



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 04:58 AM BST

PDB ID : 6JLO  
Title : XFEL structure of cyanobacterial photosystem II (2F state, dataset2)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2019-03-06  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

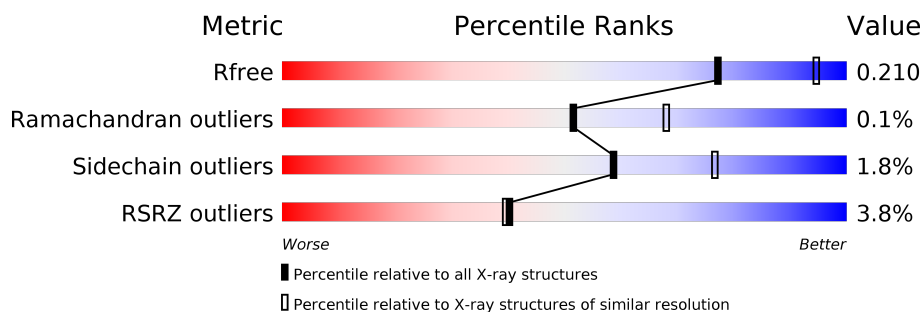
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

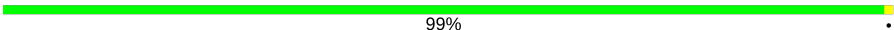

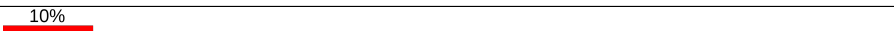
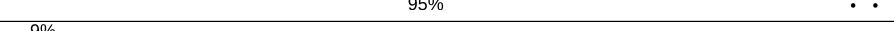



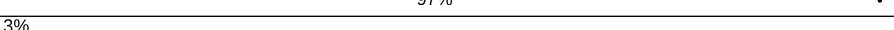
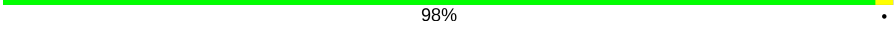


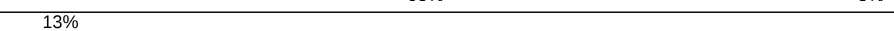
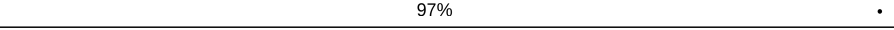



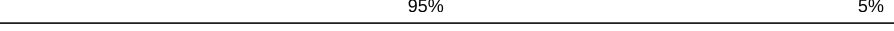
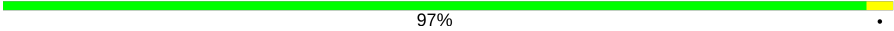
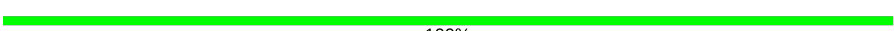





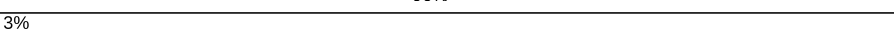
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div></div> <div>97%</div> <div>.</div> </div>
1	a	344	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	B	505	<div> <div>%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>3%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div></div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	342	 99%
5	E	84	 23% 96%
5	e	84	 10% 95%
6	F	44	 9% 77% 23%
6	f	44	 2% 70% 27%
7	H	65	 3% 97%
7	h	65	 3% 98%
8	I	38	 11% 95% 5%
8	i	38	 8% 95% 5%
9	J	39	 13% 97%
9	j	39	 18% 100%
10	K	37	 11% 100%
10	k	37	 95% 5%
11	L	37	 97%
11	l	37	 100%
12	M	36	 92% 6% 6%
12	m	36	 89% 6% 6%
13	O	244	 2% 98%
13	o	244	 2% 96%
14	T	32	 3% 88% 6% 6%
14	t	32	 3% 88% 6% 6%
15	U	104	 89% 7% 7%
15	u	104	 91% 7% 7%
16	V	137	 100%
16	v	137	 99%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	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	408	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	411	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	b	621	X	-	-	-
23	CLA	b	622	X	-	-	-
23	CLA	b	623	X	-	-	-
23	CLA	b	624	X	-	-	-
23	CLA	b	625	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	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	c	516	X	-	-	-
23	CLA	c	517	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	d	405	X	-	-	-
27	GOL	V	201	-	-	-	X
28	LMT	F	101	-	-	-	X
28	LMT	a	418	-	-	-	X
28	LMT	b	630	-	-	-	X
37	DGD	d	408	-	-	-	X

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 55695 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	54	0
			3024	1969	499	538	18			
1	a	334	Total	C	N	O	S	0	56	0
			3020	1970	497	535	18			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	14	0
			3553	2322	592	626	13			
3	c	455	Total	C	N	O	S	0	20	0
			3641	2382	606	639	14			

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	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	See sequence details	UNP P19054
K	39	TRP	VAL	See sequence details	UNP P19054
k	33	LEU	PHE	See sequence details	UNP P19054
k	39	TRP	VAL	See sequence details	UNP P19054

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

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

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

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

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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	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	4			

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



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

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

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

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

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

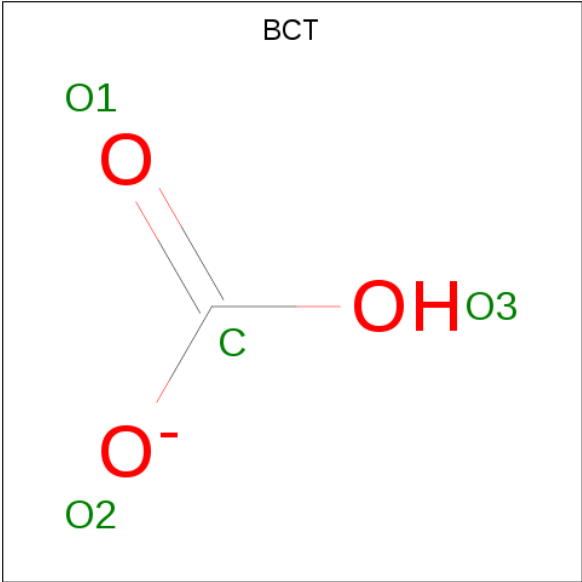
- Molecule 20 is a protein called Photosystem II protein Y.

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

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

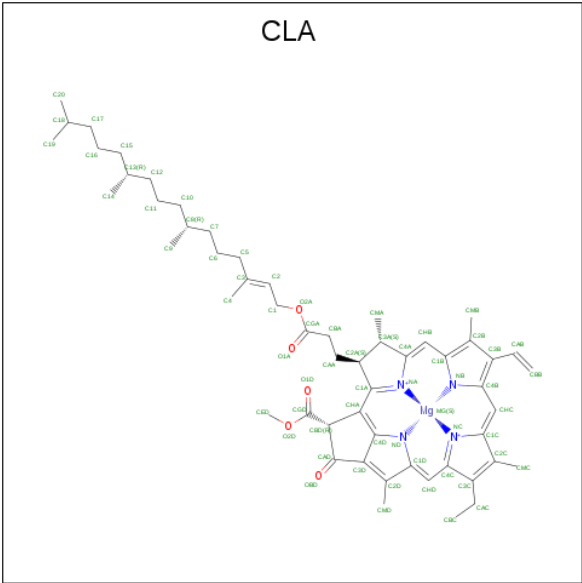
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	2
			4	4		
21	v	1	Total	Cl	0	0
			1	1		
21	a	2	Total	Cl	0	2
			4	4		
21	U	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	1
			8	2	6		
22	d	1	Total	C	O	0	1
			8	2	6		

- 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>).



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

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

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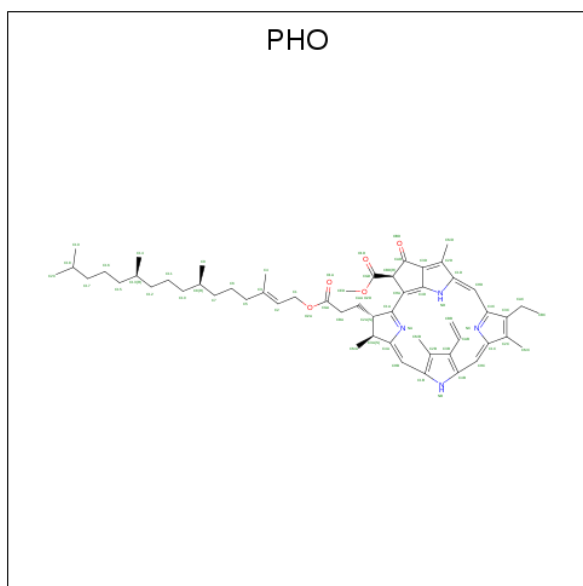
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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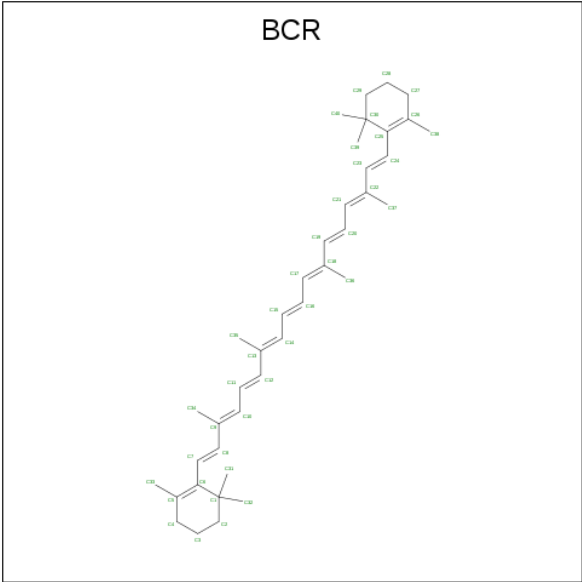
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	1
			128	110	8	10		

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



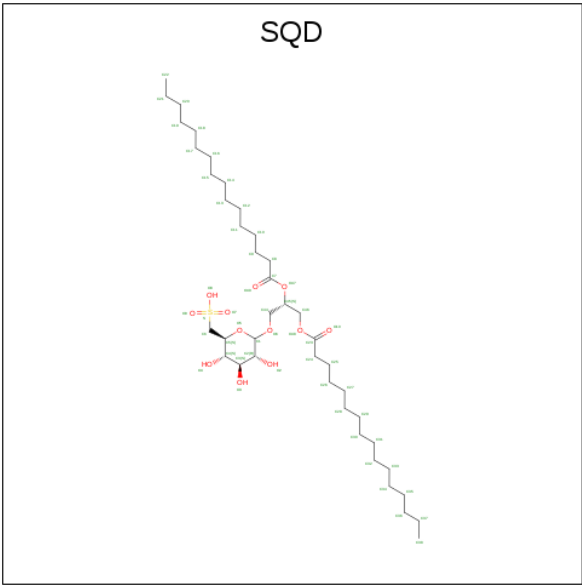
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

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



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

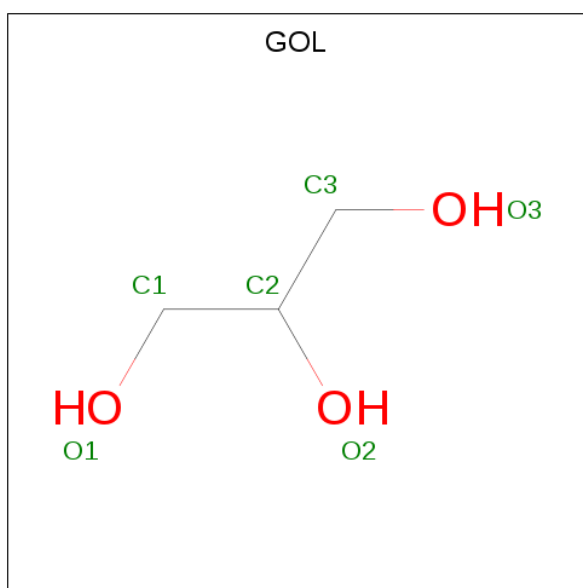
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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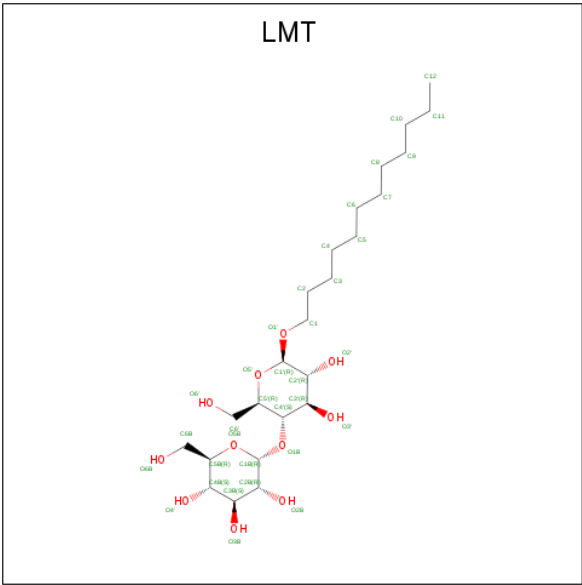
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	D	1	Total	C	O	0	0
			6	3	3		
27	F	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	T	1	Total	C	O	0	0
			6	3	3		
27	T	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			6	3	3		
27	f	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	t	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



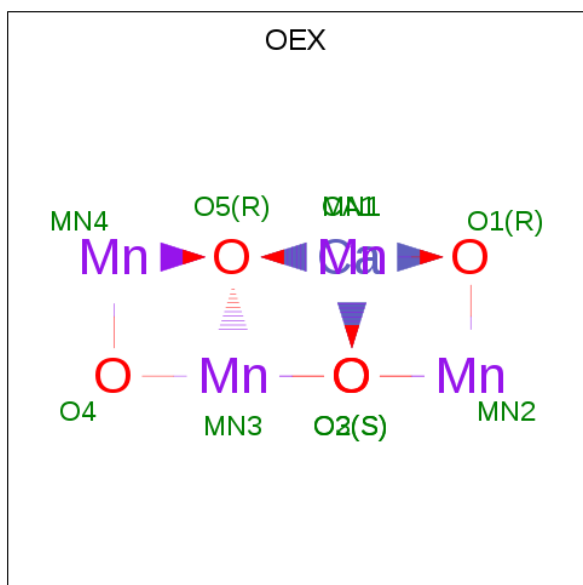
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			35	24	11		
28	B	1	Total	C	O	0	0
			25	19	6		
28	C	1	Total	C	O	0	0
			35	24	11		

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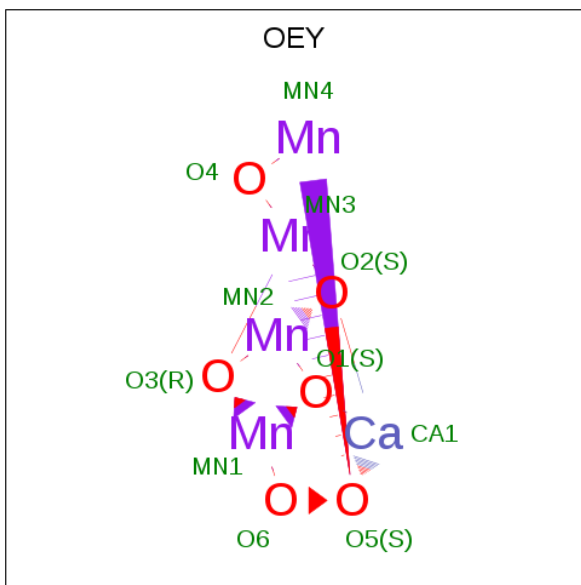
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	D	1	Total	C	O	0	0
			35	24	11		
28	F	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		
28	T	1	Total	C	O	0	0
			25	19	6		
28	a	1	Total	C	O	0	0
			35	24	11		
28	a	1	Total	C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

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



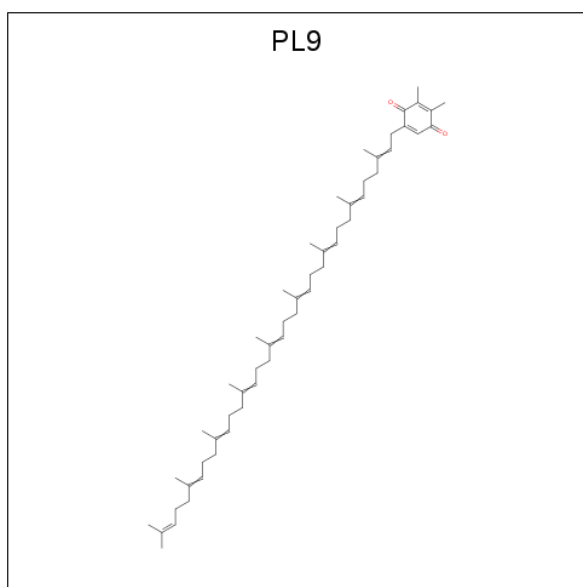
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	1
			110	106	4		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	1
			110	106	4		

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

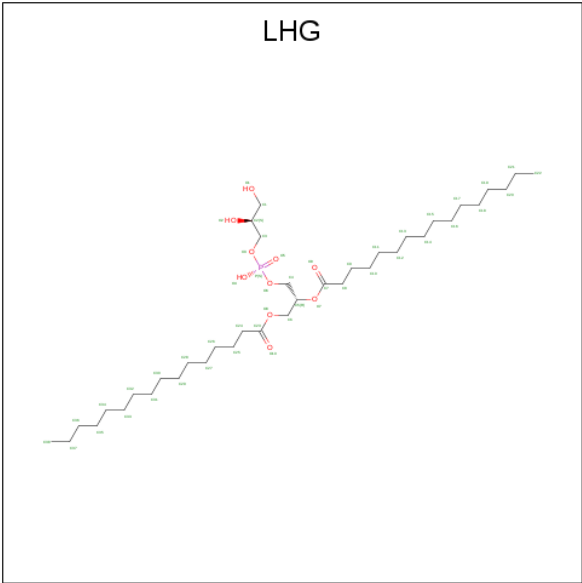
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	K	1	Total	C	O	0	0
			34	29	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	I	1	Total	C	O	0	0
			40	35	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	a	1	Total	C	O	0	0
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

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

- Molecule 33 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
33	A	1	Total	C	O	P	0	0
			42	31	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		

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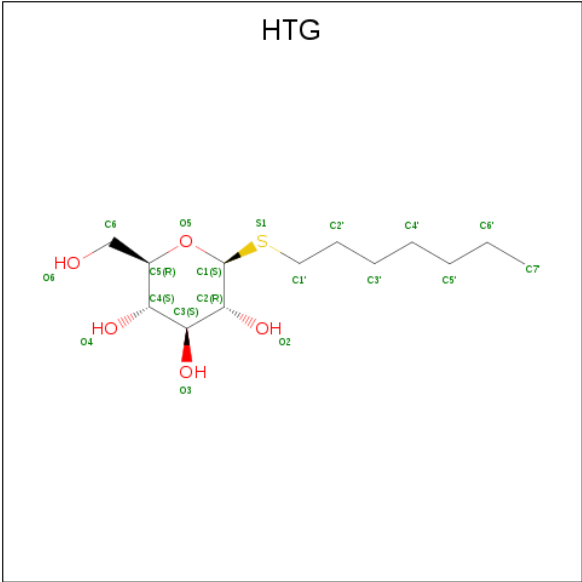
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	L	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			42	31	10	1		
33	b	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		

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

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).





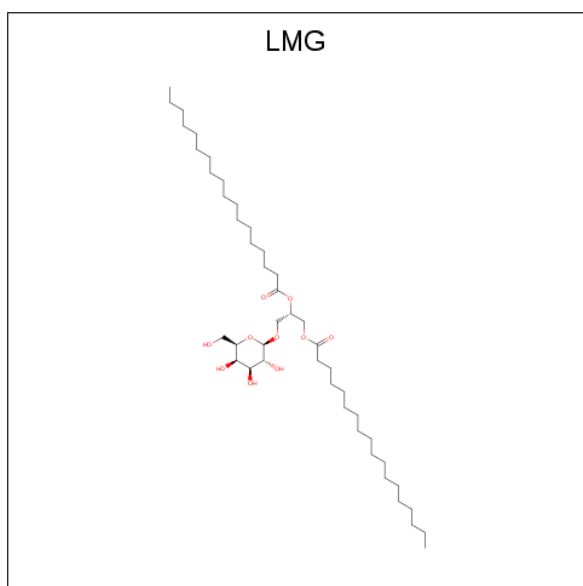
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



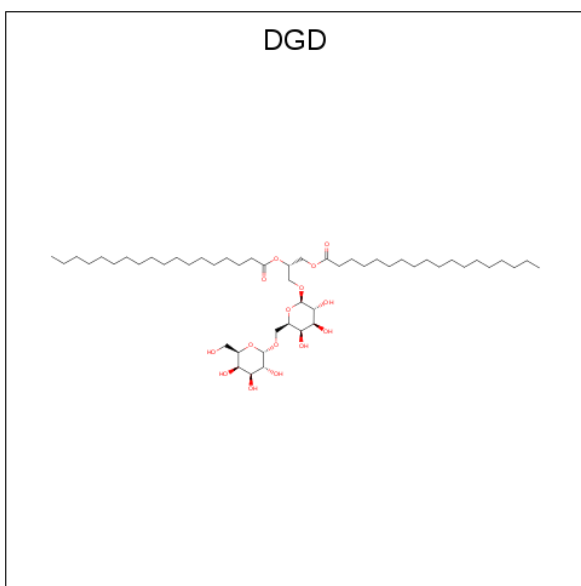
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			51	41	10			
36	C	1	Total	C	O		0	0
			51	41	10			
36	C	1	Total	C	O		0	0
			51	41	10			
36	D	1	Total	C	O		0	0
			51	41	10			
36	M	1	Total	C	O		0	0
			51	41	10			
36	Z	1	Total	C	O		0	0
			37	27	10			
36	a	1	Total	C	O		0	0
			51	41	10			
36	b	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total	C	O	0	0
			51	41	10		
36	d	1	Total	C	O	0	0
			51	41	10		
36	k	1	Total	C	O	0	0
			51	41	10		
36	z	1	Total	C	O	0	0
			39	29	10		

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



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

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

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 38  | a     | 1        | Total Fe<br>1 1 | 0       | 1       |
| 38  | D     | 1        | Total Fe<br>2 2 | 0       | 1       |

- # HEM

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

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	157	Total	O	0	14
			169	169		
41	B	287	Total	O	0	4
			291	291		
41	C	231	Total	O	0	4
			235	235		
41	D	143	Total	O	0	5
			147	147		
41	E	32	Total	O	0	1
			33	33		
41	F	11	Total	O	0	0
			11	11		
41	H	44	Total	O	0	0
			44	44		
41	I	5	Total	O	0	0
			5	5		
41	J	10	Total	O	0	0
			10	10		
41	K	10	Total	O	0	0
			10	10		
41	L	11	Total	O	0	1
			12	12		
41	M	25	Total	O	0	0
			25	25		
41	O	178	Total	O	0	2
			180	180		
41	T	16	Total	O	0	1
			17	17		
41	U	80	Total	O	0	0
			80	80		
41	V	114	Total	O	0	2
			116	116		
41	Y	4	Total	O	0	0
			4	4		

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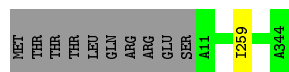
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	X	8	Total 8	O 8	0	0
41	Z	1	Total 1	O 1	0	0
41	a	151	Total 160	O 160	0	11
41	b	260	Total 263	O 263	0	3
41	c	194	Total 199	O 199	0	5
41	d	138	Total 141	O 141	0	4
41	e	20	Total 20	O 20	0	0
41	f	7	Total 7	O 7	0	0
41	h	43	Total 43	O 43	0	0
41	i	3	Total 3	O 3	0	0
41	j	6	Total 6	O 6	0	0
41	k	8	Total 8	O 8	0	0
41	l	8	Total 8	O 8	0	0
41	m	15	Total 15	O 15	0	0
41	o	155	Total 155	O 155	0	0
41	t	14	Total 14	O 14	0	0
41	u	94	Total 94	O 94	0	0
41	v	86	Total 87	O 87	0	1
41	y	1	Total 1	O 1	0	0
41	x	7	Total 7	O 7	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.

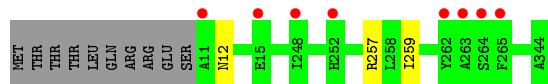
- Molecule 1: Photosystem II protein D1

Chain A:  97%



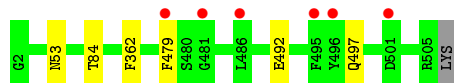
- Molecule 1: Photosystem II protein D1

Chain a:  96%



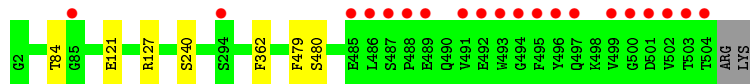
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



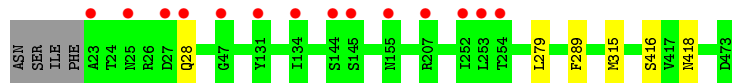
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  98%



- Molecule 3: Photosystem II CP43 reaction center protein

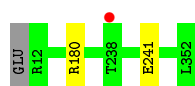
Chain C:  98%



- Molecule 3: Photosystem II CP43 reaction center protein



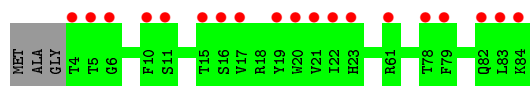
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



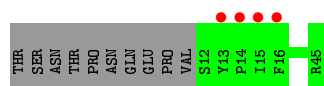
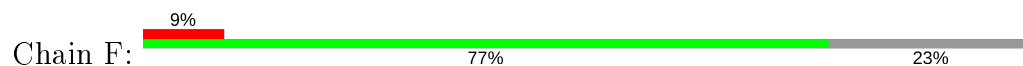
- Molecule 5: Cytochrome b559 subunit alpha



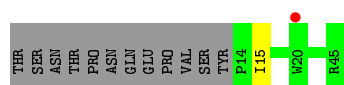
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

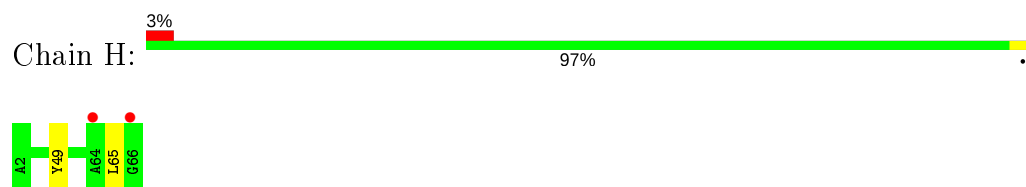


- Molecule 6: Cytochrome b559 subunit beta

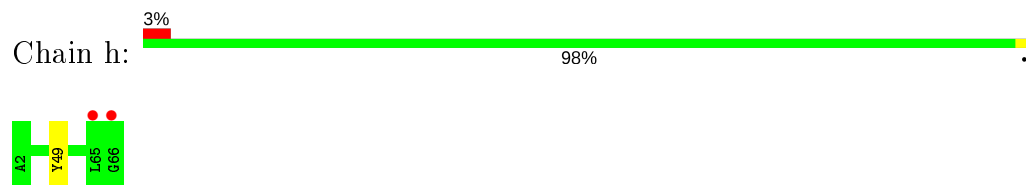




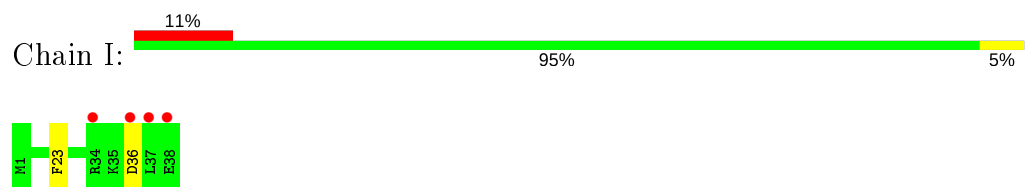
- Molecule 7: Photosystem II reaction center protein H



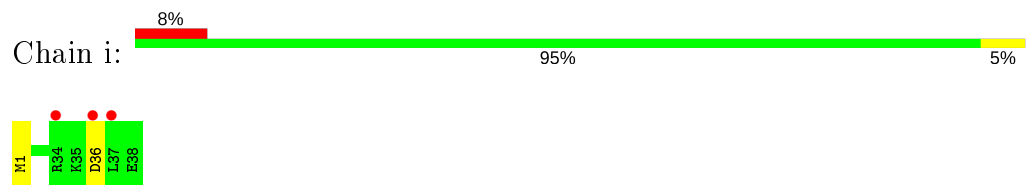
- Molecule 7: Photosystem II reaction center protein H



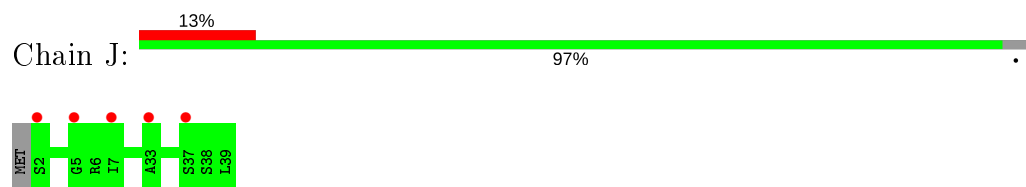
- Molecule 8: Photosystem II reaction center protein I



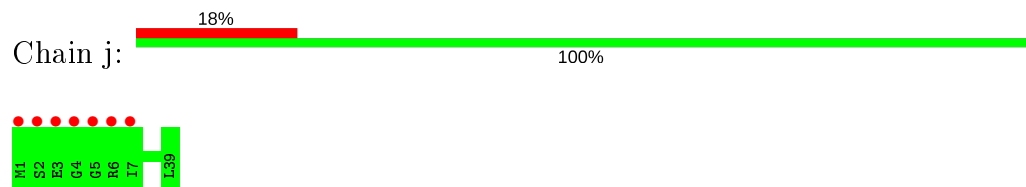
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

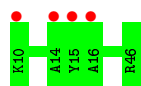


- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

Chain k: 95% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 97% .



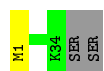
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein M

Chain M: 92% . 6%



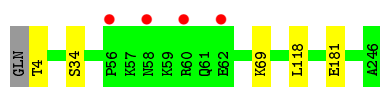
- Molecule 12: Photosystem II reaction center protein M

Chain m: 89% 6% 6%



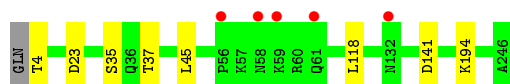
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 2% 98% .

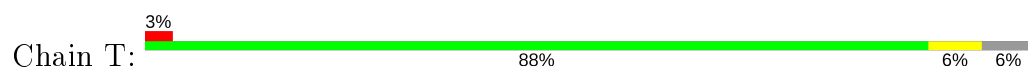


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

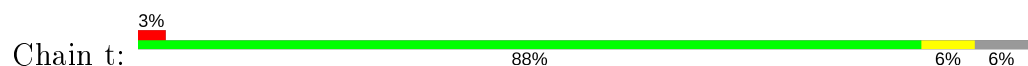
Chain o: 2% 96% .



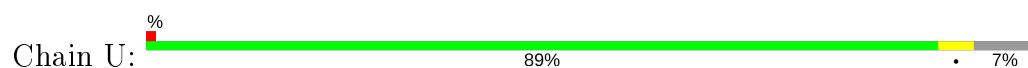
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



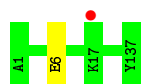
- Molecule 15: Photosystem II 12 kDa extrinsic protein



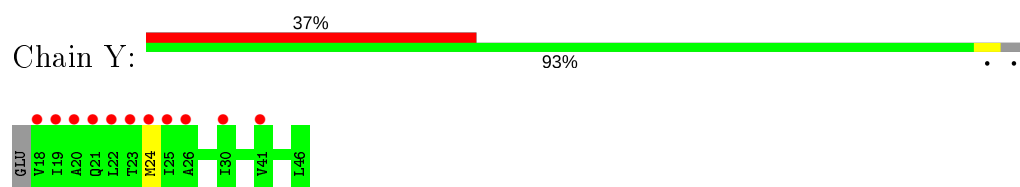
- Molecule 16: Cytochrome c-550



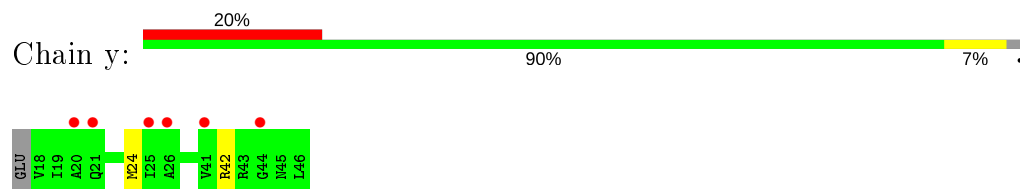
- Molecule 16: Cytochrome c-550



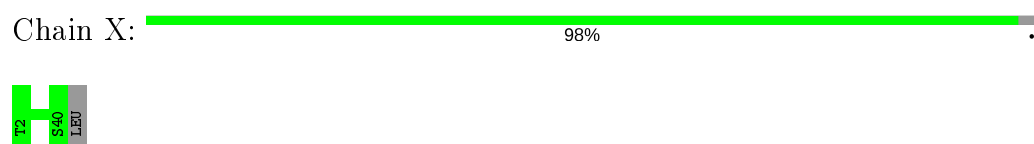
- Molecule 17: Photosystem II reaction center protein Ycf12



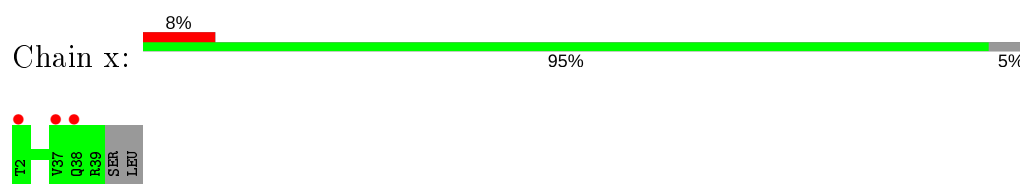
- Molecule 17: Photosystem II reaction center protein Ycf12



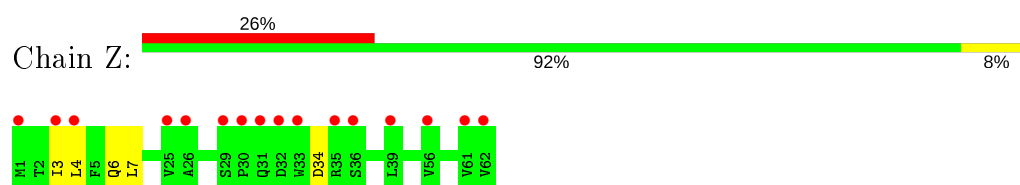
- Molecule 18: Photosystem II reaction center protein X



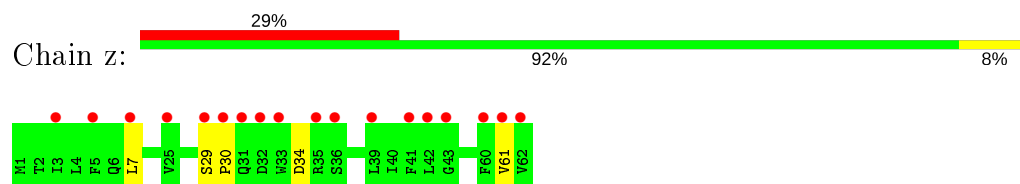
- Molecule 18: Photosystem II reaction center protein X



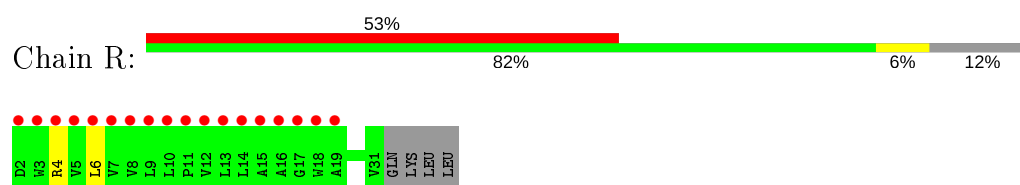
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 121.57 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.40) 99.2 (121.57-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.151 , 0.207 0.156 , 0.210	Depositor DCC
$R_{free}$ test set	17886 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 78.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	55695	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 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/3126	0.54	0/4257
1	a	0.43	0/3128	0.56	0/4260
2	B	0.43	0/4191	0.54	0/5709
2	b	0.43	0/4198	0.54	0/5720
3	C	0.38	0/3678	0.51	0/5007
3	c	0.39	0/3774	0.51	0/5135
4	D	0.46	0/2952	0.55	0/4021
4	d	0.45	0/2952	0.54	0/4021
5	E	0.33	0/693	0.48	0/944
5	e	0.33	0/695	0.50	0/948
6	F	0.39	0/284	0.51	0/387
6	f	0.40	0/265	0.53	0/360
7	H	0.36	0/535	0.54	0/728
7	h	0.35	0/524	0.52	0/713
8	I	0.34	0/311	0.50	0/419
8	i	0.36	0/311	0.52	0/419
9	J	0.36	0/278	0.41	0/376
9	j	0.32	0/286	0.46	0/386
10	K	0.35	0/303	0.50	0/416
10	k	0.35	0/303	0.49	0/416
11	L	0.42	0/319	0.49	0/433
11	l	0.45	0/319	0.50	0/433
12	M	0.46	0/270	0.59	0/368
12	m	0.44	0/262	0.60	0/357
13	O	0.38	0/1958	0.57	0/2654
13	o	0.38	0/1937	0.56	0/2625
14	T	0.44	0/266	0.52	0/362
14	t	0.50	0/266	0.52	0/362
15	U	0.38	0/785	0.54	0/1064
15	u	0.38	0/785	0.55	0/1064
16	V	0.36	0/1109	0.50	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.35	0/1098	0.51	0/1488
17	Y	0.33	0/216	0.46	0/289
17	y	0.31	0/216	0.46	0/289
18	X	0.34	0/290	0.46	0/392
18	x	0.32	0/284	0.47	0/384
19	Z	0.29	0/490	0.42	0/669
19	z	0.29	0/490	0.46	0/669
20	R	0.24	0/245	0.38	0/338
All	All	0.40	0/44392	0.53	0/60384

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/344 (112%)	378 (98%)	6 (2%)	1 (0%)	41	55
1	a	385/344 (112%)	381 (99%)	3 (1%)	1 (0%)	41	55
2	B	512/505 (101%)	503 (98%)	9 (2%)	0	100	100
2	b	513/505 (102%)	503 (98%)	9 (2%)	1 (0%)	47	62
3	C	461/455 (101%)	448 (97%)	11 (2%)	2 (0%)	34	48
3	c	473/455 (104%)	455 (96%)	16 (3%)	2 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	344 (97%)	11 (3%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	240 (96%)	9 (4%)	0	100	100
13	o	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	4	3
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5431/5384 (101%)	5280 (97%)	142 (3%)	9 (0%)	51	62

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
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	312/279 (112%)	312 (100%)	0	100	100
1	a	312/279 (112%)	310 (99%)	2 (1%)	86	94
2	B	412/403 (102%)	406 (98%)	6 (2%)	65	80
2	b	413/403 (102%)	407 (98%)	6 (2%)	65	80
3	C	361/356 (101%)	356 (99%)	5 (1%)	67	82
3	c	371/356 (104%)	361 (97%)	10 (3%)	44	65
4	D	290/277 (105%)	288 (99%)	2 (1%)	84	92
4	d	290/277 (105%)	288 (99%)	2 (1%)	84	92
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	82
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	51
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	54
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	32
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	62
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	27 (100%)	0	100	100
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	26
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	63
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	57
13	O	214/207 (103%)	208 (97%)	6 (3%)	43	63
13	o	211/207 (102%)	203 (96%)	8 (4%)	33	51
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	22
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	22
15	U	84/89 (94%)	81 (96%)	3 (4%)	35	54
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	68
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	91
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	44
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	14
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	12
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	32
20	R	25/29 (86%)	23 (92%)	2 (8%)	12	18
All	All	4506/4403 (102%)	4424 (98%)	82 (2%)	59	76

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	12	ASN
3	c	19	ASN
15	u	86	GLU

*Continued on next page...*

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Mol	Chain	Res	Type
1	a	257	ARG
2	b	240	SER

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

Mol	Chain	Res	Type
16	V	118	HIS
1	a	12	ASN
16	v	86	GLN
19	Z	58	ASN
1	a	315	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	FME	m	1	12	8,9,10	0.66	0	7,9,11	1.25	1 (14%)
14	FME	T	1	14	8,9,10	0.67	0	7,9,11	1.64	3 (42%)
12	FME	M	1	12	8,9,10	0.67	0	7,9,11	1.37	2 (28%)
14	FME	t	1	14	8,9,10	0.87	0	7,9,11	2.06	3 (42%)
8	FME	I	1	8	8,9,10	0.71	0	7,9,11	1.16	0
8	FME	i	1	8	8,9,10	0.68	0	7,9,11	1.15	1 (14%)

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

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

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

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-2.89	118.38	122.82
14	t	1	FME	O-C-CA	-2.72	117.64	124.78
14	T	1	FME	O-C-CA	-2.65	117.83	124.78
12	M	1	FME	CA-N-CN	-2.32	119.26	122.82
14	T	1	FME	C-CA-N	2.30	113.87	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

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 266 ligands modelled in this entry, 18 are unknown and 24 are monoatomic - leaving 224 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	HTG	V	206	-	19,19,19	1.04	2 (10%)	23,24,24	1.35	4 (17%)
33	LHG	L	101	-	48,48,48	0.86	2 (4%)	51,54,54	1.11	6 (11%)
23	CLA	C	504	-	59,73,73	2.04	13 (22%)	67,113,113	2.15	18 (26%)
26	SQD	A	410	-	53,54,54	0.99	3 (5%)	62,65,65	1.44	10 (16%)
23	CLA	c	508	41	59,73,73	2.00	13 (22%)	67,113,113	2.20	26 (38%)
33	LHG	d	410	-	48,48,48	0.86	2 (4%)	51,54,54	1.05	3 (5%)
28	LMT	T	104	-	25,25,36	0.57	1 (4%)	30,30,47	0.98	1 (3%)
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.58	3 (13%)
26	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.46	8 (15%)
36	LMG	b	629	-	51,51,55	0.91	2 (3%)	59,59,63	1.11	3 (5%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	7 (12%)
36	LMG	D	416	40	51,51,55	0.90	2 (3%)	59,59,63	0.96	3 (5%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.06	6 (7%)
23	CLA	C	503	-	59,73,73	2.00	13 (22%)	67,113,113	2.17	22 (32%)
23	CLA	C	507	-	59,73,73	1.97	13 (22%)	67,113,113	2.18	23 (34%)
27	GOL	a	402	-	5,5,5	0.37	0	5,5,5	0.36	0
27	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.26	0
23	CLA	b	616	41	59,73,73	1.98	13 (22%)	67,113,113	2.08	22 (32%)
28	LMT	M	104	-	36,36,36	0.55	1 (2%)	47,47,47	1.00	3 (6%)
23	CLA	c	513	-	59,73,73	2.07	13 (22%)	67,113,113	2.25	22 (32%)
36	LMG	c	522	-	51,51,55	0.94	2 (3%)	59,59,63	1.17	7 (11%)
27	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.26	0
25	BCR	Y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.80	14 (25%)
30	OYE	A	416[B]	1,3,41	0,16,16	0.00	-	-	-	-
31	PL9	d	407[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.55	14 (20%)
31	PL9	D	408[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.65	20 (29%)
36	LMG	d	416	40	51,51,55	0.91	2 (3%)	59,59,63	1.10	4 (6%)
35	HTG	b	631	-	19,19,19	0.87	1 (5%)	23,24,24	1.42	1 (4%)
27	GOL	o	301	-	5,5,5	0.41	0	5,5,5	0.32	0
31	PL9	d	407[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.66	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	GOL	a	401	-	5,5,5	0.40	0	5,5,5	0.40	0
25	BCR	B	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.43	7 (12%)
23	CLA	b	619	41	59,73,73	2.00	14 (23%)	67,113,113	2.10	22 (32%)
23	CLA	B	615	-	59,73,73	2.01	12 (20%)	67,113,113	2.18	22 (32%)
23	CLA	a	408	-	59,73,73	2.02	13 (22%)	67,113,113	2.18	25 (37%)
23	CLA	B	610	-	59,73,73	1.96	13 (22%)	67,113,113	2.15	24 (35%)
24	PHO	D	402[A]	-	67,69,69	2.15	16 (23%)	85,99,99	1.94	20 (23%)
23	CLA	A	404	-	59,73,73	2.02	12 (20%)	67,113,113	2.24	27 (40%)
31	PL9	A	417[A]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
37	DGD	c	521	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	4 (5%)
27	GOL	t	102	-	5,5,5	0.48	0	5,5,5	0.11	0
23	CLA	c	517	-	59,73,73	2.03	13 (22%)	67,113,113	2.13	24 (35%)
27	GOL	B	627	-	5,5,5	0.37	0	5,5,5	0.42	0
23	CLA	B	607	-	59,73,73	2.02	13 (22%)	67,113,113	2.26	22 (32%)
27	GOL	v	202	-	5,5,5	0.41	0	5,5,5	0.24	0
23	CLA	b	610	41	59,73,73	2.08	13 (22%)	67,113,113	2.13	19 (28%)
33	LHG	D	411	-	48,48,48	0.91	3 (6%)	51,54,54	0.90	3 (5%)
33	LHG	d	411	-	48,48,48	0.96	2 (4%)	51,54,54	1.05	2 (3%)
23	CLA	c	511	41	59,73,73	2.04	13 (22%)	67,113,113	2.17	20 (29%)
33	LHG	D	410	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	4 (7%)
23	CLA	B	608	41	59,73,73	1.98	14 (23%)	67,113,113	2.17	24 (35%)
28	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.06	3 (6%)
23	CLA	D	405	-	59,73,73	1.95	13 (22%)	67,113,113	2.26	23 (34%)
27	GOL	B	626	-	5,5,5	0.35	0	5,5,5	0.51	0
29	OEX	A	415[A]	1,3,41	0,15,15	0.00	-	-	-	-
27	GOL	A	411	-	5,5,5	0.39	0	5,5,5	0.39	0
23	CLA	B	616	-	59,73,73	2.01	12 (20%)	67,113,113	2.18	23 (34%)
37	DGD	D	409	-	52,52,67	1.03	3 (5%)	60,60,81	1.12	5 (8%)
25	BCR	d	406	-	41,41,41	1.07	1 (2%)	56,56,56	1.72	15 (26%)
27	GOL	B	629	-	5,5,5	0.42	0	5,5,5	0.45	0
23	CLA	C	511	-	59,73,73	2.06	13 (22%)	67,113,113	2.14	24 (35%)
25	BCR	c	526	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	10 (17%)
28	LMT	D	404	-	36,36,36	0.44	0	47,47,47	0.98	1 (2%)
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	8 (14%)
35	HTG	B	623	-	19,19,19	0.83	1 (5%)	23,24,24	1.47	3 (13%)
27	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.53	0
27	GOL	A	412	-	5,5,5	0.43	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	612	-	59,73,73	1.99	13 (22%)	67,113,113	2.25	23 (34%)
25	BCR	t	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.68	14 (25%)
30	OEY	a	417[B]	1,3,41	0,16,16	0.00	-	-		
27	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.76	0
24	PHO	d	402[B]	-	67,69,69	2.15	16 (23%)	85,99,99	1.99	21 (24%)
23	CLA	B	604	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	21 (31%)
25	BCR	b	628	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	10 (17%)
24	PHO	d	402[A]	-	67,69,69	2.13	16 (23%)	85,99,99	2.01	22 (25%)
23	CLA	b	623	-	59,73,73	1.98	13 (22%)	67,113,113	2.27	22 (32%)
23	CLA	c	514	-	59,73,73	2.05	13 (22%)	67,113,113	2.18	20 (29%)
23	CLA	D	406	-	59,73,73	1.97	13 (22%)	67,113,113	2.08	23 (34%)
23	CLA	C	513	-	59,73,73	2.06	13 (22%)	67,113,113	2.17	22 (32%)
28	LMT	A	414	-	36,36,36	0.59	1 (2%)	47,47,47	1.37	5 (10%)
27	GOL	V	204	-	5,5,5	0.37	0	5,5,5	0.27	0
36	LMG	k	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.05	4 (6%)
25	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.31	7 (12%)
23	CLA	B	611	41	59,73,73	2.02	14 (23%)	67,113,113	2.20	22 (32%)
23	CLA	c	515	3	59,73,73	1.97	13 (22%)	67,113,113	2.04	21 (31%)
37	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	3 (3%)
27	GOL	D	403	-	5,5,5	0.44	0	5,5,5	0.29	0
27	GOL	v	201	-	5,5,5	0.34	0	5,5,5	0.20	0
29	OEX	a	416[A]	1,3,41	0,15,15	0.00	-	-		
23	CLA	C	510	-	59,73,73	2.09	13 (22%)	67,113,113	2.09	23 (34%)
33	LHG	A	419	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
26	SQD	F	104	-	42,43,54	1.19	4 (9%)	51,54,65	1.54	9 (17%)
36	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.12	4 (8%)
39	HEM	F	102	5,6	27,50,50	0.85	2 (7%)	17,82,82	2.18	3 (17%)
35	HTG	c	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.50	3 (13%)
23	CLA	b	615	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	23 (34%)
23	CLA	A	408	-	59,73,73	1.99	13 (22%)	67,113,113	2.16	23 (34%)
25	BCR	a	412	-	41,41,41	1.05	1 (2%)	56,56,56	1.30	6 (10%)
22	BCT	A	403[A]	38	0,3,3	0.00	-	0,3,3	0.00	-
36	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	4 (6%)
28	LMT	e	102	-	36,36,36	0.49	0	47,47,47	0.82	0
36	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	5 (8%)
35	HTG	b	607	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	516	-	59,73,73	2.03	13 (22%)	67,113,113	2.33	23 (34%)
31	PL9	A	417[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.77	22 (32%)
23	CLA	C	505	41	59,73,73	2.07	14 (23%)	67,113,113	2.29	22 (32%)
25	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	12 (21%)
23	CLA	c	509	-	59,73,73	1.95	13 (22%)	67,113,113	2.09	20 (29%)
23	CLA	d	405	-	59,73,73	2.01	12 (20%)	67,113,113	2.21	25 (37%)
25	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	9 (16%)
23	CLA	a	411	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	23 (34%)
25	BCR	D	407	-	41,41,41	1.05	1 (2%)	56,56,56	1.73	12 (21%)
23	CLA	a	409	41	59,73,73	1.98	12 (20%)	67,113,113	2.18	24 (35%)
36	LMG	M	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.02	3 (5%)
39	HEM	v	206	16	27,50,50	0.87	1 (3%)	17,82,82	1.26	2 (11%)
37	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	4 (5%)
36	LMG	a	414	-	51,51,55	0.90	2 (3%)	59,59,63	1.20	6 (10%)
23	CLA	c	512	-	59,73,73	2.05	12 (20%)	67,113,113	2.28	23 (34%)
22	BCT	d	401[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	405	41	59,73,73	2.05	13 (22%)	67,113,113	2.34	23 (34%)
23	CLA	C	509	-	59,73,73	2.04	13 (22%)	67,113,113	2.17	23 (34%)
22	BCT	d	401[B]	38	0,3,3	0.00	-	0,3,3	0.00	-
31	PL9	D	408[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.74	20 (29%)
35	HTG	b	602	-	19,19,19	1.02	1 (5%)	23,24,24	1.11	2 (8%)
26	SQD	b	601	-	53,54,54	1.04	3 (5%)	62,65,65	1.58	12 (19%)
28	LMT	F	101	-	36,36,36	0.48	0	47,47,47	0.94	1 (2%)
23	CLA	B	613	-	59,73,73	2.04	13 (22%)	67,113,113	2.24	20 (29%)
39	HEM	e	101	5,6	27,50,50	0.81	1 (3%)	17,82,82	2.06	3 (17%)
33	LHG	a	419	-	41,41,48	1.03	2 (4%)	44,47,54	0.97	2 (4%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.42	2 (8%)
23	CLA	b	624	-	59,73,73	2.01	14 (23%)	67,113,113	2.05	21 (31%)
23	CLA	B	609	-	59,73,73	2.01	12 (20%)	67,113,113	2.14	22 (32%)
23	CLA	B	603	-	59,73,73	2.04	13 (22%)	67,113,113	2.36	28 (41%)
36	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.13	5 (8%)
23	CLA	b	618	-	59,73,73	1.98	13 (22%)	67,113,113	2.24	22 (32%)
25	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	11 (19%)
23	CLA	B	614	-	59,73,73	2.06	14 (23%)	67,113,113	2.18	22 (32%)
23	CLA	b	621	-	59,73,73	2.04	12 (20%)	67,113,113	2.31	24 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	DGD	d	408	-	63,63,67	0.93	2 (3%)	77,77,81	1.29	7 (9%)
28	LMT	a	418	-	36,36,36	0.43	0	47,47,47	0.76	0
24	PHO	D	402[B]	-	67,69,69	2.20	17 (25%)	85,99,99	1.85	21 (24%)
23	CLA	b	622	-	59,73,73	1.98	12 (20%)	67,113,113	2.23	25 (37%)
35	HTG	B	624	-	19,19,19	1.03	2 (10%)	23,24,24	2.12	4 (17%)
23	CLA	b	617	-	59,73,73	2.01	13 (22%)	67,113,113	2.15	22 (32%)
27	GOL	c	501	-	5,5,5	0.40	0	5,5,5	0.44	0
25	BCR	b	626	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	12 (21%)
35	HTG	b	608	-	19,19,19	1.06	2 (10%)	23,24,24	1.08	2 (8%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.41	9 (16%)
37	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	7 (9%)
25	BCR	T	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.72	15 (26%)
27	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.13	0
23	CLA	B	606	-	59,73,73	2.02	13 (22%)	67,113,113	2.15	21 (31%)
27	GOL	v	204	-	5,5,5	0.34	0	5,5,5	0.36	0
23	CLA	c	505	-	59,73,73	1.96	13 (22%)	67,113,113	2.16	23 (34%)
37	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	3 (3%)
23	CLA	b	614	-	59,73,73	1.97	13 (22%)	67,113,113	2.28	20 (29%)
23	CLA	b	611	-	59,73,73	2.04	13 (22%)	67,113,113	2.26	24 (35%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	7 (9%)
26	SQD	a	413	-	53,54,54	0.96	3 (5%)	62,65,65	1.56	12 (19%)
33	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.03	4 (7%)
25	BCR	B	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.41	6 (10%)
25	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	10 (17%)
27	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
35	HTG	B	631	-	19,19,19	1.04	1 (5%)	23,24,24	1.43	2 (8%)
27	GOL	B	630	-	5,5,5	0.34	0	5,5,5	0.41	0
36	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.34	6 (13%)
23	CLA	b	620	-	59,73,73	1.94	12 (20%)	67,113,113	2.23	23 (34%)
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.55	1 (4%)
27	GOL	v	203	-	5,5,5	0.38	0	5,5,5	0.40	0
25	BCR	A	409	-	41,41,41	1.07	1 (2%)	56,56,56	1.24	7 (12%)
28	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.91	2 (4%)
28	LMT	b	630	-	25,25,36	0.49	0	30,30,47	0.56	0
35	HTG	D	415	-	16,16,19	1.06	2 (12%)	20,21,24	1.47	1 (5%)
27	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	HEM	V	205	16	27,50,50	0.88	2 (7%)	17,82,82	1.61	3 (17%)
35	HTG	B	632	-	19,19,19	1.00	2 (10%)	23,24,24	1.31	1 (4%)
27	GOL	V	202	-	5,5,5	0.36	0	5,5,5	0.41	0
24	PHO	A	407	-	67,69,69	2.16	16 (23%)	85,99,99	1.93	24 (28%)
23	CLA	B	602	41	59,73,73	2.05	14 (23%)	67,113,113	2.12	19 (28%)
28	LMT	m	102	-	36,36,36	0.52	0	47,47,47	1.11	4 (8%)
23	CLA	C	508	41	59,73,73	1.98	13 (22%)	67,113,113	2.10	18 (26%)
35	HTG	d	414	-	16,16,19	1.19	2 (12%)	20,21,24	1.82	3 (15%)
23	CLA	d	403	41	59,73,73	2.03	13 (22%)	67,113,113	2.24	23 (34%)
28	LMT	a	404	-	36,36,36	0.57	1 (2%)	47,47,47	1.15	3 (6%)
23	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.14	20 (29%)
27	GOL	O	301	-	5,5,5	0.38	0	5,5,5	0.36	0
28	LMT	B	634	-	25,25,36	0.52	0	30,30,47	0.79	1 (3%)
23	CLA	c	506	-	59,73,73	2.02	12 (20%)	67,113,113	2.15	22 (32%)
27	GOL	V	201	-	5,5,5	0.34	0	5,5,5	0.38	0
23	CLA	B	617	-	59,73,73	1.99	12 (20%)	67,113,113	2.28	21 (31%)
27	GOL	B	635	-	5,5,5	0.38	0	5,5,5	0.44	0
28	LMT	M	105	-	36,36,36	0.48	0	47,47,47	0.85	0
23	CLA	c	510	-	59,73,73	1.98	14 (23%)	67,113,113	2.12	23 (34%)
23	CLA	A	406	41	59,73,73	1.98	11 (18%)	67,113,113	2.19	22 (32%)
27	GOL	F	103	34	5,5,5	0.38	0	5,5,5	0.18	0
31	PL9	a	415[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.82	21 (30%)
23	CLA	b	612	-	59,73,73	2.00	14 (23%)	67,113,113	2.30	22 (32%)
23	CLA	C	512	3	59,73,73	2.05	13 (22%)	67,113,113	2.12	24 (35%)
31	PL9	a	415[A]	-	55,55,55	0.61	2 (3%)	68,69,69	1.91	20 (29%)
25	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.69	14 (25%)
26	SQD	A	413	-	53,54,54	1.04	3 (5%)	62,65,65	1.14	6 (9%)
23	CLA	C	506	-	59,73,73	1.95	13 (22%)	67,113,113	2.15	17 (25%)
27	GOL	f	101	34	5,5,5	0.30	0	5,5,5	0.40	0
27	GOL	B	625	-	5,5,5	0.37	0	5,5,5	0.18	0
25	BCR	K	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	9 (16%)
23	CLA	C	514	-	59,73,73	2.03	13 (22%)	67,113,113	2.07	21 (31%)
23	CLA	b	613	-	59,73,73	2.01	13 (22%)	67,113,113	2.27	23 (34%)
33	LHG	b	634	-	48,48,48	0.97	2 (4%)	51,54,54	1.08	2 (3%)
26	SQD	B	636	-	53,54,54	1.06	3 (5%)	62,65,65	1.21	4 (6%)
27	GOL	b	605	-	5,5,5	0.36	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	625	-	59,73,73	1.96	12 (20%)	67,113,113	2.28	23 (34%)
35	HTG	C	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.81	4 (17%)
27	GOL	V	203	-	5,5,5	0.42	0	5,5,5	0.30	0
26	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.34	7 (11%)
35	HTG	b	632	-	19,19,19	1.16	2 (10%)	23,24,24	1.70	3 (13%)
23	CLA	d	404	-	59,73,73	2.00	14 (23%)	67,113,113	2.27	25 (37%)
23	CLA	B	605	-	59,73,73	1.91	12 (20%)	67,113,113	2.17	22 (32%)
22	BCT	A	403[B]	38	0,3,3	0.00	-	0,3,3	0.00	-
37	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.03	7 (9%)
27	GOL	b	603	-	5,5,5	0.37	0	5,5,5	0.50	0
33	LHG	D	412	-	48,48,48	0.97	2 (4%)	51,54,54	1.11	3 (5%)
24	PHO	a	410	-	67,69,69	2.10	17 (25%)	85,99,99	1.90	23 (27%)
27	GOL	c	502	-	5,5,5	0.39	0	5,5,5	0.42	0
23	CLA	c	507	-	59,73,73	1.97	12 (20%)	67,113,113	2.18	22 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	V	206	-	-	4/10/30/30	0/1/1/1
33	LHG	L	101	-	-	12/53/53/53	-
23	CLA	C	504	-	3/3/20/25	3/37/135/135	-
26	SQD	A	410	-	-	9/49/69/69	0/1/1/1
23	CLA	c	508	41	3/3/20/25	9/37/135/135	-
33	LHG	d	410	-	-	5/53/53/53	-
28	LMT	T	104	-	-	7/17/37/61	0/1/1/2
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
26	SQD	f	102	-	-	14/38/58/69	0/1/1/1
36	LMG	b	629	-	-	8/46/66/70	0/1/1/1
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
36	LMG	D	416	40	-	9/46/66/70	0/1/1/1
37	DGD	H	102	-	-	11/51/91/95	0/2/2/2
23	CLA	C	503	-	2/2/20/25	5/37/135/135	-
23	CLA	C	507	-	3/3/20/25	9/37/135/135	-
27	GOL	a	402	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	406	-	3/3/20/25	2/37/135/135	-
23	CLA	b	616	41	3/3/20/25	4/37/135/135	-
28	LMT	M	104	-	-	11/21/61/61	0/2/2/2
23	CLA	c	513	-	3/3/20/25	14/37/135/135	-
36	LMG	c	522	-	-	4/46/66/70	0/1/1/1
27	GOL	b	606	-	-	4/4/4/4	-
35	HTG	b	607	-	-	2/10/30/30	0/1/1/1
31	PL9	d	407[A]	-	-	8/53/73/73	0/1/1/1
31	PL9	D	408[A]	-	-	8/53/73/73	0/1/1/1
36	LMG	d	416	40	-	10/46/66/70	0/1/1/1
27	GOL	t	102	-	-	0/4/4/4	-
27	GOL	o	301	-	-	0/4/4/4	-
27	GOL	V	201	-	-	4/4/4/4	-
31	PL9	d	407[B]	-	-	7/53/73/73	0/1/1/1
27	GOL	a	401	-	-	2/4/4/4	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	b	619	41	3/3/20/25	6/37/135/135	-
23	CLA	B	615	-	3/3/20/25	18/37/135/135	-
23	CLA	a	408	-	3/3/20/25	6/37/135/135	-
23	CLA	B	610	-	3/3/20/25	4/37/135/135	-
24	PHO	D	402[A]	-	-	2/53/103/103	0/5/6/6
23	CLA	A	404	-	3/3/20/25	4/37/135/135	-
31	PL9	A	417[A]	-	-	10/53/73/73	0/1/1/1
25	BCR	d	406	-	-	5/29/63/63	0/2/2/2
37	DGD	c	521	-	-	12/51/91/95	0/2/2/2
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
23	CLA	c	517	-	2/2/20/25	4/37/135/135	-
27	GOL	B	627	-	-	2/4/4/4	-
23	CLA	B	607	-	3/3/20/25	7/37/135/135	-
27	GOL	v	202	-	-	2/4/4/4	-
23	CLA	b	610	41	3/3/20/25	13/37/135/135	-
33	LHG	D	411	-	-	9/53/53/53	-
25	BCR	t	101	-	-	3/29/63/63	0/2/2/2
23	CLA	c	511	41	3/3/20/25	4/37/135/135	-
33	LHG	D	410	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	608	41	3/3/20/25	6/37/135/135	-
37	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	D	405	-	1/1/20/25	2/37/135/135	-
27	GOL	B	626	-	-	0/4/4/4	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	616	-	3/3/20/25	9/37/135/135	-
37	DGD	D	409	-	-	19/47/67/95	0/1/1/2
23	CLA	b	621	-	3/3/20/25	2/37/135/135	-
27	GOL	B	629	-	-	2/4/4/4	-
23	CLA	C	511	-	3/3/20/25	11/37/135/135	-
25	BCR	c	526	-	-	3/29/63/63	0/2/2/2
28	LMT	D	404	-	-	8/21/61/61	0/2/2/2
25	BCR	C	515	-	-	6/29/63/63	0/2/2/2
35	HTG	B	623	-	-	6/10/30/30	0/1/1/1
27	GOL	C	525	-	-	0/4/4/4	-
27	GOL	A	412	-	-	2/4/4/4	-
23	CLA	B	612	-	3/3/20/25	5/37/135/135	-
33	LHG	d	411	-	-	13/53/53/53	-
27	GOL	C	524	-	-	0/4/4/4	-
24	PHO	d	402[B]	-	-	3/53/103/103	0/5/6/6
23	CLA	B	604	-	3/3/20/25	7/37/135/135	-
25	BCR	b	628	-	-	1/29/63/63	0/2/2/2
24	PHO	d	402[A]	-	-	3/53/103/103	0/5/6/6
23	CLA	c	514	-	3/3/20/25	10/37/135/135	-
27	GOL	B	628	-	-	2/4/4/4	-
23	CLA	C	513	-	3/3/20/25	7/37/135/135	-
28	LMT	A	414	-	-	6/21/61/61	0/2/2/2
27	GOL	V	204	-	-	2/4/4/4	-
36	LMG	k	101	-	-	17/46/66/70	0/1/1/1
25	BCR	b	627	-	-	2/29/63/63	0/2/2/2
23	CLA	B	611	41	3/3/20/25	8/37/135/135	-
23	CLA	c	515	3	3/3/20/25	4/37/135/135	-
28	LMT	C	521	-	-	10/21/61/61	0/2/2/2
27	GOL	D	403	-	-	2/4/4/4	-
27	GOL	v	201	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	HEM	V	205	16	-	0/6/54/54	-
23	CLA	C	510	-	3/3/20/25	12/37/135/135	-
33	LHG	A	419	-	-	21/46/46/53	-
26	SQD	F	104	-	-	17/38/58/69	0/1/1/1
36	LMG	z	101	-	-	15/34/54/70	0/1/1/1
39	HEM	F	102	5,6	-	0/6/54/54	-
35	HTG	c	524	-	-	0/10/30/30	0/1/1/1
23	CLA	b	615	-	3/3/20/25	10/37/135/135	-
23	CLA	A	408	-	2/2/20/25	10/37/135/135	-
25	BCR	a	412	-	-	0/29/63/63	0/2/2/2
36	LMG	C	520	-	-	13/46/66/70	0/1/1/1
28	LMT	e	102	-	-	7/21/61/61	0/2/2/2
36	LMG	C	519	-	-	11/46/66/70	0/1/1/1
23	CLA	B	605	-	3/3/20/25	2/37/135/135	-
23	CLA	c	516	-	3/3/20/25	8/37/135/135	-
31	PL9	A	417[B]	-	-	11/53/73/73	0/1/1/1
23	CLA	C	505	41	3/3/20/25	3/37/135/135	-
25	BCR	K	103	-	-	1/29/63/63	0/2/2/2
23	CLA	c	509	-	2/2/20/25	5/37/135/135	-
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
23	CLA	a	411	-	3/3/20/25	10/37/135/135	-
25	BCR	D	407	-	-	6/29/63/63	0/2/2/2
23	CLA	a	409	41	2/2/20/25	8/37/135/135	-
36	LMG	M	101	-	-	10/46/66/70	0/1/1/1
39	HEM	v	206	16	-	0/6/54/54	-
37	DGD	C	518	-	-	12/51/91/95	0/2/2/2
36	LMG	a	414	-	-	14/46/66/70	0/1/1/1
23	CLA	c	512	-	3/3/20/25	4/37/135/135	-
23	CLA	A	405	41	3/3/20/25	4/37/135/135	-
23	CLA	C	509	-	3/3/20/25	9/37/135/135	-
25	BCR	b	626	-	-	4/29/63/63	0/2/2/2
31	PL9	D	408[B]	-	-	7/53/73/73	0/1/1/1
35	HTG	b	602	-	-	3/10/30/30	0/1/1/1
26	SQD	b	601	-	-	25/49/69/69	0/1/1/1
28	LMT	F	101	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	-	3/3/20/25	3/37/135/135	-
39	HEM	e	101	5,6	-	0/6/54/54	-
33	LHG	a	419	-	-	17/46/46/53	-
35	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	b	624	-	3/3/20/25	3/37/135/135	-
23	CLA	B	609	-	2/2/20/25	1/37/135/135	-
23	CLA	B	603	-	2/2/20/25	5/37/135/135	-
36	LMG	C	501	-	-	17/46/66/70	0/1/1/1
23	CLA	d	403	41	3/3/20/25	7/37/135/135	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	614	-	3/3/20/25	9/37/135/135	-
37	DGD	d	408	-	-	28/51/91/95	0/2/2/2
28	LMT	a	418	-	-	4/21/61/61	0/2/2/2
24	PHO	D	402[B]	-	-	2/53/103/103	0/5/6/6
23	CLA	b	622	-	3/3/20/25	5/37/135/135	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
23	CLA	b	617	-	2/2/20/25	2/37/135/135	-
27	GOL	c	501	-	-	0/4/4/4	-
23	CLA	d	405	-	3/3/20/25	6/37/135/135	-
35	HTG	b	608	-	-	1/10/30/30	0/1/1/1
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2
25	BCR	T	103	-	-	3/29/63/63	0/2/2/2
27	GOL	T	101	-	-	0/4/4/4	-
23	CLA	B	606	-	3/3/20/25	3/37/135/135	-
27	GOL	v	204	-	-	2/4/4/4	-
23	CLA	c	505	-	3/3/20/25	5/37/135/135	-
37	DGD	c	520	-	-	19/51/91/95	0/2/2/2
23	CLA	b	614	-	3/3/20/25	8/37/135/135	-
23	CLA	b	611	-	2/2/20/25	4/37/135/135	-
37	DGD	c	519	-	-	14/51/91/95	0/2/2/2
26	SQD	a	413	-	-	14/49/69/69	0/1/1/1
33	LHG	d	409	-	-	5/53/53/53	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
25	BCR	c	518	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	T	102	-	-	2/4/4/4	-
35	HTG	B	631	-	-	2/10/30/30	0/1/1/1
27	GOL	B	630	-	-	4/4/4/4	-
36	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
23	CLA	b	620	-	3/3/20/25	5/37/135/135	-
35	HTG	c	523	-	-	3/10/30/30	0/1/1/1
27	GOL	v	203	-	-	2/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
28	LMT	M	102	-	-	5/21/61/61	0/2/2/2
28	LMT	b	630	-	-	4/17/37/61	0/1/1/2
35	HTG	D	415	-	-	0/7/27/30	0/1/1/1
27	GOL	b	604	-	-	0/4/4/4	-
35	HTG	B	632	-	-	1/10/30/30	0/1/1/1
27	GOL	V	202	-	-	0/4/4/4	-
23	CLA	b	623	-	3/3/20/25	19/37/135/135	-
23	CLA	B	602	41	3/3/20/25	12/37/135/135	-
23	CLA	C	508	41	3/3/20/25	5/37/135/135	-
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
23	CLA	b	618	-	2/2/20/25	3/37/135/135	-
28	LMT	a	404	-	-	5/21/61/61	0/2/2/2
23	CLA	C	502	-	3/3/20/25	11/37/135/135	-
24	PHO	A	407	-	-	3/53/103/103	0/5/6/6
28	LMT	B	634	-	-	6/17/37/61	0/1/1/2
23	CLA	c	506	-	3/3/20/25	3/37/135/135	-
27	GOL	O	301	-	-	2/4/4/4	-
23	CLA	B	617	-	3/3/20/25	6/37/135/135	-
27	GOL	B	635	-	-	0/4/4/4	-
28	LMT	M	105	-	-	7/21/61/61	0/2/2/2
23	CLA	c	510	-	3/3/20/25	14/37/135/135	-
23	CLA	A	406	41	2/2/20/25	6/37/135/135	-
27	GOL	F	103	34	-	2/4/4/4	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
31	PL9	a	415[B]	-	-	15/53/73/73	0/1/1/1
23	CLA	b	612	-	2/2/20/25	8/37/135/135	-
23	CLA	C	512	3	2/2/20/25	5/37/135/135	-

*Continued on next page...*



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PL9	a	415[A]	-	-	14/53/73/73	0/1/1/1
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	A	413	-	-	14/49/69/69	0/1/1/1
23	CLA	C	506	-	1/1/20/25	6/37/135/135	-
27	GOL	f	101	34	-	2/4/4/4	-
27	GOL	B	625	-	-	0/4/4/4	-
25	BCR	K	101	-	-	2/29/63/63	0/2/2/2
23	CLA	C	514	-	2/2/20/25	7/37/135/135	-
23	CLA	b	613	-	3/3/20/25	4/37/135/135	-
33	LHG	b	634	-	-	17/53/53/53	-
26	SQD	B	636	-	-	15/49/69/69	0/1/1/1
27	GOL	b	605	-	-	2/4/4/4	-
23	CLA	b	625	-	3/3/20/25	10/37/135/135	-
35	HTG	C	523	-	-	3/10/30/30	0/1/1/1
27	GOL	V	203	-	-	2/4/4/4	-
26	SQD	B	621	-	-	20/49/69/69	0/1/1/1
35	HTG	b	632	-	-	4/10/30/30	0/1/1/1
23	CLA	d	404	-	1/1/20/25	5/37/135/135	-
28	LMT	m	102	-	-	5/21/61/61	0/2/2/2
37	DGD	C	517	-	-	15/51/91/95	0/2/2/2
27	GOL	b	603	-	-	0/4/4/4	-
33	LHG	D	412	-	-	16/53/53/53	-
24	PHO	a	410	-	-	7/53/103/103	0/5/6/6
27	GOL	c	502	-	-	2/4/4/4	-
23	CLA	c	507	-	3/3/20/25	3/37/135/135	-

The worst 5 of 1169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3B-C2B	6.99	1.50	1.40
23	c	513	CLA	C3B-C2B	6.67	1.49	1.40
23	b	613	CLA	C3B-C2B	6.51	1.49	1.40
23	A	405	CLA	C3B-C2B	6.48	1.49	1.40
23	B	613	CLA	C3B-C2B	6.48	1.49	1.40

The worst 5 of 2361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402[B]	PHO	CMD-C2D-C1D	7.50	136.62	125.06
23	B	603	CLA	C4A-NA-C1A	-7.35	103.40	106.71
23	d	404	CLA	C4A-NA-C1A	-7.22	103.46	106.71
23	b	622	CLA	C2C-C1C-NC	7.00	116.53	109.97
23	c	516	CLA	C4A-NA-C1A	-6.92	103.59	106.71

5 of 190 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND

5 of 1351 torsion outliers are listed below:

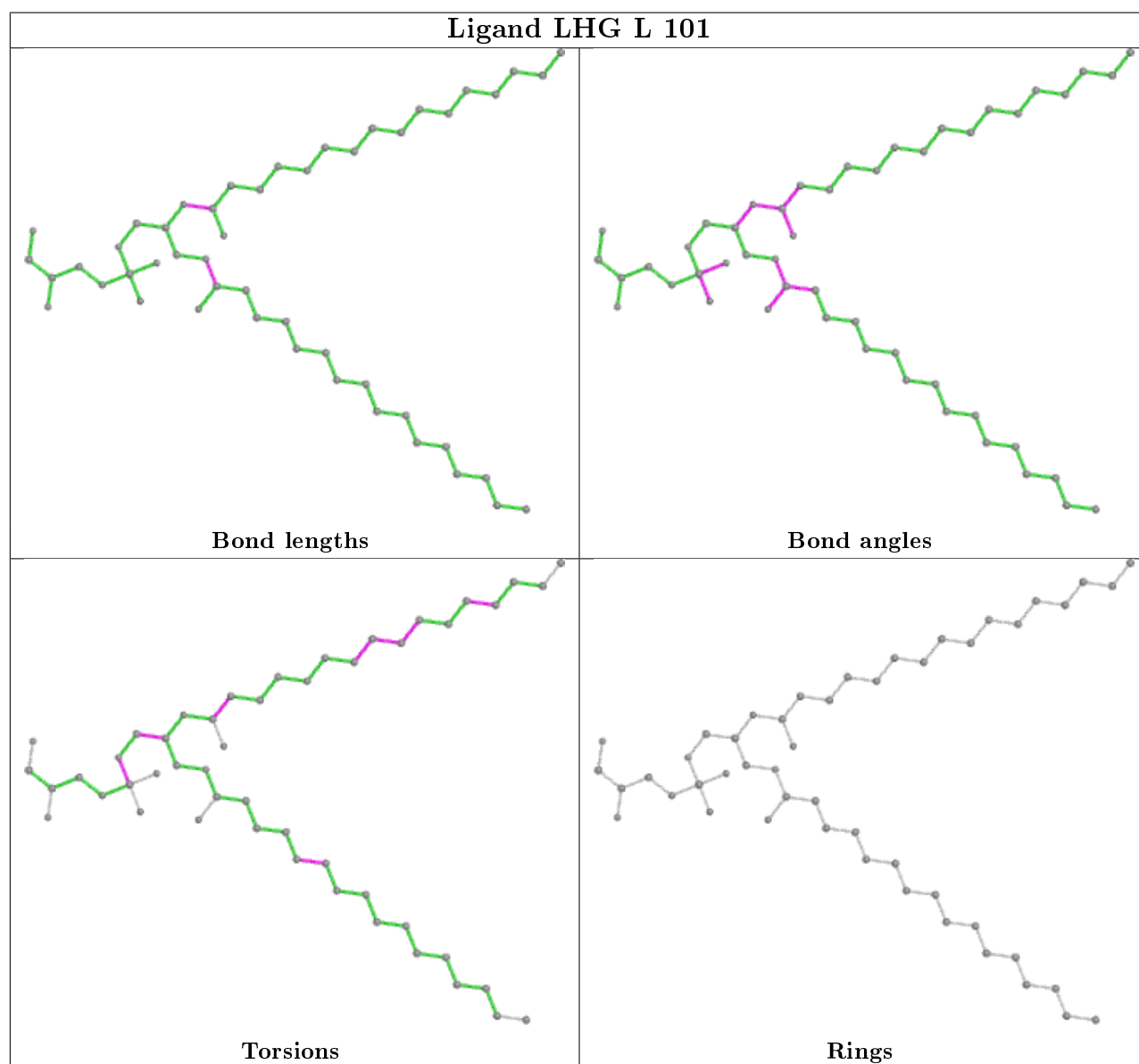
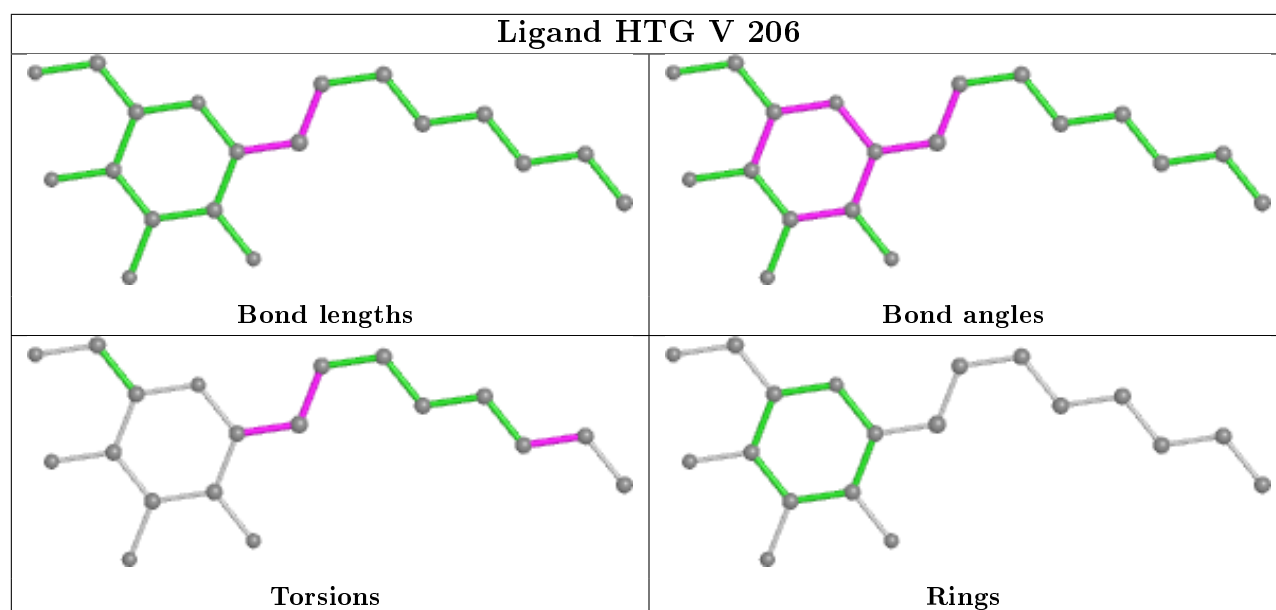
Mol	Chain	Res	Type	Atoms
35	V	206	HTG	C2-C1-S1-C1'
35	V	206	HTG	O5-C1-S1-C1'
35	V	206	HTG	C2'-C1'-S1-C1
33	L	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O4

There are no ring outliers.

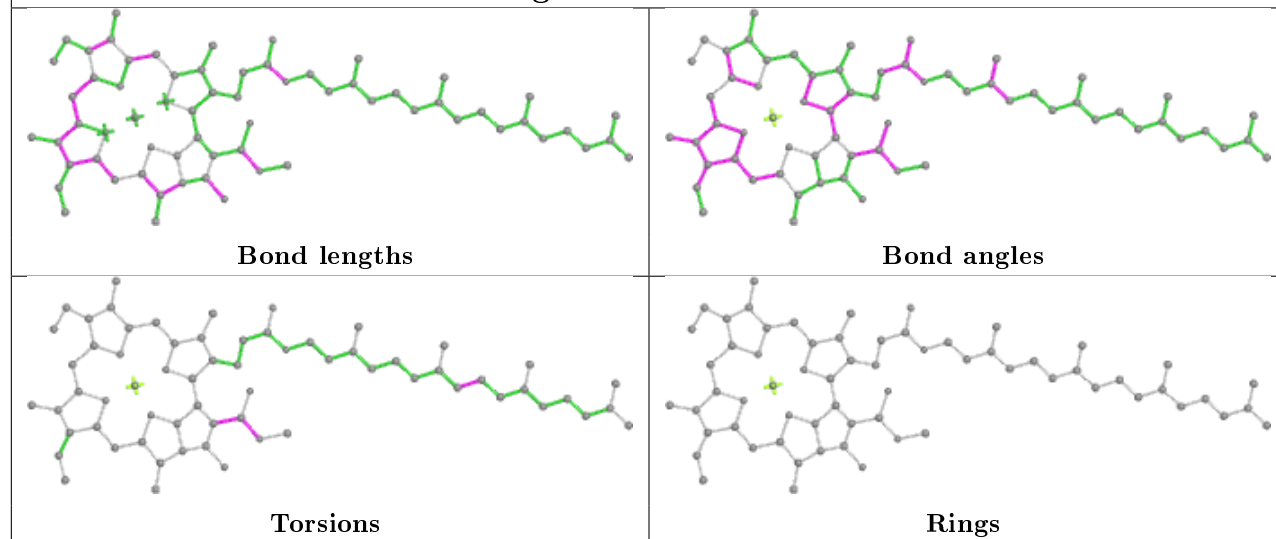
1 monomer is involved in 1 short contact:

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

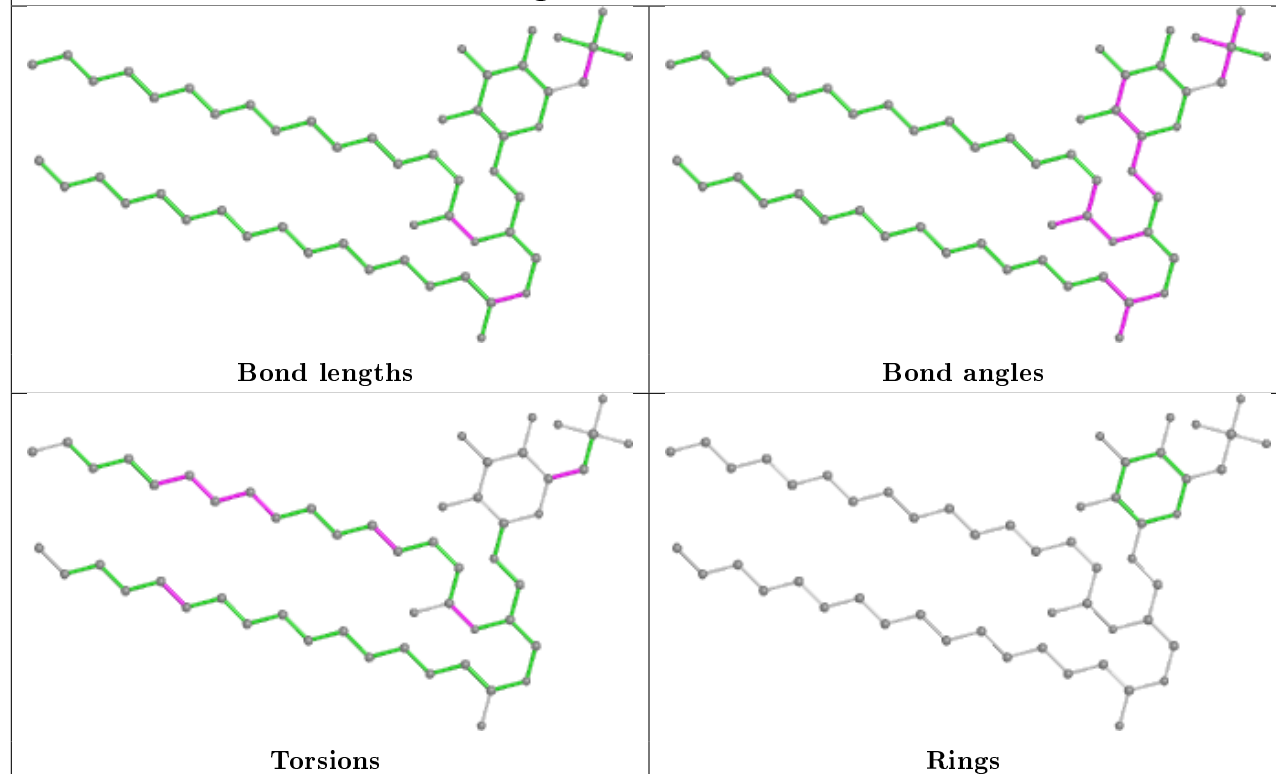
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



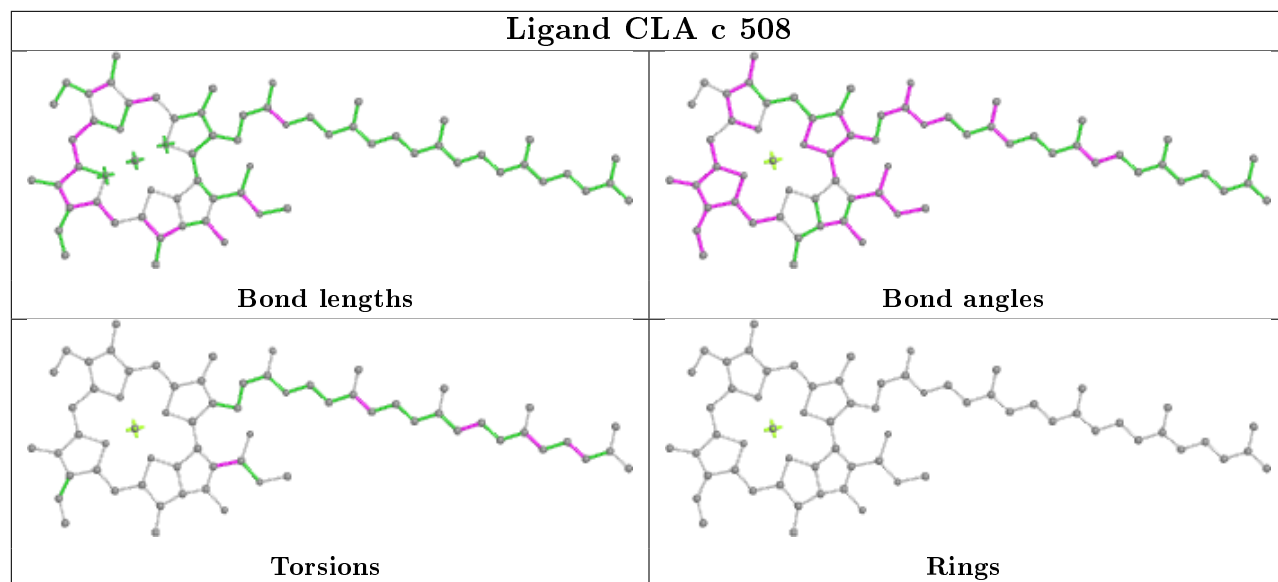
## Ligand CLA C 504



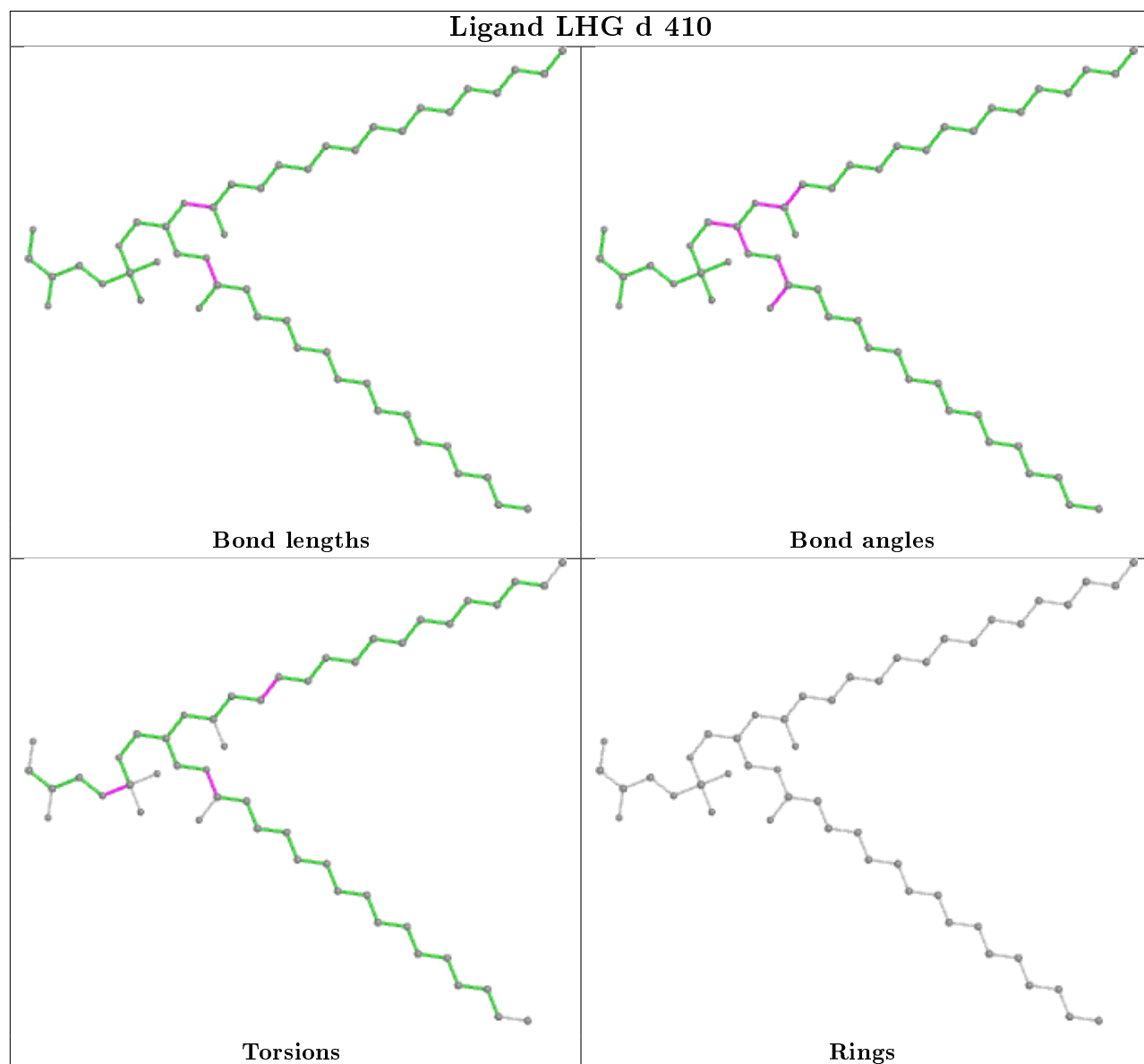
## Ligand SQD A 410

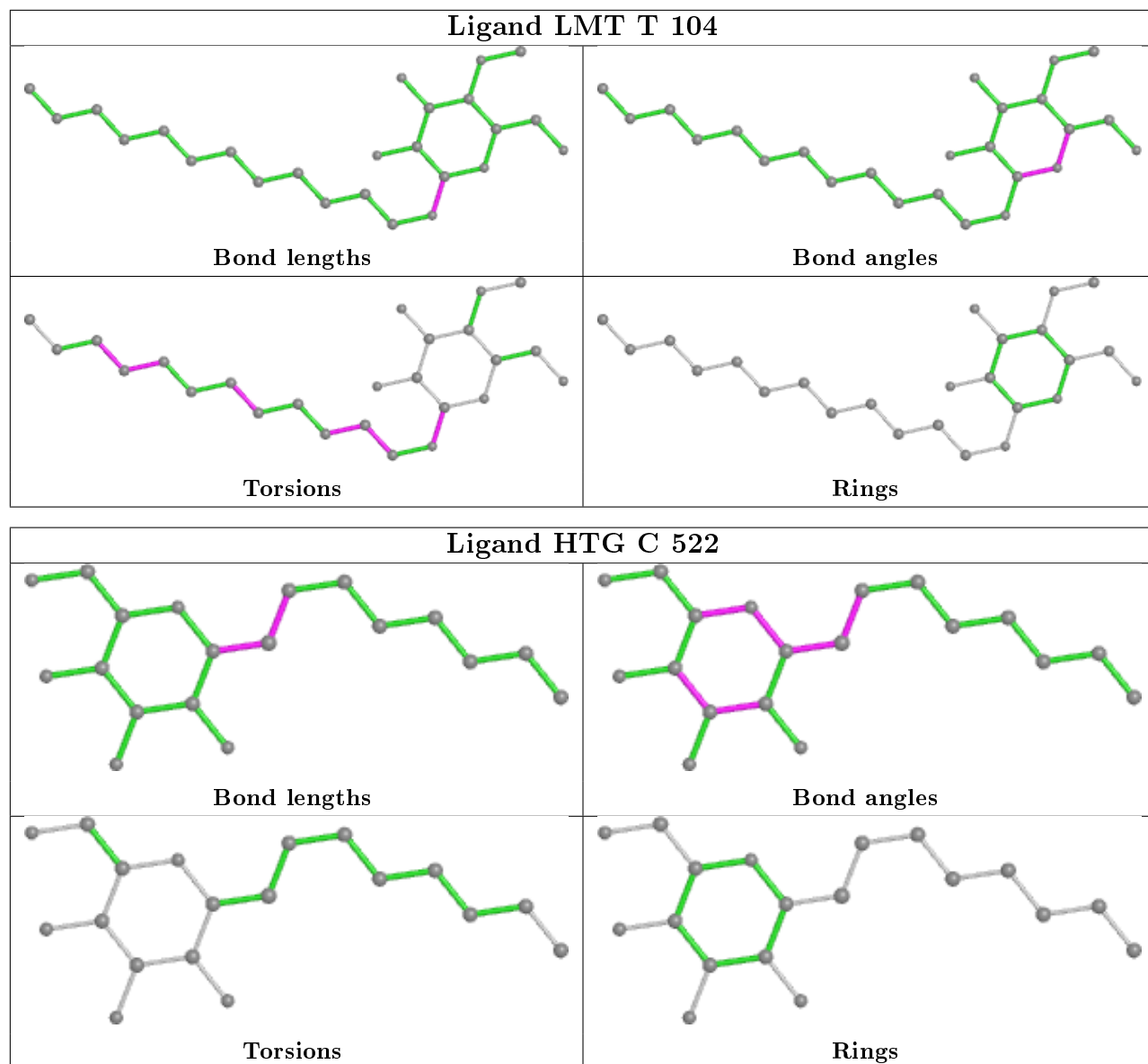


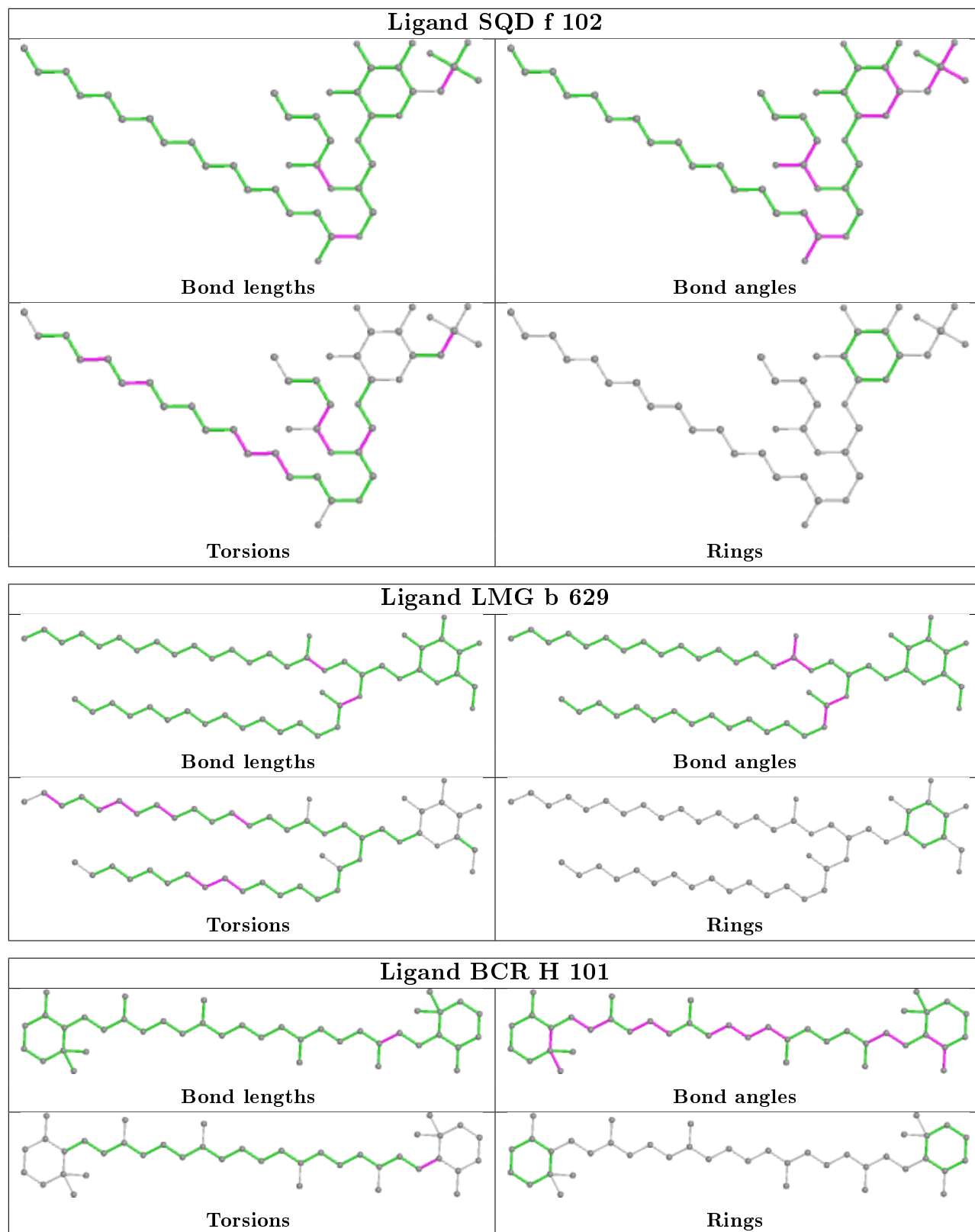
## Ligand CLA c 508

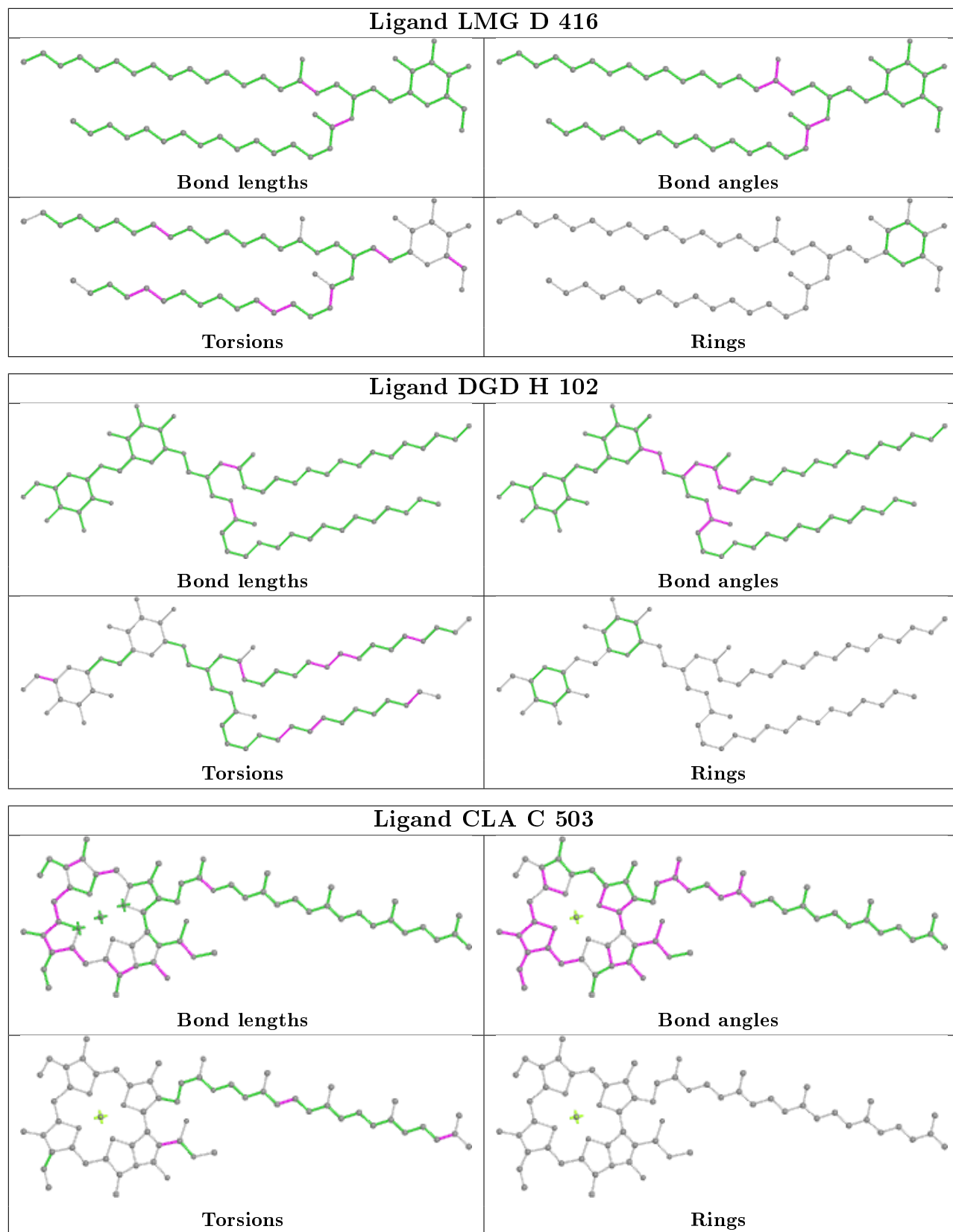


## Ligand LHG d 410

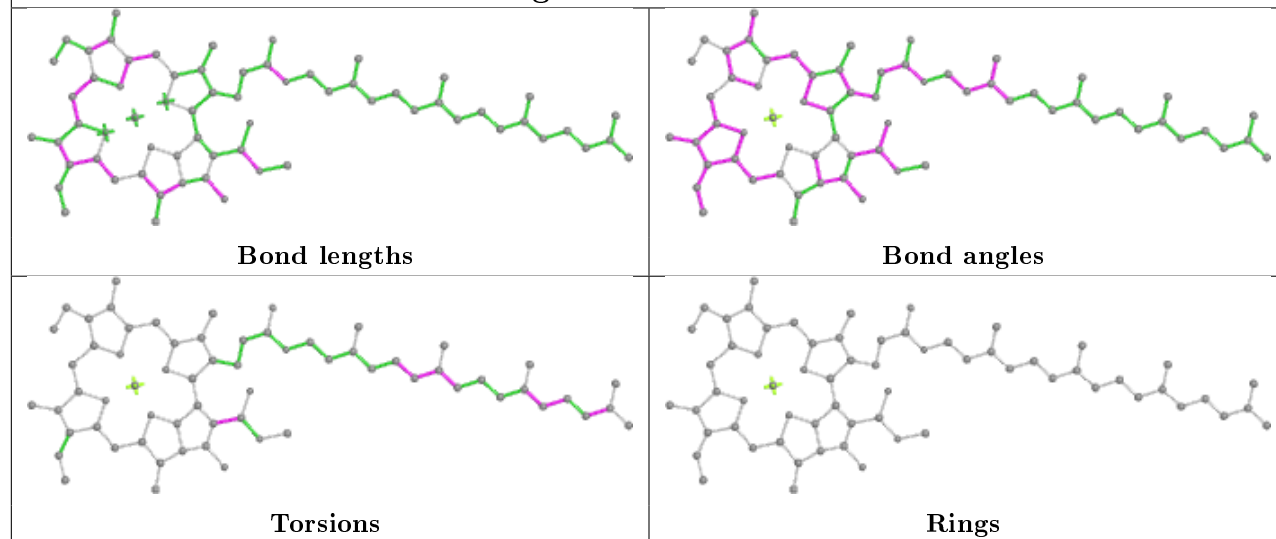
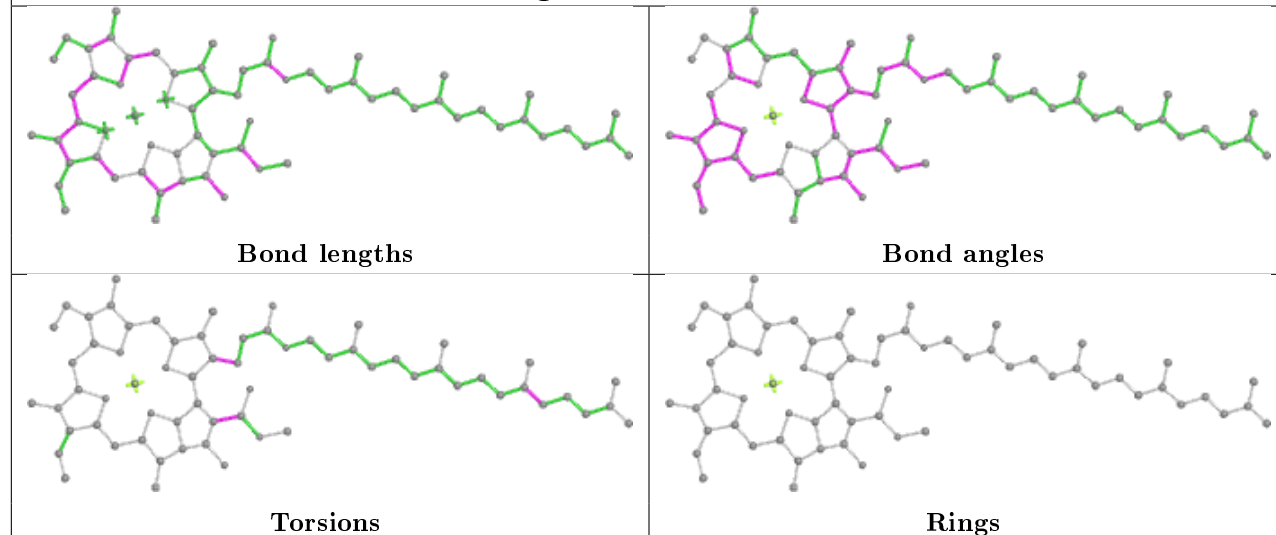
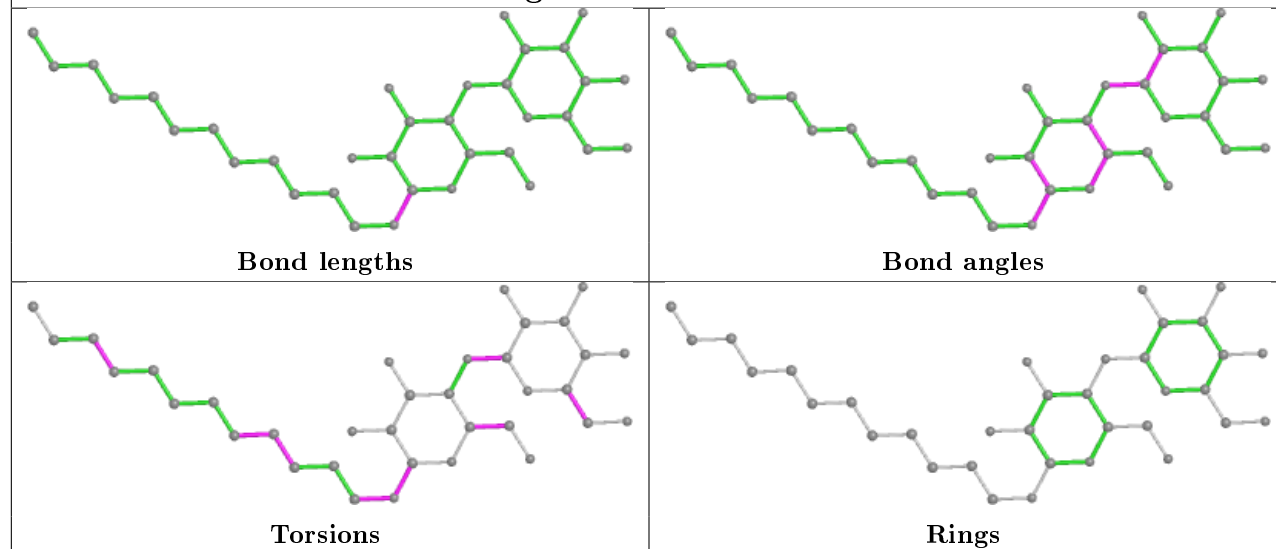


