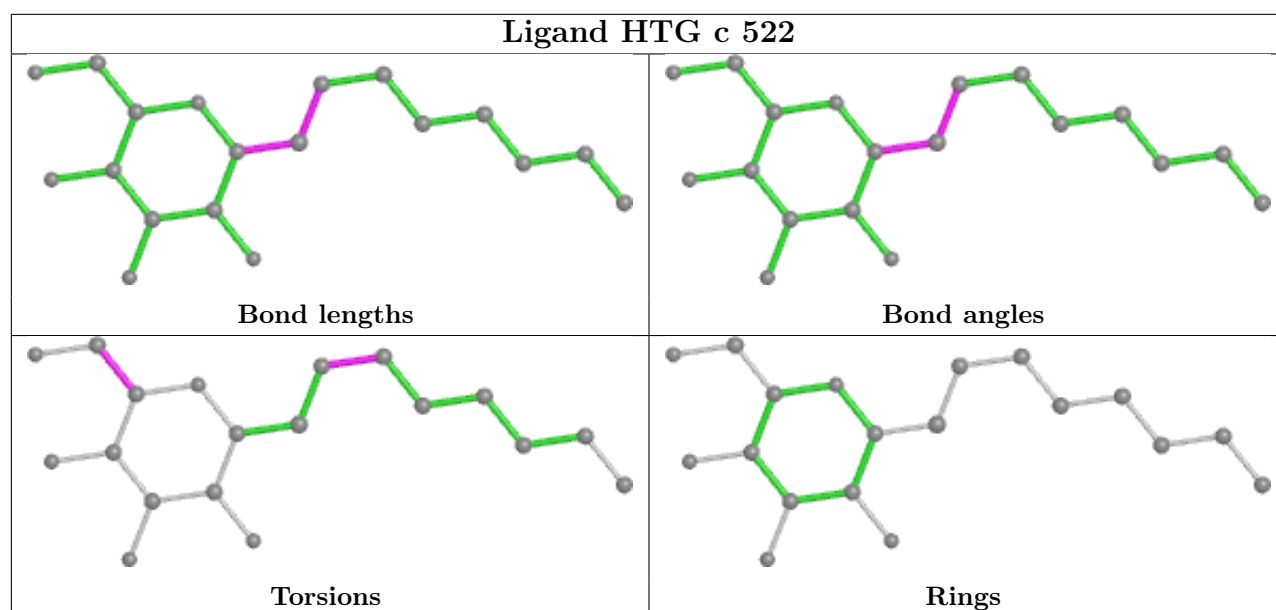


## Ligand CLA c 512

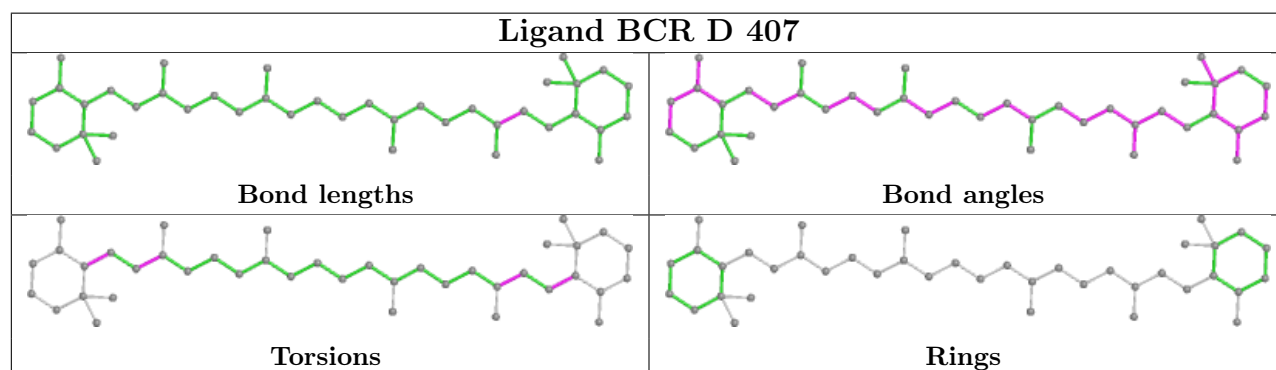
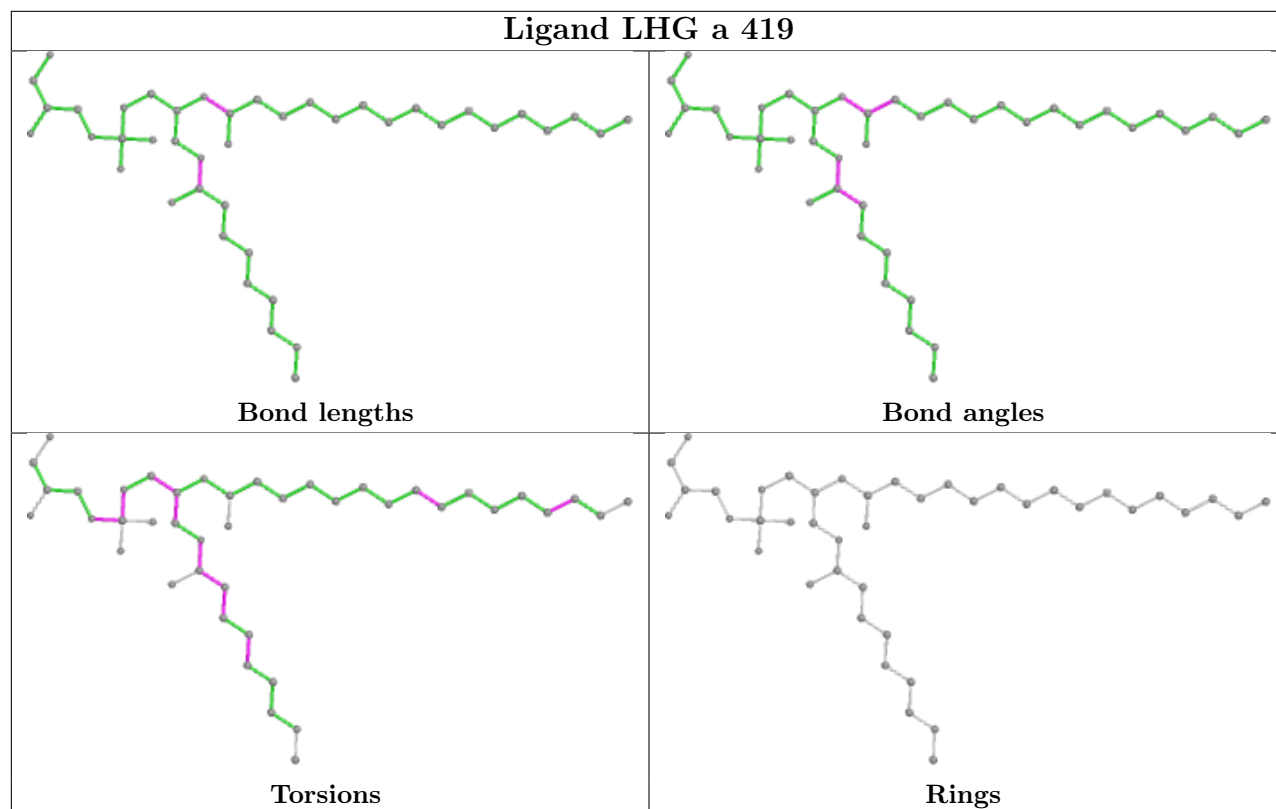
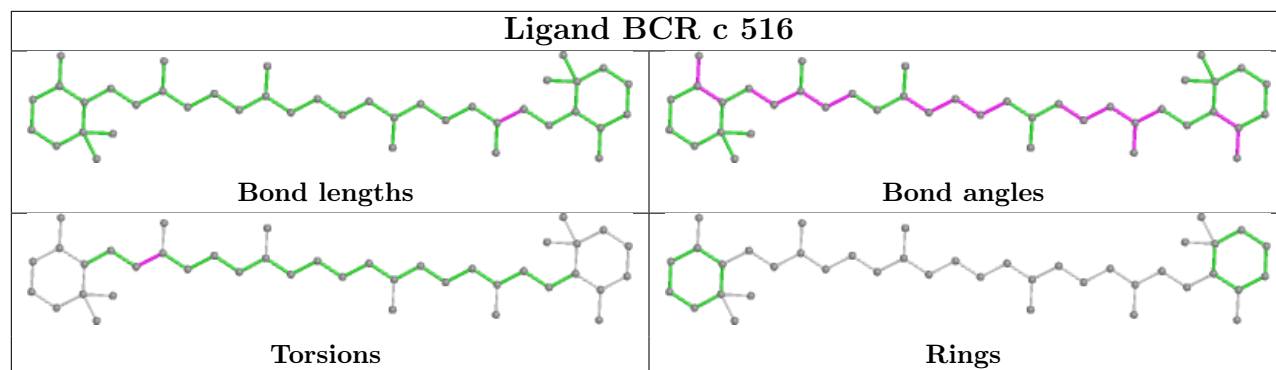


## Ligand CLA c 506

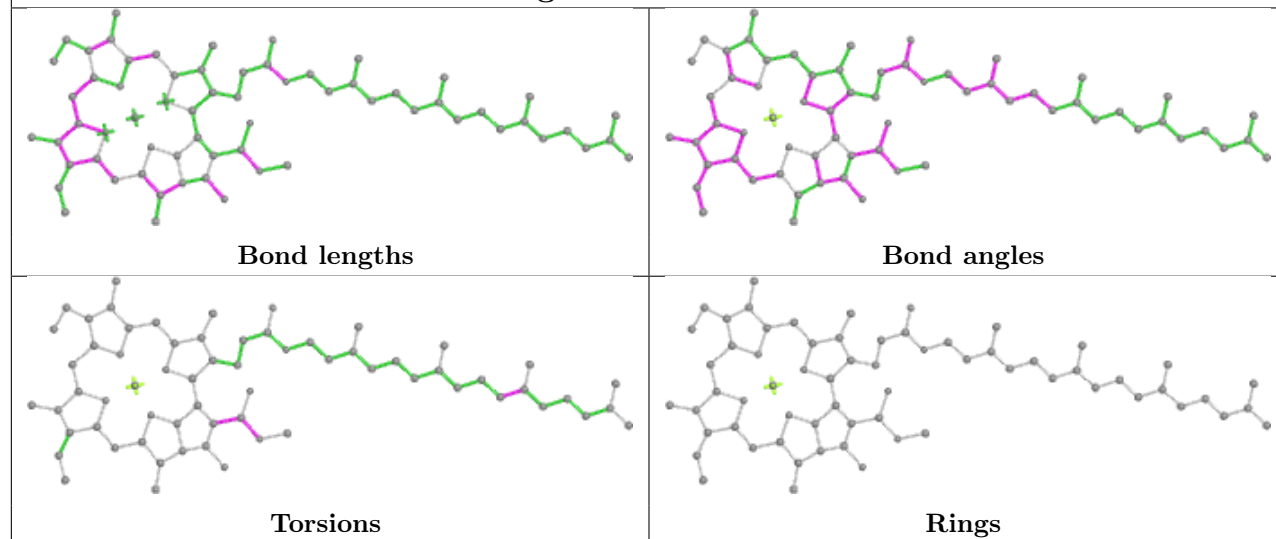




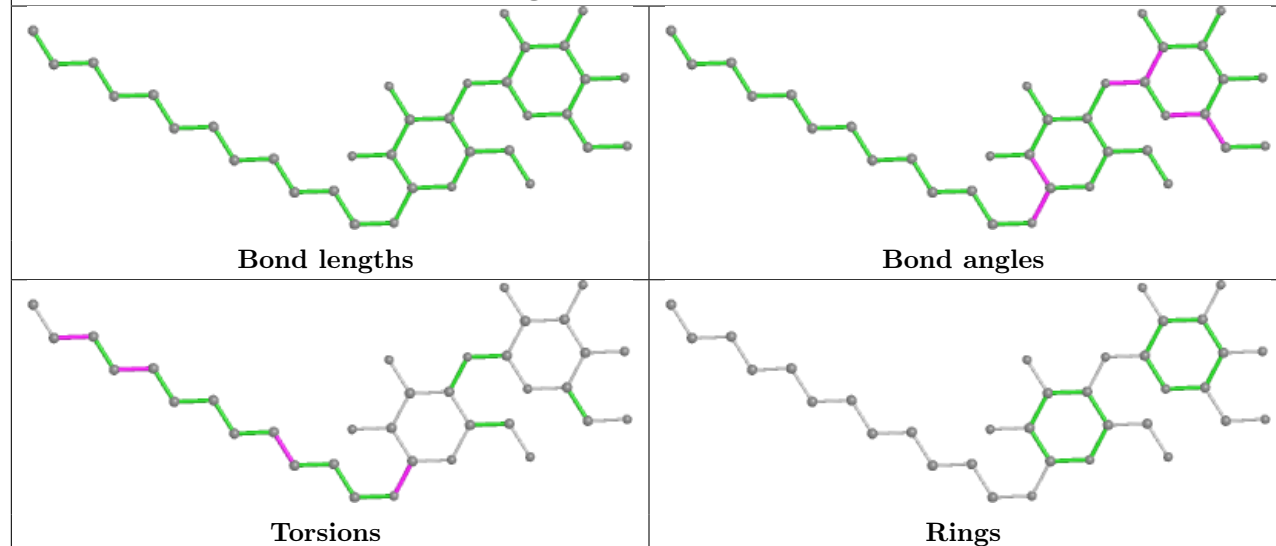




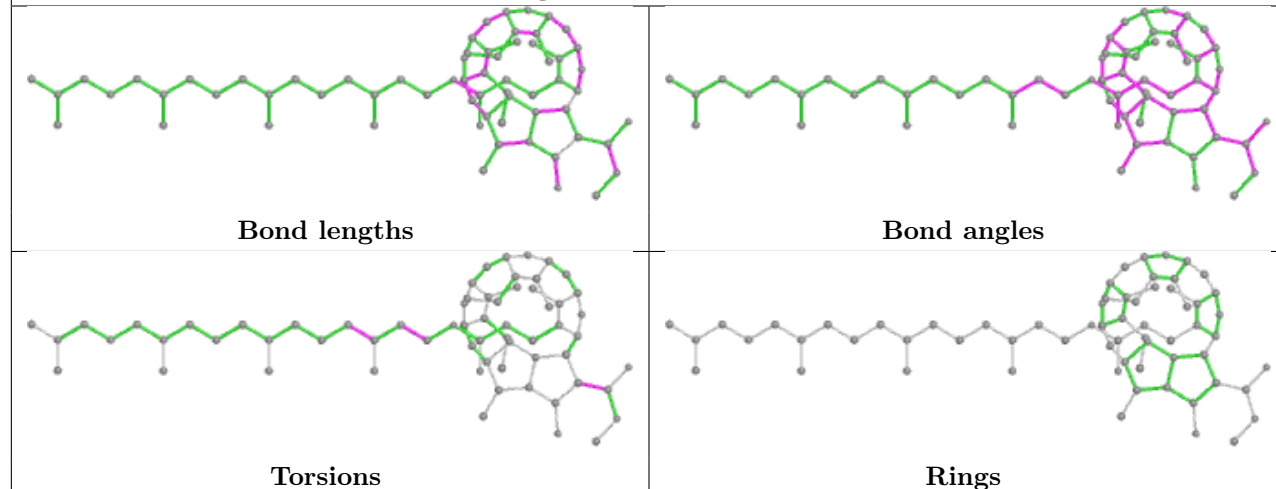
## Ligand CLA c 502

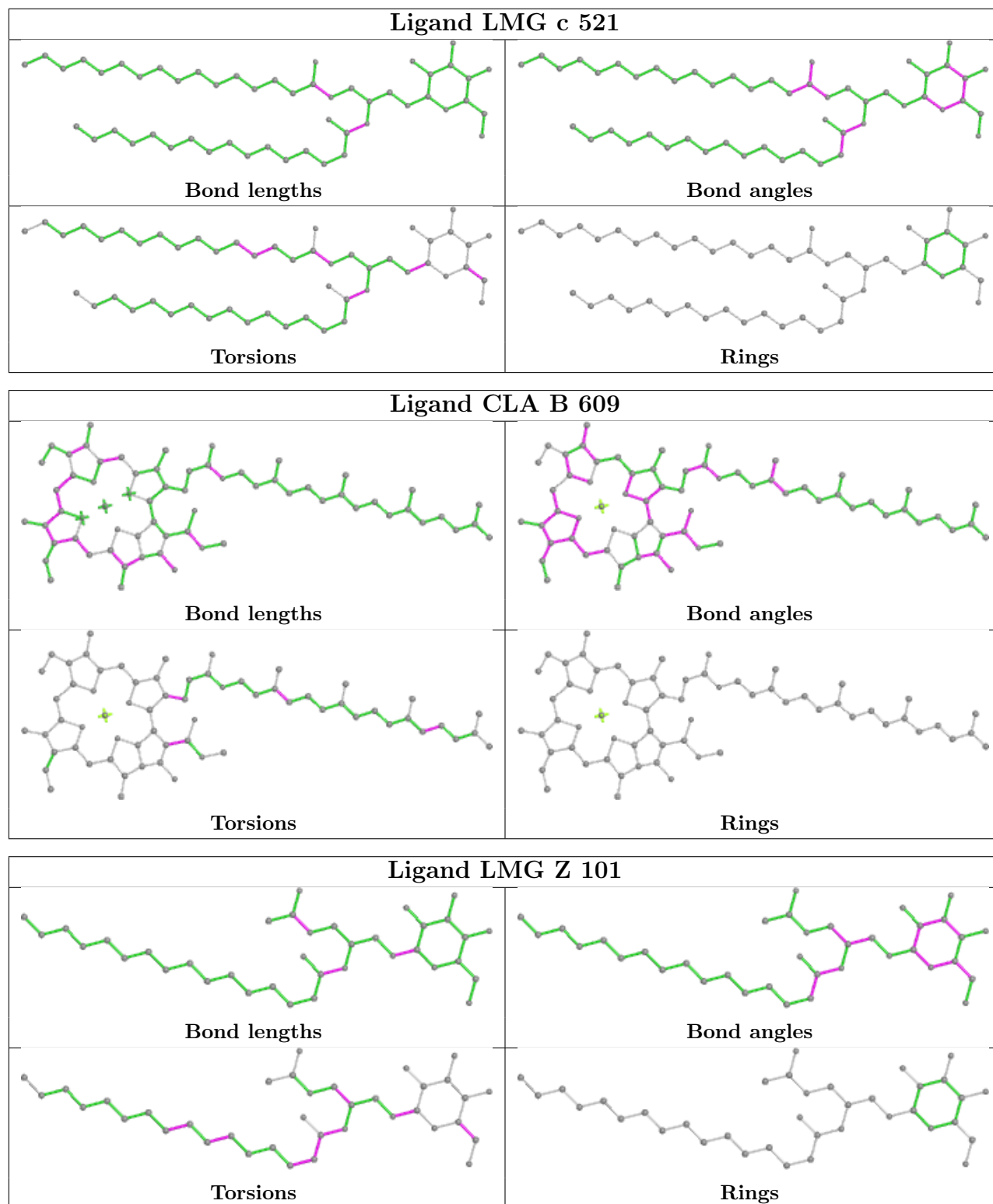


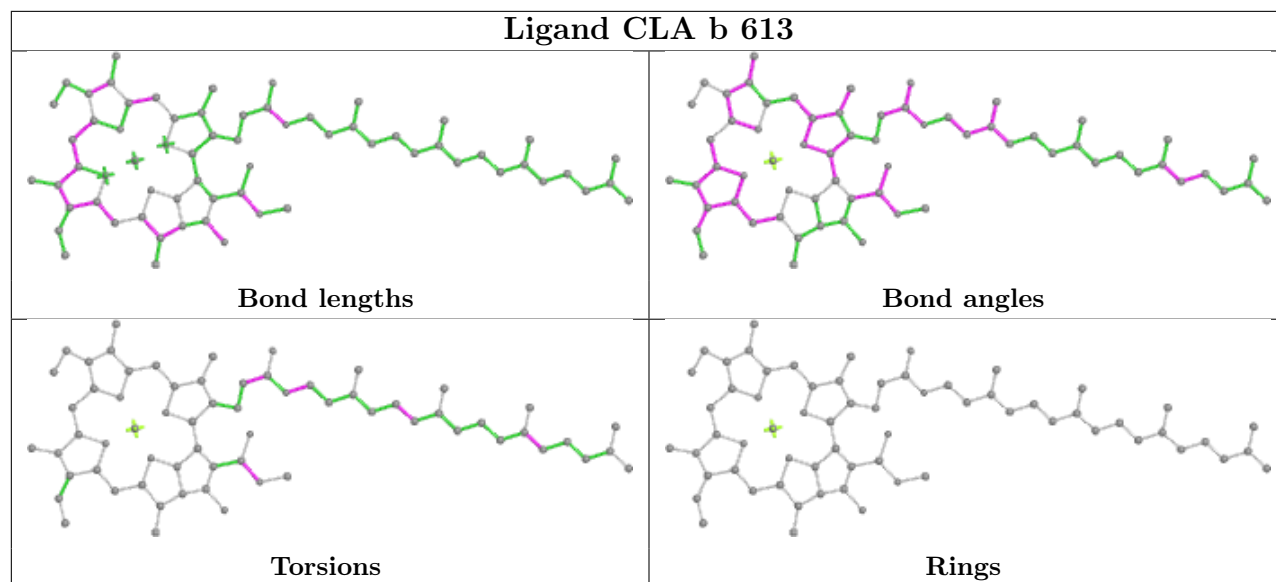
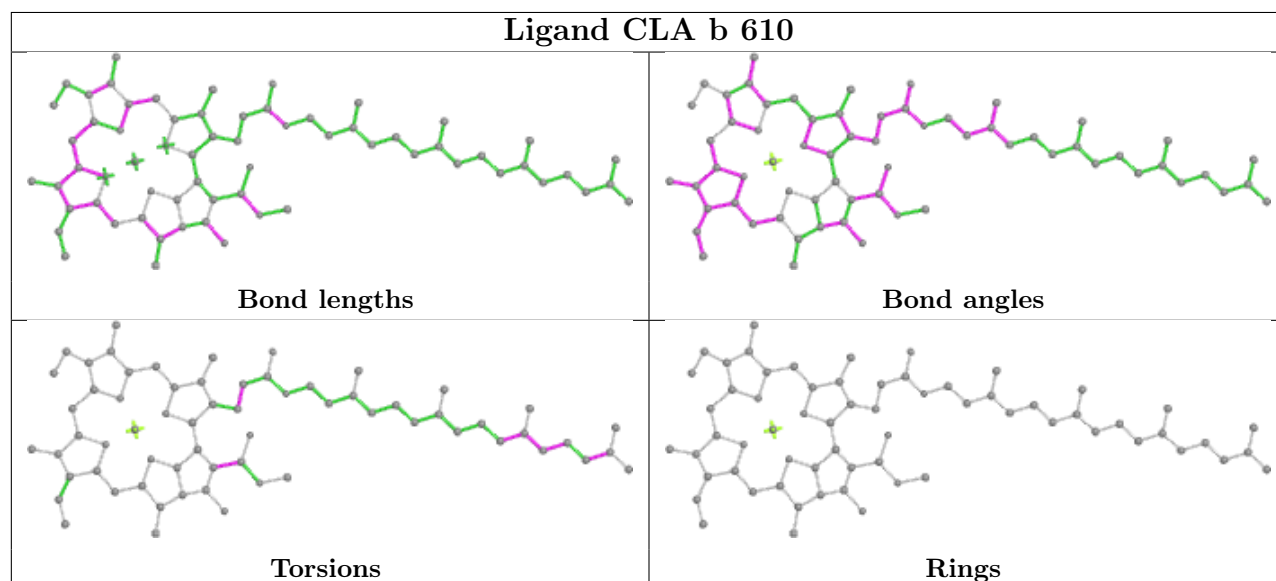
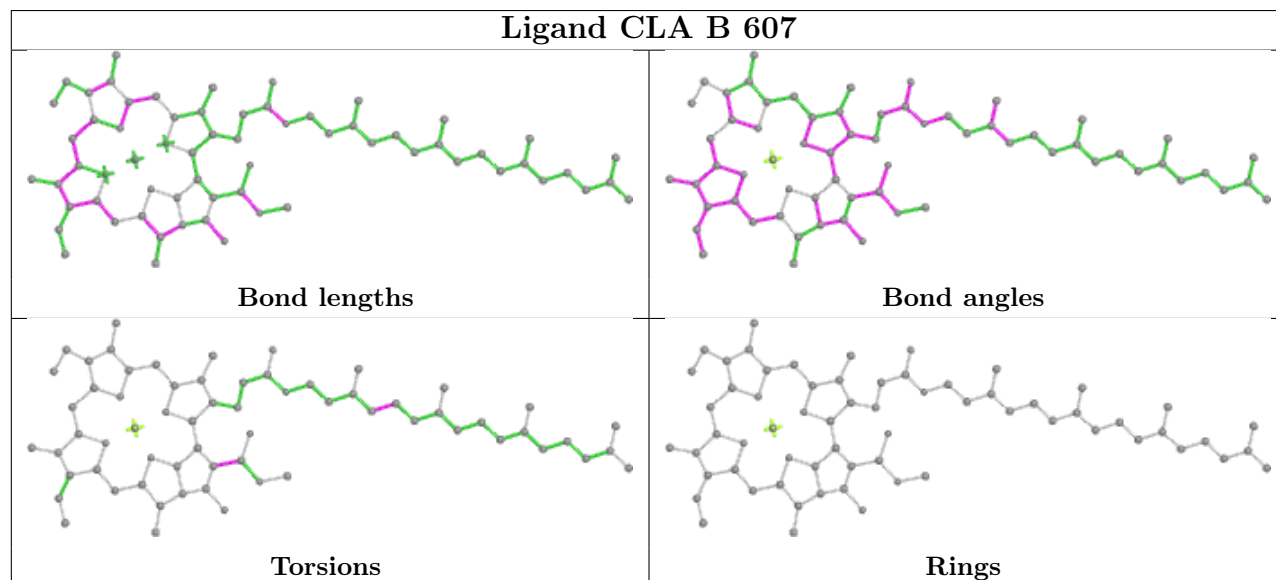
## Ligand LMT M 102

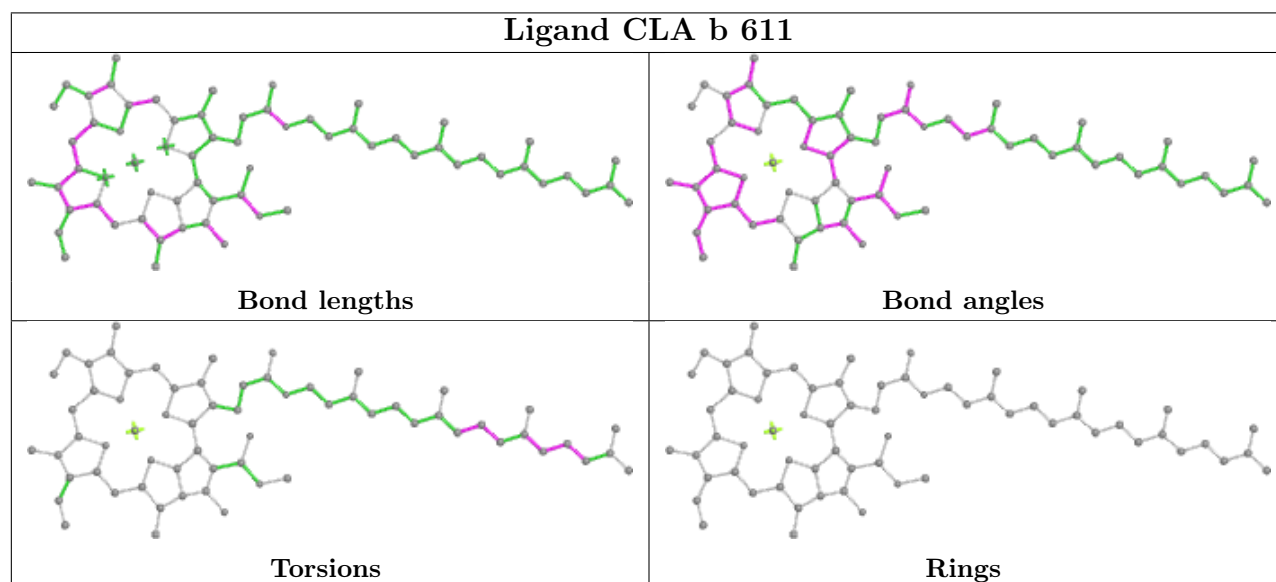
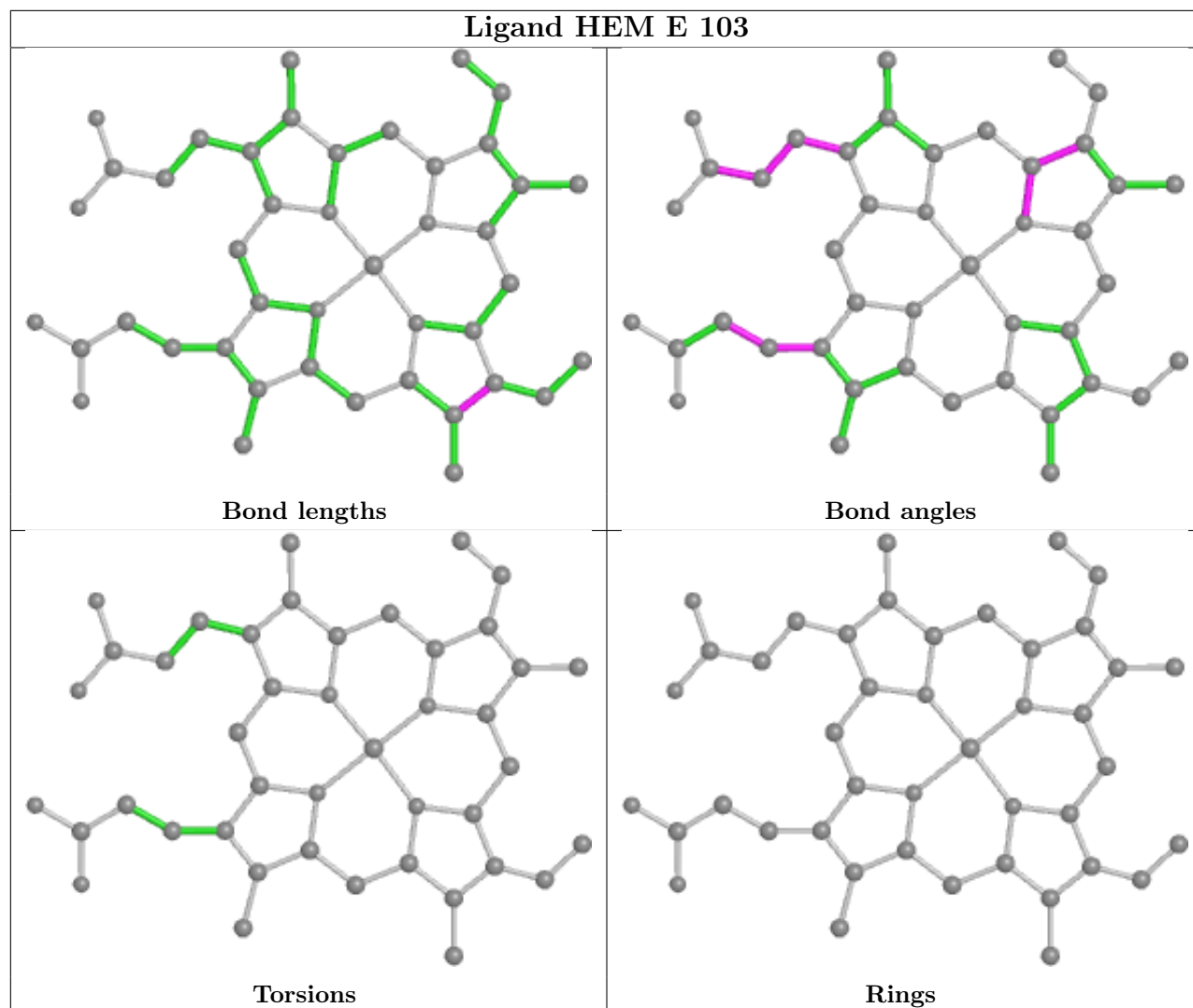


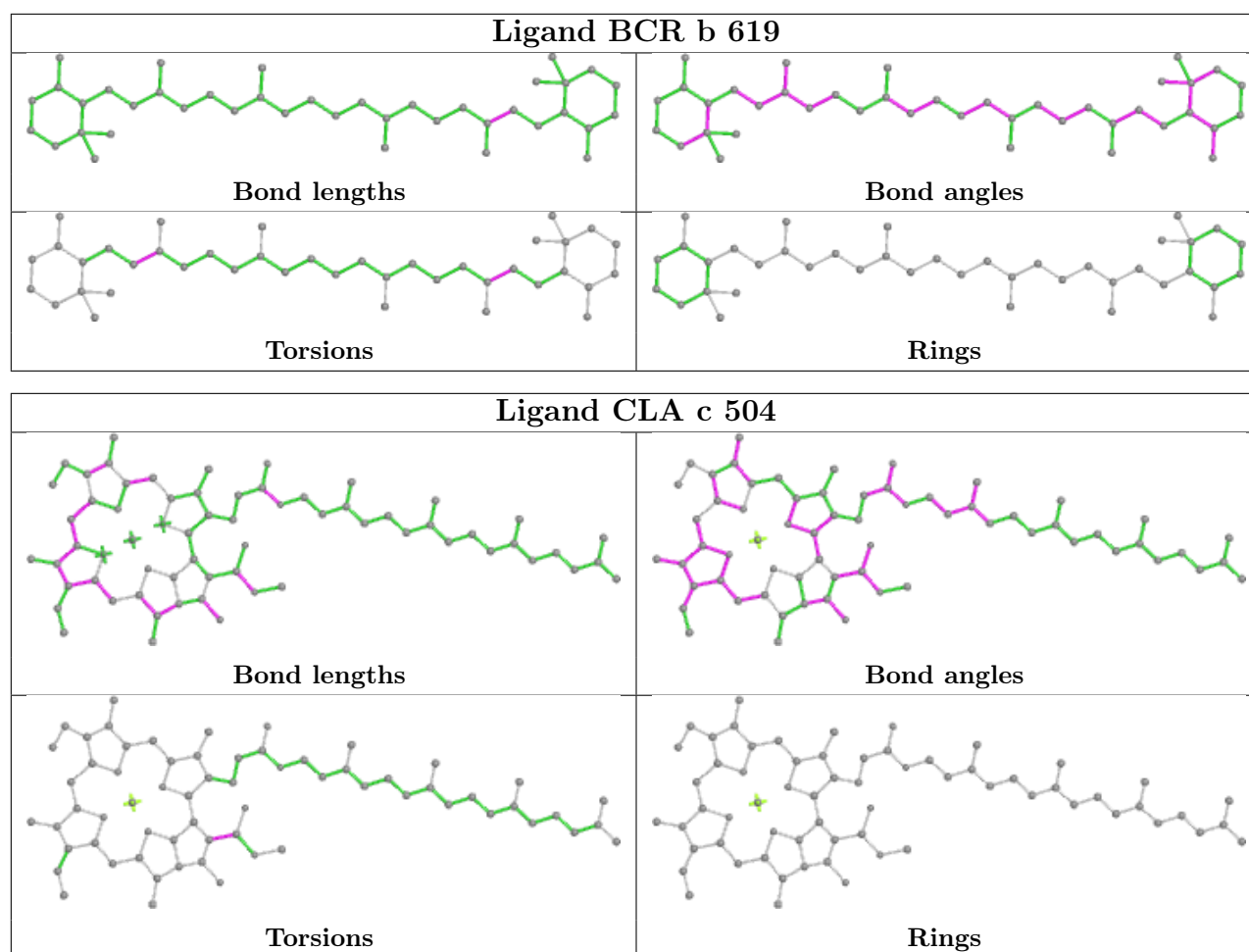
## Ligand PHO a 406





**Ligand CLA b 613****Ligand CLA b 610****Ligand CLA B 607**





## 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%)	0.29	22 (6%) 18 26	39, 48, 72, 137	0
1	a	334/344 (97%)	0.33	28 (8%) 11 16	41, 52, 80, 120	0
2	B	504/505 (99%)	-0.03	32 (6%) 20 29	41, 53, 84, 142	0
2	b	504/505 (99%)	0.20	60 (11%) 4 7	42, 56, 94, 158	0
3	C	451/455 (99%)	0.11	35 (7%) 13 19	44, 61, 87, 159	0
3	c	455/455 (100%)	0.29	47 (10%) 6 10	50, 68, 90, 125	0
4	D	342/342 (100%)	0.16	21 (6%) 21 31	39, 49, 71, 145	0
4	d	341/342 (99%)	0.18	29 (8%) 10 16	41, 54, 76, 139	0
5	E	81/84 (96%)	0.68	17 (20%) 1 1	55, 73, 102, 146	0
5	e	79/84 (94%)	0.61	16 (20%) 1 1	63, 77, 119, 148	0
6	F	34/44 (77%)	-0.15	2 (5%) 22 33	55, 66, 90, 118	0
6	f	31/44 (70%)	0.18	3 (9%) 7 12	62, 71, 101, 153	0
7	H	64/65 (98%)	-0.30	1 (1%) 72 80	49, 64, 82, 136	0
7	h	64/65 (98%)	0.37	6 (9%) 8 13	56, 68, 92, 108	0
8	I	37/38 (97%)	-0.05	2 (5%) 25 37	52, 64, 128, 151	0
8	i	37/38 (97%)	-0.18	2 (5%) 25 37	56, 64, 127, 156	0
9	J	38/39 (97%)	0.70	9 (23%) 0 1	52, 74, 136, 177	0
9	j	39/39 (100%)	0.40	5 (12%) 3 6	61, 79, 134, 165	0
10	K	37/37 (100%)	-0.43	0 100 100	61, 73, 94, 116	0
10	k	37/37 (100%)	0.22	4 (10%) 5 9	70, 77, 99, 117	0
11	L	36/37 (97%)	0.09	2 (5%) 24 35	39, 44, 100, 144	0
11	l	36/37 (97%)	0.26	1 (2%) 53 64	42, 45, 103, 123	0
12	M	32/36 (88%)	-0.01	1 (3%) 49 61	42, 47, 74, 151	0
12	m	33/36 (91%)	-0.02	2 (6%) 21 31	42, 48, 83, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.30	31 (12%) 3 6	40, 62, 117, 181	0
13	o	243/244 (99%)	0.74	56 (23%) 0 1	43, 65, 125, 174	0
14	T	29/32 (90%)	-0.12	1 (3%) 45 57	40, 45, 85, 116	0
14	t	29/32 (90%)	-0.05	2 (6%) 16 24	41, 48, 76, 139	0
15	U	96/104 (92%)	-0.17	3 (3%) 49 61	48, 59, 90, 98	0
15	u	97/104 (93%)	-0.35	0 100 100	52, 65, 85, 127	0
16	V	137/137 (100%)	-0.20	1 (0%) 87 92	45, 59, 86, 117	0
16	v	137/137 (100%)	0.38	15 (10%) 5 9	53, 74, 106, 131	0
17	X	38/40 (95%)	0.27	5 (13%) 3 5	62, 75, 100, 117	0
17	x	38/40 (95%)	0.80	8 (21%) 1 1	64, 80, 116, 164	0
18	Y	29/30 (96%)	2.20	14 (48%) 0 0	73, 92, 147, 178	0
18	y	29/30 (96%)	0.70	5 (17%) 1 2	80, 94, 124, 126	0
19	Z	62/62 (100%)	1.15	20 (32%) 0 0	75, 90, 136, 185	0
19	z	62/62 (100%)	2.03	29 (46%) 0 0	82, 101, 140, 175	0
20	R	34/34 (100%)	5.81	34 (100%) 0 0	91, 113, 146, 149	0
All	All	5283/5384 (98%)	0.28	571 (10%) 5 9	39, 59, 103, 185	0

