



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 18, 2020 – 10:58 AM BST

PDB ID : 5WS5  
Title : Native XFEL structure of photosystem II (preflash dark dataset)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2016-12-05  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

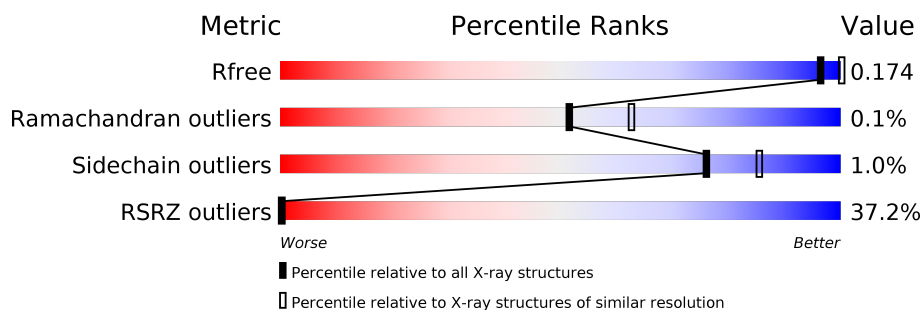
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>25%</div> <div>97%</div> </div>
1	a	344	<div> <div>33%</div> <div>96%</div> </div>
2	B	505	<div> <div>30%</div> <div>99%</div> </div>
2	b	505	<div> <div>35%</div> <div>99%</div> </div>
3	C	455	<div> <div>38%</div> <div>98%</div> </div>
3	c	455	<div> <div>39%</div> <div>99%</div> </div>
4	D	342	<div> <div>27%</div> <div>100%</div> </div>

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	X
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
26	SQD	A	412	-	-	-	X
26	SQD	B	620	-	-	-	X
26	SQD	a	413	-	-	-	X
26	SQD	b	620	-	-	-	X
26	SQD	f	102	-	-	-	X
27	GOL	v	201	-	-	-	X
29	PL9	A	414	-	-	-	X
29	PL9	a	416	-	-	-	X
30	UNL	A	415	-	-	-	X
30	UNL	B	627	-	-	-	X
30	UNL	D	413	-	-	-	X
30	UNL	I	102	-	-	-	X
30	UNL	J	101	-	-	-	X
30	UNL	K	101	-	-	-	X
30	UNL	M	102	-	-	-	X
30	UNL	b	626	-	-	-	X
30	UNL	d	409	-	-	-	X
30	UNL	d	410	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	101	-	-	-	X
30	UNL	m	102	-	-	-	X
32	LMT	A	359	-	-	-	X
32	LMT	D	404	-	-	-	X
32	LMT	E	102	-	-	-	X
32	LMT	I	101	-	-	-	X
32	LMT	M	101	-	-	-	X
32	LMT	M	103	-	-	-	X
32	LMT	a	414	-	-	-	X
32	LMT	a	420	-	-	-	X
32	LMT	b	621	-	-	-	X
32	LMT	b	627	-	-	-	X
32	LMT	e	102	-	-	-	X
32	LMT	m	103	-	-	-	X
32	LMT	t	101	-	-	-	X
33	LMG	B	621	-	-	-	X
33	LMG	C	501	-	-	-	X
33	LMG	C	521	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	a	419	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	LMG	c	521	-	-	-	X
33	LMG	z	101	-	-	-	X
34	HTG	D	414	-	-	-	X
34	HTG	b	623	-	-	-	X
34	HTG	c	522	-	-	-	X
34	HTG	d	411	-	-	-	X
35	DGD	H	102	-	-	-	X
35	DGD	h	102	-	-	-	X
37	LHG	D	409	-	-	-	X
37	LHG	E	101	-	-	-	X
37	LHG	e	101	-	-	-	X

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52545 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 D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	4	0
			2636	1730	431	460	15			

- 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	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2316	589	618	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

- 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	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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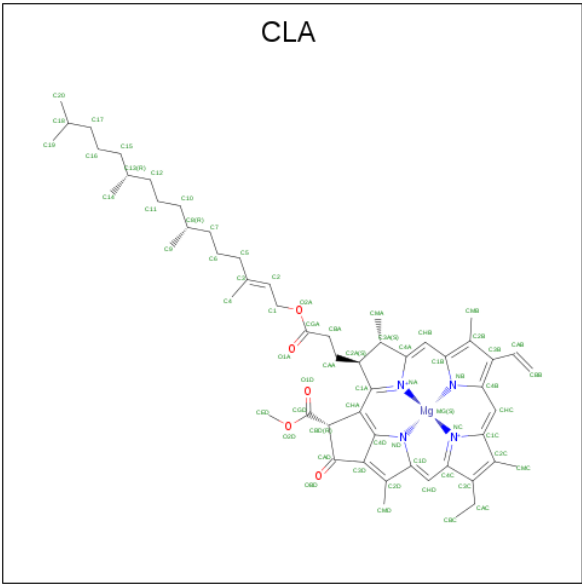
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 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

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

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

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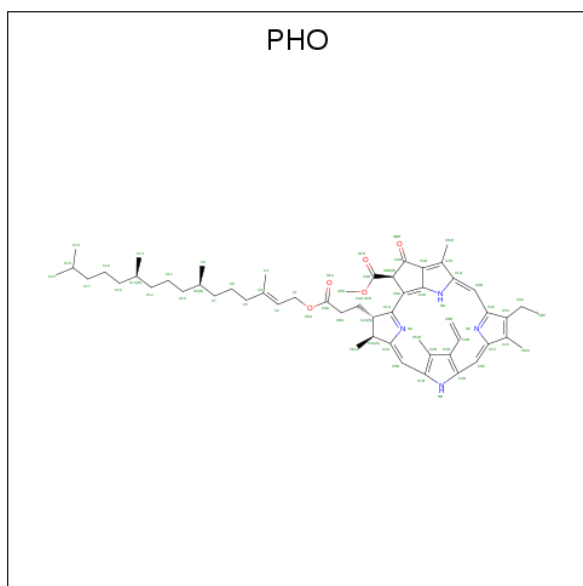
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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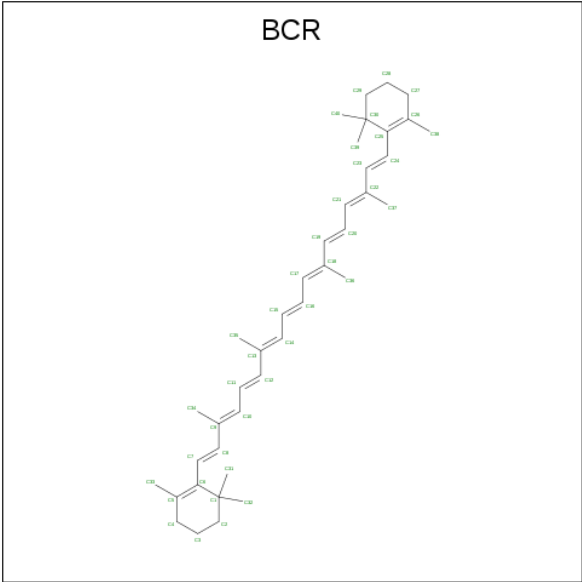
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



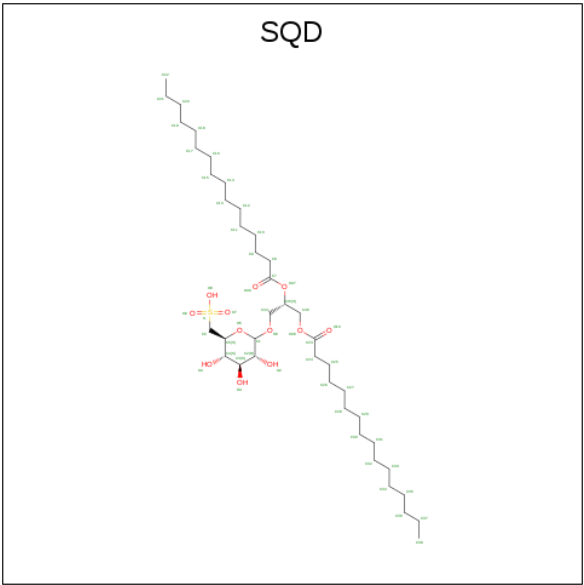
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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

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



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

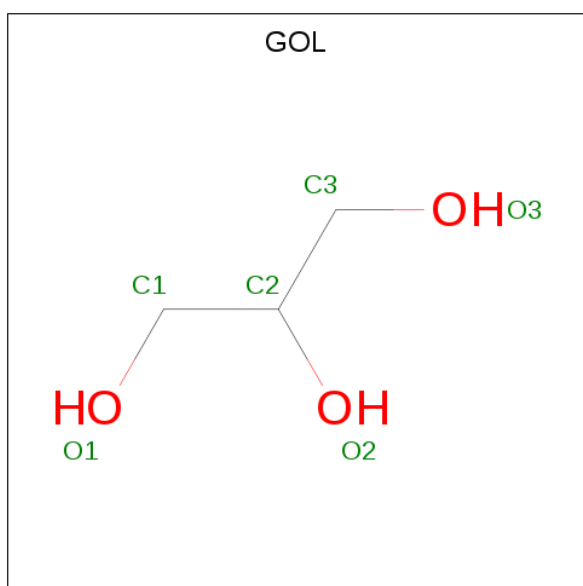
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



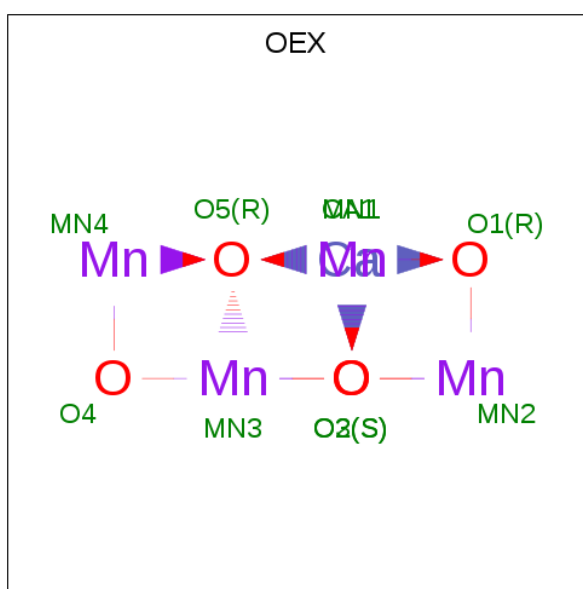
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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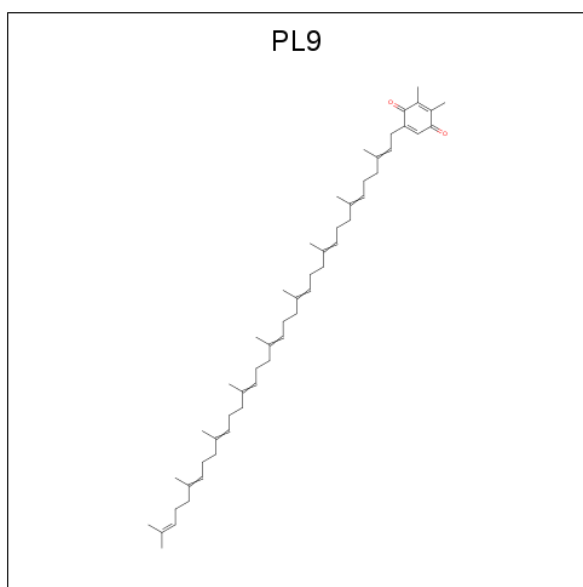
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



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

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

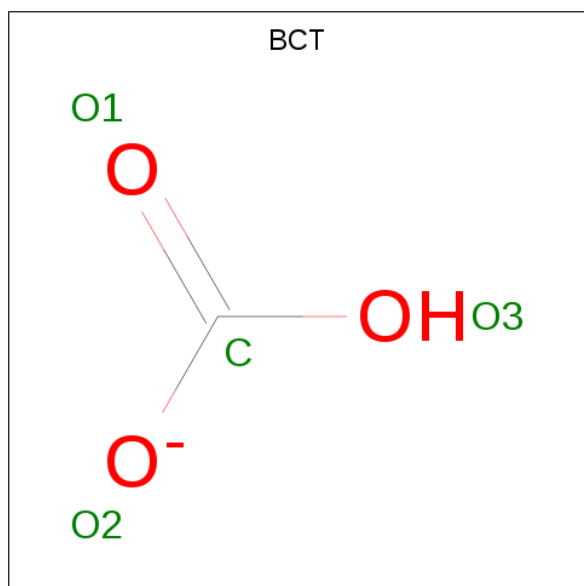
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	J	1	Total	C		0	0
			10	10			
30	i	1	Total	C	O	0	0
			40	35	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	K	1	Total	C	O	0	0
			34	29	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	I	1	Total	C	O	0	0
			40	35	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	a	1	Total	C	O	0	0
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

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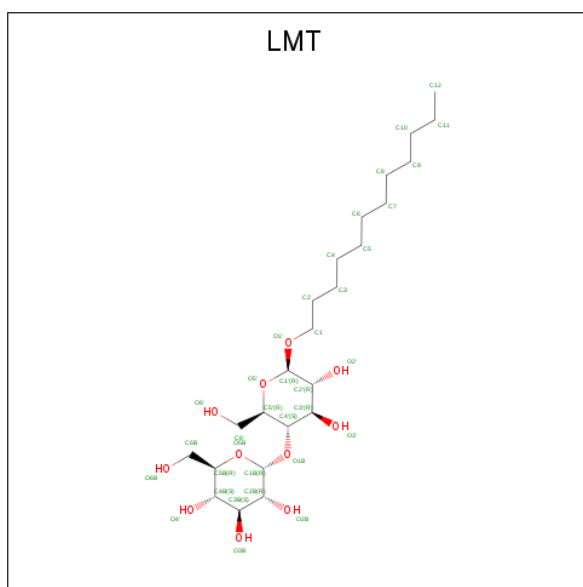
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	x	1	Total C O 18 16 2	0	0
30	A	1	Total C O 28 23 5	0	0
30	j	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	d	2	Total C O 53 47 6	0	0
30	m	1	Total C 10 10	0	0
30	b	1	Total C O 33 28 5	0	0
30	M	1	Total C 10 10	0	0

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



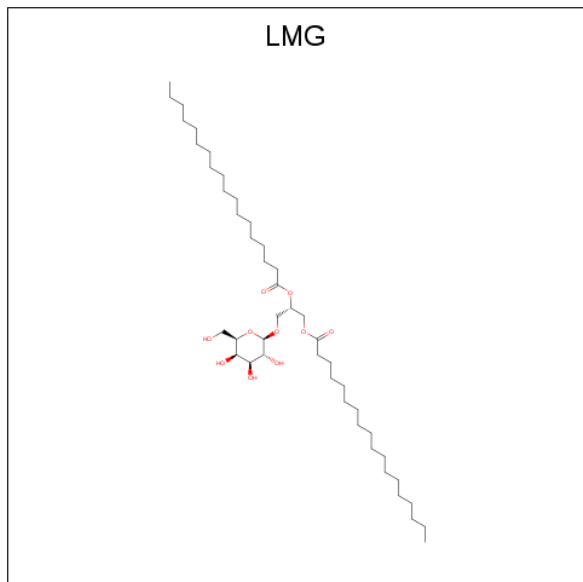
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 4 1 3	0	0
31	a	1	Total C O 4 1 3	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $\text{C}_{24}\text{H}_{46}\text{O}_{11}$ ).



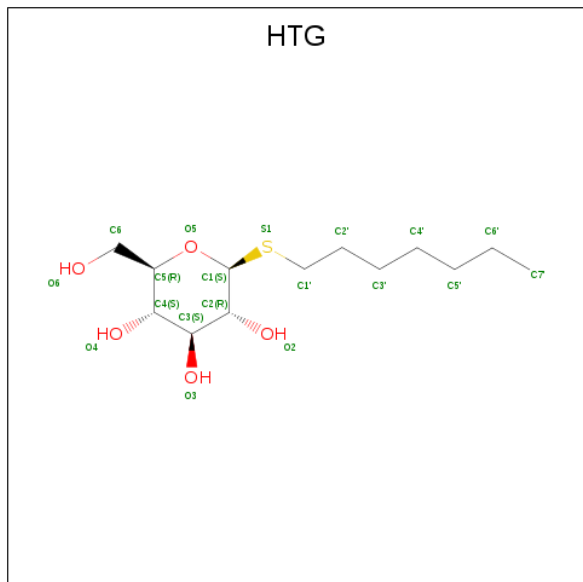
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total 35	C 24	O 11	0	0
32	D	1	Total 35	C 24	O 11	0	0
32	E	1	Total 35	C 24	O 11	0	0
32	I	1	Total 35	C 24	O 11	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	a	1	Total 35	C 24	O 11	0	0
32	a	1	Total 35	C 24	O 11	0	0
32	b	1	Total 25	C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

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



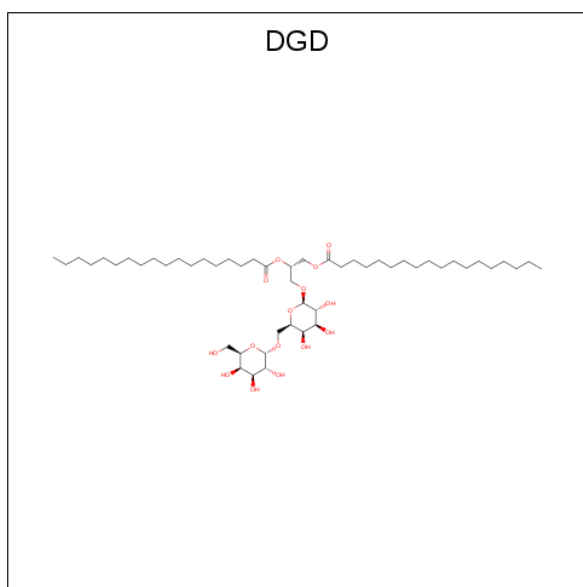
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	F	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		

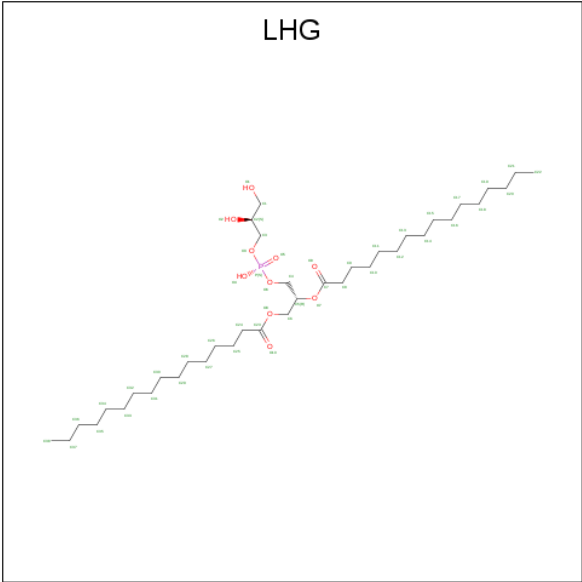
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	o	1	Total	Ca	0	0
			1	1		
36	f	1	Total	Ca	0	0
			1	1		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



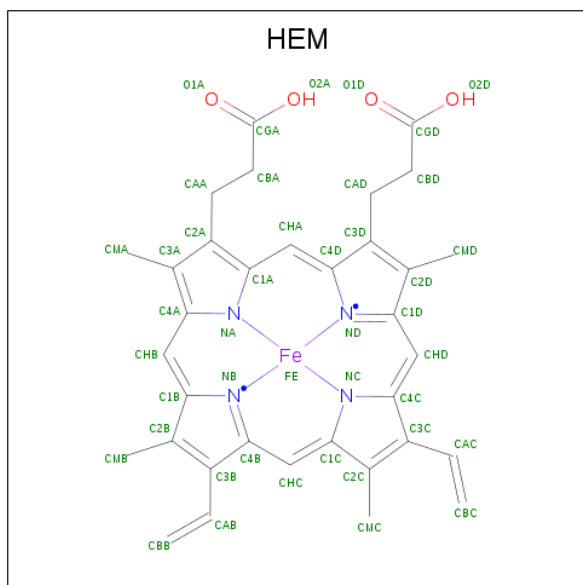
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	1	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

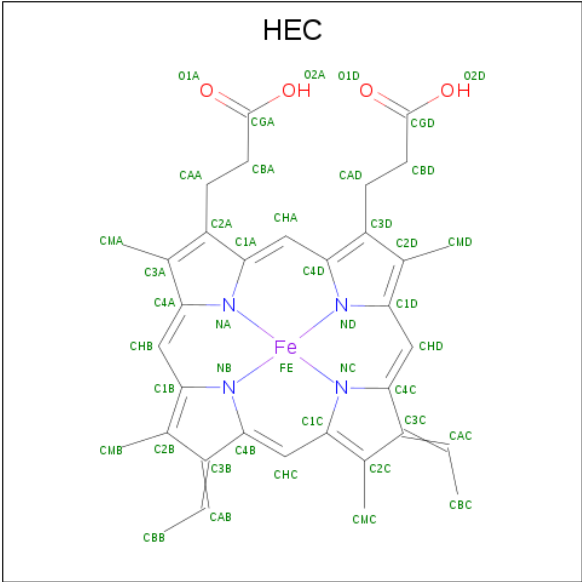


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 40 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	130	Total	O		
			130	130	0	0
41	B	167	Total	O		
			167	167	0	0
41	C	144	Total	O		
			144	144	0	0
41	D	122	Total	O		
			122	122	0	0
41	E	15	Total	O		
			15	15	0	0
41	F	4	Total	O		
			4	4	0	0
41	H	19	Total	O		
			19	19	0	0
41	I	6	Total	O		
			6	6	0	0
41	J	5	Total	O		
			5	5	0	0
41	K	6	Total	O		
			6	6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	3	Total 3	O 3	0	0
41	M	7	Total 7	O 7	0	0
41	O	71	Total 71	O 71	0	0
41	T	9	Total 9	O 9	0	0
41	U	32	Total 32	O 32	0	0
41	V	67	Total 67	O 67	0	0
41	X	1	Total 1	O 1	0	0
41	Y	1	Total 1	O 1	0	0
41	a	133	Total 133	O 133	0	0
41	b	193	Total 193	O 193	0	0
41	c	142	Total 142	O 142	0	0
41	d	114	Total 114	O 114	0	0
41	e	8	Total 8	O 8	0	0
41	f	4	Total 4	O 4	0	0
41	h	16	Total 16	O 16	0	0
41	i	3	Total 3	O 3	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	4	Total 4	O 4	0	0
41	m	15	Total 15	O 15	0	0
41	o	77	Total 77	O 77	0	0

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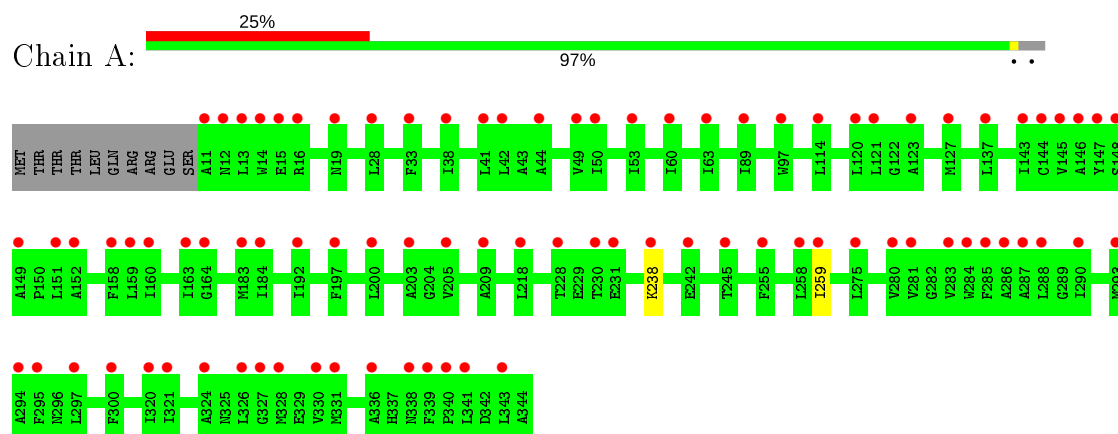
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	t	6	Total 6	O 6	0	0
41	u	47	Total 47	O 47	0	0
41	v	47	Total 47	O 47	0	0
41	x	2	Total 2	O 2	0	0
41	y	1	Total 1	O 1	0	0

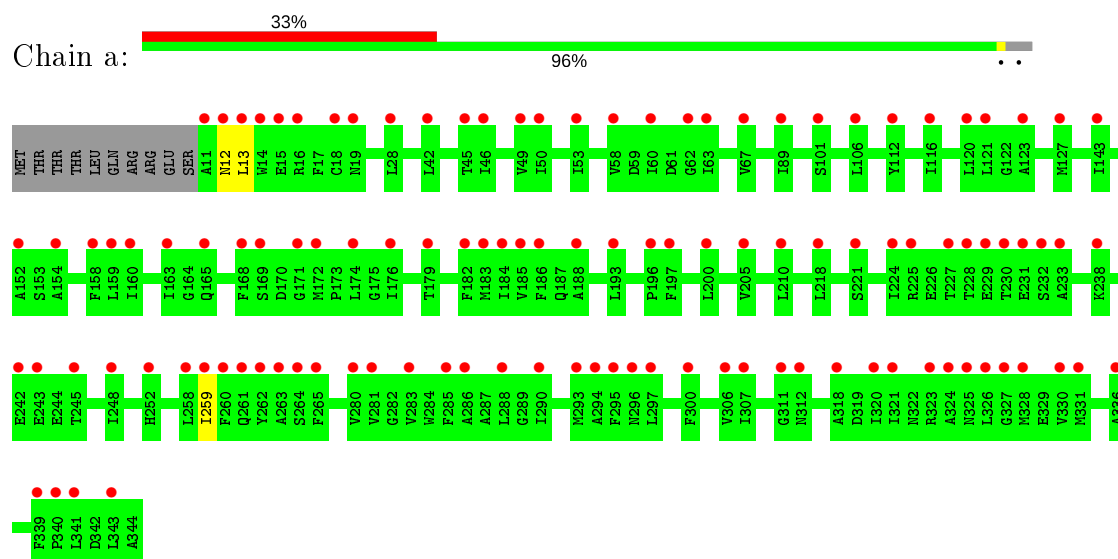
### 3 Residue-property plots [i](#)

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 D1 protein

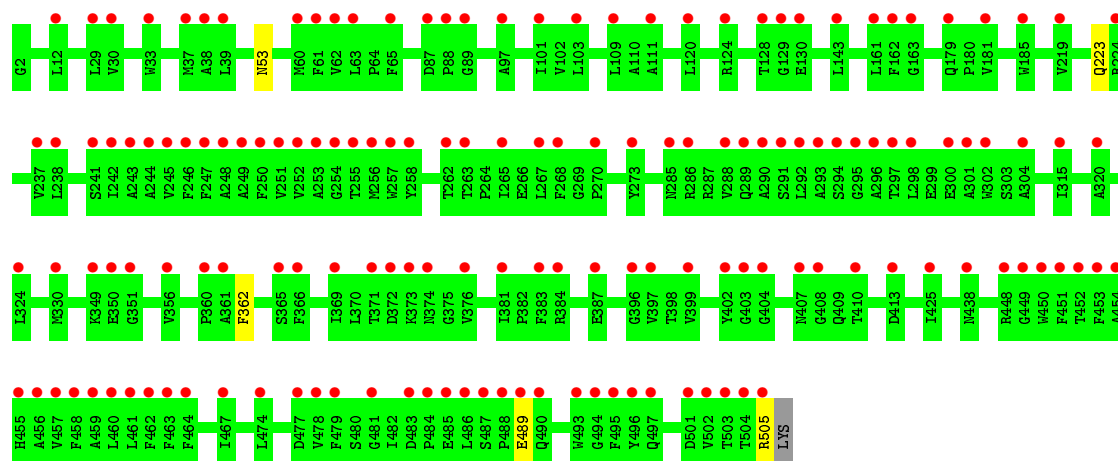


- Molecule 1: Photosystem II D1 protein

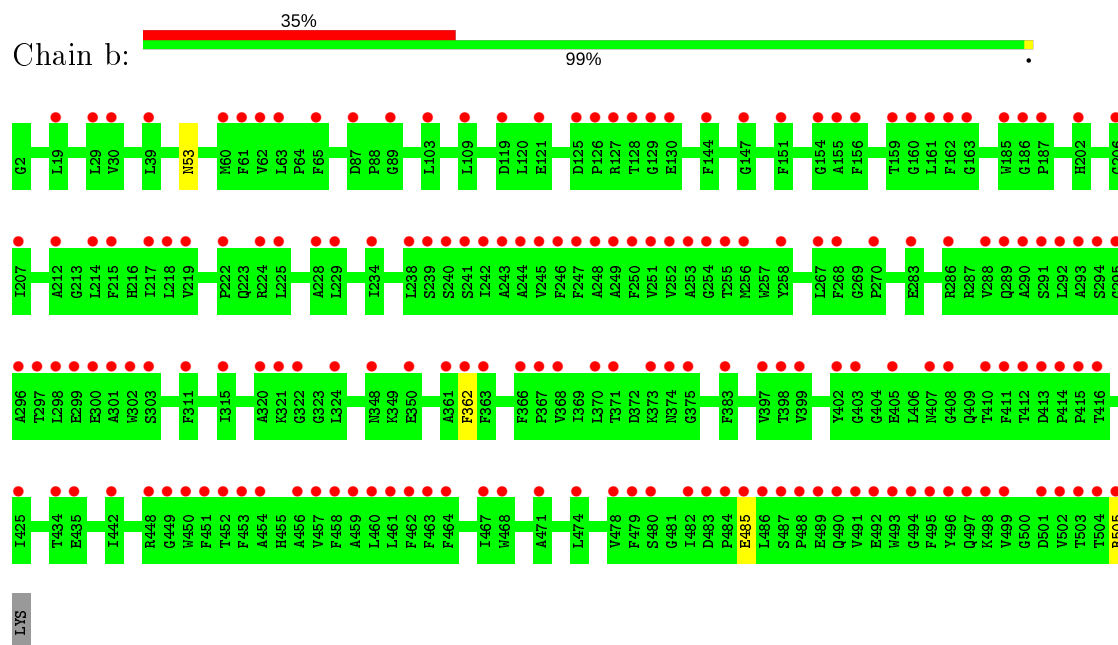


- Molecule 2: Photosystem II CP47 reaction center protein

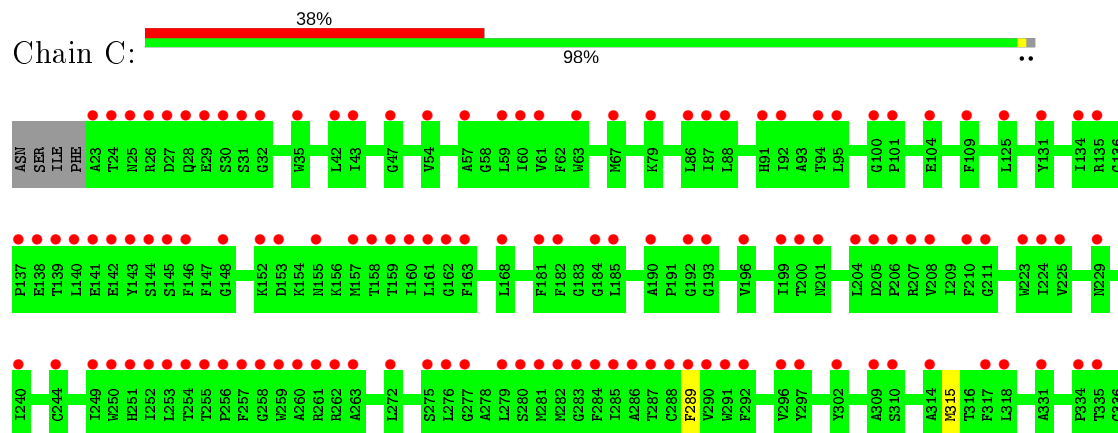


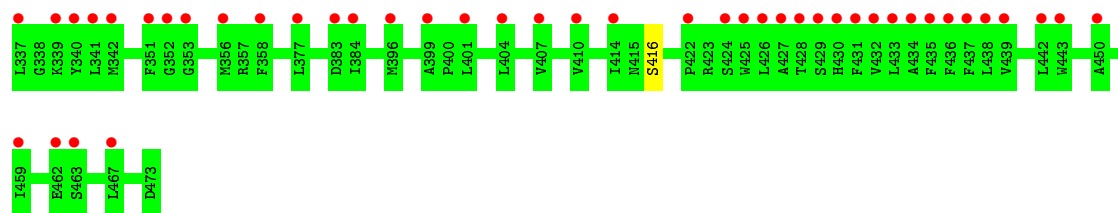


• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II CP43 protein

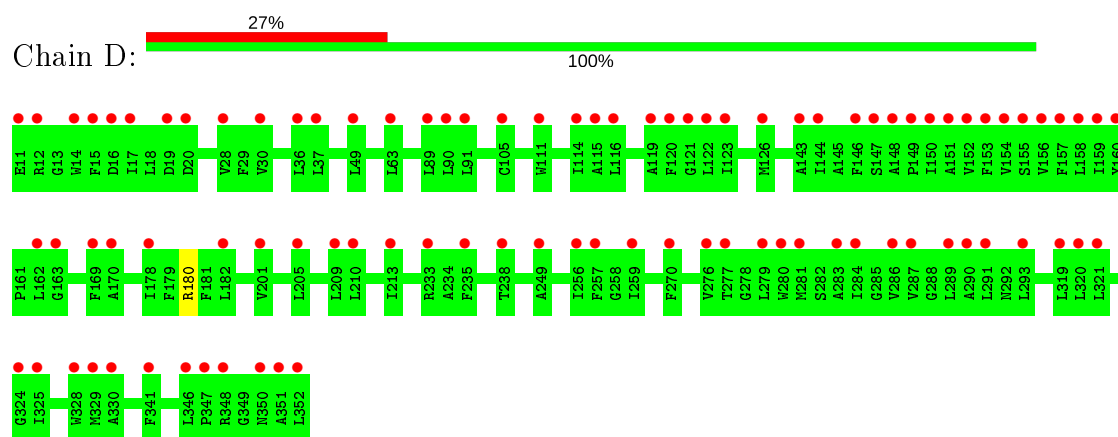




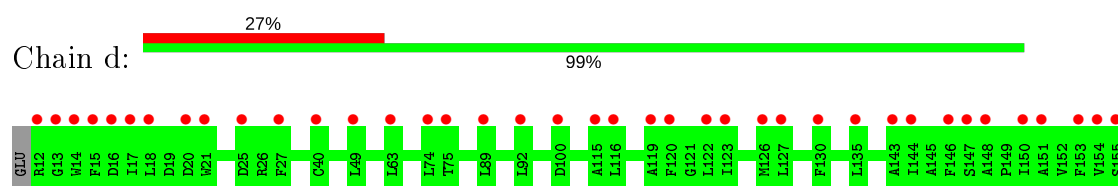
• Molecule 3: Photosystem II CP43 protein



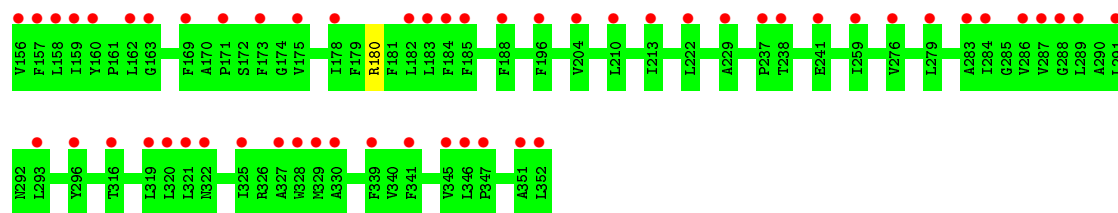
• Molecule 4: Photosystem II D2 protein



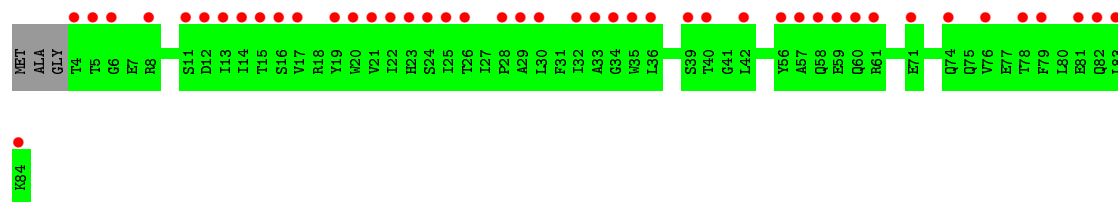
• Molecule 4: Photosystem II D2 protein



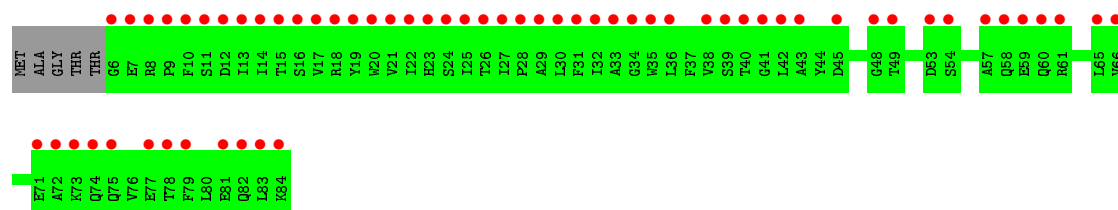
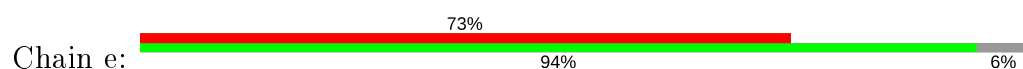




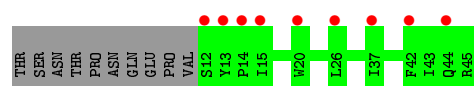
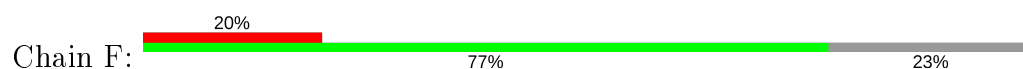
• Molecule 5: Cytochrome b559 subunit alpha



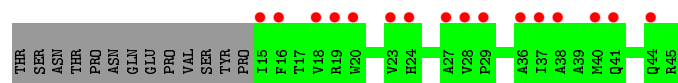
• Molecule 5: Cytochrome b559 subunit alpha



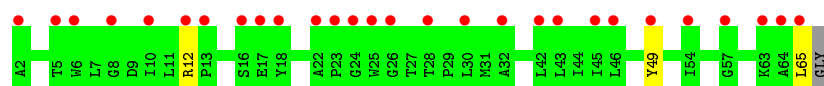
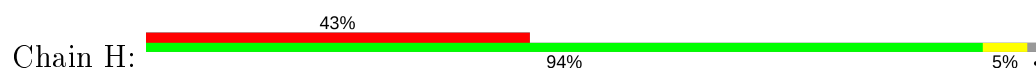
• Molecule 6: Cytochrome b559 subunit beta



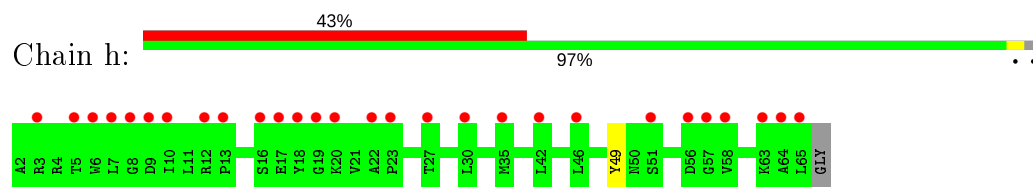
• Molecule 6: Cytochrome b559 subunit beta



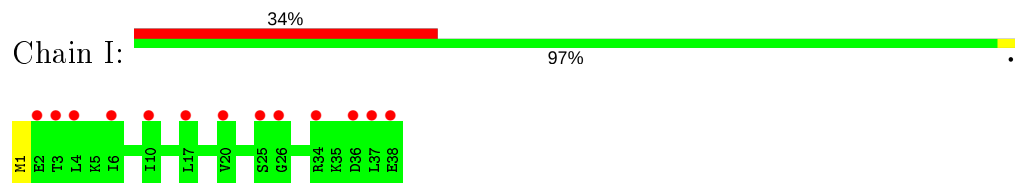
• Molecule 7: Photosystem II reaction center protein H



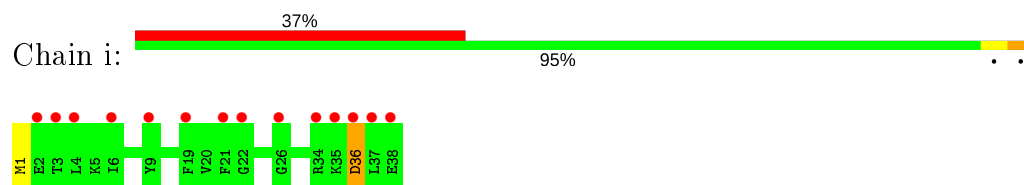
- Molecule 7: Photosystem II reaction center protein H



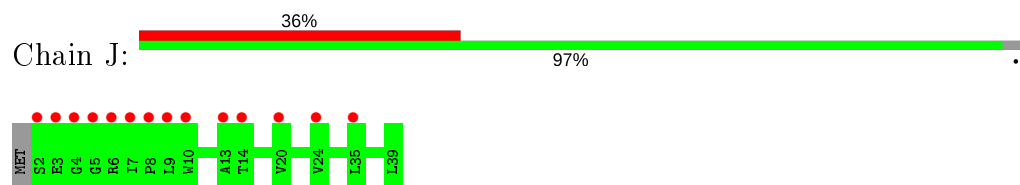
- Molecule 8: Photosystem II reaction center protein I



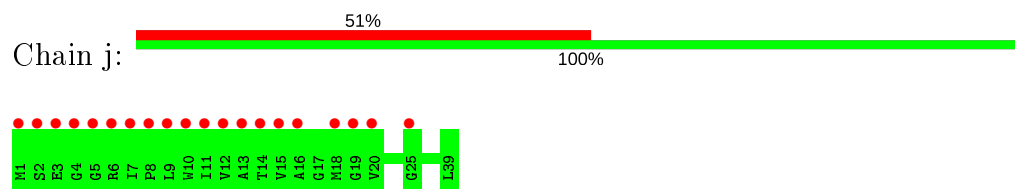
- Molecule 8: Photosystem II reaction center protein I



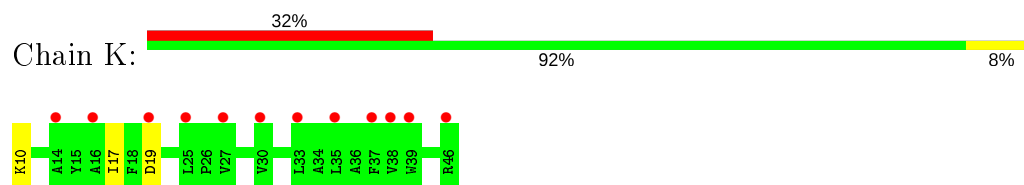
- Molecule 9: Photosystem II reaction center protein J



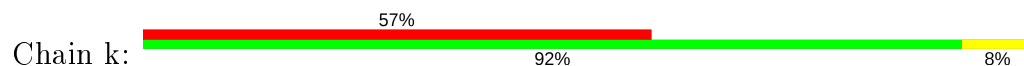
- Molecule 9: Photosystem II reaction center protein J

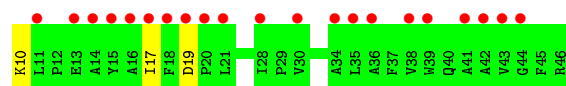


- Molecule 10: Photosystem II protein K

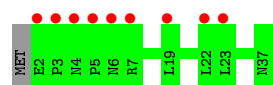


- Molecule 10: Photosystem II protein K

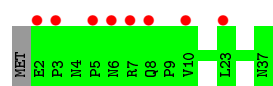




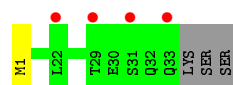
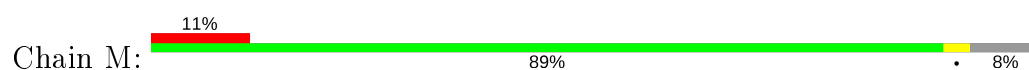
- Molecule 11: Photosystem II reaction center protein L



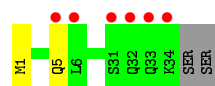
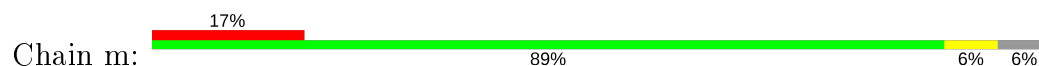
- Molecule 11: Photosystem II reaction center protein L



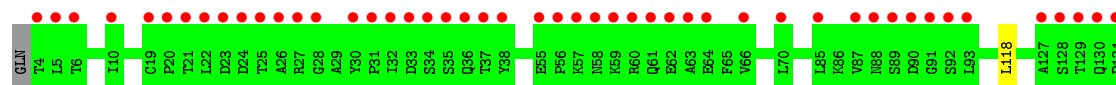
- Molecule 12: Photosystem II protein M



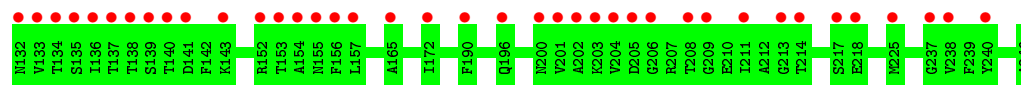
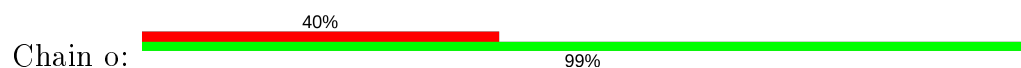
- Molecule 12: Photosystem II protein M

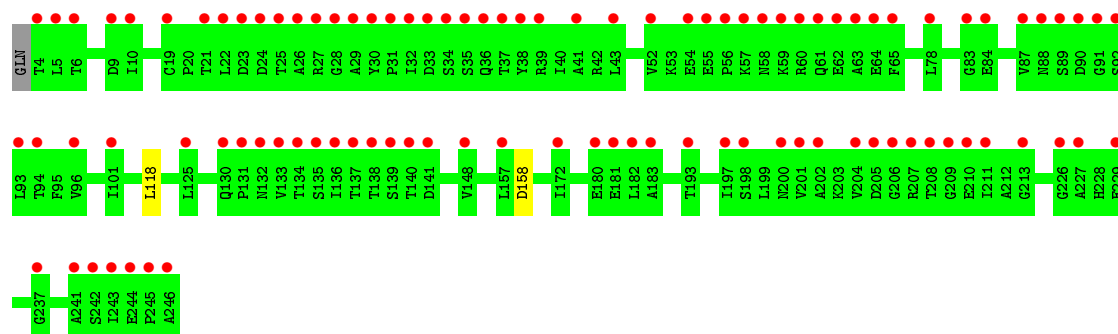


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

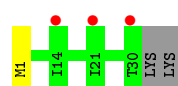


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

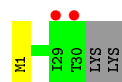
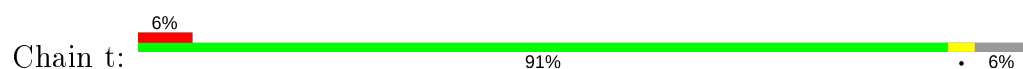




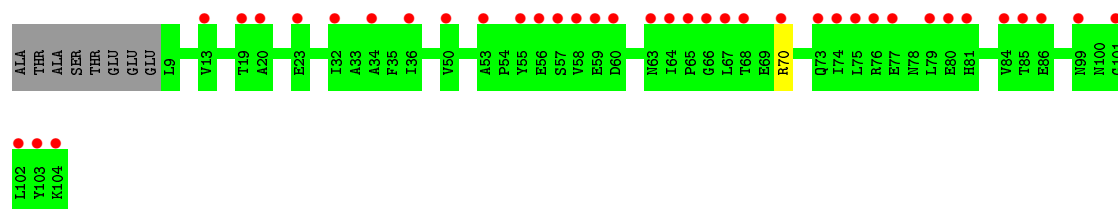
- Molecule 14: Photosystem II reaction center protein T



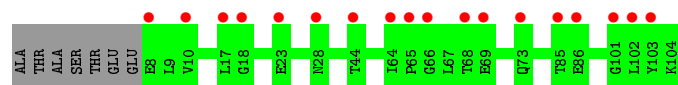
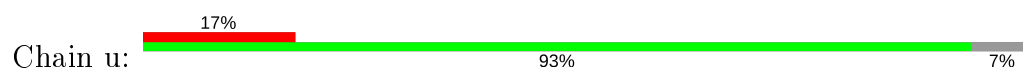
- Molecule 14: Photosystem II reaction center protein T



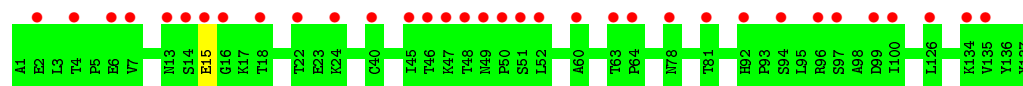
- Molecule 15: Photosystem II 12 kDa extrinsic protein



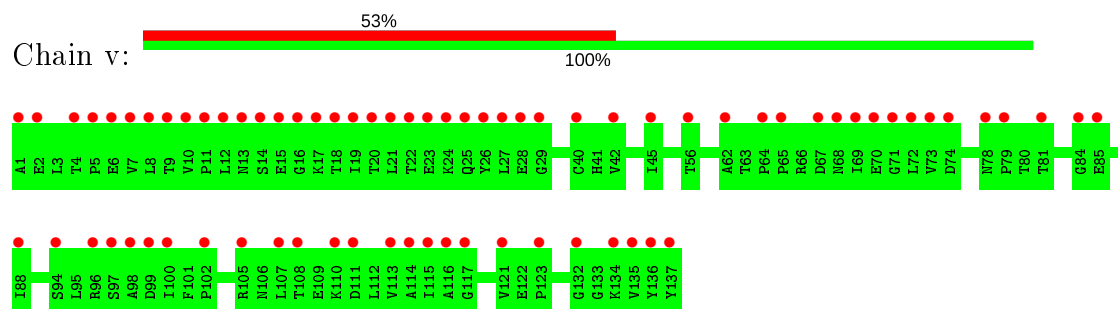
- Molecule 15: Photosystem II 12 kDa extrinsic protein



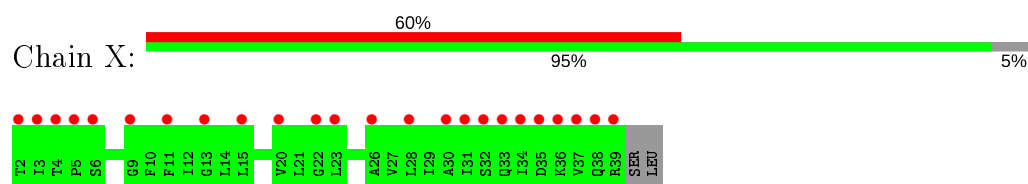
- Molecule 16: Cytochrome c-550



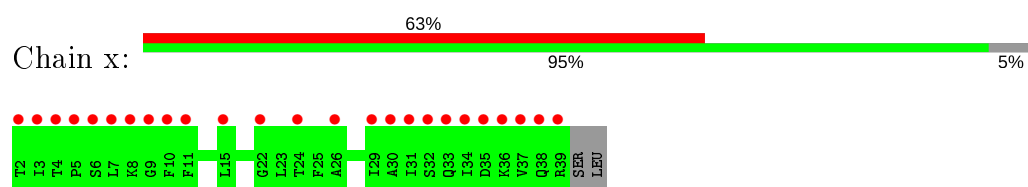
- Molecule 16: Cytochrome c-550



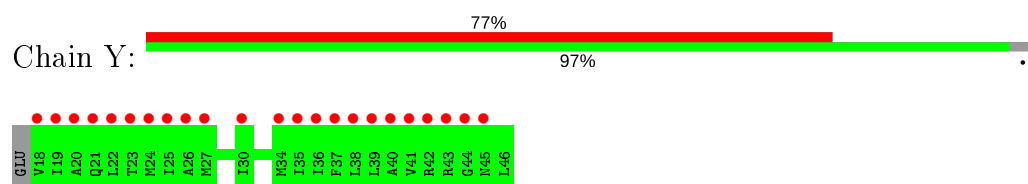
- Molecule 17: Photosystem II reaction center protein X



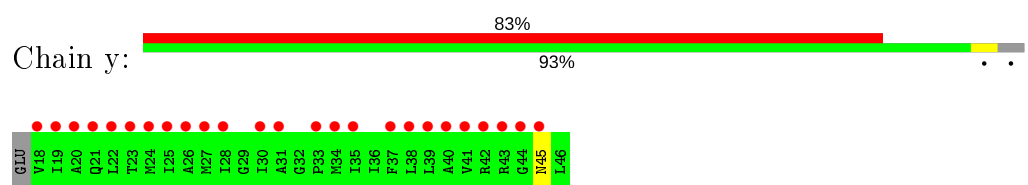
- Molecule 17: Photosystem II reaction center protein X



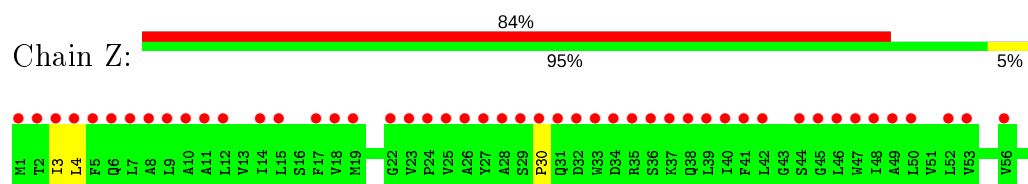
- Molecule 18: Photosystem II reaction center protein Ycf12



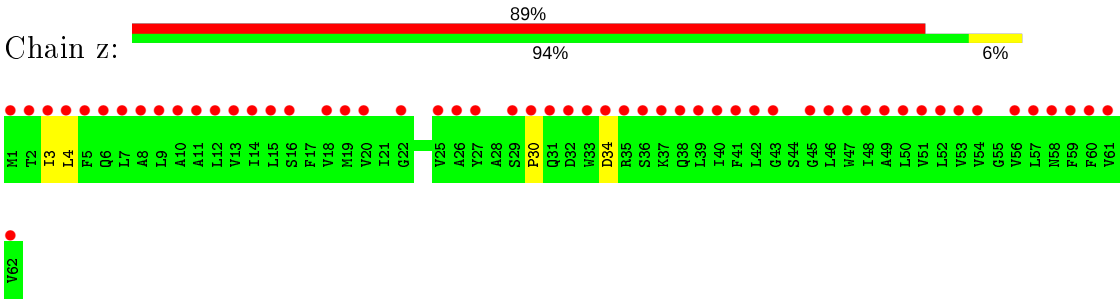
- Molecule 18: Photosystem II reaction center protein Ycf12



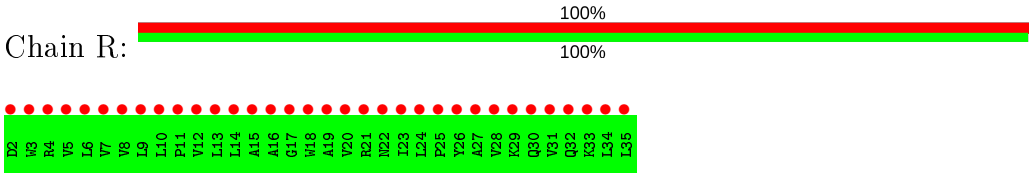
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.70 Å   229.89 Å   285.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.35 47.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 100.0 (47.31-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.34 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.133   ,   0.171 0.138   ,   0.174	Depositor DCC
$R_{free}$ test set	17041 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 83.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	52545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, LMG, FE2, HEC, 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	0.48	0/2728	0.58	0/3719
1	a	0.45	0/2733	0.56	0/3727
2	B	0.46	0/4171	0.56	0/5683
2	b	0.44	0/4138	0.54	0/5640
3	C	0.43	0/3626	0.53	0/4936
3	c	0.40	0/3662	0.53	0/4985
4	D	0.48	0/2827	0.56	0/3852
4	d	0.46	0/2818	0.55	0/3840
5	E	0.40	0/687	0.53	0/936
5	e	0.38	0/667	0.52	0/908
6	F	0.41	0/284	0.53	0/387
6	f	0.42	0/257	0.52	0/349
7	H	0.40	0/530	0.56	0/723
7	h	0.36	0/519	0.53	0/708
8	I	0.40	0/311	0.50	0/419
8	i	0.40	0/311	0.50	0/419
9	J	0.36	0/278	0.49	0/376
9	j	0.34	0/283	0.47	0/383
10	K	0.38	0/303	0.54	0/416
10	k	0.36	0/303	0.53	0/416
11	L	0.46	0/311	0.49	0/423
11	l	0.42	0/311	0.47	0/423
12	M	0.48	0/261	0.64	0/357
12	m	0.47	0/262	0.62	0/357
13	O	0.41	0/1926	0.59	0/2611
13	o	0.42	0/1910	0.60	1/2589 (0.0%)
14	T	0.56	0/257	0.56	0/349
14	t	0.49	0/257	0.52	0/349
15	U	0.41	0/776	0.55	0/1052
15	u	0.42	0/785	0.59	0/1064
16	V	0.40	0/1085	0.52	0/1473



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.38	0/1085	0.50	0/1473
17	X	0.34	0/284	0.49	0/384
17	x	0.32	0/284	0.50	0/384
18	Y	0.31	0/216	0.46	0/289
18	y	0.31	0/216	0.50	0/289
19	Z	0.32	0/490	0.43	0/669
19	z	0.31	0/490	0.43	0/669
20	R	0.28	0/279	0.40	0/383
All	All	0.43	0/42921	0.55	1/58409 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.22	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	41	47
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	41	47
2	B	510/505 (101%)	505 (99%)	5 (1%)	0	100	100
2	b	506/505 (100%)	500 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	34	38
3	c	457/455 (100%)	446 (98%)	9 (2%)	2 (0%)	34	38
4	D	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	2
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	238 (97%)	7 (3%)	0	100	100
13	o	243/244 (100%)	237 (98%)	6 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	9	7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	7
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5251/5384 (98%)	5147 (98%)	95 (2%)	9 (0%)	51	56

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
1	a	259	ILE
3	c	416[A]	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	272/279 (98%)	270 (99%)	2 (1%)	84	91
1	a	273/279 (98%)	271 (99%)	2 (1%)	84	91
2	B	410/403 (102%)	405 (99%)	5 (1%)	71	82
2	b	406/403 (101%)	402 (99%)	4 (1%)	76	85
3	C	356/356 (100%)	354 (99%)	2 (1%)	86	93
3	c	360/356 (101%)	355 (99%)	5 (1%)	67	78
4	D	278/277 (100%)	277 (100%)	1 (0%)	91	95
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	95
5	E	73/73 (100%)	73 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	55/54 (102%)	51 (93%)	4 (7%)	14	14
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	68
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	52
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	6
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	6
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	46
13	O	210/207 (101%)	209 (100%)	1 (0%)	88	94
13	o	208/207 (100%)	207 (100%)	1 (0%)	88	94
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	82 (99%)	1 (1%)	71	82
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	87
16	v	117/117 (100%)	117 (100%)	0	100	100
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	21 (96%)	1 (4%)	27	33
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	41
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	22
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4357/4403 (99%)	4312 (99%)	45 (1%)	76	85

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	3	ILE

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Mol	Chain	Res	Type
2	b	362	PHE
18	y	45	ASN
1	a	12	ASN
2	b	485	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	73	GLN
2	b	53	ASN
12	m	5	GLN
13	O	130	GLN
13	o	124	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.50	2 (28%)
14	FME	T	1	14	8,9,10	0.60	0	7,9,11	1.53	2 (28%)
12	FME	M	1	12	8,9,10	0.59	0	7,9,11	1.46	2 (28%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.09	1 (14%)
14	FME	t	1	14	8,9,10	0.61	0	7,9,11	1.66	2 (28%)
8	FME	i	1	8	8,9,10	0.57	0	7,9,11	1.39	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.67	117.79	124.78
14	t	1	FME	CA-N-CN	-2.55	118.89	122.82
12	m	1	FME	CA-N-CN	-2.50	118.98	122.82
14	T	1	FME	CG-CB-CA	2.38	119.57	112.95
12	M	1	FME	O-C-CA	-2.33	118.67	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 214 ligands modelled in this entry, 18 are unknown and 15 are monoatomic - leaving 181 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$
32	LMT	b	627	-	25,25,36	0.53	1 (4%)	30,30,47	0.76	0
23	CLA	b	610	41	59,73,73	1.96	14 (23%)	67,113,113	2.29	23 (34%)
33	LMG	z	101	-	39,39,55	1.06	2 (5%)	47,47,63	1.10	4 (8%)
28	OEX	a	415	1,3,41	0,15,15	0.00	-	-	-	-
23	CLA	C	512	3	59,73,73	2.05	12 (20%)	67,113,113	2.16	21 (31%)
40	HEC	V	202	16	26,50,50	1.49	4 (15%)	18,82,82	1.64	3 (16%)
32	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.87	0
23	CLA	B	612	2	59,73,73	1.98	13 (22%)	67,113,113	2.40	27 (40%)
34	HTG	V	203	-	11,11,19	0.24	0	15,15,24	1.09	1 (6%)
26	SQD	f	102	-	42,43,54	1.17	3 (7%)	51,54,65	1.46	9 (17%)
23	CLA	C	511	3	59,73,73	1.97	14 (23%)	67,113,113	2.33	24 (35%)
23	CLA	B	610	41	59,73,73	2.01	14 (23%)	67,113,113	2.27	25 (37%)
37	LHG	L	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.08	2 (3%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.52	13 (23%)
23	CLA	c	508	41	59,73,73	1.97	12 (20%)	67,113,113	2.18	20 (29%)
23	CLA	B	607	41	59,73,73	1.99	14 (23%)	67,113,113	2.23	22 (32%)
35	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.23	6 (7%)
23	CLA	d	402	4	59,73,73	1.95	13 (22%)	67,113,113	2.27	25 (37%)
23	CLA	b	609	2	59,73,73	1.95	13 (22%)	67,113,113	2.27	22 (32%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.32	5 (8%)
25	BCR	c	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.83	15 (26%)
23	CLA	b	606	2	59,73,73	1.92	12 (20%)	67,113,113	2.26	23 (34%)
32	LMT	t	102	-	26,26,36	0.57	1 (3%)	31,31,47	0.95	2 (6%)
27	GOL	V	201	-	5,5,5	0.41	0	5,5,5	0.49	0
23	CLA	a	405	1	59,73,73	1.99	13 (22%)	67,113,113	2.33	29 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.51	10 (17%)
34	HTG	b	625	-	19,19,19	0.94	2 (10%)	23,24,24	1.41	3 (13%)
34	HTG	c	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.56	1 (4%)
33	LMG	D	415	39	51,51,55	0.87	2 (3%)	59,59,63	0.89	3 (5%)
34	HTG	b	622	-	19,19,19	1.04	1 (5%)	23,24,24	1.73	5 (21%)
37	LHG	d	406	-	48,48,48	0.88	2 (4%)	51,54,54	1.09	4 (7%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	12 (21%)
23	CLA	b	614	2	59,73,73	1.91	13 (22%)	67,113,113	2.24	22 (32%)
32	LMT	a	420	-	36,36,36	0.49	1 (2%)	47,47,47	0.91	0
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	12 (21%)
32	LMT	M	101	-	36,36,36	0.49	0	47,47,47	1.06	3 (6%)
23	CLA	a	409	1	59,73,73	1.94	14 (23%)	67,113,113	2.28	26 (38%)
35	DGD	h	102	-	63,63,67	0.84	2 (3%)	77,77,81	0.98	4 (5%)
25	BCR	a	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.61	12 (21%)
29	PL9	d	405	-	55,55,55	0.65	1 (1%)	68,69,69	1.82	19 (27%)
35	DGD	c	518	-	63,63,67	0.89	3 (4%)	77,77,81	0.97	3 (3%)
33	LMG	c	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	4 (6%)
34	HTG	B	626	-	19,19,19	1.00	2 (10%)	23,24,24	1.54	4 (17%)
26	SQD	F	101	-	42,43,54	1.17	4 (9%)	51,54,65	1.78	11 (21%)
37	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
25	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	C	508	41	59,73,73	1.95	12 (20%)	67,113,113	2.15	20 (29%)
27	GOL	b	624	-	5,5,5	0.29	0	5,5,5	0.54	0
35	DGD	c	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.14	6 (7%)
23	CLA	b	602	2	59,73,73	1.98	13 (22%)	67,113,113	2.31	25 (37%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.58	9 (16%)
23	CLA	c	504	3	59,73,73	1.94	13 (22%)	67,113,113	2.20	19 (28%)
23	CLA	B	613	2	59,73,73	2.06	15 (25%)	67,113,113	2.28	22 (32%)
24	PHO	A	353	-	67,69,69	2.06	16 (23%)	85,99,99	2.14	25 (29%)
34	HTG	B	623	-	19,19,19	0.91	1 (5%)	23,24,24	1.48	3 (13%)
28	OEX	A	413	1,3,41	0,15,15	0.00	-	-	-	-
27	GOL	c	501	-	5,5,5	0.31	0	5,5,5	0.43	0
23	CLA	A	404	1	59,73,73	2.00	14 (23%)	67,113,113	2.34	25 (37%)
38	HEM	e	87	5,6	27,50,50	0.89	1 (3%)	17,82,82	1.88	4 (23%)
23	CLA	b	605	2	59,73,73	1.94	14 (23%)	67,113,113	2.30	22 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	512	3	59,73,73	1.96	12 (20%)	67,113,113	2.25	21 (31%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	4 (6%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.57	13 (23%)
25	BCR	C	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.64	13 (23%)
32	LMT	D	404	-	36,36,36	0.43	0	47,47,47	1.09	4 (8%)
23	CLA	C	513	3	59,73,73	2.01	13 (22%)	67,113,113	2.28	20 (29%)
34	HTG	b	623	-	19,19,19	1.05	2 (10%)	23,24,24	1.74	3 (13%)
33	LMG	d	412	39	51,51,55	0.88	2 (3%)	59,59,63	1.06	3 (5%)
26	SQD	a	413	-	53,54,54	1.05	3 (5%)	62,65,65	1.21	8 (12%)
23	CLA	B	604	2	59,73,73	1.87	12 (20%)	67,113,113	2.31	23 (34%)
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
27	GOL	C	523	-	5,5,5	0.47	0	5,5,5	0.13	0
31	BCT	A	348	21	0,3,3	0.00	-	0,3,3	0.00	-
35	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	1.00	5 (6%)
23	CLA	b	611	2	59,73,73	1.95	12 (20%)	67,113,113	2.32	23 (34%)
32	LMT	e	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.91	2 (4%)
26	SQD	B	620	-	53,54,54	1.02	3 (5%)	62,65,65	1.47	9 (14%)
25	BCR	d	404	-	41,41,41	1.08	1 (2%)	56,56,56	1.86	15 (26%)
32	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.92	2 (4%)
23	CLA	b	601	41	59,73,73	2.06	14 (23%)	67,113,113	2.14	21 (31%)
31	BCT	a	404	21	0,3,3	0.00	-	0,3,3	0.00	-
32	LMT	t	101	-	25,25,36	0.53	1 (4%)	30,30,47	1.03	1 (3%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.68	13 (23%)
27	GOL	B	625	-	5,5,5	0.60	0	5,5,5	0.76	0
33	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.48	8 (17%)
23	CLA	B	603	2	59,73,73	1.95	13 (22%)	67,113,113	2.50	26 (38%)
37	LHG	D	410	-	48,48,48	0.86	3 (6%)	51,54,54	0.98	3 (5%)
38	HEM	E	103	5,6	27,50,50	0.86	1 (3%)	17,82,82	2.54	3 (17%)
37	LHG	d	407	-	48,48,48	0.87	3 (6%)	51,54,54	1.00	3 (5%)
23	CLA	B	611	2	59,73,73	1.99	14 (23%)	67,113,113	2.25	23 (34%)
23	CLA	A	406	41	59,73,73	1.95	13 (22%)	67,113,113	2.13	24 (35%)
23	CLA	C	504	3	59,73,73	1.94	13 (22%)	67,113,113	2.17	22 (32%)
27	GOL	a	412	-	5,5,5	0.33	0	5,5,5	0.47	0
24	PHO	a	353	-	67,69,69	2.14	16 (23%)	85,99,99	2.03	22 (25%)
32	LMT	a	414	-	36,36,36	0.55	1 (2%)	47,47,47	1.10	4 (8%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	509	3	59,73,73	2.05	12 (20%)	67,113,113	2.32	22 (32%)
29	PL9	D	408	-	55,55,55	0.65	1 (1%)	68,69,69	1.77	17 (25%)
37	LHG	D	409	-	48,48,48	0.90	3 (6%)	51,54,54	1.17	6 (11%)
37	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	7 (12%)
24	PHO	a	408	-	67,69,69	2.02	17 (25%)	85,99,99	2.02	24 (28%)
23	CLA	a	406	41	59,73,73	1.99	12 (20%)	67,113,113	2.24	22 (32%)
32	LMT	b	621	-	25,25,36	0.48	0	30,30,47	0.72	0
24	PHO	A	407	-	67,69,69	2.06	17 (25%)	85,99,99	2.02	23 (27%)
27	GOL	a	418	-	5,5,5	0.36	0	5,5,5	0.68	0
25	BCR	K	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.62	12 (21%)
35	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	1.04	6 (7%)
23	CLA	B	615	2	59,73,73	1.93	11 (18%)	67,113,113	2.21	24 (35%)
25	BCR	b	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.52	13 (23%)
25	BCR	B	617	-	41,41,41	1.01	1 (2%)	56,56,56	1.56	10 (17%)
23	CLA	B	602	2	59,73,73	2.02	12 (20%)	67,113,113	2.36	27 (40%)
34	HTG	B	622	-	19,19,19	1.03	1 (5%)	23,24,24	1.54	5 (21%)
23	CLA	B	605	2	59,73,73	1.92	12 (20%)	67,113,113	2.40	27 (40%)
23	CLA	c	511	3	59,73,73	1.94	13 (22%)	67,113,113	2.27	25 (37%)
34	HTG	d	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.68	1 (5%)
23	CLA	A	408	1	59,73,73	2.01	14 (23%)	67,113,113	2.24	26 (38%)
32	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.10	3 (6%)
23	CLA	D	405	4	59,73,73	1.91	12 (20%)	67,113,113	2.31	24 (35%)
23	CLA	B	609	2	59,73,73	1.97	13 (22%)	67,113,113	2.15	19 (28%)
23	CLA	b	608	2	59,73,73	2.04	13 (22%)	67,113,113	2.19	26 (38%)
23	CLA	B	606	2	59,73,73	1.88	13 (22%)	67,113,113	2.44	25 (37%)
26	SQD	A	410	-	53,54,54	0.94	3 (5%)	62,65,65	1.94	12 (19%)
23	CLA	C	514	3	59,73,73	2.00	12 (20%)	67,113,113	2.14	23 (34%)
23	CLA	a	407	41	59,73,73	1.95	12 (20%)	67,113,113	2.21	23 (34%)
23	CLA	C	509	3	59,73,73	2.04	13 (22%)	67,113,113	2.30	22 (32%)
23	CLA	C	506	3	59,73,73	1.91	13 (22%)	67,113,113	2.26	22 (32%)
23	CLA	c	505	41	59,73,73	2.01	15 (25%)	67,113,113	2.21	25 (37%)
34	HTG	D	414	-	16,16,19	1.03	2 (12%)	20,21,24	1.60	1 (5%)
34	HTG	C	522	-	19,19,19	0.93	1 (5%)	23,24,24	1.41	2 (8%)
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	c	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.16	5 (8%)
23	CLA	b	612	2	59,73,73	1.98	15 (25%)	67,113,113	2.34	20 (29%)
23	CLA	B	601	41	59,73,73	2.05	13 (22%)	67,113,113	2.22	23 (34%)
33	LMG	a	419	-	51,51,55	0.91	2 (3%)	59,59,63	1.13	5 (8%)
23	CLA	c	507	3	59,73,73	2.00	13 (22%)	67,113,113	2.22	22 (32%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.44	10 (17%)
32	LMT	A	359	-	36,36,36	0.58	1 (2%)	47,47,47	0.87	1 (2%)
35	DGD	c	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.06	6 (7%)
23	CLA	b	615	2	59,73,73	1.95	12 (20%)	67,113,113	2.13	21 (31%)
23	CLA	b	607	41	59,73,73	1.92	13 (22%)	67,113,113	2.16	22 (32%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.52	6 (10%)
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.15	5 (11%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.26	4 (6%)
23	CLA	B	616	2	59,73,73	1.98	13 (22%)	67,113,113	2.17	20 (29%)
23	CLA	C	503	3	59,73,73	1.95	13 (22%)	67,113,113	2.18	21 (31%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	5 (8%)
23	CLA	C	502	3	59,73,73	1.92	13 (22%)	67,113,113	2.24	22 (32%)
23	CLA	C	510	3	59,73,73	2.04	15 (25%)	67,113,113	2.17	23 (34%)
23	CLA	b	604	2	59,73,73	1.92	12 (20%)	67,113,113	2.29	21 (31%)
29	PL9	A	414	-	55,55,55	0.63	1 (1%)	68,69,69	2.00	23 (33%)
23	CLA	A	405	41	59,73,73	2.00	12 (20%)	67,113,113	2.29	25 (37%)
27	GOL	B	624	-	5,5,5	0.36	0	5,5,5	0.54	0
29	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.99	21 (30%)
23	CLA	D	406	4	59,73,73	1.99	13 (22%)	67,113,113	2.19	22 (32%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.56	9 (14%)
25	BCR	B	618	-	41,41,41	0.92	1 (2%)	56,56,56	1.62	16 (28%)
40	HEC	v	202	16	26,50,50	1.58	4 (15%)	18,82,82	1.87	6 (33%)
23	CLA	c	503	3	59,73,73	1.93	13 (22%)	67,113,113	2.20	22 (32%)
23	CLA	c	502	3	59,73,73	1.99	13 (22%)	67,113,113	2.19	24 (35%)
23	CLA	c	510	3	59,73,73	2.04	12 (20%)	67,113,113	2.30	26 (38%)
23	CLA	C	505	41	59,73,73	1.96	13 (22%)	67,113,113	2.25	23 (34%)
37	LHG	D	411	-	48,48,48	0.89	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	b	603	2	59,73,73	2.02	13 (22%)	67,113,113	2.43	25 (37%)
23	CLA	d	403	4	59,73,73	1.99	13 (22%)	67,113,113	2.18	27 (40%)
32	LMT	m	103	-	36,36,36	0.47	0	47,47,47	0.92	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	D	407	-	41,41,41	1.04	1 (2%)	56,56,56	1.92	16 (28%)
23	CLA	c	513	3	59,73,73	1.99	12 (20%)	67,113,113	2.31	24 (35%)
27	GOL	v	201	-	5,5,5	0.40	0	5,5,5	0.36	0
23	CLA	C	507	3	59,73,73	1.97	14 (23%)	67,113,113	2.25	27 (40%)
26	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.70	13 (20%)
26	SQD	A	412	-	53,54,54	1.01	3 (5%)	62,65,65	1.20	9 (14%)
25	BCR	t	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.74	15 (26%)
23	CLA	b	616	2	59,73,73	1.95	12 (20%)	67,113,113	2.28	22 (32%)
23	CLA	B	608	2	59,73,73	1.94	14 (23%)	67,113,113	2.28	24 (35%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.19	6 (10%)
23	CLA	b	613	2	59,73,73	2.02	15 (25%)	67,113,113	2.31	24 (35%)
23	CLA	c	514	3	59,73,73	1.99	13 (22%)	67,113,113	2.13	23 (34%)
27	GOL	A	411	-	5,5,5	0.39	0	5,5,5	0.22	0
23	CLA	B	614	2	59,73,73	1.94	13 (22%)	67,113,113	2.45	24 (35%)
23	CLA	c	506	3	59,73,73	1.92	12 (20%)	67,113,113	2.20	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
32	LMT	b	627	-	-	8/17/37/61	0/1/1/2
23	CLA	b	610	41	3/3/20/25	7/37/135/135	-
33	LMG	z	101	-	-	8/34/54/70	0/1/1/1
23	CLA	C	512	3	3/3/20/25	4/37/135/135	-
40	HEC	V	202	16	-	0/6/54/54	-
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
23	CLA	B	612	2	3/3/20/25	4/37/135/135	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	C	511	3	3/3/20/25	12/37/135/135	-
23	CLA	B	610	41	3/3/20/25	5/37/135/135	-
37	LHG	L	101	-	-	19/53/53/53	-
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
23	CLA	c	508	41	3/3/20/25	6/37/135/135	-
23	CLA	B	607	41	3/3/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	517	-	-	13/51/91/95	0/2/2/2
23	CLA	b	609	2	2/2/20/25	7/37/135/135	-
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
23	CLA	b	606	2	3/3/20/25	10/37/135/135	-
32	LMT	t	102	-	-	5/17/38/61	0/1/1/2
27	GOL	V	201	-	-	2/4/4/4	-
23	CLA	a	405	1	3/3/20/25	2/37/135/135	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2
34	HTG	b	625	-	-	4/10/30/30	0/1/1/1
34	HTG	c	522	-	-	4/10/30/30	0/1/1/1
33	LMG	D	415	39	-	10/46/66/70	0/1/1/1
34	HTG	b	622	-	-	4/10/30/30	0/1/1/1
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	b	614	2	3/3/20/25	13/37/135/135	-
32	LMT	a	420	-	-	4/21/61/61	0/2/2/2
37	LHG	d	406	-	-	6/53/53/53	-
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
23	CLA	a	409	1	3/3/20/25	11/37/135/135	-
35	DGD	h	102	-	-	9/51/91/95	0/2/2/2
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
35	DGD	c	518	-	-	12/51/91/95	0/2/2/2
23	CLA	d	402	4	1/1/20/25	3/37/135/135	-
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
26	SQD	F	101	-	-	13/38/58/69	0/1/1/1
37	LHG	d	408	-	-	15/53/53/53	-
25	BCR	c	516	-	-	3/29/63/63	0/2/2/2
34	HTG	D	414	-	-	0/7/27/30	0/1/1/1
23	CLA	C	508	41	3/3/20/25	6/37/135/135	-
27	GOL	b	624	-	-	0/4/4/4	-
35	DGD	c	517	-	-	21/51/91/95	0/2/2/2
23	CLA	b	602	2	2/2/20/25	3/37/135/135	-
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	504	3	3/3/20/25	2/37/135/135	-
23	CLA	B	613	2	3/3/20/25	7/37/135/135	-
23	CLA	C	503	3	3/3/20/25	7/37/135/135	-
34	HTG	B	623	-	-	4/10/30/30	0/1/1/1
27	GOL	c	501	-	-	0/4/4/4	-
23	CLA	A	404	1	3/3/20/25	3/37/135/135	-
38	HEM	e	87	5,6	-	1/6/54/54	-
24	PHO	A	407	-	-	3/53/103/103	0/5/6/6
23	CLA	c	512	3	3/3/20/25	5/37/135/135	-
33	LMG	B	621	-	-	15/46/66/70	0/1/1/1
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
25	BCR	C	516	-	-	1/29/63/63	0/2/2/2
32	LMT	D	404	-	-	7/21/61/61	0/2/2/2
23	CLA	C	513	3	3/3/20/25	11/37/135/135	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
33	LMG	d	412	39	-	7/46/66/70	0/1/1/1
26	SQD	a	413	-	-	18/49/69/69	0/1/1/1
23	CLA	B	604	2	3/3/20/25	8/37/135/135	-
35	DGD	C	518	-	-	17/51/91/95	0/2/2/2
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	b	611	2	3/3/20/25	4/37/135/135	-
35	DGD	H	102	-	-	13/51/91/95	0/2/2/2
32	LMT	e	102	-	-	7/21/61/61	0/2/2/2
26	SQD	B	620	-	-	18/49/69/69	0/1/1/1
25	BCR	d	404	-	-	6/29/63/63	0/2/2/2
32	LMT	M	103	-	-	10/21/61/61	0/2/2/2
23	CLA	b	601	41	3/3/20/25	17/37/135/135	-
32	LMT	t	101	-	-	6/17/37/61	0/1/1/2
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
27	GOL	B	625	-	-	4/4/4/4	-
33	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
23	CLA	B	603	2	2/2/20/25	5/37/135/135	-
25	BCR	D	407	-	-	7/29/63/63	0/2/2/2
38	HEM	E	103	5,6	-	0/6/54/54	-
37	LHG	d	407	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	611	2	3/3/20/25	2/37/135/135	-
23	CLA	A	406	41	2/2/20/25	7/37/135/135	-
23	CLA	C	504	3	3/3/20/25	3/37/135/135	-
27	GOL	a	412	-	-	4/4/4/4	-
24	PHO	a	353	-	-	5/53/103/103	0/5/6/6
32	LMT	a	414	-	-	7/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	509	3	3/3/20/25	3/37/135/135	-
29	PL9	D	408	-	-	7/53/73/73	0/1/1/1
37	LHG	D	409	-	-	11/53/53/53	-
37	LHG	l	101	-	-	17/53/53/53	-
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	PHO	a	408	-	-	5/53/103/103	0/5/6/6
23	CLA	a	406	41	2/2/20/25	7/37/135/135	-
32	LMT	b	621	-	-	7/17/37/61	0/1/1/2
23	CLA	b	605	2	3/3/20/25	5/37/135/135	-
27	GOL	a	418	-	-	2/4/4/4	-
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
35	DGD	C	519	-	-	13/51/91/95	0/2/2/2
23	CLA	B	615	2	3/3/20/25	8/37/135/135	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	602	2	2/2/20/25	7/37/135/135	-
34	HTG	B	622	-	-	5/10/30/30	0/1/1/1
23	CLA	B	605	2	3/3/20/25	7/37/135/135	-
23	CLA	c	511	3	3/3/20/25	10/37/135/135	-
34	HTG	d	411	-	-	0/7/27/30	0/1/1/1
23	CLA	A	408	1	3/3/20/25	11/37/135/135	-
32	LMT	I	101	-	-	9/21/61/61	0/2/2/2
23	CLA	B	609	2	2/2/20/25	4/37/135/135	-
23	CLA	b	608	2	2/2/20/25	4/37/135/135	-
23	CLA	B	606	2	2/2/20/25	8/37/135/135	-
26	SQD	A	410	-	-	15/49/69/69	0/1/1/1
23	CLA	C	514	3	3/3/20/25	5/37/135/135	-
23	CLA	a	407	41	2/2/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	509	3	3/3/20/25	4/37/135/135	-
23	CLA	C	506	3	1/1/20/25	7/37/135/135	-
23	CLA	c	505	41	3/3/20/25	6/37/135/135	-
37	LHG	D	410	-	-	14/53/53/53	-
34	HTG	C	522	-	-	1/10/30/30	0/1/1/1
37	LHG	e	101	-	-	12/46/46/53	-
33	LMG	c	521	-	-	8/46/66/70	0/1/1/1
23	CLA	b	612	2	3/3/20/25	4/37/135/135	-
23	CLA	B	601	41	3/3/20/25	13/37/135/135	-
33	LMG	a	419	-	-	12/46/66/70	0/1/1/1
23	CLA	c	507	3	3/3/20/25	10/37/135/135	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
32	LMT	A	359	-	-	3/21/61/61	0/2/2/2
35	DGD	c	519	-	-	7/51/91/95	0/2/2/2
23	CLA	b	615	2	3/3/20/25	5/37/135/135	-
23	CLA	b	607	41	3/3/20/25	4/37/135/135	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
37	LHG	E	101	-	-	19/46/46/53	-
33	LMG	C	521	-	-	9/46/66/70	0/1/1/1
23	CLA	B	616	2	3/3/20/25	7/37/135/135	-
24	PHO	A	353	-	-	3/53/103/103	0/5/6/6
33	LMG	C	520	-	-	13/46/66/70	0/1/1/1
33	LMG	c	520	-	-	15/46/66/70	0/1/1/1
23	CLA	C	502	3	3/3/20/25	4/37/135/135	-
23	CLA	C	510	3	3/3/20/25	4/37/135/135	-
23	CLA	b	604	2	3/3/20/25	6/37/135/135	-
29	PL9	A	414	-	-	16/53/73/73	0/1/1/1
23	CLA	A	405	41	3/3/20/25	4/37/135/135	-
27	GOL	B	624	-	-	4/4/4/4	-
29	PL9	a	416	-	-	16/53/73/73	0/1/1/1
23	CLA	D	406	4	3/3/20/25	7/37/135/135	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
40	HEC	v	202	16	-	0/6/54/54	-
23	CLA	c	503	3	3/3/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	502	3	3/3/20/25	5/37/135/135	-
23	CLA	c	510	3	3/3/20/25	12/37/135/135	-
23	CLA	C	505	41	3/3/20/25	6/37/135/135	-
37	LHG	D	411	-	-	14/53/53/53	-
23	CLA	b	603	2	2/2/20/25	4/37/135/135	-
23	CLA	d	403	4	3/3/20/25	7/37/135/135	-
32	LMT	m	103	-	-	6/21/61/61	0/2/2/2
23	CLA	c	514	3	3/3/20/25	6/37/135/135	-
23	CLA	c	513	3	3/3/20/25	10/37/135/135	-
27	GOL	v	201	-	-	2/4/4/4	-
23	CLA	C	507	3	3/3/20/25	12/37/135/135	-
26	SQD	a	411	-	-	10/49/69/69	0/1/1/1
26	SQD	A	412	-	-	11/49/69/69	0/1/1/1
25	BCR	t	103	-	-	6/29/63/63	0/2/2/2
23	CLA	b	616	2	3/3/20/25	12/37/135/135	-
23	CLA	B	608	2	2/2/20/25	3/37/135/135	-
33	LMG	m	101	-	-	14/46/66/70	0/1/1/1
23	CLA	b	613	2	3/3/20/25	7/37/135/135	-
23	CLA	D	405	4	1/1/20/25	3/37/135/135	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	614	2	3/3/20/25	12/37/135/135	-
23	CLA	c	506	3	1/1/20/25	5/37/135/135	-

The worst 5 of 1132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3B-C2B	6.94	1.50	1.40
23	D	405	CLA	C3B-C2B	6.74	1.49	1.40
23	C	512	CLA	C3B-C2B	6.62	1.49	1.40
23	B	603	CLA	C3B-C2B	6.53	1.49	1.40
23	b	612	CLA	C3B-C2B	6.51	1.49	1.40

The worst 5 of 2350 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C4A-NA-C1A	-8.66	102.81	106.71
23	b	602	CLA	C4A-NA-C1A	-7.71	103.24	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C4A-NA-C1A	-7.67	103.26	106.71
23	C	504	CLA	C4A-NA-C1A	-7.54	103.31	106.71
38	E	103	HEM	CAD-CBD-CGD	7.42	125.12	112.67

5 of 190 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND

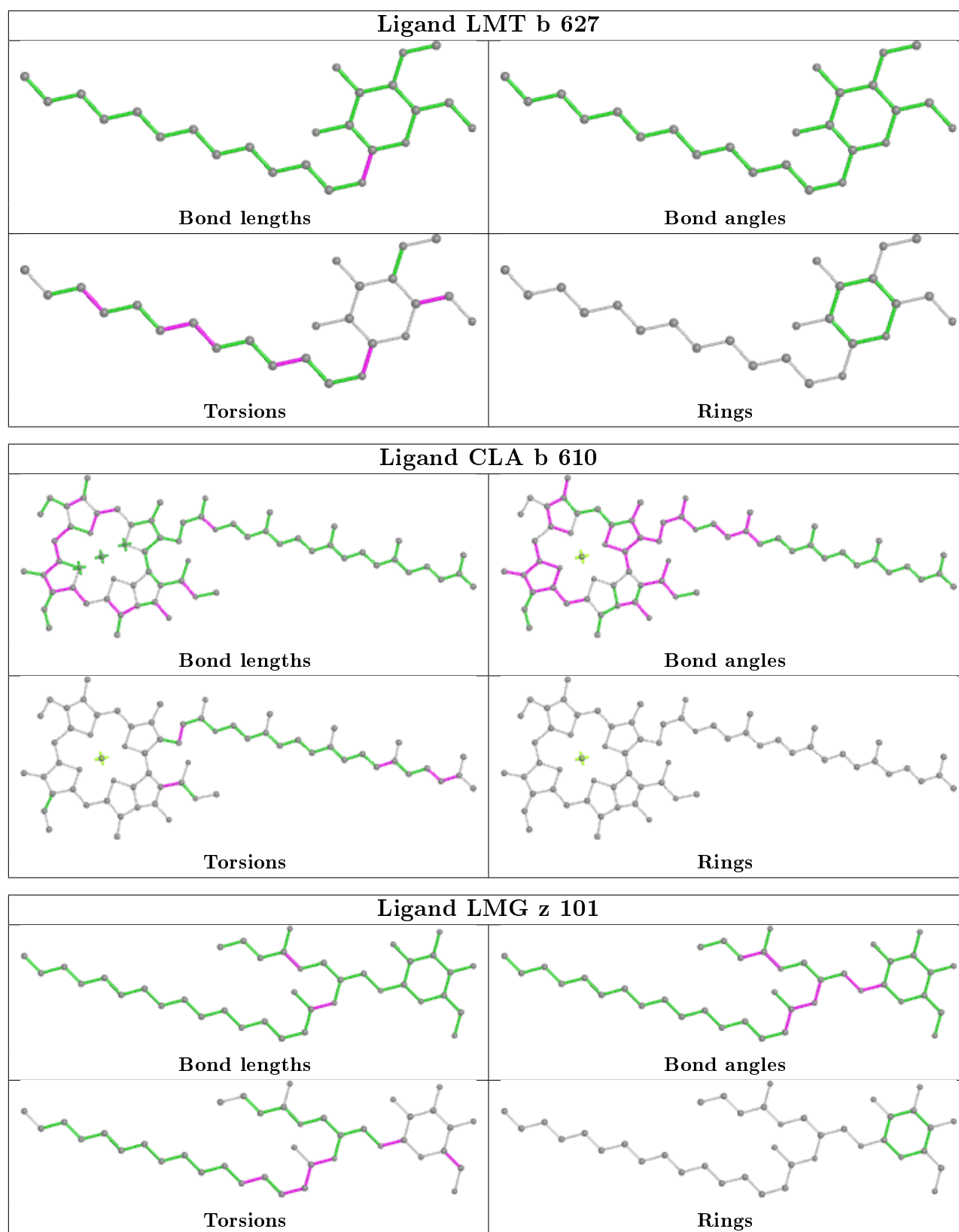
5 of 1213 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	b	627	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	O5'-C1'-O1'-C1
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	C11-C10-O7-C8
32	E	102	LMT	C2'-C1'-O1'-C1

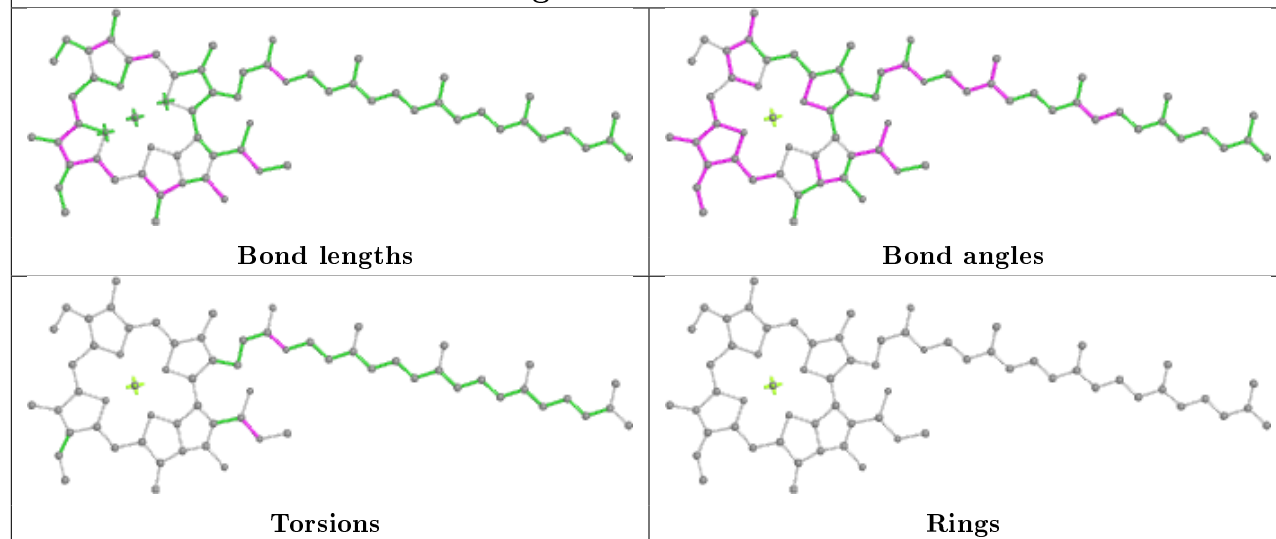
There are no ring outliers.

No monomer is involved in short contacts.

