



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 23, 2022 – 06:28 PM JST

PDB ID : 7YQ2  
Title : Crystal structure of photosystem II expressing psbA2 gene only  
Authors : Nakajima, Y.; Suga, M.; Shen, J.R.  
Deposited on : 2022-08-05  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.31.3  
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) : 2.31.3

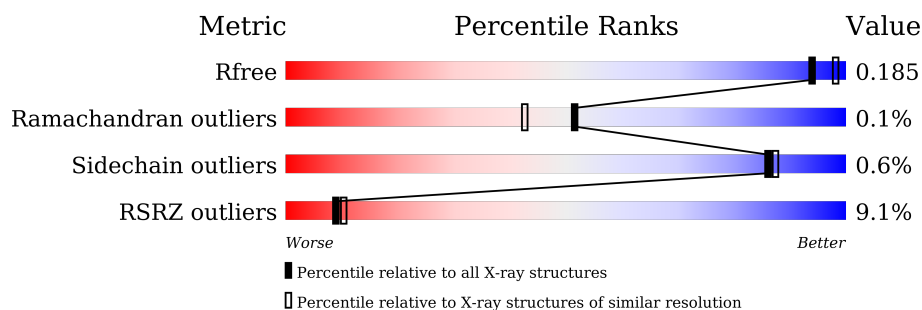
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	360	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	a	360	<div> <div>8%</div> <div>93%</div> <div>7%</div> </div>
2	B	510	<div> <div>6%</div> <div>99%</div> <div>.</div> </div>
2	b	510	<div> <div>9%</div> <div>98%</div> <div>.</div> </div>
3	C	461	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>
3	c	461	<div> <div>6%</div> <div>98%</div> <div>.</div> </div>
4	D	352	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	

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Mol	Chain	Length	Quality of chain
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	413	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
30	UNL	A	415	-	-	-	X
30	UNL	A	418	-	-	-	X
30	UNL	B	627	-	-	-	X
30	UNL	T	102	-	-	-	X
30	UNL	a	418	-	-	-	X
30	UNL	h	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	UNL	h	106	-	-	-	X
30	UNL	t	103	-	-	-	X
31	LMT	c	922	-	-	-	X
32	GOL	B	637	-	-	-	X
32	GOL	O	304	-	-	-	X
34	DMS	O	312	-	-	-	X
36	HTG	B	625	-	-	-	X
36	HTG	c	924	-	-	-	X
36	HTG	c	943	-	-	-	X
36	HTG	d	420	-	-	-	X

## 2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 55630 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2607	1712	427	455	13			
1	a	336	Total	C	N	O	S	0	3	0
			2632	1727	431	461	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	8	0
			3995	2623	665	694	13			
2	b	504	Total	C	N	O	S	0	9	0
			3961	2600	656	692	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	6	0
			3507	2295	586	613	13			
3	c	456	Total	C	N	O	S	0	3	0
			3532	2314	589	616	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
			2713	1799	439	463	12			
4	d	342	Total	C	N	O	S	0	2	0
			2724	1806	442	463	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	1	0
			629	413	102	114			
5	e	79	Total	C	N	O	0	2	0
			644	423	102	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	32	Total	C	N	O	S	0	1	0
			263	179	44	39	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			505	336	81	86	2			
7	h	65	Total	C	N	O	S	0	1	0
			516	343	85	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total	C	N	O	S	0	0	0
			301	205	47	48	1			
8	i	37	Total	C	N	O	S	0	0	0
			297	203	47	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			270	182	40	46	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	2	0
			311	209	49	52	1			
11	l	37	Total	C	N	O	S	0	1	0
			305	205	48	51	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			270	182	39	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			274	184	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	10	0
			1895	1190	313	388	4			
13	o	243	Total	C	N	O	S	0	5	0
			1879	1177	311	387	4			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			767	487	129	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	4	0
			1089	691	181	213	4			
16	v	137	Total	C	N	O	S	0	2	0
			1070	678	178	210	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			
17	y	30	Total	C	N	O	S	0	1	0
			229	152	38	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	S	0	0	0
			286	191	46	49				
18	x	39	Total	C	N	O	S	0	0	0
			286	191	46	49				

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

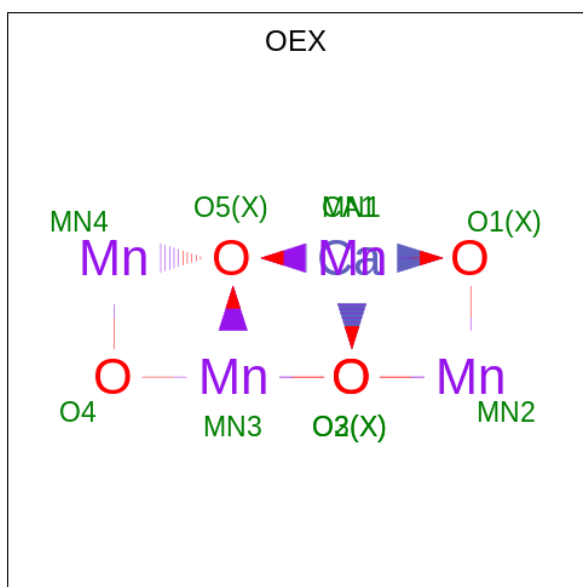
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			458	317	67	72	2			
19	z	62	Total	C	N	O	S	0	0	0
			455	312	67	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			228	150	41	37				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).





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

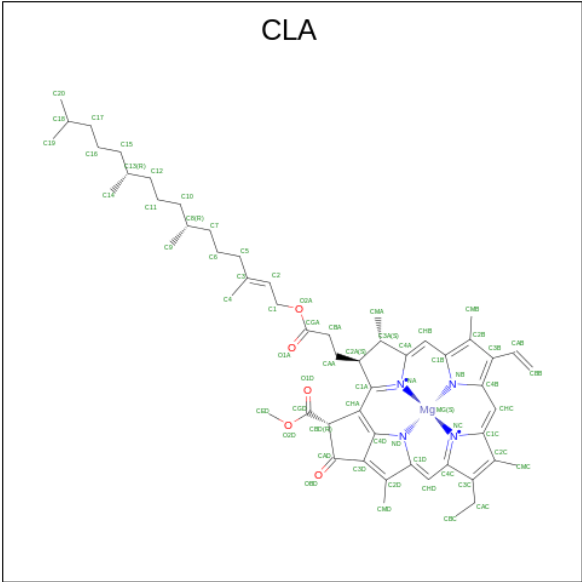
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 24 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
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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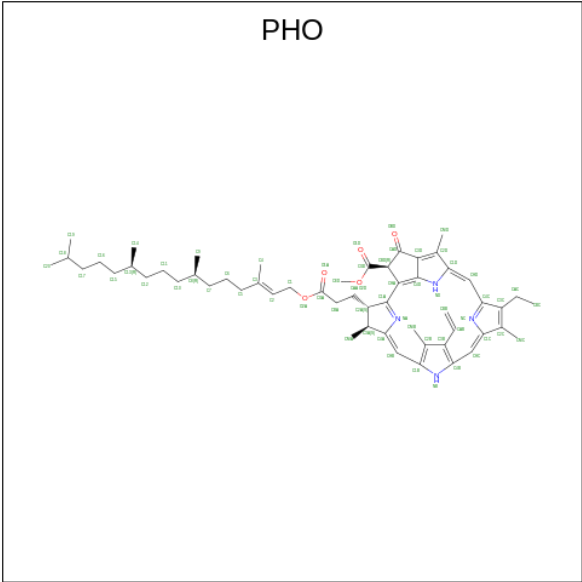
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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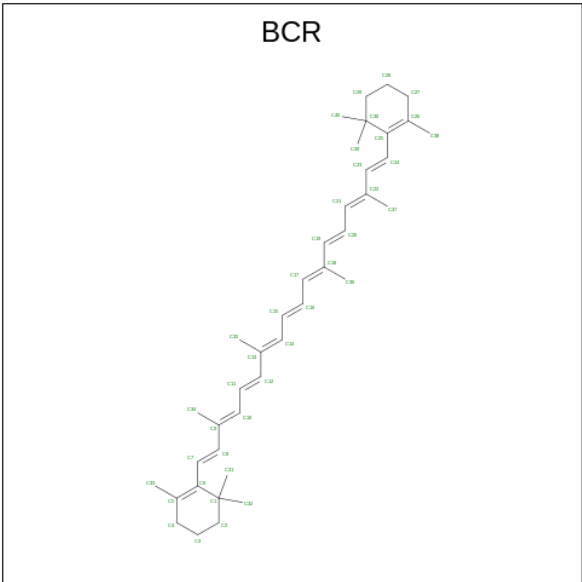
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



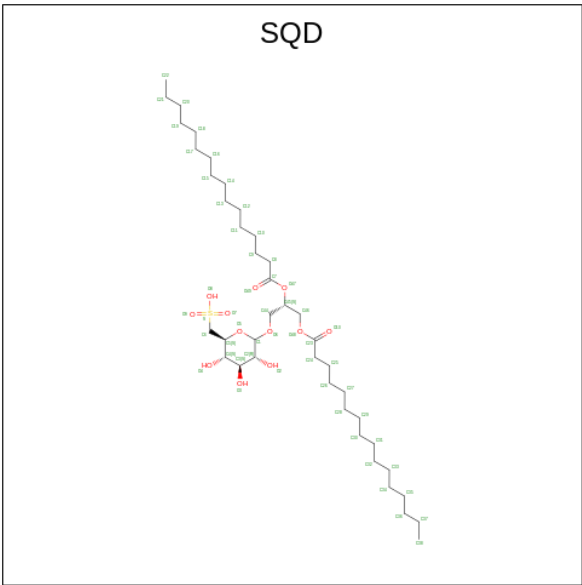
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

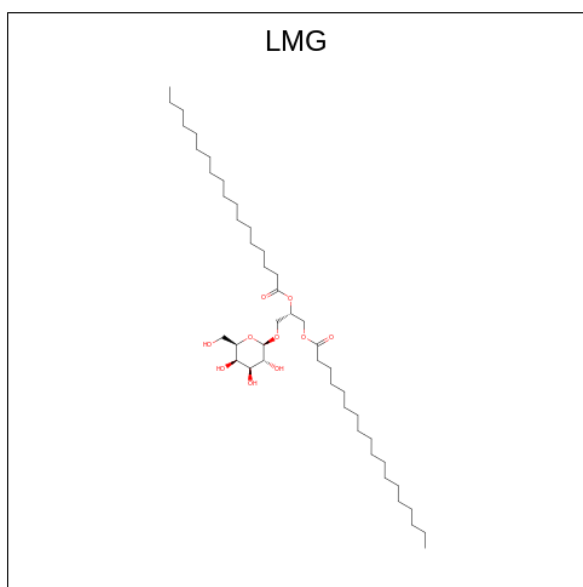
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			37	25	11	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		
27	l	1	Total	C	O	S	0	0
			54	41	12	1		

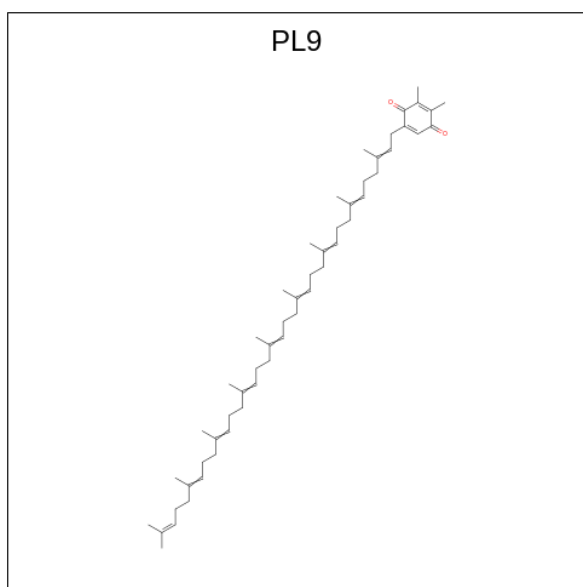
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	D	1	Total	C	O	0	0
			51	41	10		
28	a	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	d	1	Total	C	O	0	0
			51	41	10		

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



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

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

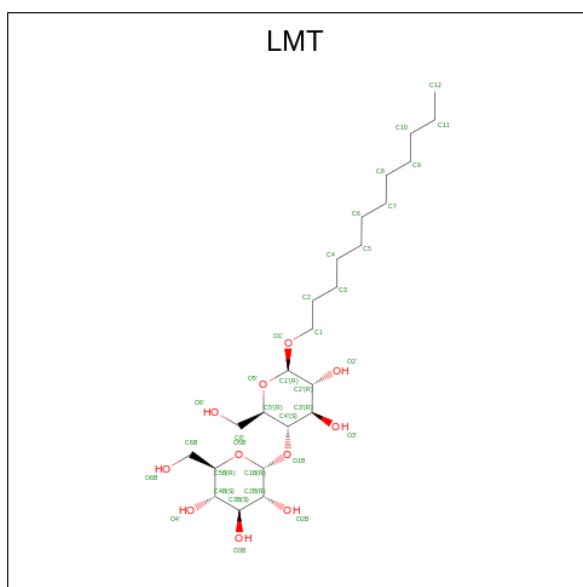
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	4	Total	C	O	0	0
			57	52	5		
30	B	4	Total	C		0	0
			24	24			
30	C	3	Total	C	O	0	0
			54	49	5		
30	D	3	Total	C	O	0	0
			60	55	5		
30	E	4	Total	C		0	0
			22	22			
30	H	2	Total	C	O	0	0
			24	22	2		
30	I	7	Total	C		0	0
			79	79			
30	J	3	Total	C		0	0
			36	36			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	T	1	Total C 15 15	0	0
30	X	1	Total C 16 16	0	0
30	Z	3	Total C 20 20	0	0
30	a	2	Total C O 45 40 5	0	0
30	b	8	Total C O 87 85 2	0	0
30	c	6	Total C O 47 45 2	0	0
30	d	3	Total C O 65 58 7	0	0
30	e	2	Total C 15 15	0	0
30	h	3	Total C 29 29	0	0
30	i	5	Total C O 66 64 2	0	0
30	j	3	Total C 15 15	0	0
30	k	2	Total C O 39 34 5	0	0
30	l	1	Total C 13 13	0	0
30	m	1	Total C 11 11	0	0
30	t	1	Total C 12 12	0	0
30	y	1	Total C 4 4	0	0
30	x	4	Total C O 39 37 2	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



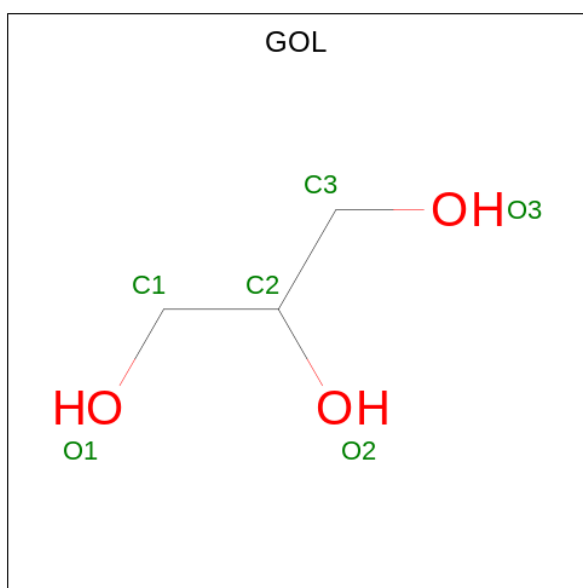
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total 35	C 24	O 11	0	0
31	A	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 24	C 18	O 6	0	0
31	F	1	Total 24	C 18	O 6	0	0
31	J	1	Total 24	C 18	O 6	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	M	1	Total 25	C 19	O 6	0	0
31	Z	1	Total 35	C 24	O 11	0	0
31	a	1	Total 35	C 24	O 11	0	0
31	b	1	Total 35	C 24	O 11	0	0
31	c	1	Total 35	C 24	O 11	0	0
31	c	1	Total 35	C 24	O 11	0	0
31	e	1	Total 24	C 18	O 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	j	1	Total	C	O	0	0
			24	18	6		
31	m	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			23	18	5		
31	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



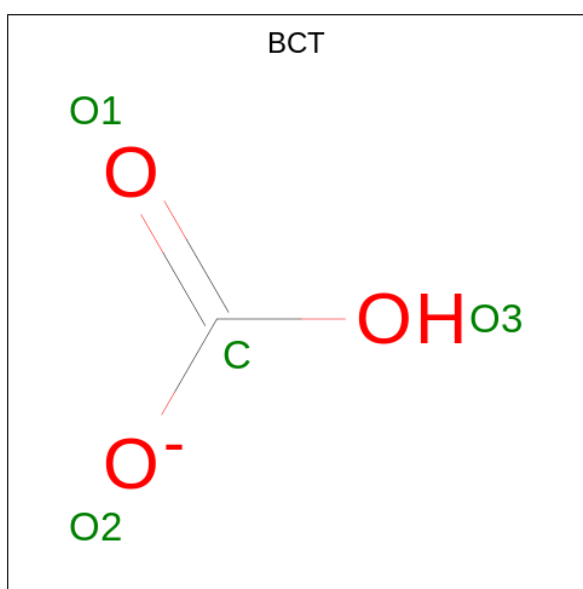
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			6	3	3		
32	B	1	Total	C	O	0	0
			6	3	3		
32	B	1	Total	C	O	0	0
			6	3	3		
32	C	1	Total	C	O	0	0
			6	3	3		
32	O	1	Total	C	O	0	0
			6	3	3		
32	V	1	Total	C	O	0	0
			6	3	3		

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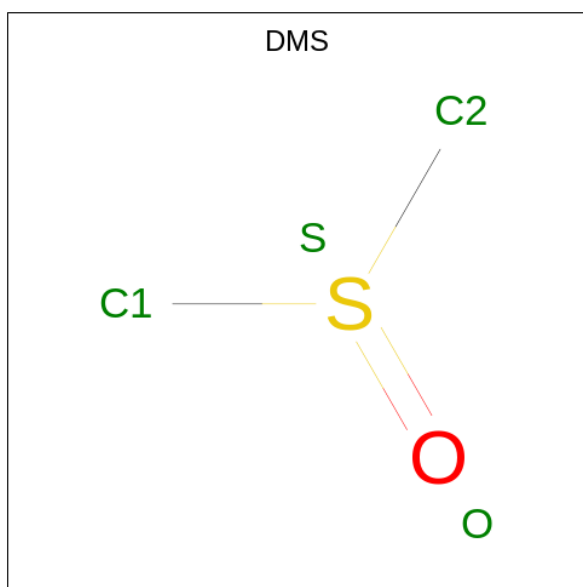
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	V	1	Total	C	O	0	0
			6	3	3		
32	a	1	Total	C	O	0	0
			6	3	3		
32	b	1	Total	C	O	0	0
			6	3	3		
32	c	1	Total	C	O	0	0
			6	3	3		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 34 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $\text{C}_2\text{H}_6\text{OS}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	H	1	Total 4	C 2	O 1	S 1	0	0
34	K	1	Total 4	C 2	O 1	S 1	0	0
34	L	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	e	1	Total 4	C 2	O 1	S 1	0	0
34	e	1	Total 4	C 2	O 1	S 1	0	0
34	e	1	Total 4	C 2	O 1	S 1	0	0
34	h	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	i	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	y	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

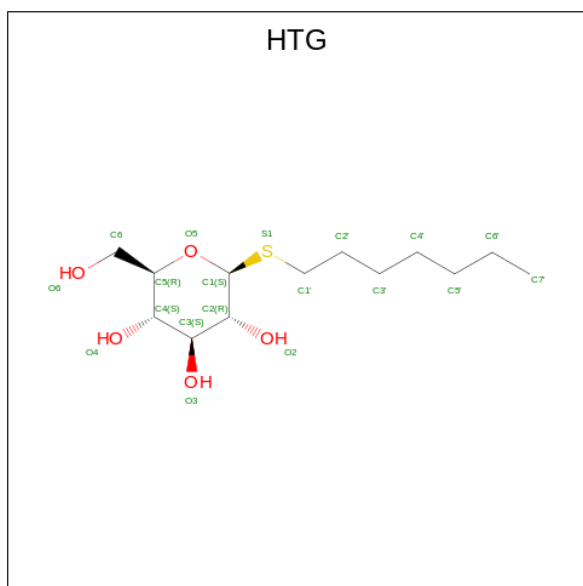
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total	Ca	0	0
			1	1		
35	V	1	Total	Ca	0	0
			1	1		
35	b	1	Total	Ca	0	0
			1	1		
35	c	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		
35	v	1	Total	Ca	0	0
			1	1		

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		

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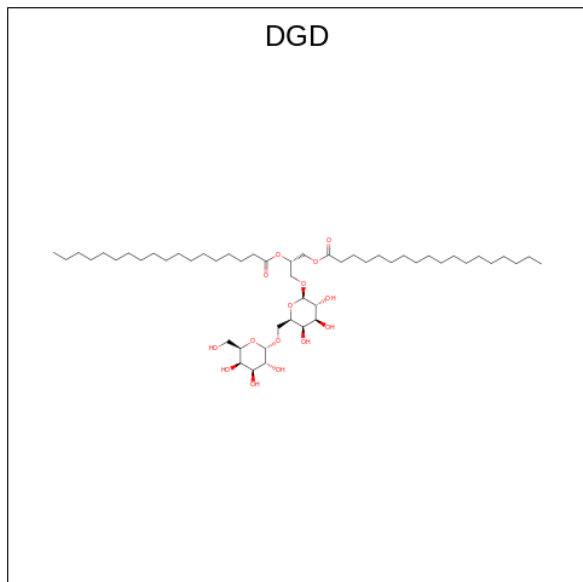
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	U	1	Total	C			0	0
			4	4				
36	V	1	Total	C	O	S	0	0
			13	7	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			17	11	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	v	1	Total	C	O	S	0	0
			19	13	5	1		
36	y	1	Total	C	O	S	0	0
			19	13	5	1		

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



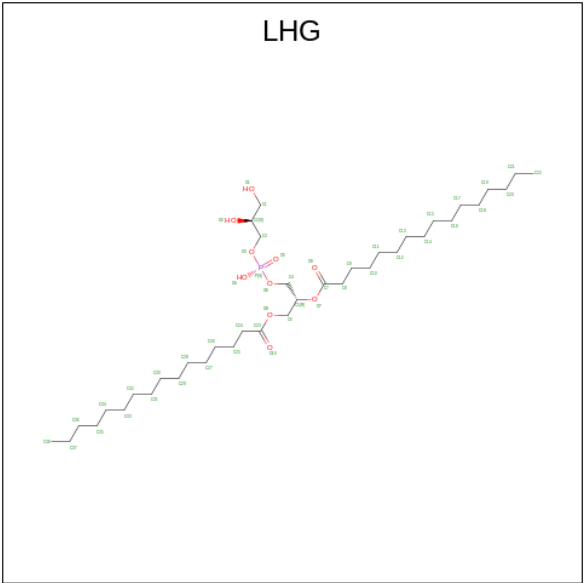
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	C	1	Total	C	O		0	0
			62	47	15			
37	C	1	Total	C	O		0	0
			62	47	15			
37	C	1	Total	C	O		0	0
			62	47	15			
37	D	1	Total	C	O		0	0
			52	42	10			
37	H	1	Total	C	O		0	0
			62	47	15			
37	c	1	Total	C	O		0	0
			62	47	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	d	1	Total	C	O	0	0
			50	41	9		
37	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 38 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
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			46	35	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		
38	L	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		

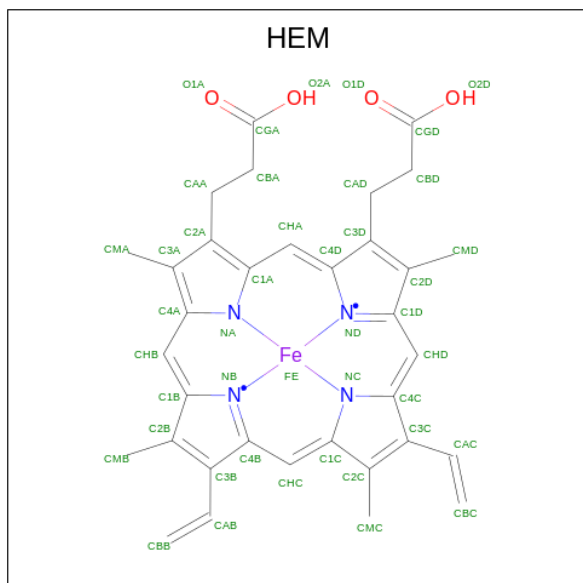
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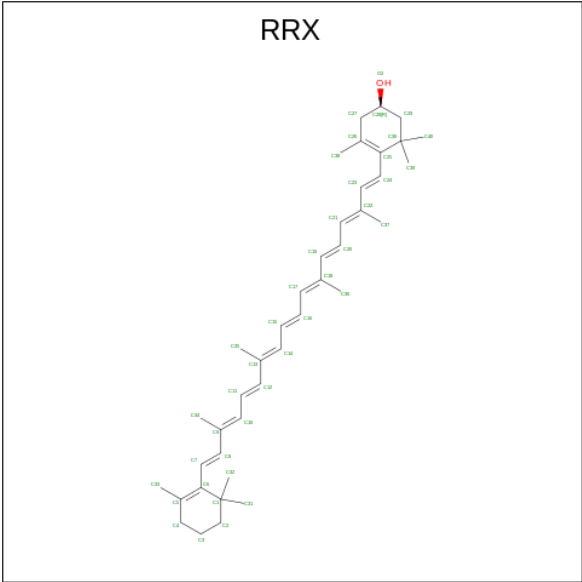
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	d	1	Total	C	O	P	0	0
			47	36	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 40 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).

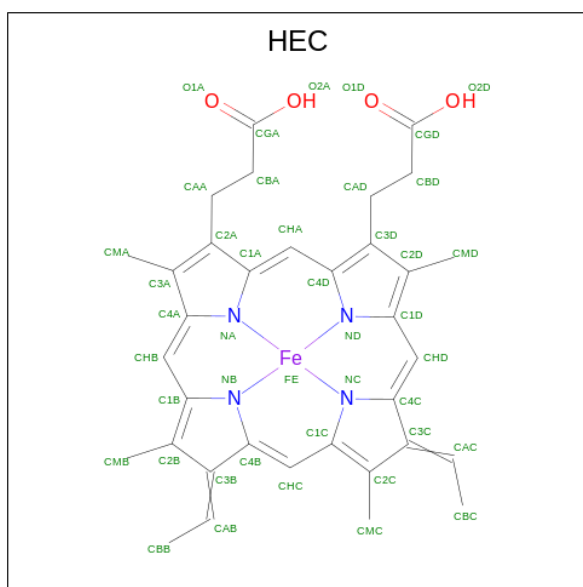


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	H	1	Total	C	O	0	0
			41	40	1		
40	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 42 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	158	Total	O		
			159	159	0	1
43	B	406	Total	O		
			411	411	0	6
43	C	293	Total	O		
			295	295	0	2
43	D	173	Total	O		
			177	177	0	4
43	E	35	Total	O		
			35	35	0	0
43	F	15	Total	O		
			15	15	0	0
43	H	51	Total	O		
			51	51	0	0
43	I	11	Total	O		
			11	11	0	0
43	J	15	Total	O		
			15	15	0	0
43	K	9	Total	O		
			9	9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	L	16	Total 16	O 16	0	0
43	M	20	Total 20	O 20	0	0
43	O	217	Total 224	O 224	0	7
43	T	14	Total 14	O 14	0	0
43	U	116	Total 117	O 117	0	1
43	V	153	Total 157	O 157	0	4
43	Y	6	Total 6	O 6	0	0
43	X	22	Total 22	O 22	0	0
43	Z	4	Total 4	O 4	0	0
43	a	157	Total 159	O 159	0	2
43	b	394	Total 399	O 399	0	5
43	c	316	Total 320	O 320	0	5
43	d	170	Total 172	O 172	0	2
43	e	38	Total 39	O 39	0	1
43	f	12	Total 12	O 12	0	0
43	h	51	Total 52	O 52	0	1
43	i	12	Total 12	O 12	0	0
43	j	12	Total 12	O 12	0	0
43	k	6	Total 6	O 6	0	0
43	l	20	Total 20	O 20	0	0
43	m	20	Total 20	O 20	0	0

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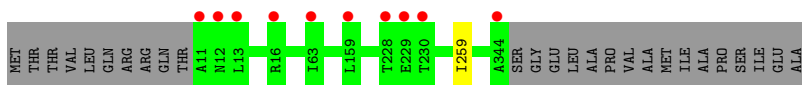
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	o	194	Total 198	O 198	0	4
43	t	23	Total 24	O 24	0	1
43	u	117	Total 119	O 119	0	2
43	v	116	Total 118	O 118	0	2
43	y	8	Total 8	O 8	0	0
43	x	14	Total 14	O 14	0	0
43	z	6	Total 6	O 6	0	0

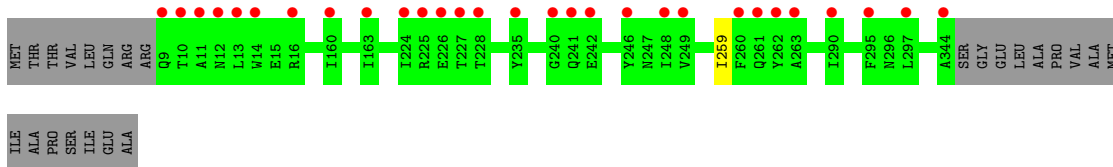
### 3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 2



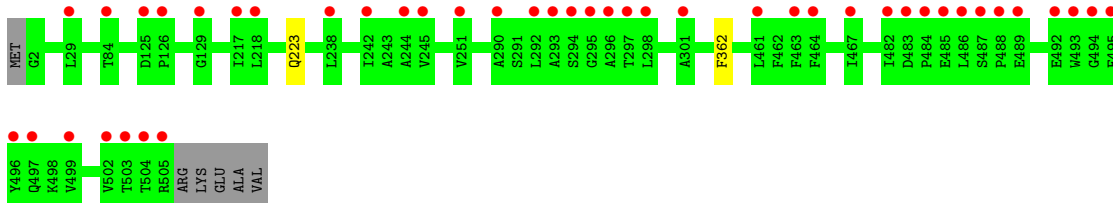
- Molecule 1: Photosystem II protein D1 2



- Molecule 2: Photosystem II CP47 reaction center protein

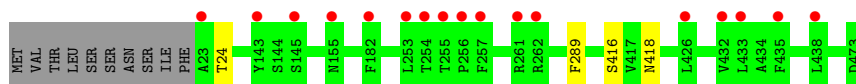


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein



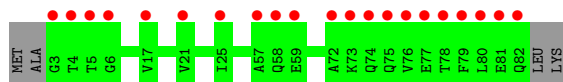
- Molecule 4: Photosystem II D2 protein



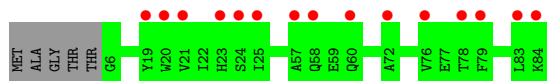
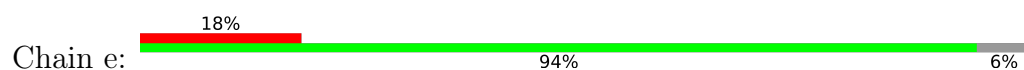
- Molecule 4: Photosystem II D2 protein



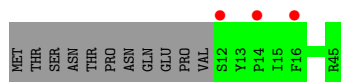
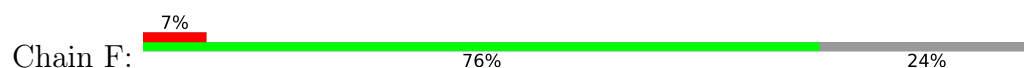
- Molecule 5: Cytochrome b559 subunit alpha



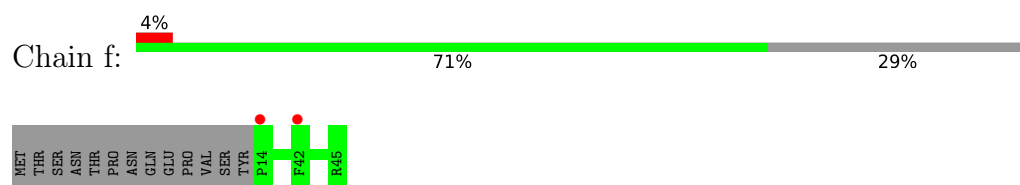
- Molecule 5: Cytochrome b559 subunit alpha



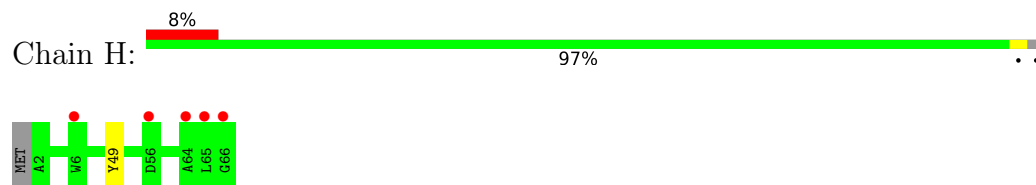
- Molecule 6: Cytochrome b559 subunit beta



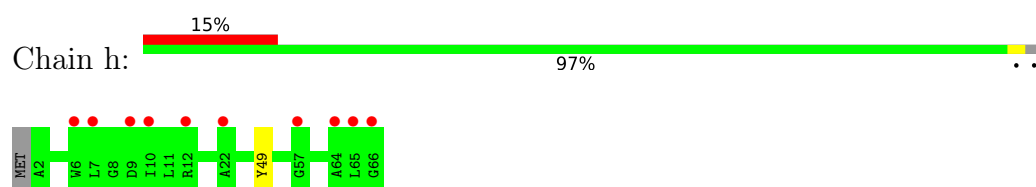
- Molecule 6: Cytochrome b559 subunit beta



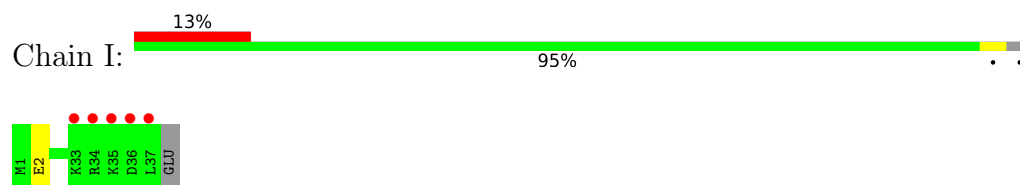
- Molecule 7: Photosystem II reaction center protein H



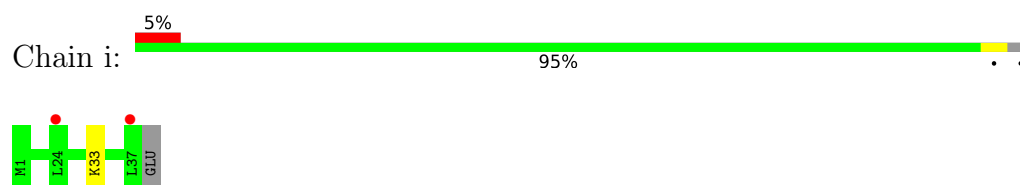
- Molecule 7: Photosystem II reaction center protein H



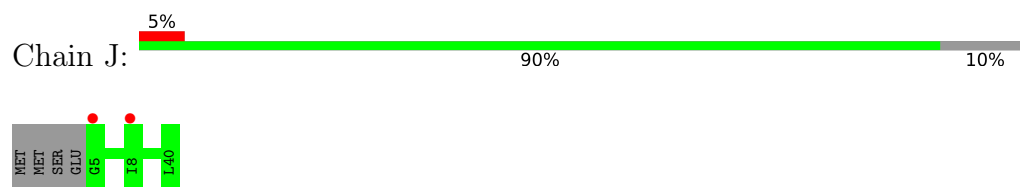
- Molecule 8: Photosystem II reaction center protein I



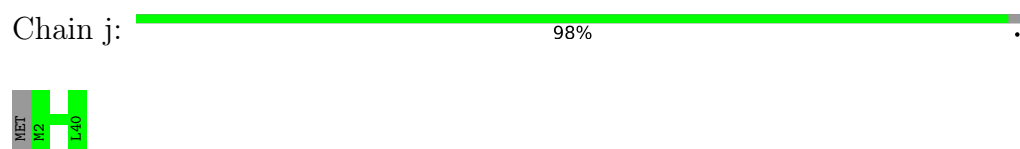
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

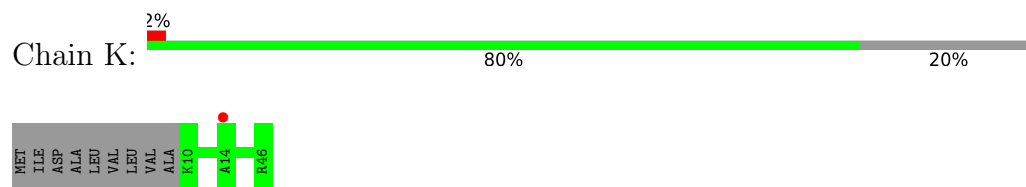


- Molecule 9: Photosystem II reaction center protein J

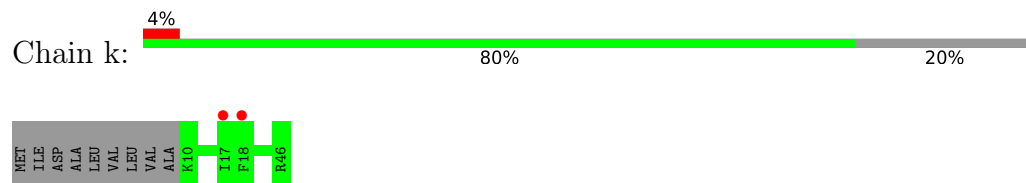




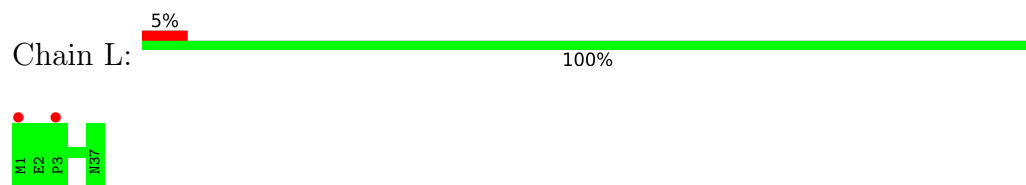
- Molecule 10: Photosystem II reaction center protein K



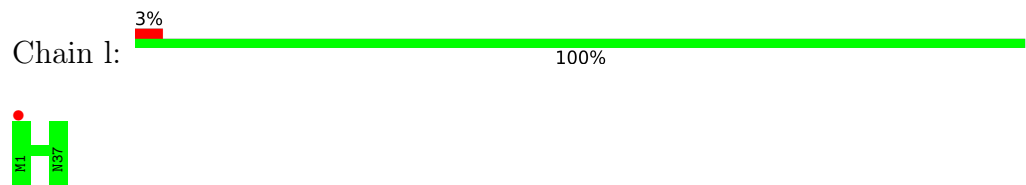
- Molecule 10: Photosystem II reaction center protein K



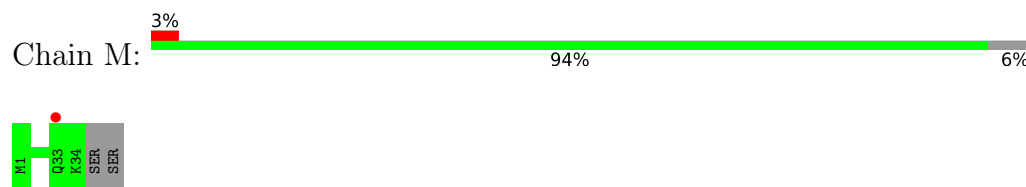
- Molecule 11: Photosystem II reaction center protein L



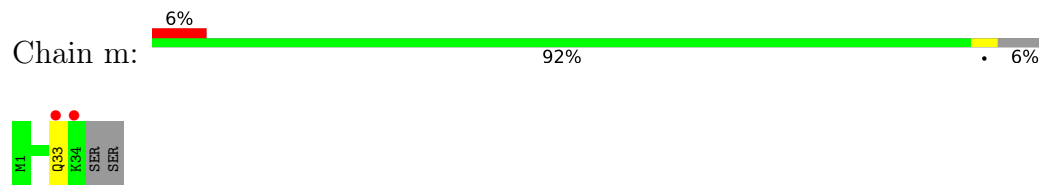
- Molecule 11: Photosystem II reaction center protein L



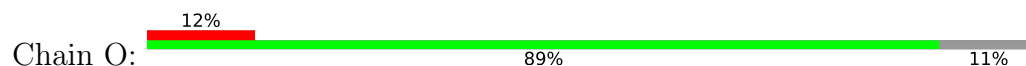
- Molecule 12: Photosystem II reaction center protein M

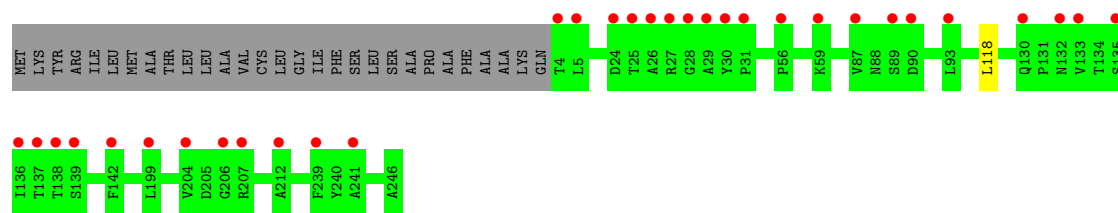


- Molecule 12: Photosystem II reaction center protein M

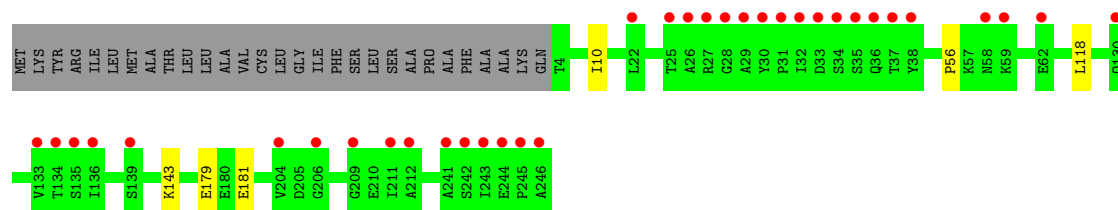
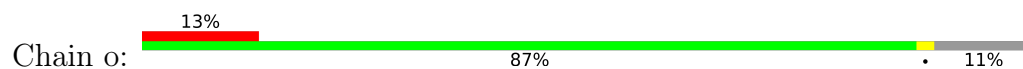


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

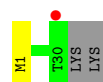




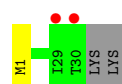
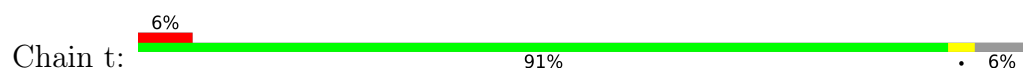
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



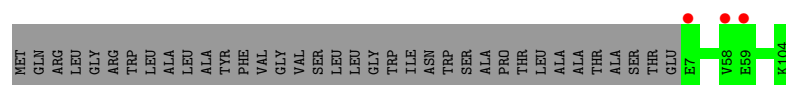
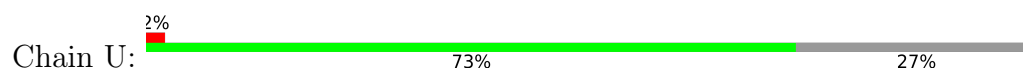
- Molecule 14: Photosystem II reaction center protein T



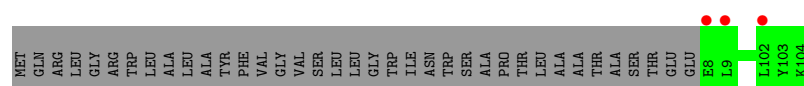
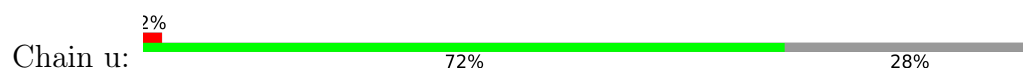
- Molecule 14: Photosystem II reaction center protein T



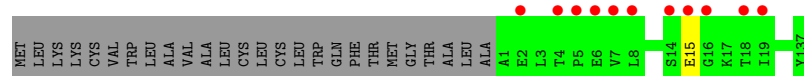
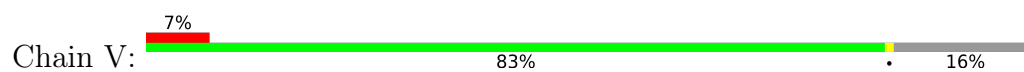
- Molecule 15: Photosystem II 12 kDa extrinsic protein



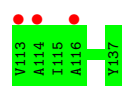
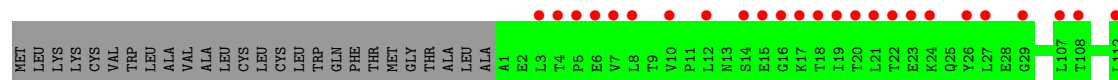
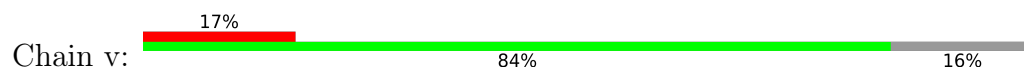
- Molecule 15: Photosystem II 12 kDa extrinsic protein



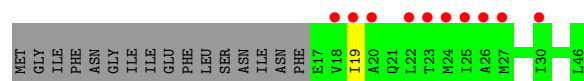
- Molecule 16: Cytochrome c-550



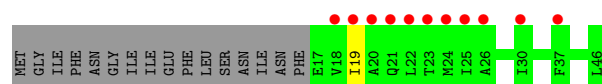
- Molecule 16: Cytochrome c-550



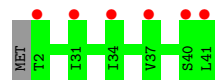
- Molecule 17: Photosystem II reaction center protein Ycf12



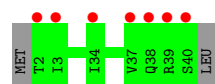
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

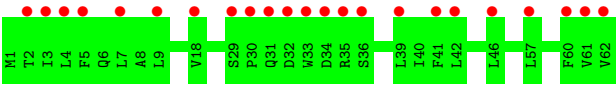


- Molecule 18: Photosystem II reaction center X protein

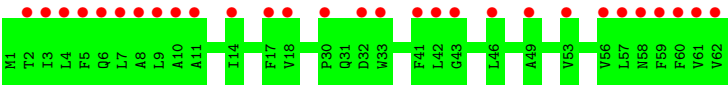


- Molecule 19: Photosystem II reaction center protein Z

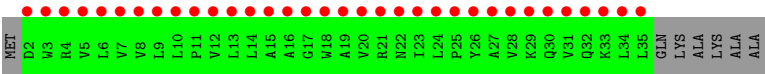
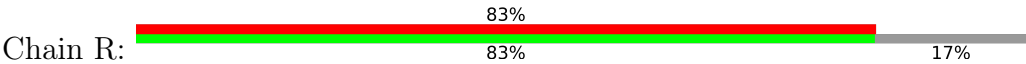




● Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.14Å 228.17Å 286.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 48.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.90) 99.8 (48.98-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.151 , 0.184 0.151 , 0.185	Depositor DCC
$R_{free}$ test set	31121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 73.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	55630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: CA, HEM, LMG, CLA, GOL, PHO, HTG, DMS, UNL, RRX, HEC, LMT, MG, SQD, BCT, CL, FE2, OEX, BCR, LHG, DGD, PL9, FME

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	0.45	0/2693	0.54	0/3680
1	a	0.43	0/2723	0.54	0/3719
2	B	0.42	0/4156	0.54	0/5665
2	b	0.41	0/4122	0.54	0/5623
3	C	0.39	0/3638	0.51	0/4954
3	c	0.39	0/3655	0.51	0/4976
4	D	0.48	0/2811	0.56	1/3833 (0.0%)
4	d	0.44	0/2825	0.54	1/3850 (0.0%)
5	E	0.37	0/651	0.49	0/892
5	e	0.32	0/669	0.49	0/913
6	F	0.36	0/284	0.46	0/387
6	f	0.37	0/274	0.44	0/372
7	H	0.36	0/518	0.51	0/706
7	h	0.32	0/532	0.48	0/723
8	I	0.31	0/298	0.43	0/403
8	i	0.33	0/294	0.47	0/398
9	J	0.36	0/257	0.47	0/349
9	j	0.33	0/276	0.49	0/374
10	K	0.34	0/299	0.43	0/412
10	k	0.33	0/299	0.45	0/412
11	L	0.47	0/324	0.53	0/441
11	l	0.48	0/315	0.48	0/428
12	M	0.41	0/266	0.53	0/363
12	m	0.39	0/270	0.51	0/368
13	O	0.37	0/1956	0.57	0/2653
13	o	0.38	0/1925	0.58	0/2611
14	T	0.48	0/266	0.53	0/362
14	t	0.42	0/266	0.52	0/362
15	U	0.40	0/778	0.55	0/1057
15	u	0.40	0/785	0.56	0/1064
16	V	0.39	0/1122	0.54	0/1522

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.32	0/1097	0.51	0/1491
17	Y	0.29	0/219	0.43	0/294
17	y	0.26	0/233	0.42	0/312
18	X	0.28	0/289	0.42	0/391
18	x	0.28	0/289	0.44	0/391
19	Z	0.31	0/459	0.39	0/630
19	z	0.29	0/456	0.37	0/626
20	R	0.26	0/232	0.46	0/321
All	All	0.40	0/42821	0.53	2/58328 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	272	LEU	CA-CB-CG	5.83	128.70	115.30
4	D	272	LEU	CA-CB-CG	5.05	126.93	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/360 (93%)	329 (98%)	4 (1%)	1 (0%)	41	31
1	a	337/360 (94%)	332 (98%)	4 (1%)	1 (0%)	41	31
2	B	511/510 (100%)	503 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	511/510 (100%)	503 (98%)	8 (2%)	0	100	100
3	C	455/461 (99%)	445 (98%)	8 (2%)	2 (0%)	34	24
3	c	457/461 (99%)	446 (98%)	10 (2%)	1 (0%)	47	38
4	D	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
4	d	342/352 (97%)	335 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	79 (100%)	0	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	251/272 (92%)	246 (98%)	5 (2%)	0	100	100
13	o	246/272 (90%)	241 (98%)	5 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	96/134 (72%)	93 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	139/163 (85%)	136 (98%)	3 (2%)	0	100	100
16	v	137/163 (84%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/46 (61%)	28 (100%)	0	0	100	100
17	y	29/46 (63%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	X	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5292/5691 (93%)	5194 (98%)	93 (2%)	5 (0%)	51	42

All (5) Ramachandran outliers are listed below:

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

### 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	266/290 (92%)	266 (100%)	0	100	100
1	a	271/290 (93%)	271 (100%)	0	100	100
2	B	405/407 (100%)	404 (100%)	1 (0%)	93	94
2	b	397/407 (98%)	395 (100%)	2 (0%)	88	89
3	C	357/362 (99%)	354 (99%)	3 (1%)	81	82
3	c	358/362 (99%)	355 (99%)	3 (1%)	81	82
4	D	275/283 (97%)	274 (100%)	1 (0%)	91	91
4	d	277/283 (98%)	275 (99%)	2 (1%)	84	84
5	E	65/73 (89%)	65 (100%)	0	100	100
5	e	68/73 (93%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	52/55 (94%)	51 (98%)	1 (2%)	57	53
7	h	54/55 (98%)	53 (98%)	1 (2%)	57	53
8	I	32/34 (94%)	31 (97%)	1 (3%)	40	32
8	i	31/34 (91%)	30 (97%)	1 (3%)	39	30
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	36/35 (103%)	36 (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	31/32 (97%)	30 (97%)	1 (3%)	39	30
13	O	211/228 (92%)	210 (100%)	1 (0%)	88	89
13	o	208/228 (91%)	201 (97%)	7 (3%)	37	28
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	81/112 (72%)	81 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	121/138 (88%)	119 (98%)	2 (2%)	60	57
16	v	117/138 (85%)	117 (100%)	0	100	100
17	Y	22/37 (60%)	21 (96%)	1 (4%)	27	18
17	y	24/37 (65%)	23 (96%)	1 (4%)	30	20
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	45/51 (88%)	45 (100%)	0	100	100
19	z	44/51 (86%)	44 (100%)	0	100	100
20	R	16/33 (48%)	16 (100%)	0	100	100
All	All	4289/4639 (92%)	4260 (99%)	29 (1%)	86	84

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	416	SER
13	o	181	GLU
4	d	180	ARG
13	o	143	LYS
4	d	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	332	GLN
17	y	21	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
14	FME	t	1	14	8,9,10	0.99	0	7,9,11	1.48	1 (14%)
12	FME	m	1	12	8,9,10	0.95	0	7,9,11	0.83	0
19	FME	Z	1	19	8,9,10	0.91	0	7,9,11	1.01	0
8	FME	I	1	8	8,9,10	0.91	0	7,9,11	0.97	0
14	FME	T	1	14	8,9,10	0.99	0	7,9,11	1.40	1 (14%)
19	FME	z	1	19	8,9,10	0.90	0	7,9,11	1.05	0
12	FME	M	1	12	8,9,10	1.00	0	7,9,11	0.47	0
8	FME	i	1	8	8,9,10	0.92	0	7,9,11	0.86	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	4/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
19	FME	Z	1	19	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
19	FME	z	1	19	-	2/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.59	114.41	109.73
14	t	1	FME	C-CA-N	2.11	113.55	109.73

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
19	Z	1	FME	CA-CB-CG-SD
14	t	1	FME	N-CA-CB-CG
14	t	1	FME	O-C-CA-CB
19	z	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 414 ligands modelled in this entry, 15 are monoatomic and 77 are unknown - leaving 322 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
34	DMS	c	931	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
24	CLA	b	615	-	65,73,73	2.46	18 (27%)	76,113,113	2.46	30 (39%)
26	BCR	b	621	-	41,41,41	0.74	0	56,56,56	1.47	9 (16%)
34	DMS	A	426	-	3,3,3	2.67	1 (33%)	3,3,3	0.61	0
34	DMS	v	208	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
28	LMG	c	920	-	51,51,55	0.94	2 (3%)	59,59,63	1.12	4 (6%)
34	DMS	u	201	-	3,3,3	2.66	1 (33%)	3,3,3	0.82	0
26	BCR	c	916	-	41,41,41	0.76	0	56,56,56	1.38	7 (12%)
34	DMS	O	302	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
24	CLA	B	616	-	65,73,73	2.44	18 (27%)	76,113,113	2.49	24 (31%)
31	LMT	c	922	-	36,36,36	0.50	1 (2%)	47,47,47	1.24	4 (8%)
34	DMS	O	305	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
37	DGD	c	918	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
24	CLA	C	504	43	65,73,73	2.35	19 (29%)	76,113,113	2.54	26 (34%)
26	BCR	k	103	-	41,41,41	0.72	0	56,56,56	1.30	6 (10%)
24	CLA	b	609	-	65,73,73	2.29	18 (27%)	76,113,113	2.62	25 (32%)
24	CLA	C	510	-	65,73,73	2.49	21 (32%)	76,113,113	2.51	30 (39%)
27	SQD	a	415	-	53,54,54	0.95	3 (5%)	62,65,65	1.68	11 (17%)
34	DMS	b	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
24	CLA	C	502	-	65,73,73	2.57	20 (30%)	76,113,113	2.49	26 (34%)
36	HTG	B	629	-	19,19,19	1.00	2 (10%)	23,24,24	1.46	3 (13%)
38	LHG	D	407	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
24	CLA	c	909	-	65,73,73	2.40	18 (27%)	76,113,113	2.65	27 (35%)
36	HTG	C	536	-	19,19,19	1.09	2 (10%)	23,24,24	1.29	1 (4%)
37	DGD	c	917	-	63,63,67	0.84	2 (3%)	77,77,81	1.13	4 (5%)
24	CLA	B	614	-	65,73,73	2.31	18 (27%)	76,113,113	2.57	28 (36%)
34	DMS	o	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.64	0
36	HTG	y	102	-	19,19,19	1.07	2 (10%)	23,24,24	1.19	1 (4%)
26	BCR	K	101	-	41,41,41	0.74	0	56,56,56	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	L	102	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
26	BCR	b	622	-	41,41,41	0.85	0	56,56,56	1.10	4 (7%)
24	CLA	a	410	43	65,73,73	2.29	20 (30%)	76,113,113	2.62	26 (34%)
34	DMS	d	418	-	3,3,3	2.66	1 (33%)	3,3,3	0.47	0
34	DMS	O	308	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
24	CLA	c	911	-	65,73,73	2.47	20 (30%)	76,113,113	2.42	23 (30%)
24	CLA	C	513	-	65,73,73	2.42	19 (29%)	76,113,113	2.44	25 (32%)
34	DMS	C	526	-	3,3,3	2.63	1 (33%)	3,3,3	0.40	0
24	CLA	a	413	-	65,73,73	2.20	19 (29%)	76,113,113	2.54	29 (38%)
34	DMS	B	633	-	3,3,3	2.60	1 (33%)	3,3,3	0.38	0
34	DMS	H	104	7	3,3,3	2.65	1 (33%)	3,3,3	0.56	0
38	LHG	D	406	-	48,48,48	0.82	2 (4%)	51,54,54	1.19	7 (13%)
24	CLA	d	404	-	65,73,73	2.56	20 (30%)	76,113,113	2.53	26 (34%)
34	DMS	b	645	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
34	DMS	C	535	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
26	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.32	5 (8%)
24	CLA	c	903	-	65,73,73	2.41	18 (27%)	76,113,113	2.43	24 (31%)
34	DMS	b	647	-	3,3,3	2.67	1 (33%)	3,3,3	0.60	0
34	DMS	b	638	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
31	LMT	A	417	-	36,36,36	0.47	0	47,47,47	1.19	3 (6%)
34	DMS	v	207	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
24	CLA	C	506	-	65,73,73	2.57	20 (30%)	76,113,113	2.45	26 (34%)
24	CLA	B	611	43	65,73,73	2.46	19 (29%)	76,113,113	2.52	27 (35%)
24	CLA	C	505	-	65,73,73	2.68	19 (29%)	76,113,113	2.26	20 (26%)
36	HTG	B	630	-	19,19,19	1.01	2 (10%)	23,24,24	1.35	3 (13%)
24	CLA	b	608	-	65,73,73	2.72	20 (30%)	76,113,113	2.54	25 (32%)
34	DMS	c	930	-	3,3,3	2.53	1 (33%)	3,3,3	0.36	0
34	DMS	o	306	-	3,3,3	2.70	1 (33%)	3,3,3	0.67	0
24	CLA	b	618	-	65,73,73	2.38	19 (29%)	76,113,113	2.60	26 (34%)
31	LMT	B	626	-	24,24,36	0.47	0	29,29,47	1.13	2 (6%)
24	CLA	b	610	-	65,73,73	2.48	18 (27%)	76,113,113	2.47	25 (32%)
34	DMS	a	422	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
32	GOL	O	304	-	5,5,5	0.82	0	5,5,5	1.06	0
37	DGD	D	405	-	52,52,67	0.92	2 (3%)	60,60,81	1.17	6 (10%)
34	DMS	a	420	-	3,3,3	2.51	1 (33%)	3,3,3	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
31	LMT	Z	101	-	36,36,36	0.42	0	47,47,47	0.91	1 (2%)
34	DMS	i	106	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
24	CLA	C	508	-	65,73,73	2.53	18 (27%)	76,113,113	2.45	25 (32%)
24	CLA	d	401	43	65,73,73	2.34	17 (26%)	76,113,113	2.65	29 (38%)
34	DMS	c	934	-	3,3,3	2.69	1 (33%)	3,3,3	0.54	0
34	DMS	b	639	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
38	LHG	l	103	-	48,48,48	0.89	2 (4%)	51,54,54	1.04	5 (9%)
31	LMT	j	102	-	24,24,36	0.54	1 (4%)	29,29,47	0.90	0
34	DMS	A	425	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
25	PHO	A	409	-	51,69,69	1.89	7 (13%)	47,99,99	1.83	8 (17%)
34	DMS	U	204	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
34	DMS	A	423	-	3,3,3	2.42	1 (33%)	3,3,3	0.73	0
34	DMS	o	302	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
32	GOL	a	419	-	5,5,5	1.11	0	5,5,5	0.65	0
34	DMS	V	209	-	3,3,3	2.60	1 (33%)	3,3,3	0.58	0
34	DMS	C	529	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.07	3 (6%)
24	CLA	c	904	-	65,73,73	2.72	20 (30%)	76,113,113	2.27	26 (34%)
31	LMT	M	101	-	36,36,36	0.39	0	47,47,47	0.81	1 (2%)
34	DMS	C	524	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
26	BCR	a	414	-	41,41,41	0.79	0	56,56,56	1.28	4 (7%)
24	CLA	b	614	43	65,73,73	2.29	19 (29%)	76,113,113	2.44	25 (32%)
26	BCR	B	620	-	41,41,41	0.68	0	56,56,56	1.24	7 (12%)
27	SQD	A	412	-	53,54,54	0.96	3 (5%)	62,65,65	1.69	12 (19%)
36	HTG	B	624	-	19,19,19	0.78	1 (5%)	23,24,24	1.44	2 (8%)
34	DMS	b	631	-	3,3,3	2.38	1 (33%)	3,3,3	0.42	0
31	LMT	M	102	-	25,25,36	0.48	0	30,30,47	0.93	1 (3%)
37	DGD	c	919	-	63,63,67	0.84	2 (3%)	77,77,81	0.96	4 (5%)
24	CLA	B	609	-	65,73,73	2.44	19 (29%)	76,113,113	2.36	24 (31%)
34	DMS	O	313	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
34	DMS	e	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
24	CLA	B	603	-	65,73,73	2.36	19 (29%)	76,113,113	2.63	29 (38%)
34	DMS	C	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
34	DMS	c	932	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	D	403	-	41,41,41	0.83	0	56,56,56	1.68	9 (16%)
24	CLA	b	617	-	65,73,73	2.49	19 (29%)	76,113,113	2.54	25 (32%)
31	LMT	c	927	-	36,36,36	0.43	0	47,47,47	0.89	3 (6%)
34	DMS	c	935	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
24	CLA	B	602	43	65,73,73	2.39	21 (32%)	76,113,113	2.42	26 (34%)
28	LMG	a	416	-	51,51,55	0.95	3 (5%)	59,59,63	1.29	9 (15%)
28	LMG	c	921	-	51,51,55	0.96	2 (3%)	59,59,63	1.20	6 (10%)
28	LMG	b	624	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
31	LMT	m	103	-	36,36,36	0.40	0	47,47,47	0.81	2 (4%)
24	CLA	C	509	-	65,73,73	2.49	20 (30%)	76,113,113	2.46	26 (34%)
36	HTG	b	602	-	19,19,19	1.02	2 (10%)	23,24,24	1.38	3 (13%)
29	PL9	d	407	-	55,55,55	0.76	1 (1%)	68,69,69	1.51	13 (19%)
36	HTG	c	941	-	19,19,19	1.00	1 (5%)	23,24,24	1.84	5 (21%)
36	HTG	B	623	-	19,19,19	1.09	1 (5%)	23,24,24	1.24	1 (4%)
24	CLA	c	910	-	65,73,73	2.44	19 (29%)	76,113,113	2.49	28 (36%)
24	CLA	B	606	-	65,73,73	2.35	20 (30%)	76,113,113	2.50	26 (34%)
27	SQD	b	601	-	53,54,54	1.05	4 (7%)	62,65,65	1.61	12 (19%)
34	DMS	b	641	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
24	CLA	b	607	-	65,73,73	2.43	20 (30%)	76,113,113	2.46	25 (32%)
34	DMS	V	214	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
24	CLA	B	605	-	65,73,73	2.33	20 (30%)	76,113,113	2.55	24 (31%)
24	CLA	c	905	43	65,73,73	2.24	20 (30%)	76,113,113	2.65	29 (38%)
37	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.89	3 (3%)
34	DMS	y	101	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
24	CLA	c	907	-	65,73,73	2.49	20 (30%)	76,113,113	2.46	24 (31%)
31	LMT	e	101	-	24,24,36	0.46	0	29,29,47	0.64	0
34	DMS	o	304	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
40	RRX	H	101	-	42,42,42	0.71	0	57,58,58	1.34	7 (12%)
40	RRX	h	101	-	42,42,42	0.73	0	57,58,58	1.30	7 (12%)
36	HTG	C	520	-	19,19,19	1.01	2 (10%)	23,24,24	1.29	1 (4%)
24	CLA	c	906	-	65,73,73	2.39	18 (27%)	76,113,113	2.36	25 (32%)
34	DMS	a	424	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
36	HTG	U	201	-	3,3,19	0.34	0	2,2,24	0.71	0
31	LMT	A	421	-	36,36,36	0.43	0	47,47,47	0.99	1 (2%)
28	LMG	d	412	41	51,51,55	0.90	2 (3%)	59,59,63	0.89	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	c	928	-	19,19,19	1.07	2 (10%)	23,24,24	1.49	3 (13%)
34	DMS	O	314	-	3,3,3	2.67	1 (33%)	3,3,3	0.64	0
27	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.11	3 (4%)
34	DMS	b	643	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
28	LMG	B	621	-	51,51,55	0.95	2 (3%)	59,59,63	1.11	5 (8%)
34	DMS	B	642	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
26	BCR	C	515	-	41,41,41	0.71	0	56,56,56	1.45	7 (12%)
28	LMG	C	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.19	6 (10%)
34	DMS	o	305	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
34	DMS	b	632	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
34	DMS	B	641	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
34	DMS	d	415	-	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
36	HTG	O	316	-	19,19,19	0.89	2 (10%)	23,24,24	1.29	2 (8%)
32	GOL	A	419	-	5,5,5	0.99	0	5,5,5	1.00	0
26	BCR	c	915	-	41,41,41	0.74	0	56,56,56	1.37	6 (10%)
34	DMS	B	644	-	3,3,3	2.59	1 (33%)	3,3,3	0.32	0
34	DMS	c	937	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
34	DMS	d	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
24	CLA	a	409	-	65,73,73	2.41	20 (30%)	76,113,113	2.53	26 (34%)
32	GOL	B	637	-	5,5,5	0.95	0	5,5,5	0.90	0
34	DMS	v	209	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
38	LHG	D	408	-	45,45,48	0.90	2 (4%)	48,51,54	0.95	4 (8%)
26	BCR	B	636	-	41,41,41	0.72	0	56,56,56	1.58	12 (21%)
36	HTG	d	420	-	19,19,19	1.01	2 (10%)	23,24,24	1.45	2 (8%)
34	DMS	B	643	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
34	DMS	D	415	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
25	PHO	A	408	-	51,69,69	1.75	7 (13%)	47,99,99	1.66	9 (19%)
36	HTG	d	414	-	19,19,19	1.04	2 (10%)	23,24,24	1.70	3 (13%)
31	LMT	a	402	-	36,36,36	0.42	0	47,47,47	1.13	4 (8%)
31	LMT	b	625	-	36,36,36	0.40	0	47,47,47	1.27	6 (12%)
33	BCT	A	422	22	2,3,3	0.64	0	2,3,3	0.61	0
34	DMS	h	105	-	3,3,3	2.65	1 (33%)	3,3,3	0.37	0
31	LMT	F	103	-	24,24,36	0.45	0	29,29,47	0.58	0
26	BCR	T	101	-	41,41,41	0.71	0	56,56,56	1.69	12 (21%)
24	CLA	c	912	3	65,73,73	2.39	18 (27%)	76,113,113	2.42	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	V	215	-	19,19,19	1.03	1 (5%)	23,24,24	2.17	3 (13%)
21	OEX	A	401	1,43,3	0,15,15	-	-	-		
38	LHG	d	411	-	46,46,48	0.88	2 (4%)	49,52,54	1.02	4 (8%)
24	CLA	b	619	-	65,73,73	2.43	20 (30%)	76,113,113	2.39	27 (35%)
37	DGD	C	516	-	63,63,67	0.83	3 (4%)	77,77,81	1.10	5 (6%)
34	DMS	C	534	-	3,3,3	2.65	1 (33%)	3,3,3	0.42	0
24	CLA	B	613	-	65,73,73	2.32	20 (30%)	76,113,113	2.40	21 (27%)
26	BCR	A	411	-	41,41,41	0.77	0	56,56,56	1.35	4 (7%)
24	CLA	B	612	-	65,73,73	2.46	16 (24%)	76,113,113	2.62	29 (38%)
34	DMS	O	315	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
24	CLA	C	501	-	65,73,73	2.32	19 (29%)	76,113,113	2.50	24 (31%)
21	OEX	a	404	1,43,3	0,15,15	-	-	-		
24	CLA	b	606	-	65,73,73	2.49	20 (30%)	76,113,113	2.50	28 (36%)
34	DMS	o	303	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
32	GOL	V	207	-	5,5,5	1.02	0	5,5,5	0.86	0
34	DMS	c	926	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
29	PL9	A	414	-	55,55,55	0.60	1 (1%)	68,69,69	1.90	20 (29%)
39	HEM	F	102	6,5	41,50,50	1.90	6 (14%)	45,82,82	1.71	7 (15%)
42	HEC	v	202	16	32,50,50	2.33	6 (18%)	24,82,82	1.64	5 (20%)
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.49	6 (11%)
32	GOL	V	206	-	5,5,5	0.85	0	5,5,5	0.96	0
34	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
34	DMS	O	311	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
34	DMS	b	646	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
24	CLA	A	406	43	65,73,73	2.34	20 (30%)	76,113,113	2.69	24 (31%)
34	DMS	D	416	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
34	DMS	c	933	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
37	DGD	H	102	-	63,63,67	0.89	3 (4%)	77,77,81	0.99	7 (9%)
34	DMS	b	644	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
24	CLA	D	402	-	65,73,73	2.27	19 (29%)	76,113,113	2.49	25 (32%)
26	BCR	d	406	-	41,41,41	0.82	0	56,56,56	1.71	10 (17%)
33	BCT	d	402[B]	22	2,3,3	0.68	0	2,3,3	0.47	0
32	GOL	c	929	-	5,5,5	1.00	0	5,5,5	0.93	0
34	DMS	A	427	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
24	CLA	B	607	-	65,73,73	2.52	20 (30%)	76,113,113	2.49	27 (35%)
34	DMS	B	639	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	C	530	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
34	DMS	B	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
34	DMS	O	312	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
24	CLA	d	405	-	65,73,73	2.29	20 (30%)	76,113,113	2.60	26 (34%)
24	CLA	A	407	43	65,73,73	2.16	20 (30%)	76,113,113	2.65	26 (34%)
31	LMT	m	102	-	36,36,36	0.44	0	47,47,47	0.87	0
36	HTG	V	204	-	12,13,19	0.61	0	16,18,24	2.11	5 (31%)
34	DMS	V	201	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
36	HTG	d	419	-	19,19,19	1.05	2 (10%)	23,24,24	1.27	1 (4%)
36	HTG	D	412	-	19,19,19	1.05	2 (10%)	23,24,24	1.46	3 (13%)
37	DGD	C	518	-	63,63,67	0.82	2 (3%)	77,77,81	0.99	4 (5%)
34	DMS	u	202	-	3,3,3	2.61	1 (33%)	3,3,3	0.72	0
42	HEC	V	203	16	32,50,50	2.16	6 (18%)	24,82,82	1.85	5 (20%)
27	SQD	l	101	-	53,54,54	1.03	4 (7%)	62,65,65	1.35	5 (8%)
34	DMS	O	309	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
24	CLA	C	507	43	65,73,73	2.56	20 (30%)	76,113,113	2.51	25 (32%)
34	DMS	e	102	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
24	CLA	C	503	-	65,73,73	2.70	19 (29%)	76,113,113	2.37	22 (28%)
36	HTG	C	521	-	19,19,19	1.05	2 (10%)	23,24,24	1.50	2 (8%)
24	CLA	c	908	43	65,73,73	2.51	20 (30%)	76,113,113	2.59	28 (36%)
24	CLA	B	604	-	65,73,73	2.33	20 (30%)	76,113,113	2.62	26 (34%)
31	LMT	B	622	-	36,36,36	0.43	0	47,47,47	1.58	10 (21%)
34	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	0.49	0
27	SQD	F	101	-	36,37,54	0.95	2 (5%)	44,47,65	1.94	9 (20%)
34	DMS	V	213	-	3,3,3	2.67	1 (33%)	3,3,3	0.63	0
38	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	5 (9%)
34	DMS	B	647	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
36	HTG	b	627	-	19,19,19	1.11	2 (10%)	23,24,24	1.71	3 (13%)
34	DMS	c	938	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
24	CLA	B	610	-	65,73,73	2.57	18 (27%)	76,113,113	2.37	24 (31%)
24	CLA	A	410	-	65,73,73	2.22	18 (27%)	76,113,113	2.62	26 (34%)
36	HTG	c	942	-	19,19,19	1.02	2 (10%)	23,24,24	1.32	4 (17%)
36	HTG	O	303	-	19,19,19	1.09	1 (5%)	23,24,24	1.15	2 (8%)
34	DMS	B	634	-	3,3,3	2.69	1 (33%)	3,3,3	0.73	0
34	DMS	V	205	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	v	204	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
24	CLA	B	608	43	65,73,73	2.27	18 (27%)	76,113,113	2.44	23 (30%)
34	DMS	D	413	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
34	DMS	D	414	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
38	LHG	d	410	-	48,48,48	0.86	2 (4%)	51,54,54	0.91	3 (5%)
24	CLA	c	914	-	65,73,73	2.55	19 (29%)	76,113,113	2.33	25 (32%)
34	DMS	a	423	-	3,3,3	2.68	1 (33%)	3,3,3	0.66	0
26	BCR	Y	101	-	41,41,41	0.78	0	56,56,56	1.53	10 (17%)
25	PHO	a	412	-	51,69,69	1.80	8 (15%)	47,99,99	1.80	8 (17%)
34	DMS	U	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
24	CLA	C	512	-	65,73,73	2.58	19 (29%)	76,113,113	2.39	27 (35%)
26	BCR	k	102	-	41,41,41	0.76	0	56,56,56	1.54	8 (14%)
36	HTG	C	537	-	19,19,19	0.99	2 (10%)	23,24,24	1.48	3 (13%)
29	PL9	a	417	-	55,55,55	0.62	1 (1%)	68,69,69	1.80	17 (25%)
34	DMS	O	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
29	PL9	D	404	-	55,55,55	0.72	1 (1%)	68,69,69	1.58	14 (20%)
34	DMS	V	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.64	0
26	BCR	B	619	-	41,41,41	0.88	0	56,56,56	1.15	6 (10%)
36	HTG	B	631	-	19,19,19	0.98	1 (5%)	23,24,24	1.77	2 (8%)
34	DMS	a	425	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
32	GOL	B	638	-	5,5,5	1.06	0	5,5,5	1.20	1 (20%)
34	DMS	B	632	-	3,3,3	2.45	1 (33%)	3,3,3	0.38	0
34	DMS	b	642	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
34	DMS	e	103	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
26	BCR	C	514	-	41,41,41	0.74	0	56,56,56	1.35	7 (12%)
36	HTG	b	626	-	19,19,19	0.85	1 (5%)	23,24,24	1.28	3 (13%)
34	DMS	v	205	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
34	DMS	K	102	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
34	DMS	C	532	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
34	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
37	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.06	6 (7%)
28	LMG	A	413	-	51,51,55	0.95	2 (3%)	59,59,63	1.16	6 (10%)
34	DMS	T	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
24	CLA	b	620	-	65,73,73	2.50	18 (27%)	76,113,113	2.55	26 (34%)
24	CLA	c	913	-	65,73,73	2.60	19 (29%)	76,113,113	2.51	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	V	211	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
34	DMS	d	416	-	3,3,3	2.66	1 (33%)	3,3,3	0.43	0
24	CLA	D	401	-	65,73,73	2.19	20 (30%)	76,113,113	2.74	25 (32%)
24	CLA	C	511	3	65,73,73	2.55	18 (27%)	76,113,113	2.41	26 (34%)
38	LHG	L	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.12	3 (5%)
34	DMS	V	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
24	CLA	b	605	43	65,73,73	2.51	19 (29%)	76,113,113	2.38	26 (34%)
34	DMS	v	210	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	v	206	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
34	DMS	c	939	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
25	PHO	a	411	-	51,69,69	1.70	7 (13%)	47,99,99	1.72	10 (21%)
37	DGD	d	408	-	50,50,67	0.95	2 (4%)	58,58,81	1.38	8 (13%)
28	LMG	C	523	-	51,51,55	0.94	2 (3%)	59,59,63	1.27	8 (13%)
34	DMS	U	203	-	3,3,3	2.68	1 (33%)	3,3,3	0.86	0
31	LMT	J	102	-	24,24,36	0.51	0	29,29,47	0.76	0
24	CLA	B	617	-	65,73,73	2.40	19 (29%)	76,113,113	2.58	27 (35%)
34	DMS	c	936	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
31	LMT	t	101	-	23,23,36	0.46	0	26,27,47	1.00	1 (3%)
24	CLA	b	616	-	65,73,73	2.24	18 (27%)	76,113,113	2.64	25 (32%)
36	HTG	c	924	-	19,19,19	1.04	2 (10%)	23,24,24	1.30	2 (8%)
27	SQD	A	416	-	53,54,54	1.04	3 (5%)	62,65,65	1.11	5 (8%)
24	CLA	c	902	-	65,73,73	2.46	18 (27%)	76,113,113	2.67	27 (35%)
28	LMG	D	409	41	51,51,55	0.83	2 (3%)	59,59,63	0.90	4 (6%)
24	CLA	B	615	-	65,73,73	2.20	18 (27%)	76,113,113	2.64	27 (35%)
24	CLA	b	613	-	65,73,73	2.58	21 (32%)	76,113,113	2.31	23 (30%)
24	CLA	b	612	-	65,73,73	2.77	20 (30%)	76,113,113	2.40	23 (30%)
34	DMS	A	424	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
34	DMS	v	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.40	0
34	DMS	a	421	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
32	GOL	C	525	-	5,5,5	0.92	0	5,5,5	0.97	0
34	DMS	C	533	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
34	DMS	O	306	-	3,3,3	2.67	1 (33%)	3,3,3	0.47	0
36	HTG	b	603	-	19,19,19	1.02	2 (10%)	23,24,24	1.40	3 (13%)
26	BCR	b	623	-	41,41,41	0.76	1 (2%)	56,56,56	1.46	13 (23%)
36	HTG	c	923	-	19,19,19	1.03	2 (10%)	23,24,24	1.53	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	B	625	-	19,19,19	1.01	1 (5%)	23,24,24	1.94	4 (17%)
31	LMT	t	102	-	36,36,36	0.43	0	47,47,47	0.85	1 (2%)
36	HTG	v	211	-	19,19,19	1.06	2 (10%)	23,24,24	1.63	4 (17%)
33	BCT	a	408[A]	22	2,3,3	0.65	0	2,3,3	0.75	0
34	DMS	B	646	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
36	HTG	c	943	-	17,17,19	1.05	2 (11%)	21,22,24	1.42	1 (4%)
34	DMS	c	940	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
24	CLA	A	405	-	65,73,73	2.56	18 (27%)	76,113,113	2.47	25 (32%)
24	CLA	b	611	43	65,73,73	2.31	19 (29%)	76,113,113	2.41	25 (32%)
39	HEM	f	101	6,5	41,50,50	1.95	8 (19%)	45,82,82	1.68	8 (17%)
32	GOL	b	637	-	5,5,5	0.91	0	5,5,5	0.97	0
34	DMS	O	310	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0

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
36	HTG	c	942	-	-	2/10/30/30	0/1/1/1
26	BCR	T	101	-	-	2/29/63/63	0/2/2/2
24	CLA	b	615	-	1/1/15/20	2/37/115/115	-
32	GOL	a	419	-	-	2/4/4/4	-
24	CLA	c	912	3	-	0/37/115/115	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
36	HTG	O	303	-	-	2/10/30/30	0/1/1/1
36	HTG	V	215	-	-	1/10/30/30	0/1/1/1
38	LHG	E	101	-	-	10/46/46/53	-
24	CLA	B	608	43	1/1/15/20	1/37/115/115	-
24	CLA	c	904	-	1/1/15/20	4/37/115/115	-
31	LMT	M	101	-	-	3/21/61/61	0/2/2/2
38	LHG	d	411	-	-	9/51/51/53	-
38	LHG	d	410	-	-	11/53/53/53	-
24	CLA	c	914	-	1/1/15/20	3/37/115/115	-
24	CLA	b	619	-	1/1/15/20	7/37/115/115	-
28	LMG	c	920	-	-	8/46/66/70	0/1/1/1
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
26	BCR	a	414	-	-	1/29/63/63	0/2/2/2
24	CLA	b	614	43	1/1/15/20	3/37/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	BCR	c	916	-	-	3/29/63/63	0/2/2/2
27	SQD	A	412	-	-	9/49/69/69	0/1/1/1
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
24	CLA	B	613	-	1/1/15/20	2/37/115/115	-
26	BCR	A	411	-	-	1/29/63/63	0/2/2/2
25	PHO	a	412	-	-	1/37/103/103	0/5/6/6
24	CLA	B	612	-	1/1/15/20	2/37/115/115	-
31	LMT	M	102	-	-	7/17/37/61	0/1/1/2
24	CLA	B	616	-	1/1/15/20	10/37/115/115	-
24	CLA	C	512	-	1/1/15/20	5/37/115/115	-
37	DGD	c	919	-	-	9/51/91/95	0/2/2/2
31	LMT	c	922	-	-	7/21/61/61	0/2/2/2
24	CLA	C	501	-	1/1/15/20	3/37/115/115	-
24	CLA	B	609	-	-	2/37/115/115	-
24	CLA	b	606	-	1/1/15/20	8/37/115/115	-
26	BCR	k	102	-	-	4/29/63/63	0/2/2/2
36	HTG	C	537	-	-	2/10/30/30	0/1/1/1
37	DGD	c	918	-	-	16/51/91/95	0/2/2/2
24	CLA	C	504	43	1/1/15/20	5/37/115/115	-
26	BCR	k	103	-	-	1/29/63/63	0/2/2/2
24	CLA	b	609	-	1/1/15/20	2/37/115/115	-
29	PL9	a	417	-	-	11/53/73/73	0/1/1/1
32	GOL	V	207	-	-	1/4/4/4	-
24	CLA	B	603	-	1/1/15/20	4/37/115/115	-
24	CLA	C	510	-	1/1/15/20	4/37/115/115	-
29	PL9	D	404	-	-	2/53/73/73	0/1/1/1
27	SQD	a	415	-	-	6/49/69/69	0/1/1/1
29	PL9	A	414	-	-	10/53/73/73	0/1/1/1
24	CLA	C	502	-	-	3/37/115/115	-
36	HTG	c	923	-	-	1/10/30/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
39	HEM	F	102	6,5	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	B	631	-	-	1/10/30/30	0/1/1/1
26	BCR	D	403	-	-	7/29/63/63	0/2/2/2
42	HEC	v	202	16	-	2/10/54/54	-
36	HTG	B	629	-	-	2/10/30/30	0/1/1/1
32	GOL	B	638	-	-	4/4/4/4	-
24	CLA	b	617	-	1/1/15/20	2/37/115/115	-
31	LMT	c	927	-	-	11/21/61/61	0/2/2/2
38	LHG	D	407	-	-	5/53/53/53	-
27	SQD	f	102	-	-	16/38/58/69	0/1/1/1
24	CLA	c	909	-	1/1/15/20	8/37/115/115	-
32	GOL	V	206	-	-	4/4/4/4	-
36	HTG	C	536	-	-	1/10/30/30	0/1/1/1
24	CLA	B	602	43	1/1/15/20	12/37/115/115	-
37	DGD	c	917	-	-	13/51/91/95	0/2/2/2
24	CLA	B	614	-	1/1/15/20	6/37/115/115	-
28	LMG	a	416	-	-	18/46/66/70	0/1/1/1
28	LMG	c	921	-	-	1/46/66/70	0/1/1/1
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
28	LMG	b	624	-	-	11/46/66/70	0/1/1/1
31	LMT	m	103	-	-	2/21/61/61	0/2/2/2
36	HTG	b	626	-	-	2/10/30/30	0/1/1/1
24	CLA	C	509	-	1/1/15/20	7/37/115/115	-
36	HTG	b	602	-	-	2/10/30/30	0/1/1/1
29	PL9	d	407	-	-	7/53/73/73	0/1/1/1
36	HTG	y	102	-	-	3/10/30/30	0/1/1/1
36	HTG	c	941	-	-	1/10/30/30	0/1/1/1
36	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	c	910	-	1/1/15/20	8/37/115/115	-
24	CLA	B	606	-	1/1/15/20	3/37/115/115	-
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
24	CLA	A	406	43	-	5/37/115/115	-
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	CLA	a	410	43	-	6/37/115/115	-
27	SQD	b	601	-	-	17/49/69/69	0/1/1/1
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	C	517	-	-	15/51/91/95	0/2/2/2
24	CLA	b	607	-	1/1/15/20	3/37/115/115	-
24	CLA	B	605	-	1/1/15/20	1/37/115/115	-
24	CLA	c	905	43	1/1/15/20	5/37/115/115	-
28	LMG	A	413	-	-	16/46/66/70	0/1/1/1
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2
24	CLA	c	907	-	1/1/15/20	8/37/115/115	-
24	CLA	b	620	-	1/1/15/20	6/37/115/115	-
24	CLA	c	911	-	1/1/15/20	2/37/115/115	-
24	CLA	c	913	-	1/1/15/20	3/37/115/115	-
31	LMT	e	101	-	-	3/15/35/61	0/1/1/2
24	CLA	D	402	-	1/1/15/20	5/37/115/115	-
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
24	CLA	C	513	-	-	6/37/115/115	-
40	RRX	H	101	-	-	3/29/65/65	0/2/2/2
40	RRX	h	101	-	-	2/29/65/65	0/2/2/2
24	CLA	D	401	-	1/1/15/20	3/37/115/115	-
24	CLA	c	906	-	1/1/15/20	4/37/115/115	-
36	HTG	C	520	-	-	3/10/30/30	0/1/1/1
24	CLA	C	511	3	1/1/15/20	3/37/115/115	-
32	GOL	c	929	-	-	2/4/4/4	-
38	LHG	L	101	-	-	14/53/53/53	-
24	CLA	b	605	43	1/1/15/20	5/37/115/115	-
24	CLA	B	607	-	1/1/15/20	7/37/115/115	-
24	CLA	a	413	-	1/1/15/20	7/37/115/115	-
38	LHG	D	406	-	-	9/53/53/53	-
24	CLA	d	404	-	1/1/15/20	4/37/115/115	-
36	HTG	U	201	-	-	0/1/1/30	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	c	903	-	1/1/15/20	5/37/115/115	-
31	LMT	A	421	-	-	8/21/61/61	0/2/2/2
28	LMG	d	412	41	-	8/46/66/70	0/1/1/1
36	HTG	c	928	-	-	0/10/30/30	0/1/1/1
27	SQD	a	401	-	-	19/49/69/69	0/1/1/1
25	PHO	a	411	-	-	4/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	d	408	-	-	20/44/64/95	0/1/1/2
28	LMG	C	523	-	-	9/46/66/70	0/1/1/1
31	LMT	A	417	-	-	6/21/61/61	0/2/2/2
31	LMT	J	102	-	-	3/15/35/61	0/1/1/2
24	CLA	B	617	-	1/1/15/20	11/37/115/115	-
24	CLA	d	405	-	1/1/15/20	5/37/115/115	-
28	LMG	B	621	-	-	13/46/66/70	0/1/1/1
24	CLA	A	407	43	-	6/37/115/115	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
31	LMT	t	101	-	-	3/15/31/61	0/1/1/2
36	HTG	V	204	-	-	3/4/24/30	0/1/1/1
24	CLA	C	506	-	1/1/15/20	6/37/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
36	HTG	d	419	-	-	1/10/30/30	0/1/1/1
28	LMG	C	519	-	-	14/46/66/70	0/1/1/1
24	CLA	b	616	-	1/1/15/20	4/37/115/115	-
36	HTG	c	924	-	-	0/10/30/30	0/1/1/1
24	CLA	B	611	43	1/1/15/20	3/37/115/115	-
36	HTG	D	412	-	-	3/10/30/30	0/1/1/1
24	CLA	C	505	-	1/1/15/20	3/37/115/115	-
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
36	HTG	B	630	-	-	1/10/30/30	0/1/1/1
24	CLA	b	608	-	1/1/15/20	2/37/115/115	-
42	HEC	V	203	16	-	2/10/54/54	-
27	SQD	A	416	-	-	12/49/69/69	0/1/1/1
24	CLA	c	902	-	1/1/15/20	1/37/115/115	-
28	LMG	D	409	41	-	4/46/66/70	0/1/1/1
24	CLA	B	615	-	1/1/15/20	4/37/115/115	-
24	CLA	b	618	-	1/1/15/20	13/37/115/115	-
27	SQD	l	101	-	-	22/49/69/69	0/1/1/1
24	CLA	b	613	-	1/1/15/20	0/37/115/115	-
24	CLA	C	507	43	1/1/15/20	8/37/115/115	-
24	CLA	b	612	-	-	2/37/115/115	-
31	LMT	B	626	-	-	10/15/35/61	0/1/1/2
36	HTG	O	316	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	503	-	1/1/15/20	3/37/115/115	-
24	CLA	b	610	-	1/1/15/20	4/37/115/115	-
32	GOL	O	304	-	-	2/4/4/4	-
32	GOL	C	525	-	-	1/4/4/4	-
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
37	DGD	D	405	-	-	20/47/67/95	0/1/1/2
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
36	HTG	C	521	-	-	2/10/30/30	0/1/1/1
24	CLA	c	908	43	1/1/15/20	5/37/115/115	-
31	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
24	CLA	B	604	-	1/1/15/20	4/37/115/115	-
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
26	BCR	c	915	-	-	1/29/63/63	0/2/2/2
32	GOL	A	419	-	-	2/4/4/4	-
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	C	508	-	1/1/15/20	6/37/115/115	-
24	CLA	d	401	43	1/1/15/20	5/37/115/115	-
38	LHG	l	103	-	-	14/53/53/53	-
31	LMT	t	102	-	-	9/21/61/61	0/2/2/2
24	CLA	a	409	-	1/1/15/20	3/37/115/115	-
32	GOL	B	637	-	-	4/4/4/4	-
36	HTG	v	211	-	-	1/10/30/30	0/1/1/1
38	LHG	D	408	-	-	8/50/50/53	-
26	BCR	B	636	-	-	1/29/63/63	0/2/2/2
36	HTG	d	420	-	-	3/10/30/30	0/1/1/1
27	SQD	F	101	-	-	10/31/51/69	0/1/1/1
31	LMT	j	102	-	-	3/15/35/61	0/1/1/2
38	LHG	d	409	-	-	8/53/53/53	-
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
36	HTG	b	627	-	-	3/10/30/30	0/1/1/1
36	HTG	c	943	-	-	2/8/28/30	0/1/1/1
36	HTG	d	414	-	-	4/10/30/30	0/1/1/1
24	CLA	A	405	-	1/1/15/20	2/37/115/115	-
31	LMT	a	402	-	-	7/21/61/61	0/2/2/2
25	PHO	A	409	-	-	0/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	b	625	-	-	7/21/61/61	0/2/2/2
24	CLA	b	611	43	1/1/15/20	1/37/115/115	-
24	CLA	B	610	-	1/1/15/20	5/37/115/115	-
39	HEM	f	101	6,5	-	1/12/54/54	-
24	CLA	A	410	-	-	8/37/115/115	-
32	GOL	b	637	-	-	0/4/4/4	-
31	LMT	F	103	-	-	4/15/35/61	0/1/1/2

The worst 5 of 1653 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	MG-NA	10.97	2.32	2.06
24	C	507	CLA	MG-NA	10.43	2.31	2.06
24	C	511	CLA	MG-NA	10.27	2.30	2.06
24	C	503	CLA	MG-NA	10.00	2.30	2.06
24	b	612	CLA	MG-ND	-9.99	1.86	2.05

The worst 5 of 2413 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	909	CLA	C1D-ND-C4D	-11.30	98.31	106.33
24	D	401	CLA	C1D-ND-C4D	-11.21	98.37	106.33
24	b	616	CLA	C1D-ND-C4D	-10.86	98.62	106.33
24	A	406	CLA	C1D-ND-C4D	-10.74	98.71	106.33
24	c	902	CLA	C1D-ND-C4D	-10.67	98.75	106.33

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND

5 of 1032 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6

*Continued on next page...*

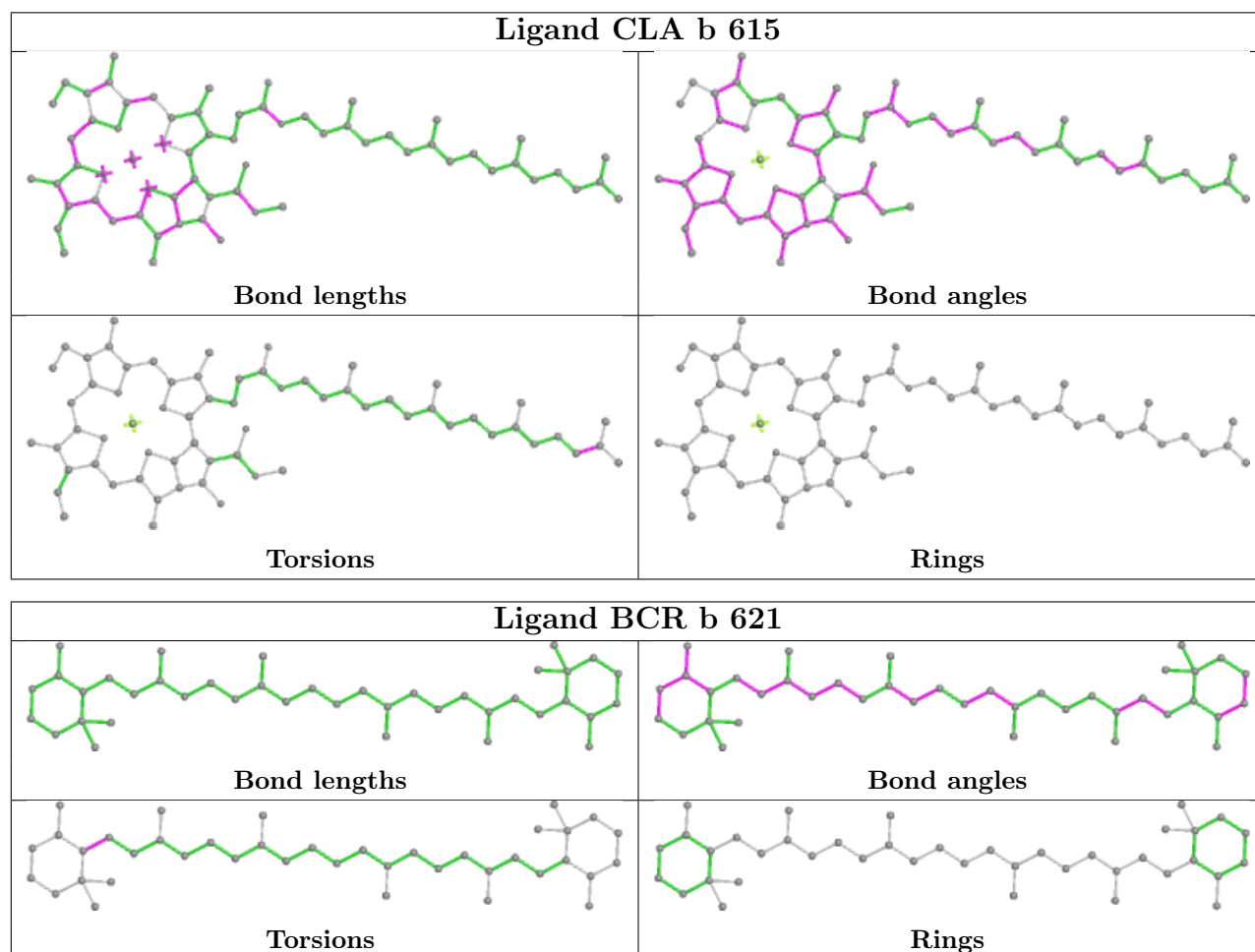
*Continued from previous page...*

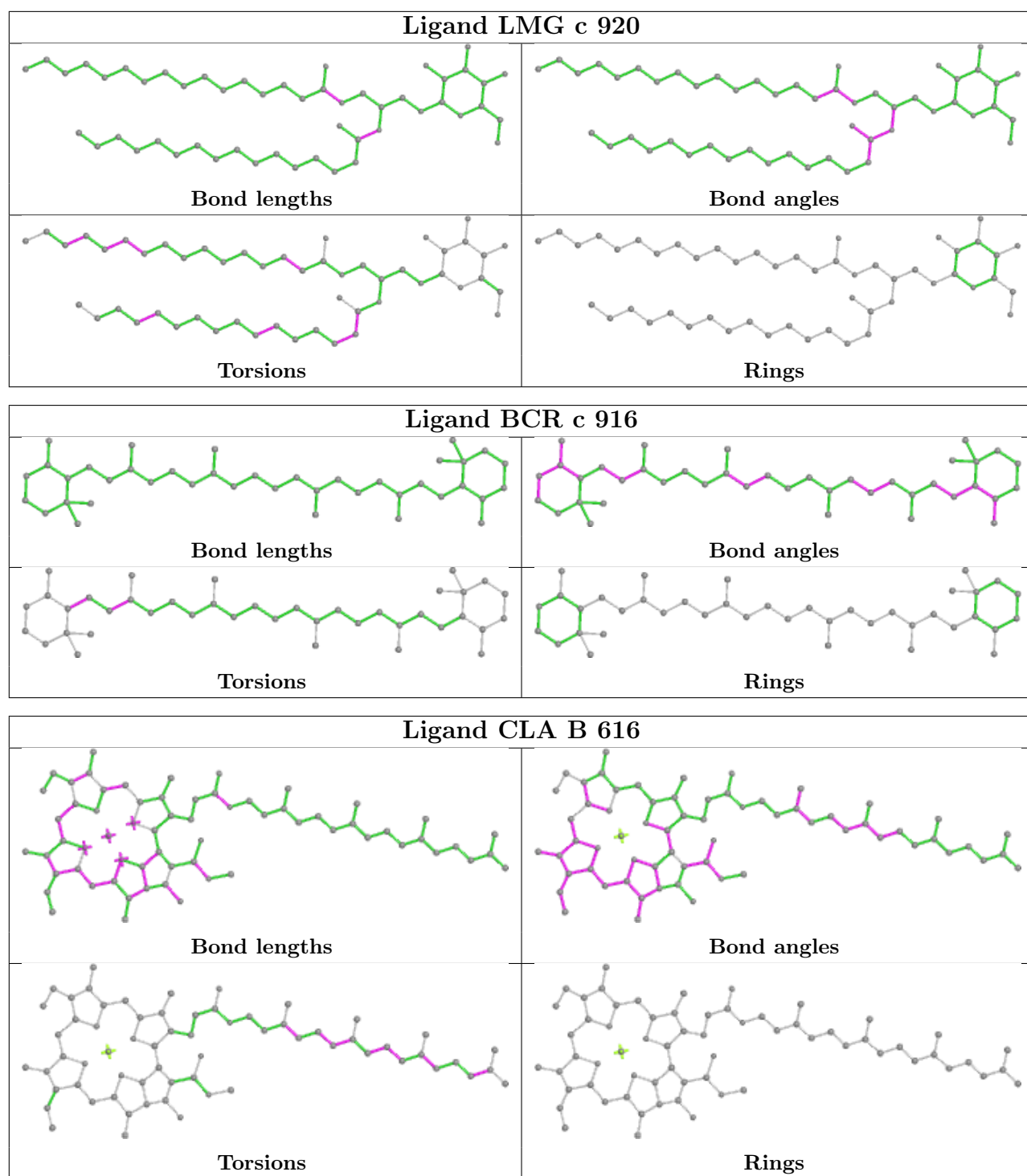
Mol	Chain	Res	Type	Atoms
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D

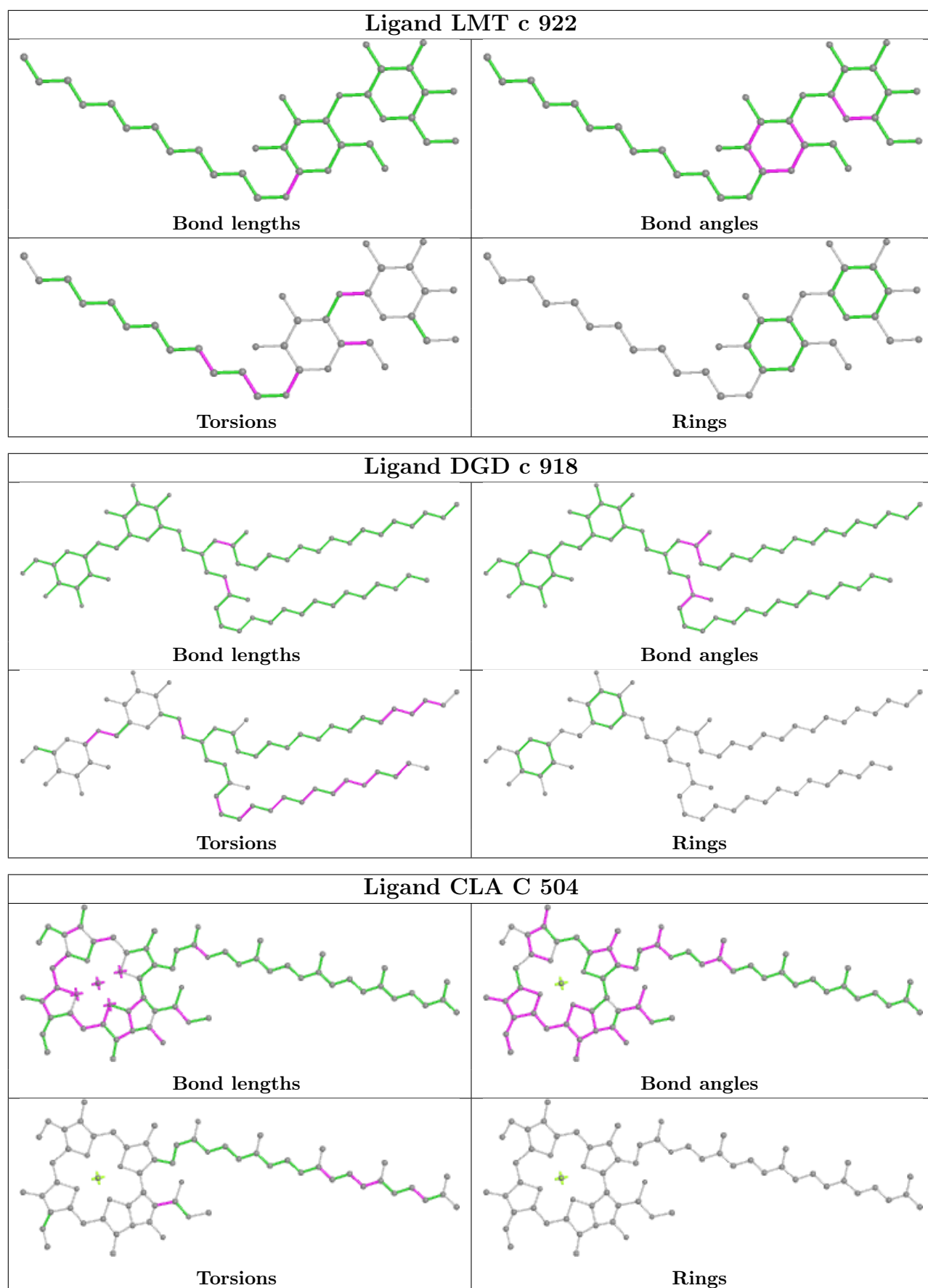
There are no ring outliers.

