



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 04:16 PM BST

PDB ID : 6JLP
Title : XFEL structure of cyanobacterial photosystem II (3F state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

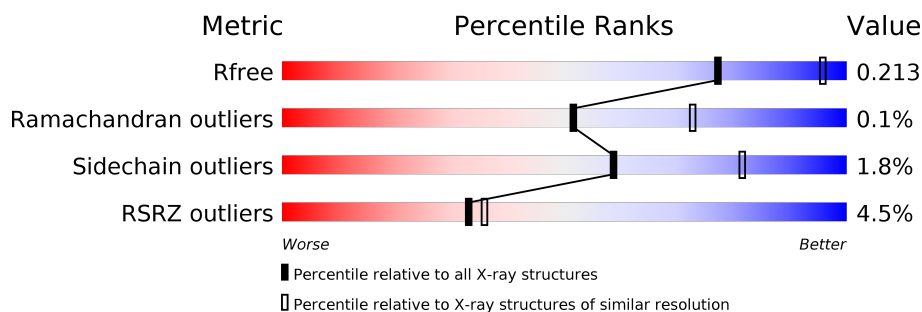
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



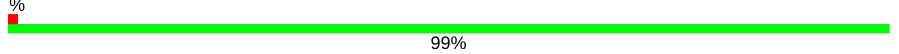
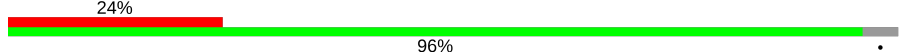
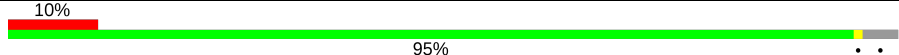
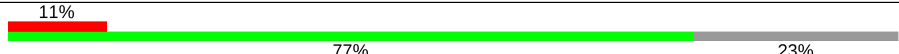
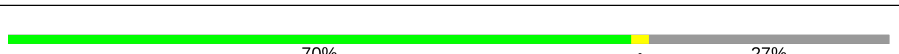
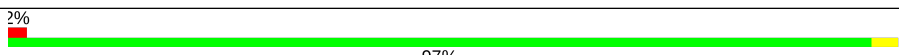
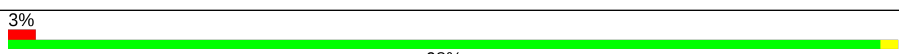
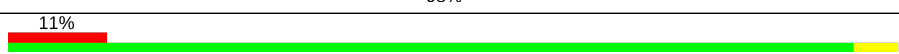
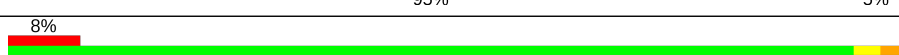
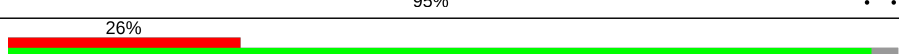
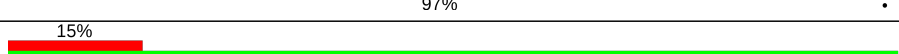
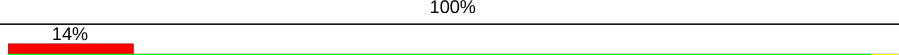
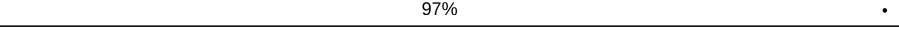
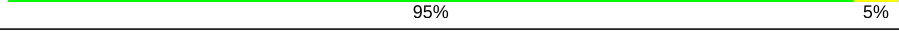
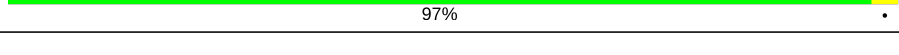
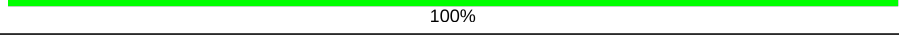


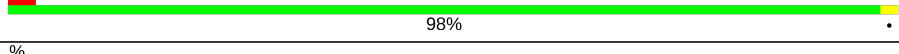
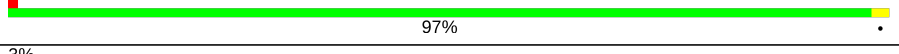





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div></div> <div>97%</div> <div>.</div> </div>
1	a	344	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
2	B	505	<div> <div>2%</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>5%</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>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	d	342	% 
5	E	84	24% 
5	e	84	10% 
6	F	44	11% 
6	f	44	70% 
7	H	65	2% 
7	h	65	3% 
8	I	38	11% 
8	i	38	8% 
9	J	39	26% 
9	j	39	15% 
10	K	37	14% 
10	k	37	95% 
11	L	37	97% 
11	l	37	100% 
12	M	36	86% 
12	m	36	89% 
13	O	244	3% 
13	o	244	% 
14	T	32	3% 
14	t	32	88% 
15	U	104	% 
15	u	104	90% 
16	V	137	% 
16	v	137	% 

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	407	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	-	-	-

Continued on next page...

Continued from previous page...

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	406	X	-	-	-
23	CLA	D	407	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	a	412	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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	d	405	X	-	-	-
26	GOL	V	202	-	-	-	X
27	LMT	C	521	-	-	-	X
27	LMT	F	101	-	-	-	X
27	LMT	a	419	-	-	-	X
27	LMT	b	630	-	-	-	X
34	DGD	d	408	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 55697 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	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			

Continued on next page...

Continued from previous page...

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	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		0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O		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		98	0	0
			239	163	41	35				

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		
21	a	1	Total	Fe	0	1
			1	1		

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

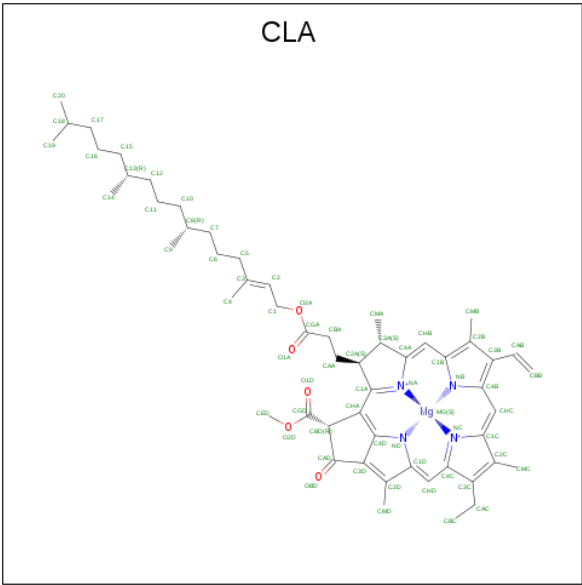
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

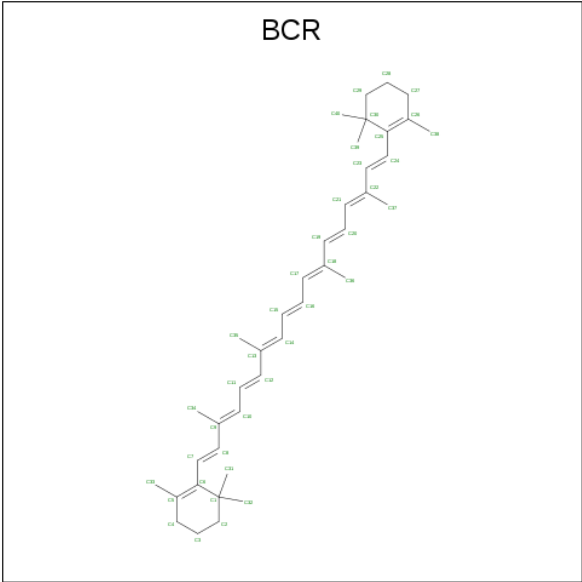
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

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	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



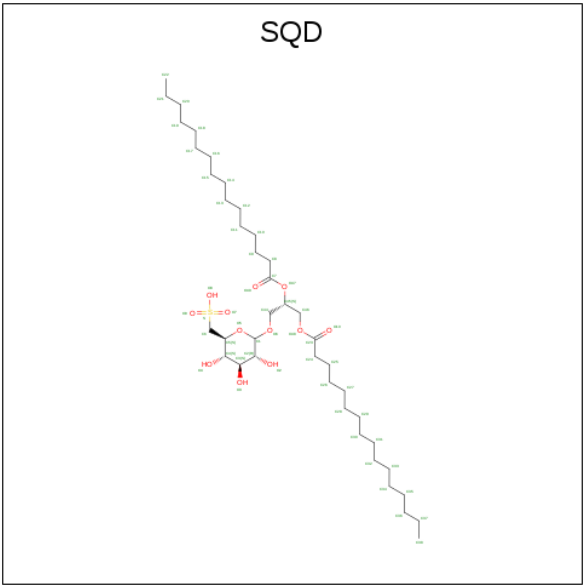
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



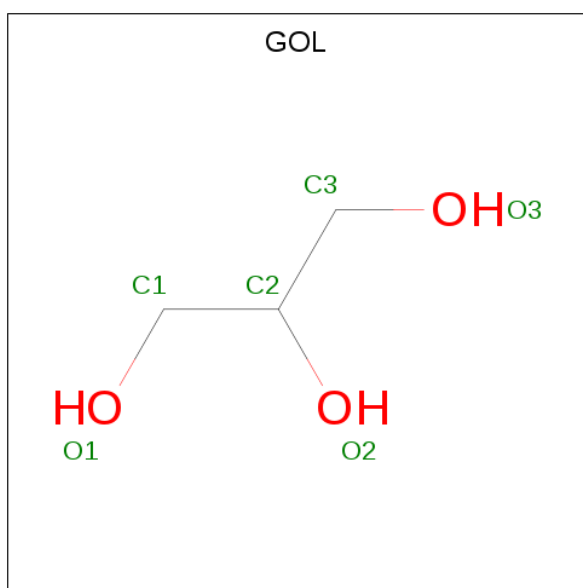
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O S 54 41 12 1	0	0
25	A	1	Total C O S 54 41 12 1	0	0
25	B	1	Total C O S 54 41 12 1	0	0

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

Continued from previous page...

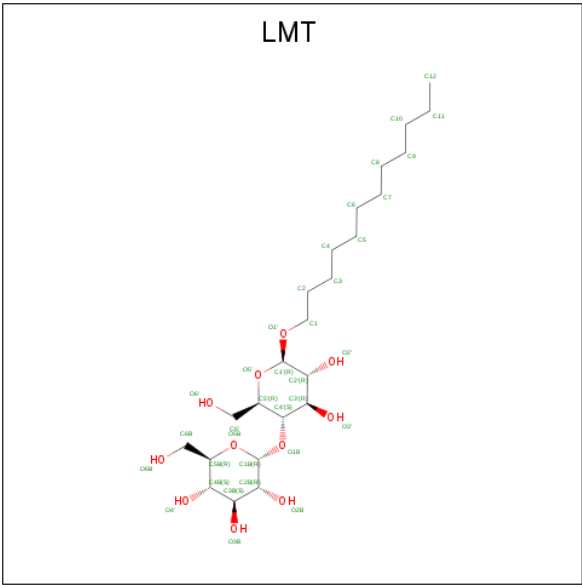
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	0
			6	3	3		
26	D	1	Total	C	O	0	0
			6	3	3		
26	F	1	Total	C	O	0	0
			6	3	3		
26	O	1	Total	C	O	0	0
			6	3	3		
26	T	1	Total	C	O	0	0
			6	3	3		
26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

Continued on next page...

Continued from previous page...

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

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



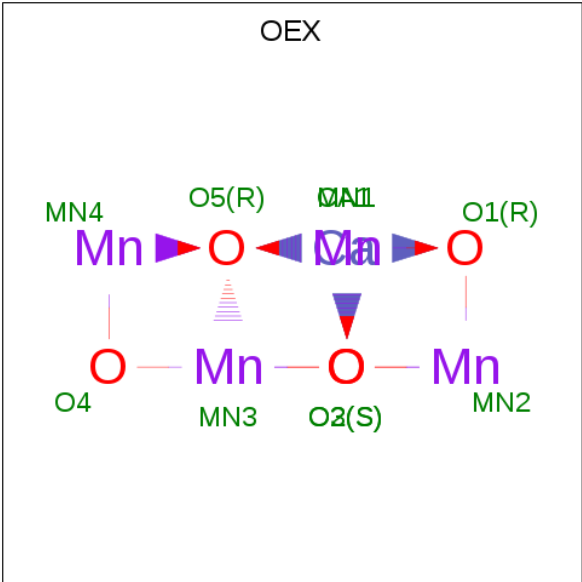
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			35	24	11		
27	C	1	Total	C	O	0	0
			35	24	11		
27	D	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

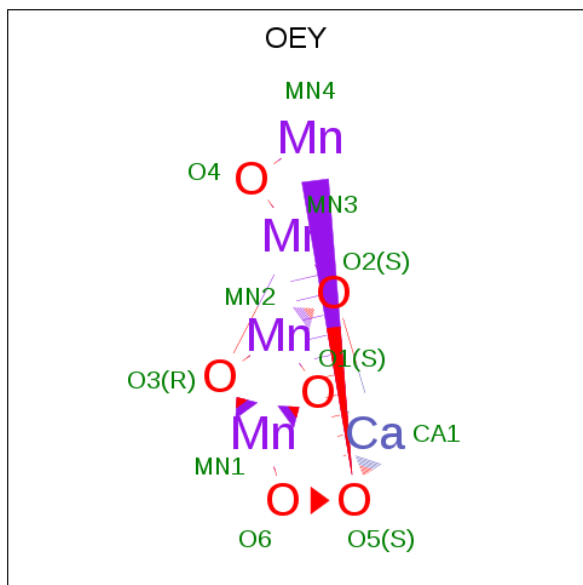
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	F	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	T	1	Total	C	O	0	0
			25	19	6		
27	a	1	Total	C	O	0	0
			35	24	11		
27	a	1	Total	C	O	0	0
			35	24	11		
27	b	1	Total	C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

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



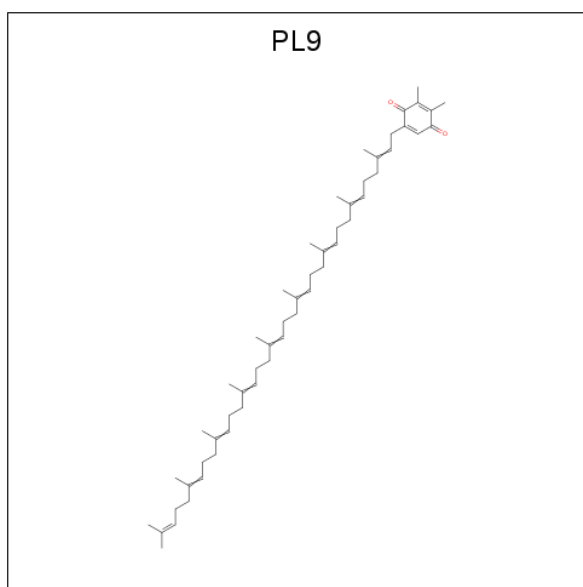
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 29 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

- Molecule 30 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
30	A	1	Total	C	O	0	1
			110	106	4		
30	D	1	Total	C	O	0	1
			110	106	4		
30	a	1	Total	C	O	0	1
			110	106	4		
30	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

Continued on next page...

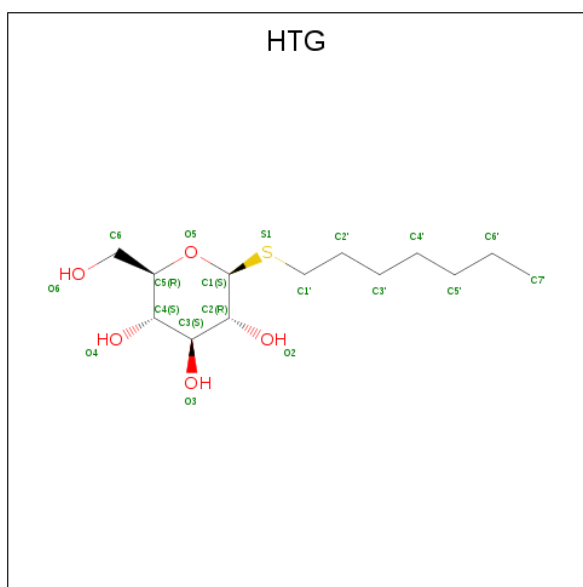
Continued from previous page...

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

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

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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



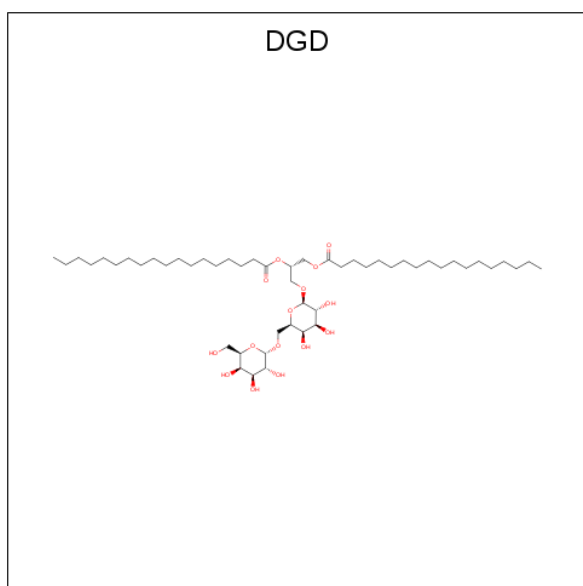
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	D	1	Total 16	C 10	O 5	S 1	0	0
33	V	1	Total 19	C 13	O 5	S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

Continued on next page...

Continued from previous page...

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

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



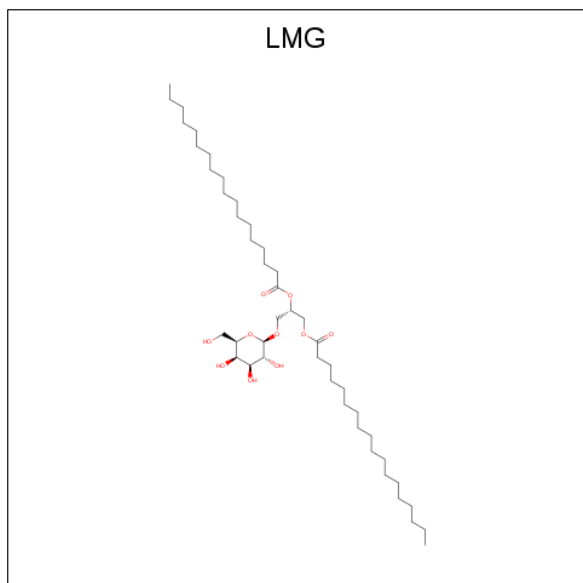
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	D	1	Total	C	O		0	0
			52	42	10			
34	c	1	Total	C	O		0	0
			62	47	15			
34	c	1	Total	C	O		0	0
			62	47	15	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

Continued on next page...

Continued from previous page...

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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



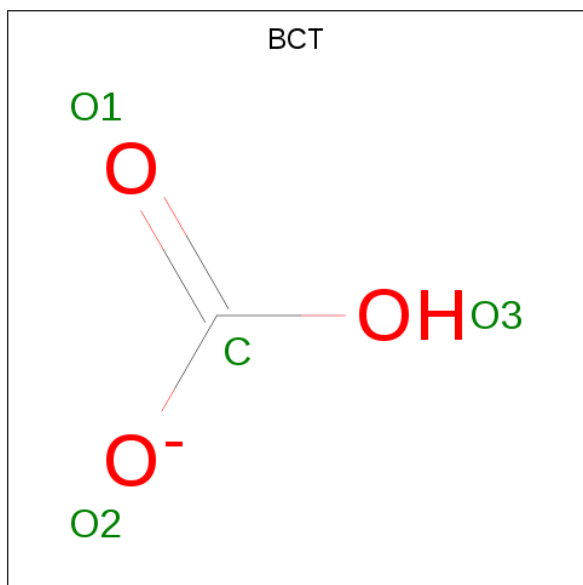
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			51	41	10		
35	C	1	Total	C	O	0	0
			51	41	10		
35	C	1	Total	C	O	0	0
			51	41	10		
35	D	1	Total	C	O	0	0
			51	41	10		
35	M	1	Total	C	O	0	0
			51	41	10		
35	Z	1	Total	C	O	0	0
			37	27	10		
35	a	1	Total	C	O	0	0
			51	41	10		
35	b	1	Total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

Continued on next page...

Continued from previous page...

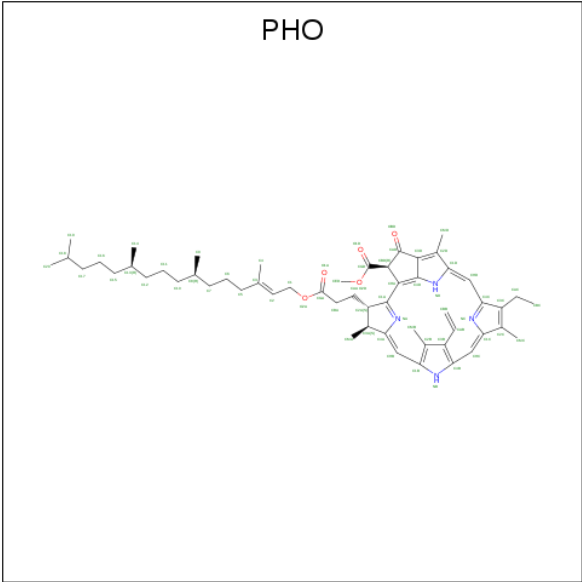
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	c	1	Total	C	O	0	0
			51	41	10		
35	d	1	Total	C	O	0	0
			51	41	10		
35	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 36 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



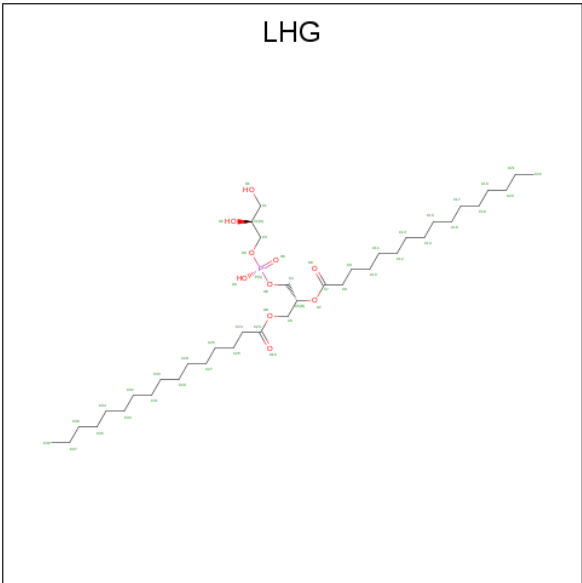
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D	1	Total	C	O	0	1
			8	2	6		
36	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 37 is PHEOPHYTIN A (three-letter code: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



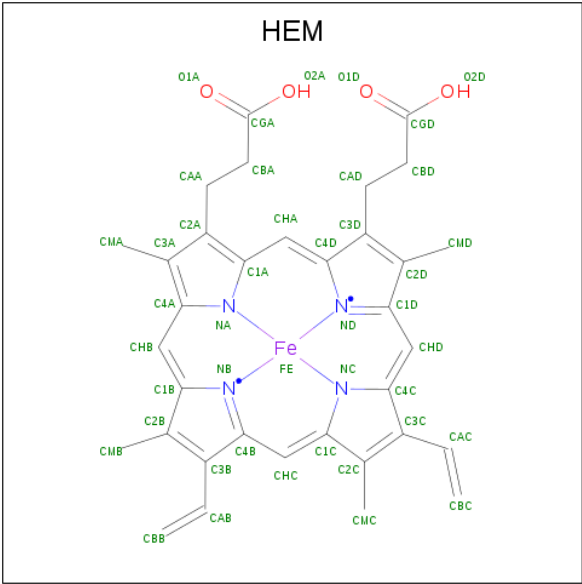
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	N	O	0	0
			64	55	4	5		
37	D	1	Total	C	N	O	0	1
			128	110	8	10		
37	a	1	Total	C	N	O	0	0
			64	55	4	5		
37	d	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

Continued on next page...

Continued from previous page...

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	160	Total 172	O 172	0	14
41	B	286	Total 290	O 290	0	4
41	C	218	Total 222	O 222	0	5
41	D	146	Total 150	O 150	0	5
41	E	34	Total 35	O 35	0	1
41	F	11	Total 11	O 11	0	0
41	H	40	Total 40	O 40	0	0
41	I	6	Total 6	O 6	0	0
41	J	10	Total 10	O 10	0	0
41	K	9	Total 9	O 9	0	0
41	L	15	Total 16	O 16	0	1
41	M	23	Total 23	O 23	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	O	180	Total 182	O 182	0	2
41	T	16	Total 17	O 17	0	1
41	U	79	Total 79	O 79	0	0
41	V	122	Total 124	O 124	0	2
41	Y	4	Total 4	O 4	0	0
41	X	10	Total 10	O 10	0	0
41	Z	1	Total 1	O 1	0	0
41	a	146	Total 155	O 155	0	12
41	b	259	Total 262	O 262	0	3
41	c	204	Total 209	O 209	0	6
41	d	142	Total 145	O 145	0	3
41	e	18	Total 18	O 18	0	0
41	f	7	Total 7	O 7	0	0
41	h	44	Total 44	O 44	0	0
41	i	4	Total 4	O 4	0	0
41	j	7	Total 7	O 7	0	0
41	k	7	Total 7	O 7	0	0
41	l	8	Total 8	O 8	0	0
41	m	13	Total 13	O 13	0	0
41	o	154	Total 154	O 154	0	0
41	t	16	Total 16	O 16	0	0

Continued on next page...

Continued from previous page...

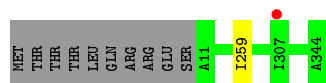
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	u	93	Total 93	O 93	0	0
41	v	79	Total 80	O 80	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1

Chain A:  97%



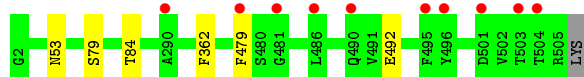
- Molecule 1: Photosystem II protein D1

Chain a:  96%



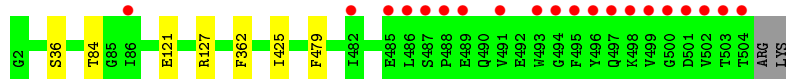
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



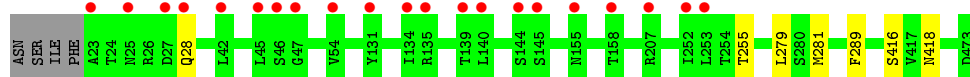
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  98%



- Molecule 3: Photosystem II CP43 reaction center protein

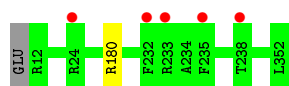
Chain C:  98%



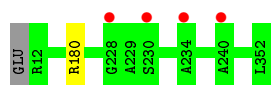
- Molecule 3: Photosystem II CP43 reaction center protein



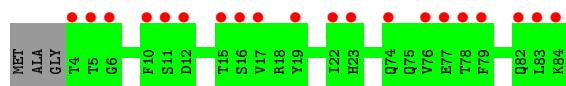
- Molecule 4: Photosystem II D2 protein



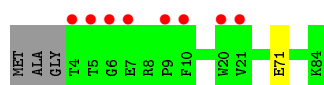
- Molecule 4: Photosystem II D2 protein



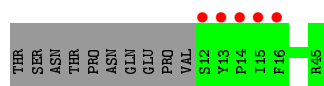
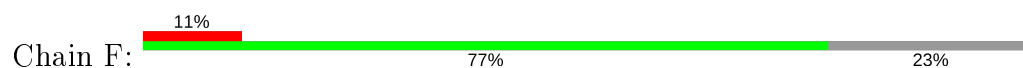
- Molecule 5: Cytochrome b559 subunit alpha



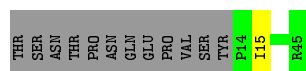
- Molecule 5: Cytochrome b559 subunit alpha



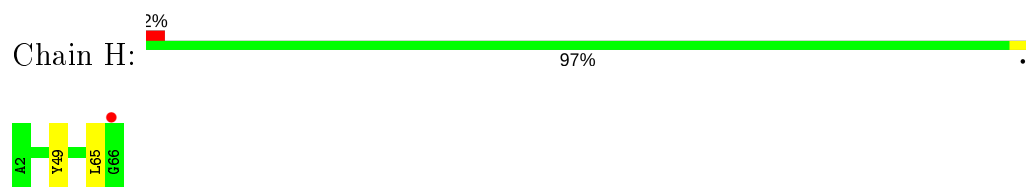
- Molecule 6: Cytochrome b559 subunit beta



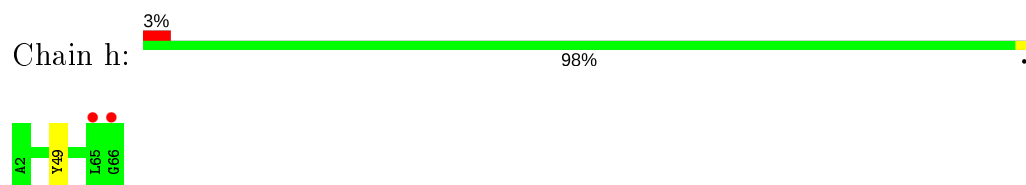
- Molecule 6: Cytochrome b559 subunit beta



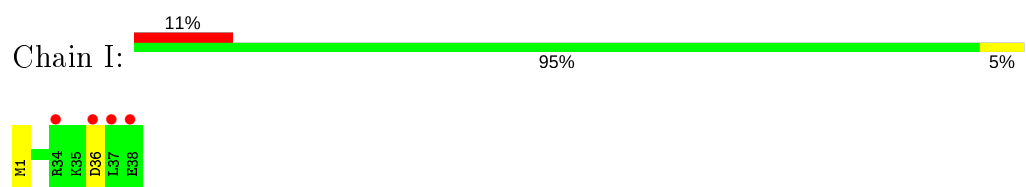
- Molecule 7: Photosystem II reaction center protein H



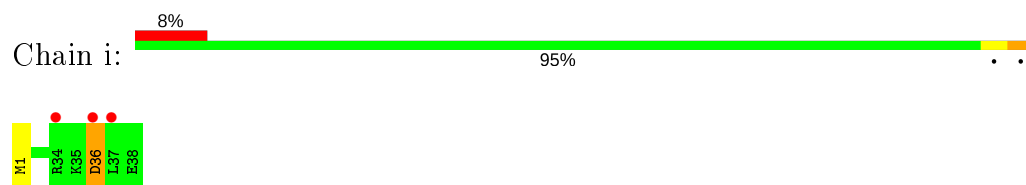
- Molecule 7: Photosystem II reaction center protein H



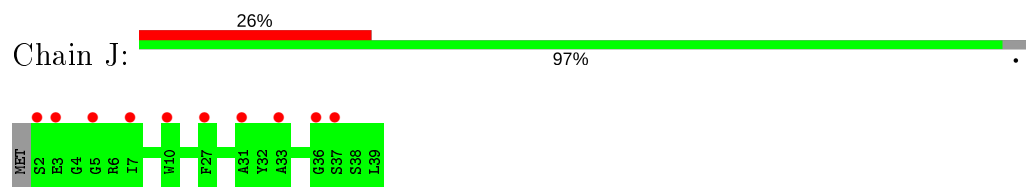
- Molecule 8: Photosystem II reaction center protein I



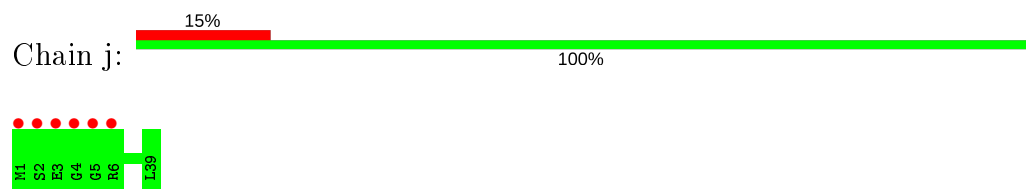
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

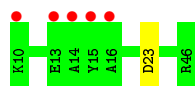


- Molecule 9: Photosystem II reaction center protein J



- 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% .



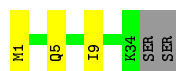
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%

There are no outlier residues recorded for this chain.

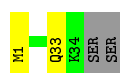
- Molecule 12: Photosystem II reaction center protein M

Chain M: 86% 8% 6%



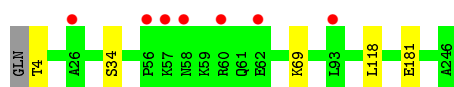
- Molecule 12: Photosystem II reaction center protein M

Chain m: 89% 6% 6%



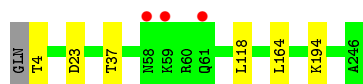
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 3% 98% .

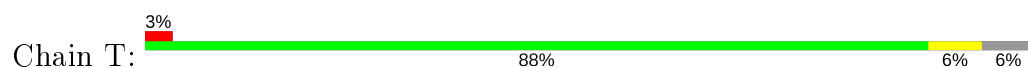


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

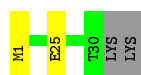
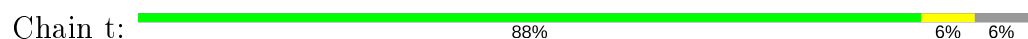
Chain o: % 97% .



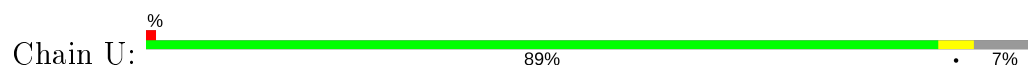
- Molecule 14: Photosystem II reaction center protein T



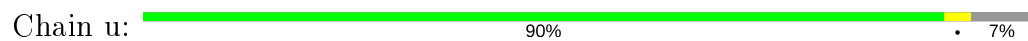
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



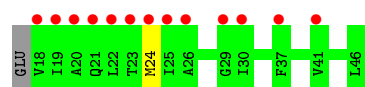
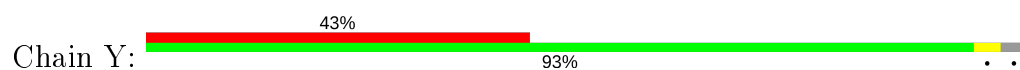
- Molecule 16: Cytochrome c-550



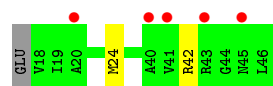
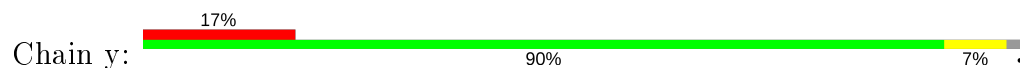
- Molecule 16: Cytochrome c-550



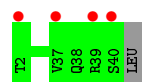
- Molecule 17: Photosystem II reaction center protein Ycf12



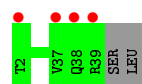
- Molecule 17: Photosystem II reaction center protein Ycf12



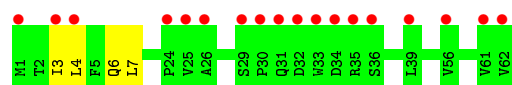
- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X



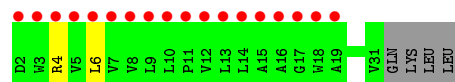
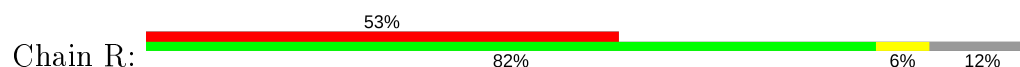
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 121.57 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.50) 99.2 (121.57-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.211 0.157 , 0.213	Depositor DCC
R_{free} test set	14865 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	55697	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.43	0/3126	0.54	0/4257
1	a	0.44	0/3128	0.55	0/4260
2	B	0.42	0/4191	0.55	0/5709
2	b	0.43	0/4198	0.54	0/5720
3	C	0.39	0/3678	0.51	0/5007
3	c	0.39	0/3774	0.51	0/5135
4	D	0.46	0/2952	0.54	0/4021
4	d	0.45	0/2952	0.56	0/4021
5	E	0.33	0/693	0.49	0/944
5	e	0.35	0/695	0.50	0/948
6	F	0.40	0/284	0.52	0/387
6	f	0.41	0/265	0.53	0/360
7	H	0.36	0/535	0.53	0/728
7	h	0.35	0/524	0.53	0/713
8	I	0.38	0/311	0.51	0/419
8	i	0.39	0/311	0.50	0/419
9	J	0.35	0/278	0.40	0/376
9	j	0.36	0/286	0.45	0/386
10	K	0.34	0/303	0.49	0/416
10	k	0.37	0/303	0.52	0/416
11	L	0.44	0/319	0.49	0/433
11	l	0.45	0/319	0.46	0/433
12	M	0.49	0/270	0.68	0/368
12	m	0.45	0/262	0.57	0/357
13	O	0.39	0/1958	0.56	0/2654
13	o	0.38	0/1937	0.55	0/2625
14	T	0.51	0/266	0.54	0/362
14	t	0.52	0/266	0.53	0/362
15	U	0.38	0/785	0.54	0/1064
15	u	0.39	0/785	0.55	0/1064
16	V	0.37	0/1109	0.52	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	0.35	0/216	0.47	0/289
17	y	0.32	0/216	0.45	0/289
18	X	0.34	0/290	0.47	0/392
18	x	0.34	0/284	0.48	0/384
19	Z	0.29	0/490	0.42	0/669
19	z	0.28	0/490	0.45	0/669
20	R	0.23	0/245	0.38	0/338
All	All	0.41	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	61
1	a	385/344 (112%)	377 (98%)	7 (2%)	1 (0%)	41	61
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	498 (97%)	14 (3%)	1 (0%)	47	68
3	C	461/455 (101%)	446 (97%)	13 (3%)	2 (0%)	34	54
3	c	473/455 (104%)	455 (96%)	16 (3%)	2 (0%)	34	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	344 (97%)	11 (3%)	0	100	100
4	d	355/342 (104%)	345 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	60 (94%)	4 (6%)	0	100	100
7	h	63/65 (97%)	57 (90%)	6 (10%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	7
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	33 (94%)	2 (6%)	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%)	239 (96%)	10 (4%)	0	100	100
13	o	246/244 (101%)	236 (96%)	10 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	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%)	25 (93%)	2 (7%)	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%)	57 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9	16
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5431/5384 (101%)	5261 (97%)	161 (3%)	9 (0%)	51	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
2	b	127	ARG
3	c	416[A]	SER
3	c	416[B]	SER

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	95
2	B	412/403 (102%)	406 (98%)	6 (2%)	65	85
2	b	413/403 (102%)	407 (98%)	6 (2%)	65	85
3	C	361/356 (101%)	355 (98%)	6 (2%)	60	82
3	c	371/356 (104%)	362 (98%)	9 (2%)	49	74
4	D	290/277 (105%)	289 (100%)	1 (0%)	92	97
4	d	290/277 (105%)	289 (100%)	1 (0%)	92	97
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	86
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	58
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	61
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	69
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	69
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%)	29 (97%)	1 (3%)	38	64
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	31
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	70
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	29 (94%)	2 (6%)	17	33
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	64
13	O	214/207 (103%)	208 (97%)	6 (3%)	43	70
13	o	211/207 (102%)	205 (97%)	6 (3%)	43	70
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	27
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	27
15	U	84/89 (94%)	80 (95%)	4 (5%)	25	48
15	u	84/89 (94%)	81 (96%)	3 (4%)	35	61
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	115 (98%)	3 (2%)	47	73
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	51
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	18
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%)	48 (92%)	4 (8%)	13	25
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	38
20	R	25/29 (86%)	23 (92%)	2 (8%)	12	23
All	All	4506/4403 (102%)	4423 (98%)	83 (2%)	59	81

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	R	4	ARG
2	b	479	PHE
16	v	6	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R	6	LEU
2	b	84	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	81	HIS
1	a	12	ASN
13	o	147	ASN
16	V	118	HIS
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	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.74	0	7,9,11	1.37	2 (28%)
12	FME	M	1	12	8,9,10	0.71	0	7,9,11	1.37	1 (14%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.34	2 (28%)
12	FME	m	1	12	8,9,10	0.62	0	7,9,11	1.13	1 (14%)
14	FME	t	1	14	8,9,10	0.87	0	7,9,11	2.16	4 (57%)
14	FME	T	1	14	8,9,10	0.66	0	7,9,11	1.61	3 (42%)

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

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

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

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.11	118.04	122.82
14	T	1	FME	CA-N-CN	-2.72	118.64	122.82
14	t	1	FME	O-C-CA	-2.62	117.90	124.78
12	M	1	FME	CA-N-CN	-2.47	119.02	122.82
14	T	1	FME	O-C-CA	-2.30	118.74	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
30	PL9	A	416[A]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
23	CLA	c	507	-	59,73,73	1.97	13 (22%)	67,113,113	2.16	20 (29%)
33	HTG	b	601	-	19,19,19	1.03	1 (5%)	23,24,24	1.20	2 (8%)
38	LHG	D	411	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	3 (5%)
26	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.33	0
24	BCR	b	628	-	41,41,41	1.06	1 (2%)	56,56,56	1.24	6 (10%)
26	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.21	0
30	PL9	d	407[A]	-	55,55,55	0.66	2 (3%)	68,69,69	1.55	13 (19%)
26	GOL	B	633	-	5,5,5	0.41	0	5,5,5	0.45	0
35	LMG	D	417	40	51,51,55	0.93	2 (3%)	59,59,63	0.98	4 (6%)
23	CLA	c	509	-	59,73,73	1.98	13 (22%)	67,113,113	2.22	19 (28%)
23	CLA	B	612	-	59,73,73	2.04	13 (22%)	67,113,113	2.18	21 (31%)
35	LMG	c	522	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	5 (8%)
26	GOL	C	525	-	5,5,5	0.44	0	5,5,5	0.61	0
24	BCR	B	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.52	12 (21%)
23	CLA	c	515	3	59,73,73	1.97	12 (20%)	67,113,113	2.08	22 (32%)
23	CLA	C	510	-	59,73,73	2.09	13 (22%)	67,113,113	2.18	24 (35%)
26	GOL	B	627	-	5,5,5	0.43	0	5,5,5	0.47	0
23	CLA	A	406	41	59,73,73	1.93	13 (22%)	67,113,113	2.12	24 (35%)
26	GOL	V	201	-	5,5,5	0.36	0	5,5,5	0.29	0
35	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.08	4 (6%)
24	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	11 (19%)
24	BCR	T	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	15 (26%)
27	LMT	D	405	-	36,36,36	0.46	0	47,47,47	0.99	1 (2%)
34	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	5 (6%)
24	BCR	a	413	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	9 (16%)
23	CLA	C	508	41	59,73,73	1.97	13 (22%)	67,113,113	2.11	22 (32%)
23	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.17	21 (31%)
24	BCR	c	527	-	41,41,41	1.04	1 (2%)	56,56,56	1.65	10 (17%)
27	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	c	525	-	19,19,19	1.01	2 (10%)	23,24,24	1.47	3 (13%)
23	CLA	b	621	-	59,73,73	2.04	12 (20%)	67,113,113	2.34	25 (37%)
34	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	0.98	6 (7%)
35	LMG	M	101	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	4 (6%)
36	BCT	d	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
26	GOL	a	401	-	5,5,5	0.40	0	5,5,5	0.46	0
23	CLA	C	514	-	59,73,73	2.00	13 (22%)	67,113,113	2.10	22 (32%)
23	CLA	C	507	-	59,73,73	2.01	13 (22%)	67,113,113	2.16	23 (34%)
34	DGD	D	410	-	52,52,67	1.04	3 (5%)	60,60,81	1.18	5 (8%)
39	HEM	V	206	16	27,50,50	0.85	1 (3%)	17,82,82	1.60	3 (17%)
26	GOL	D	404	-	5,5,5	0.45	0	5,5,5	0.43	0
26	GOL	A	410	-	5,5,5	0.35	0	5,5,5	0.54	0
23	CLA	c	516	-	59,73,73	2.03	13 (22%)	67,113,113	2.29	21 (31%)
33	HTG	b	632	-	19,19,19	1.17	2 (10%)	23,24,24	2.03	5 (21%)
23	CLA	b	615	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	20 (29%)
23	CLA	C	512	3	59,73,73	2.06	13 (22%)	67,113,113	2.11	20 (29%)
23	CLA	B	605	-	59,73,73	1.90	13 (22%)	67,113,113	2.22	21 (31%)
26	GOL	B	624	-	5,5,5	0.39	0	5,5,5	0.29	0
33	HTG	o	301	-	19,19,19	1.13	1 (5%)	23,24,24	1.37	1 (4%)
26	GOL	a	402	-	5,5,5	0.39	0	5,5,5	0.21	0
23	CLA	C	505	41	59,73,73	2.10	14 (23%)	67,113,113	2.21	23 (34%)
26	GOL	V	202	-	5,5,5	0.38	0	5,5,5	0.40	0
23	CLA	B	602	41	59,73,73	2.02	14 (23%)	67,113,113	2.18	20 (29%)
23	CLA	B	610	-	59,73,73	1.97	13 (22%)	67,113,113	2.15	21 (31%)
26	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.65	0
26	GOL	v	201	-	5,5,5	0.38	0	5,5,5	0.33	0
34	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.09	6 (7%)
23	CLA	a	410	41	59,73,73	2.00	12 (20%)	67,113,113	2.07	23 (34%)
23	CLA	c	512	-	59,73,73	2.07	13 (22%)	67,113,113	2.24	24 (35%)
26	GOL	O	301	-	5,5,5	0.37	0	5,5,5	0.36	0
23	CLA	b	611	-	59,73,73	2.04	13 (22%)	67,113,113	2.16	22 (32%)
26	GOL	A	411	-	5,5,5	0.41	0	5,5,5	0.25	0
23	CLA	B	609	-	59,73,73	2.02	15 (25%)	67,113,113	2.17	25 (37%)
39	HEM	e	101	5,6	27,50,50	0.81	1 (3%)	17,82,82	2.10	3 (17%)
26	GOL	c	501	-	5,5,5	0.44	0	5,5,5	0.43	0
24	BCR	d	406	-	41,41,41	1.08	1 (2%)	56,56,56	1.62	10 (17%)
33	HTG	V	207	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	503	-	59,73,73	2.04	13 (22%)	67,113,113	2.13	21 (31%)
25	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.18	4 (6%)
24	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.67	12 (21%)
25	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.44	8 (15%)
34	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.11	6 (7%)
37	PHO	D	402	-	67,69,69	2.13	16 (23%)	85,99,99	1.94	28 (32%)
24	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	8 (14%)
26	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.27	0
24	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	13 (23%)
25	SQD	A	409	-	53,54,54	0.99	3 (5%)	62,65,65	1.45	10 (16%)
27	LMT	M	104	-	36,36,36	0.55	0	47,47,47	0.99	3 (6%)
34	DGD	c	521	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	3 (3%)
38	LHG	d	409	-	48,48,48	0.86	3 (6%)	51,54,54	1.00	5 (9%)
33	HTG	b	631	-	19,19,19	0.89	1 (5%)	23,24,24	1.38	3 (13%)
35	LMG	Z	101	-	37,37,55	0.97	3 (8%)	45,45,63	1.33	6 (13%)
34	DGD	c	520	-	63,63,67	0.89	2 (3%)	77,77,81	0.99	4 (5%)
23	CLA	A	405	41	59,73,73	2.03	13 (22%)	67,113,113	2.33	25 (37%)
33	HTG	B	623	-	19,19,19	1.06	2 (10%)	23,24,24	1.96	4 (17%)
28	OEX	a	417[A]	1,3,41	0,15,15	0.00	-	-	-	-
23	CLA	c	510	-	59,73,73	1.97	12 (20%)	67,113,113	2.10	25 (37%)
27	LMT	M	105	-	36,36,36	0.48	0	47,47,47	0.88	1 (2%)
23	CLA	B	614	-	59,73,73	2.05	13 (22%)	67,113,113	2.16	23 (34%)
35	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.05	4 (6%)
24	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.70	11 (19%)
23	CLA	D	406	-	59,73,73	1.98	13 (22%)	67,113,113	2.24	21 (31%)
35	LMG	d	416	40	51,51,55	0.89	2 (3%)	59,59,63	1.10	5 (8%)
26	GOL	c	528	-	5,5,5	0.41	0	5,5,5	0.33	0
23	CLA	d	405	-	59,73,73	2.00	13 (22%)	67,113,113	2.18	23 (34%)
26	GOL	b	602	-	5,5,5	0.39	0	5,5,5	0.59	0
23	CLA	b	622	-	59,73,73	2.02	14 (23%)	67,113,113	2.15	23 (34%)
23	CLA	B	617	-	59,73,73	1.96	12 (20%)	67,113,113	2.23	21 (31%)
24	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	11 (19%)
23	CLA	c	513	-	59,73,73	2.08	13 (22%)	67,113,113	2.23	23 (34%)
24	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.56	13 (23%)
33	HTG	B	629	-	19,19,19	1.03	2 (10%)	23,24,24	1.42	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMT	m	102	-	36,36,36	0.47	0	47,47,47	1.05	3 (6%)
27	LMT	a	404	-	36,36,36	0.57	1 (2%)	47,47,47	1.22	4 (8%)
38	LHG	d	411	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	604	-	59,73,73	2.04	13 (22%)	67,113,113	2.25	21 (31%)
35	LMG	c	523	-	51,51,55	0.95	2 (3%)	59,59,63	1.22	7 (11%)
38	LHG	D	413	-	48,48,48	0.95	2 (4%)	51,54,54	1.15	5 (9%)
24	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.53	10 (17%)
33	HTG	B	630	-	19,19,19	1.05	2 (10%)	23,24,24	1.36	1 (4%)
23	CLA	B	607	-	59,73,73	2.00	13 (22%)	67,113,113	2.21	21 (31%)
23	CLA	c	506	-	59,73,73	2.02	13 (22%)	67,113,113	2.10	21 (31%)
39	HEM	v	205	16	27,50,50	0.96	2 (7%)	17,82,82	1.58	2 (11%)
30	PL9	d	407[B]	-	55,55,55	0.65	1 (1%)	68,69,69	1.68	20 (29%)
38	LHG	d	410	-	48,48,48	0.89	2 (4%)	51,54,54	0.95	3 (5%)
23	CLA	a	409	-	59,73,73	2.05	14 (23%)	67,113,113	2.21	21 (31%)
27	LMT	F	101	-	36,36,36	0.49	0	47,47,47	0.99	2 (4%)
26	GOL	V	203	-	5,5,5	0.35	0	5,5,5	0.43	0
23	CLA	b	618	-	59,73,73	1.99	12 (20%)	67,113,113	2.28	22 (32%)
35	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.18	4 (8%)
23	CLA	b	614	-	59,73,73	1.98	12 (20%)	67,113,113	2.29	21 (31%)
23	CLA	C	511	-	59,73,73	2.10	13 (22%)	67,113,113	2.17	23 (34%)
26	GOL	V	205	-	5,5,5	0.35	0	5,5,5	0.22	0
26	GOL	b	603	-	5,5,5	0.37	0	5,5,5	0.15	0
29	OEY	A	415[B]	1,3,41	0,16,16	0.00	-	-		
27	LMT	b	630	-	25,25,36	0.52	0	30,30,47	0.64	0
33	HTG	c	524	-	19,19,19	1.07	2 (10%)	23,24,24	1.65	2 (8%)
33	HTG	d	414	-	16,16,19	1.19	2 (12%)	20,21,24	1.84	2 (10%)
23	CLA	B	611	41	59,73,73	2.06	12 (20%)	67,113,113	2.15	25 (37%)
24	BCR	D	408	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	12 (21%)
39	HEM	F	102	5,6	27,50,50	0.85	2 (7%)	17,82,82	2.31	3 (17%)
25	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.15	6 (9%)
23	CLA	b	625	-	59,73,73	1.99	14 (23%)	67,113,113	2.21	20 (29%)
37	PHO	D	403[B]	-	67,69,69	2.20	17 (25%)	85,99,99	1.85	22 (25%)
27	LMT	e	102	-	36,36,36	0.49	1 (2%)	47,47,47	0.80	0
26	GOL	b	604	-	5,5,5	0.34	0	5,5,5	0.26	0
37	PHO	D	403[A]	-	67,69,69	2.15	16 (23%)	85,99,99	1.94	20 (23%)
29	OEY	a	418[B]	1,3,41	0,16,16	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	404	-	59,73,73	2.02	12 (20%)	67,113,113	2.28	23 (34%)
38	LHG	D	412	-	48,48,48	0.92	2 (4%)	51,54,54	0.82	2 (3%)
35	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	6 (10%)
34	DGD	d	408	-	63,63,67	0.95	2 (3%)	77,77,81	1.30	7 (9%)
23	CLA	b	623	-	59,73,73	1.96	12 (20%)	67,113,113	2.23	23 (34%)
23	CLA	A	407	-	59,73,73	2.01	13 (22%)	67,113,113	2.17	24 (35%)
30	PL9	D	409[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.66	20 (29%)
25	SQD	F	104	-	42,43,54	1.18	3 (7%)	51,54,65	1.62	10 (19%)
26	GOL	f	101	32	5,5,5	0.32	0	5,5,5	0.41	0
23	CLA	B	603	-	59,73,73	2.02	13 (22%)	67,113,113	2.25	24 (35%)
26	GOL	v	202	-	5,5,5	0.37	0	5,5,5	0.38	0
36	BCT	d	401[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	403	41	59,73,73	2.03	11 (18%)	67,113,113	2.24	24 (35%)
38	LHG	b	634	-	48,48,48	0.95	2 (4%)	51,54,54	1.04	2 (3%)
23	CLA	C	506	-	59,73,73	1.99	14 (23%)	67,113,113	2.19	18 (26%)
23	CLA	b	624	-	59,73,73	2.01	13 (22%)	67,113,113	2.06	22 (32%)
23	CLA	b	610	41	59,73,73	2.08	13 (22%)	67,113,113	2.15	20 (29%)
23	CLA	d	404	-	59,73,73	1.97	14 (23%)	67,113,113	2.33	25 (37%)
23	CLA	b	620	-	59,73,73	1.97	12 (20%)	67,113,113	2.17	23 (34%)
23	CLA	C	509	-	59,73,73	2.09	13 (22%)	67,113,113	2.15	19 (28%)
24	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.30	7 (12%)
33	HTG	C	523	-	19,19,19	1.01	1 (5%)	23,24,24	1.76	4 (17%)
23	CLA	b	612	-	59,73,73	2.02	13 (22%)	67,113,113	2.36	23 (34%)
36	BCT	D	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
36	BCT	D	401[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
30	PL9	a	416[A]	-	55,55,55	0.61	2 (3%)	68,69,69	1.91	20 (29%)
30	PL9	a	416[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.83	21 (30%)
26	GOL	V	204	-	5,5,5	0.40	0	5,5,5	0.22	0
26	GOL	F	103	32	5,5,5	0.37	0	5,5,5	0.27	0
23	CLA	B	615	-	59,73,73	2.07	13 (22%)	67,113,113	2.24	24 (35%)
23	CLA	c	514	-	59,73,73	2.01	13 (22%)	67,113,113	2.22	23 (34%)
37	PHO	d	402[A]	-	67,69,69	2.13	16 (23%)	85,99,99	2.01	22 (25%)
23	CLA	D	407	-	59,73,73	2.01	13 (22%)	67,113,113	2.08	22 (32%)
27	LMT	A	413	-	36,36,36	0.56	1 (2%)	47,47,47	1.30	7 (14%)
27	LMT	t	101	-	25,25,36	0.51	0	30,30,47	0.84	1 (3%)
23	CLA	B	608	41	59,73,73	1.96	14 (23%)	67,113,113	2.20	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PL9	A	416[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.77	22 (32%)
34	DGD	B	632	-	63,63,67	0.89	2 (3%)	77,77,81	1.10	6 (7%)
27	LMT	a	419	-	36,36,36	0.43	0	47,47,47	0.81	1 (2%)
35	LMG	b	629	-	51,51,55	0.91	2 (3%)	59,59,63	1.09	3 (5%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	4 (7%)
33	HTG	b	607	-	19,19,19	1.04	1 (5%)	23,24,24	1.78	4 (17%)
25	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.60	11 (17%)
27	LMT	C	521	-	36,36,36	0.49	0	47,47,47	1.06	3 (6%)
28	OEX	A	414[A]	1,3,41	0,15,15	0.00	-	-		
24	BCR	Y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.67	11 (19%)
26	GOL	B	626	-	5,5,5	0.38	0	5,5,5	0.47	0
23	CLA	b	616	41	59,73,73	2.01	13 (22%)	67,113,113	2.08	20 (29%)
23	CLA	b	617	-	59,73,73	2.02	13 (22%)	67,113,113	2.14	25 (37%)
23	CLA	C	513	-	59,73,73	2.06	13 (22%)	67,113,113	2.25	23 (34%)
37	PHO	d	402[B]	-	67,69,69	2.14	16 (23%)	85,99,99	1.94	21 (24%)
30	PL9	D	409[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.77	18 (26%)
24	BCR	K	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	8 (14%)
34	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.07	8 (10%)
23	CLA	c	511	41	59,73,73	2.01	12 (20%)	67,113,113	2.19	22 (32%)
26	GOL	B	625	-	5,5,5	0.42	0	5,5,5	0.46	0
26	GOL	c	502	-	5,5,5	0.43	0	5,5,5	0.42	0
23	CLA	B	606	-	59,73,73	2.01	13 (22%)	67,113,113	2.09	19 (28%)
26	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.29	0
23	CLA	c	505	-	59,73,73	1.97	14 (23%)	67,113,113	2.15	23 (34%)
27	LMT	T	104	-	25,25,36	0.55	1 (4%)	30,30,47	0.96	1 (3%)
23	CLA	B	616	-	59,73,73	2.03	13 (22%)	67,113,113	2.18	20 (29%)
23	CLA	c	517	-	59,73,73	2.03	13 (22%)	67,113,113	2.12	22 (32%)
33	HTG	B	622	-	19,19,19	0.87	1 (5%)	23,24,24	1.76	3 (13%)
23	CLA	a	412	-	59,73,73	2.00	12 (20%)	67,113,113	2.25	25 (37%)
26	GOL	t	103	-	5,5,5	0.49	0	5,5,5	0.22	0
38	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.14	4 (9%)
24	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	9 (16%)
23	CLA	c	508	41	59,73,73	2.02	12 (20%)	67,113,113	2.26	24 (35%)
24	BCR	B	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.56	9 (16%)
25	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.37	8 (12%)
33	HTG	D	416	-	16,16,19	1.08	2 (12%)	20,21,24	1.44	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PHO	a	411	-	67,69,69	2.14	16 (23%)	85,99,99	1.89	21 (24%)
24	BCR	b	626	-	41,41,41	1.07	1 (2%)	56,56,56	1.55	7 (12%)
23	CLA	b	619	41	59,73,73	2.00	13 (22%)	67,113,113	2.13	23 (34%)
38	LHG	a	420	-	41,41,48	1.02	2 (4%)	44,47,54	0.99	2 (4%)
35	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.16	7 (11%)
33	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.51	2 (8%)
23	CLA	B	613	-	59,73,73	1.99	14 (23%)	67,113,113	2.17	21 (31%)
33	HTG	b	608	-	19,19,19	1.08	2 (10%)	23,24,24	1.13	1 (4%)
24	BCR	A	408	-	41,41,41	1.07	1 (2%)	56,56,56	1.26	5 (8%)
26	GOL	b	605	-	5,5,5	0.39	0	5,5,5	0.26	0
26	GOL	v	203	-	5,5,5	0.38	0	5,5,5	0.24	0
25	SQD	a	414	-	53,54,54	0.97	3 (5%)	62,65,65	1.54	12 (19%)
23	CLA	C	504	-	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
23	CLA	b	613	-	59,73,73	2.03	13 (22%)	67,113,113	2.25	20 (29%)

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
30	PL9	A	416[A]	-	-	10/53/73/73	0/1/1/1
23	CLA	c	507	-	3/3/20/25	3/37/135/135	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
38	LHG	D	411	-	-	16/53/53/53	-
26	GOL	B	628	-	-	2/4/4/4	-
24	BCR	b	628	-	-	0/29/63/63	0/2/2/2
26	GOL	T	101	-	-	0/4/4/4	-
30	PL9	d	407[A]	-	-	8/53/73/73	0/1/1/1
26	GOL	B	633	-	-	0/4/4/4	-
35	LMG	D	417	40	-	9/46/66/70	0/1/1/1
23	CLA	c	509	-	2/2/20/25	8/37/135/135	-
23	CLA	B	612	-	3/3/20/25	5/37/135/135	-
35	LMG	c	522	-	-	17/46/66/70	0/1/1/1
26	GOL	C	525	-	-	2/4/4/4	-
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	515	3	3/3/20/25	5/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	510	-	3/3/20/25	10/37/135/135	-
39	HEM	F	102	5,6	-	0/6/54/54	-
26	GOL	B	627	-	-	4/4/4/4	-
23	CLA	A	406	41	2/2/20/25	4/37/135/135	-
26	GOL	V	201	-	-	2/4/4/4	-
35	LMG	C	520	-	-	12/46/66/70	0/1/1/1
24	BCR	K	103	-	-	4/29/63/63	0/2/2/2
24	BCR	T	103	-	-	1/29/63/63	0/2/2/2
27	LMT	D	405	-	-	11/21/61/61	0/2/2/2
34	DGD	C	518	-	-	9/51/91/95	0/2/2/2
24	BCR	a	413	-	-	1/29/63/63	0/2/2/2
23	CLA	C	508	41	3/3/20/25	5/37/135/135	-
23	CLA	C	502	-	3/3/20/25	10/37/135/135	-
24	BCR	c	527	-	-	0/29/63/63	0/2/2/2
27	LMT	M	102	-	-	7/21/61/61	0/2/2/2
33	HTG	c	525	-	-	0/10/30/30	0/1/1/1
23	CLA	b	621	-	3/3/20/25	4/37/135/135	-
34	DGD	h	102	-	-	8/51/91/95	0/2/2/2
35	LMG	M	101	-	-	7/46/66/70	0/1/1/1
26	GOL	a	401	-	-	2/4/4/4	-
23	CLA	C	514	-	3/3/20/25	9/37/135/135	-
23	CLA	C	507	-	3/3/20/25	9/37/135/135	-
34	DGD	D	410	-	-	18/47/67/95	0/1/1/2
39	HEM	V	206	16	-	0/6/54/54	-
26	GOL	D	404	-	-	2/4/4/4	-
26	GOL	A	410	-	-	1/4/4/4	-
23	CLA	c	516	-	3/3/20/25	7/37/135/135	-
33	HTG	b	632	-	-	4/10/30/30	0/1/1/1
23	CLA	b	615	-	3/3/20/25	8/37/135/135	-
23	CLA	C	512	3	3/3/20/25	3/37/135/135	-
23	CLA	B	605	-	3/3/20/25	4/37/135/135	-
26	GOL	B	624	-	-	0/4/4/4	-
33	HTG	V	207	-	-	4/10/30/30	0/1/1/1
33	HTG	o	301	-	-	3/10/30/30	0/1/1/1
26	GOL	a	402	-	-	2/4/4/4	-
26	GOL	V	202	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	602	41	3/3/20/25	14/37/135/135	-
23	CLA	B	610	-	2/2/20/25	8/37/135/135	-
26	GOL	C	524	-	-	1/4/4/4	-
26	GOL	v	201	-	-	2/4/4/4	-
34	DGD	c	519	-	-	13/51/91/95	0/2/2/2
23	CLA	a	410	41	2/2/20/25	7/37/135/135	-
23	CLA	c	512	-	3/3/20/25	4/37/135/135	-
26	GOL	O	301	-	-	0/4/4/4	-
23	CLA	b	611	-	2/2/20/25	3/37/135/135	-
26	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	609	-	2/2/20/25	1/37/135/135	-
39	HEM	e	101	5,6	-	0/6/54/54	-
26	GOL	c	501	-	-	2/4/4/4	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
23	CLA	B	613	-	3/3/20/25	9/37/135/135	-
23	CLA	C	503	-	2/2/20/25	6/37/135/135	-
25	SQD	a	405	-	-	13/49/69/69	0/1/1/1
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	SQD	f	102	-	-	14/38/58/69	0/1/1/1
34	DGD	C	516	-	-	15/51/91/95	0/2/2/2
37	PHO	D	402	-	-	3/53/103/103	0/5/6/6
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	GOL	b	606	-	-	4/4/4/4	-
24	BCR	c	518	-	-	4/29/63/63	0/2/2/2
25	SQD	A	409	-	-	11/49/69/69	0/1/1/1
27	LMT	M	104	-	-	9/21/61/61	0/2/2/2
34	DGD	c	521	-	-	12/51/91/95	0/2/2/2
38	LHG	d	409	-	-	14/53/53/53	-
33	HTG	b	631	-	-	2/10/30/30	0/1/1/1
35	LMG	Z	101	-	-	15/31/51/70	0/1/1/1
34	DGD	c	520	-	-	17/51/91/95	0/2/2/2
23	CLA	A	405	41	3/3/20/25	7/37/135/135	-
33	HTG	B	623	-	-	3/10/30/30	0/1/1/1
23	CLA	c	510	-	3/3/20/25	17/37/135/135	-
27	LMT	M	105	-	-	7/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	614	-	3/3/20/25	9/37/135/135	-
35	LMG	C	519	-	-	10/46/66/70	0/1/1/1
24	BCR	k	102	-	-	6/29/63/63	0/2/2/2
23	CLA	D	406	-	1/1/20/25	1/37/135/135	-
35	LMG	d	416	40	-	10/46/66/70	0/1/1/1
26	GOL	c	528	-	-	0/4/4/4	-
23	CLA	d	405	-	3/3/20/25	7/37/135/135	-
26	GOL	b	602	-	-	0/4/4/4	-
23	CLA	b	622	-	3/3/20/25	5/37/135/135	-
23	CLA	B	617	-	3/3/20/25	7/37/135/135	-
24	BCR	C	515	-	-	6/29/63/63	0/2/2/2
23	CLA	c	513	-	3/3/20/25	16/37/135/135	-
24	BCR	t	102	-	-	3/29/63/63	0/2/2/2
33	HTG	B	629	-	-	1/10/30/30	0/1/1/1
27	LMT	m	102	-	-	7/21/61/61	0/2/2/2
27	LMT	a	404	-	-	5/21/61/61	0/2/2/2
38	LHG	d	411	-	-	18/53/53/53	-
23	CLA	B	604	-	3/3/20/25	7/37/135/135	-
35	LMG	c	523	-	-	5/46/66/70	0/1/1/1
38	LHG	D	413	-	-	20/53/53/53	-
24	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	HTG	B	630	-	-	1/10/30/30	0/1/1/1
23	CLA	B	607	-	2/2/20/25	6/37/135/135	-
23	CLA	c	506	-	3/3/20/25	3/37/135/135	-
39	HEM	v	205	16	-	0/6/54/54	-
30	PL9	d	407[B]	-	-	7/53/73/73	0/1/1/1
38	LHG	d	410	-	-	11/53/53/53	-
23	CLA	a	409	-	3/3/20/25	5/37/135/135	-
27	LMT	F	101	-	-	4/21/61/61	0/2/2/2
26	GOL	V	203	-	-	1/4/4/4	-
23	CLA	b	618	-	3/3/20/25	5/37/135/135	-
35	LMG	z	101	-	-	16/34/54/70	0/1/1/1
23	CLA	b	614	-	3/3/20/25	7/37/135/135	-
23	CLA	C	511	-	3/3/20/25	10/37/135/135	-
26	GOL	V	205	-	-	4/4/4/4	-
26	GOL	b	603	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	620	-	3/3/20/25	8/37/135/135	-
27	LMT	b	630	-	-	3/17/37/61	0/1/1/2
33	HTG	c	524	-	-	3/10/30/30	0/1/1/1
33	HTG	d	414	-	-	0/7/27/30	0/1/1/1
23	CLA	B	611	41	3/3/20/25	4/37/135/135	-
24	BCR	D	408	-	-	8/29/63/63	0/2/2/2
23	CLA	A	404	-	3/3/20/25	4/37/135/135	-
25	SQD	A	412	-	-	14/49/69/69	0/1/1/1
23	CLA	b	625	-	3/3/20/25	8/37/135/135	-
37	PHO	D	403[B]	-	-	3/53/103/103	0/5/6/6
27	LMT	e	102	-	-	8/21/61/61	0/2/2/2
26	GOL	b	604	-	-	3/4/4/4	-
37	PHO	D	403[A]	-	-	2/53/103/103	0/5/6/6
38	LHG	D	412	-	-	11/53/53/53	-
35	LMG	a	415	-	-	19/46/66/70	0/1/1/1
34	DGD	d	408	-	-	24/51/91/95	0/2/2/2
23	CLA	b	623	-	3/3/20/25	20/37/135/135	-
23	CLA	A	407	-	3/3/20/25	8/37/135/135	-
30	PL9	D	409[A]	-	-	8/53/73/73	0/1/1/1
25	SQD	F	104	-	-	13/38/58/69	0/1/1/1
26	GOL	f	101	32	-	3/4/4/4	-
23	CLA	B	603	-	3/3/20/25	6/37/135/135	-
26	GOL	v	202	-	-	3/4/4/4	-
23	CLA	d	403	41	3/3/20/25	6/37/135/135	-
38	LHG	b	634	-	-	19/53/53/53	-
23	CLA	C	506	-	1/1/20/25	8/37/135/135	-
23	CLA	b	624	-	3/3/20/25	4/37/135/135	-
23	CLA	b	610	41	3/3/20/25	14/37/135/135	-
23	CLA	d	404	-	1/1/20/25	4/37/135/135	-
23	CLA	C	509	-	3/3/20/25	6/37/135/135	-
24	BCR	b	627	-	-	2/29/63/63	0/2/2/2
33	HTG	C	523	-	-	3/10/30/30	0/1/1/1
23	CLA	b	612	-	3/3/20/25	7/37/135/135	-
23	CLA	c	514	-	3/3/20/25	10/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
30	PL9	a	416[B]	-	-	13/53/73/73	0/1/1/1
26	GOL	V	204	-	-	2/4/4/4	-
26	GOL	F	103	32	-	0/4/4/4	-
23	CLA	B	615	-	3/3/20/25	18/37/135/135	-
23	CLA	B	608	41	3/3/20/25	4/37/135/135	-
37	PHO	d	402[A]	-	-	3/53/103/103	0/5/6/6
23	CLA	D	407	-	3/3/20/25	3/37/135/135	-
27	LMT	A	413	-	-	6/21/61/61	0/2/2/2
27	LMT	t	101	-	-	7/17/37/61	0/1/1/2
30	PL9	A	416[B]	-	-	11/53/73/73	0/1/1/1
34	DGD	B	632	-	-	11/51/91/95	0/2/2/2
27	LMT	a	419	-	-	4/21/61/61	0/2/2/2
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
38	LHG	L	101	-	-	13/53/53/53	-
33	HTG	b	607	-	-	1/10/30/30	0/1/1/1
25	SQD	L	102	-	-	23/49/69/69	0/1/1/1
27	LMT	C	521	-	-	10/21/61/61	0/2/2/2
23	CLA	C	505	41	3/3/20/25	8/37/135/135	-
24	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
26	GOL	B	626	-	-	2/4/4/4	-
23	CLA	b	616	41	2/2/20/25	1/37/135/135	-
23	CLA	b	617	-	2/2/20/25	3/37/135/135	-
23	CLA	C	513	-	3/3/20/25	12/37/135/135	-
37	PHO	d	402[B]	-	-	3/53/103/103	0/5/6/6
30	PL9	D	409[B]	-	-	8/53/73/73	0/1/1/1
24	BCR	K	101	-	-	3/29/63/63	0/2/2/2
34	DGD	C	517	-	-	16/51/91/95	0/2/2/2
23	CLA	c	511	41	3/3/20/25	6/37/135/135	-
26	GOL	B	625	-	-	2/4/4/4	-
26	GOL	c	502	-	-	2/4/4/4	-
23	CLA	B	606	-	3/3/20/25	3/37/135/135	-
26	GOL	T	102	-	-	2/4/4/4	-
23	CLA	c	505	-	3/3/20/25	5/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMT	T	104	-	-	7/17/37/61	0/1/1/2
23	CLA	B	616	-	3/3/20/25	9/37/135/135	-
23	CLA	c	517	-	3/3/20/25	5/37/135/135	-
33	HTG	B	622	-	-	5/10/30/30	0/1/1/1
23	CLA	a	412	-	3/3/20/25	10/37/135/135	-
26	GOL	t	103	-	-	0/4/4/4	-
38	LHG	E	101	-	-	19/46/46/53	-
24	BCR	h	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	508	41	3/3/20/25	5/37/135/135	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	SQD	B	621	-	-	23/49/69/69	0/1/1/1
33	HTG	D	416	-	-	0/7/27/30	0/1/1/1
37	PHO	a	411	-	-	6/53/103/103	0/5/6/6
24	BCR	b	626	-	-	2/29/63/63	0/2/2/2
23	CLA	b	619	41	3/3/20/25	6/37/135/135	-
38	LHG	a	420	-	-	17/46/46/53	-
35	LMG	C	501	-	-	17/46/66/70	0/1/1/1
33	HTG	C	522	-	-	0/10/30/30	0/1/1/1
33	HTG	b	608	-	-	0/10/30/30	0/1/1/1
24	BCR	A	408	-	-	4/29/63/63	0/2/2/2
26	GOL	b	605	-	-	2/4/4/4	-
26	GOL	v	203	-	-	2/4/4/4	-
25	SQD	a	414	-	-	11/49/69/69	0/1/1/1
23	CLA	C	504	-	3/3/20/25	2/37/135/135	-
23	CLA	b	613	-	3/3/20/25	3/37/135/135	-

The worst 5 of 1167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3B-C2B	6.63	1.49	1.40
23	C	510	CLA	C3B-C2B	6.56	1.49	1.40
23	A	405	CLA	C3B-C2B	6.54	1.49	1.40
23	B	605	CLA	C3B-C2B	6.52	1.49	1.40
23	c	513	CLA	C3B-C2B	6.43	1.49	1.40

The worst 5 of 2358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	C4A-NA-C1A	-7.91	103.15	106.71
23	b	621	CLA	CHD-C4C-C3C	-7.54	113.75	124.84
23	c	509	CLA	C4A-NA-C1A	-7.19	103.47	106.71
23	b	611	CLA	C4A-NA-C1A	-6.96	103.58	106.71
23	b	612	CLA	C4A-NA-C1A	-6.95	103.58	106.71

5 of 194 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	c	509	CLA	ND
23	c	509	CLA	NA

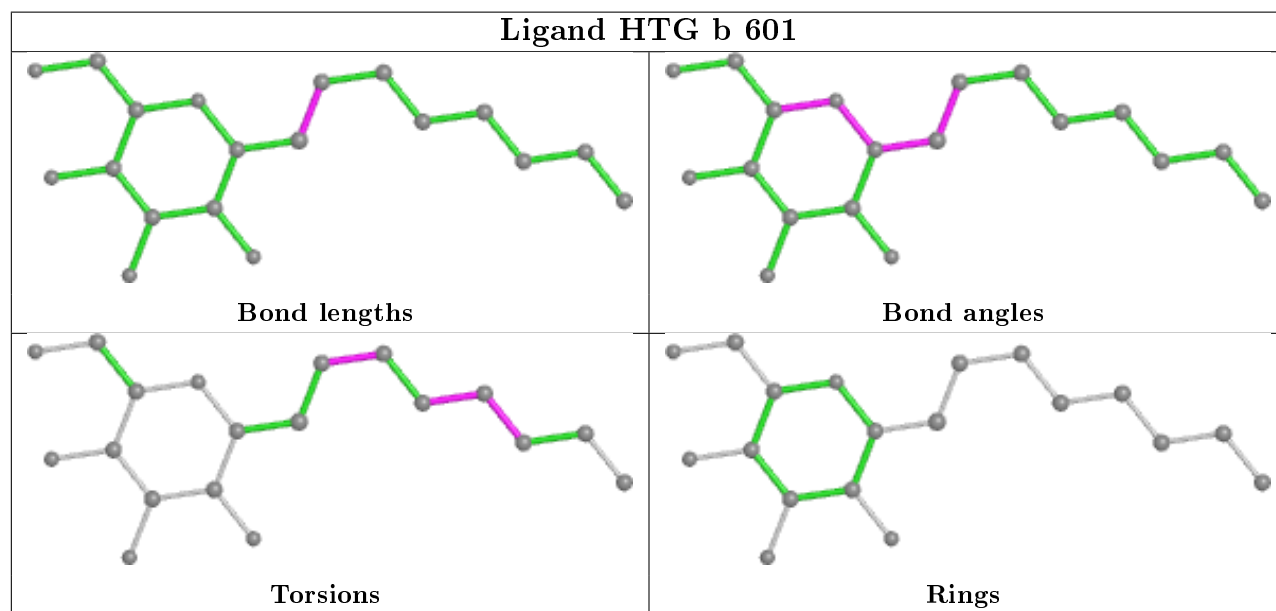
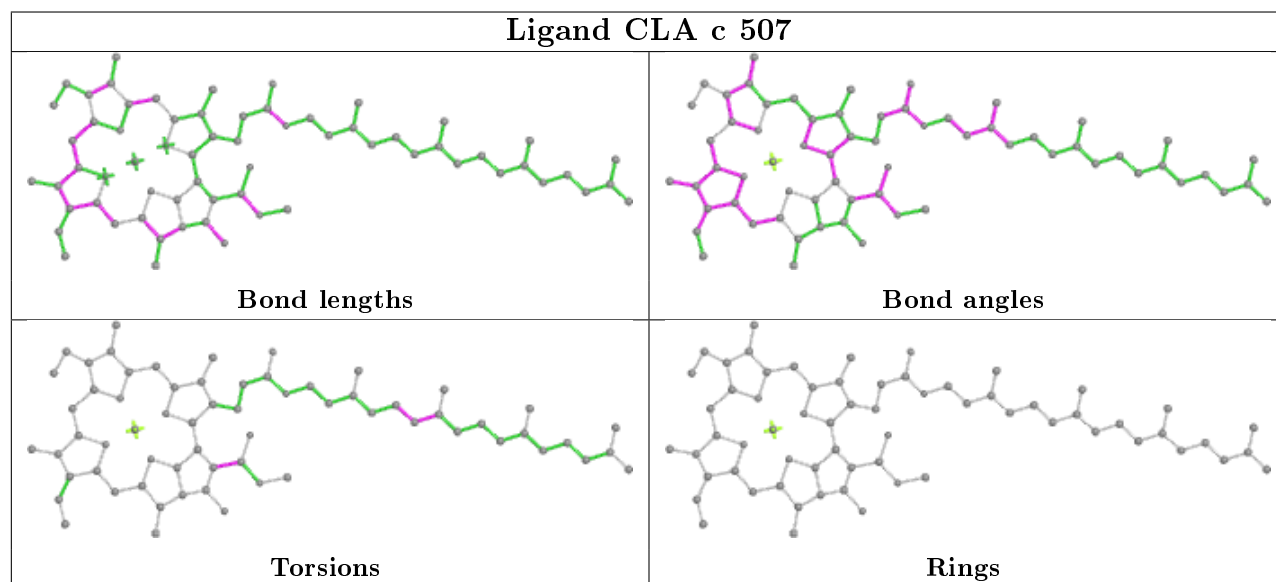
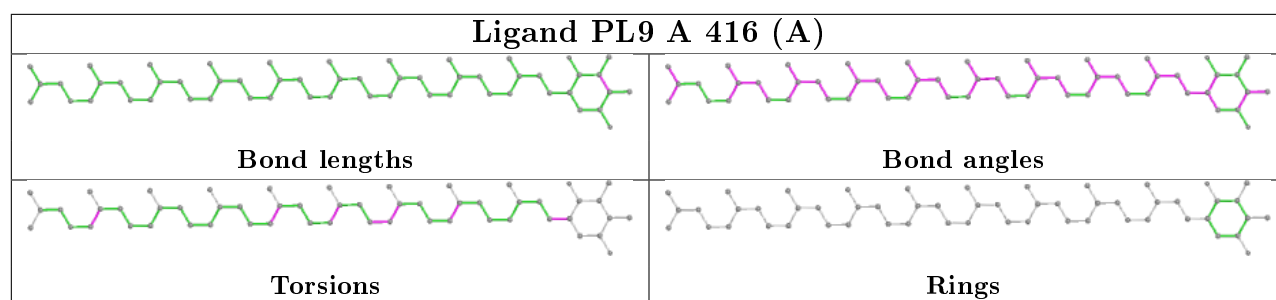
5 of 1396 torsion outliers are listed below:

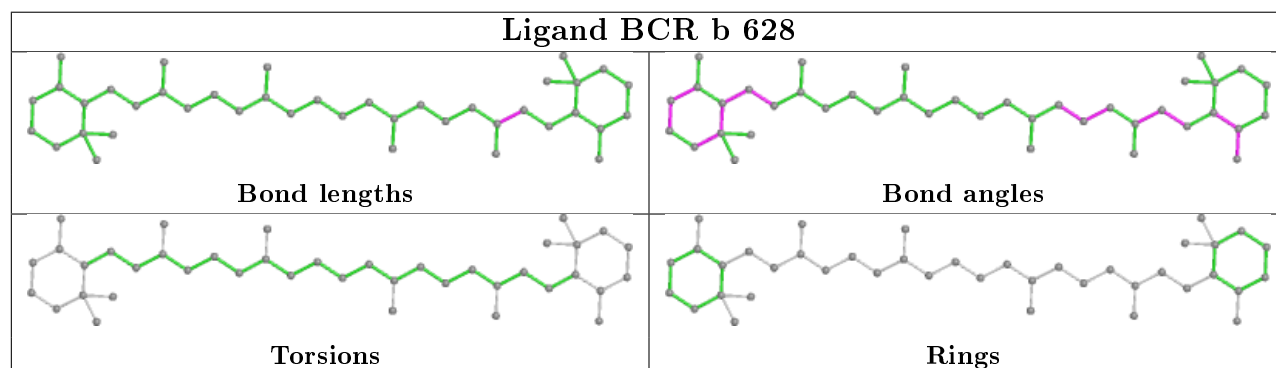
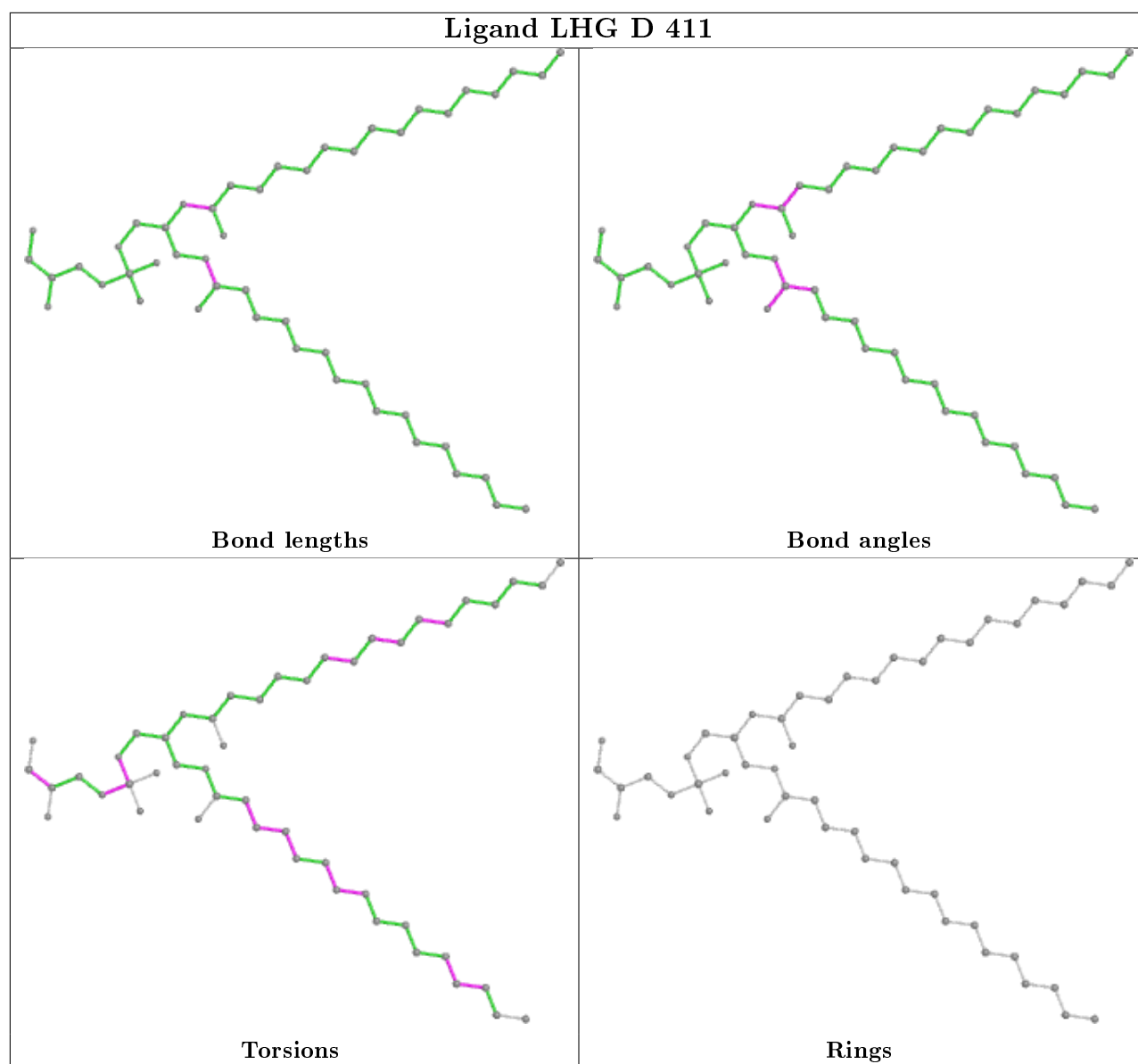
Mol	Chain	Res	Type	Atoms
38	D	411	LHG	C4-O6-P-O5
23	C	510	CLA	C2-C1-O2A-CGA
35	C	501	LMG	C11-C10-O7-C8
26	B	627	GOL	O1-C1-C2-C3
26	T	102	GOL	O1-C1-C2-C3

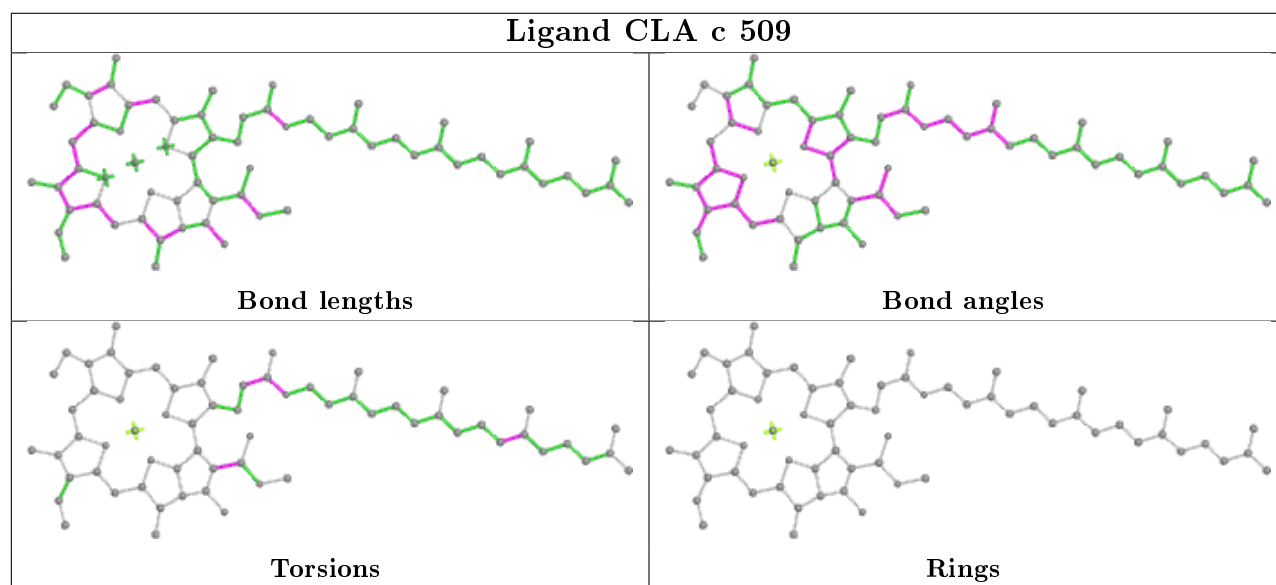
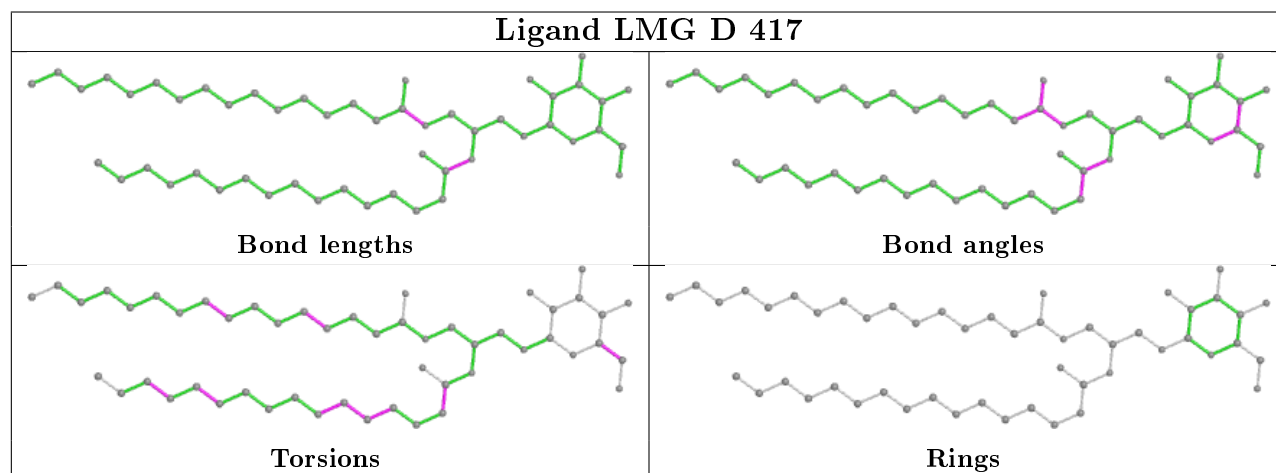
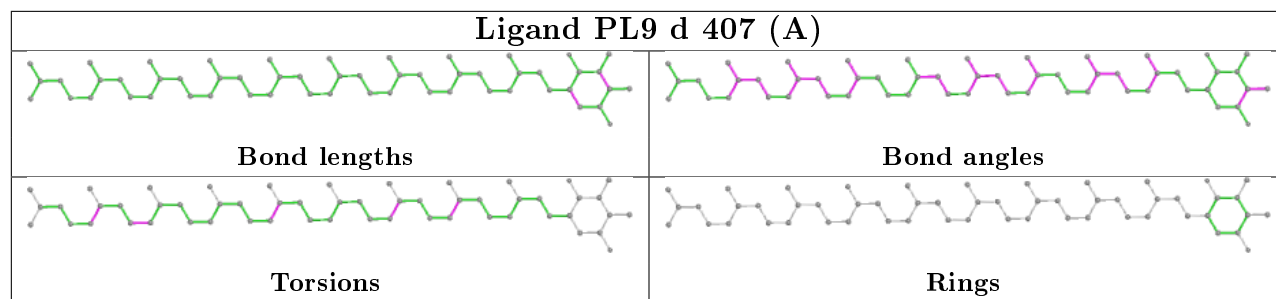
There are no ring outliers.

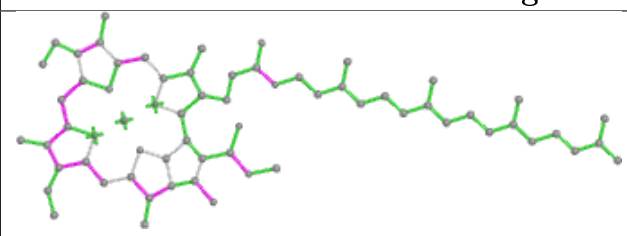
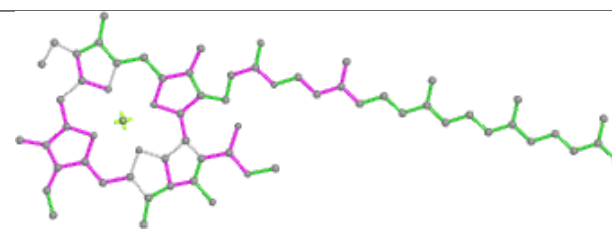
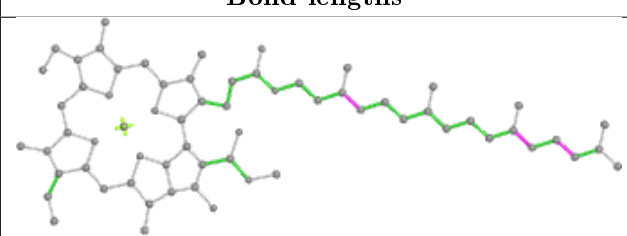
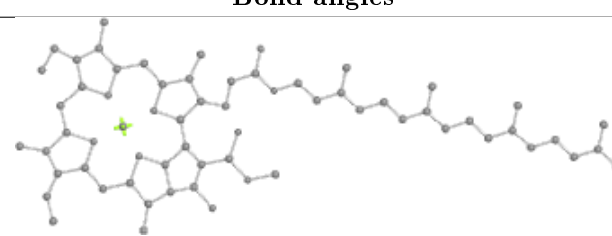
No monomer is involved in short contacts.