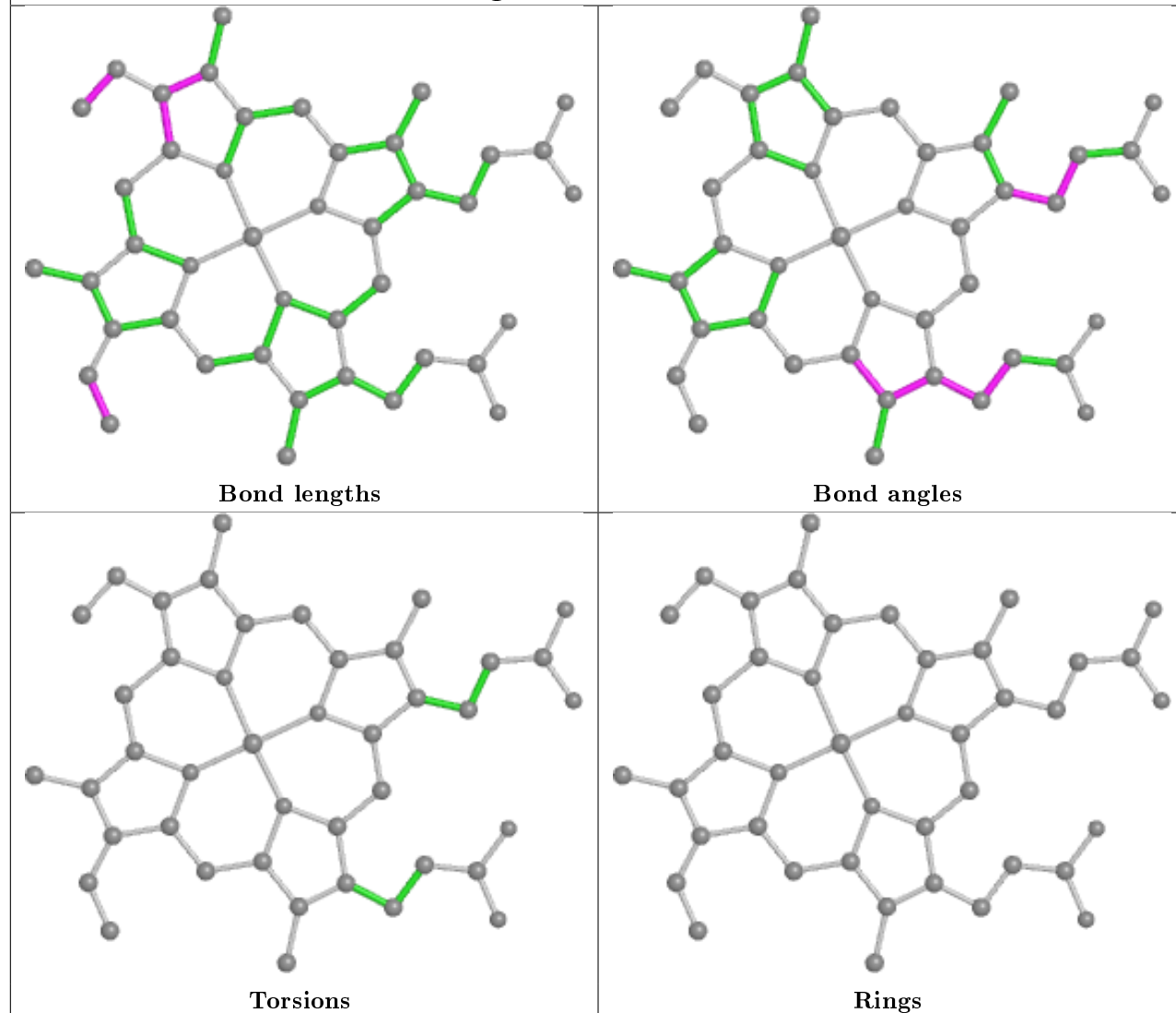
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

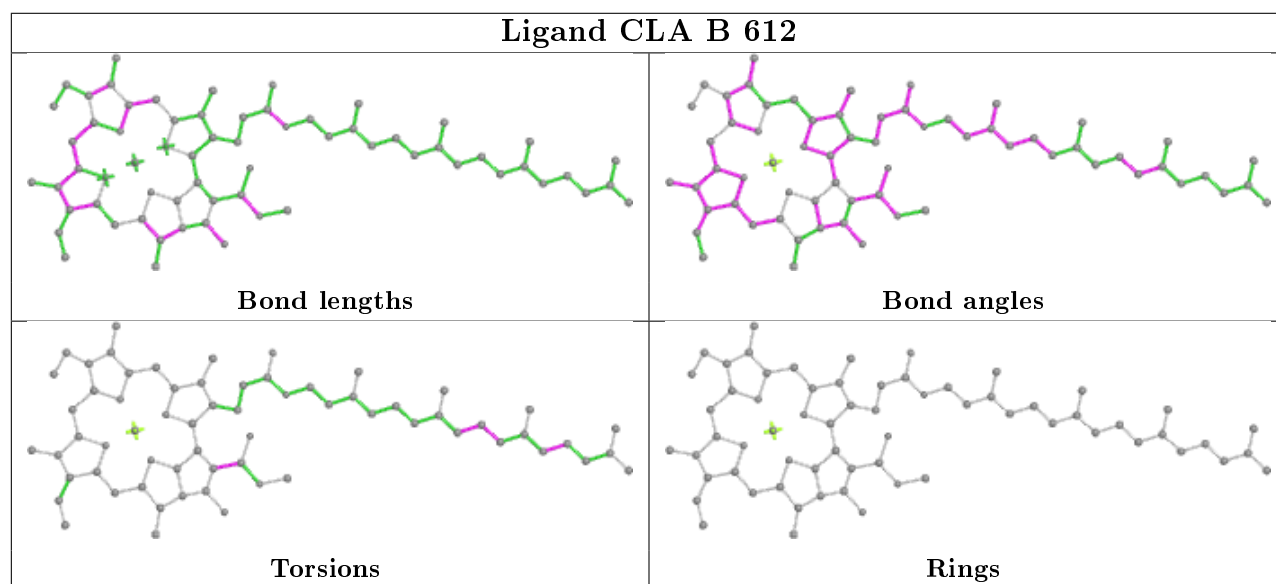
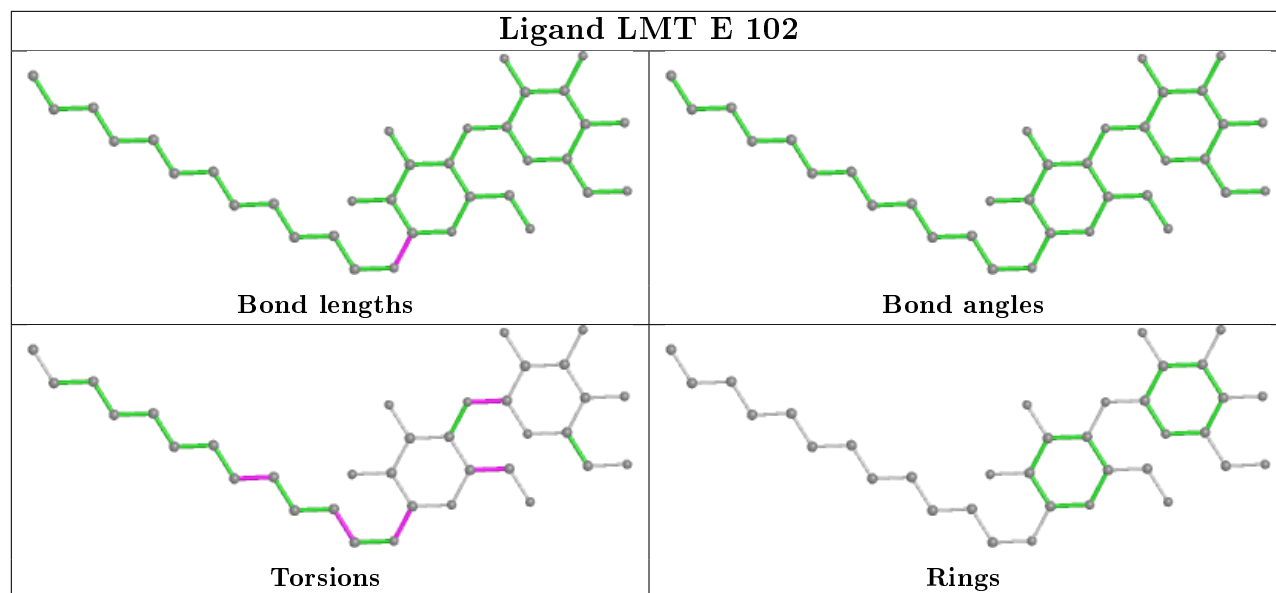


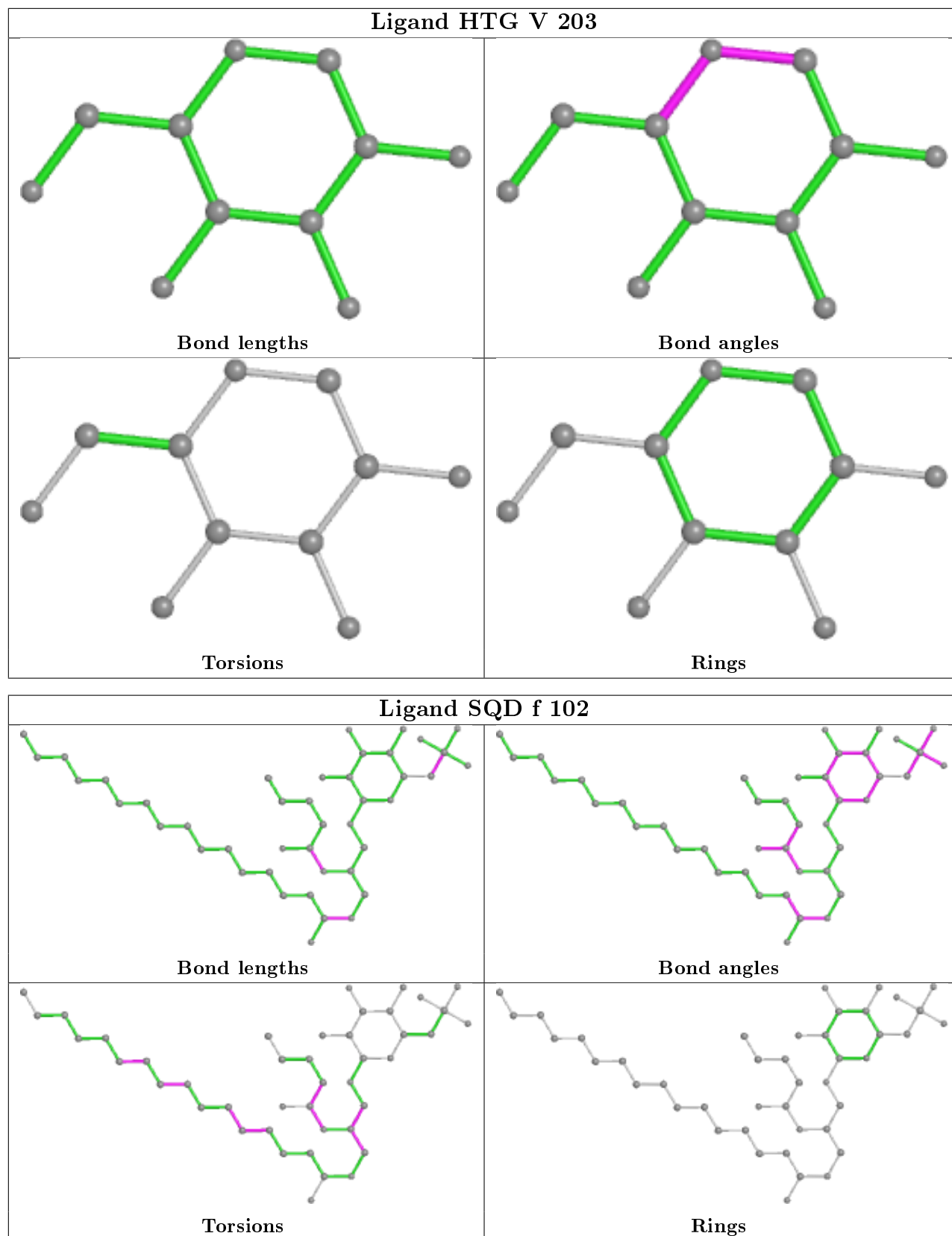
## Ligand CLA C 512

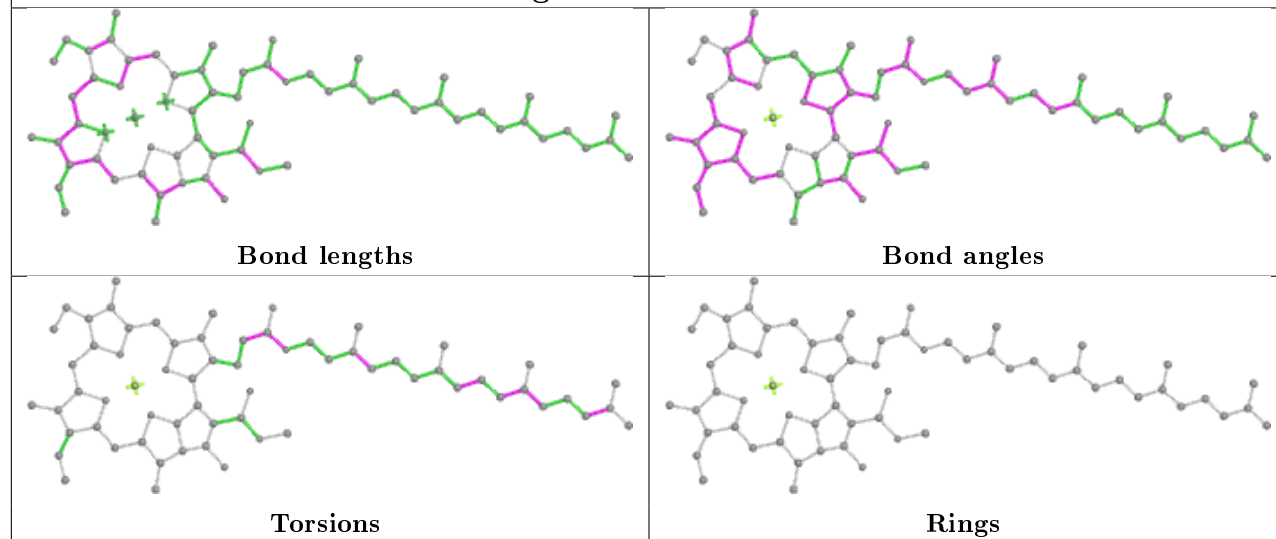
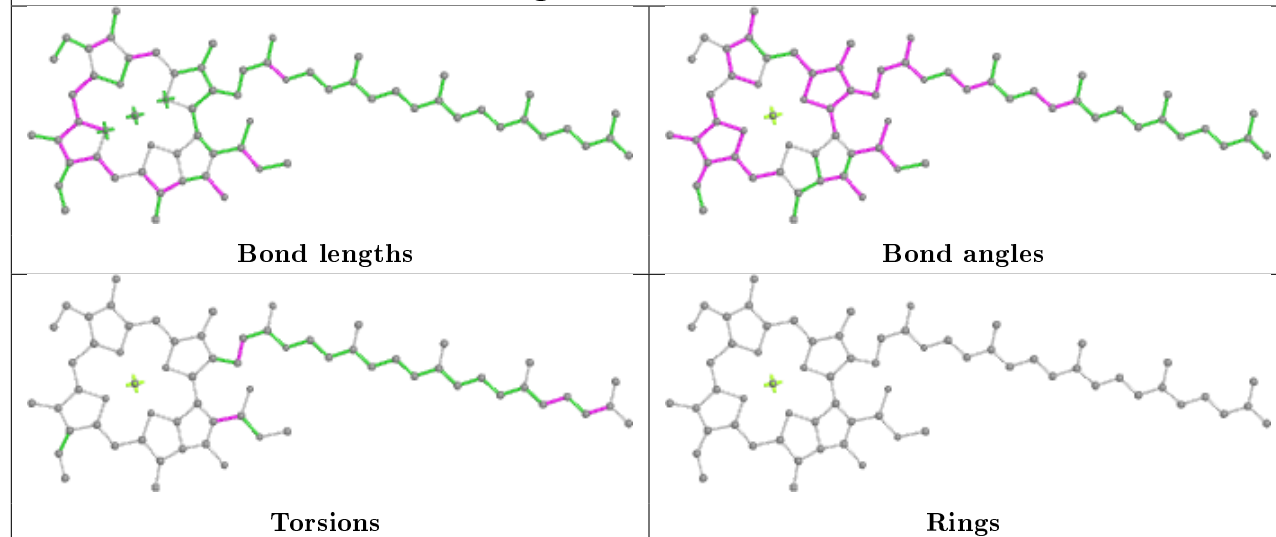


## Ligand HEC V 202

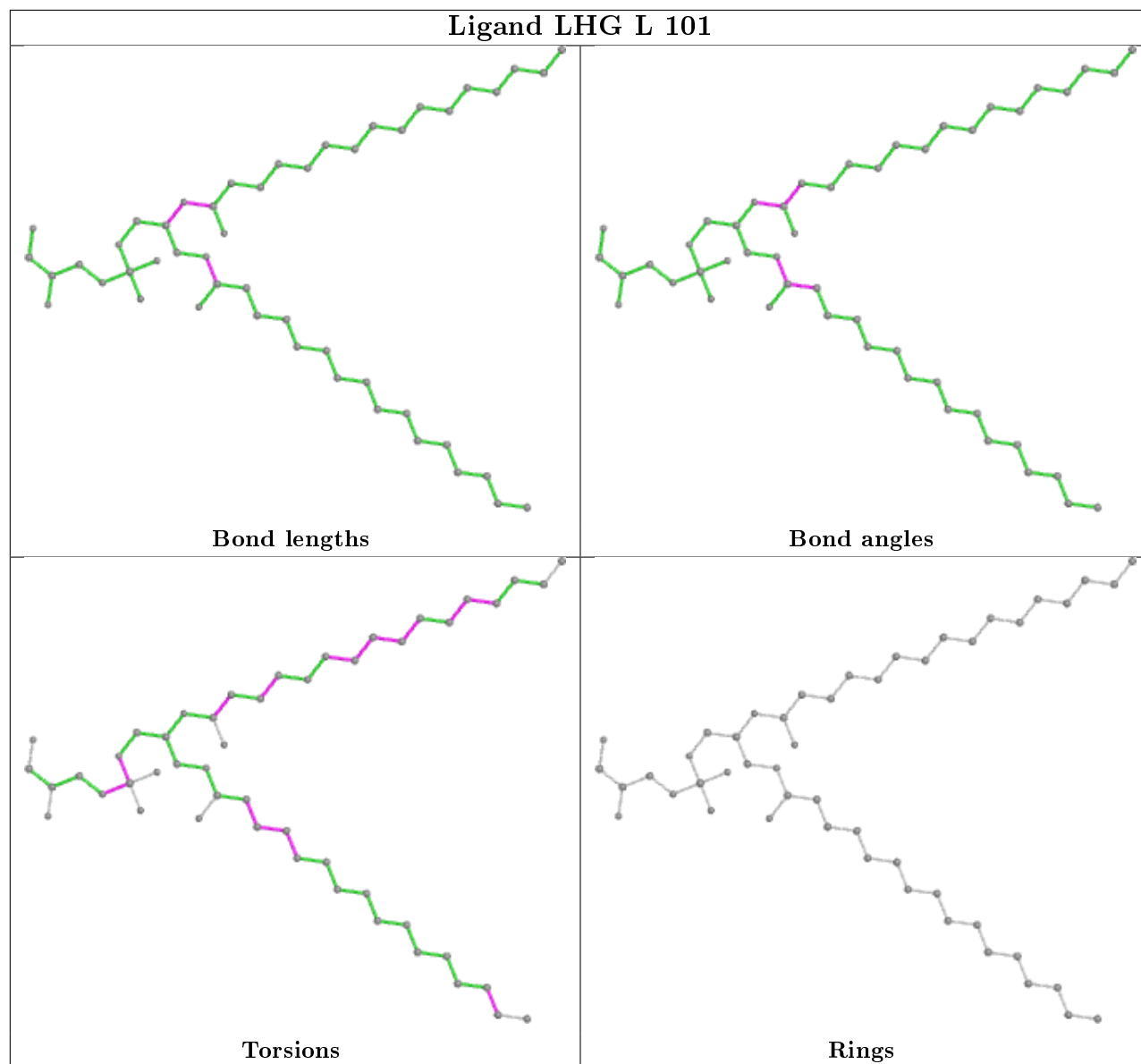




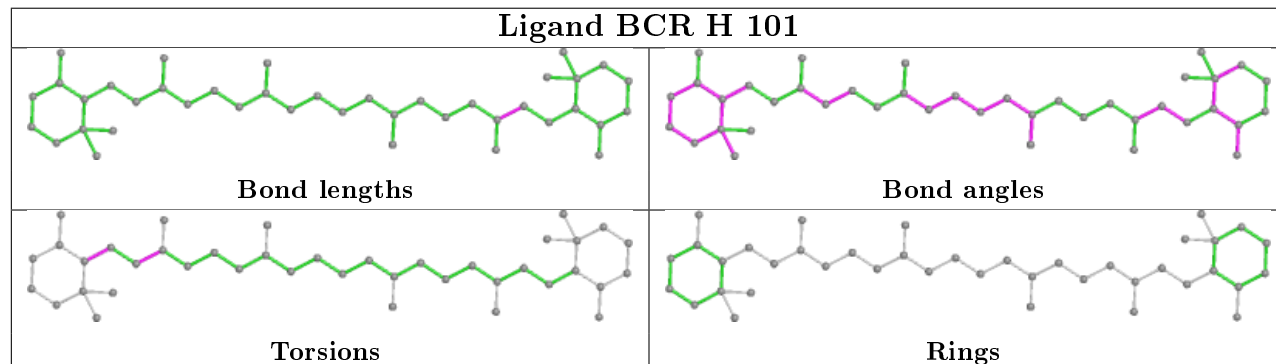


**Ligand CLA C 511****Ligand CLA B 610**

## Ligand LHG L 101

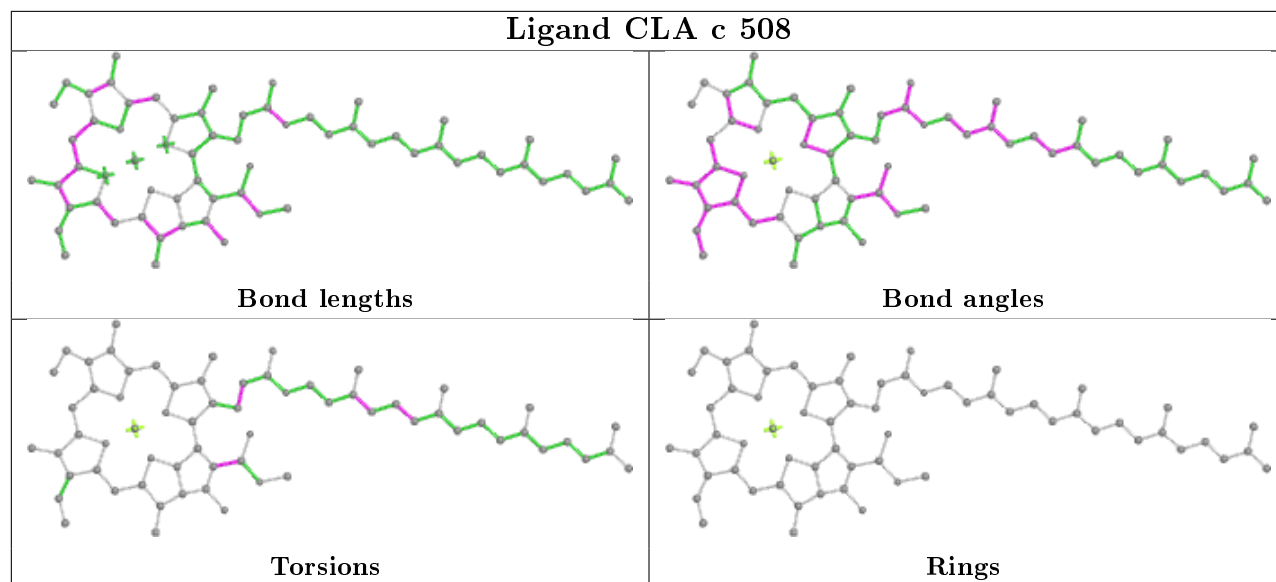


## Ligand BCR H 101

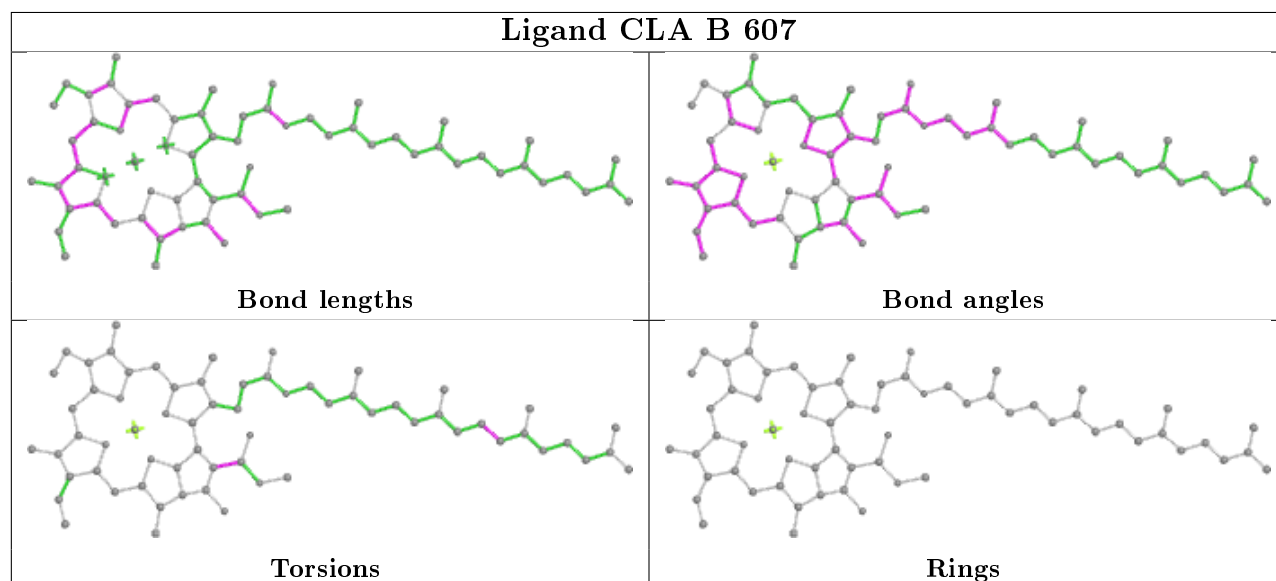




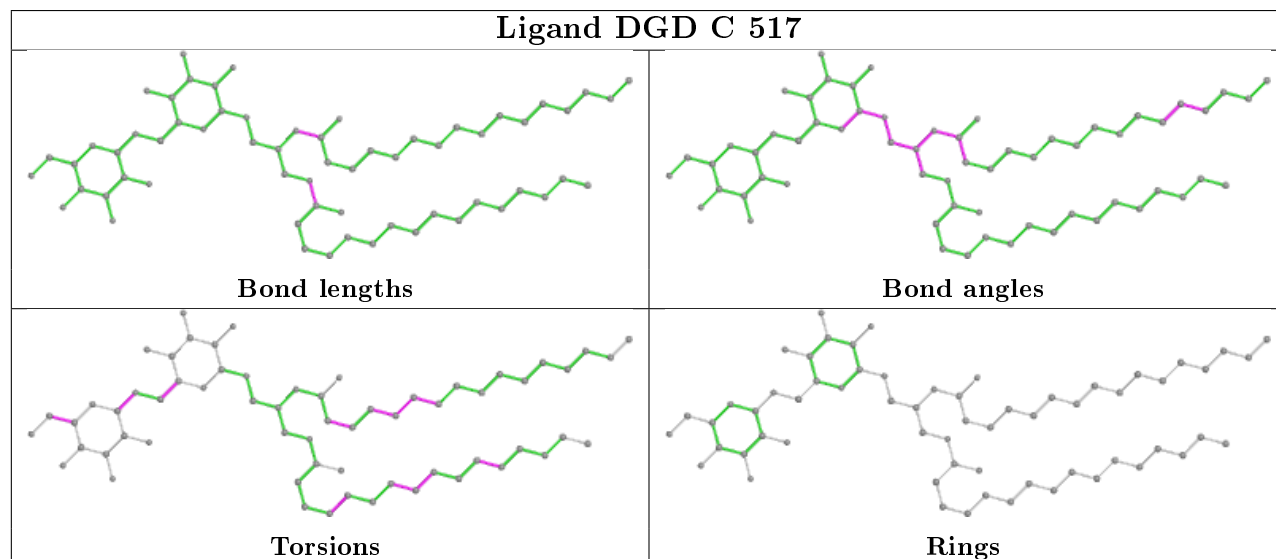
## Ligand CLA c 508

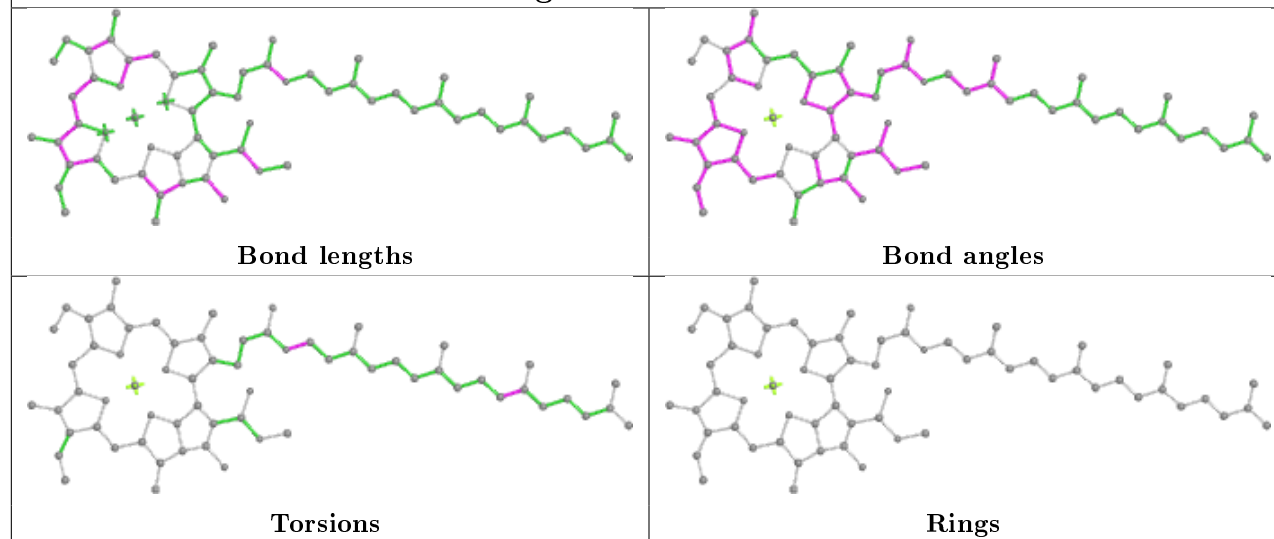
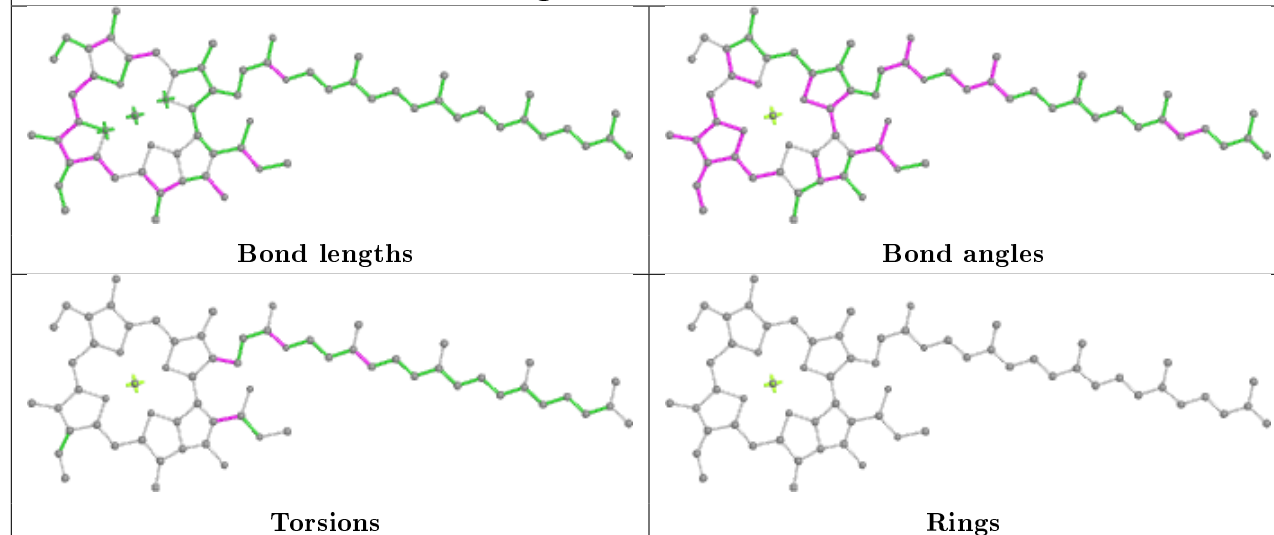
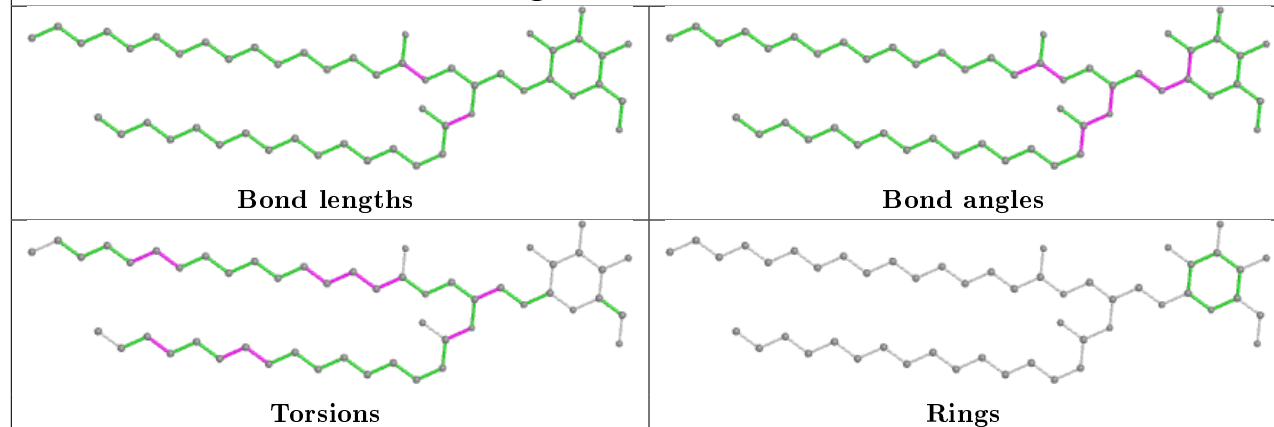


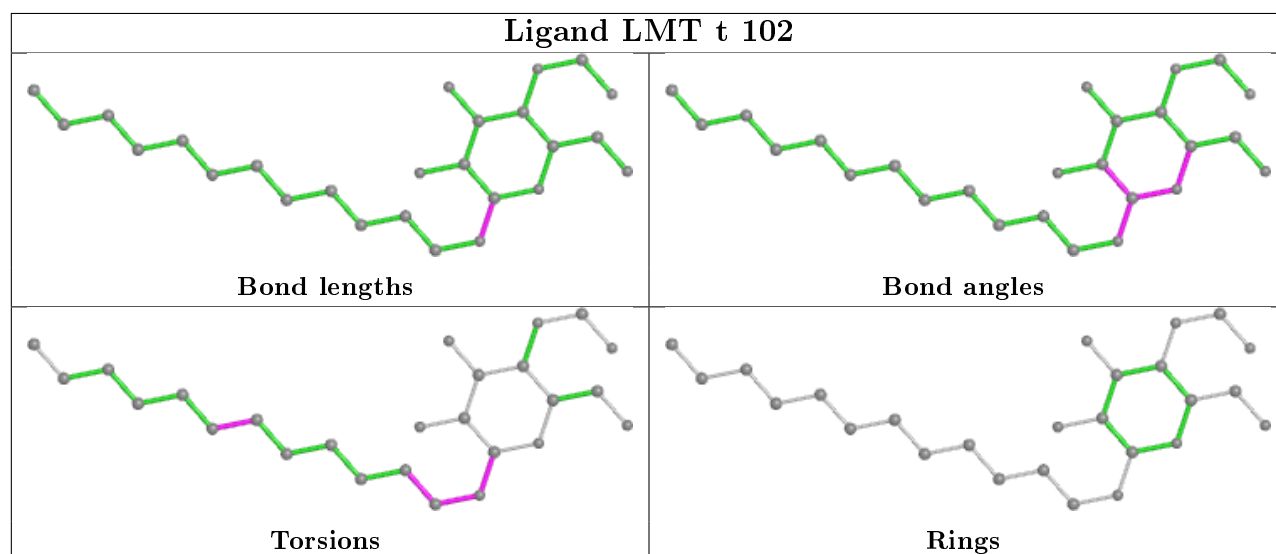
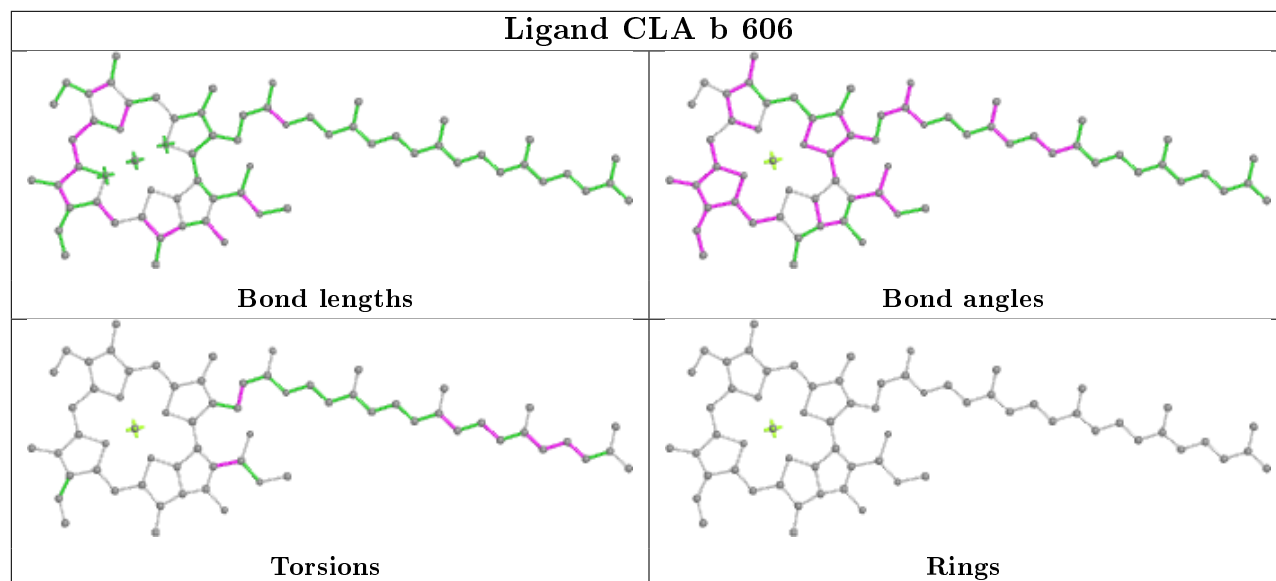
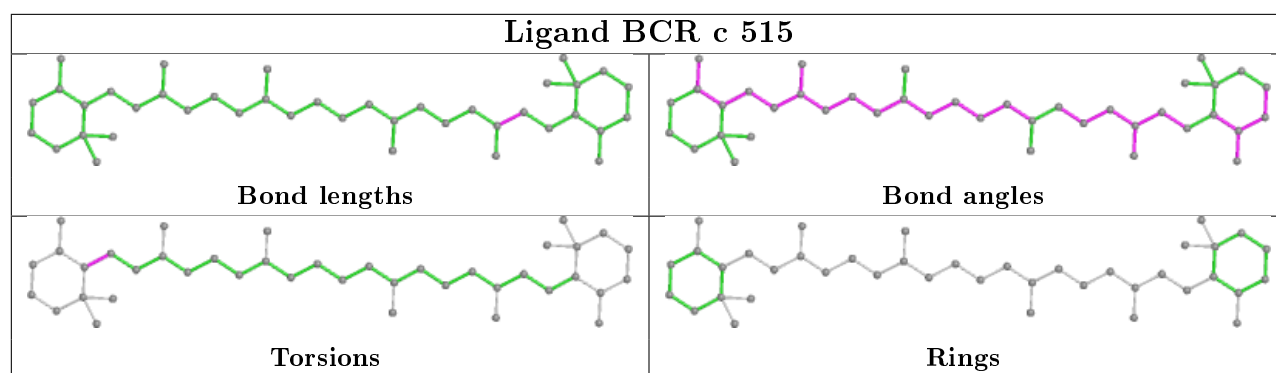
## Ligand CLA B 607

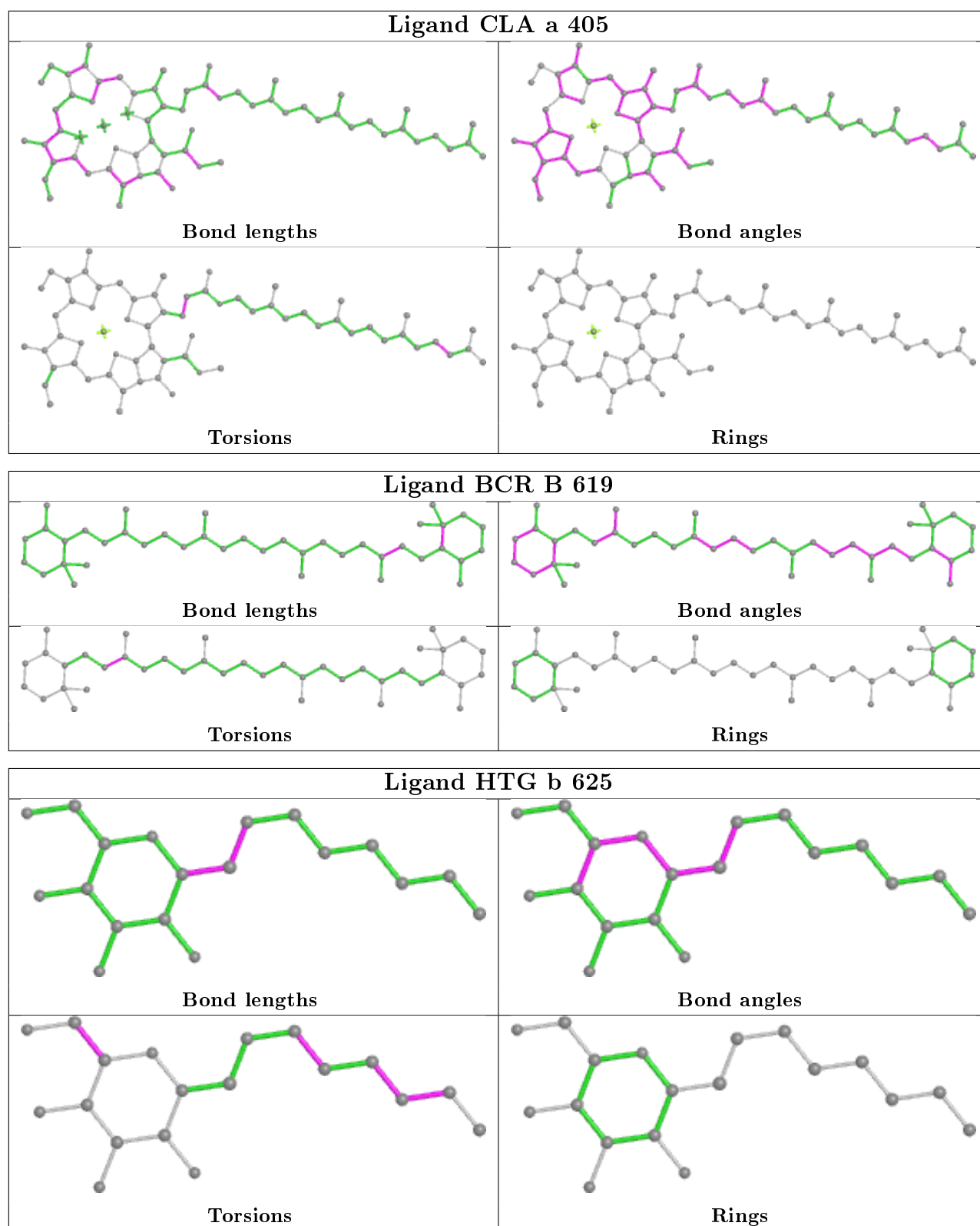


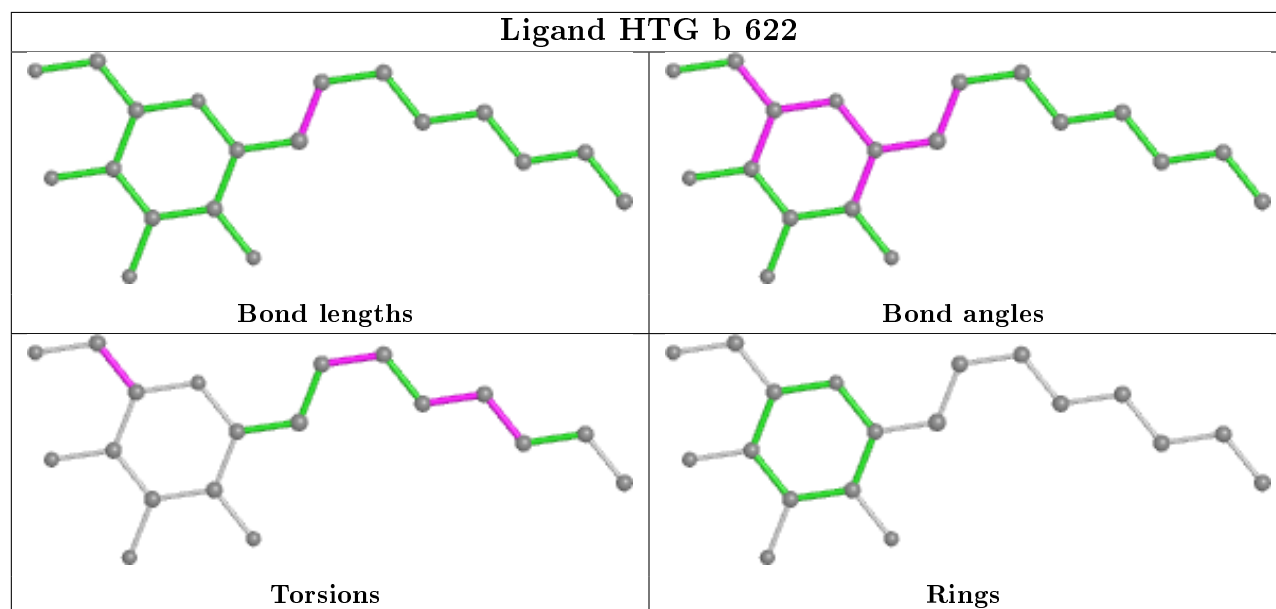
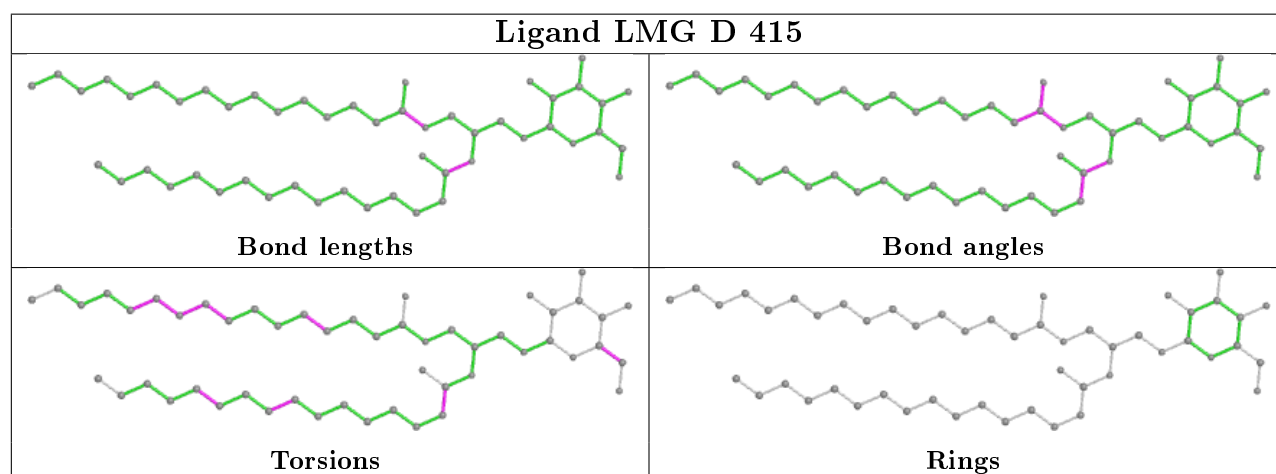
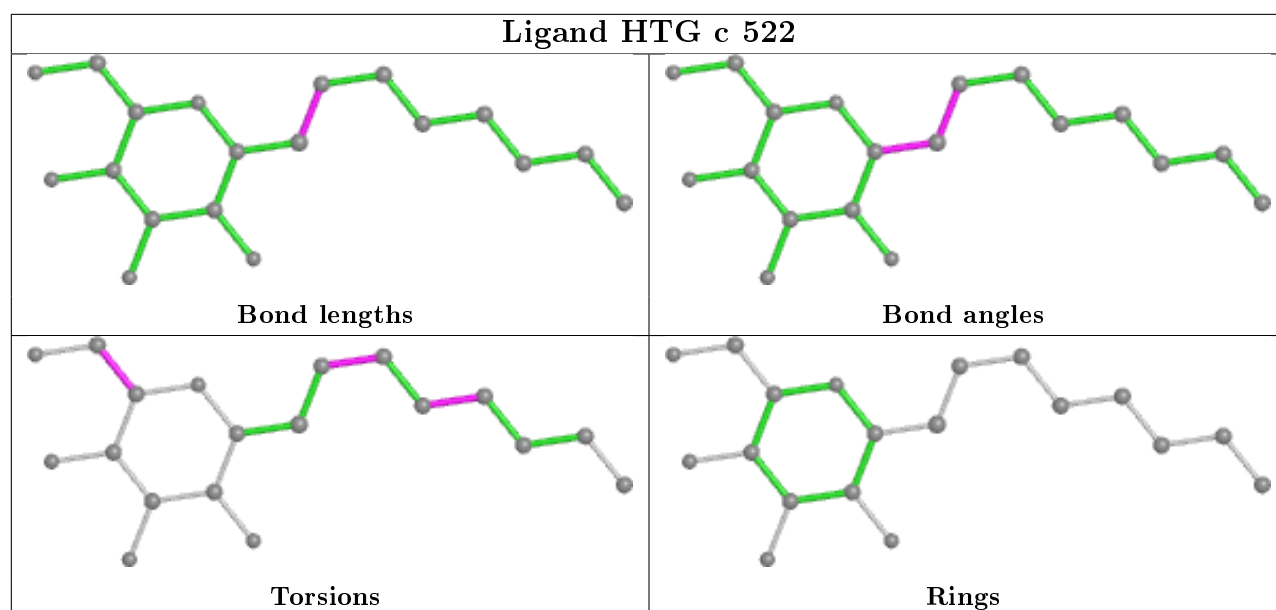
## Ligand DGD C 517



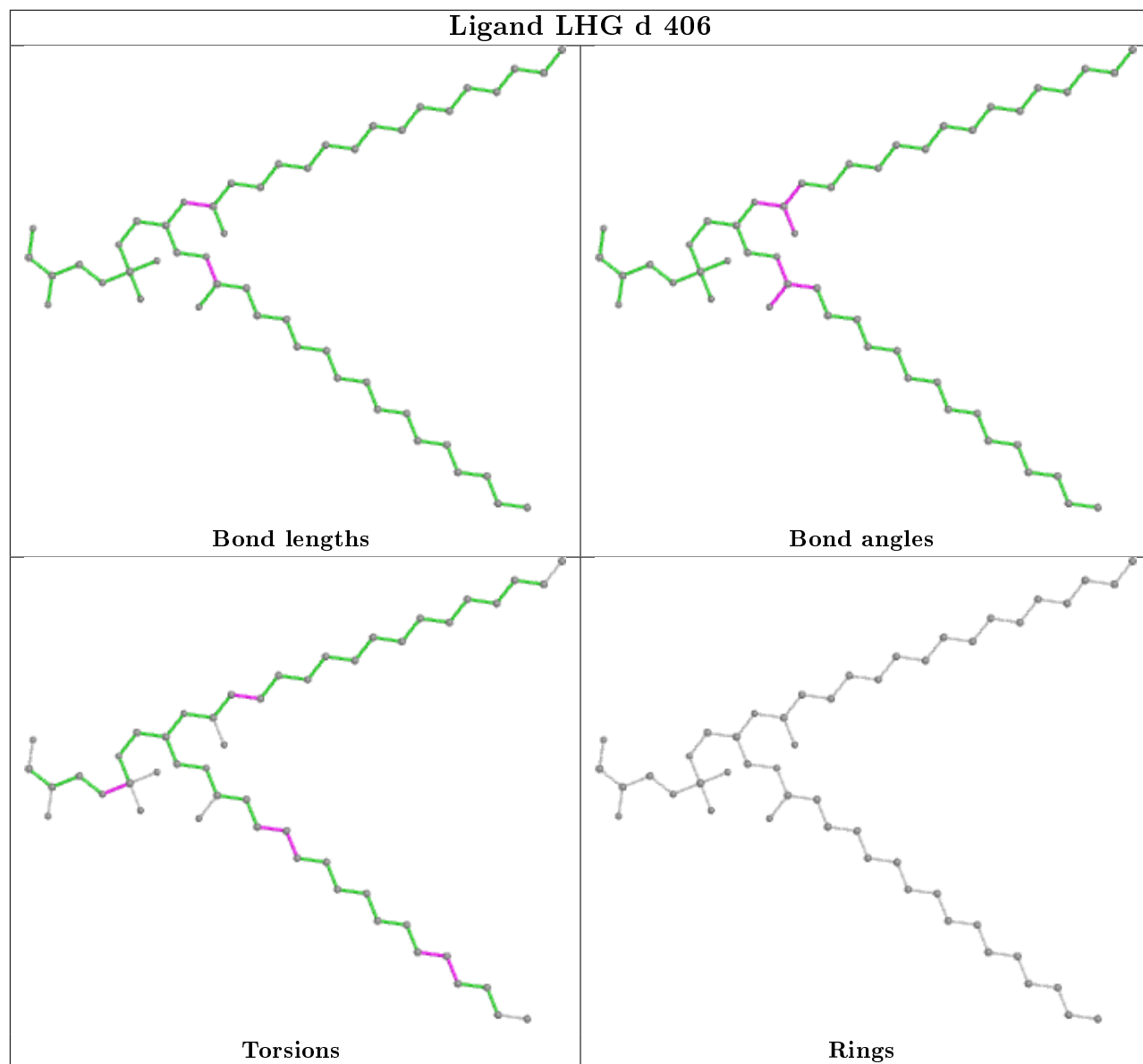
**Ligand CLA d 402****Ligand CLA b 609****Ligand LMG C 501**



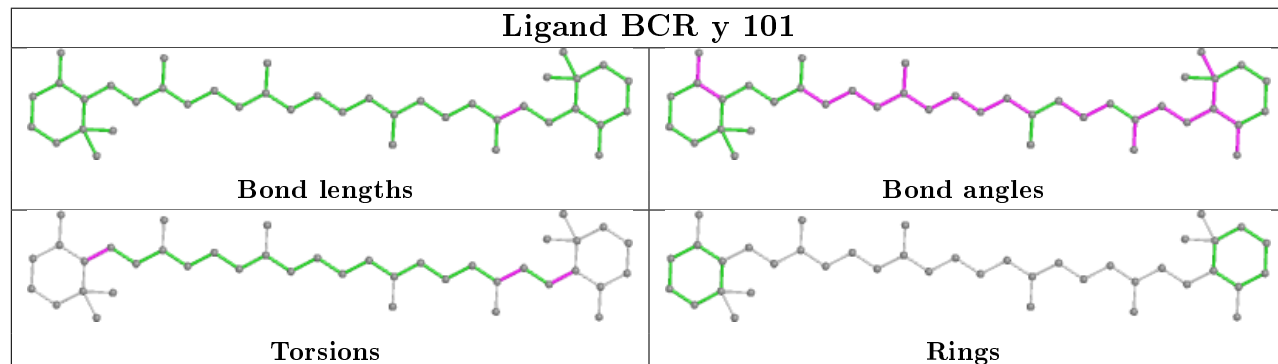




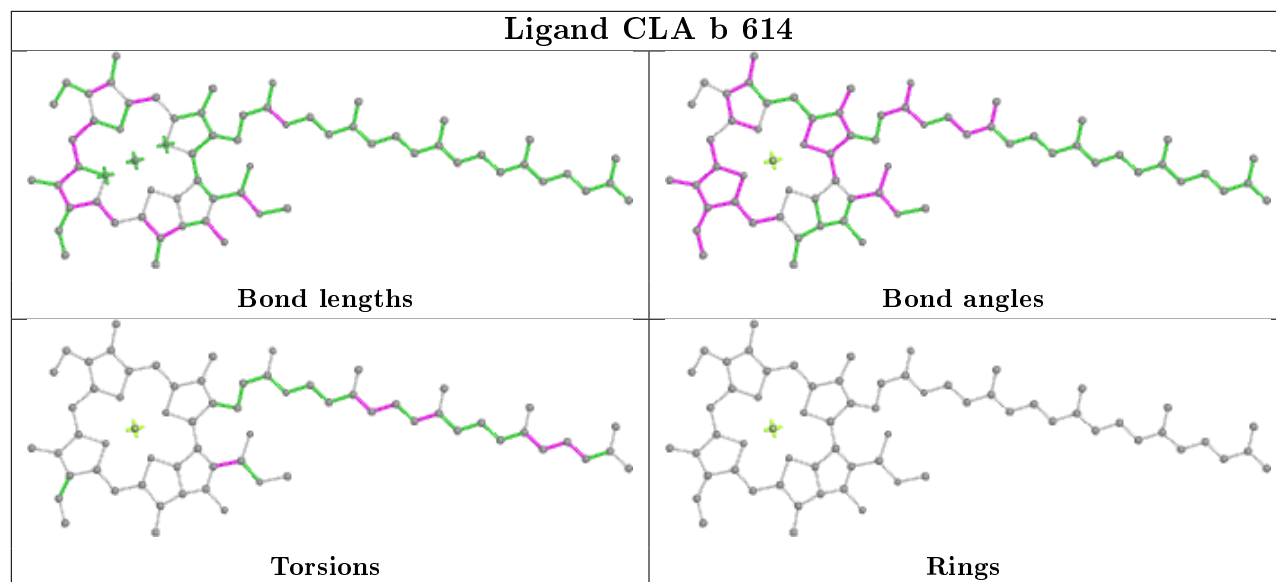
## Ligand LHG d 406



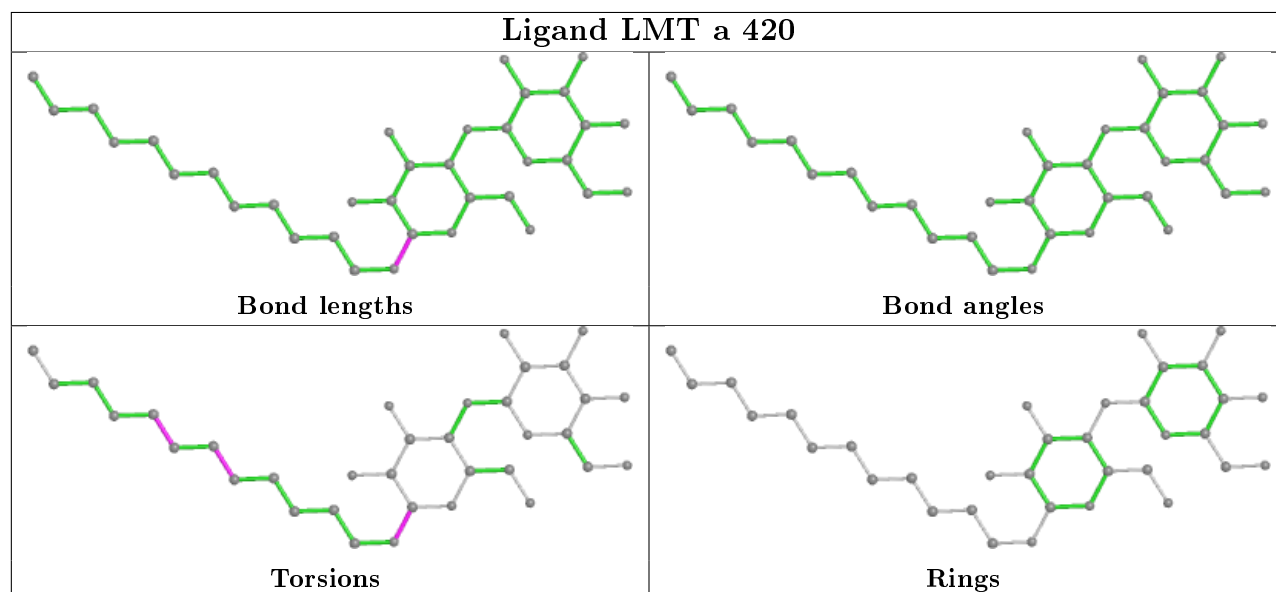
## Ligand BCR y 101



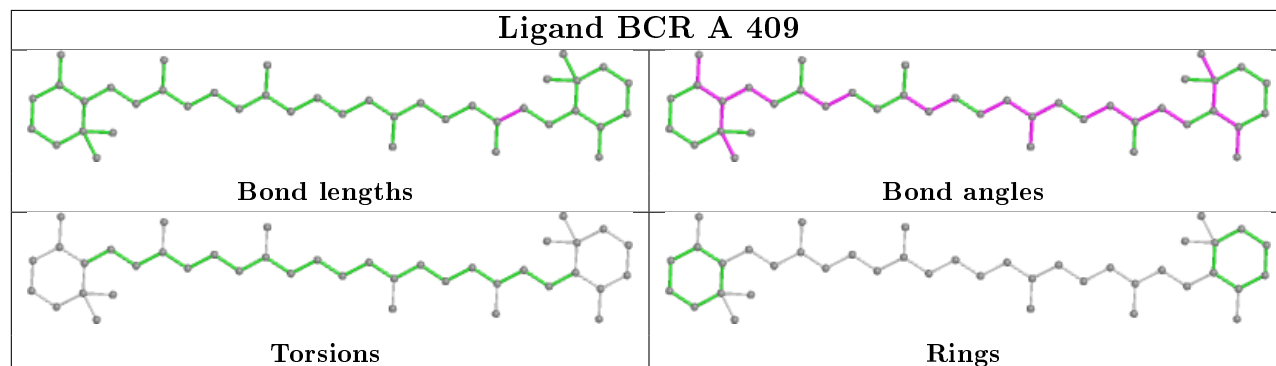
## Ligand CLA b 614

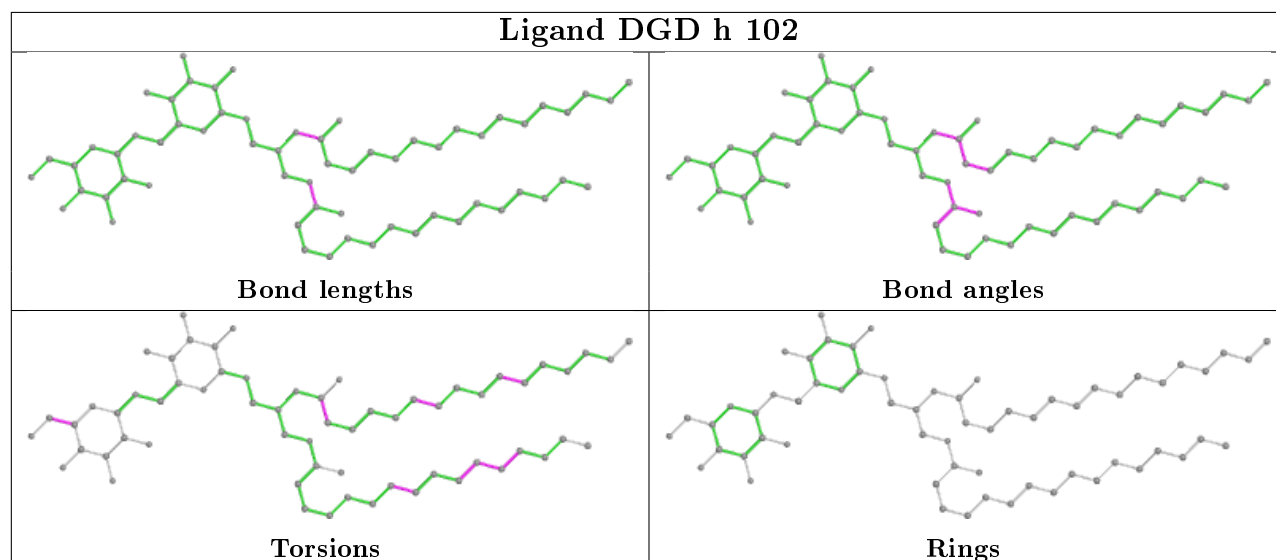
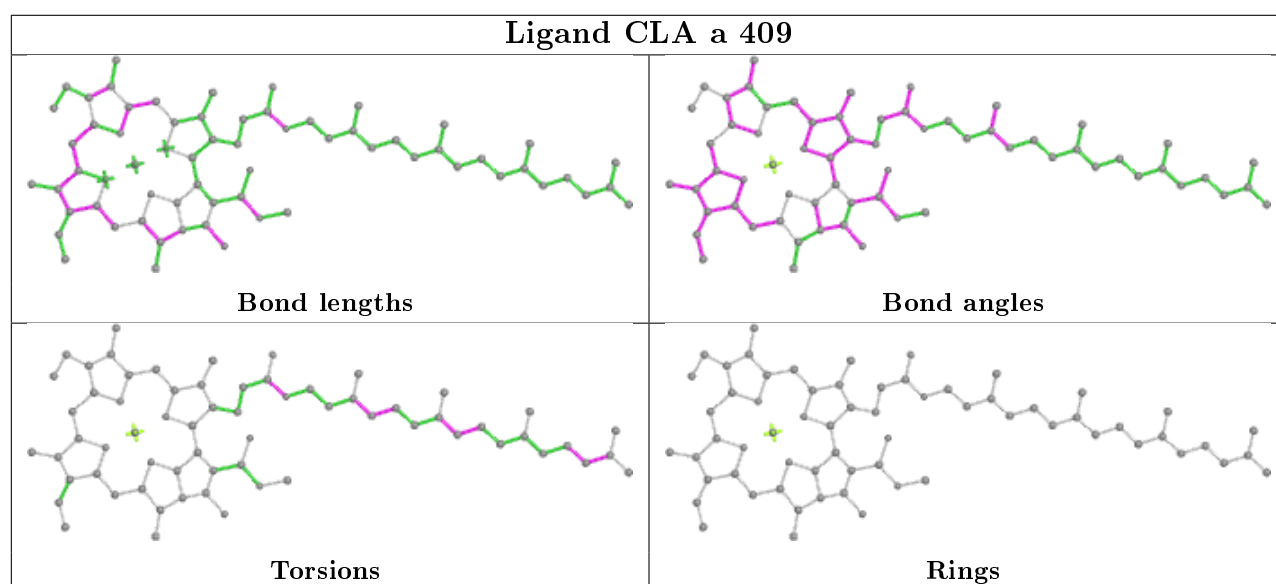
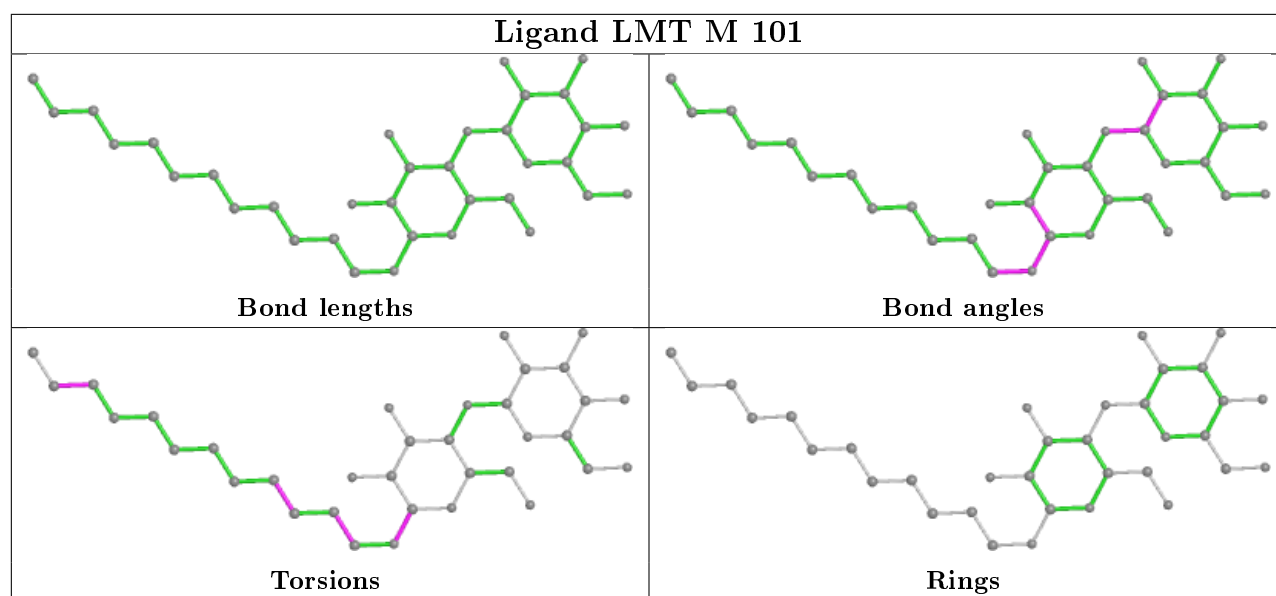


## Ligand LMT a 420

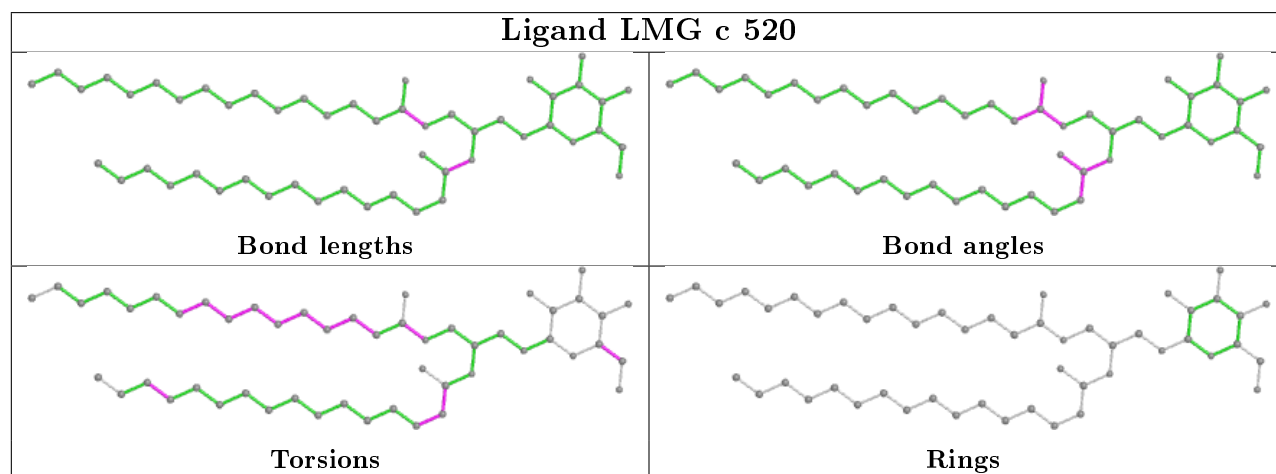
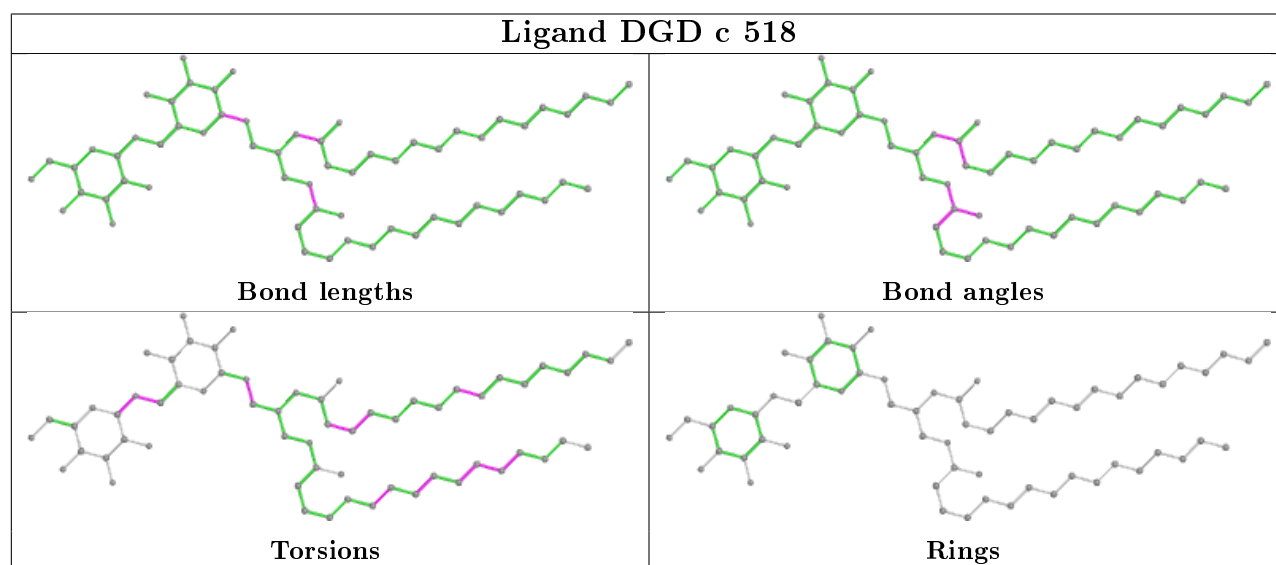
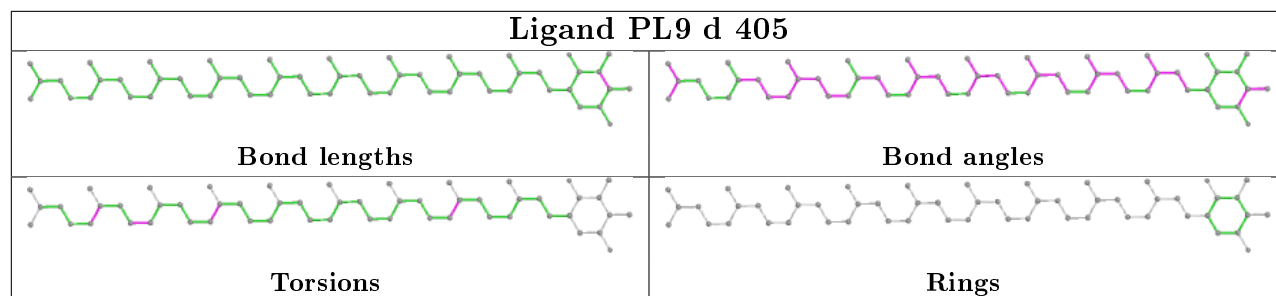
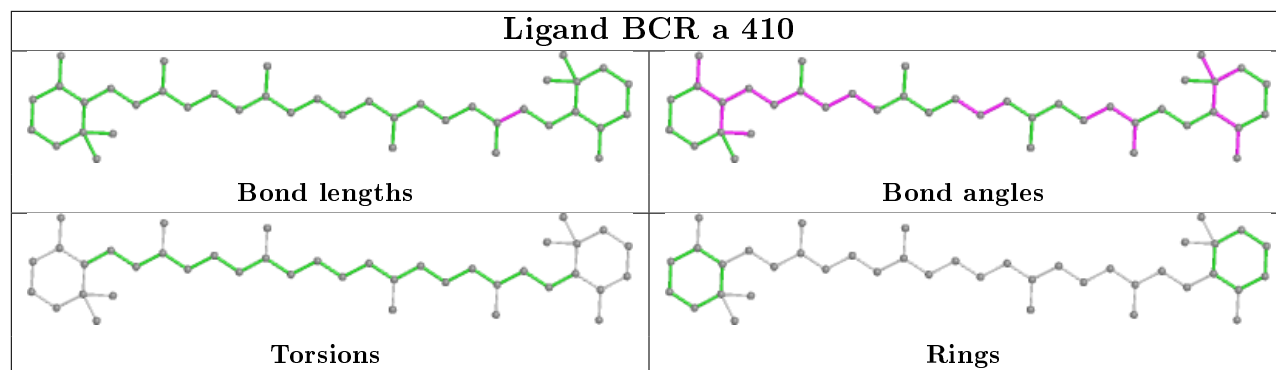


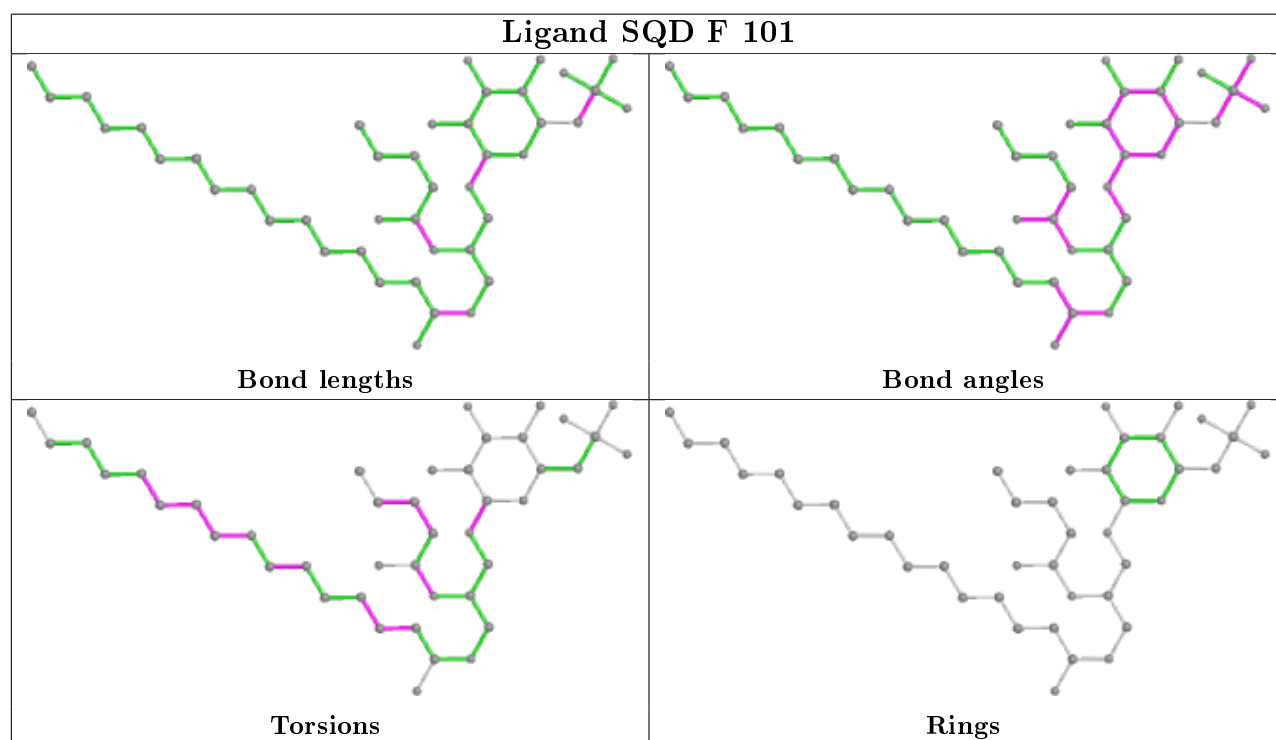
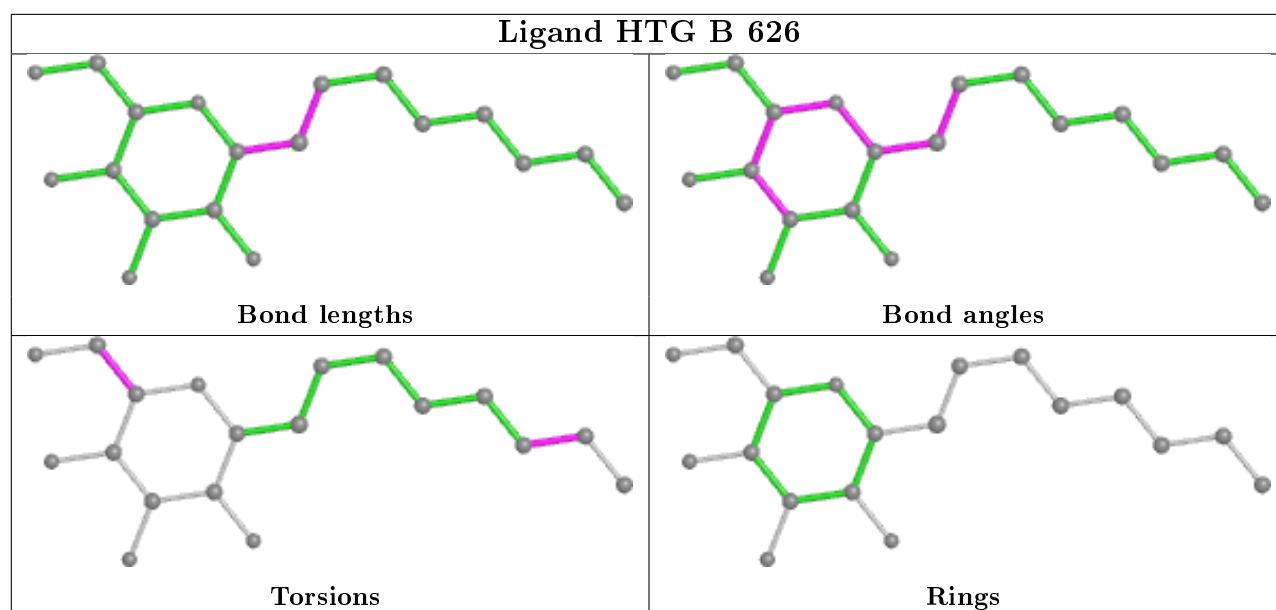
## Ligand BCR A 409



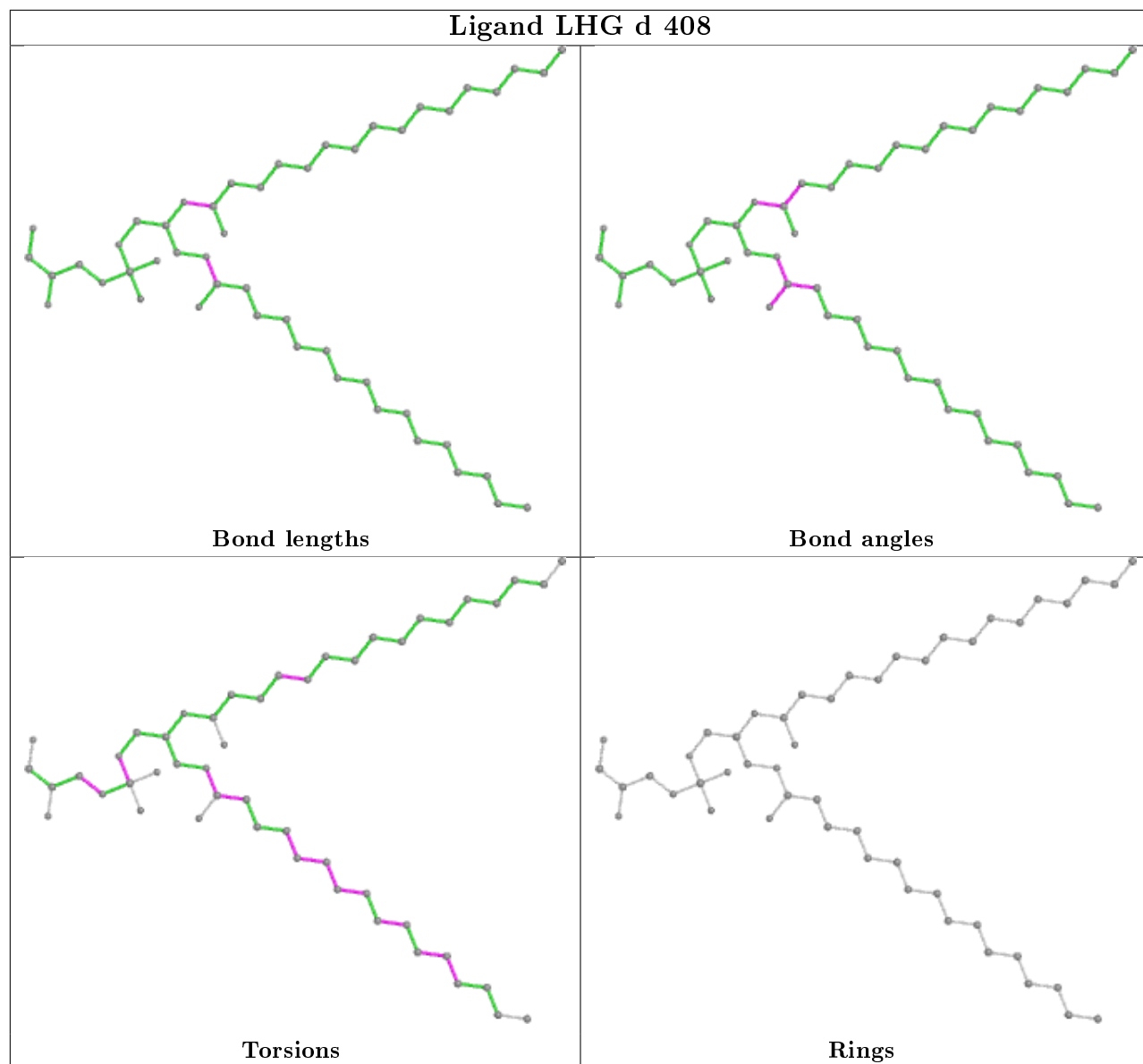




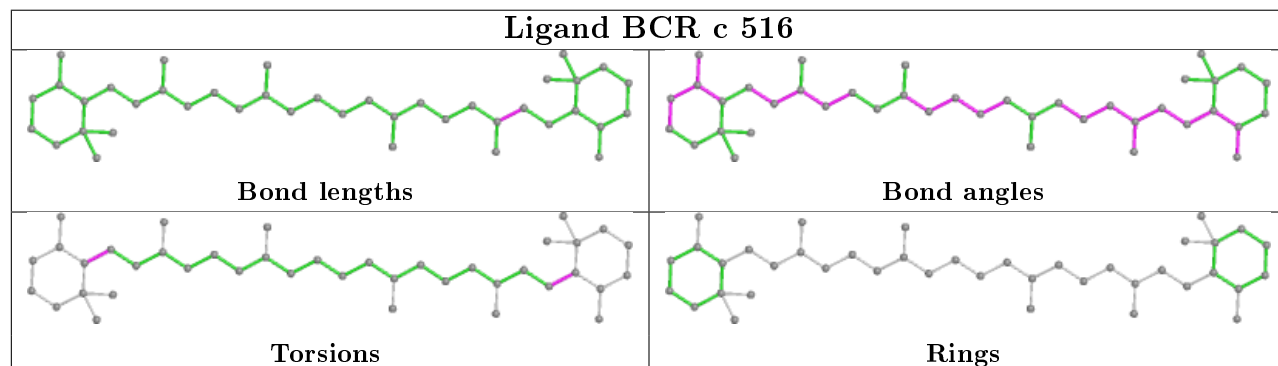


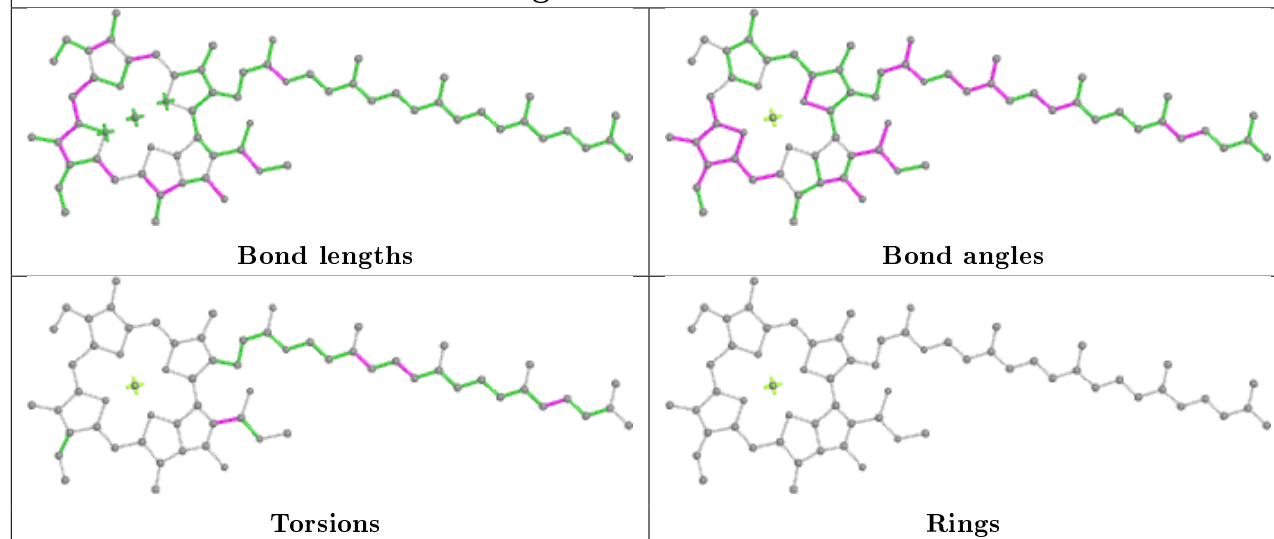
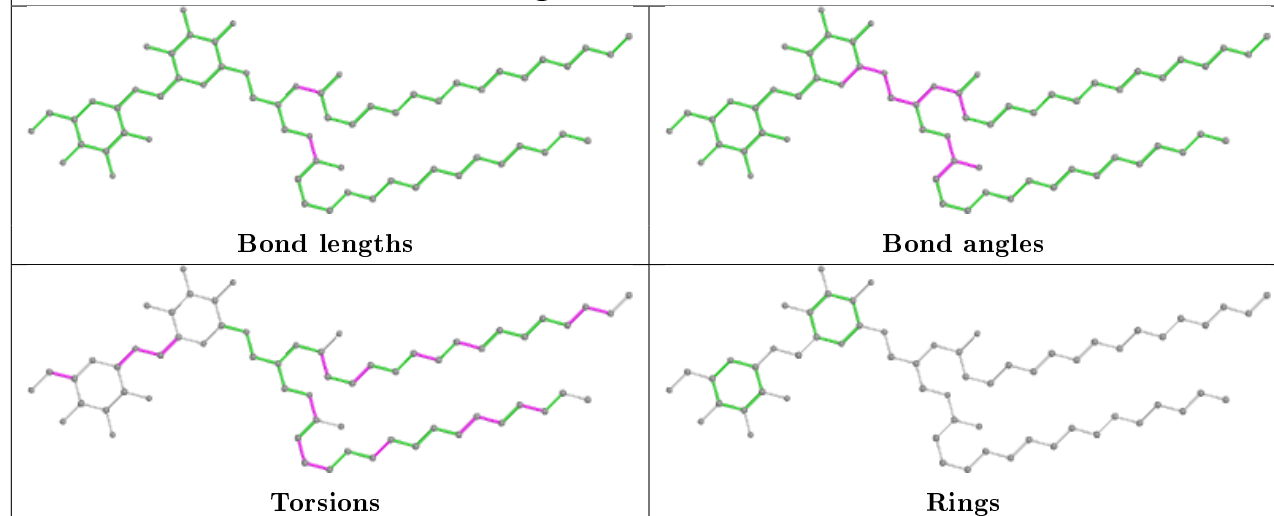
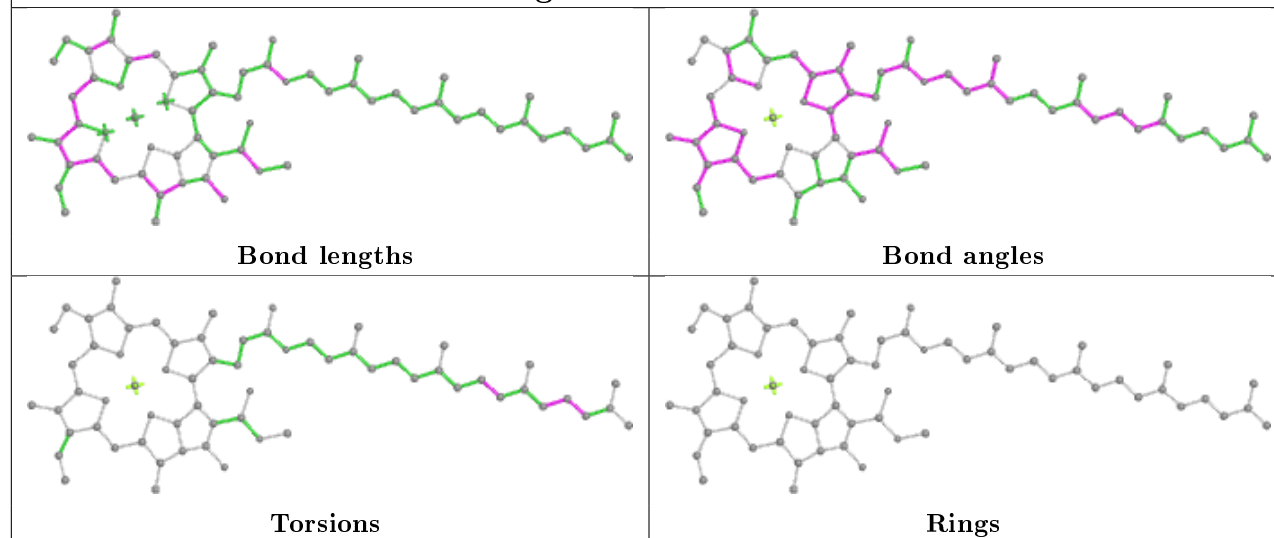


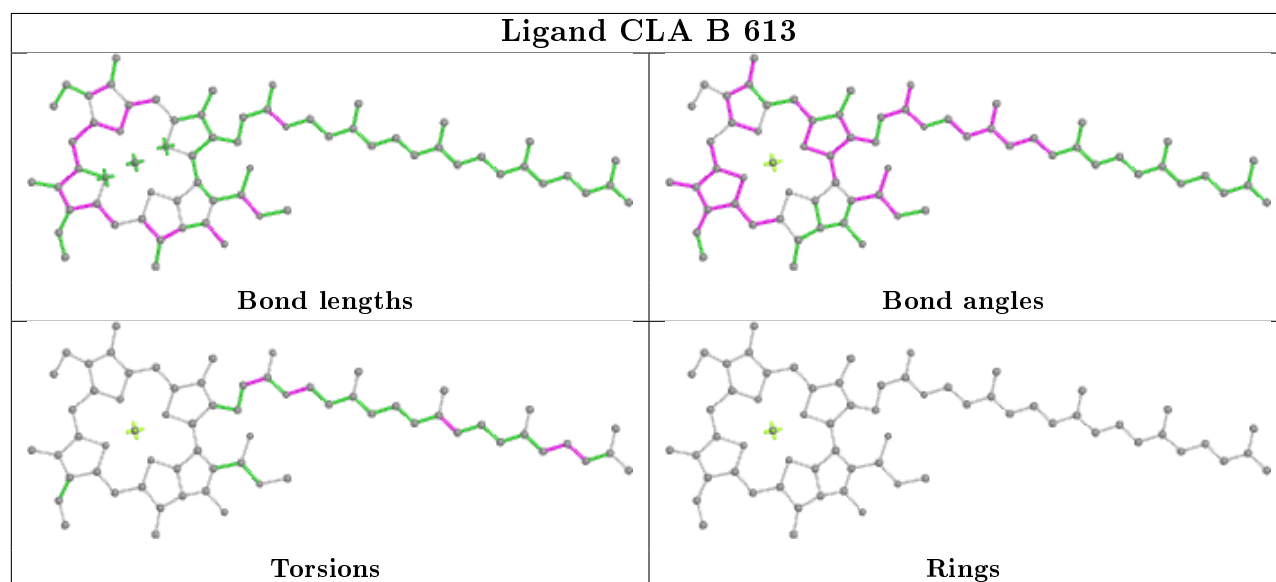
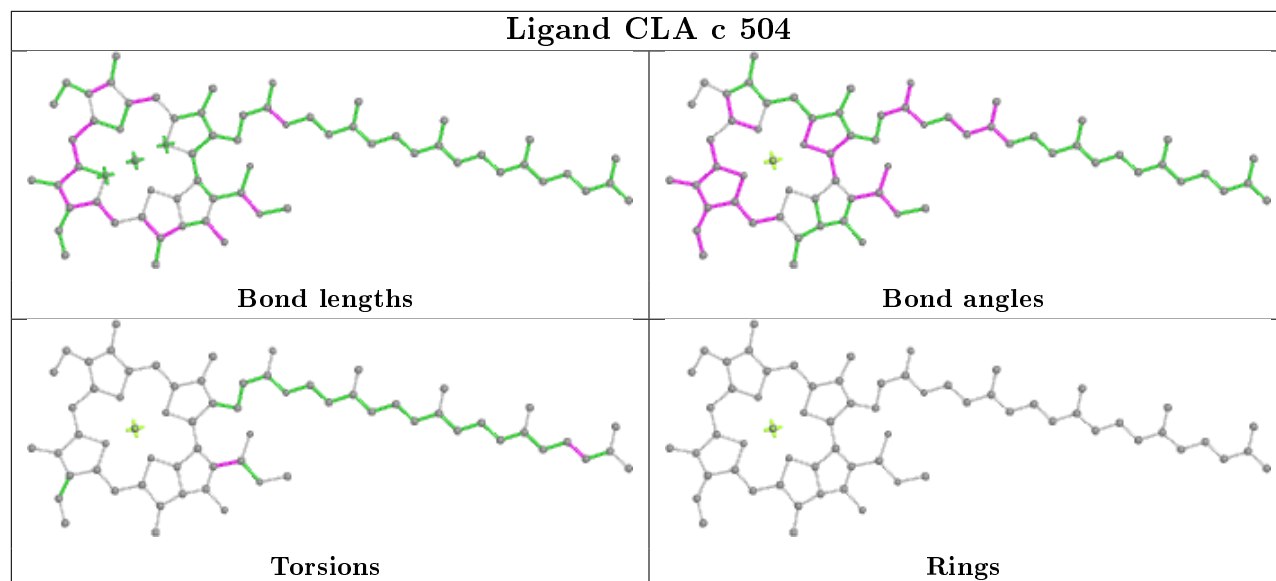
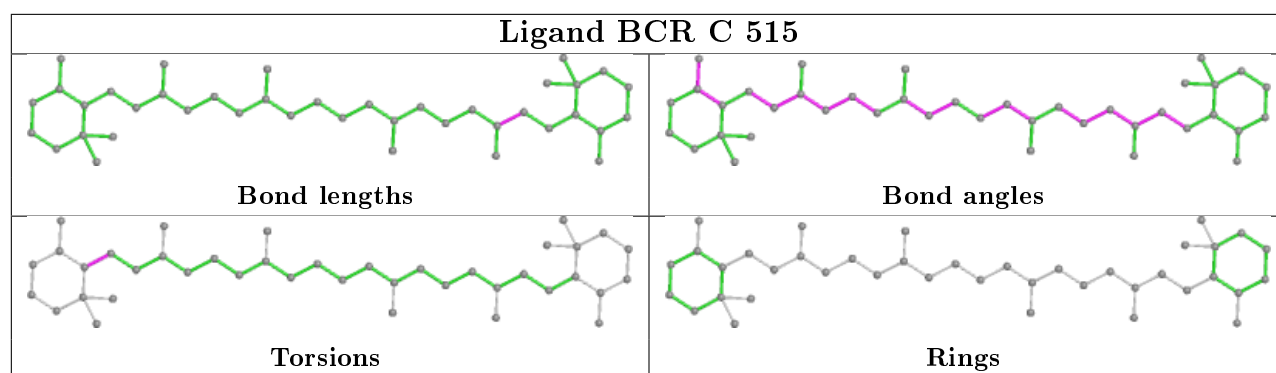
## Ligand LHG d 408

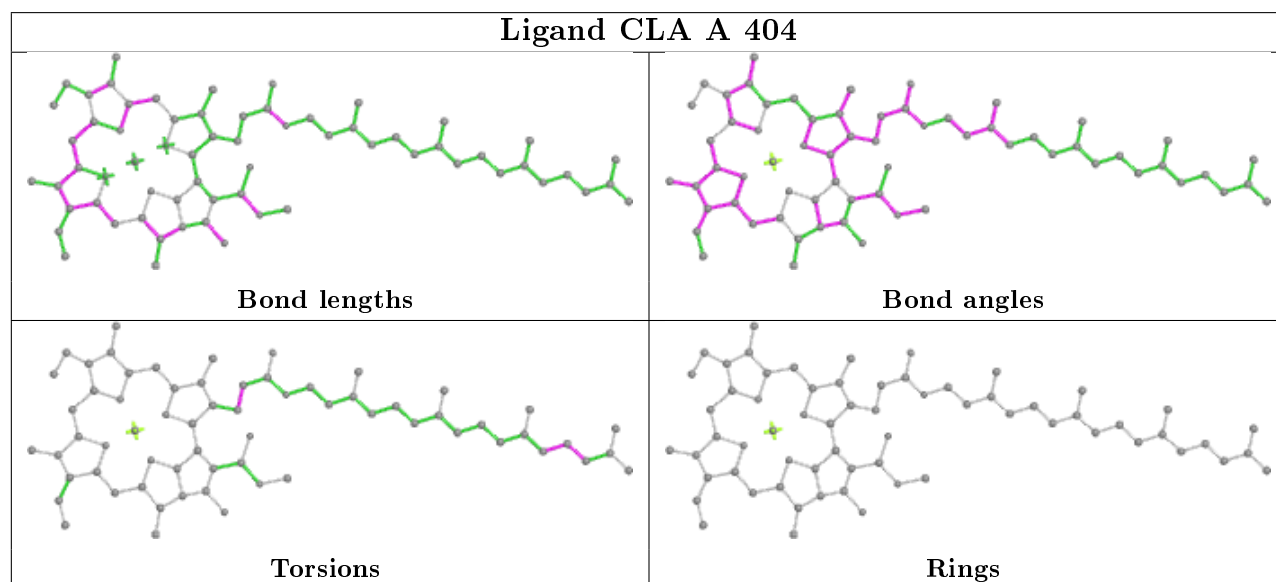
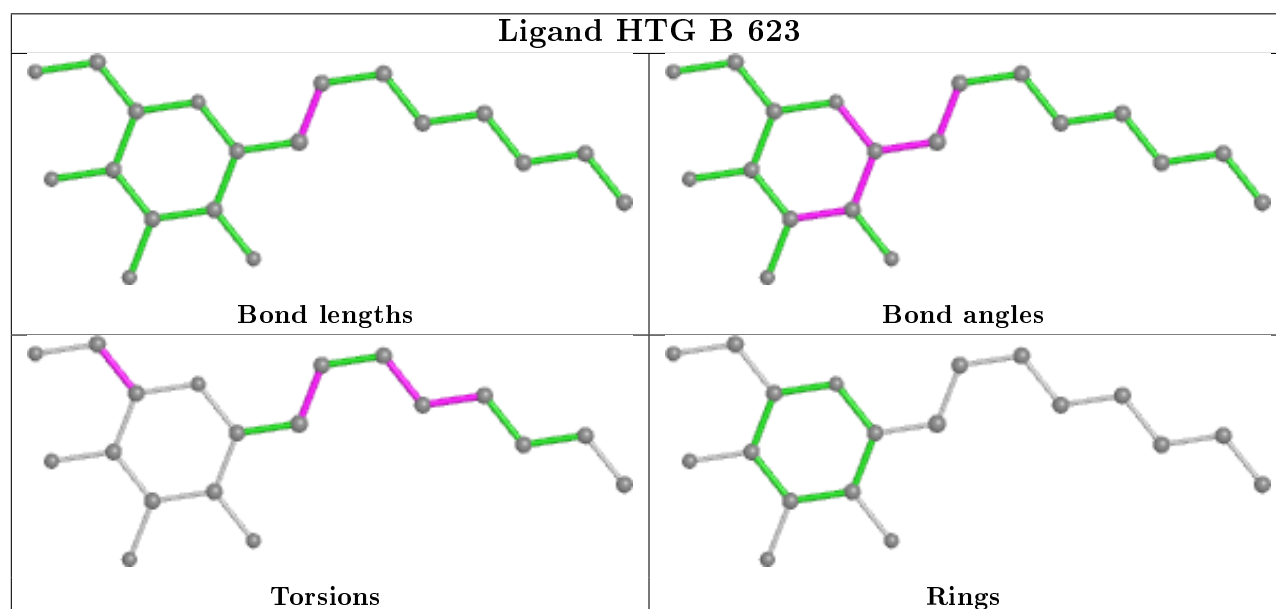
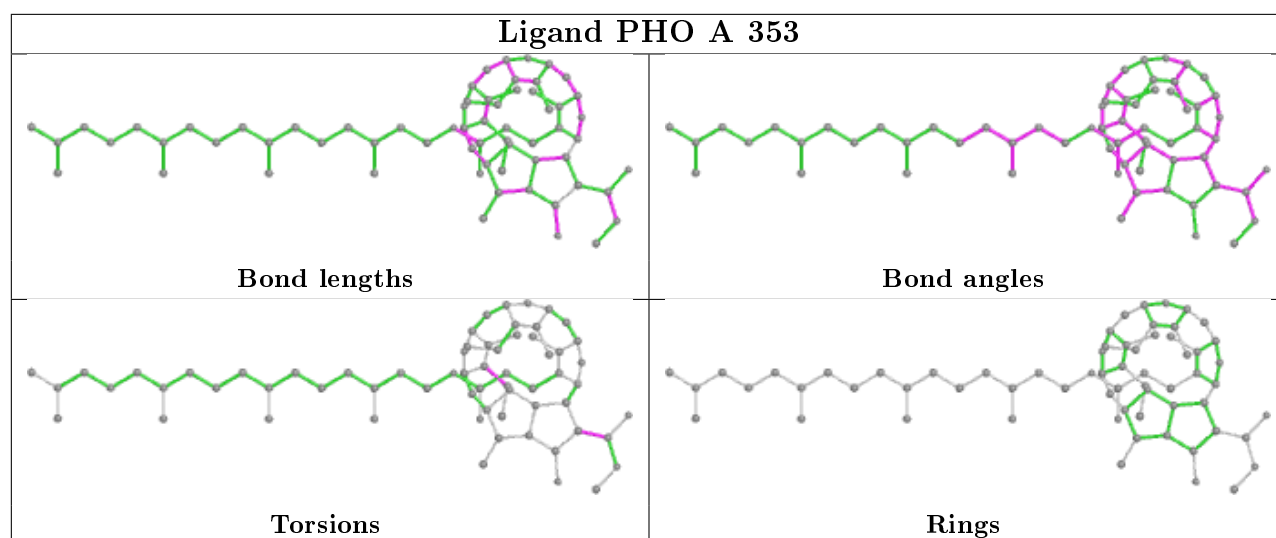