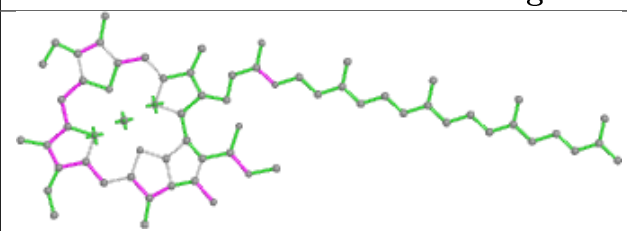
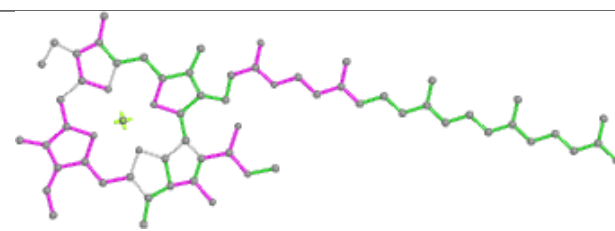
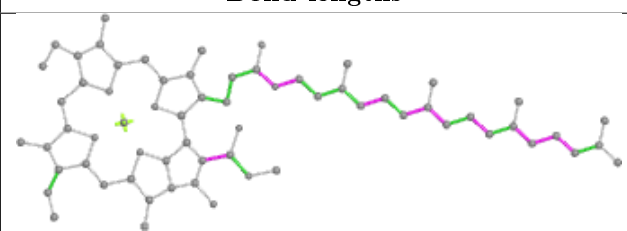
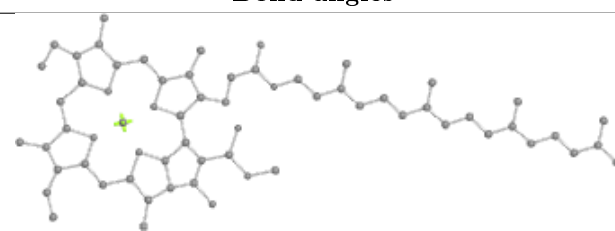


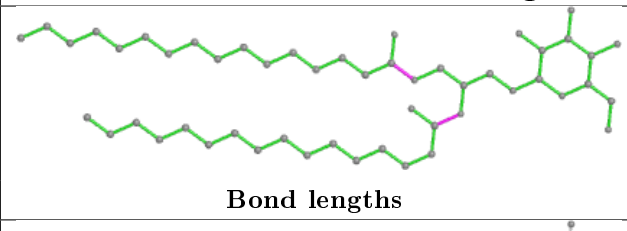
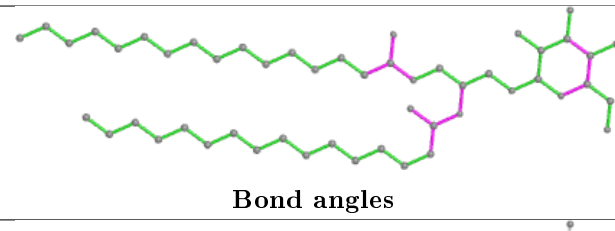
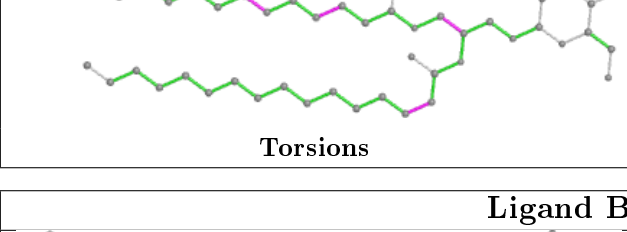



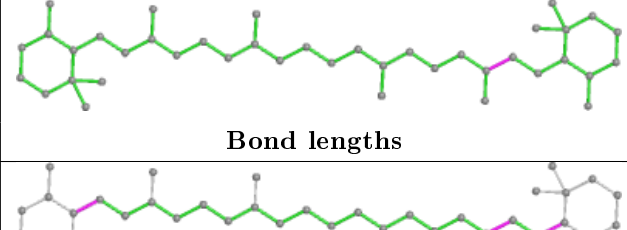
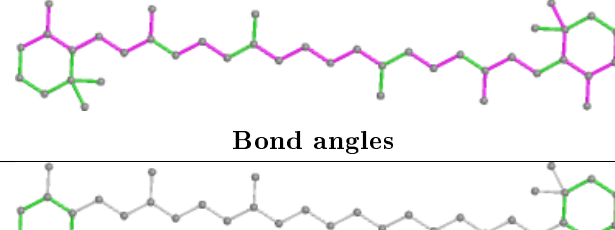
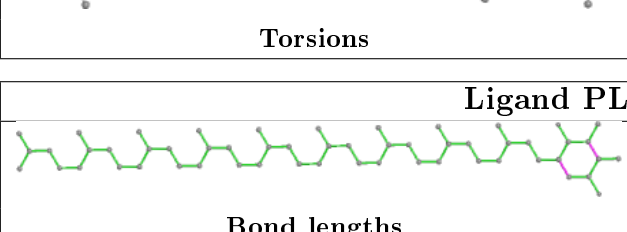
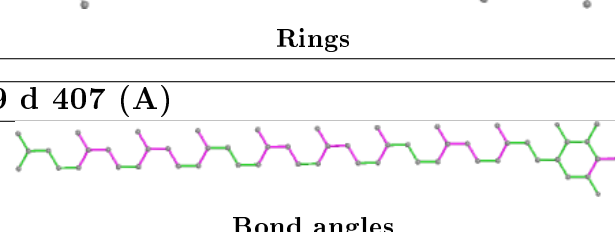


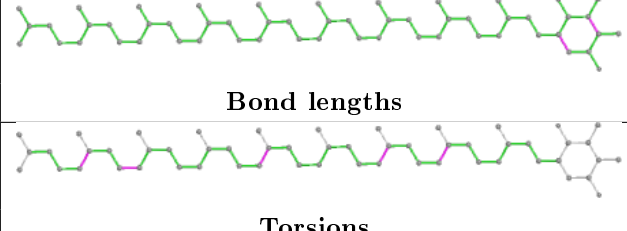
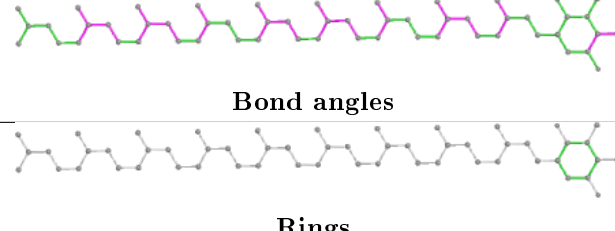




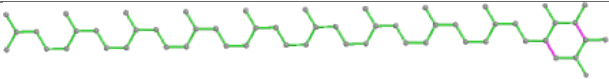
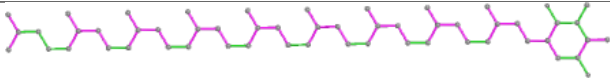
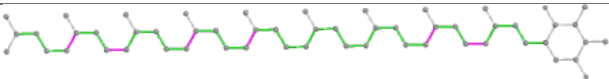
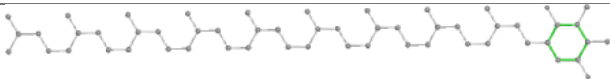
**Ligand CLA C 507****Ligand CLA b 616****Ligand LMT M 104**

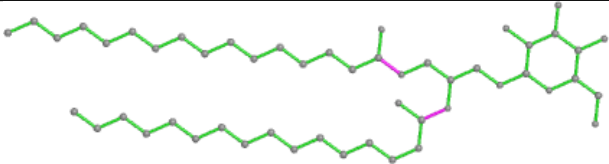
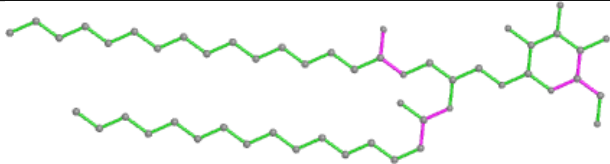
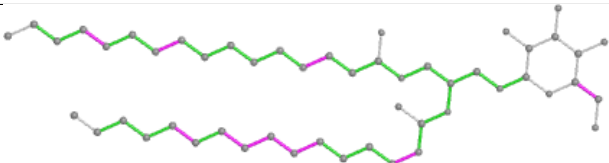
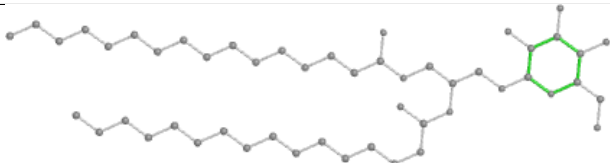
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

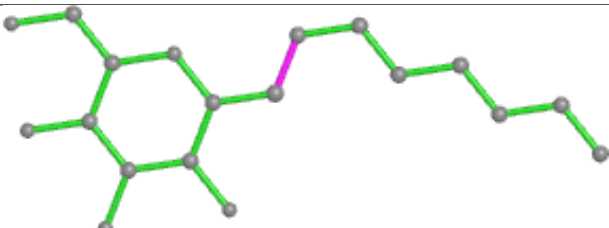
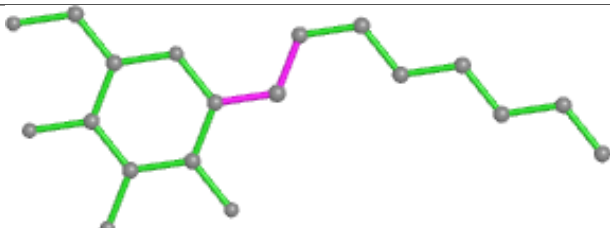
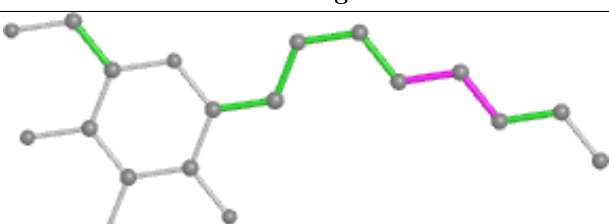
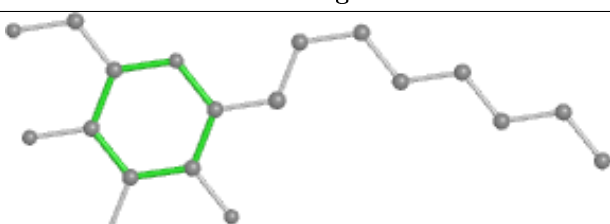
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

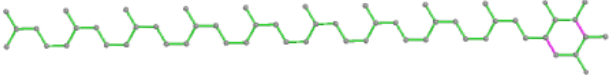
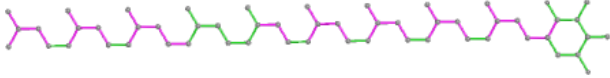
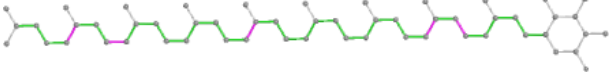
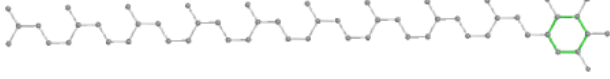
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

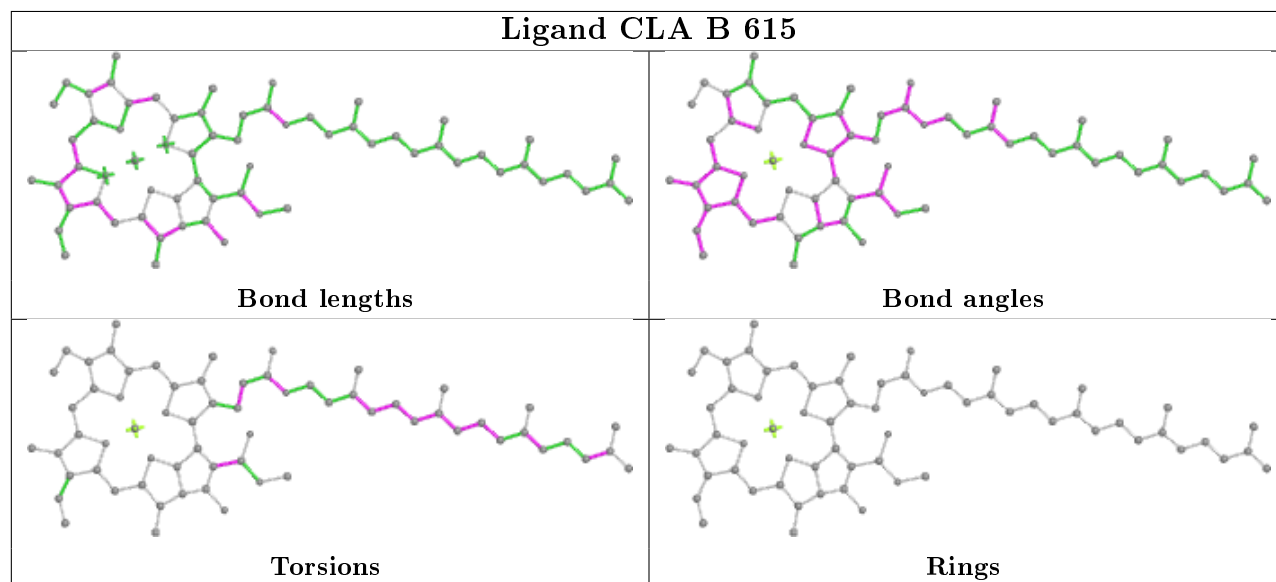
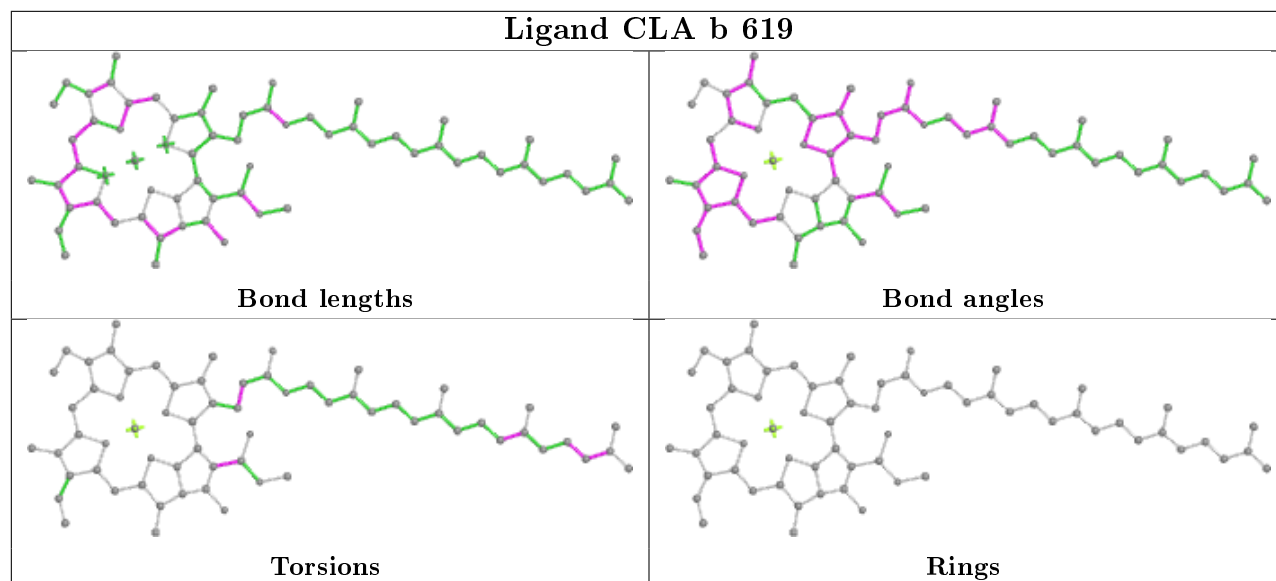
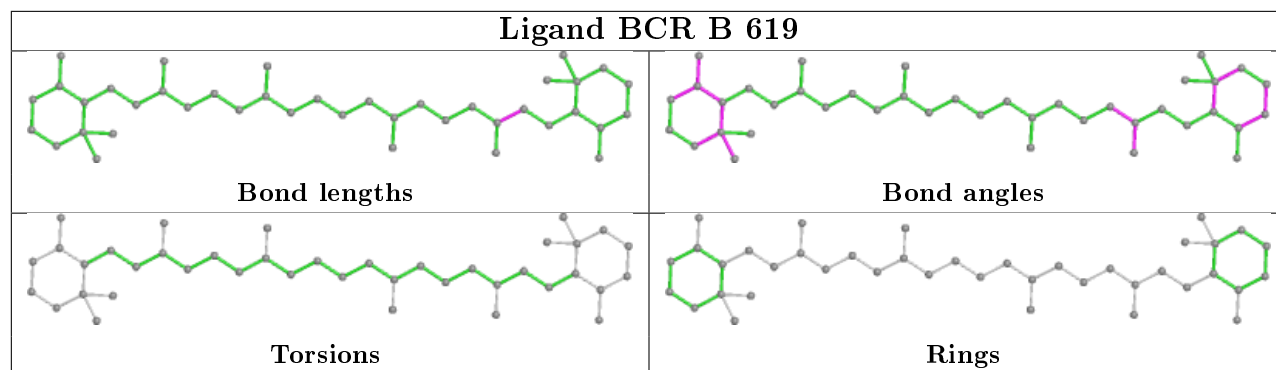
Ligand PL9 d 407 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 408 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

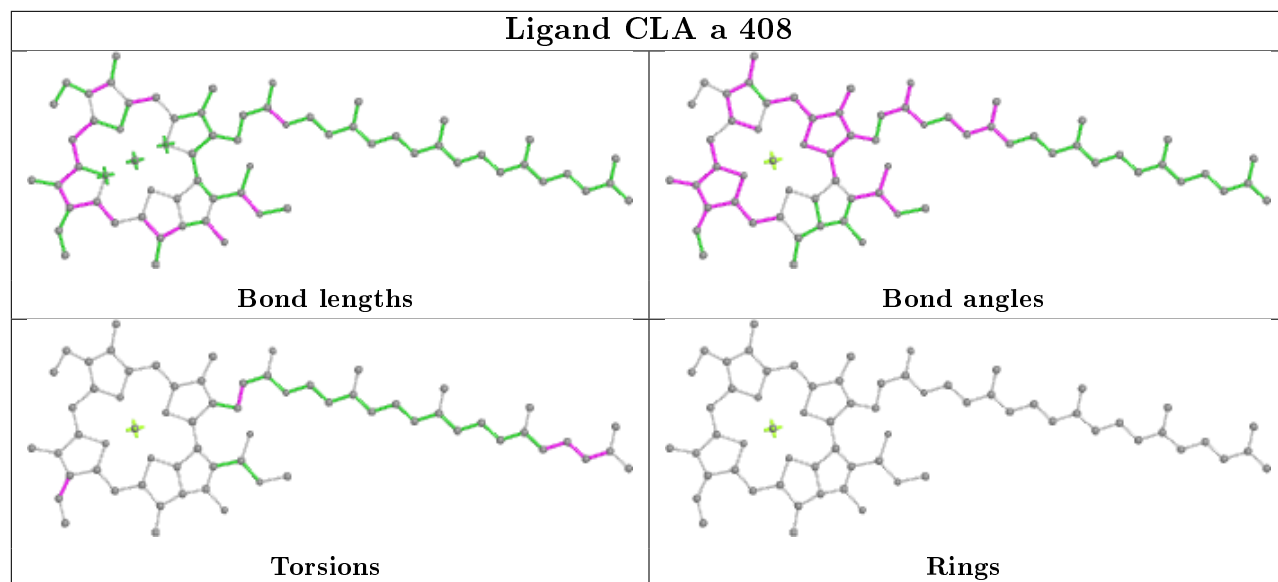
Ligand LMG d 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG b 631	
 Bond lengths	 Bond angles
 Torsions	 Rings

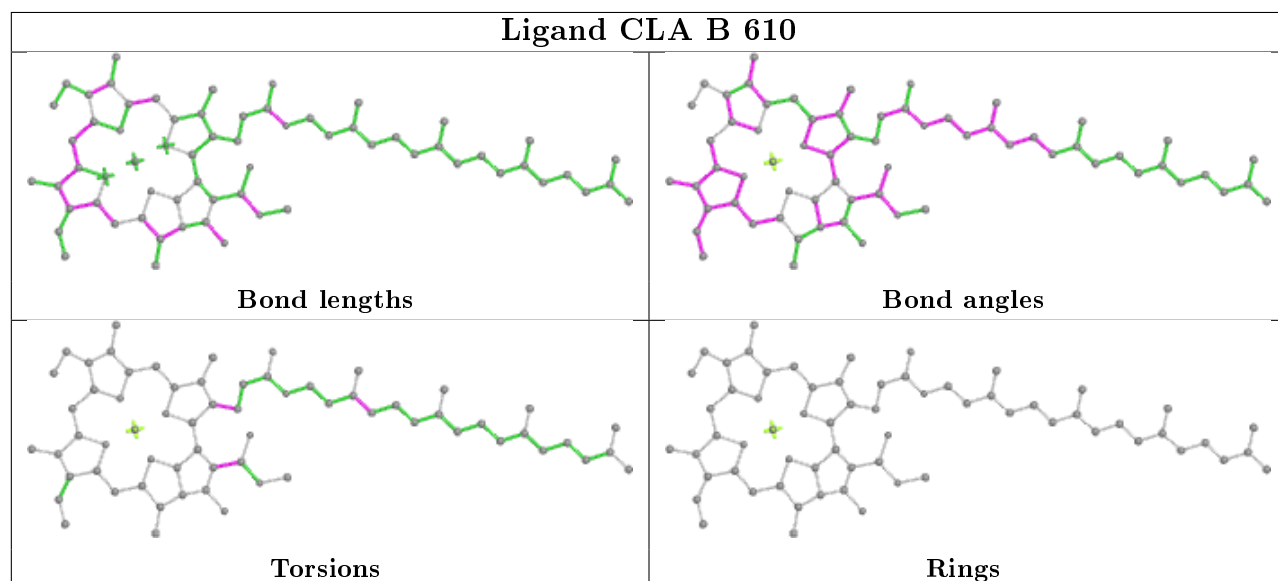
Ligand PL9 d 407 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings



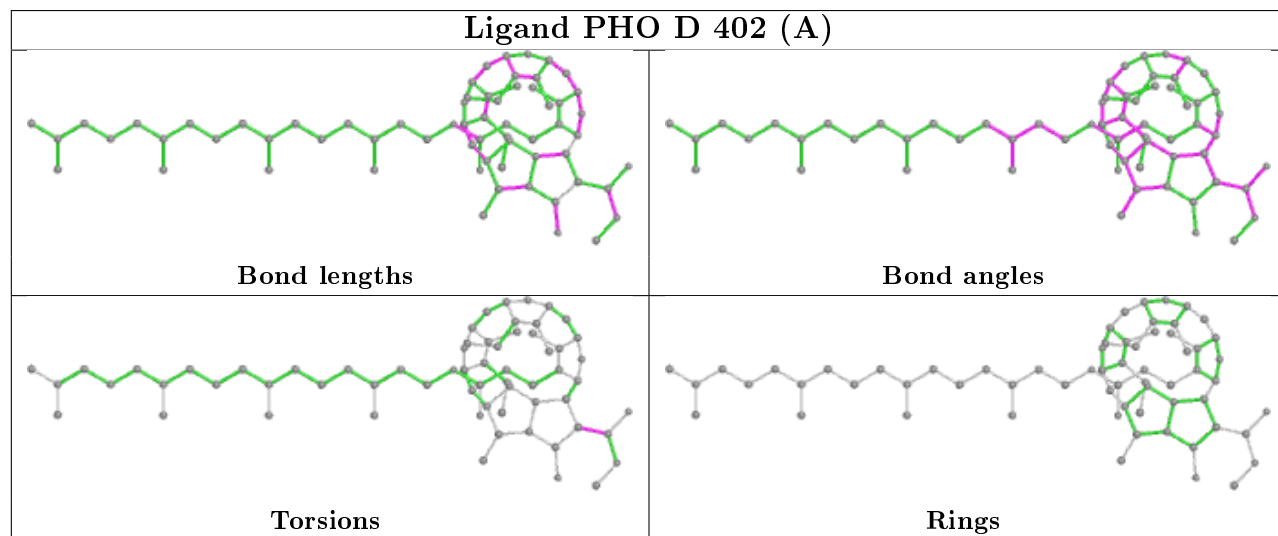
## Ligand CLA a 408

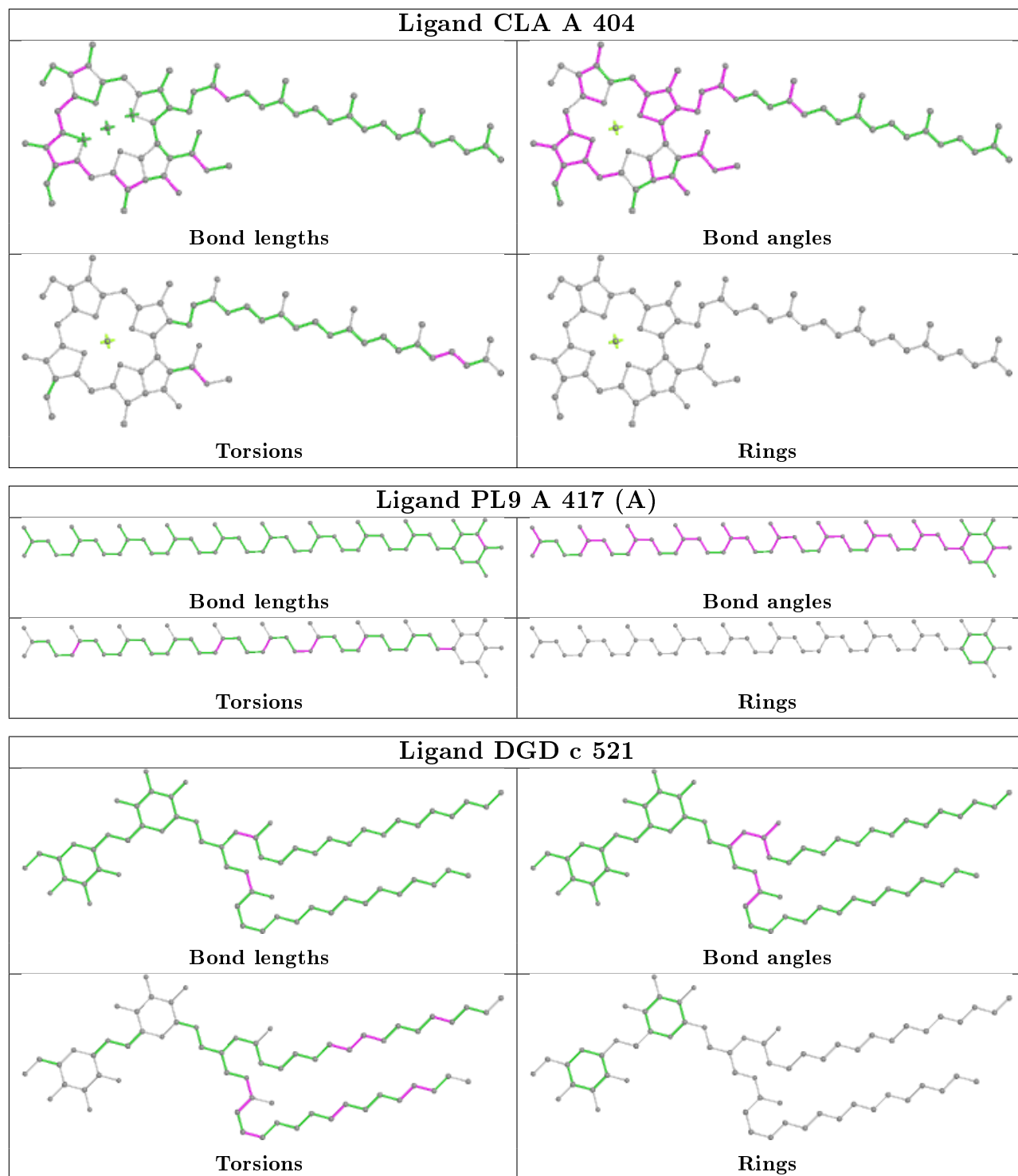


## Ligand CLA B 610

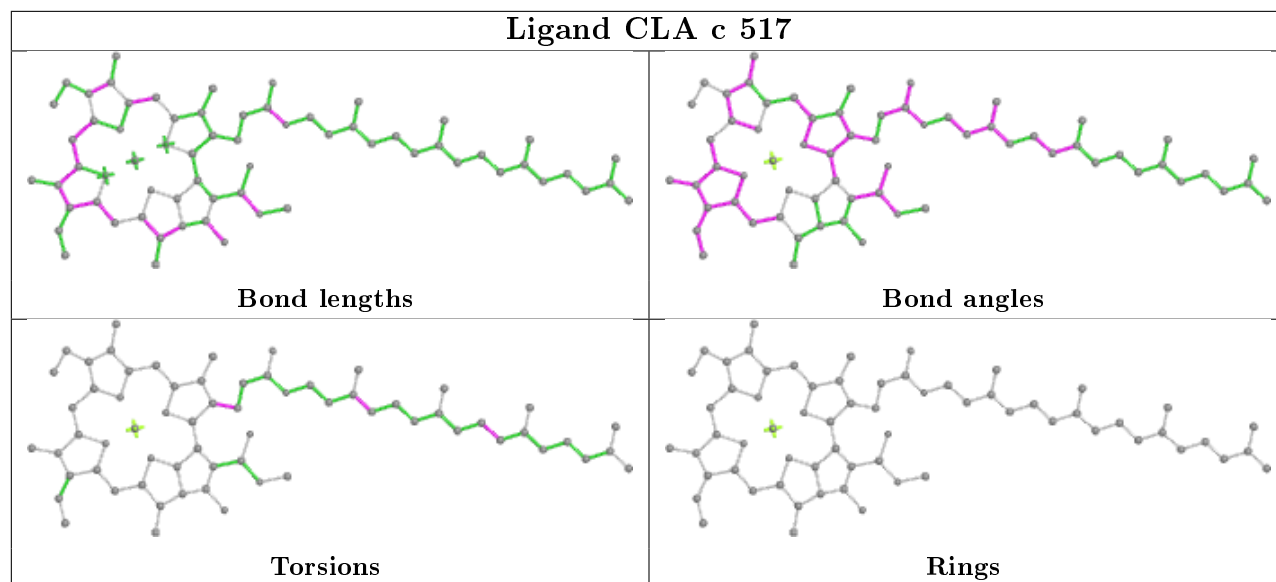


## Ligand PHO D 402 (A)

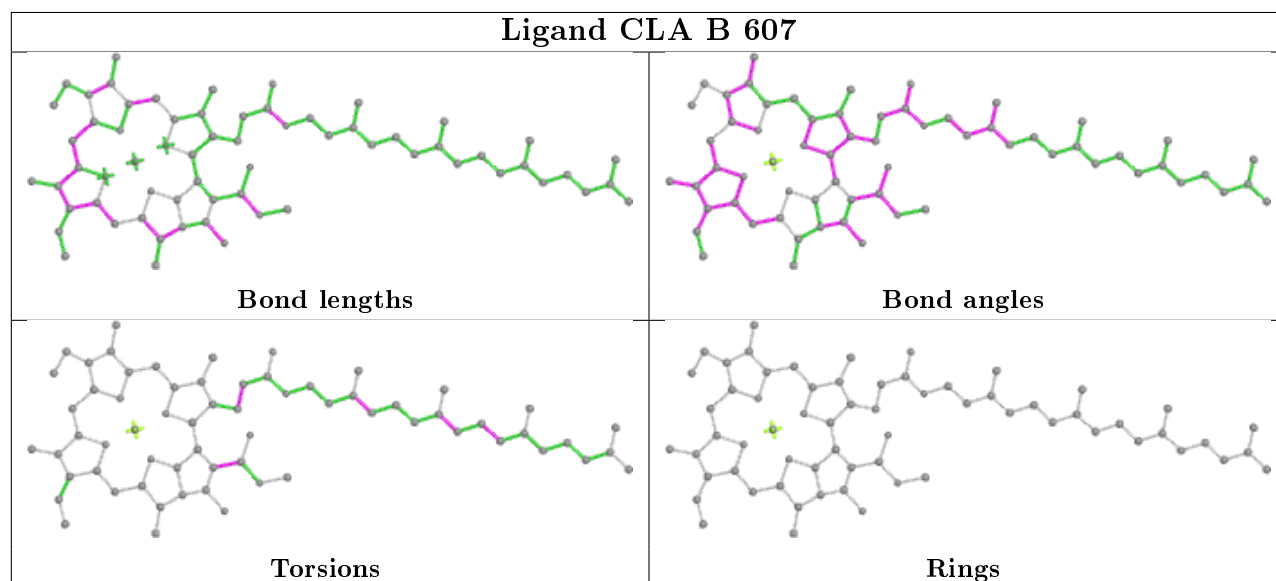




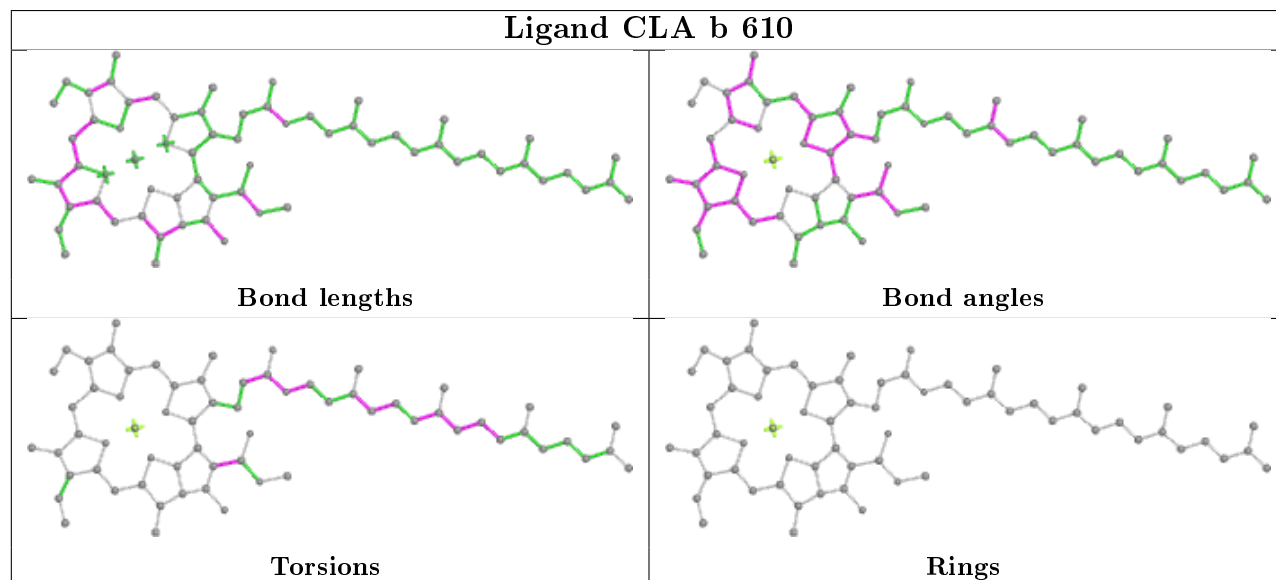
## Ligand CLA c 517

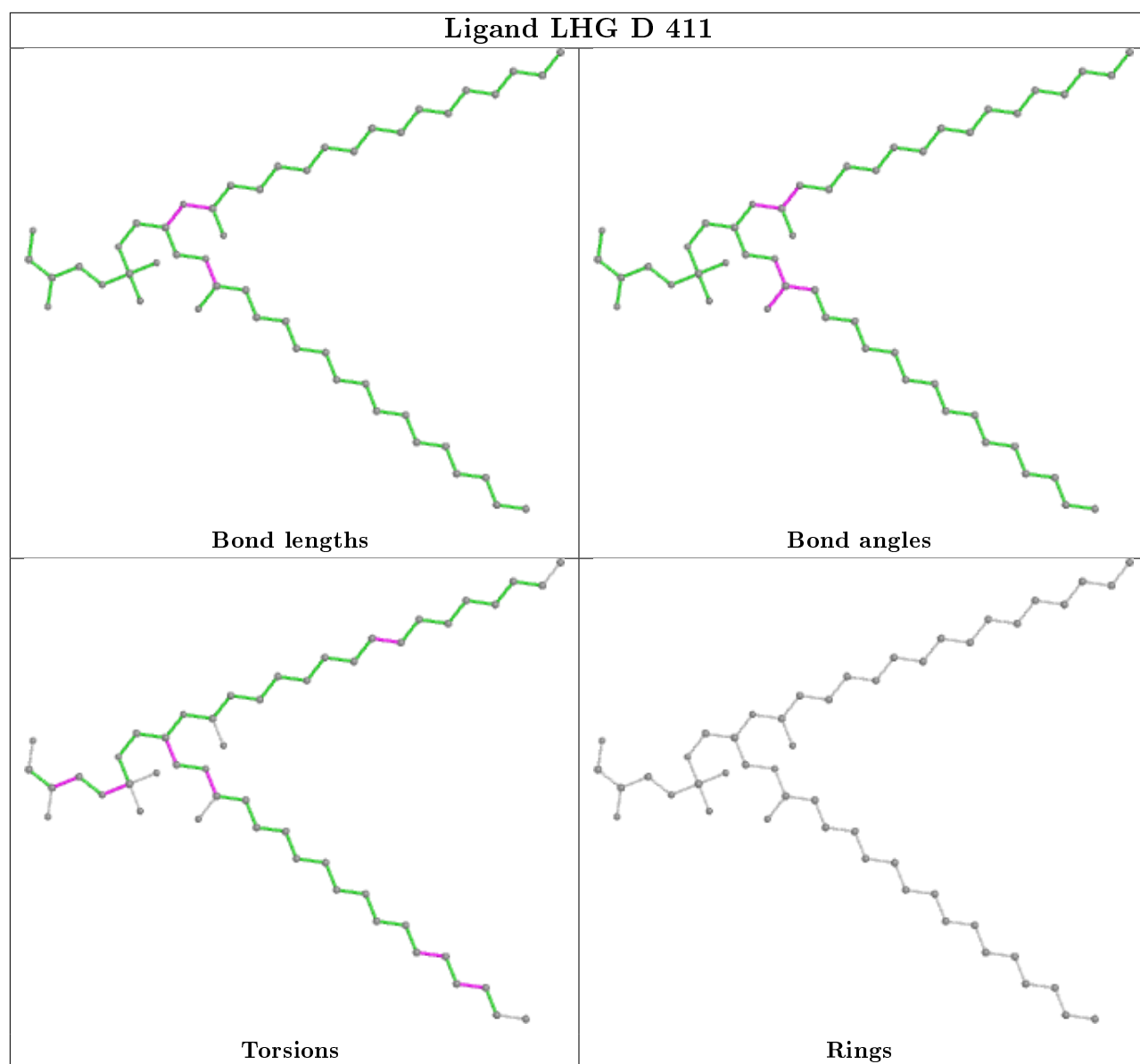


## Ligand CLA B 607



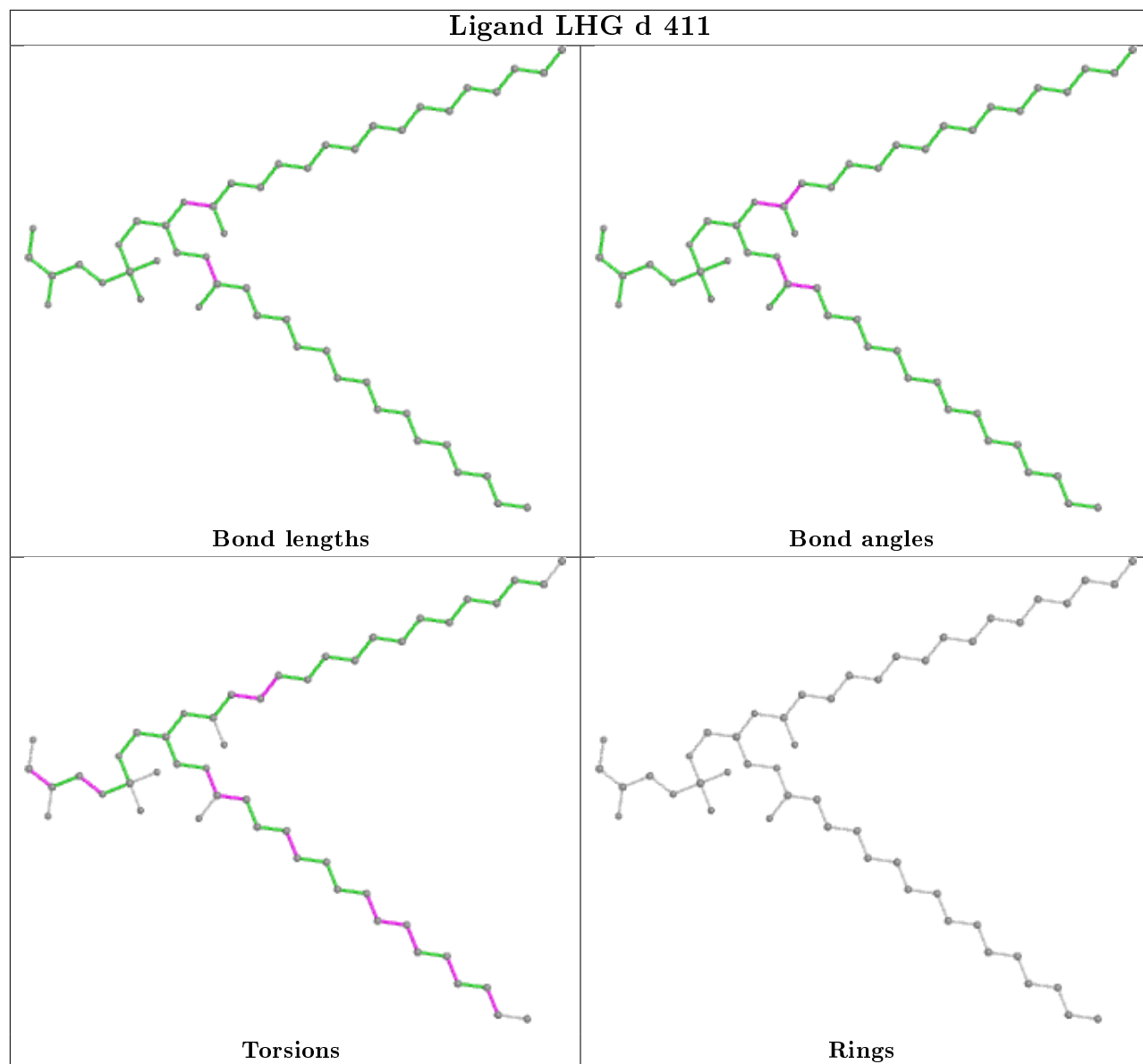
## Ligand CLA b 610



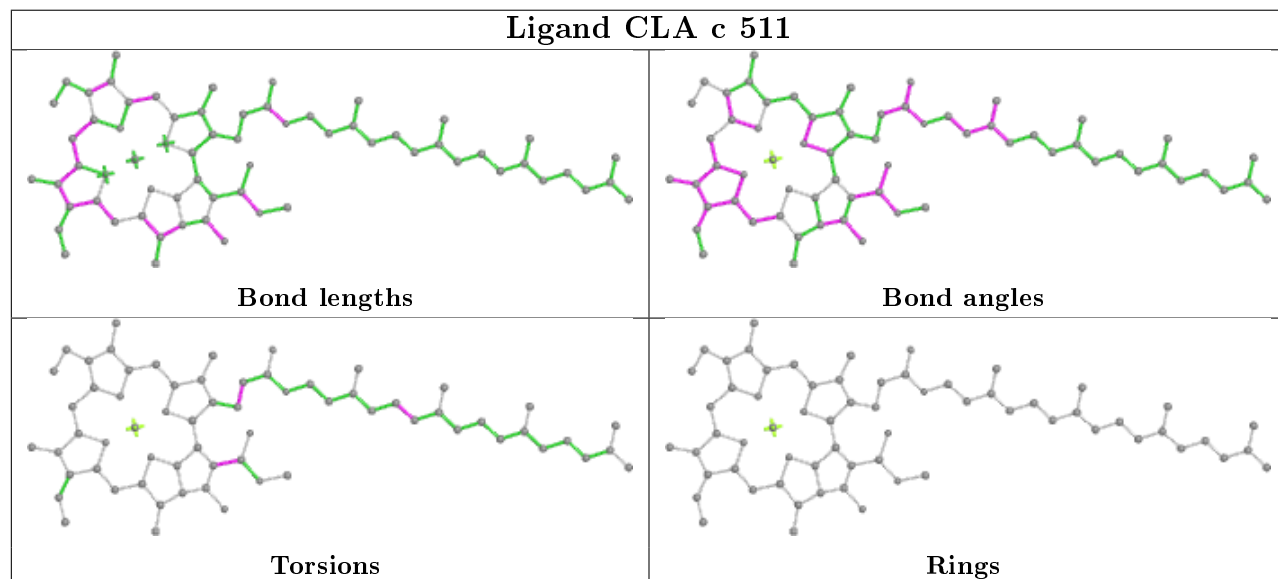


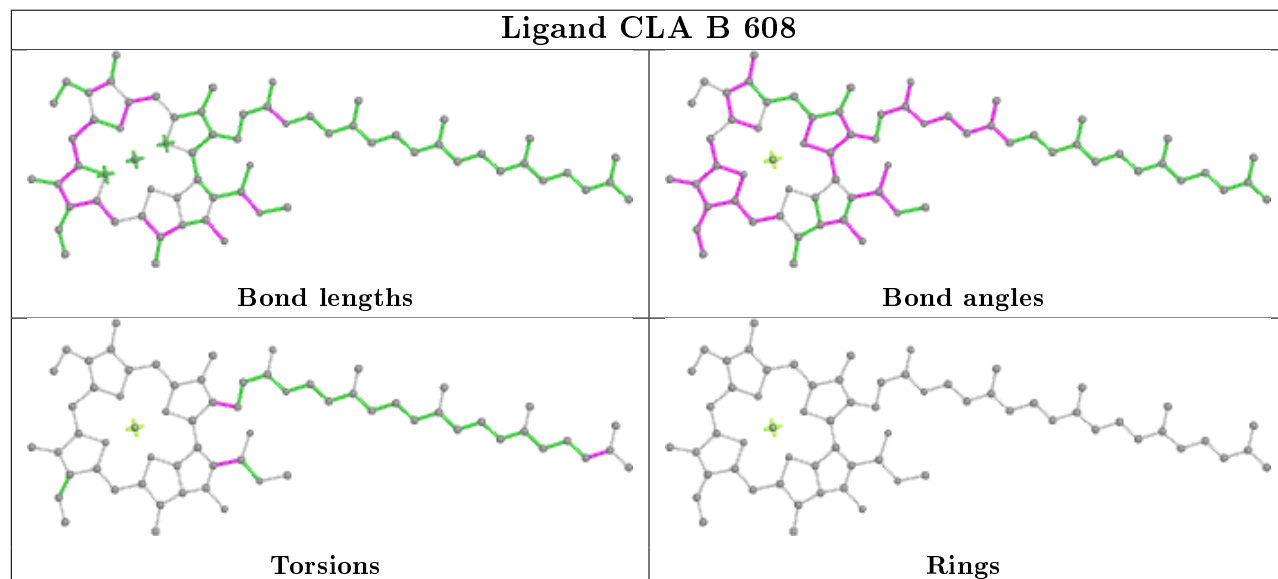
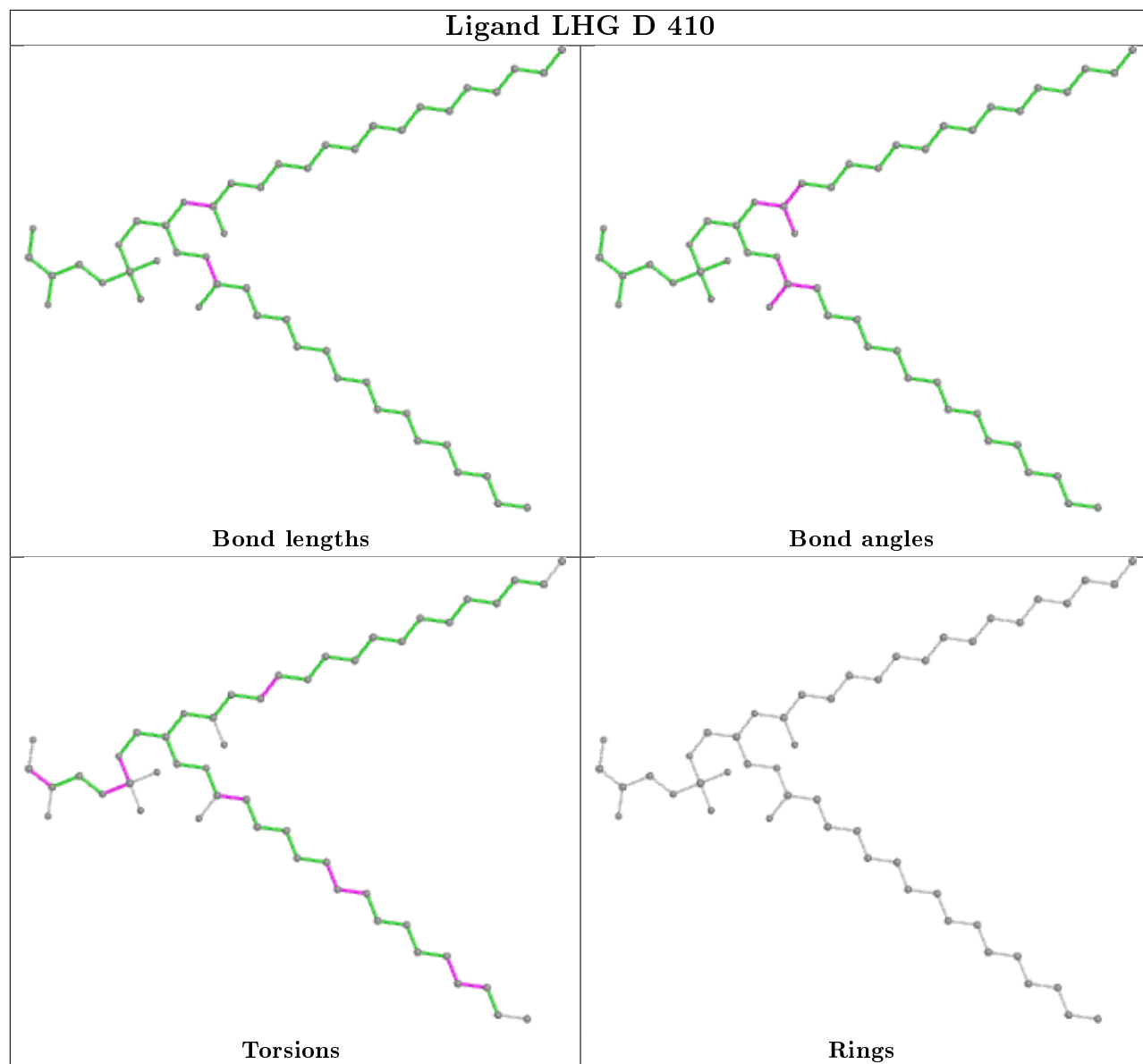


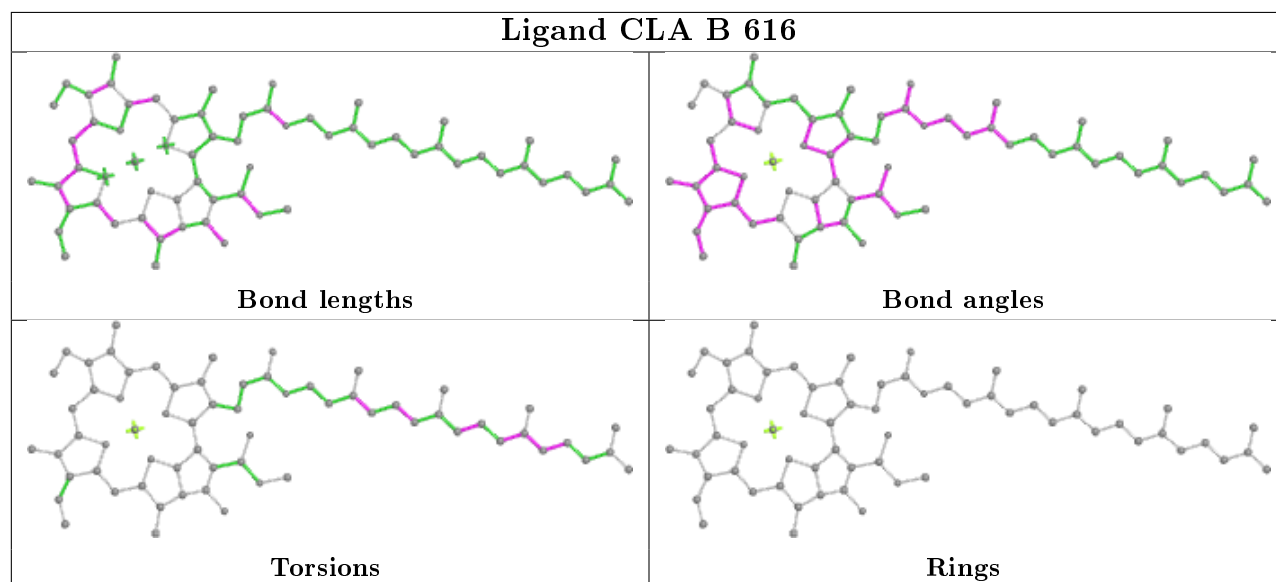
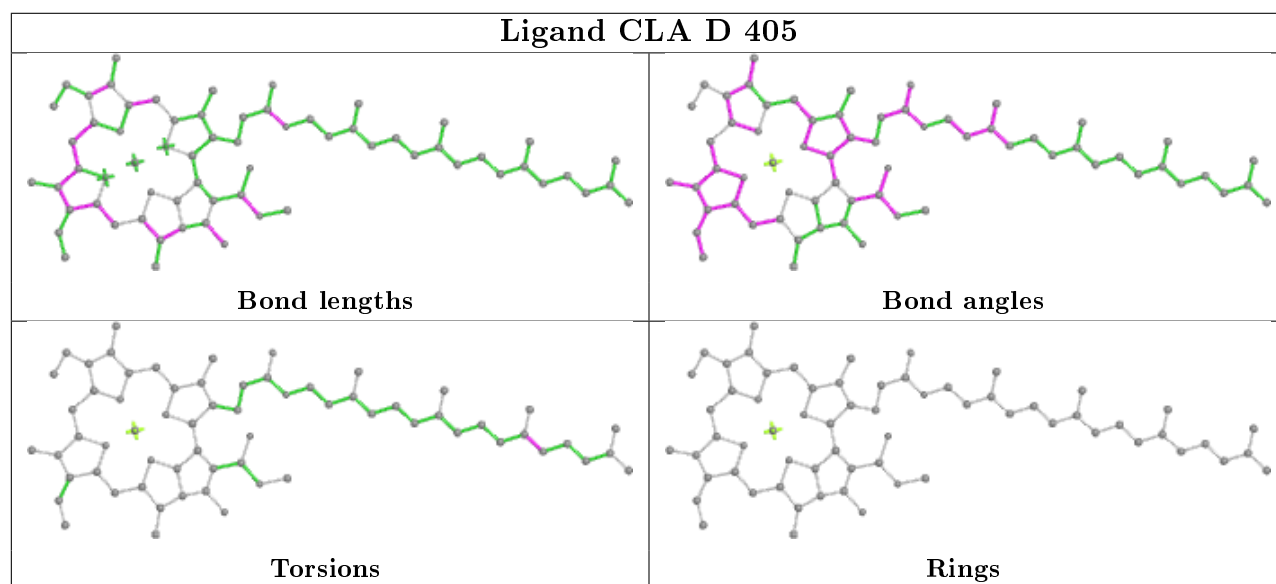
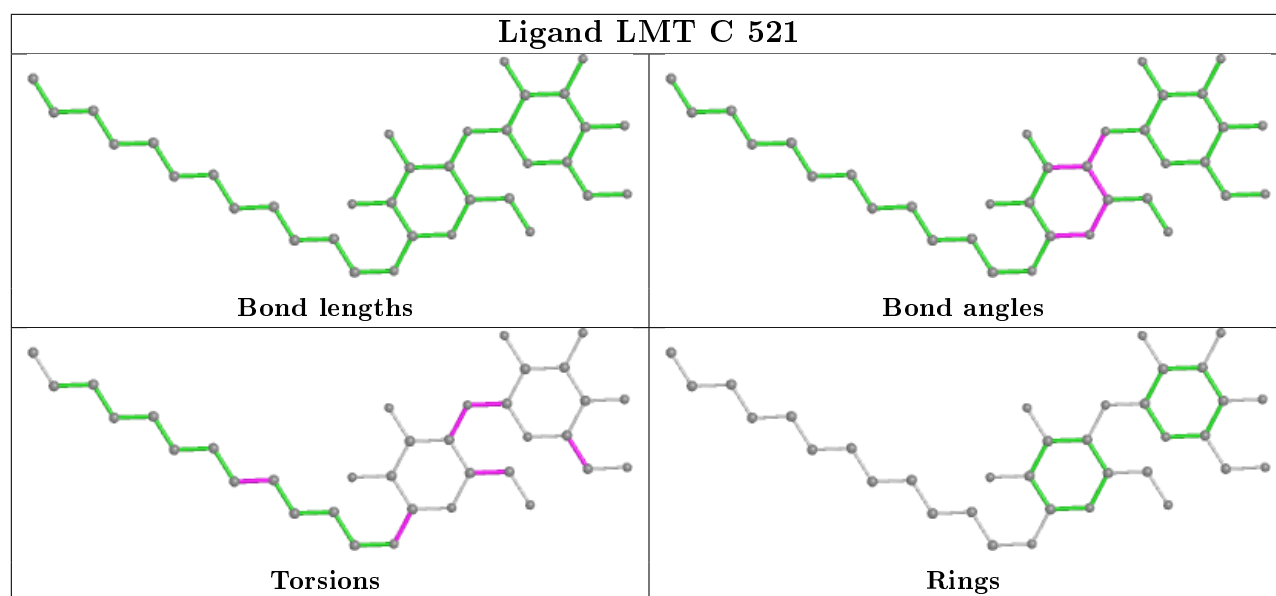
## Ligand LHG d 411

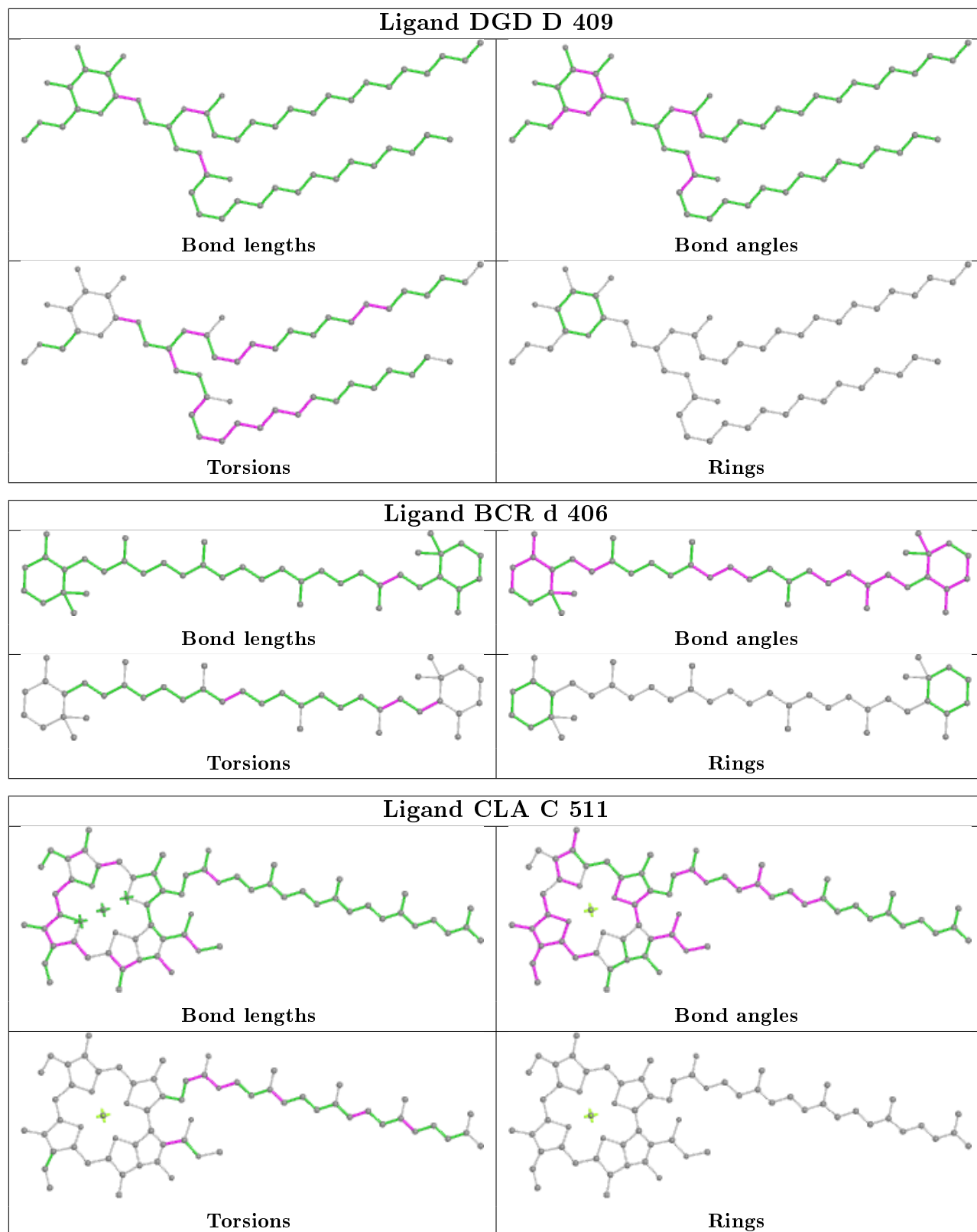


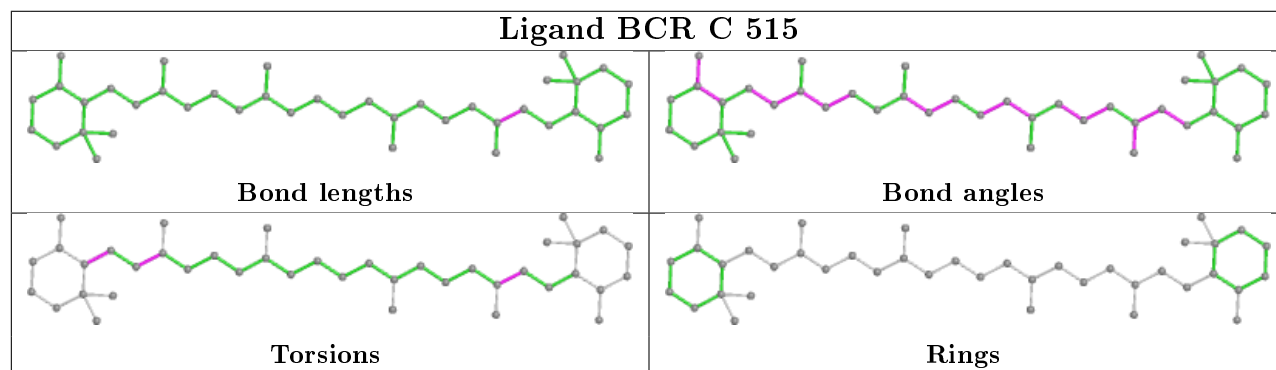
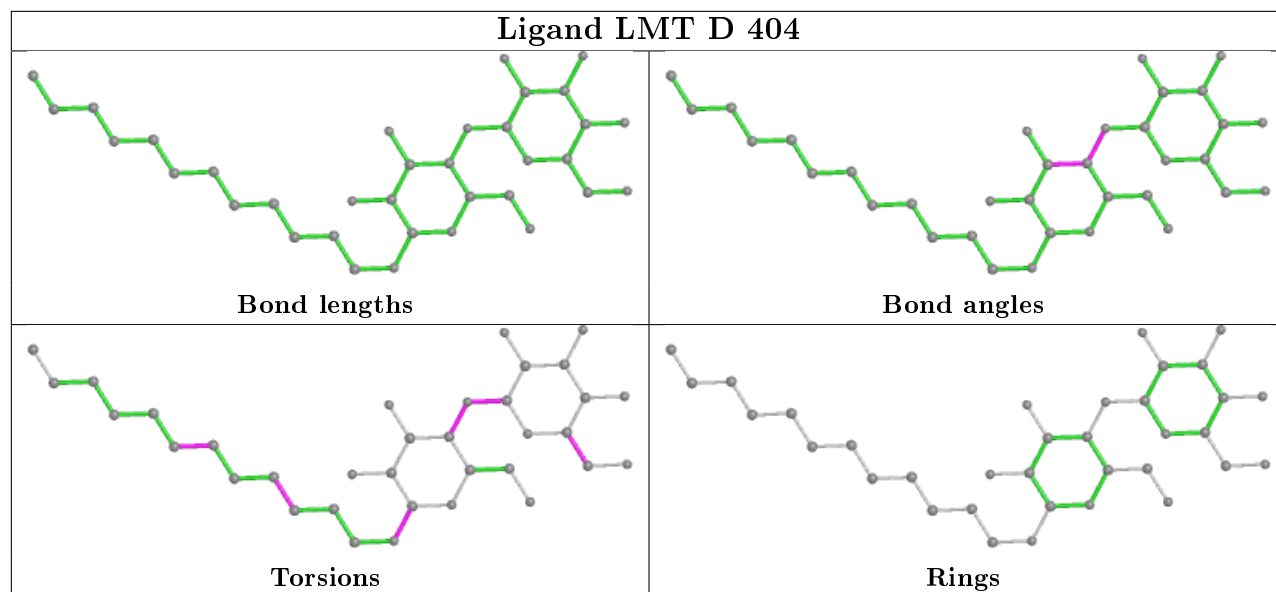
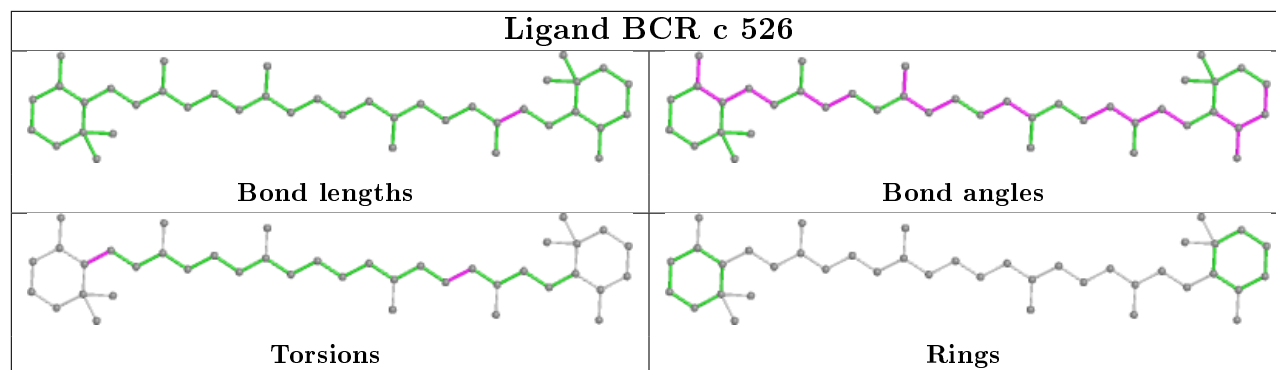
## Ligand CLA c 511

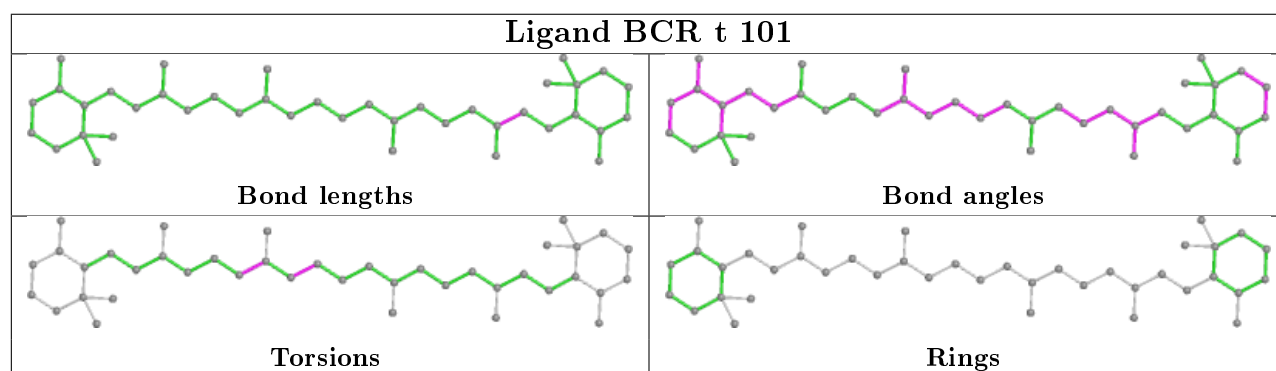
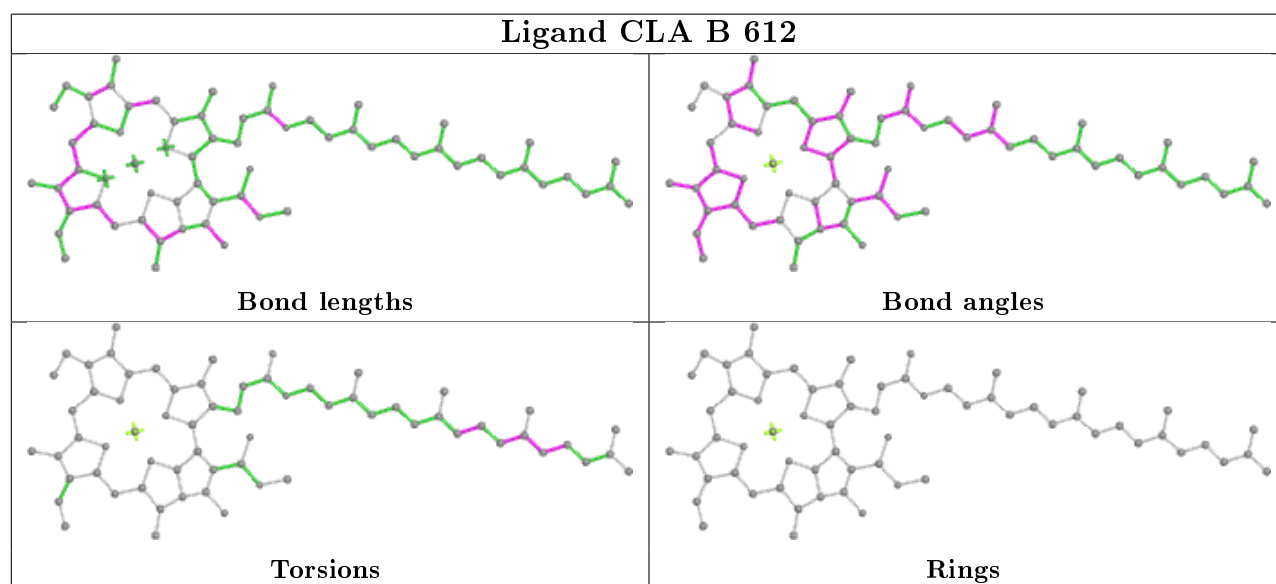
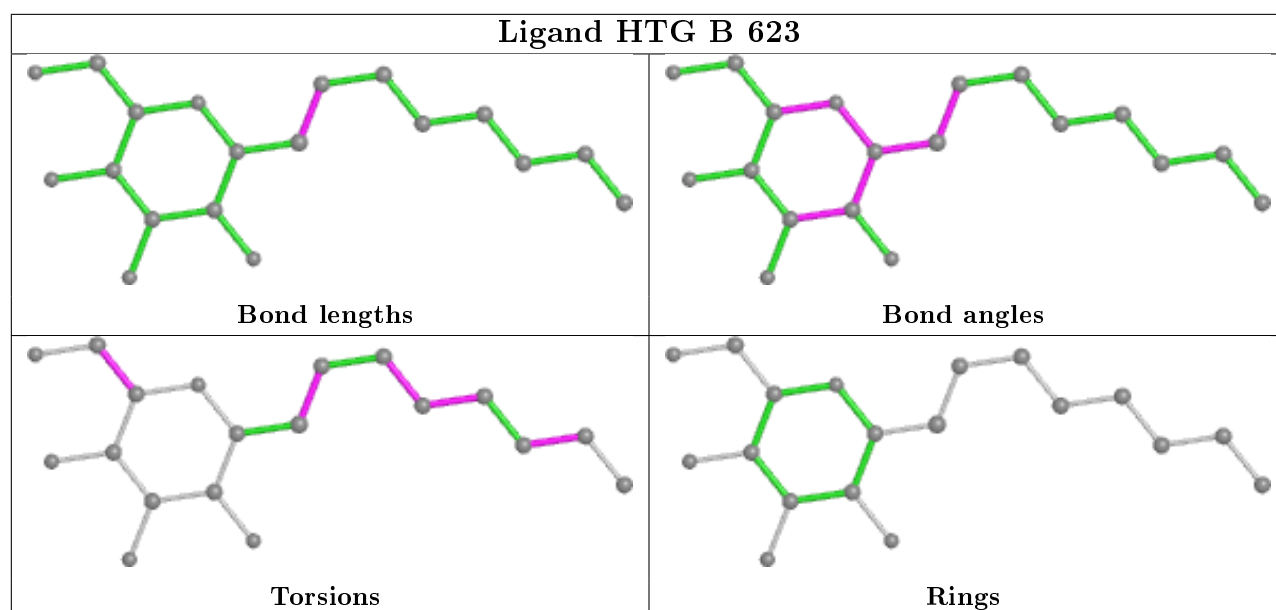


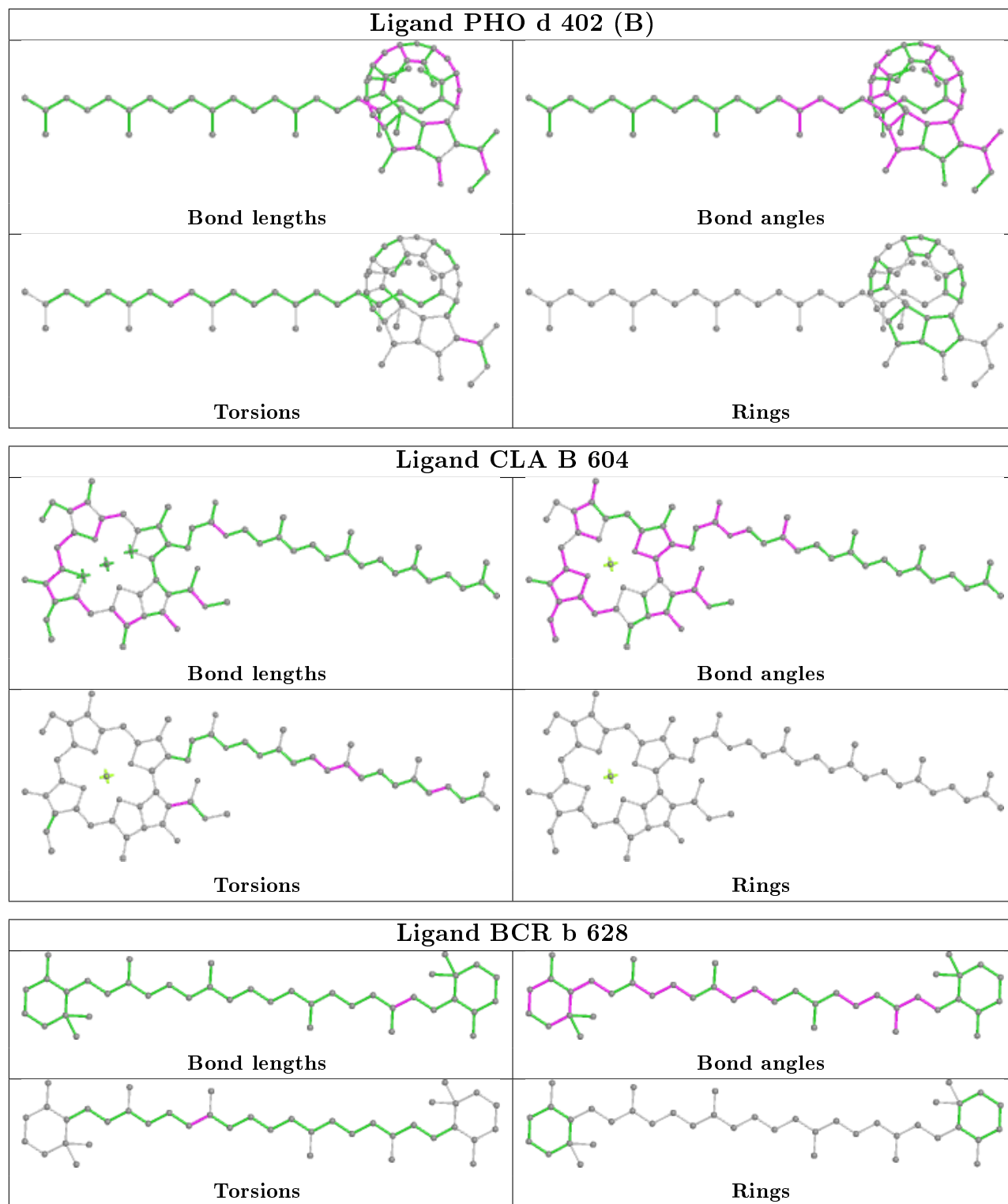


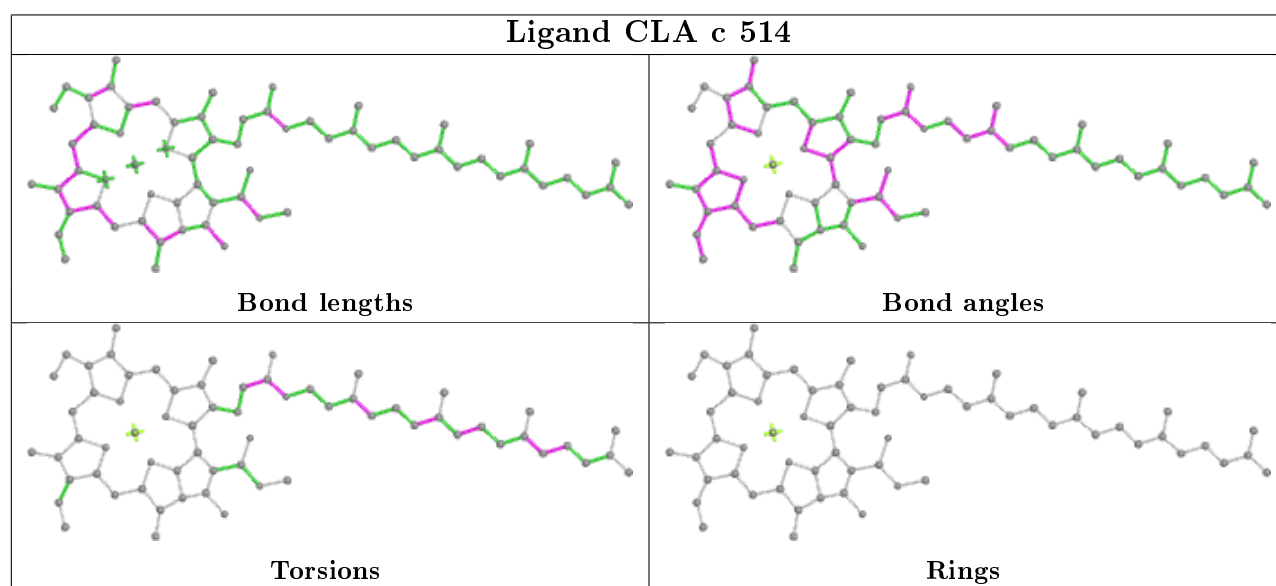
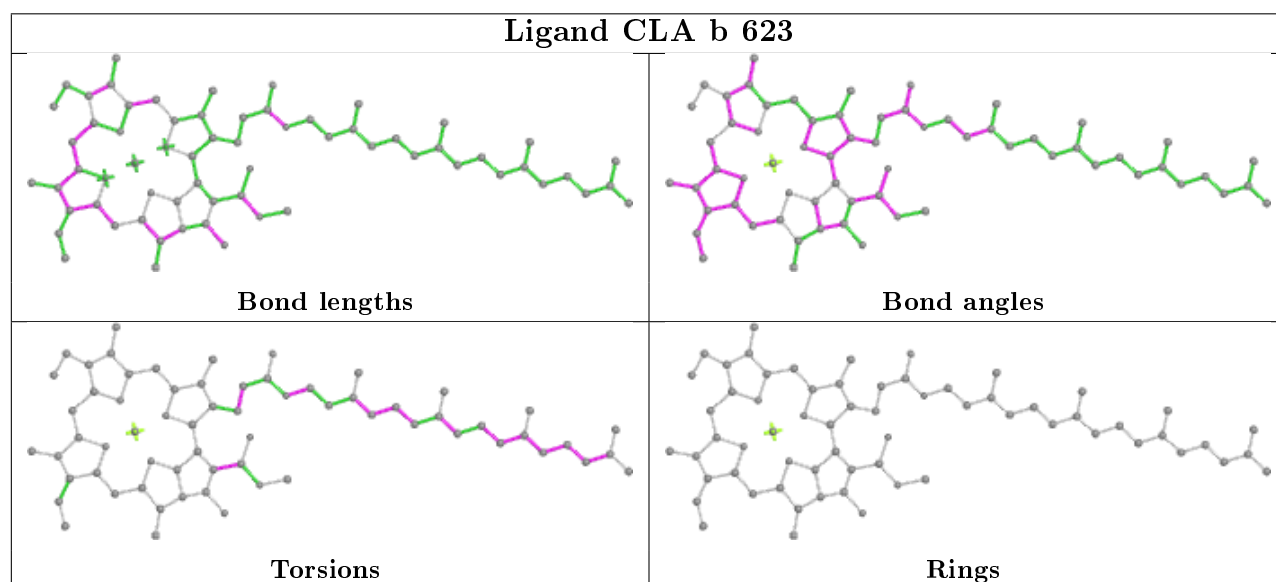
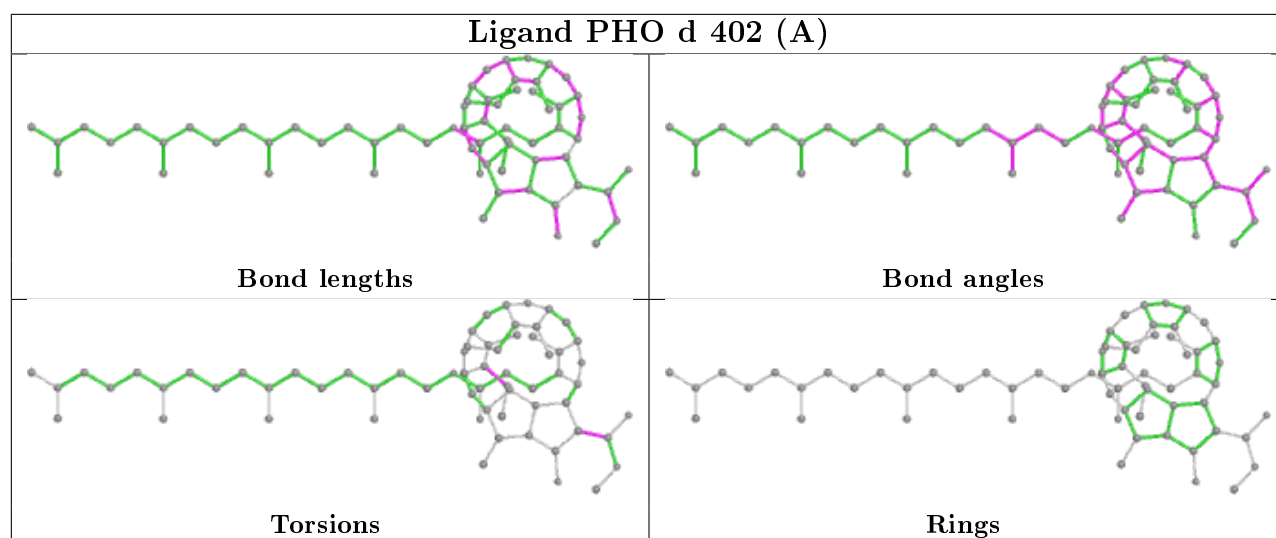






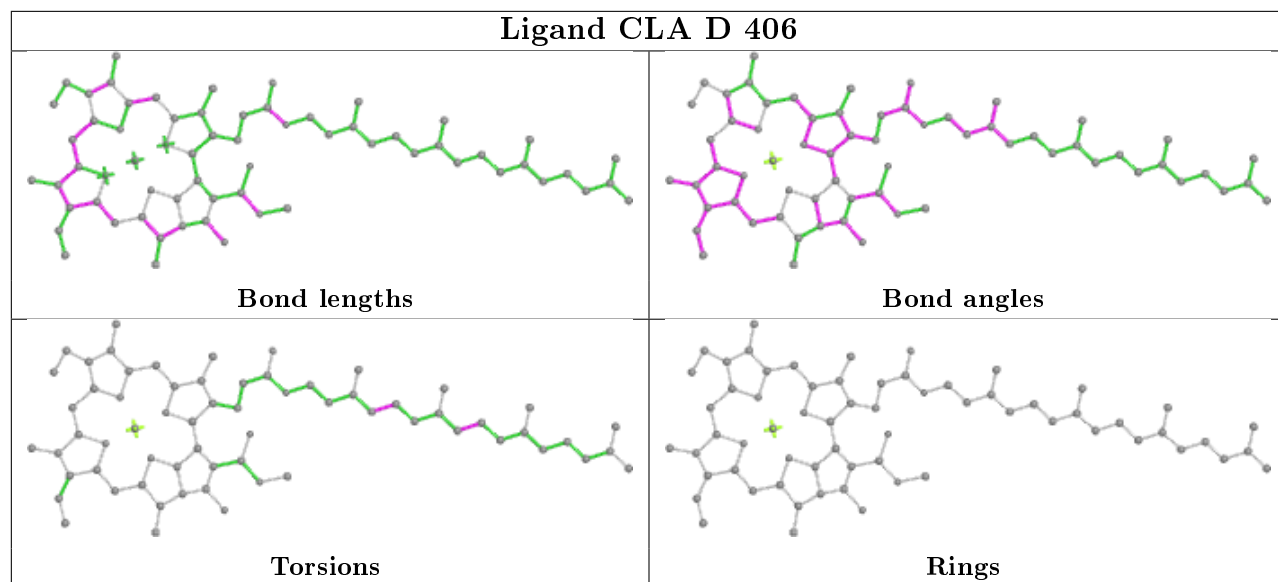




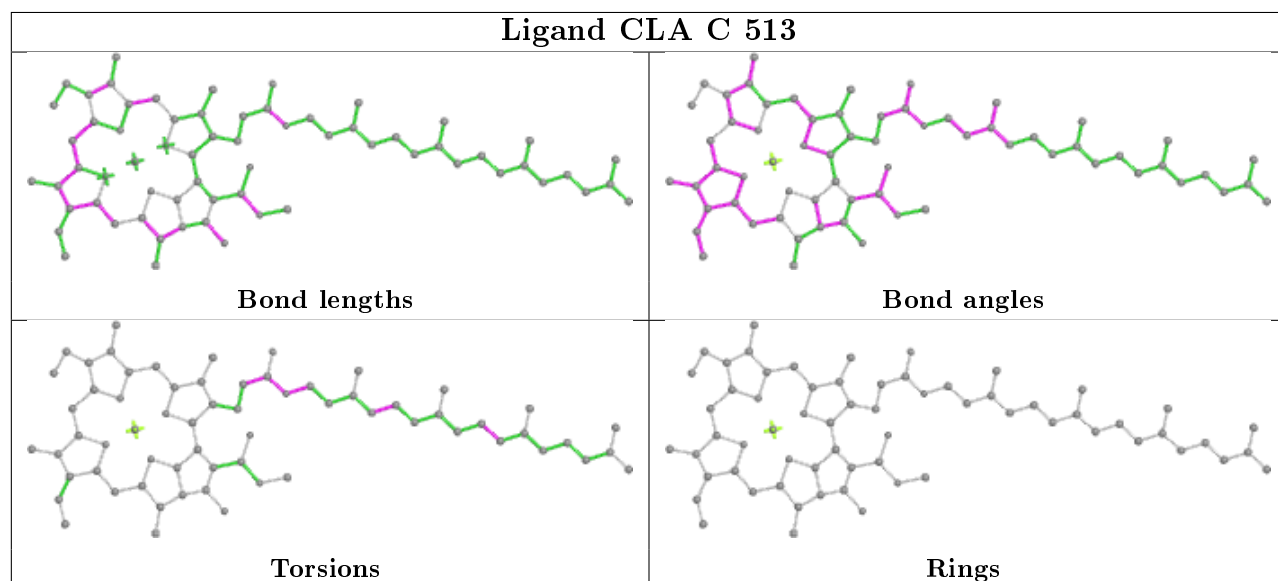




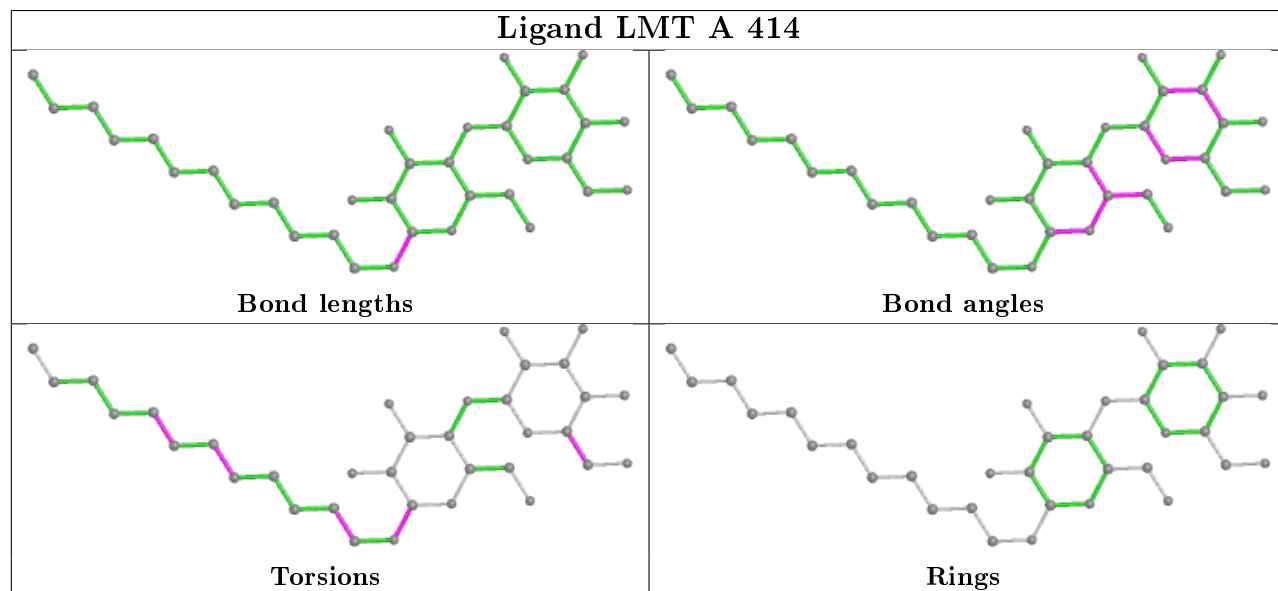
## Ligand CLA D 406

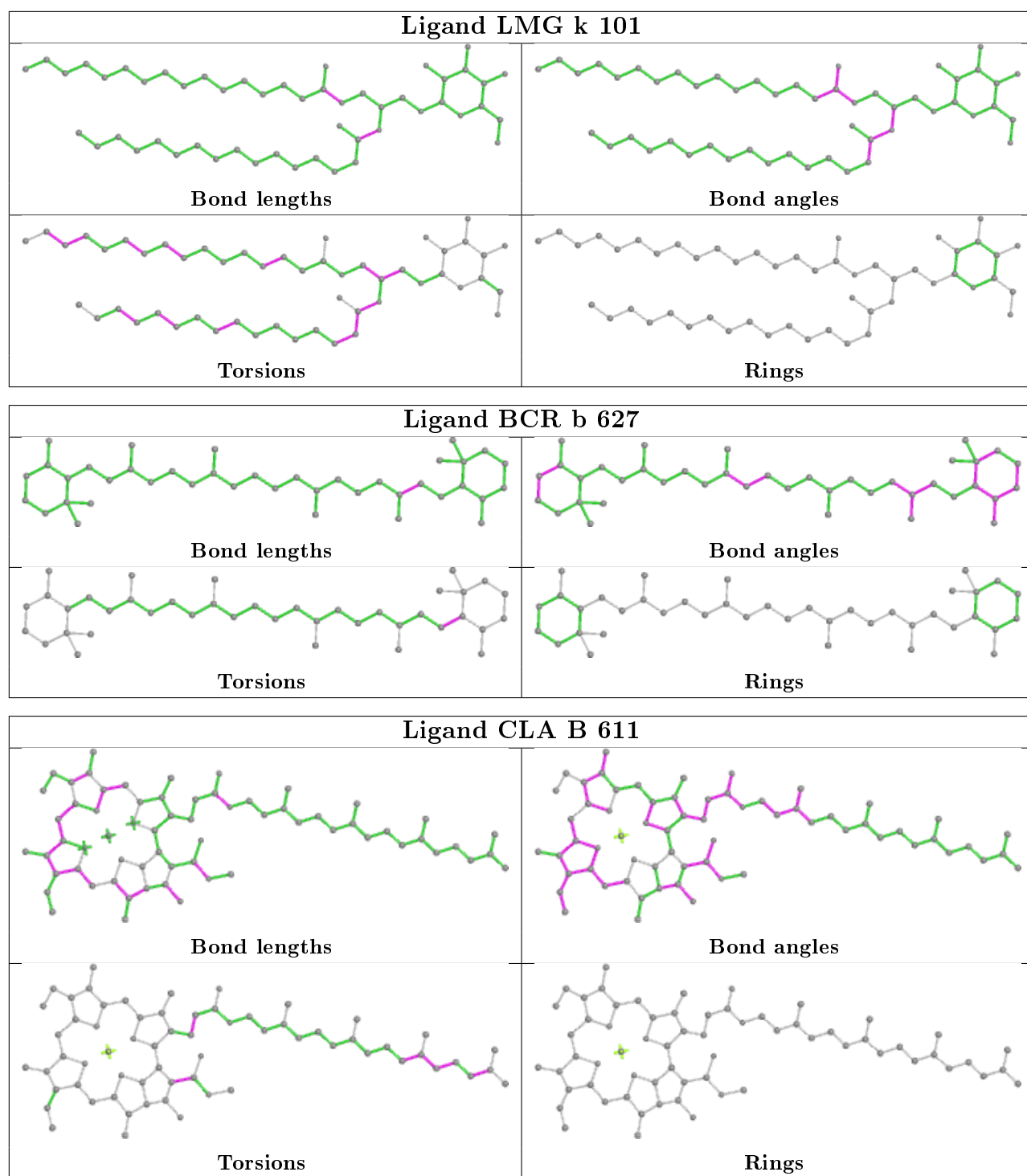


## Ligand CLA C 513

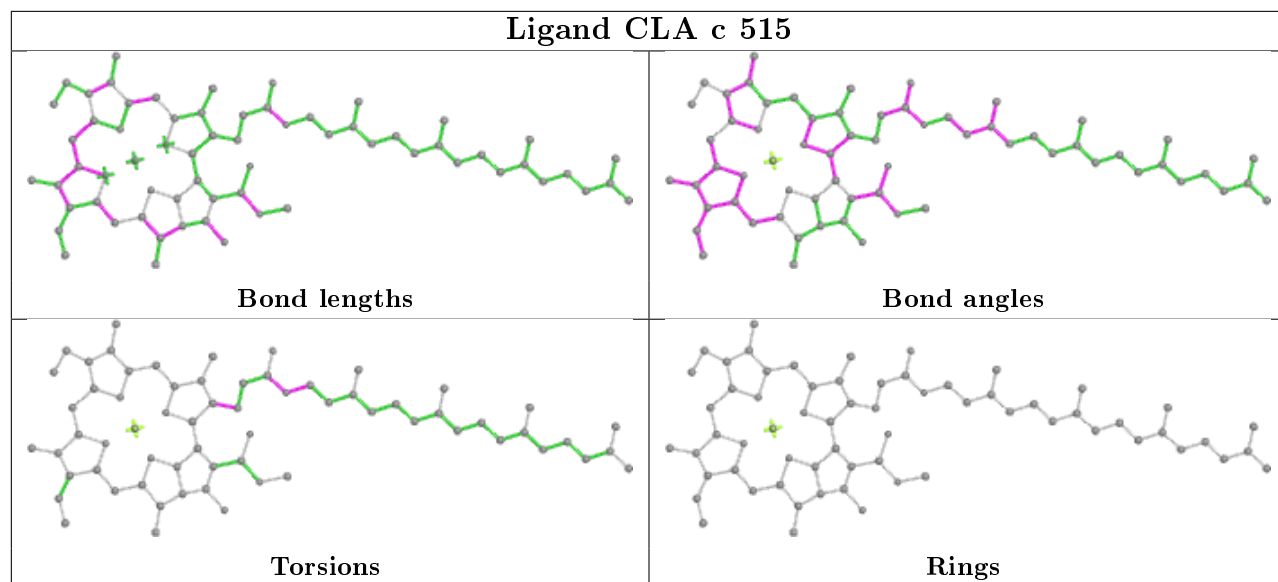


## Ligand LMT A 414

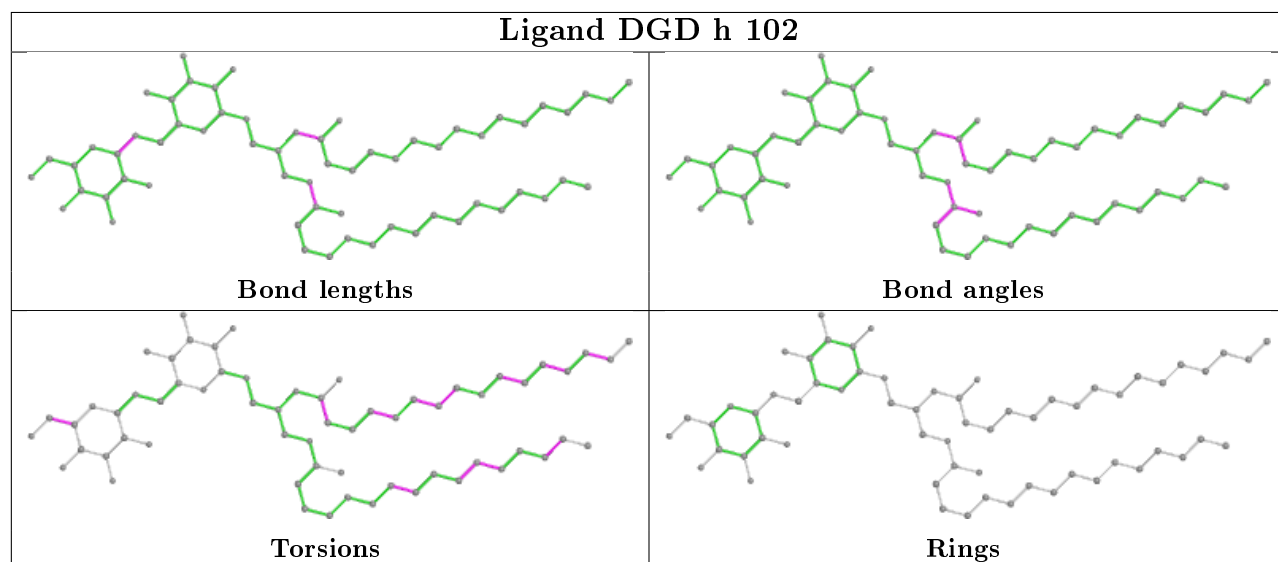




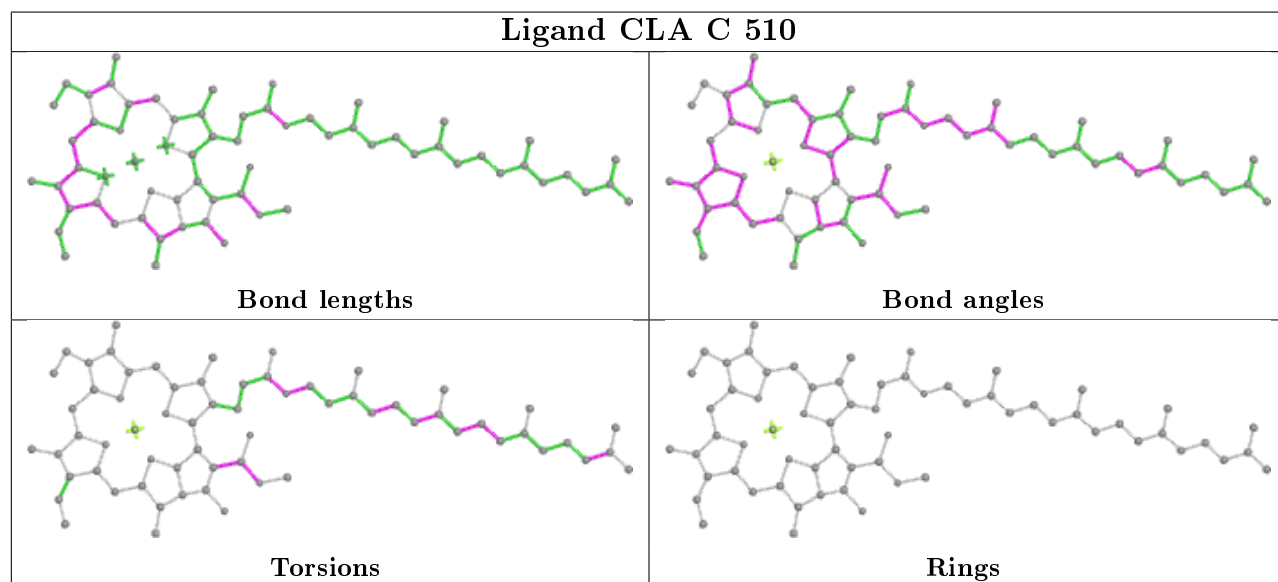
## Ligand CLA c 515

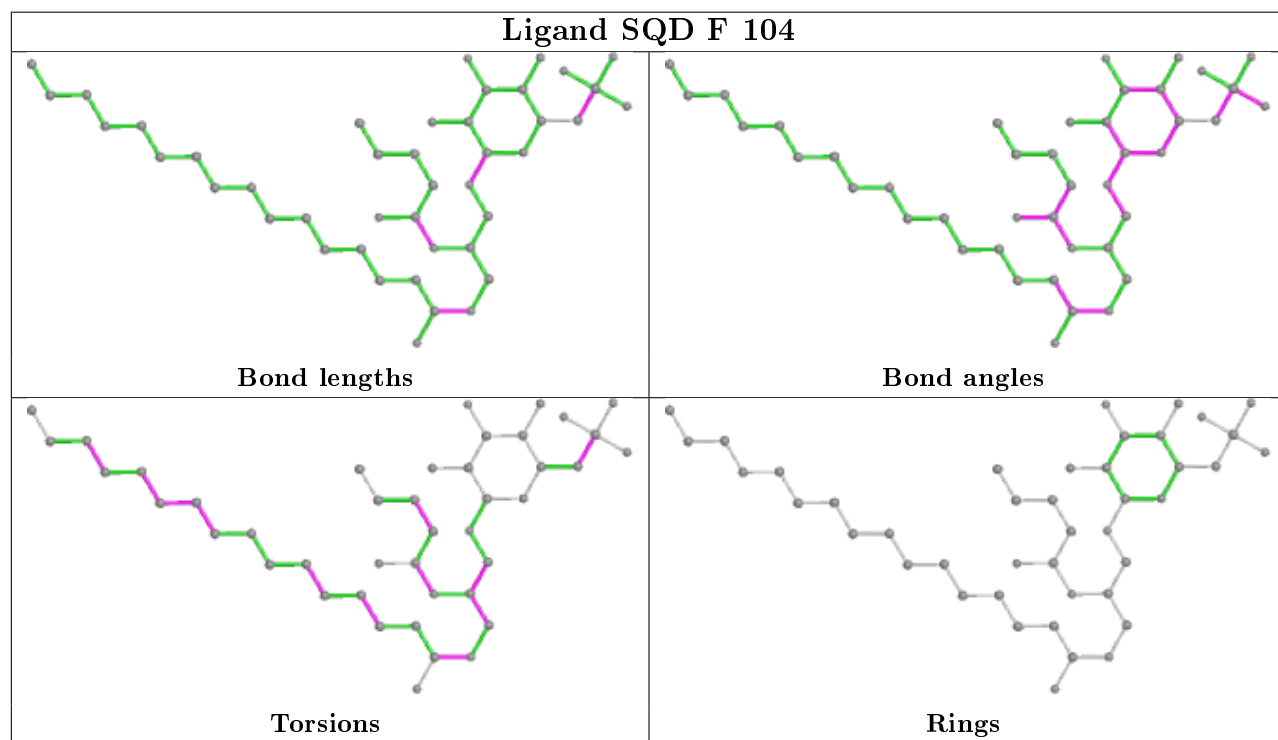
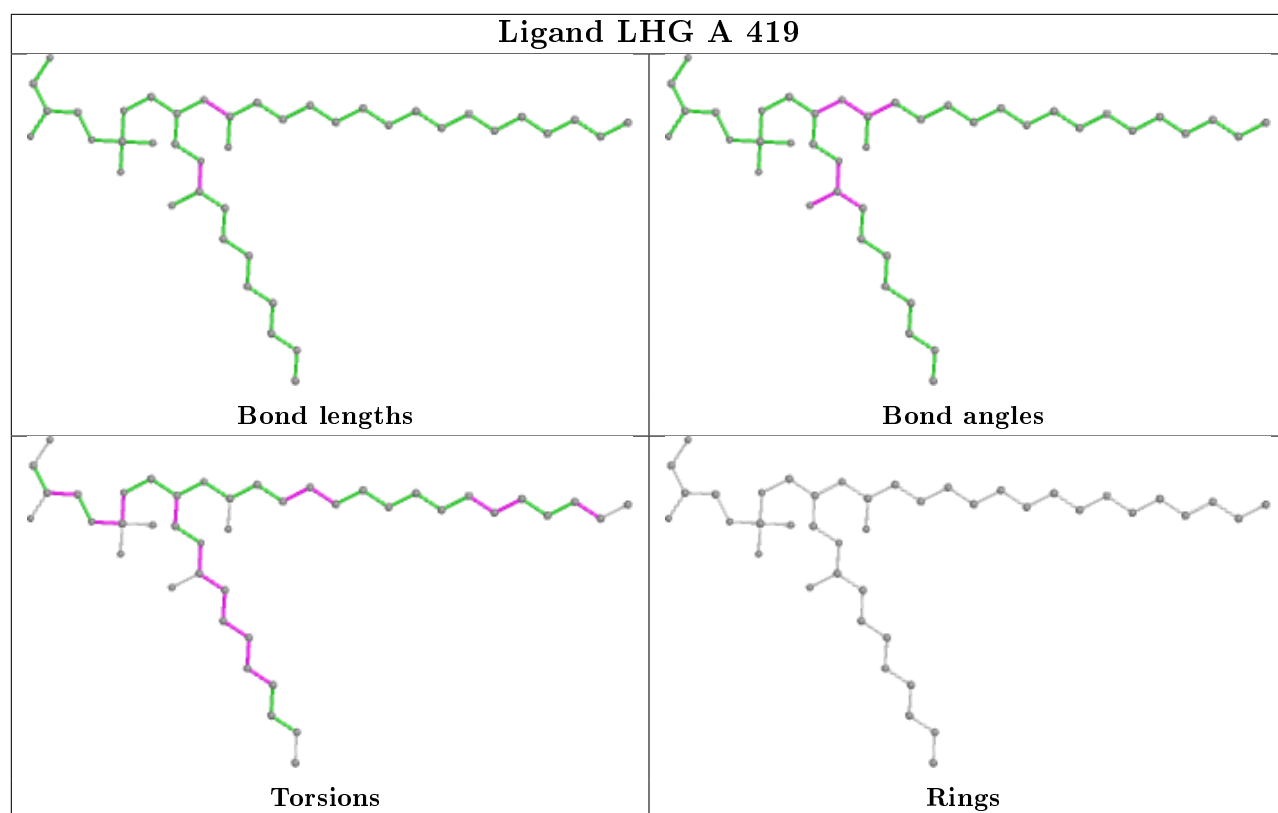