The worst 5 of 571 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Y	19	ILE	11.8
20	R	6	LEU	11.3
1	A	11	ALA	8.4
20	R	18	TRP	8.2
17	x	38	GLN	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	FME	i	1	10/11	0.97	0.10	54,67,72,79	0
12	FME	M	1	10/11	0.98	0.12	38,58,80,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	FME	T	1	10/11	0.98	0.09	44,46,68,71	0
8	FME	I	1	10/11	0.98	0.13	56,66,73,76	0
12	FME	m	1	10/11	0.98	0.08	40,57,77,93	0
14	FME	t	1	10/11	0.98	0.08	39,46,70,75	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
31	LMG	C	521	51/55	0.44	0.48	77,131,166,170	0
33	HTG	b	622	19/19	0.47	0.57	90,147,155,155	0
34	LMT	E	102	35/35	0.49	0.39	117,161,175,176	0
30	UNL	j	101	10/-	0.50	0.43	86,94,101,102	0
30	UNL	A	414	28/-	0.51	0.43	93,105,126,127	0
34	LMT	C	525	35/35	0.56	0.55	97,149,164,168	0
34	LMT	a	412	35/35	0.56	0.45	70,139,150,152	0
34	LMT	D	403	35/35	0.57	0.40	70,135,146,152	0
34	LMT	e	101	35/35	0.59	0.60	114,176,180,181	0
34	LMT	m	103	35/35	0.61	0.43	68,104,116,119	0
29	PL9	A	413	55/55	0.62	0.39	80,108,117,118	0
30	UNL	J	101	10/-	0.63	0.31	76,91,99,100	0
33	HTG	D	413	16/19	0.64	0.33	91,119,132,136	0
31	LMG	c	521	51/55	0.64	0.39	78,133,158,163	0
34	LMT	M	102	35/35	0.65	0.29	58,107,138,142	0
34	LMT	M	104	35/35	0.66	0.29	80,152,175,176	0
30	UNL	I	101	40/-	0.69	0.28	73,109,155,156	0
32	LHG	a	419	42/49	0.69	0.38	98,142,173,177	0
30	UNL	i	101	40/-	0.69	0.31	75,103,153,163	0
32	LHG	E	101	42/49	0.70	0.27	80,126,141,143	0
31	LMG	Z	101	37/55	0.70	0.30	79,133,167,170	0
30	UNL	C	526	34/-	0.70	0.32	90,120,133,134	0
36	CA	F	101	1/1	0.70	0.05	129,129,129,129	0
30	UNL	b	625	33/-	0.71	0.39	67,101,152,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	a	415	30/-	0.73	0.28	102,114,136,145	0
34	LMT	D	404	35/35	0.74	0.30	73,118,133,134	0
34	LMT	a	418	35/35	0.74	0.51	119,152,162,163	0
26	GOL	B	626	6/6	0.74	0.25	91,105,106,108	0
26	GOL	B	627	6/6	0.74	0.33	109,114,117,119	0
26	GOL	O	302	6/6	0.74	0.26	84,85,88,89	0
30	UNL	c	525	32/-	0.75	0.39	90,115,132,135	0
33	HTG	B	621	19/19	0.76	0.26	65,82,115,116	0
33	HTG	B	622	19/19	0.76	0.41	76,96,106,106	0
27	SQD	f	102	43/54	0.76	0.47	119,138,168,171	0
30	UNL	d	411	36/-	0.77	0.26	75,100,133,136	0
30	UNL	m	102	10/-	0.77	0.26	65,72,99,100	0
34	LMT	b	620	25/35	0.78	0.22	92,128,152,154	0
34	LMT	b	626	25/35	0.78	0.25	52,77,134,137	0
29	PL9	a	414	55/55	0.78	0.31	90,117,133,138	0
30	UNL	B	625	33/-	0.78	0.23	59,113,154,157	0
33	HTG	b	621	19/19	0.78	0.24	68,82,114,118	0
31	LMG	z	101	39/55	0.79	0.31	86,136,147,149	0
27	SQD	L	102	54/54	0.80	0.22	64,92,116,121	0
31	LMG	a	417	51/55	0.80	0.23	62,96,110,122	0
33	HTG	h	101	16/19	0.81	0.30	99,136,147,148	0
30	UNL	M	103	10/-	0.82	0.27	66,78,91,94	0
34	LMT	B	628	25/35	0.82	0.22	54,82,139,141	0
34	LMT	t	101	26/35	0.82	0.21	80,119,138,141	0
33	HTG	c	522	19/19	0.82	0.31	118,141,149,151	0
30	UNL	D	412	40/-	0.83	0.24	61,93,130,131	0
27	SQD	A	411	54/54	0.83	0.17	67,87,125,127	0
25	BCR	h	102	40/40	0.84	0.18	56,67,80,84	0
26	GOL	b	623	6/6	0.84	0.21	89,99,105,112	0
31	LMG	C	520	51/55	0.85	0.23	61,92,114,119	0
26	GOL	c	526	6/6	0.85	0.53	117,120,128,129	0
25	BCR	H	101	40/40	0.85	0.18	50,69,79,81	0
31	LMG	m	101	51/55	0.86	0.23	52,72,99,103	0
27	SQD	B	620	54/54	0.86	0.18	62,94,126,130	0
33	HTG	V	202	11/19	0.87	0.47	117,124,127,128	0
30	UNL	x	101	18/-	0.87	0.19	71,80,124,127	0
31	LMG	M	101	51/55	0.87	0.20	53,72,94,115	0
33	HTG	C	522	19/19	0.87	0.29	114,127,137,138	0
23	CLA	C	514	65/65	0.87	0.21	69,80,114,116	0
36	CA	O	301	1/1	0.87	0.16	116,116,116,116	0
26	GOL	A	410	6/6	0.88	0.19	71,74,79,88	0
27	SQD	a	411	54/54	0.88	0.15	69,96,137,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	LMG	A	415	51/55	0.88	0.20	63,90,109,114	0
35	DGD	C	518	62/66	0.88	0.20	51,67,124,134	0
35	DGD	h	103	62/66	0.88	0.25	52,65,73,75	0
26	GOL	v	202	6/6	0.88	0.24	62,91,95,95	0
31	LMG	c	520	51/55	0.88	0.25	69,96,133,136	0
32	LHG	A	416	49/49	0.89	0.23	44,63,85,88	0
35	DGD	C	519	62/66	0.90	0.19	47,62,104,119	0
35	DGD	H	102	62/66	0.90	0.23	45,60,78,83	0
23	CLA	C	513	65/65	0.90	0.17	63,73,122,125	0
30	UNL	D	411	17/-	0.90	0.30	64,81,117,117	0
30	UNL	X	101	18/-	0.90	0.14	63,76,94,95	0
23	CLA	B	602	65/65	0.91	0.15	46,55,75,83	0
23	CLA	C	505	65/65	0.91	0.17	49,57,95,109	0
26	GOL	b	627	6/6	0.91	0.24	99,99,102,103	0
29	PL9	d	406	55/55	0.91	0.20	40,48,59,67	0
27	SQD	C	501	54/54	0.91	0.20	58,86,115,118	0
26	GOL	c	501	6/6	0.91	0.28	62,73,78,81	0
25	BCR	k	101	40/40	0.91	0.15	65,77,87,88	0
23	CLA	c	513	65/65	0.92	0.16	70,88,122,129	0
23	CLA	c	514	65/65	0.92	0.27	71,91,124,127	0
31	LMG	D	414	51/55	0.92	0.19	51,74,116,126	0
32	LHG	b	628	49/49	0.92	0.18	43,59,69,83	0
27	SQD	D	415	43/54	0.92	0.22	76,114,135,142	0
23	CLA	B	609	65/65	0.92	0.13	50,59,74,85	0
23	CLA	C	507	65/65	0.92	0.14	58,72,128,137	0
23	CLA	b	602	65/65	0.92	0.20	49,59,75,86	0
35	DGD	c	518	62/66	0.92	0.21	56,76,120,133	0
35	DGD	c	519	62/66	0.92	0.18	55,64,105,112	0
25	BCR	k	102	40/40	0.92	0.12	64,75,91,97	0
23	CLA	c	503	65/65	0.92	0.28	55,62,77,89	0
23	CLA	c	504	65/65	0.92	0.23	58,69,78,82	0
36	CA	c	524	1/1	0.92	0.04	90,90,90,90	0
23	CLA	c	508	65/65	0.93	0.15	58,70,81,90	0
23	CLA	C	508	65/65	0.93	0.13	55,64,78,87	0
26	GOL	a	410	6/6	0.93	0.24	66,73,88,94	0
23	CLA	b	609	65/65	0.93	0.14	53,62,76,93	0
23	CLA	d	404	65/65	0.93	0.14	54,64,120,126	0
23	CLA	c	505	65/65	0.93	0.28	56,65,106,116	0
33	HTG	b	624	19/19	0.93	0.12	68,80,100,107	0
30	UNL	d	410	17/-	0.93	0.18	69,82,99,100	0
33	HTG	B	624	19/19	0.94	0.10	68,83,91,99	0
23	CLA	b	612	65/65	0.94	0.19	44,52,64,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	616	65/65	0.94	0.17	47,61,122,124	0
31	LMG	d	412	51/55	0.94	0.13	57,72,117,133	0
23	CLA	b	601	65/65	0.94	0.20	65,83,126,136	0
23	CLA	B	614	65/65	0.94	0.15	38,48,100,107	0
25	BCR	C	515	40/40	0.94	0.14	67,80,90,93	0
35	DGD	C	517	62/66	0.94	0.24	48,58,103,108	0
23	CLA	D	406	65/65	0.94	0.17	50,59,132,135	0
32	LHG	L	101	49/49	0.94	0.16	42,56,69,95	0
25	BCR	Y	101	40/40	0.94	0.11	61,70,82,89	0
25	BCR	c	515	40/40	0.94	0.15	75,86,94,95	0
32	LHG	d	407	49/49	0.94	0.27	48,66,80,86	0
32	LHG	d	408	49/49	0.94	0.15	43,54,73,84	0
32	LHG	d	409	49/49	0.94	0.22	60,69,125,134	0
25	BCR	d	405	40/40	0.94	0.13	58,69,91,104	0
27	SQD	a	409	54/54	0.94	0.20	71,87,124,125	0
36	CA	v	201	1/1	0.94	0.28	117,117,117,117	0
39	MG	J	102	1/1	0.94	0.11	61,61,61,61	0
32	LHG	D	409	49/49	0.95	0.15	44,53,73,86	0
32	LHG	D	410	49/49	0.95	0.18	50,64,123,134	0
25	BCR	T	101	40/40	0.95	0.14	43,54,64,64	0
23	CLA	b	614	65/65	0.95	0.15	40,48,112,114	0
25	BCR	b	618	40/40	0.95	0.22	39,55,72,77	0
23	CLA	C	502	65/65	0.95	0.14	53,60,73,81	0
23	CLA	c	502	65/65	0.95	0.13	57,66,80,84	0
23	CLA	C	504	65/65	0.95	0.14	55,63,74,79	0
23	CLA	B	601	65/65	0.95	0.24	57,78,119,129	0
23	CLA	B	611	65/65	0.95	0.17	40,45,64,75	0
29	PL9	D	408	55/55	0.95	0.18	39,49,61,70	0
23	CLA	c	506	65/65	0.95	0.14	50,62,85,89	0
26	GOL	B	623	6/6	0.95	0.14	73,86,93,97	0
23	CLA	B	603	65/65	0.95	0.14	44,52,68,73	0
23	CLA	c	509	65/65	0.95	0.25	53,63,127,129	0
35	DGD	c	517	62/66	0.95	0.21	51,65,96,104	0
23	CLA	c	512	65/65	0.95	0.13	60,72,86,94	0
23	CLA	b	604	65/65	0.95	0.24	40,48,108,117	0
23	CLA	b	607	65/65	0.95	0.18	38,45,78,87	0
23	CLA	C	511	65/65	0.95	0.22	53,62,85,92	0
23	CLA	b	610	65/65	0.95	0.16	50,56,70,78	0
25	BCR	C	516	40/40	0.95	0.14	54,64,79,83	0
36	CA	o	301	1/1	0.95	0.13	104,104,104,104	0
23	CLA	C	512	65/65	0.95	0.13	58,68,84,91	0
25	BCR	K	101	40/40	0.95	0.14	63,74,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
39	MG	j	102	1/1	0.95	0.07	68,68,68,68	0
23	CLA	b	606	65/65	0.96	0.12	46,55,120,127	0
23	CLA	A	408	65/65	0.96	0.12	44,51,115,124	0
23	CLA	c	510	65/65	0.96	0.19	60,66,87,92	0
25	BCR	t	102	40/40	0.96	0.15	42,59,74,75	0
23	CLA	c	511	65/65	0.96	0.32	58,66,75,79	0
23	CLA	C	503	65/65	0.96	0.18	50,59,82,93	0
23	CLA	B	610	65/65	0.96	0.15	47,53,67,83	0
23	CLA	b	611	65/65	0.96	0.22	43,50,70,82	0
26	GOL	C	523	6/6	0.96	0.15	60,63,69,69	0
23	CLA	B	606	65/65	0.96	0.12	44,53,102,110	0
24	PHO	A	407	64/64	0.96	0.15	38,43,53,62	0
24	PHO	D	402	64/64	0.96	0.26	41,51,56,57	0
25	BCR	A	409	40/40	0.96	0.12	40,50,59,61	0
25	BCR	B	618	40/40	0.96	0.16	43,54,71,76	0
25	BCR	B	619	40/40	0.96	0.10	48,59,76,80	0
23	CLA	B	607	65/65	0.96	0.17	37,46,67,75	0
23	CLA	b	615	65/65	0.96	0.12	47,56,78,82	0
25	BCR	D	407	40/40	0.96	0.17	52,63,101,108	0
23	CLA	a	407	65/65	0.96	0.16	46,55,130,131	0
23	CLA	B	616	65/65	0.96	0.17	47,58,137,141	0
23	CLA	C	509	65/65	0.96	0.19	50,58,123,136	0
23	CLA	b	603	65/65	0.96	0.17	47,54,76,85	0
25	BCR	b	617	40/40	0.96	0.16	41,48,59,64	0
23	CLA	C	510	65/65	0.96	0.13	56,64,85,88	0
25	BCR	b	619	40/40	0.96	0.11	49,59,85,92	0
23	CLA	b	605	65/65	0.96	0.16	42,49,69,75	0
23	CLA	c	507	65/65	0.96	0.12	61,74,127,135	0
23	CLA	b	608	65/65	0.97	0.21	50,57,73,78	0
24	PHO	a	416	64/64	0.97	0.19	45,52,58,65	0
25	BCR	c	516	40/40	0.97	0.10	57,69,76,79	0
23	CLA	C	506	65/65	0.97	0.15	50,57,90,94	0
23	CLA	a	405	65/65	0.97	0.21	45,53,124,126	0
23	CLA	B	613	65/65	0.97	0.22	39,47,87,92	0
23	CLA	A	406	65/65	0.97	0.22	40,48,104,113	0
23	CLA	b	613	65/65	0.97	0.28	40,48,81,86	0
23	CLA	B	615	65/65	0.97	0.12	46,52,78,89	0
23	CLA	B	608	65/65	0.97	0.19	45,53,70,73	0
23	CLA	B	604	65/65	0.97	0.19	38,45,105,110	0
23	CLA	B	605	65/65	0.97	0.12	40,46,61,72	0
23	CLA	d	402	65/65	0.97	0.16	40,46,62,68	0
25	BCR	a	408	40/40	0.97	0.10	42,50,58,61	0

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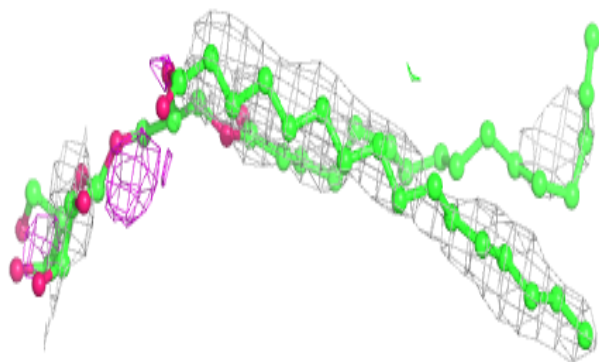
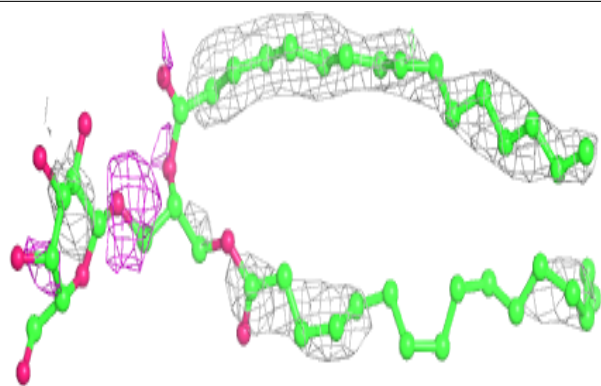
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
38	HEM	f	101	43/43	0.97	0.20	70,83,119,127	0
23	CLA	A	404	65/65	0.97	0.23	39,42,67,72	0
23	CLA	B	612	65/65	0.97	0.16	42,50,61,66	0
40	HEC	v	203	43/43	0.97	0.11	59,65,70,75	0
25	BCR	B	617	40/40	0.98	0.13	40,50,60,62	0
23	CLA	D	405	65/65	0.98	0.26	38,44,62,70	0
23	CLA	A	405	65/65	0.98	0.18	38,44,54,56	0
37	BCT	D	401	4/4	0.98	0.07	59,64,65,66	0
37	BCT	d	401	4/4	0.98	0.09	57,58,64,67	0
38	HEM	E	103	43/43	0.98	0.12	62,71,86,98	0
24	PHO	a	406	64/64	0.98	0.15	40,47,52,55	0
36	CA	C	524	1/1	0.98	0.21	72,72,72,72	0
23	CLA	d	403	65/65	0.98	0.24	42,47,71,80	0
40	HEC	V	201	43/43	0.98	0.09	50,53,58,62	0
23	CLA	a	404	65/65	0.98	0.20	43,46,67,80	0
36	CA	c	523	1/1	0.99	0.10	81,81,81,81	0
21	FE2	A	401	1/1	0.99	0.03	61,61,61,61	0
21	FE2	a	401	1/1	0.99	0.02	61,61,61,61	0
22	CL	A	403	1/1	0.99	0.13	45,45,45,45	0
22	CL	a	403	1/1	0.99	0.13	49,49,49,49	0
28	OEX	A	412	10/10	0.99	0.11	44,49,53,56	0
28	OEX	a	413	10/10	1.00	0.11	45,54,55,56	0
22	CL	A	402	1/1	1.00	0.06	40,40,40,40	0
22	CL	a	402	1/1	1.00	0.10	48,48,48,48	0

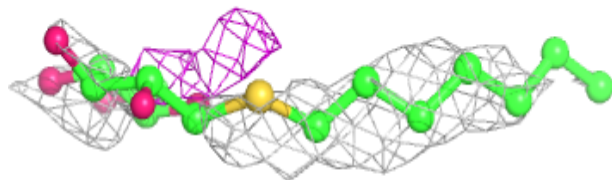
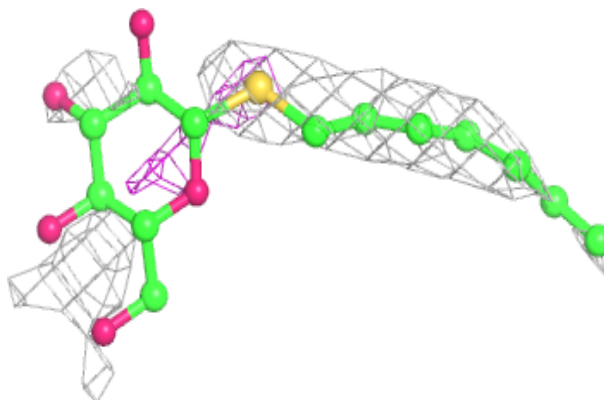
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMG C 521:**

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

**Electron density around HTG b 622:**

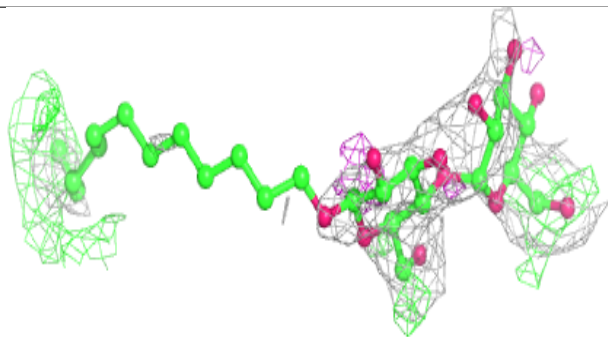
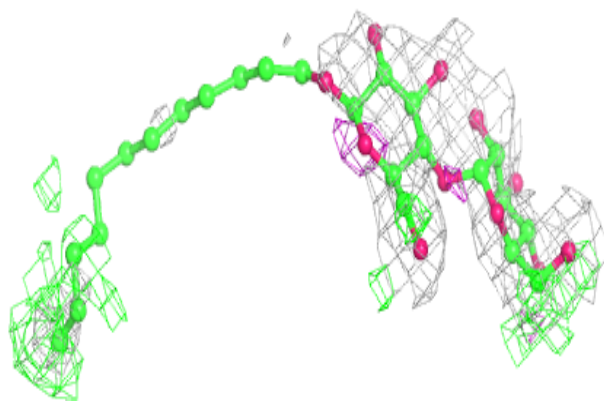
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



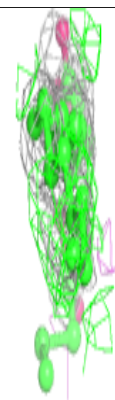
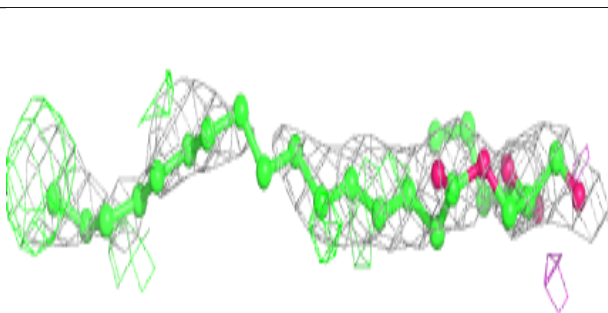
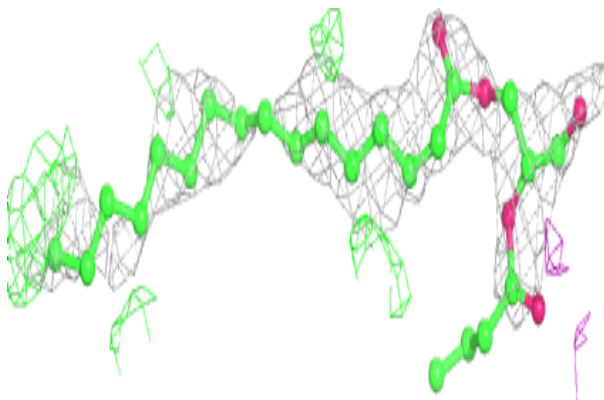


**Electron density around LMT E 102:**

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

**Electron density around UNL A 414:**

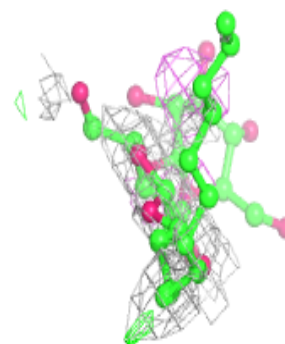
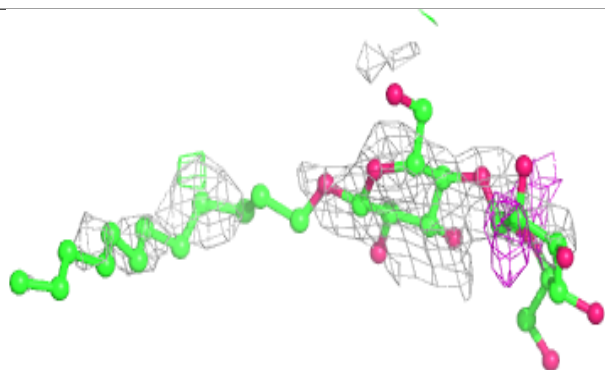
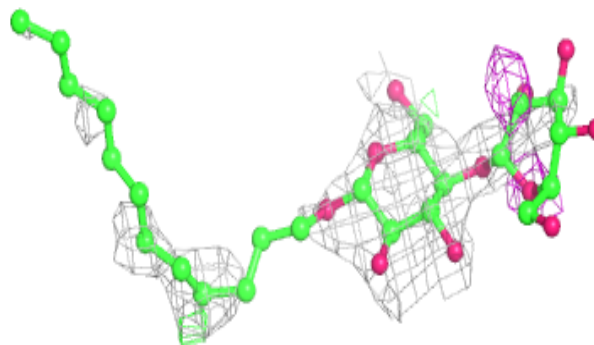
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



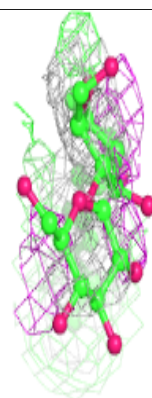
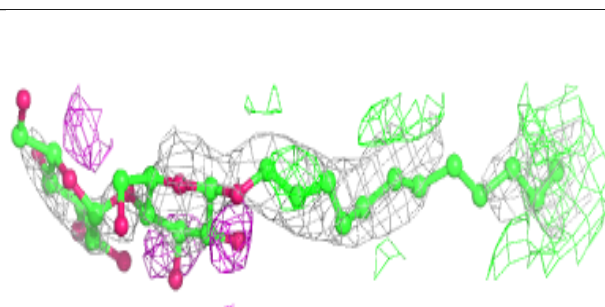
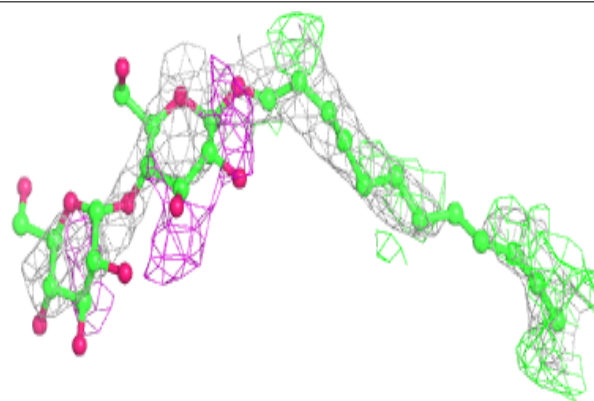


**Electron density around LMT C 525:**

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

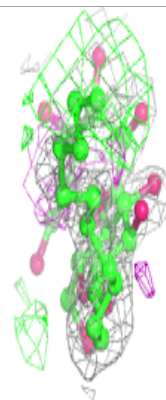
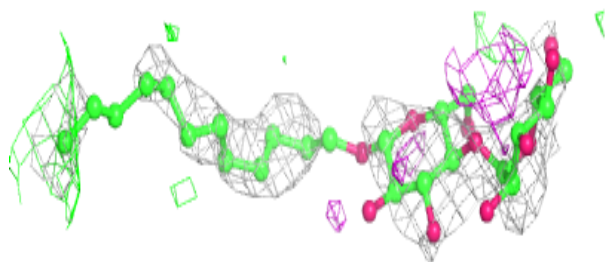
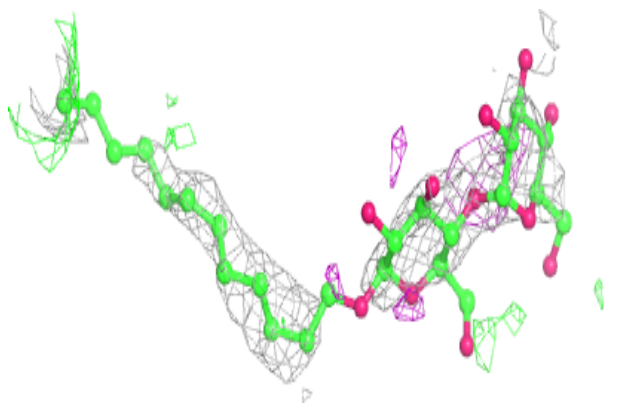
**Electron density around LMT a 412:**

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

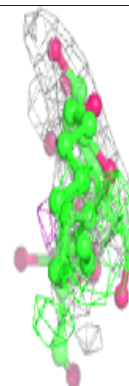
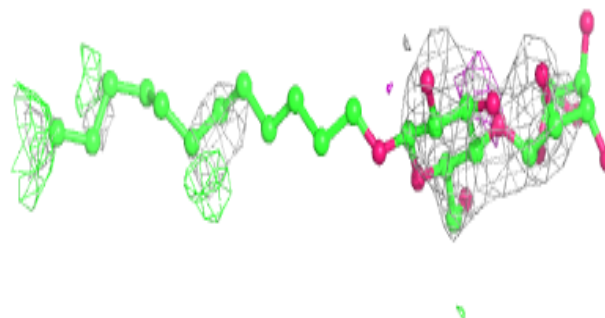
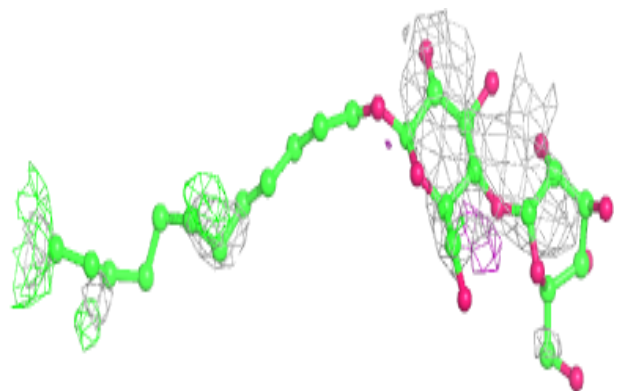


**Electron density around LMT D 403:**

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

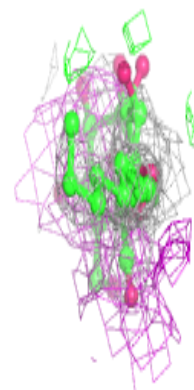
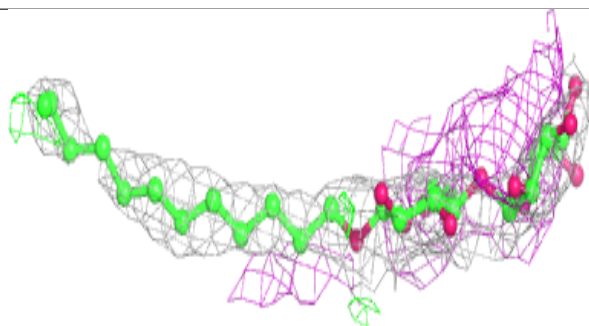
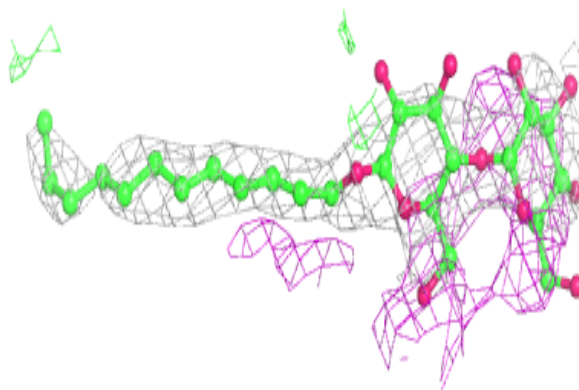
**Electron density around LMT e 101:**

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

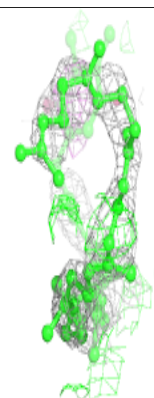
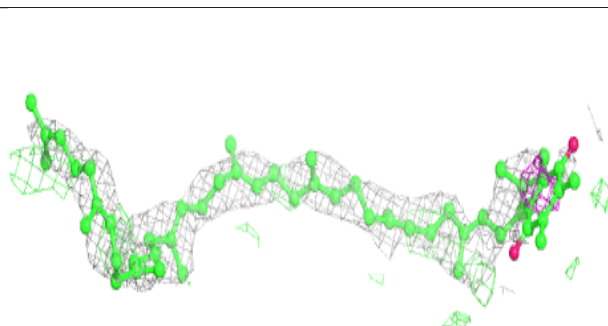
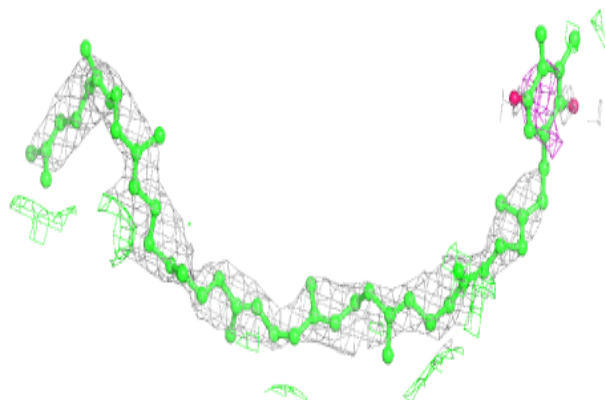


**Electron density around LMT m 103:**

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

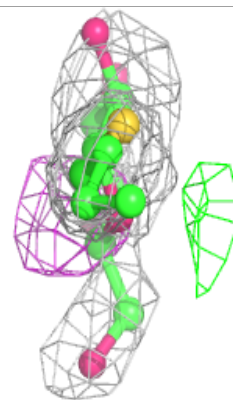
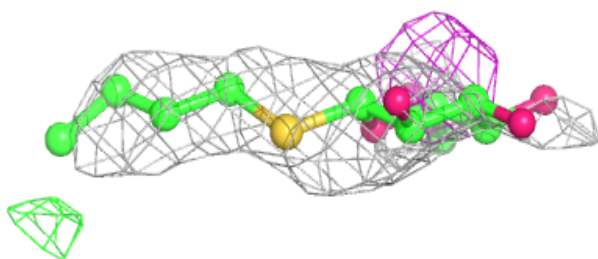
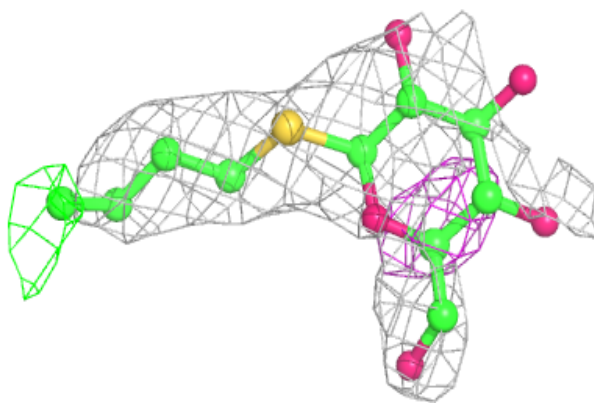
**Electron density around PL9 A 413:**

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

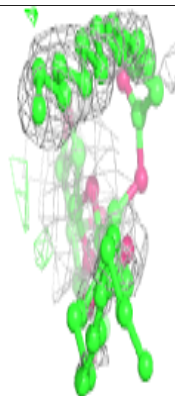
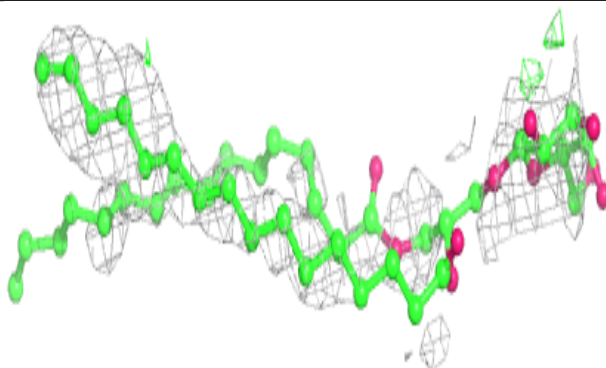
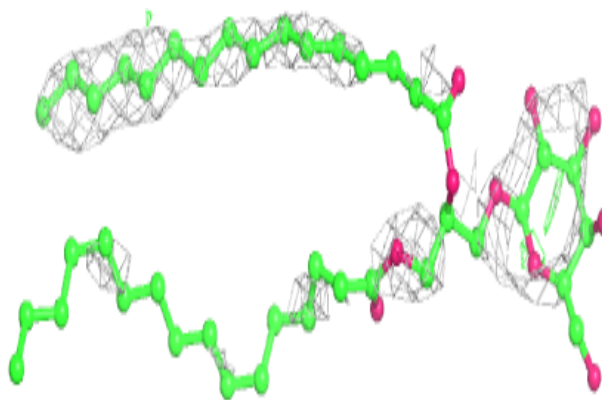


**Electron density around HTG D 413:**

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

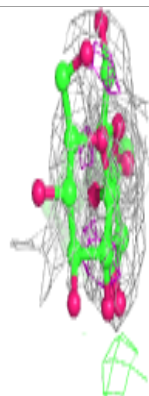
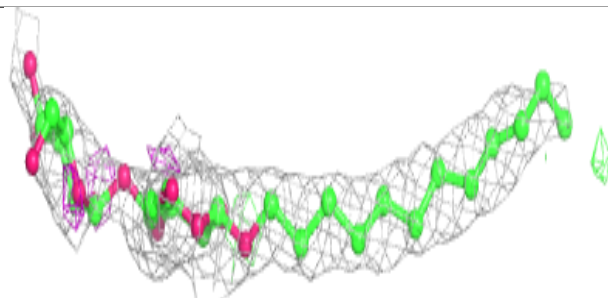
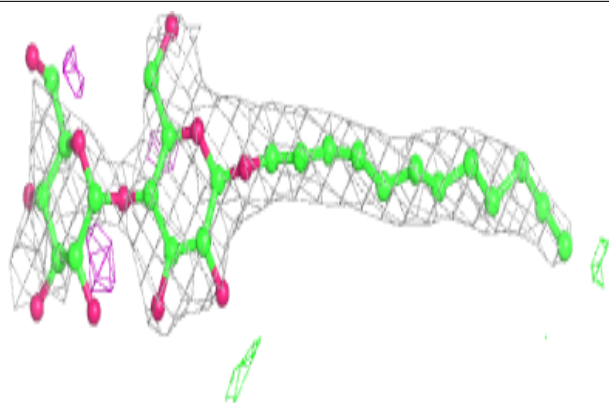
**Electron density around LMG c 521:**

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

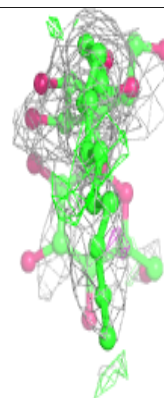
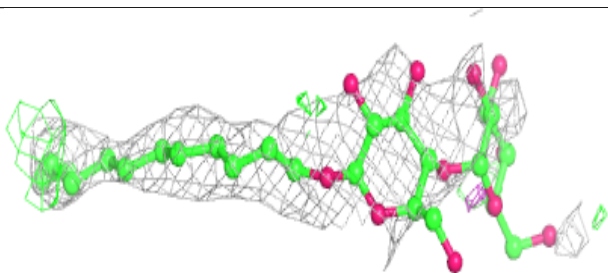
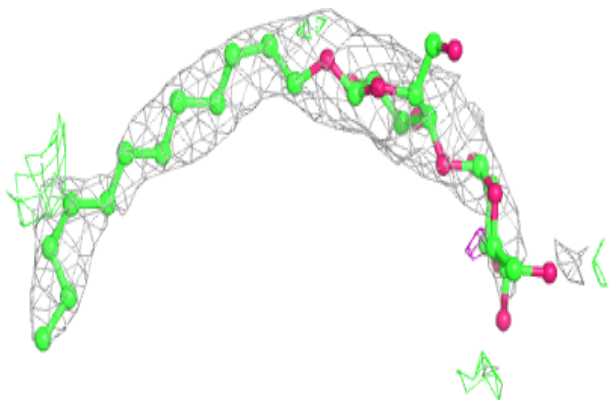


**Electron density around LMT M 102:**

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

**Electron density around LMT M 104:**

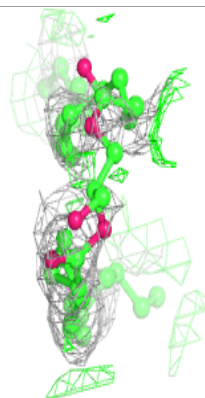
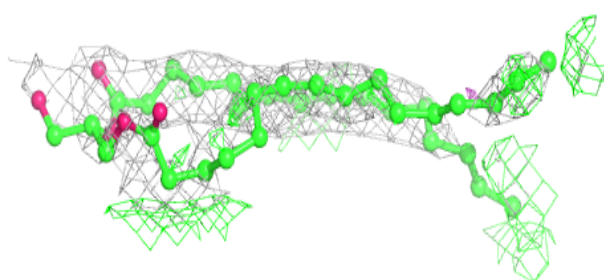
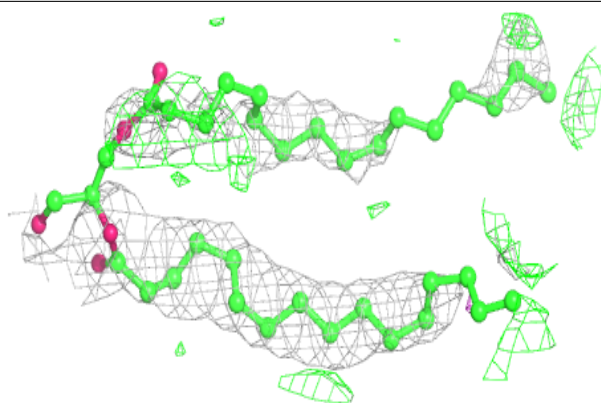
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



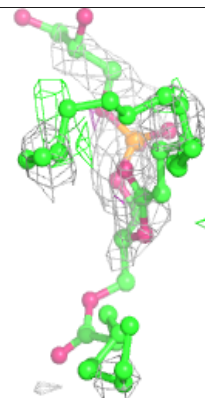
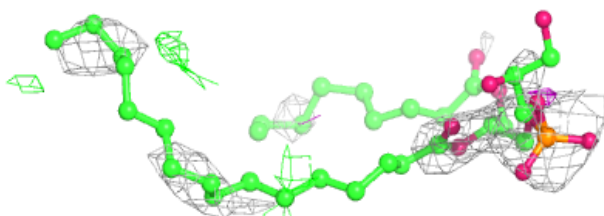
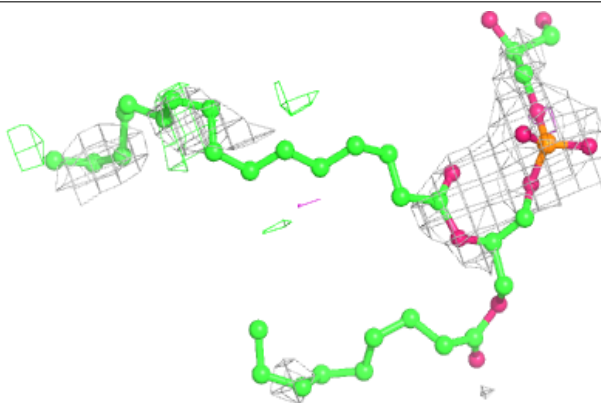


**Electron density around UNL I 101:**

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

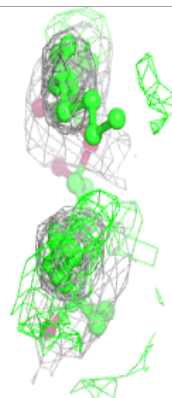
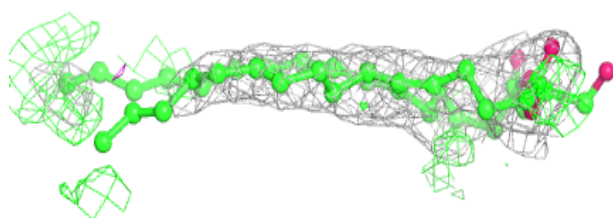
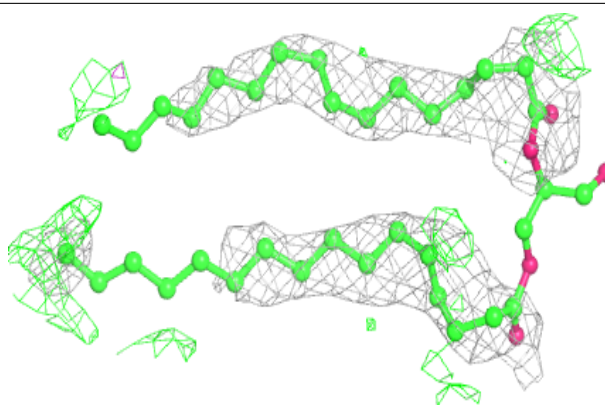
**Electron density around LHG a 419:**

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

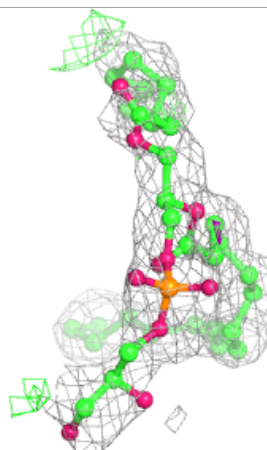
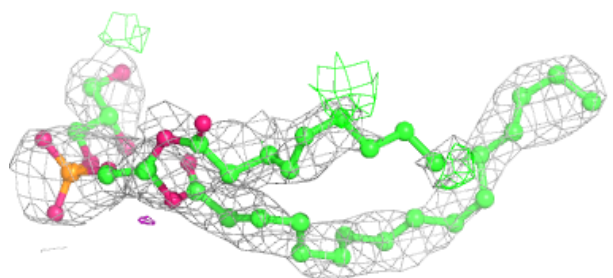
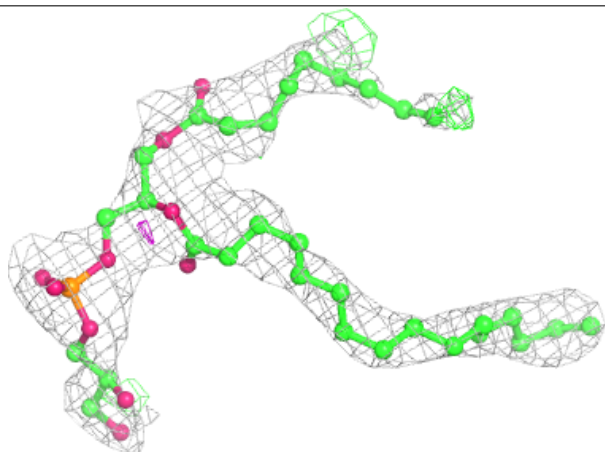


**Electron density around UNL i 101:**

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

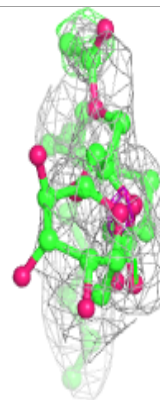
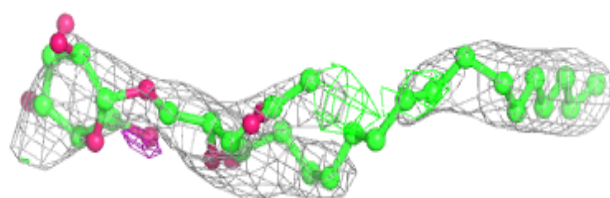
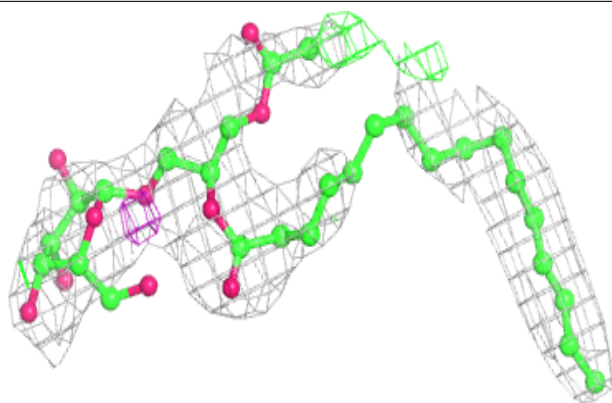
**Electron density around LHG E 101:**

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

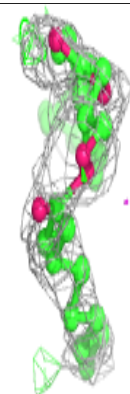
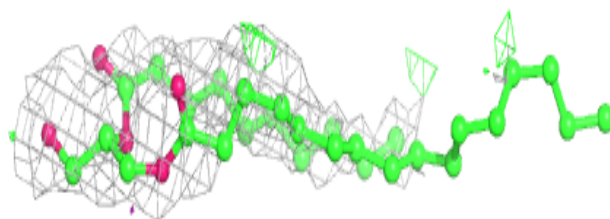
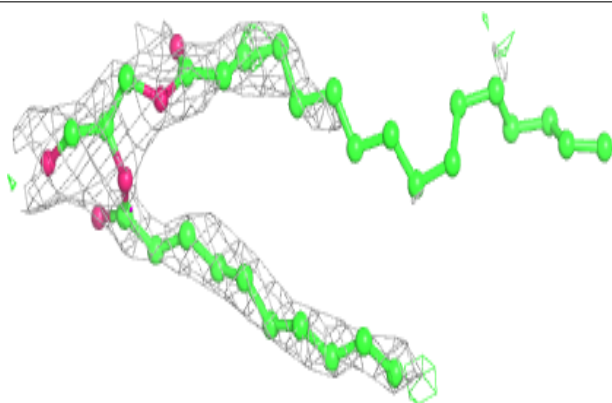


**Electron density around LMG Z 101:**

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

**Electron density around UNL C 526:**

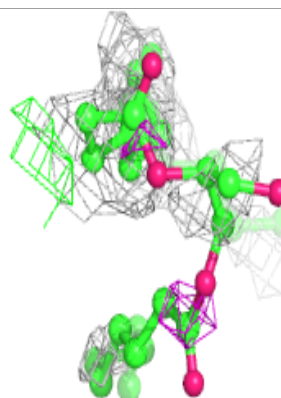
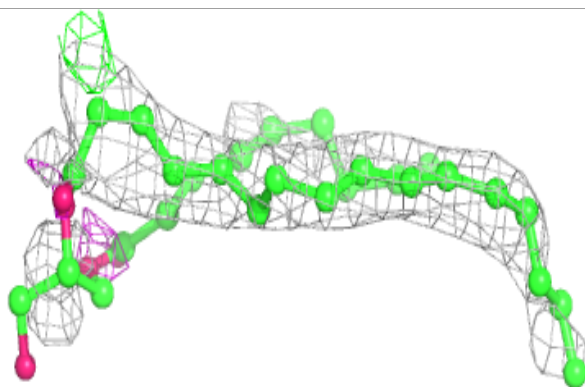
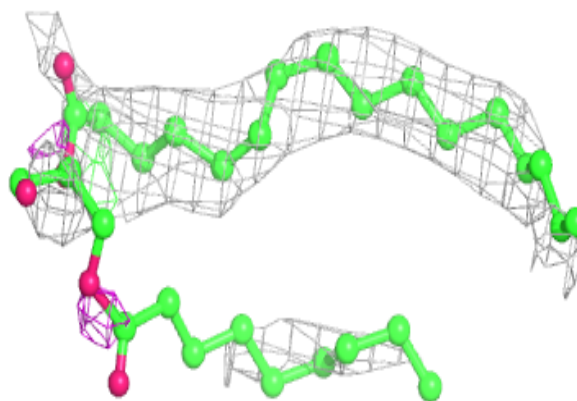
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



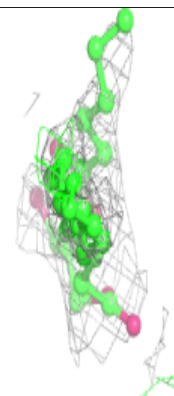
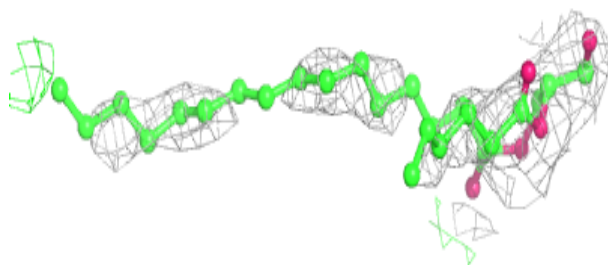
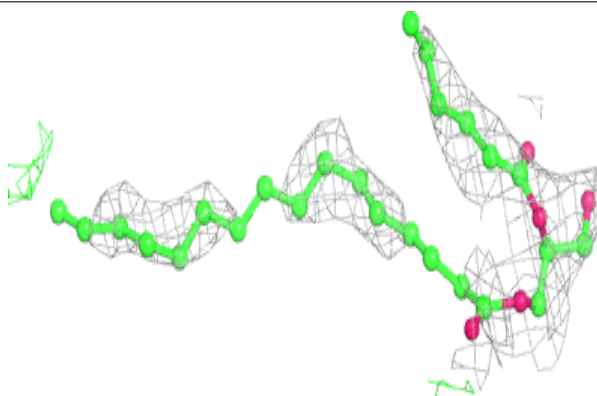