## Ligand BCR c 516

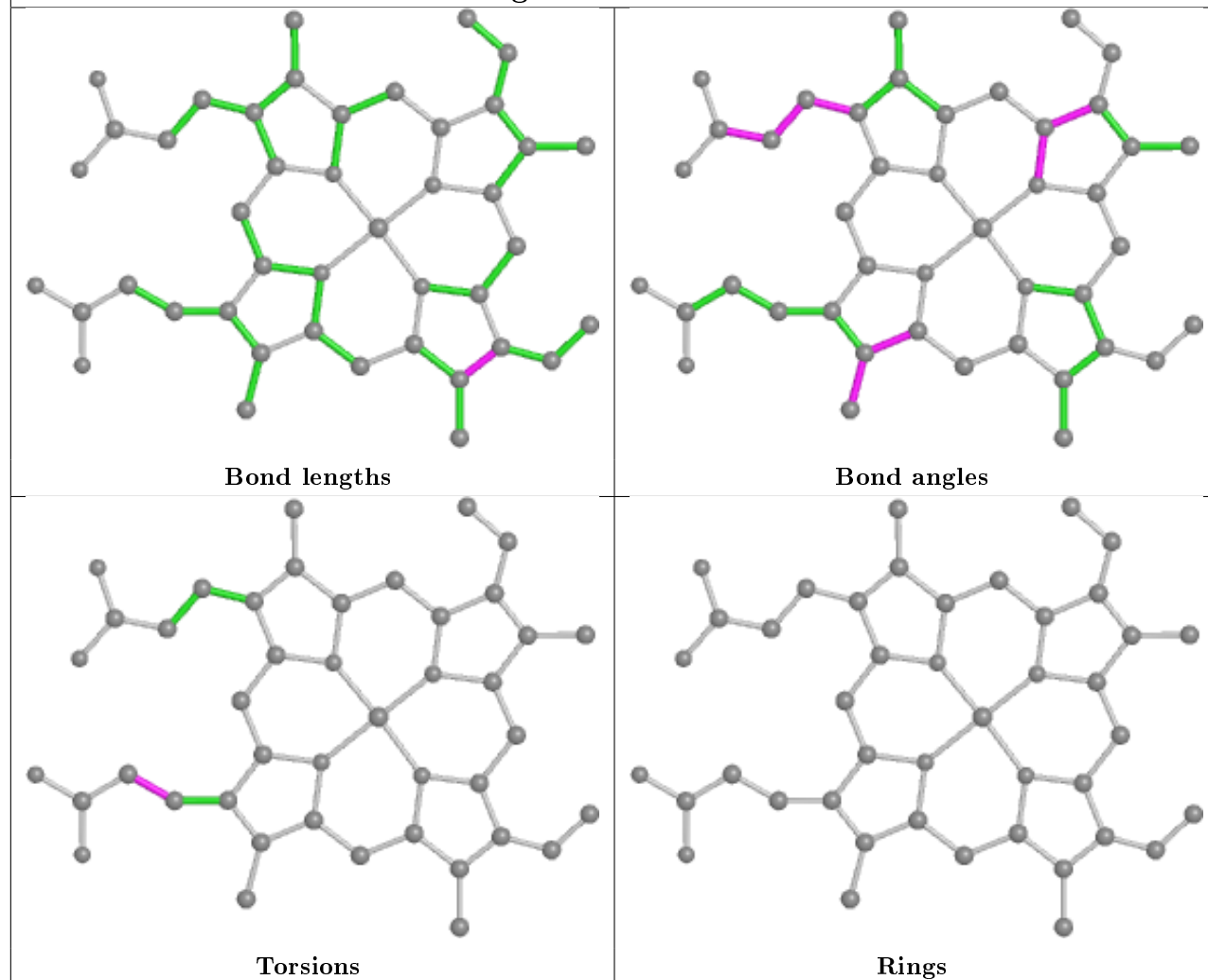


**Ligand CLA C 508****Ligand DGD c 517****Ligand CLA b 602**

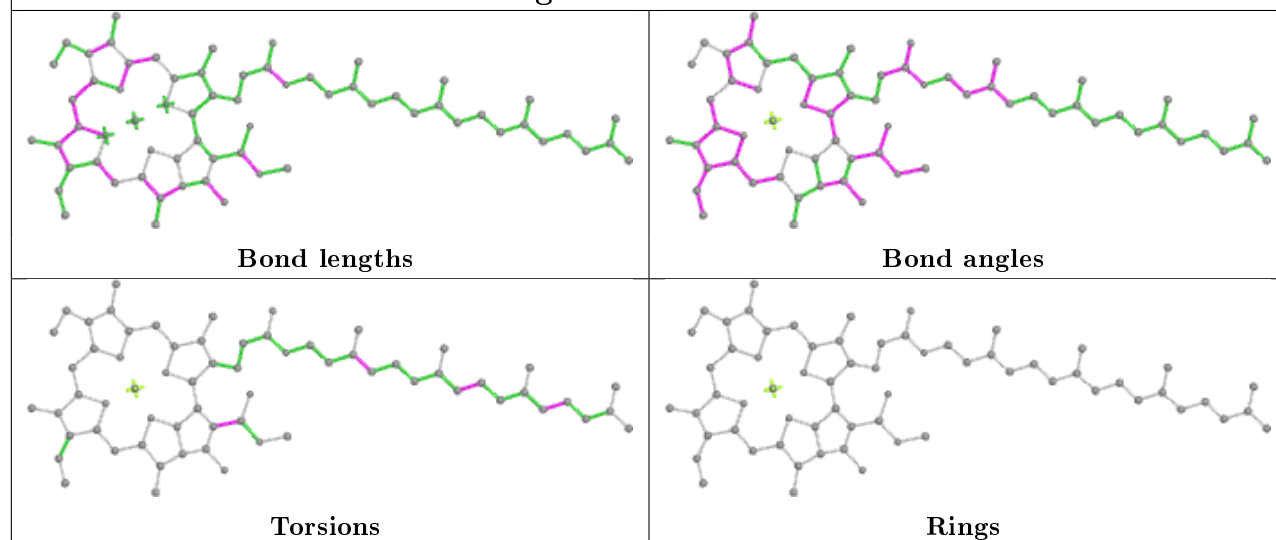


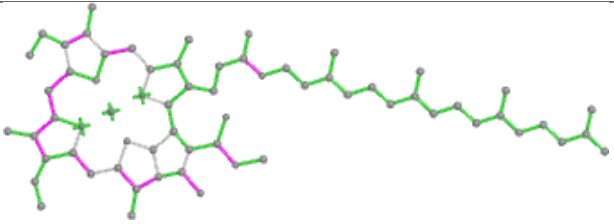
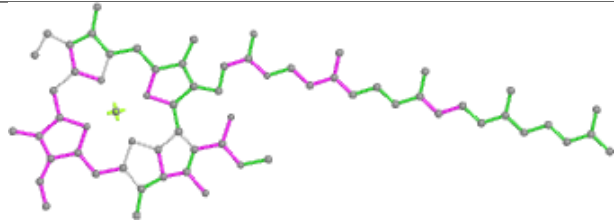
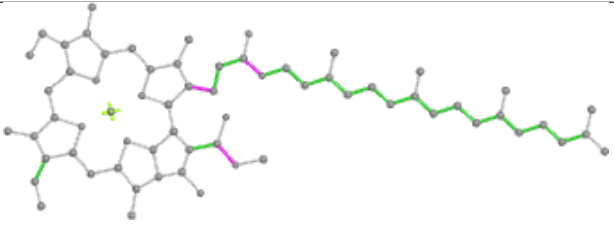
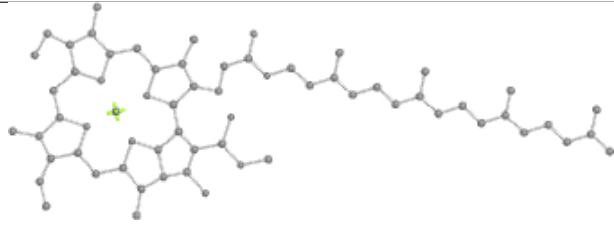
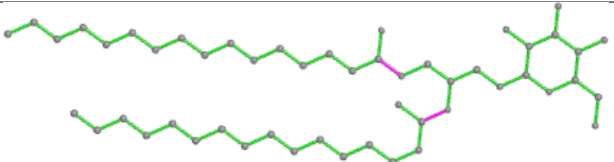
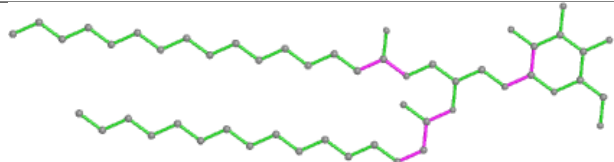
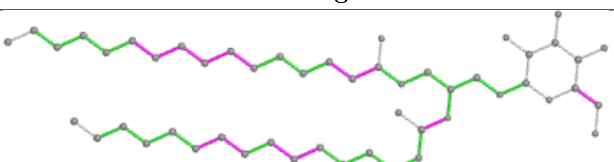
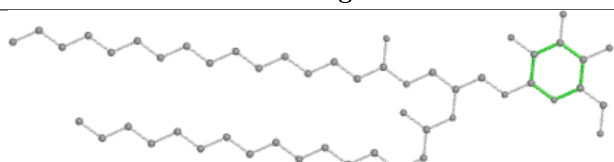
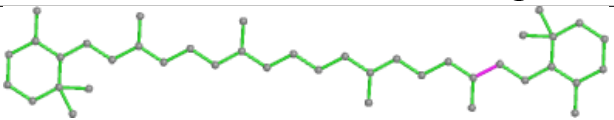
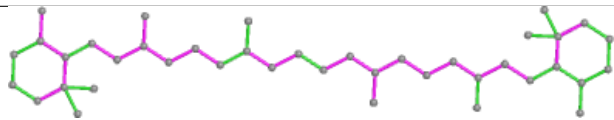
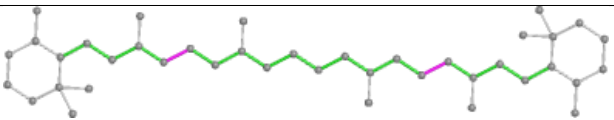
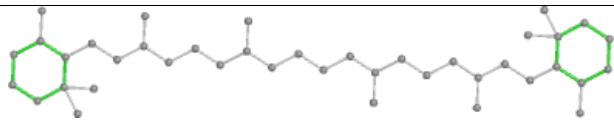


## Ligand HEM e 87

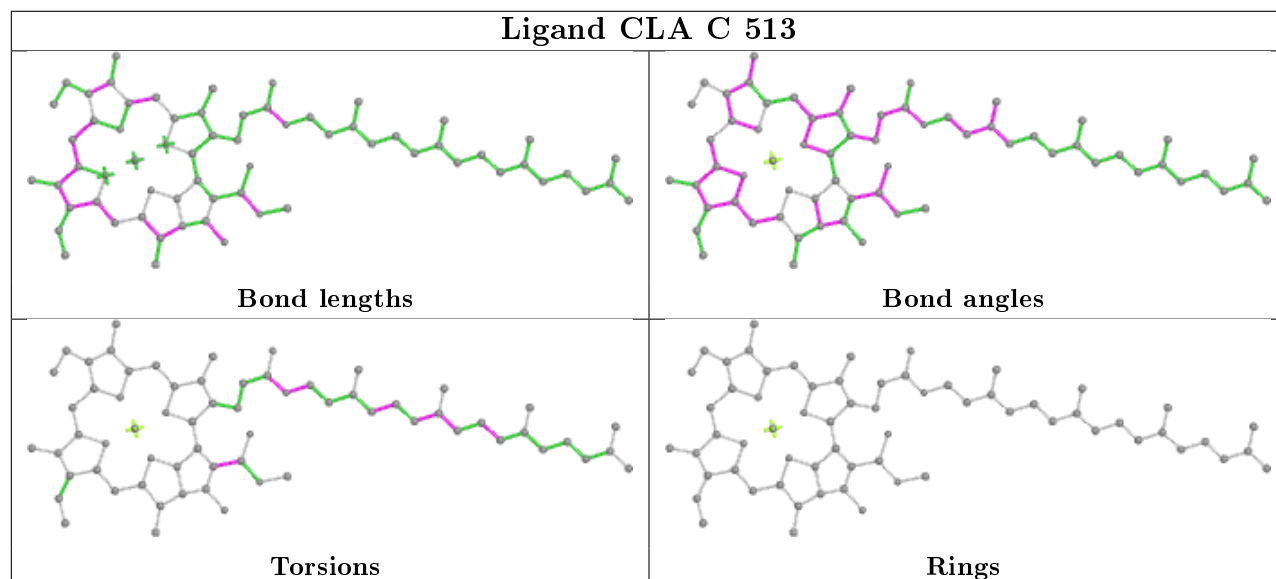
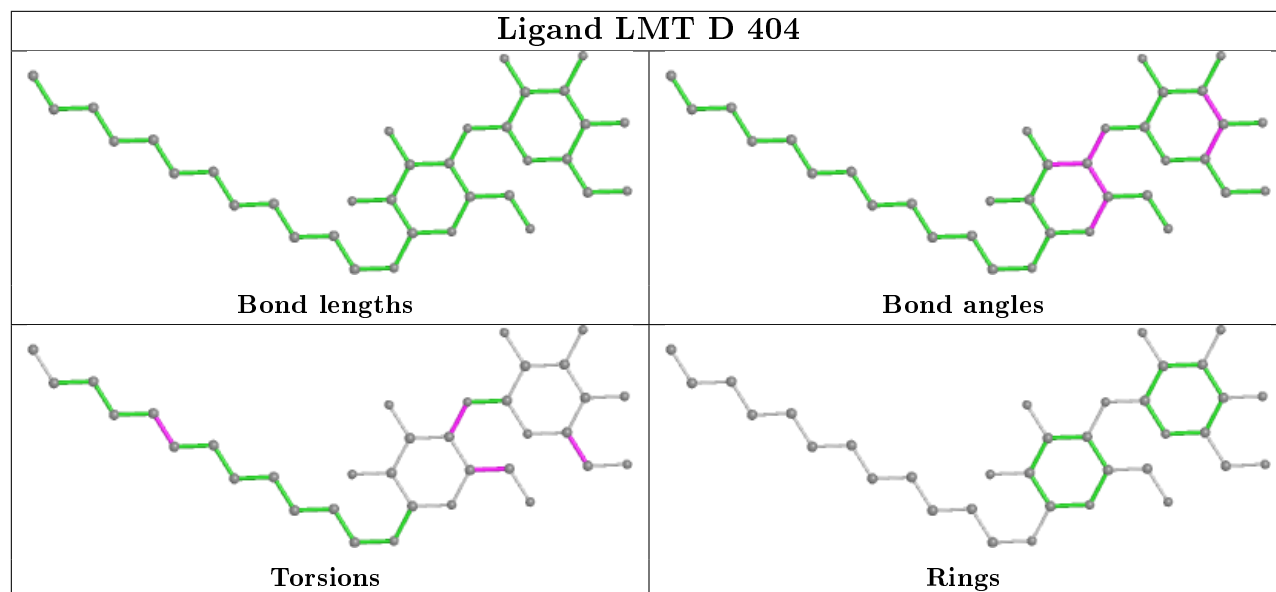
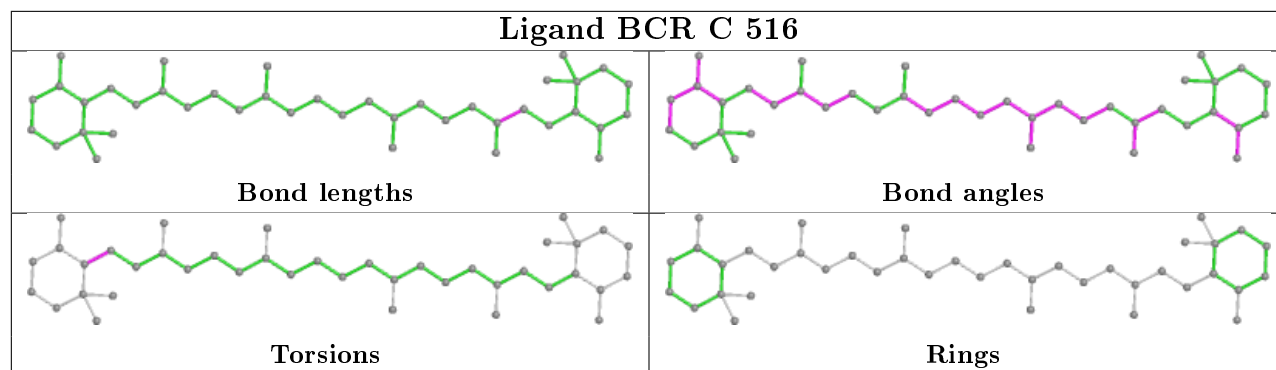


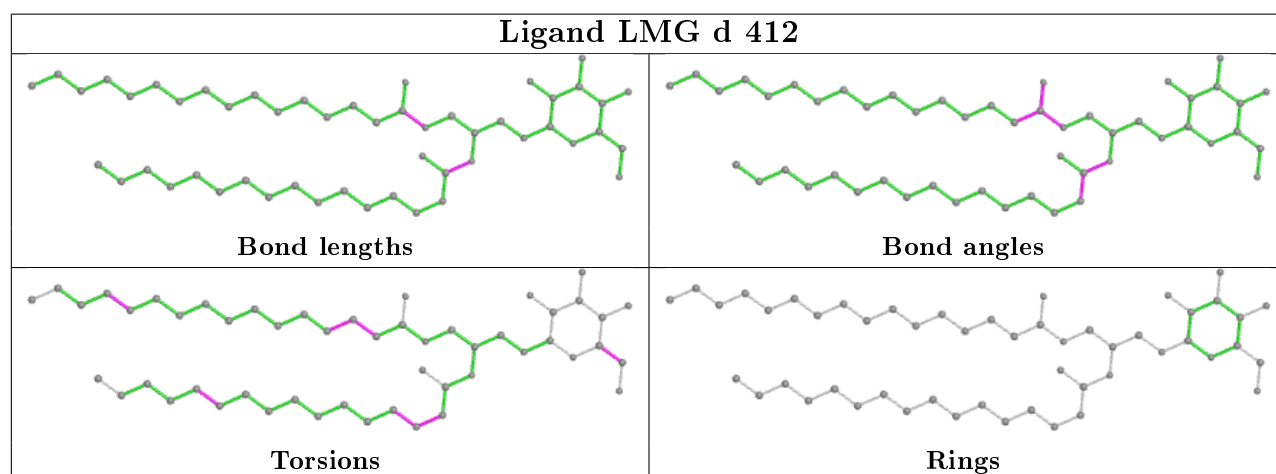
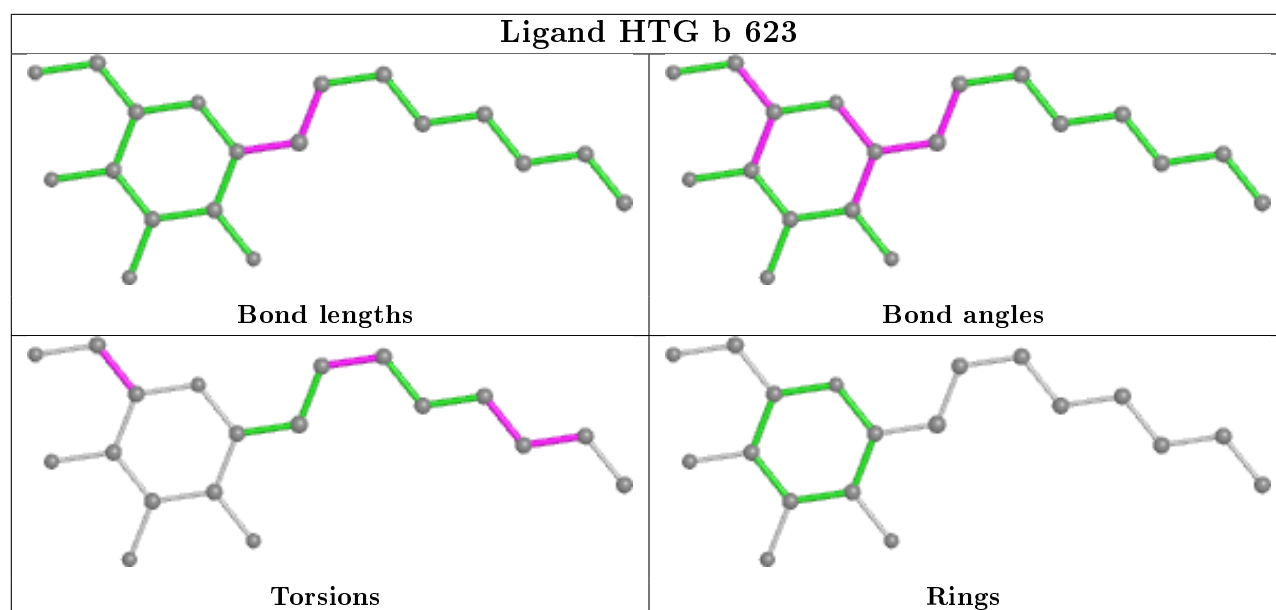
## Ligand CLA b 605

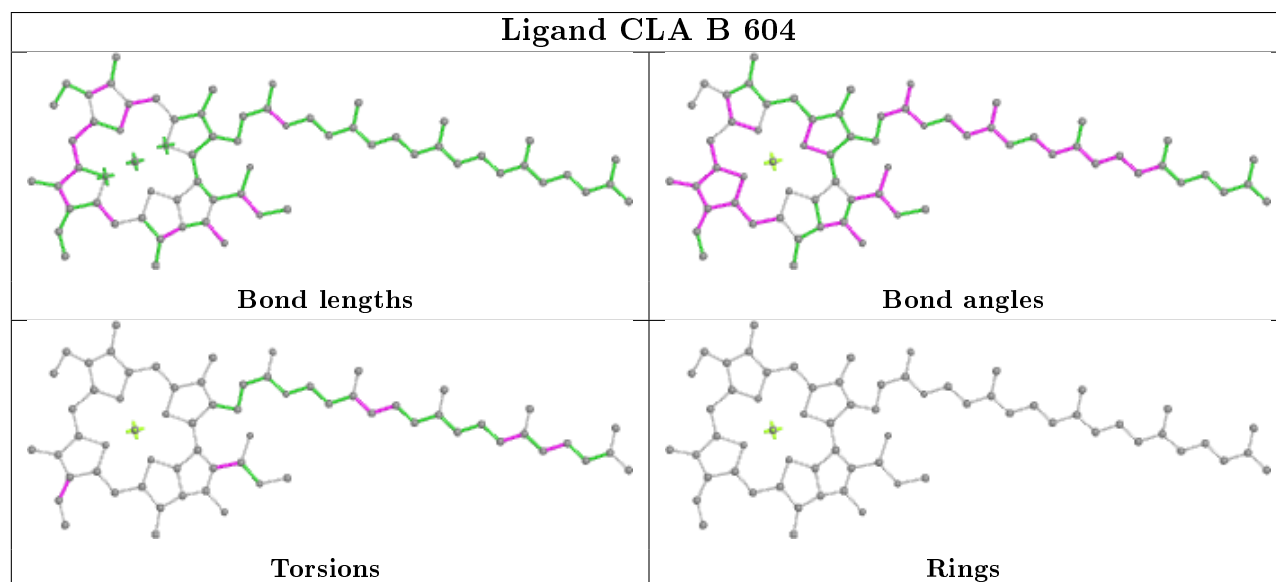
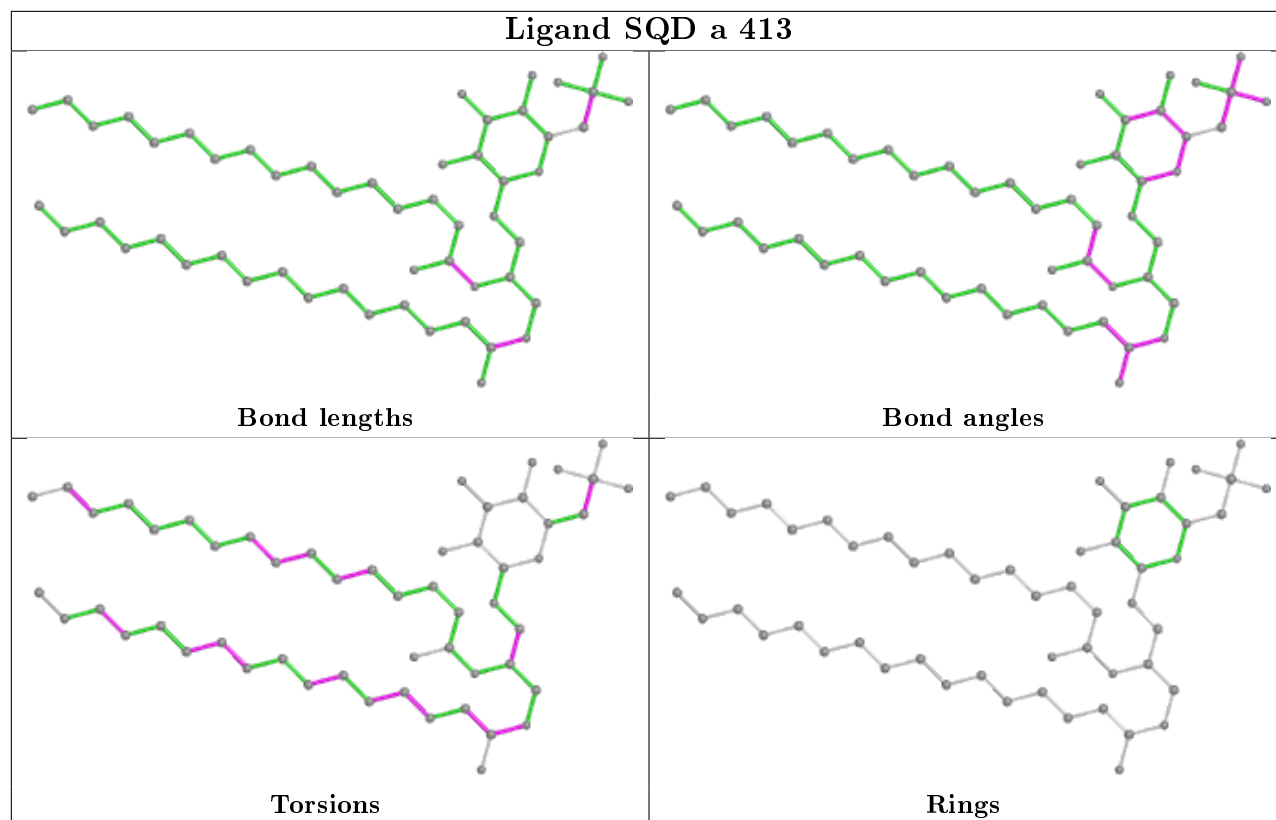


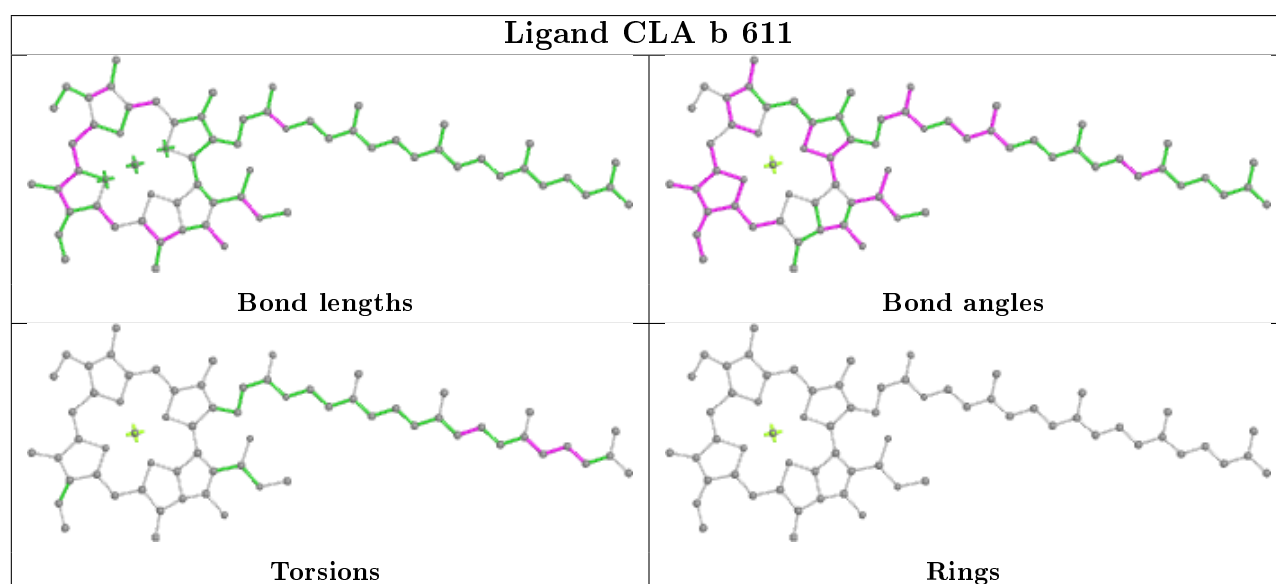
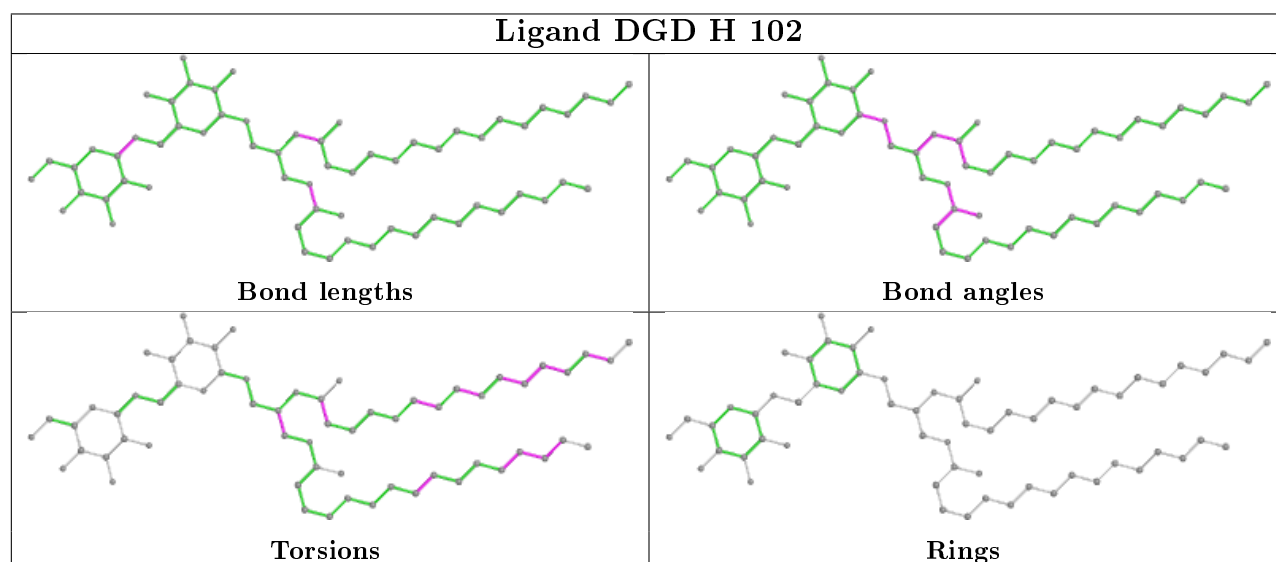
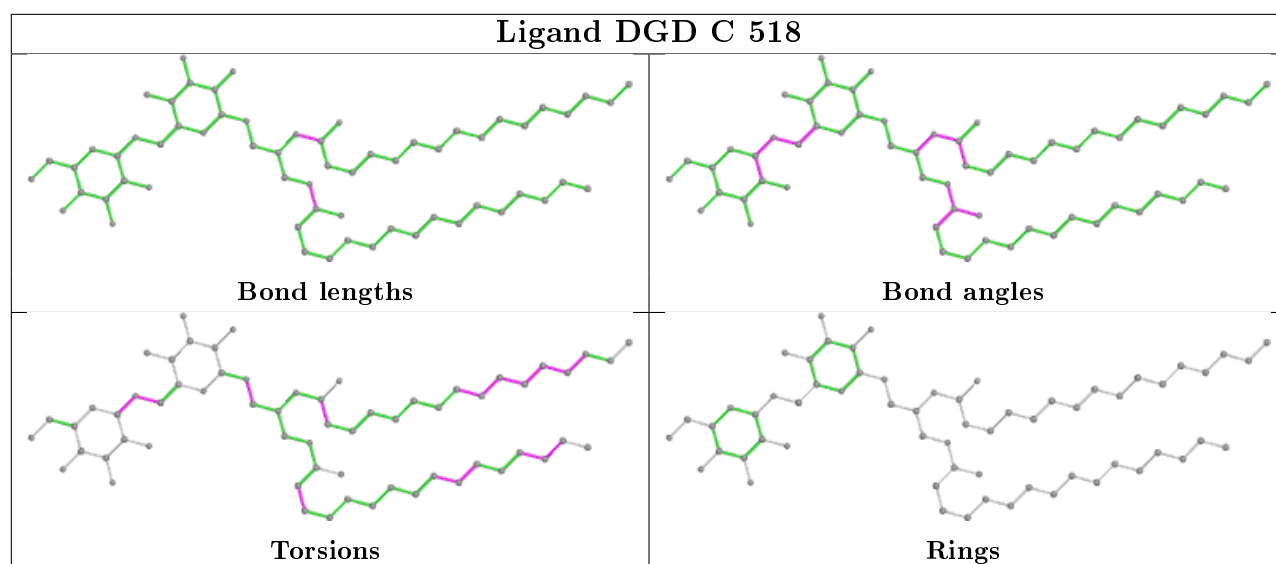
Ligand CLA c 512	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG B 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR k 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

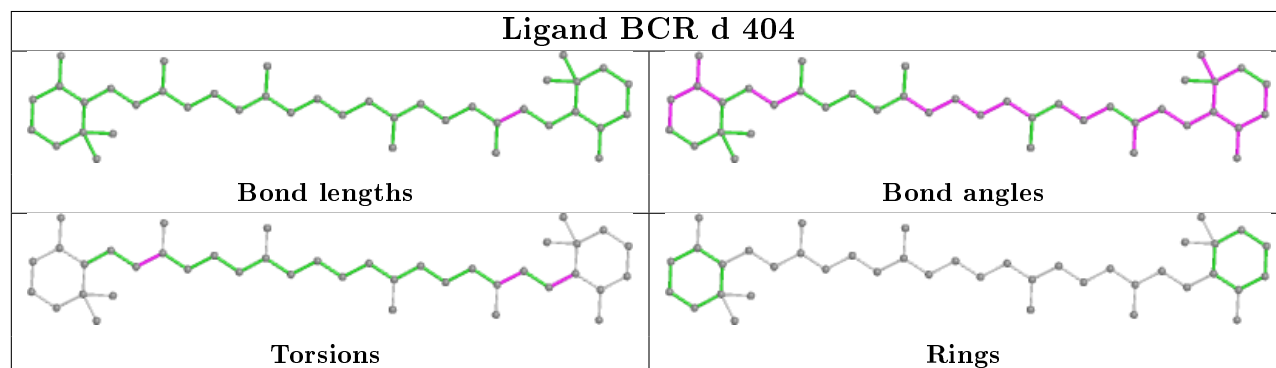
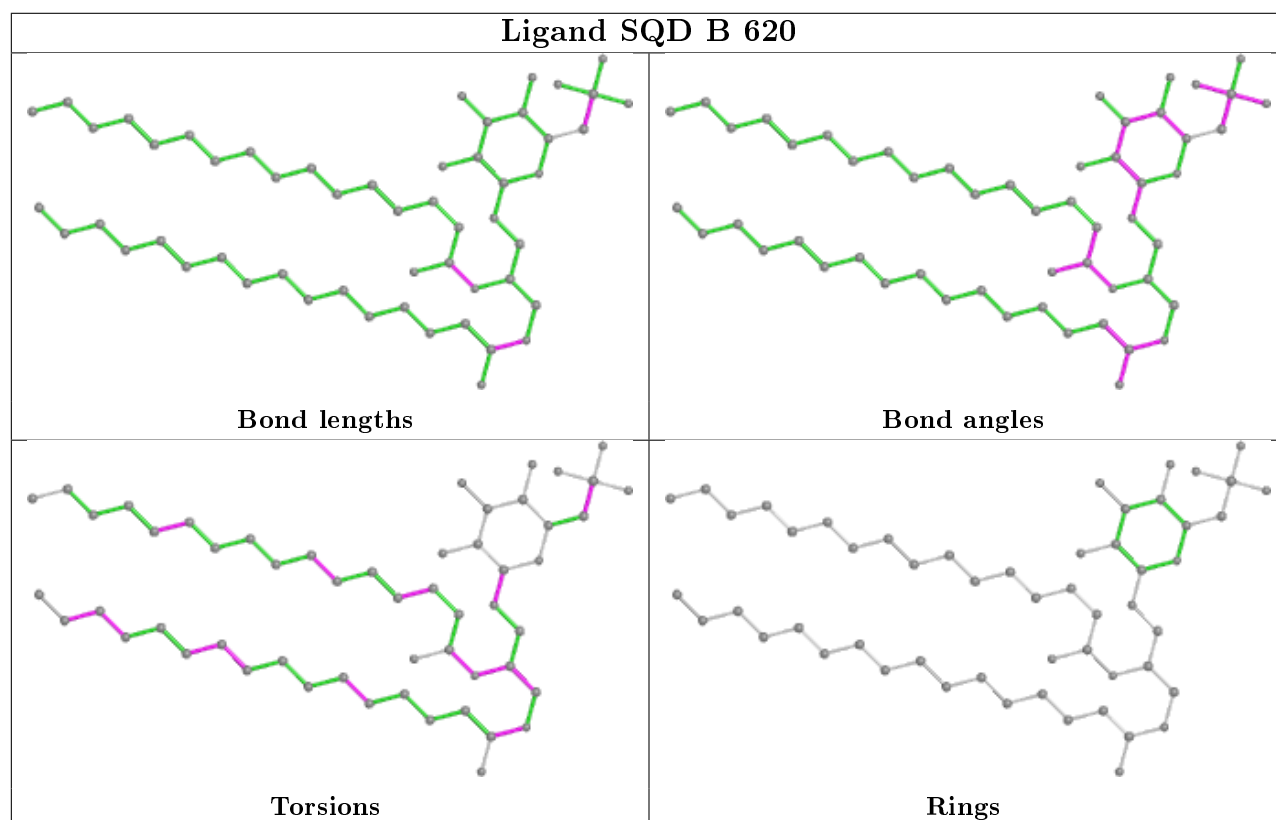
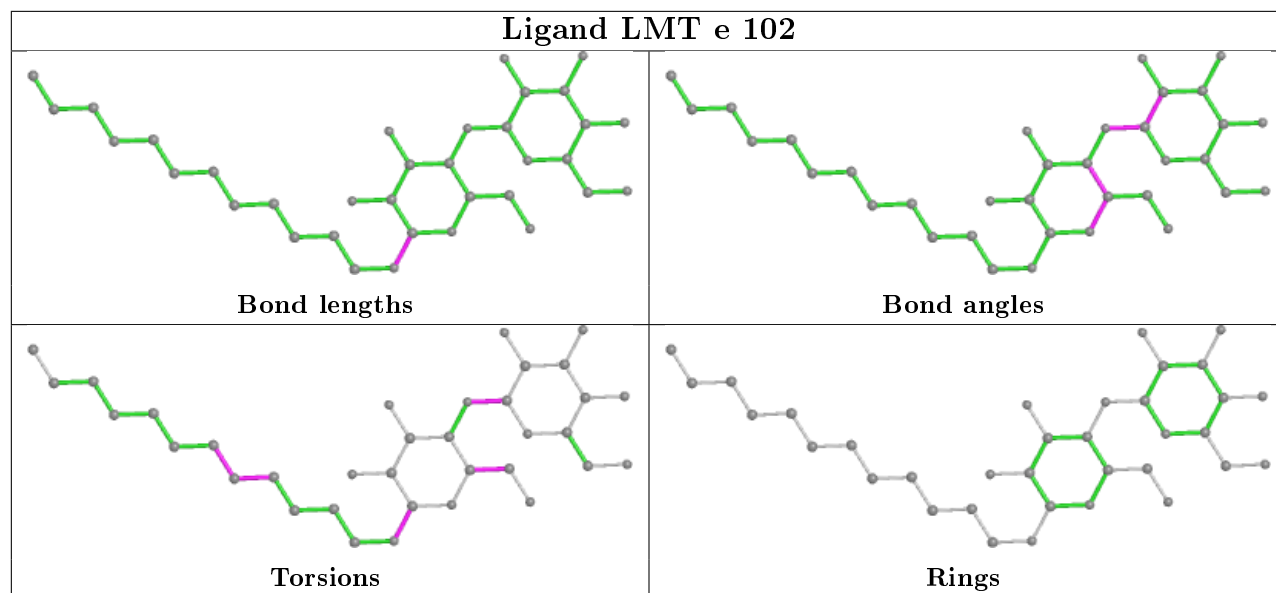


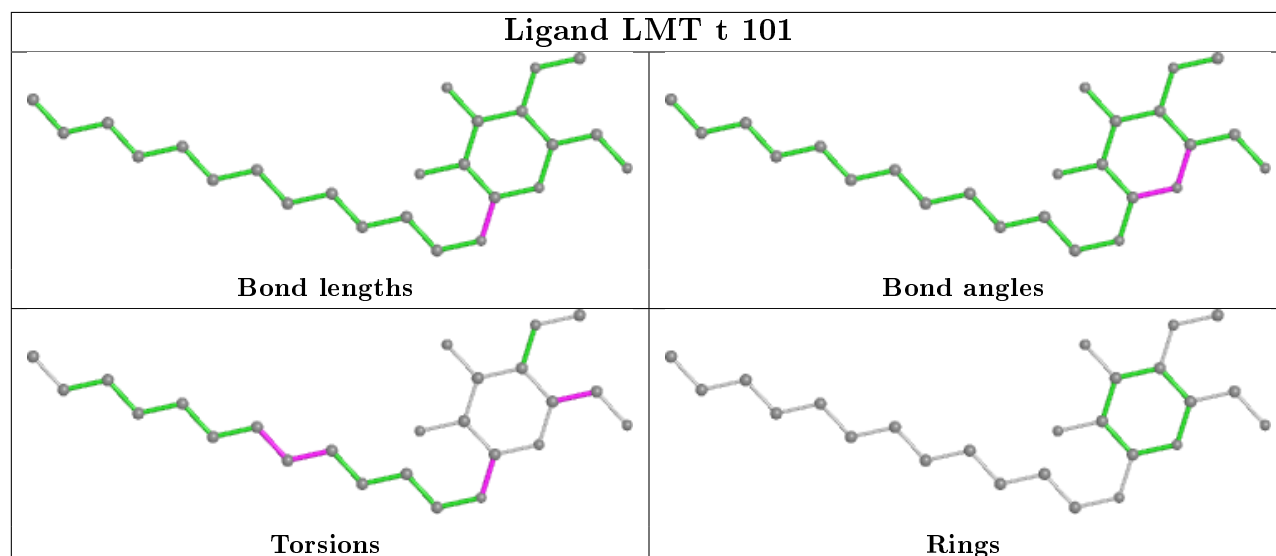
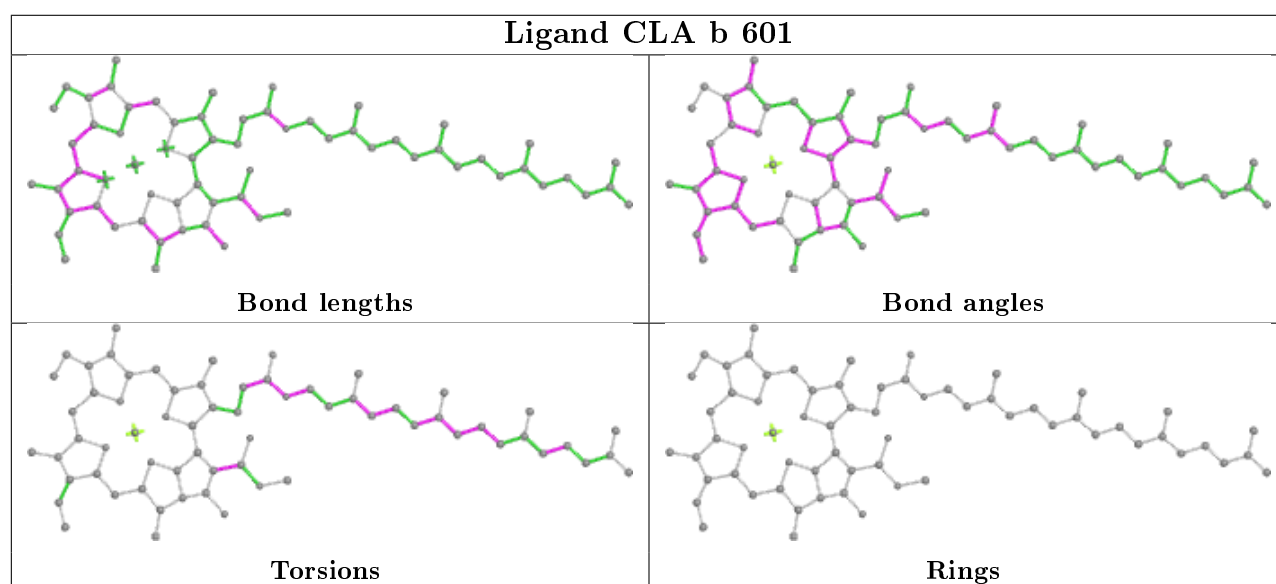
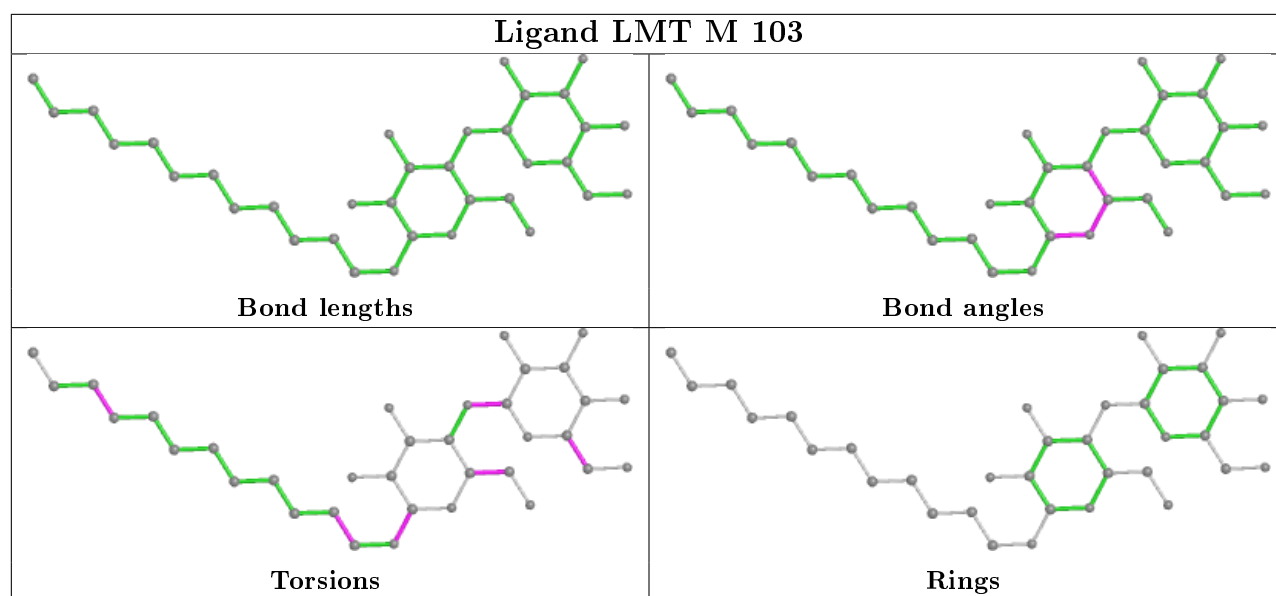


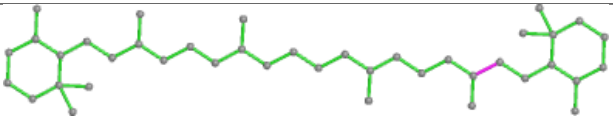
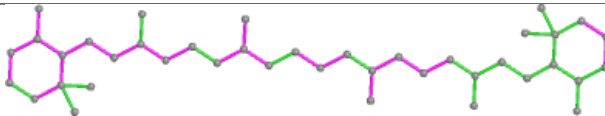
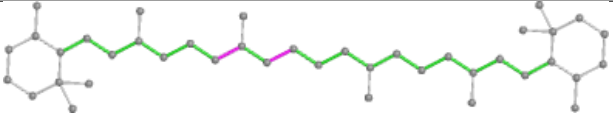
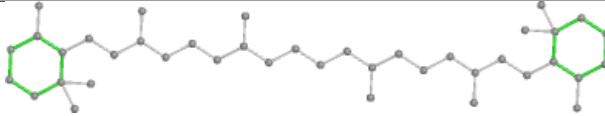


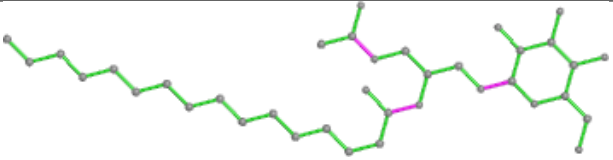
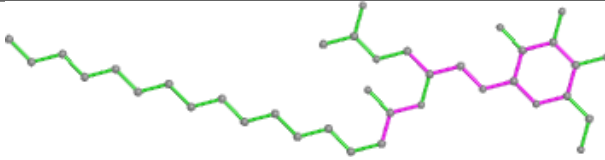
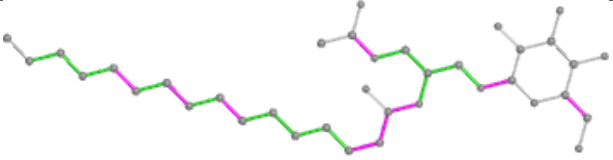
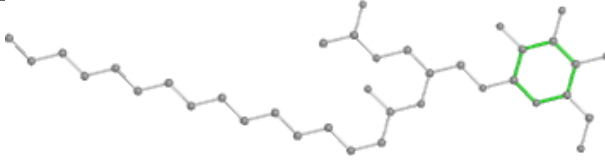


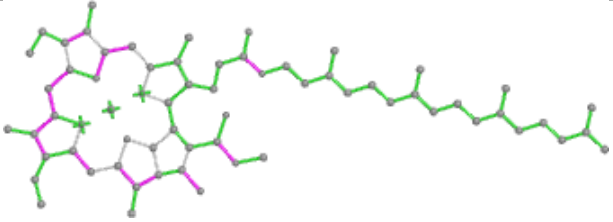
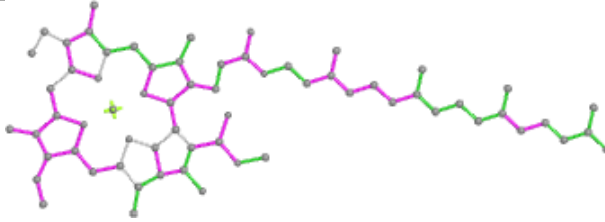
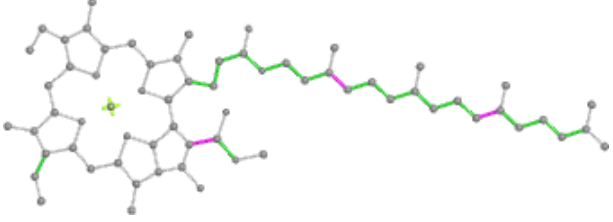
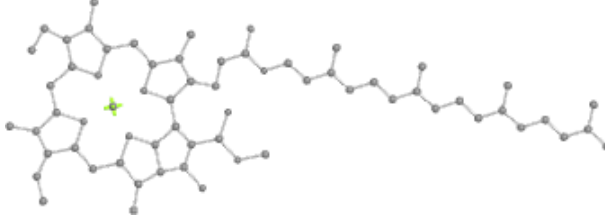


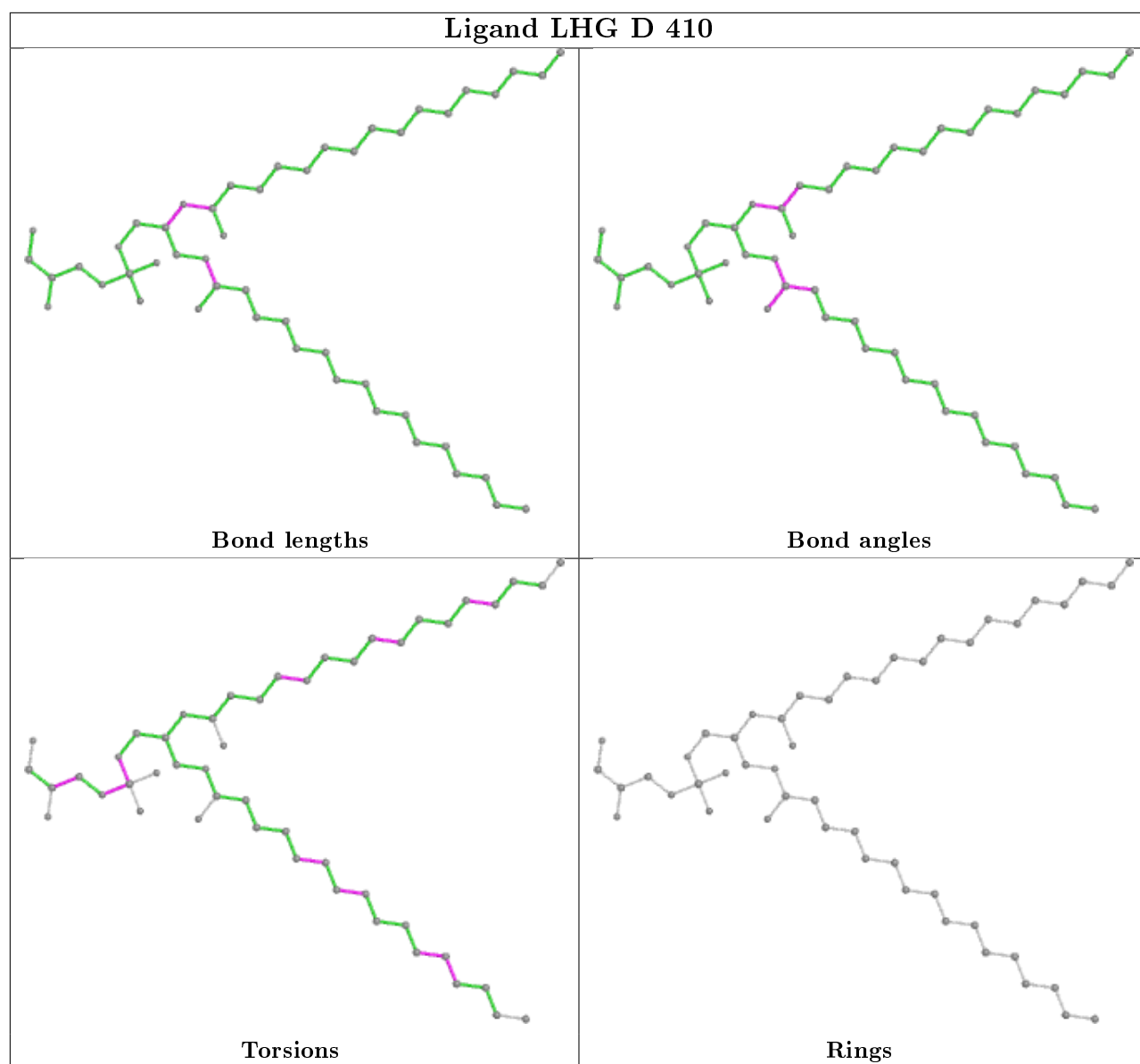




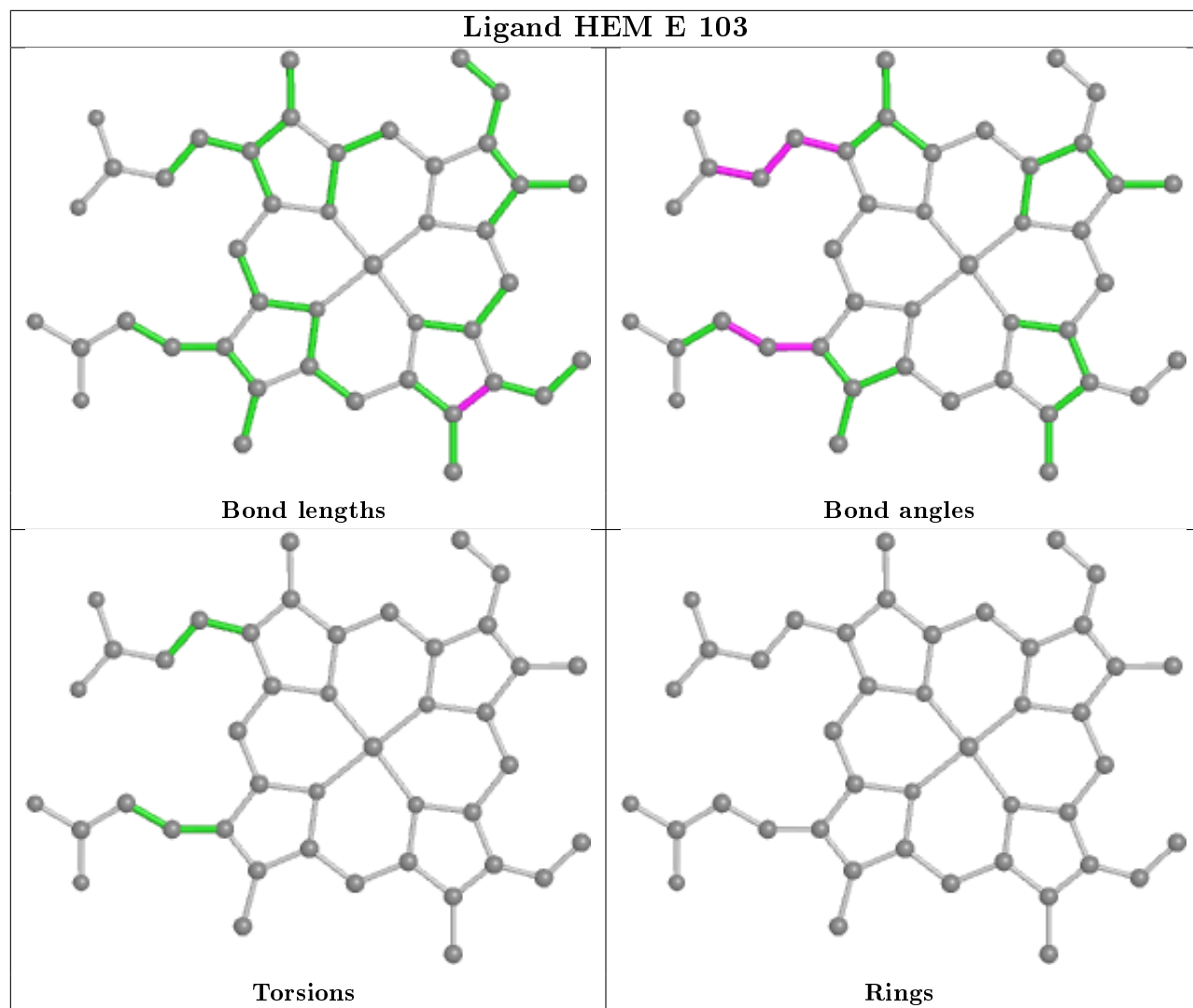
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

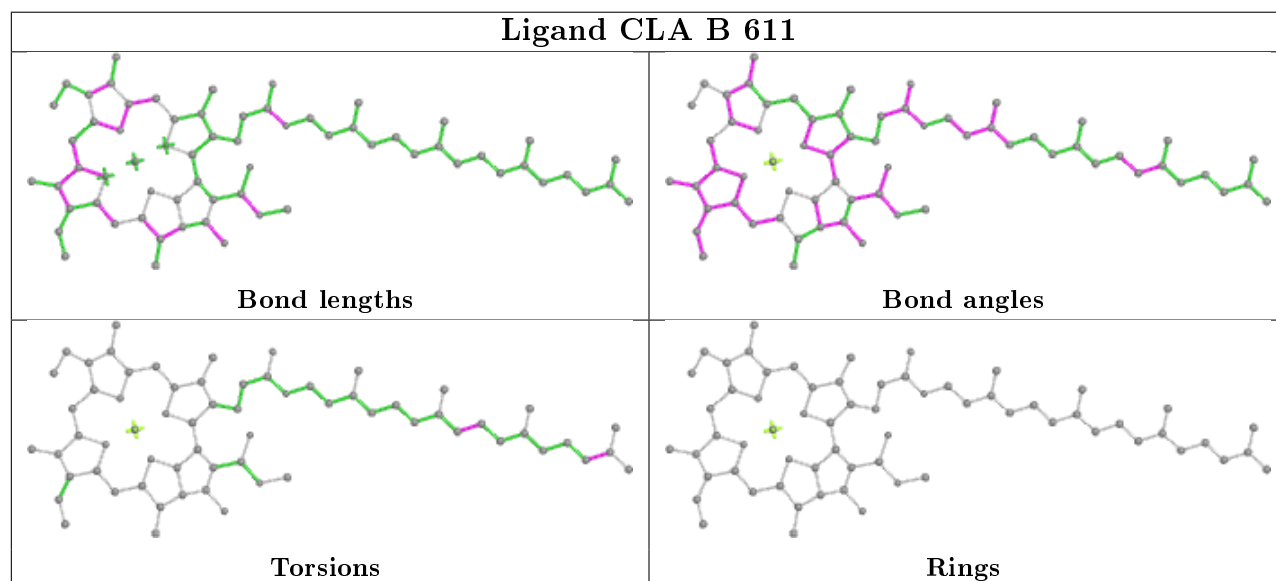
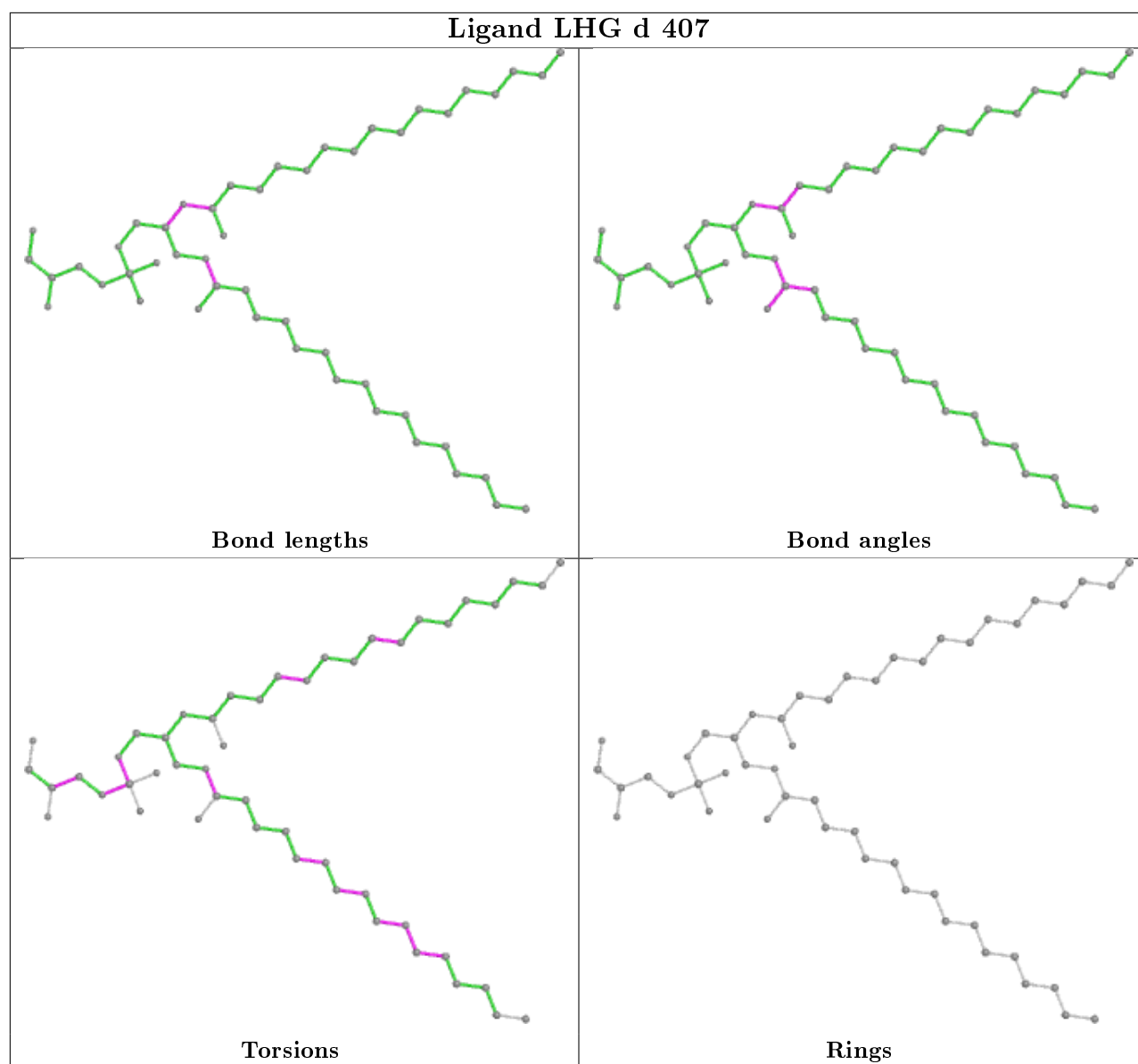
Ligand LMG Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

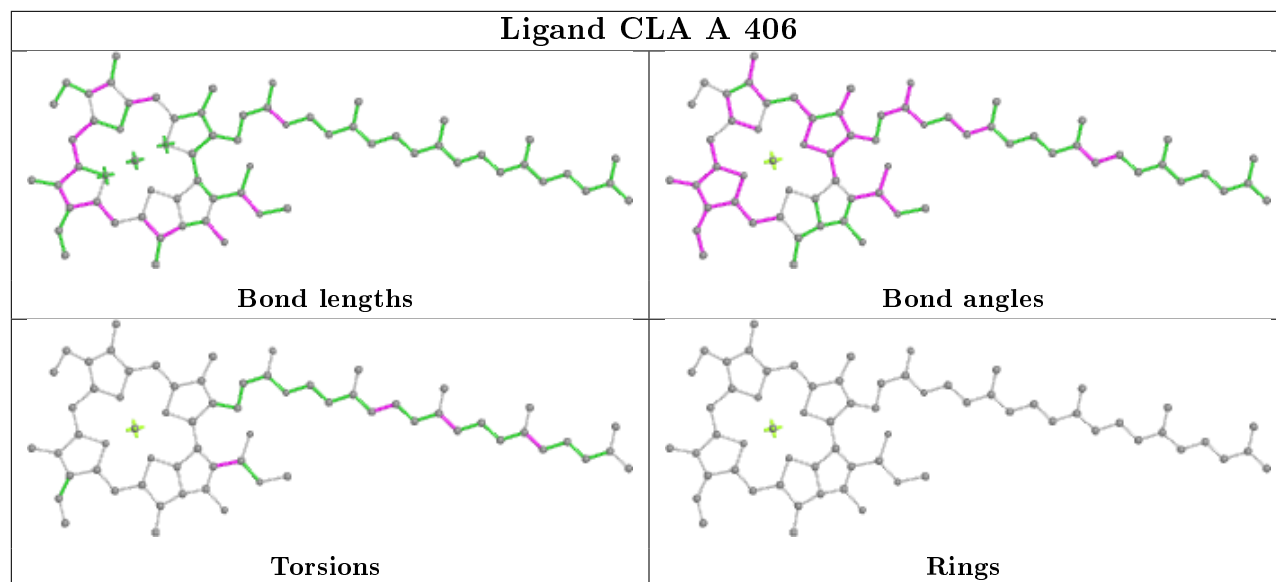
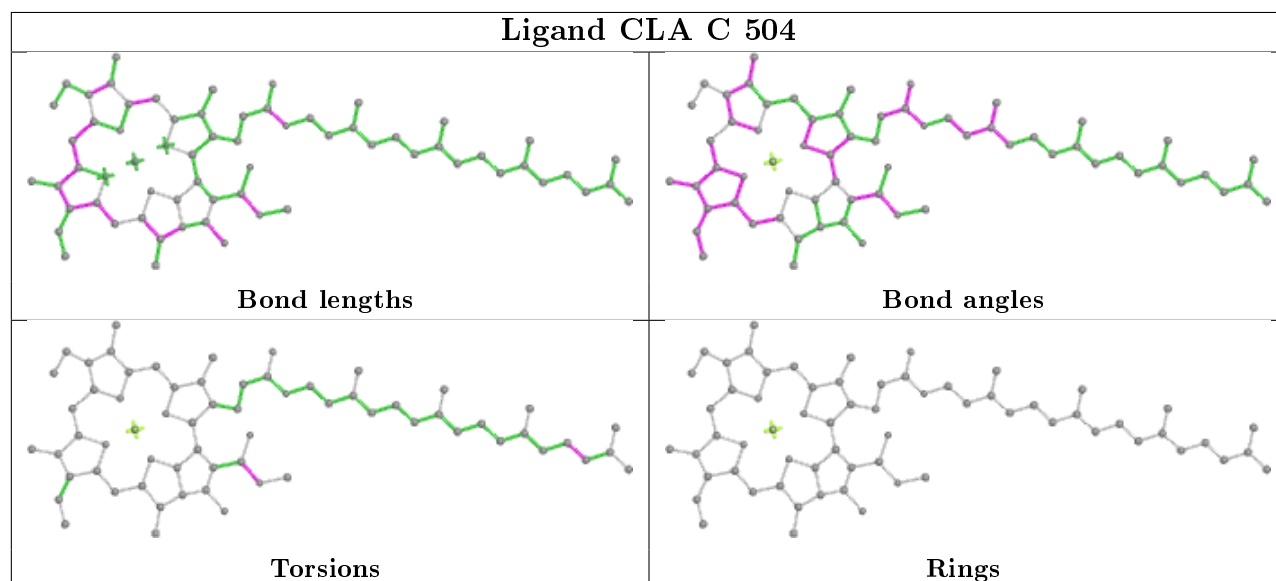
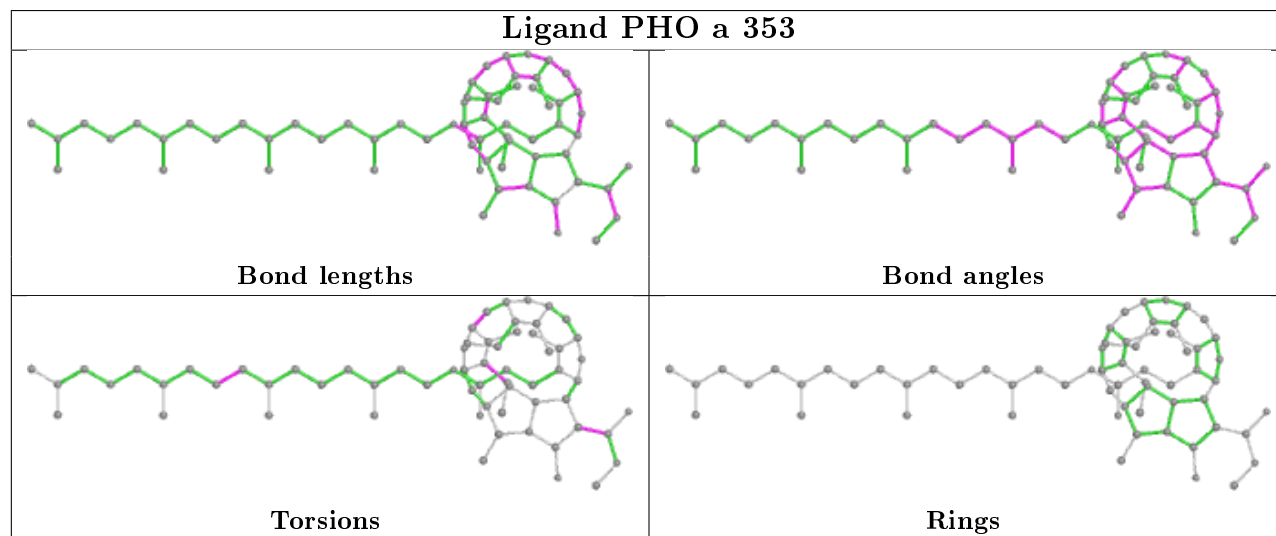
Ligand CLA B 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

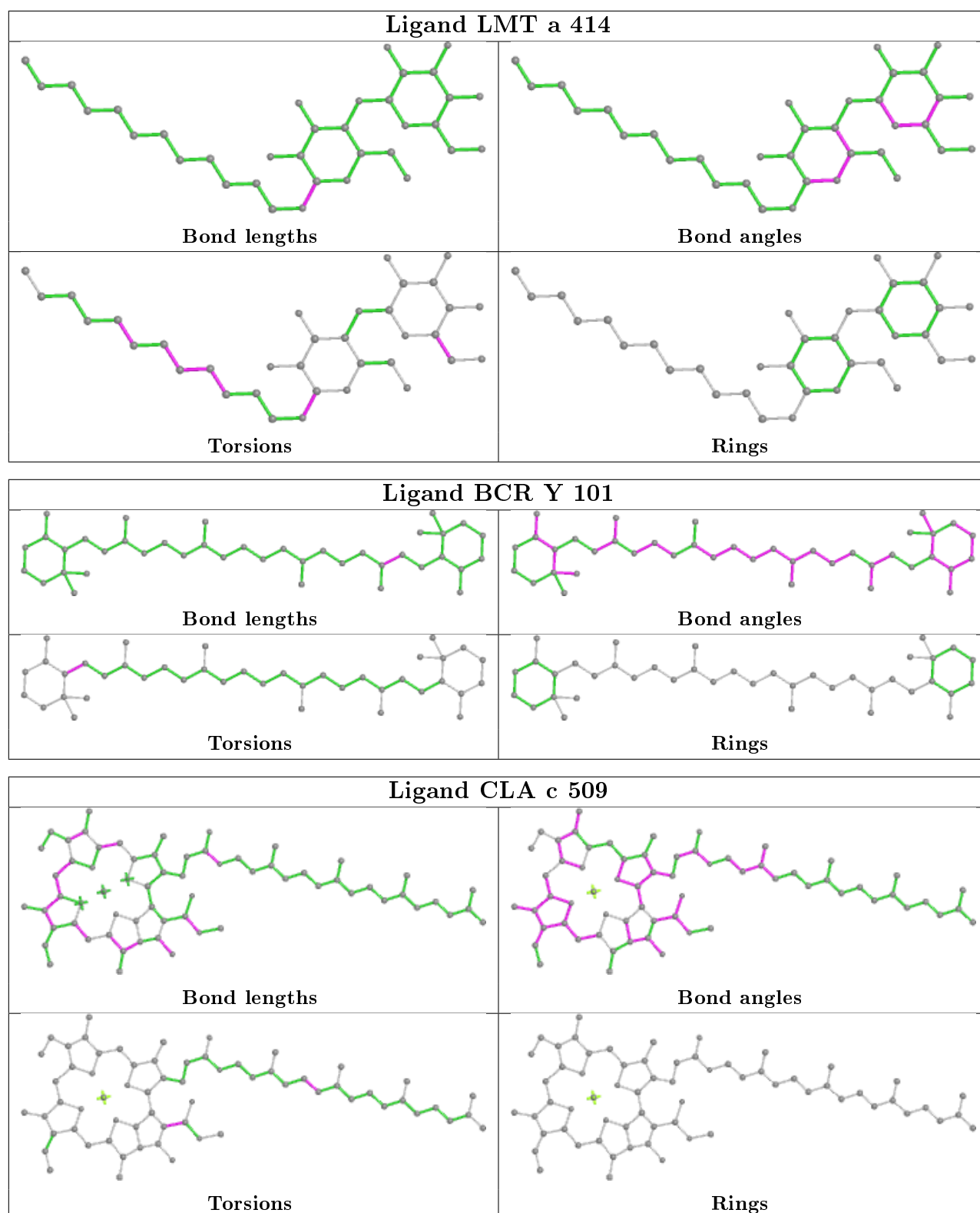


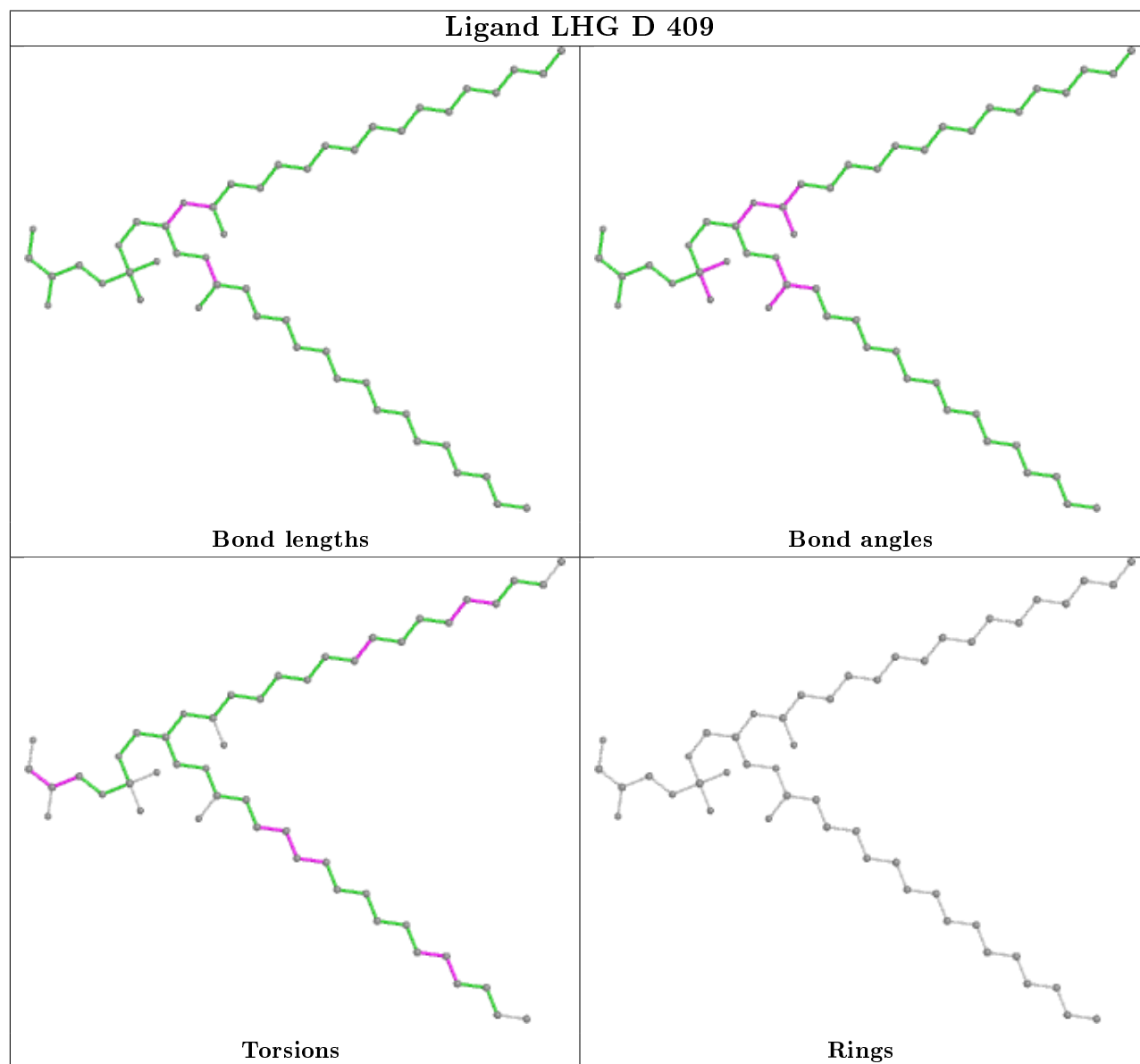
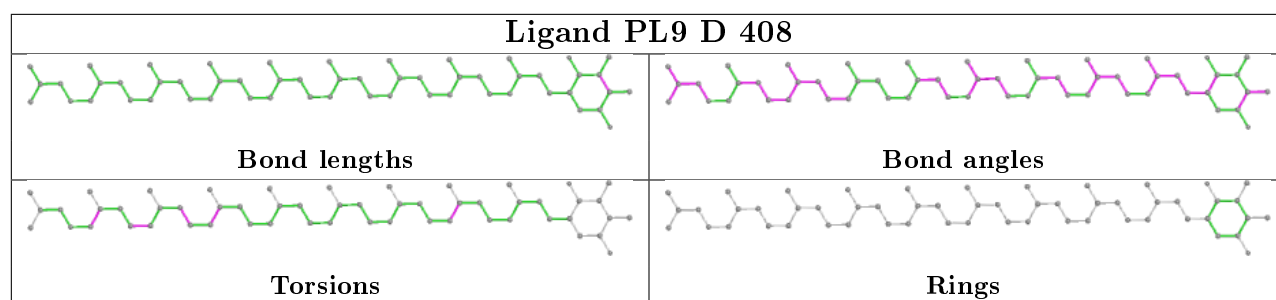




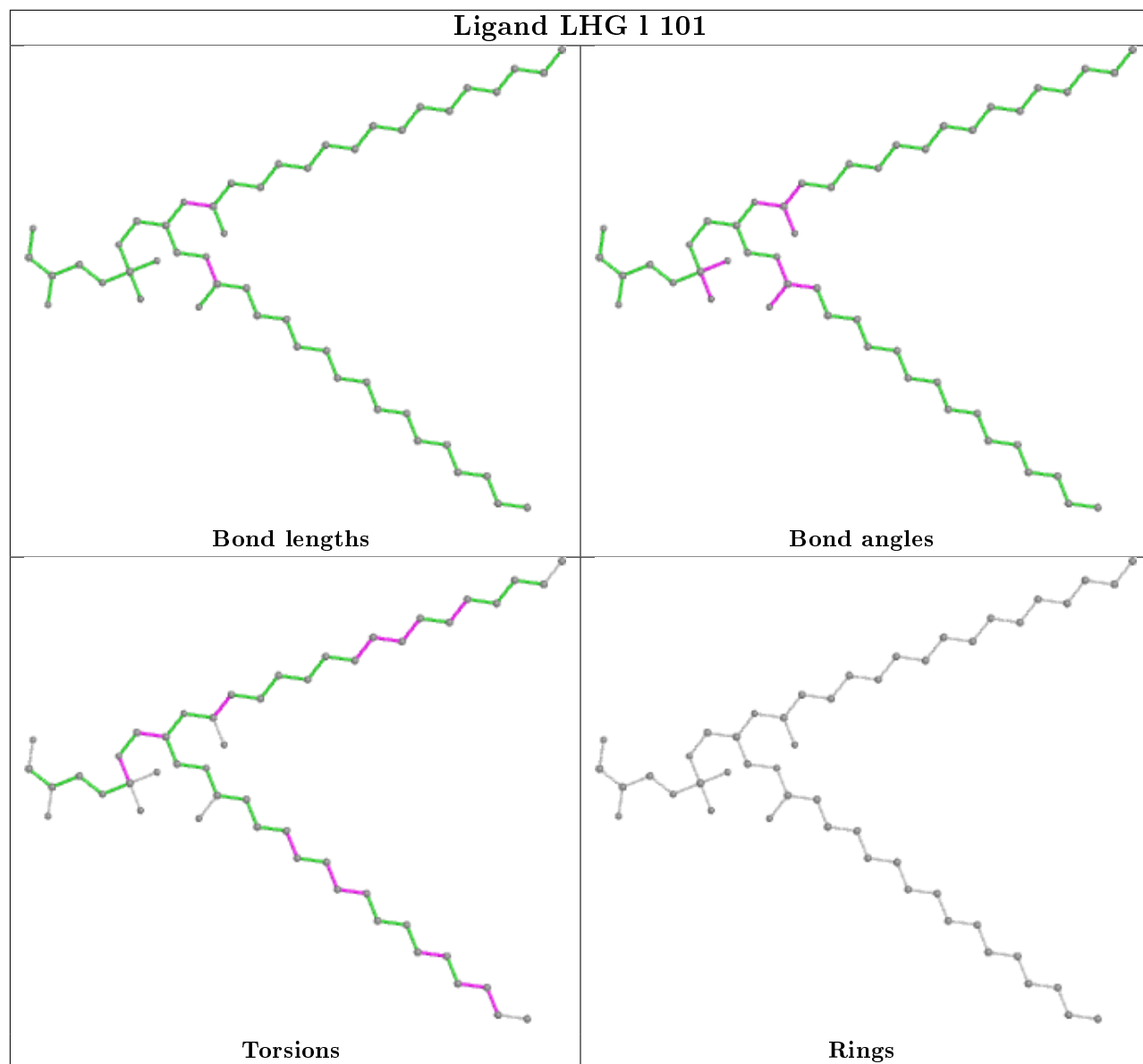


**Ligand CLA A 406****Ligand CLA C 504****Ligand PHO a 353**

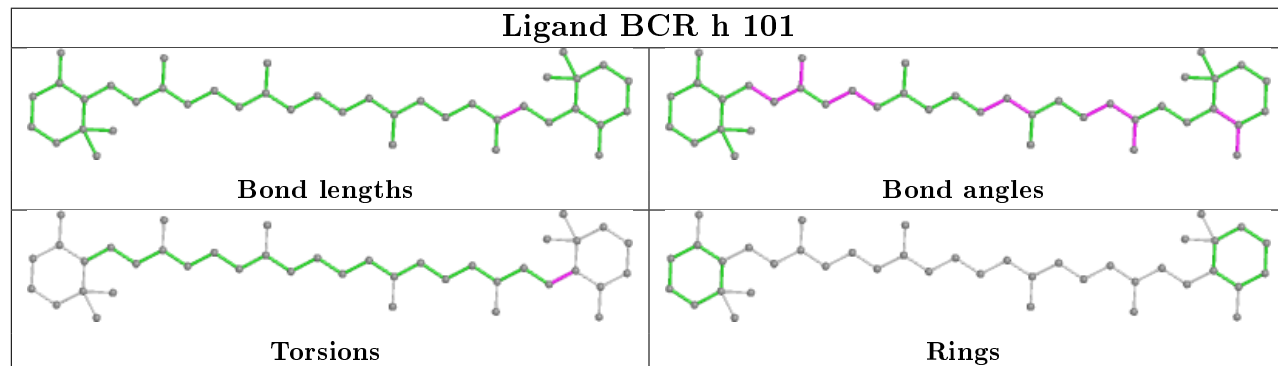


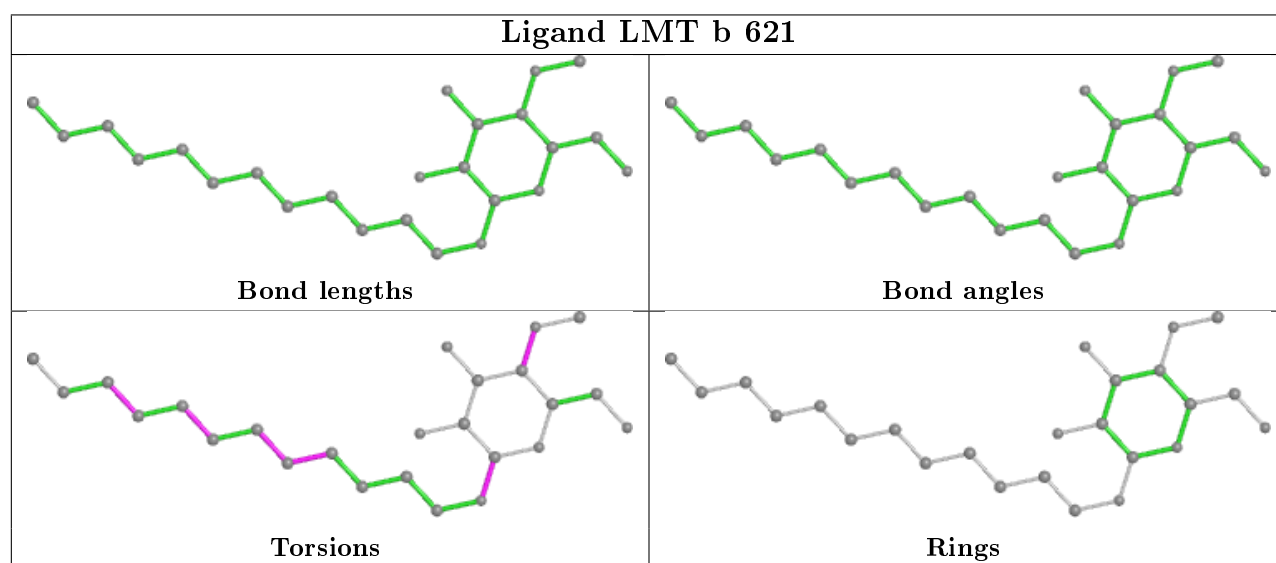
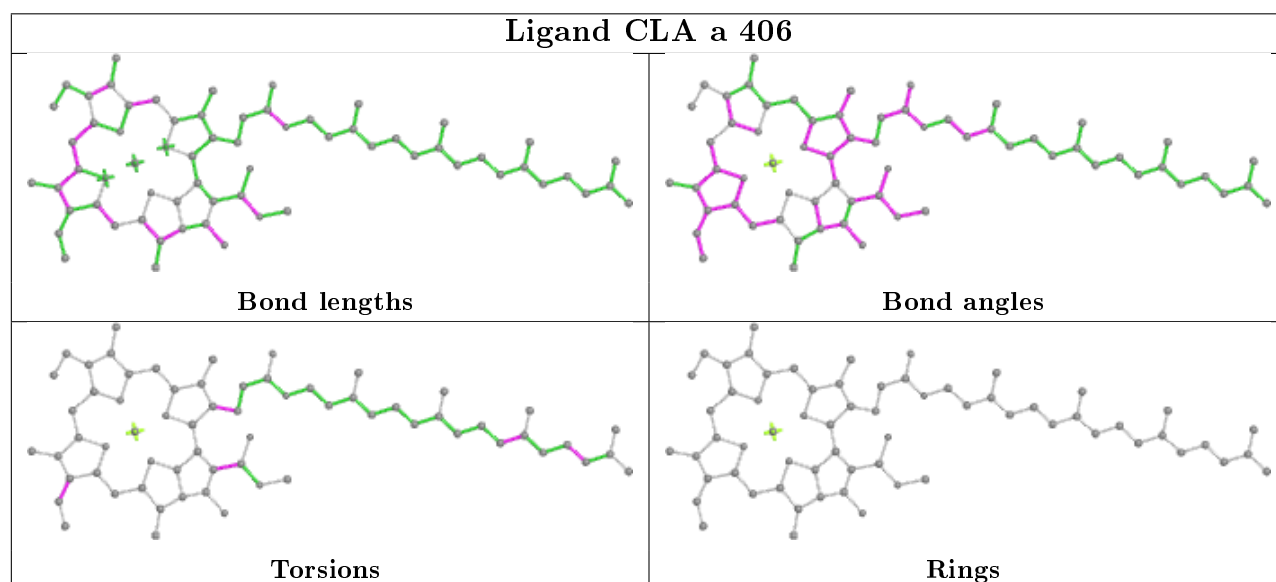
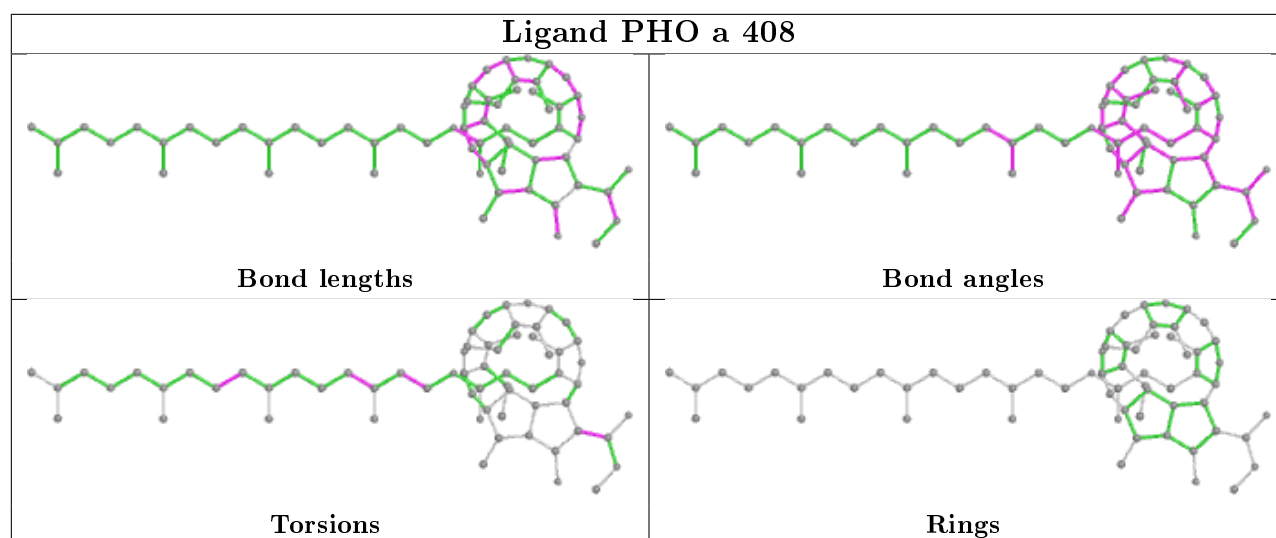


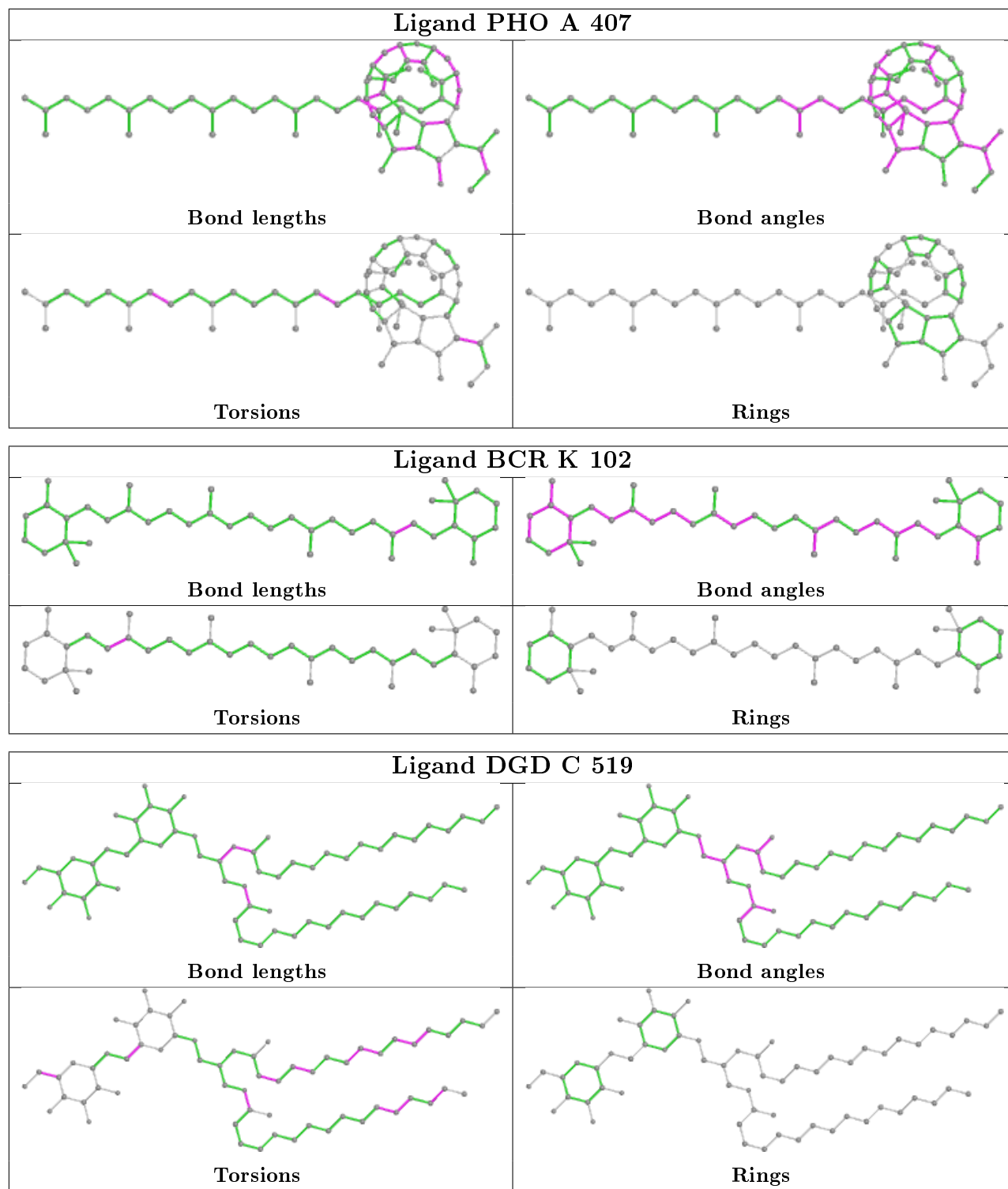
## Ligand LHG 1 101



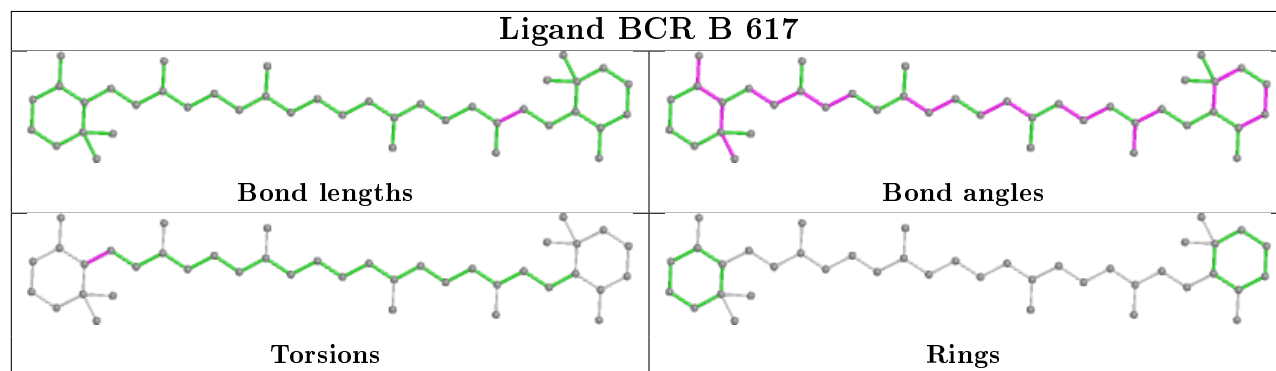
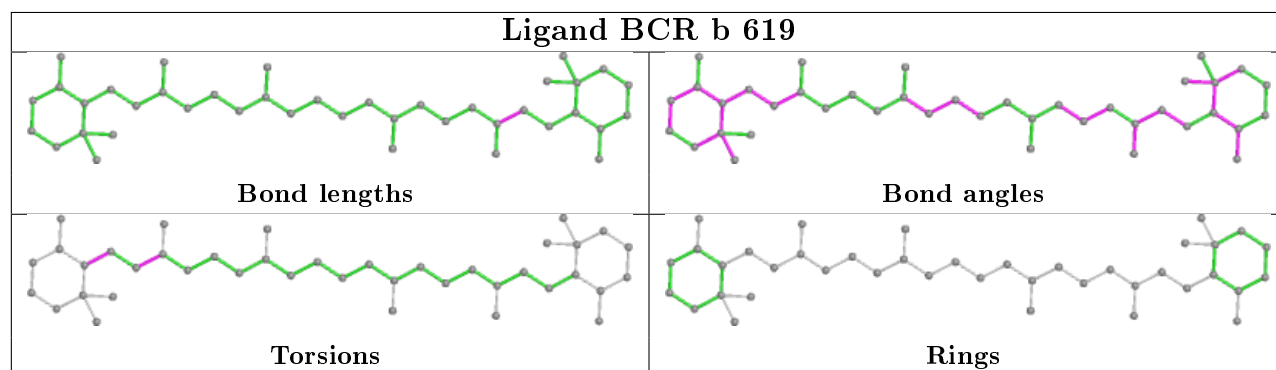
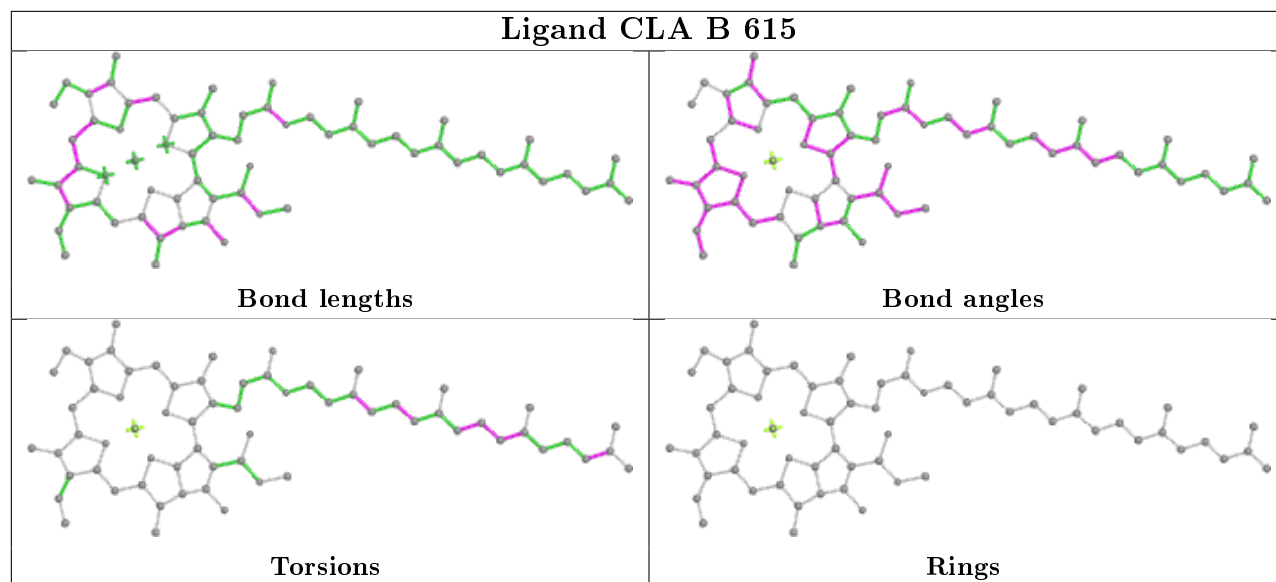
## Ligand BCR h 101