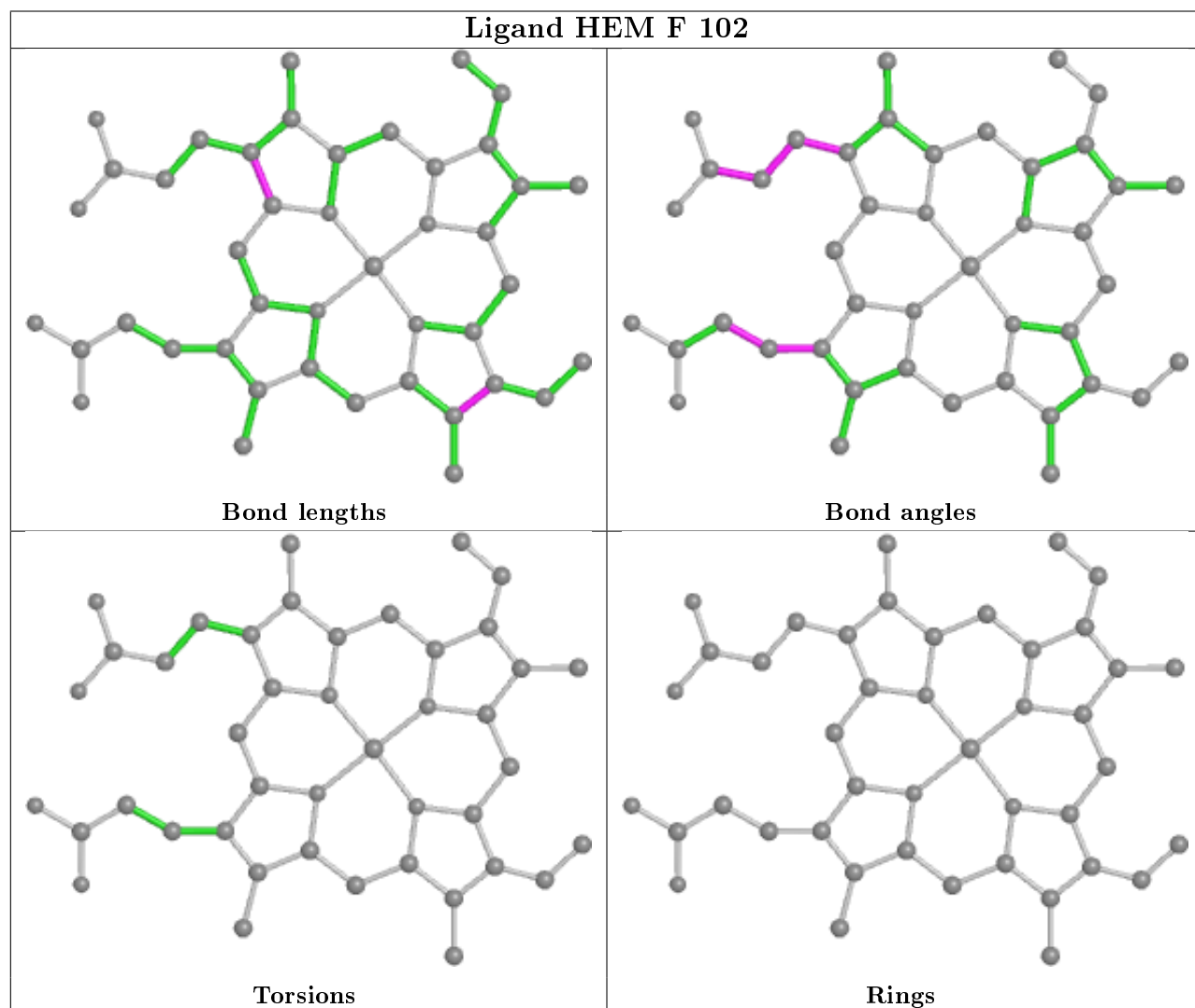
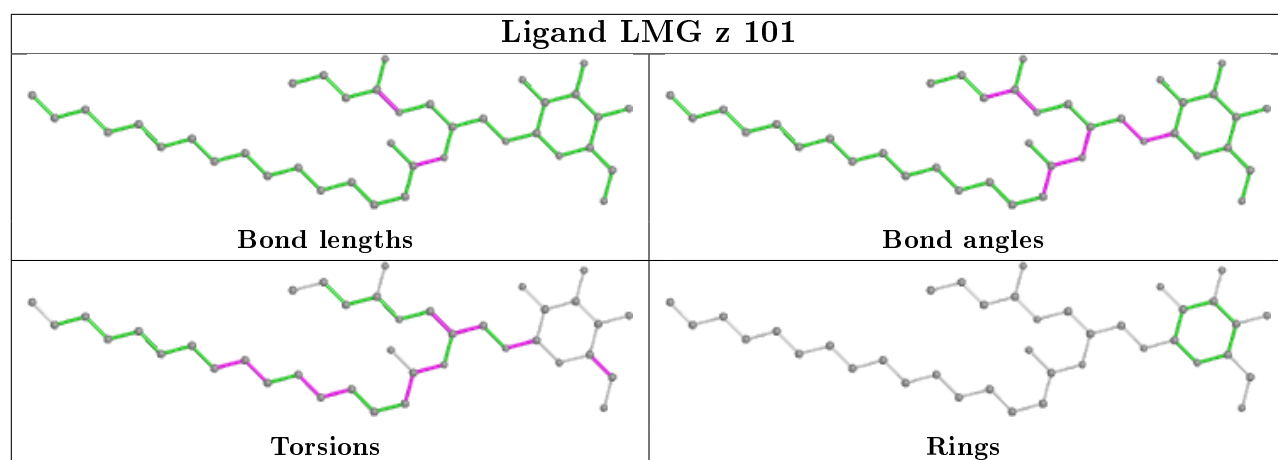
## Ligand DGD h 102

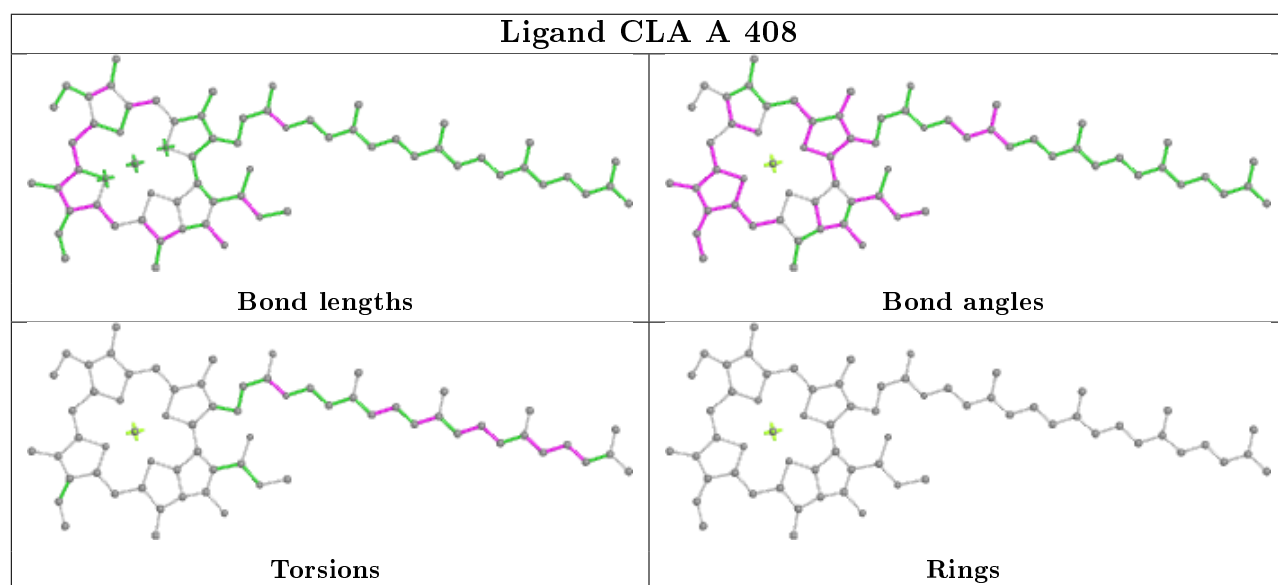
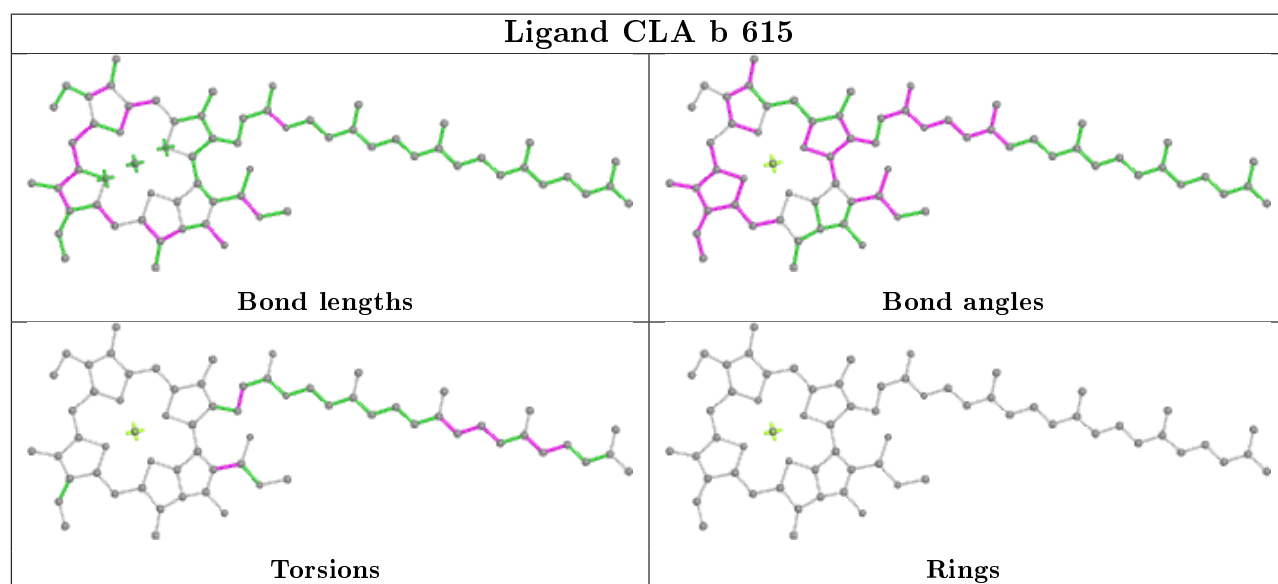
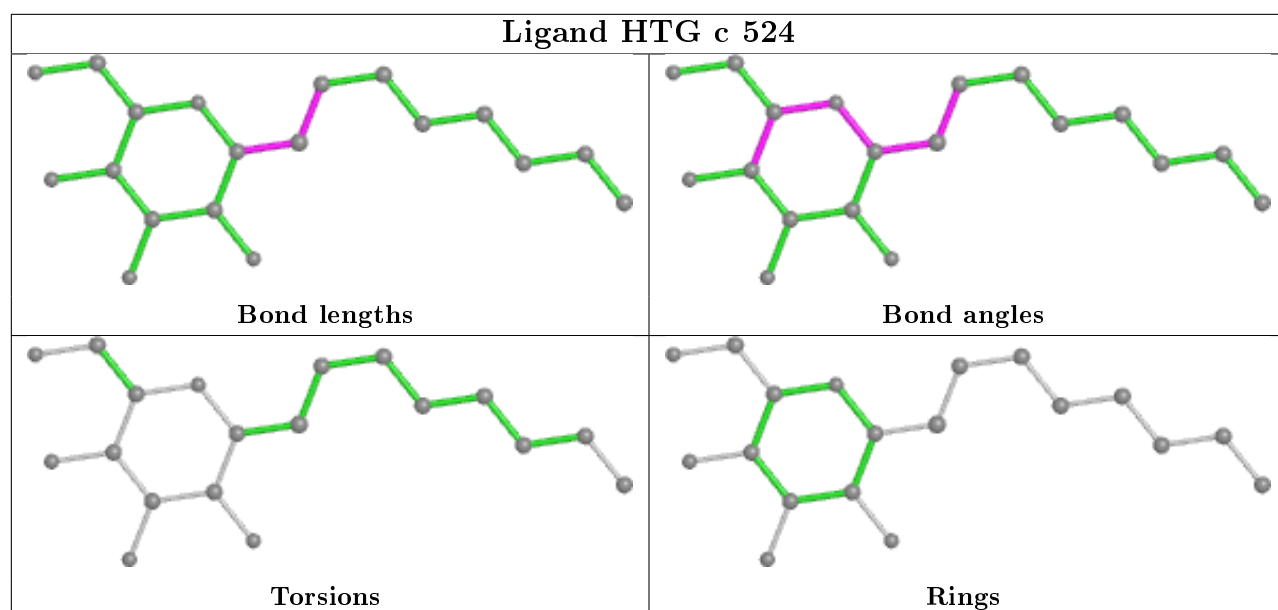


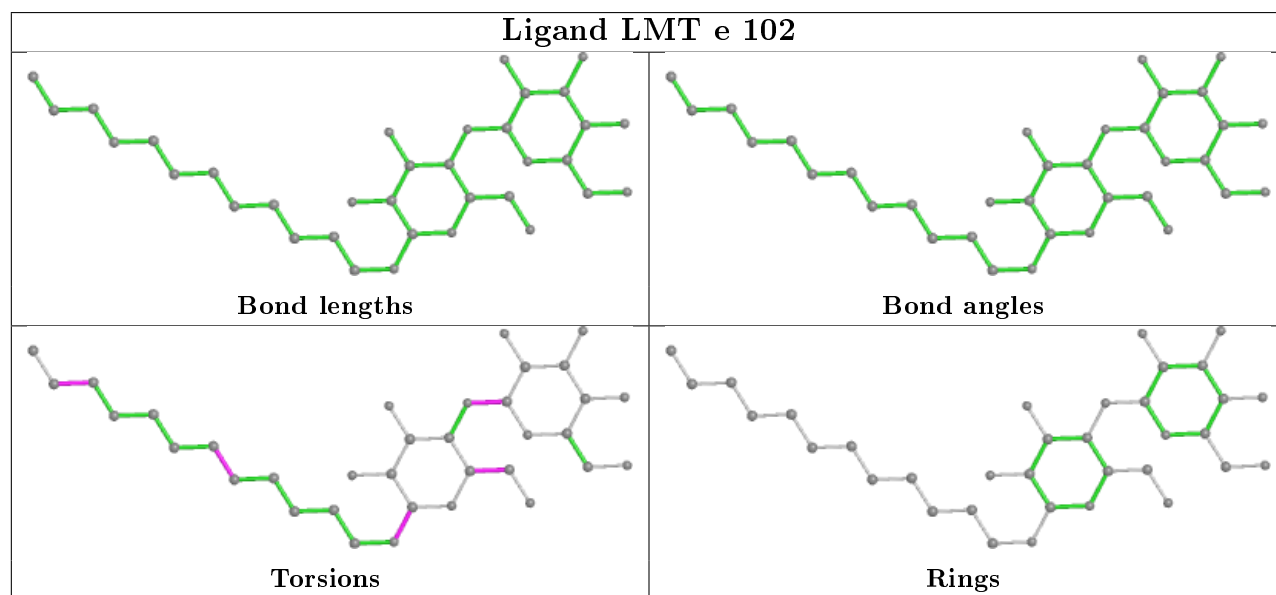
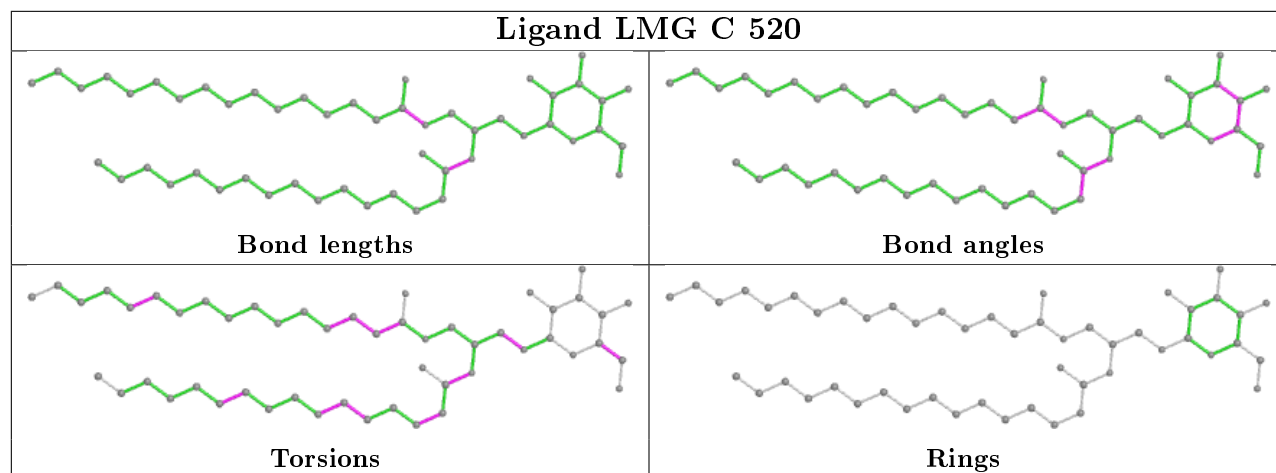
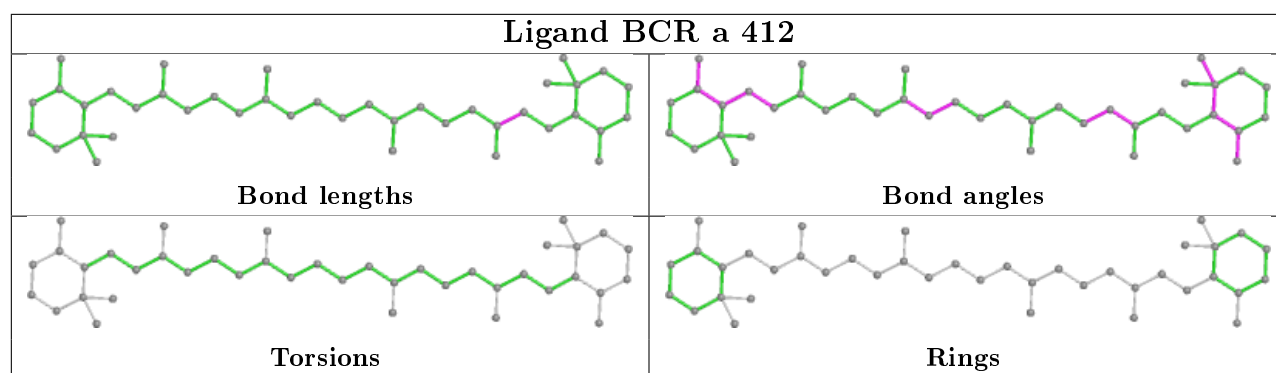
## Ligand CLA C 510

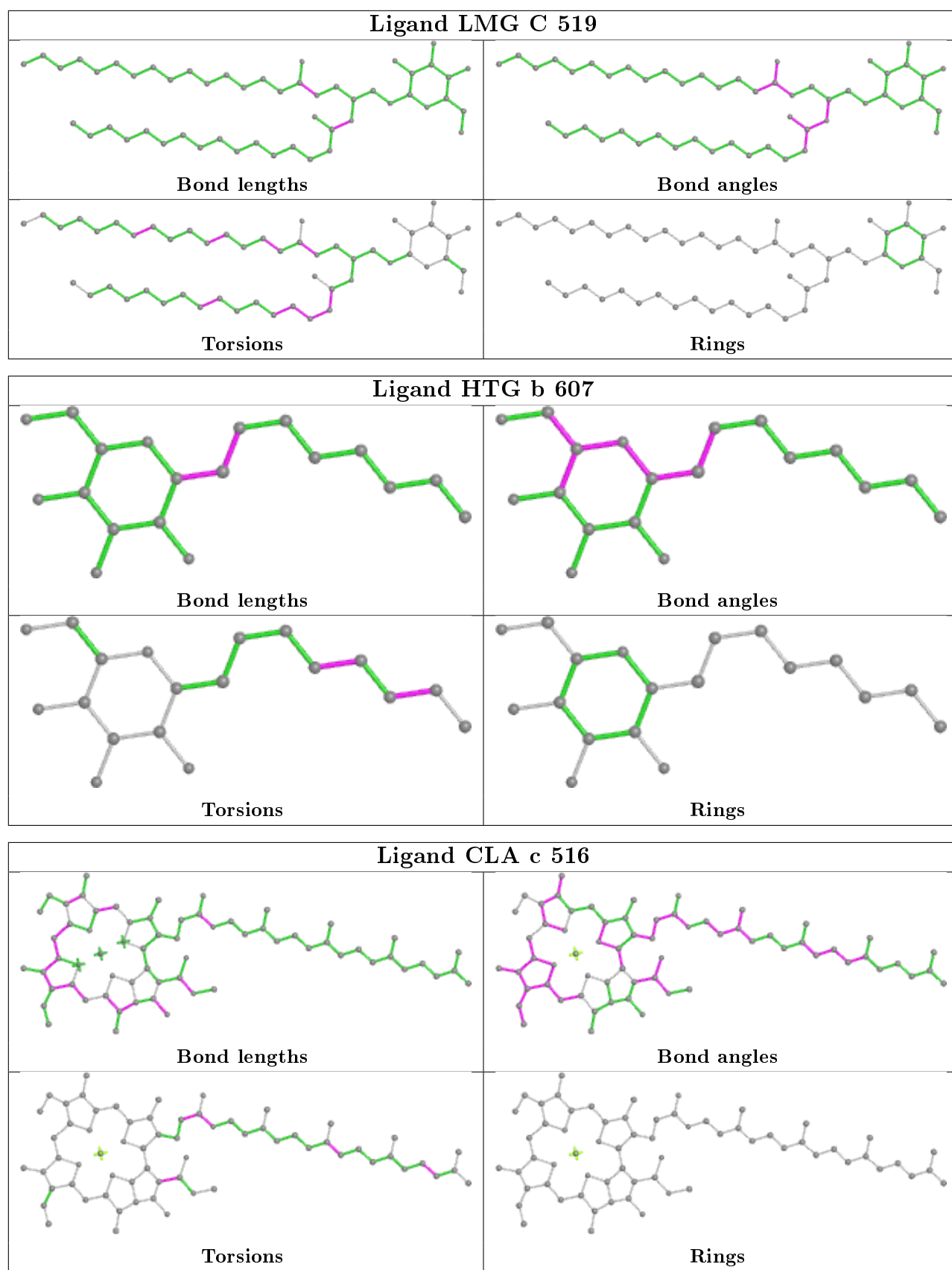




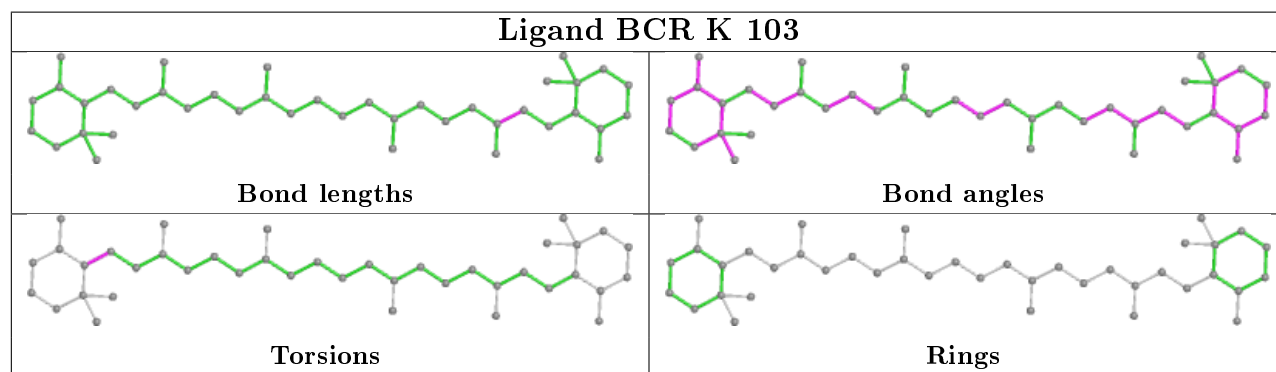
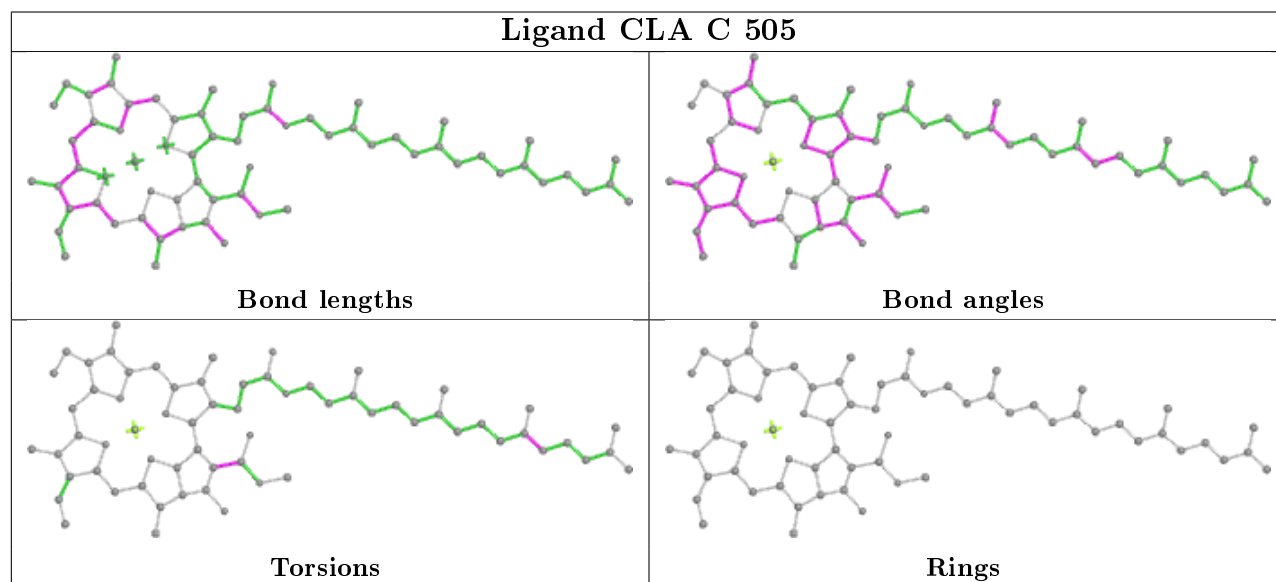
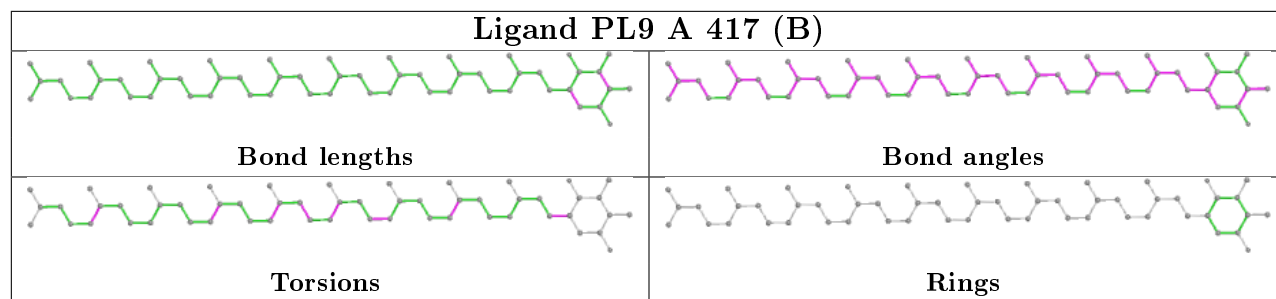




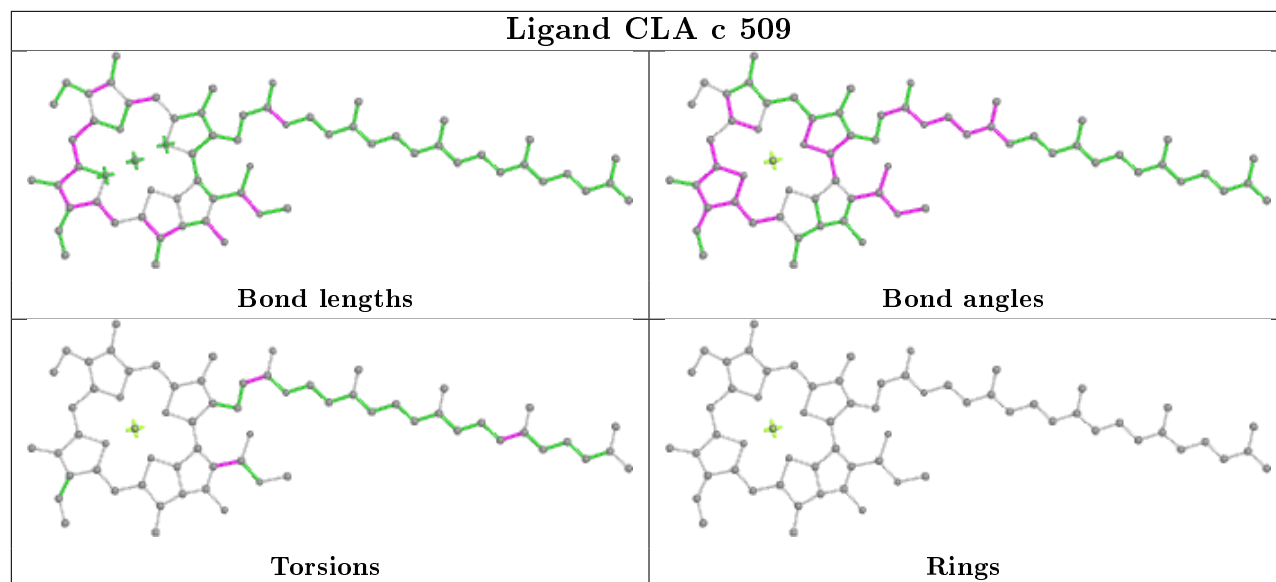




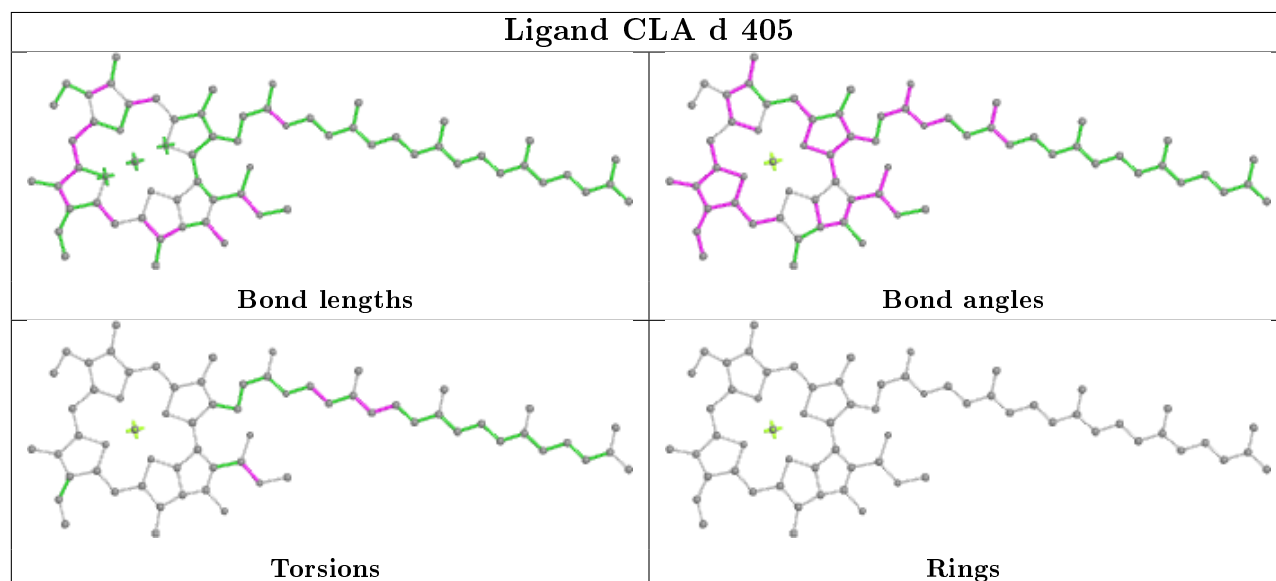




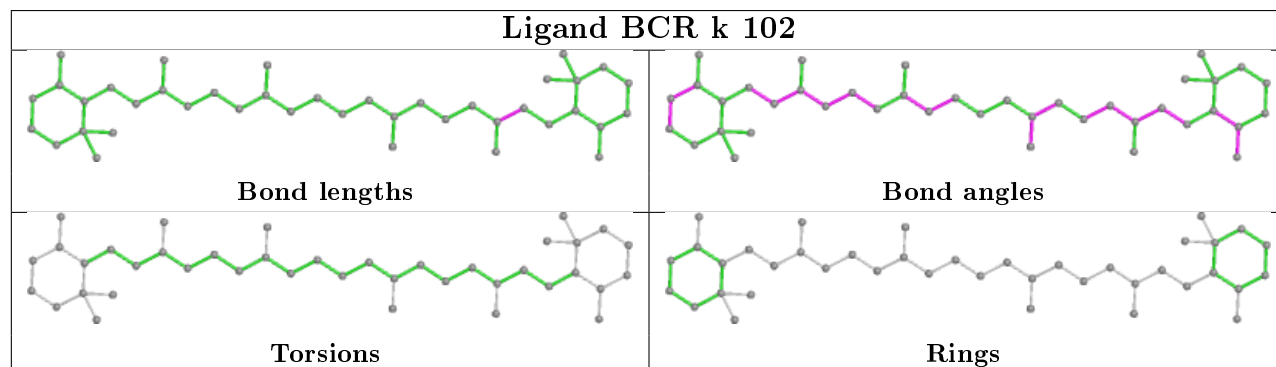
## Ligand CLA c 509

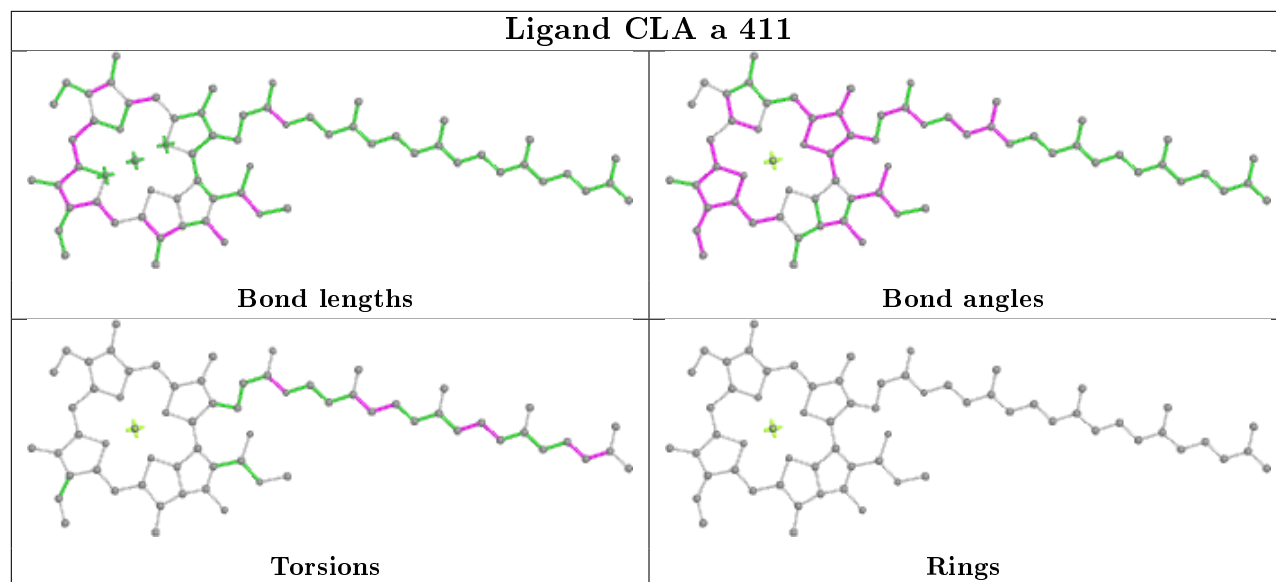
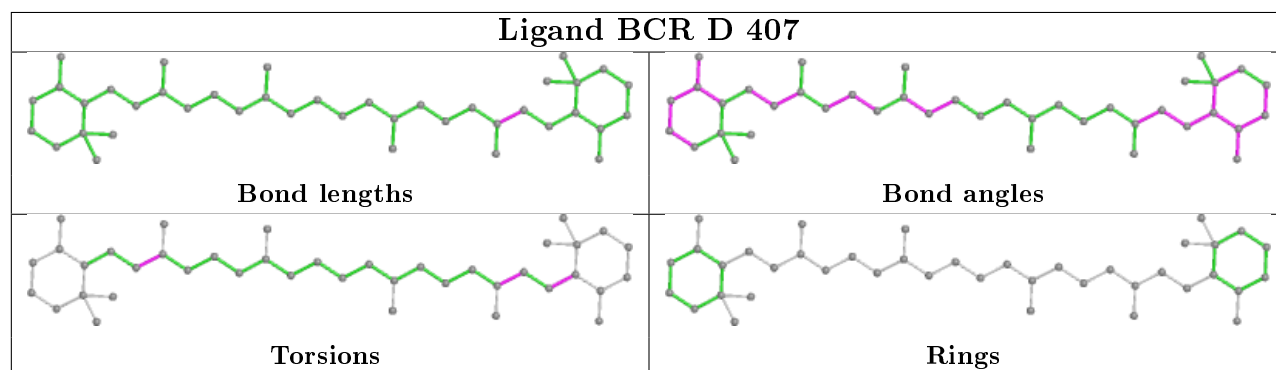
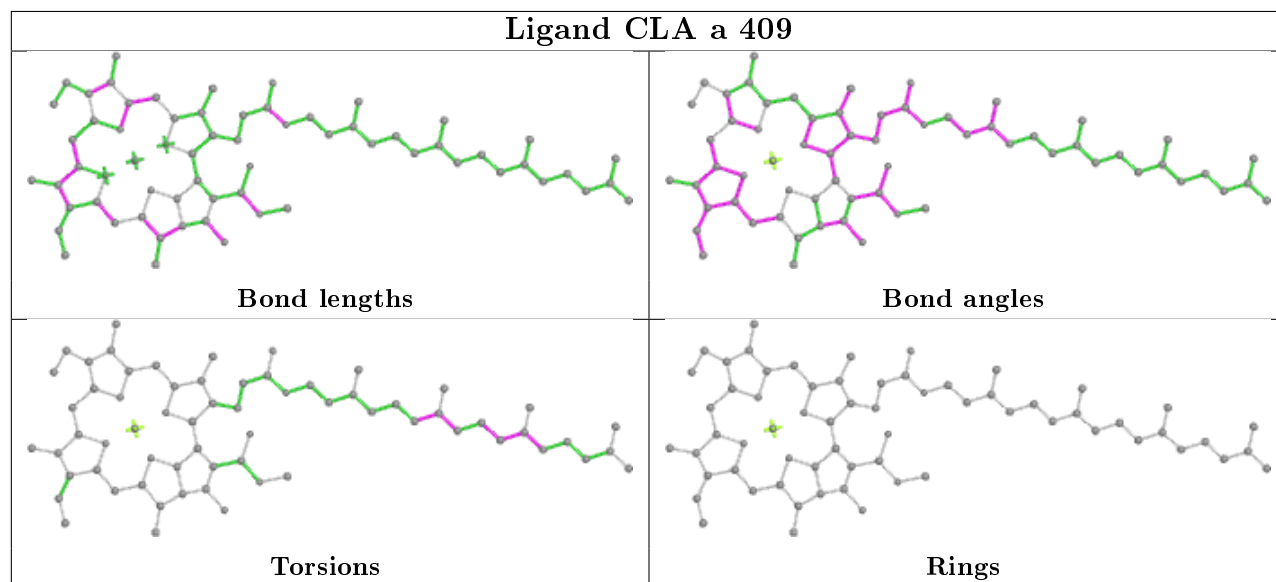


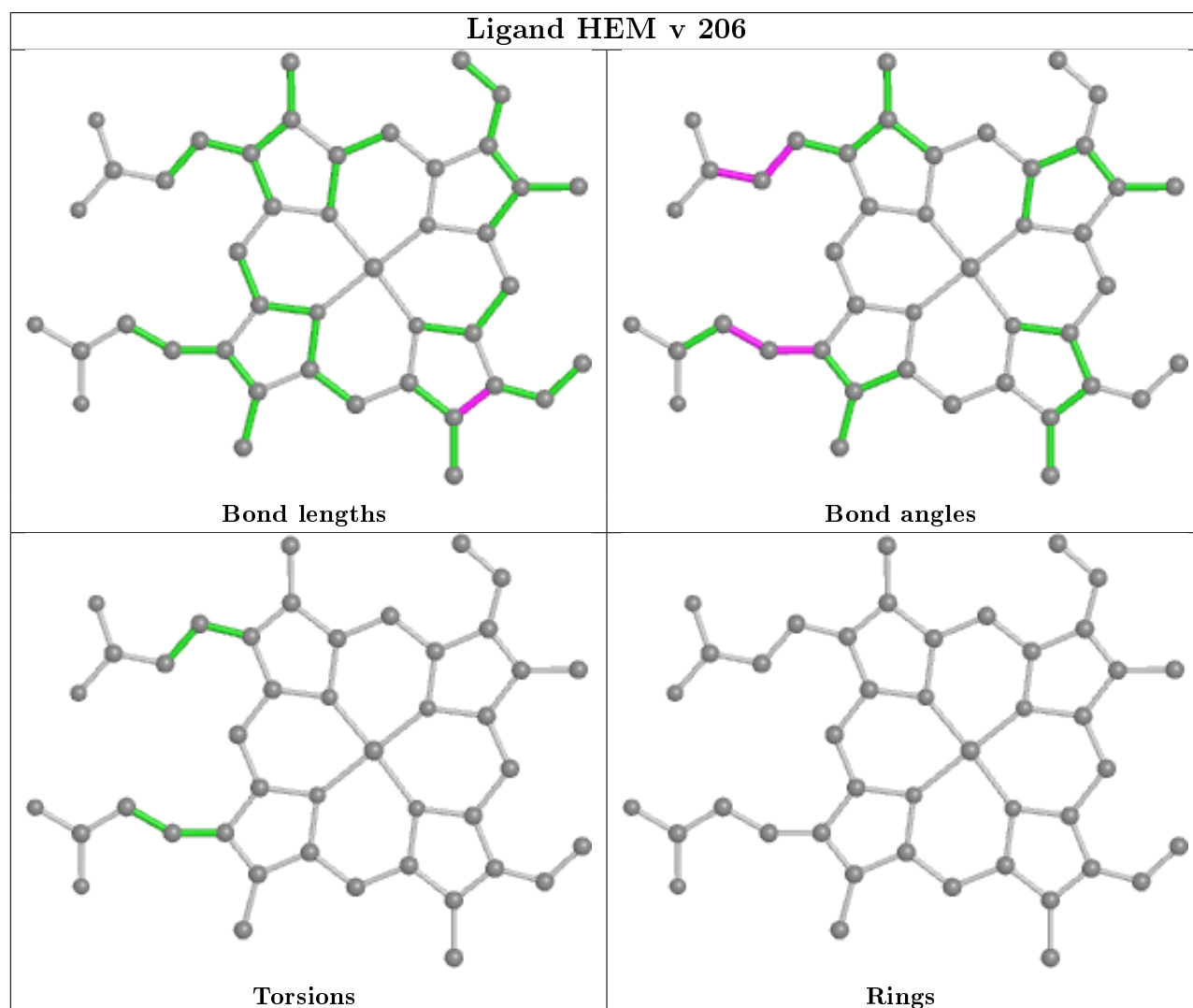
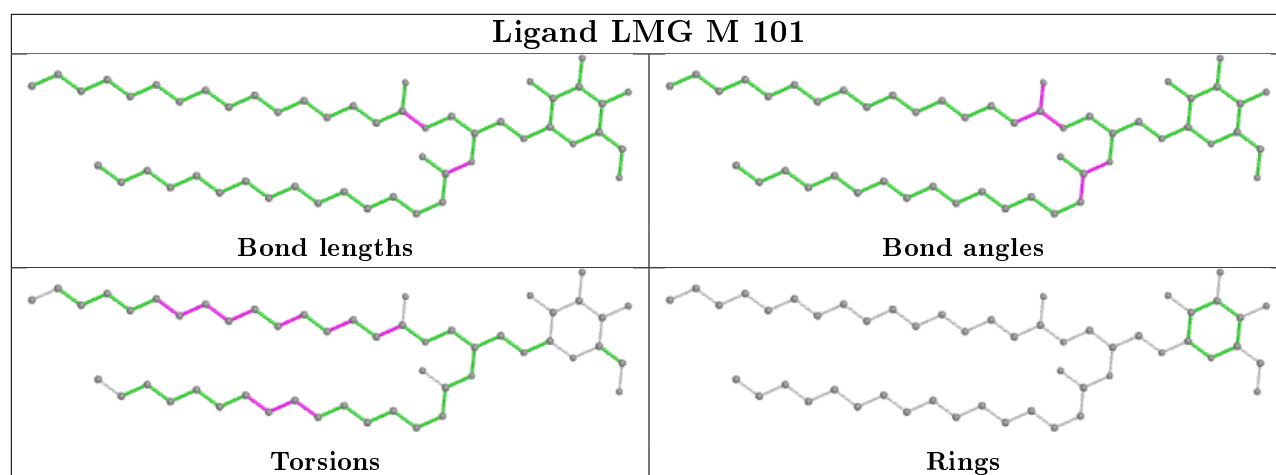
## Ligand CLA d 405

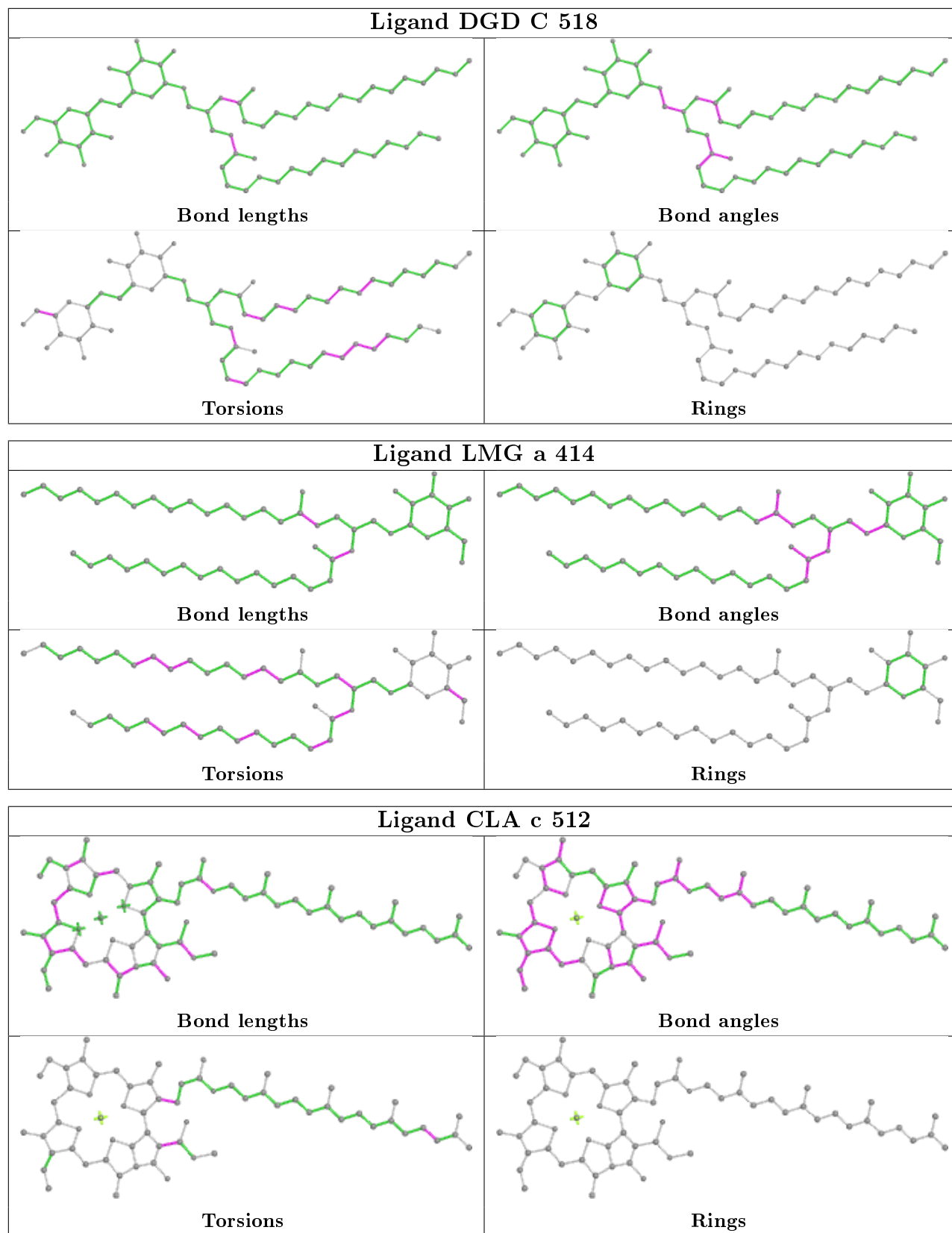


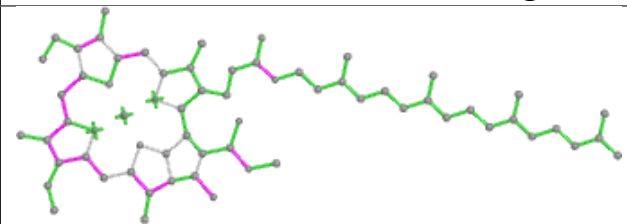
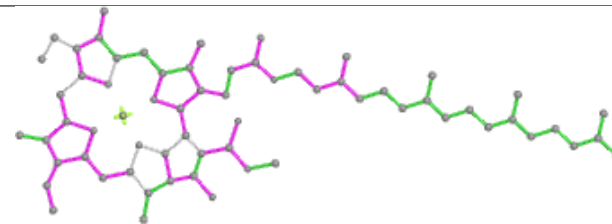
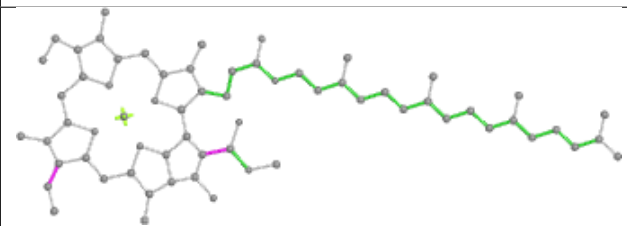
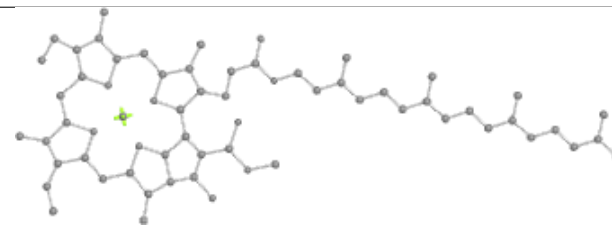
## Ligand BCR k 102

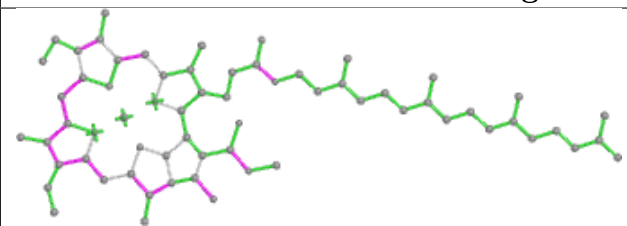
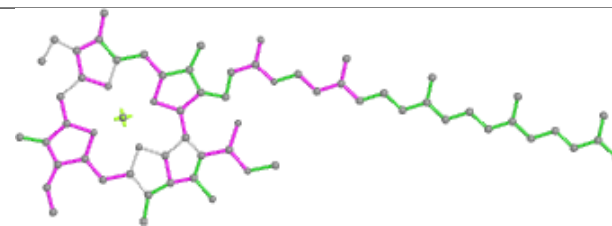
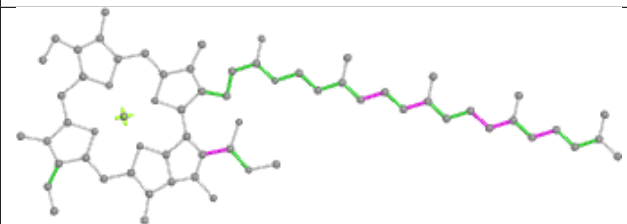
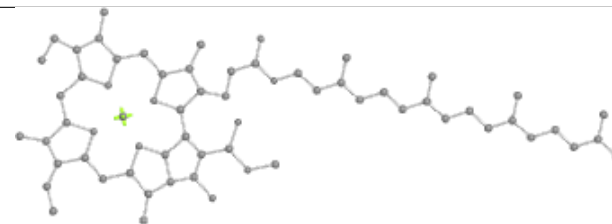


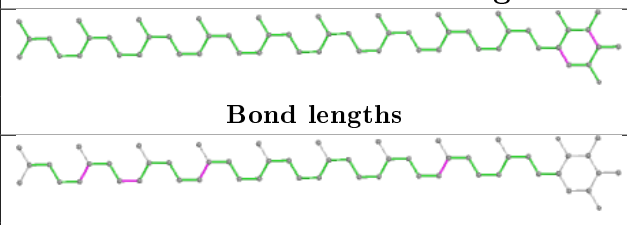
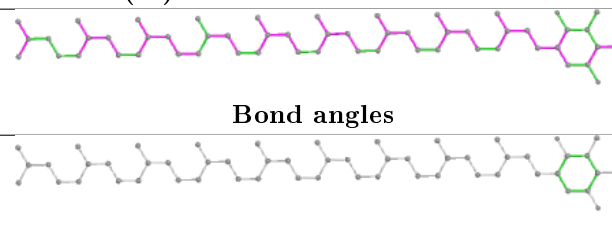
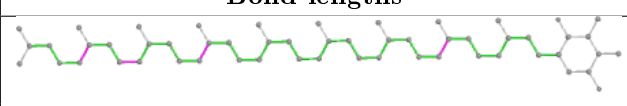
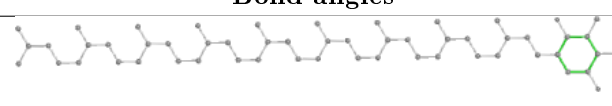
**Ligand CLA a 411****Ligand BCR D 407****Ligand CLA a 409**

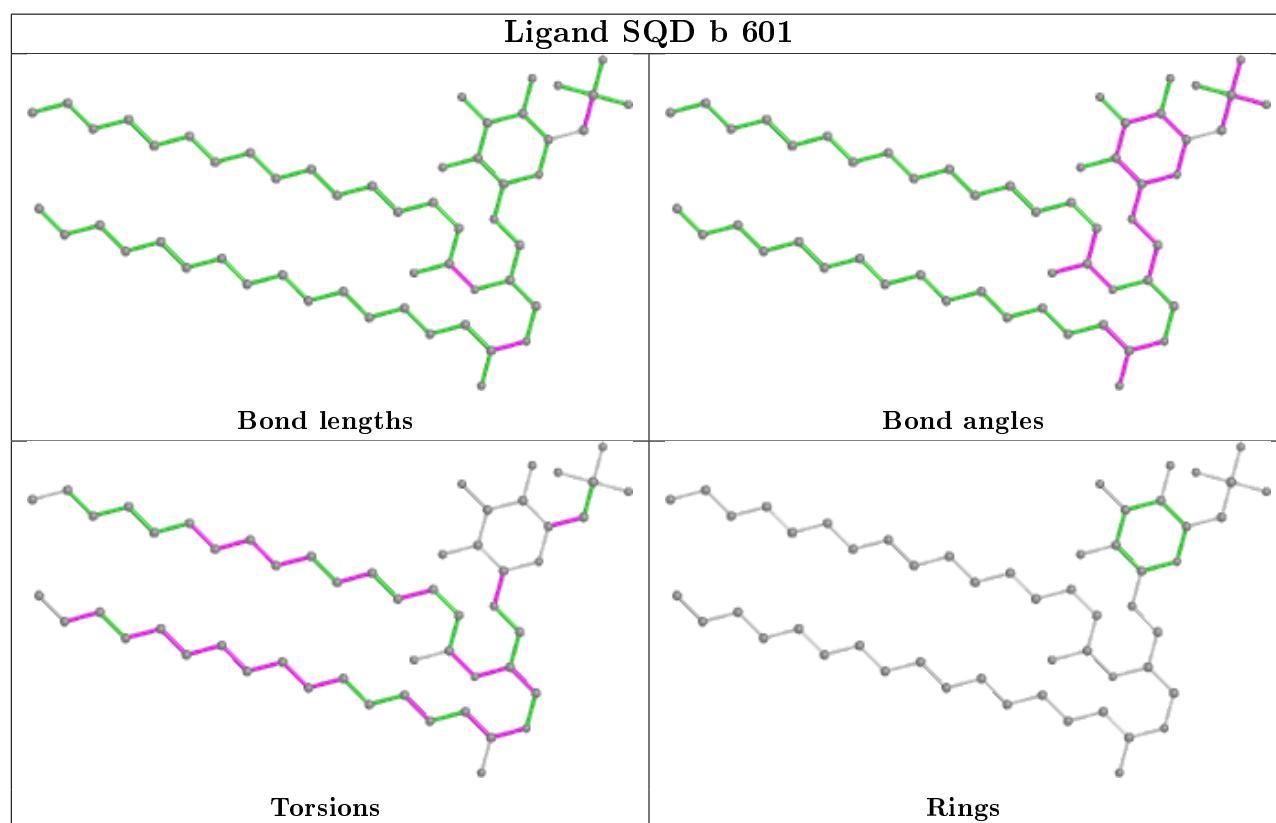
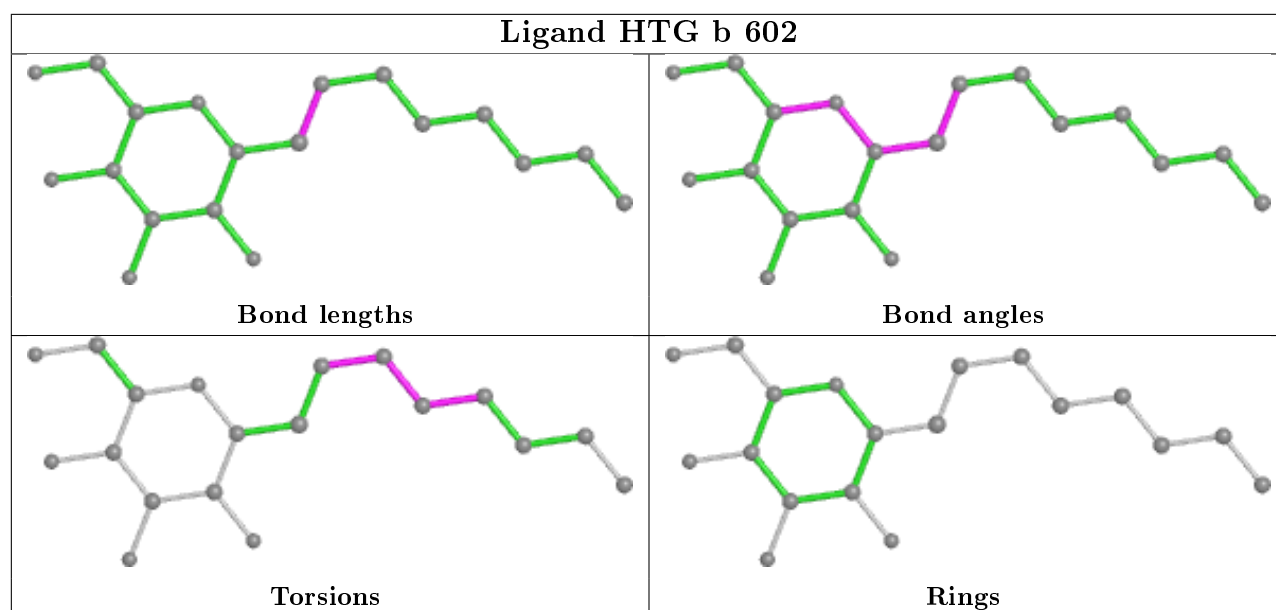


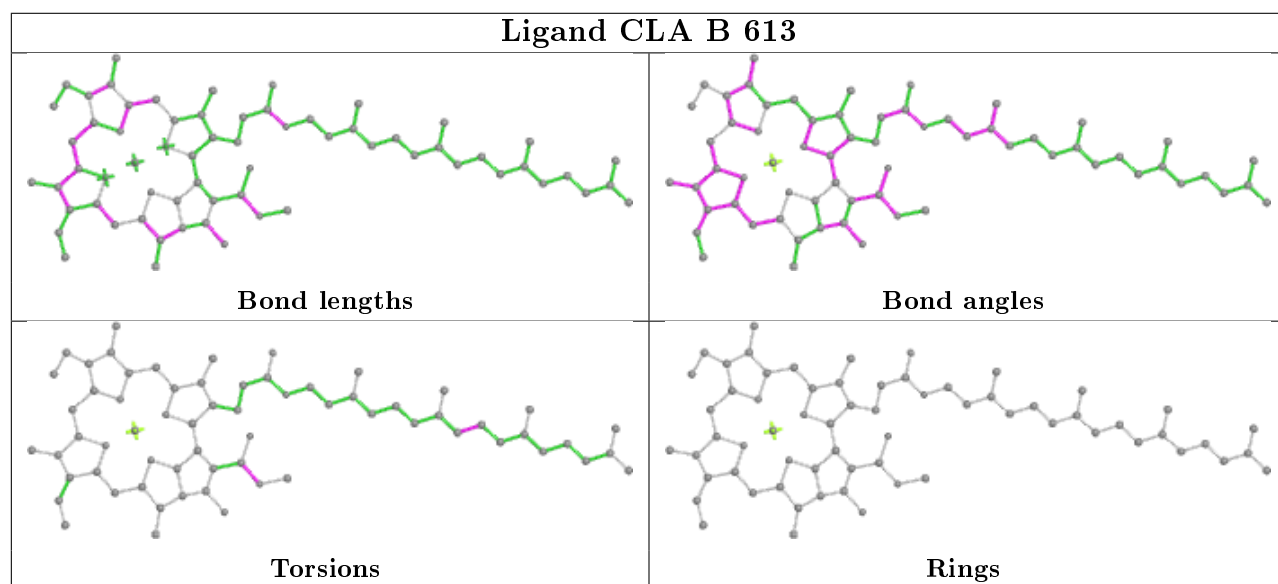
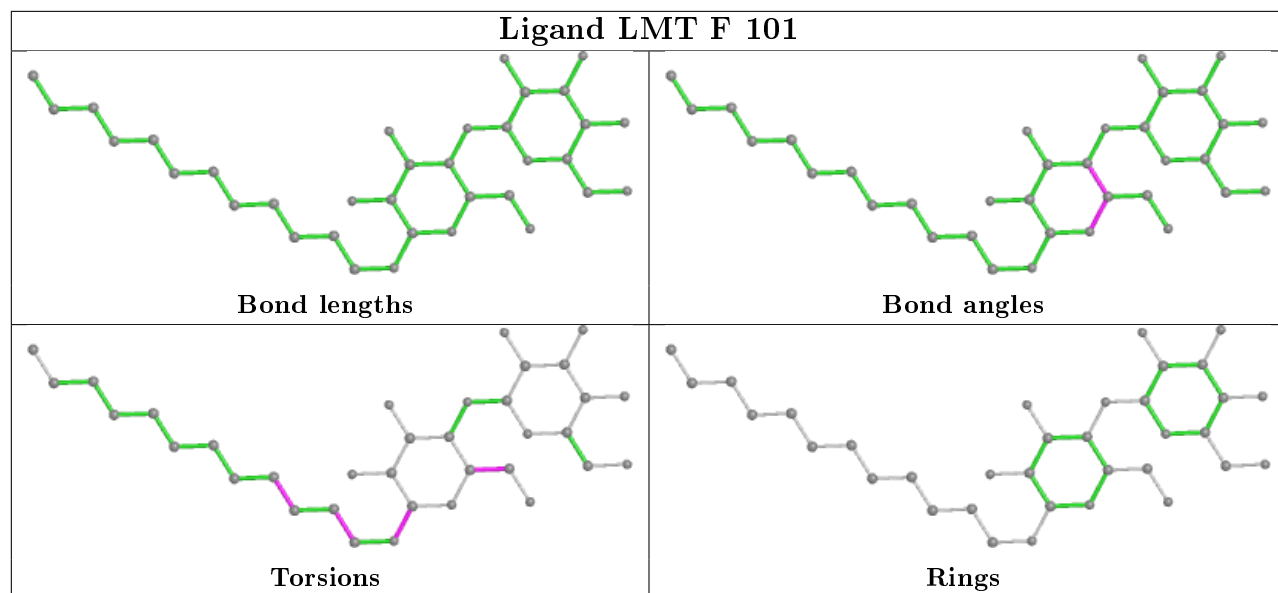


Ligand CLA A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

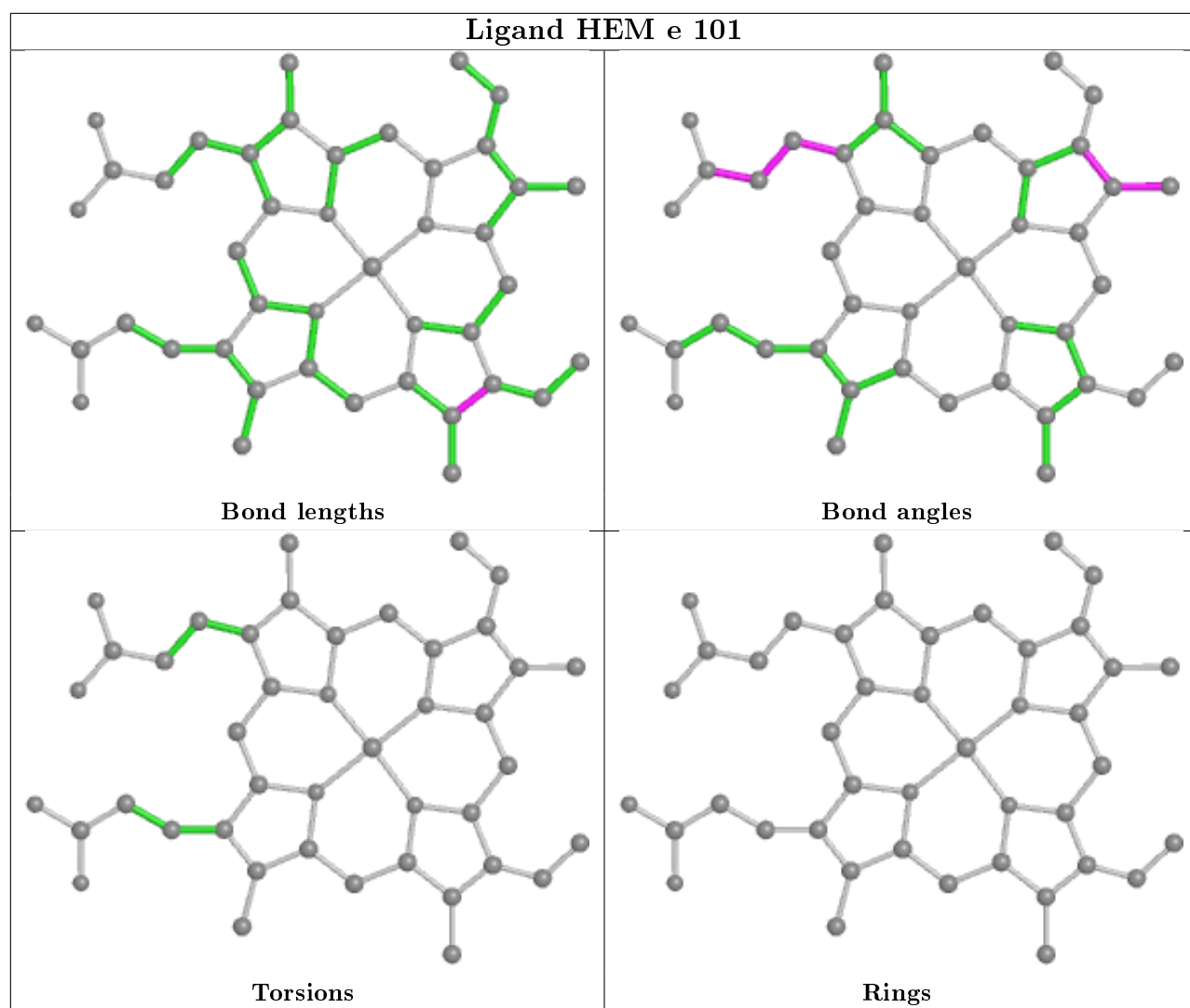
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

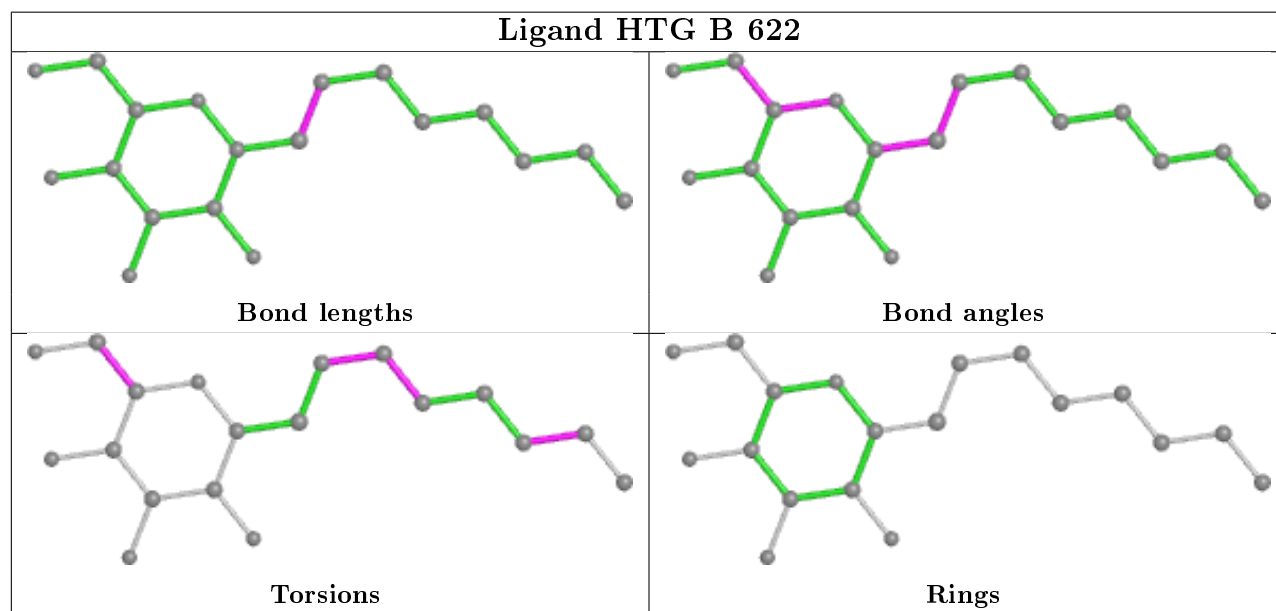
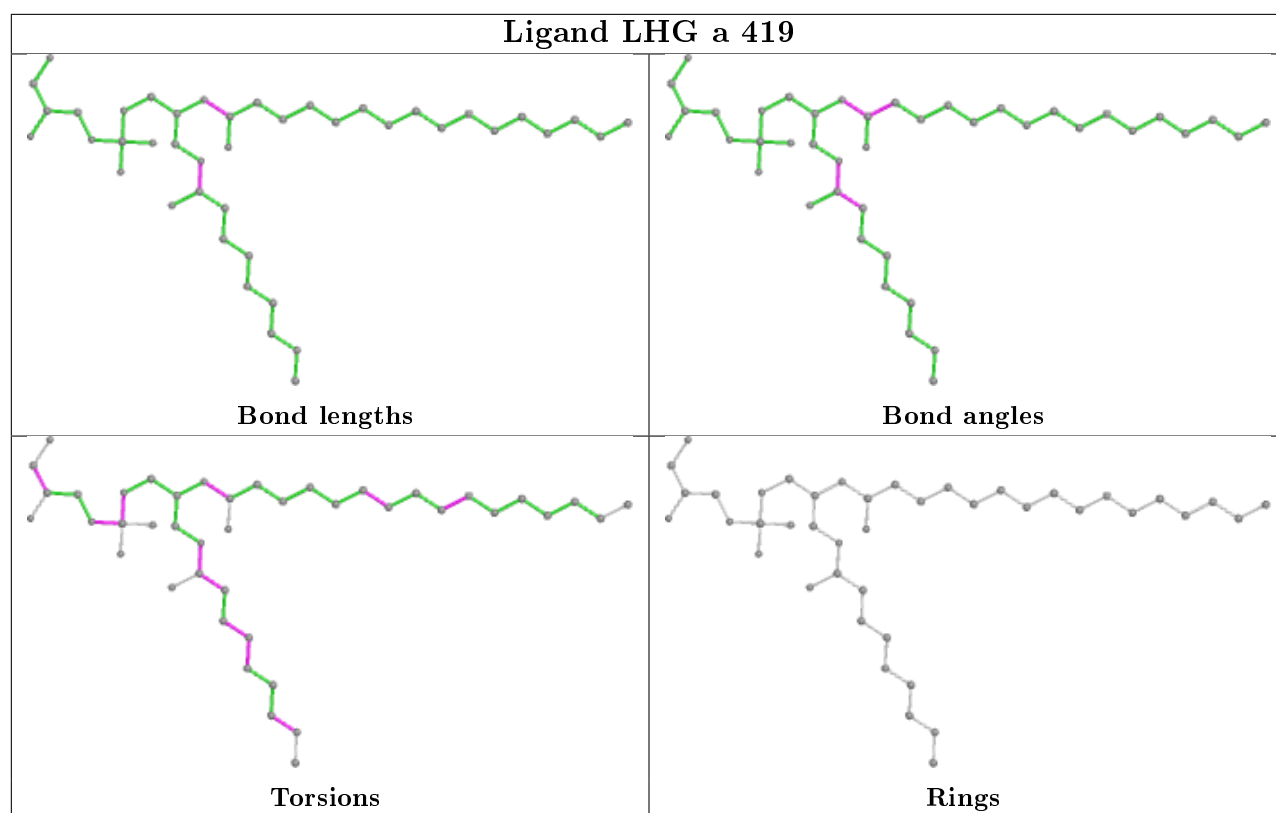
Ligand PL9 D 408 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings



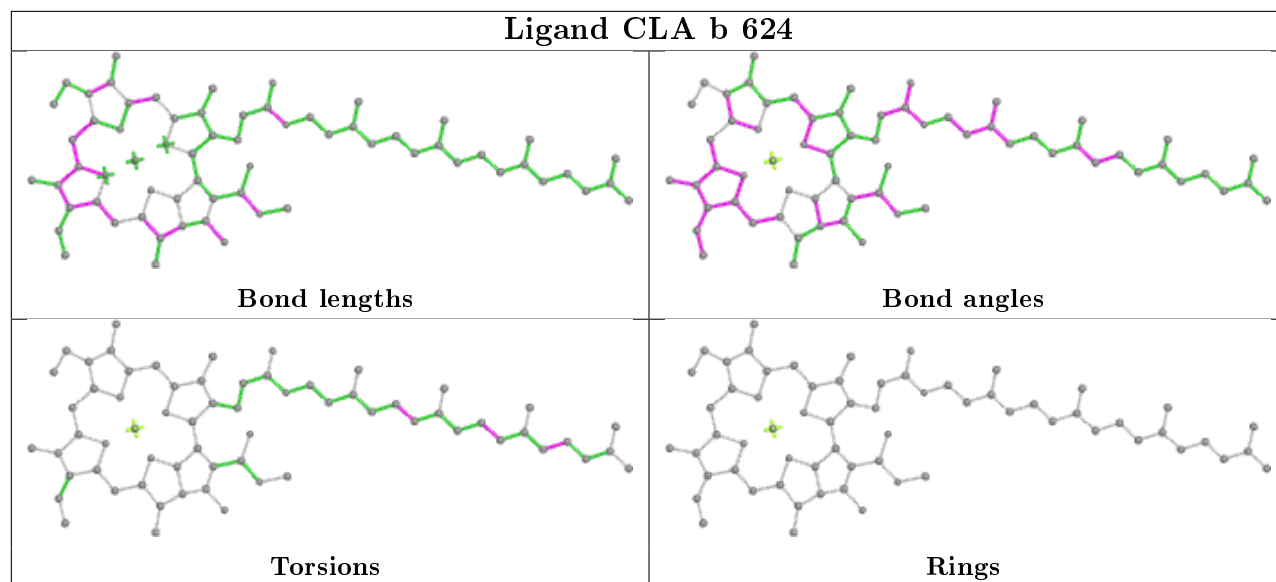




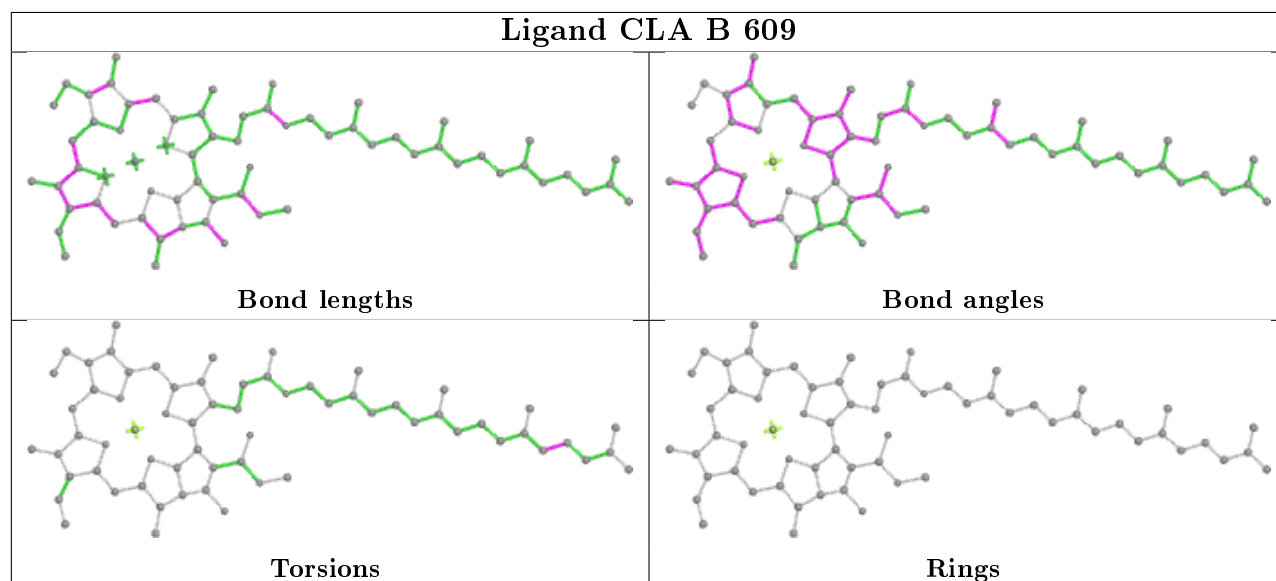




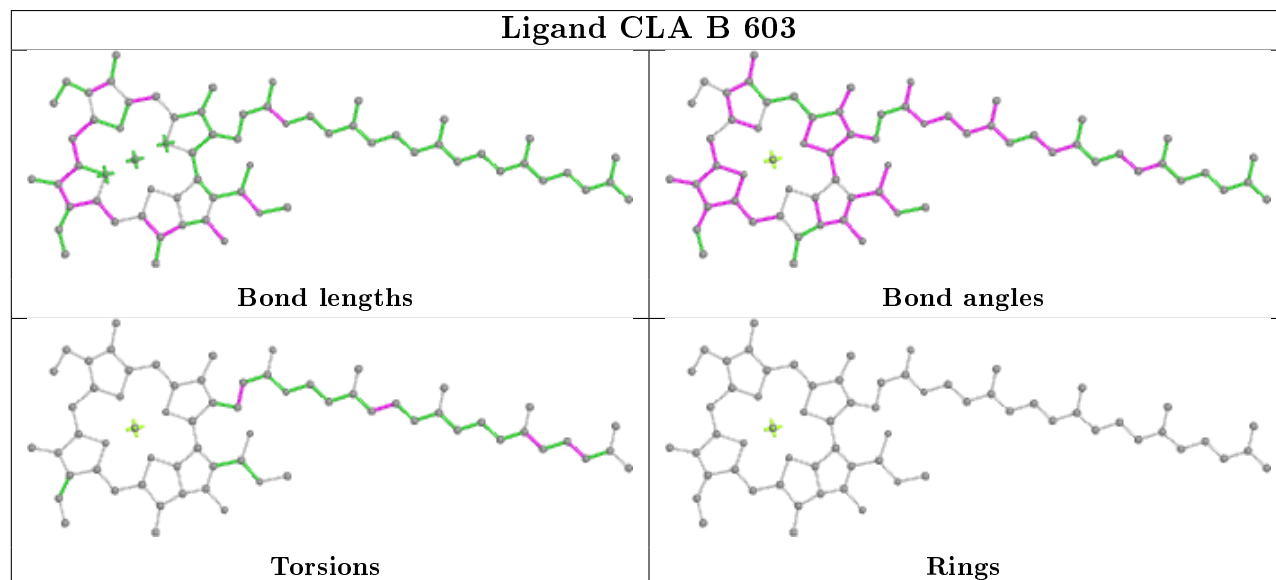
## Ligand CLA b 624

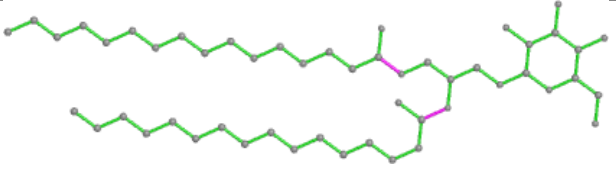
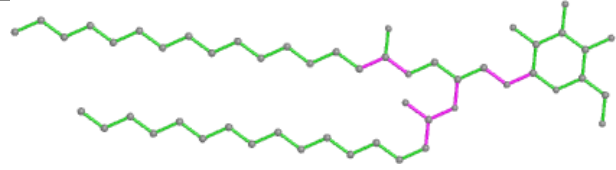
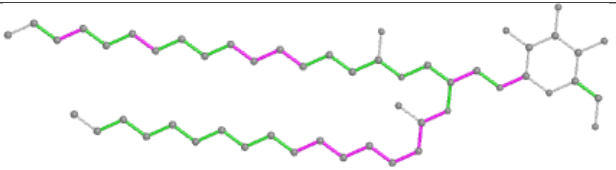
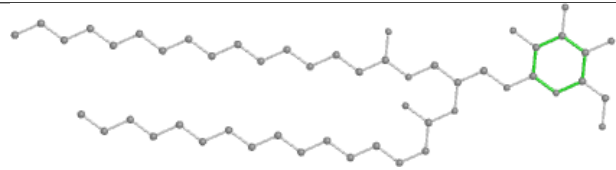


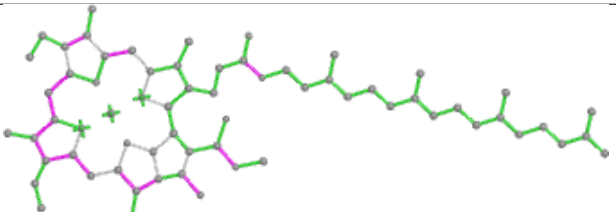
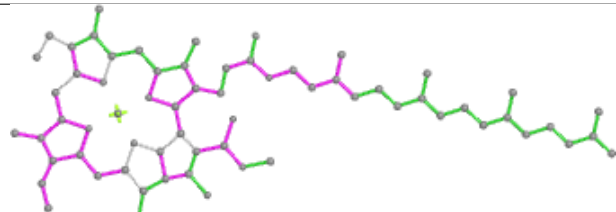
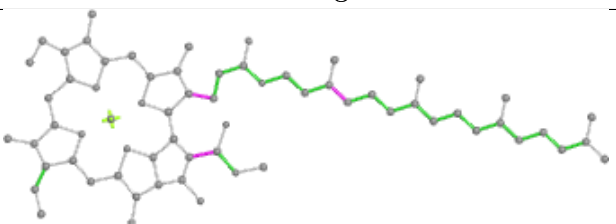
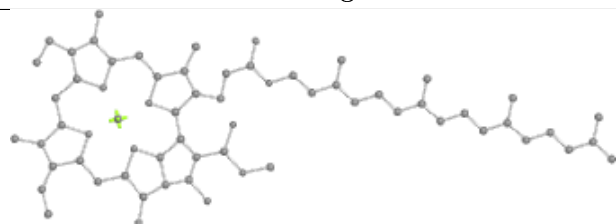
## Ligand CLA B 609


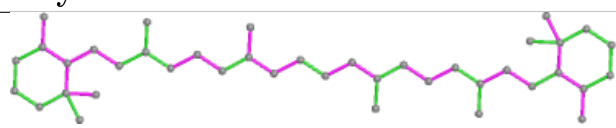
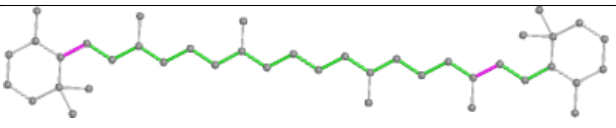
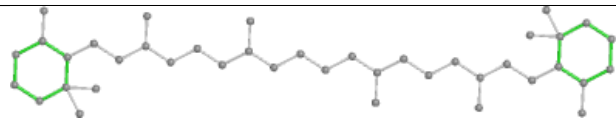


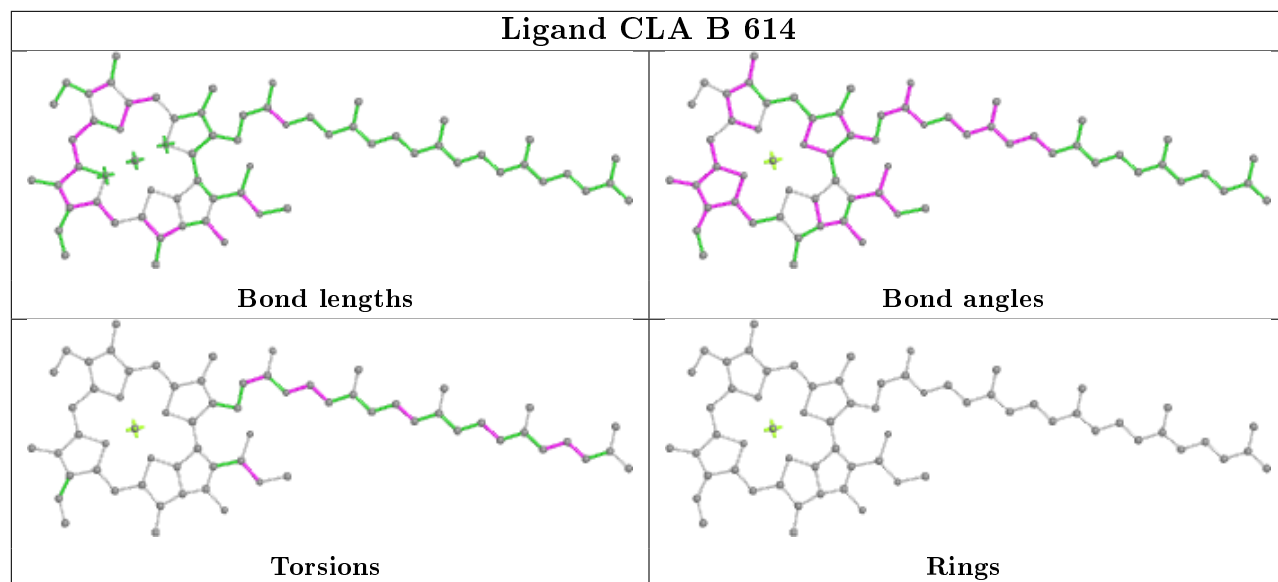
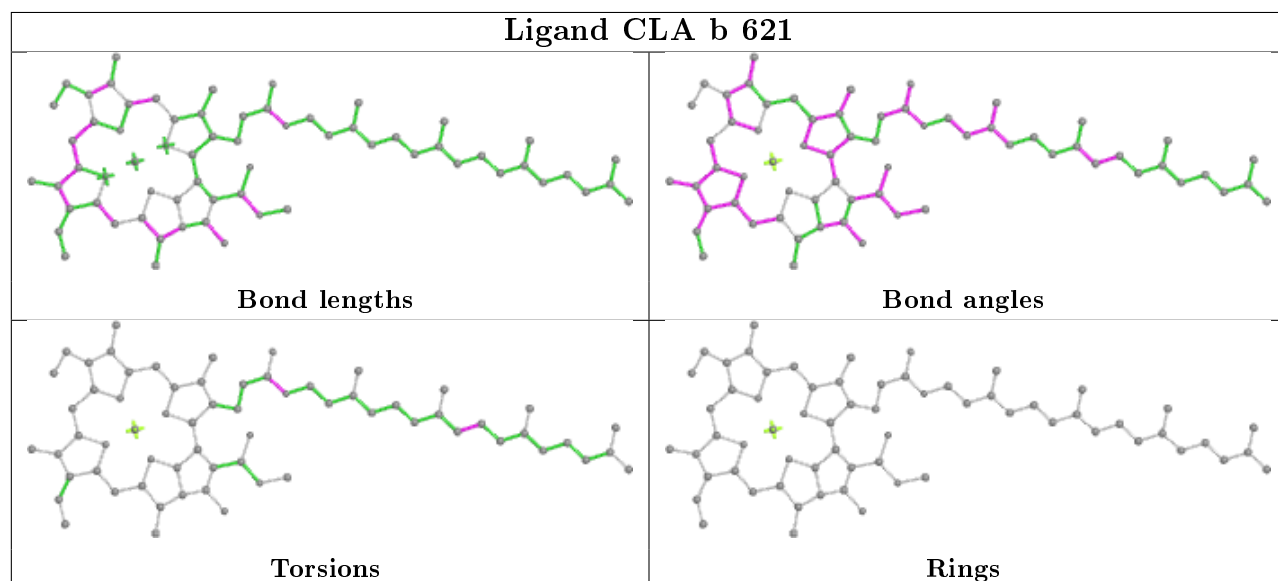
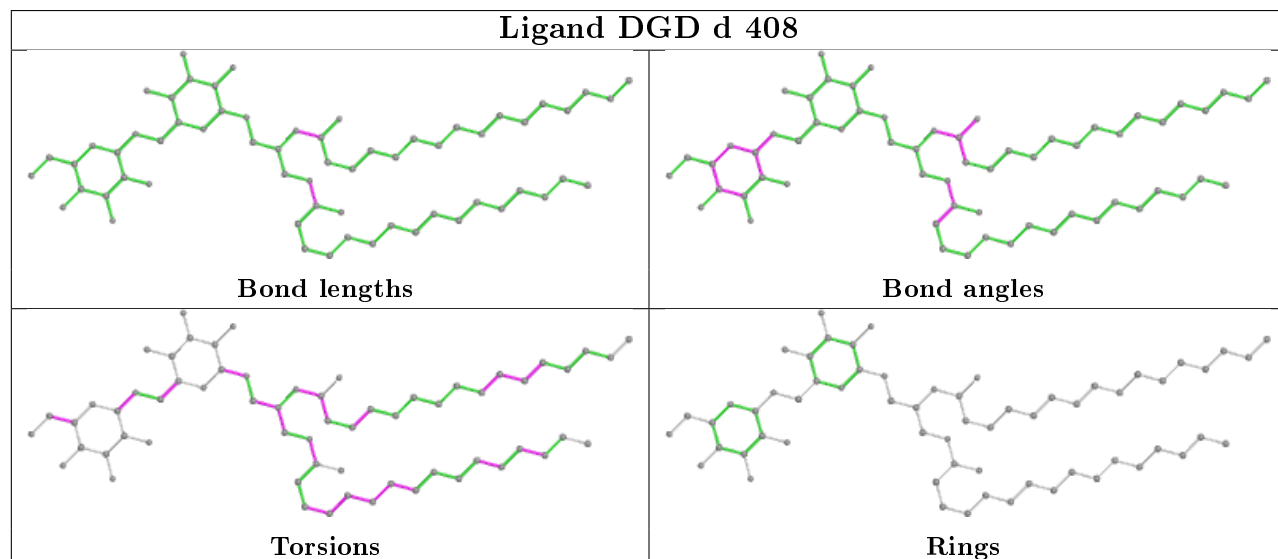
## Ligand CLA B 603