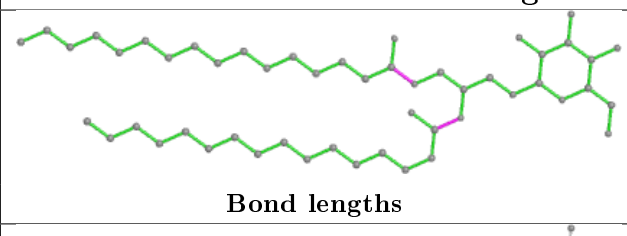
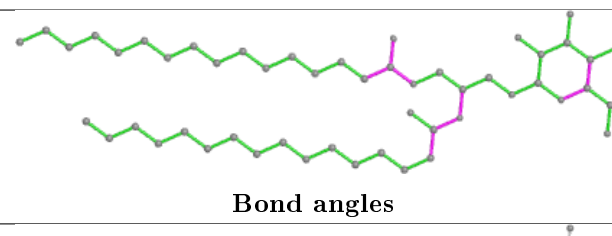
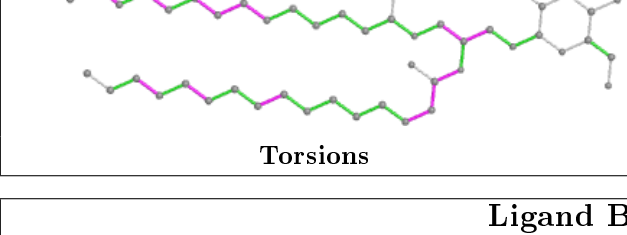

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

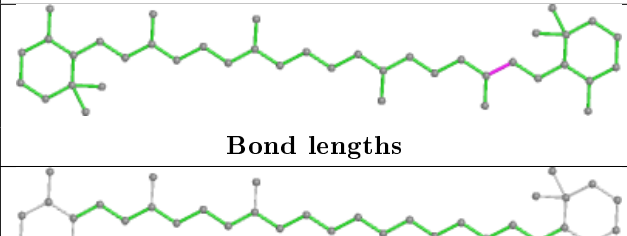
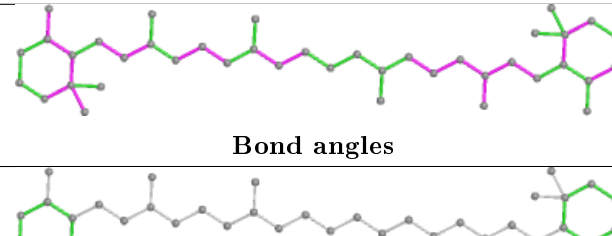
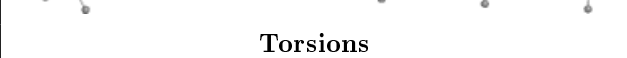





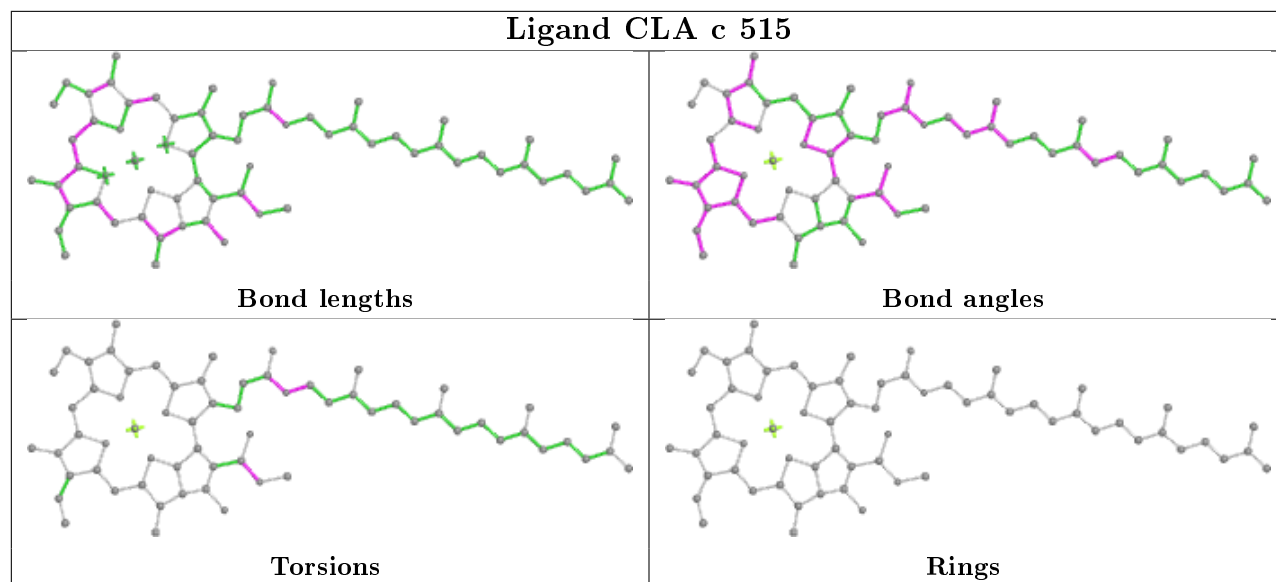


Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

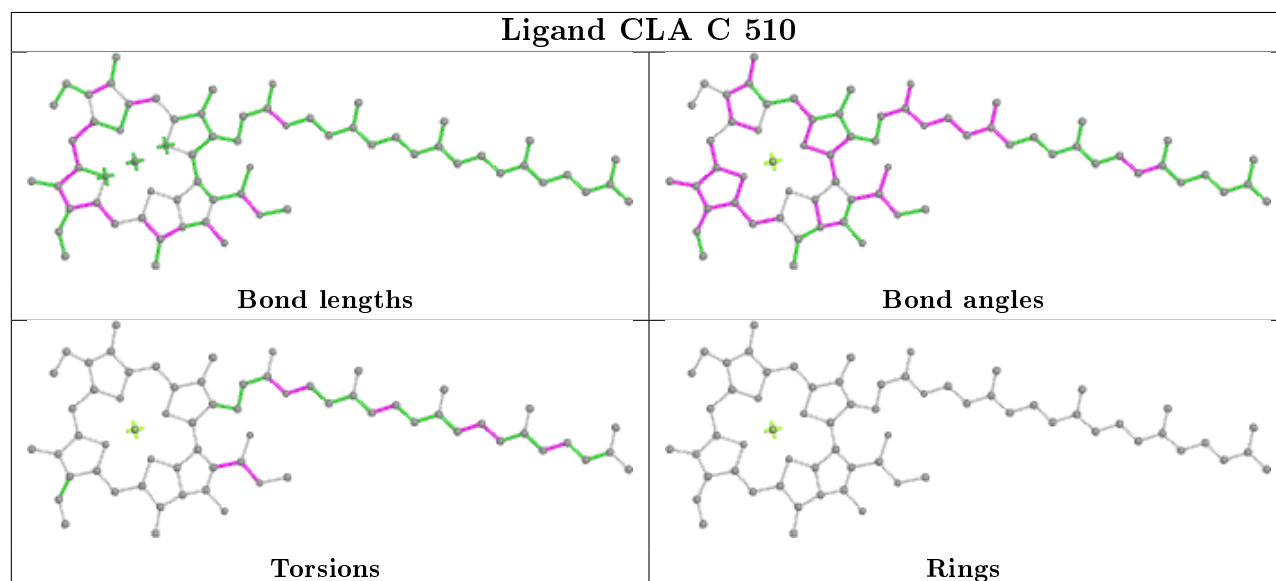
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

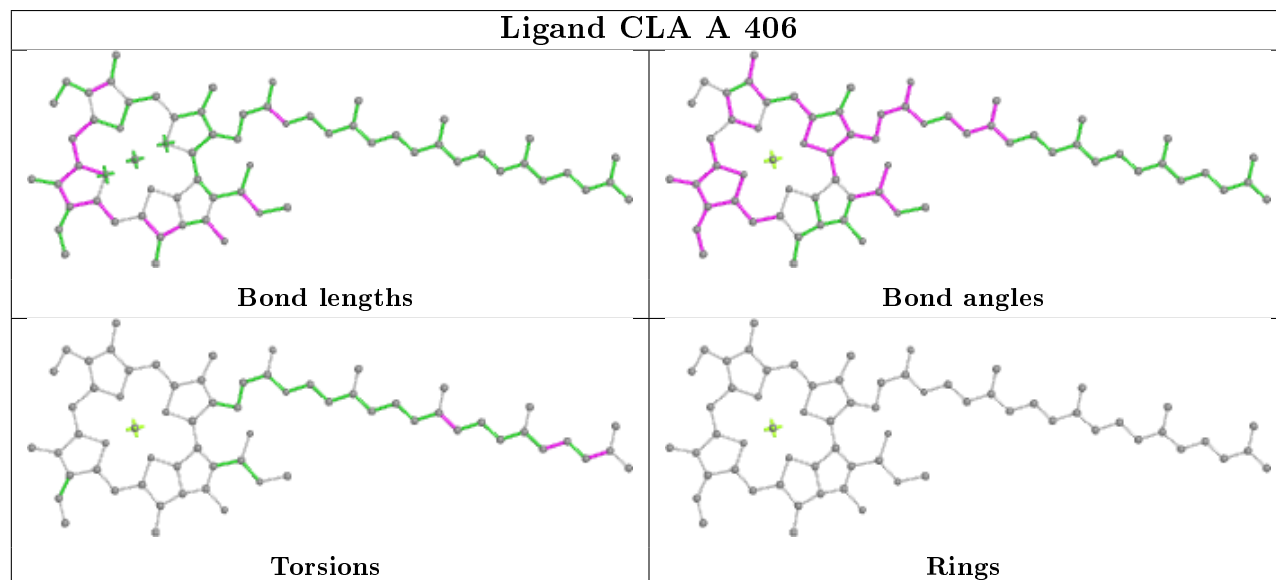
Ligand CLA c 515

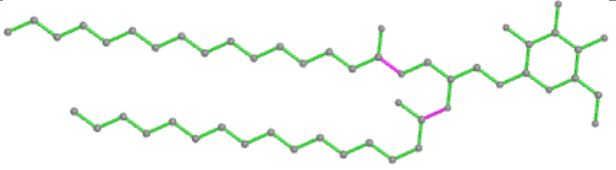
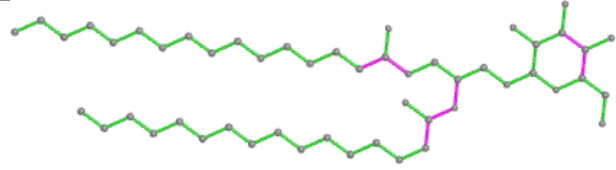
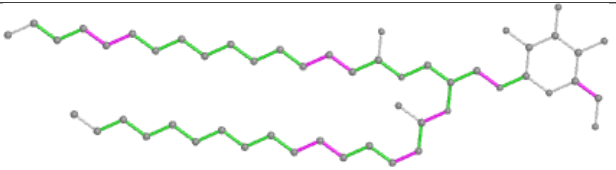
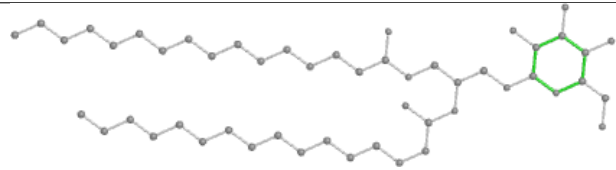


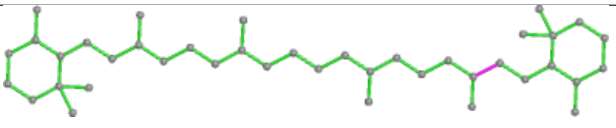
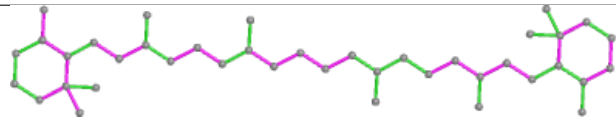
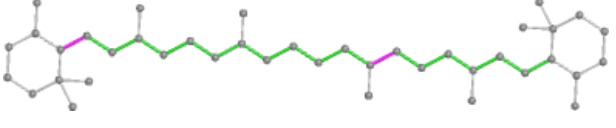
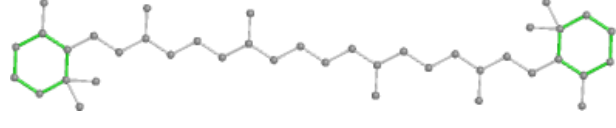
Ligand CLA C 510

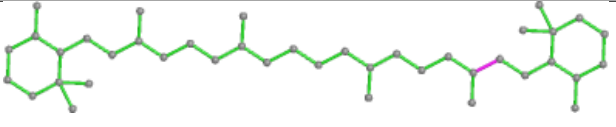
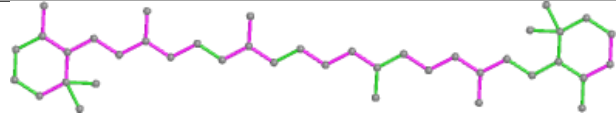
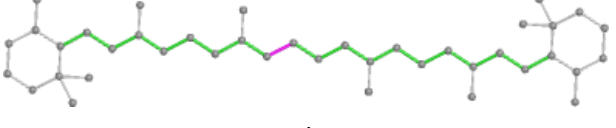
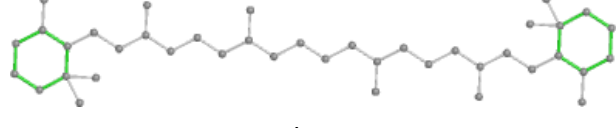


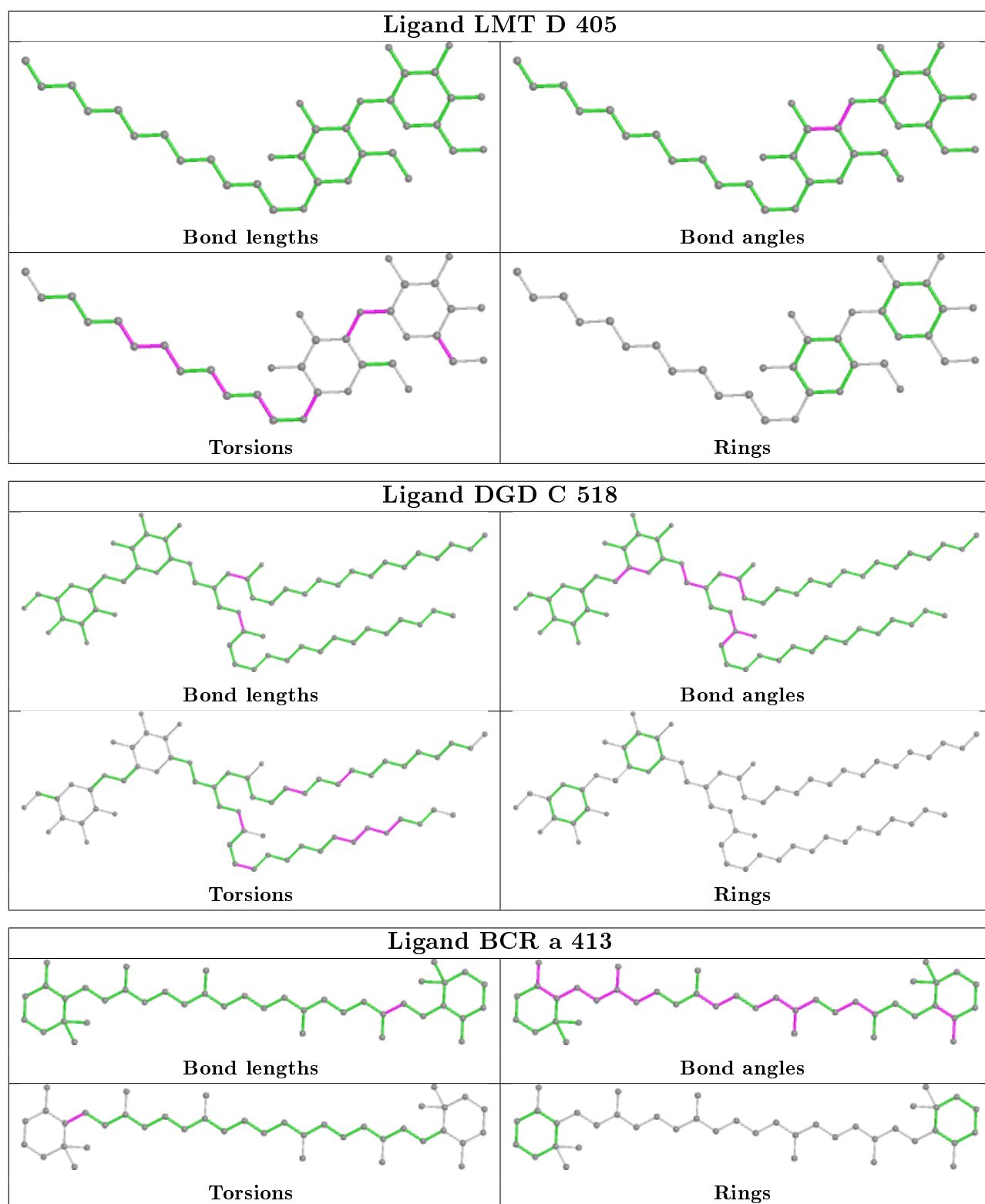
Ligand CLA A 406



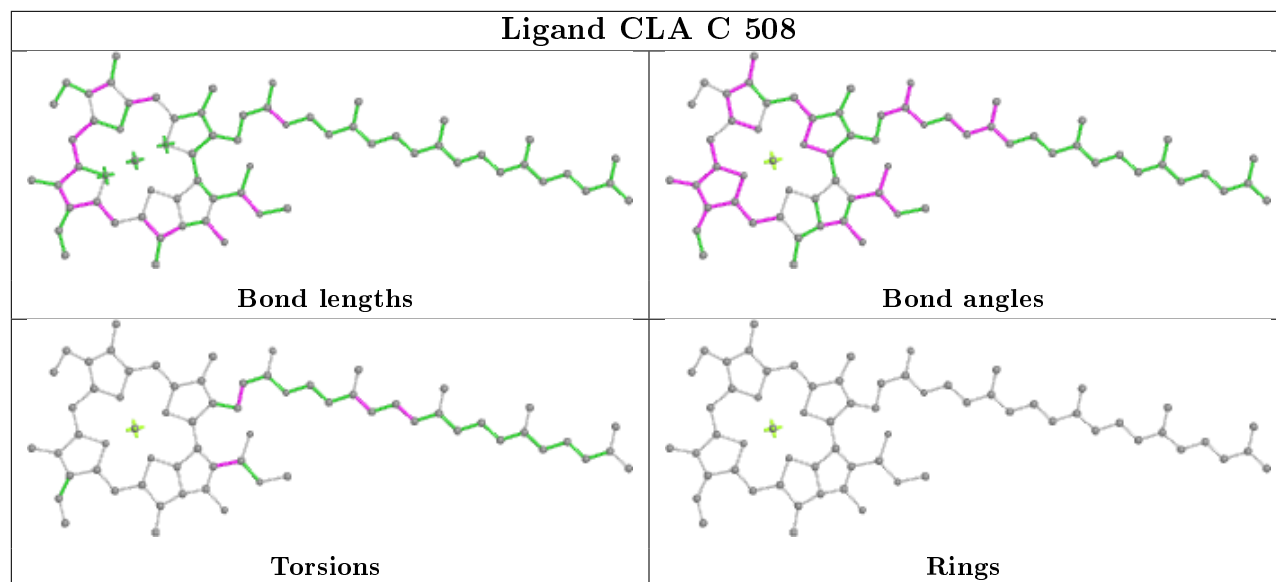
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

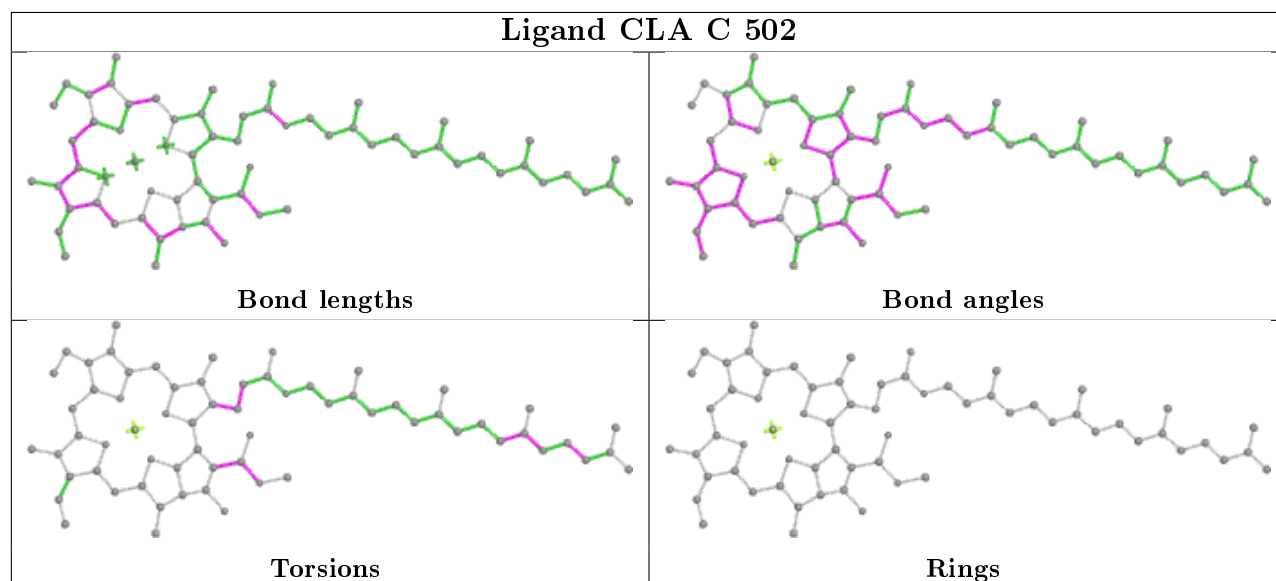
Ligand BCR T 103	
	
Bond lengths	Bond angles
	
Torsions	Rings



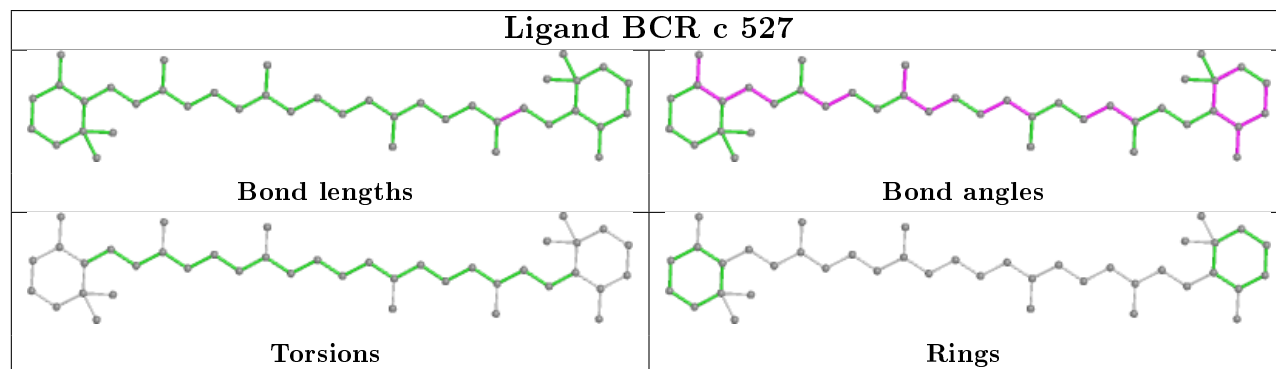
Ligand CLA C 508

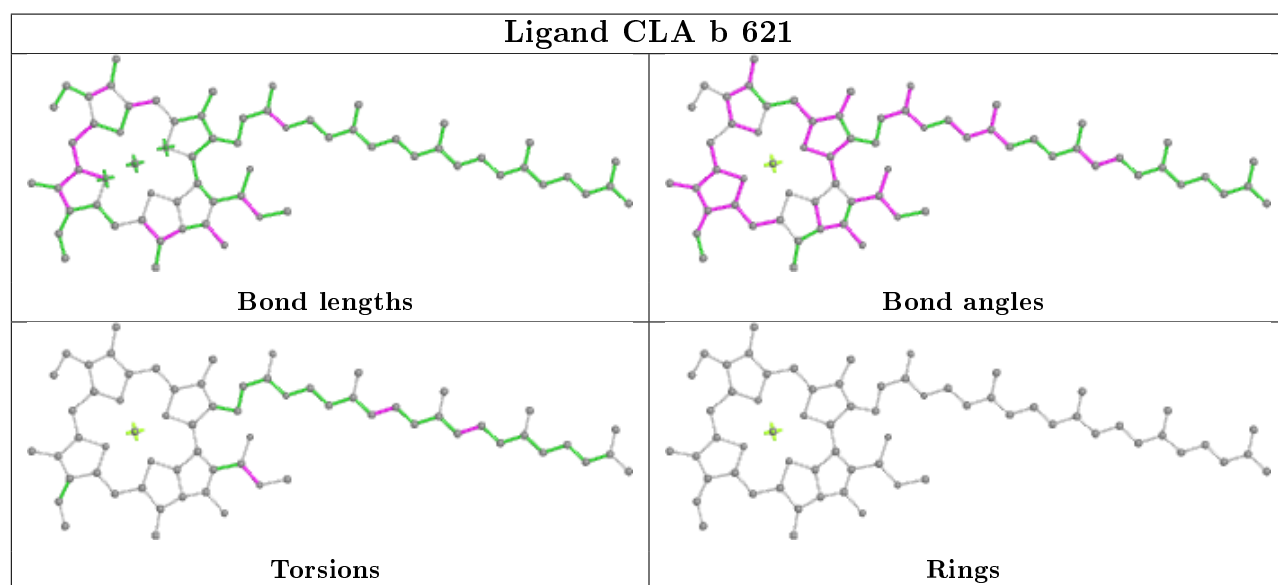
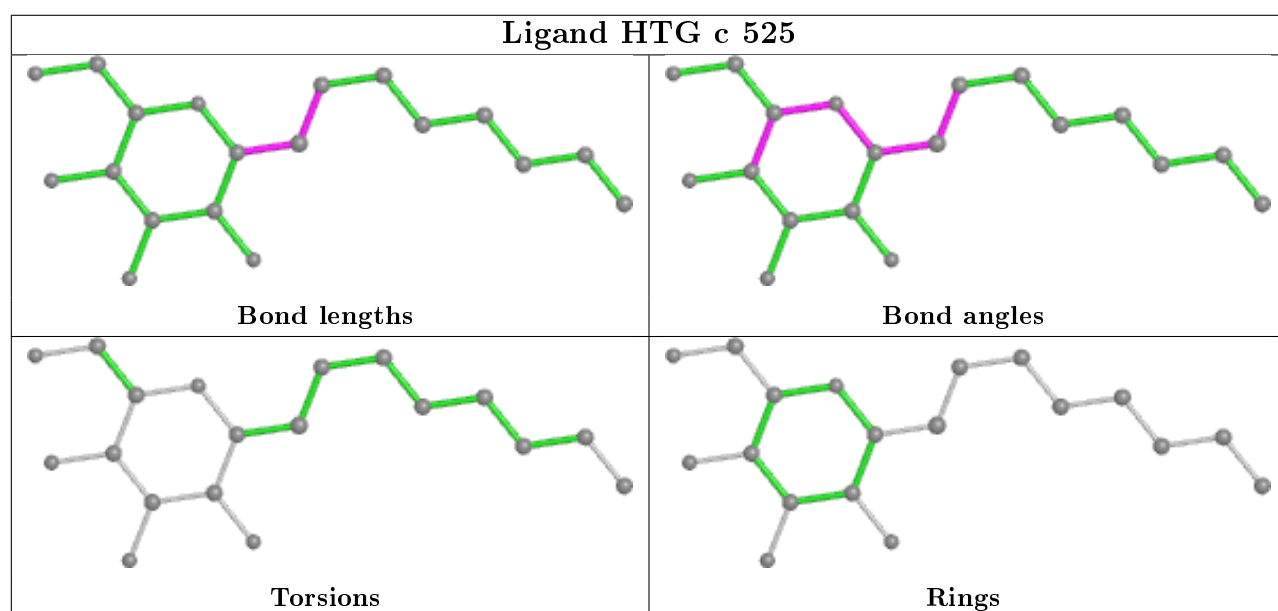
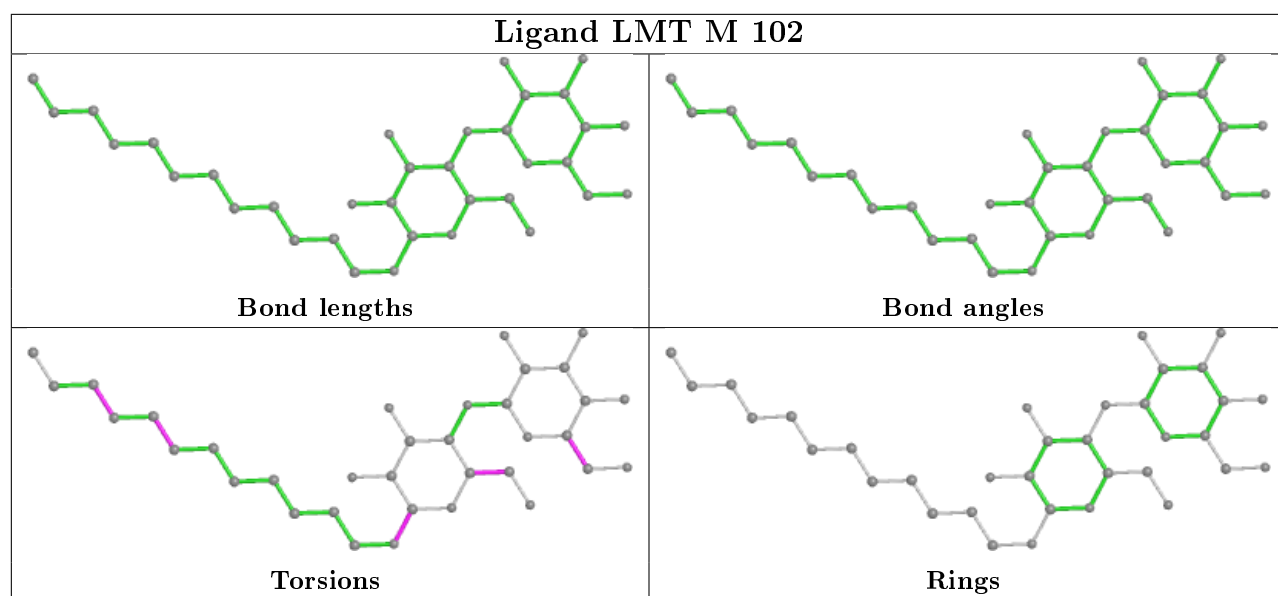


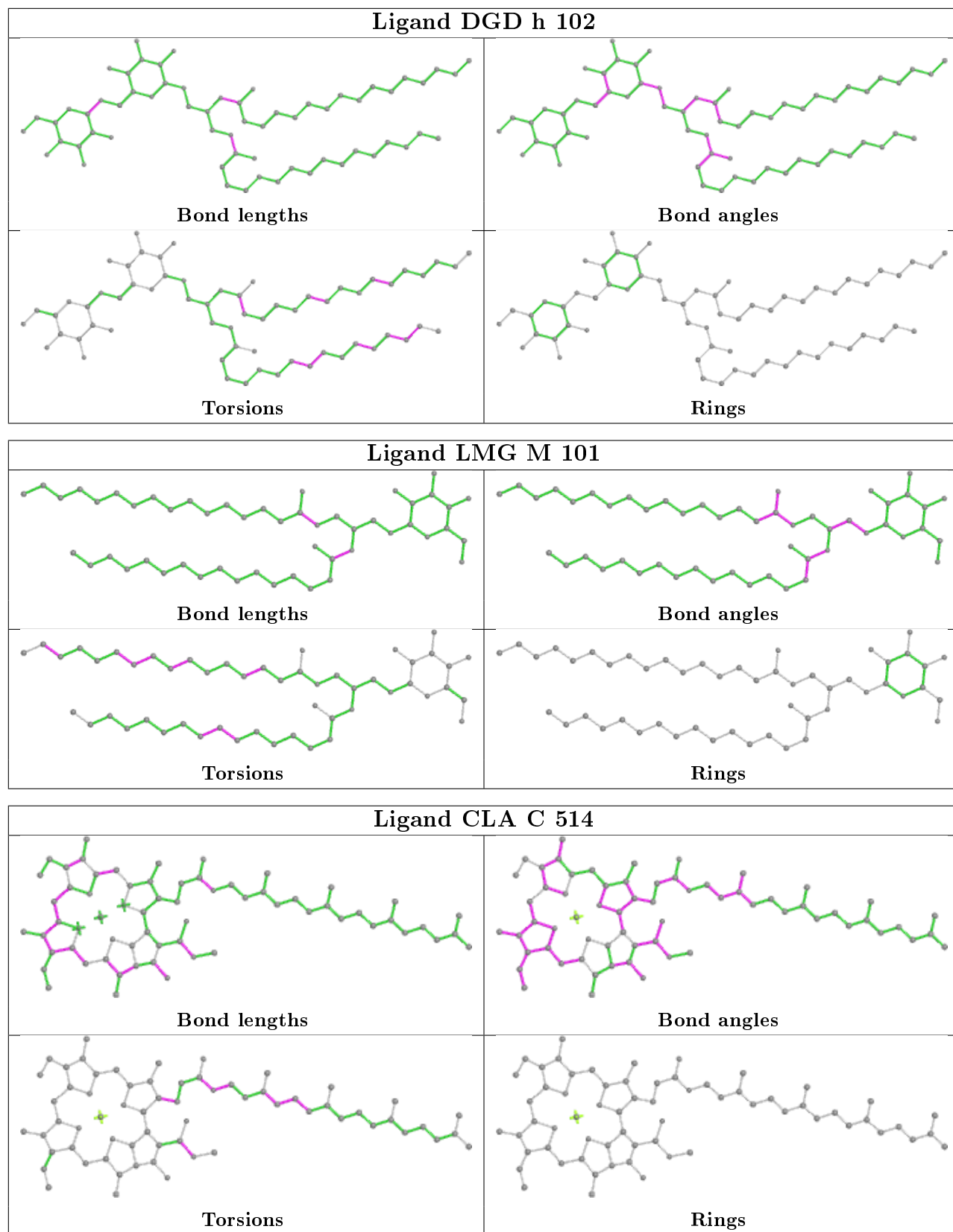
Ligand CLA C 502

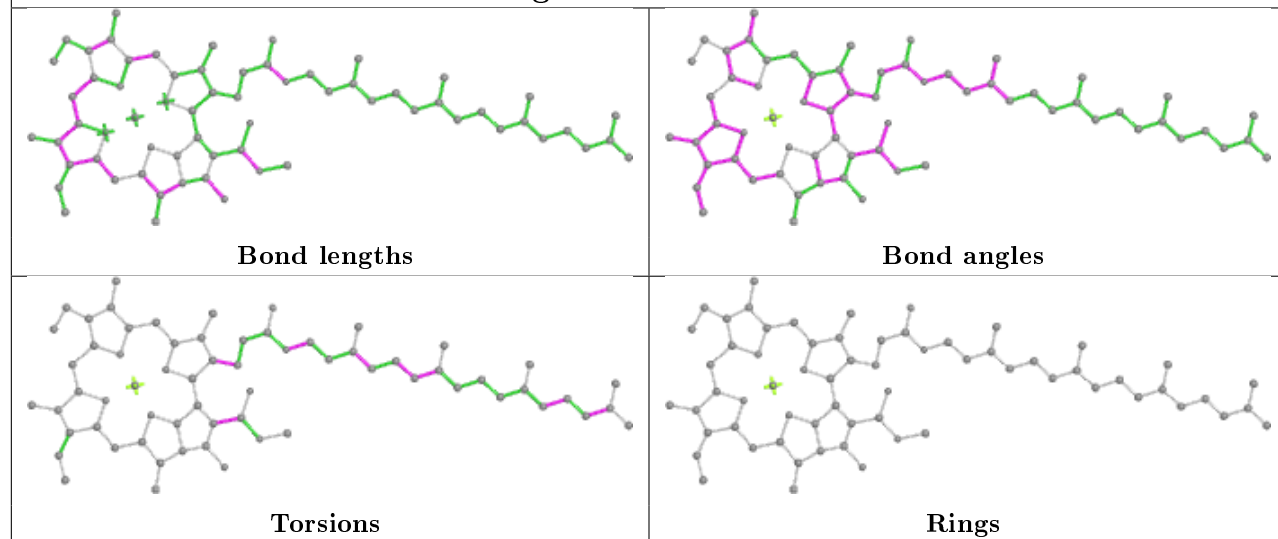
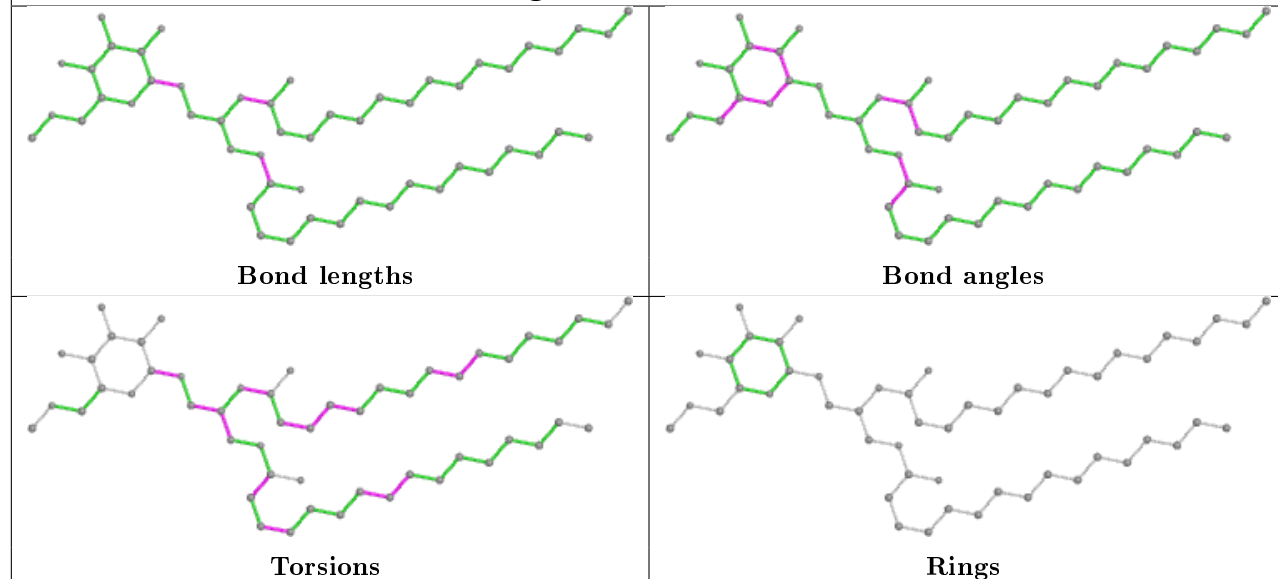


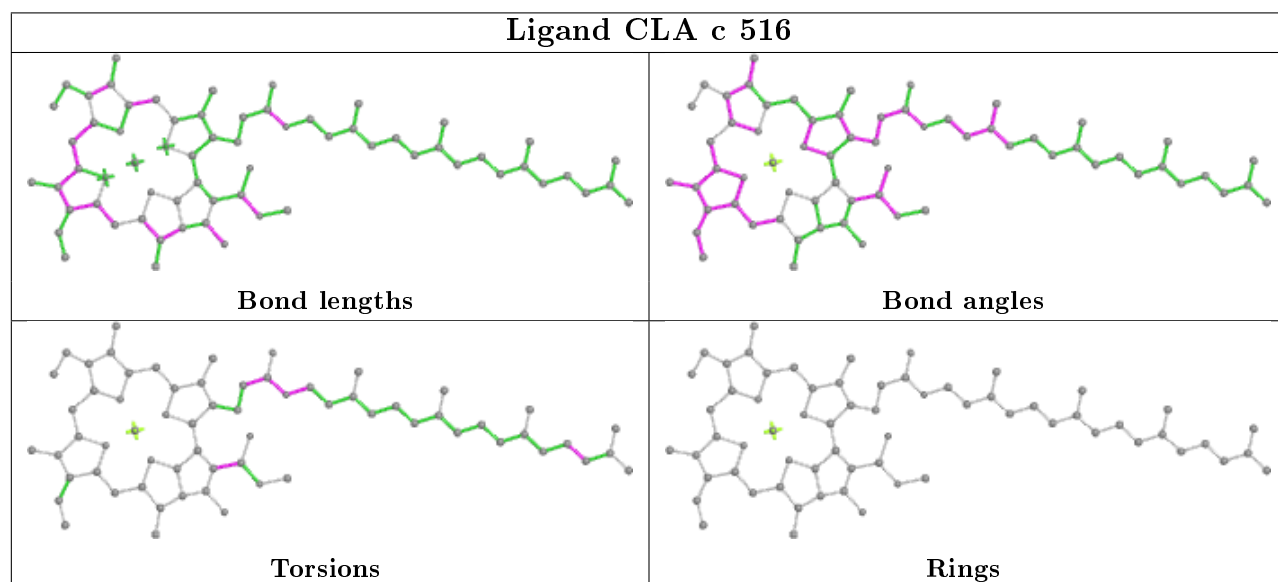
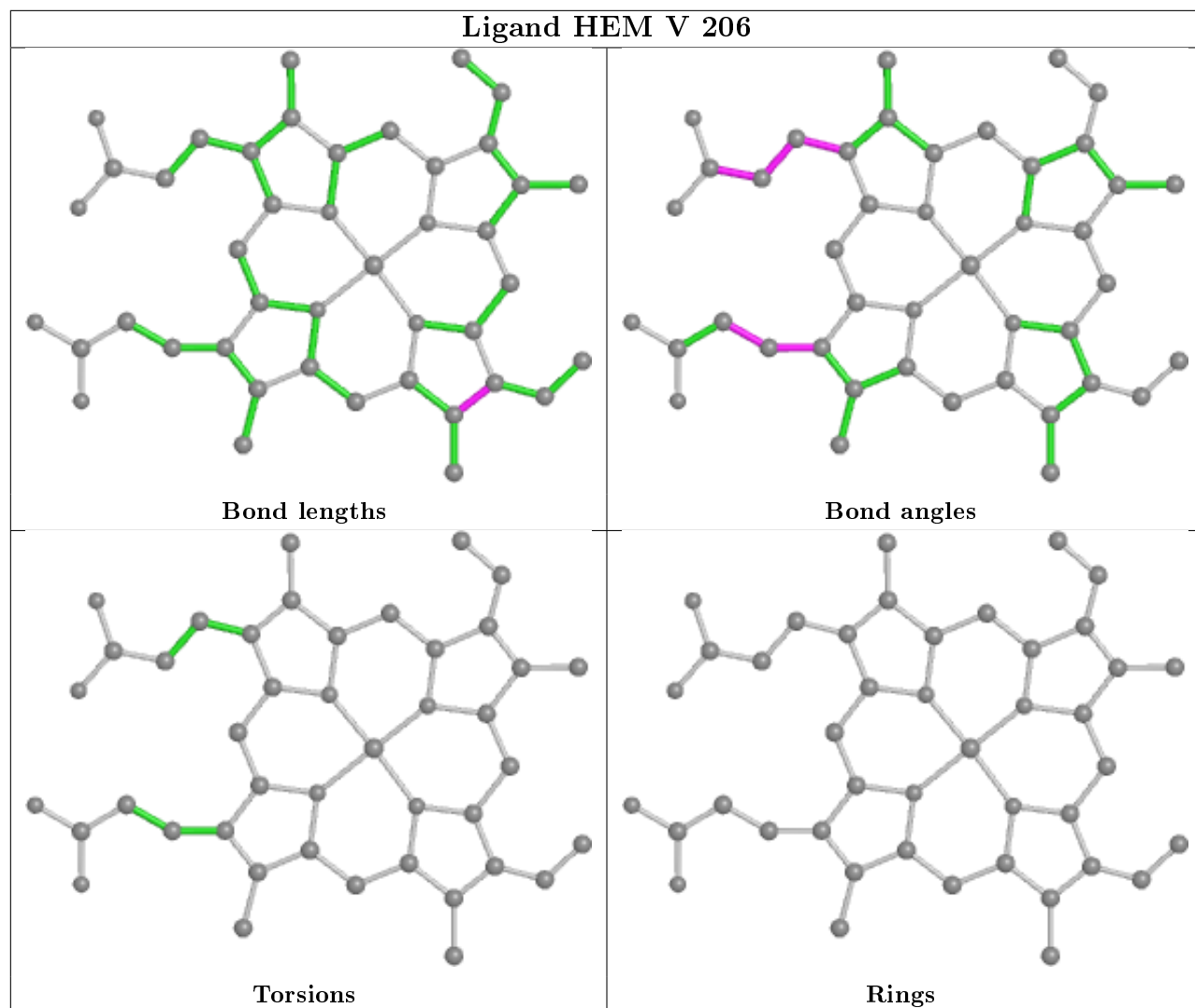
Ligand BCR c 527

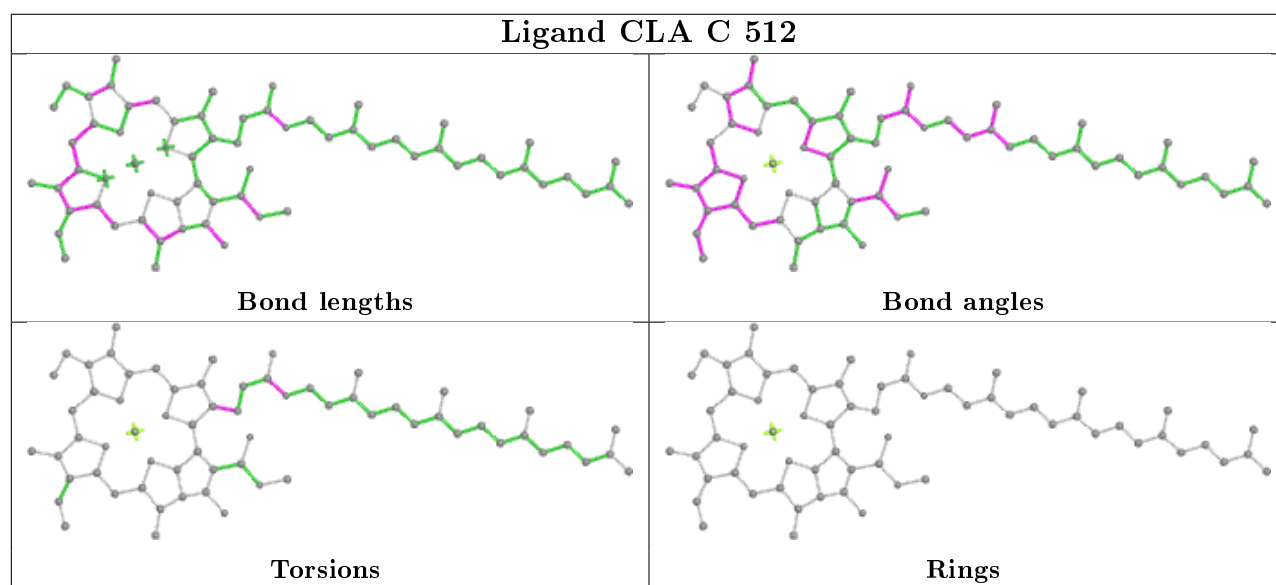
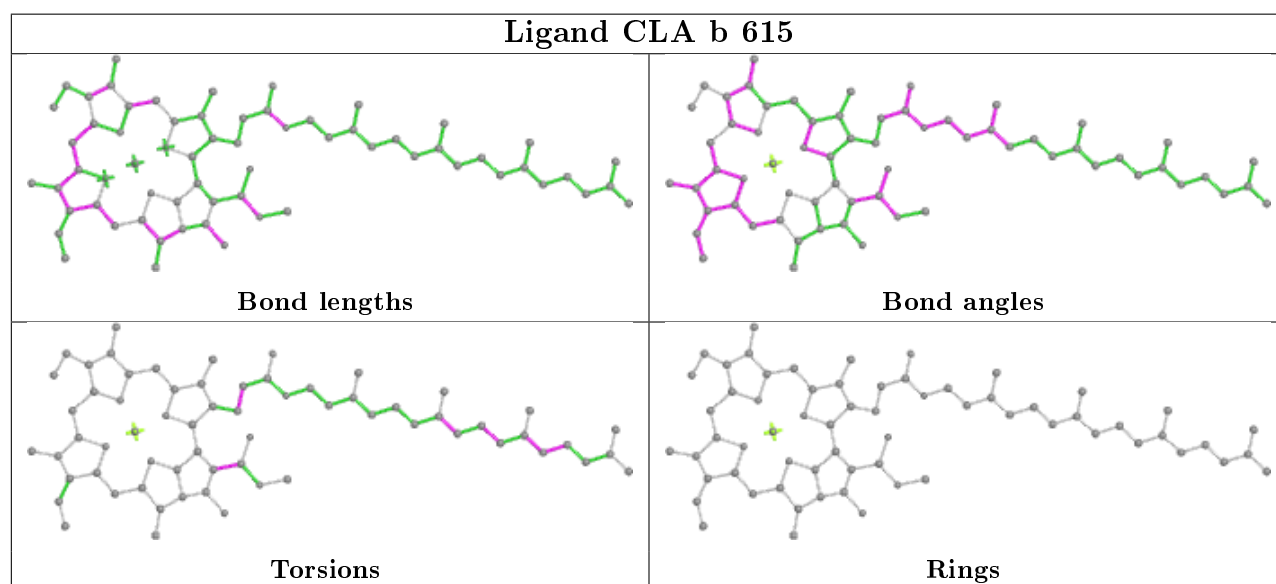
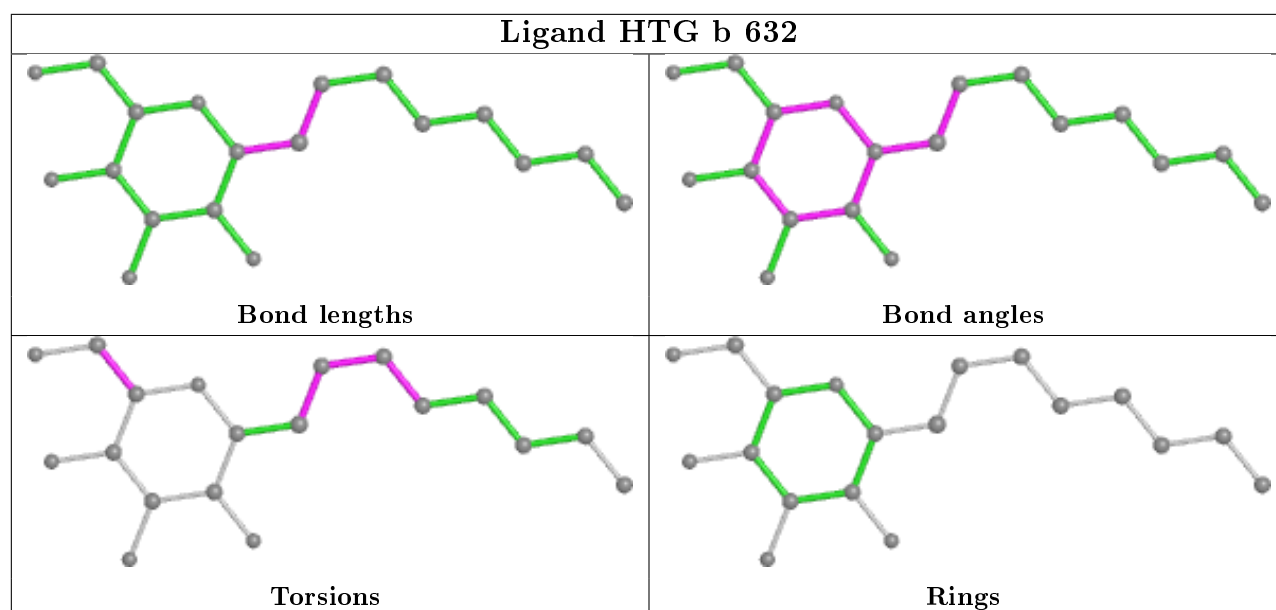




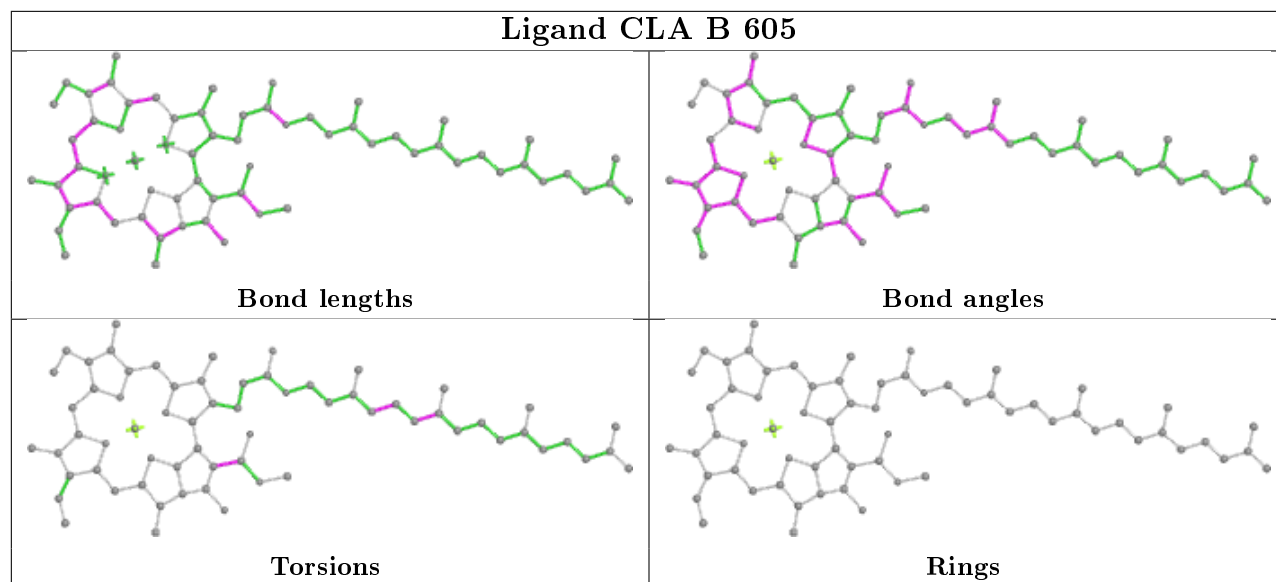


Ligand CLA C 507**Ligand DGD D 410**

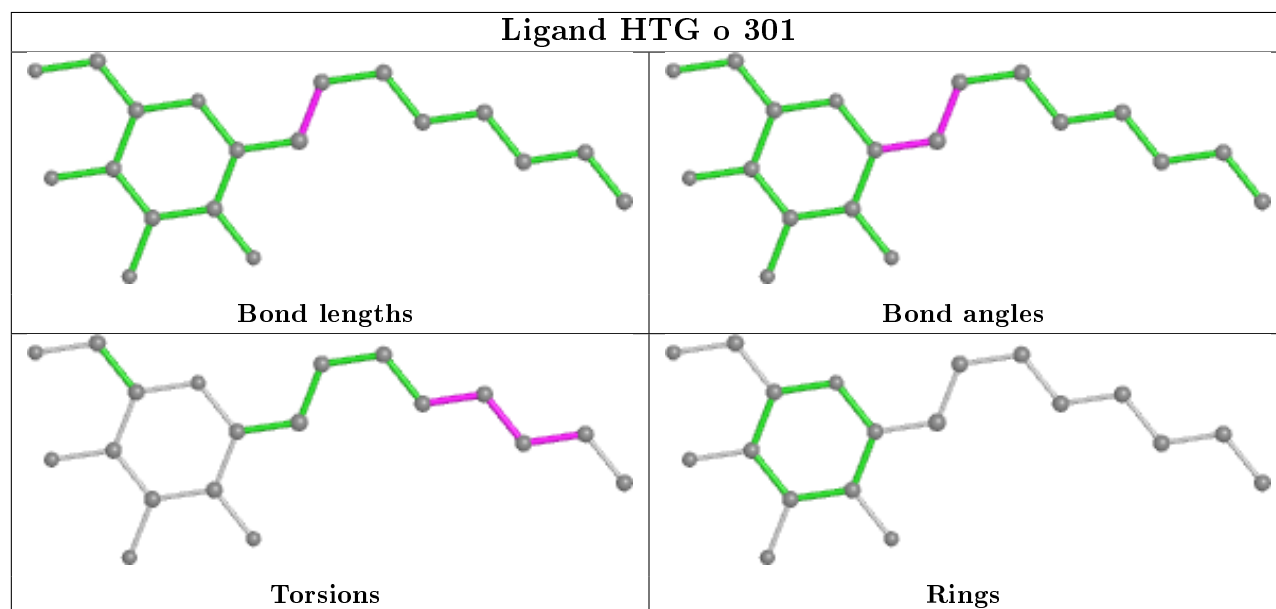




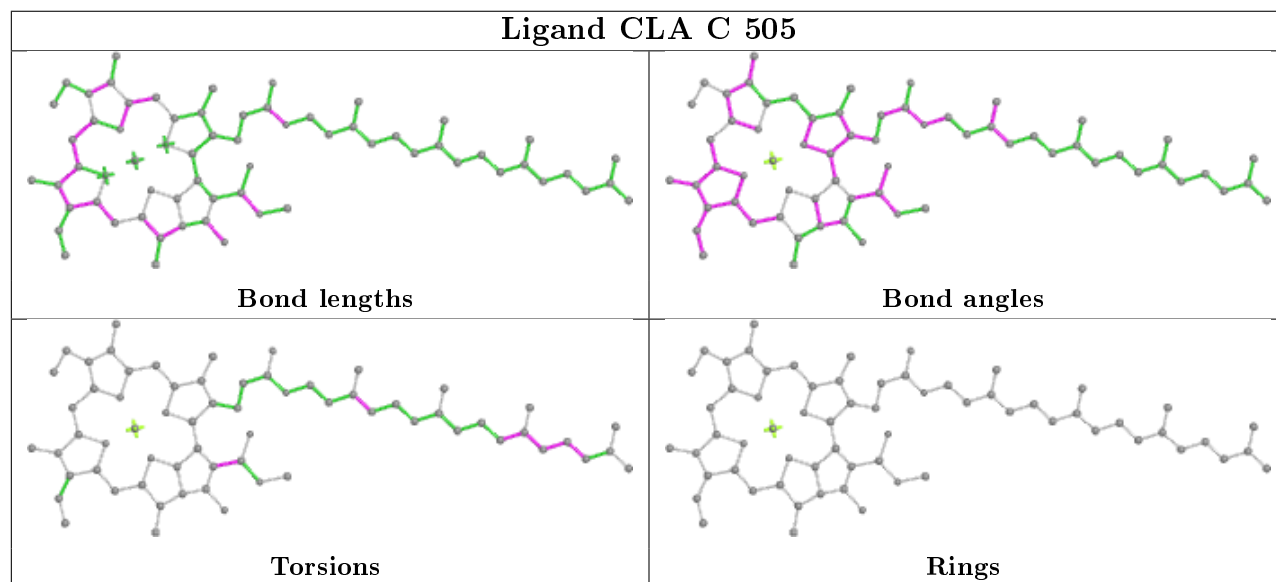
Ligand CLA B 605

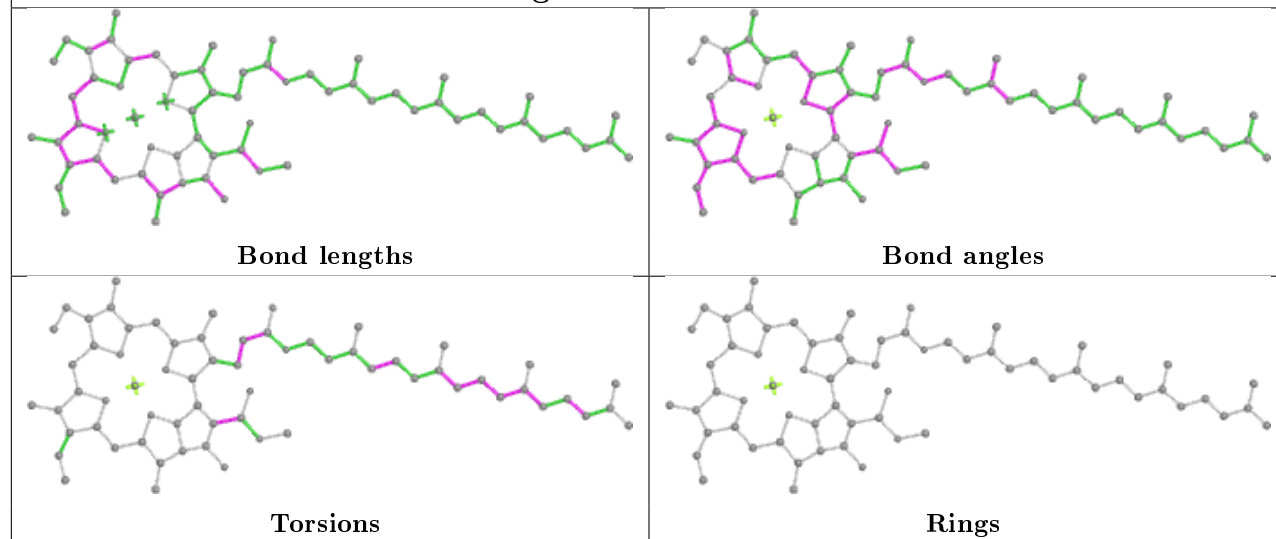
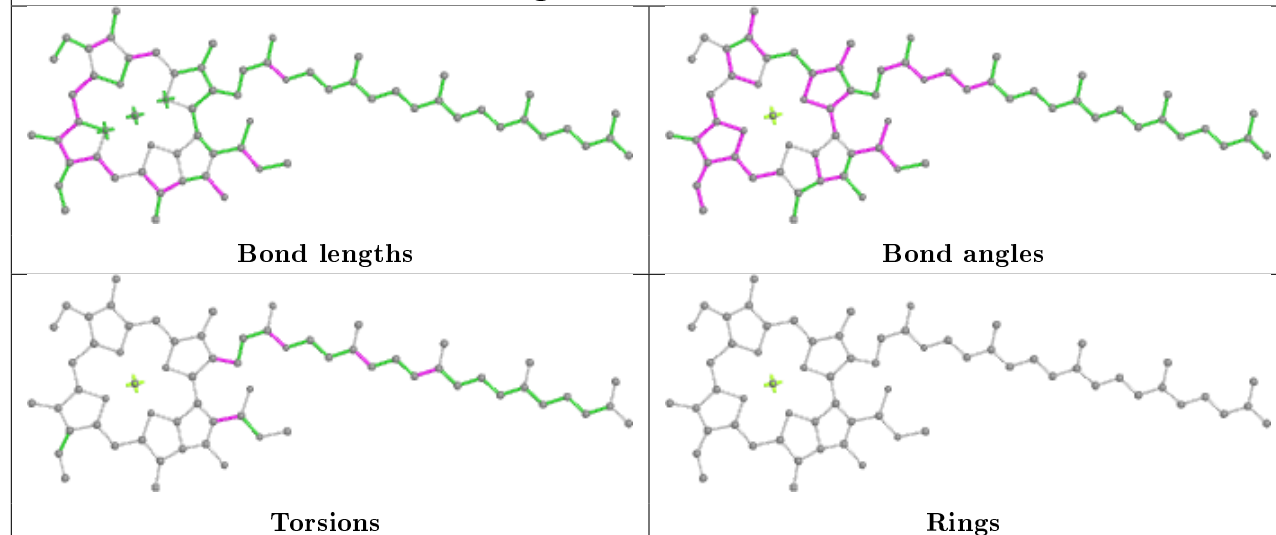
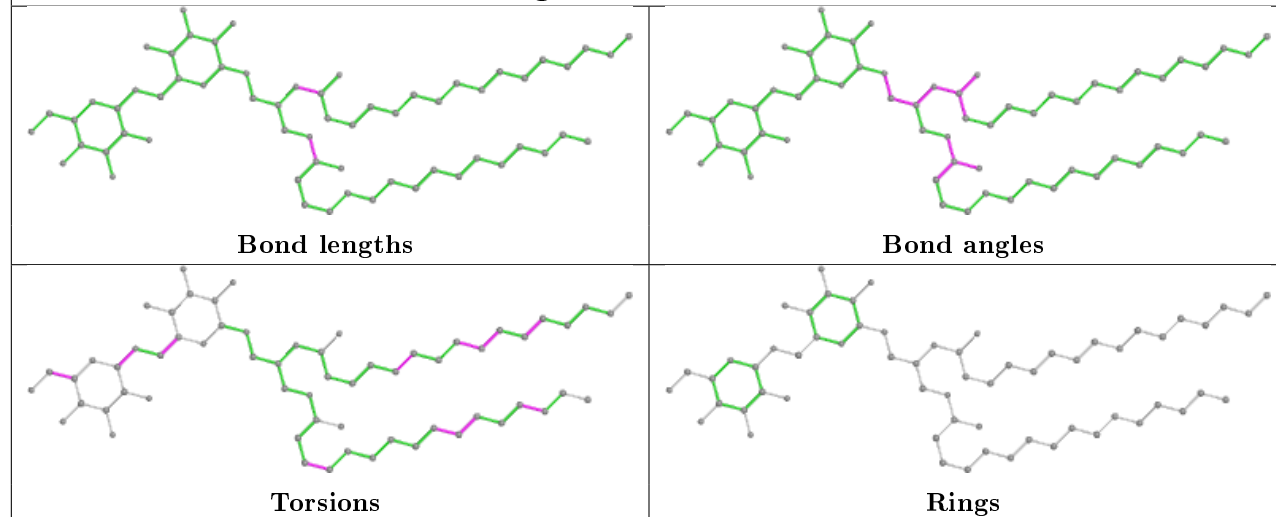


Ligand HTG o 301

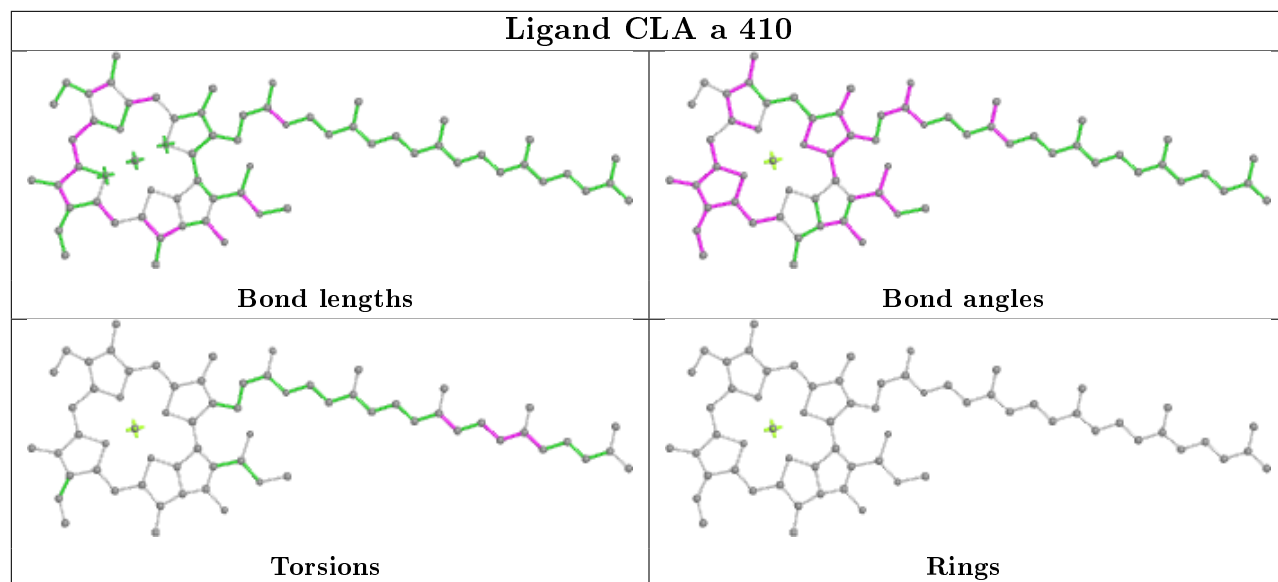


Ligand CLA C 505

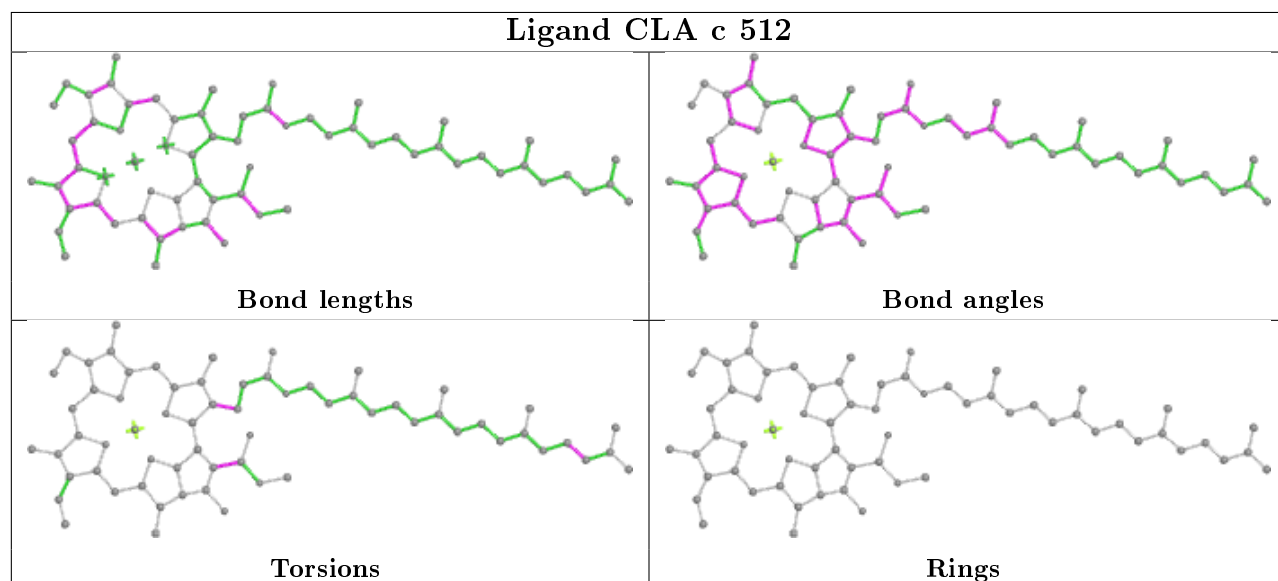


Ligand CLA B 602**Ligand CLA B 610****Ligand DGD c 519**

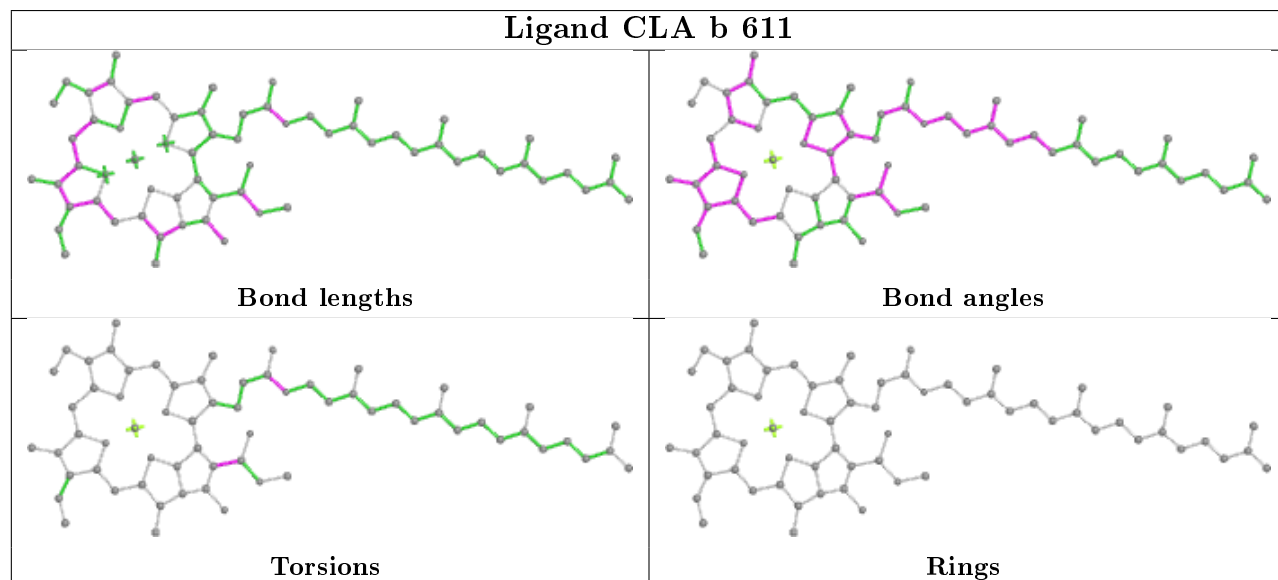
Ligand CLA a 410



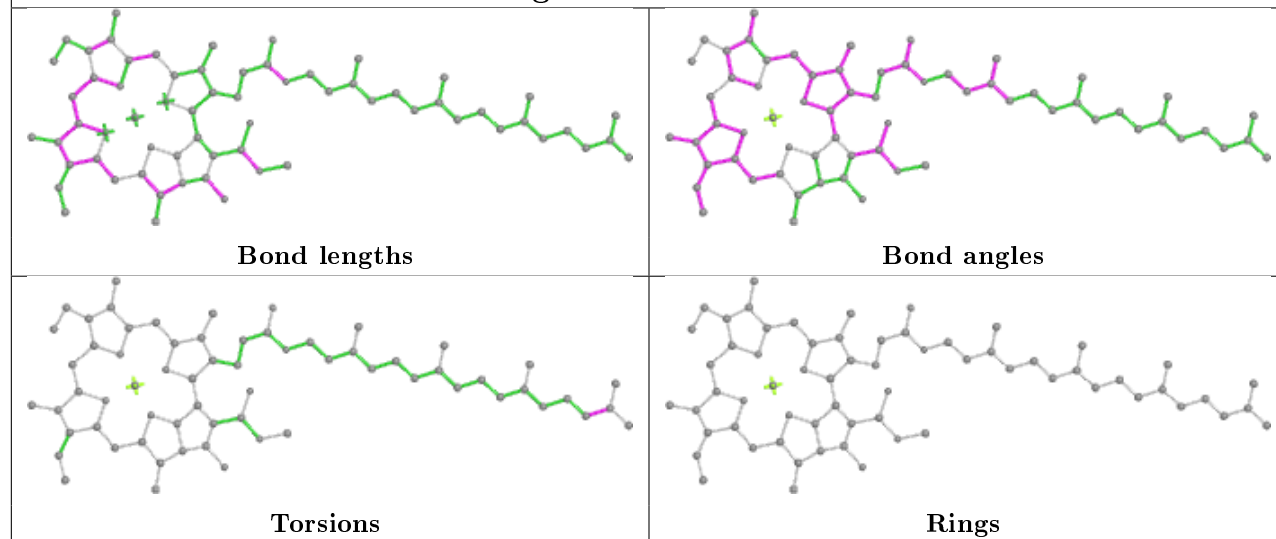
Ligand CLA c 512



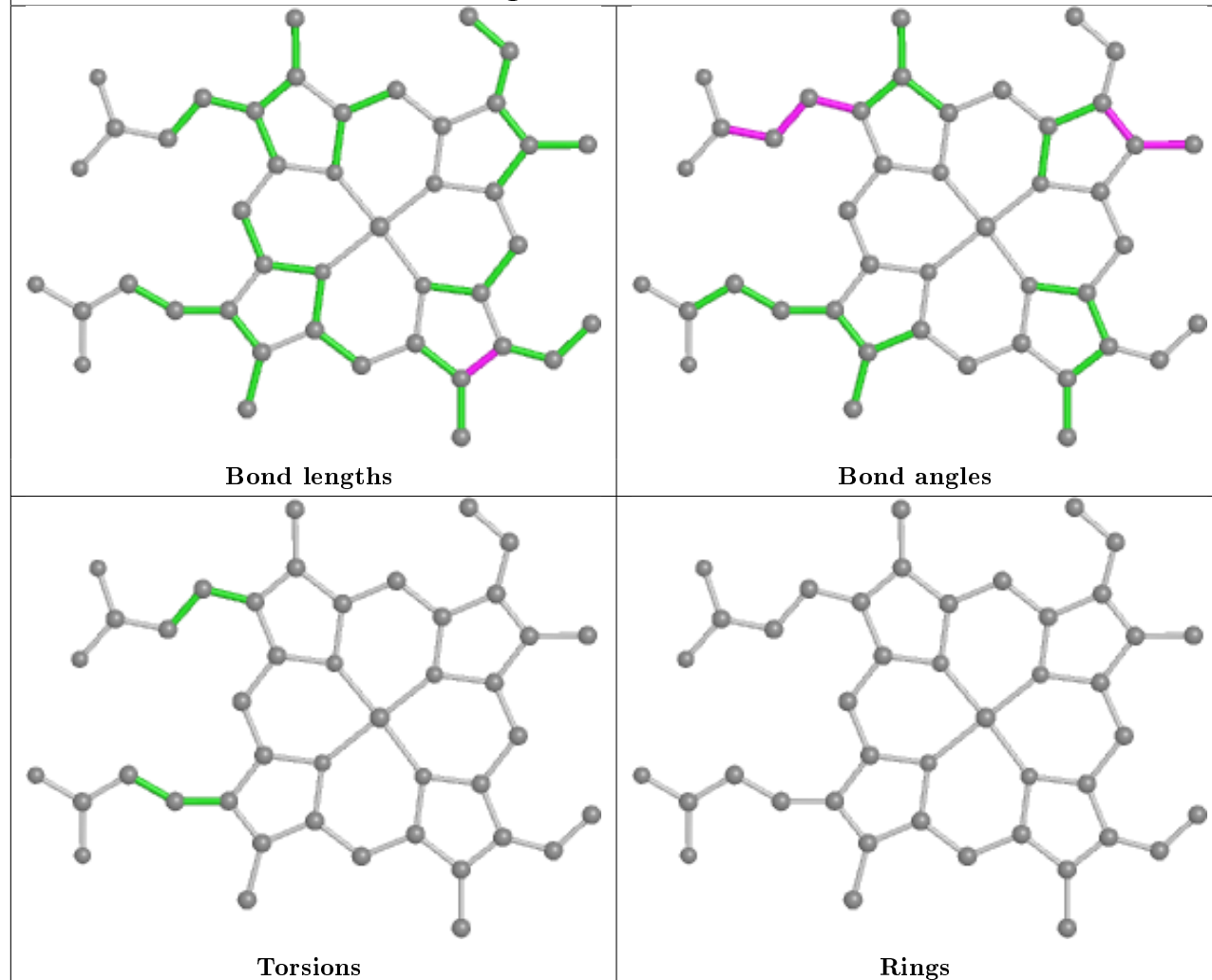
Ligand CLA b 611



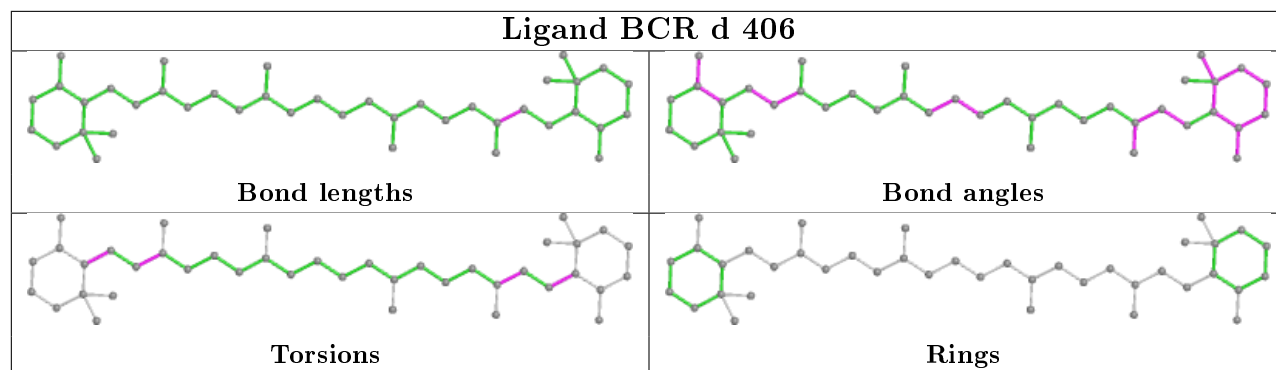
Ligand CLA B 609



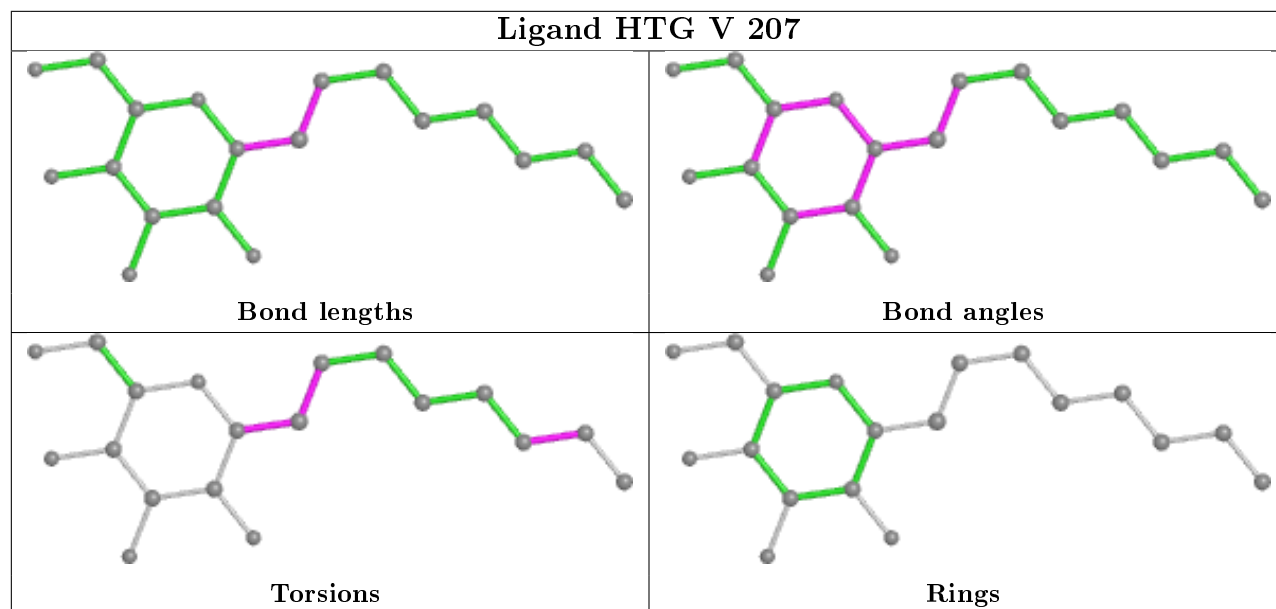
Ligand HEM e 101



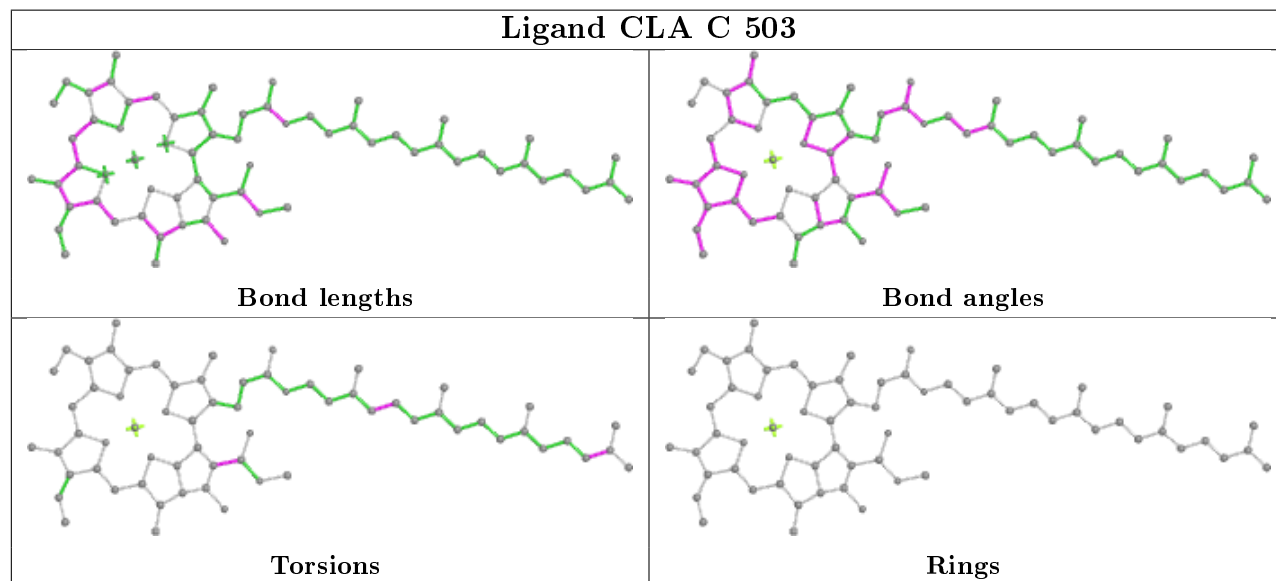
Ligand BCR d 406

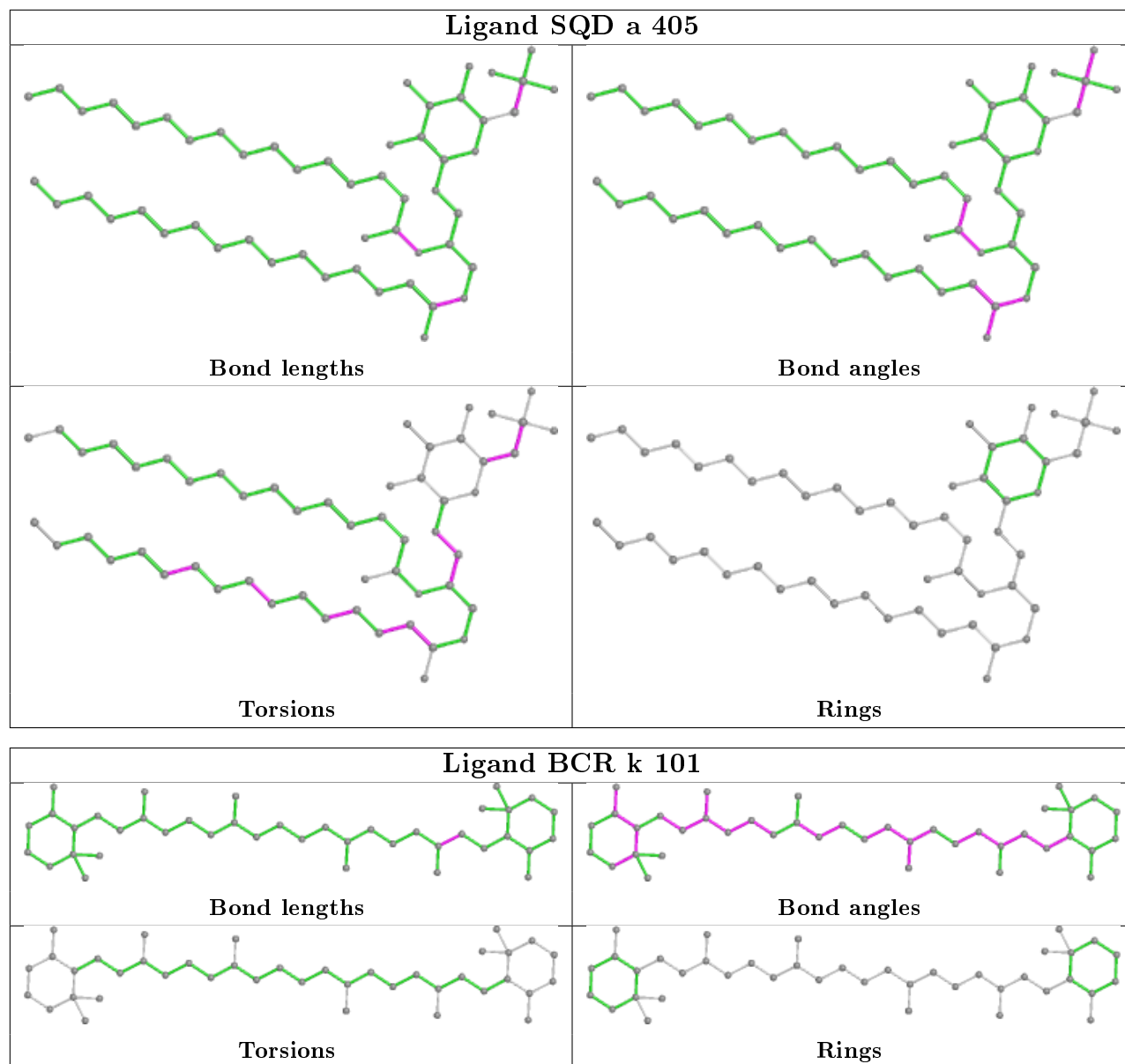


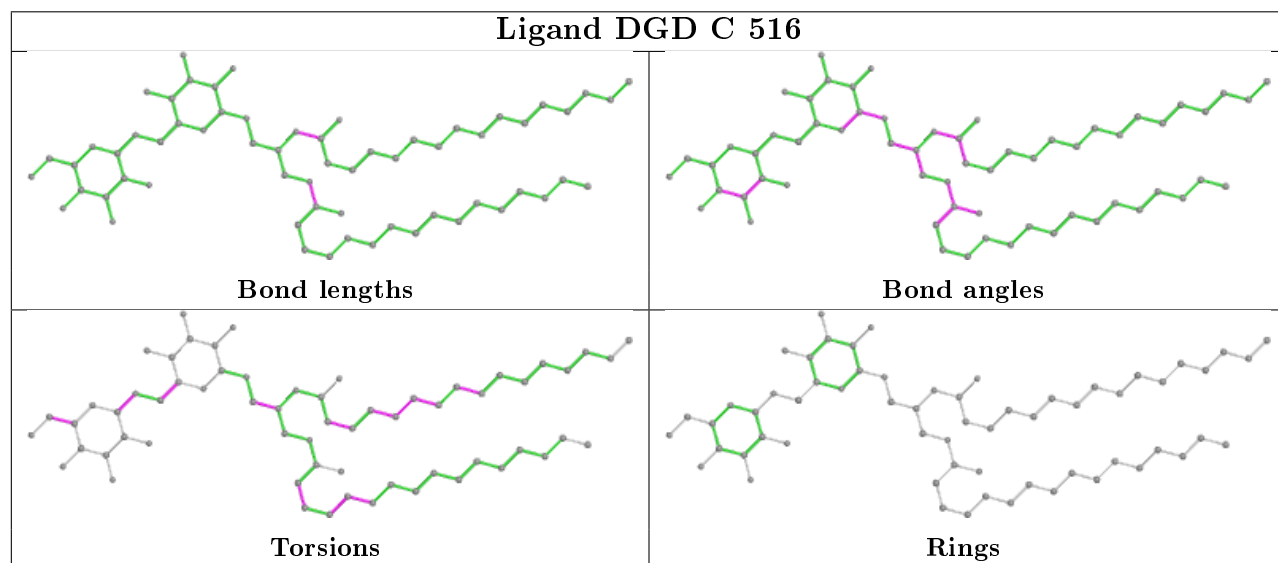
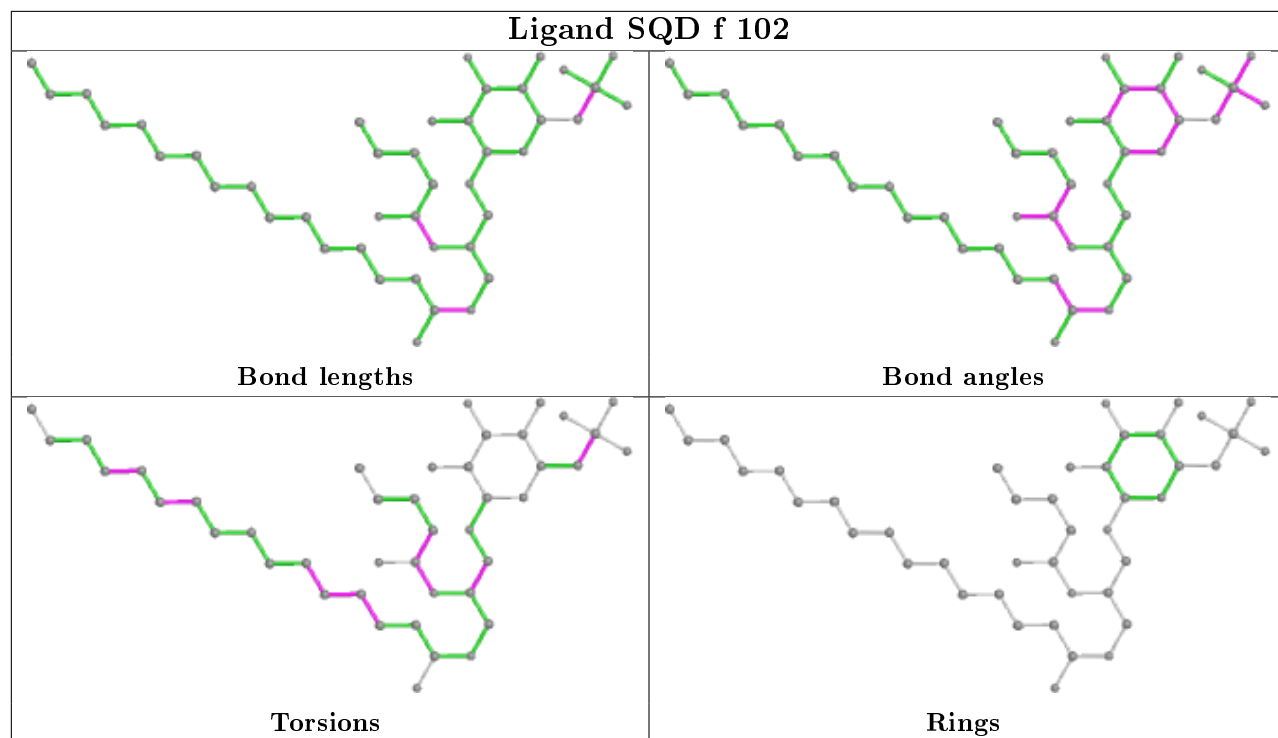
Ligand HTG V 207

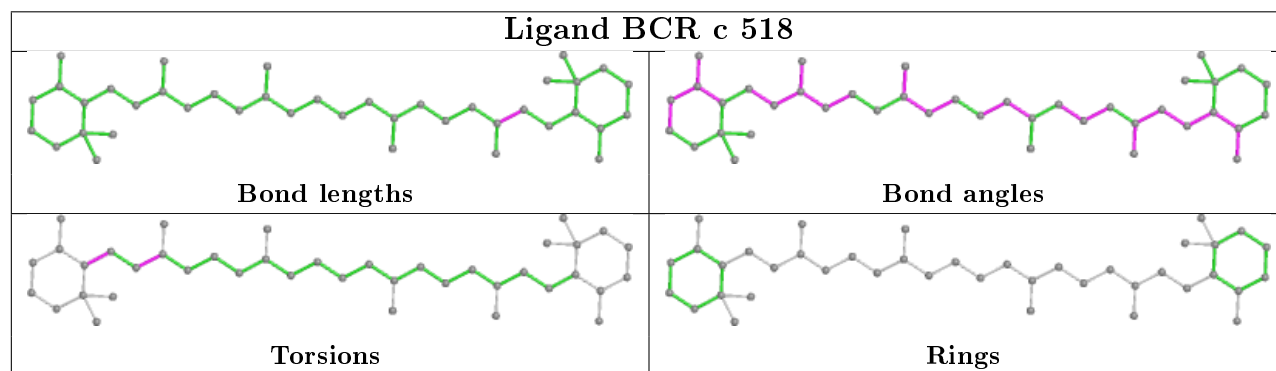
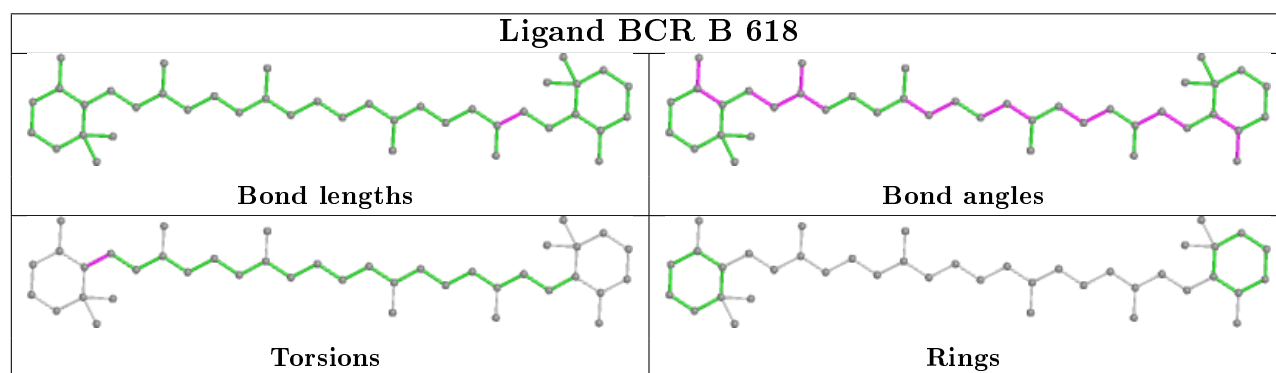
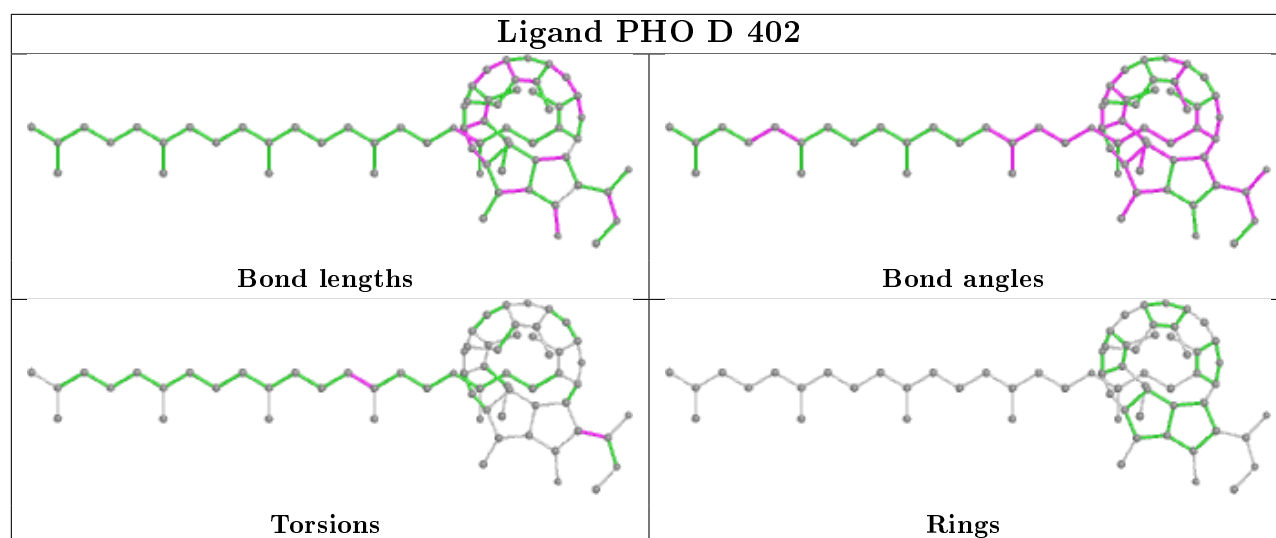


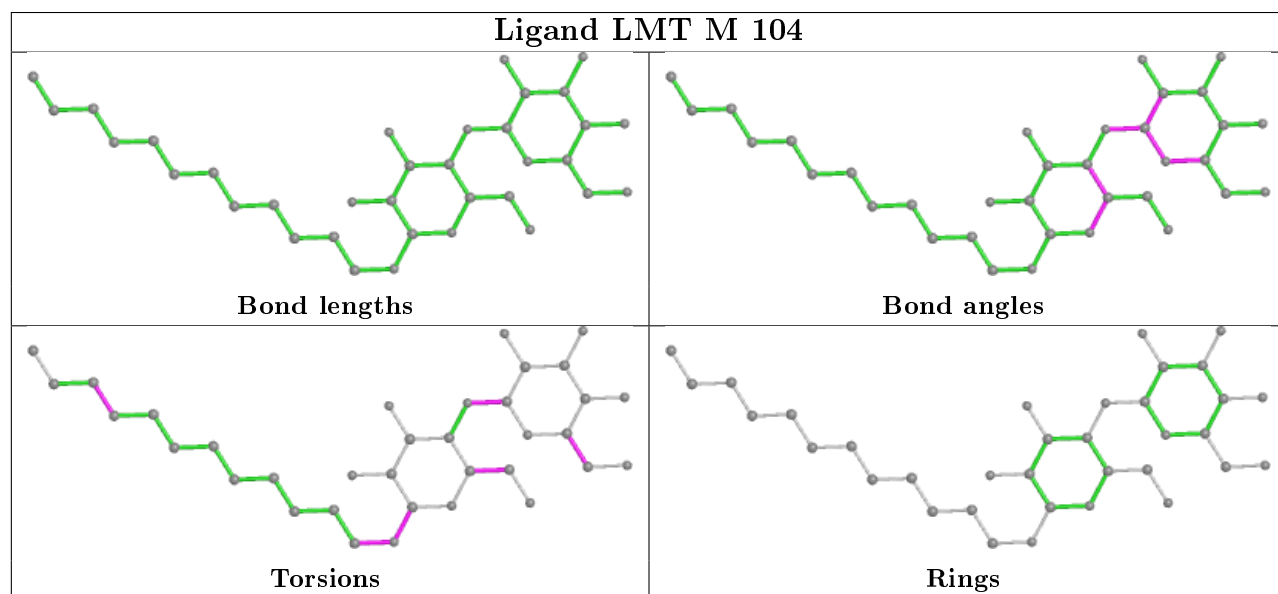
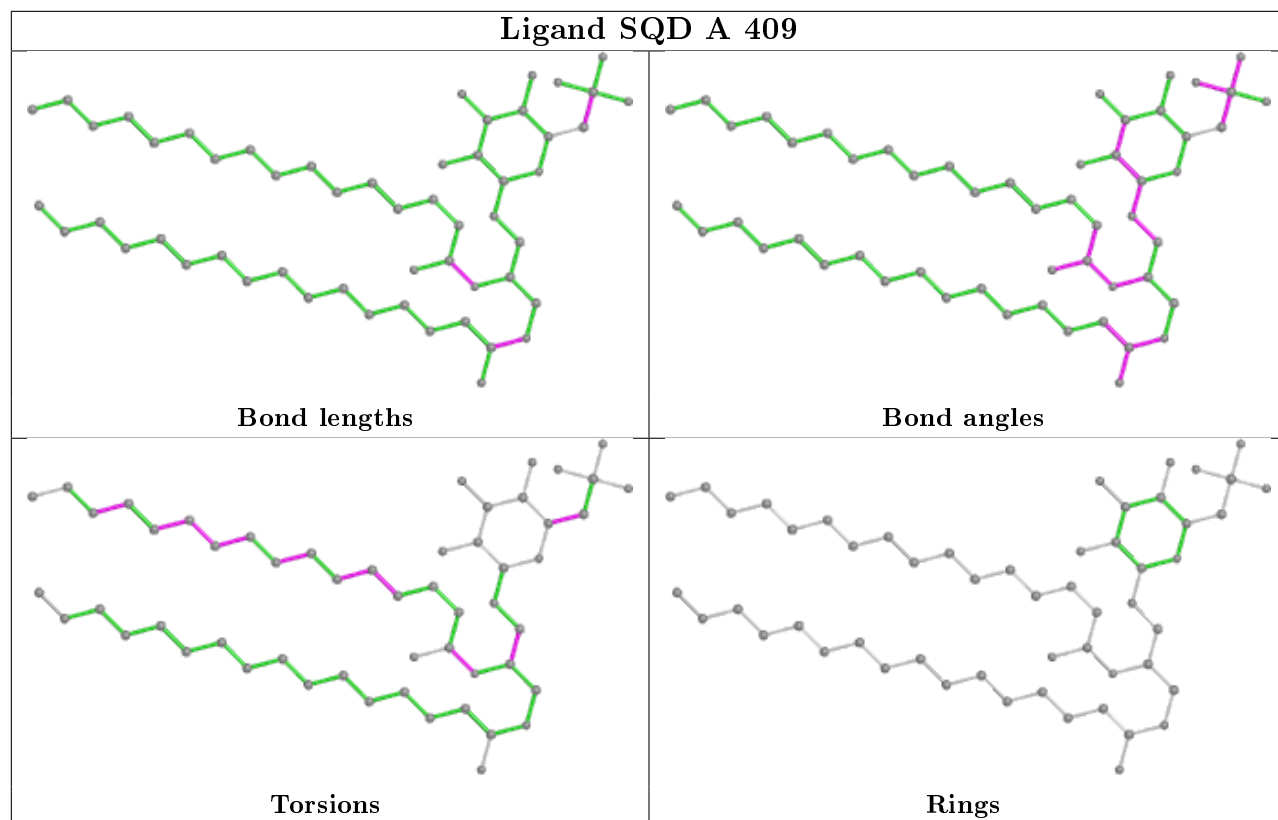
Ligand CLA C 503

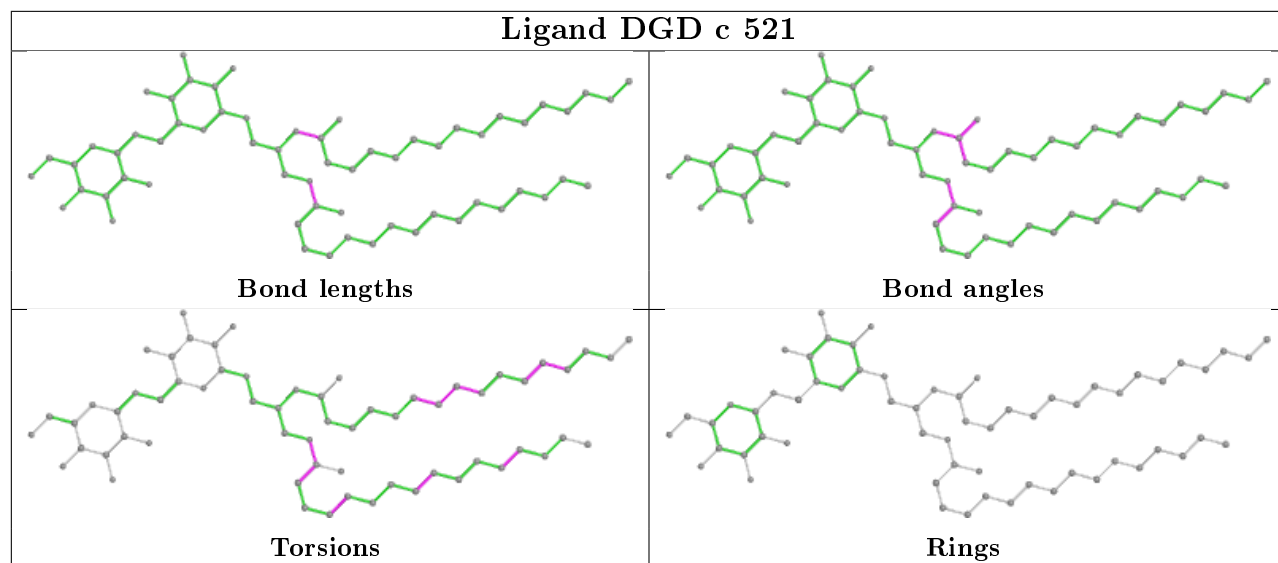
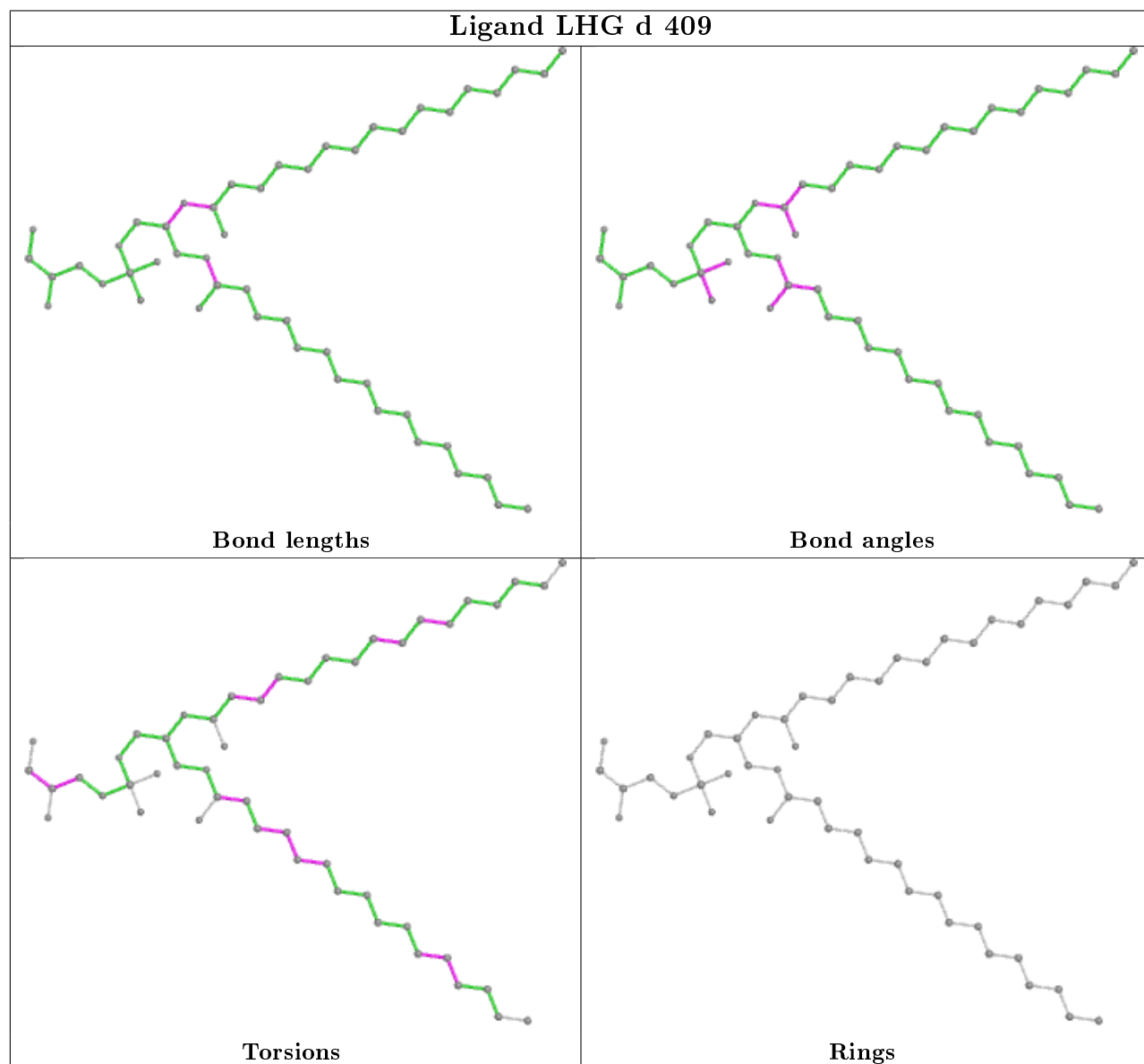


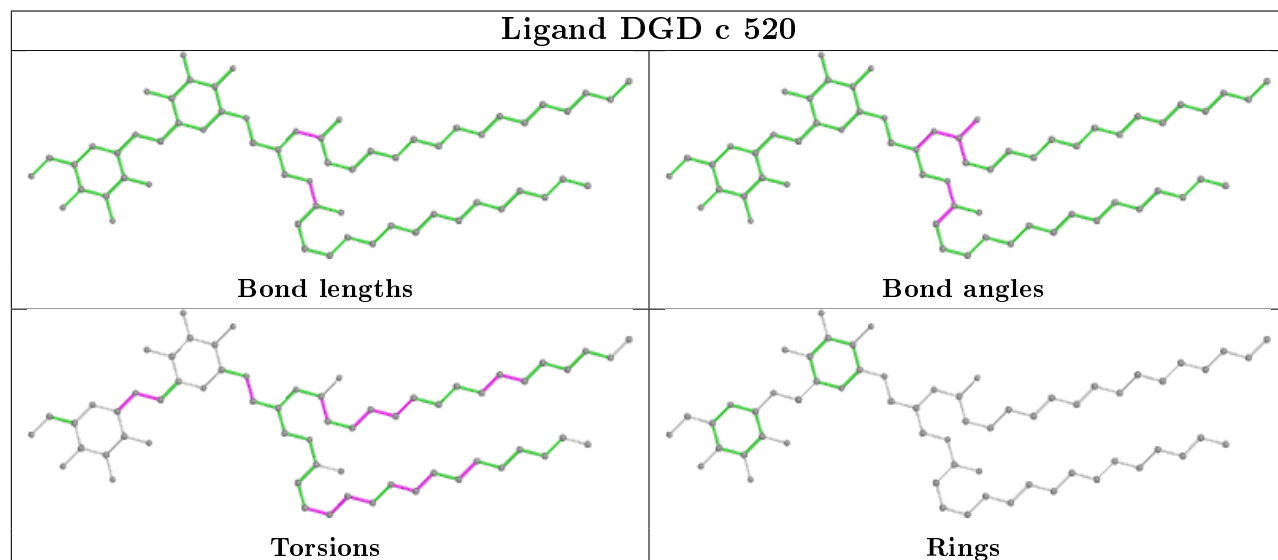
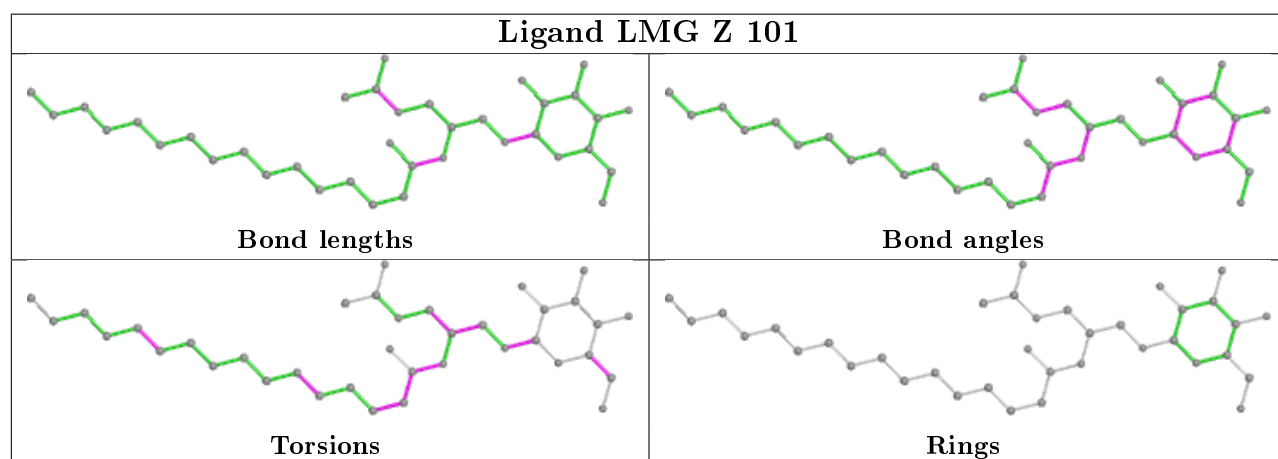
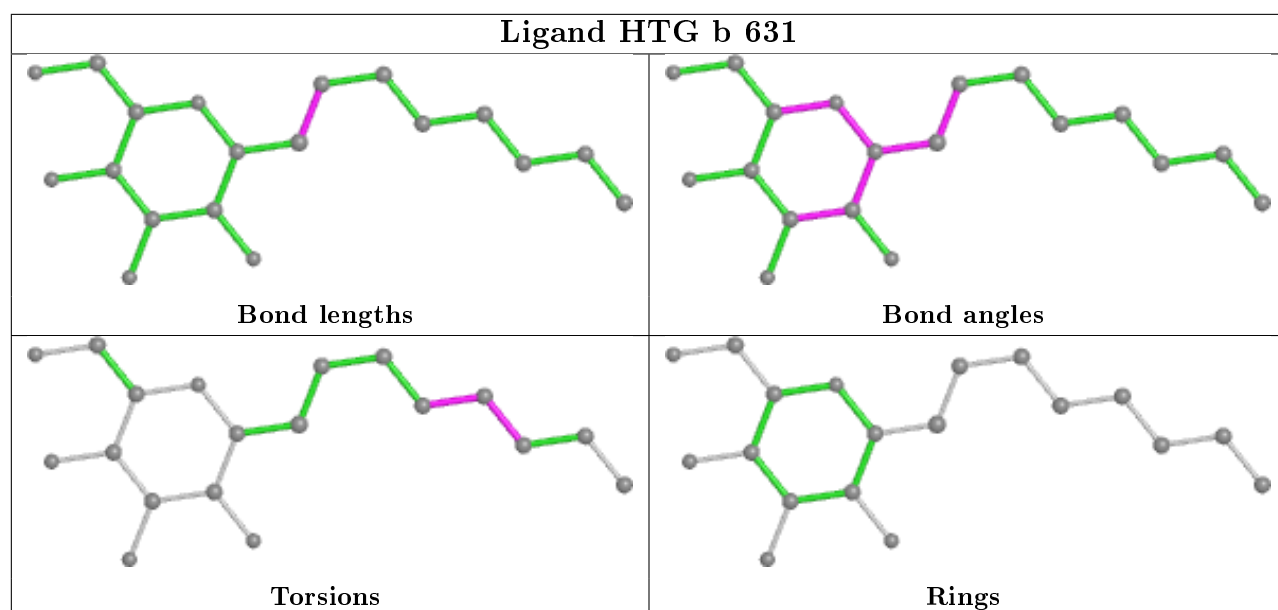