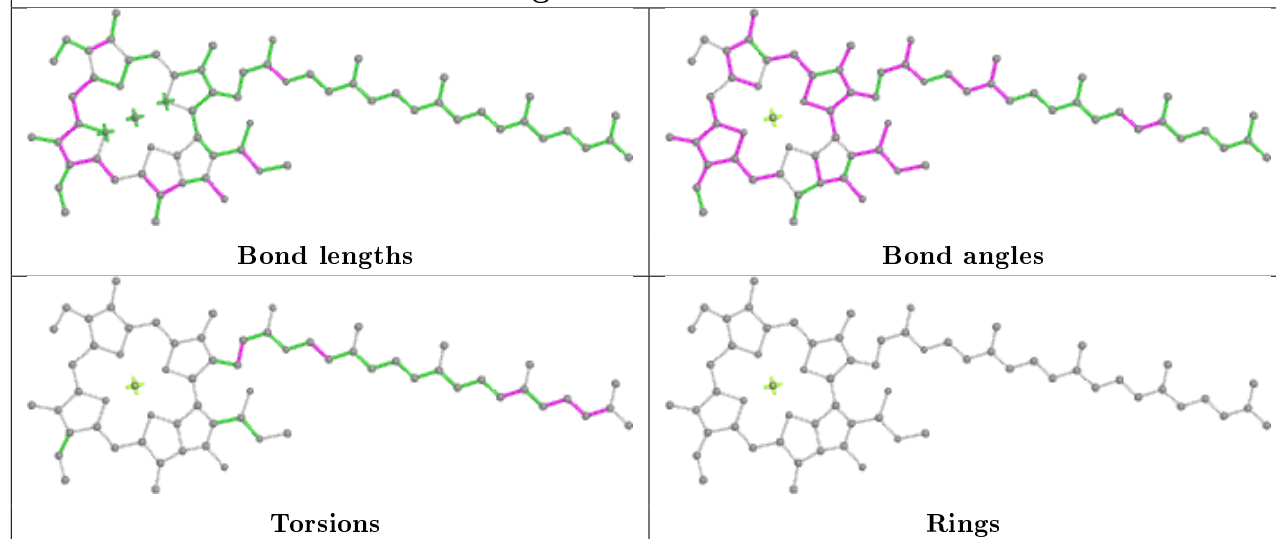




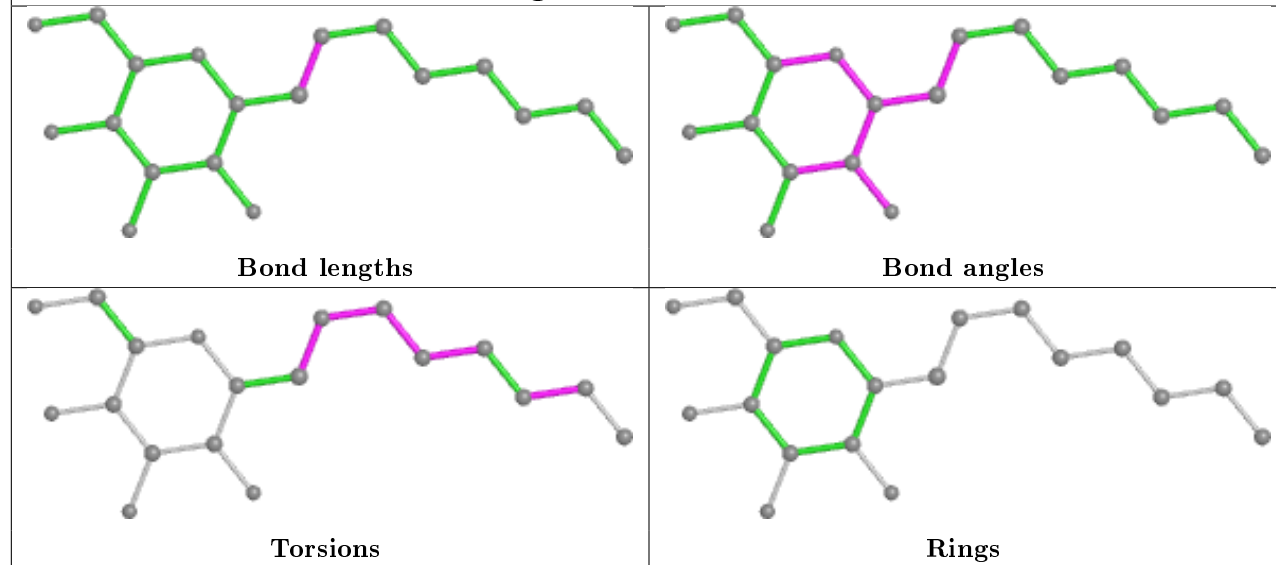




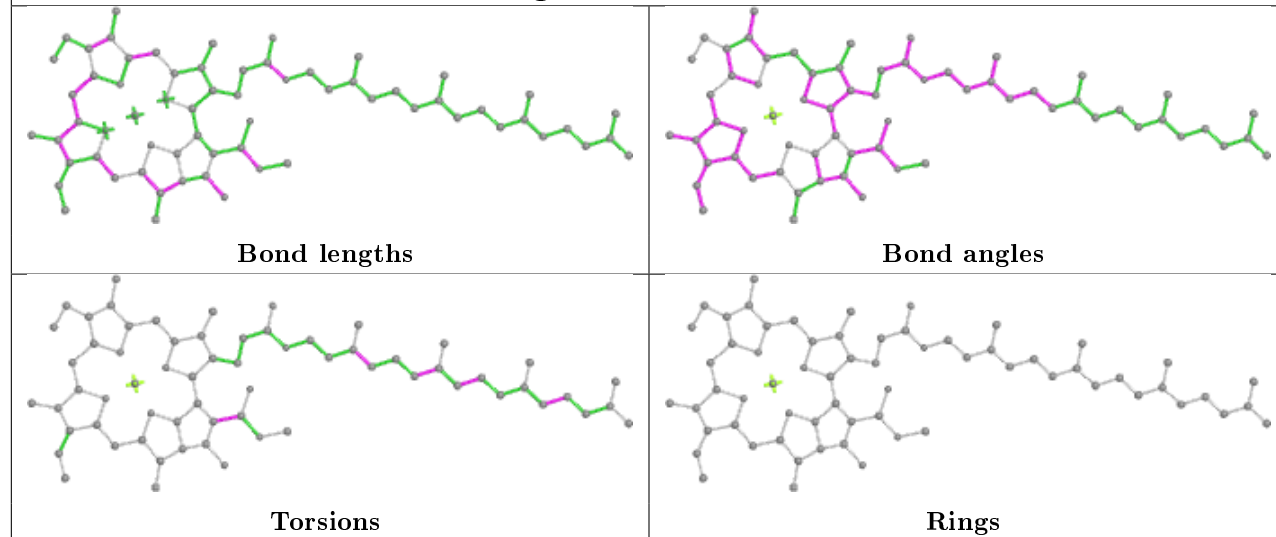
## Ligand CLA B 602



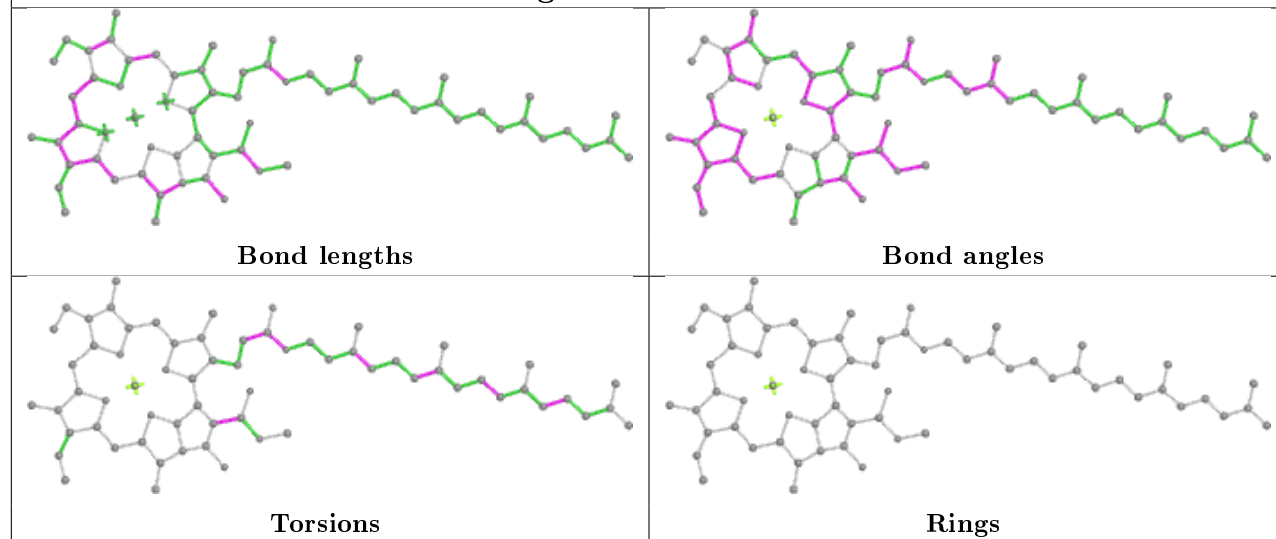
## Ligand HTG B 622



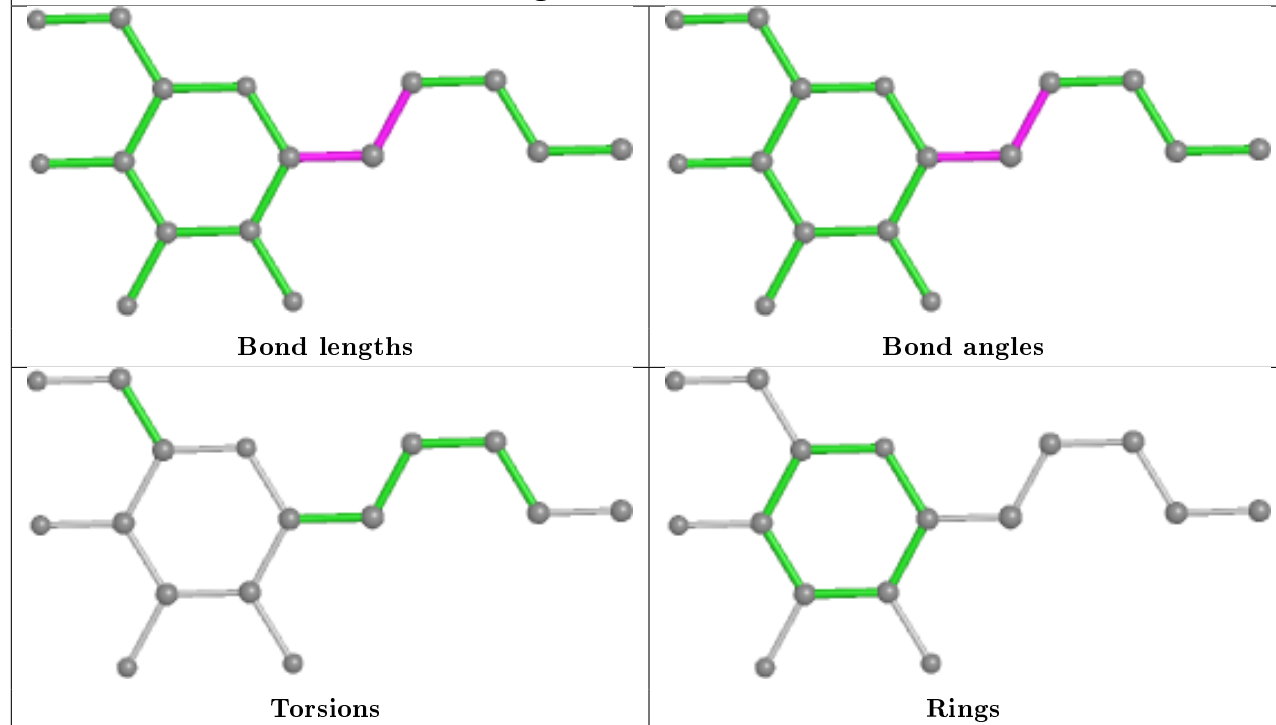
## Ligand CLA B 605



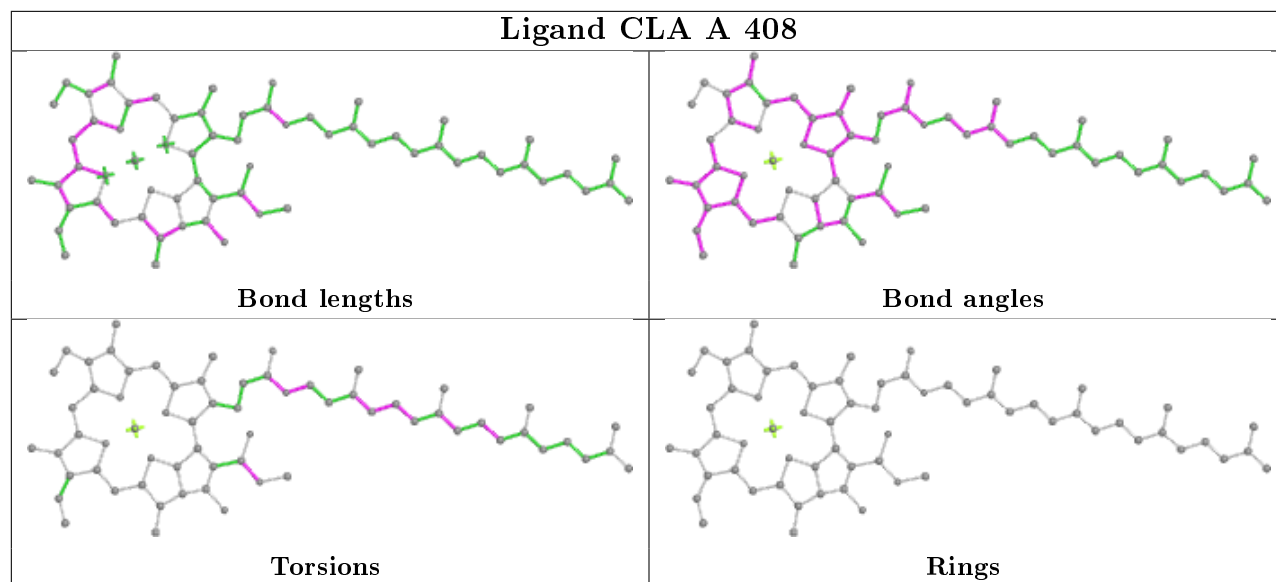
## Ligand CLA c 511



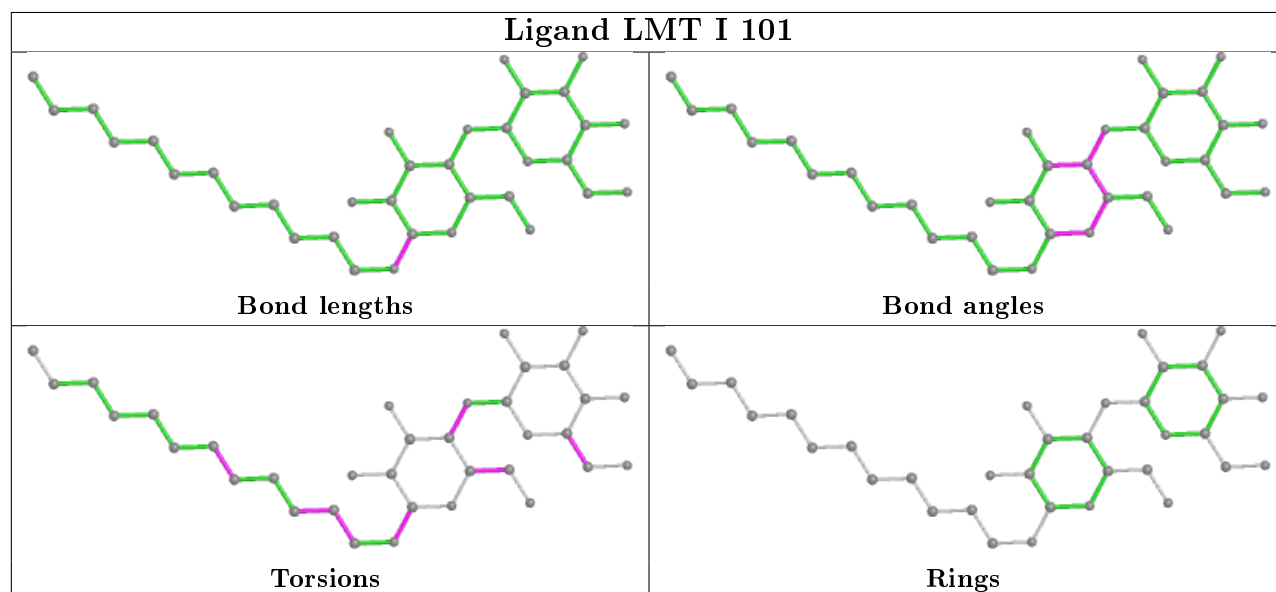
## Ligand HTG d 411



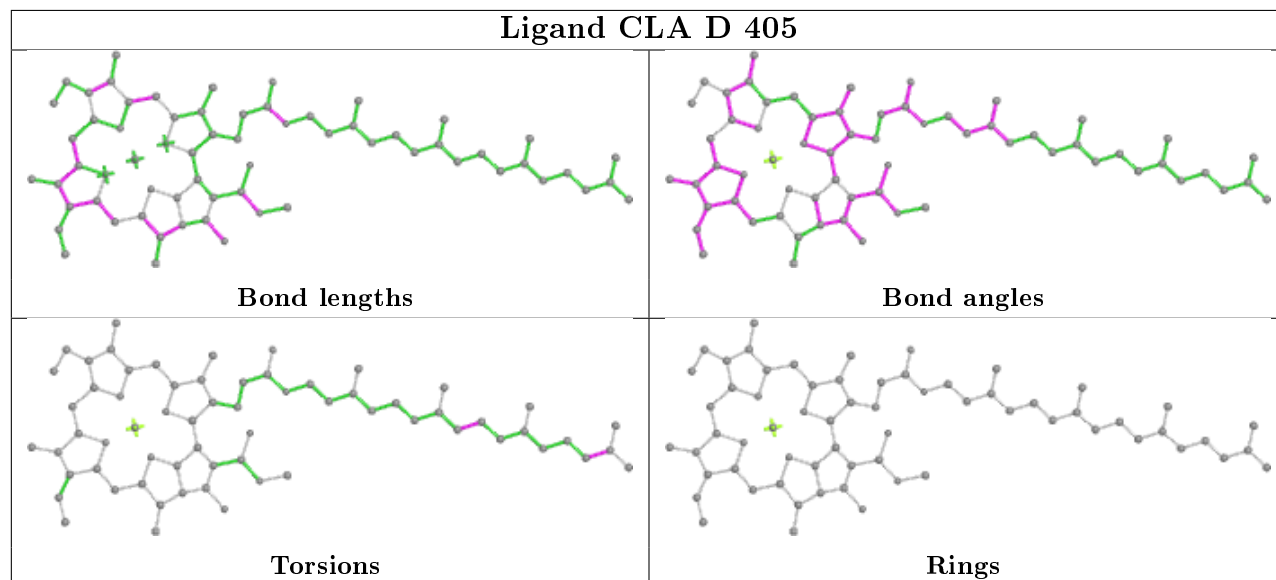
## Ligand CLA A 408

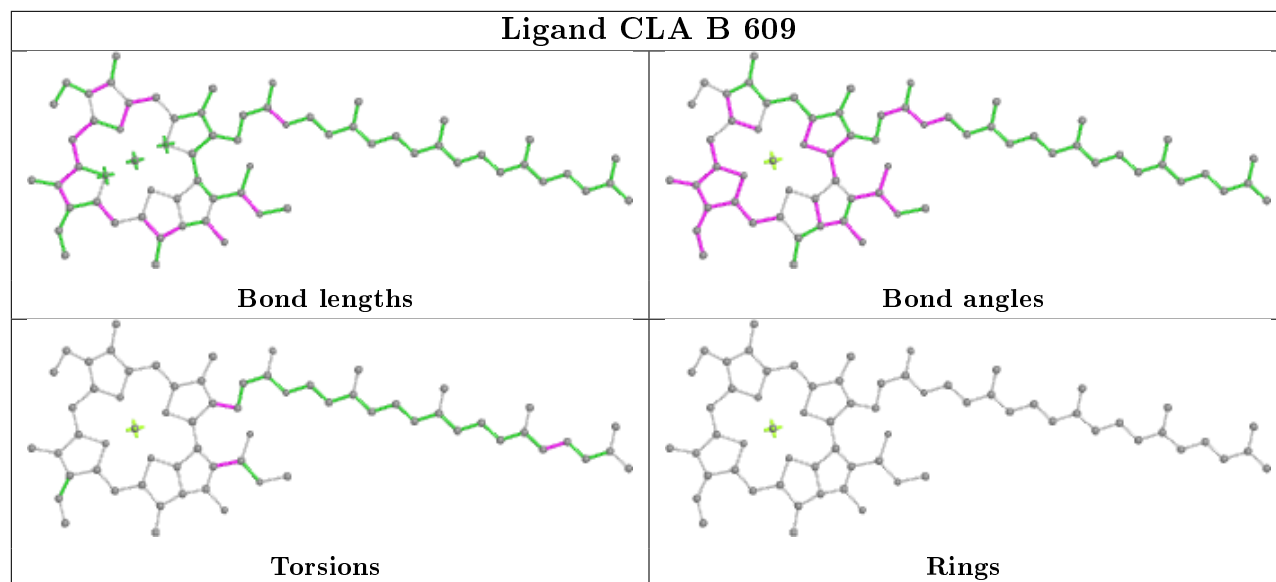
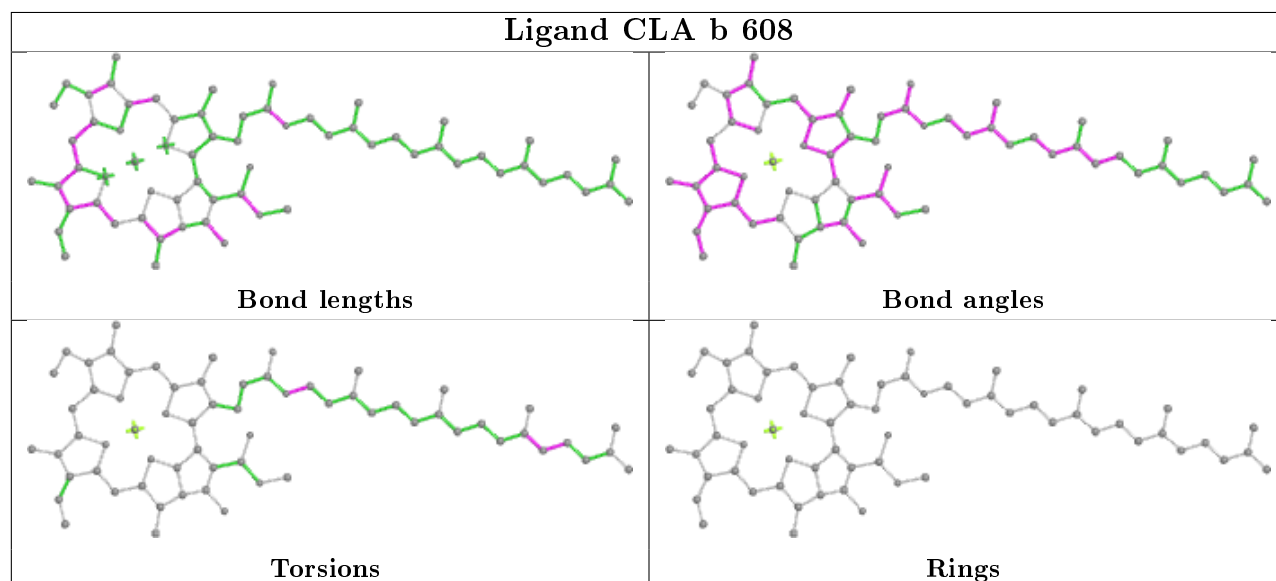
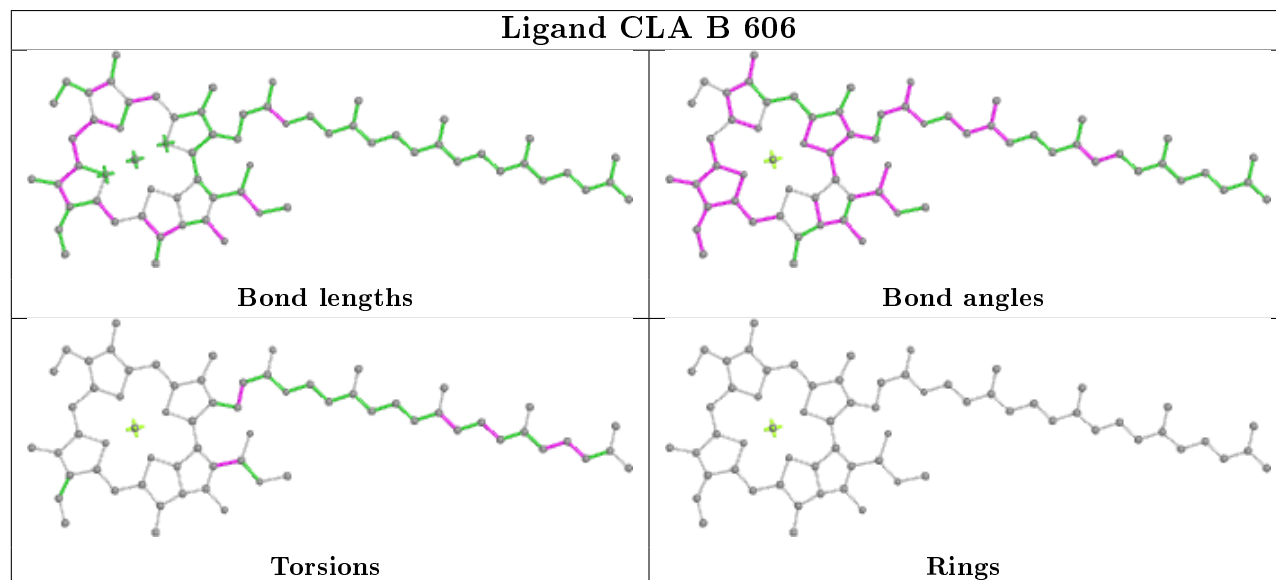


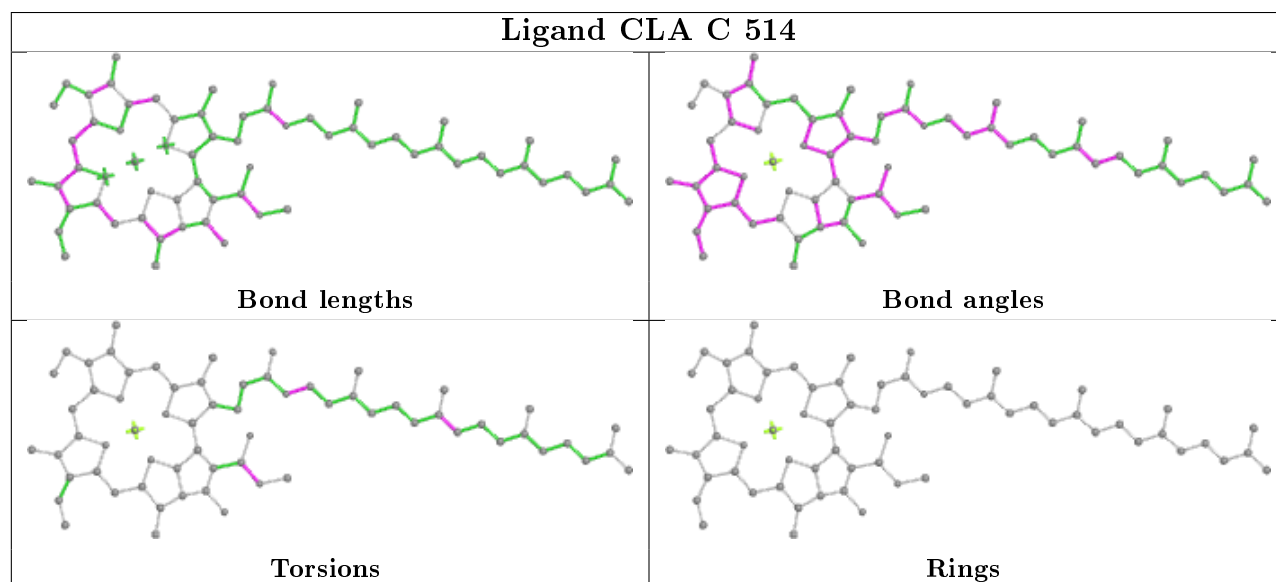
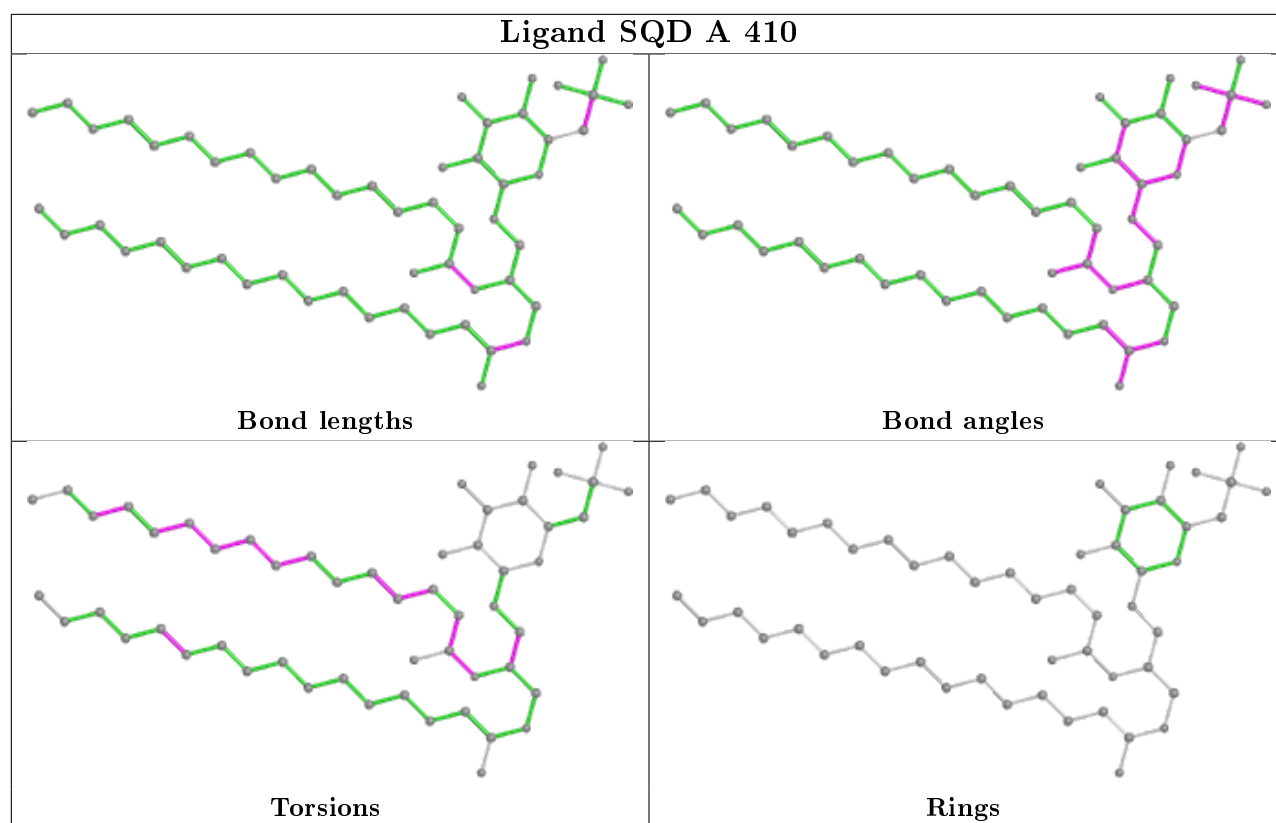
## Ligand LMT I 101



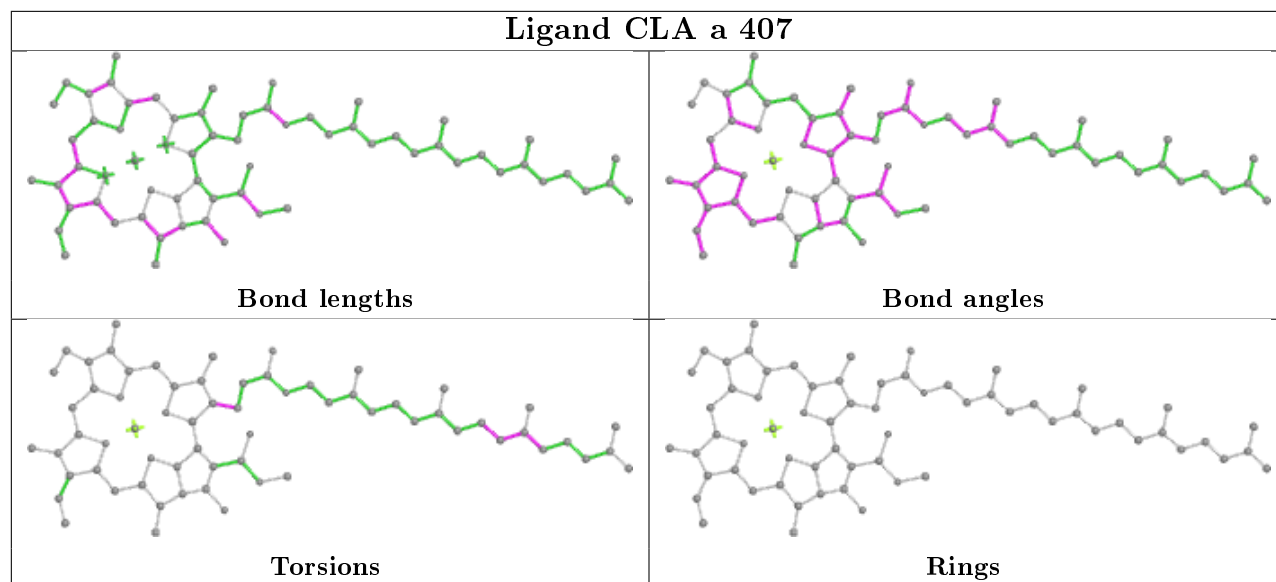
## Ligand CLA D 405



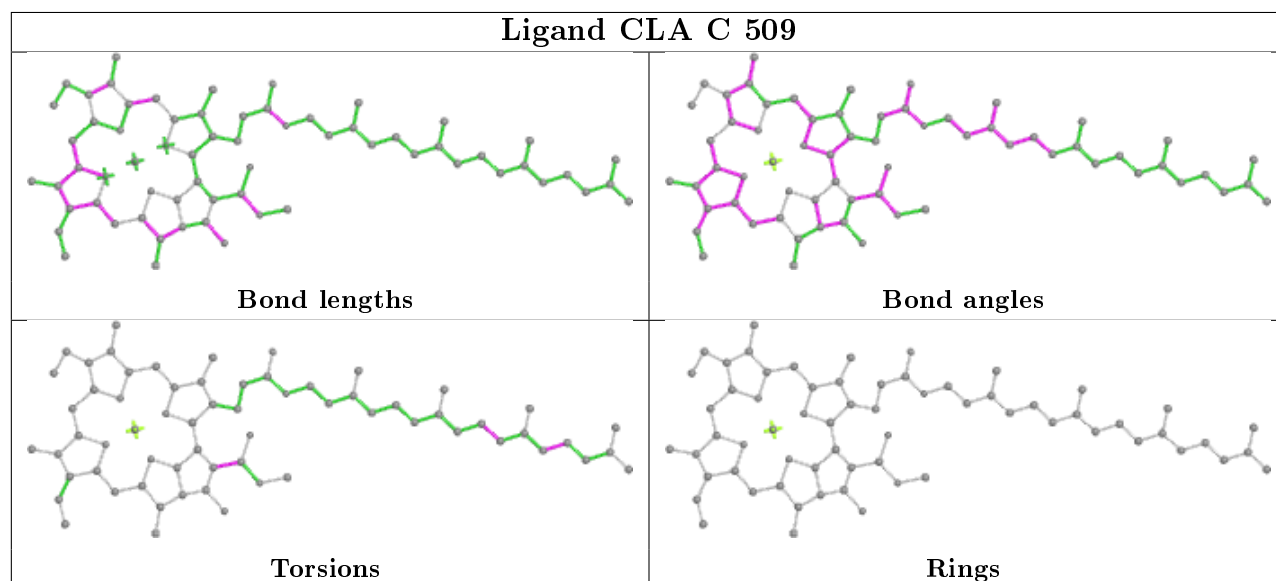
**Ligand CLA B 609****Ligand CLA b 608****Ligand CLA B 606**



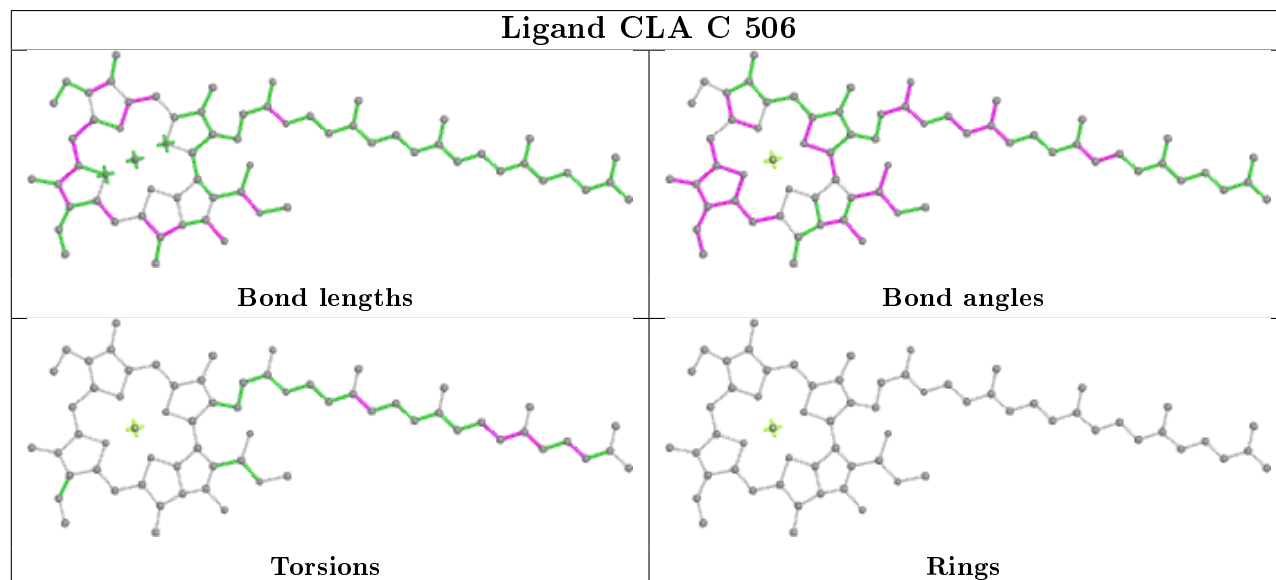
## Ligand CLA a 407



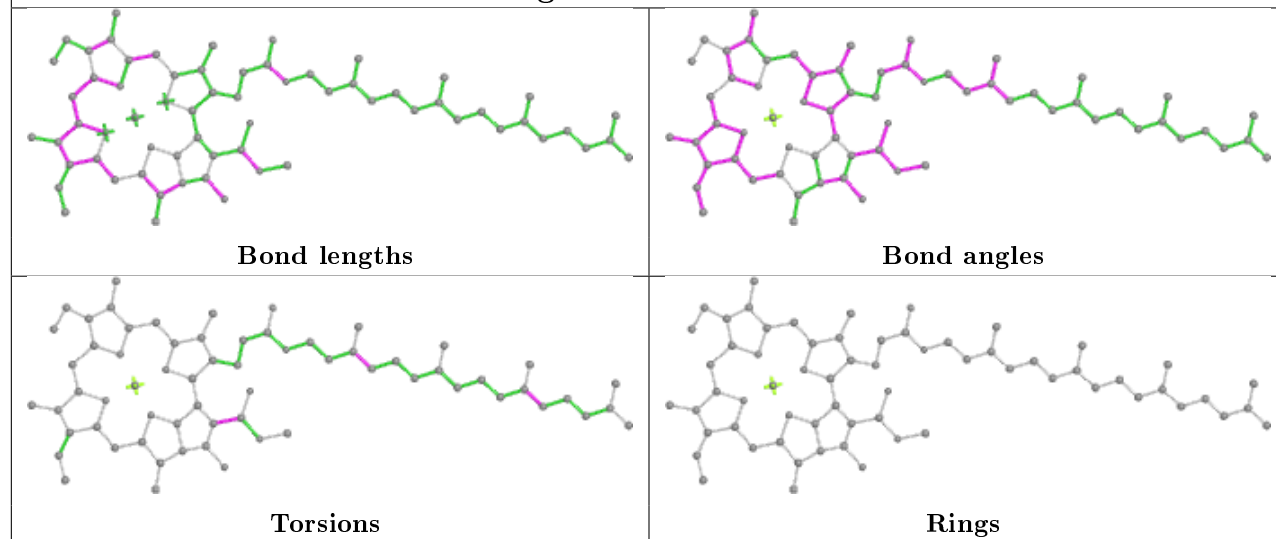
## Ligand CLA C 509



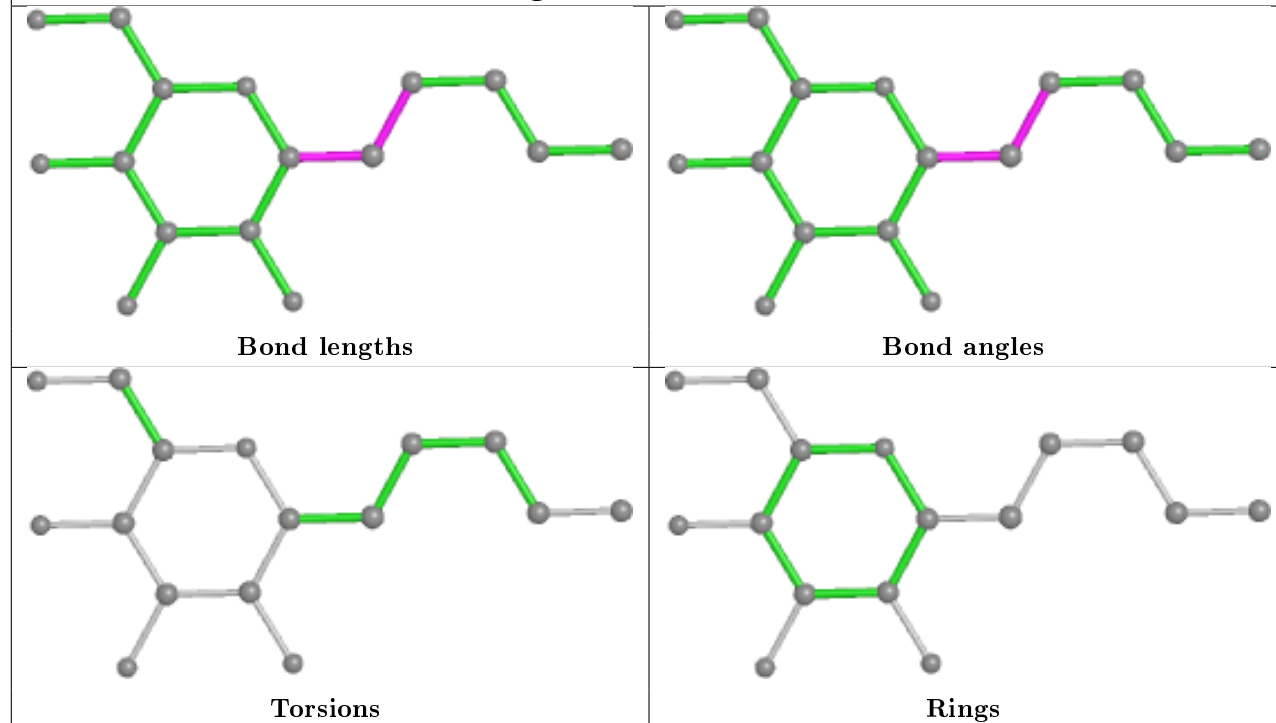
## Ligand CLA C 506



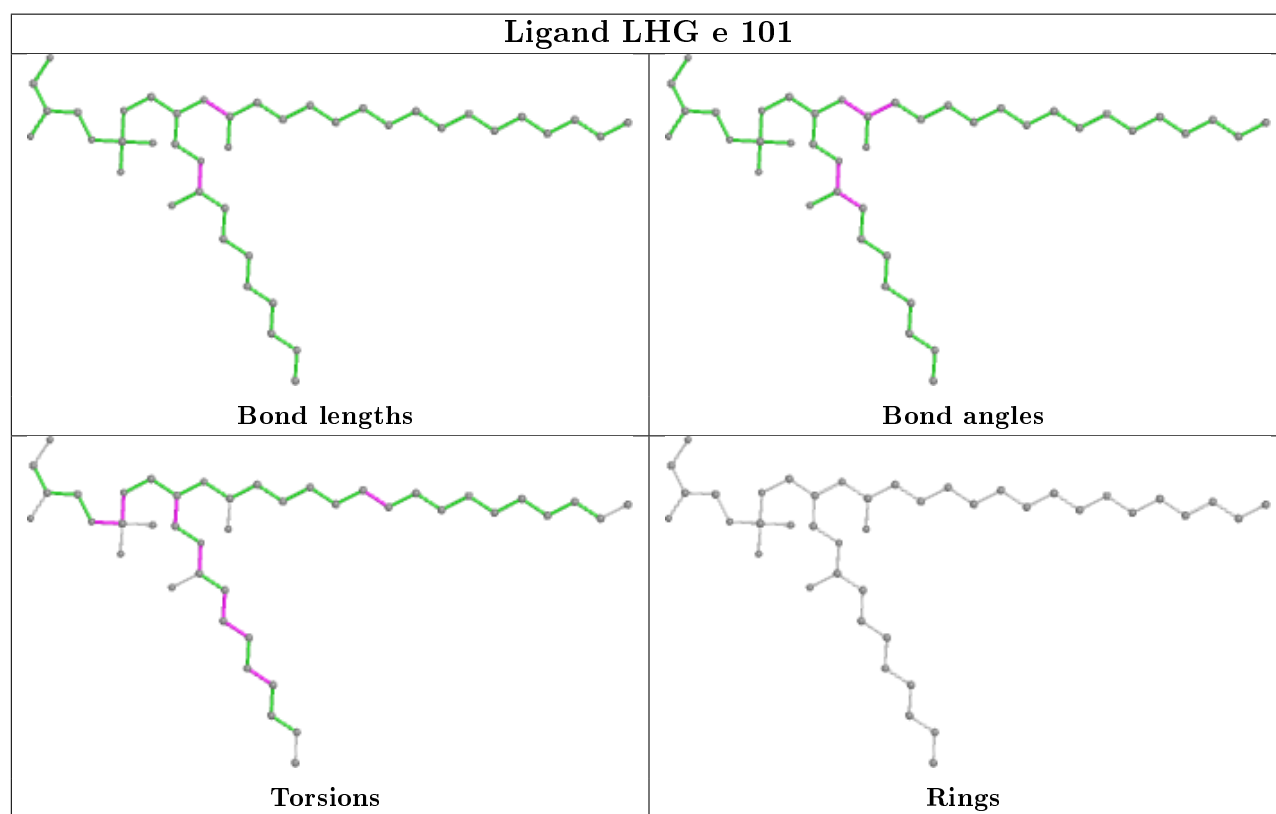
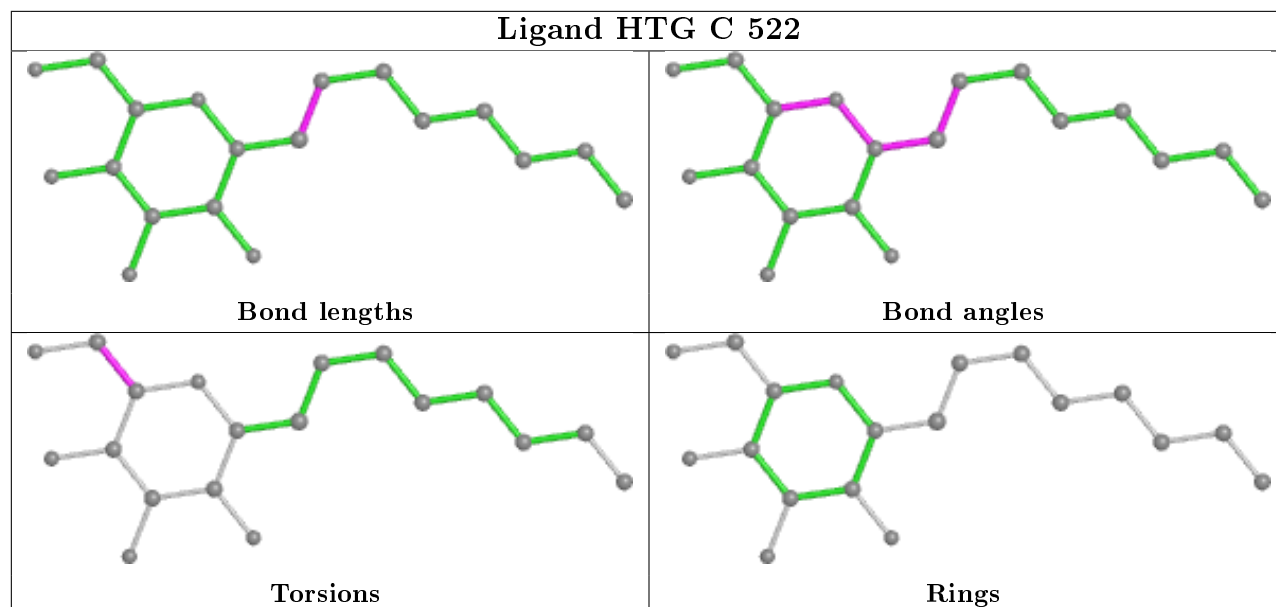
## Ligand CLA c 505

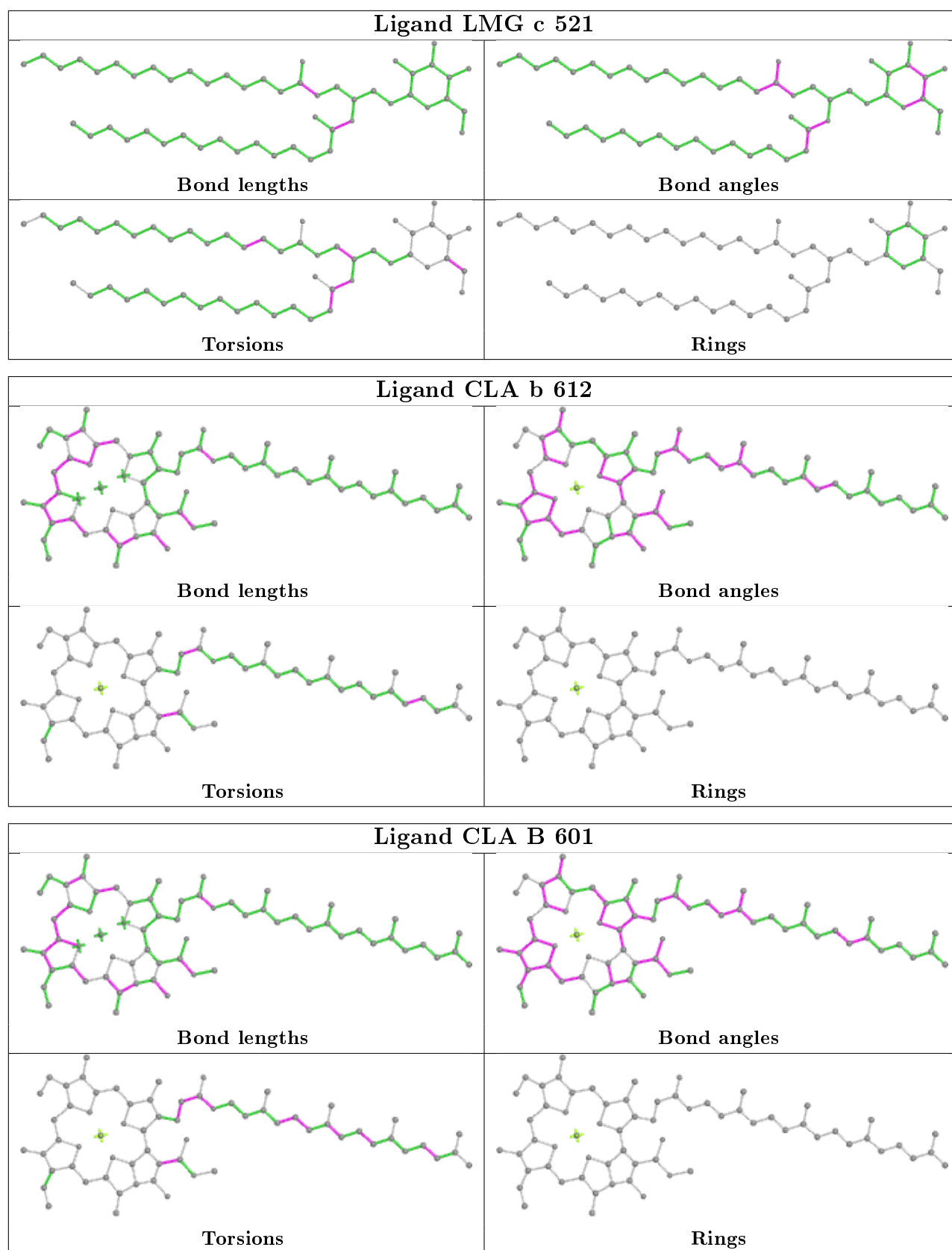


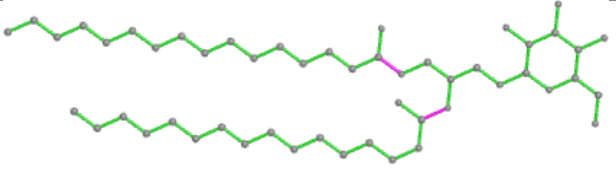
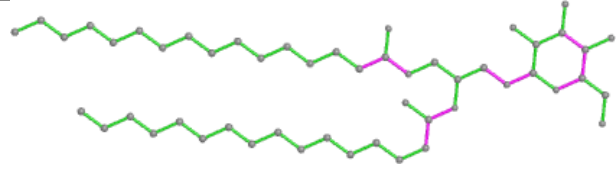
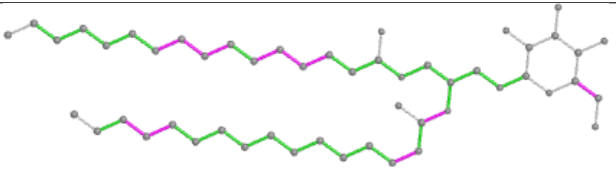
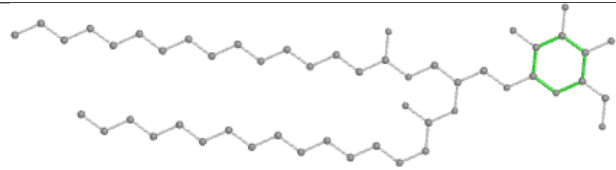
## Ligand HTG D 414

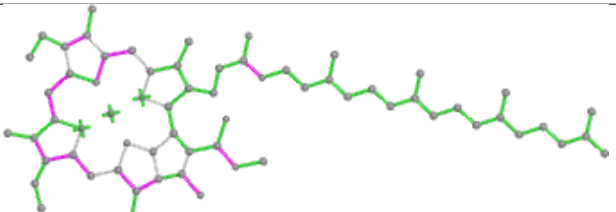
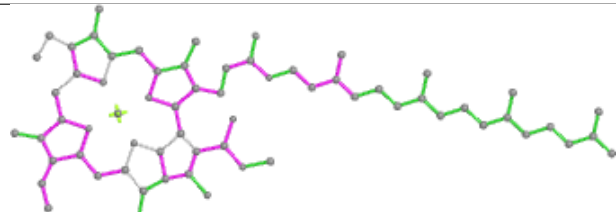
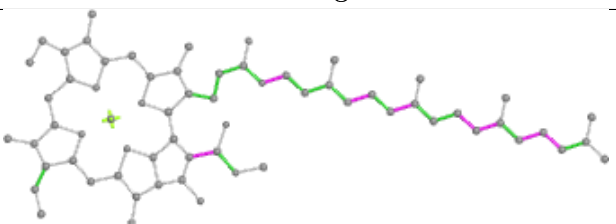
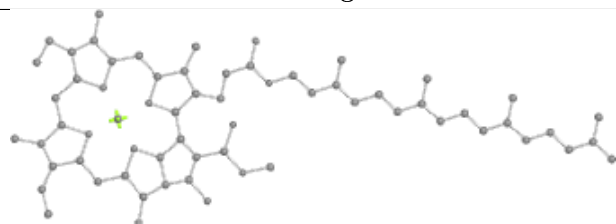



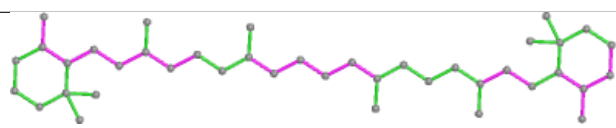
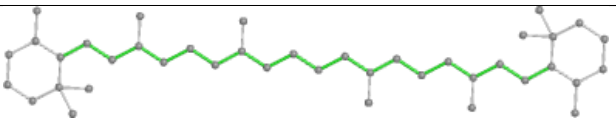
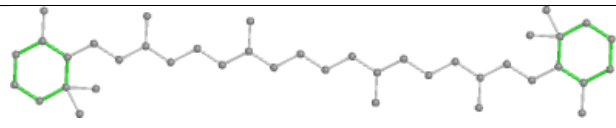


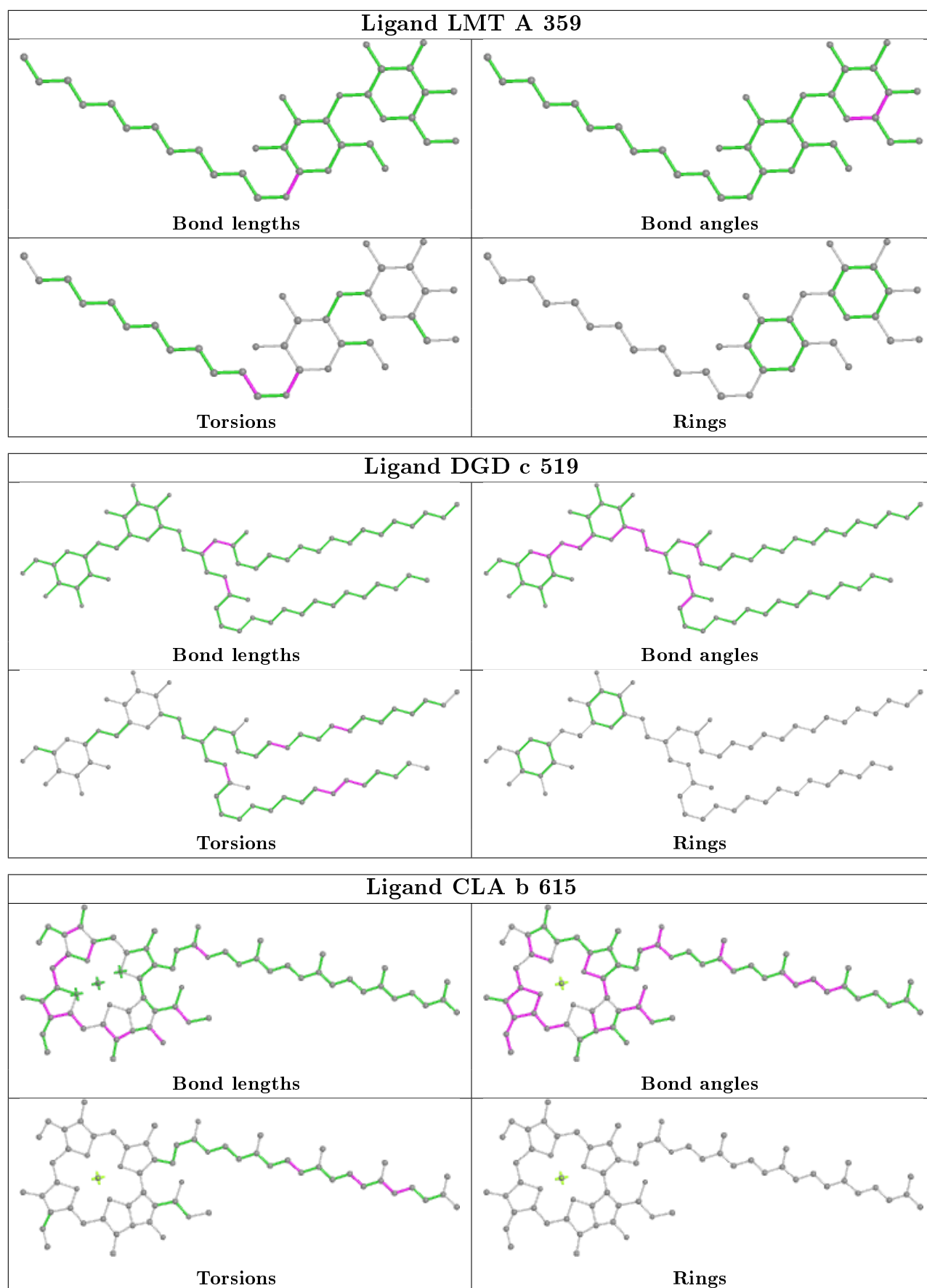


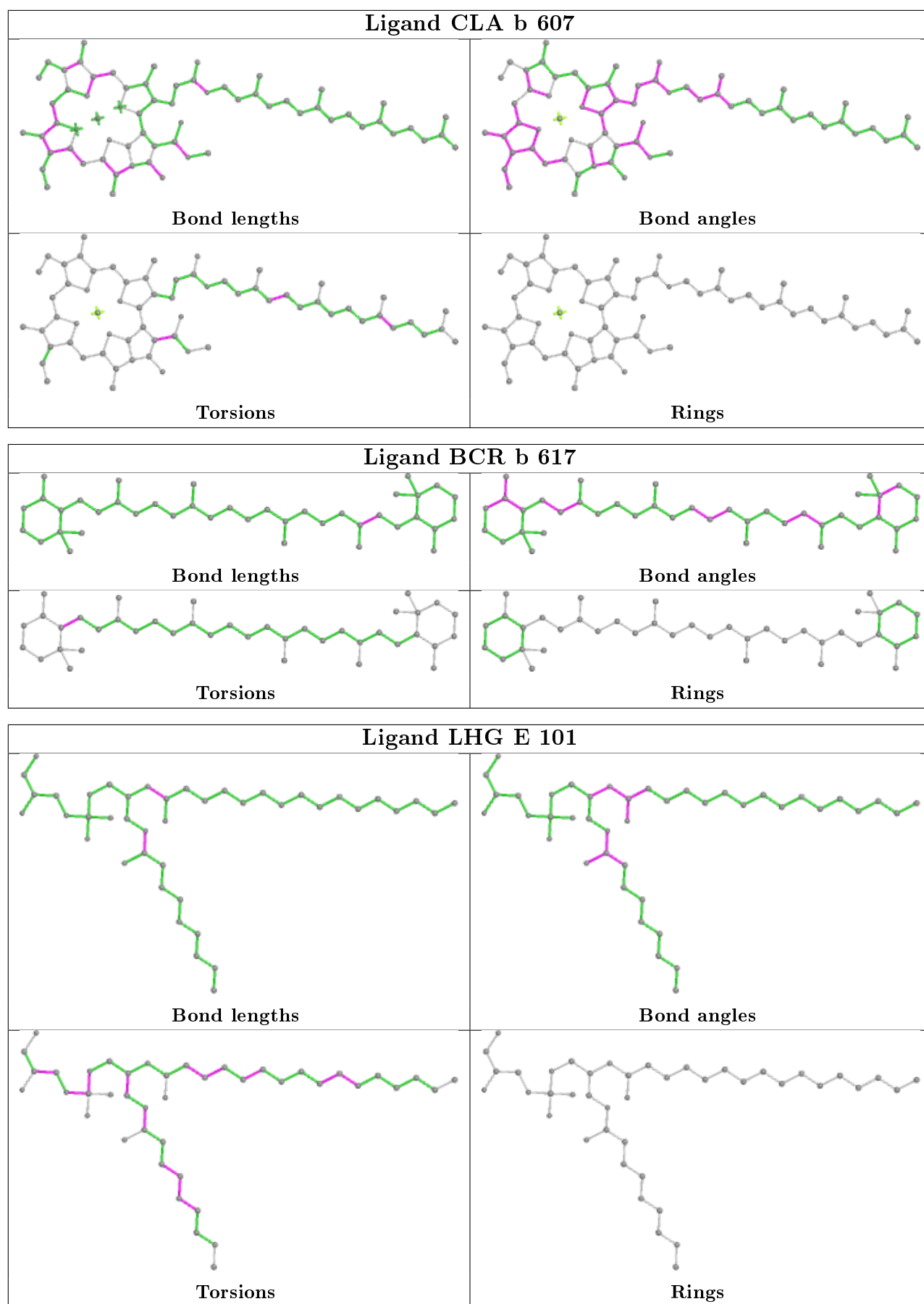


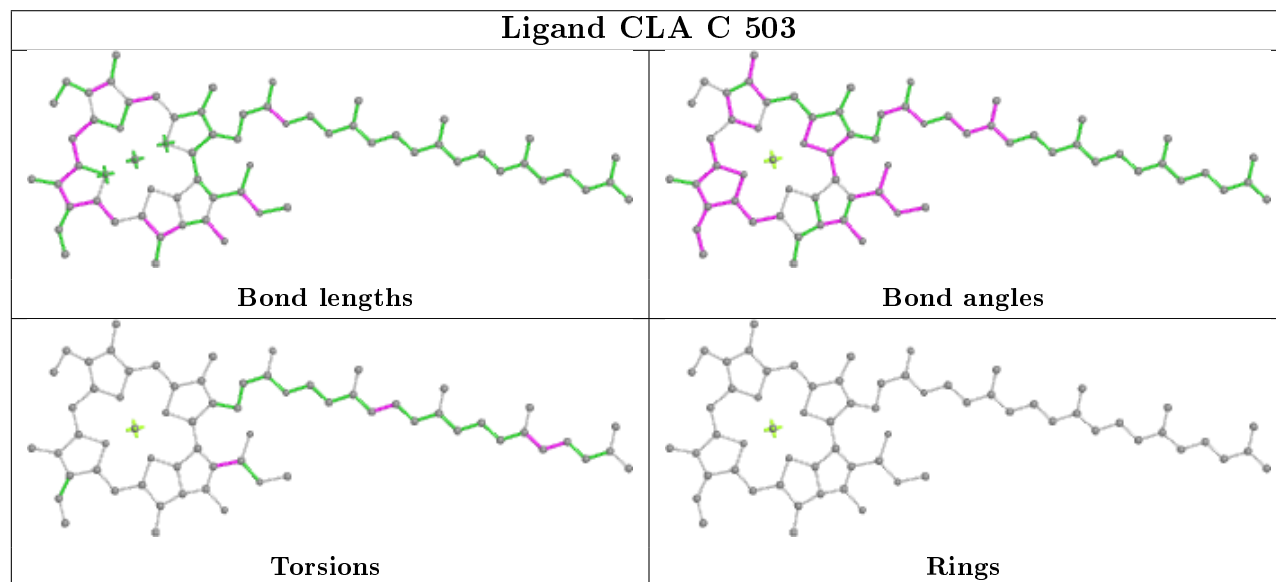
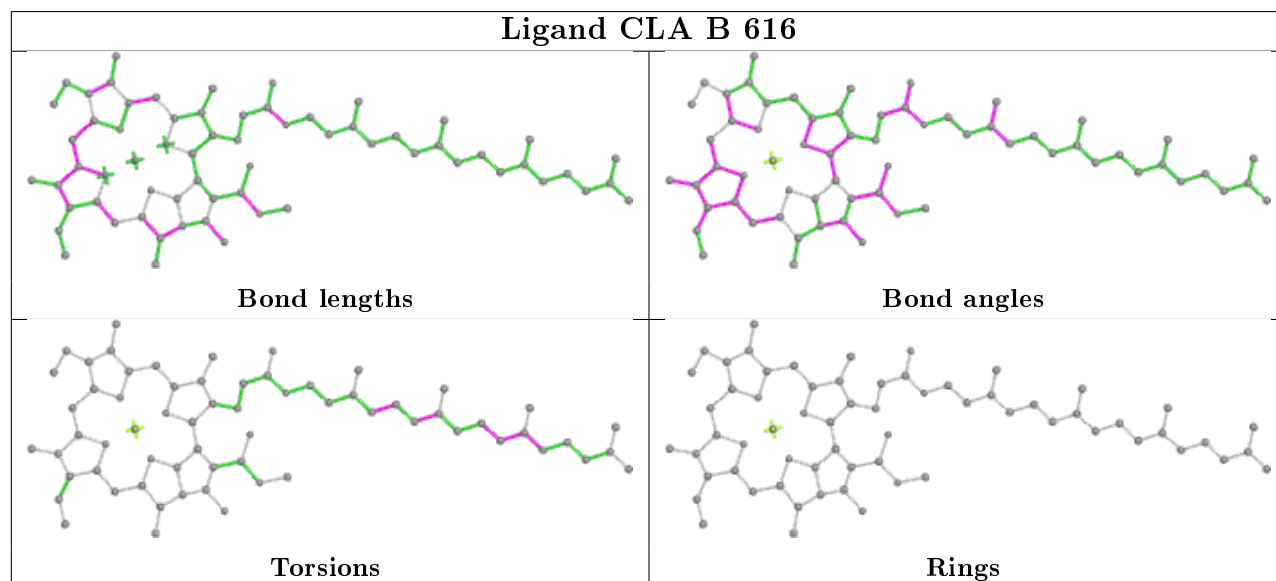
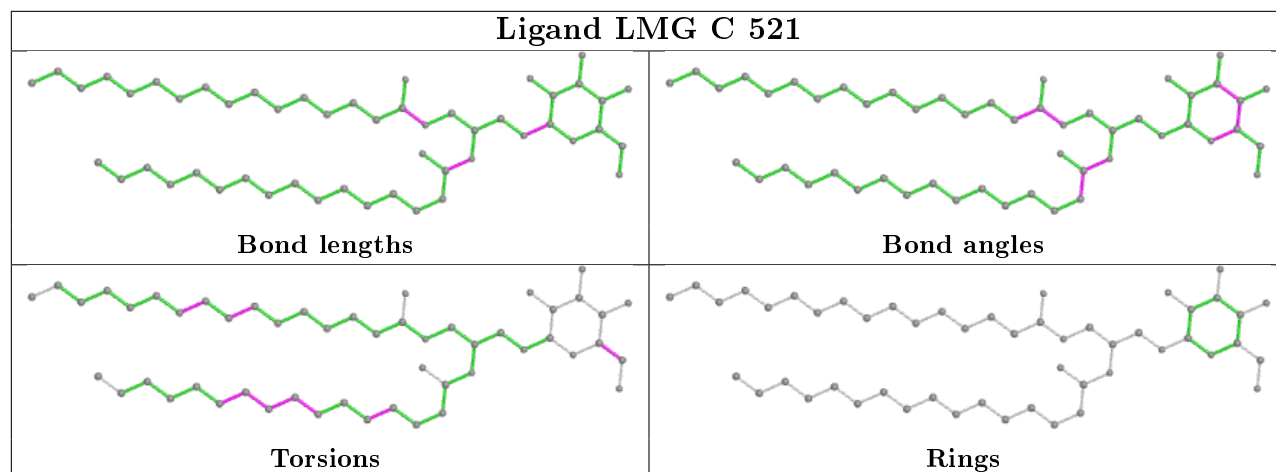
Ligand LMG a 419	
	
Bond lengths	Bond angles
	
Torsions	Rings

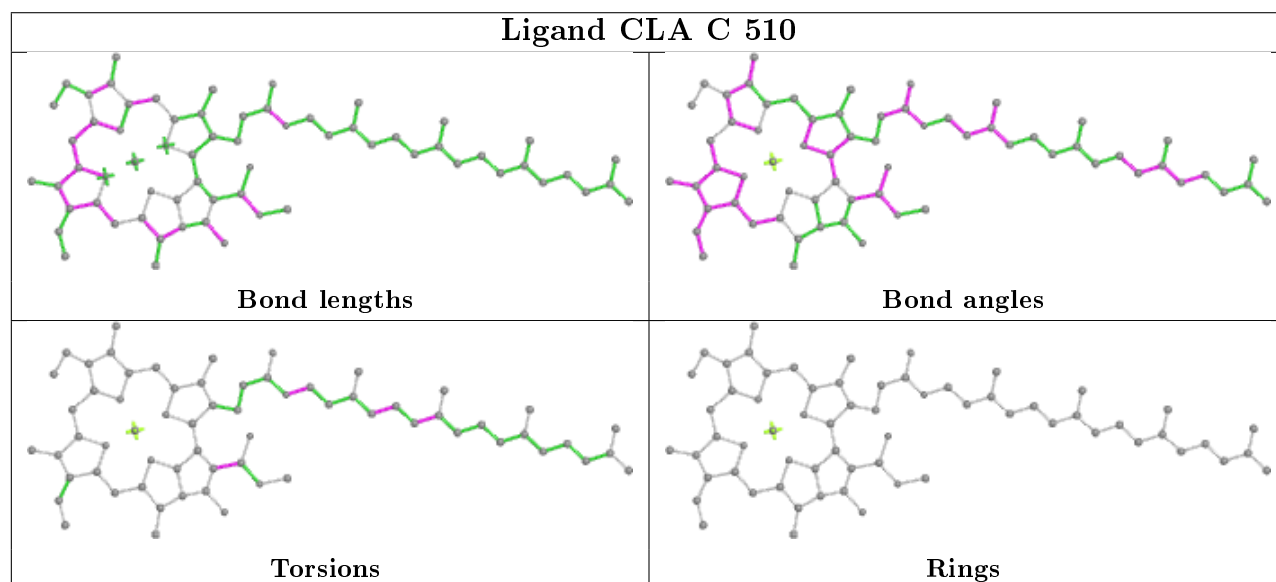
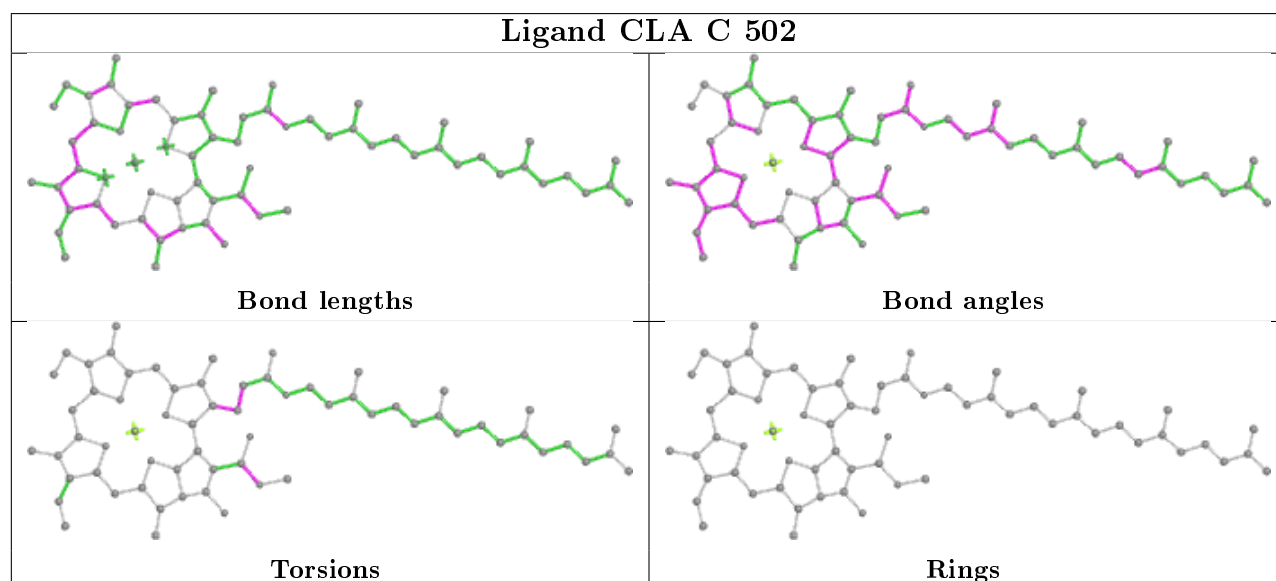
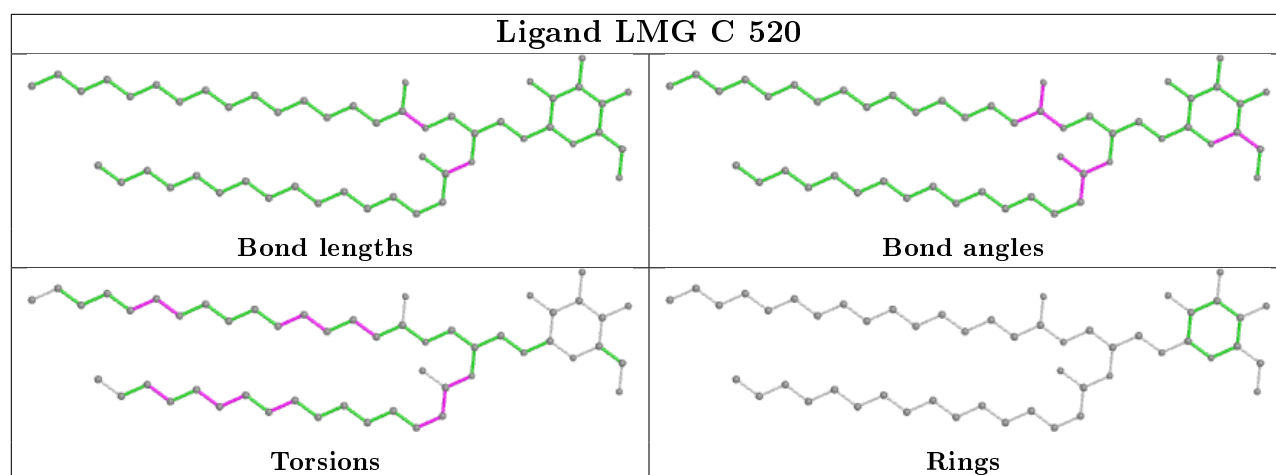
Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

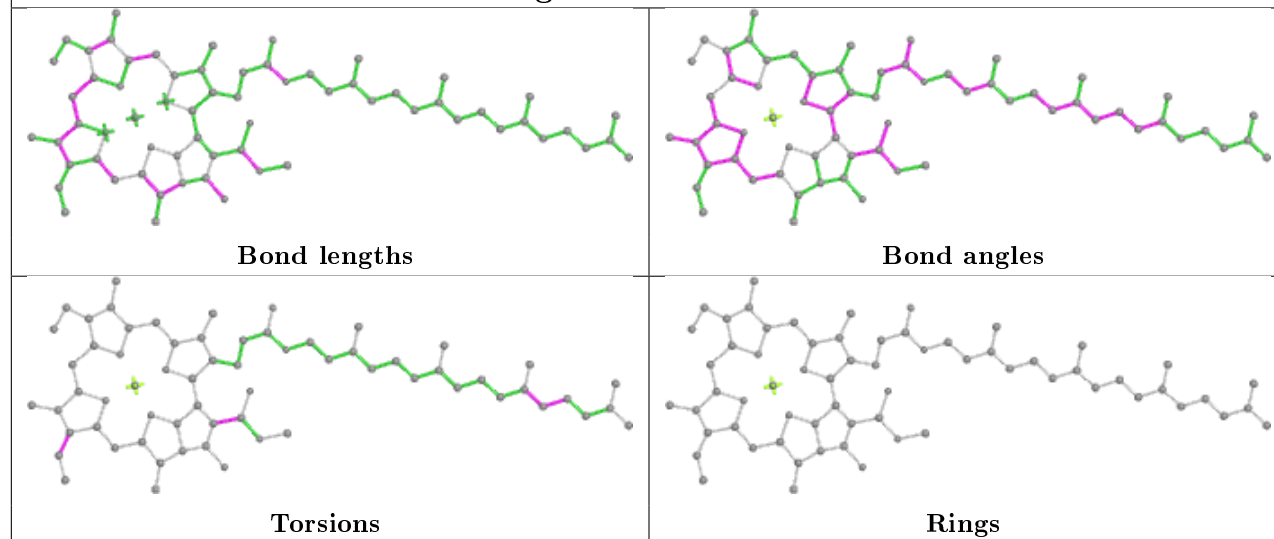
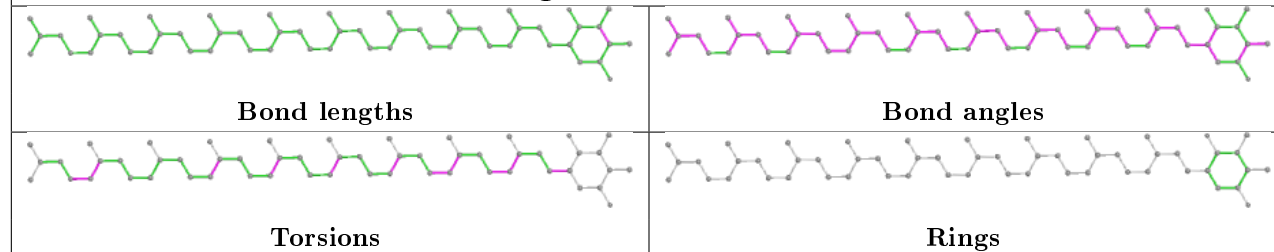
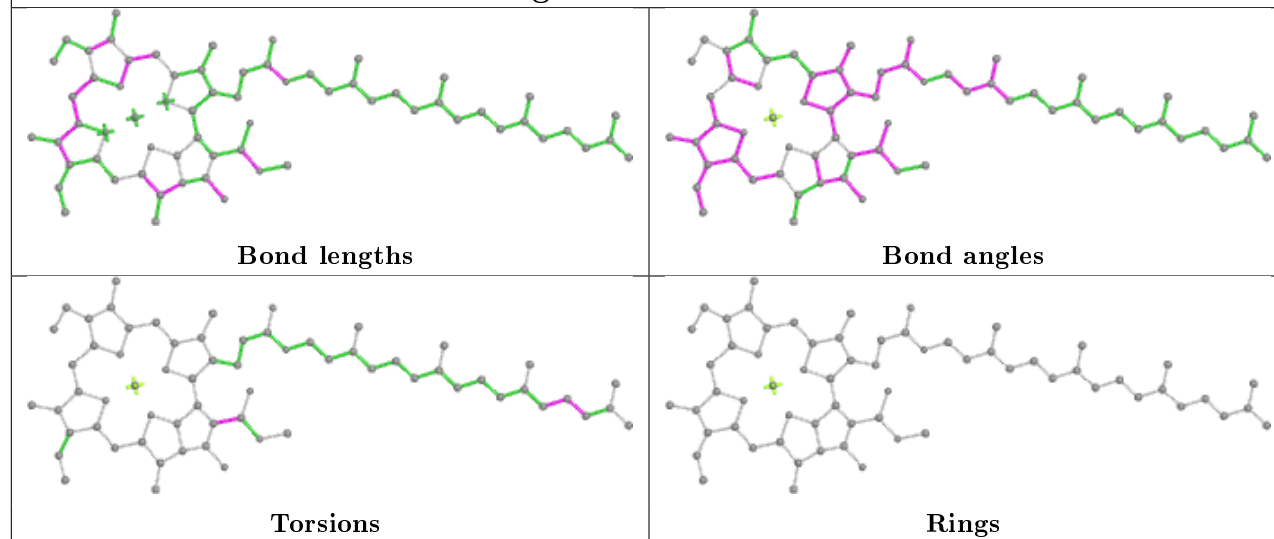
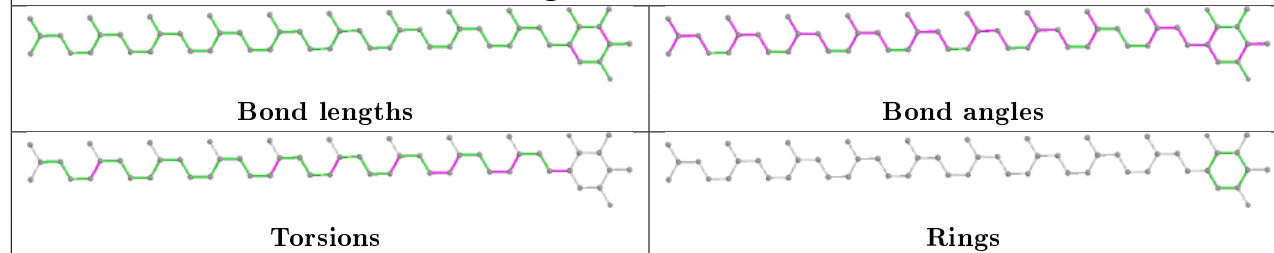
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



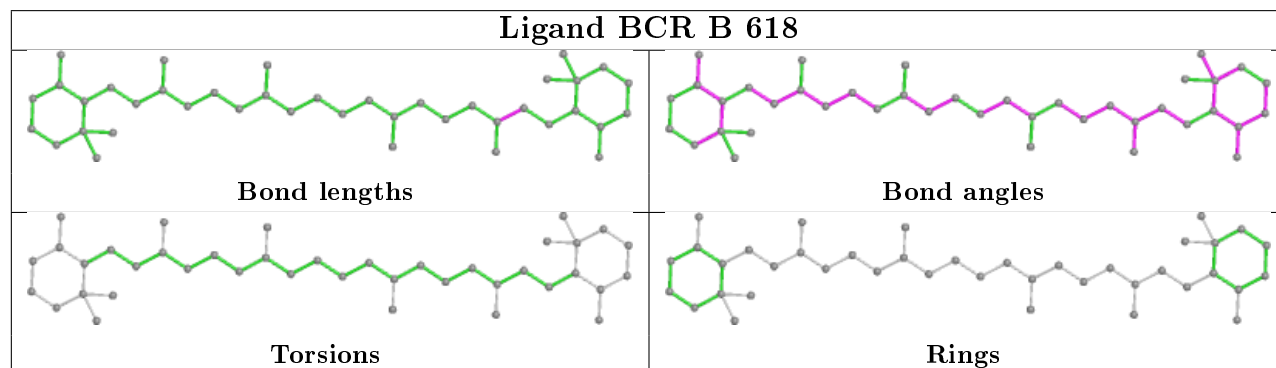
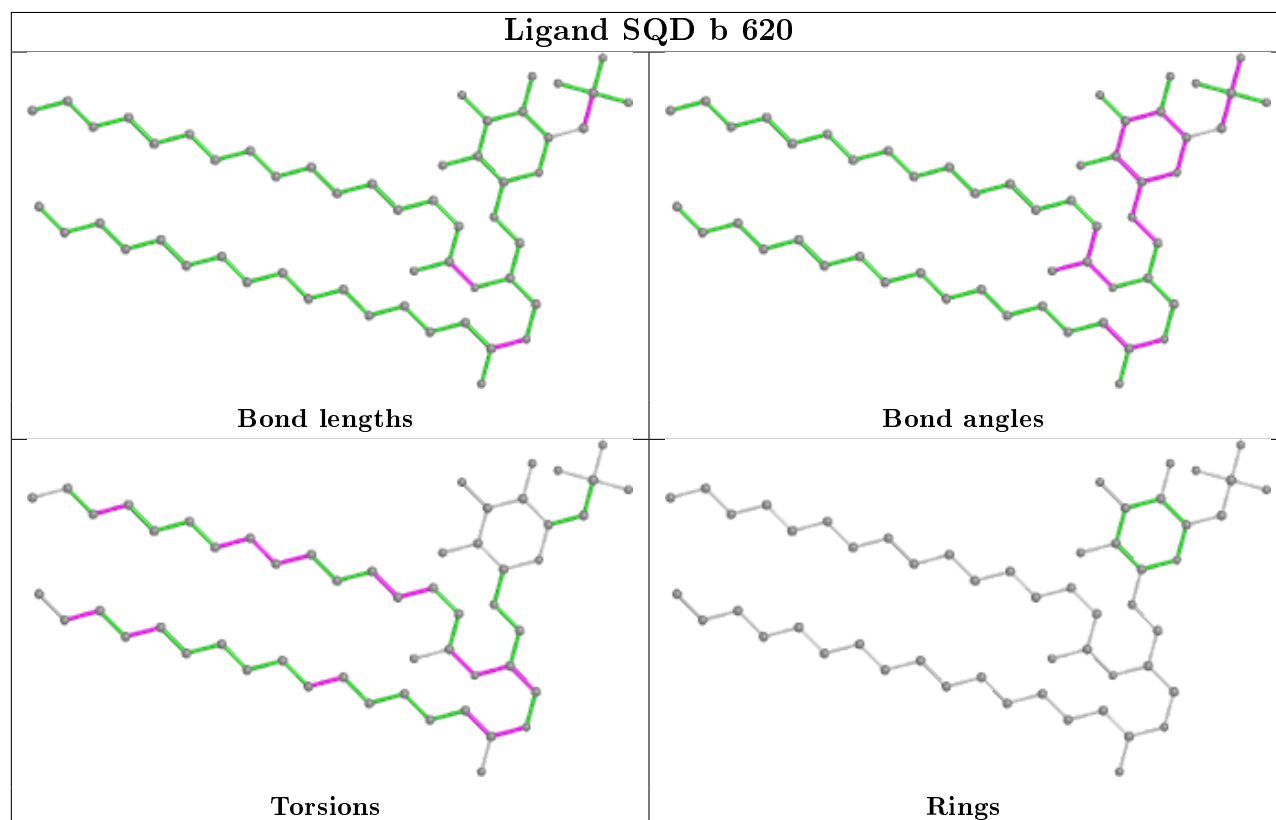
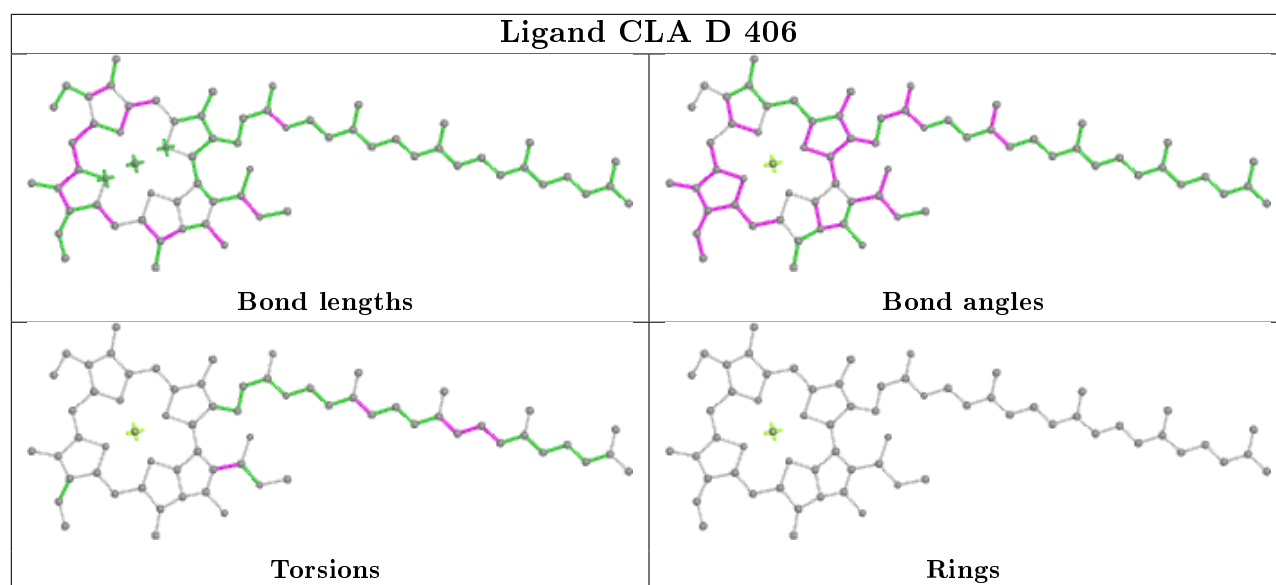