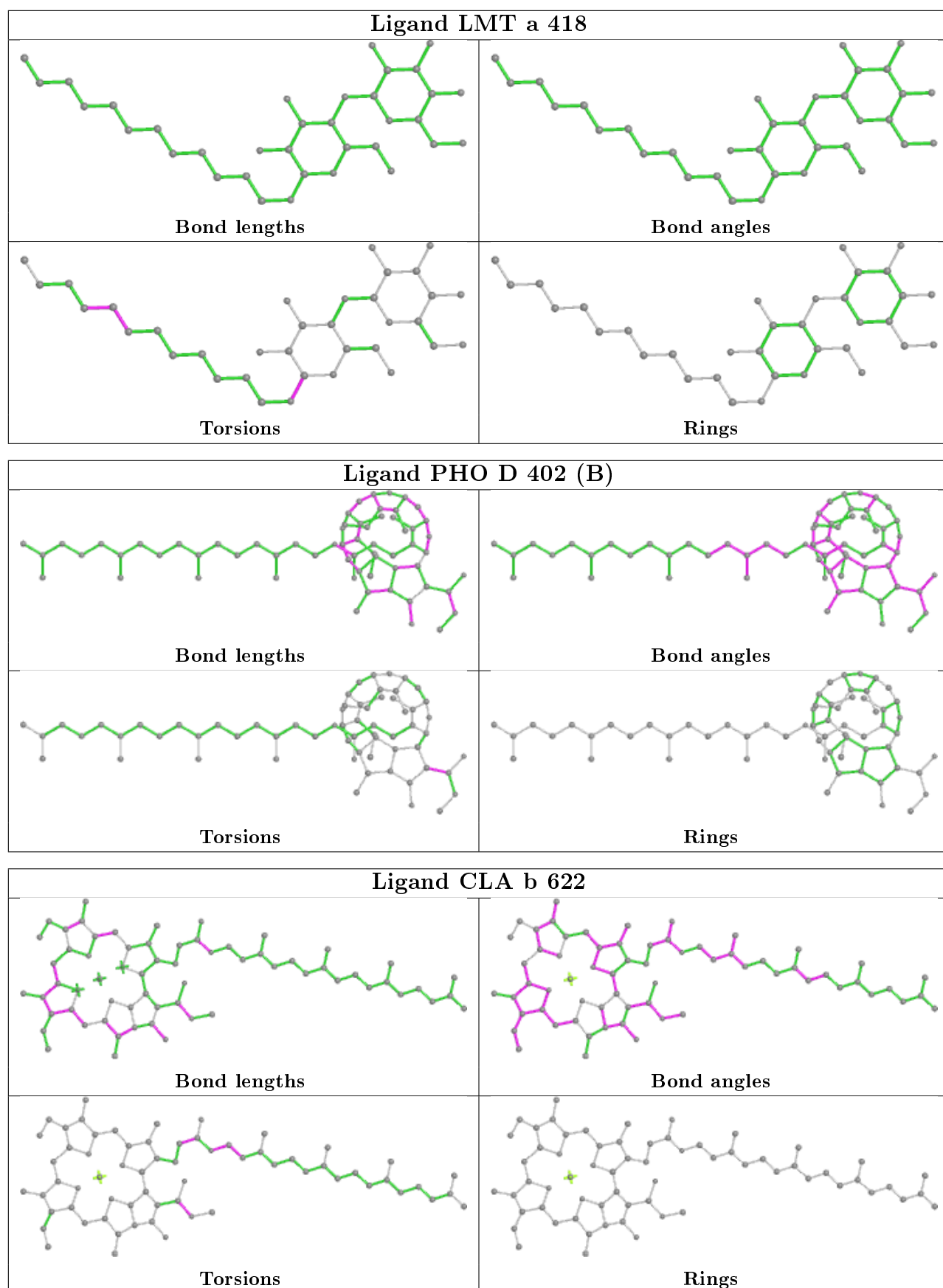


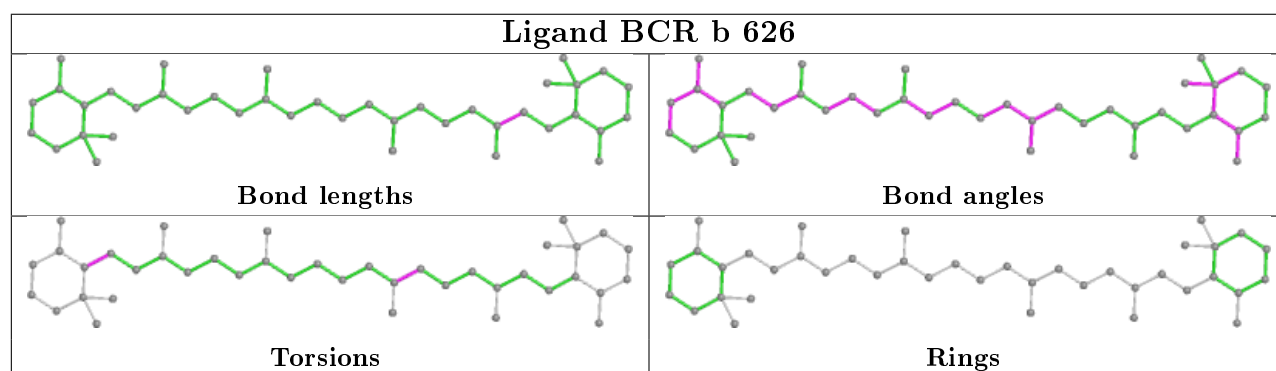
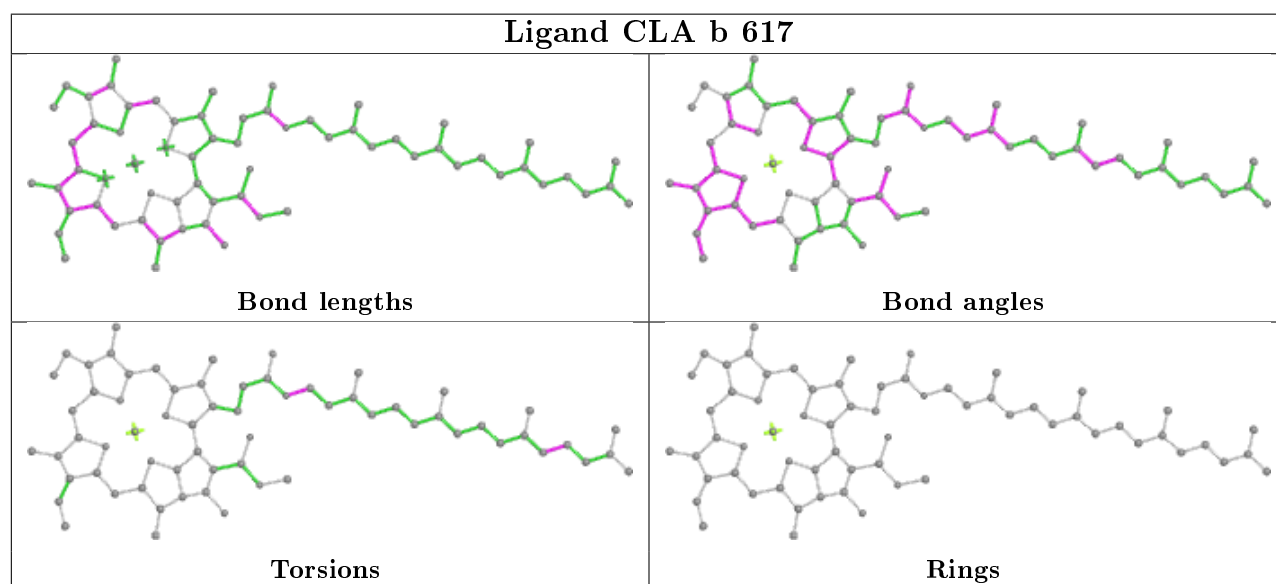
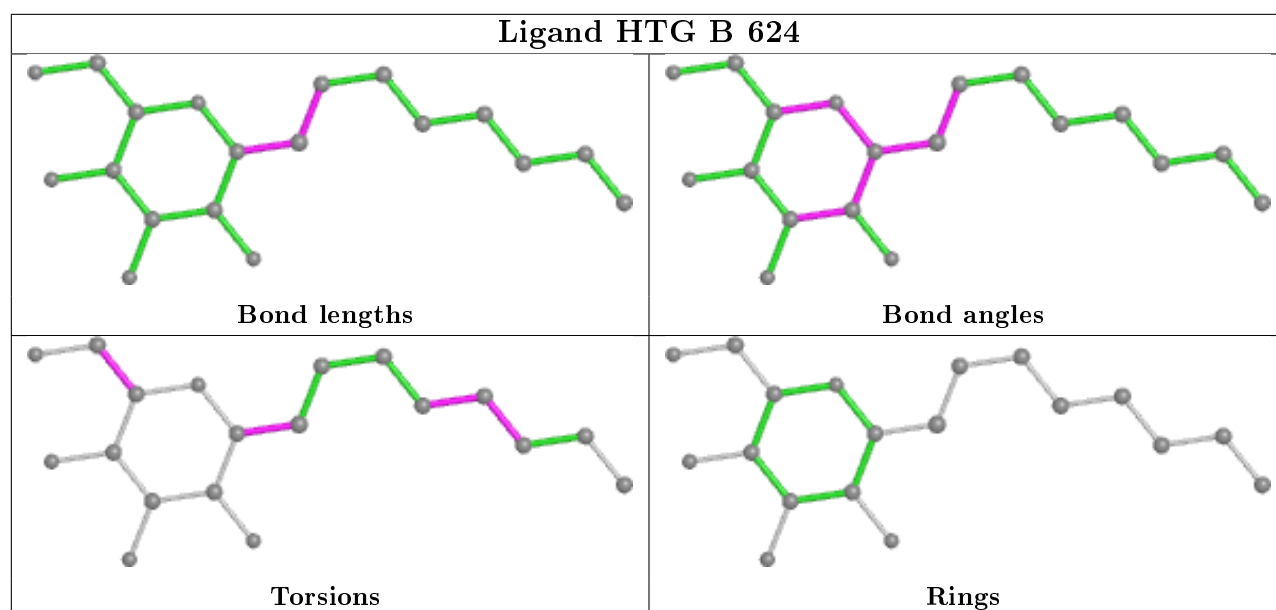
Ligand LMG C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

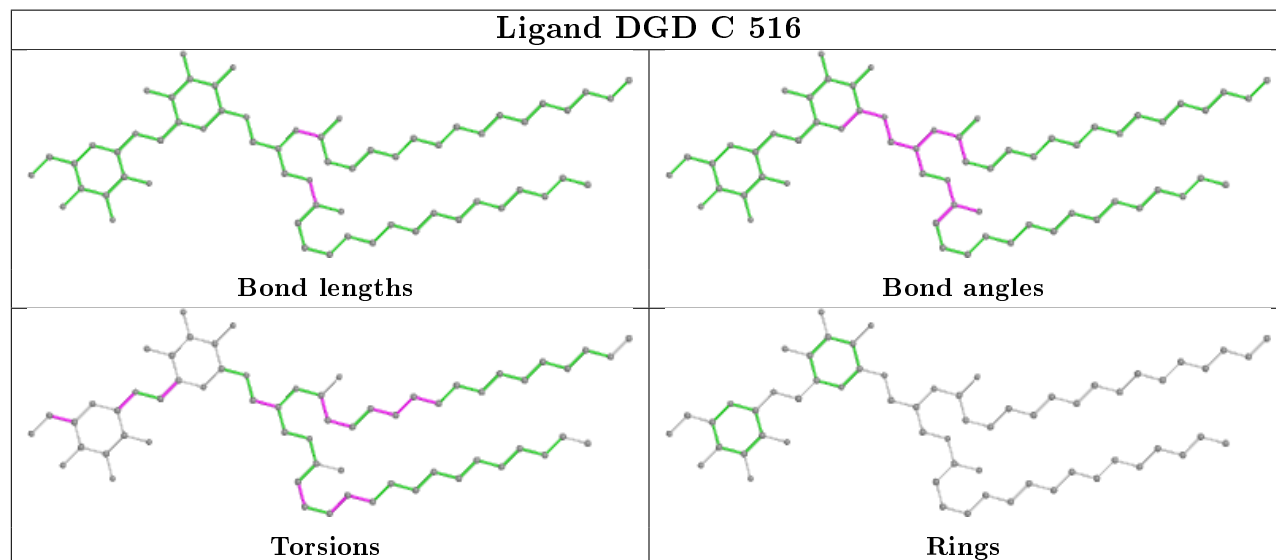
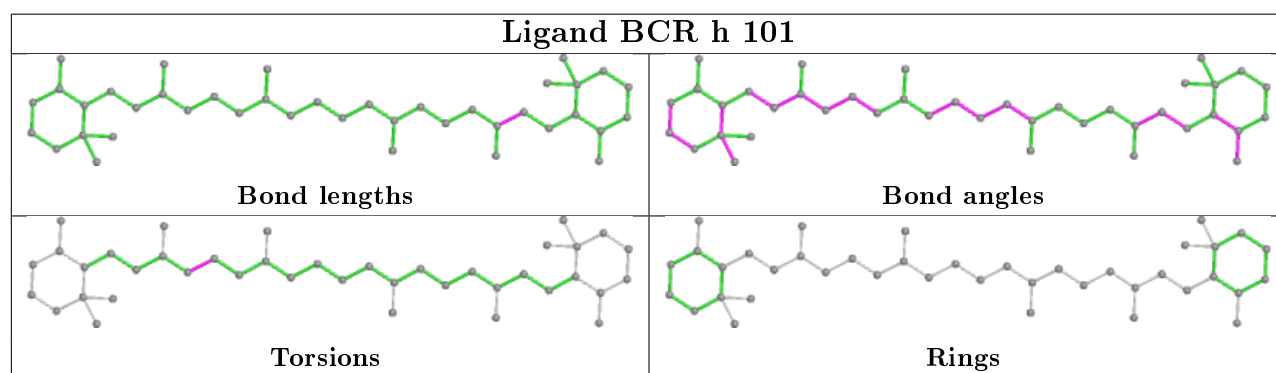
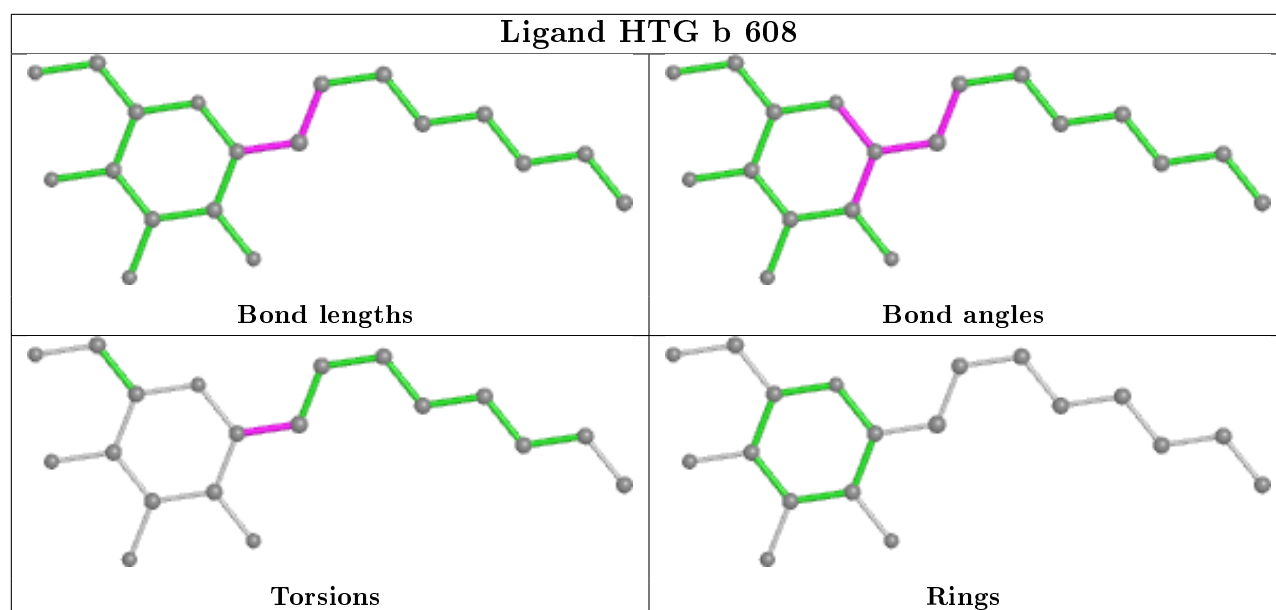
Ligand CLA b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

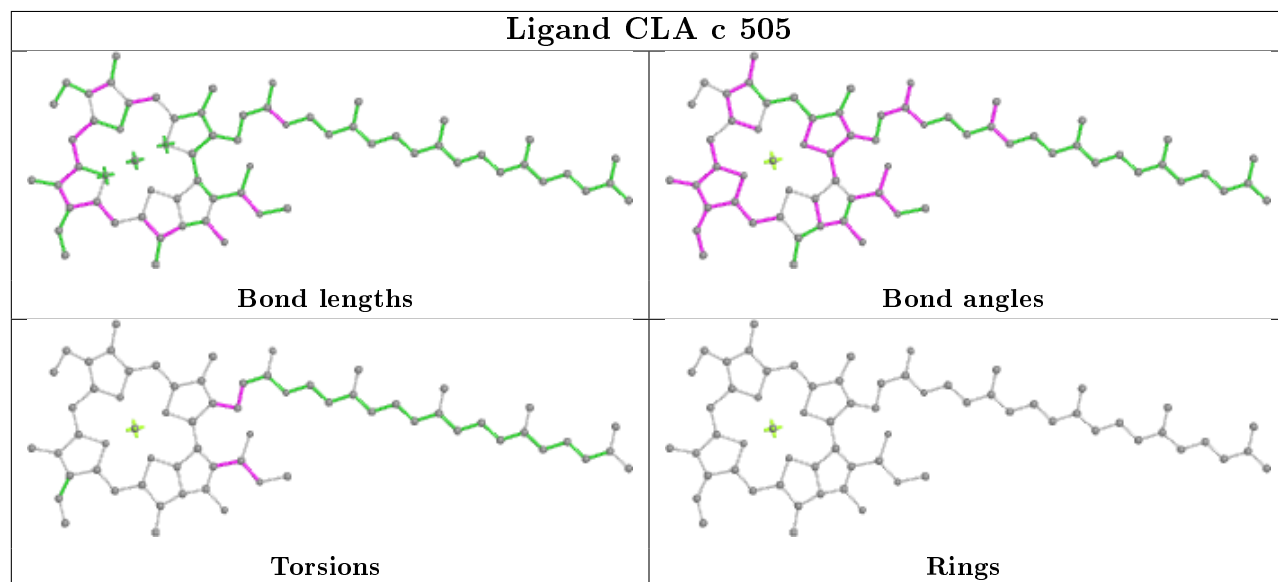
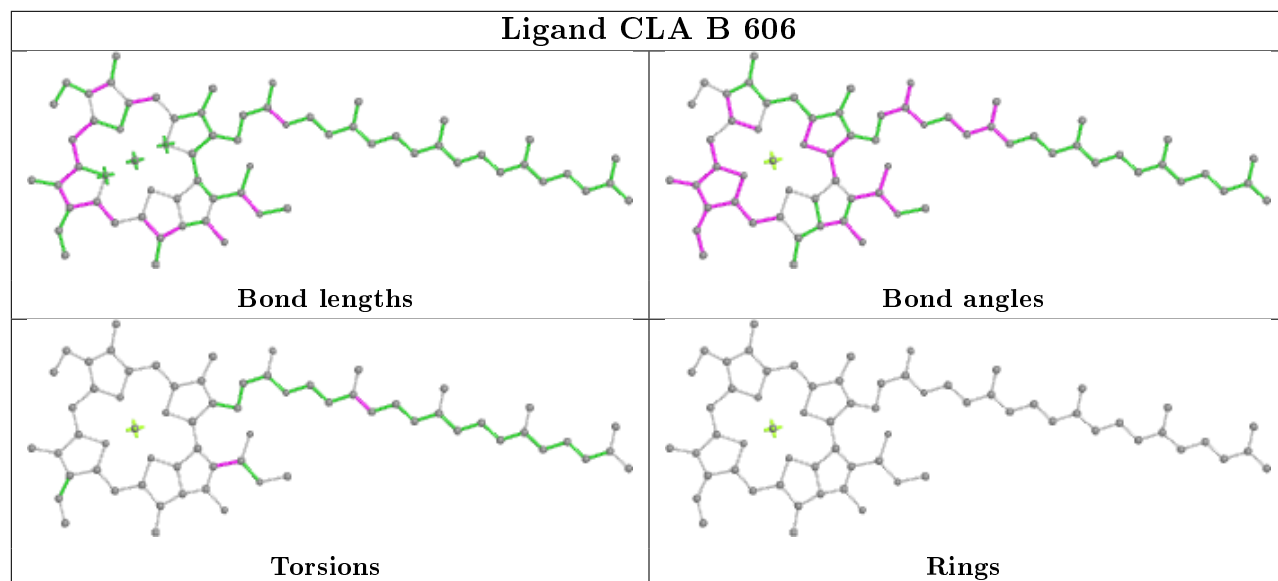
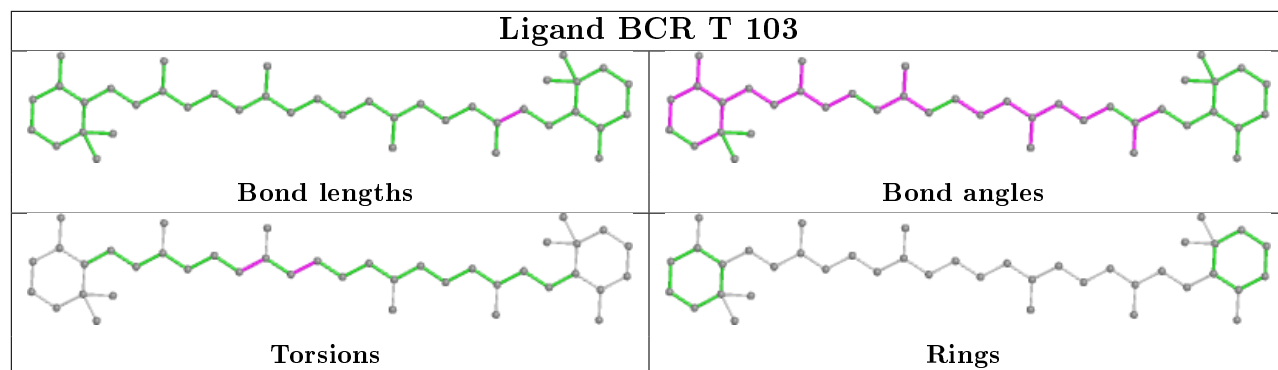
**Ligand CLA B 614****Ligand CLA b 621****Ligand DGD d 408**



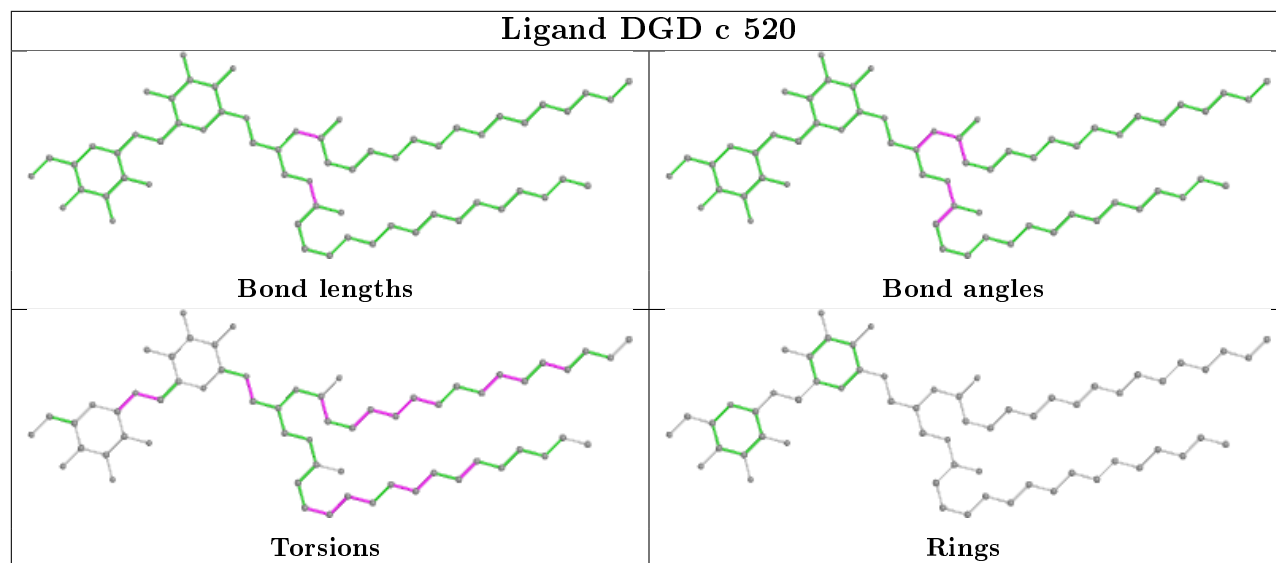




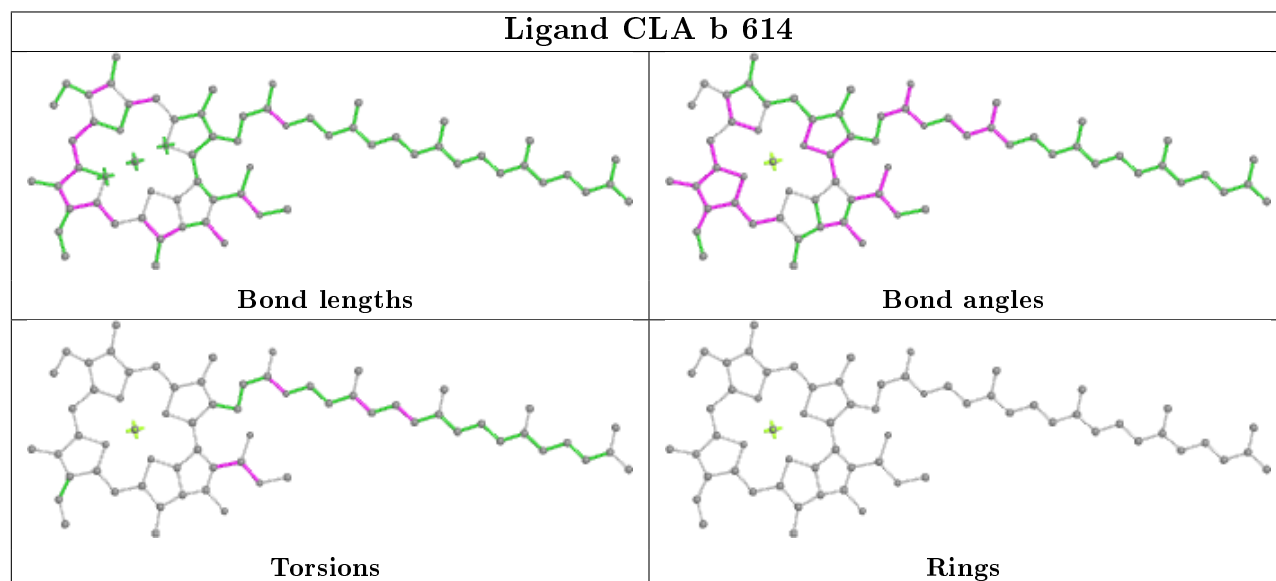




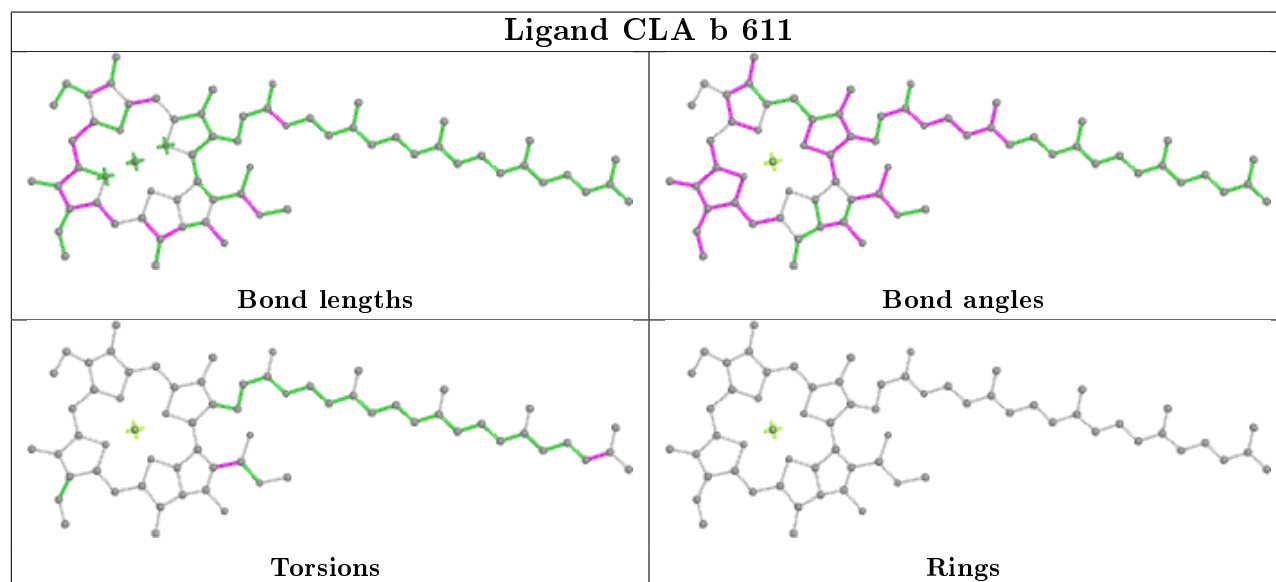
## Ligand DGD c 520

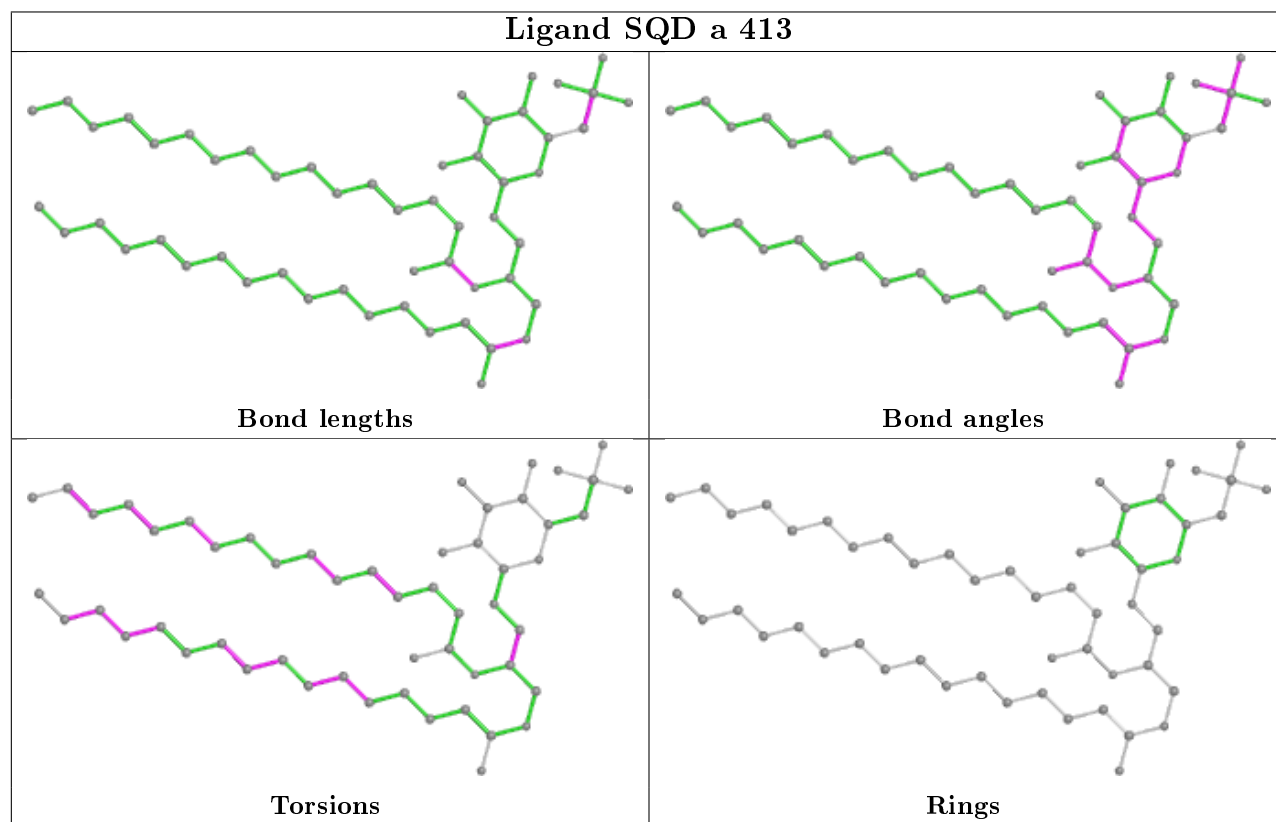
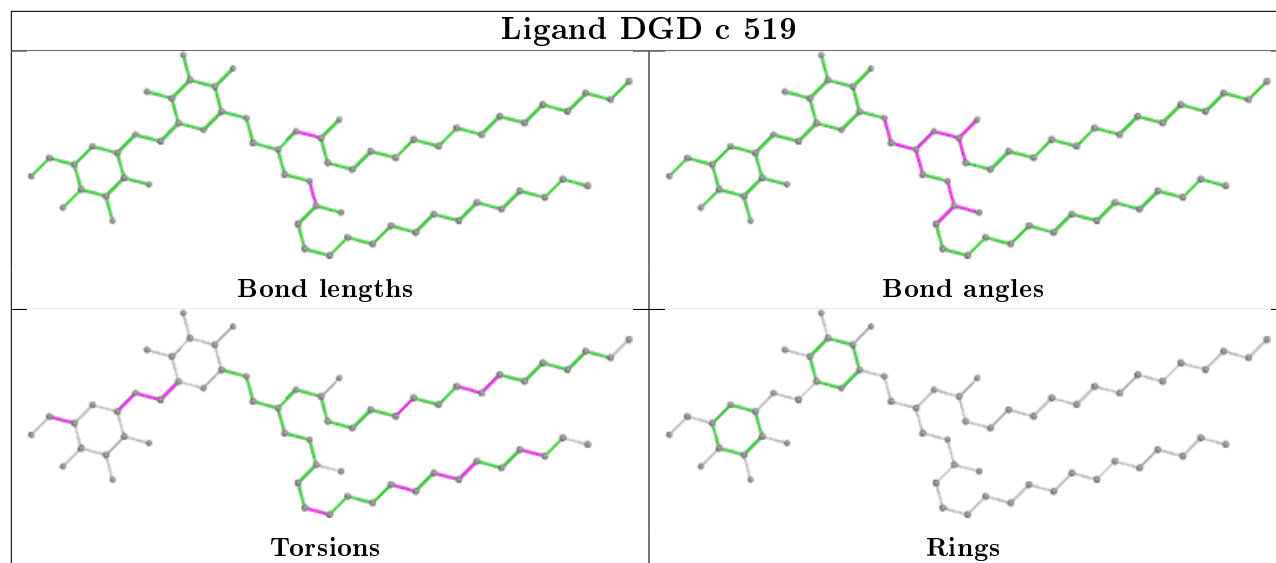


## Ligand CLA b 614

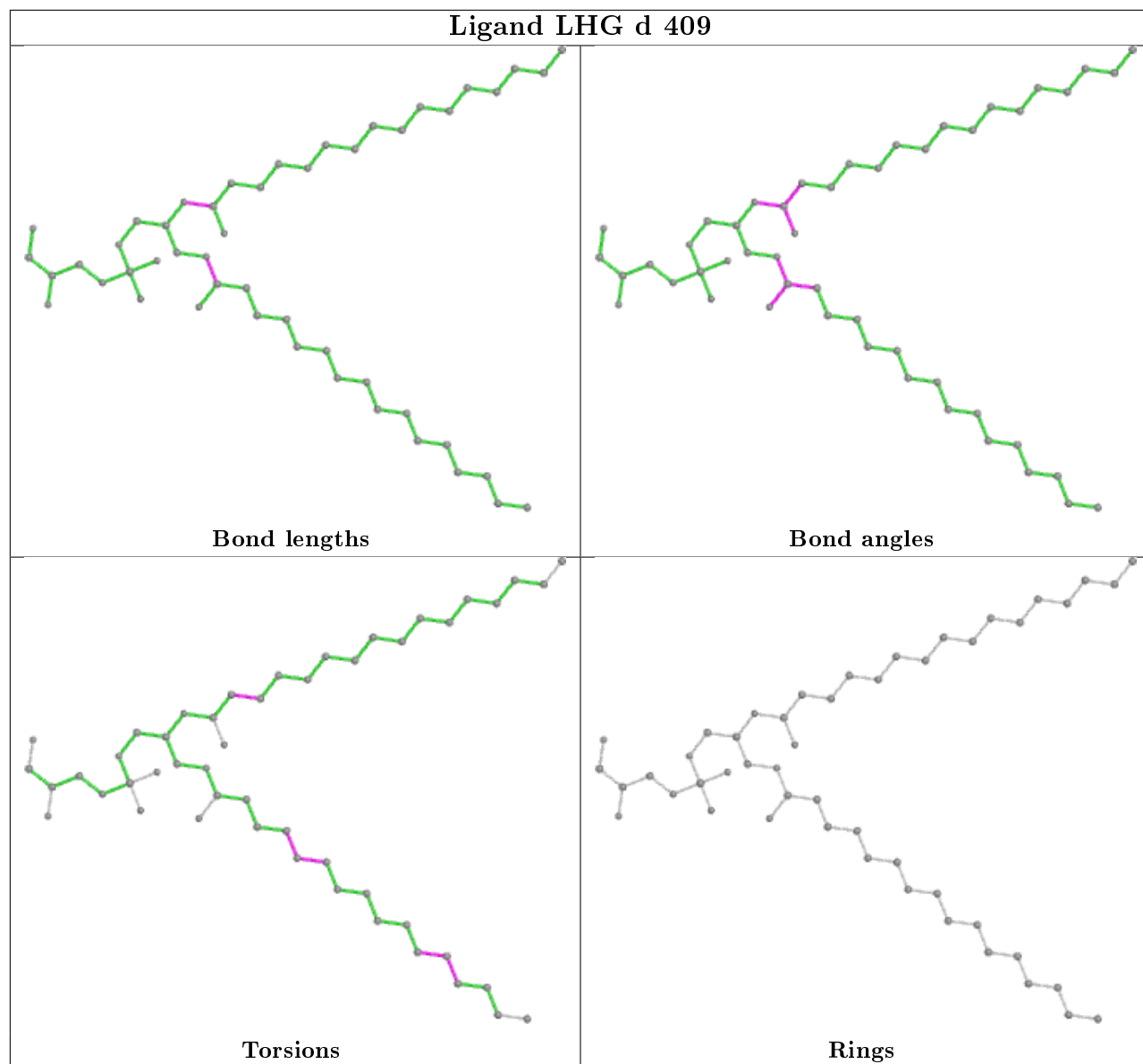


## Ligand CLA b 611

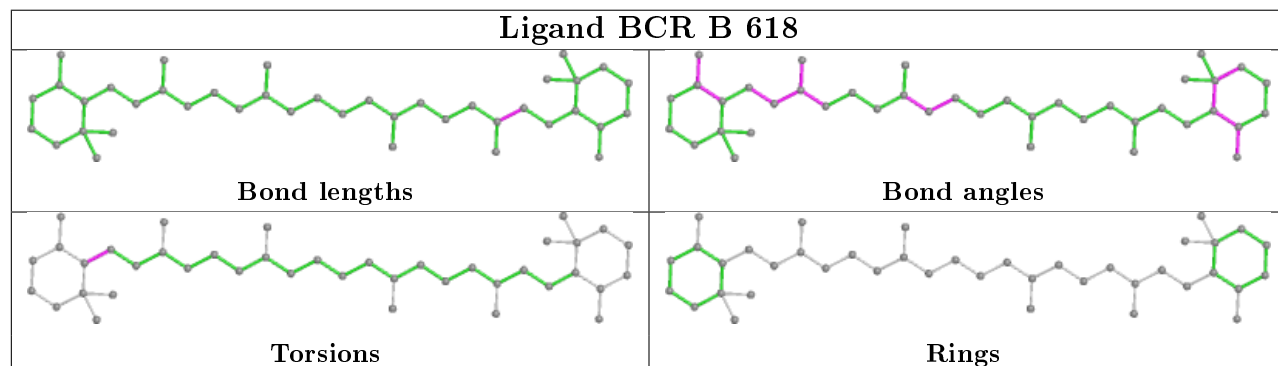




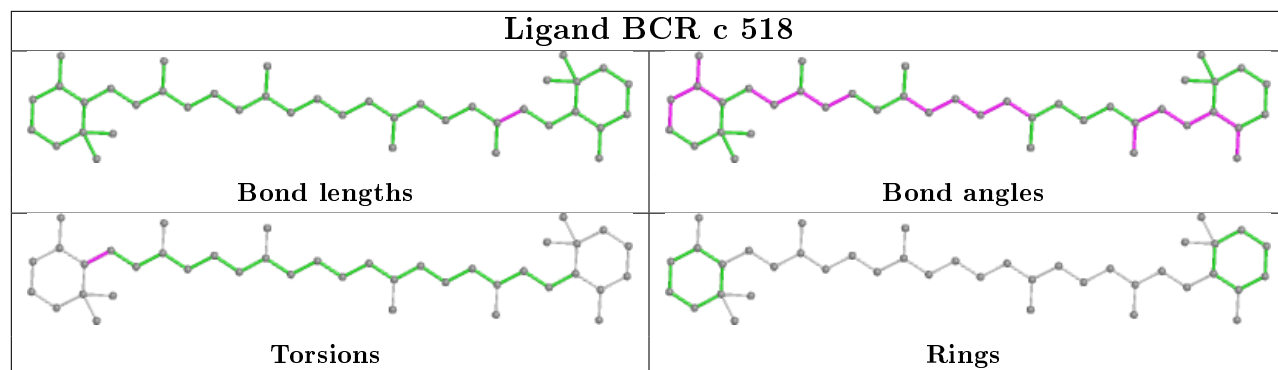
## Ligand LHG d 409



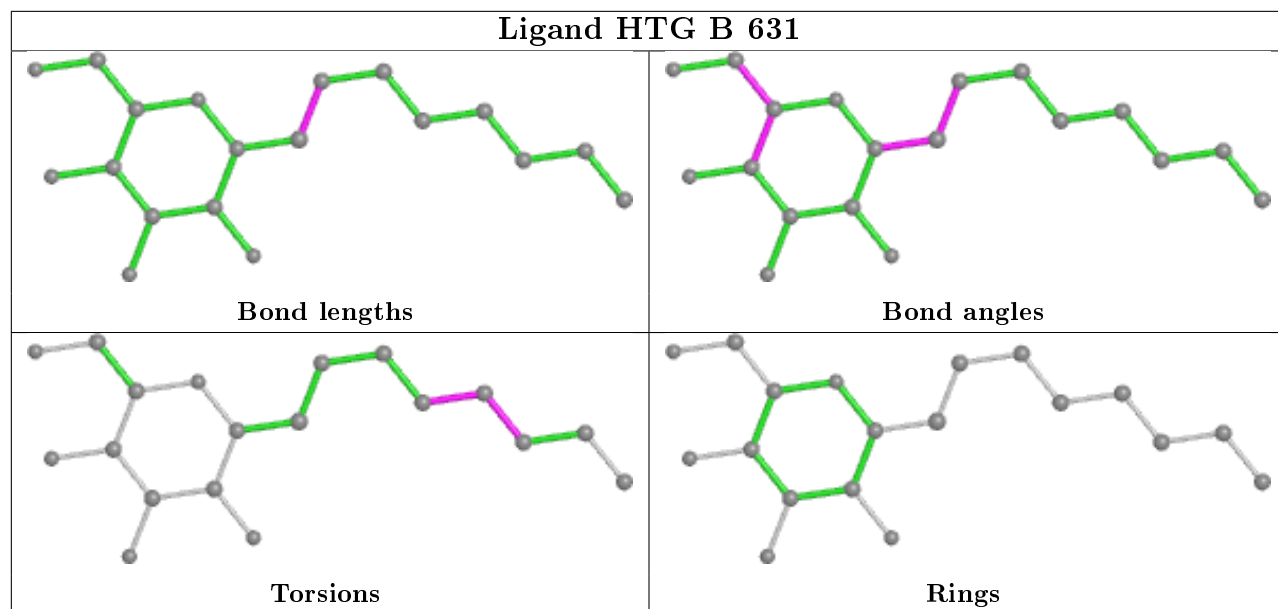
## Ligand BCR B 618



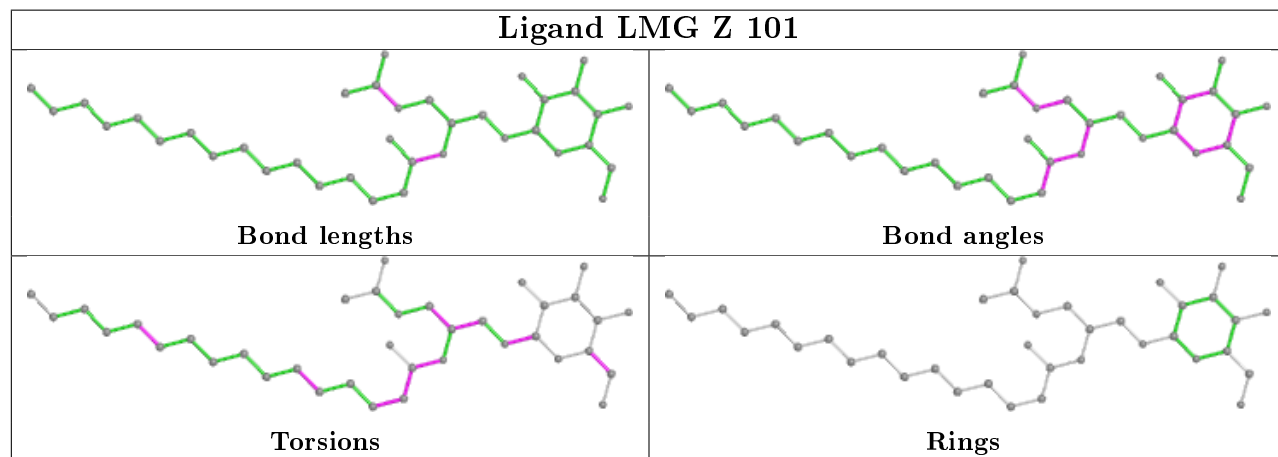
## Ligand BCR c 518



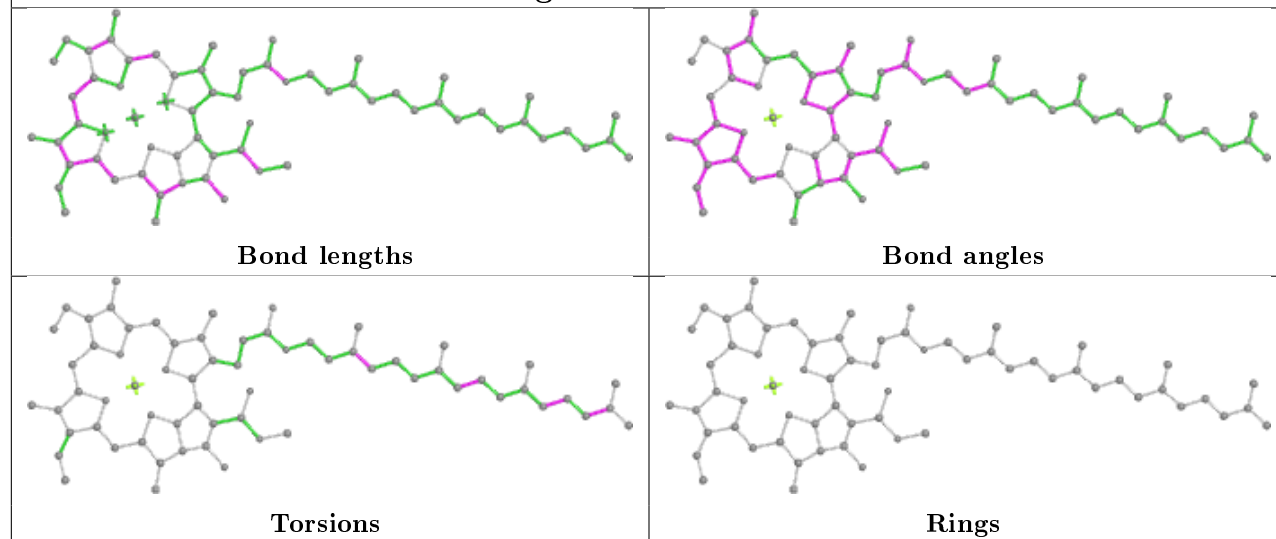
## Ligand HTG B 631



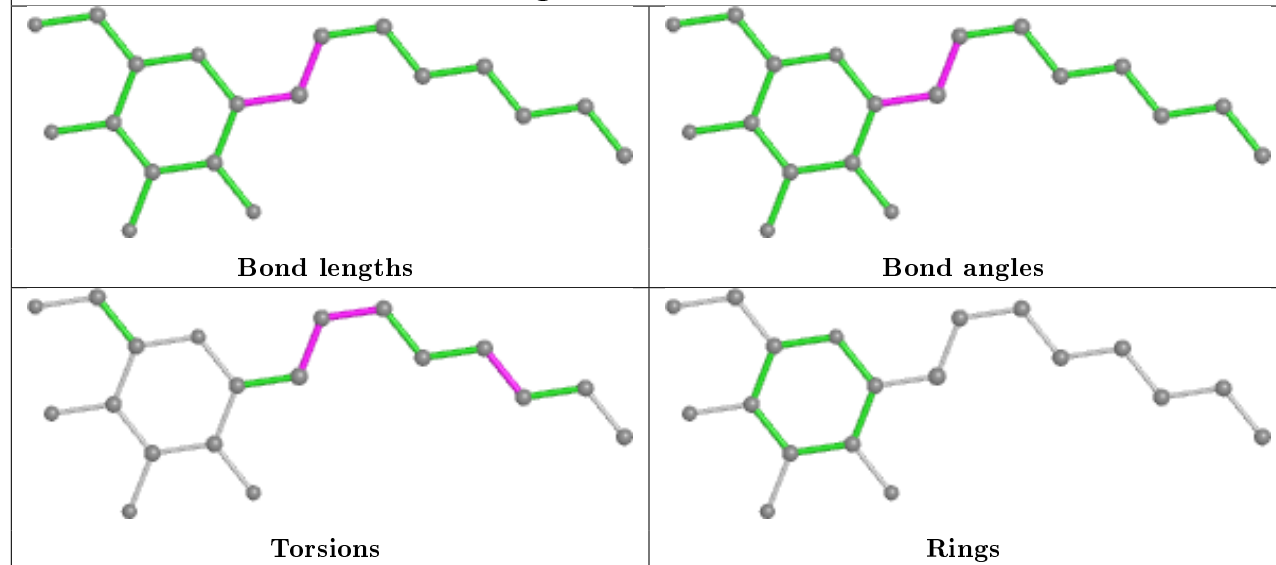
## Ligand LMG Z 101



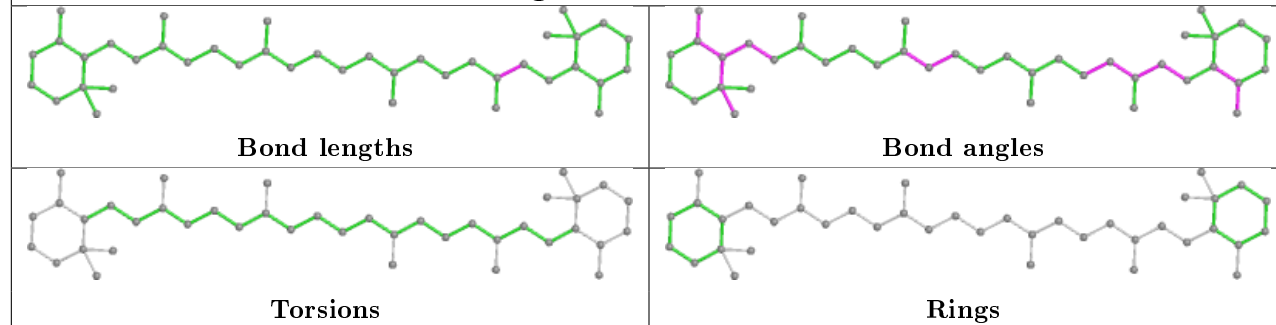
## Ligand CLA b 620

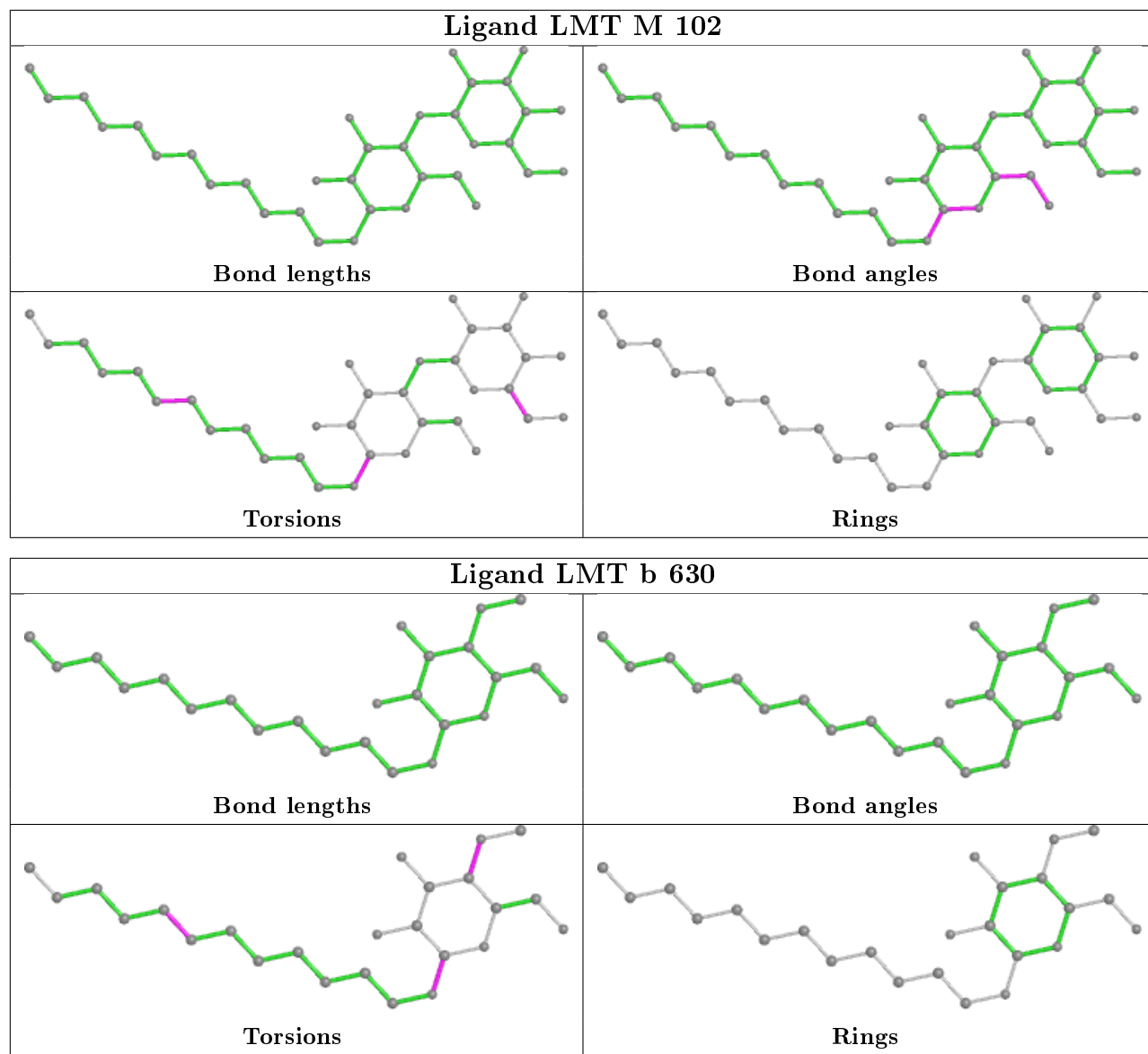


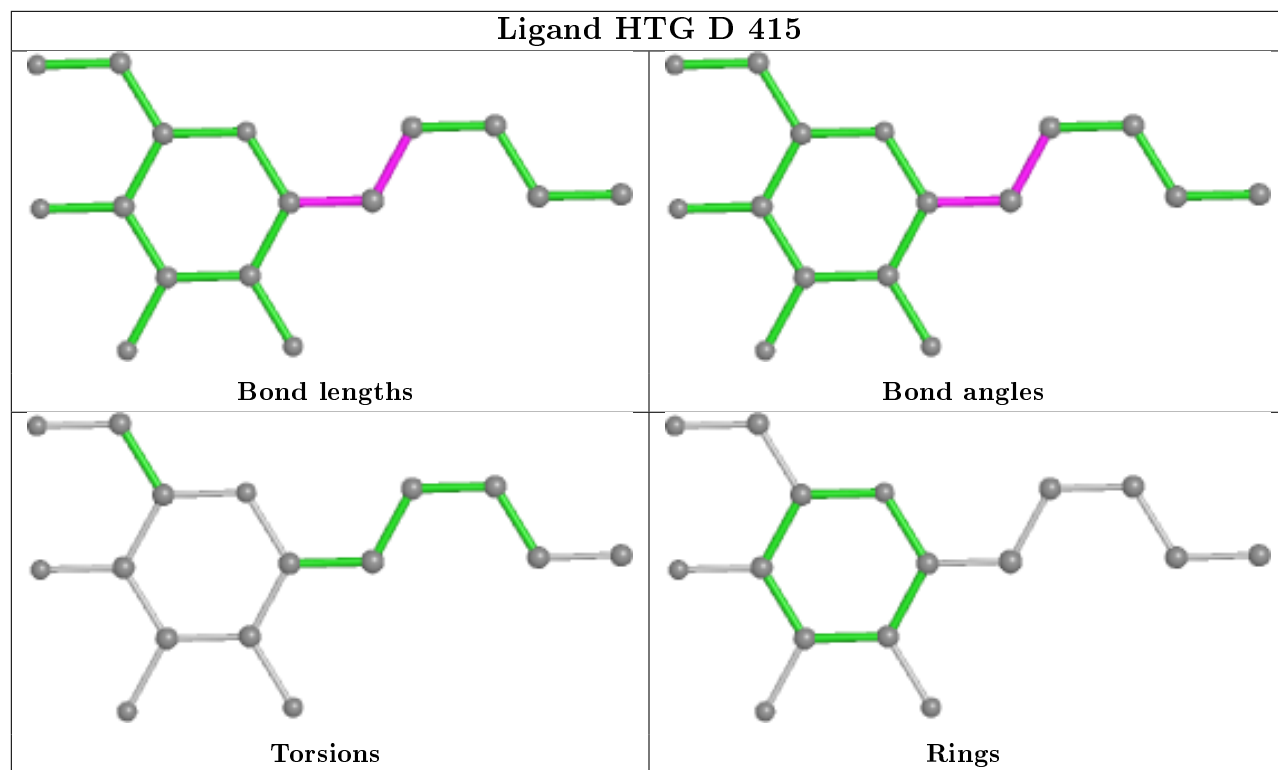
## Ligand HTG c 523



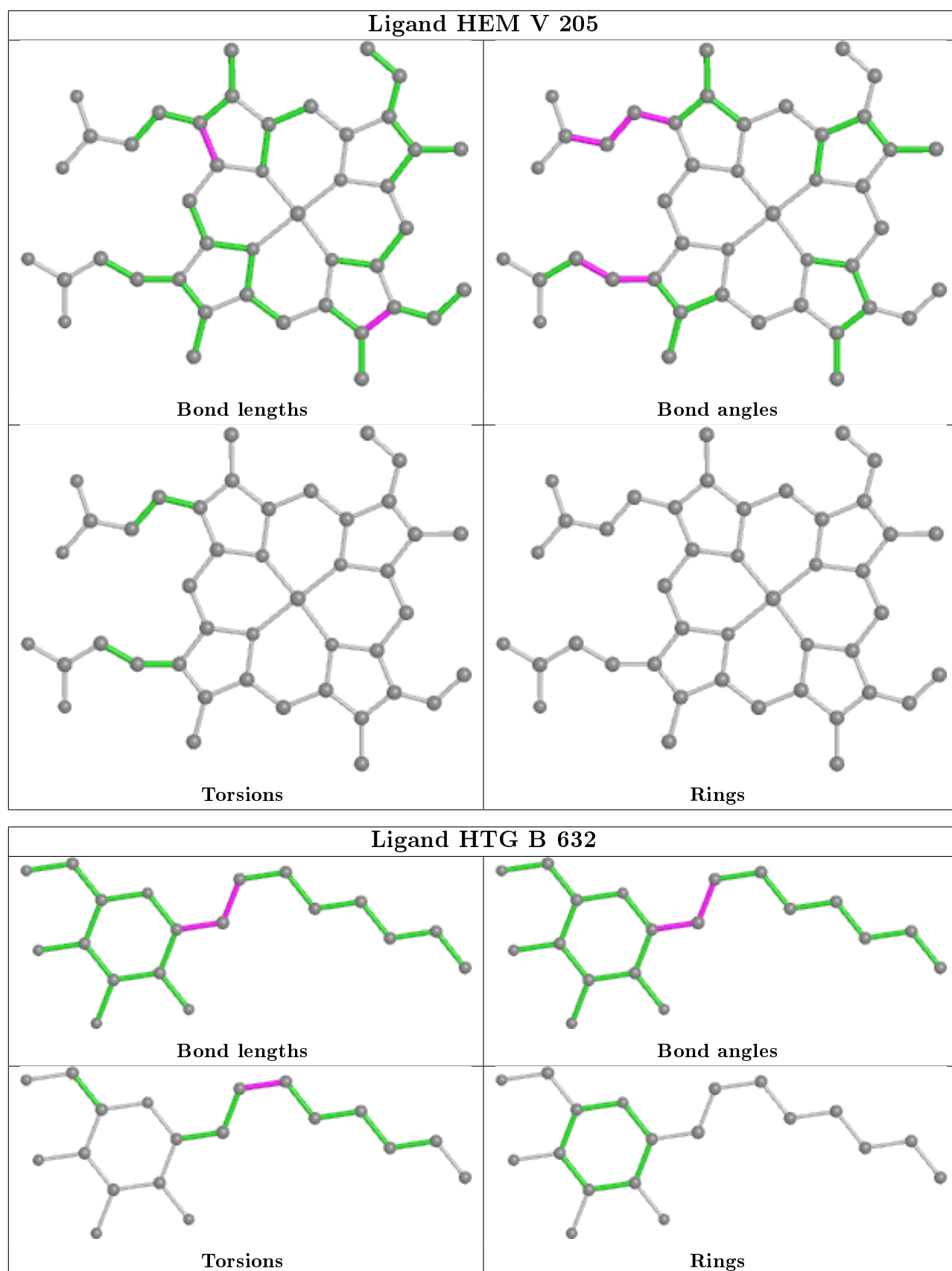
## Ligand BCR A 409

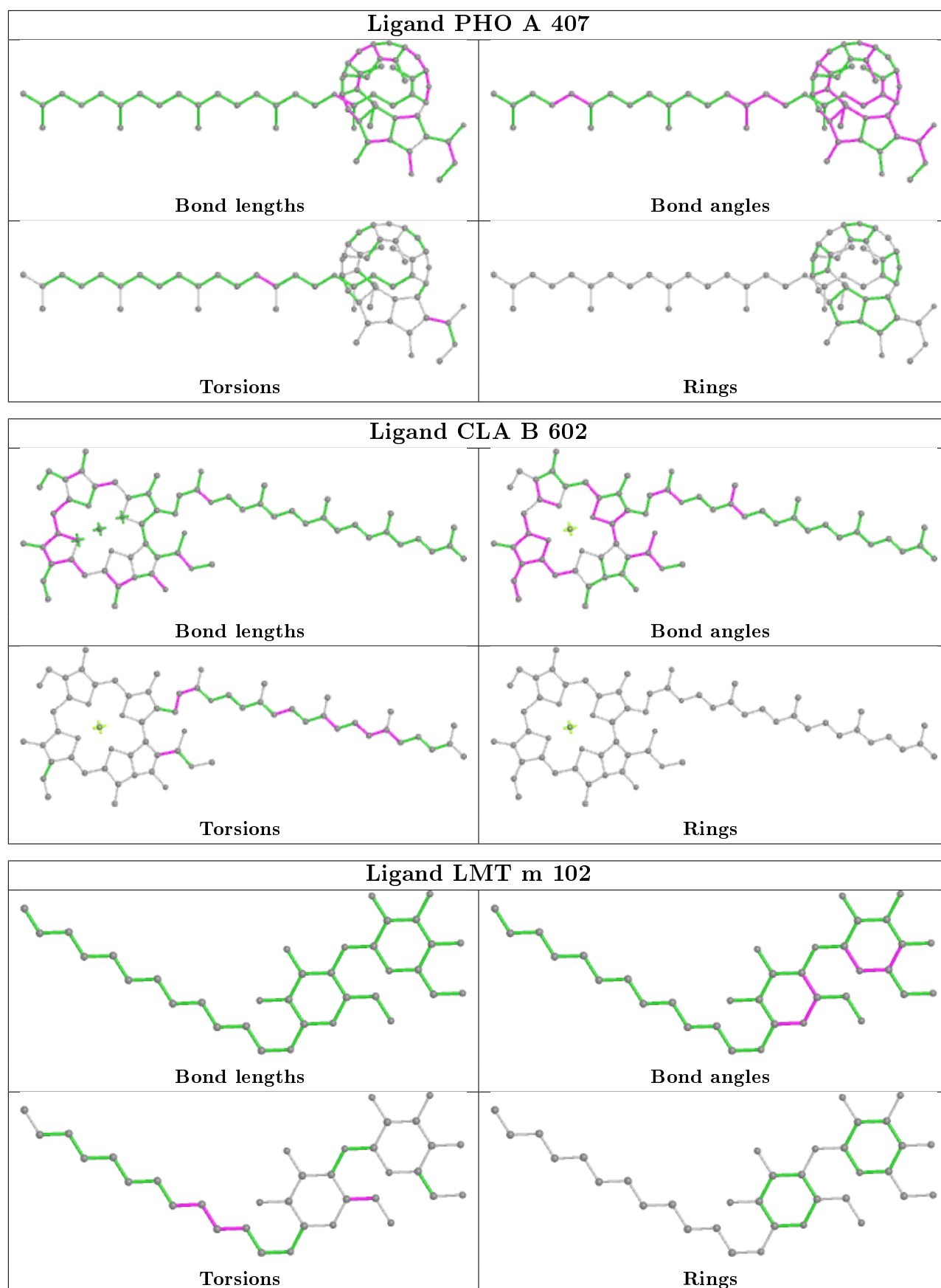




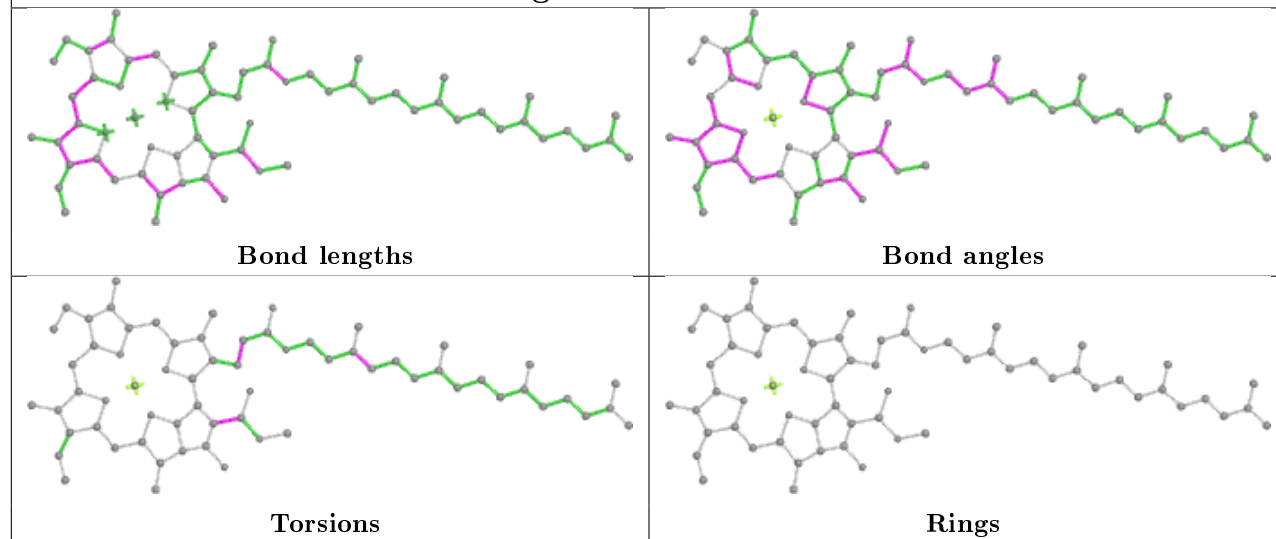




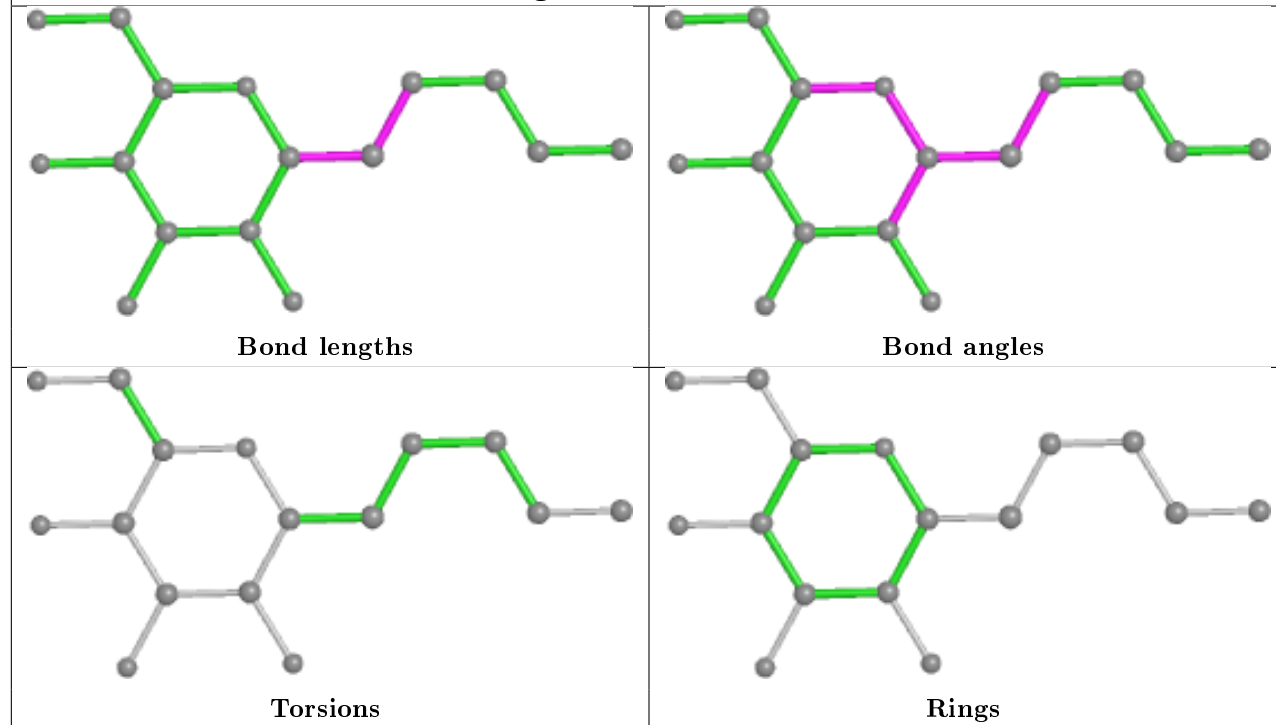




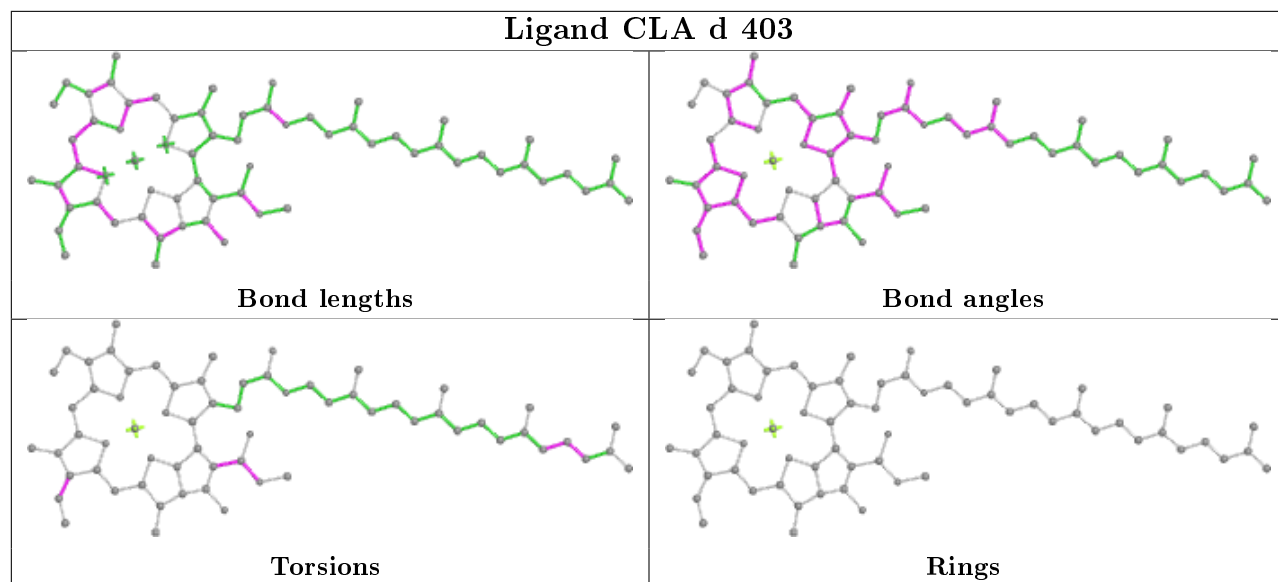
## Ligand CLA C 508



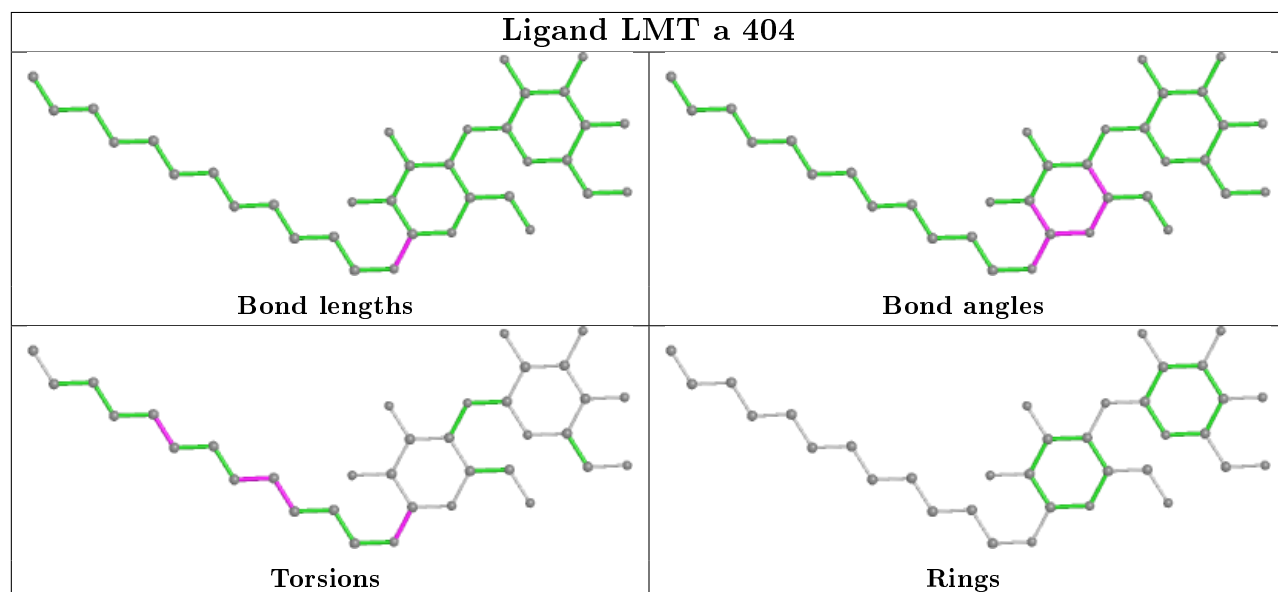
## Ligand HTG d 414



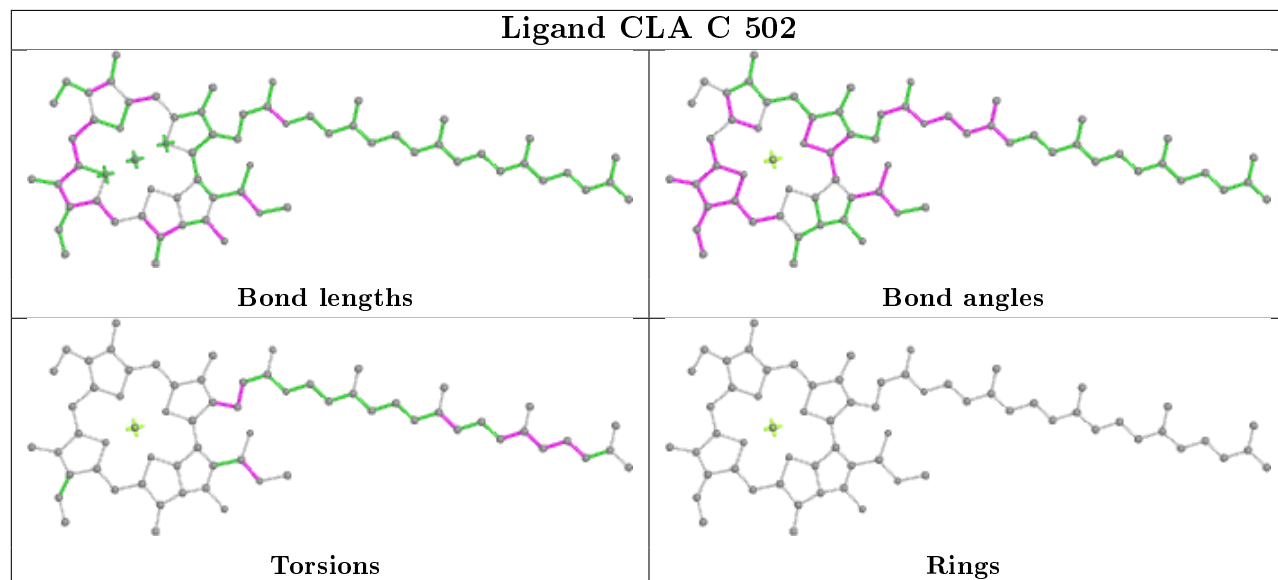
## Ligand CLA d 403

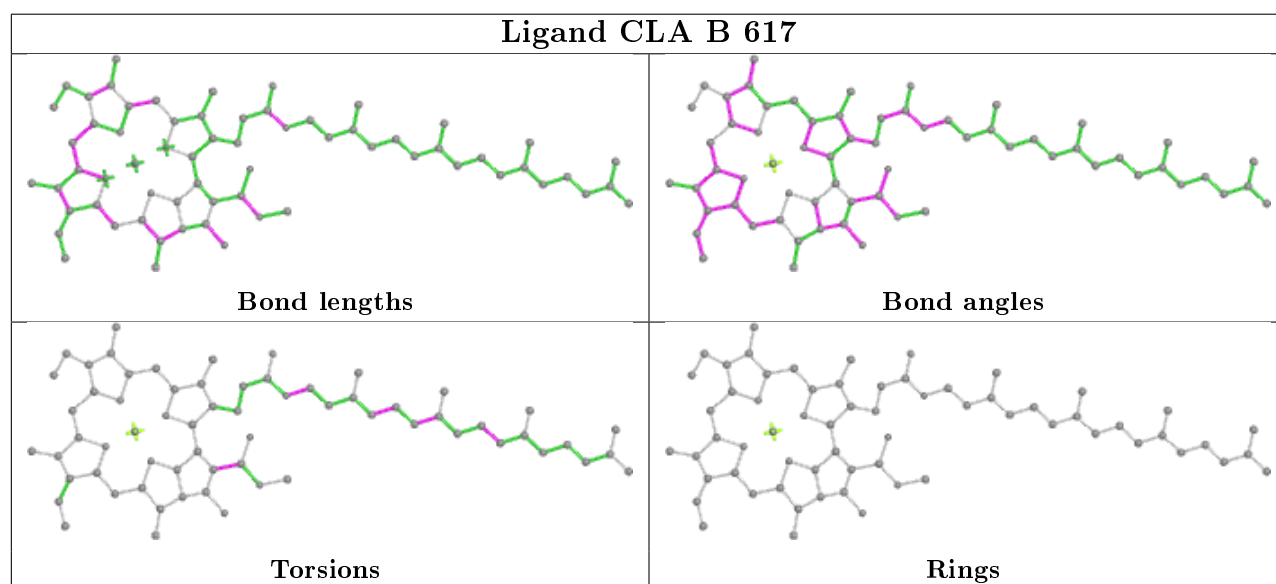
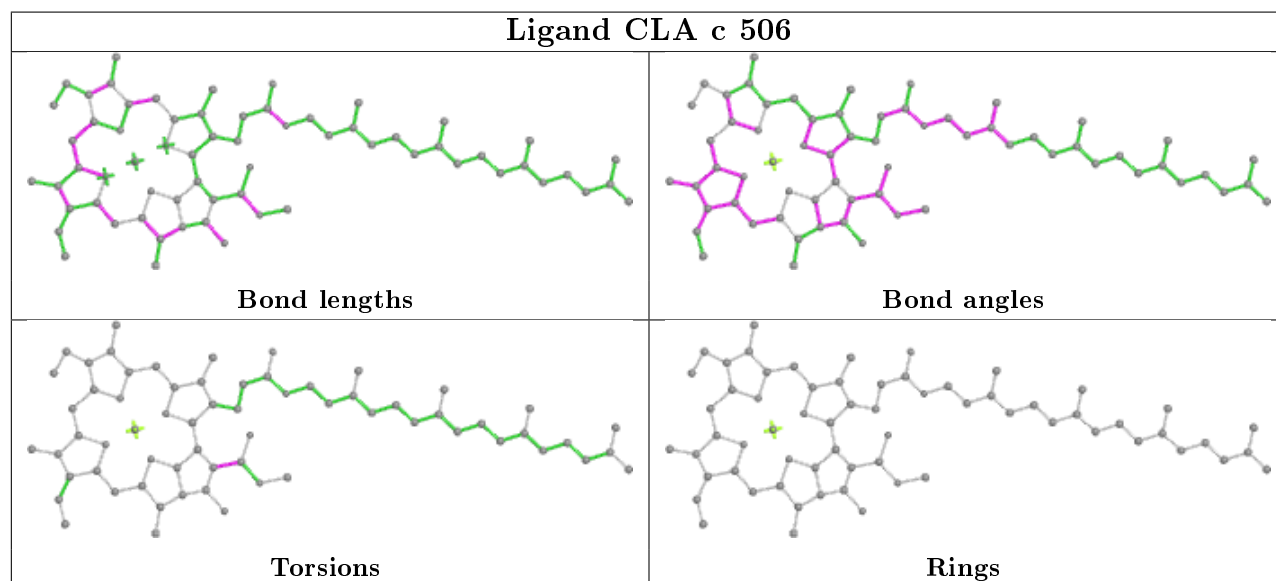
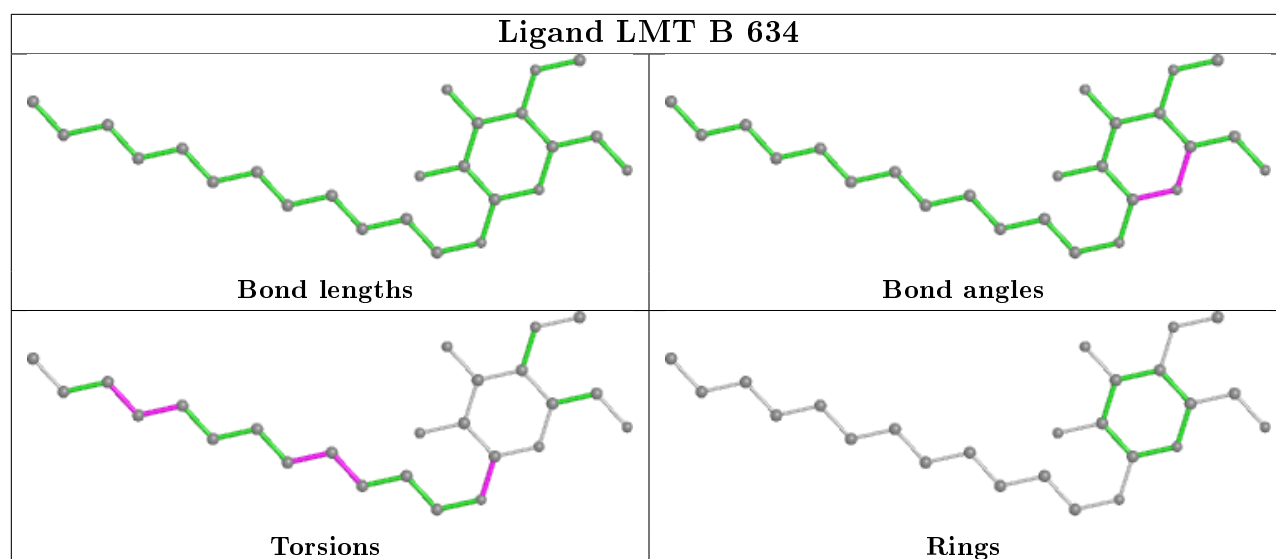


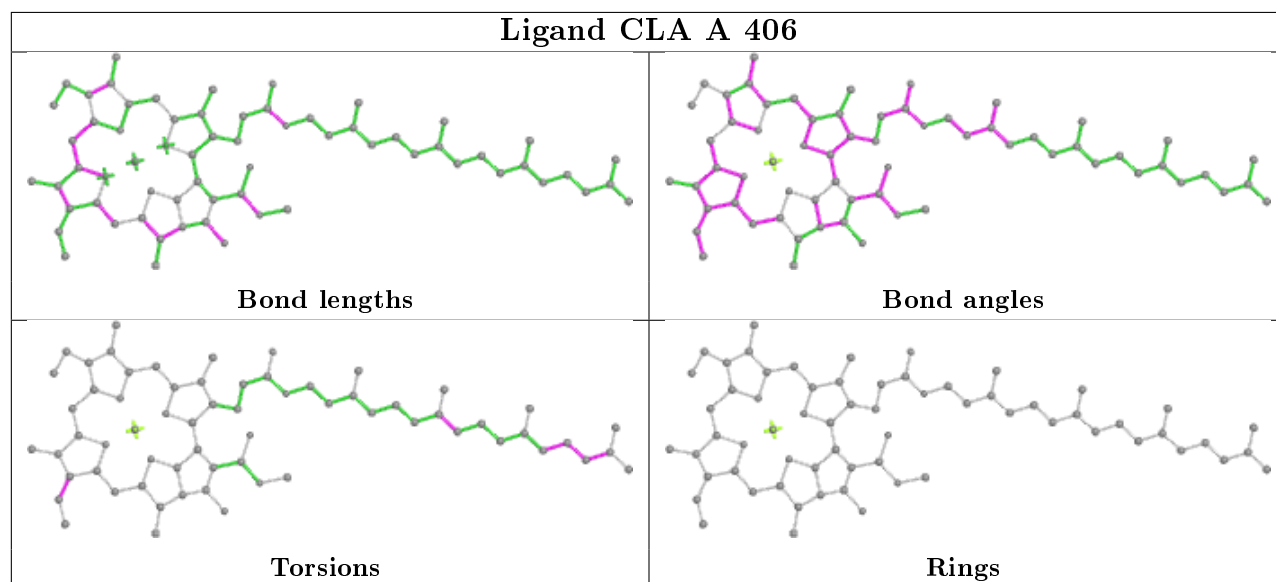
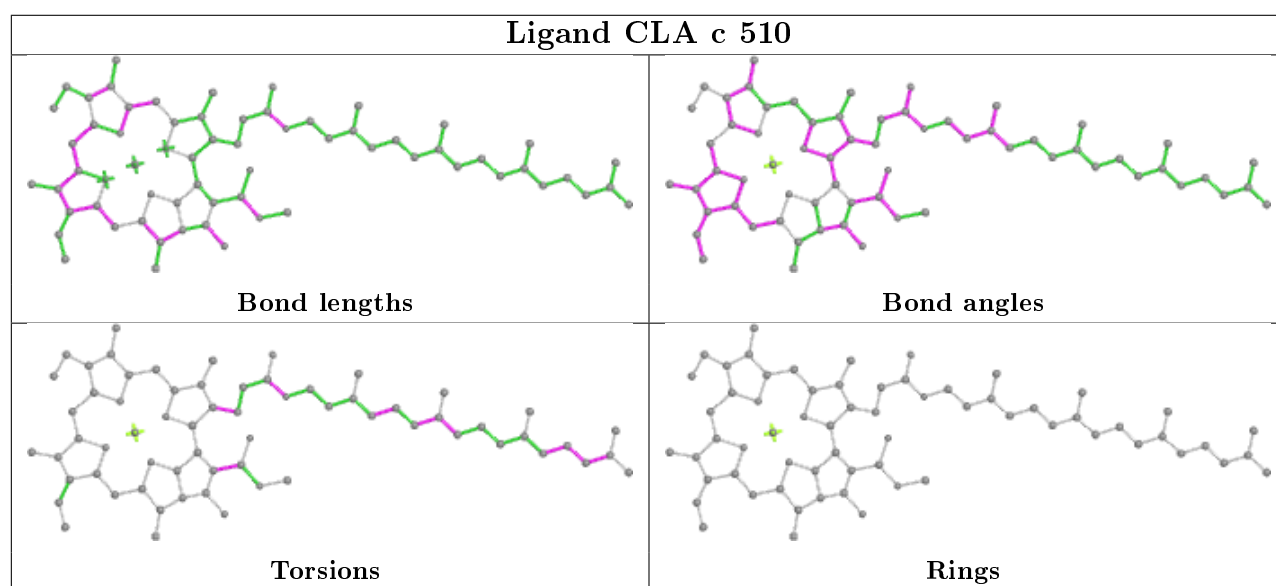
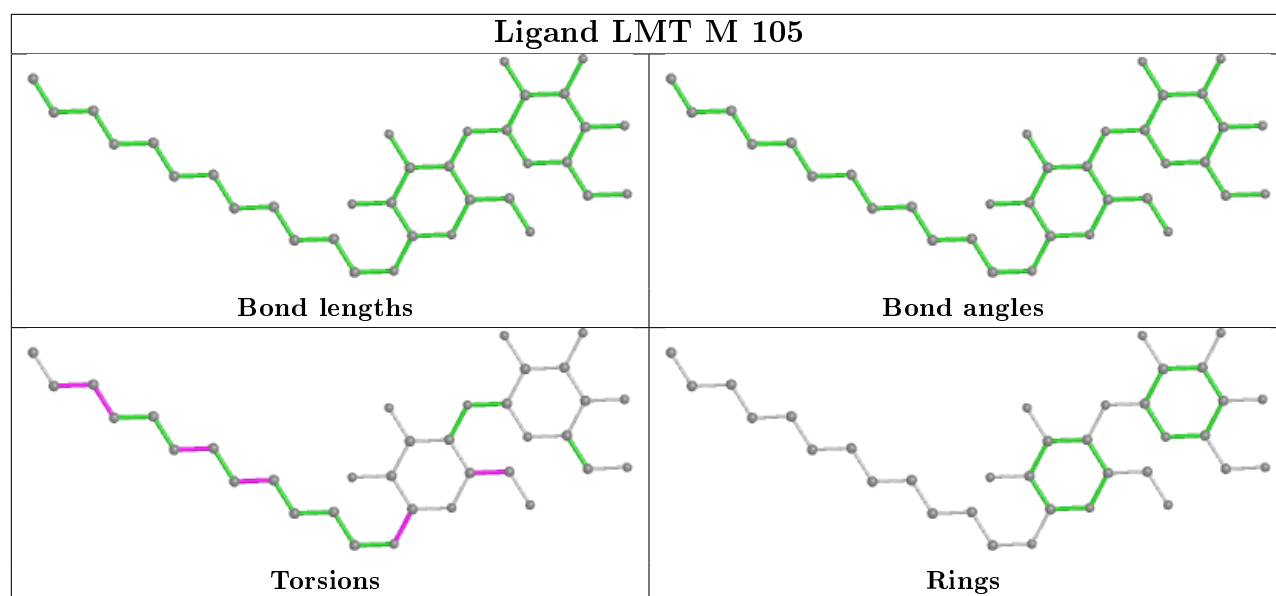
## Ligand LMT a 404

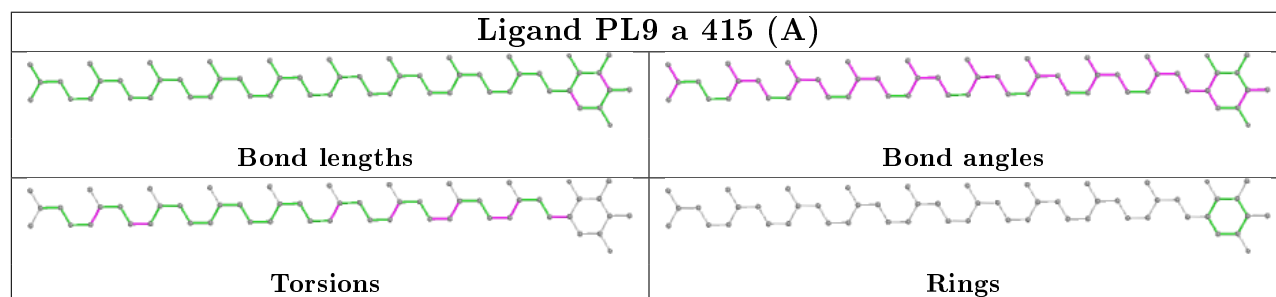
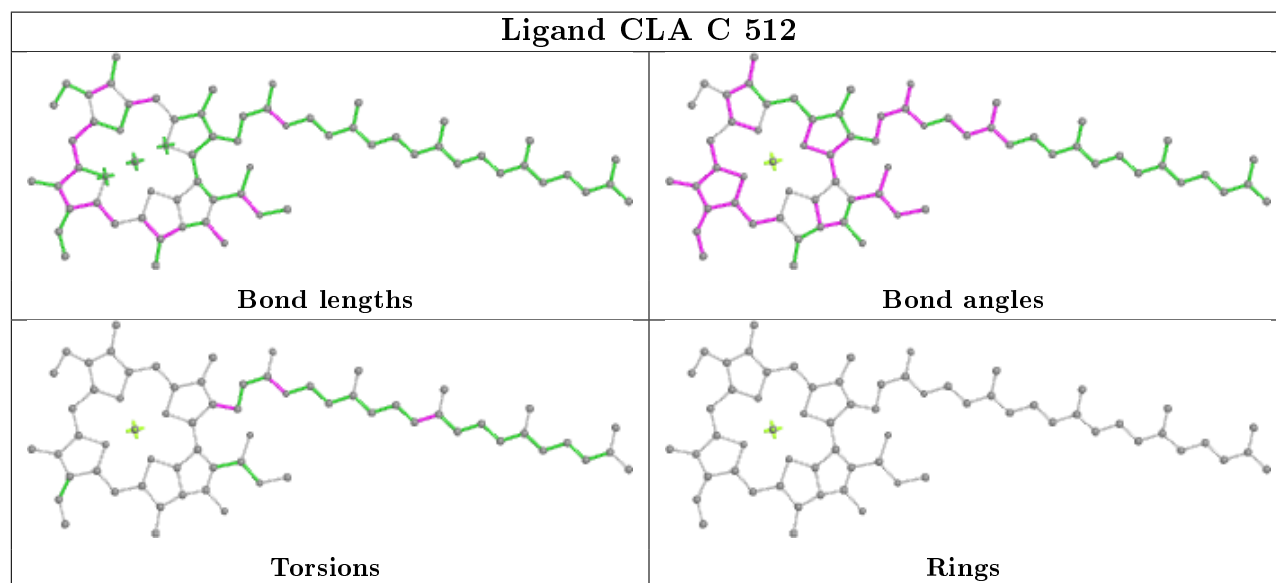
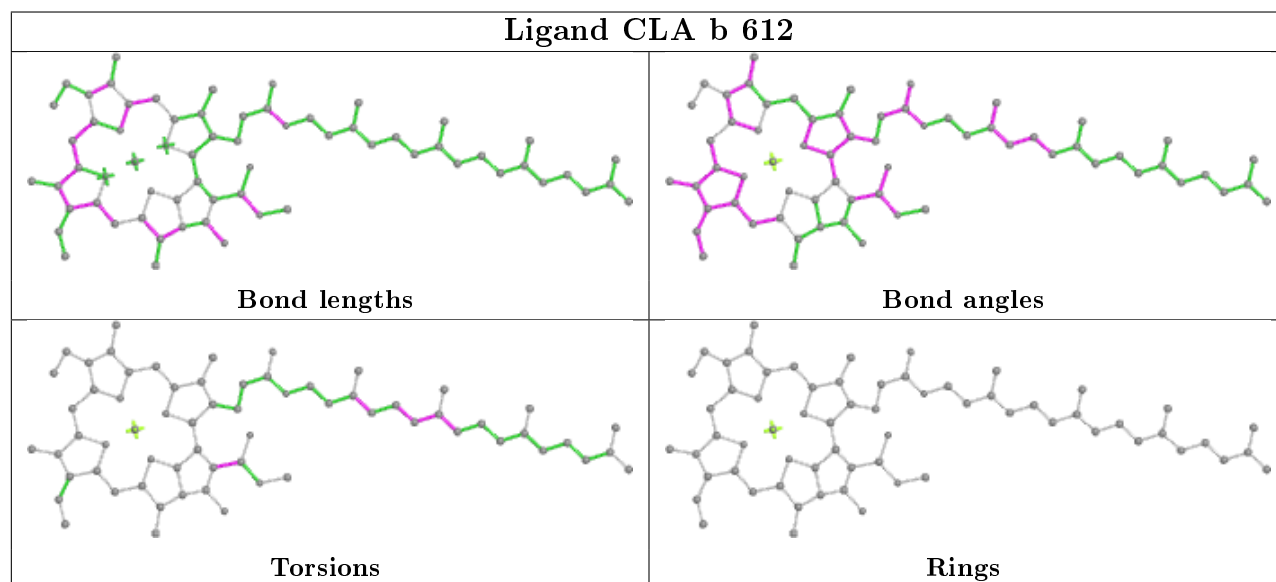
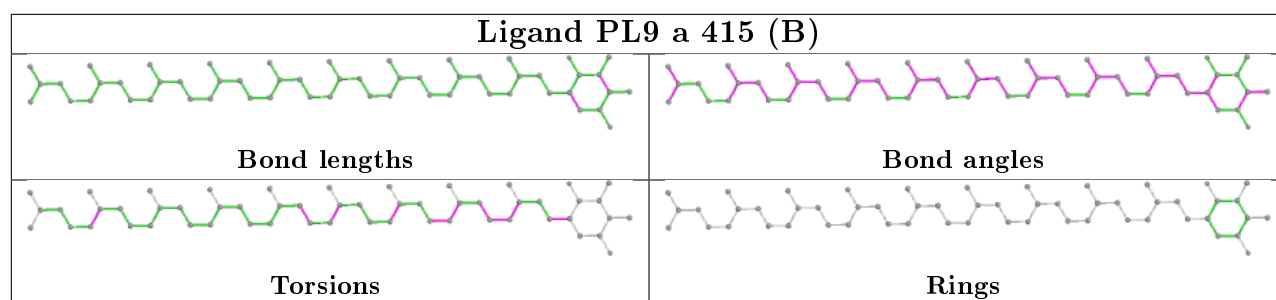


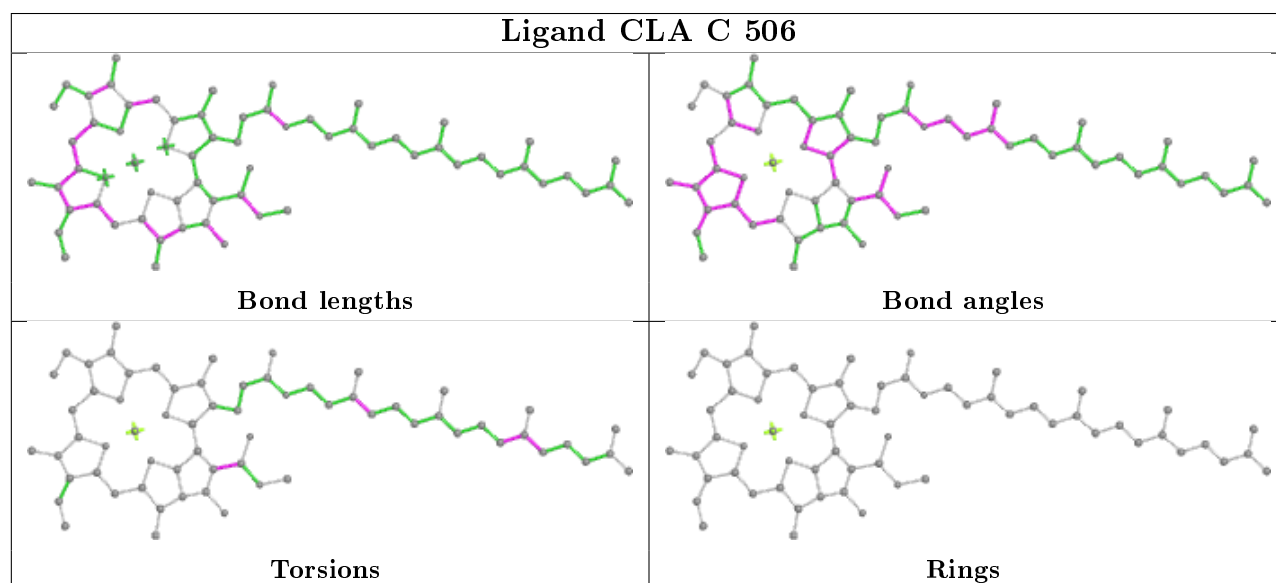
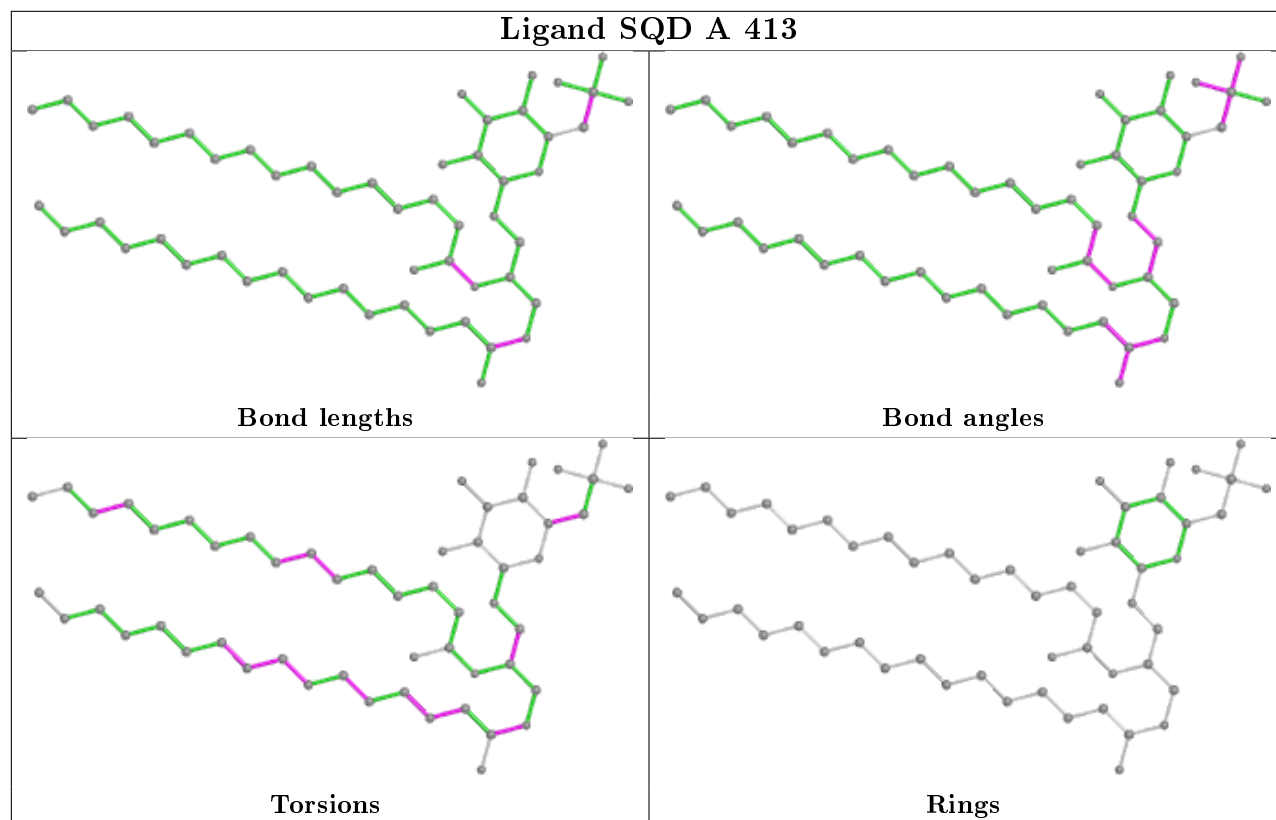
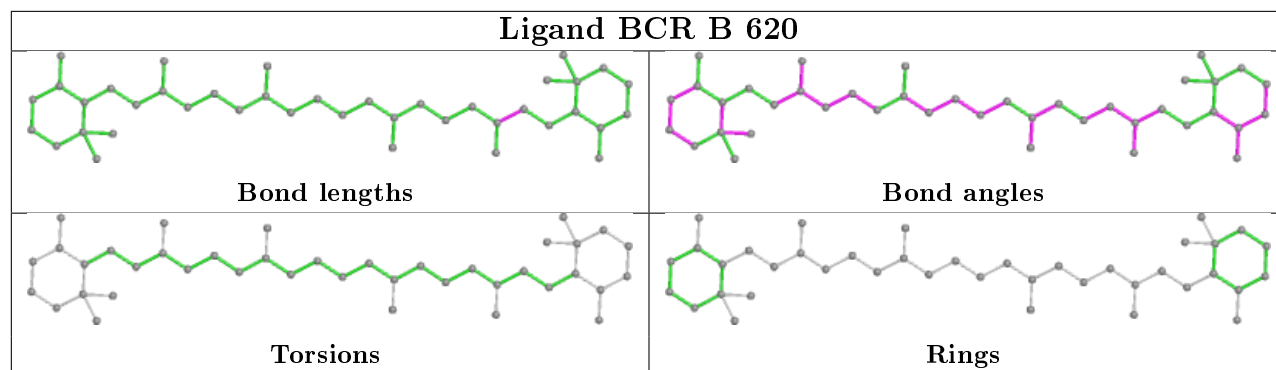
## Ligand CLA C 502