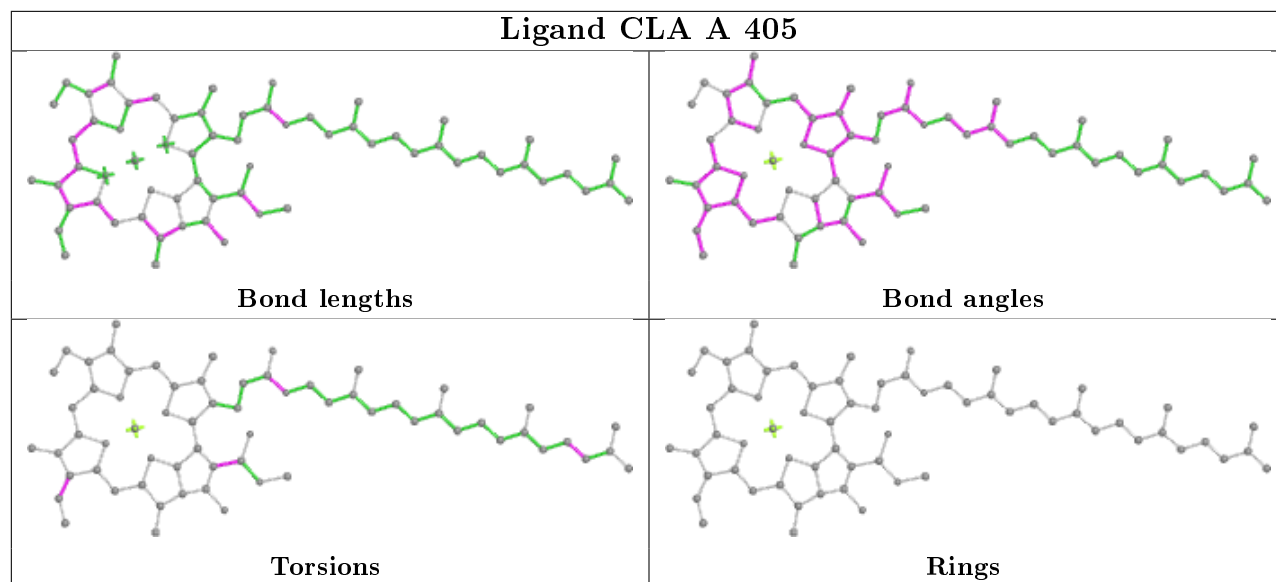




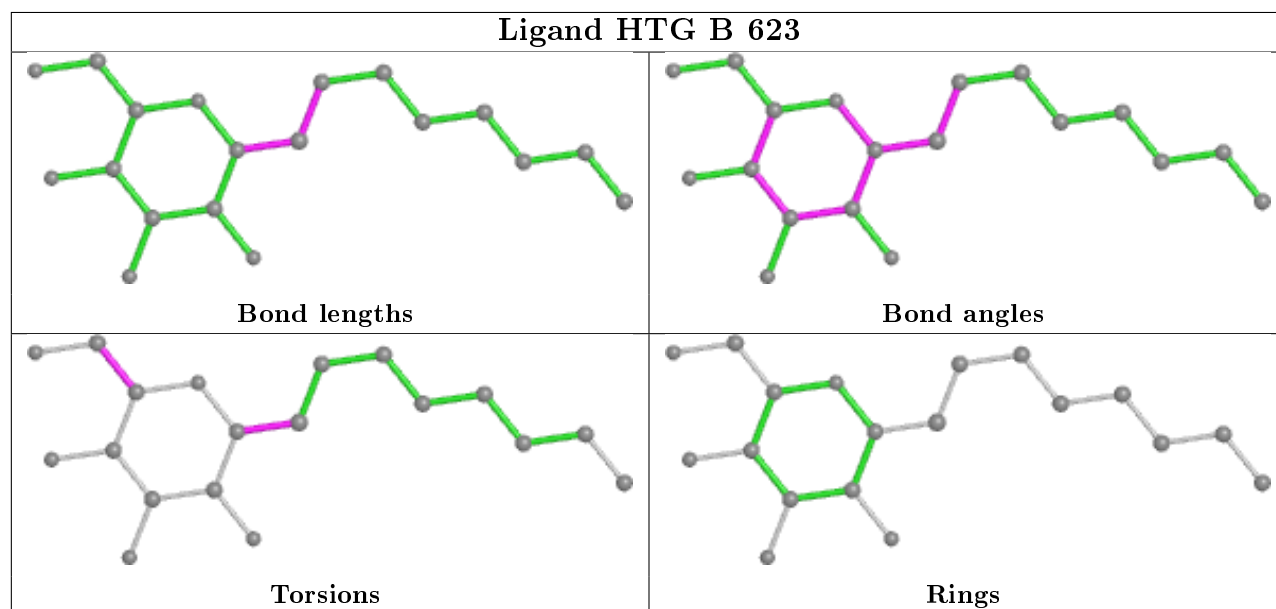
Ligand DGD c 521**Ligand LHG d 409**



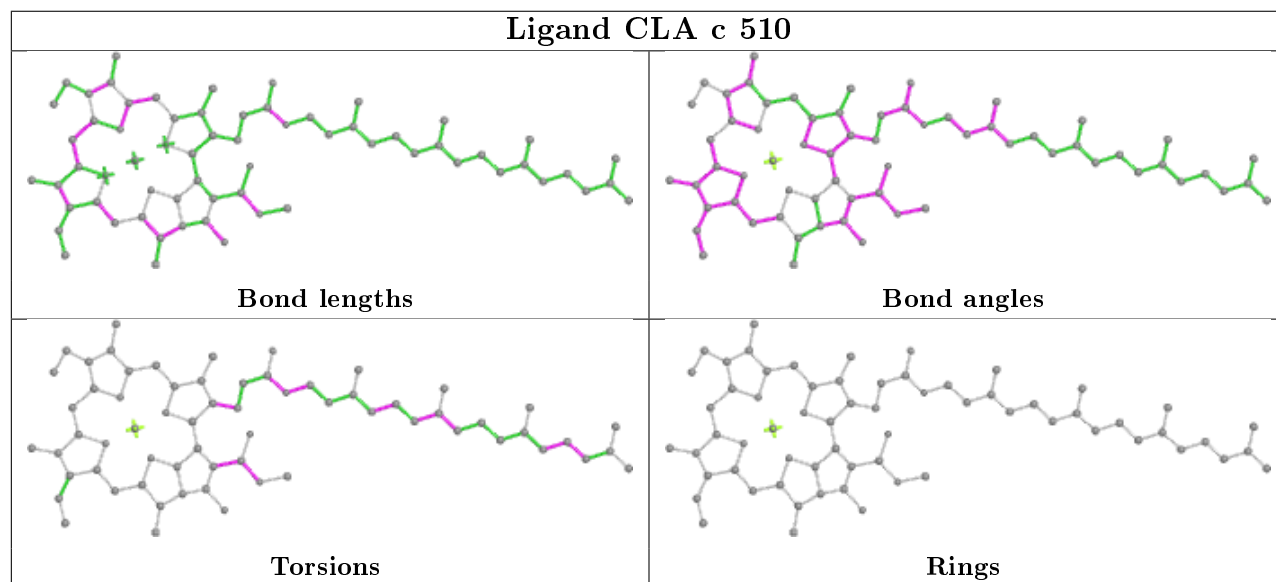
Ligand CLA A 405

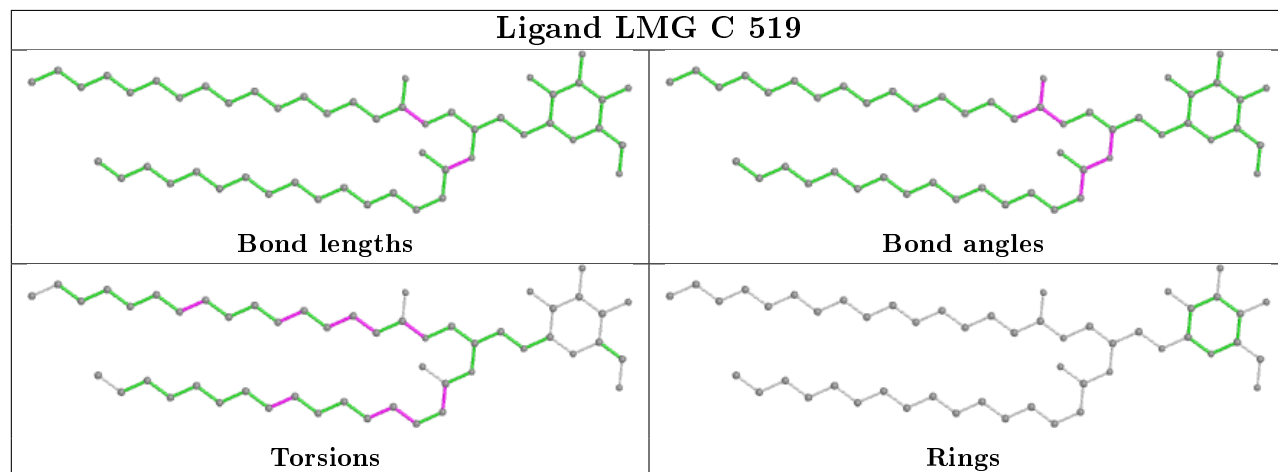
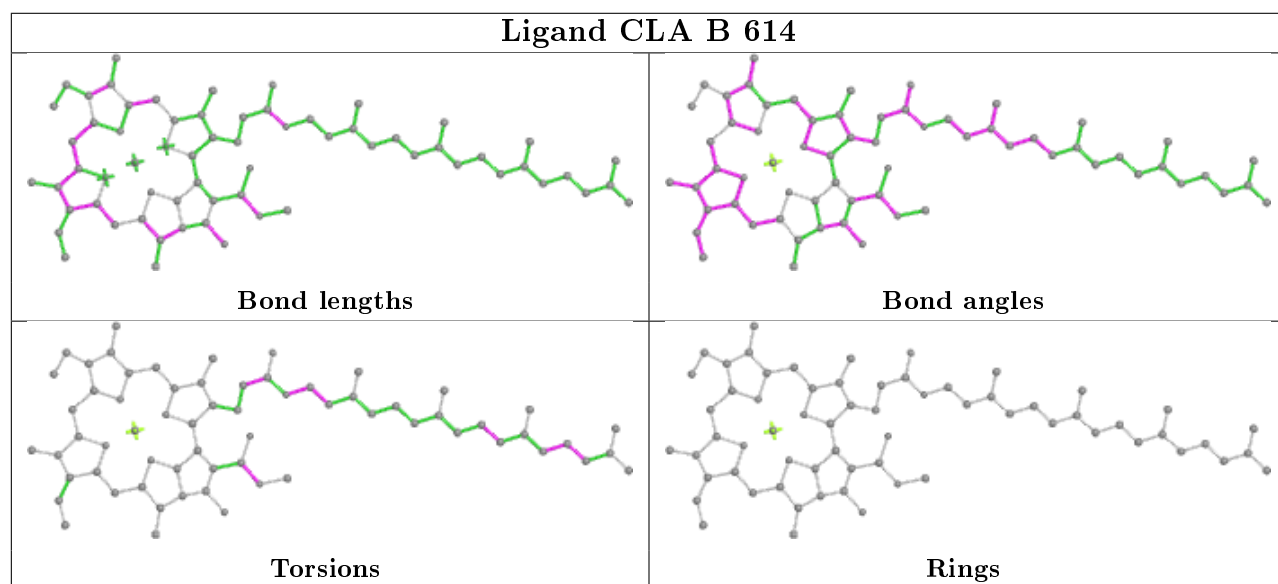
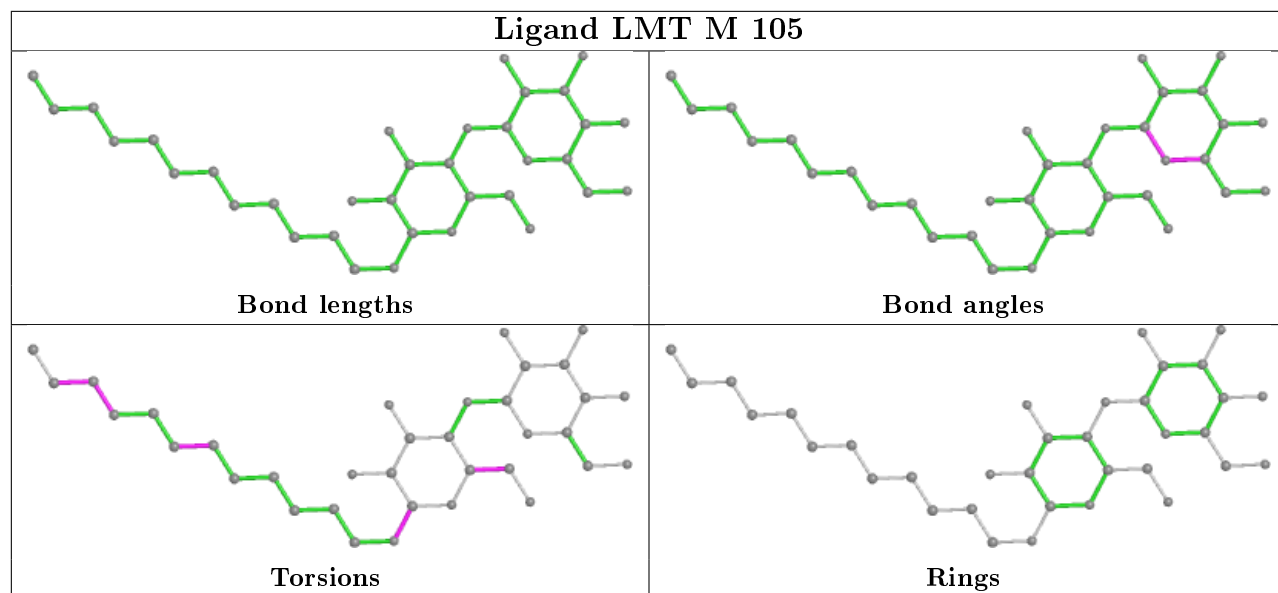


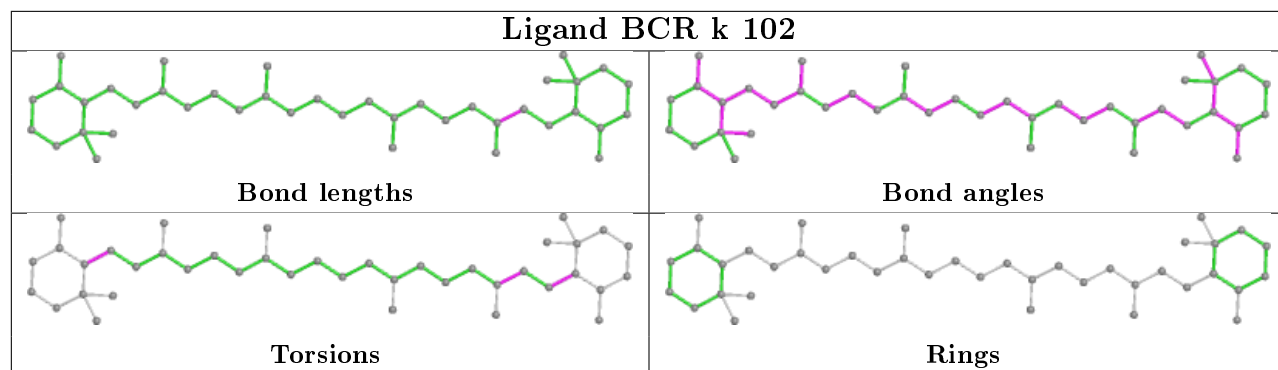
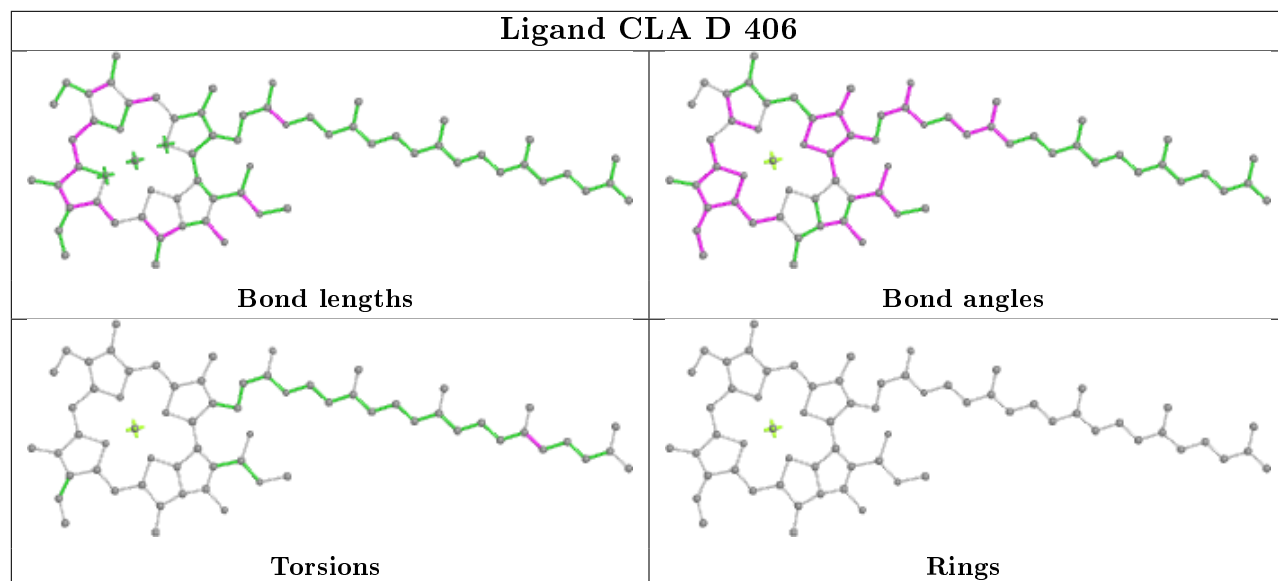
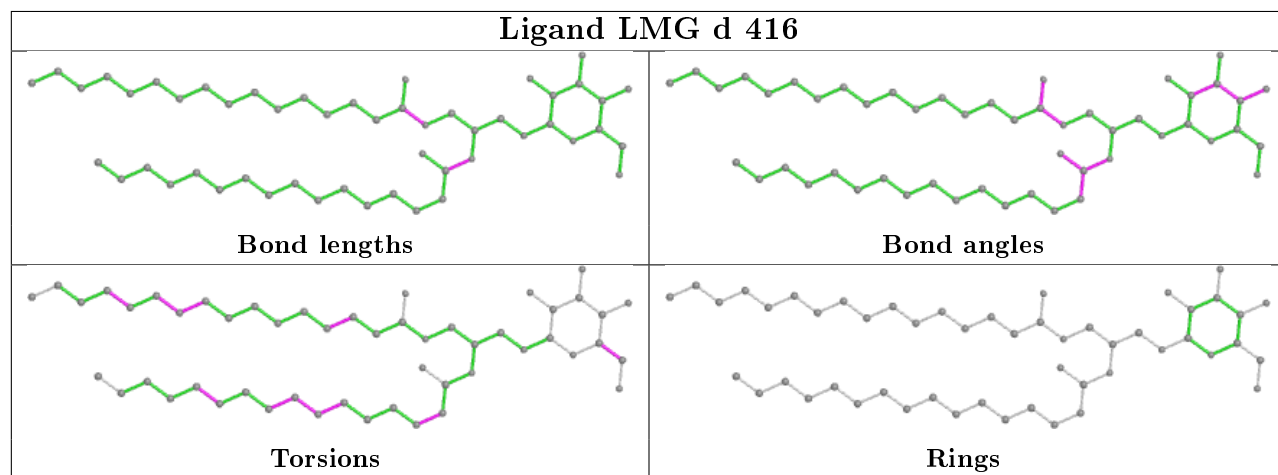
Ligand HTG B 623

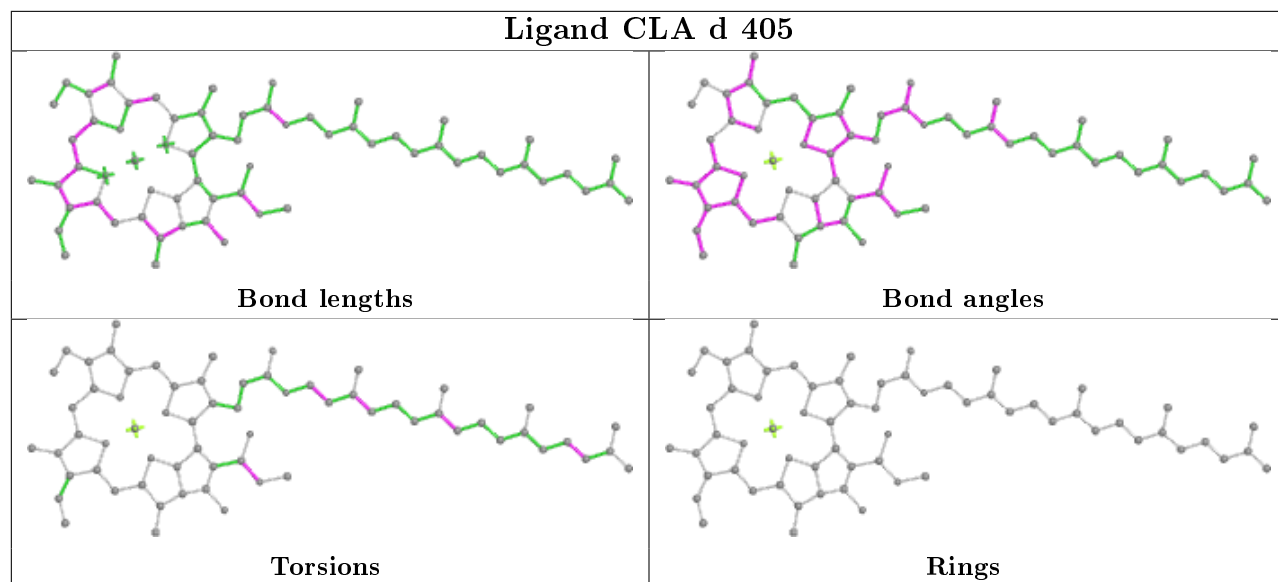
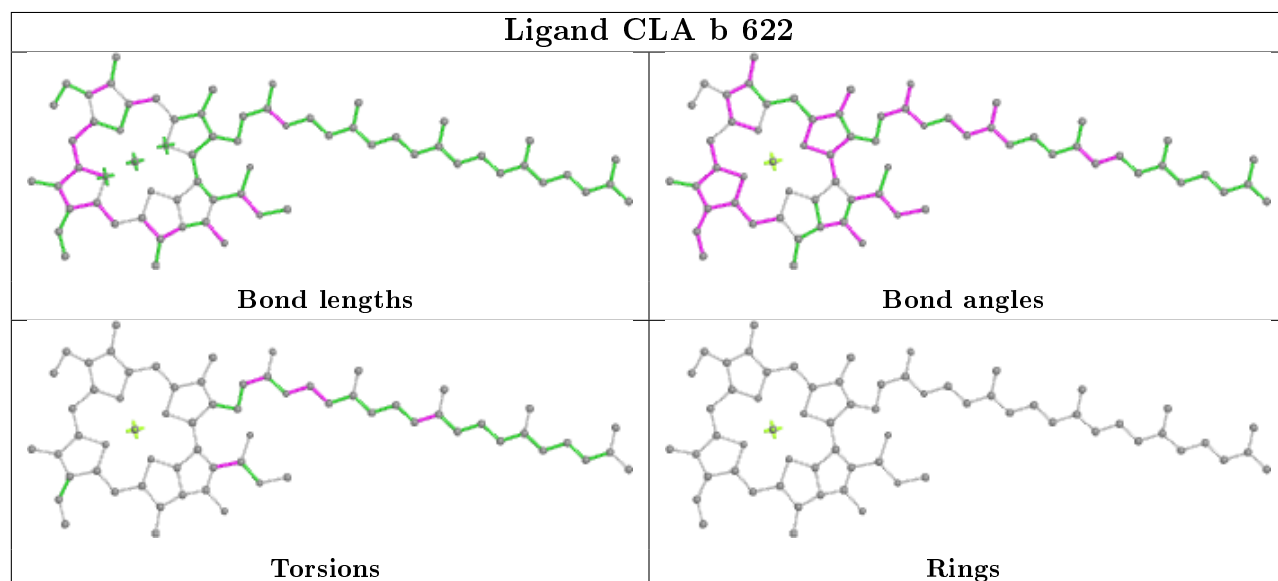
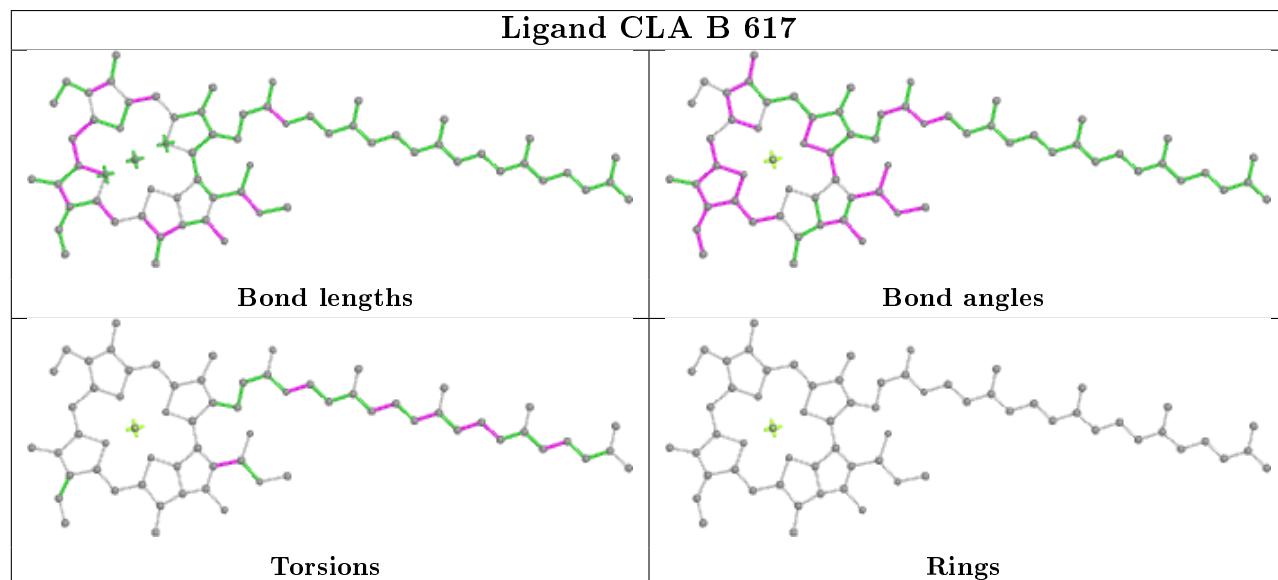


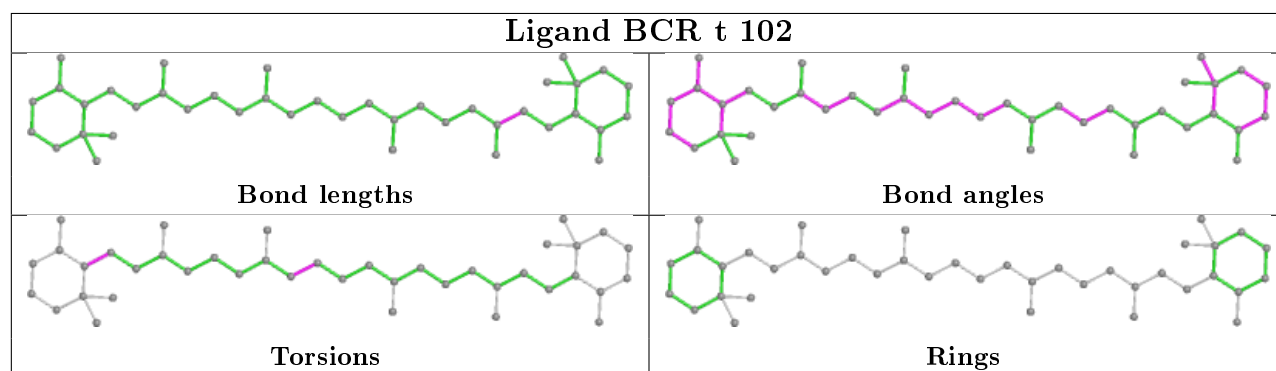
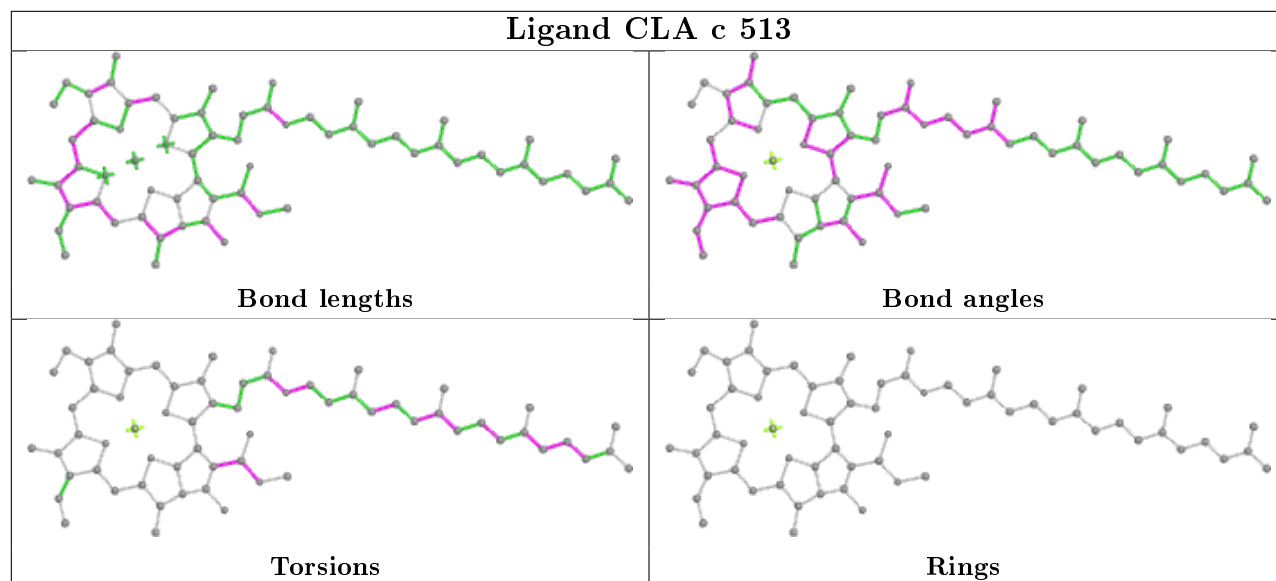
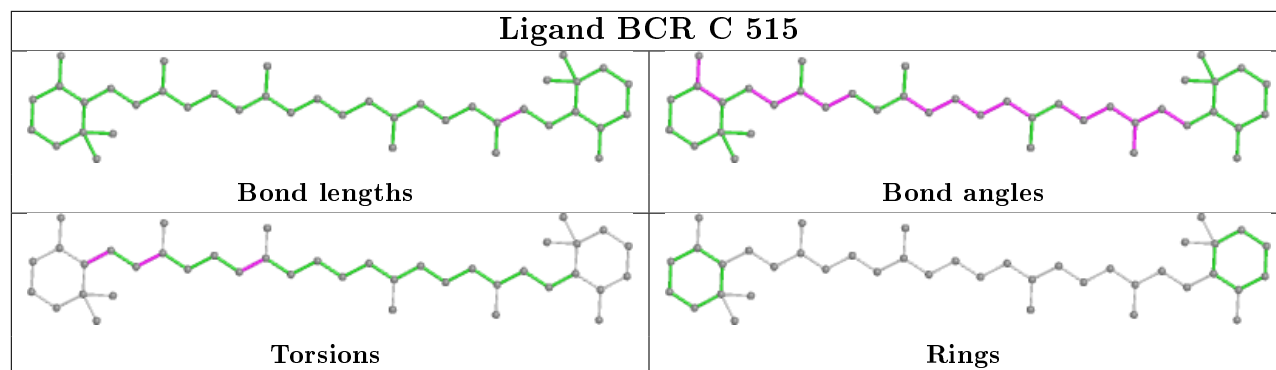
Ligand CLA c 510

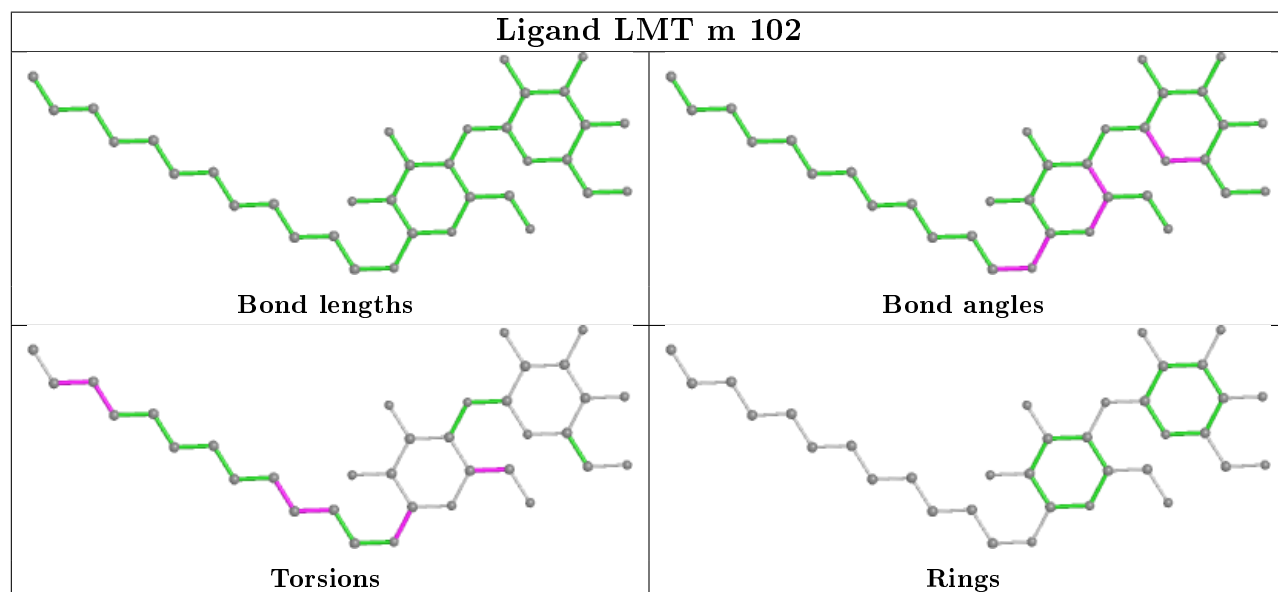
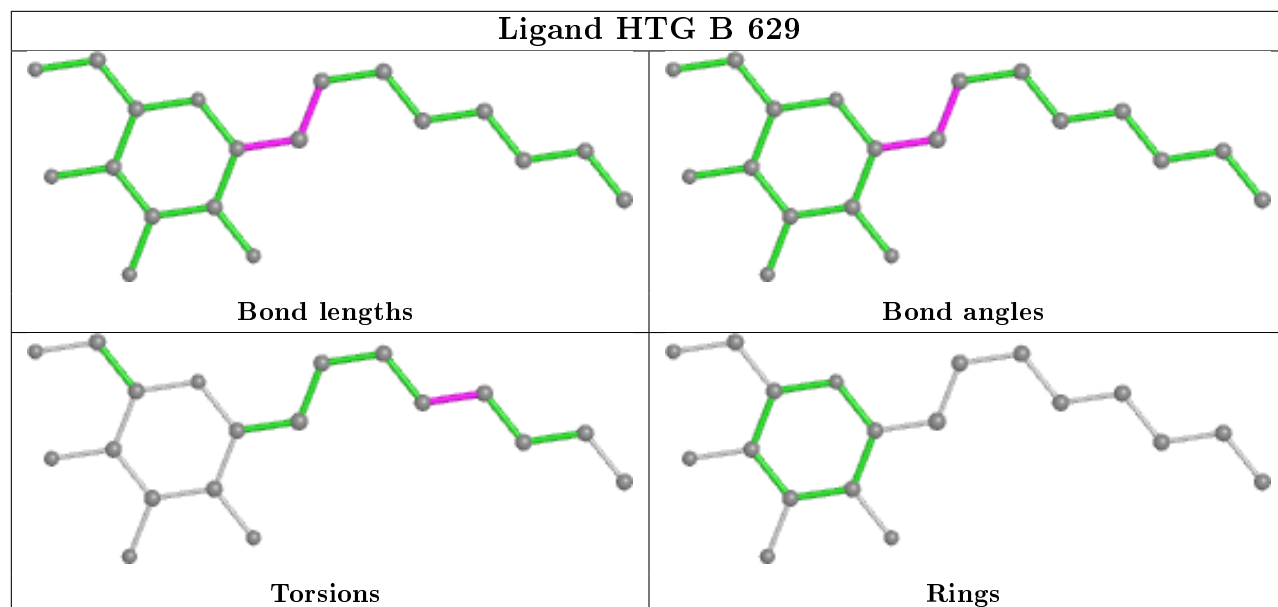


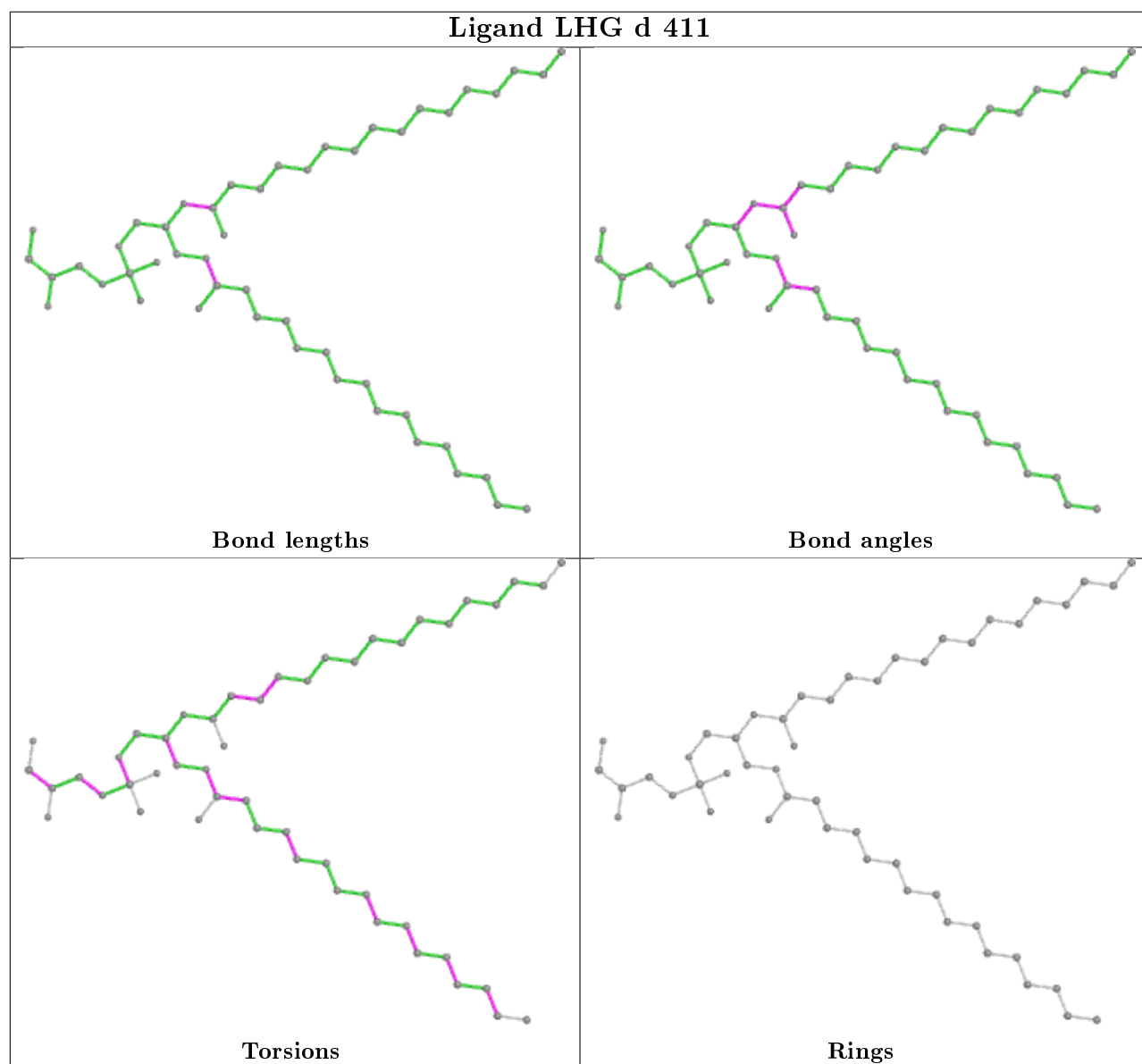
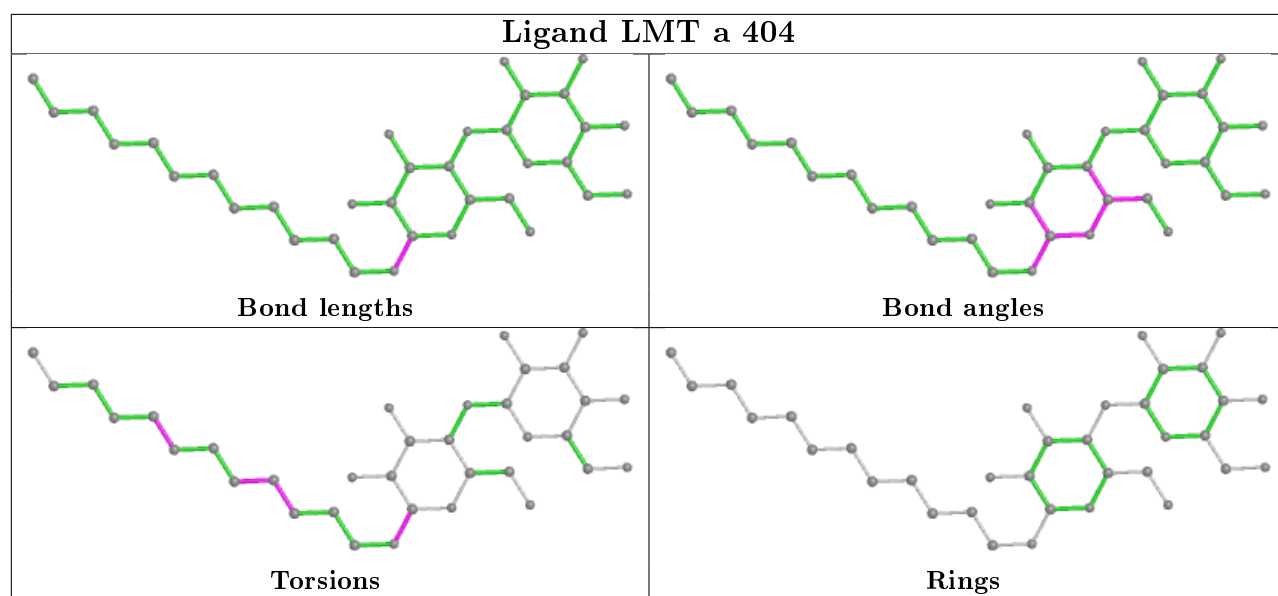


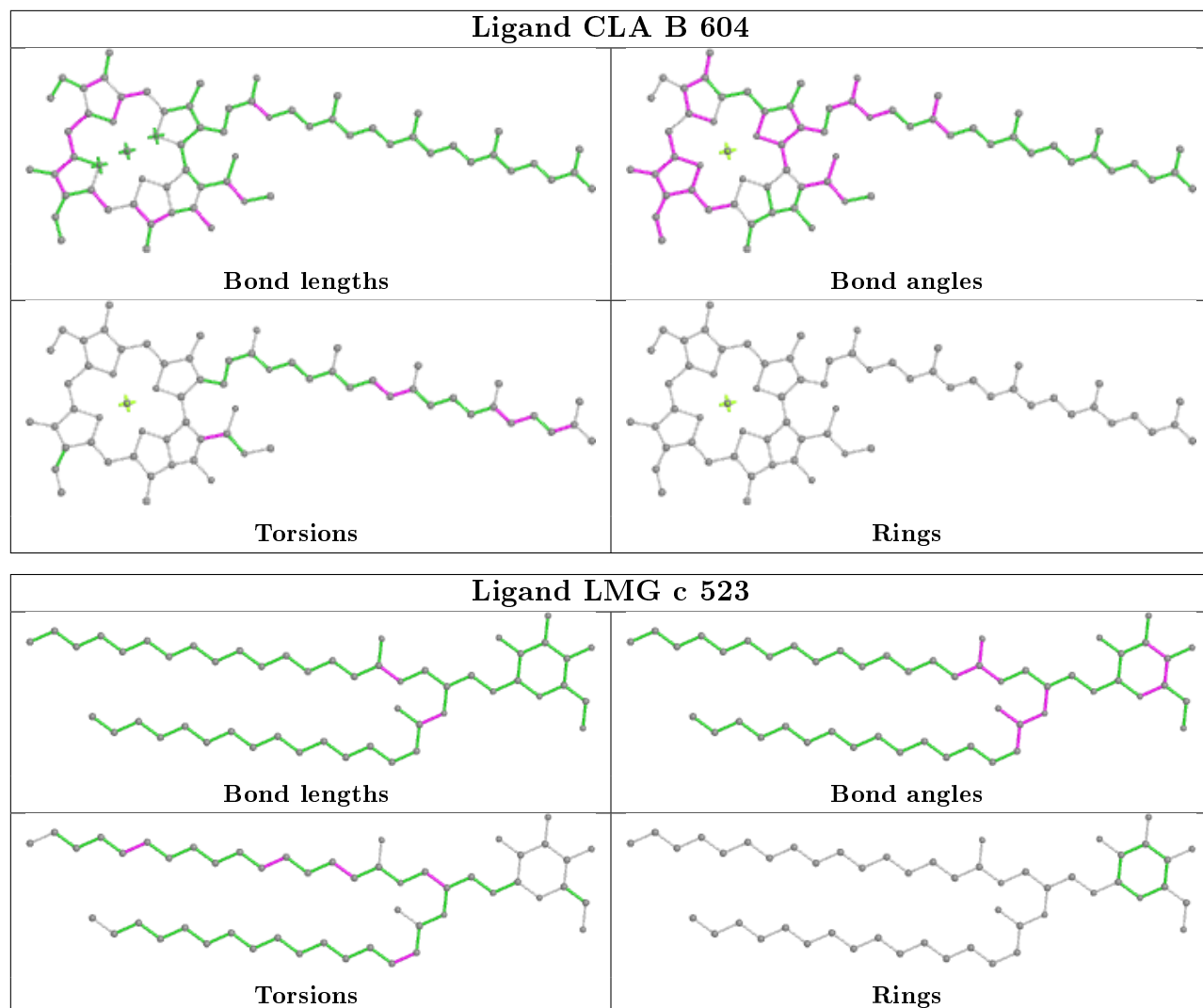
Ligand BCR k 102**Ligand CLA D 406****Ligand LMG d 416**

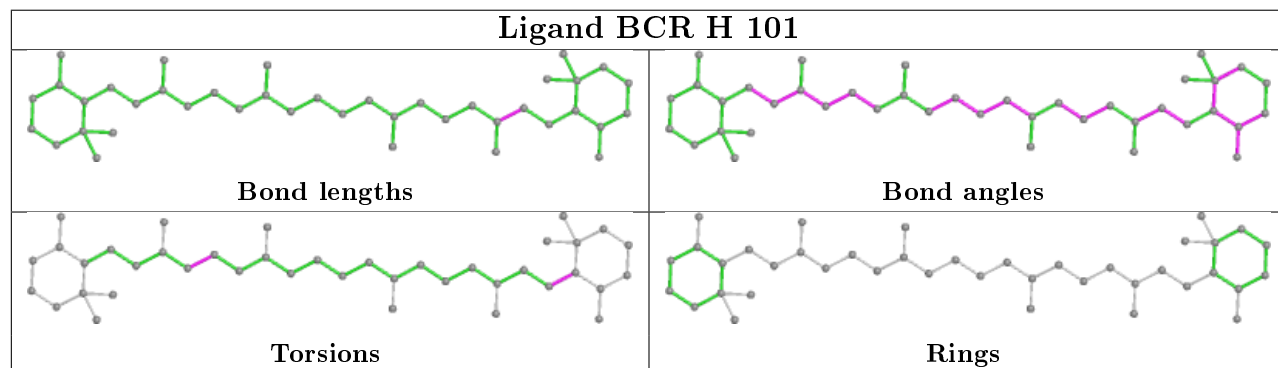
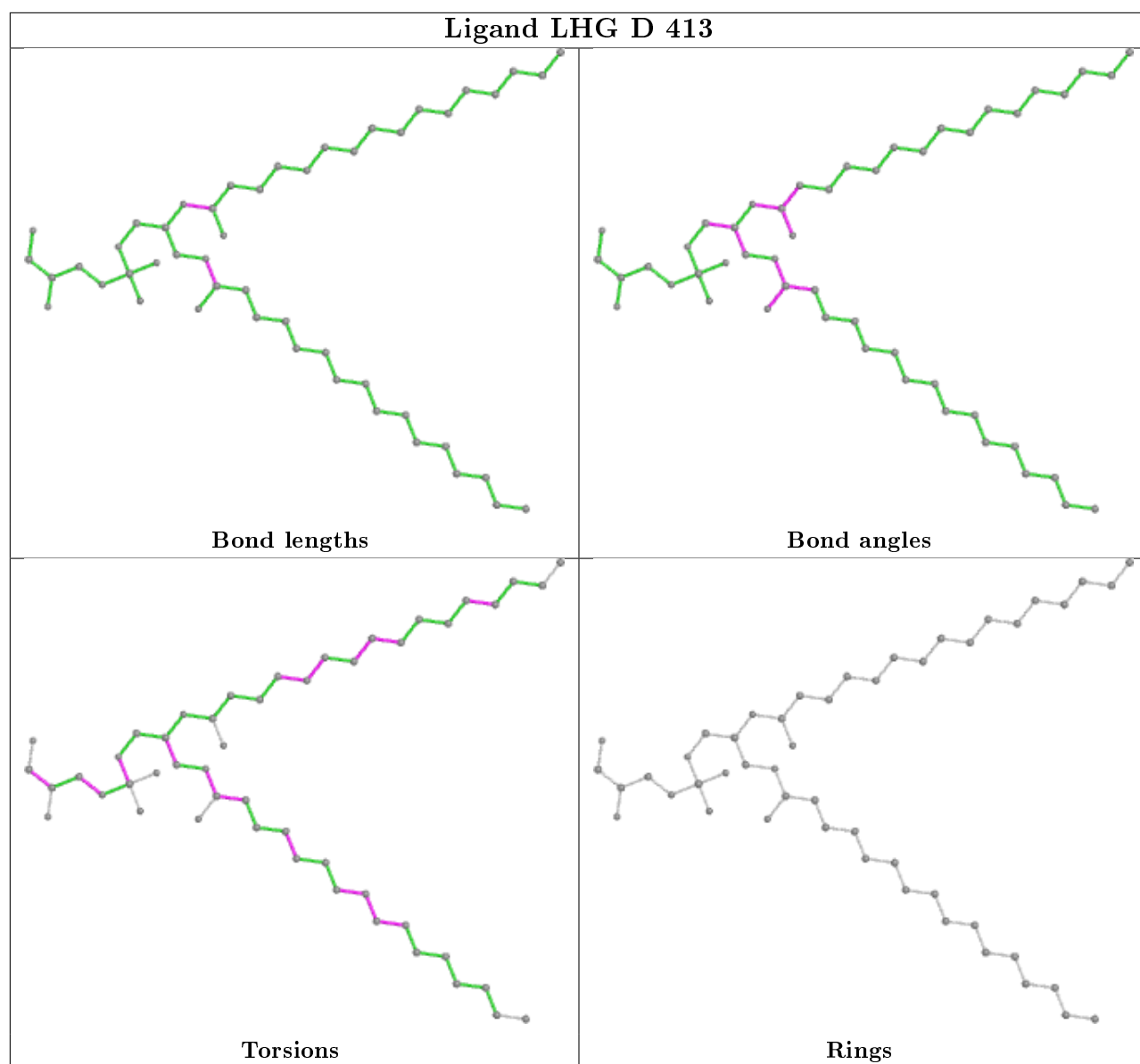
Ligand CLA d 405**Ligand CLA b 622****Ligand CLA B 617**

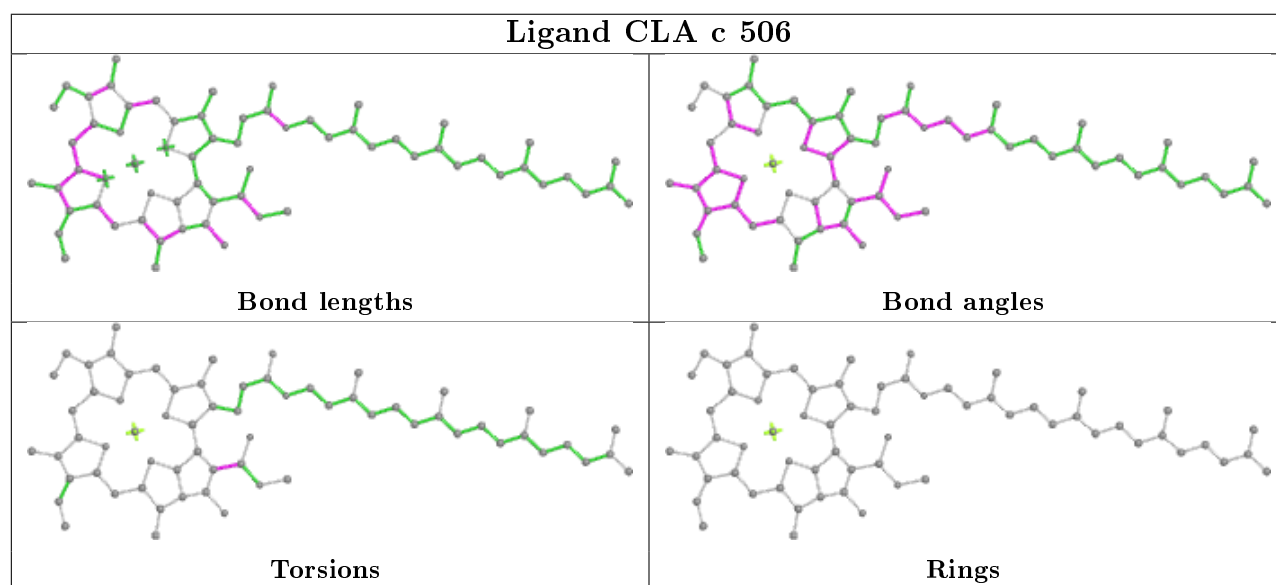
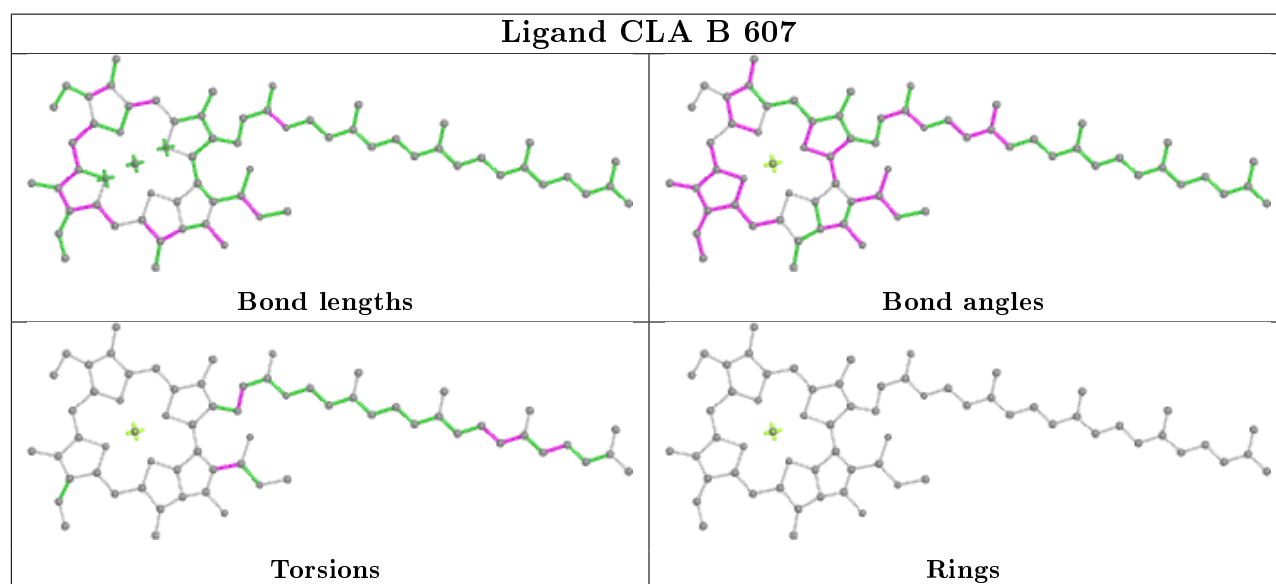
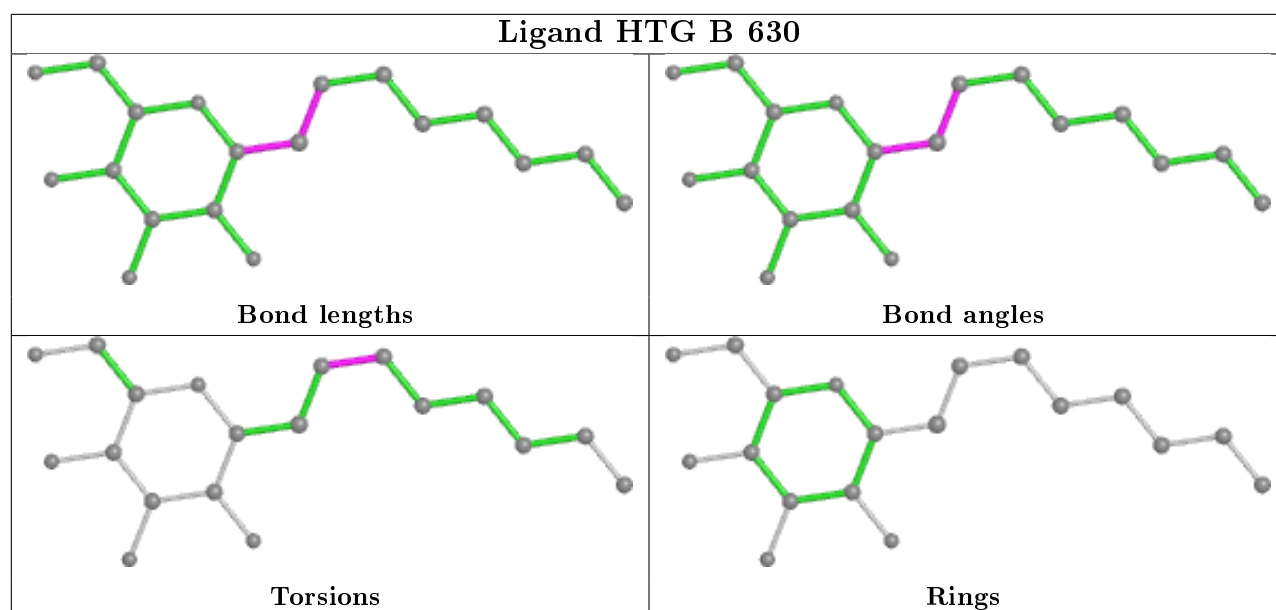


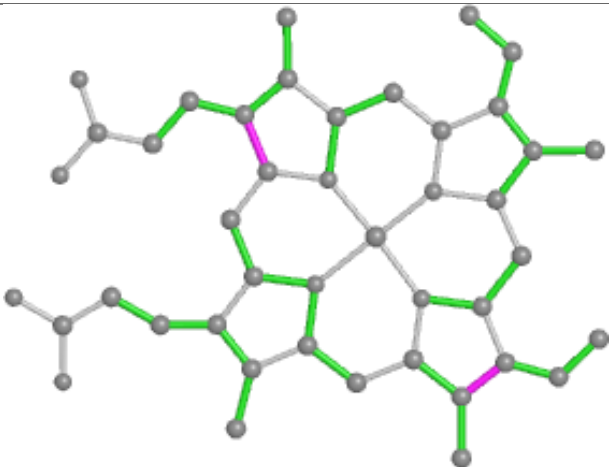
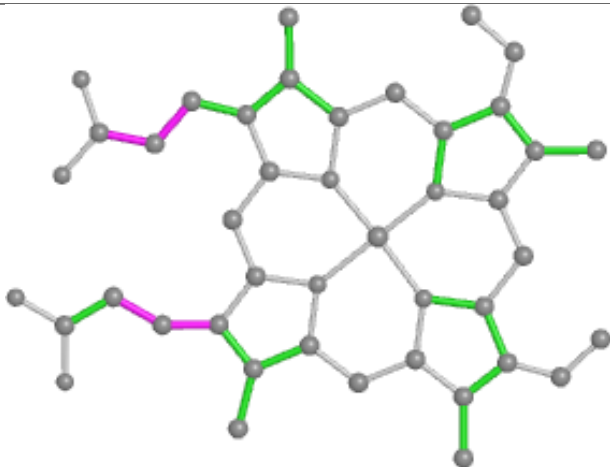
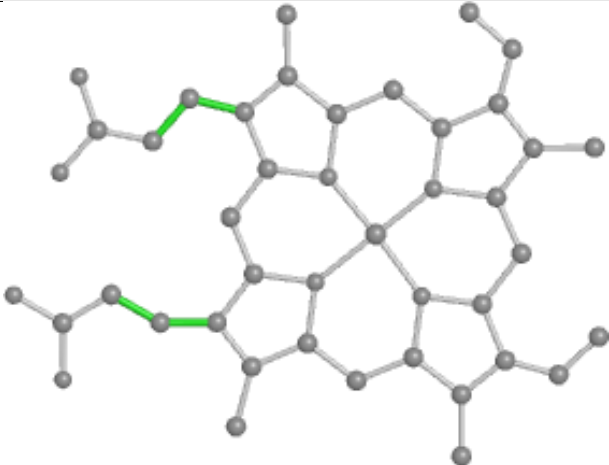
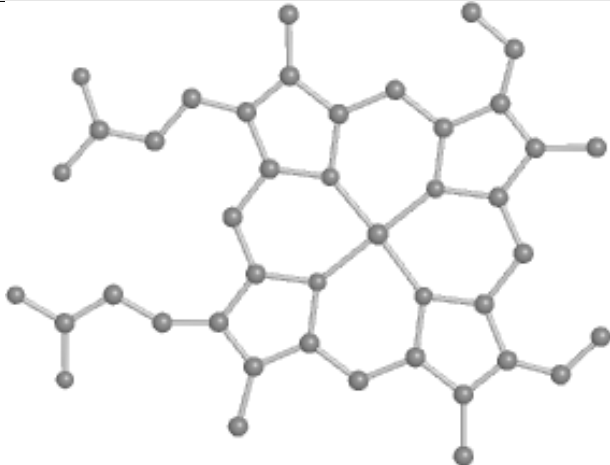


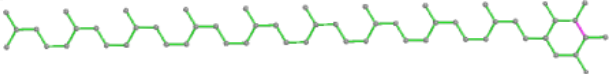
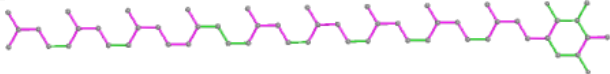
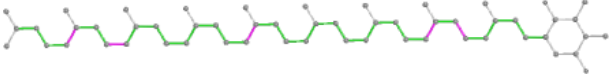
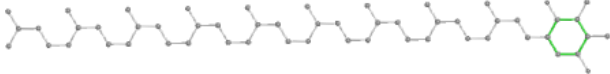


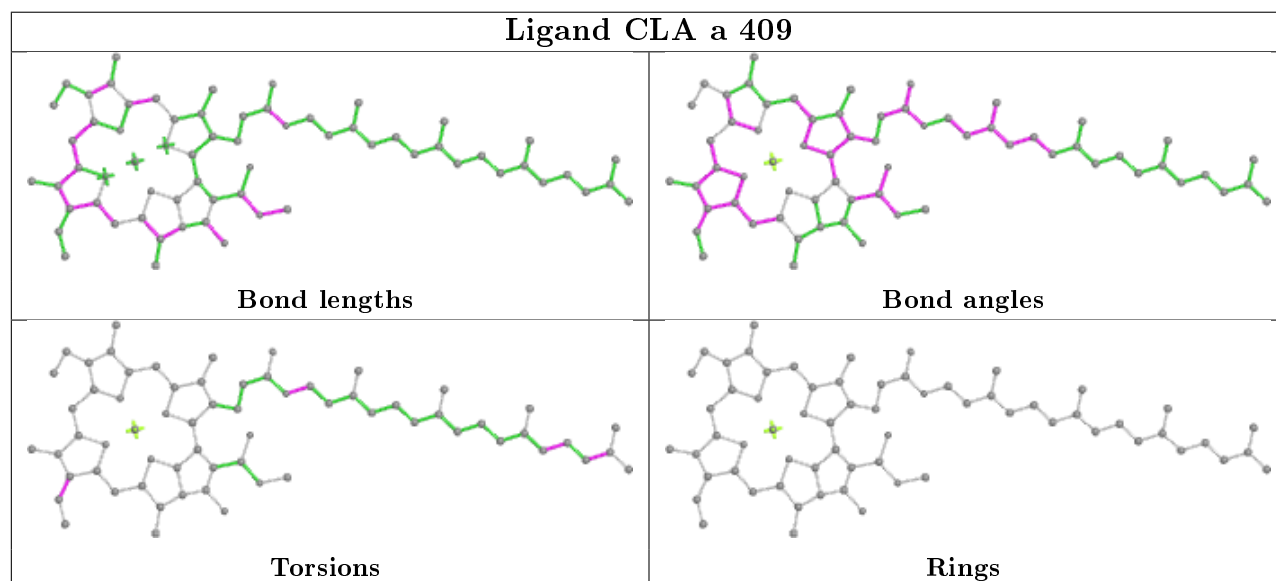
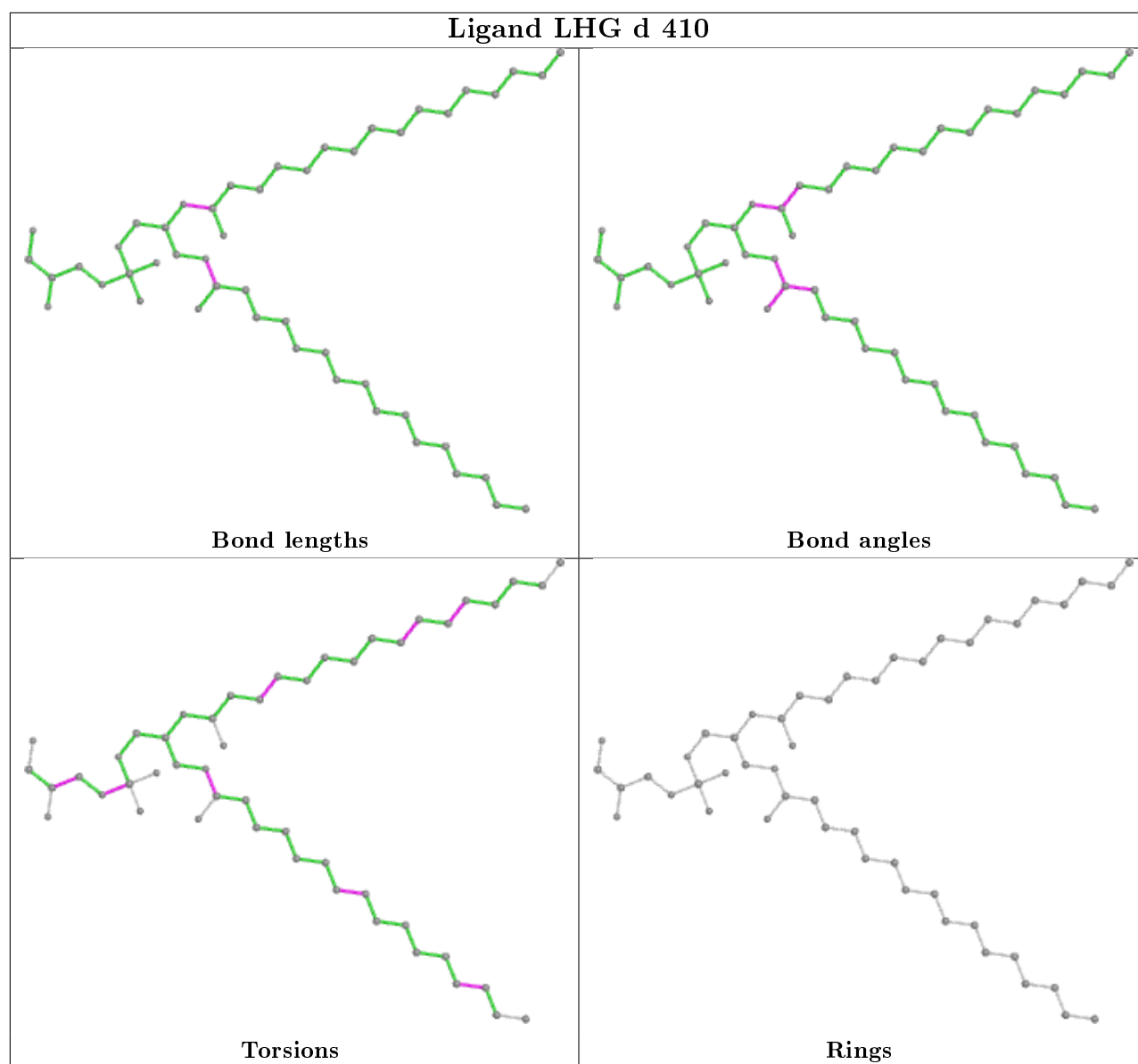


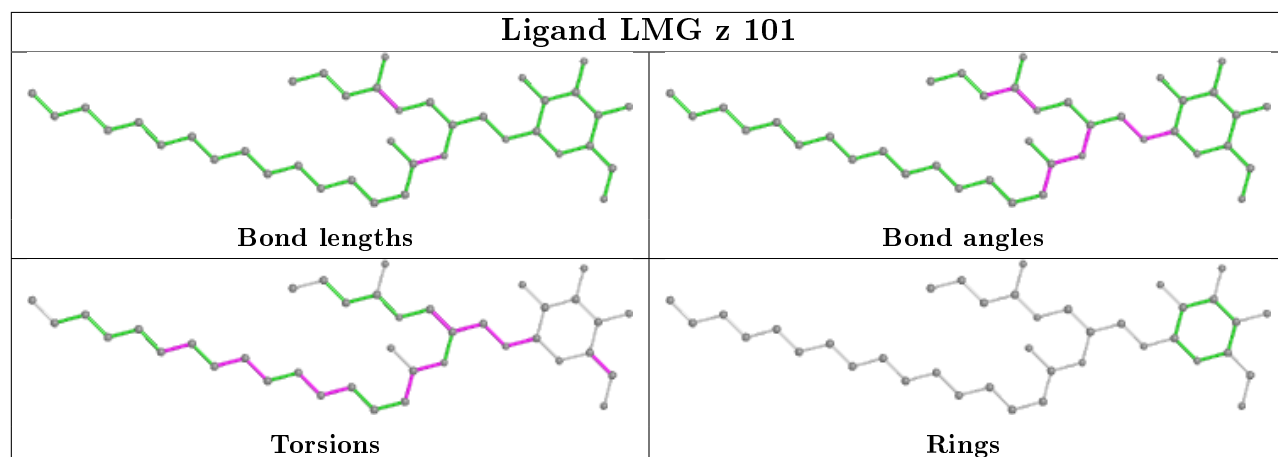
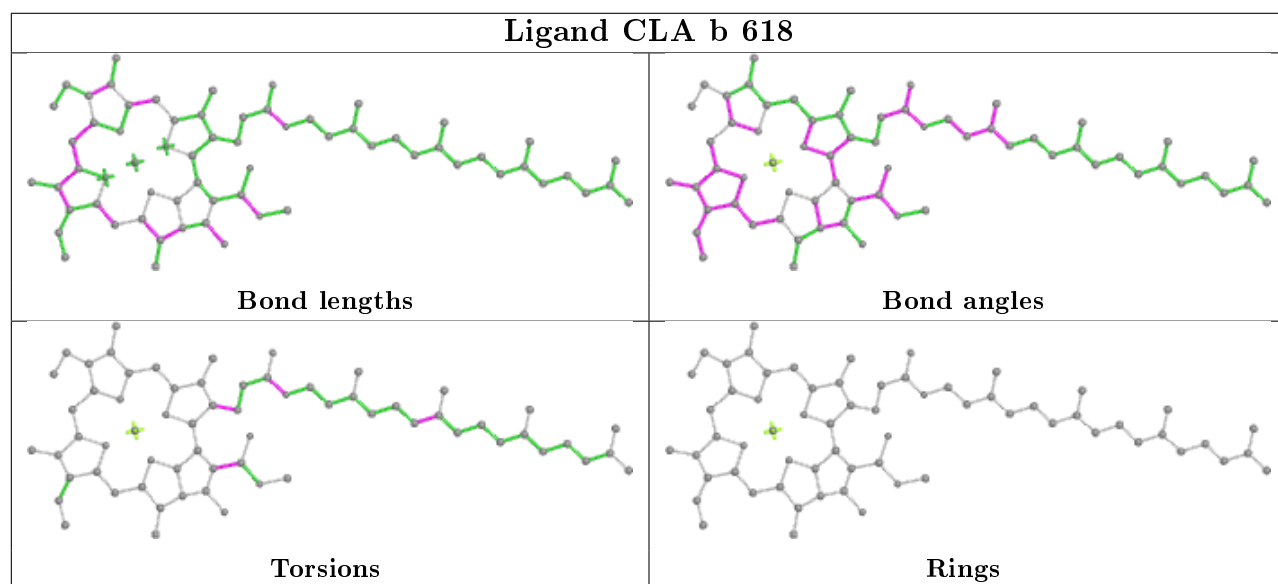
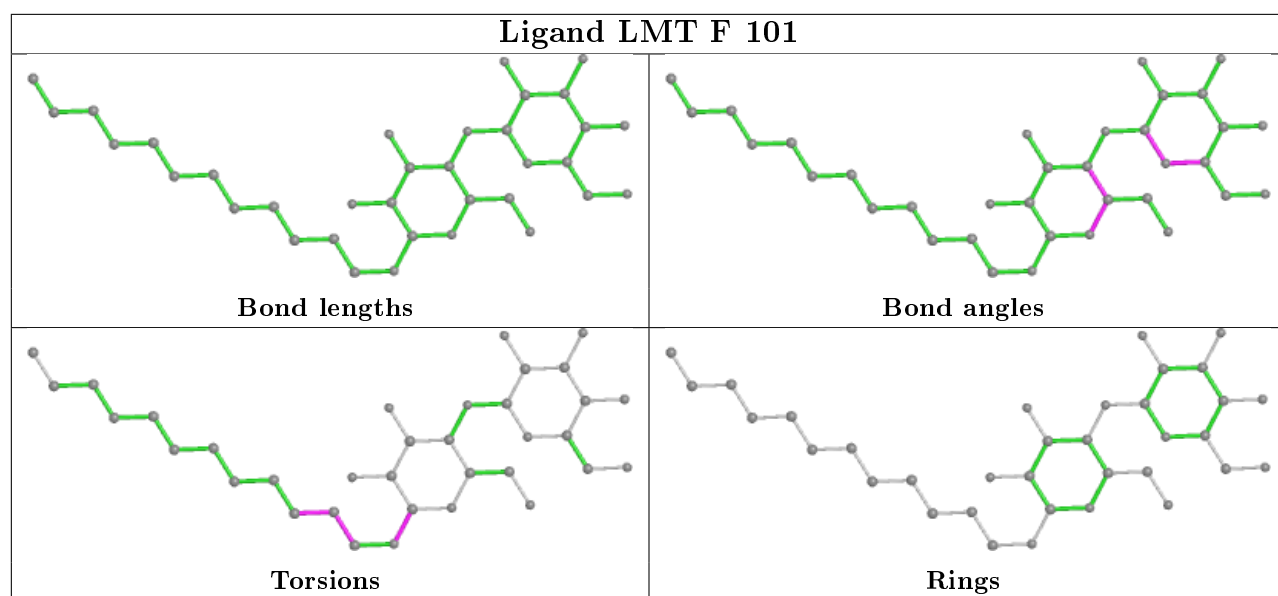




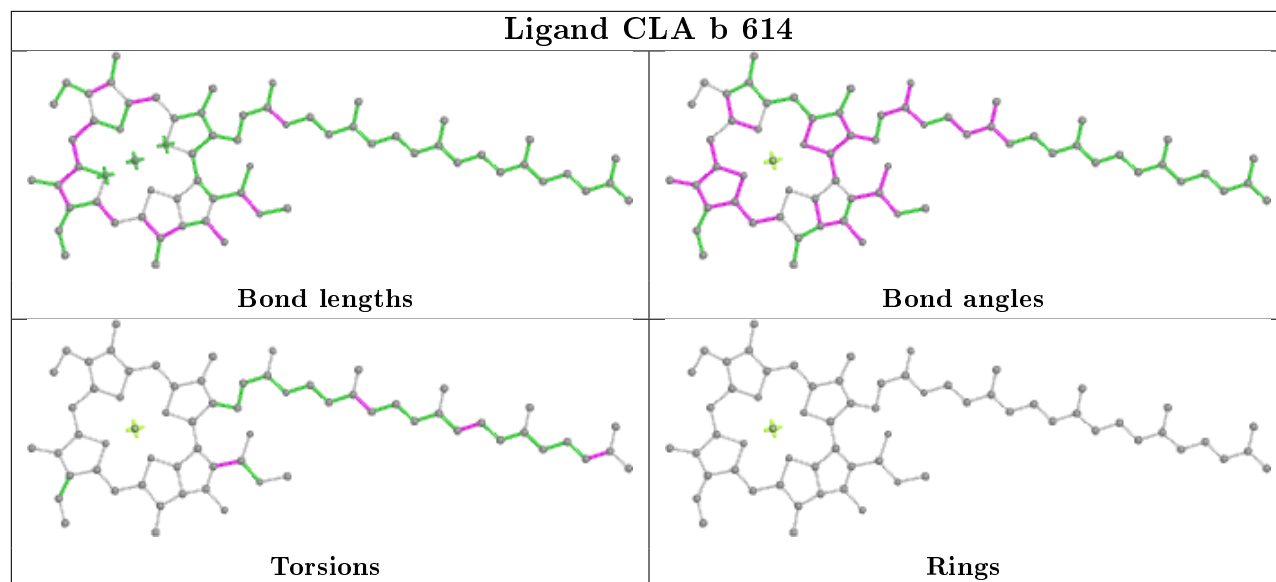
Ligand HEM v 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

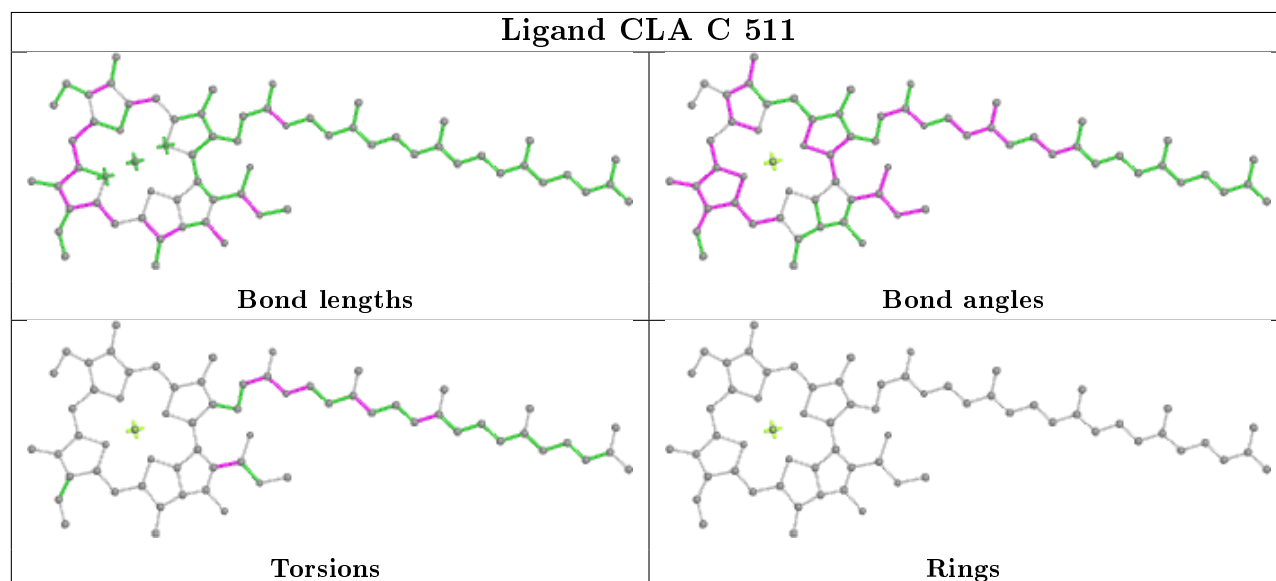




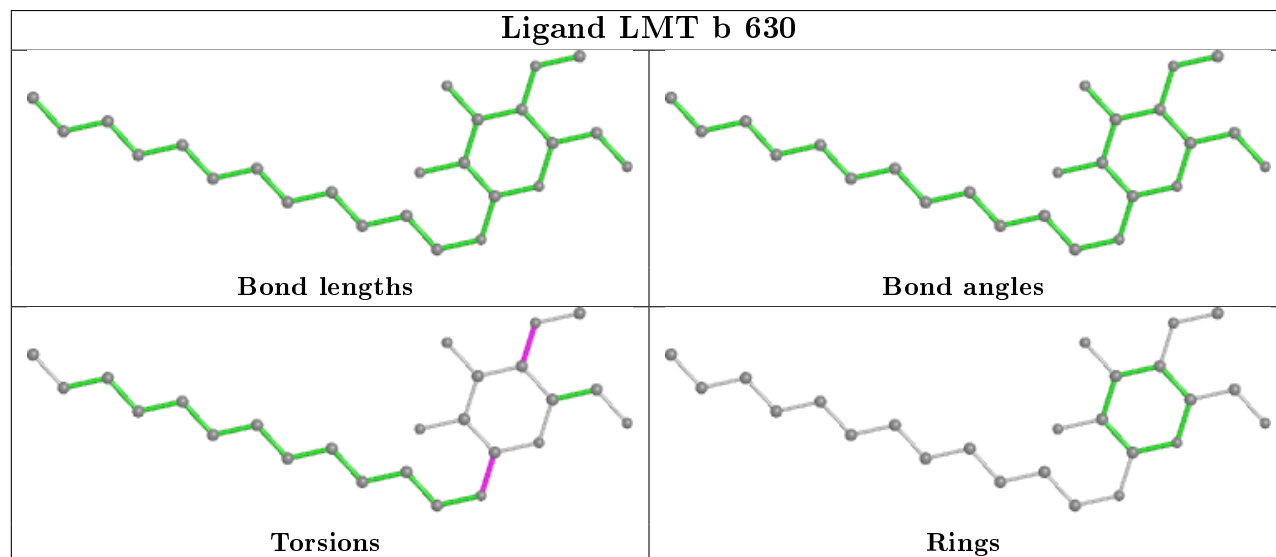
Ligand CLA b 614

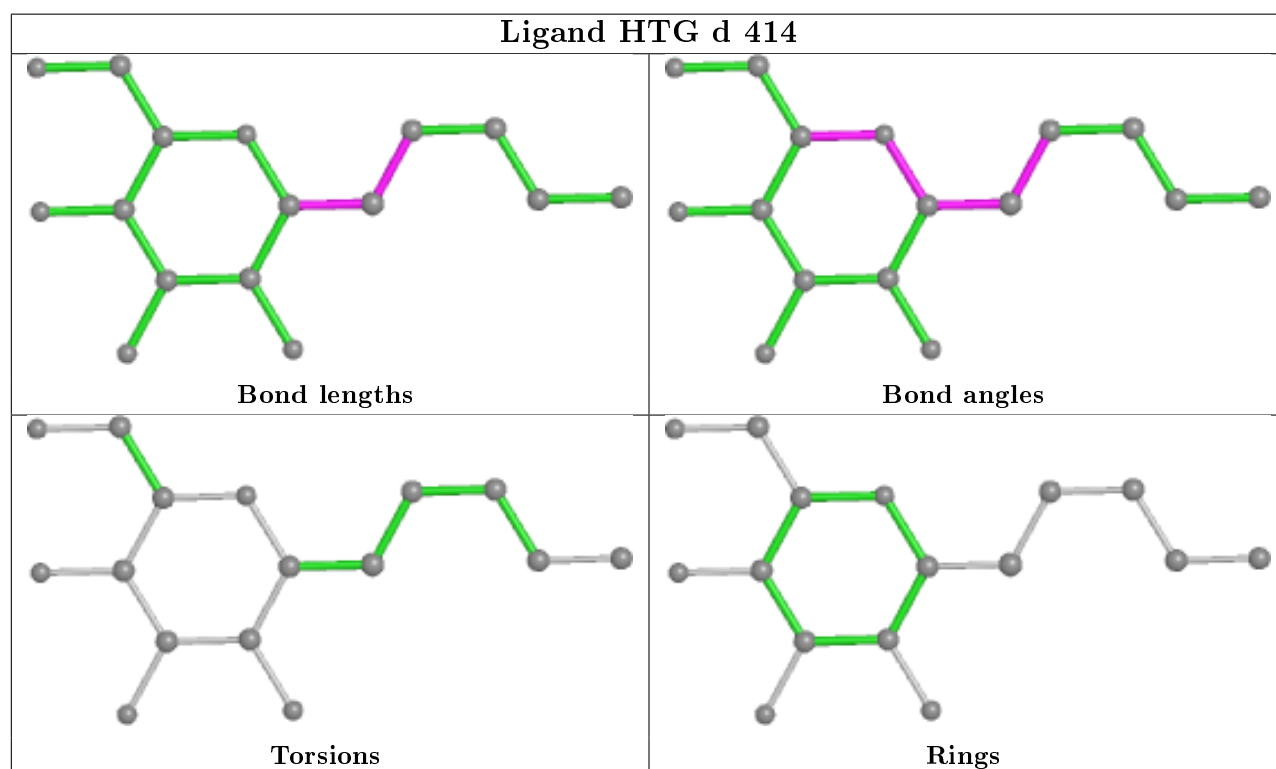
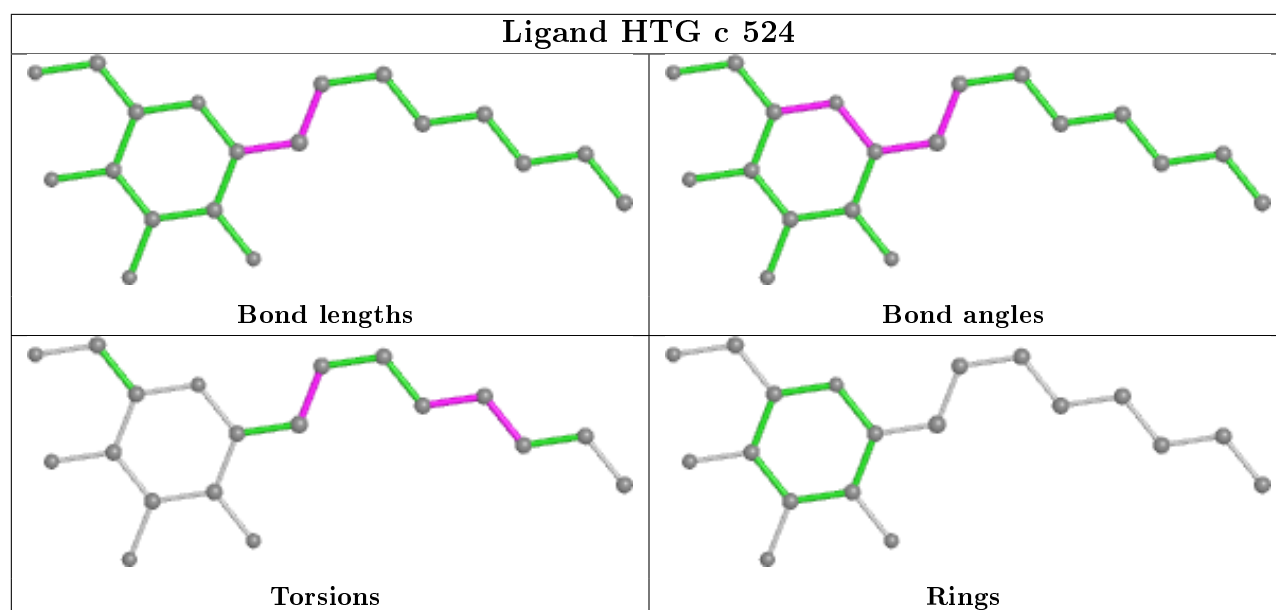


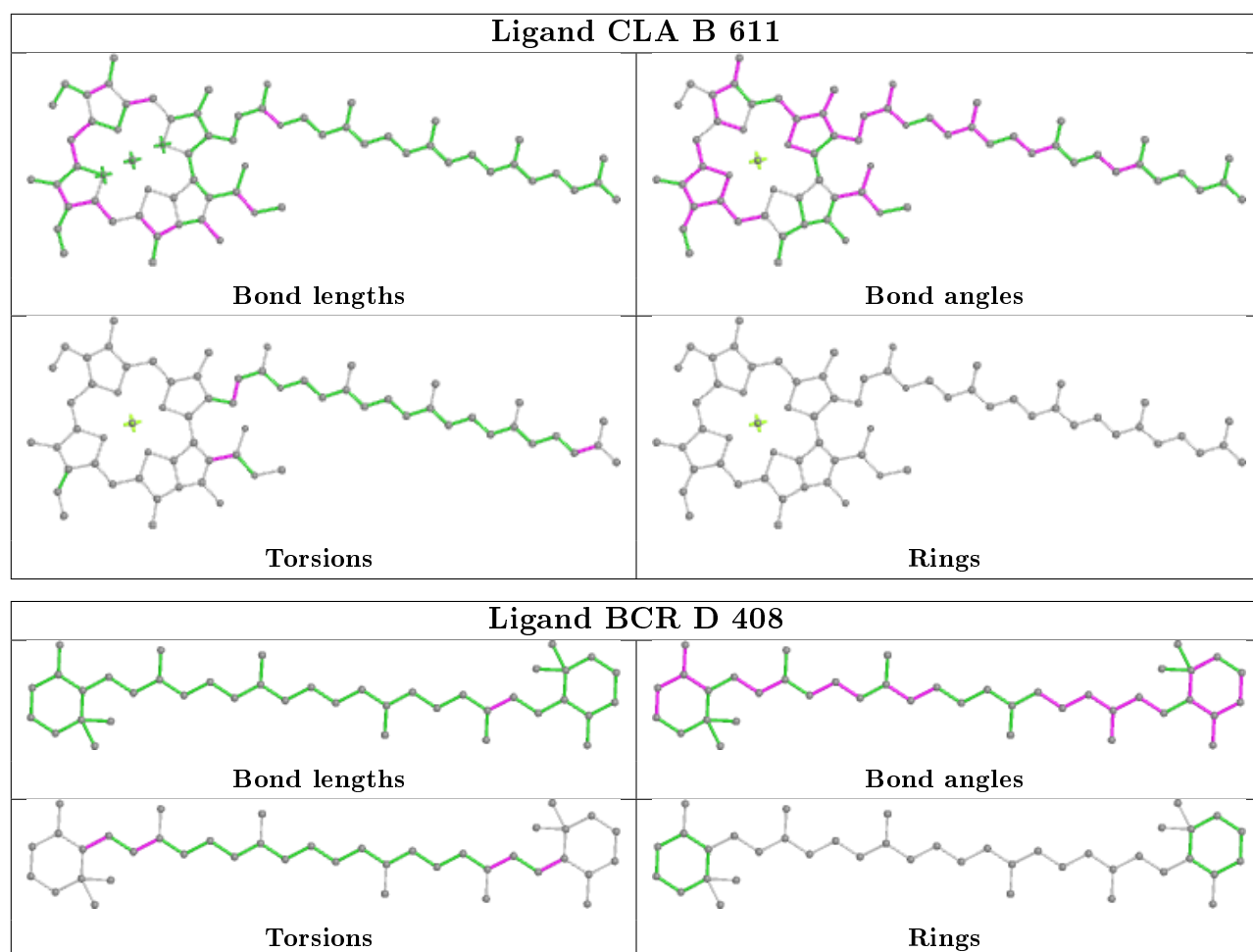
Ligand CLA C 511

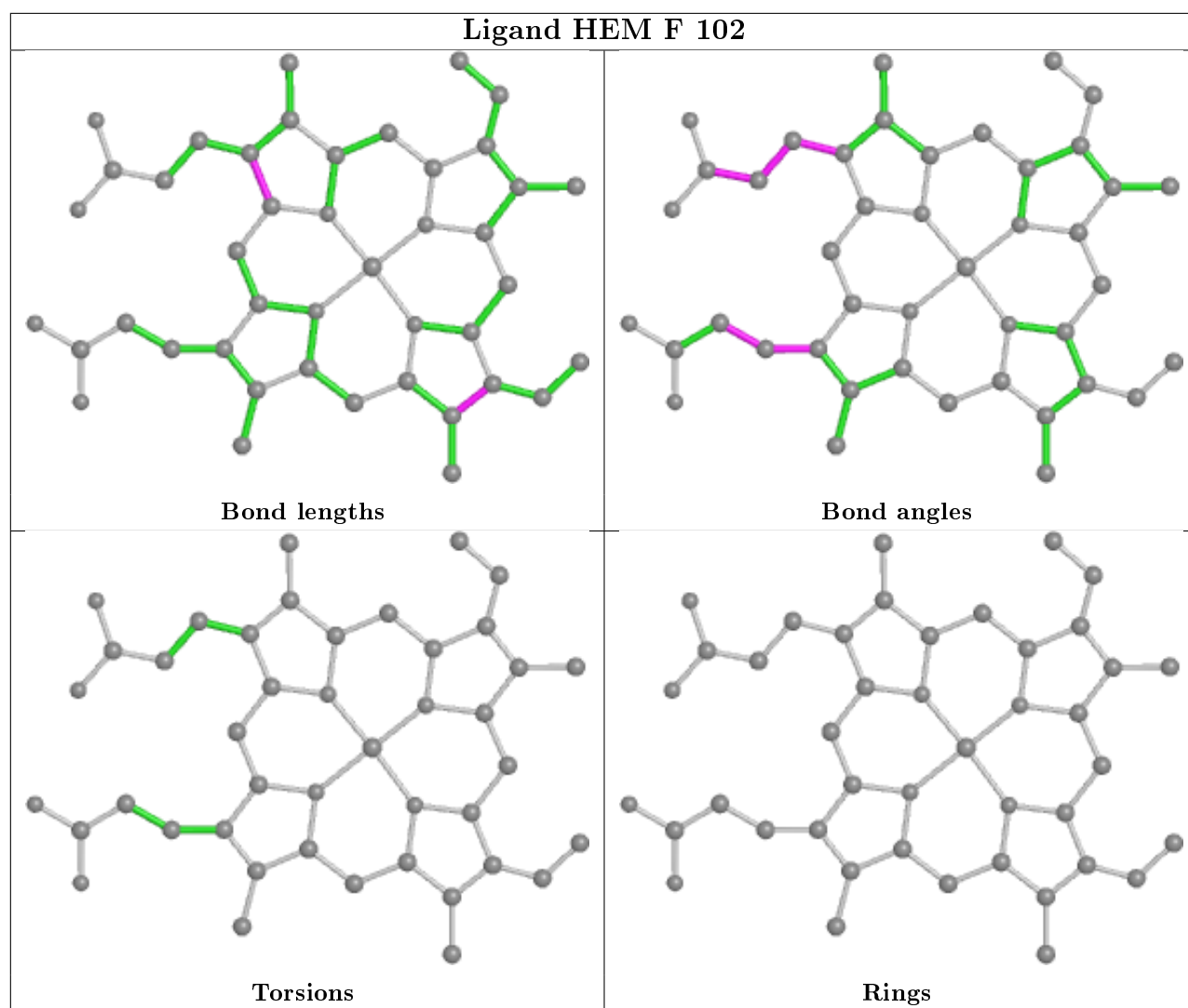


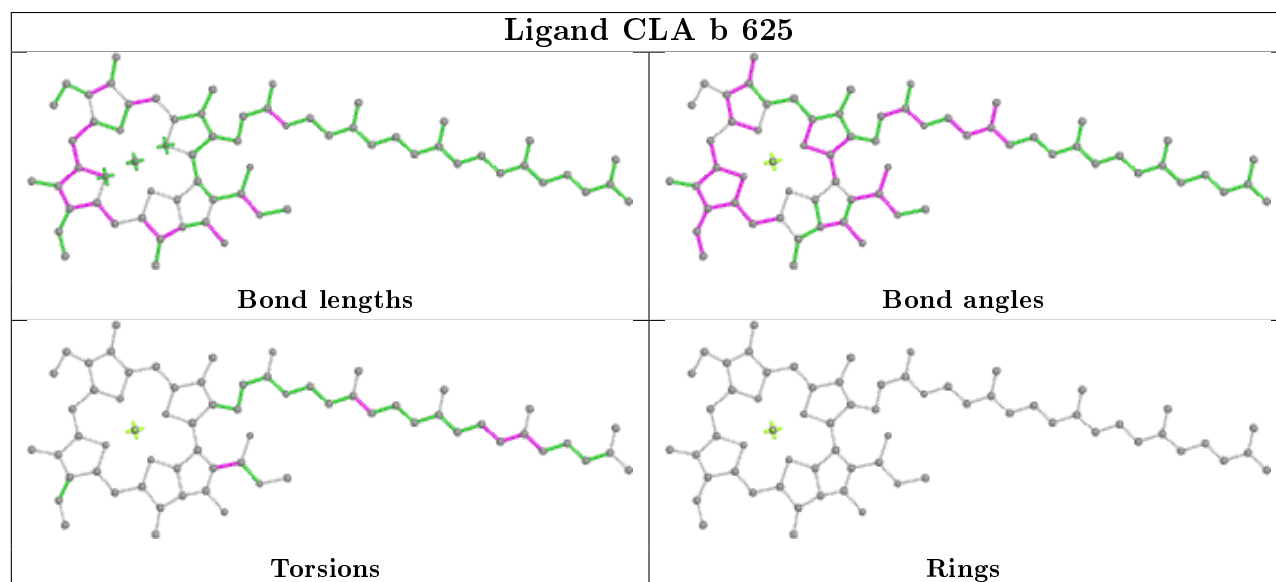
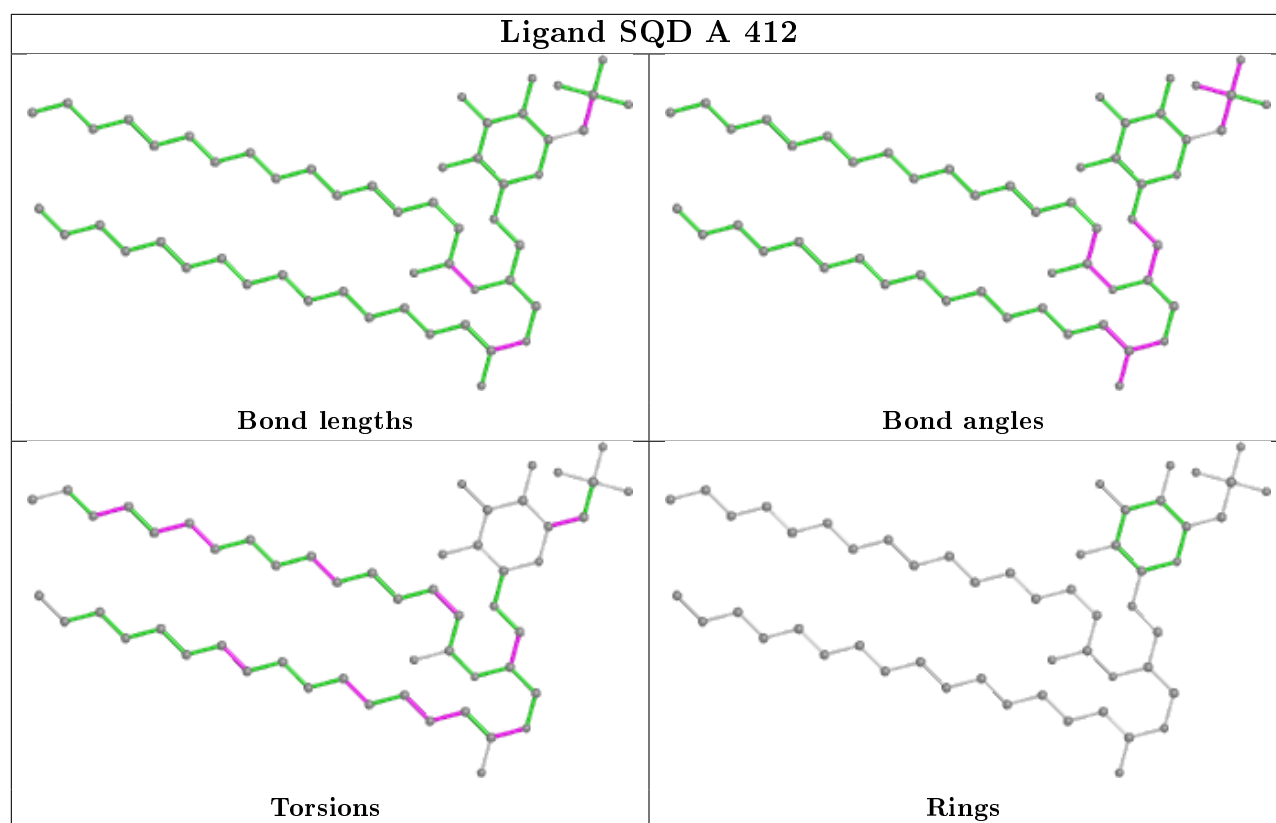
Ligand LMT b 630

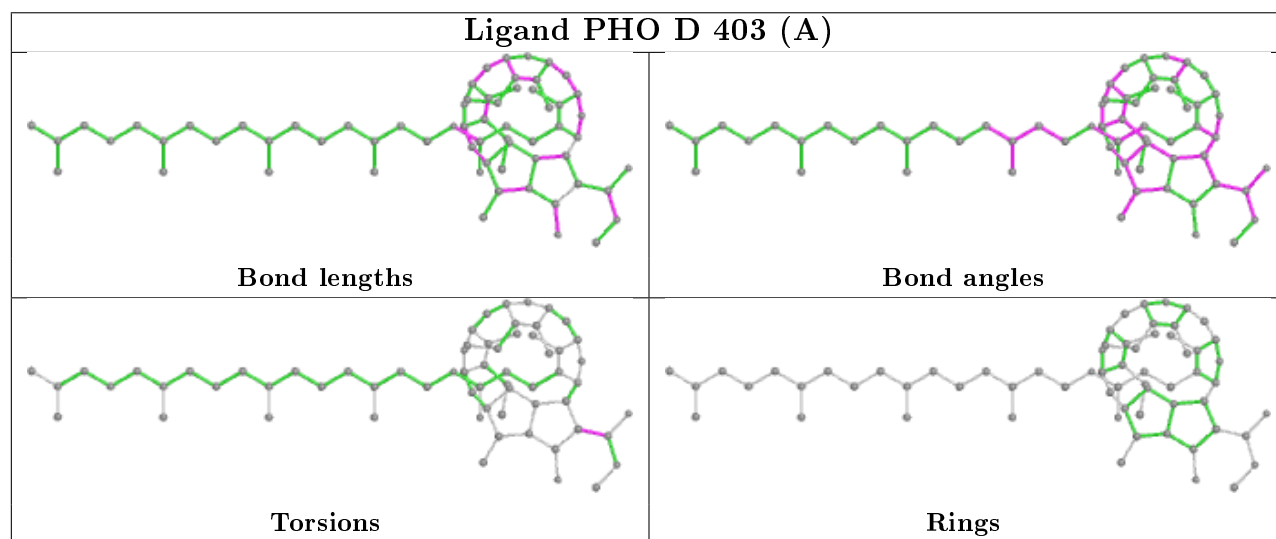
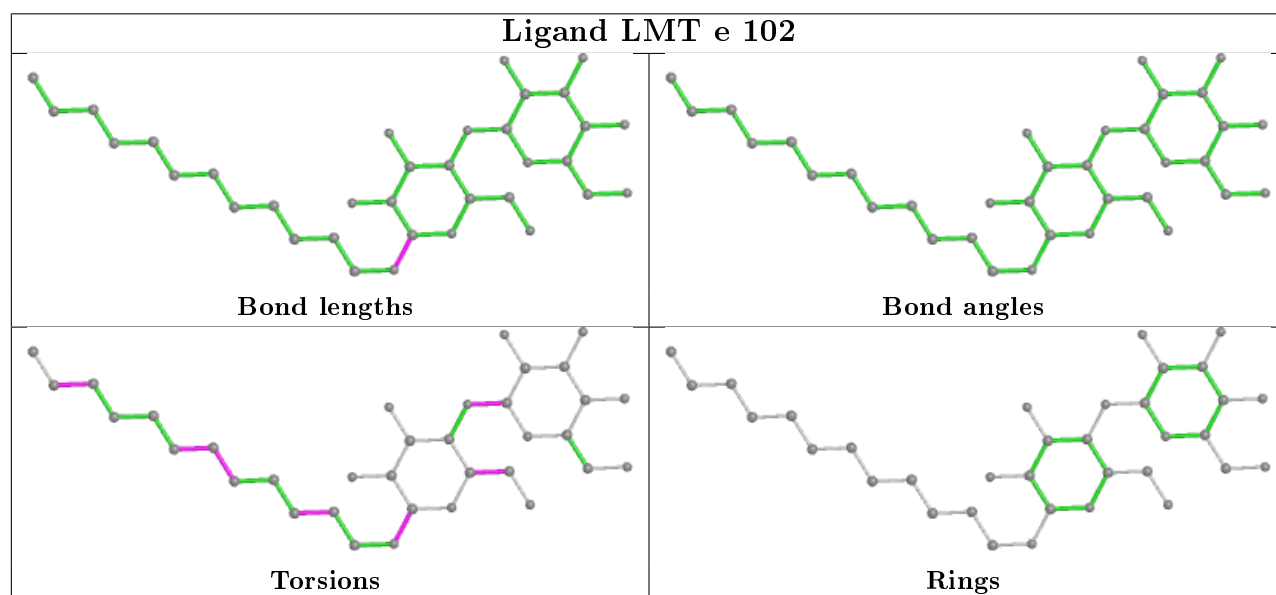
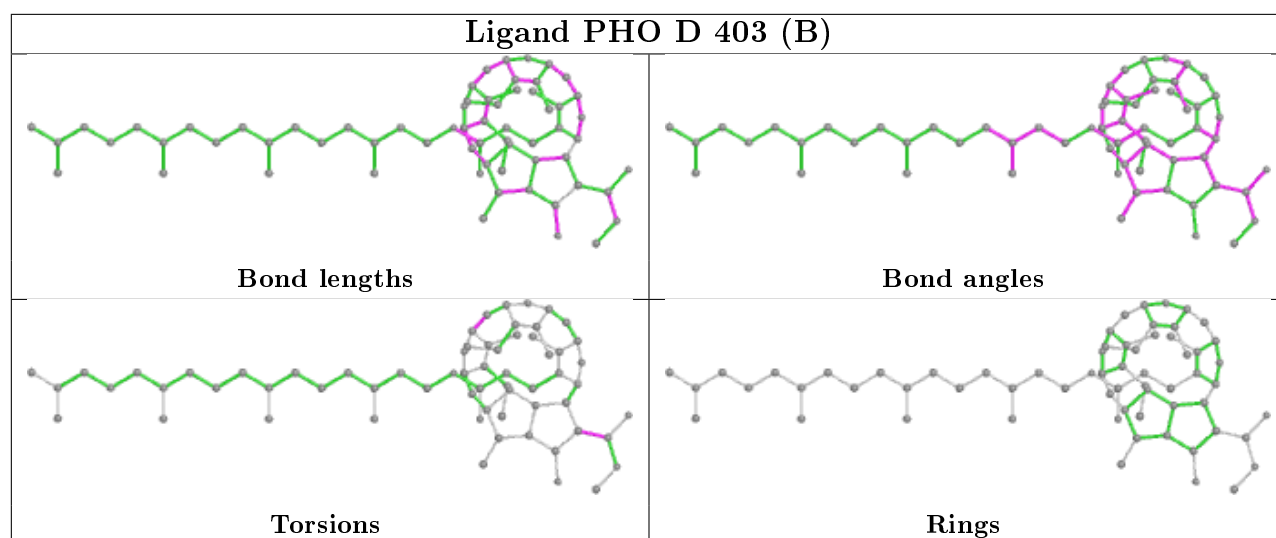