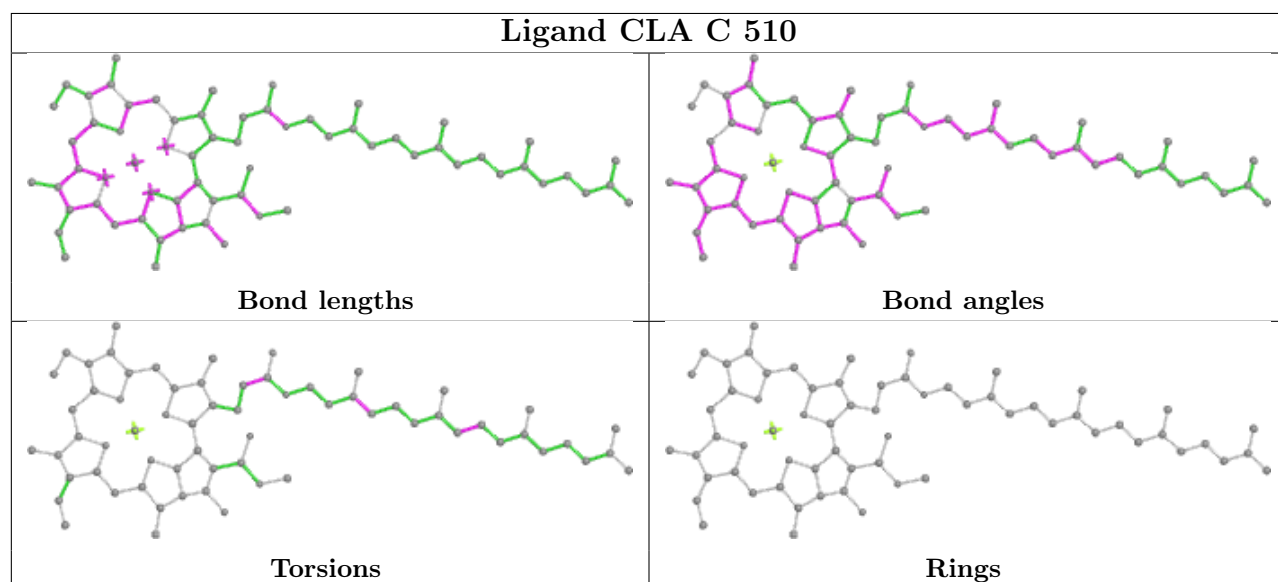
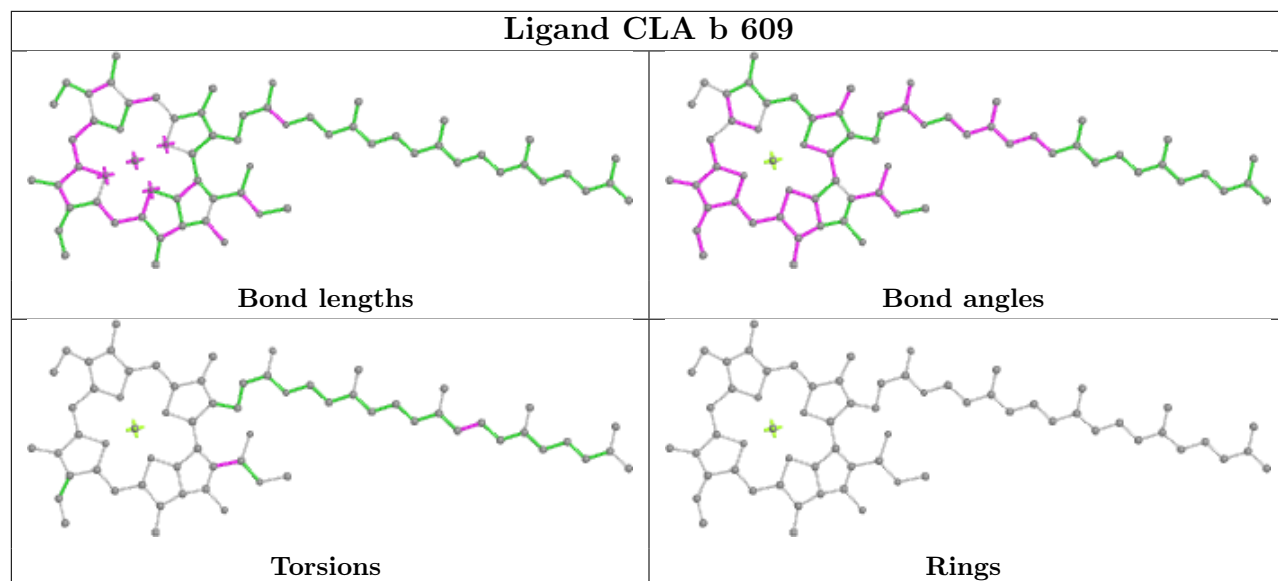
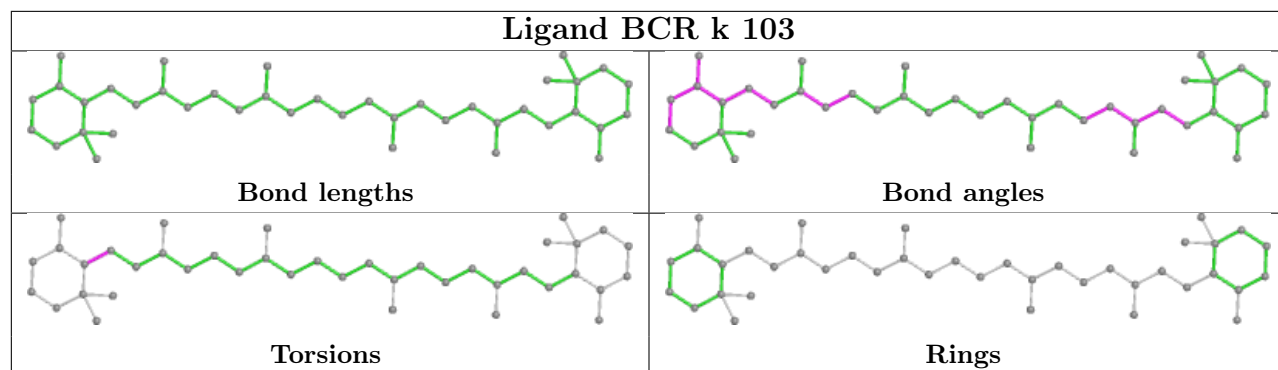
No monomer is involved in short contacts.

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

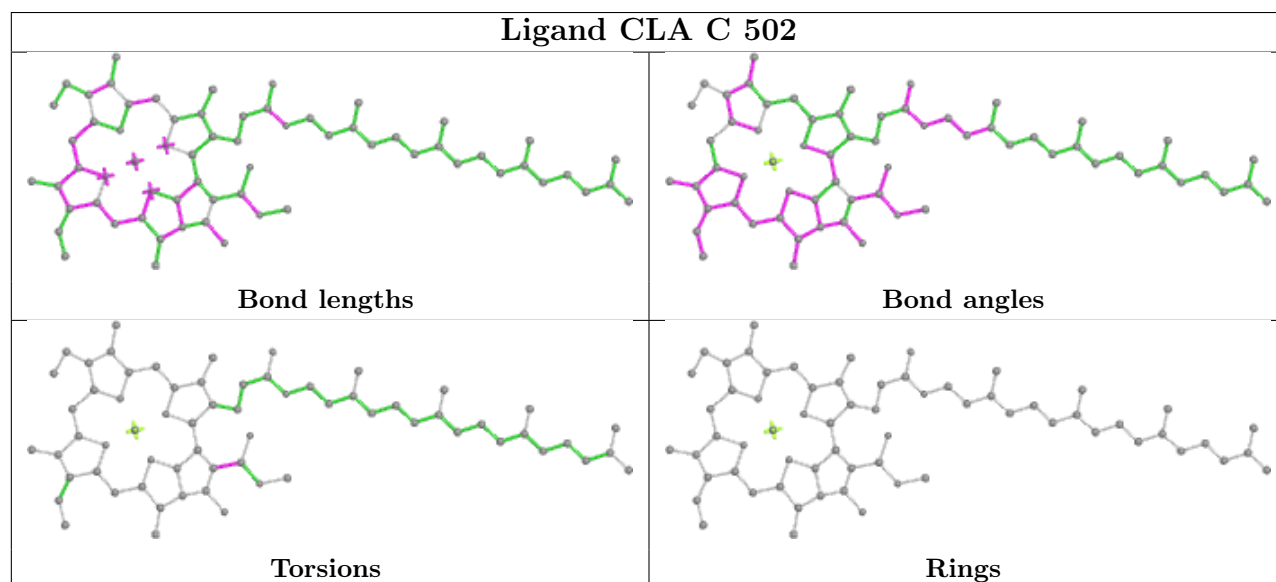
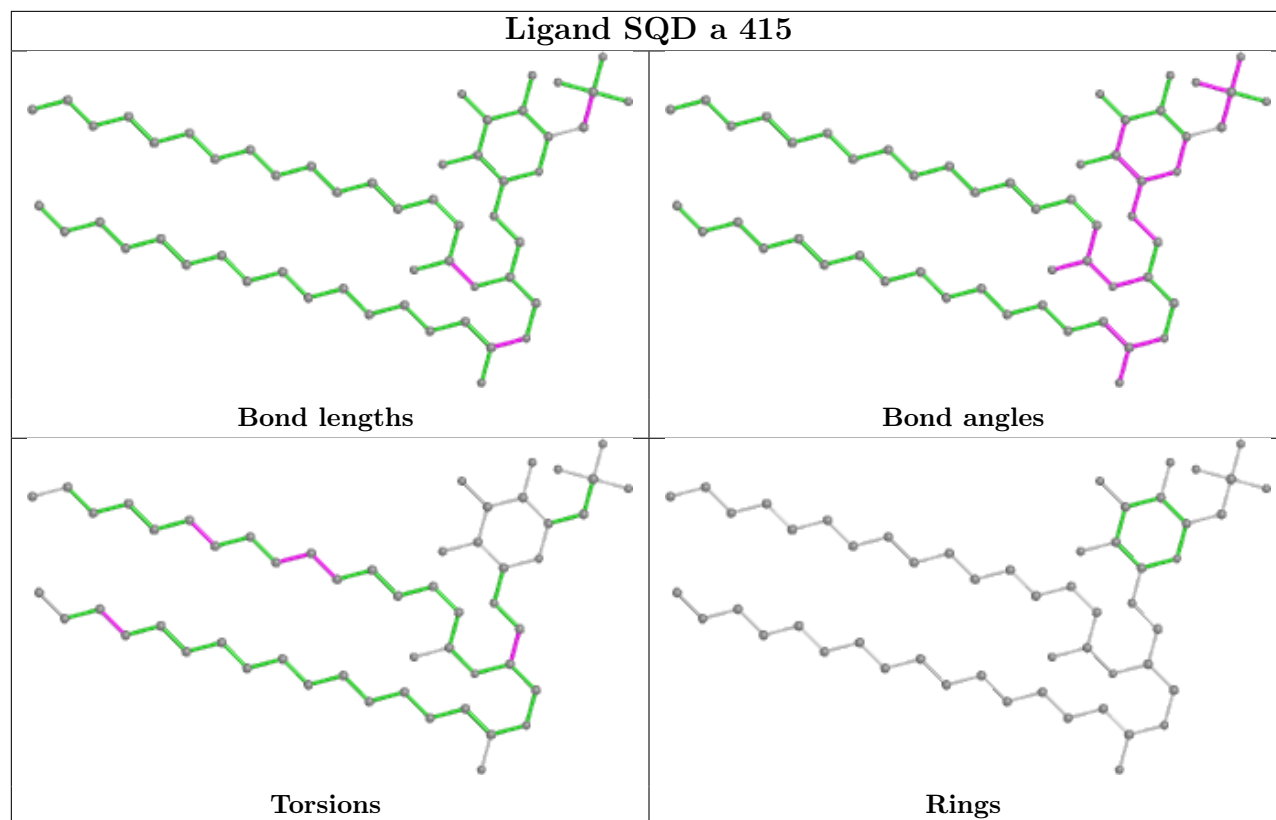


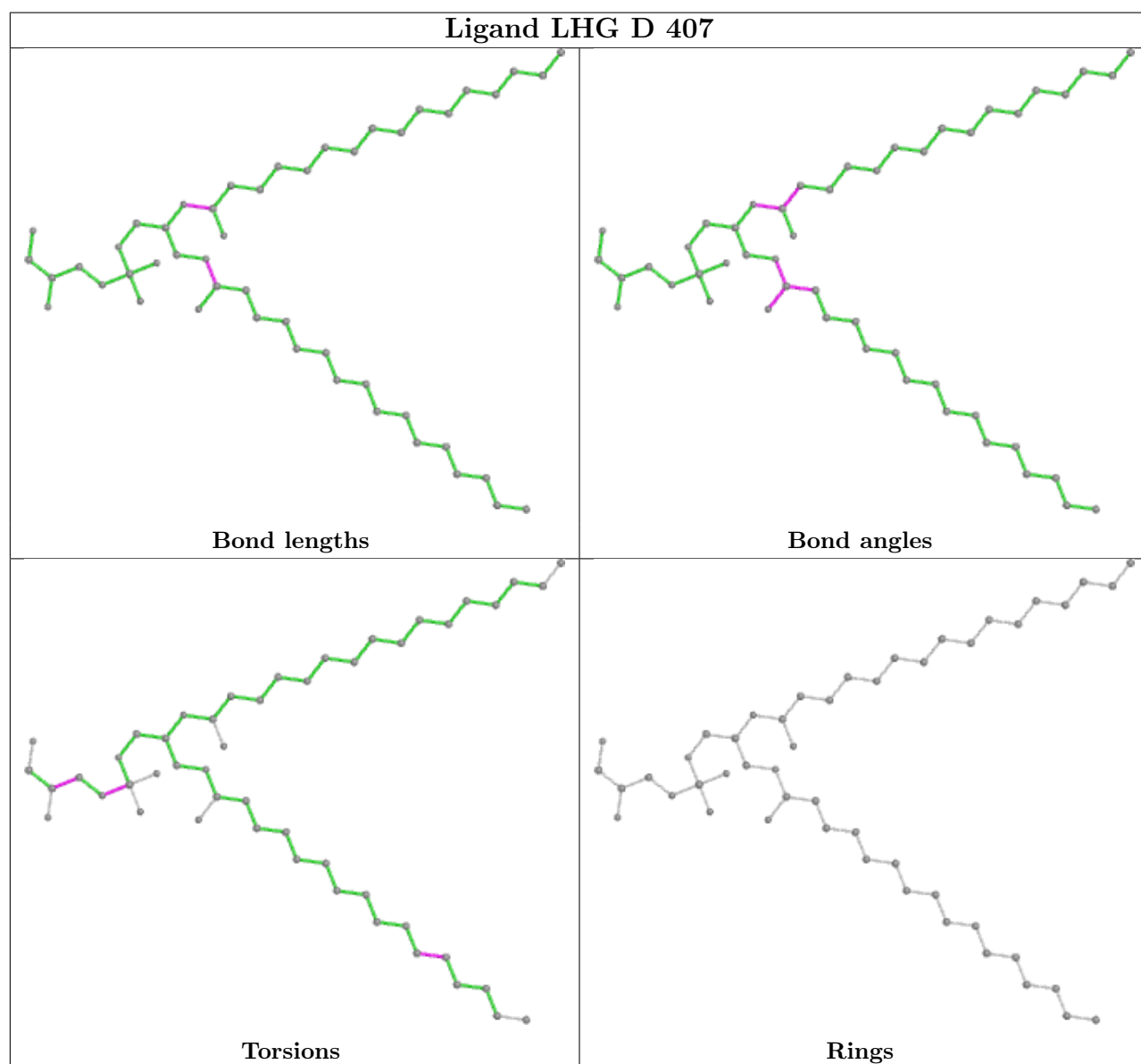
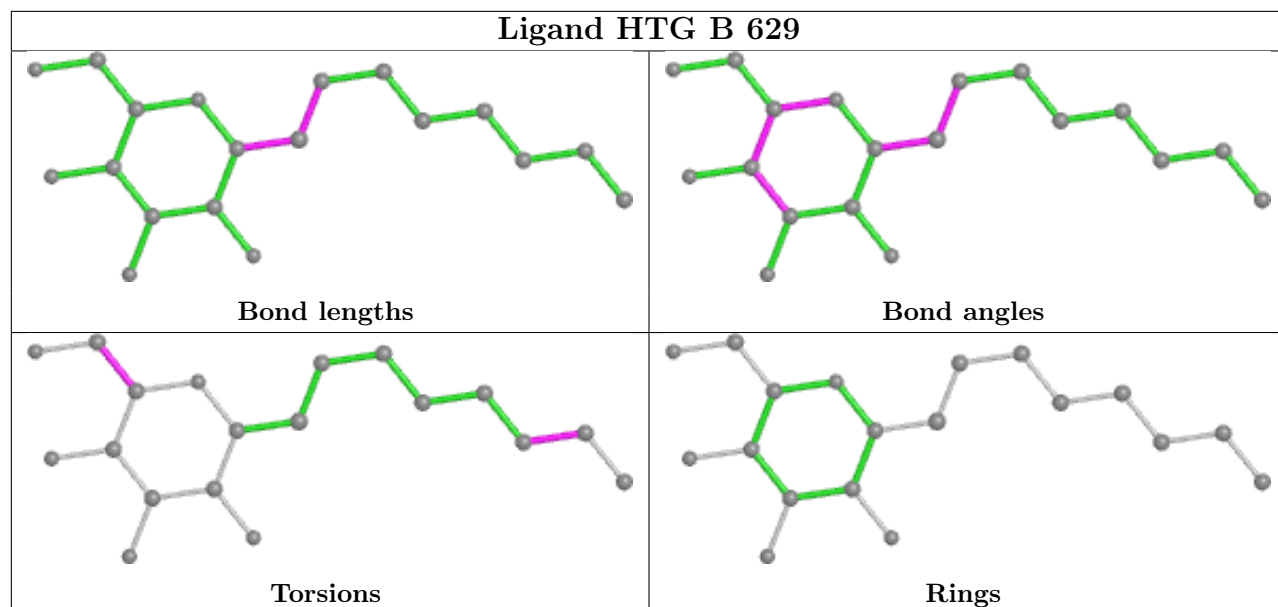




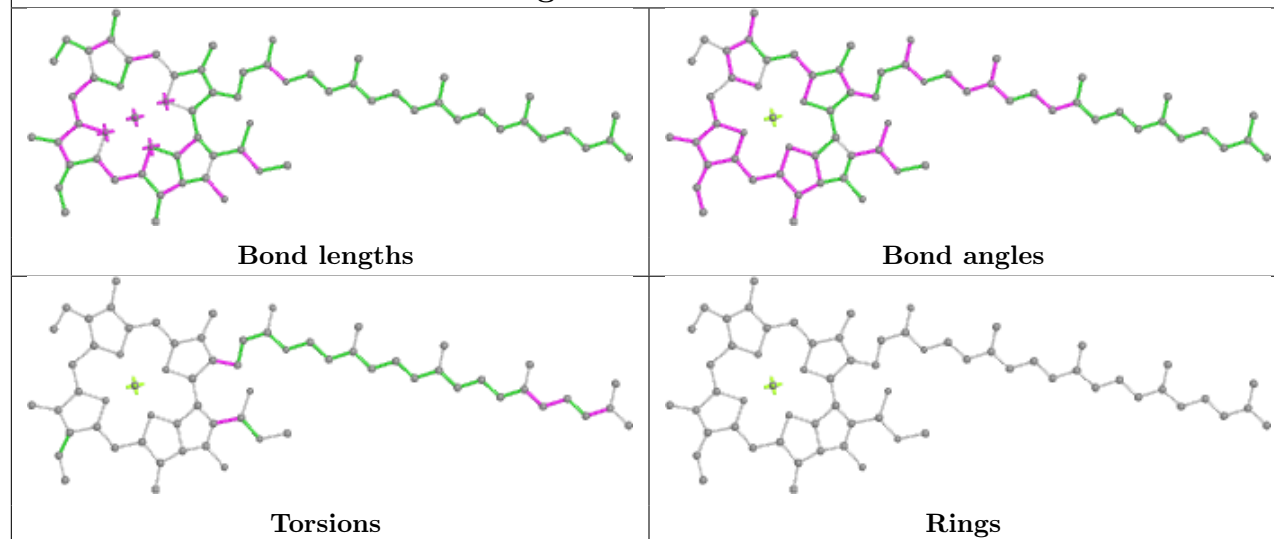




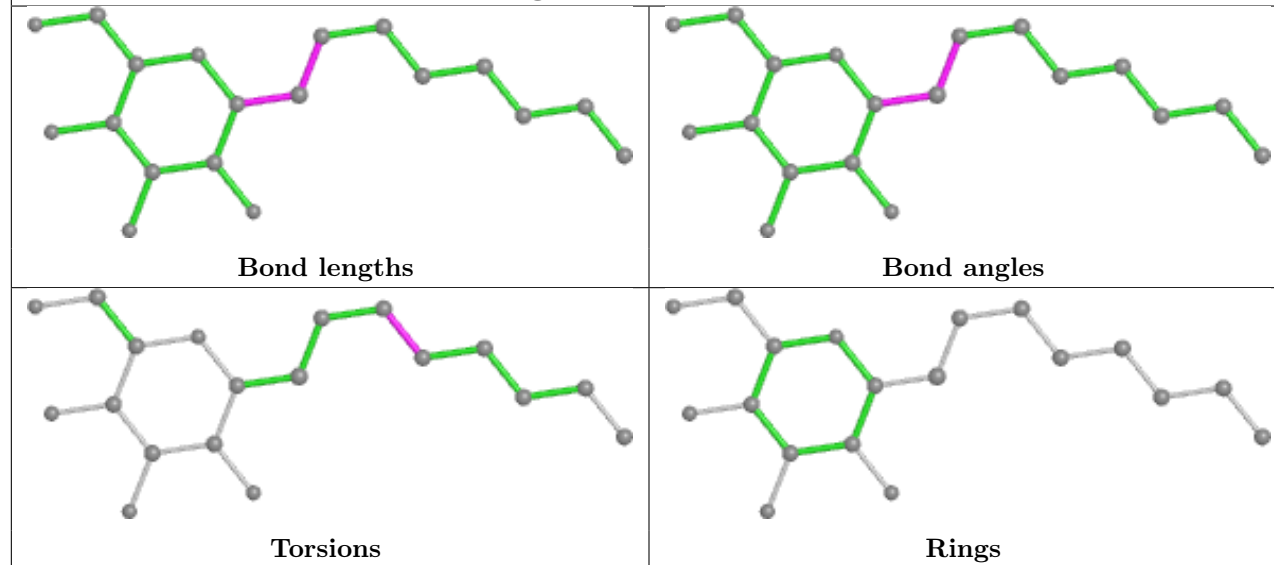




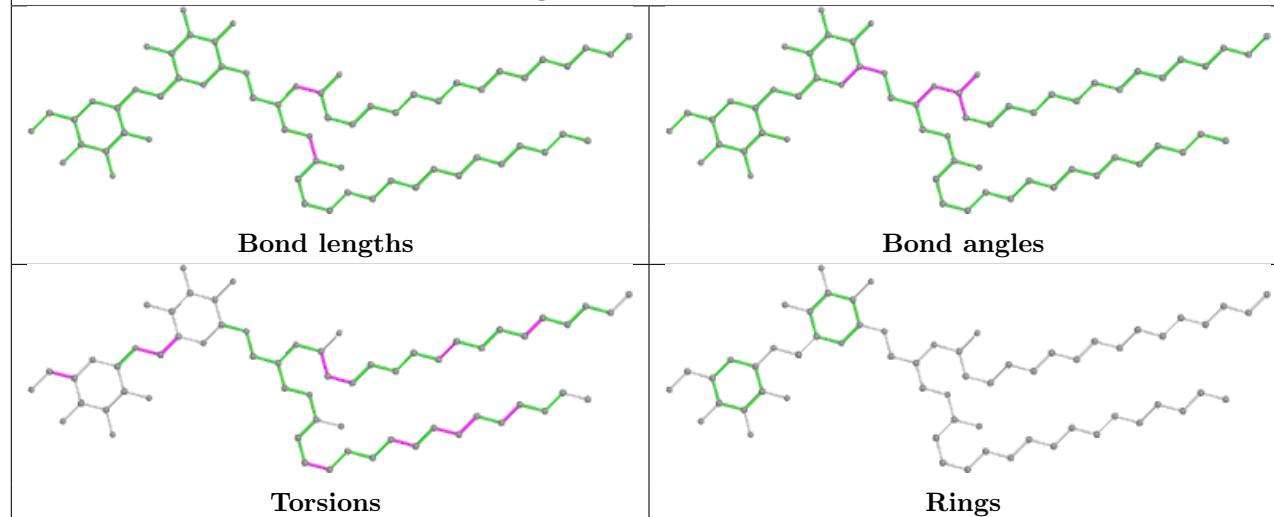
## Ligand CLA c 909



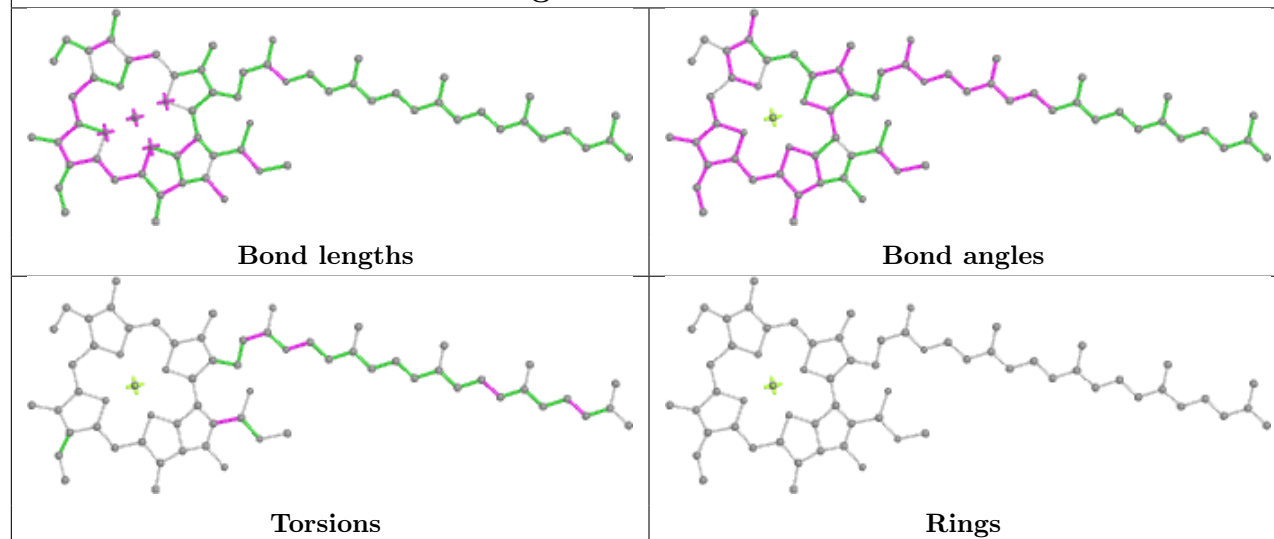
## Ligand HTG C 536



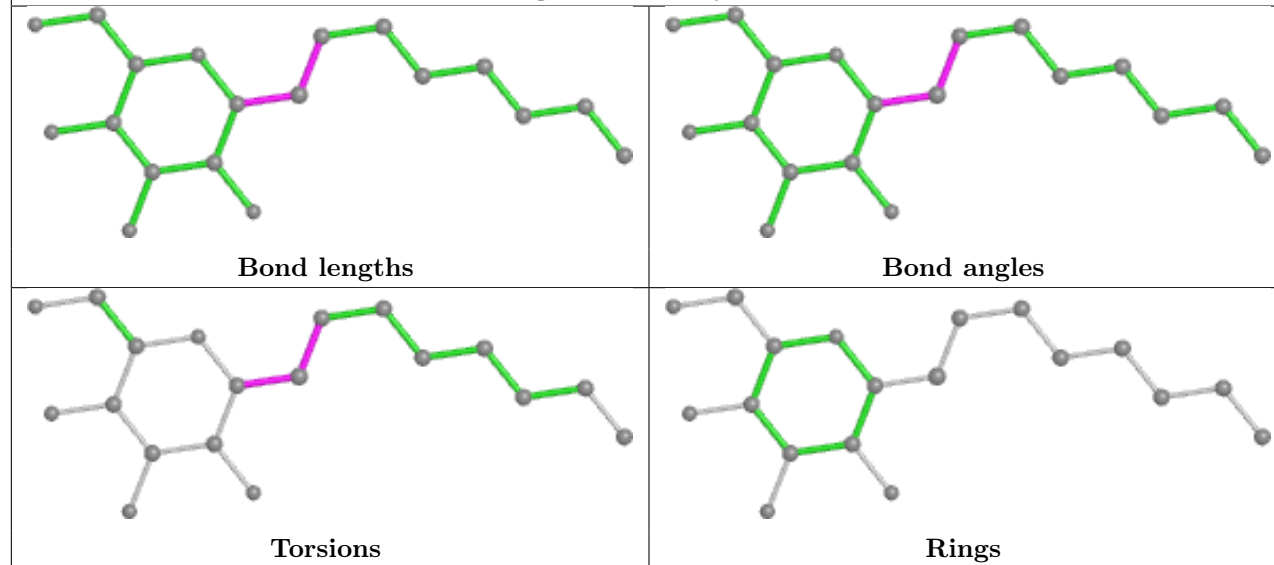
## Ligand DGD c 917



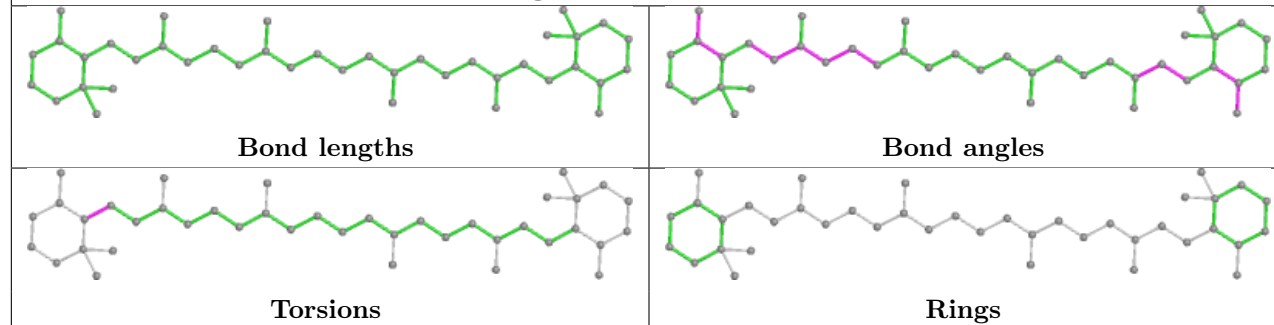
## Ligand CLA B 614

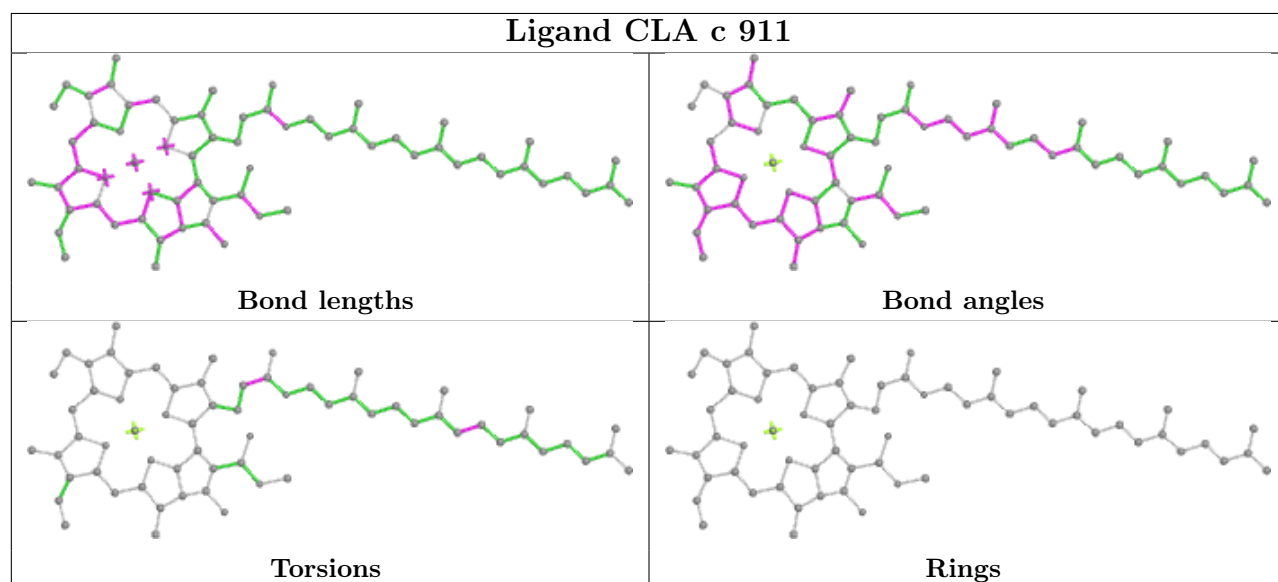
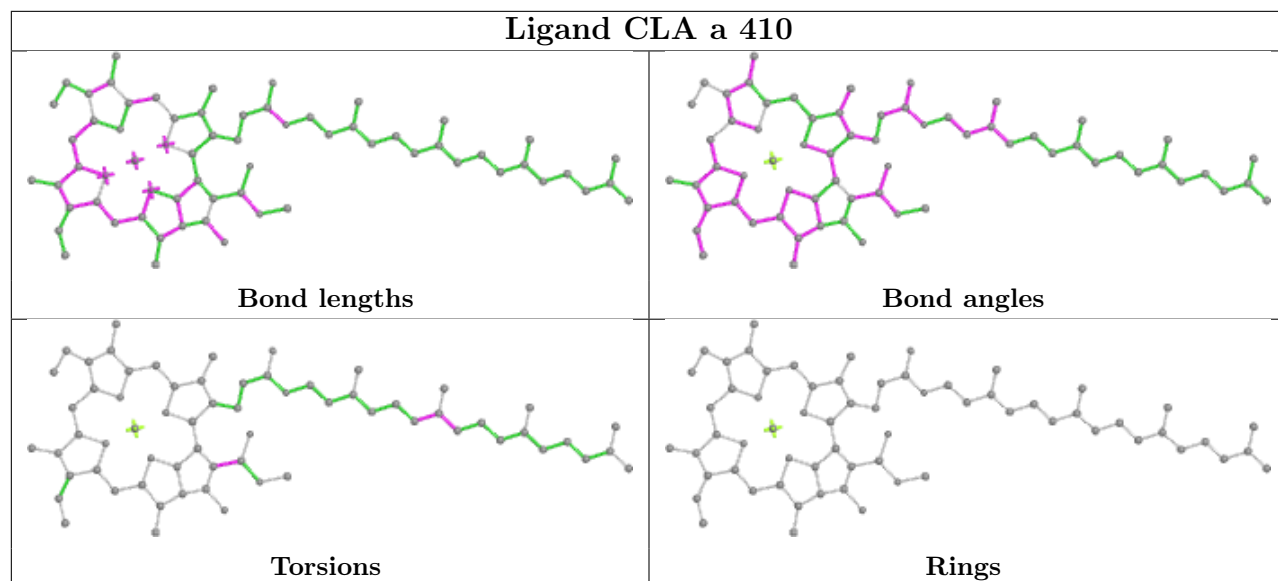
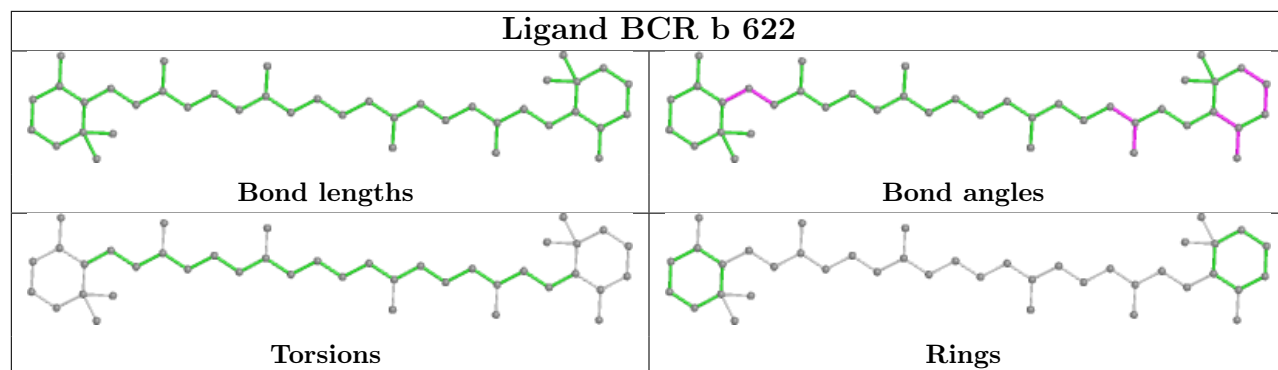


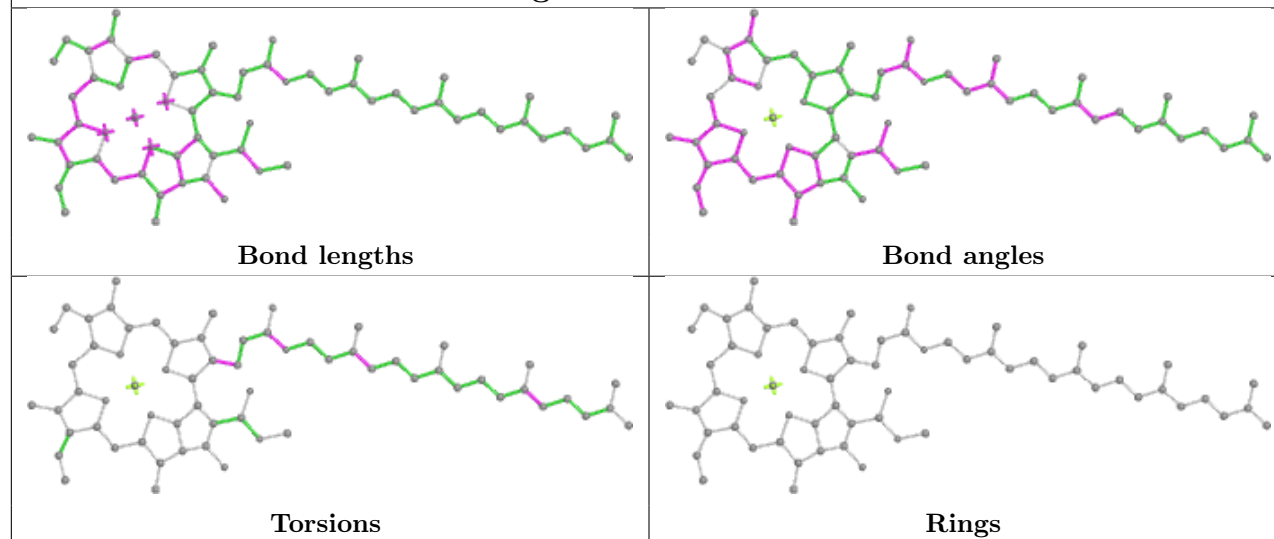
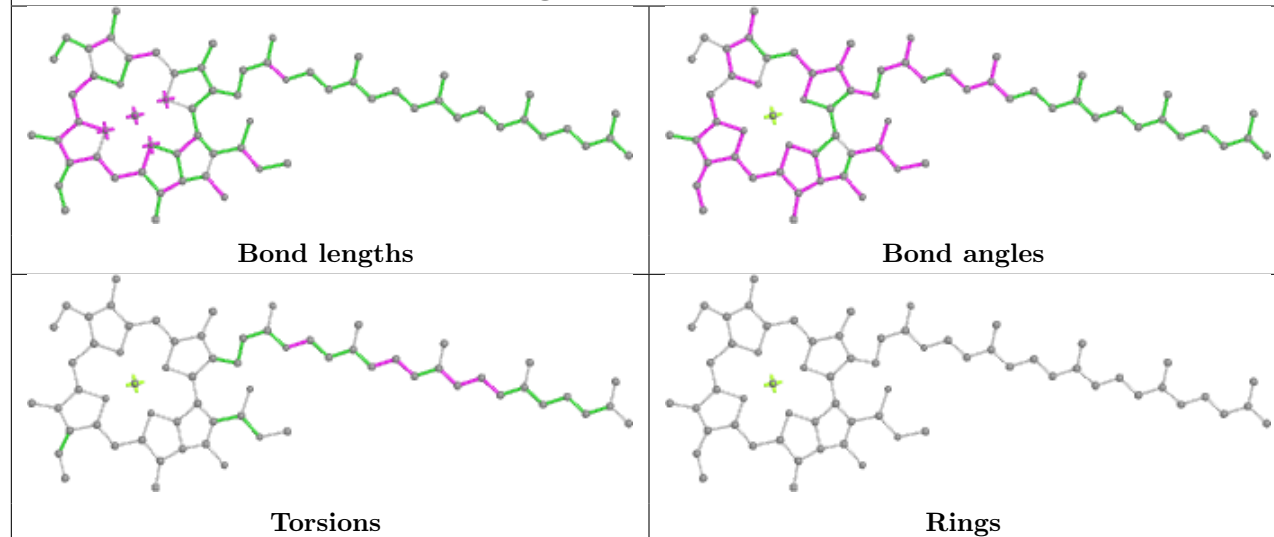
## Ligand HTG y 102

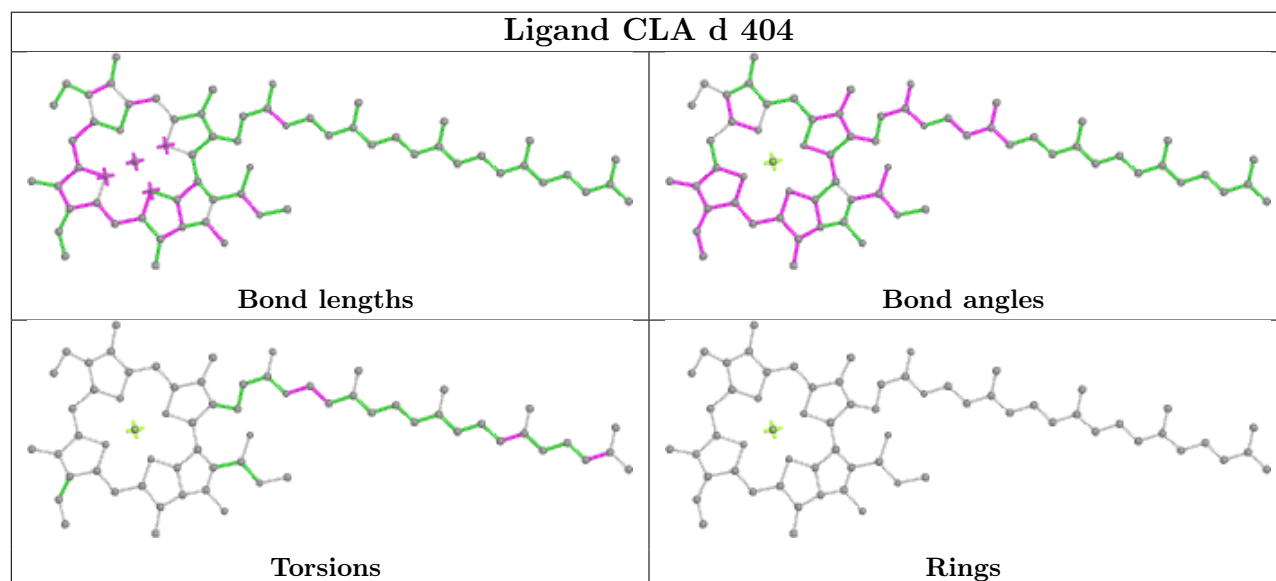
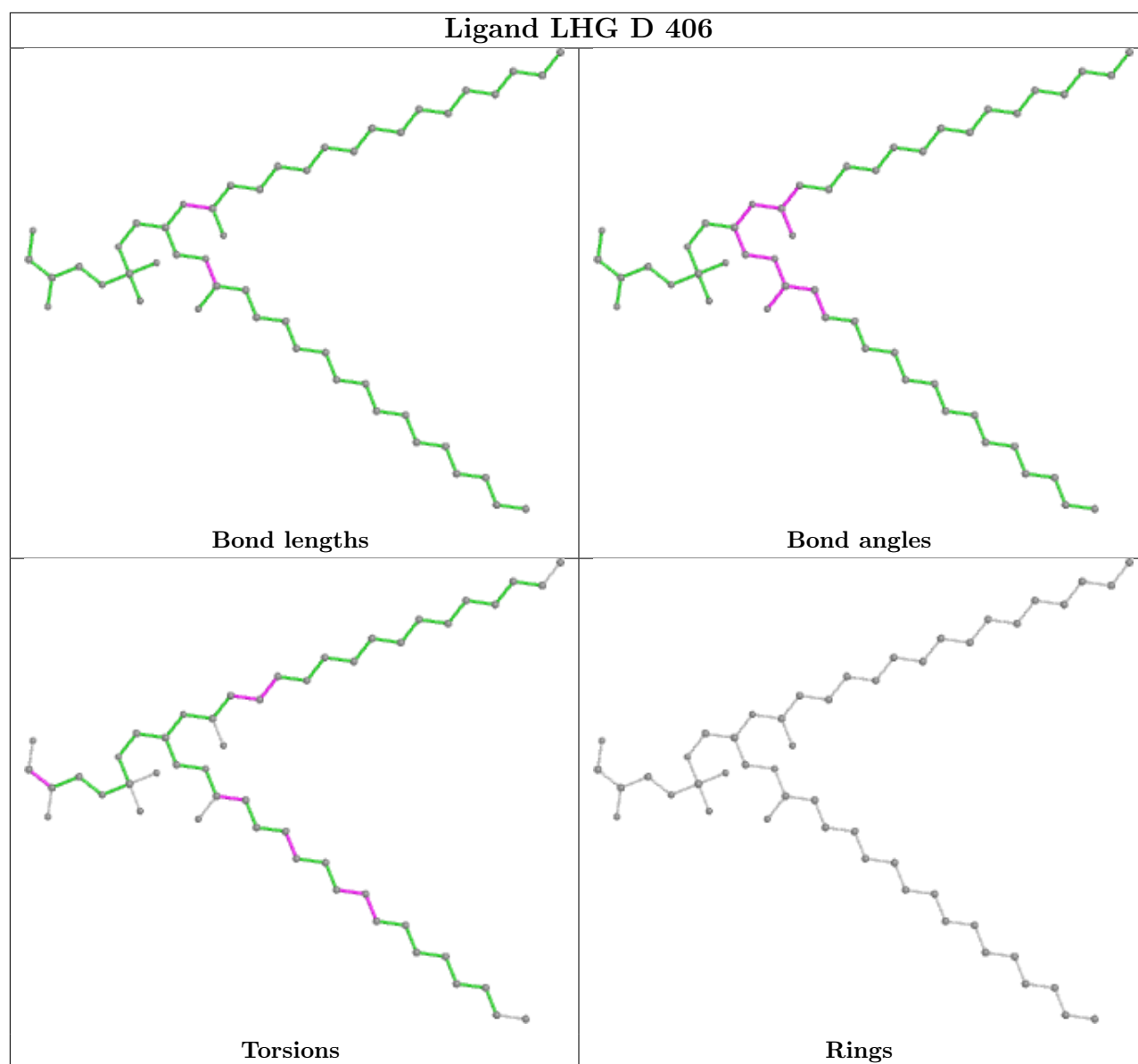


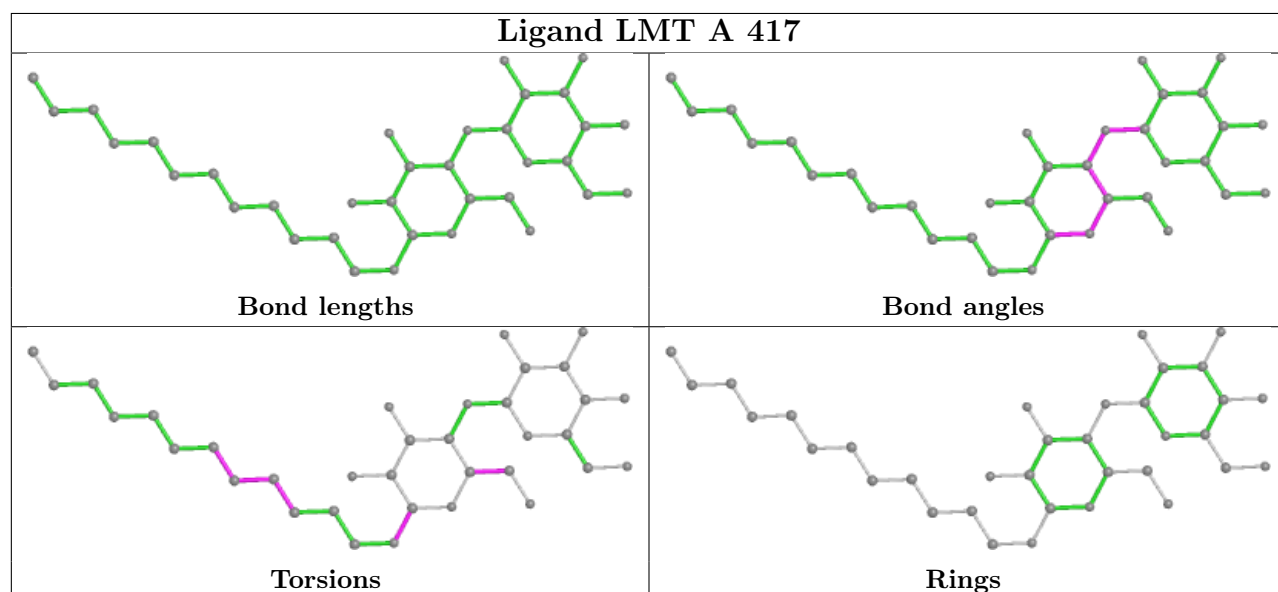
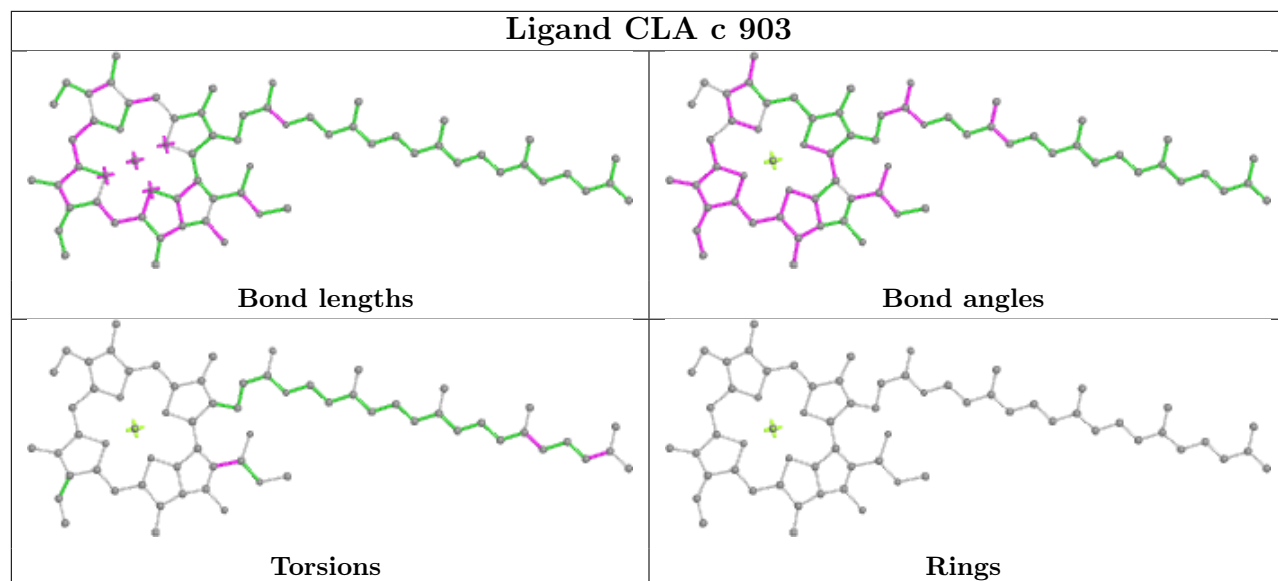
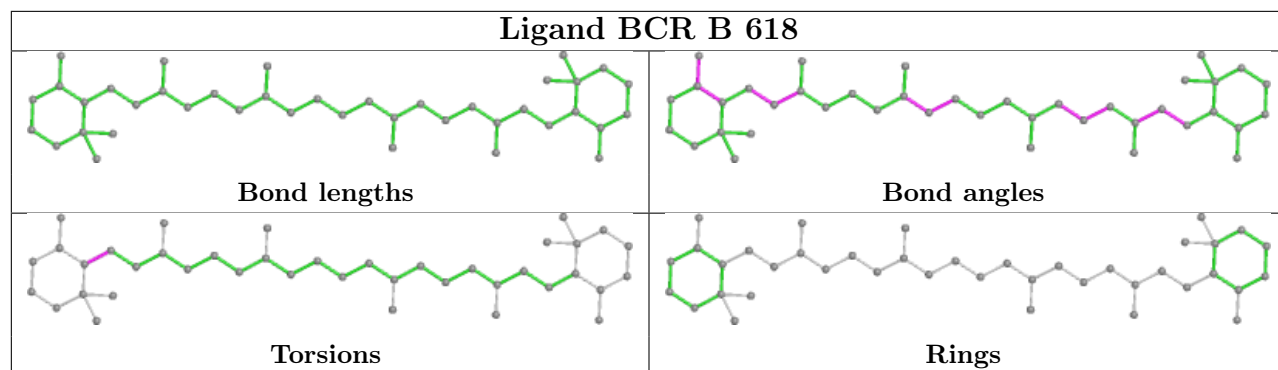
## Ligand BCR K 101





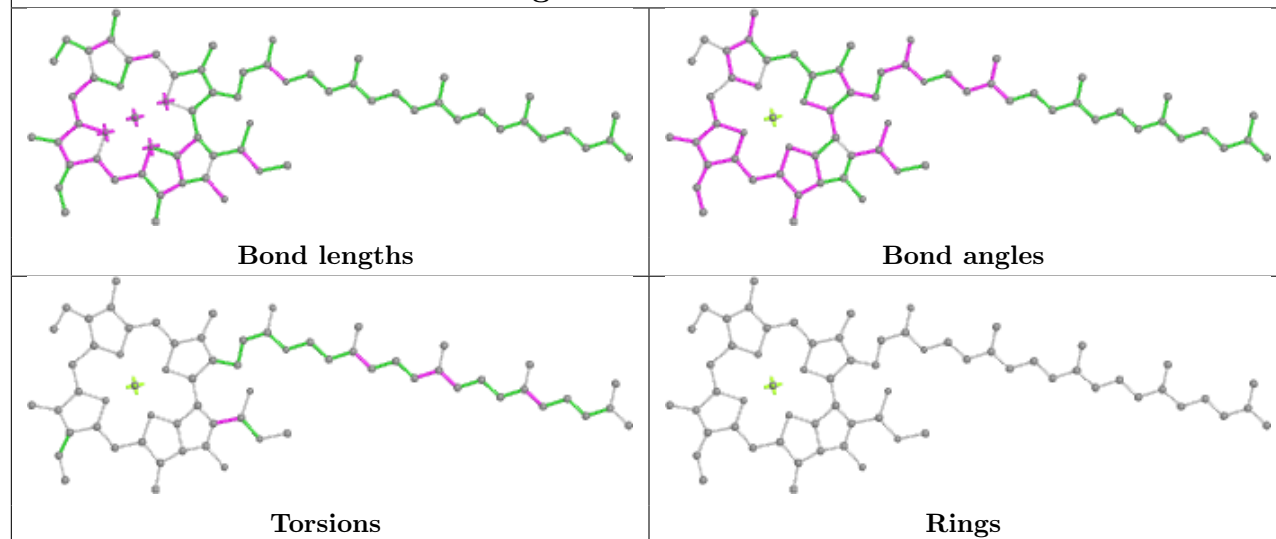
**Ligand CLA C 513****Ligand CLA a 413**



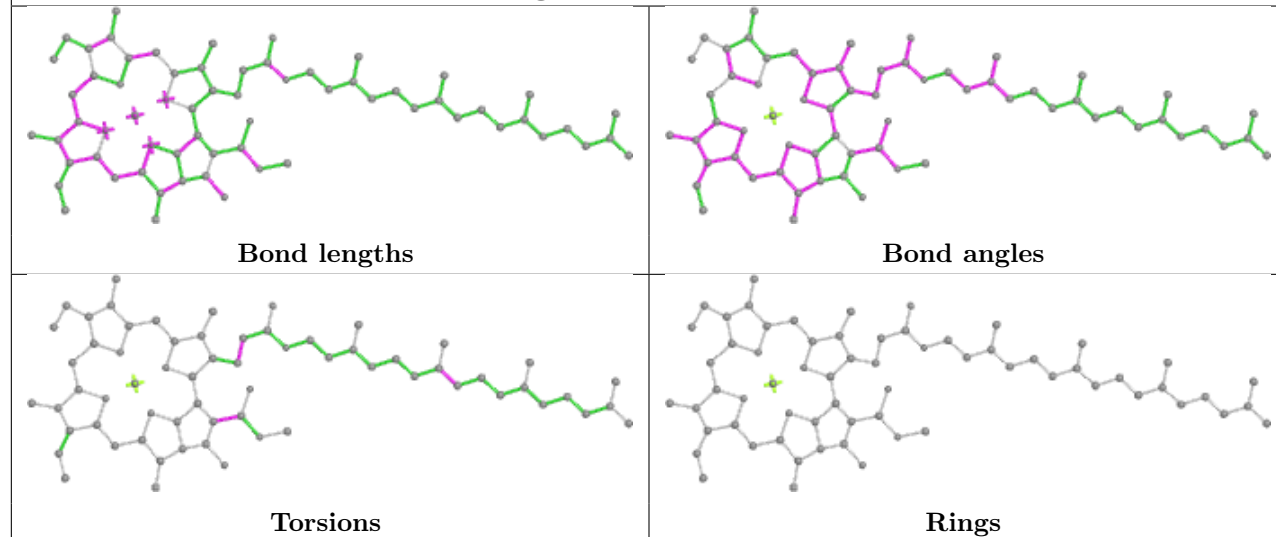




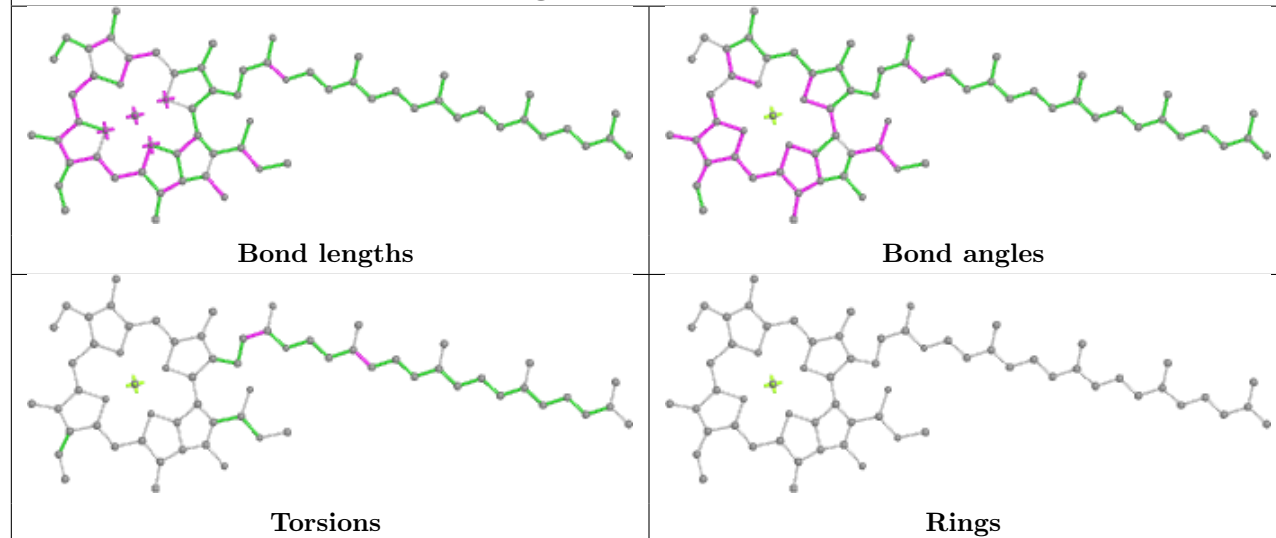
## Ligand CLA C 506

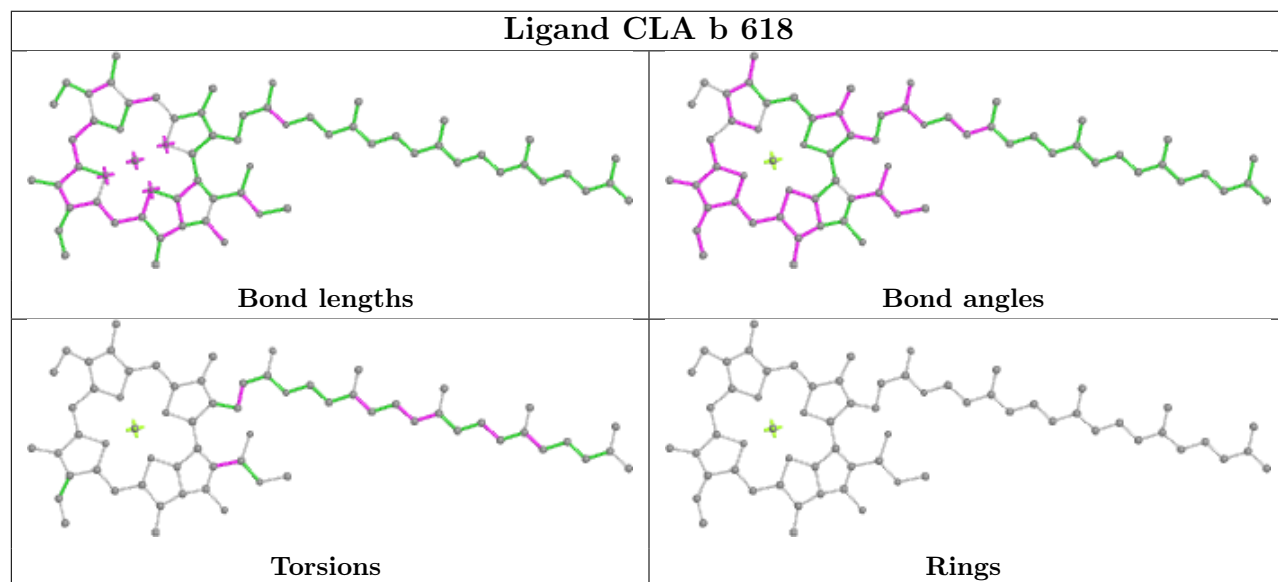
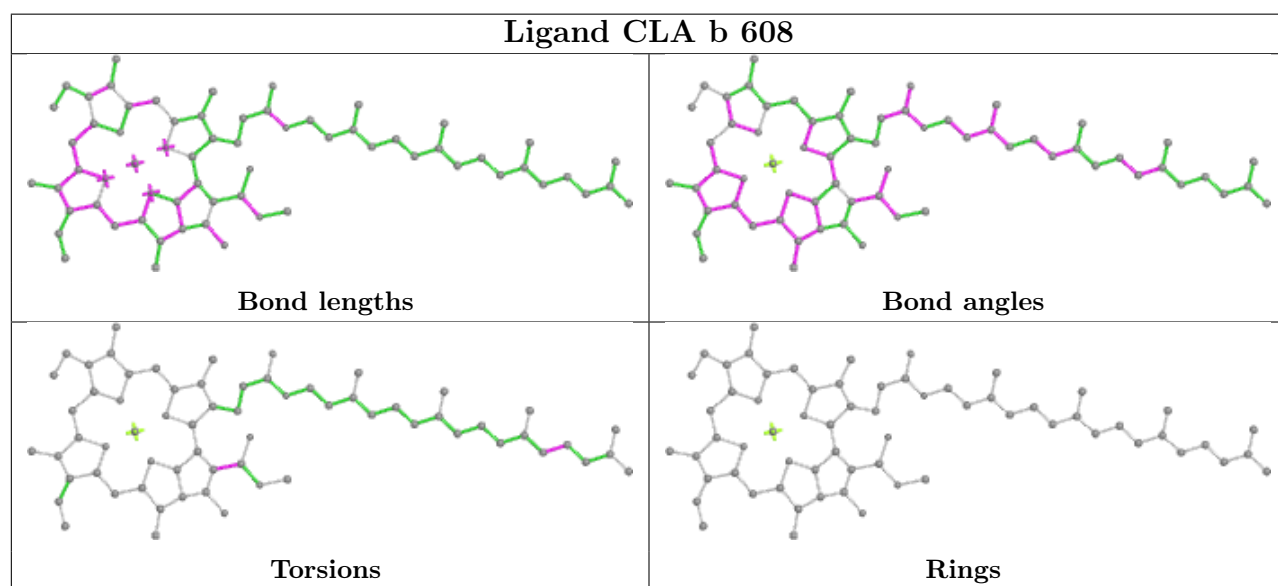
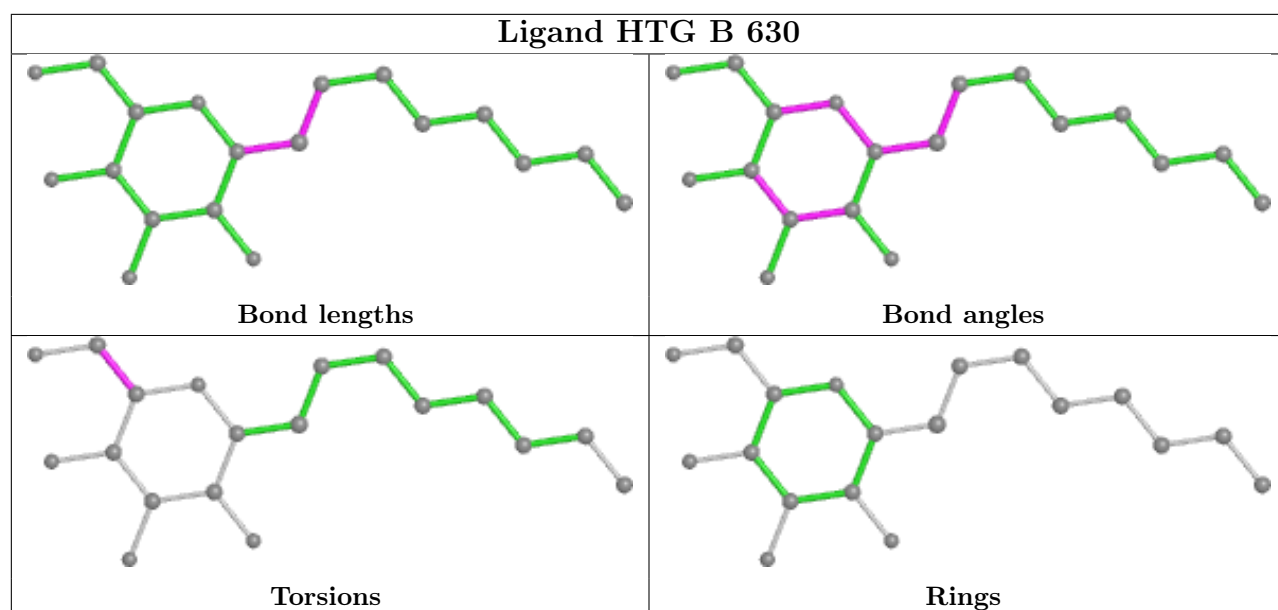


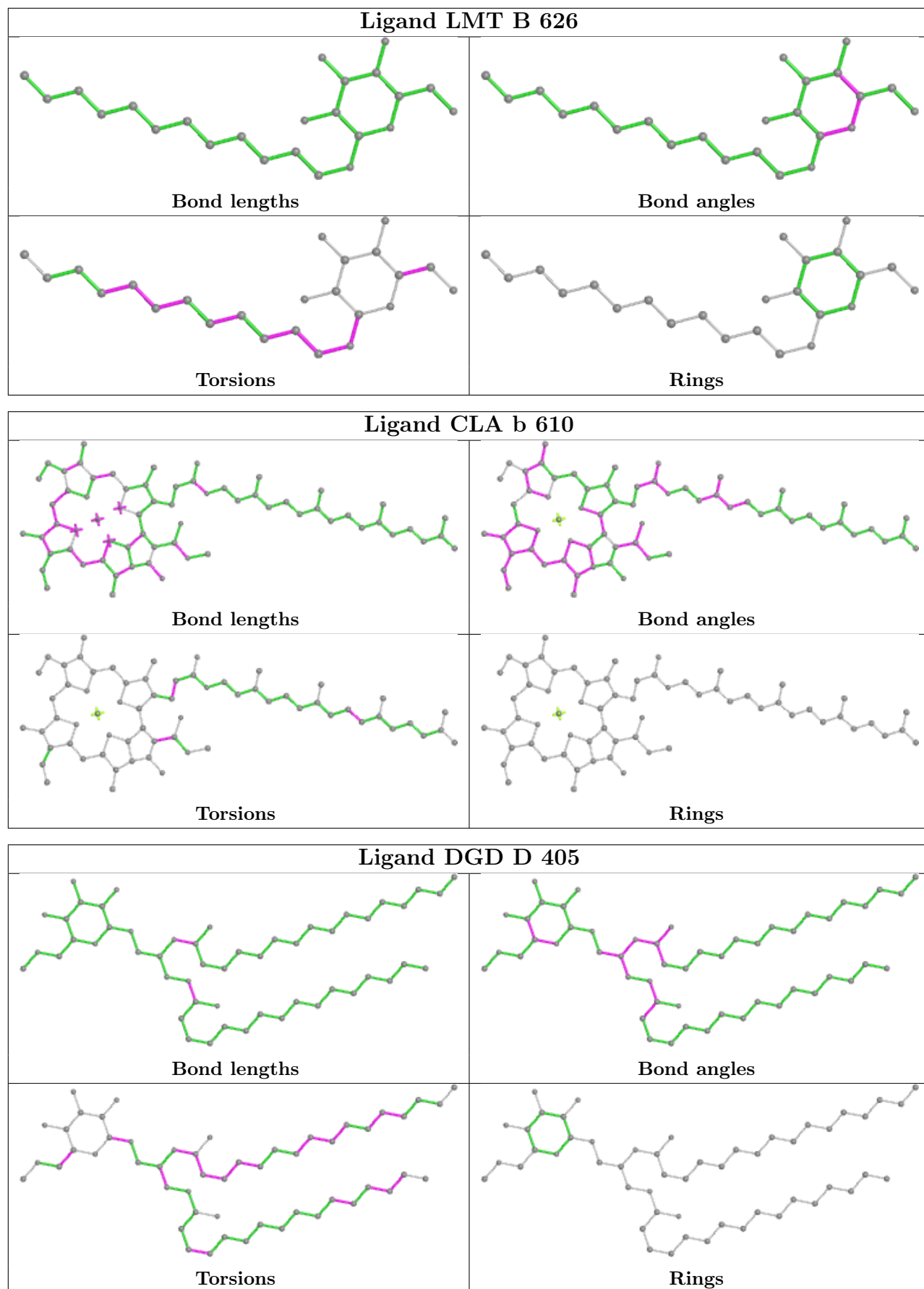
## Ligand CLA B 611

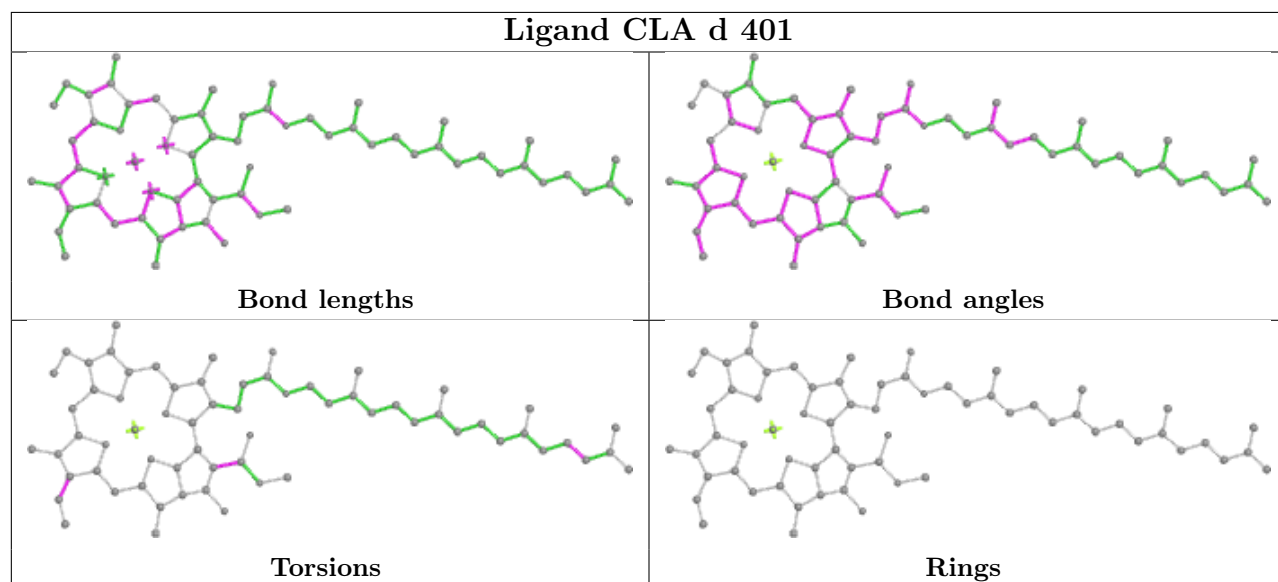
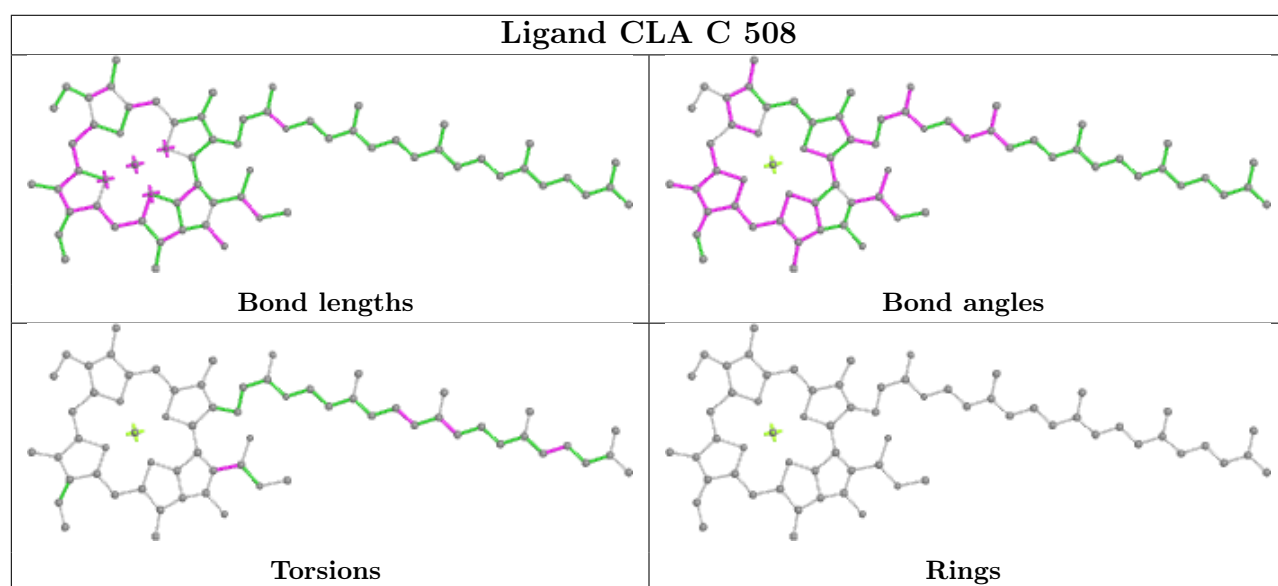
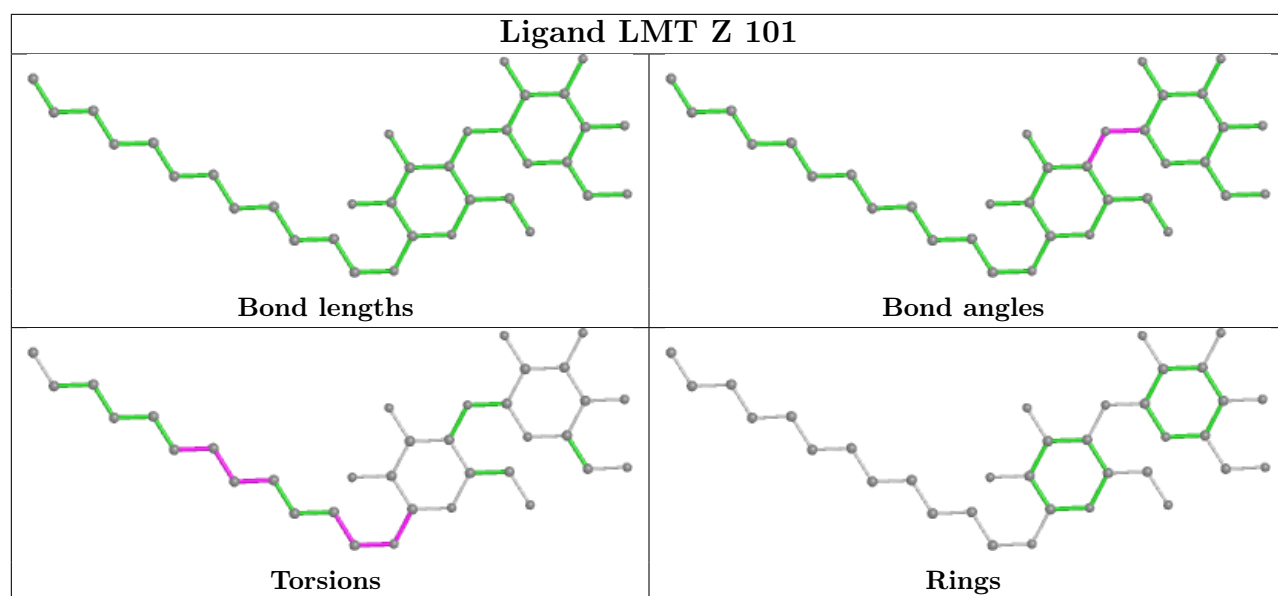