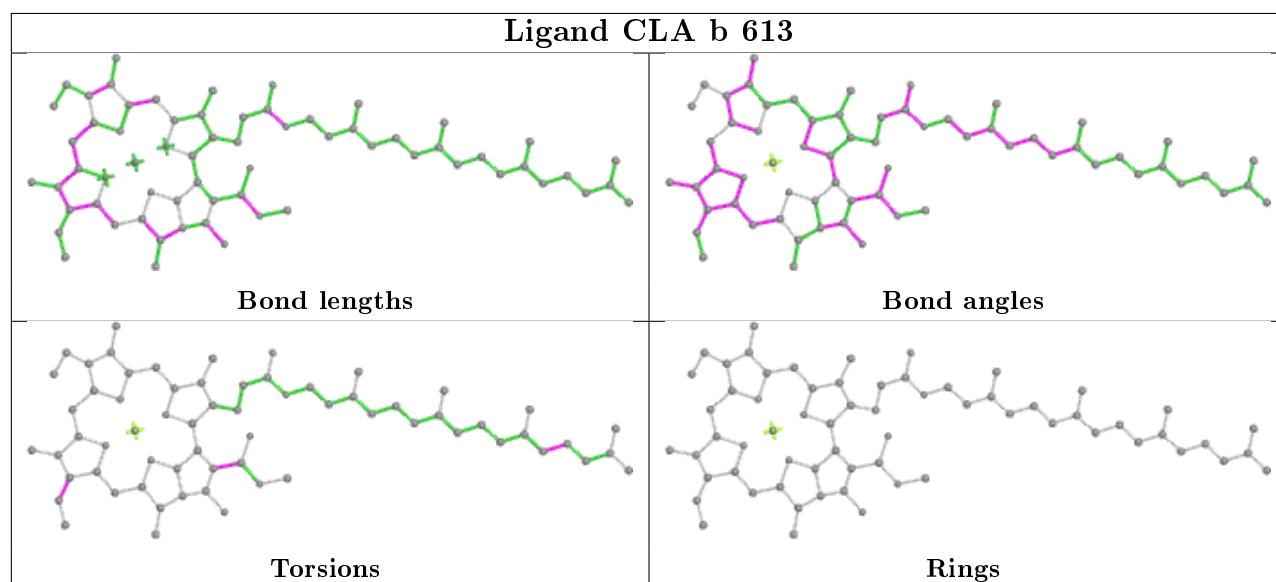
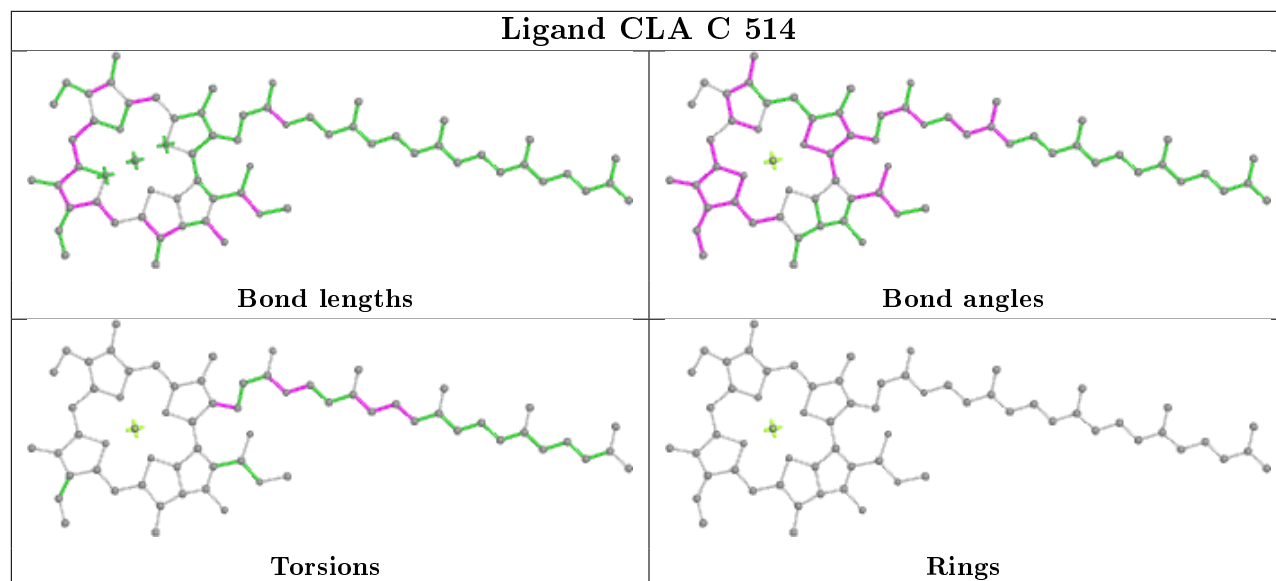
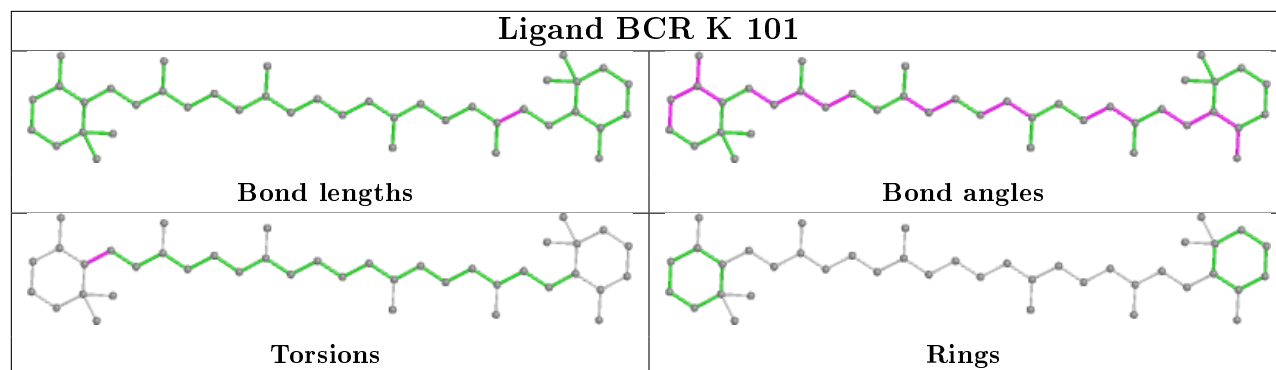


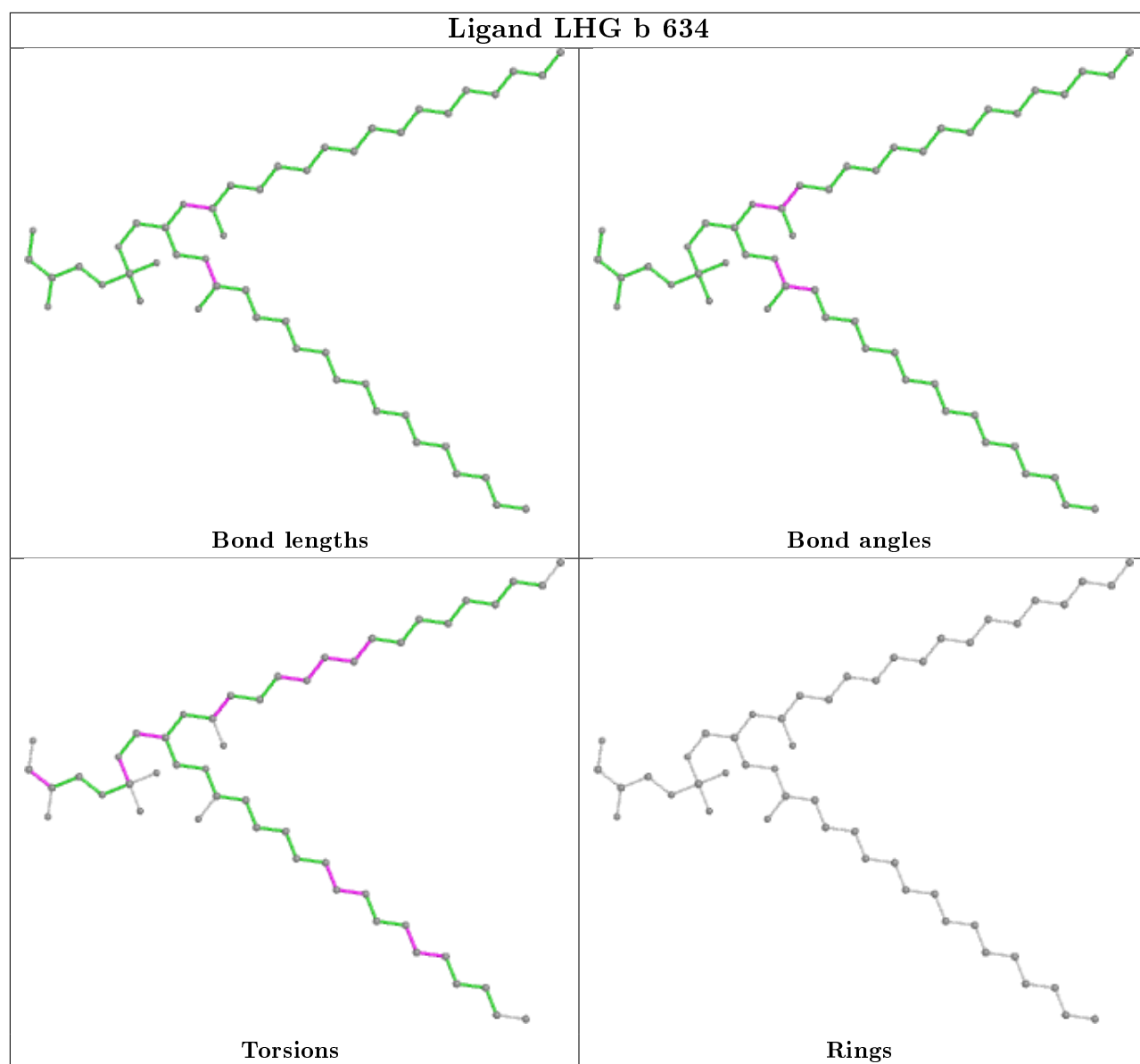


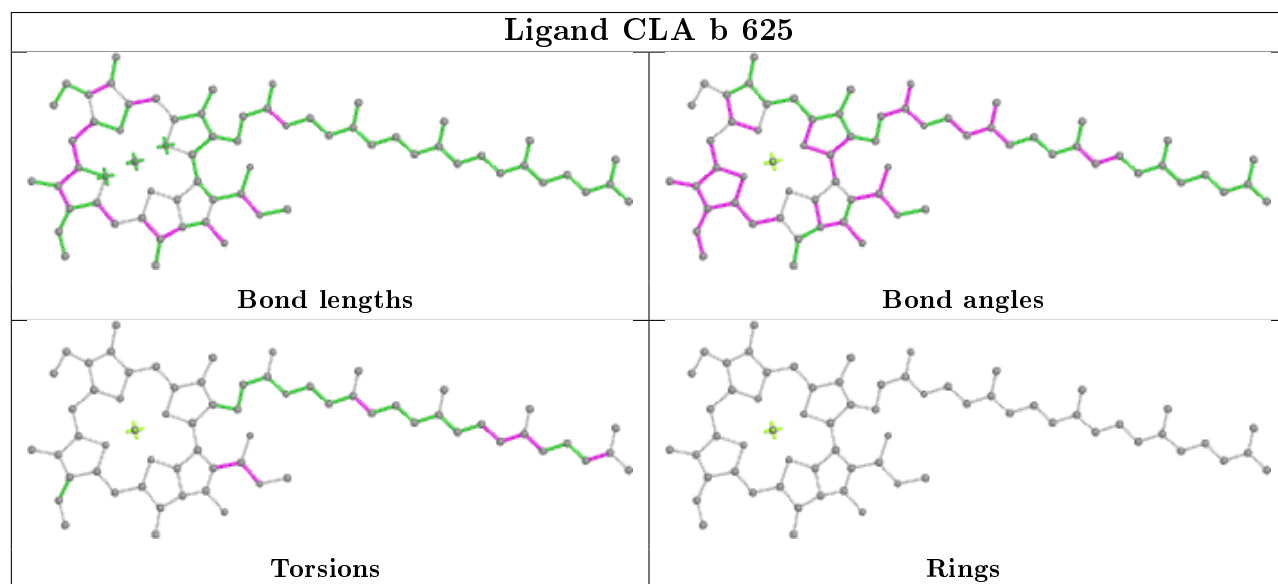
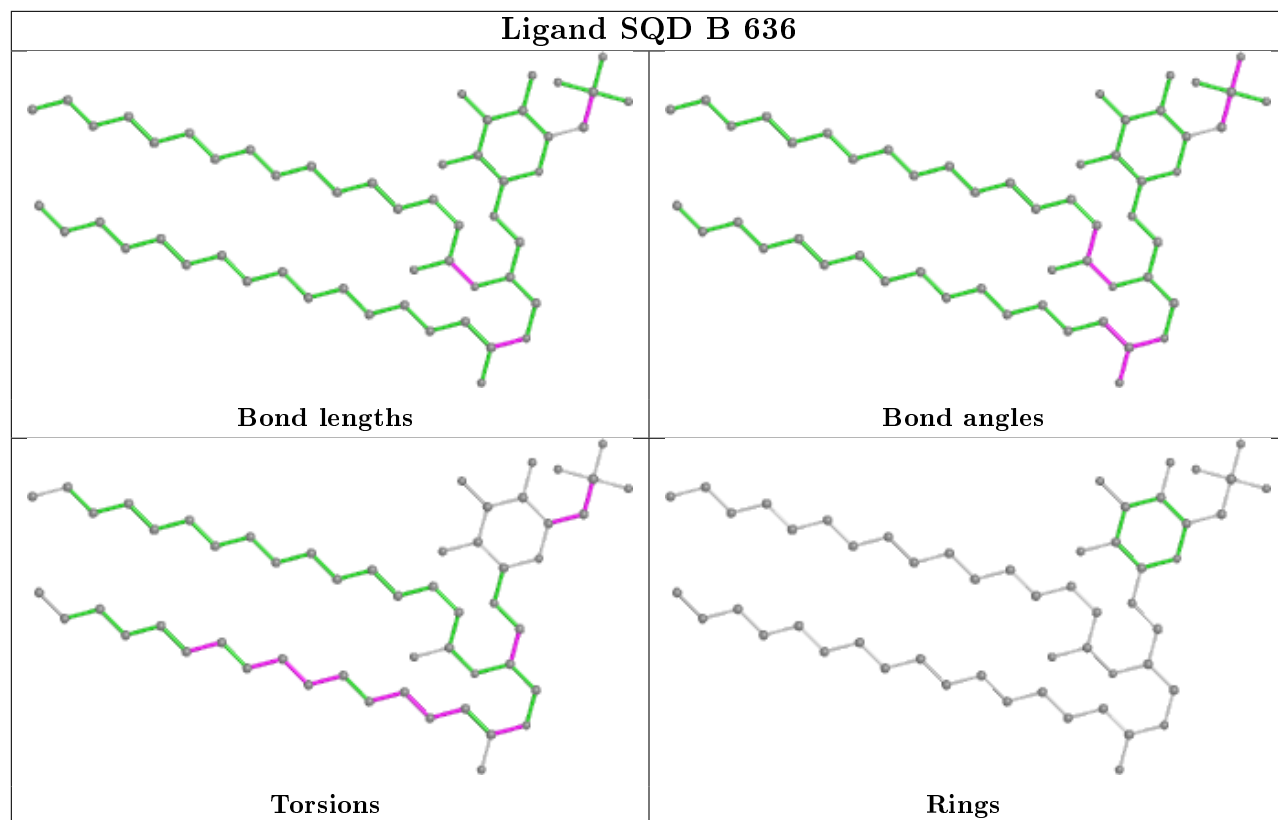


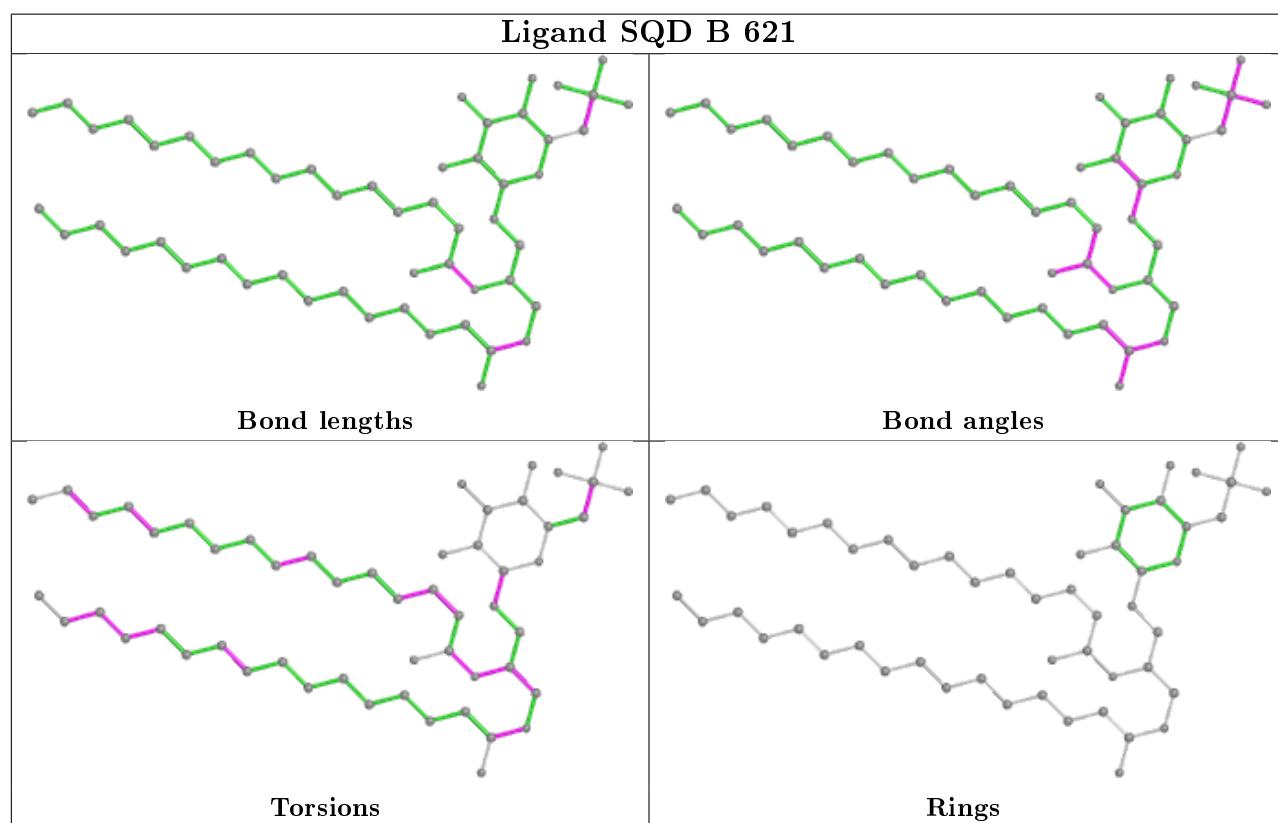
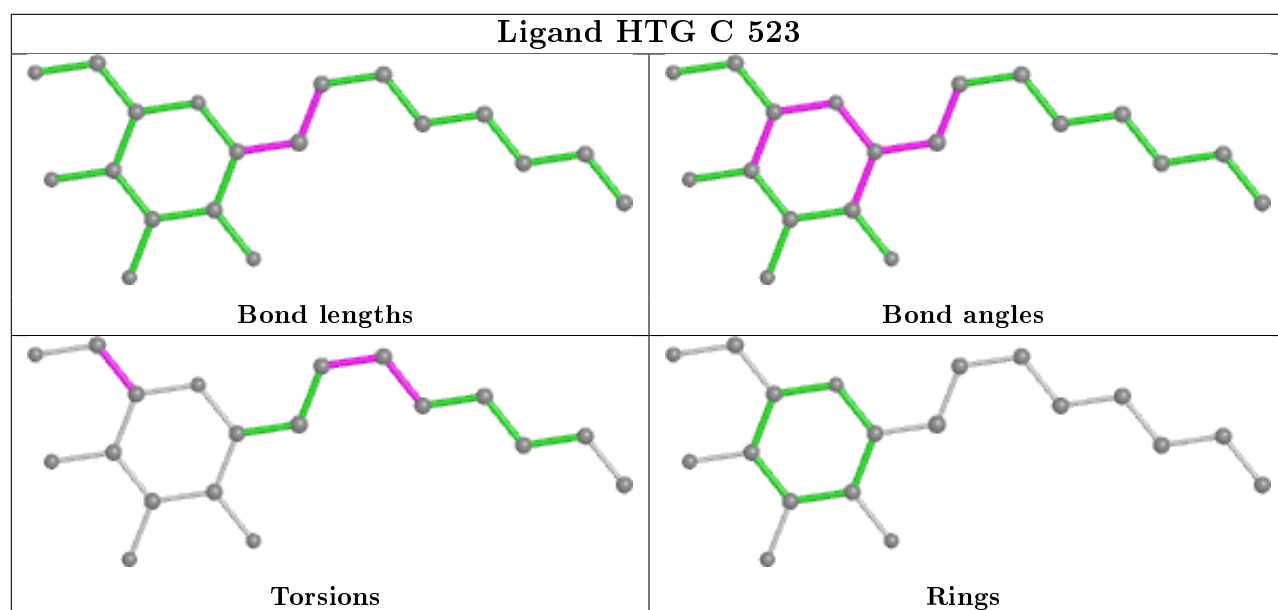


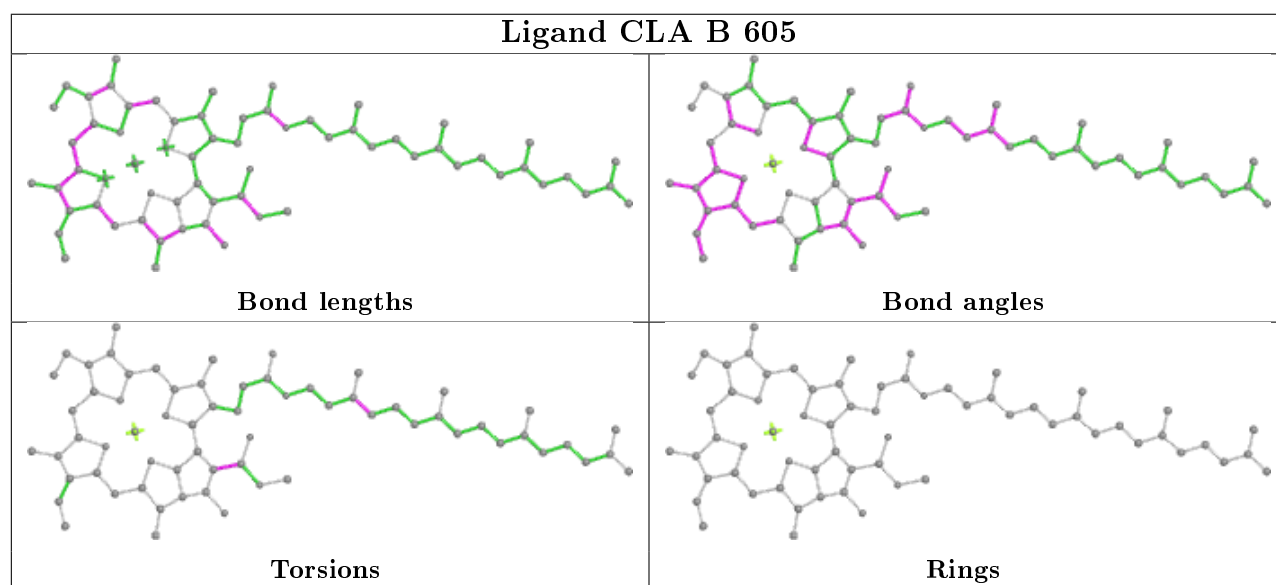
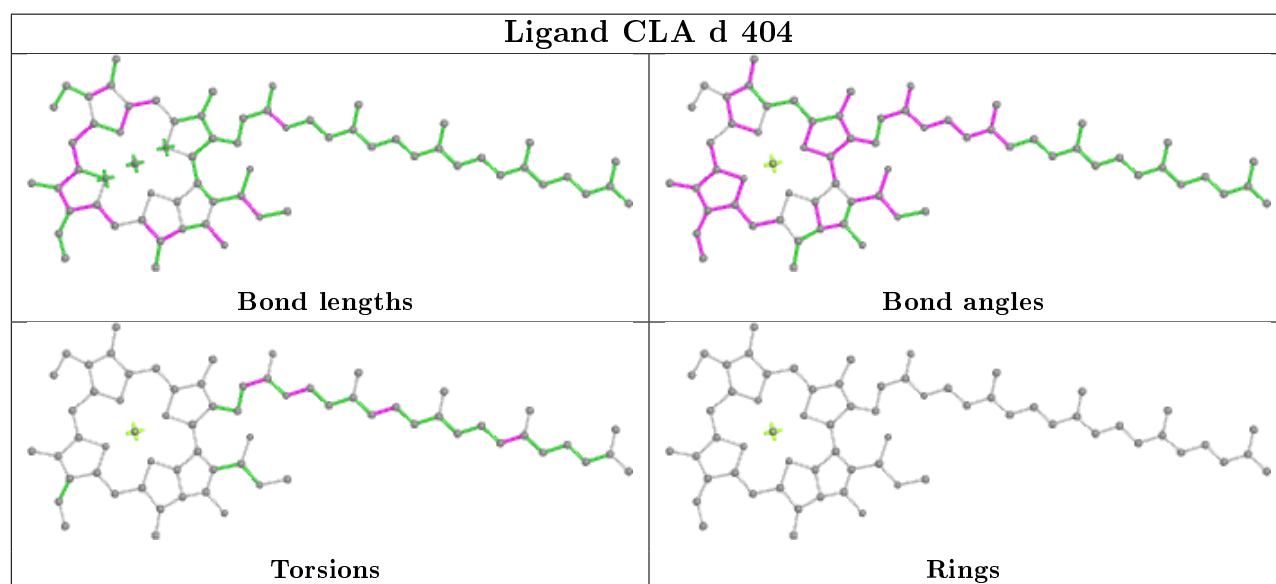
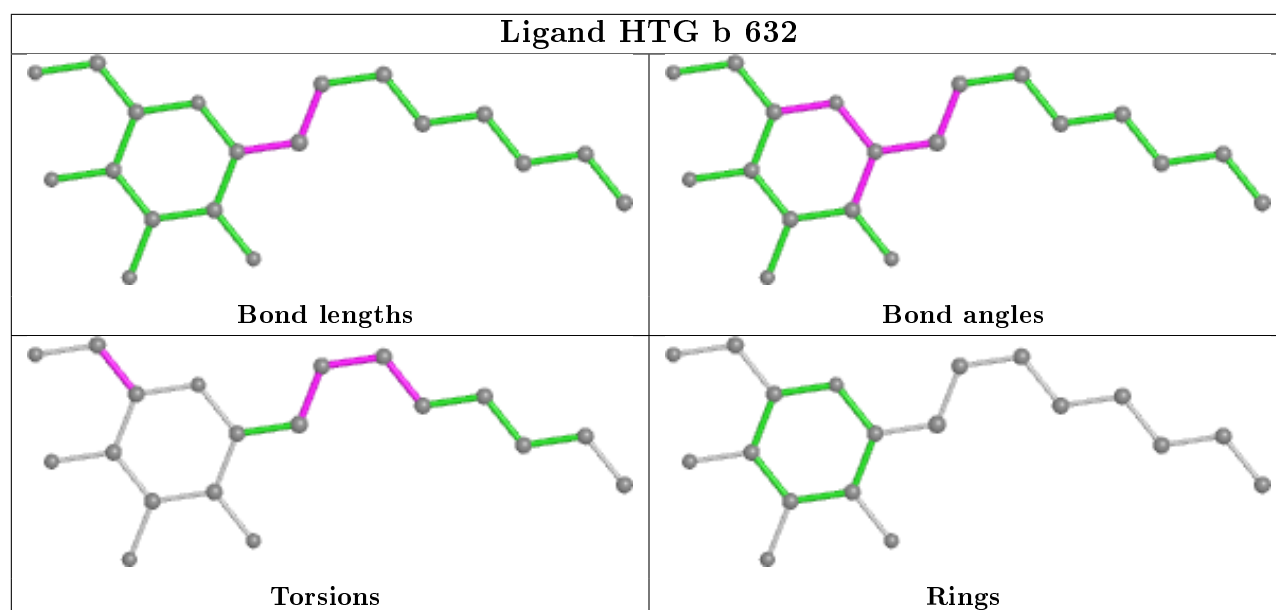


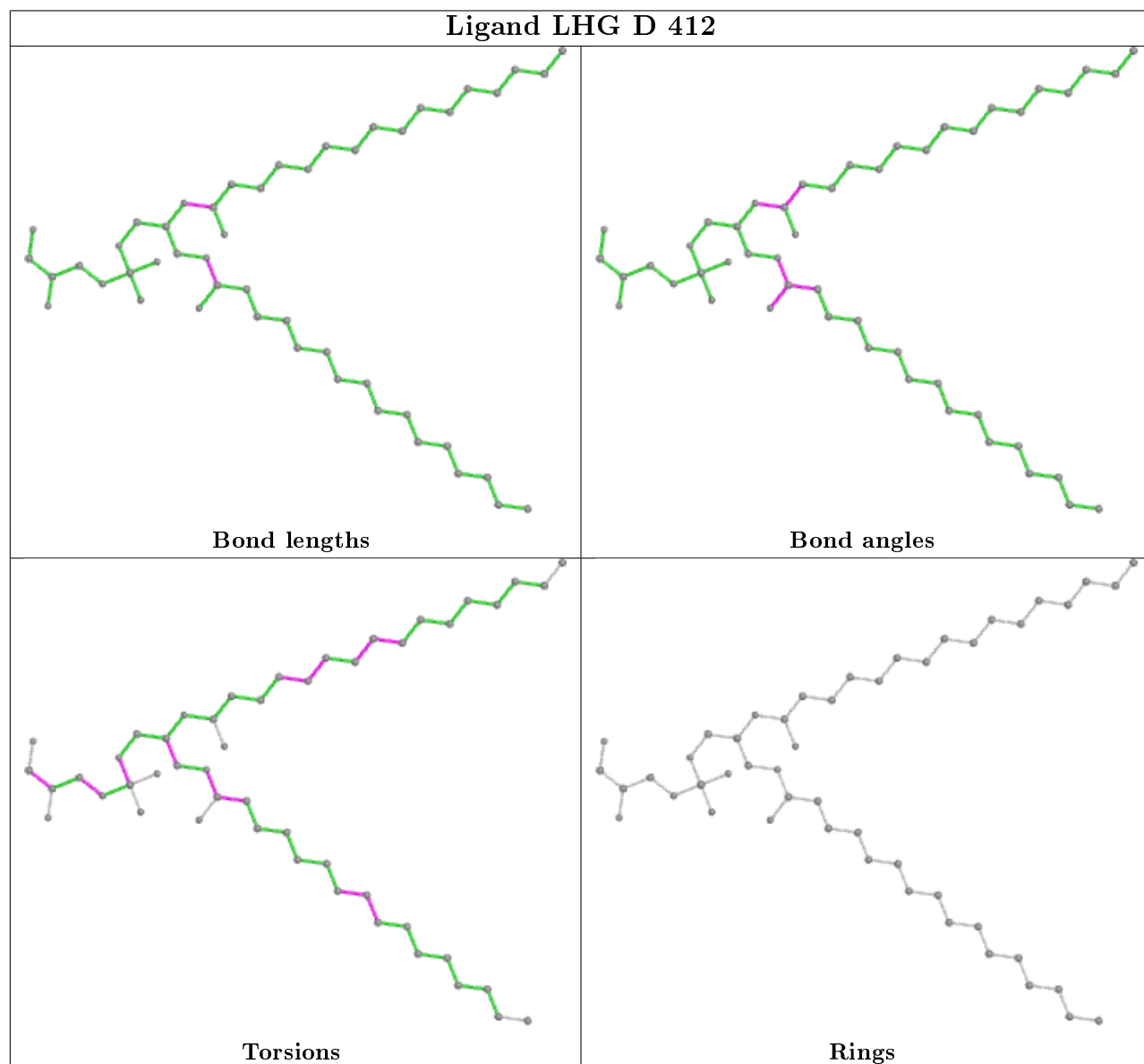
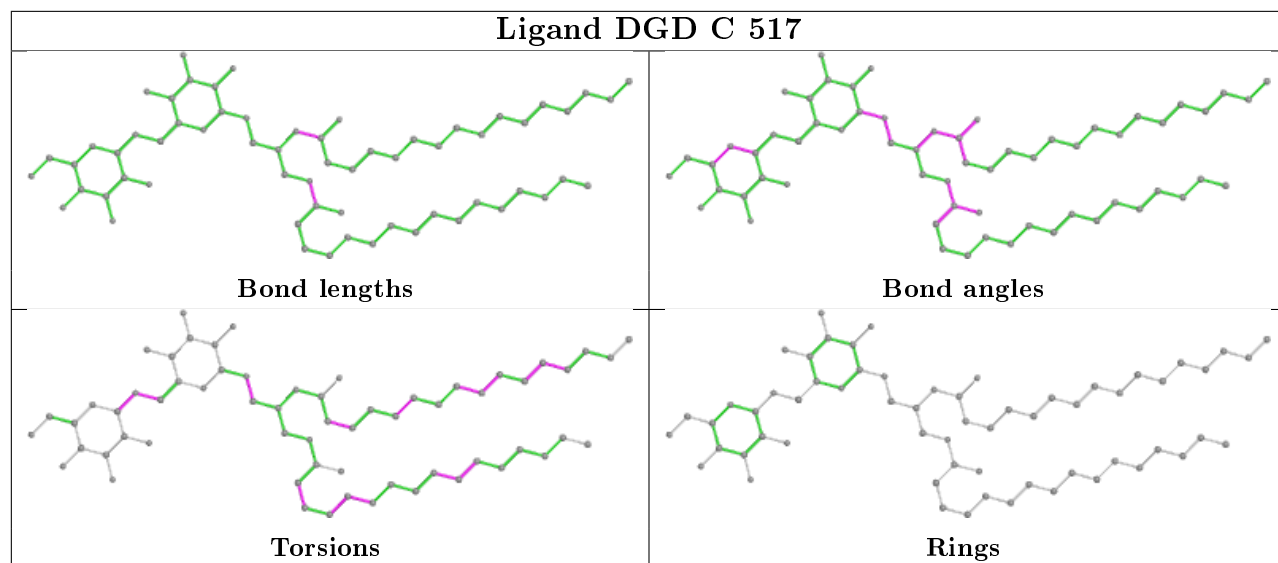


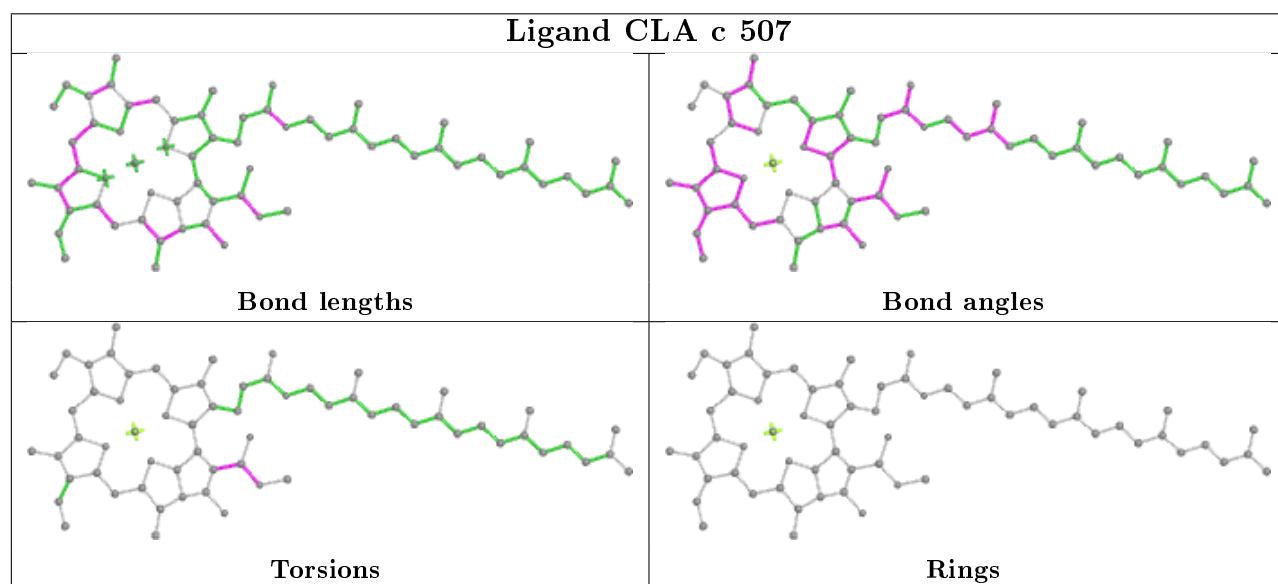
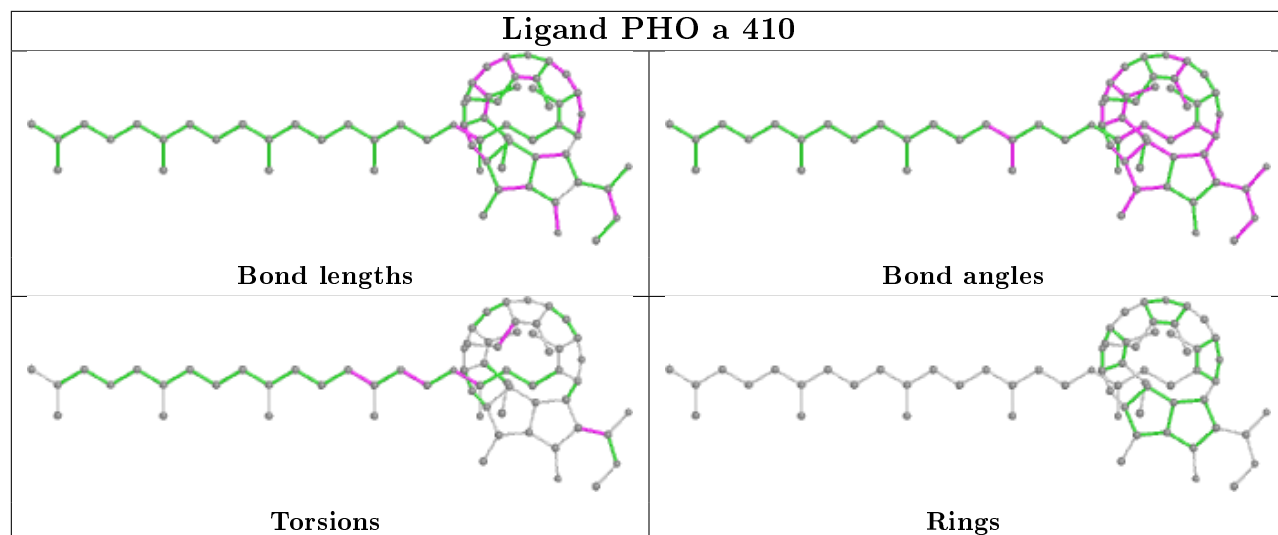


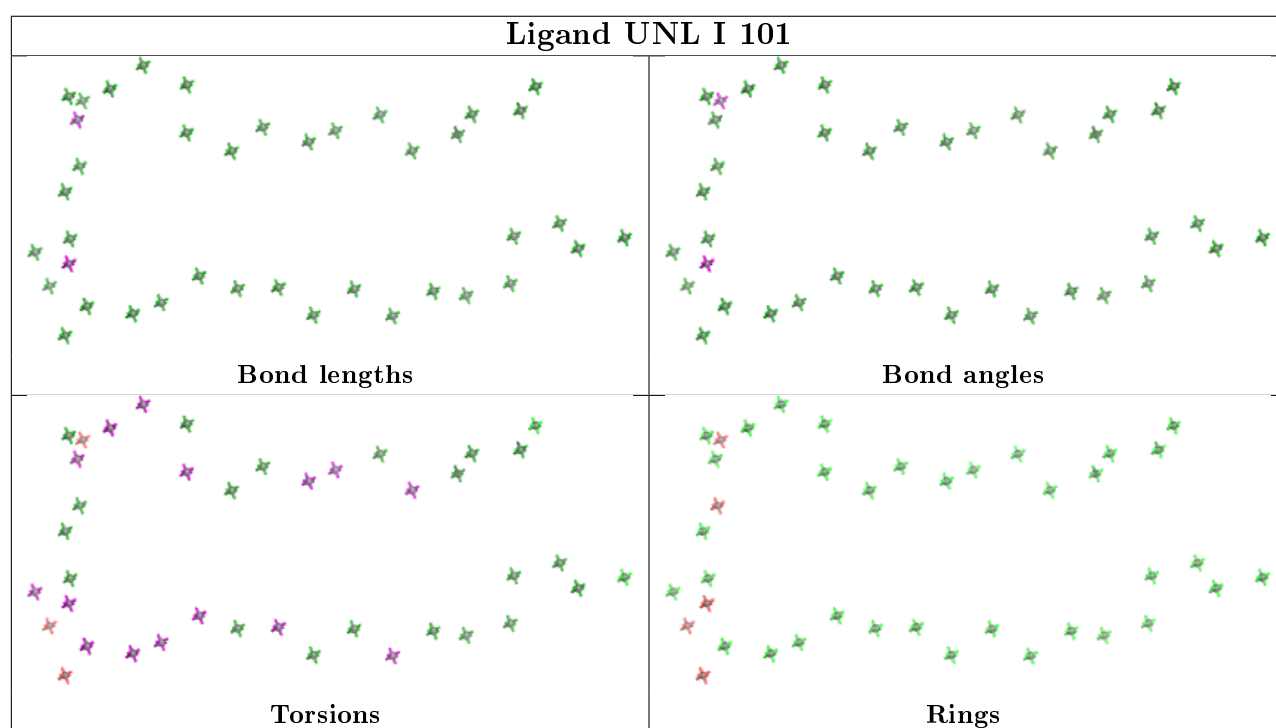
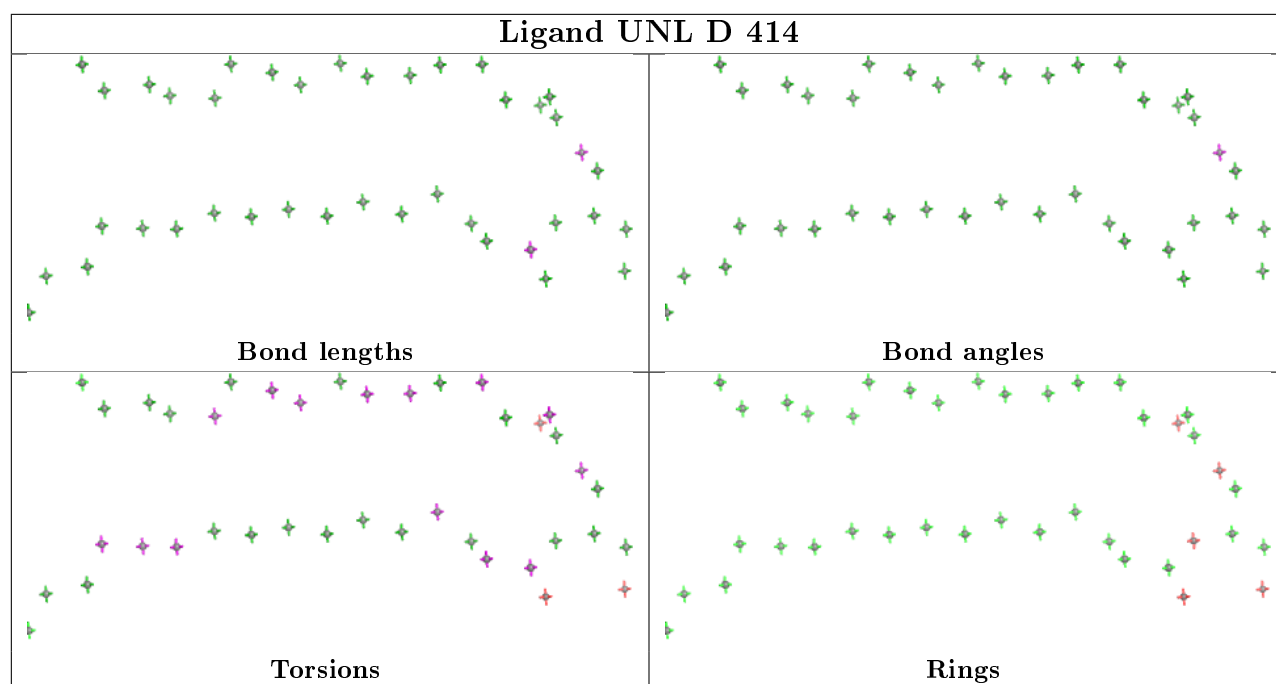




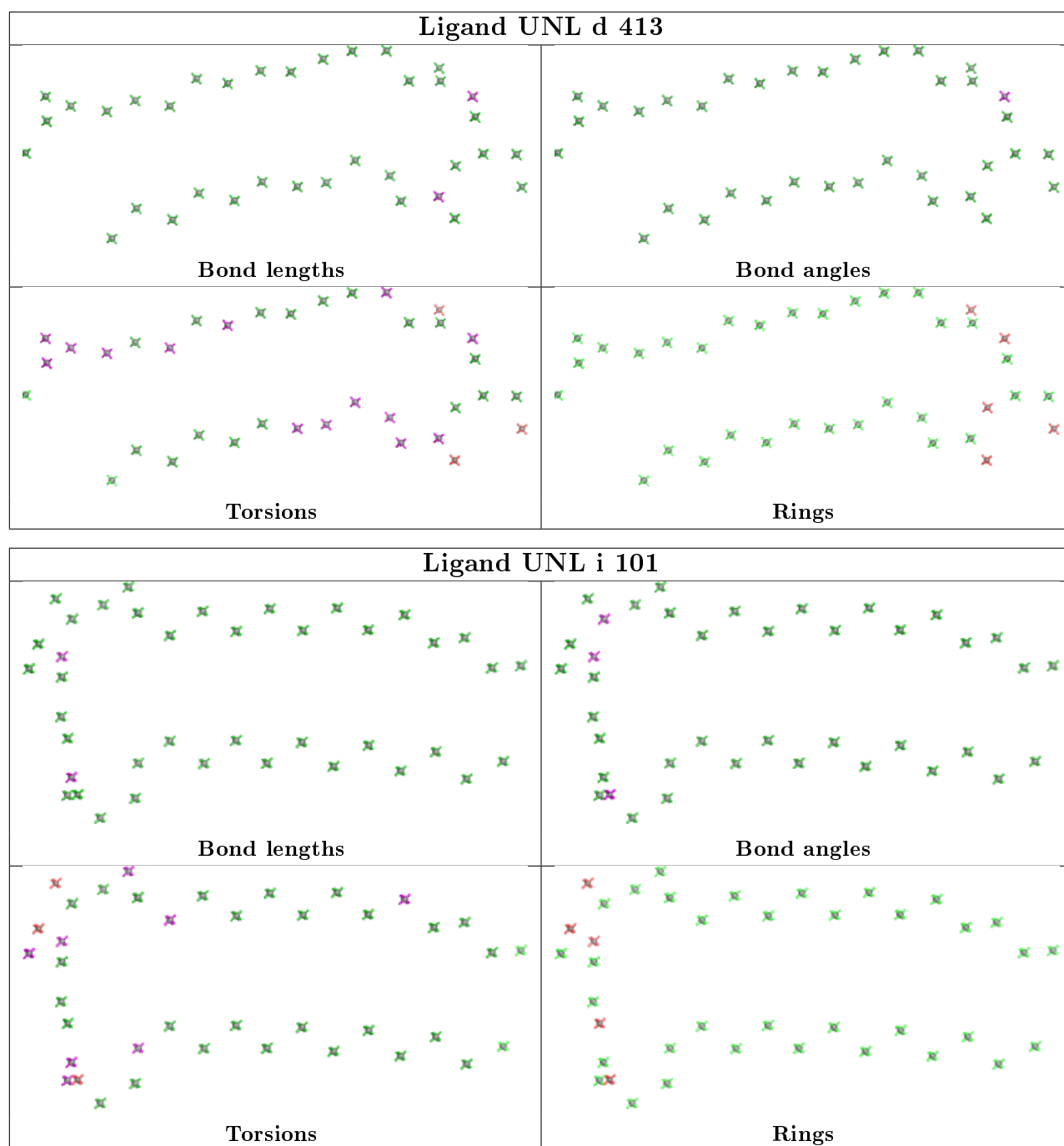


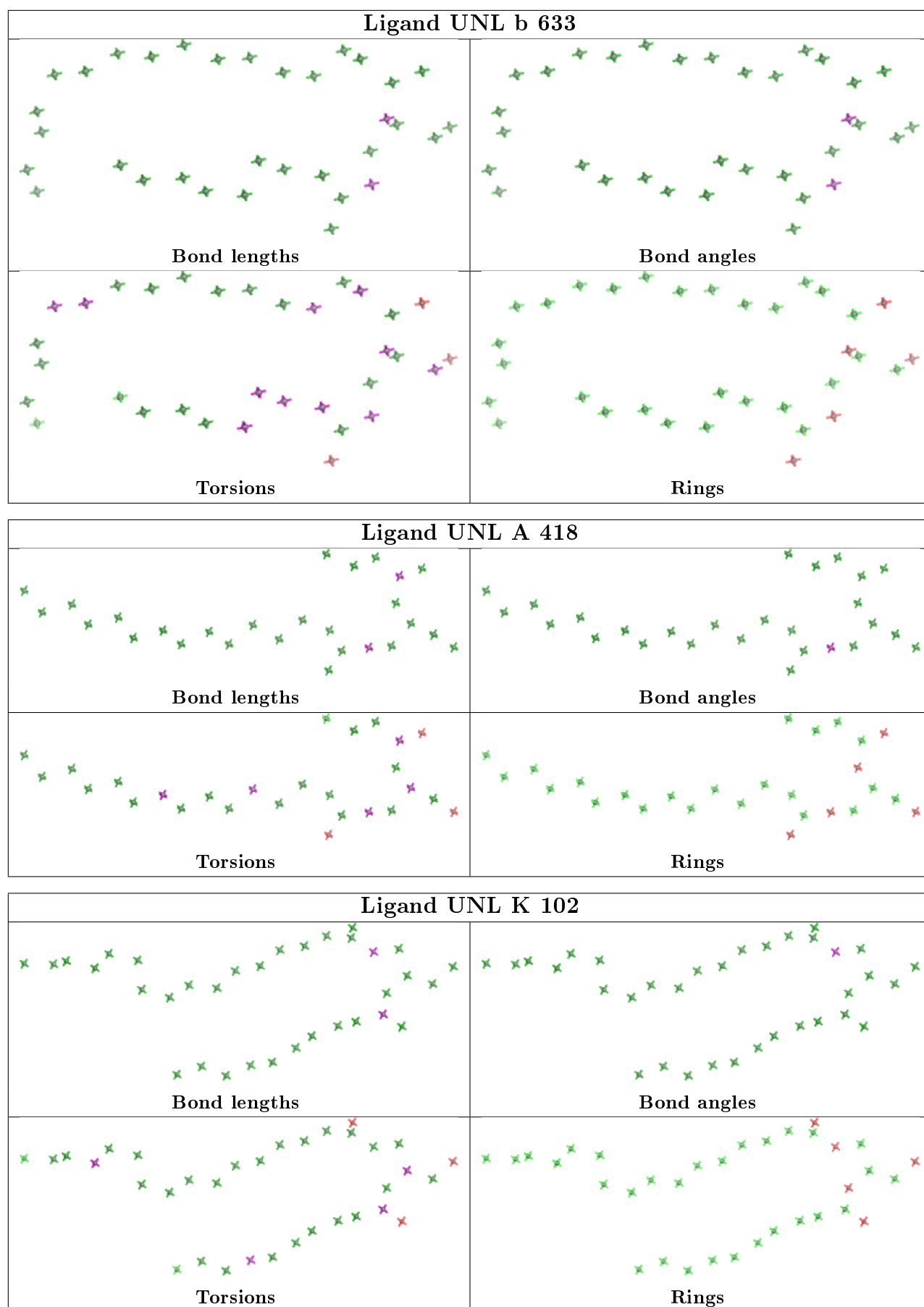


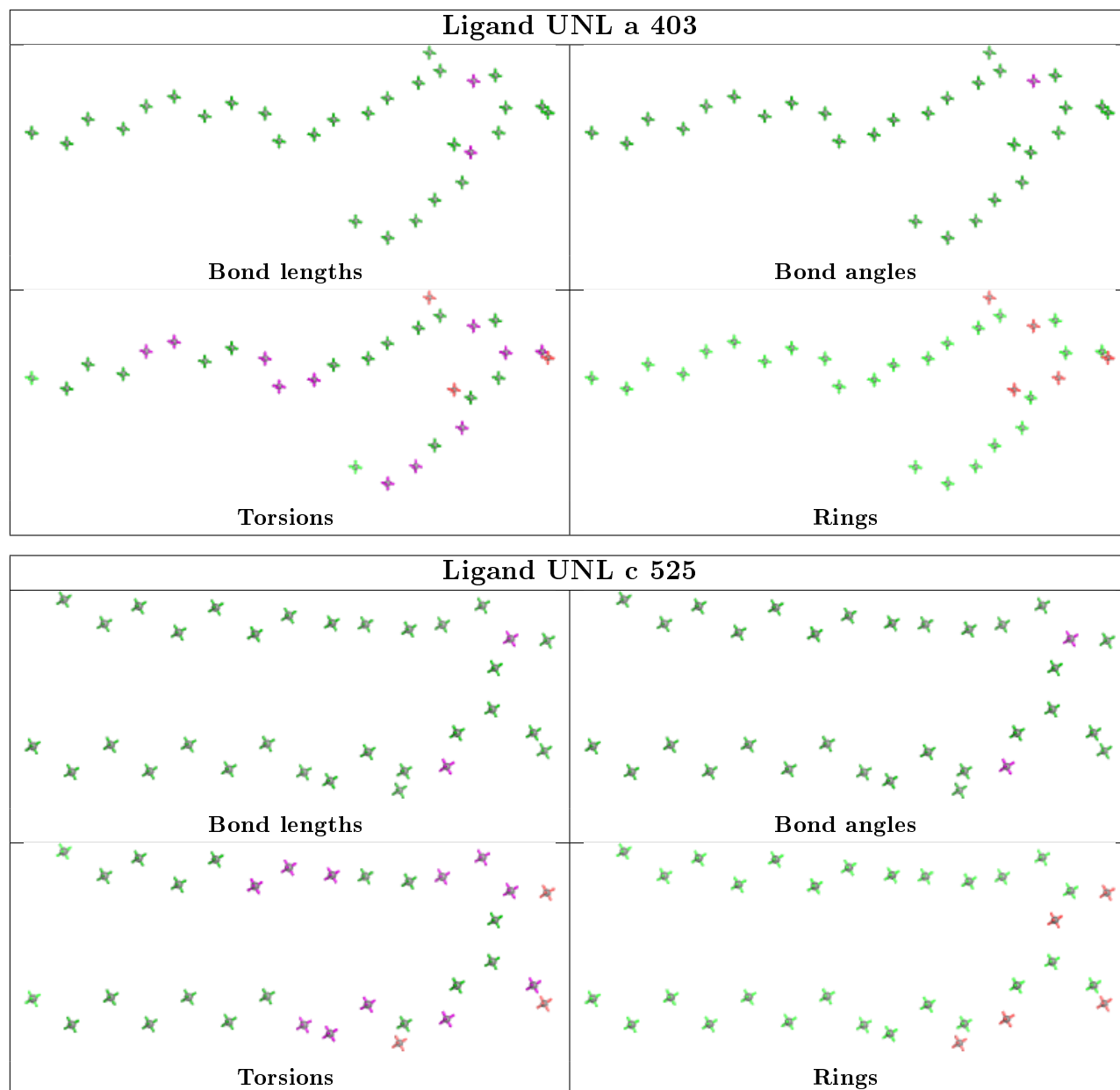


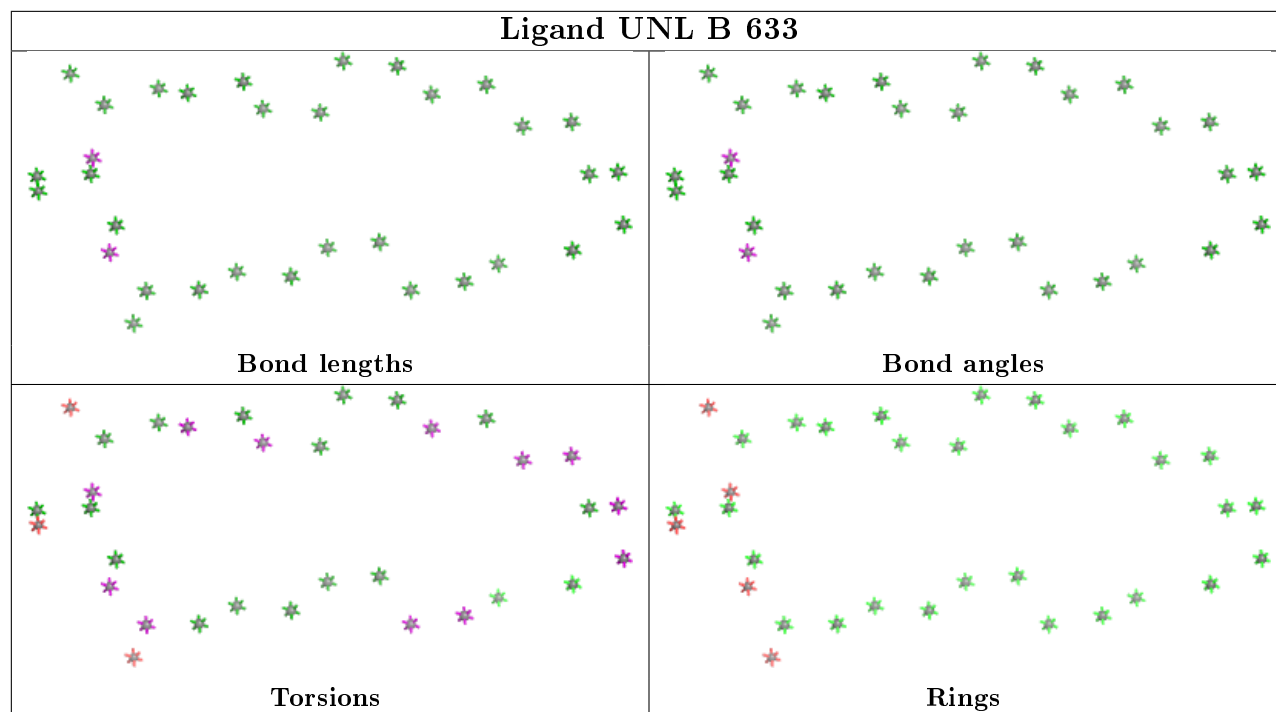












## 5.7 Other polymers [i](#)

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%)	-0.02	0 100 100	36, 48, 81, 127	0
1	a	334/344 (97%)	0.17	8 (2%) 59 57	37, 49, 86, 157	0
2	B	504/505 (99%)	0.03	6 (1%) 79 77	37, 53, 90, 153	0
2	b	503/505 (99%)	0.14	20 (3%) 38 37	40, 53, 102, 199	0
3	C	451/455 (99%)	0.09	14 (3%) 49 47	42, 63, 89, 152	0
3	c	455/455 (100%)	-0.01	3 (0%) 87 86	46, 66, 87, 137	0
4	D	341/342 (99%)	-0.03	1 (0%) 94 93	36, 49, 80, 132	0
4	d	341/342 (99%)	0.03	1 (0%) 94 93	36, 51, 81, 118	0
5	E	81/84 (96%)	1.17	19 (23%) 0 0	58, 84, 115, 160	0
5	e	81/84 (96%)	0.56	8 (9%) 7 6	60, 81, 131, 187	0
6	F	34/44 (77%)	0.43	4 (11%) 4 4	59, 72, 119, 124	0
6	f	32/44 (72%)	0.05	1 (3%) 49 47	59, 69, 132, 147	0
7	H	65/65 (100%)	-0.02	2 (3%) 49 47	54, 65, 89, 158	0
7	h	65/65 (100%)	-0.00	2 (3%) 49 47	53, 65, 84, 165	0
8	I	37/38 (97%)	0.30	4 (10%) 5 5	51, 65, 133, 192	0
8	i	37/38 (97%)	0.24	3 (8%) 12 11	52, 63, 125, 165	0
9	J	38/39 (97%)	0.76	5 (13%) 3 3	59, 78, 159, 185	0
9	j	39/39 (100%)	0.55	7 (17%) 1 1	58, 71, 156, 185	0
10	K	37/37 (100%)	0.47	4 (10%) 5 5	64, 78, 100, 110	0
10	k	37/37 (100%)	0.19	0 100 100	62, 77, 98, 117	0
11	L	37/37 (100%)	-0.01	0 100 100	37, 43, 99, 128	0
11	l	37/37 (100%)	0.05	0 100 100	39, 45, 105, 131	0
12	M	33/36 (91%)	0.07	0 100 100	35, 44, 74, 122	0
12	m	33/36 (91%)	0.28	0 100 100	35, 45, 82, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.05	4 (1%) 72 70	39, 59, 106, 157	0
13	o	243/244 (99%)	-0.01	5 (2%) 63 61	40, 62, 116, 177	0
14	T	29/32 (90%)	0.13	1 (3%) 45 44	38, 45, 77, 142	0
14	t	29/32 (90%)	0.17	1 (3%) 45 44	39, 46, 72, 149	0
15	U	97/104 (93%)	-0.11	1 (1%) 82 80	44, 58, 91, 126	0
15	u	97/104 (93%)	-0.14	0 100 100	47, 61, 83, 126	0
16	V	137/137 (100%)	-0.01	1 (0%) 87 86	44, 59, 84, 114	0
16	v	137/137 (100%)	-0.02	1 (0%) 87 86	47, 69, 102, 141	0
17	Y	29/30 (96%)	3.53	11 (37%) 0 0	79, 96, 194, 213	0
17	y	29/30 (96%)	1.12	6 (20%) 1 0	79, 97, 147, 168	0
18	X	39/40 (97%)	0.13	0 100 100	63, 75, 126, 149	0
18	x	38/40 (95%)	0.44	3 (7%) 12 11	64, 72, 135, 162	0
19	Z	62/62 (100%)	1.23	16 (25%) 0 0	81, 99, 134, 146	0
19	z	62/62 (100%)	1.08	18 (29%) 0 0	80, 98, 144, 190	0
20	R	18/34 (52%)	5.70	18 (100%) 0 0	104, 152, 180, 185	0
All	All	5275/5384 (97%)	0.16	198 (3%) 40 39	35, 58, 110, 213	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	20.2
17	Y	19	ILE	14.8
17	Y	20	ALA	12.6
20	R	8	VAL	10.4
20	R	18	TRP	9.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	T	1	10/11	0.91	0.15	38,51,69,90	0
8	FME	i	1	10/11	0.92	0.14	40,61,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	FME	m	1	10/11	0.95	0.16	35,51,99,110	0
14	FME	t	1	10/11	0.96	0.14	32,41,50,93	0
8	FME	I	1	10/11	0.97	0.15	42,55,62,63	0
12	FME	M	1	10/11	0.98	0.19	37,50,94,100	0

### 6.3 Carbohydrates

There are no monosaccharides in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	CA	b	609	1/1	0.23	0.07	147,147,147,147	0
28	LMT	F	101	35/35	0.24	0.57	133,168,178,179	0
37	DGD	d	408	62/66	0.31	0.47	83,130,177,185	0
32	UNL	J	101	10/-	0.36	0.27	80,97,103,105	0
28	LMT	b	630	25/35	0.46	0.44	84,108,161,164	0
33	LHG	a	419	42/49	0.54	0.33	83,141,183,185	0
28	LMT	a	418	35/35	0.54	0.40	97,135,160,164	0
37	DGD	D	409	52/66	0.55	0.36	75,108,154,165	0
32	UNL	K	102	34/-	0.56	0.25	91,128,136,139	0
26	SQD	f	102	43/54	0.57	0.33	102,125,159,165	0
28	LMT	C	521	35/35	0.58	0.36	102,138,166,166	0
28	LMT	m	102	35/35	0.60	0.25	50,108,132,133	0
32	UNL	a	403	30/-	0.61	0.30	75,97,125,131	0
33	LHG	A	419	42/49	0.61	0.29	77,120,144,148	0
32	UNL	c	525	32/-	0.62	0.24	80,99,140,150	0
28	LMT	a	404	35/35	0.62	0.30	57,98,122,147	0
35	HTG	d	414	16/19	0.64	0.22	83,103,113,126	0
36	LMG	C	519	51/55	0.65	0.24	61,104,123,126	0
36	LMG	Z	101	37/55	0.65	0.32	80,131,148,151	0
32	UNL	j	101	10/-	0.65	0.26	69,87,97,98	0
35	HTG	D	415	16/19	0.66	0.30	74,138,159,163	0
28	LMT	A	414	35/35	0.66	0.26	56,91,113,122	0
28	LMT	e	102	35/35	0.66	0.30	92,137,158,159	0
32	UNL	A	418	28/-	0.67	0.25	64,91,111,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	LMT	M	105	35/35	0.67	0.27	58,95,126,127	0
28	LMT	D	404	35/35	0.69	0.29	78,132,156,159	0
28	LMT	M	104	35/35	0.70	0.27	54,102,153,155	0
36	LMG	z	101	39/55	0.70	0.28	80,131,153,162	0
35	HTG	c	524	19/19	0.70	0.28	82,117,127,131	0
32	UNL	m	101	10/-	0.70	0.37	58,66,81,82	0
34	CA	B	601	1/1	0.71	0.07	123,123,123,123	0
28	LMT	B	634	25/35	0.71	0.32	56,85,147,154	0
28	LMT	T	104	25/35	0.71	0.31	47,81,132,142	0
32	UNL	B	633	33/-	0.72	0.29	60,86,131,134	0
27	GOL	v	202	6/6	0.73	0.22	86,100,101,109	0
32	UNL	b	633	33/-	0.73	0.27	56,92,143,145	0
35	HTG	B	624	19/19	0.73	0.26	74,126,137,186	0
37	DGD	C	517	62/66	0.73	0.23	52,73,103,110	0
27	GOL	V	201	6/6	0.74	0.48	83,92,94,96	0
35	HTG	C	523	19/19	0.74	0.28	87,108,129,139	0
35	HTG	b	632	19/19	0.76	0.22	84,140,154,155	0
31	PL9	A	417[B]	55/55	0.76	0.29	85,107,122,125	55
31	PL9	A	417[A]	55/55	0.76	0.29	85,107,123,125	55
36	LMG	C	520	51/55	0.77	0.31	67,119,131,134	0
31	PL9	a	415[A]	55/55	0.77	0.27	91,111,122,122	55
26	SQD	b	601	54/54	0.77	0.22	49,79,130,144	0
32	UNL	M	103	10/-	0.77	0.29	54,61,84,85	0
35	HTG	b	608	19/19	0.77	0.20	58,111,145,147	0
32	UNL	i	101	40/-	0.77	0.26	67,89,140,142	0
35	HTG	B	632	19/19	0.77	0.21	57,113,139,189	0
31	PL9	a	415[B]	55/55	0.77	0.27	92,111,122,123	55
32	UNL	d	413	36/-	0.78	0.26	60,91,132,138	0
27	GOL	b	606	6/6	0.78	0.21	79,90,98,98	0
36	LMG	b	629	51/55	0.78	0.21	43,57,75,87	0
26	SQD	F	104	43/54	0.78	0.24	90,122,138,144	0
27	GOL	O	301	6/6	0.79	0.23	83,92,94,97	0
26	SQD	B	636	54/54	0.79	0.23	45,81,130,132	0
27	GOL	t	102	6/6	0.80	0.41	71,91,105,109	0
36	LMG	M	101	51/55	0.80	0.21	40,60,77,89	0
36	LMG	c	522	51/55	0.80	0.24	64,114,125,127	0
23	CLA	C	514	65/65	0.80	0.28	64,87,119,126	0
32	UNL	I	101	40/-	0.80	0.26	51,88,154,155	0
28	LMT	M	102	35/35	0.81	0.21	44,94,118,130	0
26	SQD	A	413	54/54	0.81	0.23	56,80,130,138	0
21	CL	v	205	1/1	0.81	0.09	124,124,124,124	0
35	HTG	b	631	19/19	0.82	0.26	71,83,97,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	SQD	B	621	54/54	0.82	0.23	48,81,143,150	0
37	DGD	h	102	62/66	0.82	0.21	38,58,80,85	0
23	CLA	C	505	65/65	0.82	0.22	47,65,96,110	0
32	UNL	X	101	18/-	0.82	0.18	61,78,113,117	0
36	LMG	k	101	51/55	0.83	0.23	67,96,122,125	0
35	HTG	B	623	19/19	0.83	0.21	62,78,91,92	0
34	CA	F	105	1/1	0.83	0.04	112,112,112,112	0
23	CLA	c	517	65/65	0.84	0.22	85,97,108,112	0
35	HTG	b	607	19/19	0.84	0.20	49,81,95,101	0
36	LMG	C	501	51/55	0.84	0.20	58,91,106,111	0
37	DGD	H	102	62/66	0.84	0.20	42,58,97,102	0
37	DGD	C	518	62/66	0.84	0.19	49,66,88,97	0
32	UNL	D	414	40/-	0.84	0.21	59,87,128,135	0
34	CA	f	103	1/1	0.84	0.13	135,135,135,135	0
35	HTG	c	523	19/19	0.85	0.17	92,106,118,124	0
27	GOL	V	204	6/6	0.85	0.13	96,100,106,117	0
27	GOL	T	101	6/6	0.85	0.41	69,87,92,93	0
35	HTG	B	631	19/19	0.85	0.17	52,94,118,125	0
27	GOL	a	402	6/6	0.85	0.23	96,103,108,109	0
26	SQD	a	413	54/54	0.86	0.17	53,88,106,109	0
26	SQD	A	410	54/54	0.86	0.21	54,94,105,109	0
35	HTG	C	522	19/19	0.86	0.17	86,100,123,126	0
36	LMG	a	414	51/55	0.86	0.21	60,86,102,110	0
35	HTG	b	602	19/19	0.86	0.19	49,64,75,79	0
32	UNL	d	415	18/-	0.86	0.20	67,74,111,117	0
27	GOL	f	101	6/6	0.87	0.18	95,101,102,103	0
23	CLA	c	510	65/65	0.87	0.18	56,74,97,104	0
37	DGD	c	520	62/66	0.87	0.19	52,65,117,131	0
36	LMG	D	416	51/55	0.88	0.18	52,75,120,131	0
23	CLA	c	511	65/65	0.88	0.17	52,68,77,82	0
23	CLA	b	616	65/65	0.88	0.20	29,42,51,58	0
27	GOL	C	524	6/6	0.88	0.41	81,88,106,110	0
27	GOL	T	102	6/6	0.88	0.43	100,114,116,120	0
33	LHG	D	412	49/49	0.88	0.24	53,70,117,124	0
27	GOL	c	502	6/6	0.88	0.43	76,97,108,111	0
23	CLA	C	512	65/65	0.89	0.17	57,76,93,108	0
35	HTG	V	206	19/19	0.89	0.32	77,106,125,227	0
27	GOL	o	301	6/6	0.89	0.19	84,90,99,104	0
23	CLA	C	507	65/65	0.89	0.17	54,78,117,123	0
23	CLA	B	607	65/65	0.89	0.17	35,53,96,98	0
27	GOL	B	635	6/6	0.89	0.16	57,59,66,69	0
23	CLA	b	611	65/65	0.89	0.19	42,54,61,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	LMG	d	416	51/55	0.89	0.19	55,68,107,118	0
23	CLA	c	507	65/65	0.89	0.17	52,65,76,93	0
23	CLA	B	614	65/65	0.90	0.18	31,43,66,84	0
23	CLA	c	509	65/65	0.90	0.16	43,55,72,76	0
23	CLA	c	508	65/65	0.90	0.16	51,65,81,89	0
23	CLA	b	615	65/65	0.90	0.17	41,54,92,97	0
27	GOL	A	411	6/6	0.90	0.15	54,57,60,70	0
23	CLA	c	512	65/65	0.90	0.15	46,58,125,136	0
23	CLA	c	515	65/65	0.90	0.17	55,71,88,95	0
23	CLA	b	610	65/65	0.90	0.19	52,80,123,129	0
27	GOL	A	412	6/6	0.90	0.21	76,82,86,90	0
37	DGD	c	521	62/66	0.90	0.17	48,62,94,109	0
21	CL	U	201	1/1	0.90	0.07	116,116,116,116	0
35	HTG	B	622	19/19	0.90	0.18	48,68,85,91	0
33	LHG	D	410	49/49	0.90	0.23	40,53,65,67	0
23	CLA	b	618	65/65	0.90	0.18	46,55,65,68	0
23	CLA	C	513	65/65	0.90	0.17	61,83,93,101	0
27	GOL	v	203	6/6	0.91	0.23	93,105,109,120	0
25	BCR	K	101	40/40	0.91	0.15	62,87,98,98	0
33	LHG	d	411	49/49	0.91	0.20	49,64,116,122	0
23	CLA	C	511	65/65	0.91	0.15	54,71,81,84	0
25	BCR	c	526	40/40	0.91	0.16	68,87,98,99	0
25	BCR	H	101	40/40	0.91	0.18	43,64,79,81	0
27	GOL	F	103	6/6	0.91	0.31	104,108,111,111	0
23	CLA	C	504	65/65	0.91	0.20	50,66,79,84	0
23	CLA	B	602	65/65	0.91	0.19	52,74,118,137	0
23	CLA	C	509	65/65	0.91	0.15	49,66,130,139	0
23	CLA	b	624	65/65	0.91	0.16	43,53,73,79	0
23	CLA	B	610	65/65	0.91	0.18	45,54,62,68	0
23	CLA	C	502	65/65	0.91	0.15	50,63,78,92	0
37	DGD	C	516	62/66	0.92	0.17	42,55,89,91	0
23	CLA	c	513	65/65	0.92	0.17	54,68,82,91	0
23	CLA	B	616	65/65	0.92	0.17	40,54,71,78	0
33	LHG	b	634	49/49	0.92	0.21	38,52,68,85	0
33	LHG	d	410	49/49	0.92	0.23	37,48,64,91	0
23	CLA	b	625	65/65	0.92	0.17	44,61,111,117	0
23	CLA	c	516	65/65	0.92	0.17	62,77,93,97	0
37	DGD	c	519	62/66	0.92	0.18	41,60,100,103	0
23	CLA	c	514	65/65	0.92	0.15	51,63,72,82	0
25	BCR	y	101	40/40	0.92	0.16	56,72,84,92	0
22	BCT	A	403[B]	4/4	0.92	0.24	72,82,83,95	4
27	GOL	D	403	6/6	0.92	0.27	52,56,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	BCT	A	403[A]	4/4	0.92	0.24	76,81,81,92	4
23	CLA	D	406	65/65	0.92	0.15	45,61,114,119	0
25	BCR	Y	101	40/40	0.92	0.17	65,78,92,103	0
23	CLA	B	613	65/65	0.93	0.15	34,45,54,58	0
23	CLA	b	623	65/65	0.93	0.18	33,46,93,110	0
23	CLA	B	608	65/65	0.93	0.18	28,43,57,64	0
33	LHG	d	409	49/49	0.93	0.22	41,55,68,69	0
23	CLA	C	508	65/65	0.93	0.16	51,70,83,91	0
23	CLA	B	605	65/65	0.93	0.16	32,44,76,81	0
23	CLA	d	403	65/65	0.93	0.17	36,44,51,62	0
23	CLA	A	404	65/65	0.93	0.16	33,40,53,66	0
23	CLA	b	617	65/65	0.93	0.16	41,56,64,70	0
27	GOL	b	605	6/6	0.93	0.22	67,86,109,116	0
23	CLA	d	405	65/65	0.93	0.18	49,59,108,118	0
23	CLA	b	620	65/65	0.93	0.17	33,47,57,64	0
27	GOL	V	203	6/6	0.93	0.26	64,71,80,84	0
23	CLA	b	621	65/65	0.93	0.15	36,47,56,65	0
23	CLA	C	510	65/65	0.93	0.15	54,73,88,95	0
23	CLA	B	603	65/65	0.93	0.16	41,52,63,70	0
27	GOL	B	629	6/6	0.93	0.27	51,65,75,83	0
23	CLA	B	615	65/65	0.93	0.20	32,45,99,106	0
23	CLA	b	612	65/65	0.93	0.16	41,54,64,70	0
23	CLA	a	408	65/65	0.93	0.19	35,42,50,62	0
25	BCR	b	627	40/40	0.93	0.18	34,47,64,72	0
32	UNL	d	412	17/-	0.94	0.23	59,72,96,98	0
31	PL9	d	407[B]	55/55	0.94	0.21	34,44,54,60	55
23	CLA	B	612	65/65	0.94	0.18	32,44,55,60	0
25	BCR	h	101	40/40	0.94	0.17	52,67,77,78	0
33	LHG	D	411	49/49	0.94	0.21	32,49,73,81	0
23	CLA	C	506	65/65	0.94	0.14	48,58,74,83	0
27	GOL	V	202	6/6	0.94	0.20	54,67,81,83	0
23	CLA	b	619	65/65	0.94	0.17	42,54,63,70	0
27	GOL	B	627	6/6	0.94	0.22	71,79,86,91	0
23	CLA	c	505	65/65	0.94	0.15	52,66,75,79	0
32	UNL	D	413	17/-	0.94	0.19	50,76,96,100	0
25	BCR	d	406	40/40	0.94	0.20	51,64,84,86	0
25	BCR	k	102	40/40	0.94	0.16	59,75,87,90	0
23	CLA	a	411	65/65	0.94	0.19	39,57,122,128	0
23	CLA	B	609	65/65	0.94	0.19	41,51,67,70	0
25	BCR	D	407	40/40	0.94	0.17	51,65,105,115	0
23	CLA	D	405	65/65	0.94	0.17	31,42,64,67	0
27	GOL	B	626	6/6	0.94	0.23	53,67,81,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	B	617	65/65	0.94	0.20	43,58,134,136	0
33	LHG	L	101	49/49	0.94	0.21	41,50,59,62	0
27	GOL	C	525	6/6	0.94	0.20	56,58,70,72	0
22	BCT	d	401[A]	4/4	0.94	0.23	74,74,76,78	4
31	PL9	d	407[A]	55/55	0.94	0.21	33,44,54,60	55
22	BCT	d	401[B]	4/4	0.94	0.23	73,74,76,78	4
23	CLA	A	406	65/65	0.95	0.15	34,45,102,111	0
24	PHO	D	402[B]	64/64	0.95	0.17	36,48,58,63	64
23	CLA	b	622	65/65	0.95	0.19	34,47,60,67	0
31	PL9	D	408[A]	55/55	0.95	0.22	31,43,50,58	55
39	HEM	F	102	43/43	0.95	0.17	60,81,105,113	0
25	BCR	A	409	40/40	0.95	0.17	36,47,55,56	0
40	MG	J	102	1/1	0.95	0.12	64,64,64,64	0
25	BCR	K	103	40/40	0.95	0.16	59,74,89,92	0
23	CLA	C	503	65/65	0.95	0.15	45,65,72,76	0
23	CLA	A	408	65/65	0.95	0.15	38,56,120,128	0
25	BCR	T	103	40/40	0.95	0.15	30,50,64,66	0
39	HEM	e	101	43/43	0.95	0.19	72,91,130,138	0
23	CLA	B	611	65/65	0.95	0.19	40,57,67,70	0
23	CLA	b	613	65/65	0.95	0.16	33,45,71,77	0
23	CLA	B	606	65/65	0.95	0.16	35,44,57,61	0
27	GOL	v	204	6/6	0.95	0.25	63,69,78,81	0
23	CLA	a	409	65/65	0.95	0.18	37,48,109,116	0
27	GOL	a	401	6/6	0.95	0.19	52,63,72,75	0
23	CLA	b	614	65/65	0.95	0.17	35,46,60,65	0
27	GOL	B	628	6/6	0.95	0.29	61,71,81,83	0
24	PHO	D	402[A]	64/64	0.95	0.17	37,49,59,63	64
24	PHO	A	407	64/64	0.95	0.16	30,41,50,55	0
25	BCR	C	515	40/40	0.95	0.17	50,64,76,78	0
23	CLA	d	404	65/65	0.95	0.17	35,43,58,69	0
24	PHO	d	402[B]	64/64	0.95	0.18	39,50,56,59	64
23	CLA	c	506	65/65	0.95	0.14	48,62,79,87	0
23	CLA	A	405	65/65	0.95	0.16	30,40,48,53	0
23	CLA	B	604	65/65	0.95	0.18	46,55,63,66	0
24	PHO	d	402[A]	64/64	0.95	0.18	37,51,57,59	64
31	PL9	D	408[B]	55/55	0.95	0.22	32,43,51,56	55
25	BCR	B	620	40/40	0.96	0.19	41,52,62,66	0
21	CL	A	402[A]	1/1	0.96	0.11	44,44,44,44	1
34	CA	c	504	1/1	0.96	0.07	85,85,85,85	0
25	BCR	a	412	40/40	0.96	0.18	37,47,54,57	0
25	BCR	b	628	40/40	0.96	0.18	40,59,69,70	0
25	BCR	B	619	40/40	0.96	0.18	36,48,61,67	0

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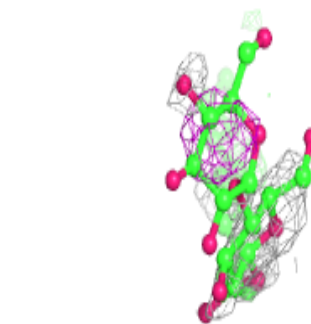
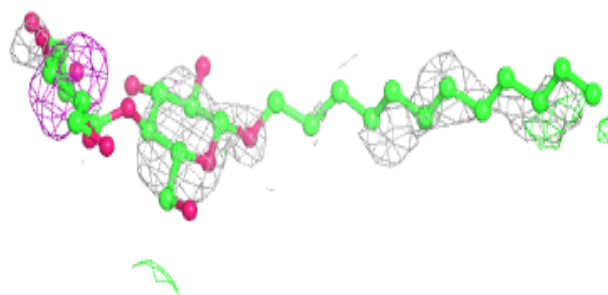
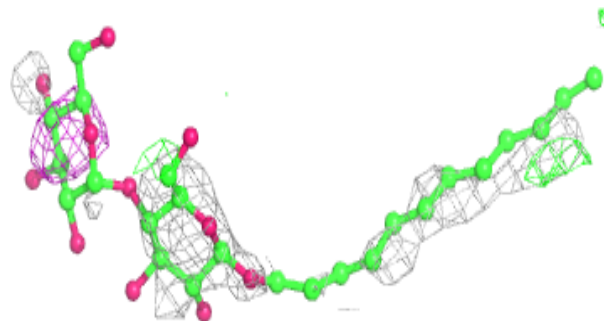
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	c	518	40/40	0.96	0.19	52,64,77,80	0
25	BCR	t	101	40/40	0.96	0.19	33,52,66,68	0
27	GOL	b	604	6/6	0.96	0.15	63,68,80,82	0
25	BCR	B	618	40/40	0.96	0.20	34,45,56,58	0
24	PHO	a	410	64/64	0.96	0.19	36,44,50,53	0
21	CL	A	402[B]	1/1	0.96	0.11	46,46,46,46	1
27	GOL	v	201	6/6	0.96	0.18	72,80,88,97	0
34	CA	O	302	1/1	0.97	0.04	96,96,96,96	0
25	BCR	b	626	40/40	0.97	0.18	38,47,56,58	0
39	HEM	v	206	43/43	0.97	0.14	55,68,73,77	0
27	GOL	B	625	6/6	0.97	0.18	53,63,67,79	0
27	GOL	b	603	6/6	0.97	0.22	58,75,83,86	0
40	MG	j	102	1/1	0.97	0.15	71,71,71,71	0
27	GOL	B	630	6/6	0.97	0.35	50,85,91,96	0
39	HEM	V	205	43/43	0.97	0.13	46,53,60,62	0
34	CA	C	526	1/1	0.97	0.11	88,88,88,88	0
29	OEX	a	416[A]	10/10	0.98	0.15	41,48,53,56	10
34	CA	o	302	1/1	0.98	0.05	96,96,96,96	0
27	GOL	c	501	6/6	0.98	0.24	56,62,65,68	0
30	OEY	a	417[B]	11/11	0.98	0.16	40,48,57,78	11
30	OEY	A	416[B]	11/11	0.99	0.13	43,53,64,72	11
38	FE2	D	401[A]	1/1	0.99	0.08	70,70,70,70	1
34	CA	c	503	1/1	0.99	0.08	78,78,78,78	0
21	CL	a	406[A]	1/1	0.99	0.16	46,46,46,46	1
38	FE2	a	405[B]	1/1	0.99	0.10	62,62,62,62	0
21	CL	a	407[A]	1/1	0.99	0.13	52,52,52,52	1
29	OEX	A	415[A]	10/10	0.99	0.12	47,56,62,72	10
21	CL	a	407[B]	1/1	0.99	0.13	47,47,47,47	1
38	FE2	D	401[B]	1/1	0.99	0.08	69,69,69,69	1
21	CL	a	406[B]	1/1	0.99	0.16	47,47,47,47	1
21	CL	A	401[A]	1/1	1.00	0.17	42,42,42,42	1
21	CL	A	401[B]	1/1	1.00	0.17	39,39,39,39	1

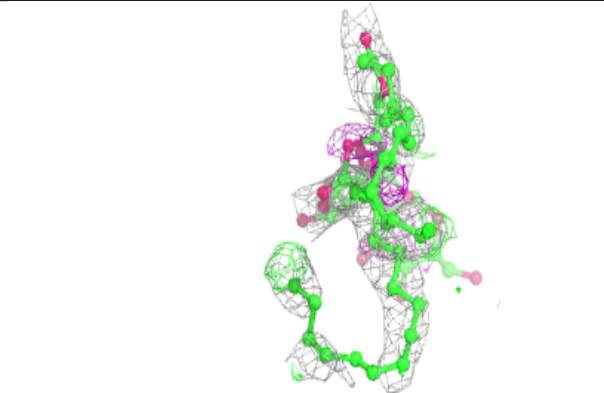
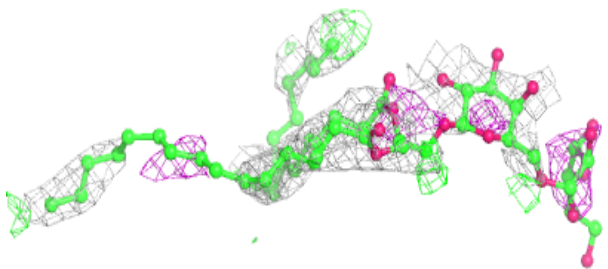
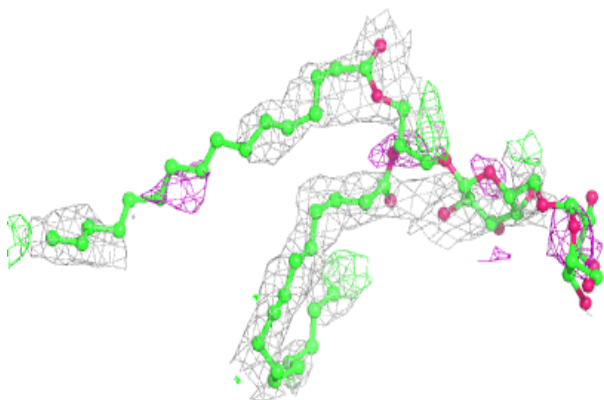
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT 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)

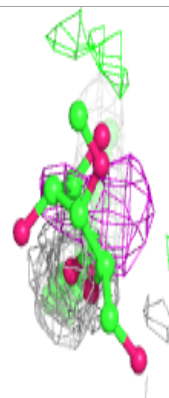
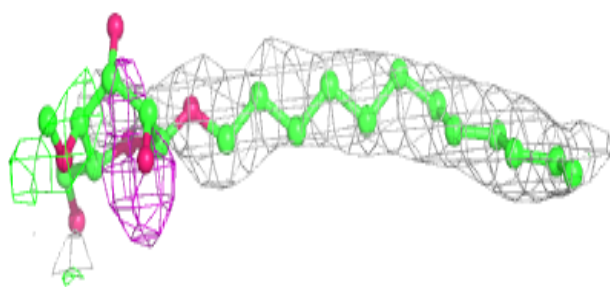
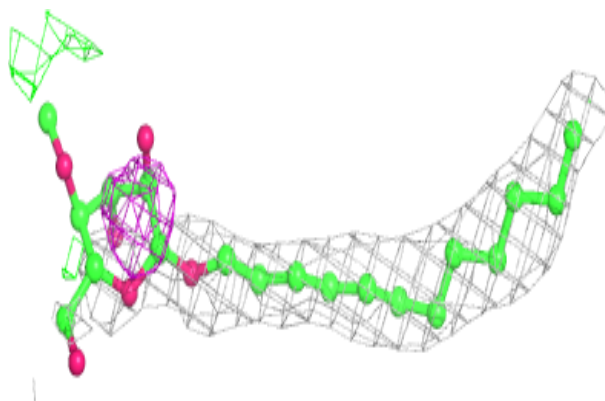
**Electron density around DGD d 408:**

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



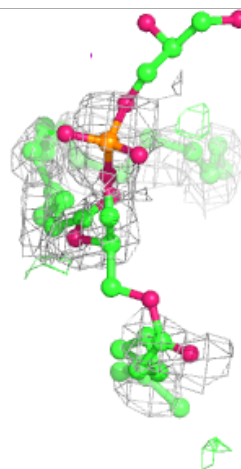
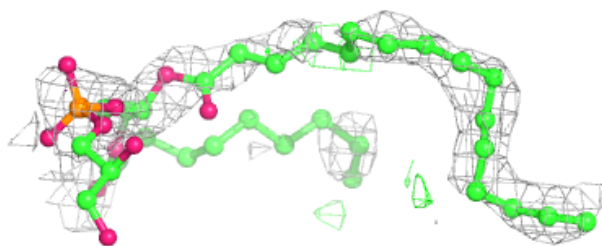
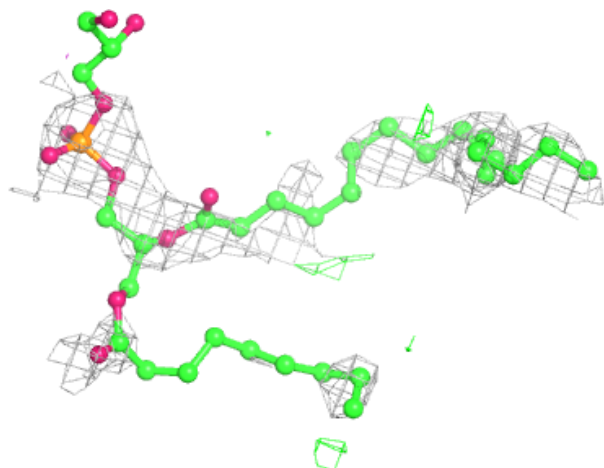
**Electron density around LMT b 630:**

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



**Electron density around LHG a 419:**

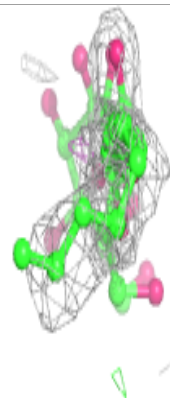
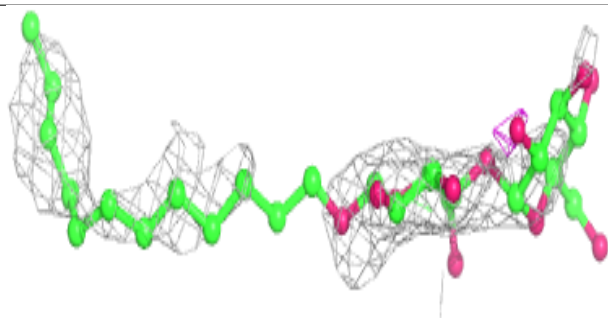
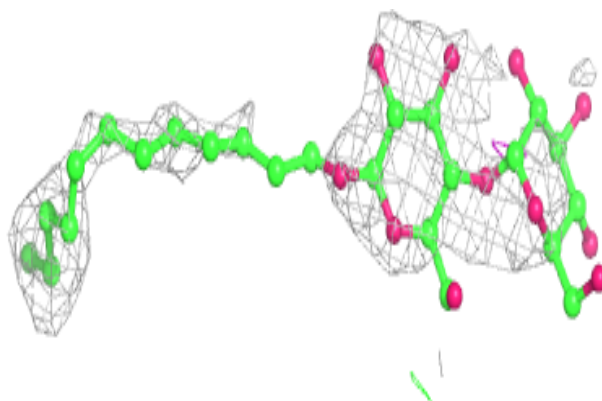
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



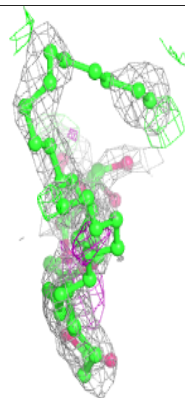
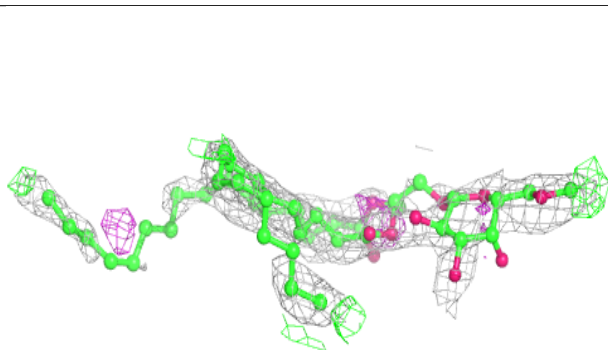
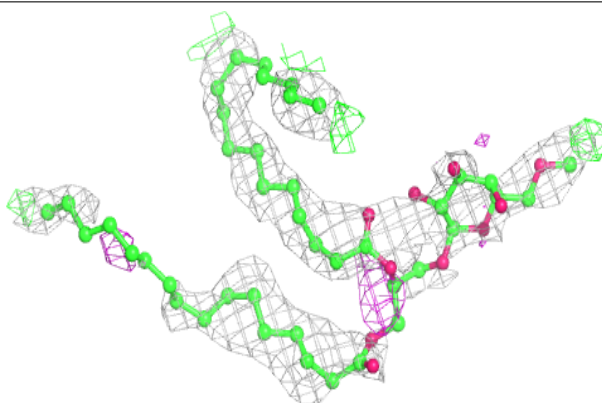


**Electron density around LMT a 418:**

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

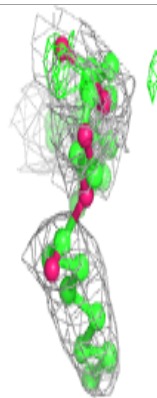
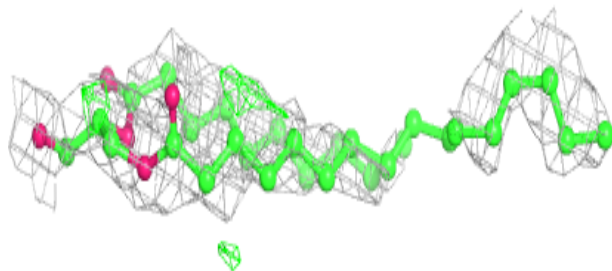
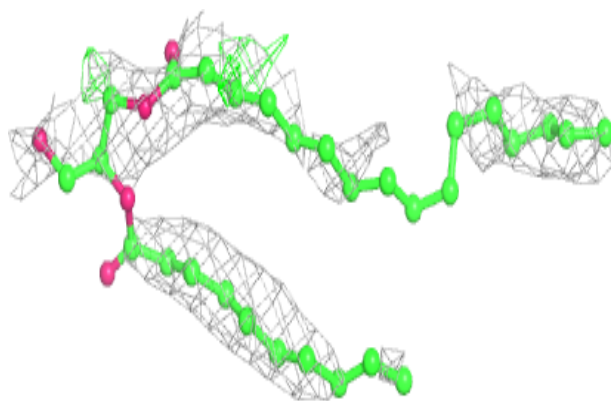
**Electron density around DGD D 409:**

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

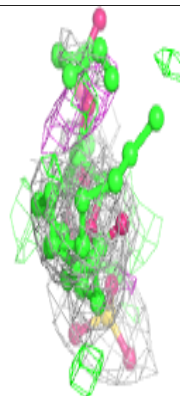
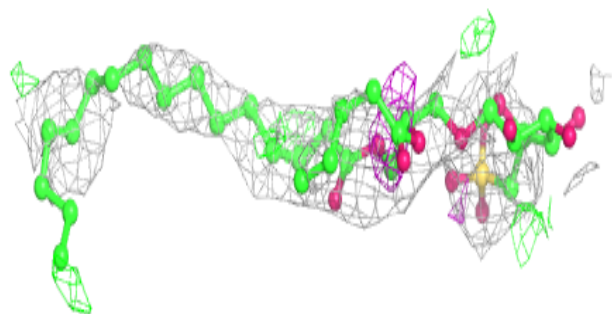
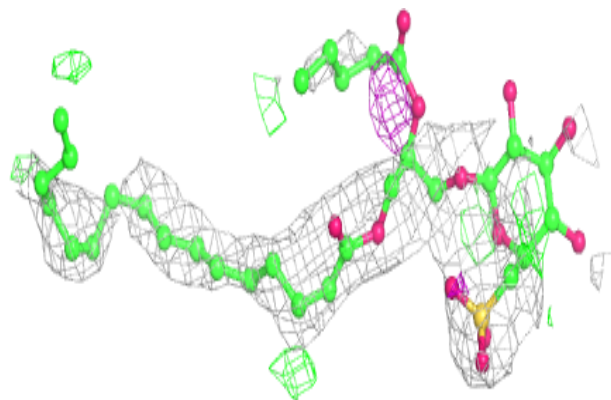


**Electron density around UNL K 102:**

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

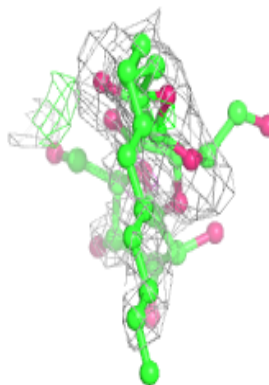
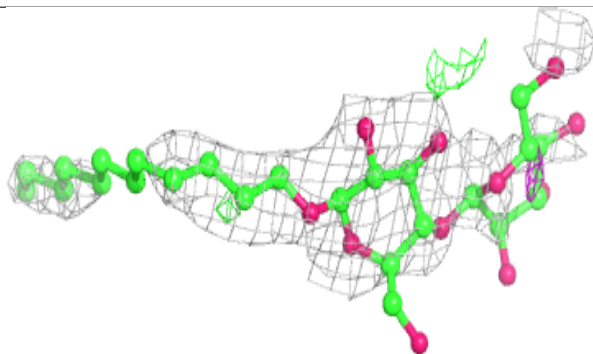
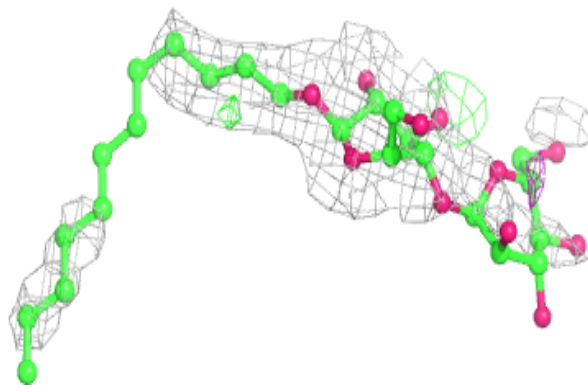
**Electron density around SQD f 102:**

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

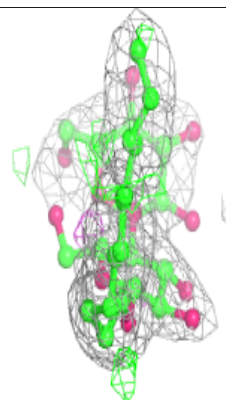
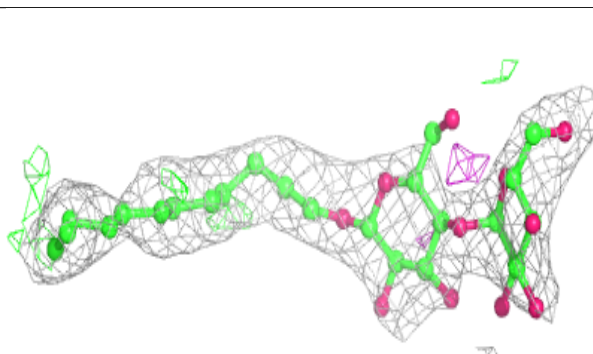
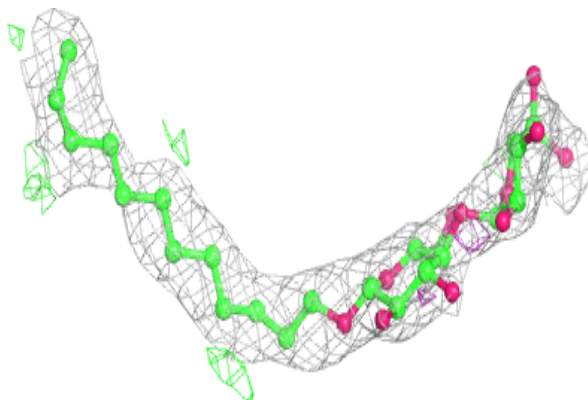


**Electron density around LMT C 521:**

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

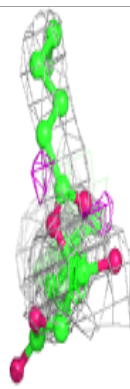
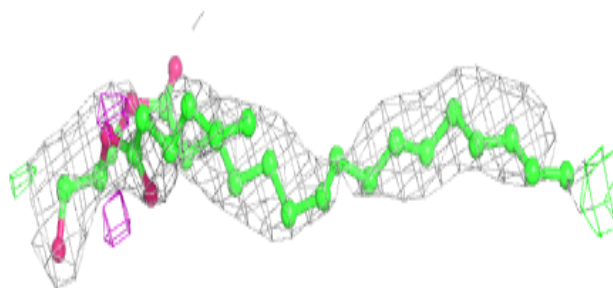
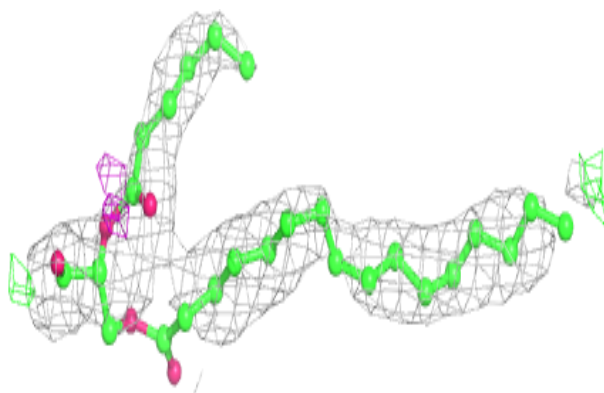
**Electron density around LMT m 102:**

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



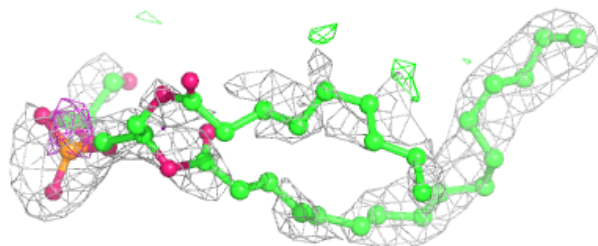
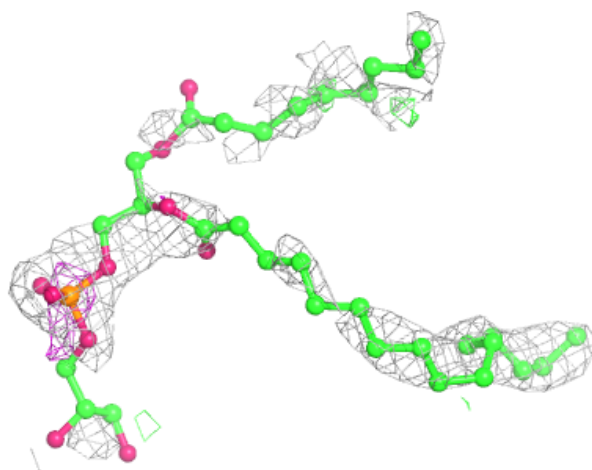
**Electron density around UNL a 403:**

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



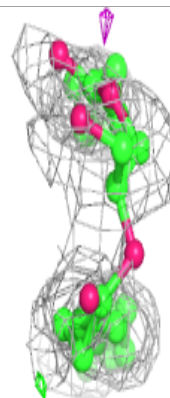
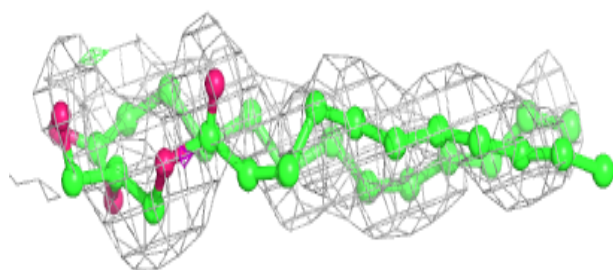
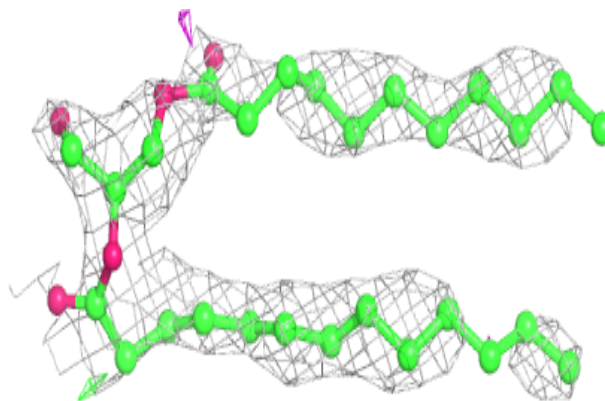
**Electron density around LHG A 419:**

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

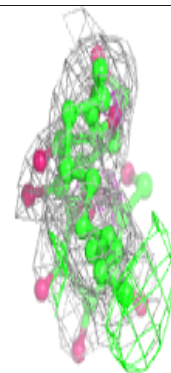
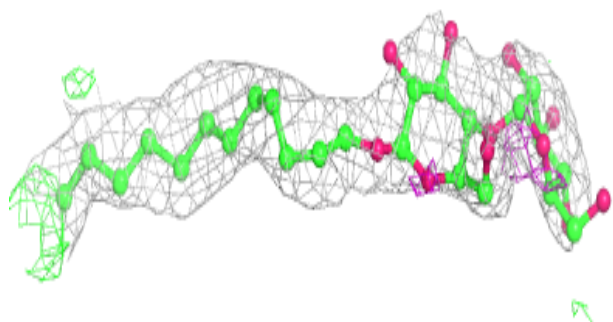
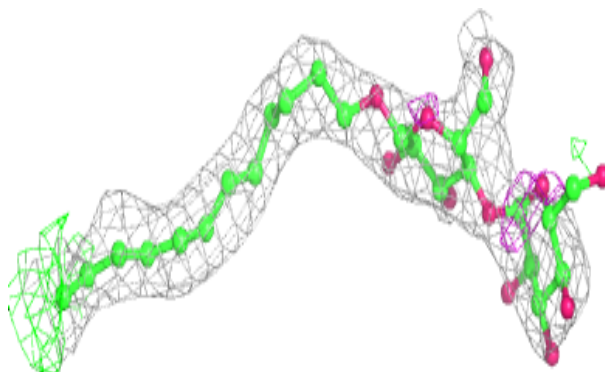