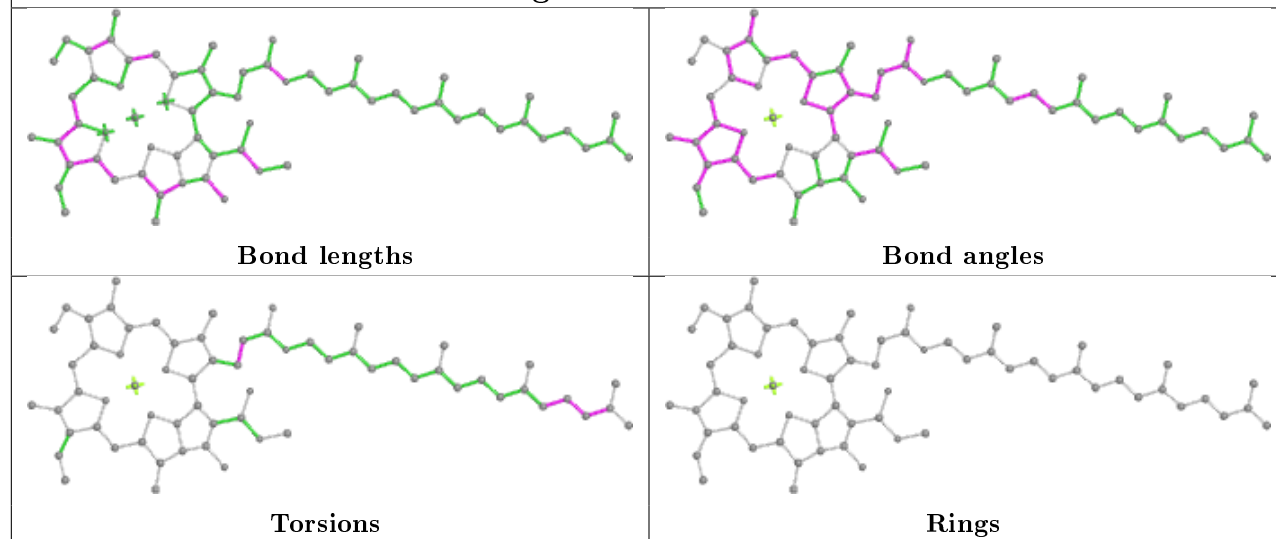
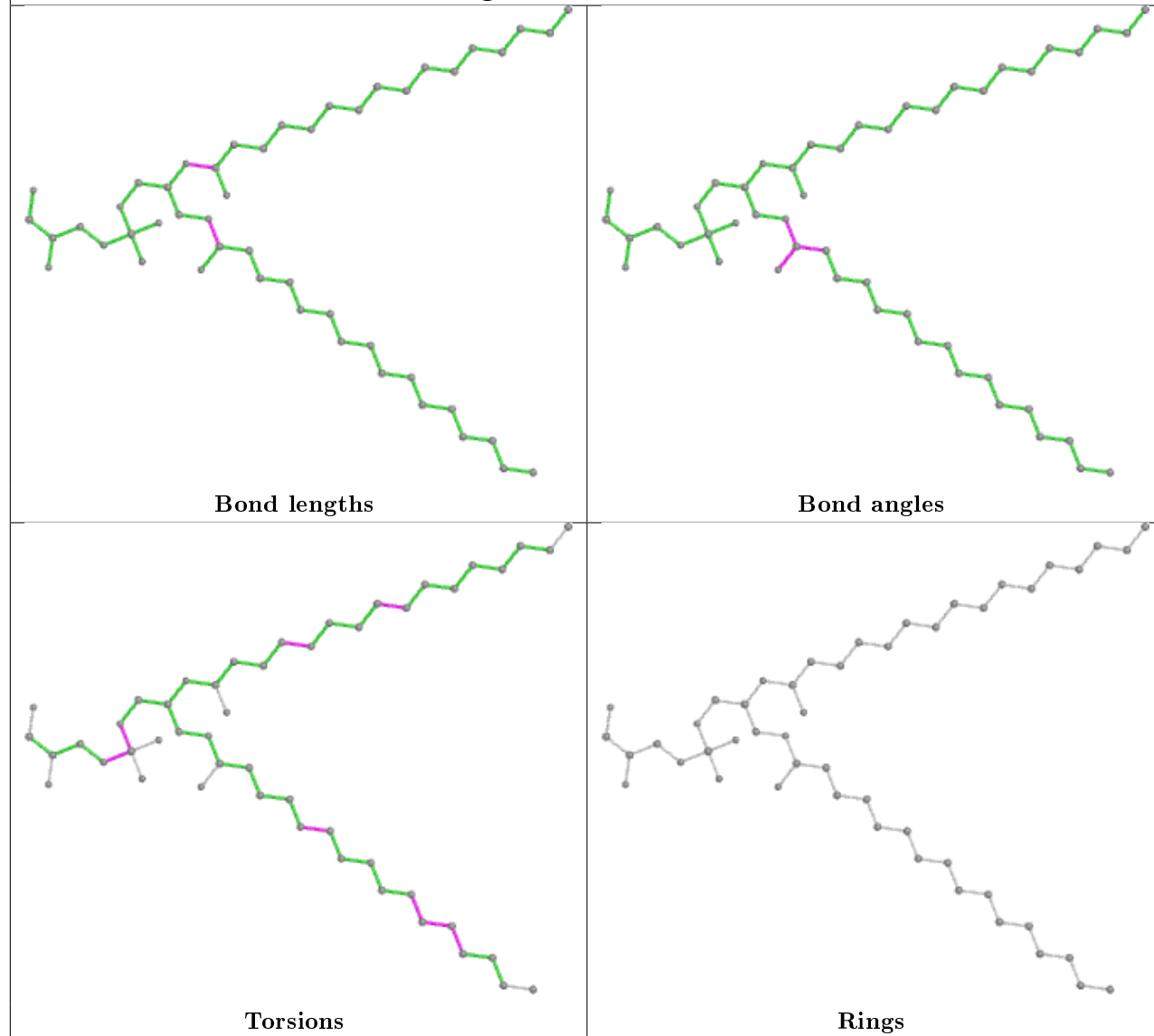


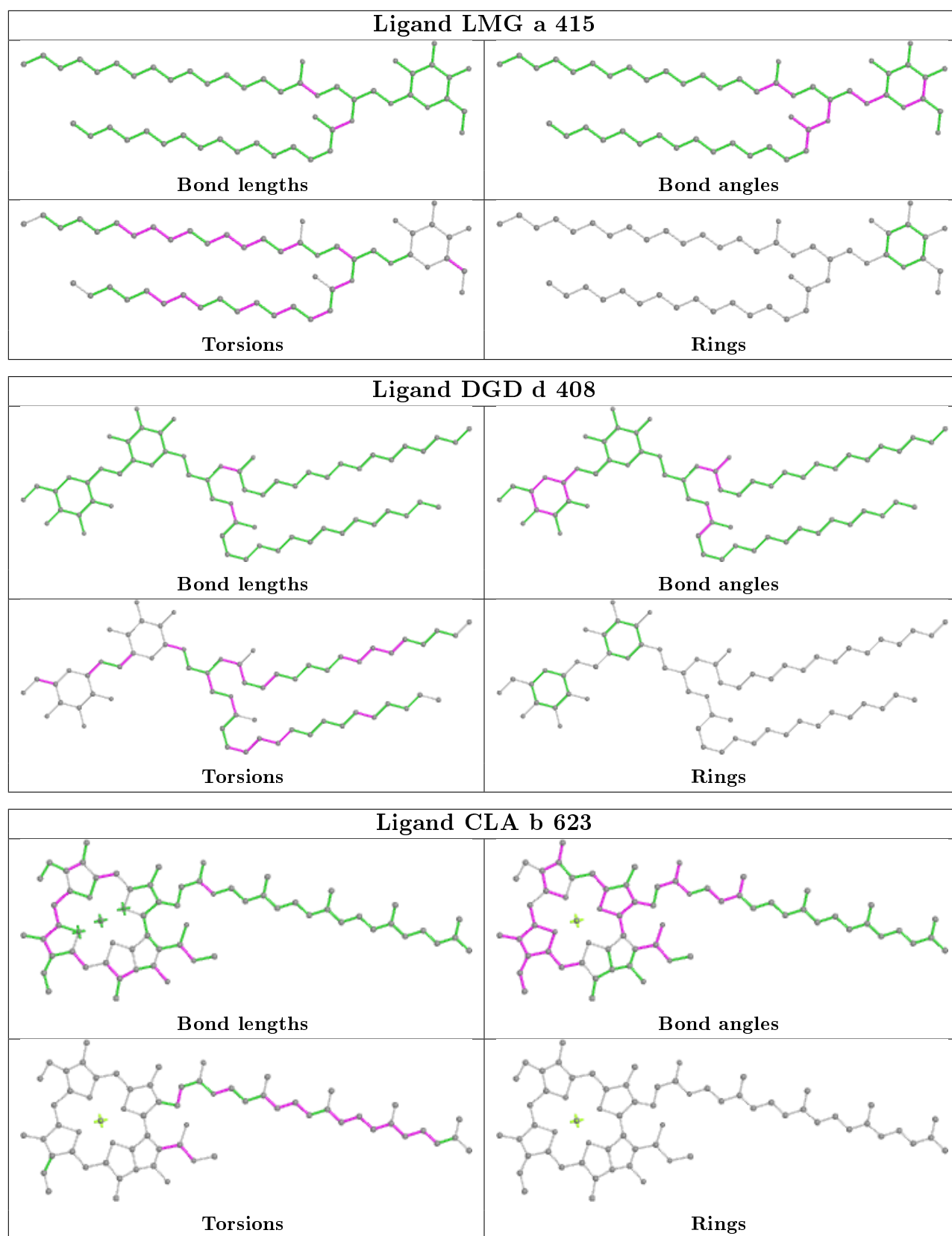


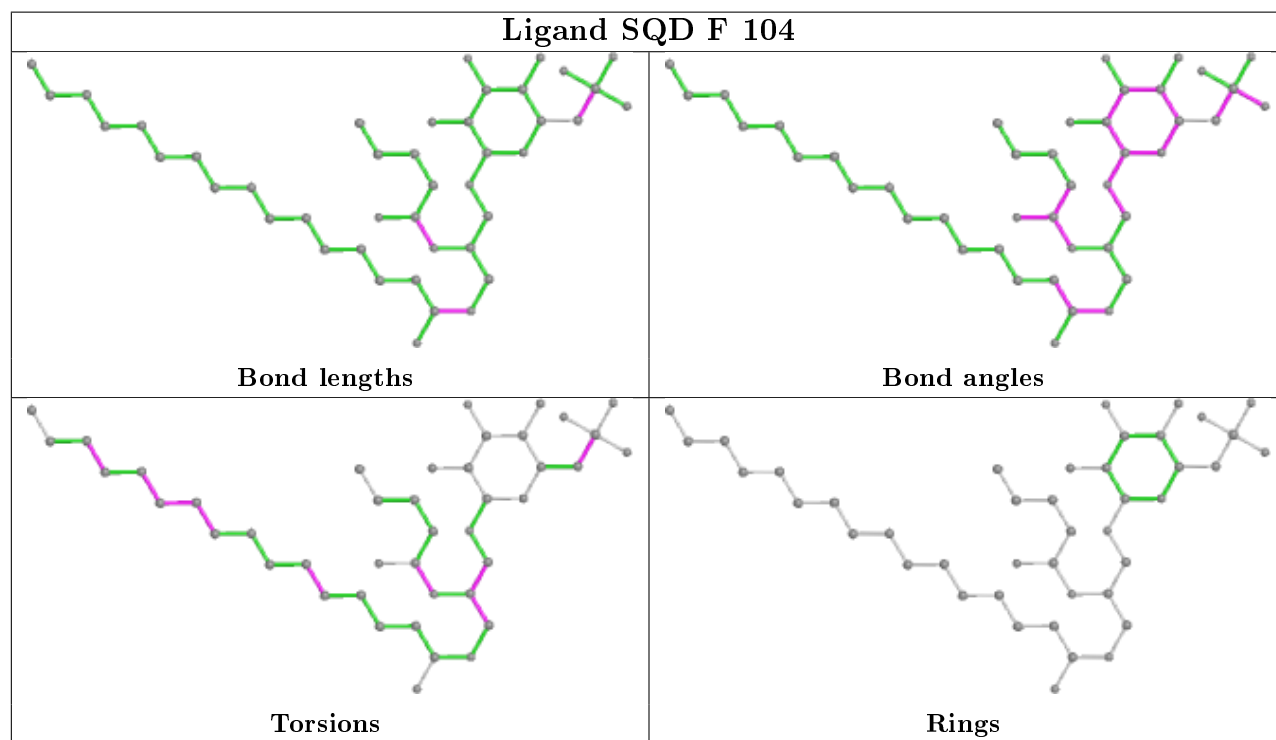
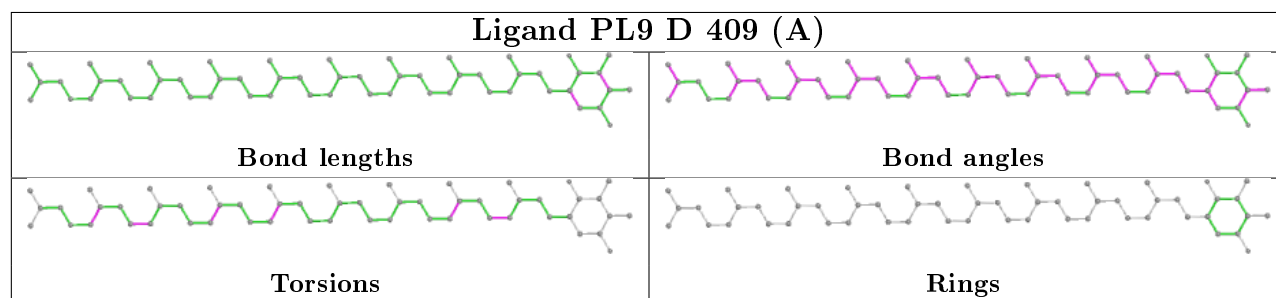
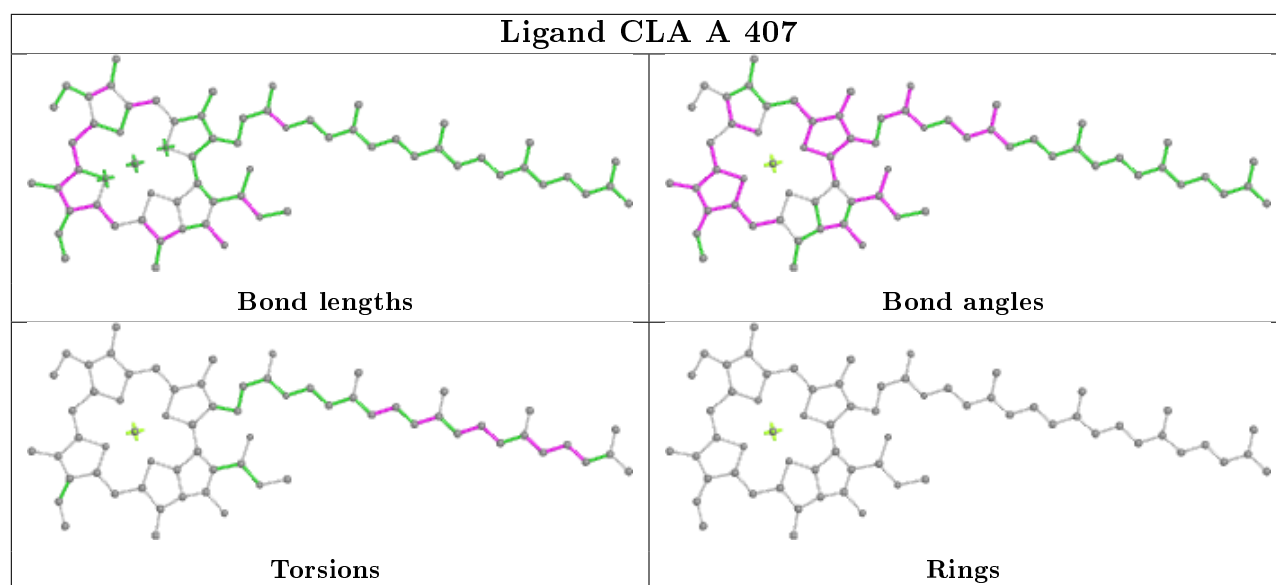


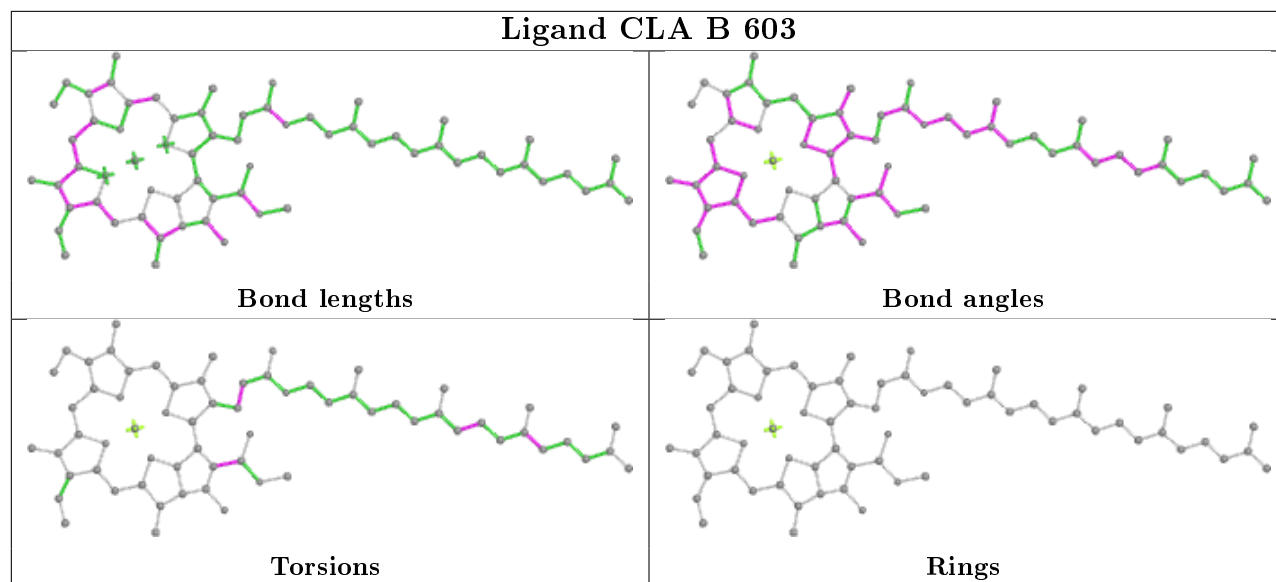
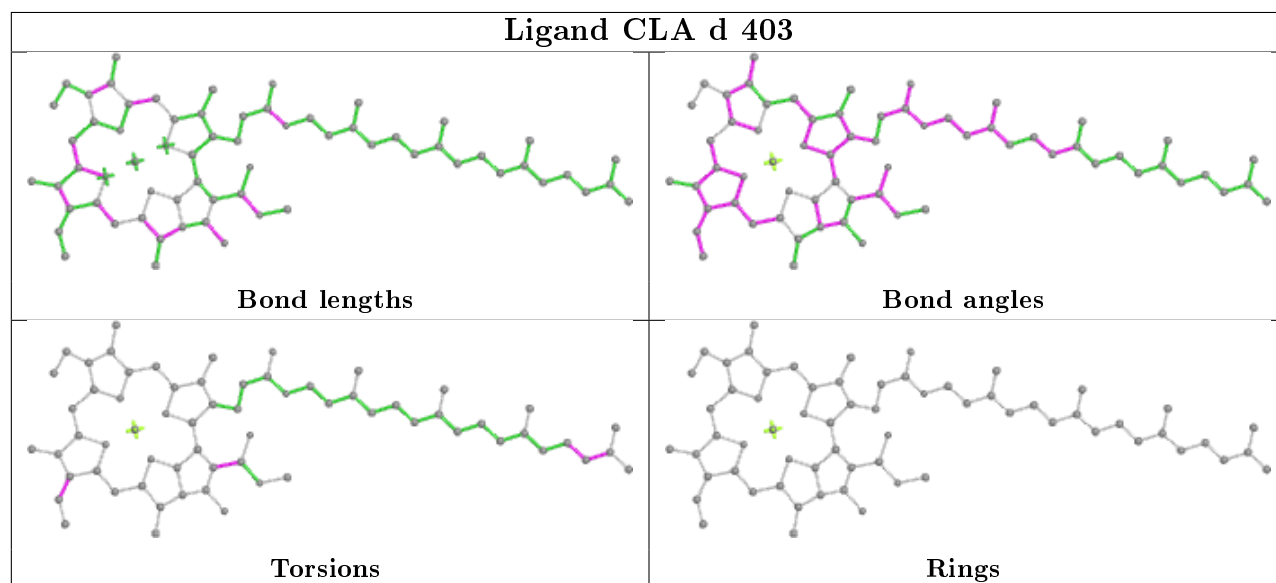




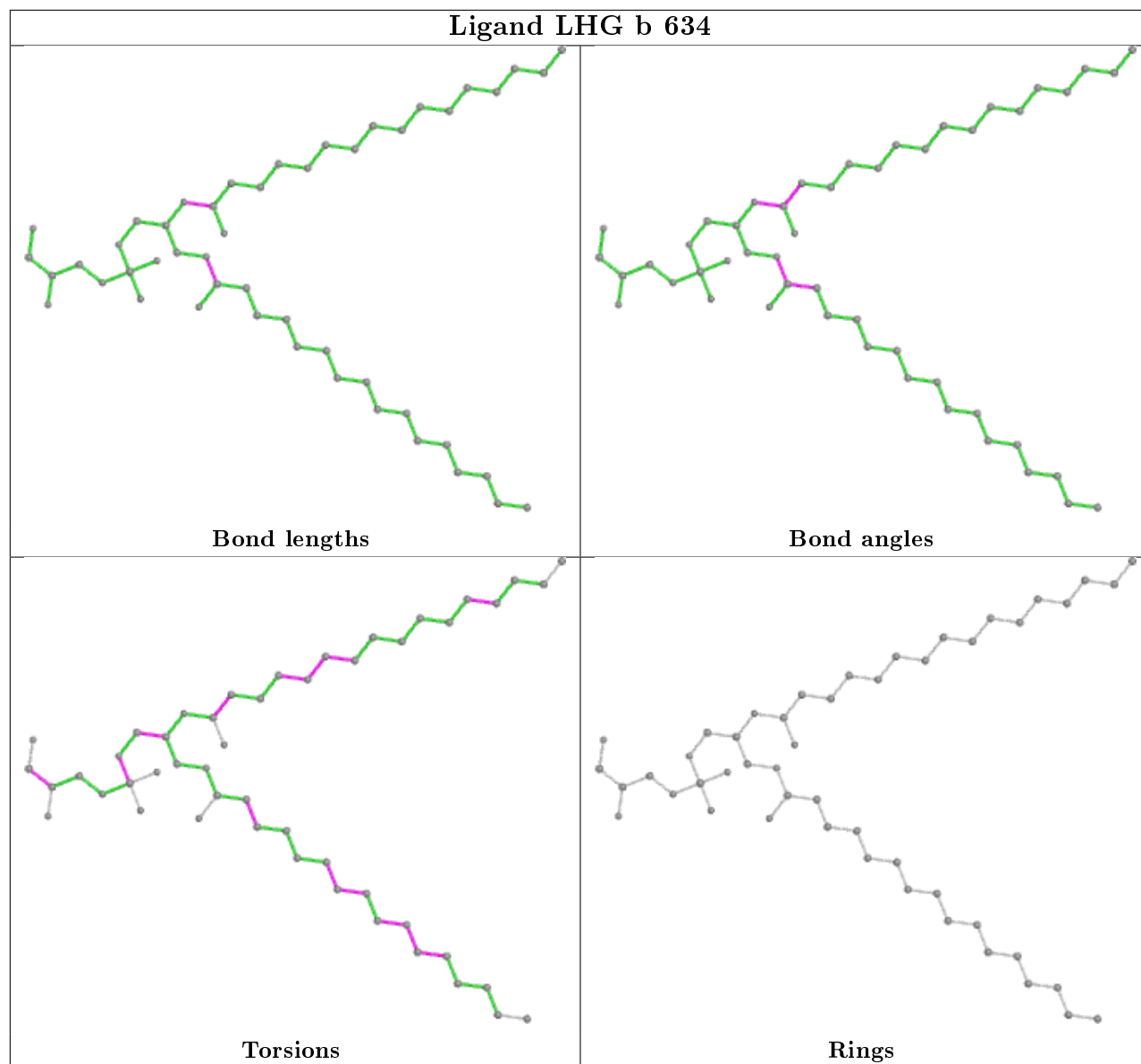
Ligand CLA A 404**Ligand LHG D 412**



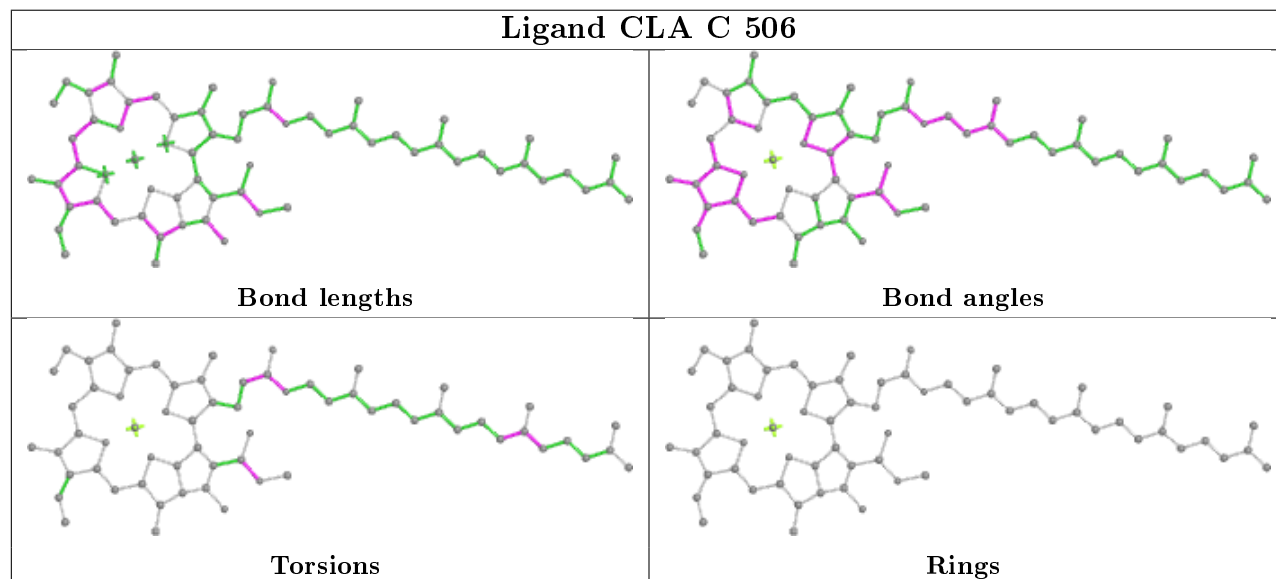


Ligand CLA B 603**Ligand CLA d 403**

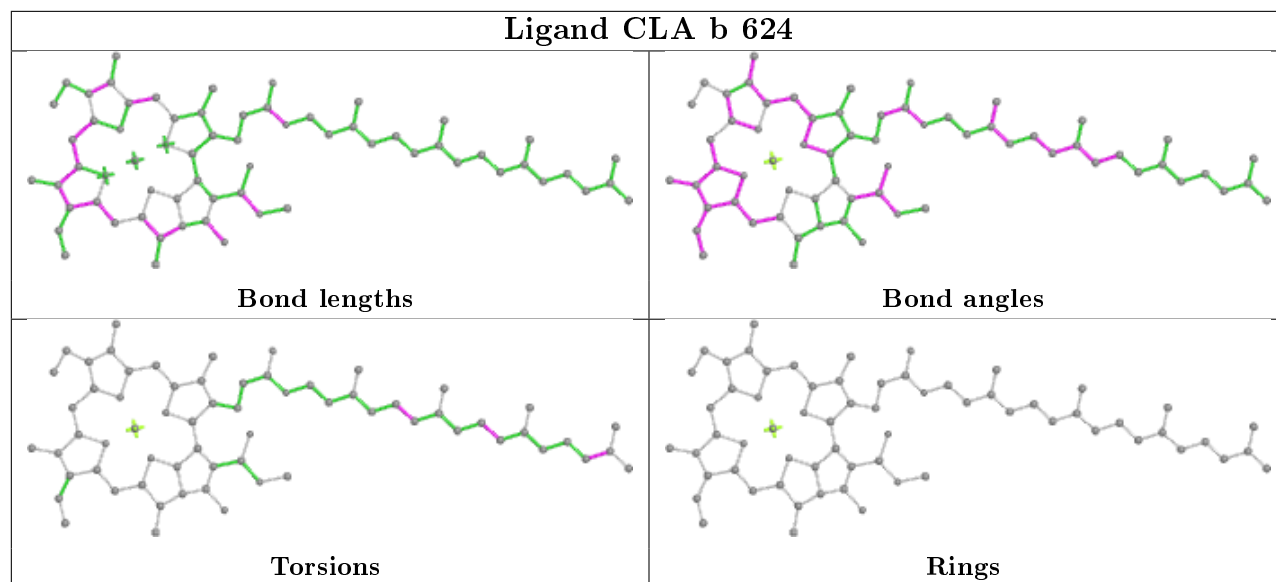
Ligand LHG b 634



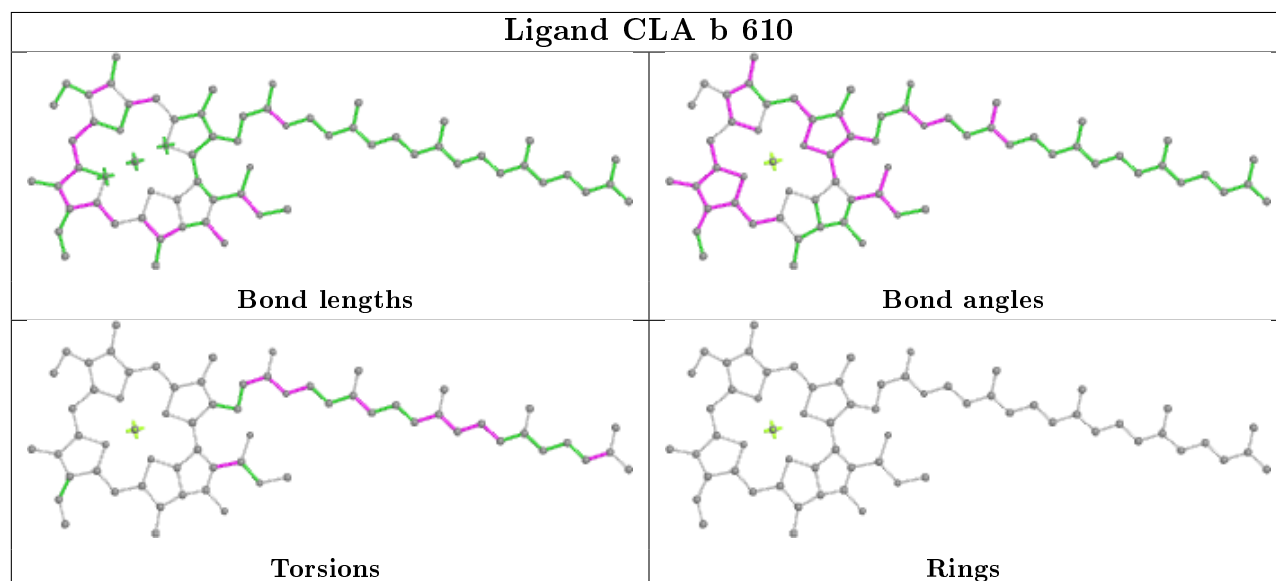
Ligand CLA C 506



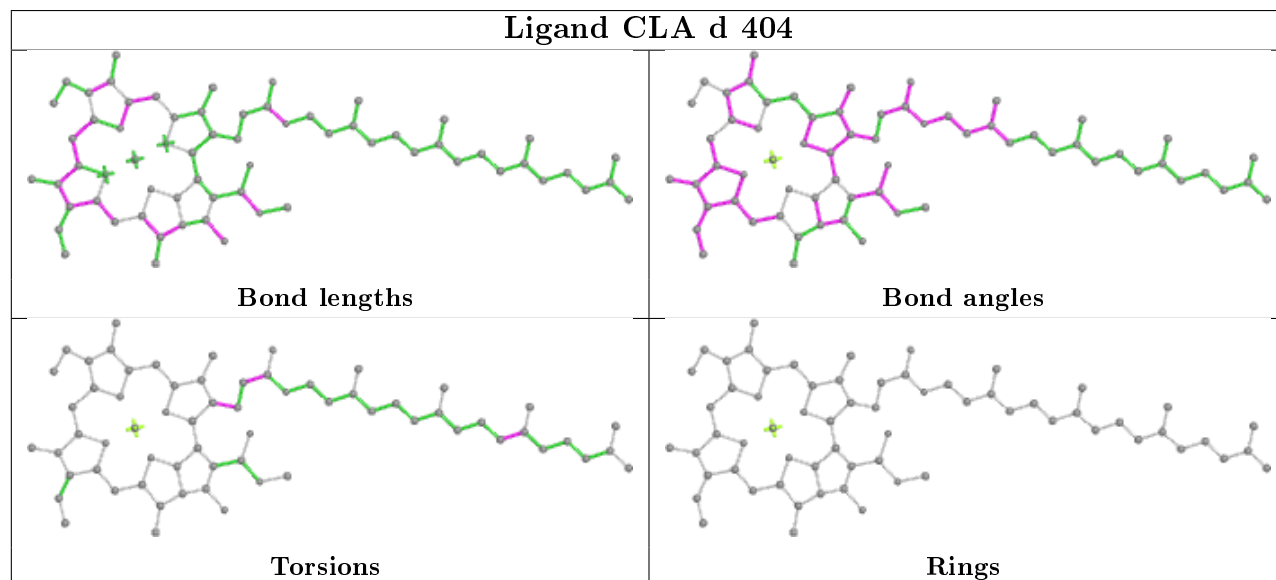
Ligand CLA b 624

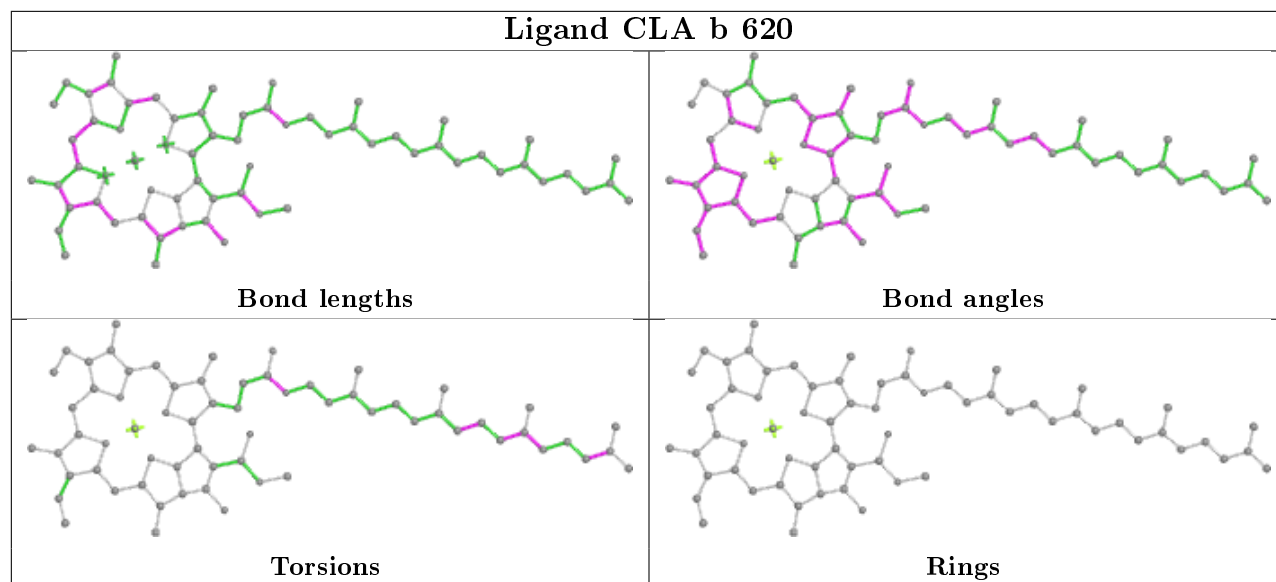
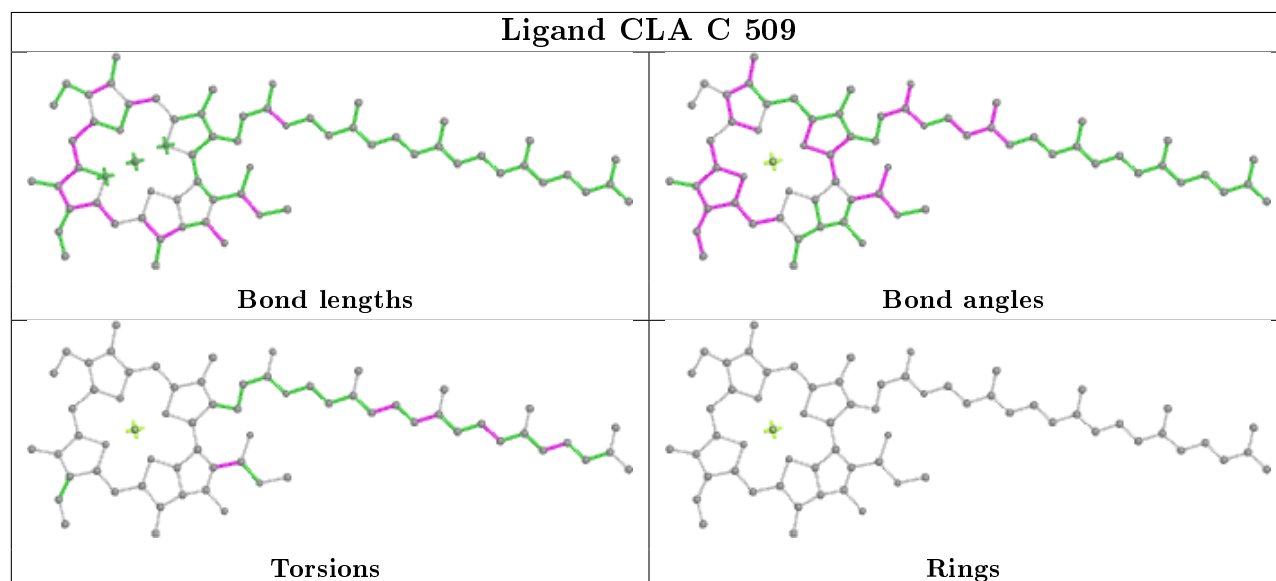
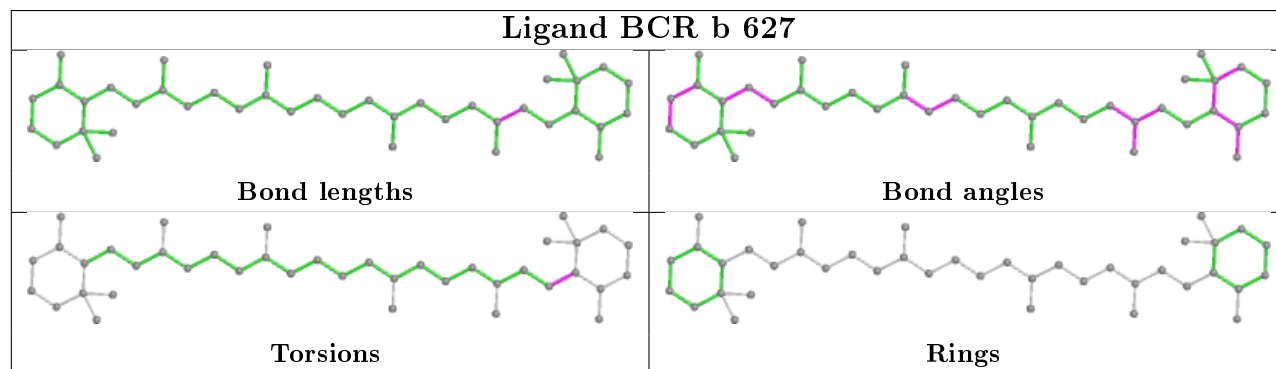


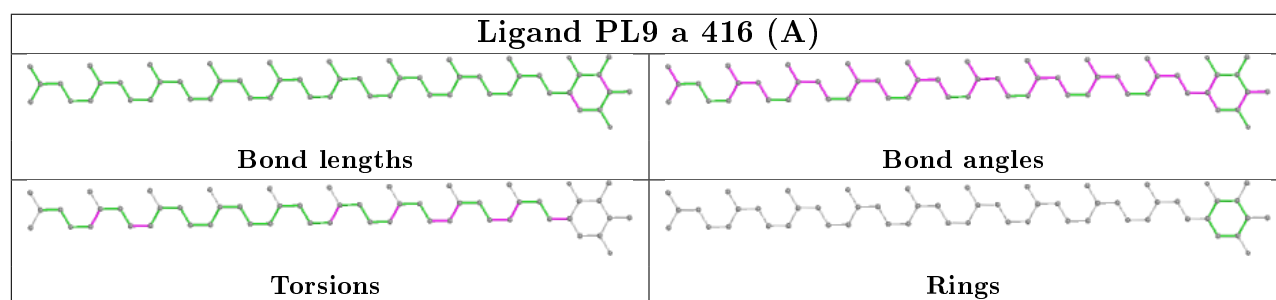
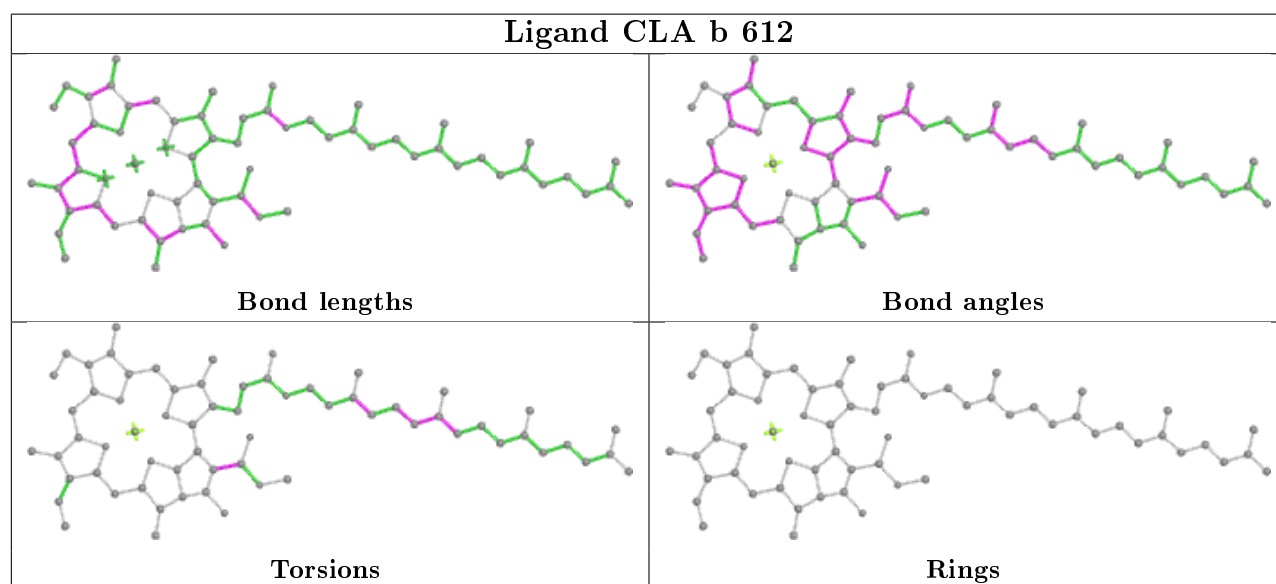
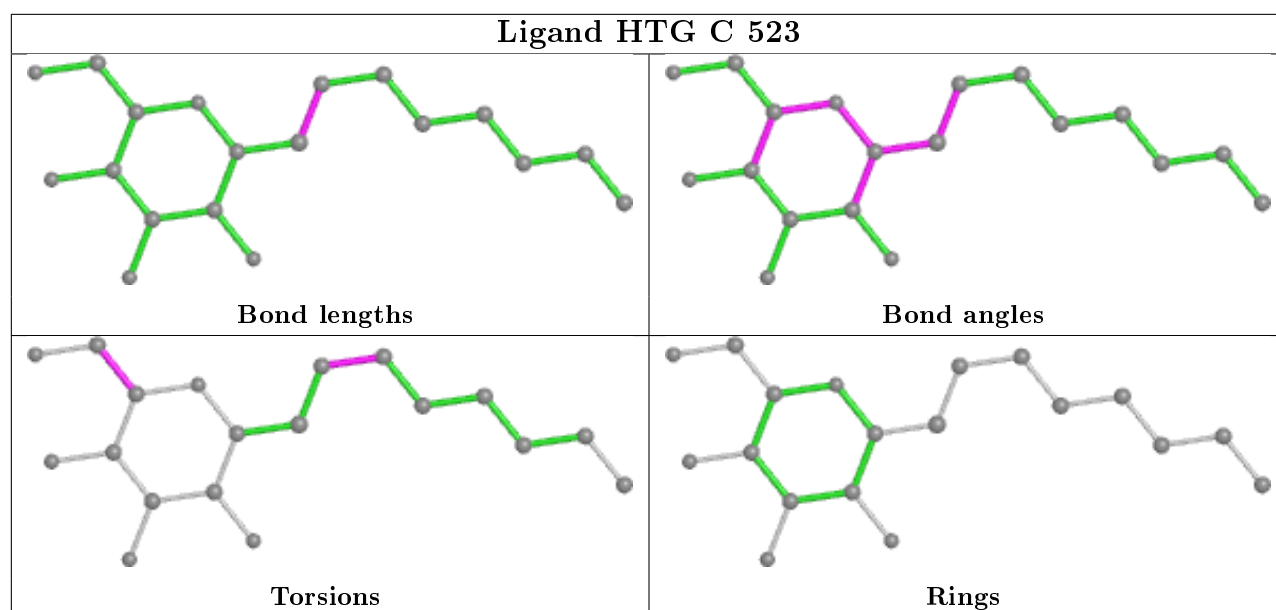
Ligand CLA b 610

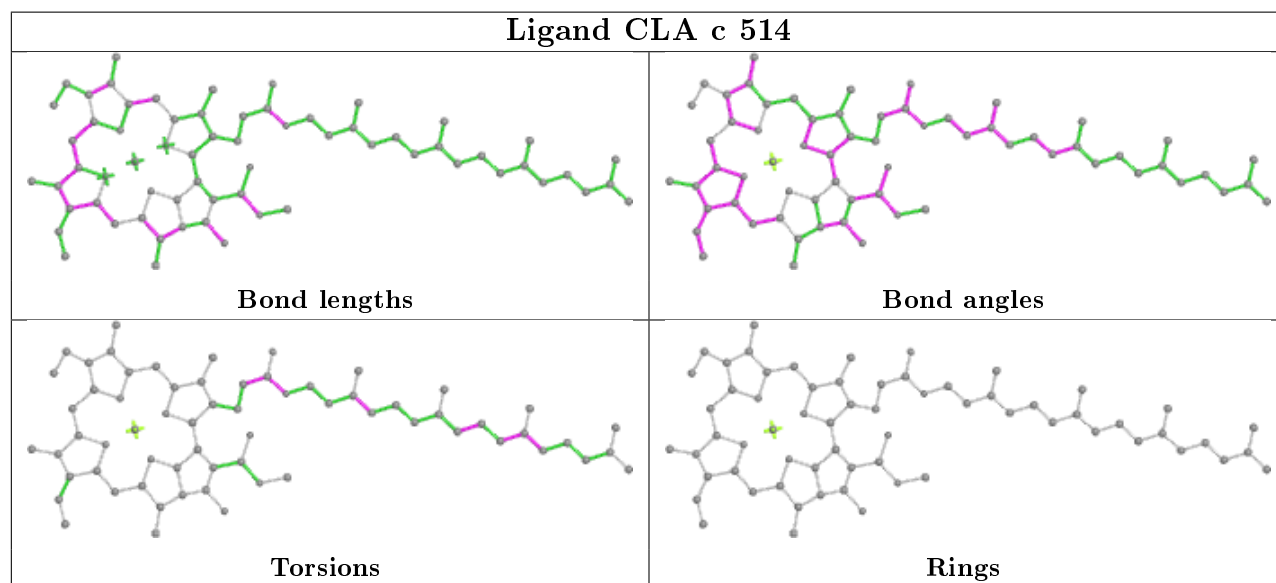
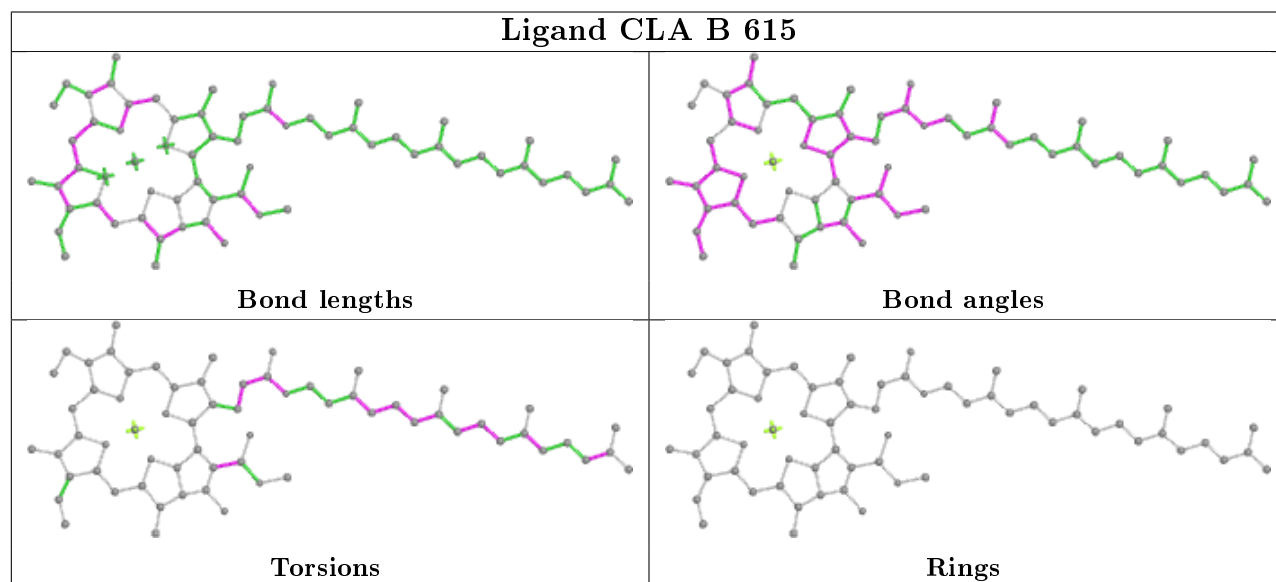
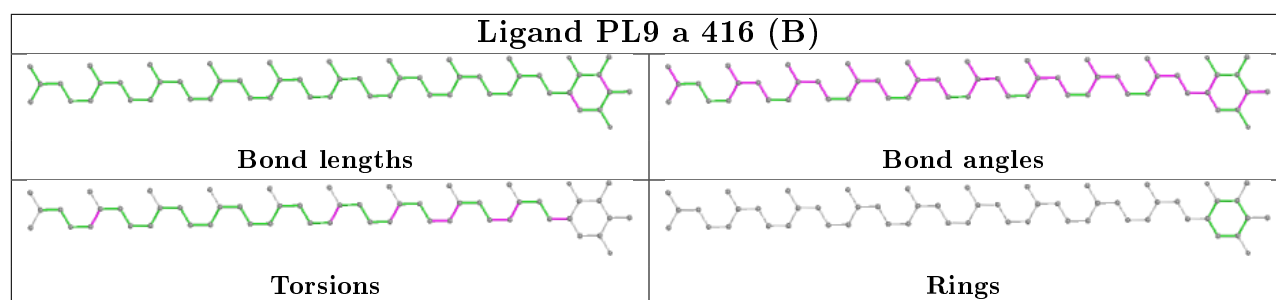


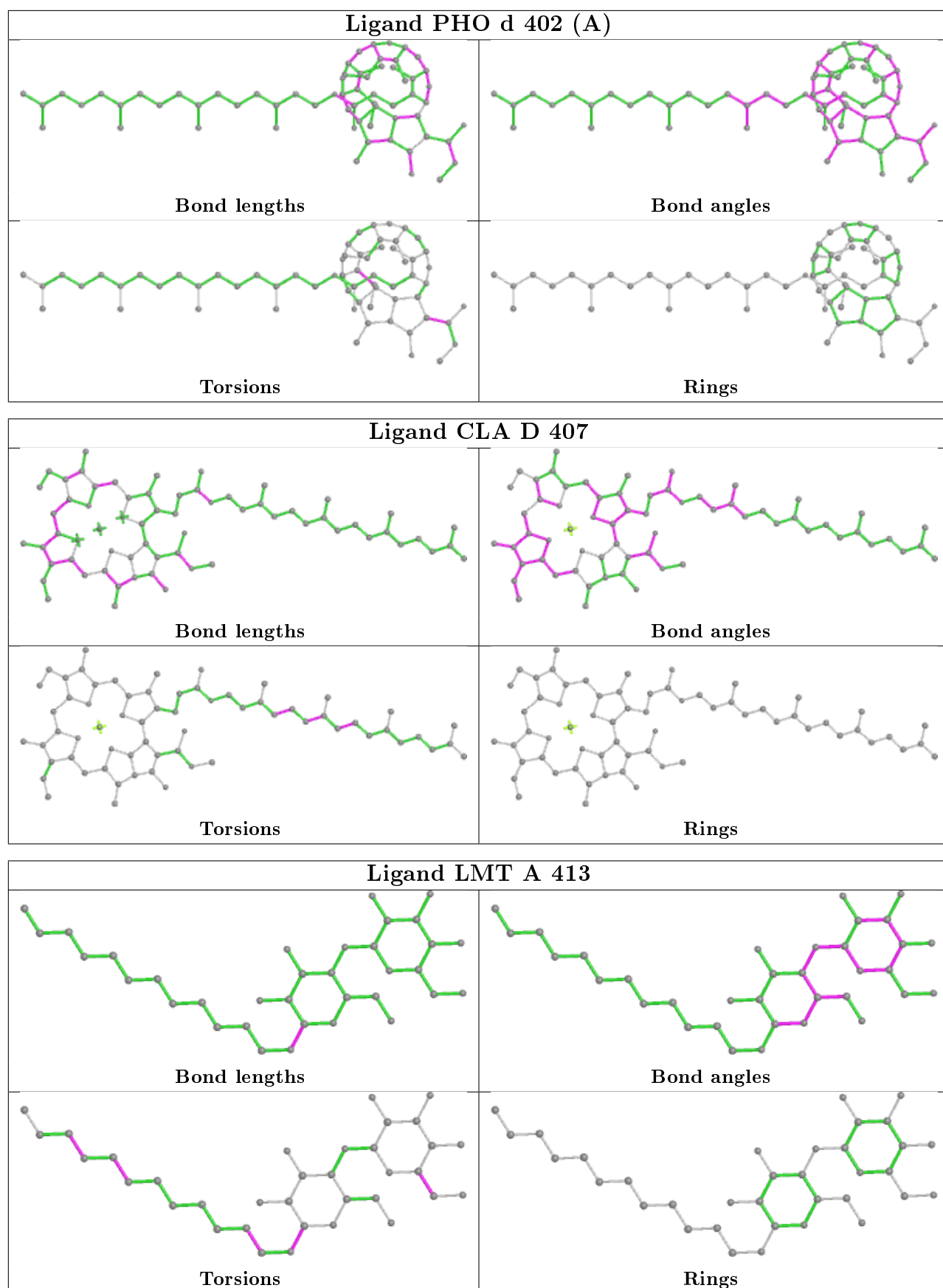
Ligand CLA d 404

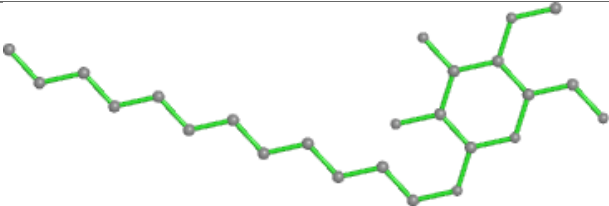
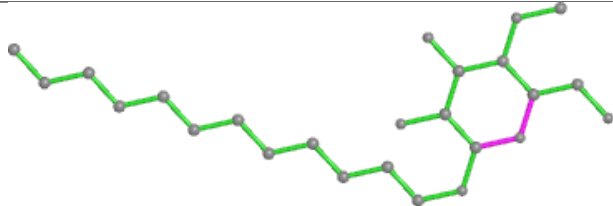
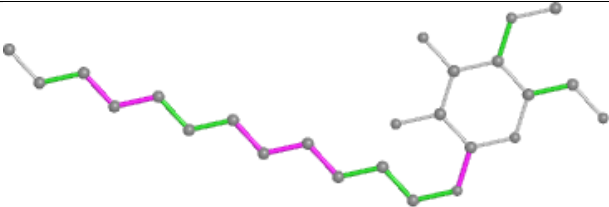
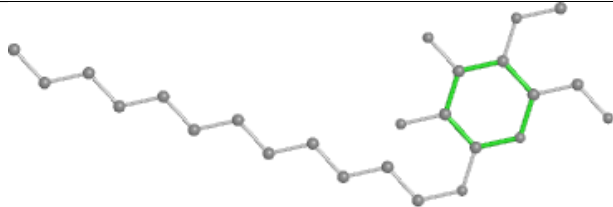


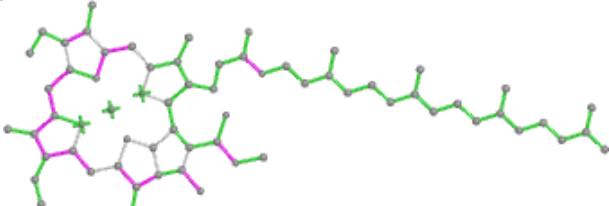
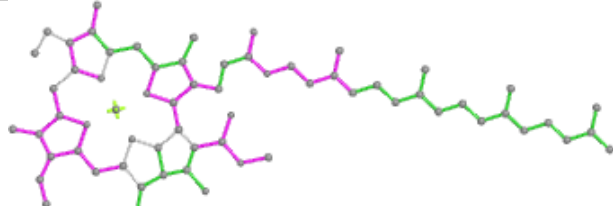
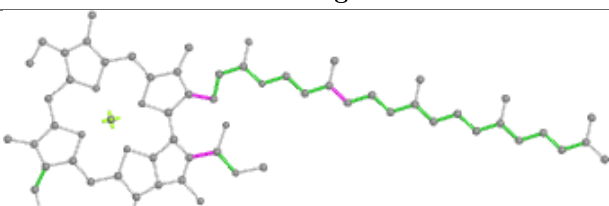
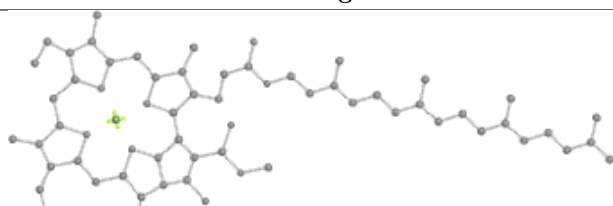
Ligand CLA b 620**Ligand CLA C 509****Ligand BCR b 627**

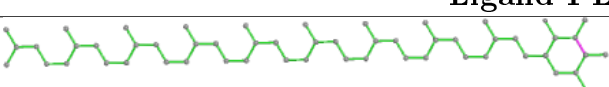
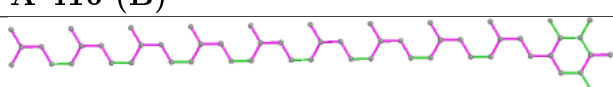
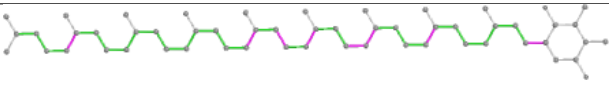
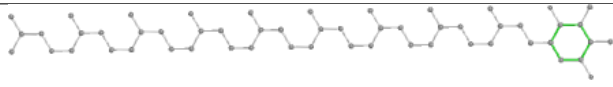


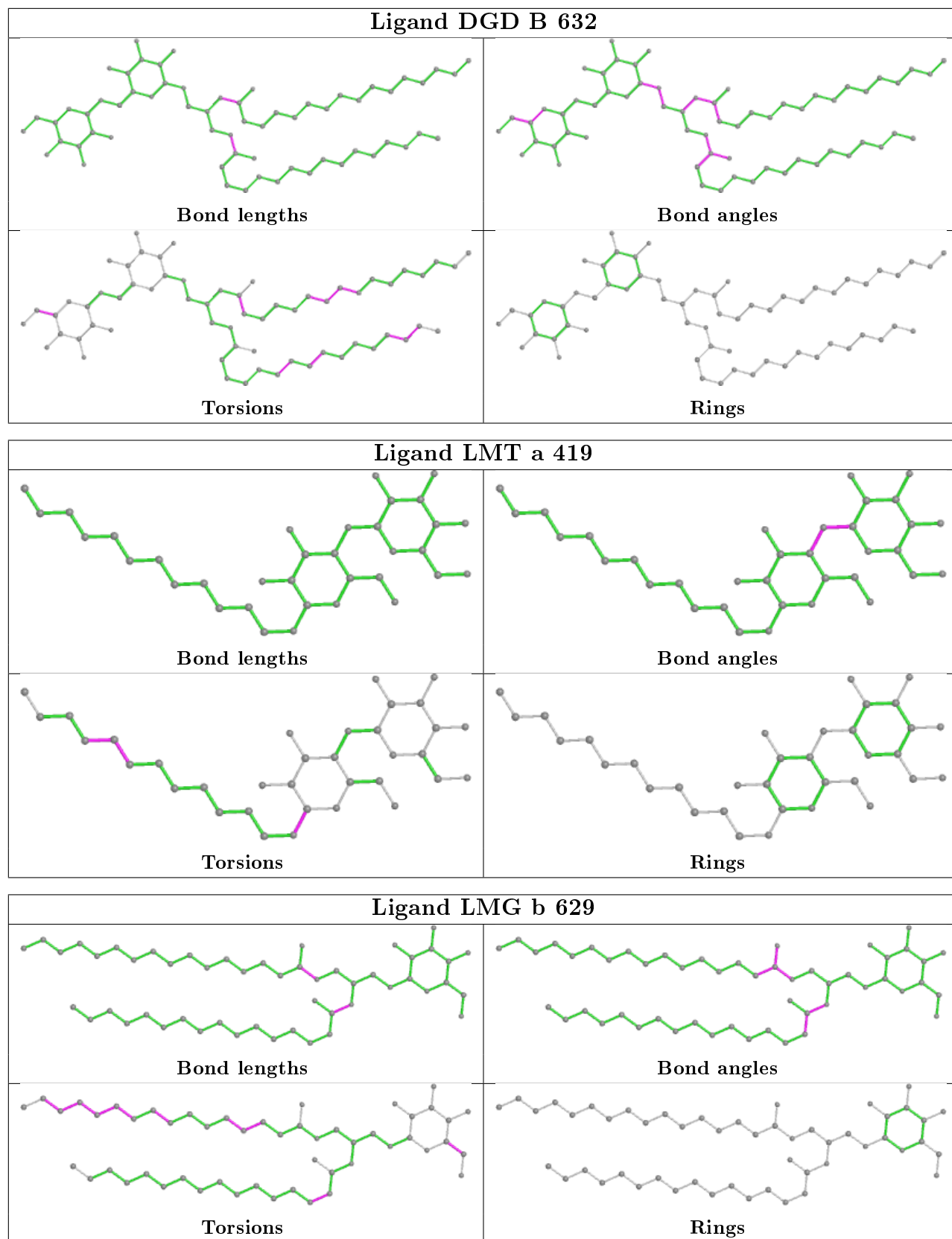




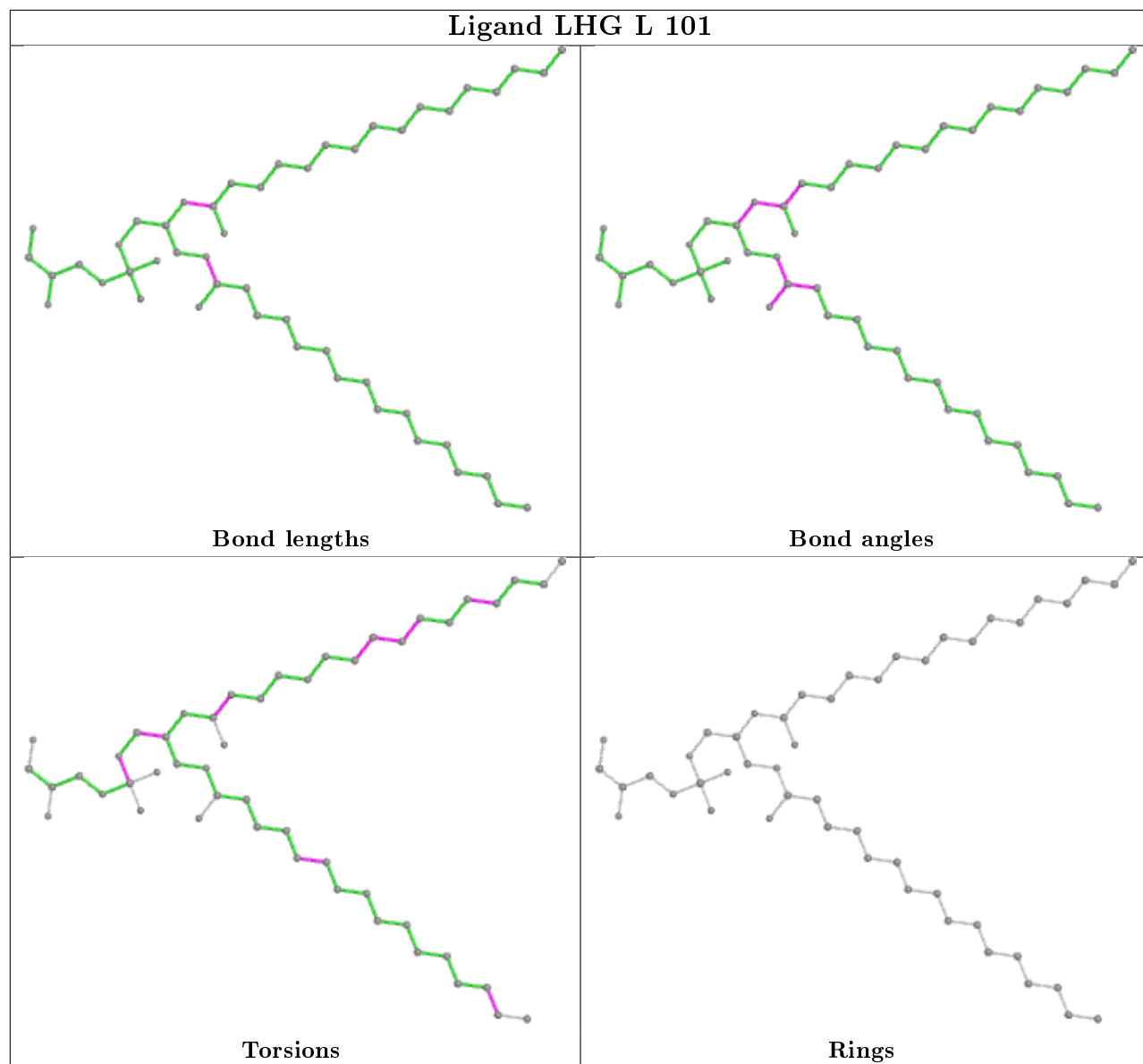
Ligand LMT t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

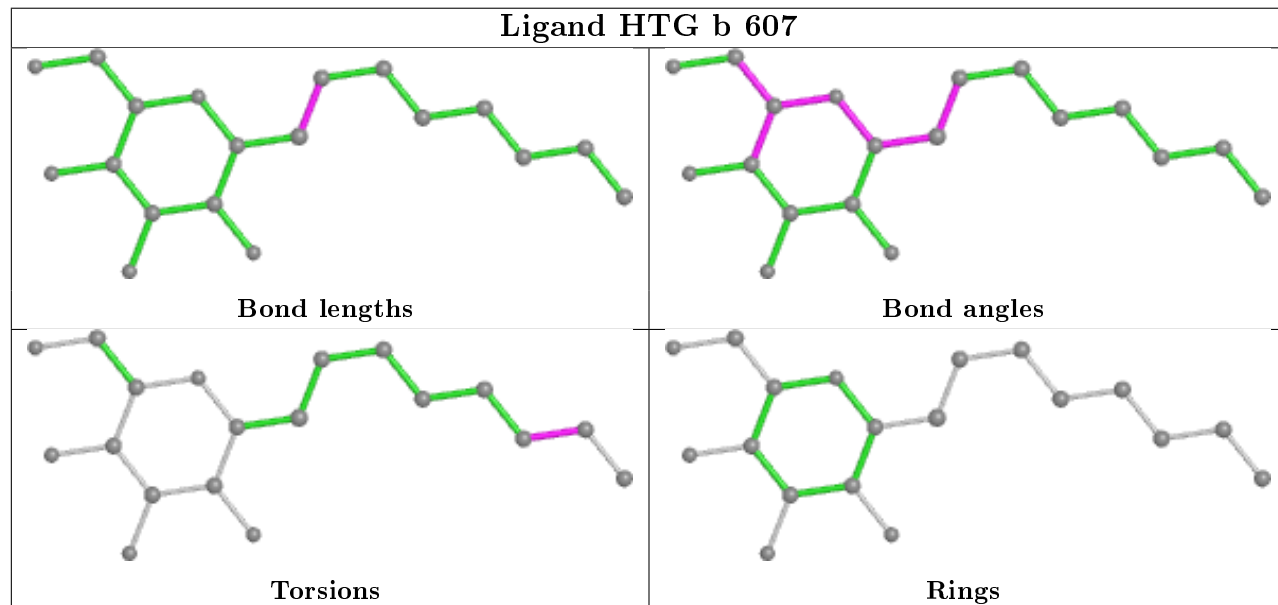
Ligand PL9 A 416 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

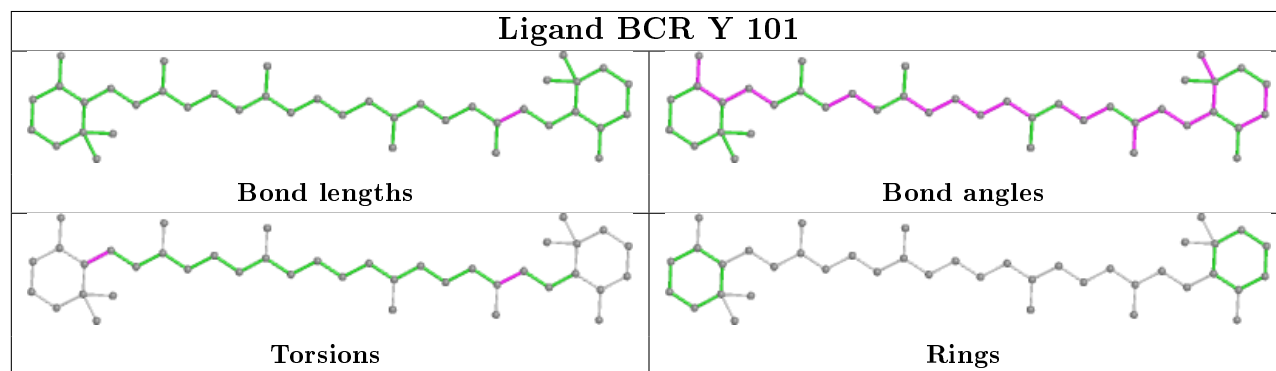
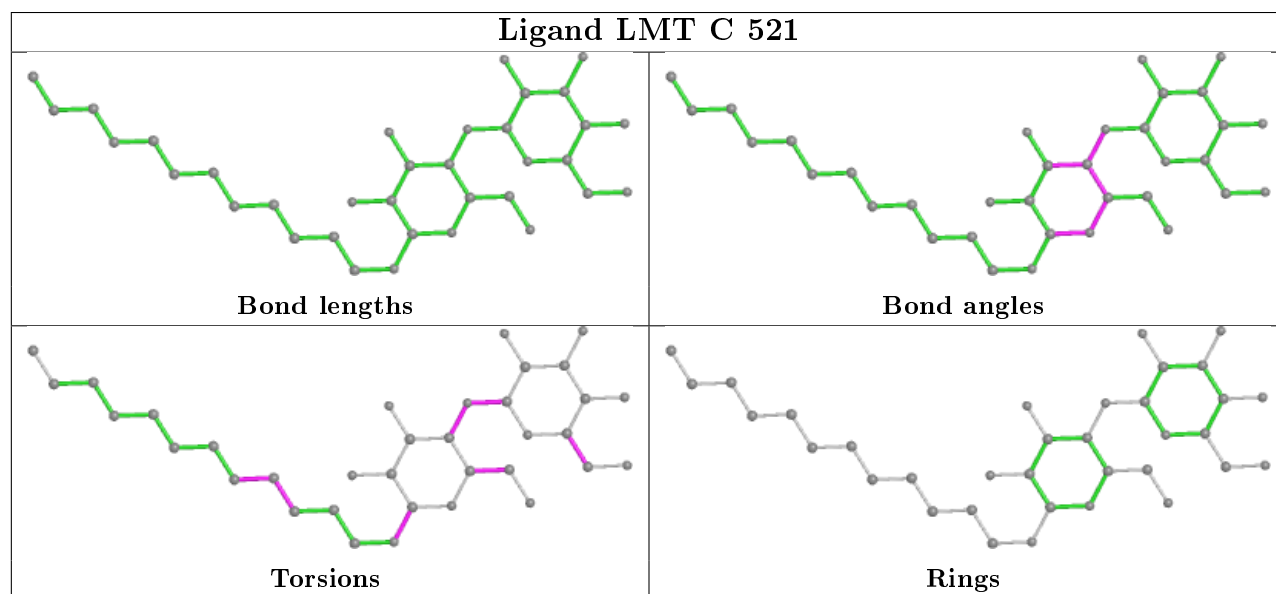
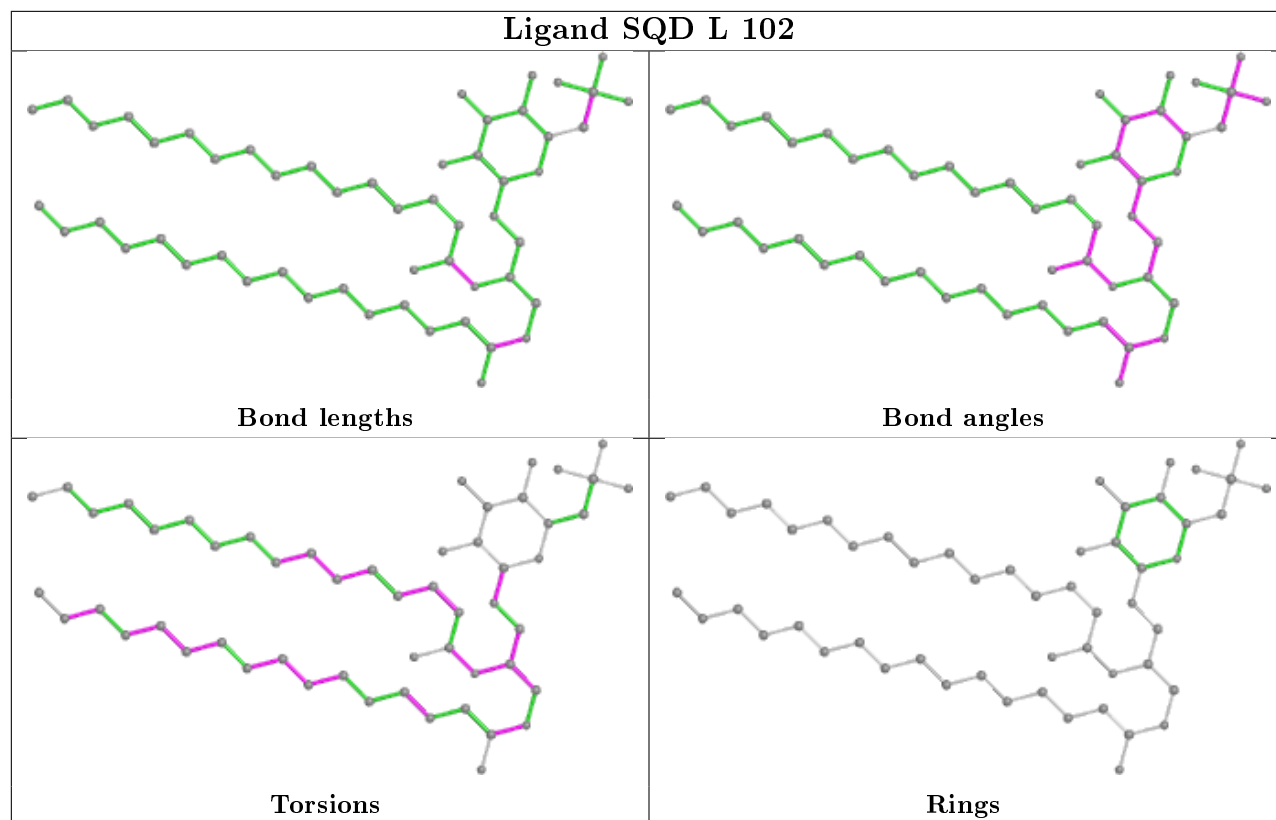


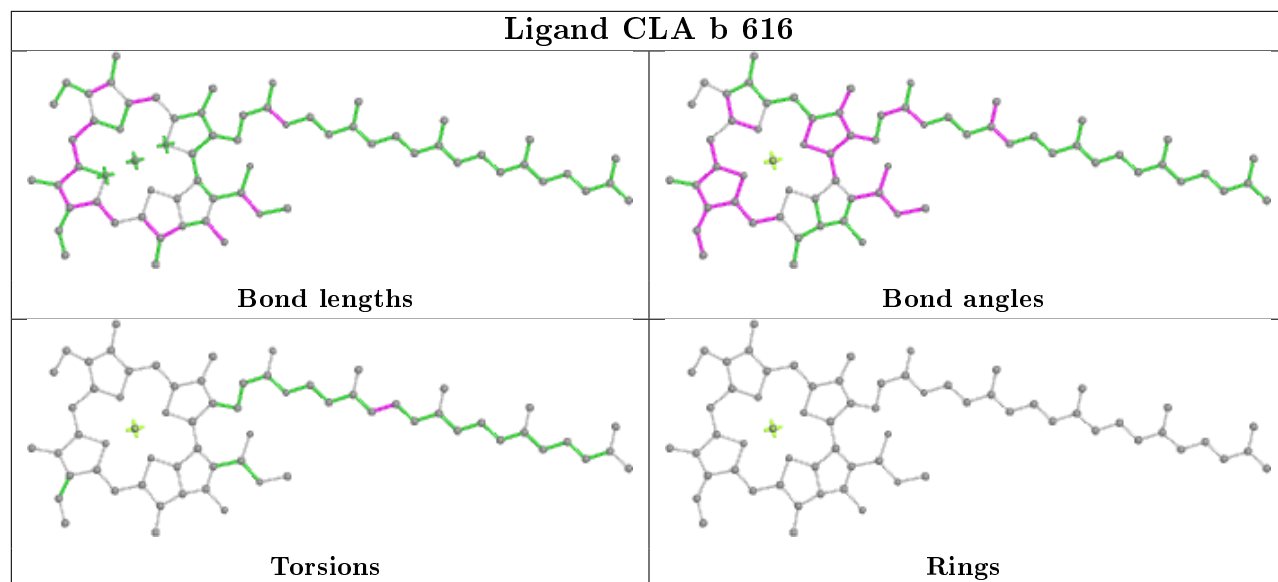
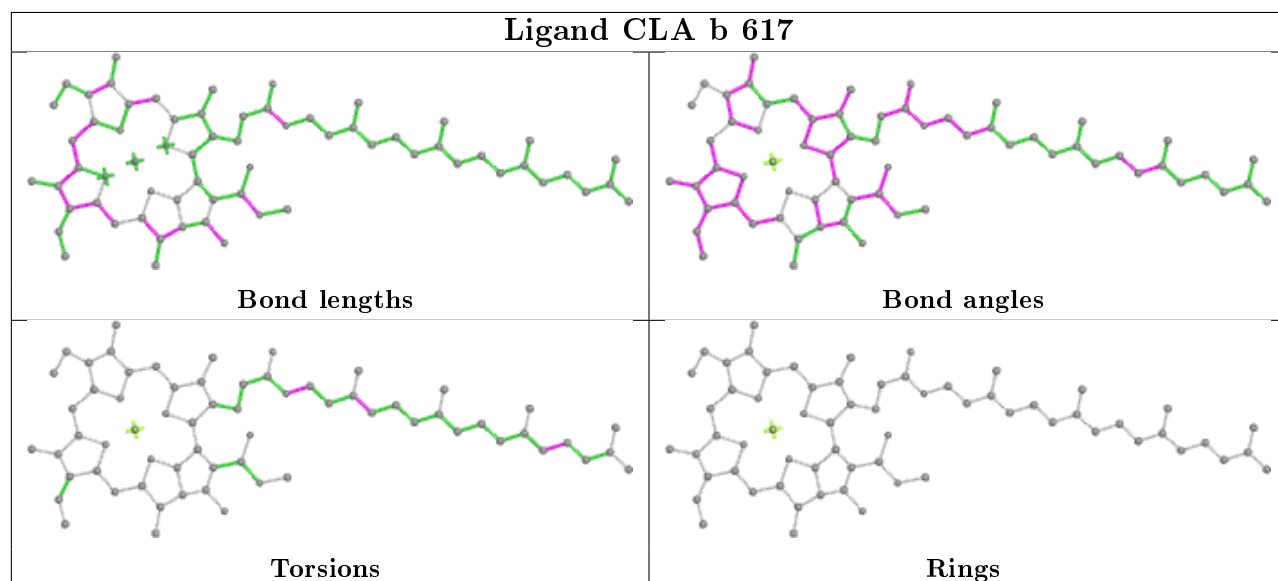
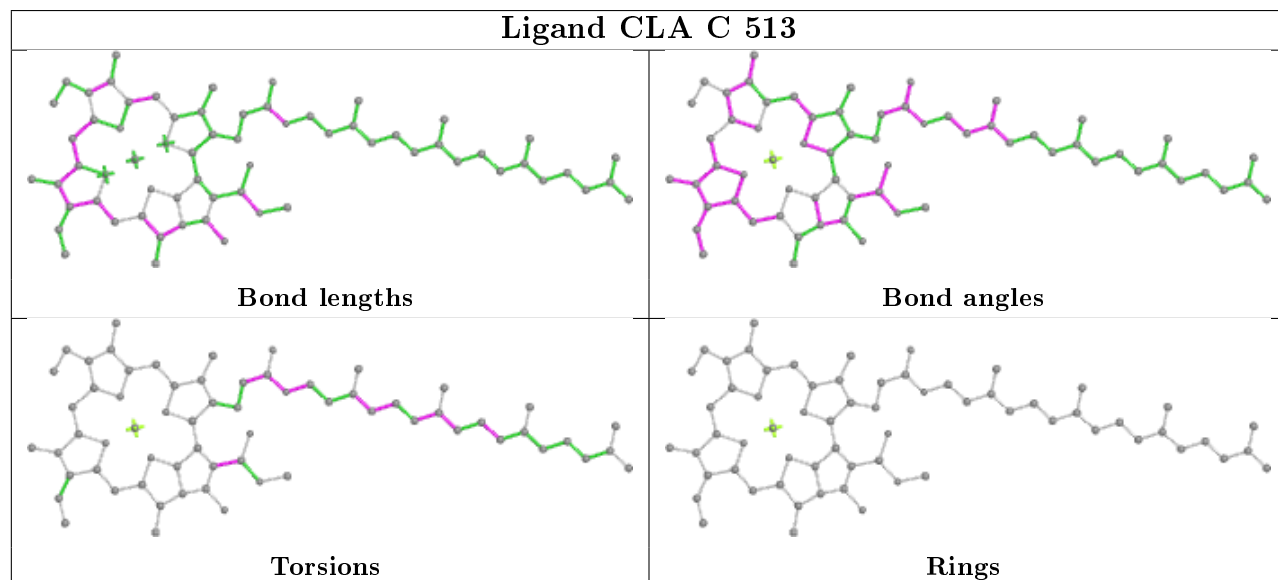
Ligand LHG L 101

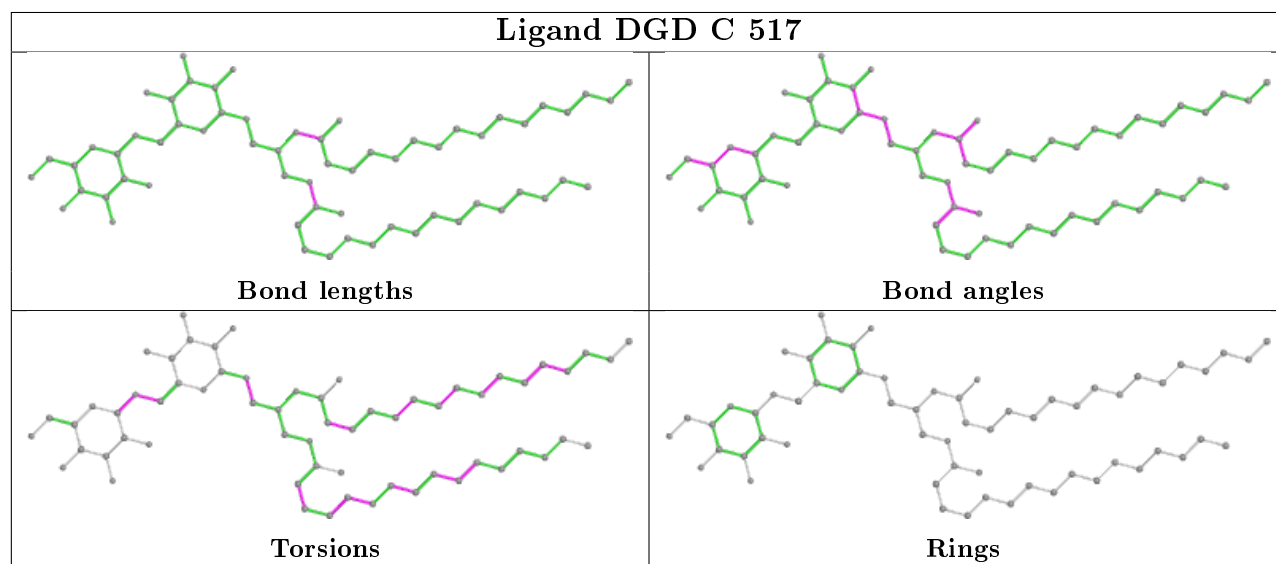
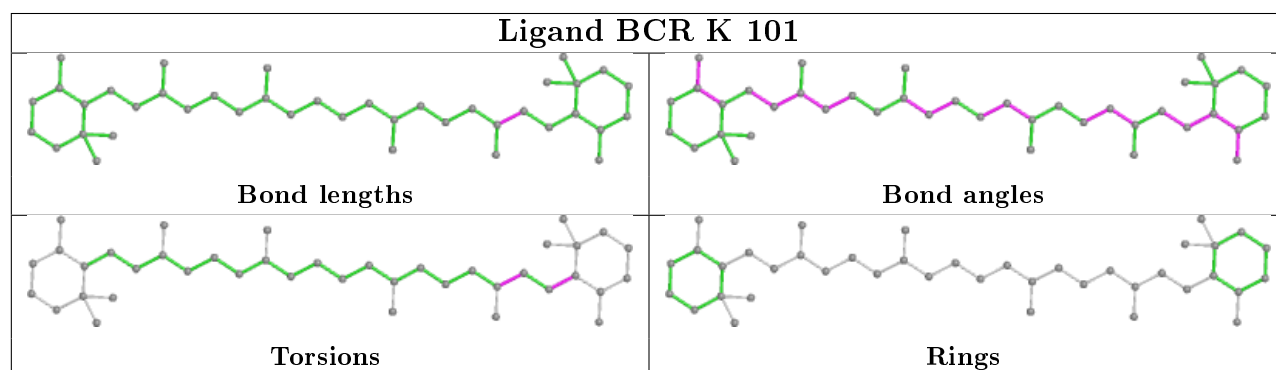
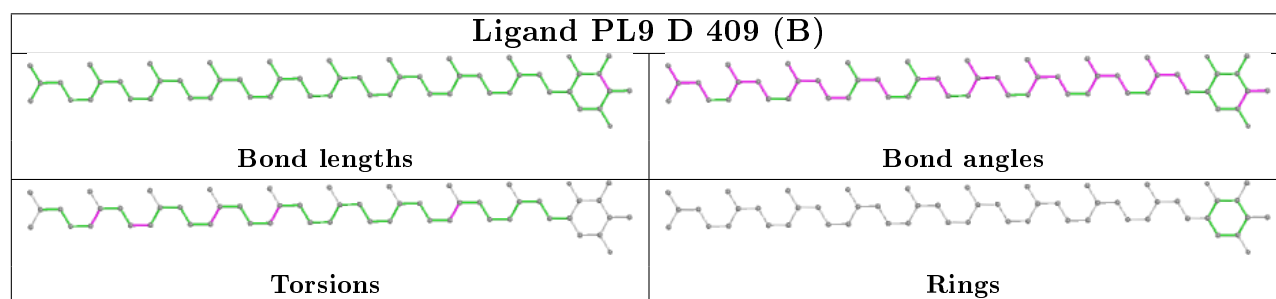
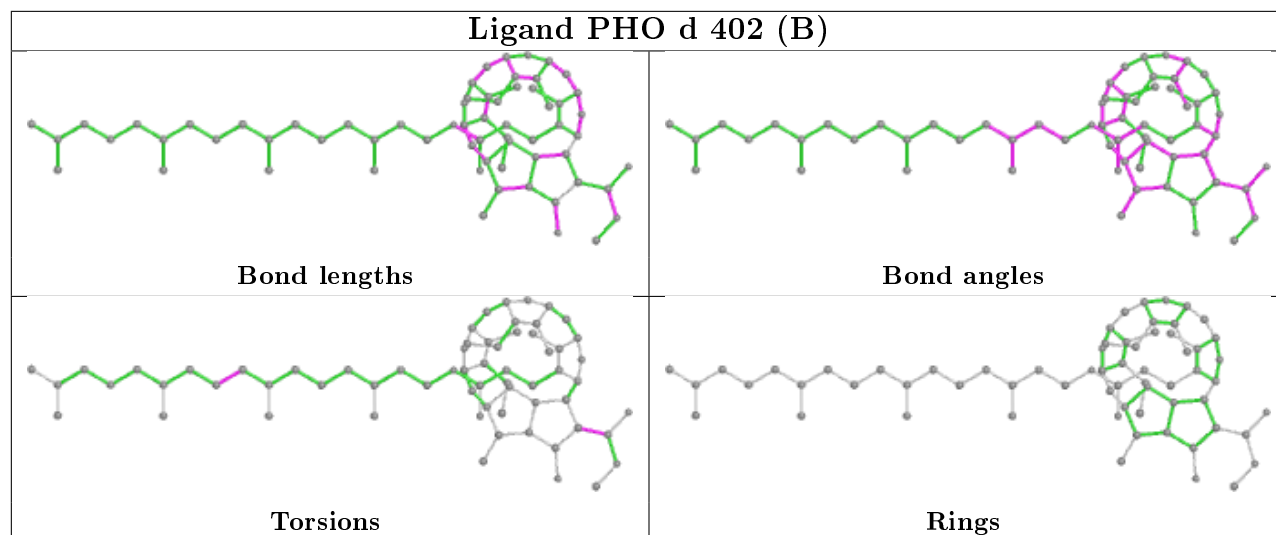


Ligand HTG b 607

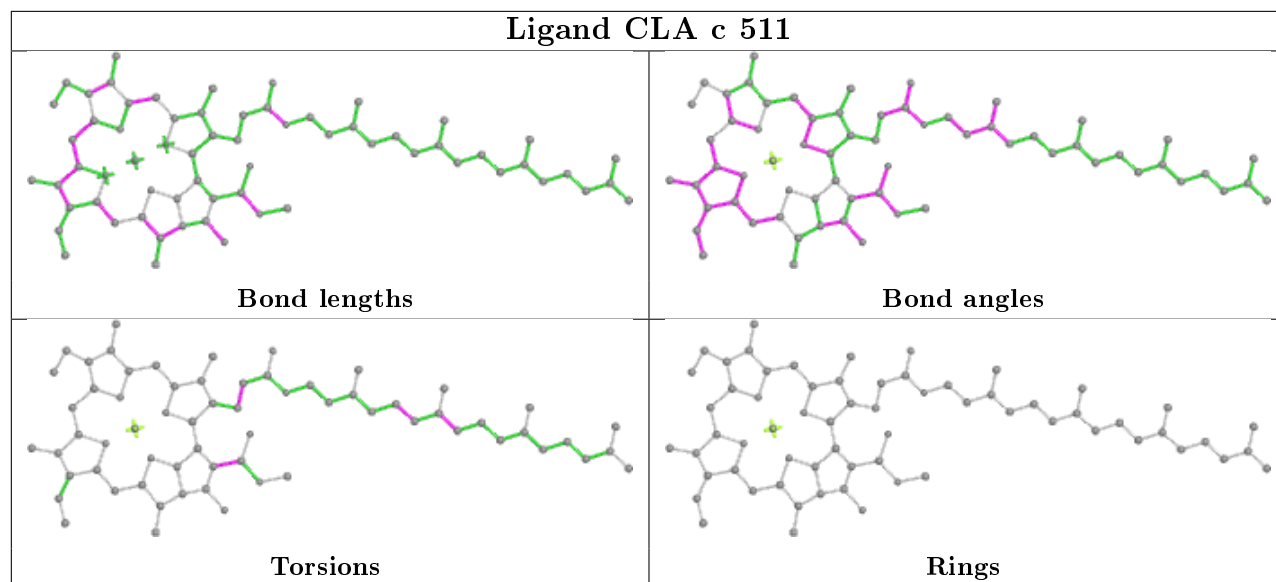




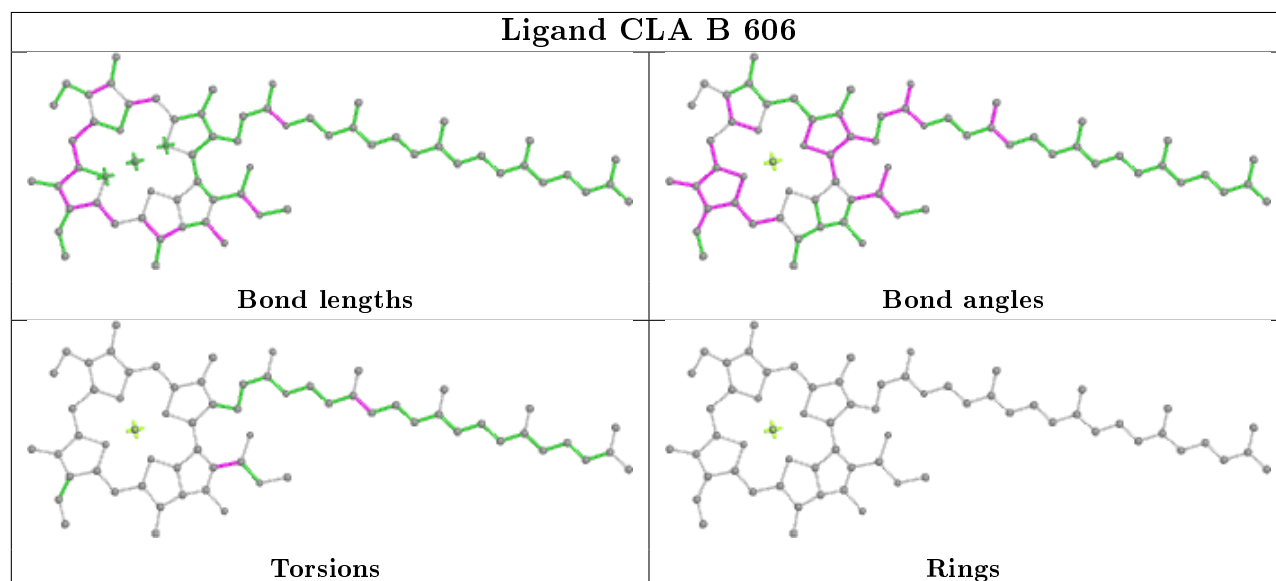
Ligand CLA b 616**Ligand CLA b 617****Ligand CLA C 513**



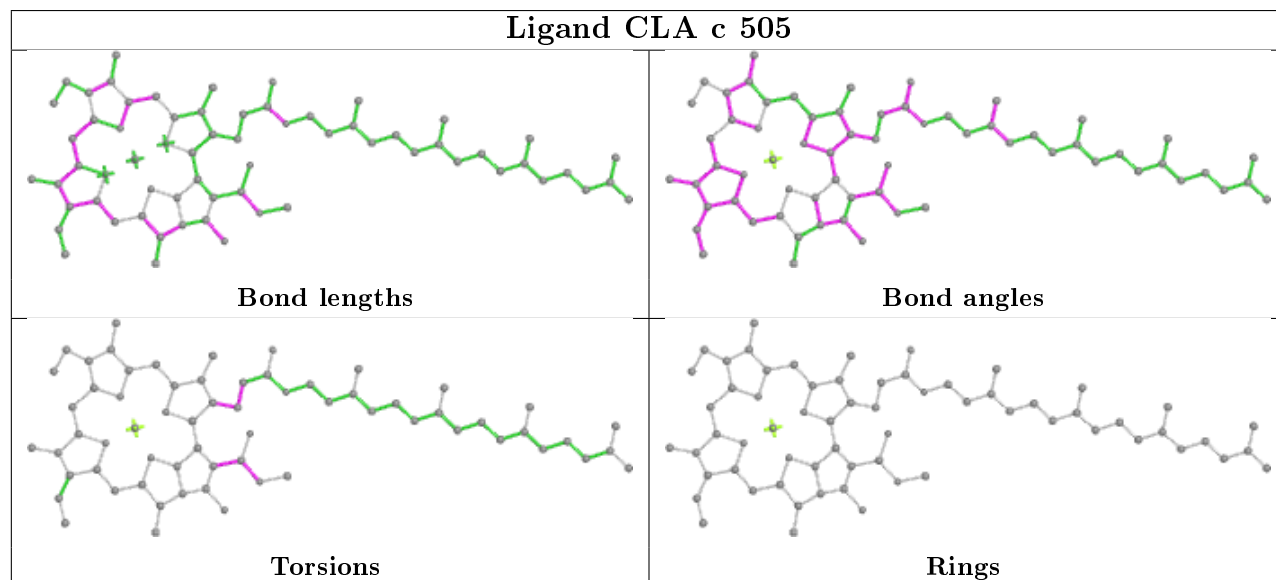
Ligand CLA c 511

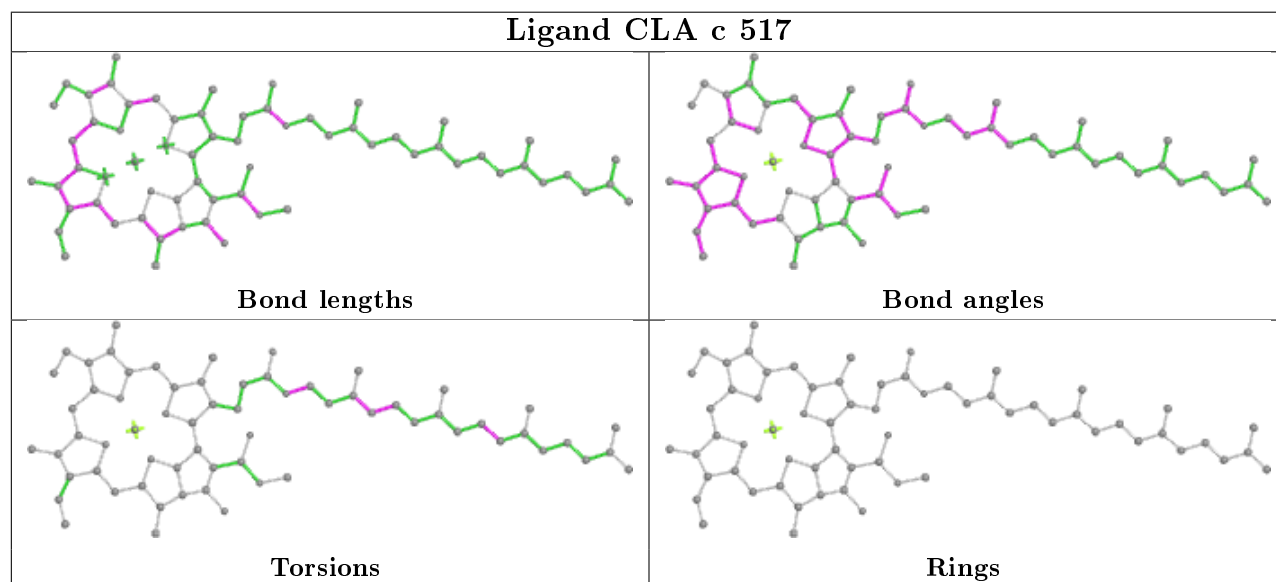
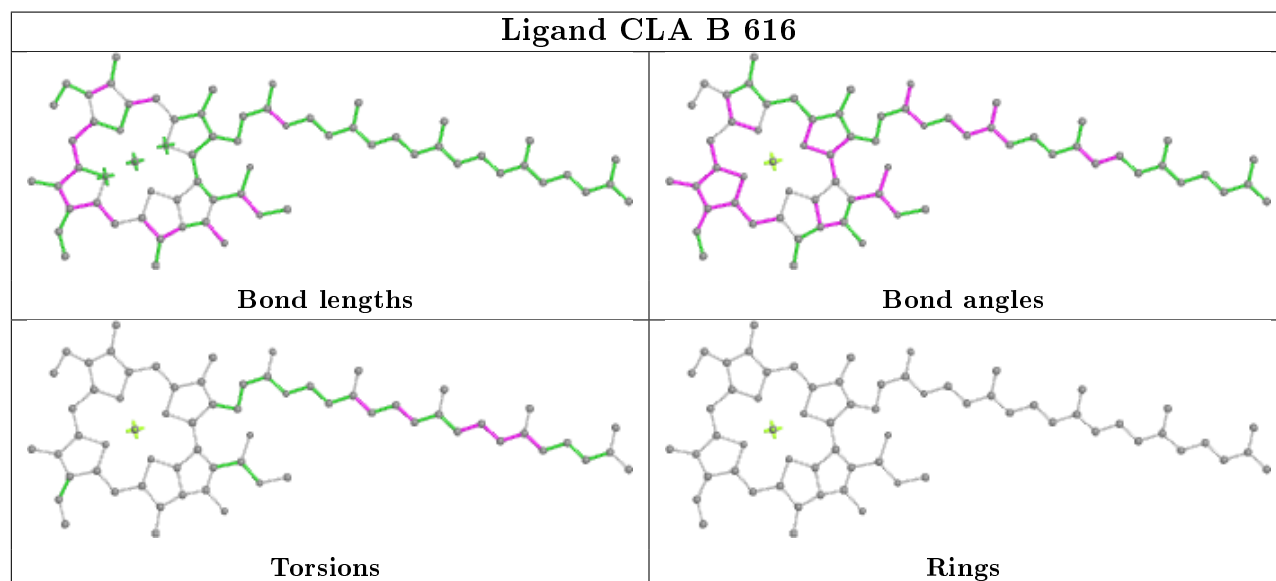
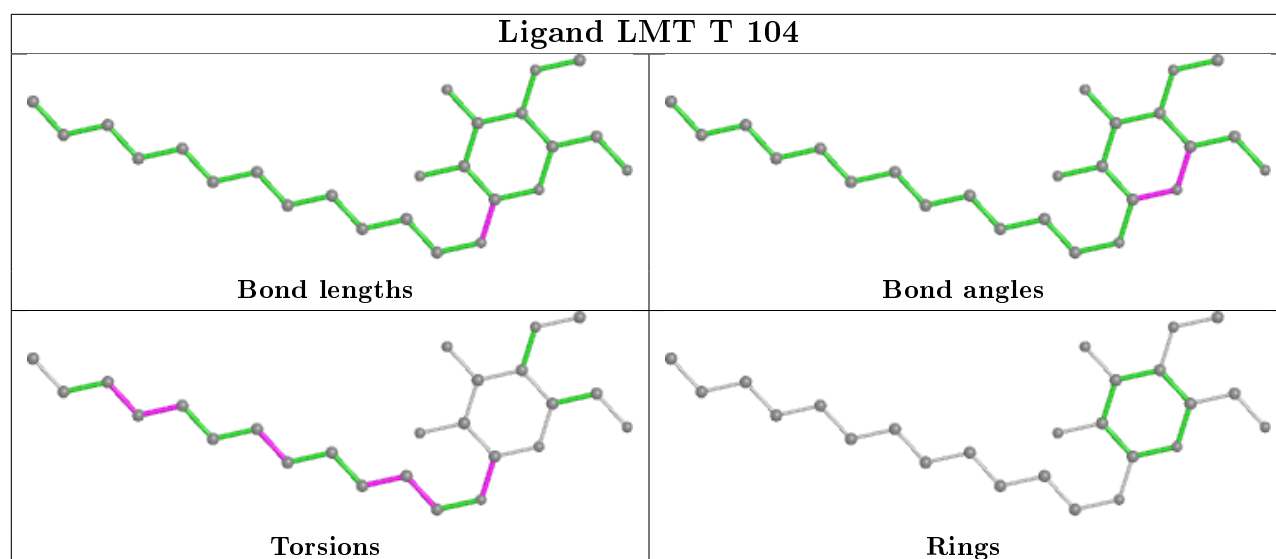