**Electron density around UNL b 625:**

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

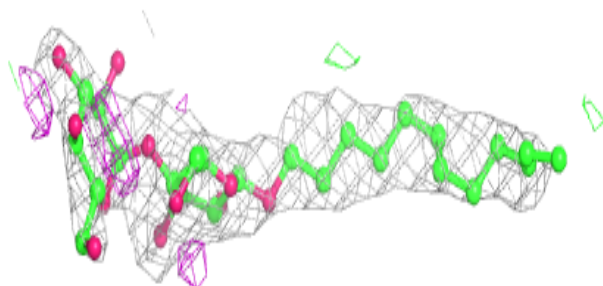
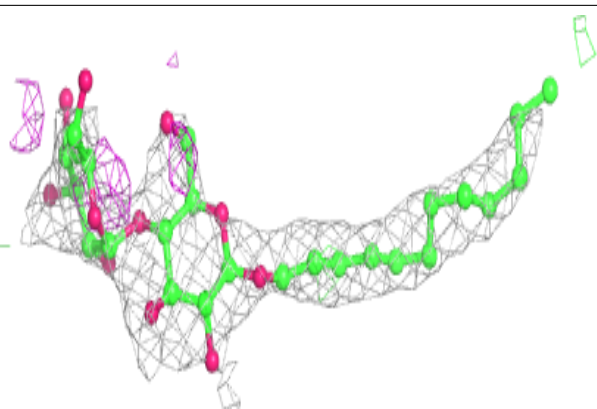
**Electron density around UNL a 415:**

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

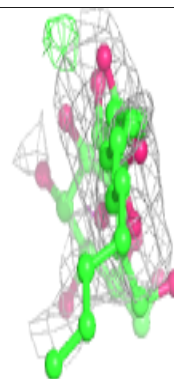
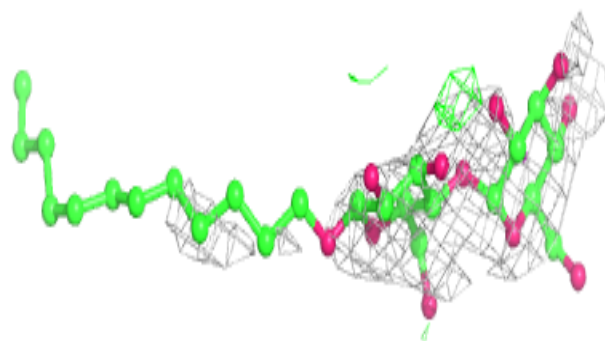
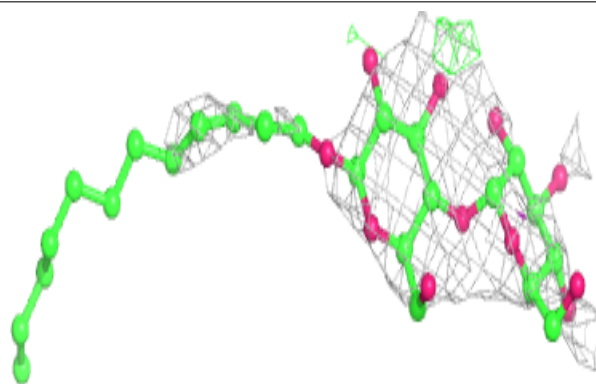


**Electron density around LMT D 404:**

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

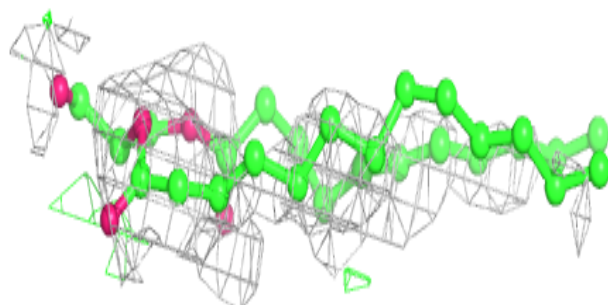
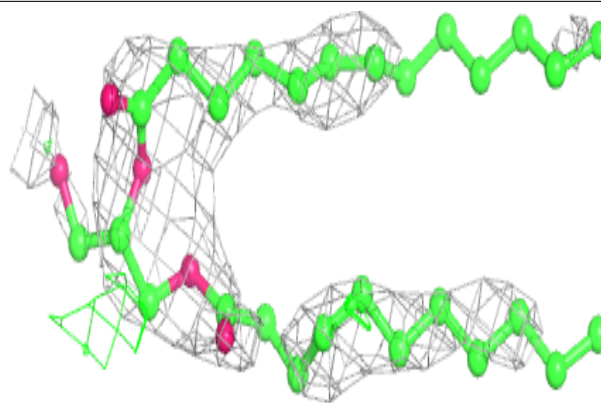
**Electron density around LMT a 418:**

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

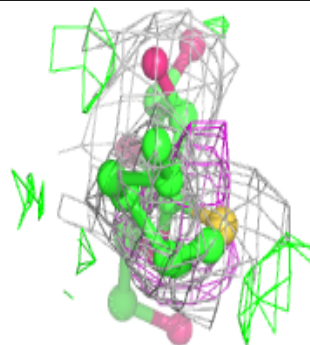
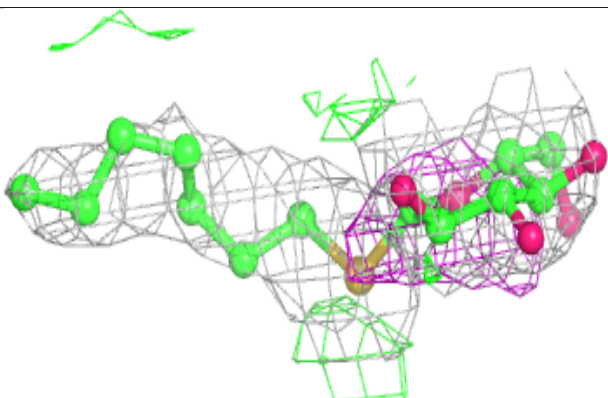
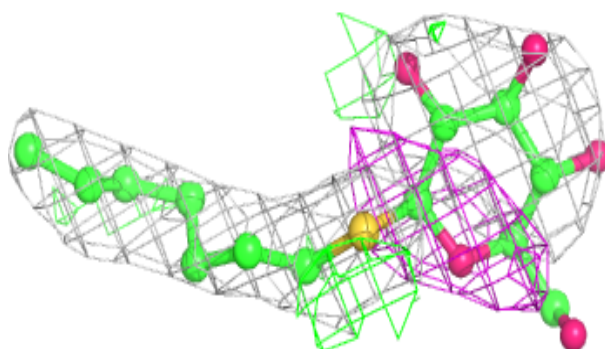


**Electron density around UNL c 525:**

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

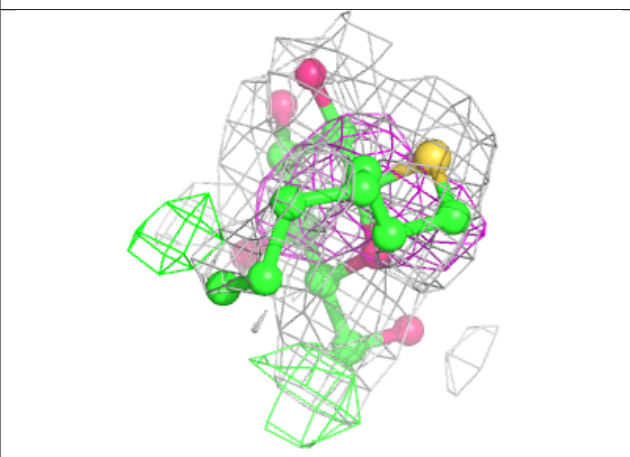
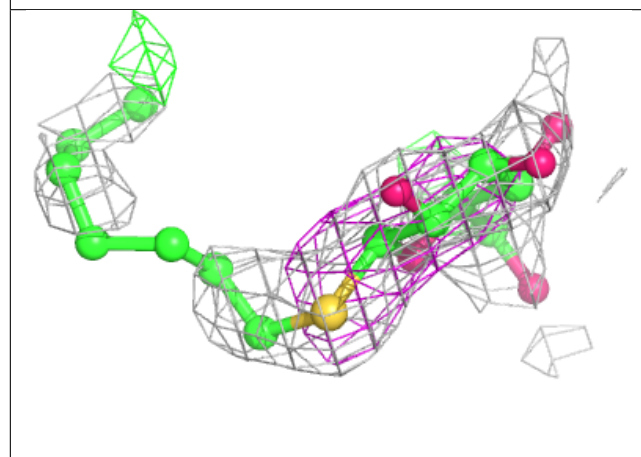
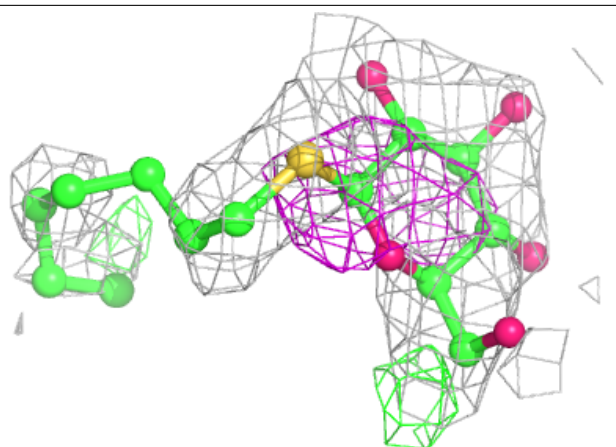
**Electron density around HTG B 621:**

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

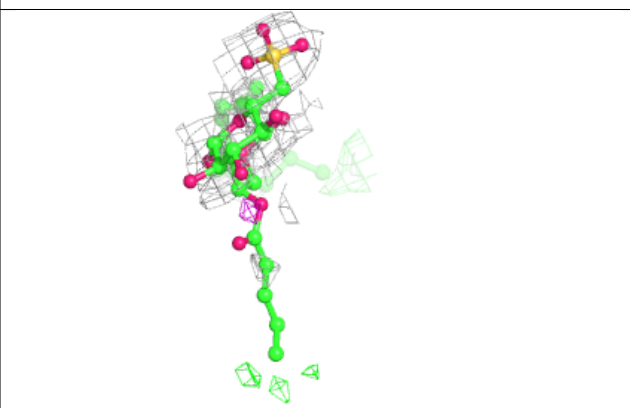
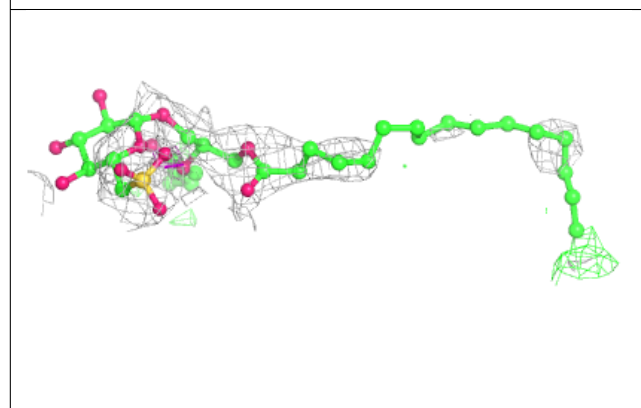
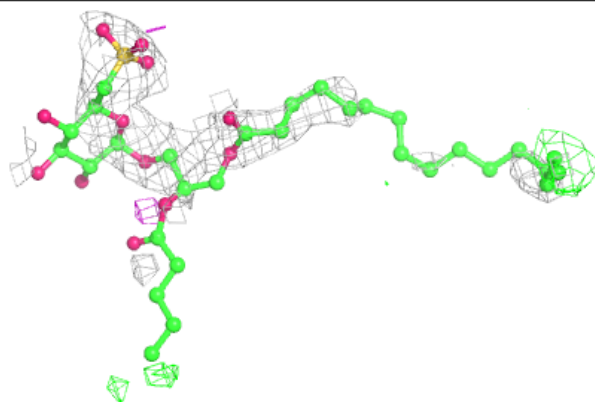


**Electron density around HTG B 622:**

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

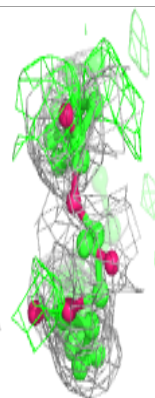
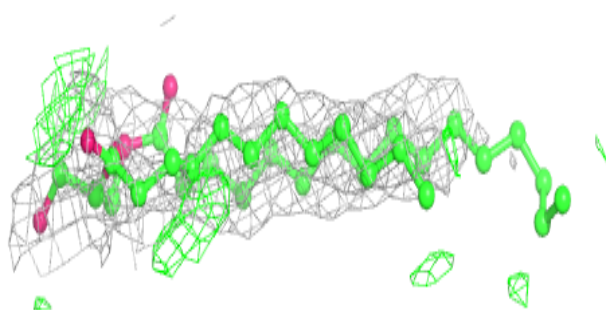
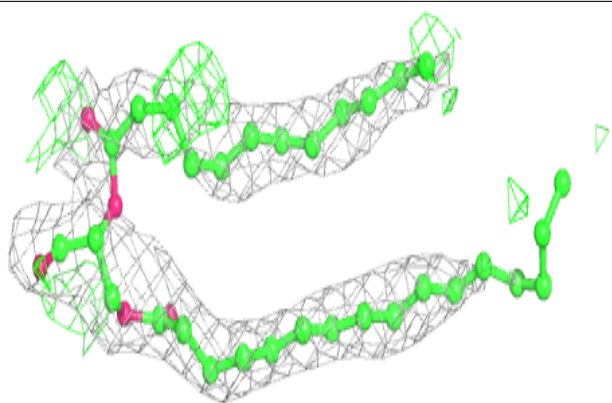
**Electron density around SQD f 102:**

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

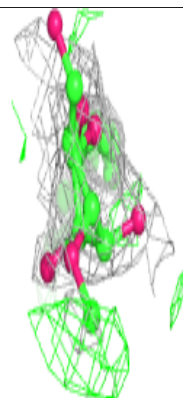
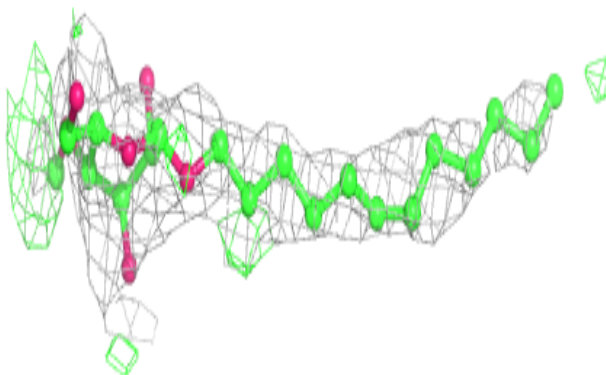
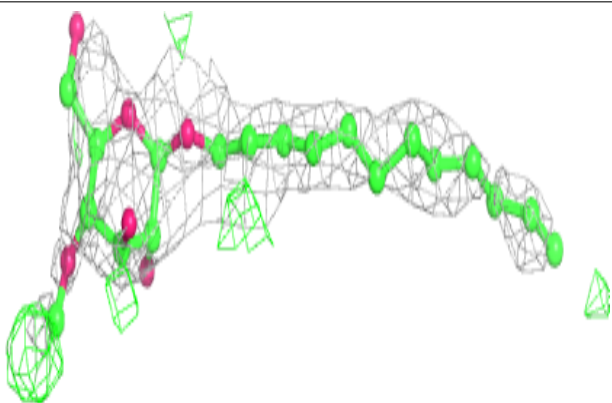


**Electron density around UNL d 411:**

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

**Electron density around LMT b 620:**

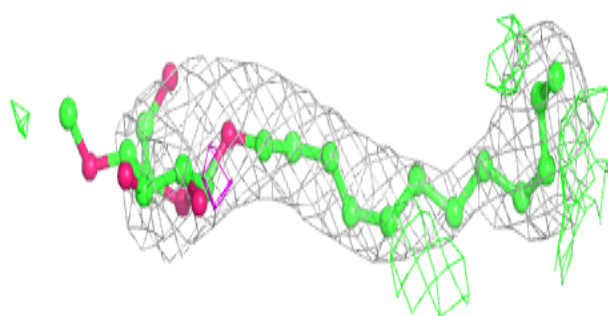
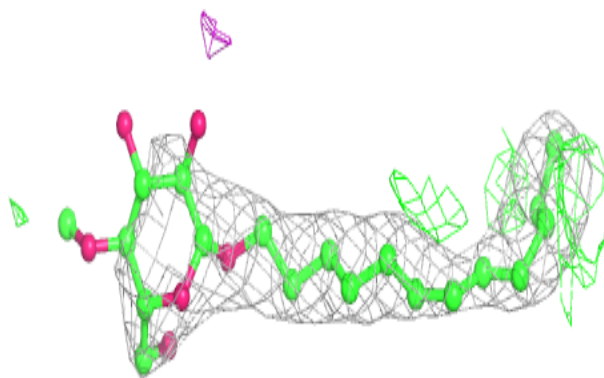
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



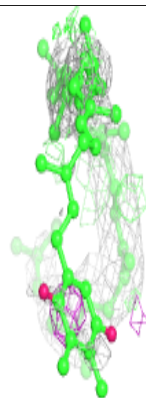
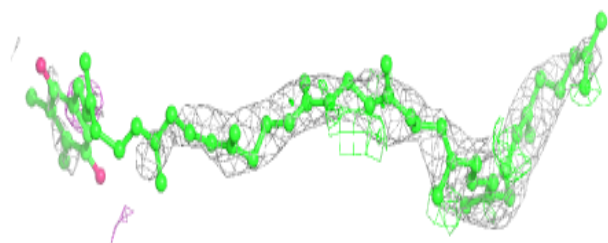
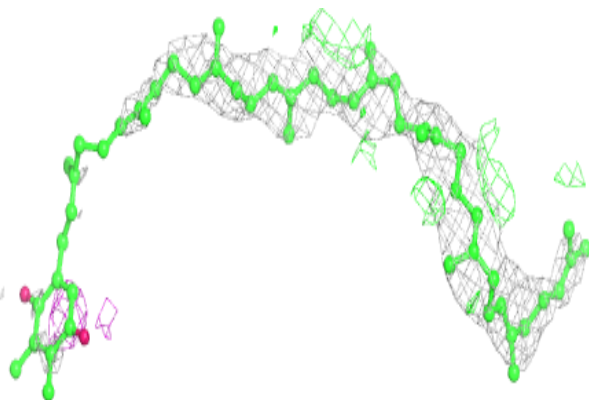


**Electron density around LMT b 626:**

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

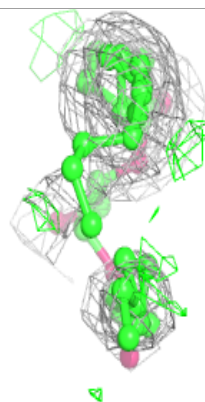
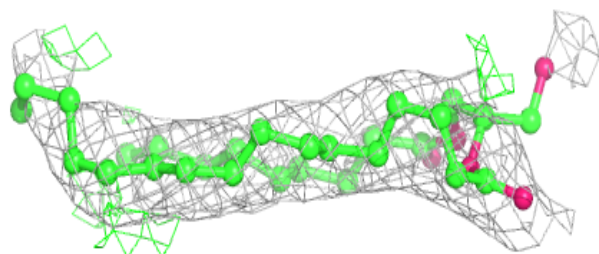
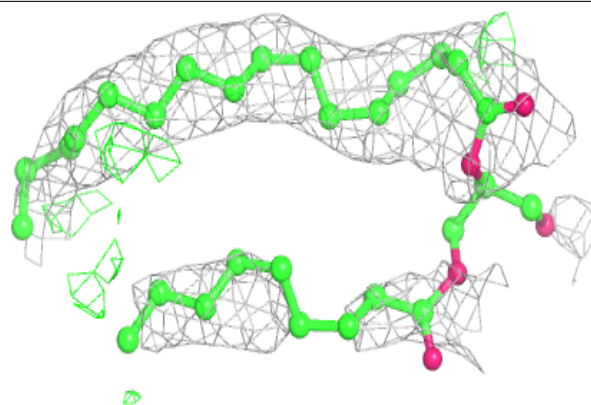
**Electron density around PL9 a 414:**

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

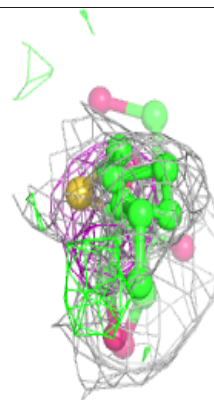
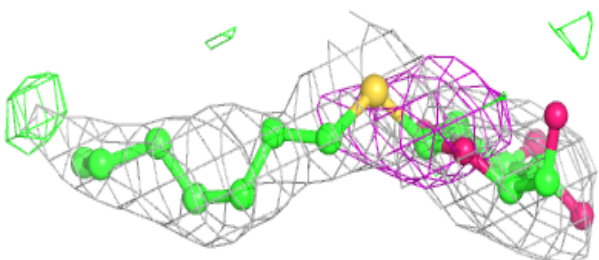
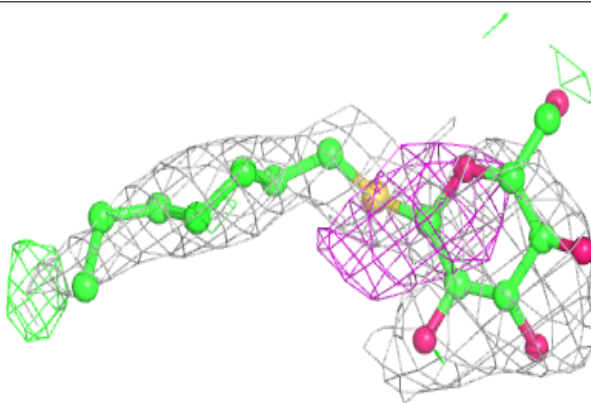


**Electron density around UNL B 625:**

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

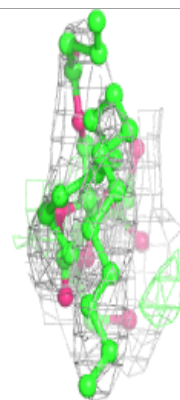
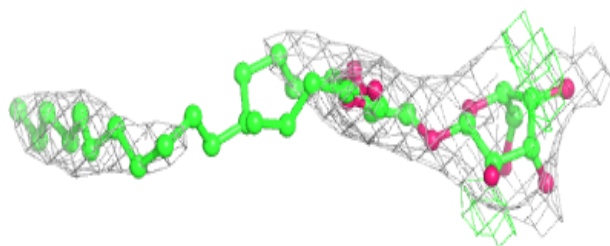
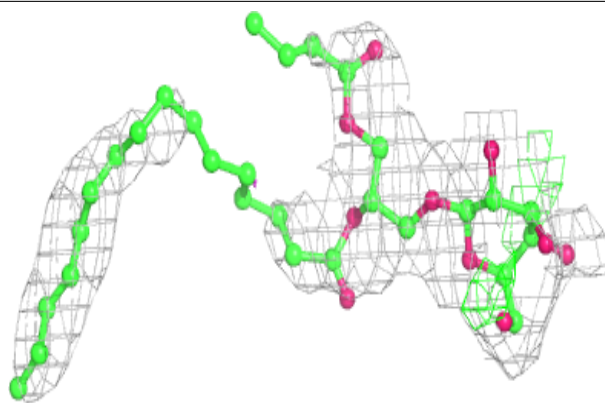
**Electron density around HTG b 621:**

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

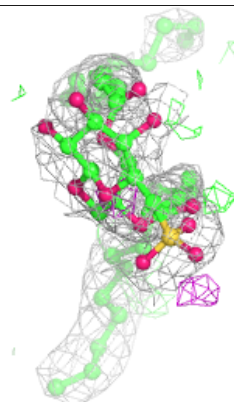
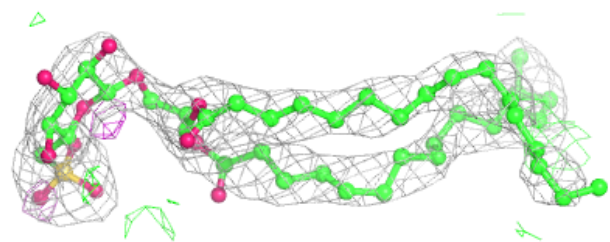
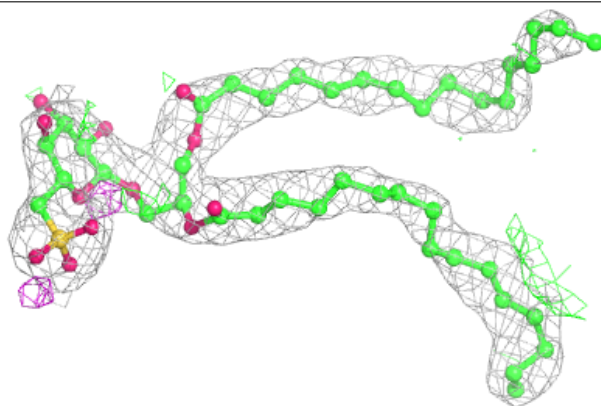


**Electron density around LMG z 101:**

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

**Electron density around SQD L 102:**

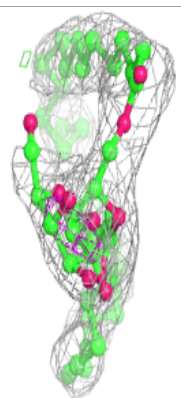
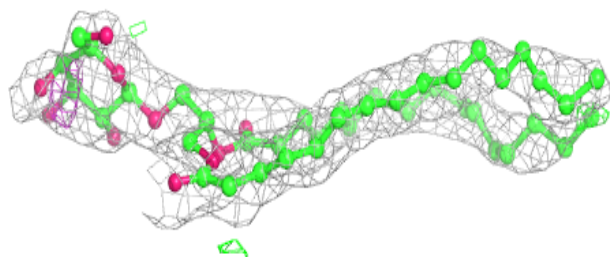
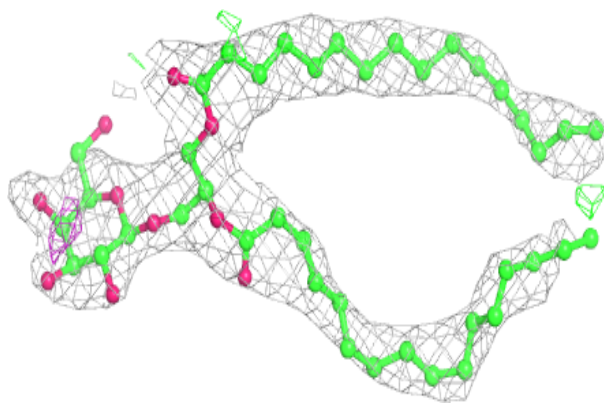
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



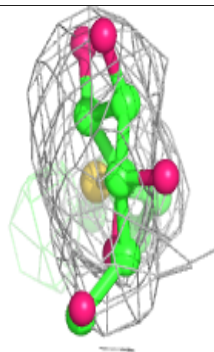
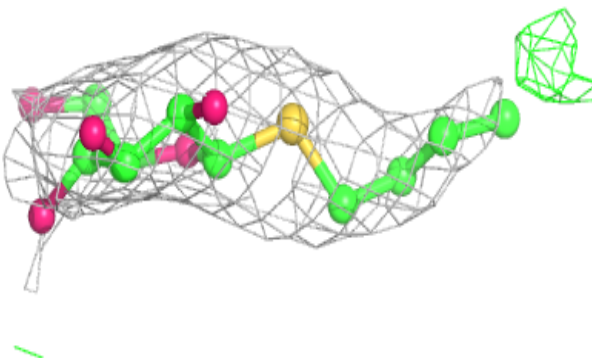
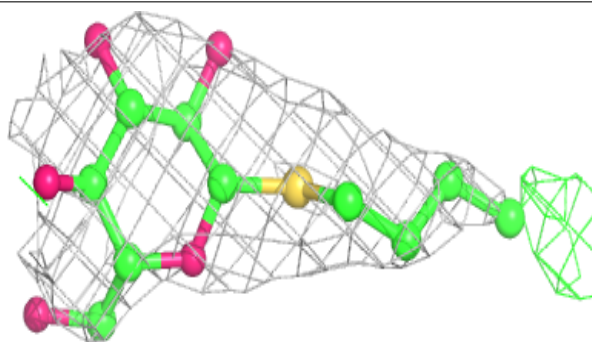


**Electron density around LMG a 417:**

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

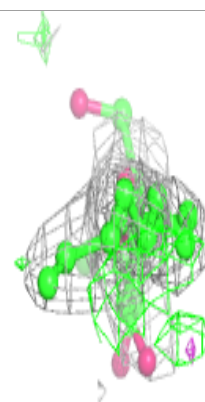
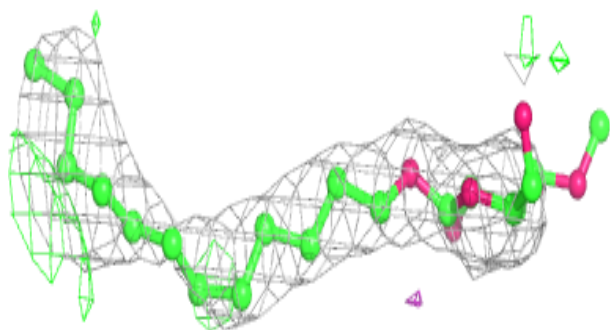
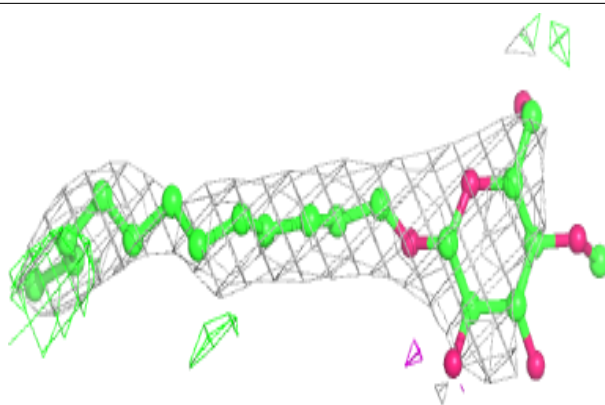
**Electron density around HTG h 101:**

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

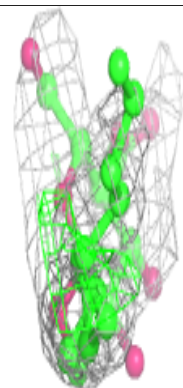
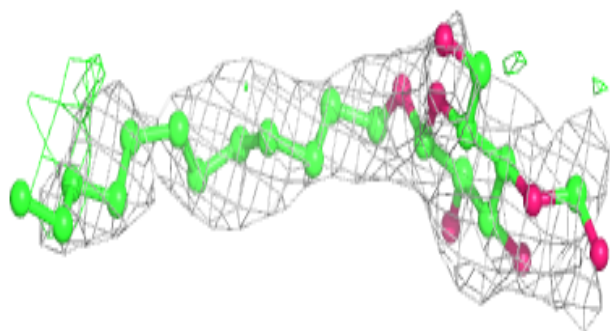
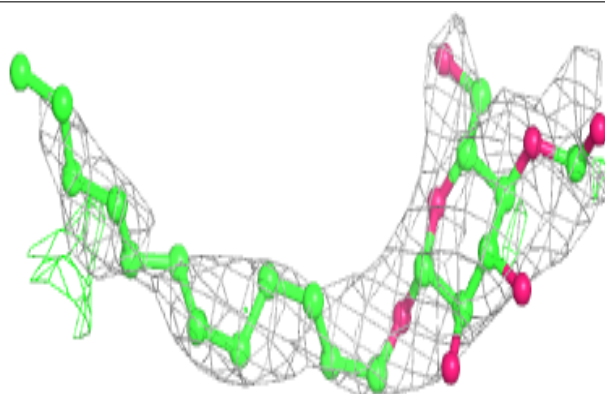


**Electron density around LMT B 628:**

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

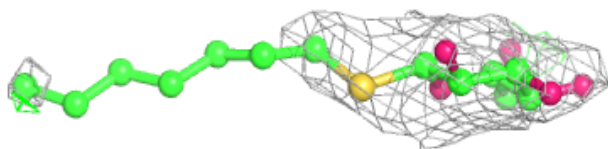
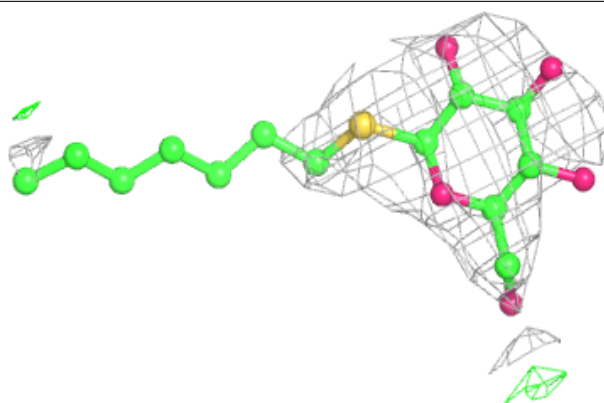
**Electron density around LMT t 101:**

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

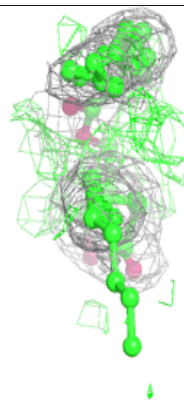
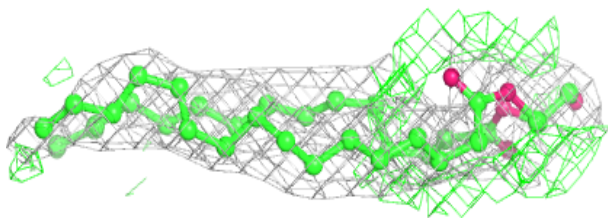
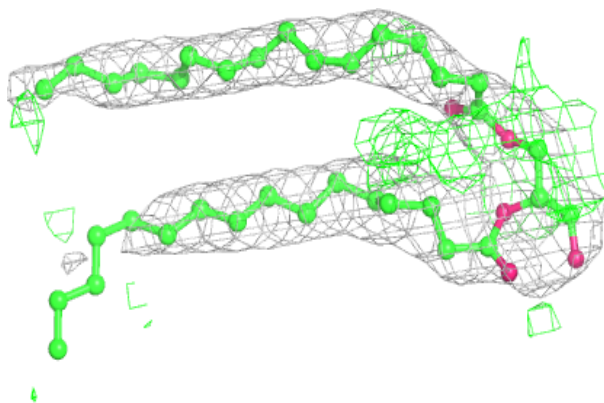


**Electron density around HTG c 522:**

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

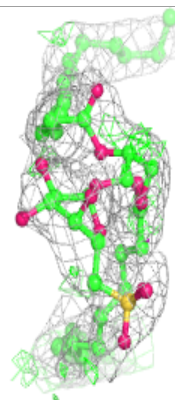
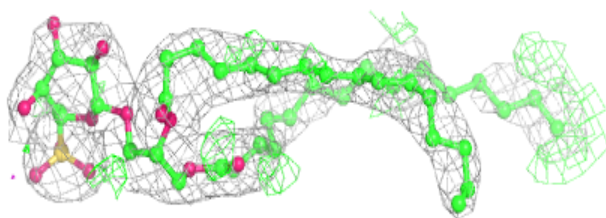
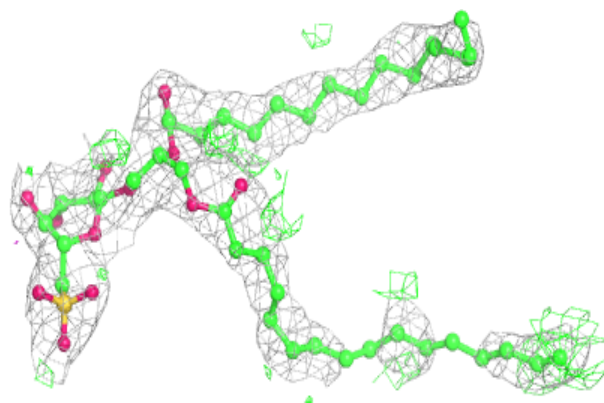
**Electron density around UNL D 412:**

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

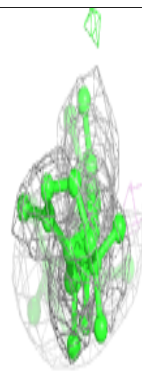
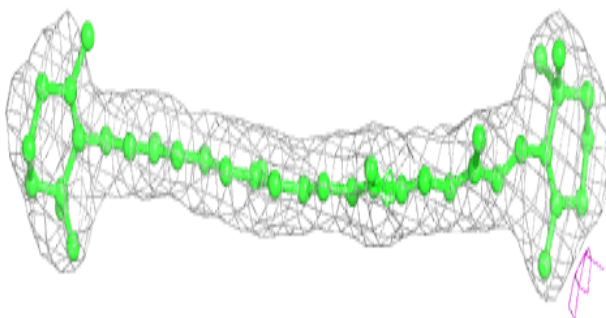
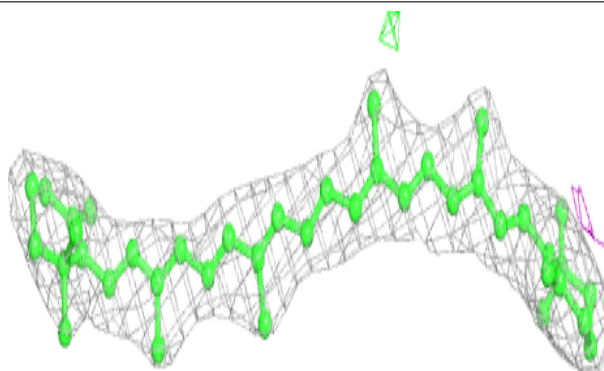


**Electron density around SQD A 411:**

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

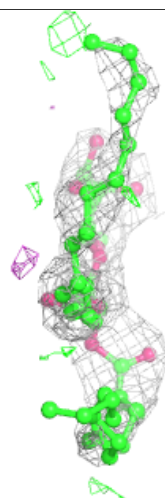
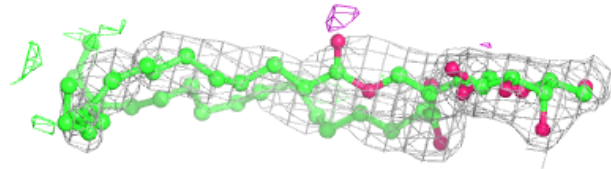
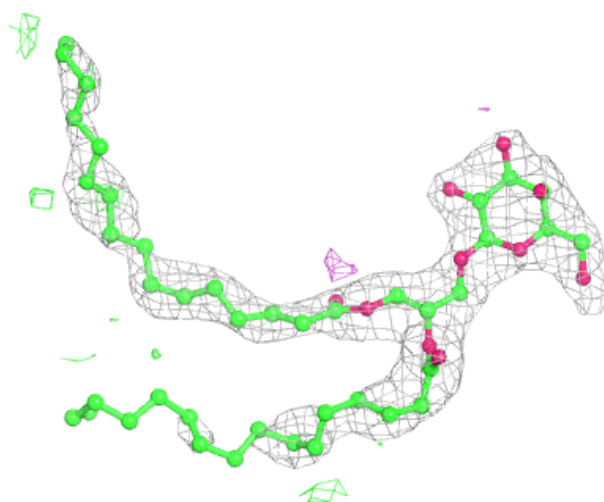
**Electron density around BCR h 102:**

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



**Electron density around LMG C 520:**

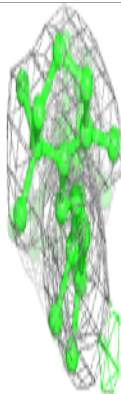
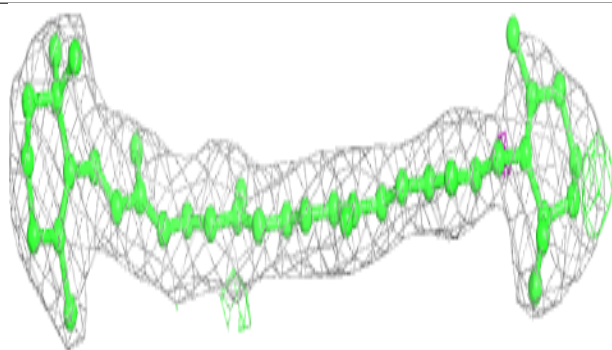
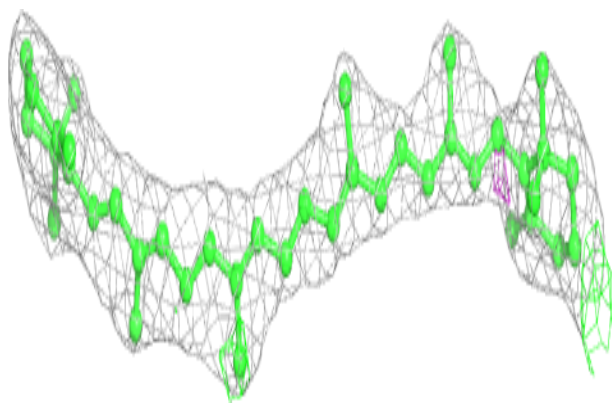
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



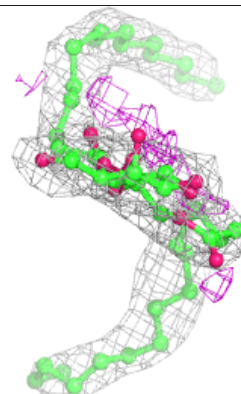
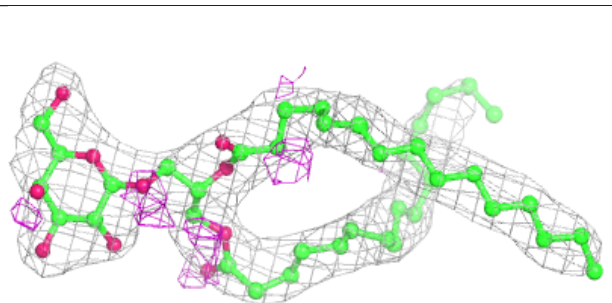
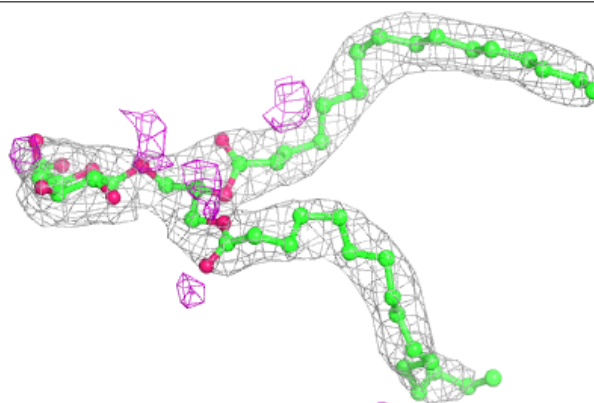


**Electron density around BCR H 101:**

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

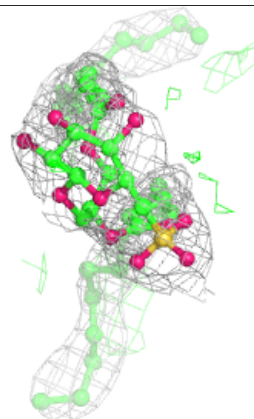
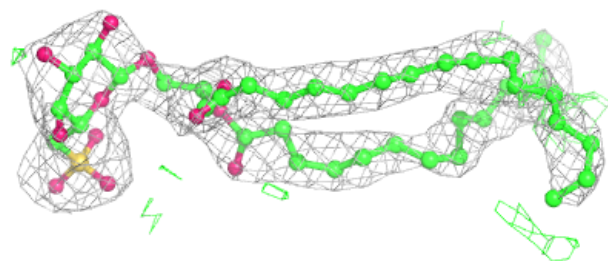
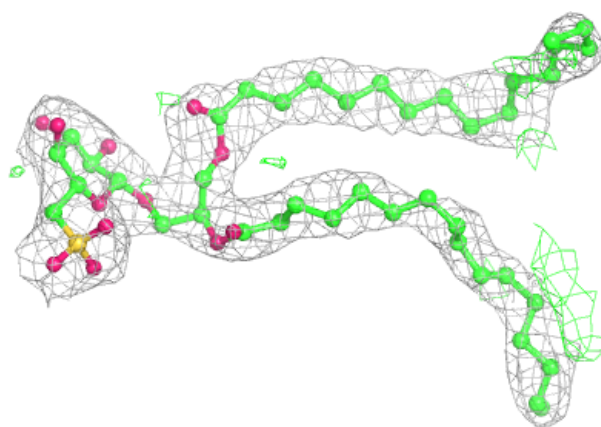
**Electron density around LMG m 101:**

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



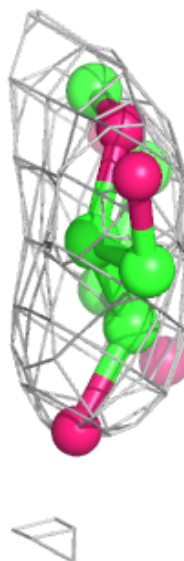
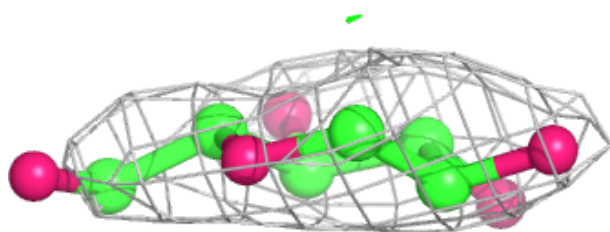
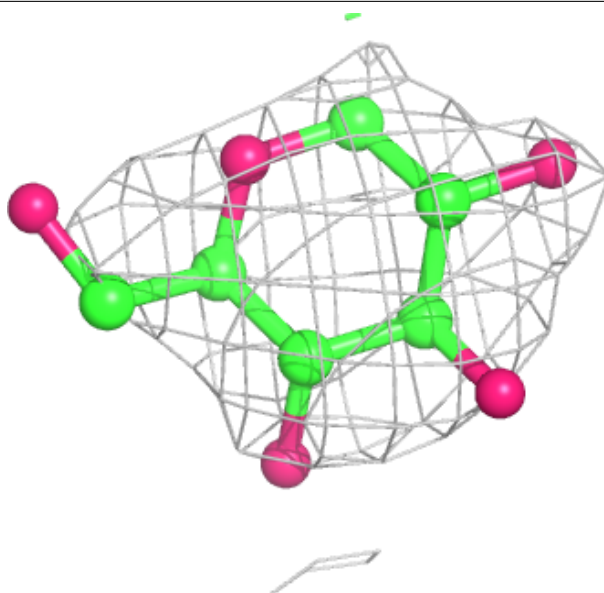
**Electron density around SQD B 620:**