**Electron density around UNL c 525:**

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

**Electron density around LMT a 404:**

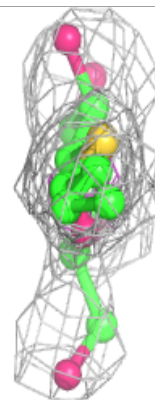
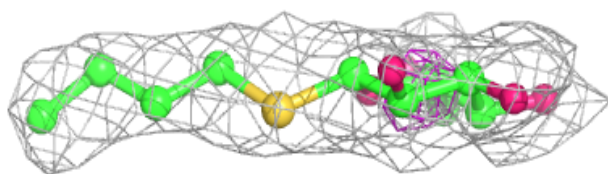
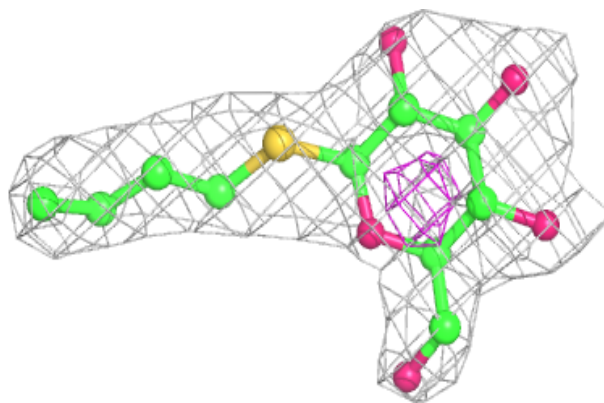
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





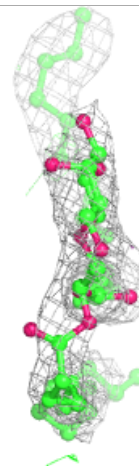
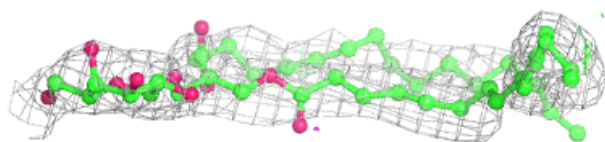
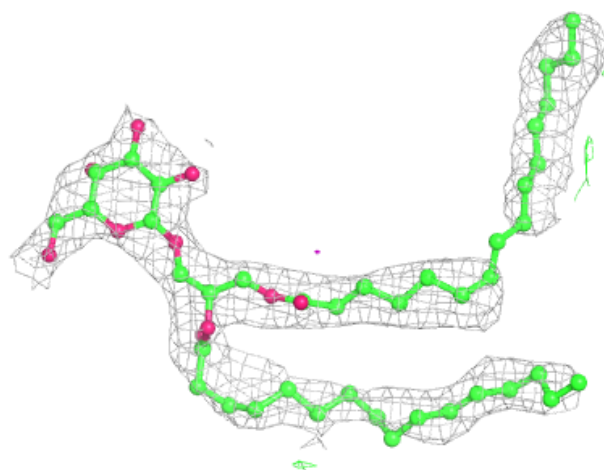
**Electron density around HTG d 414:**

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



**Electron density around LMG C 519:**

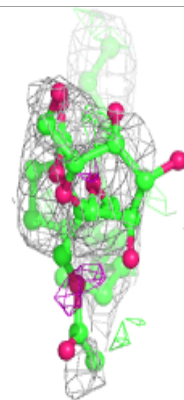
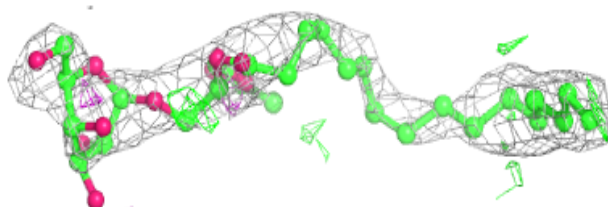
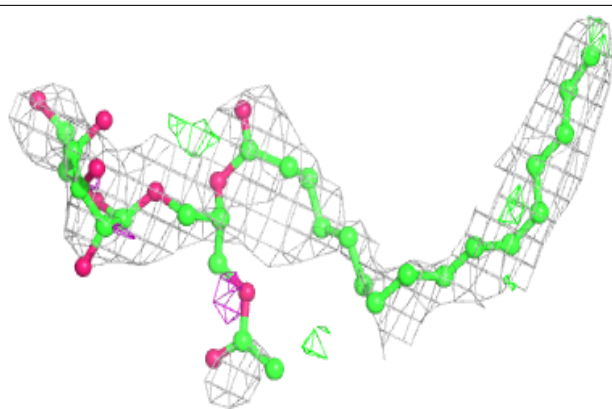
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



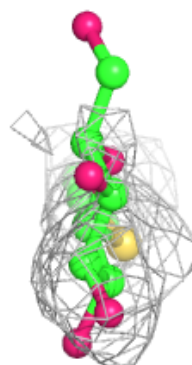
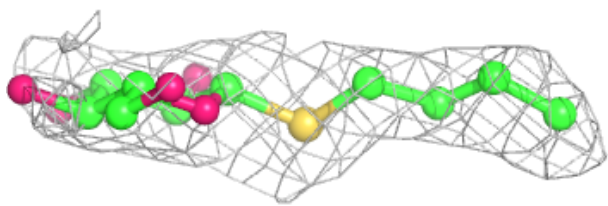
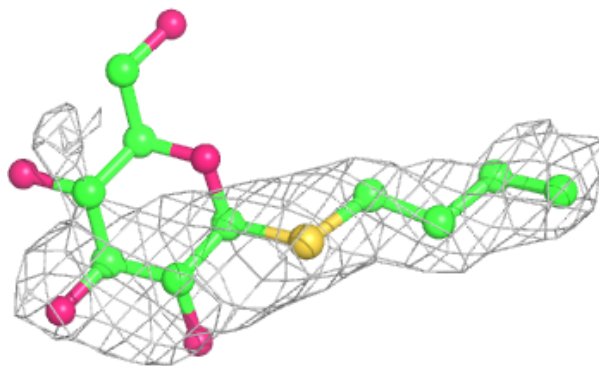


**Electron density around LMG Z 101:**

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

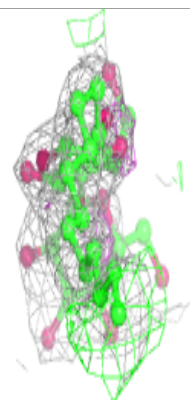
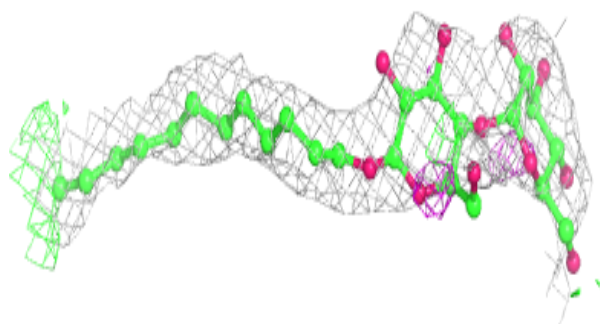
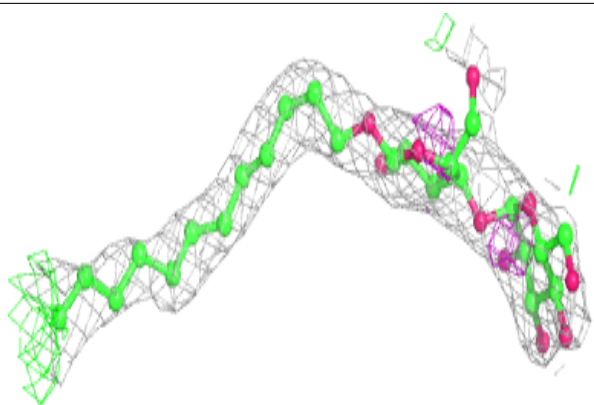
**Electron density around HTG D 415:**

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

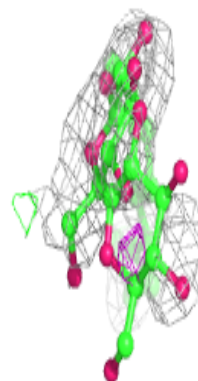
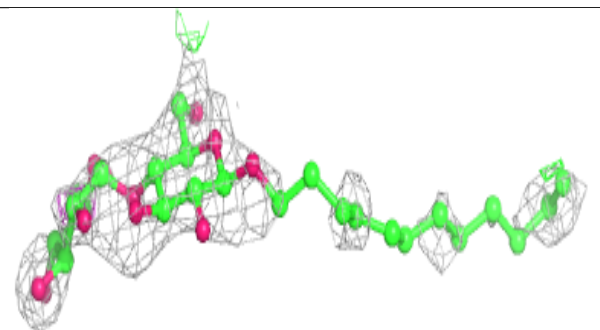
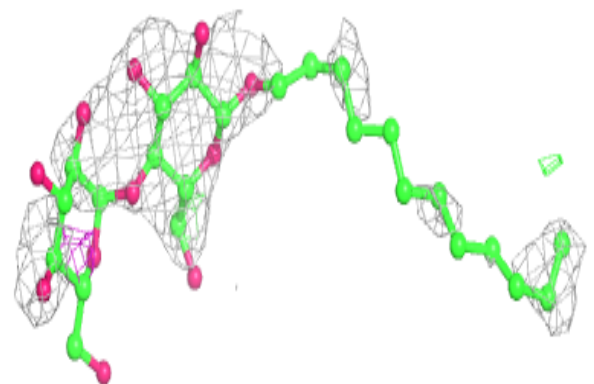


**Electron density around LMT A 414:**

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

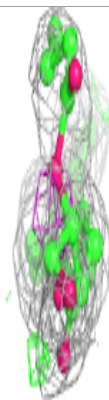
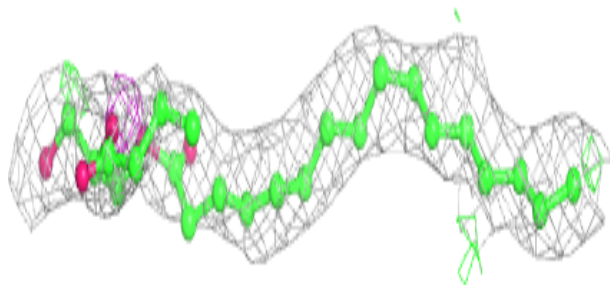
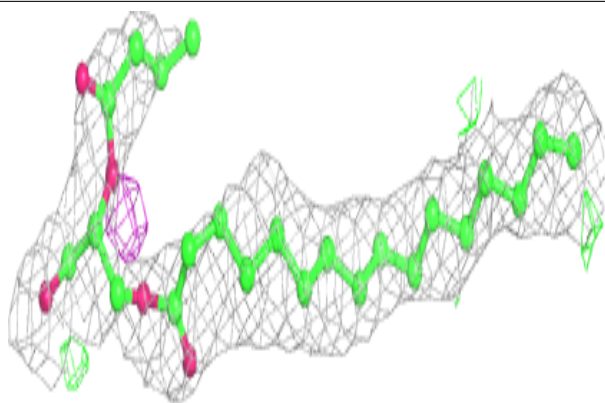
**Electron density around LMT e 102:**

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

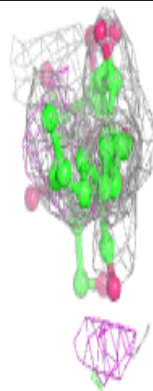
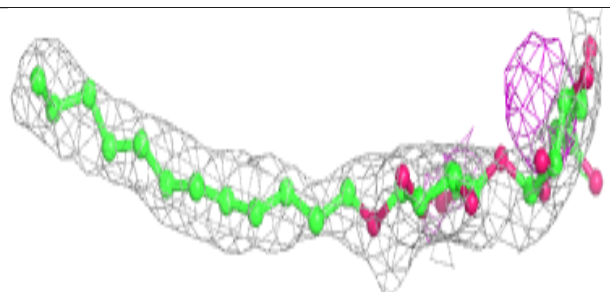
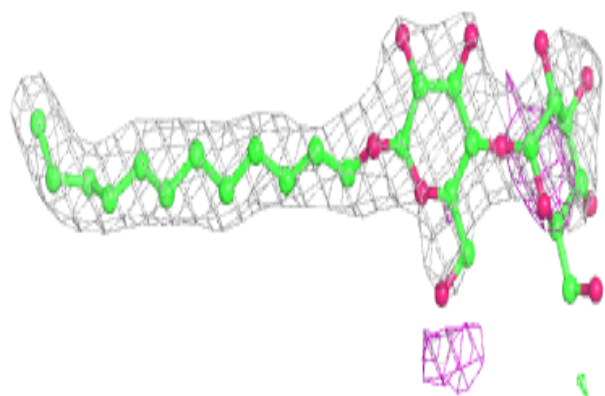


**Electron density around UNL A 418:**

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

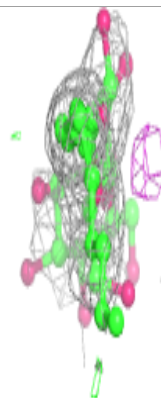
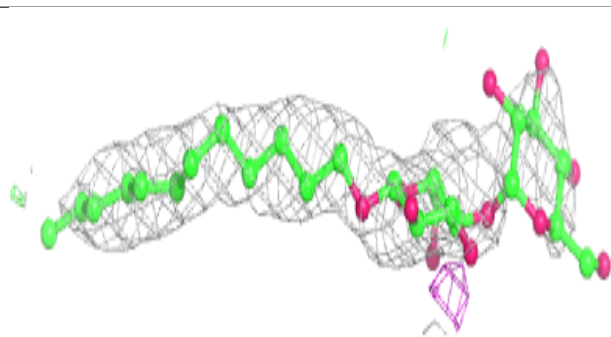
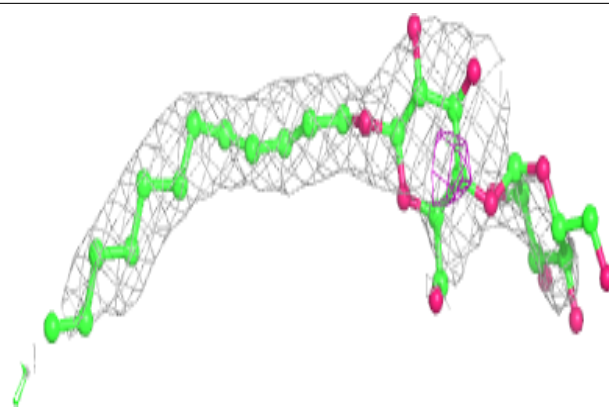
**Electron density around LMT M 105:**

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

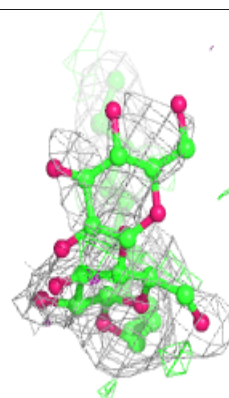
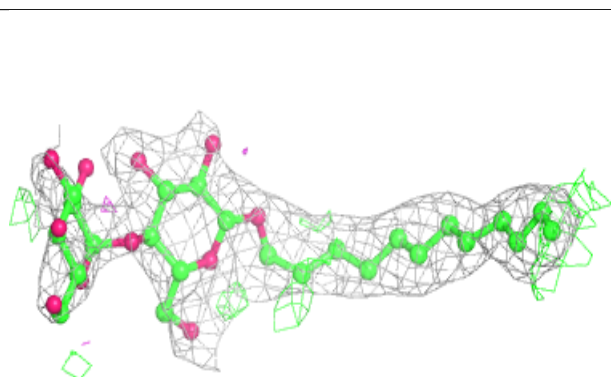
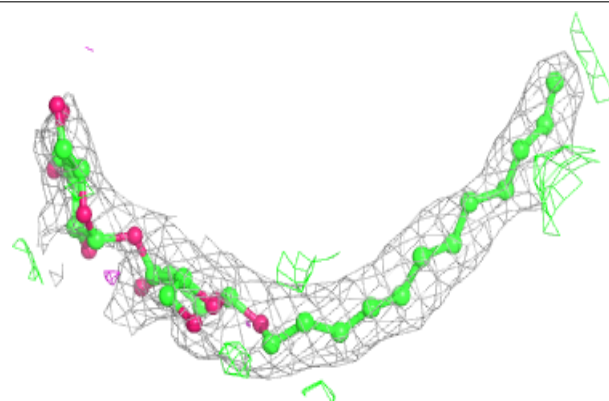


**Electron density around LMT D 404:**

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

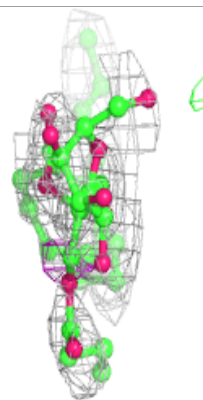
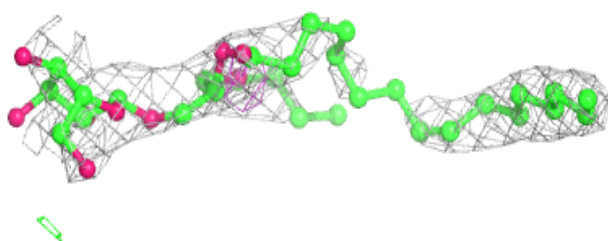
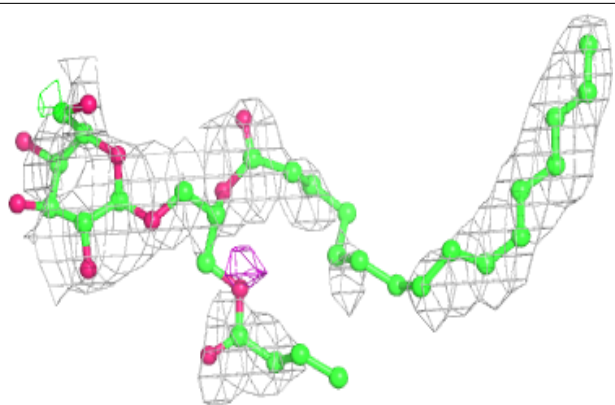
**Electron density around LMT M 104:**

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

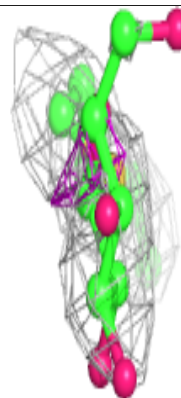
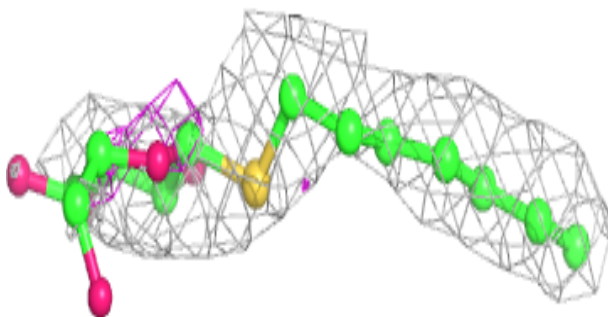
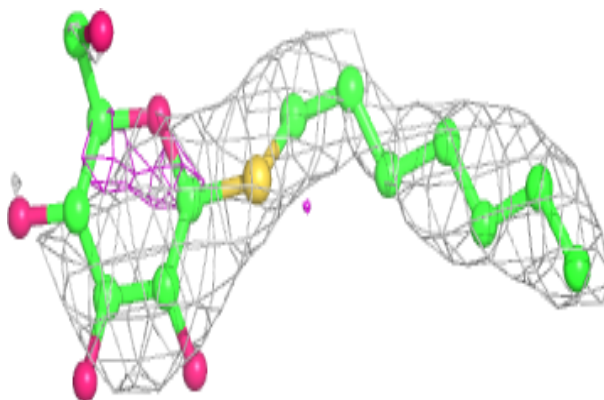


**Electron density around LMG z 101:**

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

**Electron density around HTG c 524:**

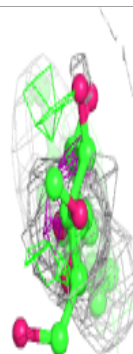
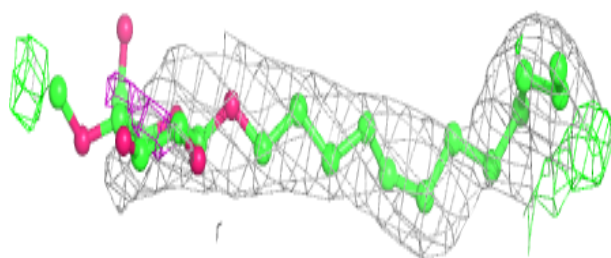
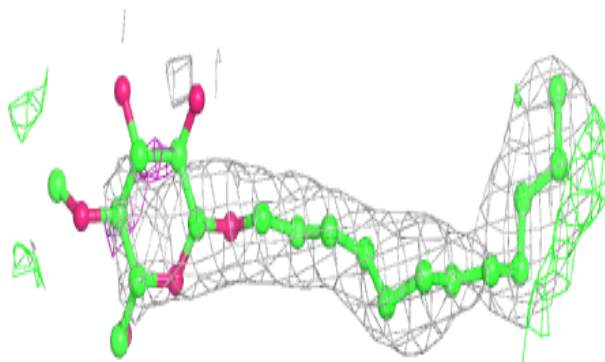
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



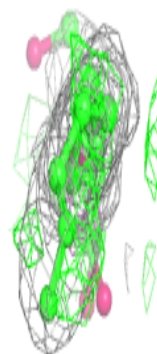
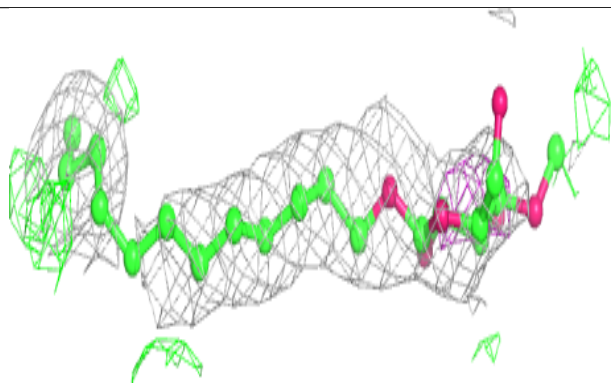
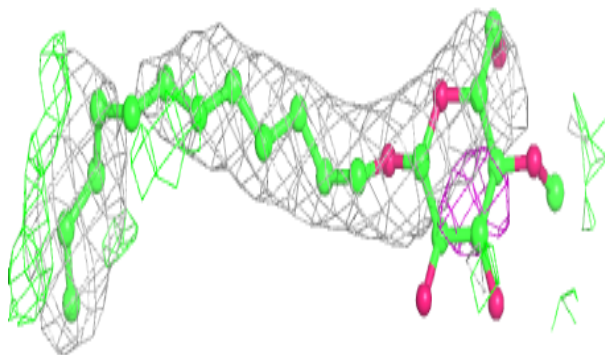


**Electron density around LMT B 634:**

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

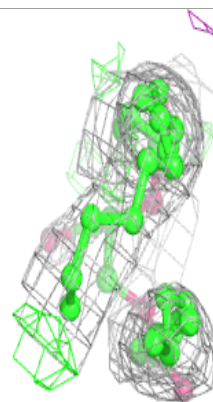
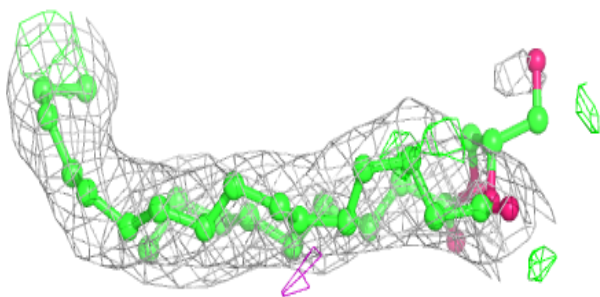
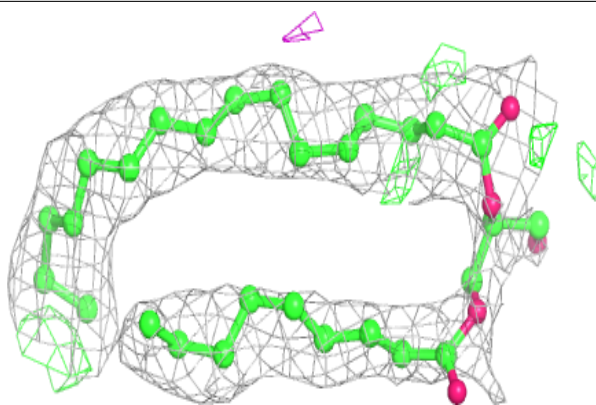
**Electron density around LMT T 104:**

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

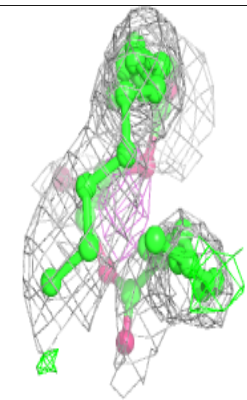
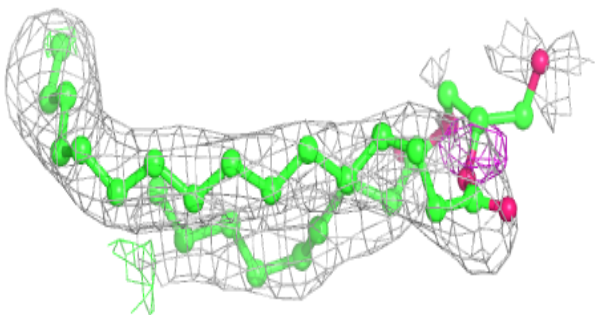
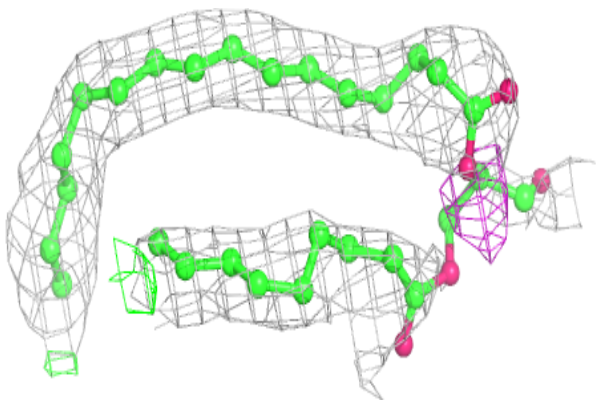


**Electron density around UNL B 633:**

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

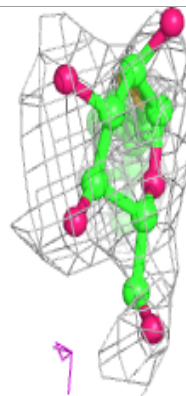
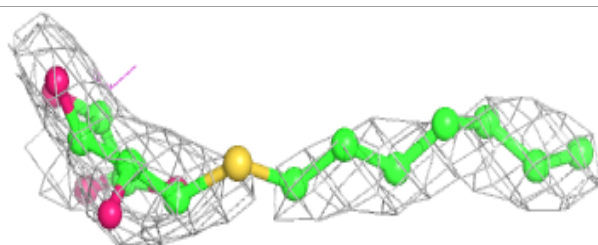
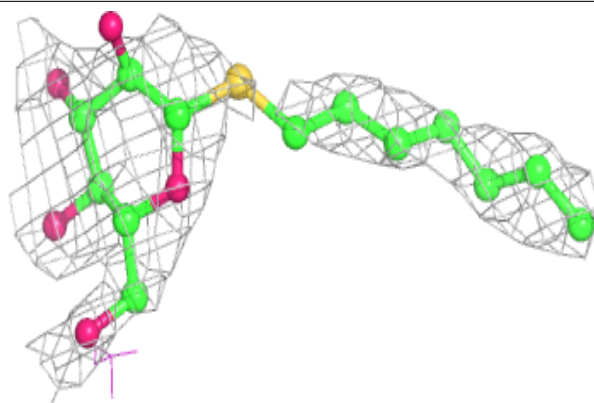
**Electron density around UNL b 633:**

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

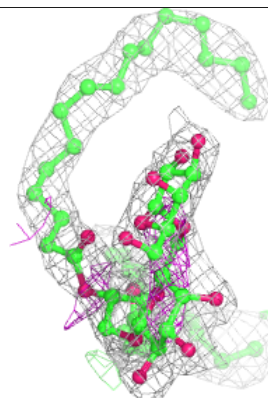
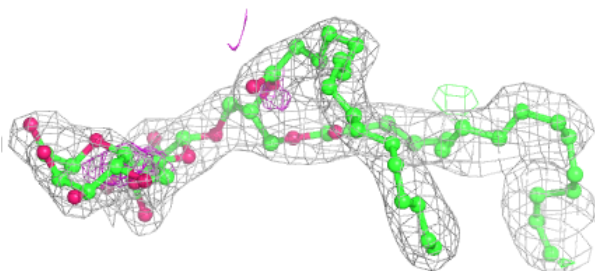
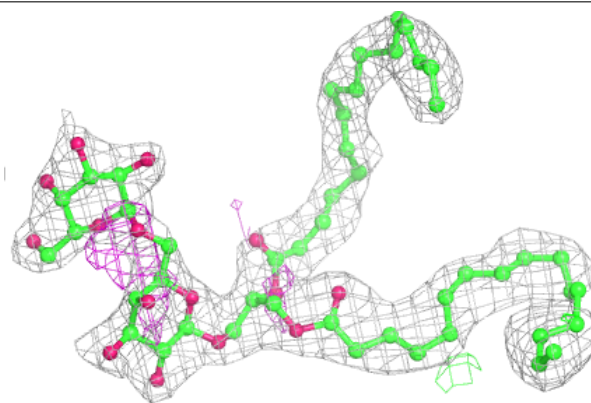


**Electron density around HTG B 624:**

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

**Electron density around DGD C 517:**

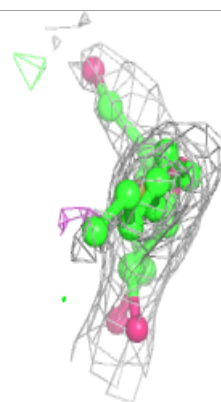
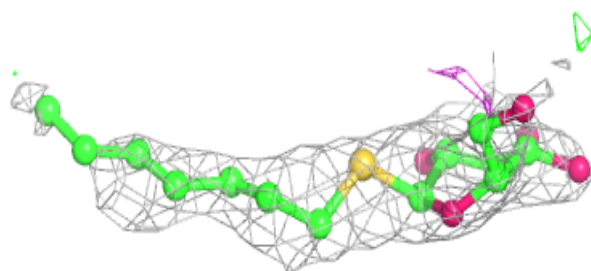
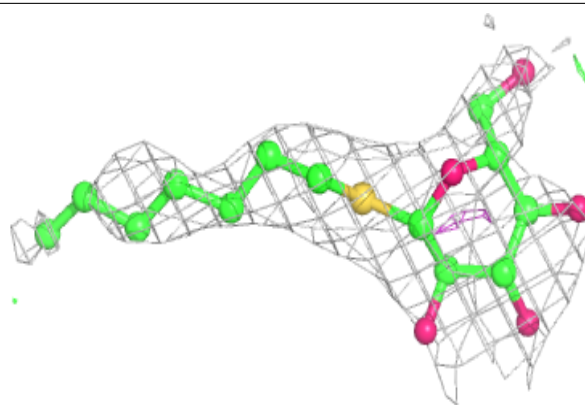
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



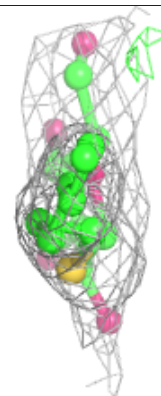
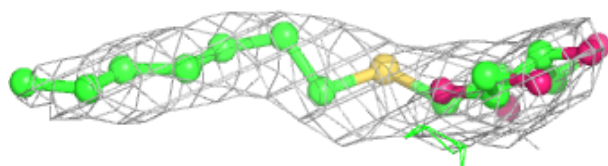
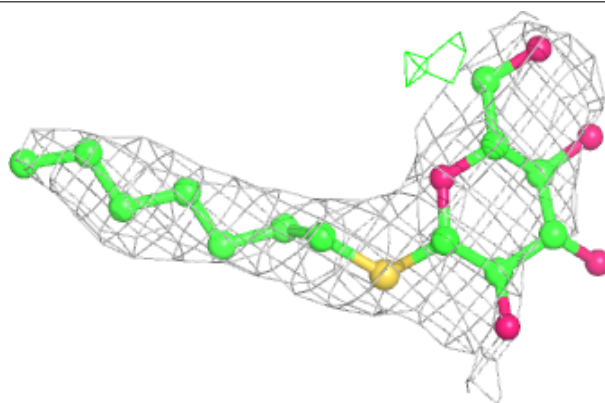


**Electron density around HTG C 523:**

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

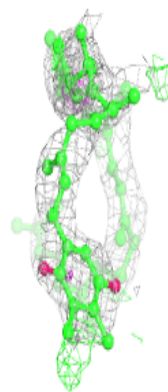
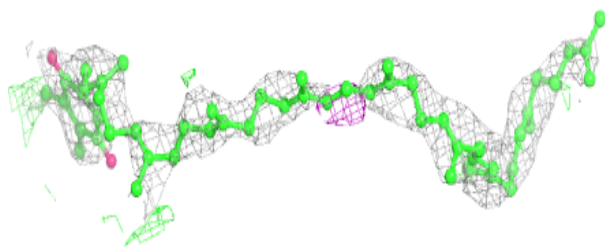
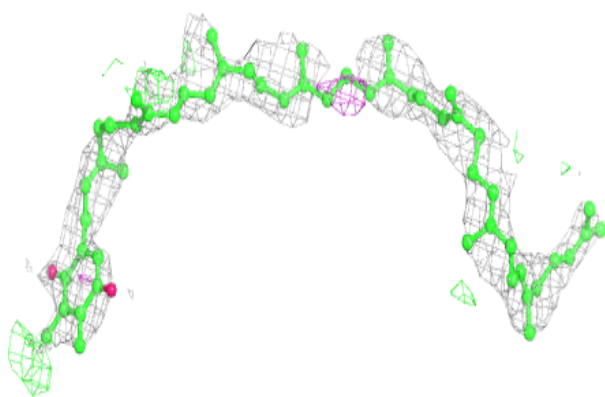
**Electron density around HTG b 632:**

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

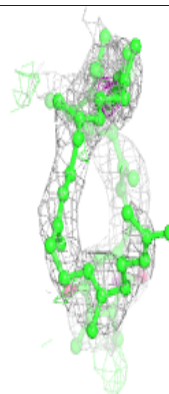
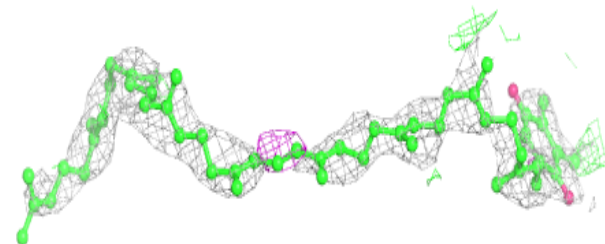
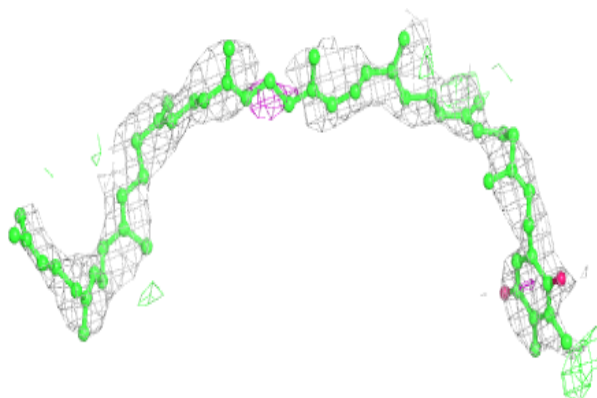


**Electron density around PL9 A 417 (B):**

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

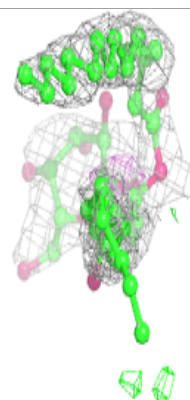
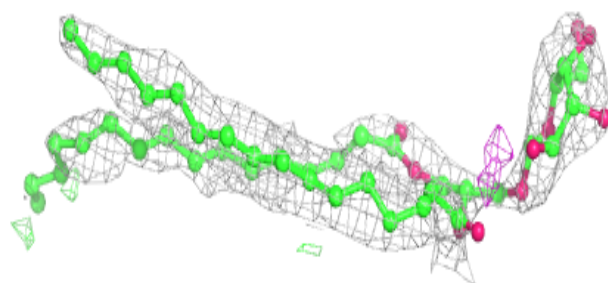
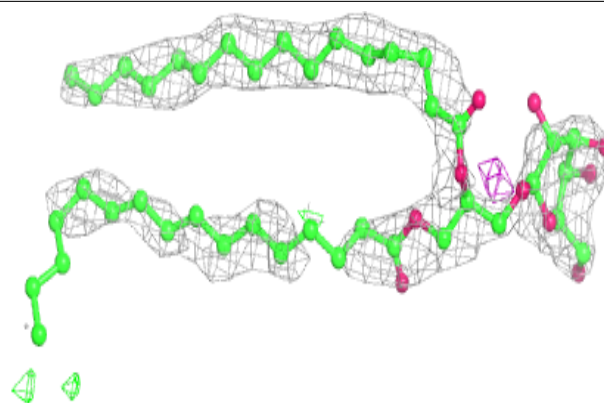
**Electron density around PL9 A 417 (A):**

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

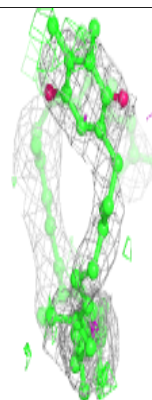
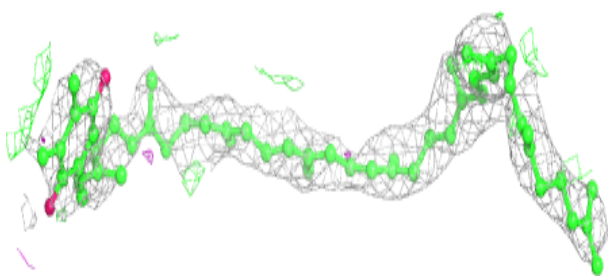
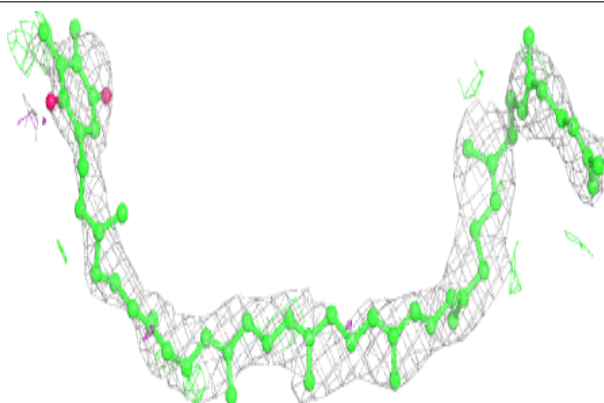


**Electron density around LMG C 520:**

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

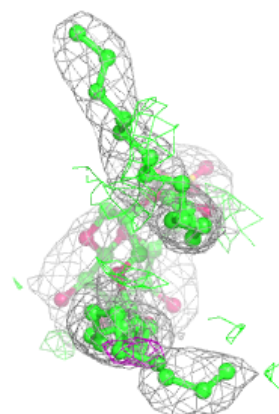
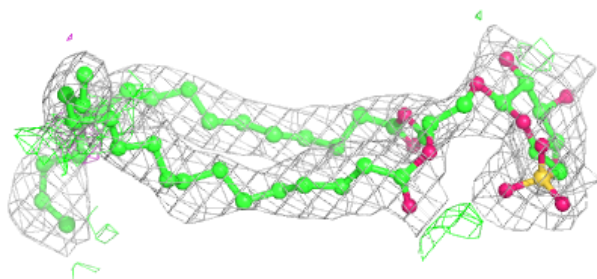
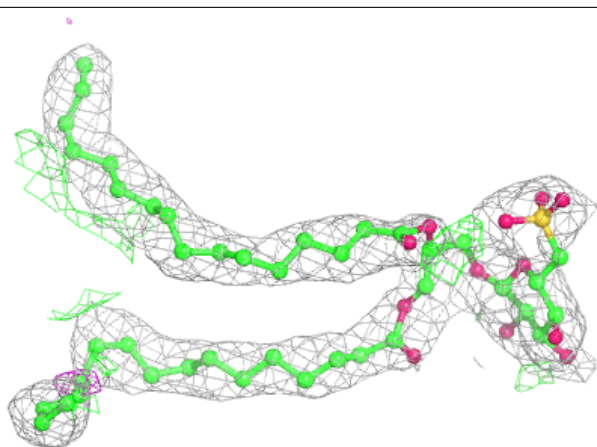
**Electron density around PL9 a 415 (A):**

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

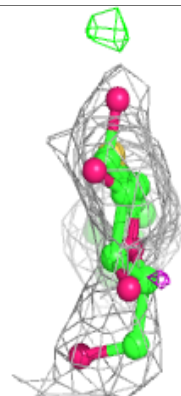
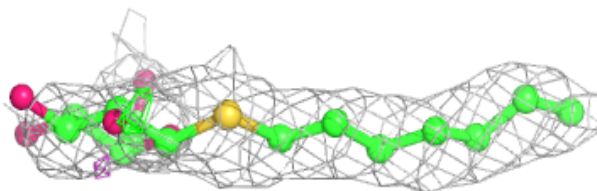
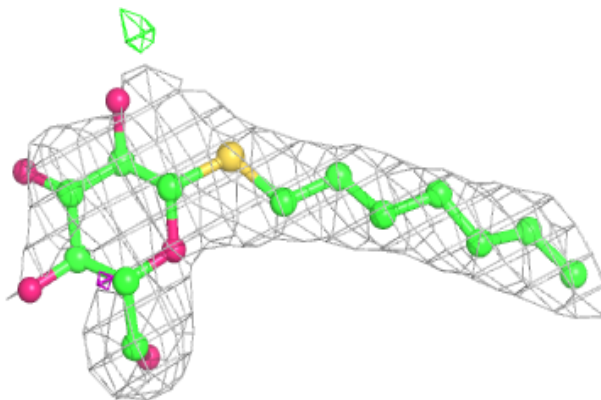


**Electron density around SQD b 601:**

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

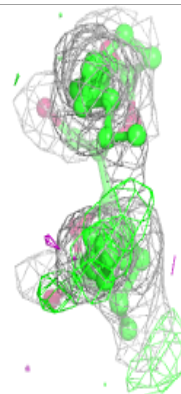
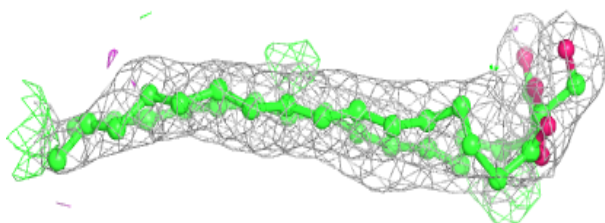
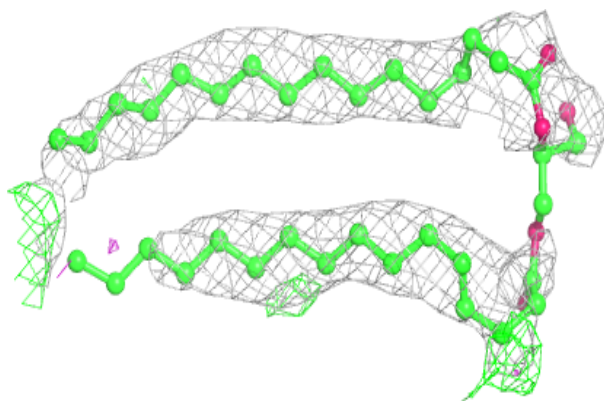
**Electron density around HTG b 608:**

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

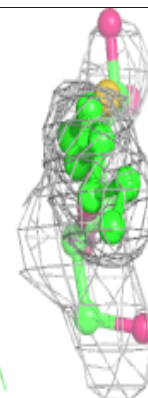
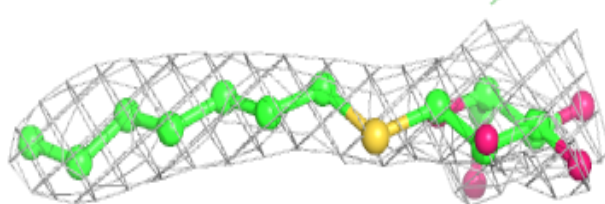
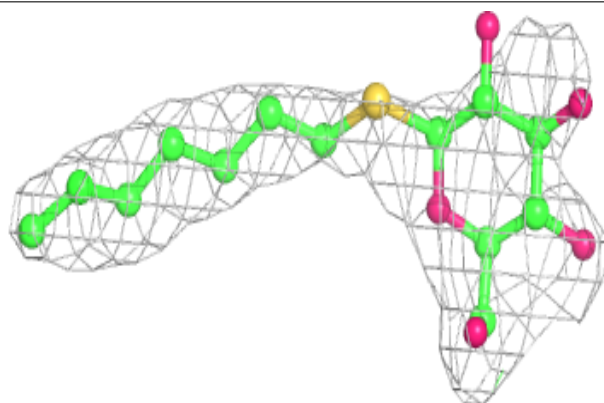


**Electron density around UNL i 101:**

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

**Electron density around HTG B 632:**

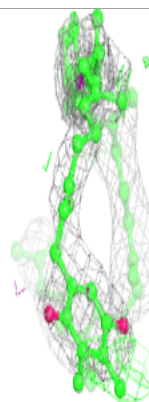
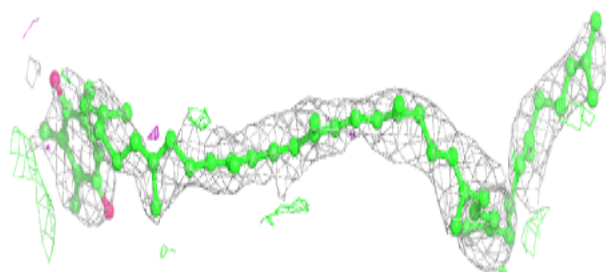
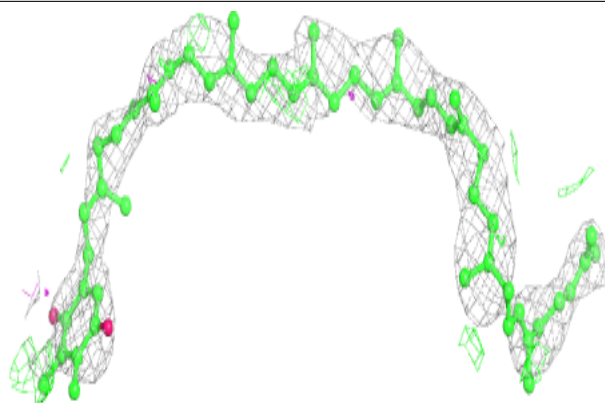
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



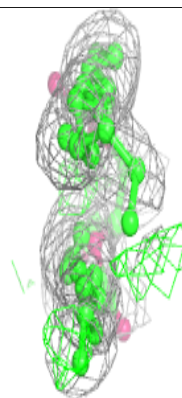
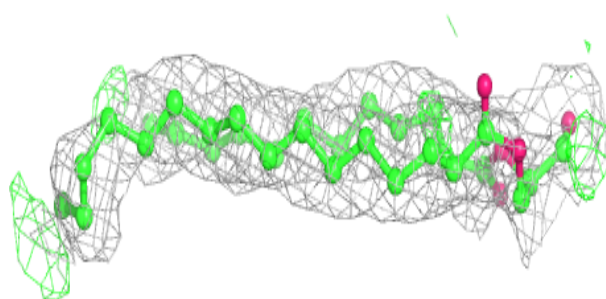
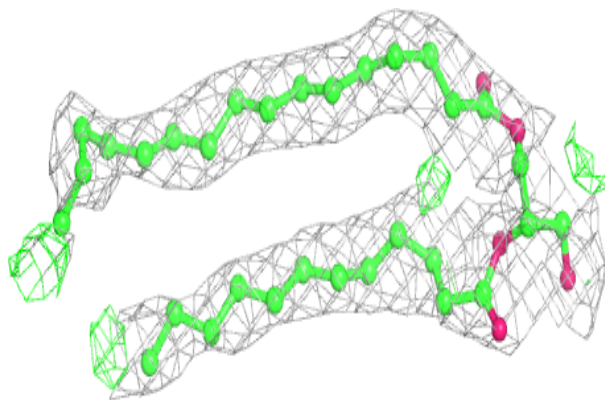


**Electron density around PL9 a 415 (B):**

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

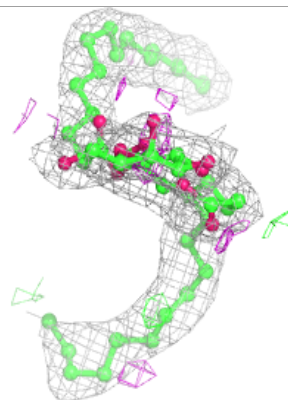
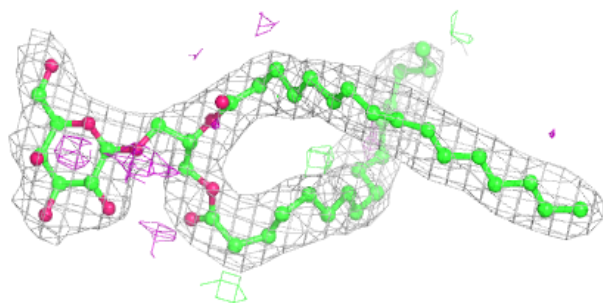
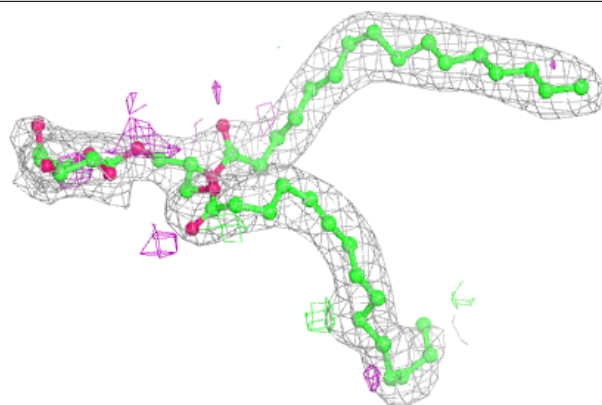
**Electron density around UNL d 413:**

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

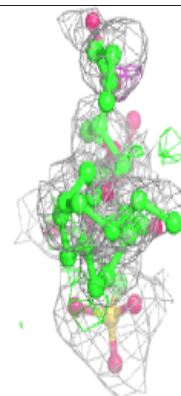
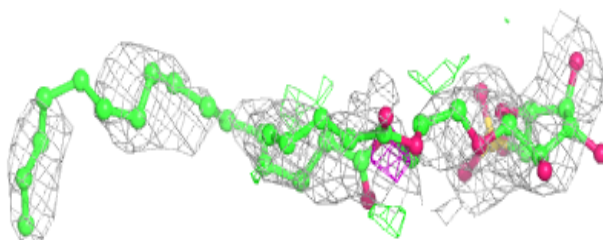
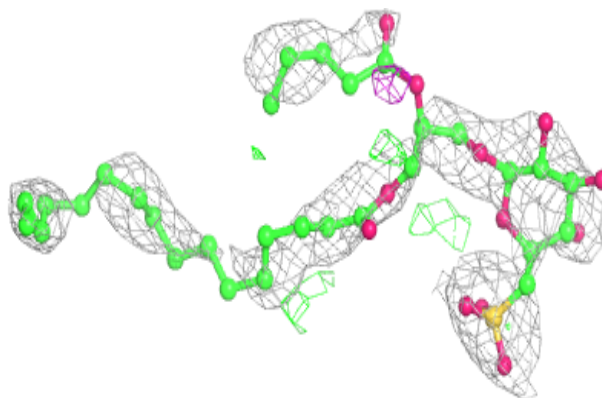


**Electron density around LMG b 629:**

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

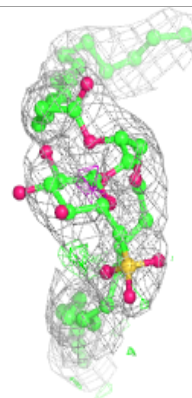
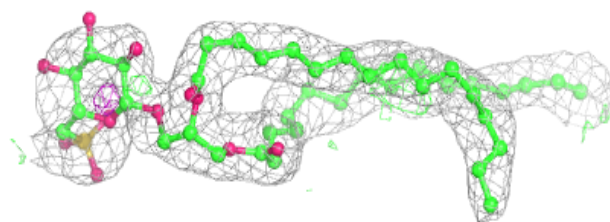
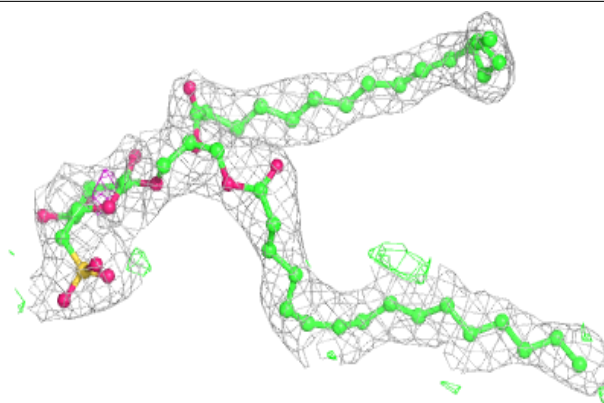
**Electron density around SQD F 104:**

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

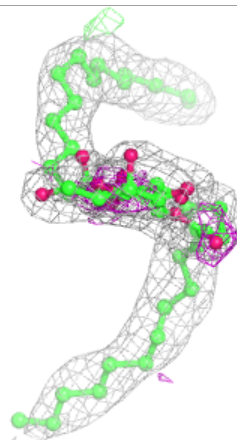
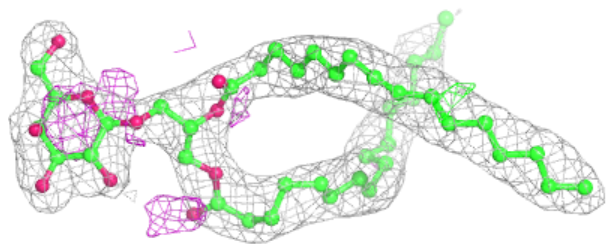
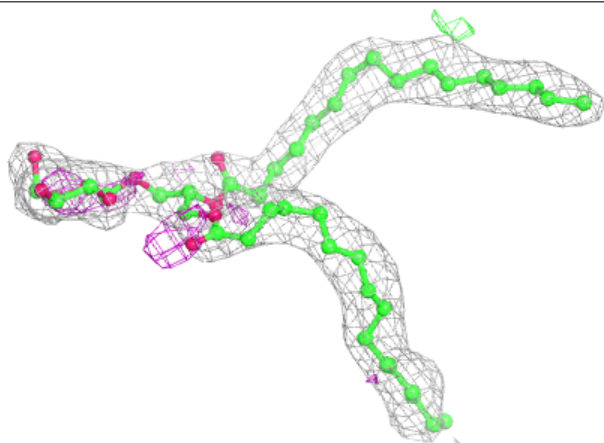


**Electron density around SQD B 636:**

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

**Electron density around LMG M 101:**

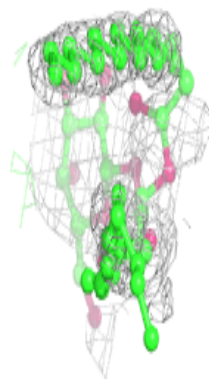
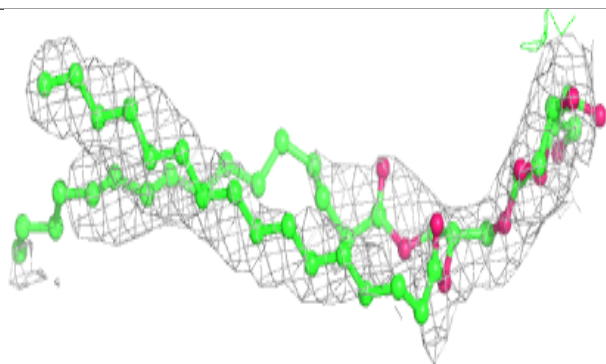
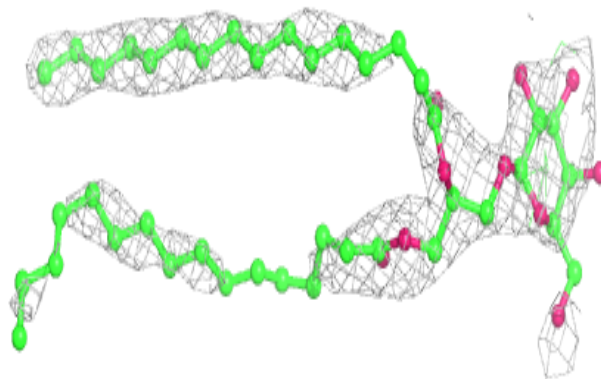
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



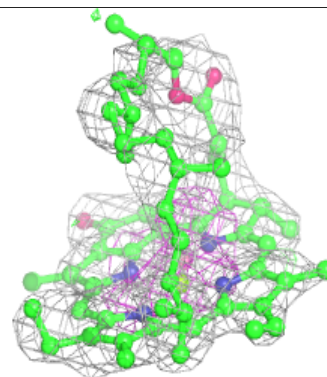
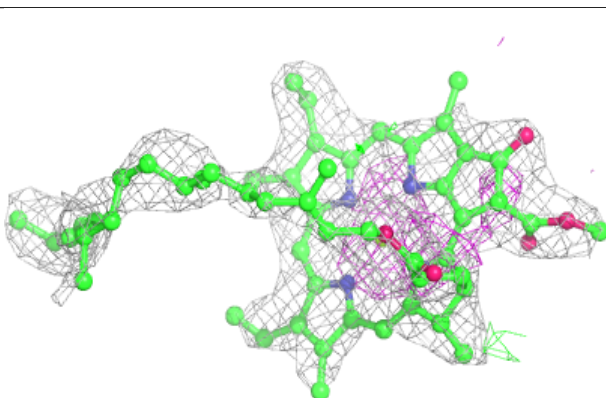
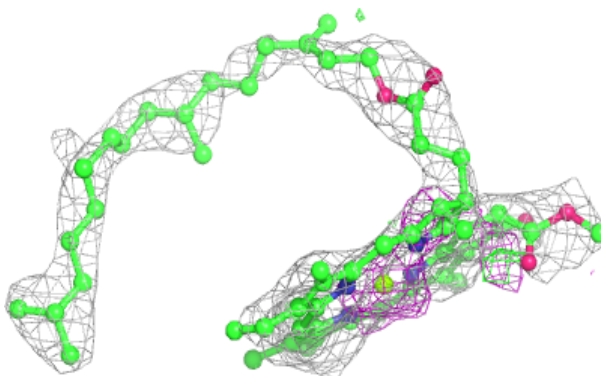


**Electron density around LMG c 522:**

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

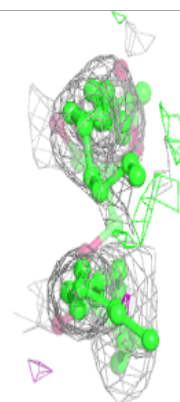
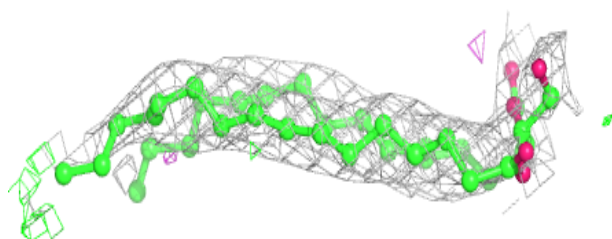
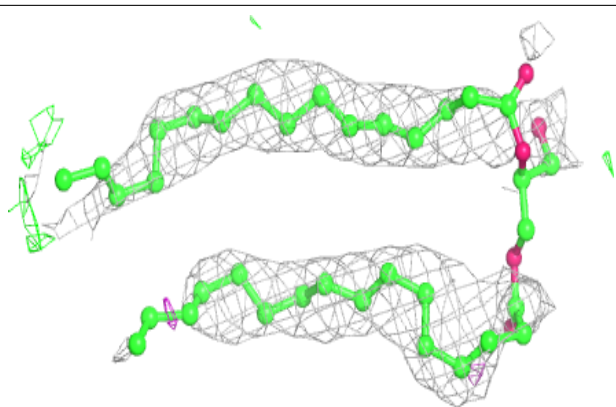
**Electron density around CLA C 514:**

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

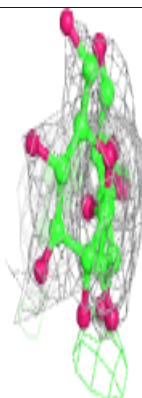
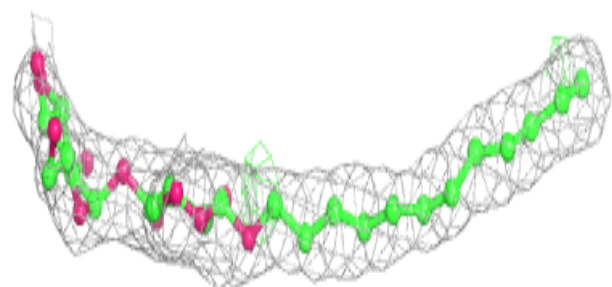
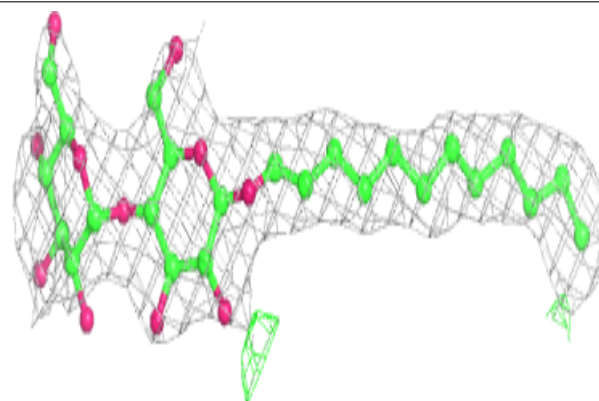


**Electron density around UNL I 101:**

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

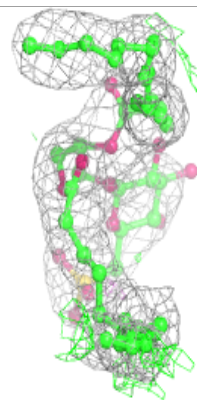
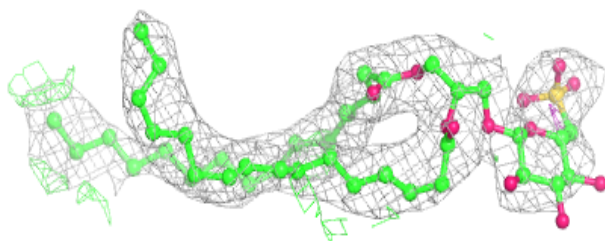
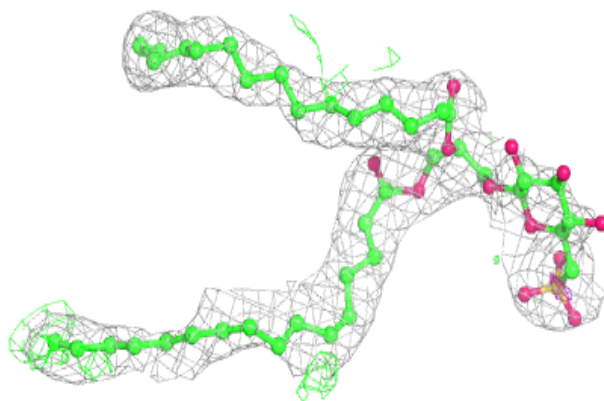
**Electron density around LMT M 102:**

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

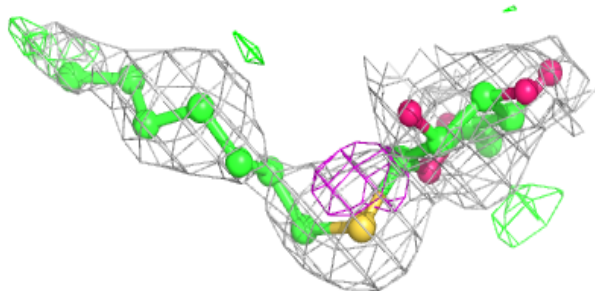
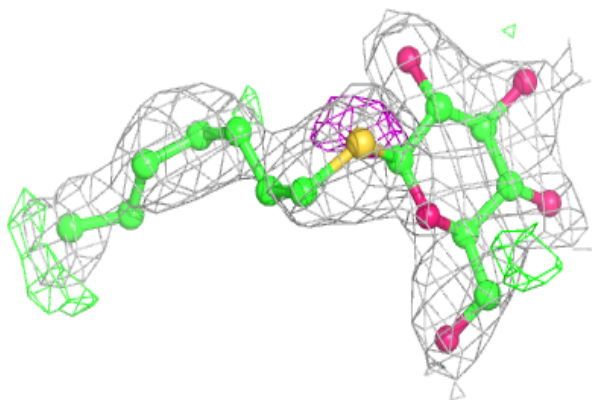


**Electron density around SQD A 413:**

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

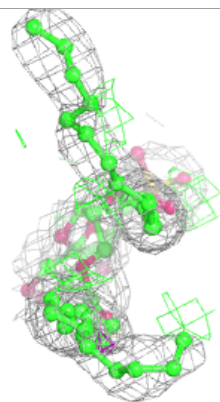
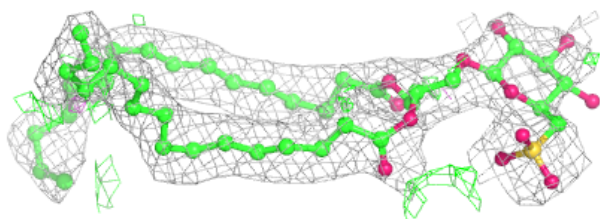
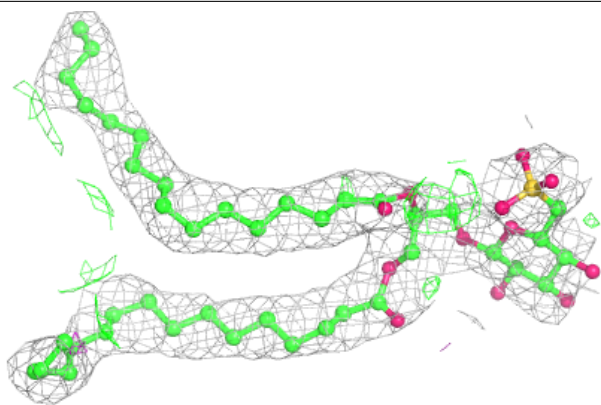
**Electron density around HTG b 631:**

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

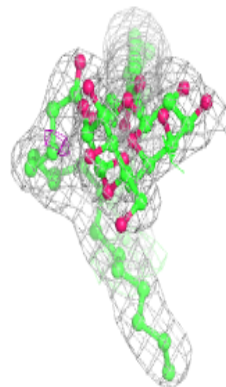
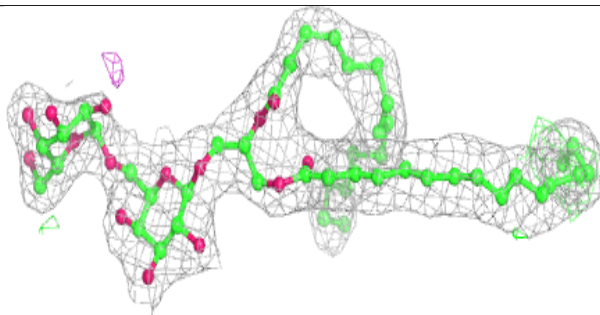
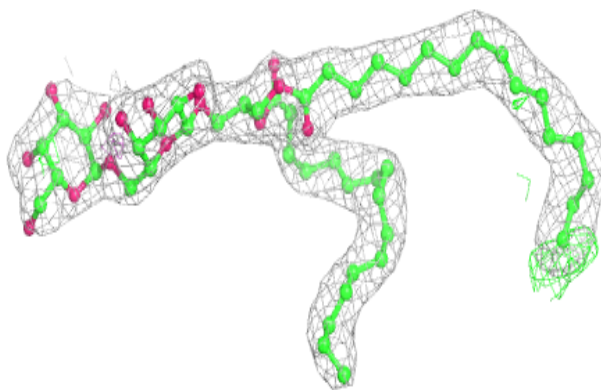


**Electron density around SQD B 621:**

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

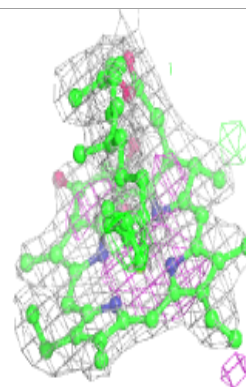
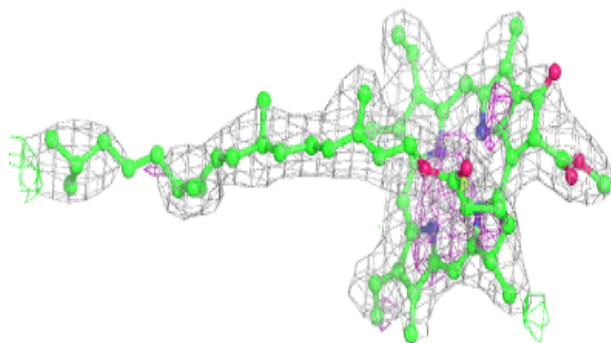
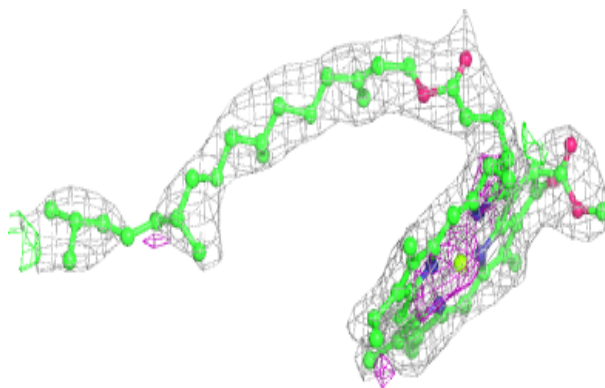
**Electron density around DGD h 102:**

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



**Electron density around CLA C 505:**

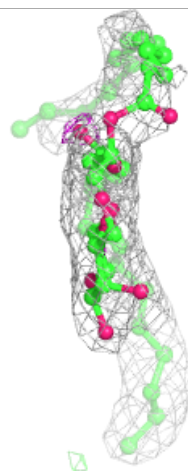
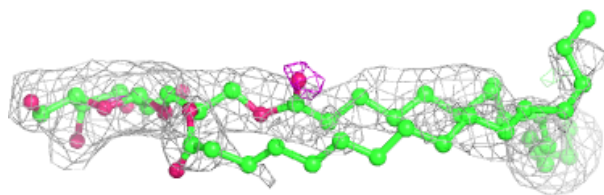
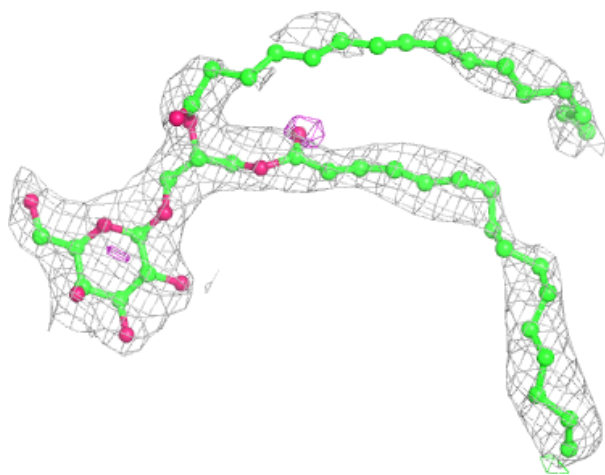
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





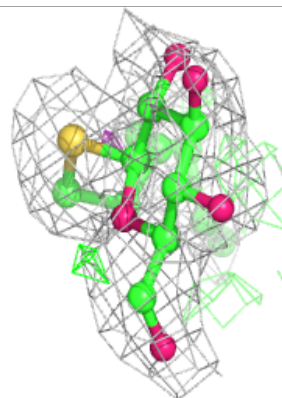
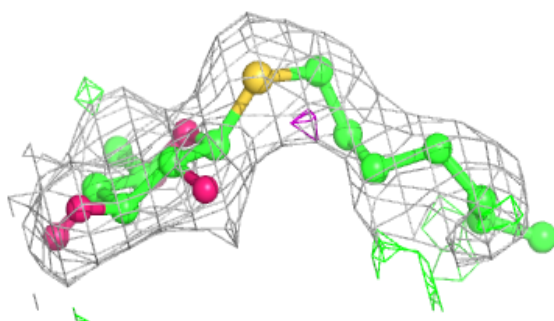
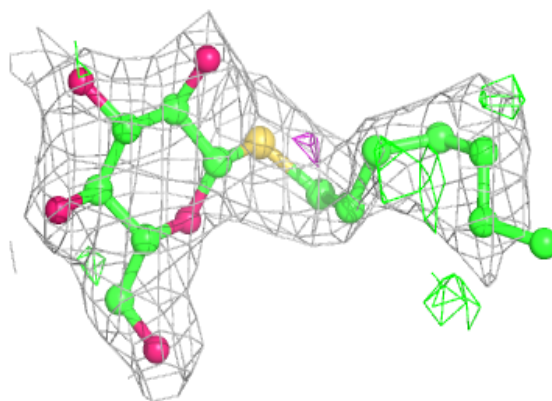
**Electron density around LMG k 101:**

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

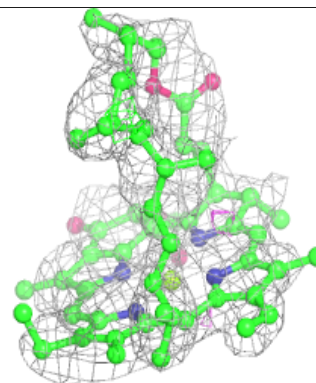
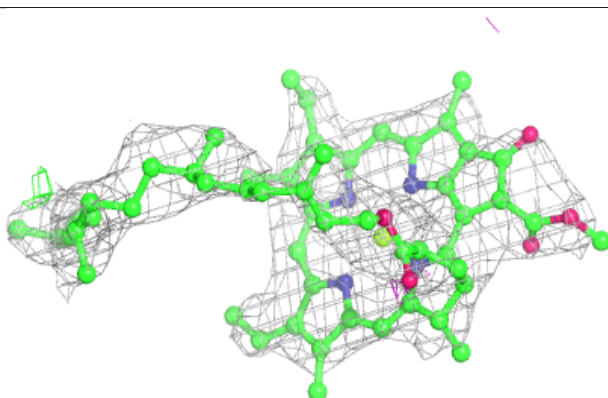
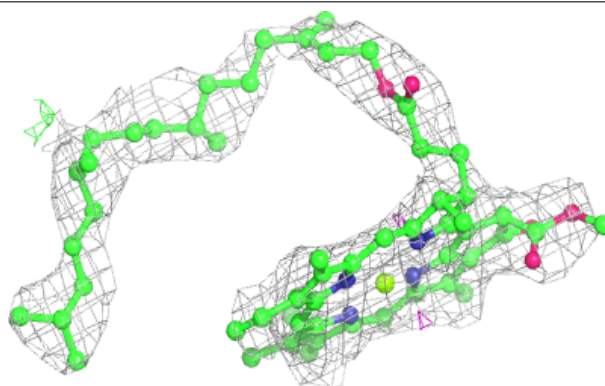


**Electron density around HTG B 623:**

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

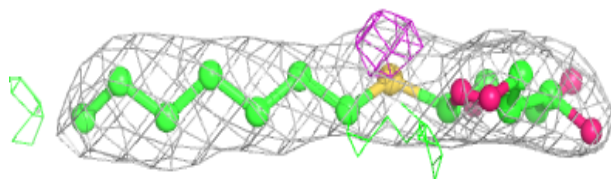
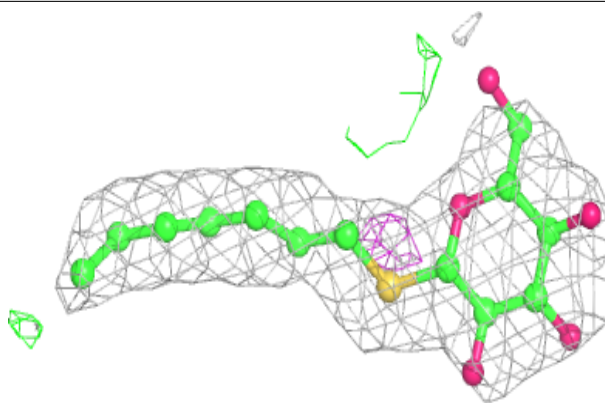
**Electron density around CLA c 517:**

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

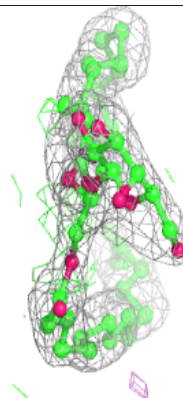
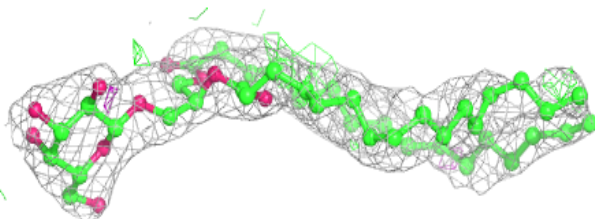
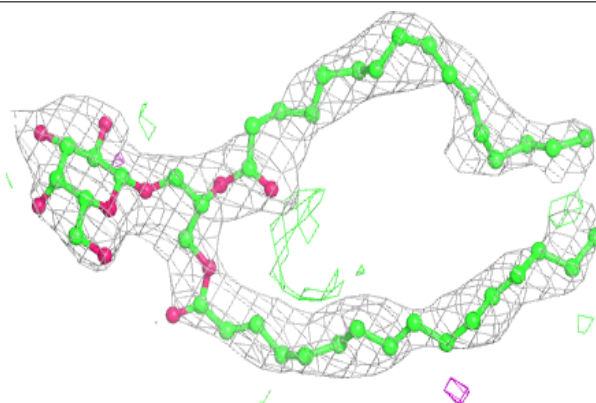


**Electron density around HTG b 607:**

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

**Electron density around LMG C 501:**

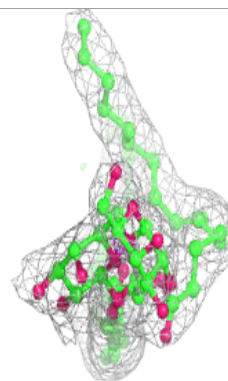
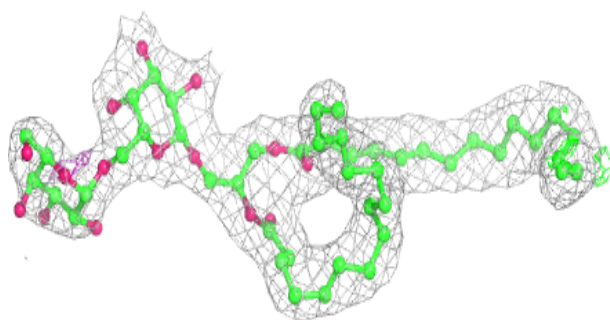
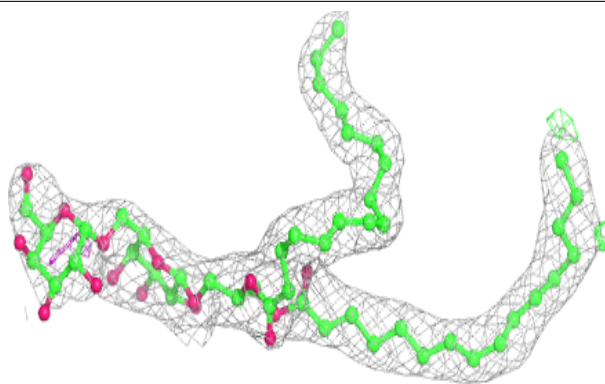
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



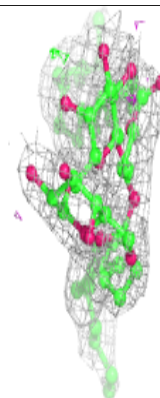
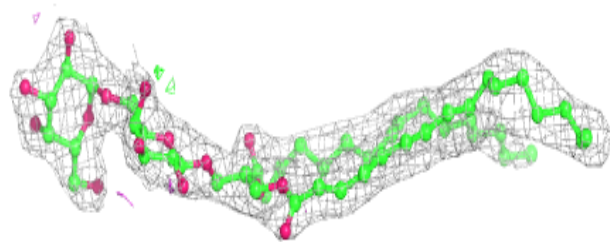
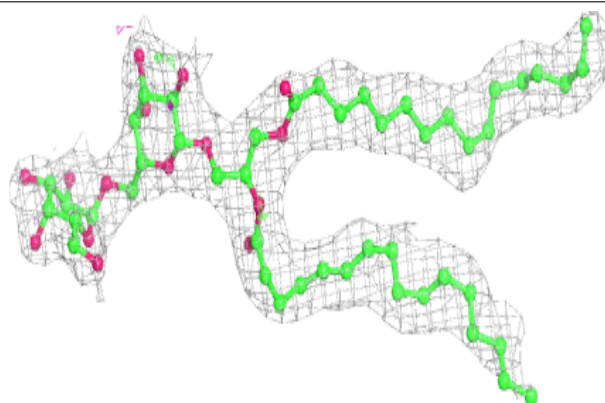


**Electron density around DGD H 102:**

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

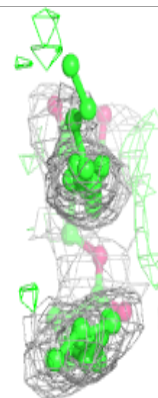
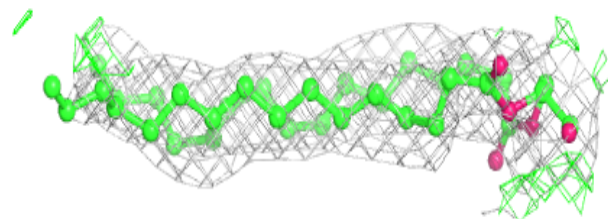
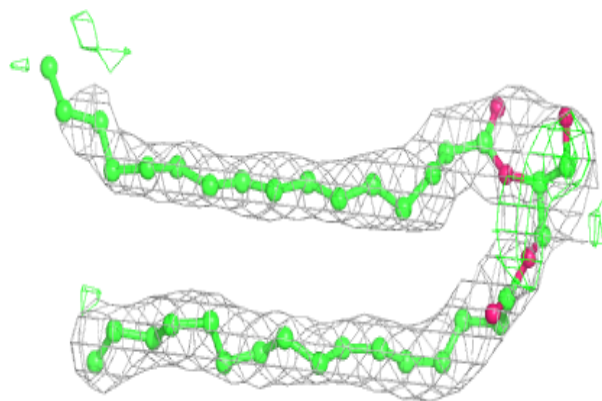
**Electron density around DGD C 518:**

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

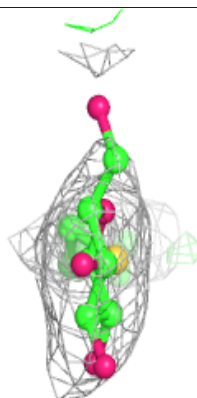
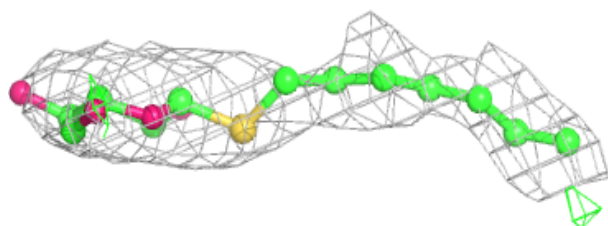
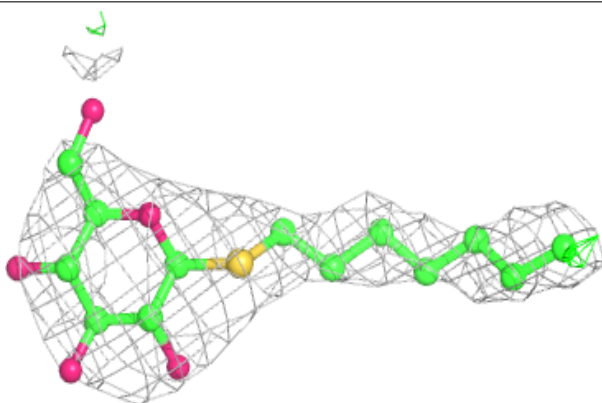


**Electron density around UNL D 414:**

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

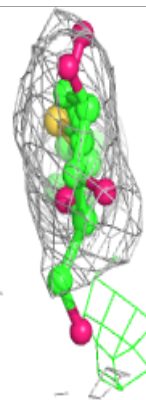
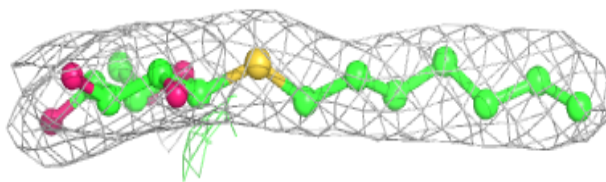
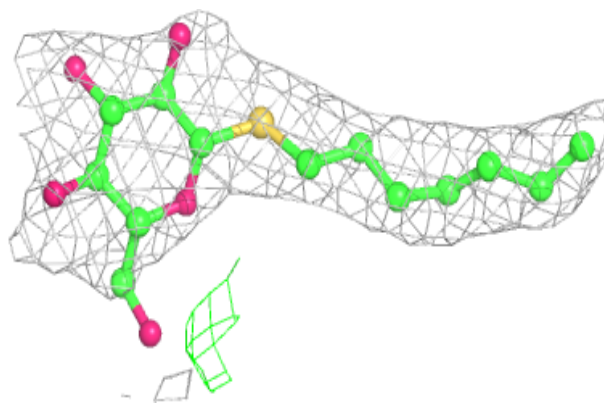
**Electron density around HTG c 523:**

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



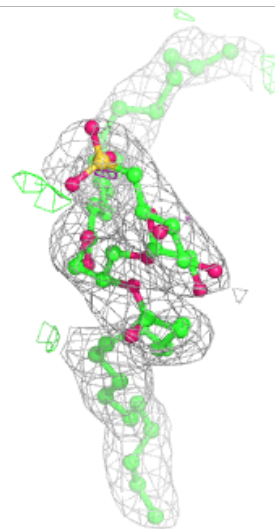
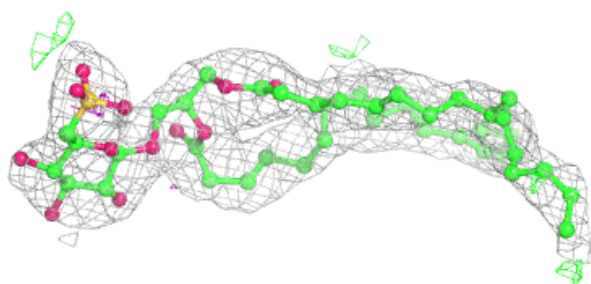
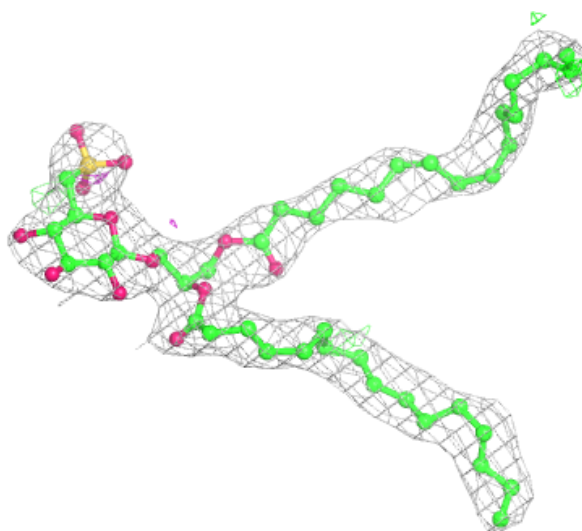
**Electron density around HTG B 631:**

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



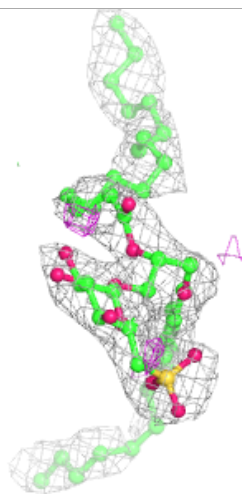
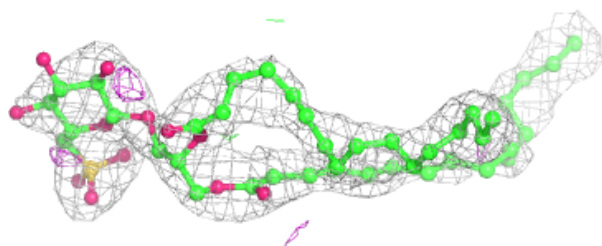
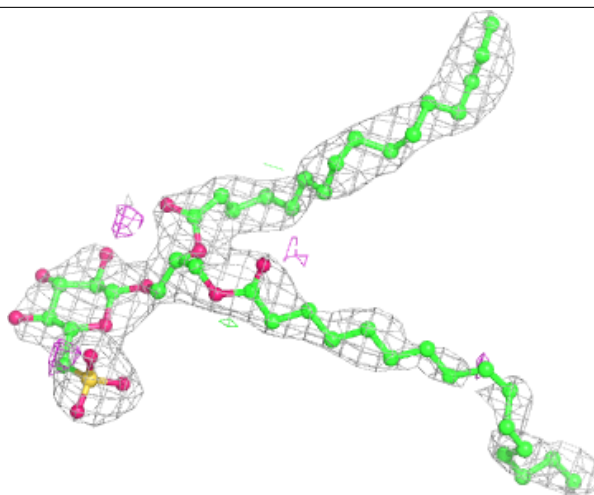
**Electron density around SQD a 413:**

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



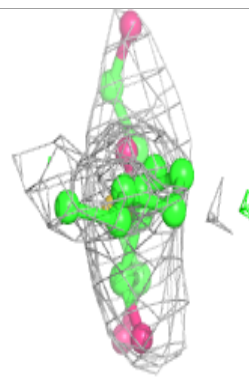
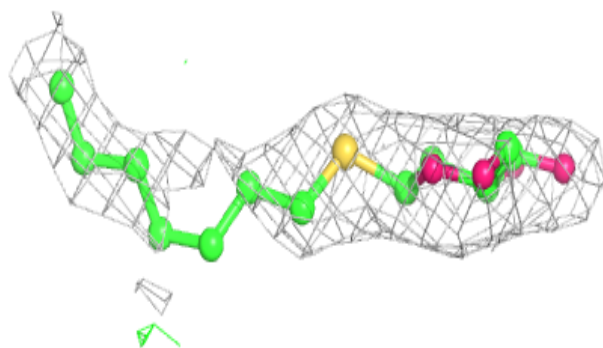
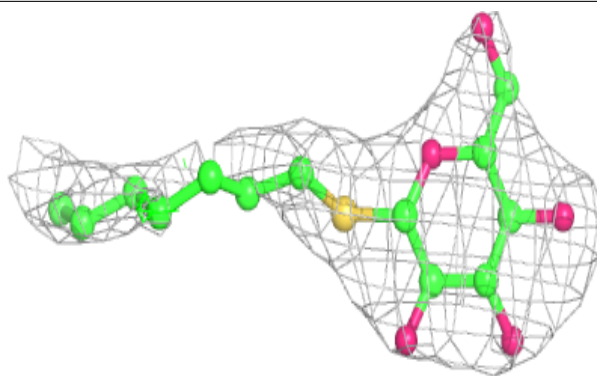
**Electron density around SQD A 410:**

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

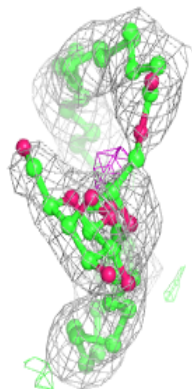
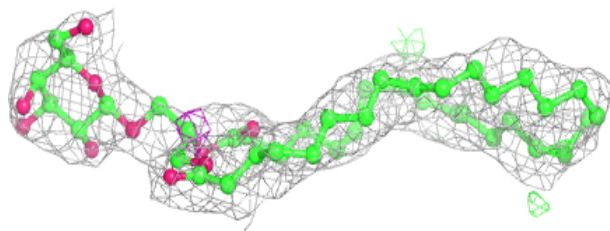
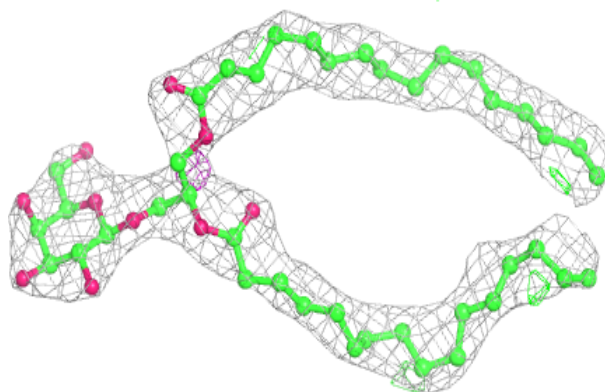


**Electron density around HTG C 522:**

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

**Electron density around LMG a 414:**

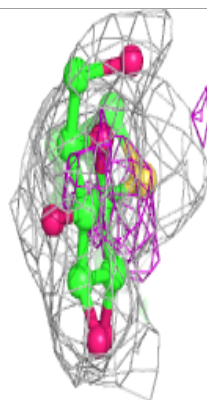
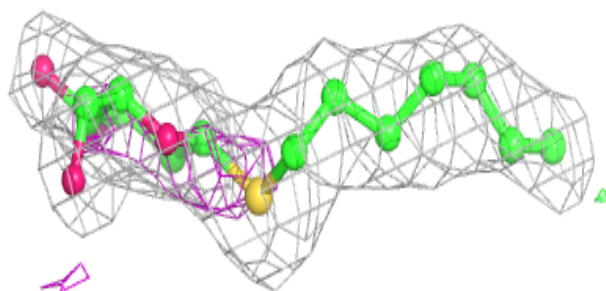
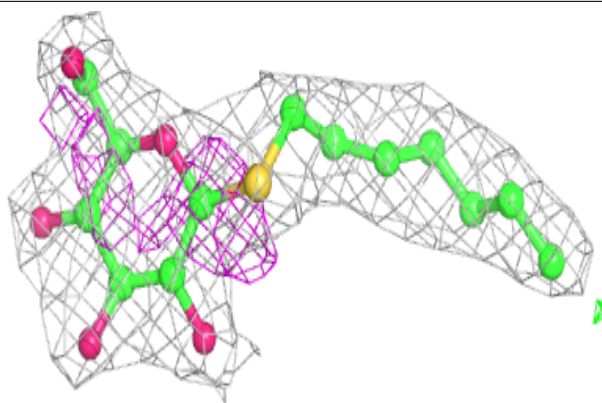
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



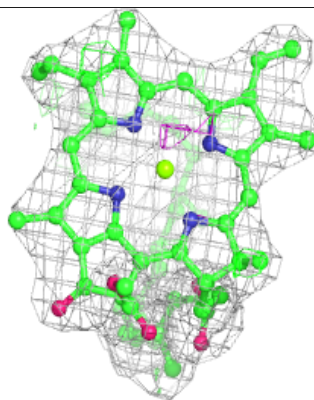
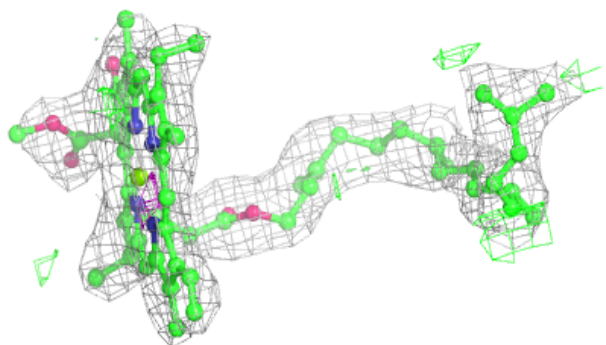
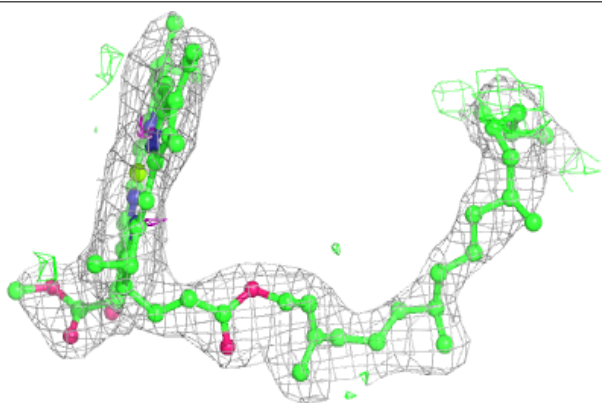


**Electron density around HTG b 602:**

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

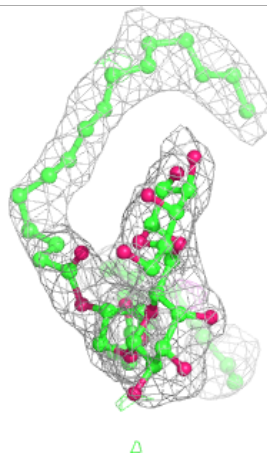
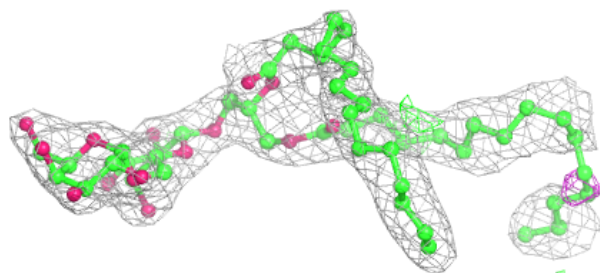
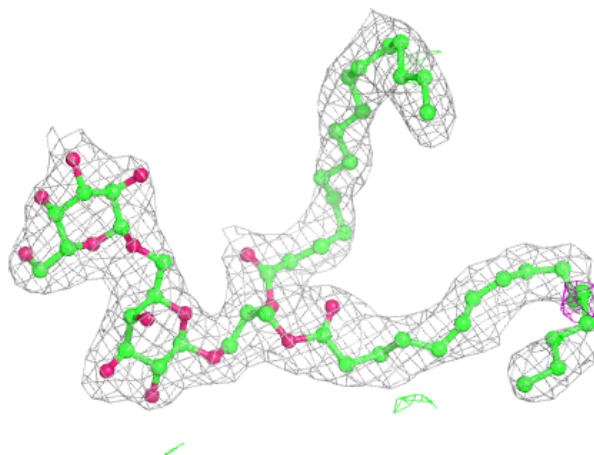
**Electron density around CLA c 510:**

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

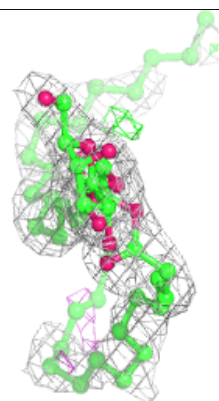
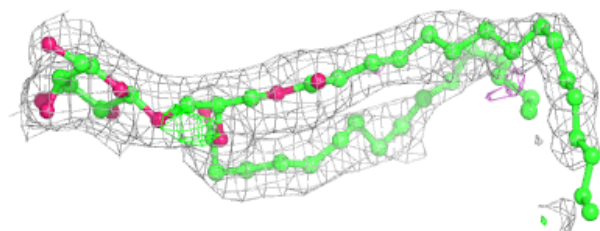
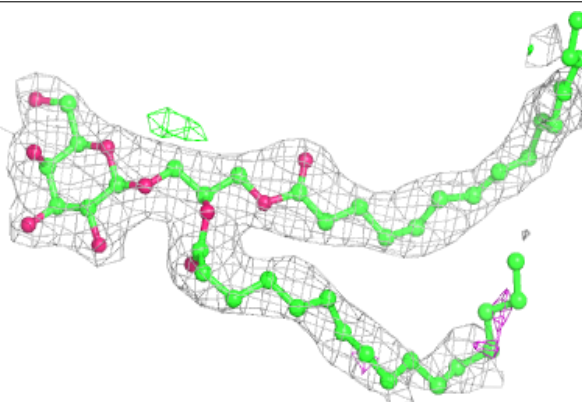


**Electron density around DGD c 520:**

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

**Electron density around LMG D 416:**

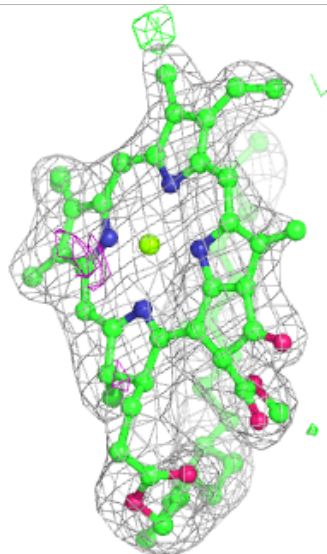
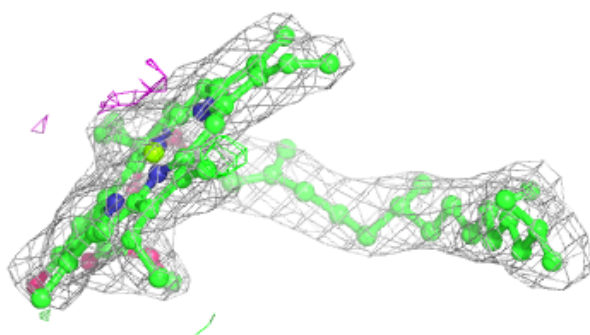
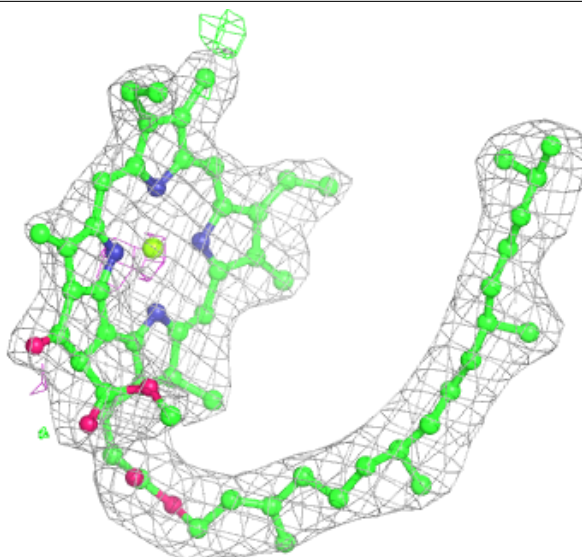
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





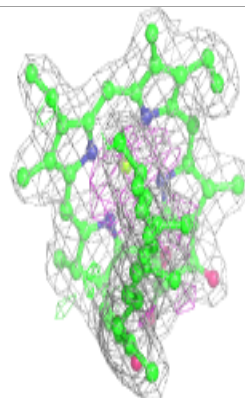
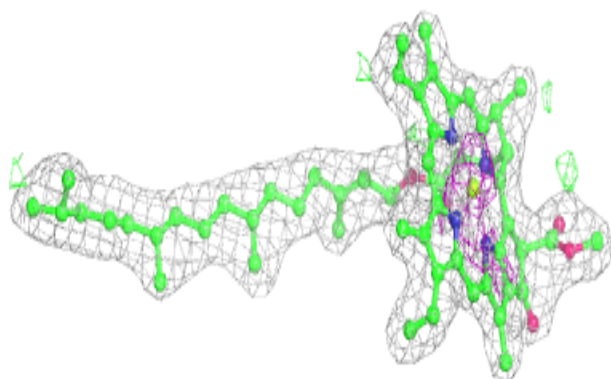
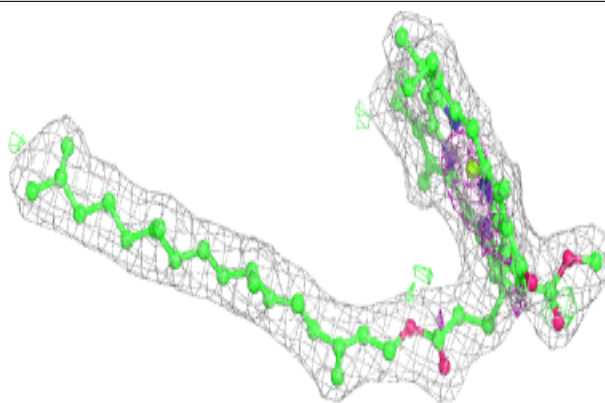
**Electron density around CLA c 511:**