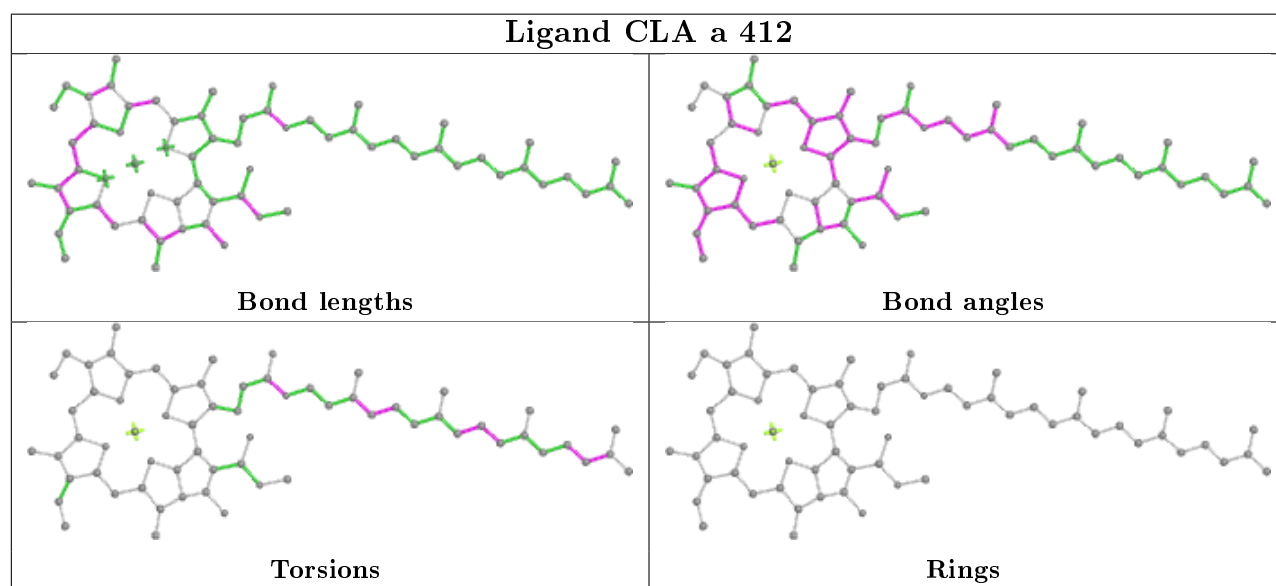
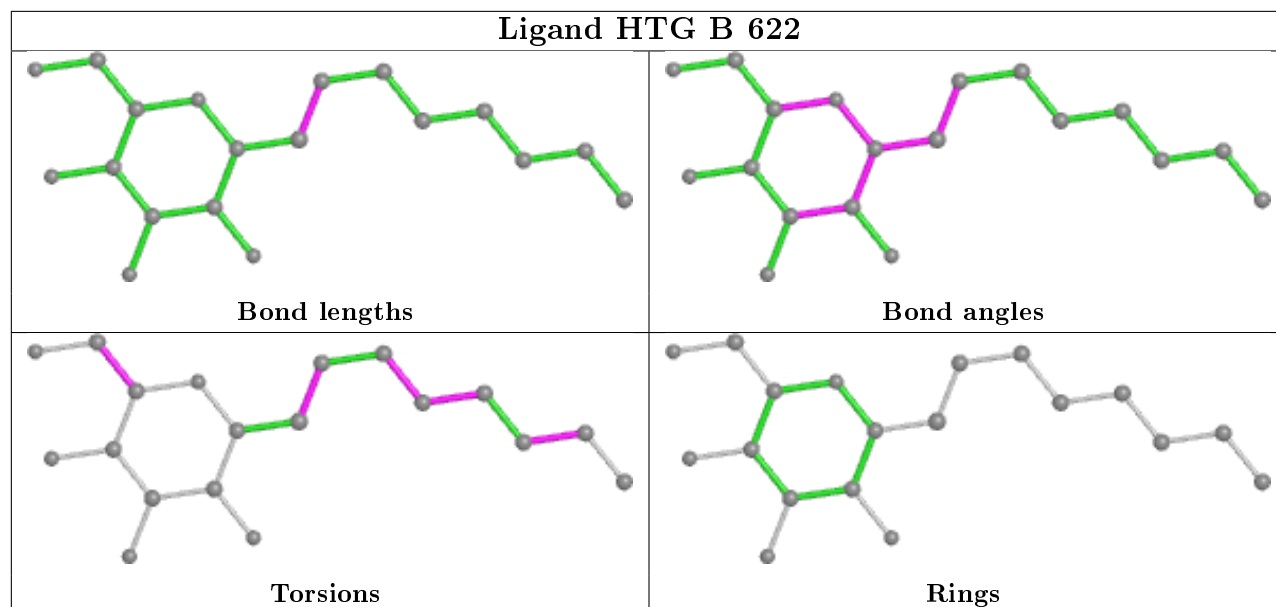
Ligand CLA B 606

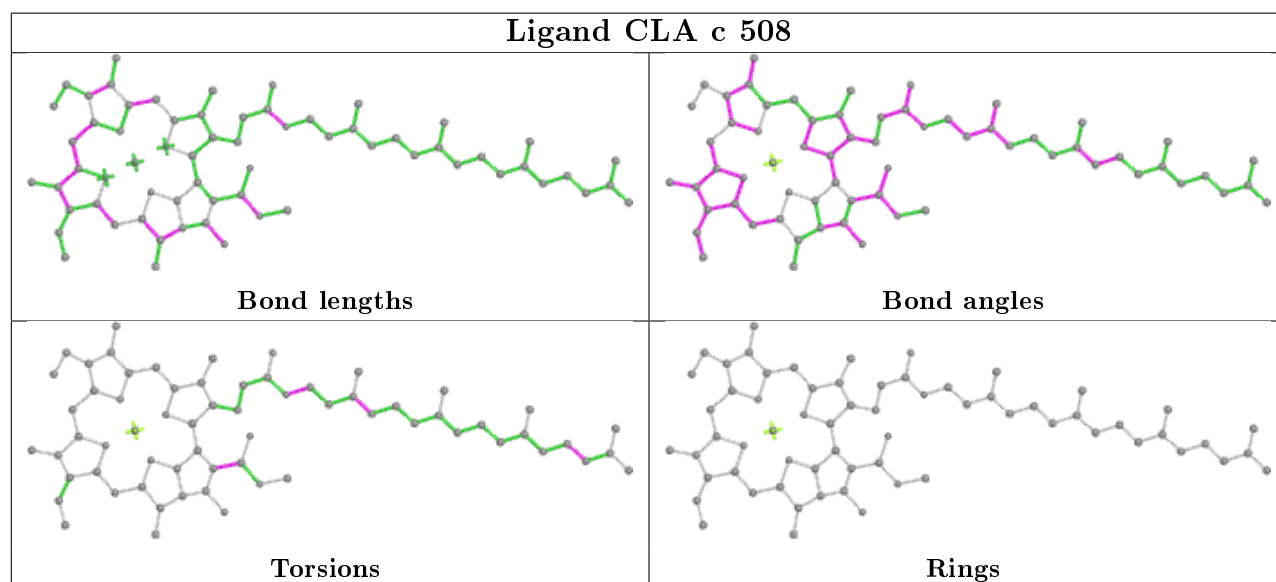
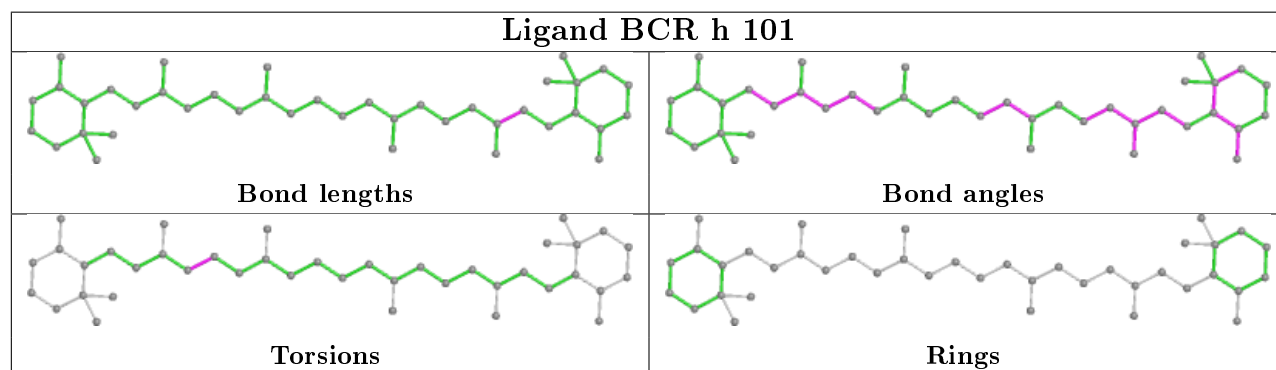
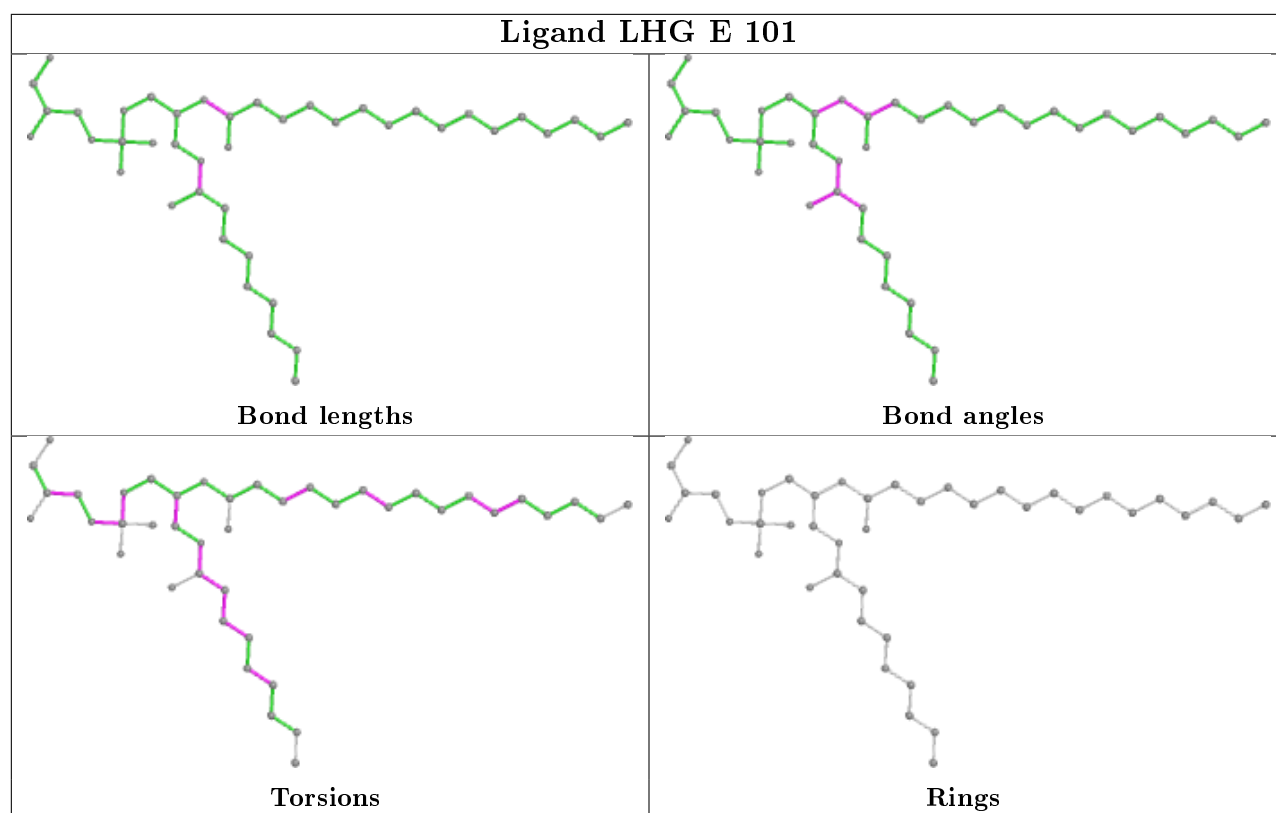


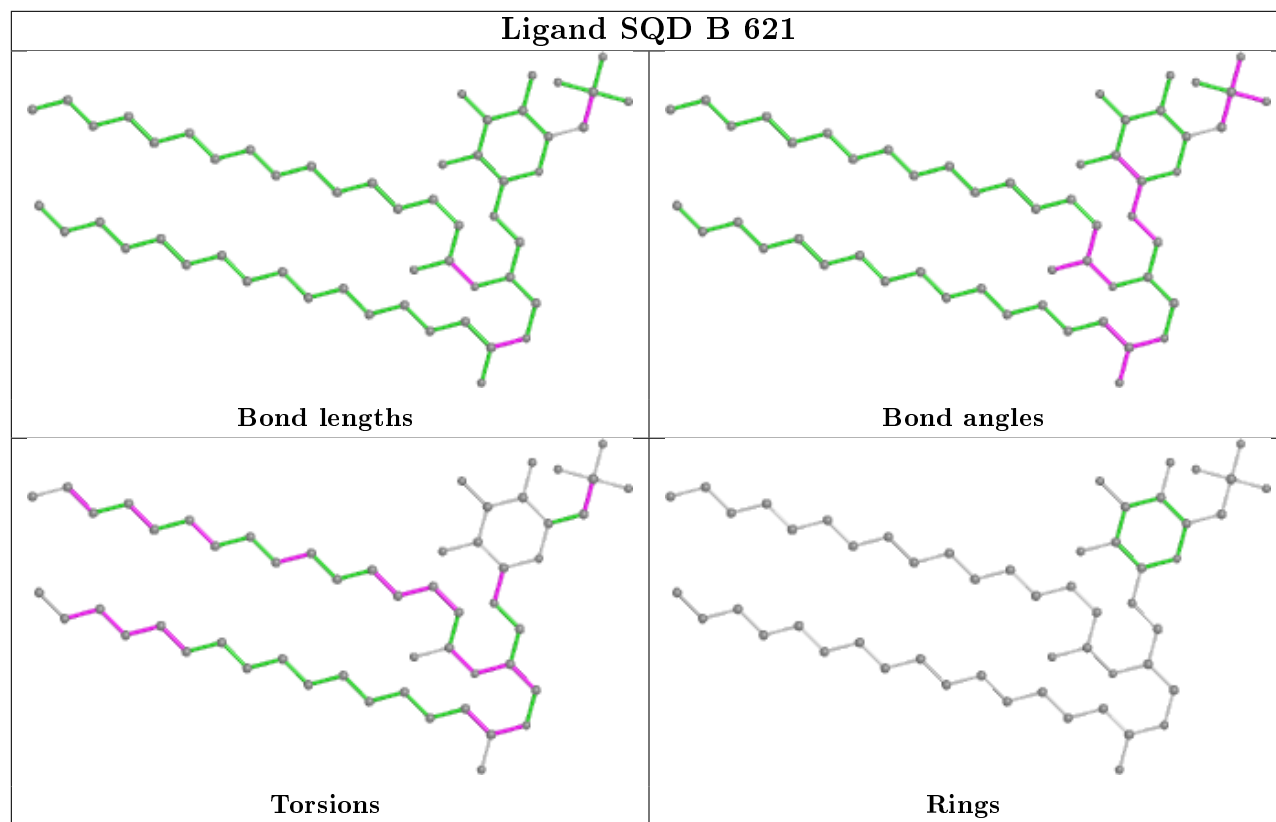
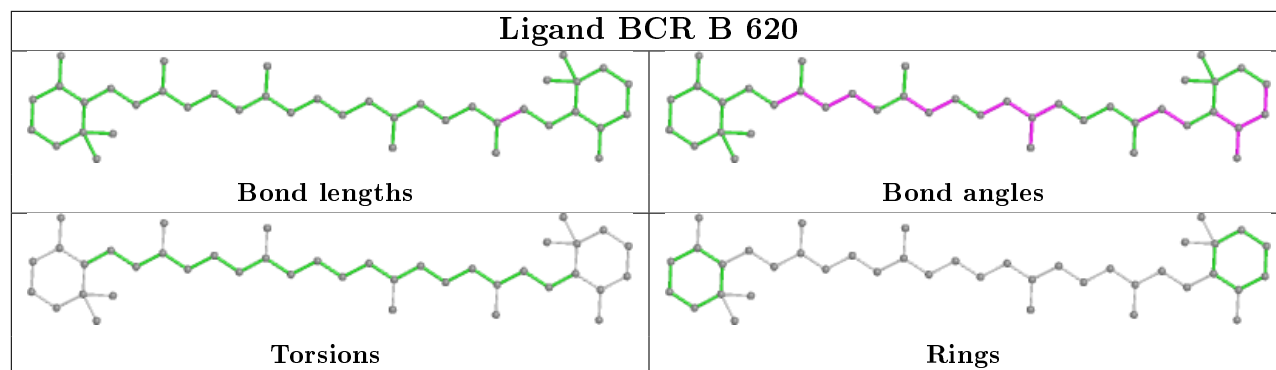
Ligand CLA c 505

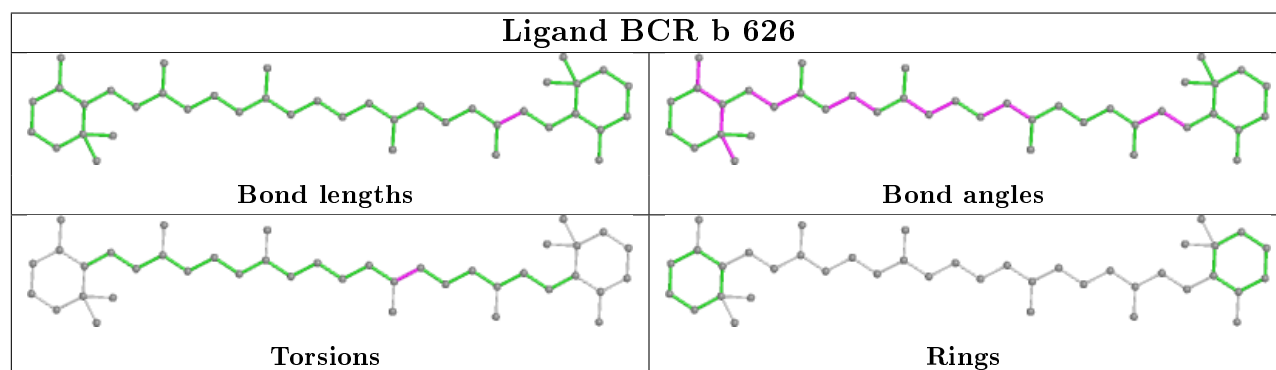
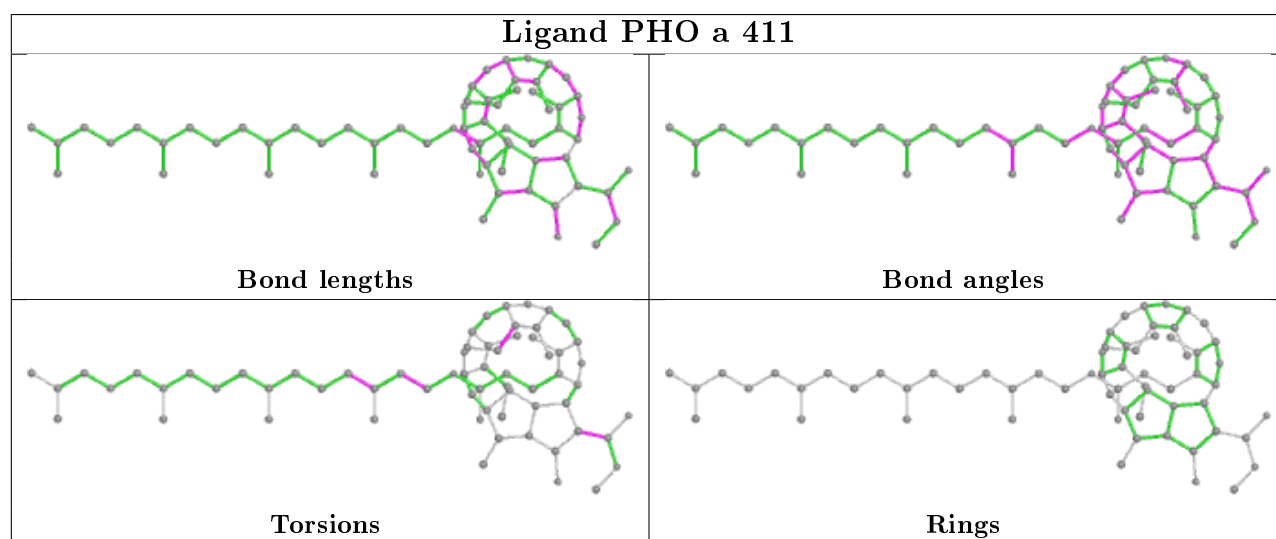
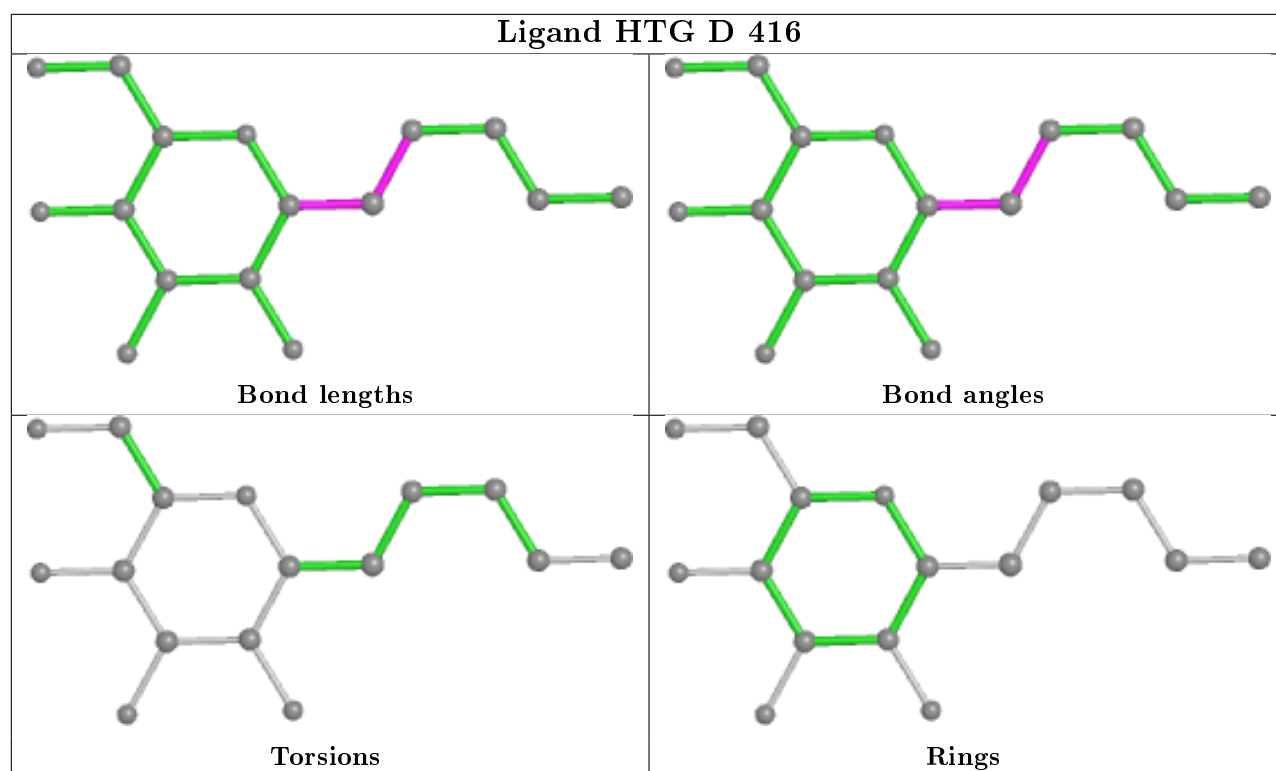


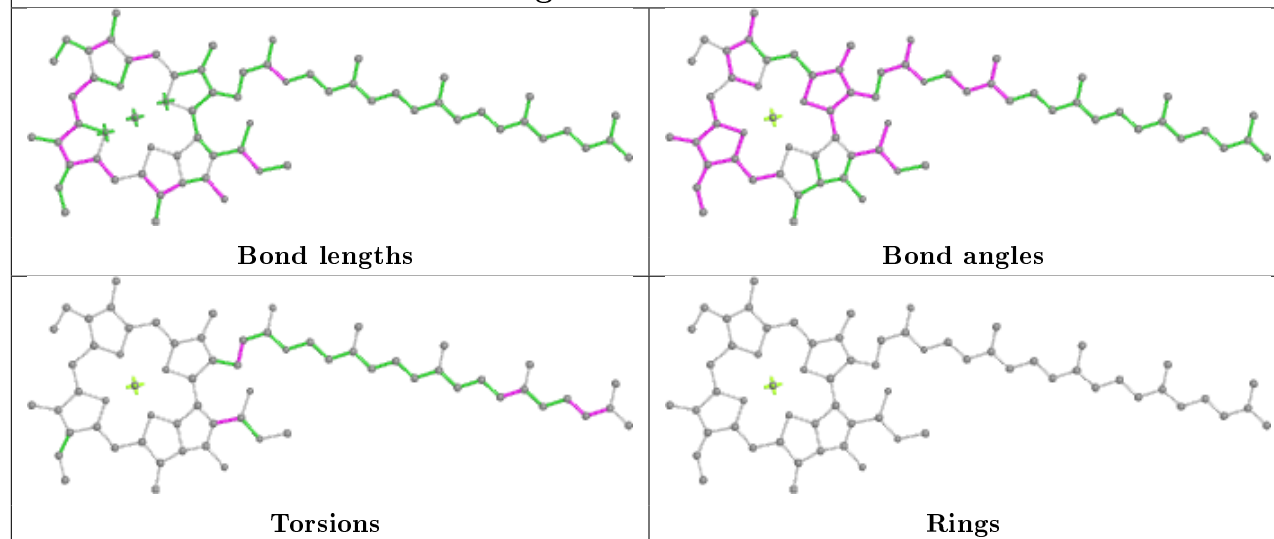
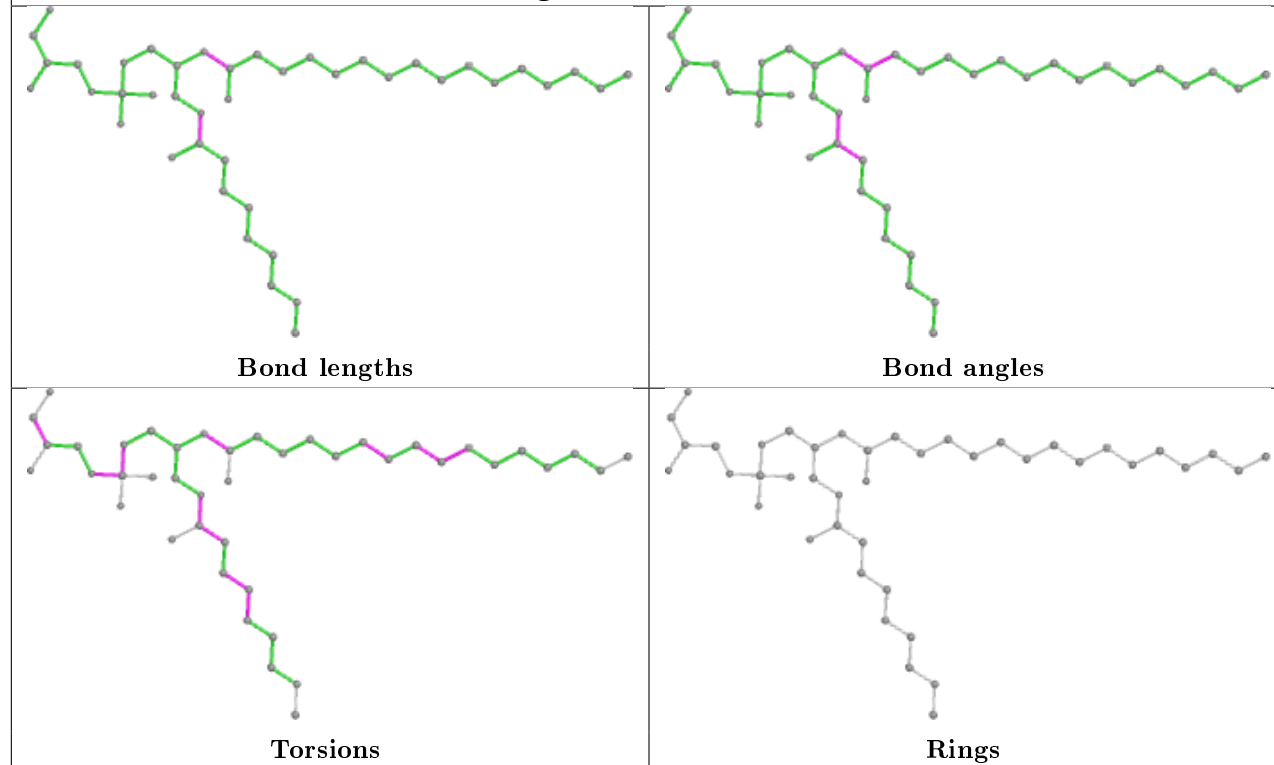


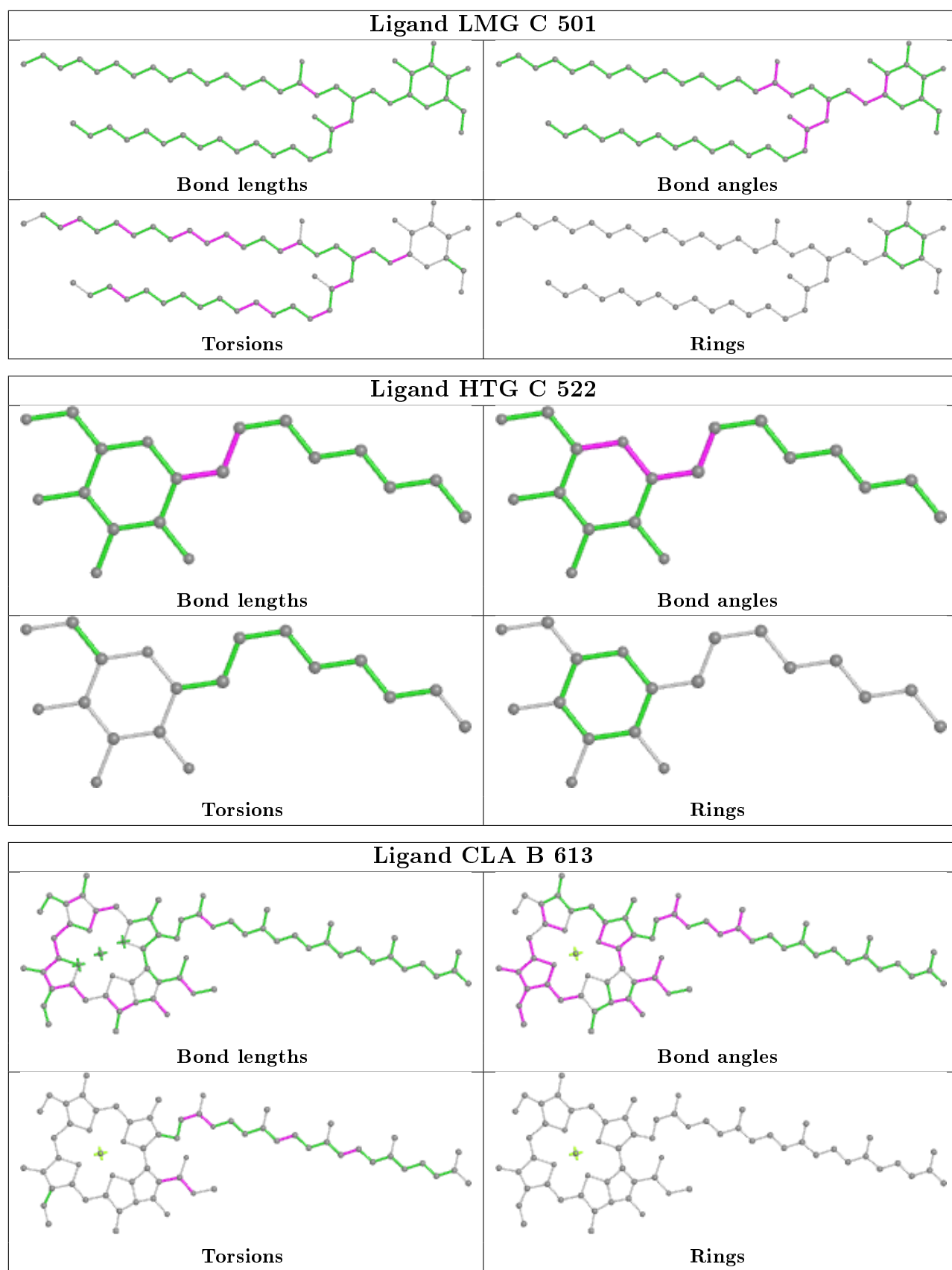


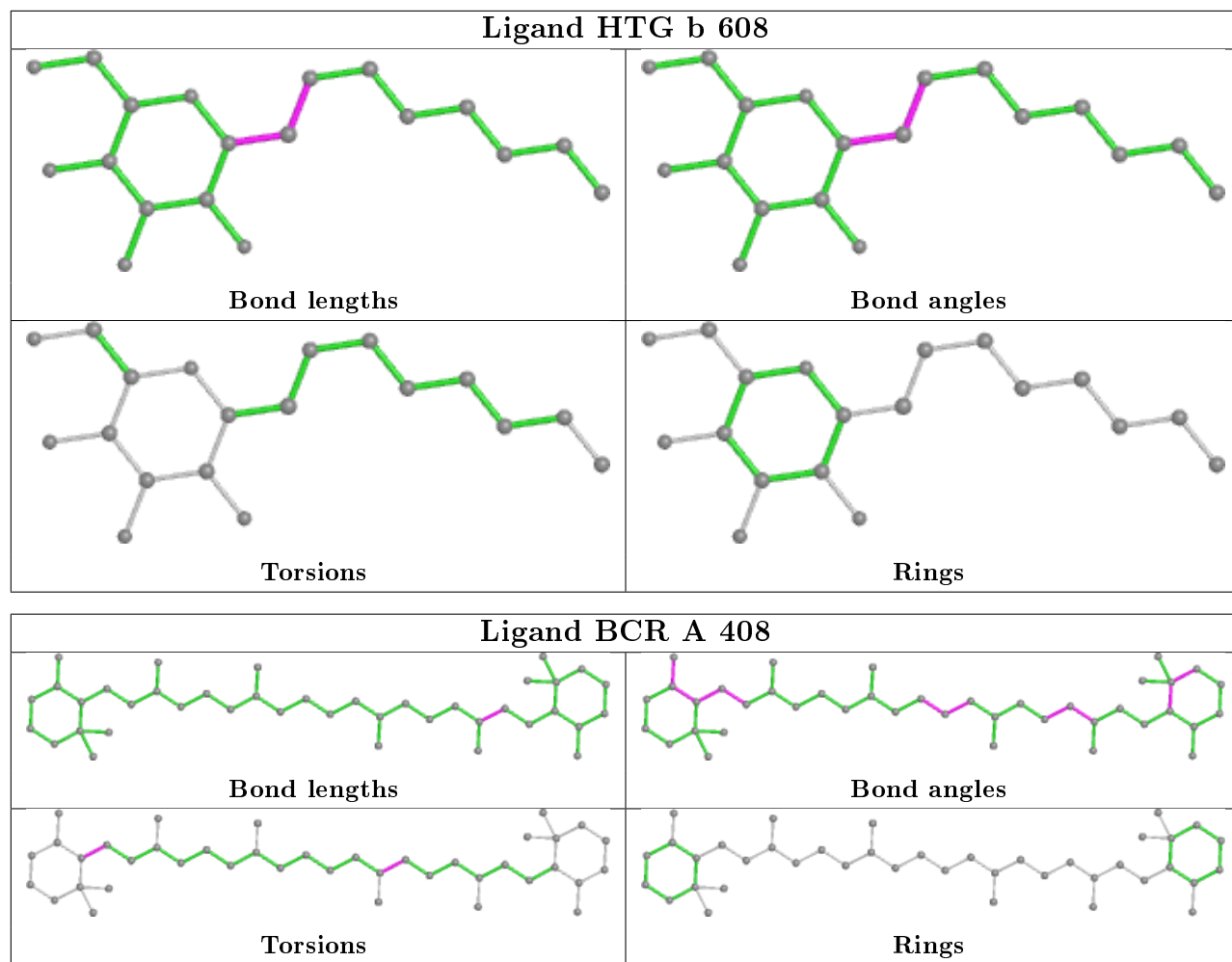


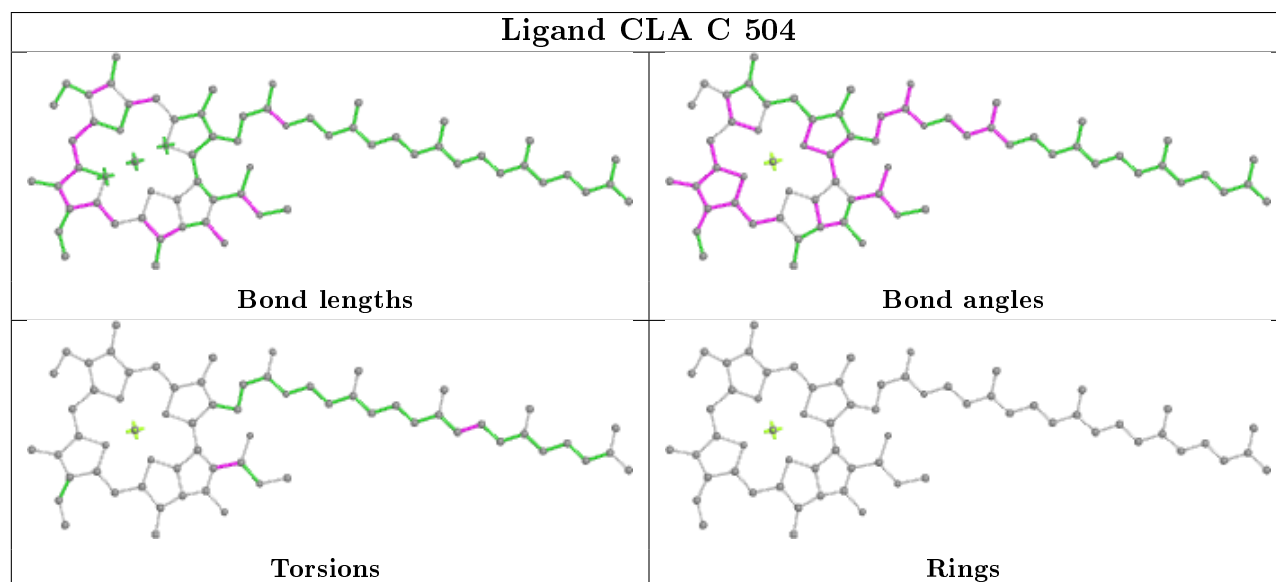
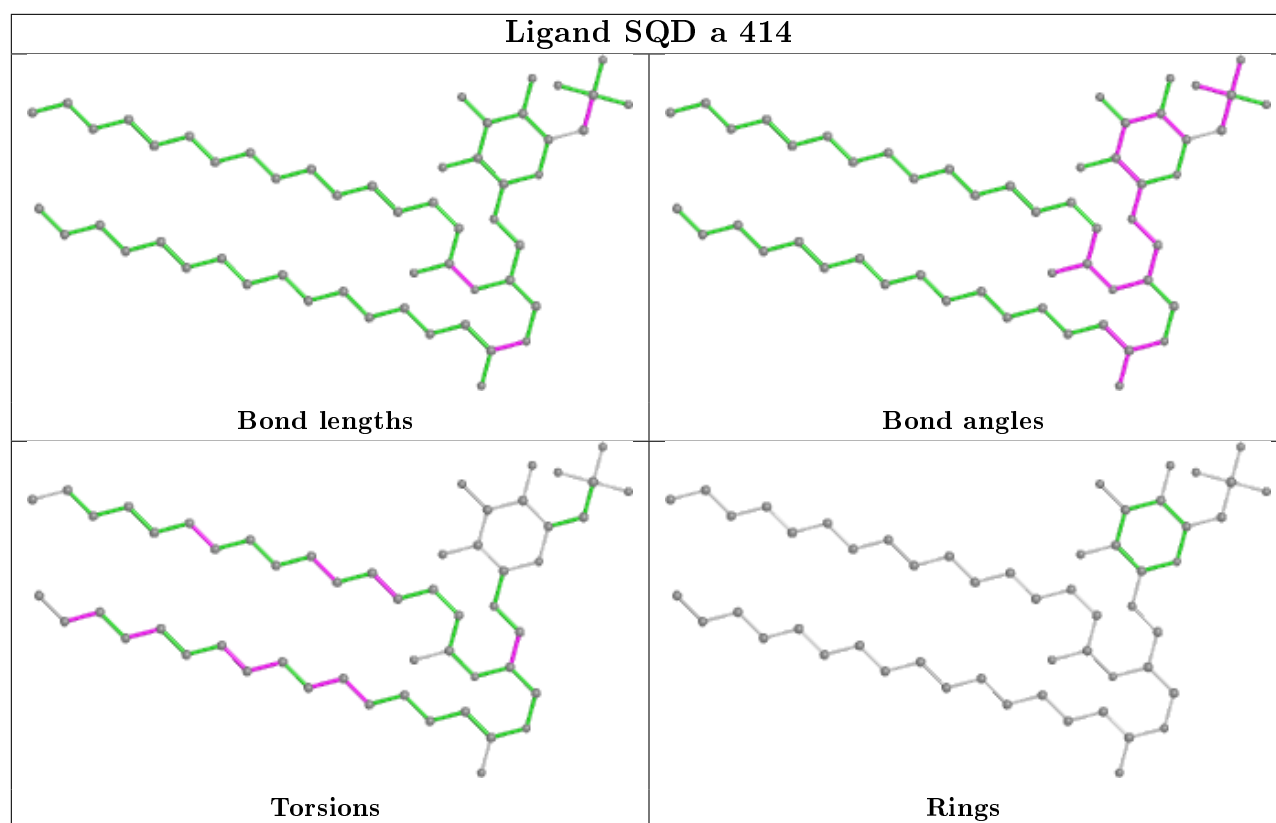


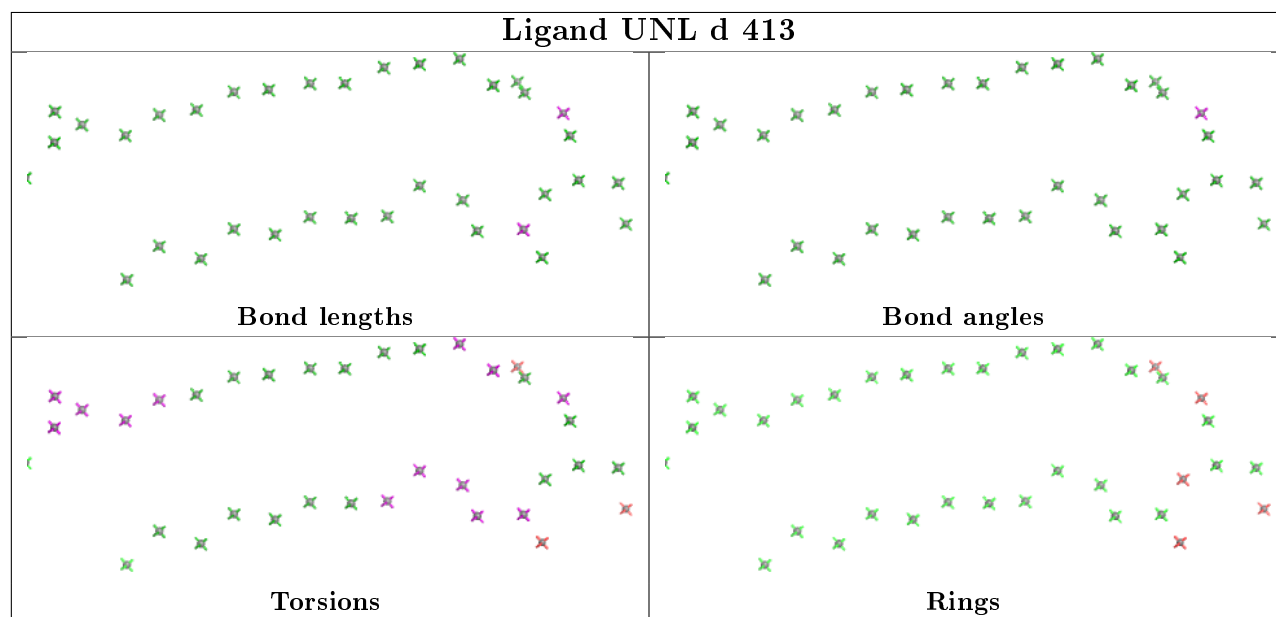
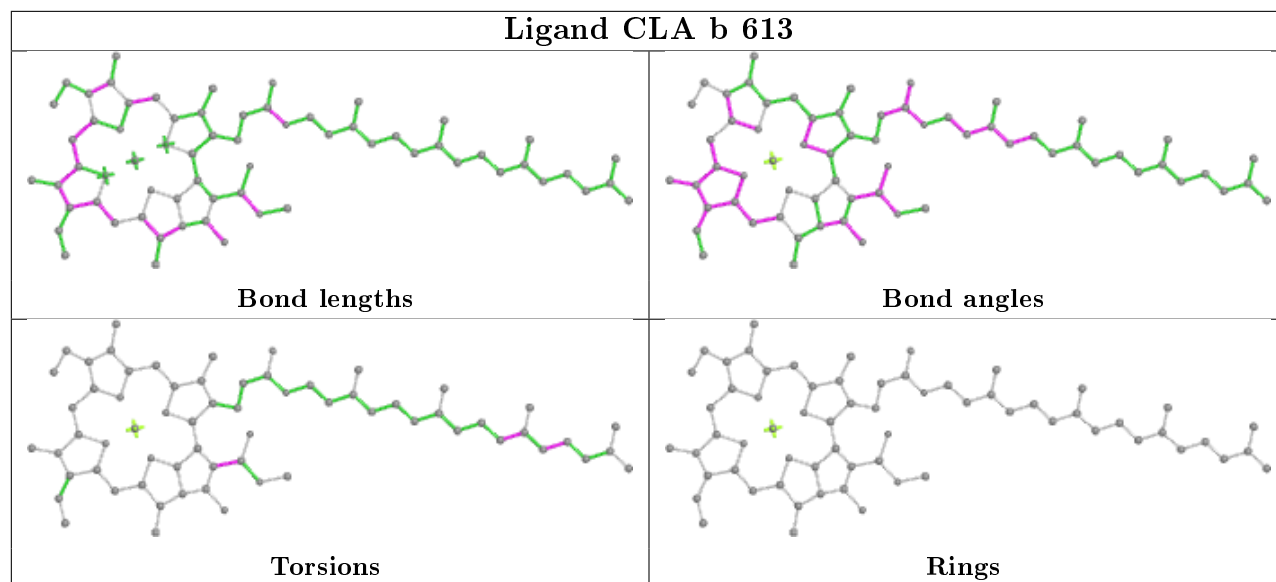


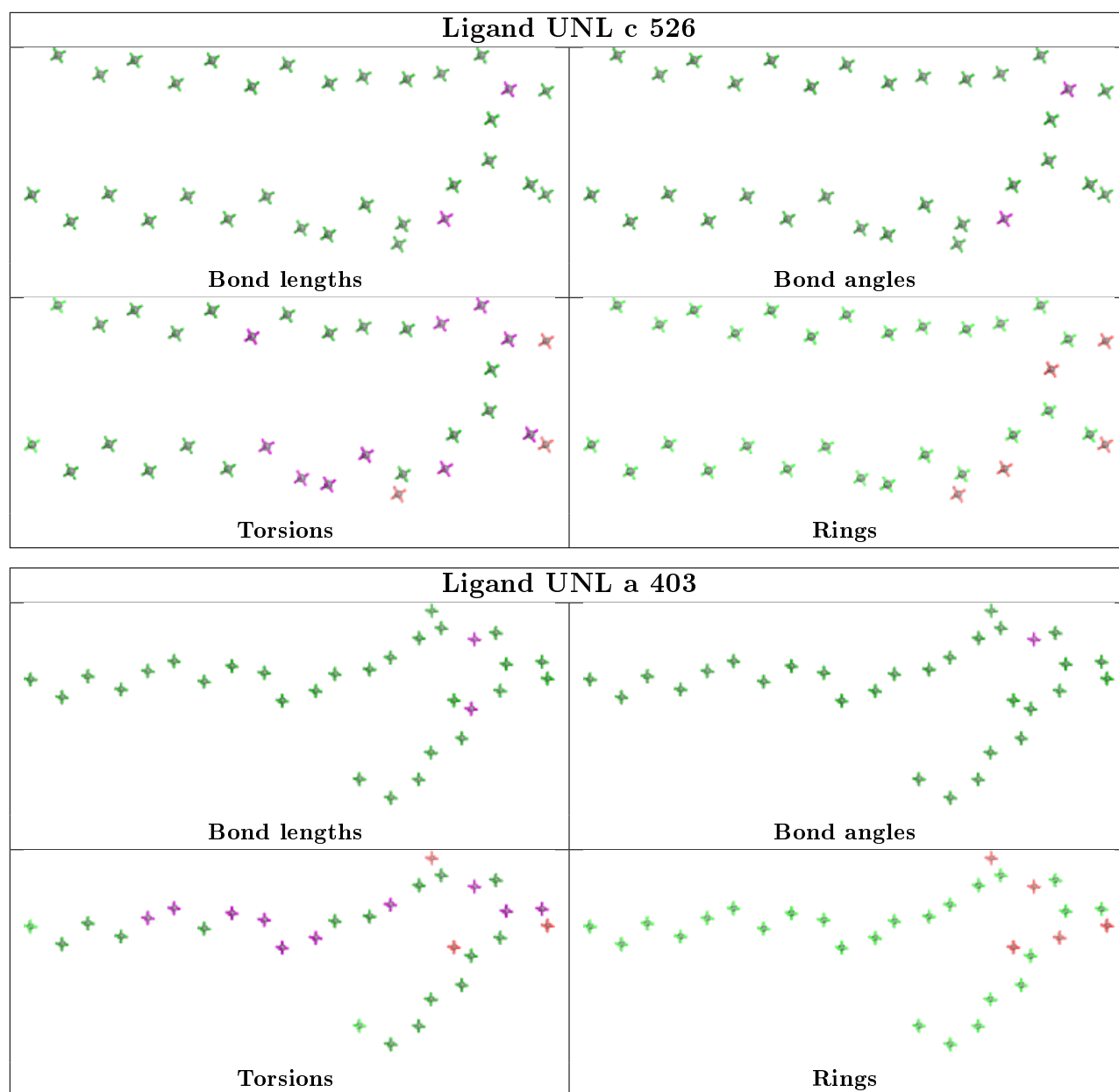
Ligand CLA b 619**Ligand LHG a 420**

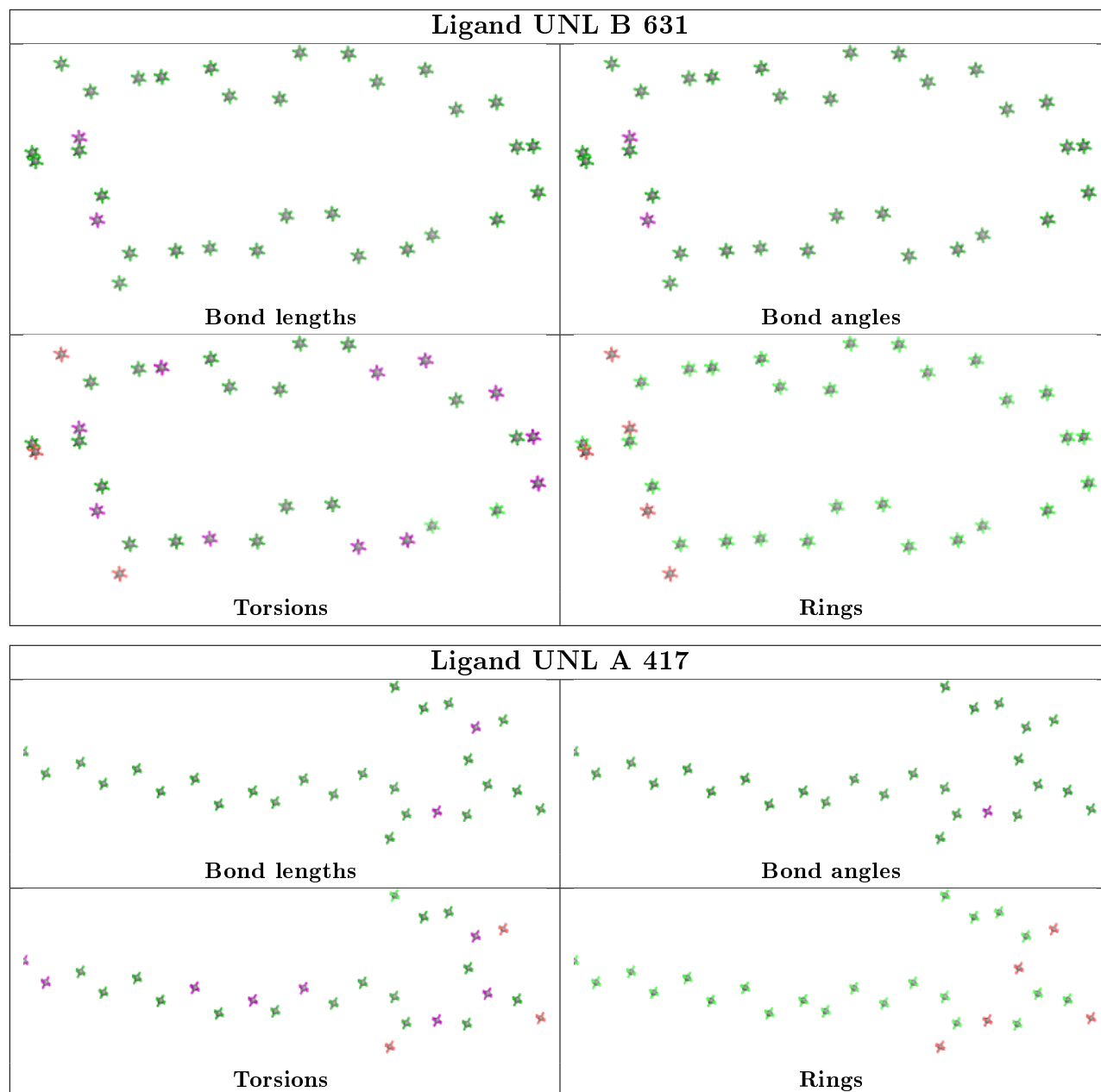


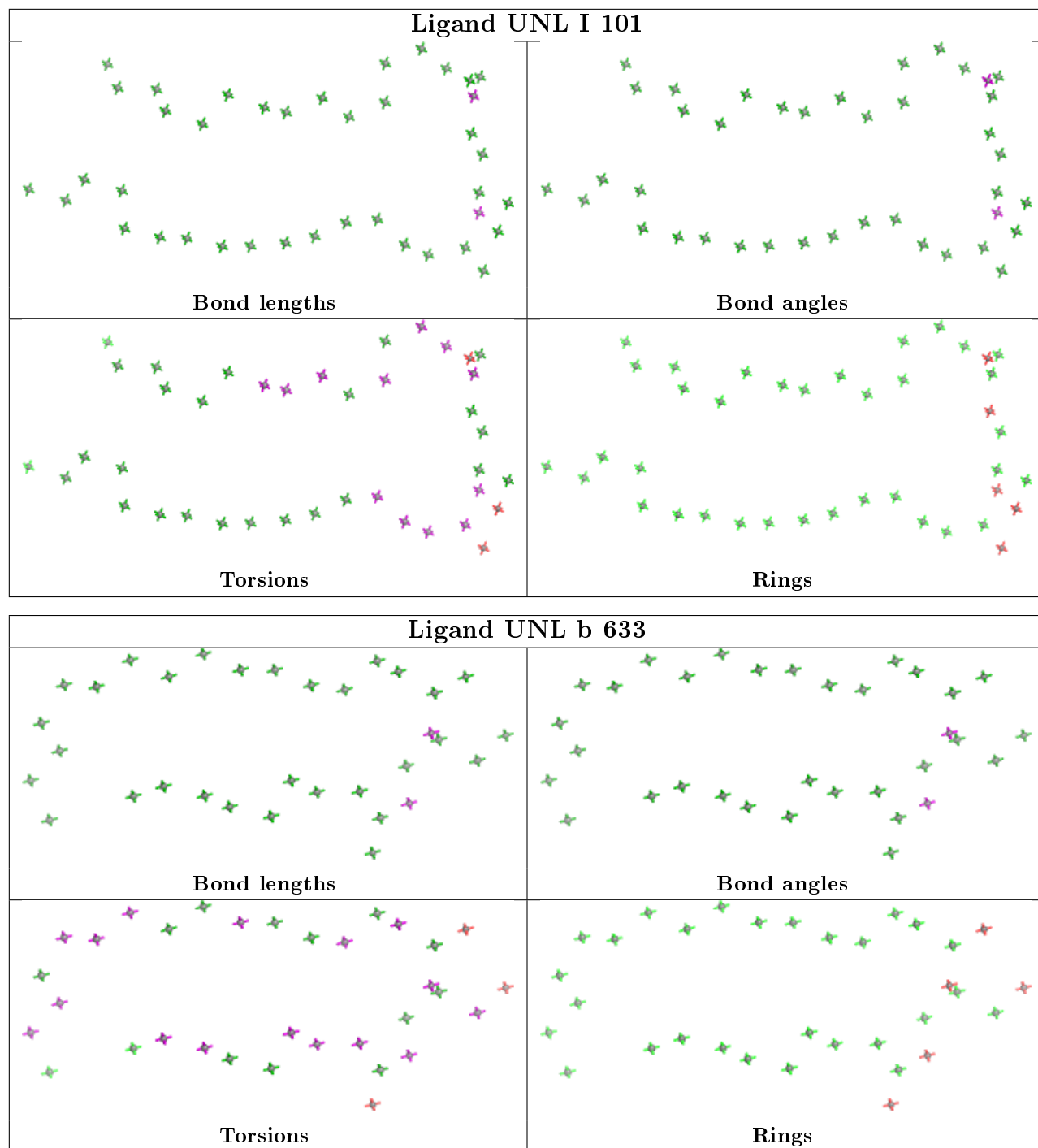


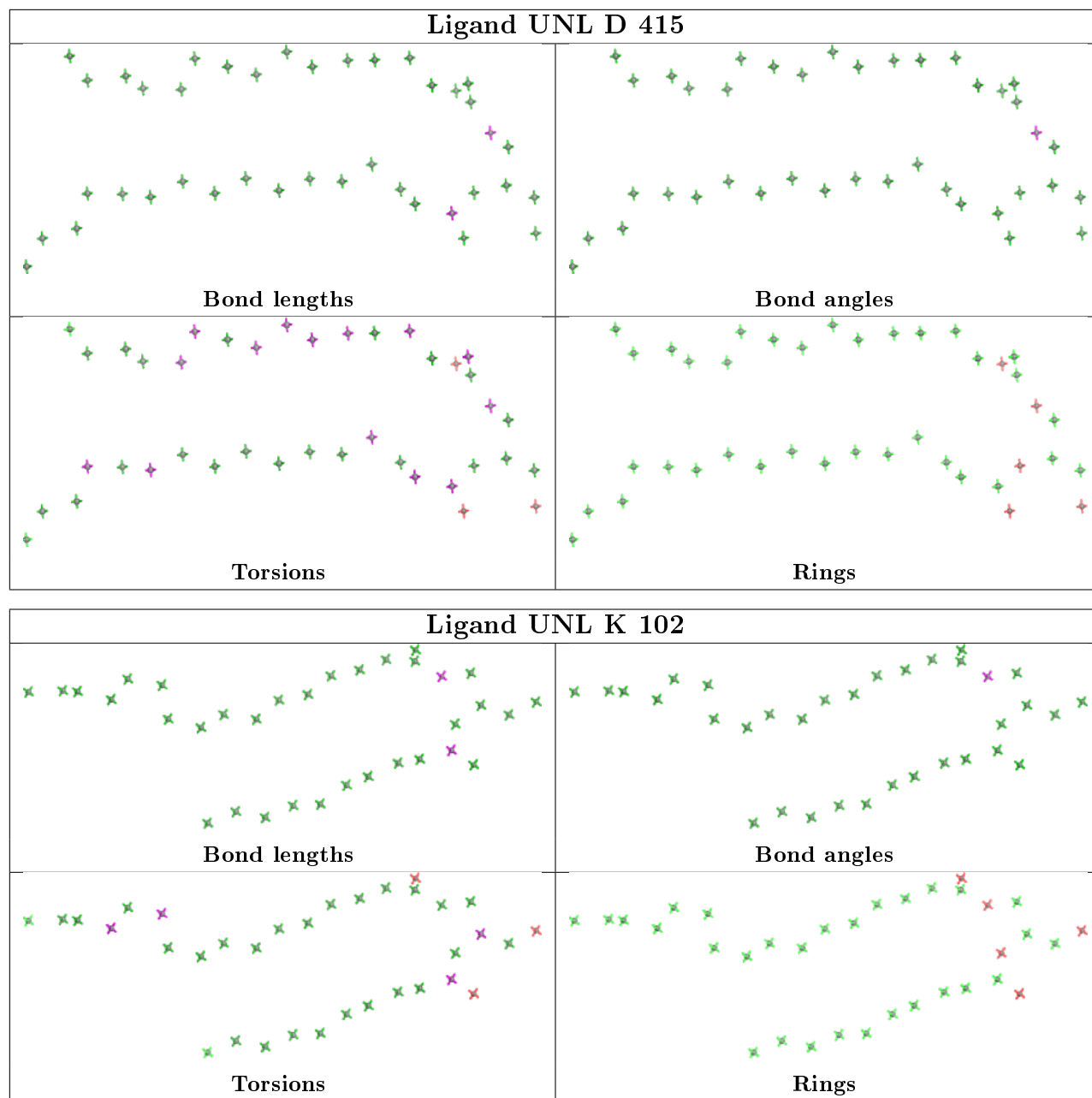


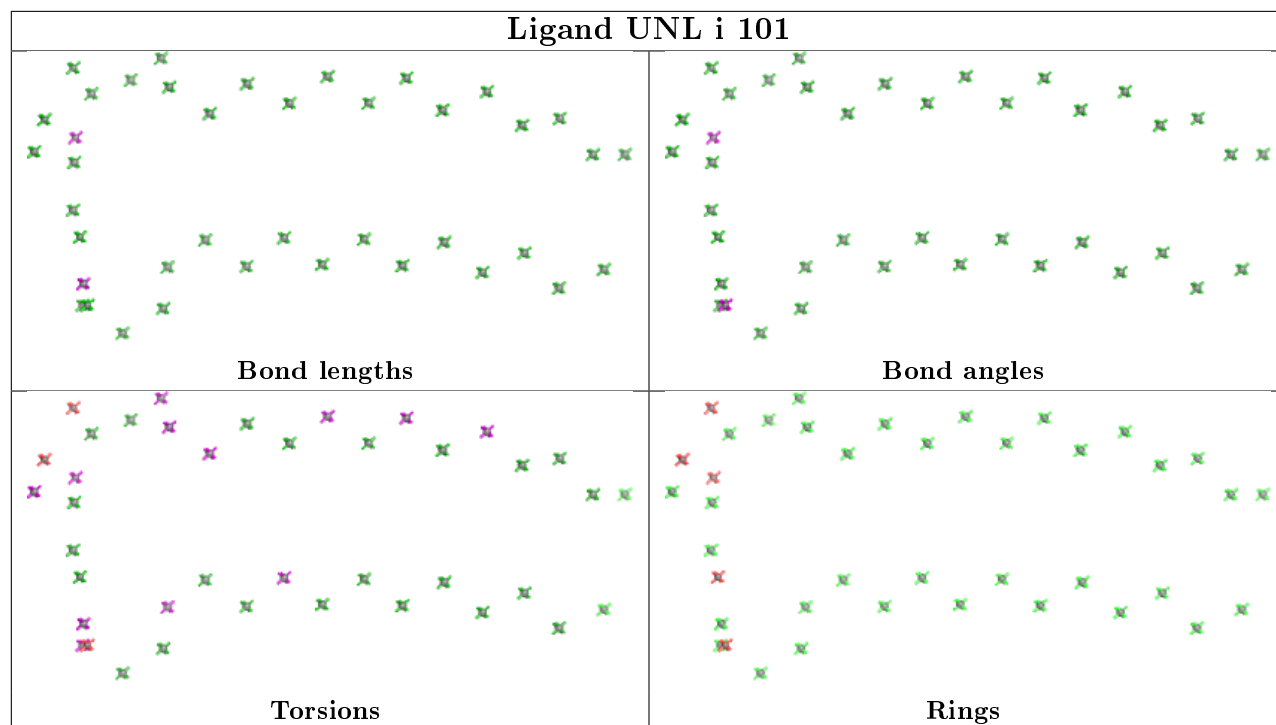












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	0.19	1 (0%) 94 94	36, 47, 80, 129	0
1	a	334/344 (97%)	0.31	13 (3%) 39 42	36, 49, 88, 147	0
2	B	504/505 (99%)	0.21	10 (1%) 65 68	38, 52, 93, 149	0
2	b	503/505 (99%)	0.30	20 (3%) 38 41	37, 53, 104, 202	0
3	C	451/455 (99%)	0.34	21 (4%) 31 33	42, 62, 91, 136	0
3	c	455/455 (100%)	0.16	4 (0%) 84 86	46, 66, 87, 123	0
4	D	341/342 (99%)	0.13	5 (1%) 73 75	34, 49, 82, 143	0
4	d	341/342 (99%)	0.21	4 (1%) 79 80	36, 51, 77, 115	0
5	E	81/84 (96%)	1.26	20 (24%) 0 0	56, 85, 117, 162	0
5	e	81/84 (96%)	0.70	8 (9%) 7 7	58, 79, 131, 187	0
6	F	34/44 (77%)	0.62	5 (14%) 2 2	58, 72, 120, 130	0
6	f	32/44 (72%)	0.11	0 100 100	58, 68, 128, 159	0
7	H	65/65 (100%)	0.18	1 (1%) 73 75	52, 65, 85, 166	0
7	h	65/65 (100%)	0.11	2 (3%) 49 52	52, 65, 85, 169	0
8	I	37/38 (97%)	0.46	4 (10%) 5 5	50, 64, 136, 194	0
8	i	37/38 (97%)	0.36	3 (8%) 12 12	48, 61, 131, 164	0
9	J	38/39 (97%)	1.17	10 (26%) 0 0	63, 79, 167, 195	0
9	j	39/39 (100%)	0.66	6 (15%) 2 1	58, 71, 149, 191	0
10	K	37/37 (100%)	0.72	5 (13%) 3 2	65, 79, 98, 119	0
10	k	37/37 (100%)	0.37	0 100 100	61, 75, 97, 119	0
11	L	37/37 (100%)	0.09	0 100 100	36, 42, 101, 127	0
11	l	37/37 (100%)	0.17	0 100 100	35, 43, 104, 138	0
12	M	33/36 (91%)	0.18	0 100 100	33, 43, 76, 131	0
12	m	33/36 (91%)	0.36	0 100 100	37, 44, 89, 122	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.29	7 (2%) 51 55	36, 58, 101, 145	0
13	o	243/244 (99%)	0.18	3 (1%) 79 80	38, 61, 115, 178	0
14	T	29/32 (90%)	0.34	1 (3%) 45 48	36, 42, 77, 145	0
14	t	29/32 (90%)	0.25	0 100 100	36, 44, 75, 144	0
15	U	97/104 (93%)	0.11	1 (1%) 82 84	45, 57, 90, 133	0
15	u	97/104 (93%)	0.07	0 100 100	46, 61, 79, 123	0
16	V	137/137 (100%)	0.23	1 (0%) 87 89	44, 59, 83, 114	0
16	v	137/137 (100%)	0.11	1 (0%) 87 89	48, 70, 103, 132	0
17	Y	29/30 (96%)	3.70	13 (44%) 0 0	80, 102, 195, 215	0
17	y	29/30 (96%)	1.01	5 (17%) 1 1	80, 94, 148, 163	0
18	X	39/40 (97%)	0.48	4 (10%) 6 6	63, 72, 125, 163	0
18	x	38/40 (95%)	0.53	4 (10%) 6 6	64, 74, 130, 159	0
19	Z	62/62 (100%)	1.45	18 (29%) 0 0	82, 99, 136, 151	0
19	z	62/62 (100%)	1.27	22 (35%) 0 0	80, 100, 152, 195	0
20	R	18/34 (52%)	5.46	18 (100%) 0 0	111, 147, 171, 187	0
All	All	5275/5384 (97%)	0.34	240 (4%) 33 36	33, 58, 110, 215	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	18.4
17	Y	19	ILE	15.8
17	Y	20	ALA	12.3
2	b	494	GLY	10.6
17	Y	21	GLN	10.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.16	38,48,56,93	0
14	FME	t	1	10/11	0.95	0.15	28,39,49,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	FME	i	1	10/11	0.95	0.15	41,58,64,68	0
12	FME	m	1	10/11	0.96	0.19	35,51,97,107	0
8	FME	I	1	10/11	0.97	0.14	39,51,61,66	0
12	FME	M	1	10/11	0.97	0.20	31,47,94,99	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LMT	F	101	35/35	0.28	0.58	133,171,182,184	0
34	DGD	d	408	62/66	0.33	0.49	87,130,176,182	0
27	LMT	b	630	25/35	0.50	0.41	85,107,156,159	0
31	UNL	J	101	10/-	0.51	0.31	70,104,114,115	0
27	LMT	a	419	35/35	0.52	0.42	98,142,160,162	0
27	LMT	C	521	35/35	0.55	0.41	103,145,170,173	0
31	UNL	j	101	10/-	0.56	0.31	59,89,101,103	0
38	LHG	a	420	42/49	0.56	0.34	92,136,181,183	0
31	UNL	c	526	32/-	0.58	0.29	82,100,140,147	0
31	UNL	K	102	34/-	0.58	0.27	94,127,136,139	0
34	DGD	D	410	52/66	0.60	0.39	74,109,157,168	0
38	LHG	E	101	42/49	0.62	0.30	89,127,142,147	0
27	LMT	a	404	35/35	0.63	0.29	55,101,126,145	0
32	CA	b	609	1/1	0.63	0.12	131,131,131,131	0
27	LMT	m	102	35/35	0.64	0.29	51,111,129,130	0
31	UNL	a	403	30/-	0.65	0.31	67,93,124,131	0
27	LMT	D	405	35/35	0.65	0.31	84,132,152,153	0
33	HTG	D	416	16/19	0.65	0.29	70,134,155,156	0
31	UNL	b	633	33/-	0.66	0.29	55,88,143,145	0
27	LMT	e	102	35/35	0.66	0.32	86,136,156,157	0
25	SQD	f	102	43/54	0.67	0.31	106,125,157,166	0
22	CL	U	201	1/1	0.67	0.10	120,120,120,120	0
33	HTG	B	630	19/19	0.68	0.25	58,118,140,169	0
35	LMG	C	519	51/55	0.68	0.26	59,102,122,125	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	HTG	d	414	16/19	0.69	0.24	75,116,122,125	0
31	UNL	A	417	28/-	0.70	0.27	63,89,113,115	0
27	LMT	M	105	35/35	0.70	0.30	50,99,119,121	0
35	LMG	Z	101	37/55	0.70	0.32	67,138,150,151	0
27	LMT	A	413	35/35	0.71	0.26	57,91,114,119	0
33	HTG	b	608	19/19	0.71	0.22	58,116,151,164	0
26	GOL	v	201	6/6	0.72	0.30	78,98,103,104	0
33	HTG	B	623	19/19	0.74	0.24	85,137,145,176	0
34	DGD	C	517	62/66	0.74	0.26	55,74,100,114	0
27	LMT	M	104	35/35	0.74	0.28	44,109,152,157	0
26	GOL	V	202	6/6	0.74	0.57	88,95,99,99	0
35	LMG	z	101	39/55	0.75	0.31	74,125,149,162	0
33	HTG	b	631	19/19	0.76	0.30	66,80,98,102	0
31	UNL	B	631	33/-	0.76	0.32	61,83,134,137	0
33	HTG	b	632	19/19	0.77	0.27	80,134,152,155	0
30	PL9	a	416[A]	55/55	0.77	0.28	91,109,122,123	55
30	PL9	a	416[B]	55/55	0.77	0.28	92,108,122,124	55
35	LMG	C	520	51/55	0.77	0.35	63,125,134,137	0
31	UNL	m	101	10/-	0.77	0.34	46,60,79,80	0
33	HTG	C	523	19/19	0.78	0.30	78,110,127,130	0
27	LMT	T	104	25/35	0.79	0.30	44,81,135,142	0
30	PL9	A	416[A]	55/55	0.79	0.29	86,107,117,119	55
26	GOL	O	301	6/6	0.79	0.17	81,84,87,87	0
32	CA	f	103	1/1	0.79	0.13	127,127,127,127	0
32	CA	B	601	1/1	0.79	0.07	131,131,131,131	0
30	PL9	A	416[B]	55/55	0.79	0.29	86,107,117,119	55
25	SQD	a	405	54/54	0.80	0.24	50,82,127,132	0
26	GOL	V	205	6/6	0.80	0.20	87,100,106,115	0
31	UNL	d	413	36/-	0.81	0.25	64,85,131,137	0
25	SQD	L	102	54/54	0.81	0.23	42,76,124,140	0
31	UNL	M	103	10/-	0.81	0.30	52,63,78,80	0
33	HTG	c	525	19/19	0.81	0.31	86,116,133,149	0
25	SQD	A	412	54/54	0.82	0.23	56,77,134,138	0
35	LMG	c	522	51/55	0.82	0.23	64,95,120,122	0
23	CLA	c	517	65/65	0.82	0.23	80,95,105,107	0
31	UNL	I	101	40/-	0.82	0.28	58,93,150,153	0
25	SQD	B	621	54/54	0.82	0.24	53,79,156,160	0
27	LMT	t	101	25/35	0.82	0.31	45,80,143,149	0
25	SQD	F	104	43/54	0.82	0.29	91,122,143,145	0
27	LMT	M	102	35/35	0.82	0.24	42,101,123,131	0
34	DGD	C	518	62/66	0.83	0.20	51,64,88,105	0
31	UNL	D	415	40/-	0.83	0.22	62,86,130,137	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	LMG	c	523	51/55	0.83	0.26	65,117,129,133	0
26	GOL	v	202	6/6	0.83	0.29	103,105,109,122	0
23	CLA	C	514	65/65	0.83	0.29	71,91,120,124	0
22	CL	v	204	1/1	0.83	0.12	120,120,120,120	0
31	UNL	i	101	40/-	0.83	0.24	50,87,139,142	0
26	GOL	a	402	6/6	0.83	0.27	103,108,108,109	0
35	LMG	M	101	51/55	0.84	0.23	39,59,75,91	0
35	LMG	b	629	51/55	0.85	0.24	40,54,76,84	0
35	LMG	C	501	51/55	0.85	0.22	62,84,103,107	0
33	HTG	b	607	19/19	0.85	0.17	53,83,94,95	0
34	DGD	h	102	62/66	0.85	0.22	36,58,75,82	0
23	CLA	C	505	65/65	0.85	0.24	47,67,101,108	0
33	HTG	c	524	19/19	0.86	0.18	99,106,117,119	0
25	SQD	A	409	54/54	0.86	0.24	55,98,108,111	0
33	HTG	B	629	19/19	0.86	0.17	48,88,113,116	0
33	HTG	C	522	19/19	0.86	0.24	84,94,135,137	0
35	LMG	a	415	51/55	0.86	0.20	59,85,101,114	0
34	DGD	B	632	62/66	0.86	0.21	43,59,89,105	0
25	SQD	a	414	54/54	0.86	0.19	56,83,104,105	0
33	HTG	B	622	19/19	0.87	0.22	63,75,85,91	0
26	GOL	C	524	6/6	0.87	0.38	88,89,103,104	0
33	HTG	b	601	19/19	0.87	0.20	49,65,76,77	0
31	UNL	X	101	18/-	0.87	0.22	69,87,109,111	0
34	DGD	c	520	62/66	0.87	0.20	49,66,111,127	0
33	HTG	V	207	19/19	0.88	0.36	80,105,126,240	0
31	UNL	d	415	18/-	0.88	0.22	67,80,109,116	0
39	HEM	F	102	43/43	0.88	0.24	59,85,111,234	0
38	LHG	D	413	49/49	0.89	0.26	51,78,118,126	0
35	LMG	D	417	51/55	0.89	0.21	50,76,125,133	0
23	CLA	c	511	65/65	0.89	0.19	52,65,77,82	0
26	GOL	T	101	6/6	0.89	0.30	58,81,84,93	0
26	GOL	T	102	6/6	0.89	0.49	107,116,118,122	0
34	DGD	c	521	62/66	0.90	0.19	51,61,98,109	0
23	CLA	b	611	65/65	0.90	0.20	43,52,62,70	0
23	CLA	B	602	65/65	0.90	0.20	53,75,112,132	0
23	CLA	c	510	65/65	0.90	0.18	57,75,99,102	0
38	LHG	D	411	49/49	0.90	0.24	40,52,64,80	0
23	CLA	b	616	65/65	0.90	0.20	29,42,50,53	0
33	HTG	o	301	19/19	0.90	0.19	51,74,87,91	0
35	LMG	d	416	51/55	0.90	0.20	53,66,107,118	0
23	CLA	c	512	65/65	0.90	0.17	47,57,115,122	0
23	CLA	C	507	65/65	0.90	0.17	59,78,118,125	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	GOL	A	411	6/6	0.90	0.20	84,86,91,92	0
23	CLA	C	512	65/65	0.90	0.20	54,76,92,97	0
26	GOL	f	101	6/6	0.90	0.23	85,90,93,96	0
23	CLA	C	502	65/65	0.91	0.17	51,62,88,93	0
34	DGD	C	516	62/66	0.91	0.18	40,56,87,95	0
23	CLA	B	607	65/65	0.91	0.18	37,52,91,95	0
23	CLA	c	507	65/65	0.91	0.18	53,64,74,93	0
26	GOL	A	410	6/6	0.91	0.20	49,56,61,66	0
23	CLA	c	508	65/65	0.91	0.17	50,64,81,86	0
23	CLA	b	618	65/65	0.91	0.20	47,55,66,73	0
23	CLA	C	513	65/65	0.91	0.17	71,87,94,97	0
32	CA	C	526	1/1	0.91	0.12	83,83,83,83	0
24	BCR	K	101	40/40	0.91	0.21	64,83,92,94	0
26	GOL	b	606	6/6	0.91	0.24	75,87,92,94	0
23	CLA	B	614	65/65	0.91	0.18	32,43,62,72	0
26	GOL	c	502	6/6	0.91	0.42	81,89,105,110	0
23	CLA	c	509	65/65	0.91	0.17	45,56,73,77	0
38	LHG	d	411	49/49	0.91	0.22	47,63,114,118	0
26	GOL	b	605	6/6	0.91	0.22	69,87,103,103	0
23	CLA	b	610	65/65	0.91	0.20	53,84,129,138	0
26	GOL	B	627	6/6	0.92	0.33	58,78,80,82	0
26	GOL	t	103	6/6	0.92	0.36	72,88,96,97	0
26	GOL	B	633	6/6	0.92	0.16	56,60,61,63	0
31	UNL	d	412	17/-	0.92	0.23	62,71,93,94	0
23	CLA	C	511	65/65	0.92	0.17	54,71,85,96	0
34	DGD	c	519	62/66	0.92	0.18	42,62,92,96	0
23	CLA	D	407	65/65	0.92	0.17	48,62,108,118	0
23	CLA	c	516	65/65	0.92	0.16	64,78,87,94	0
24	BCR	c	527	40/40	0.92	0.17	72,89,97,102	0
23	CLA	b	615	65/65	0.92	0.17	39,51,93,95	0
38	LHG	b	634	49/49	0.92	0.22	35,50,62,72	0
23	CLA	b	625	65/65	0.92	0.18	46,59,103,110	0
23	CLA	C	509	65/65	0.92	0.17	49,67,135,141	0
23	CLA	c	515	65/65	0.92	0.21	54,71,88,93	0
23	CLA	c	514	65/65	0.92	0.16	51,64,72,82	0
23	CLA	C	504	65/65	0.92	0.21	54,67,80,86	0
23	CLA	C	508	65/65	0.93	0.18	53,72,85,89	0
38	LHG	d	409	49/49	0.93	0.22	40,56,63,69	0
26	GOL	B	626	6/6	0.93	0.25	83,86,88,89	0
24	BCR	k	102	40/40	0.93	0.16	57,73,91,92	0
38	LHG	d	410	49/49	0.93	0.24	34,46,66,84	0
26	GOL	c	528	6/6	0.93	0.19	77,90,101,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	h	101	40/40	0.93	0.18	48,66,72,78	0
23	CLA	d	405	65/65	0.93	0.19	47,61,114,122	0
23	CLA	b	623	65/65	0.93	0.18	34,45,91,105	0
24	BCR	Y	101	40/40	0.93	0.19	61,79,92,106	0
26	GOL	V	204	6/6	0.93	0.31	70,71,74,75	0
23	CLA	c	513	65/65	0.93	0.17	55,68,82,88	0
26	GOL	F	103	6/6	0.93	0.30	98,110,118,121	0
23	CLA	B	615	65/65	0.93	0.20	32,45,99,102	0
23	CLA	B	610	65/65	0.93	0.17	42,55,66,79	0
24	BCR	H	101	40/40	0.93	0.18	47,60,78,78	0
23	CLA	d	403	65/65	0.93	0.18	34,41,48,51	0
23	CLA	C	510	65/65	0.93	0.18	54,74,91,95	0
23	CLA	b	624	65/65	0.93	0.17	42,53,71,76	0
23	CLA	B	608	65/65	0.93	0.18	29,43,55,67	0
23	CLA	A	404	65/65	0.94	0.18	33,39,50,61	0
23	CLA	a	409	65/65	0.94	0.19	36,42,50,72	0
30	PL9	d	407[A]	55/55	0.94	0.22	33,45,54,57	55
24	BCR	b	627	40/40	0.94	0.19	32,48,64,70	0
23	CLA	B	616	65/65	0.94	0.17	41,52,67,76	0
31	UNL	D	414	17/-	0.94	0.20	48,71,87,90	0
23	CLA	b	612	65/65	0.94	0.17	42,54,63,67	0
23	CLA	a	412	65/65	0.94	0.21	41,55,120,125	0
38	LHG	L	101	49/49	0.94	0.22	37,50,58,62	0
36	BCT	D	401[B]	4/4	0.94	0.21	75,76,81,89	4
24	BCR	k	101	40/40	0.94	0.19	59,76,86,87	0
23	CLA	D	406	65/65	0.94	0.17	32,40,65,75	0
23	CLA	B	612	65/65	0.94	0.19	34,45,53,61	0
24	BCR	K	103	40/40	0.94	0.16	62,74,82,87	0
24	BCR	d	406	40/40	0.94	0.19	52,61,83,87	0
23	CLA	b	620	65/65	0.94	0.19	34,48,58,63	0
23	CLA	b	617	65/65	0.94	0.17	44,55,66,69	0
23	CLA	B	603	65/65	0.94	0.17	43,53,60,68	0
37	PHO	d	402[B]	64/64	0.94	0.20	39,50,55,57	64
24	BCR	C	515	40/40	0.94	0.18	51,63,78,78	0
30	PL9	d	407[B]	55/55	0.94	0.22	35,45,53,58	55
37	PHO	d	402[A]	64/64	0.94	0.20	37,50,55,59	64
26	GOL	v	203	6/6	0.94	0.21	65,68,73,74	0
36	BCT	D	401[A]	4/4	0.94	0.21	76,77,81,89	4
24	BCR	D	408	40/40	0.94	0.18	49,68,101,109	0
23	CLA	A	406	65/65	0.95	0.17	35,46,104,109	0
23	CLA	A	407	65/65	0.95	0.16	42,56,118,126	0
30	PL9	D	409[A]	55/55	0.95	0.22	30,43,51,65	55

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	622	65/65	0.95	0.19	34,46,55,70	0
23	CLA	B	617	65/65	0.95	0.21	45,61,139,140	0
23	CLA	B	604	65/65	0.95	0.18	38,52,60,64	0
37	PHO	D	403[B]	64/64	0.95	0.18	39,48,54,59	64
26	GOL	V	203	6/6	0.95	0.17	51,70,86,89	0
23	CLA	B	609	65/65	0.95	0.18	40,51,63,66	0
32	CA	F	105	1/1	0.95	0.06	119,119,119,119	0
23	CLA	C	506	65/65	0.95	0.16	46,59,74,81	0
30	PL9	D	409[B]	55/55	0.95	0.22	30,43,51,61	55
23	CLA	B	605	65/65	0.95	0.17	33,43,69,75	0
23	CLA	b	619	65/65	0.95	0.18	42,54,69,72	0
23	CLA	A	405	65/65	0.95	0.17	32,39,46,51	0
23	CLA	b	614	65/65	0.95	0.17	36,45,58,64	0
23	CLA	d	404	65/65	0.95	0.17	35,43,59,65	0
23	CLA	B	606	65/65	0.95	0.16	34,44,55,62	0
37	PHO	D	403[A]	64/64	0.95	0.18	41,48,54,59	64
38	LHG	D	412	49/49	0.95	0.22	35,46,75,85	0
23	CLA	c	505	65/65	0.95	0.16	52,67,76,79	0
23	CLA	B	613	65/65	0.95	0.17	35,45,55,58	0
23	CLA	b	621	65/65	0.95	0.17	36,46,58,63	0
23	CLA	b	613	65/65	0.95	0.17	34,45,72,79	0
26	GOL	V	201	6/6	0.96	0.29	63,81,87,88	0
26	GOL	b	602	6/6	0.96	0.28	63,68,78,79	0
39	HEM	e	101	43/43	0.96	0.20	73,94,130,141	0
24	BCR	T	103	40/40	0.96	0.17	29,49,65,68	0
26	GOL	B	624	6/6	0.96	0.21	64,74,77,86	0
23	CLA	B	611	65/65	0.96	0.19	43,55,62,65	0
23	CLA	c	506	65/65	0.96	0.17	51,62,84,87	0
39	HEM	v	205	43/43	0.96	0.17	53,63,78,80	0
23	CLA	C	503	65/65	0.96	0.16	48,66,75,83	0
26	GOL	D	404	6/6	0.96	0.39	51,61,73,76	0
24	BCR	b	626	40/40	0.96	0.18	33,45,53,54	0
26	GOL	B	625	6/6	0.96	0.31	49,66,85,101	0
24	BCR	t	102	40/40	0.96	0.20	37,52,68,71	0
23	CLA	a	410	65/65	0.96	0.19	37,49,104,112	0
26	GOL	b	604	6/6	0.96	0.22	65,84,86,92	0
32	CA	O	302	1/1	0.96	0.05	90,90,90,90	0
26	GOL	B	628	6/6	0.96	0.39	55,87,89,91	0
24	BCR	A	408	40/40	0.96	0.18	33,46,55,56	0
26	GOL	a	401	6/6	0.96	0.26	53,59,71,80	0
37	PHO	D	402	64/64	0.96	0.17	31,41,49,51	0
24	BCR	a	413	40/40	0.96	0.19	34,47,57,60	0

Continued on next page...

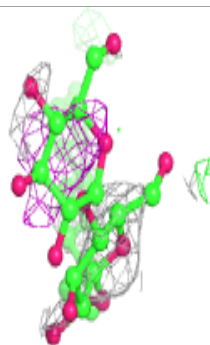
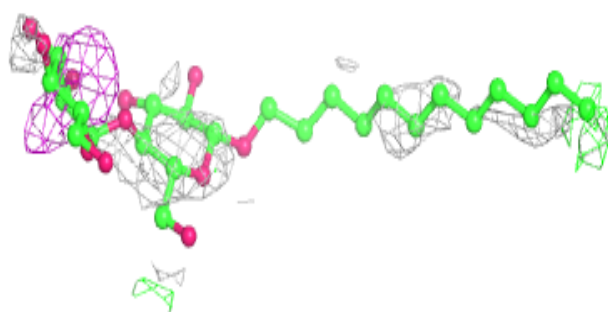
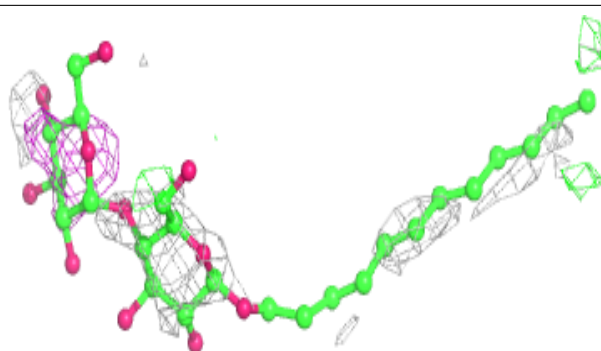
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	B	619	40/40	0.96	0.19	36,47,58,66	0
24	BCR	c	518	40/40	0.96	0.19	50,65,74,77	0
26	GOL	b	603	6/6	0.97	0.21	60,70,74,75	0
24	BCR	B	618	40/40	0.97	0.21	31,44,56,59	0
37	PHO	a	411	64/64	0.97	0.20	33,43,54,58	0
24	BCR	b	628	40/40	0.97	0.19	42,55,65,67	0
32	CA	o	302	1/1	0.97	0.06	96,96,96,96	0
40	MG	J	102	1/1	0.97	0.13	62,62,62,62	0
24	BCR	B	620	40/40	0.97	0.20	43,50,60,77	0
39	HEM	V	206	43/43	0.97	0.14	47,53,63,69	0
36	BCT	d	401[B]	4/4	0.98	0.27	71,74,75,77	4
26	GOL	c	501	6/6	0.98	0.24	55,59,61,62	0
26	GOL	C	525	6/6	0.98	0.22	53,59,63,63	0
36	BCT	d	401[A]	4/4	0.98	0.27	72,74,75,77	4
32	CA	c	504	1/1	0.98	0.06	84,84,84,84	0
22	CL	A	403[B]	1/1	0.99	0.16	44,44,44,44	1
40	MG	j	102	1/1	0.99	0.14	72,72,72,72	0
22	CL	a	408[A]	1/1	0.99	0.18	46,46,46,46	1
32	CA	c	503	1/1	0.99	0.10	79,79,79,79	0
29	OEY	a	418[B]	11/11	0.99	0.14	40,46,55,59	11
21	FE2	a	406[B]	1/1	0.99	0.09	60,60,60,60	0
21	FE2	A	401[A]	1/1	0.99	0.08	72,72,72,72	1
22	CL	a	408[B]	1/1	0.99	0.18	46,46,46,46	1
28	OEX	a	417[A]	10/10	0.99	0.13	40,47,52,54	10
22	CL	a	407[A]	1/1	0.99	0.14	43,43,43,43	1
21	FE2	A	401[B]	1/1	0.99	0.08	73,73,73,73	1
28	OEX	A	414[A]	10/10	0.99	0.15	49,56,74,80	10
22	CL	A	403[A]	1/1	0.99	0.16	44,44,44,44	1
22	CL	a	407[B]	1/1	0.99	0.14	46,46,46,46	1
29	OEY	A	415[B]	11/11	0.99	0.14	49,56,78,79	11
22	CL	A	402[A]	1/1	1.00	0.17	40,40,40,40	1
22	CL	A	402[B]	1/1	1.00	0.17	40,40,40,40	1

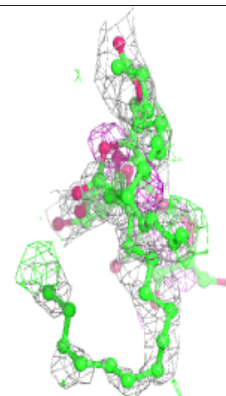
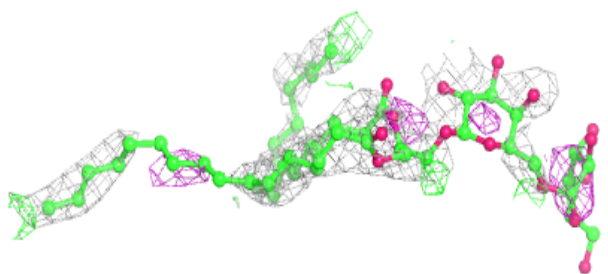
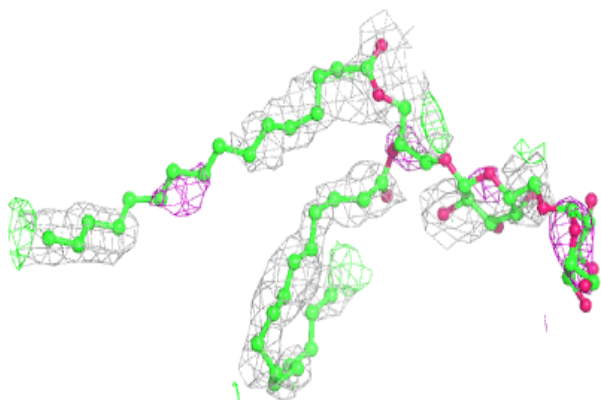
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

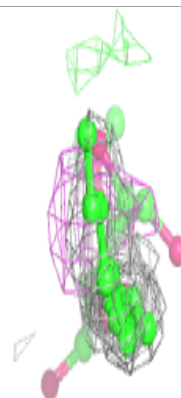
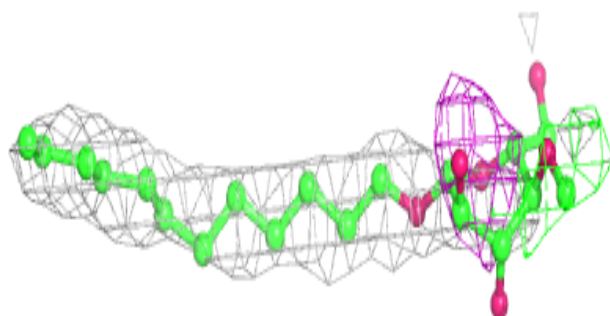
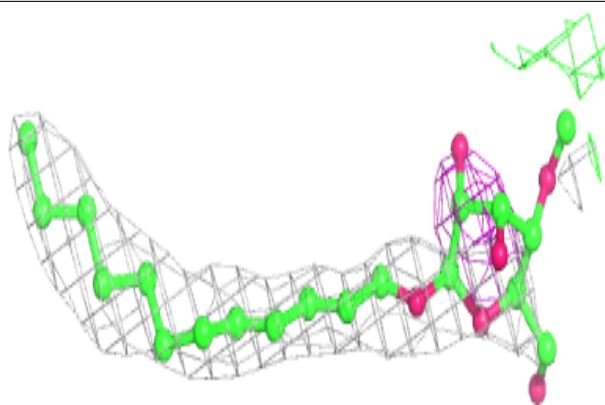
**Electron density around DGD d 408:**

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

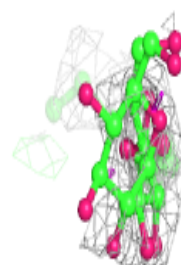
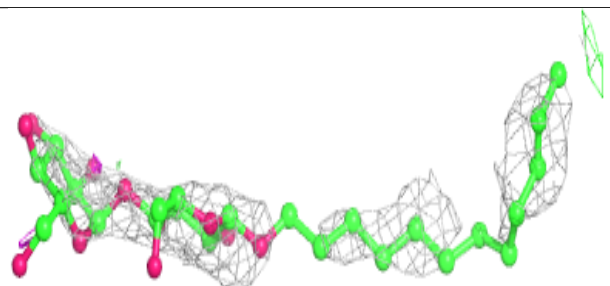
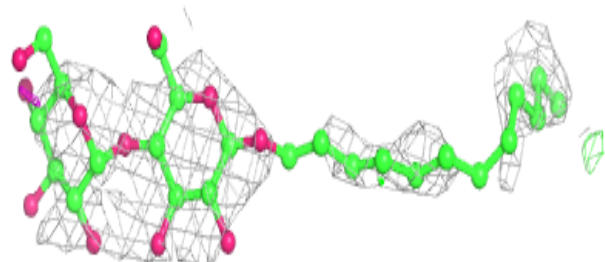


Electron density around LMT b 630:

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

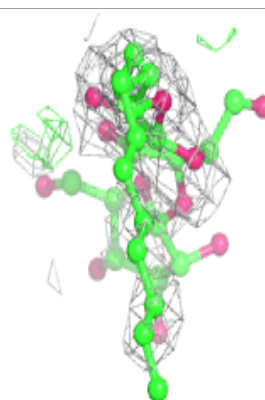
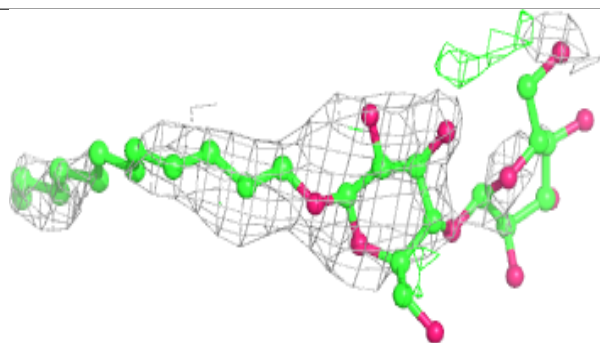
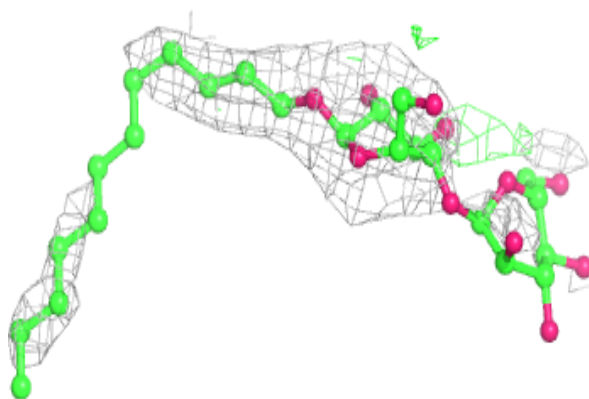
**Electron density around LMT a 419:**

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

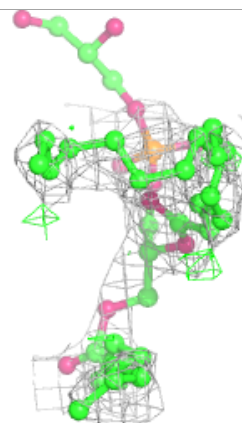
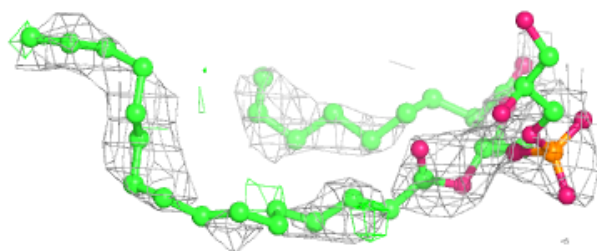
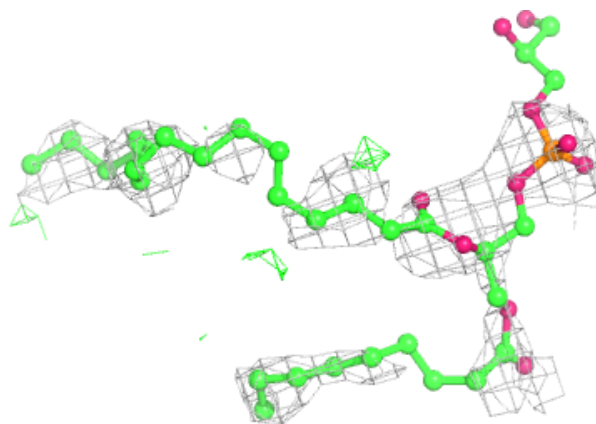


Electron density around LMT C 521:

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

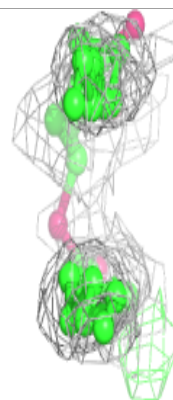
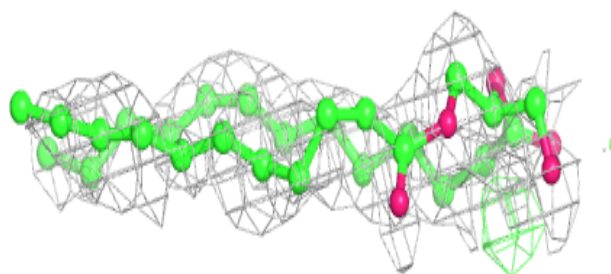
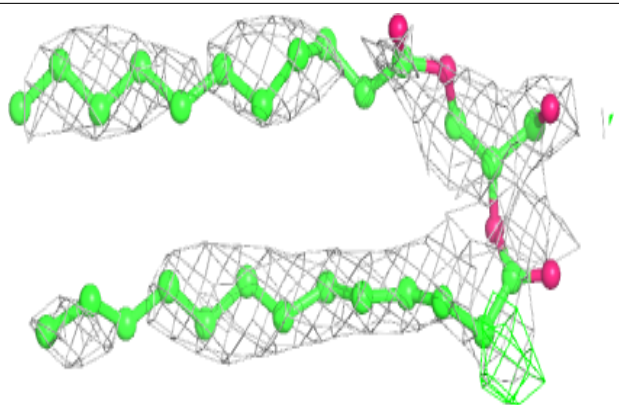
**Electron density around LHG a 420:**

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

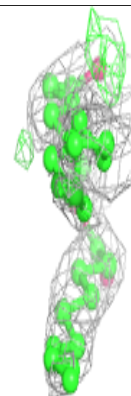
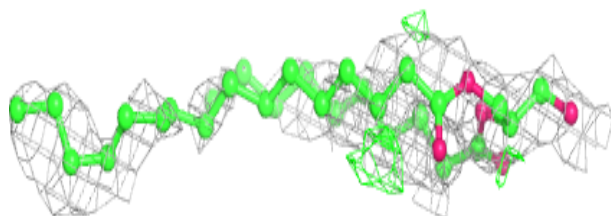
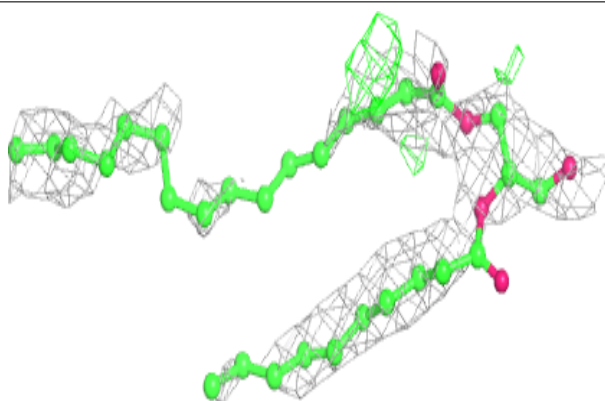


Electron density around UNL c 526:

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

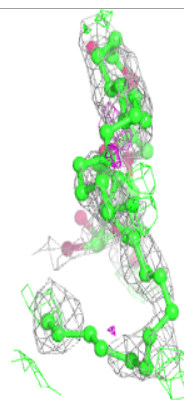
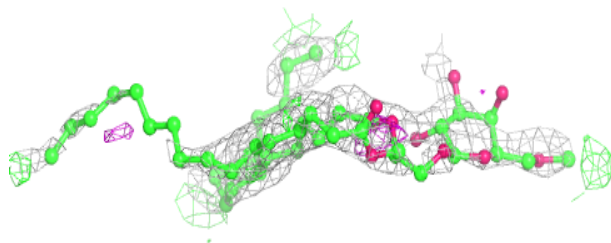
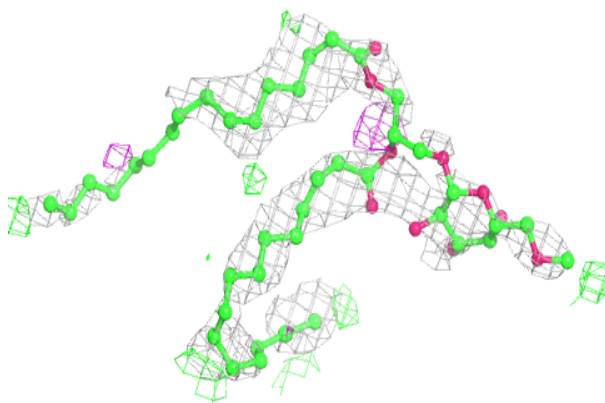
**Electron density around UNL K 102:**

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



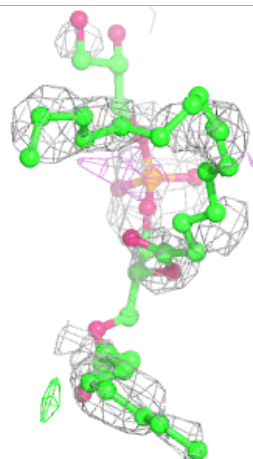
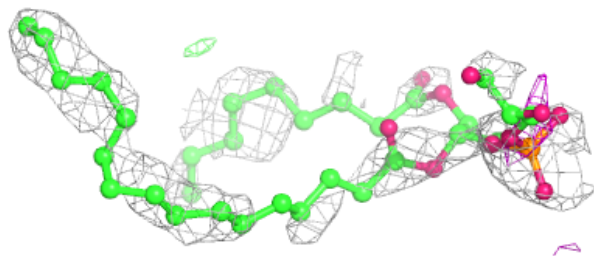
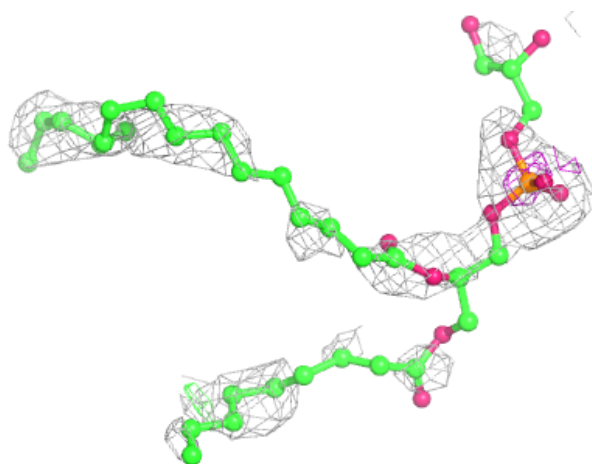
Electron density around DGD D 410:

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



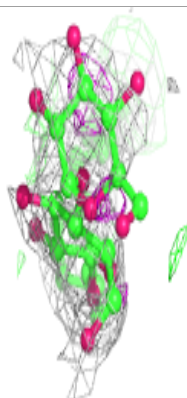
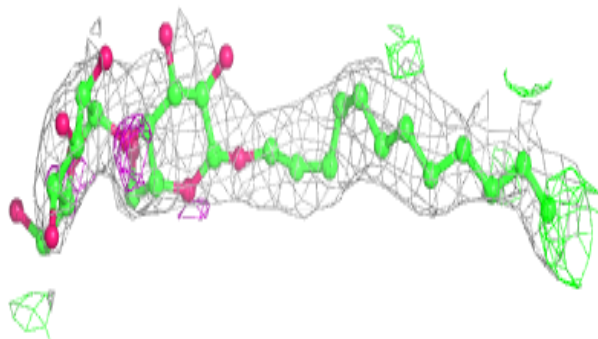
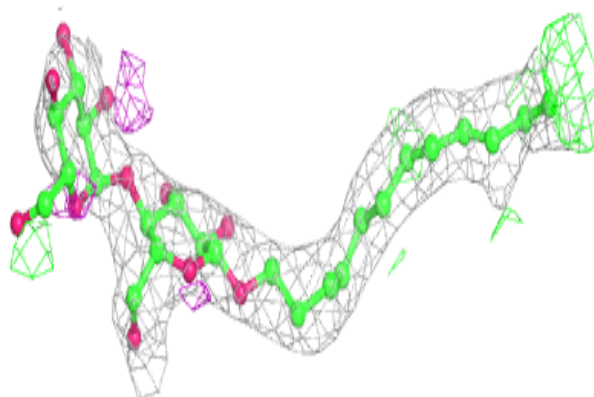
Electron density around LHG E 101:

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

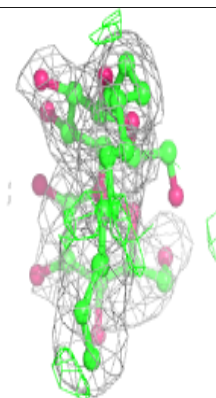
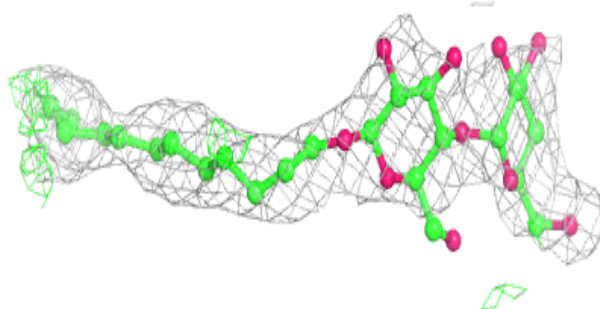
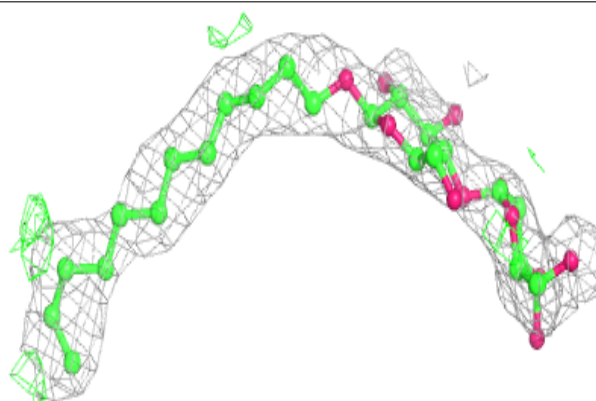


Electron density around LMT a 404:

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

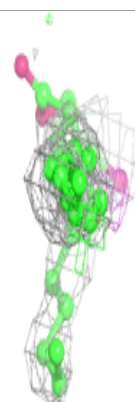
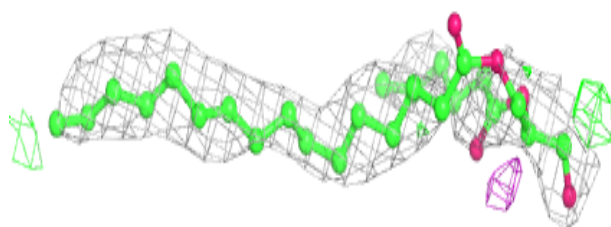
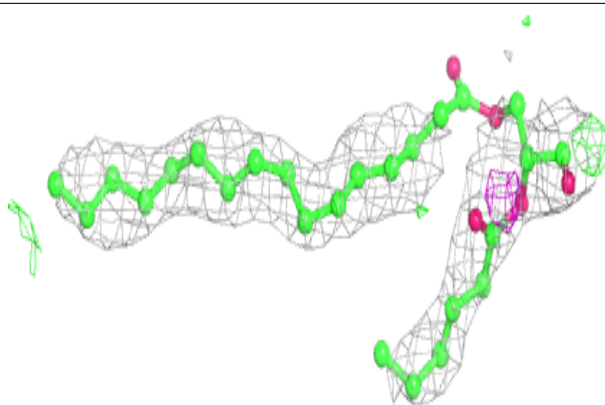
**Electron density around LMT m 102:**

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

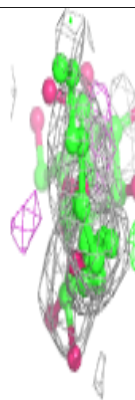
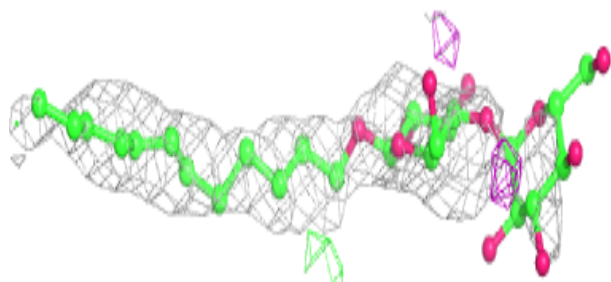
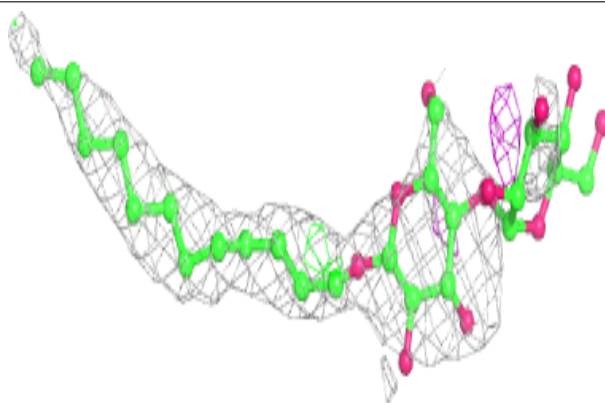


Electron density around UNL a 403:

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

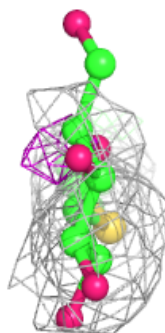
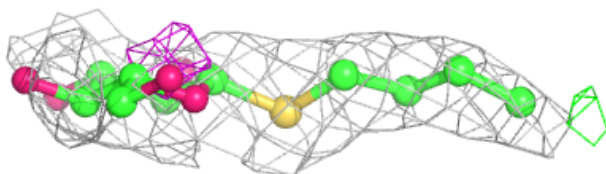
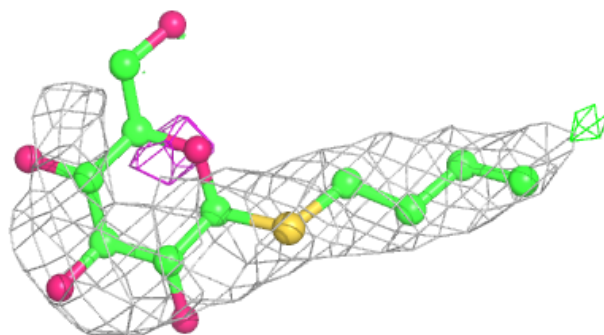
**Electron density around LMT D 405:**

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

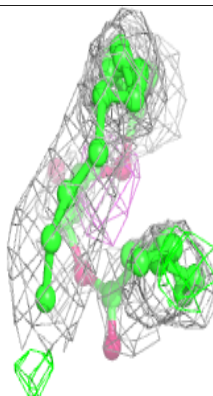
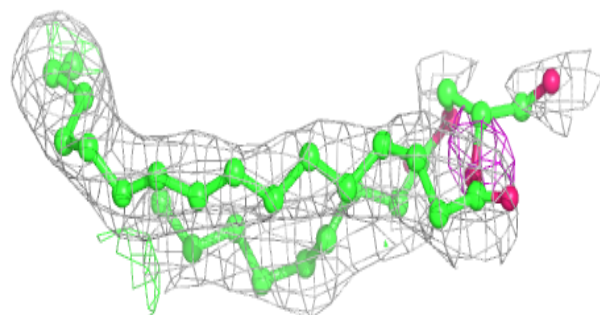
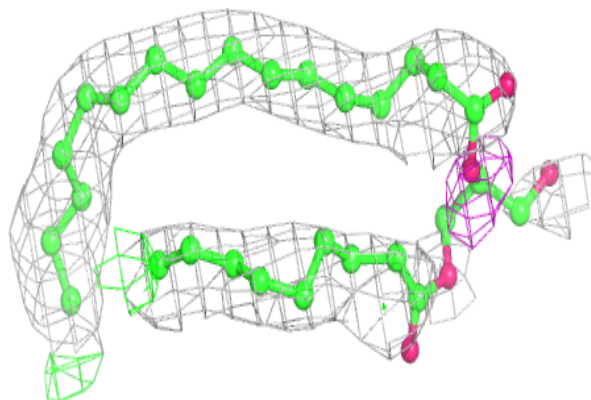


Electron density around HTG D 416:

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

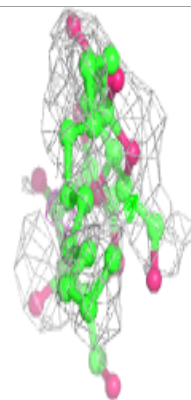
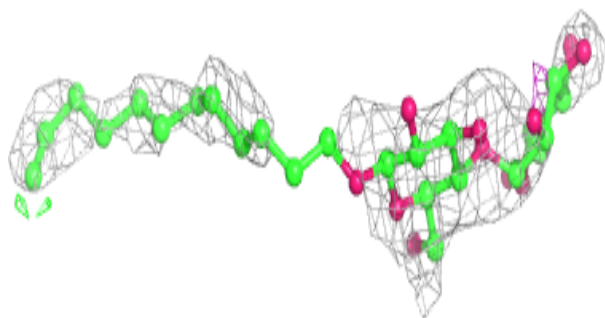
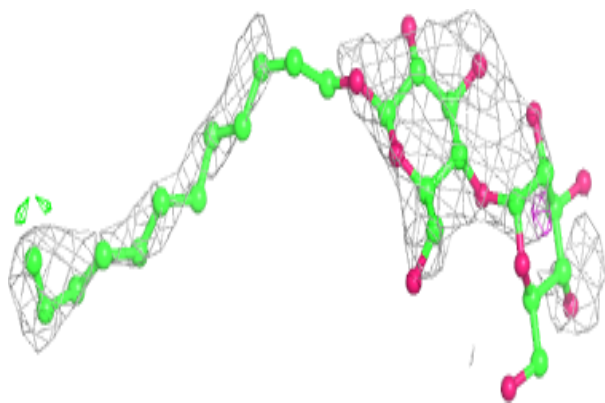
**Electron density around UNL b 633:**

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

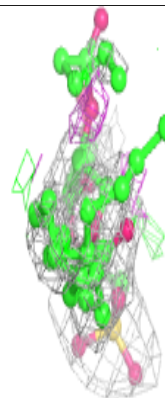
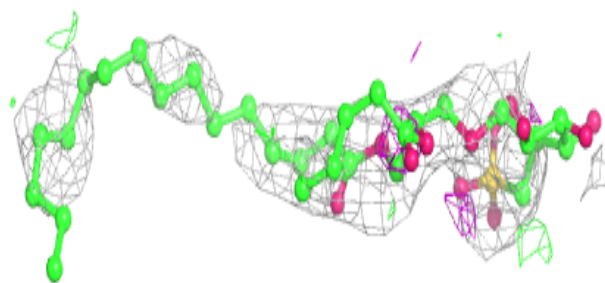
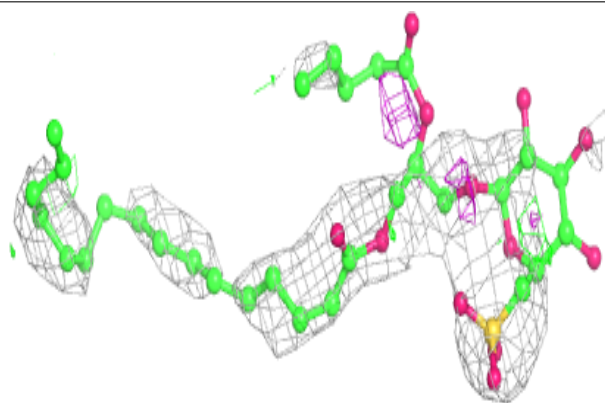


Electron density around LMT e 102:

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

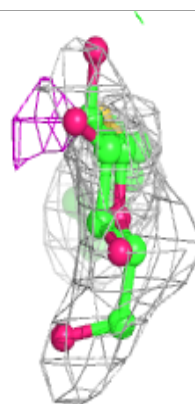
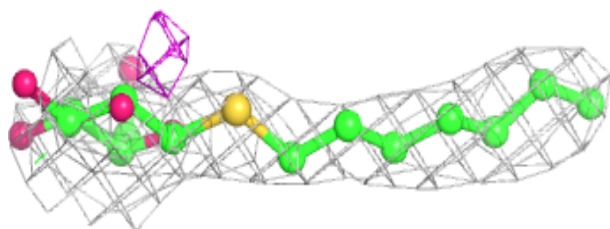
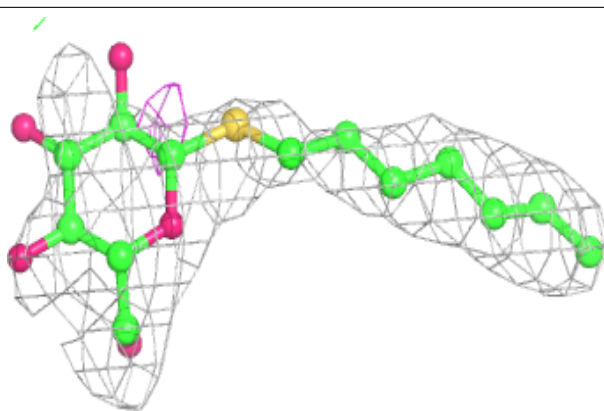
**Electron density around SQD f 102:**

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

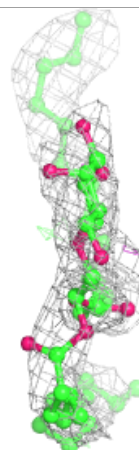
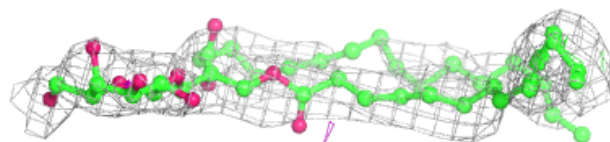
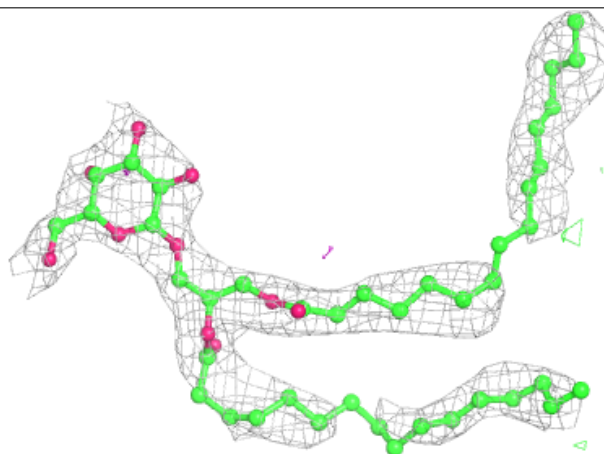


Electron density around HTG B 630:

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

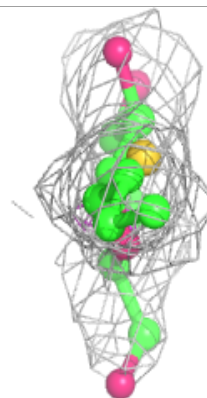
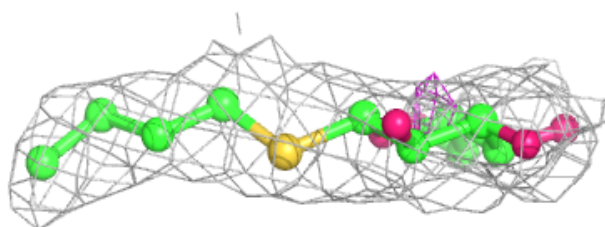
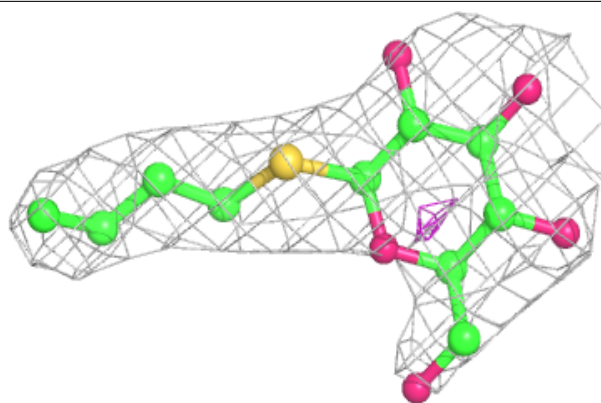
**Electron density around LMG C 519:**

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

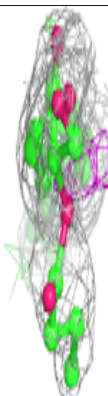
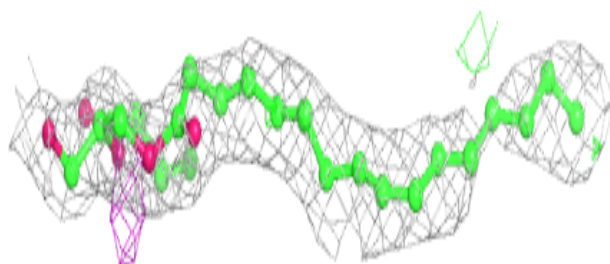
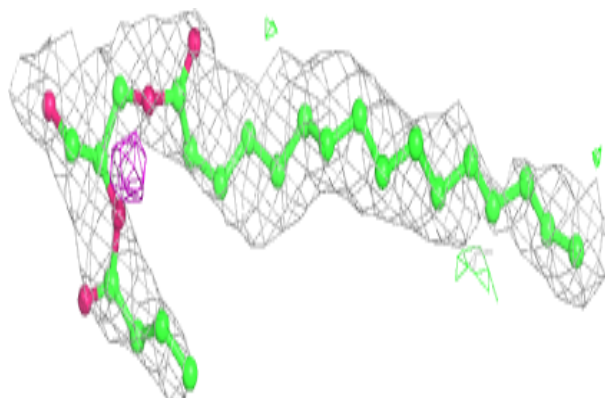


Electron density around HTG d 414:

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

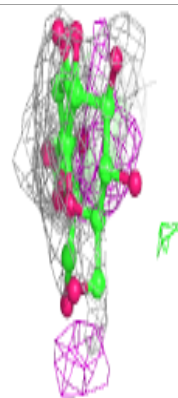
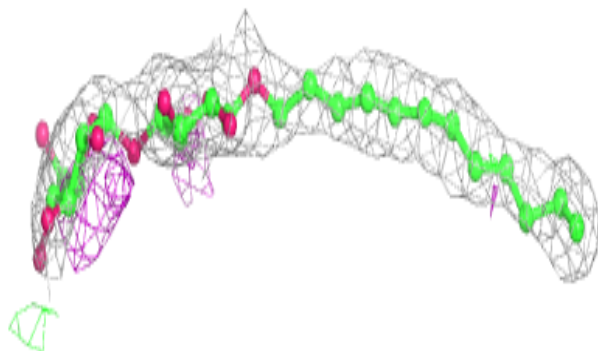
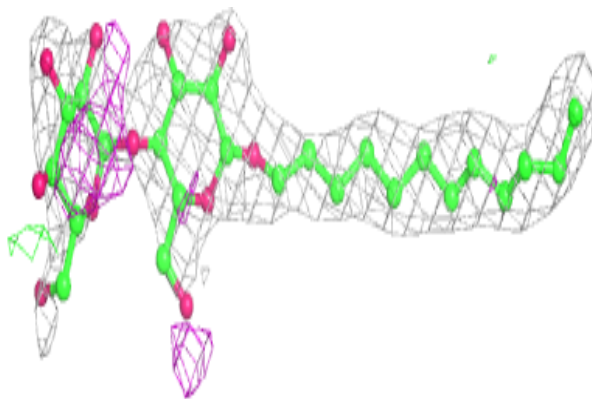
**Electron density around UNL A 417:**

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

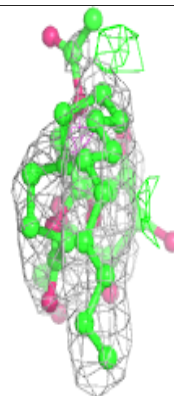
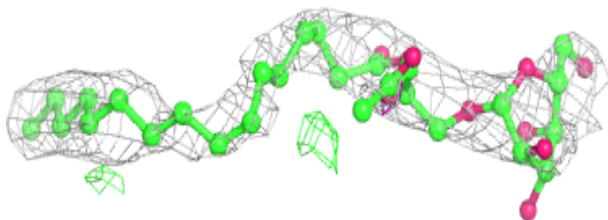
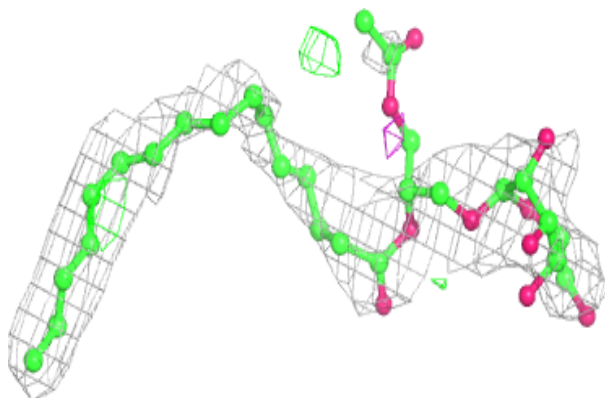


Electron density around LMT M 105:

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

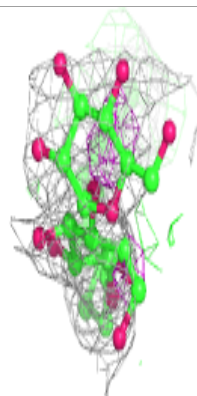
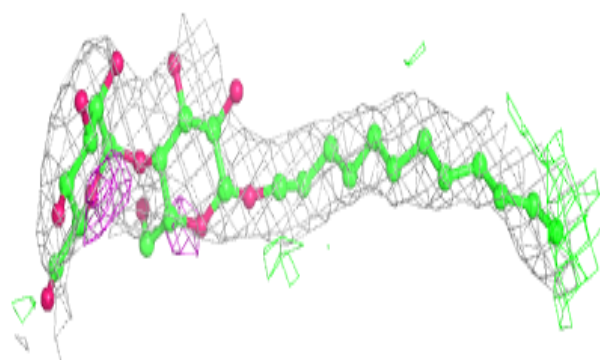
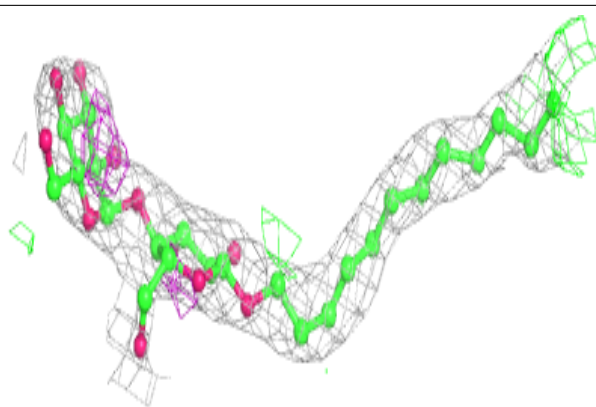
**Electron density around LMG Z 101:**

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

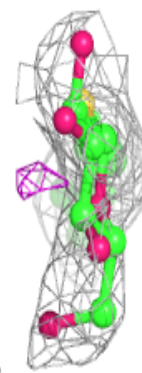
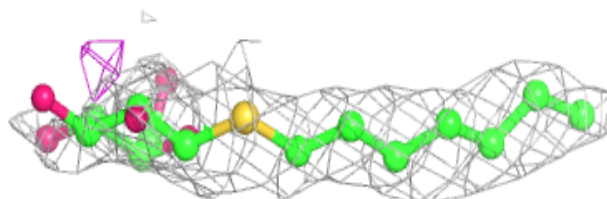
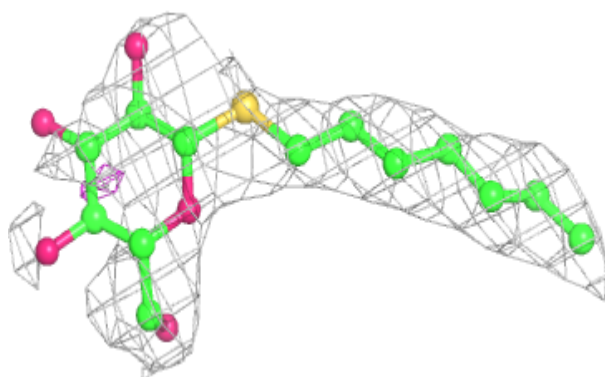


Electron density around LMT A 413:

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

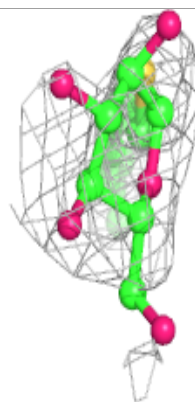
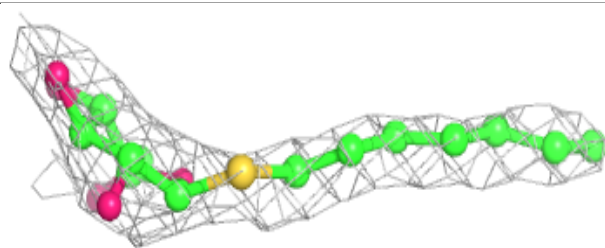
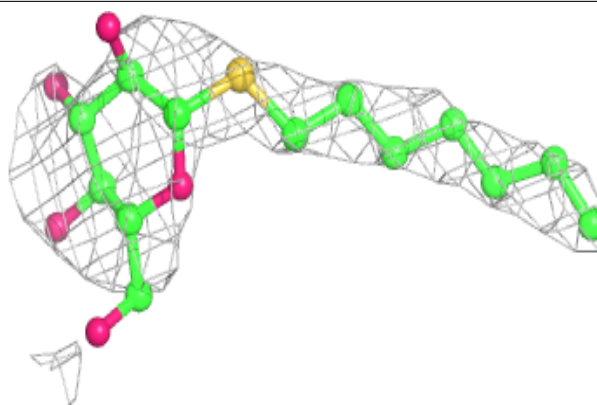
**Electron density around HTG b 608:**

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

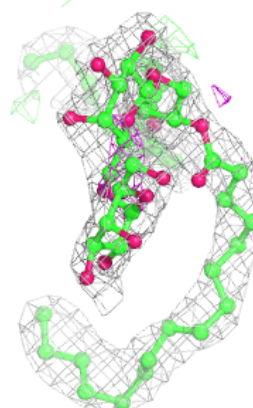
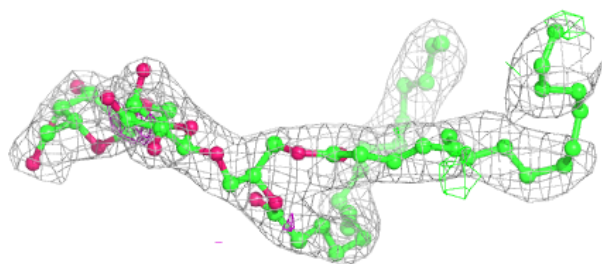
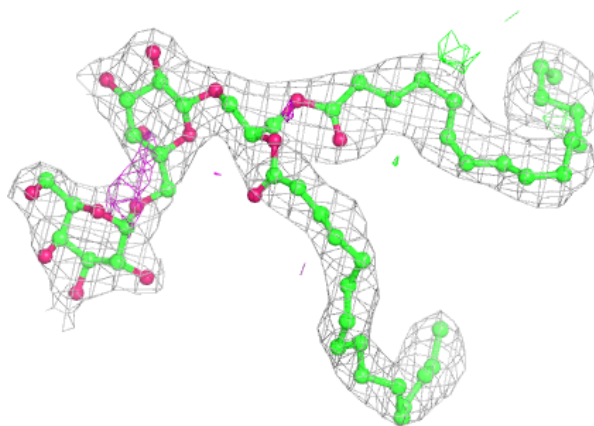


Electron density around HTG B 623:

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

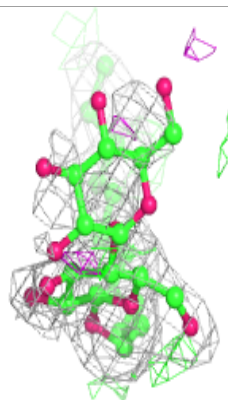
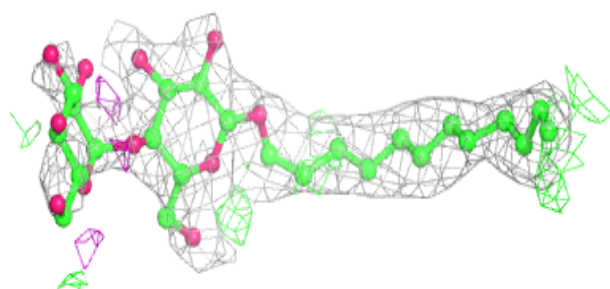
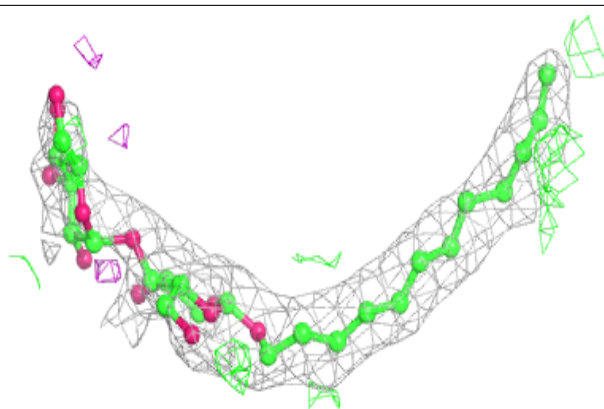
**Electron density around DGD C 517:**

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

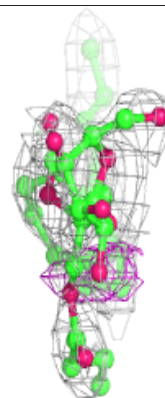
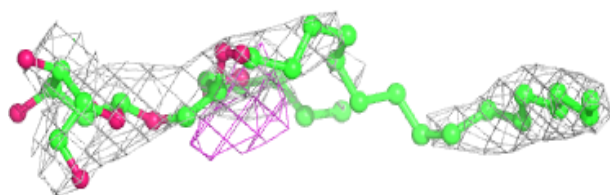
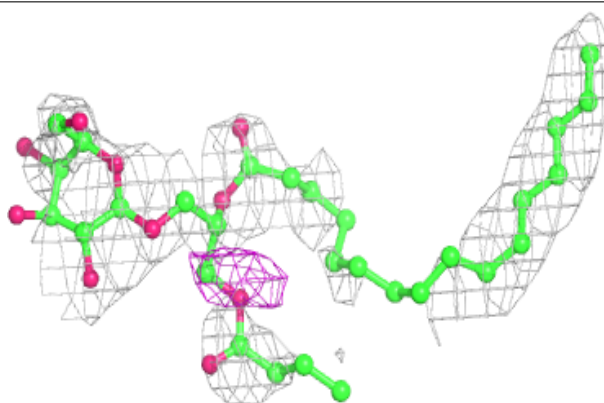


Electron density around LMT M 104:

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

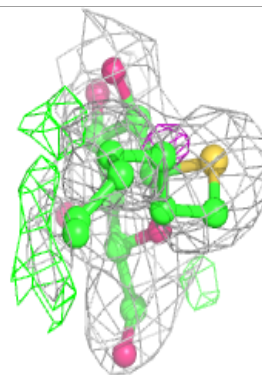
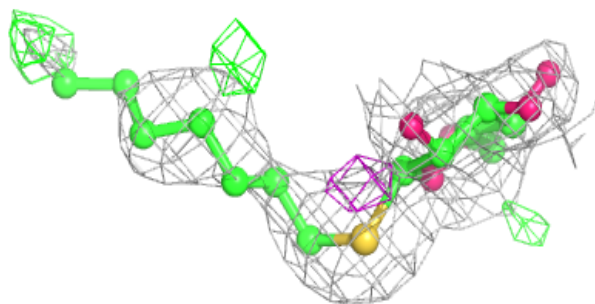
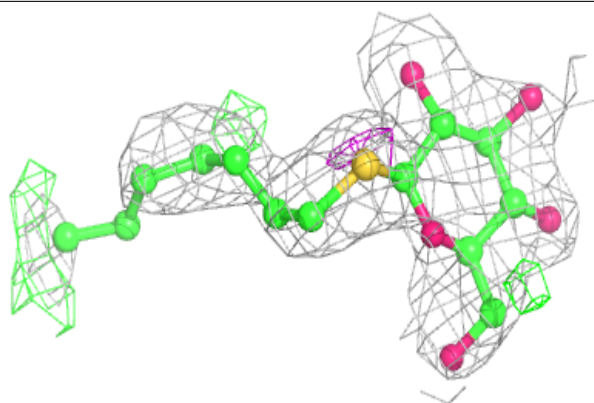
**Electron density around LMG z 101:**

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

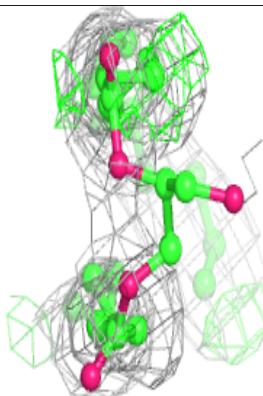
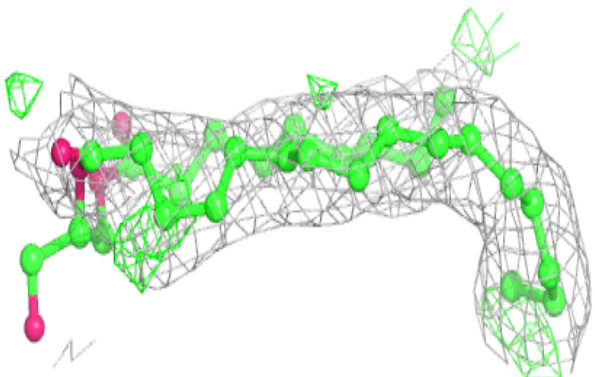
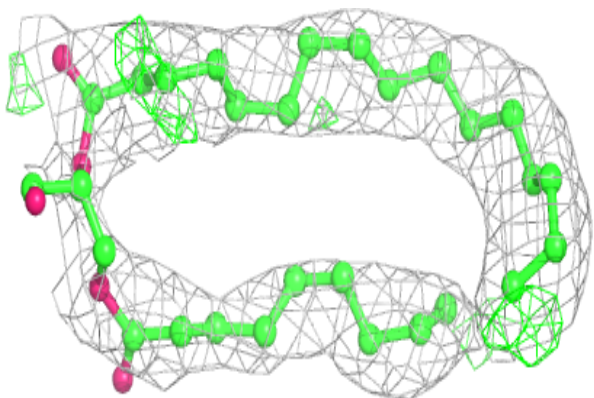


Electron density around HTG b 631:

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

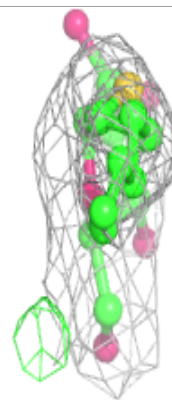
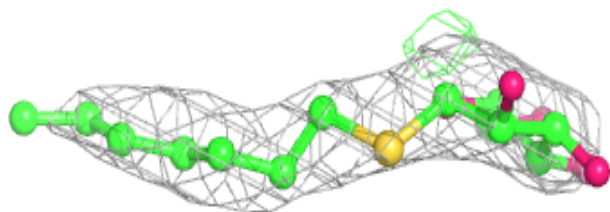
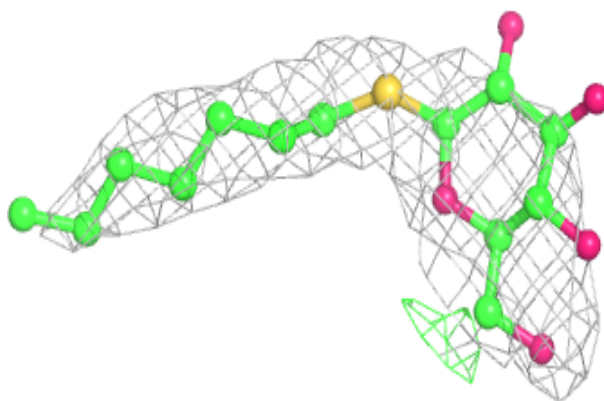
**Electron density around UNL B 631:**

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

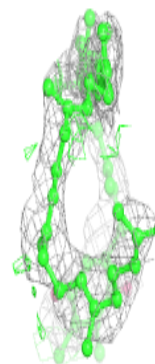
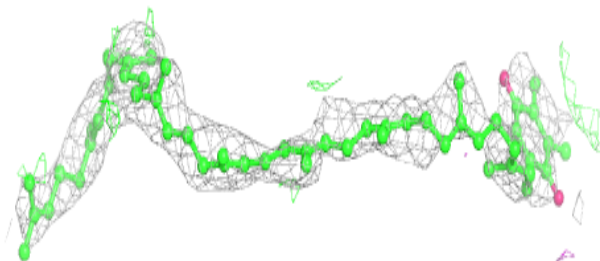
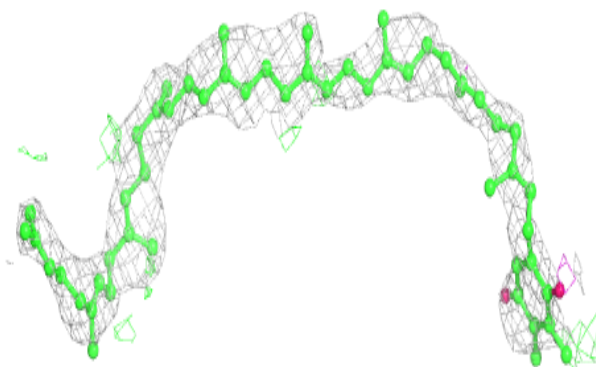


Electron density around HTG b 632:

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

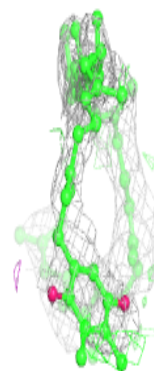
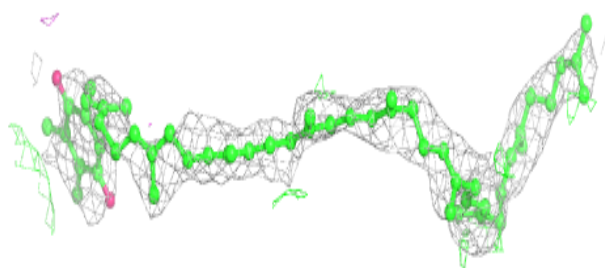
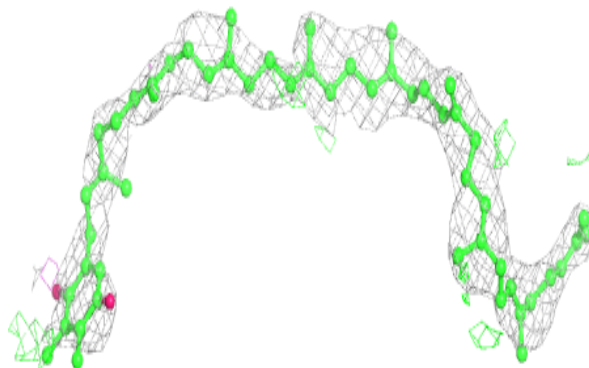
**Electron density around PL9 a 416 (A):**

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

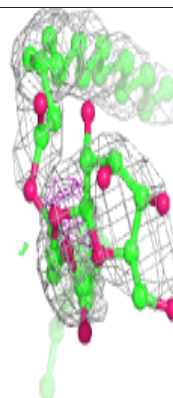
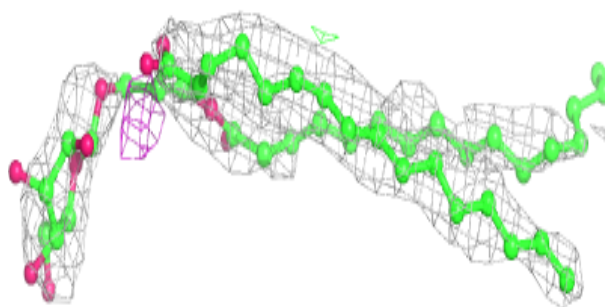
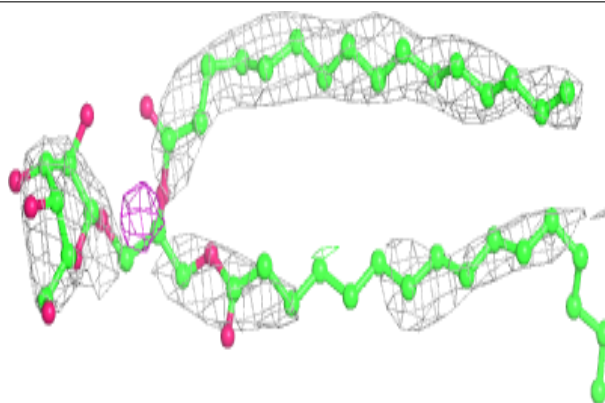


Electron density around PL9 a 416 (B):

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

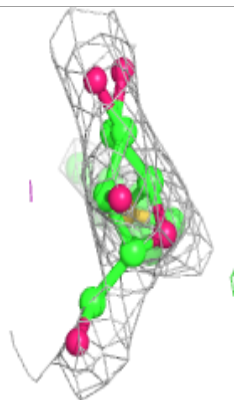
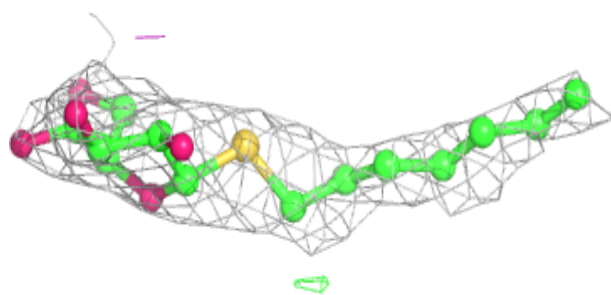
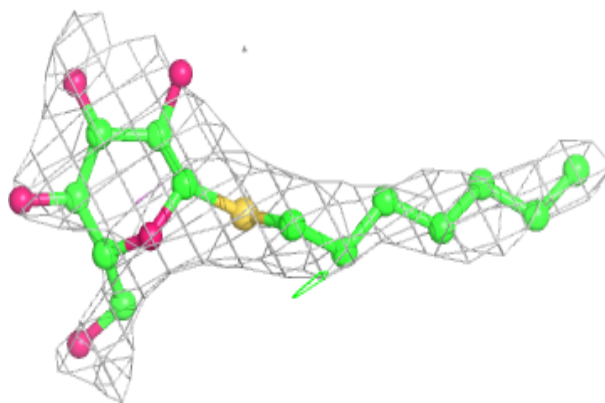
**Electron density around LMG C 520:**

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

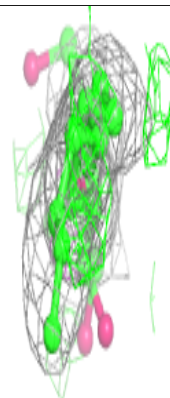
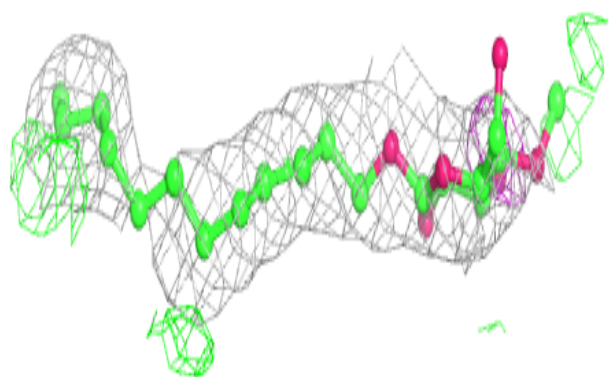
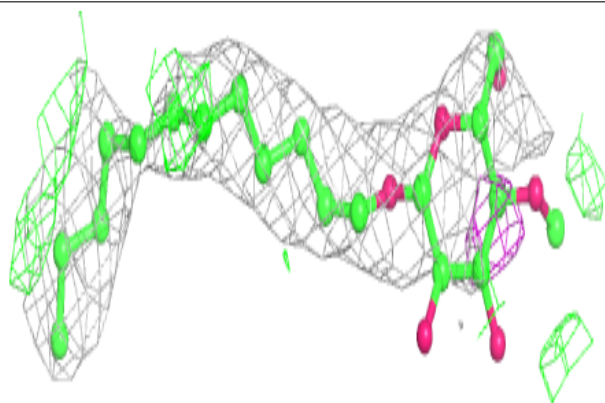


Electron density around HTG C 523:

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

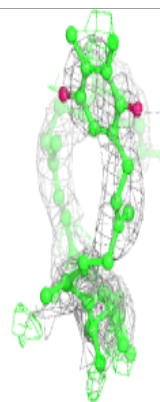
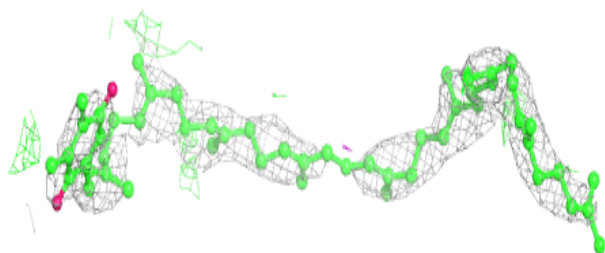
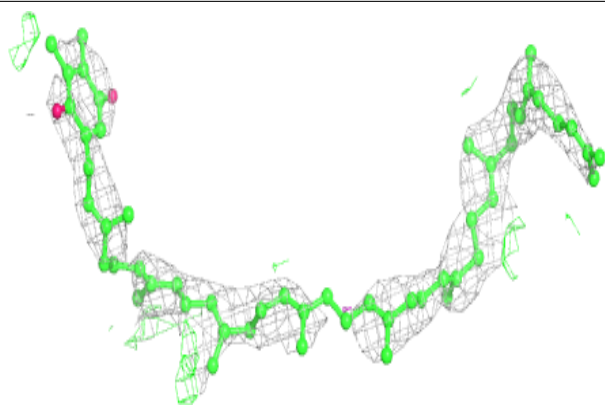
**Electron density around LMT T 104:**

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

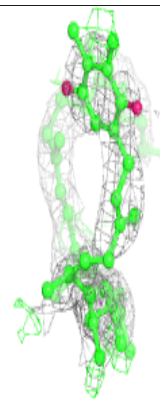
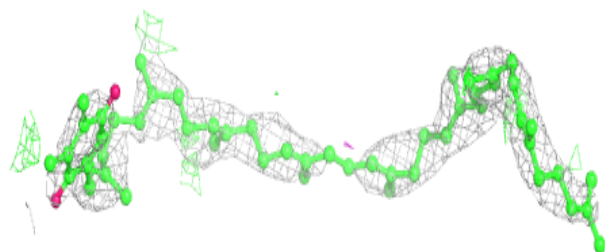
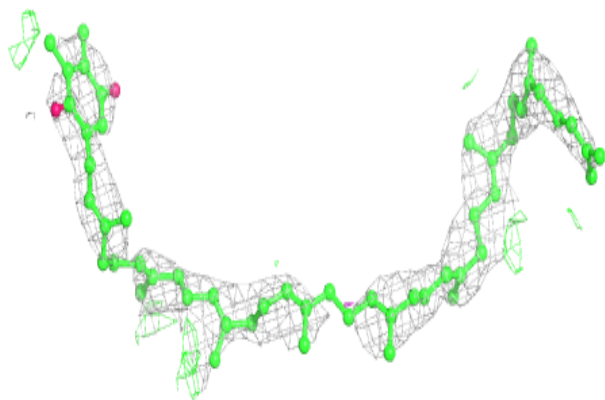


Electron density around PL9 A 416 (A):

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

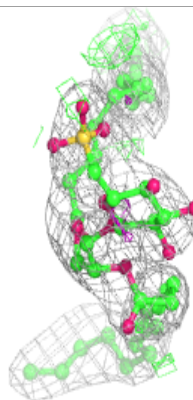
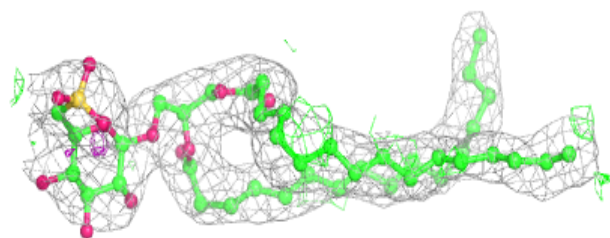
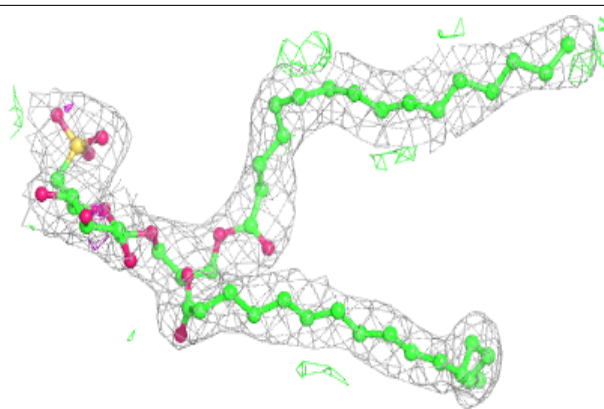
**Electron density around PL9 A 416 (B):**

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

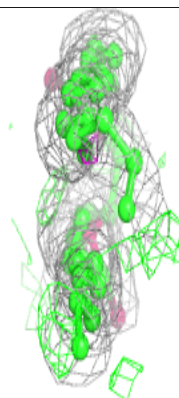
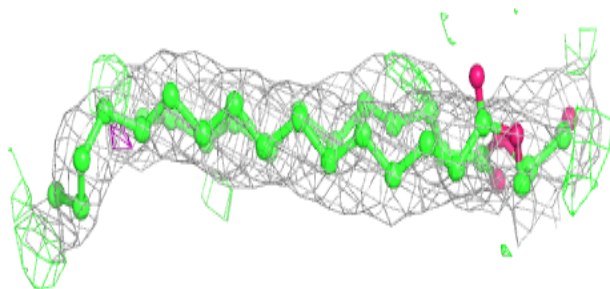
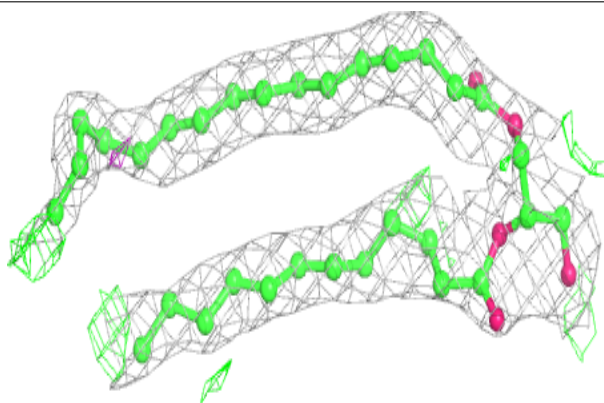


Electron density around SQD a 405:

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

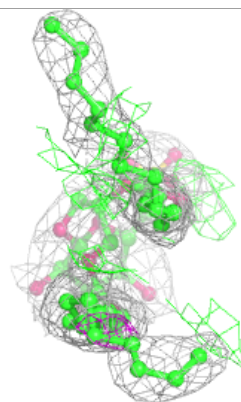
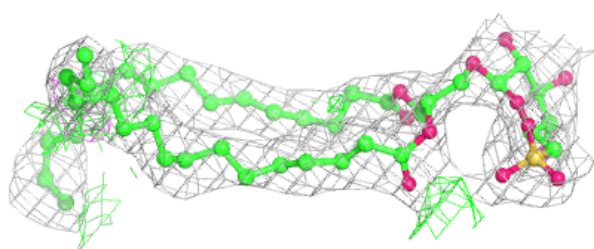
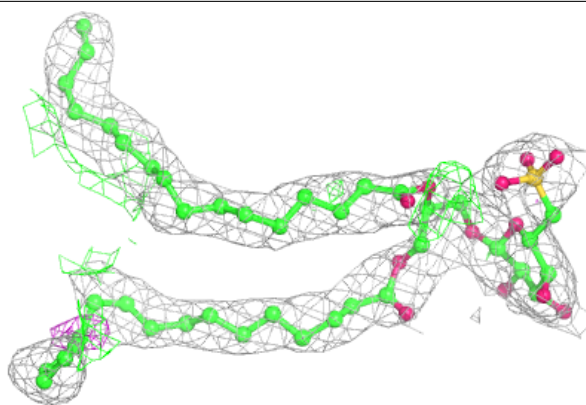
**Electron density around UNL d 413:**

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

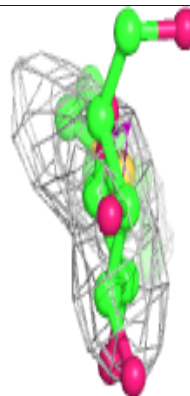
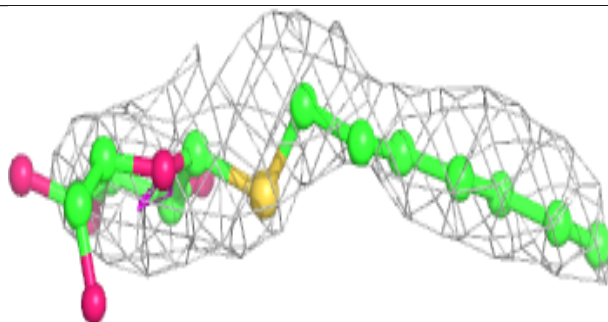
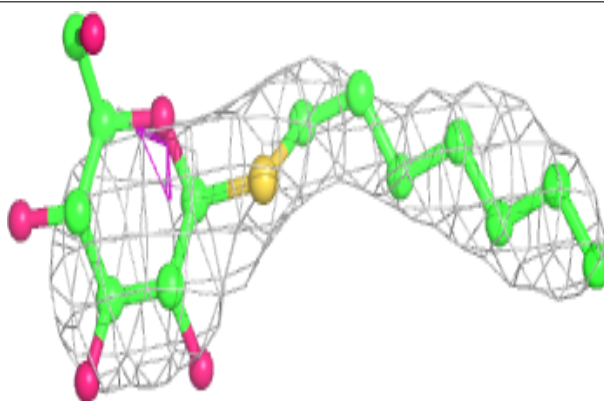


Electron density around SQD L 102:

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

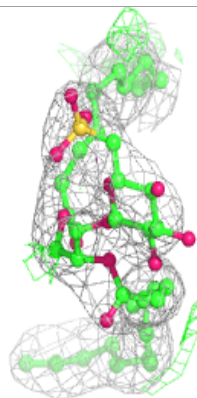
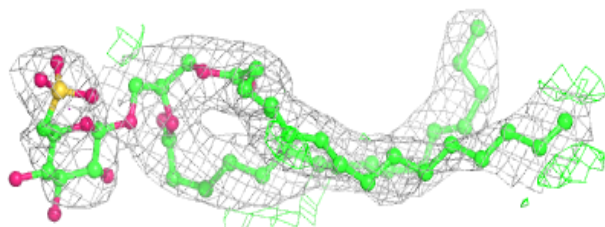
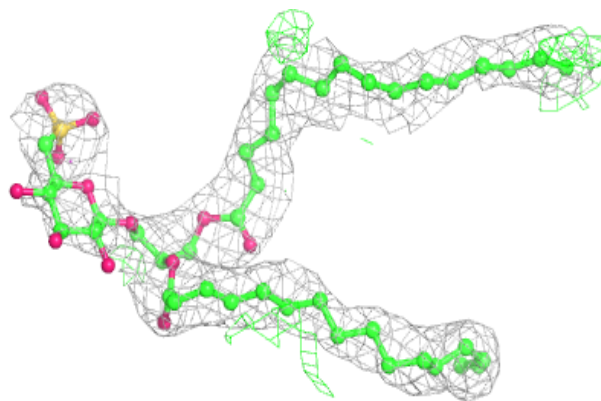
**Electron density around HTG c 525:**

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



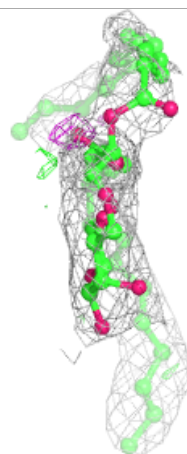
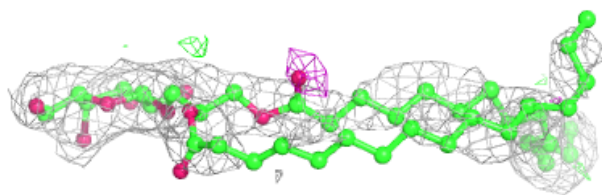
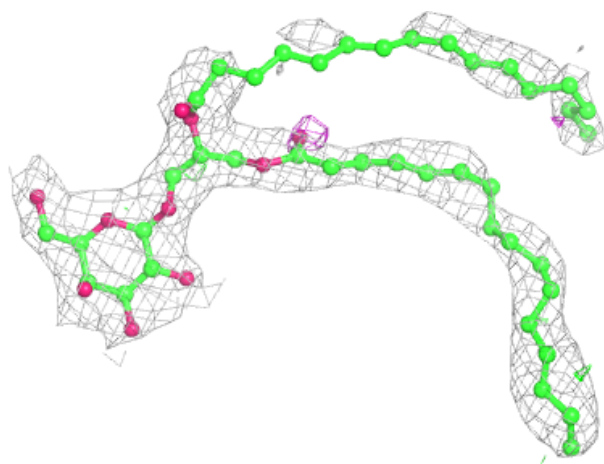
Electron density around SQD A 412:

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



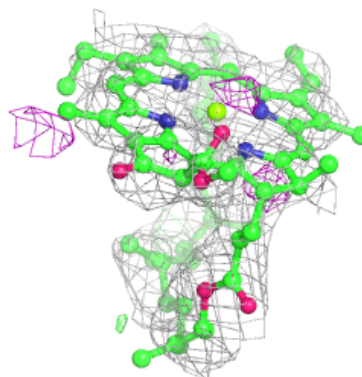
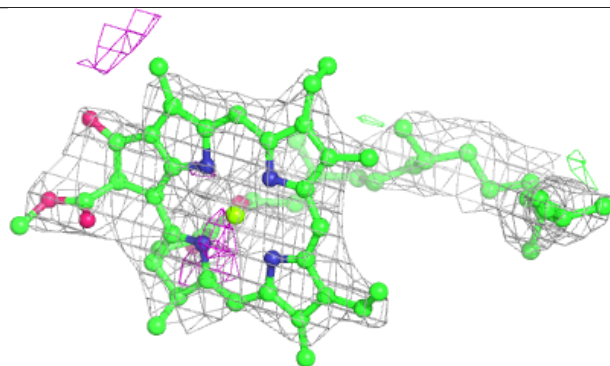
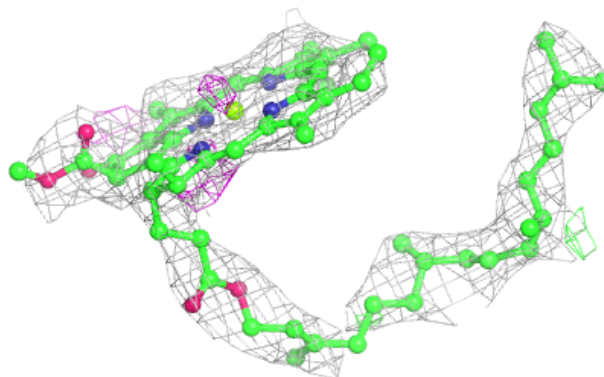
Electron density around LMG c 522:

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

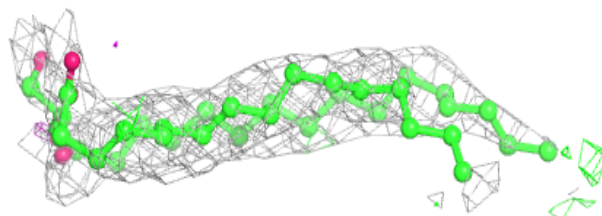
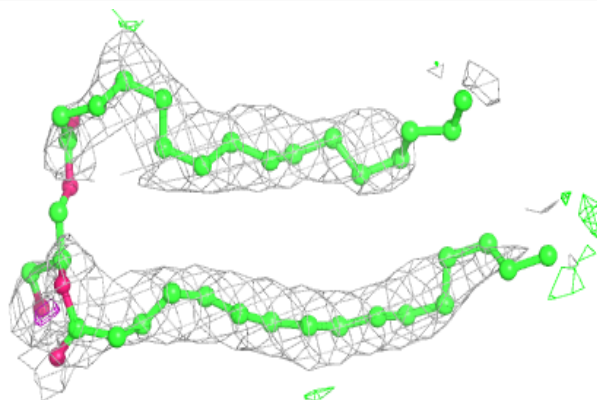


Electron density around CLA c 517:

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

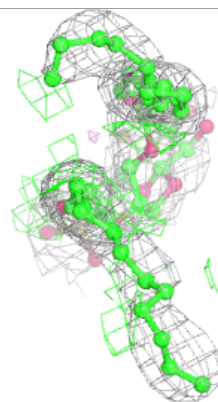
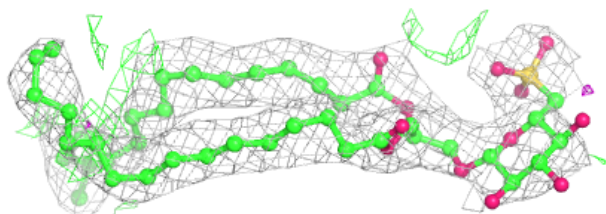
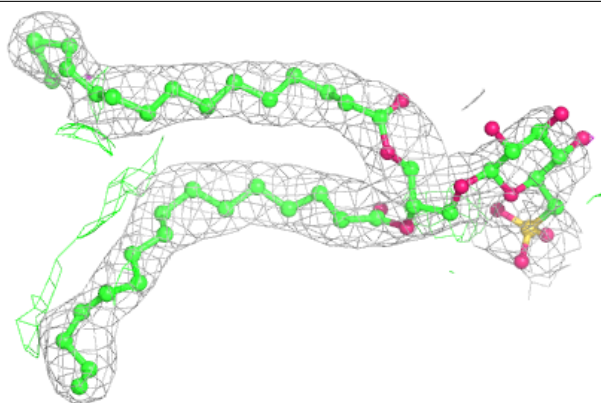
**Electron density around UNL I 101:**

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

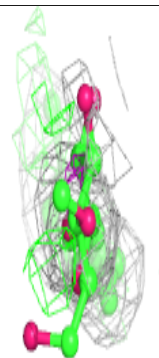
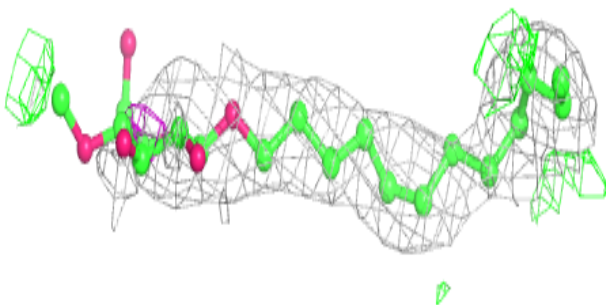
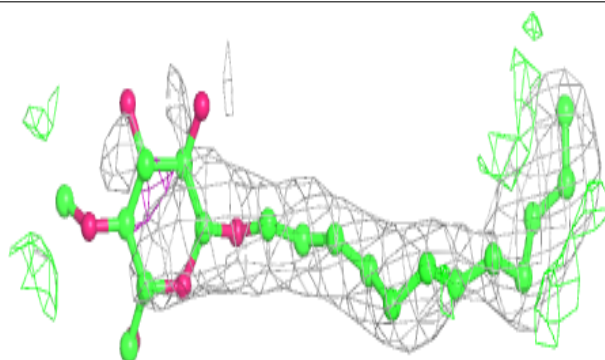


Electron density around SQD B 621:

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

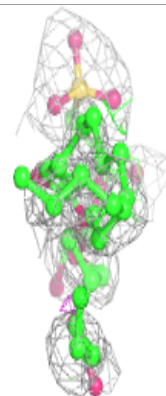
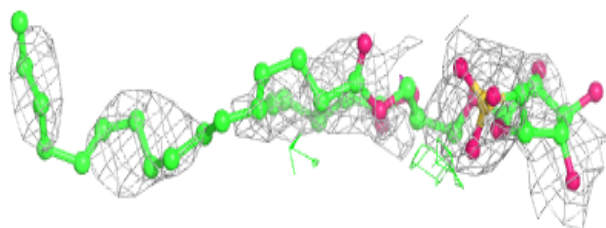
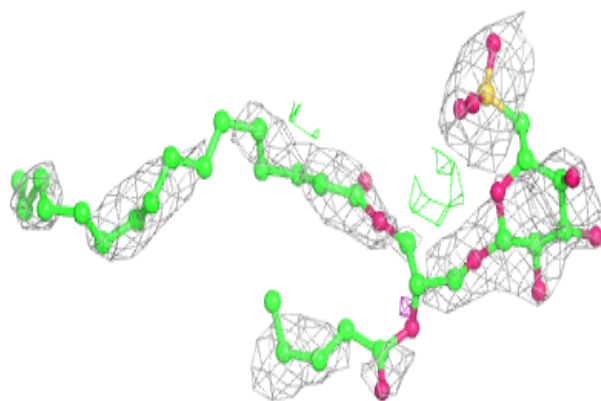
**Electron density around LMT t 101:**

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

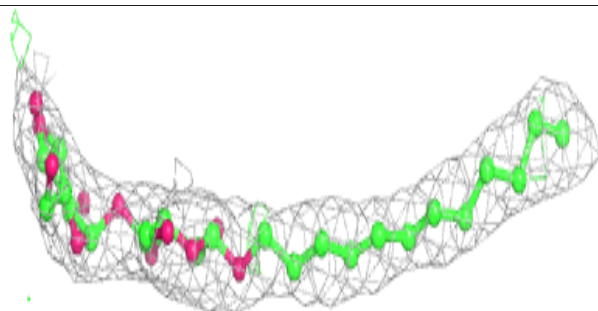
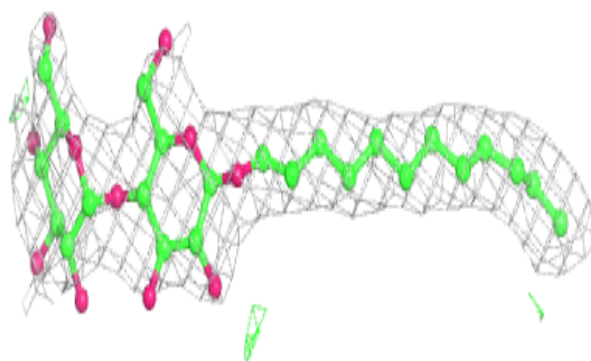


Electron density around SQD F 104:

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

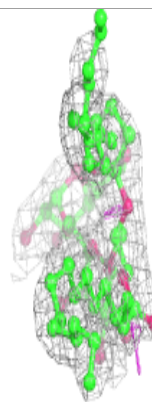
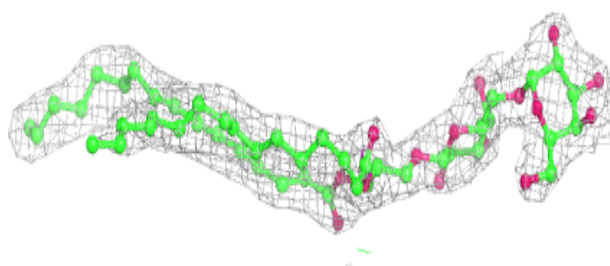
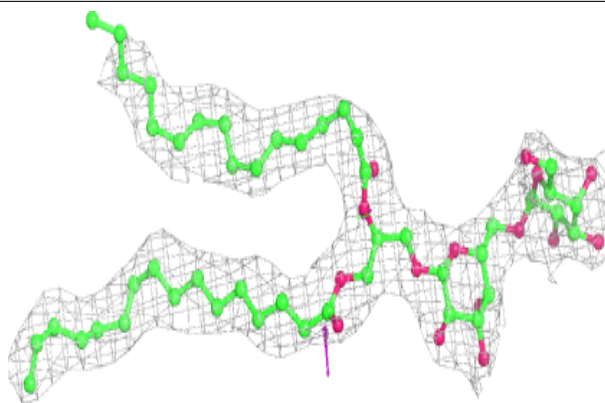
**Electron density around LMT M 102:**

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

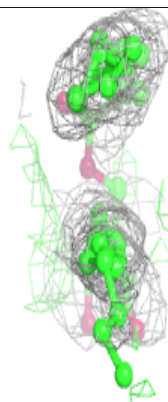
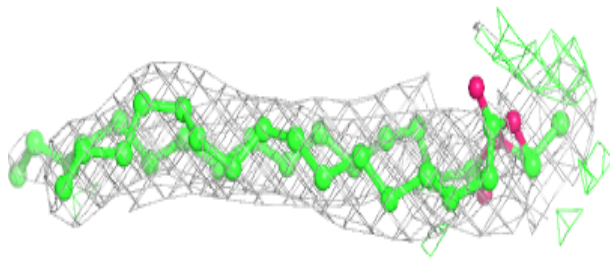
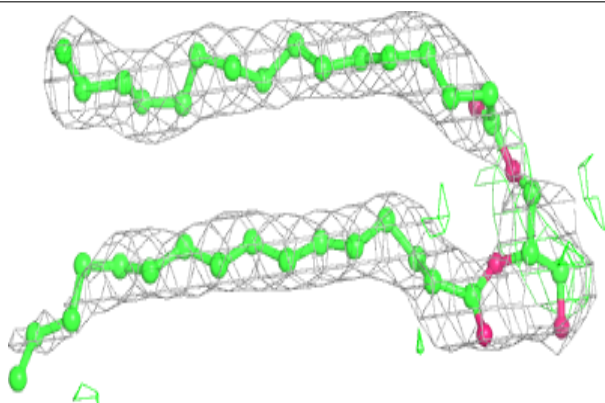


Electron density around DGD C 518:

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

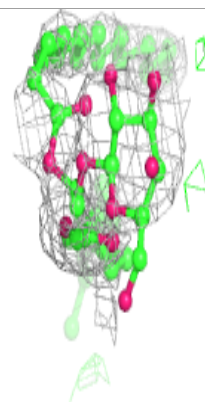
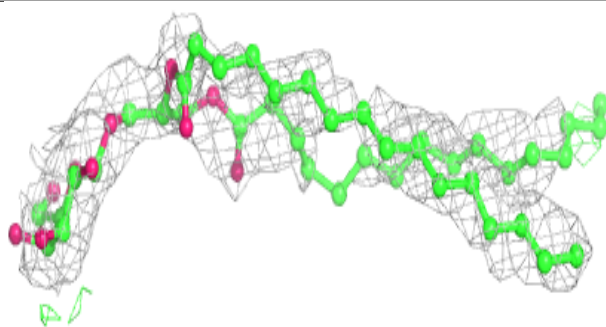
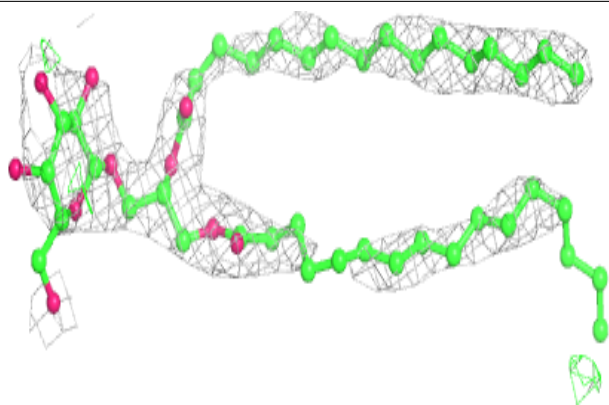
**Electron density around UNL D 415:**

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

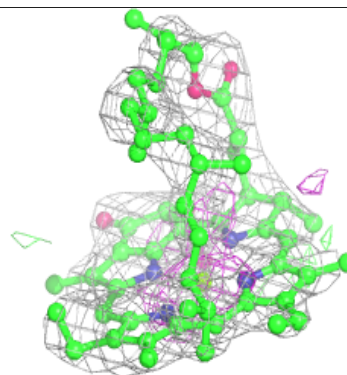
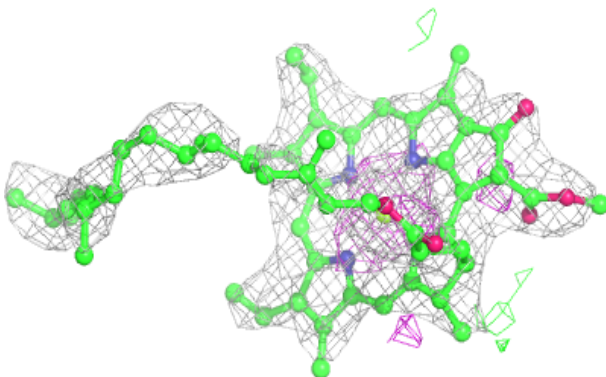
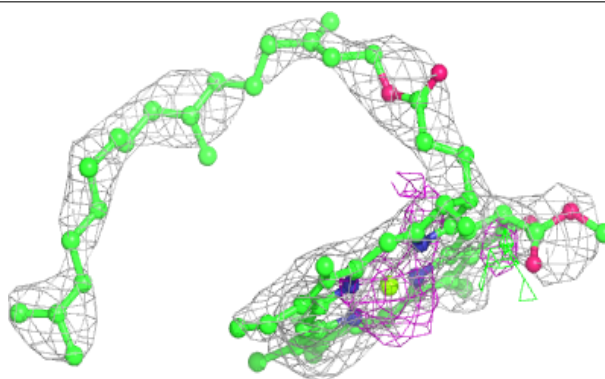


Electron density around LMG c 523:

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

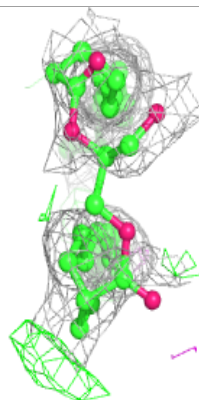
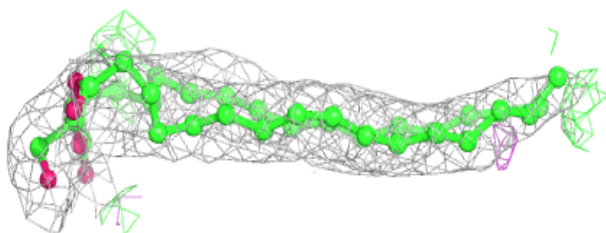
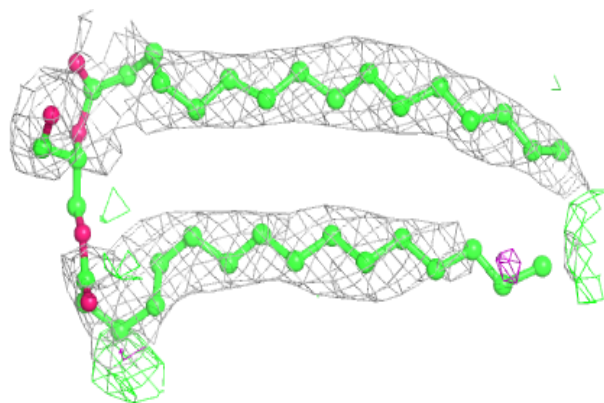
**Electron density around CLA C 514:**

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

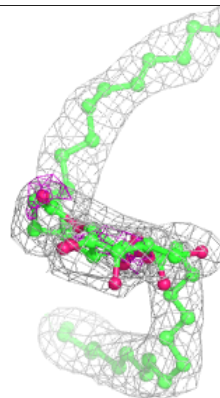
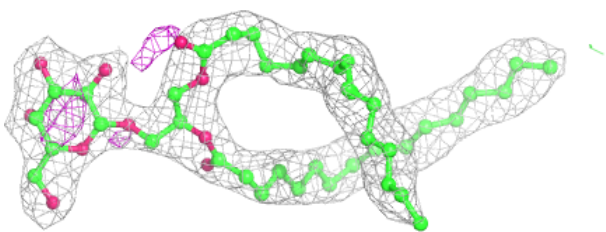
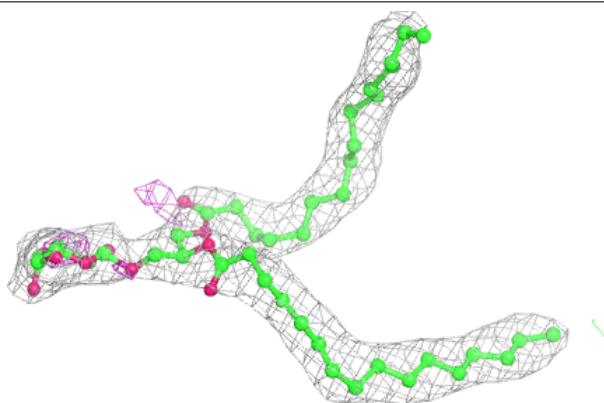


Electron density around UNL i 101:

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

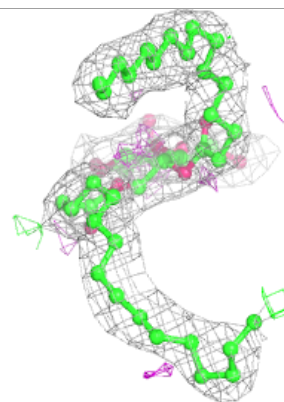
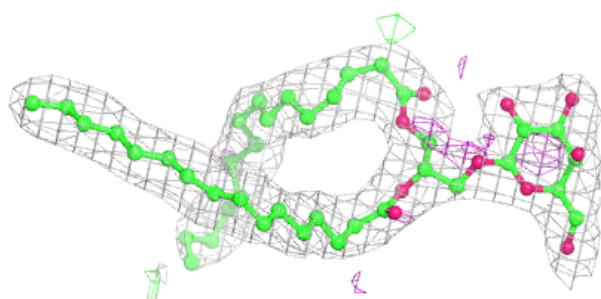
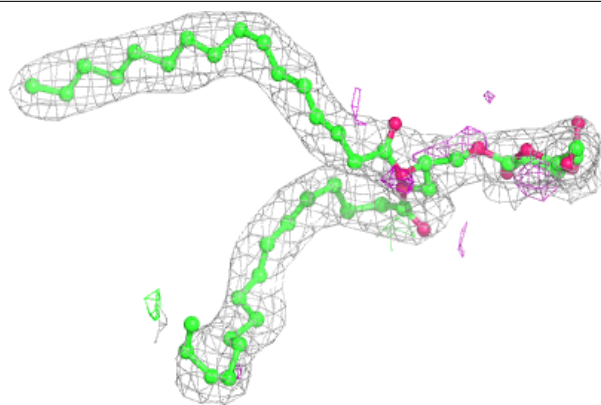
**Electron density around LMG M 101:**

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

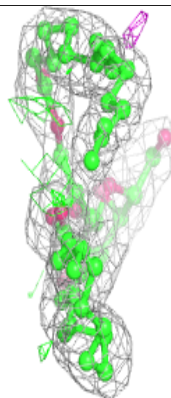
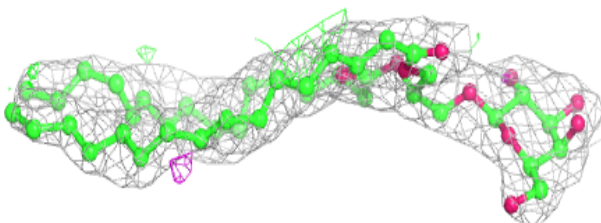
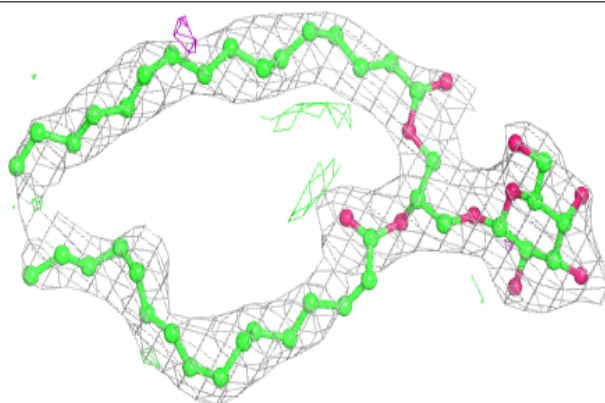


Electron density around LMG b 629:

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

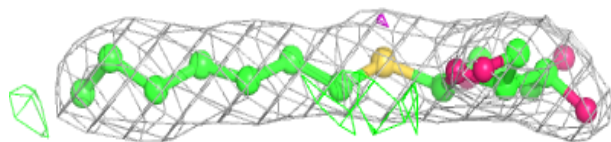
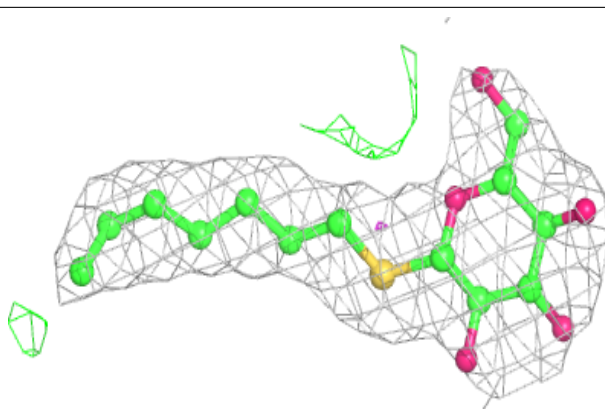
**Electron density around LMG C 501:**

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

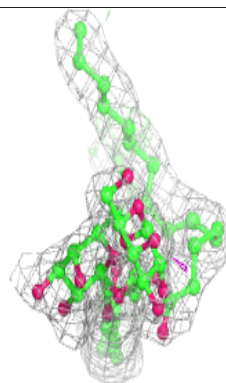
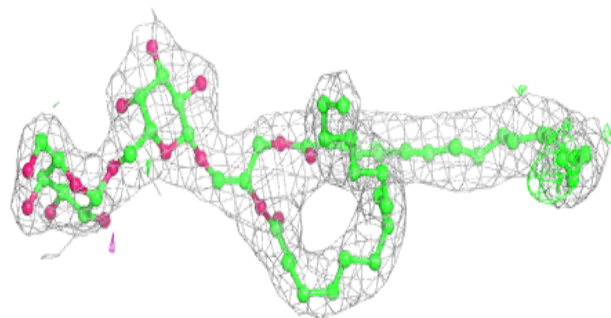
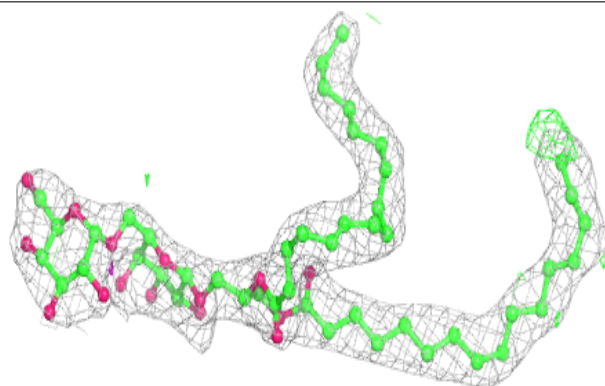


Electron density around HTG b 607:

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

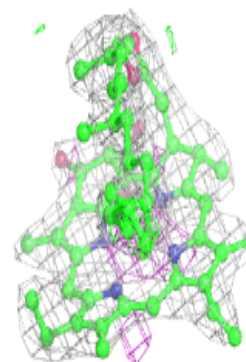
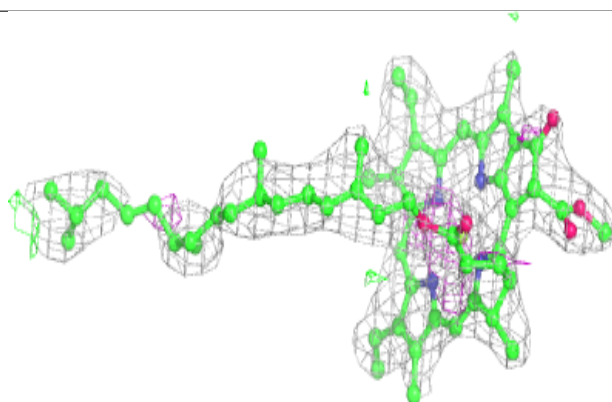
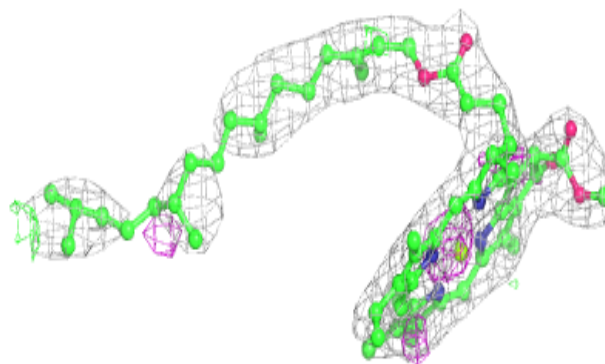
**Electron density around DGD h 102:**

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

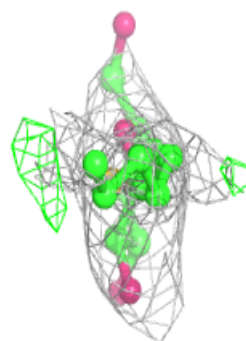
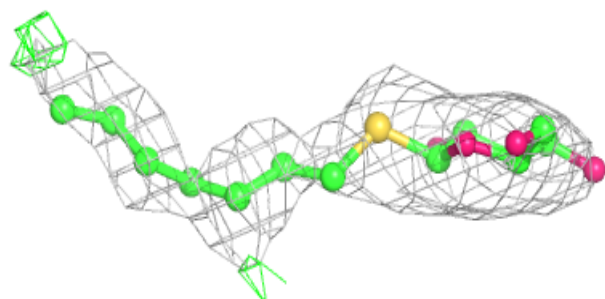
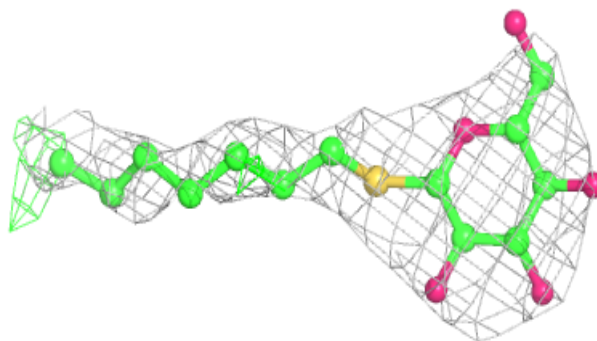


Electron density around CLA C 505:

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

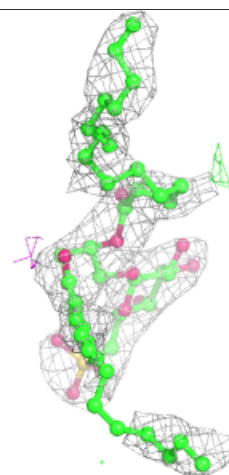
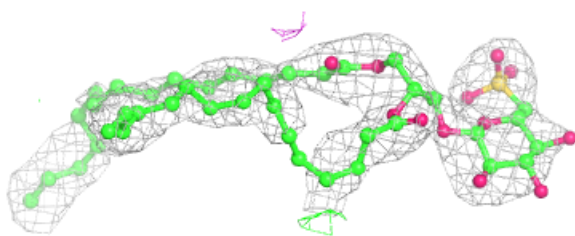
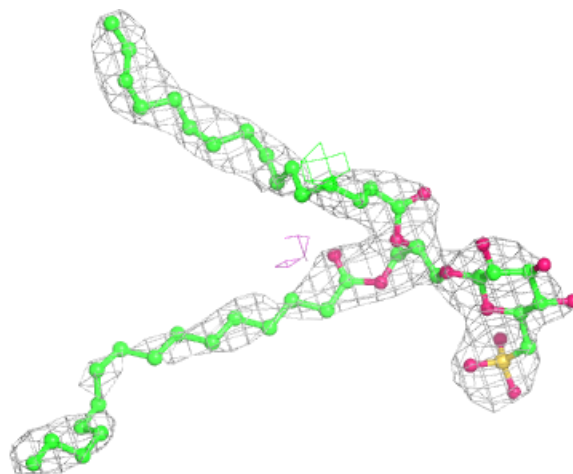
**Electron density around HTG c 524:**

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



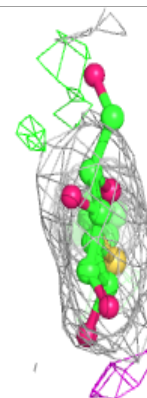
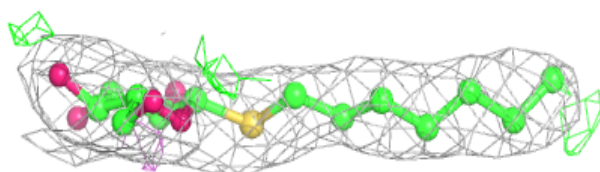
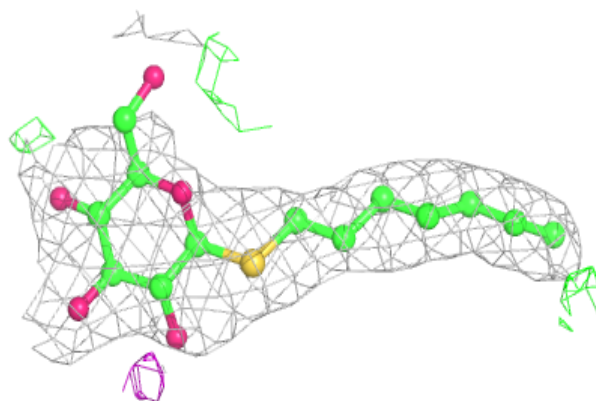
Electron density around SQD A 409:

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

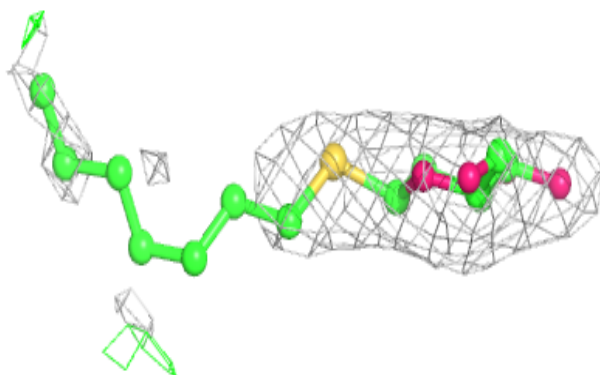
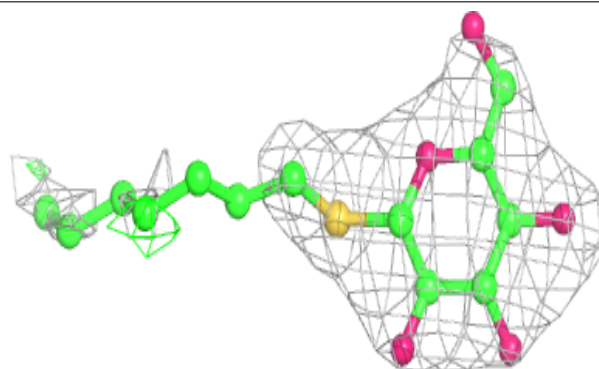


Electron density around HTG B 629:

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

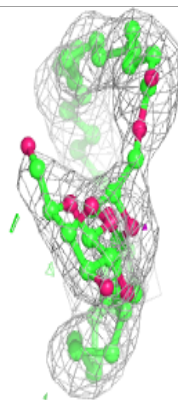
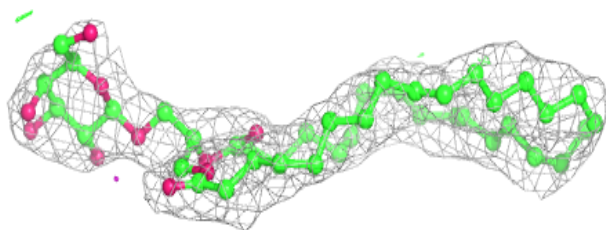
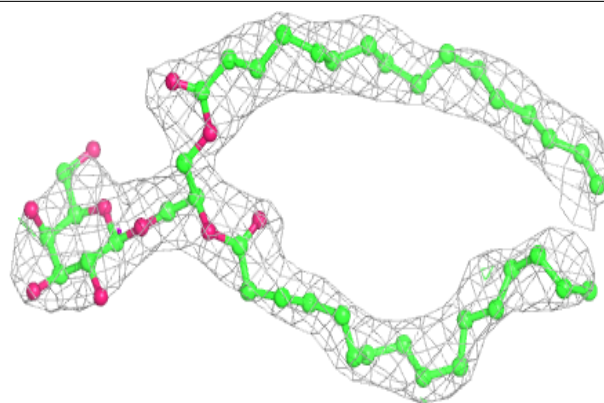
**Electron density around HTG C 522:**

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

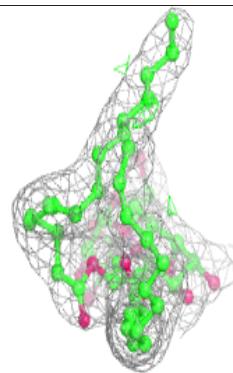
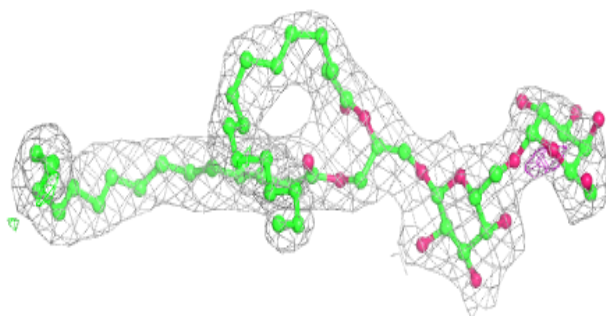
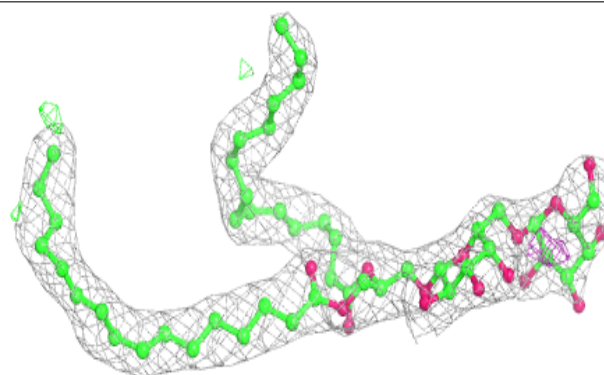


Electron density around LMG a 415:

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

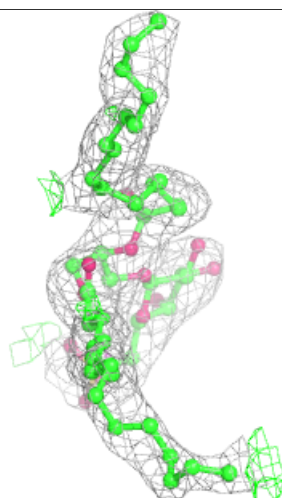
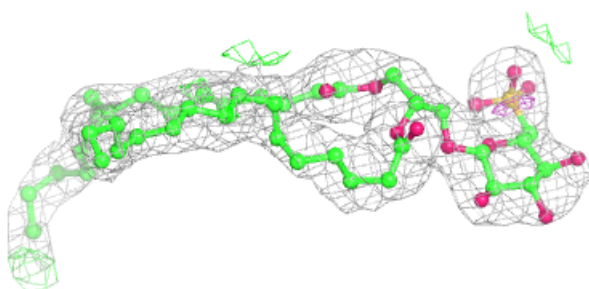
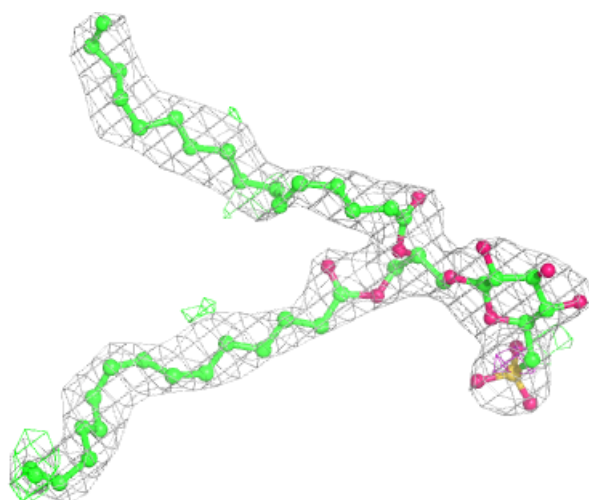
**Electron density around DGD B 632:**

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



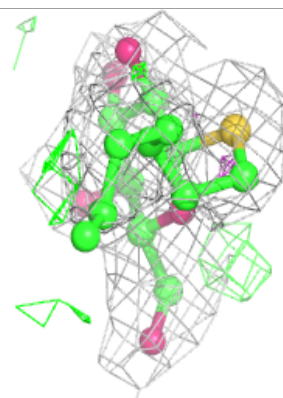
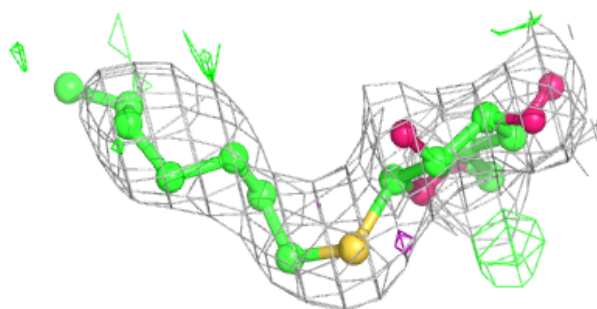
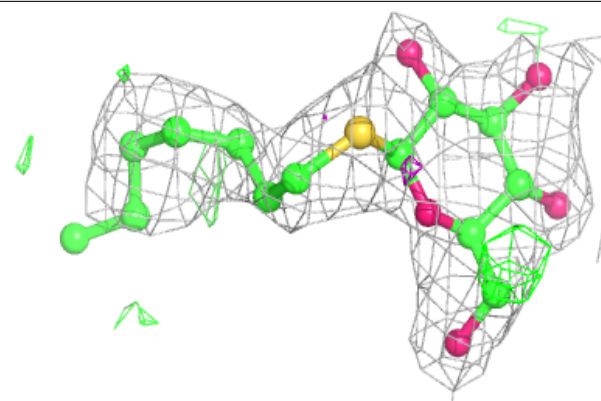
Electron density around SQD a 414:

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

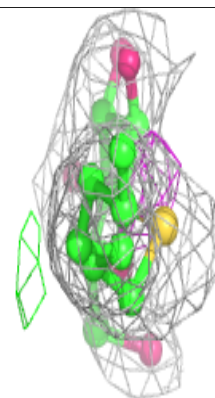
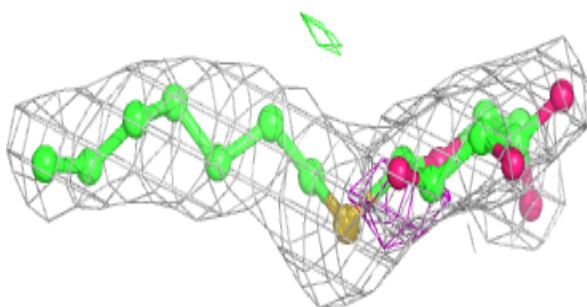
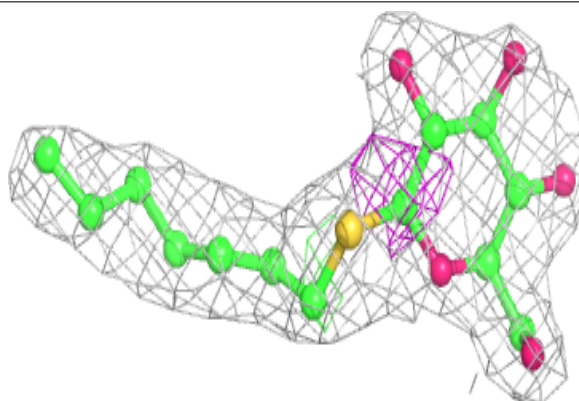


Electron density around HTG B 622:

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

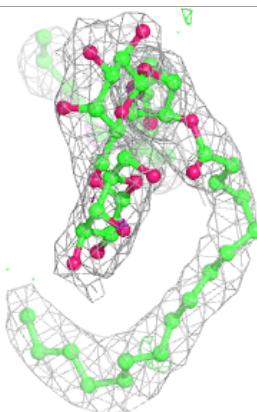
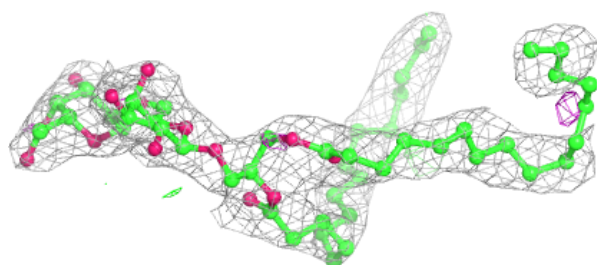
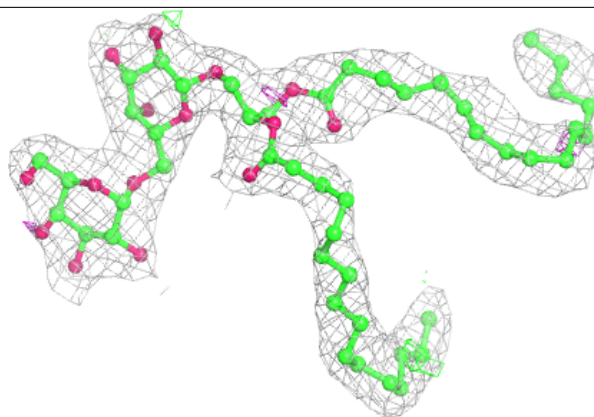
**Electron density around HTG b 601:**

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

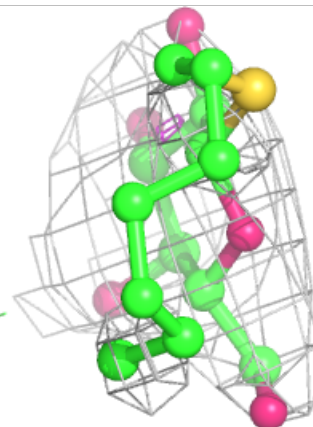
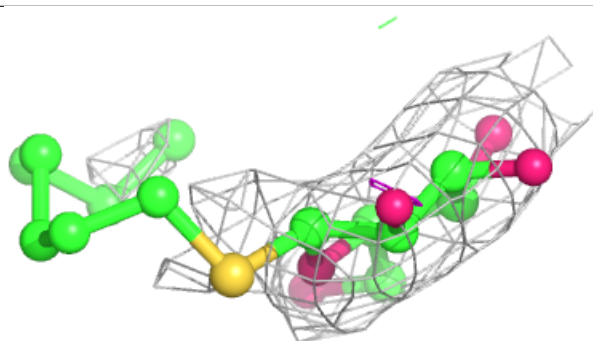
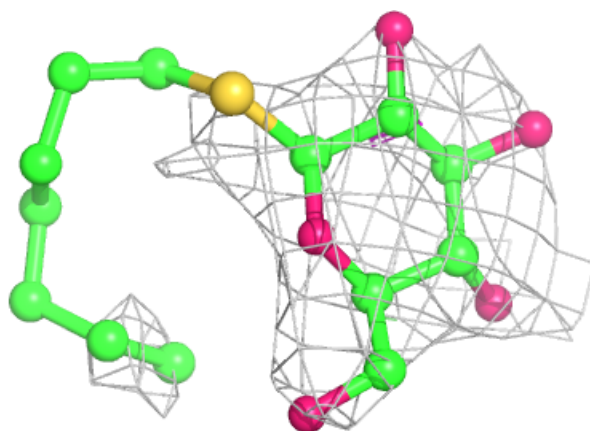


Electron density around DGD c 520:

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

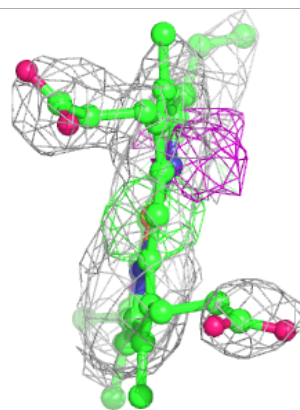
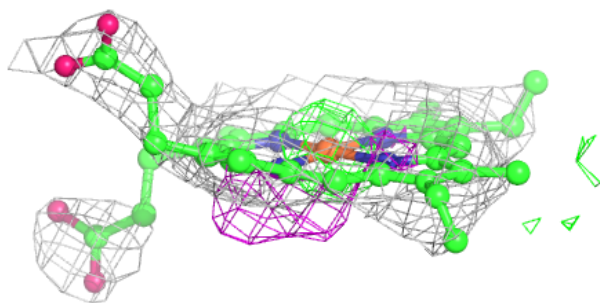
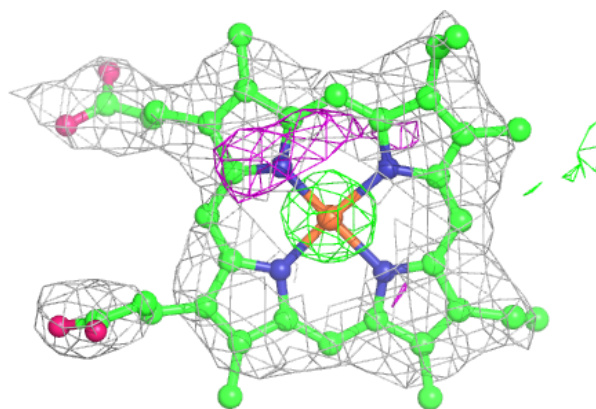
**Electron density around HTG V 207:**