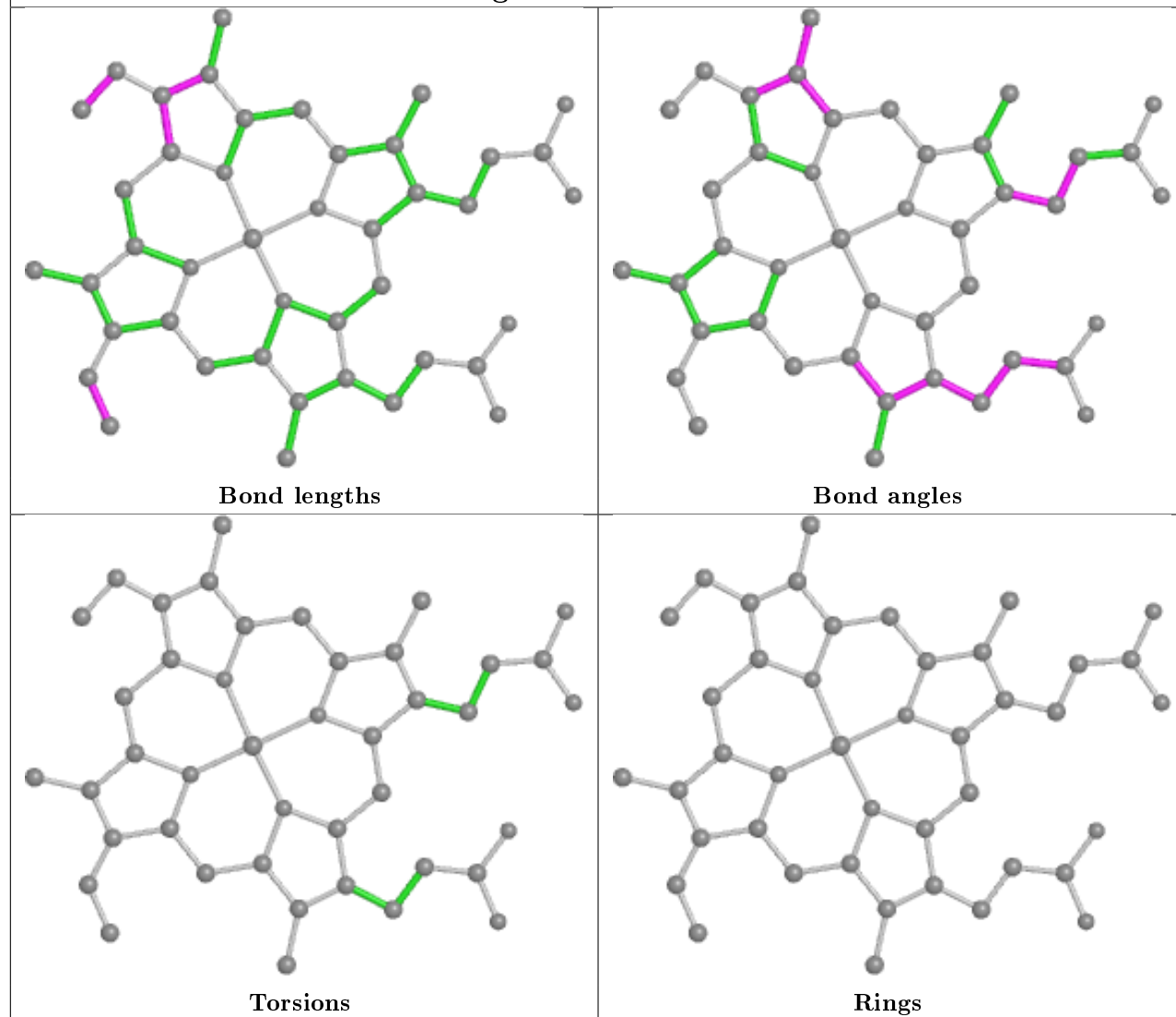


**Ligand CLA b 604****Ligand PL9 A 414****Ligand CLA A 405****Ligand PL9 a 416**

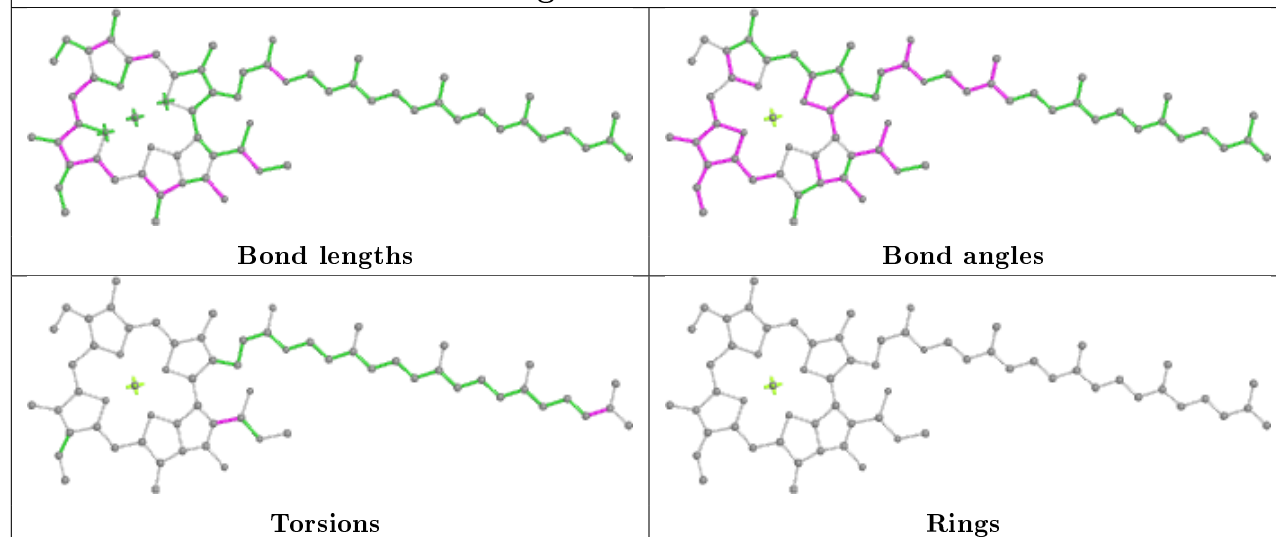




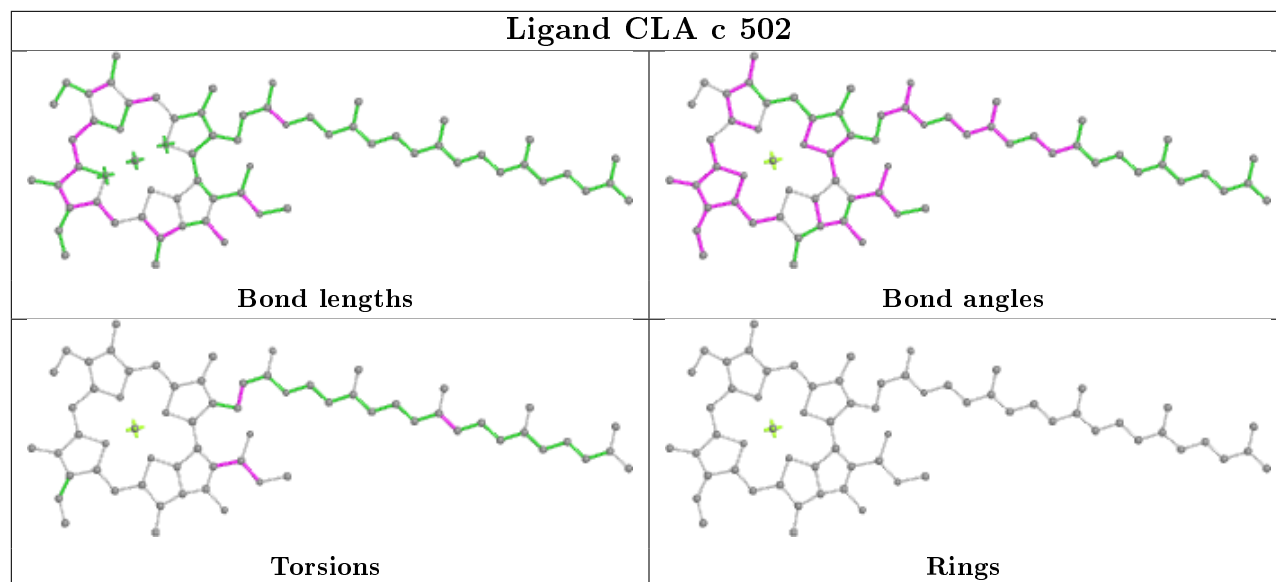
## Ligand HEC v 202



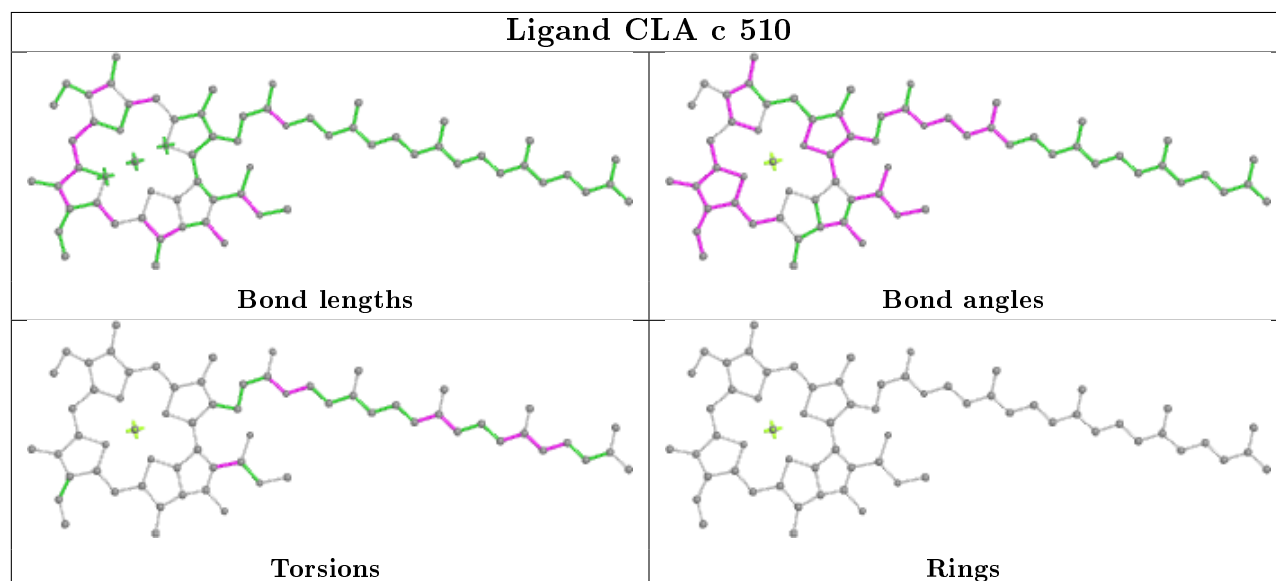
## Ligand CLA c 503



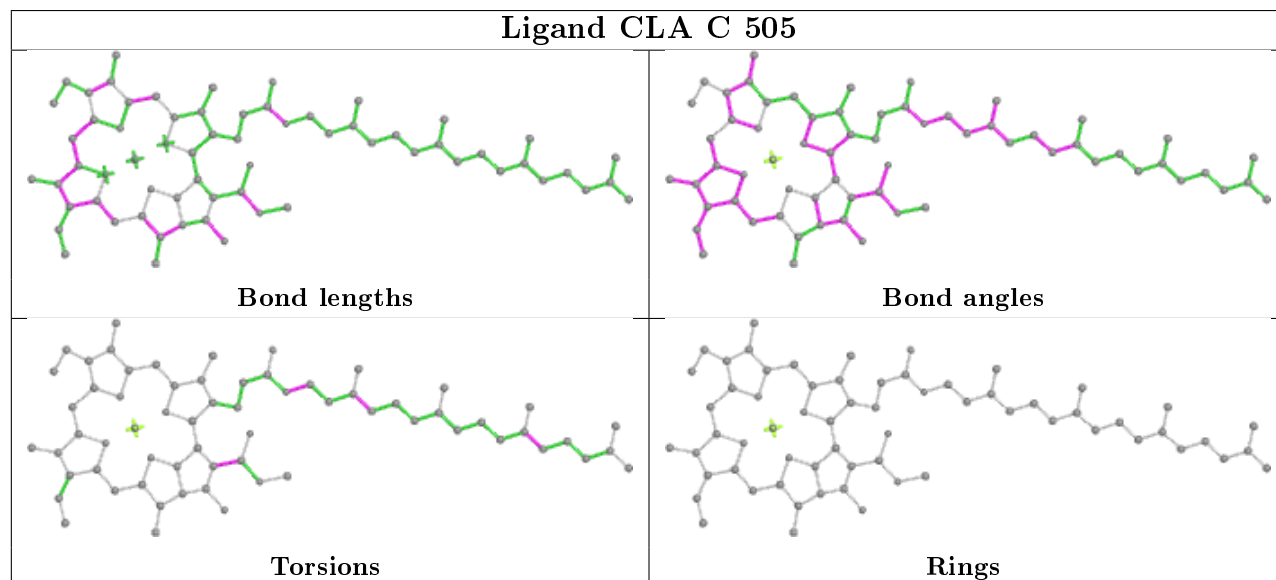
## Ligand CLA c 502

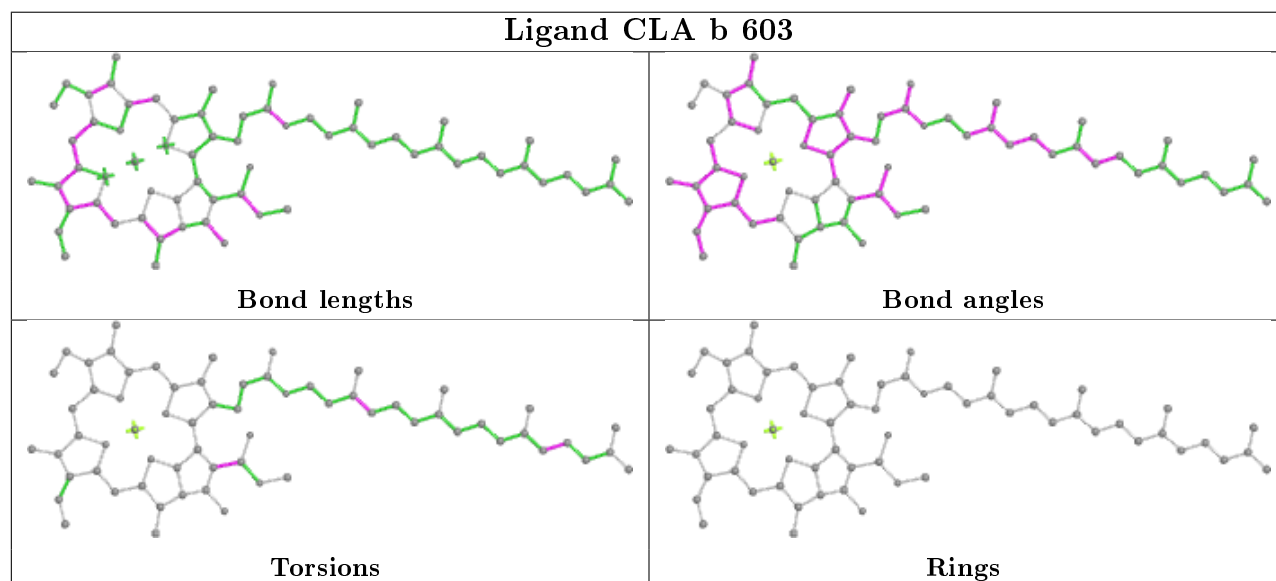
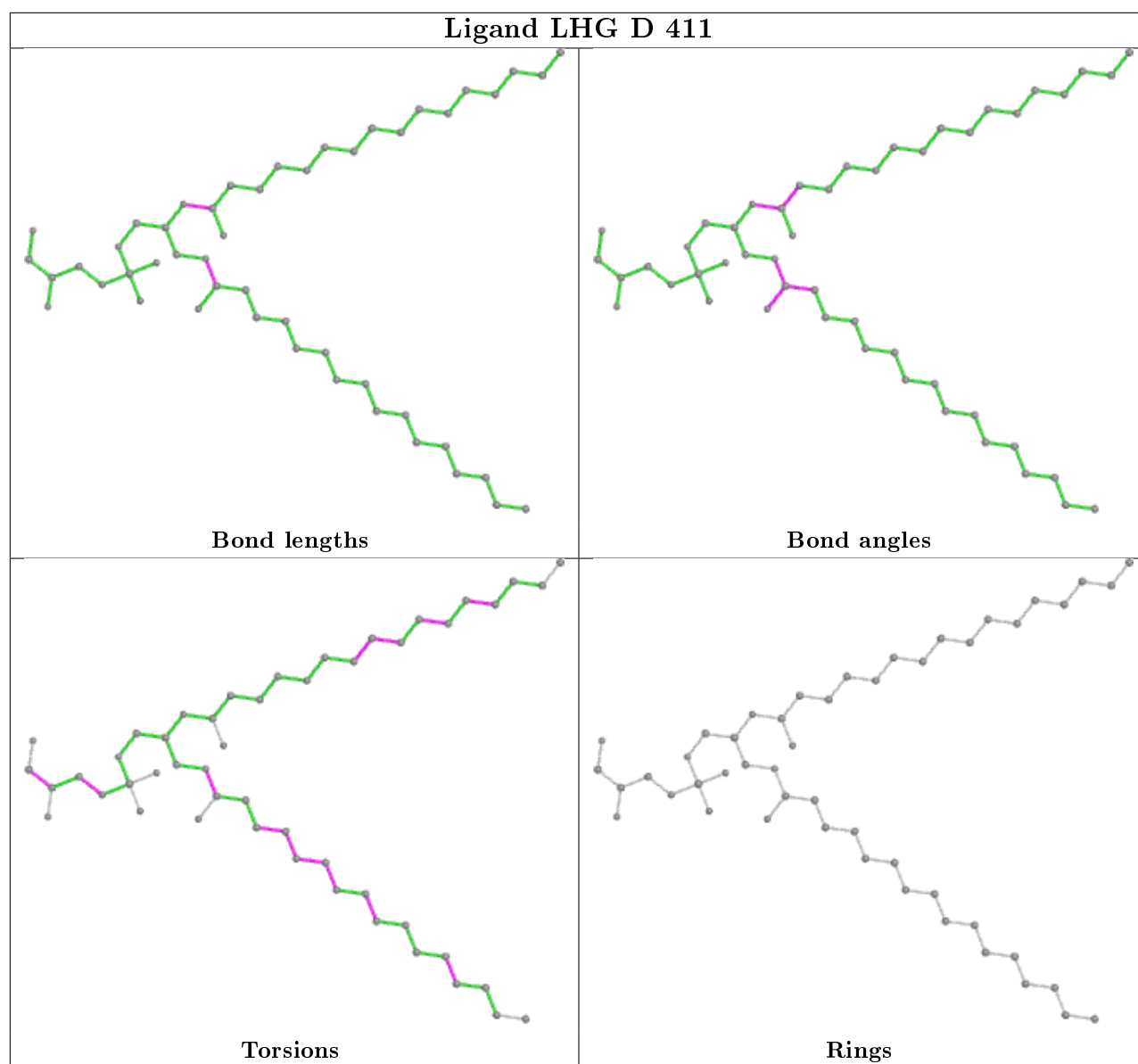


## Ligand CLA c 510

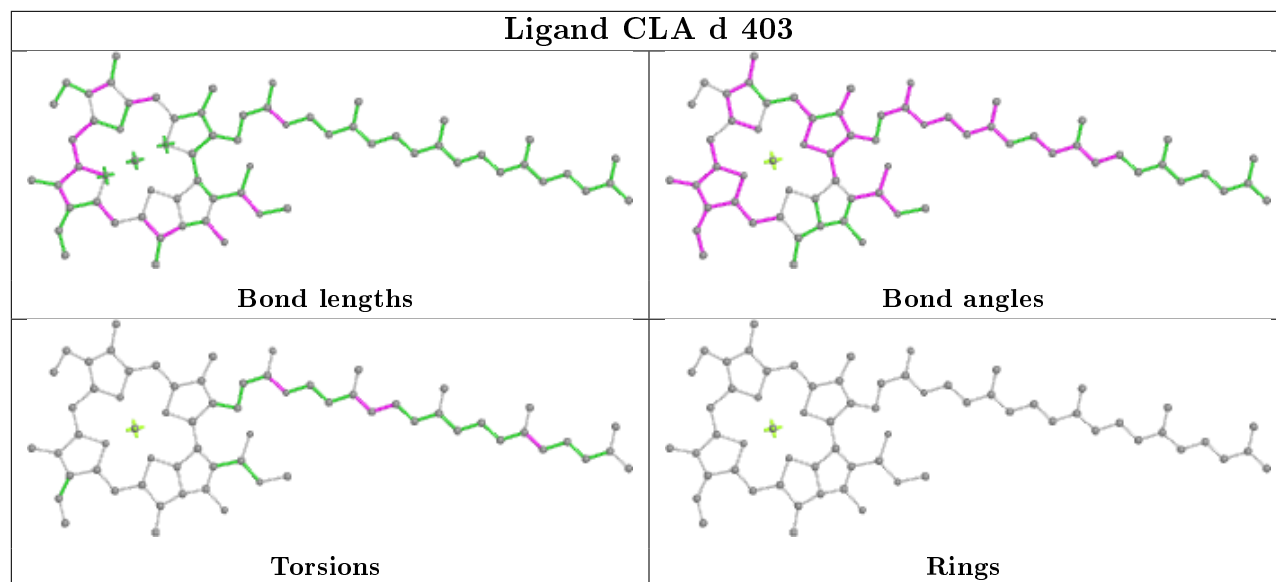


## Ligand CLA C 505

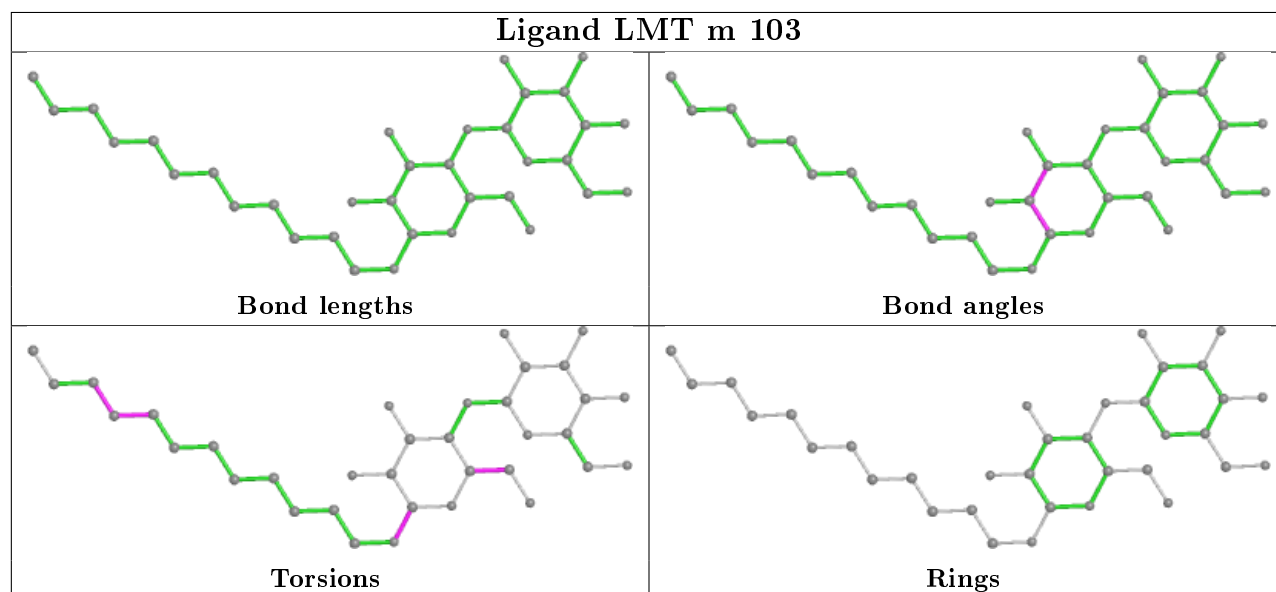




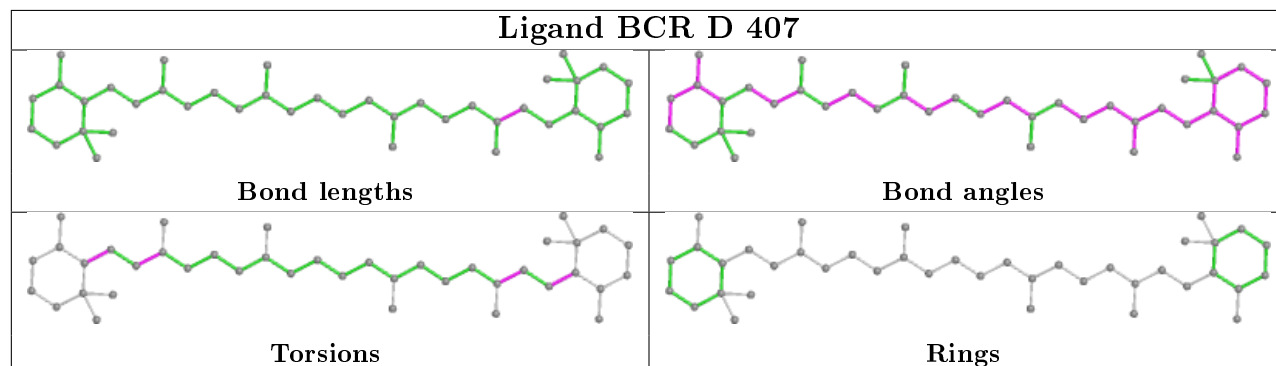
## Ligand CLA d 403

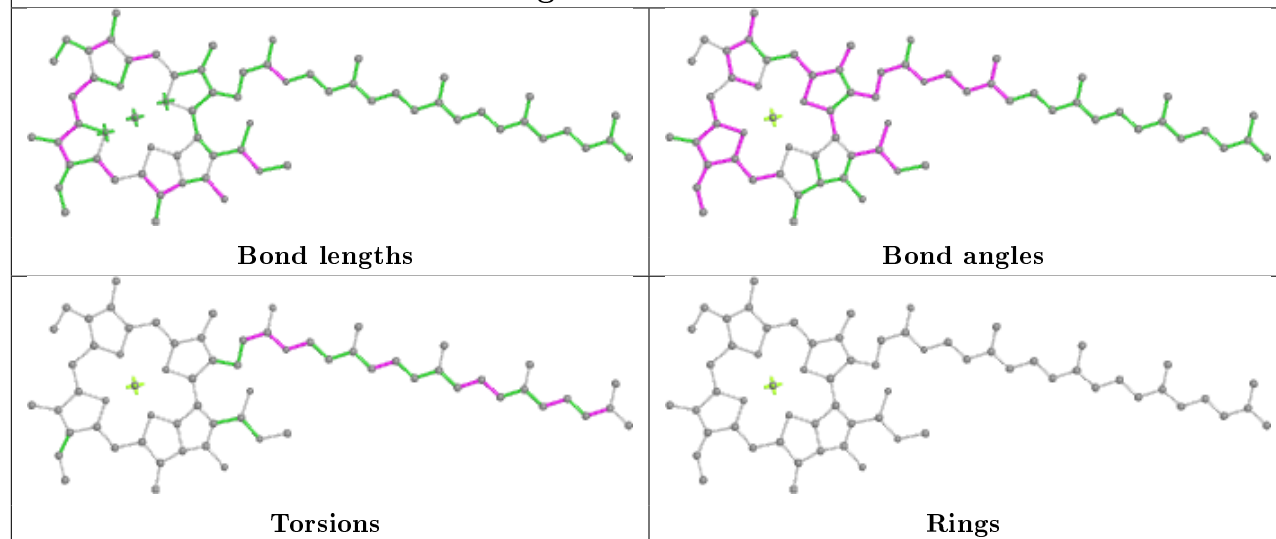
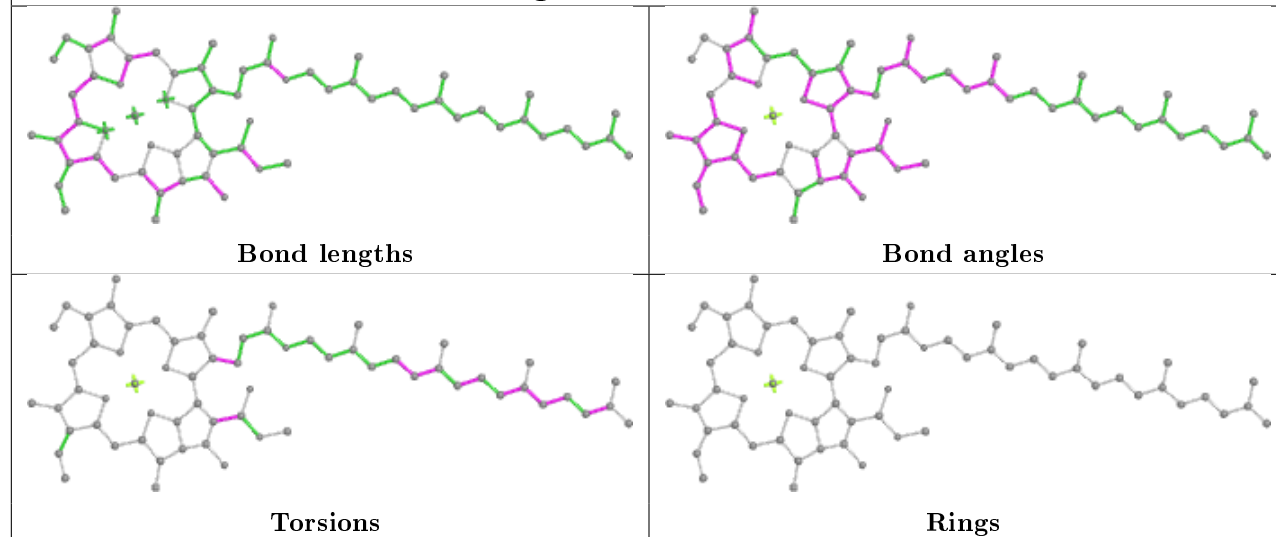


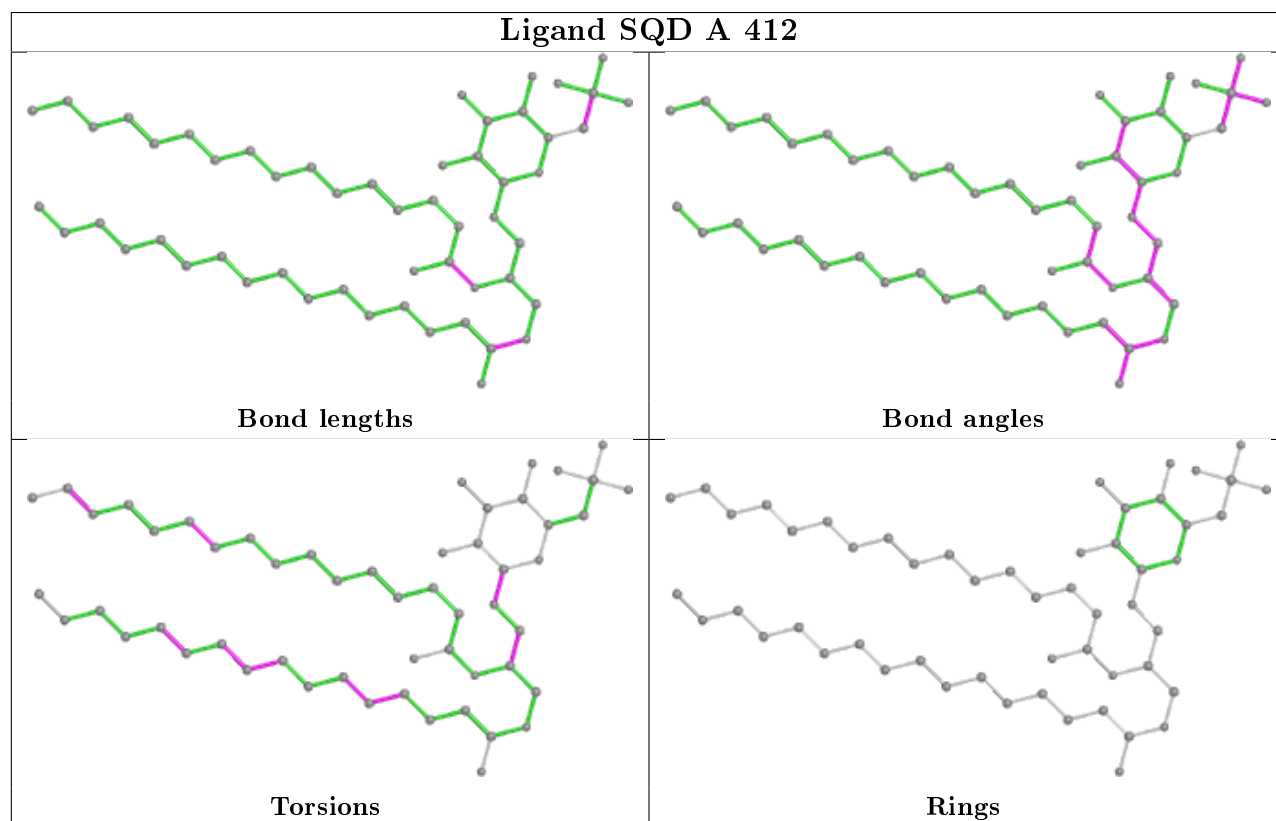
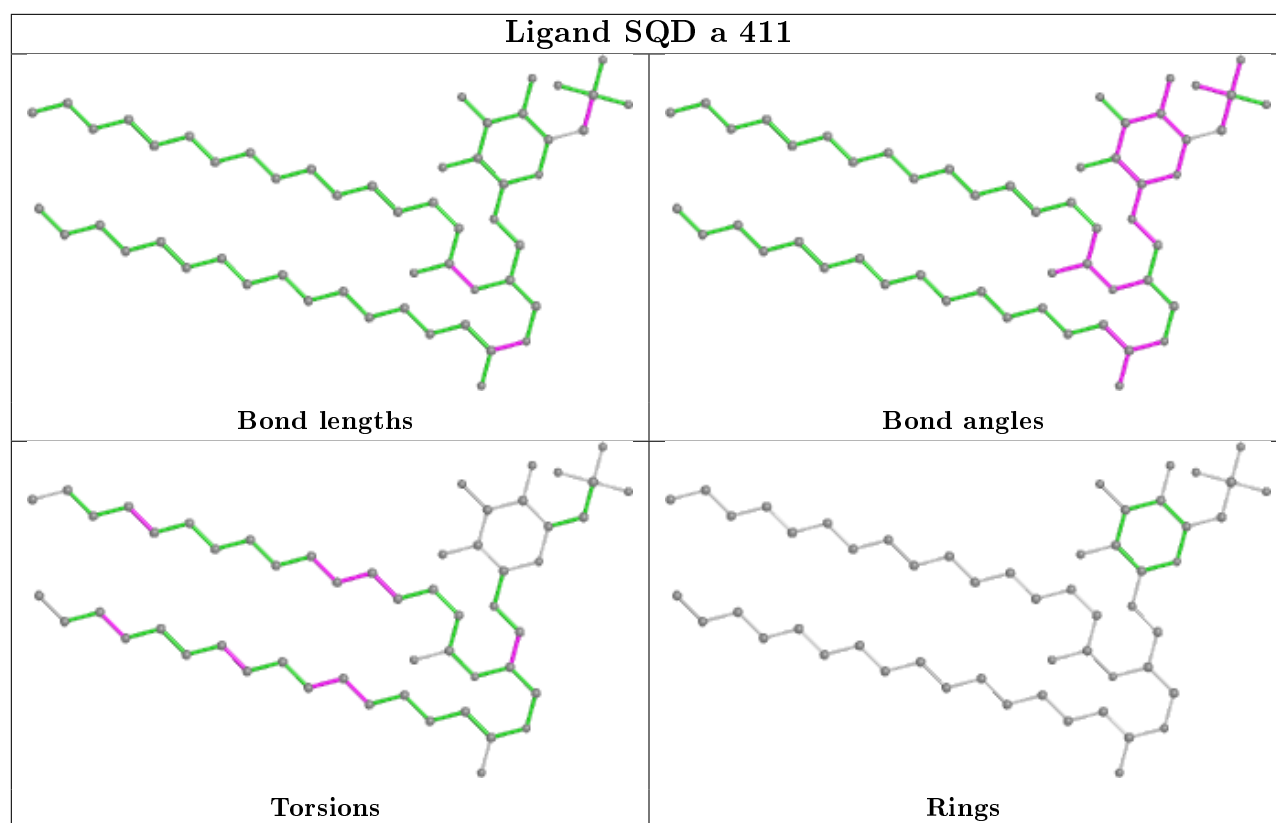
## Ligand LMT m 103

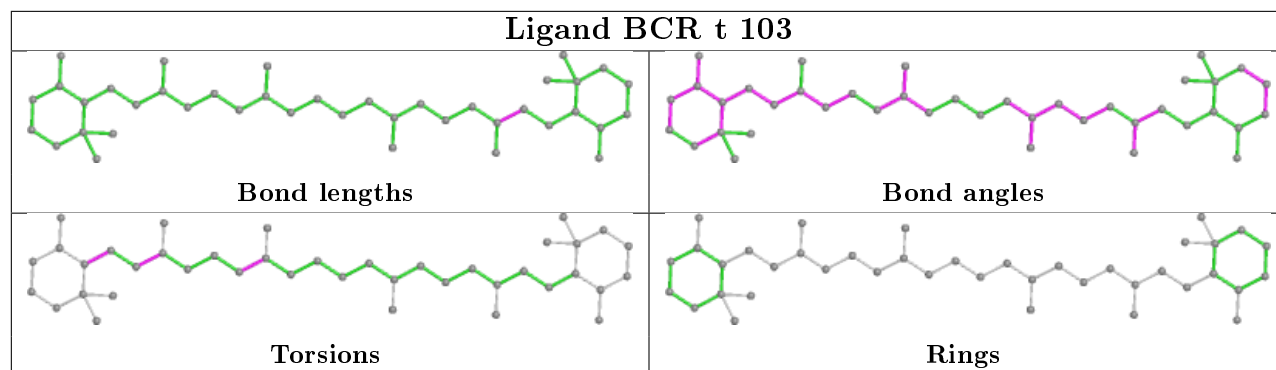
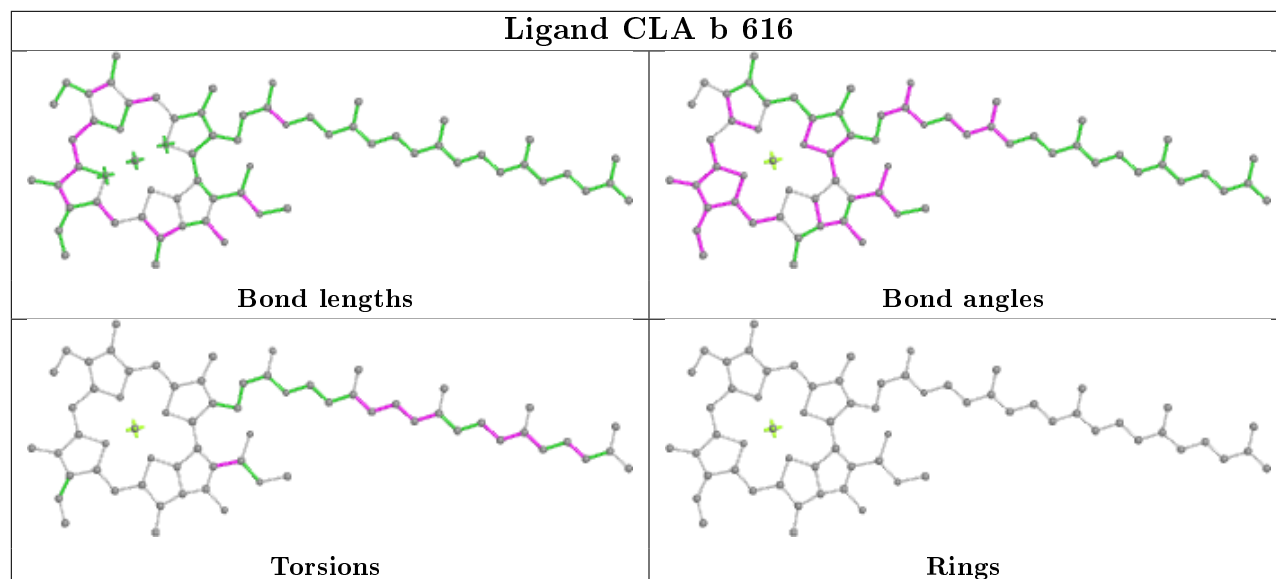
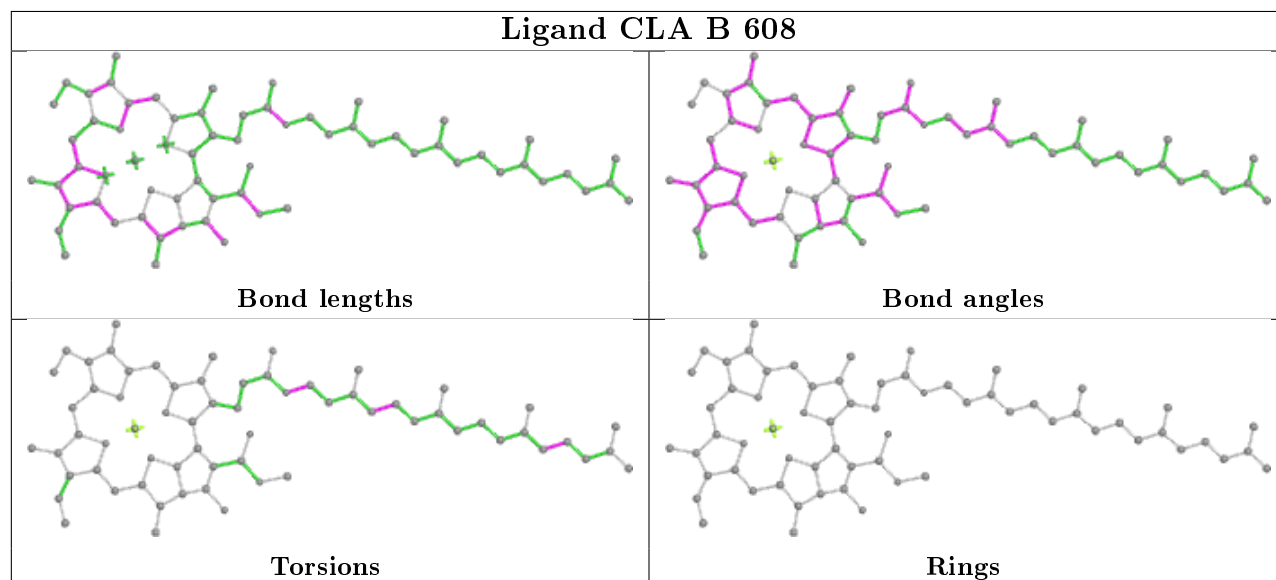


## Ligand BCR D 407

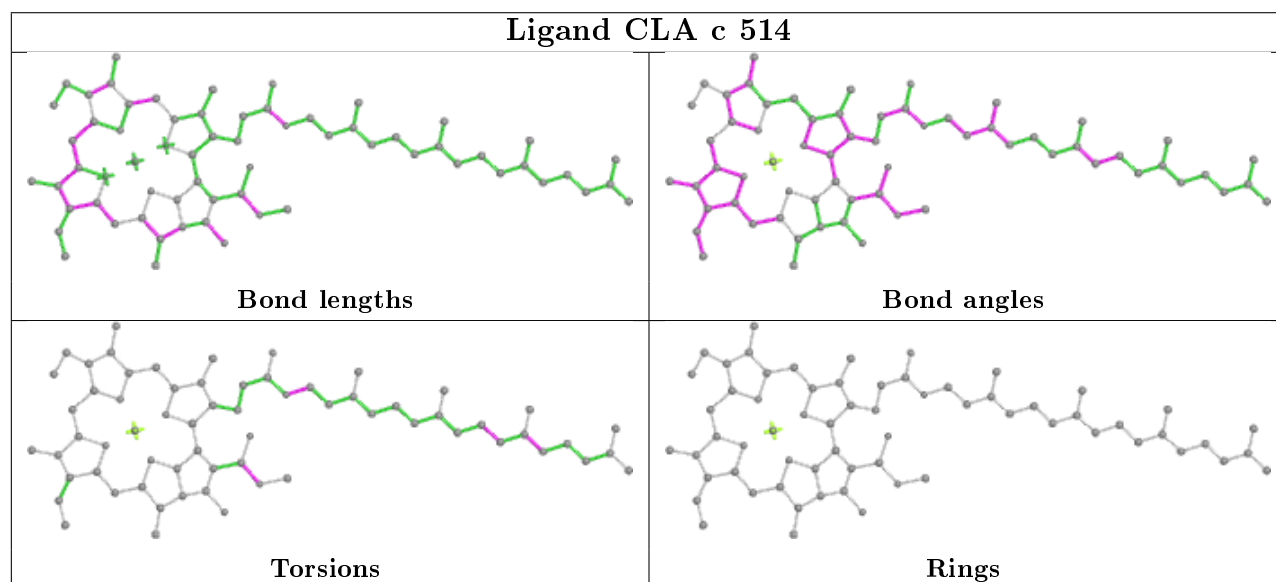
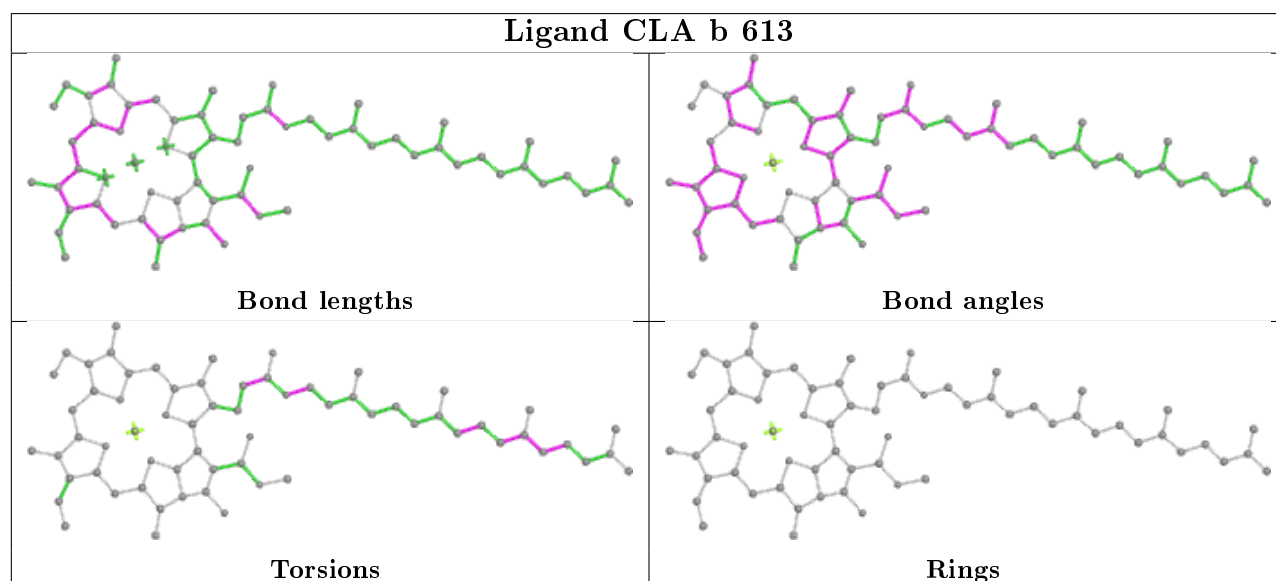
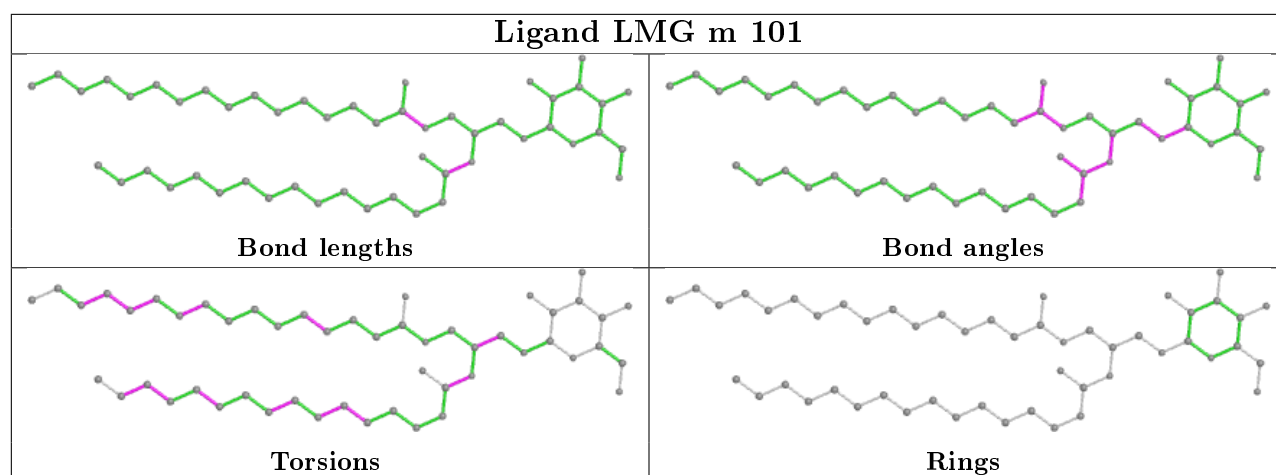


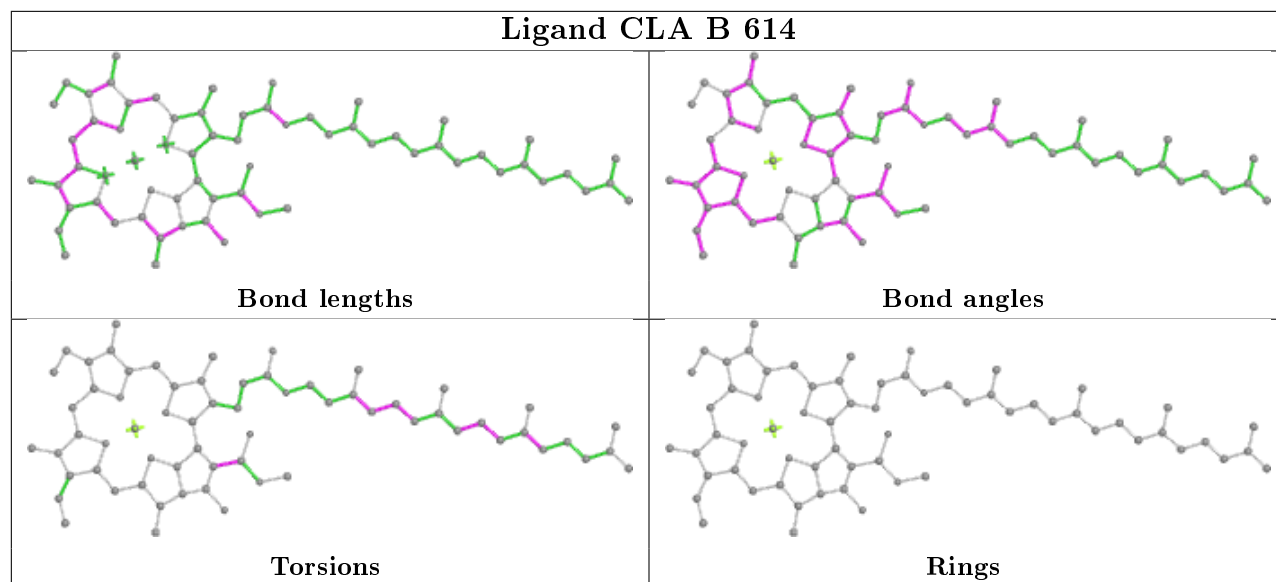
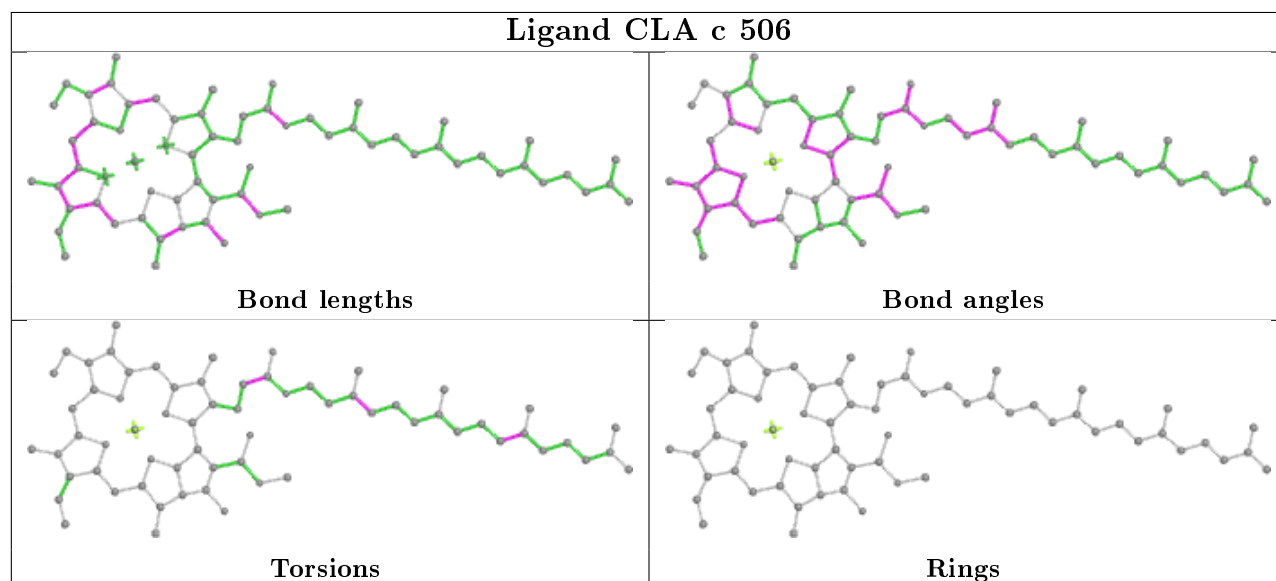
**Ligand CLA c 513****Ligand CLA C 507**

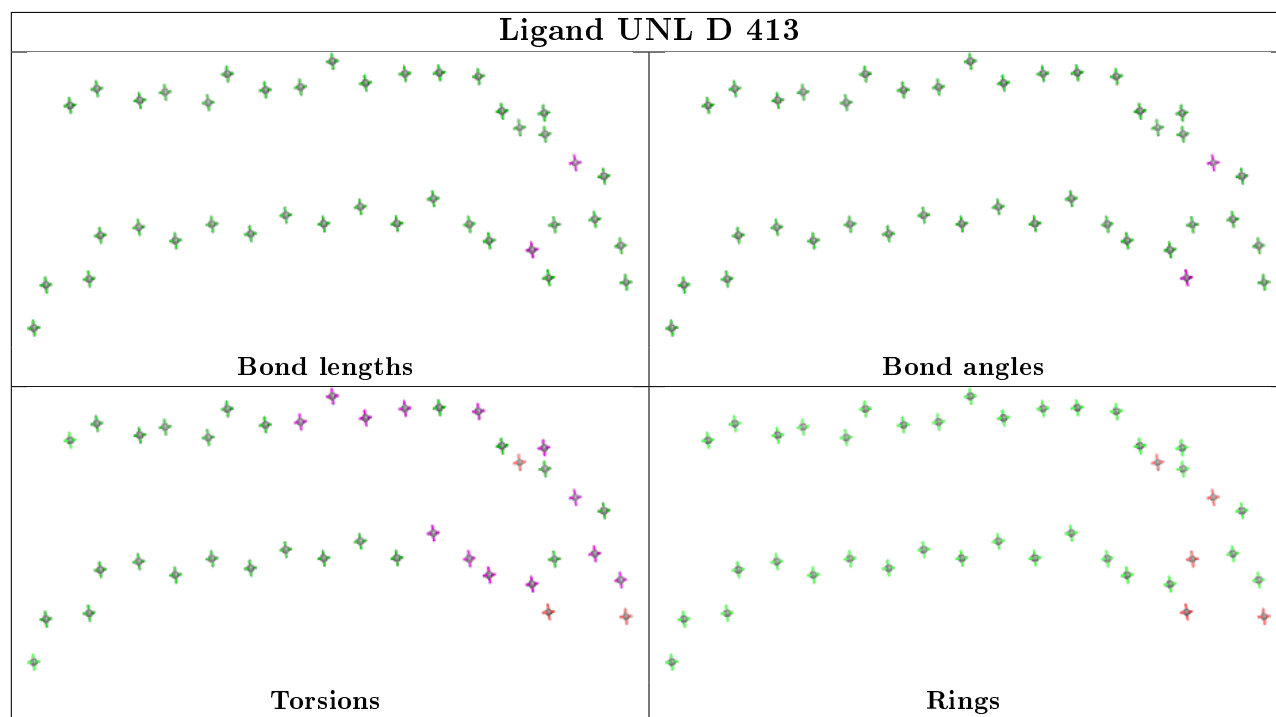
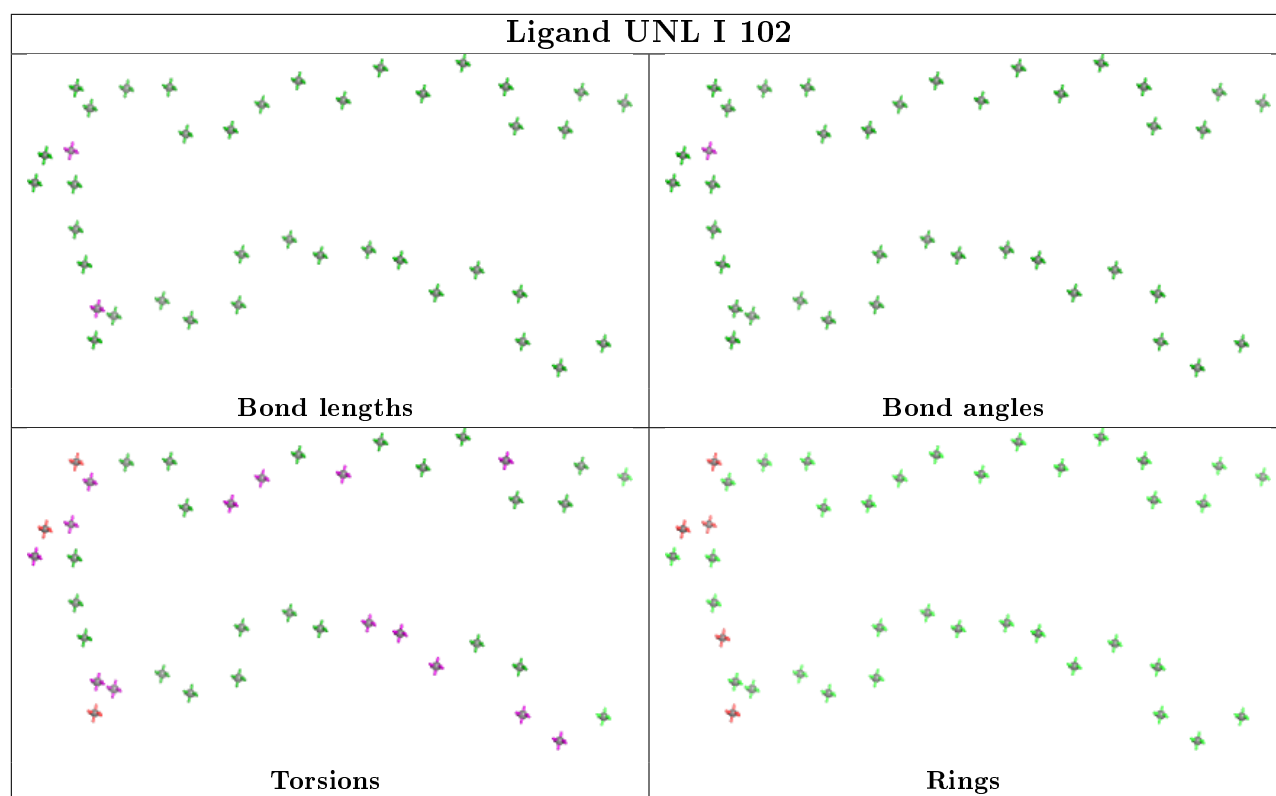


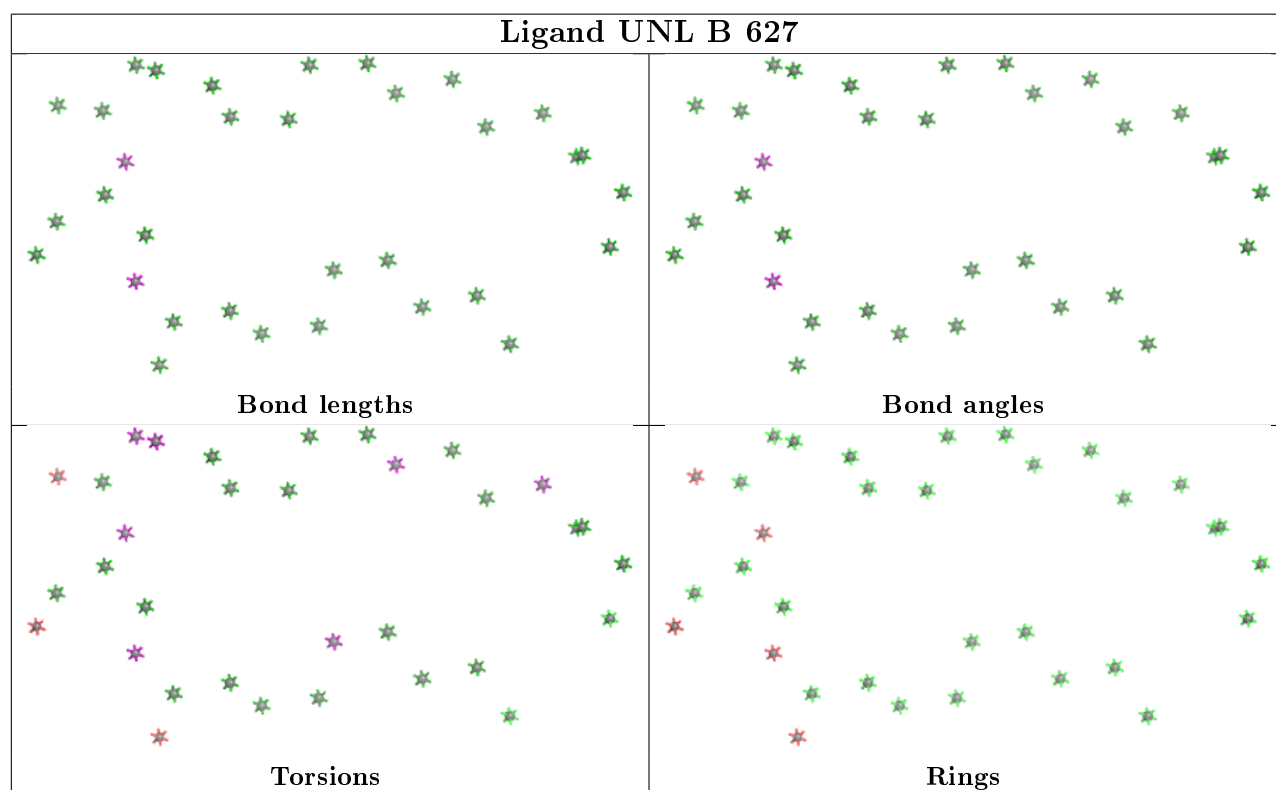
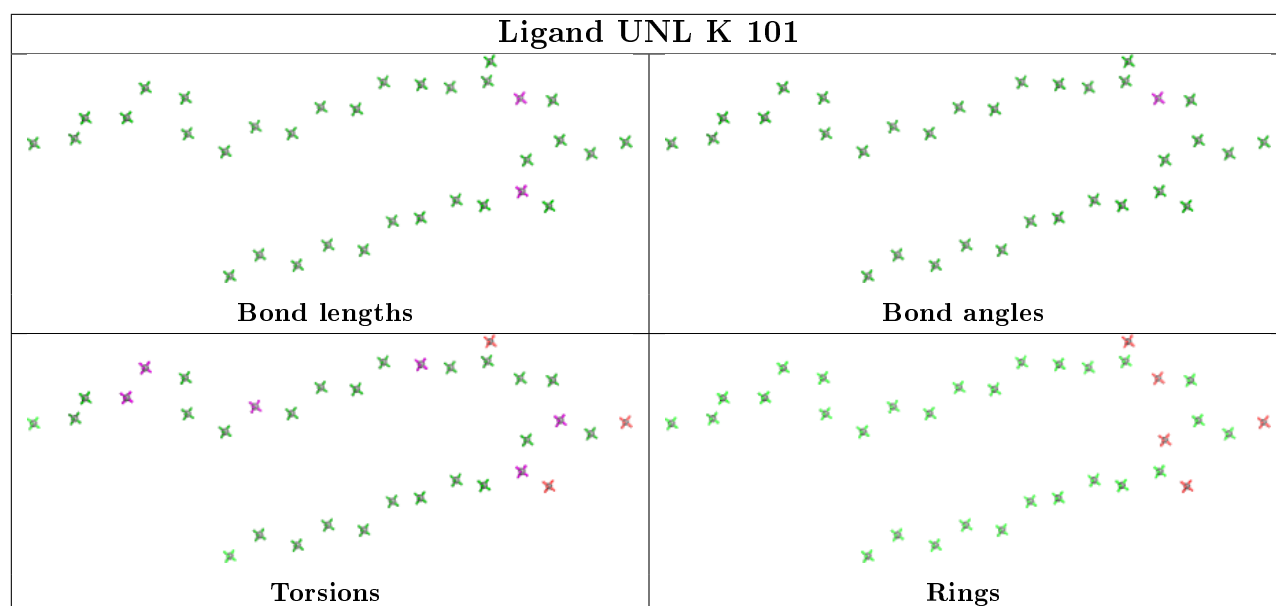
**Ligand BCR t 103****Ligand CLA b 616****Ligand CLA B 608**

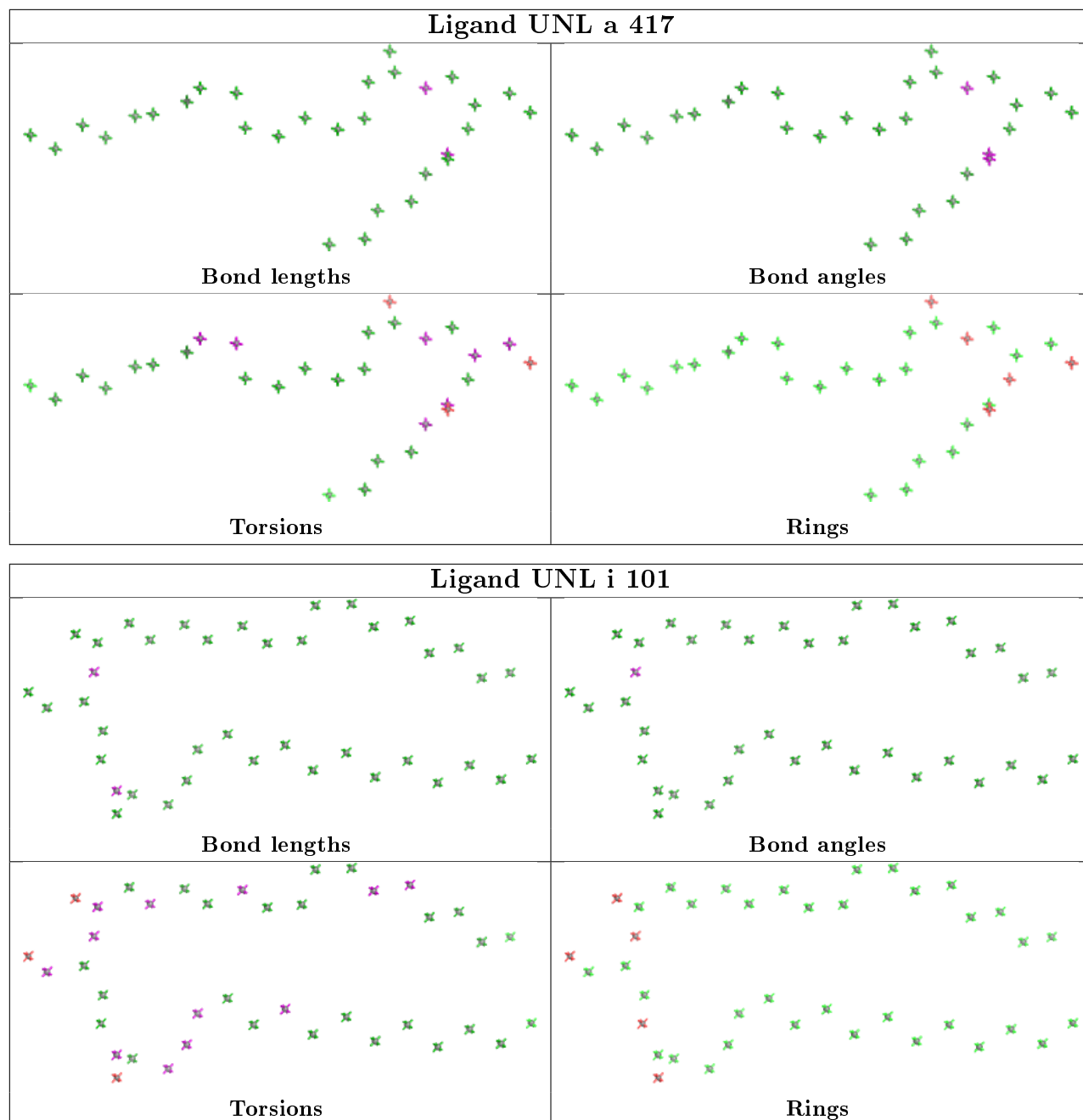


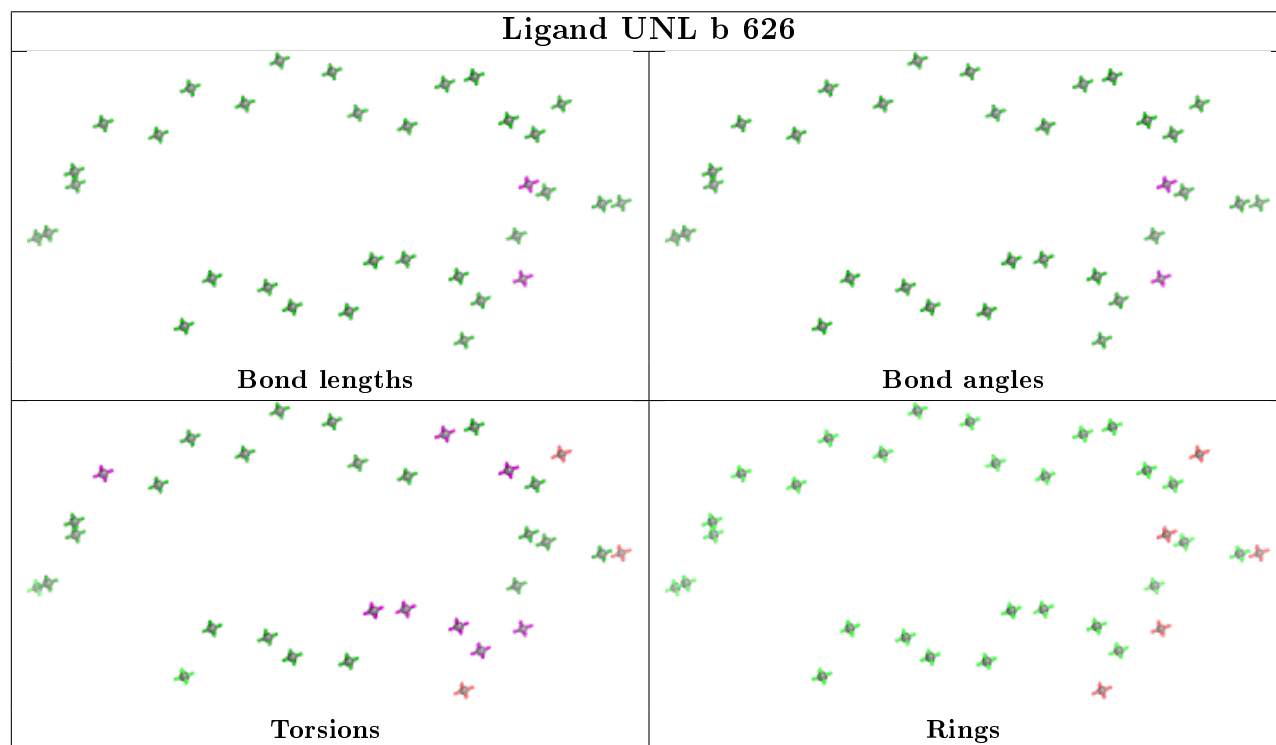
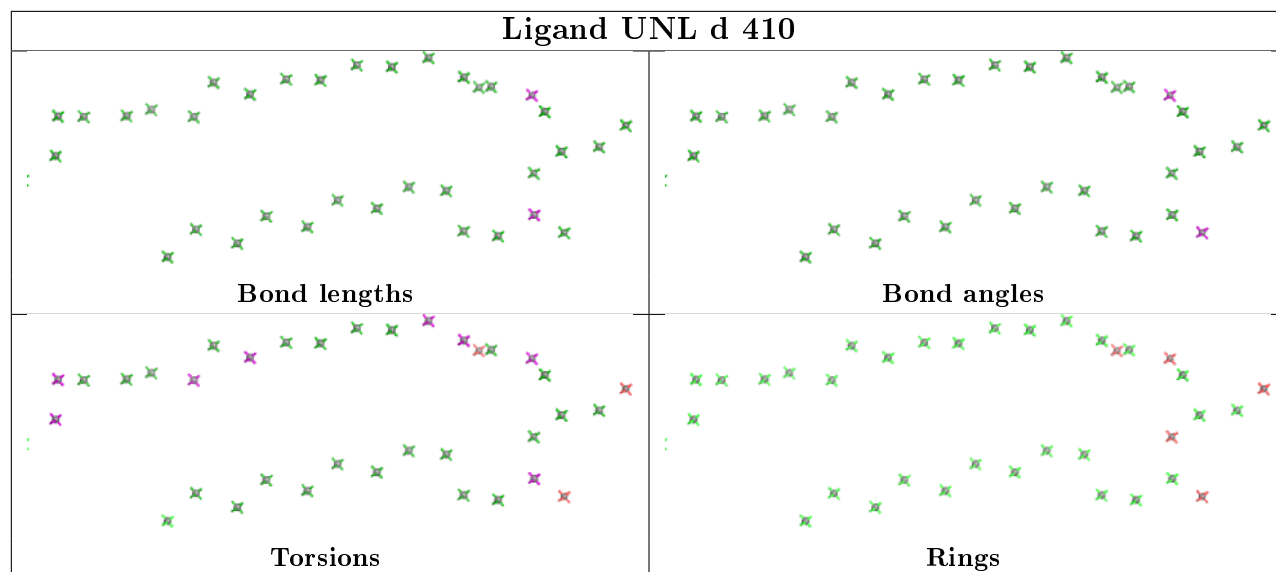


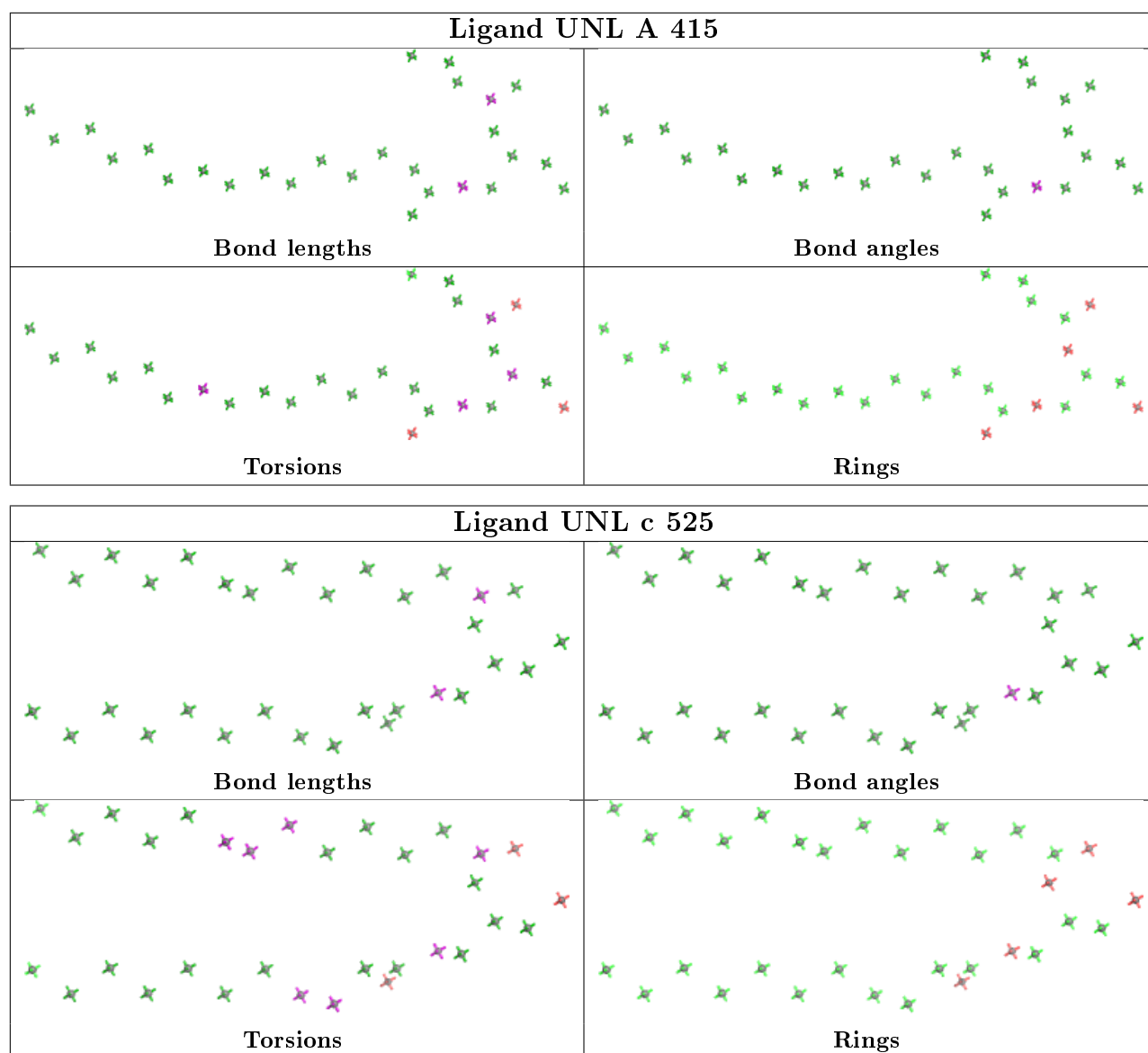
**Ligand CLA B 614****Ligand CLA c 506**











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	1.54	87 (26%) 0 0	46, 54, 76, 123	0
1	a	334/344 (97%)	1.82	114 (34%) 0 0	48, 58, 88, 134	0
2	B	504/505 (99%)	1.68	153 (30%) 0 0	47, 60, 88, 130	0
2	b	504/505 (99%)	1.85	176 (34%) 0 0	49, 63, 102, 155	0
3	C	451/455 (99%)	1.81	171 (37%) 0 0	49, 65, 86, 146	0
3	c	455/455 (100%)	1.91	179 (39%) 0 0	54, 73, 95, 133	0
4	D	342/342 (100%)	1.51	92 (26%) 0 0	46, 55, 75, 139	0
4	d	341/342 (99%)	1.56	94 (27%) 0 0	48, 60, 83, 160	0
5	E	81/84 (96%)	2.51	45 (55%) 0 0	59, 76, 104, 157	0
5	e	79/84 (94%)	3.49	61 (77%) 0 0	68, 85, 123, 148	0
6	F	34/44 (77%)	1.46	9 (26%) 0 0	62, 69, 95, 128	0
6	f	31/44 (70%)	2.58	16 (51%) 0 0	68, 75, 106, 142	0
7	H	64/65 (98%)	1.97	28 (43%) 0 0	55, 68, 84, 128	0
7	h	64/65 (98%)	2.24	28 (43%) 0 0	61, 75, 93, 140	0
8	I	37/38 (97%)	2.03	13 (35%) 0 0	59, 68, 122, 144	0
8	i	37/38 (97%)	2.08	14 (37%) 0 0	59, 70, 130, 139	0
9	J	38/39 (97%)	2.12	14 (36%) 0 0	59, 78, 130, 185	0
9	j	39/39 (100%)	2.68	20 (51%) 0 0	67, 85, 134, 172	0
10	K	37/37 (100%)	1.65	12 (32%) 0 0	68, 75, 93, 103	0
10	k	37/37 (100%)	2.27	21 (56%) 0 0	72, 82, 101, 111	0
11	L	36/37 (97%)	1.70	9 (25%) 0 1	47, 52, 103, 152	0
11	l	36/37 (97%)	1.55	8 (22%) 0 1	50, 54, 106, 151	0
12	M	32/36 (88%)	1.40	4 (12%) 3 6	48, 55, 76, 144	0
12	m	33/36 (91%)	1.54	6 (18%) 1 2	49, 55, 83, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	1.94	87 (35%) 0 0	45, 70, 117, 175	0
13	o	243/244 (99%)	2.10	98 (40%) 0 0	49, 71, 121, 168	0
14	T	29/32 (90%)	0.97	3 (10%) 6 10	49, 54, 84, 117	0
14	t	29/32 (90%)	1.21	2 (6%) 16 24	49, 56, 86, 150	0
15	U	96/104 (92%)	1.80	38 (39%) 0 0	52, 66, 90, 101	0
15	u	97/104 (93%)	1.27	18 (18%) 1 2	58, 68, 86, 131	0
16	V	137/137 (100%)	1.51	34 (24%) 0 1	52, 64, 88, 113	0
16	v	137/137 (100%)	2.40	73 (53%) 0 0	59, 76, 106, 153	0
17	X	38/40 (95%)	2.55	24 (63%) 0 0	65, 79, 102, 123	0
17	x	38/40 (95%)	3.15	25 (65%) 0 0	70, 86, 123, 162	0
18	Y	29/30 (96%)	4.39	23 (79%) 0 0	76, 92, 127, 141	0
18	y	29/30 (96%)	3.95	25 (86%) 0 0	85, 103, 127, 133	0
19	Z	62/62 (100%)	3.96	52 (83%) 0 0	75, 90, 138, 173	0
19	z	62/62 (100%)	5.00	55 (88%) 0 0	89, 104, 148, 194	0
20	R	34/34 (100%)	7.15	34 (100%) 0 0	103, 130, 154, 159	0
All	All	5283/5384 (98%)	1.96	1965 (37%) 0 0	45, 65, 107, 194	0

The worst 5 of 1965 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Y	19	ILE	13.2
2	b	494	GLY	13.1
19	z	3	ILE	13.1
20	R	18	TRP	11.5
2	b	504	THR	11.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	FME	I	1	10/11	0.81	0.23	60,72,75,79	0
8	FME	i	1	10/11	0.83	0.26	60,70,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	FME	M	1	10/11	0.85	0.21	54,65,84,92	0
12	FME	m	1	10/11	0.89	0.18	59,67,83,96	0
14	FME	t	1	10/11	0.91	0.16	49,57,68,72	0
14	FME	T	1	10/11	0.94	0.17	53,59,69,70	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	HTG	c	522	19/19	-0.14	0.64	122,143,151,152	0
32	LMT	b	621	25/35	-0.09	0.65	105,119,144,144	0
34	HTG	b	623	19/19	0.08	0.52	103,124,138,158	0
30	UNL	i	101	40/-	0.08	0.46	91,109,147,151	0
33	LMG	C	521	51/55	0.15	0.50	91,116,139,141	0
33	LMG	c	521	51/55	0.17	0.57	103,127,143,146	0
30	UNL	b	626	33/-	0.18	0.41	88,107,143,146	0
34	HTG	d	411	16/19	0.18	0.52	112,133,141,153	0
30	UNL	A	415	28/-	0.19	0.45	101,116,129,137	0
30	UNL	B	627	33/-	0.20	0.43	76,108,140,145	0
32	LMT	M	103	35/35	0.21	0.47	93,135,153,154	0
36	CA	F	102	1/1	0.21	0.15	147,147,147,147	0
26	SQD	f	102	43/54	0.21	0.56	121,146,161,163	0
32	LMT	m	103	35/35	0.21	0.46	73,95,108,111	0
32	LMT	a	414	35/35	0.22	0.57	77,121,131,134	0
32	LMT	A	359	35/35	0.22	0.56	85,123,132,134	0
32	LMT	D	404	35/35	0.23	0.47	87,111,134,136	0
32	LMT	M	101	35/35	0.25	0.43	69,95,111,113	0
32	LMT	e	102	35/35	0.26	0.65	132,156,166,171	0
37	LHG	e	101	42/49	0.26	0.56	108,140,159,166	0
30	UNL	K	101	34/-	0.29	0.59	98,118,130,146	0
32	LMT	t	101	25/35	0.29	0.57	80,99,127,128	0
30	UNL	a	417	30/-	0.29	0.39	105,118,135,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	I	102	40/-	0.33	0.44	83,112,137,141	0
34	HTG	D	414	16/19	0.33	0.50	93,117,129,133	0
33	LMG	Z	101	37/55	0.34	0.46	94,122,137,139	0
32	LMT	a	420	35/35	0.34	0.49	124,142,152,152	0
32	LMT	I	101	35/35	0.35	0.48	112,139,150,154	0
33	LMG	z	101	39/55	0.35	0.44	102,127,141,143	0
26	SQD	B	620	54/54	0.36	0.48	81,100,120,129	0
37	LHG	E	101	42/49	0.37	0.48	95,119,132,134	0
34	HTG	C	522	19/19	0.38	0.39	112,128,136,139	0
26	SQD	b	620	54/54	0.38	0.46	78,97,128,130	0
30	UNL	d	410	36/-	0.38	0.65	84,104,130,135	0
33	LMG	a	419	51/55	0.42	0.50	85,100,111,117	0
32	LMT	b	627	25/35	0.42	0.42	68,90,129,132	0
26	SQD	a	413	54/54	0.43	0.43	82,98,124,129	0
34	HTG	b	622	19/19	0.46	0.39	71,90,118,119	0
36	CA	f	103	1/1	0.47	0.14	136,136,136,136	0
30	UNL	D	413	40/-	0.48	0.43	77,100,127,131	0
33	LMG	C	501	51/55	0.49	0.49	79,98,110,117	0
34	HTG	b	625	19/19	0.50	0.33	79,86,107,111	0
34	HTG	B	622	19/19	0.51	0.40	81,91,122,125	0
32	LMT	E	102	35/35	0.51	0.53	118,142,160,165	0
26	SQD	A	412	54/54	0.53	0.41	72,92,109,117	0
35	DGD	h	102	62/66	0.54	0.49	62,72,79,84	0
30	UNL	c	525	32/-	0.55	0.34	99,116,133,137	0
33	LMG	B	621	51/55	0.56	0.41	69,78,97,108	0
29	PL9	A	414	55/55	0.59	0.50	90,112,121,124	0
29	PL9	a	416	55/55	0.59	0.44	104,118,129,130	0
27	GOL	v	201	6/6	0.60	0.84	77,89,97,99	0
34	HTG	B	623	19/19	0.60	0.37	81,103,114,114	0
33	LMG	m	101	51/55	0.60	0.36	65,77,96,113	0
35	DGD	H	102	62/66	0.62	0.51	59,68,77,78	0
32	LMT	t	102	26/35	0.63	0.28	85,105,128,129	0
33	LMG	C	520	51/55	0.63	0.40	74,94,110,120	0
23	CLA	C	514	65/65	0.63	0.32	72,85,107,112	0
30	UNL	x	101	18/-	0.63	0.27	82,91,108,111	0
23	CLA	b	602	65/65	0.63	0.35	59,66,79,89	0
30	UNL	j	101	10/-	0.63	0.57	92,102,116,117	0
33	LMG	c	520	51/55	0.64	0.38	85,101,121,129	0
27	GOL	a	418	6/6	0.64	0.34	65,79,86,90	0
26	SQD	A	410	54/54	0.65	0.40	70,87,106,114	0
35	DGD	C	518	62/66	0.65	0.34	60,71,105,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	B	609	65/65	0.65	0.29	58,64,70,74	0
36	CA	O	301	1/1	0.66	0.32	121,121,121,121	0
30	UNL	m	102	10/-	0.66	0.57	70,81,92,93	0
26	SQD	F	101	43/54	0.66	0.32	91,107,124,129	0
23	CLA	c	514	65/65	0.67	0.32	83,97,115,122	0
25	BCR	h	101	40/40	0.67	0.24	65,75,84,85	0
27	GOL	a	412	6/6	0.68	0.37	82,88,94,97	0
30	UNL	X	101	18/-	0.69	0.31	72,79,98,98	0
23	CLA	c	504	65/65	0.70	0.40	65,72,82,97	0
23	CLA	B	602	65/65	0.70	0.36	55,60,76,82	0
30	UNL	J	101	10/-	0.70	0.52	85,93,100,106	0
23	CLA	b	609	65/65	0.71	0.30	61,68,82,98	0
23	CLA	c	506	65/65	0.71	0.28	58,69,85,91	0
23	CLA	C	504	65/65	0.72	0.40	58,65,74,84	0
37	LHG	l	101	49/49	0.72	0.31	55,65,77,87	0
34	HTG	B	626	19/19	0.72	0.25	78,85,96,102	0
30	UNL	M	102	10/-	0.73	0.55	72,78,87,88	0
23	CLA	C	505	65/65	0.73	0.36	55,63,88,103	0
23	CLA	b	601	65/65	0.73	0.32	76,88,109,125	0
26	SQD	a	411	54/54	0.74	0.30	79,90,116,119	0
23	CLA	C	512	65/65	0.74	0.22	60,73,82,88	0
35	DGD	c	517	62/66	0.74	0.37	62,69,85,94	0
23	CLA	B	606	65/65	0.75	0.25	51,59,90,98	0
33	LMG	D	415	51/55	0.75	0.29	62,75,104,108	0
23	CLA	B	611	65/65	0.75	0.32	46,52,63,68	0
35	DGD	c	518	62/66	0.76	0.34	64,76,106,114	0
23	CLA	c	513	65/65	0.76	0.27	71,87,107,113	0
23	CLA	B	601	65/65	0.76	0.29	69,81,102,119	0
23	CLA	a	406	65/65	0.76	0.27	48,52,63,71	0
37	LHG	L	101	49/49	0.76	0.35	55,63,69,84	0
23	CLA	c	511	65/65	0.77	0.36	62,71,80,84	0
37	LHG	D	409	49/49	0.77	0.45	58,69,84,96	0
23	CLA	b	603	65/65	0.77	0.35	52,62,78,88	0
23	CLA	b	606	65/65	0.77	0.24	55,65,89,102	0
23	CLA	C	513	65/65	0.77	0.25	71,80,101,108	0
23	CLA	c	507	65/65	0.77	0.25	71,81,103,112	0
23	CLA	C	507	65/65	0.77	0.26	61,75,112,117	0
23	CLA	c	512	65/65	0.78	0.23	67,78,91,94	0
23	CLA	B	605	65/65	0.78	0.33	47,54,63,69	0
23	CLA	c	509	65/65	0.78	0.26	57,69,106,115	0
36	CA	o	301	1/1	0.78	0.24	107,107,107,107	0
23	CLA	C	509	65/65	0.78	0.33	54,63,97,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	DGD	C	519	62/66	0.78	0.27	57,66,90,97	0
23	CLA	B	608	65/65	0.78	0.34	51,59,69,72	0
35	DGD	C	517	62/66	0.78	0.37	55,65,89,93	0
23	CLA	b	615	65/65	0.78	0.20	56,64,74,80	0
38	HEM	E	103	43/43	0.78	0.25	65,73,87,116	0
30	UNL	d	409	17/-	0.78	0.71	78,88,109,111	0
23	CLA	B	613	65/65	0.79	0.34	47,54,80,87	0
37	LHG	d	406	49/49	0.79	0.38	60,71,88,100	0
23	CLA	C	508	65/65	0.79	0.27	59,66,77,79	0
23	CLA	B	612	65/65	0.79	0.31	47,54,61,67	0
25	BCR	H	101	40/40	0.79	0.19	58,69,79,80	0
33	LMG	d	412	51/55	0.79	0.24	69,77,107,115	0
23	CLA	C	506	65/65	0.79	0.32	55,63,81,93	0
23	CLA	A	405	65/65	0.80	0.24	44,51,59,60	0
27	GOL	b	624	6/6	0.80	0.28	93,100,106,108	0
23	CLA	b	612	65/65	0.80	0.33	53,60,66,77	0
23	CLA	D	406	65/65	0.80	0.22	55,65,105,108	0
23	CLA	B	615	65/65	0.80	0.20	48,58,74,77	0
23	CLA	b	608	65/65	0.80	0.40	57,64,79,88	0
23	CLA	b	610	65/65	0.80	0.32	57,64,73,78	0
23	CLA	C	502	65/65	0.80	0.32	56,65,71,76	0
37	LHG	d	407	49/49	0.80	0.34	55,62,72,80	0
23	CLA	b	614	65/65	0.80	0.23	49,58,92,99	0
23	CLA	b	607	65/65	0.81	0.29	47,55,76,83	0
37	LHG	D	411	49/49	0.81	0.40	60,67,105,110	0
23	CLA	c	508	65/65	0.81	0.23	64,75,83,90	0
23	CLA	C	511	65/65	0.81	0.41	58,67,77,87	0
23	CLA	B	604	65/65	0.81	0.37	44,53,90,103	0
37	LHG	d	408	49/49	0.81	0.30	64,72,102,105	0
23	CLA	a	407	65/65	0.81	0.25	52,59,102,109	0
23	CLA	c	503	65/65	0.81	0.34	59,69,79,81	0
23	CLA	c	510	65/65	0.82	0.29	61,73,84,92	0
23	CLA	b	616	65/65	0.82	0.21	58,67,97,103	0
23	CLA	A	404	65/65	0.82	0.27	43,50,60,70	0
23	CLA	B	610	65/65	0.82	0.29	52,59,69,75	0
25	BCR	c	515	40/40	0.82	0.22	86,93,98,101	0
27	GOL	V	201	6/6	0.82	0.55	64,71,83,87	0
23	CLA	B	614	65/65	0.82	0.24	48,54,87,95	0
23	CLA	d	403	65/65	0.82	0.19	58,71,98,106	0
23	CLA	B	607	65/65	0.83	0.29	44,52,69,76	0
25	BCR	B	618	40/40	0.83	0.35	53,61,74,81	0
23	CLA	a	405	65/65	0.83	0.29	48,54,64,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	605	65/65	0.83	0.30	51,57,70,72	0
23	CLA	b	604	65/65	0.83	0.32	49,56,91,101	0
37	LHG	D	410	49/49	0.83	0.38	55,61,74,84	0
23	CLA	c	505	65/65	0.83	0.32	63,71,94,111	0
23	CLA	A	406	65/65	0.83	0.23	47,54,92,96	0
25	BCR	y	101	40/40	0.83	0.16	72,79,88,91	0
30	UNL	D	412	17/-	0.83	0.46	70,84,100,106	0
24	PHO	a	353	64/64	0.83	0.27	53,60,65,67	0
23	CLA	D	405	65/65	0.83	0.26	43,50,66,81	0
24	PHO	A	353	64/64	0.83	0.30	47,56,61,64	0
34	HTG	V	203	11/19	0.84	0.50	103,119,123,128	0
23	CLA	B	603	65/65	0.84	0.34	50,58,69,75	0
23	CLA	d	402	65/65	0.84	0.27	48,55,66,78	0
23	CLA	b	611	65/65	0.84	0.28	52,58,68,75	0
25	BCR	b	618	40/40	0.84	0.33	53,62,71,76	0
23	CLA	c	502	65/65	0.84	0.29	64,72,80,84	0
25	BCR	d	404	40/40	0.84	0.20	67,78,91,92	0
25	BCR	T	101	40/40	0.85	0.31	52,62,69,72	0
38	HEM	e	87	43/43	0.85	0.39	80,94,117,126	0
23	CLA	C	503	65/65	0.85	0.38	54,62,73,86	0
39	MG	J	102	1/1	0.85	0.18	64,64,64,64	0
25	BCR	k	101	40/40	0.85	0.26	71,80,90,95	0
25	BCR	B	619	40/40	0.85	0.19	56,64,78,81	0
40	HEC	V	202	43/43	0.85	0.18	50,60,63,64	0
25	BCR	b	619	40/40	0.86	0.20	56,67,80,82	0
40	HEC	v	202	43/43	0.86	0.17	61,70,75,79	0
25	BCR	a	410	40/40	0.86	0.23	51,59,65,67	0
27	GOL	C	523	6/6	0.86	0.31	63,67,73,76	0
23	CLA	B	616	65/65	0.86	0.20	53,63,108,111	0
23	CLA	b	613	65/65	0.86	0.32	48,55,84,89	0
23	CLA	A	408	65/65	0.86	0.20	51,59,101,112	0
27	GOL	A	411	6/6	0.86	0.21	79,87,89,100	0
35	DGD	c	519	62/66	0.86	0.26	64,74,94,102	0
25	BCR	C	516	40/40	0.86	0.30	59,69,76,80	0
23	CLA	C	510	65/65	0.86	0.31	57,67,80,86	0
25	BCR	t	103	40/40	0.87	0.33	54,64,79,80	0
25	BCR	C	515	40/40	0.87	0.16	74,79,87,92	0
24	PHO	A	407	64/64	0.87	0.30	46,51,56,59	0
27	GOL	B	625	6/6	0.87	0.32	65,82,86,93	0
25	BCR	D	407	40/40	0.87	0.24	59,68,91,92	0
29	PL9	d	405	55/55	0.88	0.32	51,58,66,90	0
25	BCR	c	516	40/40	0.88	0.20	66,74,81,85	0

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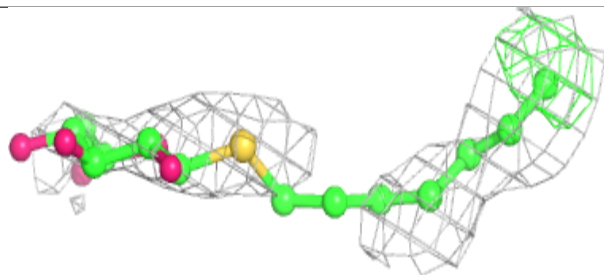
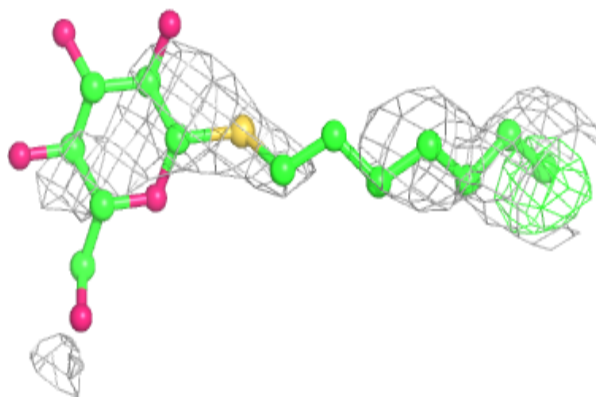
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	PHO	a	408	64/64	0.88	0.29	49,55,60,66	0
25	BCR	K	102	40/40	0.89	0.21	64,72,81,83	0
23	CLA	a	409	65/65	0.89	0.18	53,62,108,115	0
25	BCR	b	617	40/40	0.89	0.26	51,58,65,67	0
25	BCR	B	617	40/40	0.89	0.31	51,56,63,64	0
25	BCR	Y	101	40/40	0.90	0.18	67,75,80,82	0
36	CA	c	524	1/1	0.90	0.19	93,93,93,93	0
31	BCT	A	348	4/4	0.90	0.20	60,62,64,69	0
29	PL9	D	408	55/55	0.91	0.32	47,55,61,73	0
25	BCR	A	409	40/40	0.91	0.21	48,55,62,65	0
27	GOL	B	624	6/6	0.91	0.29	85,88,93,95	0
31	BCT	a	404	4/4	0.92	0.19	59,65,66,76	0
28	OEX	a	415	10/10	0.92	0.20	58,62,66,67	0
27	GOL	c	501	6/6	0.92	0.54	73,74,77,78	0
28	OEX	A	413	10/10	0.93	0.21	56,57,57,57	0
39	MG	j	102	1/1	0.94	0.17	70,70,70,70	0
36	CA	c	523	1/1	0.95	0.27	84,84,84,84	0
22	CL	a	403	1/1	0.97	0.33	58,58,58,58	0
22	CL	A	403	1/1	0.98	0.39	52,52,52,52	0
36	CA	C	524	1/1	0.99	0.24	81,81,81,81	0
21	FE2	A	401	1/1	0.99	0.05	64,64,64,64	0
21	FE2	a	401	1/1	0.99	0.08	67,67,67,67	0
22	CL	a	402	1/1	0.99	0.39	56,56,56,56	0
22	CL	A	402	1/1	0.99	0.37	51,51,51,51	0

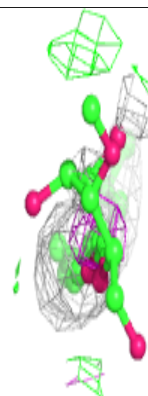
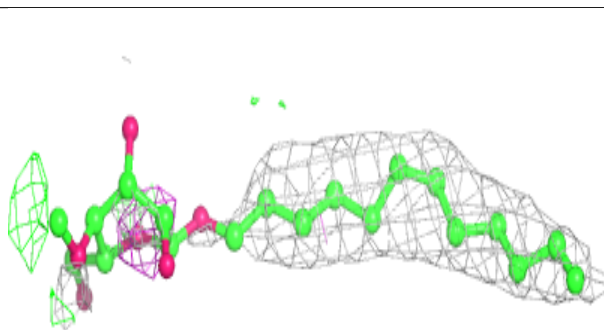
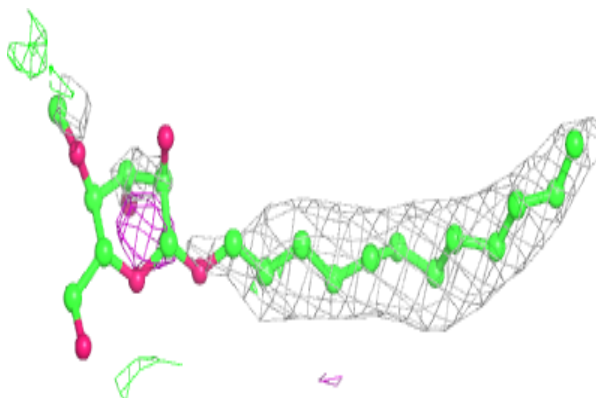
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HTG c 522:**

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

**Electron density around LMT b 621:**

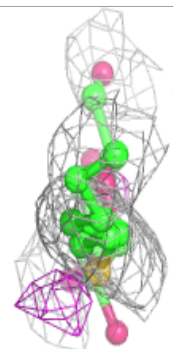
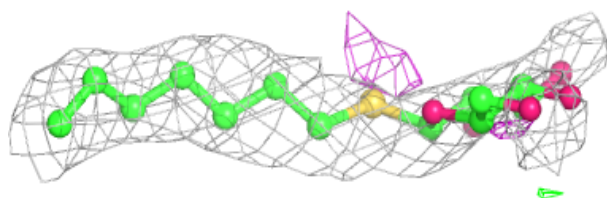
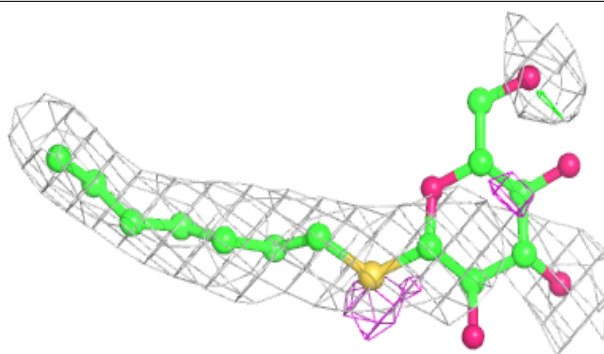
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



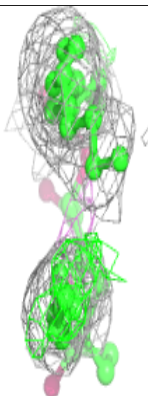
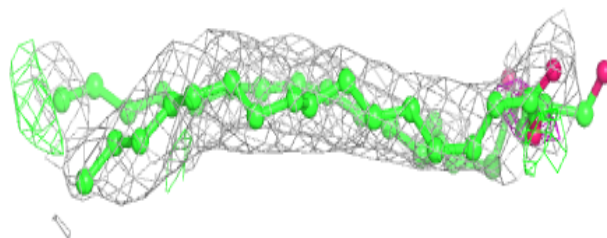
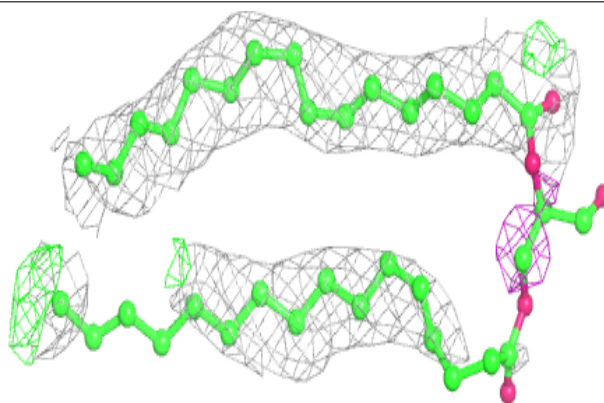


**Electron density around HTG b 623:**

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

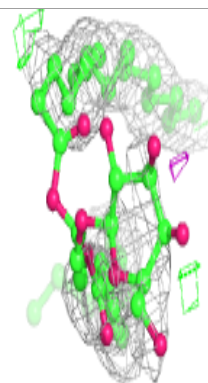
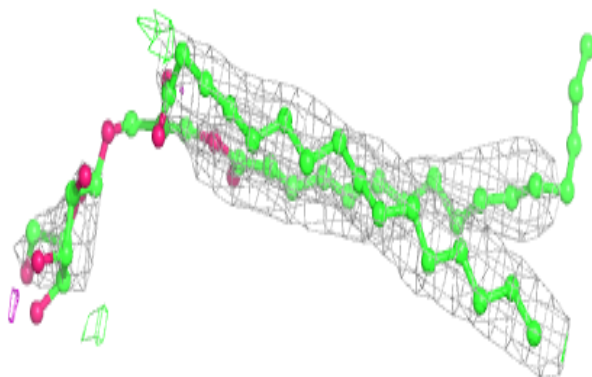
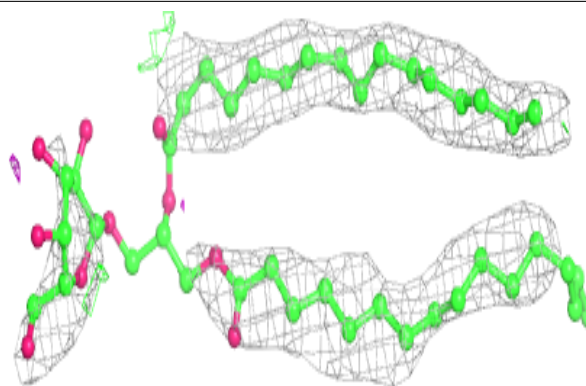
**Electron density around UNL i 101:**

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

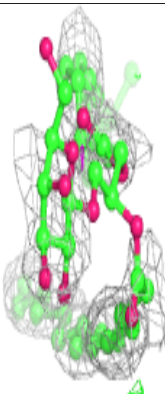
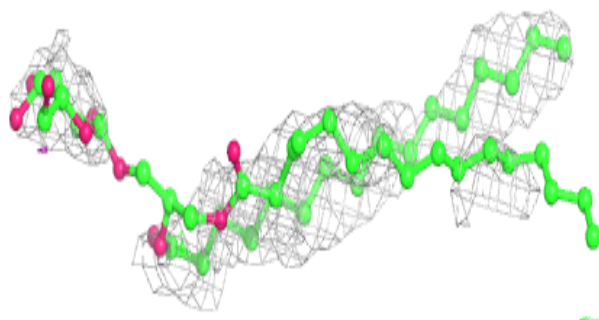
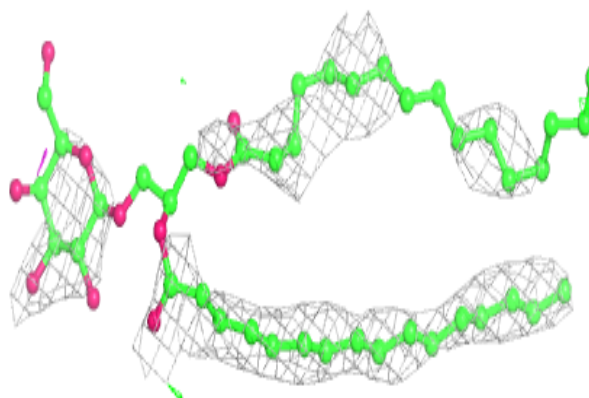