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



**Electron density around HTG V 202:**

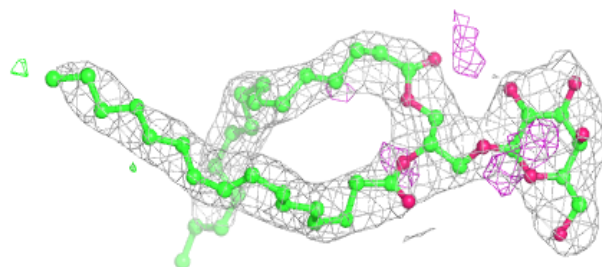
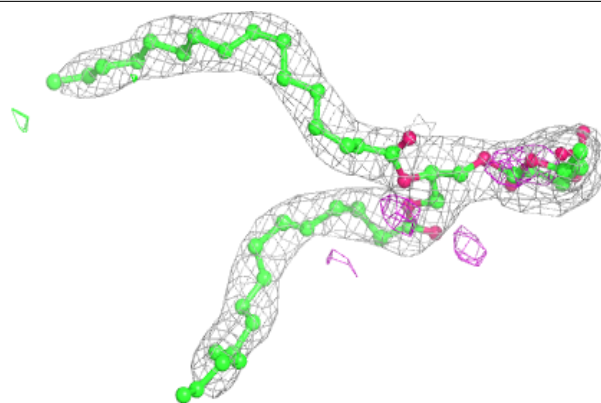
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



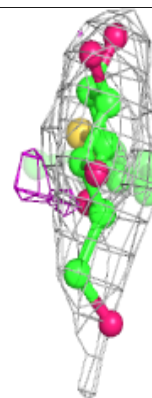
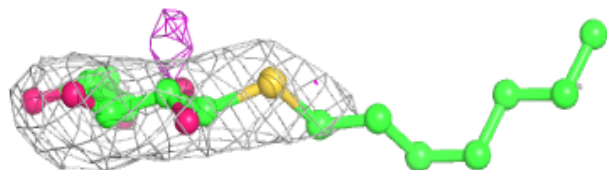
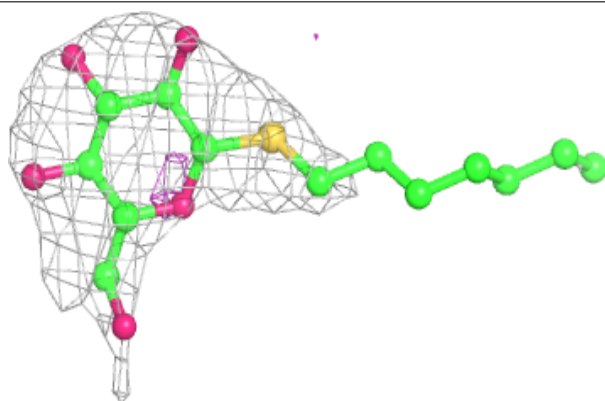


**Electron density around LMG M 101:**

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

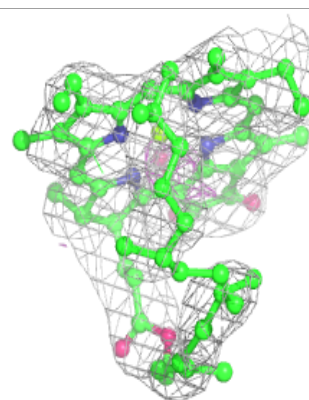
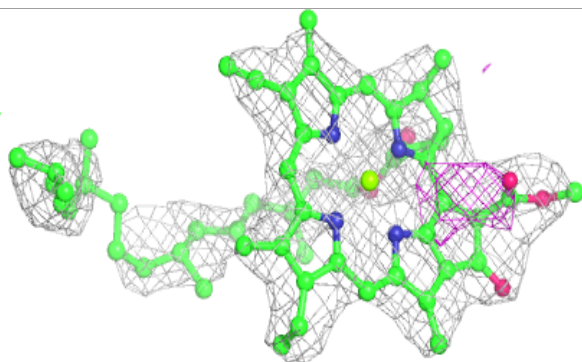
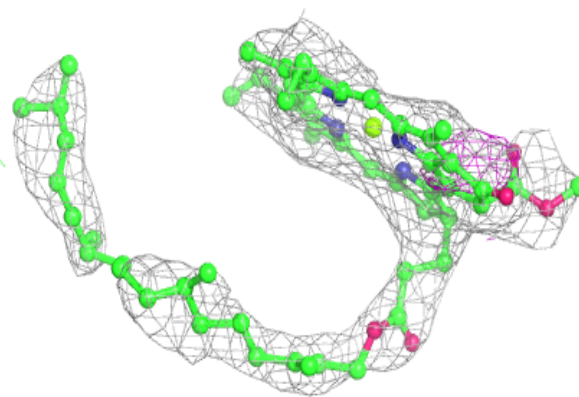
**Electron density around HTG C 522:**

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

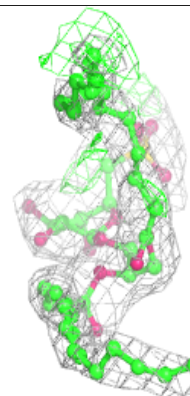
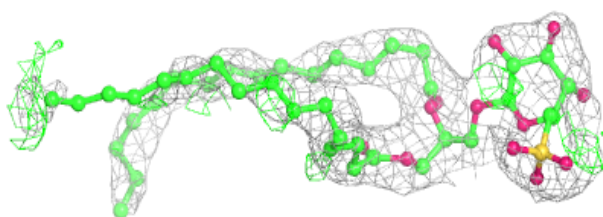
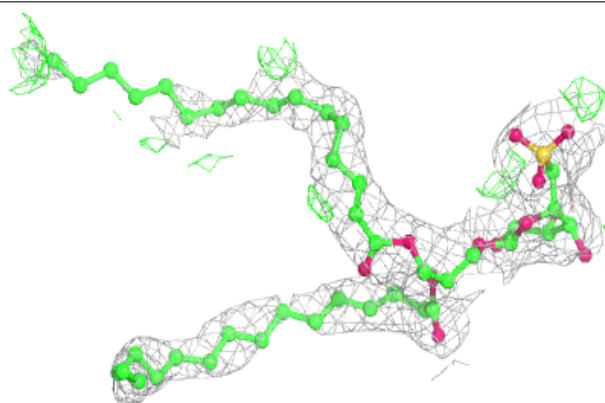


**Electron density around CLA C 514:**

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

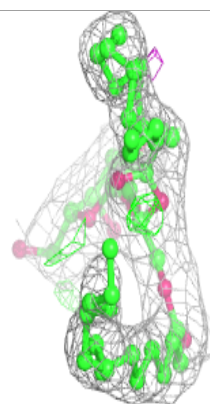
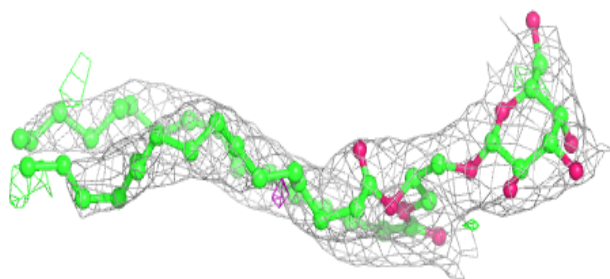
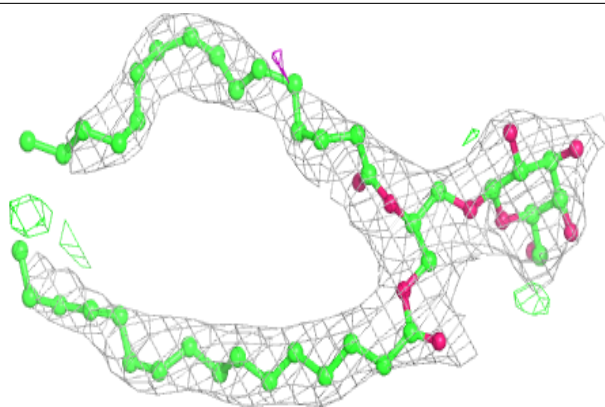
**Electron density around SQD a 411:**

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

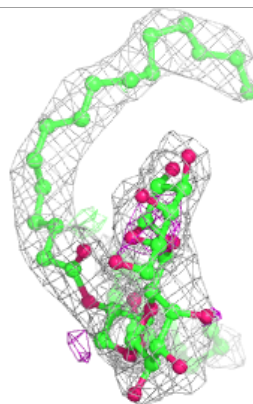
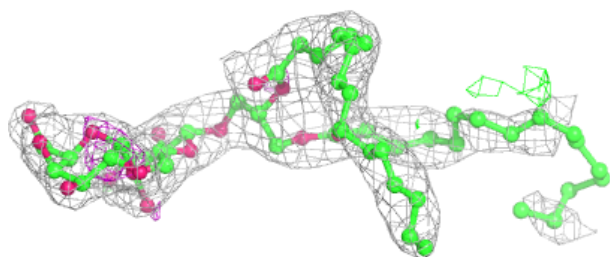
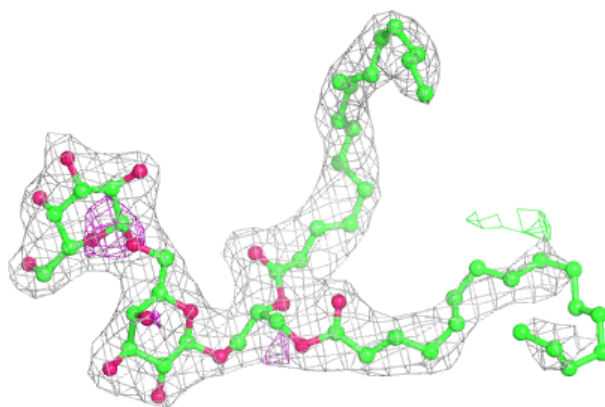


**Electron density around LMG A 415:**

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

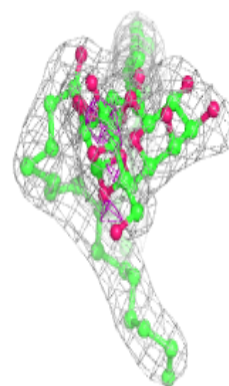
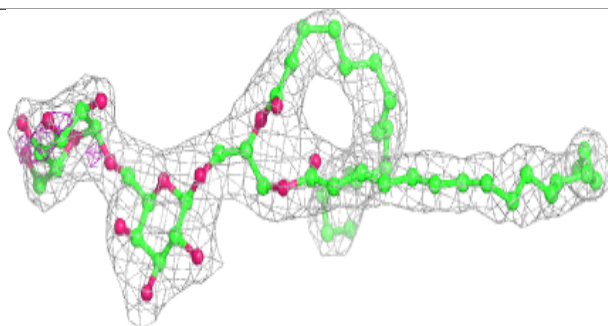
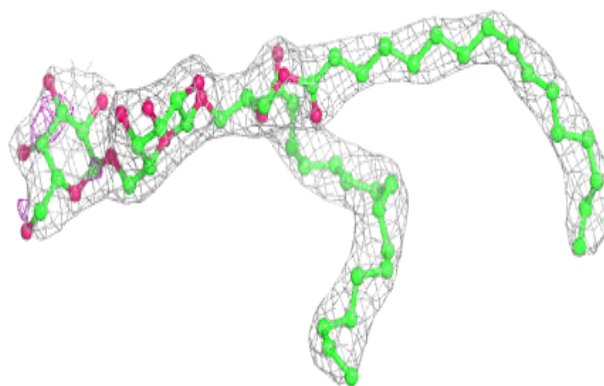
**Electron density around DGD C 518:**

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



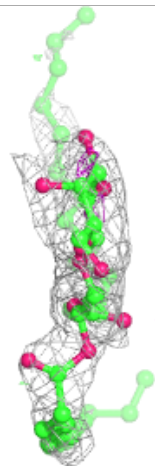
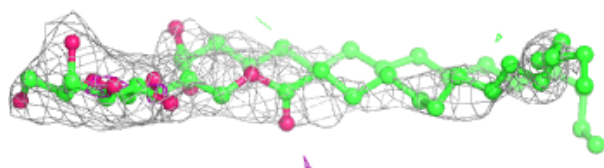
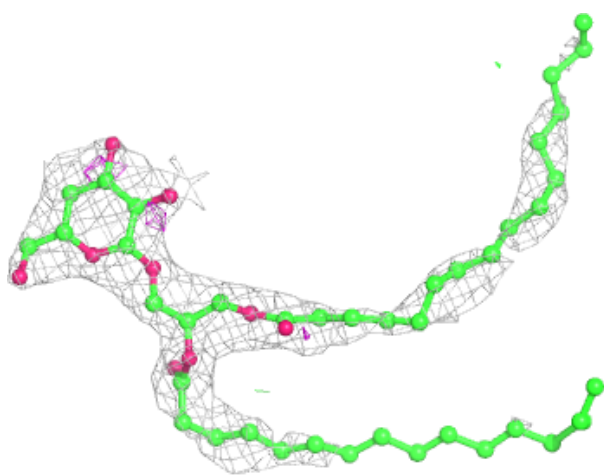
**Electron density around DGD h 103:**

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



**Electron density around LMG c 520:**

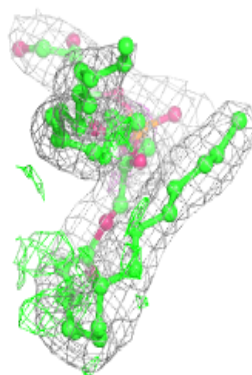
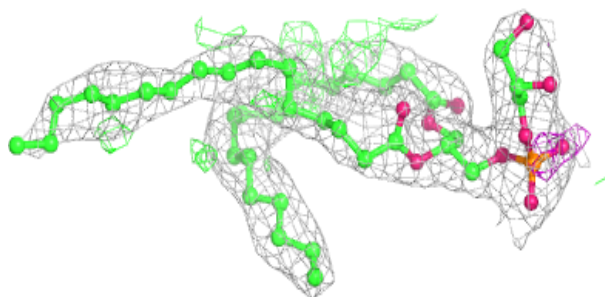
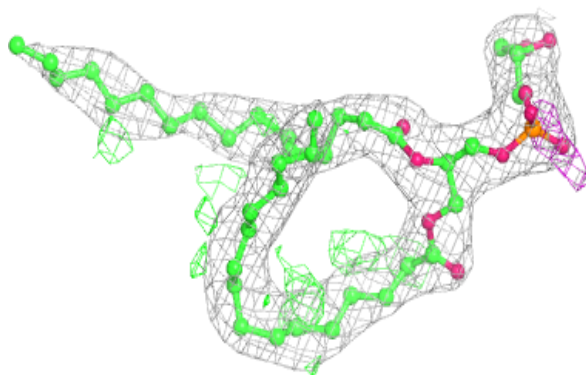
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



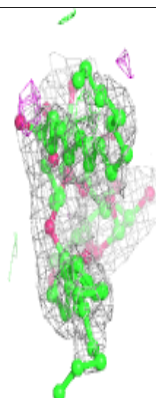
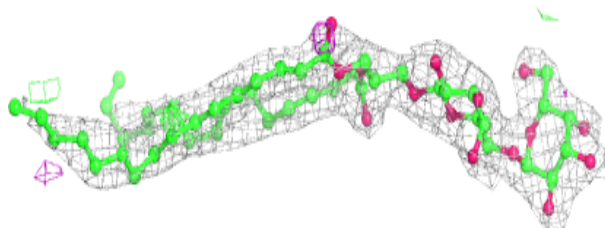
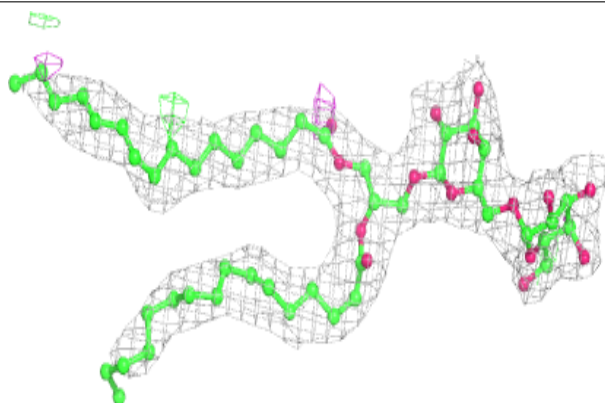


**Electron density around LHG A 416:**

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

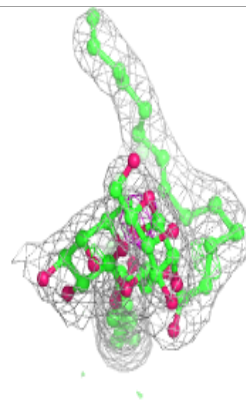
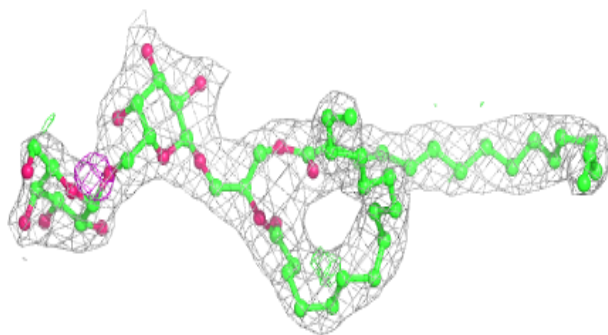
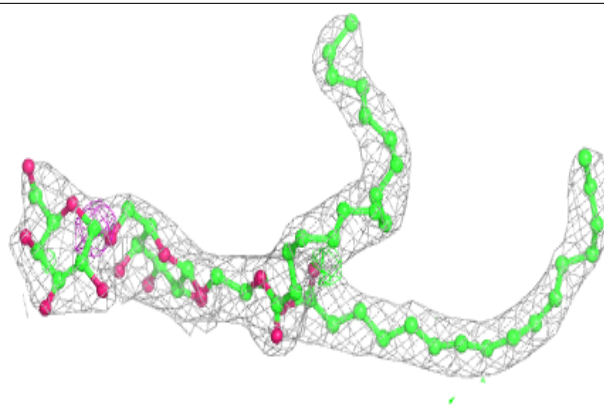
**Electron density around DGD C 519:**

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



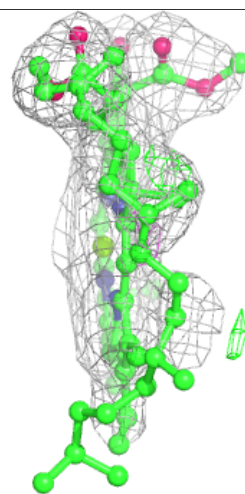
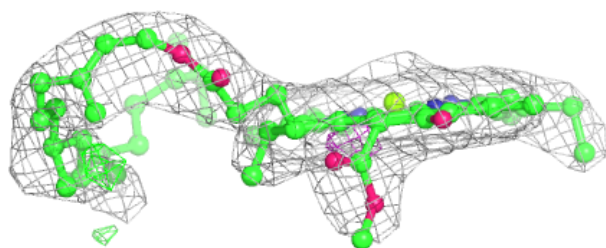
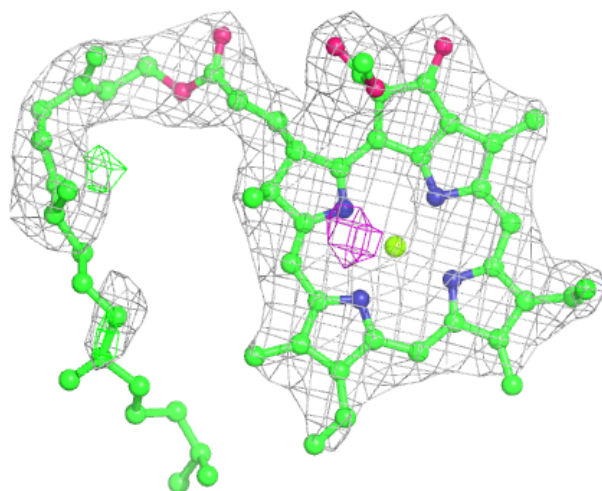
**Electron density around DGD H 102:**

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



**Electron density around CLA C 513:**

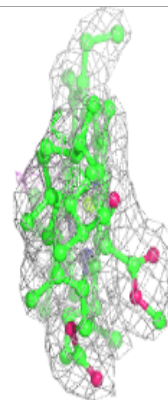
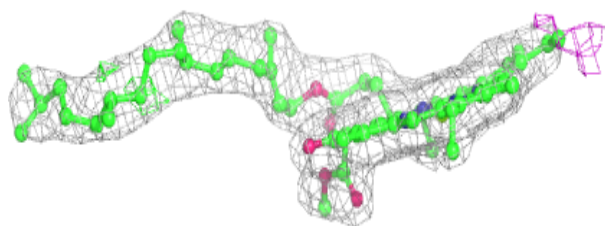
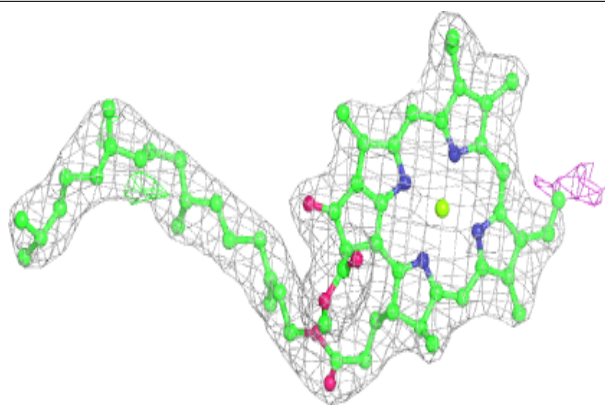
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



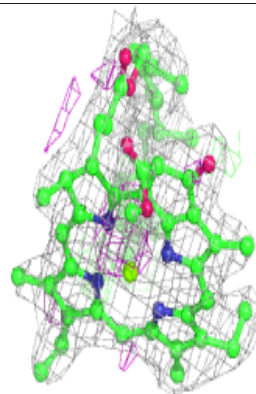
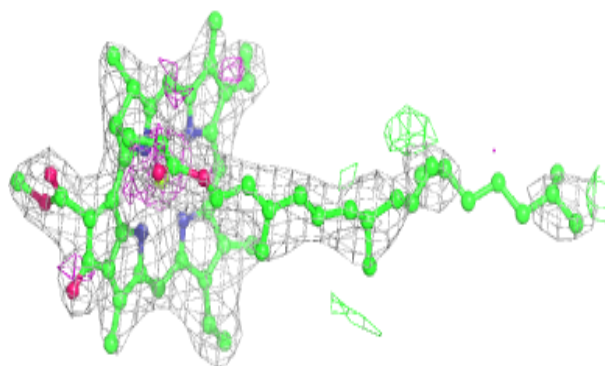
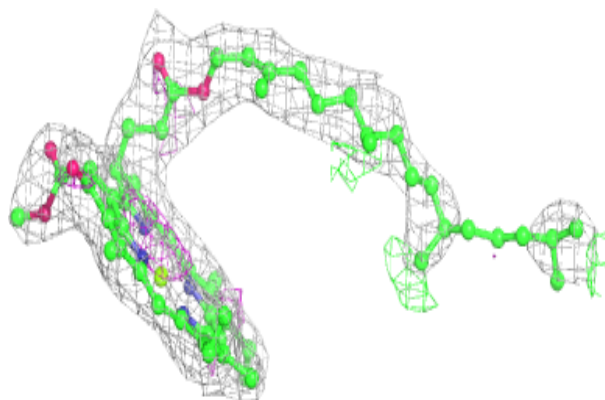


**Electron density around CLA B 602:**

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

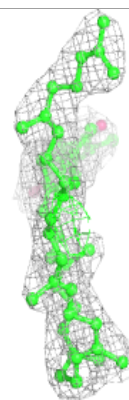
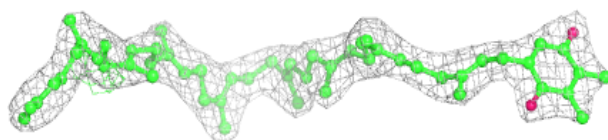
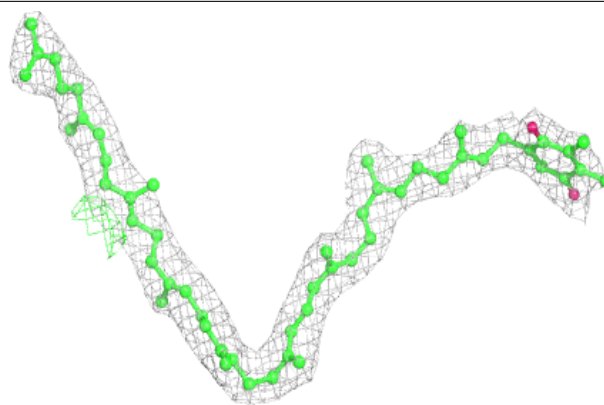
**Electron density around CLA C 505:**

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



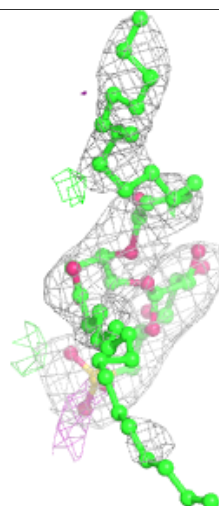
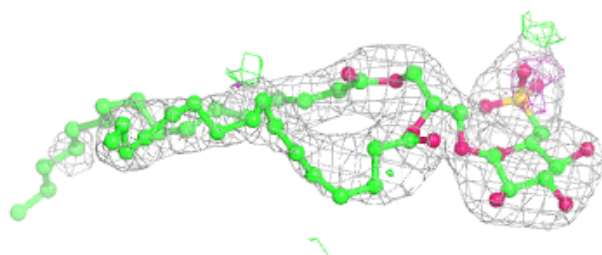
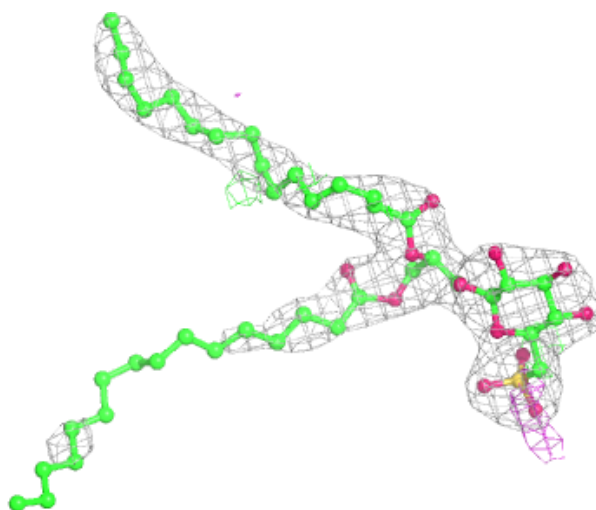
**Electron density around PL9 d 406:**

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



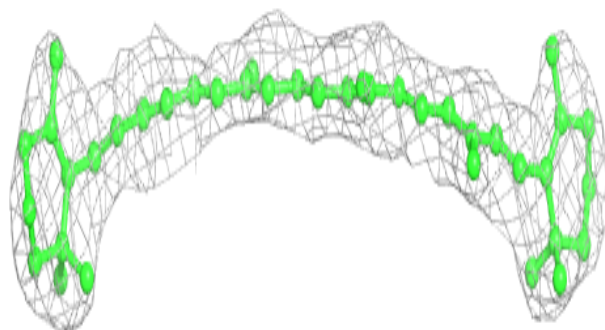
**Electron density around SQD C 501:**

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

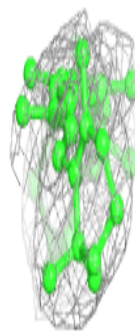
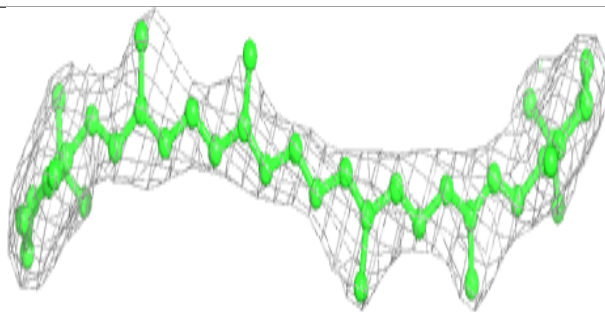


**Electron density around BCR k 101:**

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



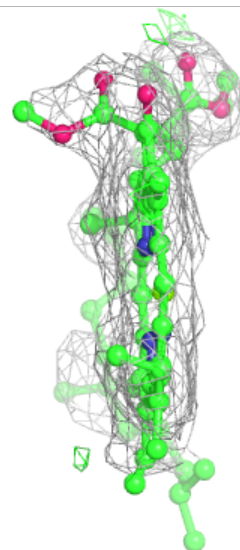
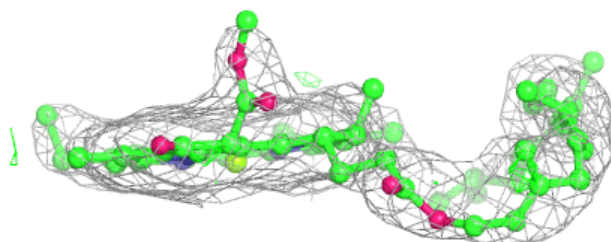
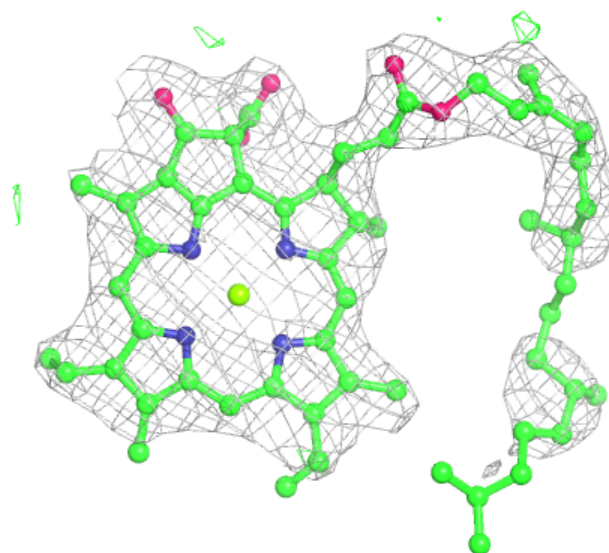
B



C

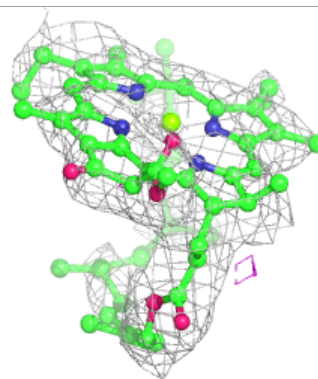
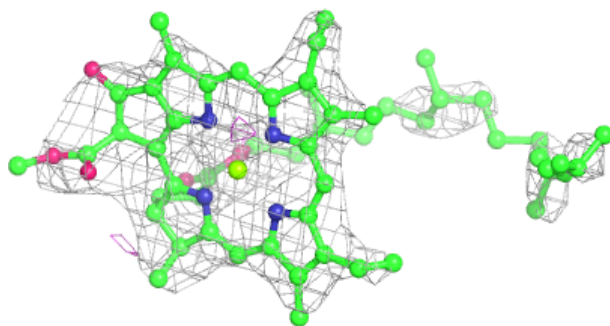
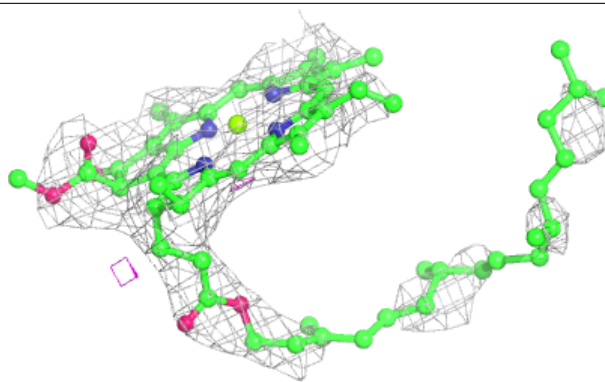
**Electron density around CLA c 513:**

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

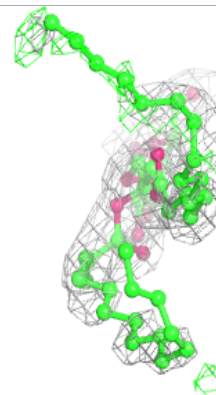
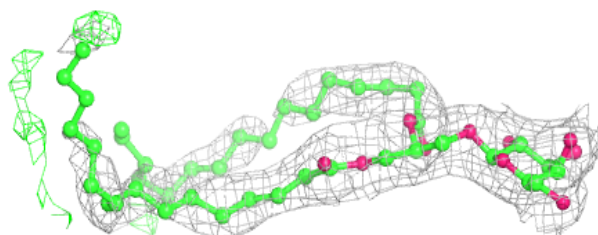
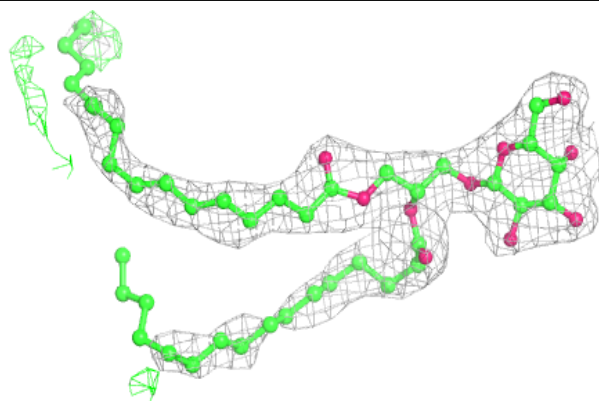


**Electron density around CLA c 514:**

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

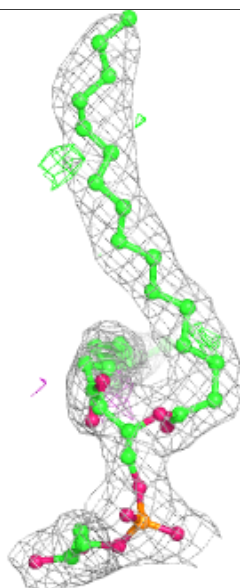
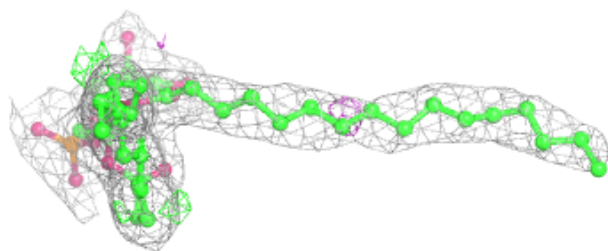
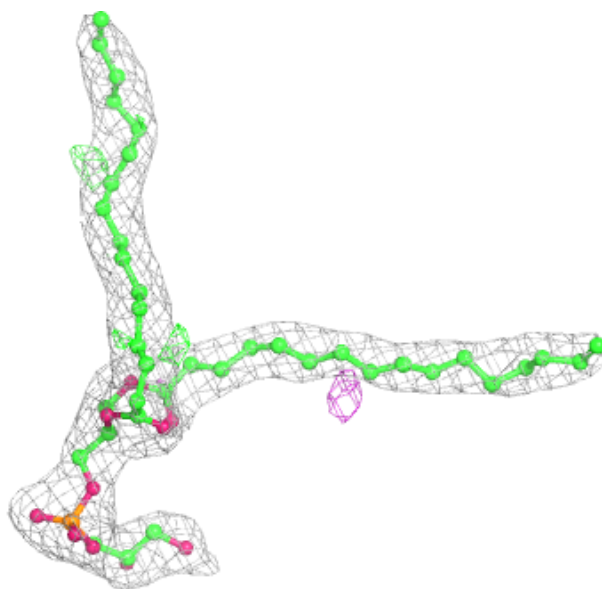
**Electron density around LMG D 414:**

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



**Electron density around LHG b 628:**

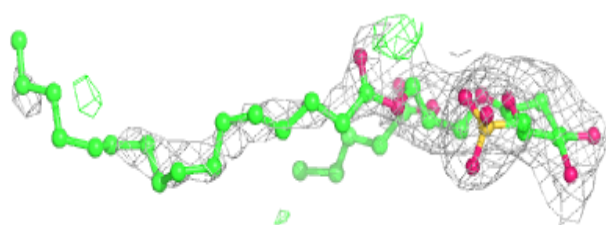
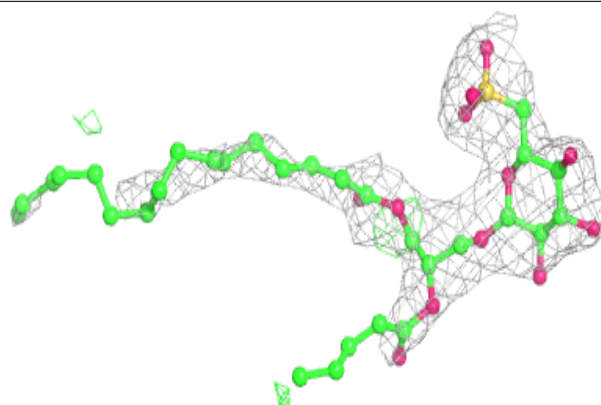
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



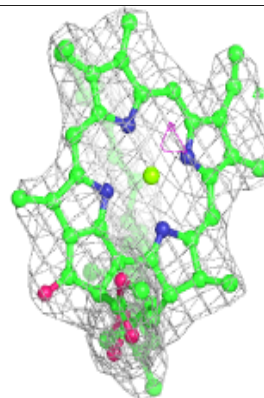
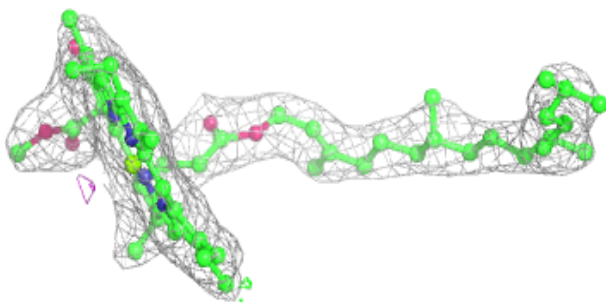
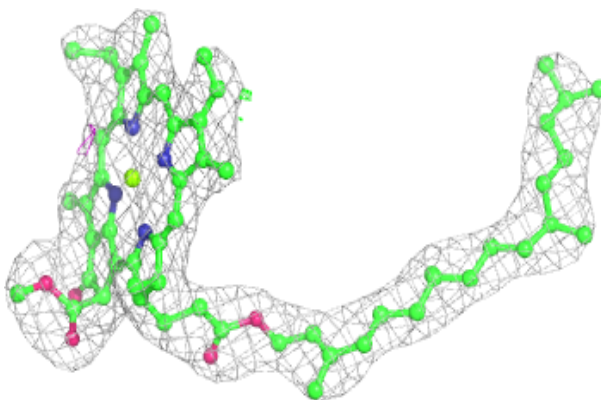


**Electron density around SQD D 415:**

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

**Electron density around CLA B 609:**

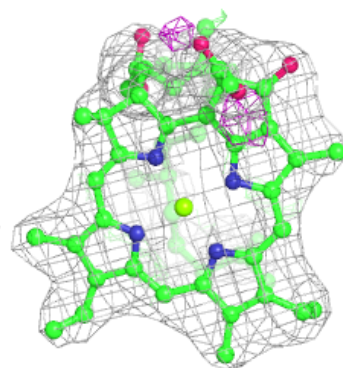
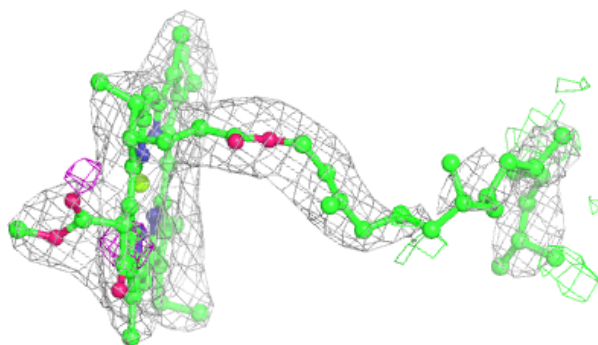
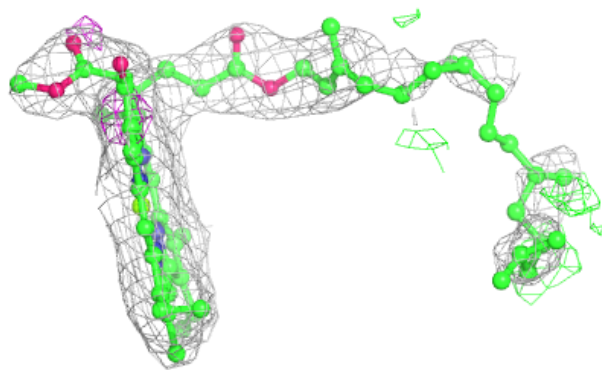
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



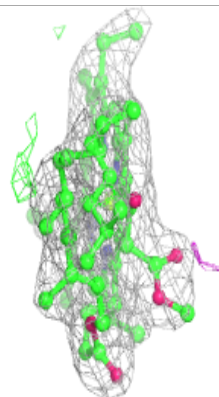
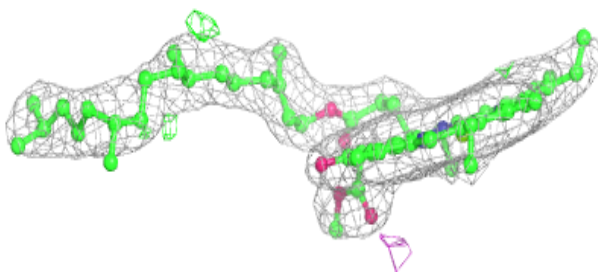
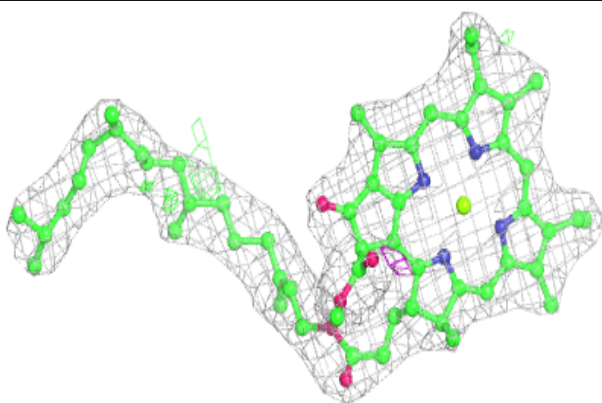


**Electron density around CLA C 507:**

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

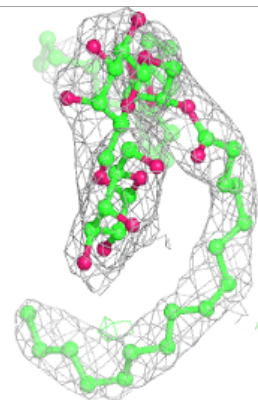
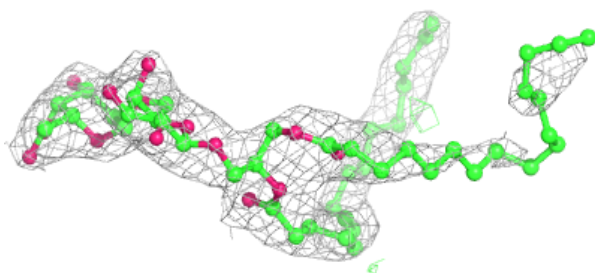
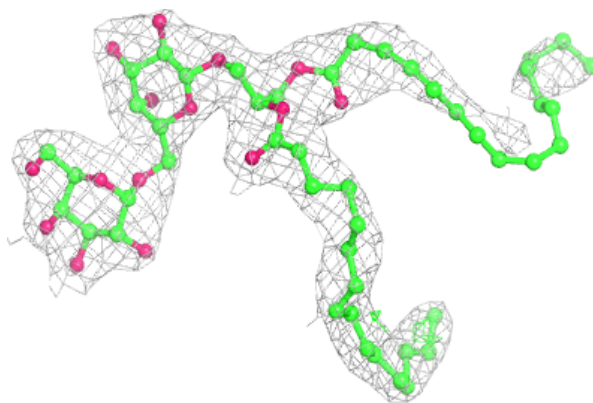
**Electron density around CLA b 602:**

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

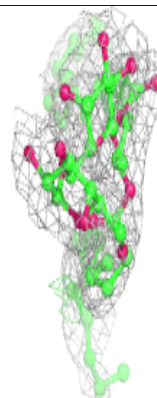
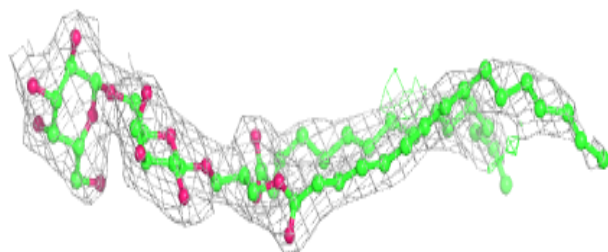
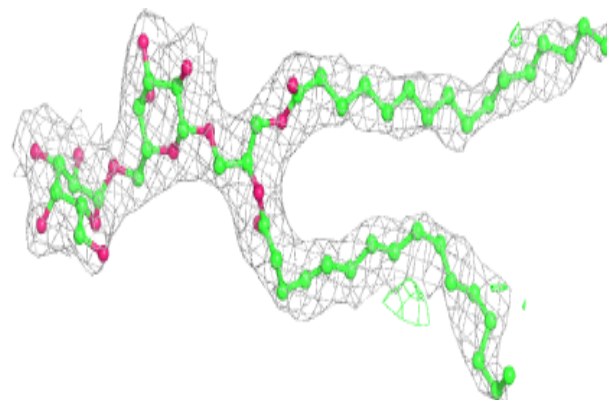


**Electron density around DGD c 518:**

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

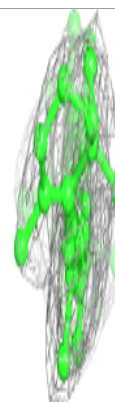
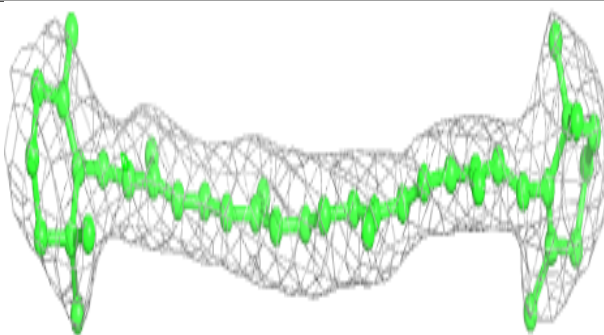
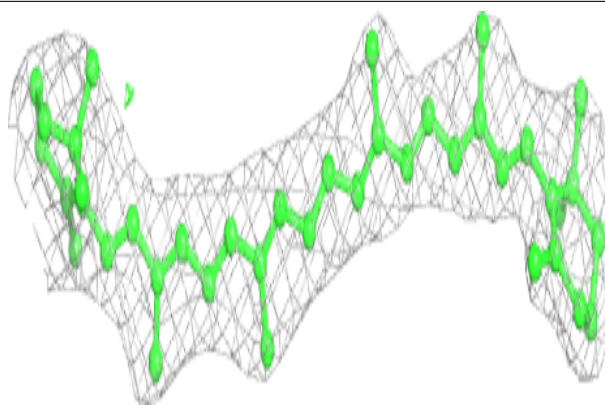
**Electron density around DGD c 519:**