## Ligand CLA C 505

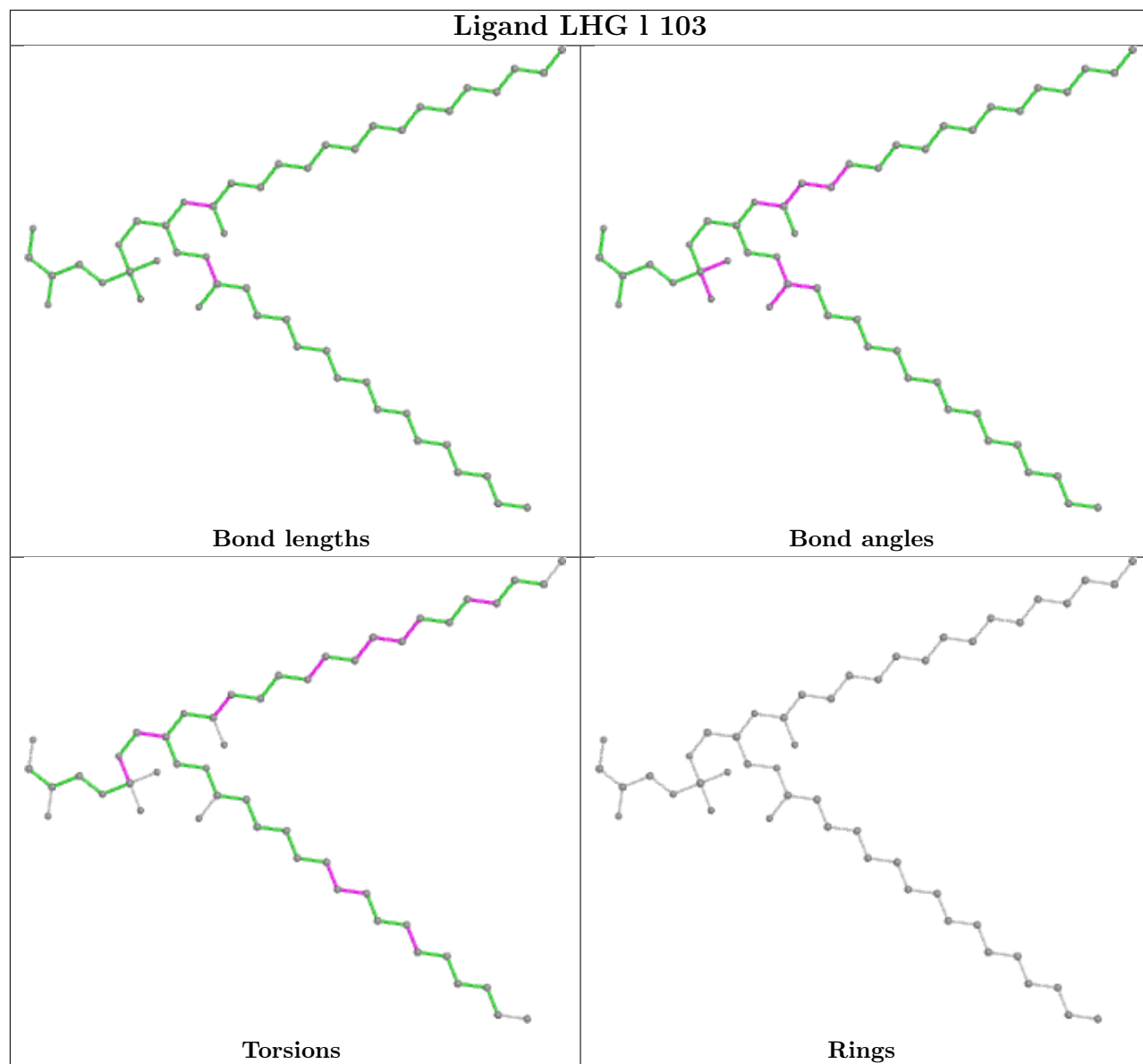




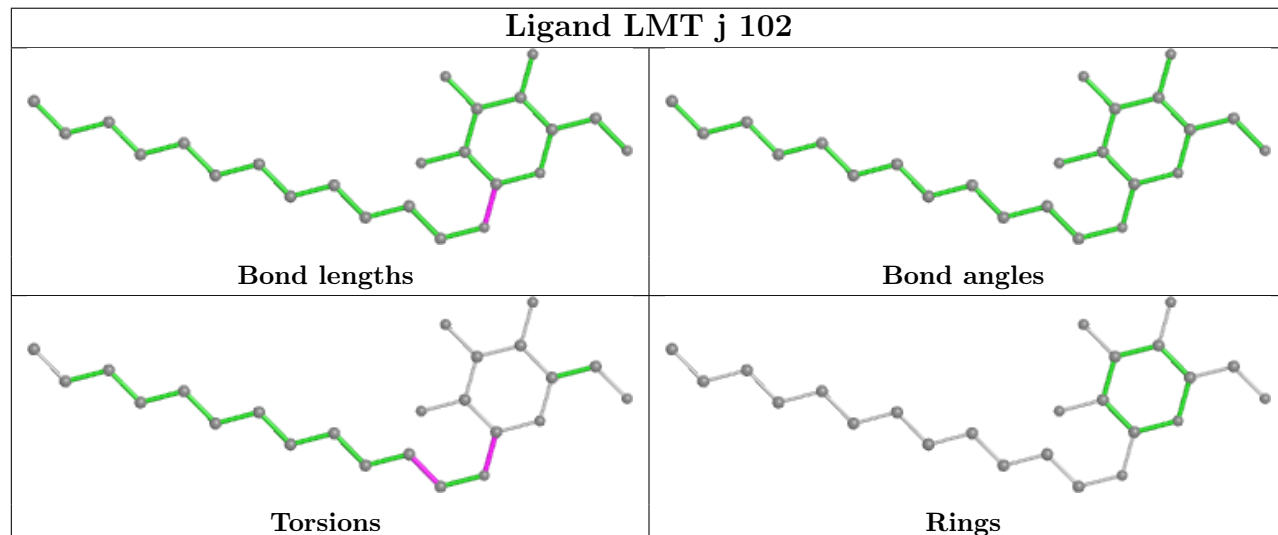


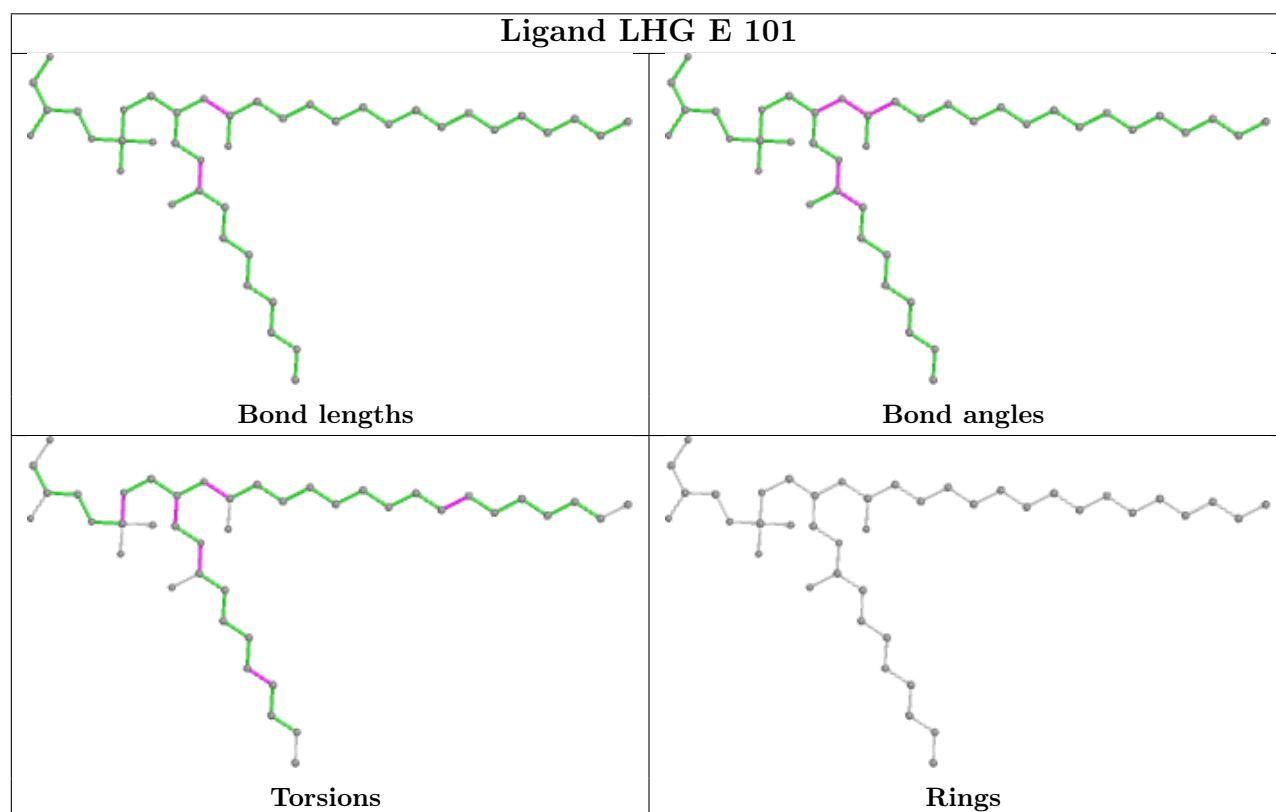
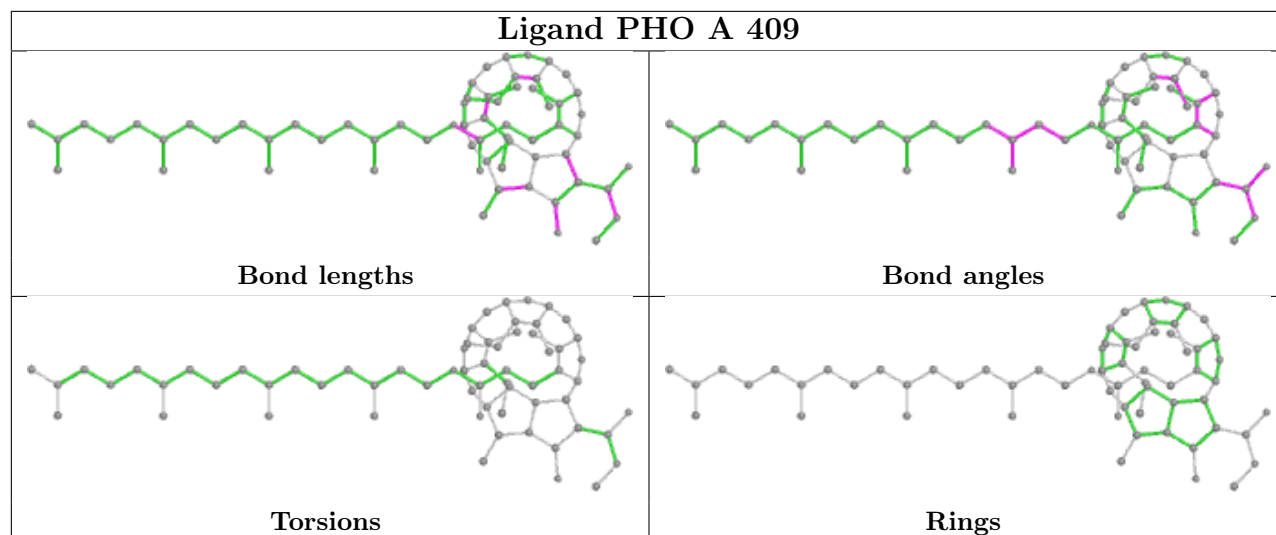


## Ligand LHG l 103

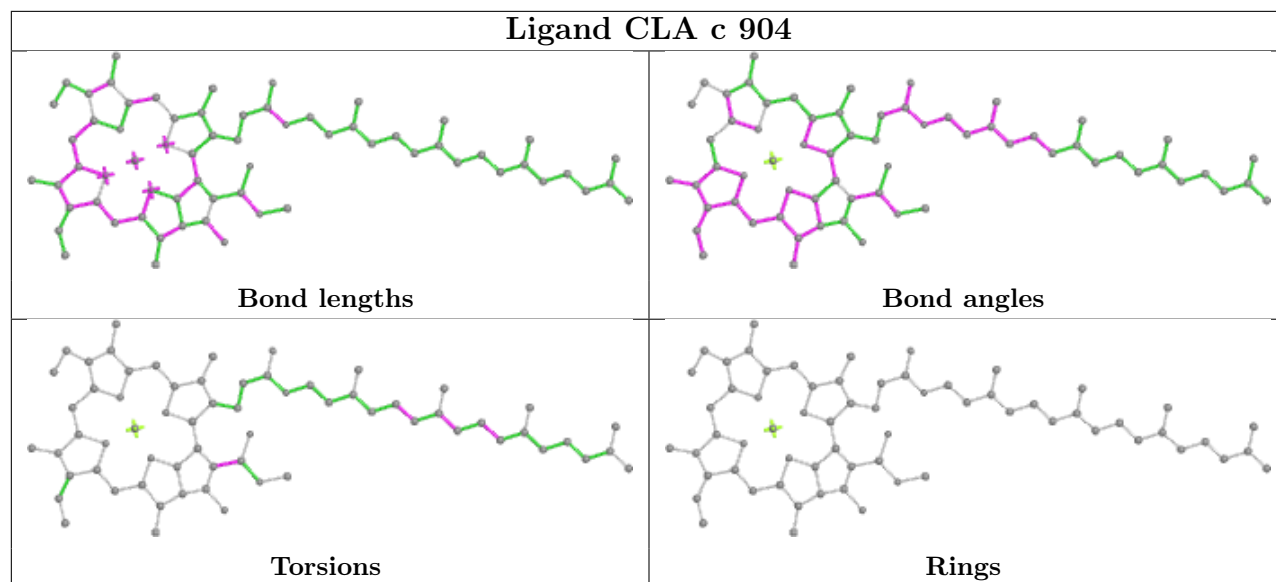


## Ligand LMT j 102

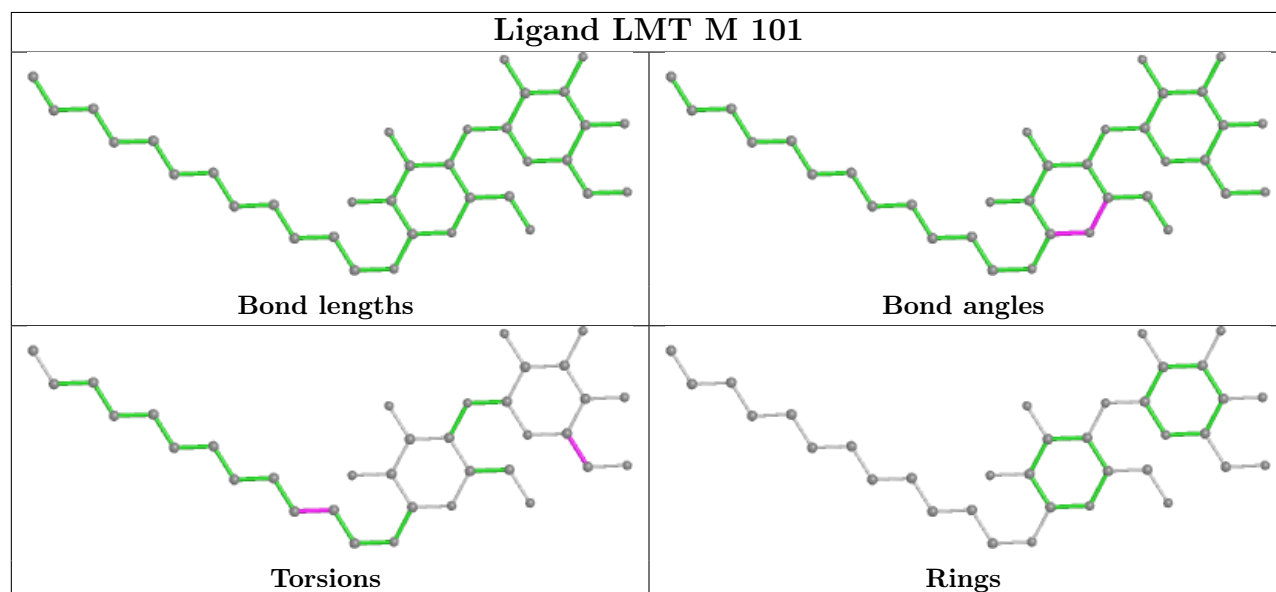




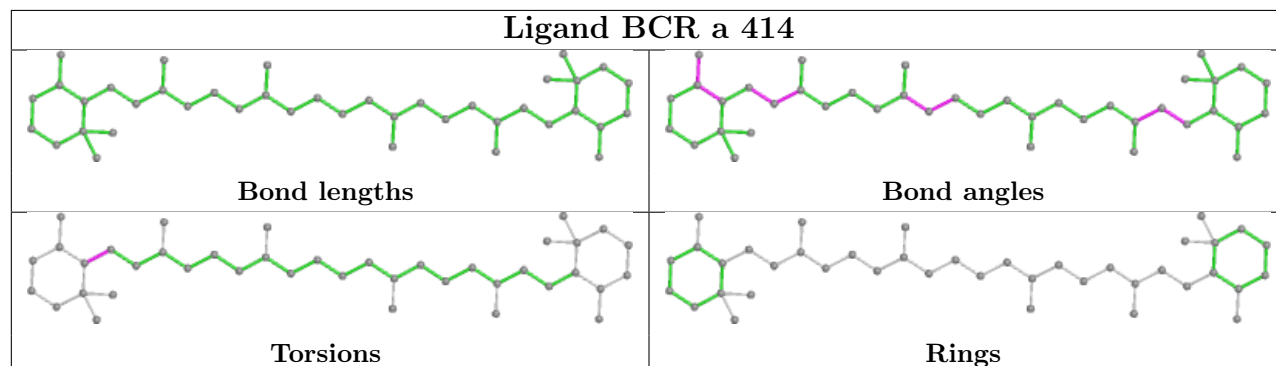
## Ligand CLA c 904



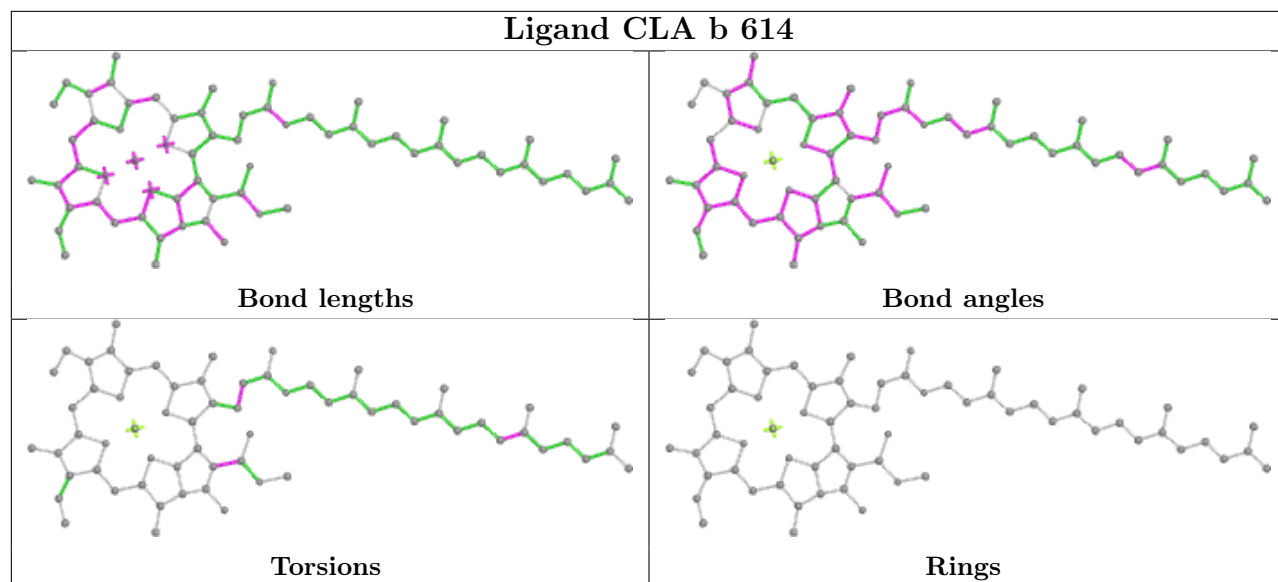
## Ligand LMT M 101



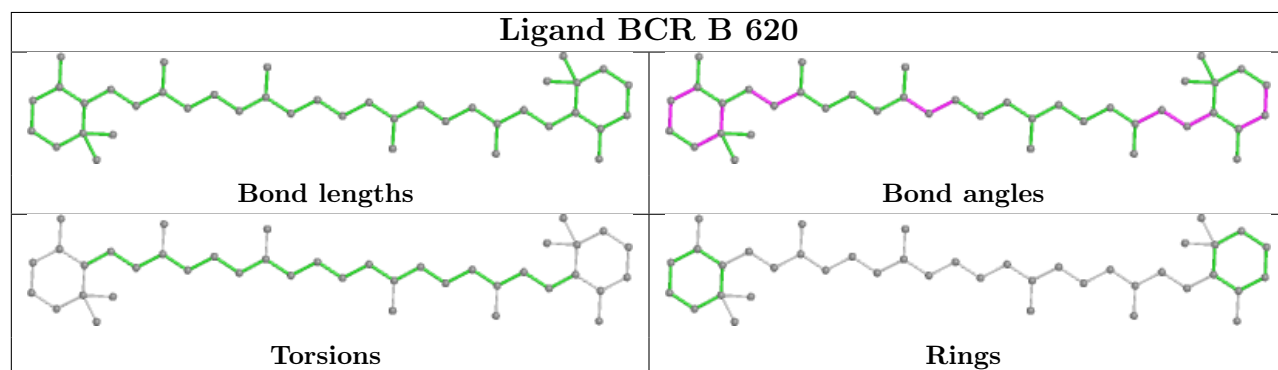
## Ligand BCR a 414



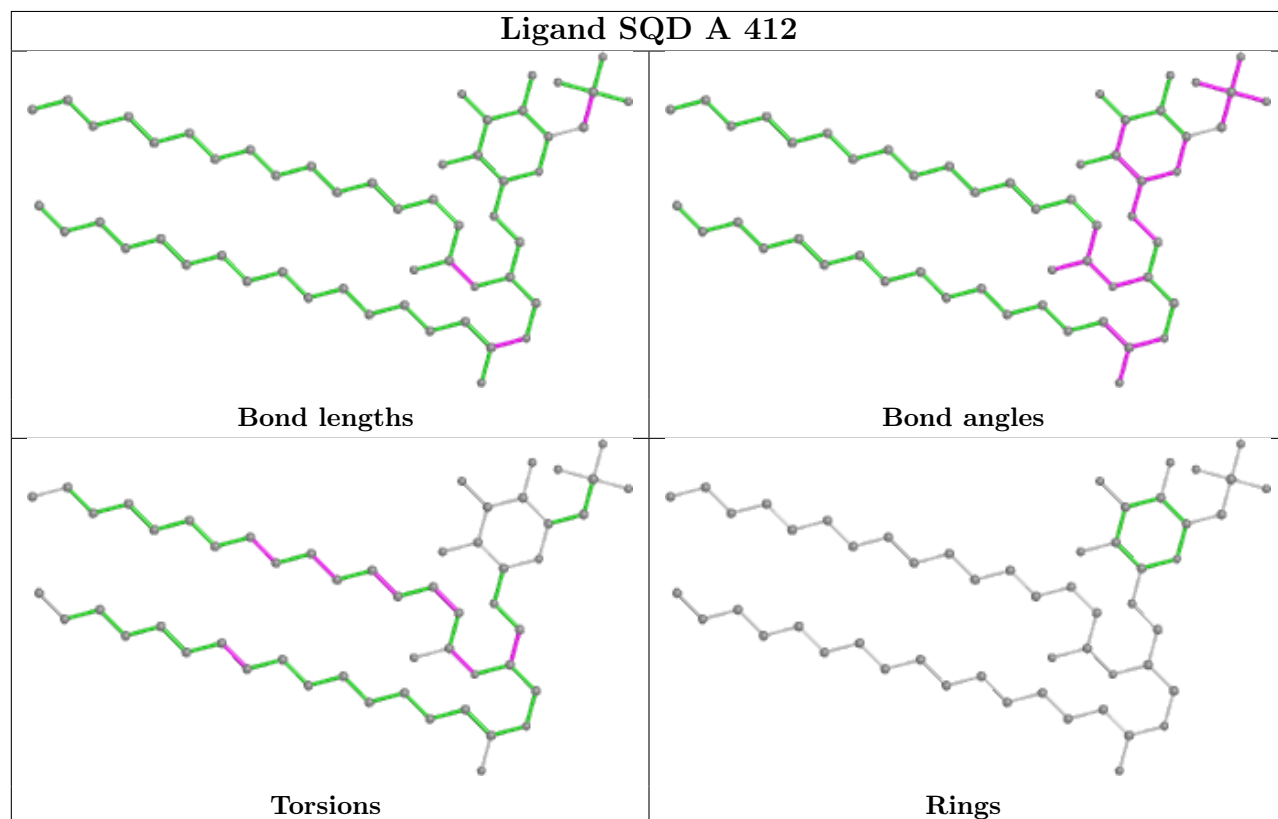
## Ligand CLA b 614



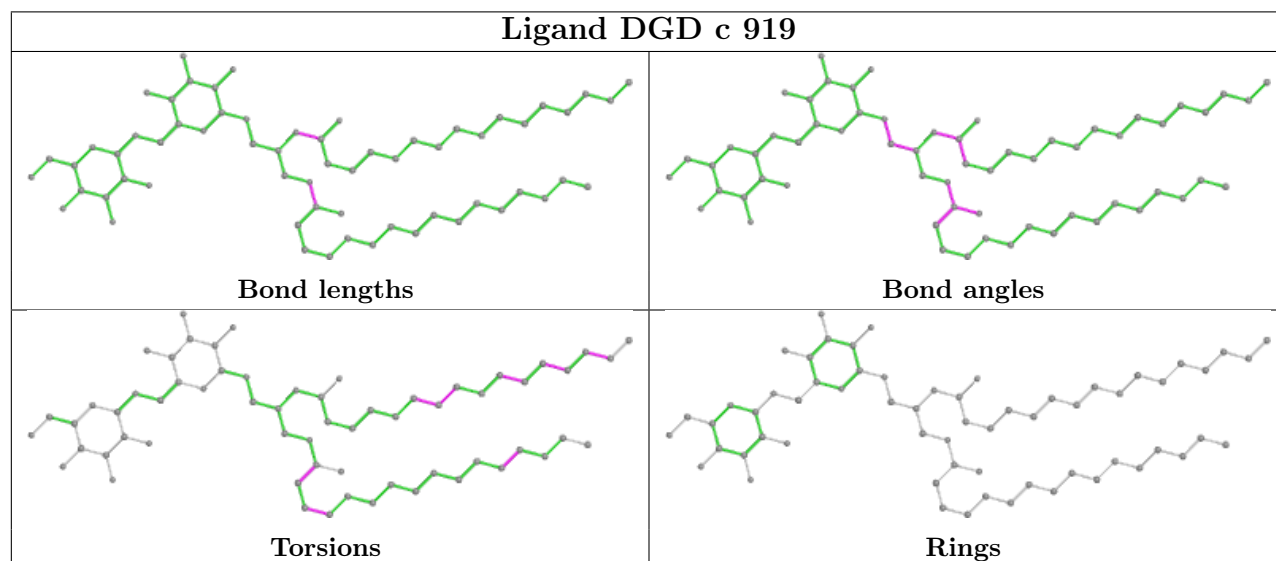
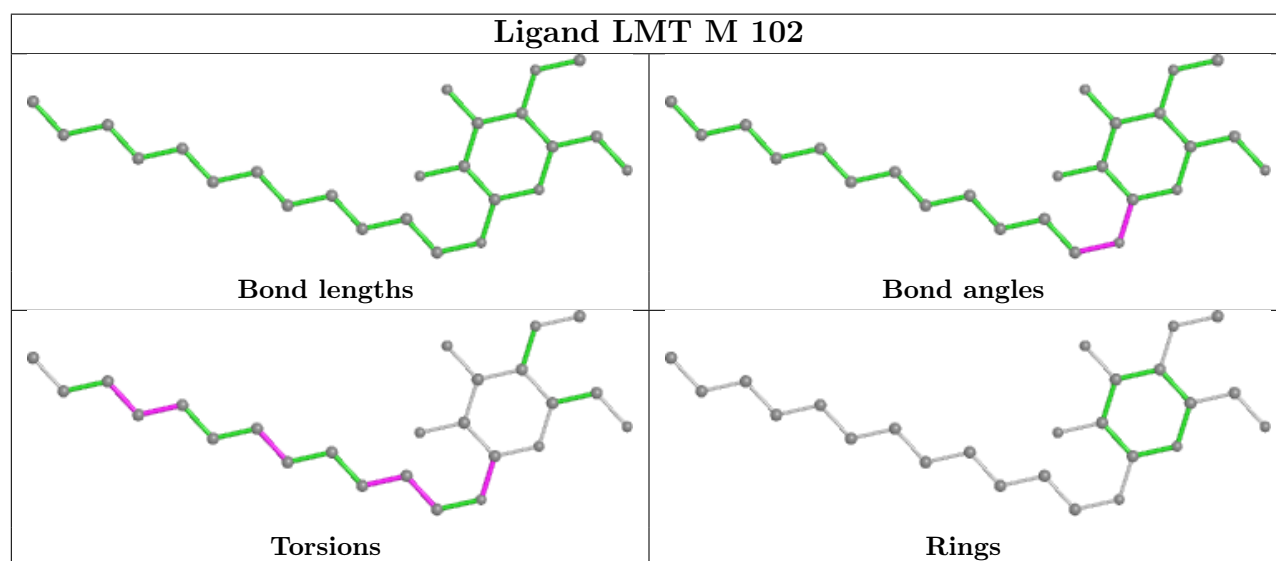
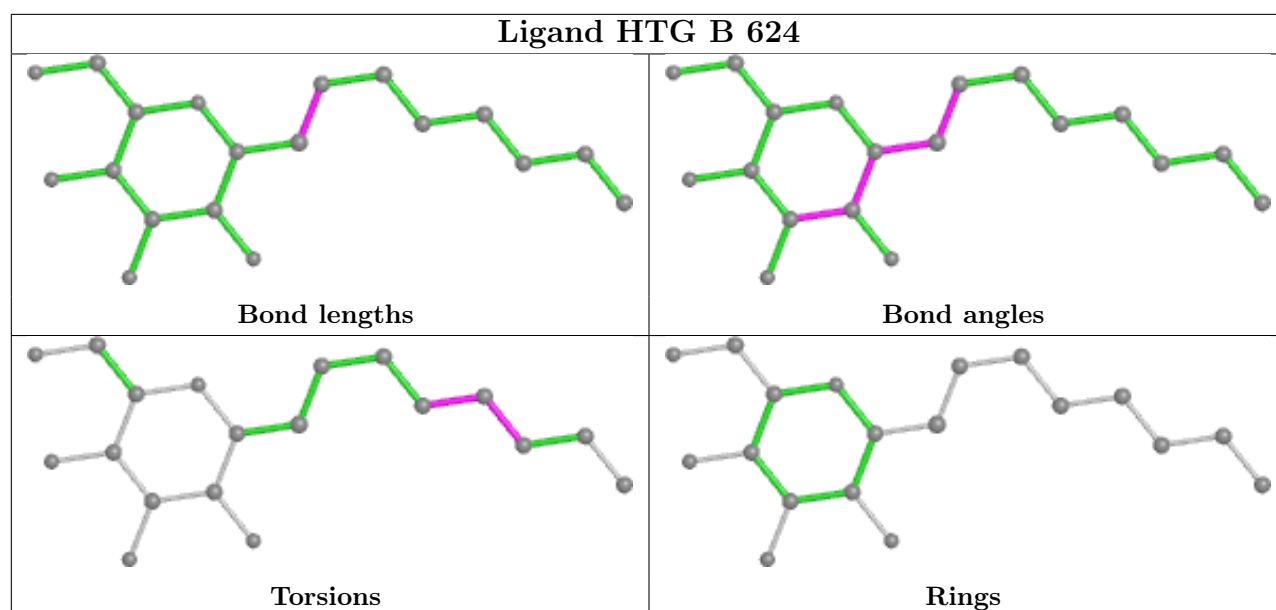
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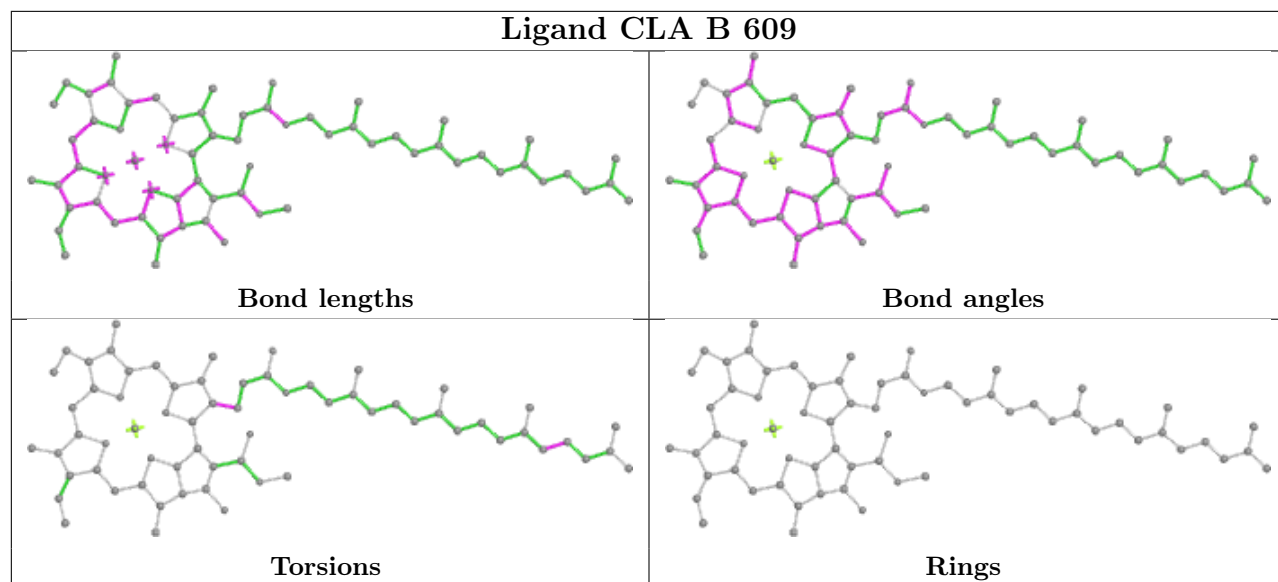
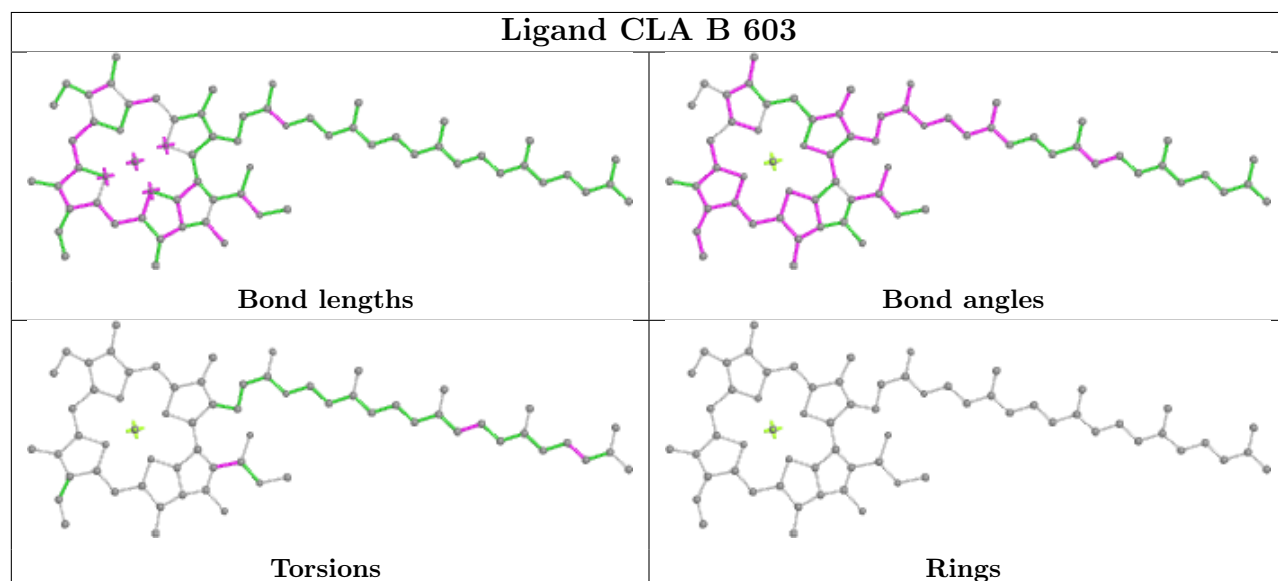
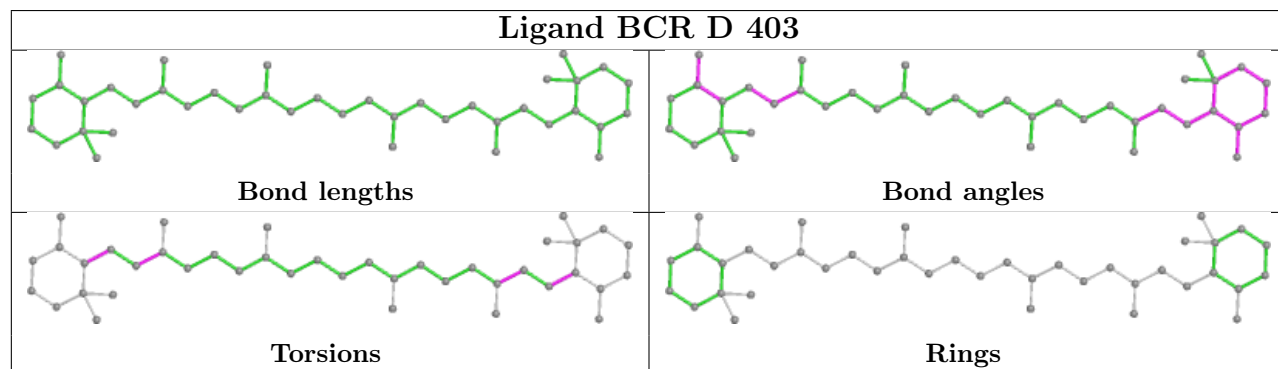


## Ligand SQD A 412

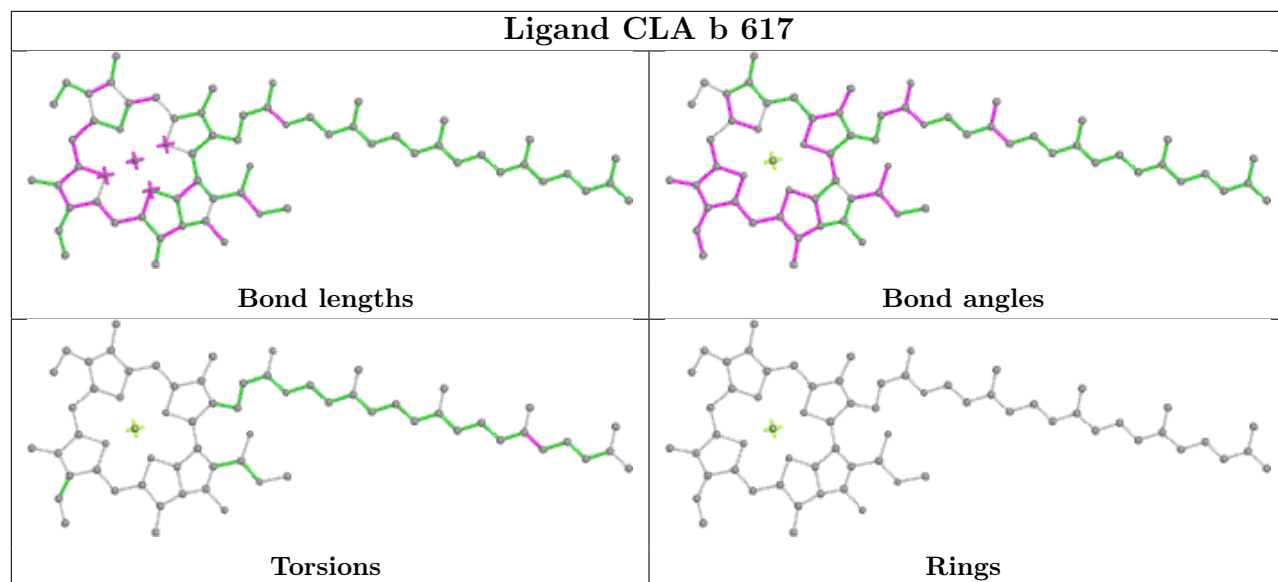




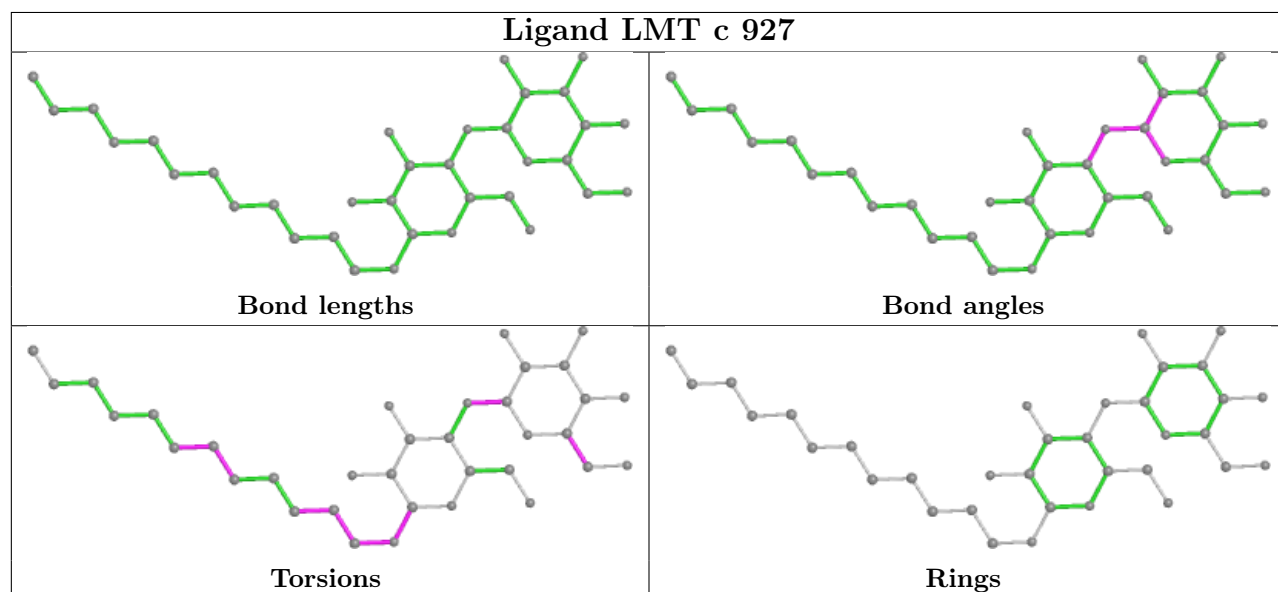


**Ligand CLA B 609****Ligand CLA B 603****Ligand BCR D 403**

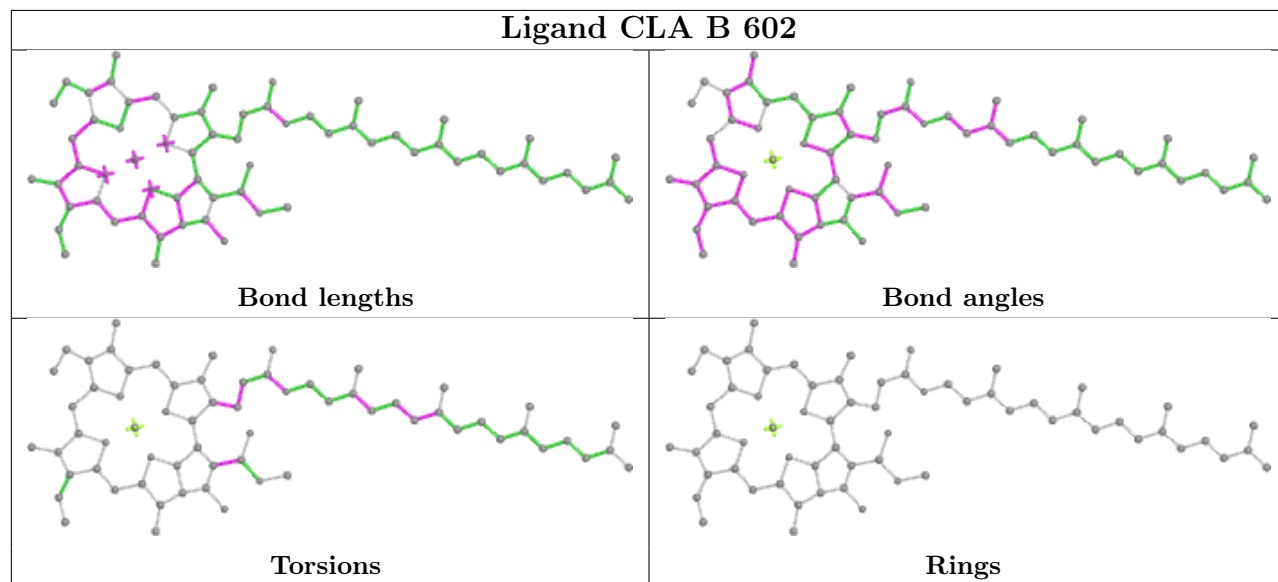
## Ligand CLA b 617

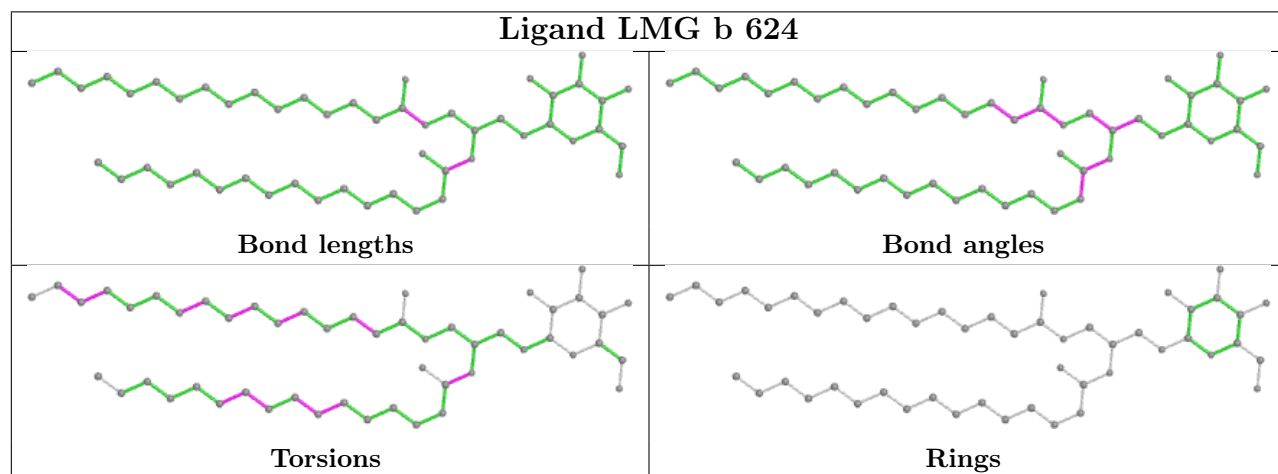
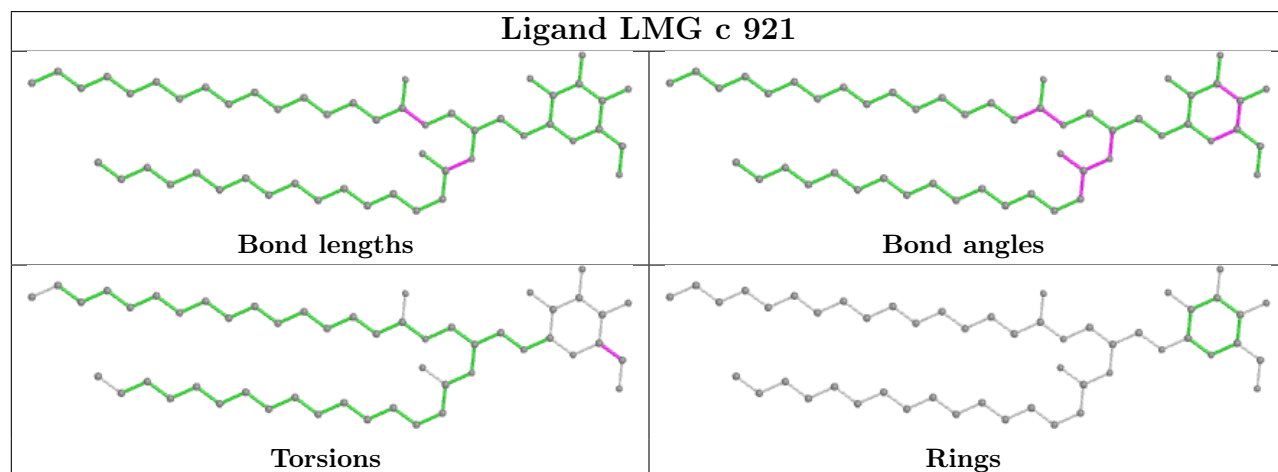
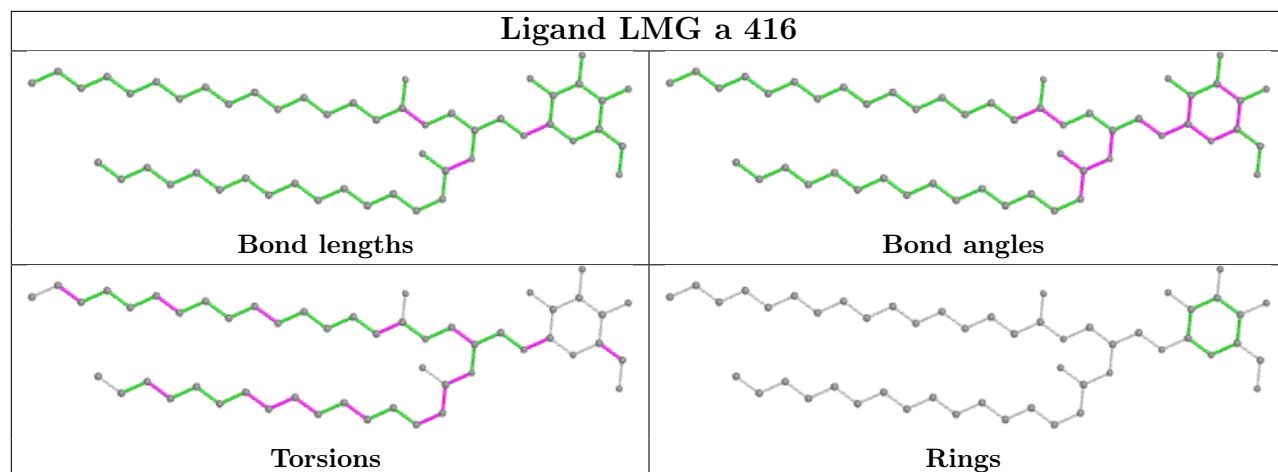


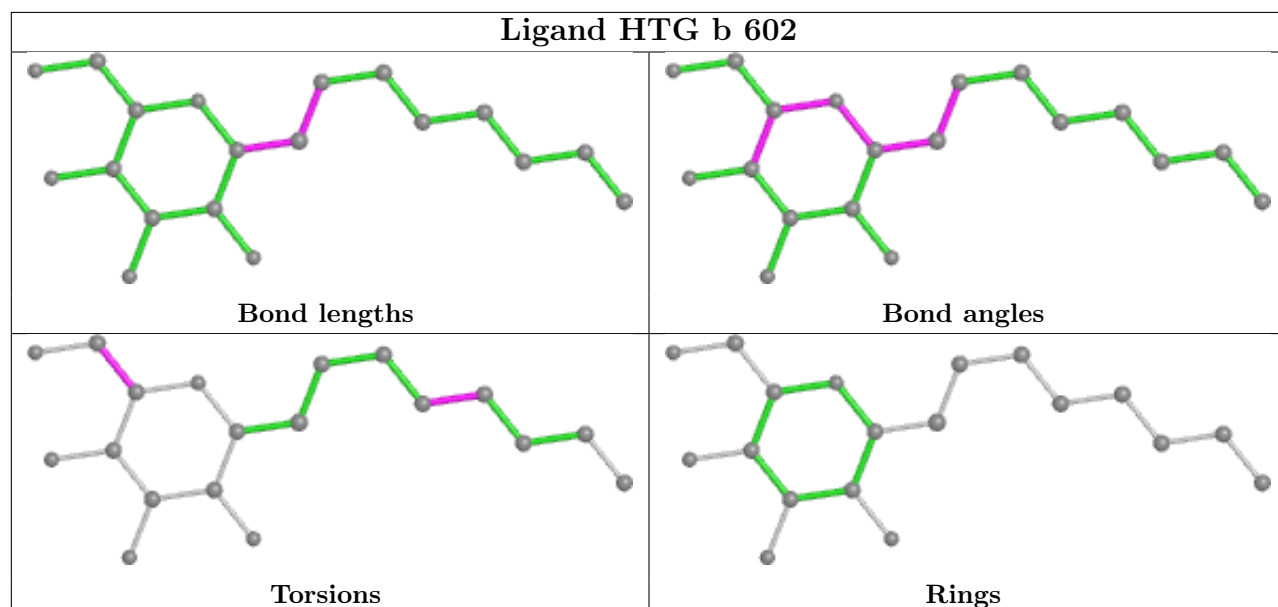
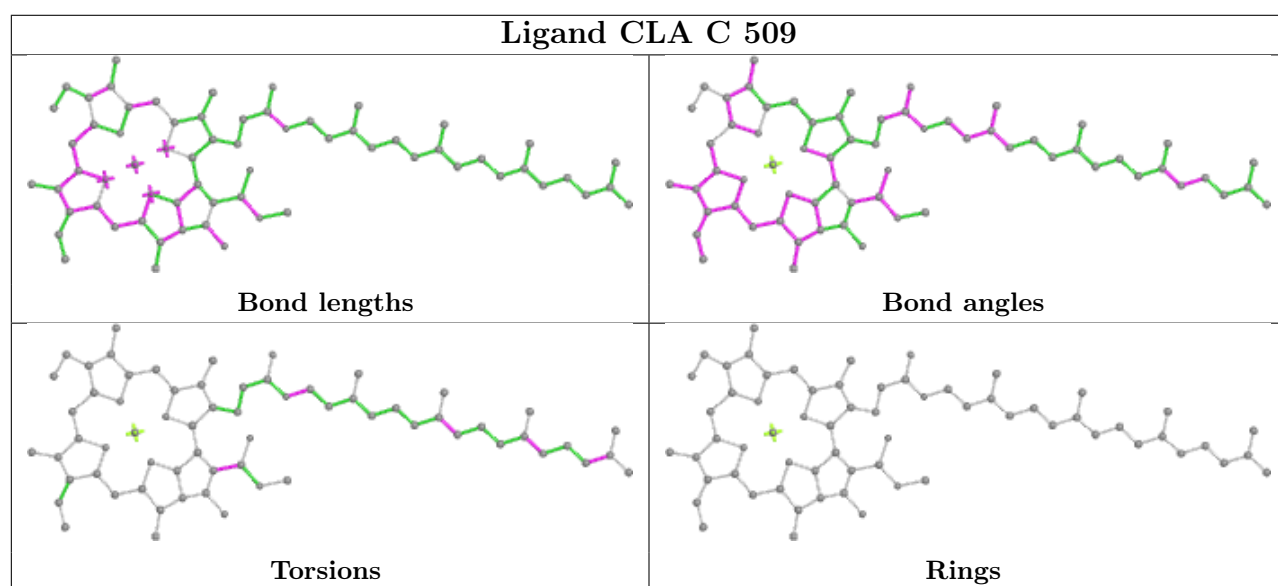
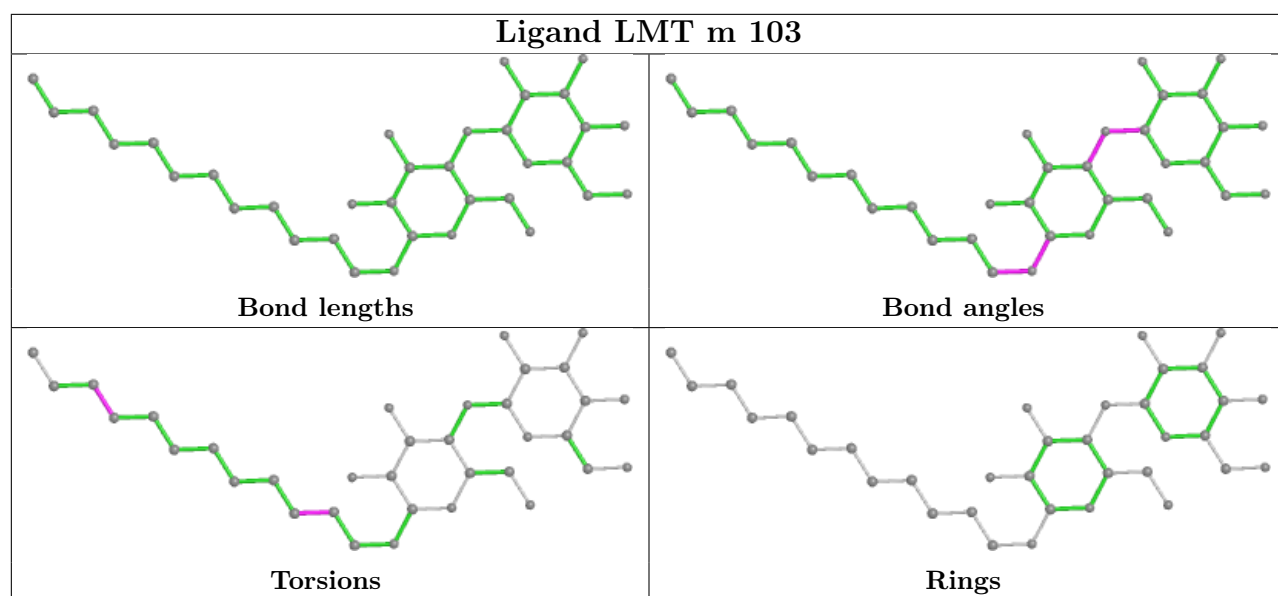
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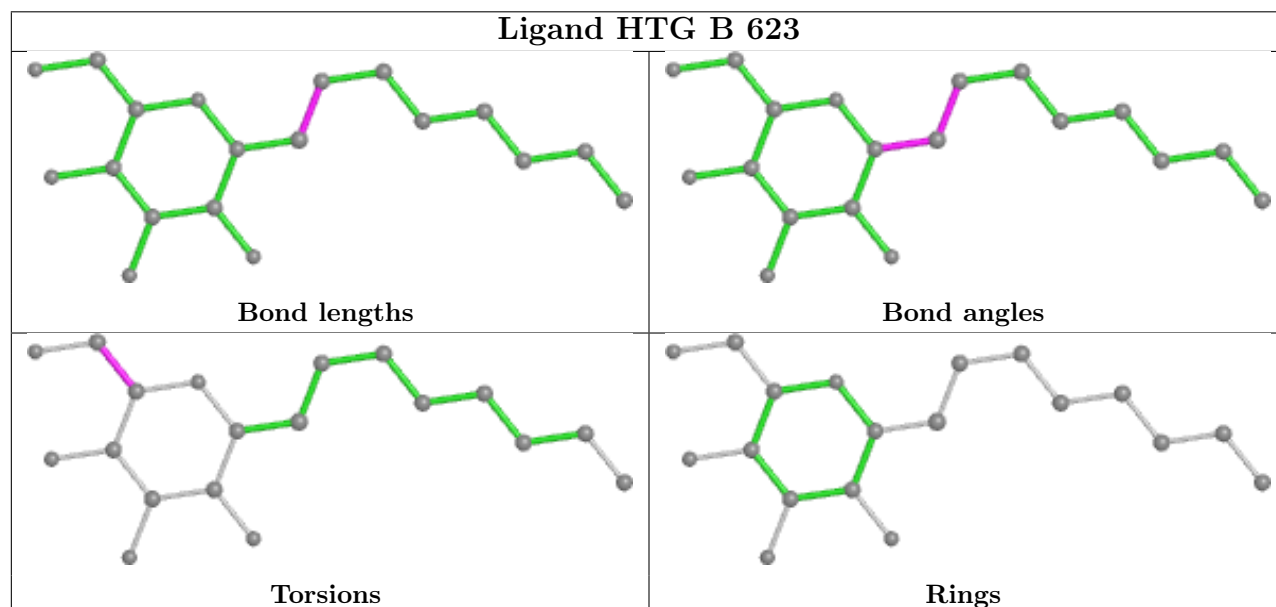
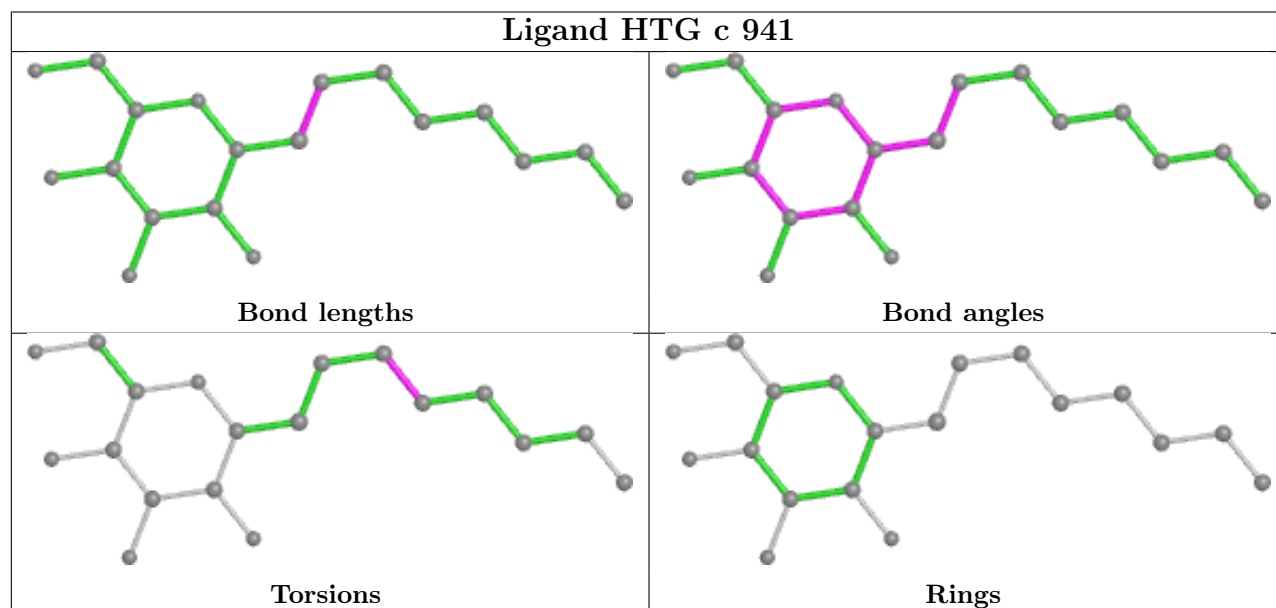
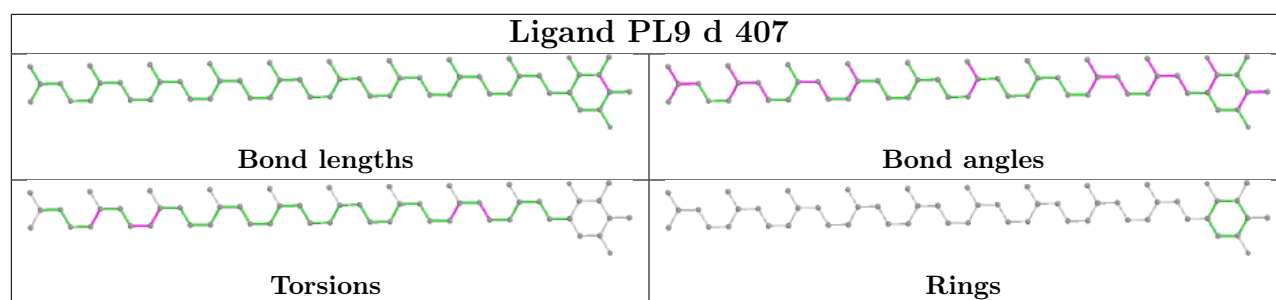


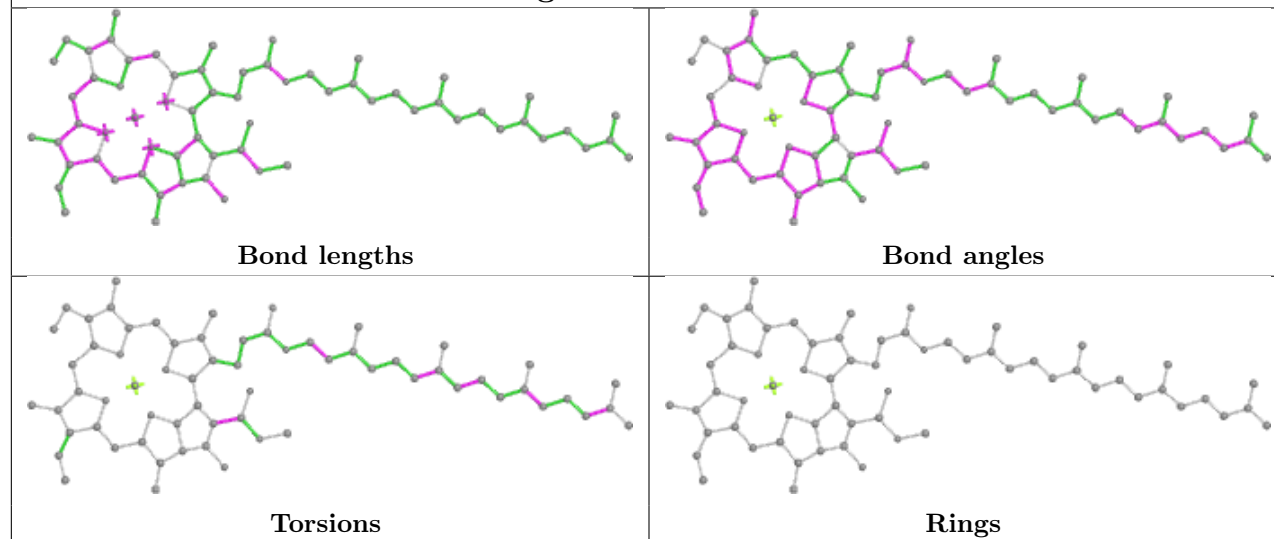
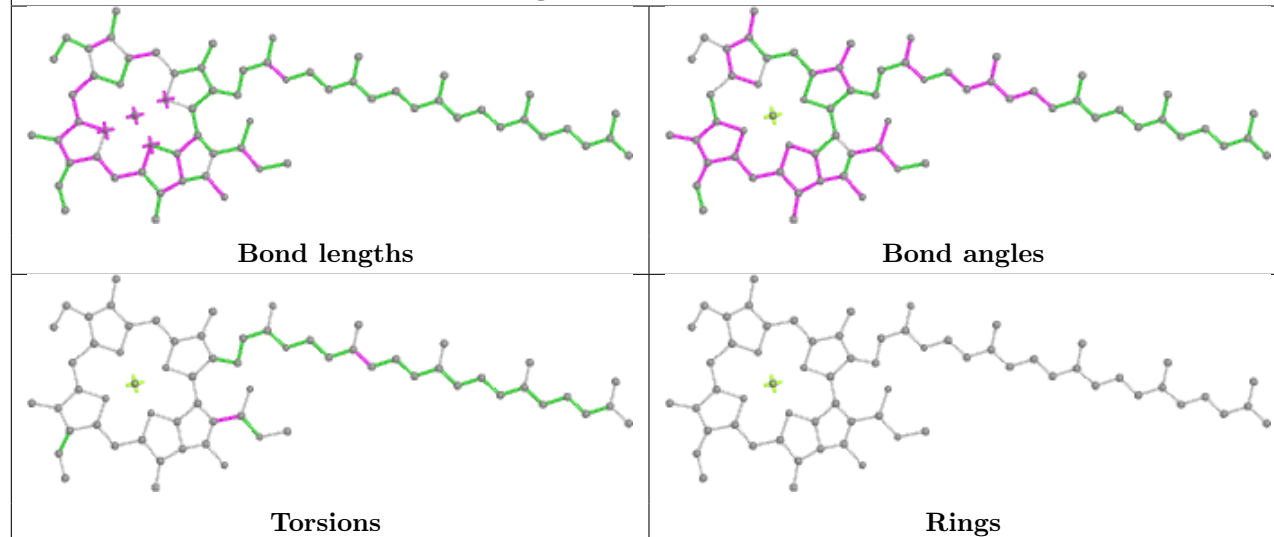
## Ligand CLA B 602

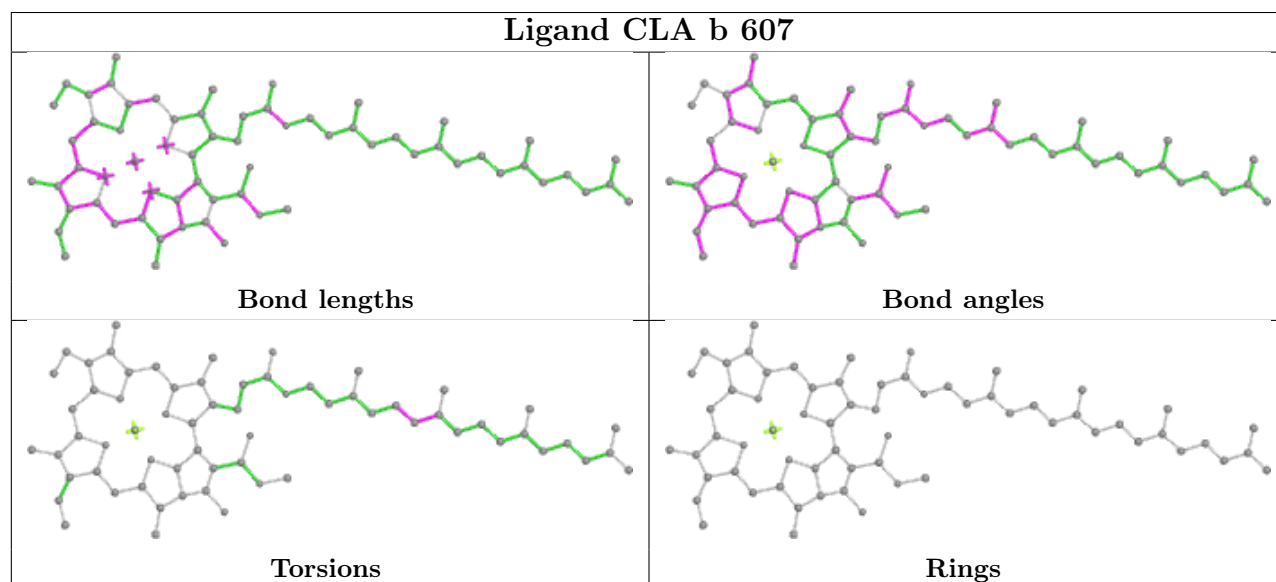
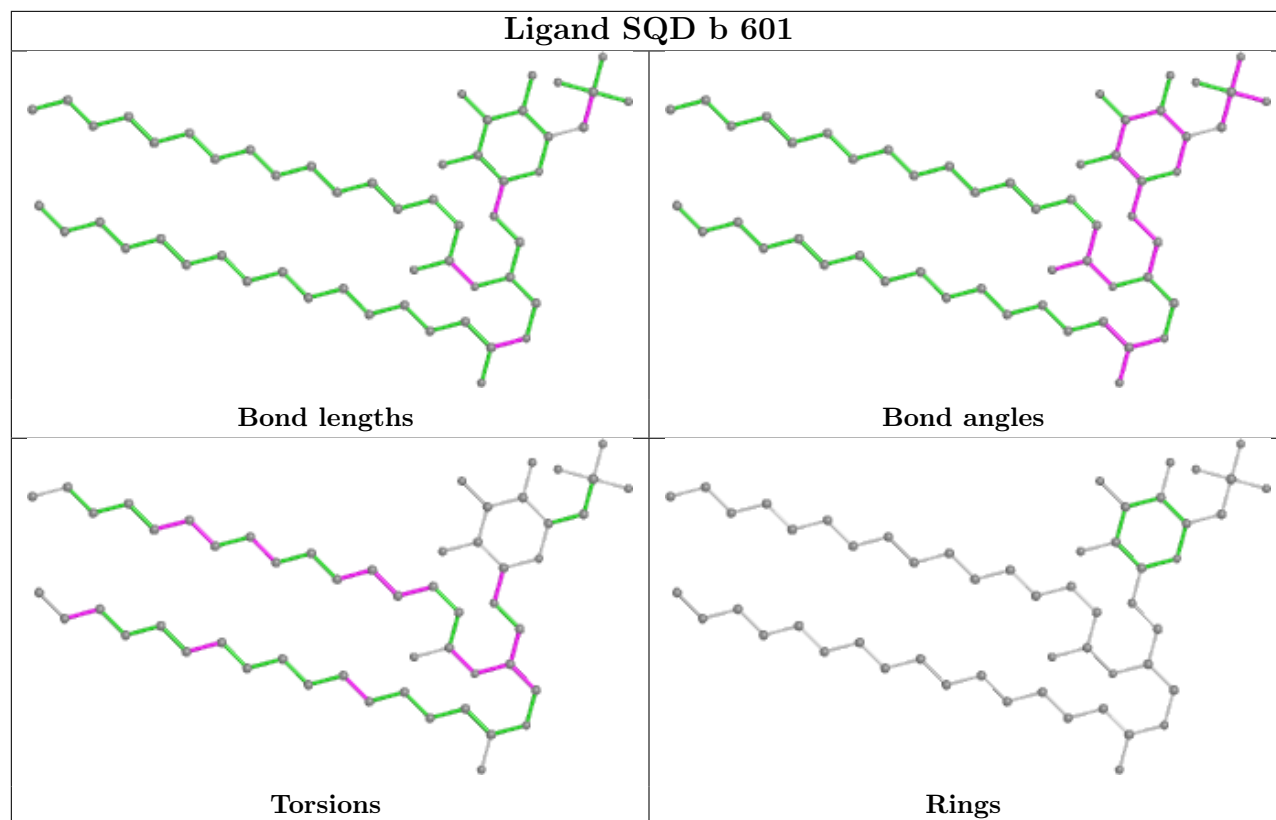




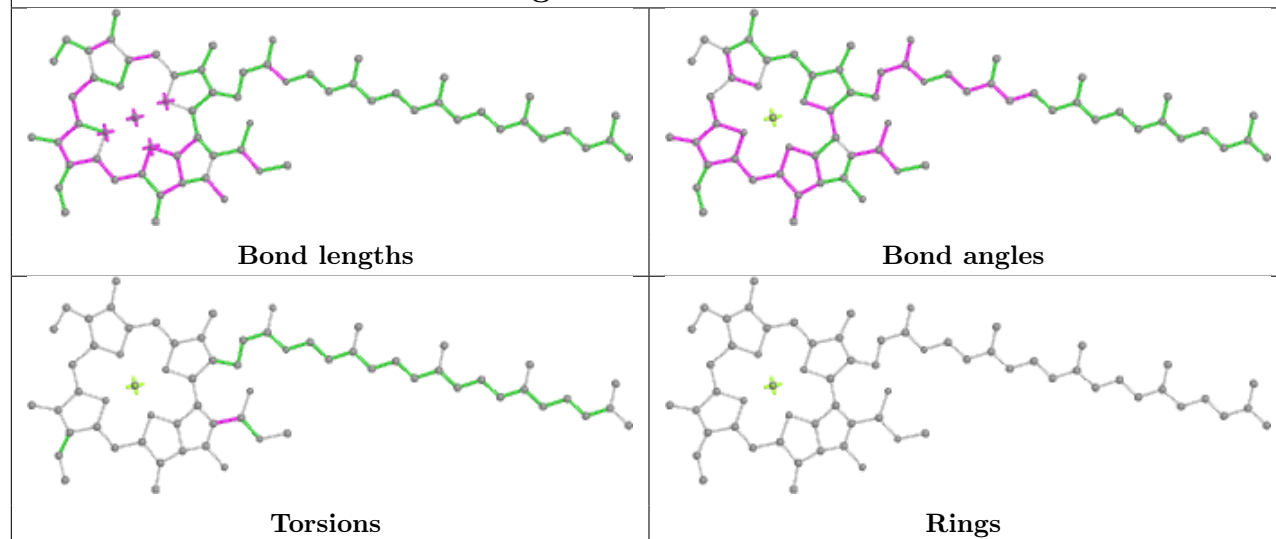
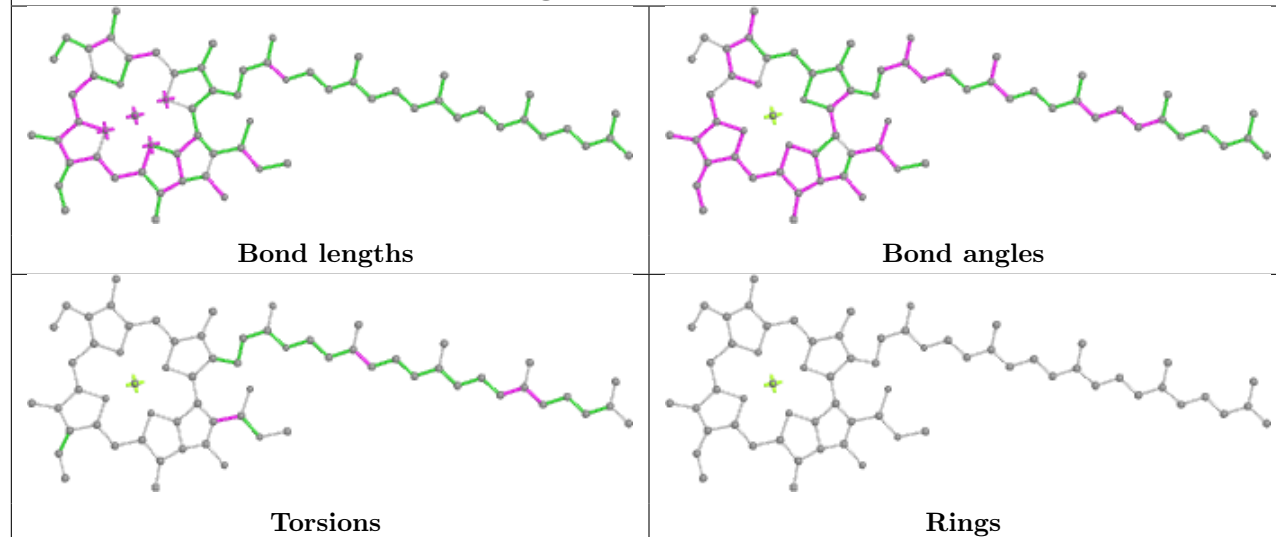
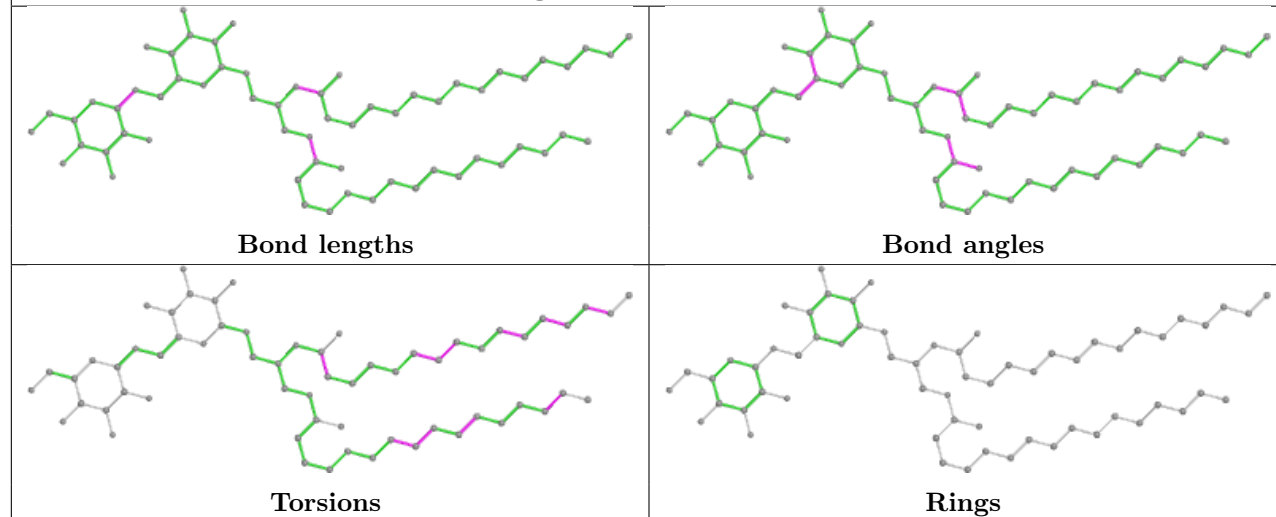




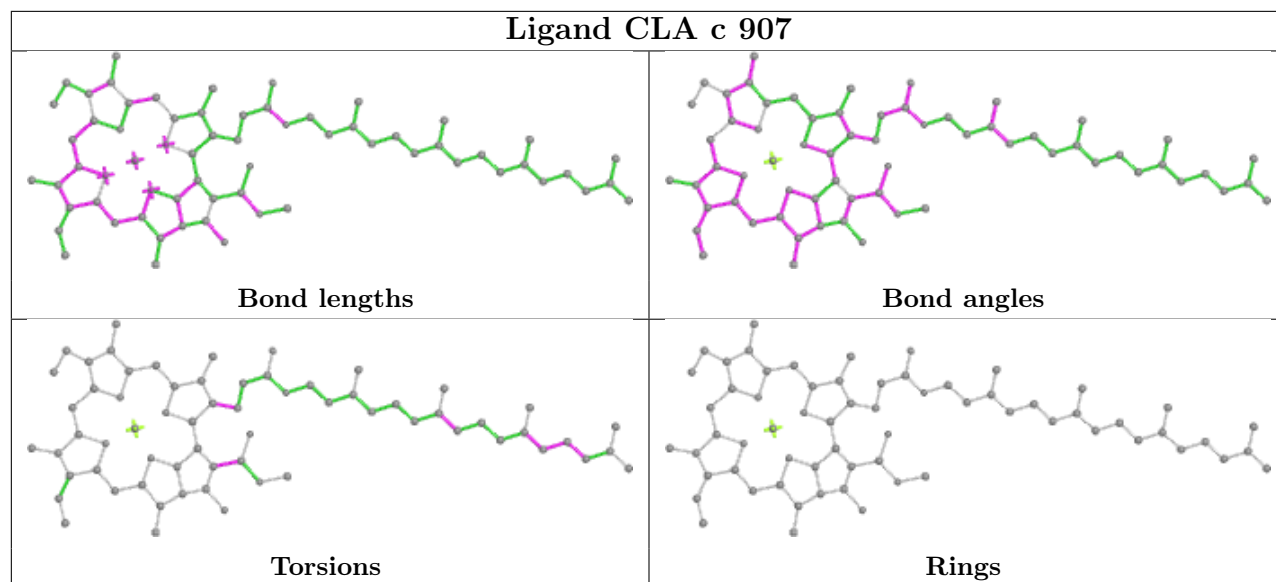
**Ligand CLA c 910****Ligand CLA B 606**



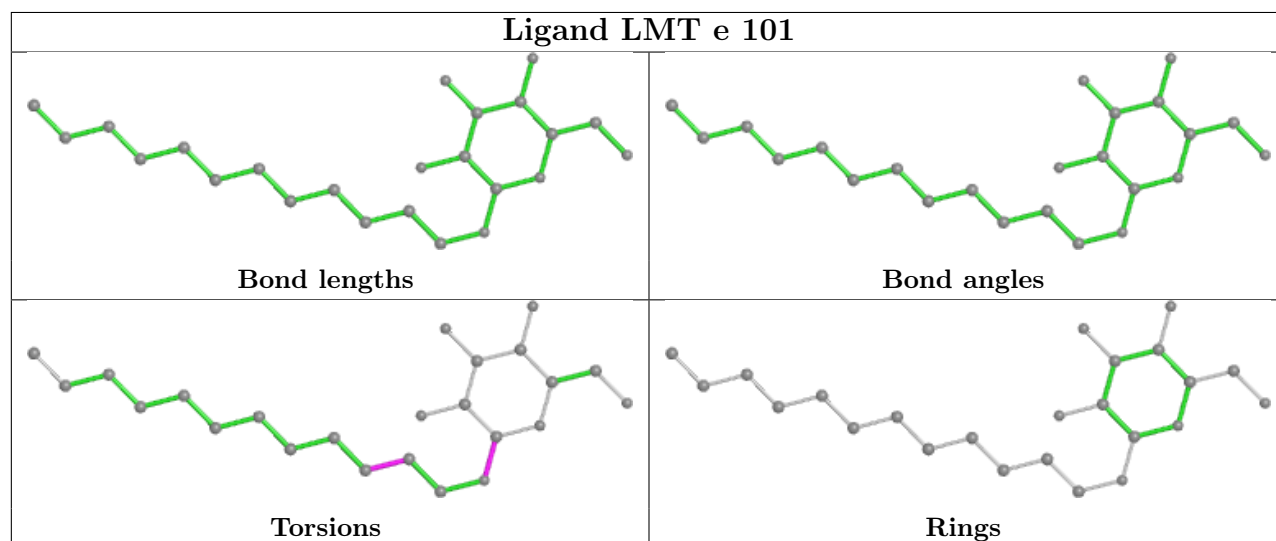


**Ligand CLA B 605****Ligand CLA c 905****Ligand DGD h 102**

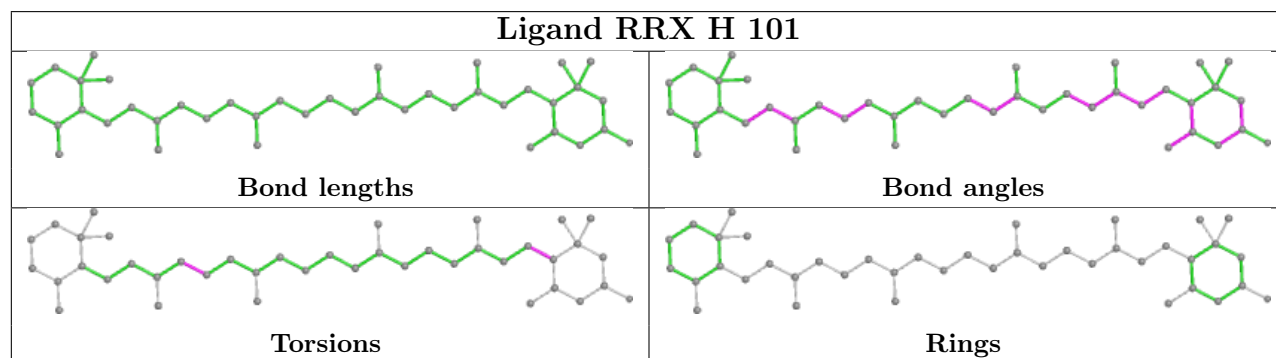
## Ligand CLA c 907



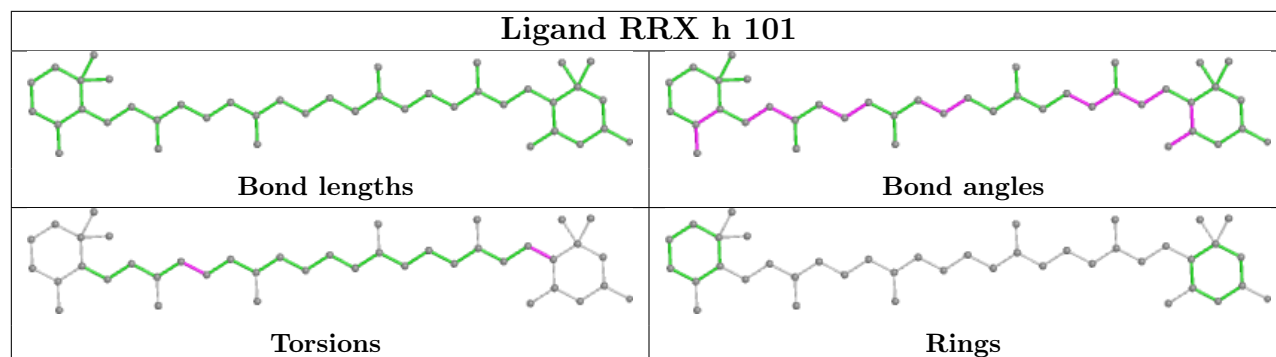
## Ligand LMT e 101



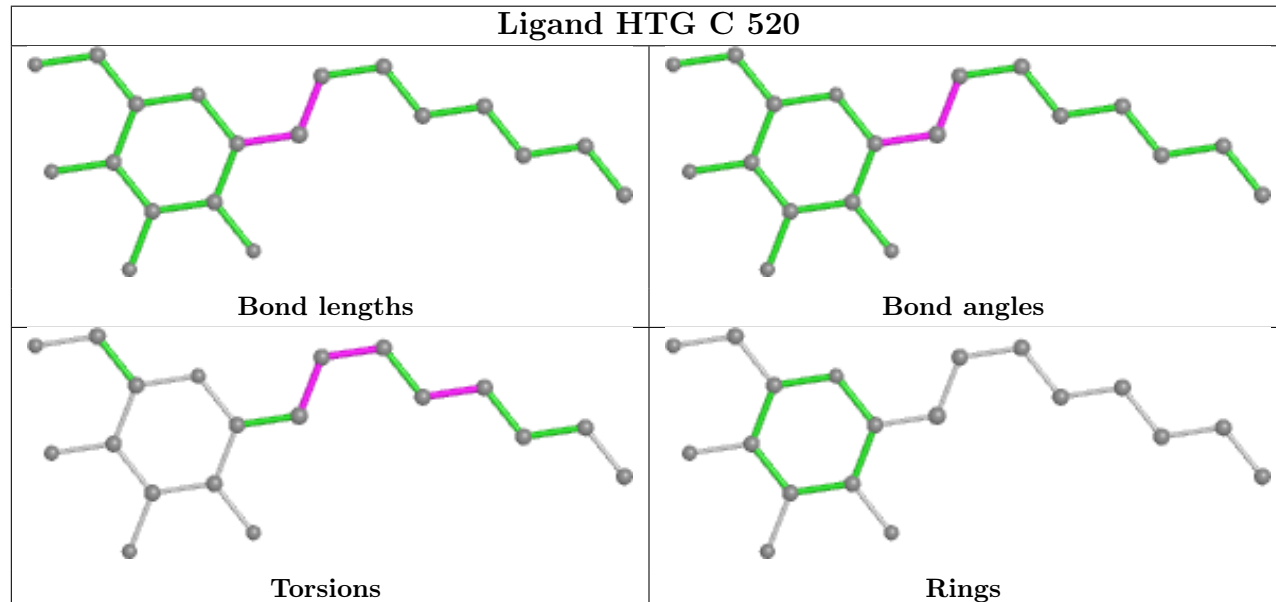
## Ligand RRX H 101



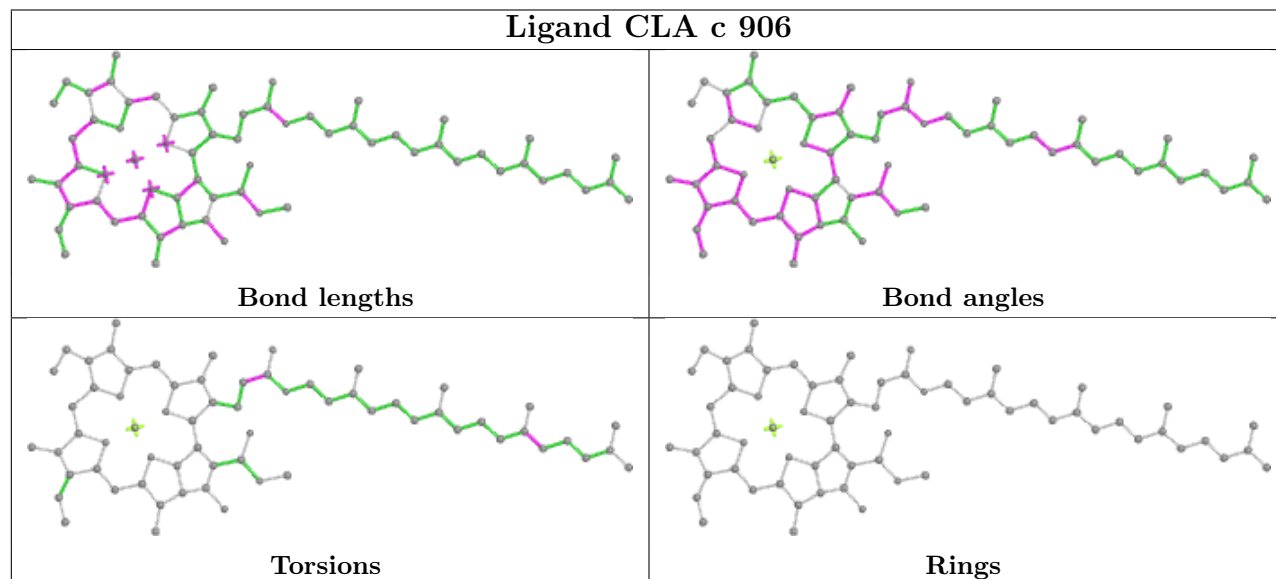
## Ligand RRX h 101

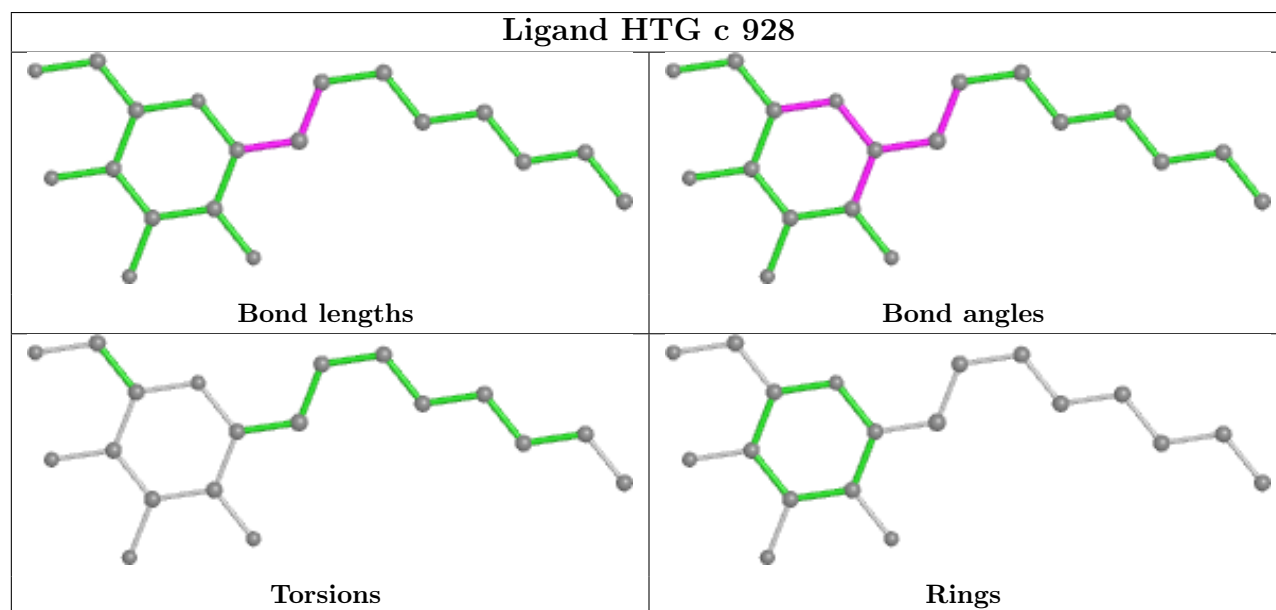
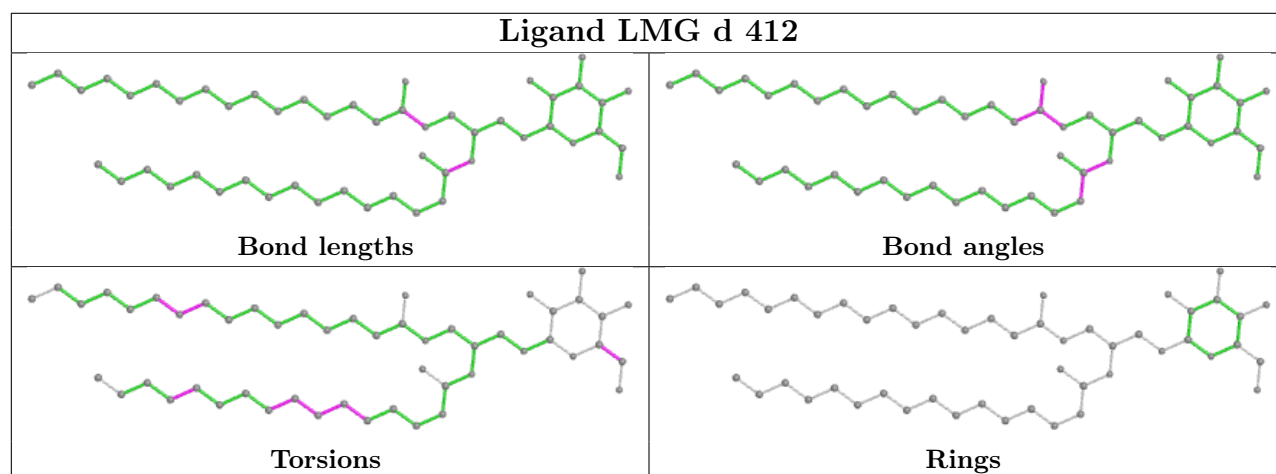
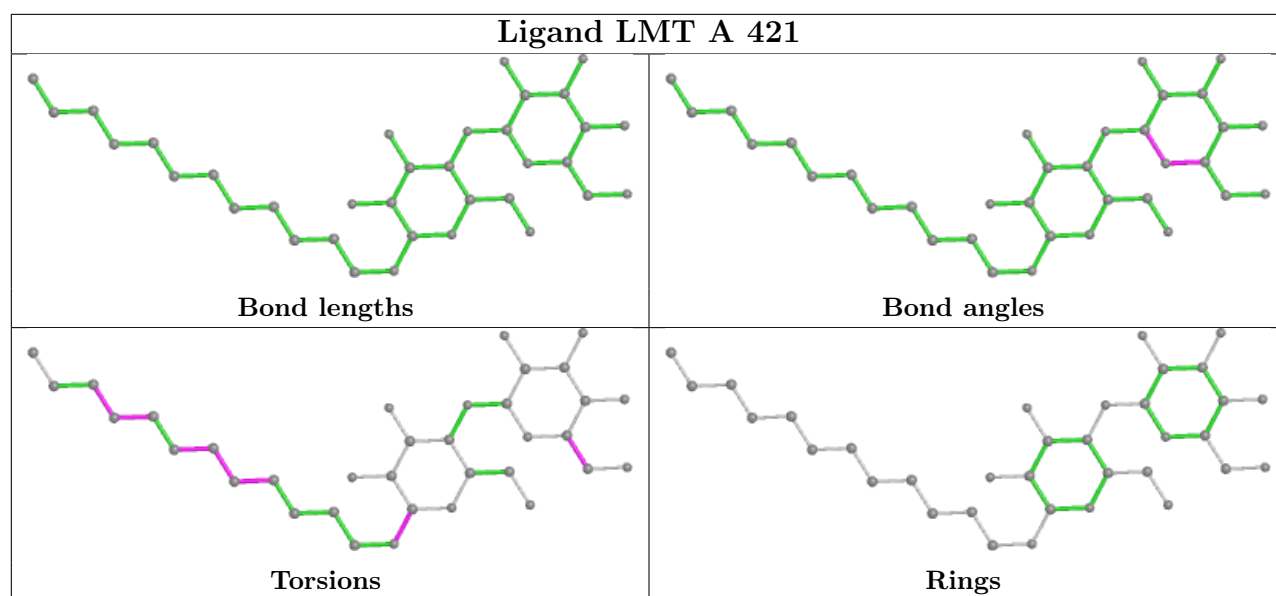