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



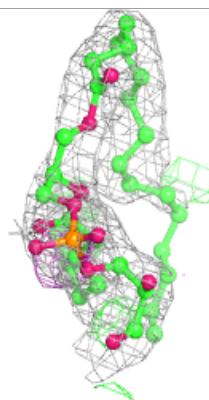
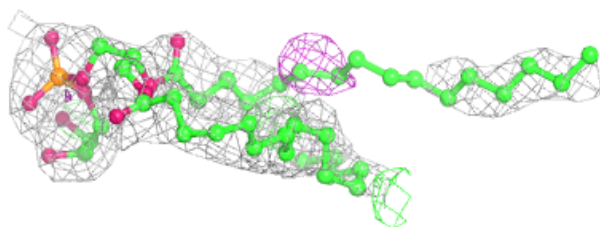
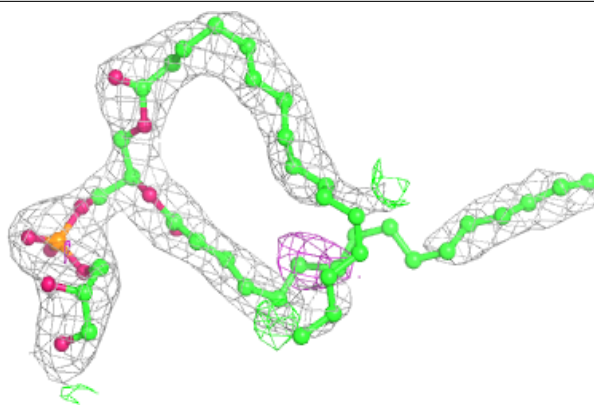
Electron density around HEM F 102:

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

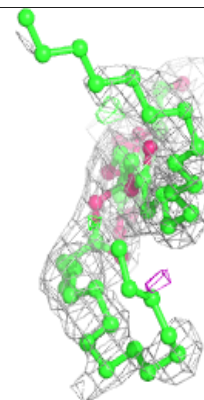
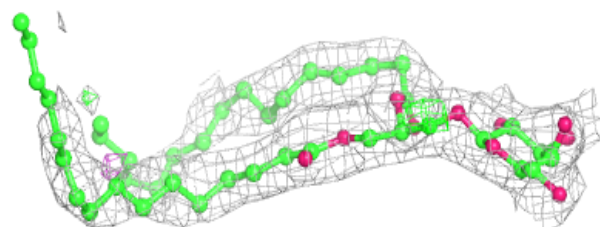
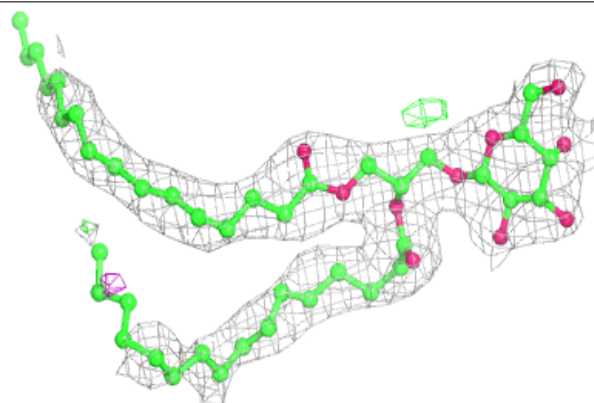


Electron density around LHG D 413:

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

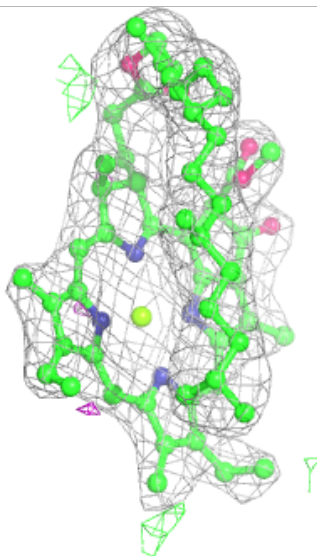
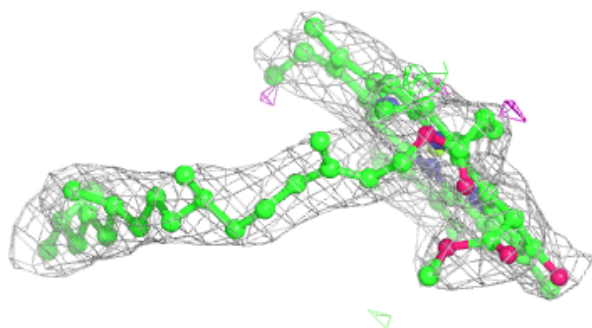
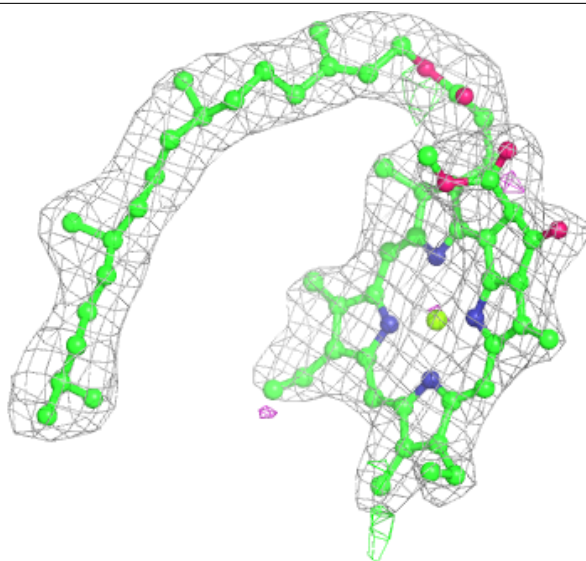
**Electron density around LMG D 417:**

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



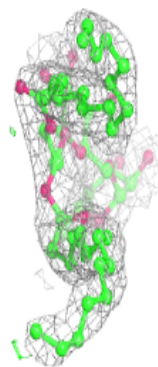
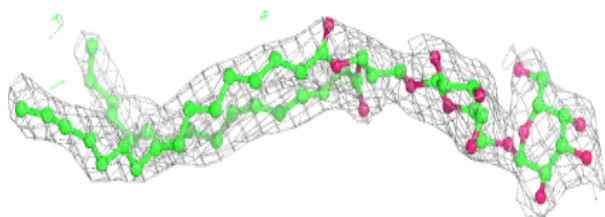
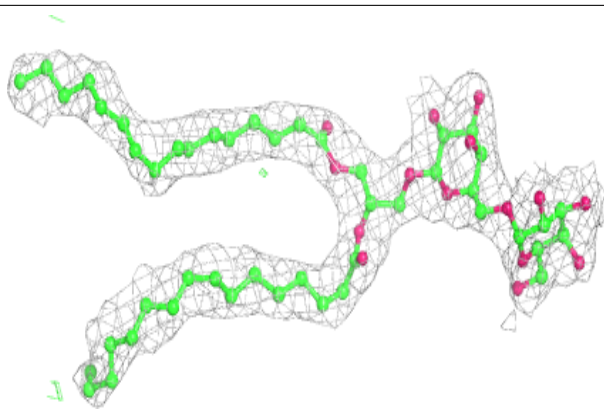
Electron density around CLA c 511:

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

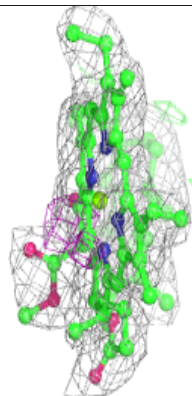
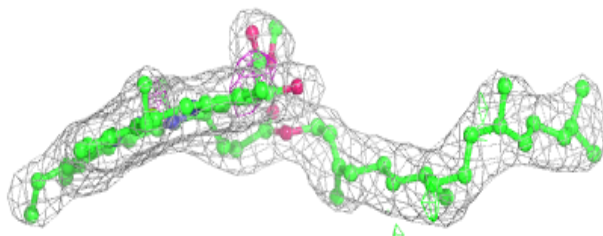
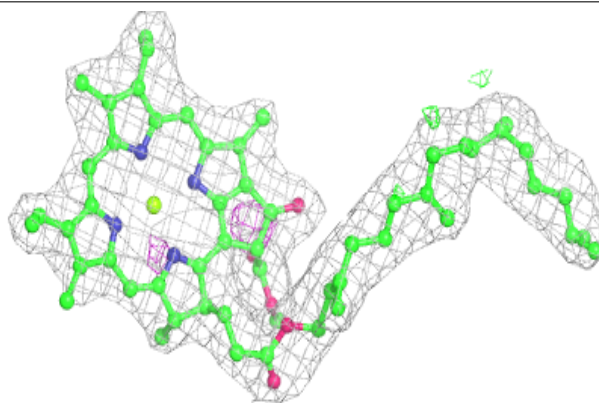


Electron density around DGD c 521:

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

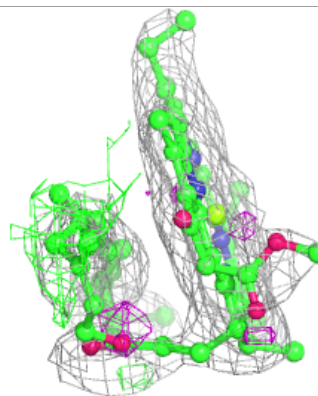
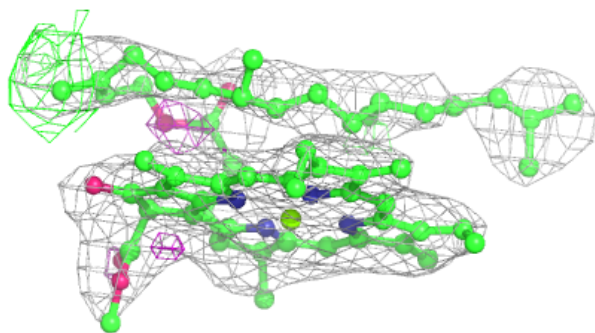
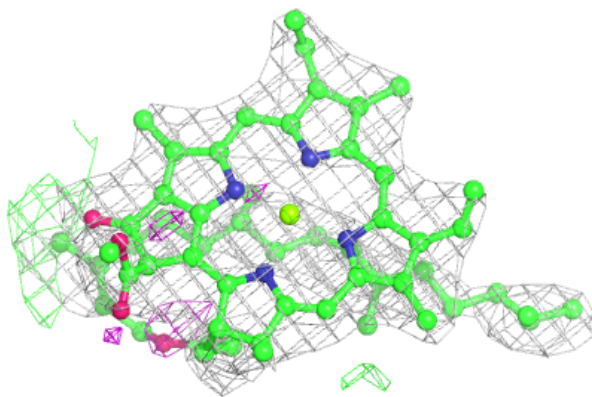
**Electron density around CLA b 611:**

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

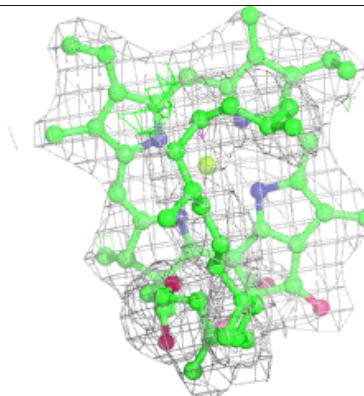
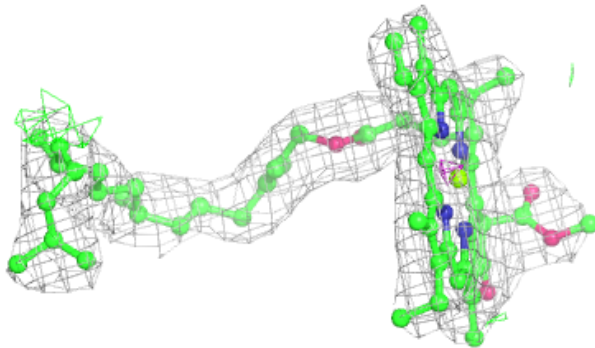
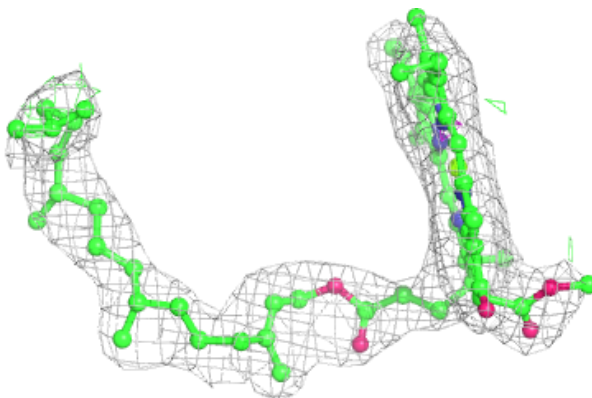


Electron density around CLA B 602:

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

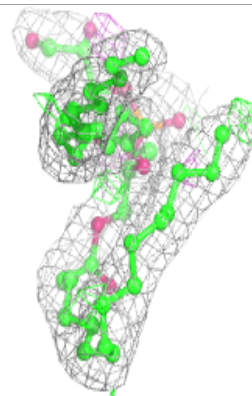
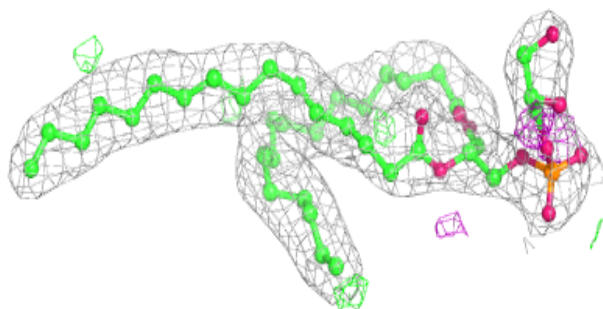
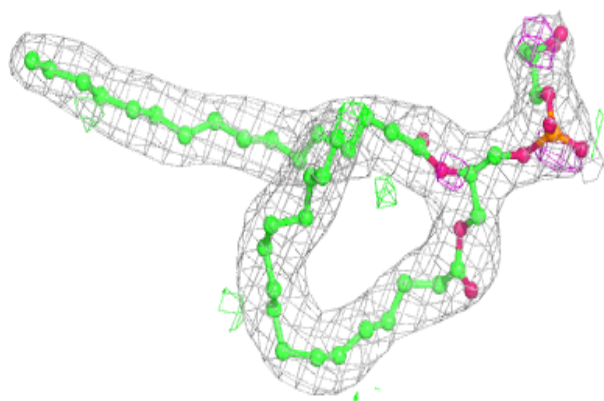
**Electron density around CLA c 510:**

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

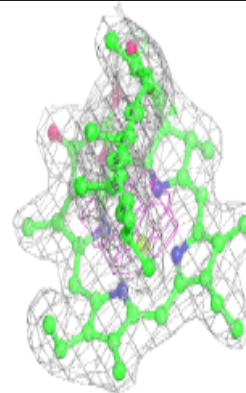
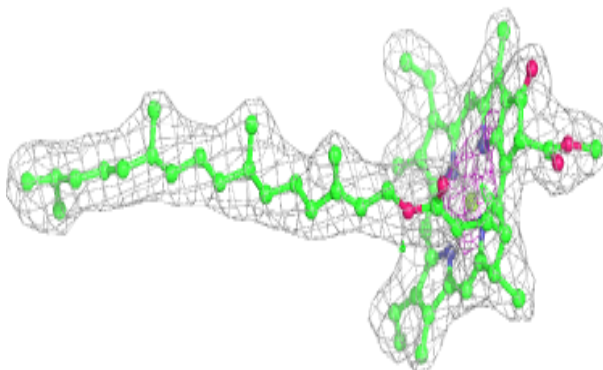
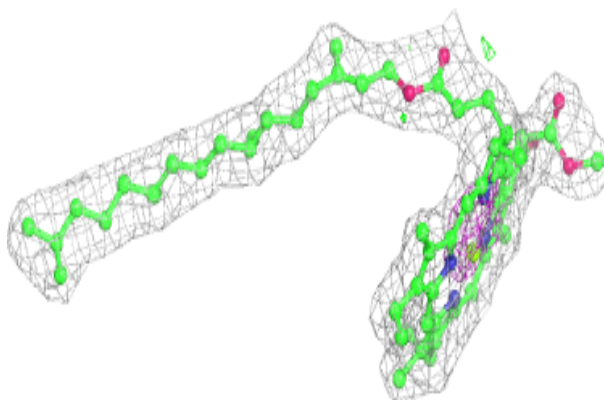


Electron density around LHG D 411:

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

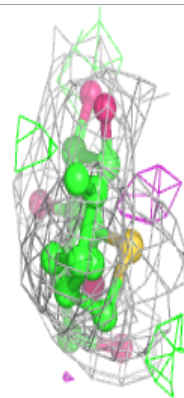
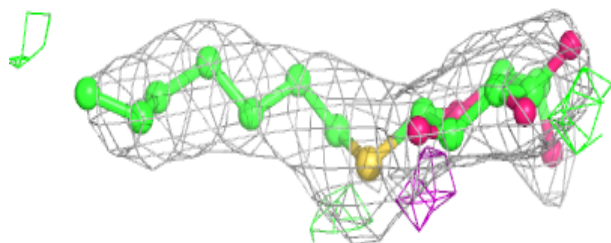
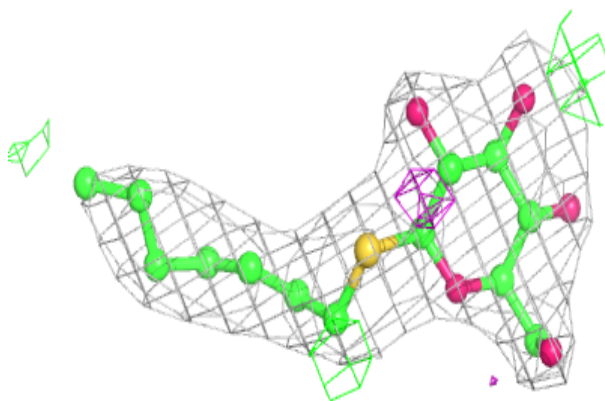
**Electron density around CLA b 616:**

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

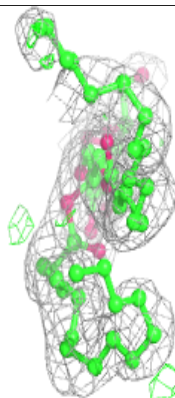
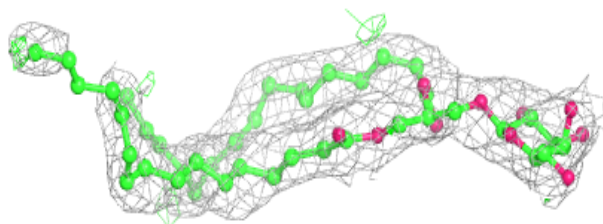
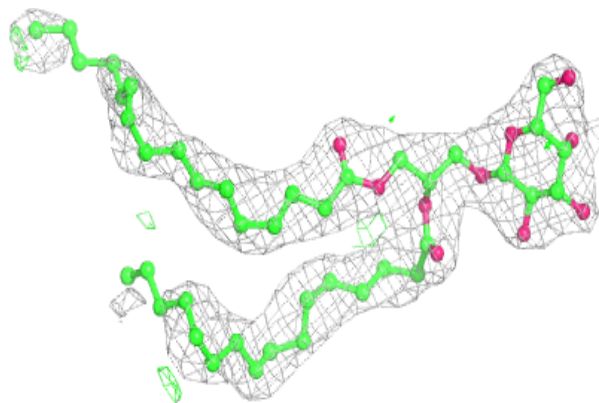


Electron density around HTG o 301:

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

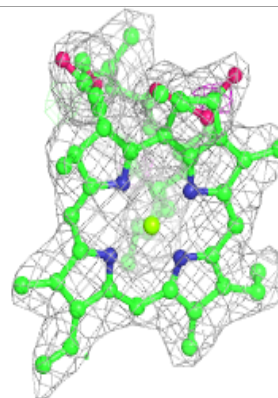
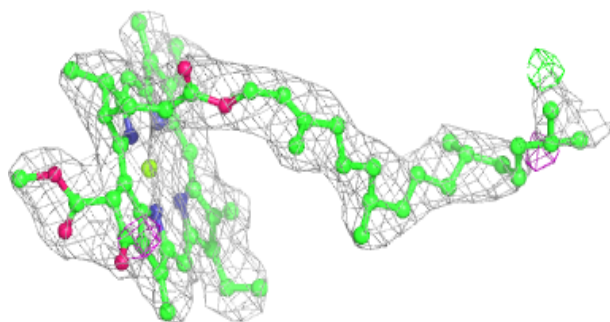
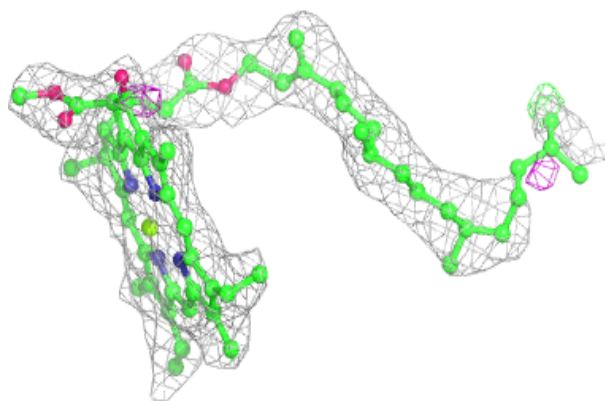
**Electron density around LMG d 416:**

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

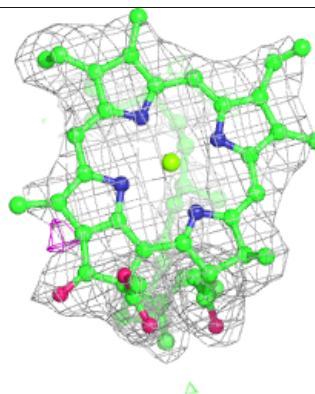
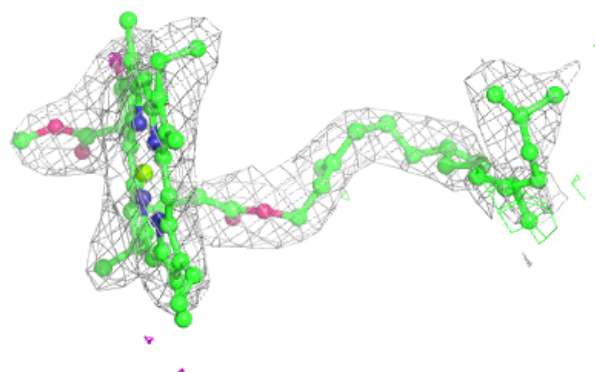
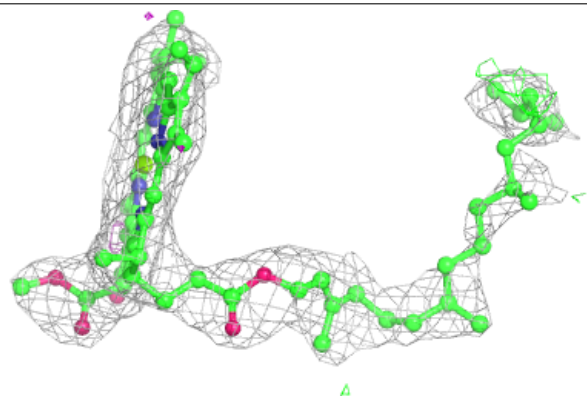


Electron density around CLA c 512:

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

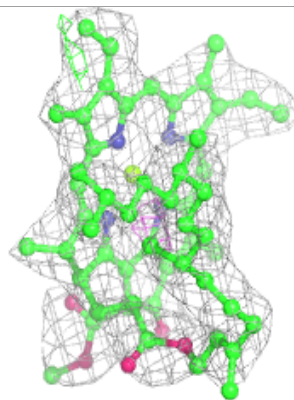
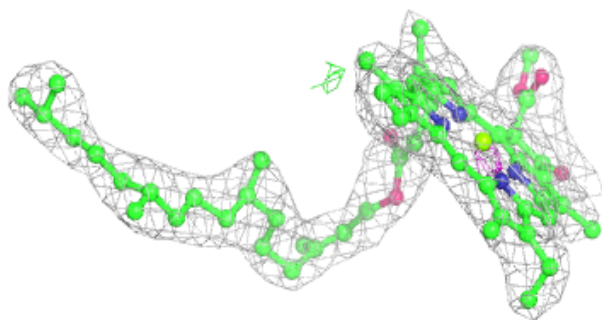
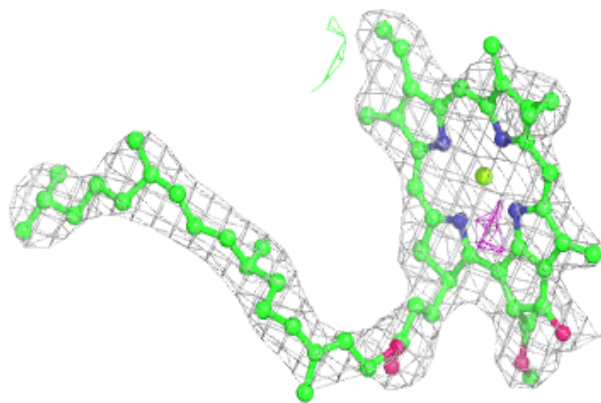
**Electron density around CLA C 507:**

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

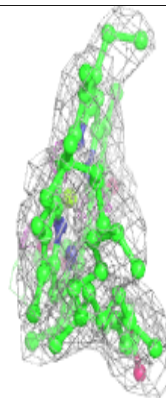
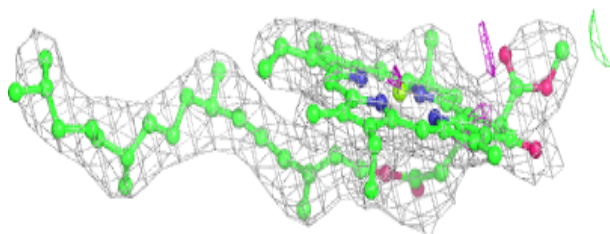
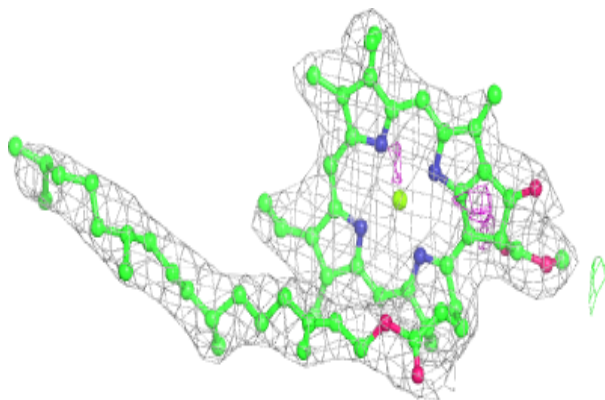


Electron density around CLA C 512:

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

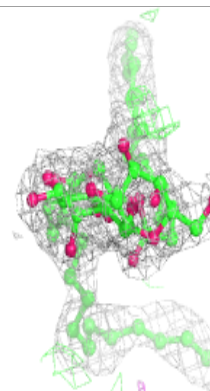
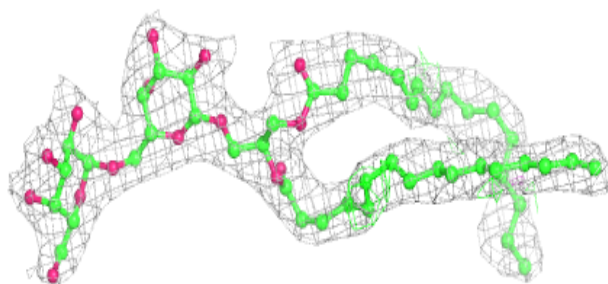
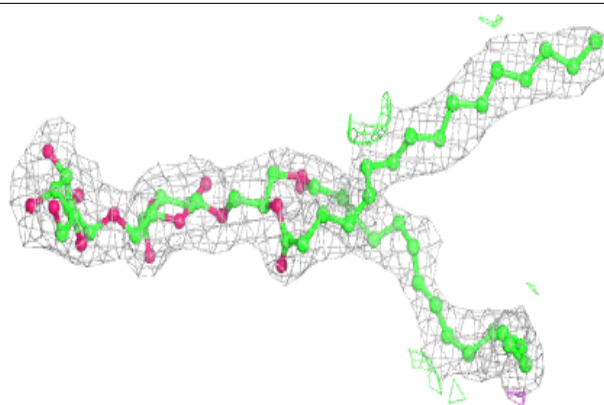
**Electron density around CLA C 502:**

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

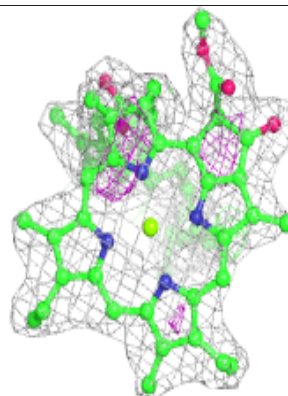
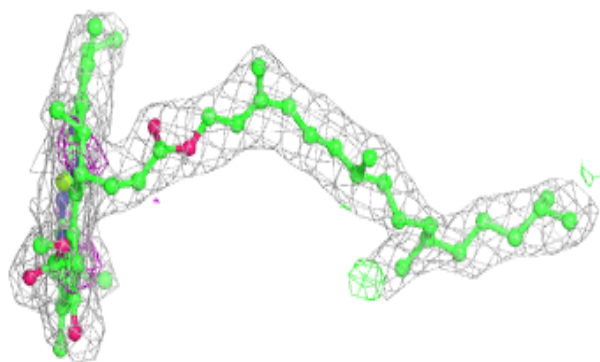
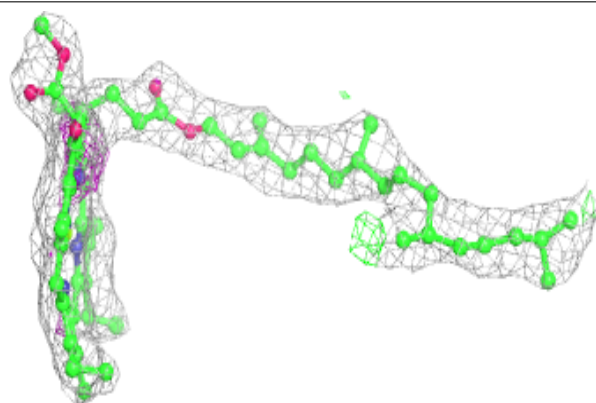


Electron density around DGD C 516:

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

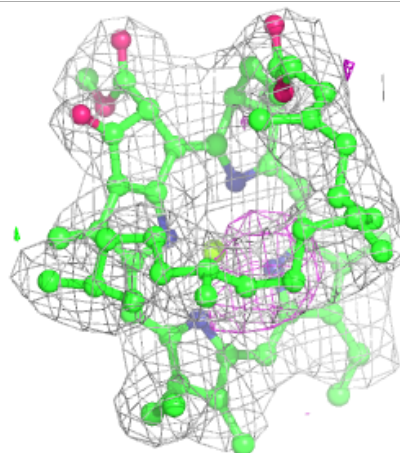
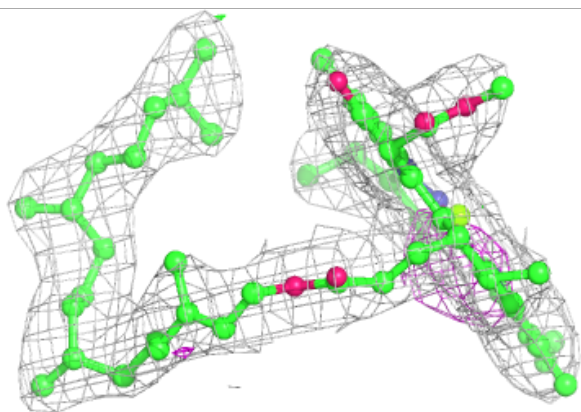
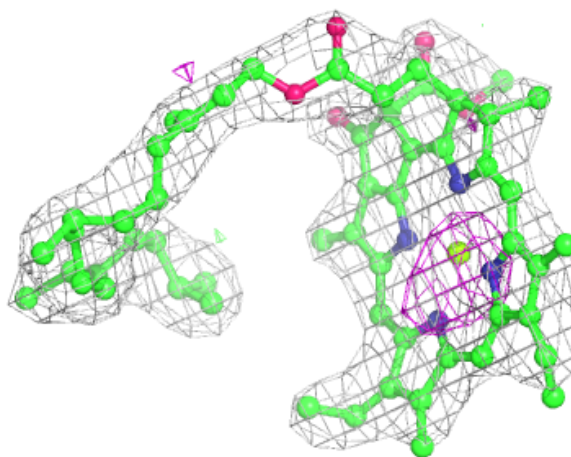
**Electron density around CLA B 607:**

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



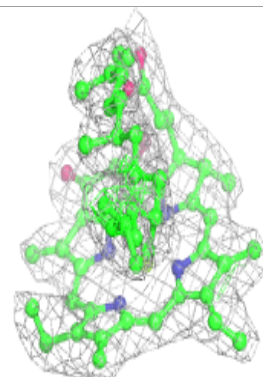
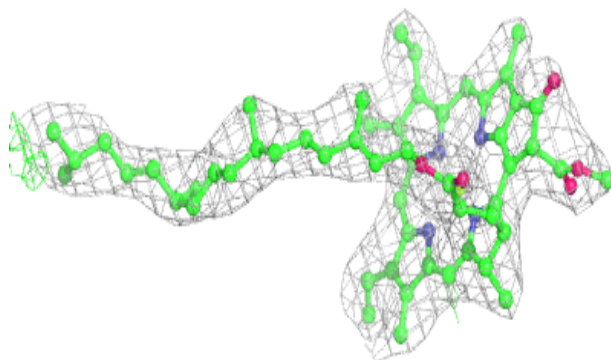
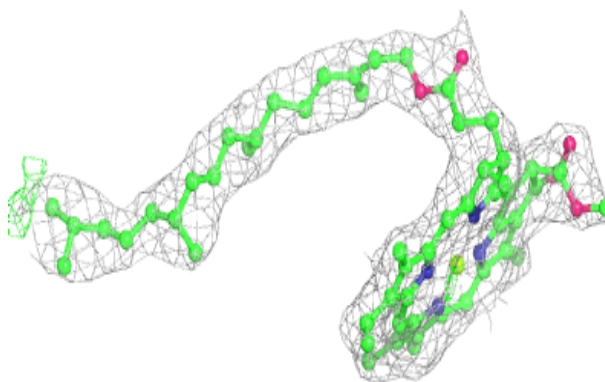
Electron density around CLA c 507:

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

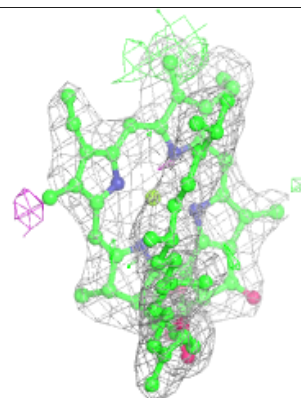
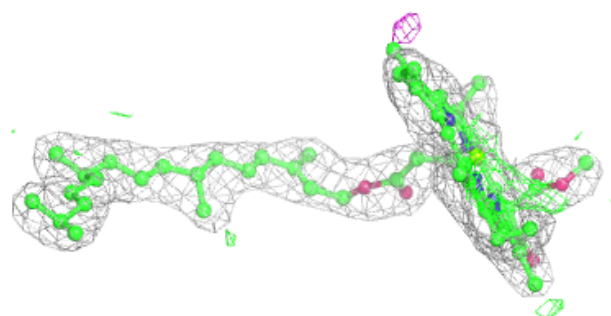
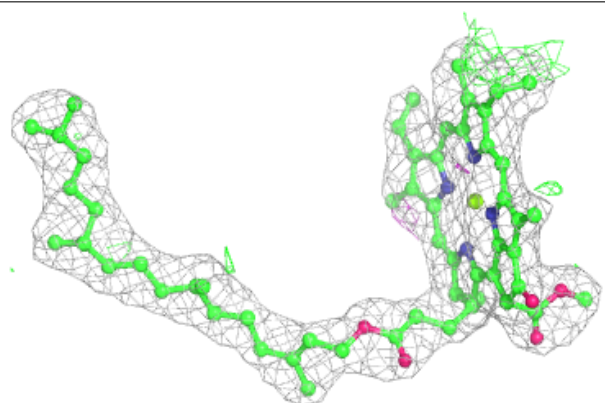


Electron density around CLA c 508:

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

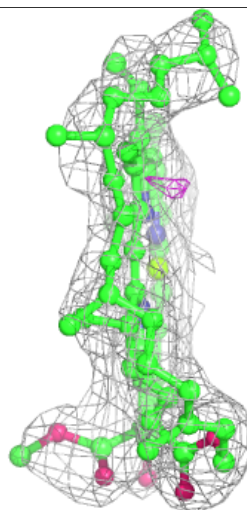
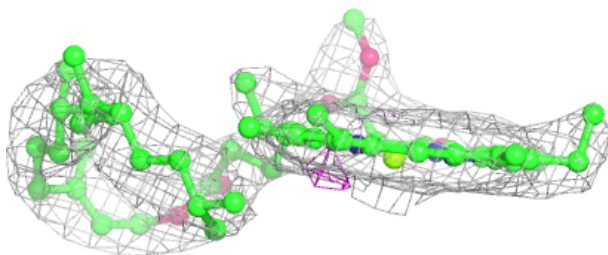
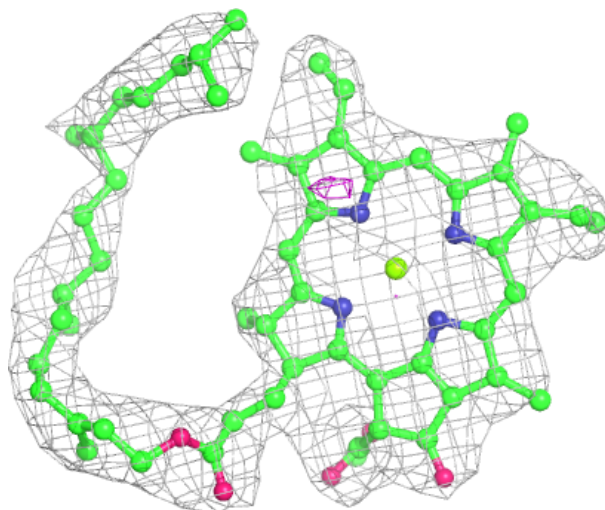
**Electron density around CLA b 618:**

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



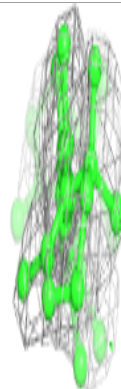
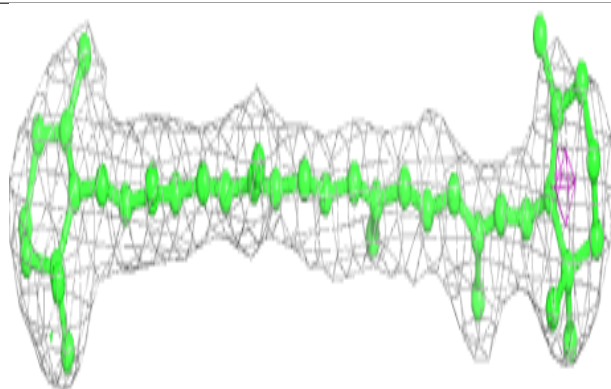
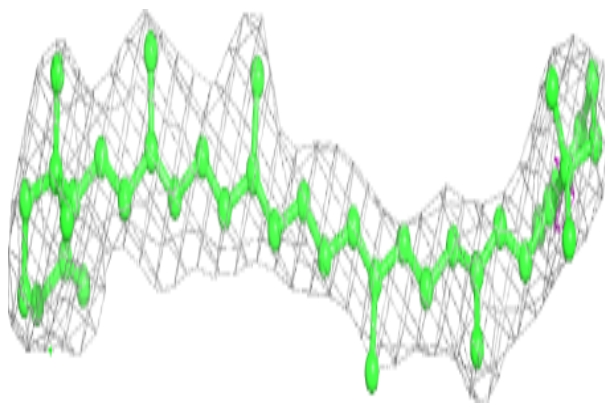
Electron density around CLA C 513:

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



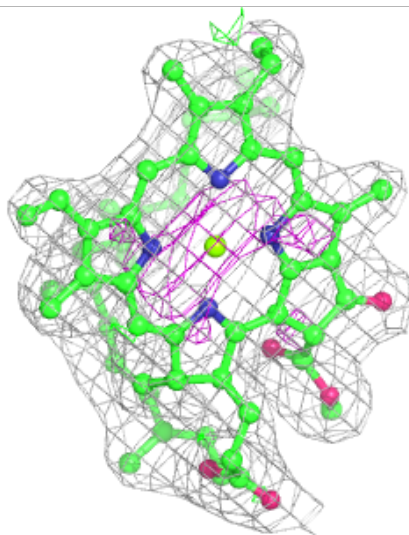
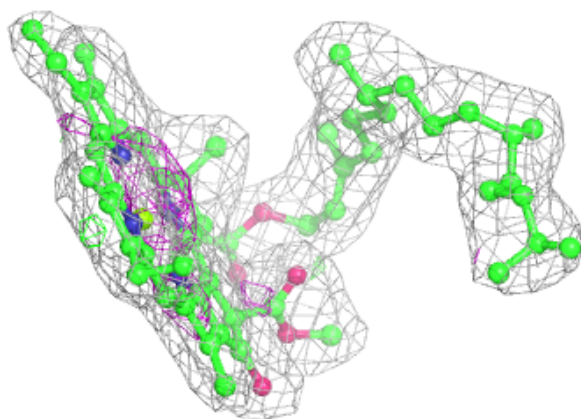
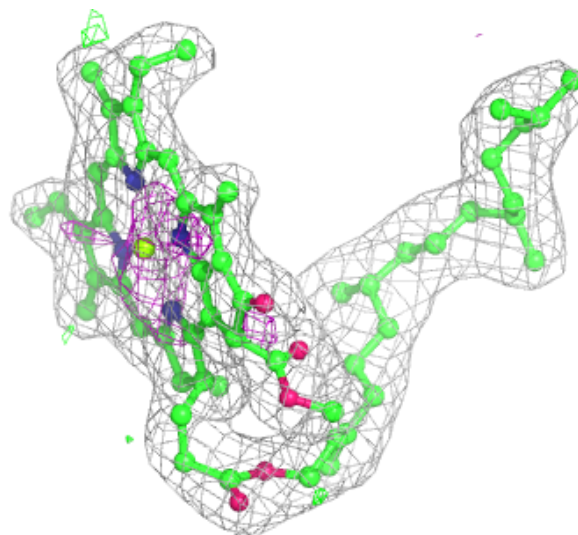
Electron density around BCR K 101:

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



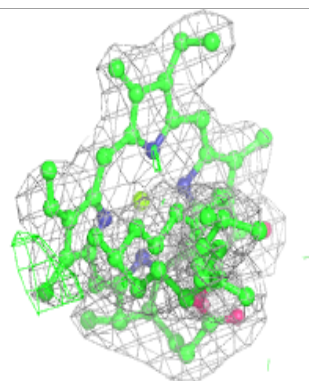
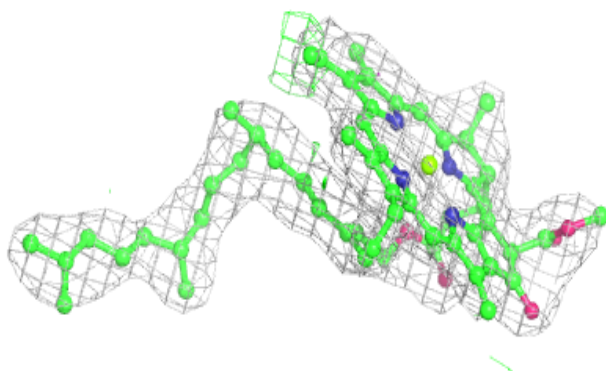
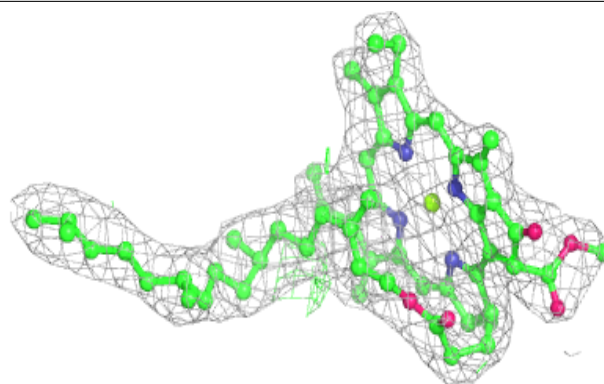
Electron density around CLA B 614:

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

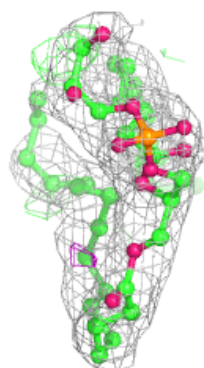
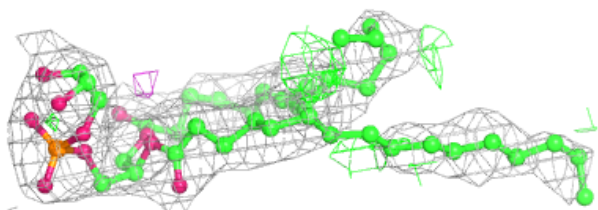
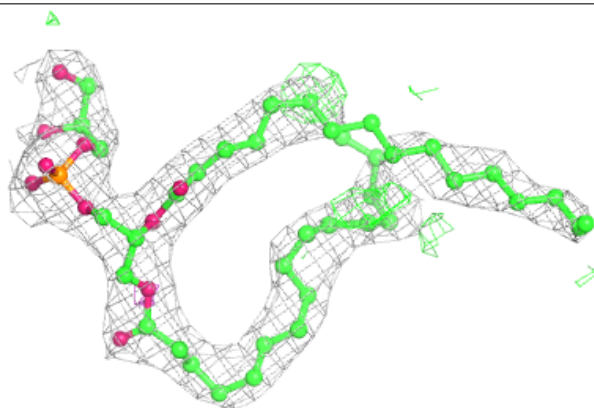


Electron density around CLA c 509:

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

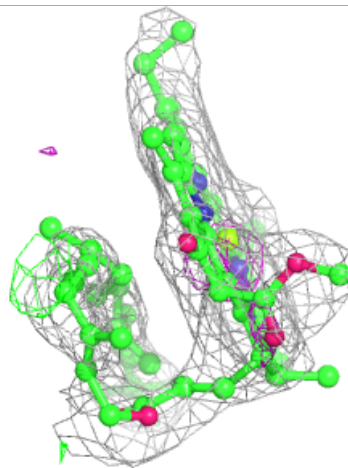
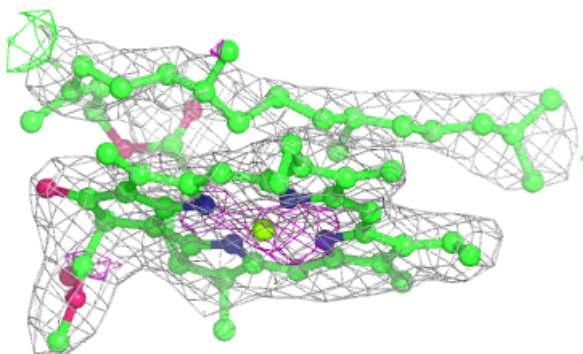
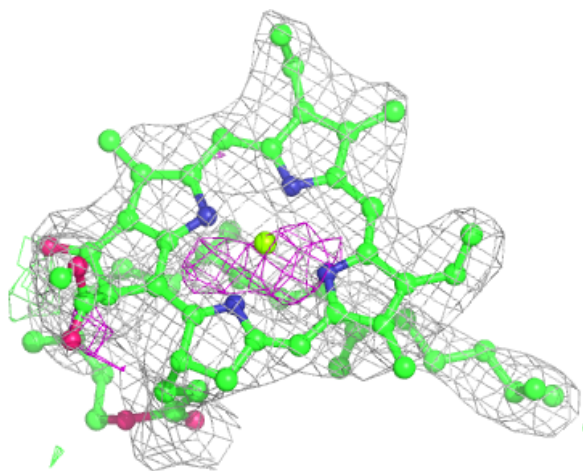
**Electron density around LHG d 411:**

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



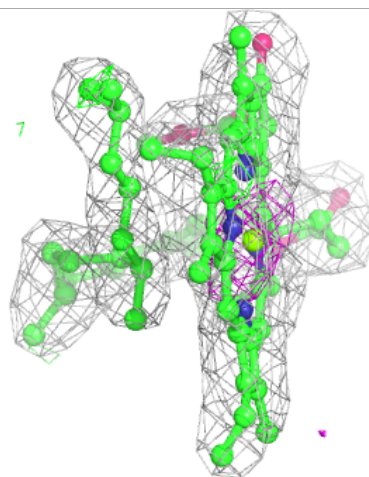
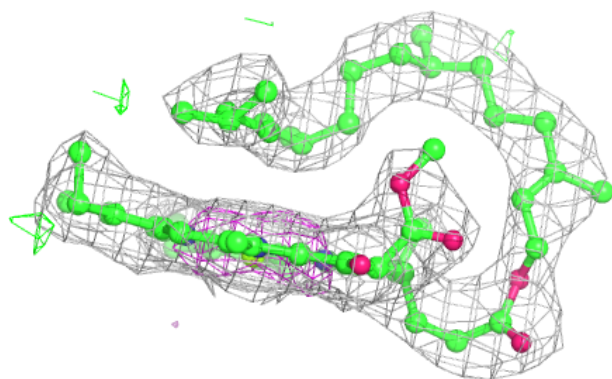
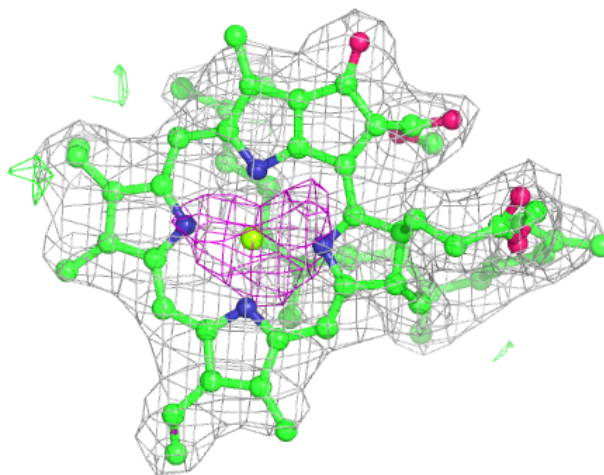
Electron density around CLA b 610:

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



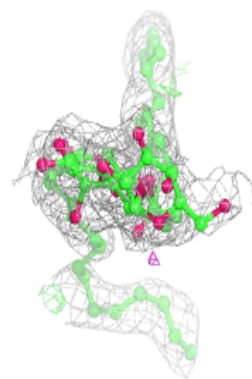
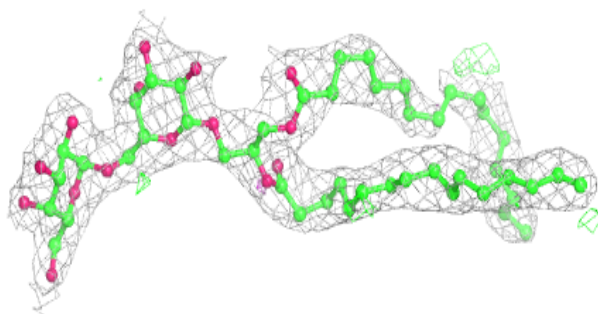
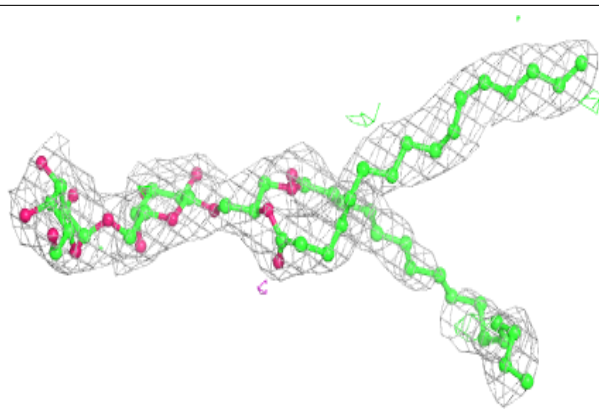
Electron density around CLA C 511:

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

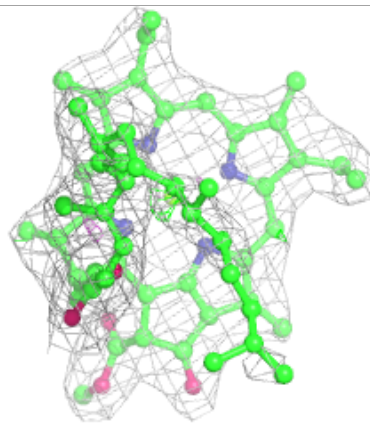
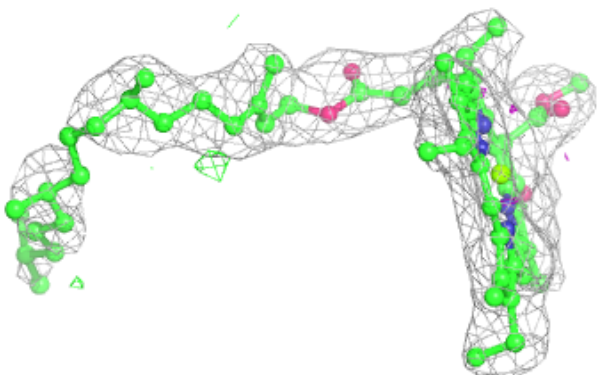
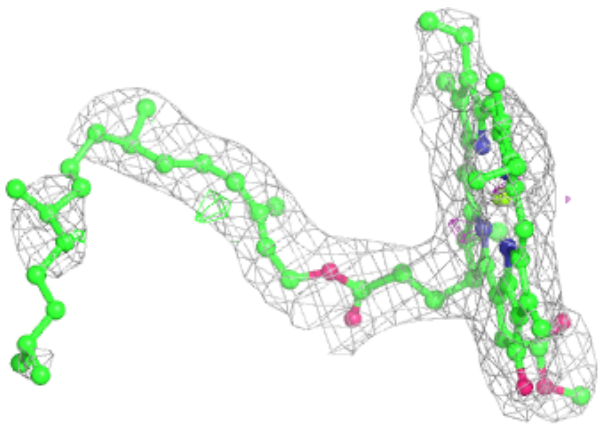


Electron density around DGD c 519:

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

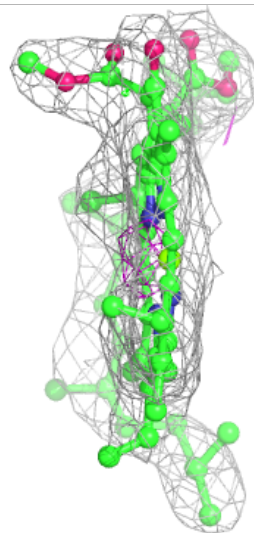
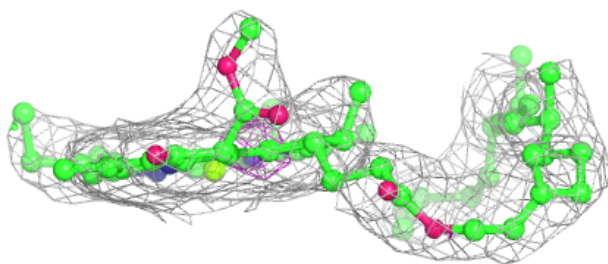
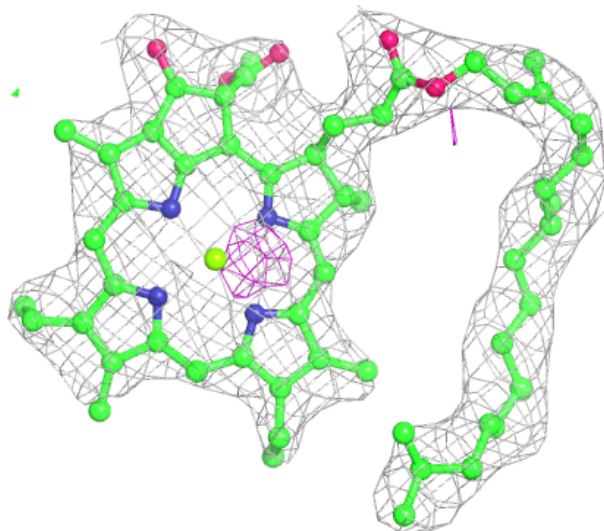
**Electron density around CLA D 407:**

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



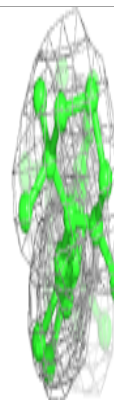
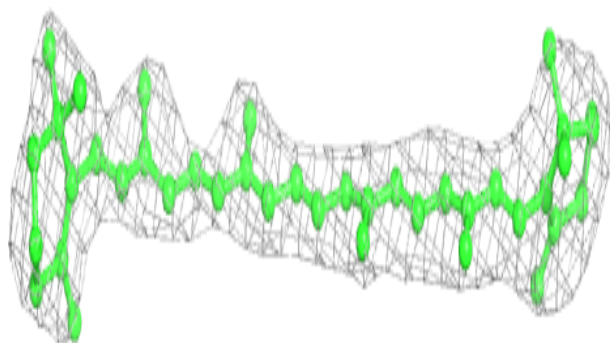
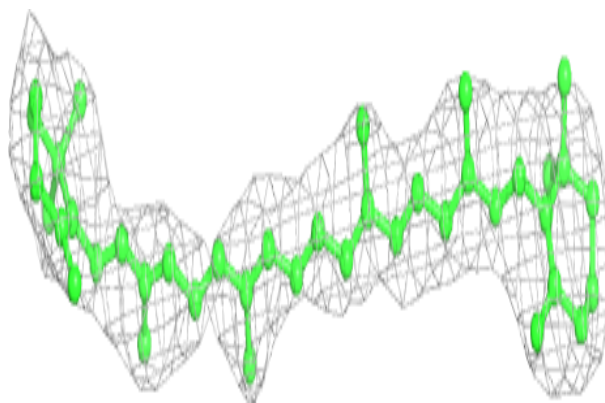
Electron density around CLA c 516:

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

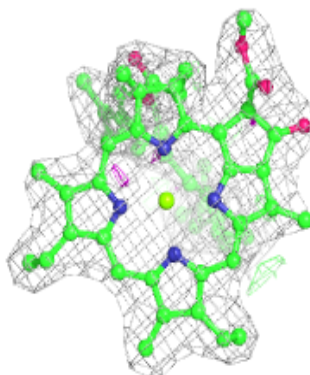
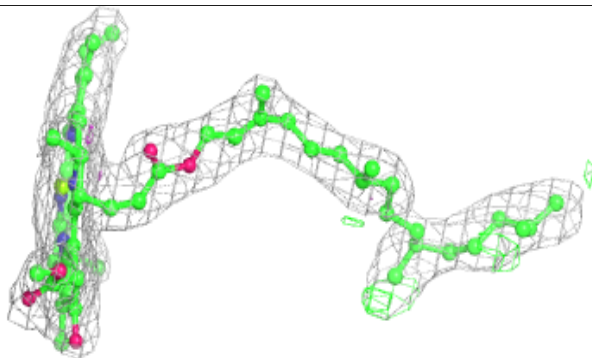
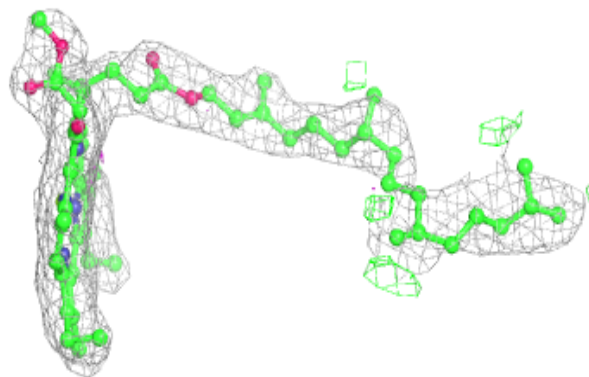


Electron density around BCR c 527:

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

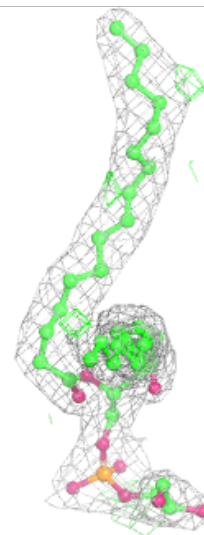
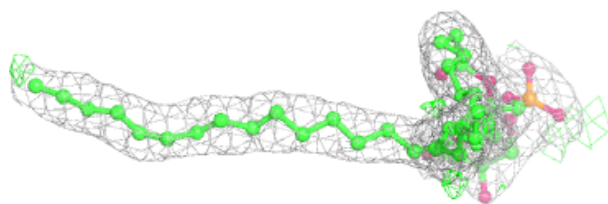
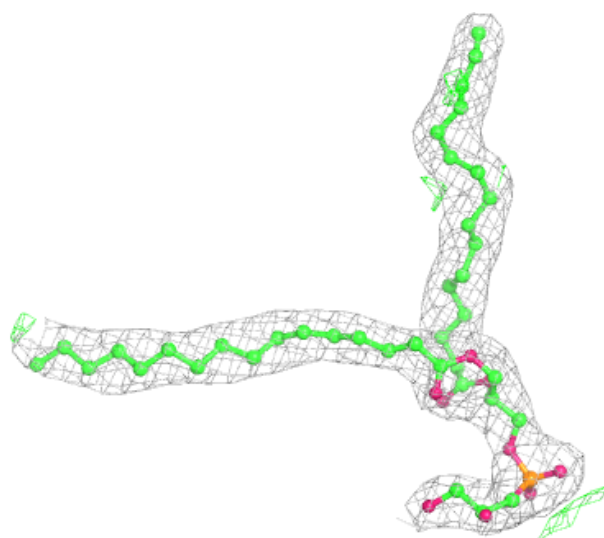
**Electron density around CLA b 615:**

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



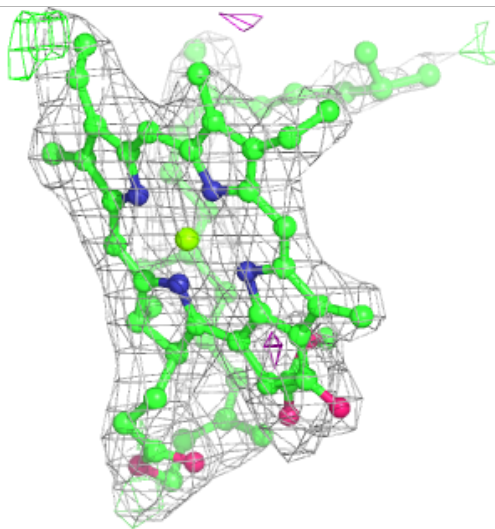
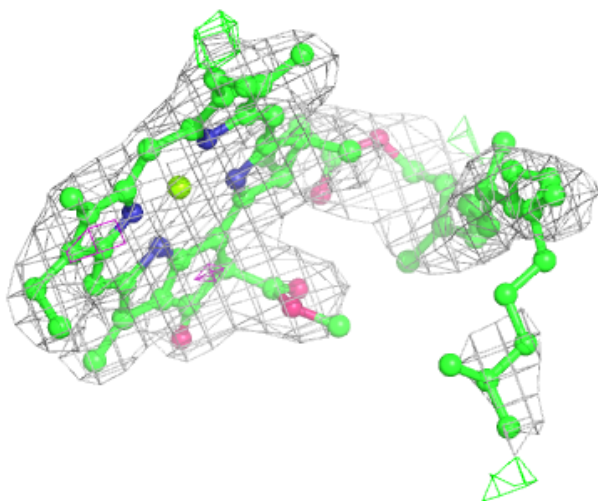
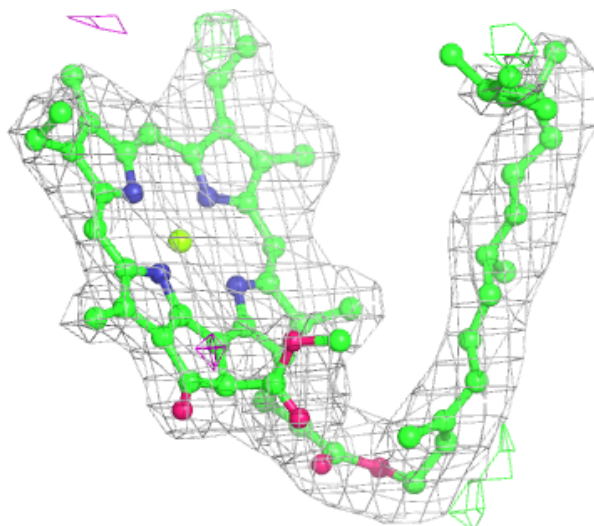
Electron density around LHG b 634:

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



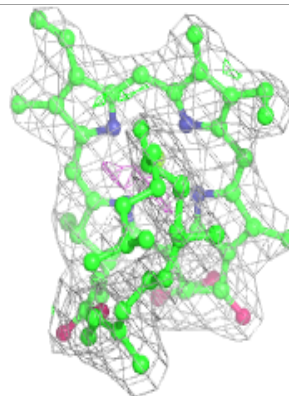
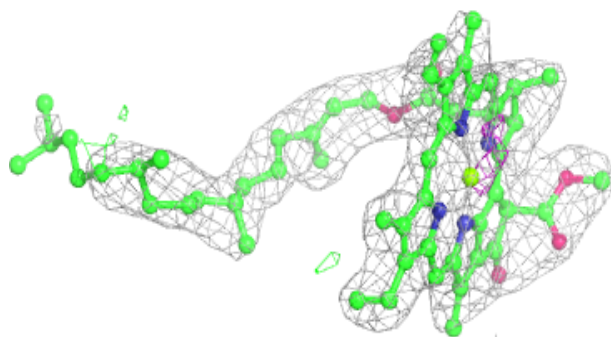
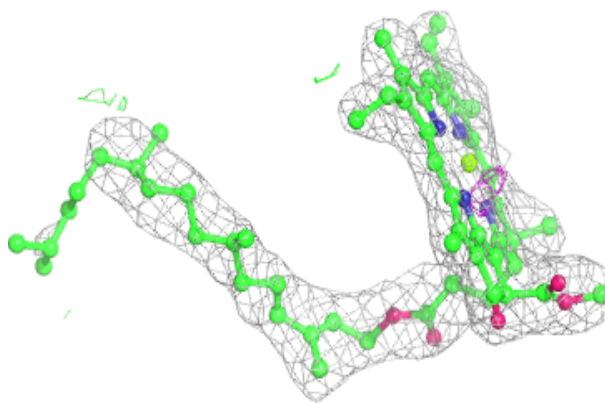
Electron density around CLA b 625:

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

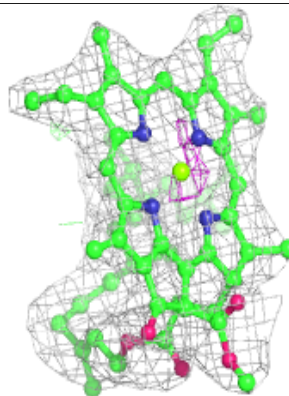
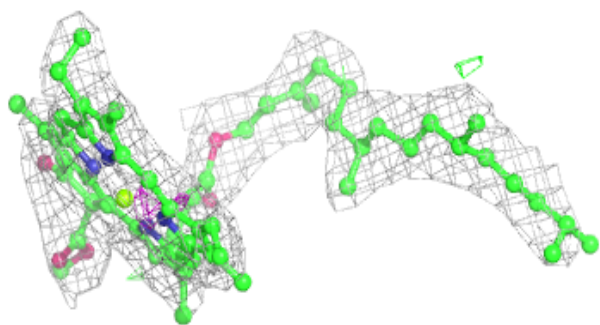
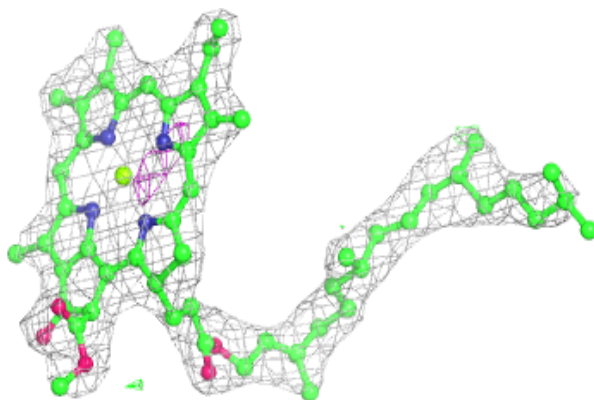


Electron density around CLA C 509:

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

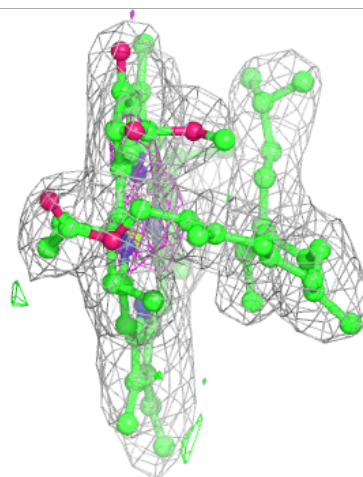
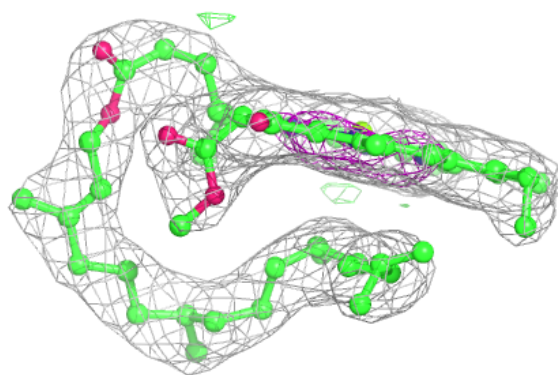
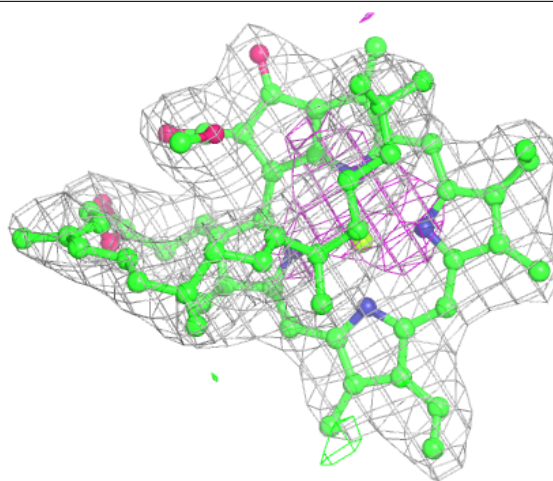
**Electron density around CLA c 515:**

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



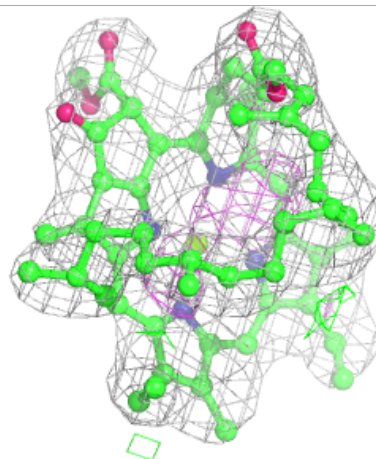
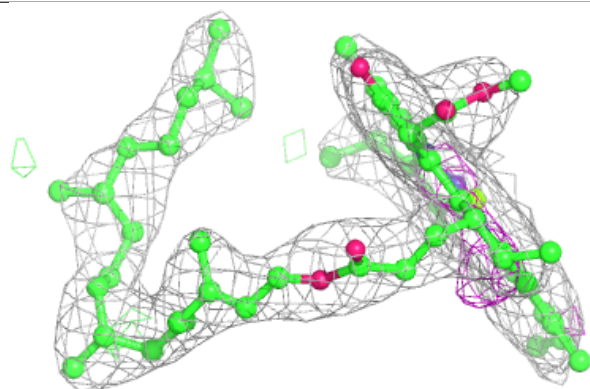
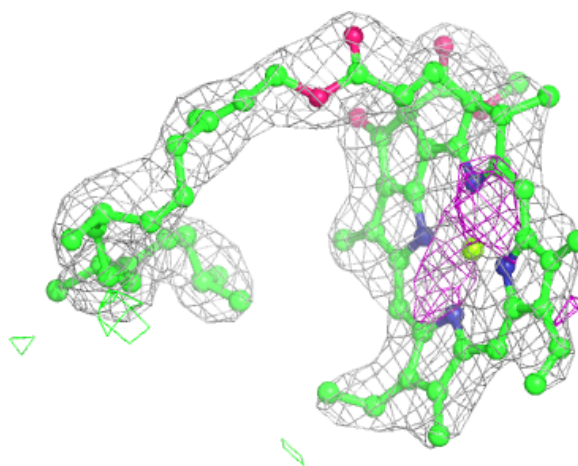
Electron density around CLA c 514:

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



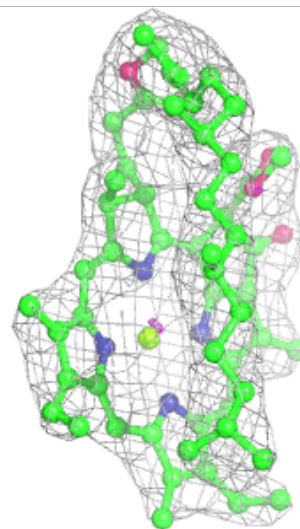
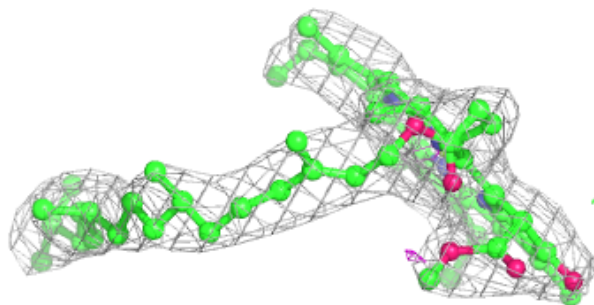
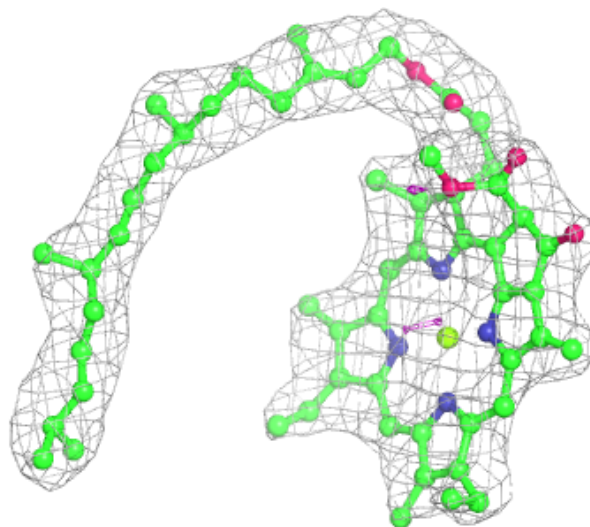
Electron density around CLA C 504:

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



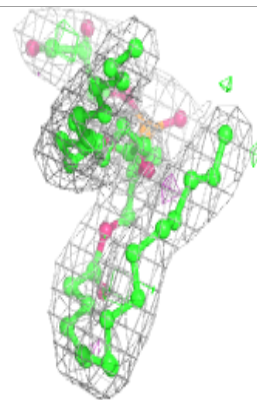
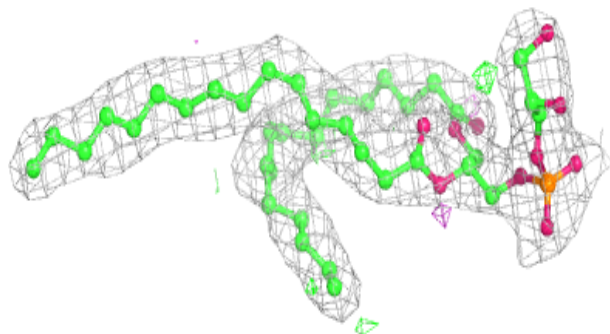
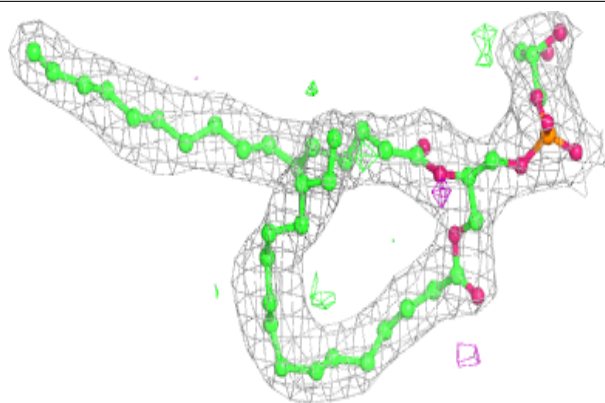
Electron density around CLA C 508:

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

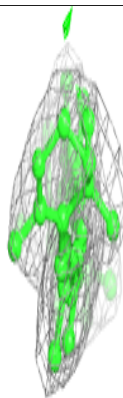
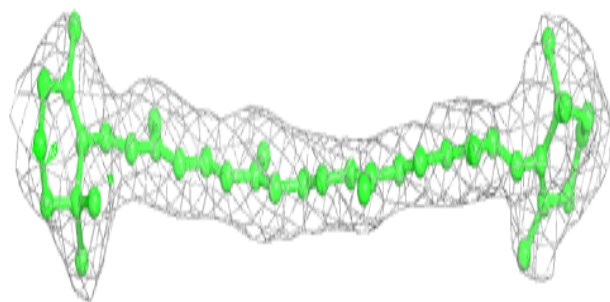
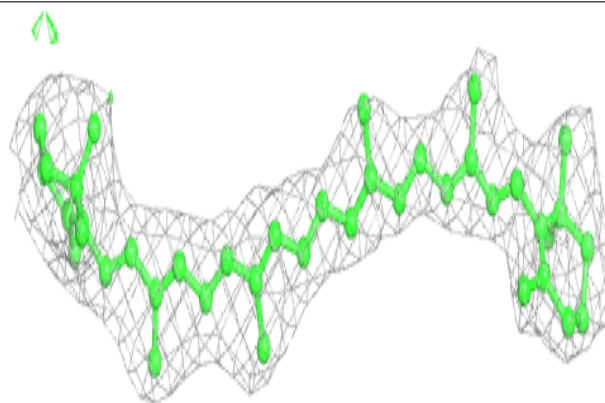


Electron density around LHG d 409:

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

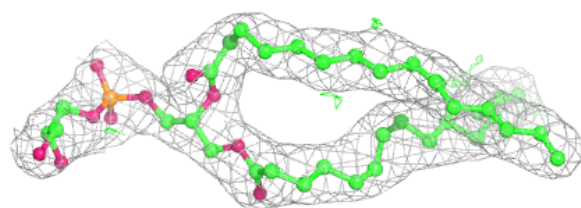
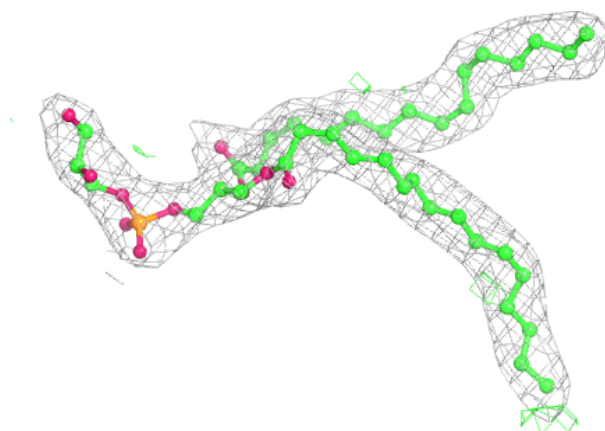
**Electron density around BCR k 102:**

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

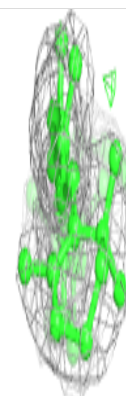
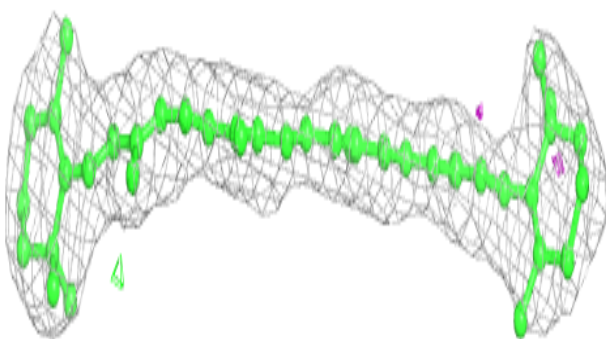
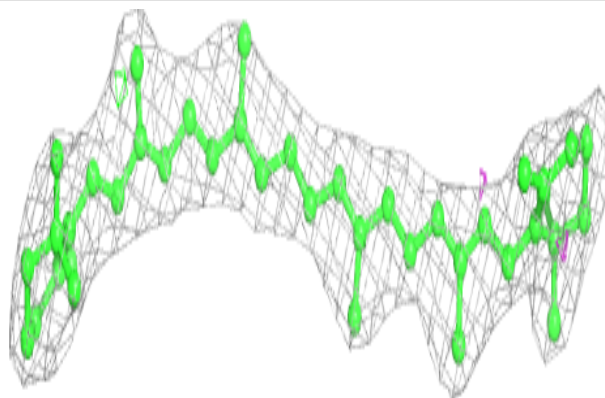


Electron density around LHG d 410:

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

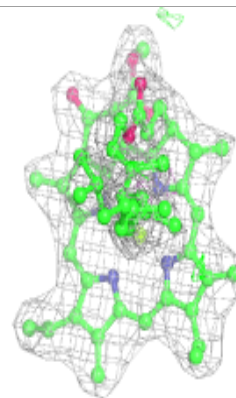
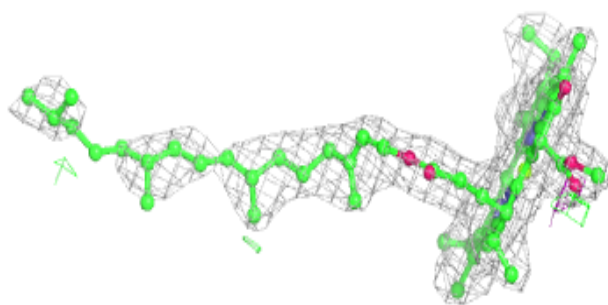
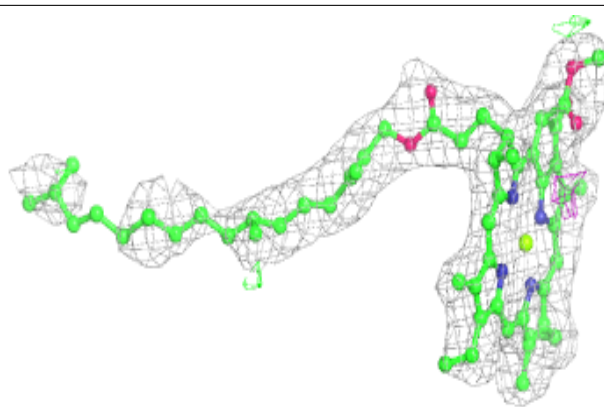
**Electron density around BCR h 101:**

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

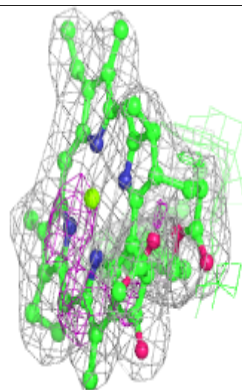
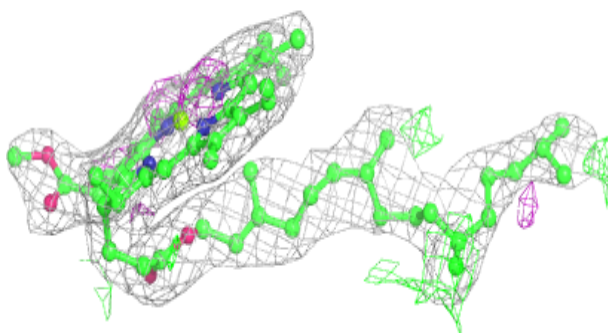
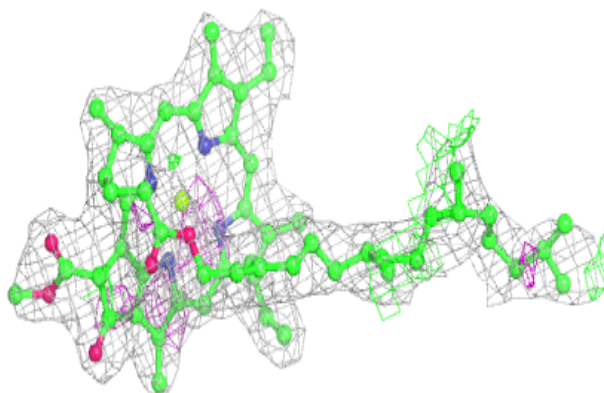


Electron density around CLA d 405:

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

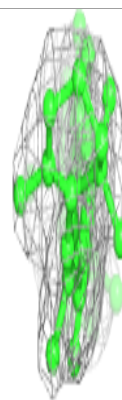
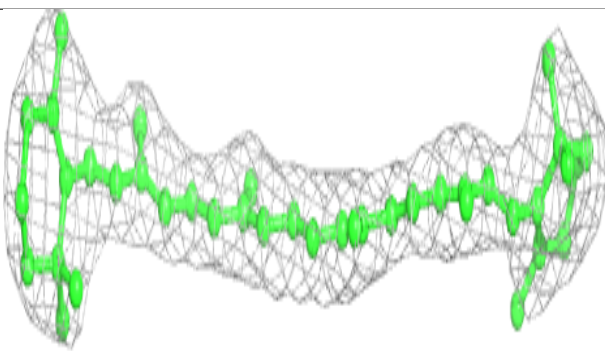
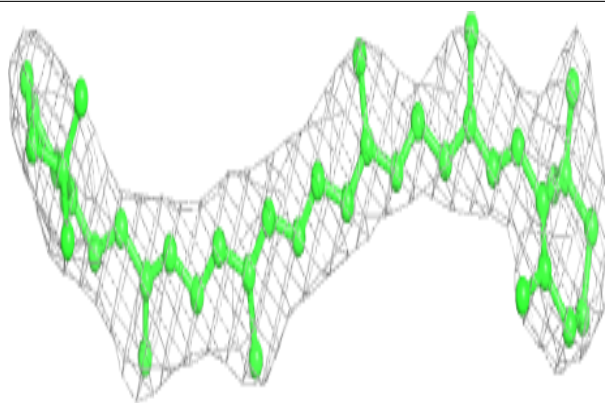
**Electron density around CLA b 623:**

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

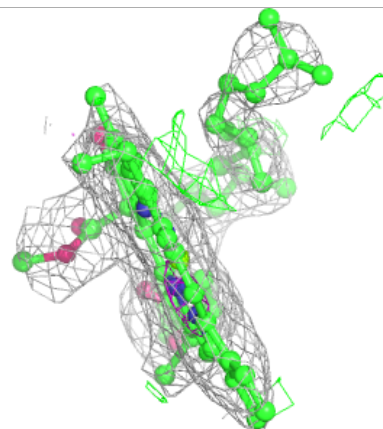
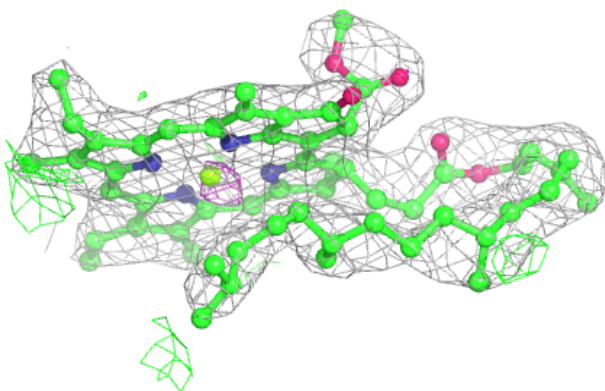
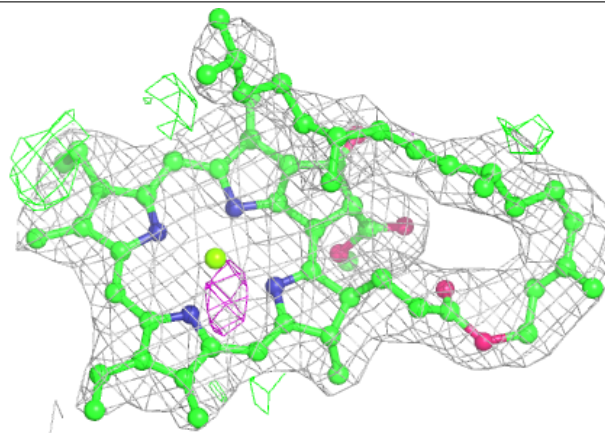


Electron density around BCR Y 101:

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

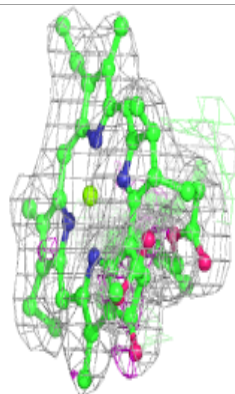
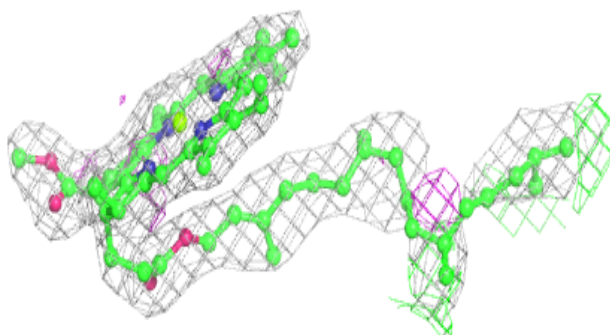
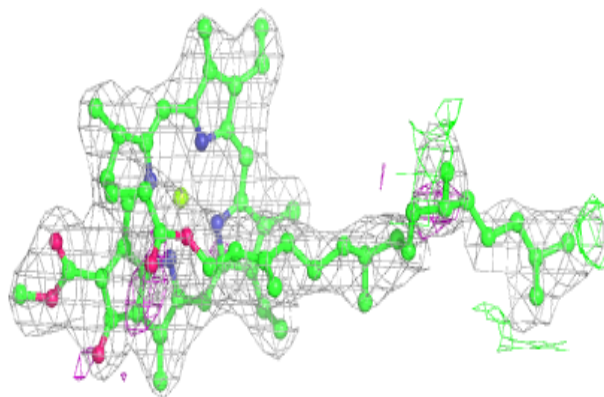
**Electron density around CLA c 513:**

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

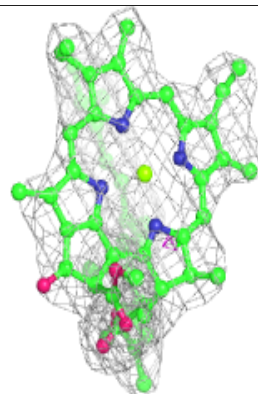
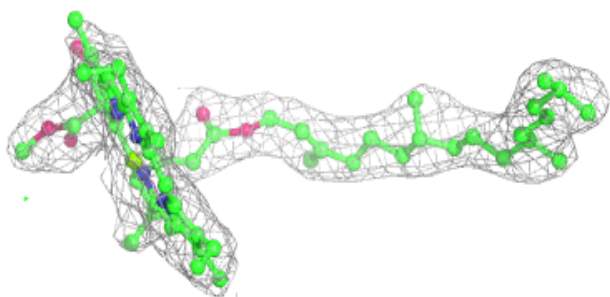
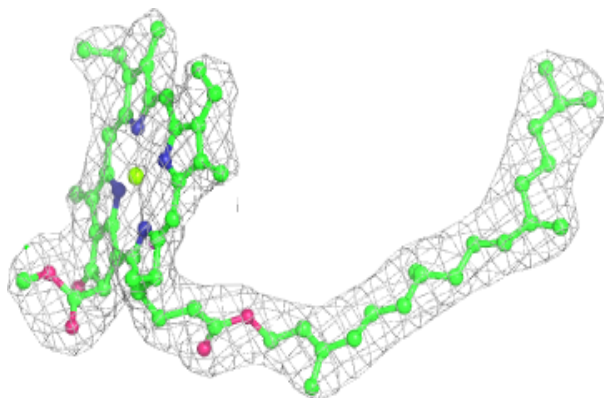


Electron density around CLA B 615:

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

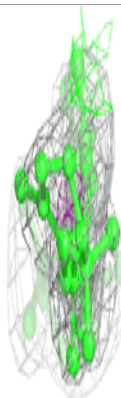
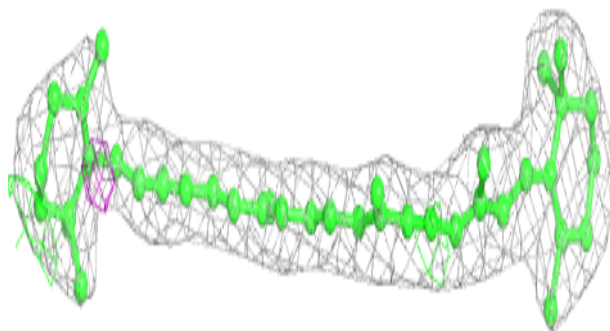
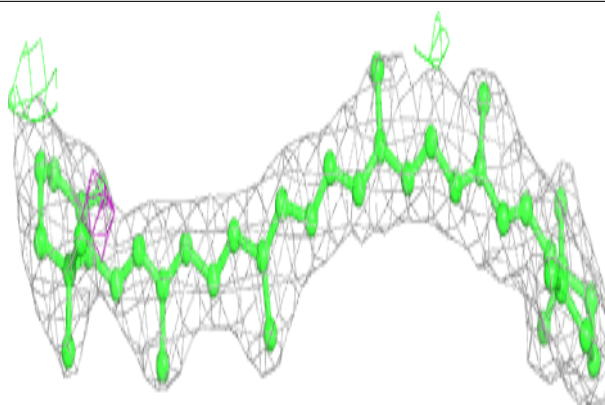
**Electron density around CLA B 610:**

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

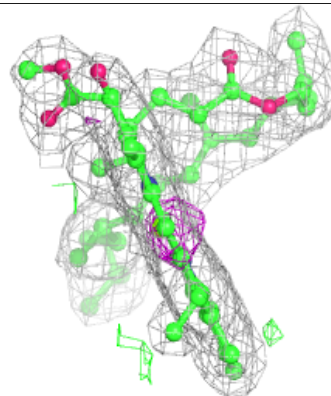
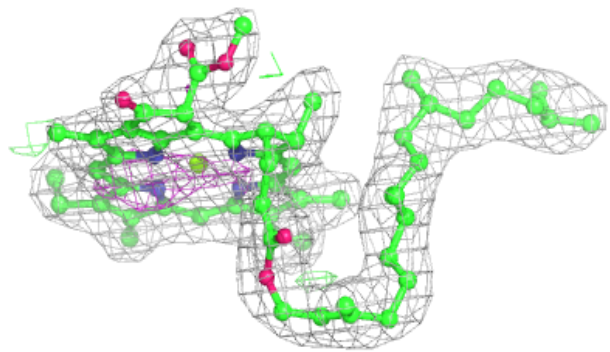
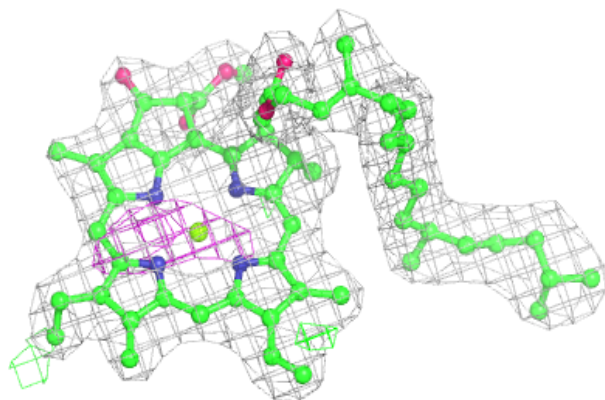


Electron density around BCR H 101:

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

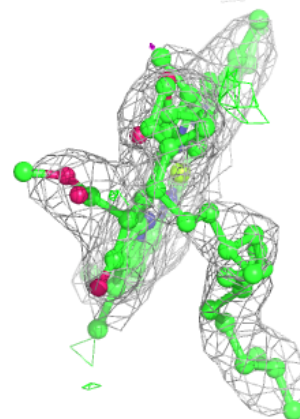
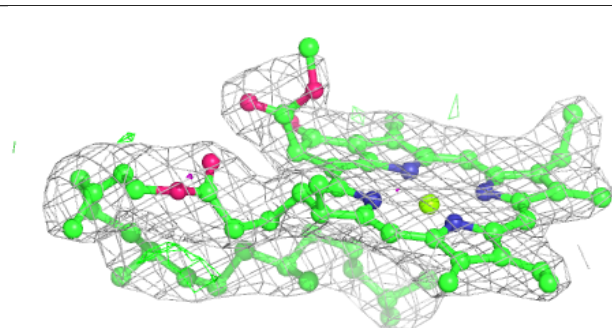
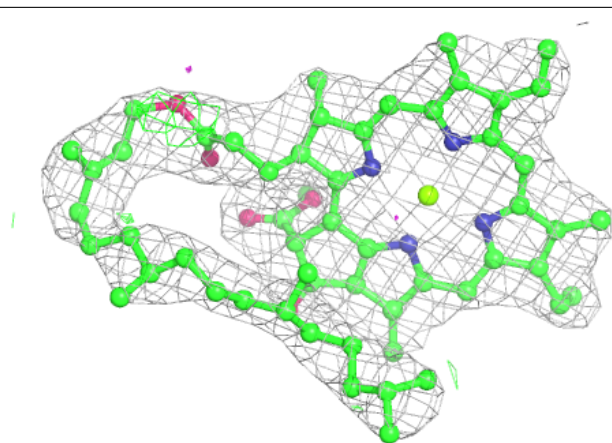
**Electron density around CLA d 403:**

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



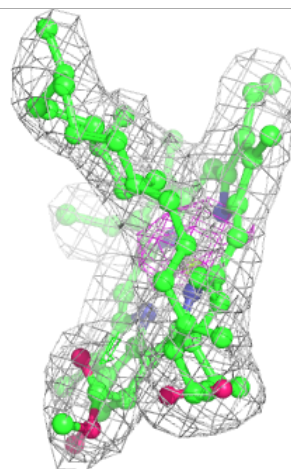
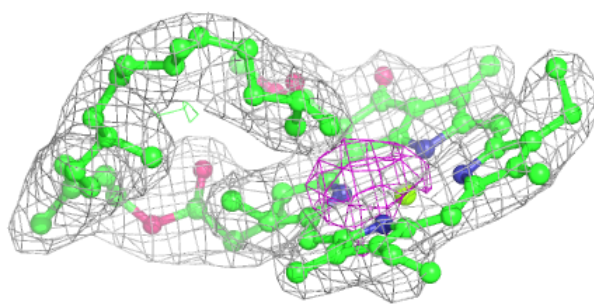
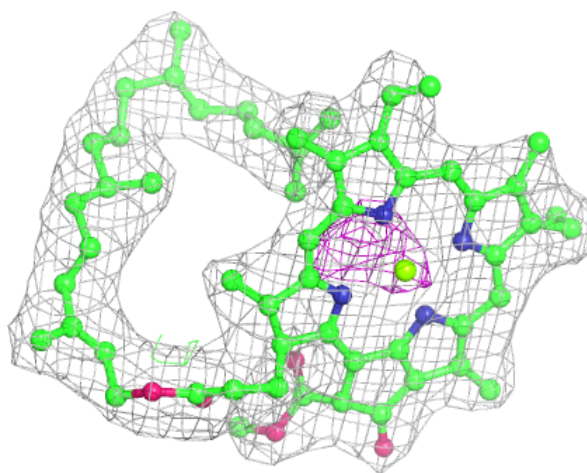
Electron density around CLA C 510:

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



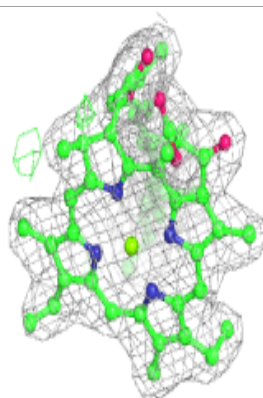
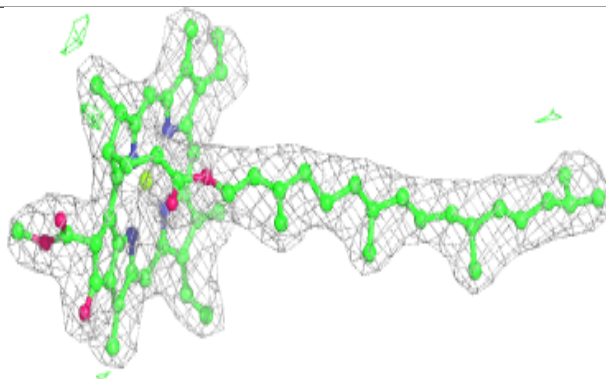
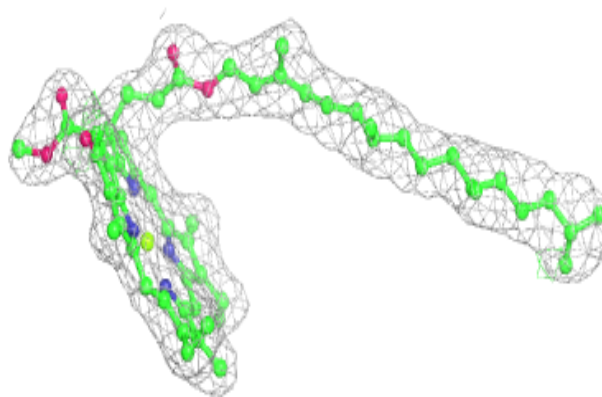
Electron density around CLA b 624:

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

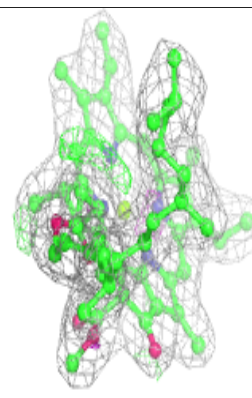
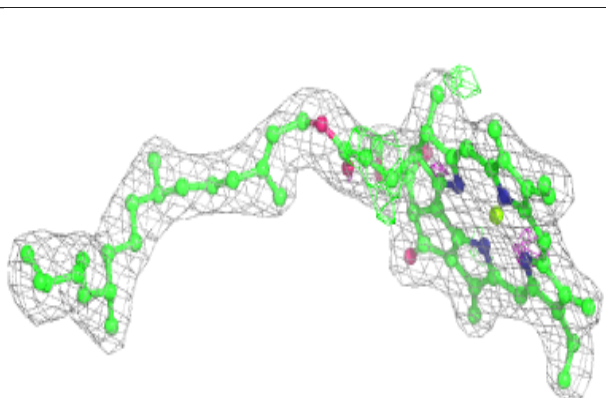
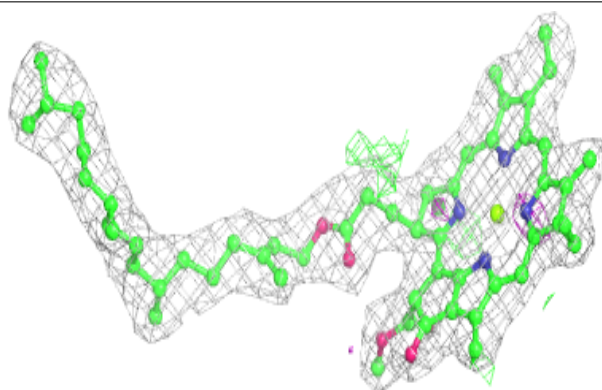


Electron density around CLA B 608:

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

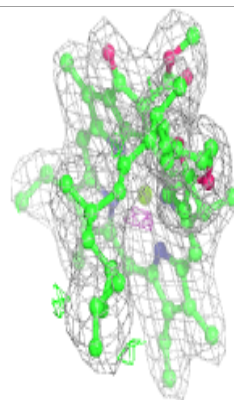
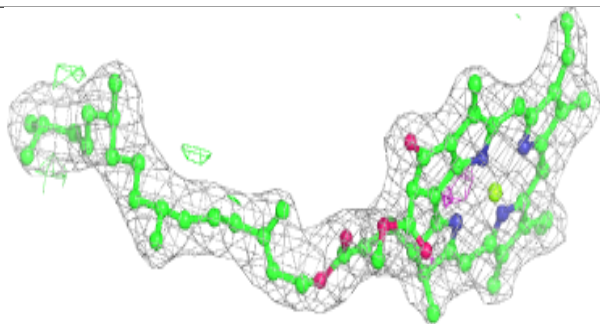
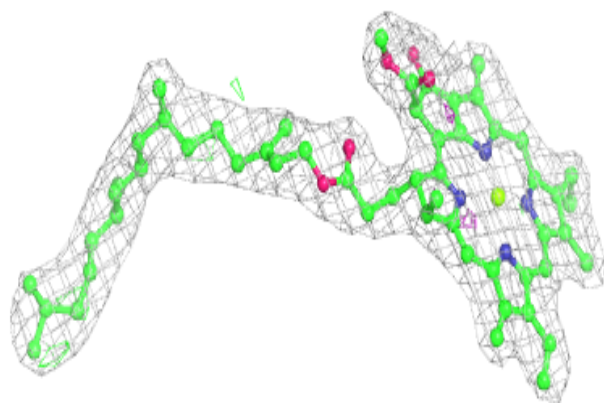
**Electron density around CLA A 404:**

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

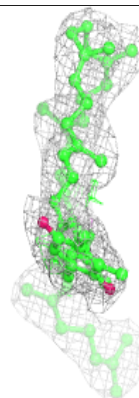
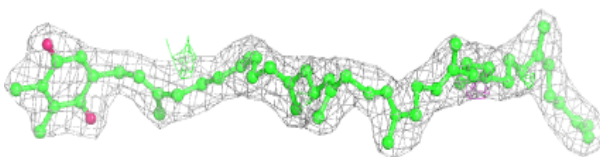
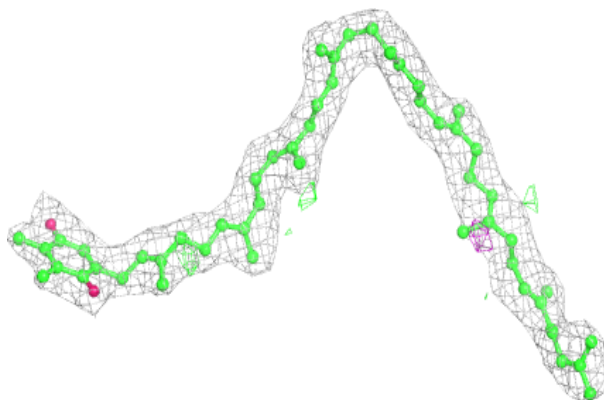


Electron density around CLA a 409:

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

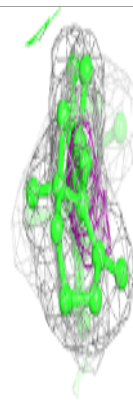
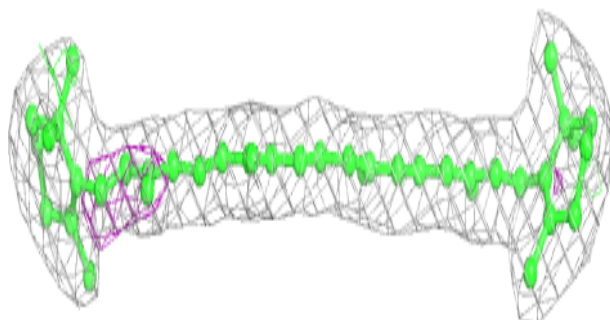
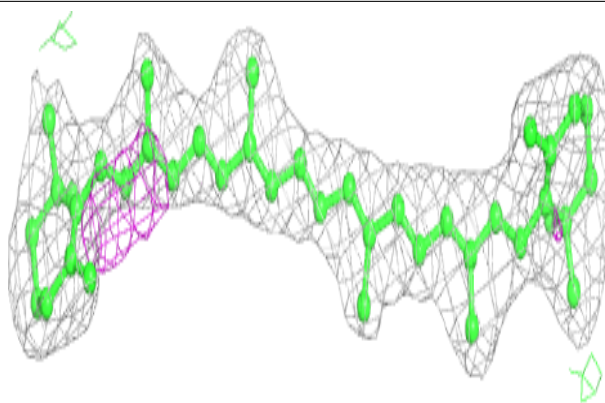
**Electron density around PL9 d 407 (A):**

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



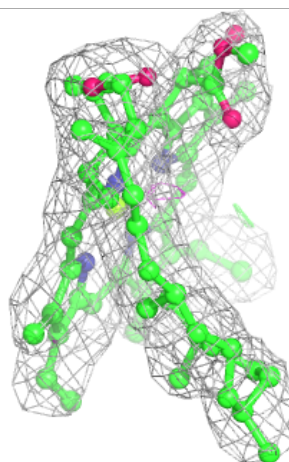
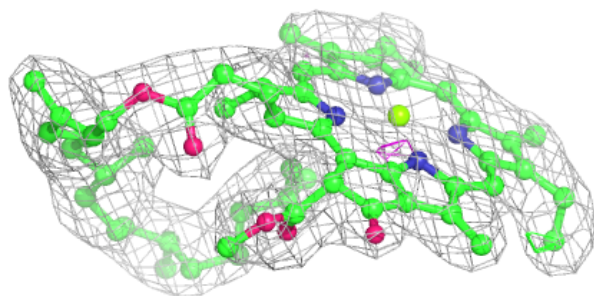
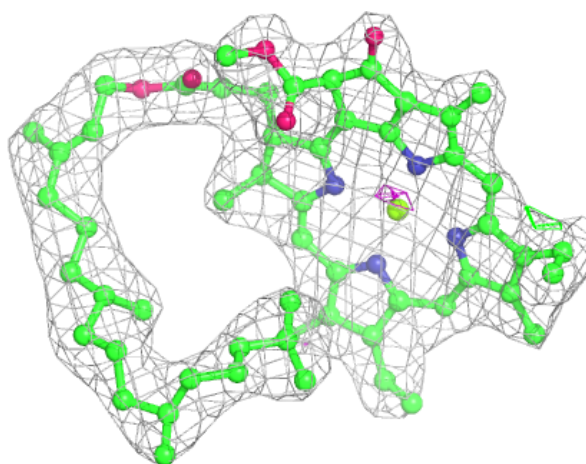
Electron density around BCR b 627:

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



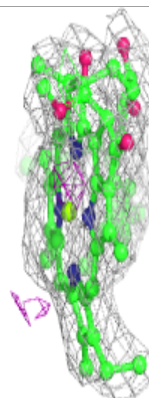
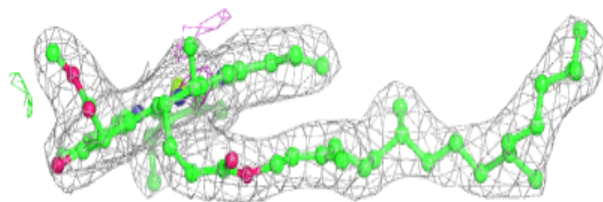
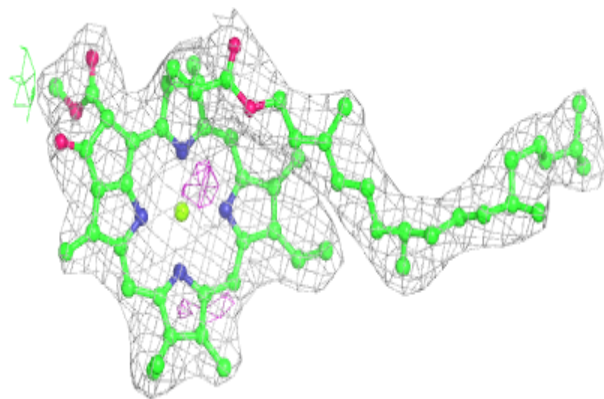
Electron density around CLA B 616:

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

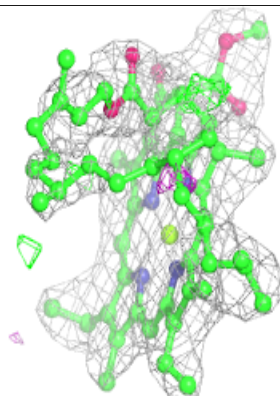
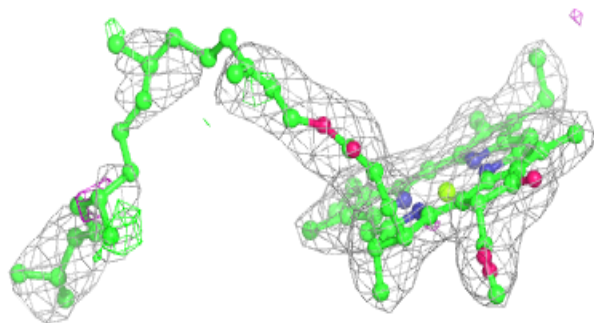
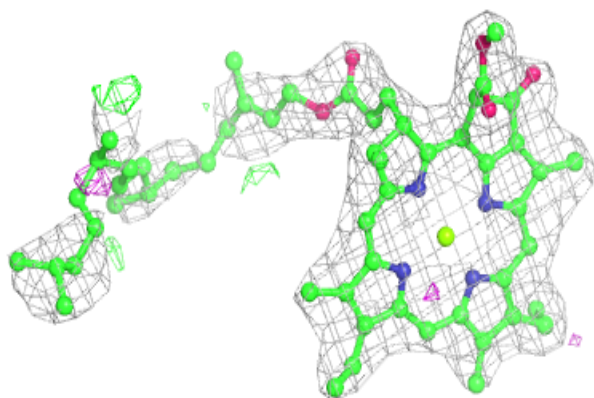


Electron density around CLA b 612:

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

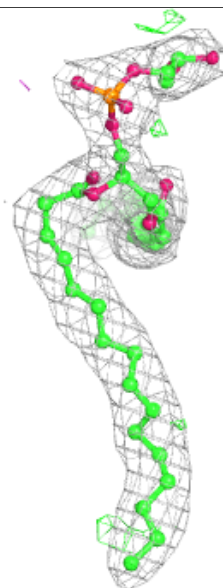
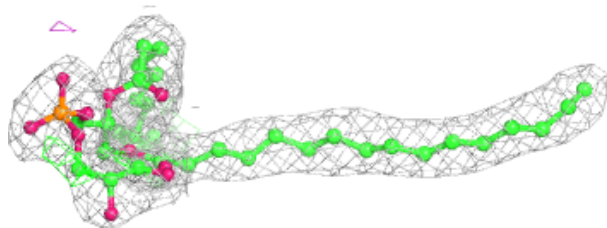
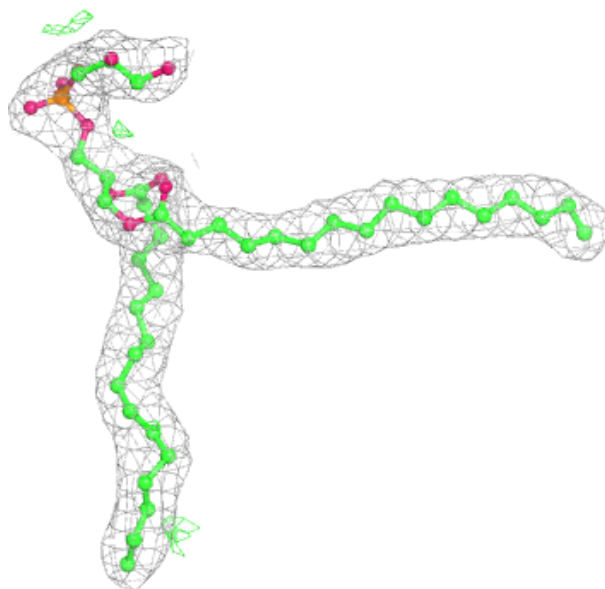
**Electron density around CLA a 412:**

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



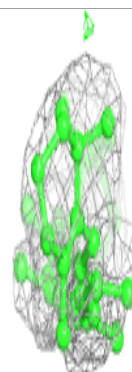
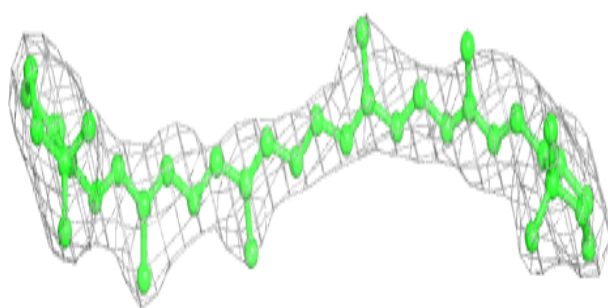
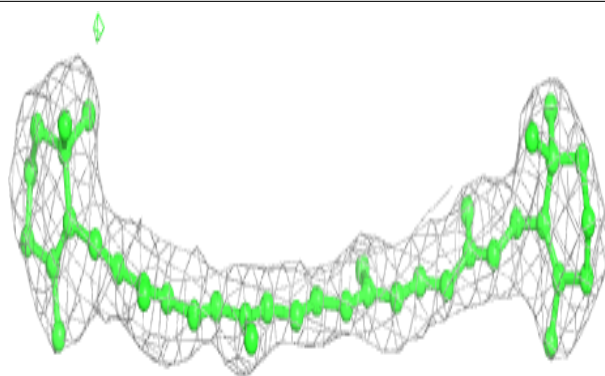
Electron density around LHG L 101:

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

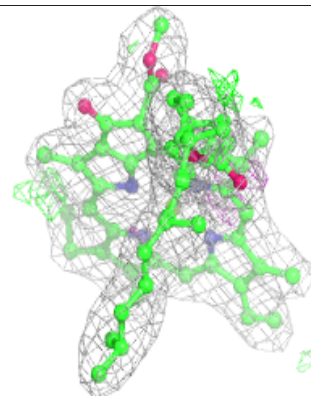
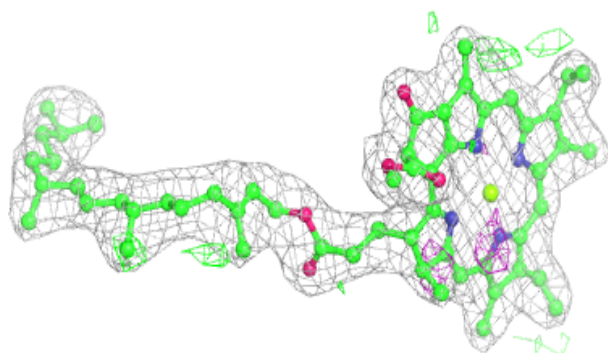
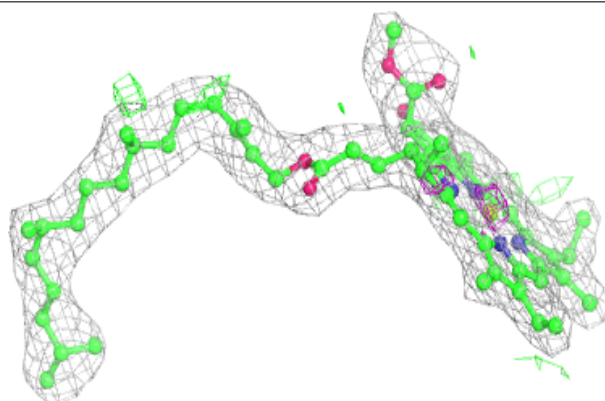


Electron density around BCR k 101:

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

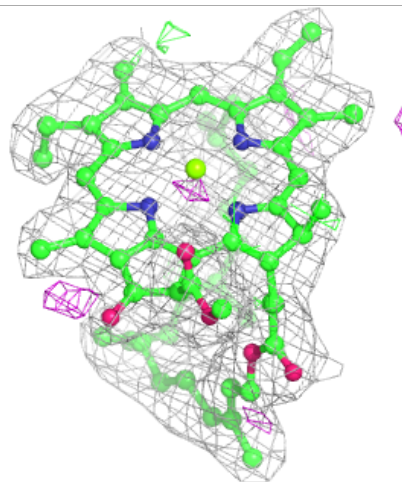
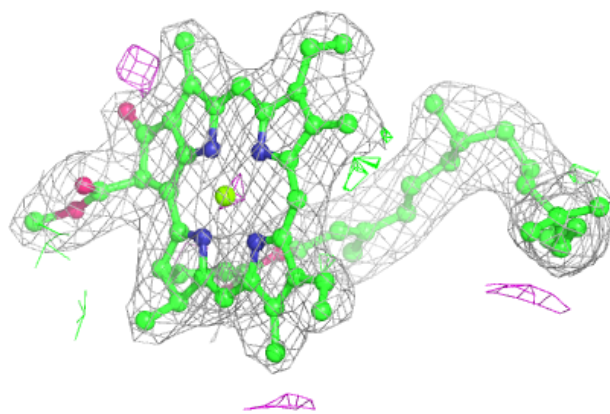
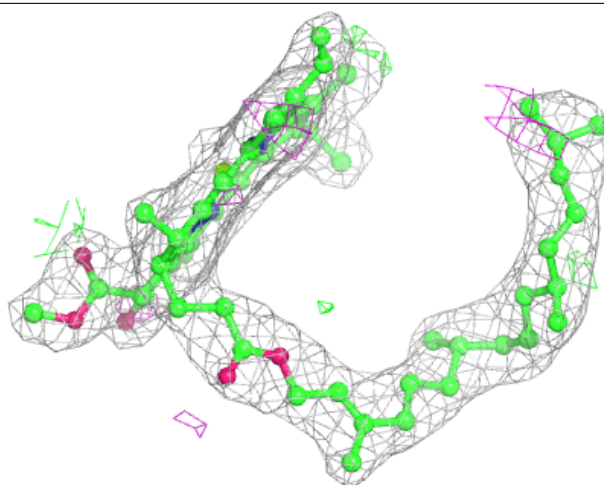
**Electron density around CLA D 406:**

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



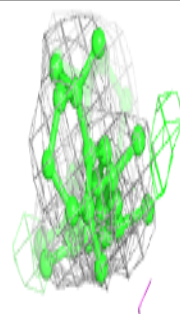
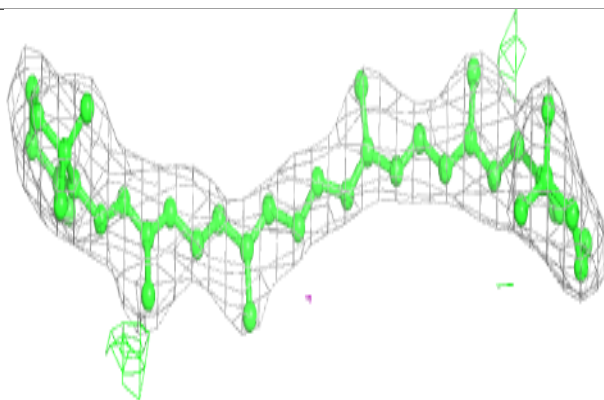
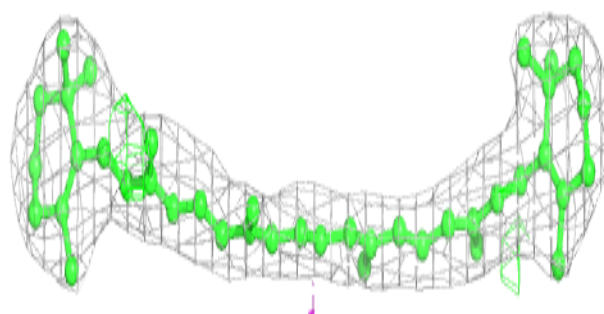
Electron density around CLA B 612:

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

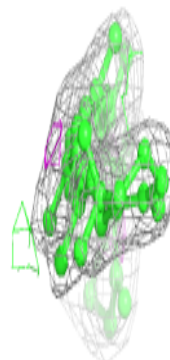
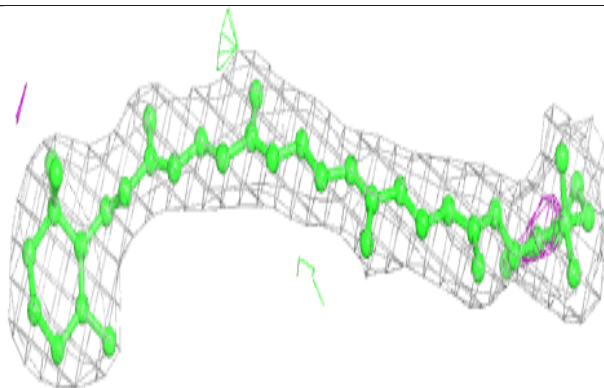
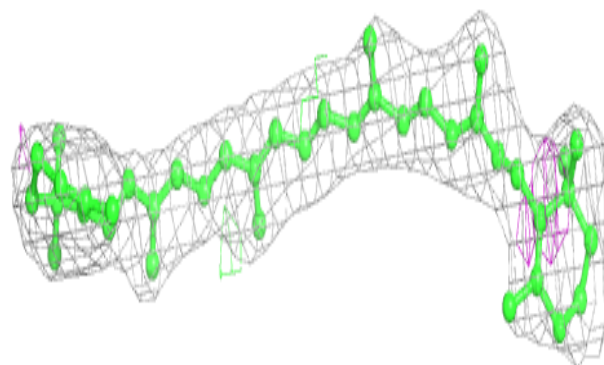


Electron density around BCR K 103:

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

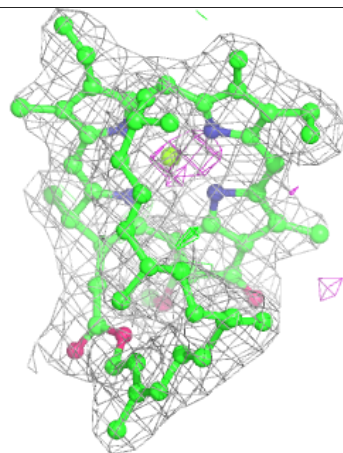
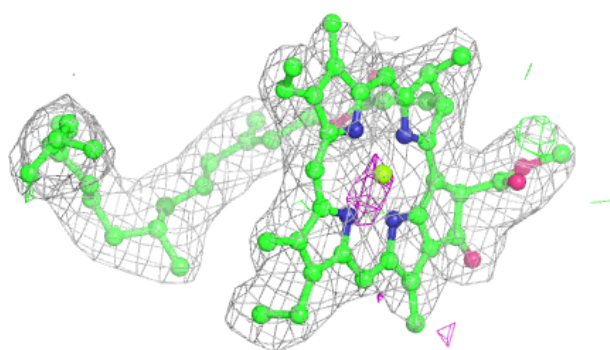
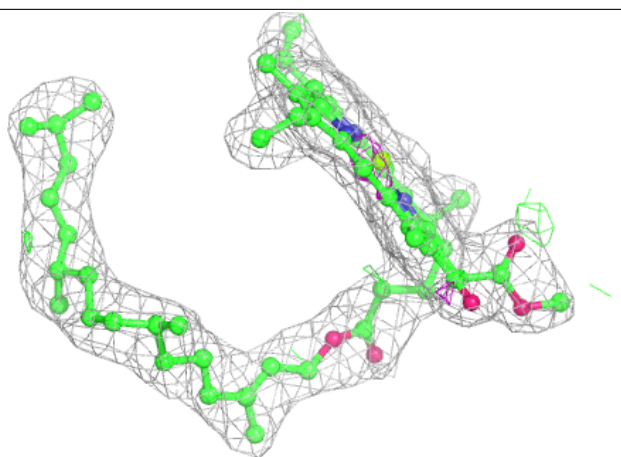
**Electron density around BCR d 406:**

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

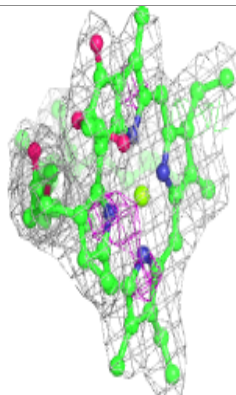
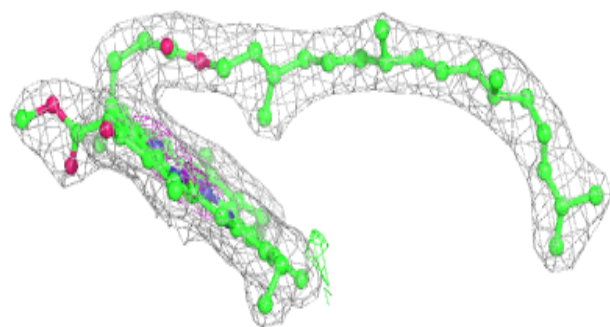
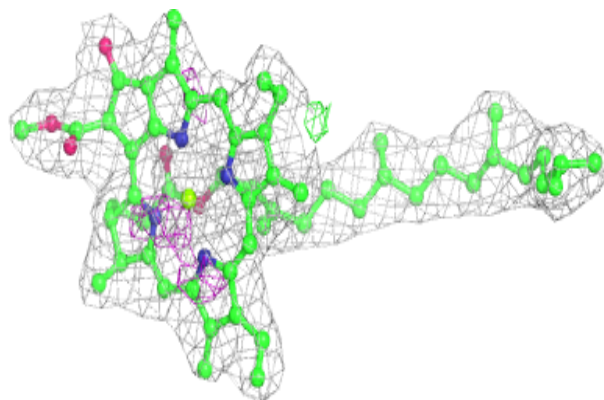


Electron density around CLA b 620:

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

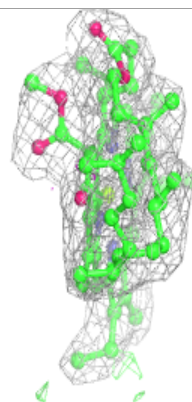
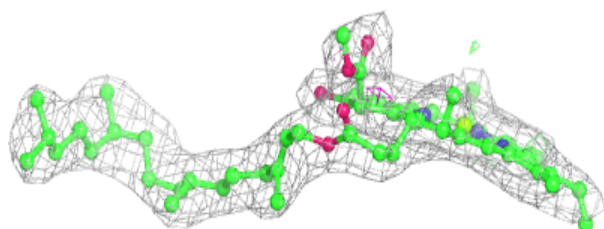
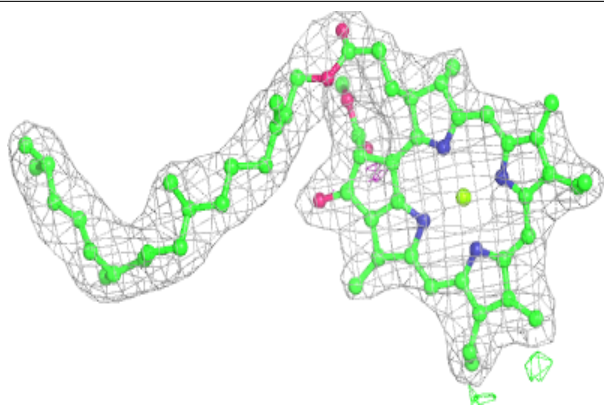
**Electron density around CLA b 617:**

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



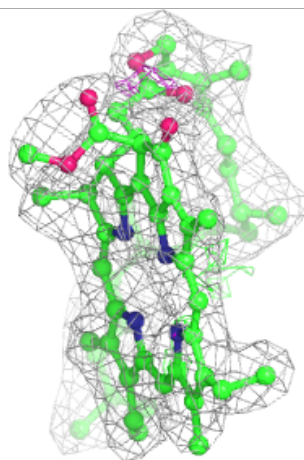
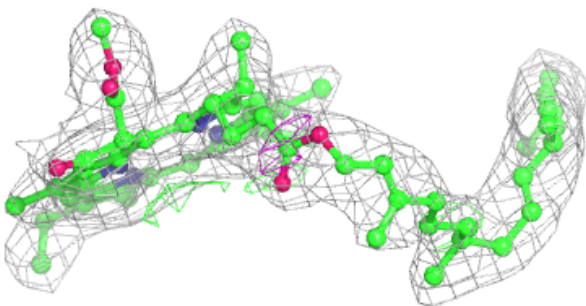
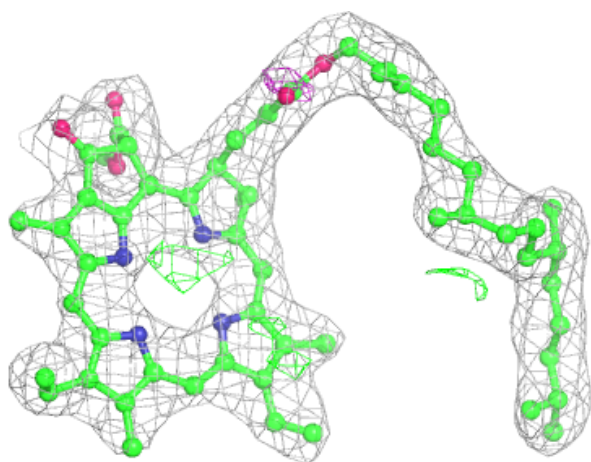
Electron density around CLA B 603:

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



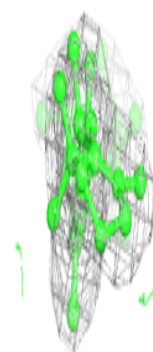
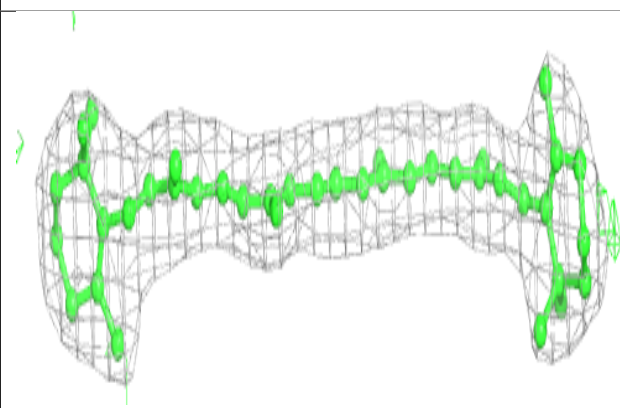
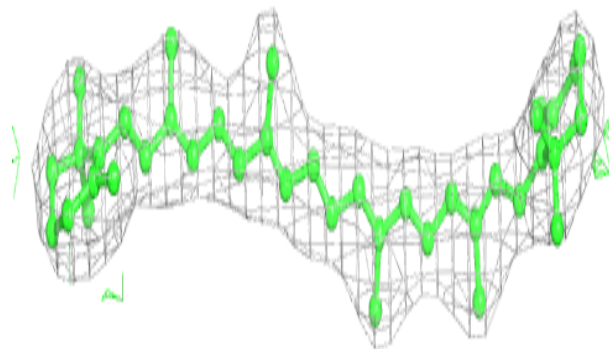
Electron density around PHO d 402 (B):

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

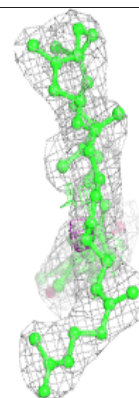
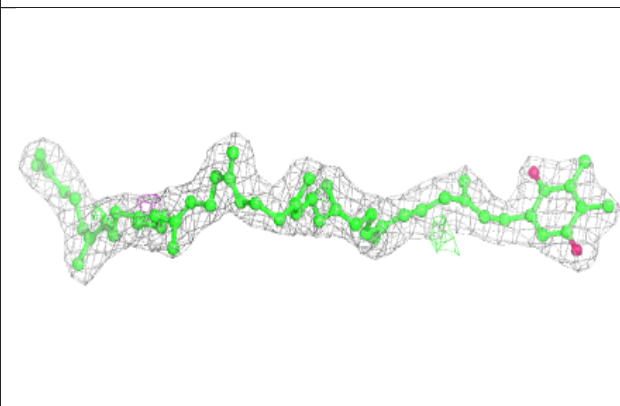
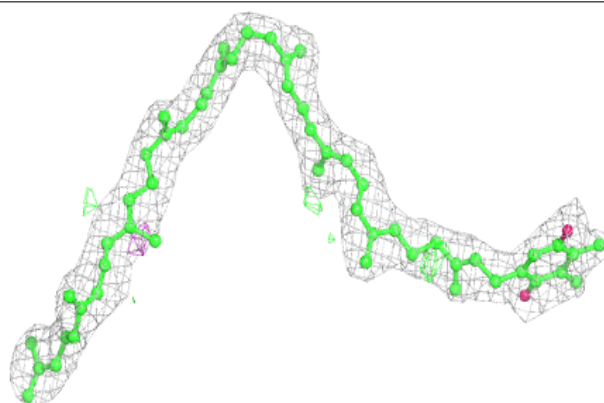


Electron density around BCR C 515:

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

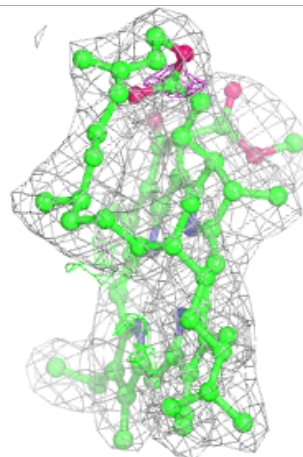
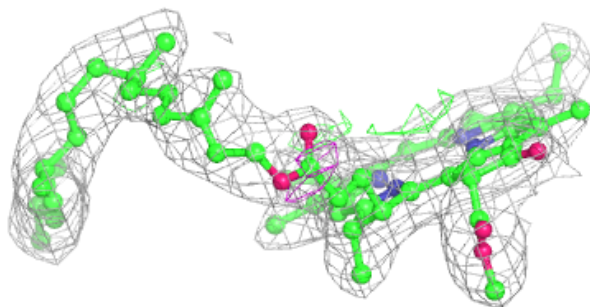
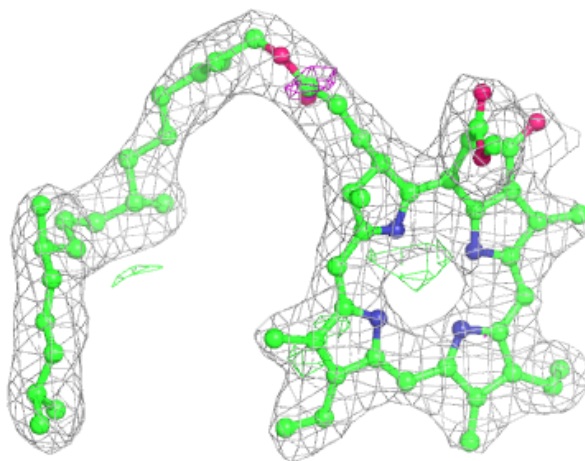
**Electron density around PL9 d 407 (B):**

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



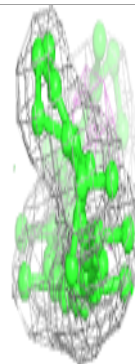
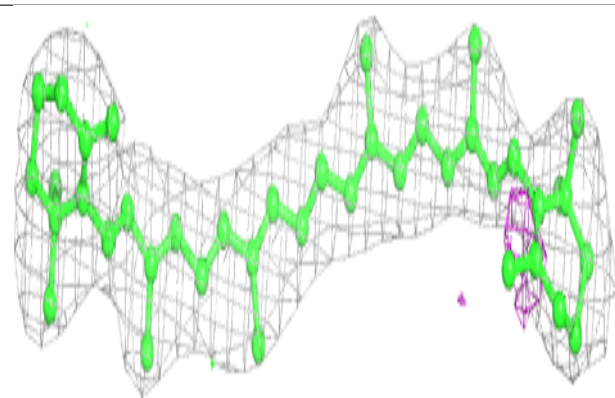
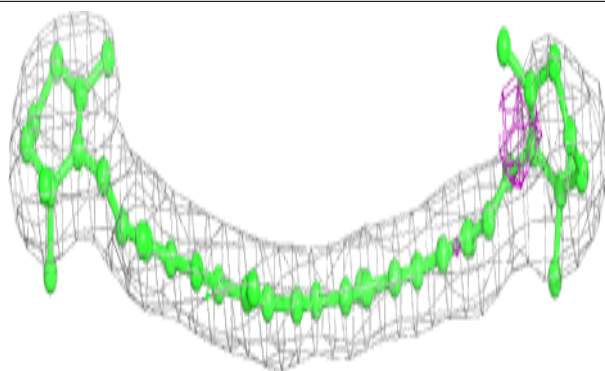
Electron density around PHO d 402 (A):

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

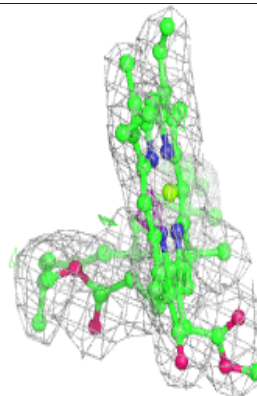
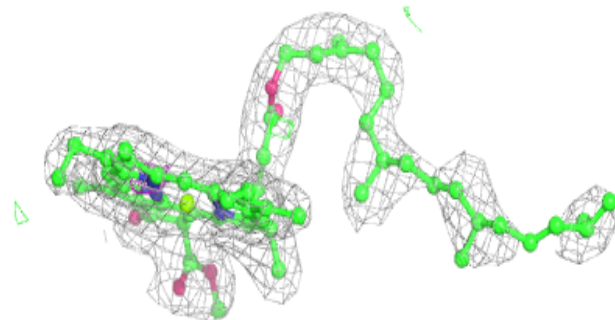
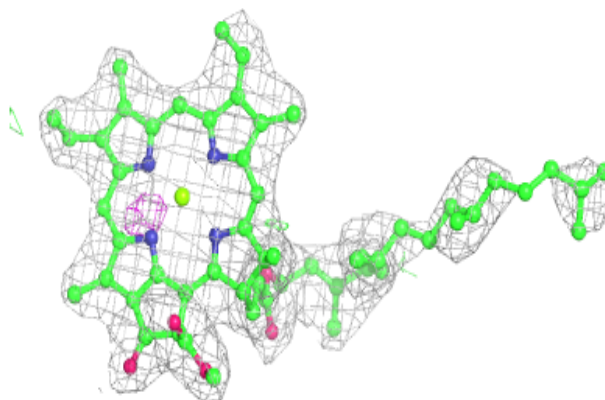


Electron density around BCR D 408:

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

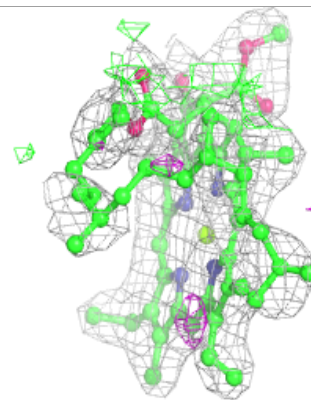
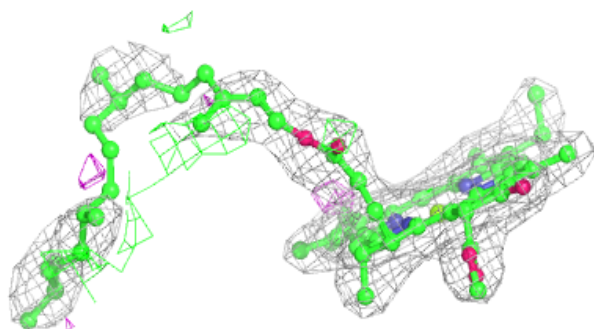
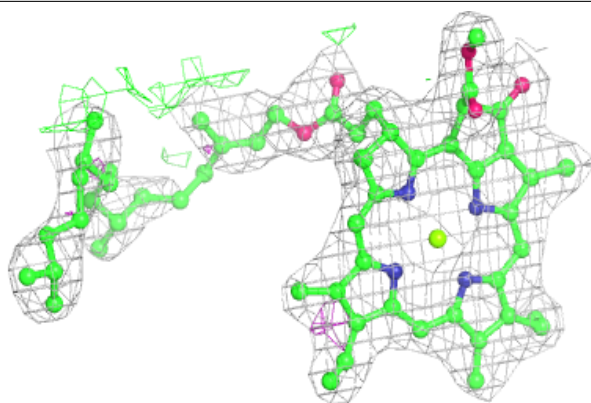
**Electron density around CLA A 406:**

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

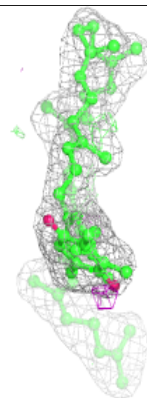
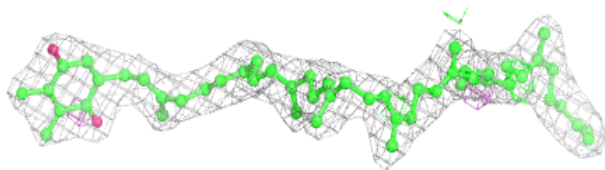
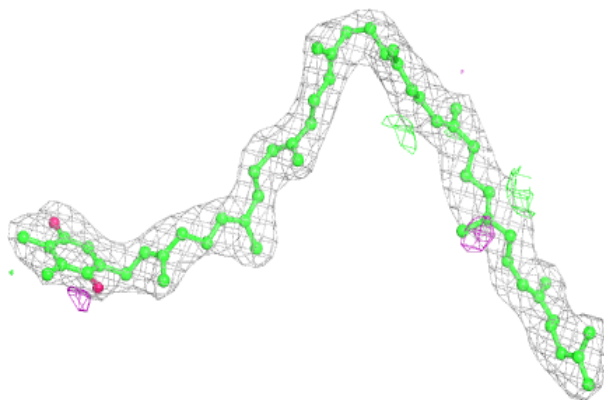


Electron density around CLA A 407:

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

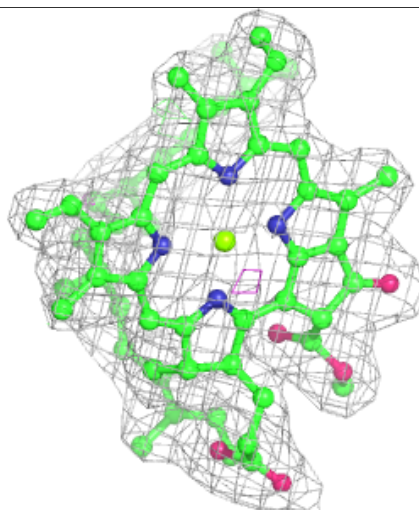
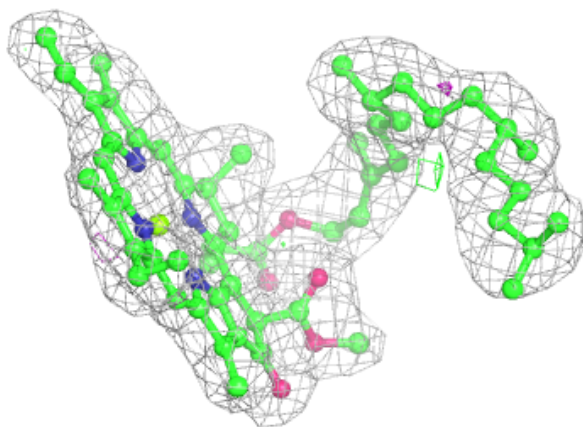
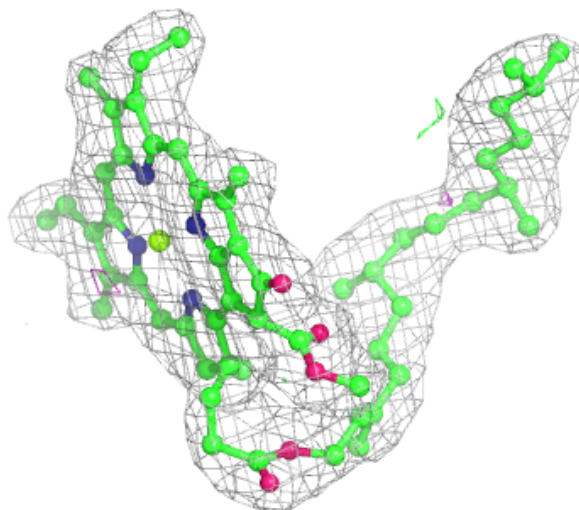
**Electron density around PL9 D 409 (A):**

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



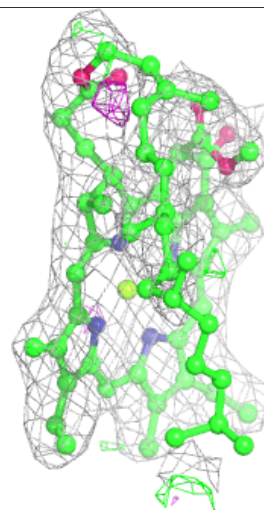
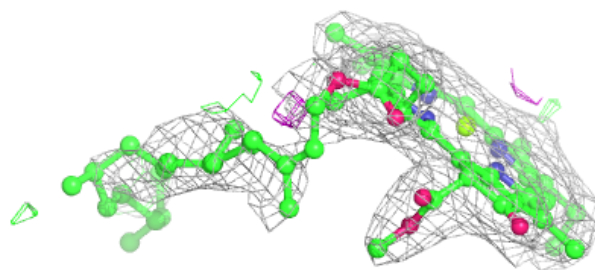
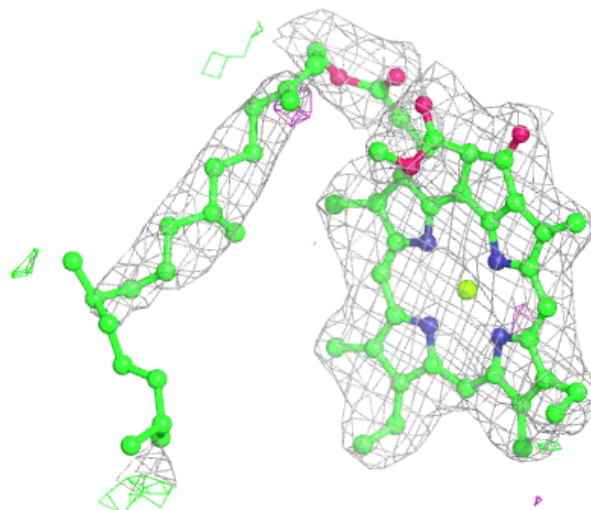
Electron density around CLA b 622:

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



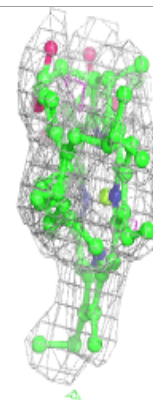
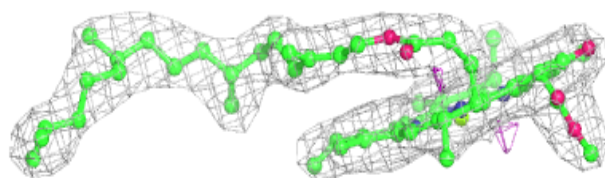
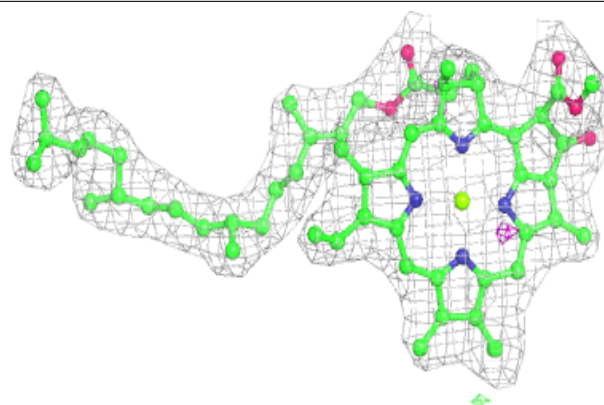
Electron density around CLA B 617:

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

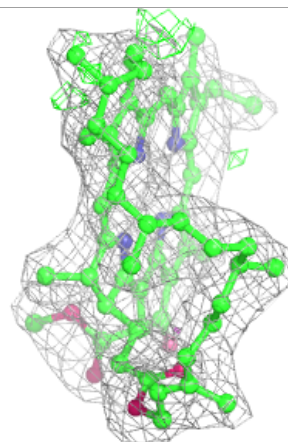
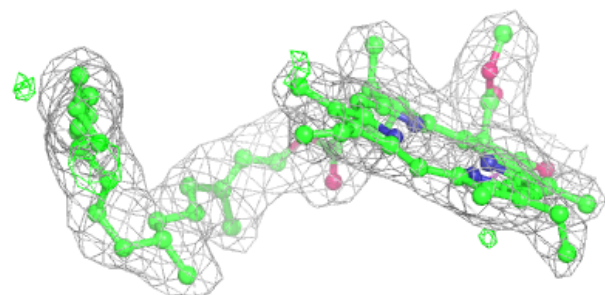
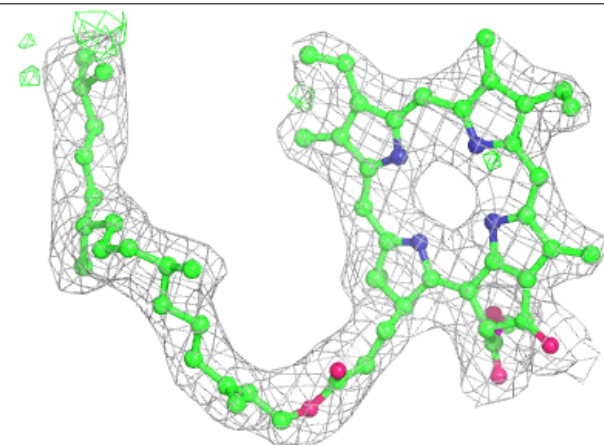


Electron density around CLA B 604:

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

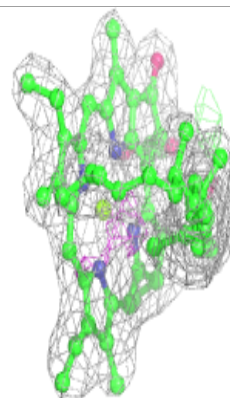
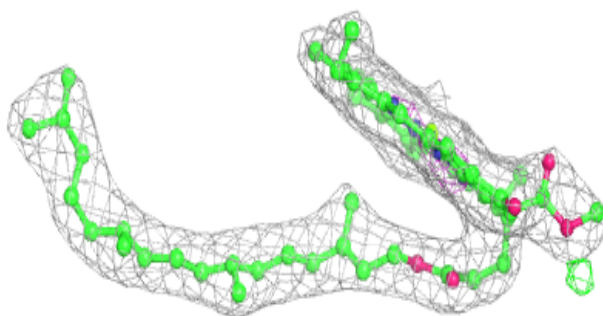
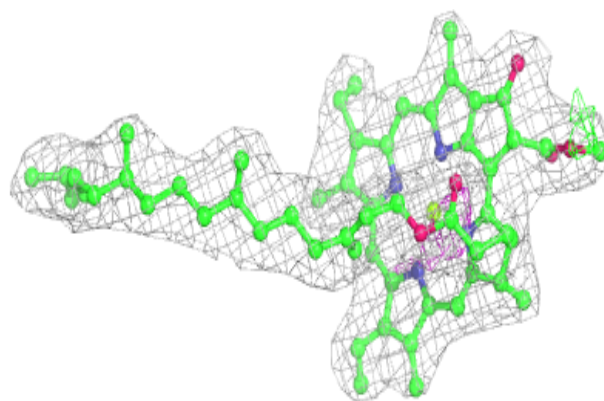
**Electron density around PHO D 403 (B):**

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

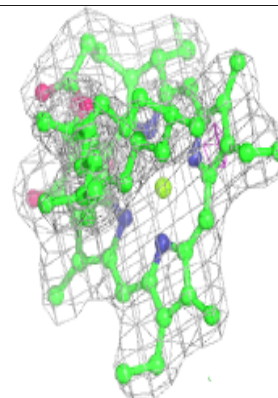
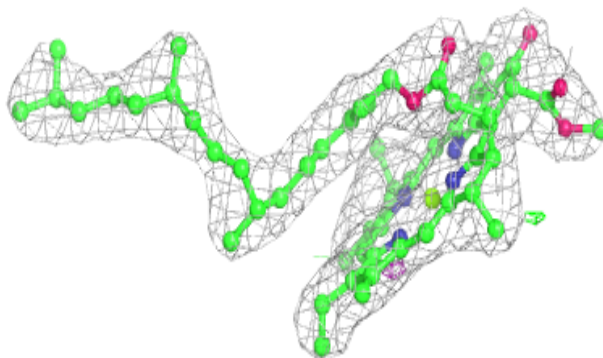
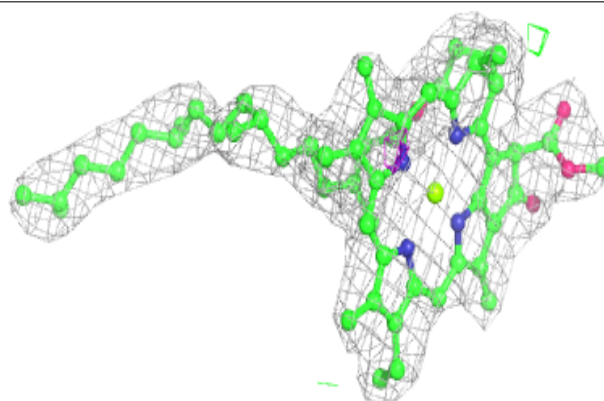


Electron density around CLA B 609:

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

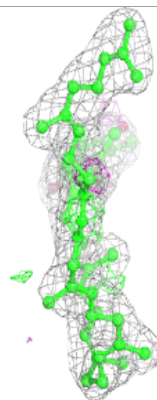
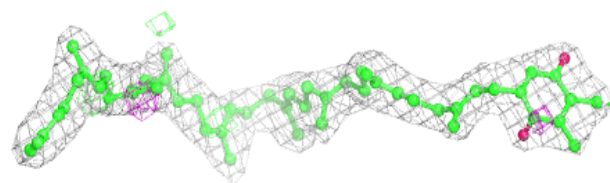
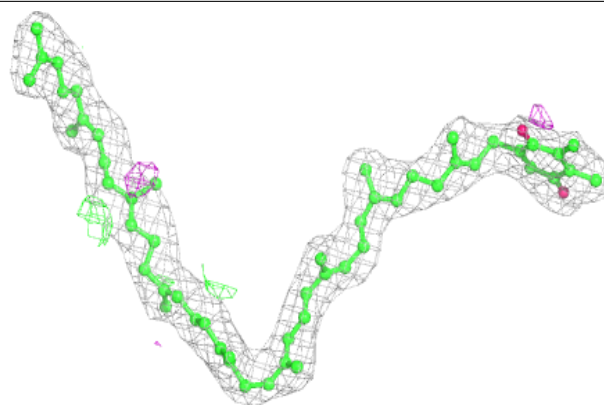
**Electron density around CLA C 506:**

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

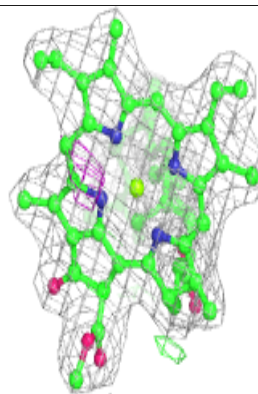
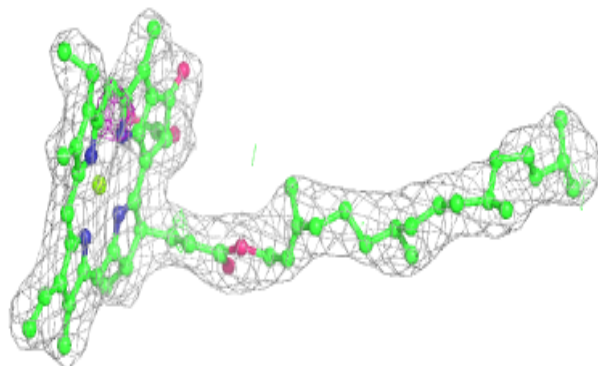
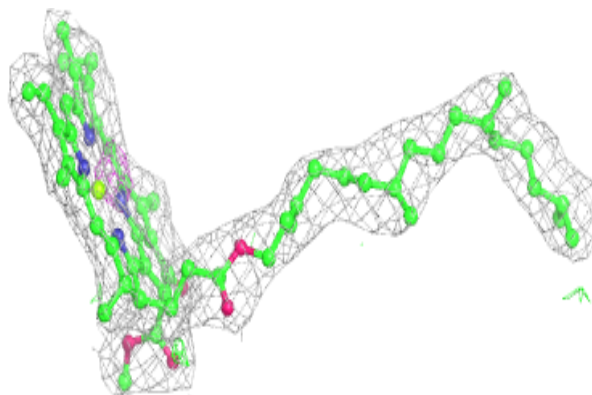


Electron density around PL9 D 409 (B):

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

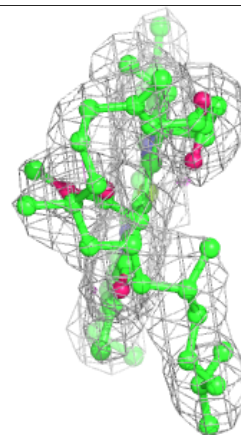
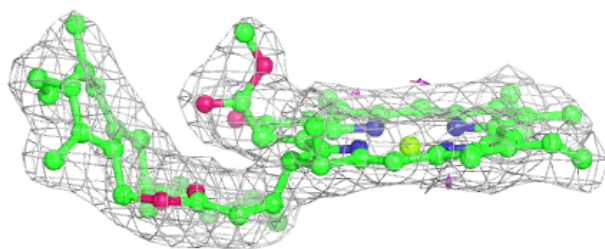
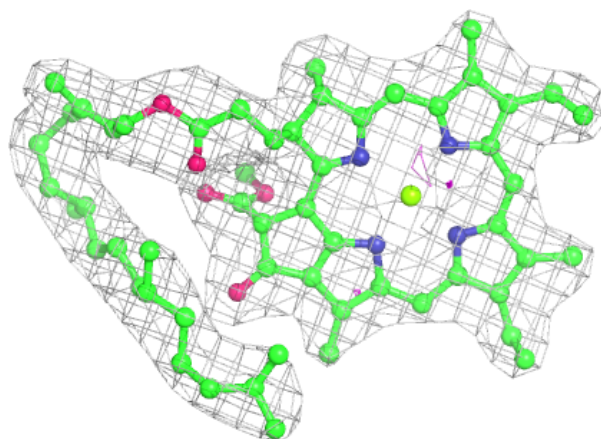
**Electron density around CLA B 605:**

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

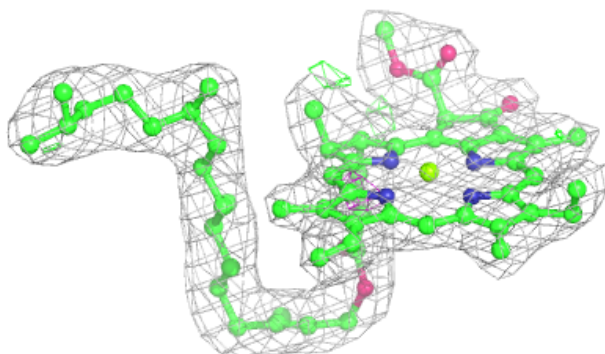
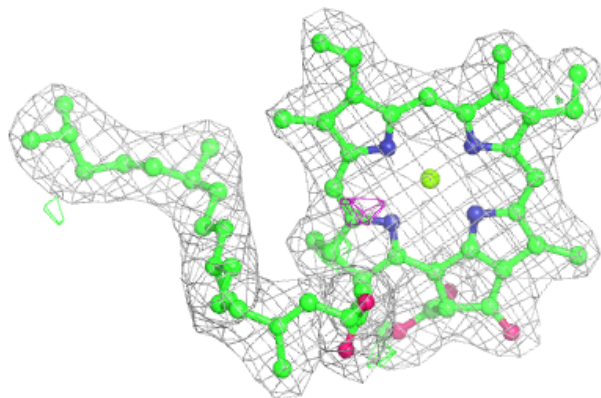


Electron density around CLA b 619:

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

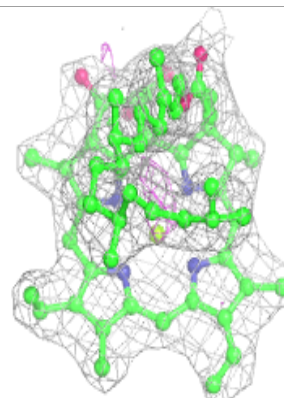
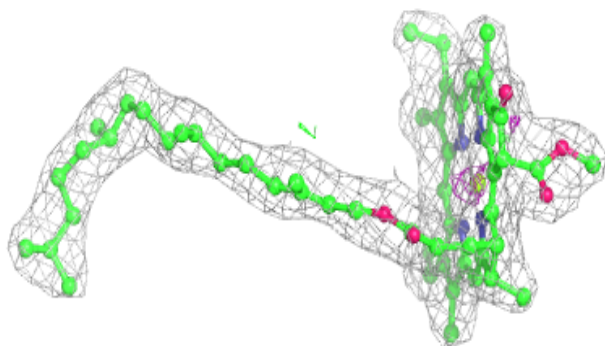
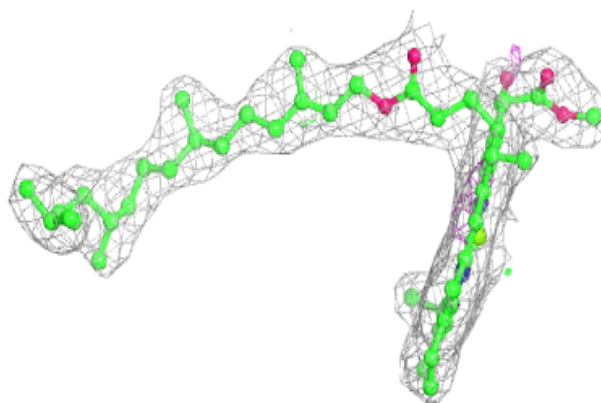
**Electron density around CLA A 405:**

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

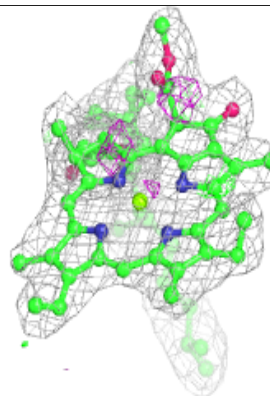
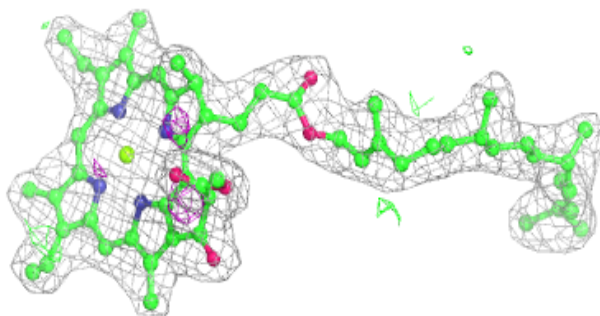
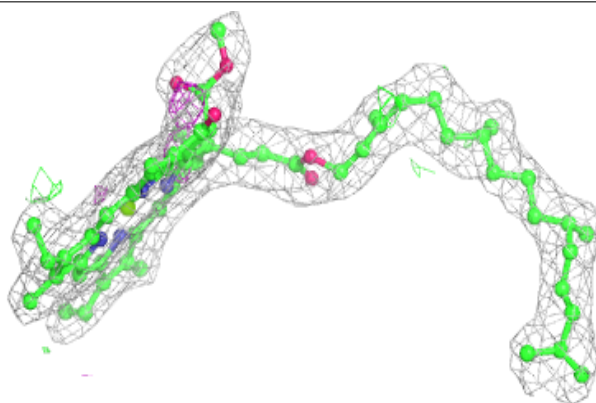


Electron density around CLA b 614:

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

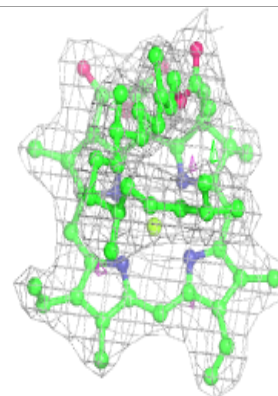
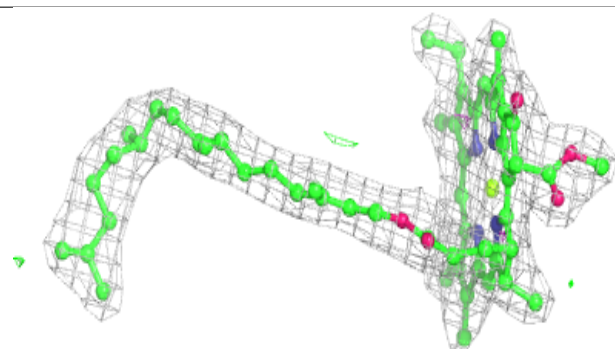
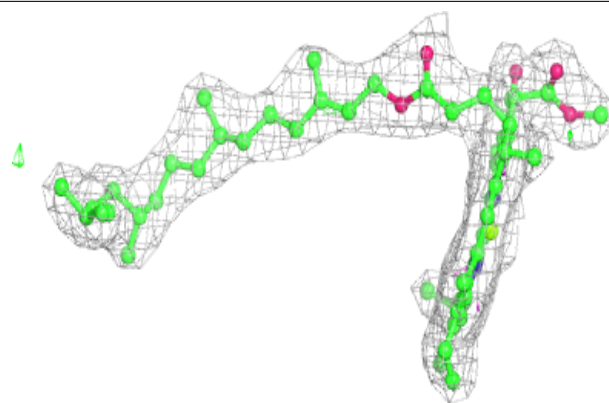
**Electron density around CLA d 404:**

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

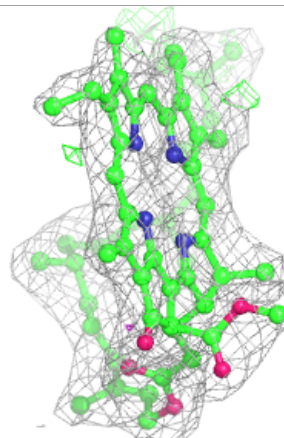
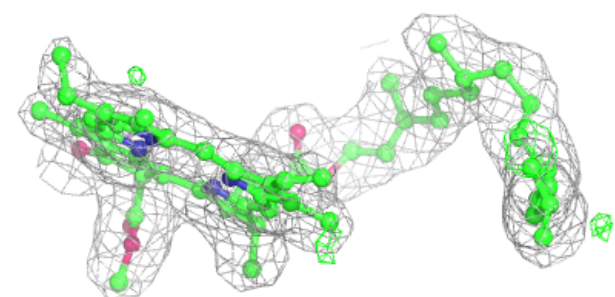
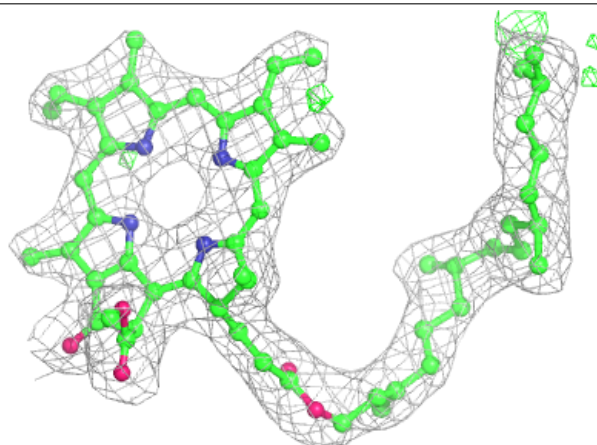


Electron density around CLA B 606:

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

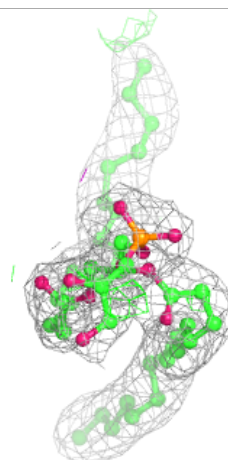
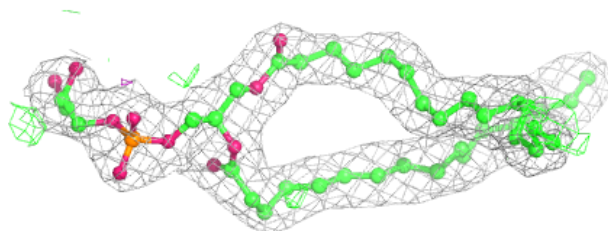
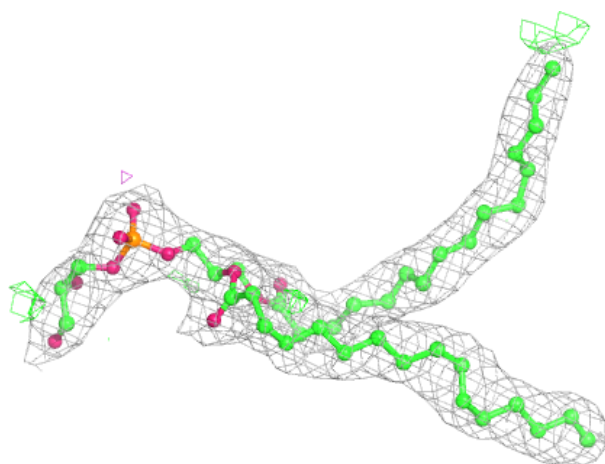
**Electron density around PHO D 403 (A):**

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



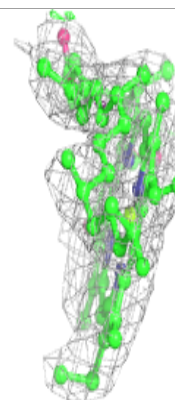
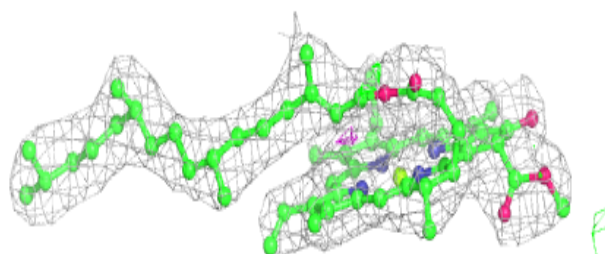
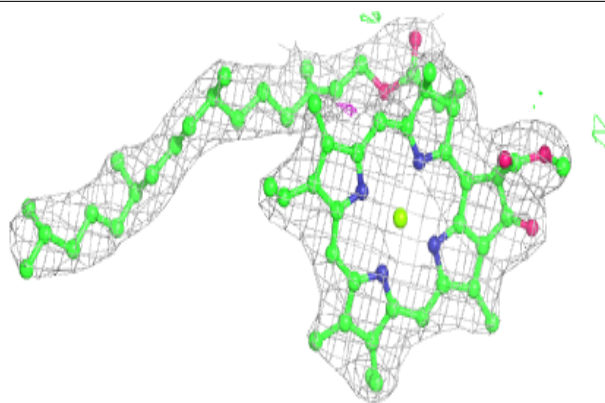
Electron density around LHG D 412:

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

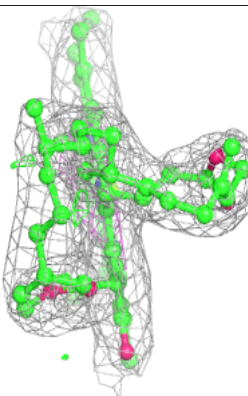
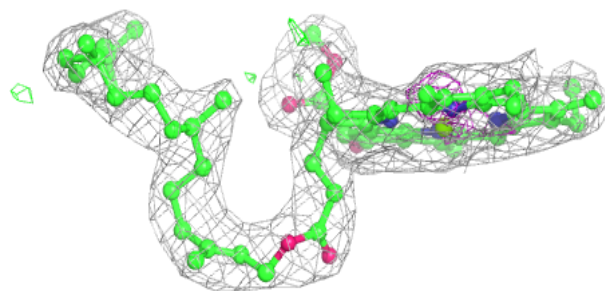
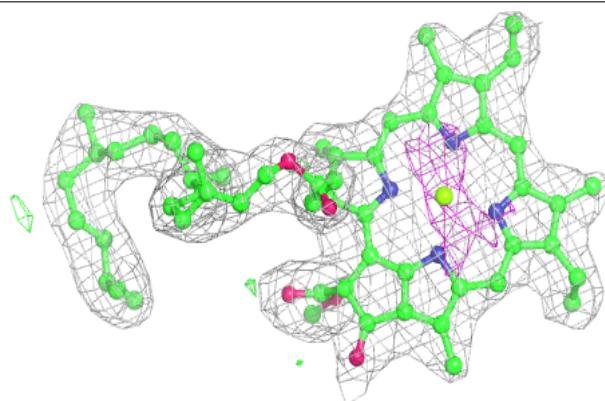


Electron density around CLA c 505:

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

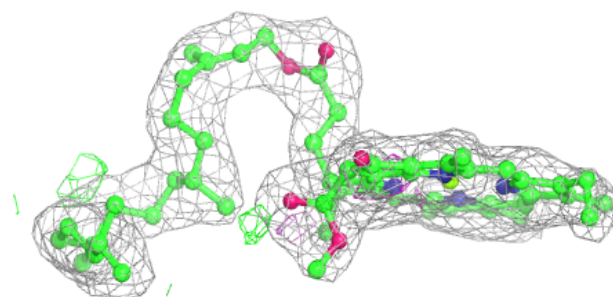
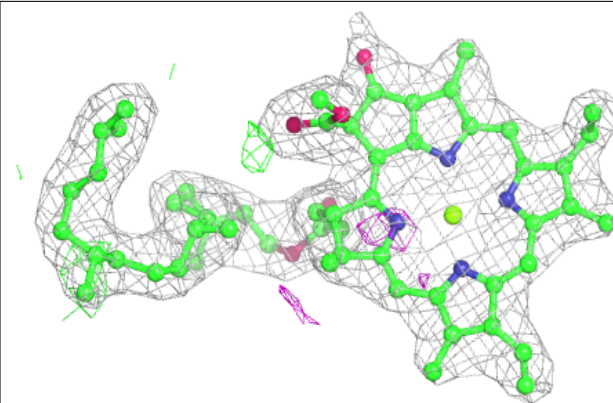
**Electron density around CLA B 613:**

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

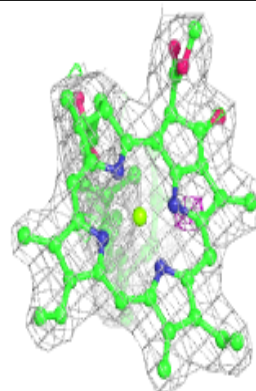
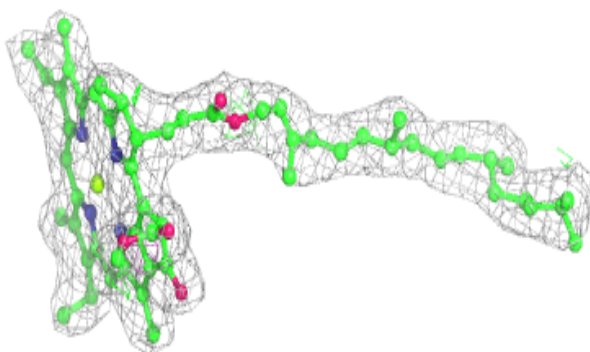
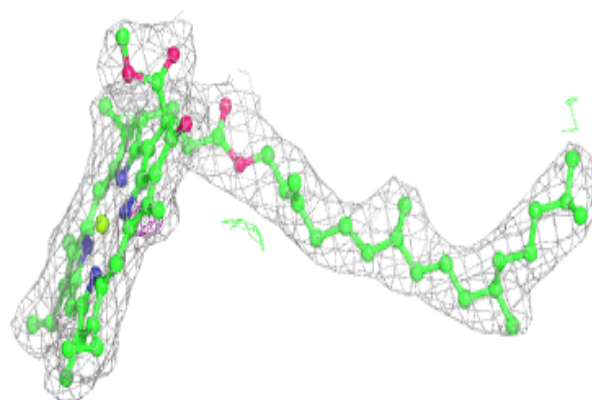


Electron density around CLA b 621:

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

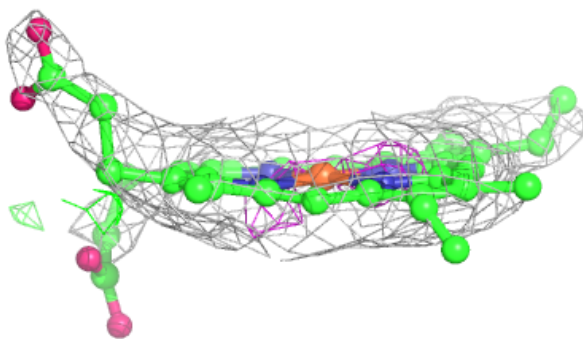
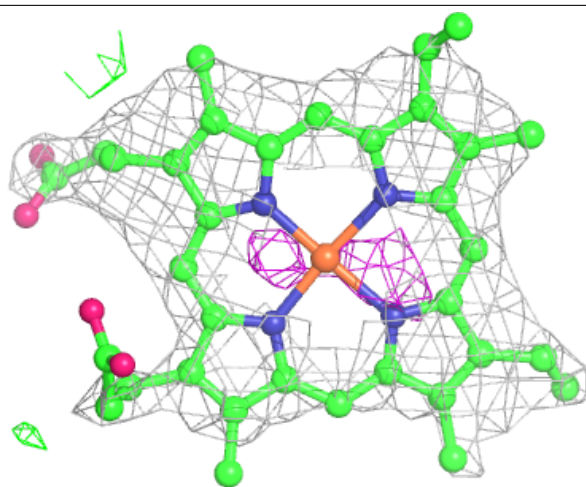
**Electron density around CLA b 613:**

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



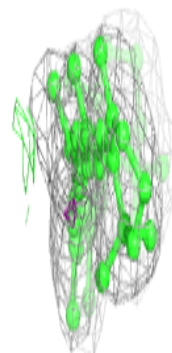
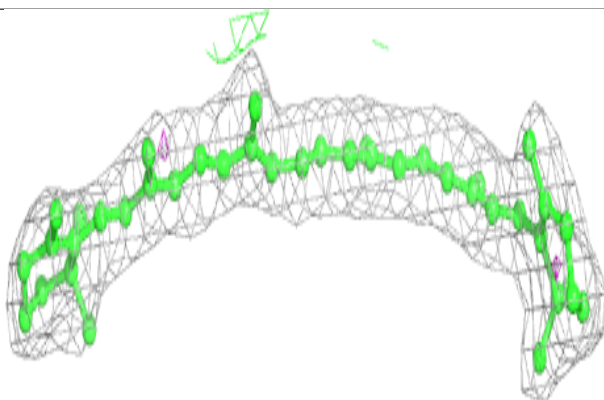
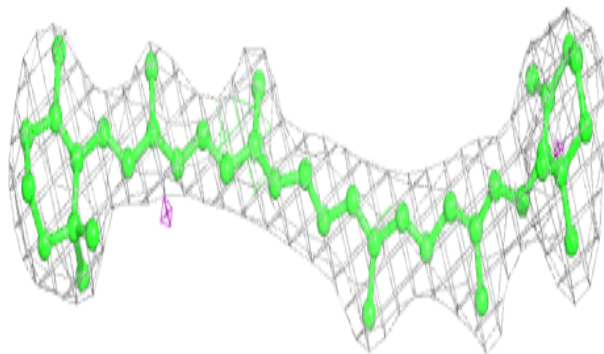
Electron density around HEM e 101:

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

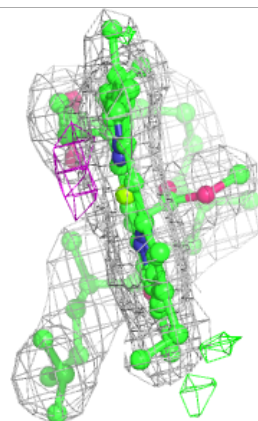
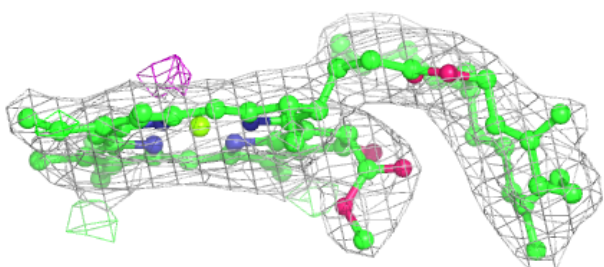
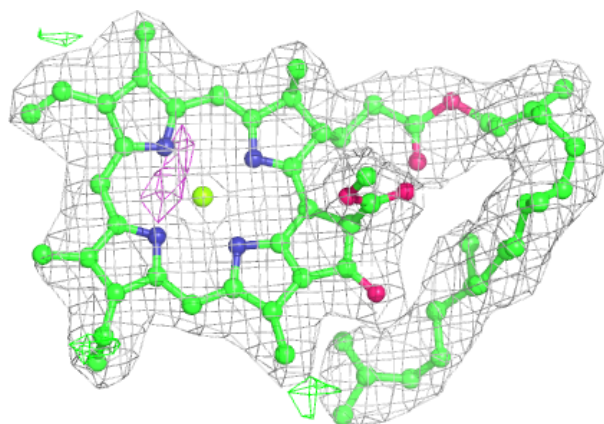


Electron density around BCR T 103:

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

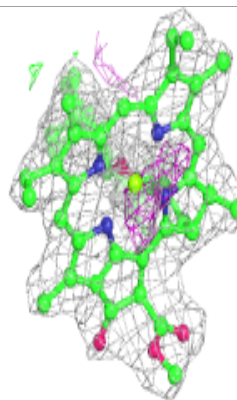
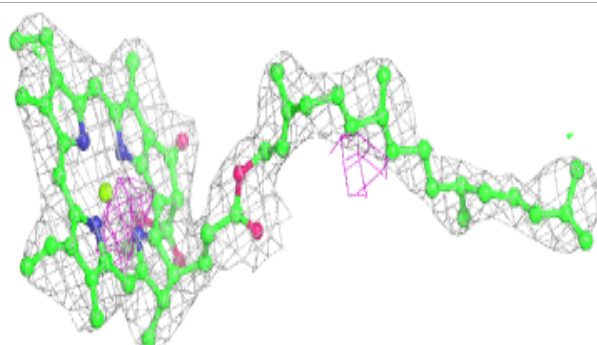
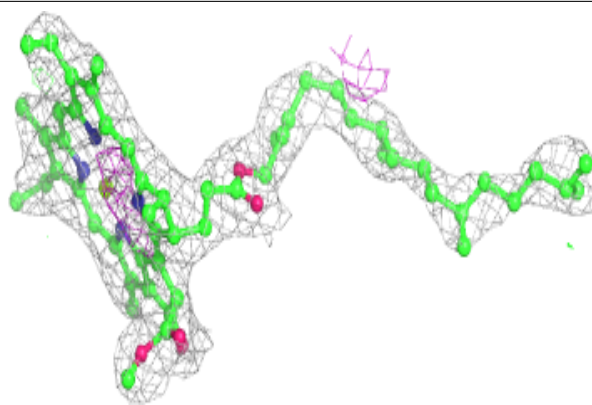
**Electron density around CLA B 611:**

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



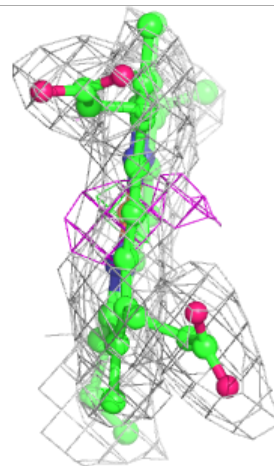
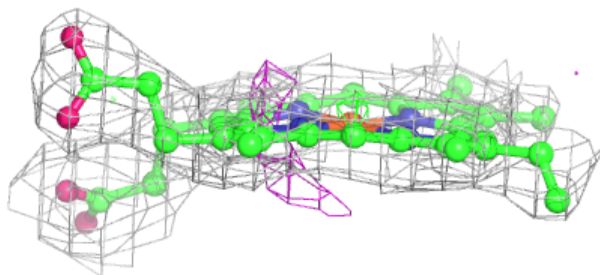
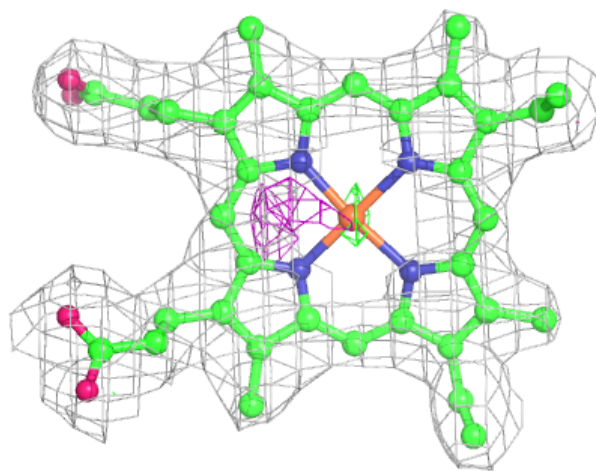
Electron density around CLA c 506:

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



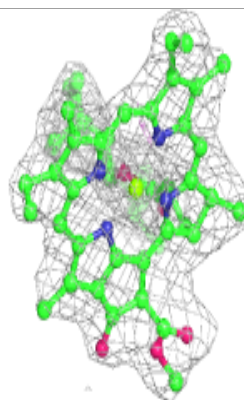
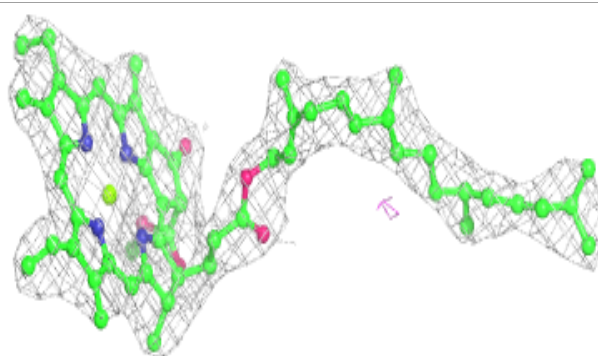
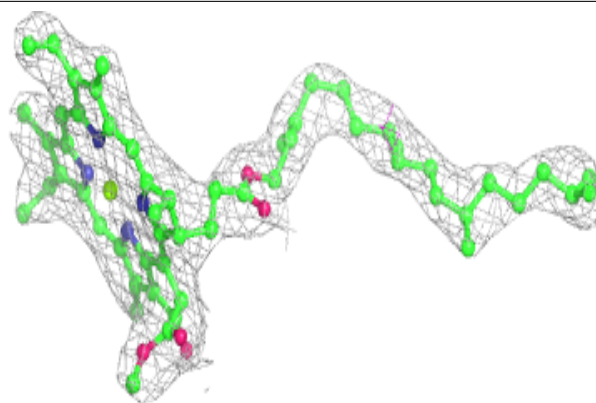
Electron density around HEM v 205:

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

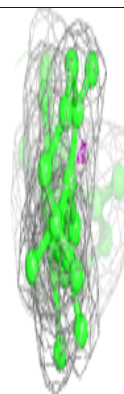
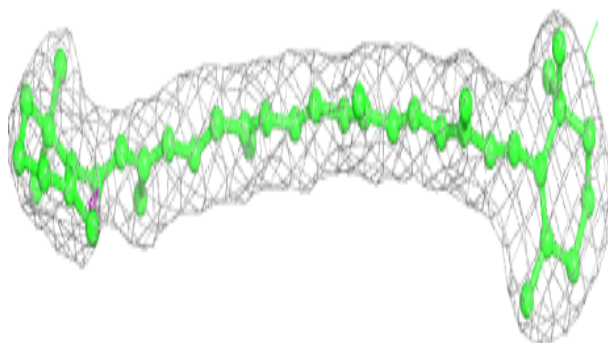
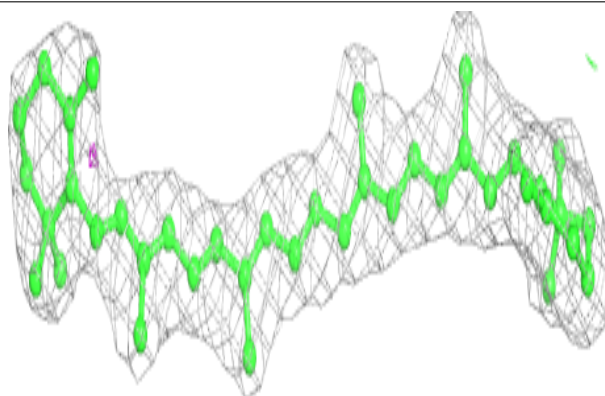


Electron density around CLA C 503:

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

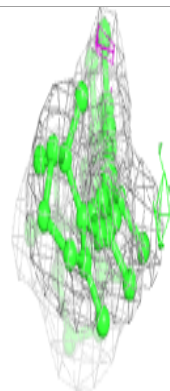
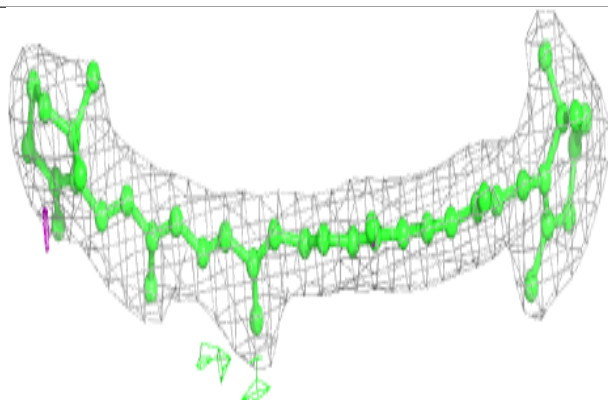
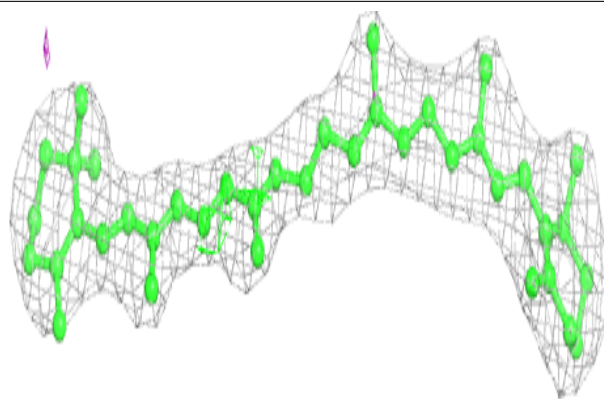
**Electron density around BCR b 626:**

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

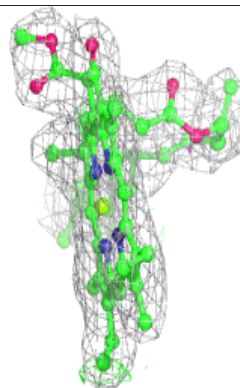
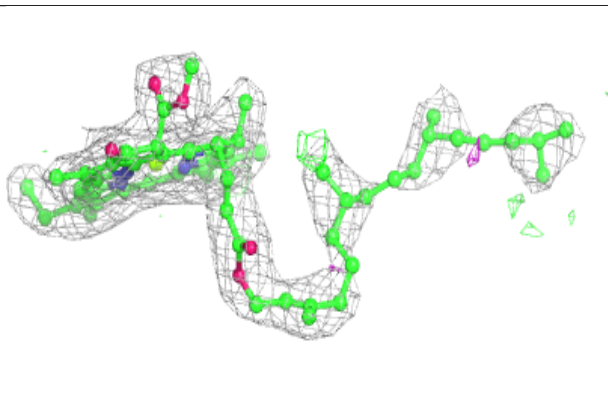
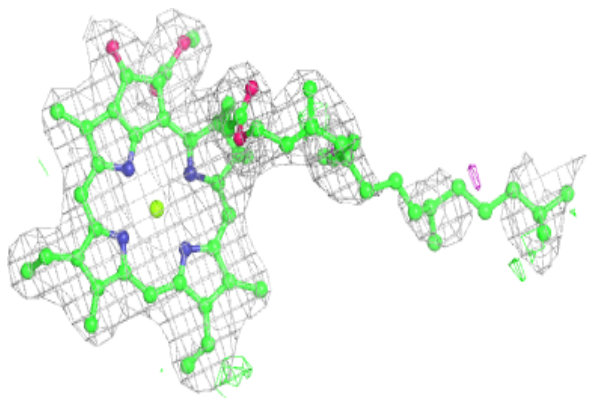


Electron density around BCR t 102:

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

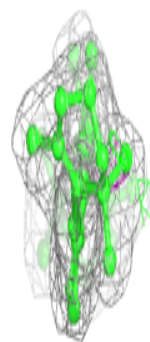
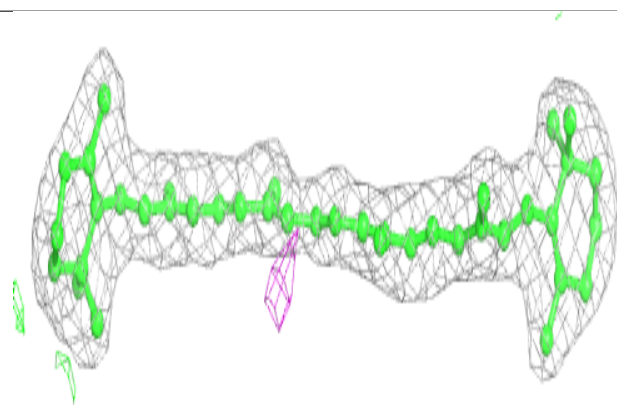
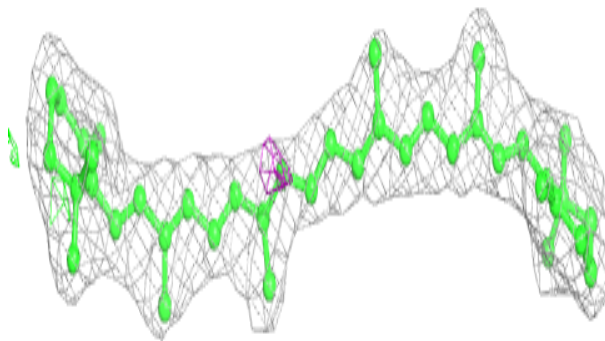
**Electron density around CLA a 410:**

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

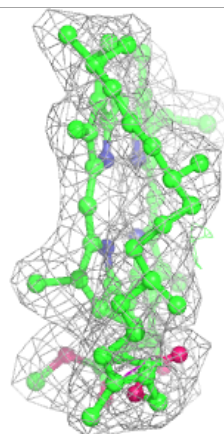
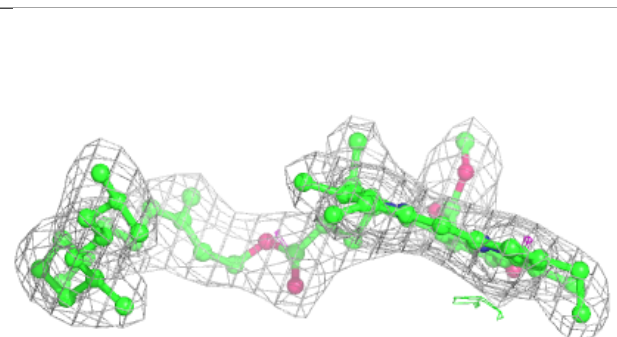
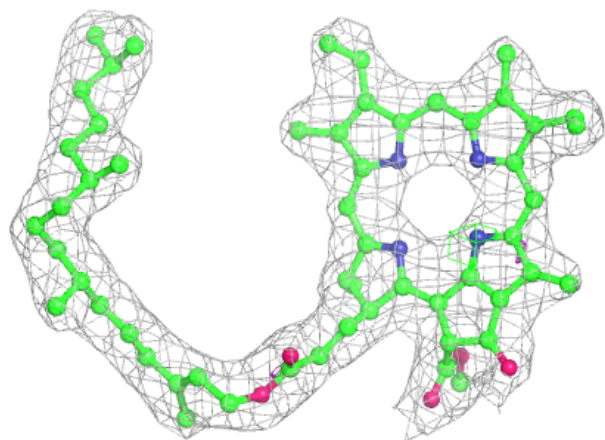


Electron density around BCR A 408:

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

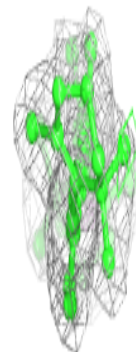
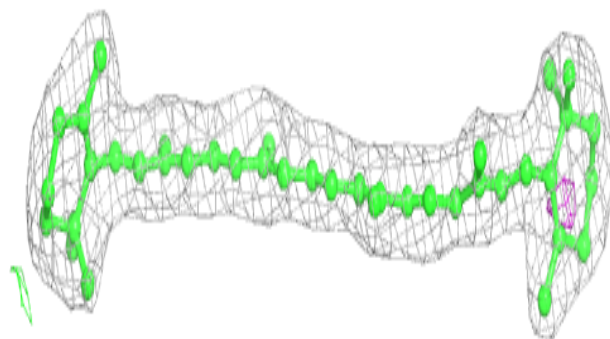
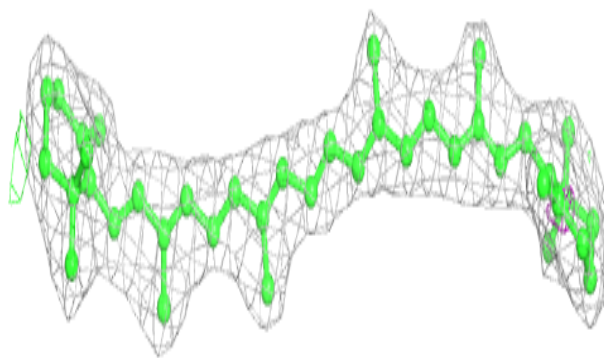
**Electron density around PHO D 402:**

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

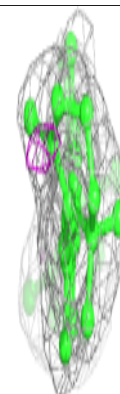
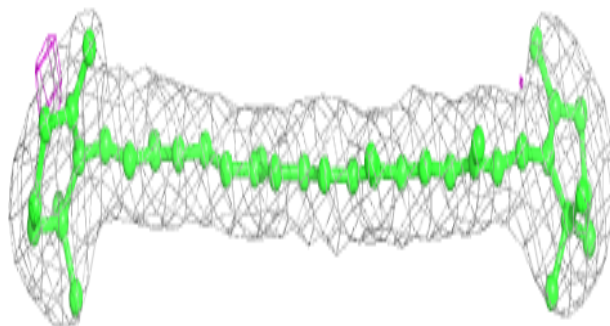
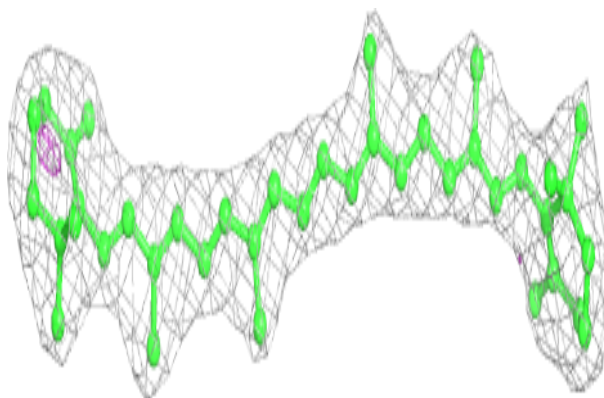


Electron density around BCR a 413:

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

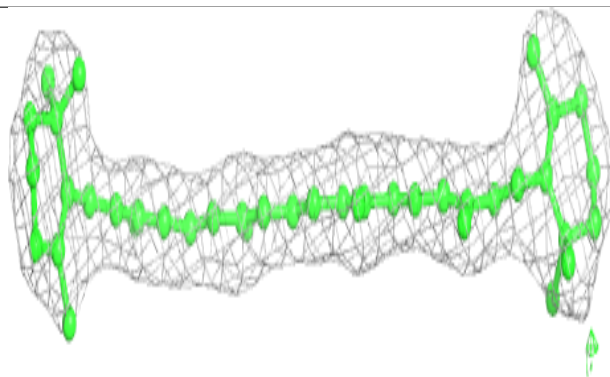
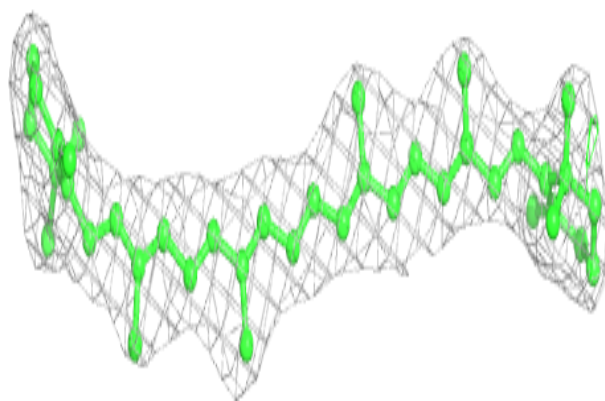
**Electron density around BCR B 619:**

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

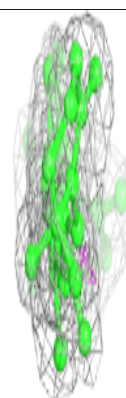
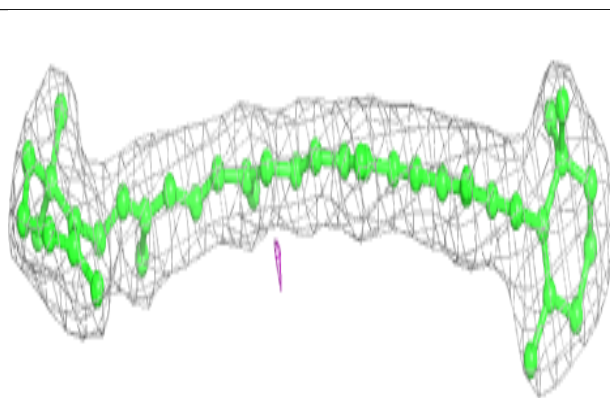
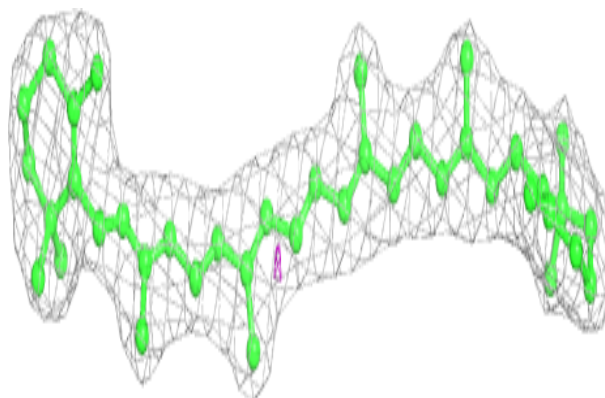


Electron density around BCR c 518:

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

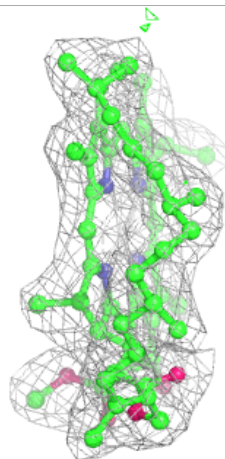
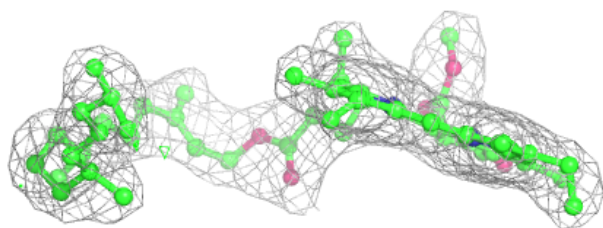
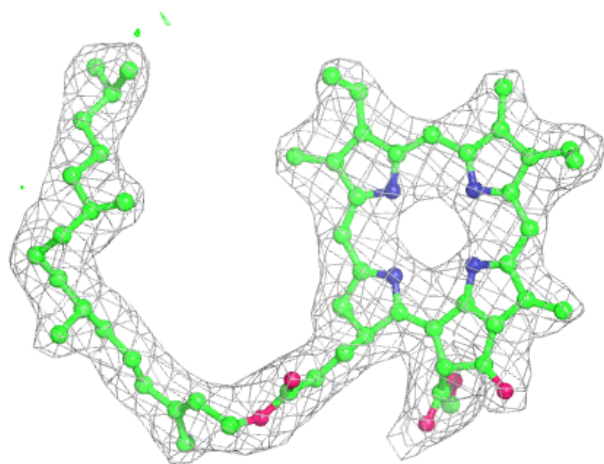
**Electron density around BCR B 618:**

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



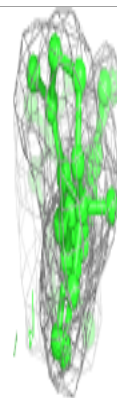
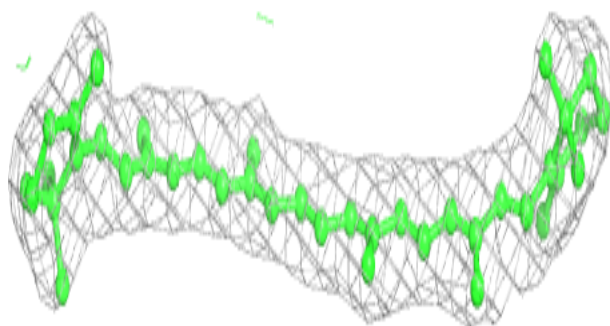
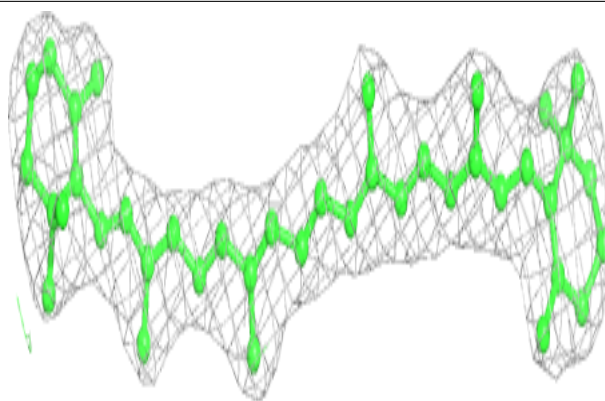
Electron density around PHO a 411:

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

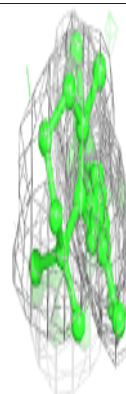
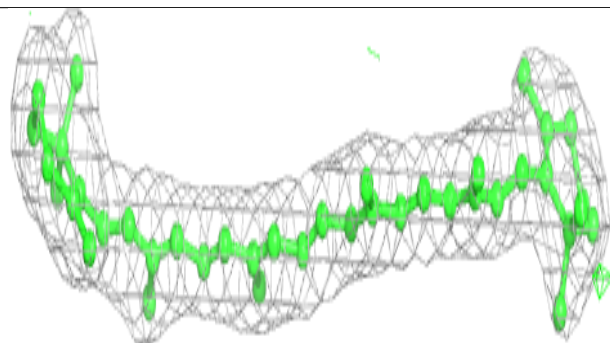
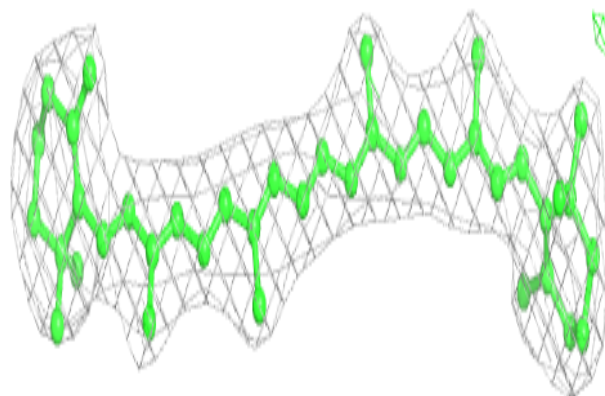


Electron density around BCR b 628:

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

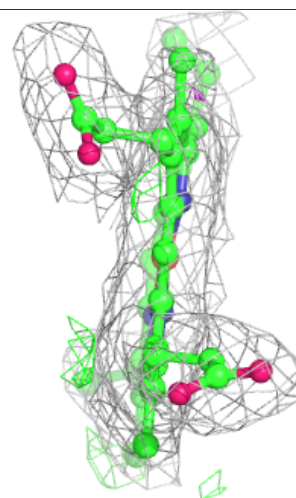
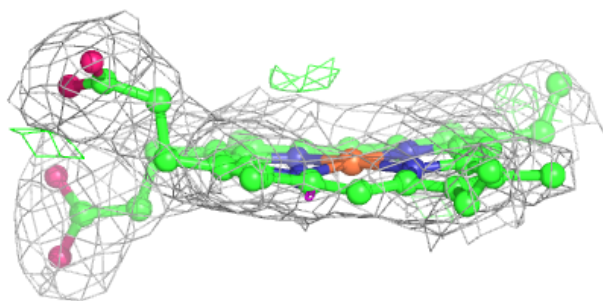
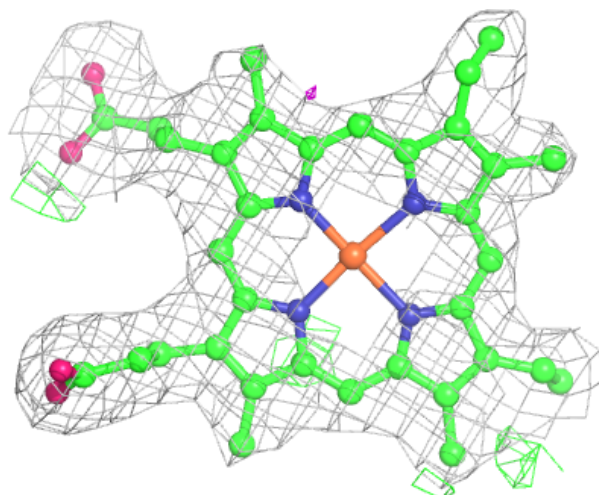
**Electron density around BCR B 620:**

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



Electron density around HEM 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.