**Electron density around LMG C 521:**

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

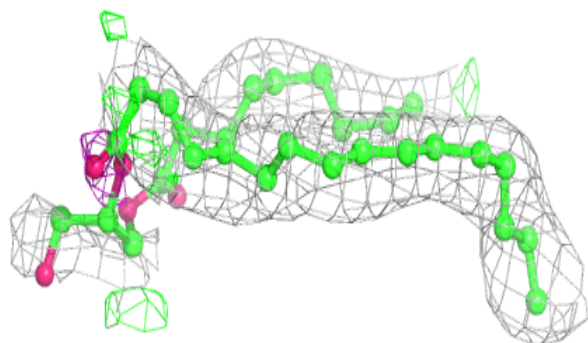
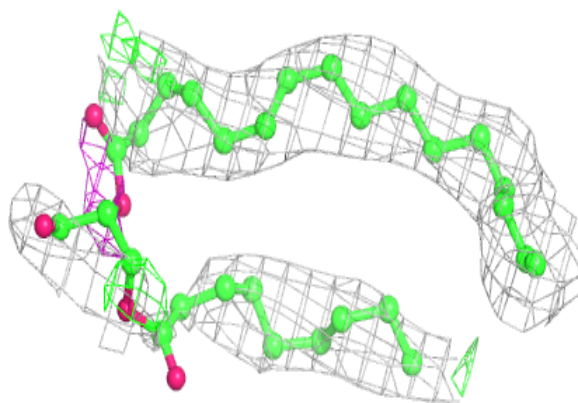
**Electron density around LMG c 521:**

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

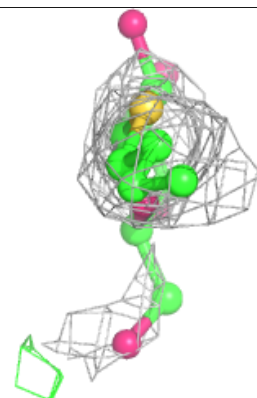
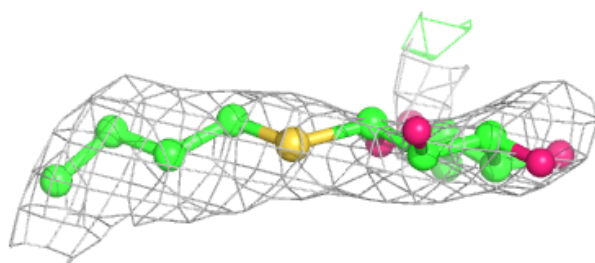
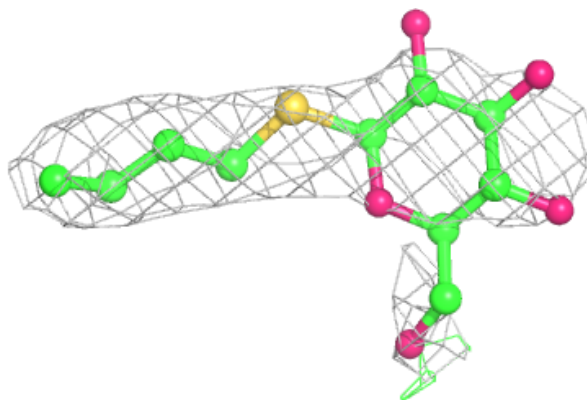


**Electron density around UNL b 626:**

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

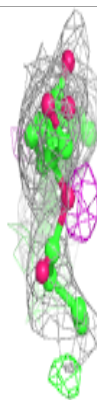
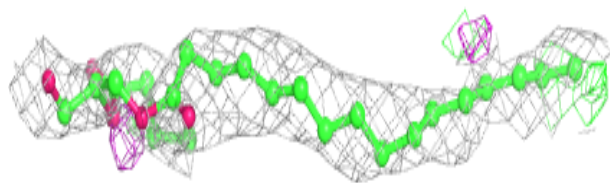
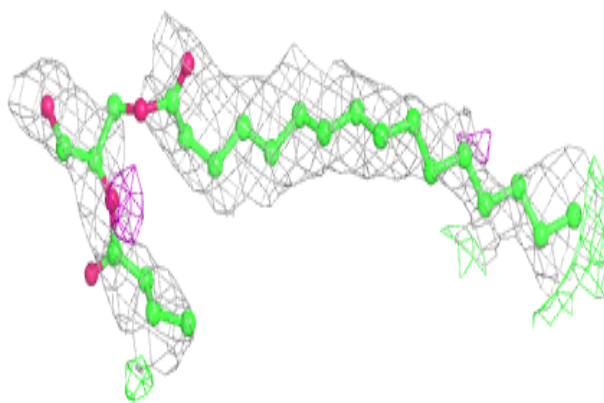
**Electron density around HTG d 411:**

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

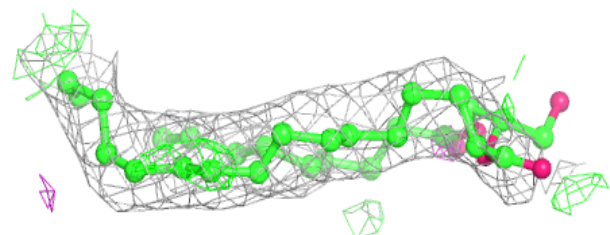
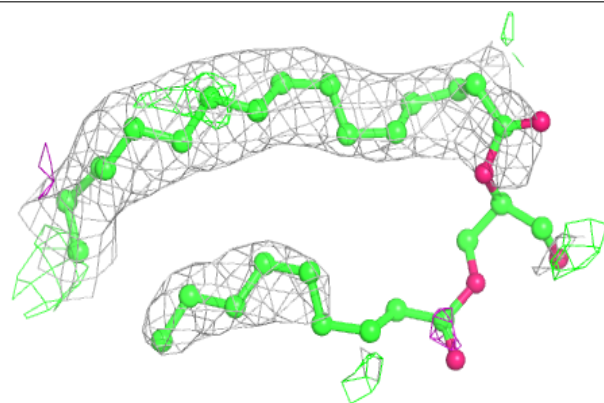


**Electron density around UNL A 415:**

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

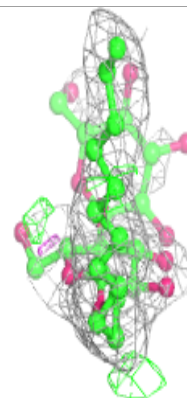
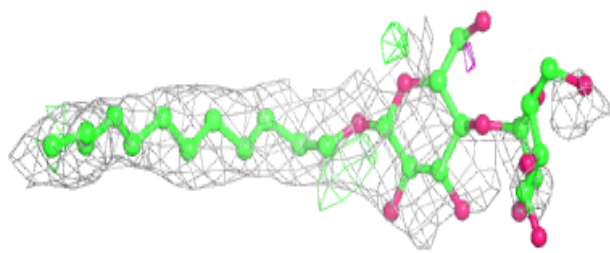
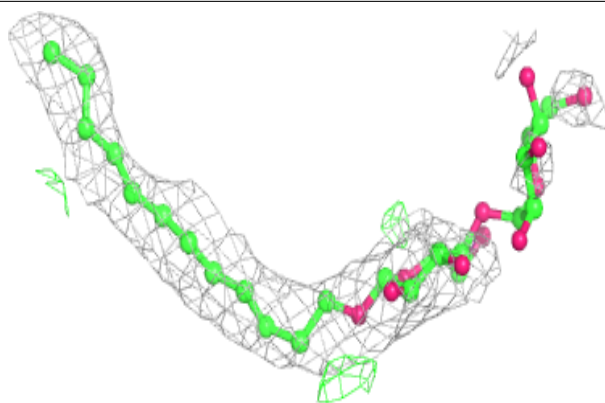
**Electron density around UNL B 627:**

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

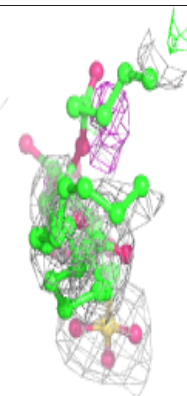
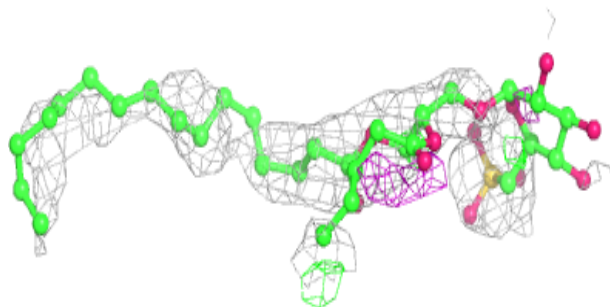
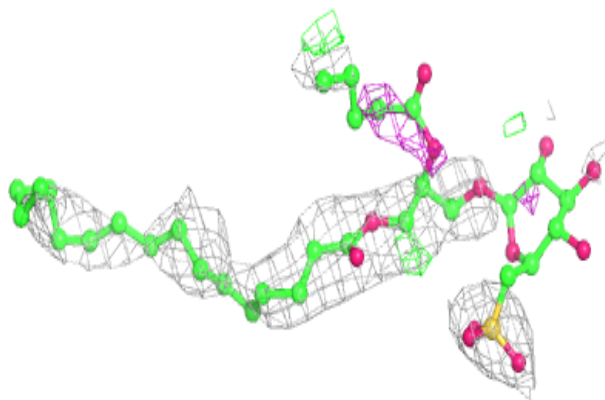


**Electron density around LMT M 103:**

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

**Electron density around SQD f 102:**

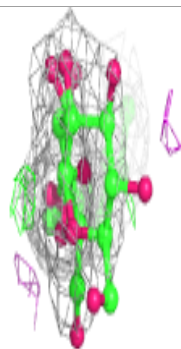
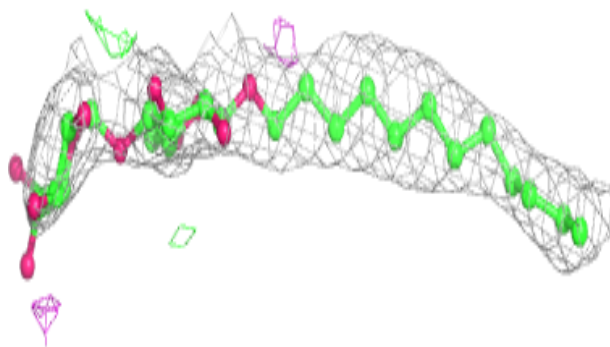
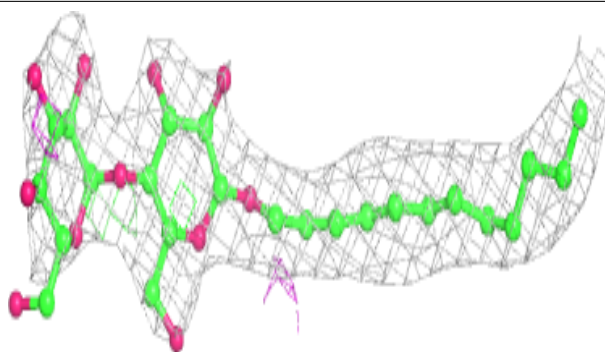
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



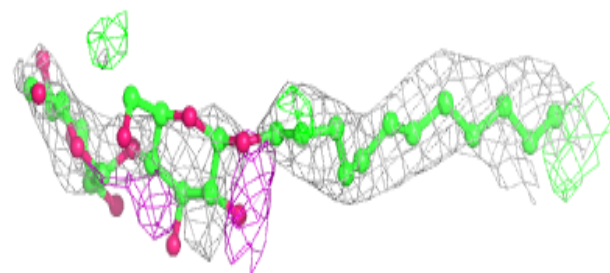
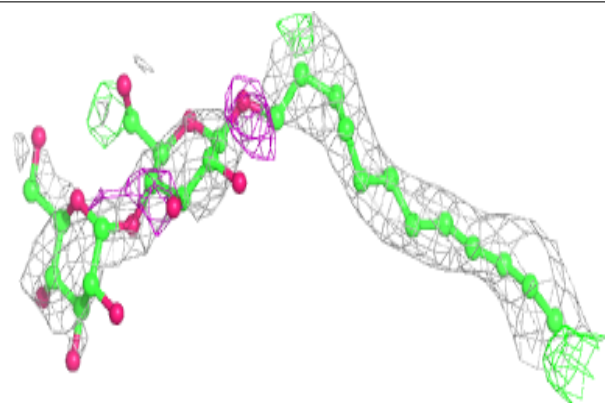


**Electron density around LMT m 103:**

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

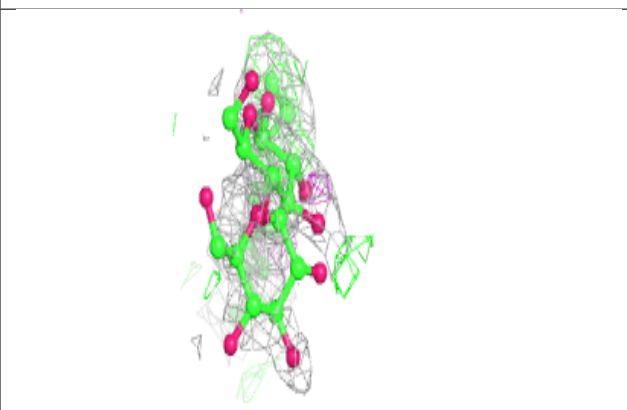
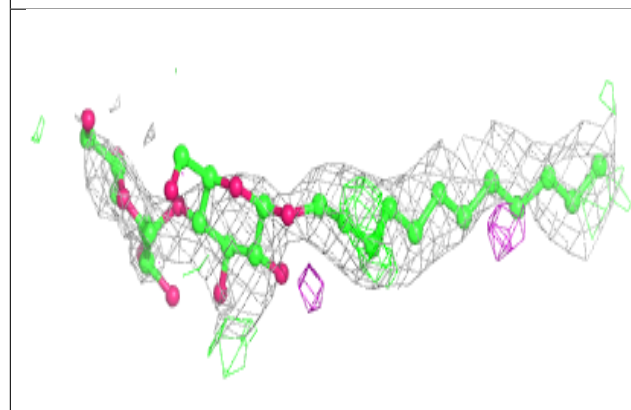
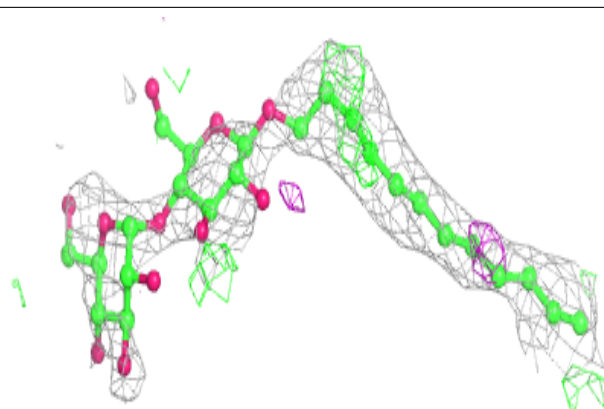
**Electron density around LMT a 414:**

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

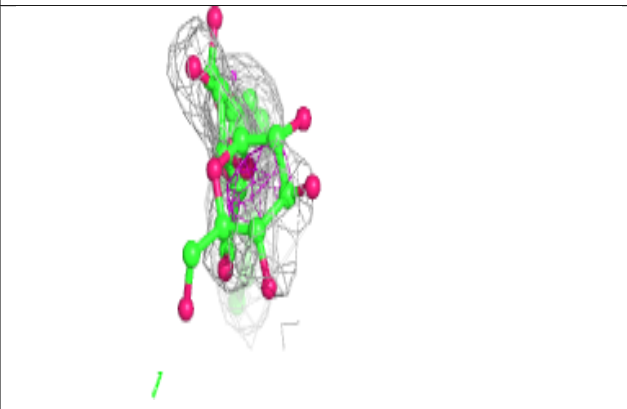
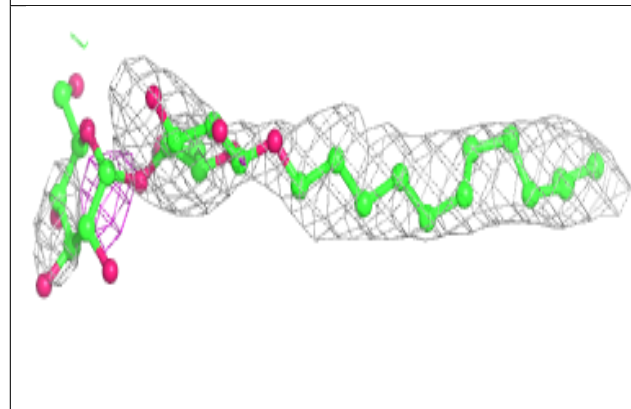
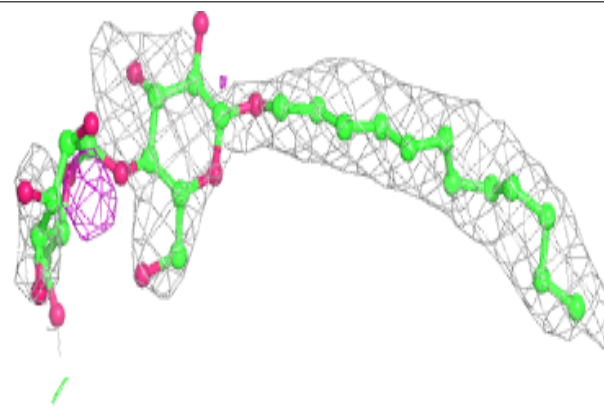


**Electron density around LMT A 359:**

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

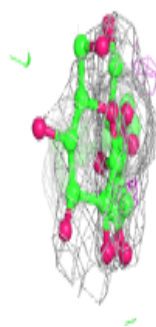
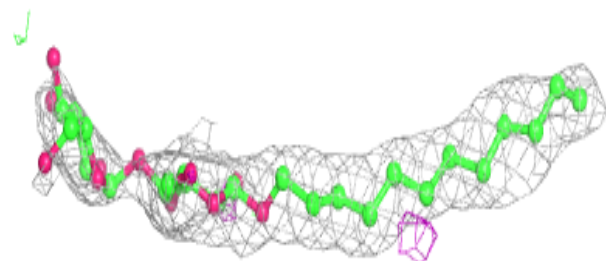
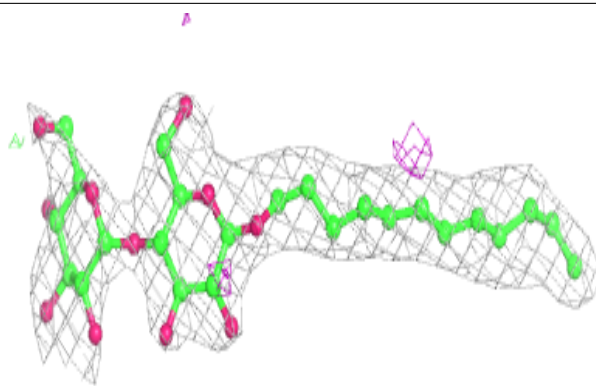
**Electron density around LMT D 404:**

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

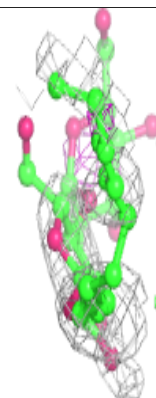
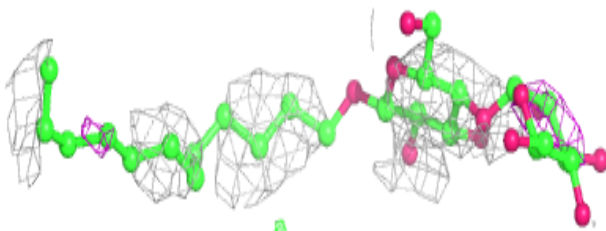
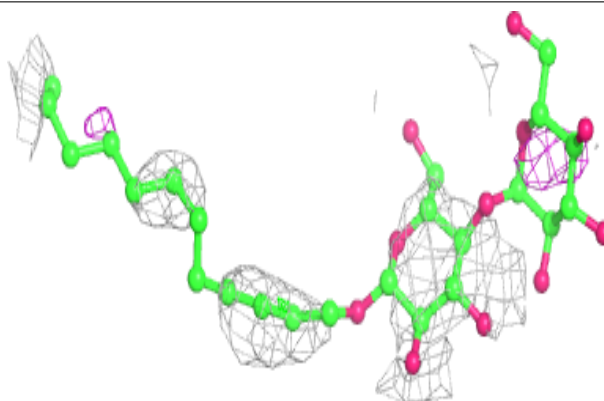


**Electron density around LMT M 101:**

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

**Electron density around LMT e 102:**

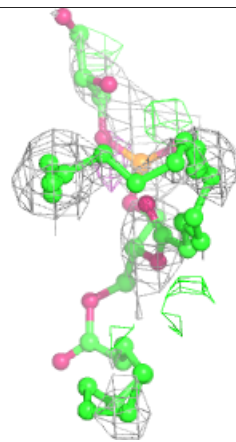
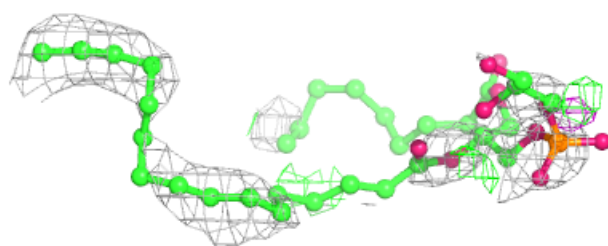
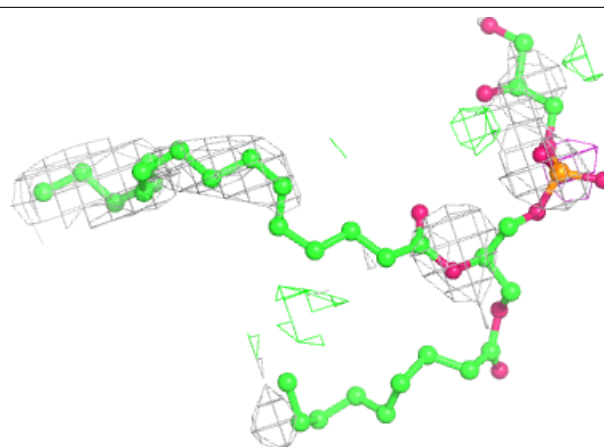
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



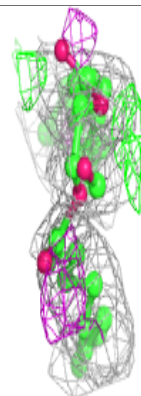
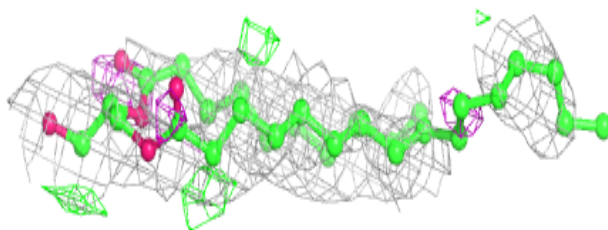
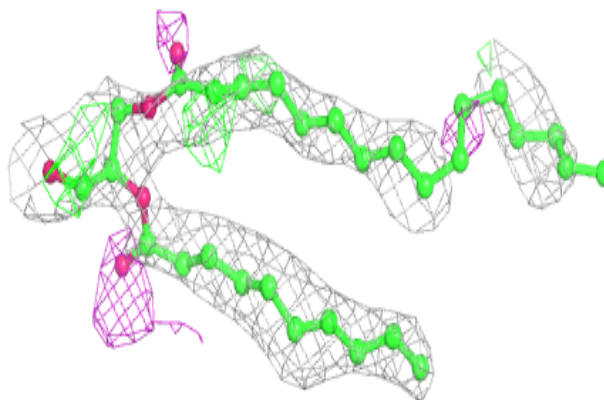


**Electron density around LHG e 101:**

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

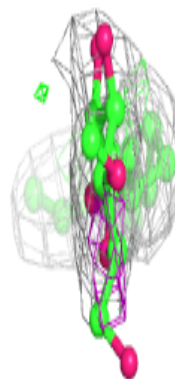
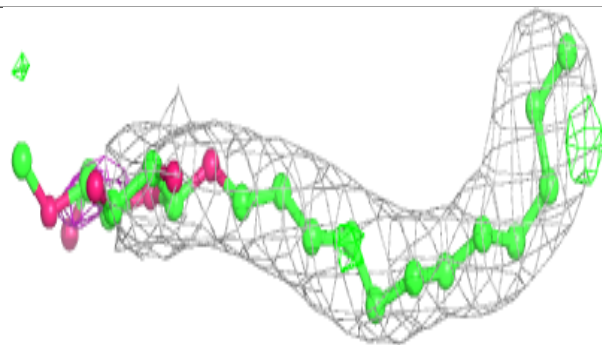
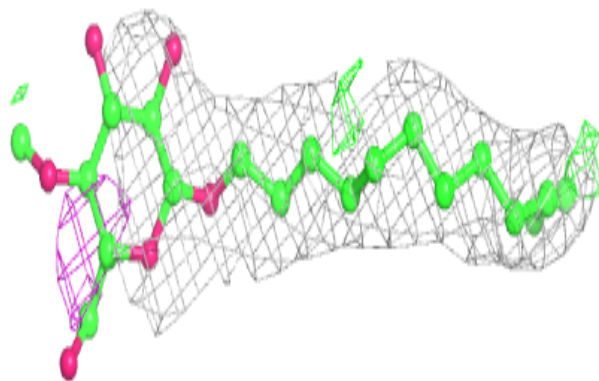
**Electron density around UNL K 101:**

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

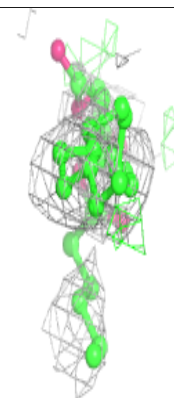
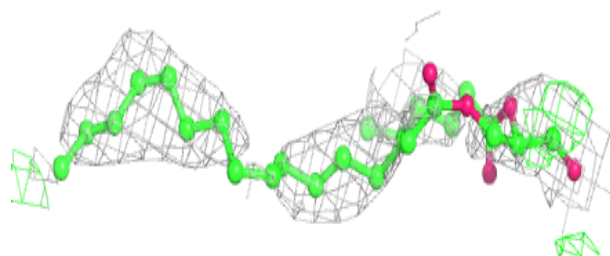
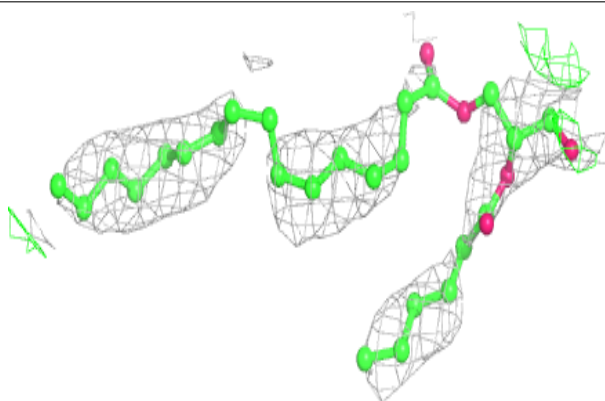


**Electron density around LMT t 101:**

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

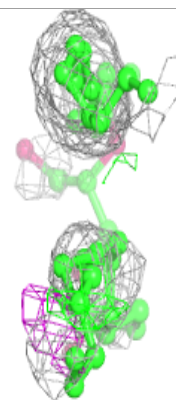
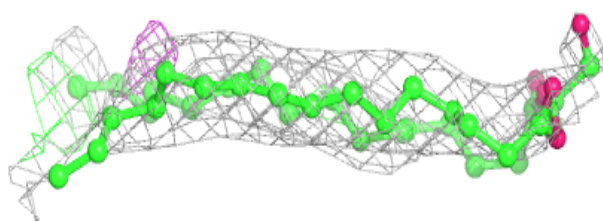
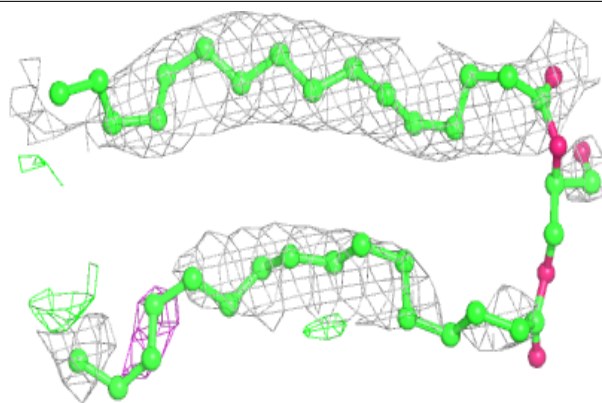
**Electron density around UNL a 417:**

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

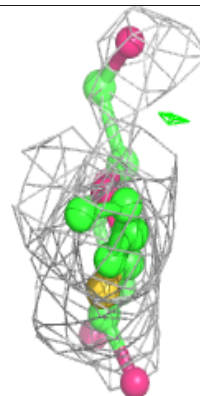
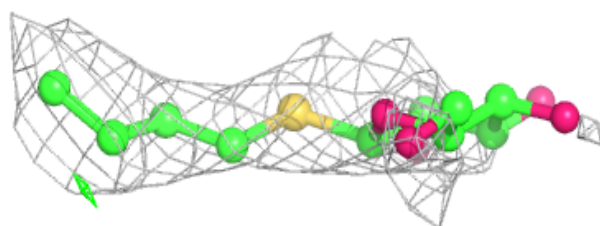
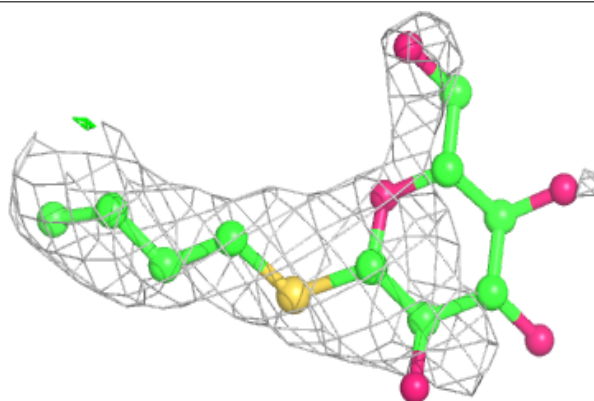


**Electron density around UNL I 102:**

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

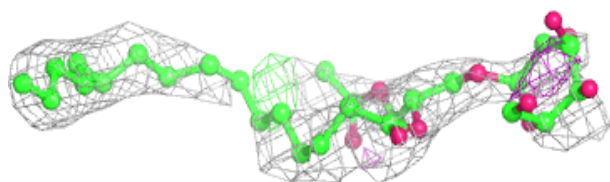
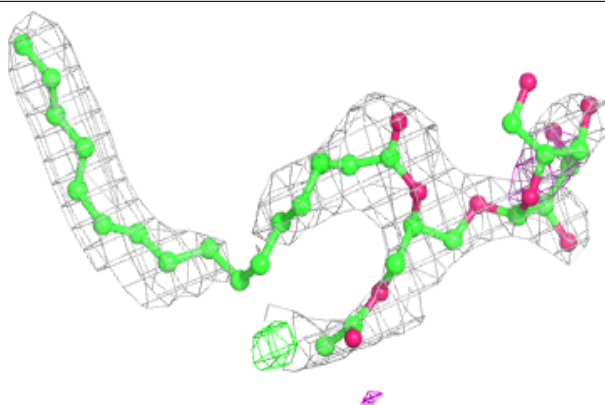
**Electron density around HTG D 414:**

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

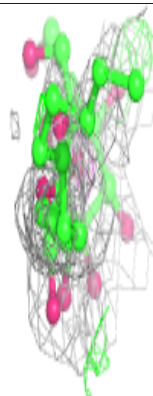
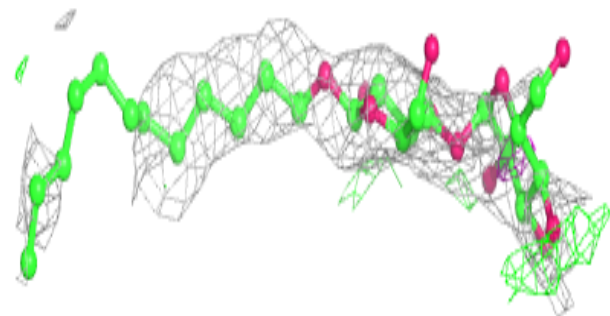
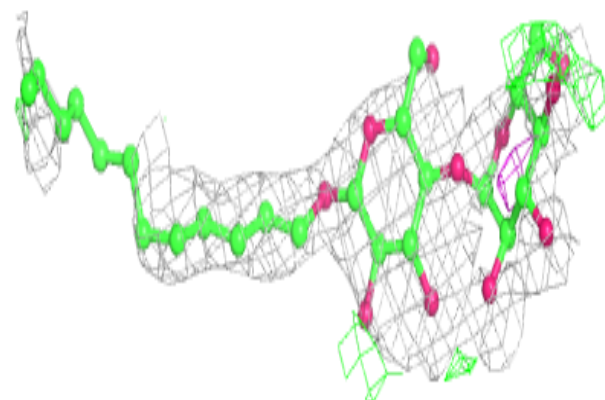


**Electron density around LMG Z 101:**

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

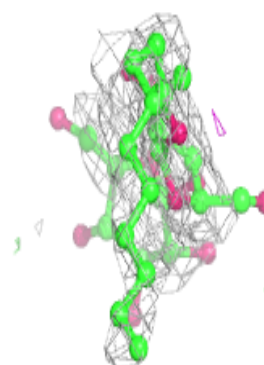
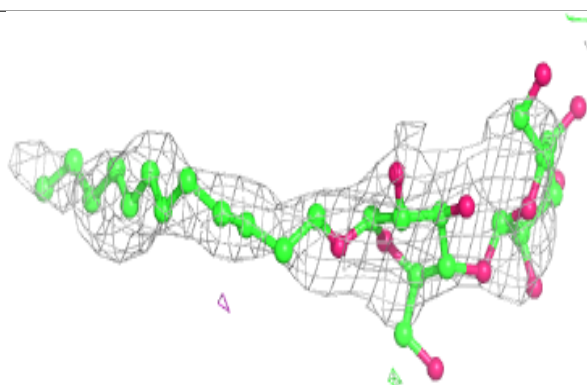
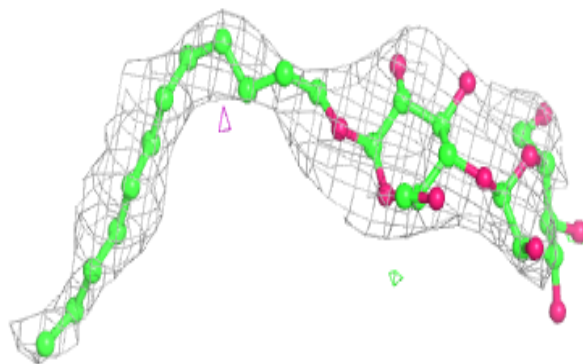
**Electron density around LMT a 420:**

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

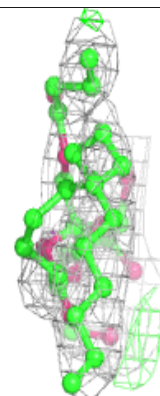
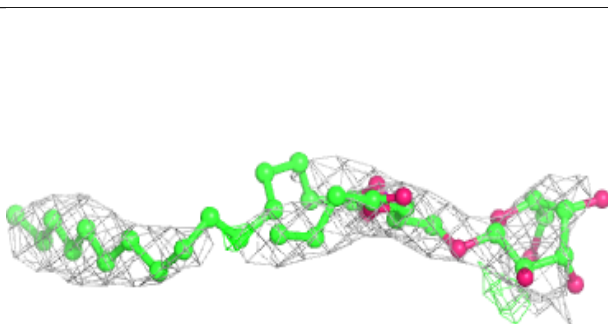
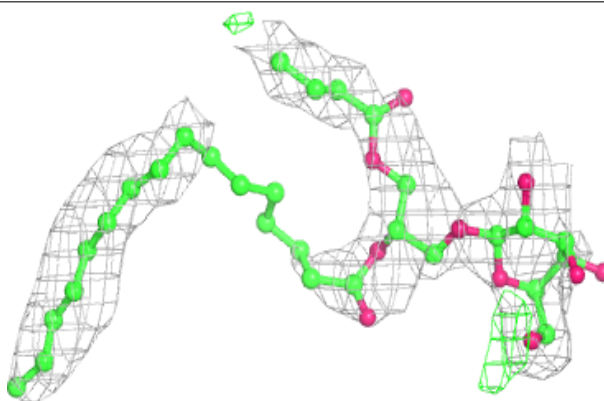


**Electron density around LMT I 101:**

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

**Electron density around LMG z 101:**

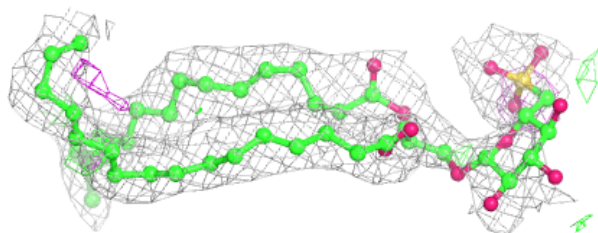
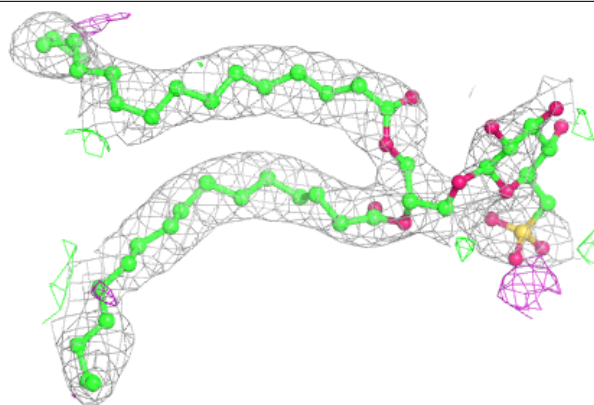
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



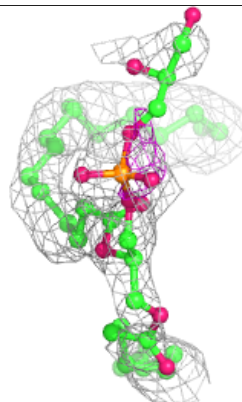
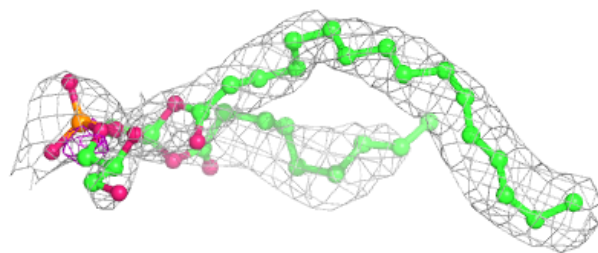
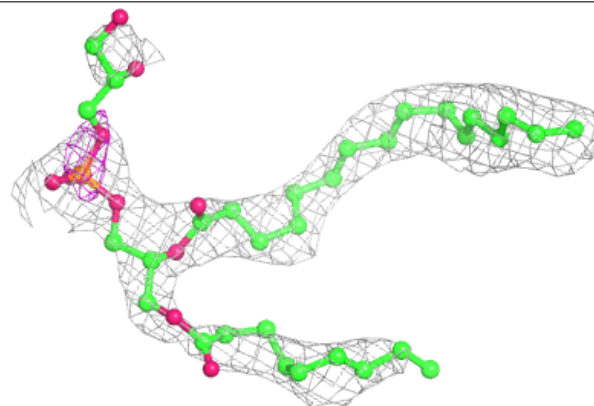


**Electron density around SQD B 620:**

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

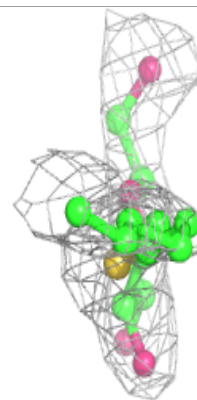
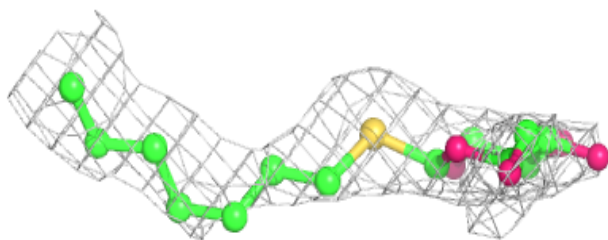
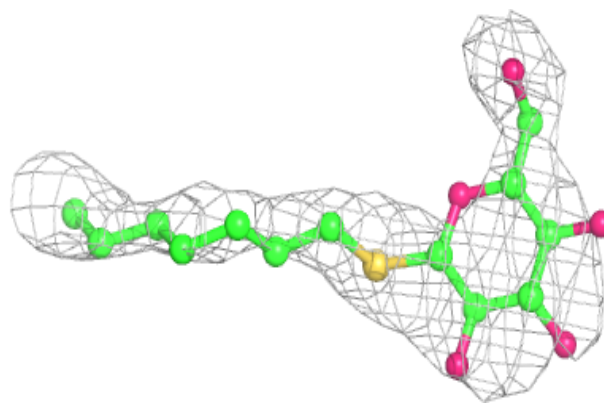
**Electron density around LHG E 101:**

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

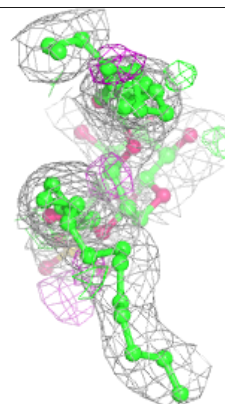
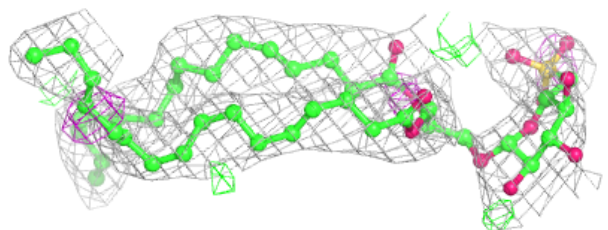
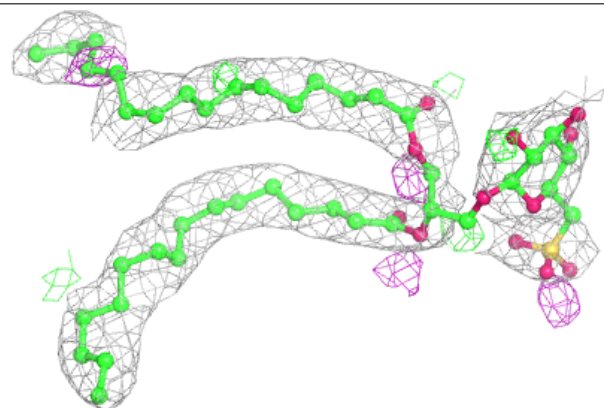


**Electron density around HTG C 522:**

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

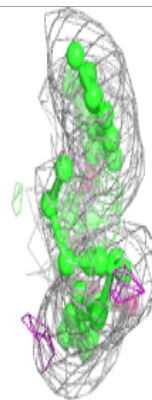
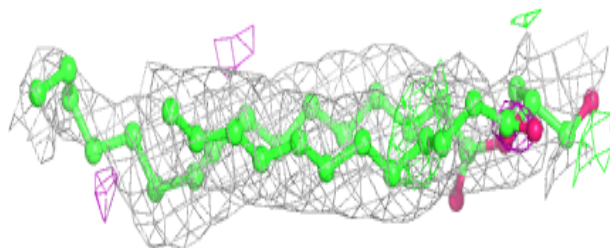
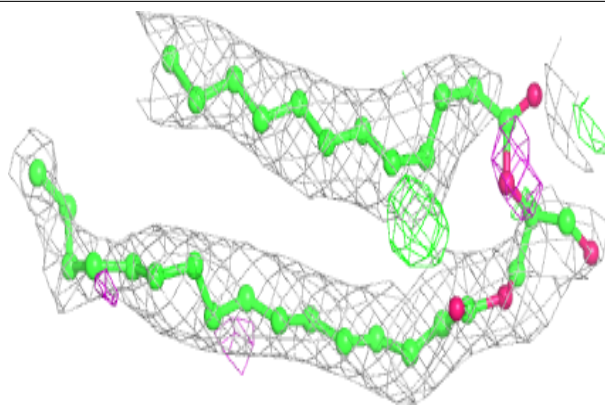
**Electron density around SQD b 620:**

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

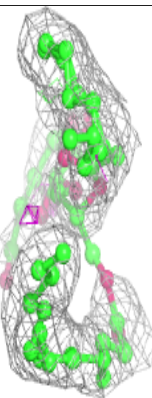
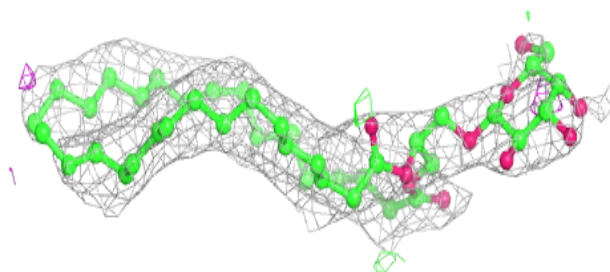
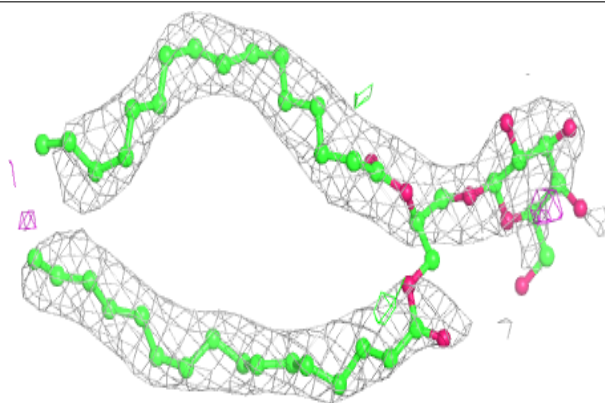


**Electron density around UNL d 410:**

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

**Electron density around LMG a 419:**

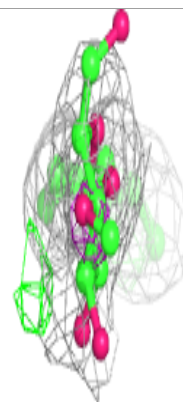
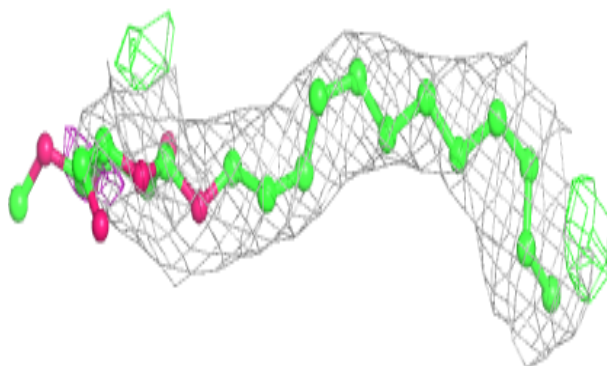
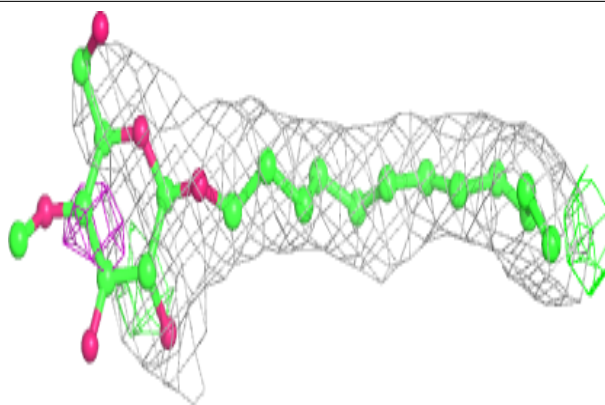
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



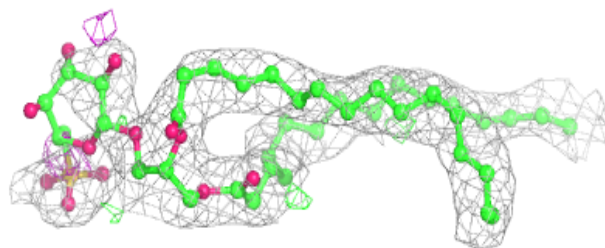
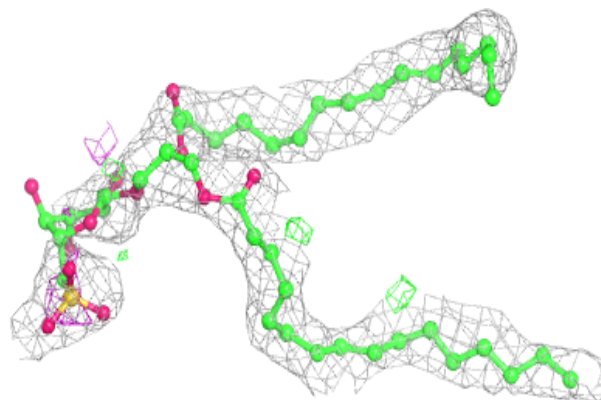


**Electron density around LMT b 627:**

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

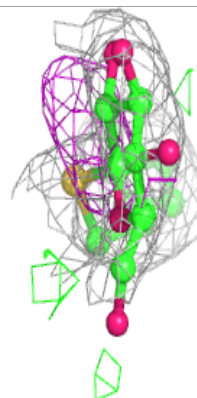
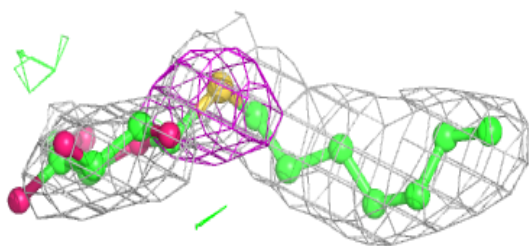
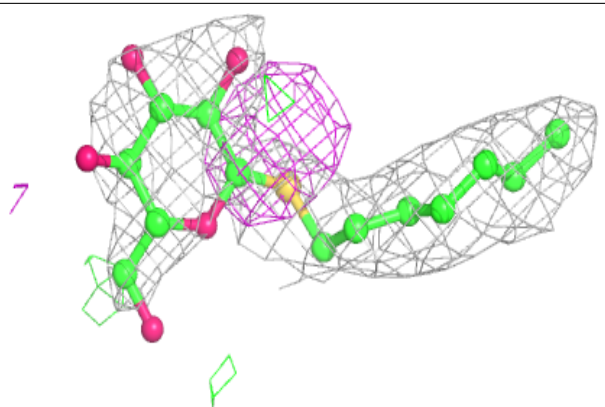
**Electron density around SQD a 413:**

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

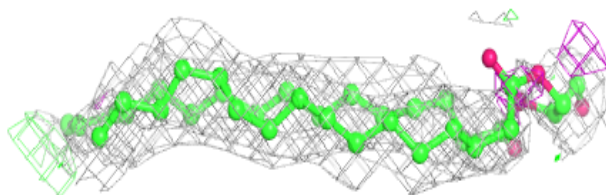
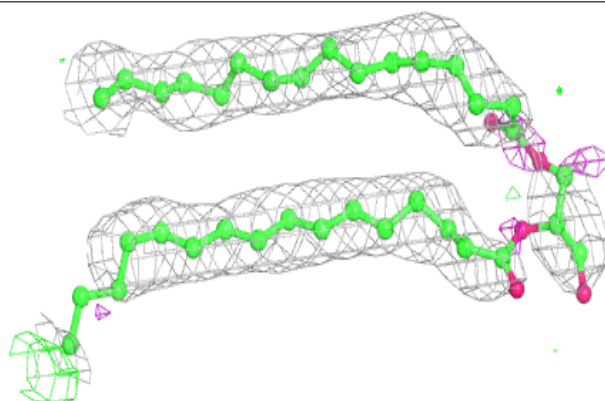


**Electron density around HTG b 622:**

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

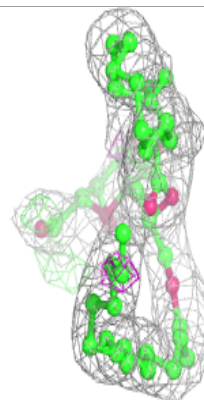
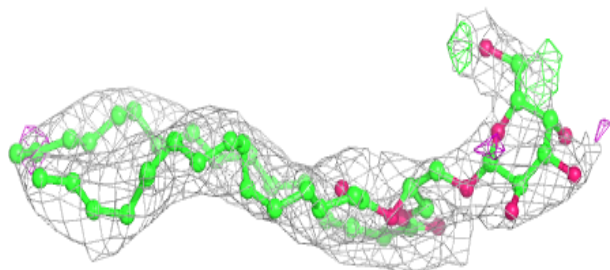
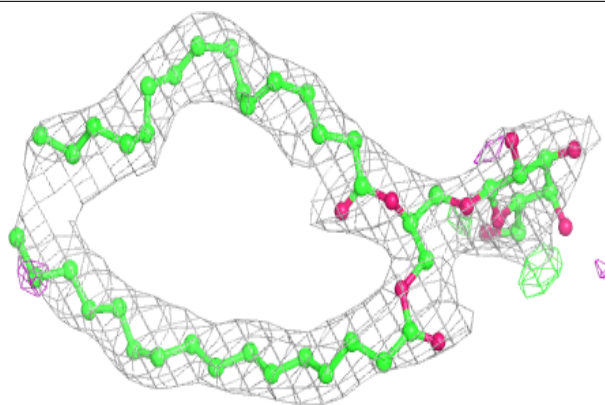
**Electron density around UNL D 413:**

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

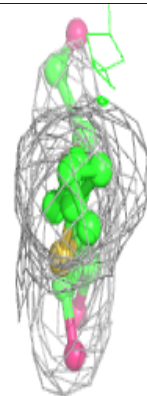
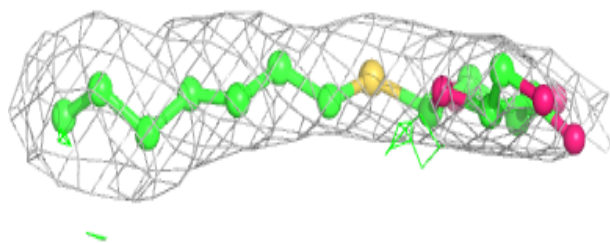
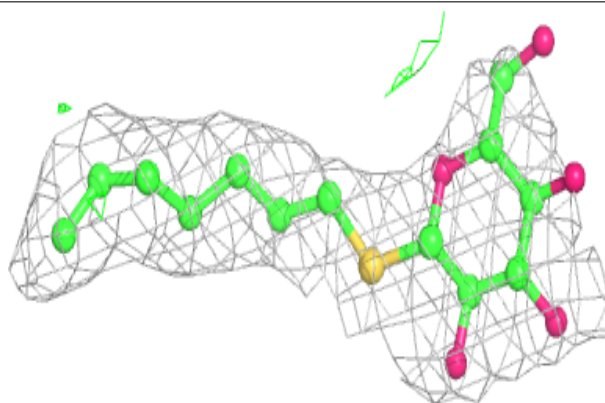


**Electron density around LMG C 501:**

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

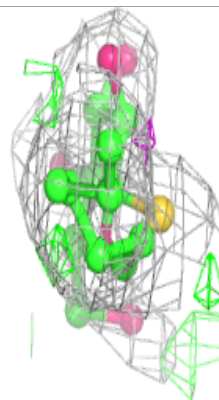
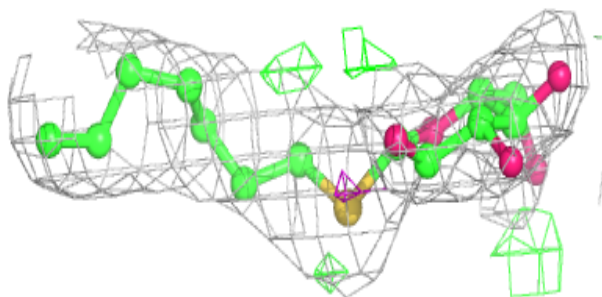
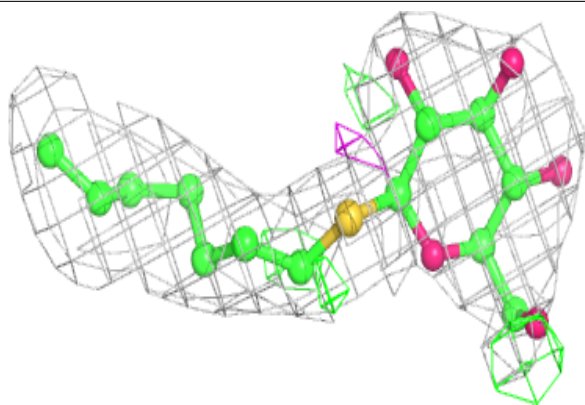
**Electron density around HTG b 625:**

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

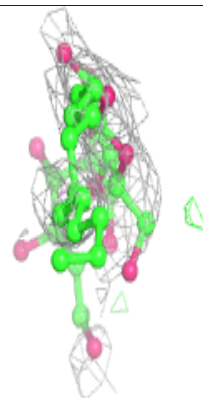
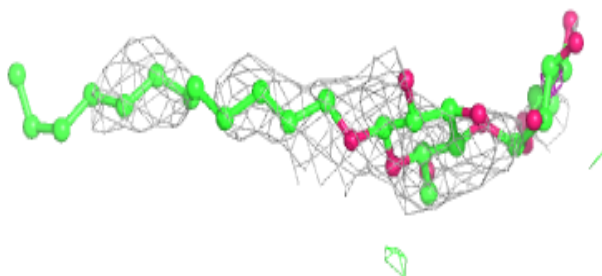
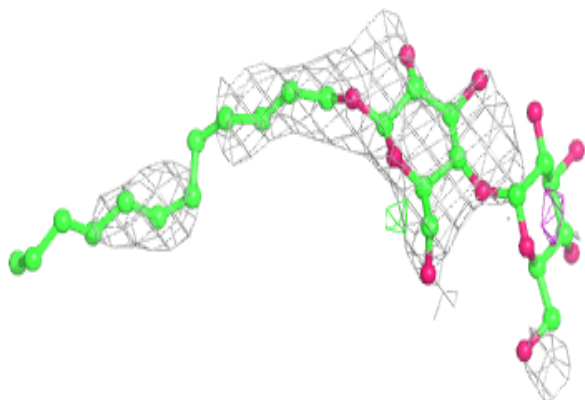


**Electron density around HTG B 622:**

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

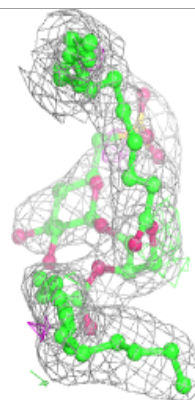
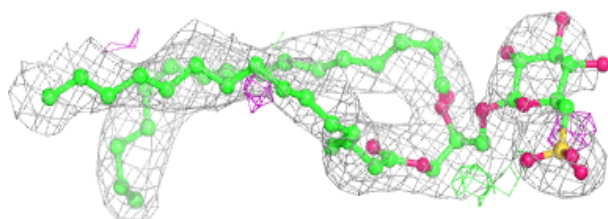
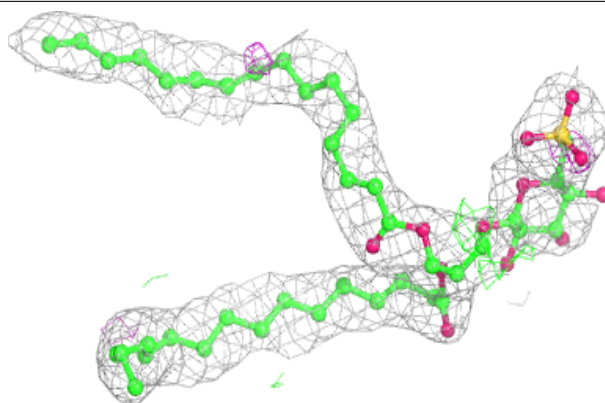
**Electron density around LMT E 102:**

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

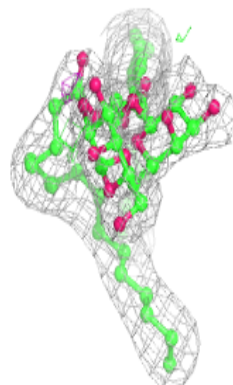
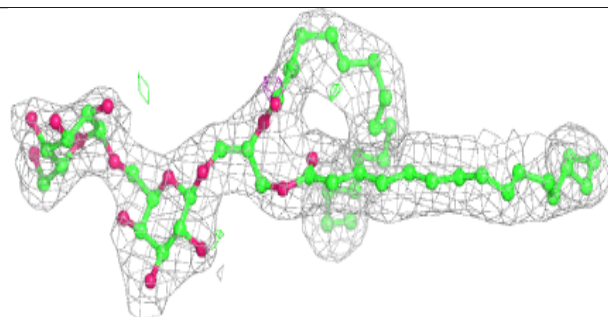
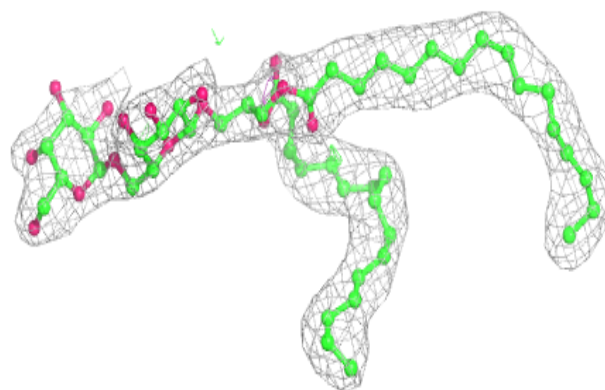


**Electron density around SQD A 412:**

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

**Electron density around DGD h 102:**

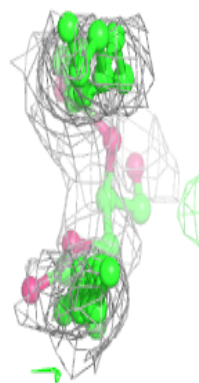
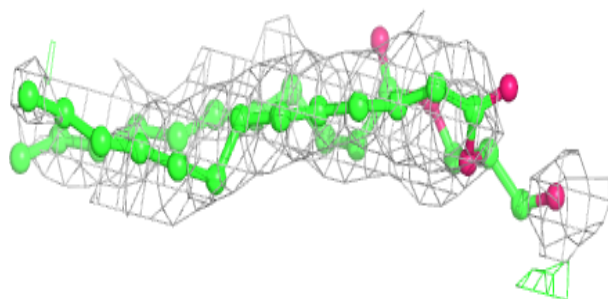
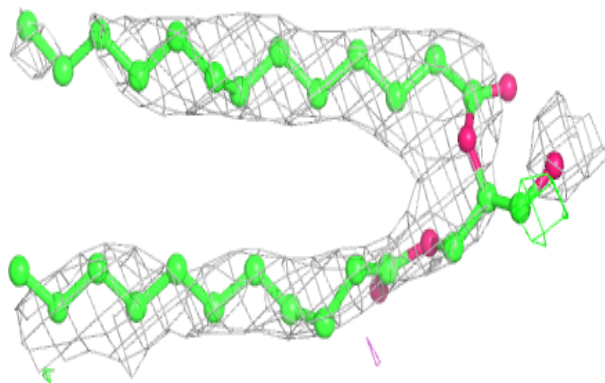
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



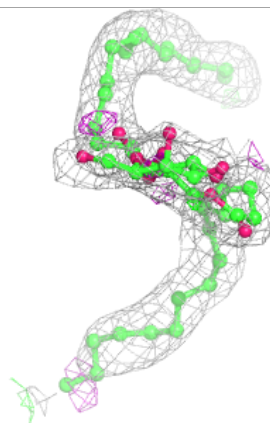
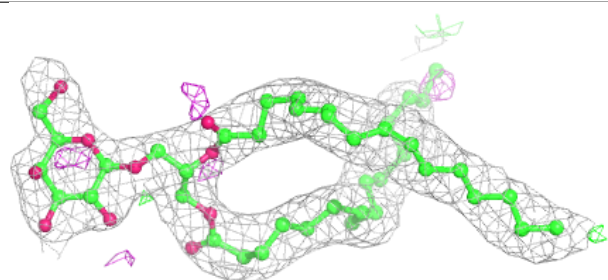
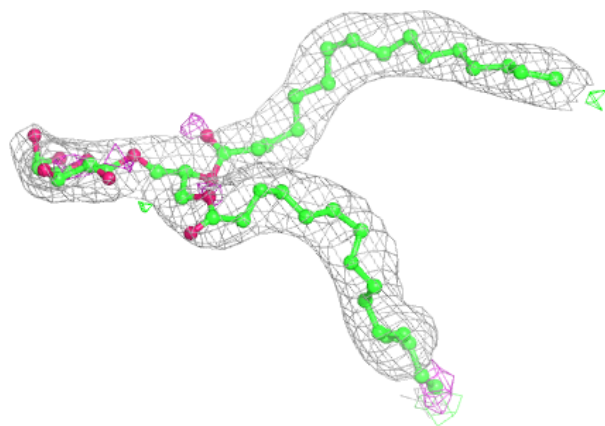


**Electron density around UNL c 525:**

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

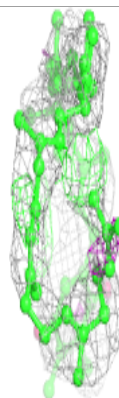
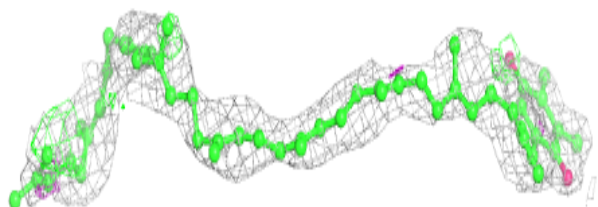
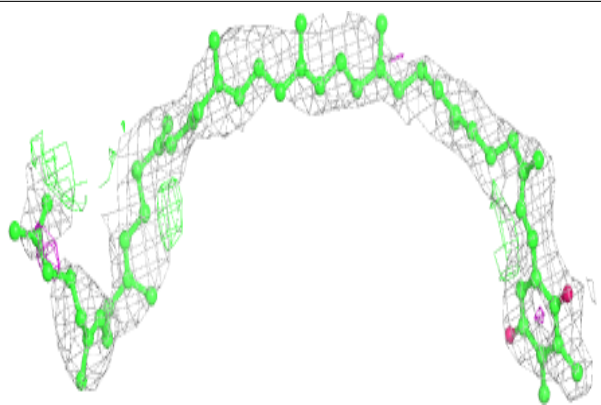
**Electron density around LMG B 621:**

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

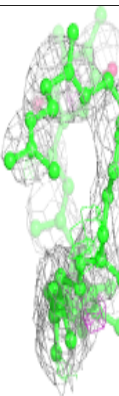
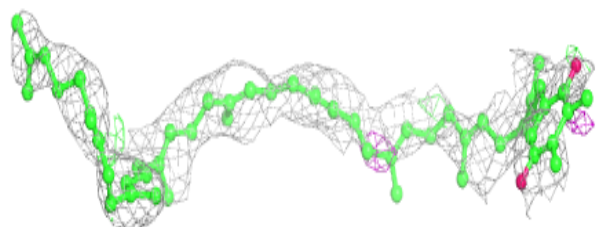
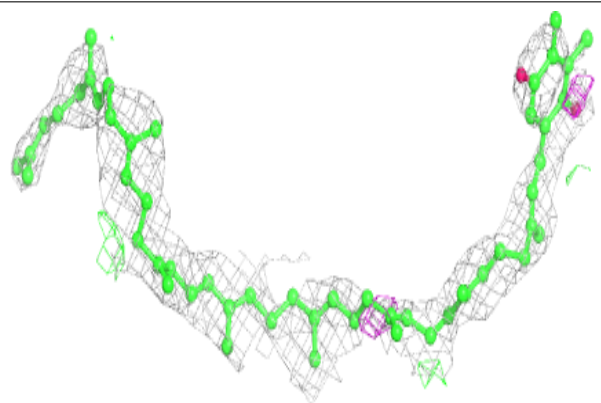


**Electron density around PL9 A 414:**

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

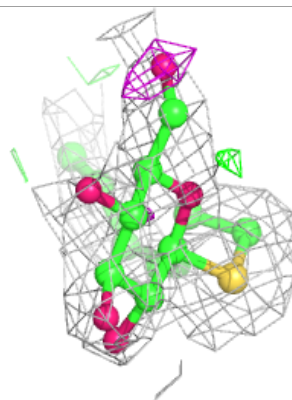
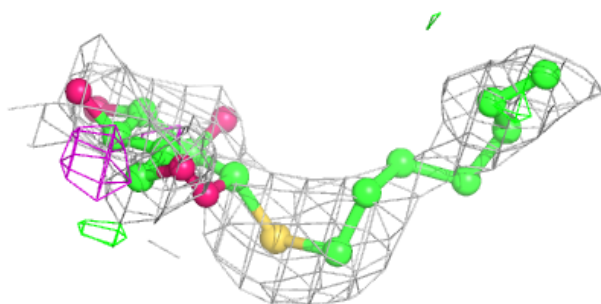
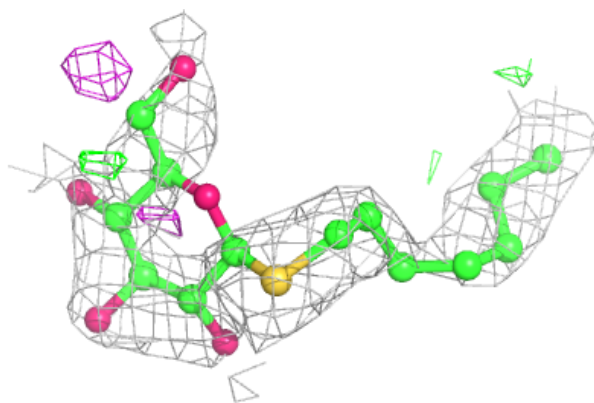
**Electron density around PL9 a 416:**

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

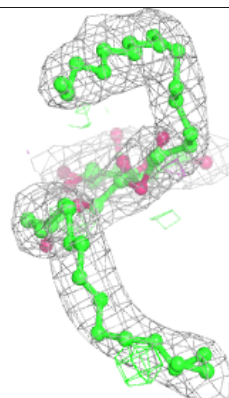
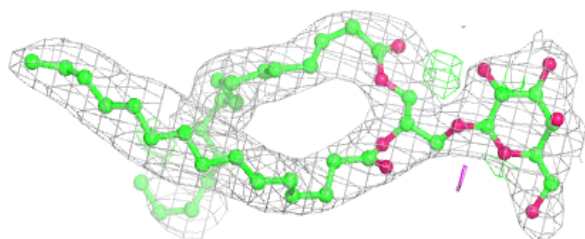
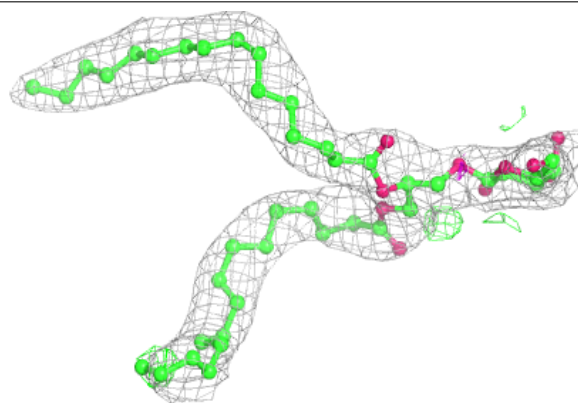


**Electron density around HTG B 623:**

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

**Electron density around LMG m 101:**

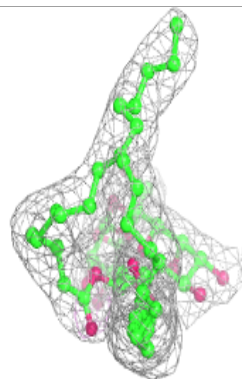
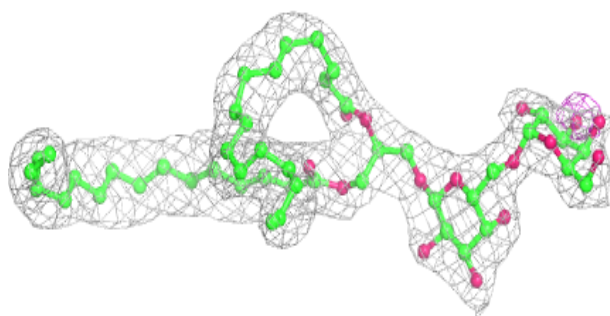
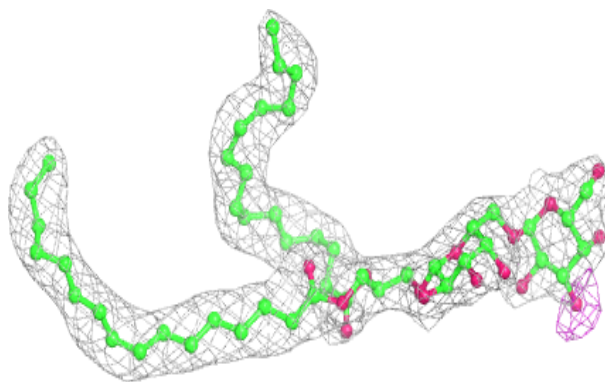
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



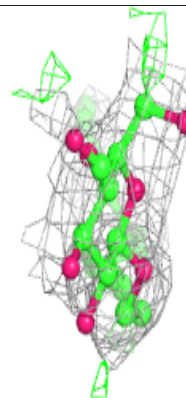
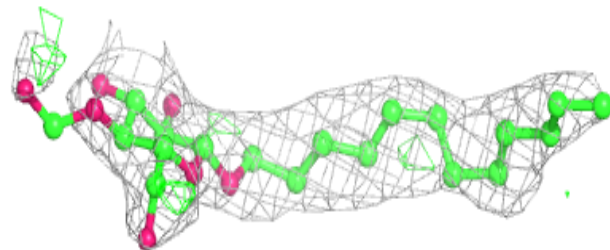
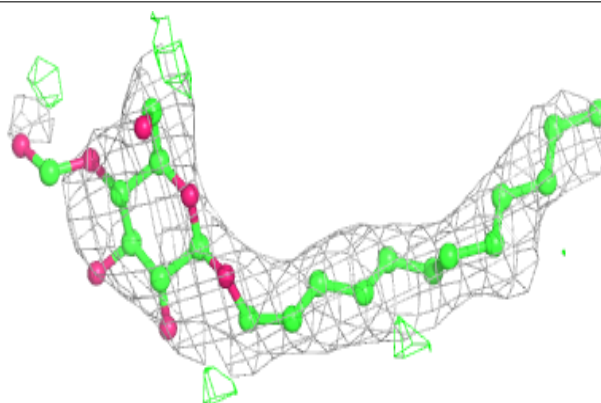


**Electron density around DGD H 102:**

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

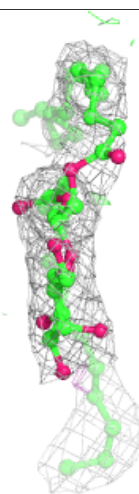
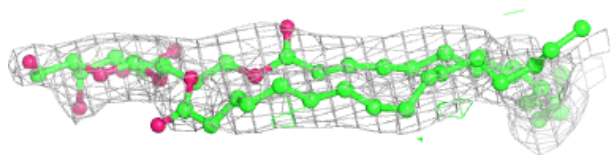
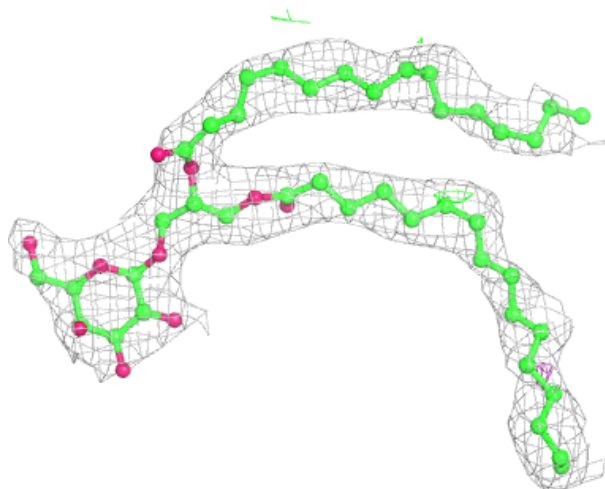
**Electron density around LMT t 102:**

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



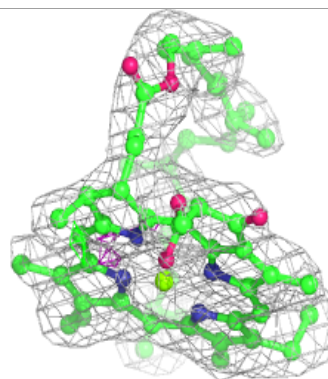
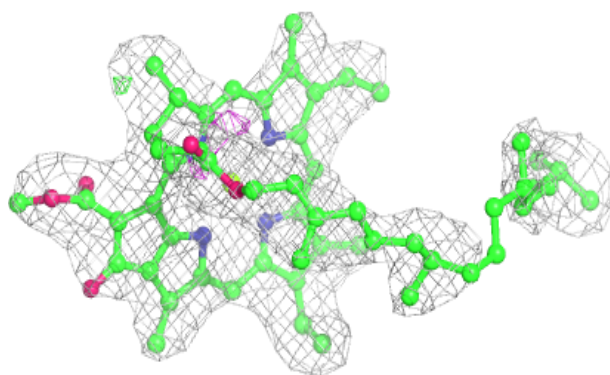
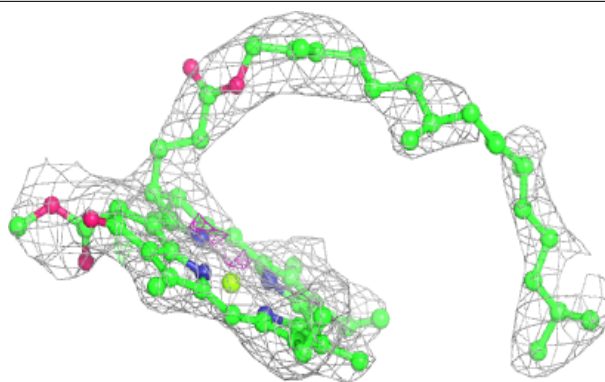
**Electron density around LMG C 520:**

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

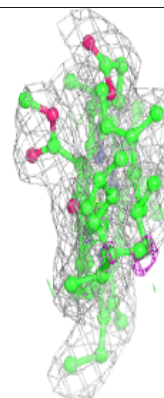
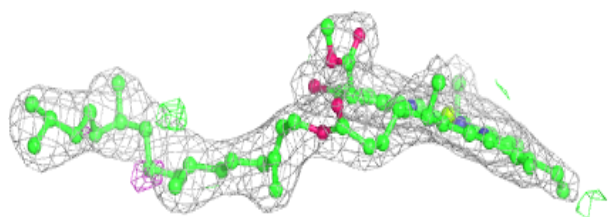
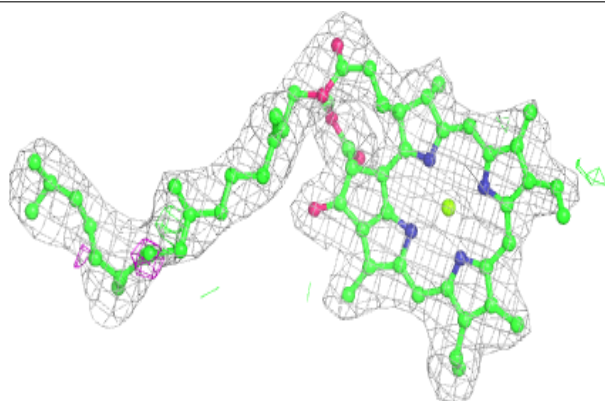


**Electron density around CLA C 514:**

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

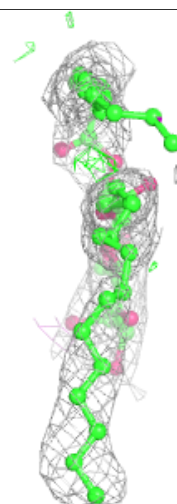
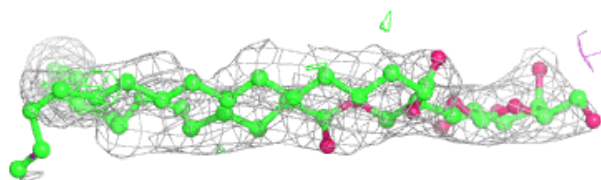
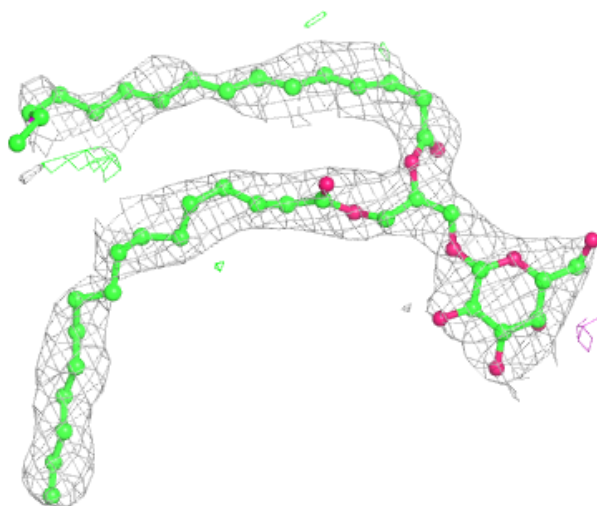
**Electron density around CLA b 602:**

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



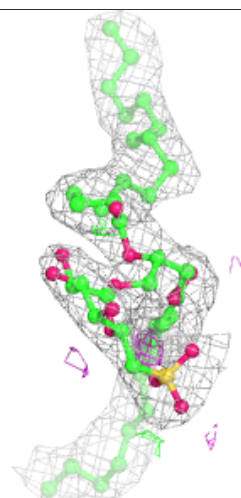
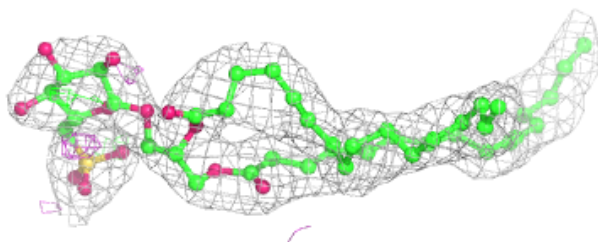
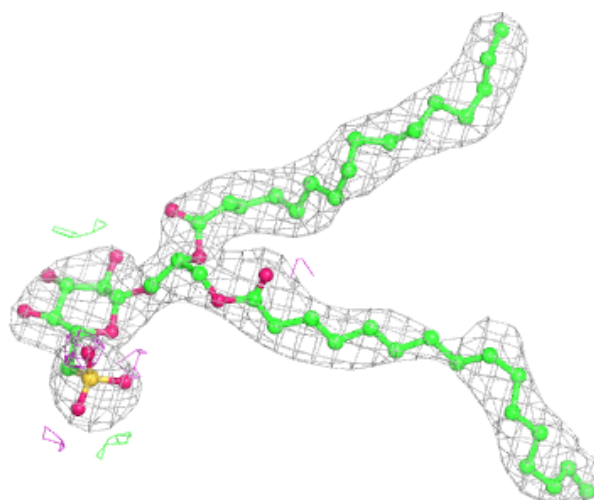
**Electron density around LMG c 520:**

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



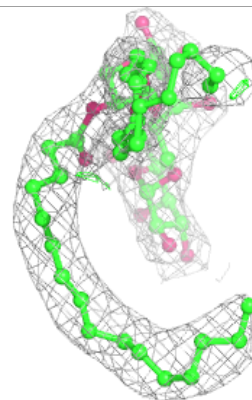
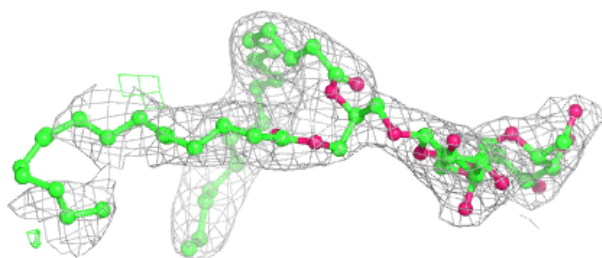
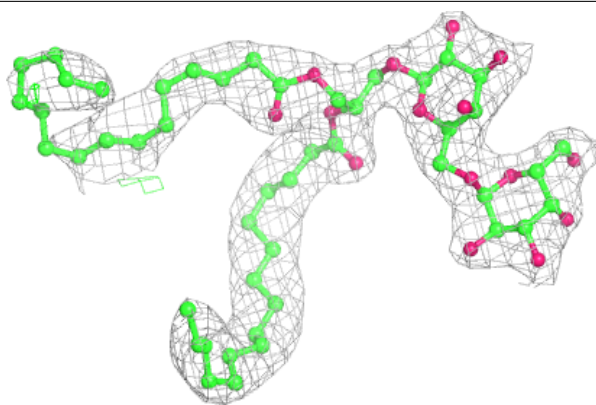
**Electron density around SQD A 410:**

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

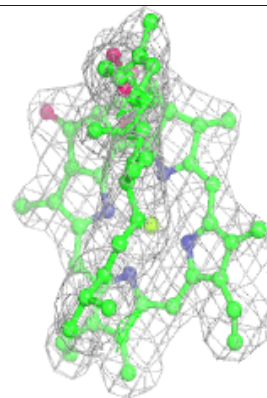
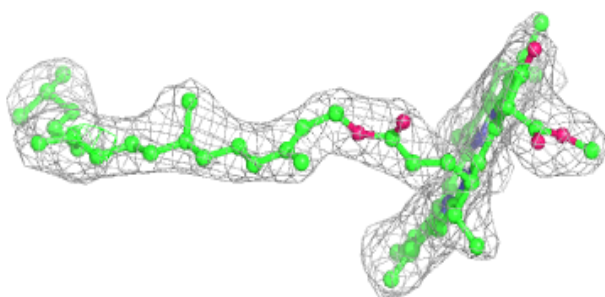
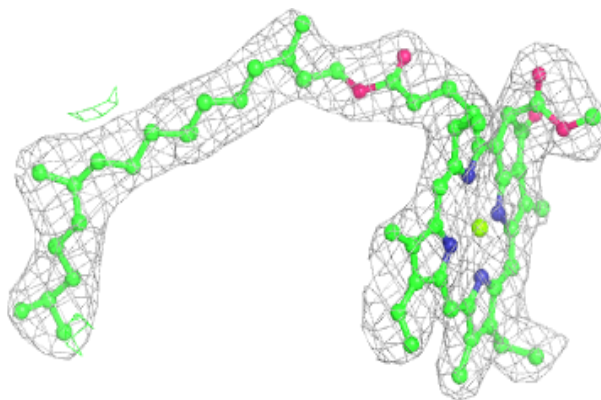


**Electron density around DGD C 518:**

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

**Electron density around CLA B 609:**

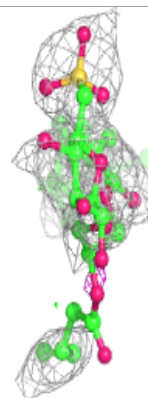
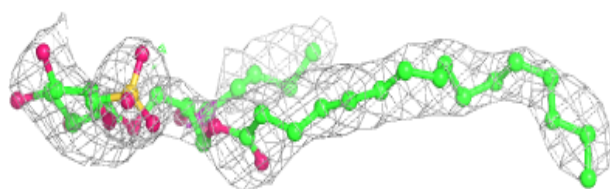
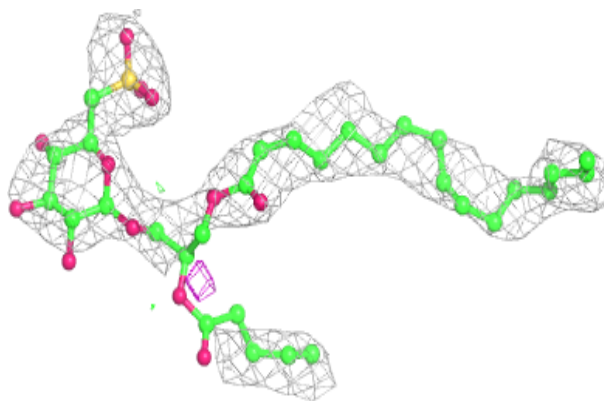
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



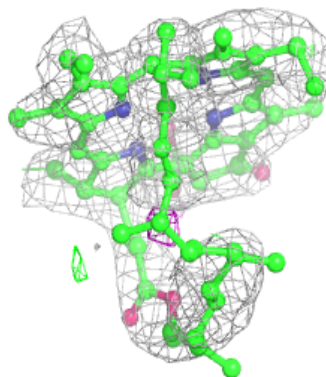
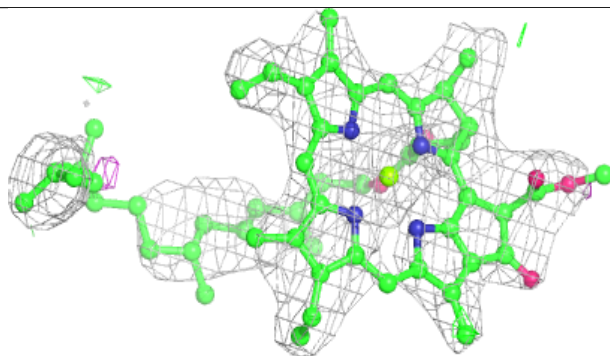
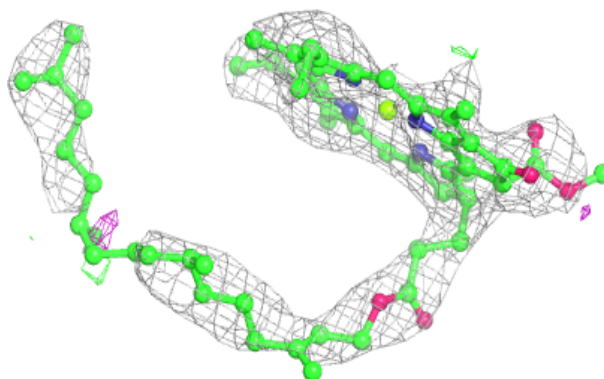


**Electron density around SQD F 101:**

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

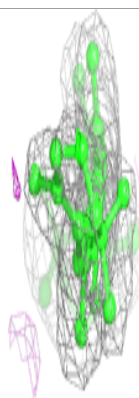
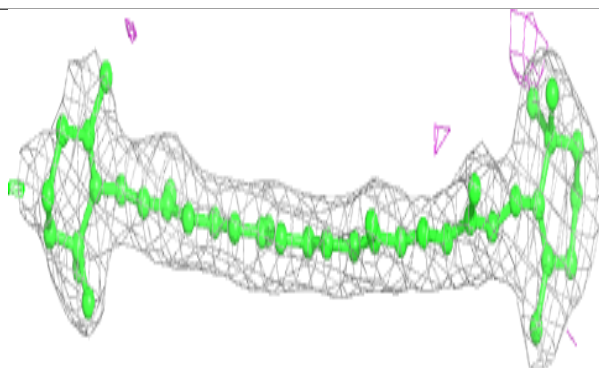
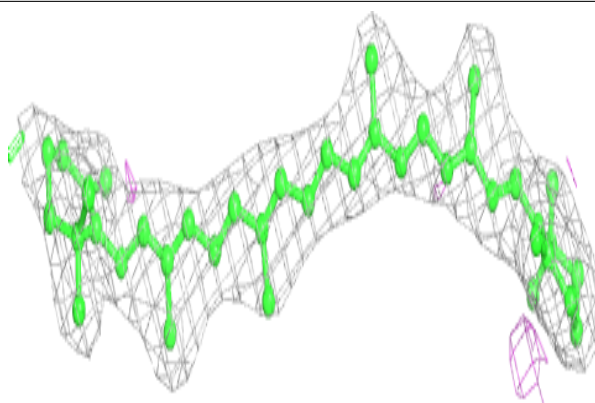
**Electron density around CLA c 514:**

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

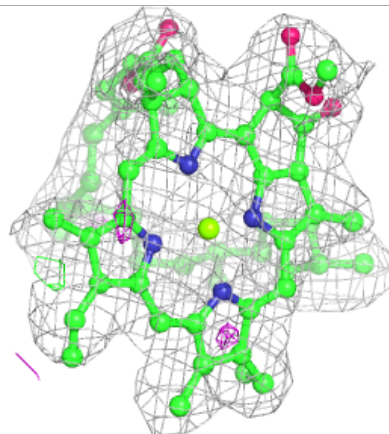
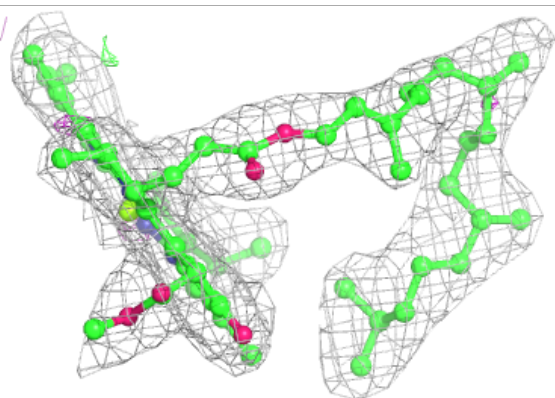
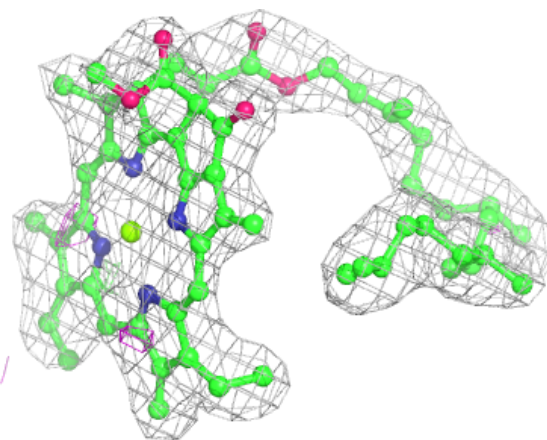


**Electron density around BCR h 101:**

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

**Electron density around CLA c 504:**

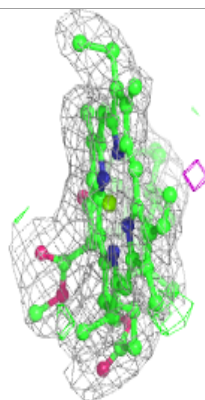
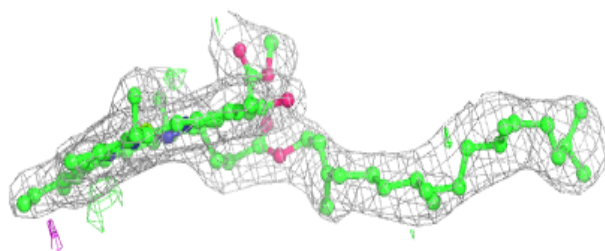
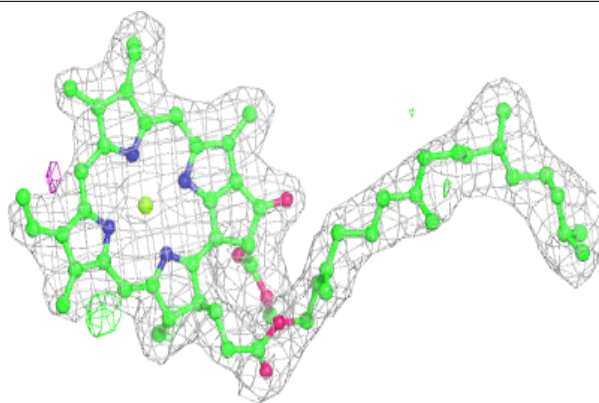
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



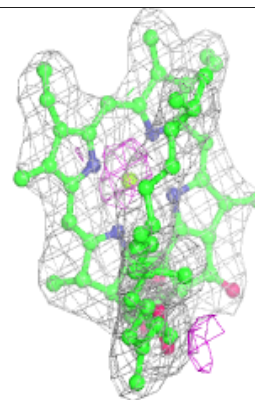
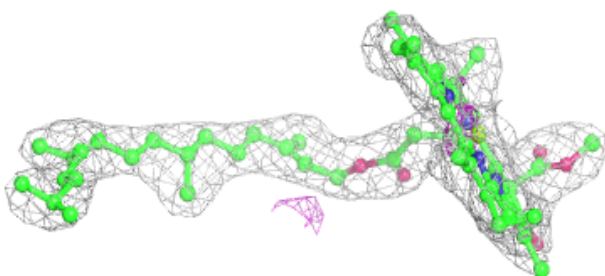
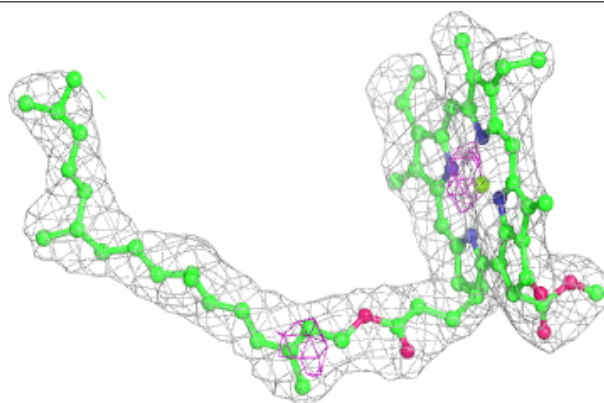


**Electron density around CLA B 602:**

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

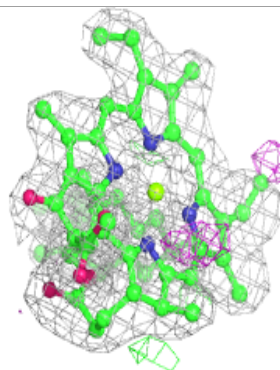
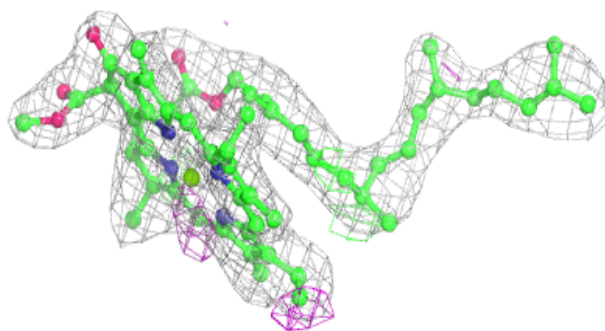
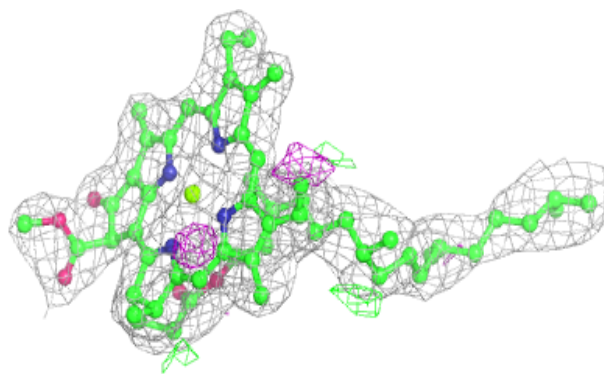
**Electron density around CLA b 609:**

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



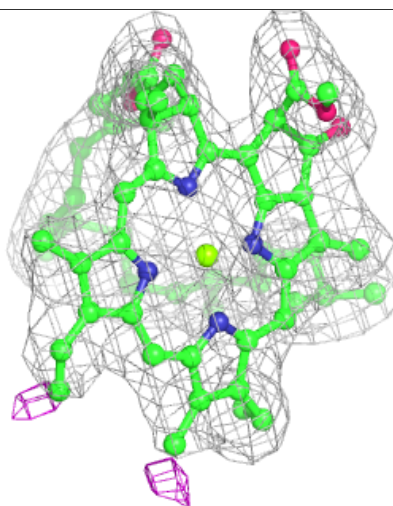
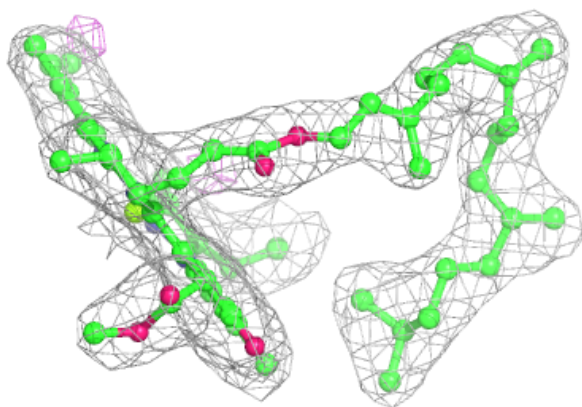
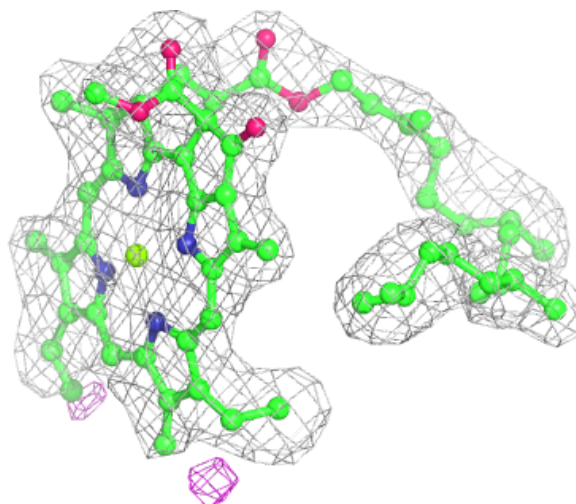
**Electron density around CLA c 506:**