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

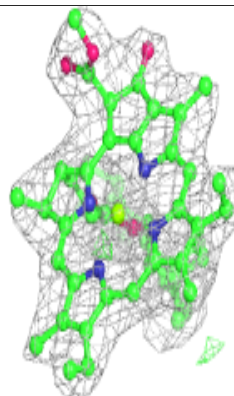
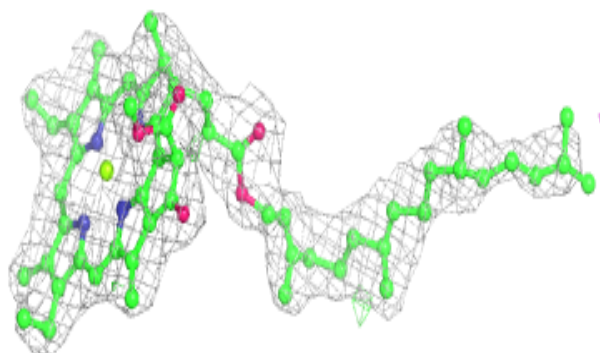
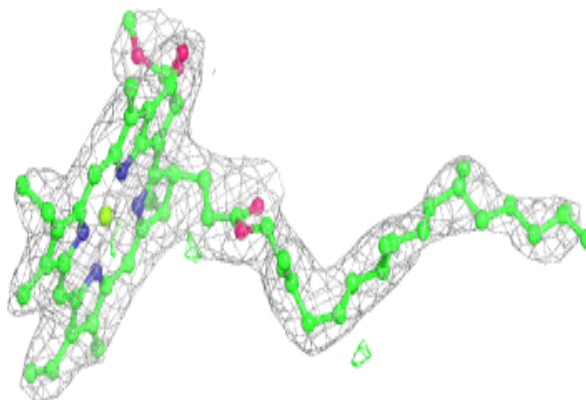


**Electron density around BCR k 102:**

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

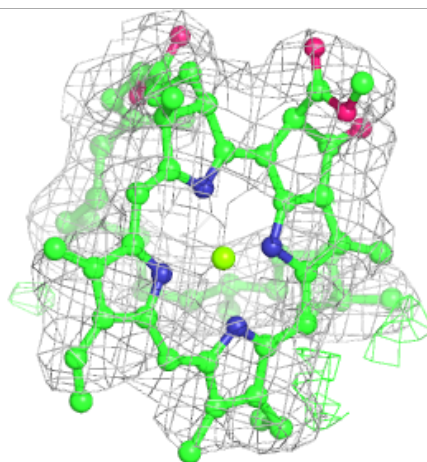
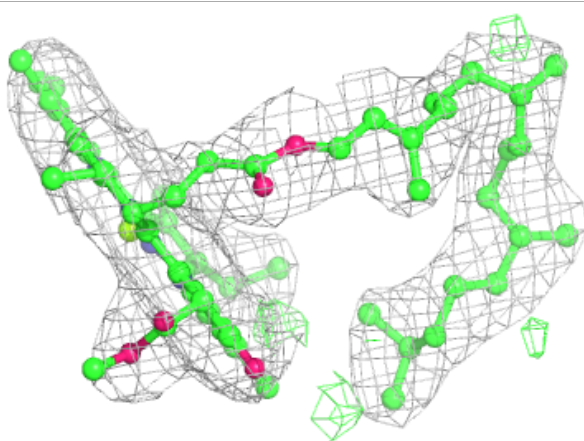
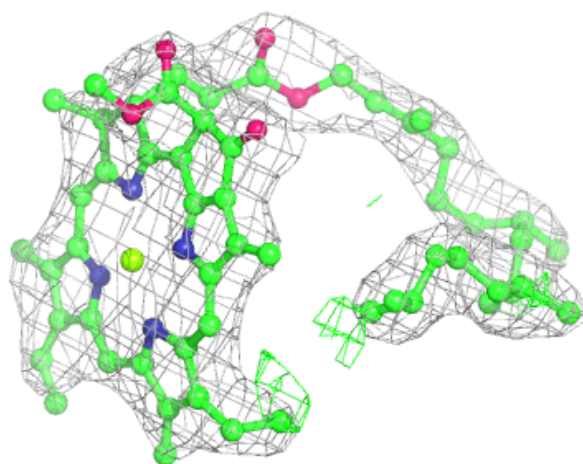
**Electron density around CLA c 503:**

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



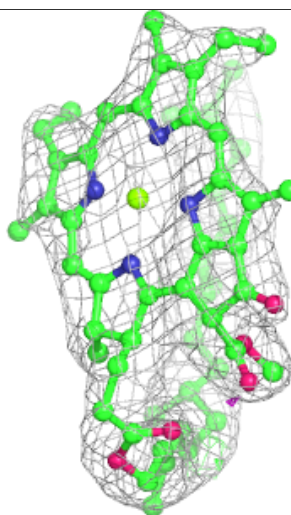
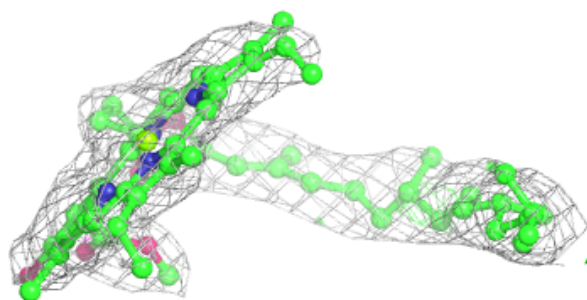
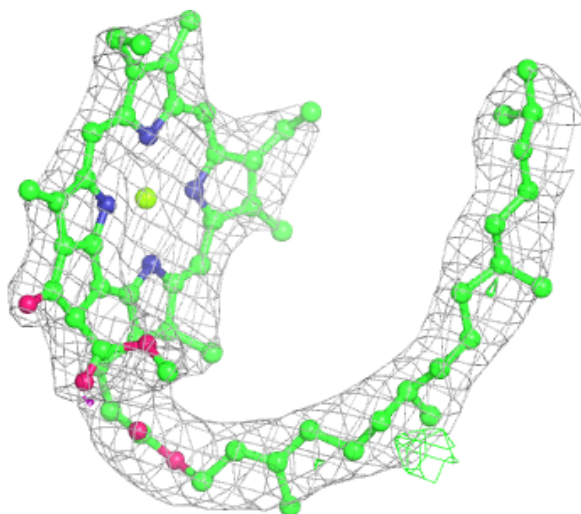
**Electron density around CLA c 504:**

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



**Electron density around CLA c 508:**

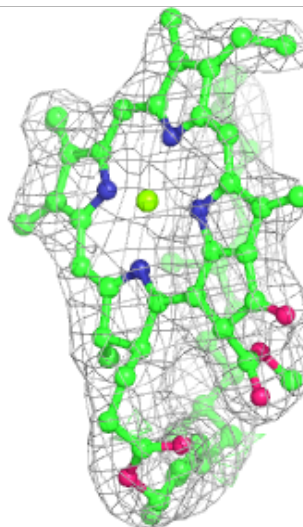
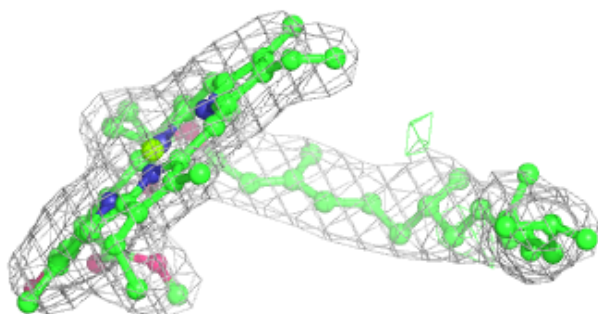
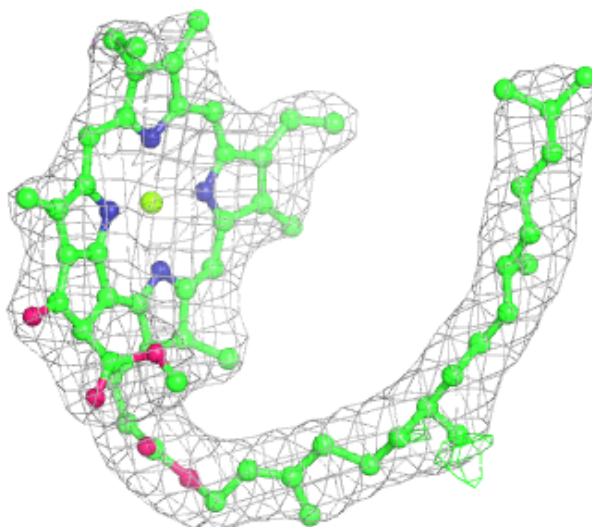
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





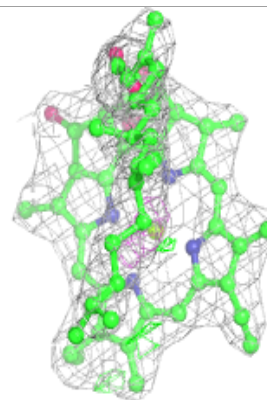
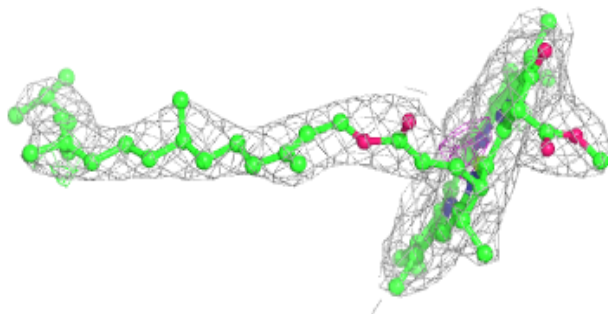
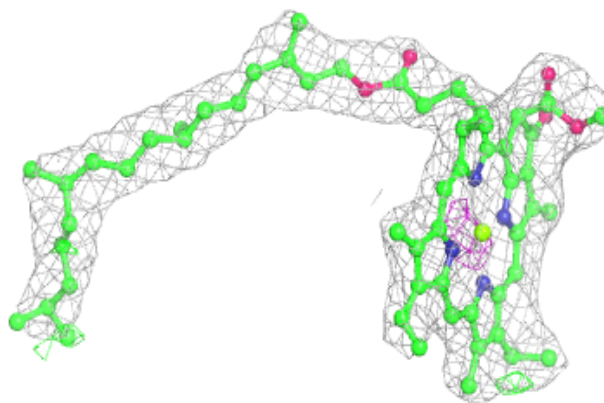
**Electron density around CLA C 508:**

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

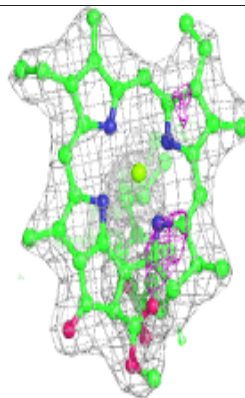
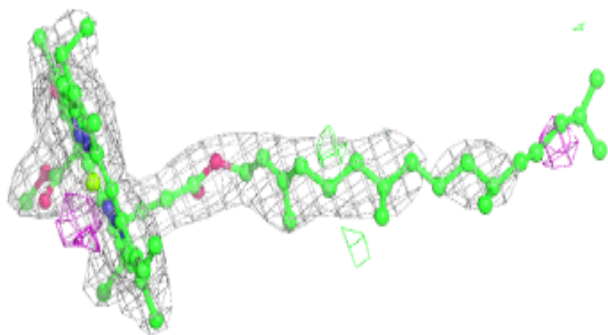
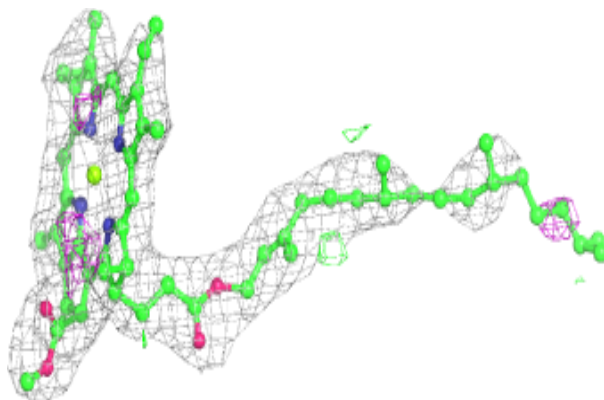


**Electron density around CLA b 609:**

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

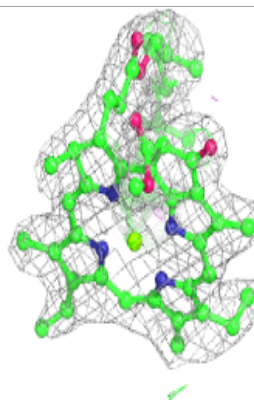
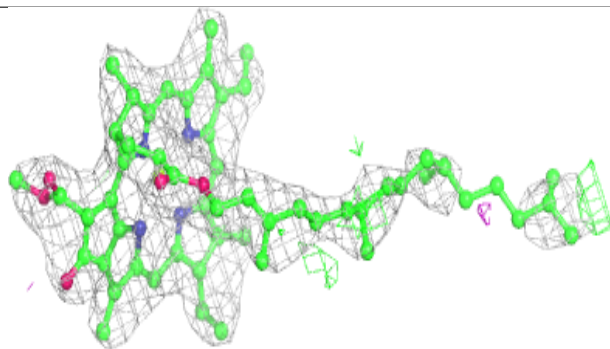
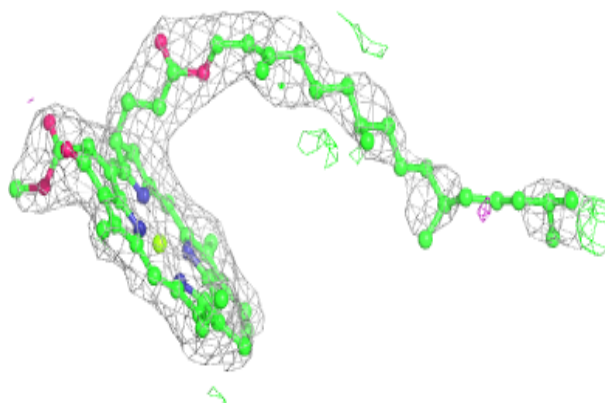
**Electron density around CLA d 404:**

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

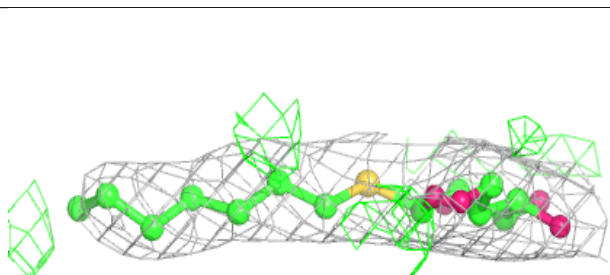
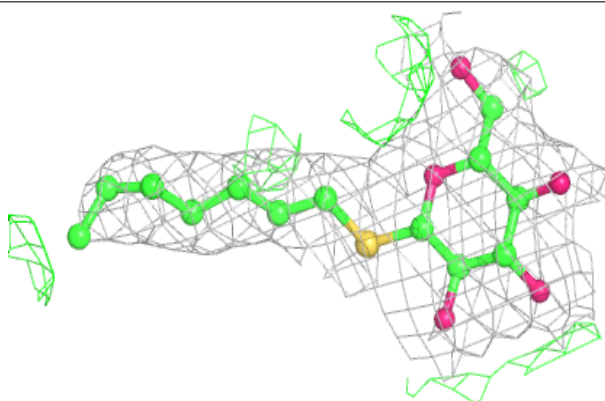


**Electron density around CLA c 505:**

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

**Electron density around HTG b 624:**

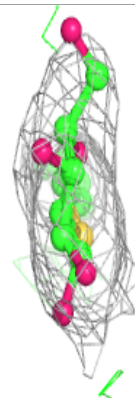
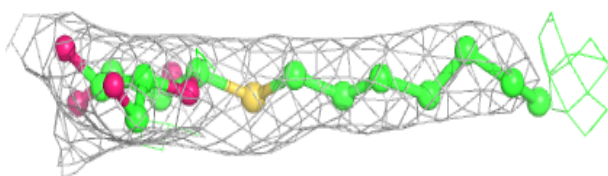
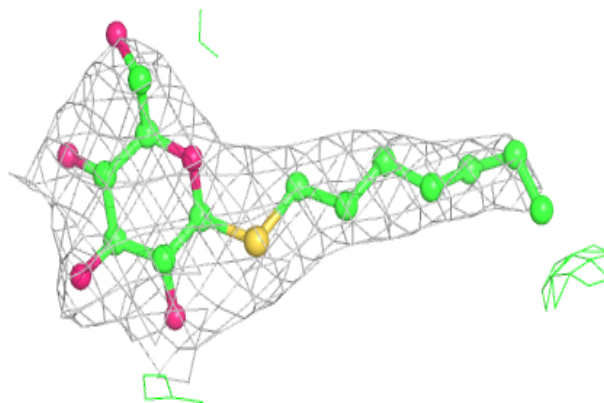
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



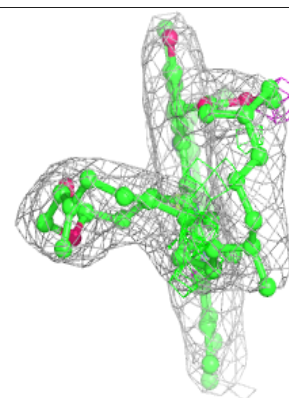
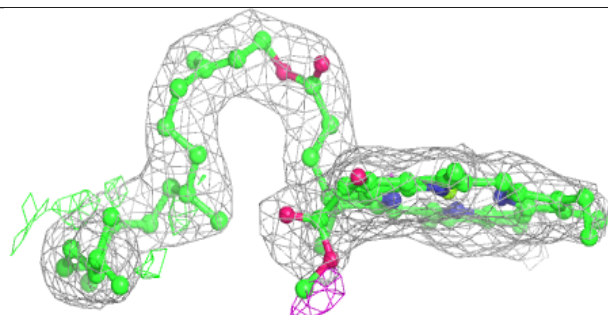
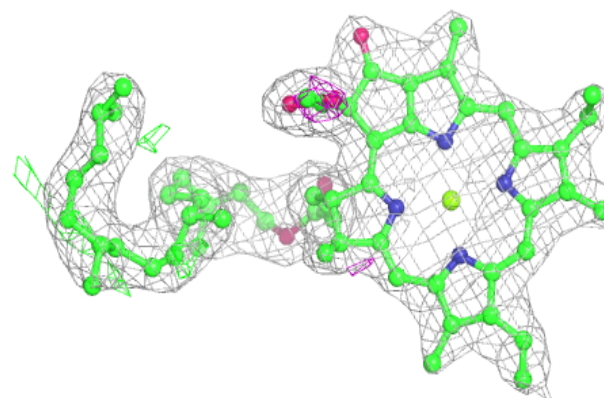


**Electron density around HTG B 624:**

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

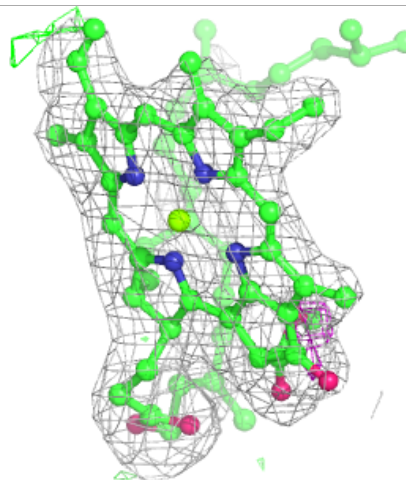
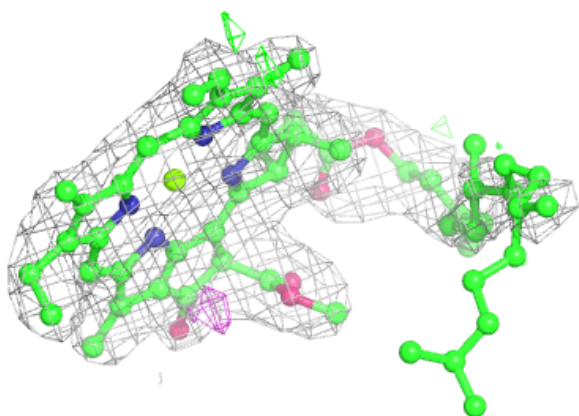
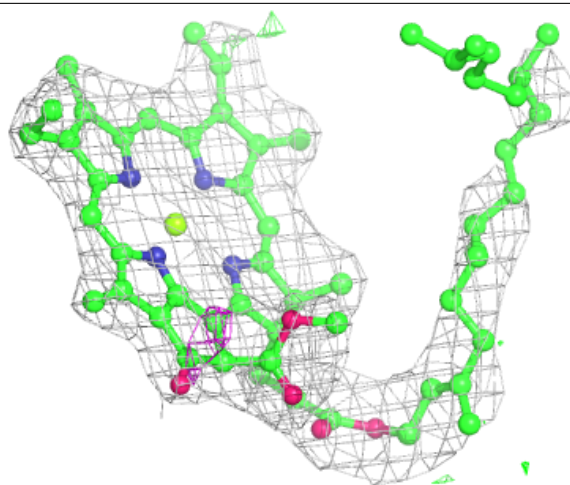
**Electron density around CLA b 612:**

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



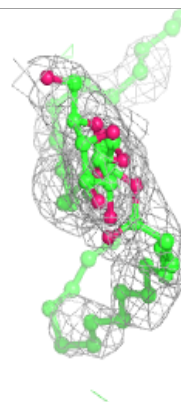
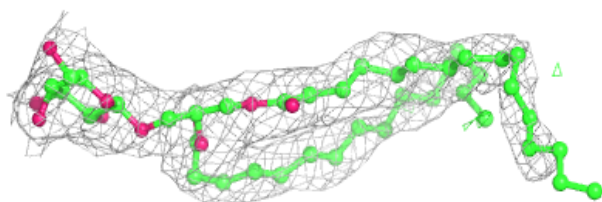
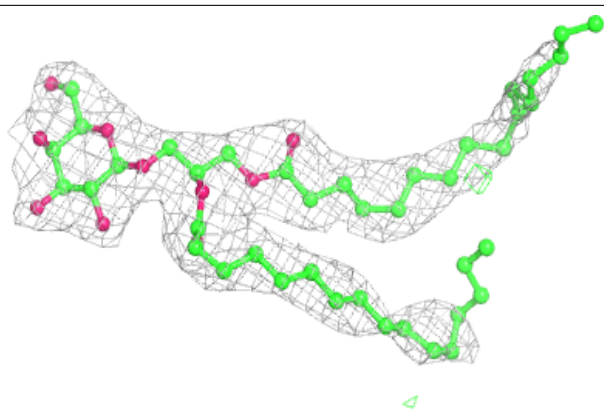
**Electron density around CLA b 616:**

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

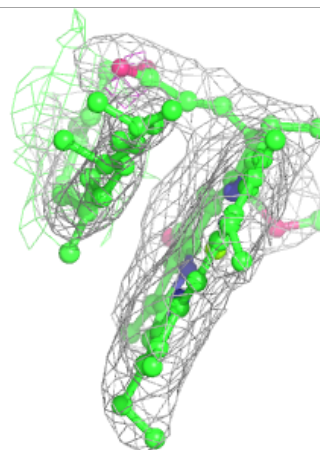
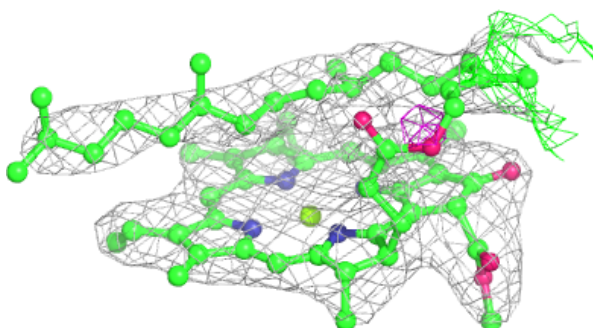
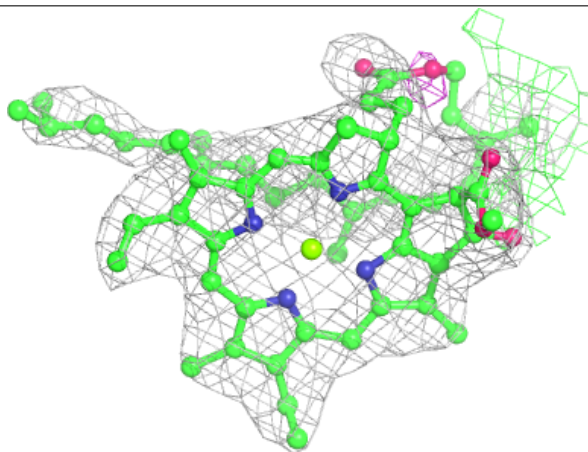


**Electron density around LMG d 412:**

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

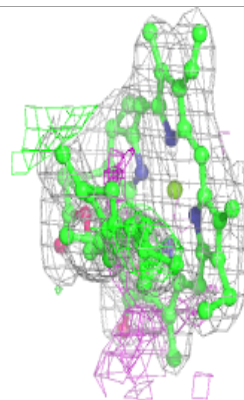
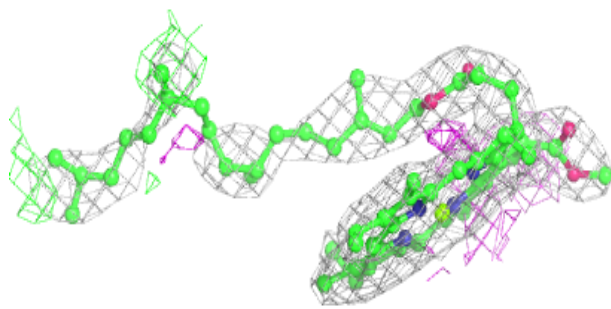
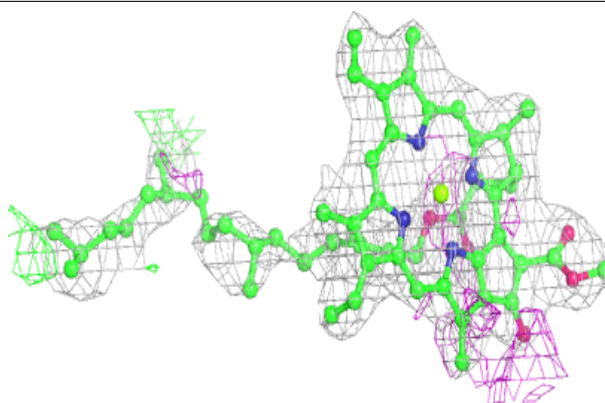
**Electron density around CLA b 601:**

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

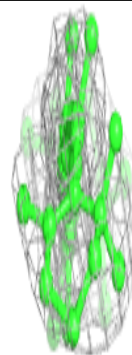
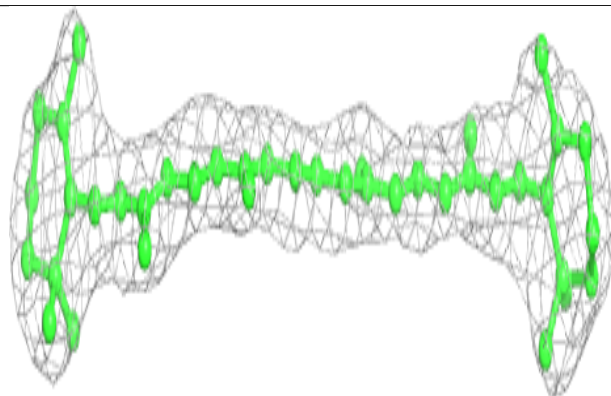
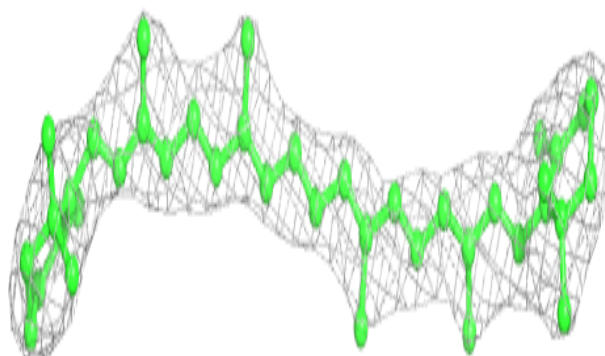


**Electron density around CLA B 614:**

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

**Electron density around BCR C 515:**

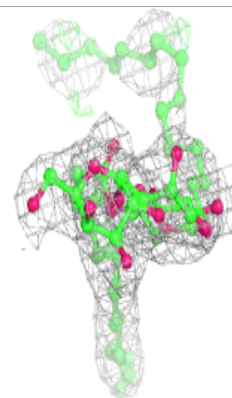
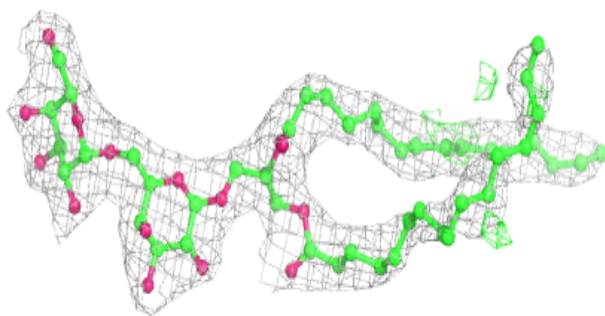
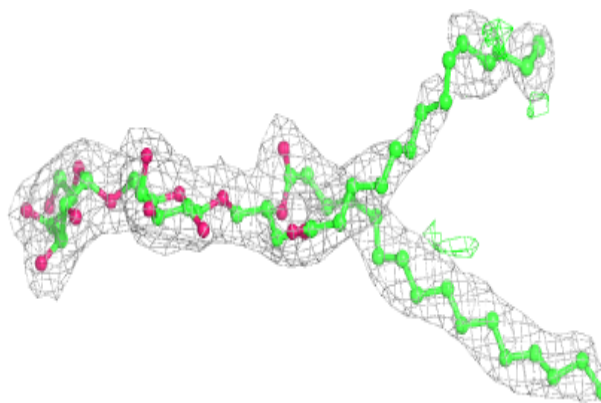
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



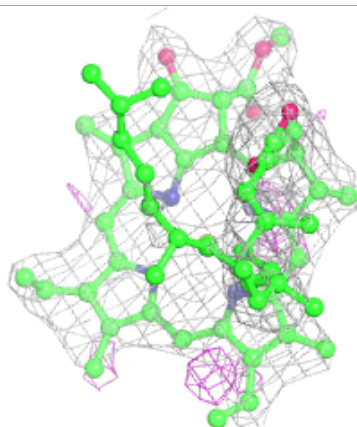
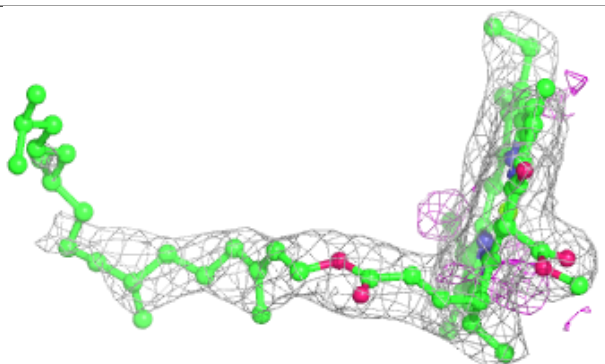
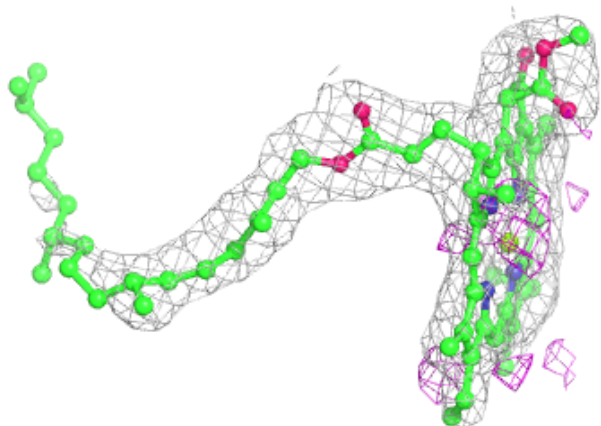


**Electron density around DGD C 517:**

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

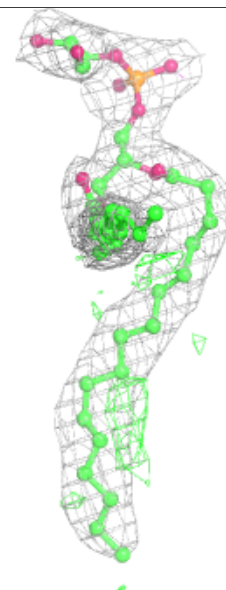
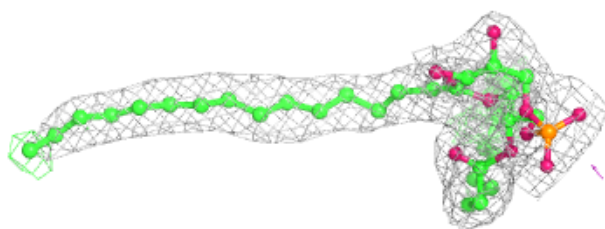
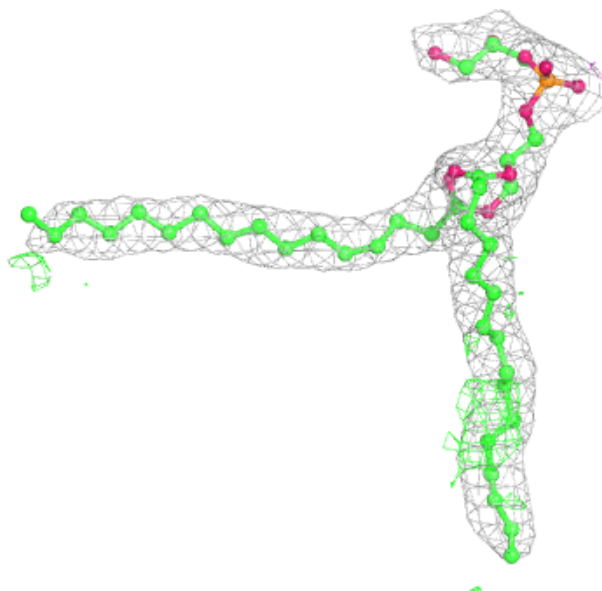
**Electron density around CLA D 406:**

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



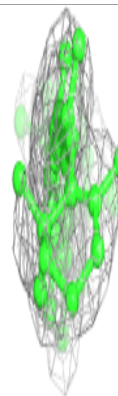
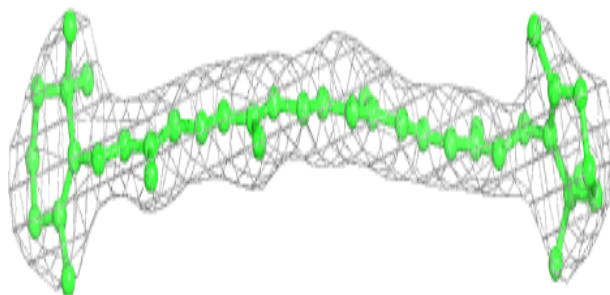
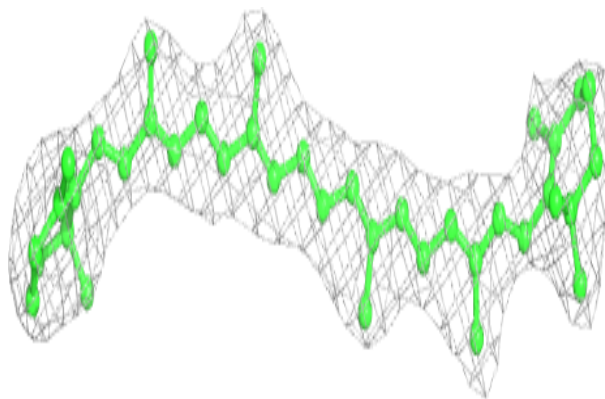
**Electron density around LHG L 101:**

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

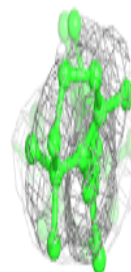
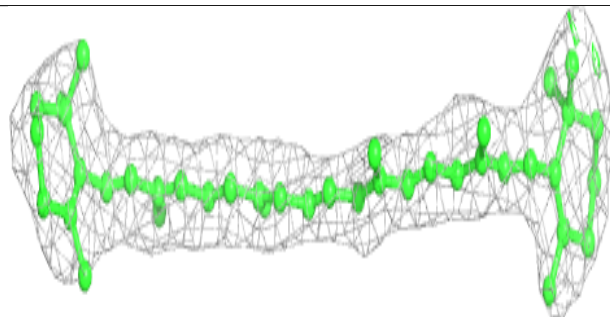
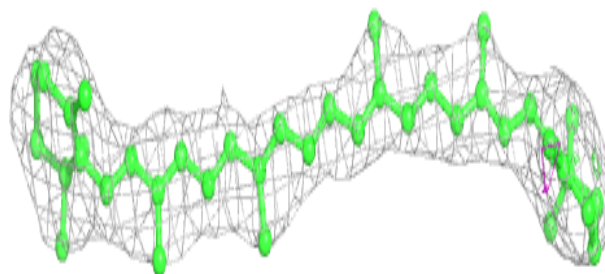


**Electron density around BCR Y 101:**

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

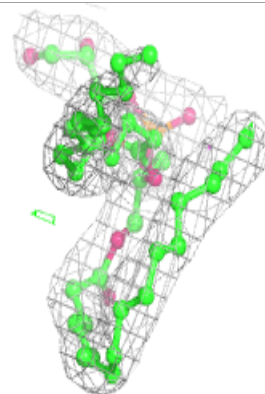
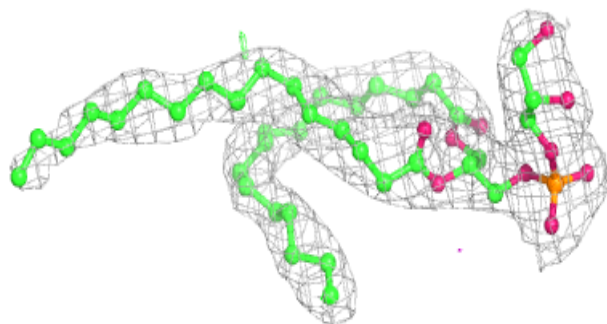
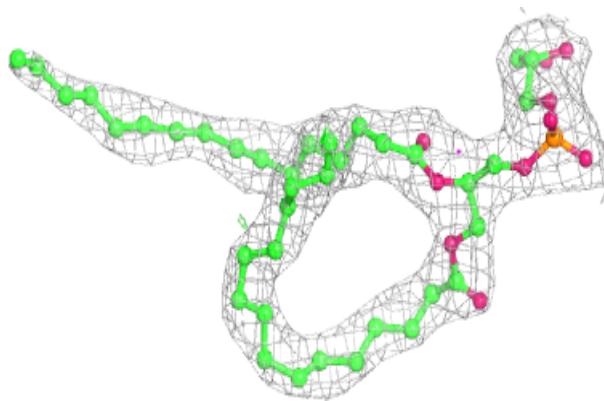
**Electron density around BCR c 515:**

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



**Electron density around LHG d 407:**

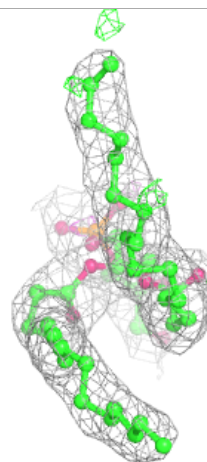
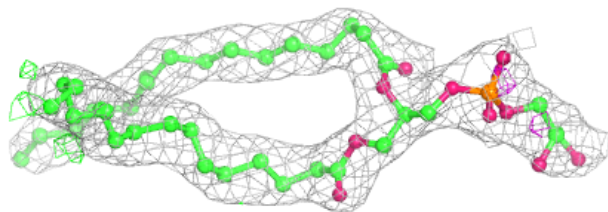
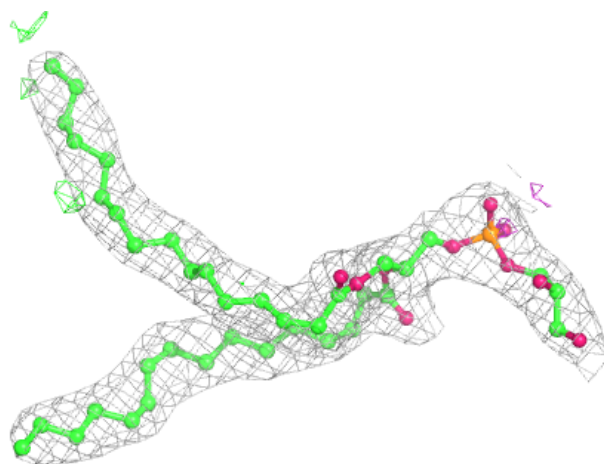
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





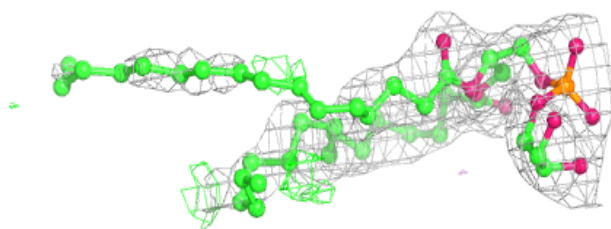
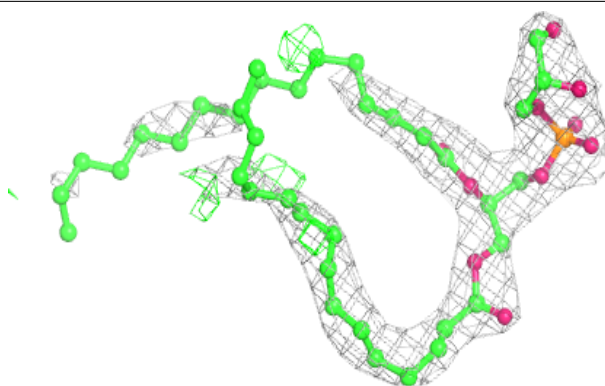
**Electron density around LHG d 408:**

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

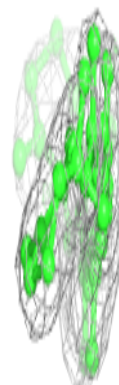
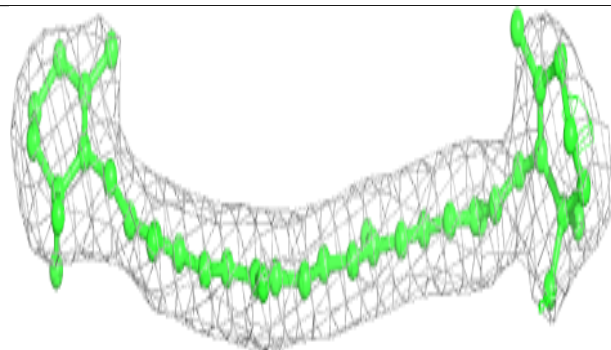
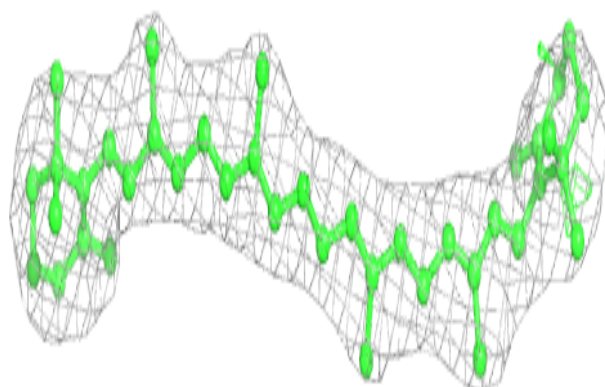


**Electron density around LHG d 409:**

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

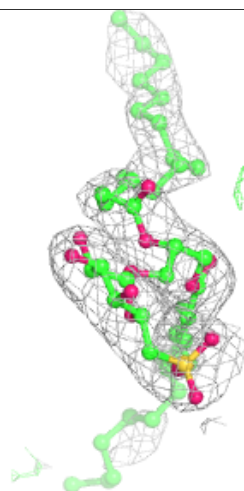
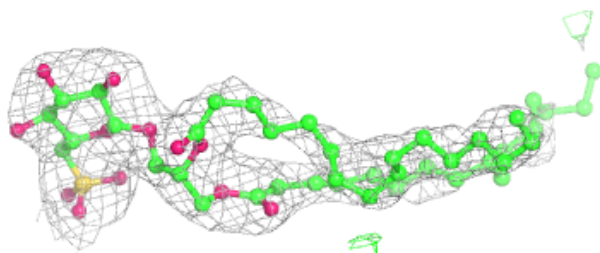
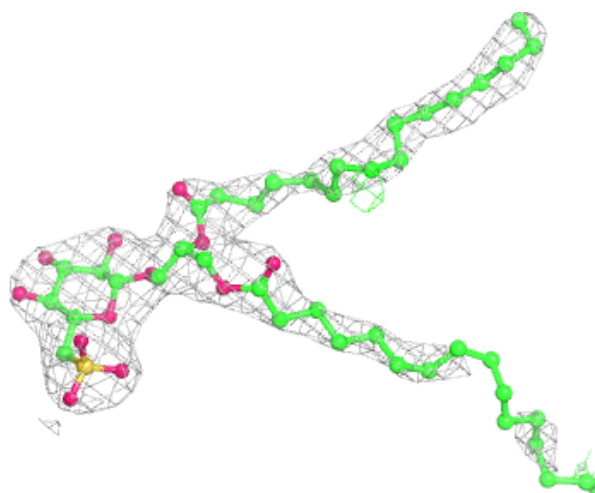
**Electron density around BCR d 405:**