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

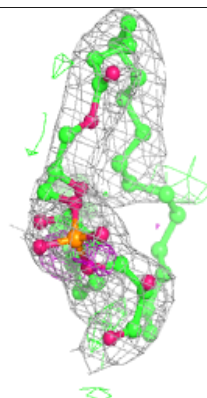
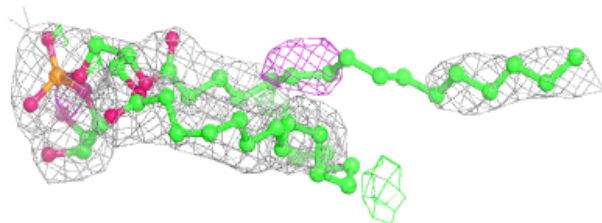
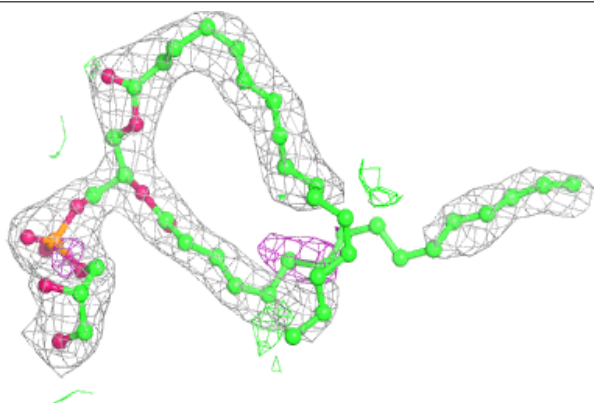


**Electron density around CLA b 616:**

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

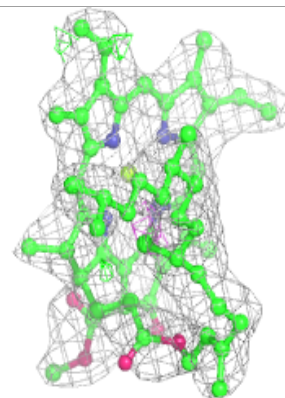
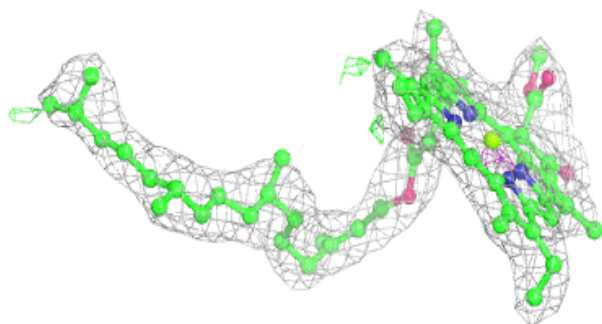
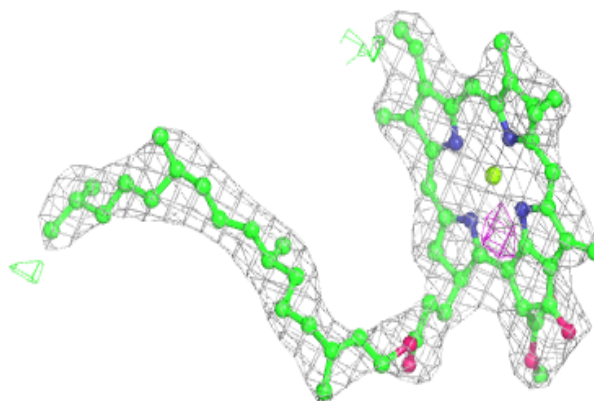
**Electron density around LHG D 412:**

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

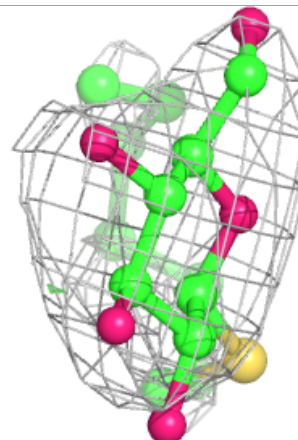
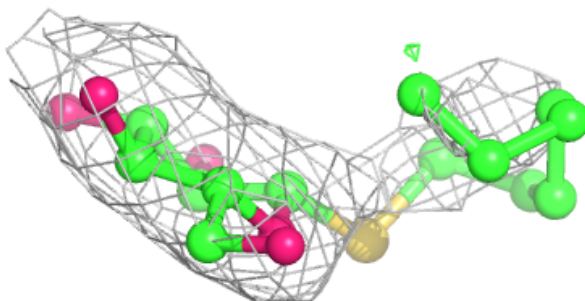
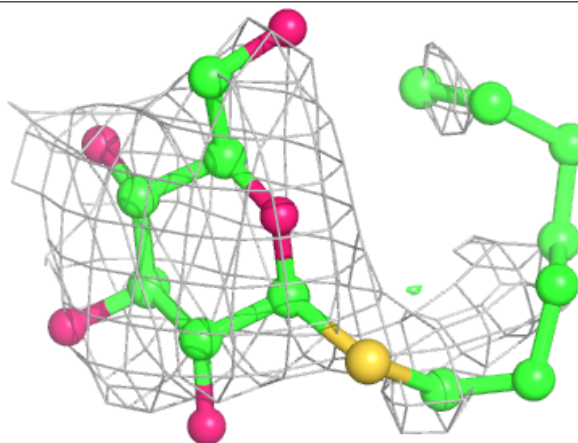


**Electron density around CLA C 512:**

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

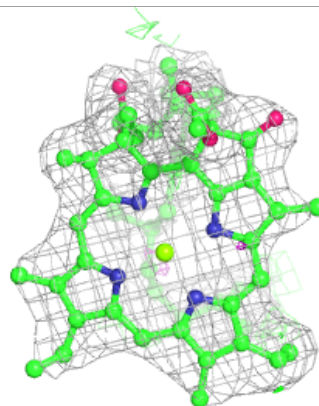
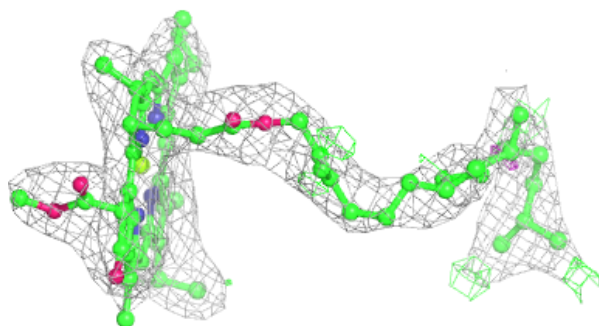
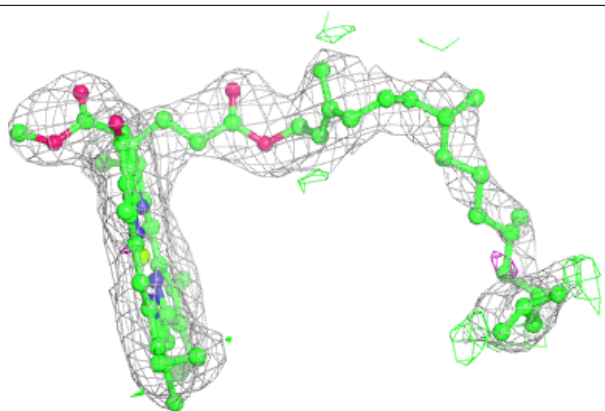
**Electron density around HTG V 206:**

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

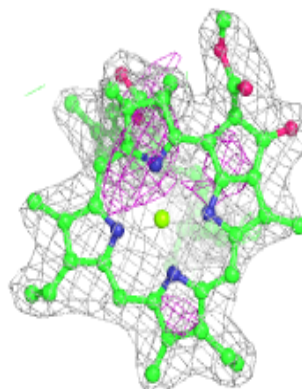
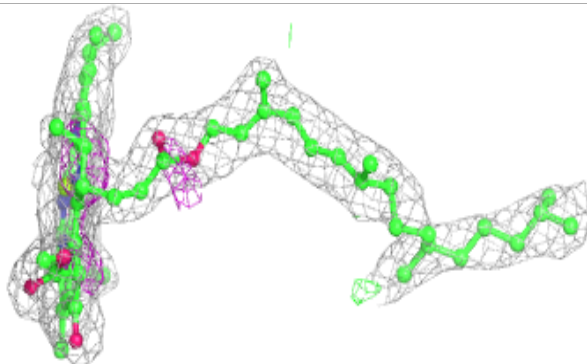
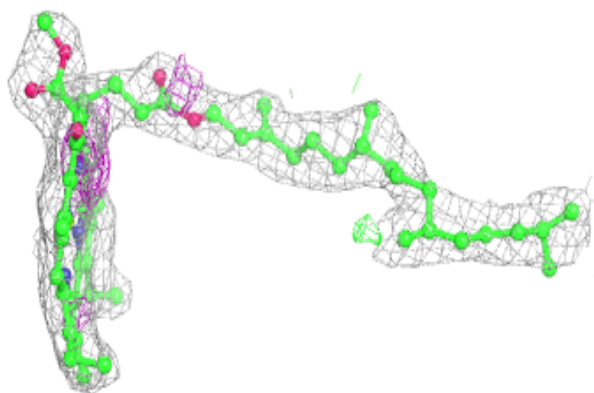


**Electron density around CLA C 507:**

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

**Electron density around CLA B 607:**

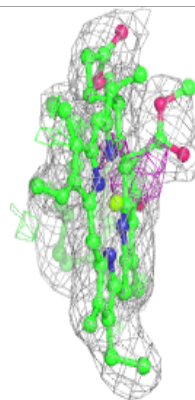
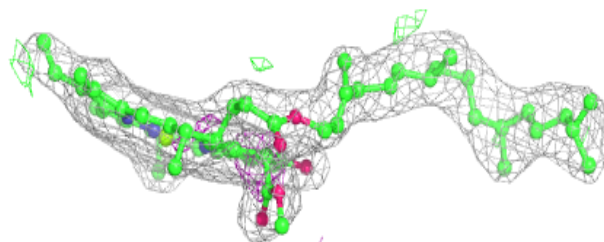
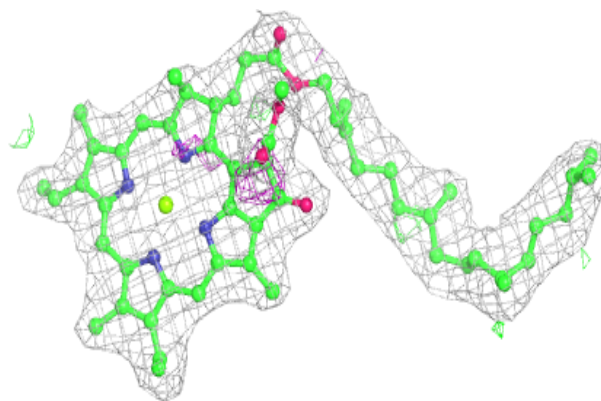
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



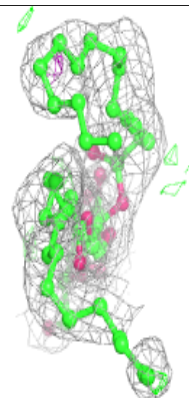
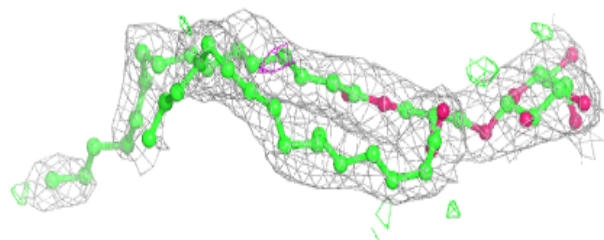
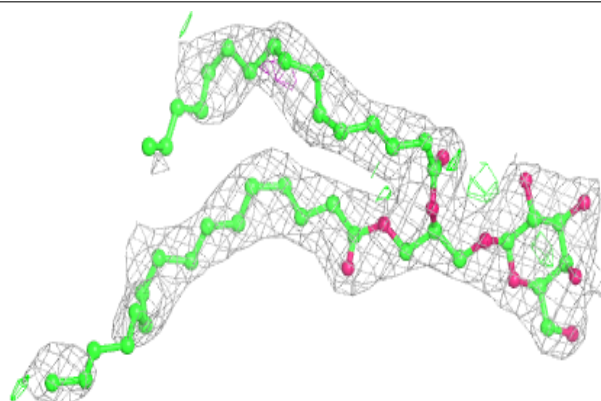


**Electron density around CLA b 611:**

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

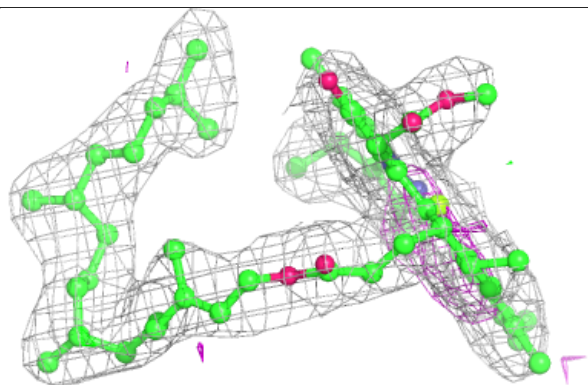
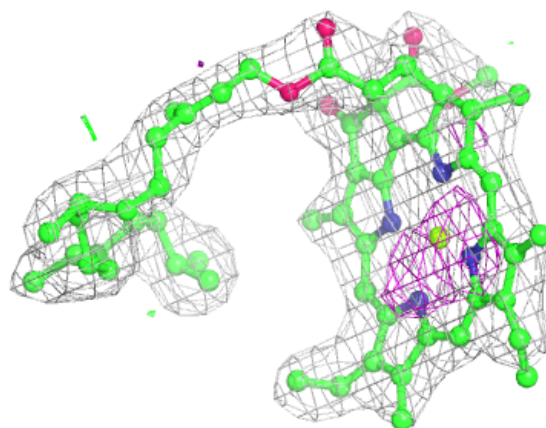
**Electron density around LMG d 416:**

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



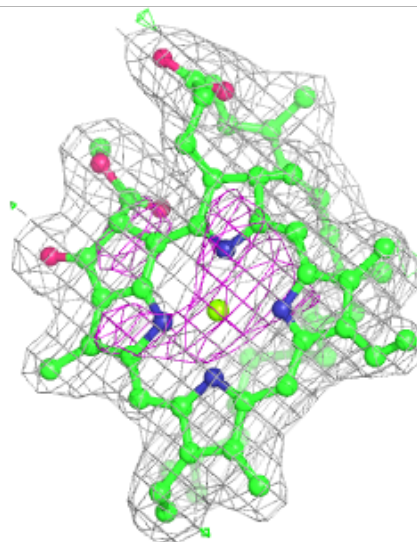
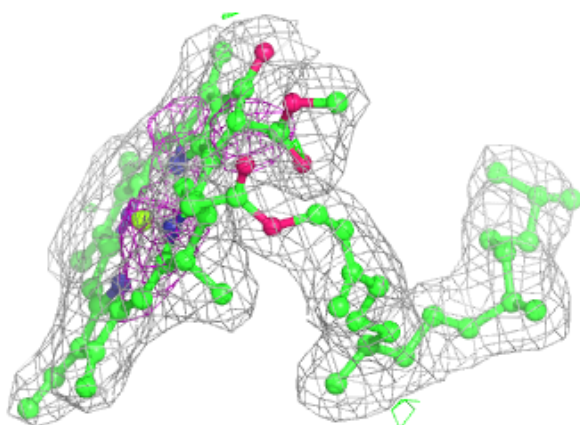
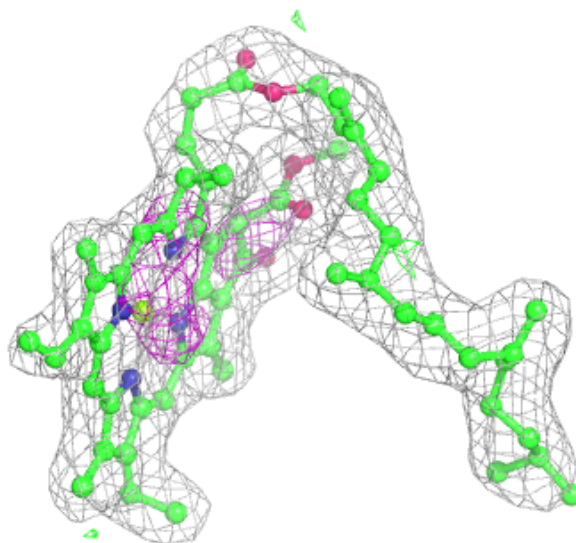
**Electron density around CLA c 507:**

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



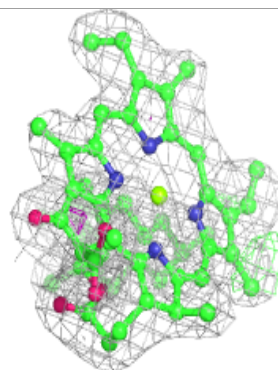
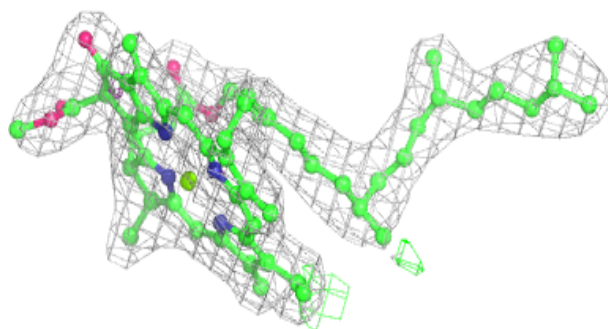
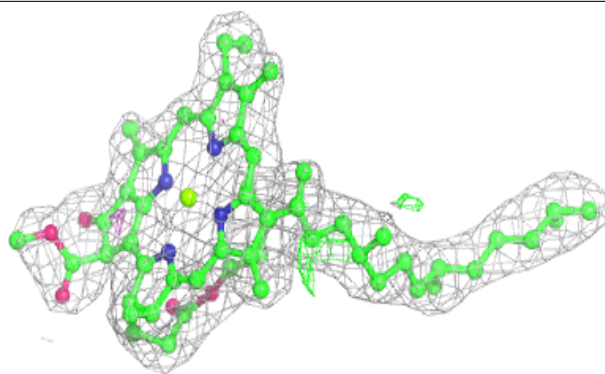
**Electron density around CLA B 614:**

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

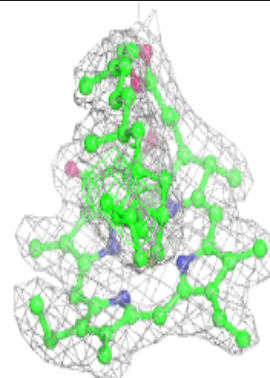
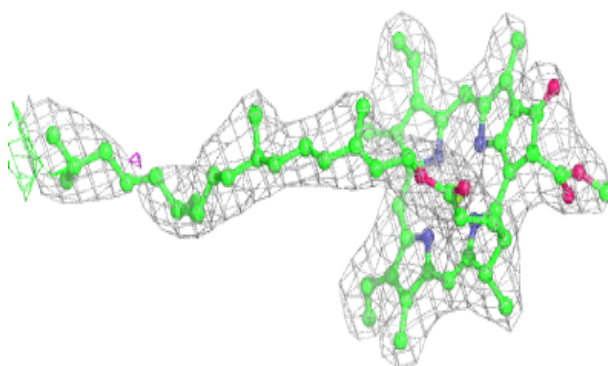
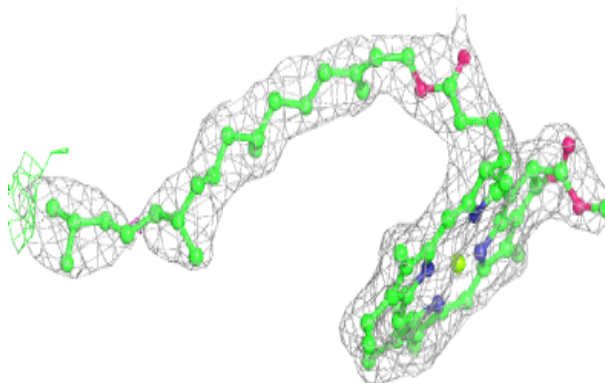


**Electron density around CLA c 509:**

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

**Electron density around CLA c 508:**

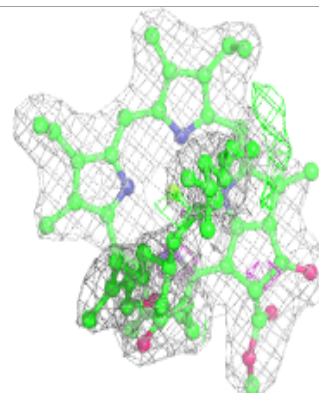
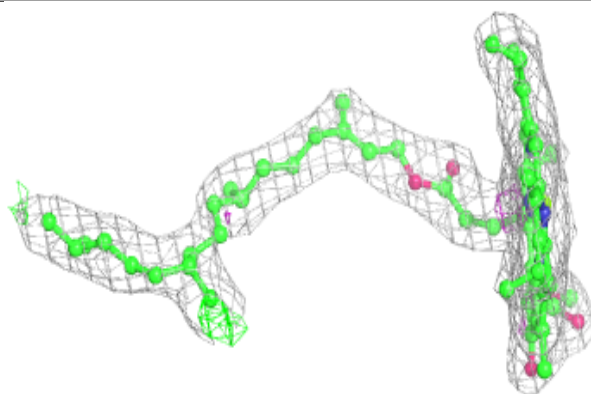
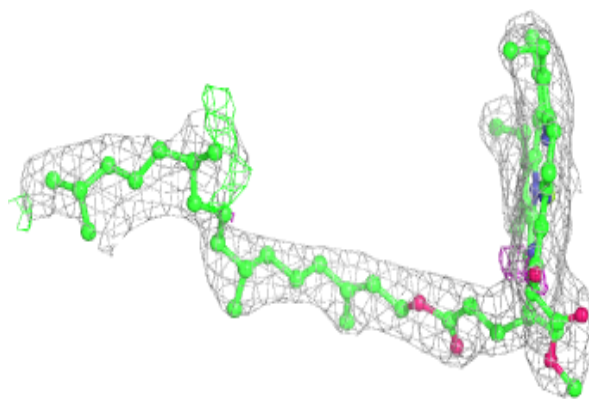
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



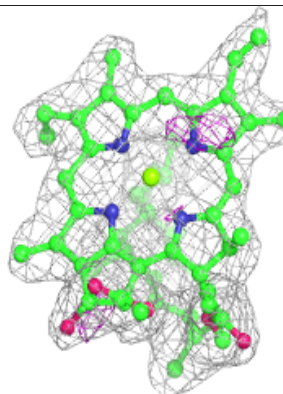
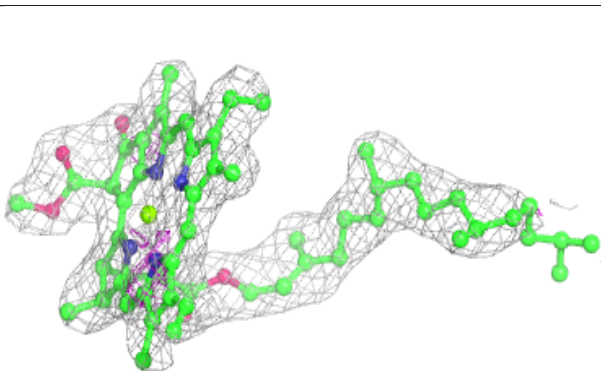
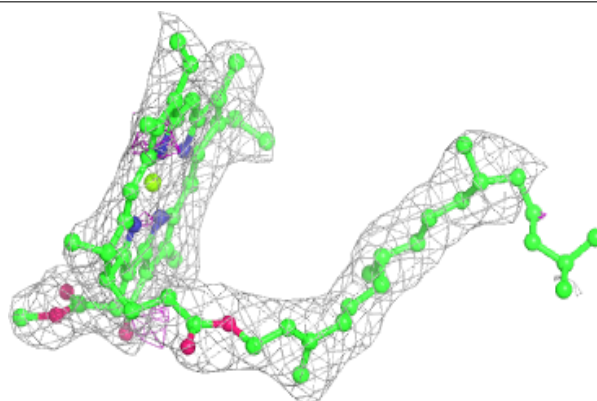


**Electron density around CLA b 615:**

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

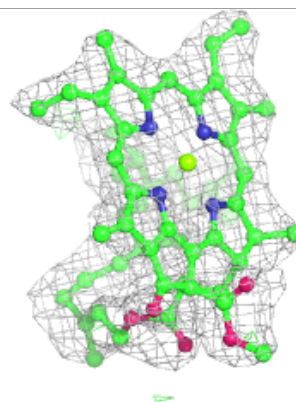
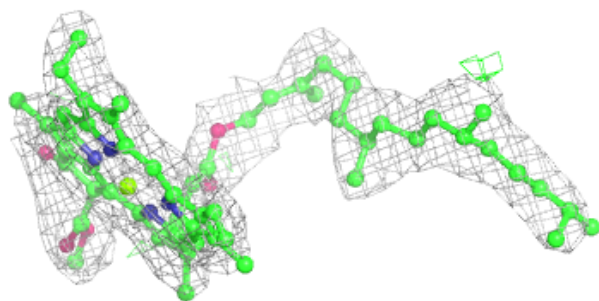
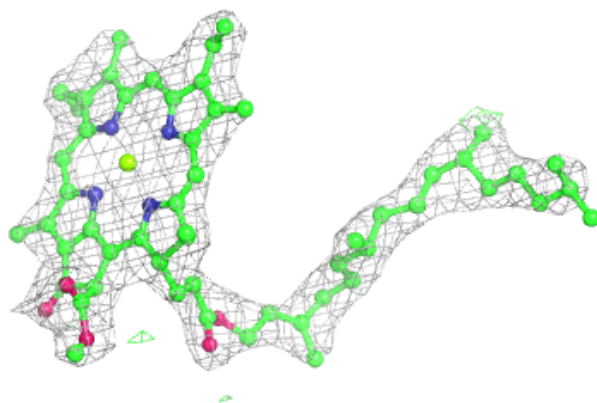
**Electron density around CLA c 512:**

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

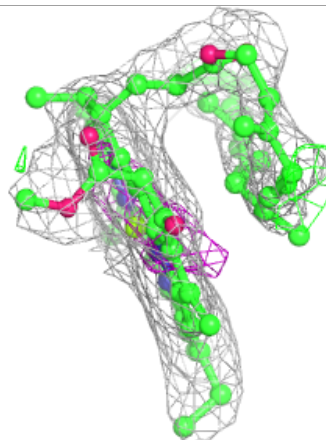
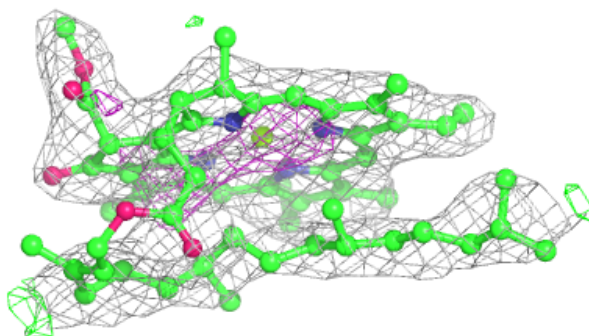
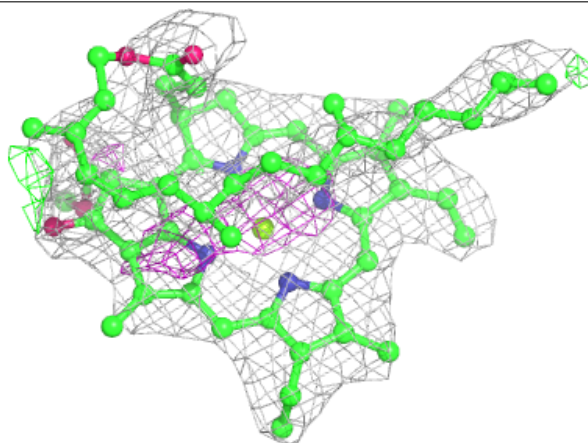


**Electron density around CLA c 515:**

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

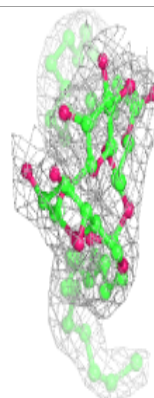
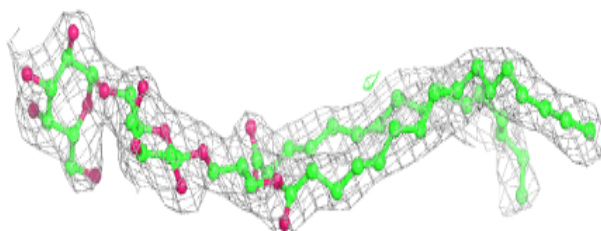
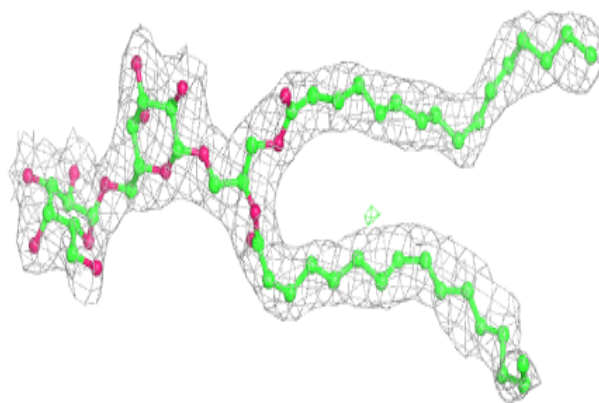
**Electron density around CLA b 610:**

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

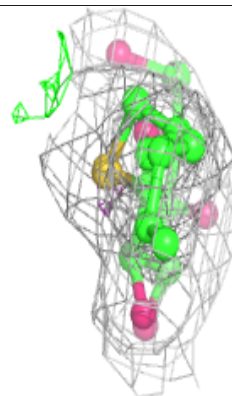
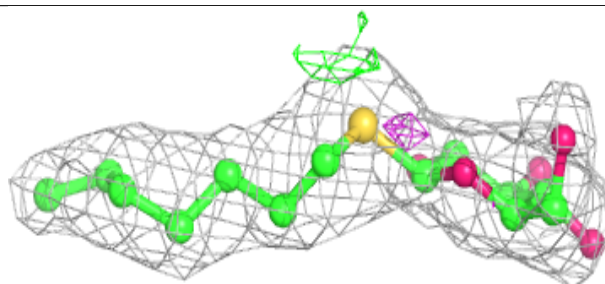
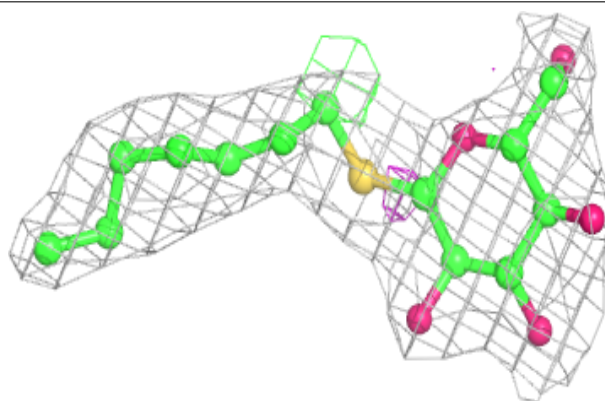


**Electron density around DGD c 521:**

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

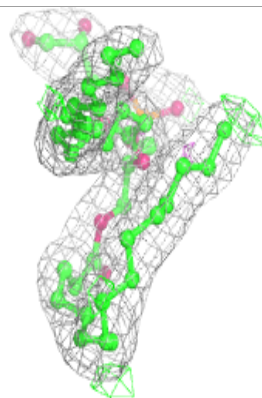
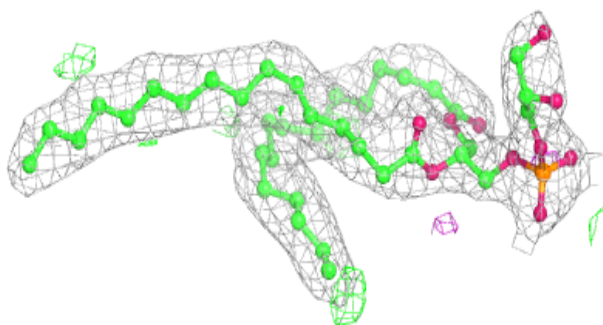
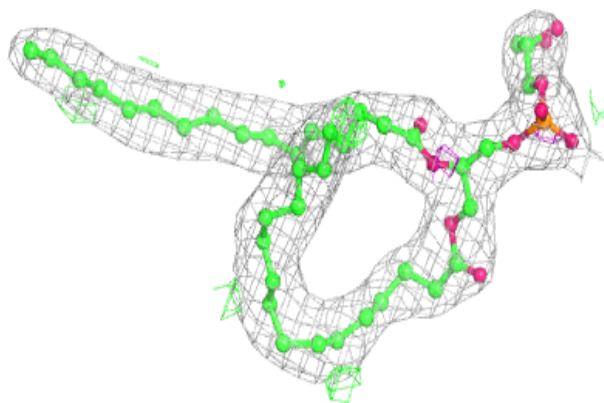
**Electron density around HTG B 622:**

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

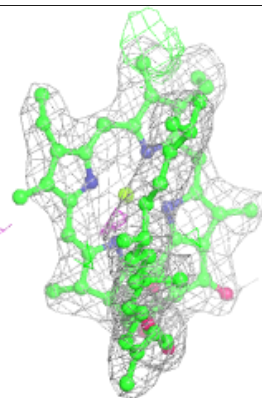
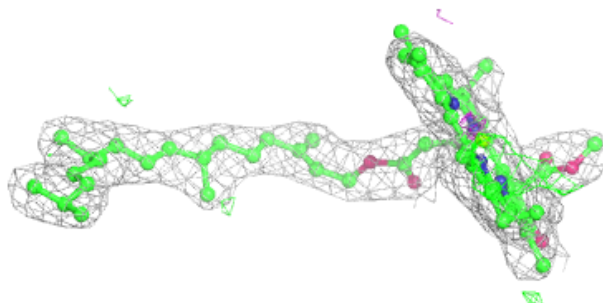
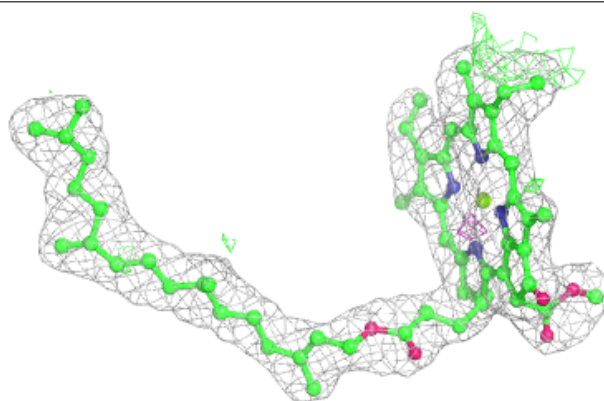


**Electron density around LHG D 410:**

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

**Electron density around CLA b 618:**

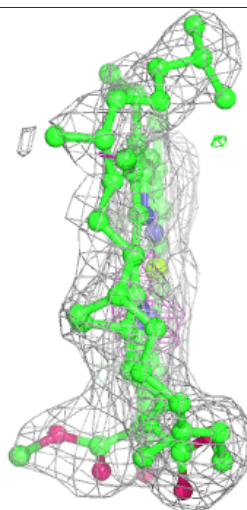
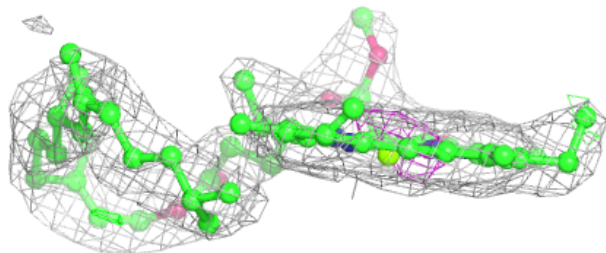
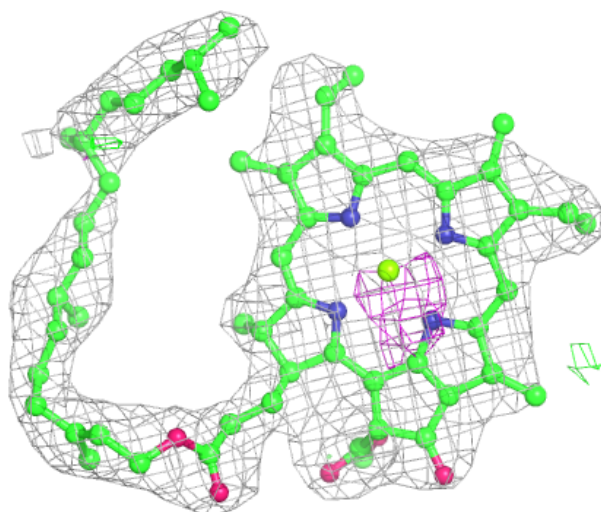
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





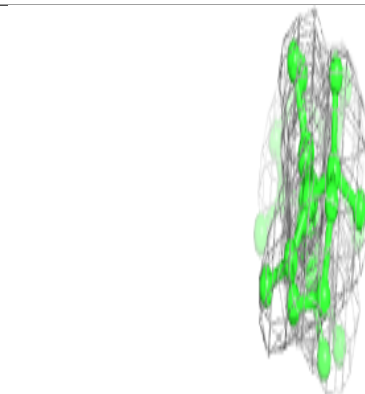
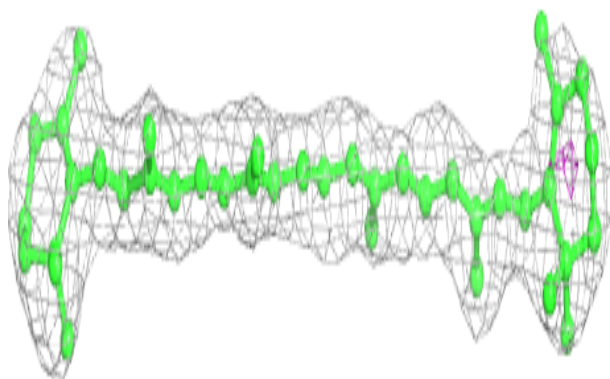
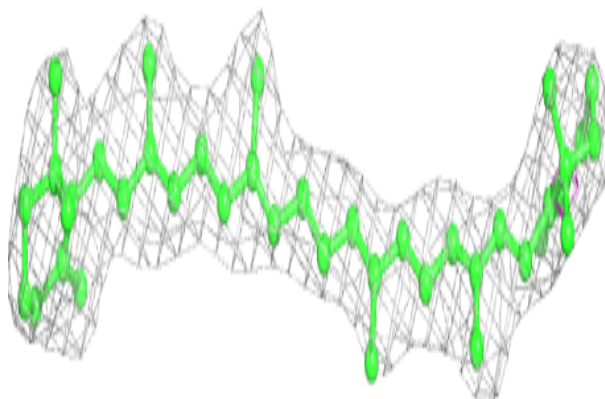
**Electron density around CLA C 513:**

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

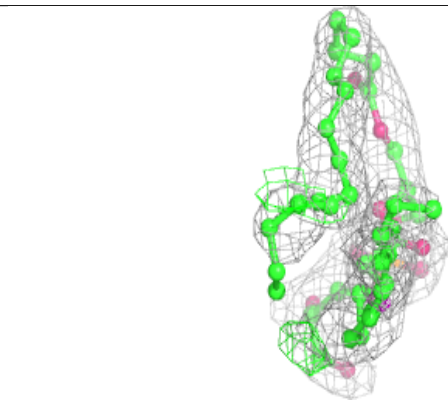
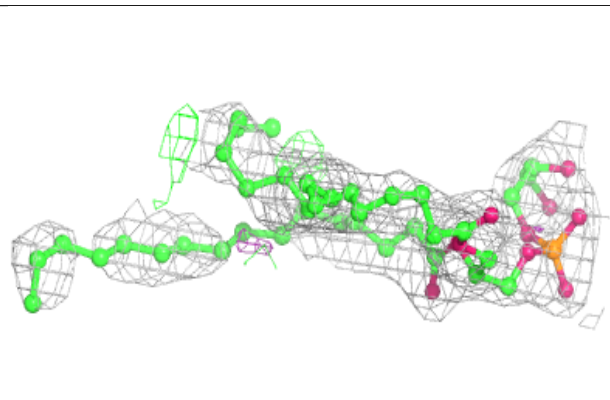
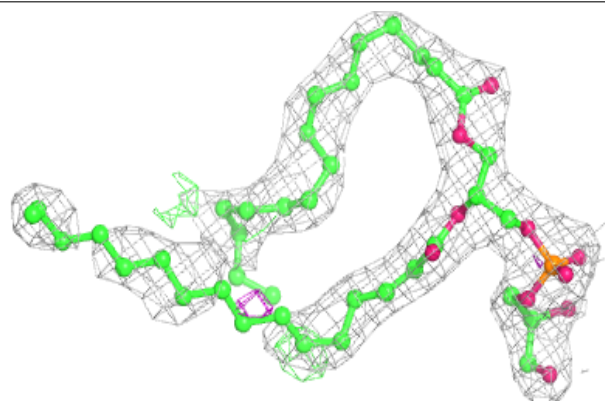


**Electron density around BCR K 101:**

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

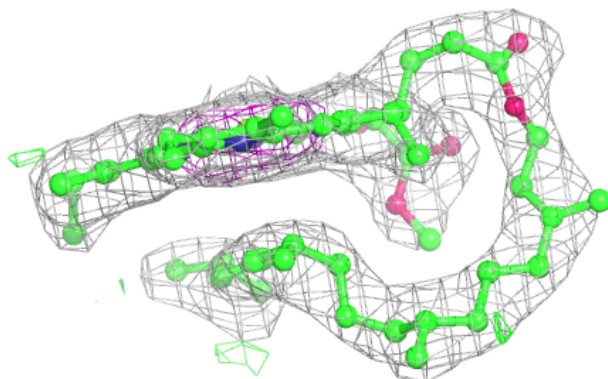
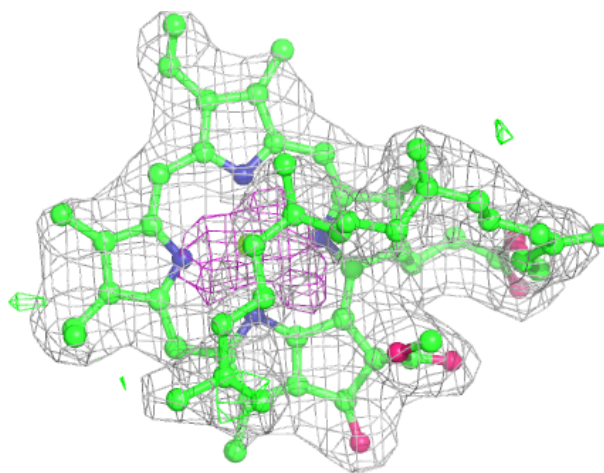
**Electron density around LHG d 411:**

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



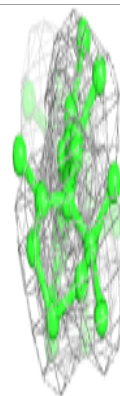
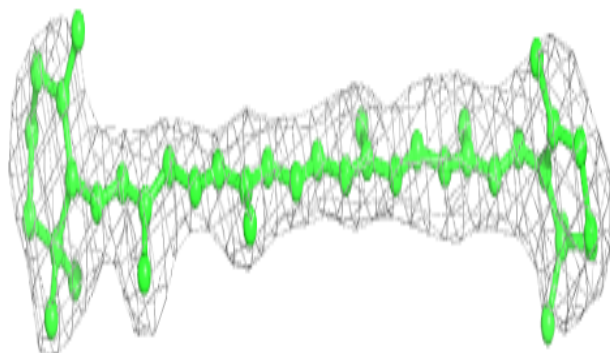
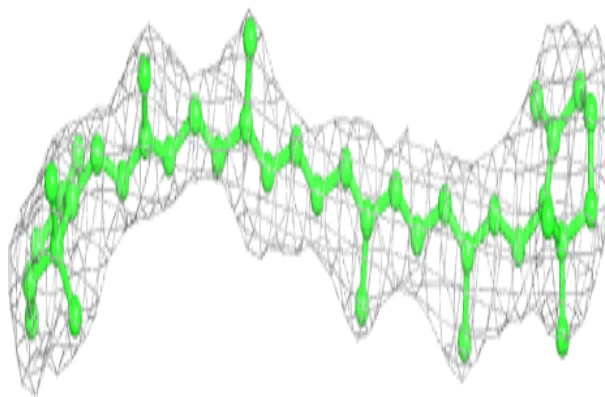
**Electron density around CLA C 511:**

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

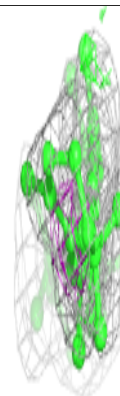
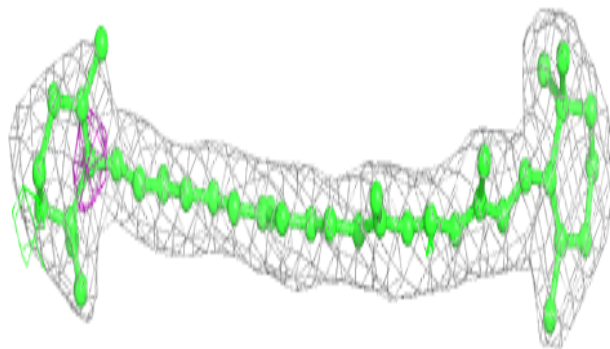
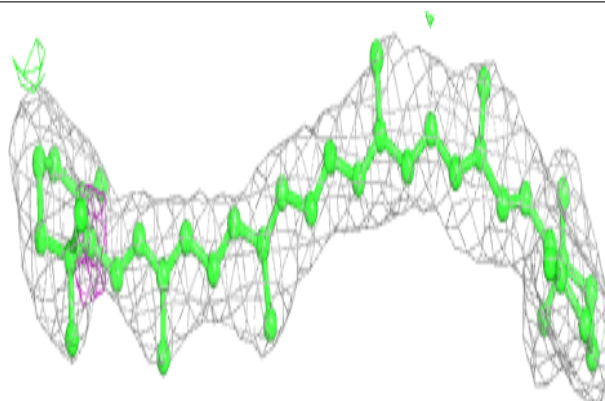


**Electron density around BCR c 526:**

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

**Electron density around BCR H 101:**

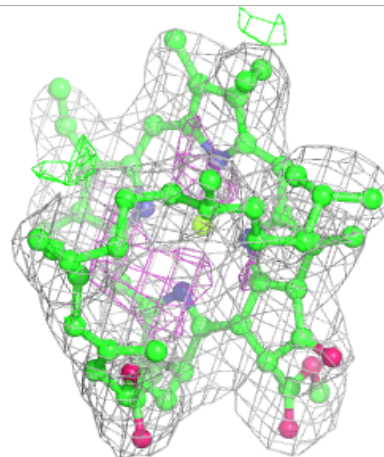
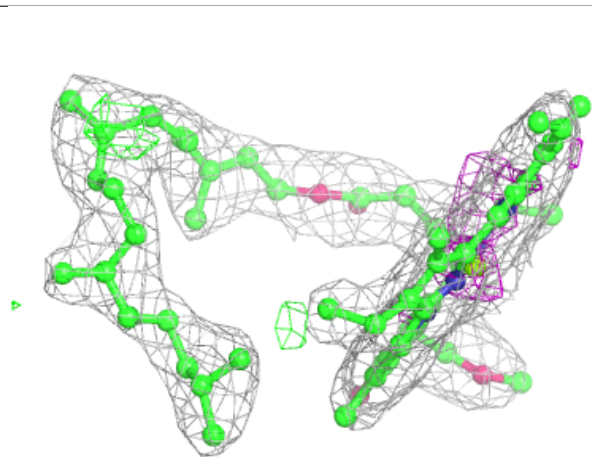
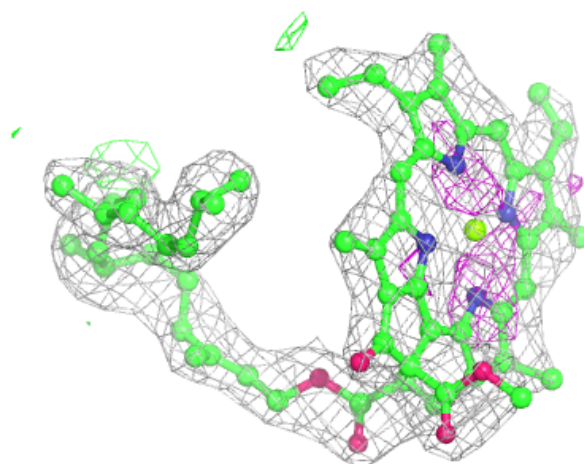
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





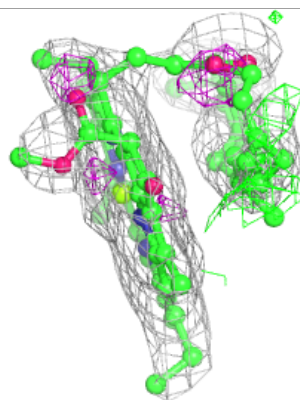
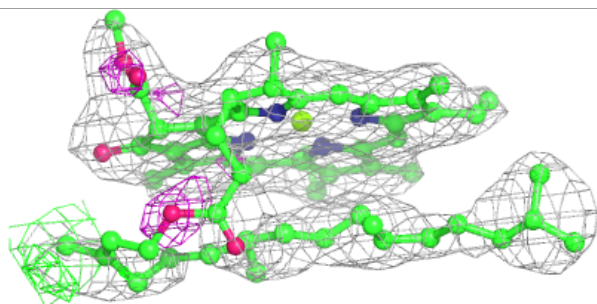
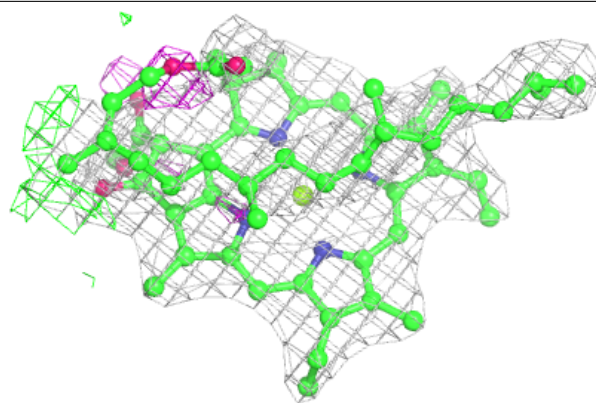
**Electron density around CLA C 504:**

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

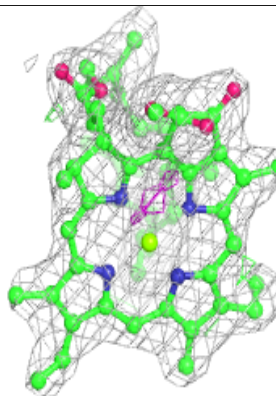
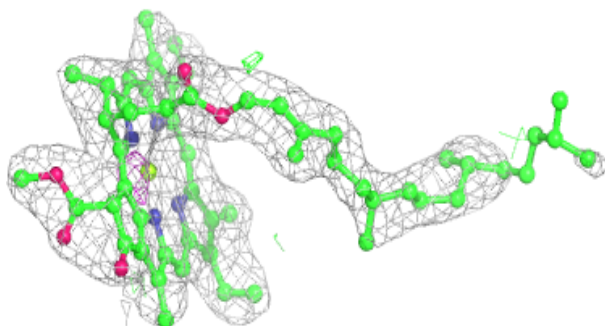
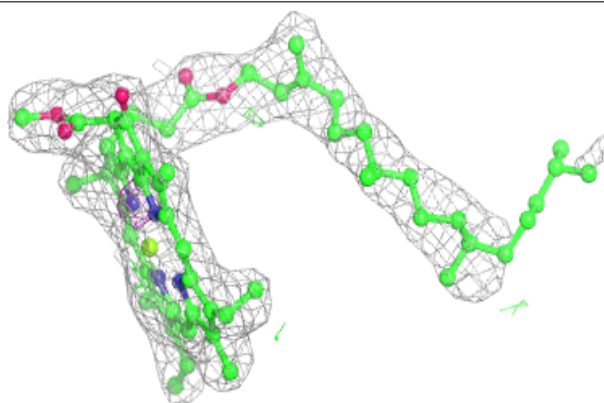


**Electron density around CLA B 602:**

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

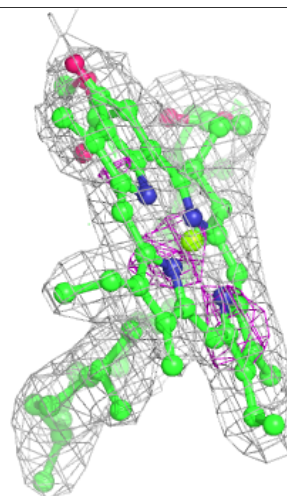
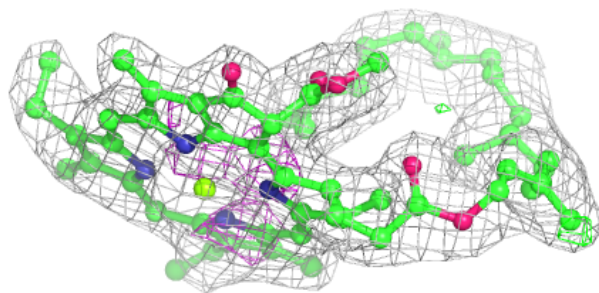
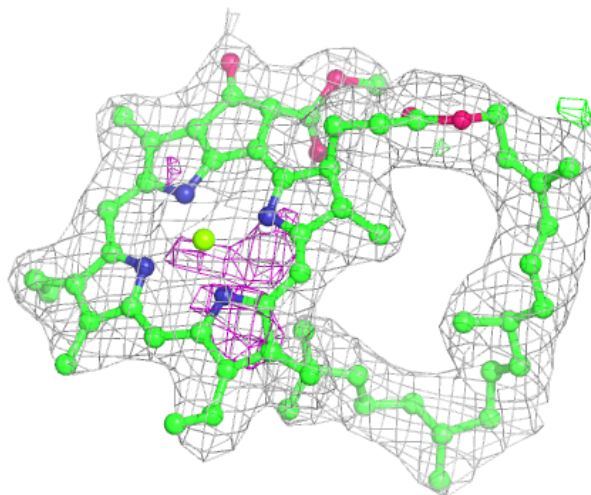
**Electron density around CLA C 509:**

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



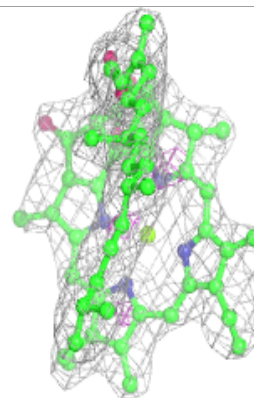
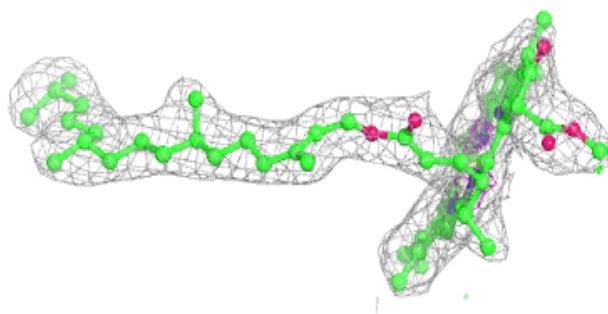
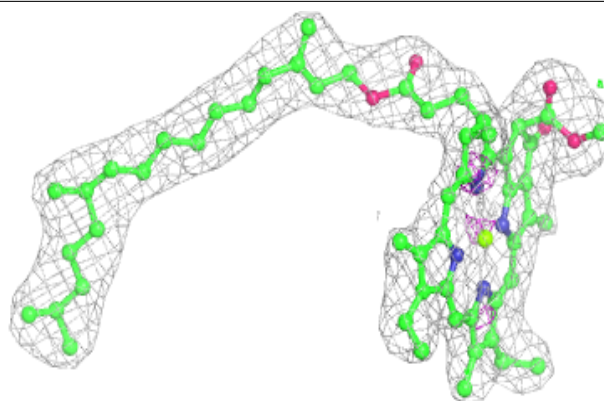
**Electron density around CLA b 624:**

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

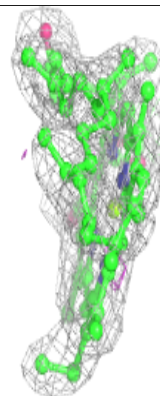
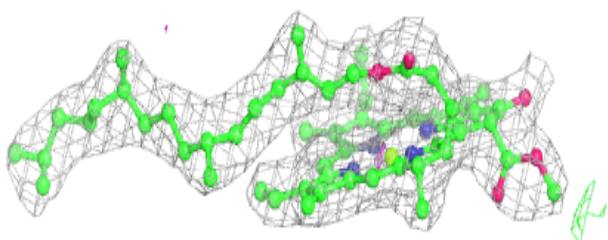
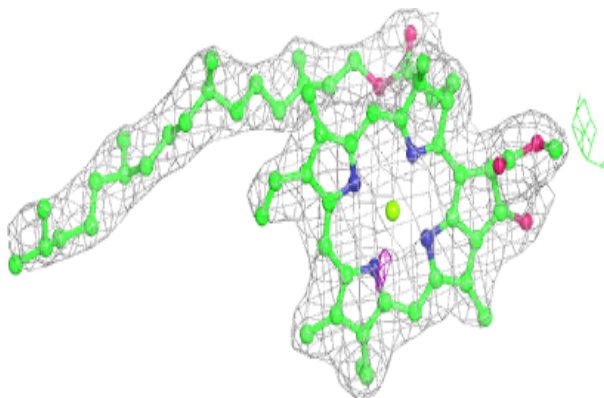


**Electron density around CLA B 610:**

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

**Electron density around CLA C 502:**

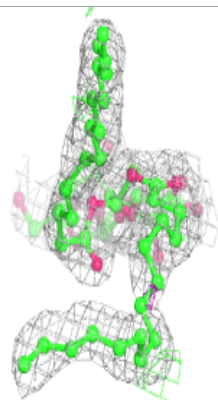
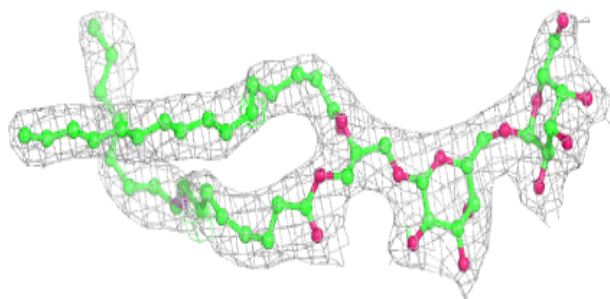
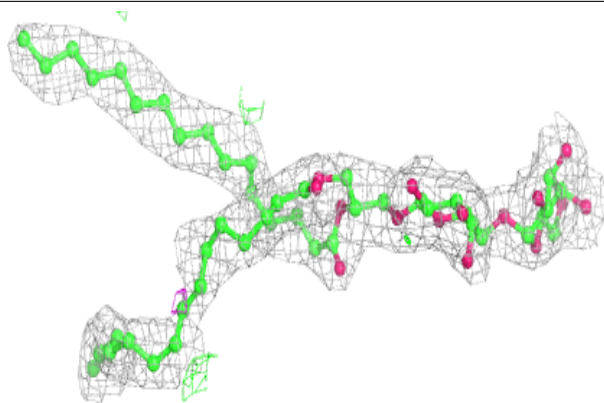
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



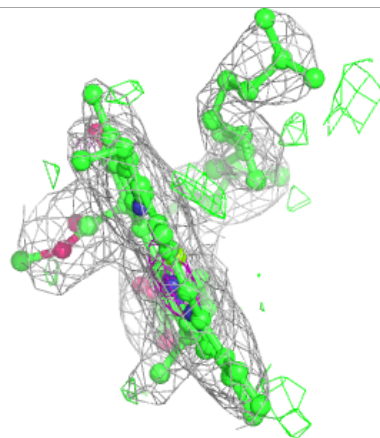
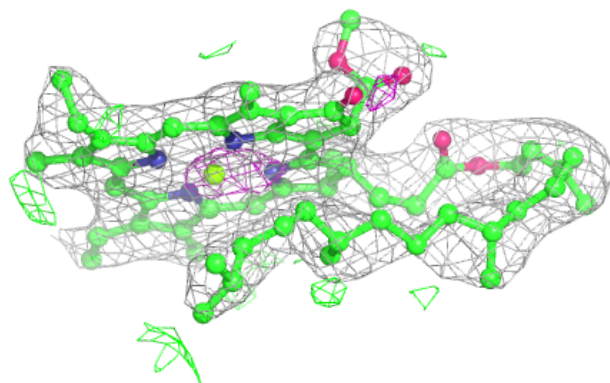
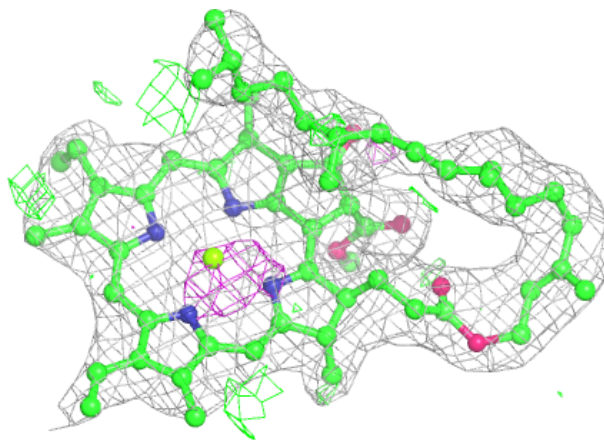


**Electron density around DGD C 516:**

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

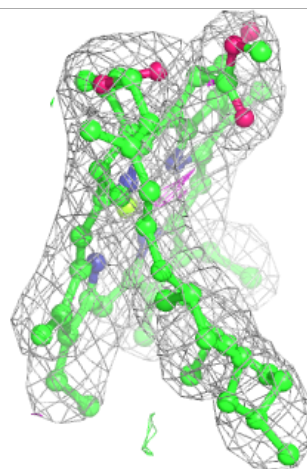
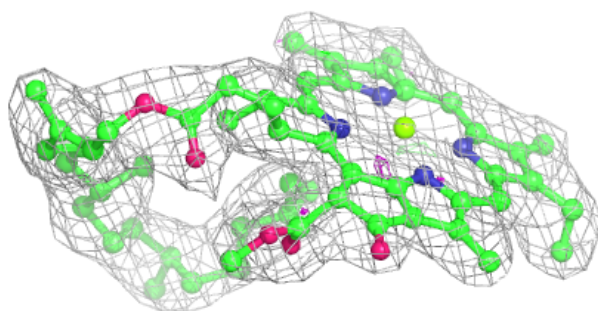
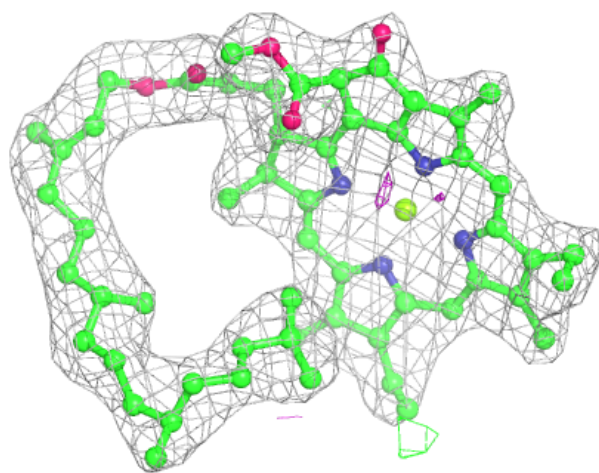
**Electron density around CLA c 513:**

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



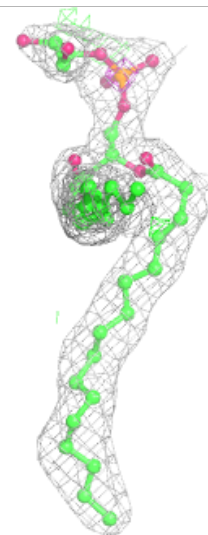
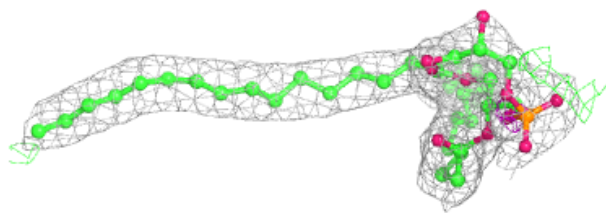
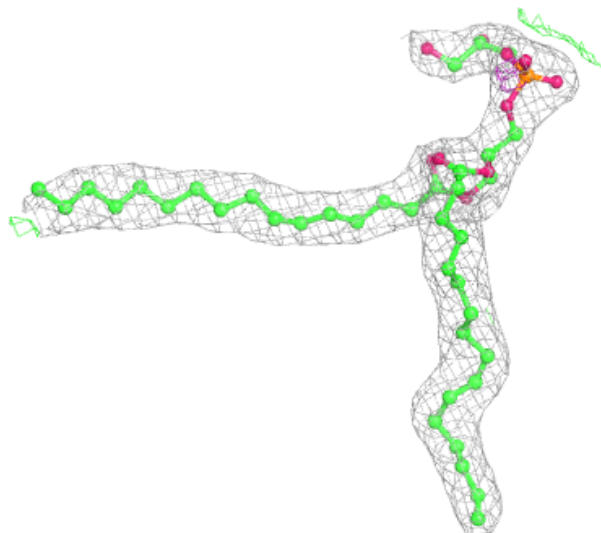
**Electron density around CLA B 616:**

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



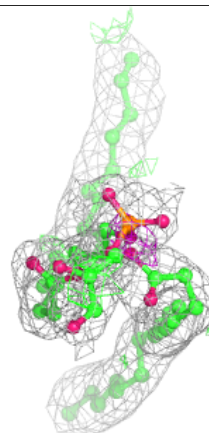
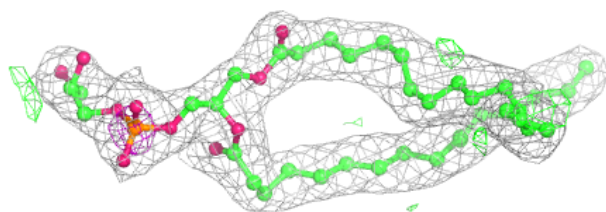
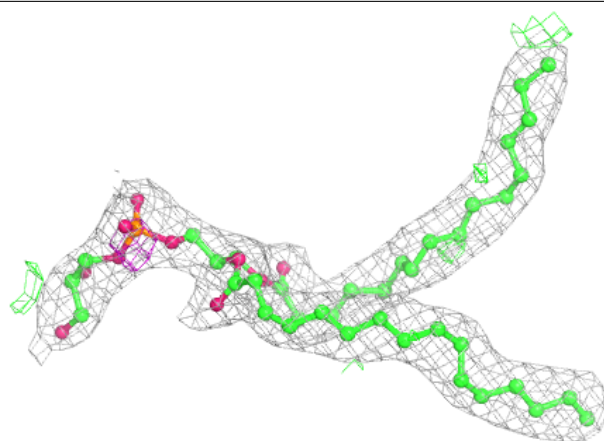
**Electron density around LHG b 634:**

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



**Electron density around LHG d 410:**

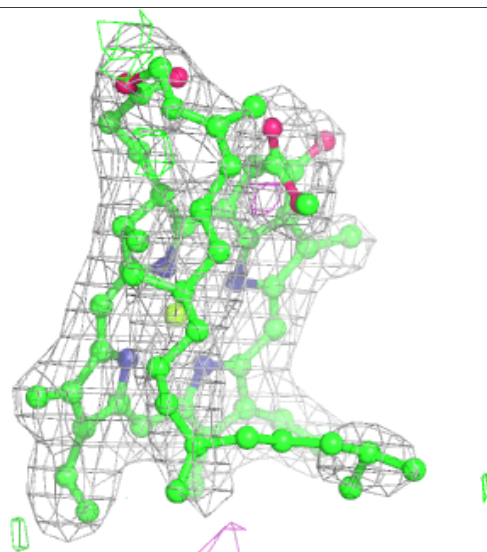
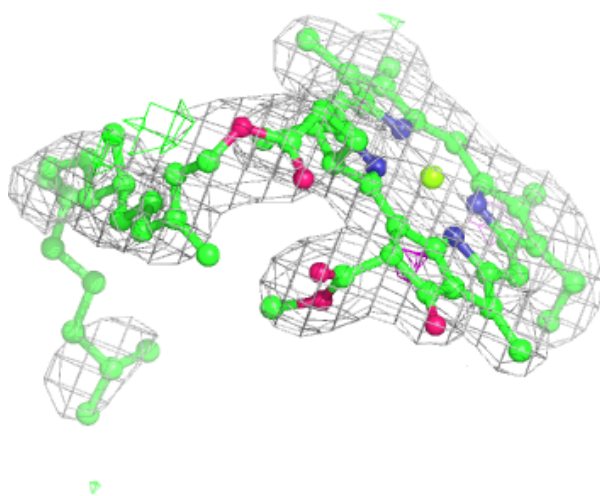
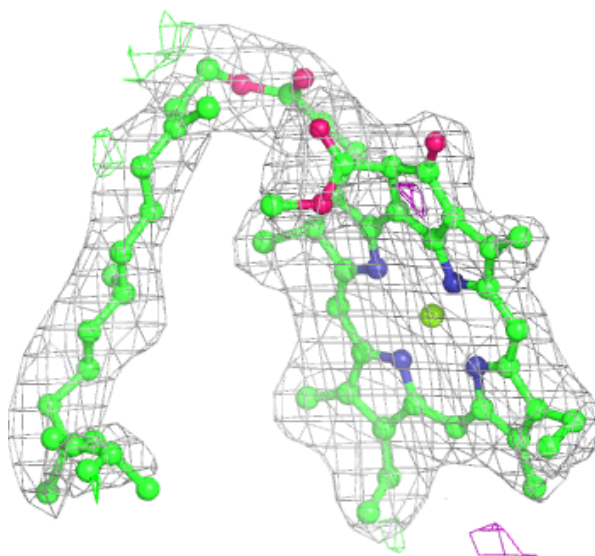
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





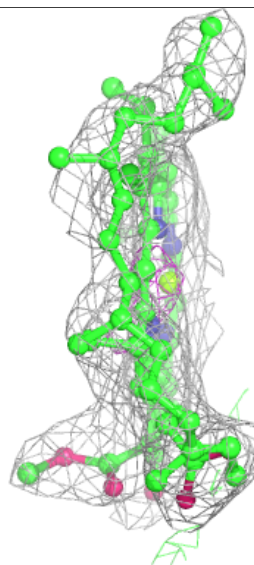
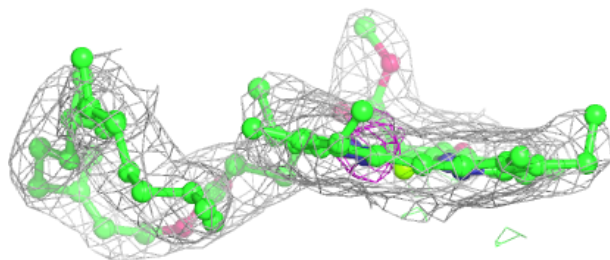
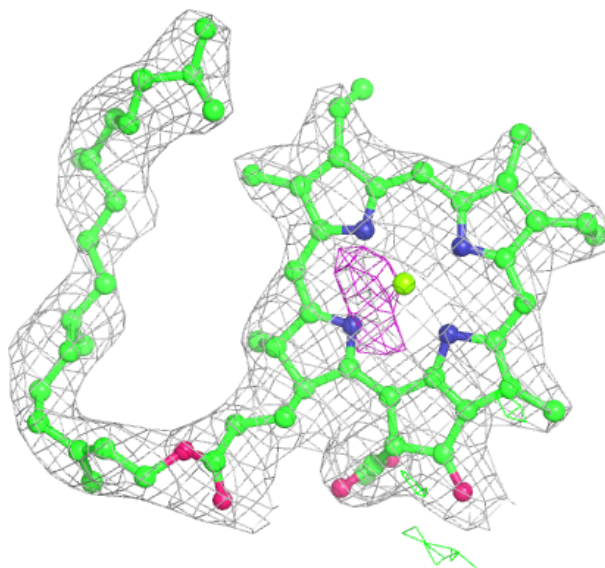
**Electron density around CLA b 625:**

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



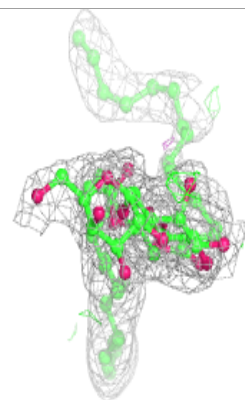
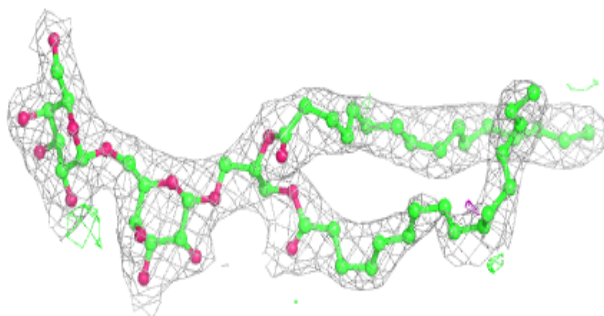
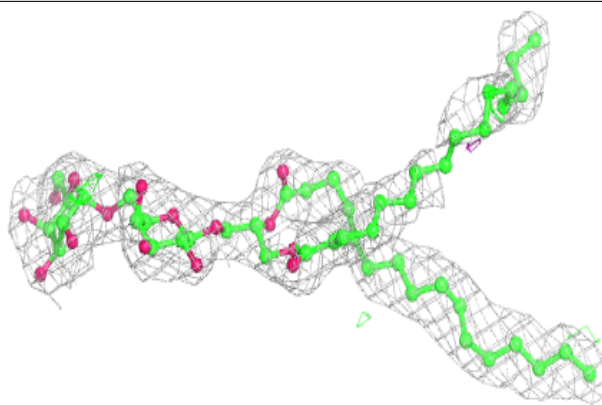
**Electron density around CLA c 516:**

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



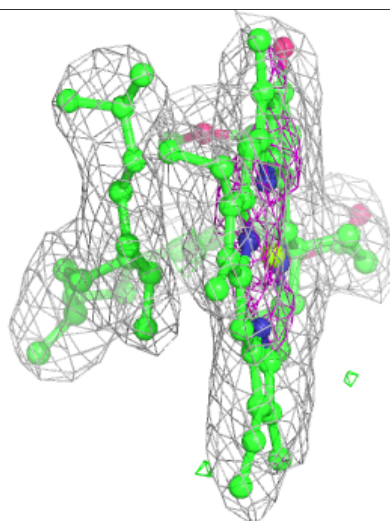
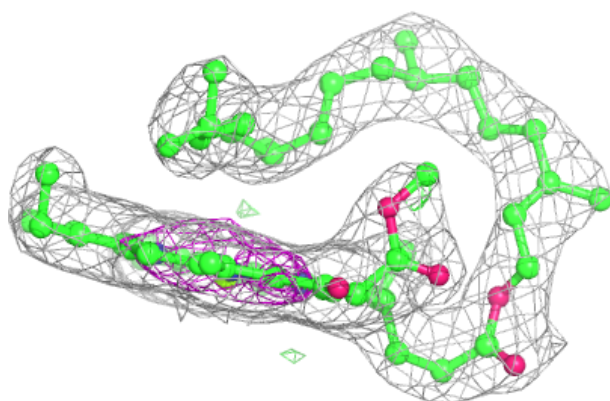
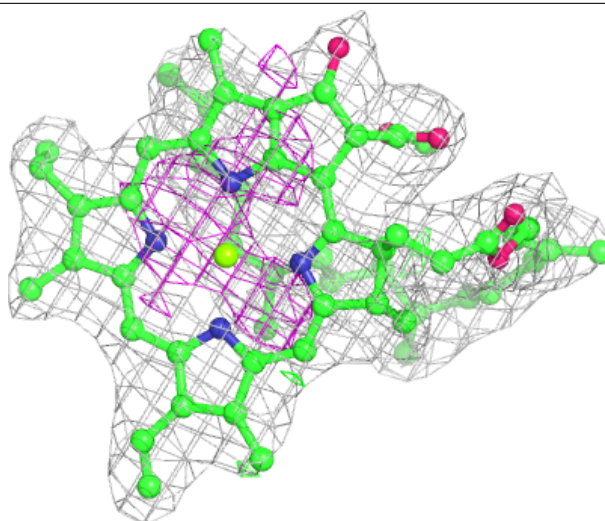
**Electron density around DGD c 519:**

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



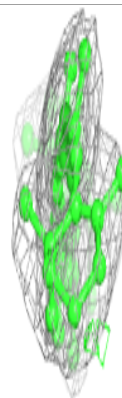
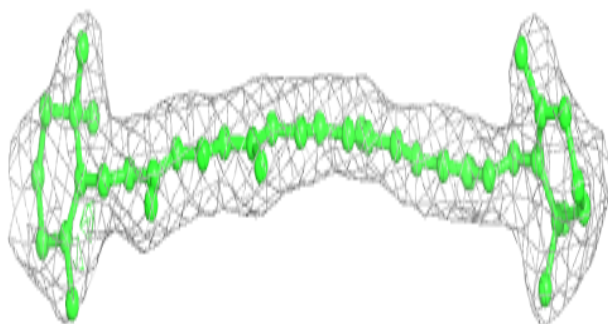
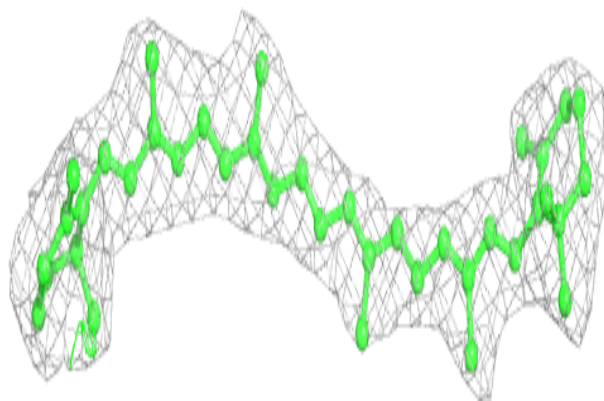
**Electron density around CLA c 514:**

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

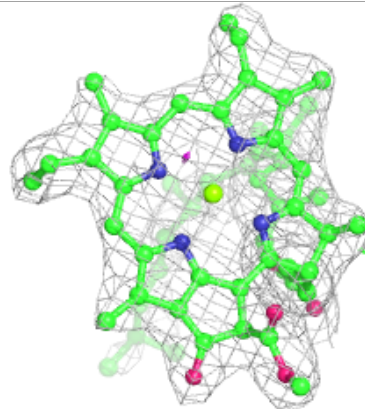
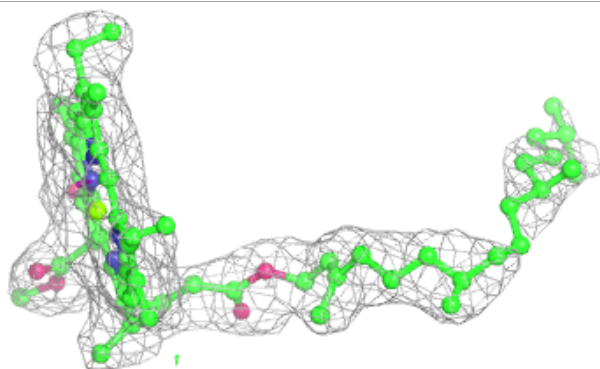
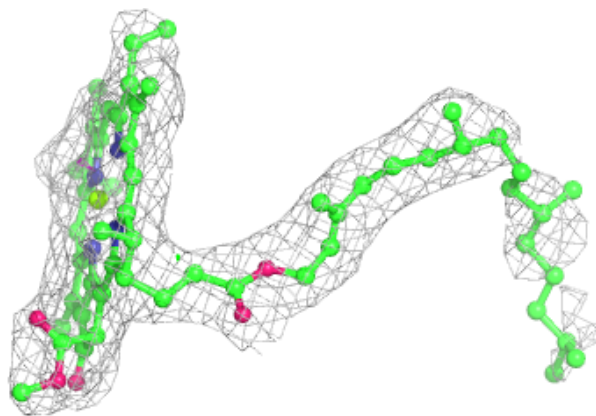


**Electron density around BCR y 101:**

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

**Electron density around CLA D 406:**

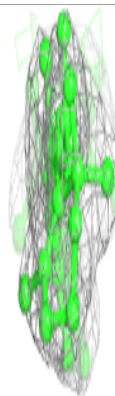
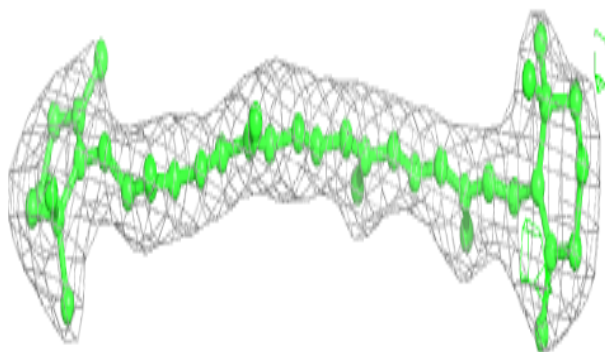
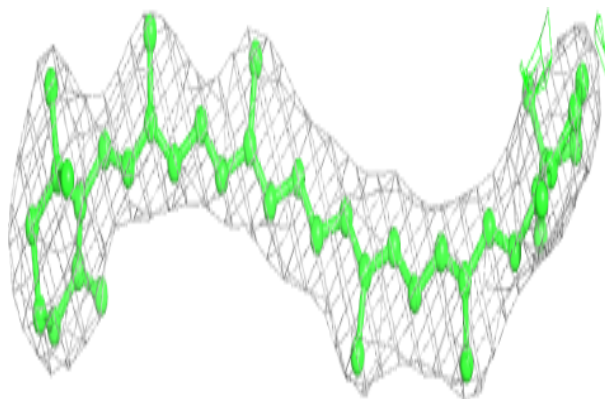
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



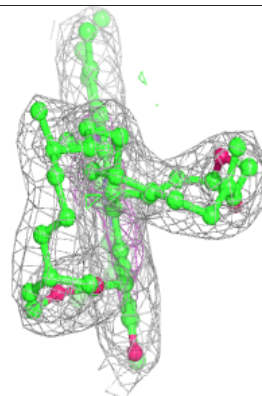
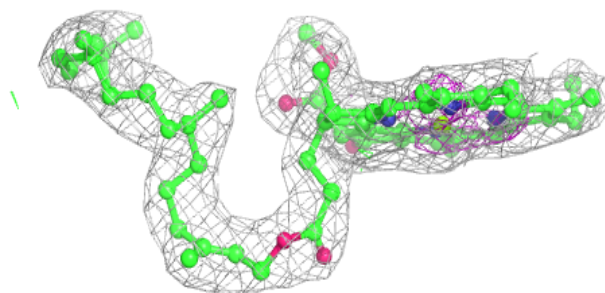
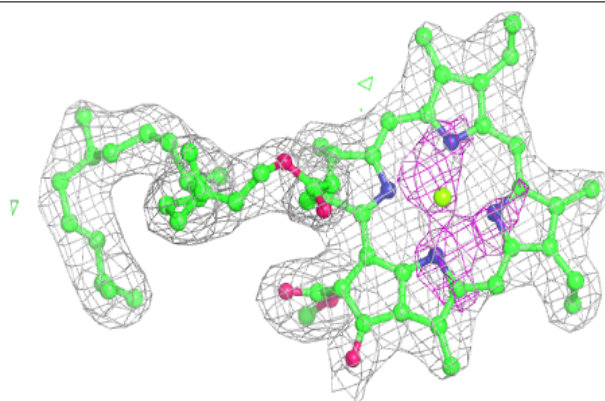


**Electron density around BCR Y 101:**

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

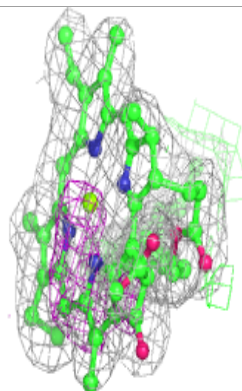
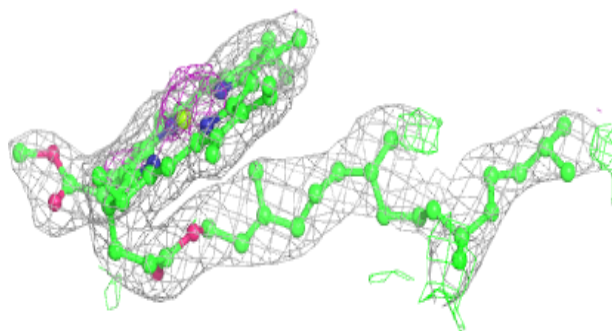
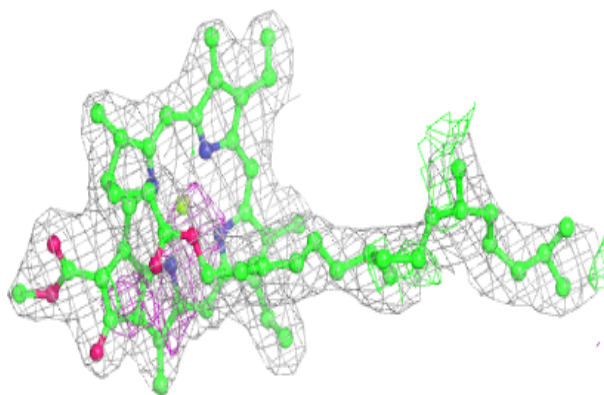
**Electron density around CLA B 613:**

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

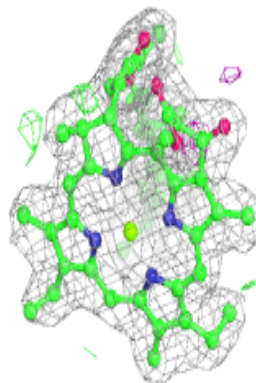
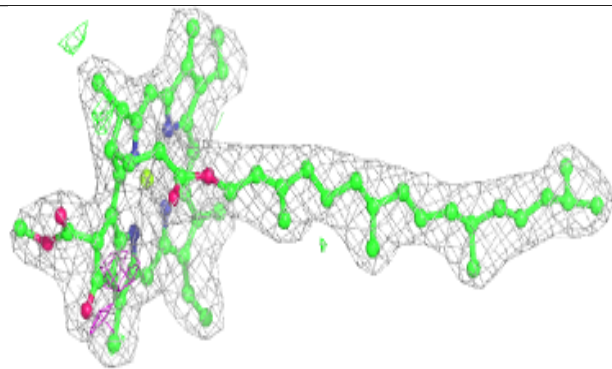
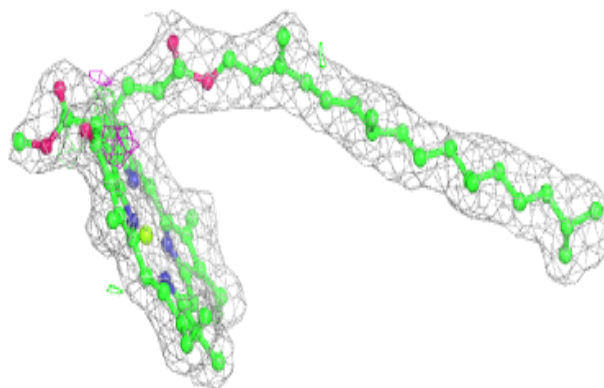


**Electron density around CLA b 623:**

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

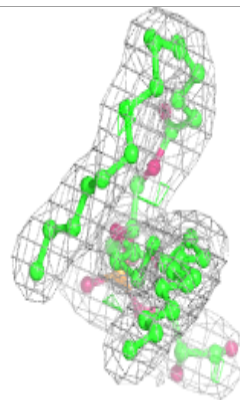
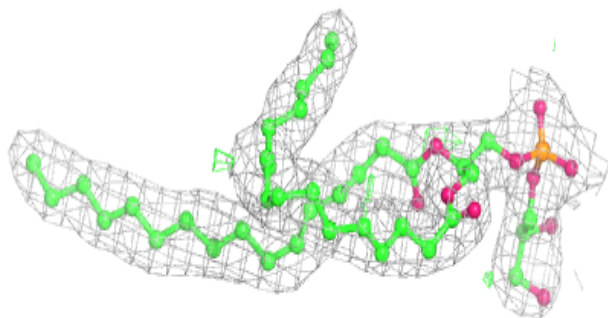
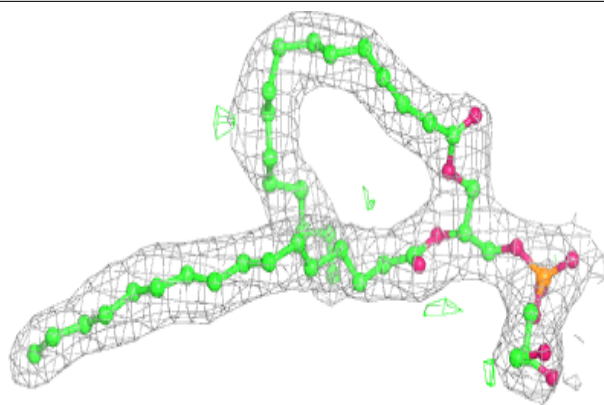
**Electron density around CLA B 608:**

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



**Electron density around LHG d 409:**

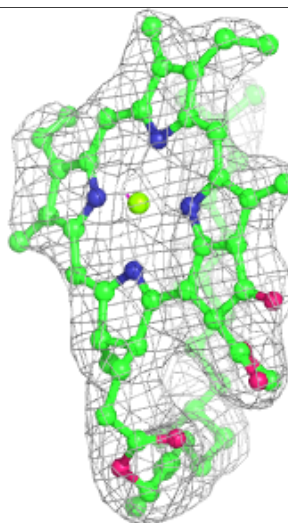
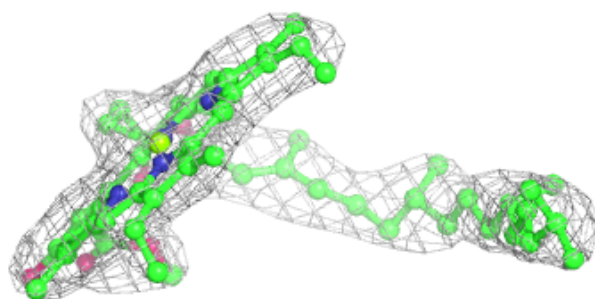
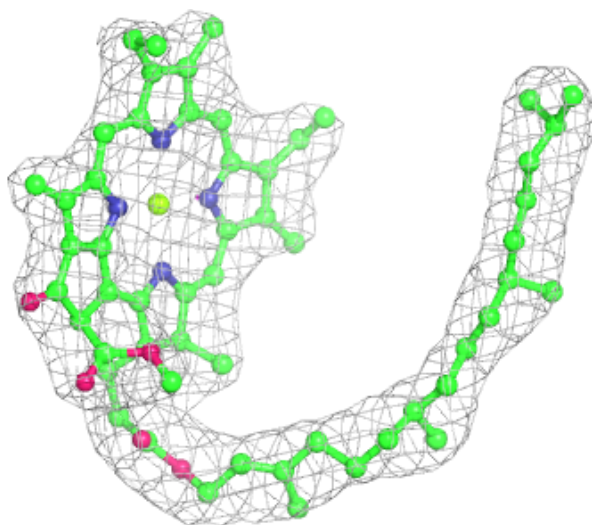
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





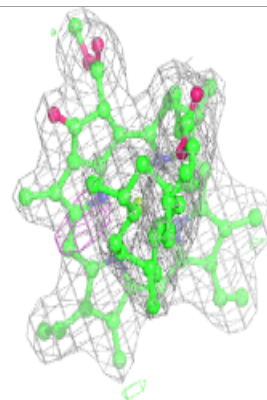
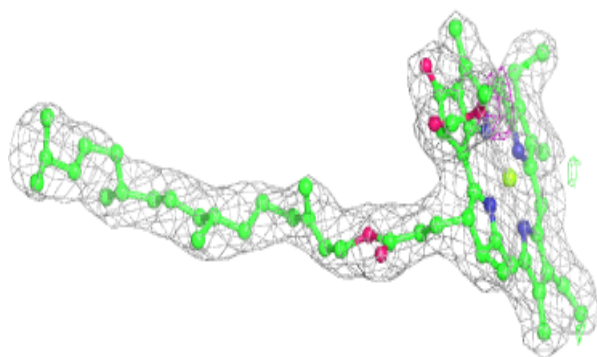
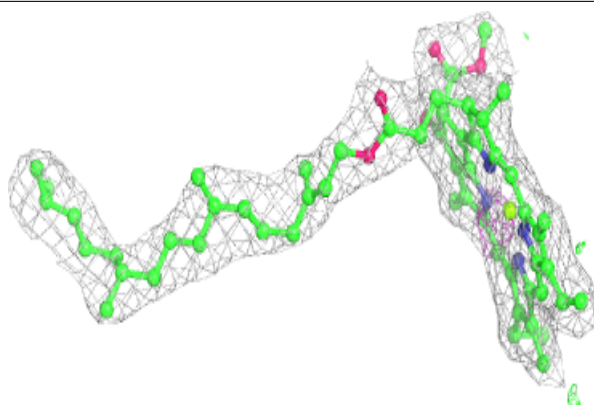
**Electron density around CLA C 508:**

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

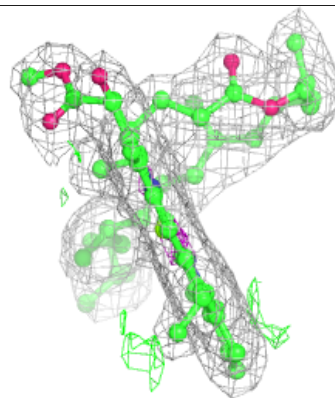
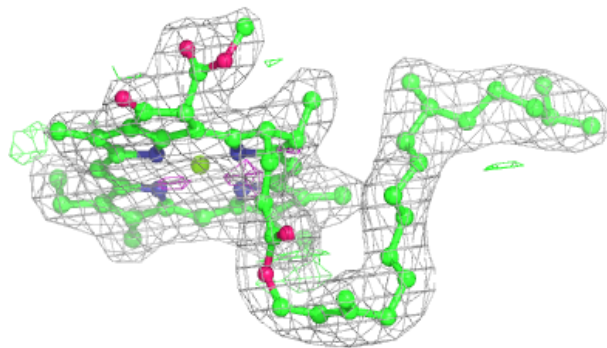
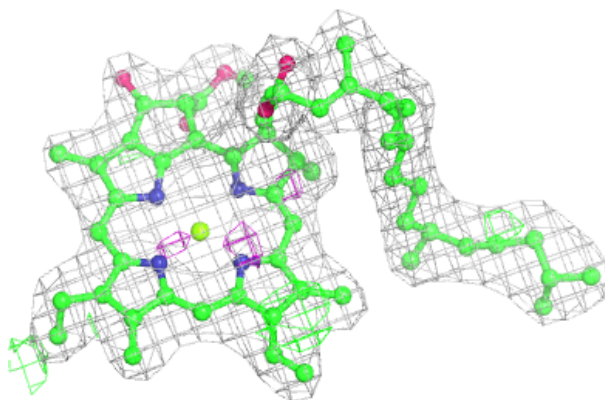


**Electron density around CLA B 605:**

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

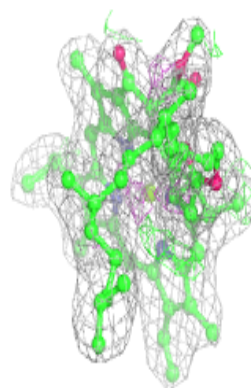
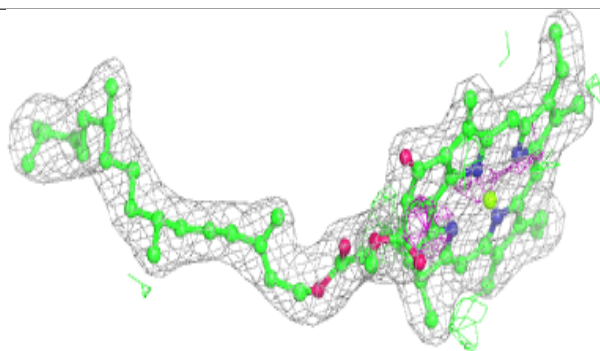
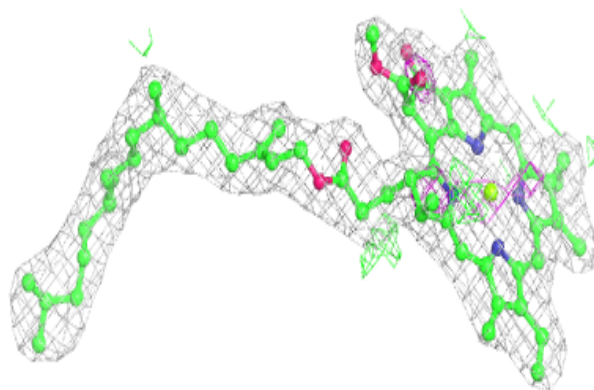
**Electron density around CLA d 403:**

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

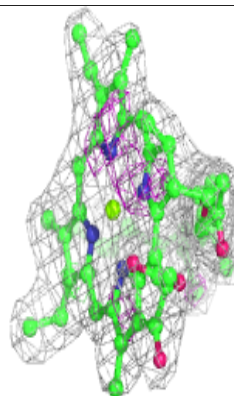
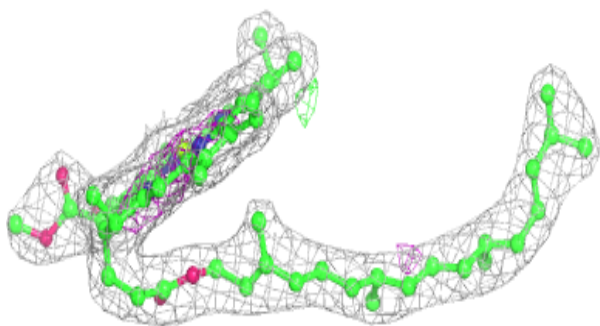
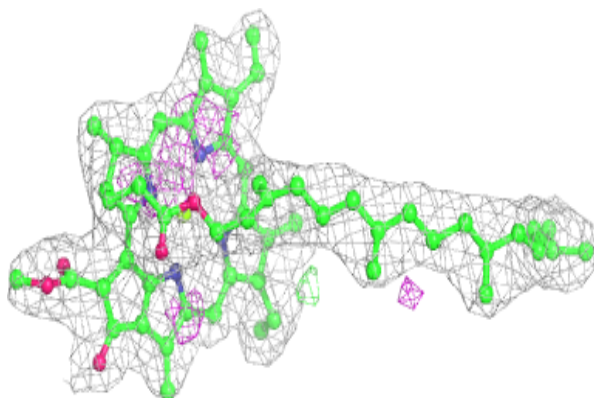


**Electron density around CLA A 404:**

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

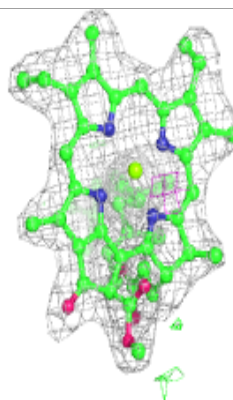
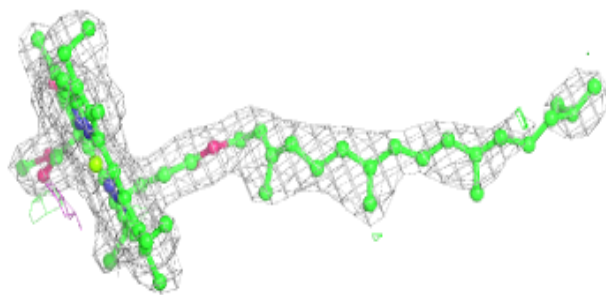
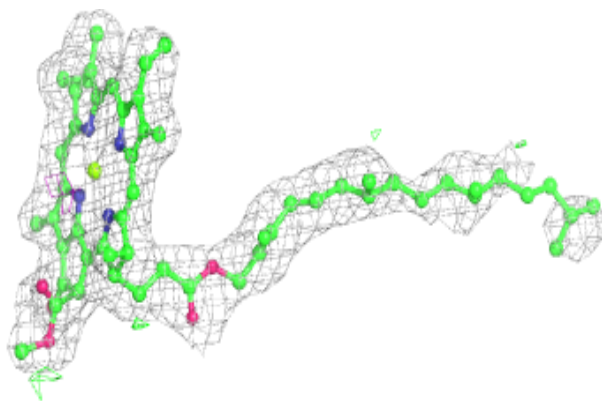
**Electron density around CLA b 617:**

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



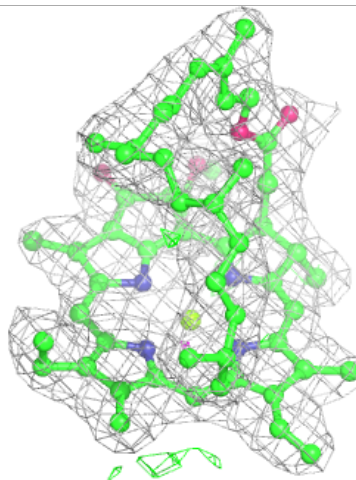
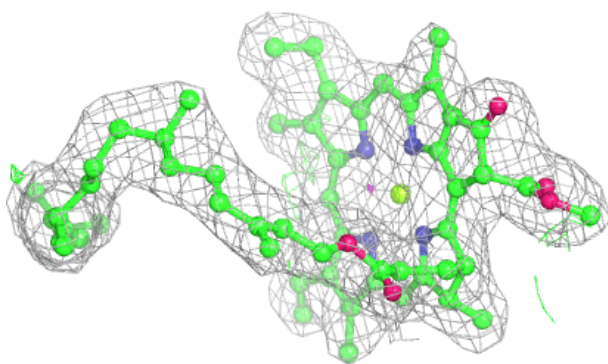
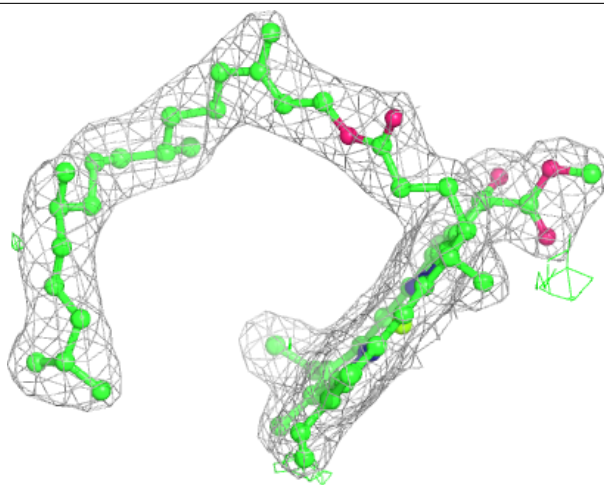
**Electron density around CLA d 405:**

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



**Electron density around CLA b 620:**

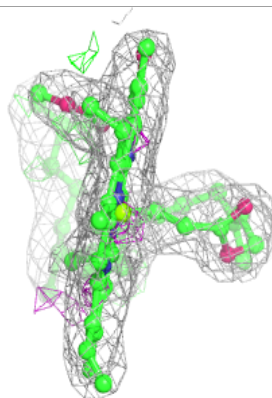
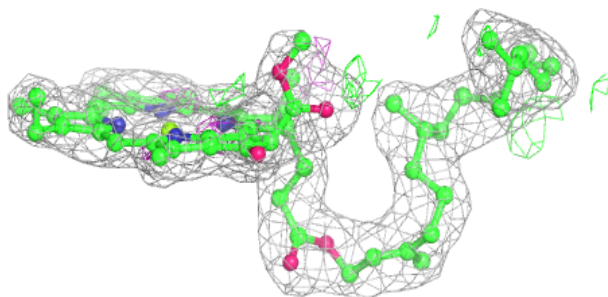
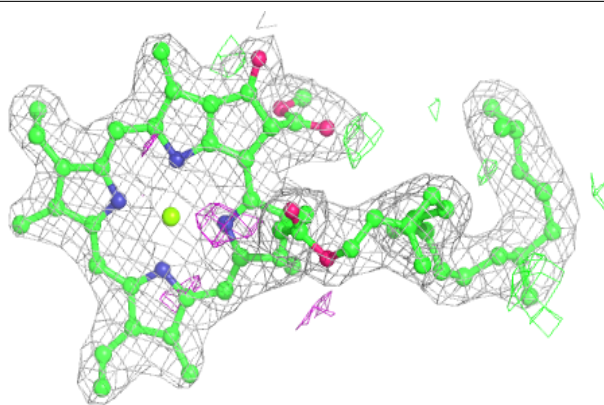
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