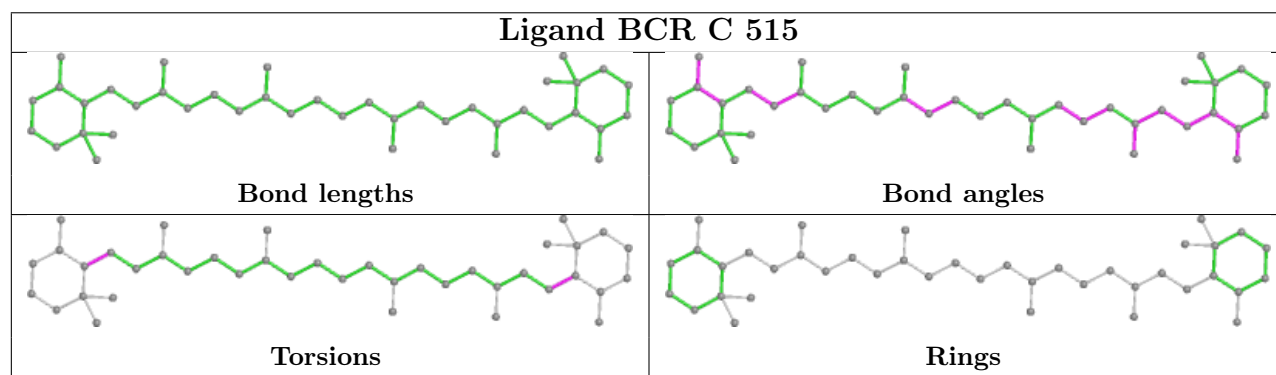
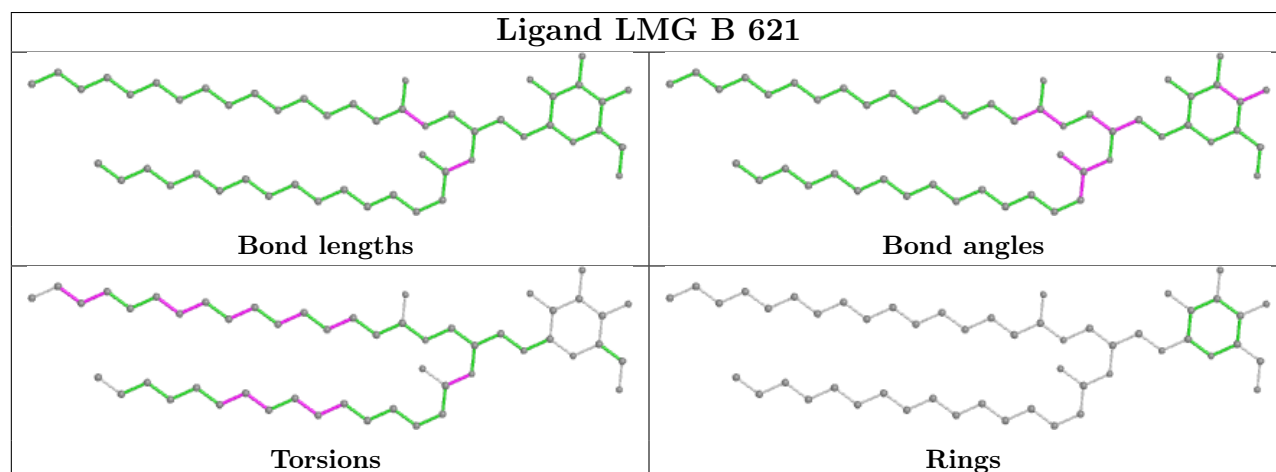
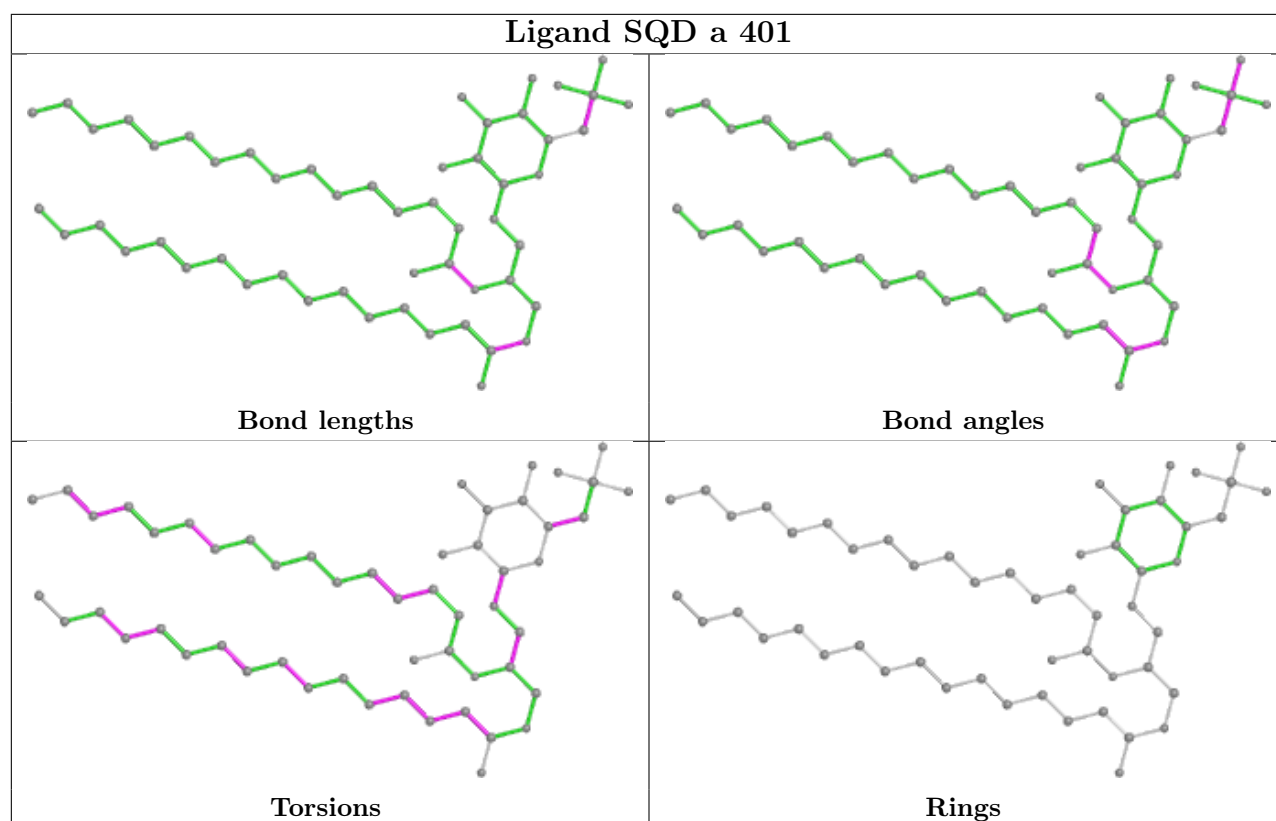
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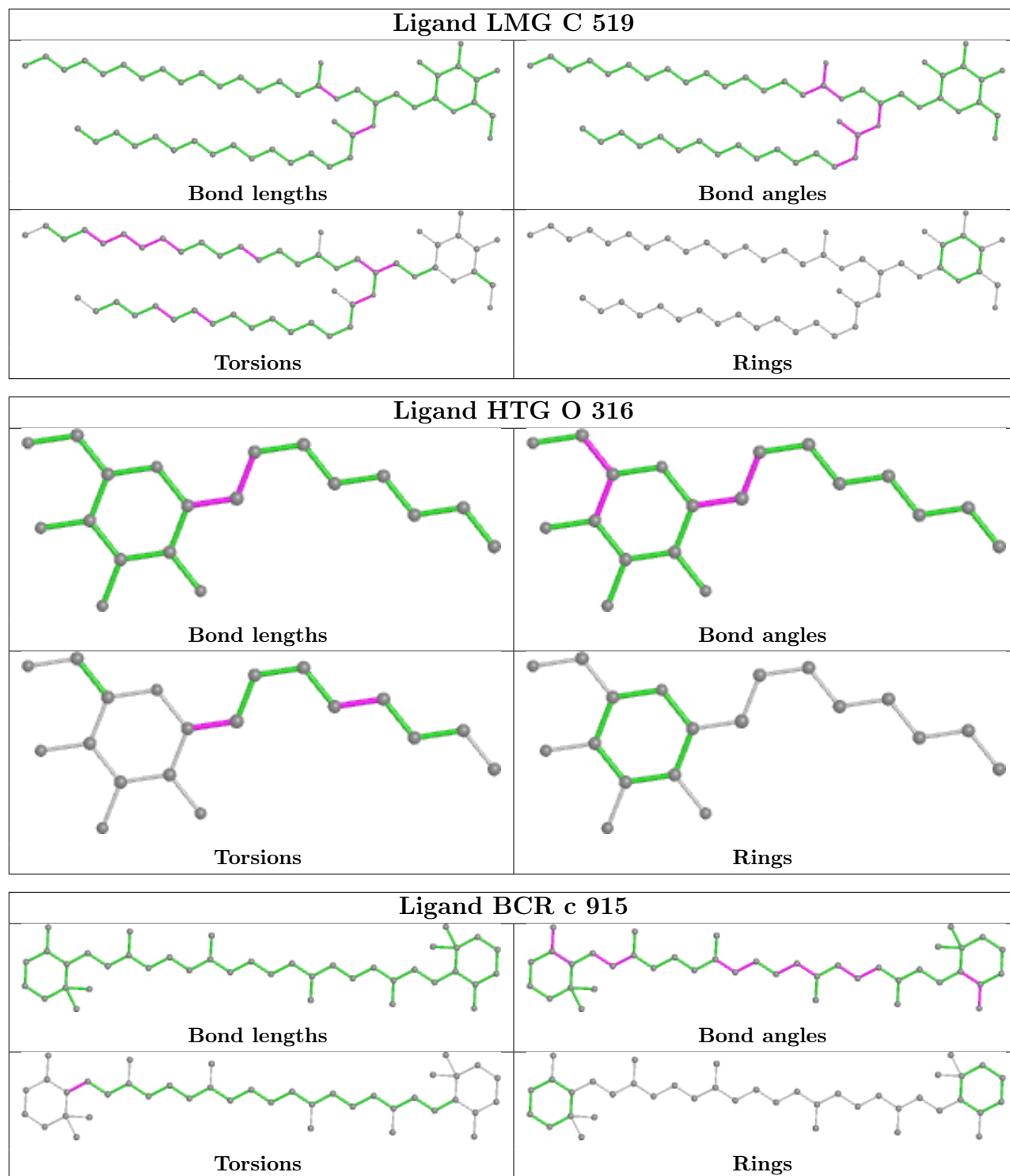


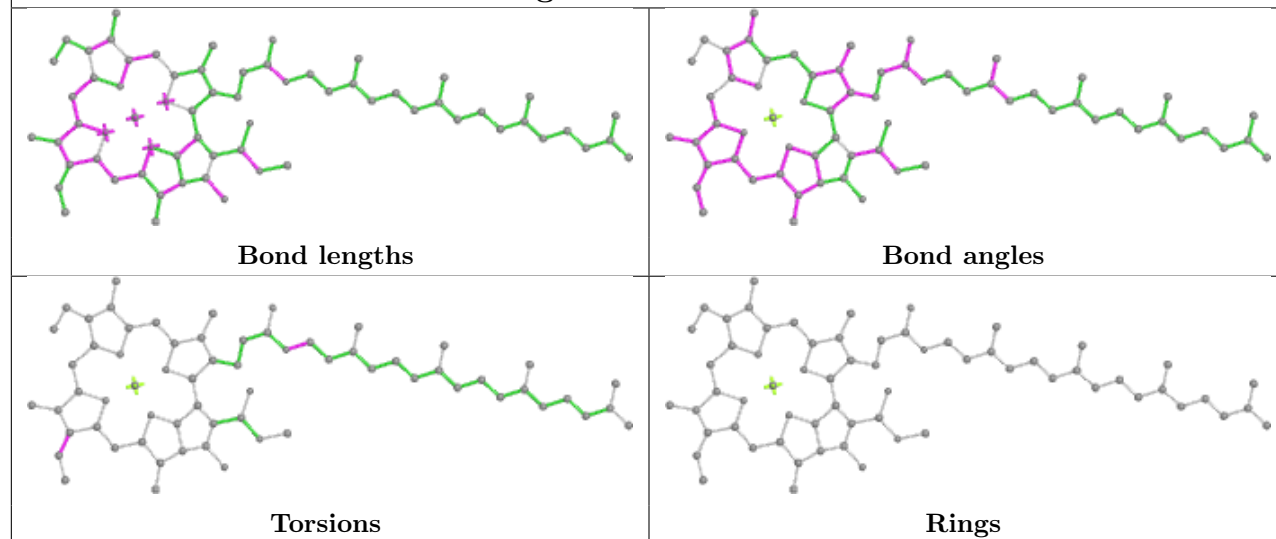
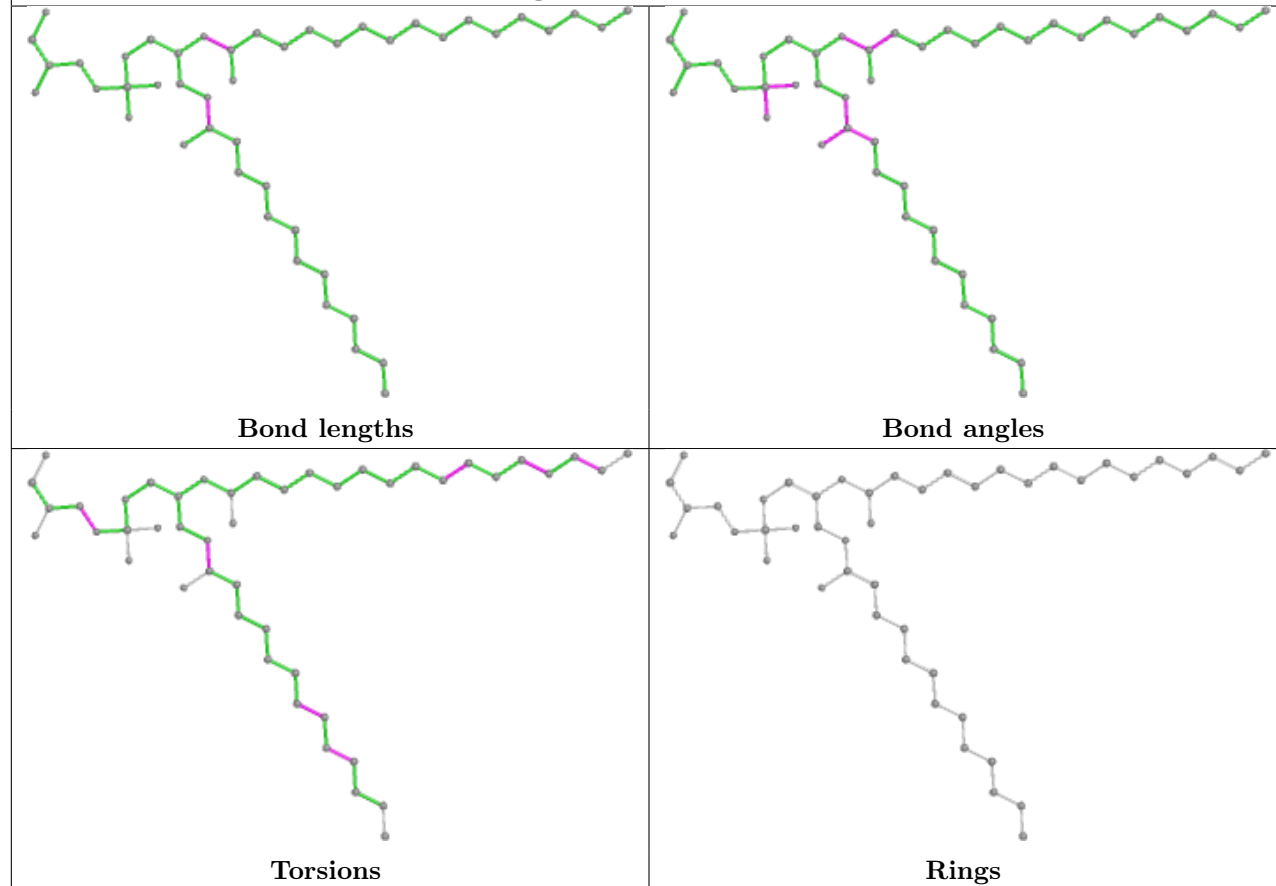
## Ligand CLA c 906

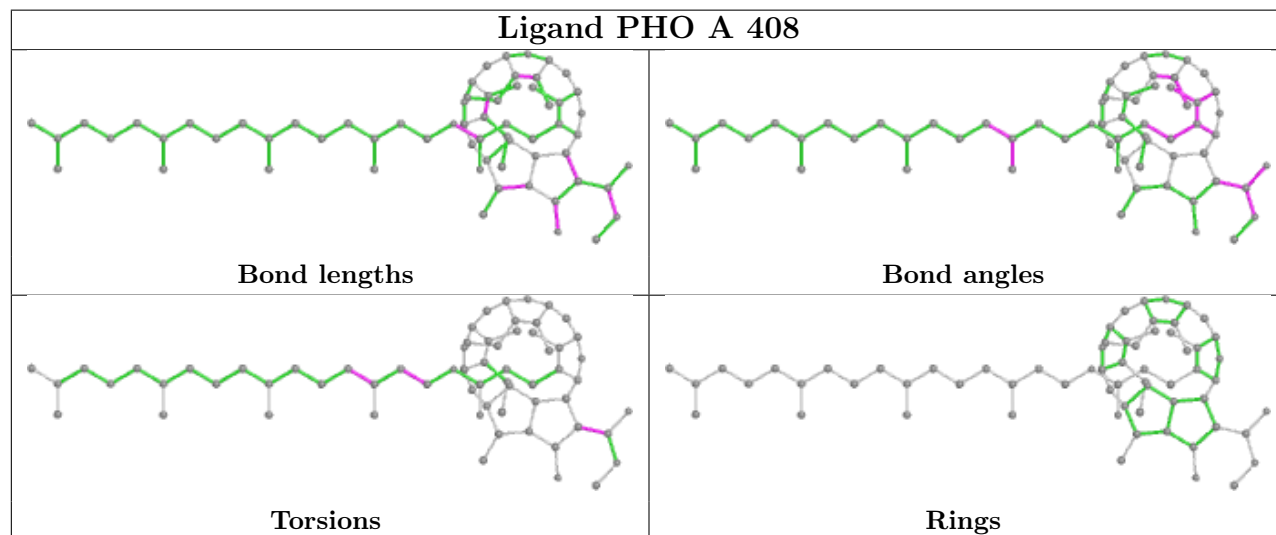
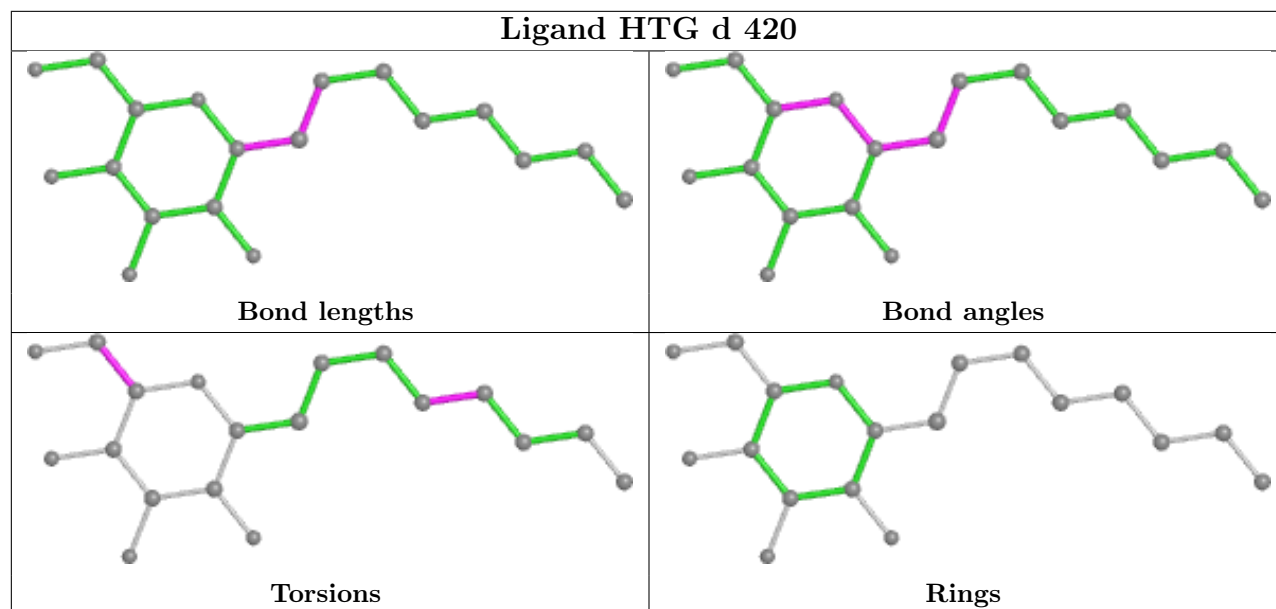
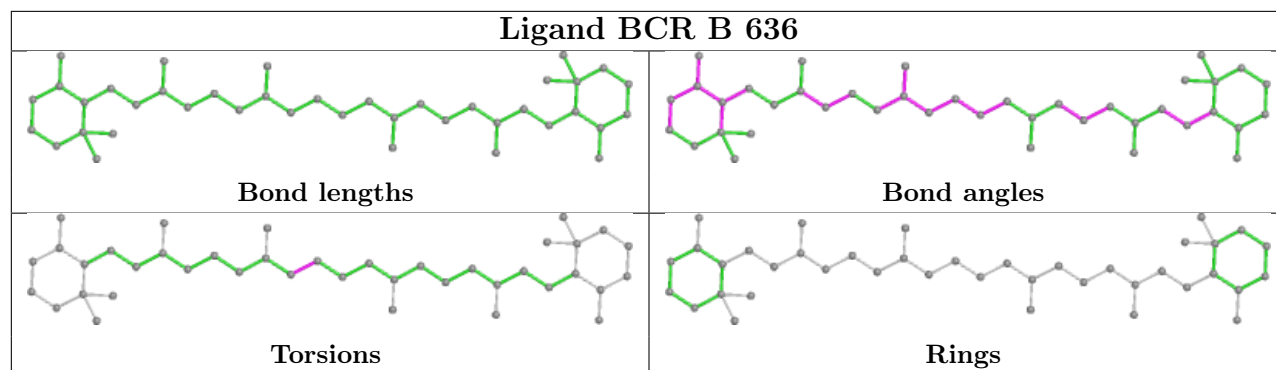




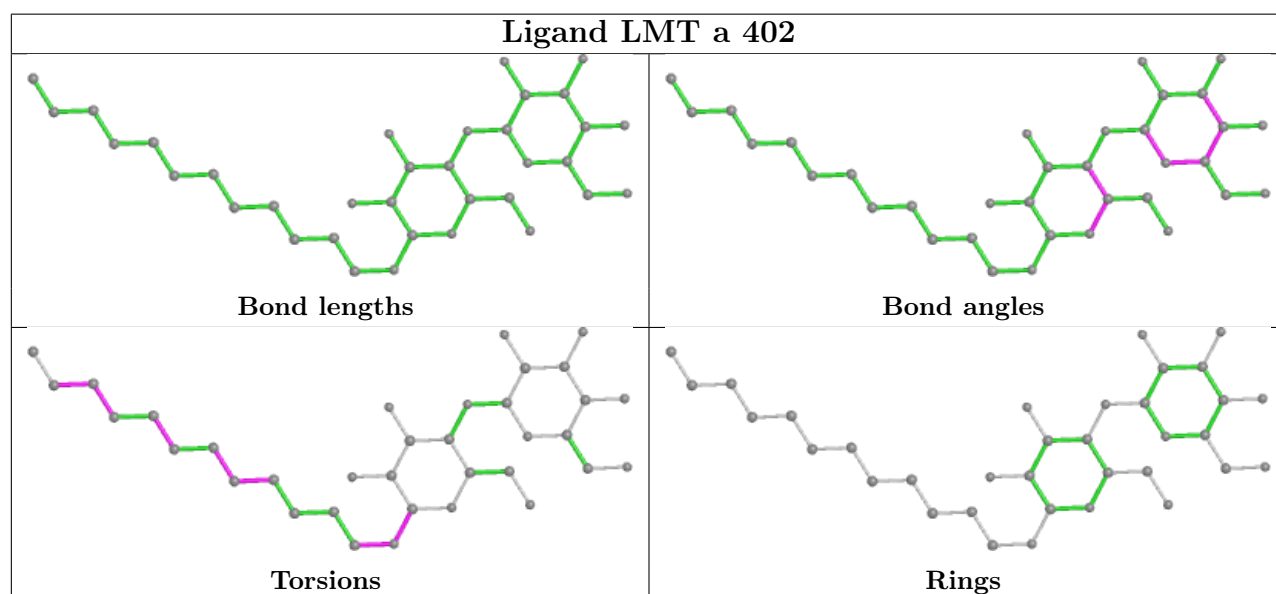
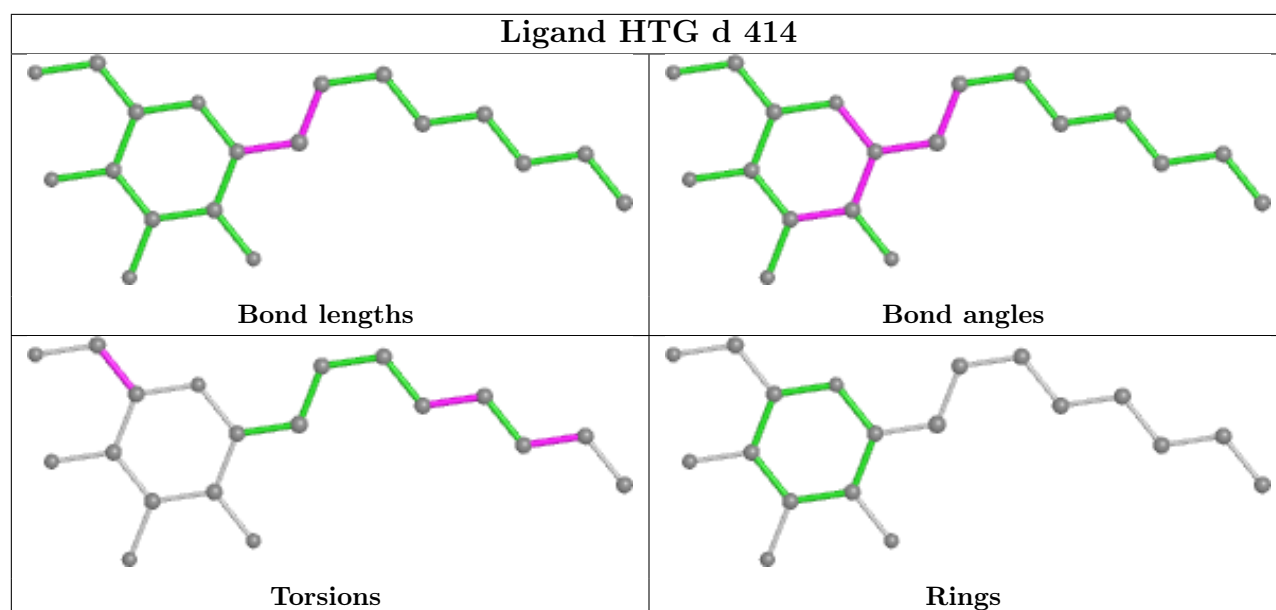


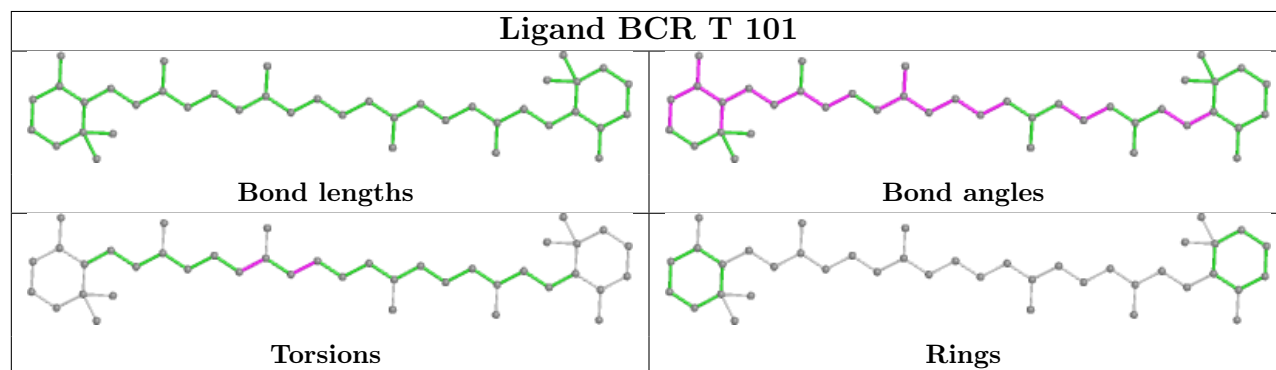
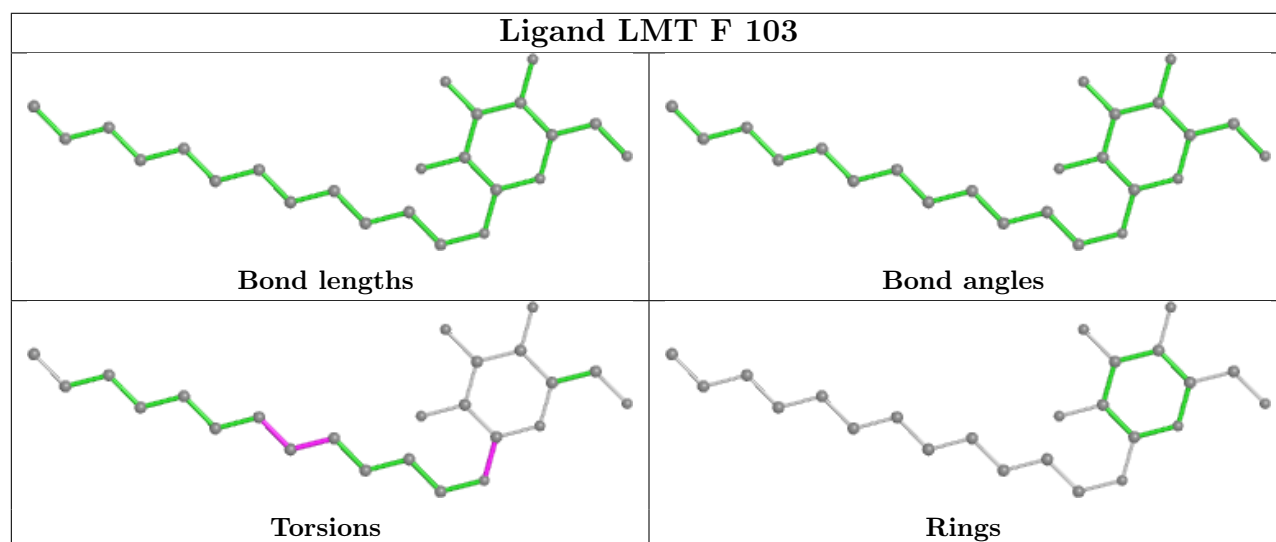
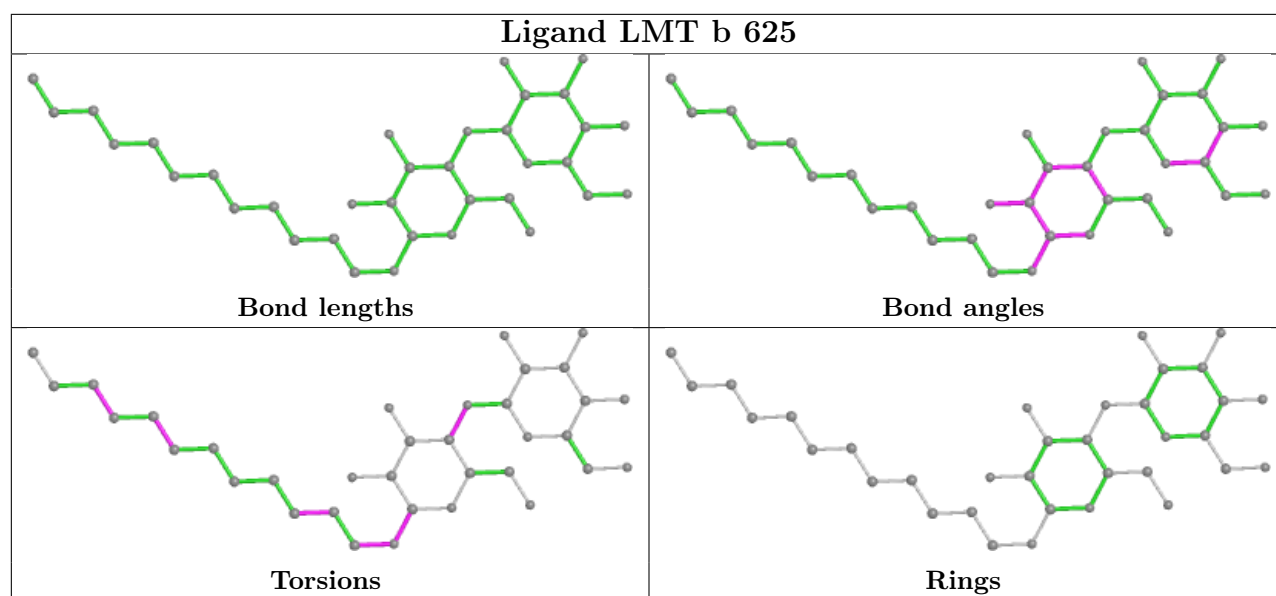


**Ligand CLA a 409****Ligand LHG D 408**

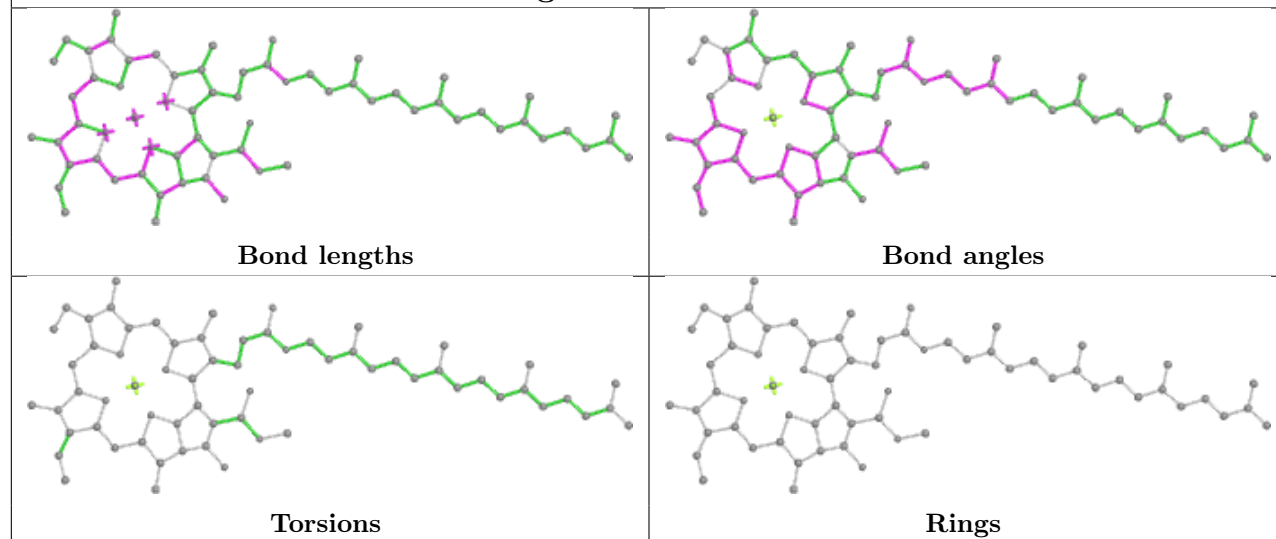




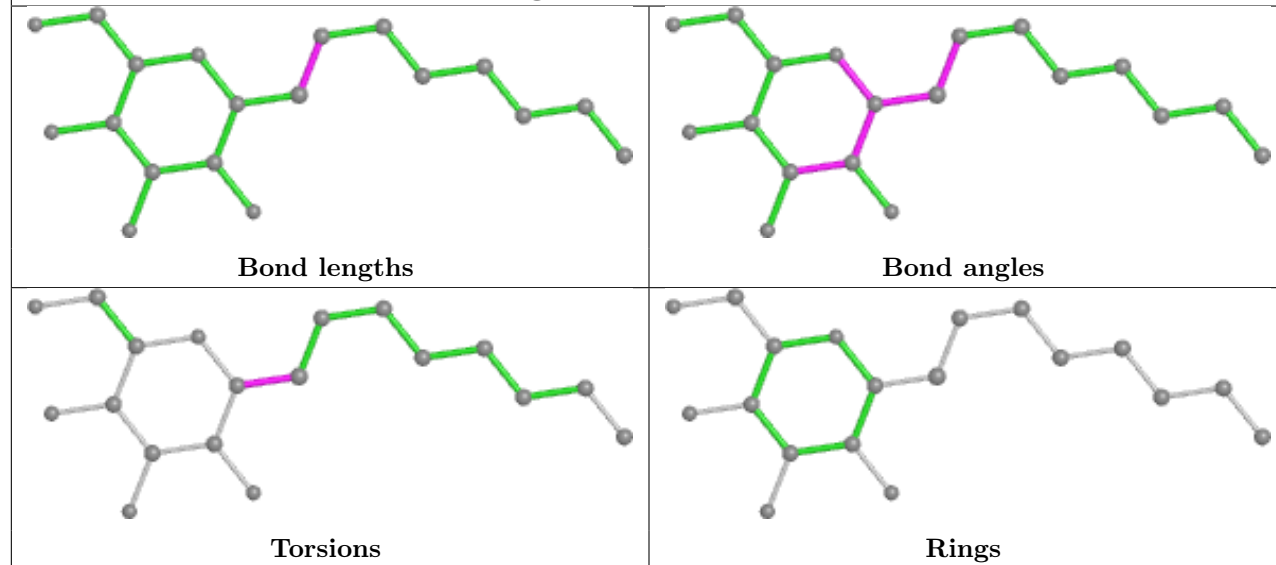




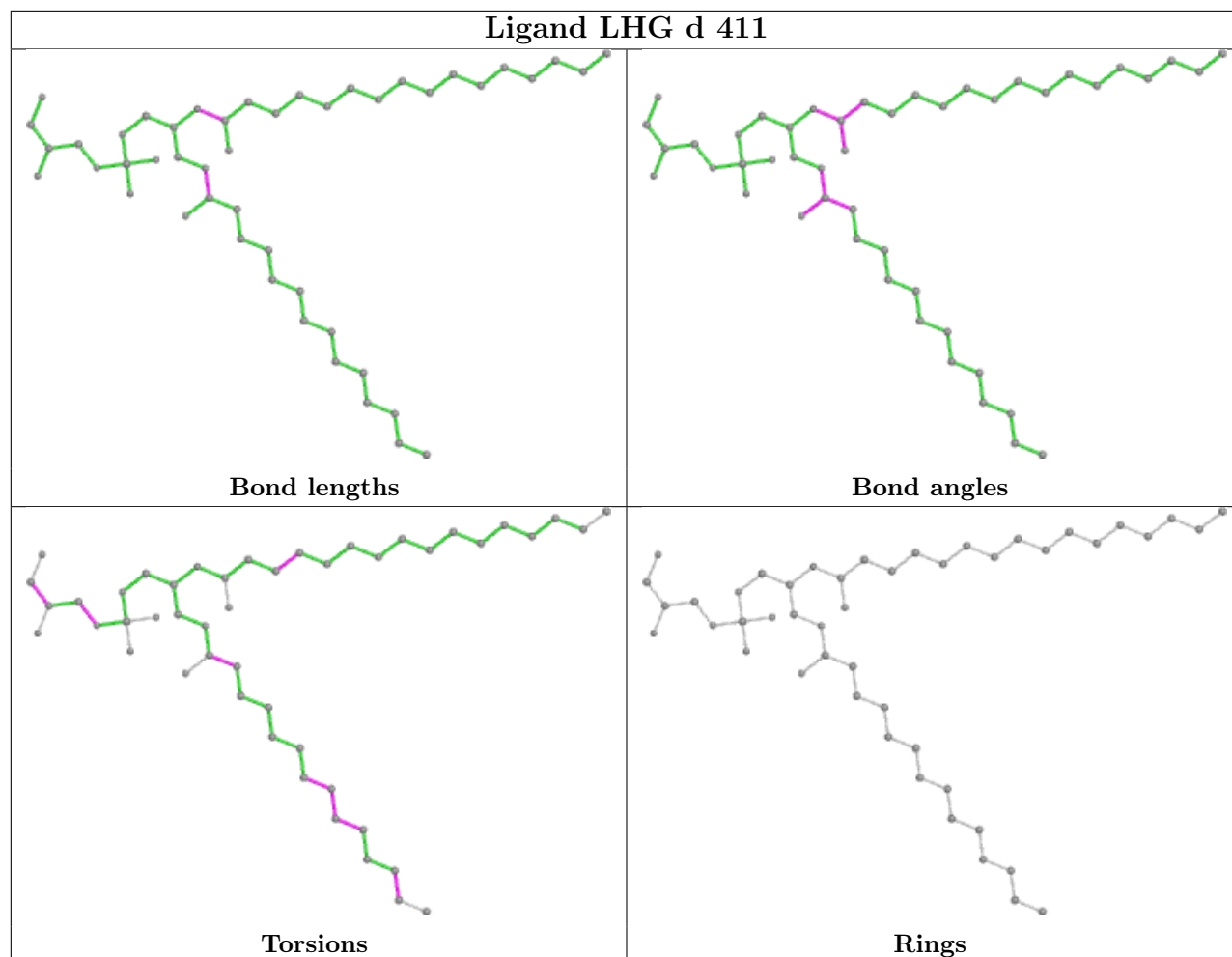
## Ligand CLA c 912



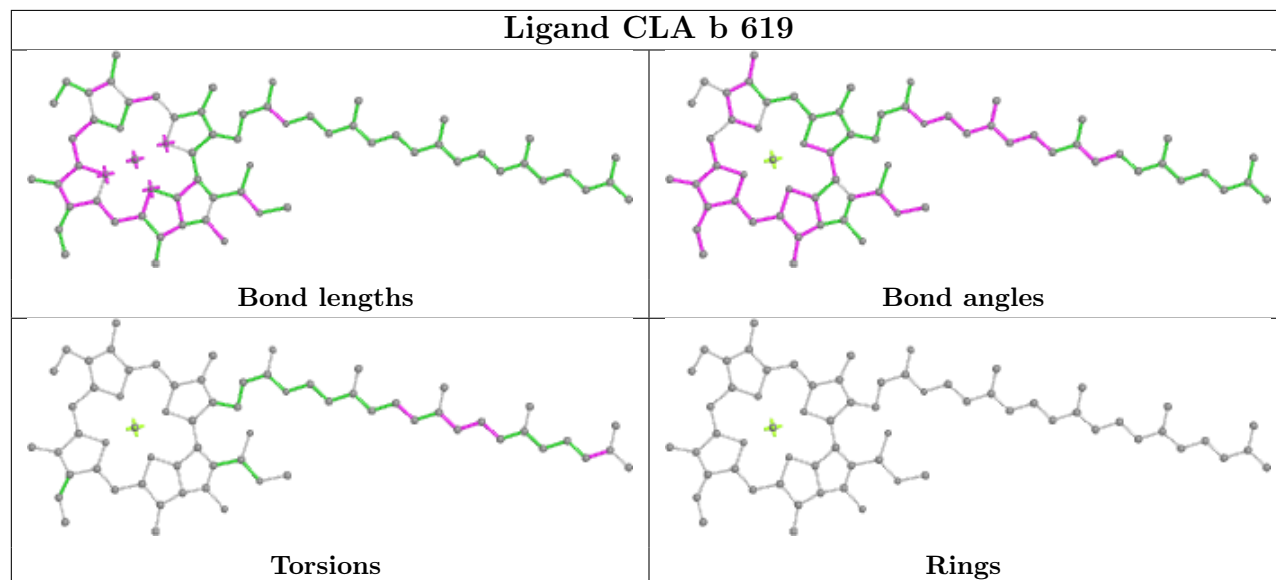
## Ligand HTG V 215

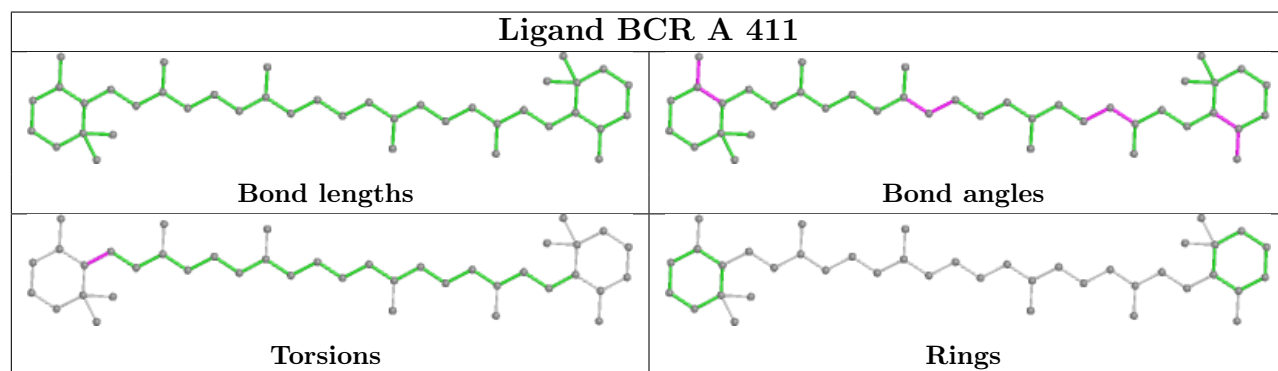
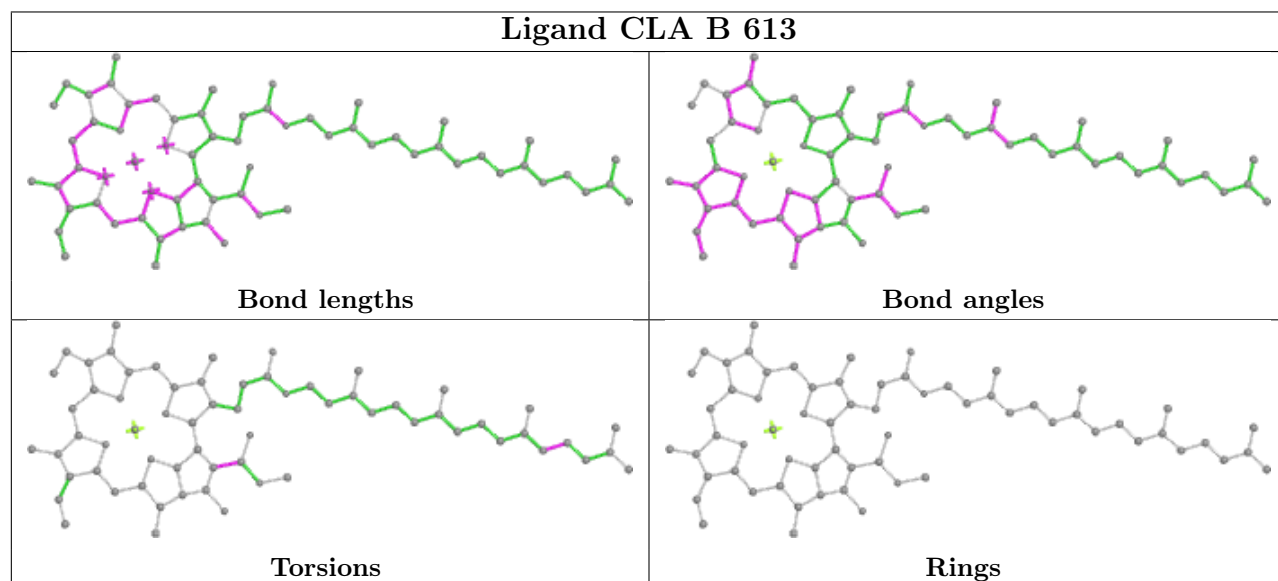
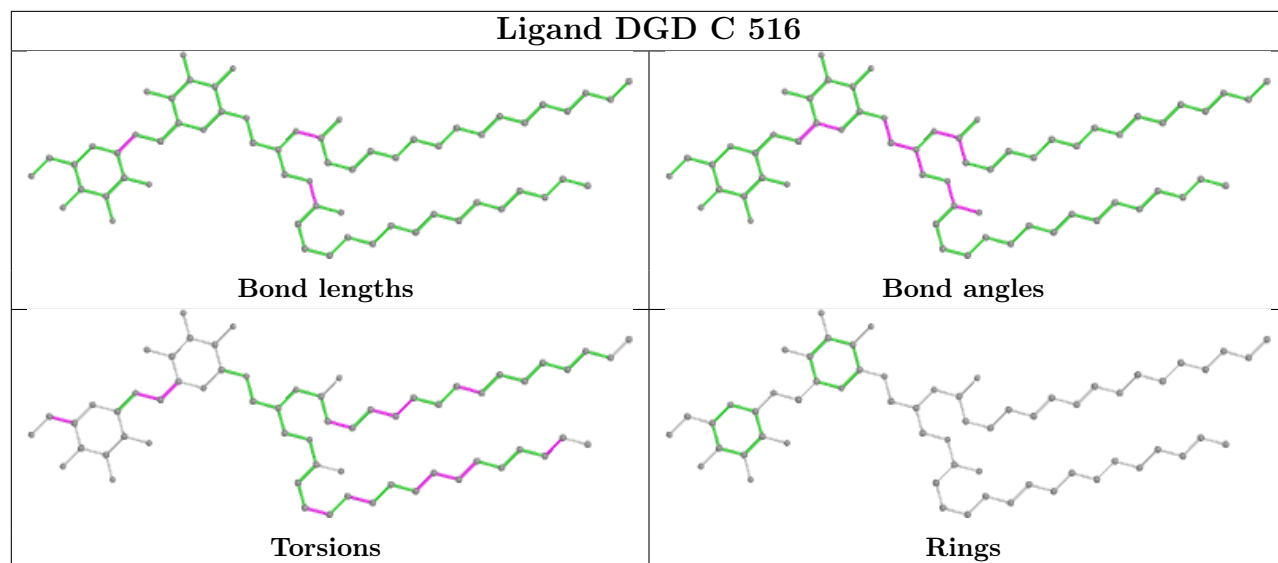


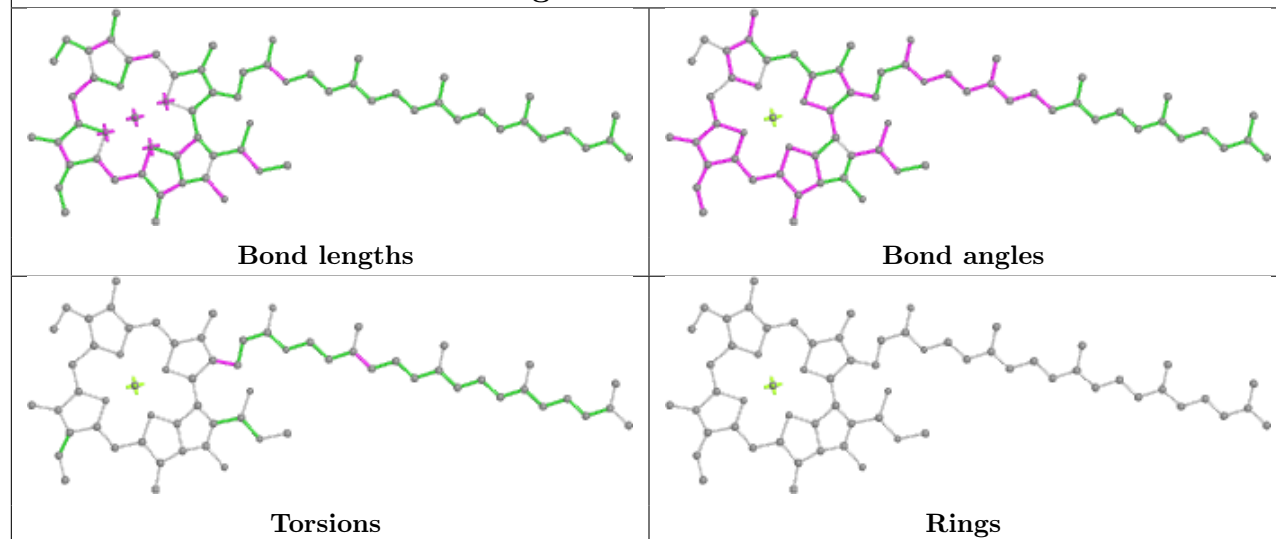
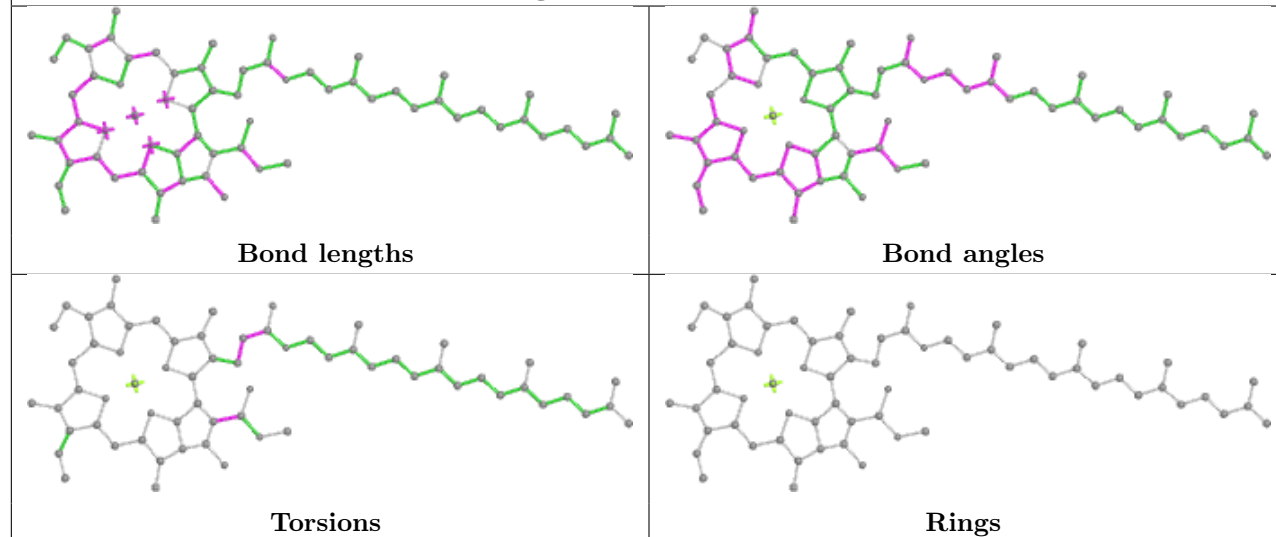
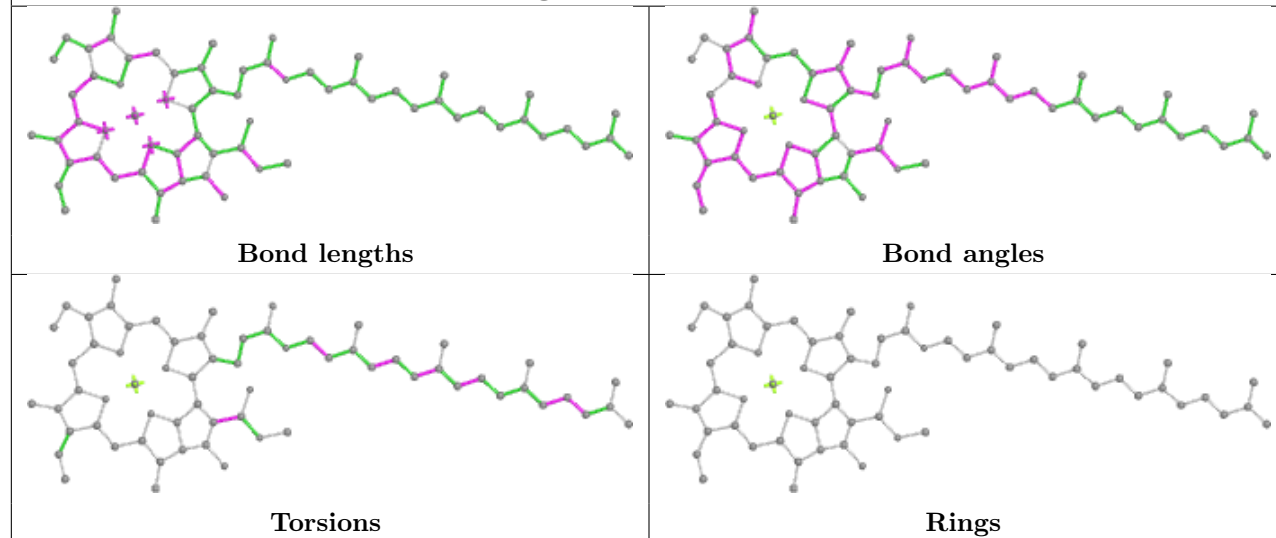
## Ligand LHG d 411

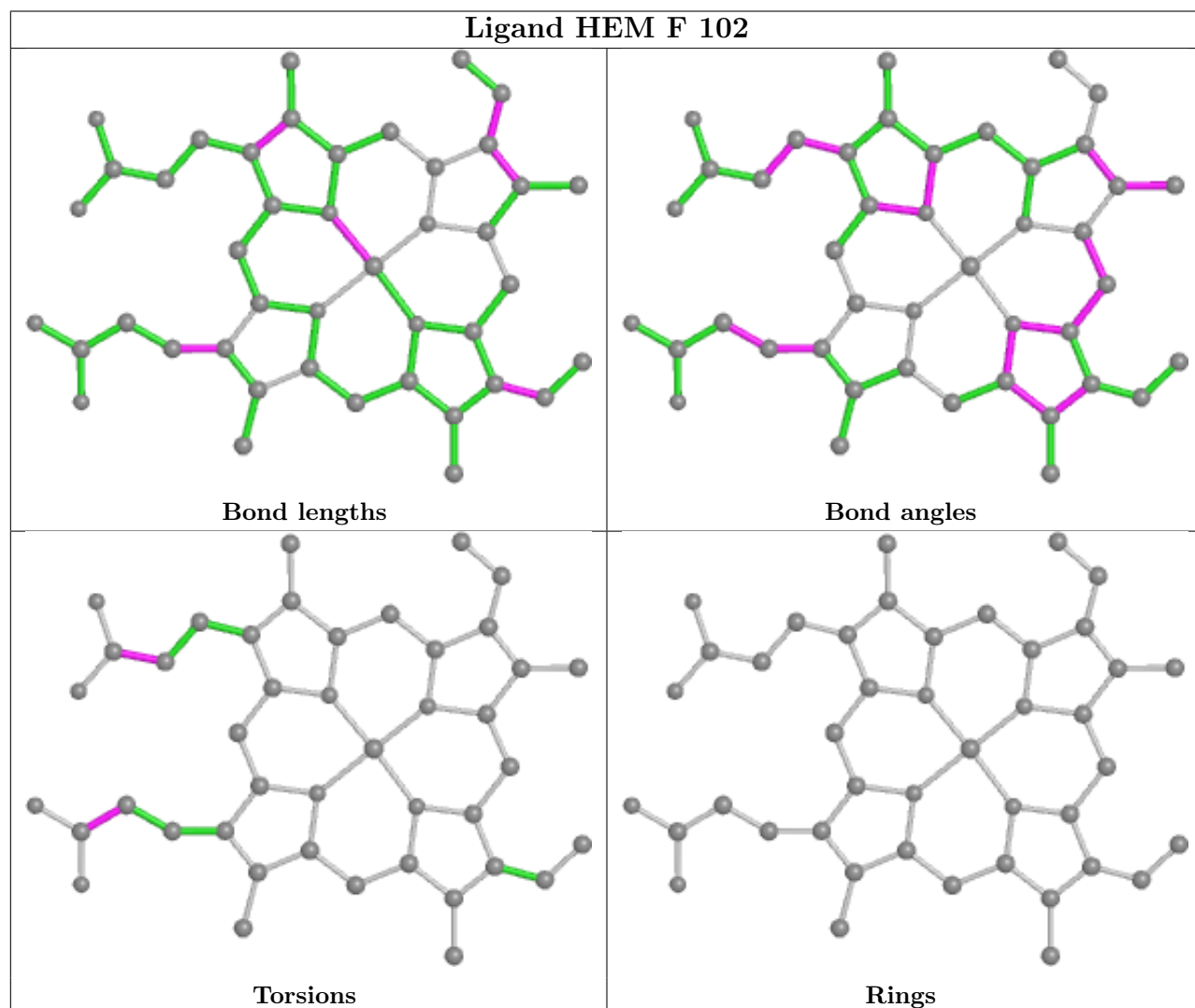
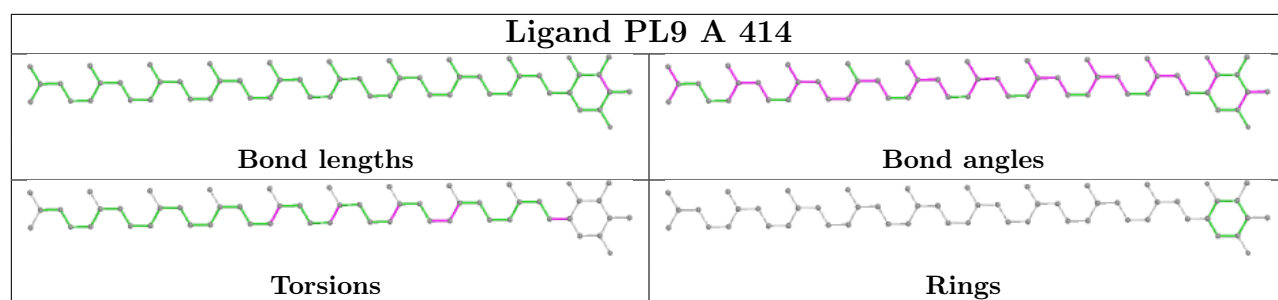


## Ligand CLA b 619

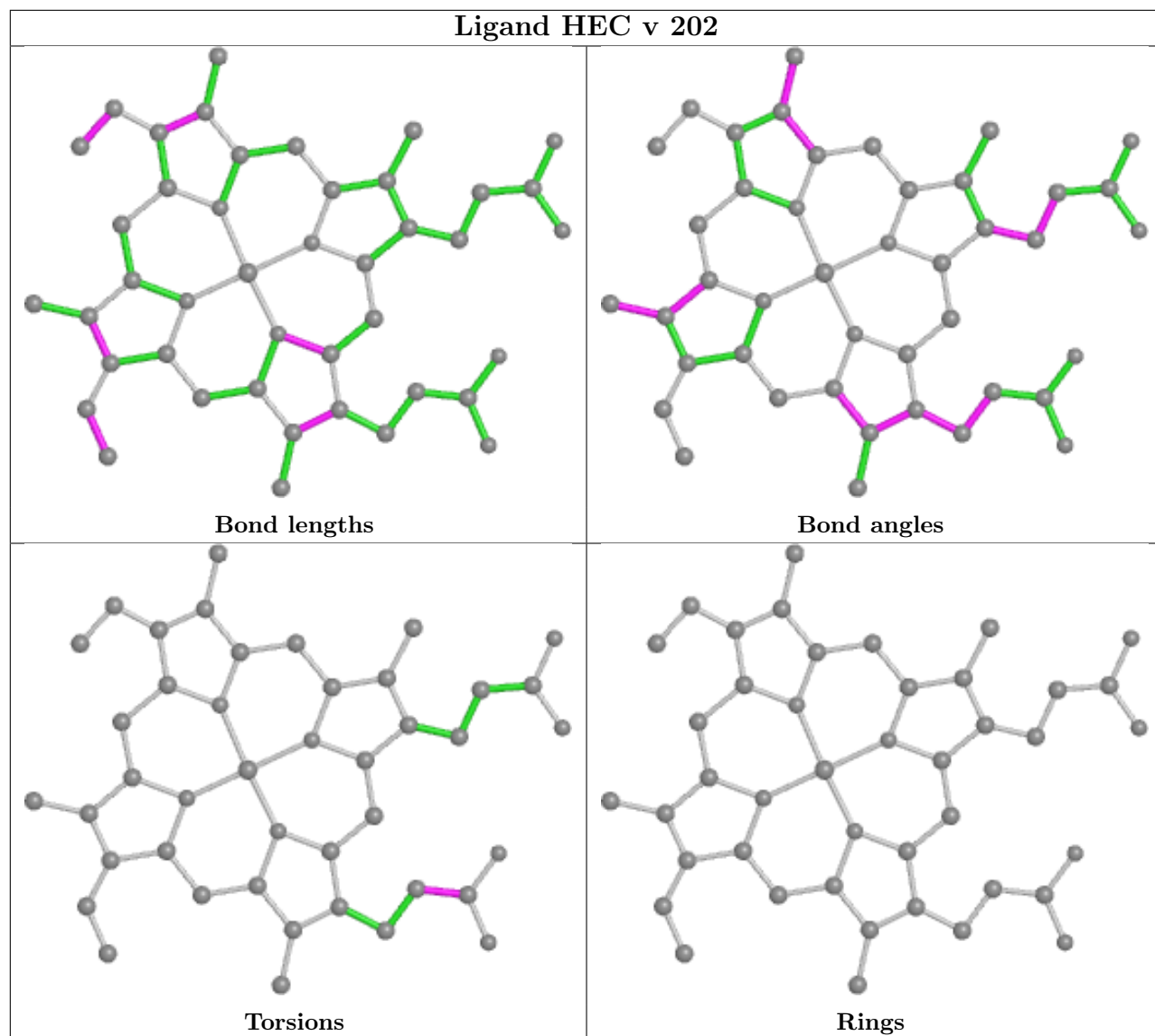




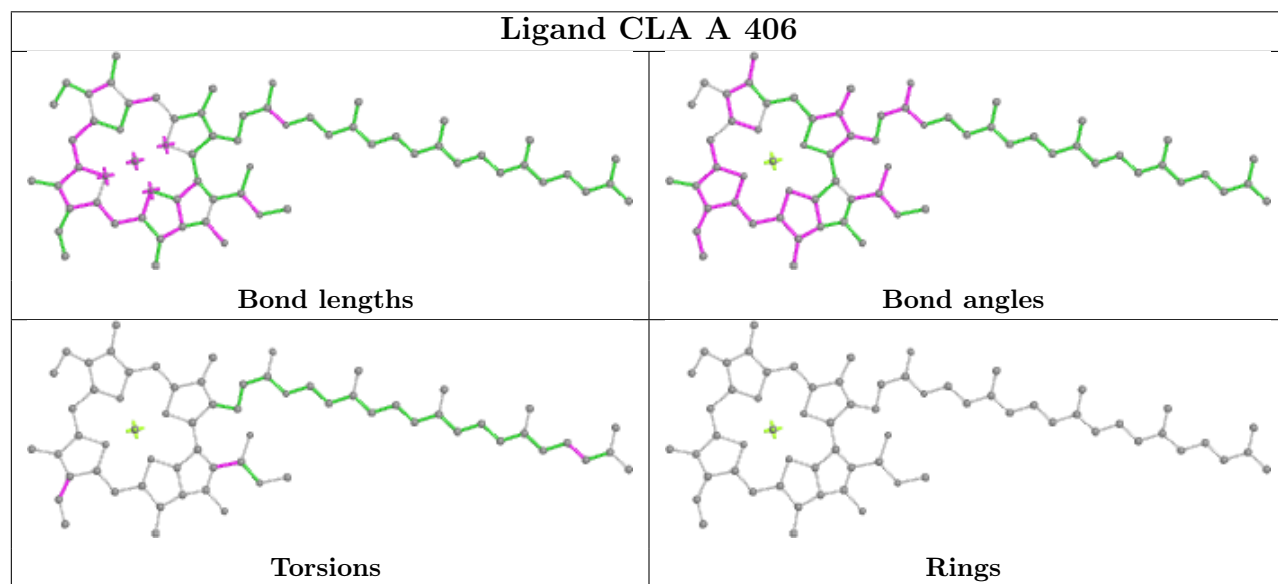
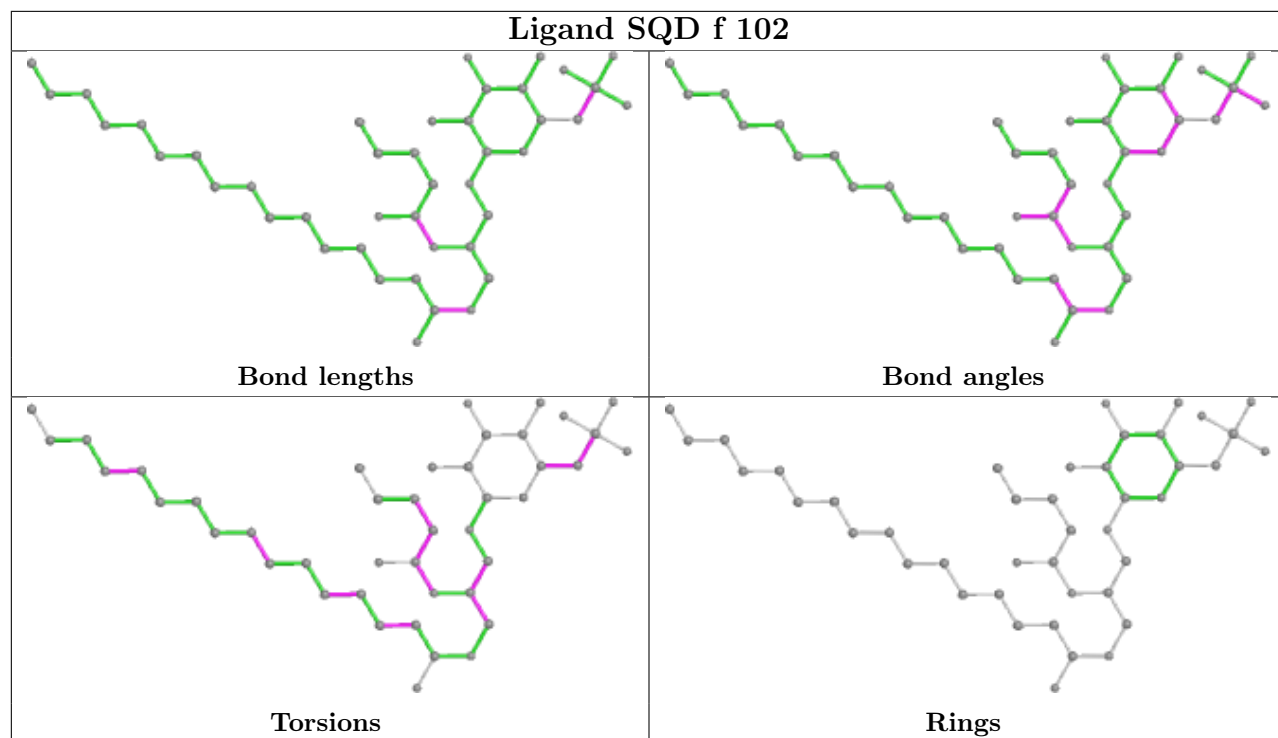
**Ligand CLA B 612****Ligand CLA C 501****Ligand CLA b 606**

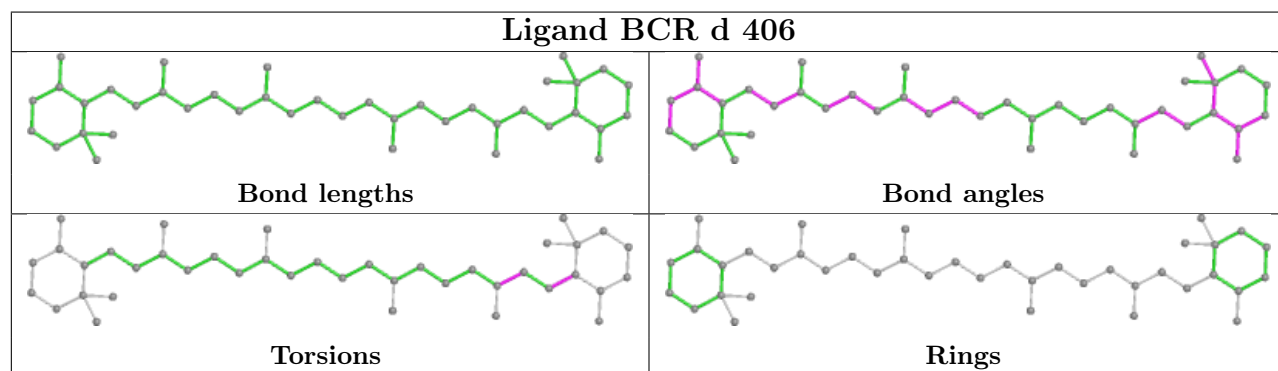
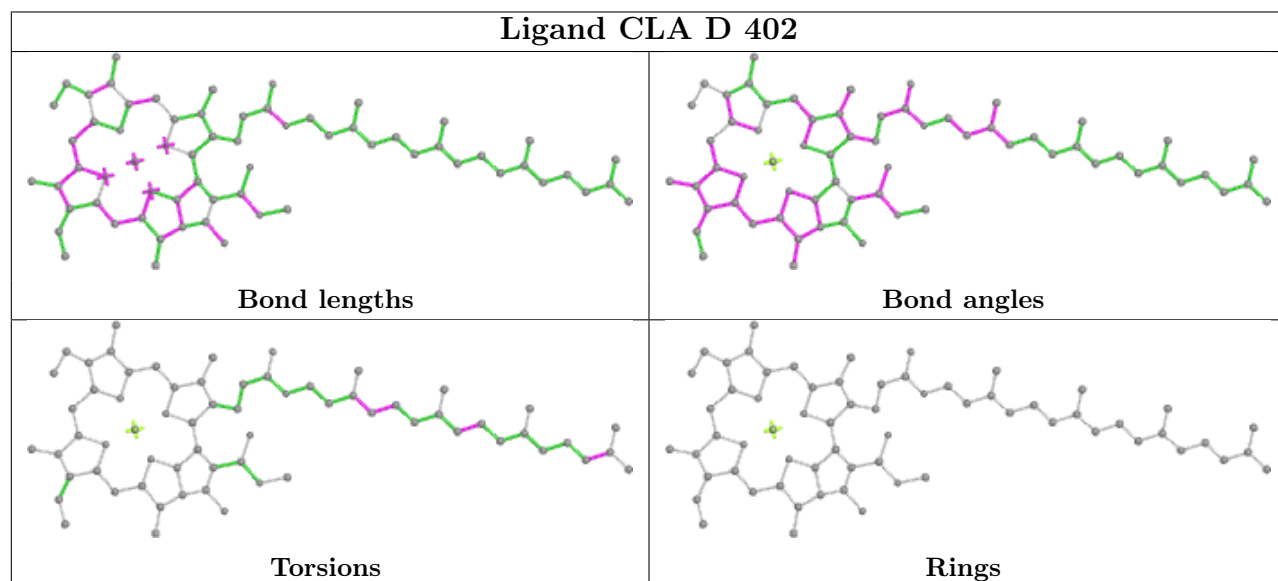
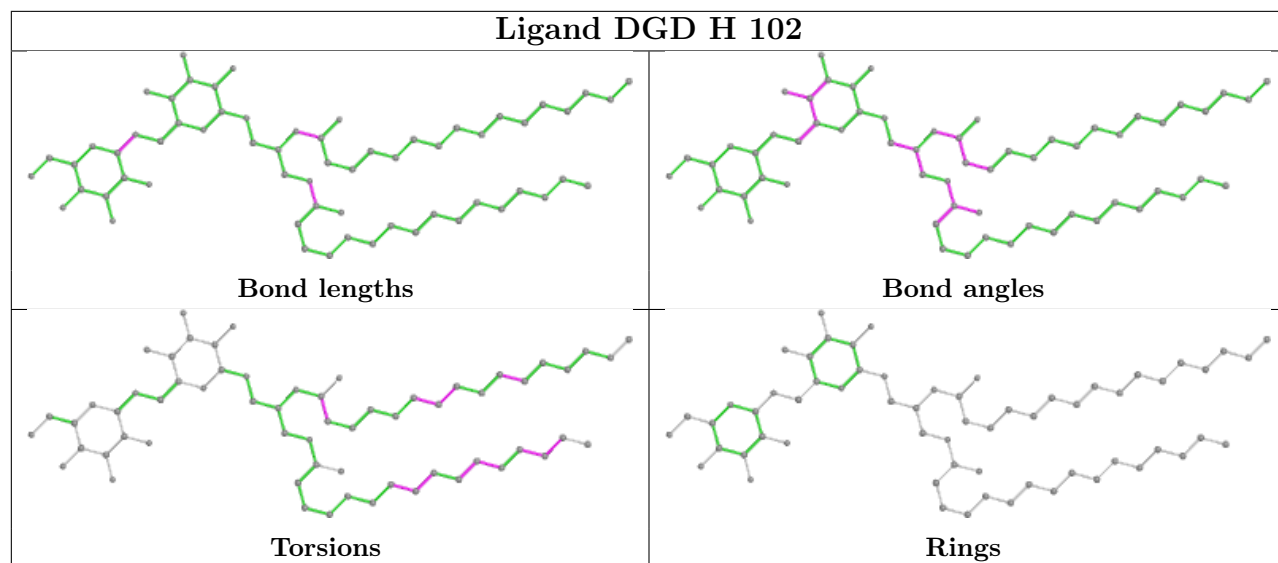


## Ligand HEC v 202

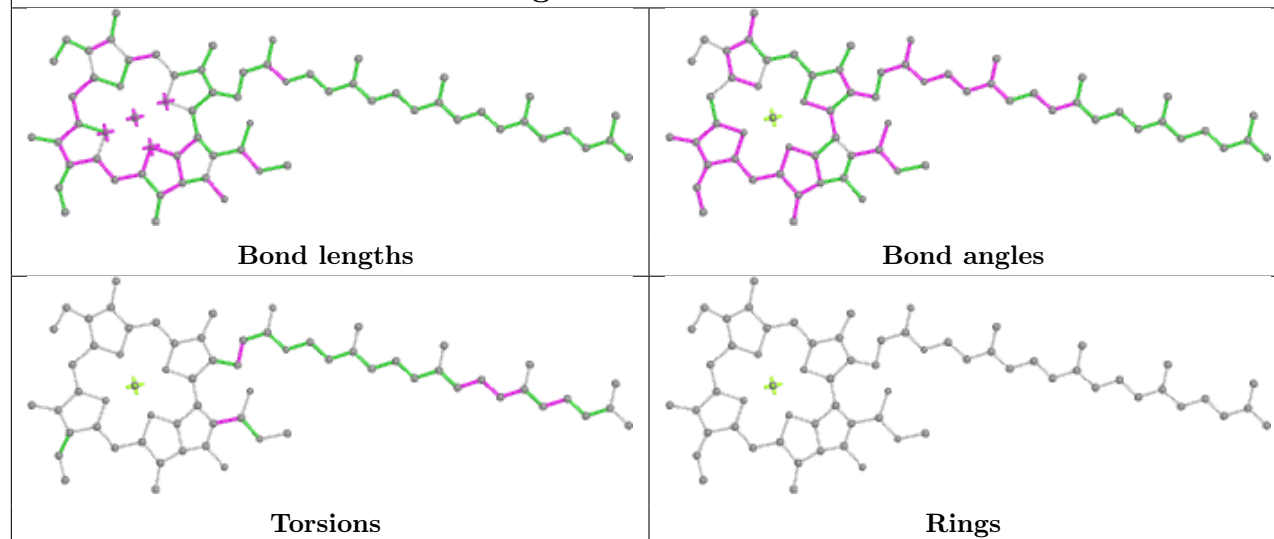




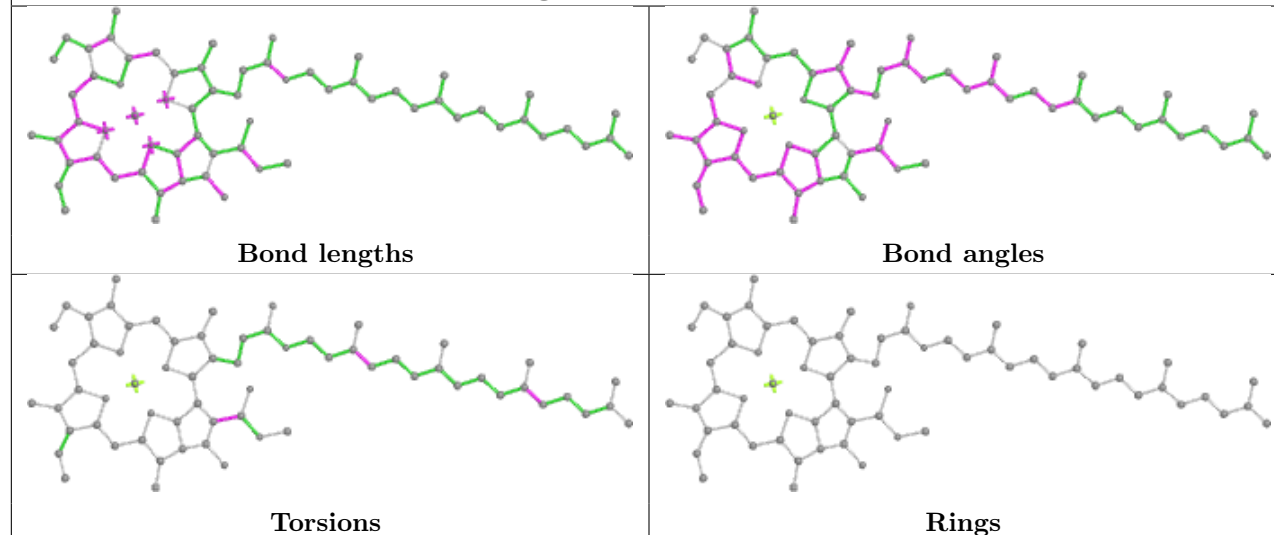




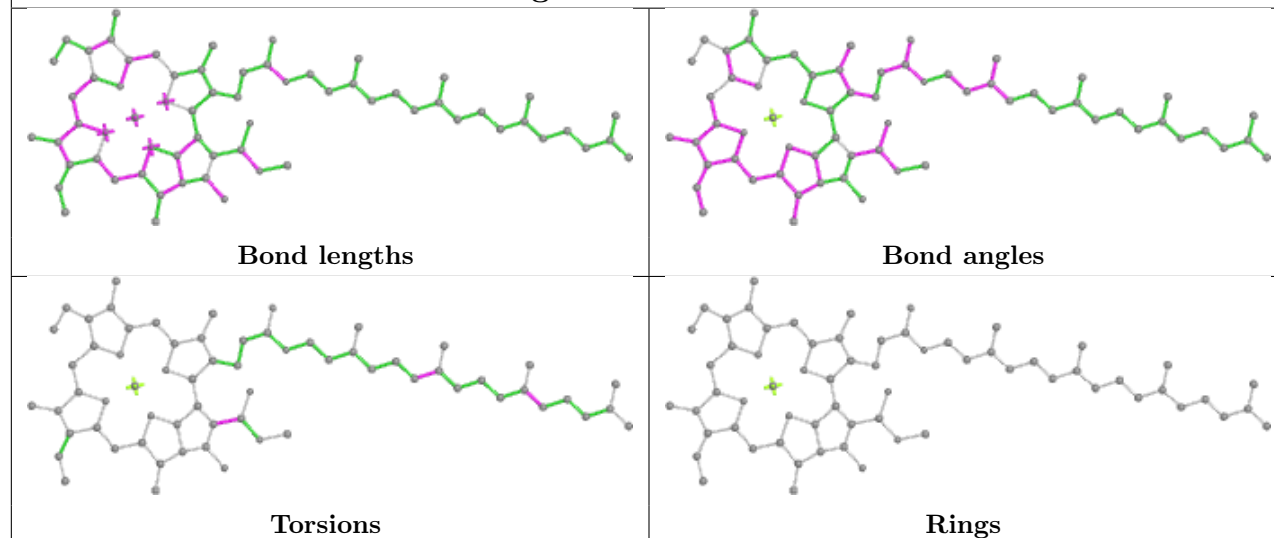
## Ligand CLA B 607

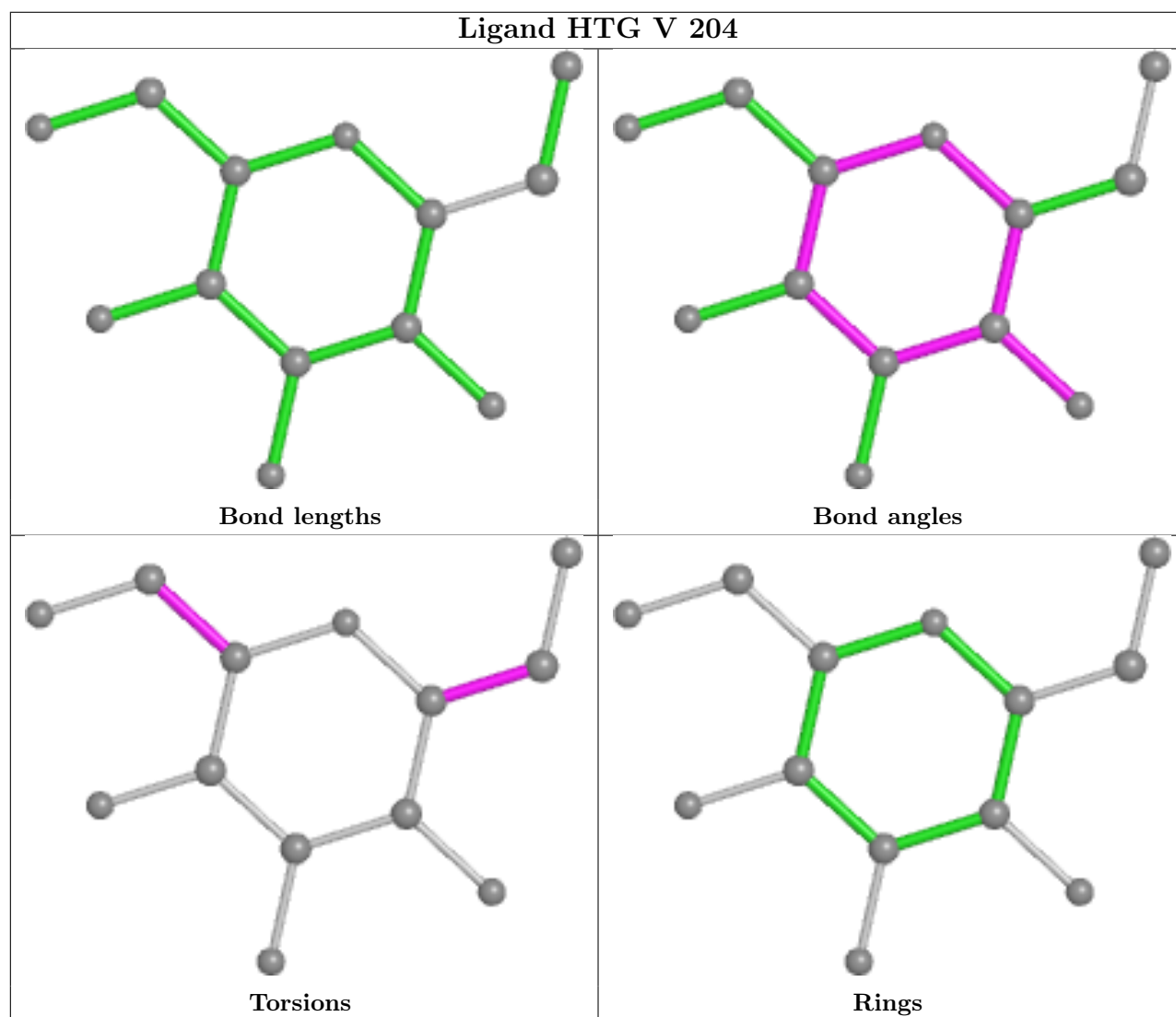
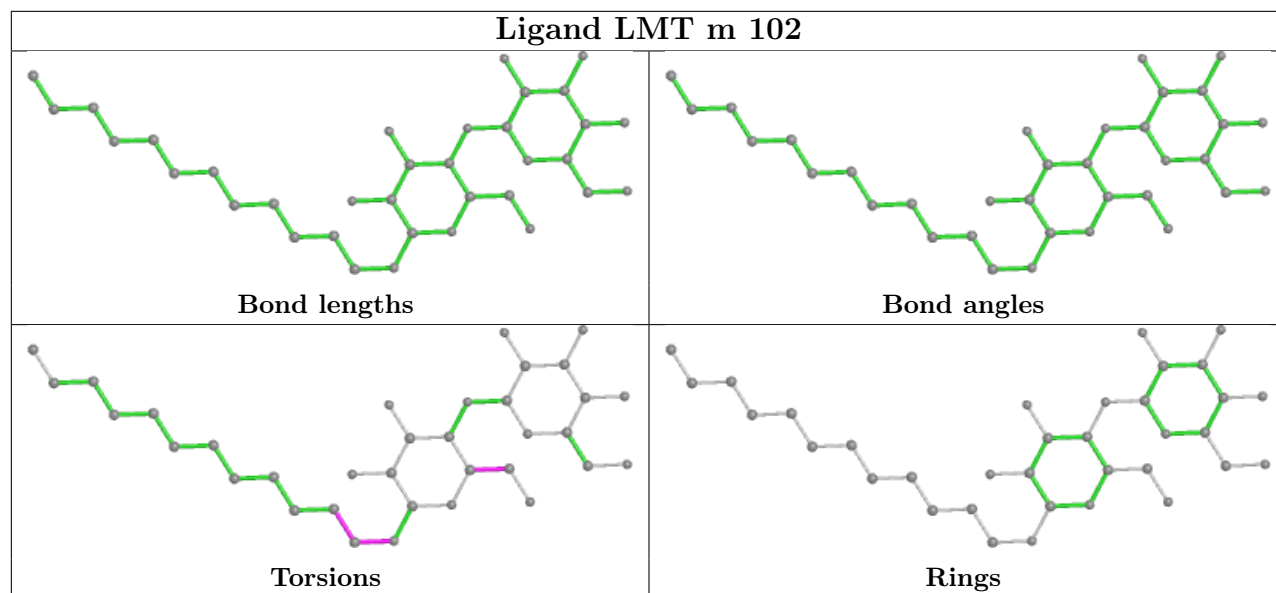