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



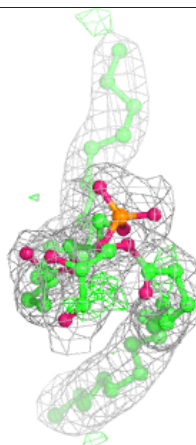
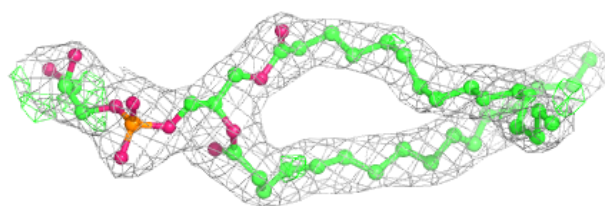
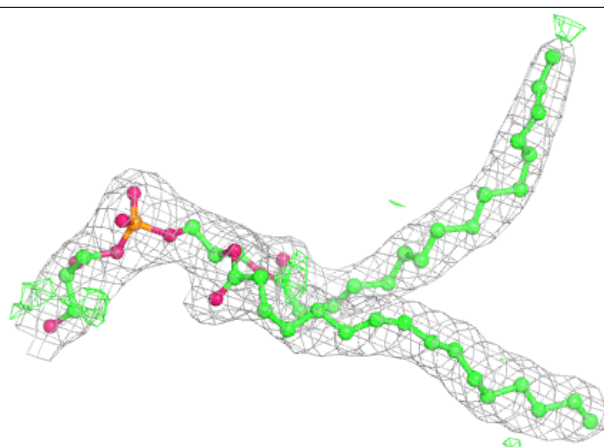
**Electron density around SQD a 409:**

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

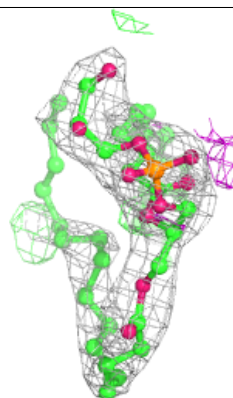
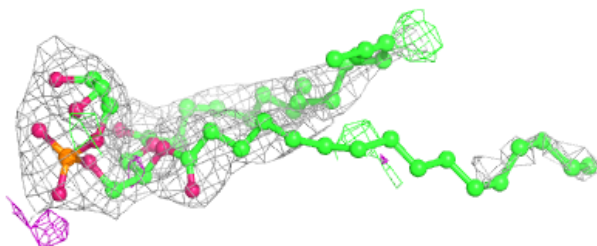
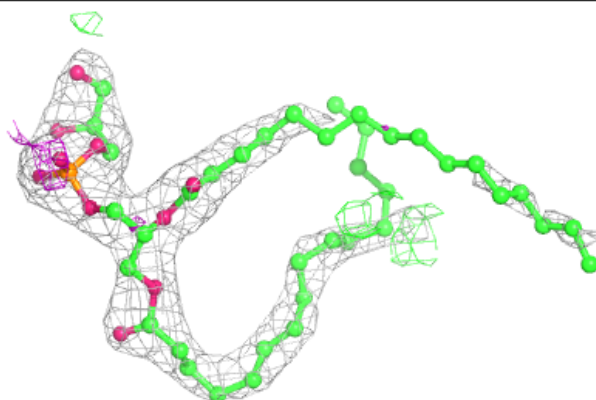


**Electron density around LHG D 409:**

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

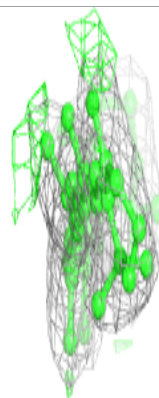
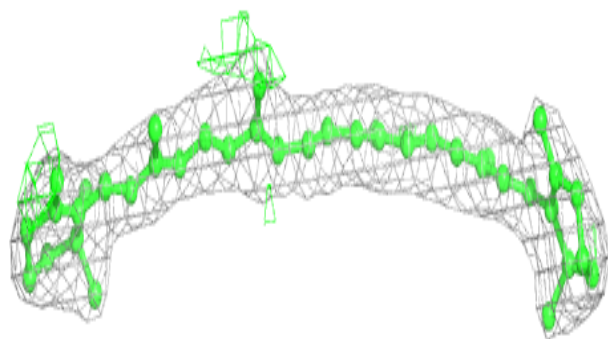
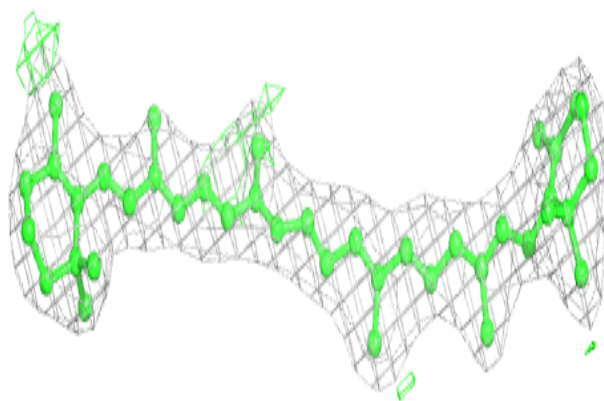
**Electron density around LHG D 410:**

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

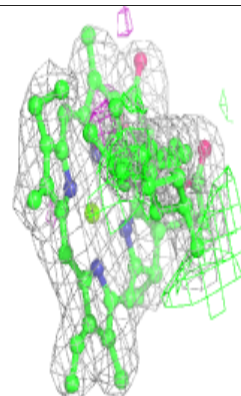
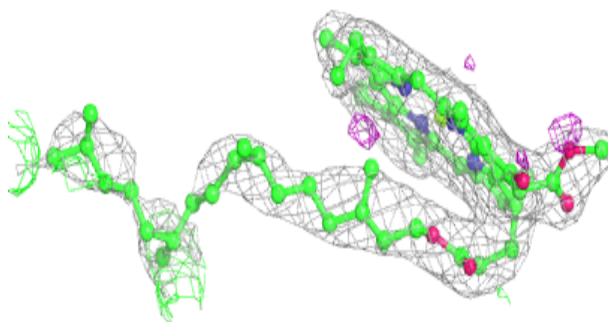
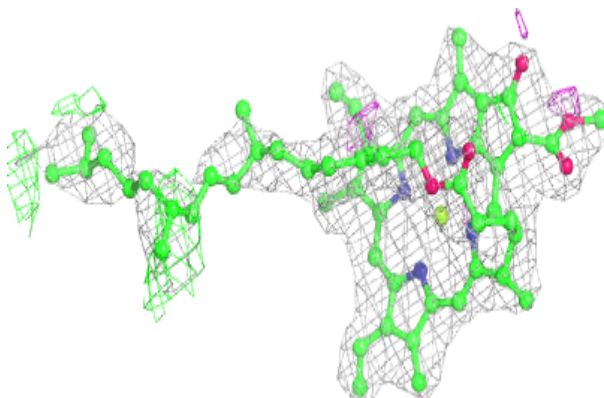


**Electron density around BCR T 101:**

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

**Electron density around CLA b 614:**

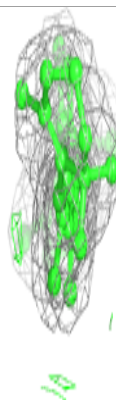
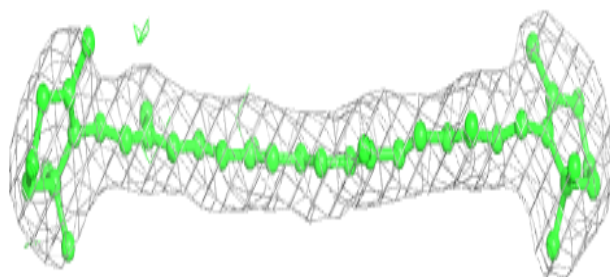
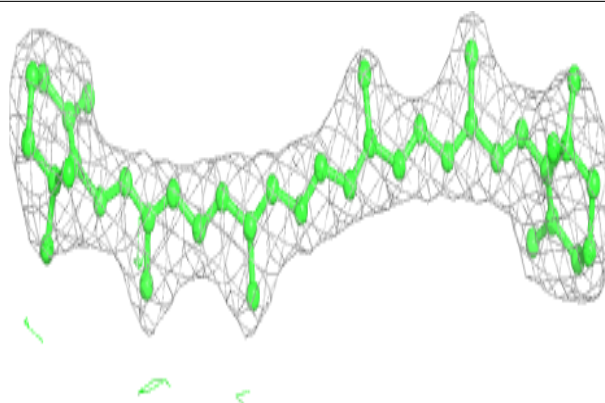
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



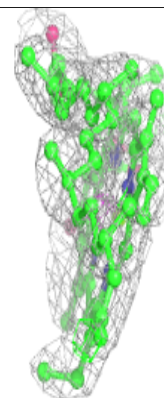
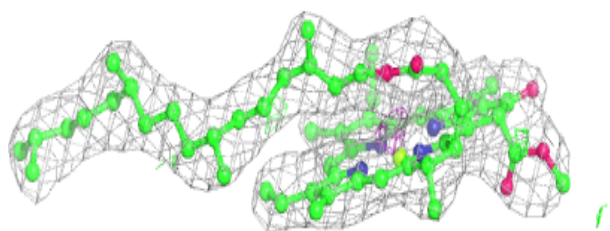
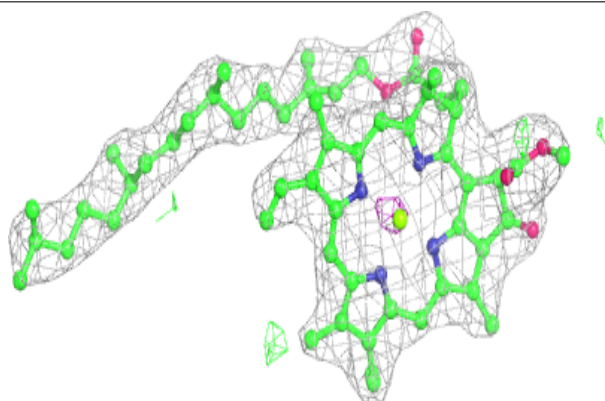


**Electron density around BCR b 618:**

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

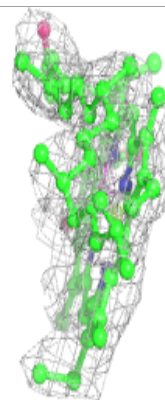
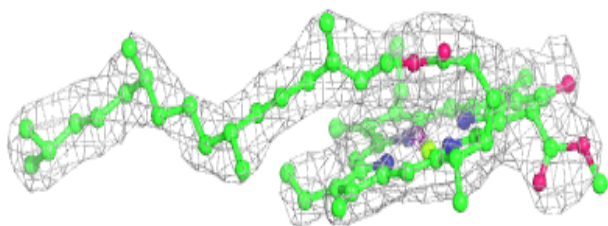
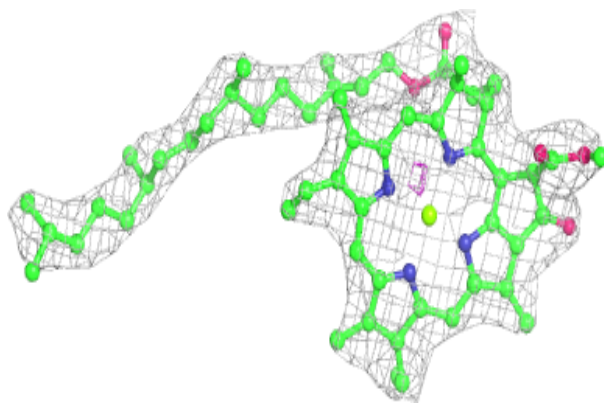
**Electron density around CLA C 502:**

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



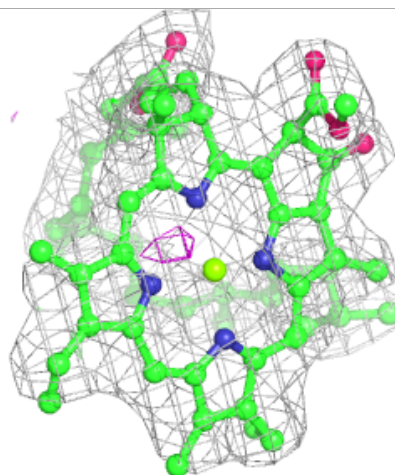
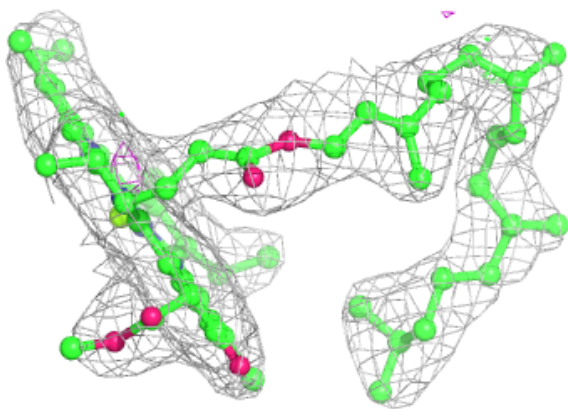
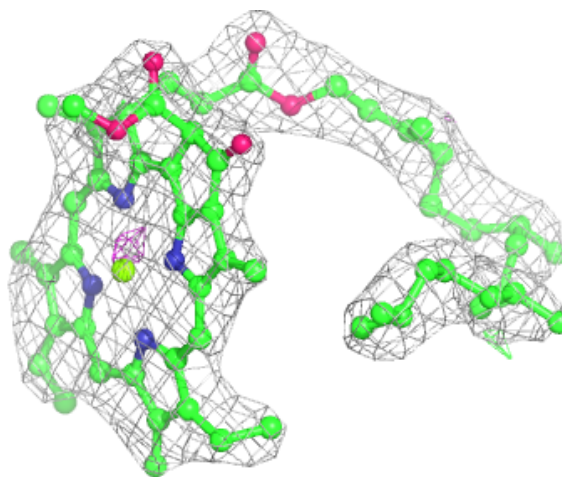
**Electron density around CLA c 502:**

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



**Electron density around CLA C 504:**

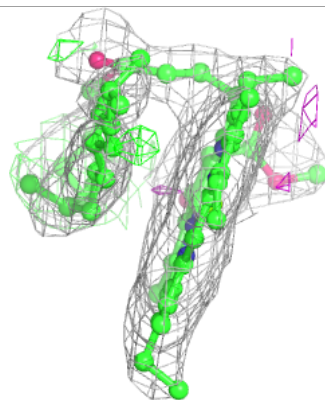
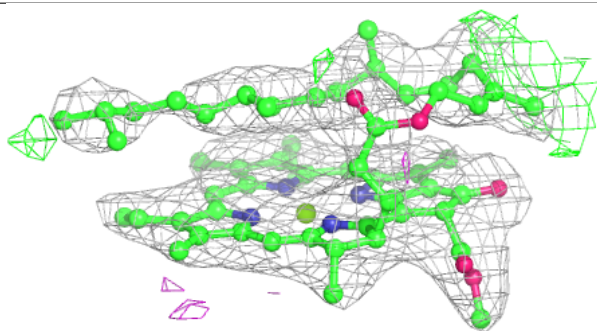
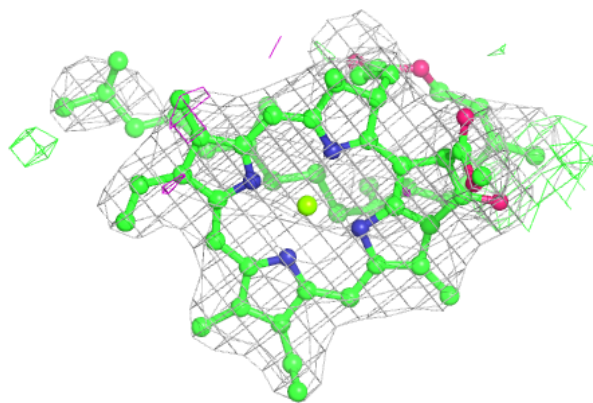
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





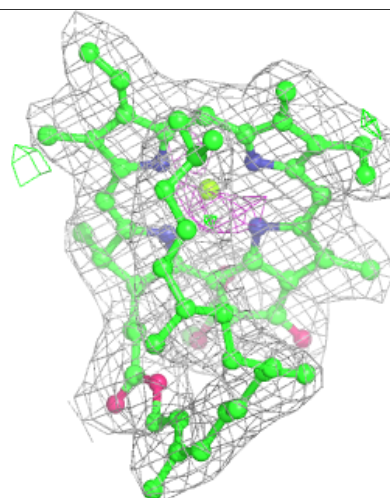
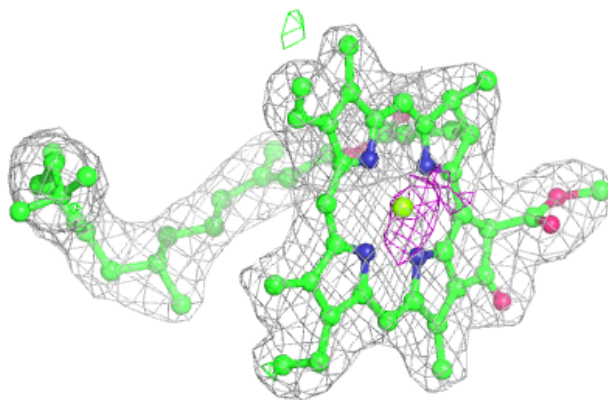
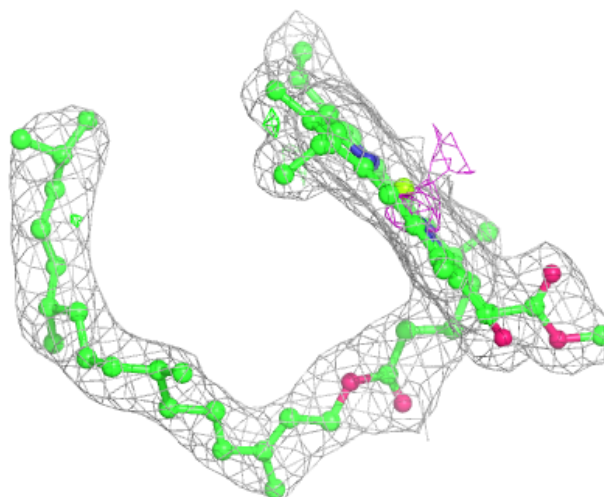
**Electron density around CLA B 601:**

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



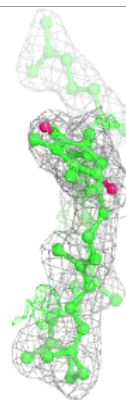
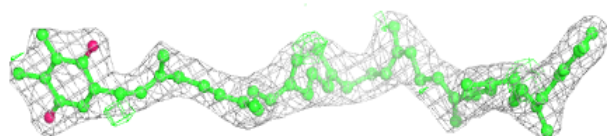
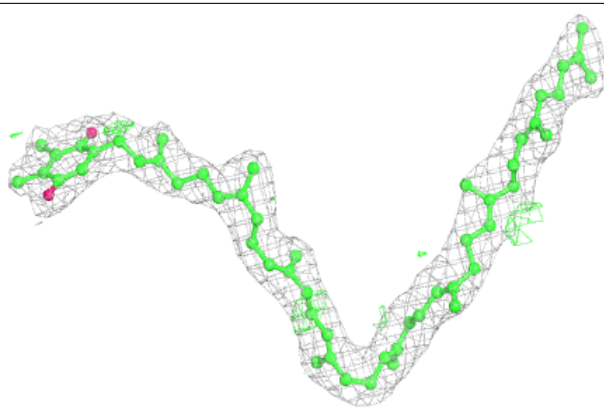
**Electron density around CLA B 611:**

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

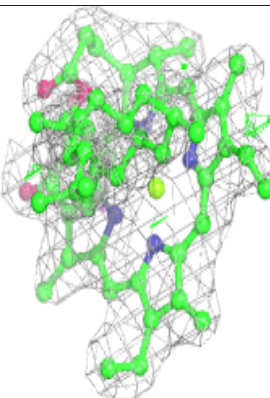
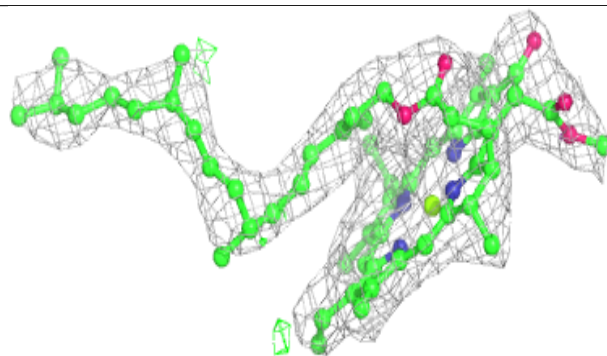
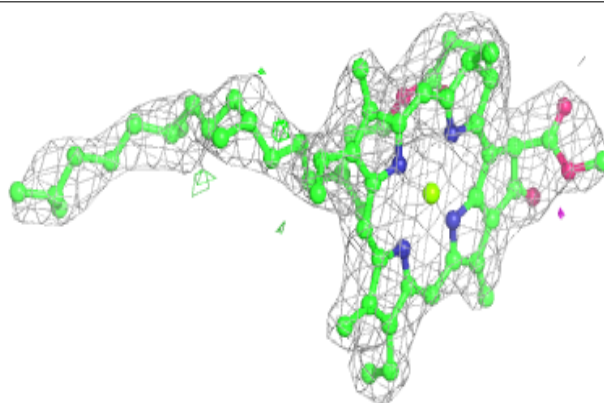


**Electron density around PL9 D 408:**

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

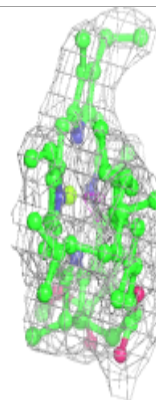
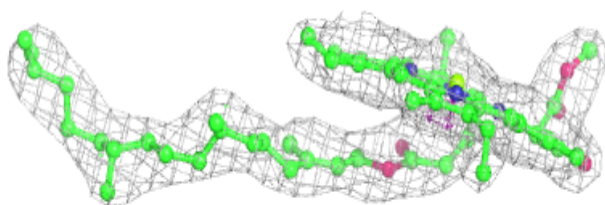
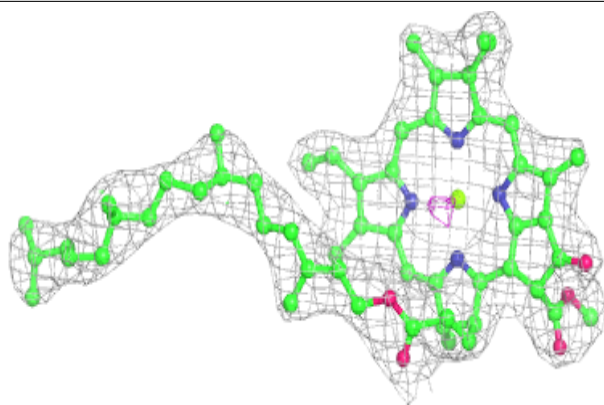
**Electron density around CLA c 506:**

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

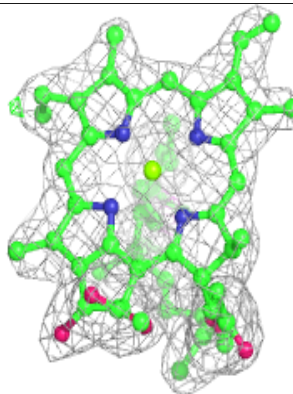
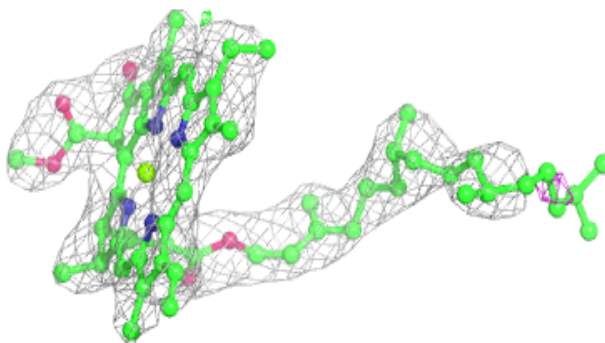
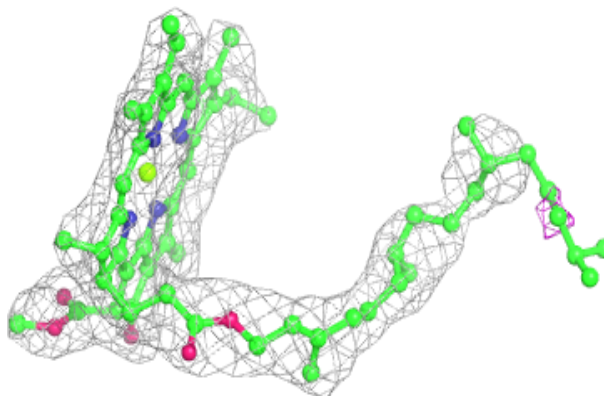


**Electron density around CLA B 603:**

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

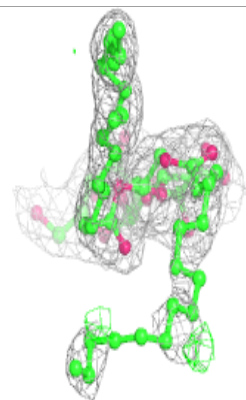
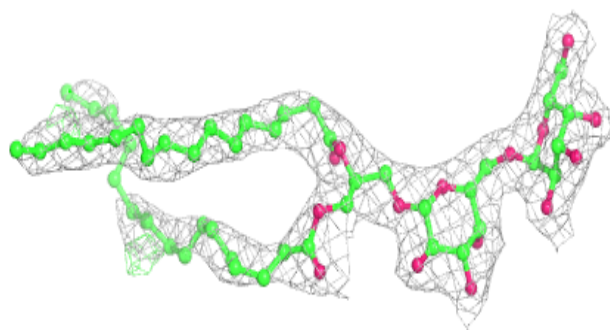
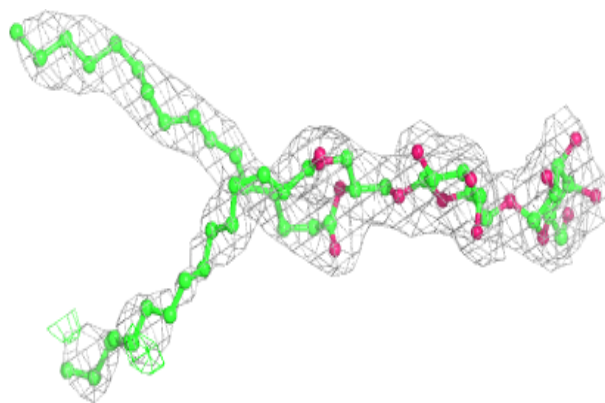
**Electron density around CLA c 509:**

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

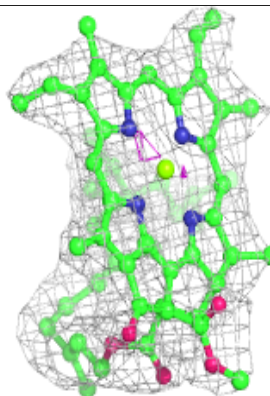
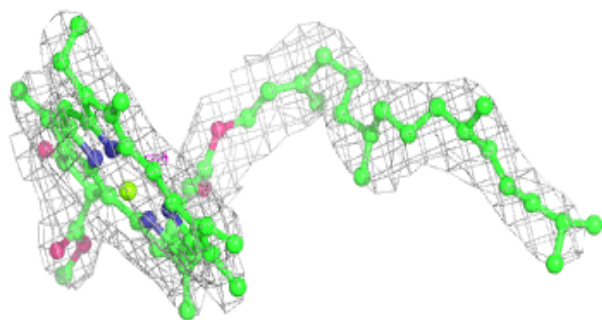
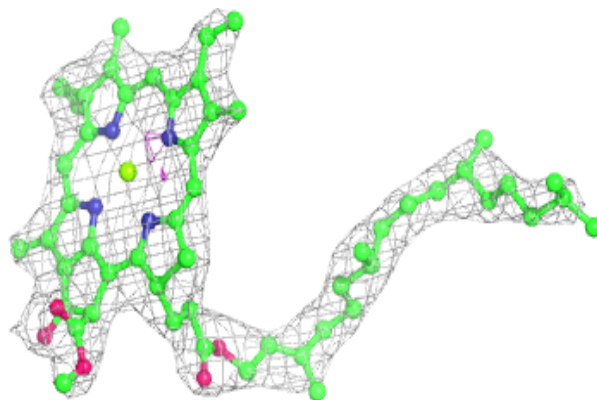


**Electron density around DGD c 517:**

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

**Electron density around CLA c 512:**

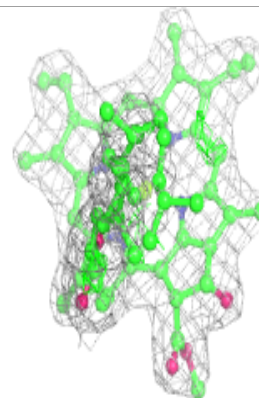
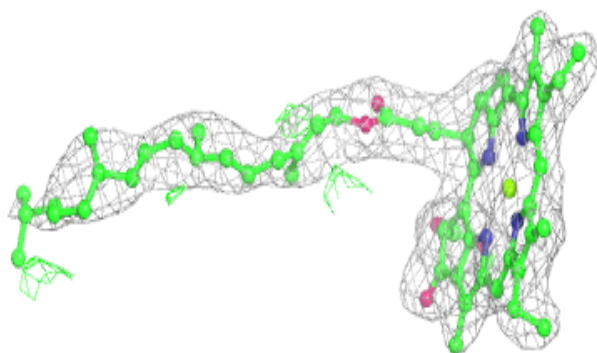
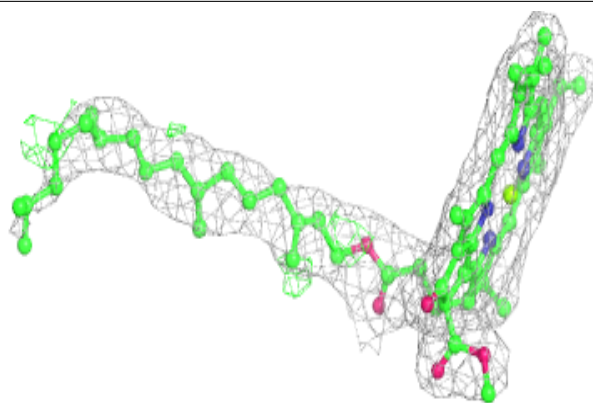
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



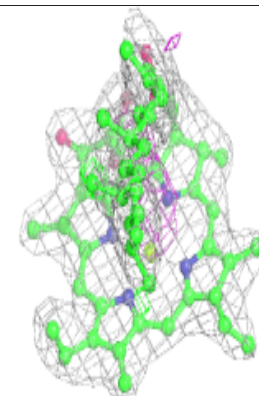
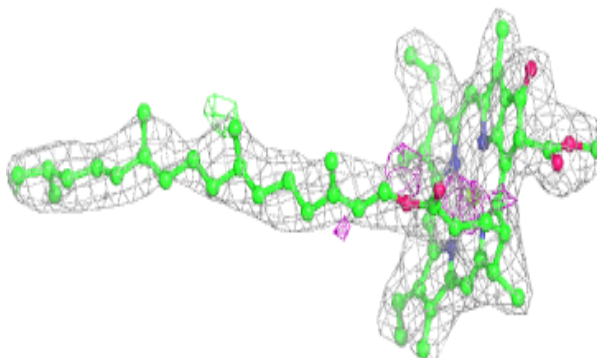
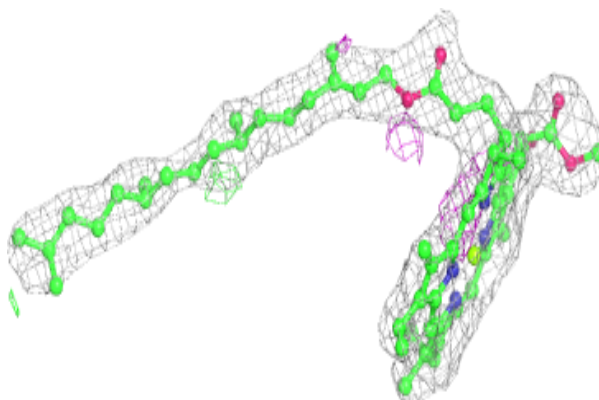


**Electron density around CLA b 604:**

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

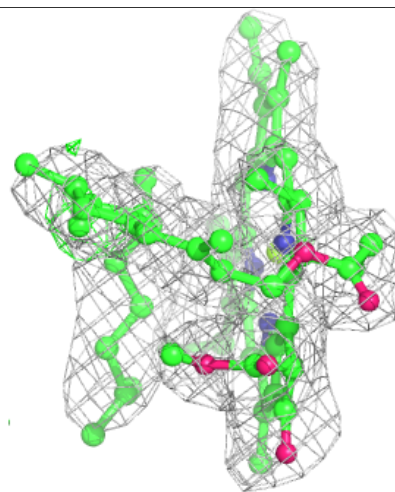
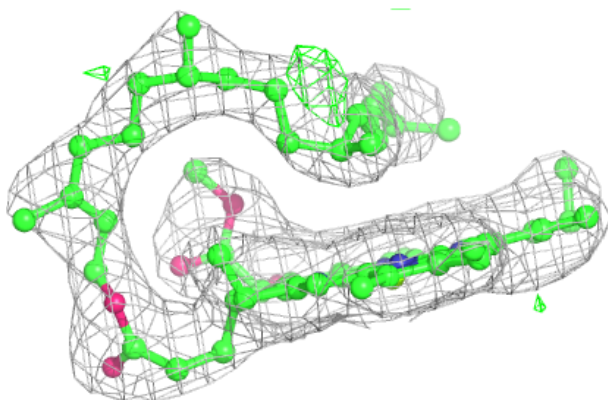
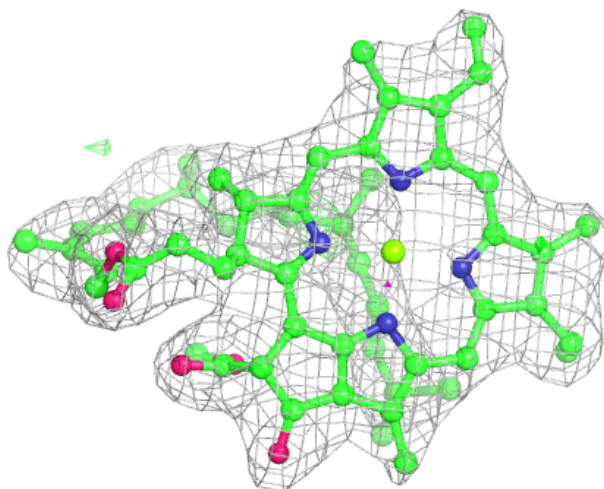
**Electron density around CLA b 607:**

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



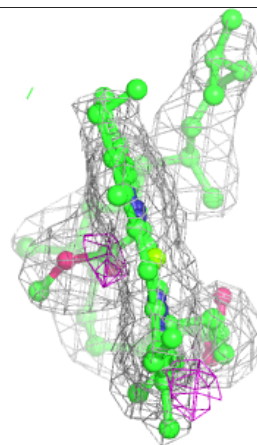
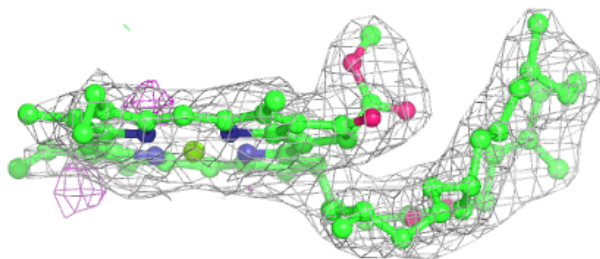
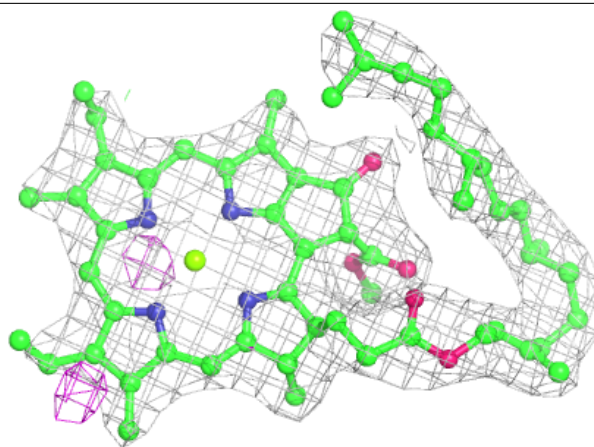
**Electron density around CLA C 511:**

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

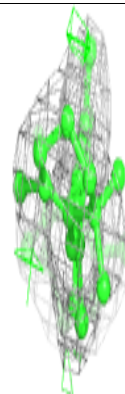
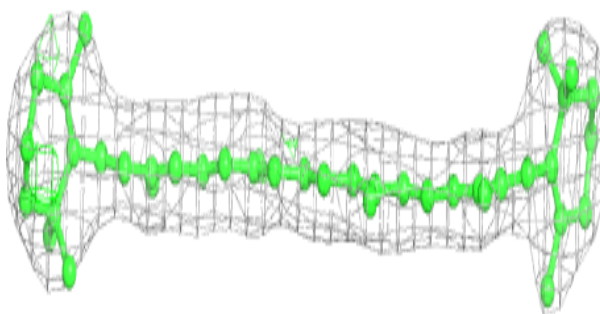
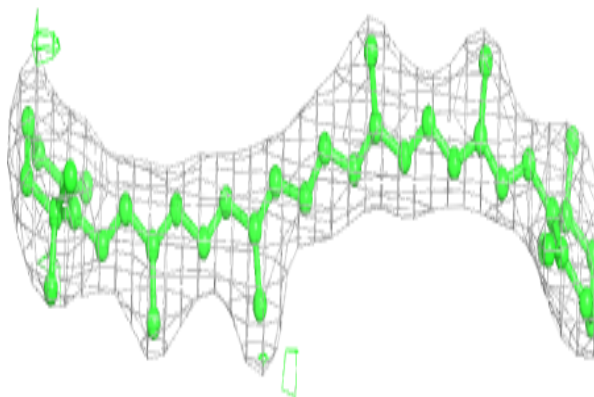


**Electron density around CLA b 610:**

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

**Electron density around BCR C 516:**

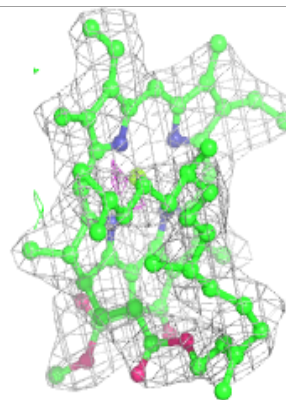
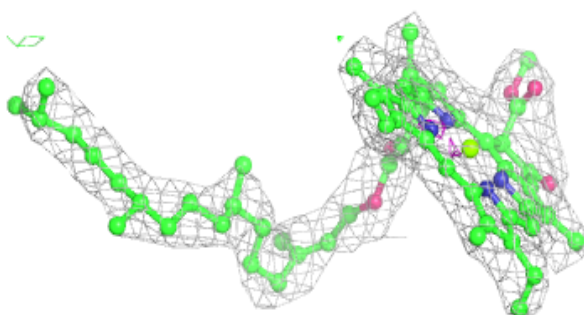
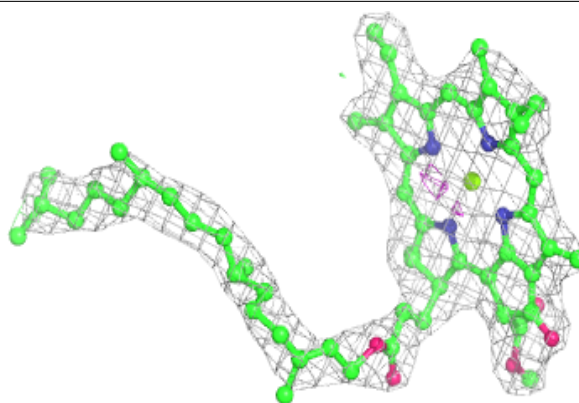
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



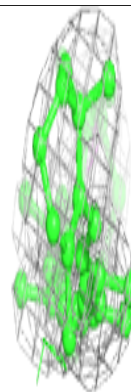
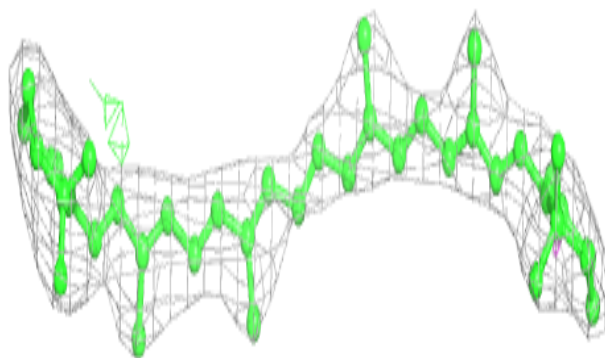
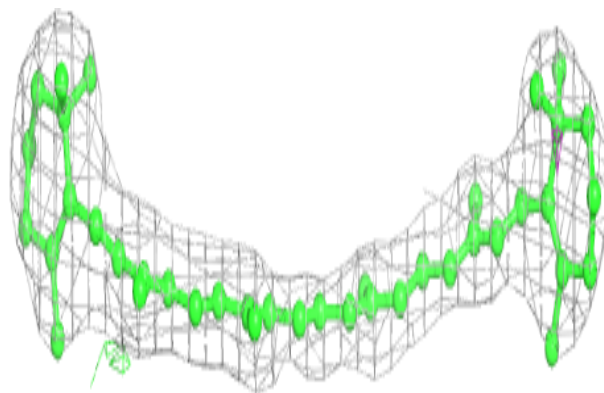


**Electron density around CLA C 512:**

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

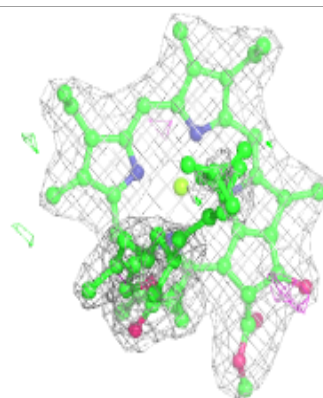
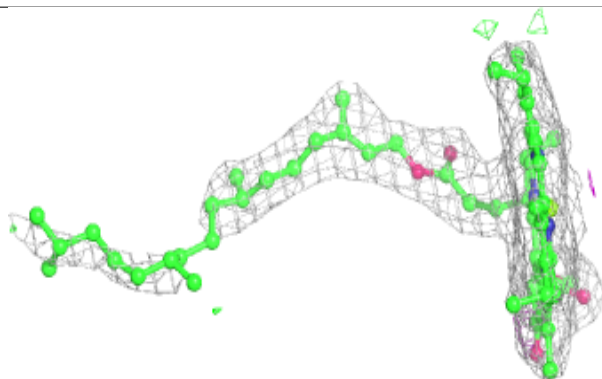
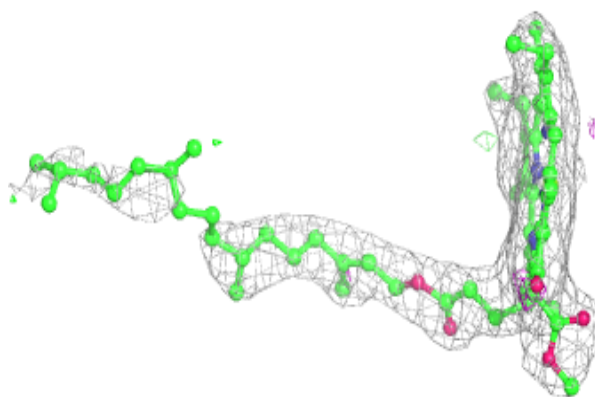
**Electron density around BCR K 101:**

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

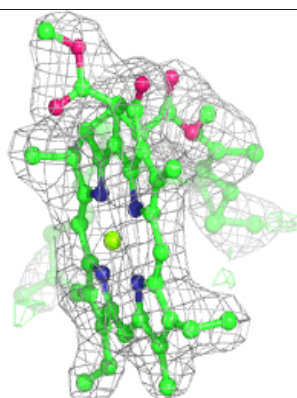
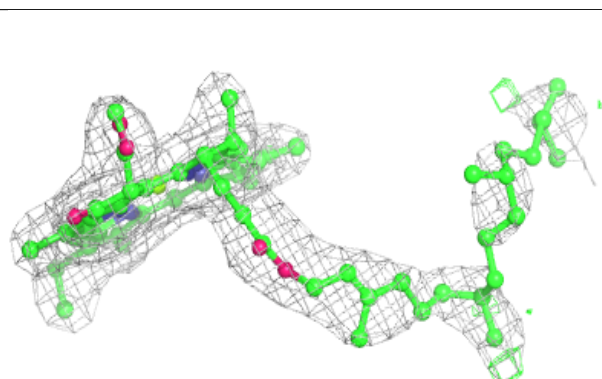
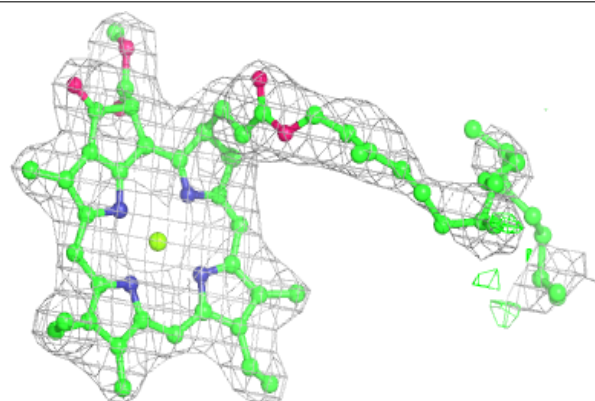


**Electron density around CLA b 606:**

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

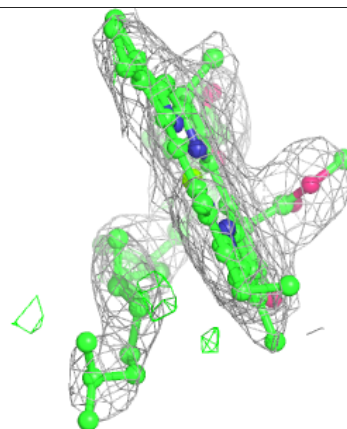
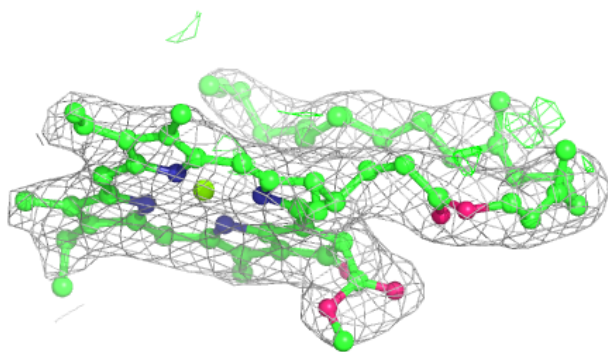
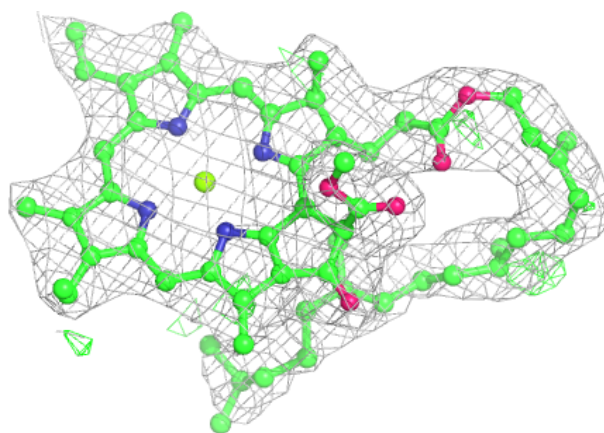
**Electron density around CLA A 408:**