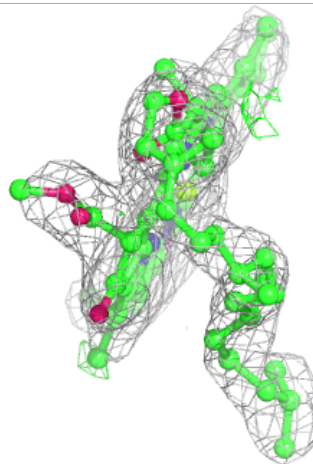
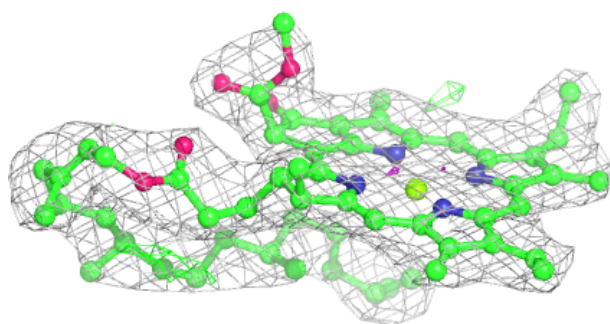
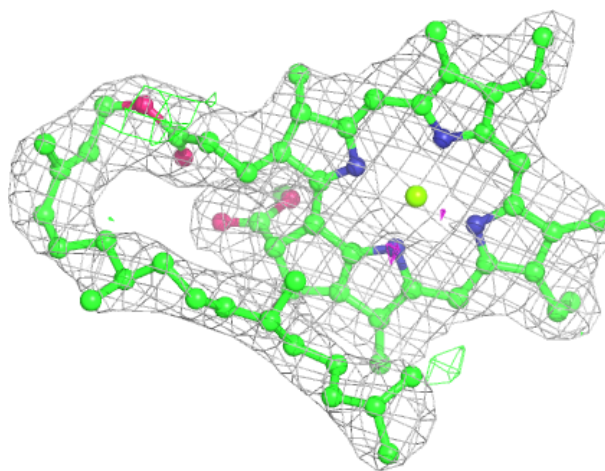
**Electron density around CLA b 621:**

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



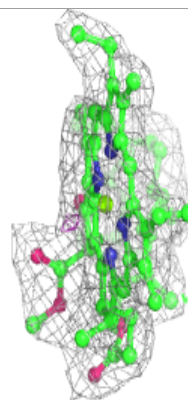
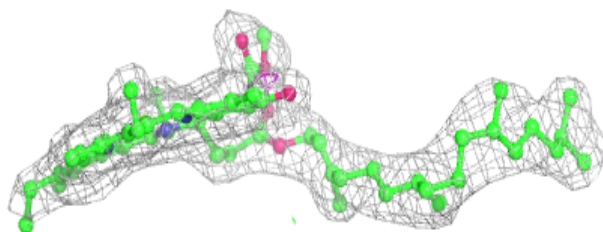
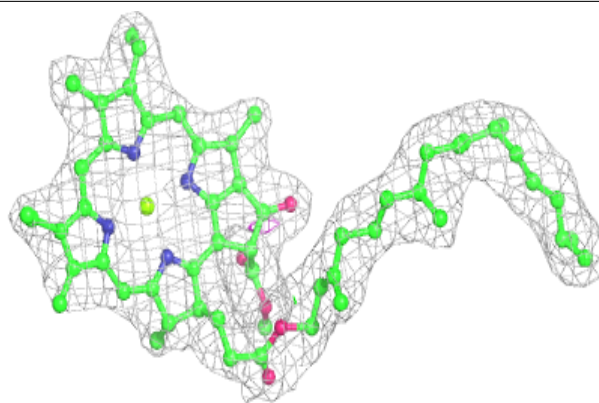
**Electron density around CLA C 510:**

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

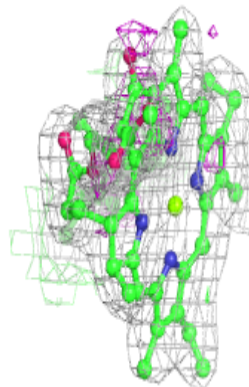
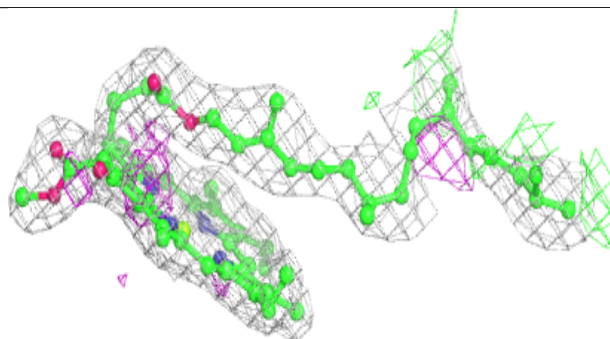
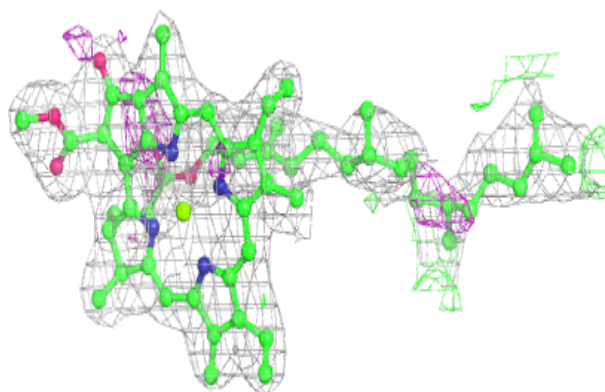


**Electron density around CLA B 603:**

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

**Electron density around CLA B 615:**

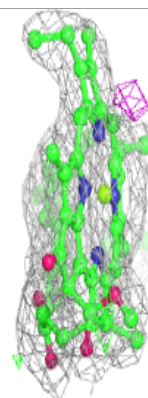
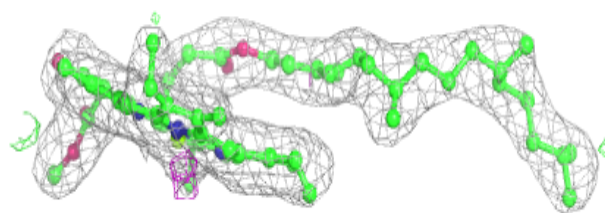
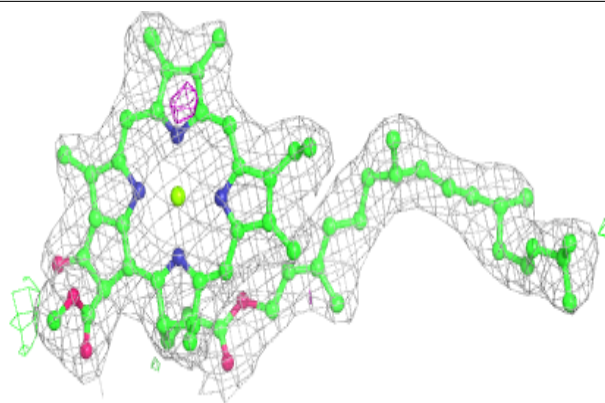
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



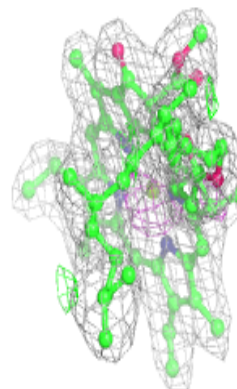
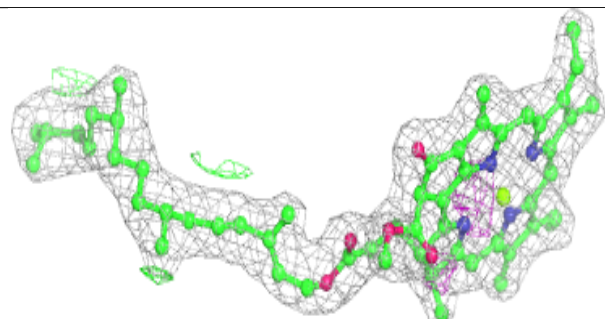
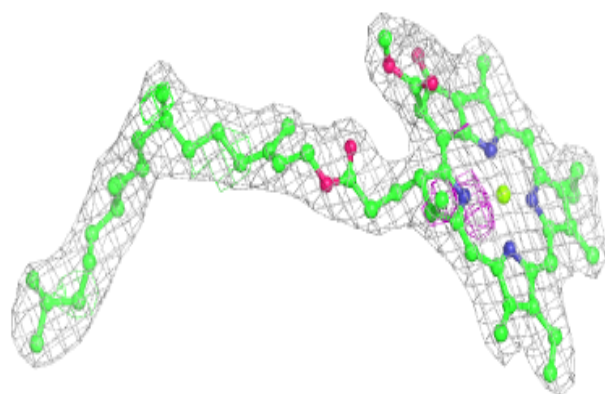


**Electron density around CLA b 612:**

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

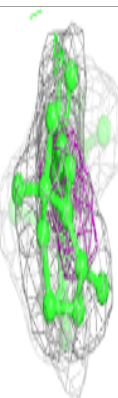
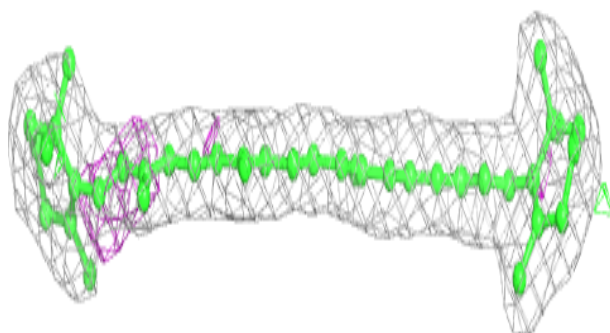
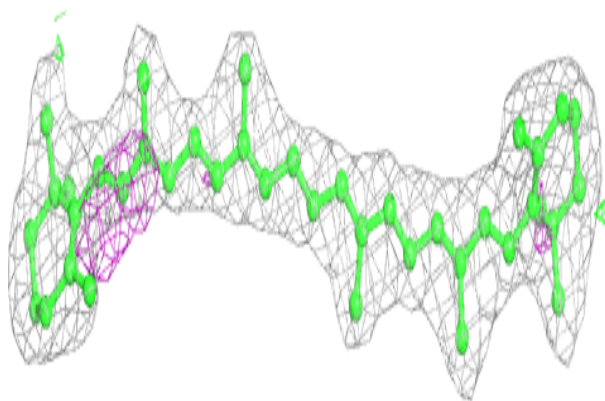
**Electron density around CLA a 408:**

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

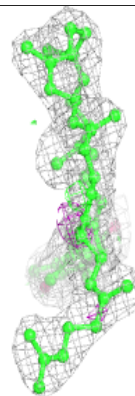
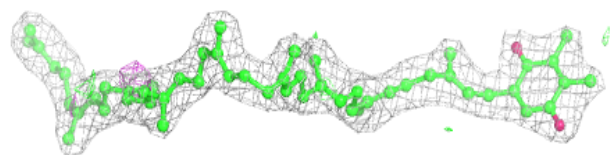
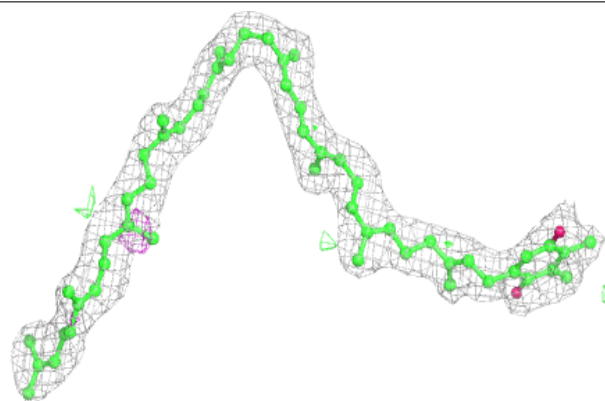


**Electron density around BCR b 627:**

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

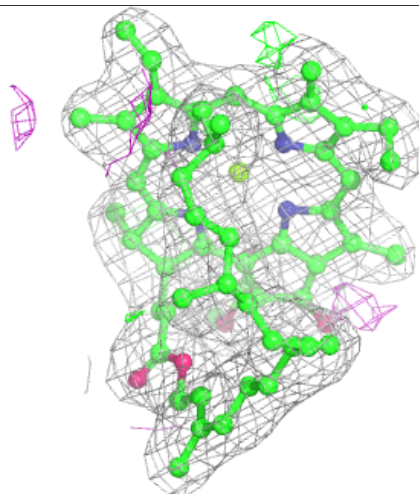
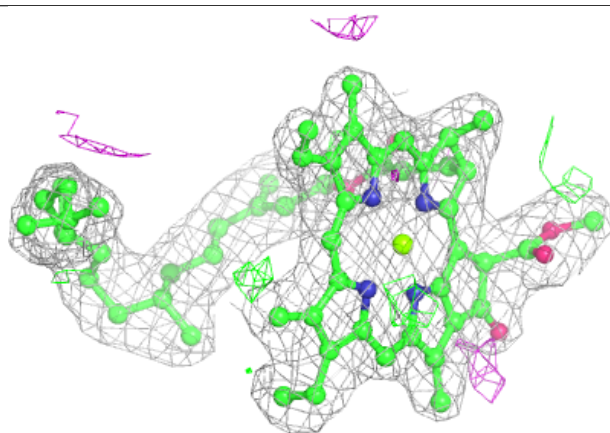
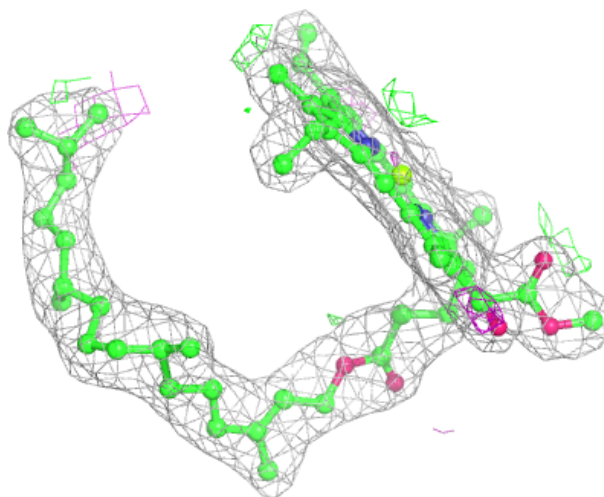
**Electron density around PL9 d 407 (B):**

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



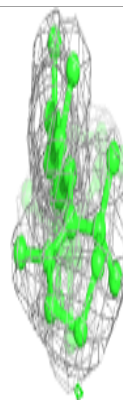
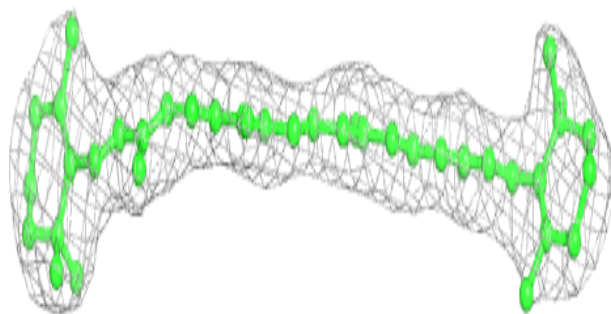
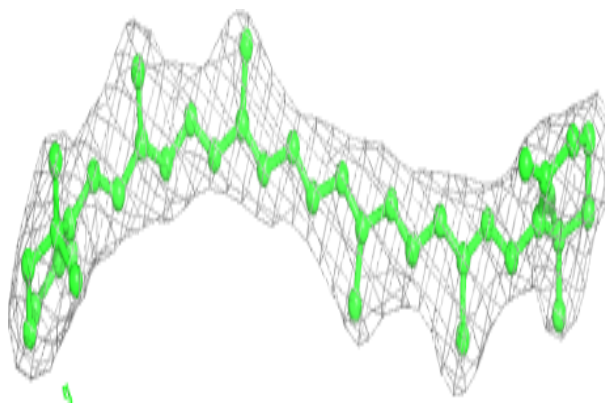
**Electron density around CLA B 612:**

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



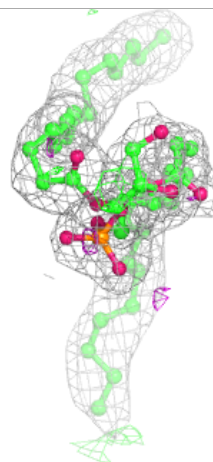
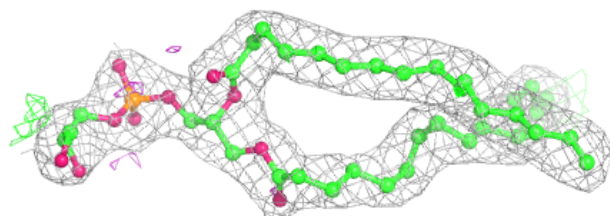
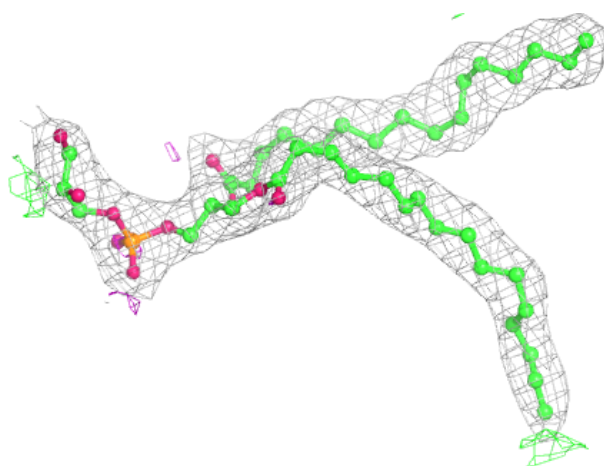
**Electron density around BCR h 101:**

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



**Electron density around LHG D 411:**

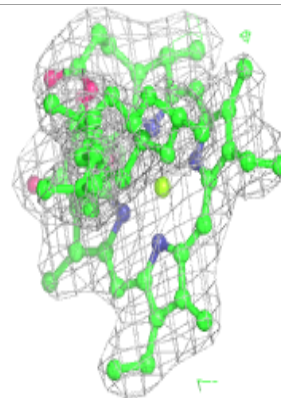
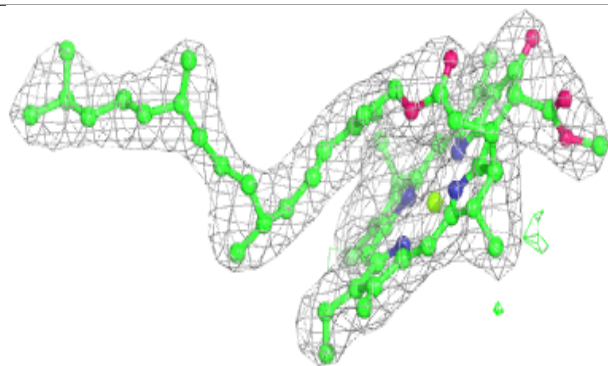
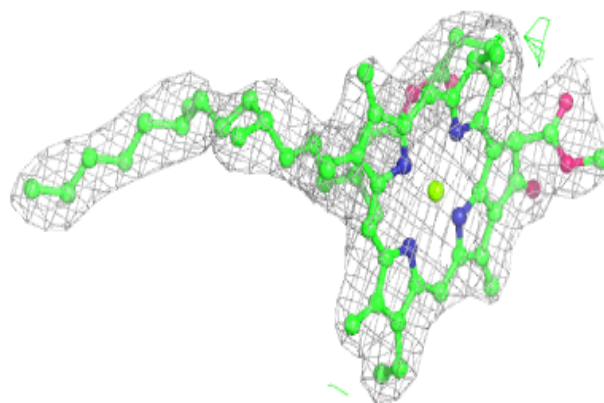
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



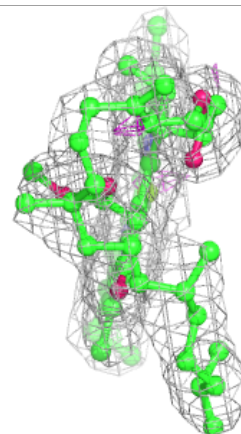
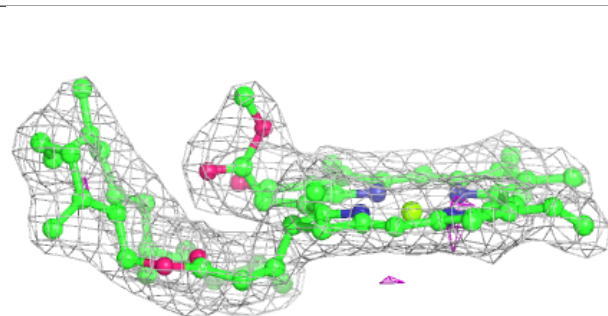
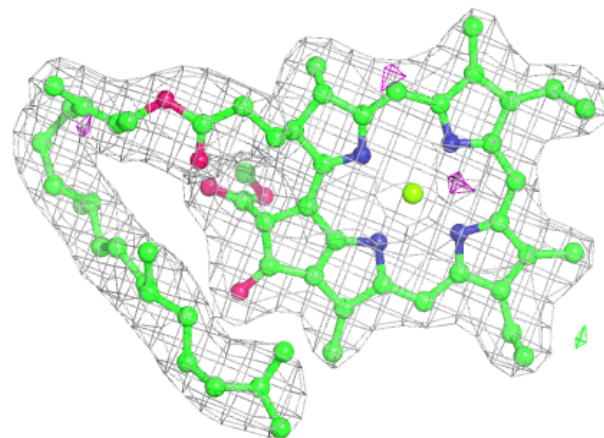


**Electron density around CLA C 506:**

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

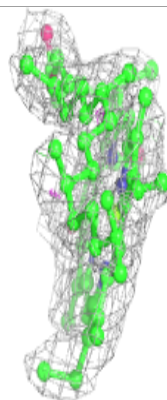
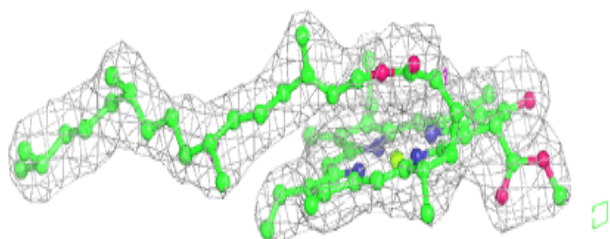
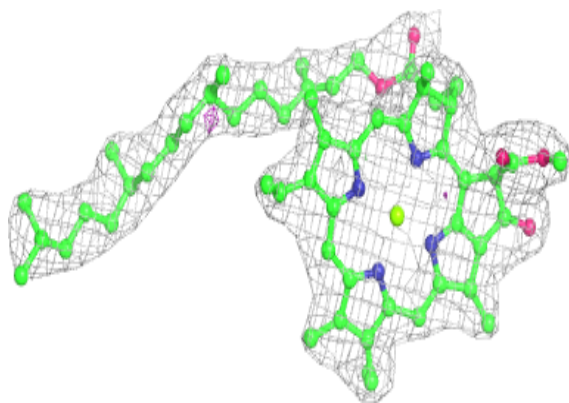
**Electron density around CLA b 619:**

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

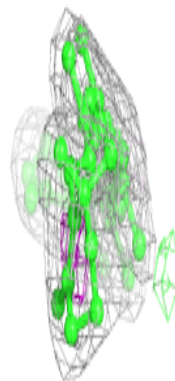
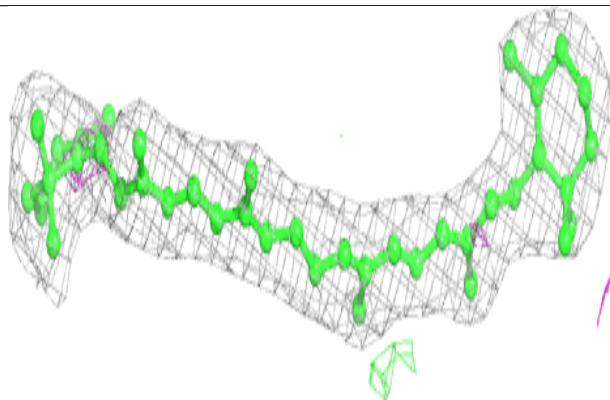
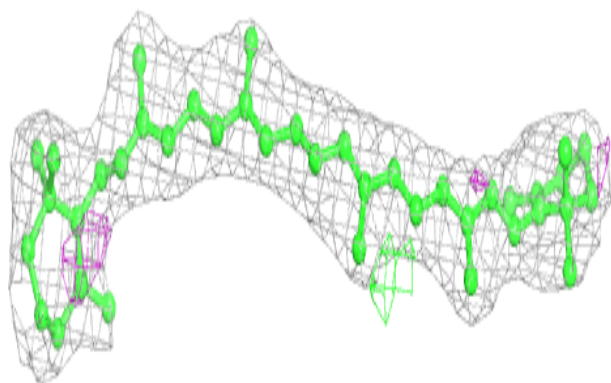


**Electron density around CLA c 505:**

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

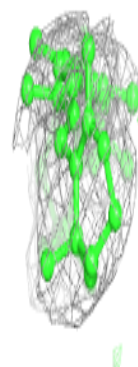
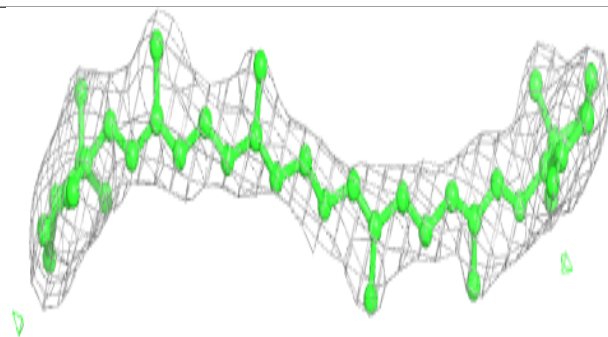
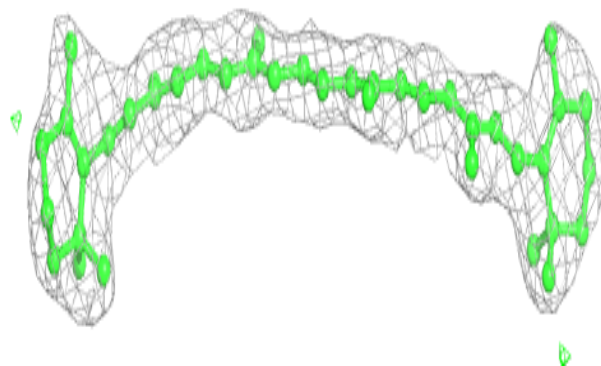
**Electron density around BCR d 406:**

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

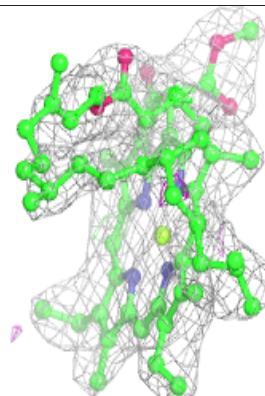
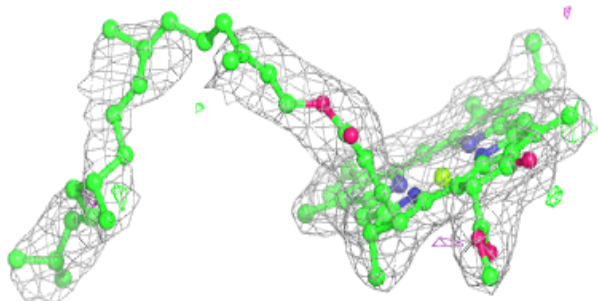
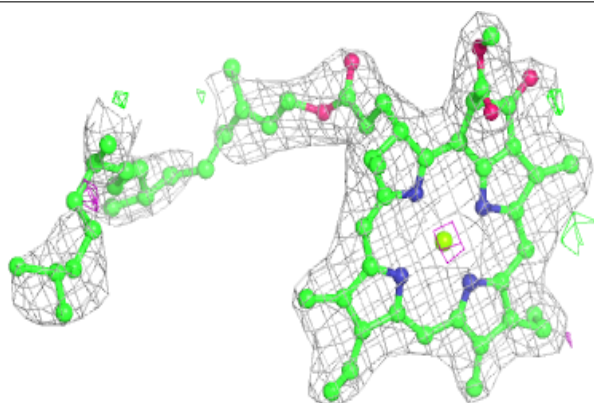


**Electron density around BCR k 102:**

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

**Electron density around CLA a 411:**

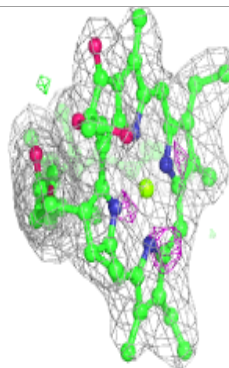
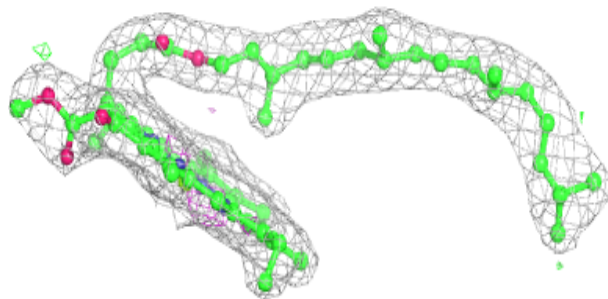
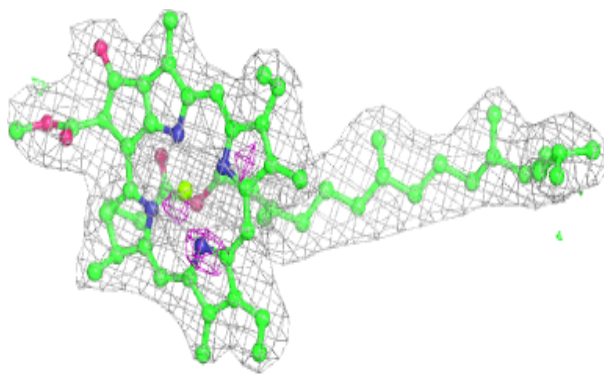
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



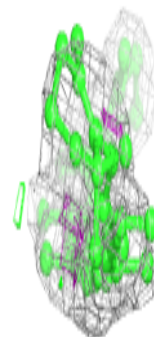
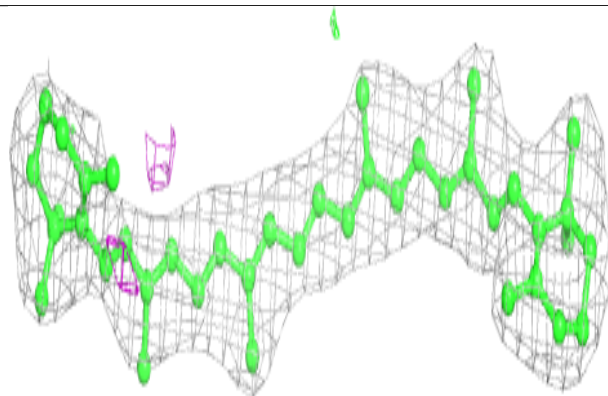
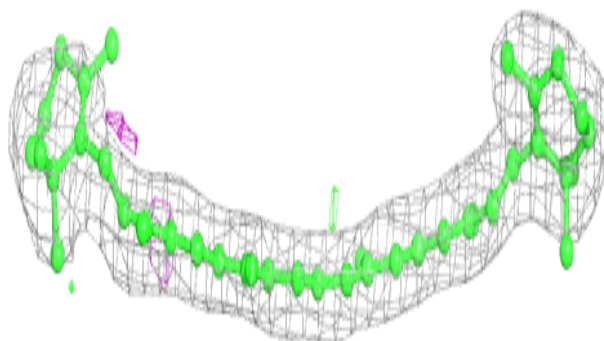


**Electron density around CLA B 609:**

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

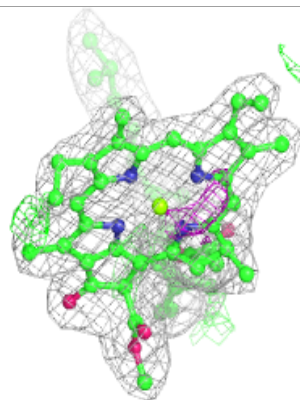
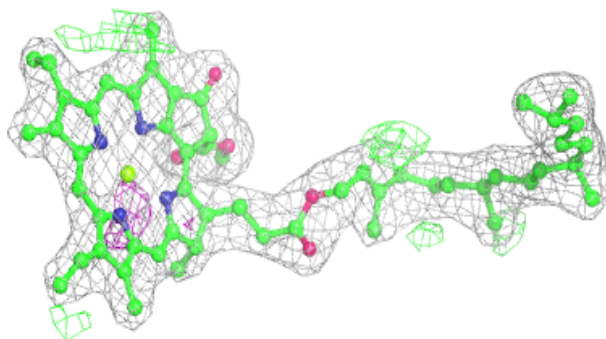
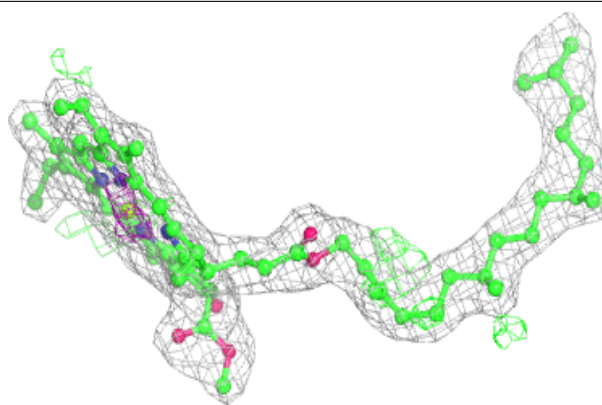
**Electron density around BCR D 407:**

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



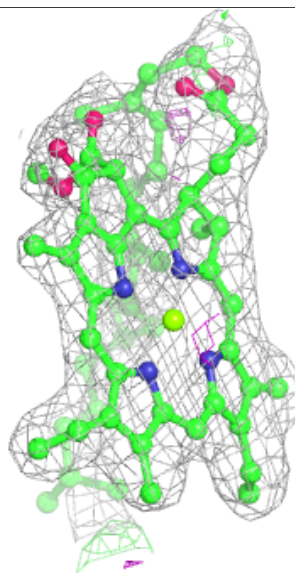
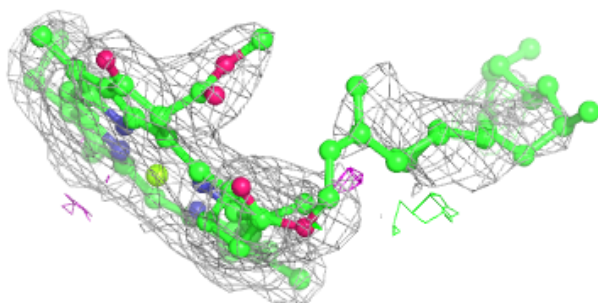
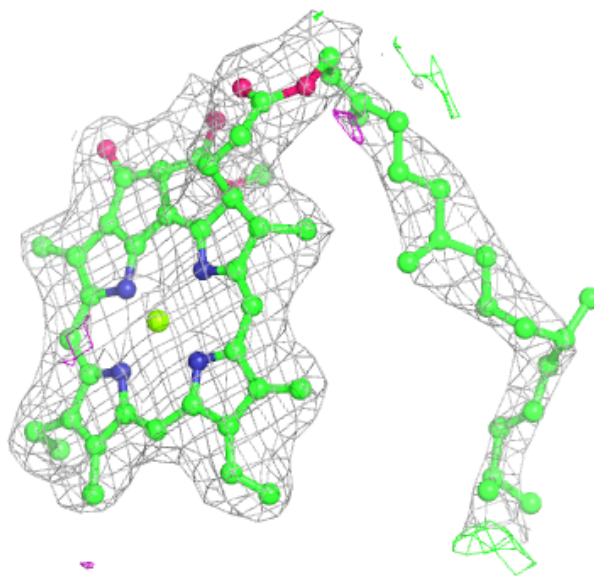
**Electron density around CLA D 405:**

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



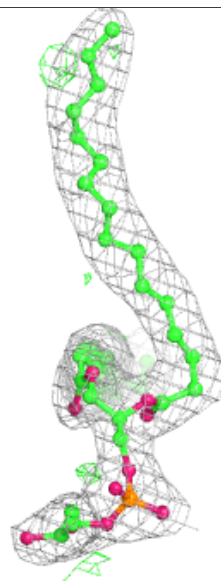
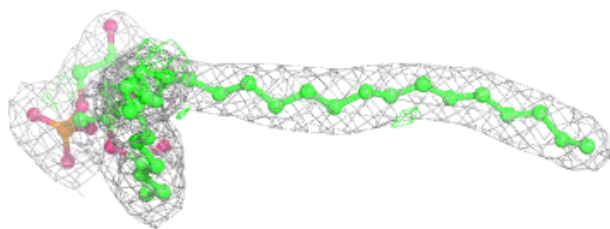
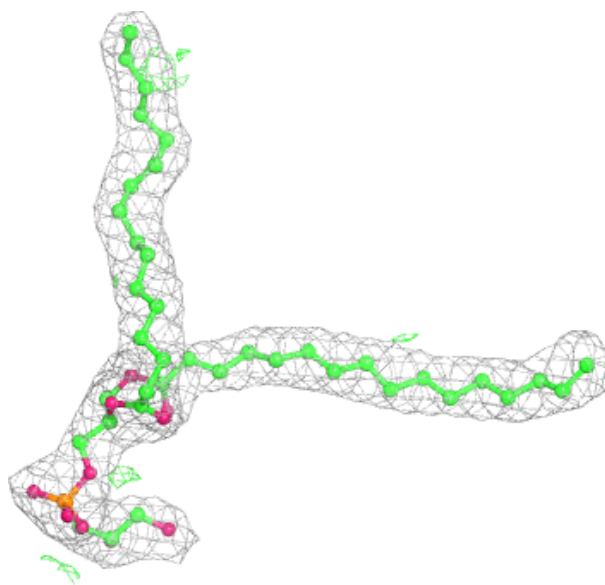
**Electron density around CLA B 617:**

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



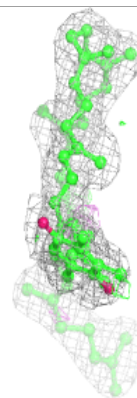
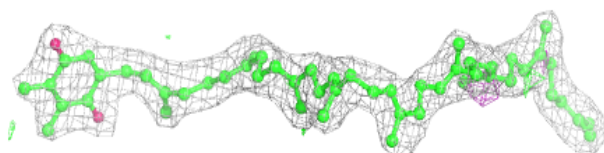
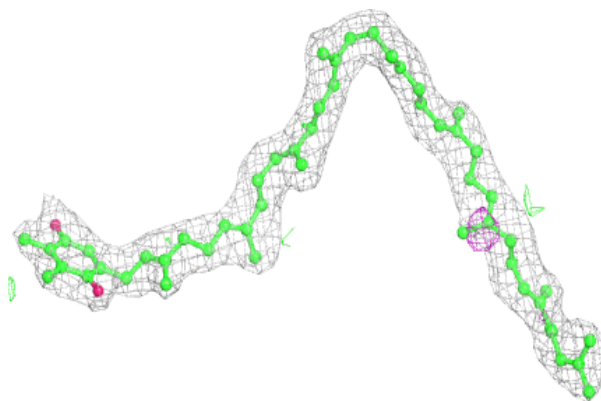
**Electron density around LHG L 101:**

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

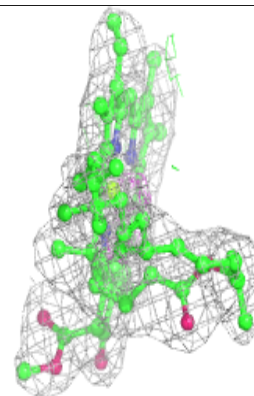
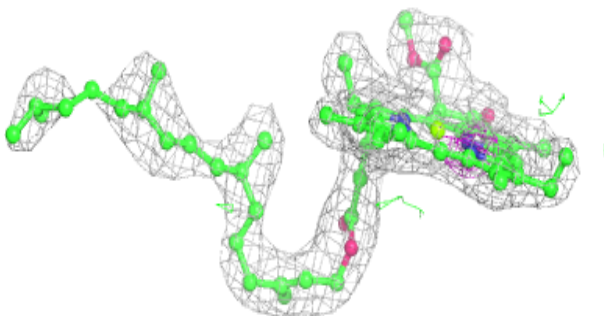
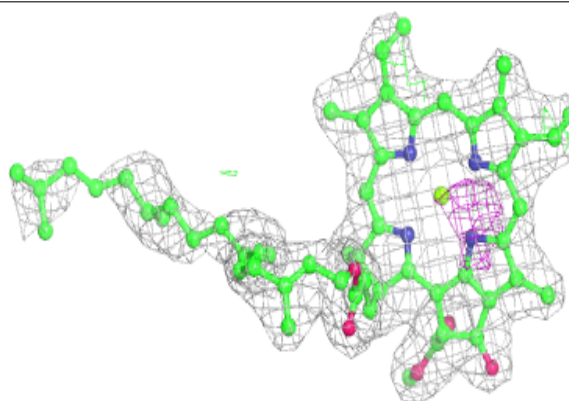


**Electron density around PL9 d 407 (A):**

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

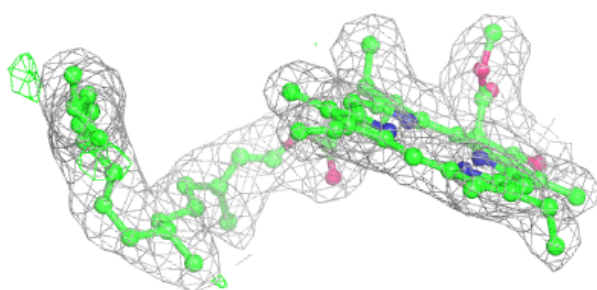
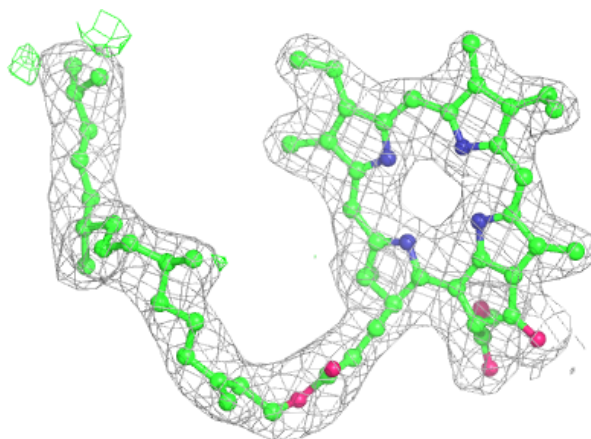
**Electron density around CLA A 406:**

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



**Electron density around PHO D 402 (B):**

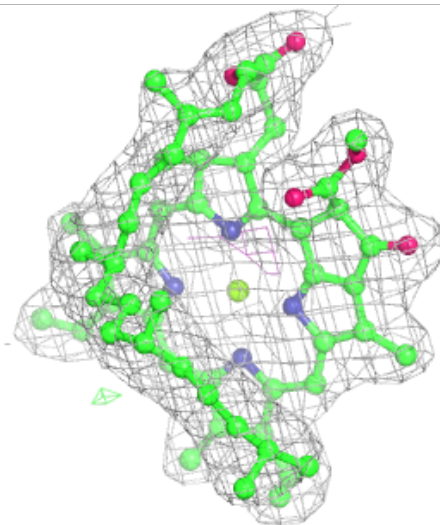
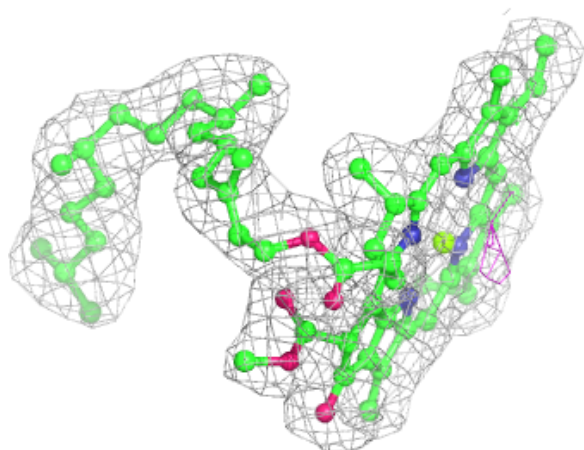
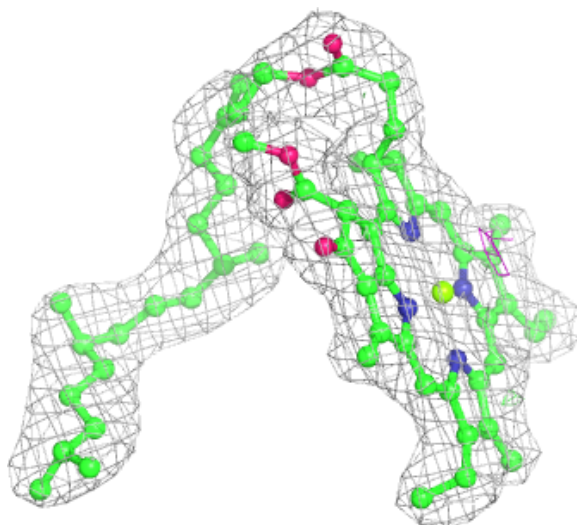
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





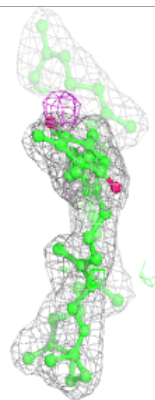
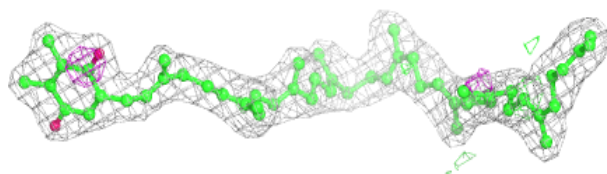
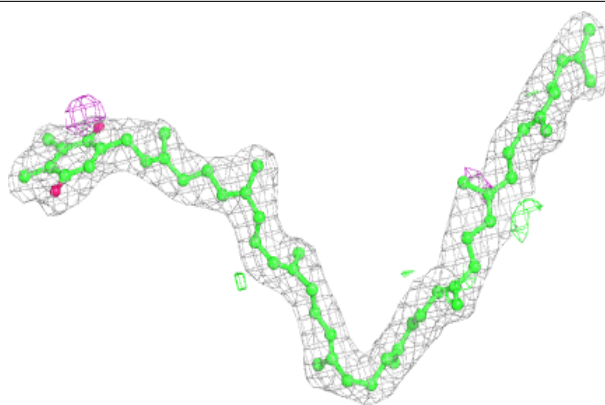
**Electron density around CLA b 622:**

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

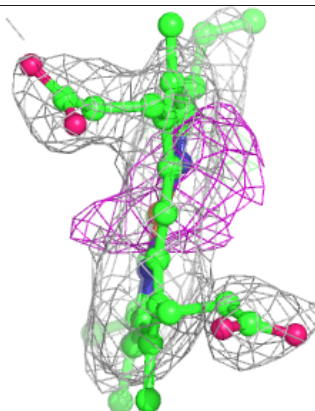
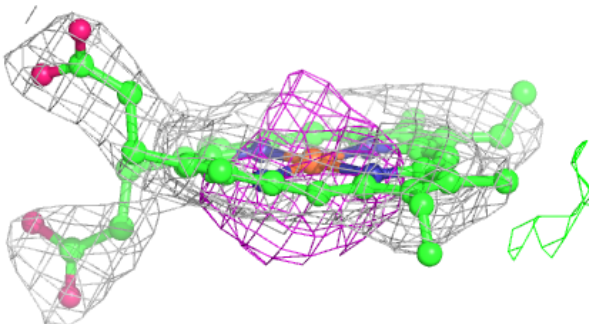
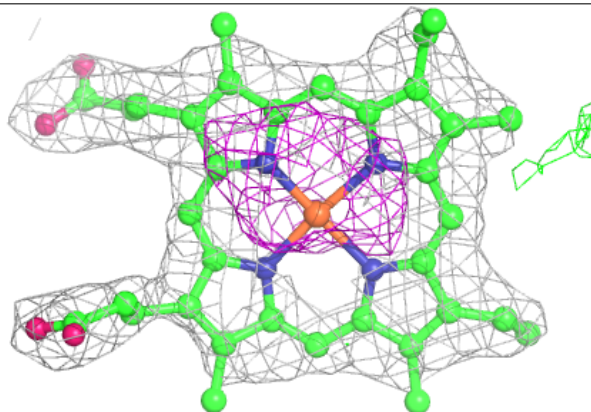


**Electron density around PL9 D 408 (A):**

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

**Electron density around HEM F 102:**

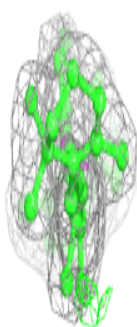
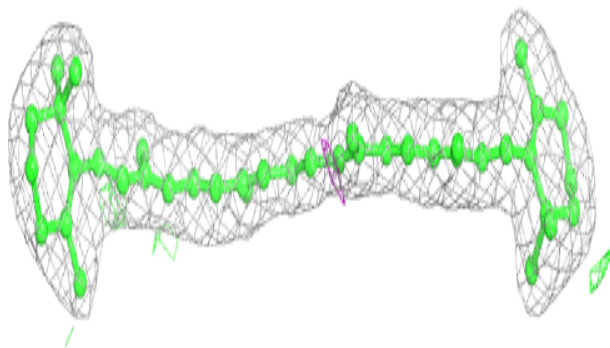
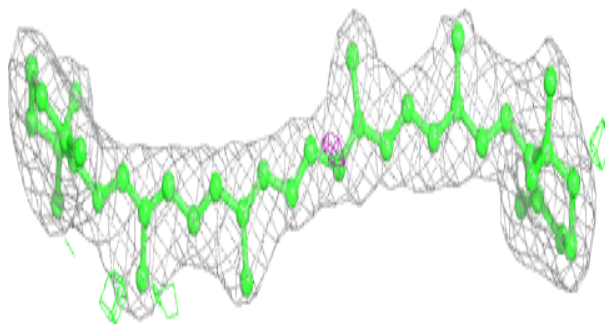
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



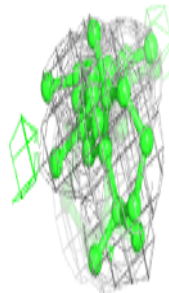
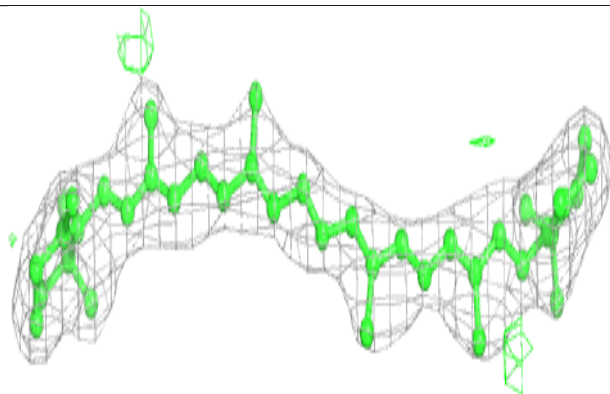
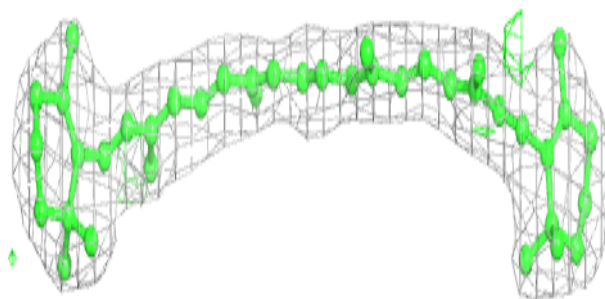


**Electron density around BCR A 409:**

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

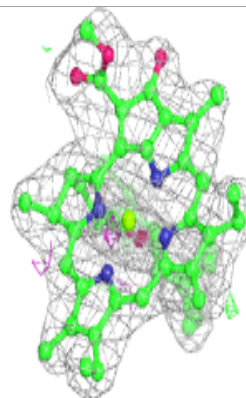
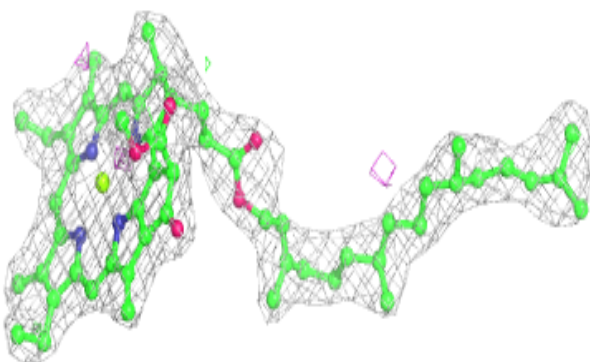
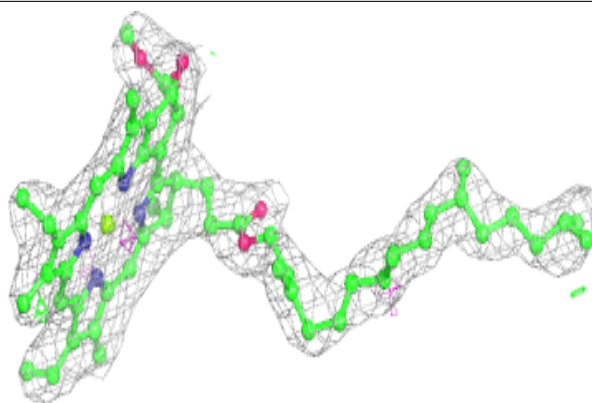
**Electron density around BCR K 103:**

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

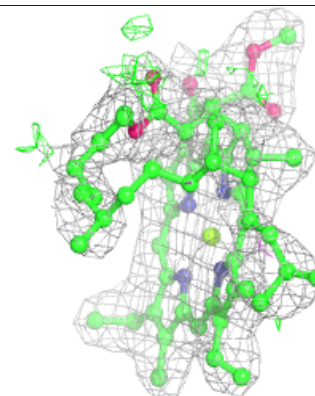
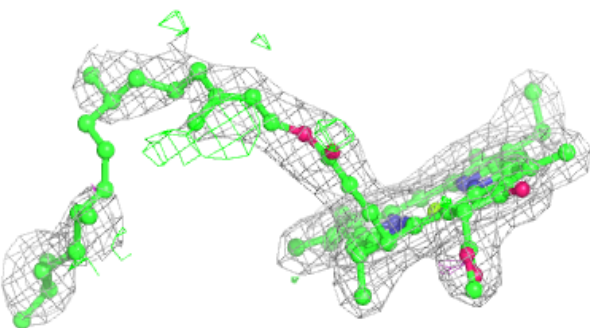
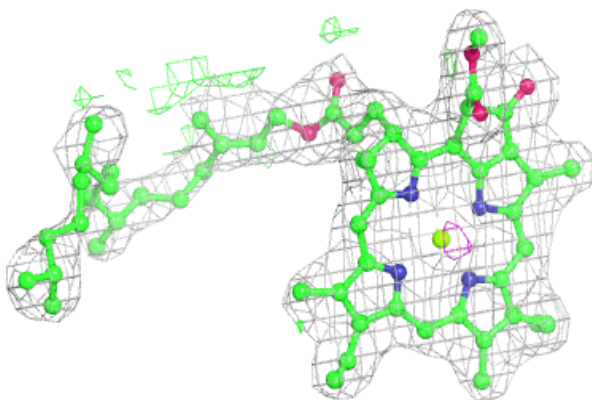


**Electron density around CLA C 503:**

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

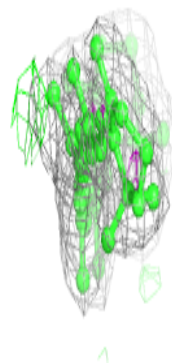
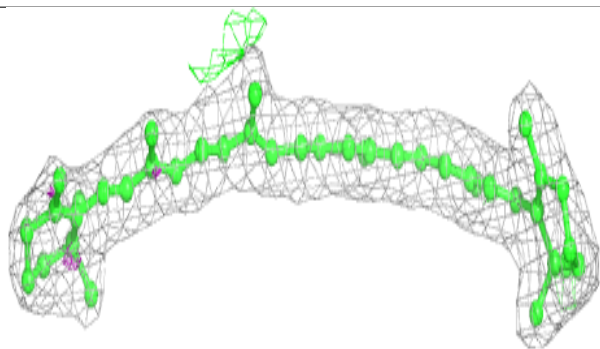
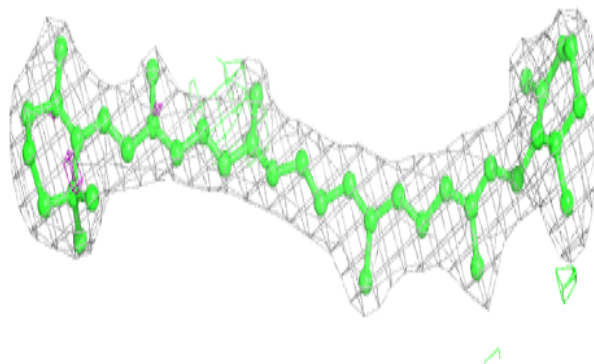
**Electron density around CLA A 408:**

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



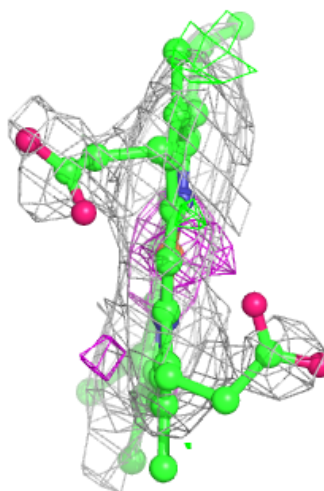
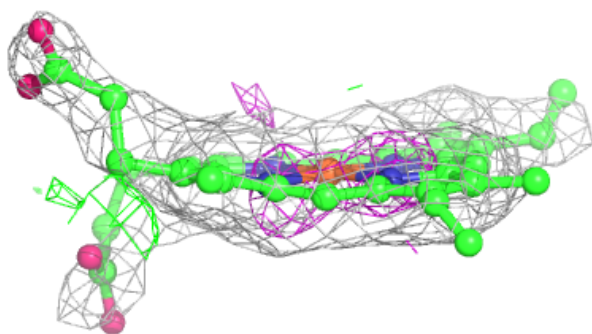
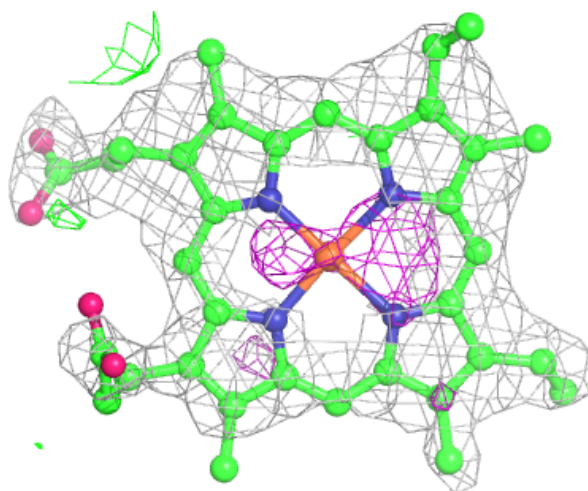
**Electron density around BCR T 103:**

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



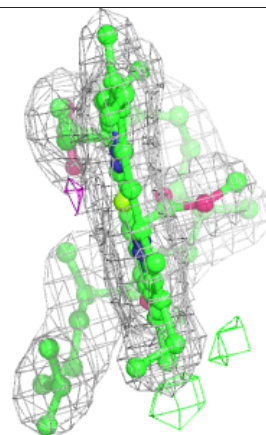
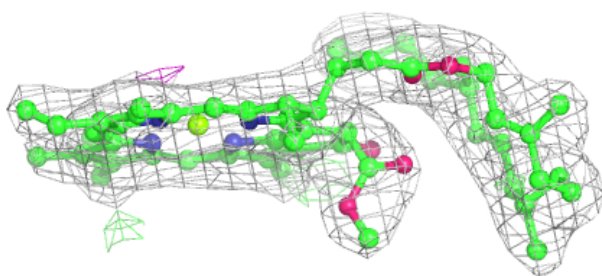
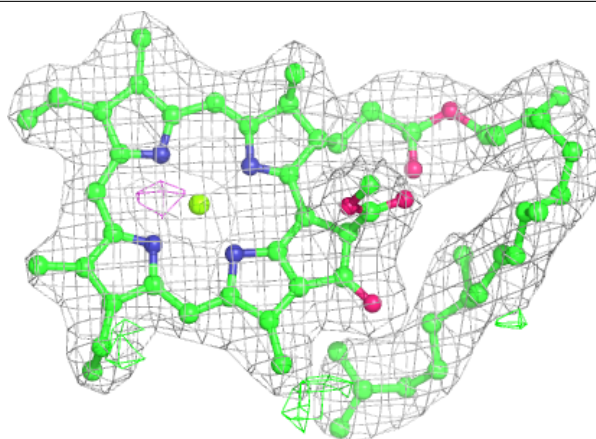
**Electron density around HEM e 101:**

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

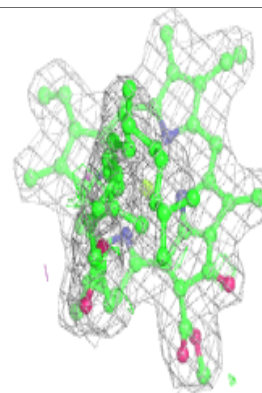
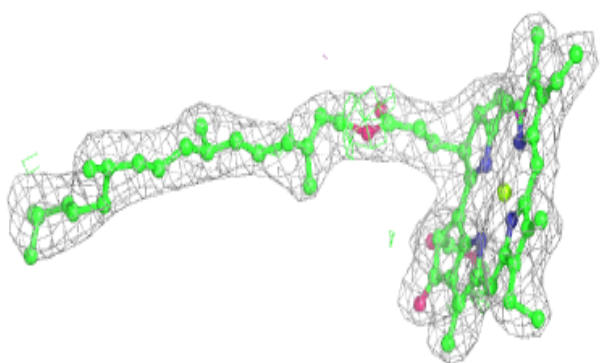
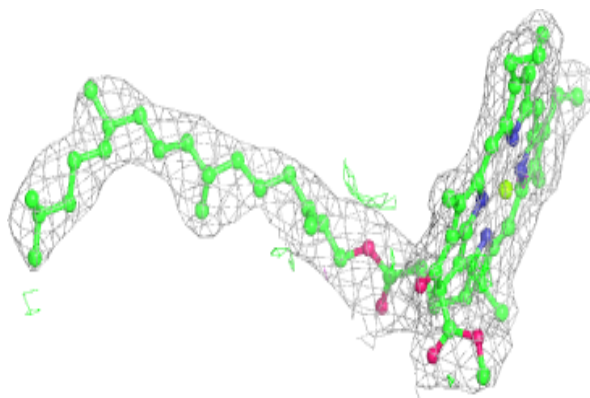


**Electron density around CLA B 611:**

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

**Electron density around CLA b 613:**

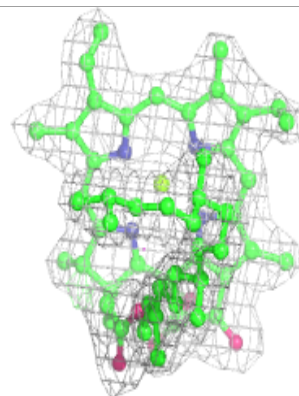
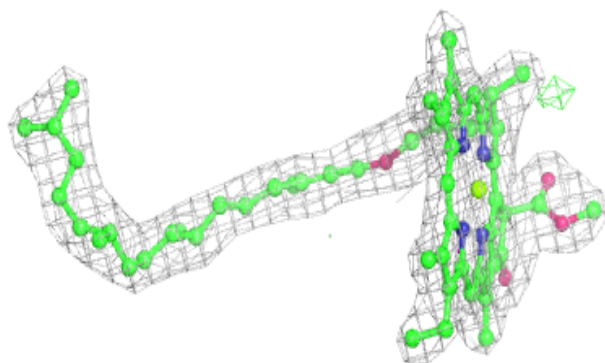
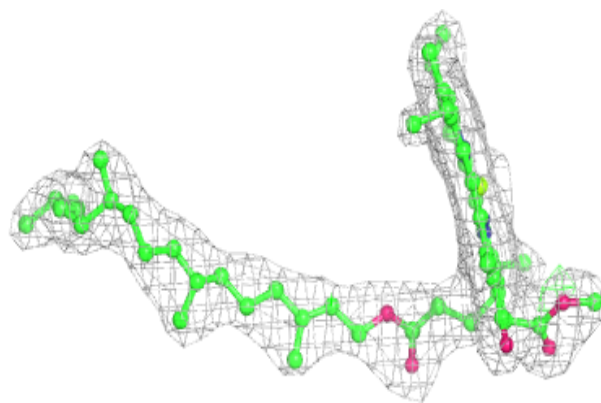
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



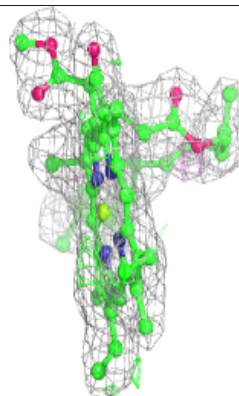
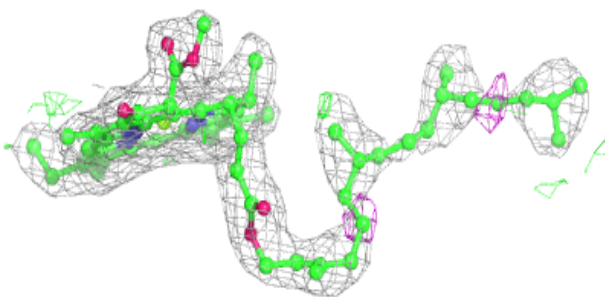
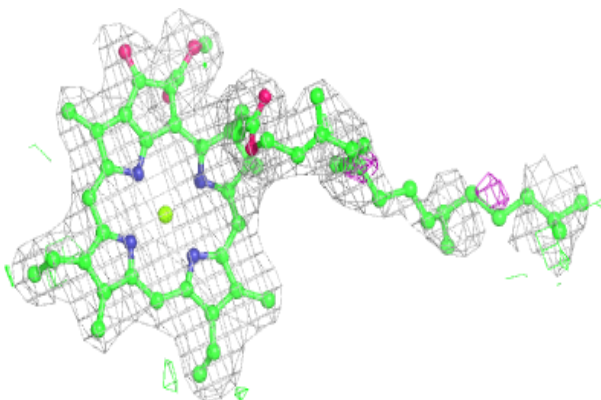


**Electron density around CLA B 606:**

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

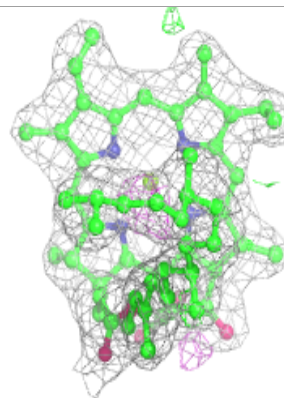
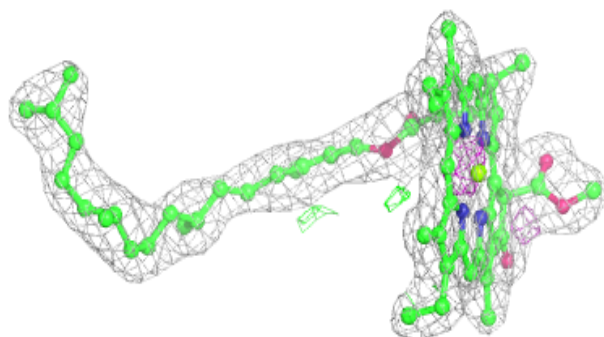
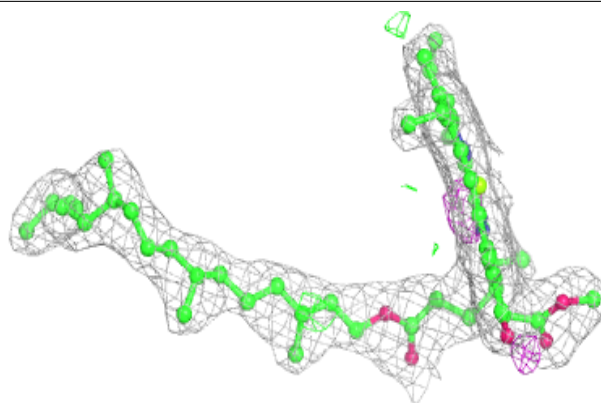
**Electron density around CLA a 409:**

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

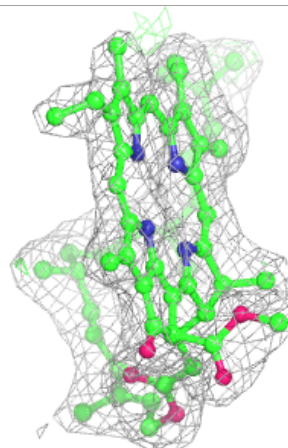
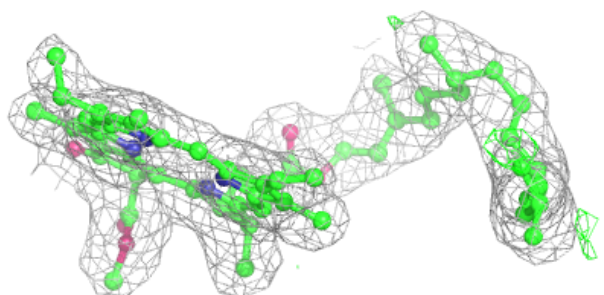
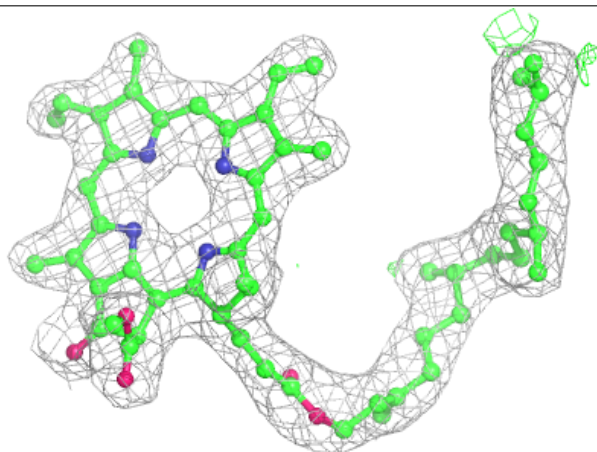


**Electron density around CLA b 614:**

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

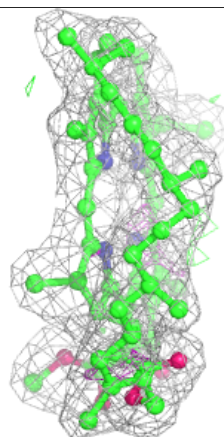
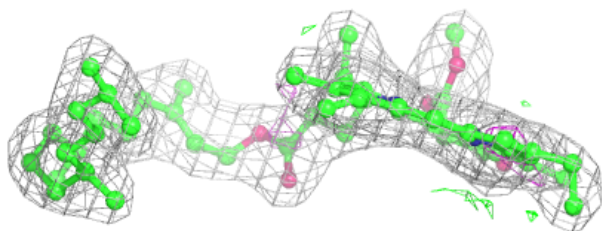
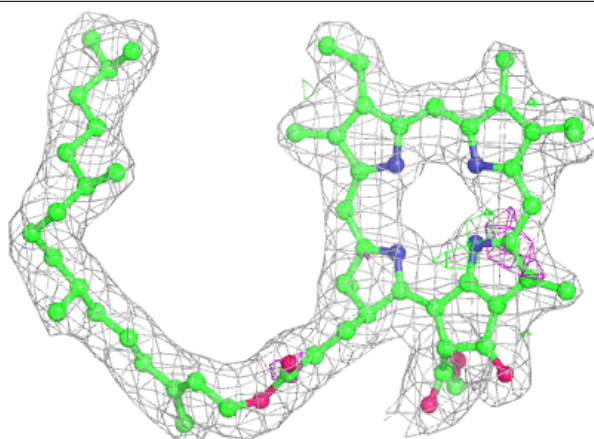
**Electron density around PHO D 402 (A):**

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

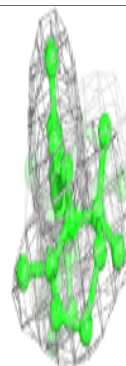
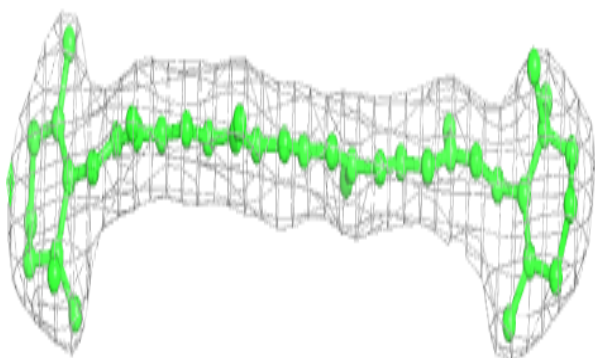
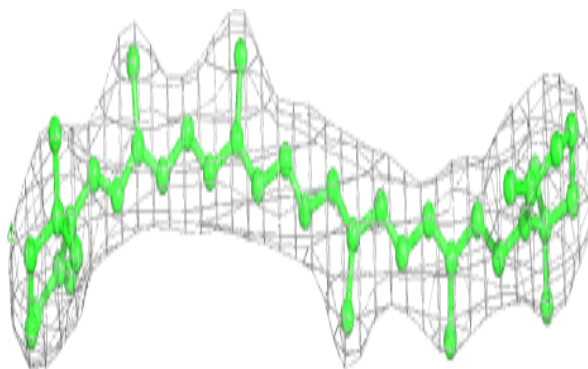


**Electron density around PHO A 407:**

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

**Electron density around BCR C 515:**

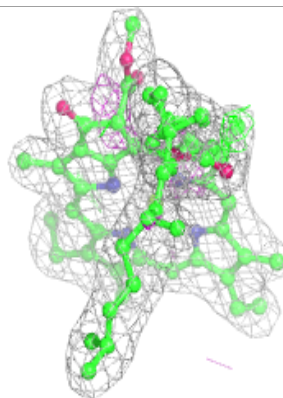
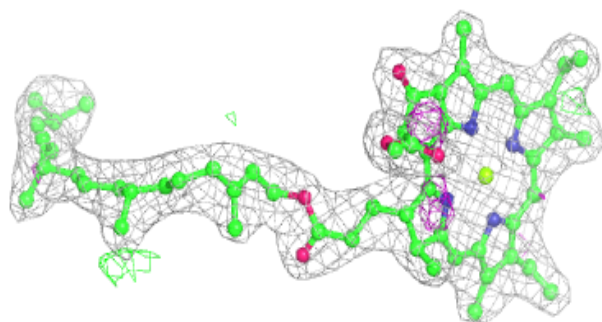
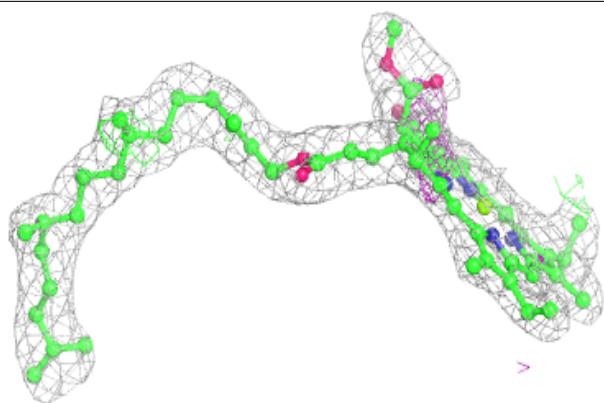
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



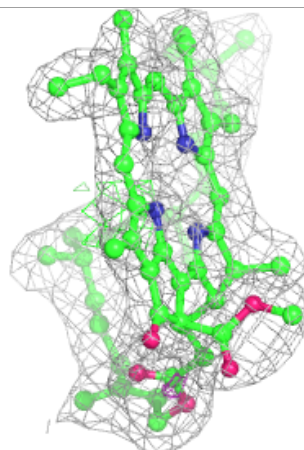
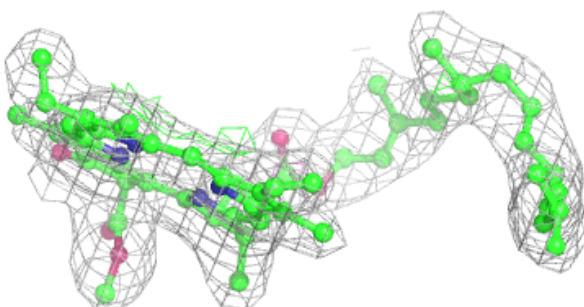
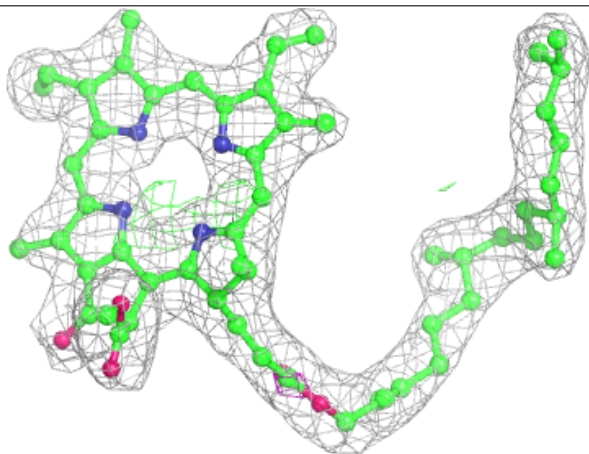


**Electron density around CLA d 404:**

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

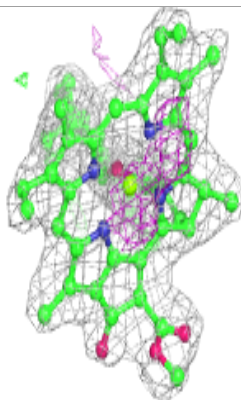
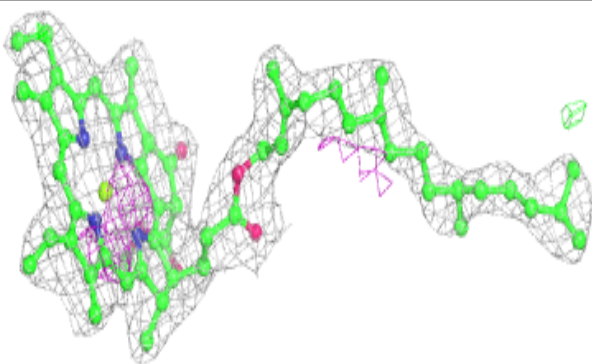
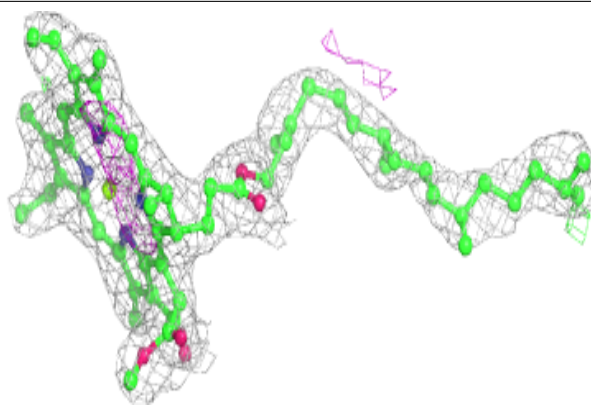
**Electron density around PHO d 402 (B):**

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

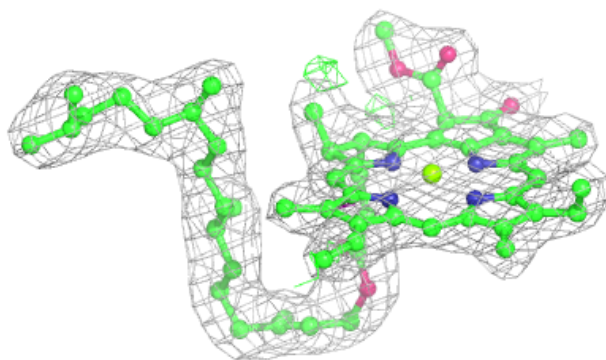
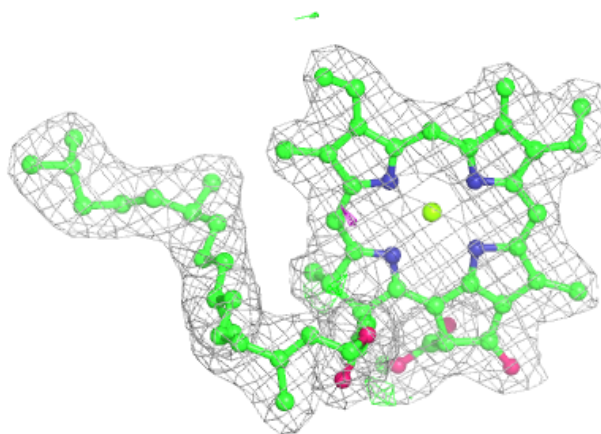


**Electron density around CLA c 506:**

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

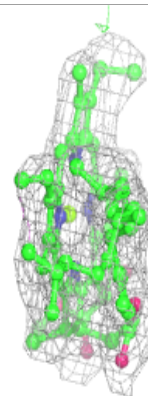
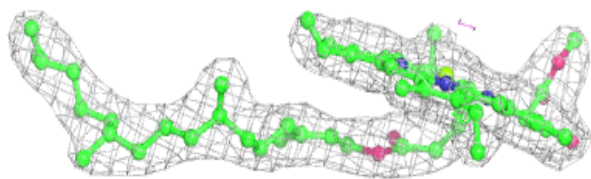
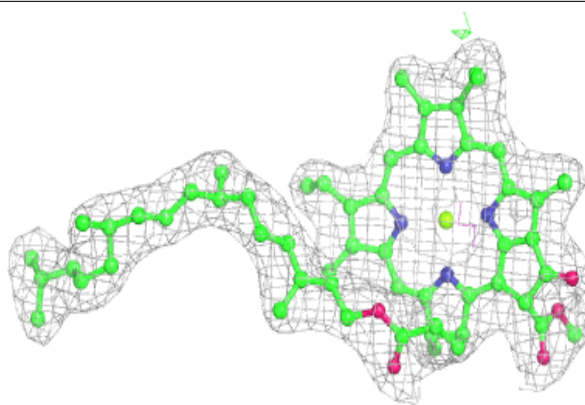
**Electron density around CLA A 405:**

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

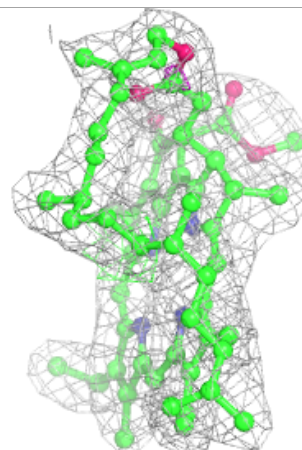
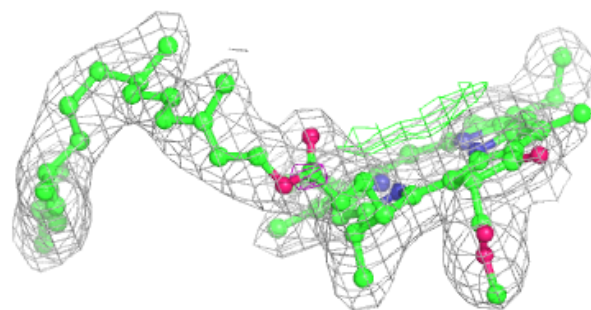
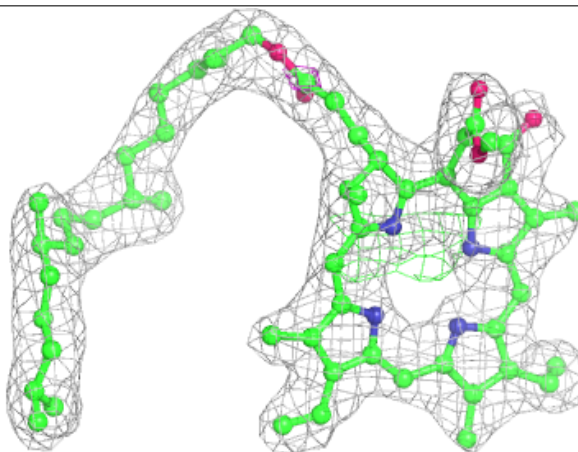


**Electron density around CLA B 604:**

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

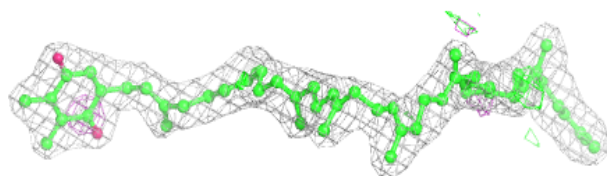
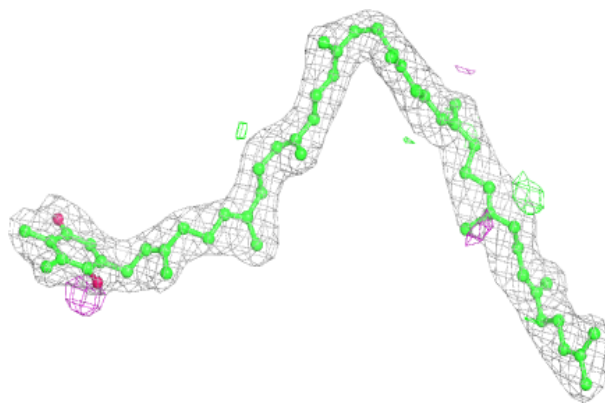
**Electron density around PHO d 402 (A):**

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

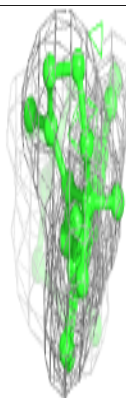
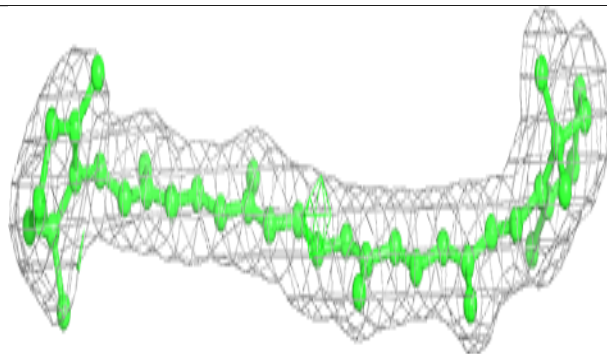
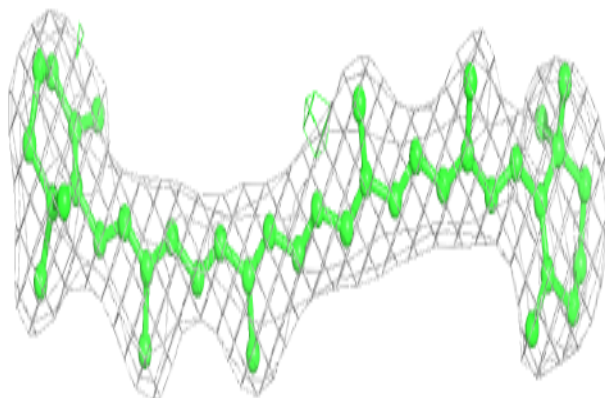


**Electron density around PL9 D 408 (B):**

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

**Electron density around BCR B 620:**

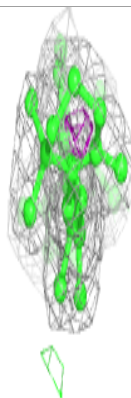
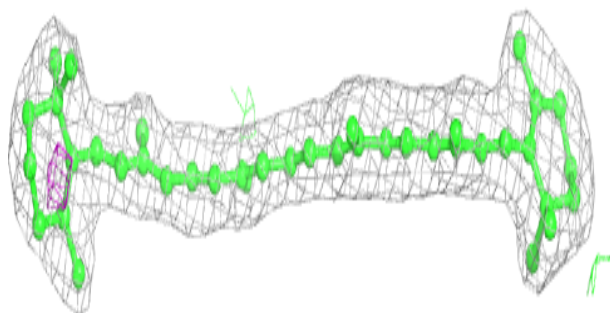
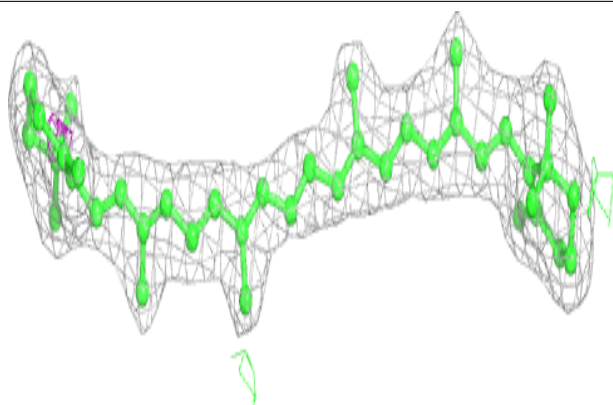
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



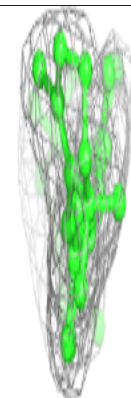
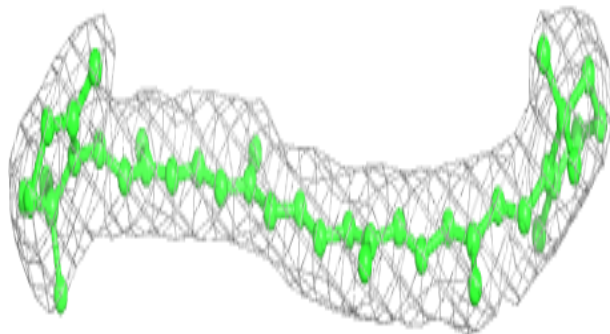
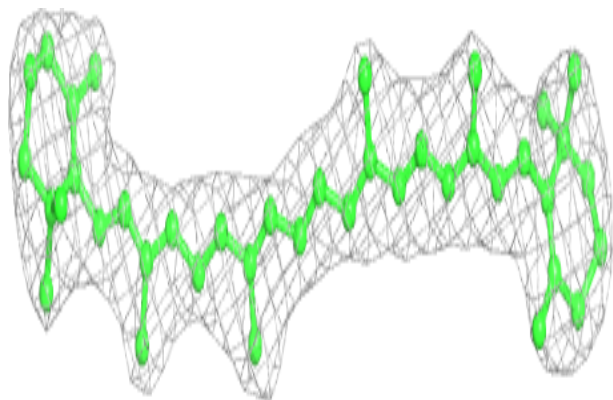


**Electron density around BCR a 412:**

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

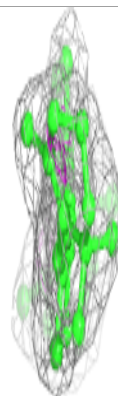
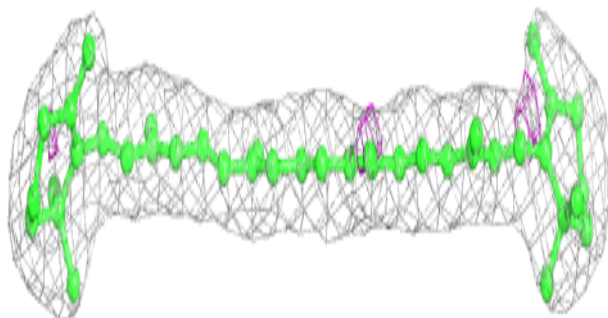
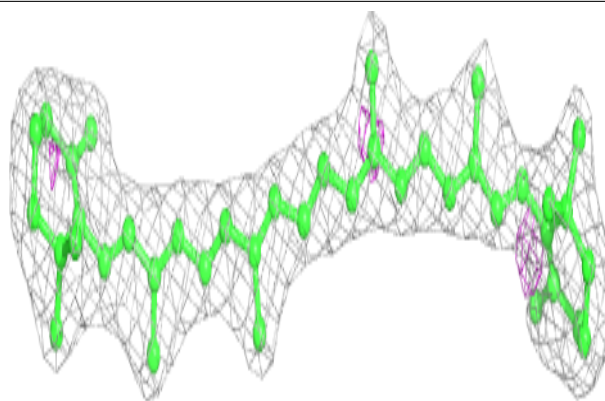
**Electron density around BCR b 628:**

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

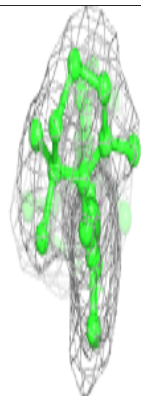
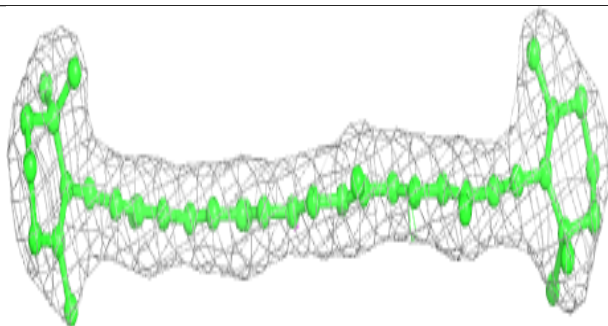
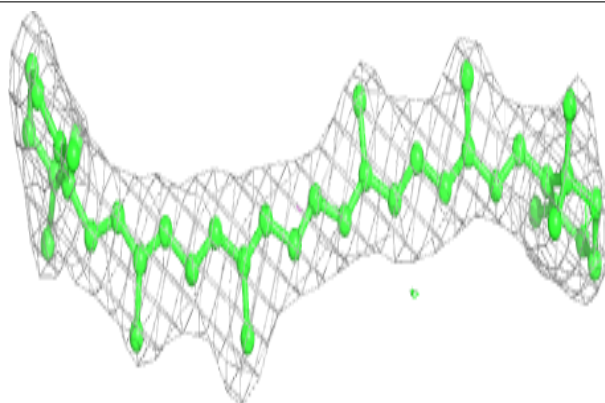


**Electron density around BCR B 619:**

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

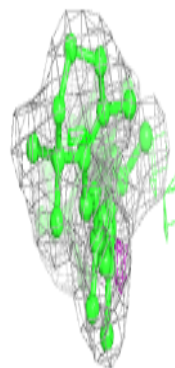
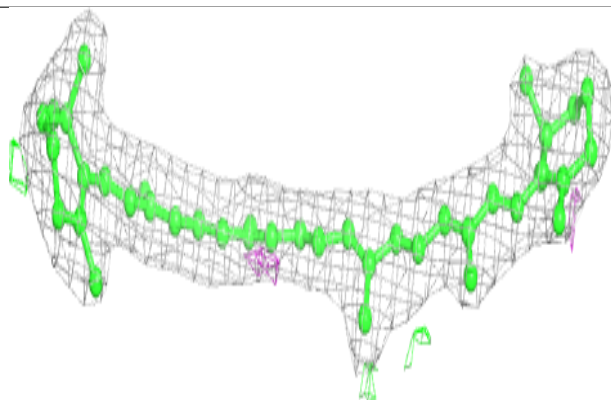
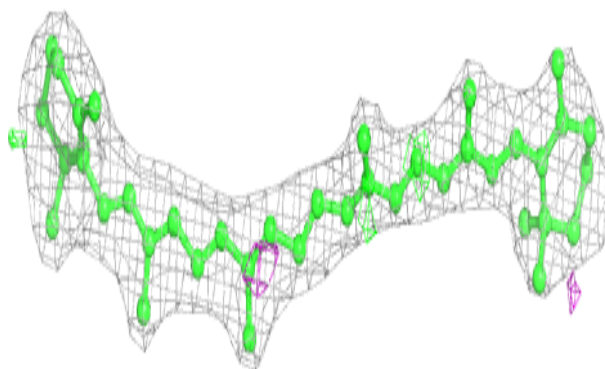
**Electron density around BCR c 518:**

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

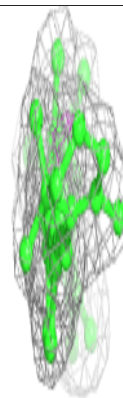
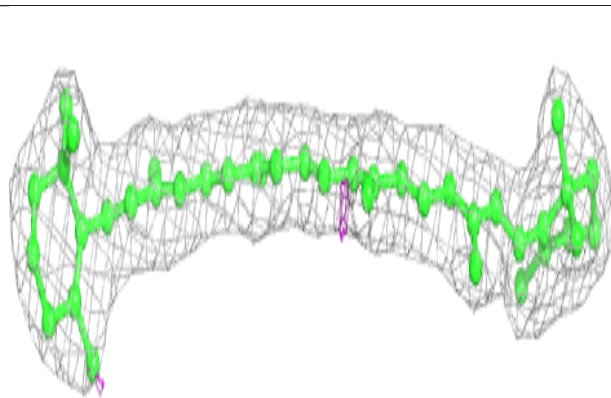
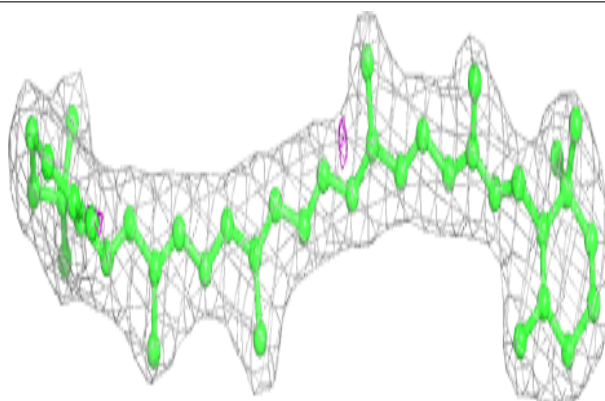


**Electron density around BCR t 101:**

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

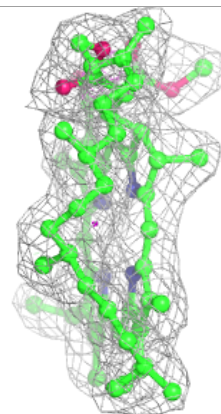
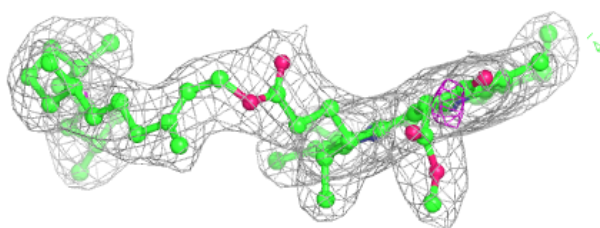
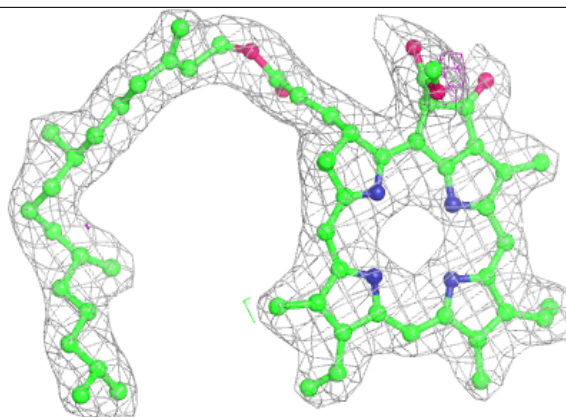
**Electron density around BCR B 618:**

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

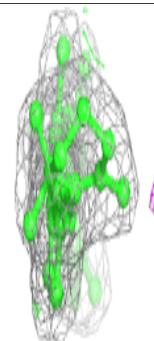
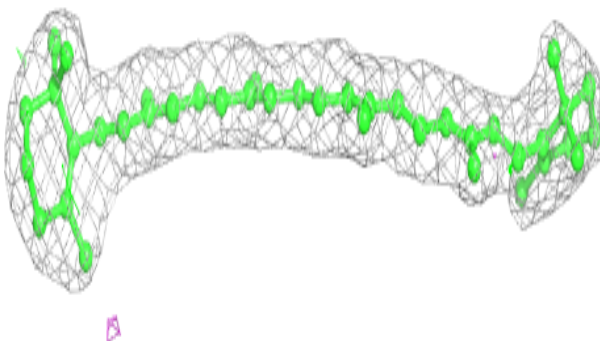
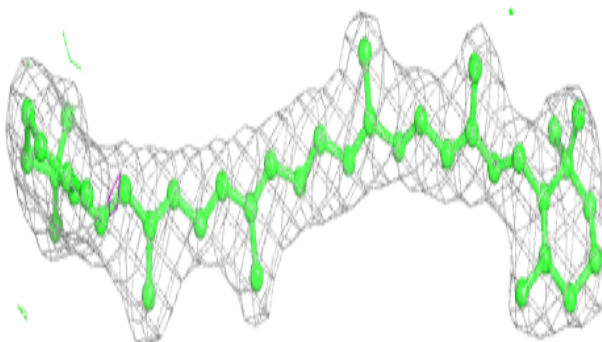


**Electron density around PHO a 410:**

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

**Electron density around BCR b 626:**

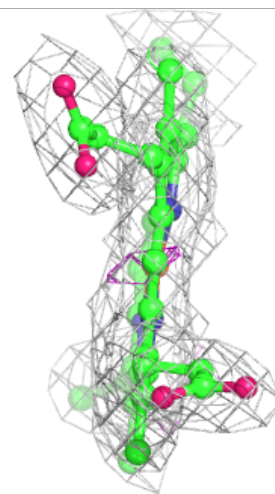
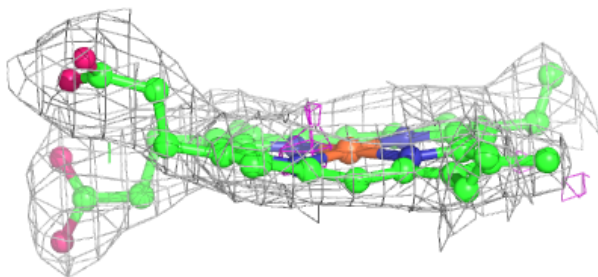
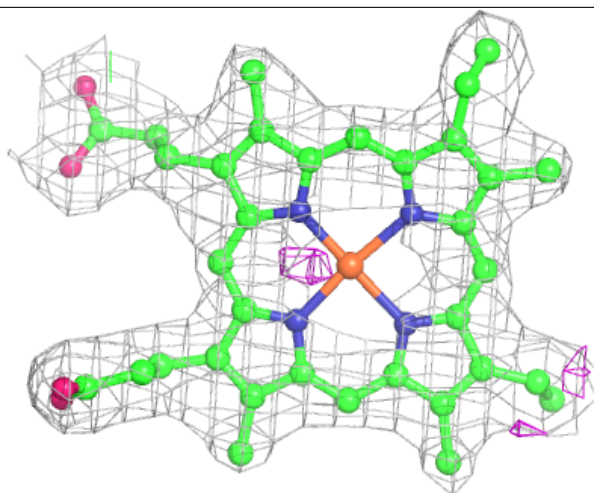
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





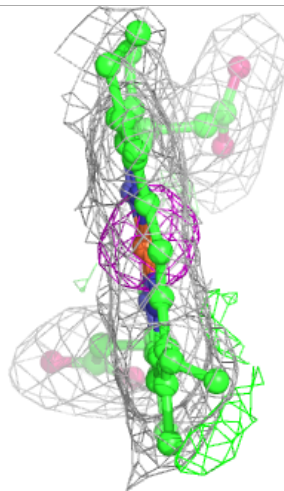
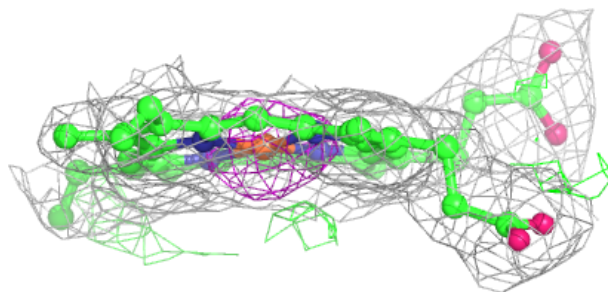
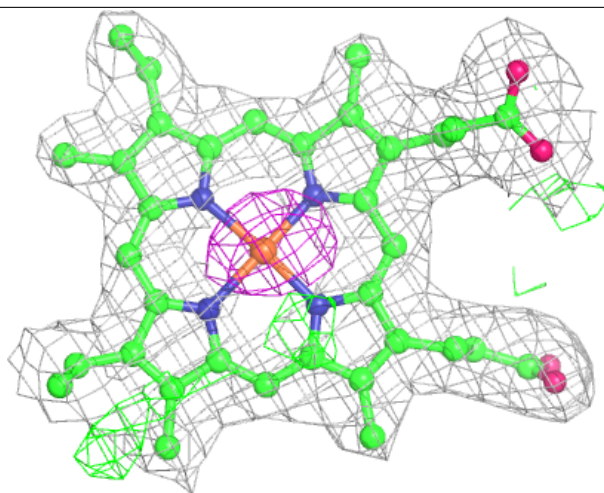
**Electron density around HEM v 206:**

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



**Electron density around HEM V 205:**

$2mF_o-DF_c$  (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.