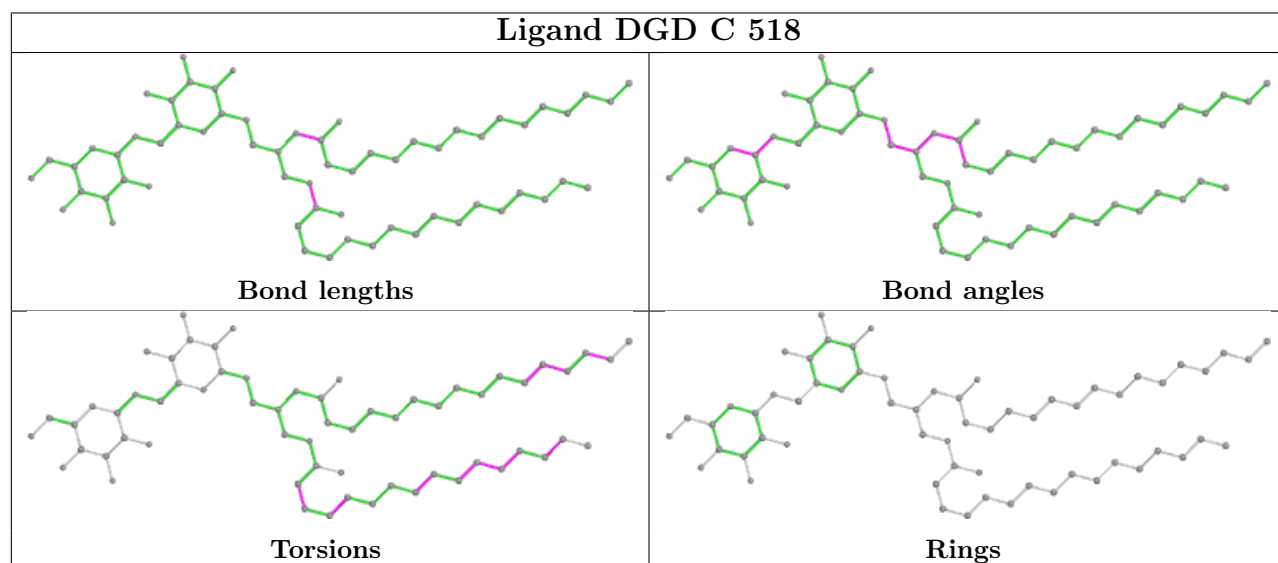
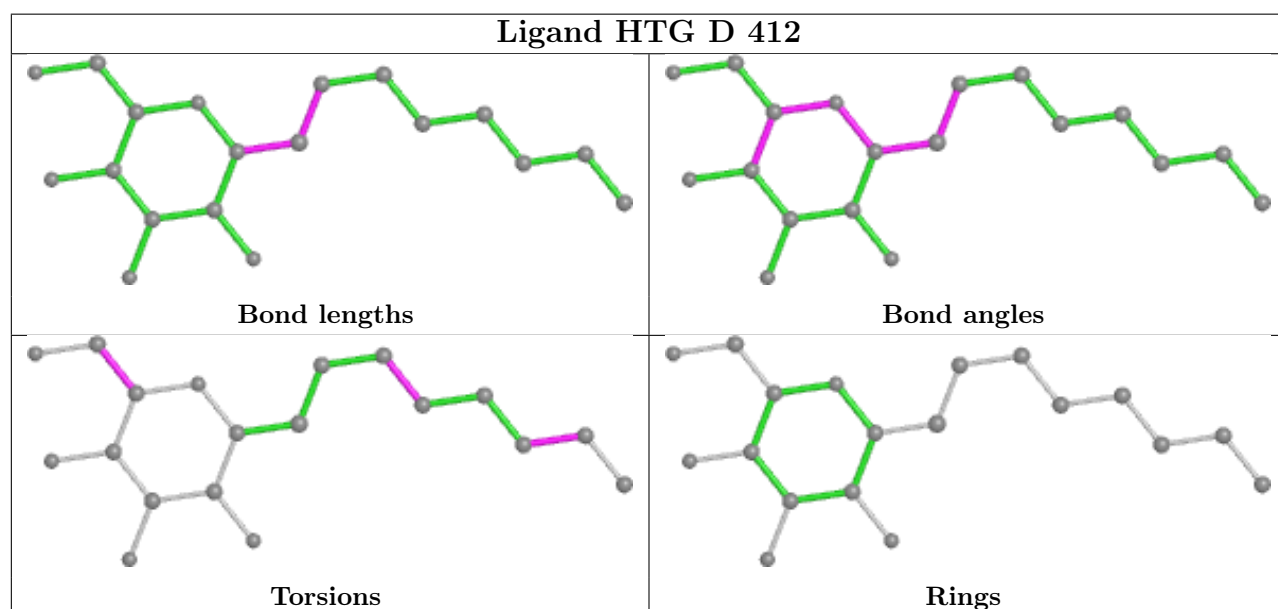
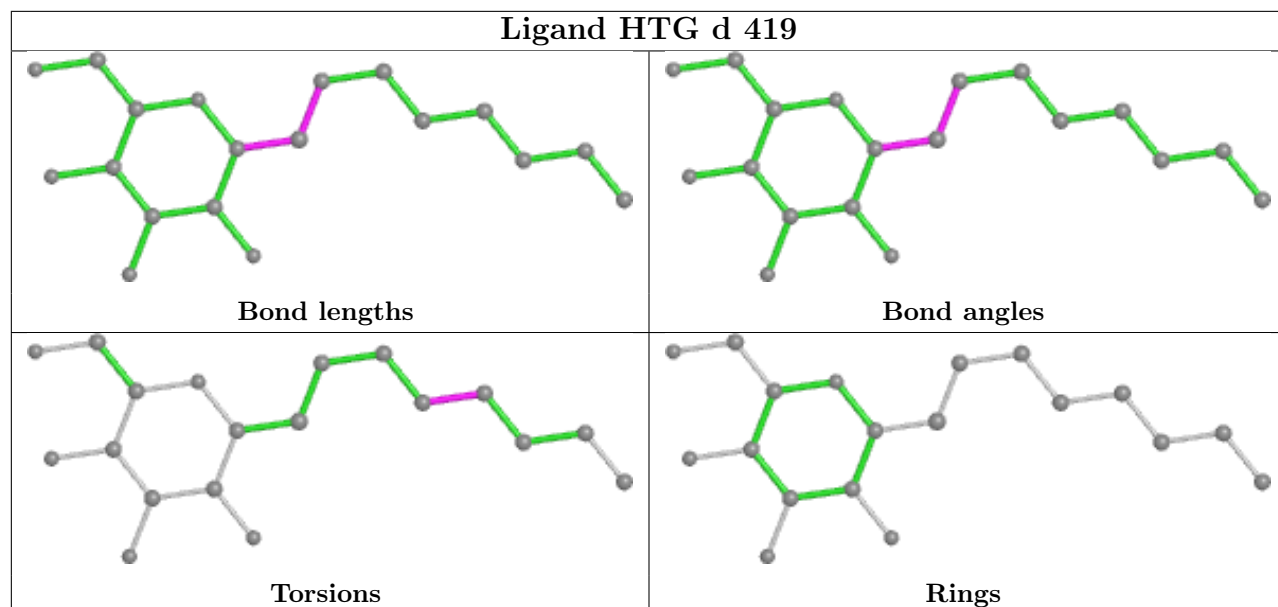
## Ligand CLA d 405

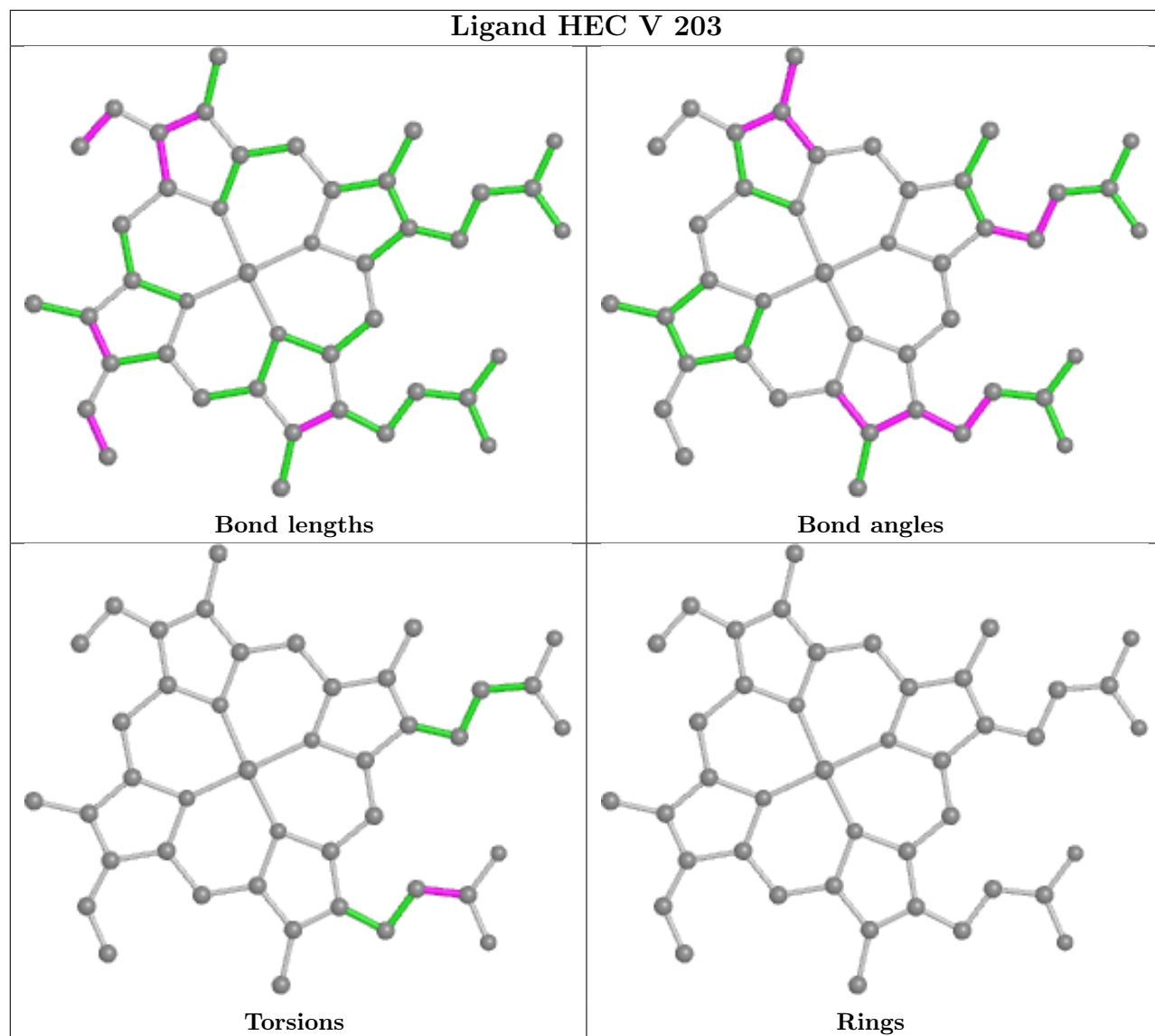


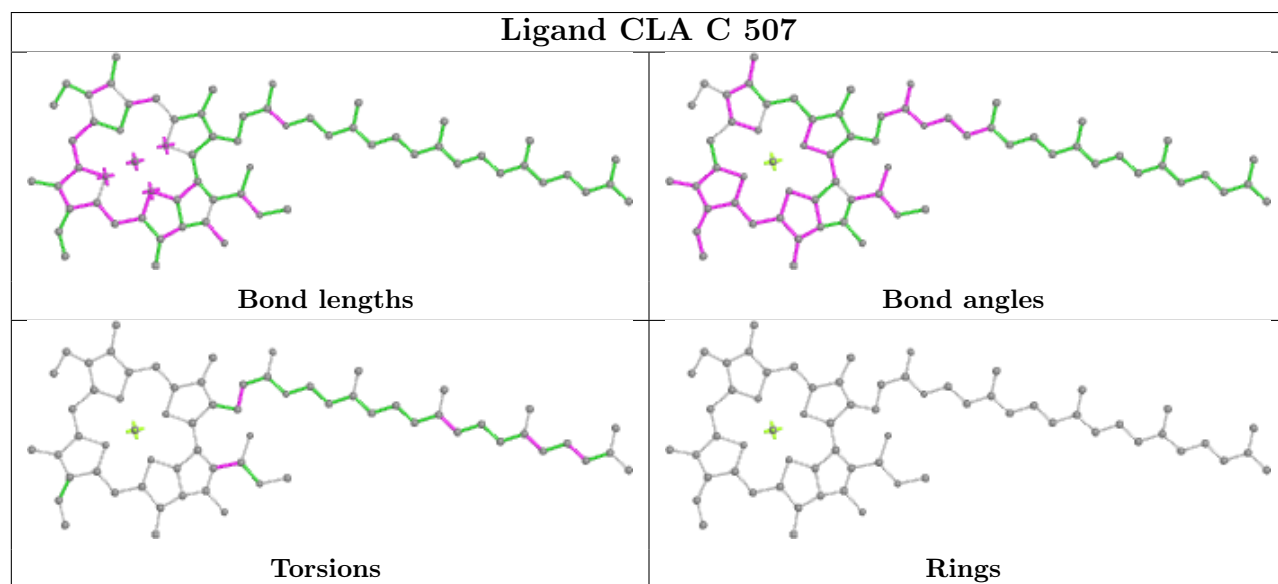
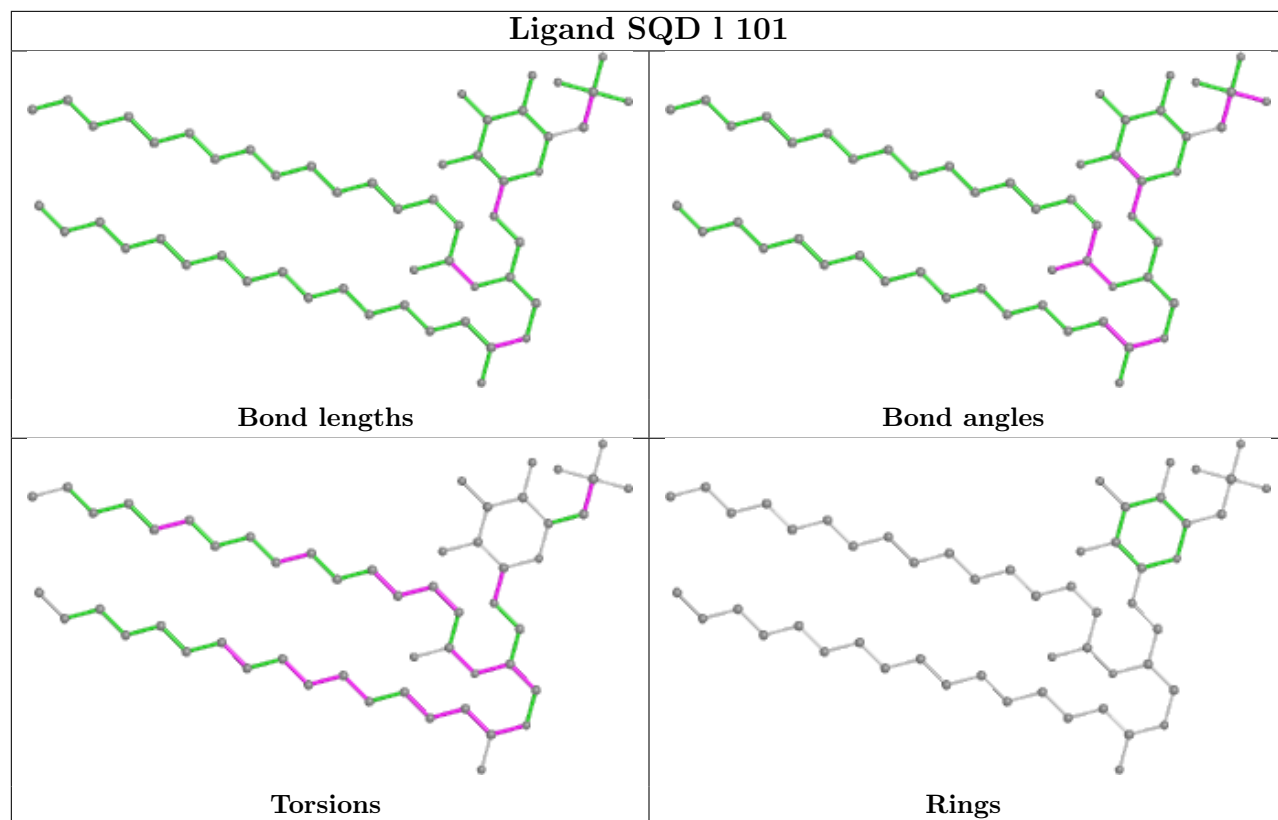
## Ligand CLA A 407



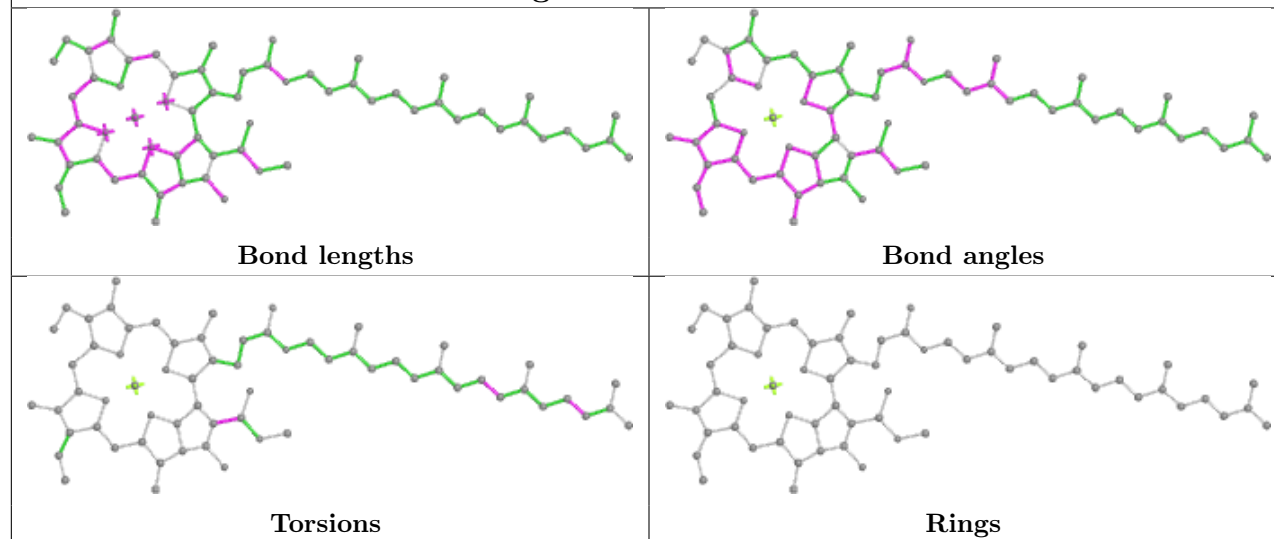




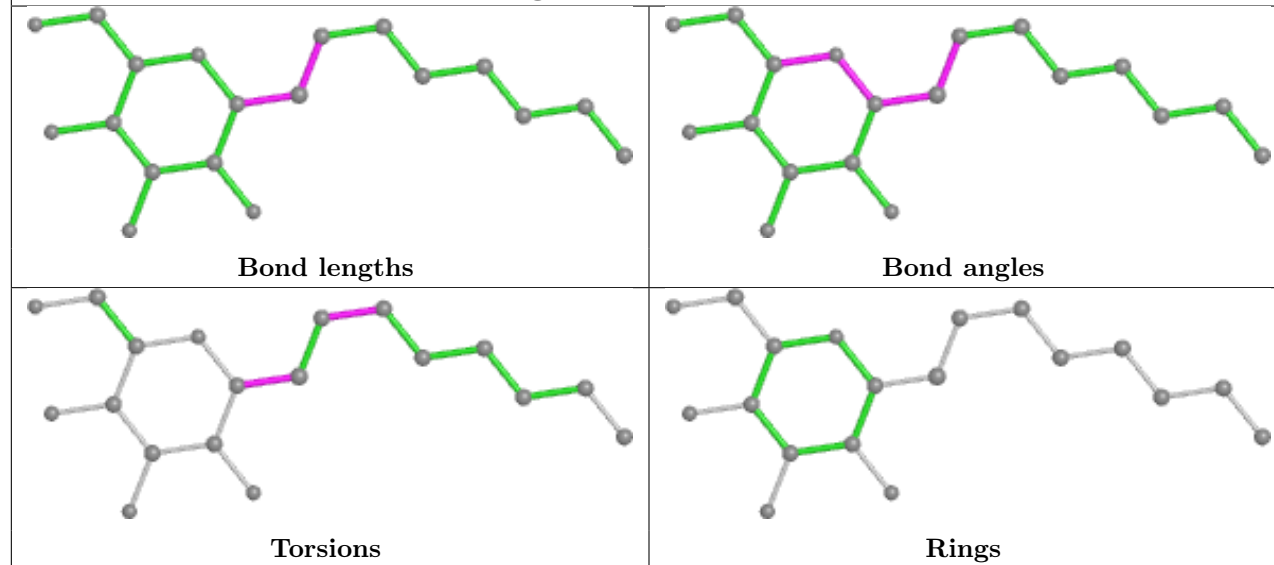




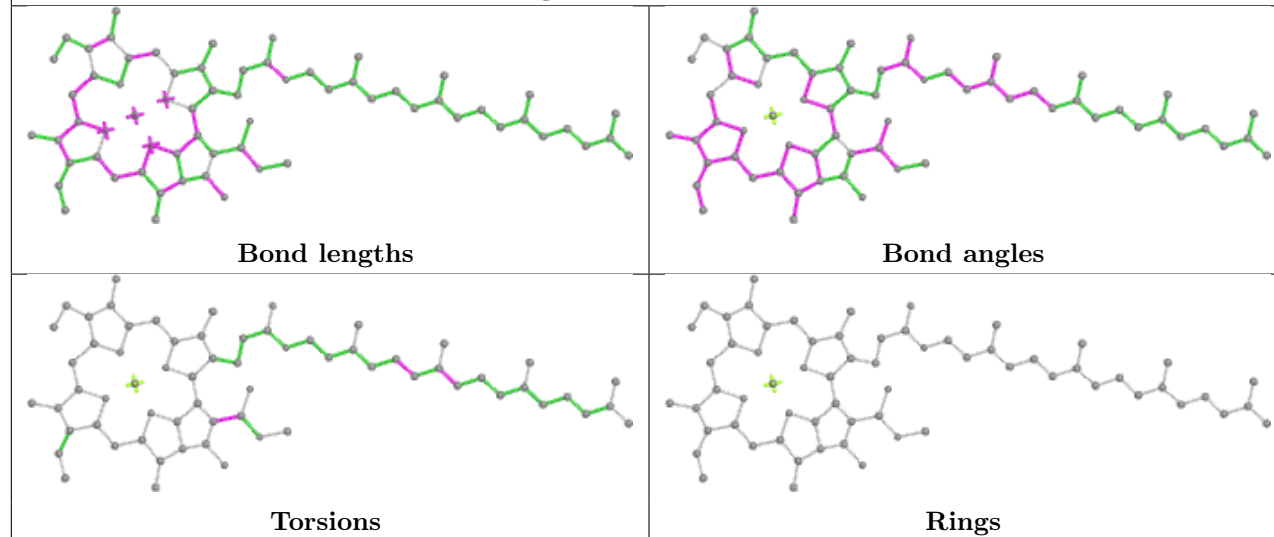
## Ligand CLA C 503



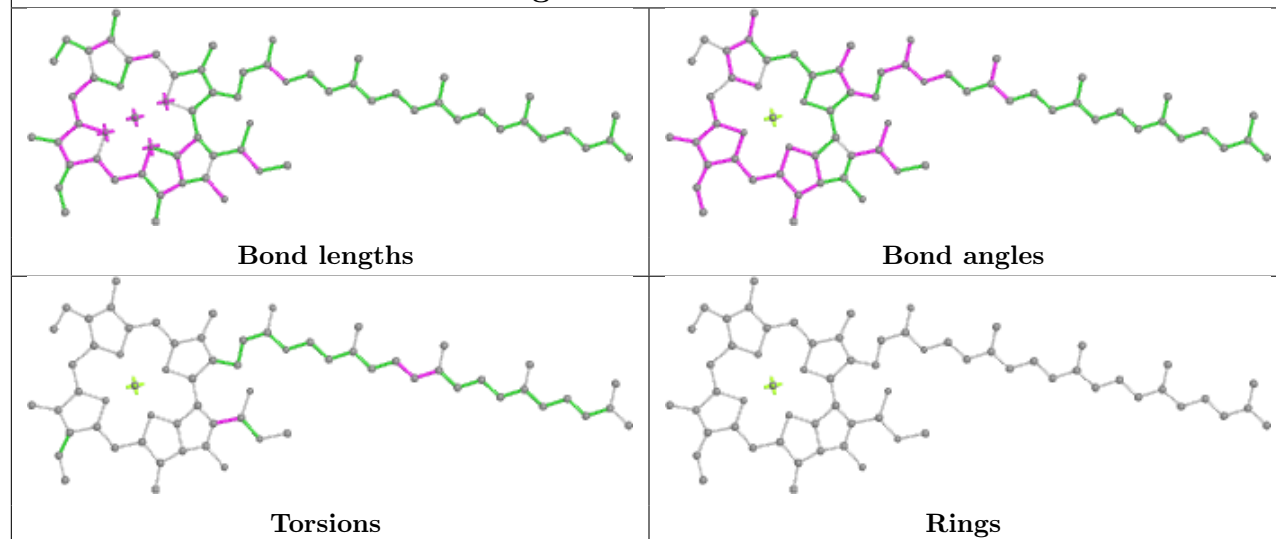
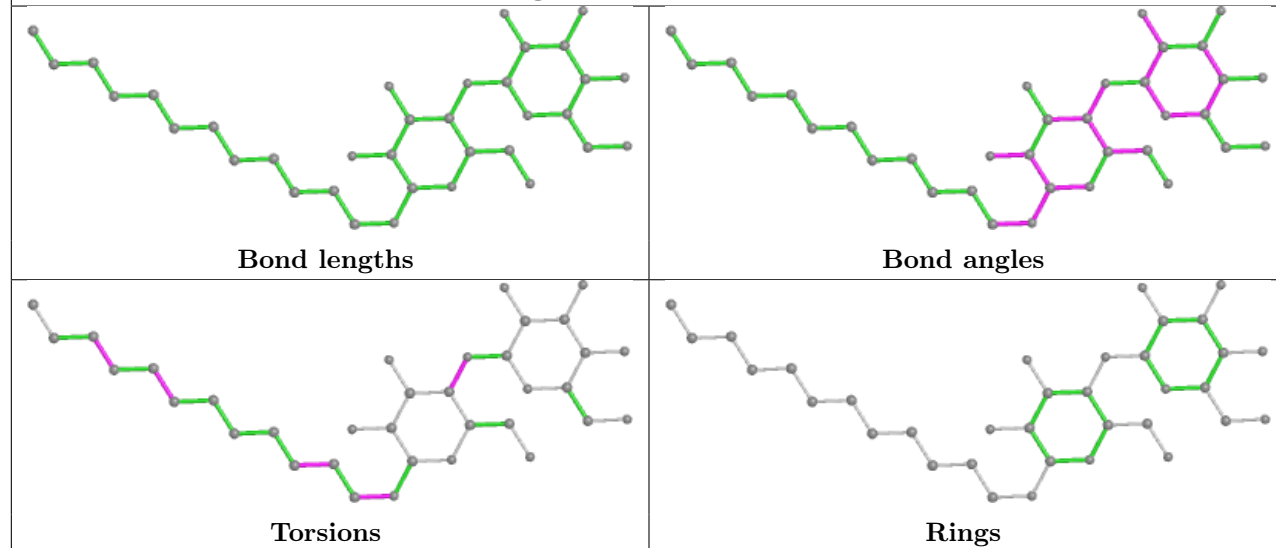
## Ligand HTG C 521

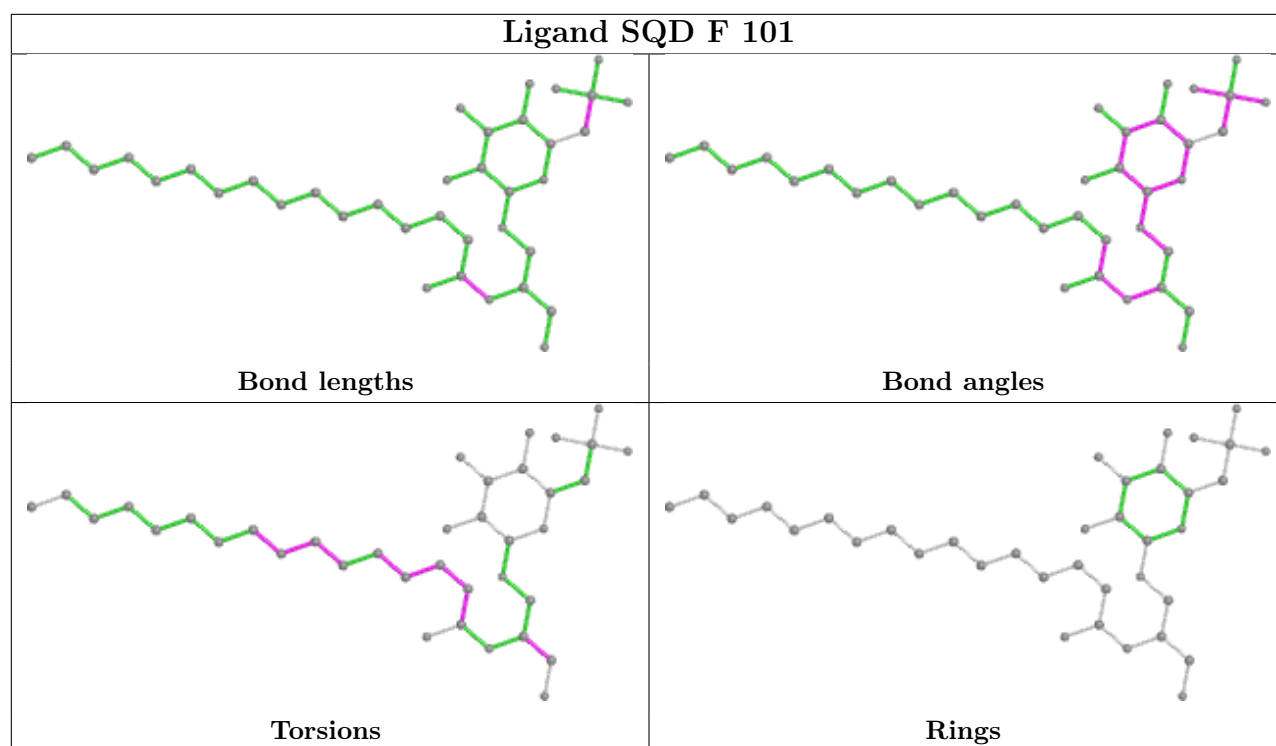


## Ligand CLA c 908

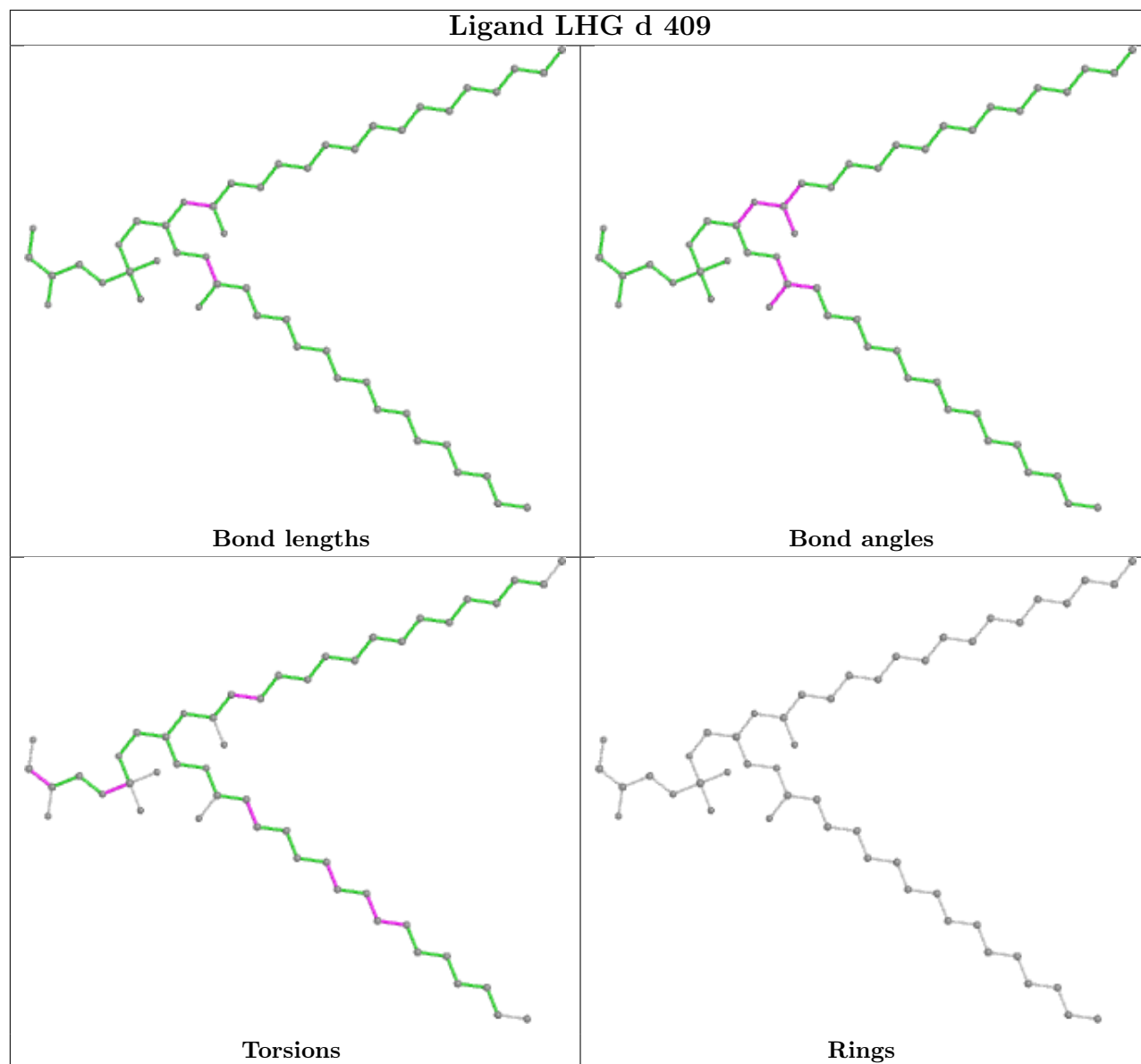




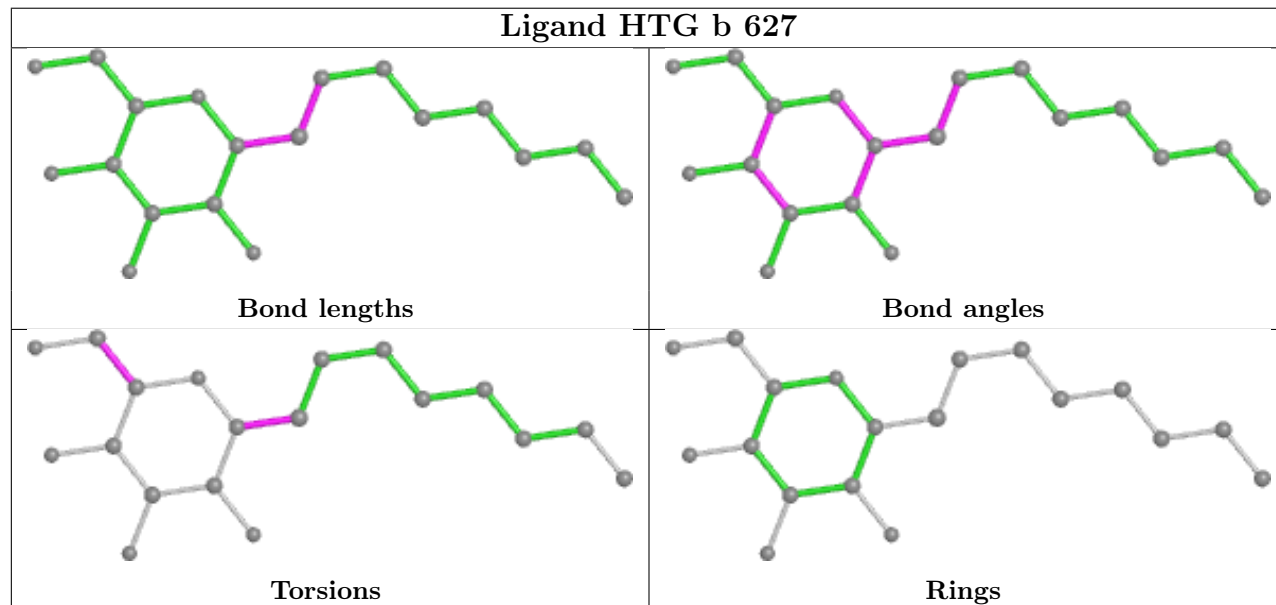
**Ligand CLA B 604****Ligand LMT B 622**



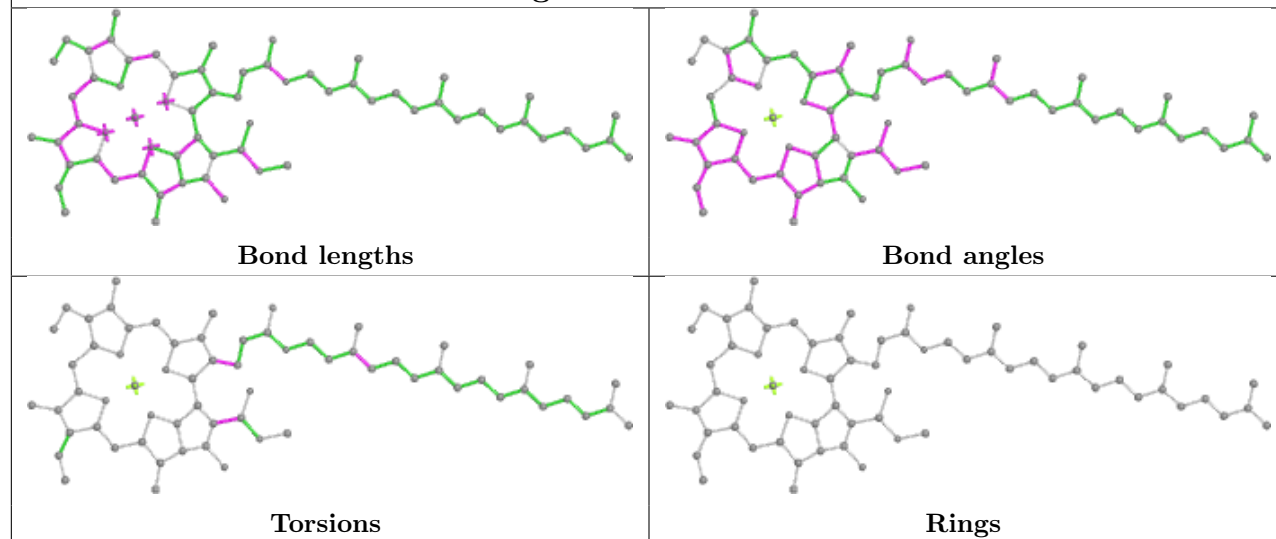
## Ligand LHG d 409



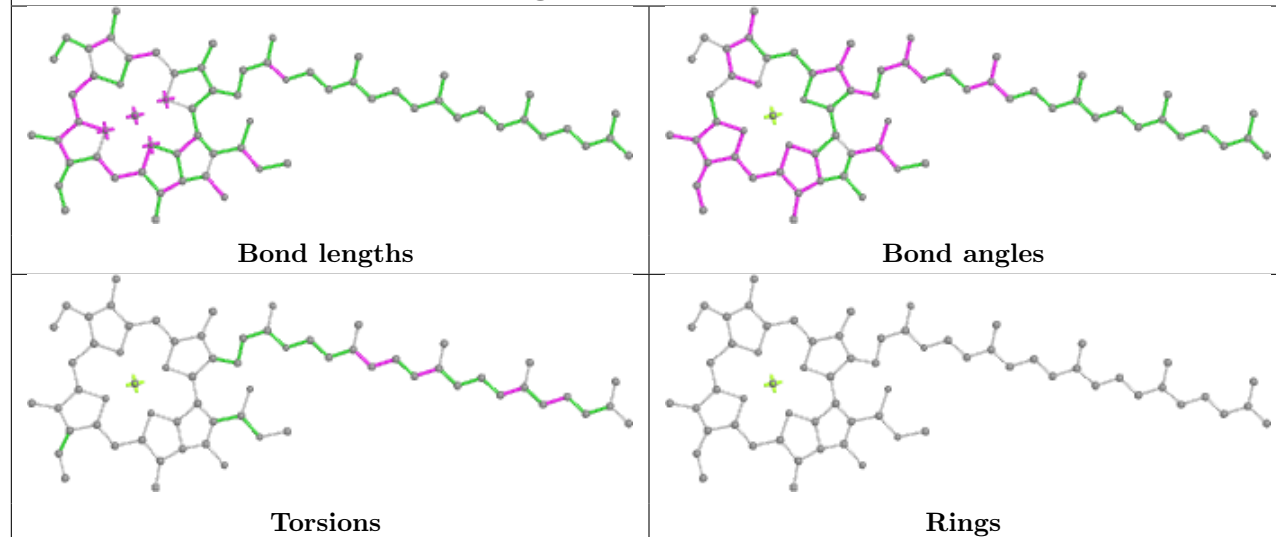
## Ligand HTG b 627



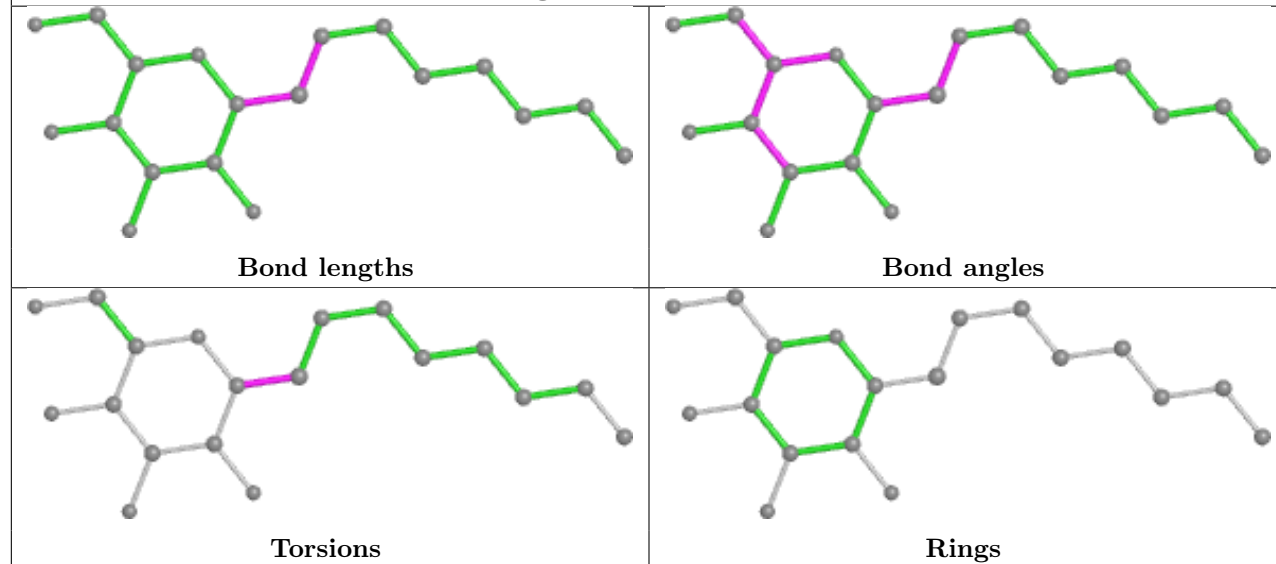
## Ligand CLA B 610

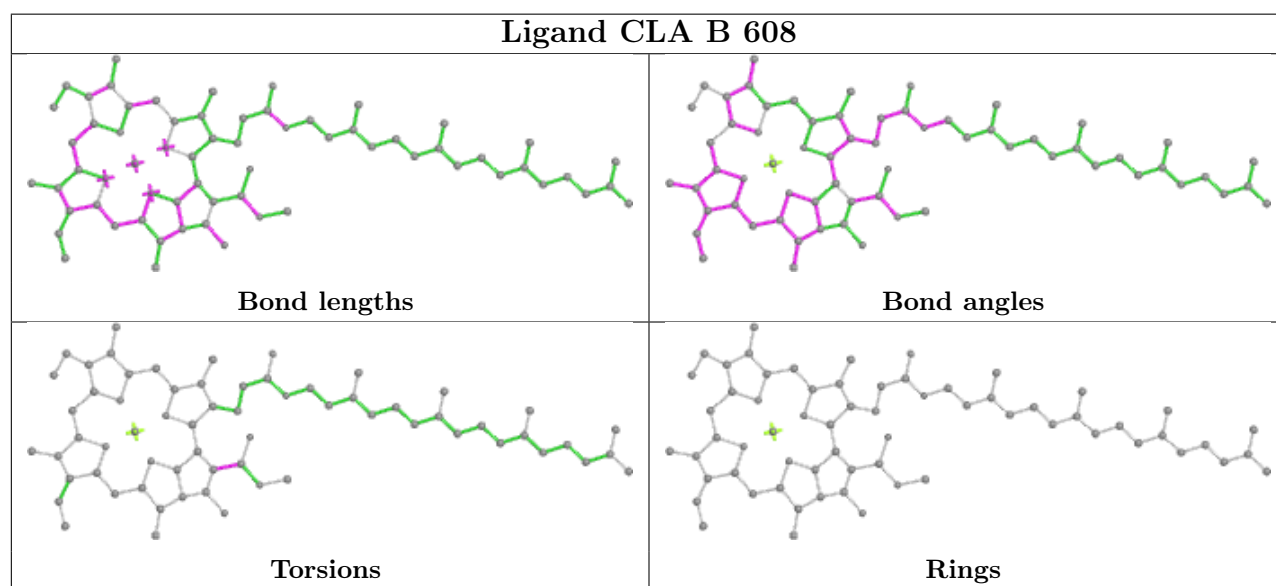
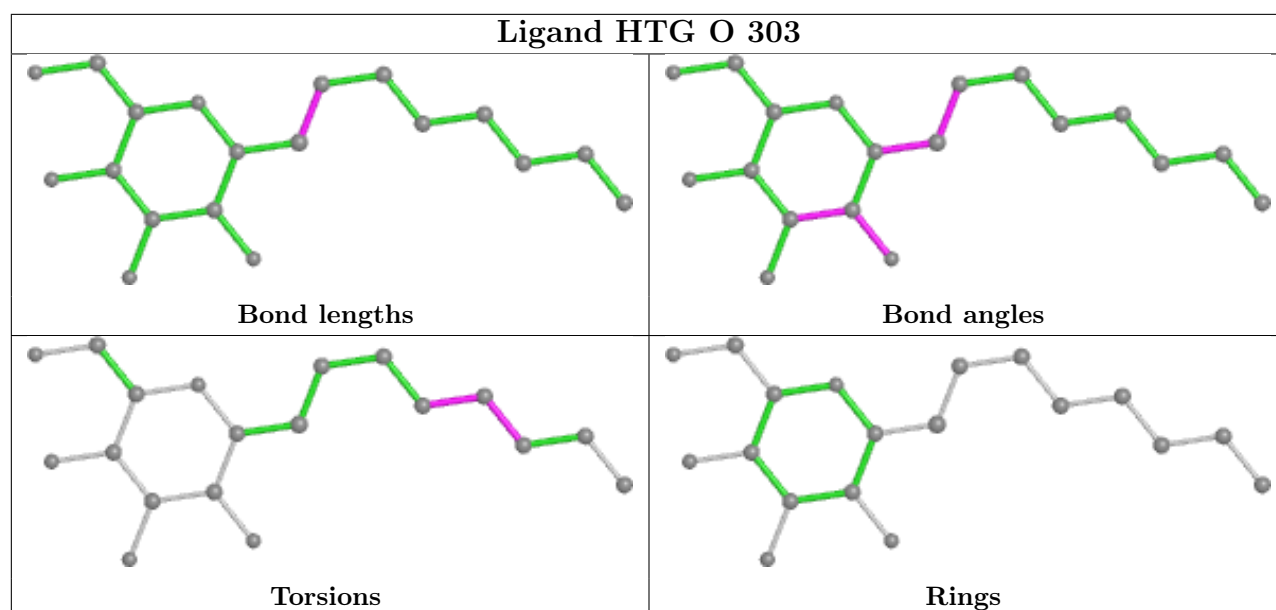


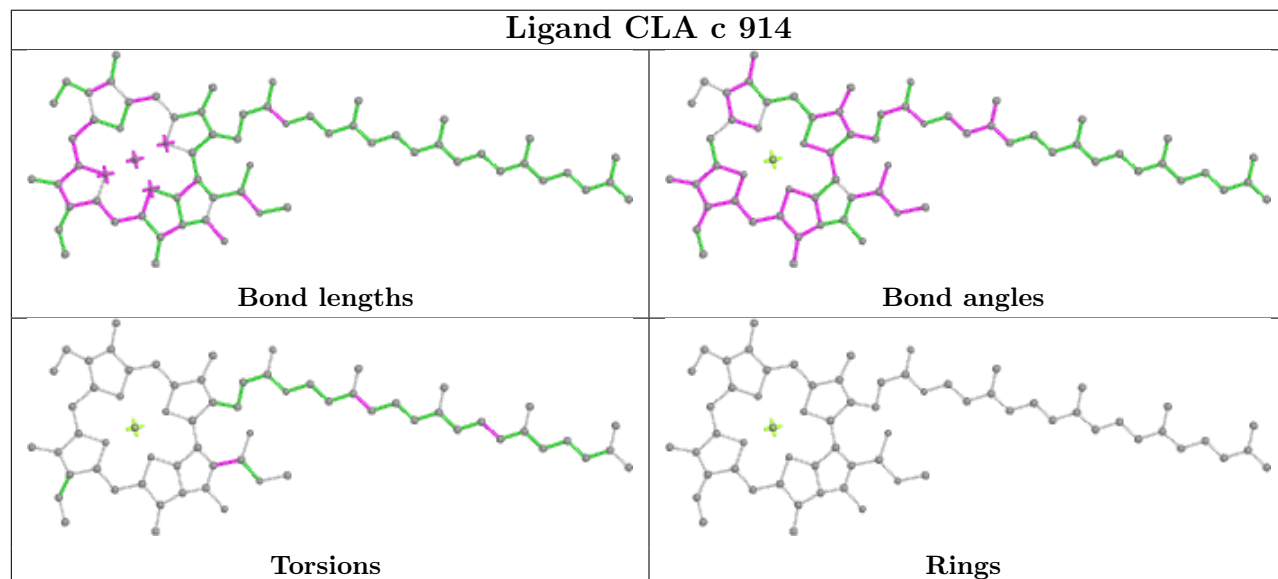
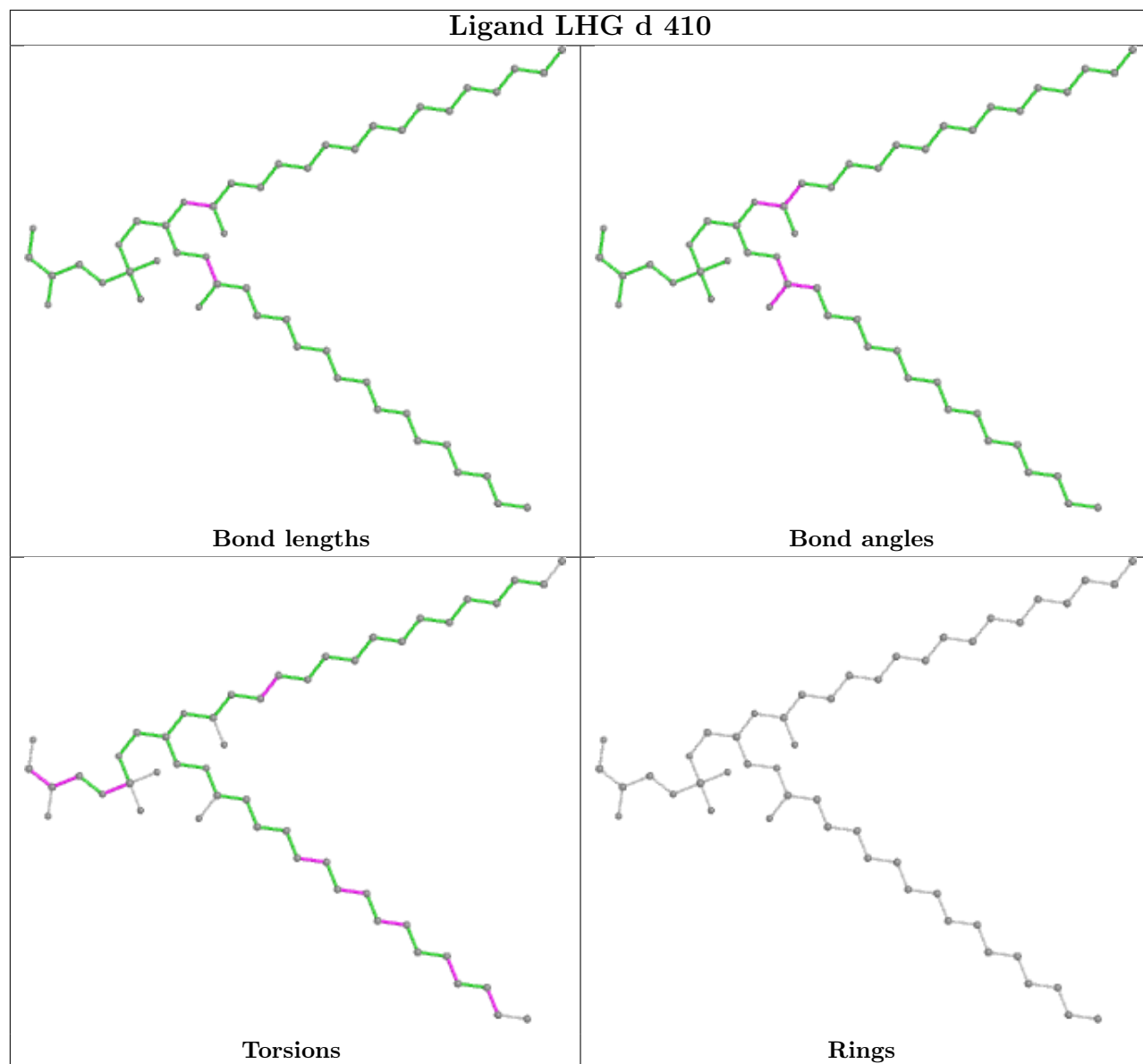
## Ligand CLA A 410

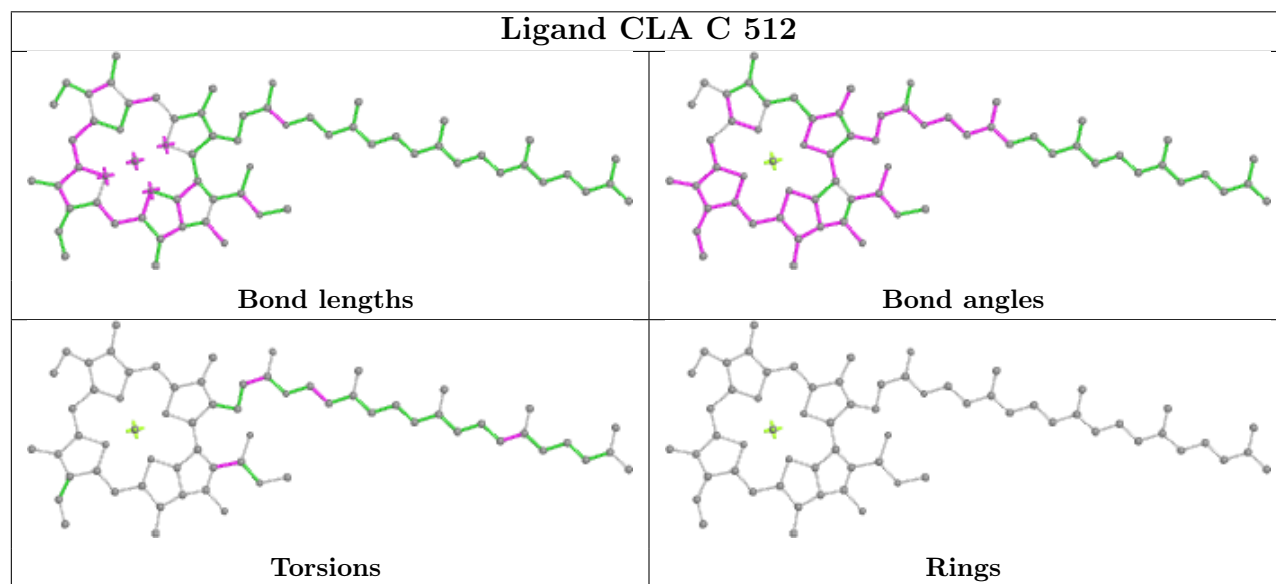
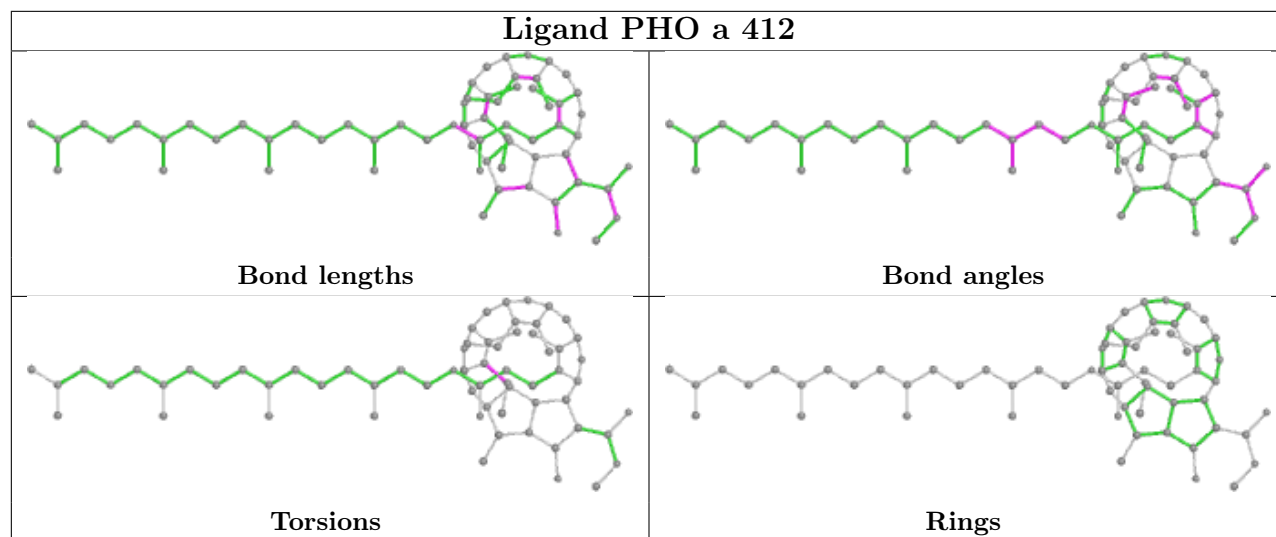
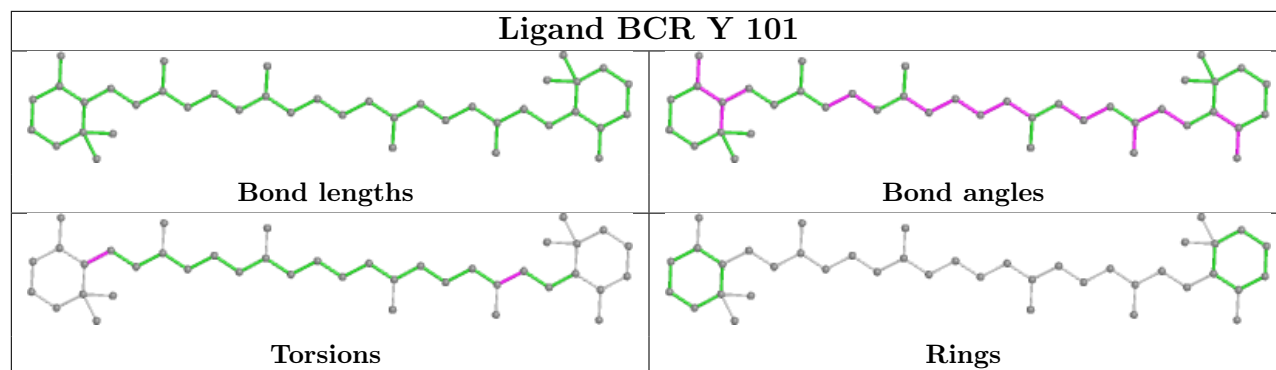


## Ligand HTG c 942

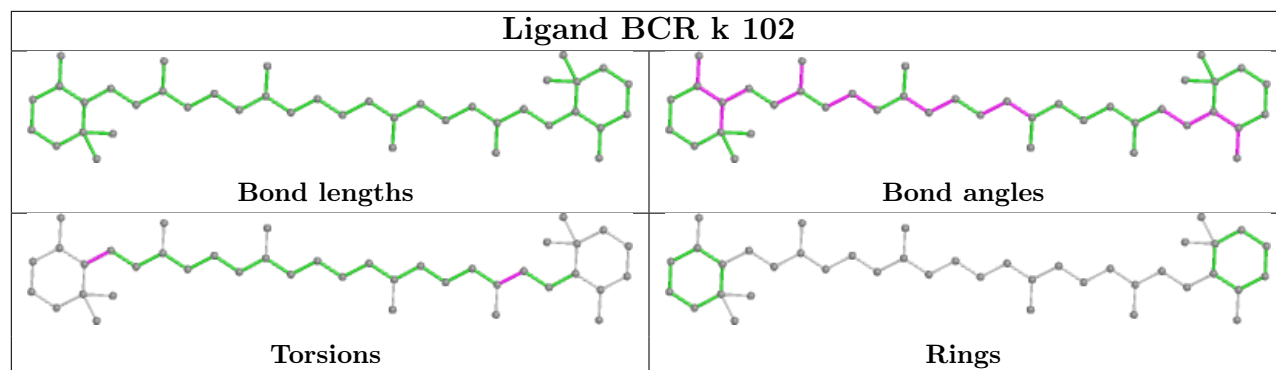




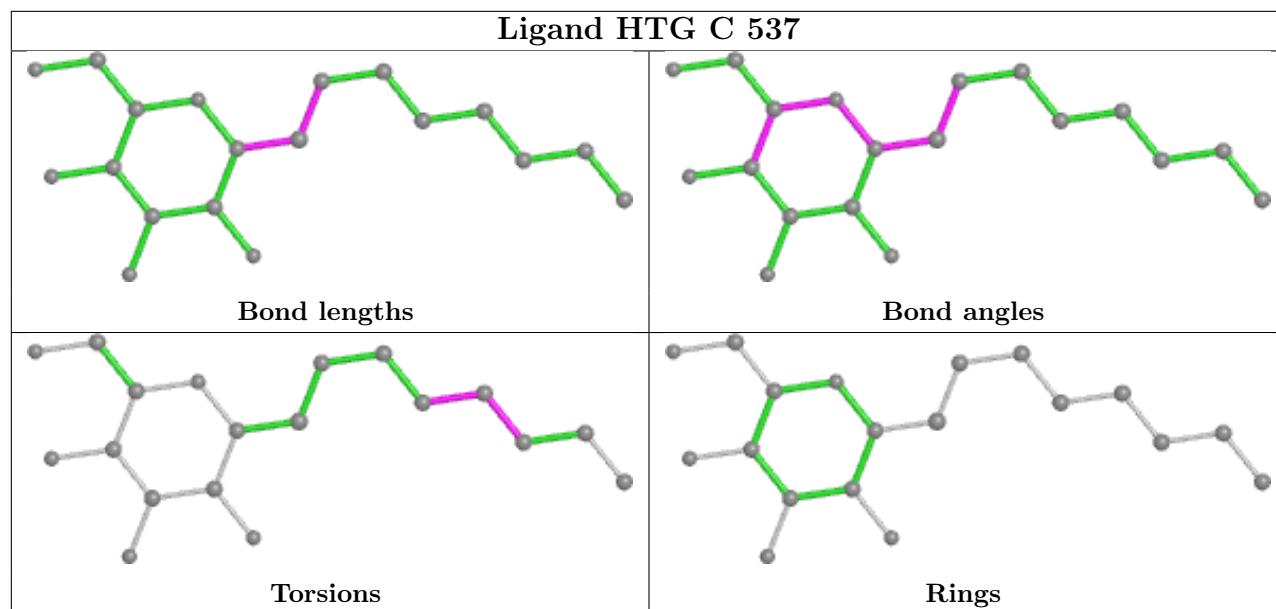




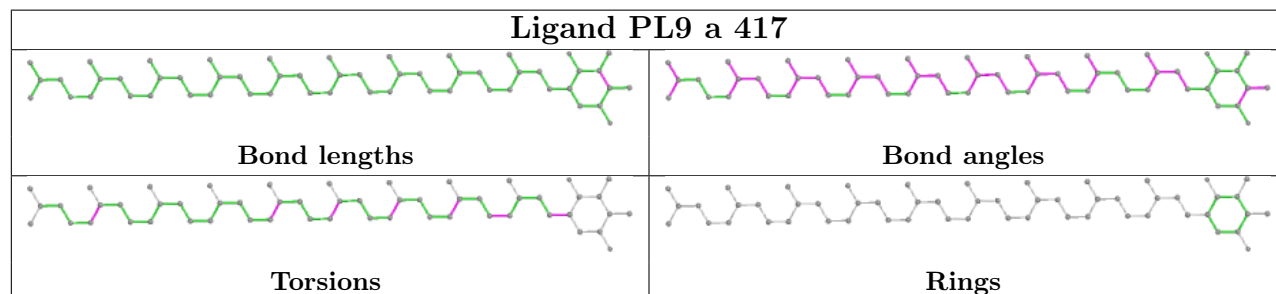
## Ligand BCR k 102



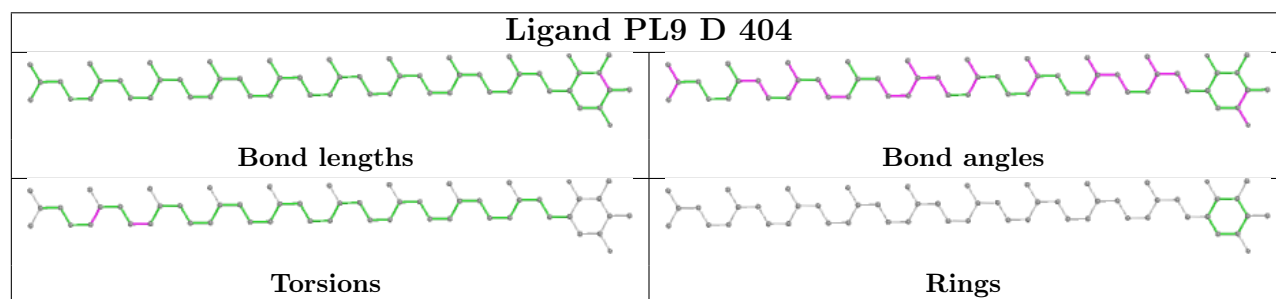
## Ligand HTG C 537



## Ligand PL9 a 417

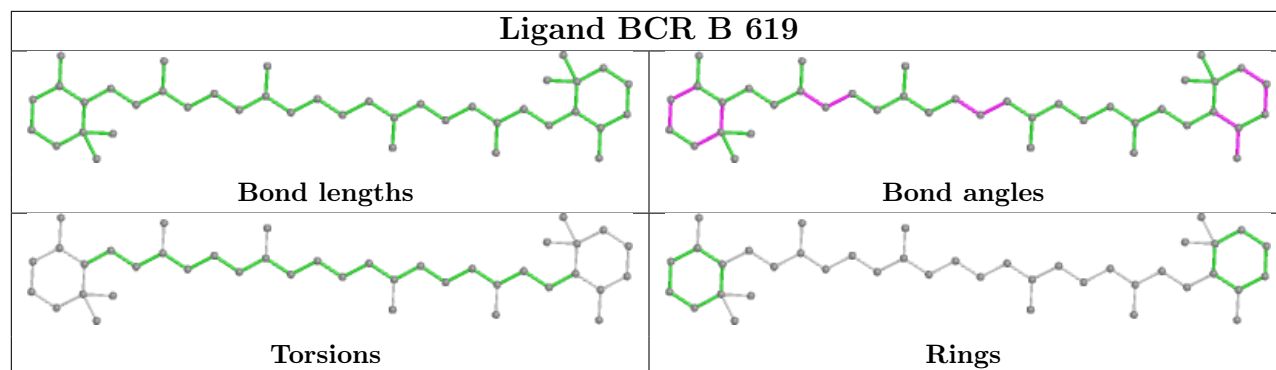


## Ligand PL9 D 404

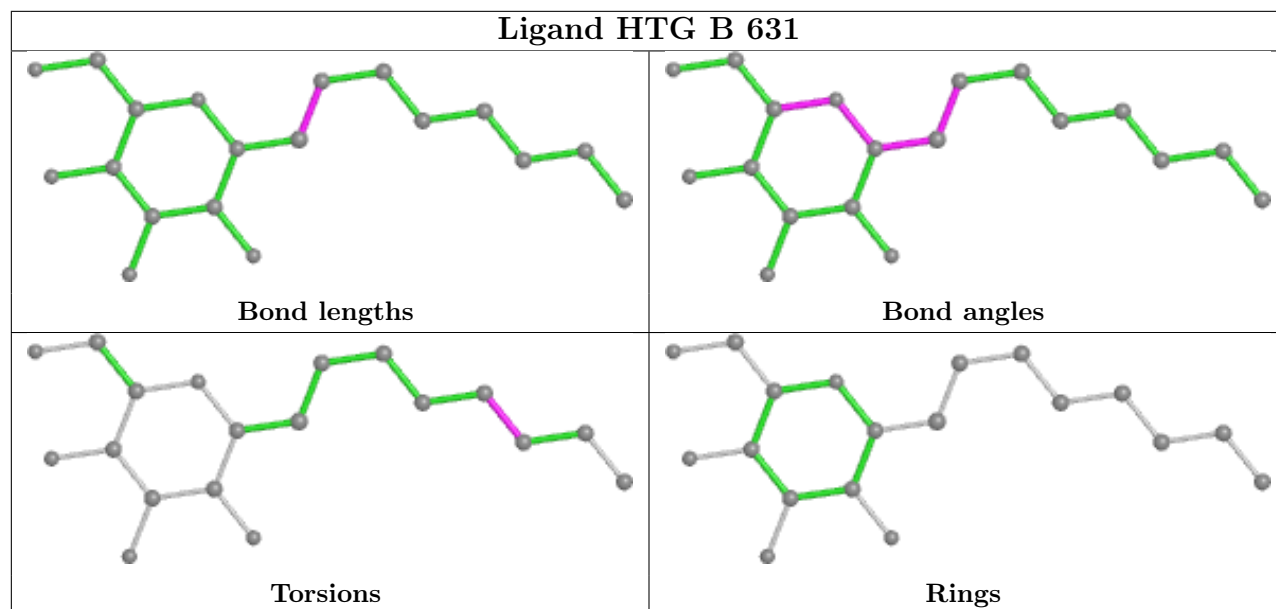




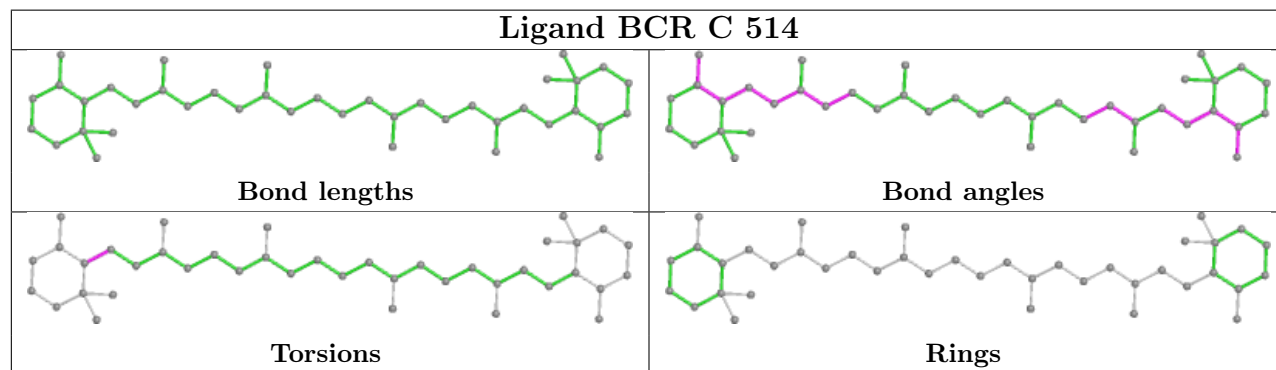
## Ligand BCR B 619

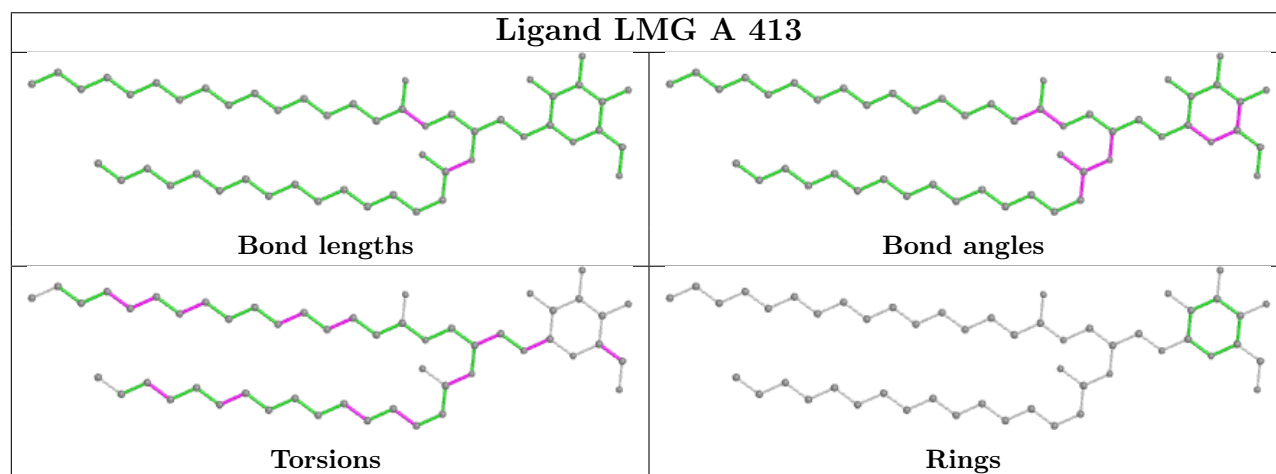
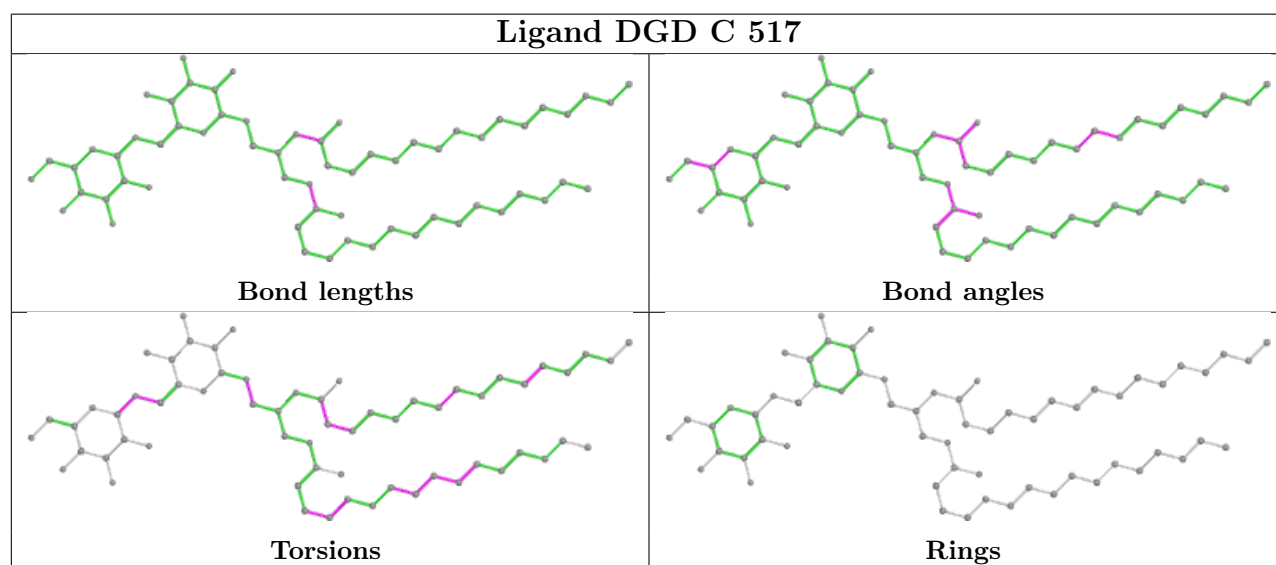
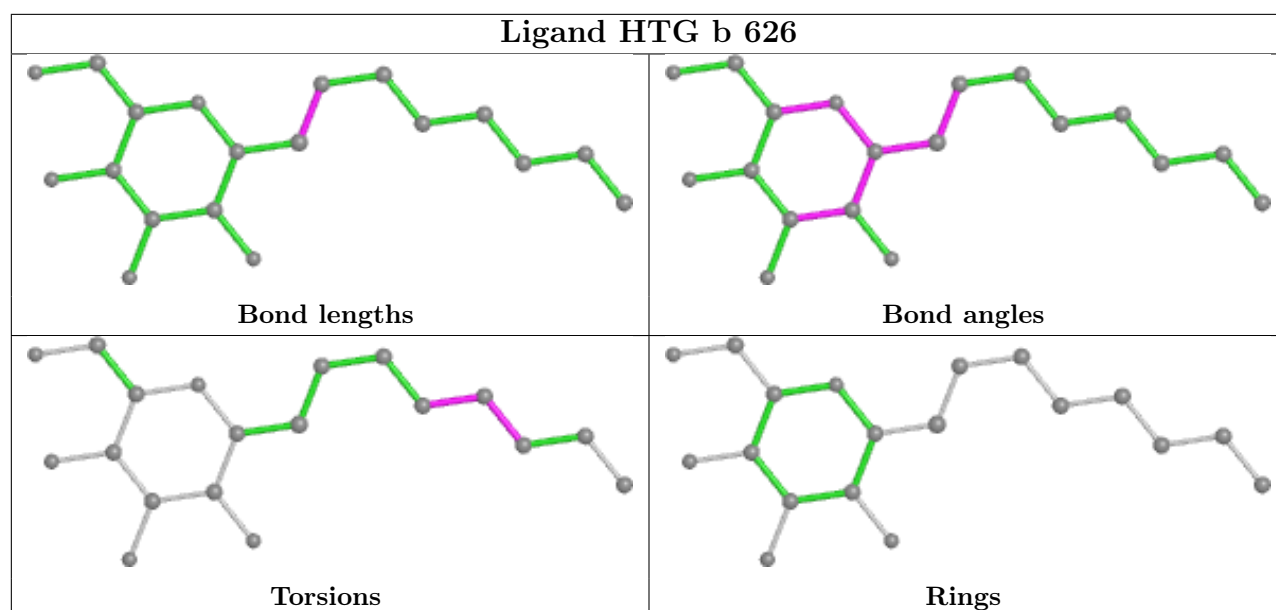