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



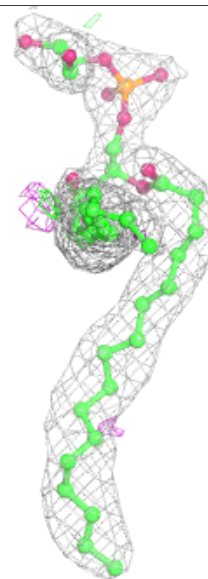
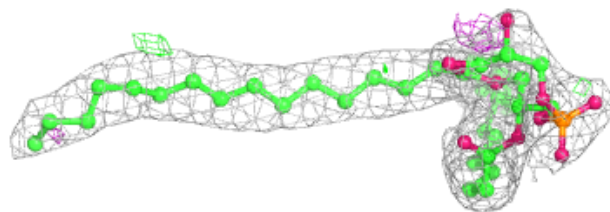
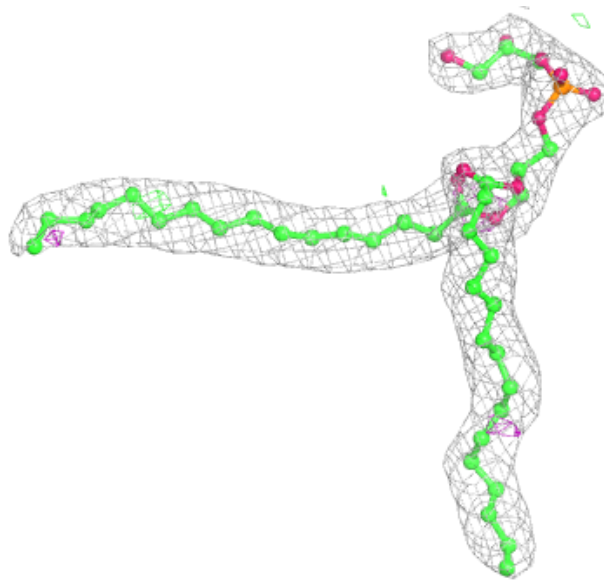
**Electron density around CLA C 504:**

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



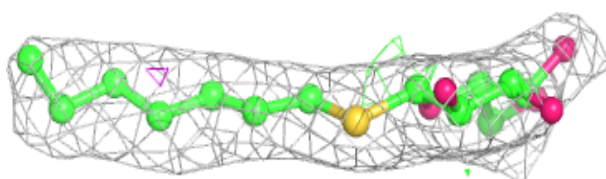
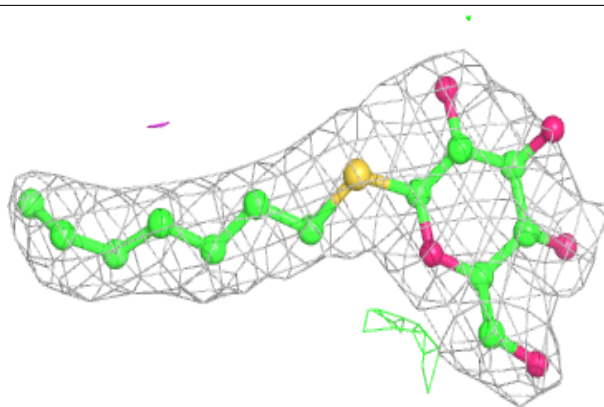
**Electron density around LHG 1 101:**

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

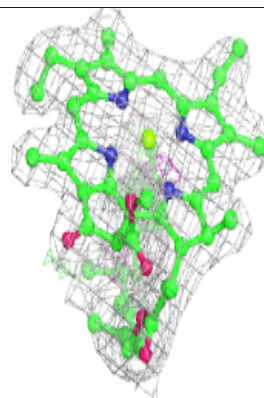
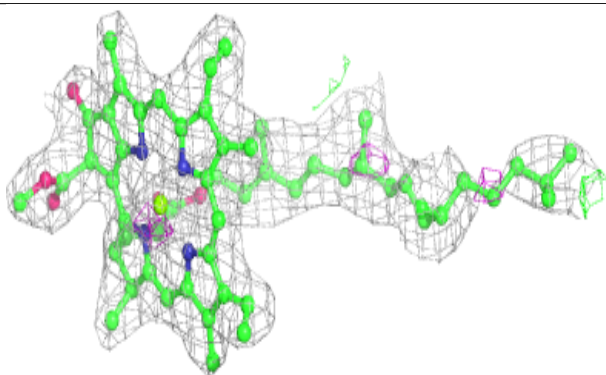
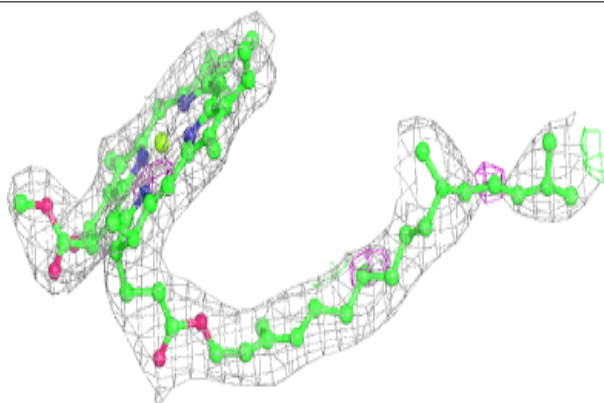


**Electron density around HTG B 626:**

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

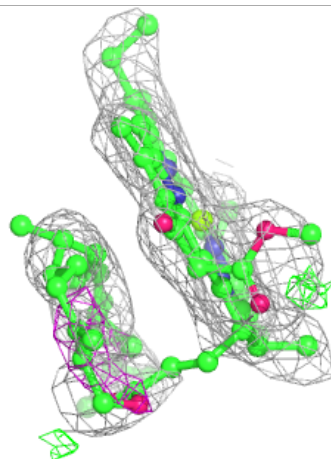
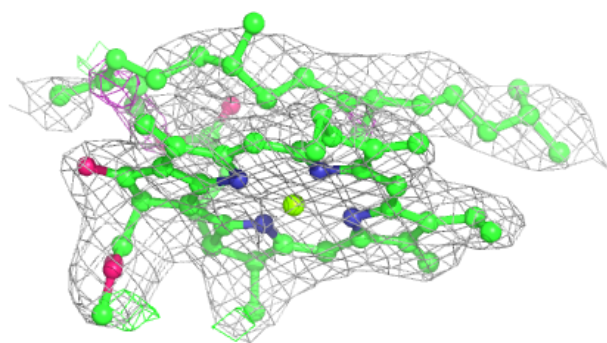
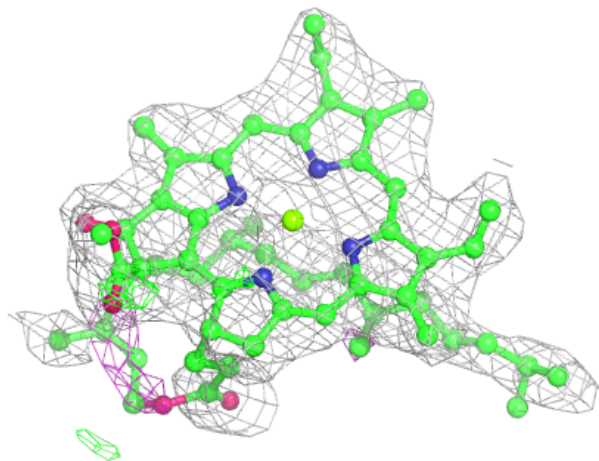
**Electron density around CLA C 505:**

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



**Electron density around CLA b 601:**

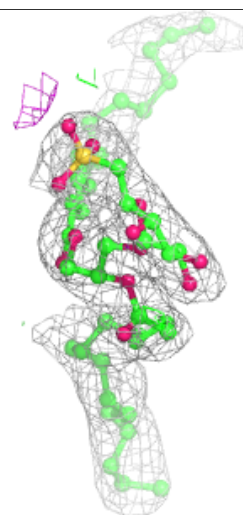
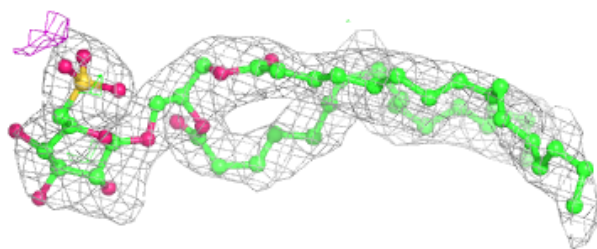
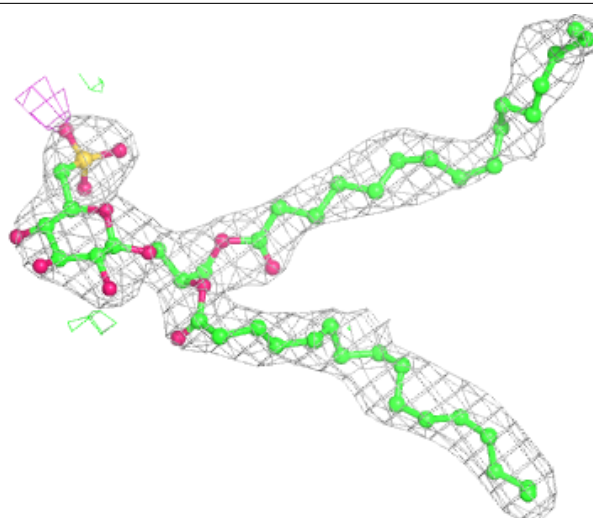
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





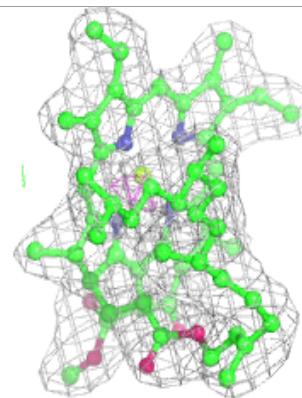
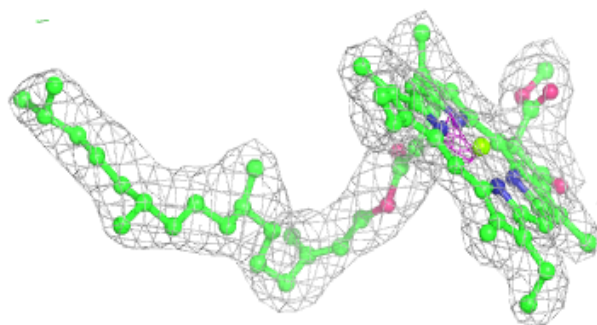
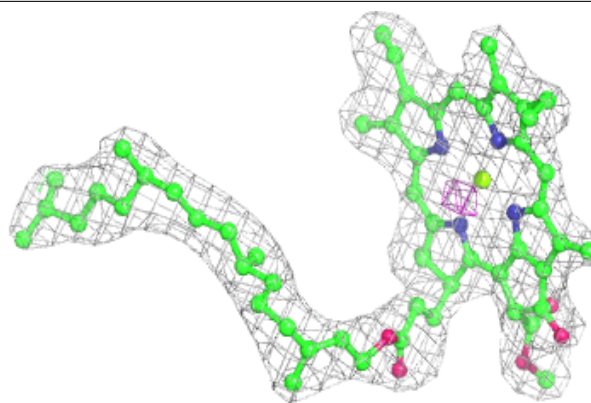
**Electron density around SQD a 411:**

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

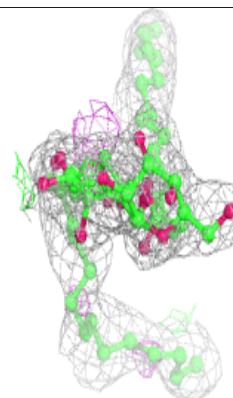
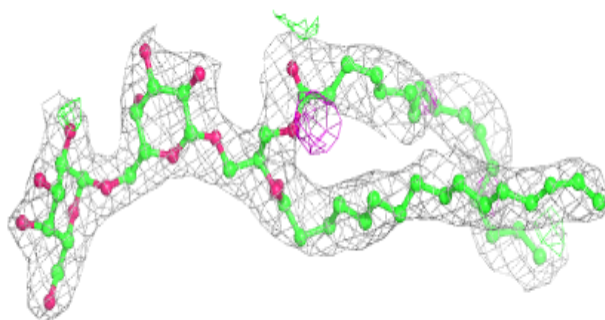
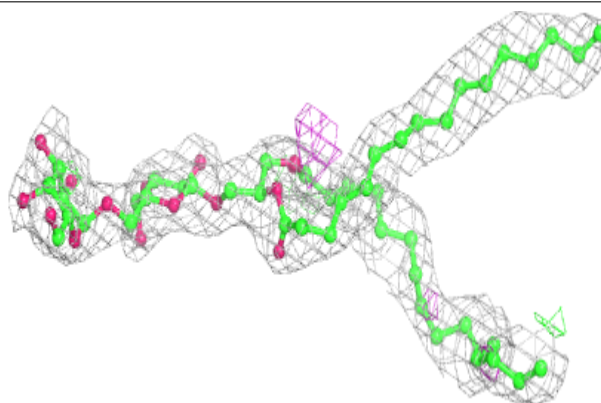


**Electron density around CLA C 512:**

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

**Electron density around DGD c 517:**

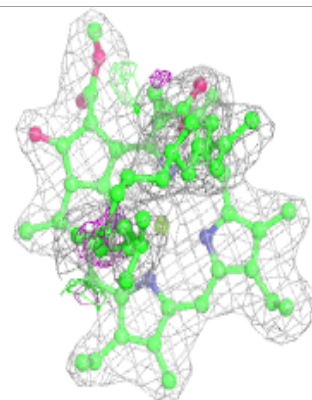
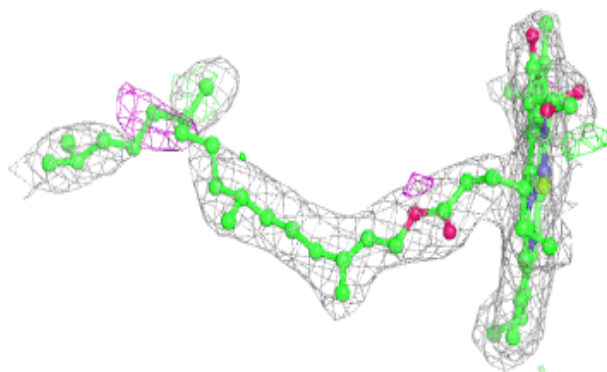
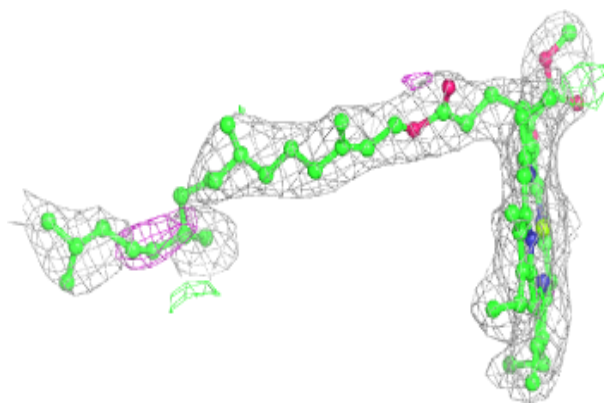
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



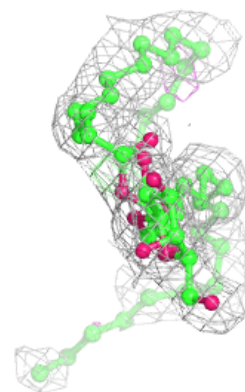
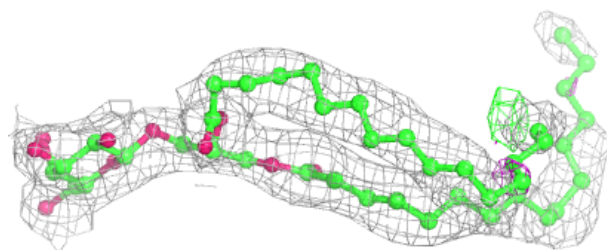
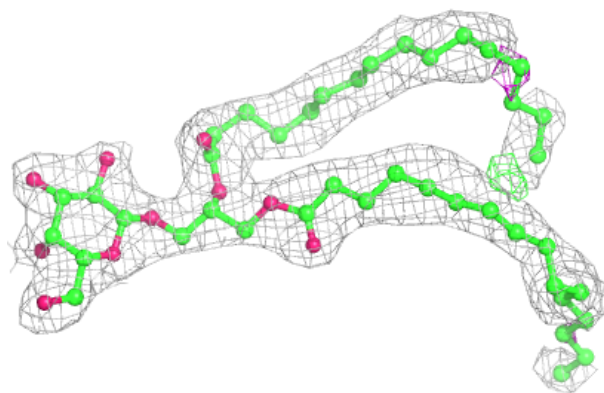


**Electron density around CLA B 606:**

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

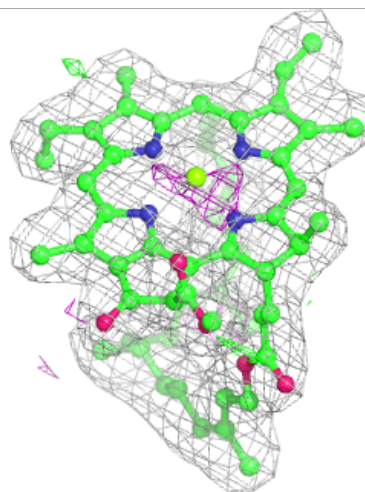
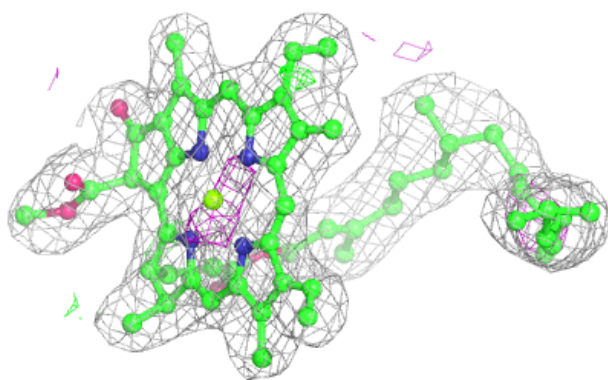
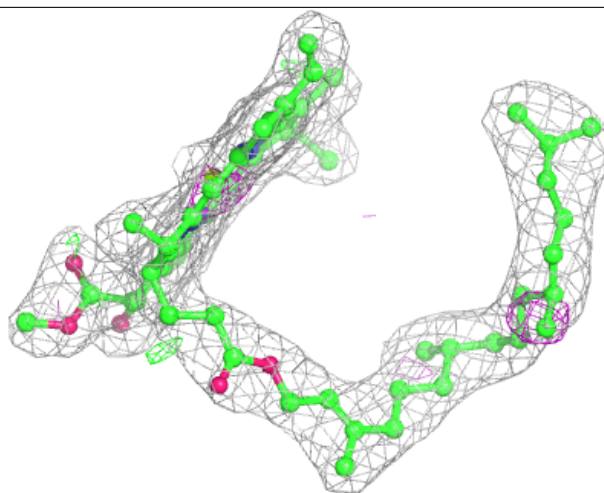
**Electron density around LMG D 415:**

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



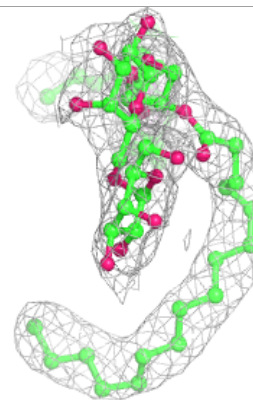
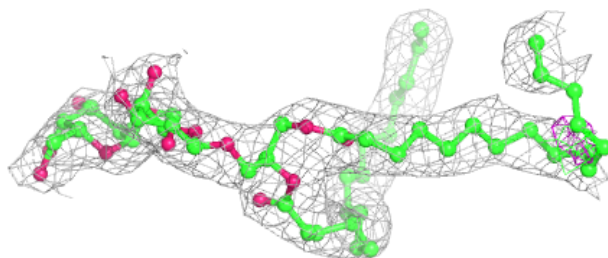
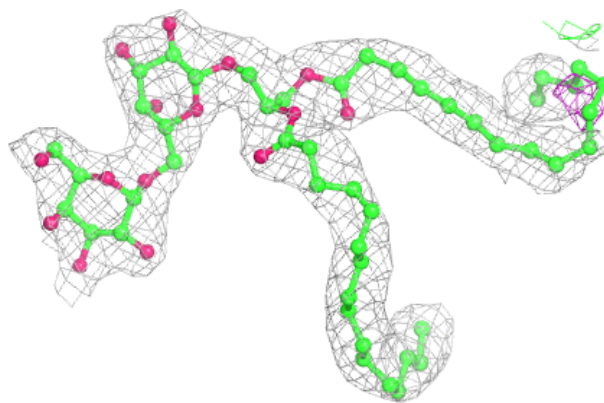
**Electron density around CLA B 611:**

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



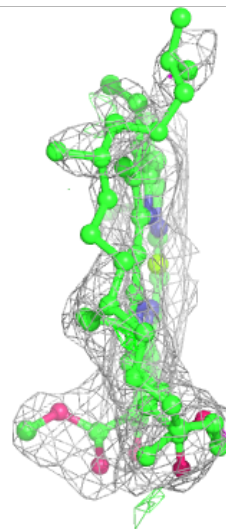
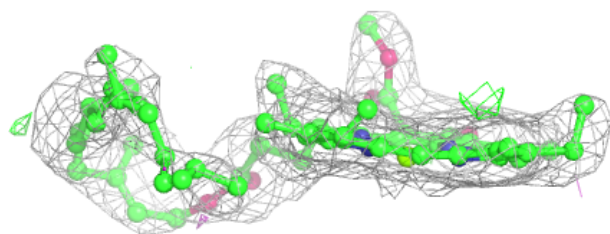
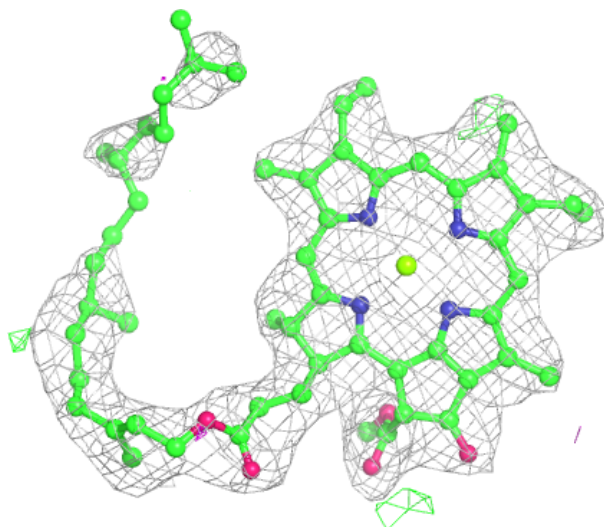
**Electron density around DGD c 518:**

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



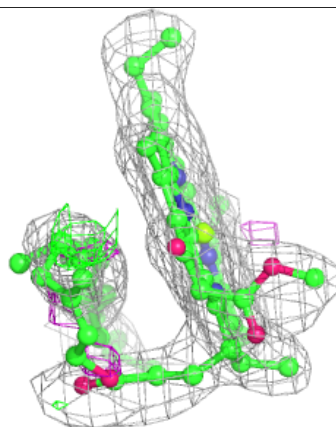
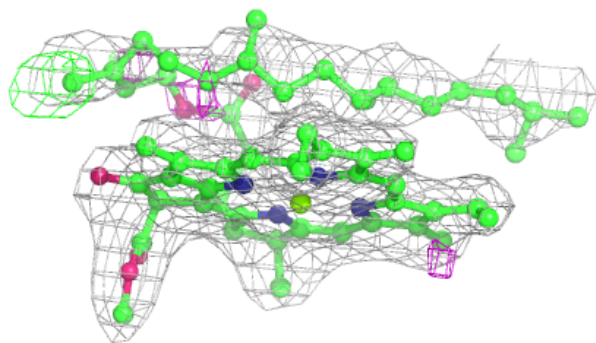
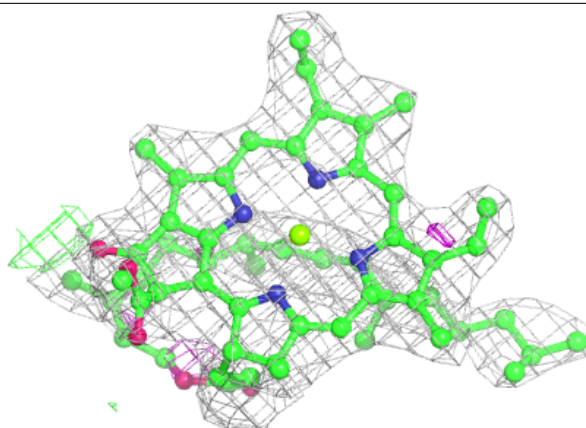
**Electron density around CLA c 513:**

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

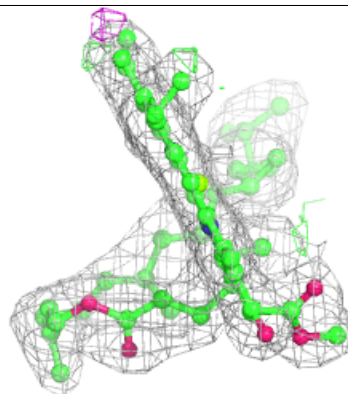
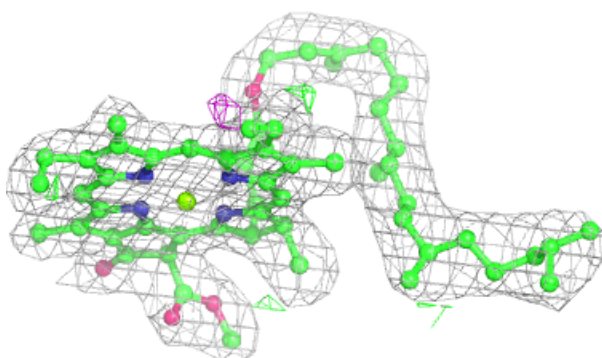
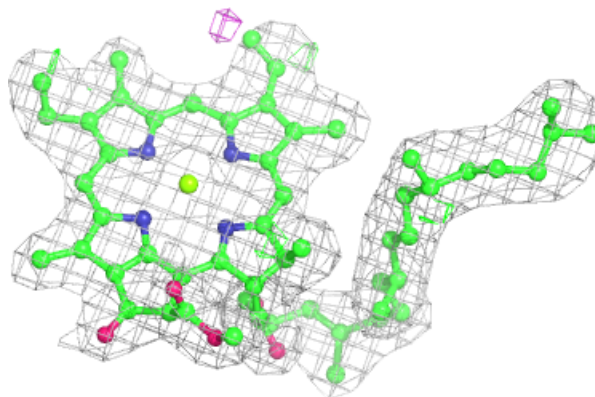


**Electron density around CLA B 601:**

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

**Electron density around CLA a 406:**

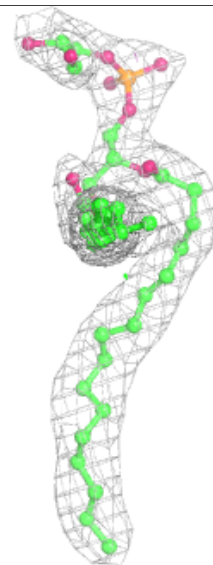
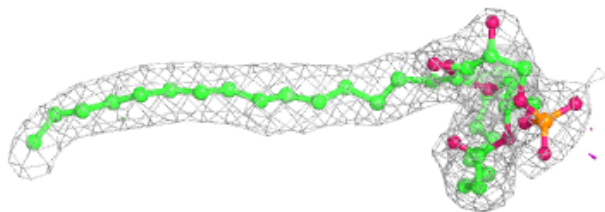
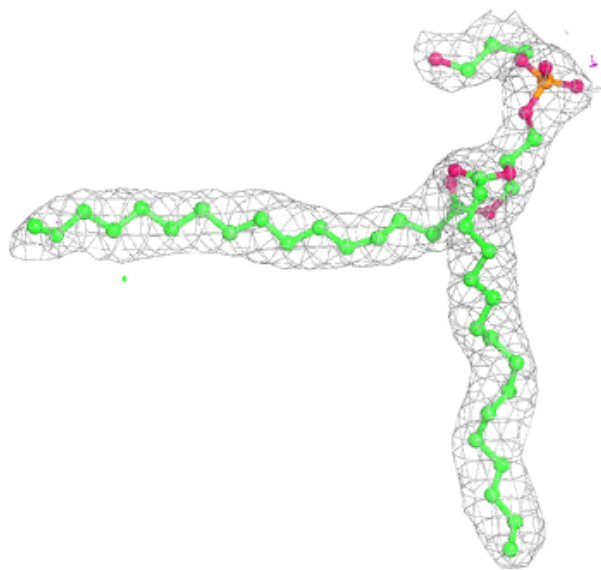
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





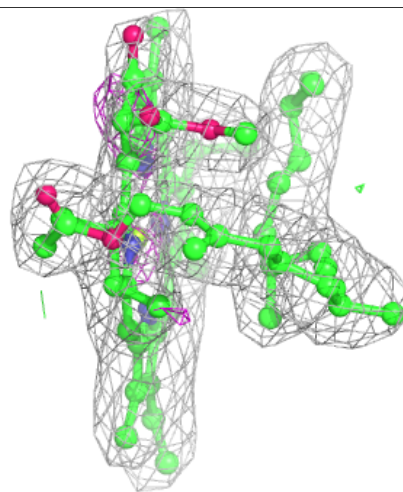
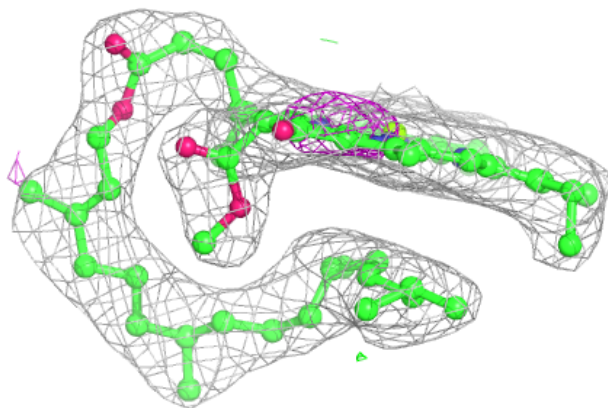
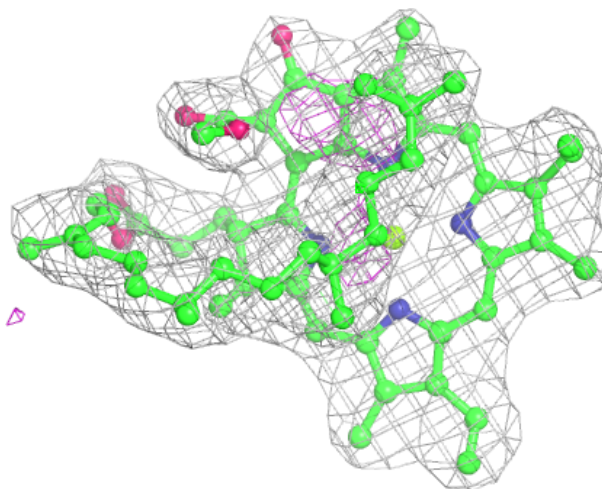
**Electron density around LHG L 101:**

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



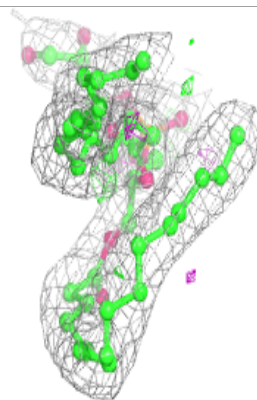
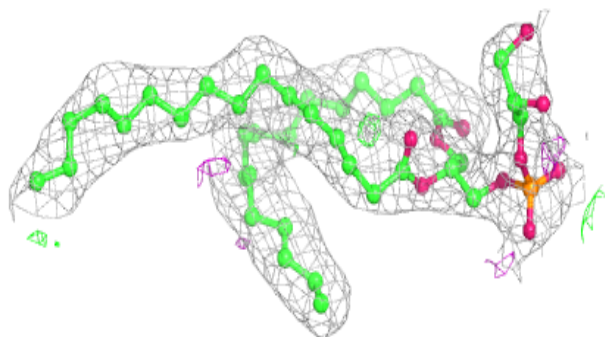
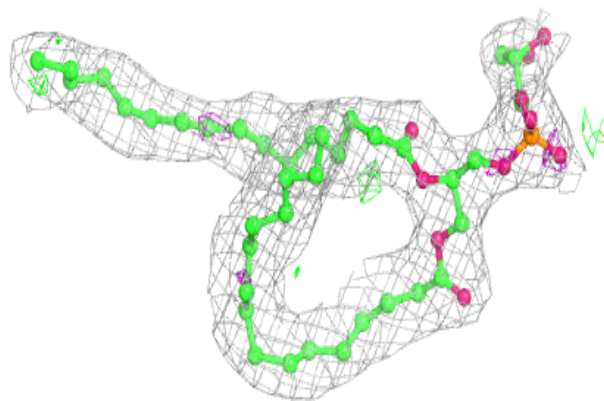
**Electron density around CLA c 511:**

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

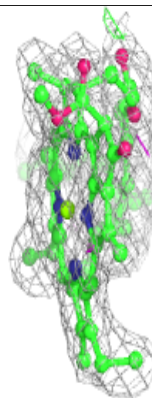
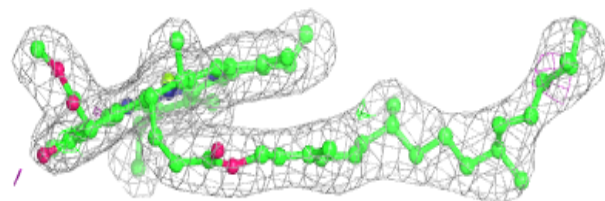
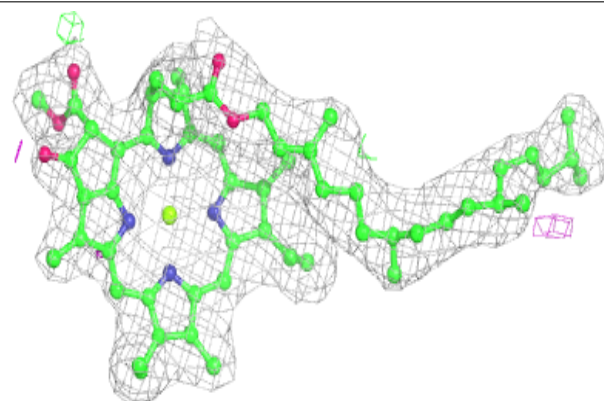


**Electron density around LHG D 409:**

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

**Electron density around CLA b 603:**

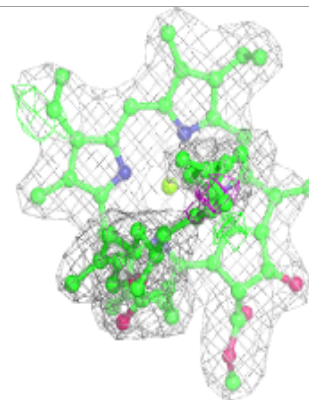
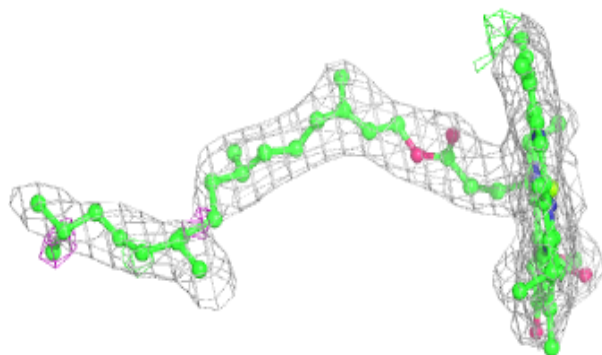
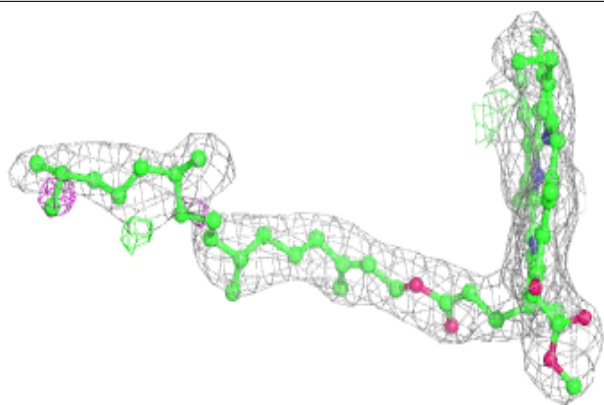
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





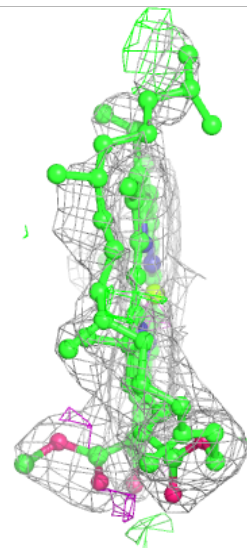
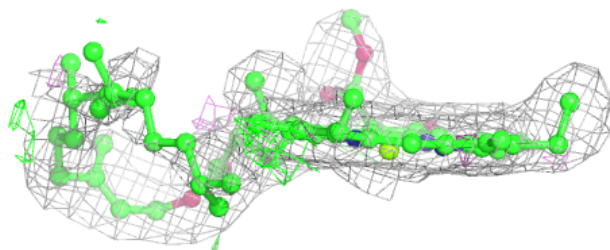
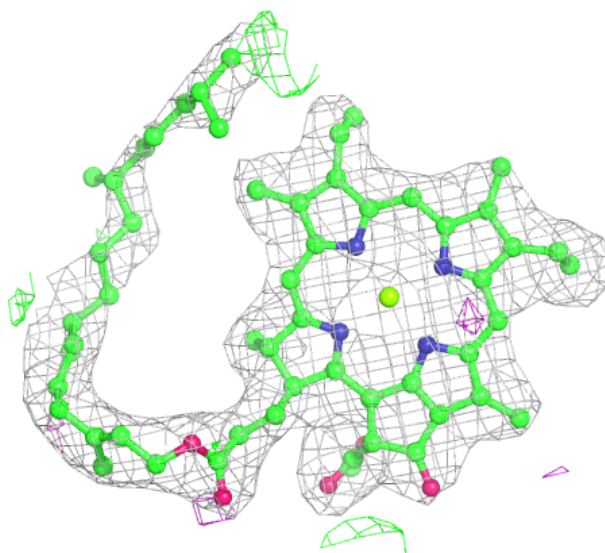
**Electron density around CLA b 606:**

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



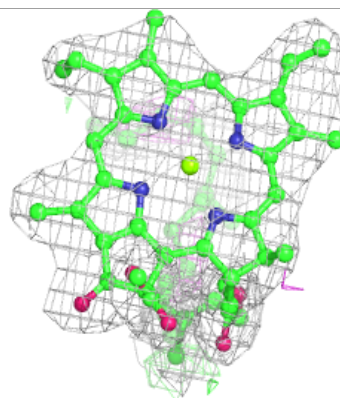
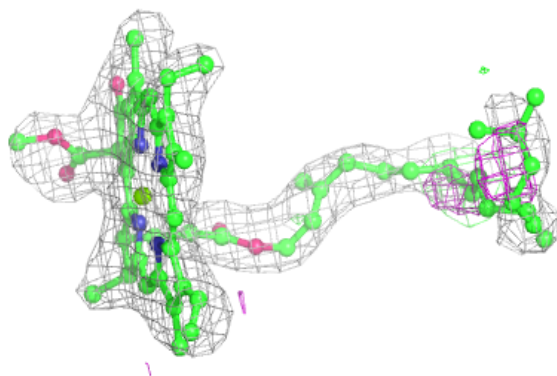
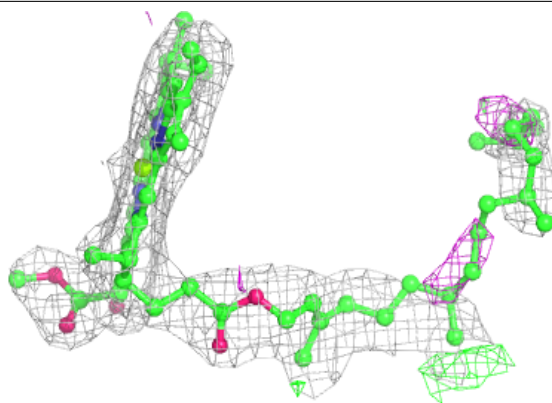
**Electron density around CLA C 513:**

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

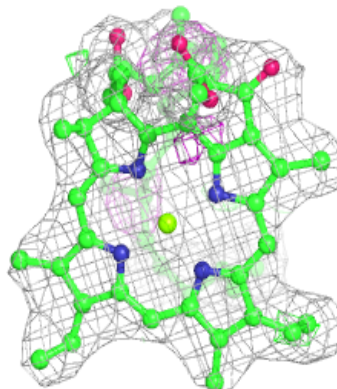
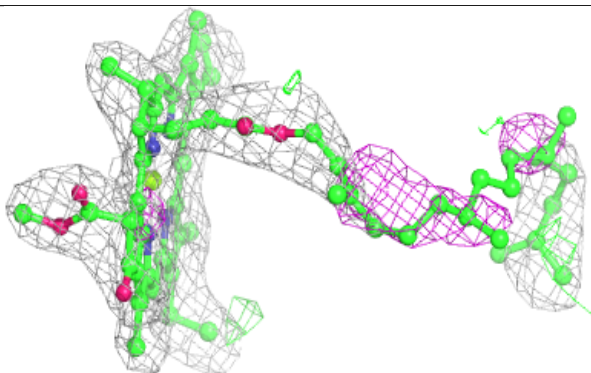
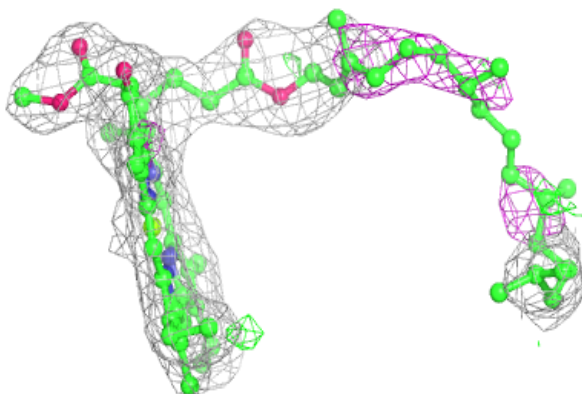


**Electron density around CLA c 507:**

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

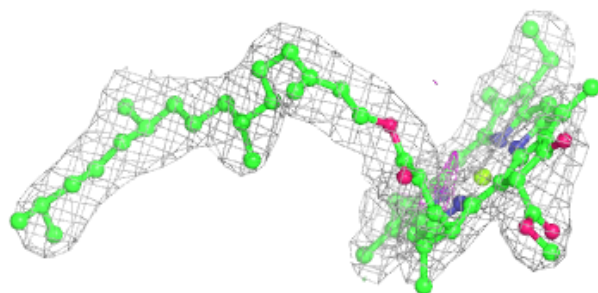
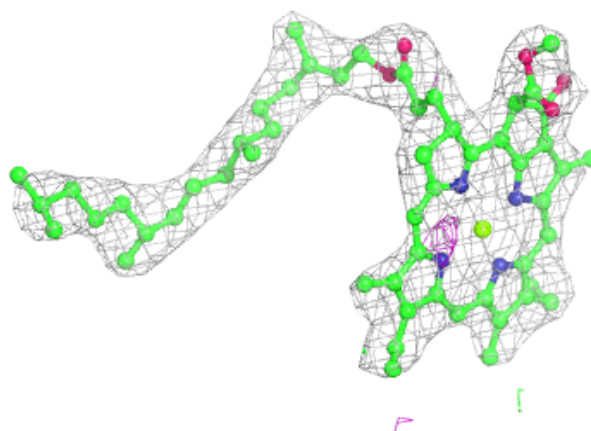
**Electron density around CLA C 507:**

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

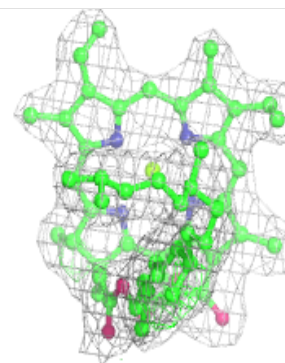
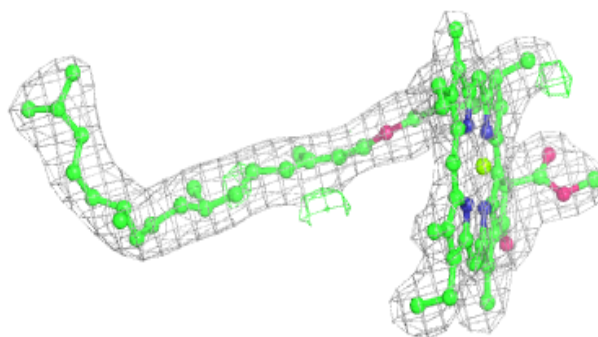
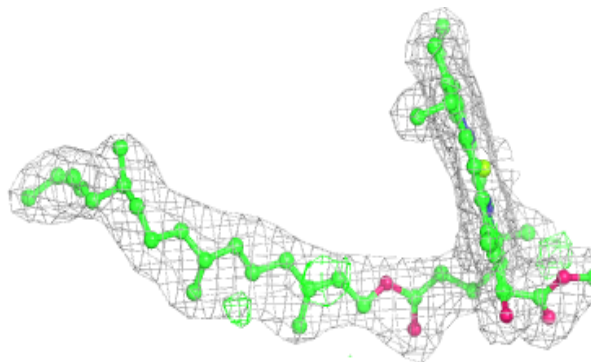


**Electron density around CLA c 512:**

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

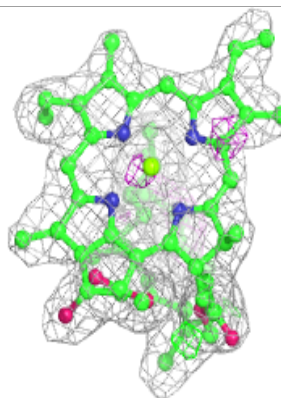
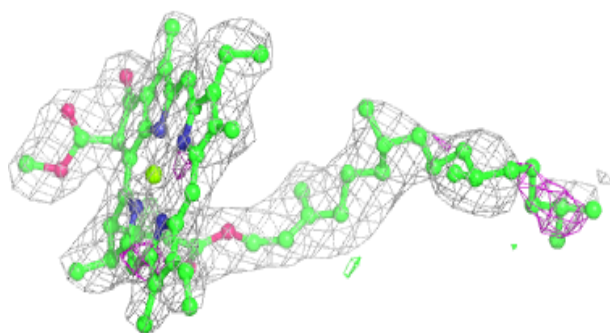
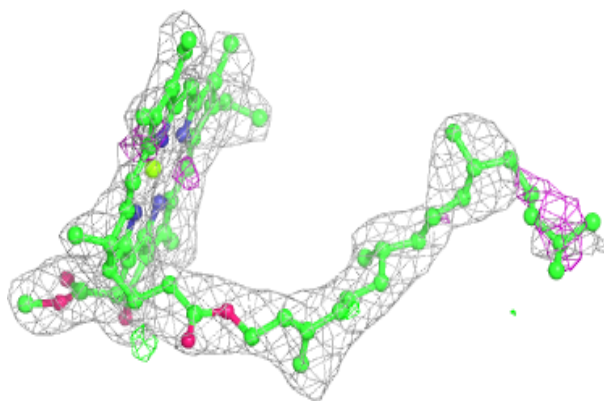
**Electron density around CLA B 605:**

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

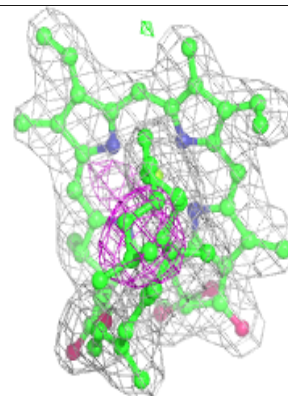
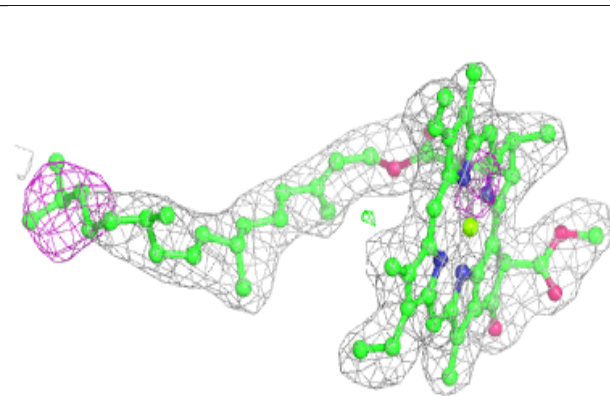
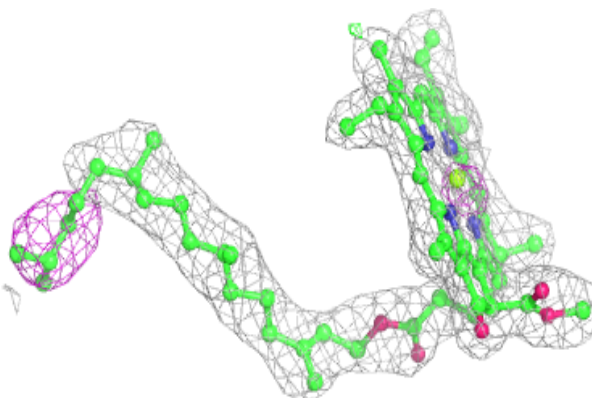


**Electron density around CLA c 509:**

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

**Electron density around CLA C 509:**

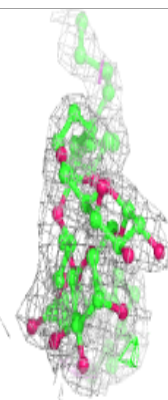
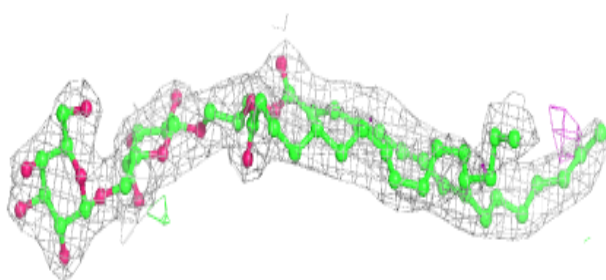
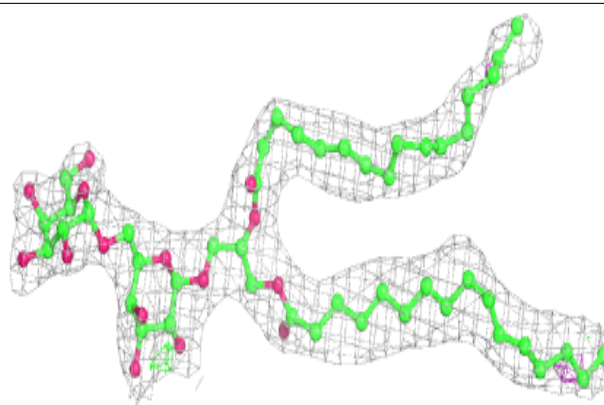
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



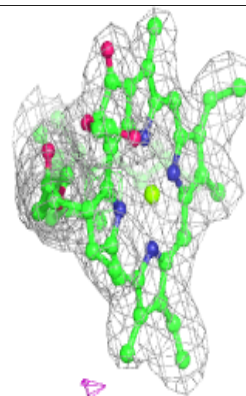
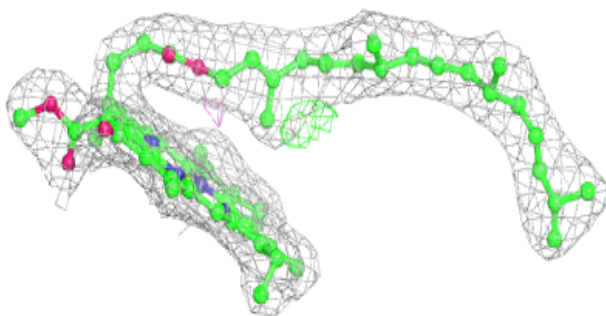
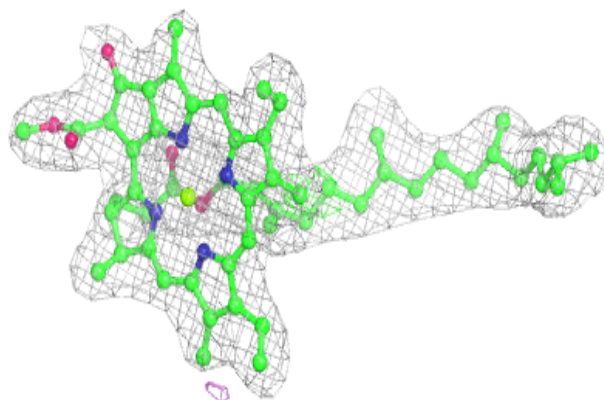


**Electron density around DGD C 519:**

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

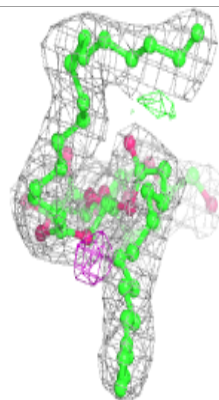
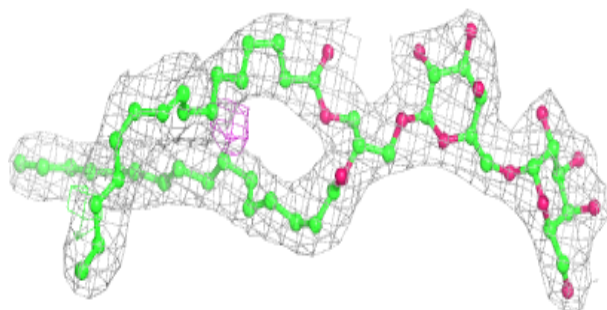
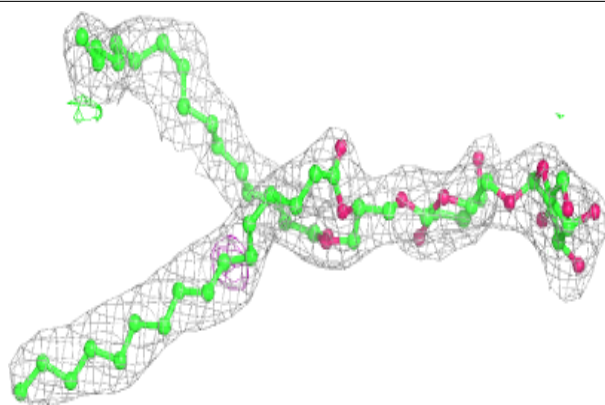
**Electron density around CLA B 608:**

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



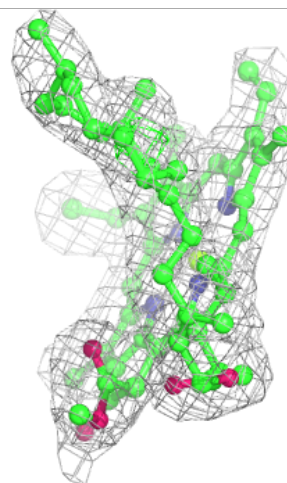
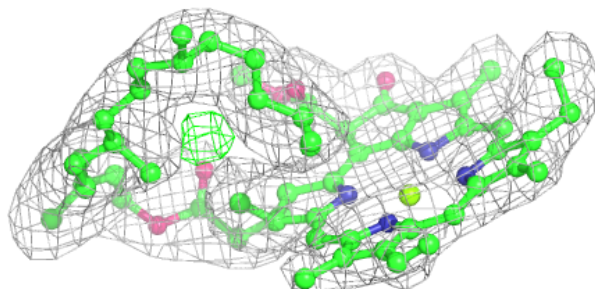
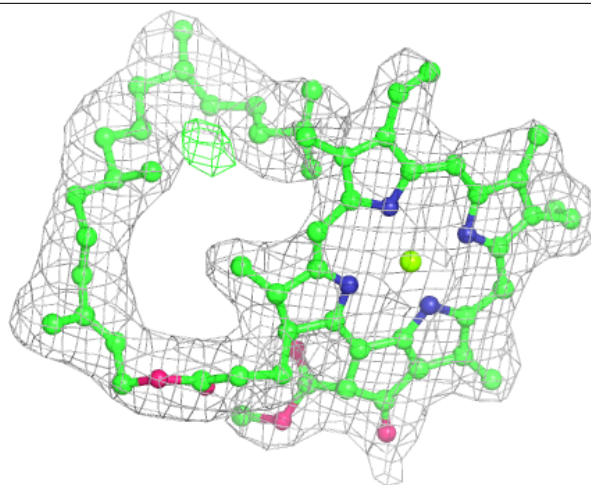
**Electron density around DGD C 517:**

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



**Electron density around CLA b 615:**

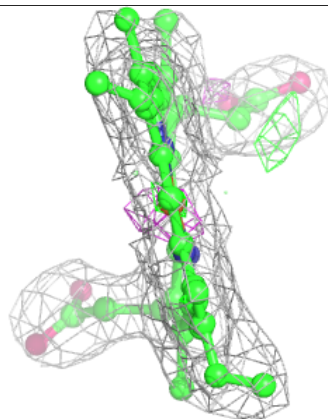
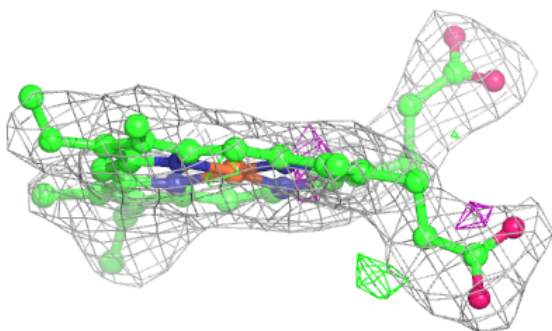
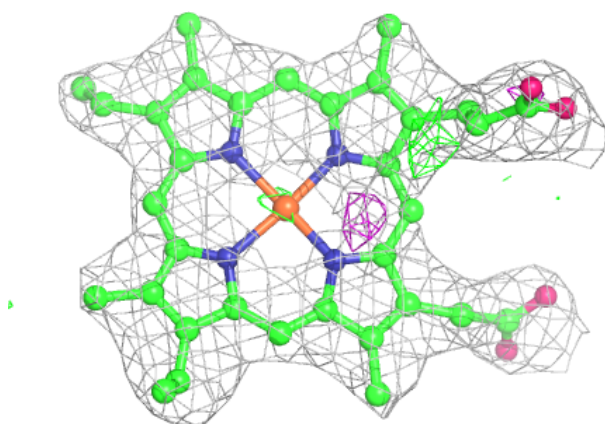
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





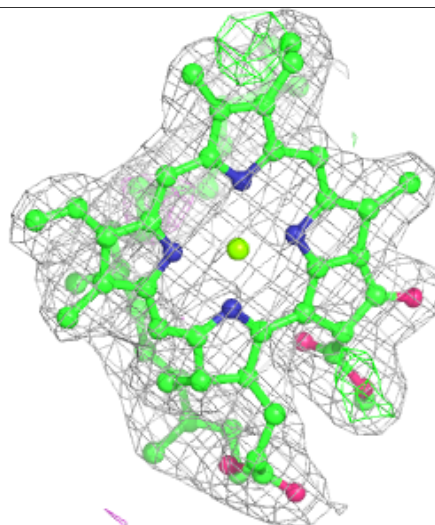
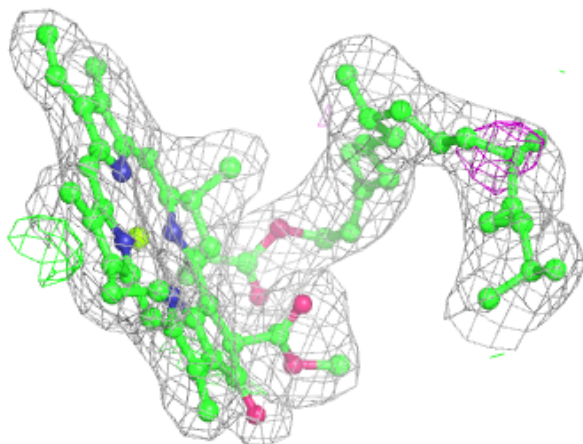
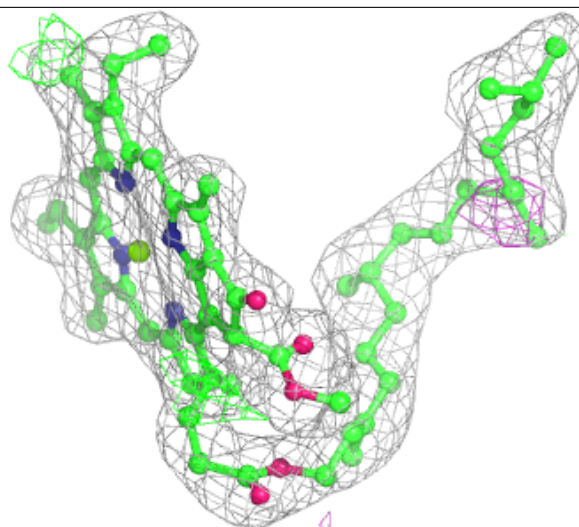
**Electron density around HEM E 103:**

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



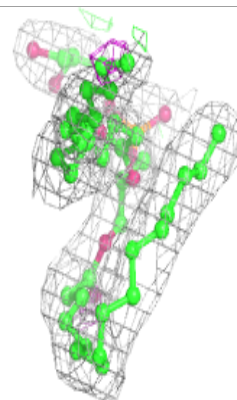
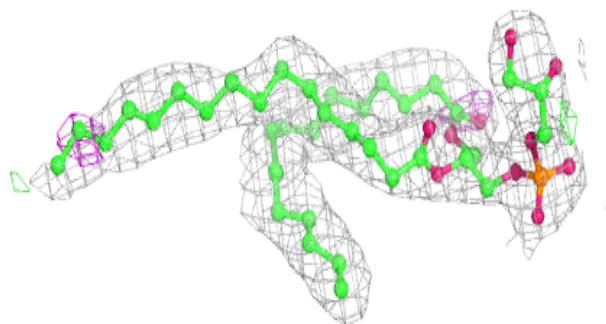
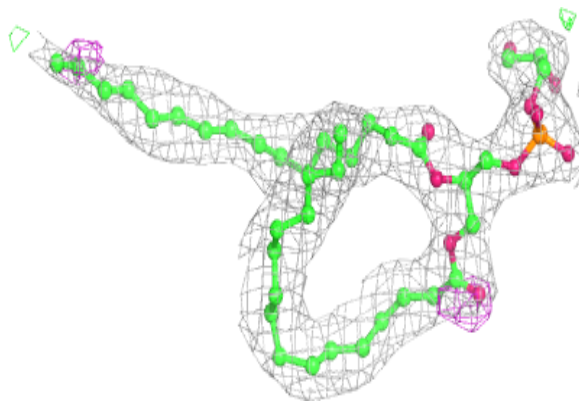
**Electron density around CLA B 613:**

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



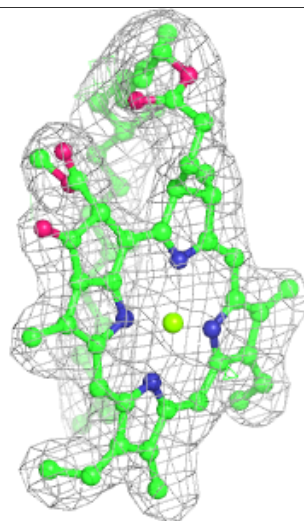
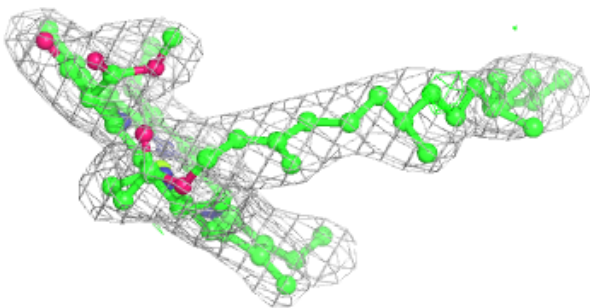
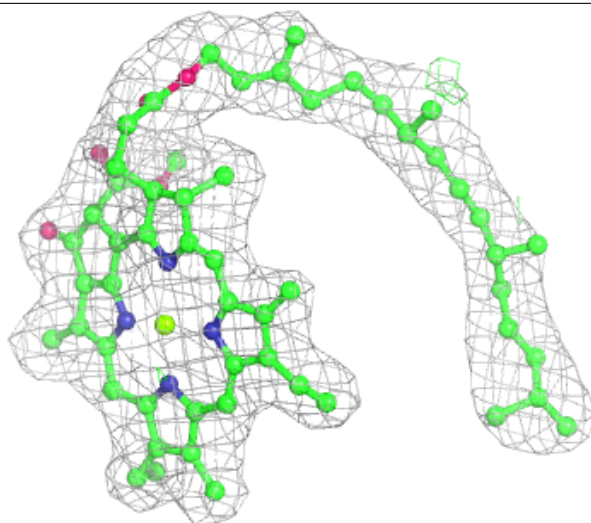
**Electron density around LHG d 406:**

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



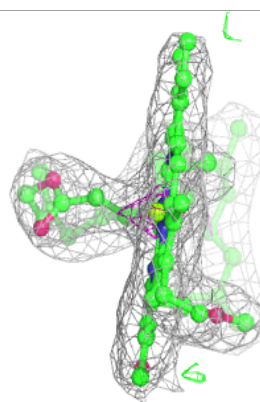
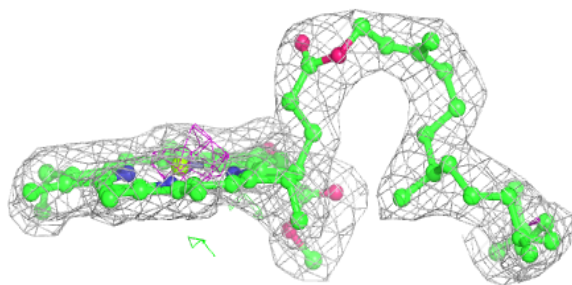
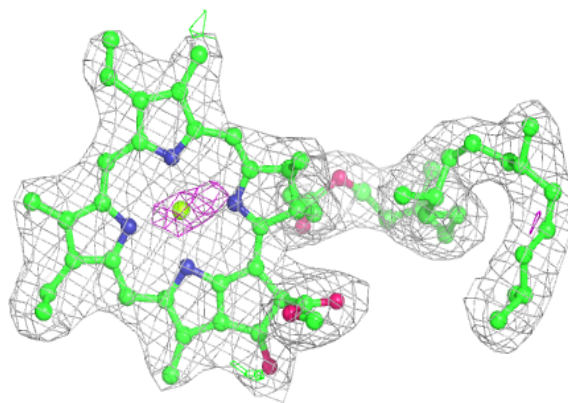
**Electron density around CLA C 508:**

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

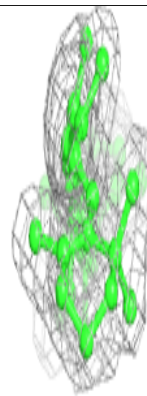
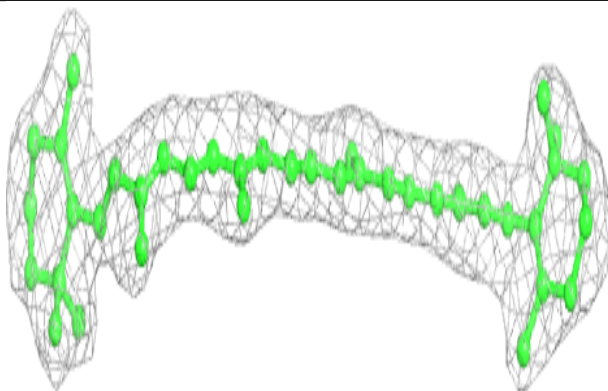
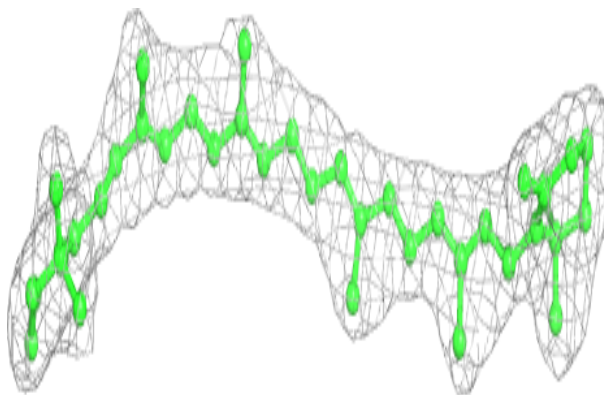


**Electron density around CLA B 612:**

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

**Electron density around BCR H 101:**

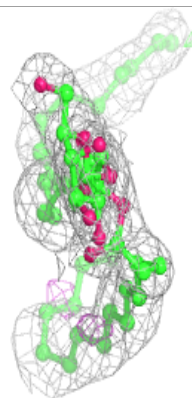
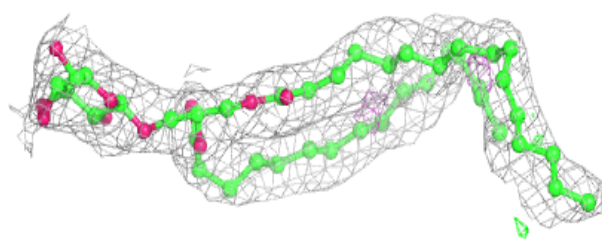
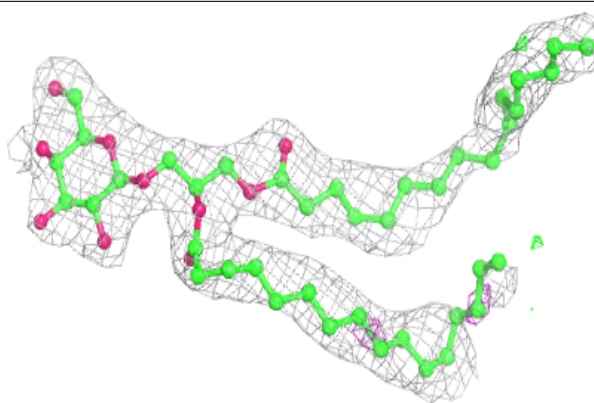
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



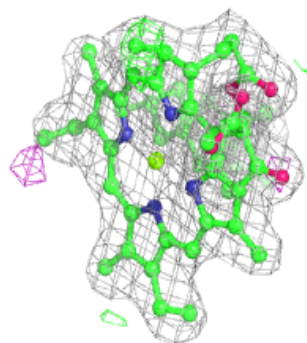
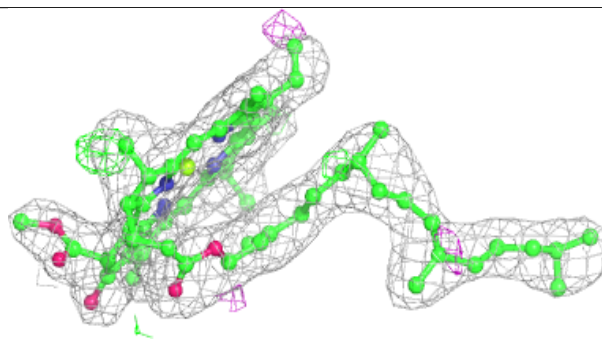
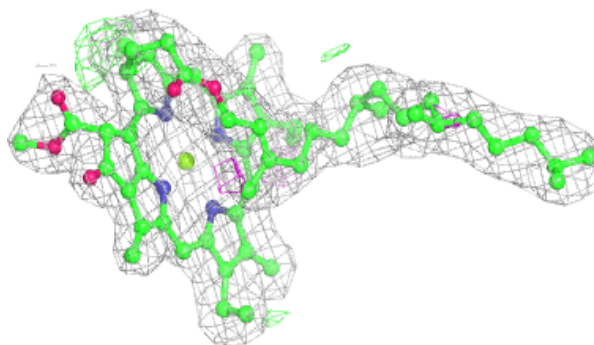


**Electron density around LMG d 412:**

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

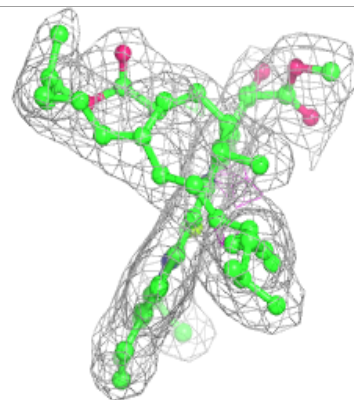
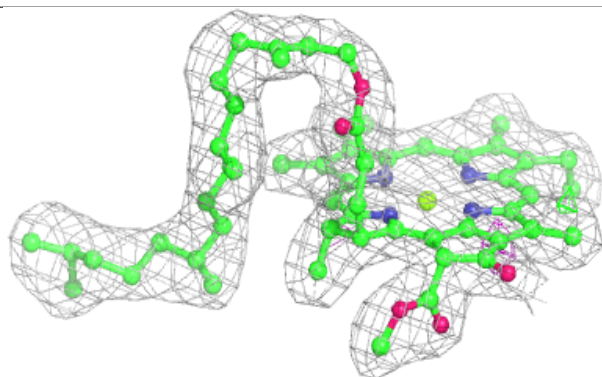
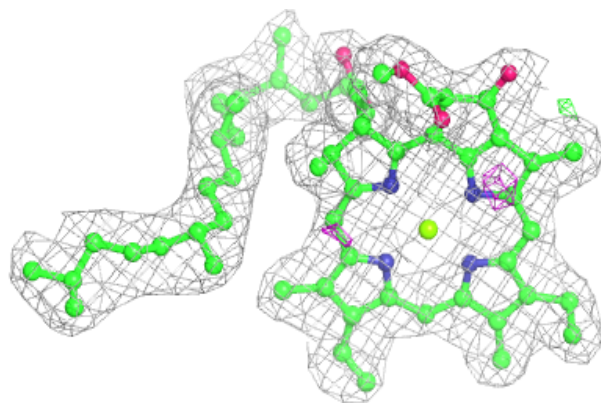
**Electron density around CLA C 506:**

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

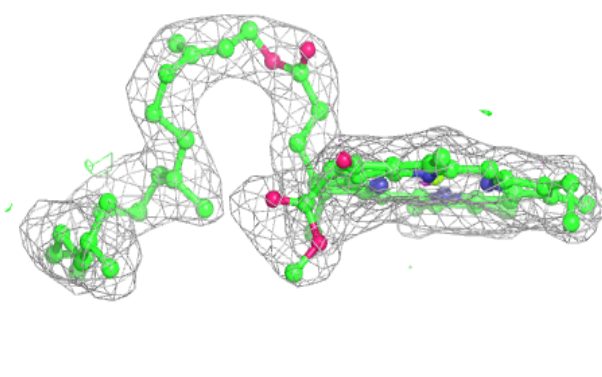
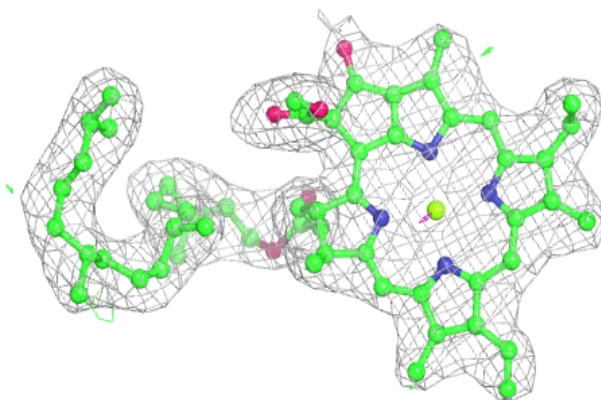


**Electron density around CLA A 405:**

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

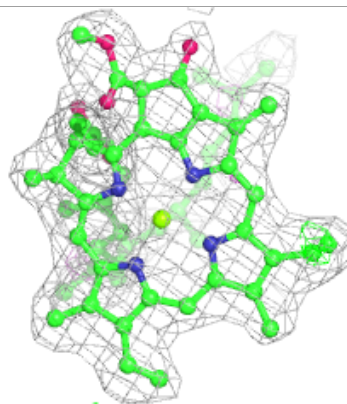
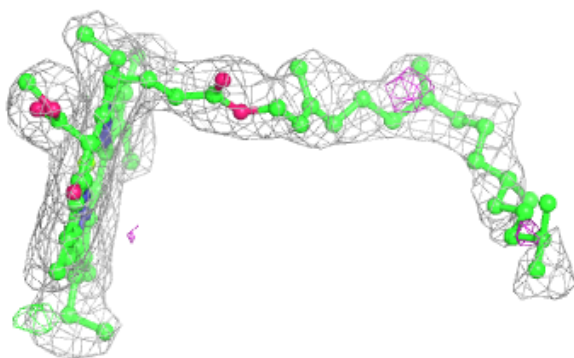
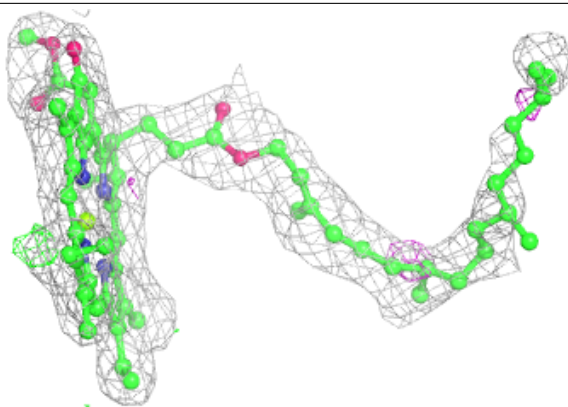
**Electron density around CLA b 612:**

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



**Electron density around CLA D 406:**

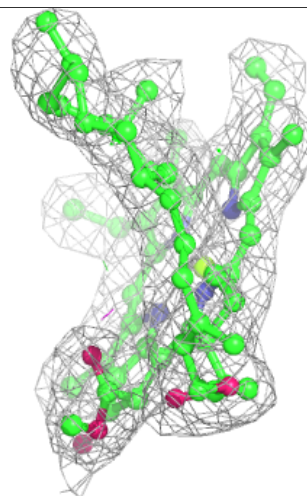
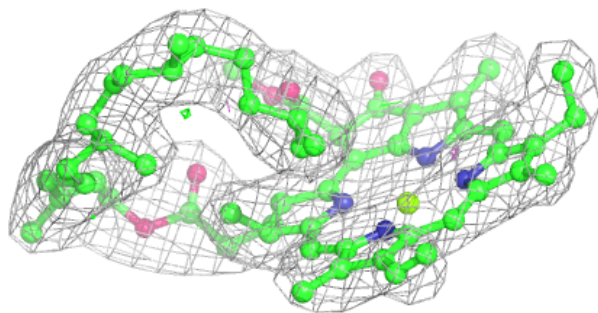
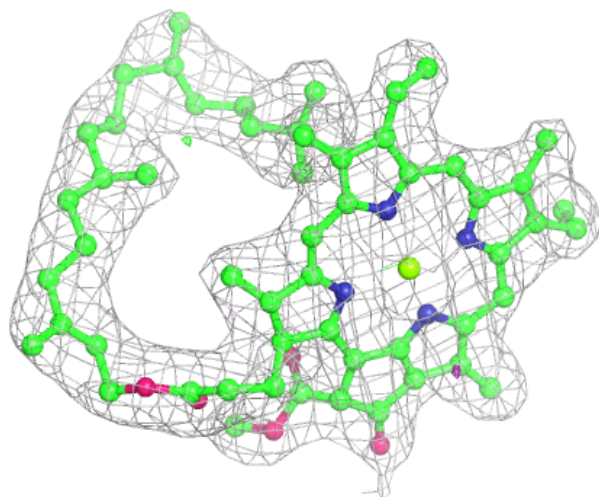
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





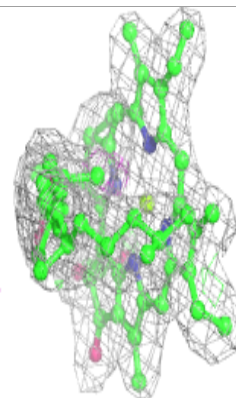
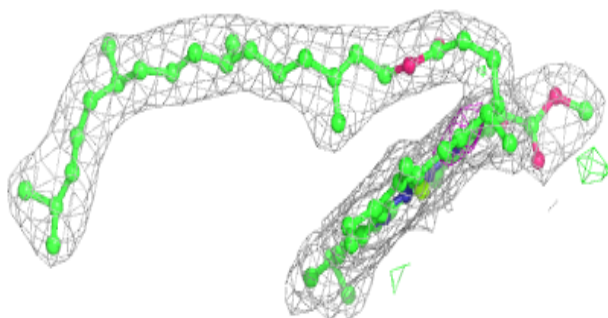
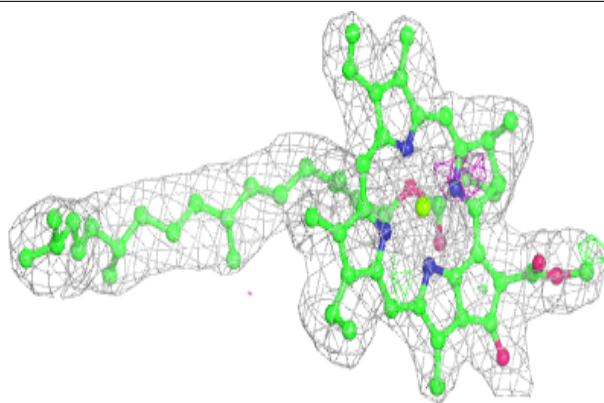
**Electron density around CLA B 615:**

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



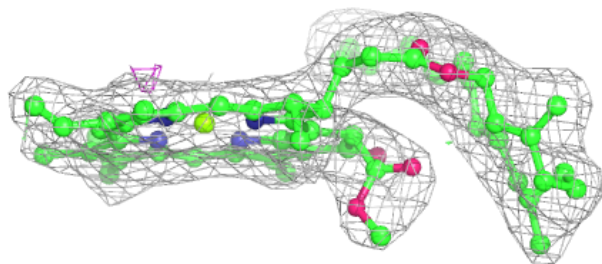
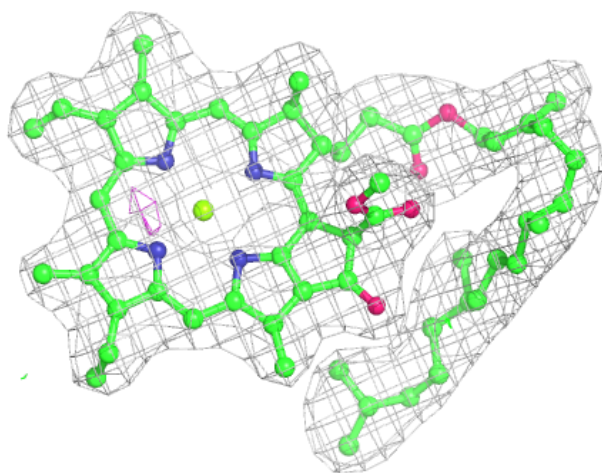
**Electron density around CLA b 608:**

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



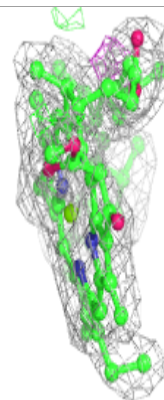
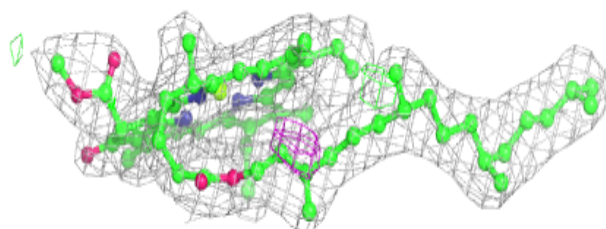
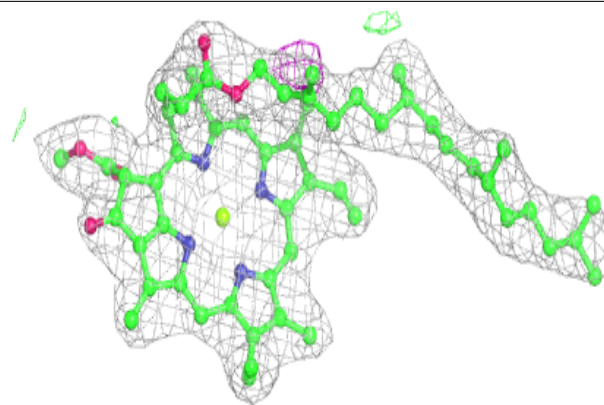
**Electron density around CLA b 610:**

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



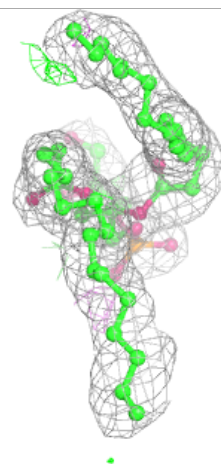
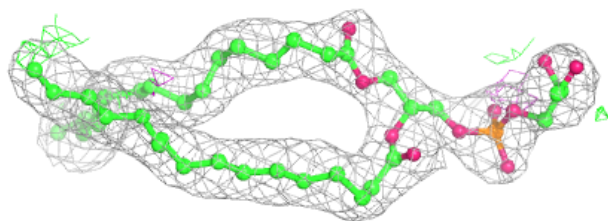
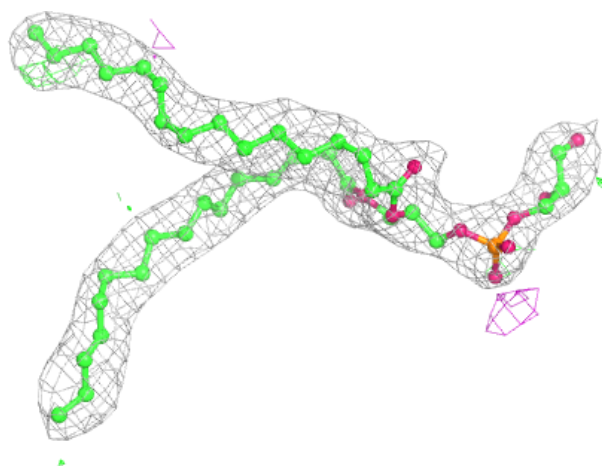
**Electron density around CLA C 502:**

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



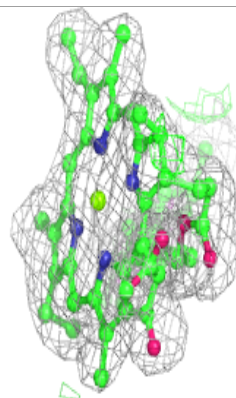
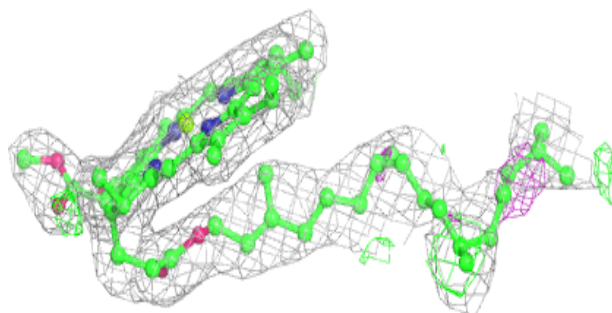
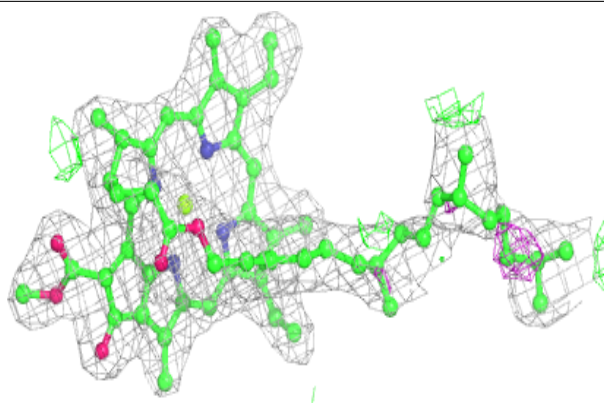
**Electron density around LHG d 407:**

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

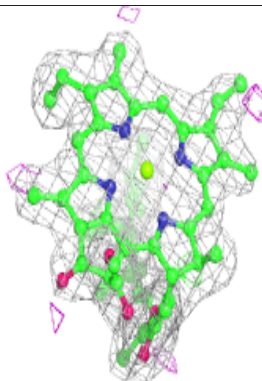
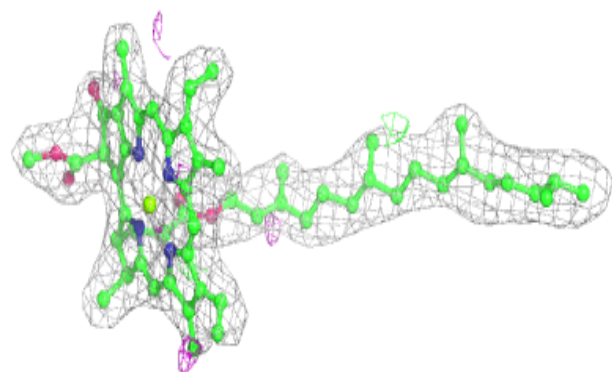
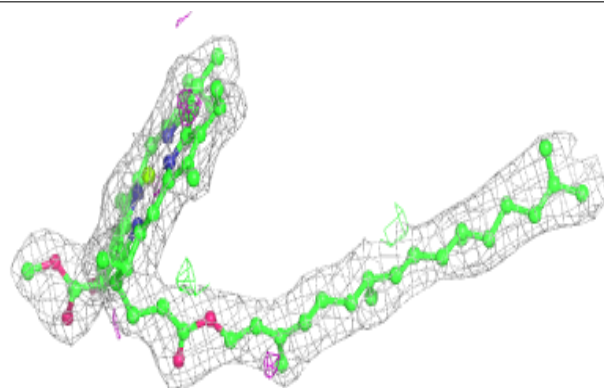


**Electron density around CLA b 614:**

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

**Electron density around CLA b 607:**

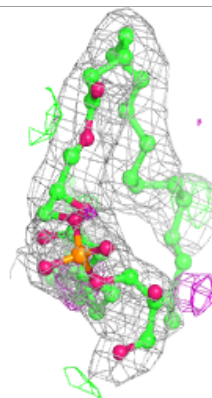
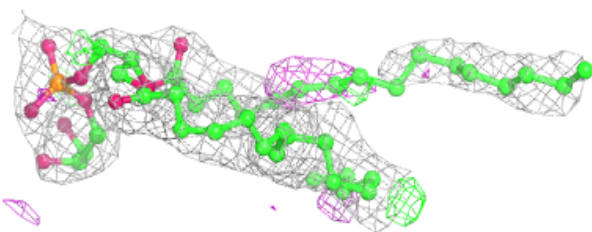
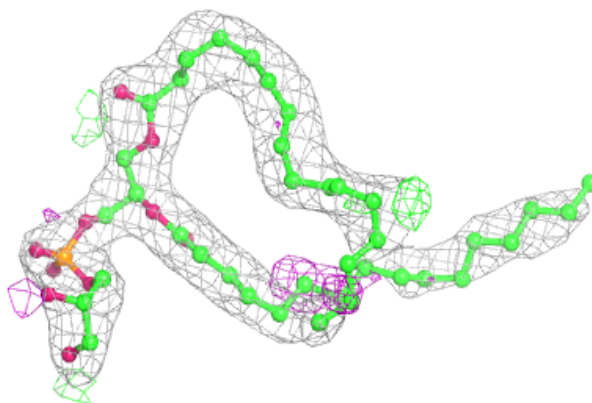
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





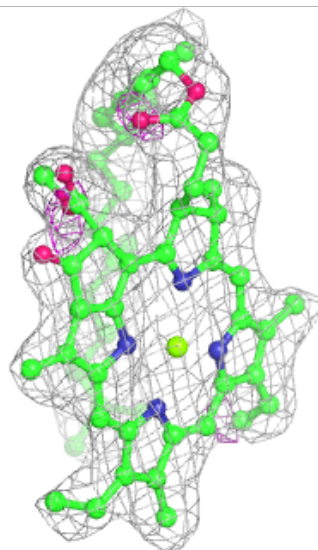
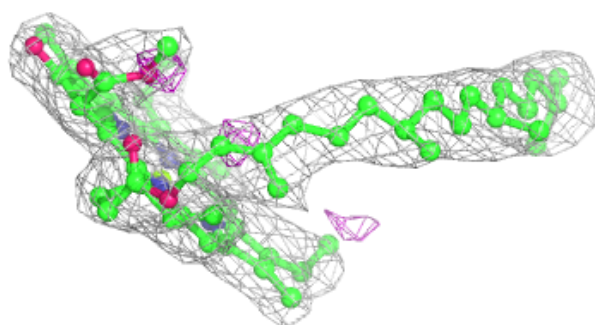
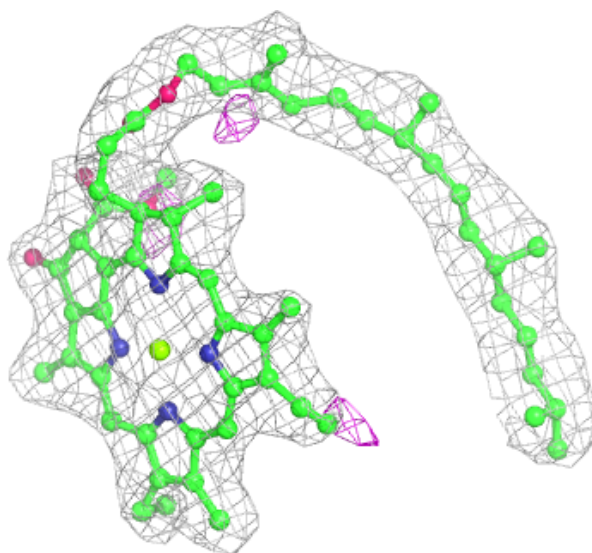
**Electron density around LHG D 411:**

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



**Electron density around CLA c 508:**

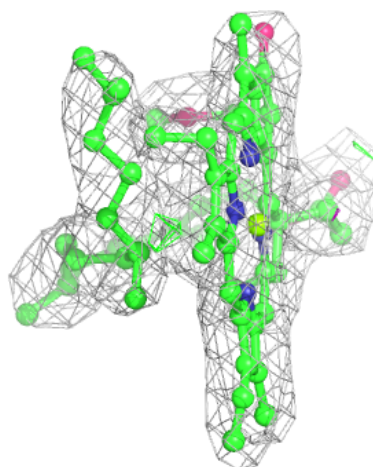
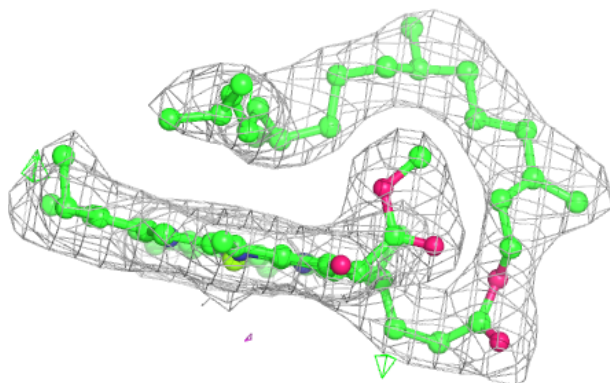
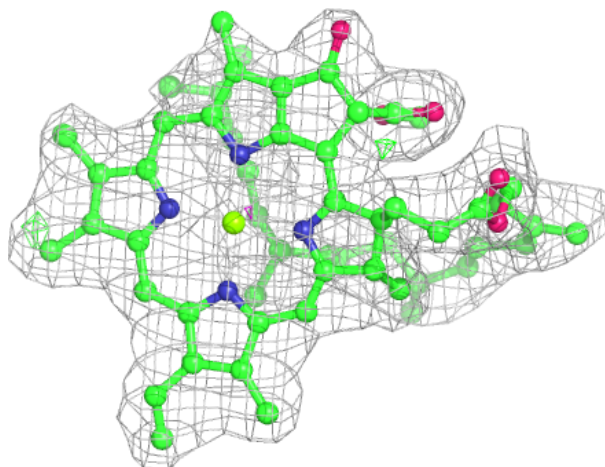
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





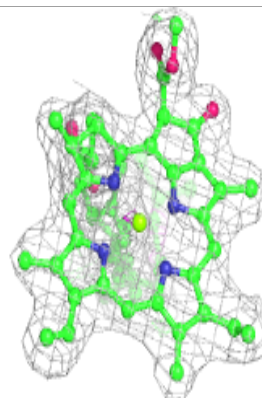
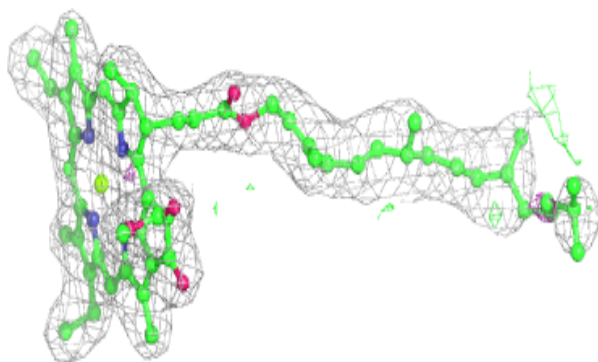
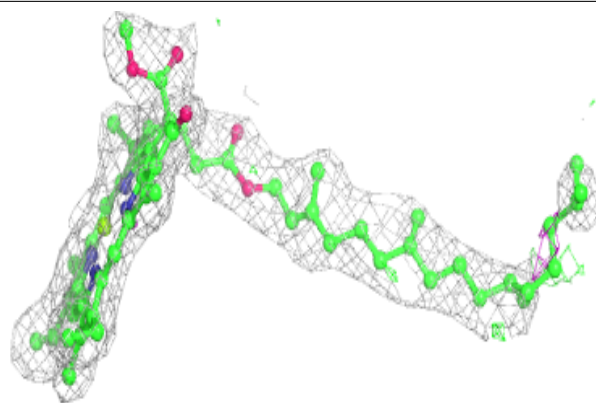
**Electron density around CLA C 511:**

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

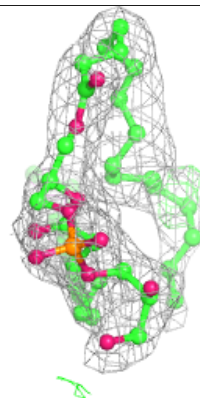
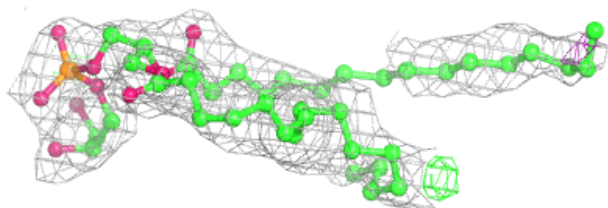


**Electron density around CLA B 604:**

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

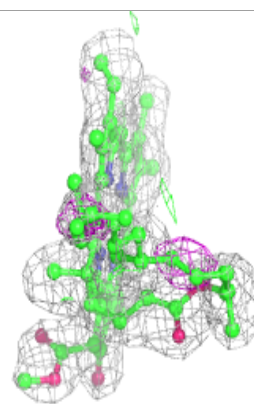
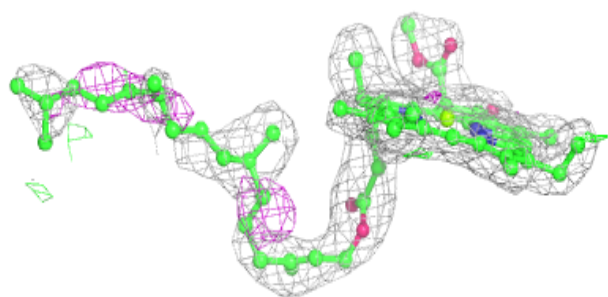
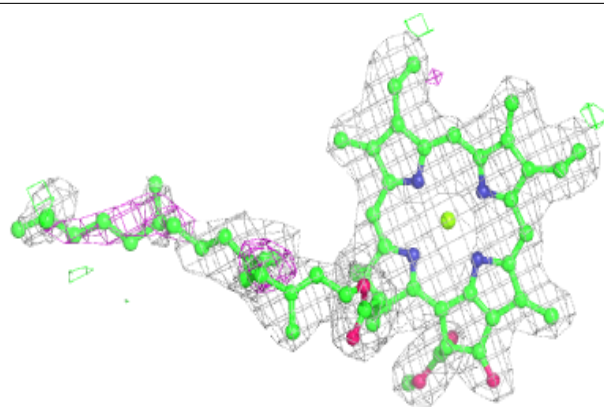
**Electron density around LHG d 408:**