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

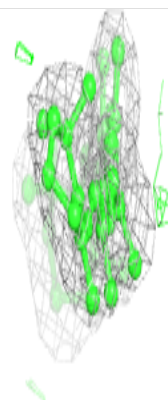
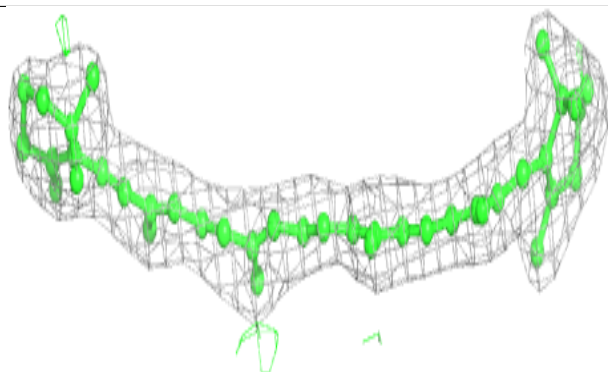
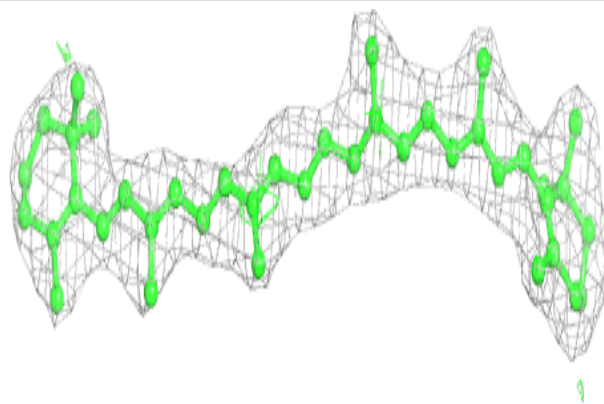


**Electron density around CLA c 510:**

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

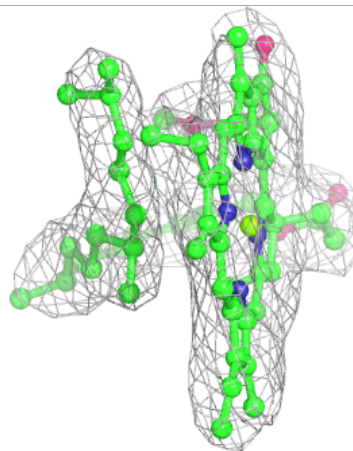
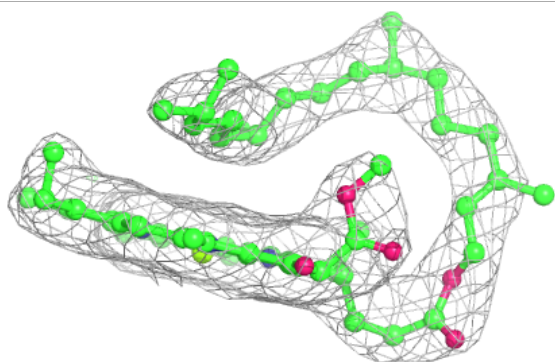
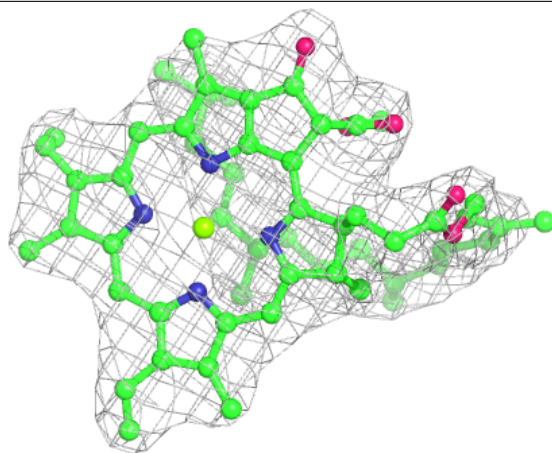
**Electron density around BCR t 102:**

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



**Electron density around CLA c 511:**

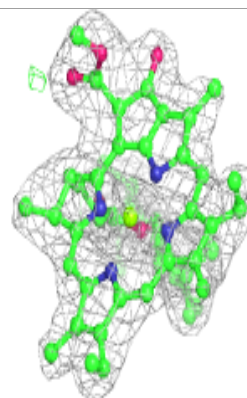
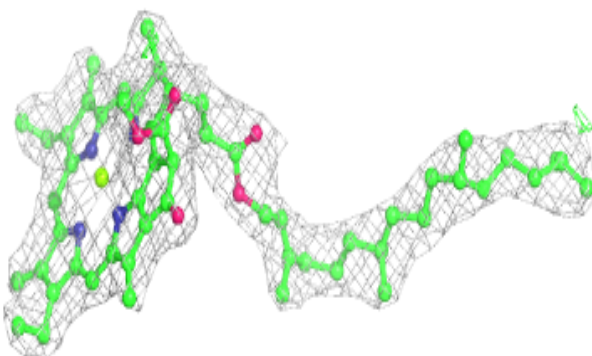
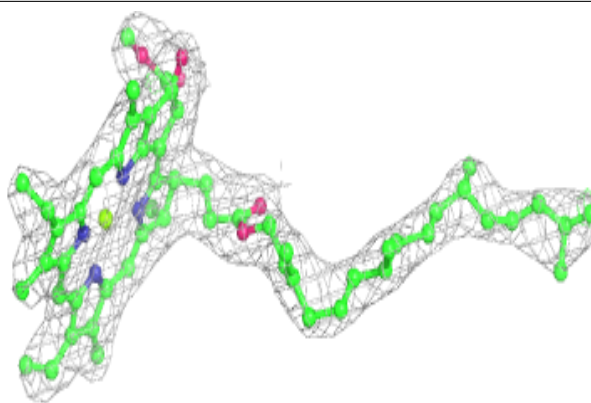
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



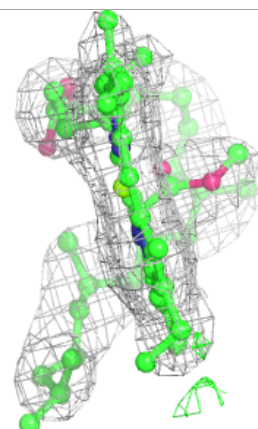
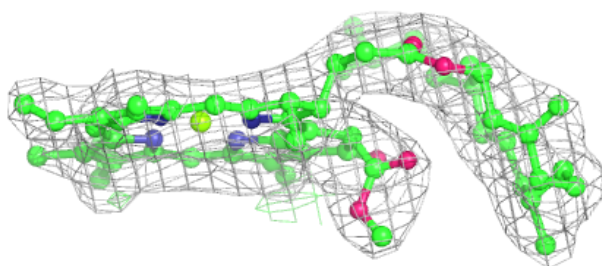
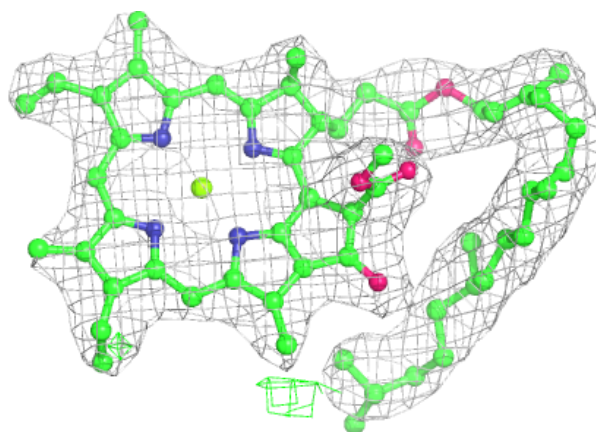


**Electron density around CLA C 503:**

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

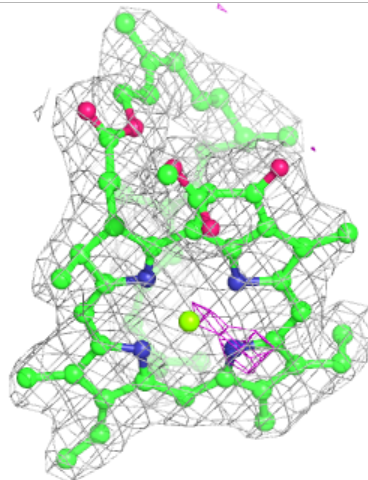
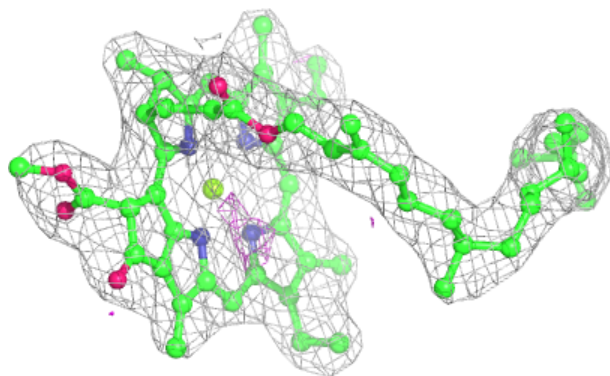
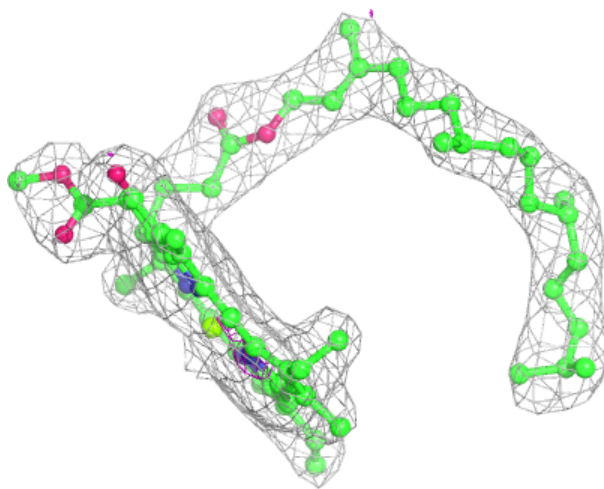
**Electron density around CLA B 610:**

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



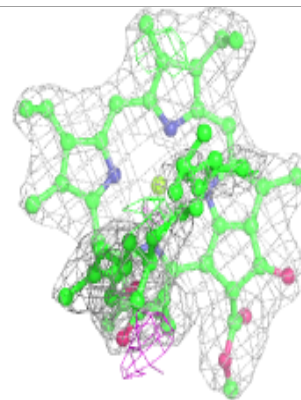
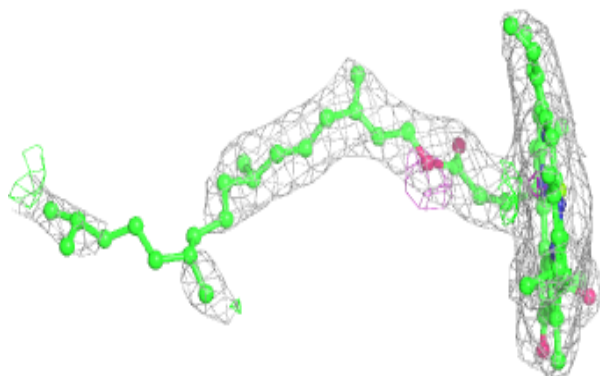
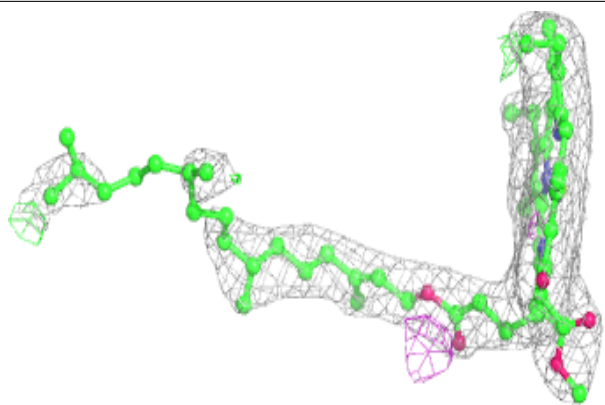
**Electron density around CLA b 611:**

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



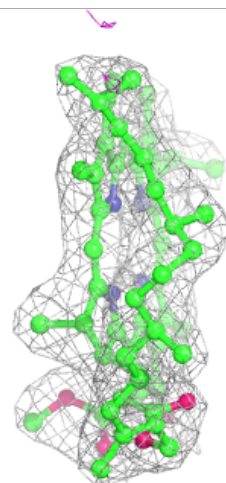
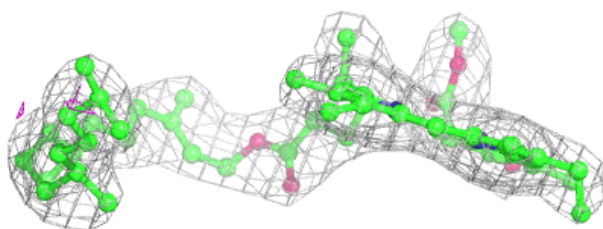
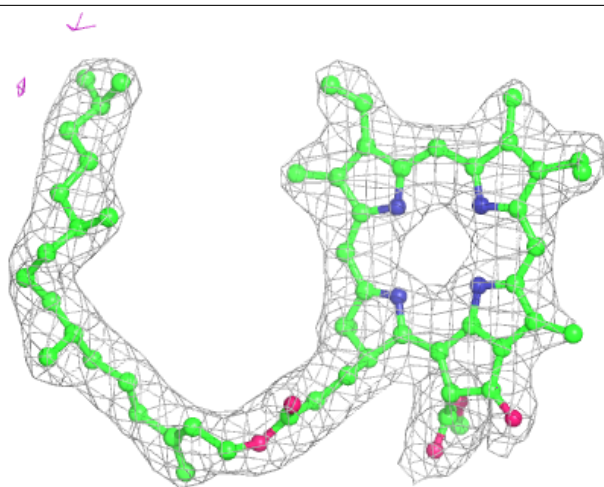
**Electron density around CLA B 606:**

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



**Electron density around PHO A 407:**

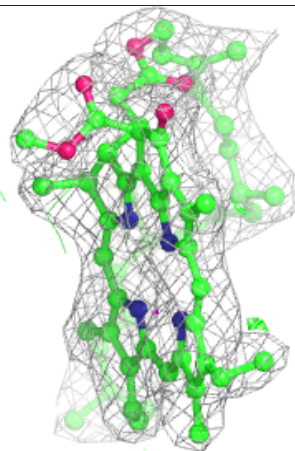
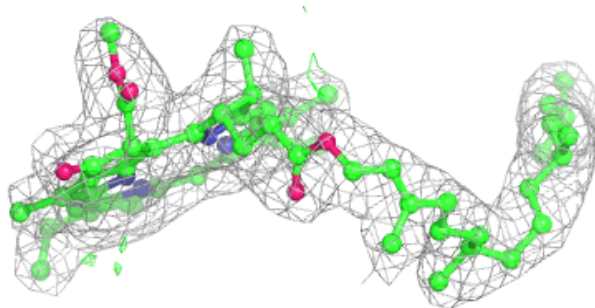
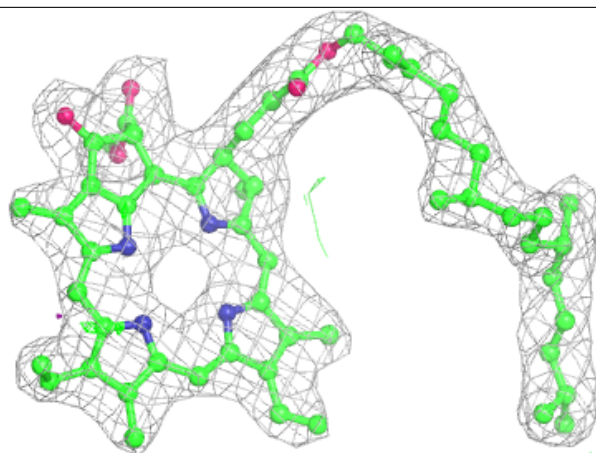
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



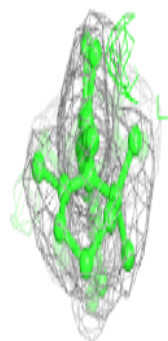
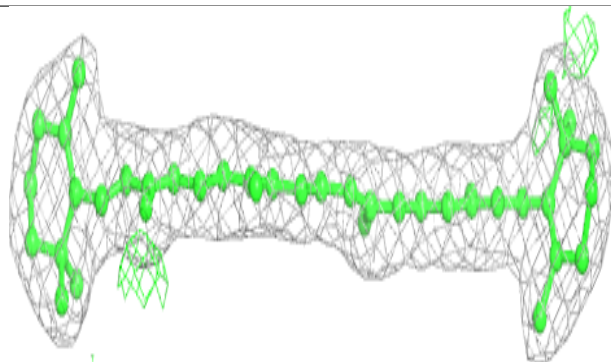
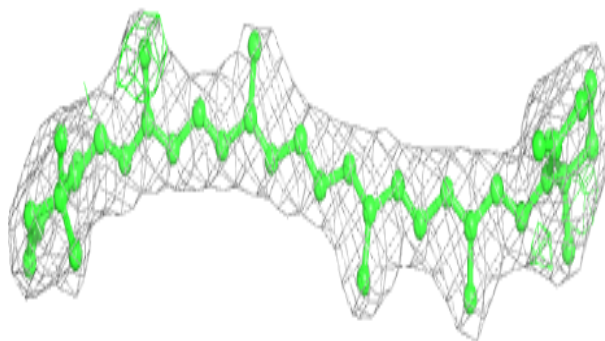


**Electron density around PHO D 402:**

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

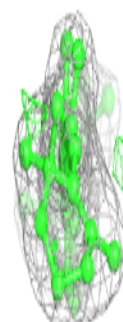
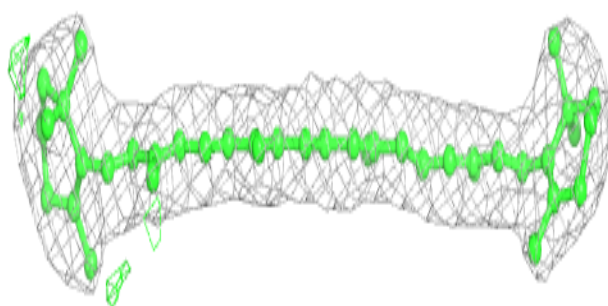
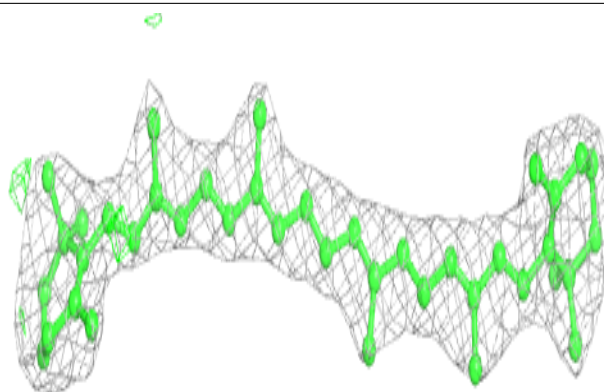
**Electron density around BCR A 409:**

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

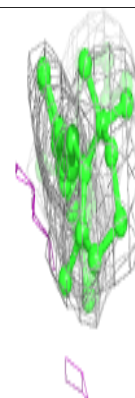
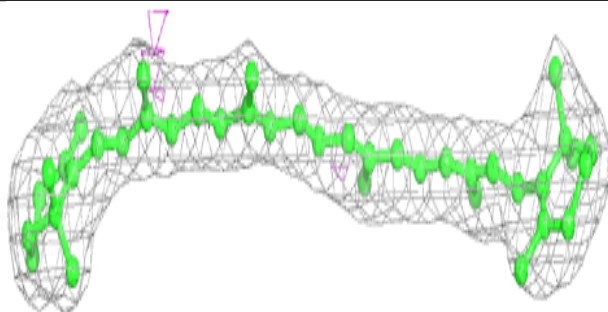
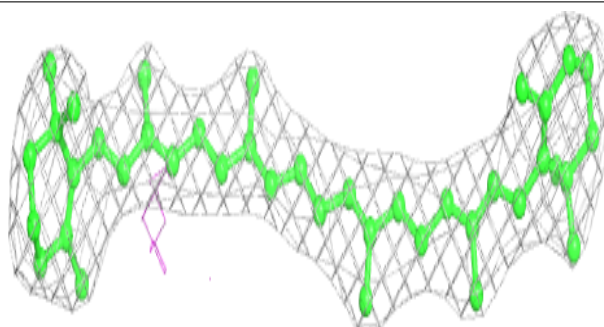


**Electron density around BCR B 618:**

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

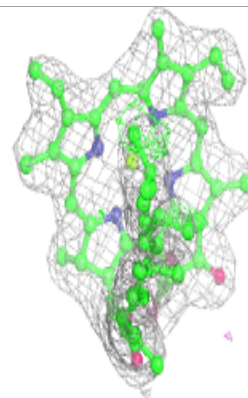
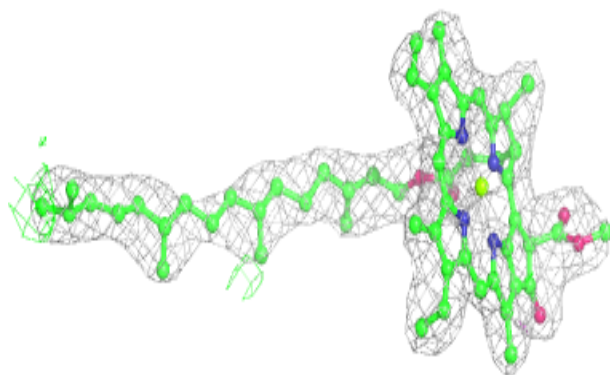
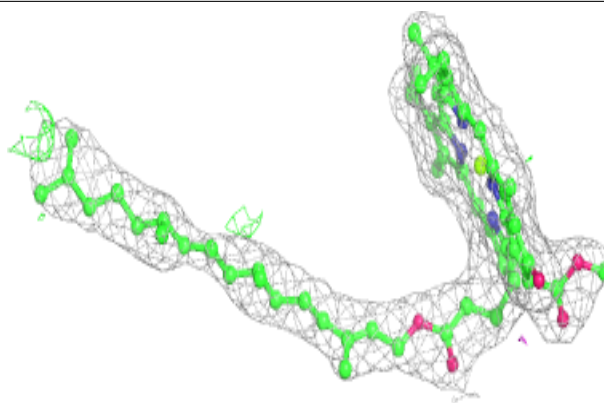
**Electron density around BCR B 619:**

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



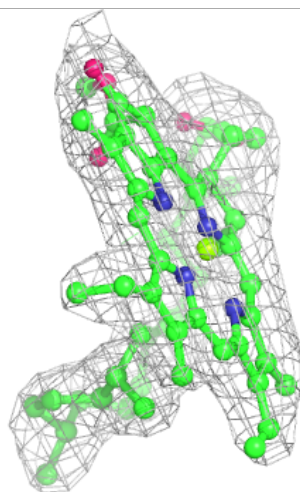
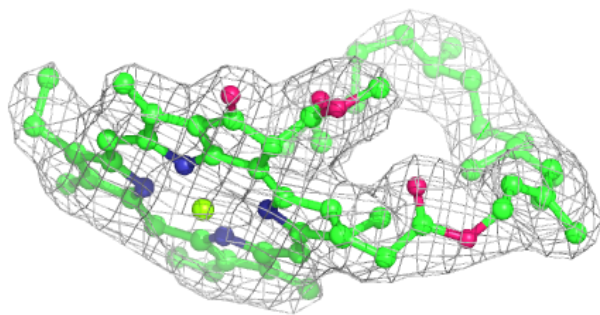
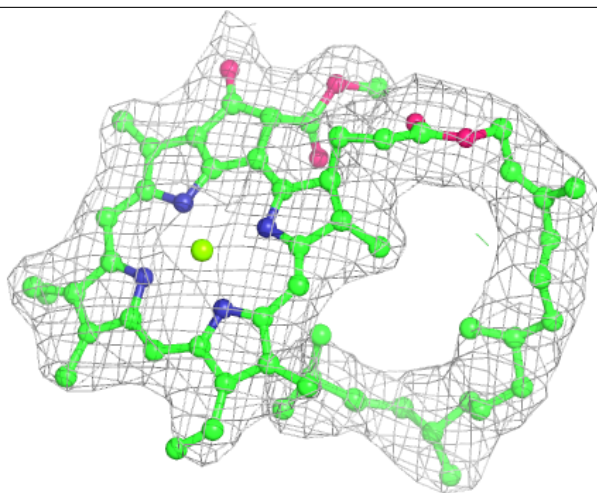
**Electron density around CLA B 607:**

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



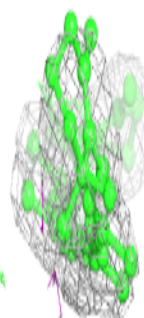
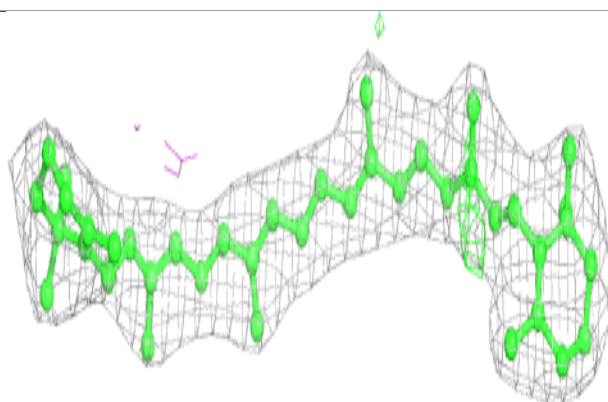
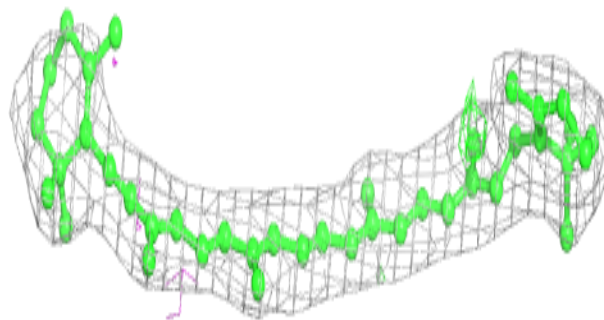
**Electron density around CLA b 615:**

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

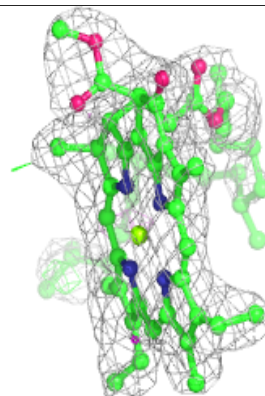
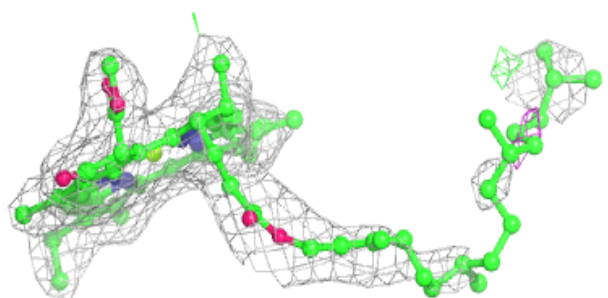
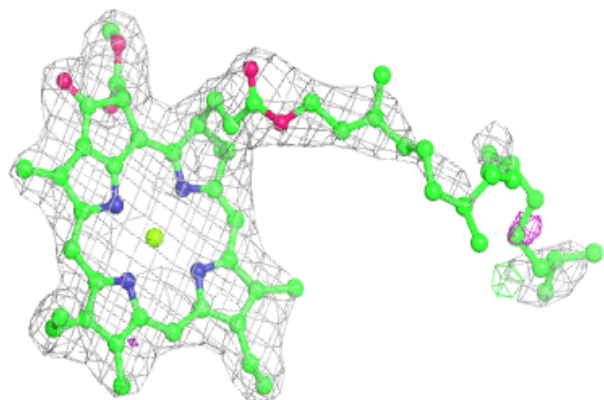


**Electron density around BCR D 407:**

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

**Electron density around CLA a 407:**

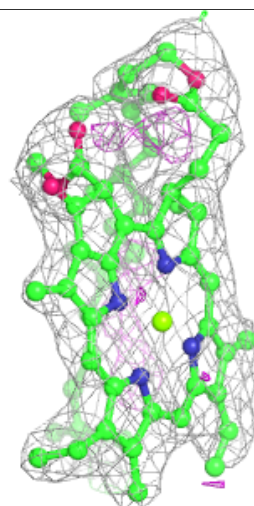
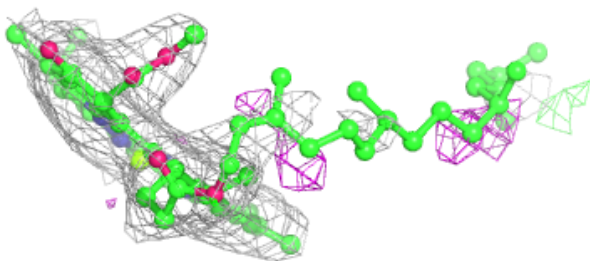
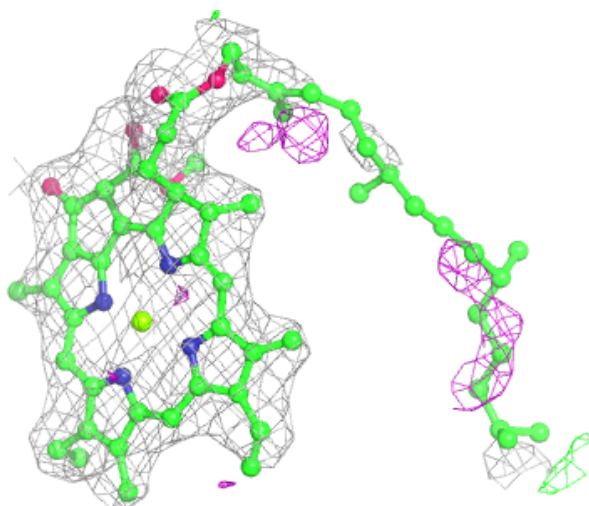
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





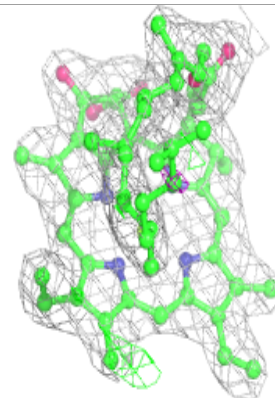
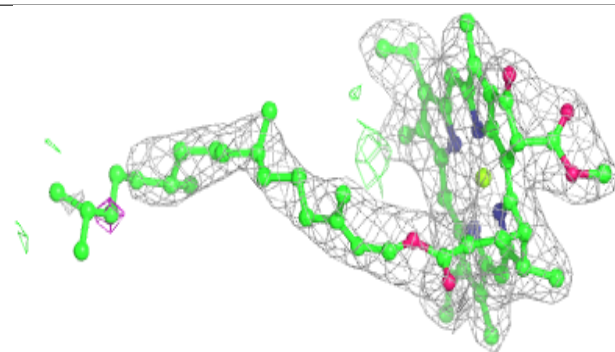
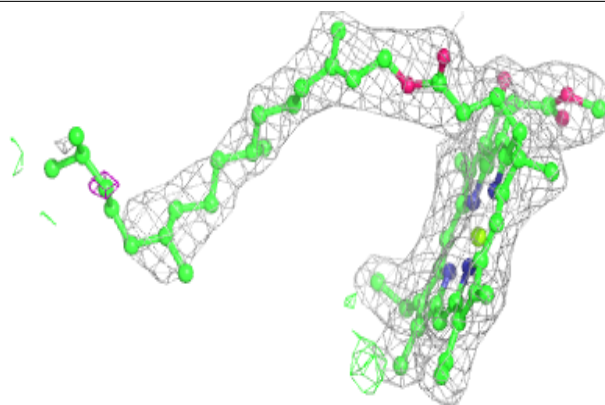
**Electron density around CLA B 616:**

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

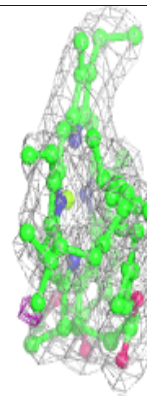
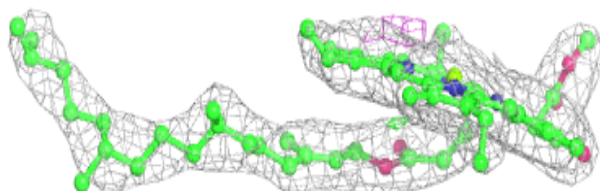
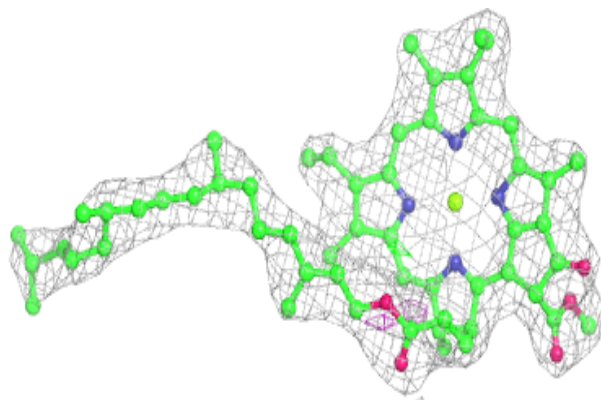


**Electron density around CLA C 509:**

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

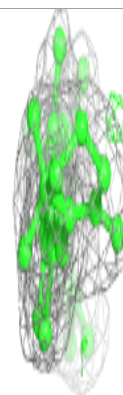
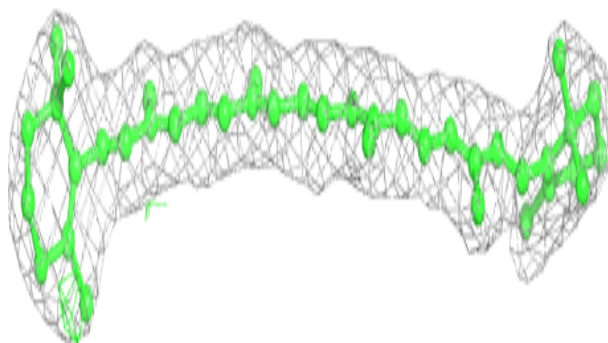
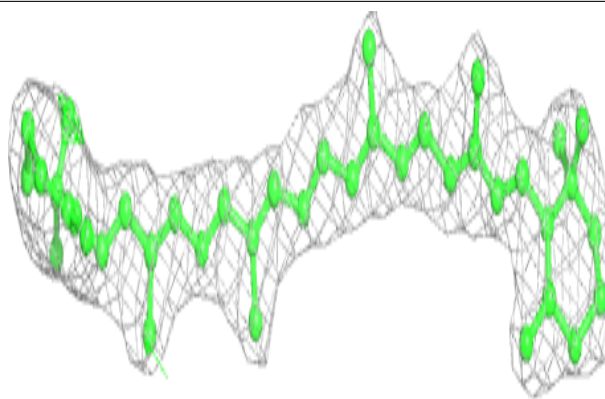
**Electron density around CLA b 603:**

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

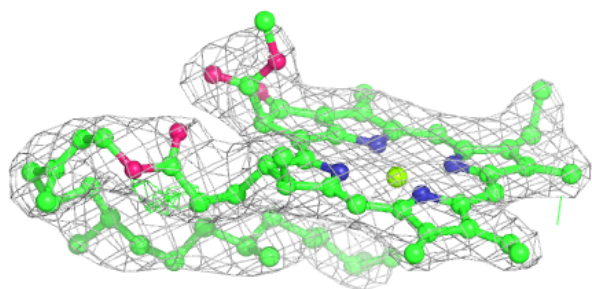
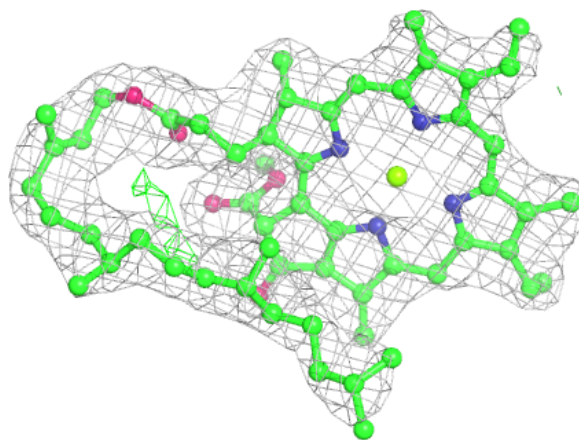


**Electron density around BCR b 617:**

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

**Electron density around CLA C 510:**

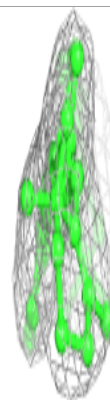
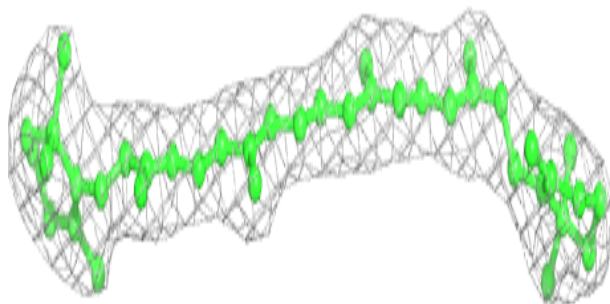
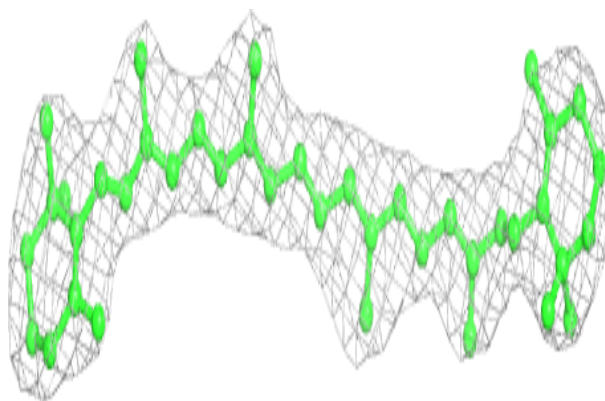
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



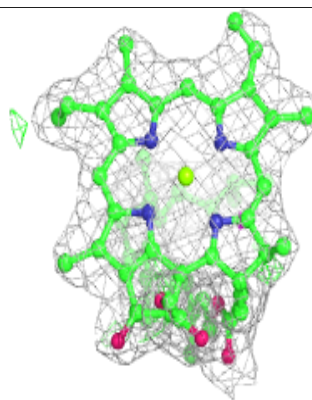
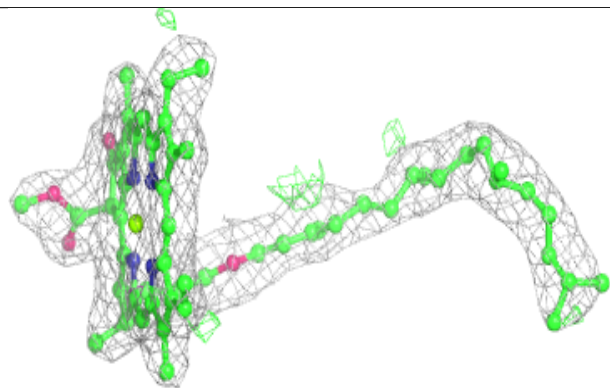
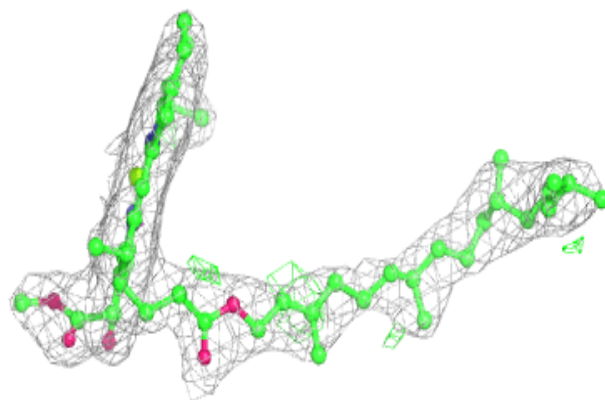


**Electron density around BCR b 619:**

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

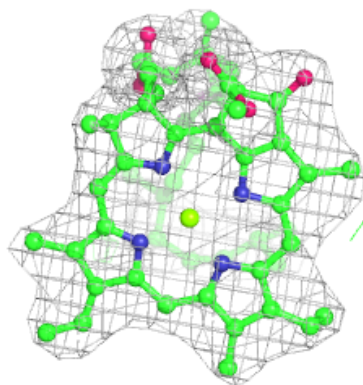
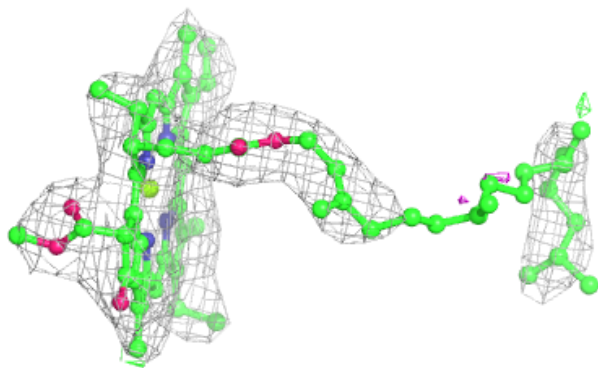
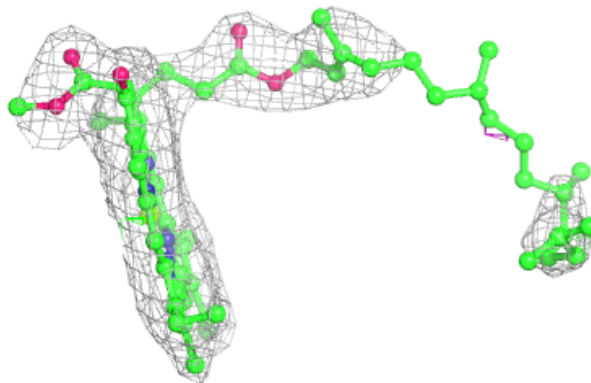
**Electron density around CLA b 605:**

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

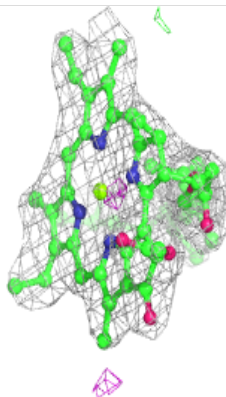
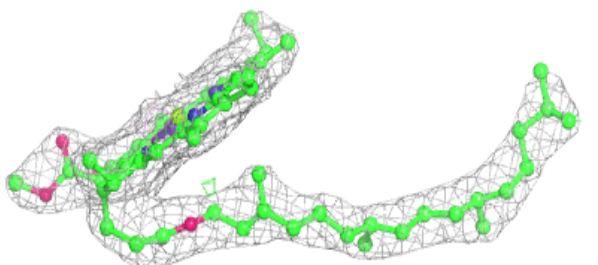
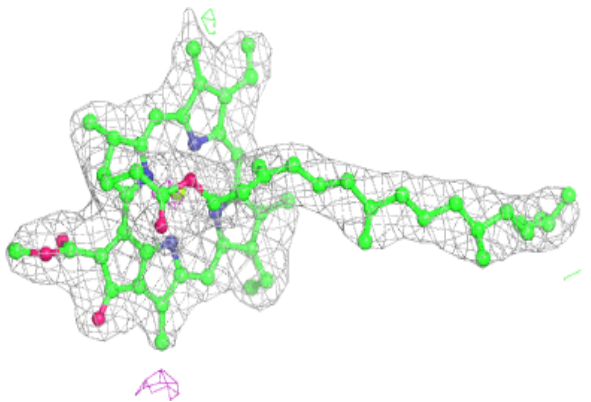


**Electron density around CLA c 507:**

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

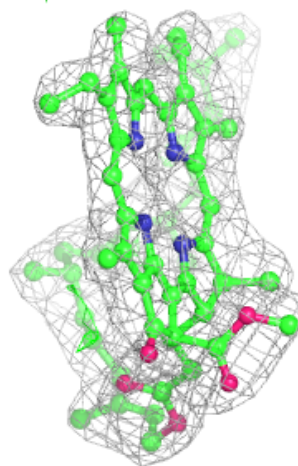
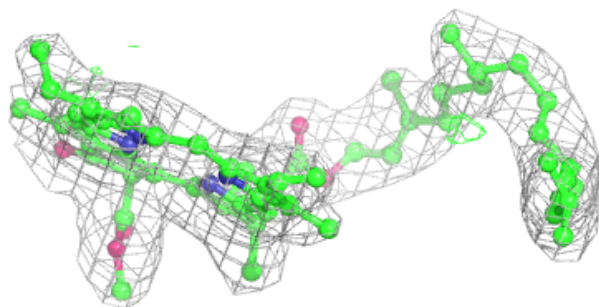
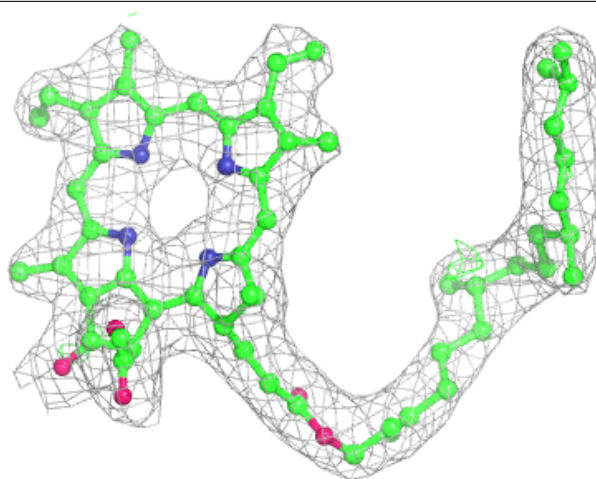
**Electron density around CLA b 608:**