## Ligand HTG B 631

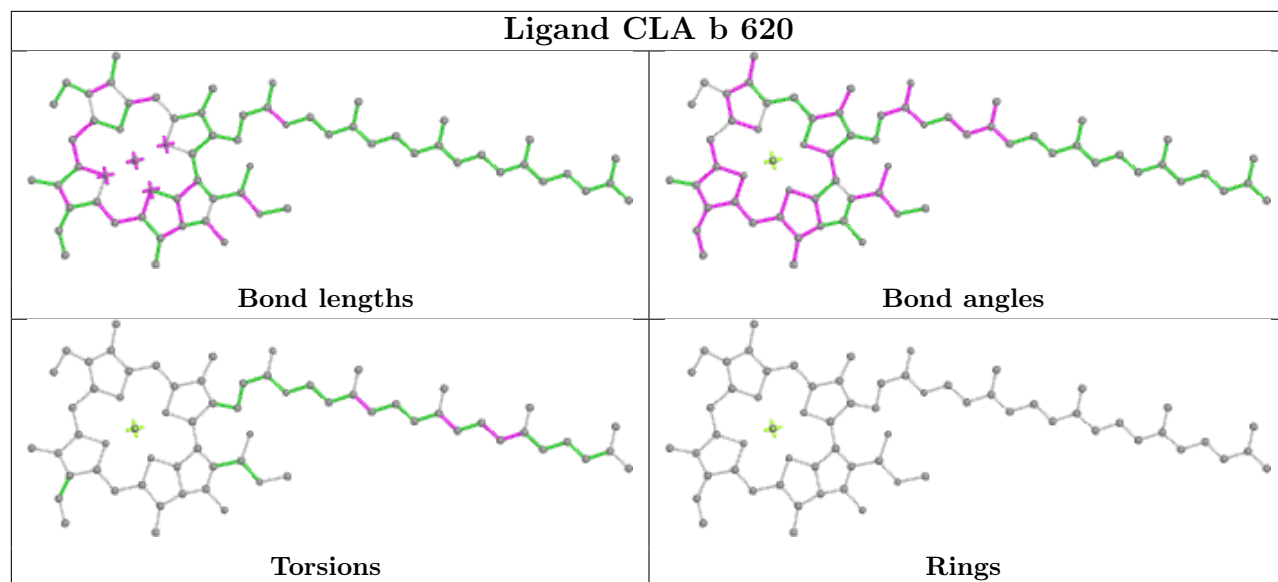


## Ligand BCR C 514

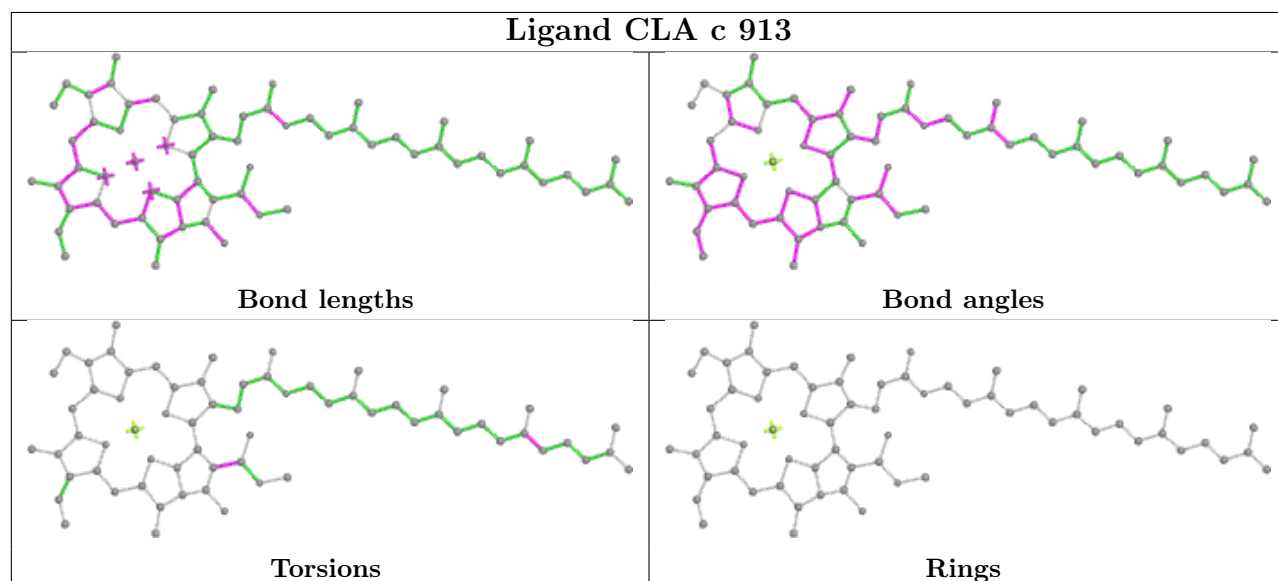




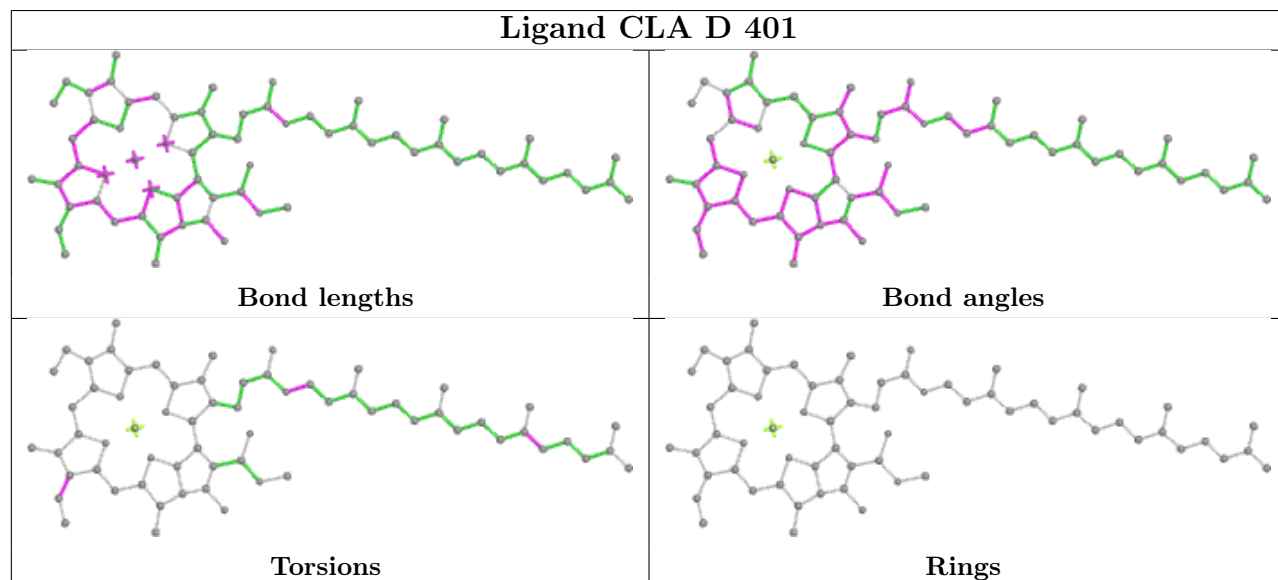
## Ligand CLA b 620



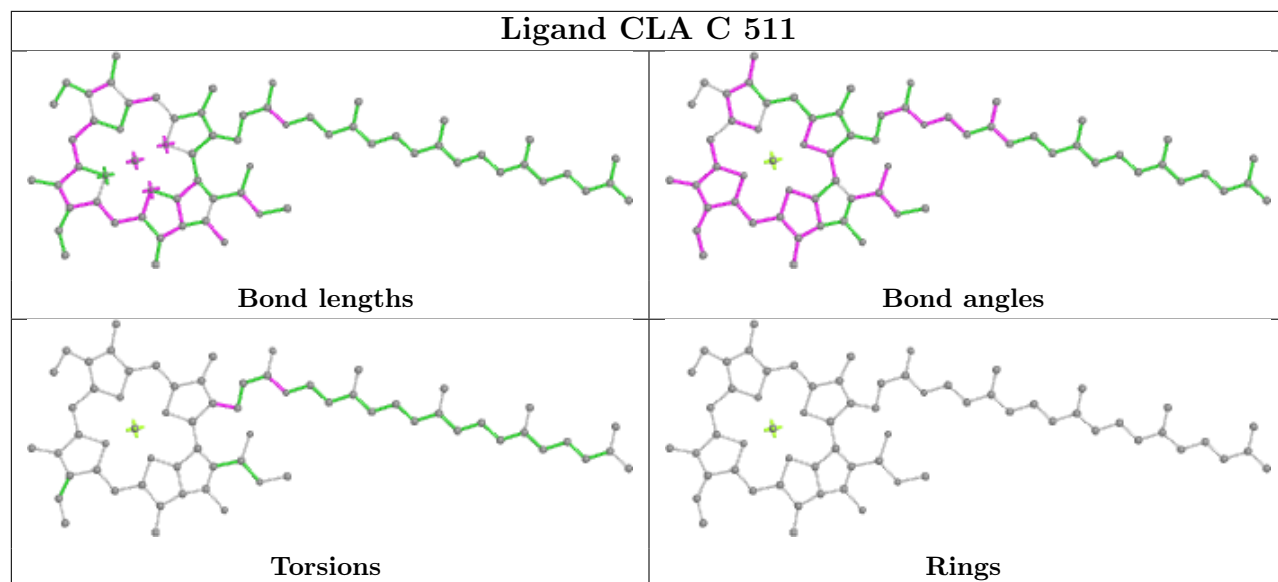
## Ligand CLA c 913



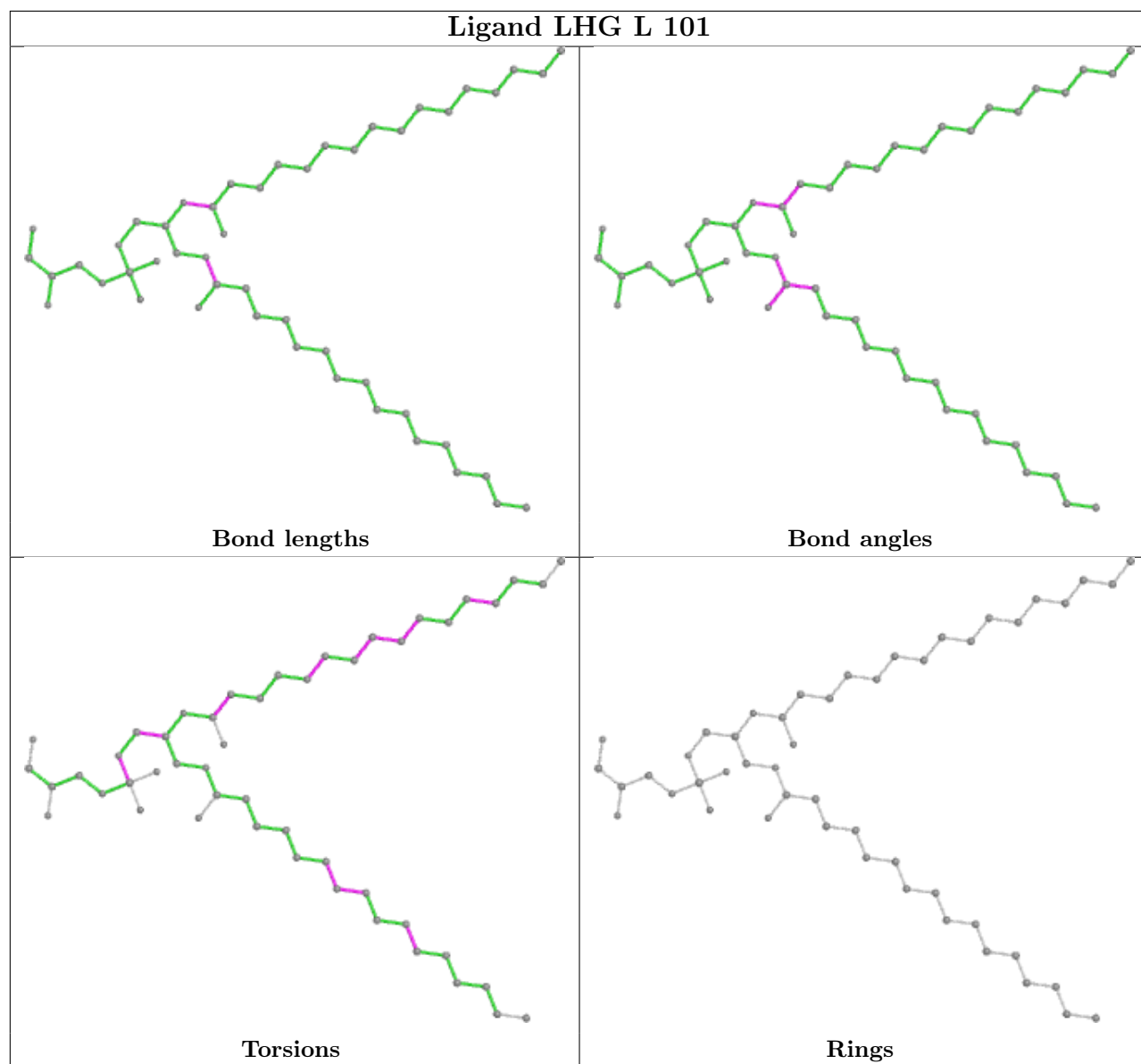
## Ligand CLA D 401



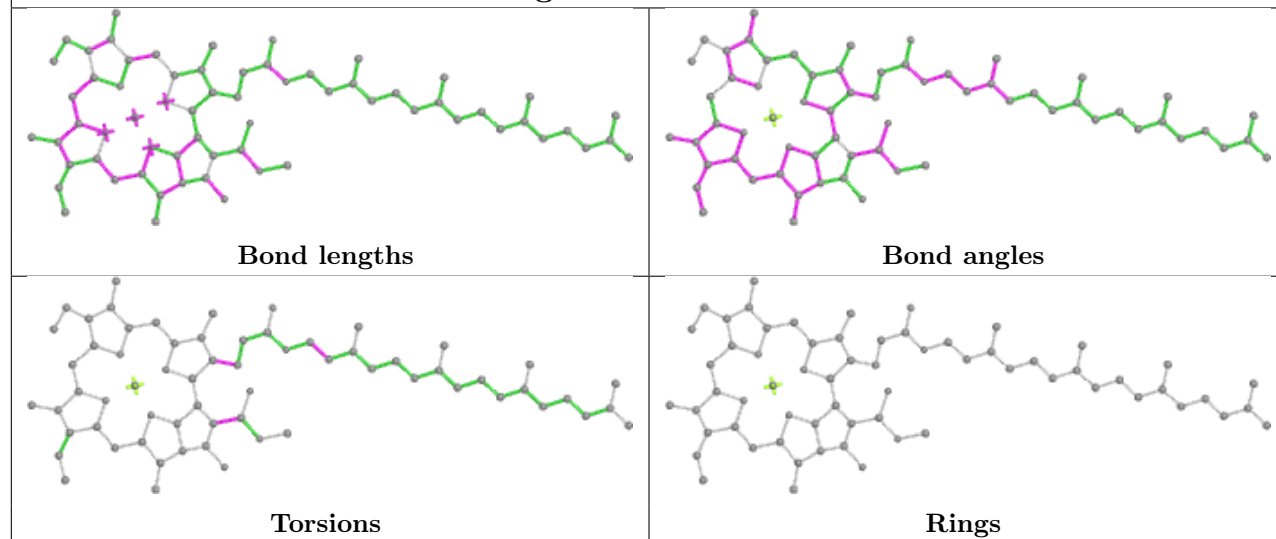
## Ligand CLA C 511



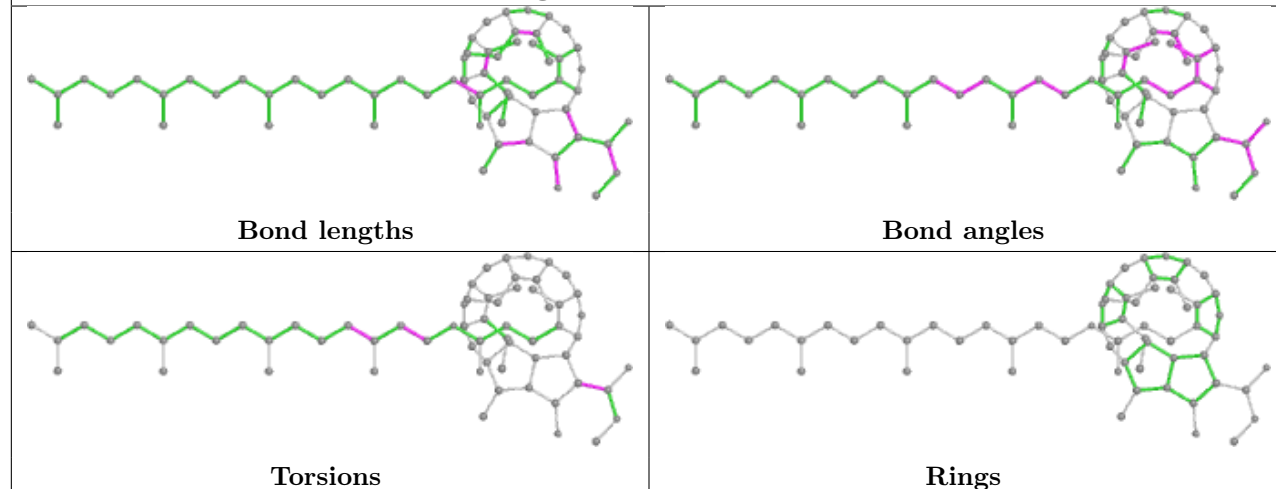
## Ligand LHG L 101



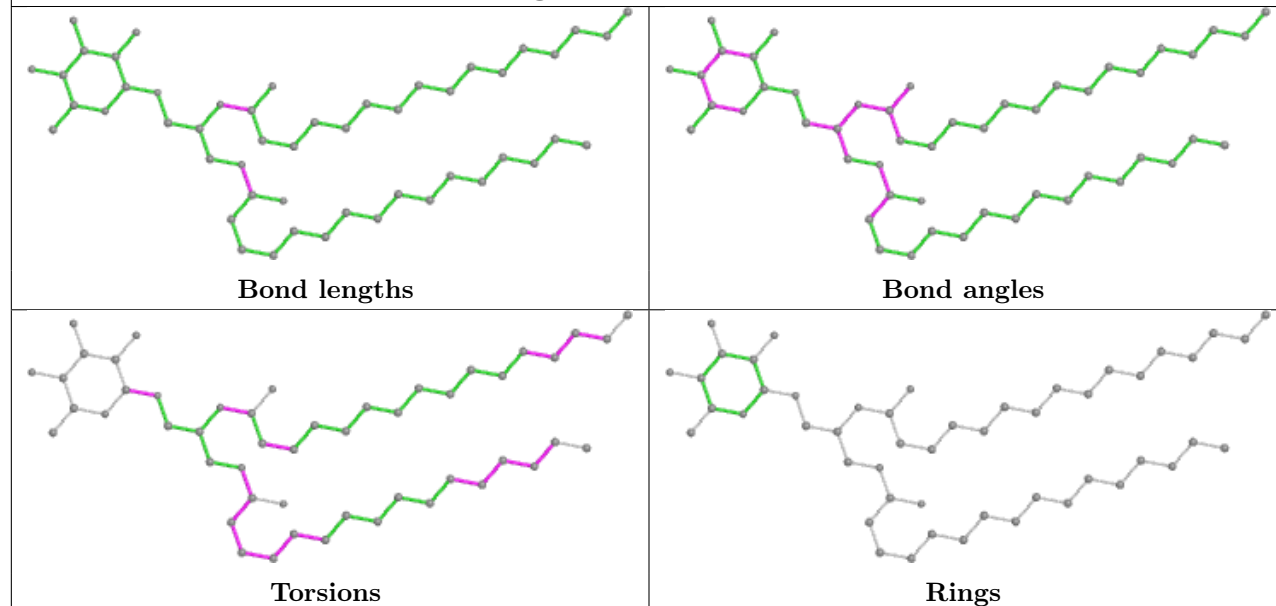
## Ligand CLA b 605

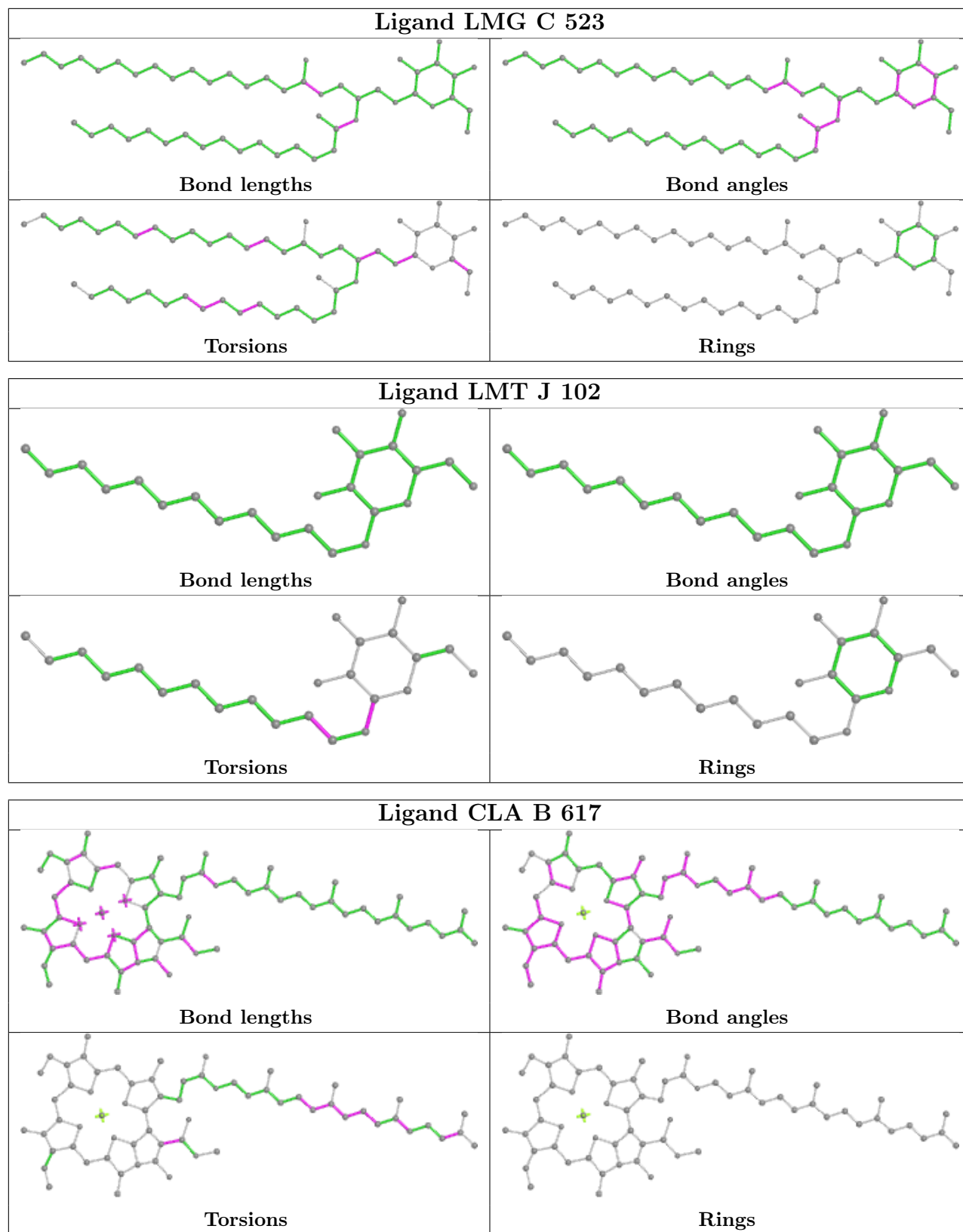


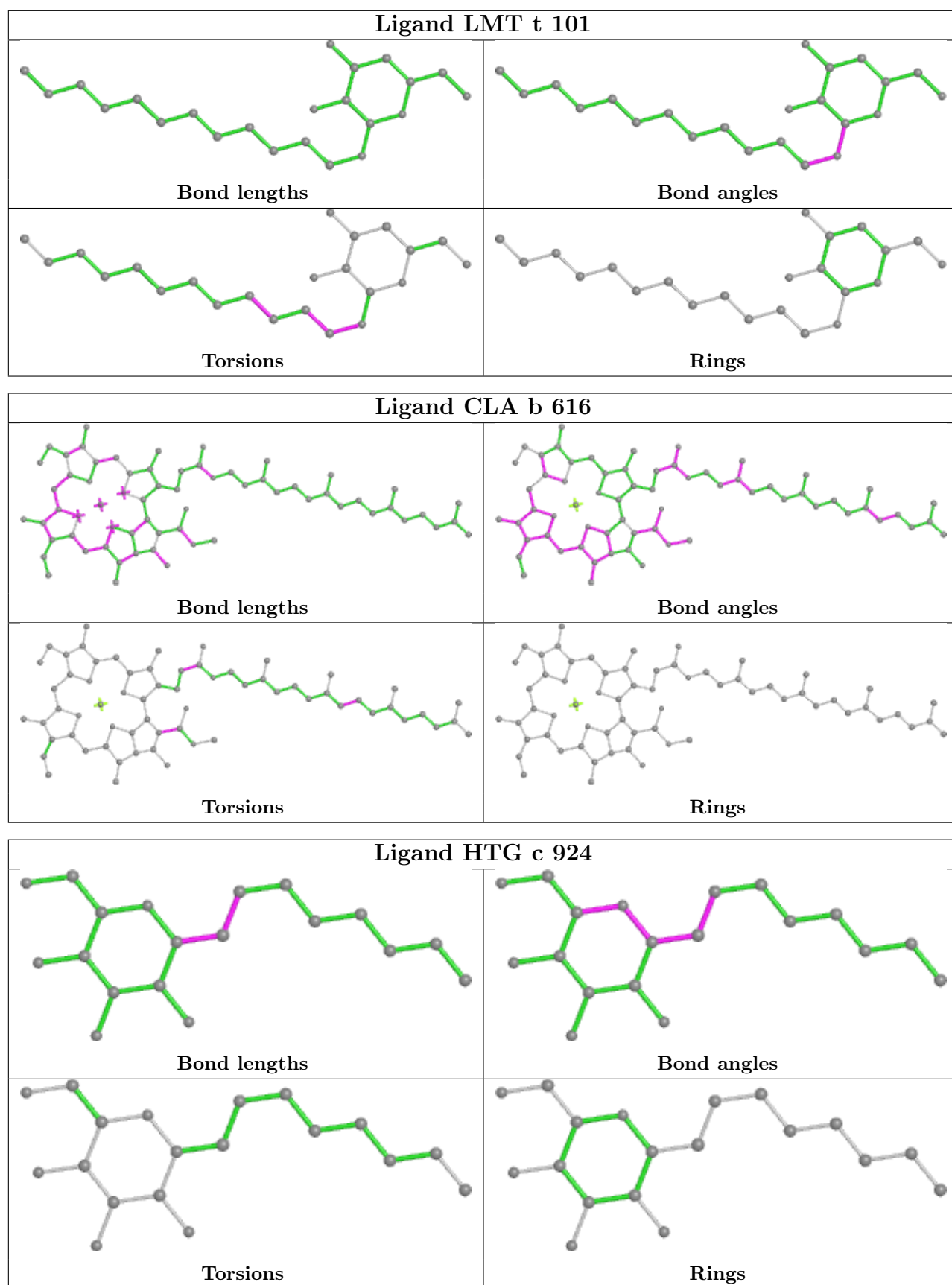
## Ligand PHO a 411

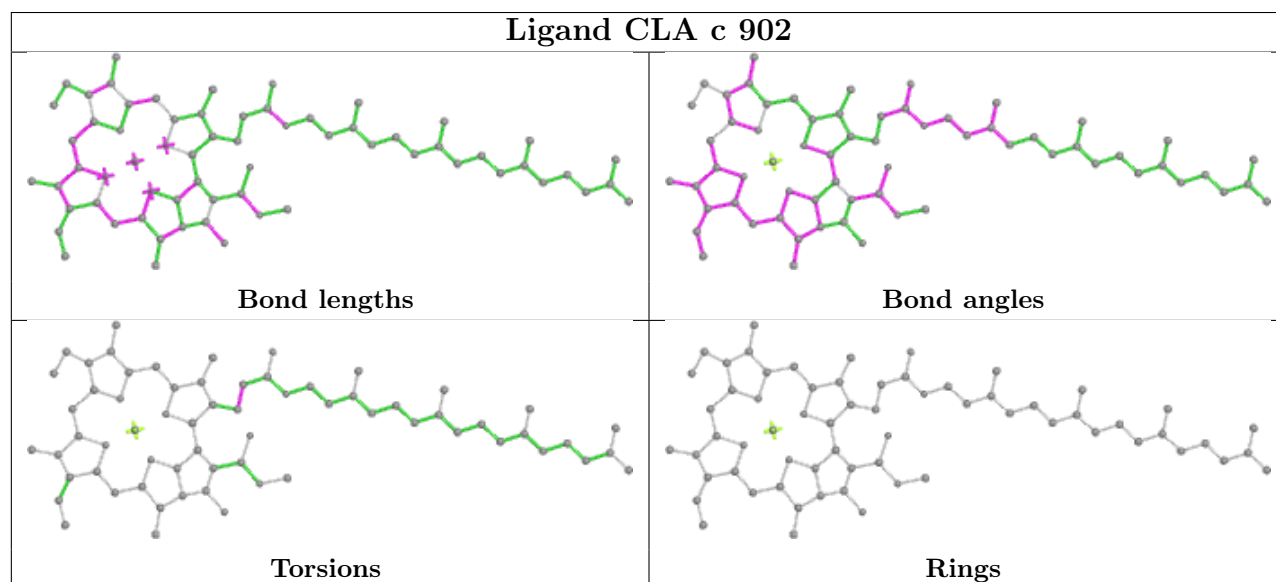
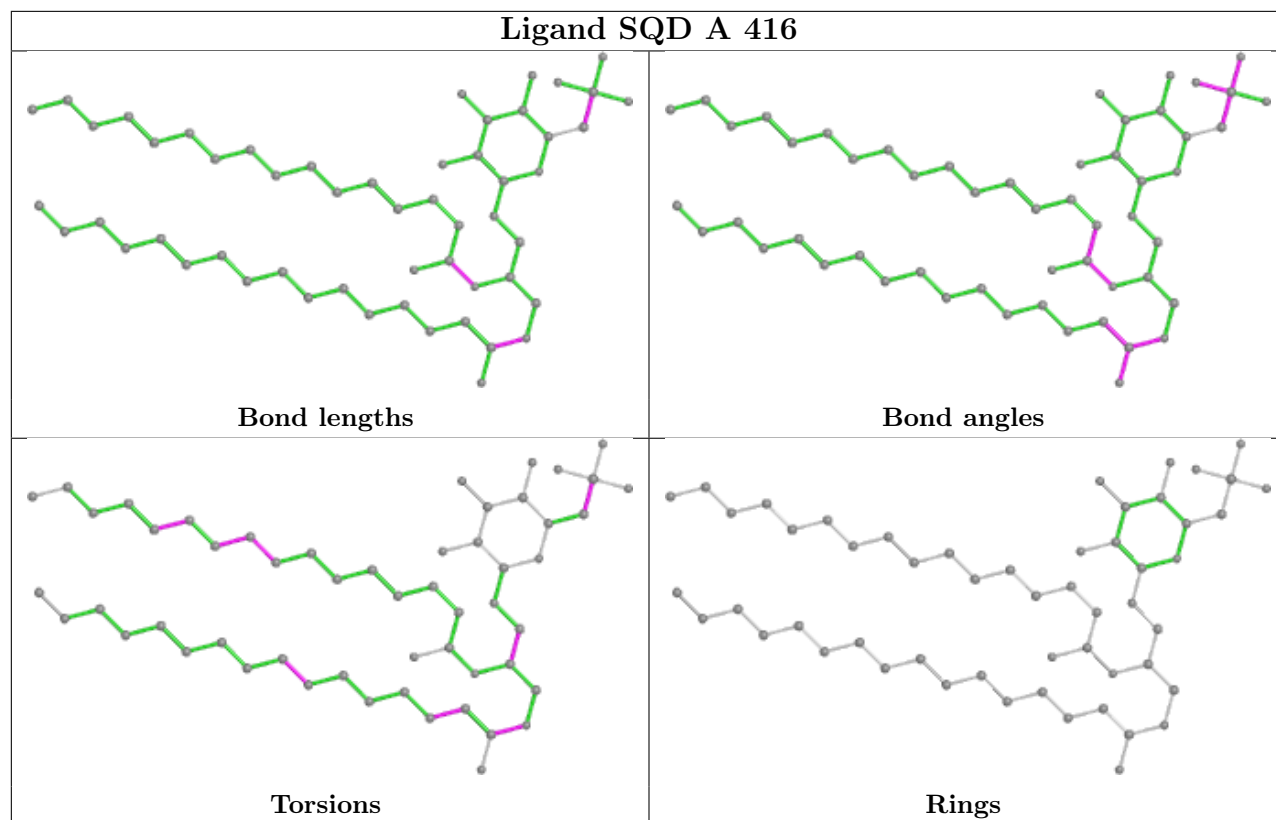


## Ligand DGD d 408

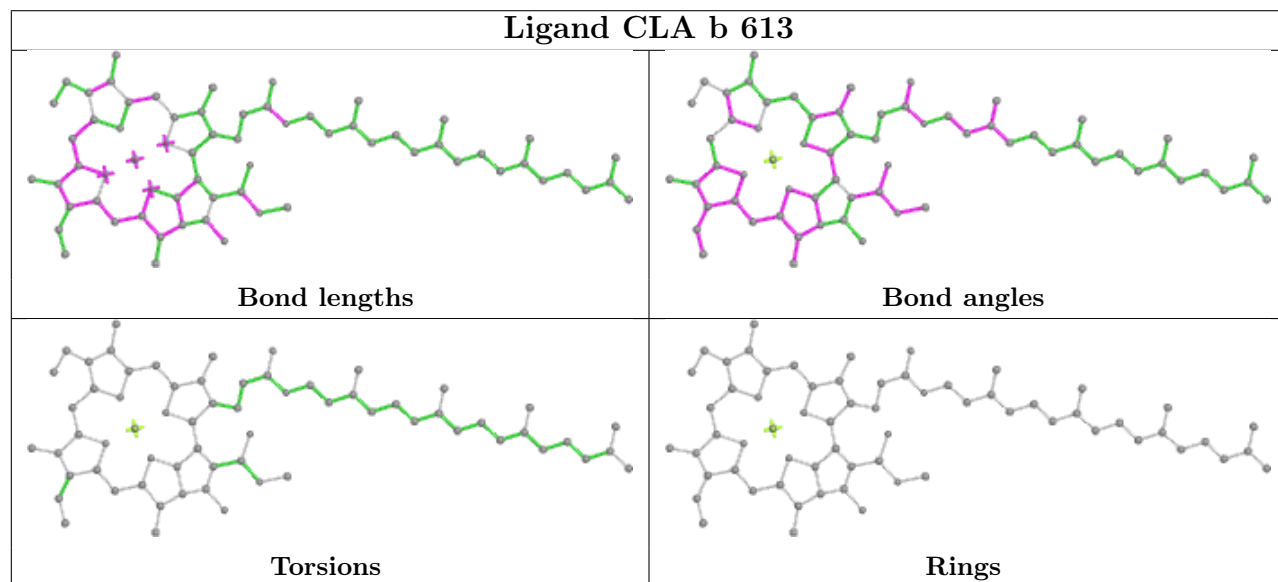
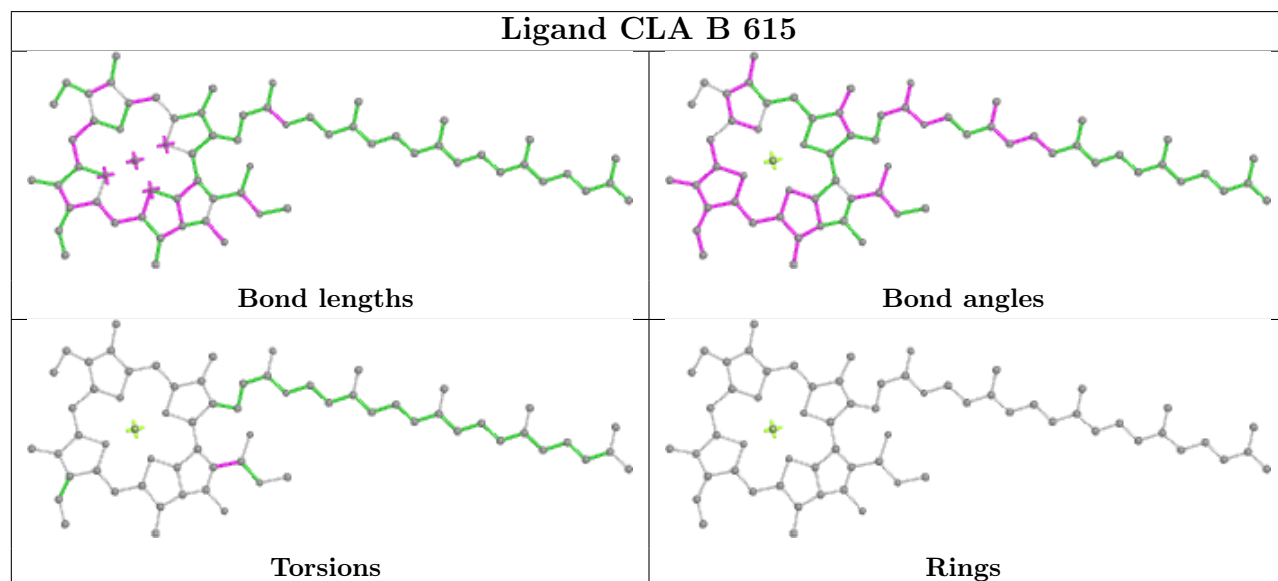
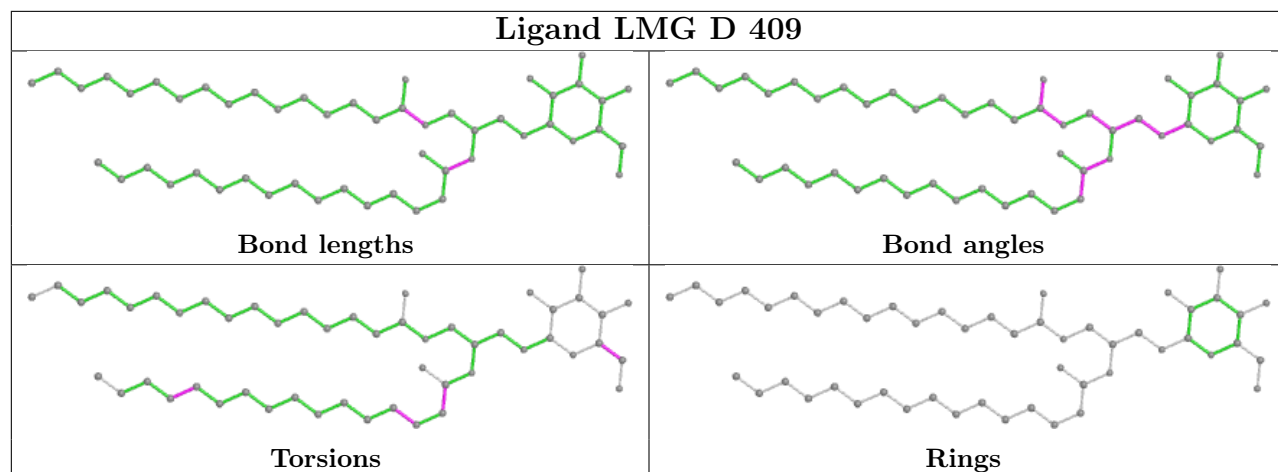




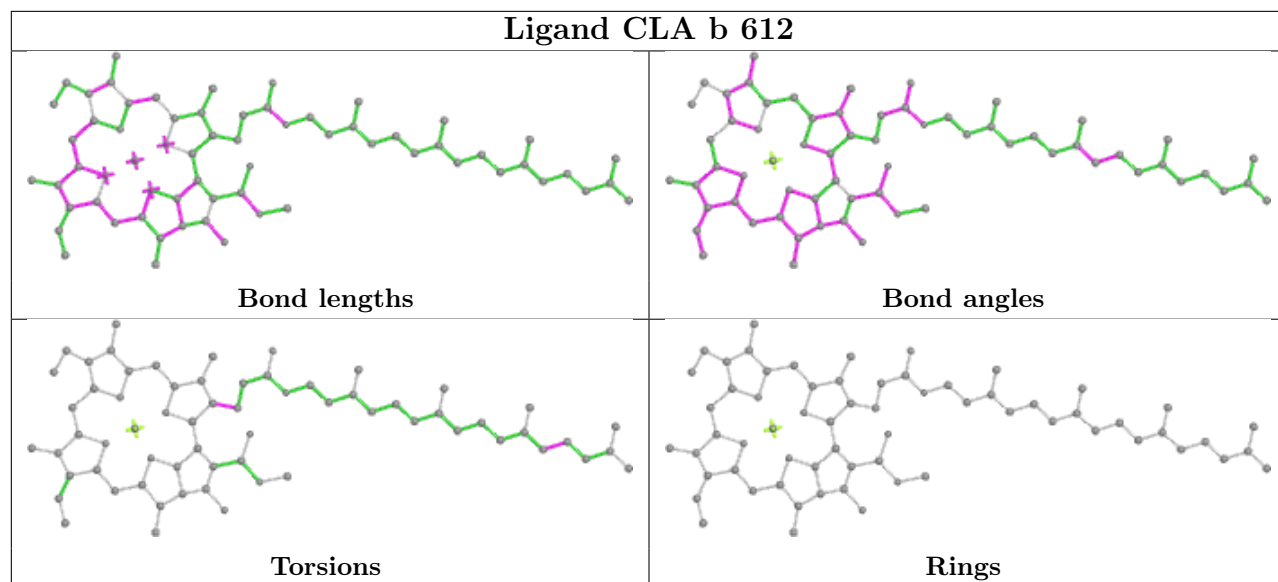




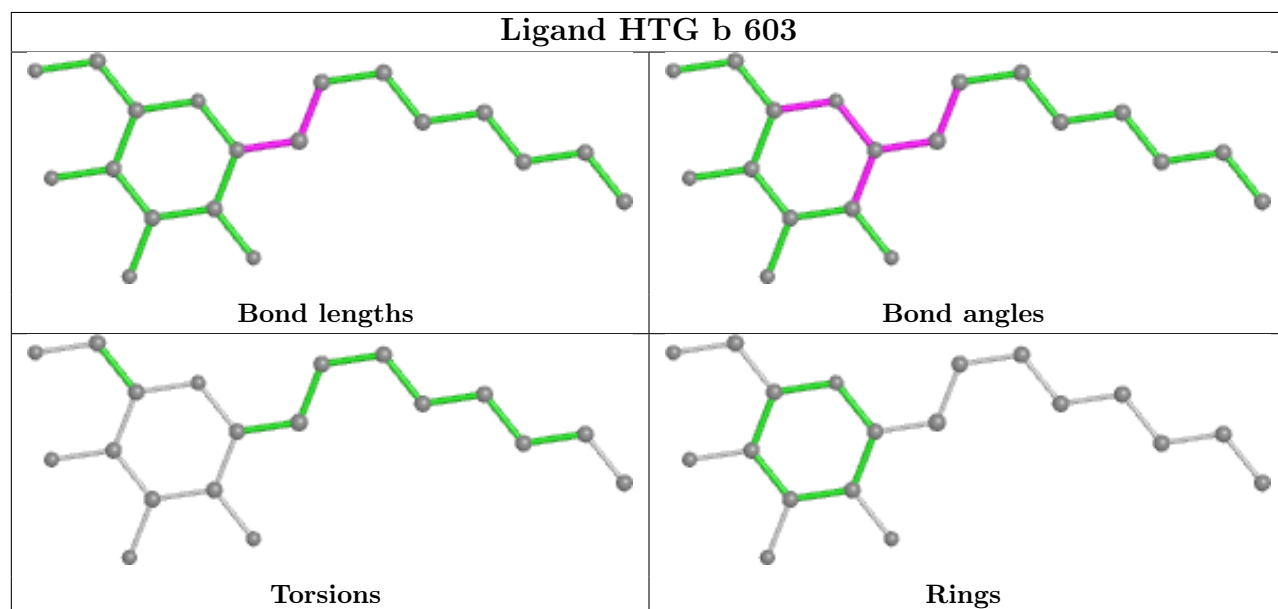




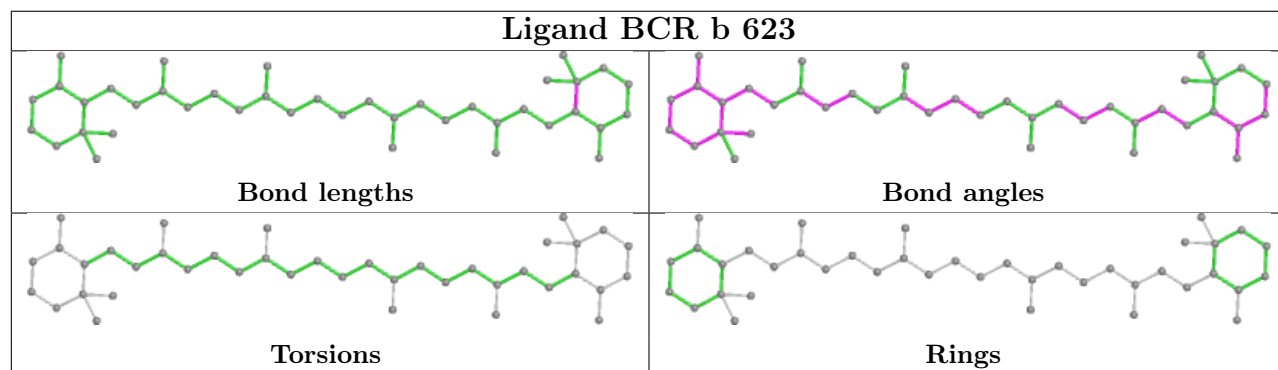
## Ligand CLA b 612

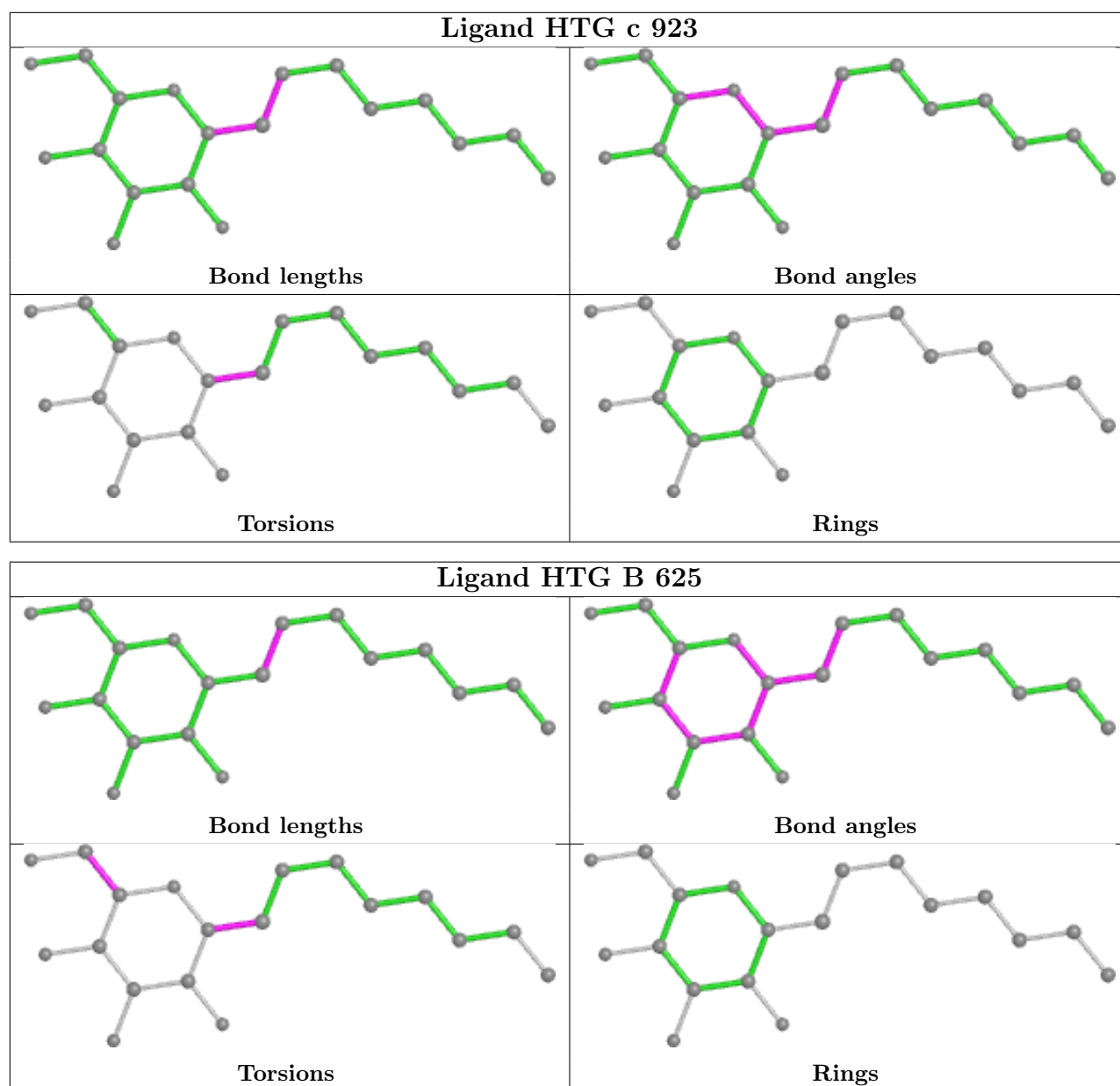


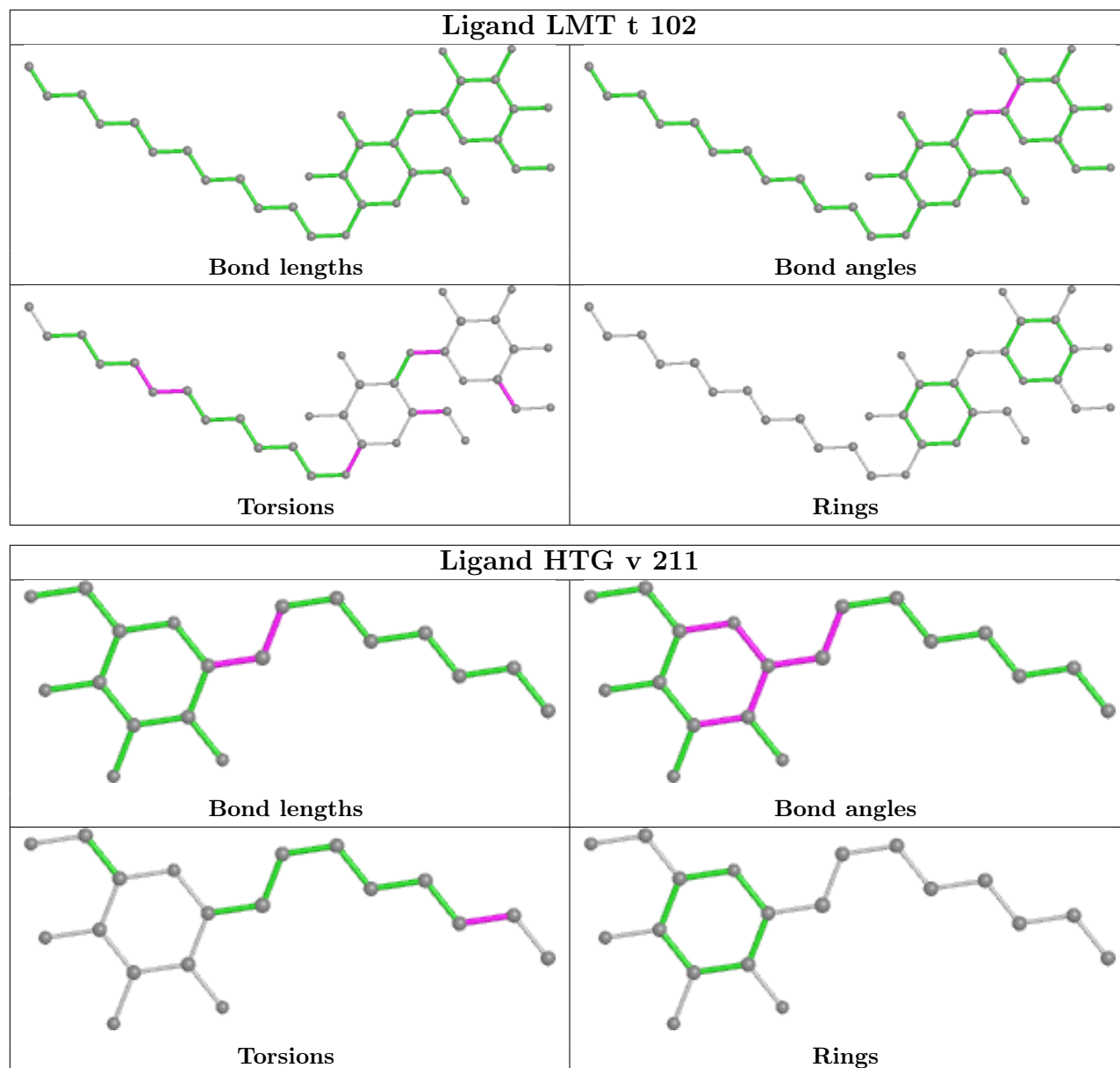
## Ligand HTG b 603

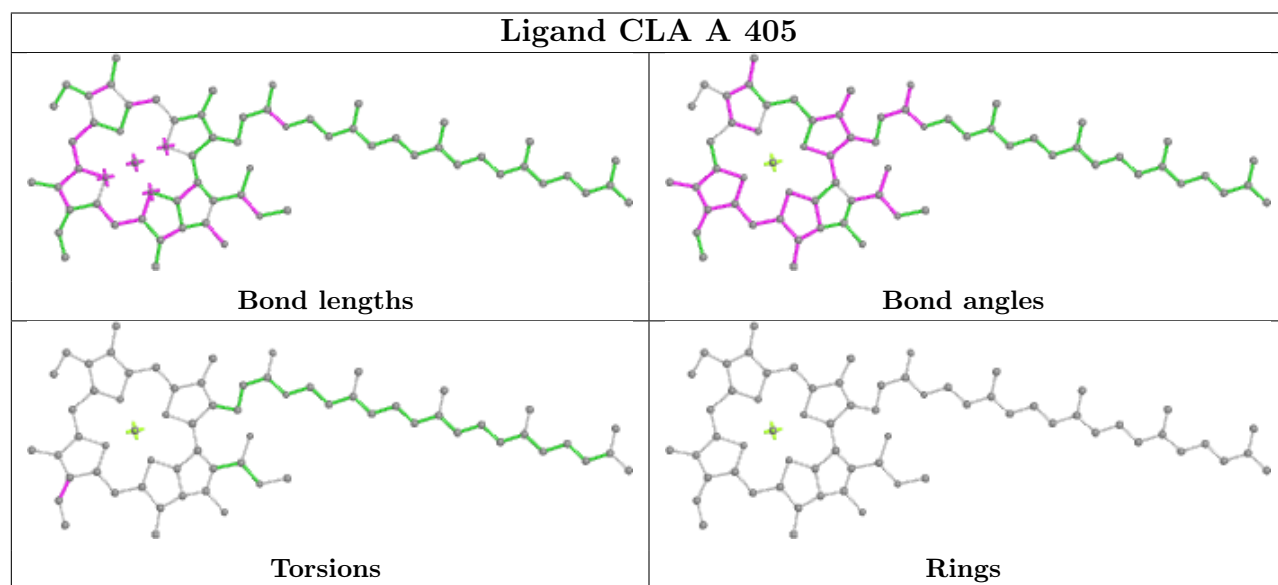
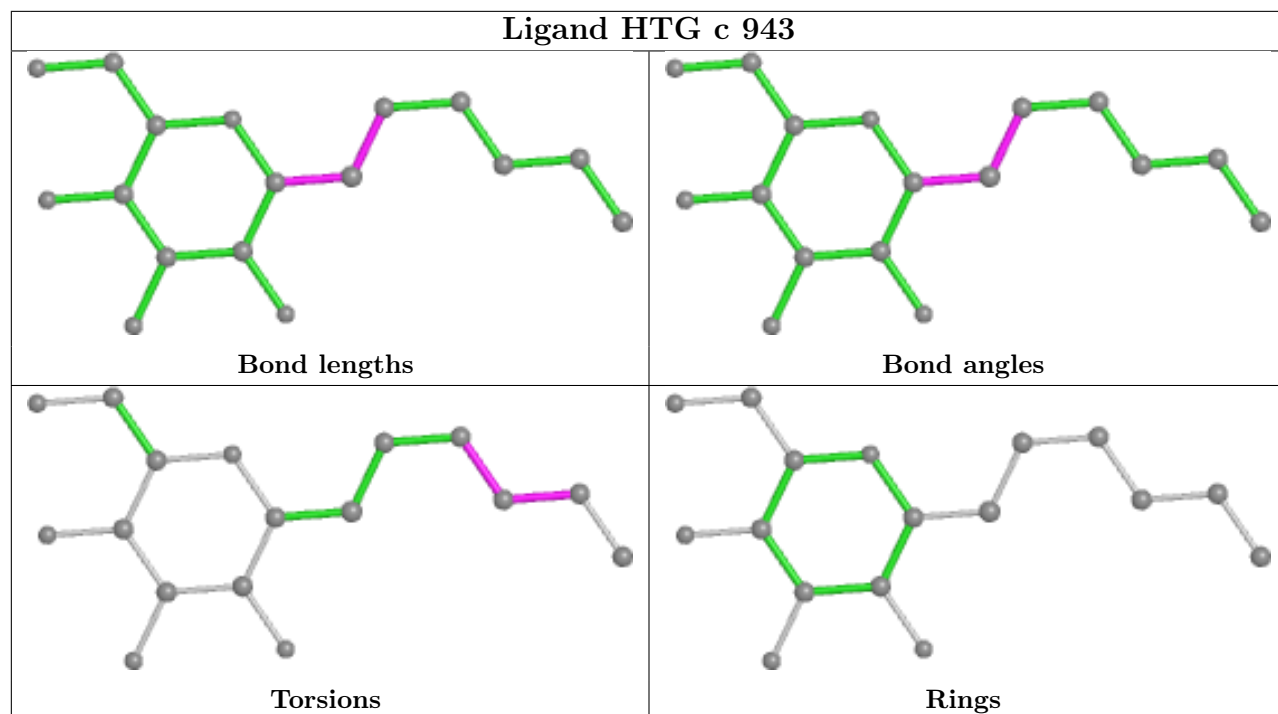


## Ligand BCR b 623

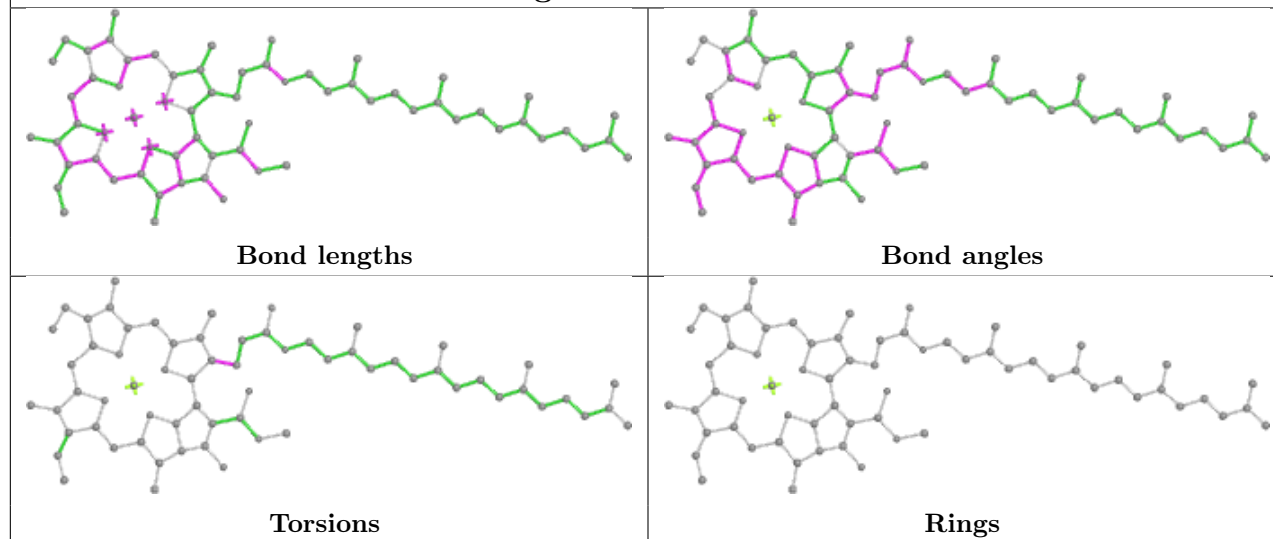




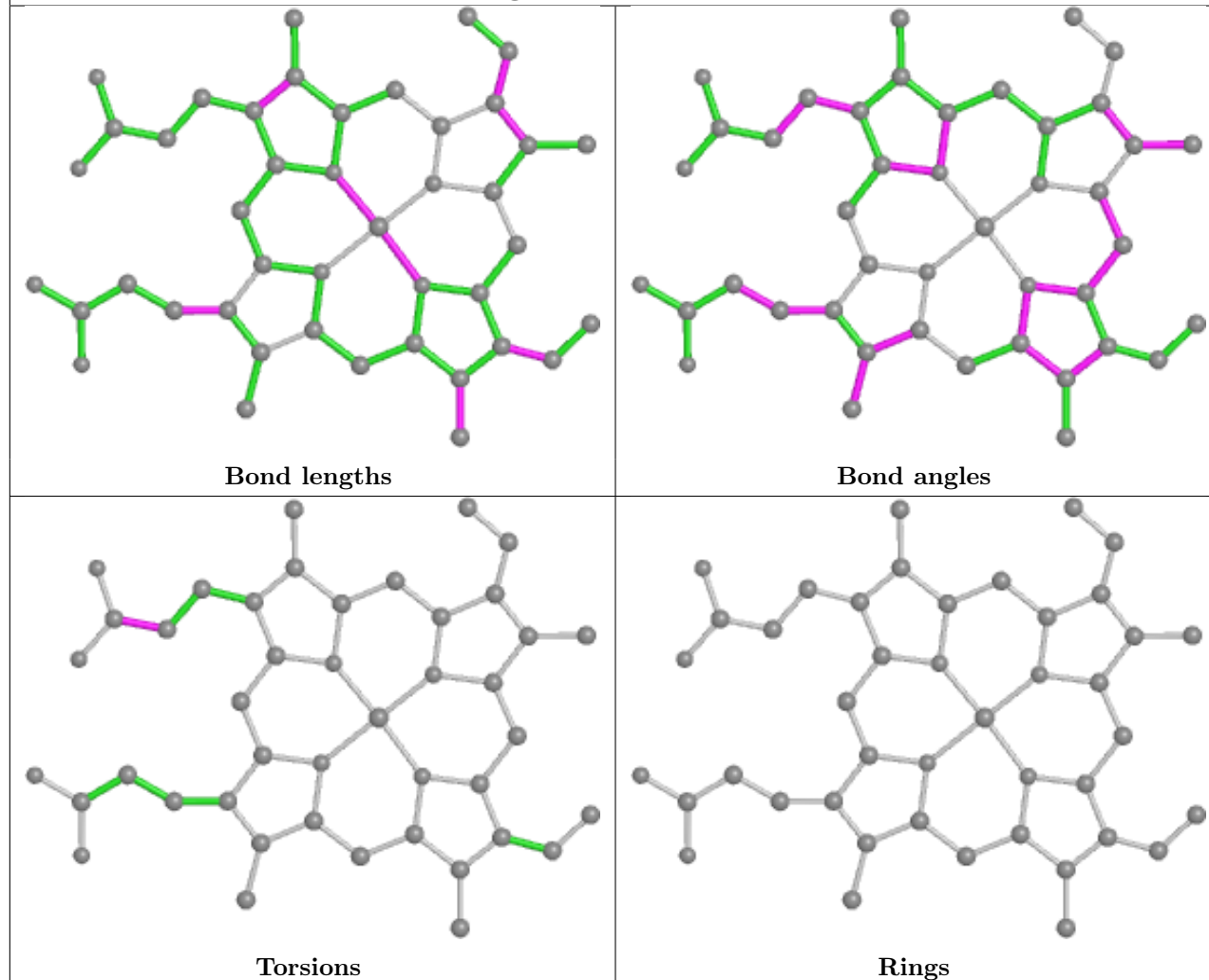




## Ligand CLA b 611



## Ligand HEM f 101



## 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	334/360 (92%)	-0.04	10 (2%) 50 53	24, 30, 52, 108	0
1	a	336/360 (93%)	0.23	29 (8%) 10 12	26, 32, 66, 131	0
2	B	505/510 (99%)	0.11	33 (6%) 18 21	26, 35, 61, 93	0
2	b	504/510 (98%)	0.17	44 (8%) 10 11	27, 38, 70, 153	0
3	C	451/461 (97%)	-0.02	17 (3%) 40 43	27, 40, 57, 104	0
3	c	456/461 (98%)	0.23	28 (6%) 21 24	30, 43, 59, 112	0
4	D	342/352 (97%)	-0.17	6 (1%) 68 71	24, 31, 48, 116	0
4	d	342/352 (97%)	-0.20	6 (1%) 68 71	25, 34, 52, 104	0
5	E	80/84 (95%)	0.98	21 (26%) 0 0	33, 54, 100, 124	0
5	e	79/84 (94%)	0.84	15 (18%) 1 1	39, 52, 98, 121	0
6	F	34/45 (75%)	-0.06	3 (8%) 10 11	35, 42, 64, 94	0
6	f	32/45 (71%)	-0.18	2 (6%) 20 22	37, 43, 82, 101	0
7	H	65/66 (98%)	0.21	5 (7%) 13 15	32, 43, 64, 121	0
7	h	65/66 (98%)	0.78	10 (15%) 2 2	35, 47, 62, 133	0
8	I	36/38 (94%)	0.47	5 (13%) 2 3	39, 46, 115, 133	0
8	i	36/38 (94%)	0.27	2 (5%) 24 27	37, 45, 86, 108	0
9	J	36/40 (90%)	-0.29	2 (5%) 24 27	33, 46, 85, 103	0
9	j	39/40 (97%)	-0.12	0 100 100	38, 49, 64, 71	0
10	K	37/46 (80%)	-0.04	1 (2%) 54 57	40, 46, 61, 68	0
10	k	37/46 (80%)	0.09	2 (5%) 25 29	40, 50, 69, 82	0
11	L	37/37 (100%)	-0.36	2 (5%) 25 29	25, 29, 75, 116	0
11	l	37/37 (100%)	-0.03	1 (2%) 54 57	26, 30, 83, 121	0
12	M	33/36 (91%)	-0.47	1 (3%) 50 53	27, 32, 75, 105	0
12	m	33/36 (91%)	0.02	2 (6%) 21 24	28, 33, 73, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	0.35	32 (13%) 3 3	24, 42, 69, 115	0
13	o	243/272 (89%)	0.39	35 (14%) 2 2	27, 44, 80, 109	0
14	T	29/32 (90%)	-0.34	1 (3%) 45 48	25, 30, 51, 120	0
14	t	29/32 (90%)	0.30	2 (6%) 16 19	27, 31, 59, 101	0
15	U	98/134 (73%)	-0.05	3 (3%) 49 51	30, 38, 61, 115	0
15	u	97/134 (72%)	-0.31	3 (3%) 49 51	34, 44, 61, 123	0
16	V	137/163 (84%)	-0.10	11 (8%) 12 13	30, 37, 58, 70	0
16	v	137/163 (84%)	0.55	28 (20%) 1 1	35, 50, 70, 87	0
17	Y	30/46 (65%)	1.61	10 (33%) 0 0	47, 60, 102, 111	0
17	y	30/46 (65%)	1.93	11 (36%) 0 0	50, 64, 96, 105	0
18	X	40/41 (97%)	1.20	6 (15%) 2 2	41, 50, 92, 125	0
18	x	39/41 (95%)	0.89	7 (17%) 1 1	44, 52, 113, 137	0
19	Z	61/62 (98%)	1.90	23 (37%) 0 0	45, 55, 85, 112	0
19	z	61/62 (98%)	2.55	29 (47%) 0 0	51, 64, 105, 121	0
20	R	34/41 (82%)	5.82	34 (100%) 0 0	60, 94, 119, 124	0
All	All	5294/5691 (93%)	0.23	482 (9%) 9 10	24, 39, 72, 153	0

The worst 5 of 482 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	X	41	LEU	15.0
8	I	37	LEU	12.9
2	b	486	LEU	12.4
7	h	65	LEU	11.2
20	R	18	TRP	9.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
19	FME	Z	1	10/11	0.90	0.23	68,82,98,101	0
19	FME	z	1	10/11	0.90	0.34	98,112,120,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	FME	t	1	10/11	0.95	0.09	30,34,59,63	0
14	FME	T	1	10/11	0.95	0.10	30,39,62,64	0
8	FME	i	1	10/11	0.97	0.13	31,40,44,47	0
12	FME	m	1	10/11	0.98	0.07	33,42,69,78	0
12	FME	M	1	10/11	0.98	0.11	31,40,71,76	0
8	FME	I	1	10/11	0.98	0.07	34,43,49,50	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
30	UNL	A	415	36/-	0.37	0.46	75,99,113,114	0
36	HTG	c	941	19/19	0.39	0.34	67,133,141,142	0
30	UNL	c	947	6/-	0.43	0.31	71,80,83,85	0
30	UNL	h	103	9/-	0.47	0.47	81,86,109,110	0
30	UNL	J	105	8/-	0.51	0.21	80,94,98,99	0
30	UNL	i	105	12/-	0.52	0.37	77,86,88,89	0
37	DGD	D	405	52/66	0.55	0.36	74,102,120,124	0
30	UNL	a	418	40/-	0.56	0.52	79,99,122,125	0
31	LMT	m	103	35/35	0.56	0.31	53,125,136,137	0
30	UNL	b	633	9/-	0.57	0.22	76,81,87,88	0
31	LMT	j	102	24/35	0.58	0.23	66,84,120,122	0
30	UNL	b	634	9/-	0.60	0.37	99,103,113,114	0
30	UNL	I	106	9/-	0.60	0.18	76,80,87,87	0
30	UNL	c	944	4/-	0.62	0.28	76,77,78,81	0
31	LMT	b	625	35/35	0.62	0.26	59,119,133,139	0
37	DGD	d	408	50/66	0.63	0.34	81,99,121,130	0
36	HTG	d	420	19/19	0.64	0.42	85,115,118,118	0
27	SQD	l	101	54/54	0.64	0.26	48,77,116,117	0
31	LMT	A	417	35/35	0.64	0.31	55,92,108,115	0
30	UNL	e	106	11/-	0.65	0.18	83,87,92,94	0
31	LMT	t	101	23/35	0.65	0.28	60,95,135,138	0
32	GOL	O	304	6/6	0.65	0.40	89,90,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	HTG	b	627	19/19	0.65	0.25	69,113,125,128	0
31	LMT	e	101	24/35	0.66	0.31	94,101,125,127	0
31	LMT	A	421	35/35	0.66	0.37	84,100,131,132	0
31	LMT	J	102	24/35	0.66	0.25	64,86,118,120	0
36	HTG	y	102	19/19	0.66	0.23	84,115,122,124	0
30	UNL	J	103	12/-	0.66	0.25	69,79,83,84	0
31	LMT	c	922	35/35	0.66	0.45	85,117,122,126	0
36	HTG	c	924	19/19	0.67	0.50	69,99,118,118	0
34	DMS	c	939	4/4	0.67	0.35	112,114,119,120	0
34	DMS	B	646	4/4	0.67	0.26	109,114,115,116	0
36	HTG	b	603	19/19	0.68	0.19	64,103,118,120	0
30	UNL	J	104	16/-	0.68	0.26	75,83,91,91	0
34	DMS	i	106	4/4	0.68	0.27	125,125,125,127	0
36	HTG	B	631	19/19	0.68	0.36	71,107,118,120	0
30	UNL	h	106	11/-	0.69	0.50	72,75,78,79	0
30	UNL	k	104	9/-	0.69	0.18	69,82,89,90	0
30	UNL	c	948	18/-	0.70	0.29	79,89,113,114	0
30	UNL	I	105	9/-	0.70	0.27	70,73,81,83	0
30	UNL	A	428	4/-	0.71	0.35	64,66,70,71	0
31	LMT	M	101	35/35	0.71	0.19	42,70,85,89	0
30	UNL	b	635	9/-	0.71	0.30	59,82,90,90	0
36	HTG	c	943	17/19	0.71	0.44	76,122,129,130	0
30	UNL	y	103	4/-	0.71	0.14	81,82,84,85	0
30	UNL	b	630	10/-	0.71	0.17	71,82,85,85	0
28	LMG	C	523	51/55	0.71	0.30	47,94,109,114	0
31	LMT	B	626	24/35	0.71	0.19	47,73,114,118	0
31	LMT	a	402	35/35	0.72	0.28	49,96,119,123	0
30	UNL	h	104	9/-	0.72	0.20	68,74,84,85	0
30	UNL	E	104	5/-	0.72	0.22	59,64,67,69	0
34	DMS	O	307	4/4	0.72	0.30	113,113,115,121	0
27	SQD	a	401	54/54	0.73	0.19	55,80,106,110	0
36	HTG	B	625	19/19	0.73	0.47	64,112,121,124	0
30	UNL	C	522	34/-	0.73	0.30	68,94,102,106	0
36	HTG	d	419	19/19	0.73	0.30	75,100,110,113	0
36	HTG	C	521	19/19	0.73	0.30	58,93,110,117	0
36	HTG	V	215	19/19	0.73	0.30	100,116,127,128	0
30	UNL	c	946	4/-	0.73	0.37	83,83,83,84	0
31	LMT	t	102	35/35	0.73	0.24	43,91,116,118	0
28	LMG	a	416	51/55	0.74	0.27	54,73,92,98	0
30	UNL	d	421	11/-	0.74	0.29	77,88,95,95	0
30	UNL	A	420	9/-	0.74	0.36	85,95,111,112	0
30	UNL	x	102	8/-	0.74	0.25	77,80,86,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
38	LHG	E	101	42/49	0.74	0.27	53,100,110,112	0
30	UNL	b	636	11/-	0.75	0.27	70,77,83,83	0
30	UNL	Z	104	8/-	0.75	0.35	69,83,102,103	0
36	HTG	D	412	19/19	0.75	0.29	68,112,130,130	0
30	UNL	l	102	13/-	0.75	0.30	55,61,77,83	0
36	HTG	B	630	19/19	0.75	0.23	56,109,116,118	0
30	UNL	A	418	8/-	0.76	0.41	70,75,82,82	0
30	UNL	b	648	5/-	0.76	0.32	73,74,76,77	0
31	LMT	m	102	35/35	0.76	0.22	34,64,85,88	0
30	UNL	T	102	15/-	0.76	0.50	78,86,92,93	0
36	HTG	C	537	19/19	0.77	0.35	84,109,123,126	0
36	HTG	d	414	19/19	0.77	0.21	67,100,117,120	0
34	DMS	d	417	4/4	0.77	0.26	106,109,109,110	0
30	UNL	I	107	11/-	0.77	0.26	65,78,88,88	0
30	UNL	b	629	16/-	0.77	0.28	59,83,97,99	0
29	PL9	A	414	55/55	0.77	0.27	53,68,102,104	0
34	DMS	c	936	4/4	0.77	0.25	119,124,124,124	0
30	UNL	B	627	8/-	0.77	0.50	63,68,78,83	0
34	DMS	A	425	4/4	0.78	0.28	94,101,101,104	0
30	UNL	I	104	12/-	0.78	0.22	70,80,92,93	0
31	LMT	Z	101	35/35	0.78	0.22	52,104,121,123	0
29	PL9	a	417	55/55	0.78	0.23	50,78,101,105	0
30	UNL	c	945	4/-	0.78	0.27	77,77,77,78	0
30	UNL	C	539	16/-	0.78	0.22	76,79,102,107	0
32	GOL	B	637	6/6	0.78	0.50	61,67,75,80	0
34	DMS	y	101	4/4	0.78	0.17	116,122,123,124	0
27	SQD	b	601	54/54	0.78	0.22	46,73,108,111	0
31	LMT	F	103	24/35	0.79	0.29	85,90,119,121	0
30	UNL	t	103	12/-	0.79	0.51	64,74,83,86	0
34	DMS	D	415	4/4	0.79	0.24	83,93,97,99	0
30	UNL	C	538	4/-	0.79	0.23	74,76,77,82	0
34	DMS	O	312	4/4	0.79	0.51	101,103,104,106	0
31	LMT	B	622	35/35	0.79	0.19	48,85,97,99	0
36	HTG	c	928	19/19	0.79	0.34	74,98,122,126	0
30	UNL	j	105	5/-	0.79	0.29	66,67,73,74	0
34	DMS	B	645	4/4	0.80	0.25	103,104,107,107	0
30	UNL	H	103	6/-	0.80	0.14	65,66,79,81	0
30	UNL	Z	102	6/-	0.80	0.23	61,72,75,77	0
30	UNL	I	102	12/-	0.80	0.23	70,82,95,98	0
28	LMG	A	413	51/55	0.80	0.24	49,74,97,102	0
34	DMS	T	103	4/4	0.80	0.28	112,112,112,112	0
34	DMS	U	202	4/4	0.80	0.42	105,108,108,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	x	104	9/-	0.80	0.19	93,95,99,102	0
34	DMS	O	302	4/4	0.81	0.21	101,104,107,108	0
36	HTG	c	942	19/19	0.81	0.22	52,78,94,100	0
30	UNL	Z	103	6/-	0.81	0.31	73,84,87,88	0
30	UNL	D	410	40/-	0.81	0.20	46,67,103,106	0
36	HTG	O	316	19/19	0.81	0.21	47,71,81,84	0
34	DMS	v	210	4/4	0.81	0.30	119,119,120,120	0
34	DMS	O	315	4/4	0.81	0.28	96,96,98,99	0
30	UNL	H	105	18/-	0.81	0.19	51,67,98,103	0
30	UNL	d	403	36/-	0.81	0.22	47,67,99,107	0
30	UNL	B	628	6/-	0.81	0.16	68,69,79,82	0
28	LMG	c	921	51/55	0.82	0.23	47,94,101,104	0
32	GOL	C	525	6/6	0.82	0.16	89,91,92,93	0
34	DMS	B	647	4/4	0.82	0.25	107,108,110,113	0
34	DMS	C	530	4/4	0.82	0.21	89,96,97,99	0
30	UNL	x	101	18/-	0.82	0.20	51,65,90,92	0
36	HTG	B	624	19/19	0.82	0.20	34,53,75,76	0
27	SQD	A	416	54/54	0.82	0.18	50,70,89,95	0
34	DMS	C	534	4/4	0.83	0.31	112,116,117,120	0
31	LMT	c	927	35/35	0.83	0.19	49,97,104,111	0
36	HTG	v	211	19/19	0.83	0.24	63,84,98,102	0
30	UNL	B	635	6/-	0.83	0.34	70,73,75,79	0
30	UNL	k	101	30/-	0.83	0.20	62,90,106,111	0
34	DMS	v	205	4/4	0.83	0.25	90,95,98,106	0
34	DMS	b	645	4/4	0.83	0.28	103,110,111,111	0
40	RRX	h	101	41/41	0.83	0.16	31,44,61,71	0
30	UNL	E	102	5/-	0.84	0.17	76,76,76,77	0
30	UNL	x	103	4/-	0.84	0.16	74,75,83,84	0
36	HTG	B	623	19/19	0.84	0.19	46,59,69,72	0
34	DMS	C	532	4/4	0.84	0.28	96,99,100,102	0
30	UNL	i	101	8/-	0.84	0.38	63,67,75,81	0
34	DMS	o	307	4/4	0.84	0.18	89,91,91,93	0
34	DMS	c	926	4/4	0.84	0.36	107,110,110,111	0
28	LMG	B	621	51/55	0.85	0.17	39,54,71,82	0
34	DMS	O	314	4/4	0.85	0.27	81,87,87,88	0
34	DMS	H	104	4/4	0.85	0.32	109,109,112,116	0
28	LMG	b	624	51/55	0.85	0.20	44,56,78,89	0
30	UNL	i	104	16/-	0.85	0.29	65,72,83,83	0
34	DMS	e	103	4/4	0.85	0.20	106,108,108,111	0
34	DMS	a	425	4/4	0.85	0.23	116,120,120,121	0
36	HTG	b	602	19/19	0.85	0.14	51,67,78,83	0
36	HTG	C	520	19/19	0.86	0.25	81,93,101,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	E	103	8/-	0.86	0.23	65,78,79,79	0
36	HTG	C	536	19/19	0.86	0.32	66,106,124,126	0
30	UNL	e	105	4/-	0.86	0.13	74,77,79,82	0
34	DMS	o	306	4/4	0.86	0.36	84,85,89,90	0
34	DMS	U	204	4/4	0.86	0.33	134,135,136,136	0
30	UNL	E	105	4/-	0.86	0.15	60,62,69,72	0
34	DMS	b	639	4/4	0.86	0.28	90,100,102,102	0
30	UNL	c	925	11/-	0.87	0.14	74,77,85,85	0
30	UNL	b	628	18/-	0.87	0.14	51,61,81,95	0
34	DMS	b	643	4/4	0.87	0.21	113,118,118,120	0
32	GOL	c	929	6/6	0.87	0.22	77,89,93,94	0
34	DMS	b	646	4/4	0.87	0.40	74,83,84,85	0
31	LMT	M	102	25/35	0.87	0.19	40,67,106,110	0
34	DMS	D	414	4/4	0.87	0.22	102,104,106,107	0
30	UNL	i	102	18/-	0.87	0.17	44,68,93,96	0
30	UNL	D	417	4/-	0.87	0.51	57,66,66,70	0
36	HTG	c	923	19/19	0.87	0.28	84,98,100,102	0
34	DMS	K	102	4/4	0.87	0.15	95,106,107,109	0
34	DMS	V	212	4/4	0.87	0.44	86,96,99,99	0
36	HTG	O	303	19/19	0.88	0.17	46,56,64,64	0
32	GOL	V	207	6/6	0.88	0.22	78,85,88,96	0
36	HTG	B	629	19/19	0.88	0.16	46,70,92,97	0
34	DMS	A	427	4/4	0.88	0.26	82,88,89,89	0
34	DMS	b	638	4/4	0.88	0.20	58,80,83,83	0
36	HTG	b	626	19/19	0.88	0.23	41,52,95,99	0
34	DMS	v	207	4/4	0.88	0.32	111,114,114,114	0
34	DMS	B	644	4/4	0.88	0.22	56,75,78,78	0
34	DMS	b	641	4/4	0.88	0.22	89,91,92,95	0
34	DMS	O	309	4/4	0.88	0.36	98,101,102,105	0
30	UNL	i	103	12/-	0.88	0.20	67,75,83,87	0
34	DMS	O	311	4/4	0.89	0.31	93,96,97,98	0
34	DMS	a	422	4/4	0.89	0.25	91,94,96,98	0
34	DMS	C	529	4/4	0.89	0.15	100,103,104,105	0
30	UNL	I	103	12/-	0.89	0.12	60,63,84,84	0
34	DMS	A	424	4/4	0.89	0.21	95,98,100,101	0
34	DMS	C	533	4/4	0.89	0.19	121,122,123,125	0
26	BCR	k	103	40/40	0.89	0.14	37,46,54,59	0
34	DMS	U	203	4/4	0.89	0.18	40,60,64,66	0
40	RRX	H	101	41/41	0.89	0.12	30,41,56,63	0
30	UNL	a	403	5/-	0.89	0.50	73,73,74,75	0
30	UNL	B	648	4/-	0.90	0.10	66,70,70,71	0
34	DMS	o	305	4/4	0.90	0.32	94,102,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	DMS	B	642	4/4	0.90	0.14	104,106,109,111	0
24	CLA	B	610	65/65	0.90	0.12	30,36,43,46	0
34	DMS	b	640	4/4	0.90	0.20	69,91,92,97	0
34	DMS	C	535	4/4	0.90	0.22	66,79,83,89	0
32	GOL	a	419	6/6	0.90	0.15	55,59,59,60	0
32	GOL	b	637	6/6	0.90	0.32	92,92,94,96	0
24	CLA	c	904	65/65	0.90	0.19	35,44,50,62	0
34	DMS	C	524	4/4	0.90	0.21	105,107,108,108	0
34	DMS	L	102	4/4	0.90	0.48	106,110,111,112	0
37	DGD	h	102	62/66	0.90	0.16	34,42,51,63	0
30	UNL	j	103	6/-	0.90	0.17	72,80,86,88	0
34	DMS	V	214	4/4	0.90	0.32	102,102,104,106	0
30	UNL	d	413	18/-	0.90	0.24	42,57,77,85	0
34	DMS	v	206	4/4	0.91	0.17	55,68,74,84	0
28	LMG	c	920	51/55	0.91	0.16	41,72,98,99	0
34	DMS	v	209	4/4	0.91	0.26	110,110,110,111	0
30	UNL	D	411	16/-	0.91	0.26	44,51,73,74	0
34	DMS	a	424	4/4	0.91	0.26	102,104,105,105	0
34	DMS	o	304	4/4	0.91	0.33	83,88,90,94	0
24	CLA	c	913	65/65	0.91	0.15	40,49,84,89	0
38	LHG	D	406	49/49	0.91	0.17	36,50,67,81	0
30	UNL	X	101	16/-	0.91	0.16	48,57,70,73	0
38	LHG	d	409	49/49	0.91	0.23	38,50,61,67	0
34	DMS	V	205	4/4	0.91	0.32	94,98,98,100	0
27	SQD	f	102	43/54	0.91	0.18	50,91,111,117	0
24	CLA	b	613	65/65	0.92	0.11	32,38,44,57	0
30	UNL	m	101	11/-	0.92	0.27	56,67,78,84	0
34	DMS	B	639	4/4	0.92	0.18	87,90,93,95	0
34	DMS	B	641	4/4	0.92	0.18	107,108,110,110	0
24	CLA	B	603	65/65	0.92	0.14	27,34,44,49	0
34	DMS	B	643	4/4	0.92	0.34	100,104,106,106	0
34	DMS	c	935	4/4	0.92	0.32	101,101,101,102	0
24	CLA	C	513	65/65	0.92	0.14	43,54,86,88	0
34	DMS	O	313	4/4	0.92	0.27	101,106,108,111	0
36	HTG	V	204	13/19	0.92	0.21	49,59,79,86	0
37	DGD	H	102	62/66	0.92	0.20	27,40,51,53	0
28	LMG	C	519	51/55	0.92	0.17	36,80,92,97	0
35	CA	V	202	1/1	0.92	0.15	89,89,89,89	0
35	CA	b	604	1/1	0.92	0.05	52,52,52,52	0
34	DMS	d	418	4/4	0.92	0.29	74,75,76,78	0
26	BCR	B	619	40/40	0.92	0.17	28,37,54,62	0
38	LHG	l	103	49/49	0.92	0.17	32,42,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	DMS	e	104	4/4	0.92	0.23	88,94,96,98	0
26	BCR	c	915	40/40	0.92	0.15	47,58,64,66	0
26	BCR	Y	101	40/40	0.93	0.10	40,44,48,54	0
34	DMS	a	423	4/4	0.93	0.21	63,76,79,85	0
34	DMS	C	531	4/4	0.93	0.11	109,111,113,116	0
26	BCR	a	414	40/40	0.93	0.11	27,33,39,41	0
34	DMS	h	105	4/4	0.93	0.19	52,53,61,80	0
26	BCR	b	622	40/40	0.93	0.17	31,39,57,64	0
24	CLA	c	903	65/65	0.93	0.22	29,38,50,61	0
24	CLA	C	512	65/65	0.93	0.10	43,50,90,92	0
30	UNL	j	104	4/-	0.93	0.29	74,75,76,78	0
32	GOL	V	206	6/6	0.93	0.31	58,69,71,83	0
37	DGD	C	517	62/66	0.93	0.14	31,43,92,101	0
34	DMS	v	203	4/4	0.93	0.25	87,94,95,96	0
26	BCR	B	636	40/40	0.93	0.14	29,41,59,59	0
27	SQD	F	101	37/54	0.93	0.22	45,71,88,92	0
26	BCR	C	514	40/40	0.93	0.11	41,49,57,57	0
34	DMS	v	208	4/4	0.93	0.25	86,89,94,98	0
34	DMS	V	211	4/4	0.93	0.12	94,94,96,99	0
26	BCR	C	515	40/40	0.93	0.10	33,42,50,54	0
34	DMS	c	937	4/4	0.93	0.13	99,101,103,103	0
34	DMS	c	938	4/4	0.93	0.27	97,97,100,104	0
26	BCR	T	101	40/40	0.93	0.14	29,42,60,63	0
27	SQD	a	415	54/54	0.94	0.14	35,65,85,87	0
24	CLA	C	507	65/65	0.94	0.11	36,42,57,66	0
24	CLA	c	914	65/65	0.94	0.17	41,53,89,96	0
25	PHO	A	409	64/64	0.94	0.15	24,30,37,42	0
36	HTG	U	201	4/19	0.94	0.12	49,51,51,56	0
26	BCR	B	618	40/40	0.94	0.17	27,35,41,41	0
24	CLA	B	607	65/65	0.94	0.11	28,34,65,71	0
24	CLA	B	602	65/65	0.94	0.23	35,52,105,110	0
24	CLA	b	605	65/65	0.94	0.18	40,54,102,107	0
24	CLA	b	606	65/65	0.94	0.11	31,36,46,56	0
26	BCR	K	101	40/40	0.94	0.10	34,43,48,49	0
24	CLA	b	610	65/65	0.94	0.10	29,37,71,80	0
34	DMS	u	202	4/4	0.94	0.23	68,80,81,86	0
24	CLA	B	615	65/65	0.94	0.13	24,32,86,95	0
24	CLA	b	614	65/65	0.94	0.10	30,36,42,61	0
24	CLA	b	619	65/65	0.94	0.10	29,37,58,65	0
32	GOL	A	419	6/6	0.94	0.20	59,61,62,66	0
29	PL9	d	407	55/55	0.94	0.15	22,29,43,56	0
32	GOL	B	638	6/6	0.94	0.32	39,58,69,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	b	623	40/40	0.94	0.12	32,41,55,58	0
24	CLA	b	620	65/65	0.94	0.13	30,41,98,102	0
34	DMS	D	416	4/4	0.94	0.19	93,94,97,98	0
26	BCR	d	406	40/40	0.94	0.10	34,41,69,72	0
35	CA	v	201	1/1	0.94	0.09	104,104,104,104	0
26	BCR	k	102	40/40	0.94	0.09	40,45,54,55	0
37	DGD	c	918	62/66	0.94	0.17	36,44,99,109	0
24	CLA	c	902	65/65	0.94	0.11	33,42,54,60	0
34	DMS	b	647	4/4	0.94	0.17	72,73,79,79	0
27	SQD	A	412	54/54	0.94	0.13	35,64,79,85	0
34	DMS	c	933	4/4	0.94	0.16	108,111,113,114	0
34	DMS	O	306	4/4	0.94	0.20	78,82,86,86	0
38	LHG	d	410	49/49	0.94	0.15	27,33,53,64	0
24	CLA	C	503	65/65	0.94	0.13	32,39,46,56	0
24	CLA	C	506	65/65	0.94	0.11	37,52,90,94	0
24	CLA	c	908	65/65	0.94	0.12	32,42,59,61	0
34	DMS	o	303	4/4	0.95	0.34	92,94,95,101	0
34	DMS	V	213	4/4	0.95	0.09	76,84,85,86	0
28	LMG	D	409	51/55	0.95	0.18	32,43,99,106	0
24	CLA	c	912	65/65	0.95	0.10	34,43,52,58	0
24	CLA	C	501	65/65	0.95	0.14	30,39,53,61	0
34	DMS	u	201	4/4	0.95	0.14	52,64,66,70	0
26	BCR	c	916	40/40	0.95	0.09	38,43,54,57	0
24	CLA	B	611	65/65	0.95	0.15	26,35,43,50	0
28	LMG	d	412	51/55	0.95	0.10	35,45,89,94	0
24	CLA	d	405	65/65	0.95	0.10	33,39,102,107	0
33	BCT	a	408[A]	4/4	0.95	0.07	31,38,39,41	4
33	BCT	d	402[B]	4/4	0.95	0.09	34,37,37,40	4
29	PL9	D	404	55/55	0.95	0.10	23,29,38,51	0
34	DMS	b	644	4/4	0.95	0.22	63,65,67,78	0
24	CLA	C	504	65/65	0.95	0.13	27,35,80,83	0
30	UNL	I	101	14/-	0.95	0.15	46,53,70,73	0
34	DMS	B	633	4/4	0.95	0.19	48,49,56,58	0
24	CLA	B	612	65/65	0.95	0.15	25,30,46,54	0
24	CLA	B	604	65/65	0.95	0.15	28,33,40,42	0
34	DMS	c	934	4/4	0.95	0.17	73,80,82,84	0
24	CLA	b	618	65/65	0.95	0.17	24,33,88,91	0
37	DGD	c	917	62/66	0.95	0.14	28,39,84,88	0
24	CLA	C	508	65/65	0.95	0.12	28,37,95,108	0
24	CLA	C	510	65/65	0.95	0.14	31,39,51,58	0
26	BCR	D	403	40/40	0.95	0.17	33,41,69,73	0
24	CLA	C	511	65/65	0.95	0.08	33,44,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	616	65/65	0.95	0.11	26,35,53,65	0
38	LHG	L	101	49/49	0.95	0.12	30,41,64,71	0
24	CLA	B	617	65/65	0.95	0.10	30,36,105,109	0
34	DMS	C	528	4/4	0.95	0.11	81,81,83,83	0
24	CLA	c	907	65/65	0.95	0.10	39,48,81,85	0
26	BCR	b	621	40/40	0.95	0.16	31,37,48,53	0
24	CLA	D	402	65/65	0.95	0.11	29,37,102,104	0
24	CLA	c	905	65/65	0.96	0.16	32,40,72,81	0
24	CLA	b	611	65/65	0.96	0.12	23,31,44,50	0
24	CLA	B	605	65/65	0.96	0.21	23,29,61,62	0
24	CLA	c	909	65/65	0.96	0.18	31,37,91,96	0
35	CA	c	901	1/1	0.96	0.06	52,52,52,52	0
34	DMS	a	421	4/4	0.96	0.12	78,84,85,89	0
24	CLA	c	910	65/65	0.96	0.25	34,40,58,64	0
34	DMS	O	305	4/4	0.96	0.10	81,82,85,88	0
34	DMS	e	102	4/4	0.96	0.15	95,95,96,99	0
24	CLA	C	509	65/65	0.96	0.12	34,41,63,67	0
24	CLA	b	616	65/65	0.96	0.18	25,33,41,42	0
37	DGD	C	516	62/66	0.96	0.17	27,38,90,95	0
34	DMS	C	527	4/4	0.96	0.19	72,74,75,77	0
37	DGD	C	518	62/66	0.96	0.12	28,37,80,85	0
24	CLA	b	617	65/65	0.96	0.21	25,31,71,77	0
24	CLA	a	413	65/65	0.96	0.11	26,34,107,111	0
24	CLA	C	505	65/65	0.96	0.13	32,39,57,63	0
34	DMS	b	642	4/4	0.96	0.08	57,63,69,73	0
24	CLA	C	502	65/65	0.96	0.14	29,36,48,63	0
24	CLA	b	607	65/65	0.96	0.12	28,35,41,44	0
26	BCR	B	620	40/40	0.96	0.09	30,37,52,55	0
34	DMS	B	634	4/4	0.96	0.11	63,64,64,65	0
24	CLA	b	608	65/65	0.96	0.17	25,31,69,74	0
34	DMS	B	640	4/4	0.96	0.30	77,78,82,86	0
34	DMS	c	931	4/4	0.96	0.24	88,88,89,92	0
34	DMS	c	932	4/4	0.96	0.16	80,88,88,89	0
34	DMS	V	201	4/4	0.96	0.21	75,76,79,88	0
24	CLA	B	608	65/65	0.96	0.12	23,29,44,50	0
34	DMS	V	210	4/4	0.97	0.09	69,71,76,76	0
24	CLA	b	612	65/65	0.97	0.14	28,35,42,45	0
24	CLA	c	906	65/65	0.97	0.12	30,37,66,74	0
24	CLA	A	406	65/65	0.97	0.08	20,26,38,53	0
24	CLA	a	410	65/65	0.97	0.13	26,32,89,95	0
24	CLA	b	615	65/65	0.97	0.20	25,31,51,55	0
34	DMS	c	940	4/4	0.97	0.22	58,63,64,66	0

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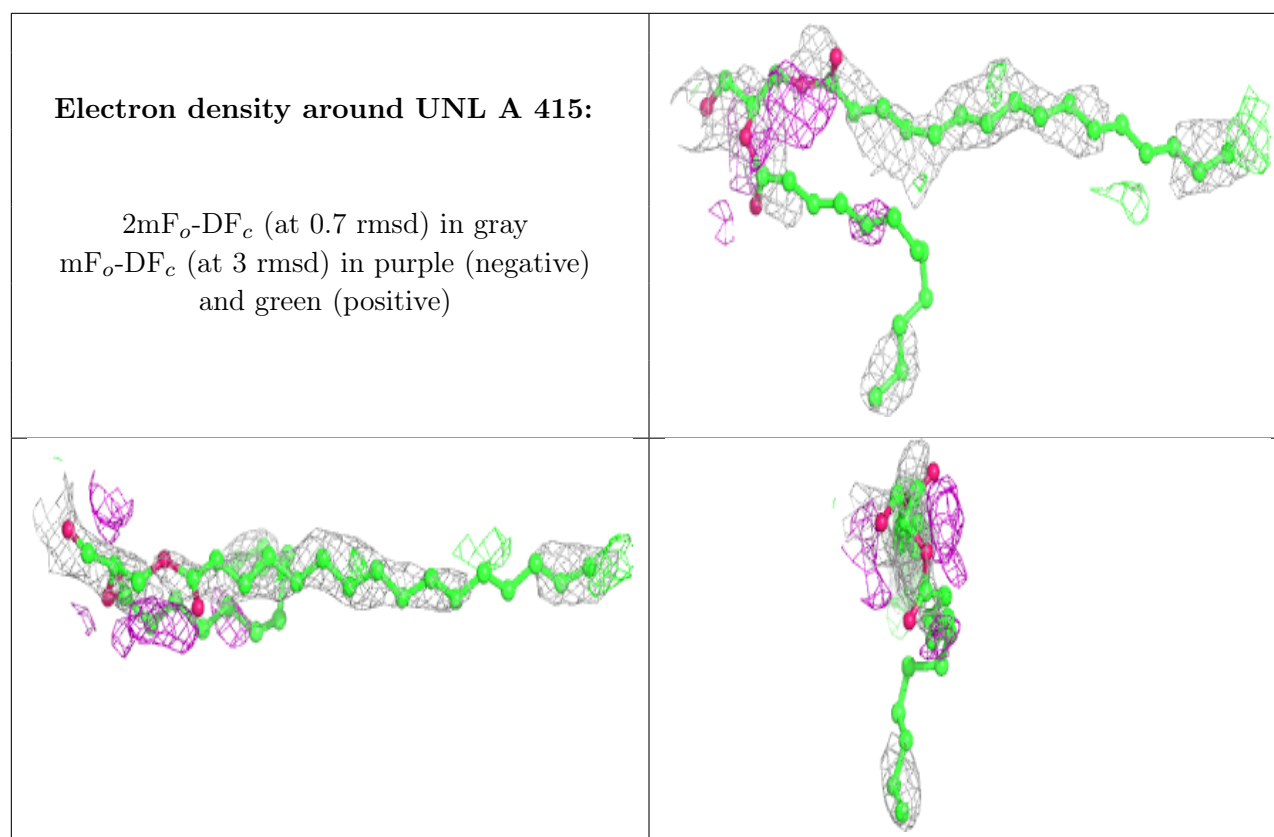
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	DMS	d	415	4/4	0.97	0.20	63,66,70,74	0
24	CLA	B	606	65/65	0.97	0.19	25,30,43,46	0
24	CLA	c	911	65/65	0.97	0.26	30,39,51,61	0
24	CLA	A	407	65/65	0.97	0.15	21,29,89,95	0
24	CLA	B	613	65/65	0.97	0.19	24,31,37,41	0
34	DMS	O	308	4/4	0.97	0.18	80,83,84,90	0
24	CLA	B	614	65/65	0.97	0.19	21,30,67,76	0
34	DMS	O	310	4/4	0.97	0.53	88,89,90,94	0
34	DMS	o	302	4/4	0.97	0.10	71,74,78,80	0
24	CLA	d	401	65/65	0.97	0.12	21,27,41,51	0
24	CLA	A	410	65/65	0.97	0.09	26,35,99,104	0
37	DGD	c	919	62/66	0.97	0.10	32,40,76,82	0
33	BCT	A	422	4/4	0.97	0.07	37,37,48,55	0
25	PHO	A	408	64/64	0.97	0.10	21,28,33,36	0
24	CLA	b	609	65/65	0.97	0.13	25,33,44,49	0
38	LHG	D	407	49/49	0.97	0.11	25,34,48,65	0
38	LHG	D	408	46/49	0.97	0.11	32,39,72,77	0
25	PHO	a	411	64/64	0.97	0.11	24,28,33,38	0
25	PHO	a	412	64/64	0.97	0.12	26,33,41,43	0
26	BCR	A	411	40/40	0.97	0.12	27,33,41,45	0
34	DMS	v	204	4/4	0.97	0.14	55,57,58,64	0
38	LHG	d	411	47/49	0.97	0.13	32,39,87,92	0
24	CLA	B	609	65/65	0.97	0.14	27,33,40,44	0
39	HEM	F	102	43/43	0.97	0.08	38,48,56,60	0
39	HEM	f	101	43/43	0.97	0.11	42,50,65,84	0
34	DMS	D	413	4/4	0.97	0.20	62,65,67,73	0
24	CLA	D	401	65/65	0.97	0.13	20,26,41,46	0
41	MG	j	101	1/1	0.97	0.18	44,44,44,44	0
42	HEC	v	202	43/43	0.97	0.10	35,41,47,48	0
24	CLA	d	404	65/65	0.98	0.13	23,28,50,57	0
34	DMS	d	416	4/4	0.98	0.13	62,64,65,72	0
34	DMS	V	209	4/4	0.98	0.12	50,59,66,67	0
34	DMS	C	526	4/4	0.98	0.12	44,46,46,50	0
24	CLA	A	405	65/65	0.98	0.10	22,26,33,54	0
35	CA	o	301	1/1	0.98	0.08	55,55,55,55	0
24	CLA	a	409	65/65	0.98	0.14	23,28,37,50	0
34	DMS	A	426	4/4	0.98	0.11	81,86,86,88	0
42	HEC	V	203	43/43	0.98	0.07	27,31,37,40	0
34	DMS	b	632	4/4	0.98	0.09	61,63,64,65	0
35	CA	O	301	1/1	0.99	0.15	56,56,56,56	0
34	DMS	V	208	4/4	0.99	0.09	50,53,56,57	0
34	DMS	B	632	4/4	0.99	0.14	28,31,33,34	0

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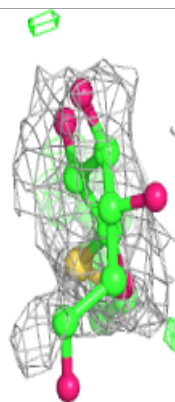
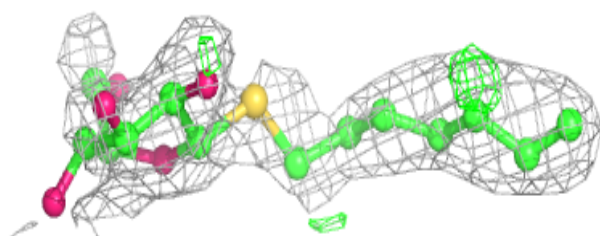
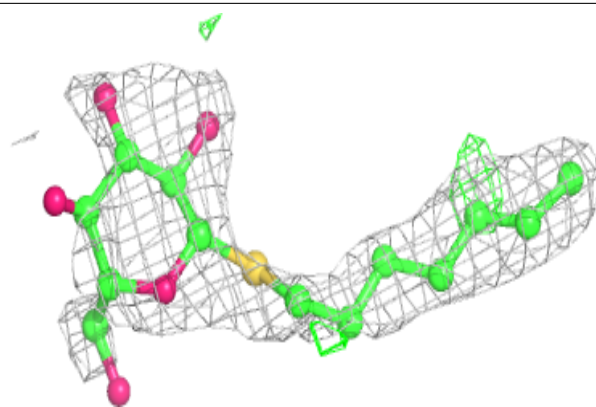
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	OEX	A	401	10/10	0.99	0.10	25,28,31,31	0
34	DMS	a	420	4/4	0.99	0.07	34,35,35,42	0
34	DMS	b	631	4/4	0.99	0.14	34,34,37,43	0
41	MG	J	101	1/1	0.99	0.08	36,36,36,36	0
34	DMS	c	930	4/4	0.99	0.10	46,49,49,50	0
34	DMS	A	423	4/4	0.99	0.11	31,34,37,48	0
35	CA	B	601	1/1	0.99	0.09	51,51,51,51	0
21	OEX	a	404	10/10	1.00	0.08	29,32,33,34	0
22	FE2	A	402	1/1	1.00	0.04	33,33,33,33	0
22	FE2	a	405	1/1	1.00	0.07	33,33,33,33	0
23	CL	A	403	1/1	1.00	0.10	26,26,26,26	0
23	CL	A	404	1/1	1.00	0.14	29,29,29,29	0
23	CL	a	406	1/1	1.00	0.10	29,29,29,29	0
23	CL	a	407	1/1	1.00	0.18	34,34,34,34	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.