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

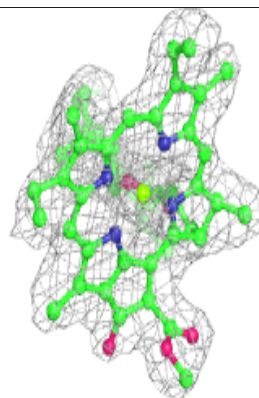
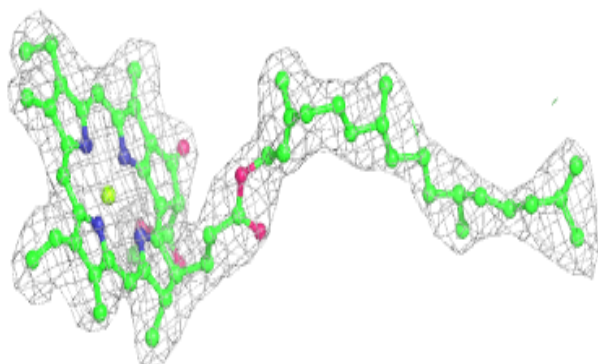
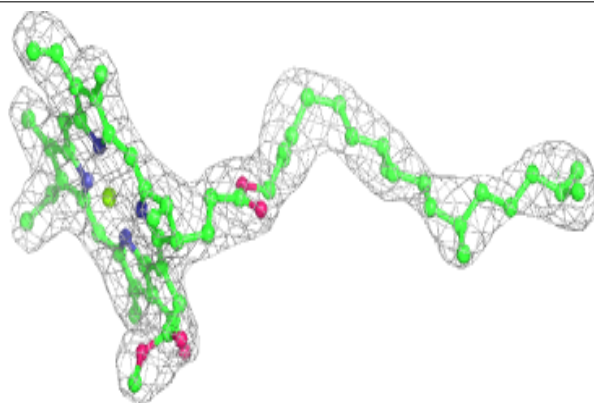


**Electron density around CLA a 407:**

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

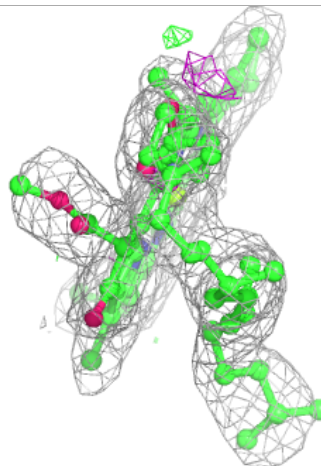
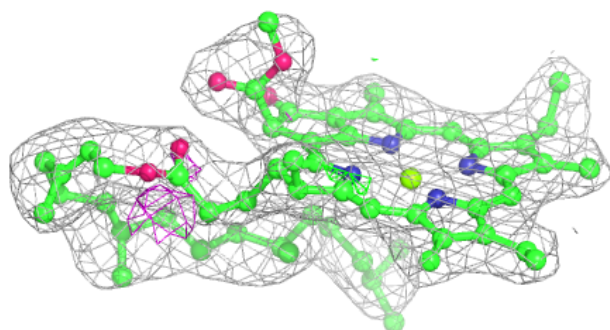
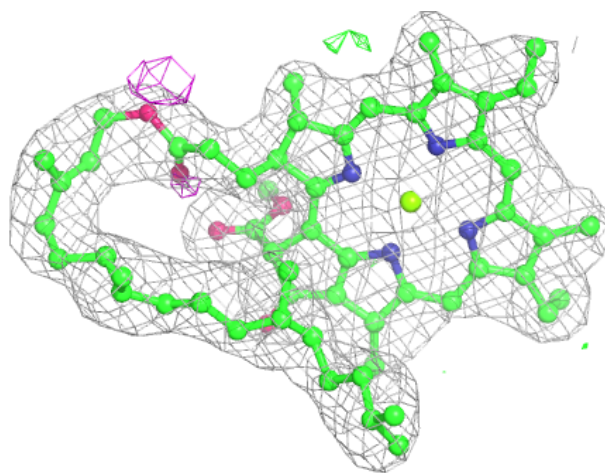
**Electron density around CLA c 503:**

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



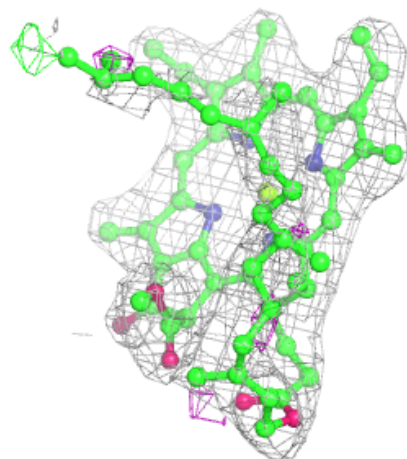
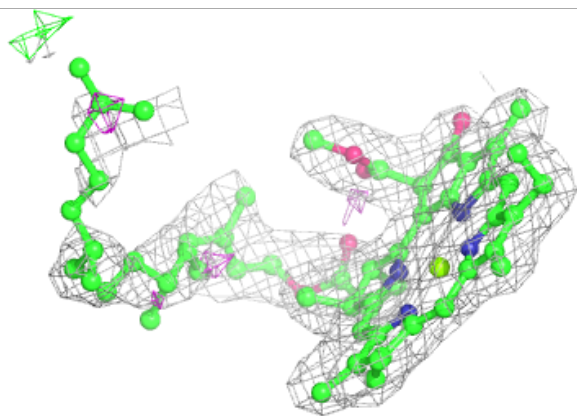
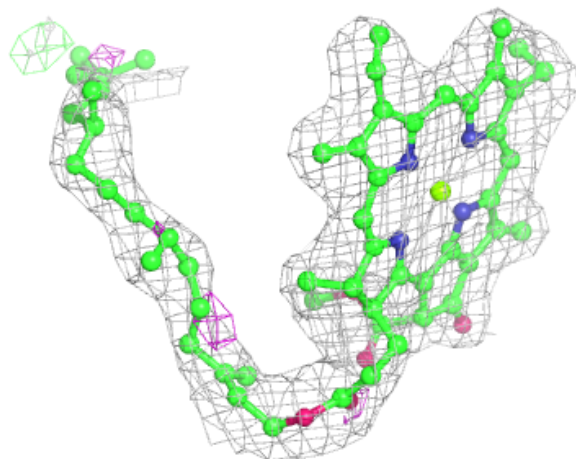
**Electron density around CLA c 510:**

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



**Electron density around CLA b 616:**

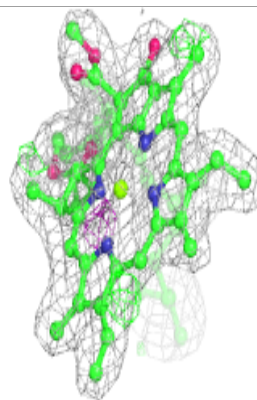
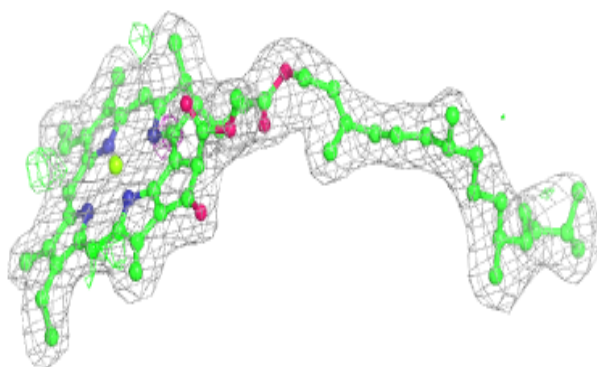
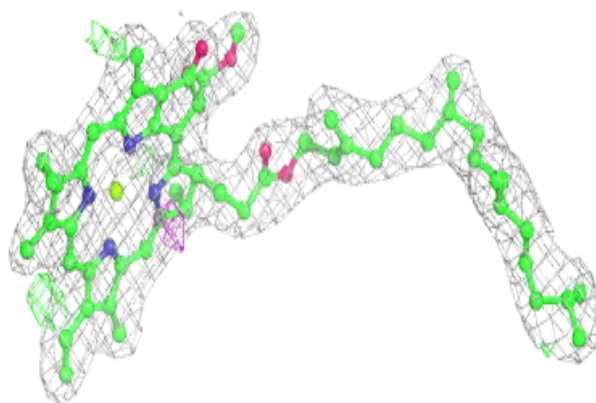
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



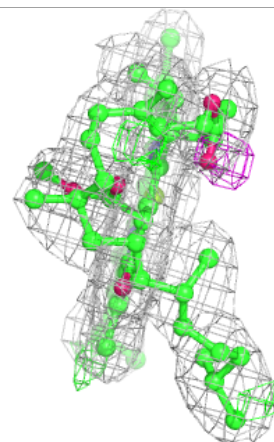
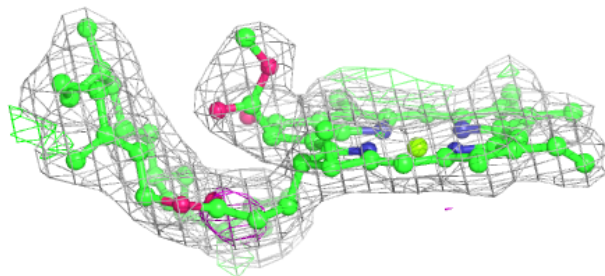
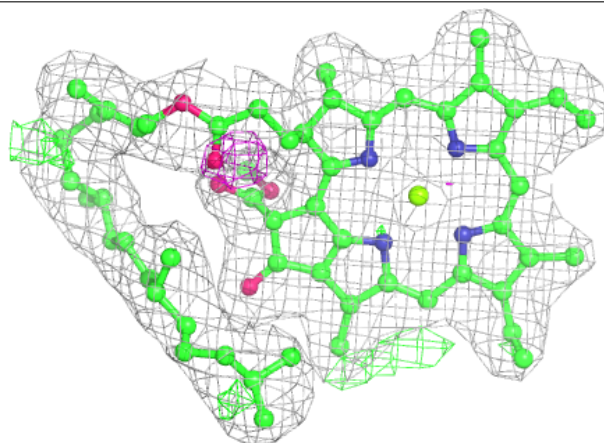


**Electron density around CLA A 404:**

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

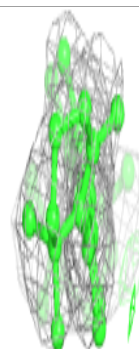
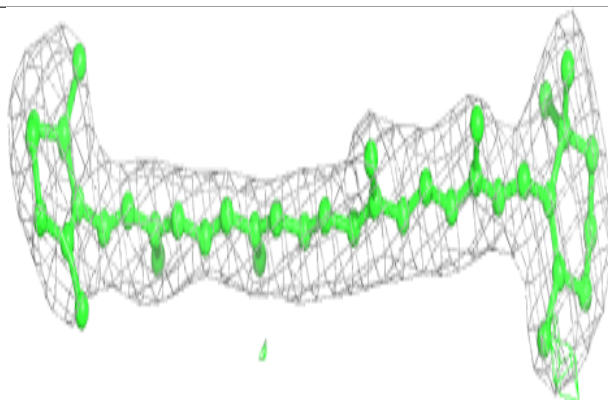
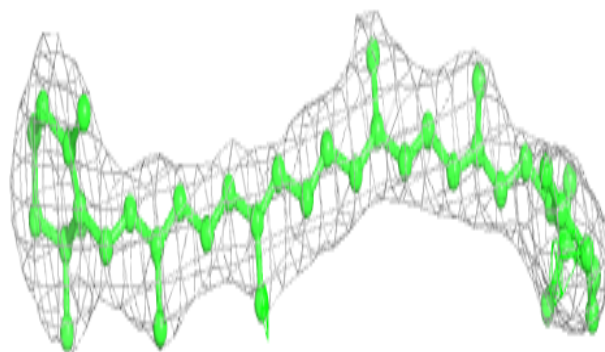
**Electron density around CLA B 610:**

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

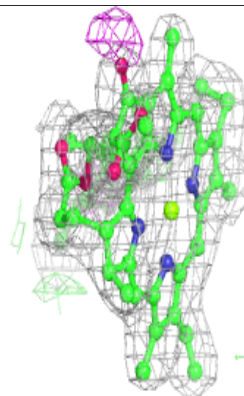
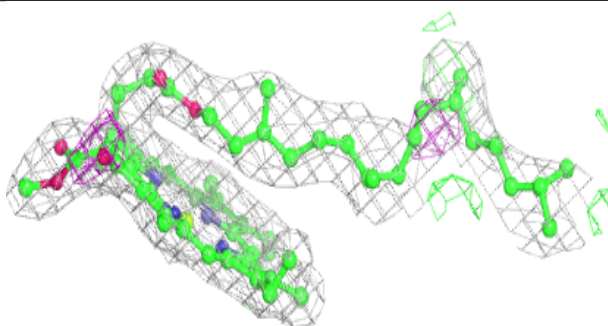
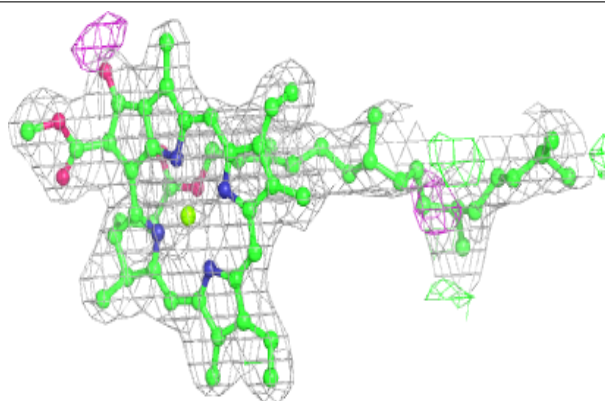


**Electron density around BCR c 515:**

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

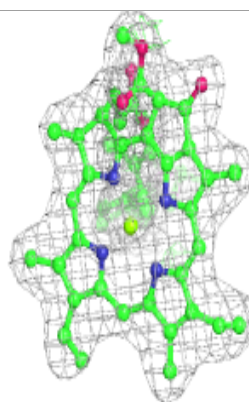
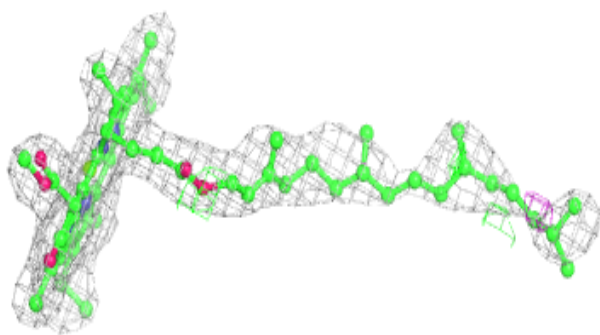
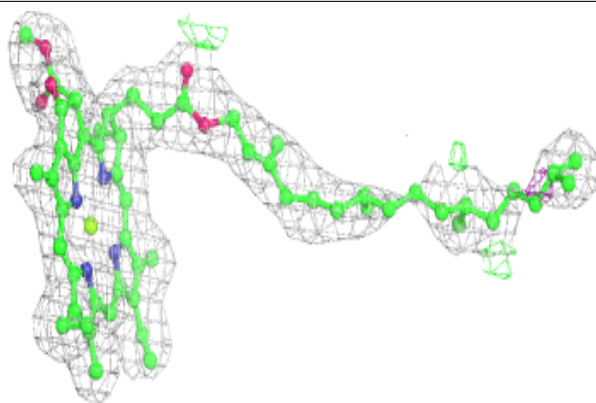
**Electron density around CLA B 614:**

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

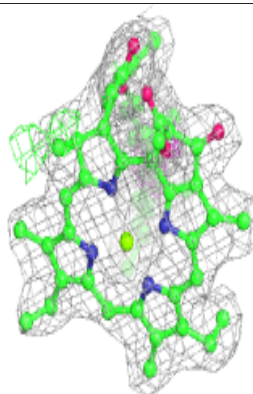
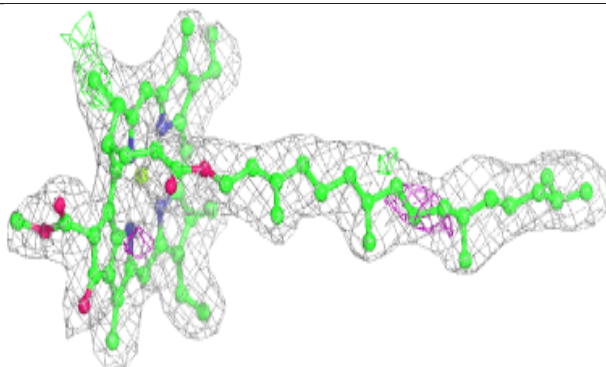
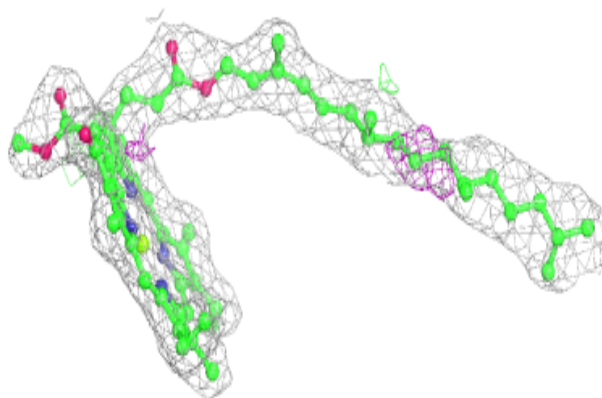


**Electron density around CLA d 403:**

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

**Electron density around CLA B 607:**

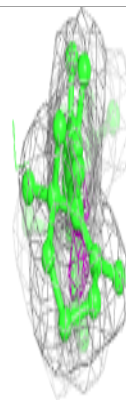
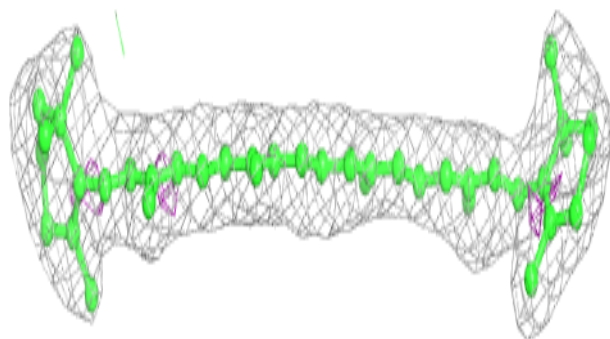
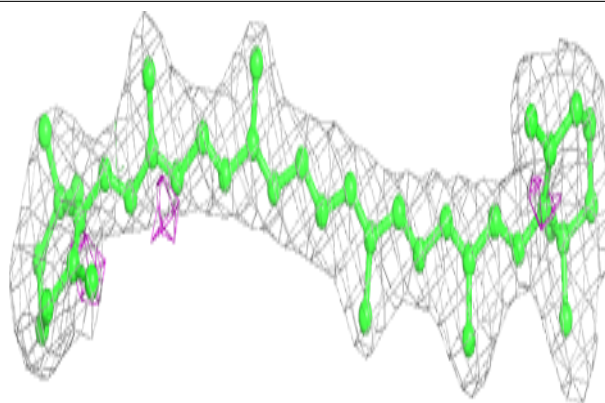
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



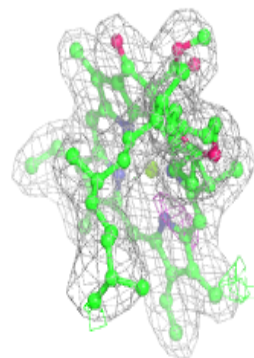
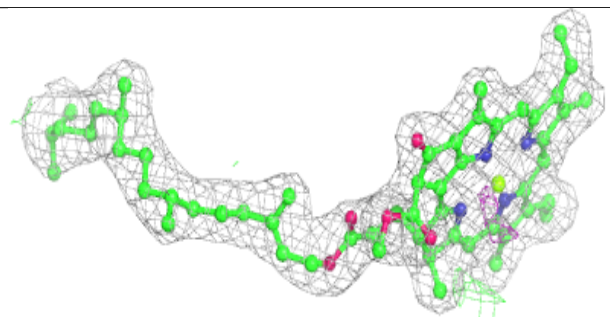
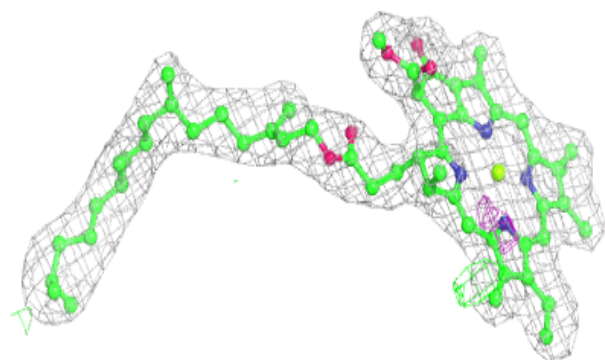


**Electron density around BCR B 618:**

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

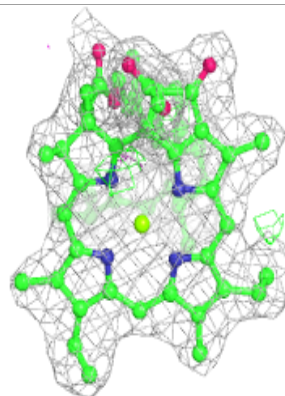
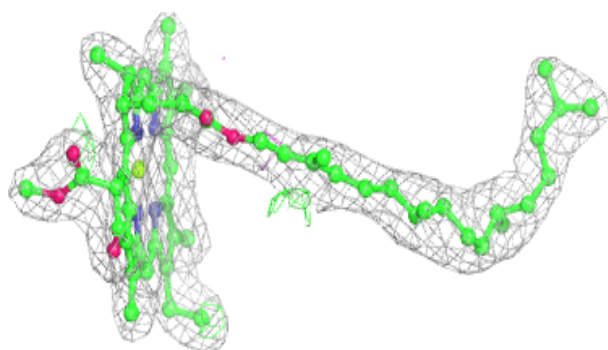
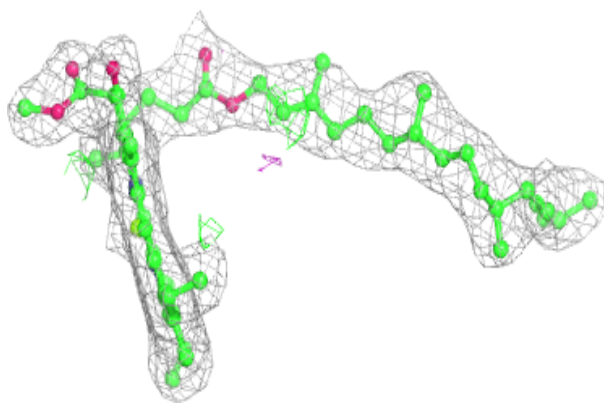
**Electron density around CLA a 405:**

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

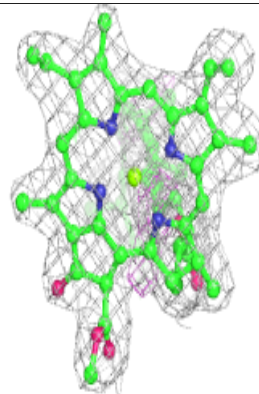
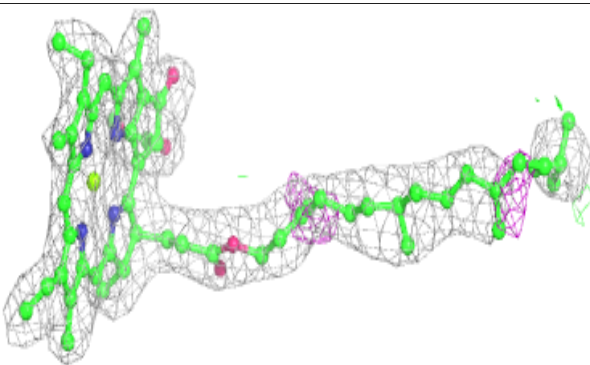
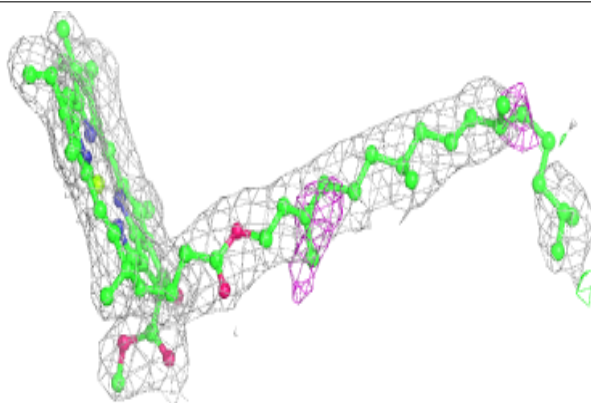


**Electron density around CLA b 605:**

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

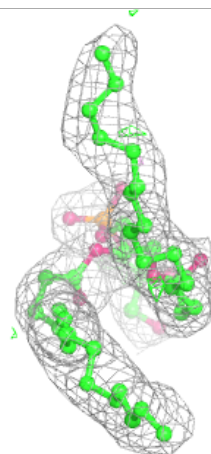
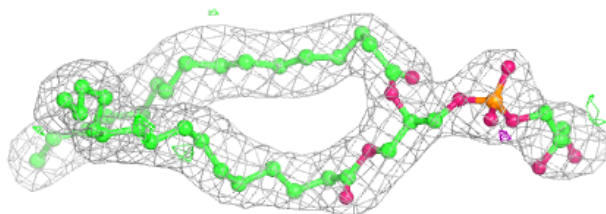
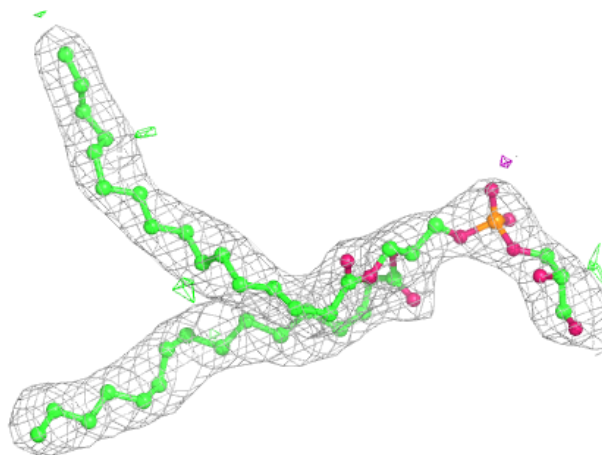
**Electron density around CLA b 604:**

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



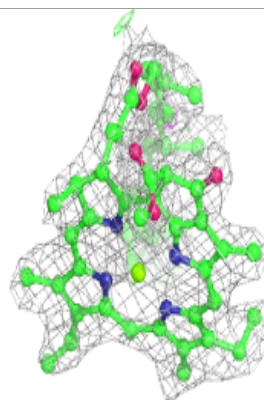
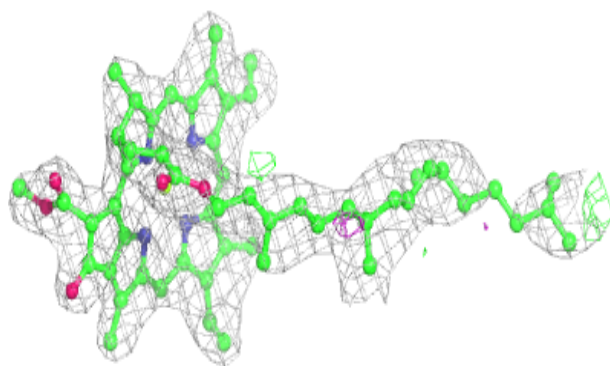
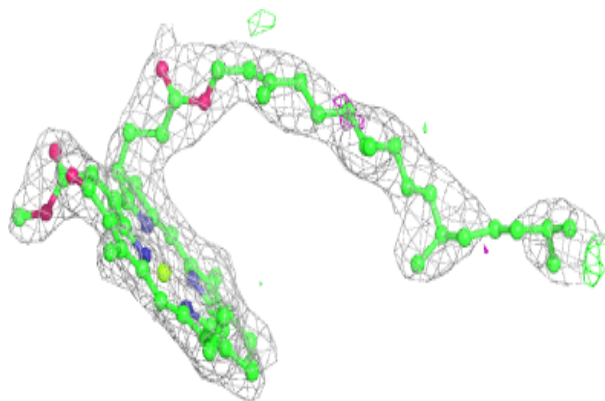
**Electron density around LHG D 410:**

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

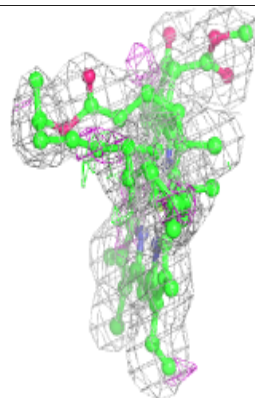
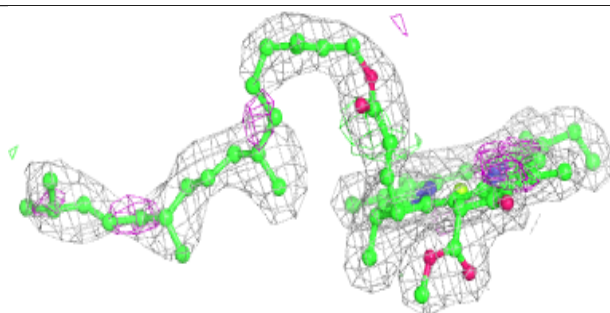
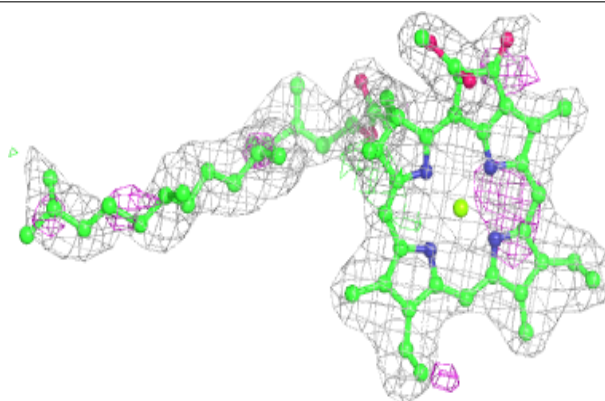


**Electron density around CLA c 505:**

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

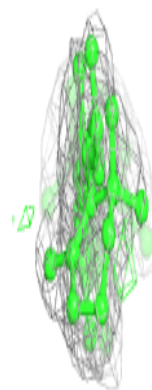
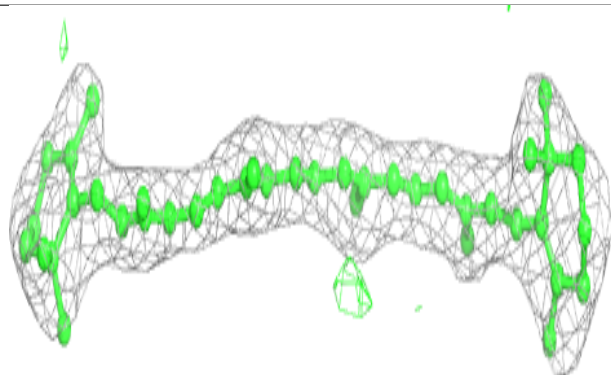
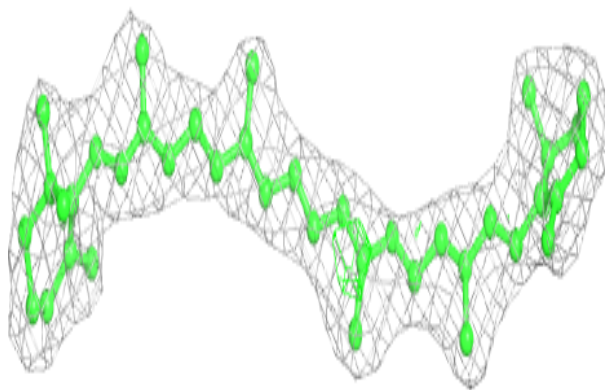
**Electron density around CLA A 406:**

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

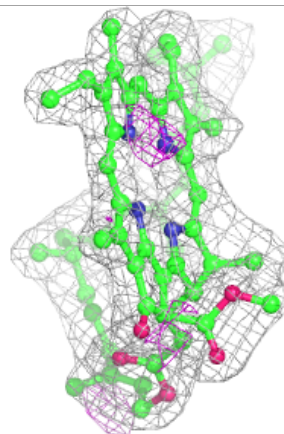
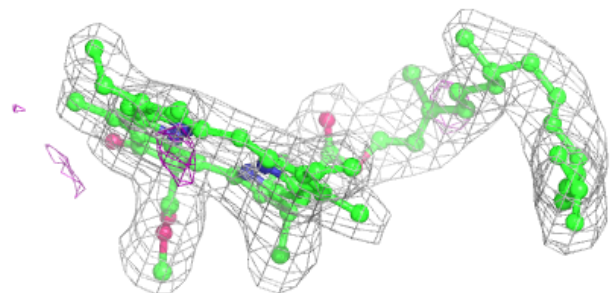
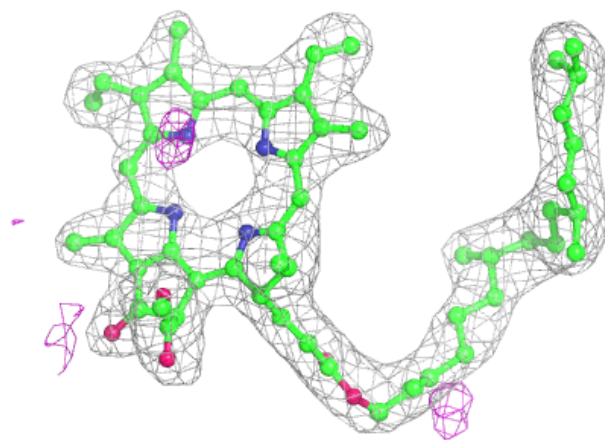


**Electron density around BCR y 101:**

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

**Electron density around PHO a 353:**

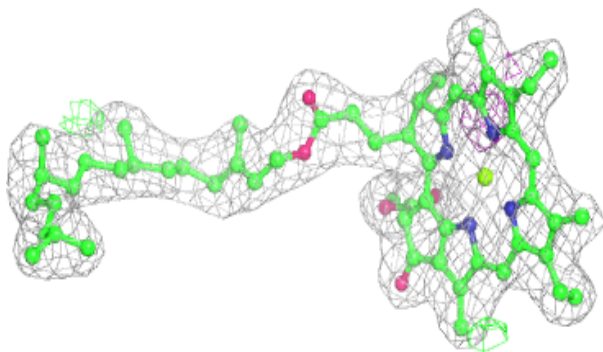
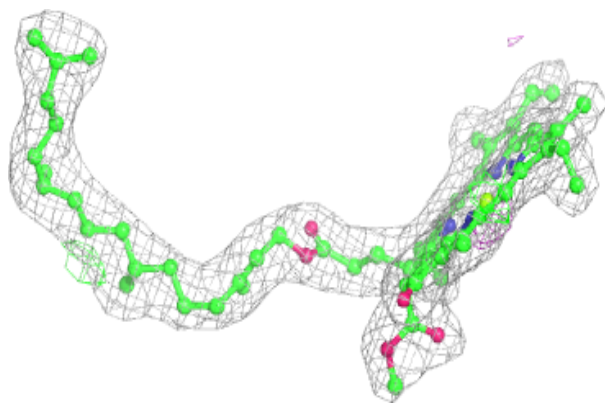
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





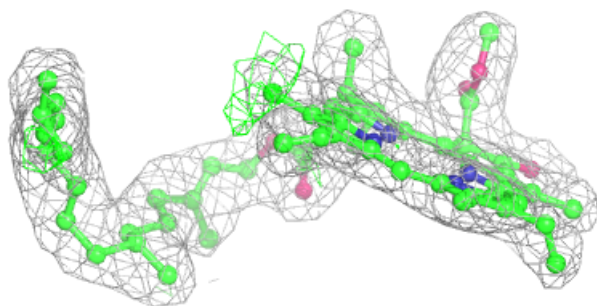
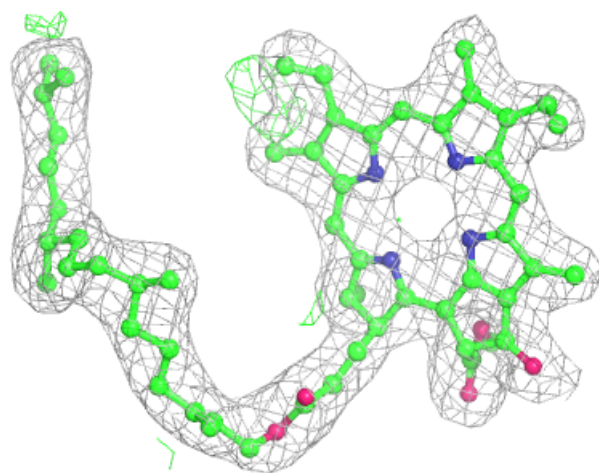
**Electron density around CLA D 405:**

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



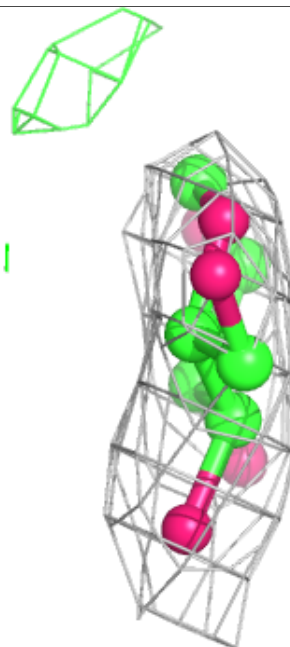
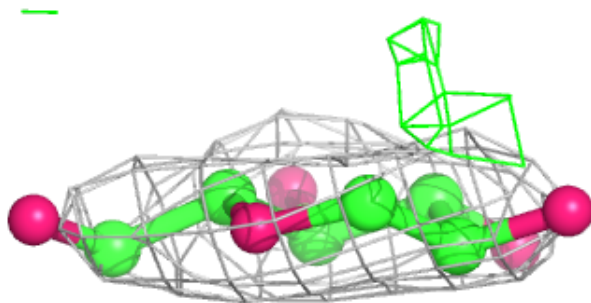
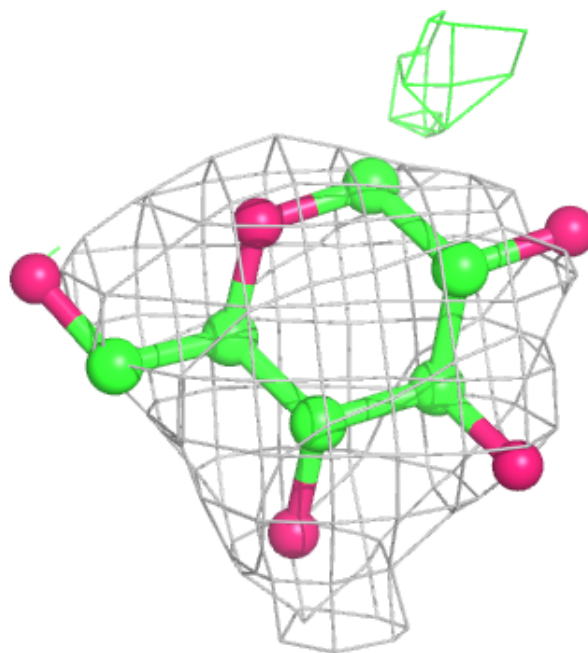
**Electron density around PHO A 353:**

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



**Electron density around HTG V 203:**

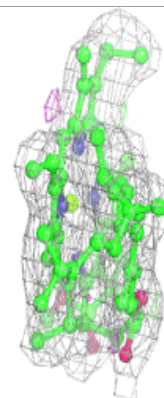
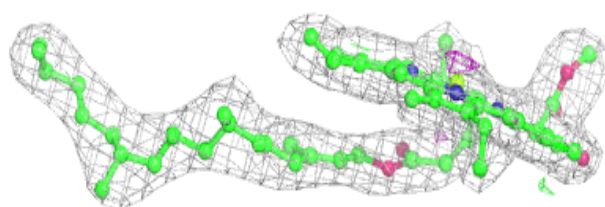
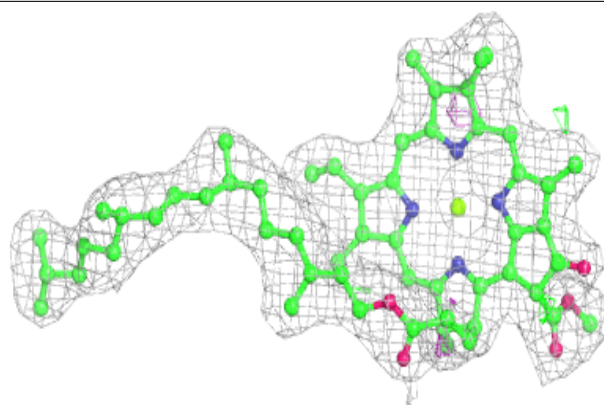
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



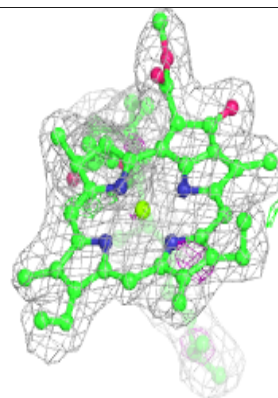
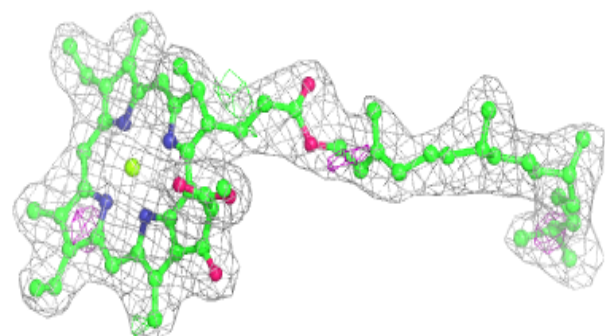
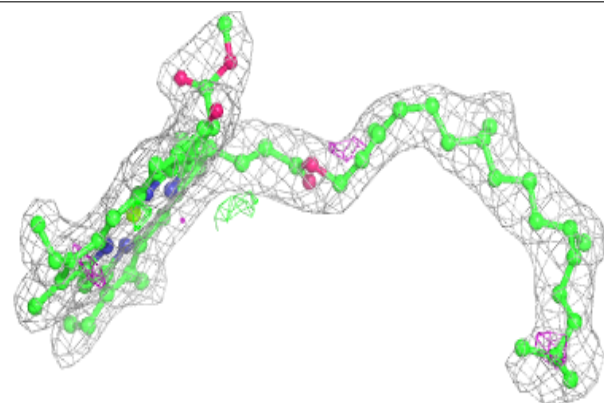


**Electron density around CLA B 603:**

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

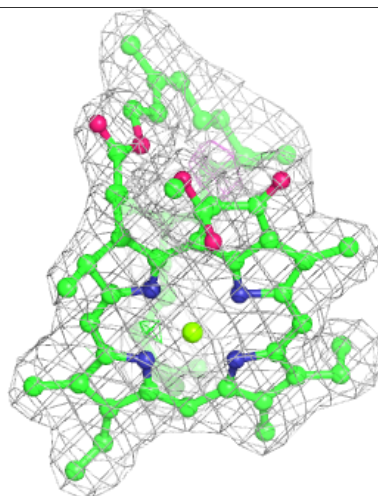
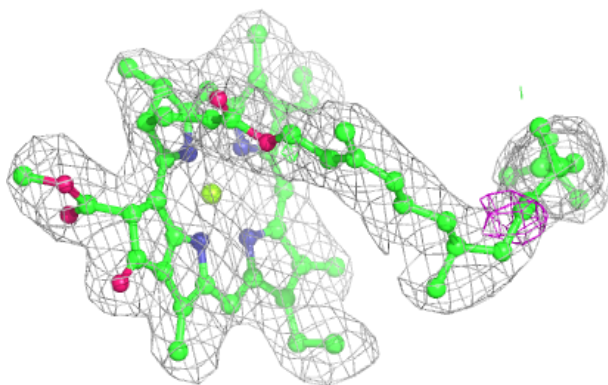
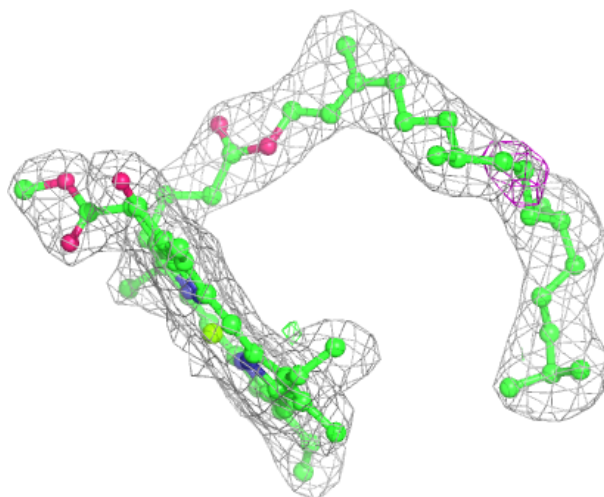
**Electron density around CLA d 402:**

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



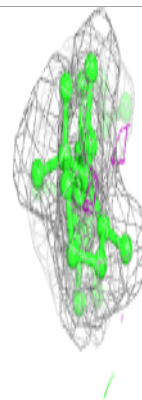
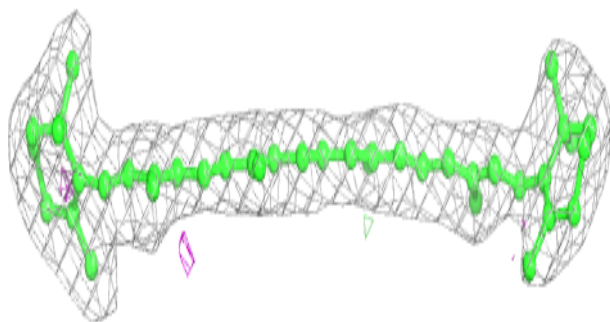
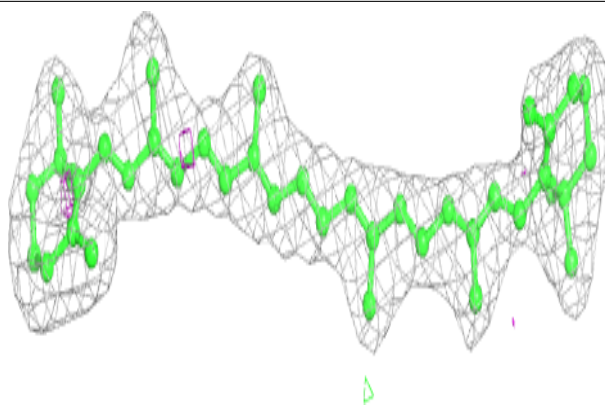
**Electron density around CLA b 611:**

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

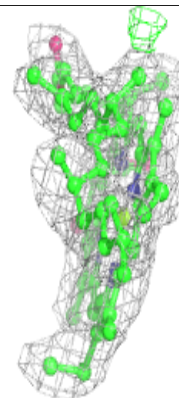
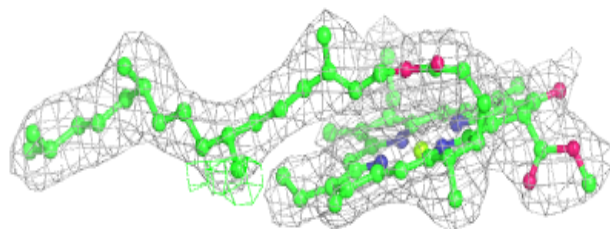
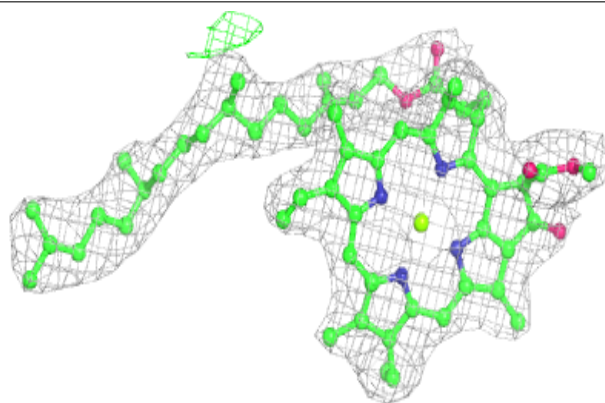


**Electron density around BCR b 618:**

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

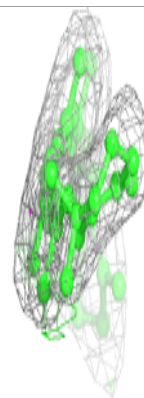
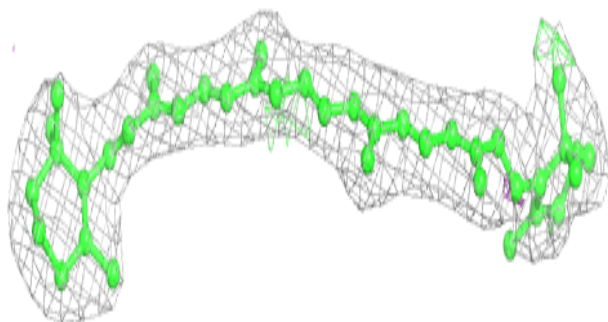
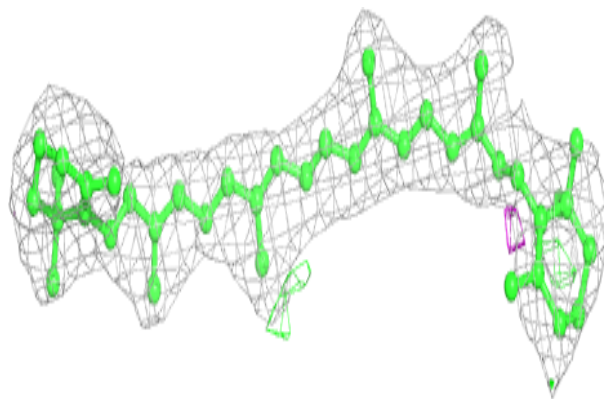
**Electron density around CLA c 502:**

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

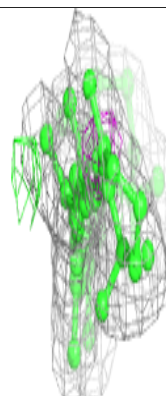
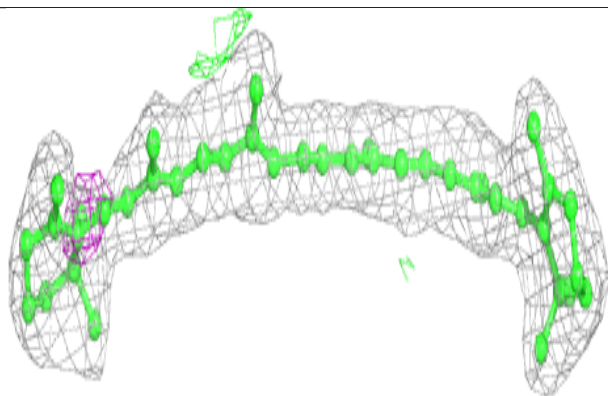
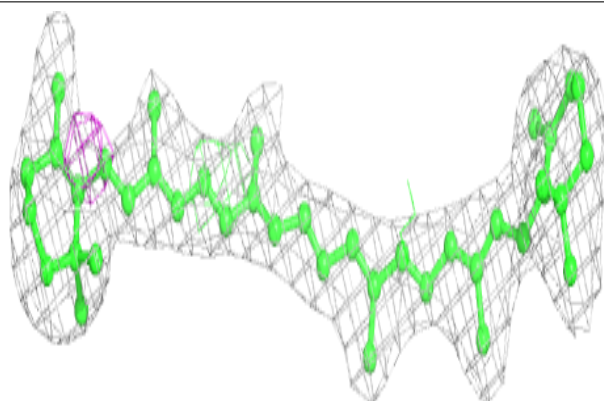


**Electron density around BCR d 404:**

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

**Electron density around BCR T 101:**

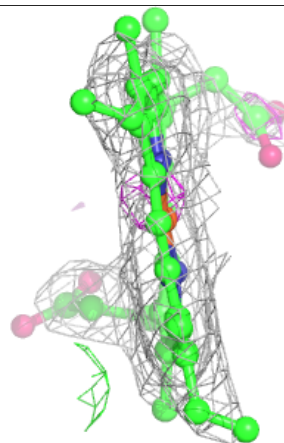
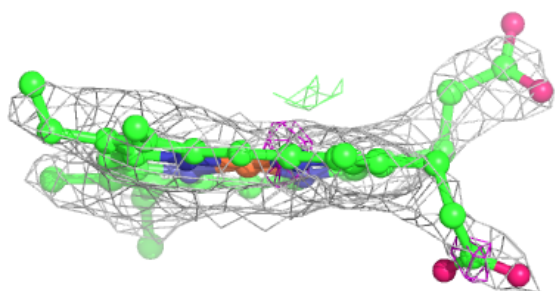
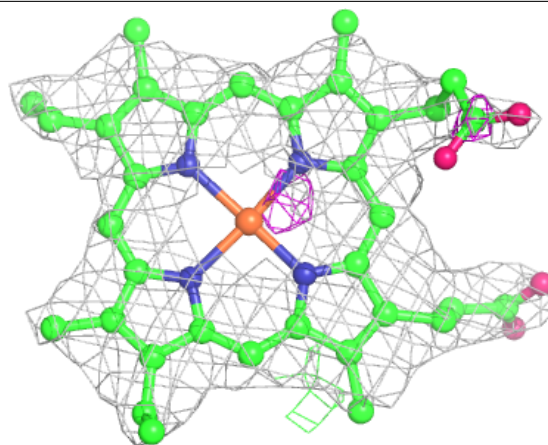
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



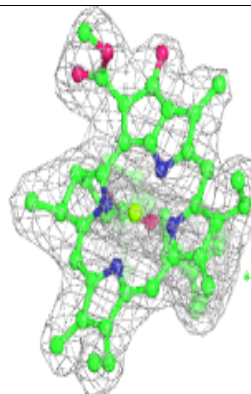
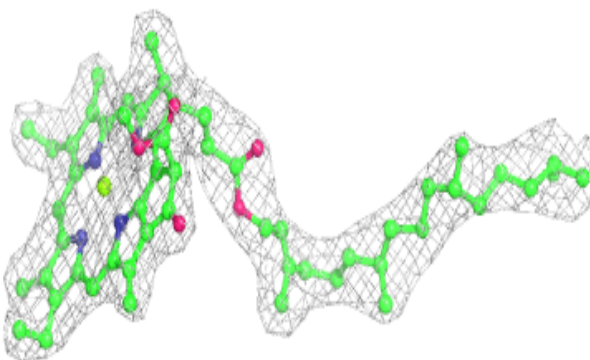
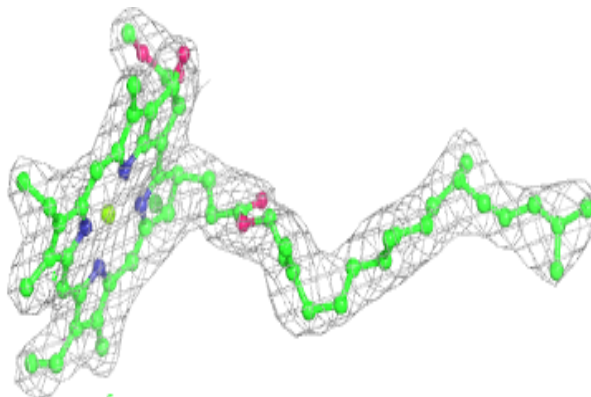


**Electron density around HEM e 87:**

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

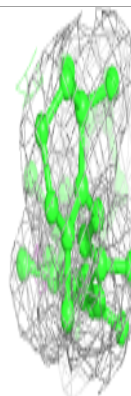
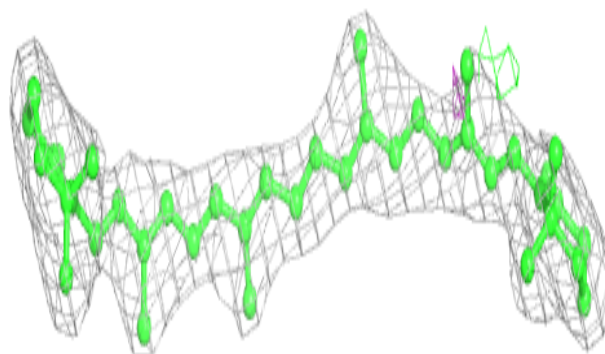
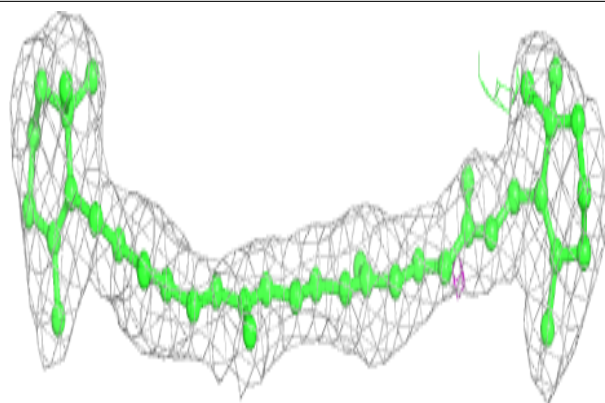
**Electron density around CLA C 503:**

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

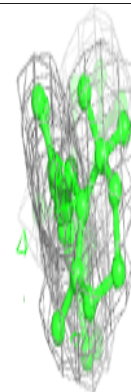
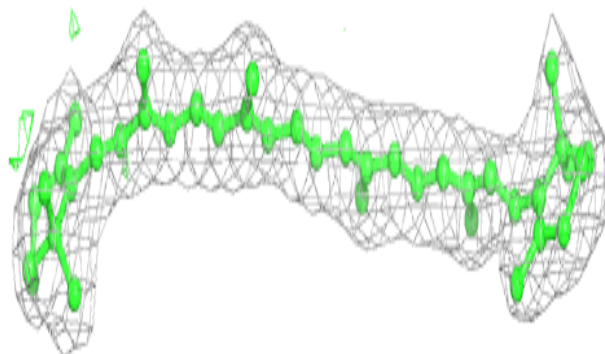
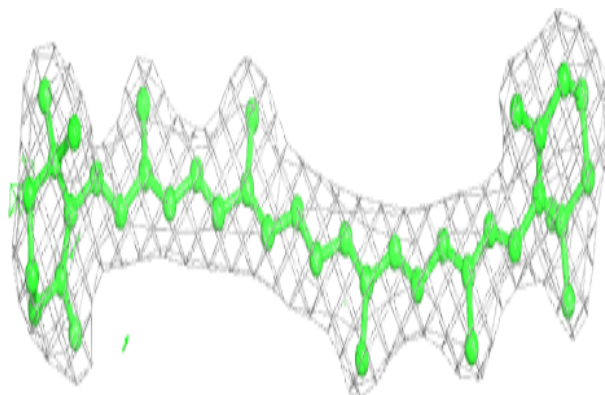


**Electron density around BCR k 101:**

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

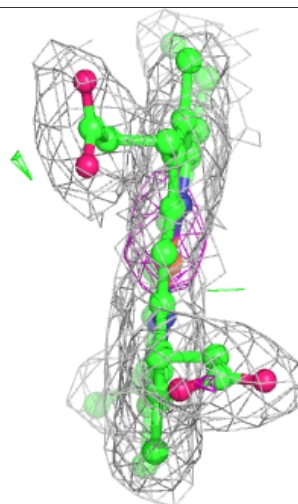
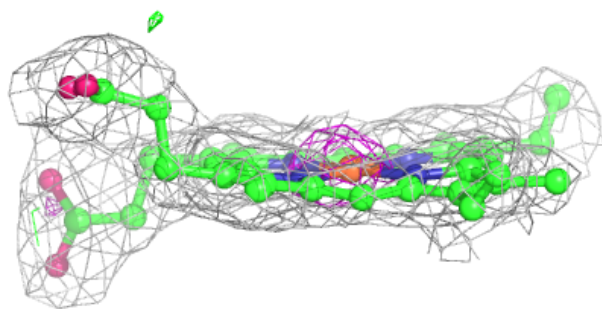
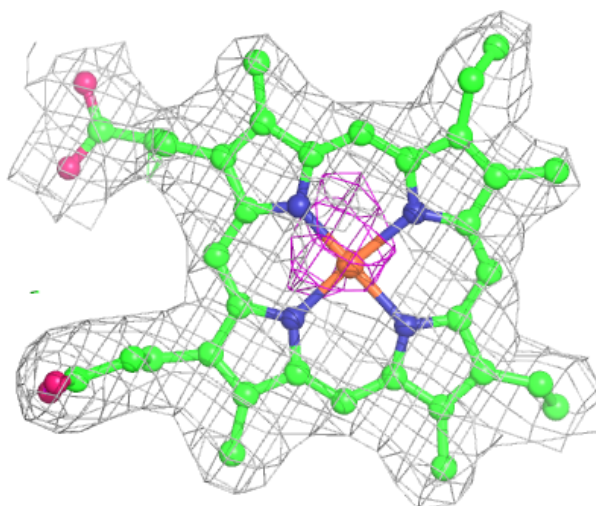
**Electron density around BCR B 619:**

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



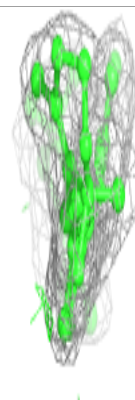
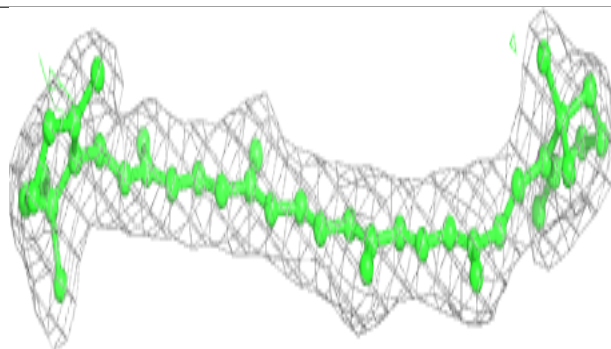
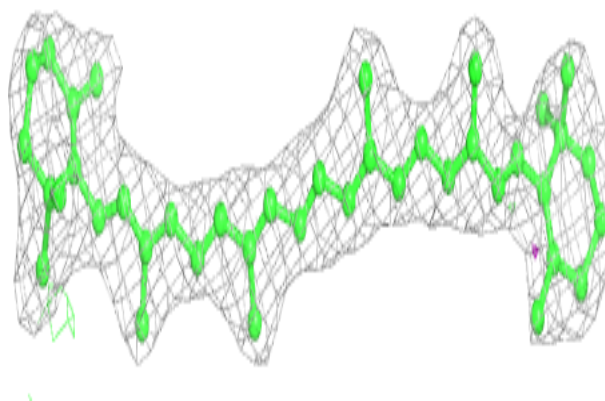
**Electron density around HEC V 202:**

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



**Electron density around BCR b 619:**

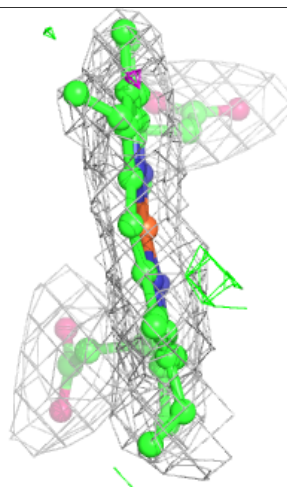
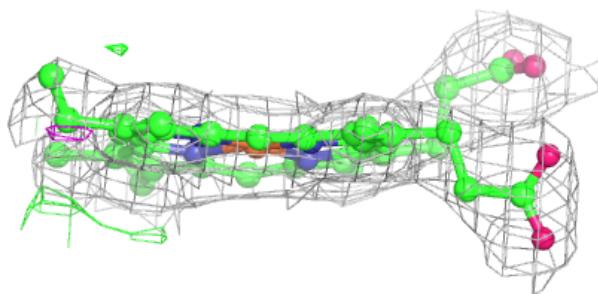
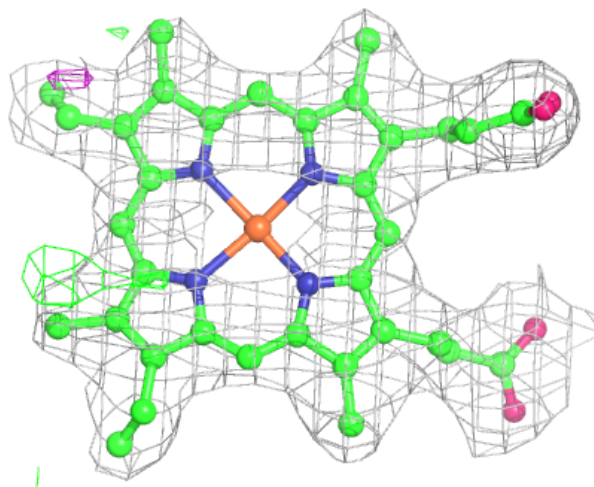
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





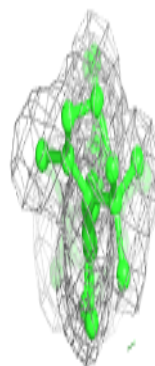
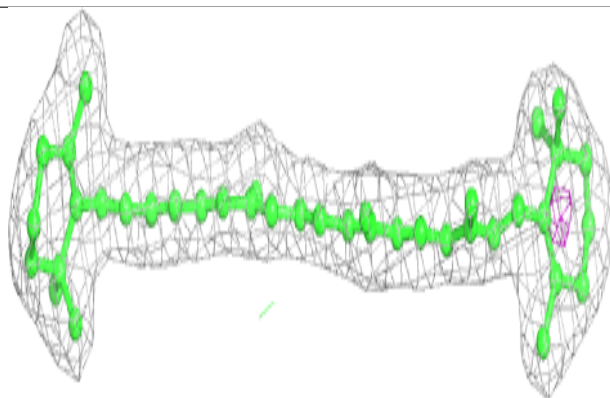
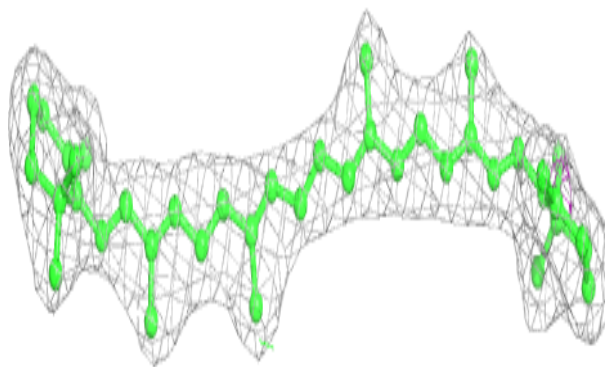
**Electron density around HEC v 202:**

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



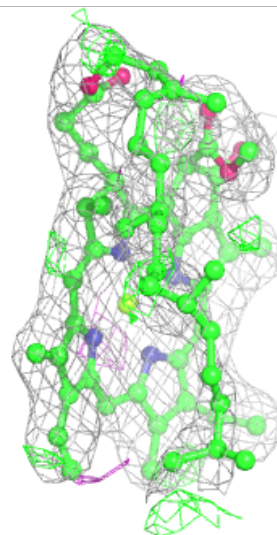
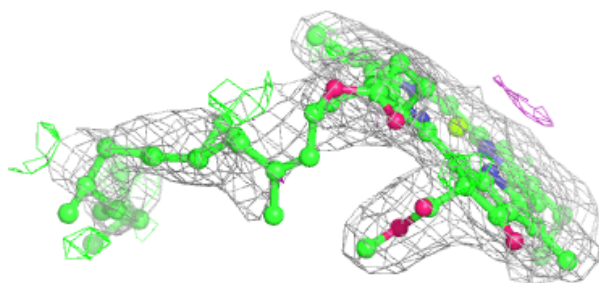
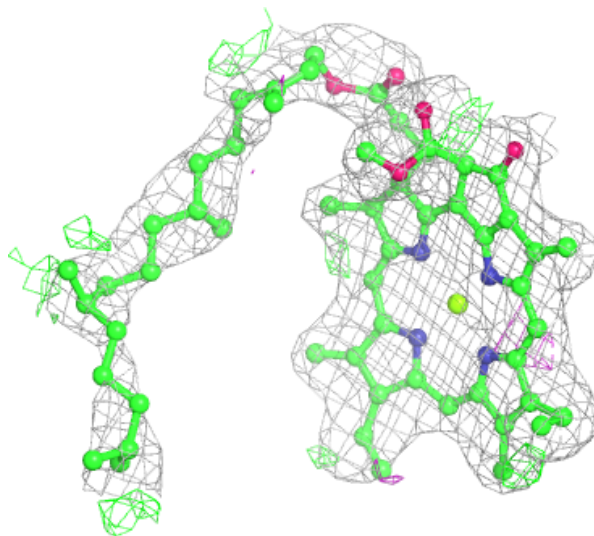
**Electron density around BCR a 410:**

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



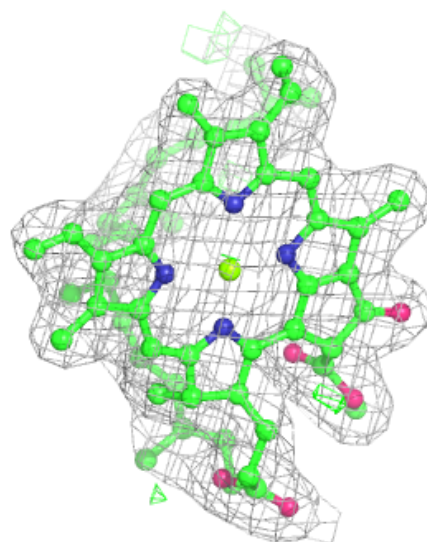
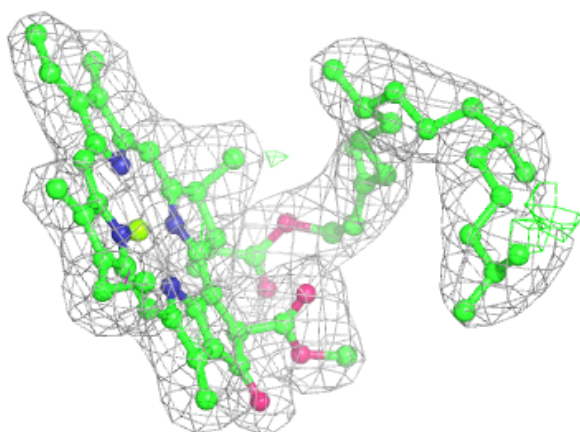
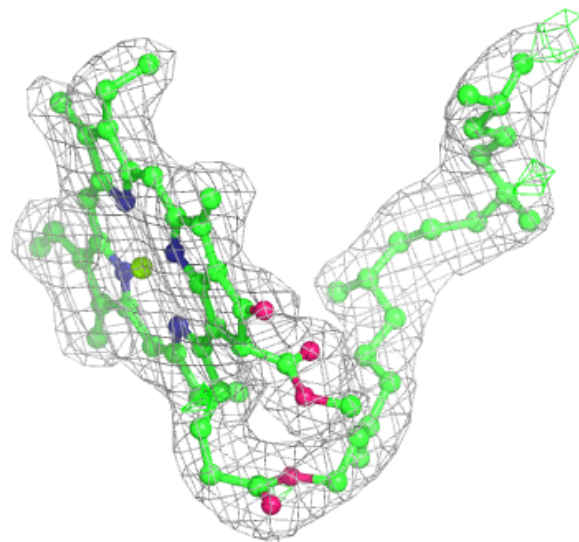
**Electron density around CLA B 616:**

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



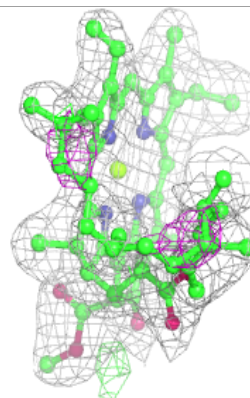
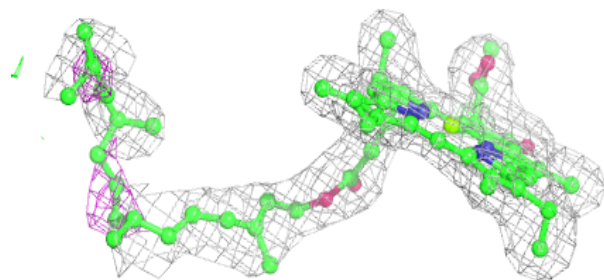
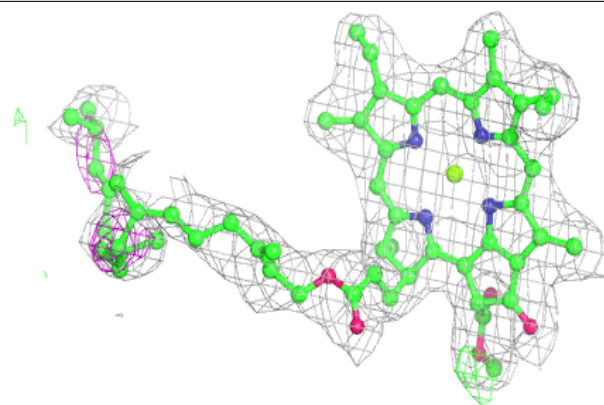
**Electron density around CLA b 613:**

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

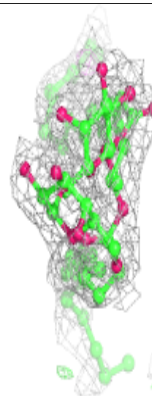
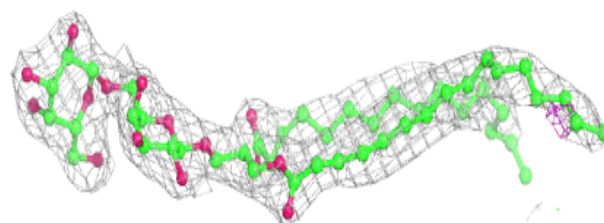
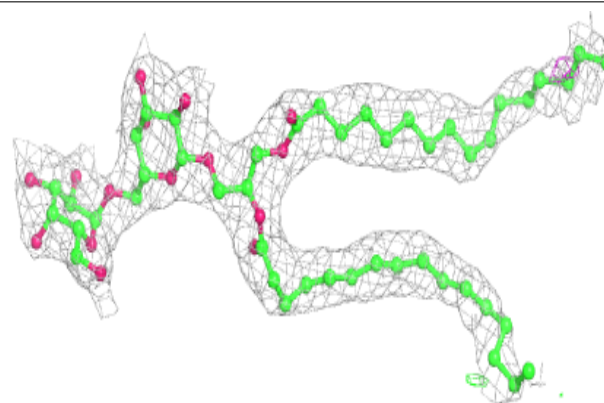


**Electron density around CLA A 408:**

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

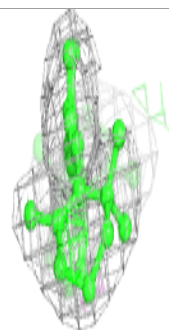
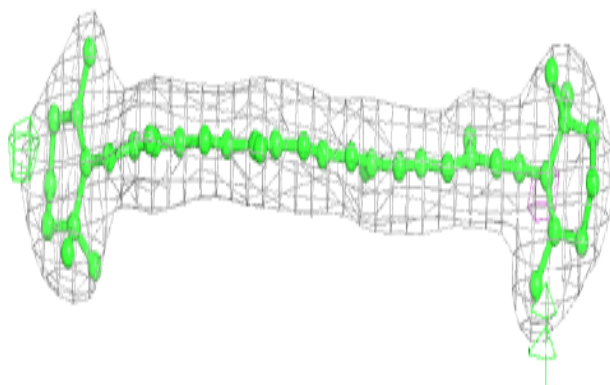
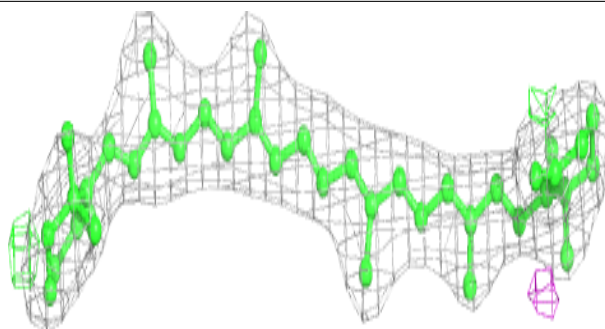
**Electron density around DGD c 519:**

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



**Electron density around BCR C 516:**

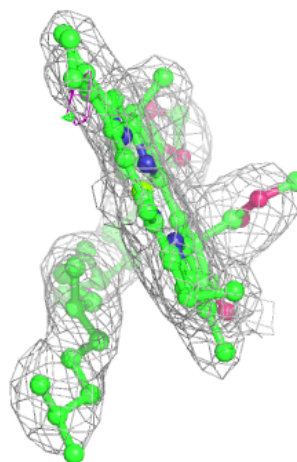
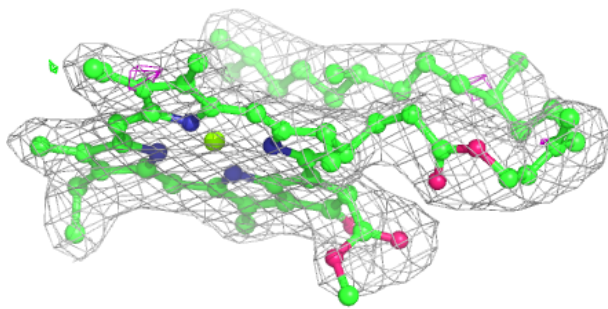
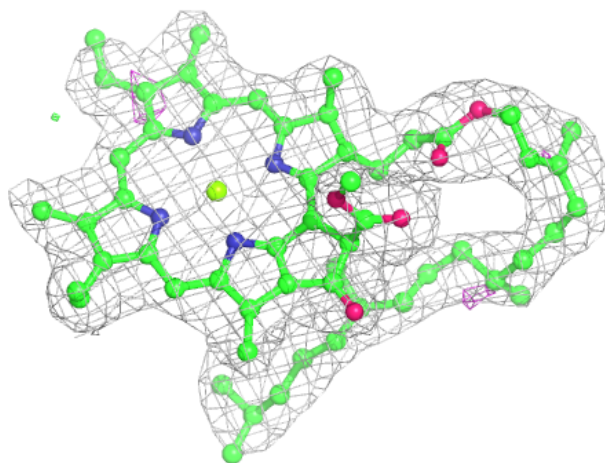
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





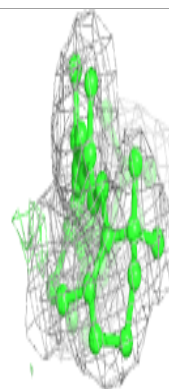
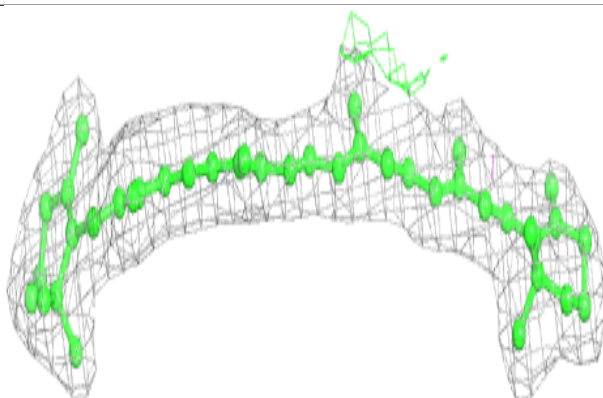
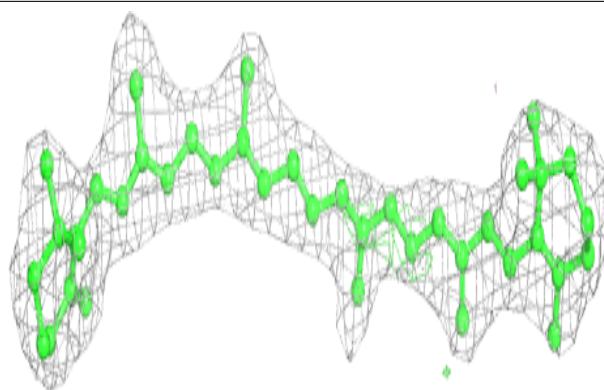
**Electron density around CLA C 510:**

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

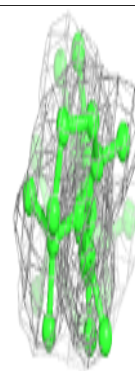
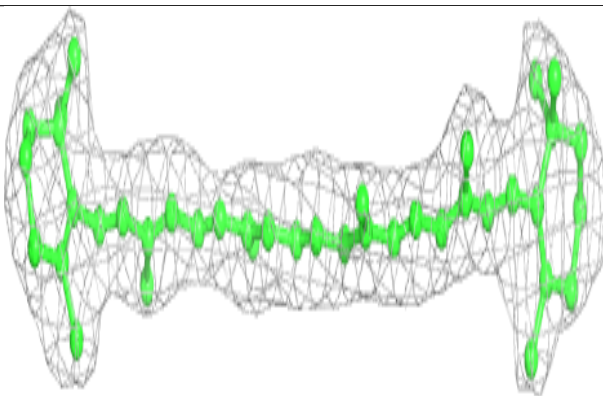
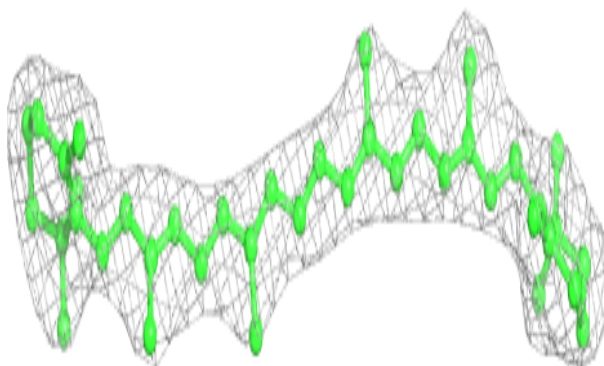


**Electron density around BCR t 103:**

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

**Electron density around BCR C 515:**

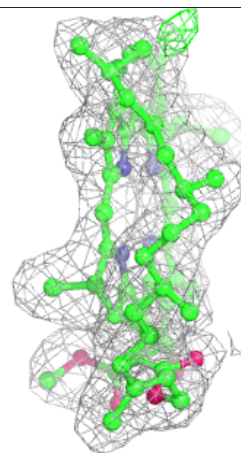
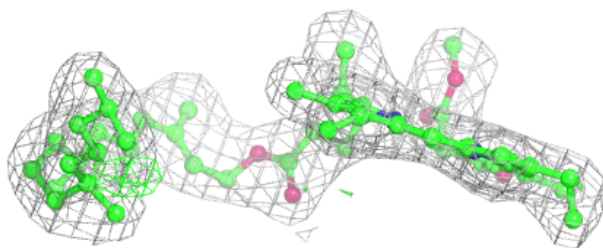
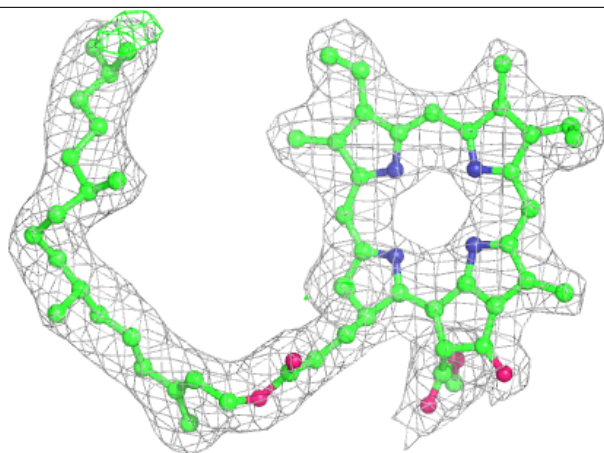
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



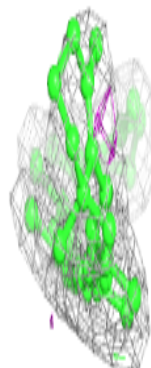
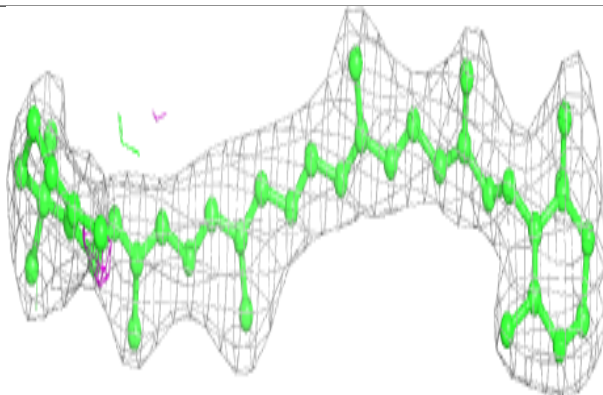
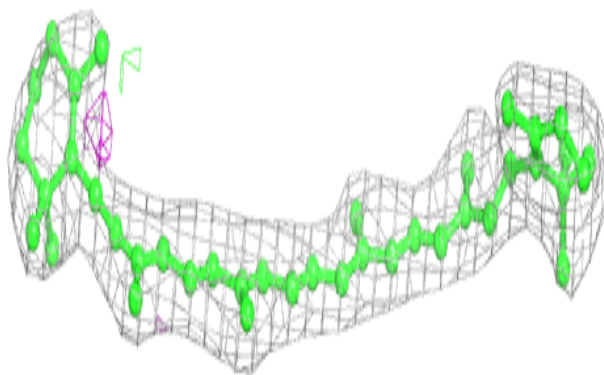


**Electron density around PHO A 407:**

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

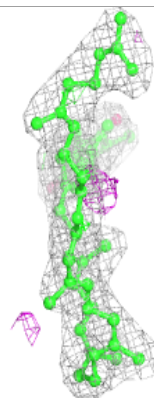
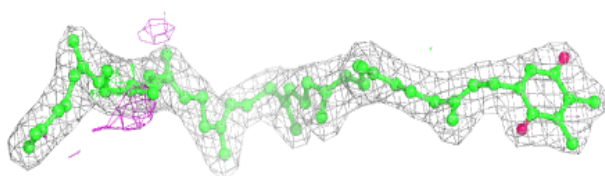
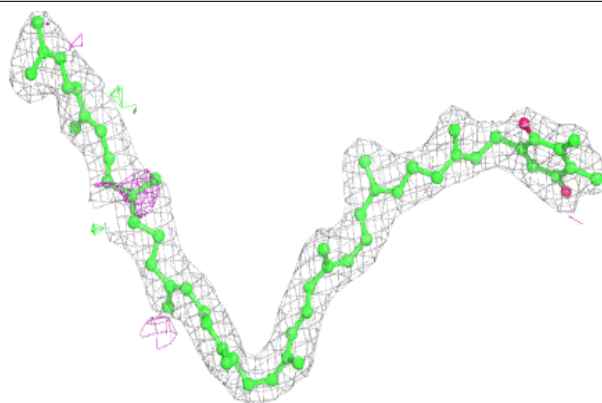
**Electron density around BCR D 407:**

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

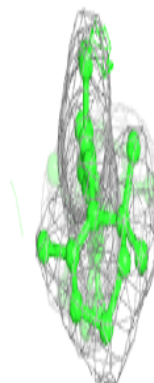
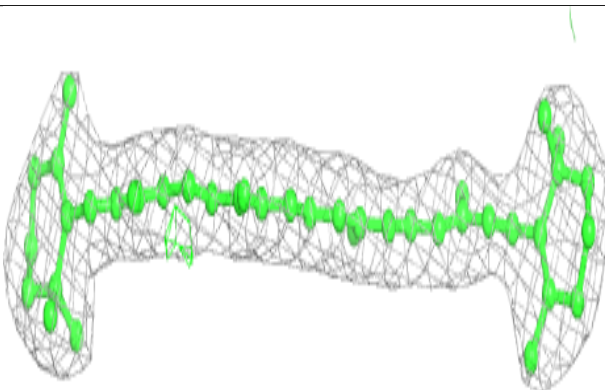
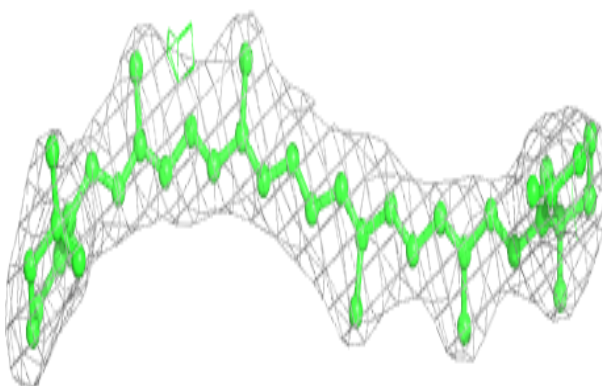


**Electron density around PL9 d 405:**

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

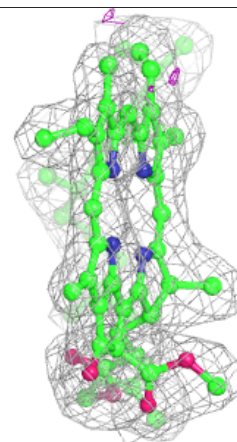
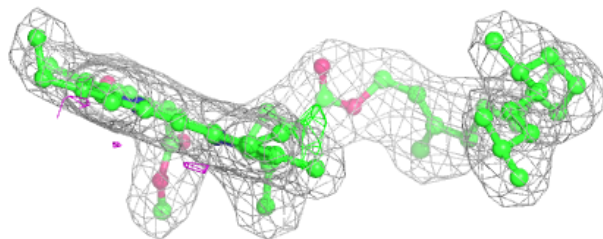
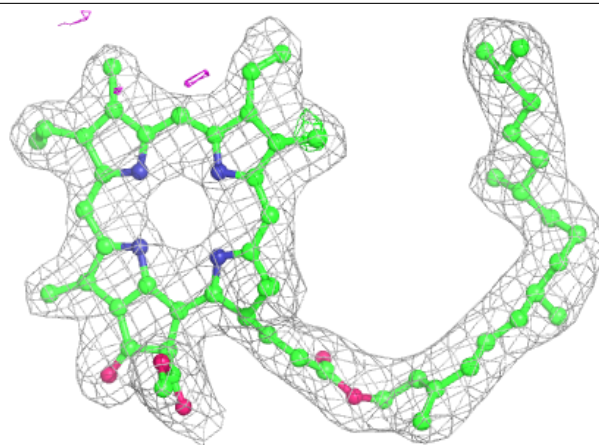
**Electron density around BCR c 516:**

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

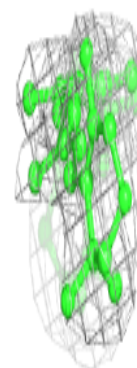
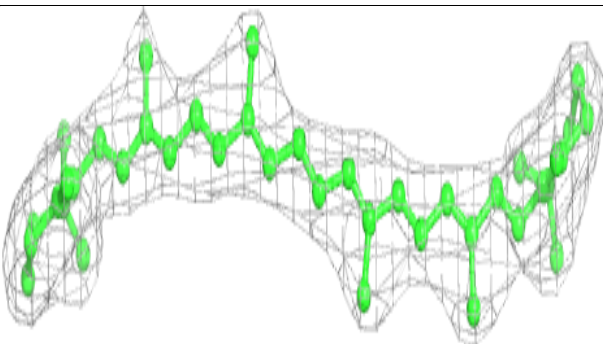
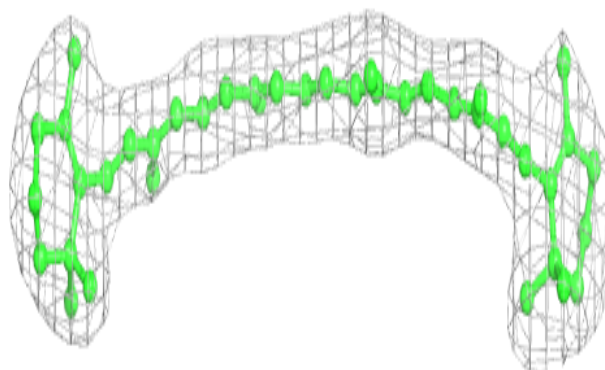


**Electron density around PHO a 408:**

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

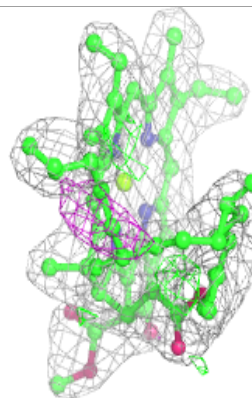
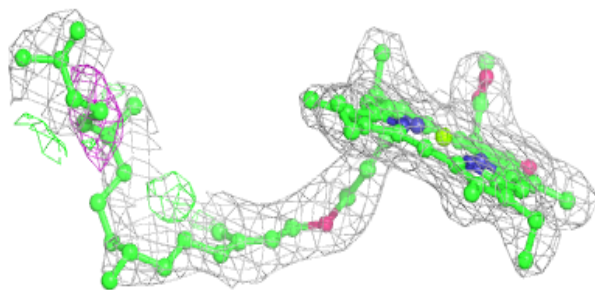
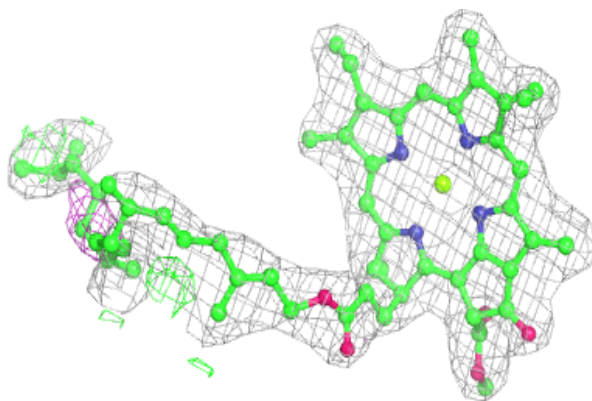
**Electron density around BCR K 102:**

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

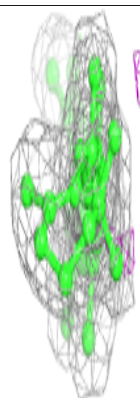
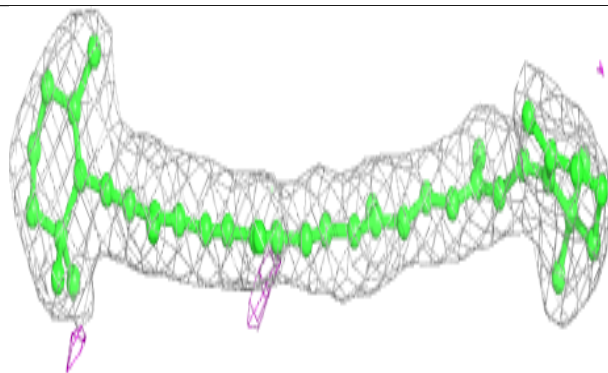
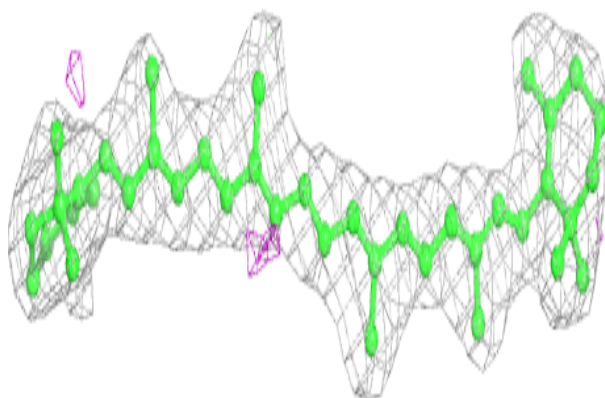


**Electron density around CLA a 409:**

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

**Electron density around BCR b 617:**

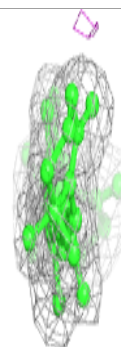
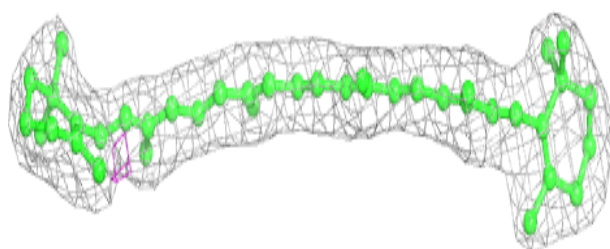
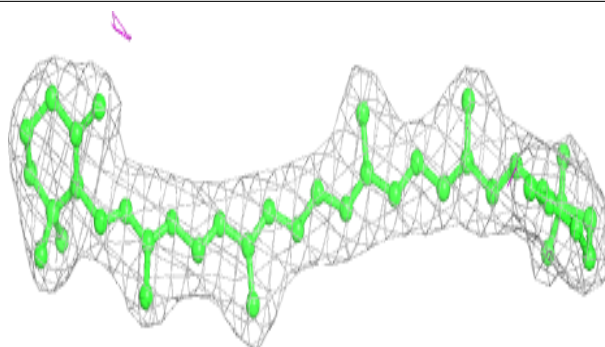
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



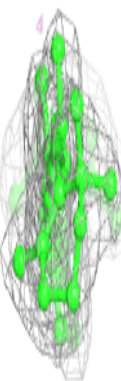
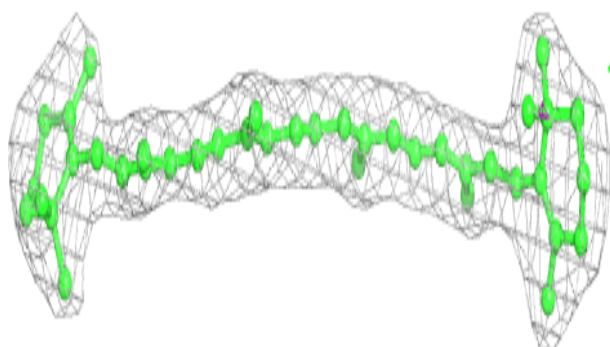
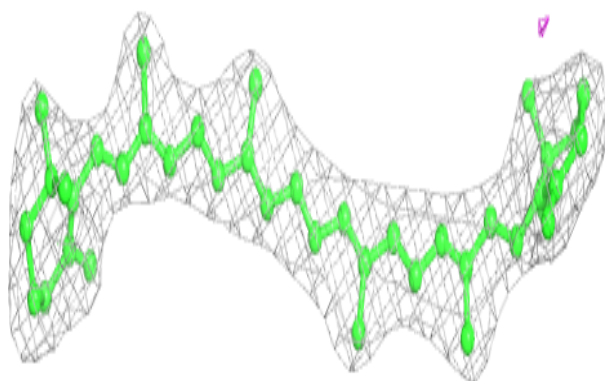


**Electron density around BCR B 617:**

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

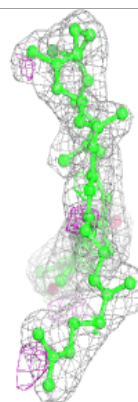
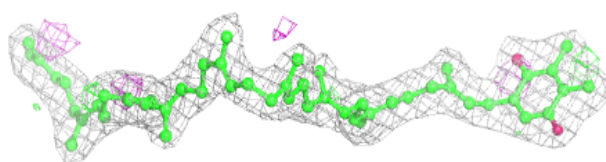
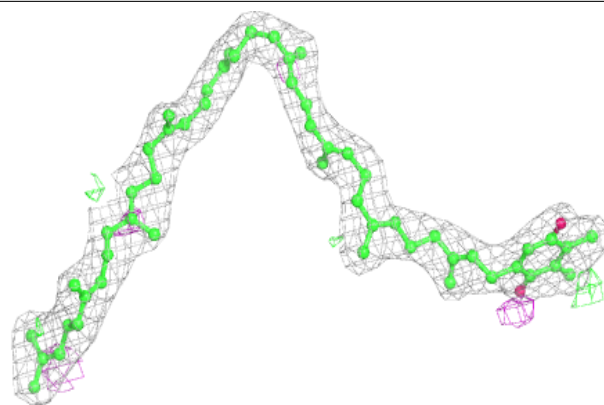
**Electron density around BCR Y 101:**

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

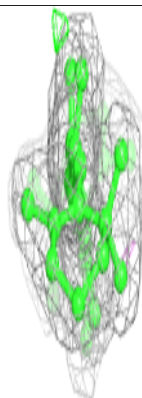
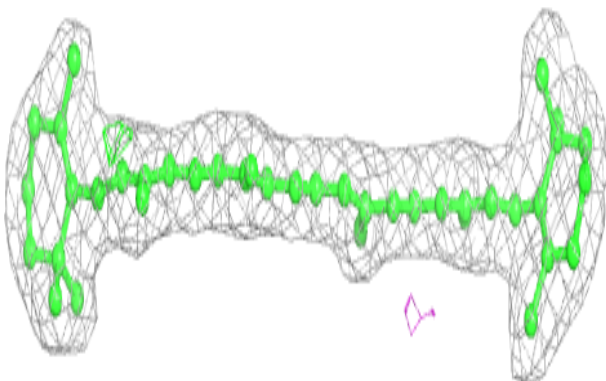
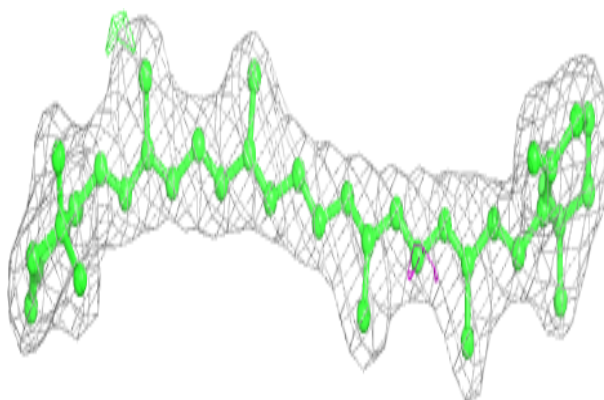


**Electron density around PL9 D 408:**

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

**Electron density around BCR 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.