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



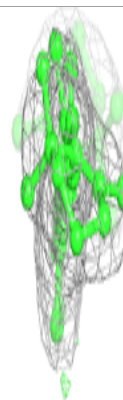
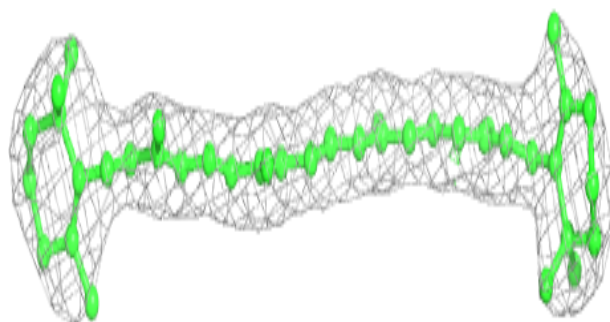
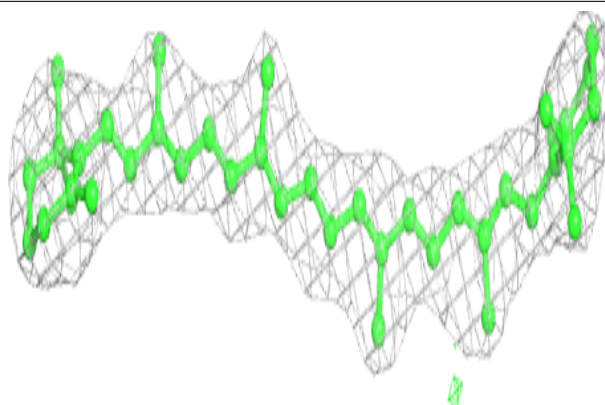
**Electron density around PHO a 416:**

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

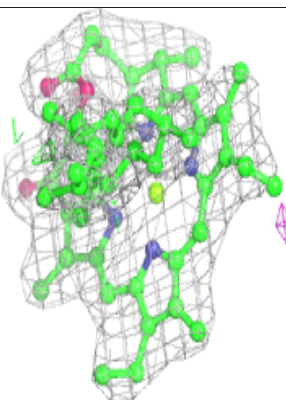
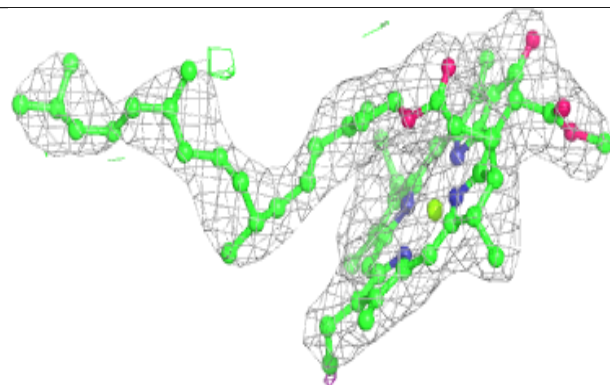
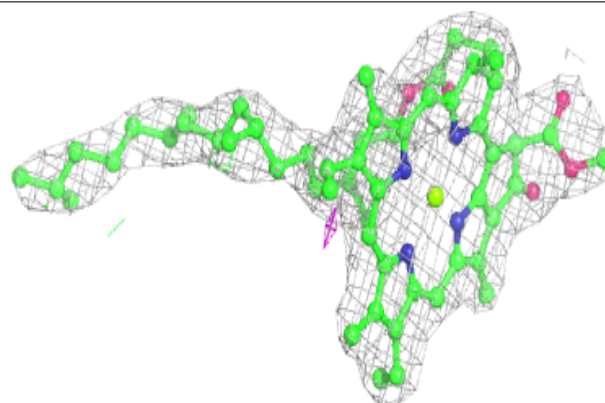


**Electron density around BCR c 516:**

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

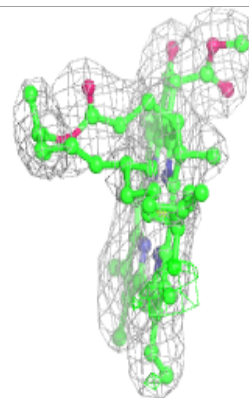
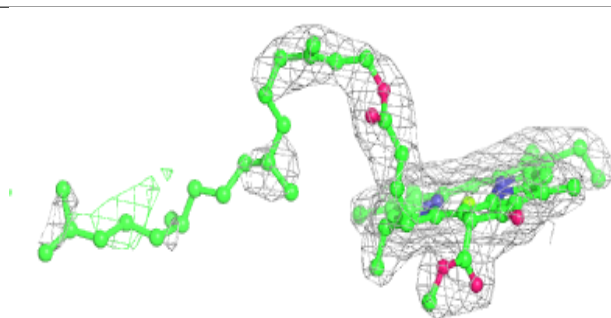
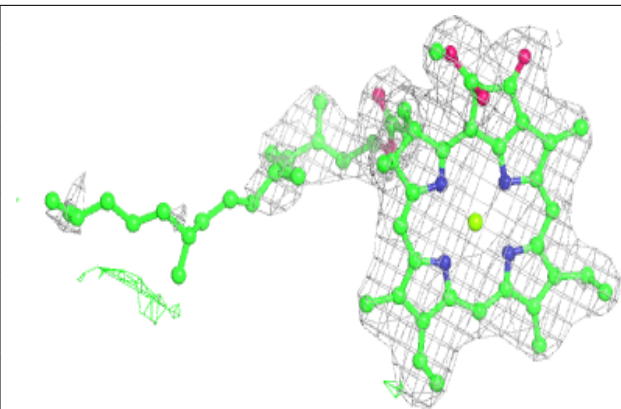
**Electron density around CLA C 506:**

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



**Electron density around CLA a 405:**

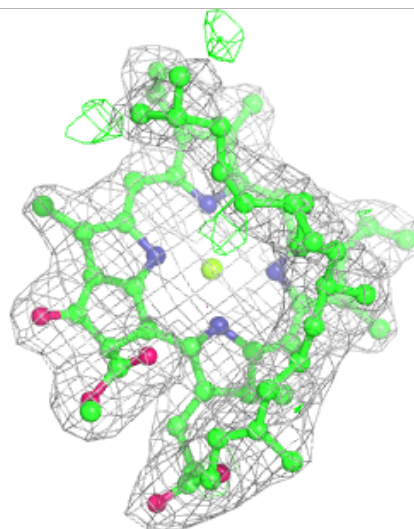
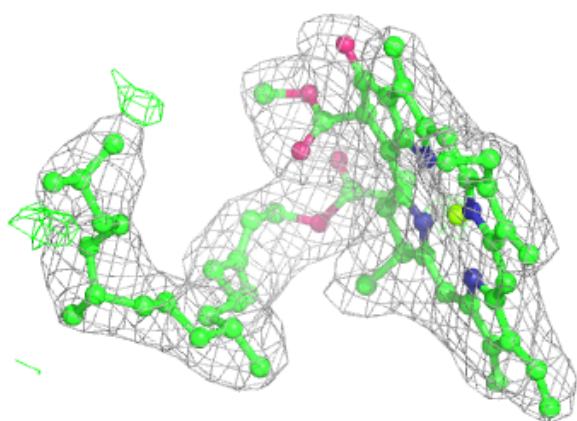
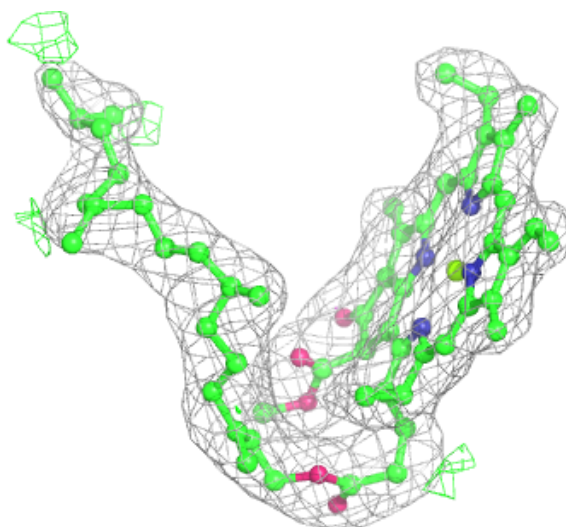
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





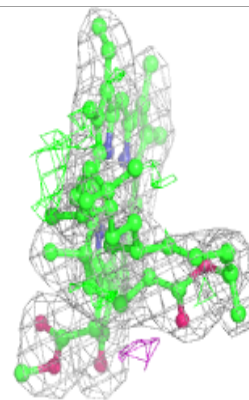
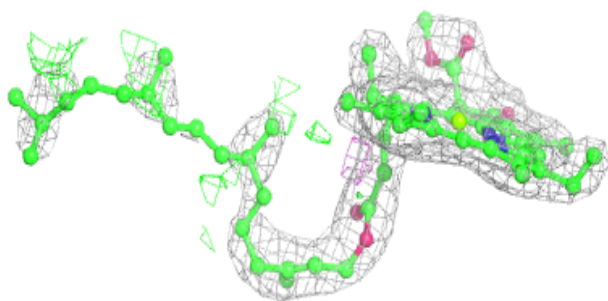
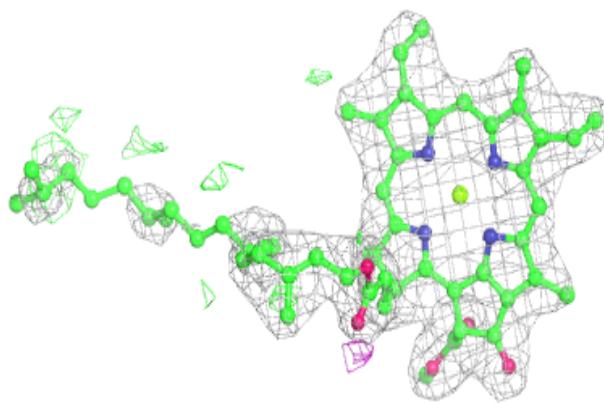
**Electron density around CLA B 613:**

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



**Electron density around CLA A 406:**

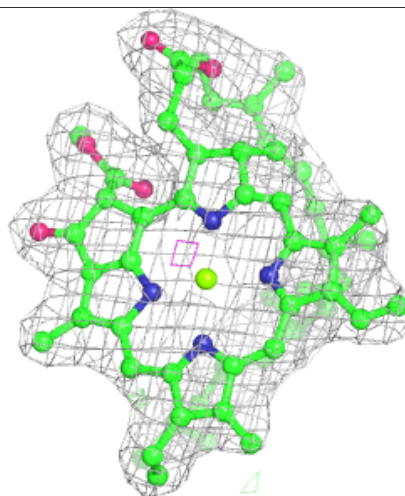
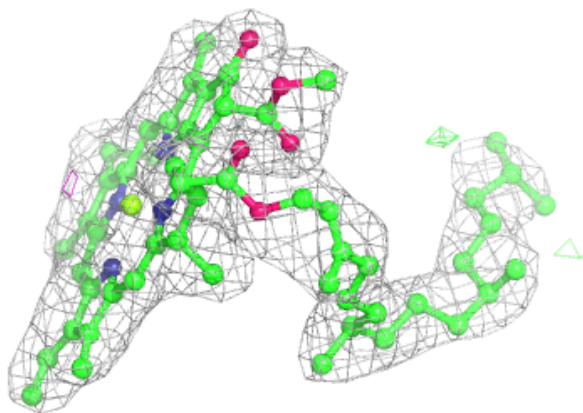
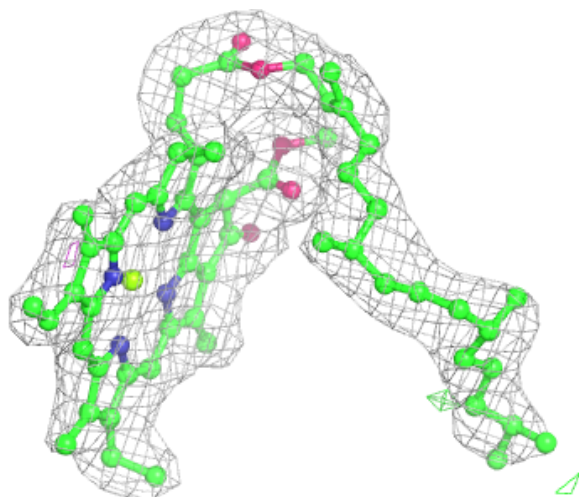
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





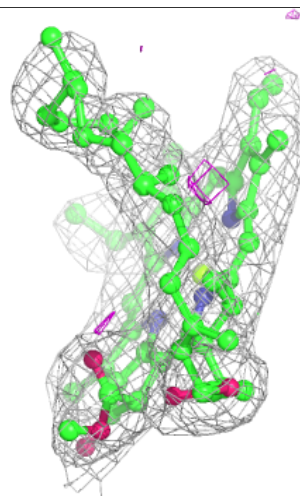
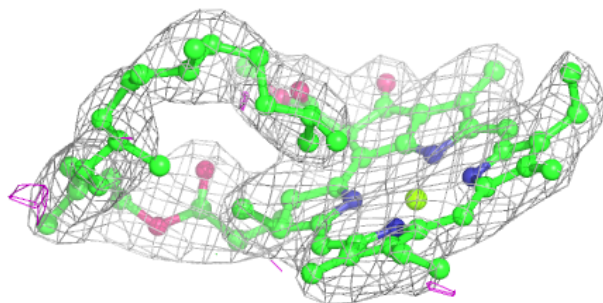
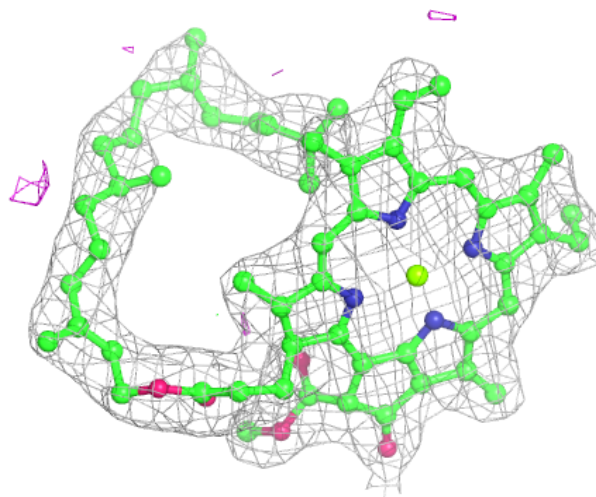
**Electron density around CLA b 613:**

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



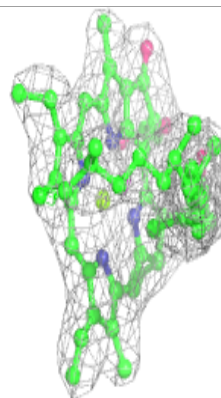
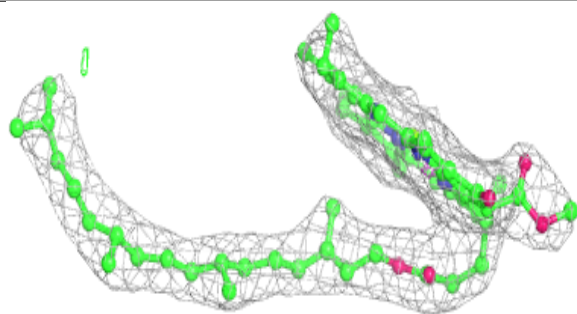
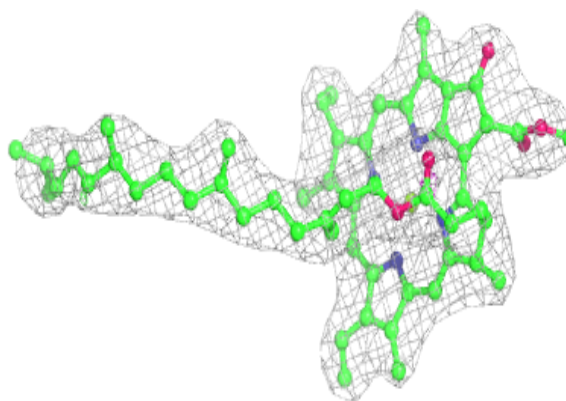
**Electron density around CLA B 615:**

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

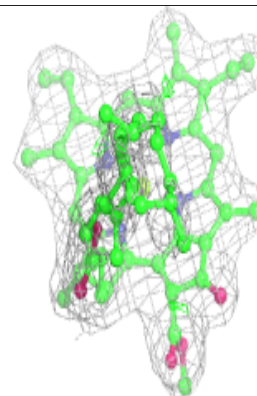
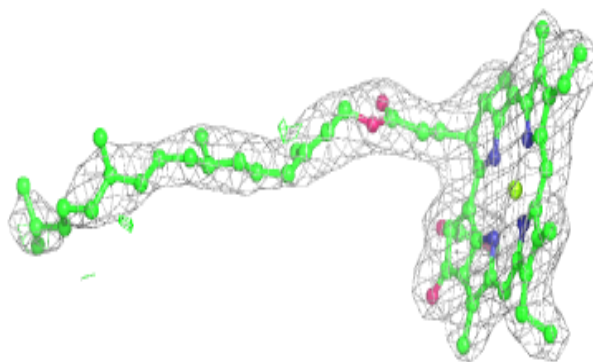
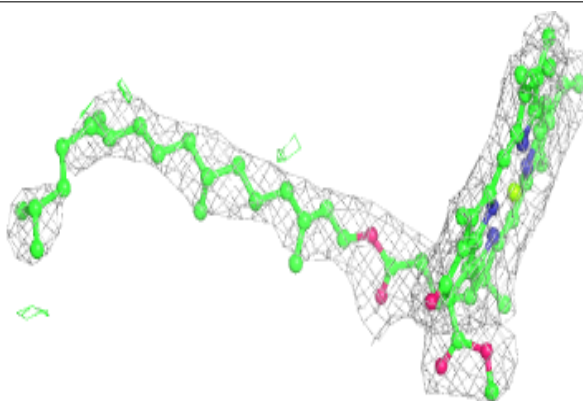


**Electron density around CLA B 608:**

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

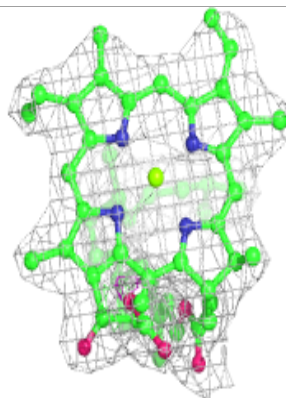
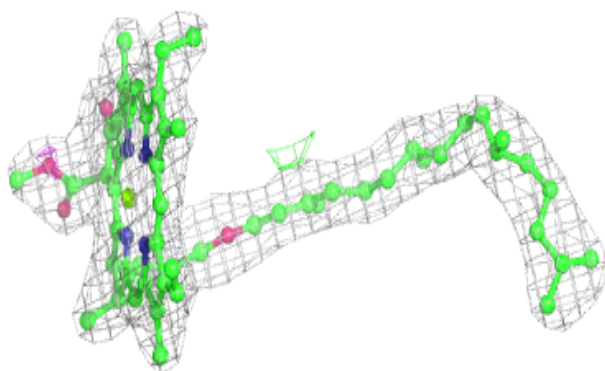
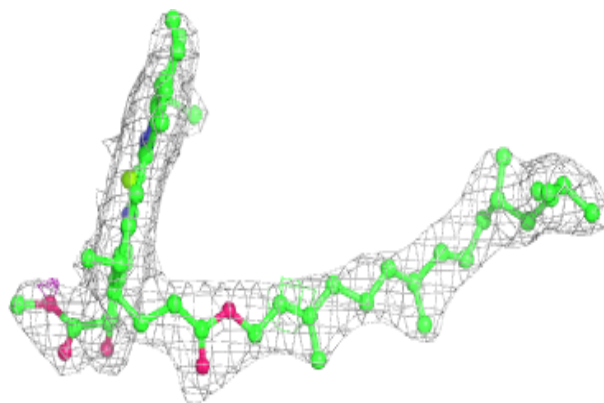
**Electron density around CLA B 604:**

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

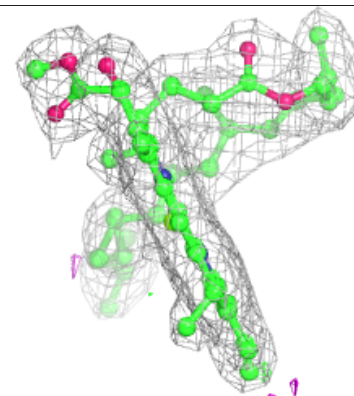
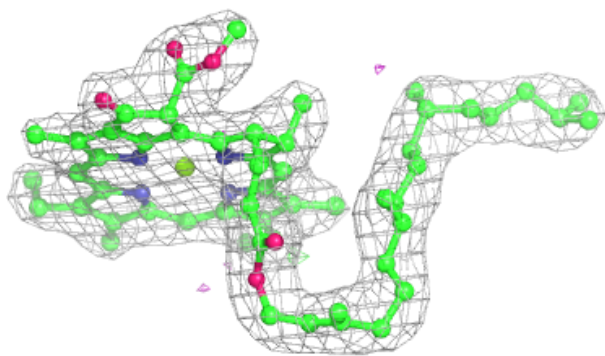
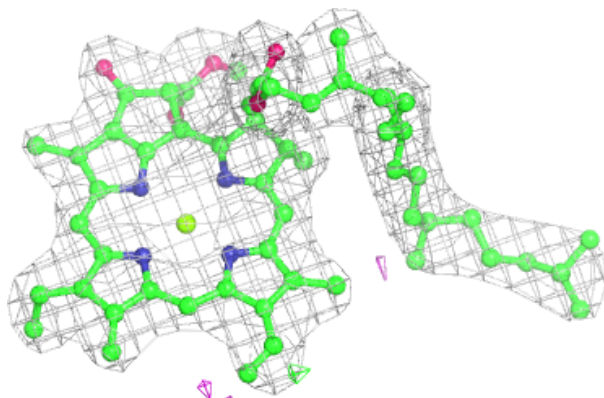


**Electron density around CLA B 605:**

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

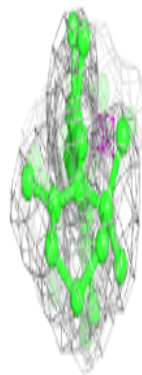
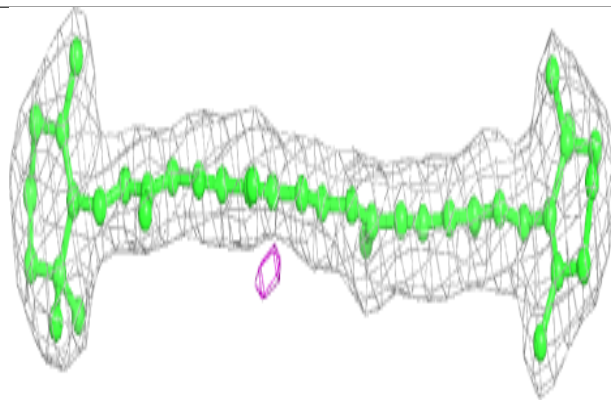
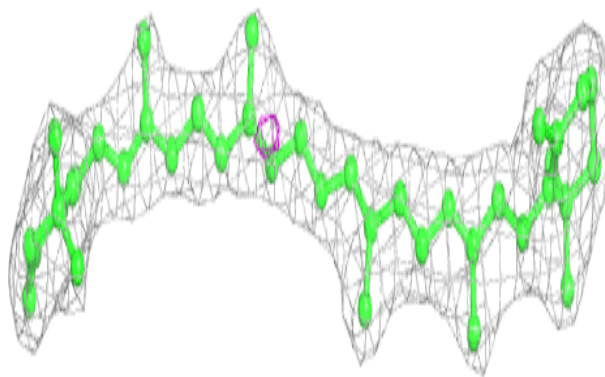
**Electron density around CLA d 402:**

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



**Electron density around BCR a 408:**

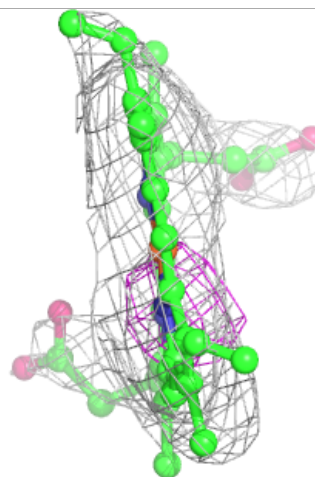
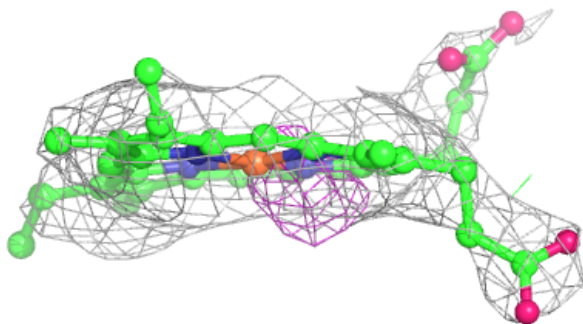
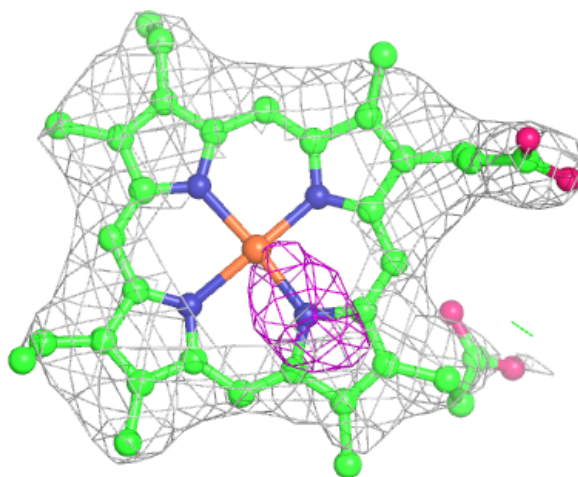
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





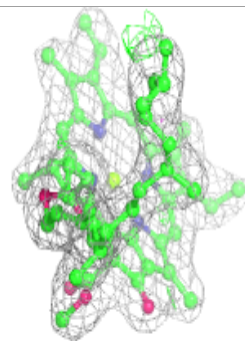
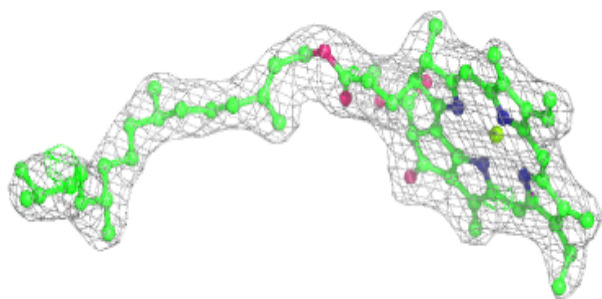
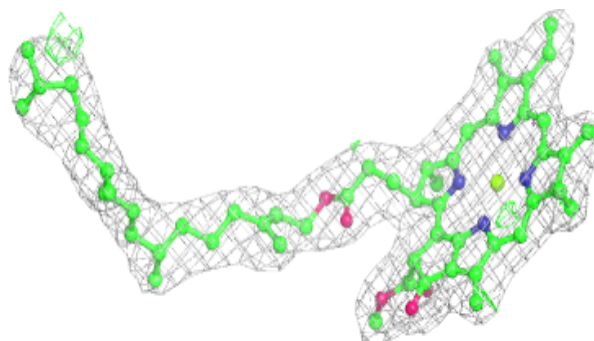
**Electron density around HEM f 101:**

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

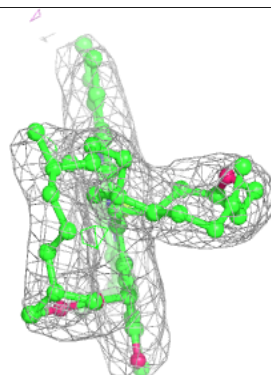
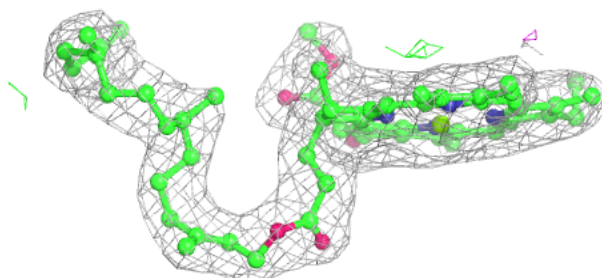
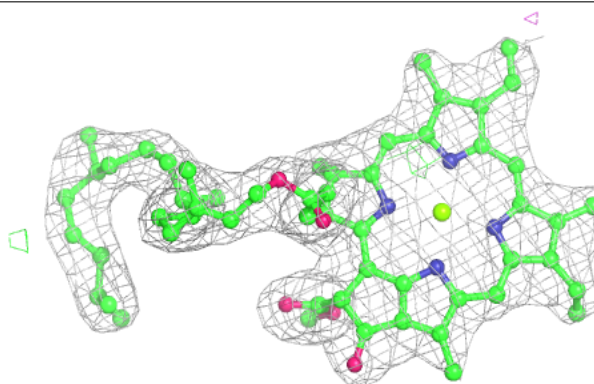


**Electron density around CLA A 404:**

$2mF_o-DF_c$  (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:**

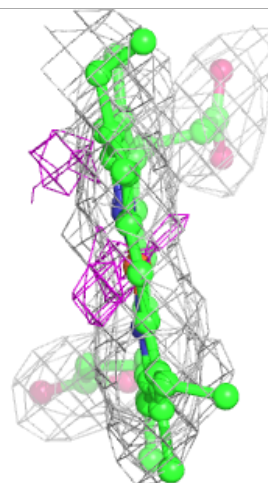
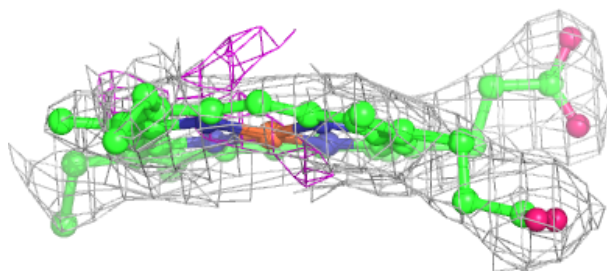
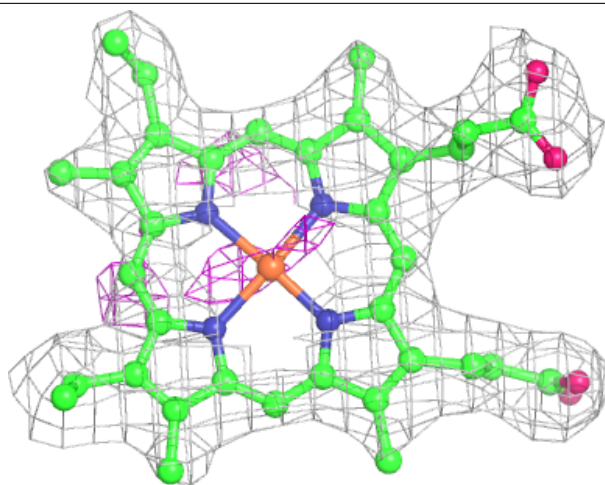
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





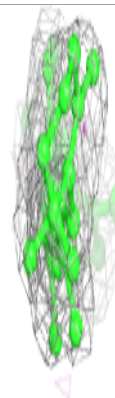
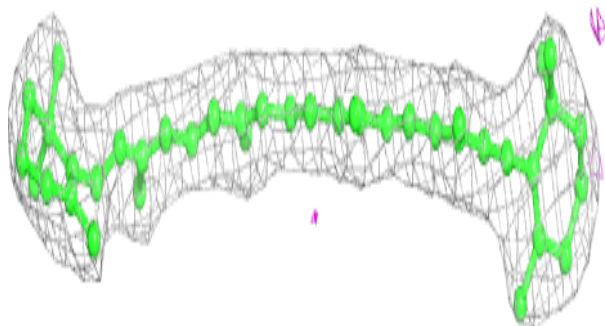
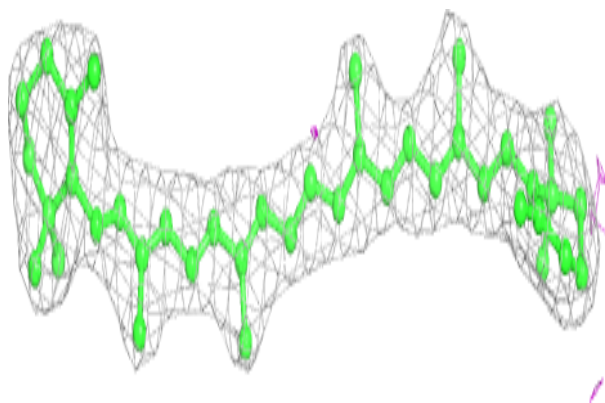
**Electron density around HEC v 203:**

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

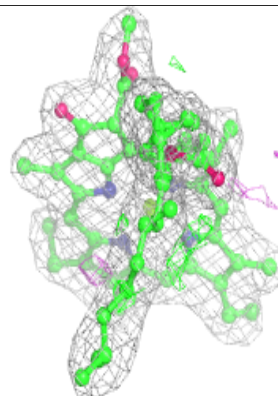
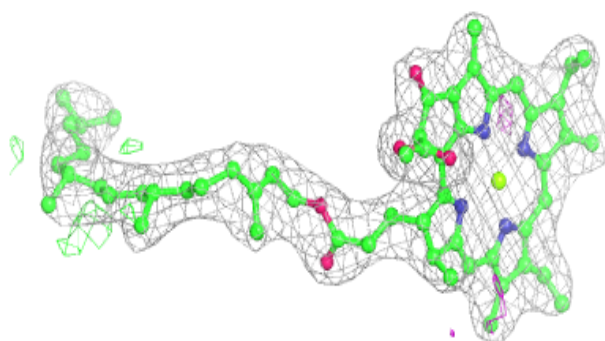
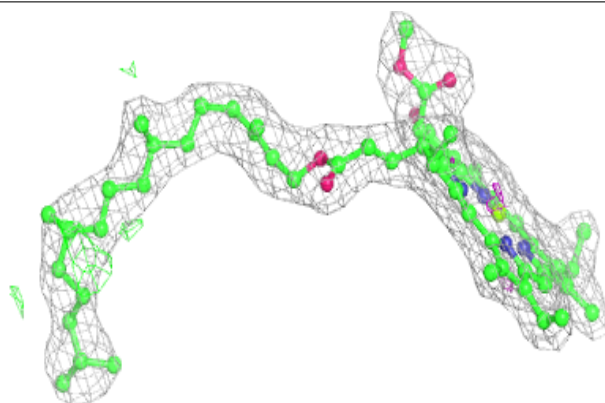


**Electron density around BCR B 617:**

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

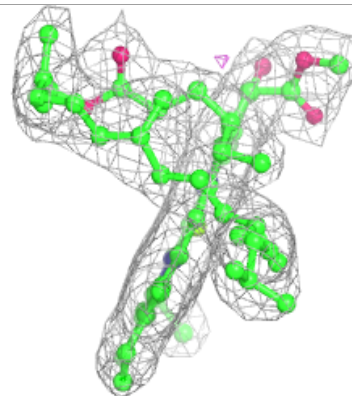
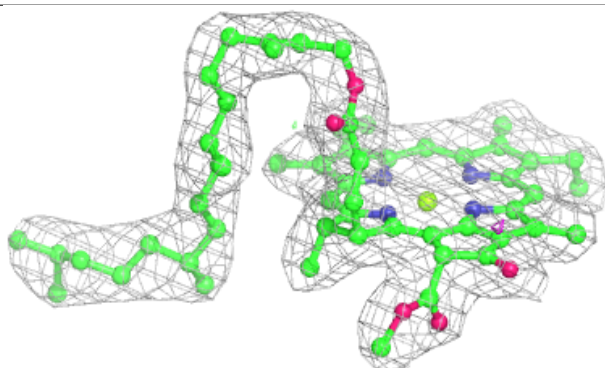
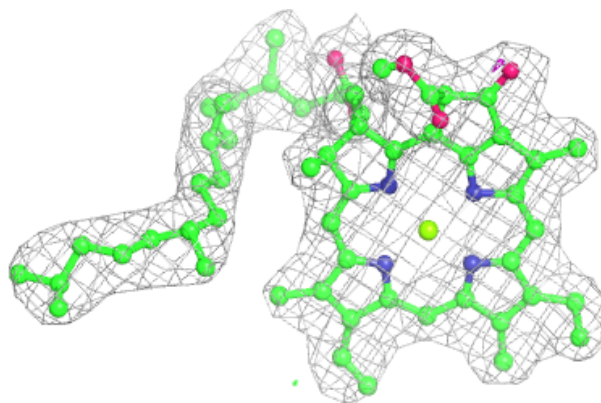
**Electron density around CLA D 405:**

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

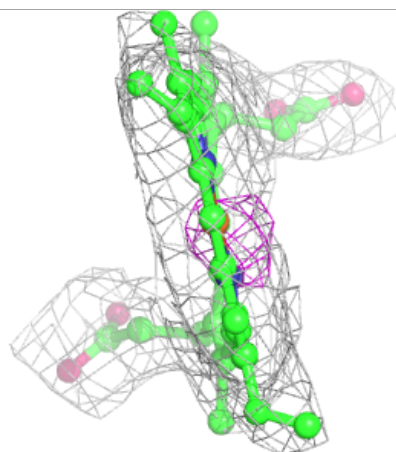
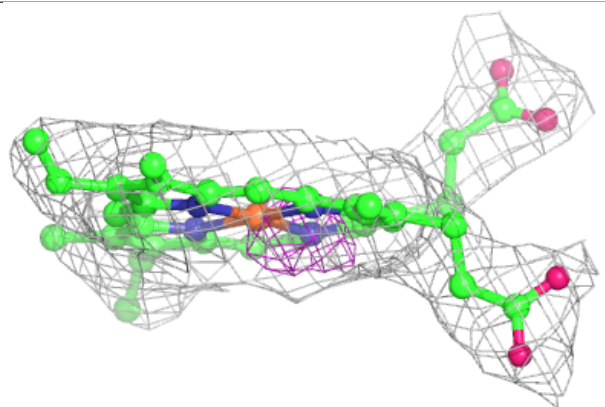
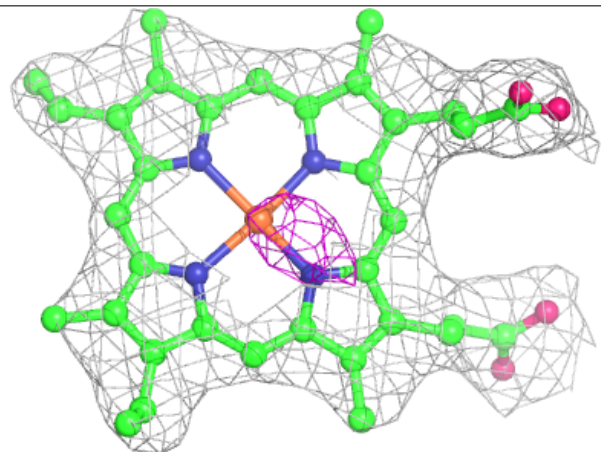


**Electron density around CLA A 405:**

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

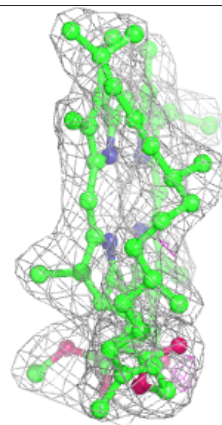
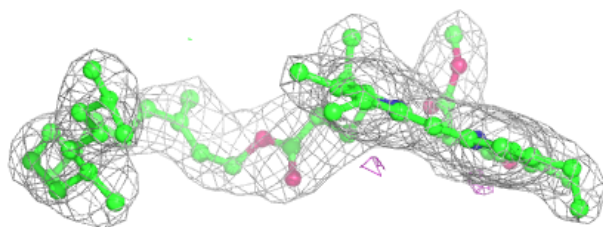
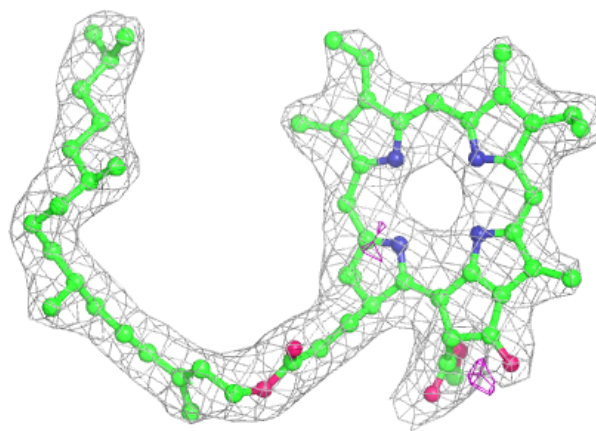
**Electron density around HEM E 103:**

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

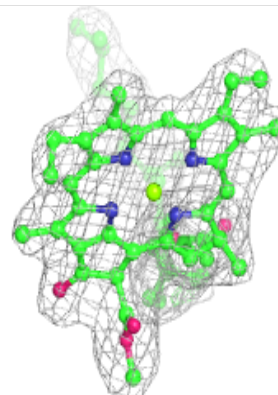
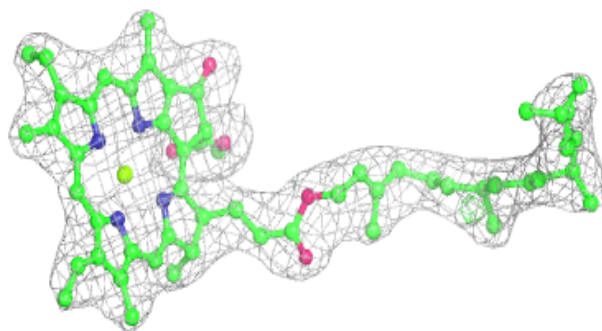
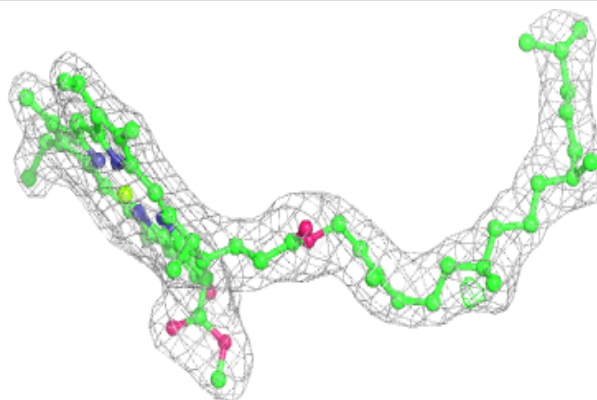


**Electron density around PHO a 406:**

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

**Electron density around CLA d 403:**

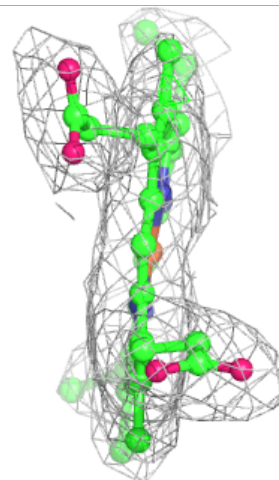
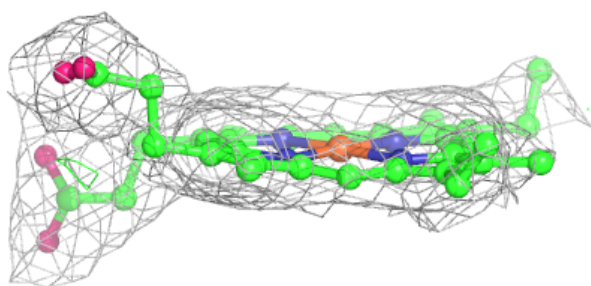
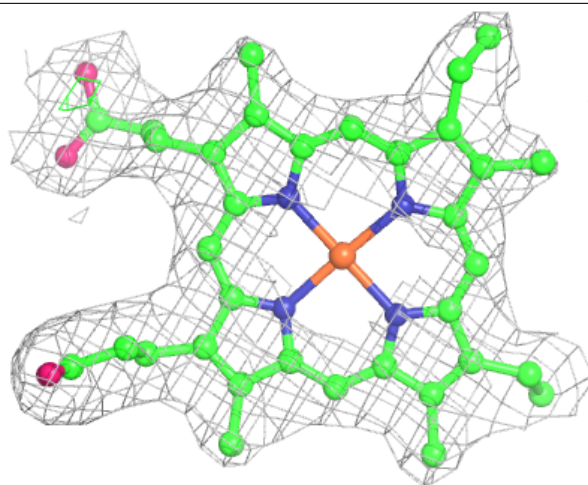
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





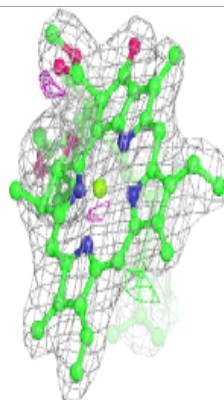
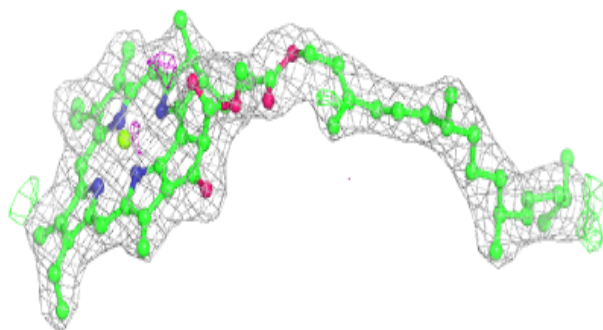
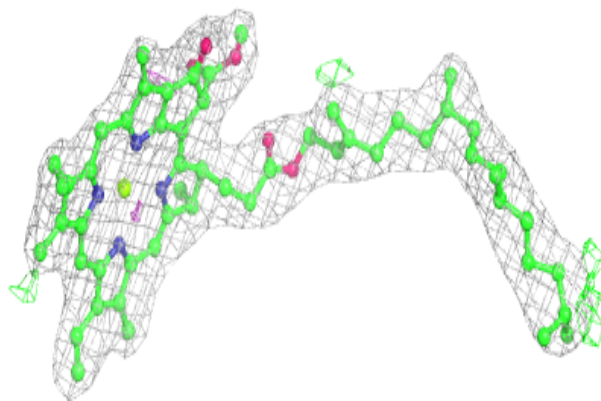
**Electron density around HEC V 201:**

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



**Electron density around CLA a 404:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.