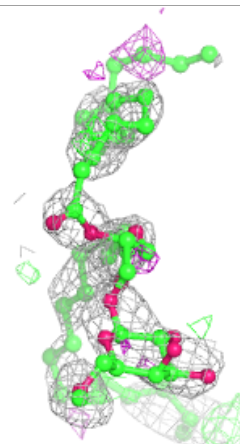
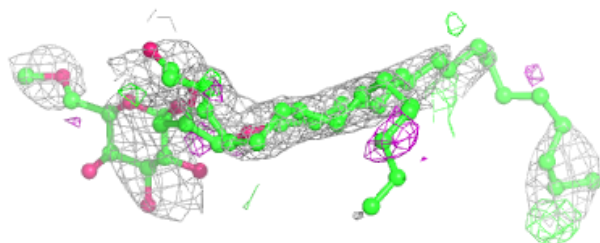
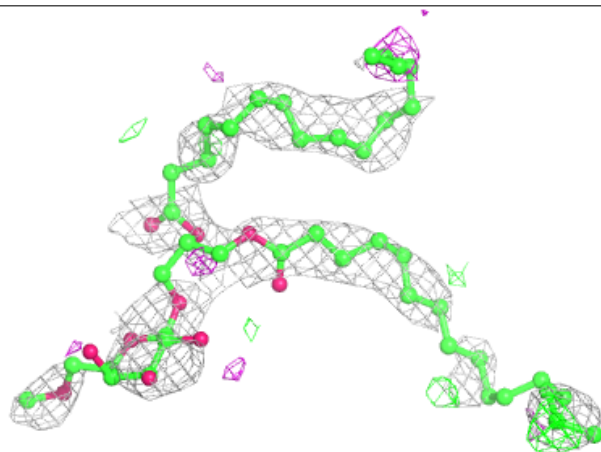


**Electron density around HTG c 941:**

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

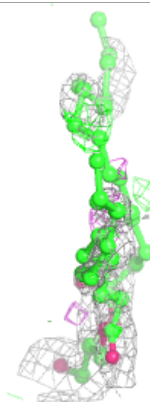
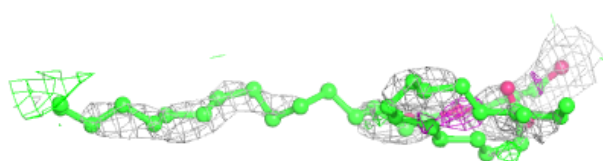
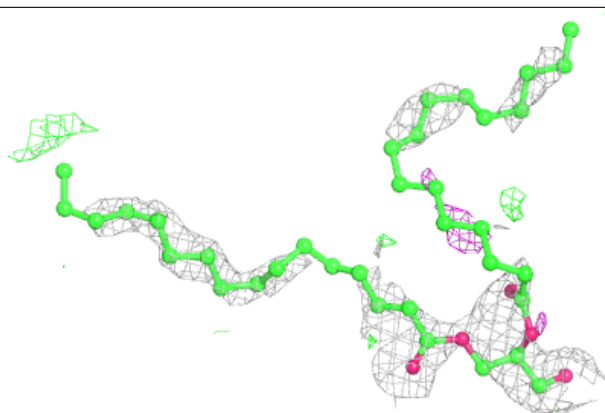
**Electron density around DGD D 405:**

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

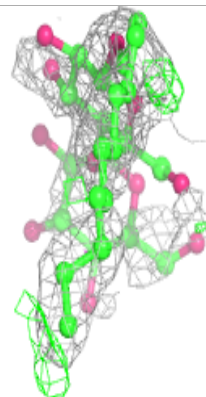
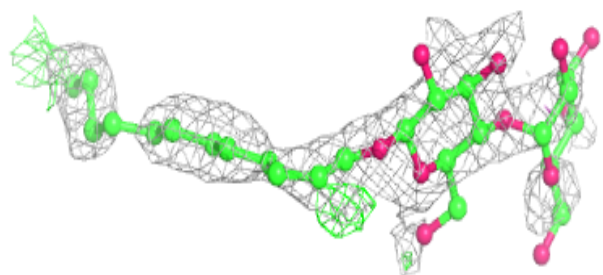
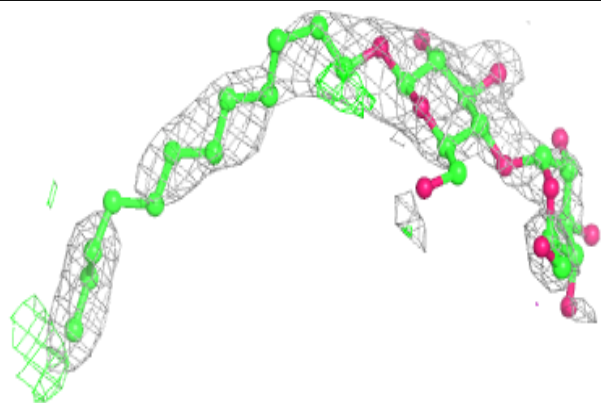


**Electron density around UNL a 418:**

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

**Electron density around LMT m 103:**

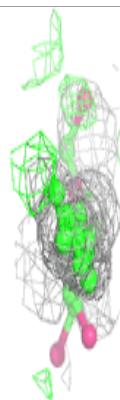
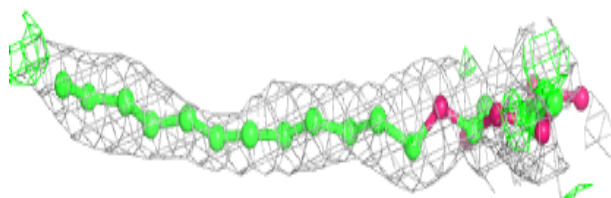
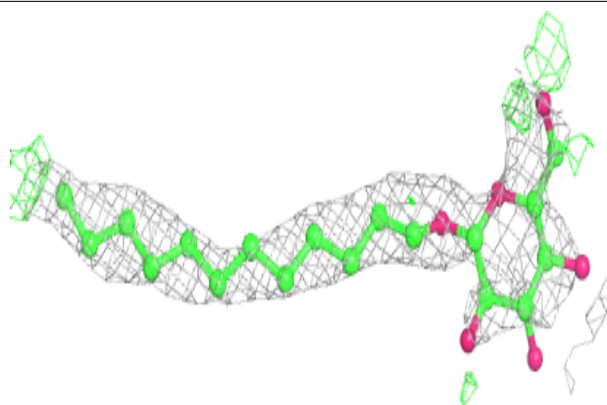
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



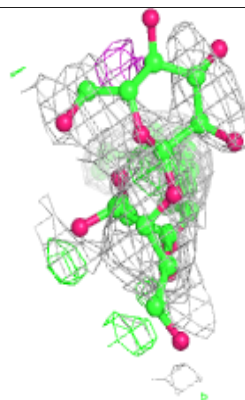
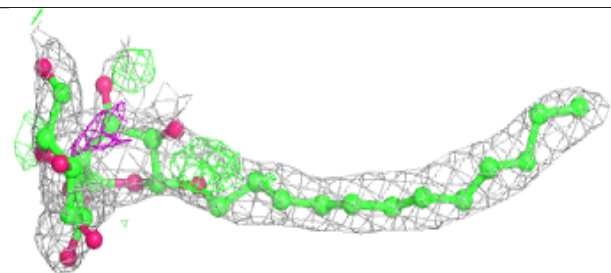
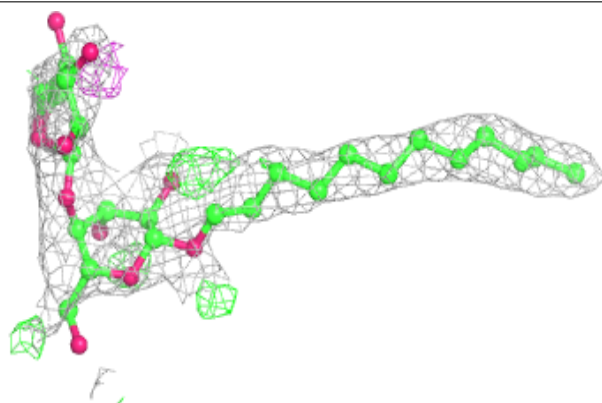


**Electron density around LMT j 102:**

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

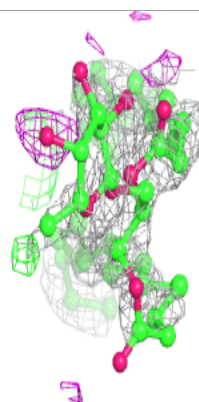
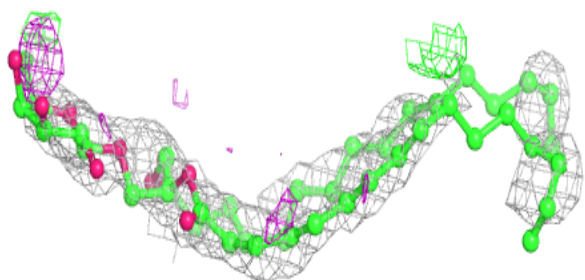
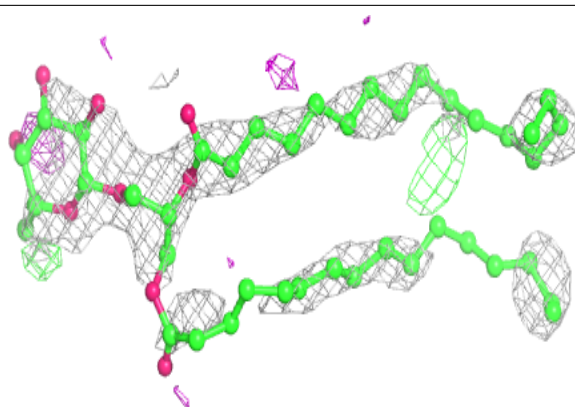
**Electron density around LMT b 625:**

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

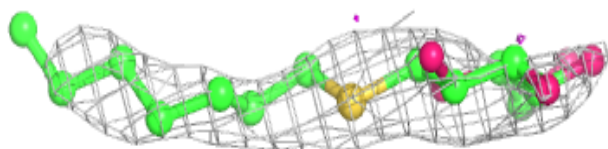
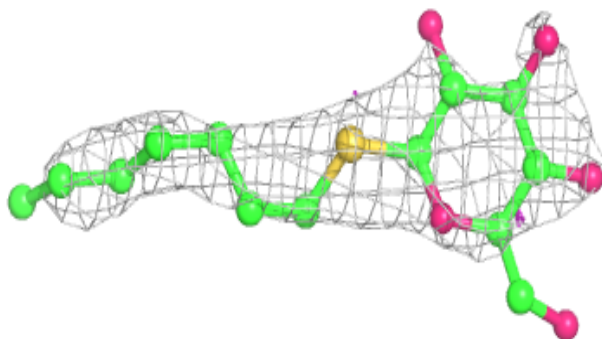


**Electron density around DGD d 408:**

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

**Electron density around HTG d 420:**

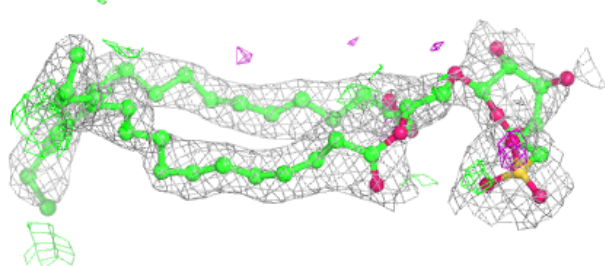
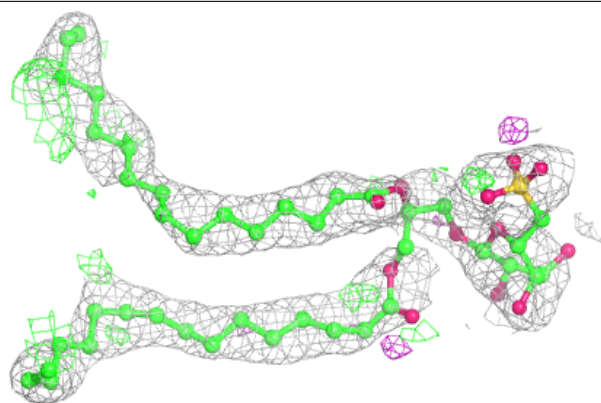
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



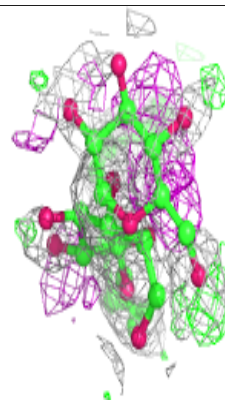
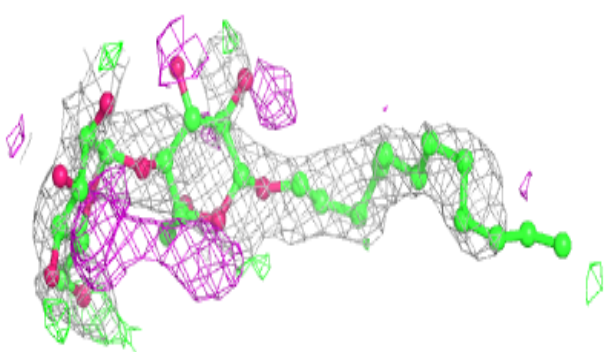
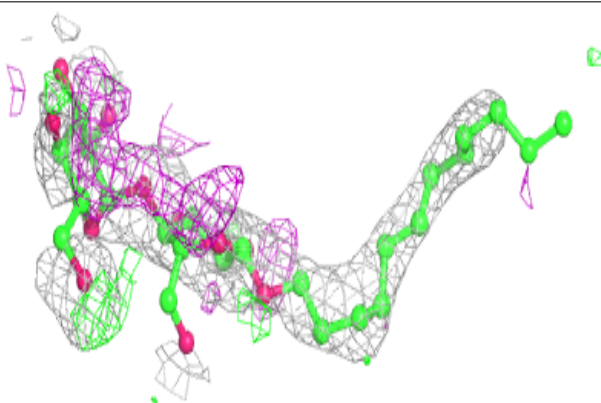


**Electron density around SQD 1 101:**

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

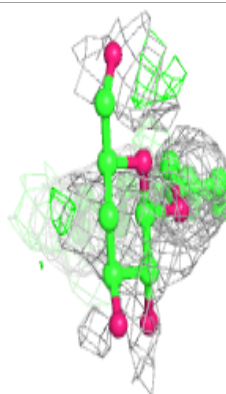
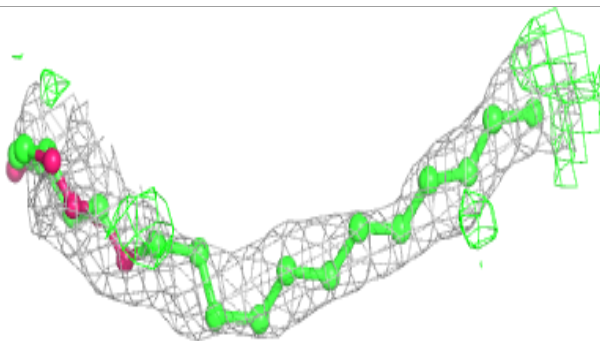
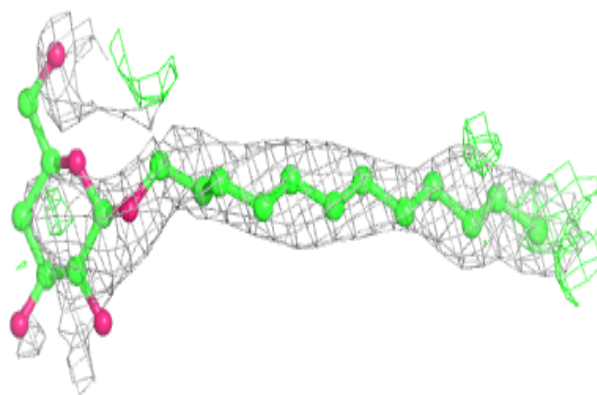
**Electron density around LMT A 417:**

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

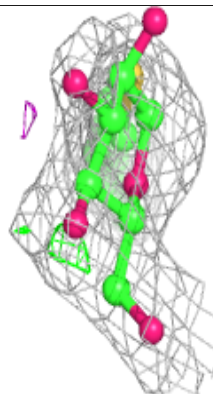
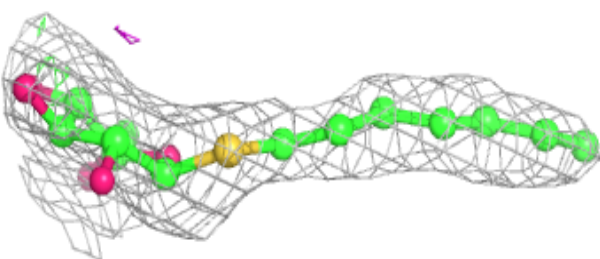
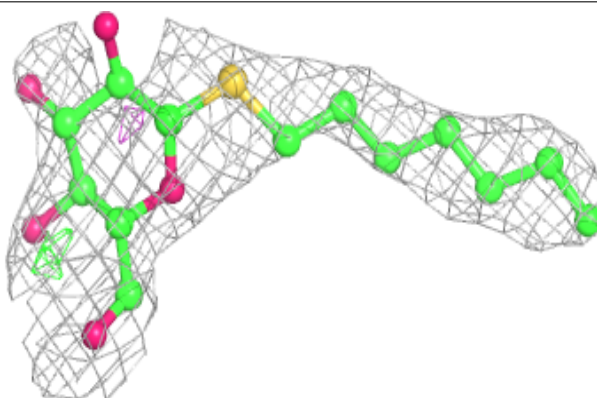


**Electron density around LMT t 101:**

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

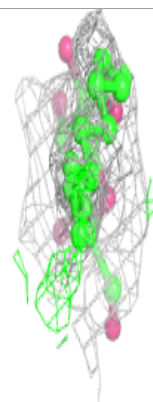
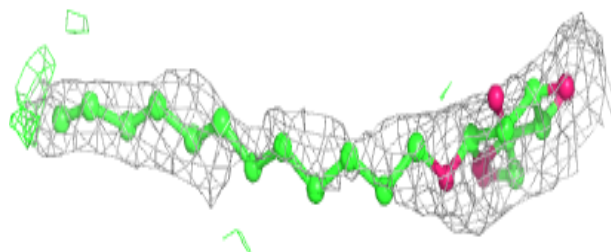
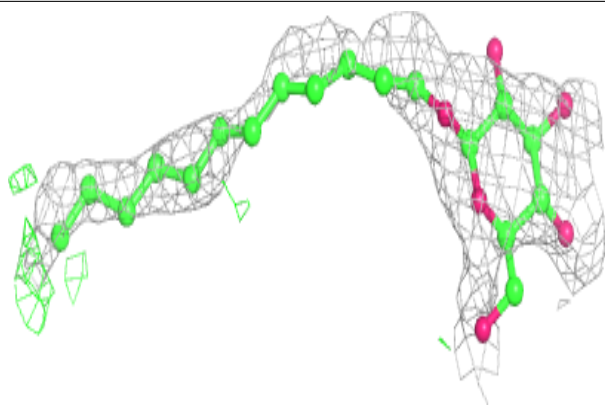
**Electron density around HTG b 627:**

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

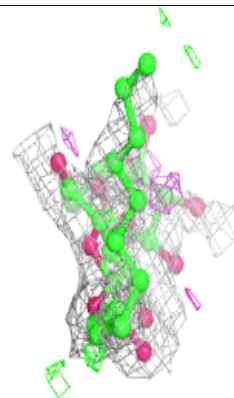
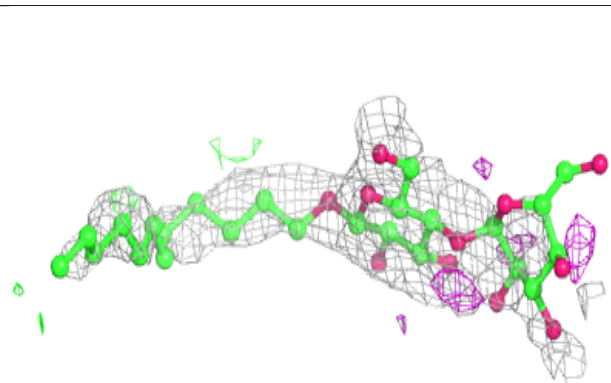
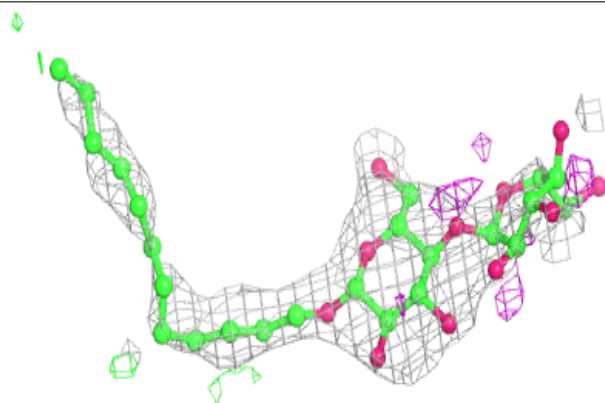


**Electron density around LMT e 101:**

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

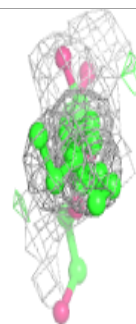
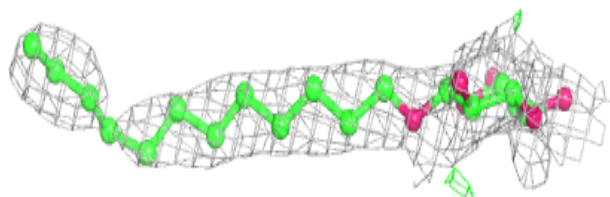
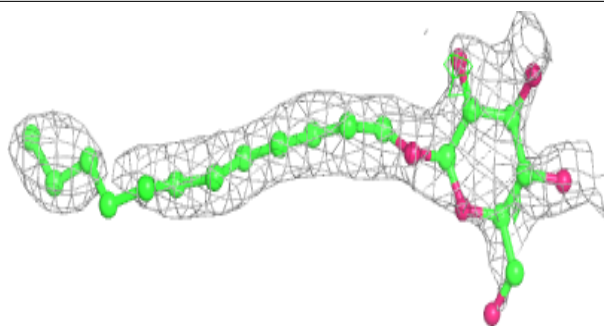
**Electron density around LMT A 421:**

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

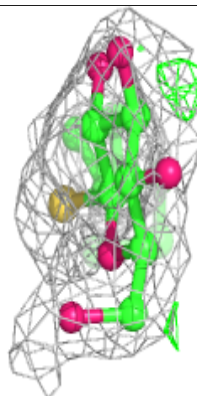
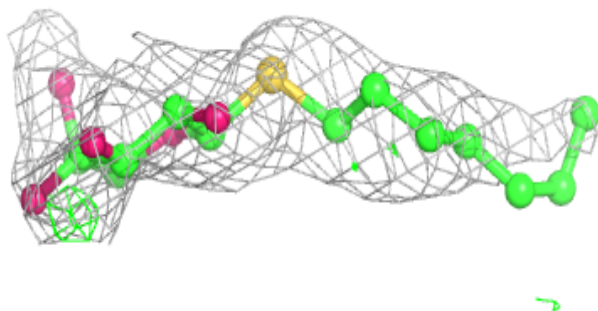
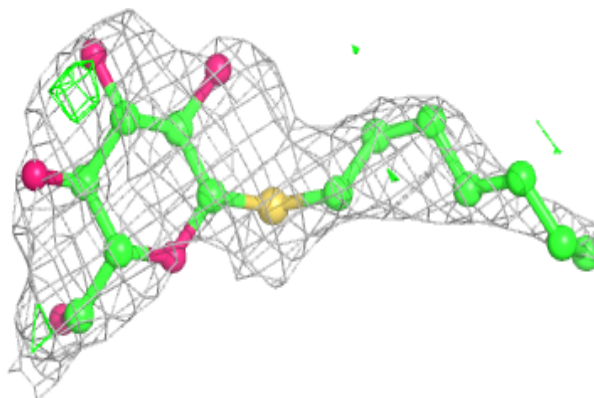


**Electron density around LMT J 102:**

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

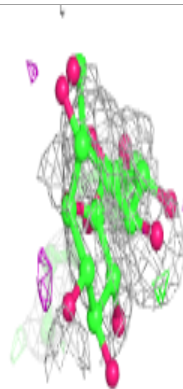
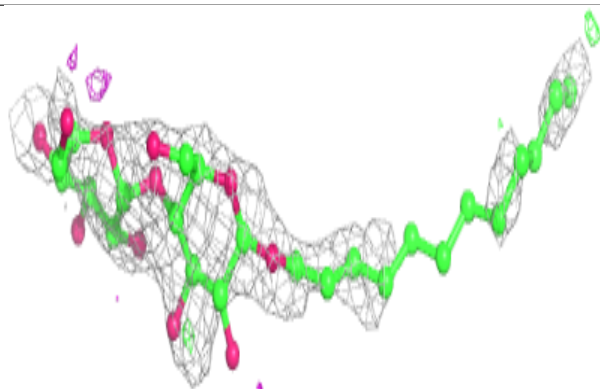
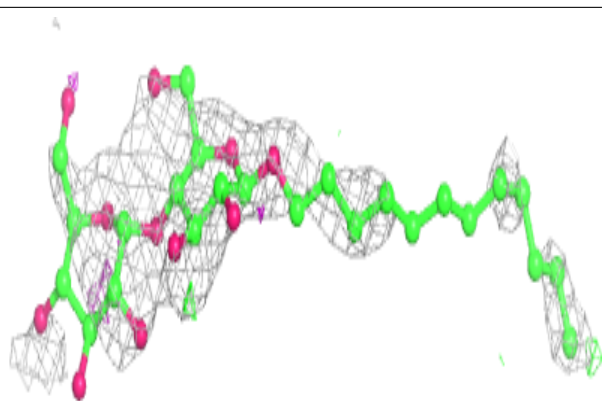
**Electron density around HTG y 102:**

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

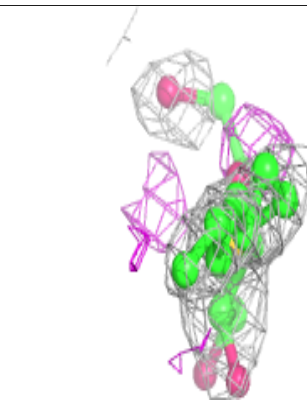
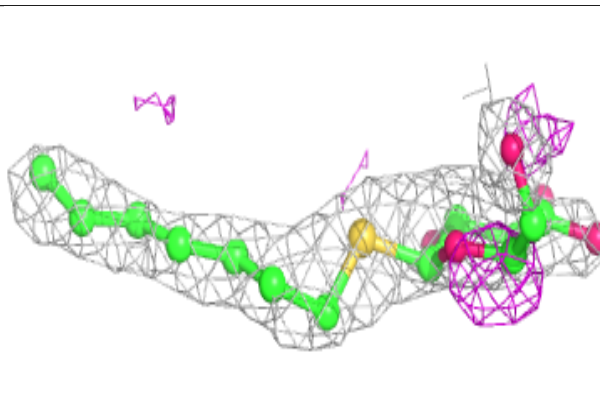
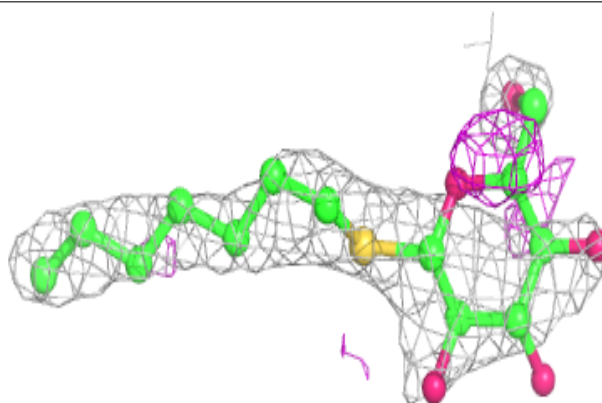


**Electron density around LMT c 922:**

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

**Electron density around HTG c 924:**

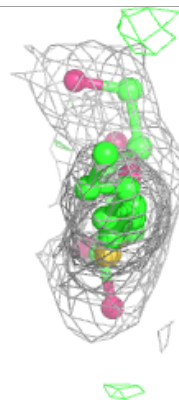
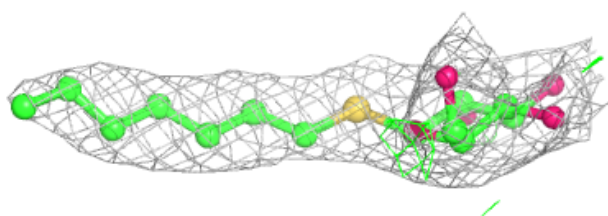
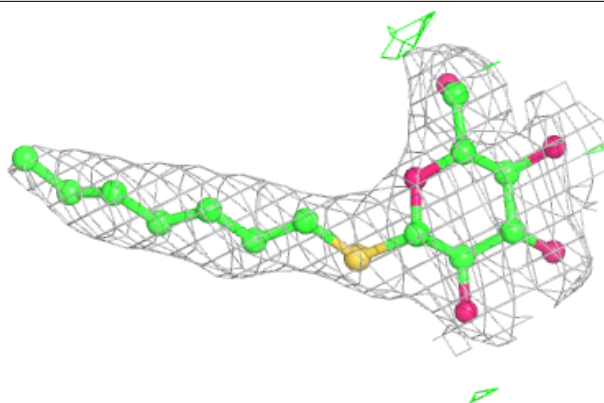
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



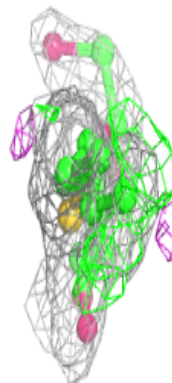
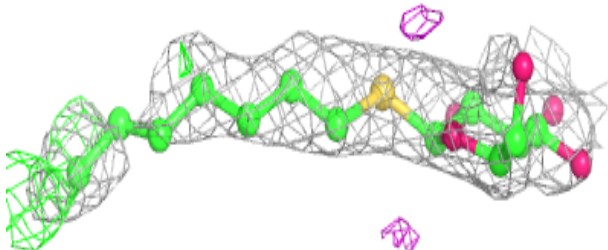
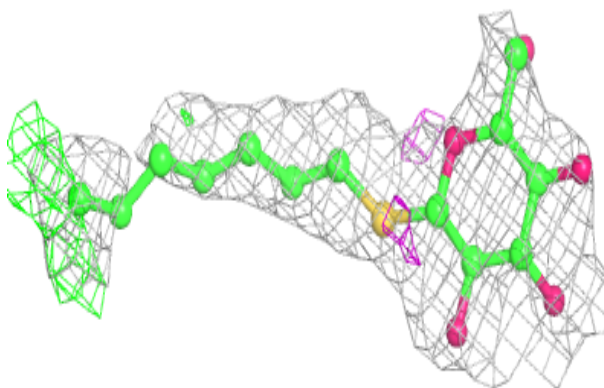


**Electron density around HTG b 603:**

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

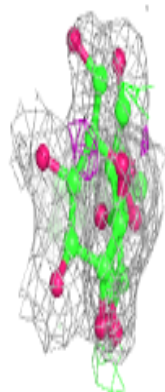
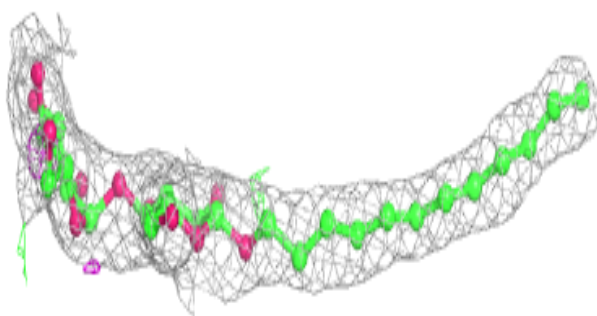
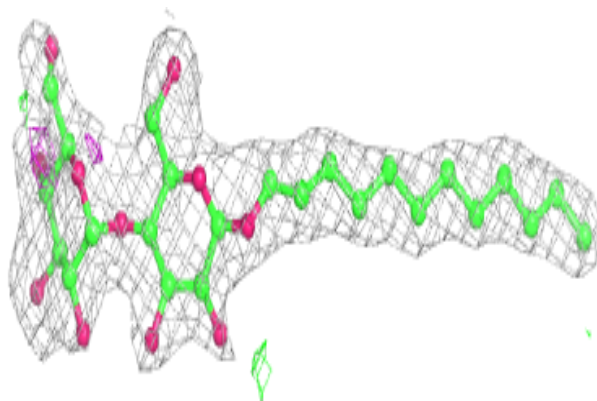
**Electron density around HTG B 631:**

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

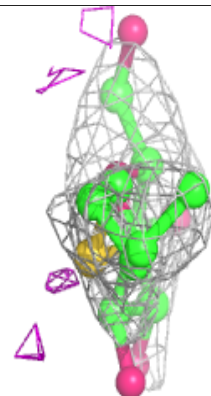
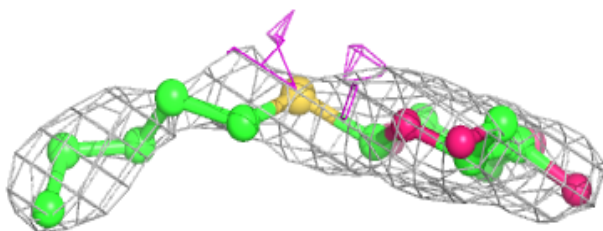
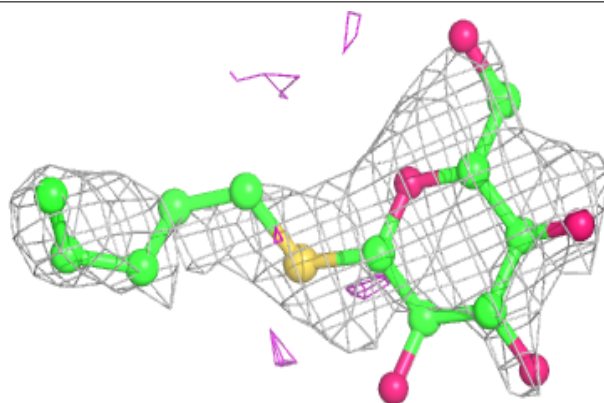


**Electron density around LMT M 101:**

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

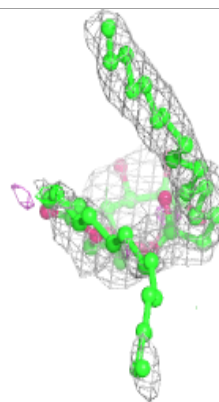
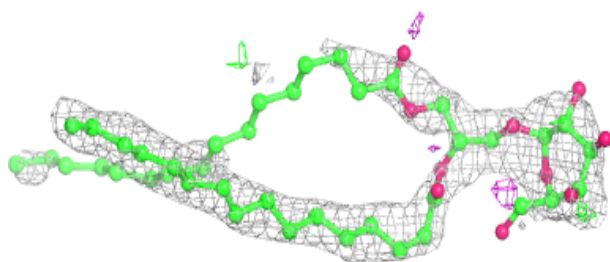
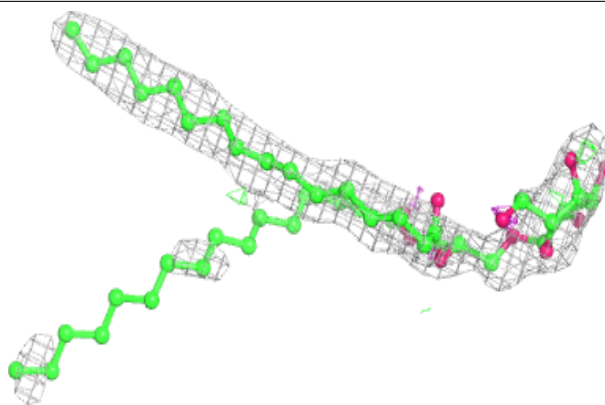
**Electron density around HTG c 943:**

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

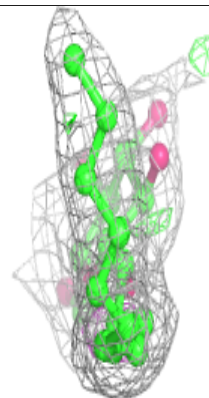
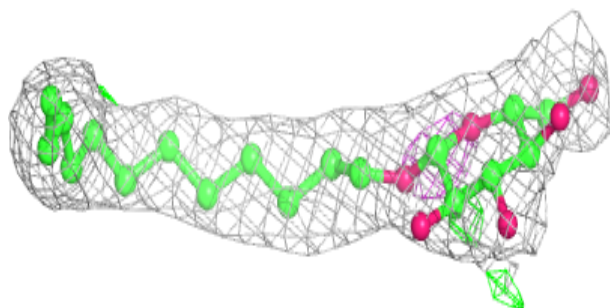
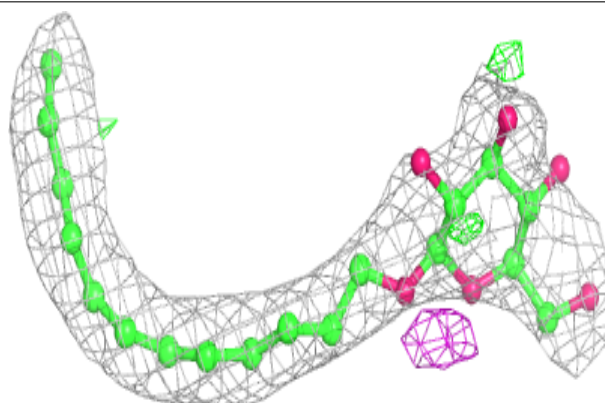


**Electron density around LMG C 523:**

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

**Electron density around LMT B 626:**

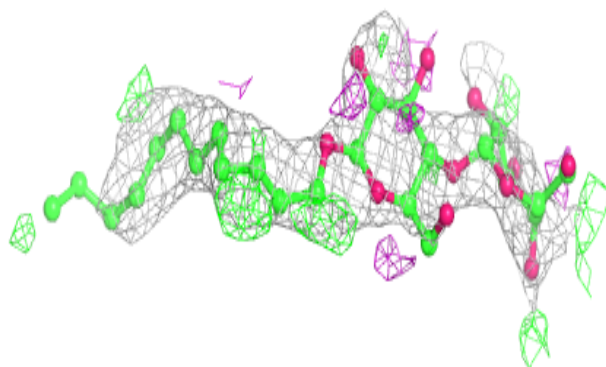
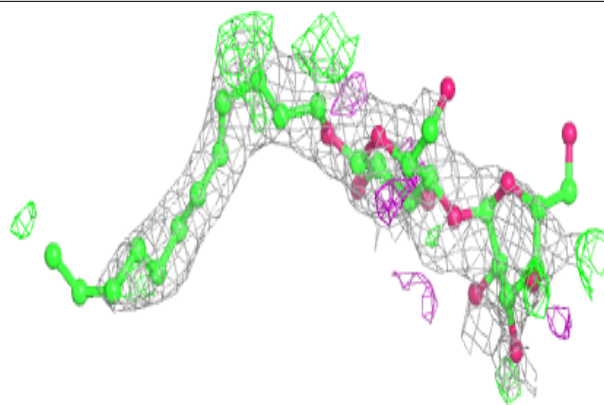
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



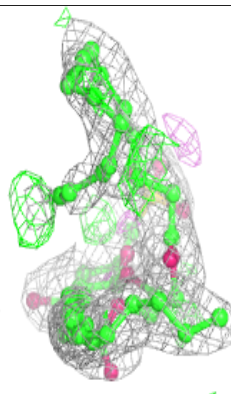
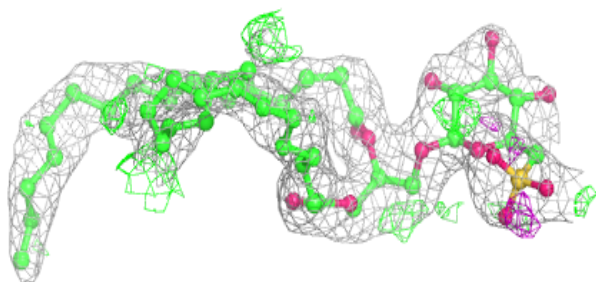
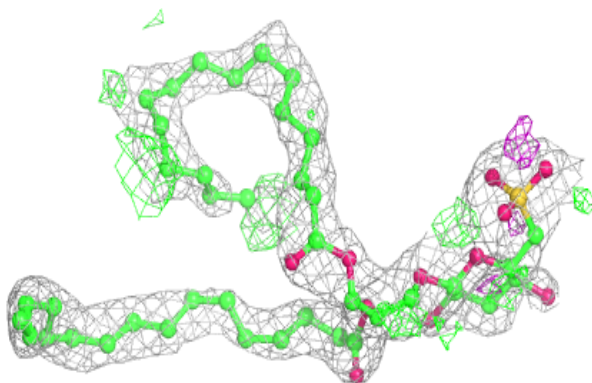


**Electron density around LMT a 402:**

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

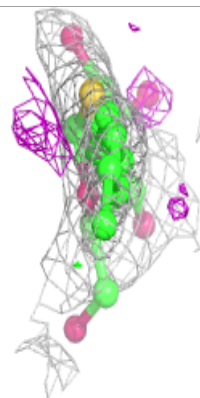
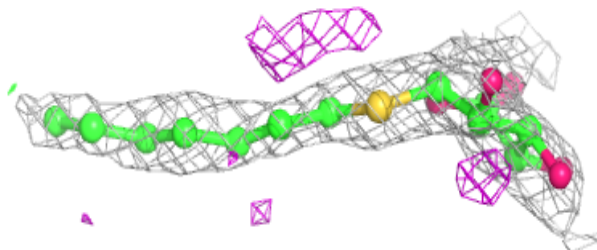
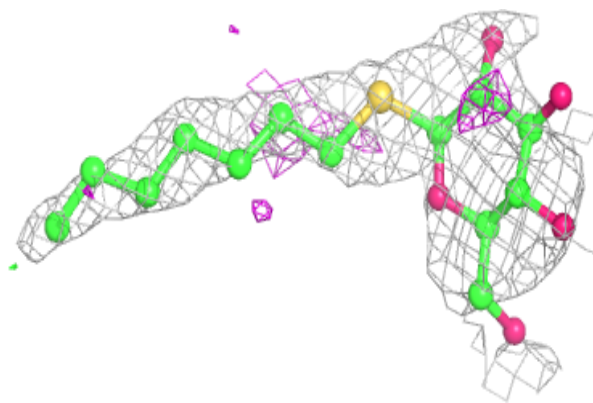
**Electron density around SQD a 401:**

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

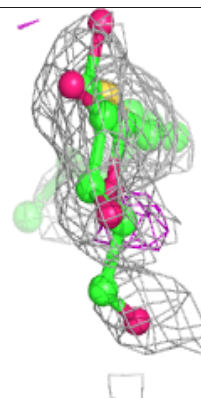
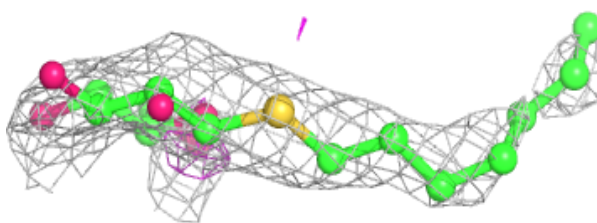
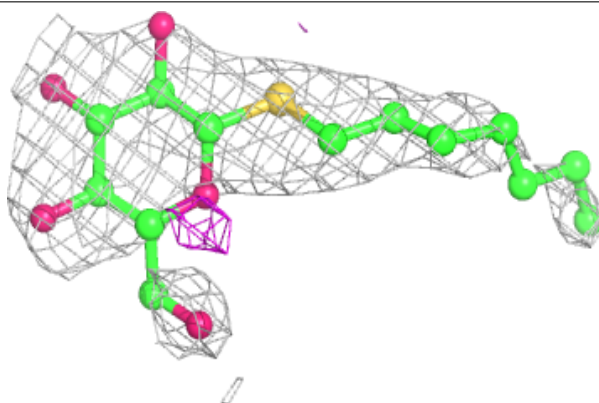


**Electron density around HTG B 625:**

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

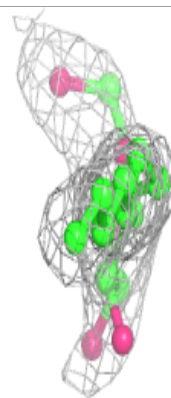
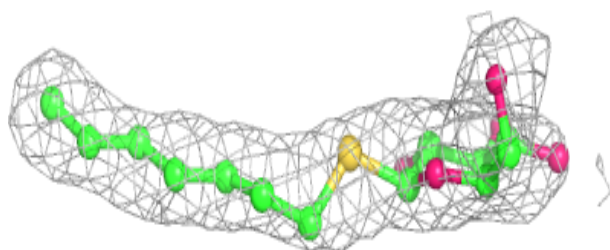
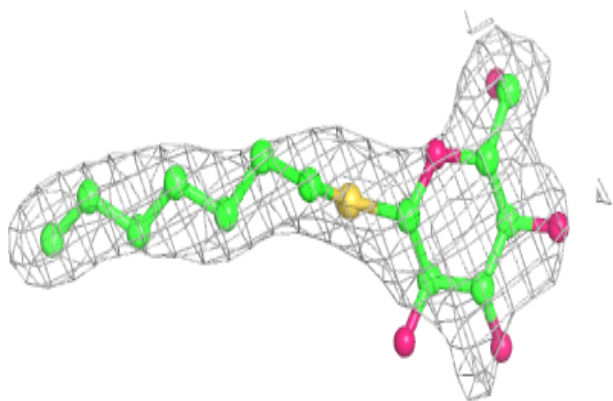
**Electron density around HTG d 419:**

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

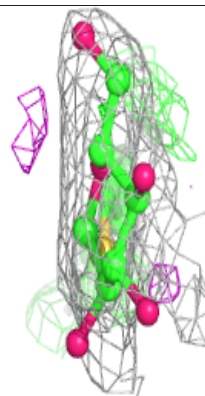
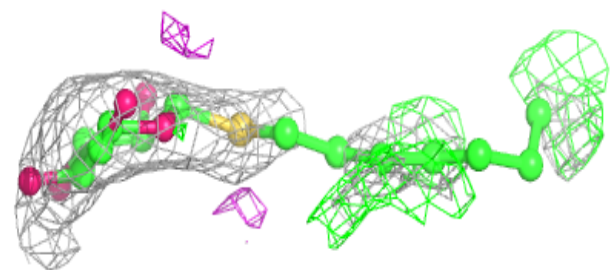
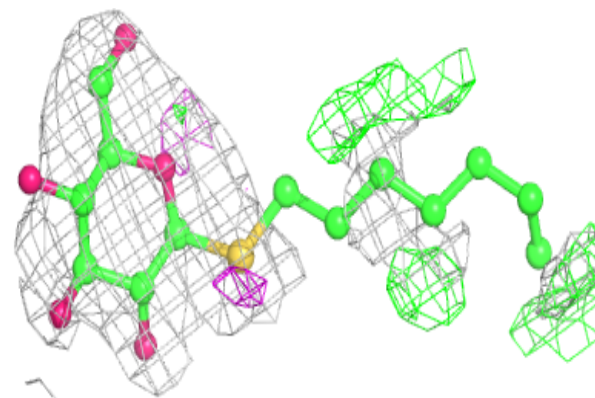


**Electron density around HTG C 521:**

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

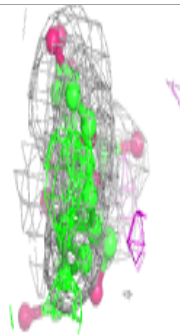
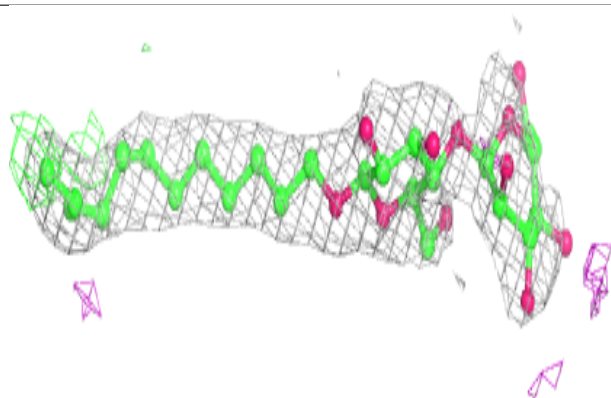
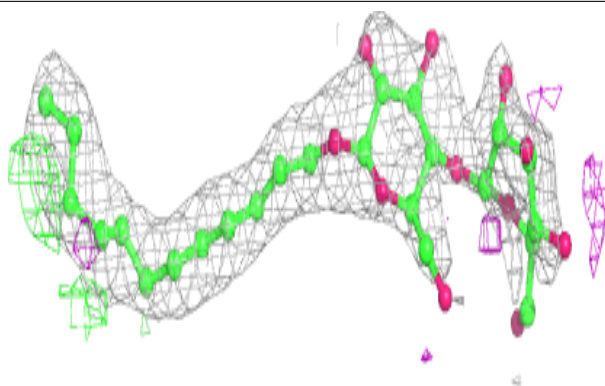
**Electron density around HTG V 215:**

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

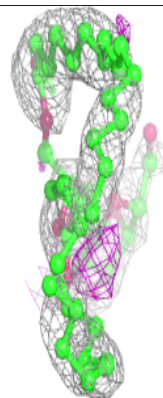
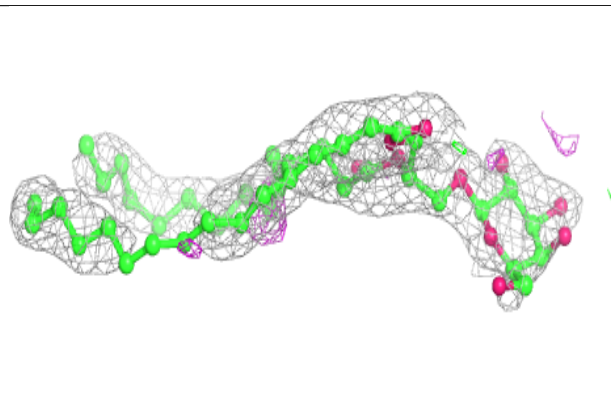
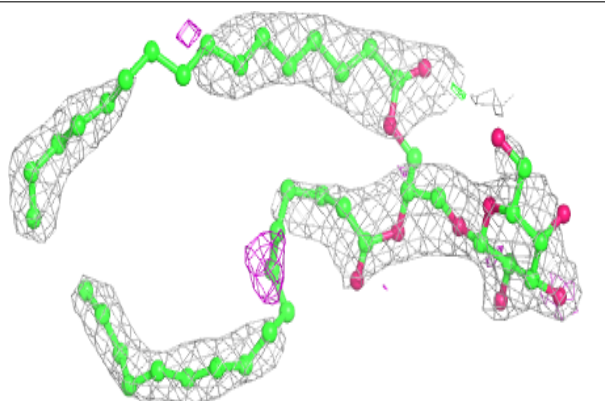


**Electron density around LMT t 102:**

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

**Electron density around LMG a 416:**

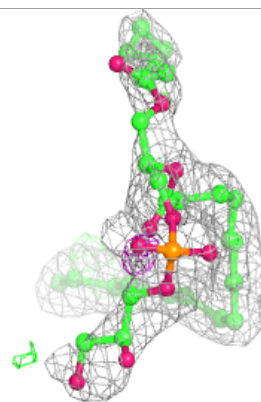
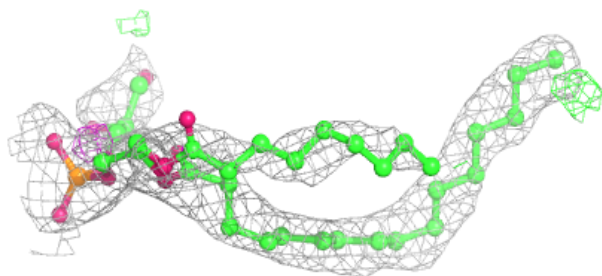
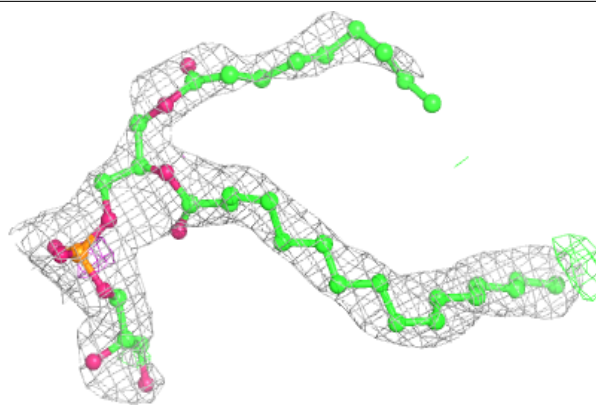
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



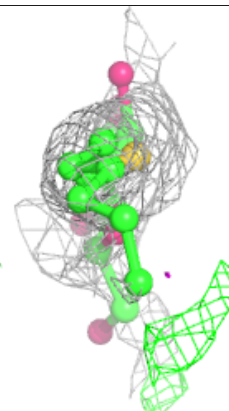
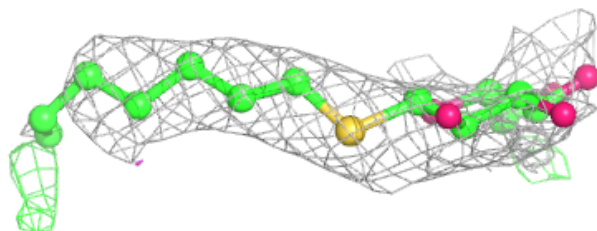
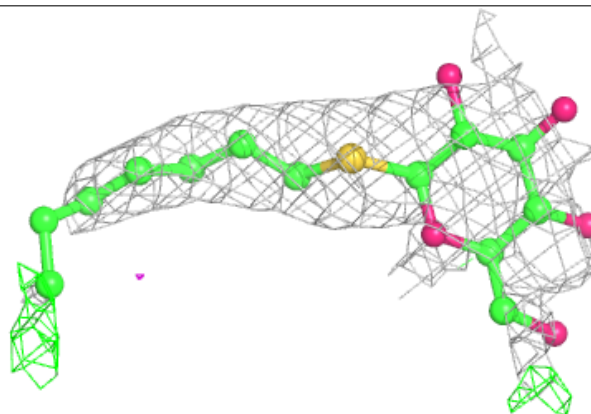


**Electron density around LHG E 101:**

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

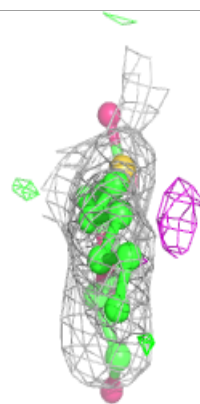
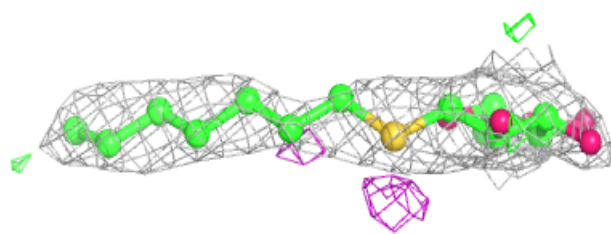
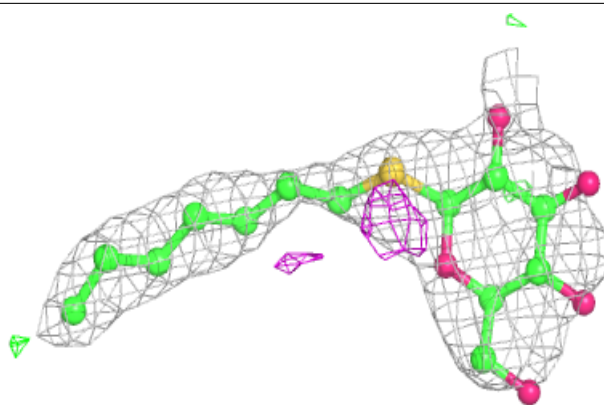
**Electron density around HTG D 412:**

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

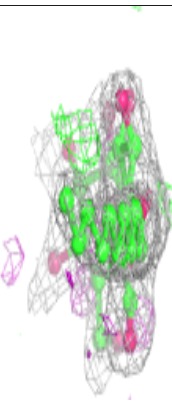
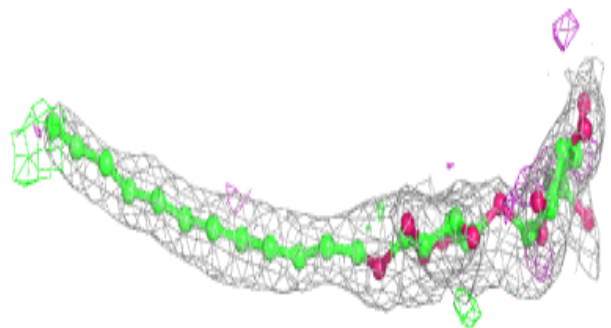
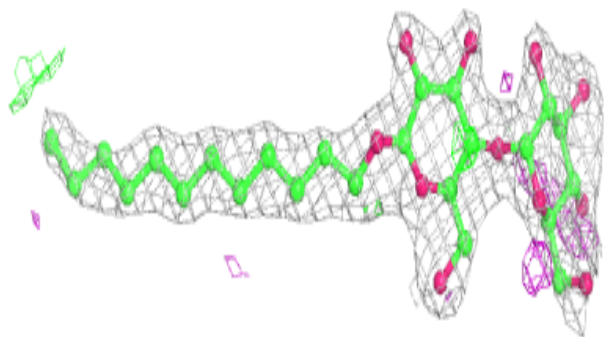


**Electron density around HTG B 630:**

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

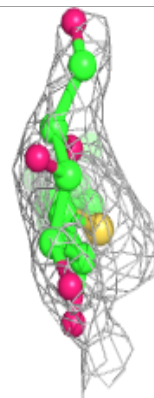
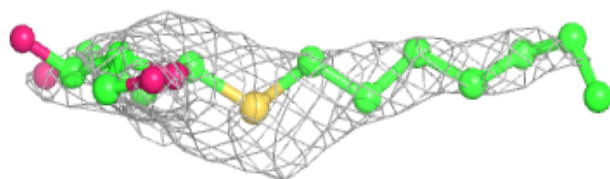
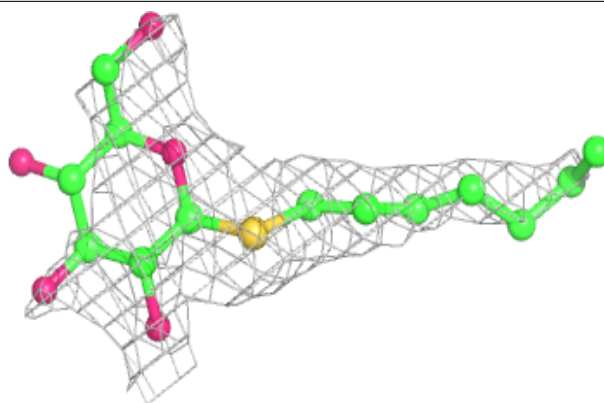
**Electron density around LMT m 102:**

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

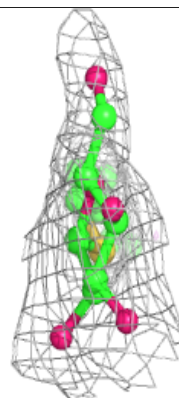
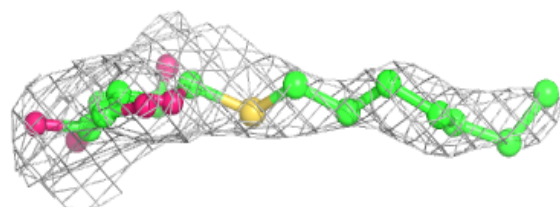
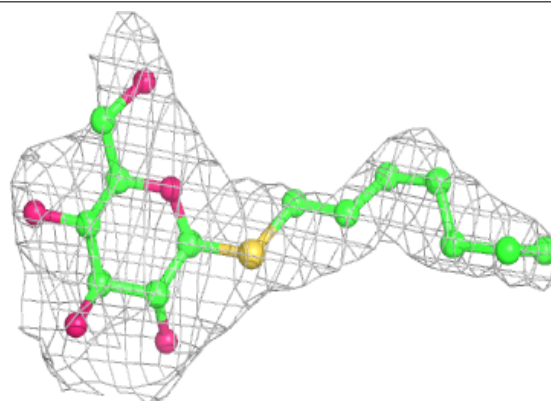


**Electron density around HTG C 537:**

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

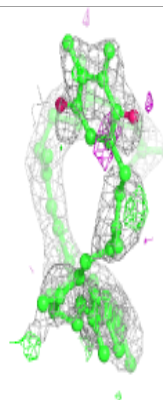
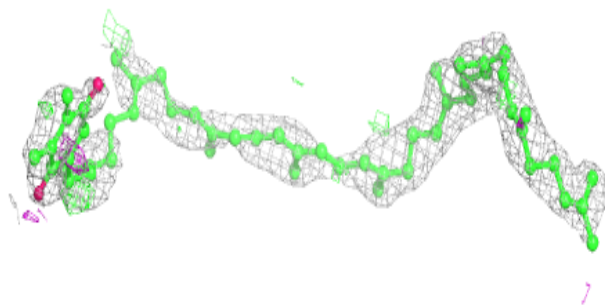
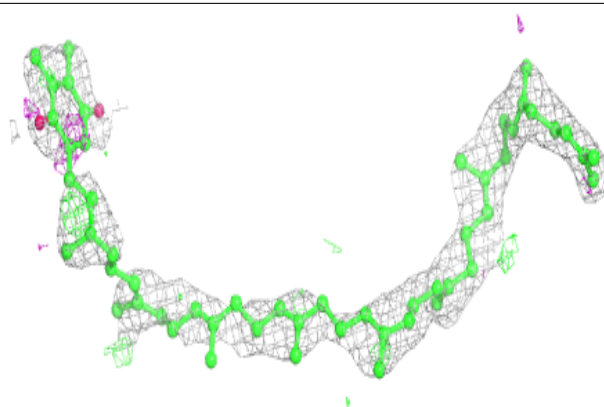
**Electron density around HTG d 414:**

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

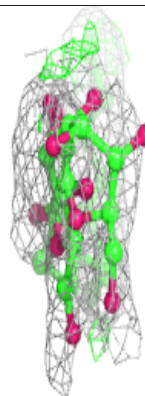
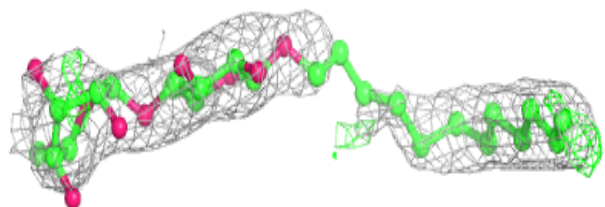
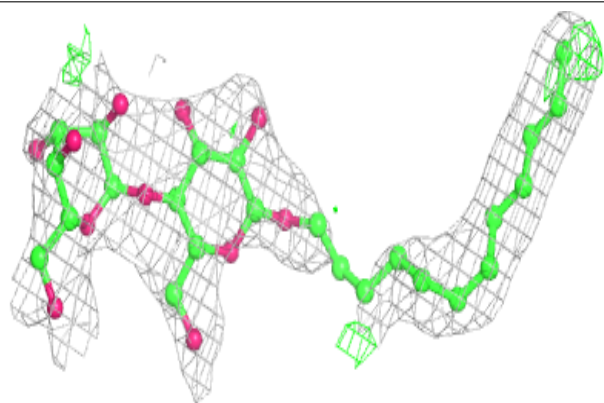


**Electron density around PL9 A 414:**

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

**Electron density around LMT Z 101:**

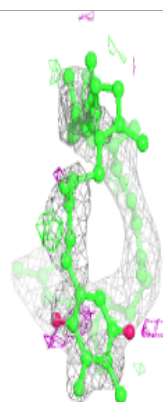
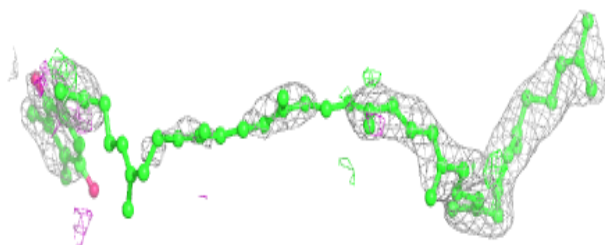
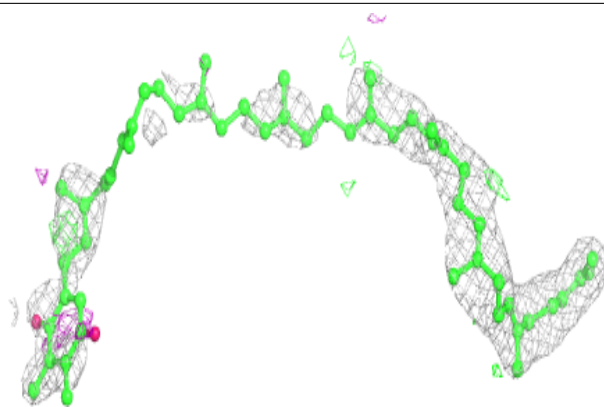
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



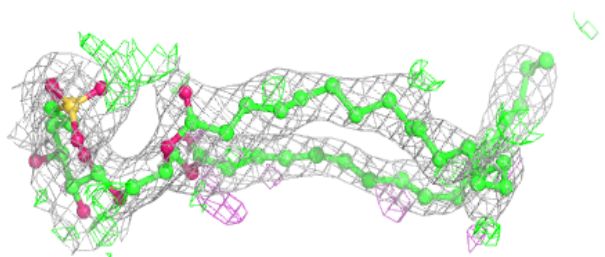
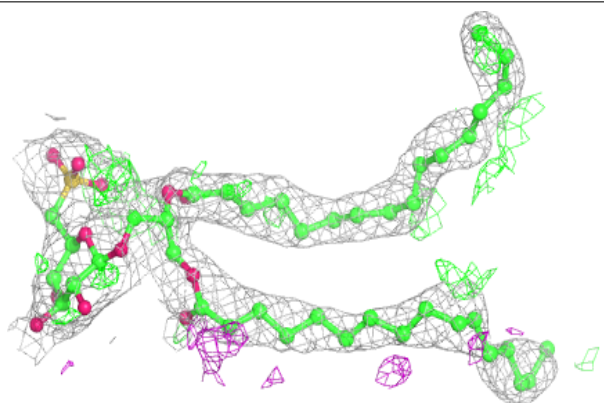


**Electron density around PL9 a 417:**

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

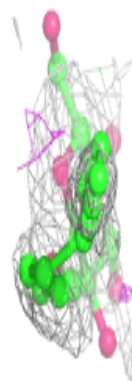
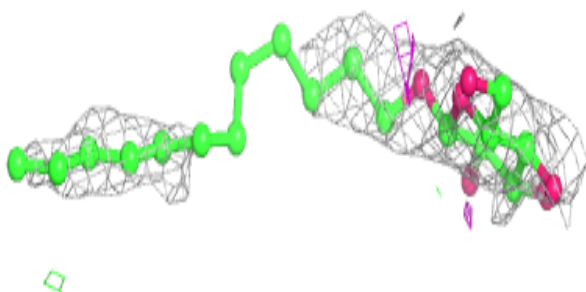
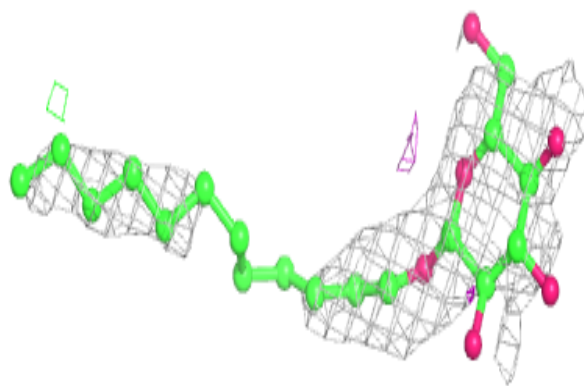
**Electron density around SQD b 601:**

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

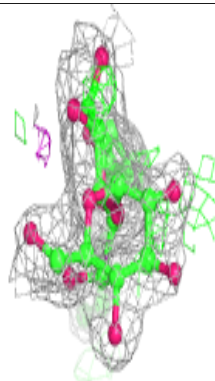
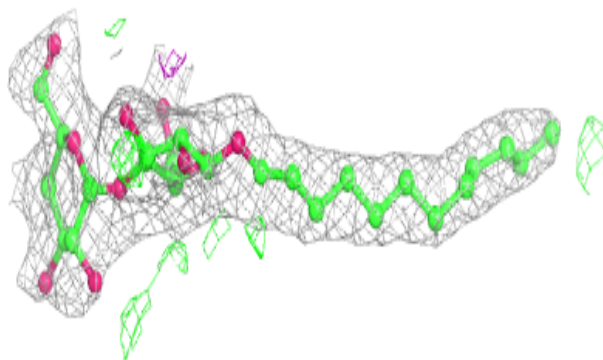
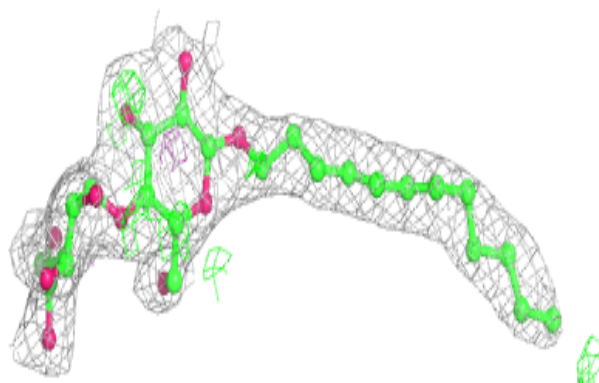


**Electron density around LMT F 103:**

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

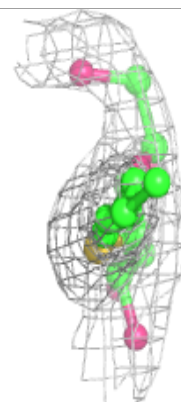
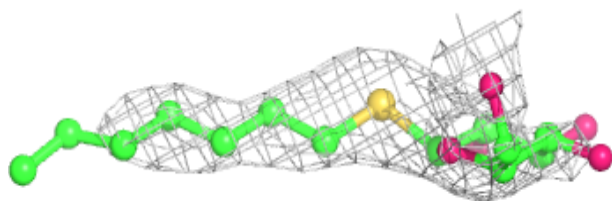
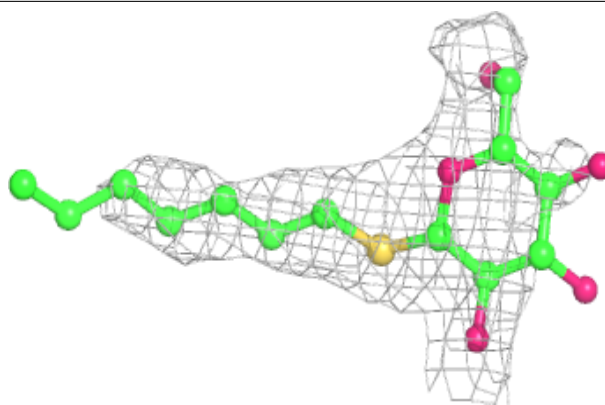
**Electron density around LMT B 622:**

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

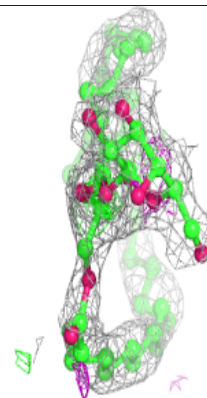
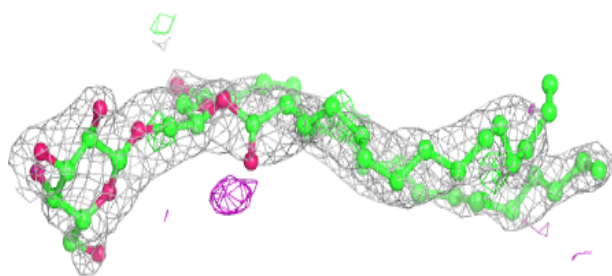
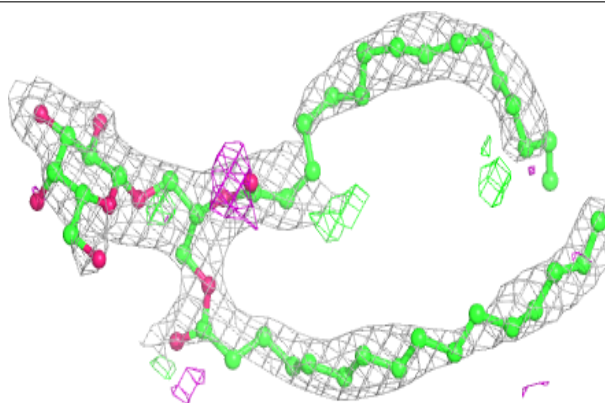


**Electron density around HTG c 928:**

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

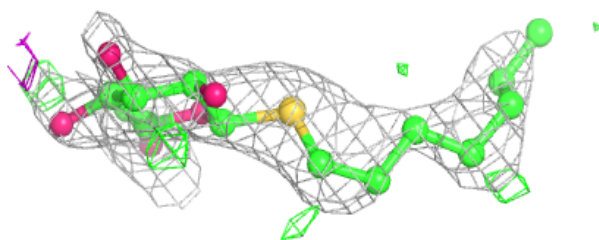
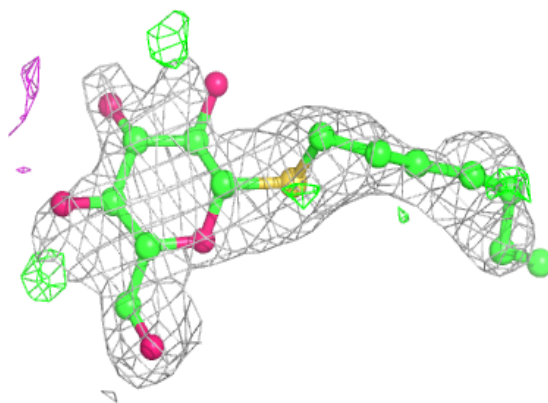
**Electron density around LMG A 413:**

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

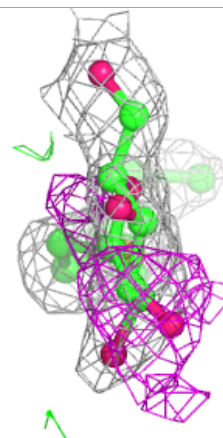
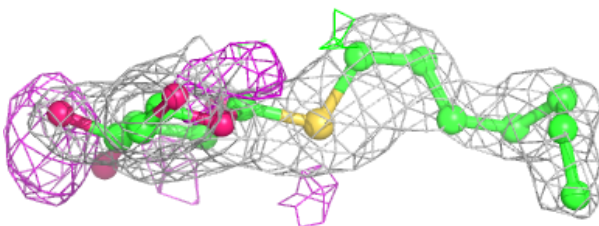
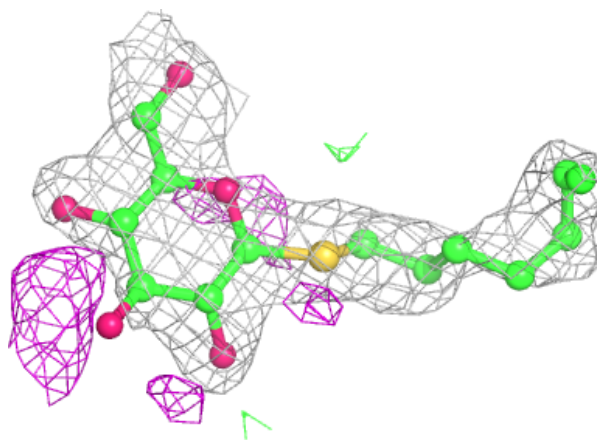


**Electron density around HTG c 942:**

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

**Electron density around HTG O 316:**

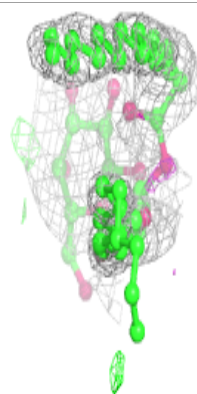
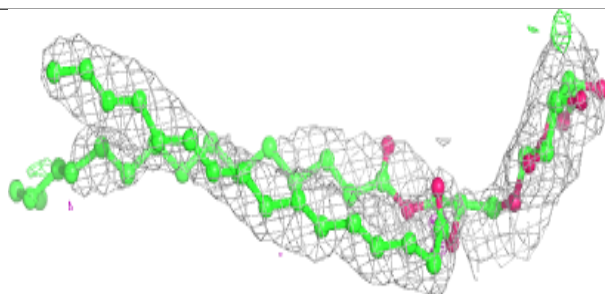
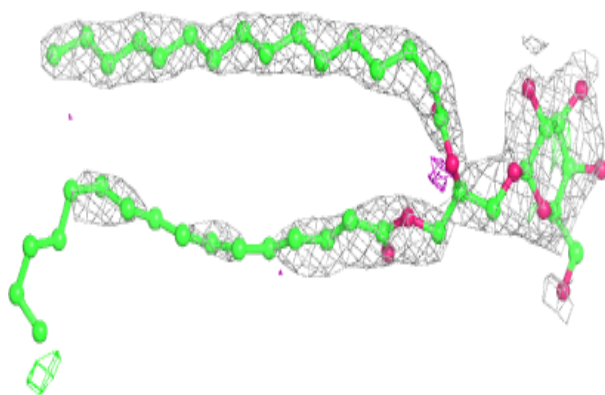
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



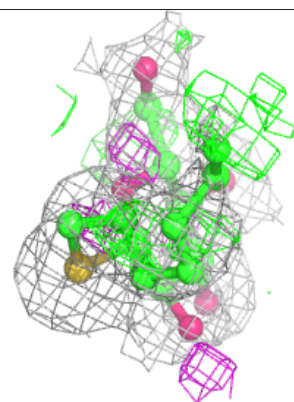
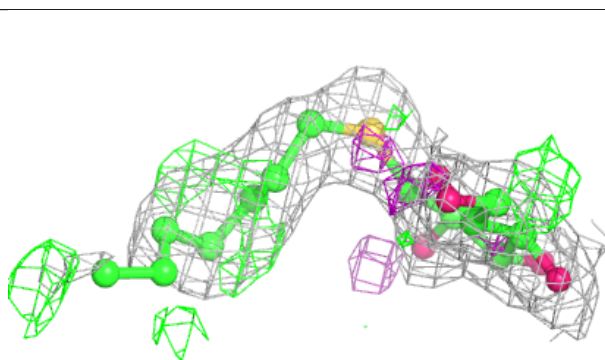
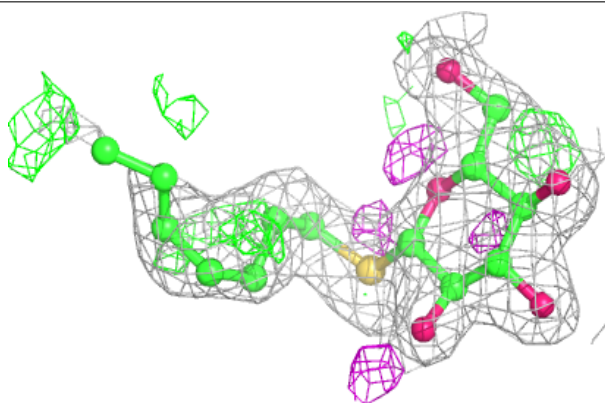


**Electron density around LMG c 921:**

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

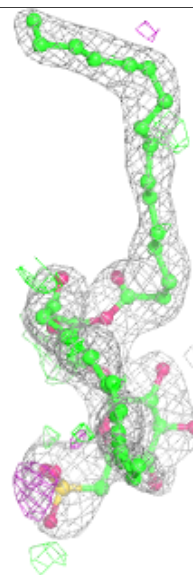
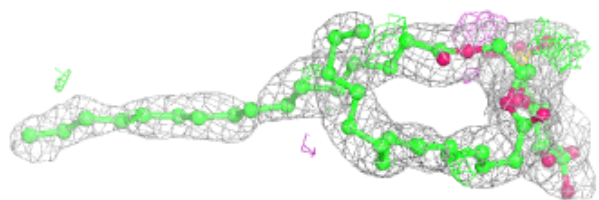
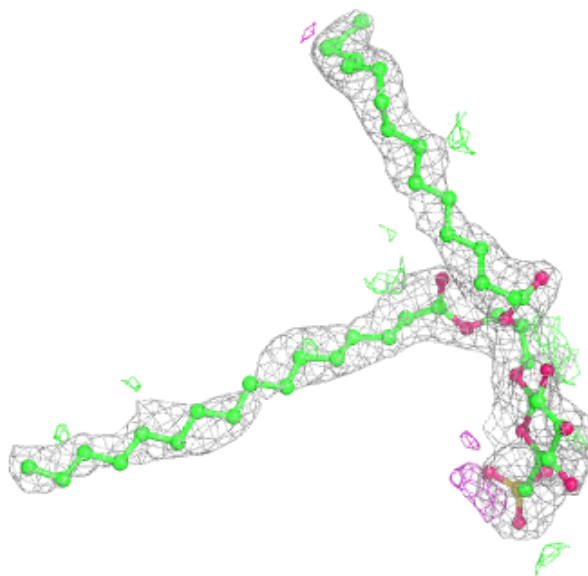
**Electron density around HTG B 624:**

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



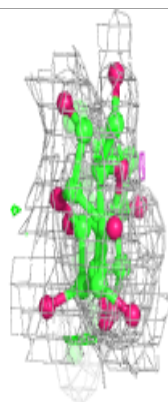
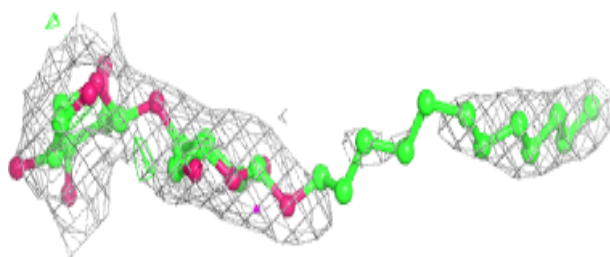
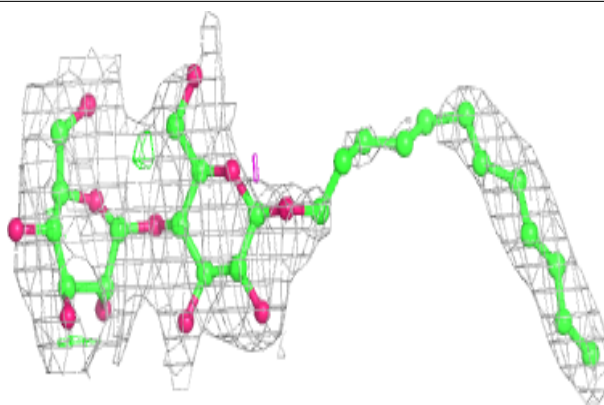
**Electron density around SQD A 416:**

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

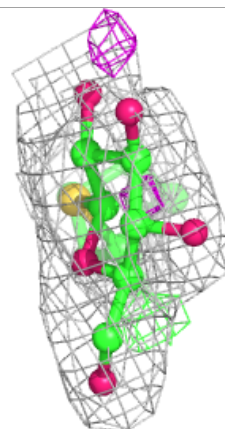
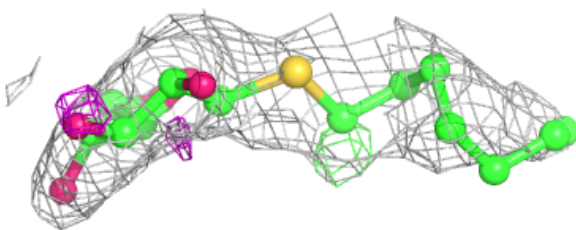
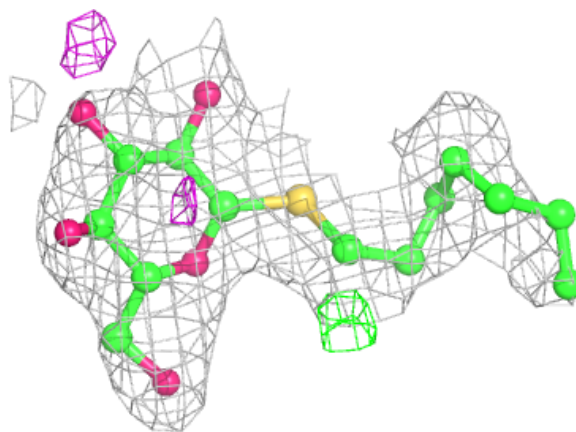


**Electron density around LMT c 927:**

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

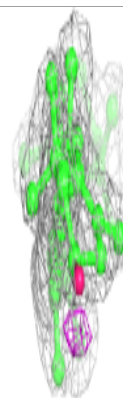
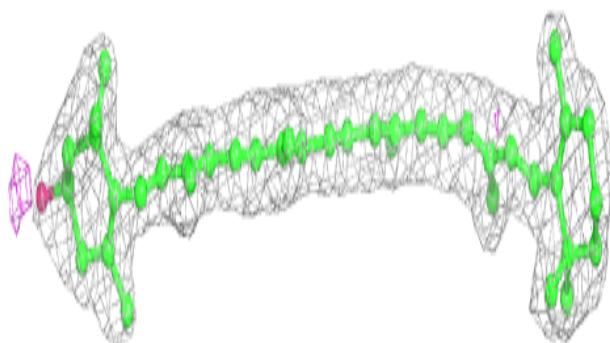
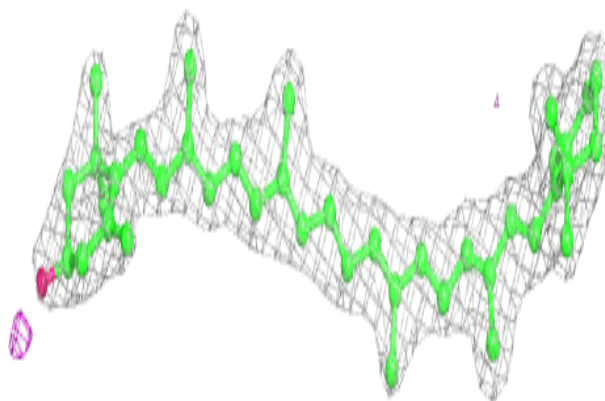
**Electron density around HTG v 211:**

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

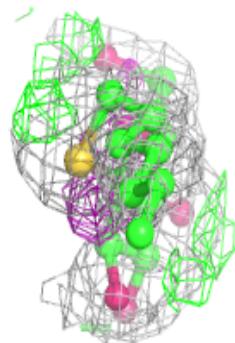
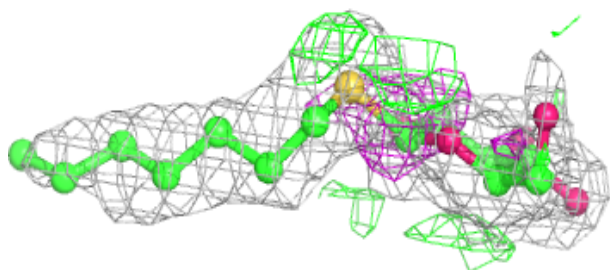
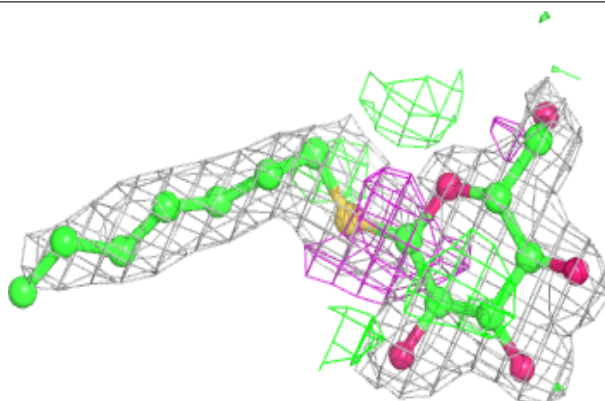


**Electron density around RRX h 101:**

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

**Electron density around HTG B 623:**

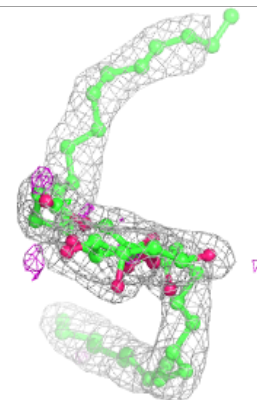
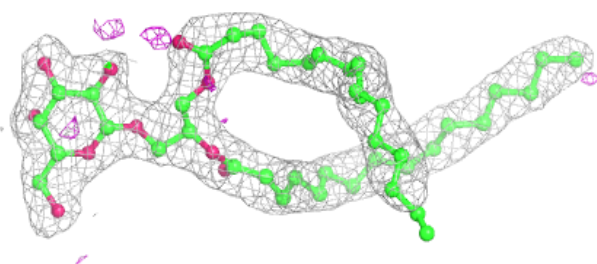
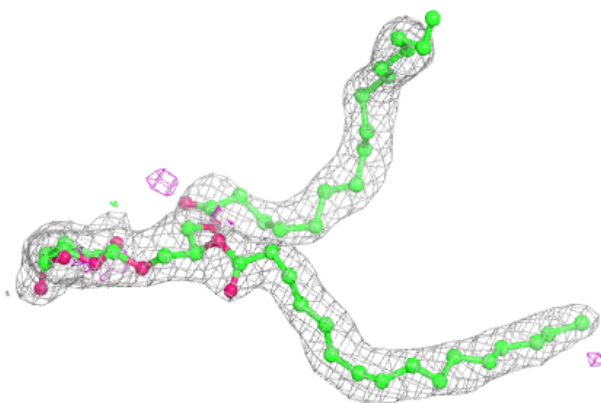
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



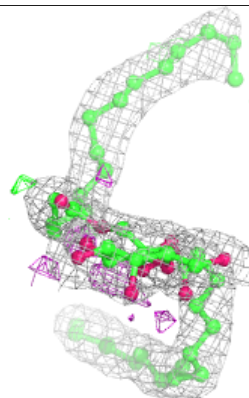
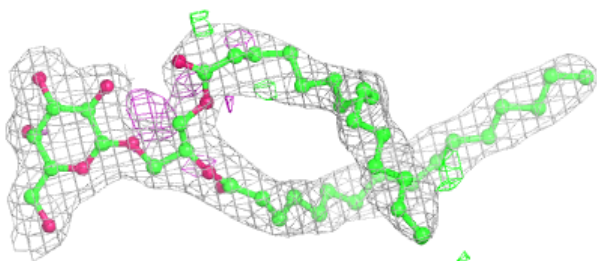
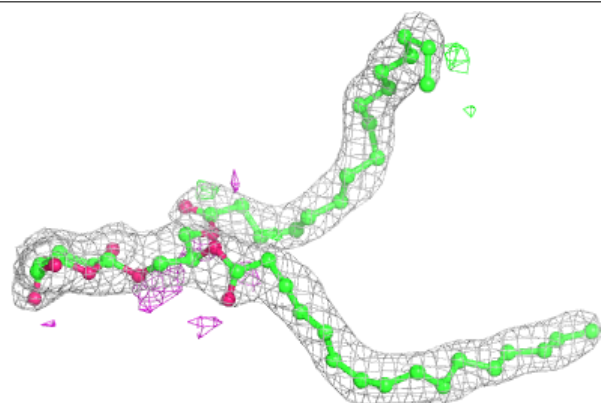


**Electron density around LMG B 621:**

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

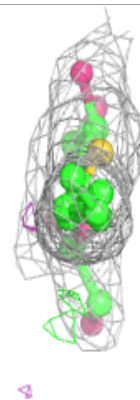
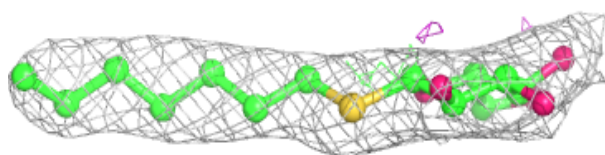
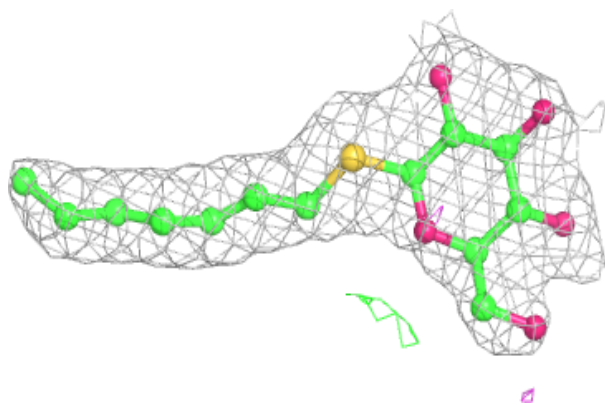
**Electron density around LMG b 624:**

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



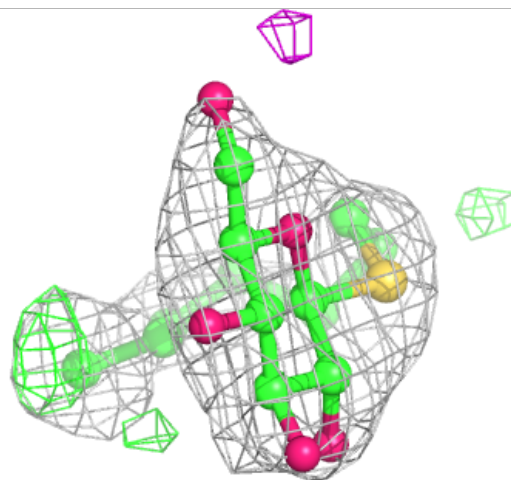
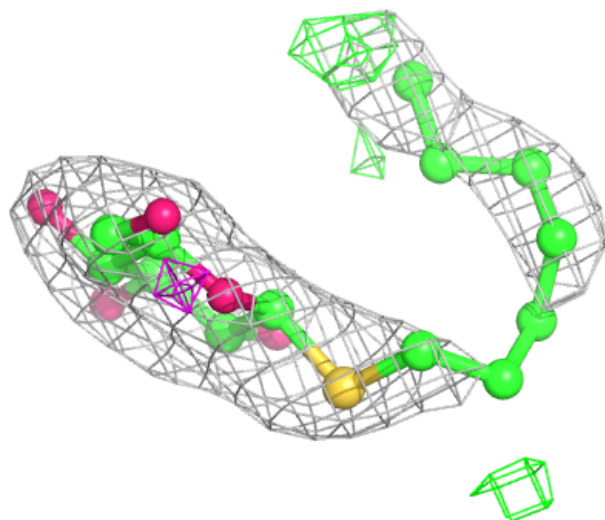
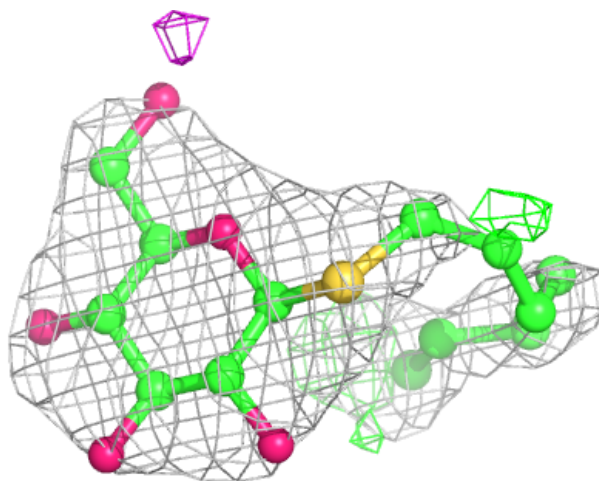
**Electron density around HTG b 602:**

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



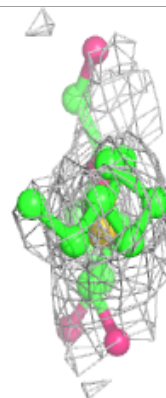
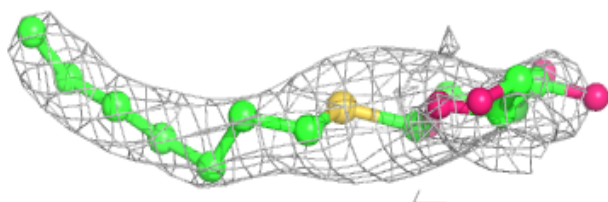
**Electron density around HTG C 520:**

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

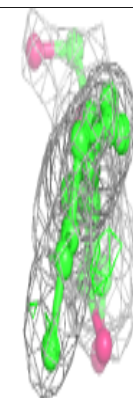
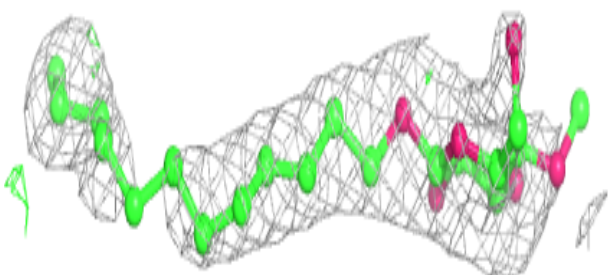
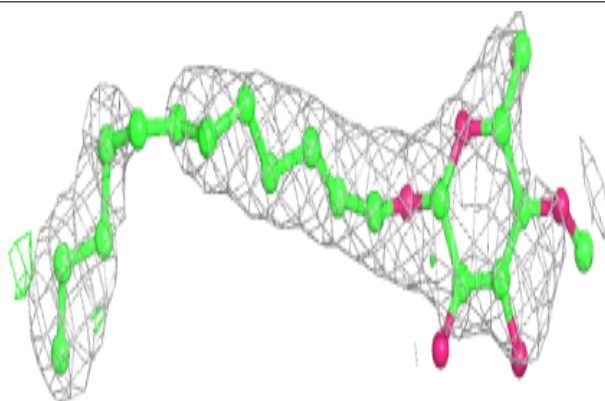


**Electron density around HTG C 536:**

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

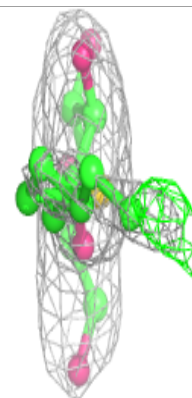
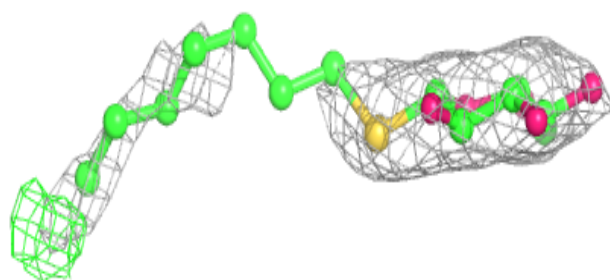
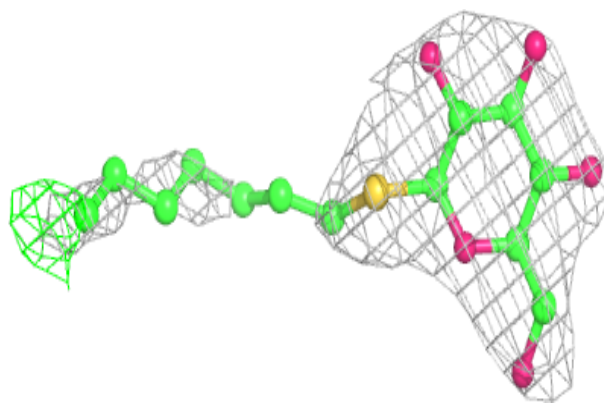
**Electron density around LMT M 102:**

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

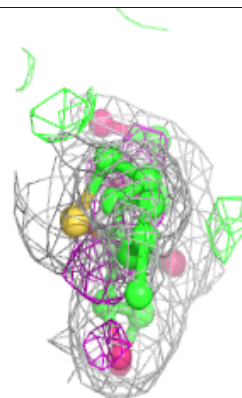
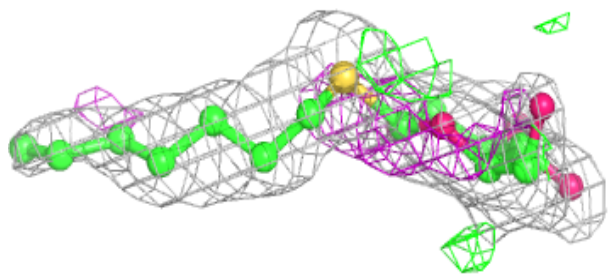
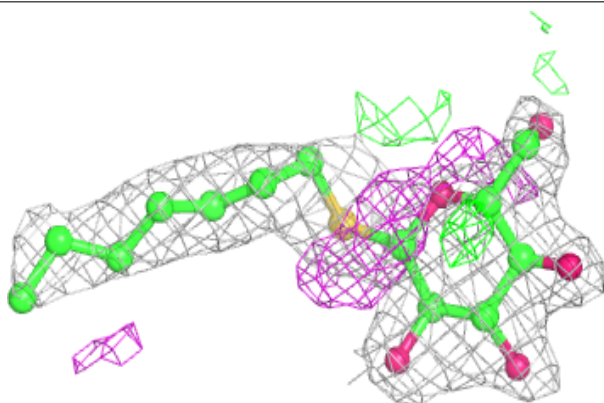


**Electron density around HTG c 923:**

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

**Electron density around HTG O 303:**

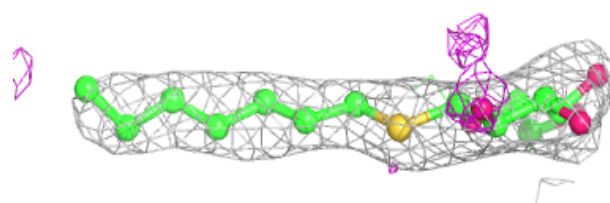
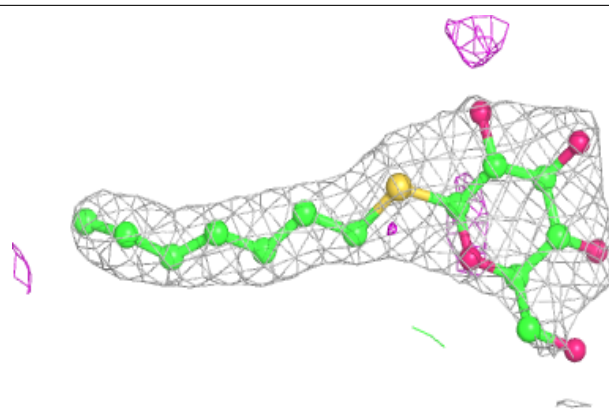
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



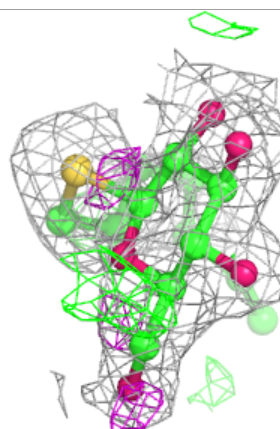
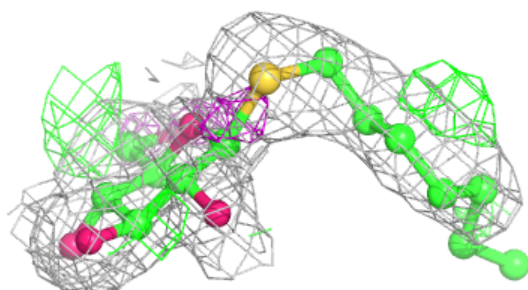
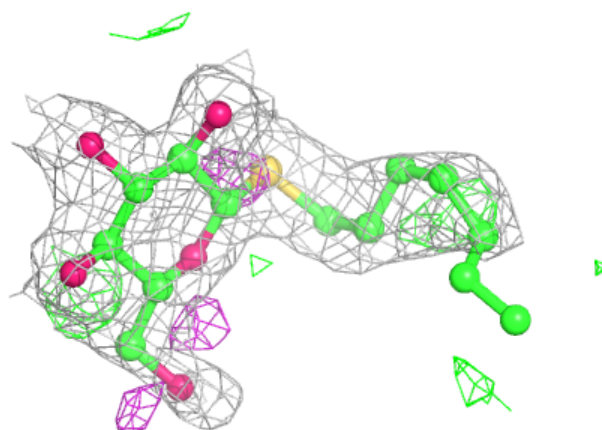


**Electron density around HTG B 629:**

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

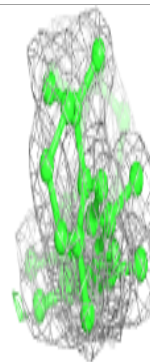
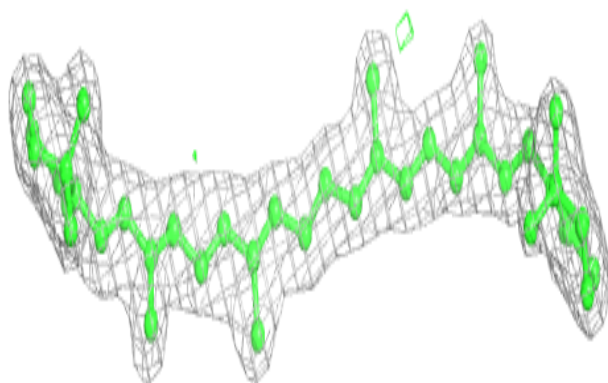
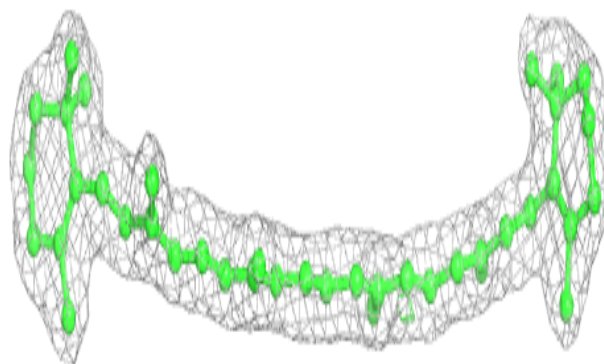
**Electron density around HTG b 626:**

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

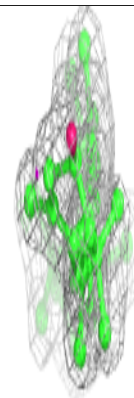
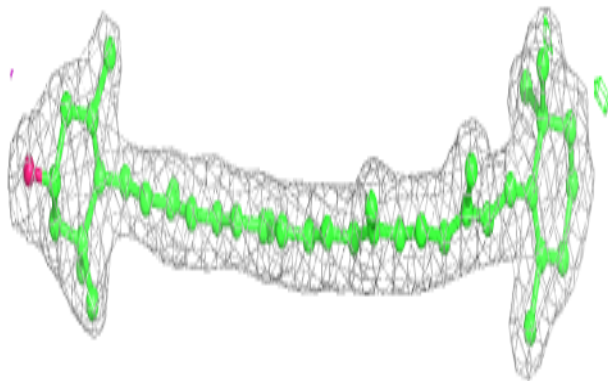
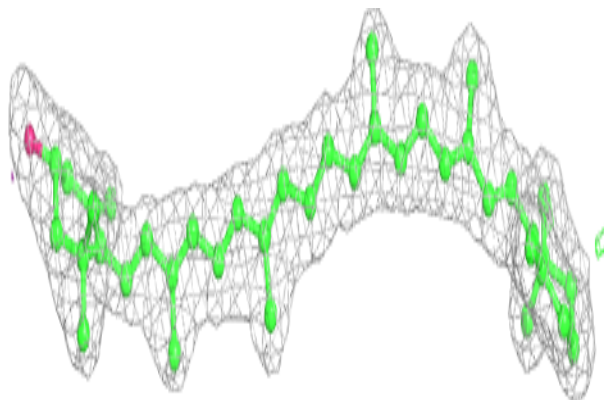


**Electron density around BCR k 103:**

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

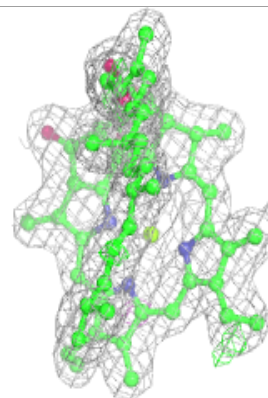
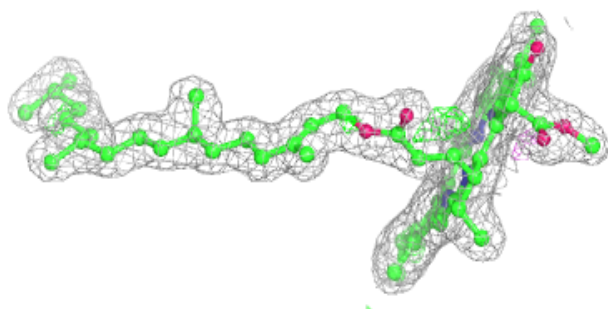
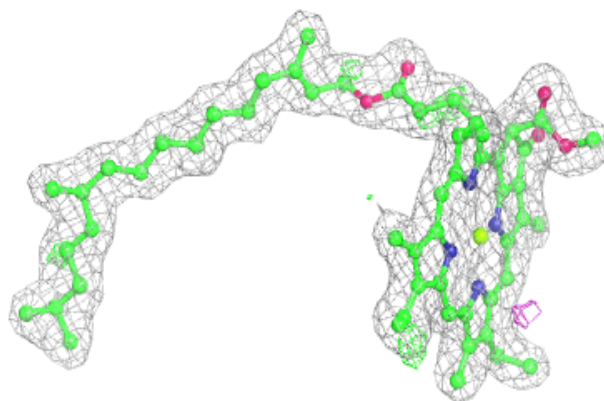
**Electron density around RRX H 101:**

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

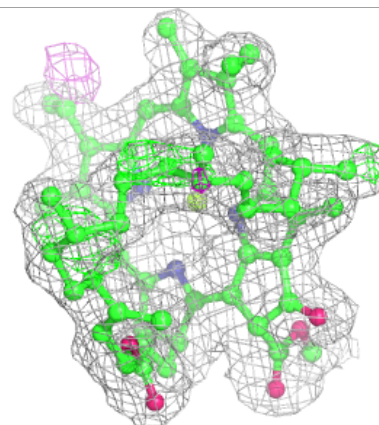
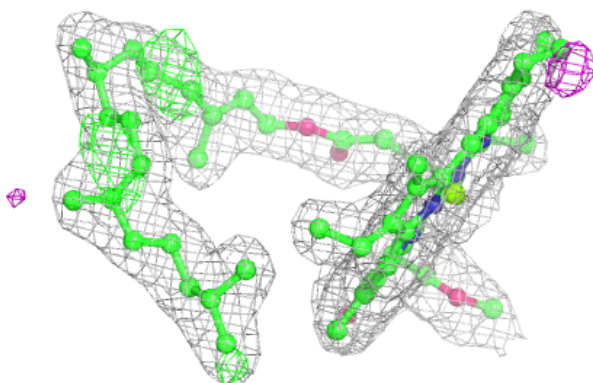
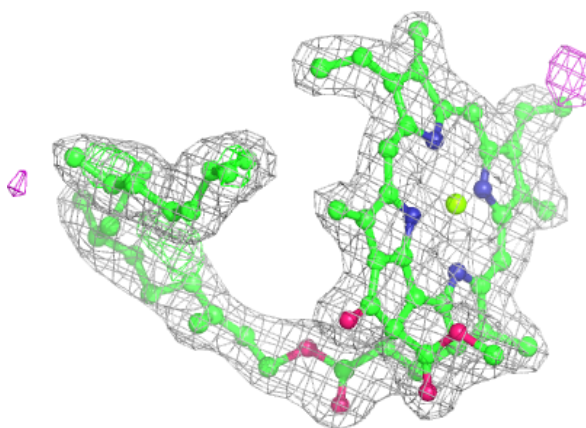


**Electron density around CLA B 610:**

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

**Electron density around CLA c 904:**

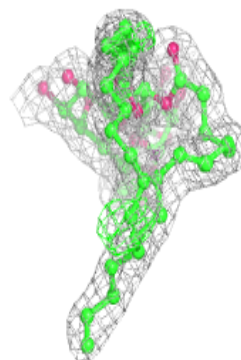
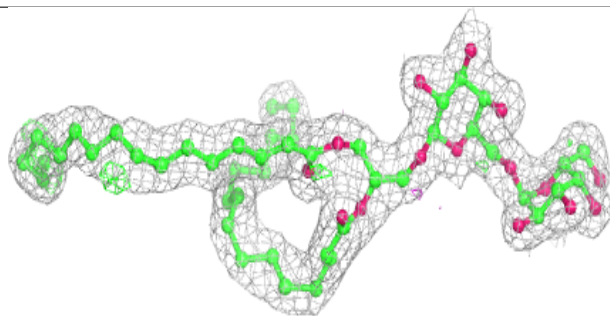
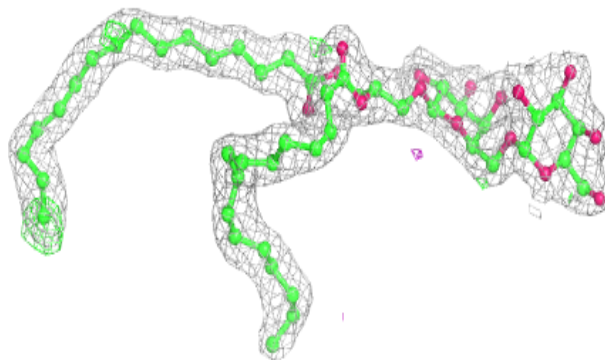
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



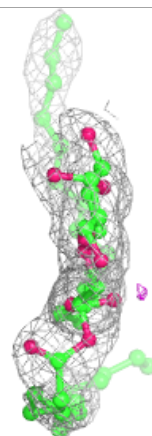
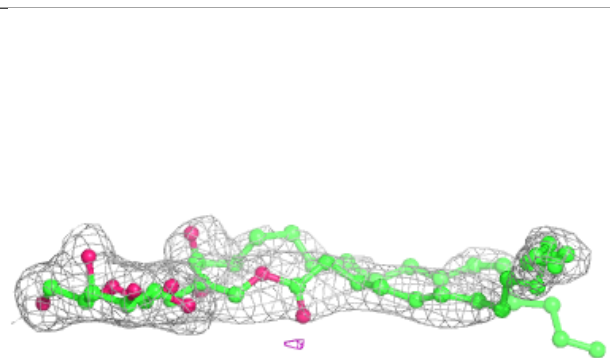
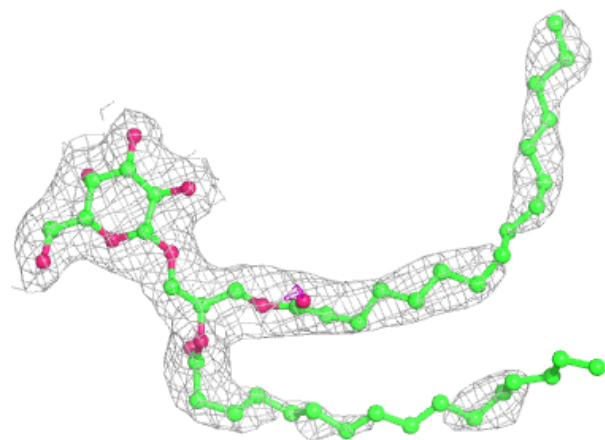


**Electron density around DGD h 102:**

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

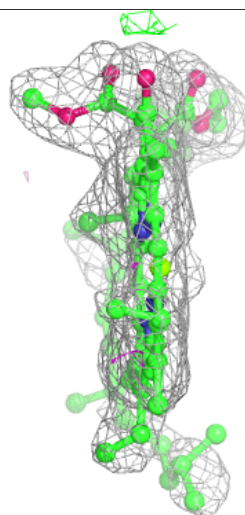
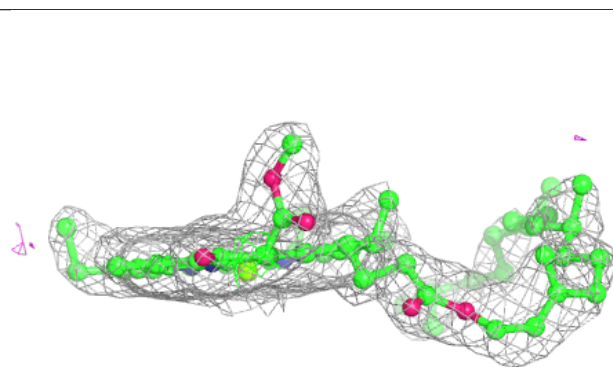
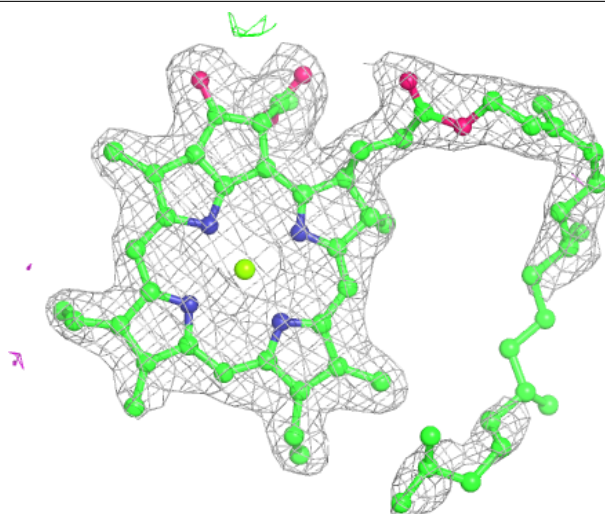
**Electron density around LMG c 920:**

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



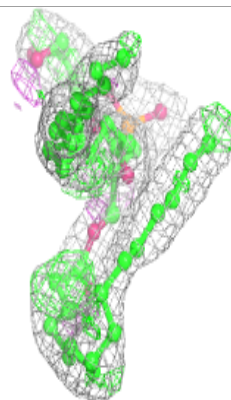
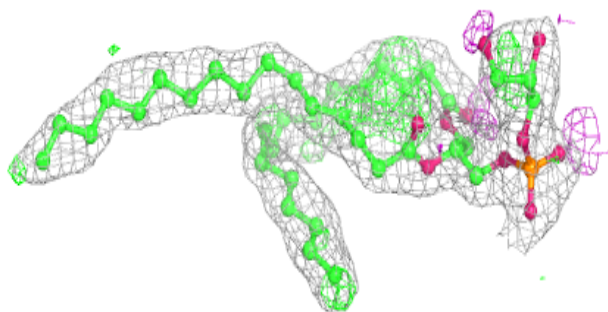
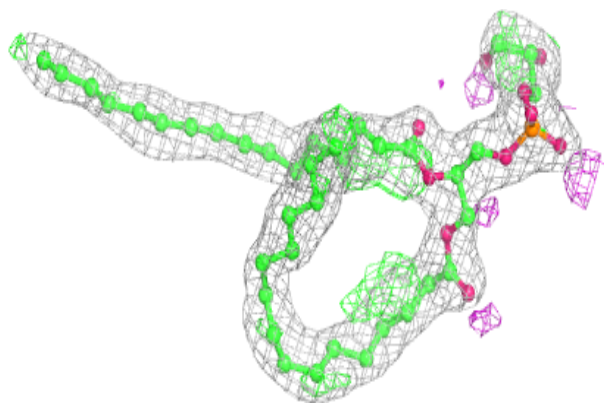
**Electron density around CLA c 913:**

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

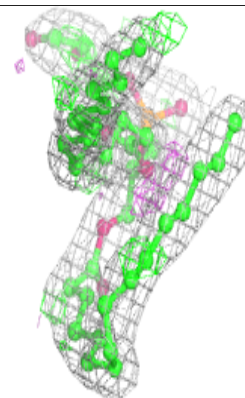
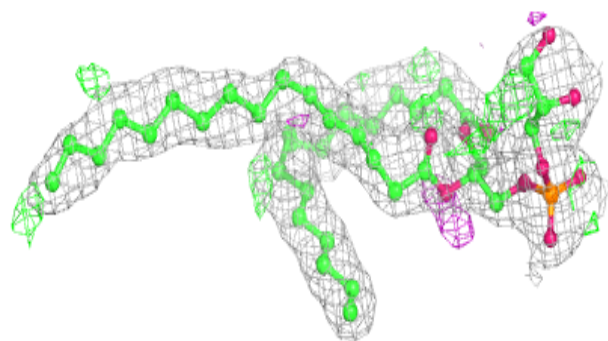
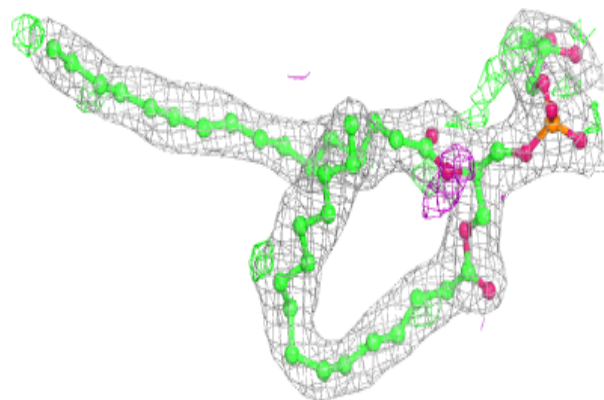


**Electron density around LHG D 406:**

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

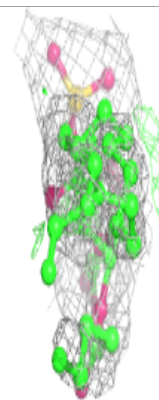
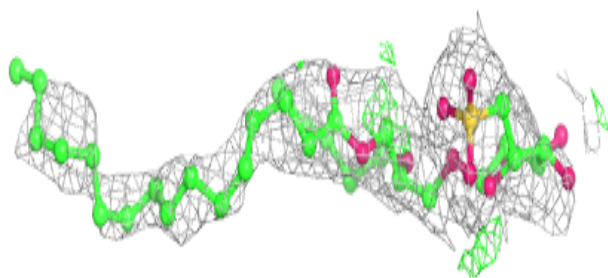
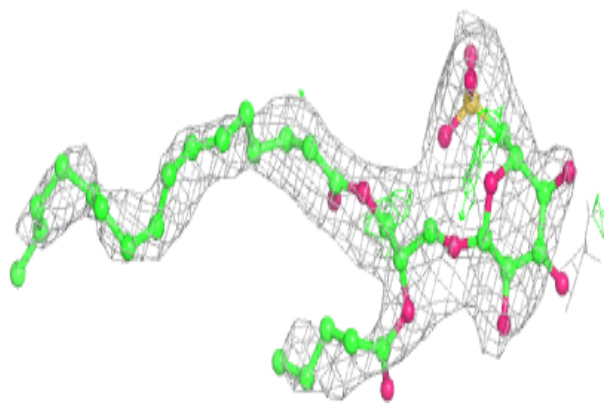
**Electron density around LHG d 409:**

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

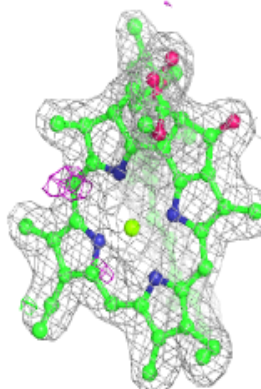
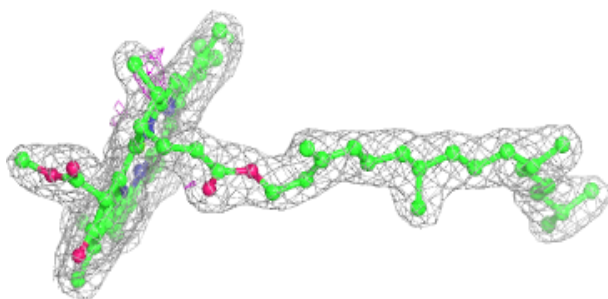
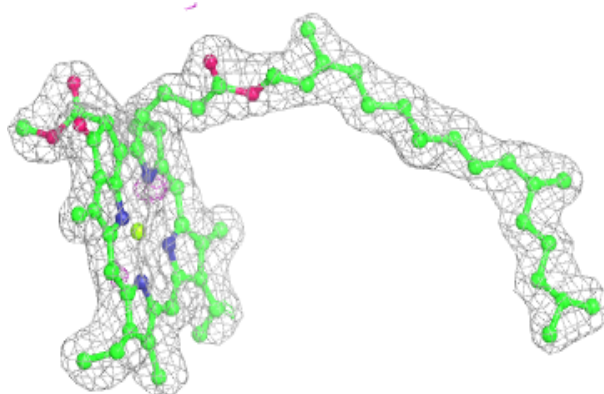


**Electron density around SQD f 102:**

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

**Electron density around CLA b 613:**

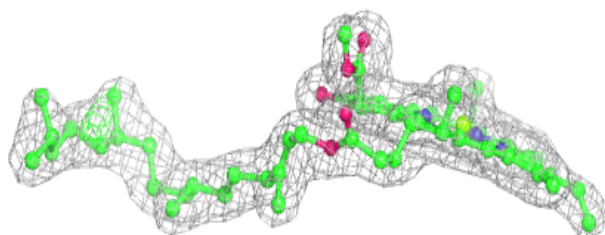
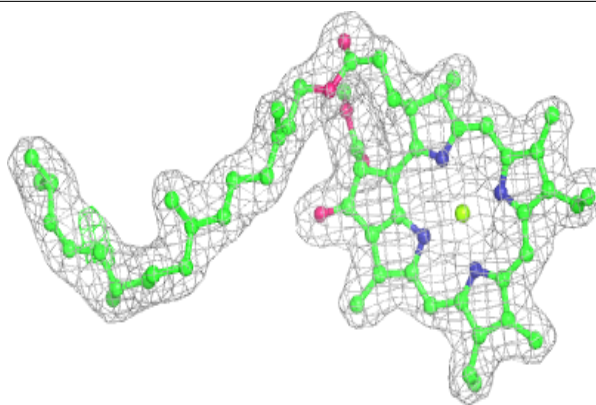
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



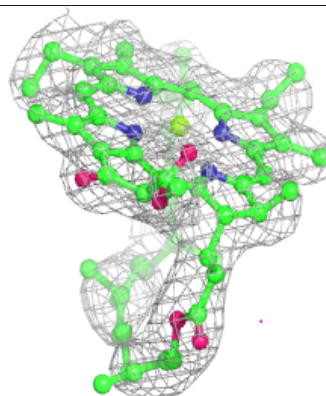
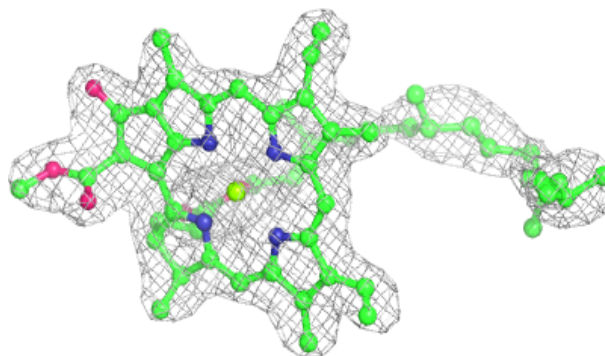
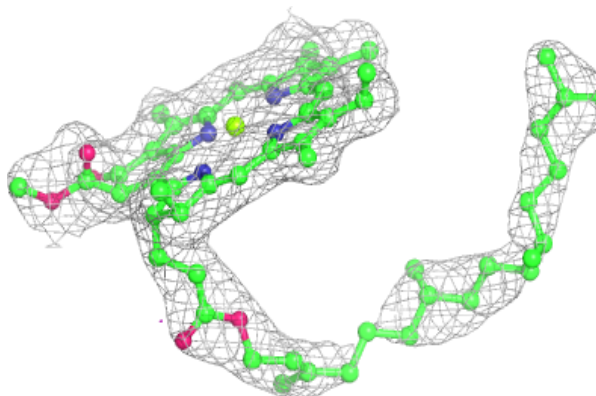


**Electron density around CLA B 603:**

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

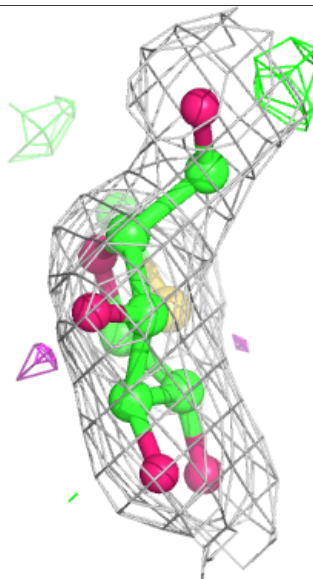
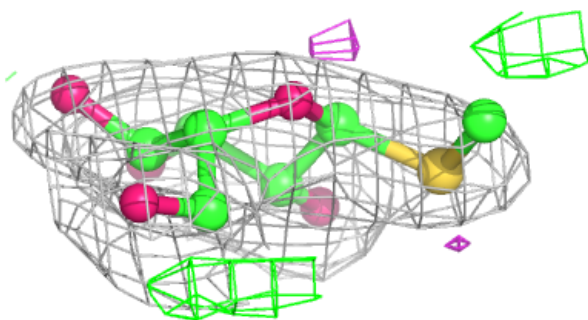
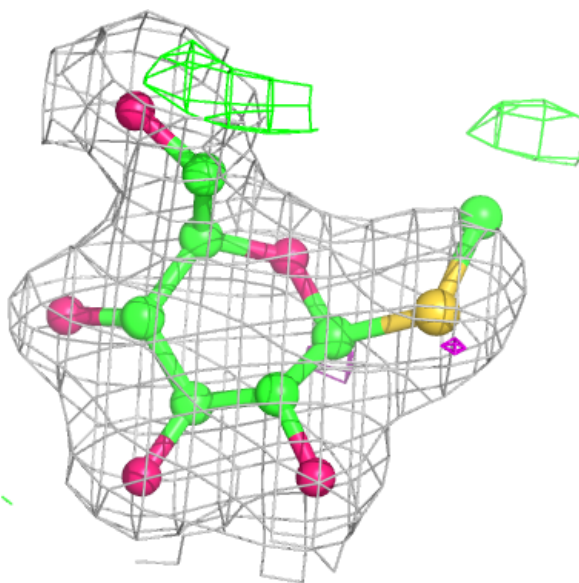
**Electron density around CLA C 513:**

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



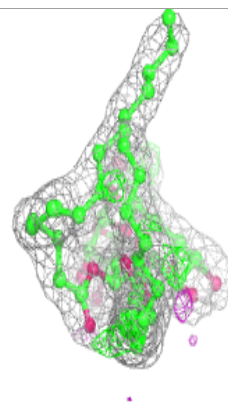
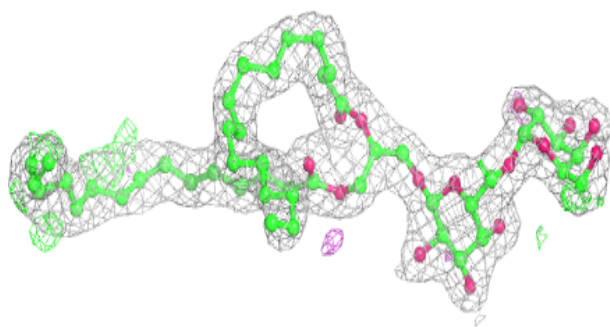
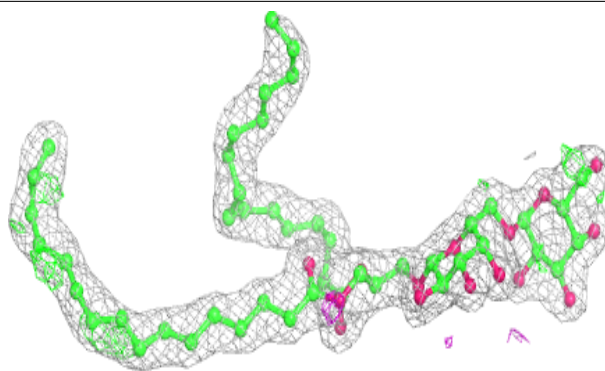
**Electron density around HTG V 204:**

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

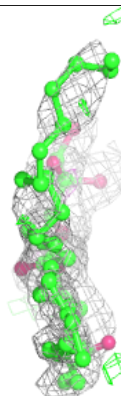
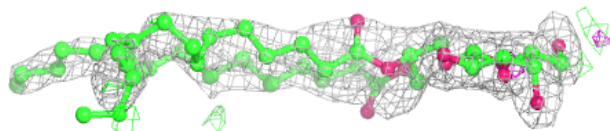
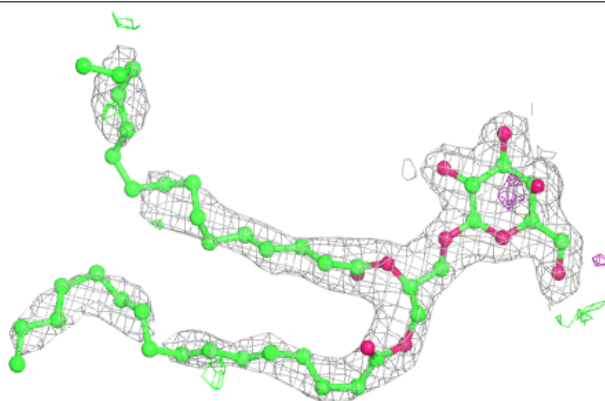


**Electron density around DGD H 102:**

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

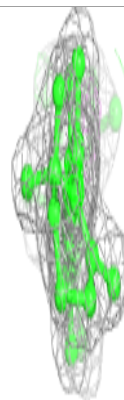
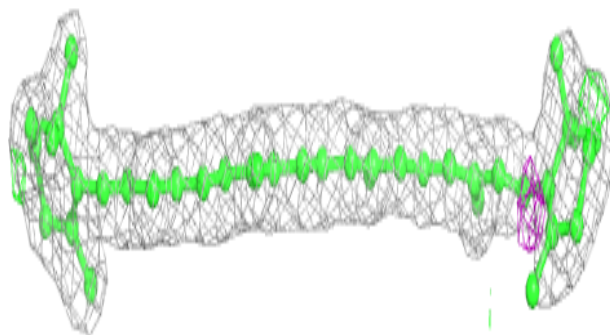
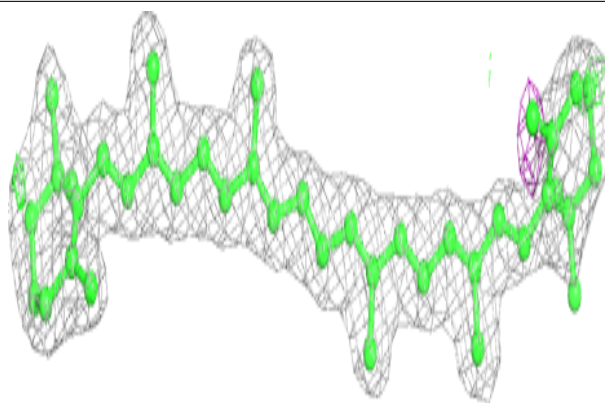
**Electron density around LMG C 519:**

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



**Electron density around BCR B 619:**

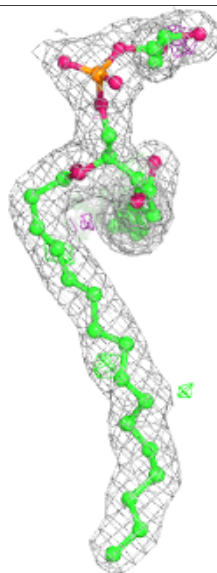
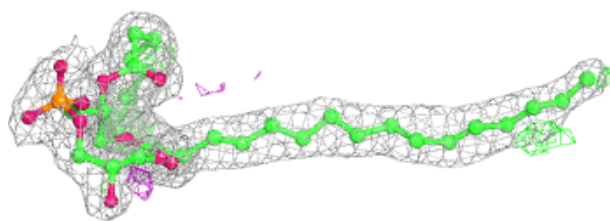
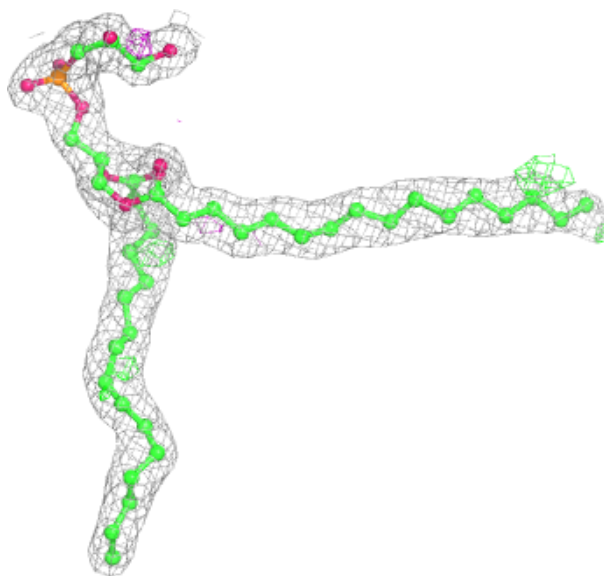
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





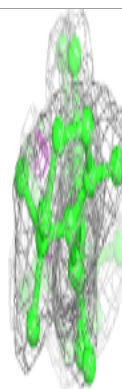
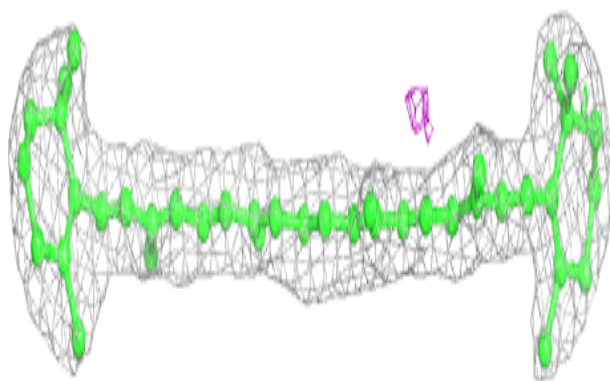
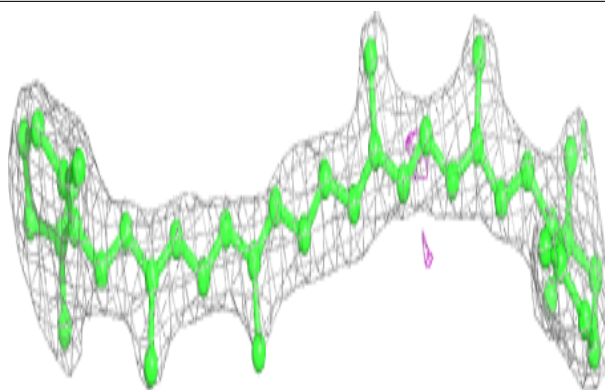
**Electron density around LHG 1 103:**

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

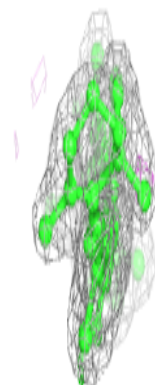
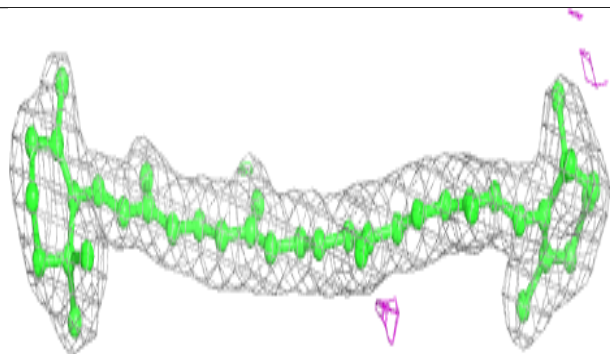
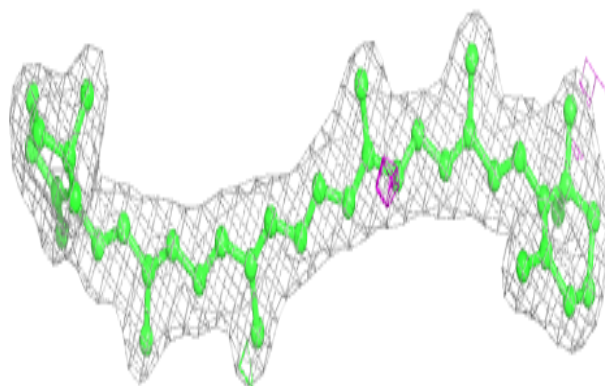


**Electron density around BCR c 915:**

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

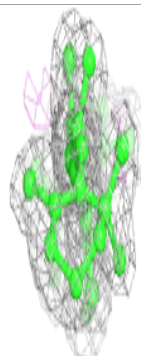
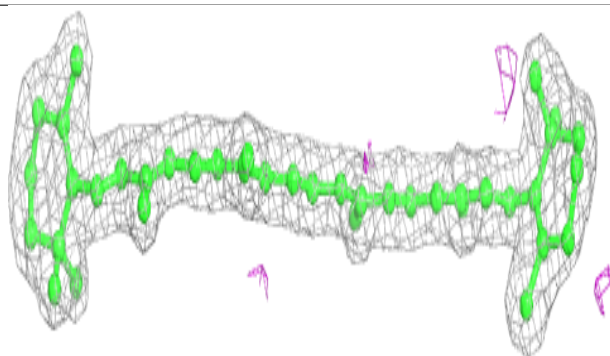
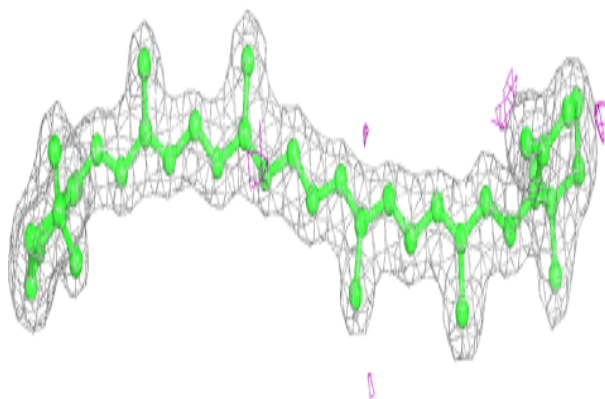
**Electron density around BCR Y 101:**

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

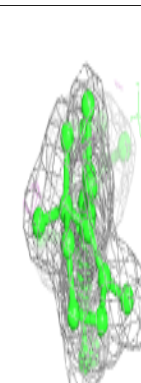
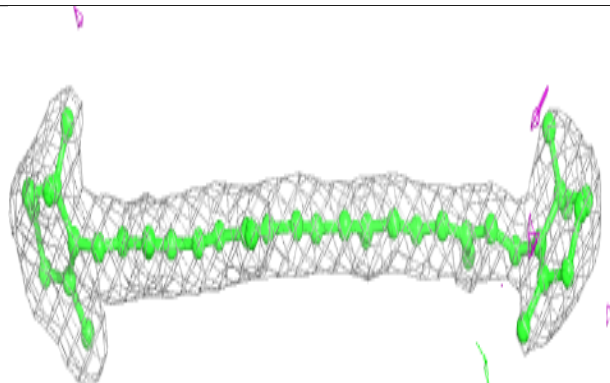
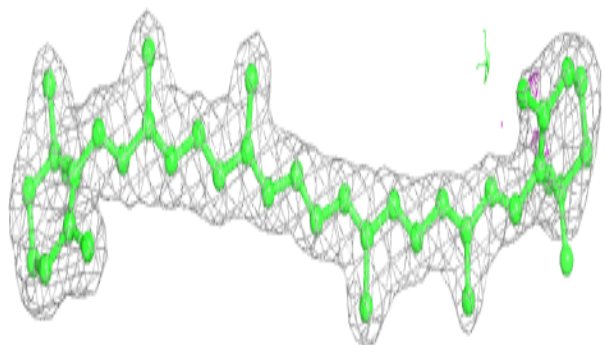


**Electron density around BCR a 414:**

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

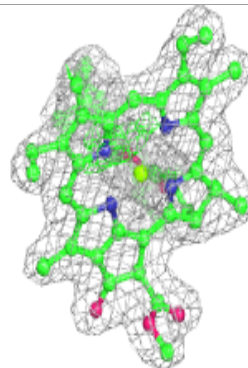
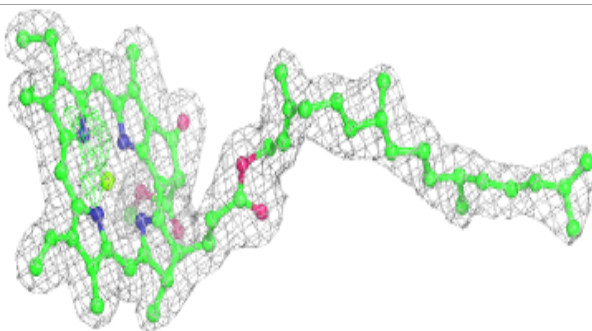
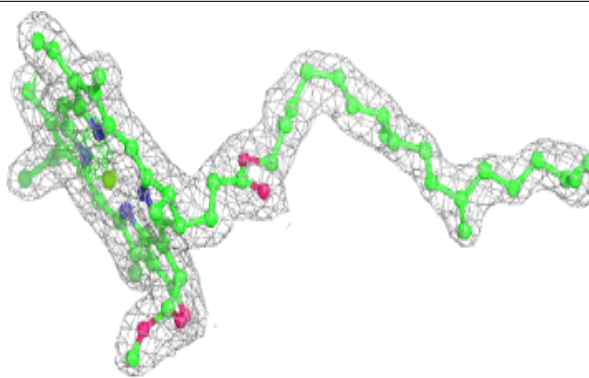
**Electron density around BCR b 622:**

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



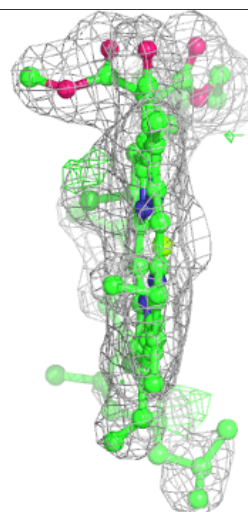
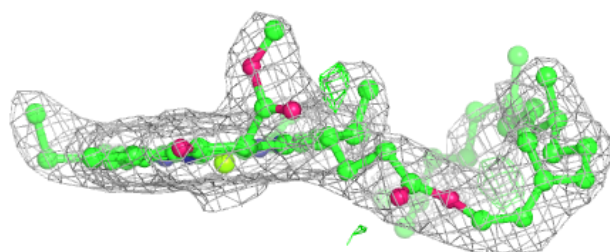
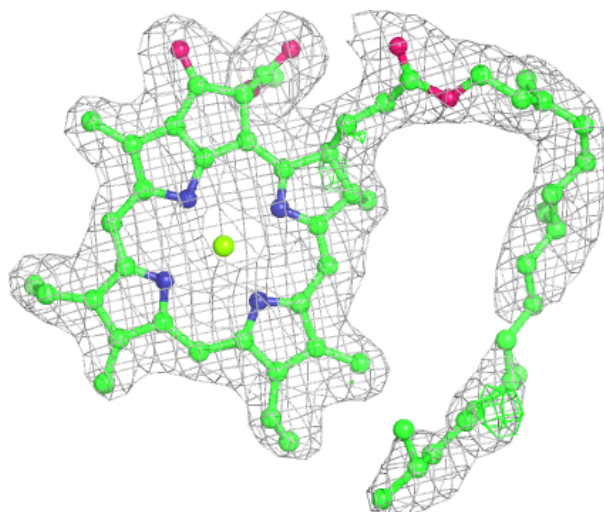
**Electron density around CLA c 903:**

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



**Electron density around CLA C 512:**

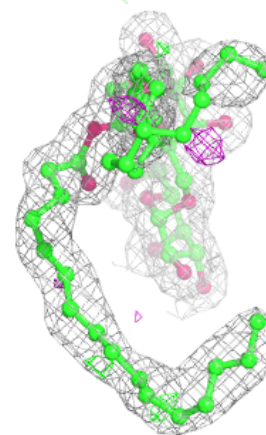
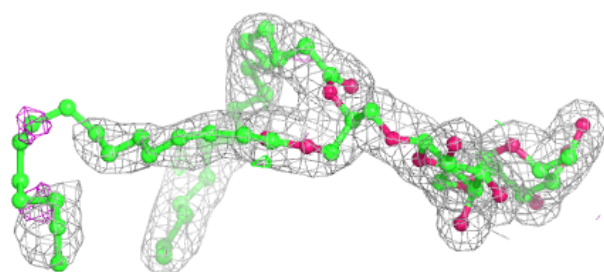
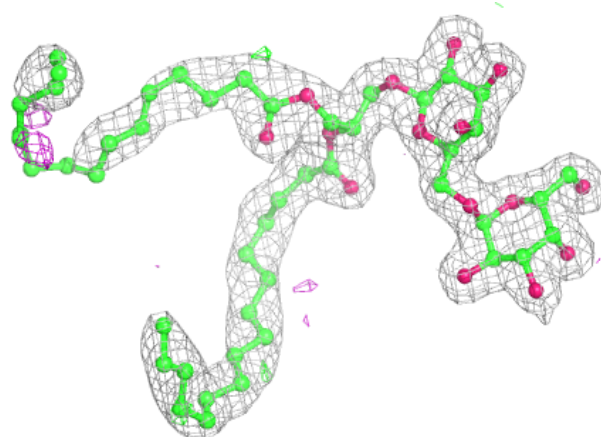
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



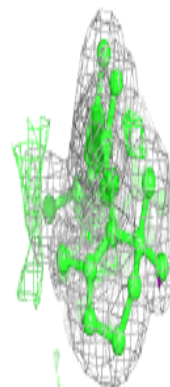
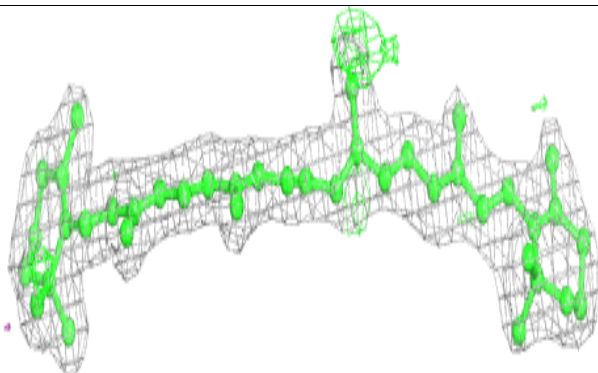
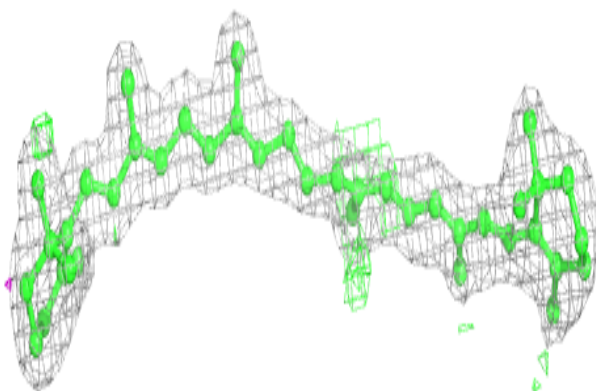


**Electron density around DGD C 517:**

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

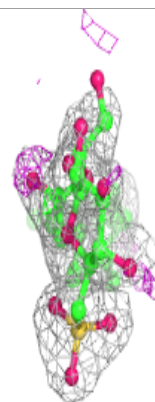
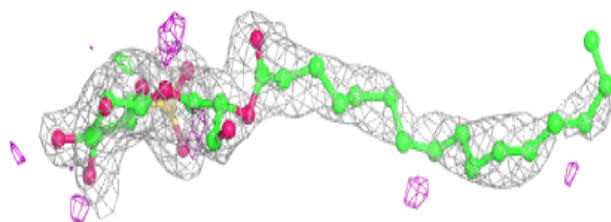
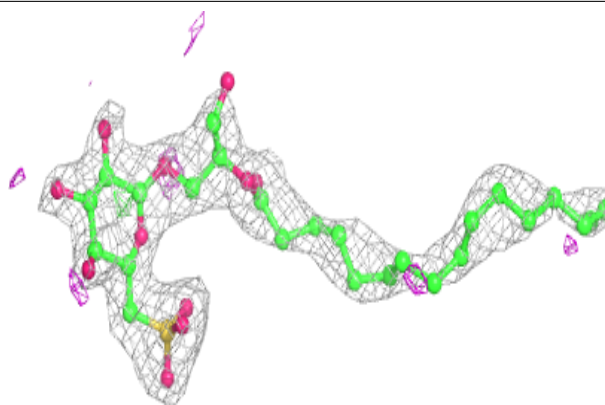
**Electron density around BCR B 636:**

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

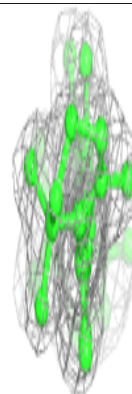
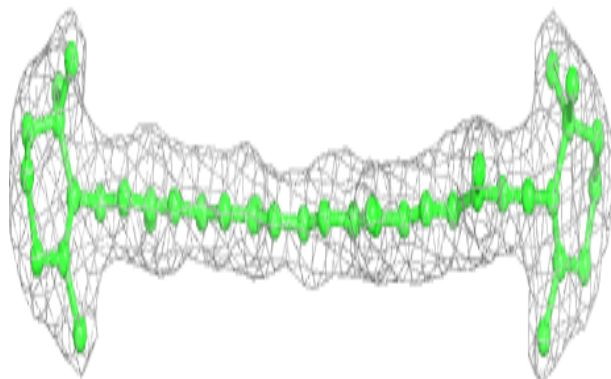
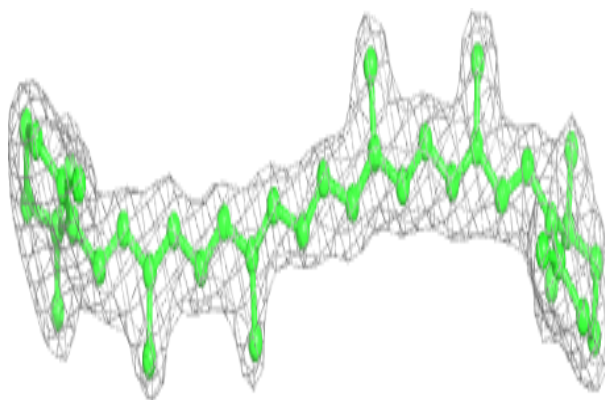


**Electron density around SQD F 101:**

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

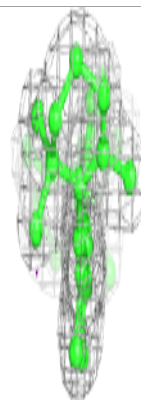
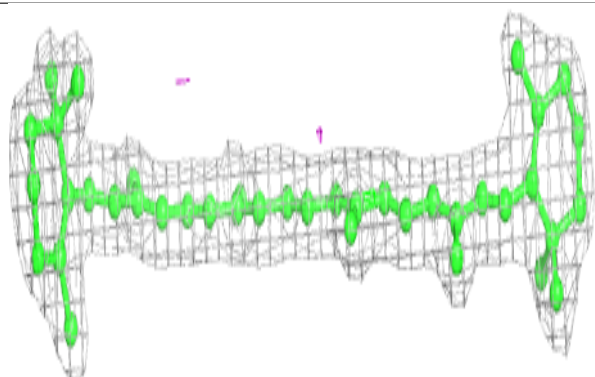
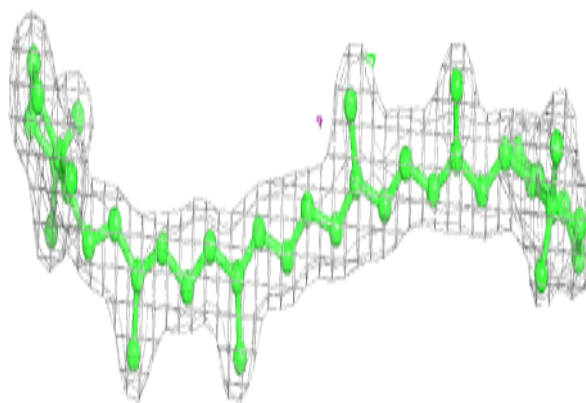
**Electron density around BCR C 514:**

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

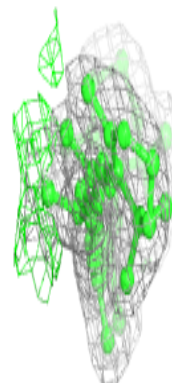
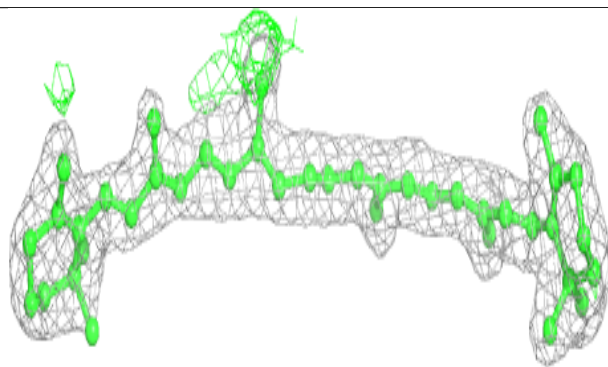
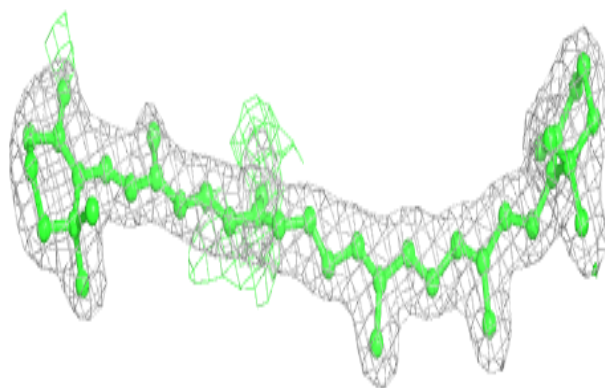


**Electron density around BCR C 515:**

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

**Electron density around BCR T 101:**

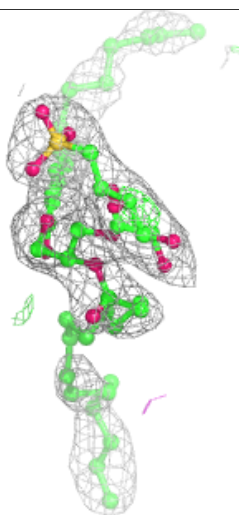
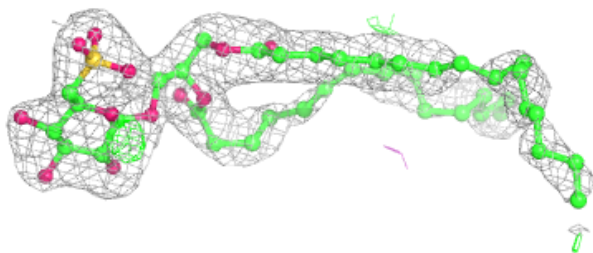
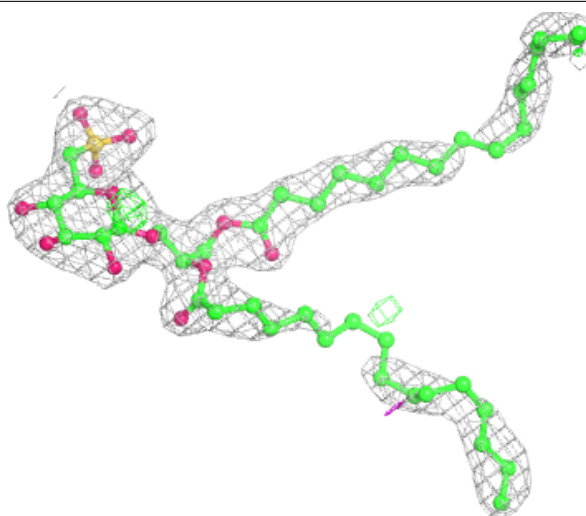
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





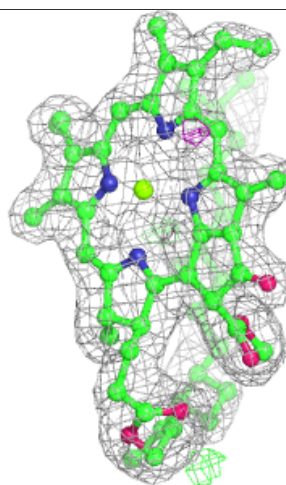
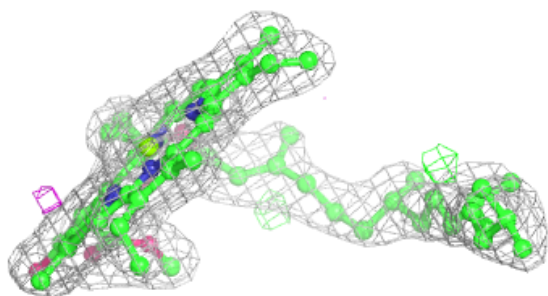
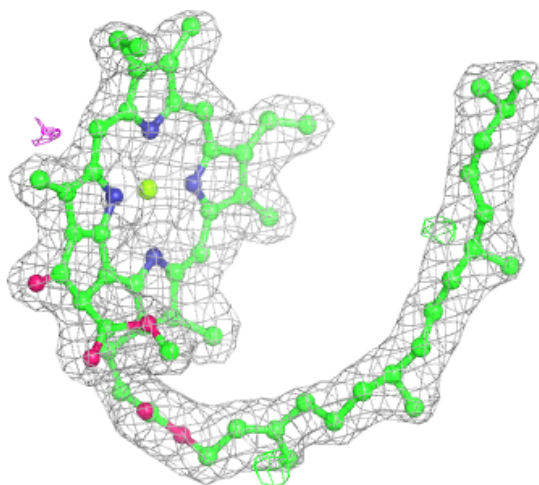
**Electron density around SQD a 415:**

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



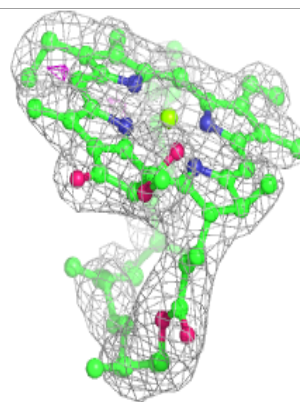
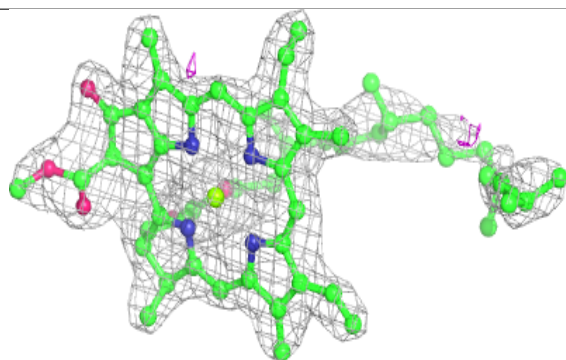
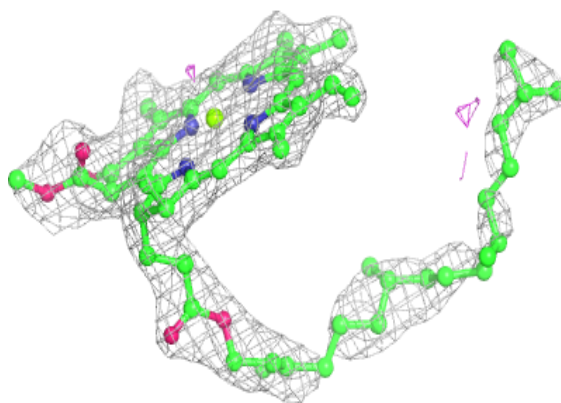
**Electron density around CLA C 507:**

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



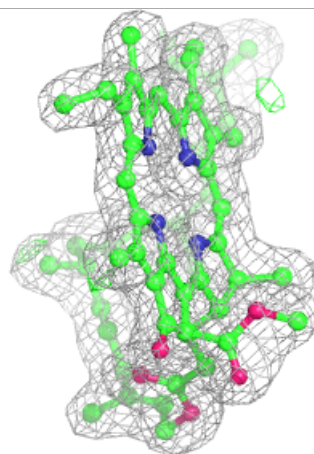
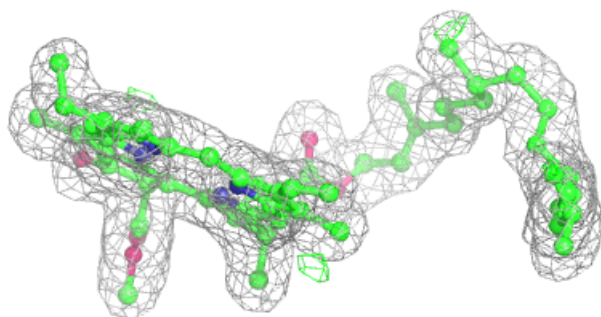
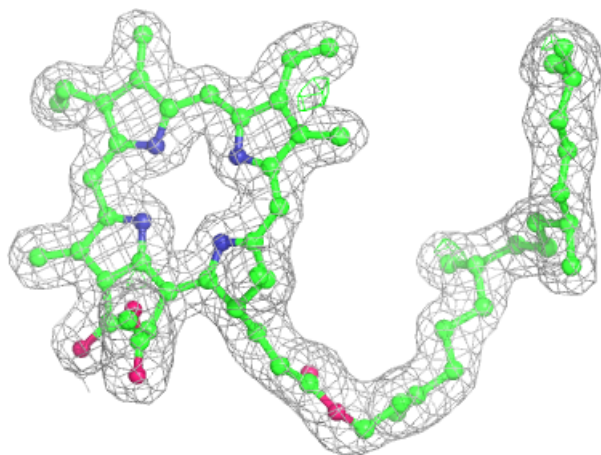
**Electron density around CLA c 914:**

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



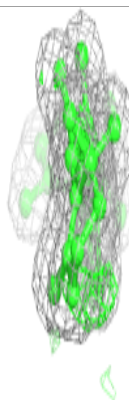
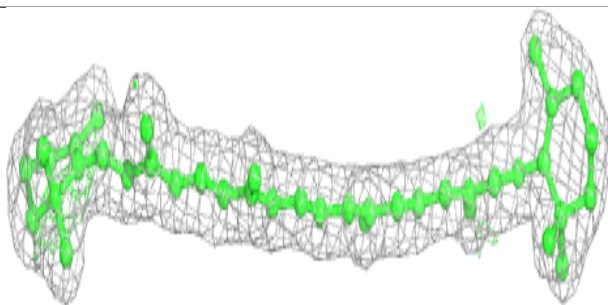
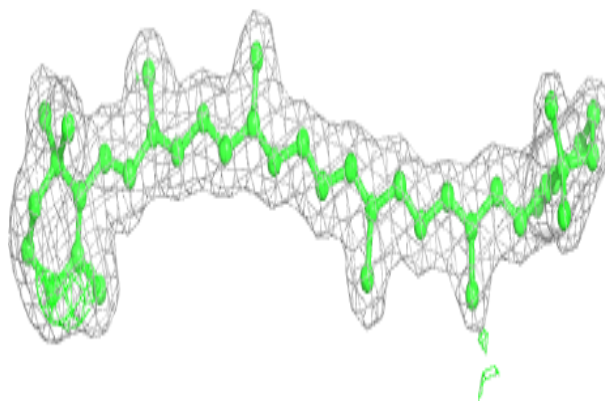
**Electron density around PHO A 409:**

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

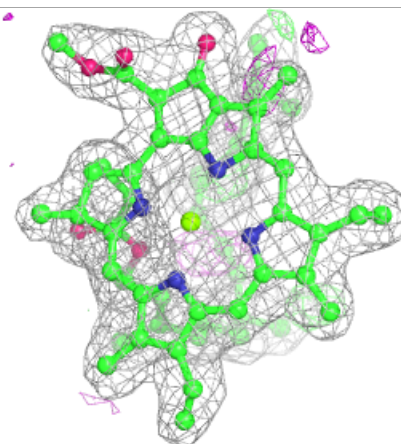
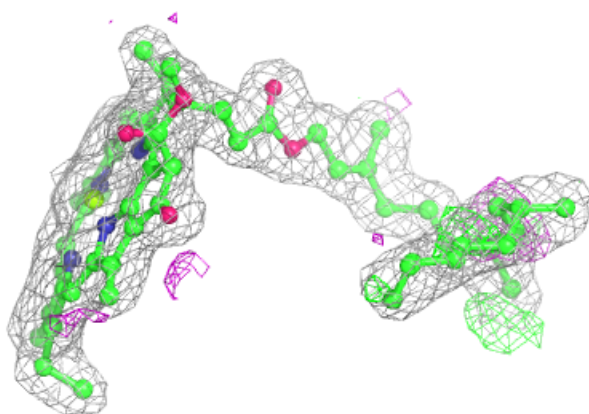
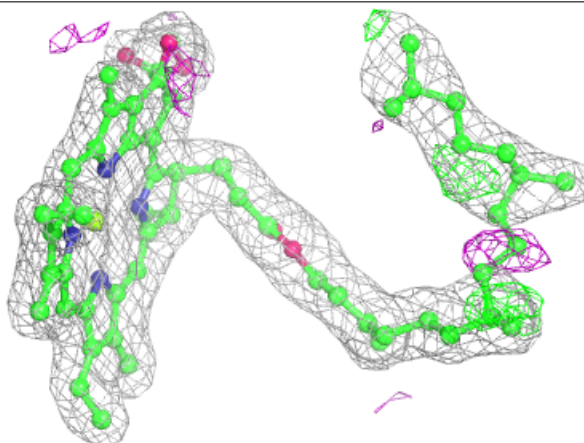


**Electron density around BCR B 618:**

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

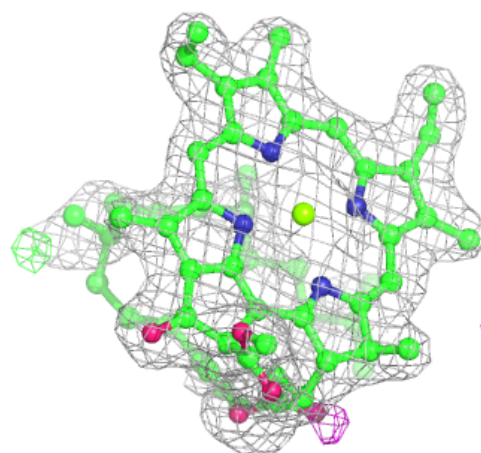
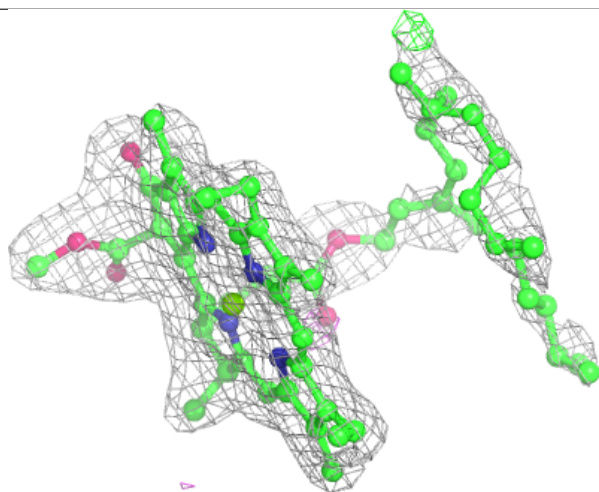
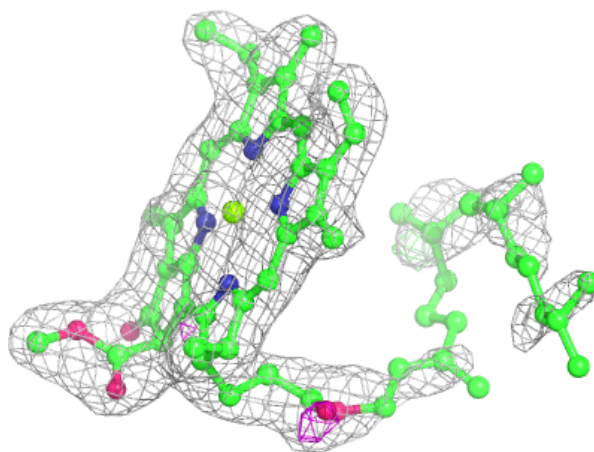
**Electron density around CLA B 607:**

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



**Electron density around CLA B 602:**

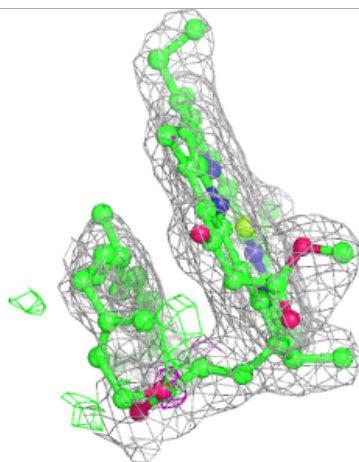
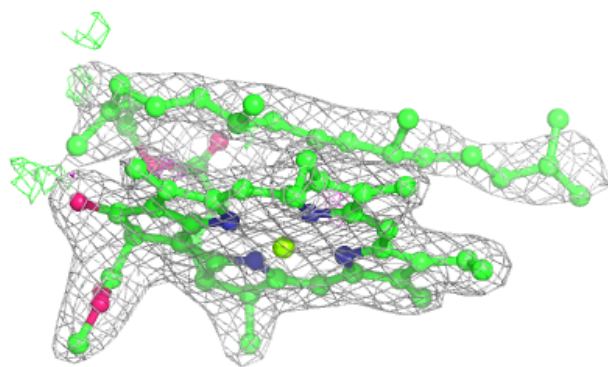
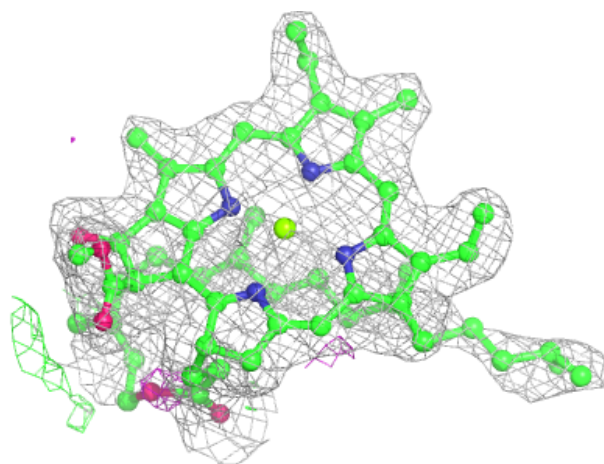
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





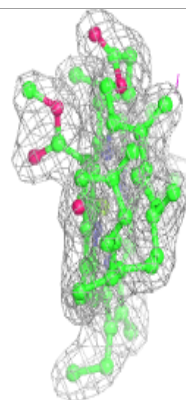
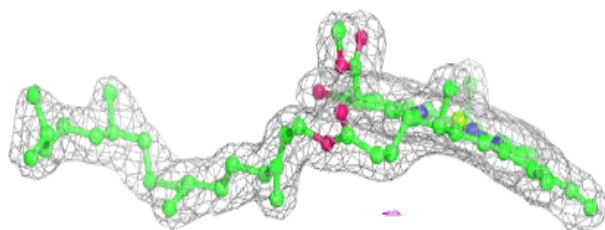
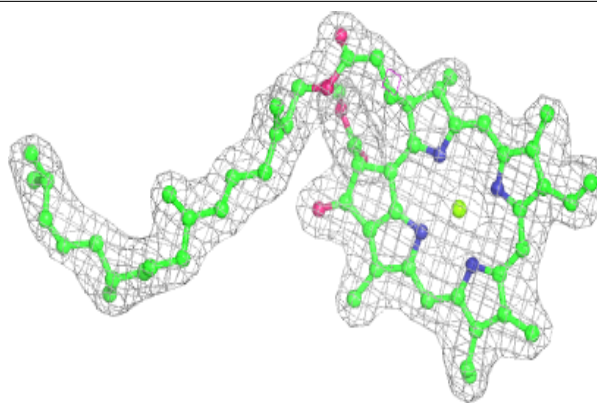
**Electron density around CLA b 605:**

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

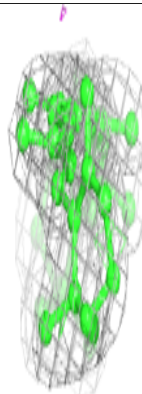
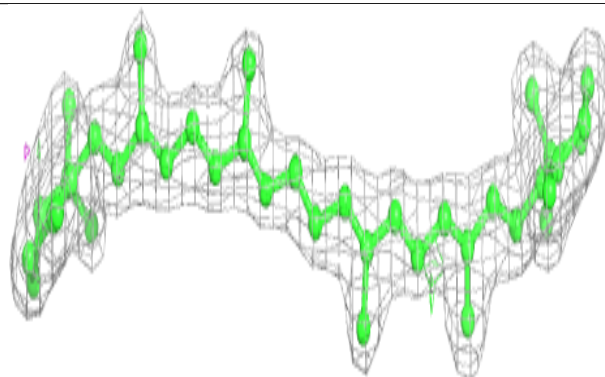
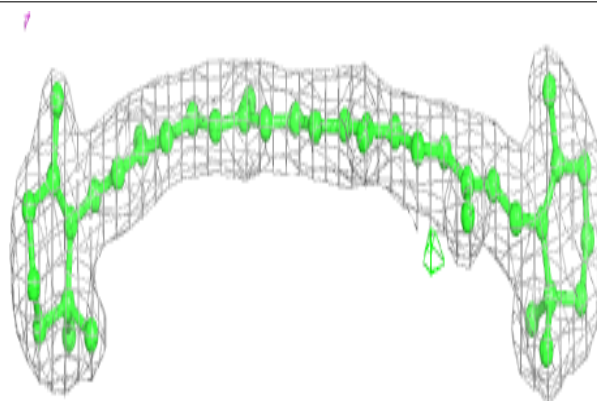


**Electron density around CLA b 606:**

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

**Electron density around BCR K 101:**

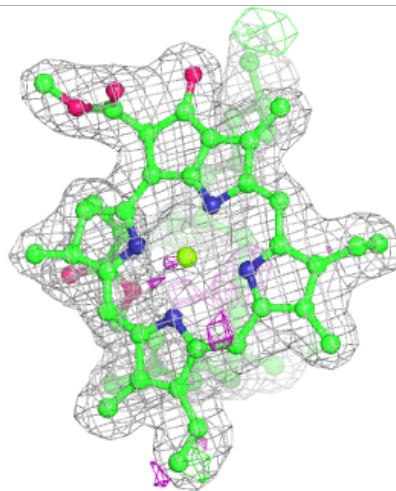
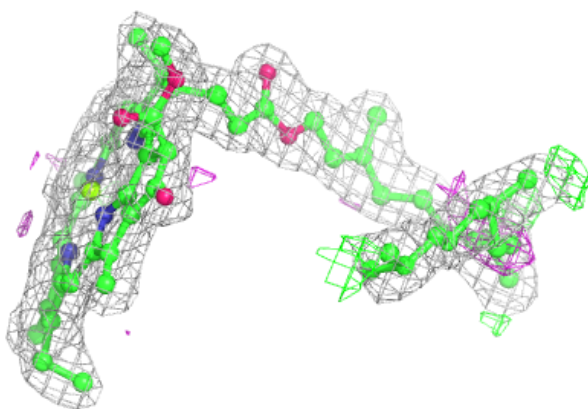
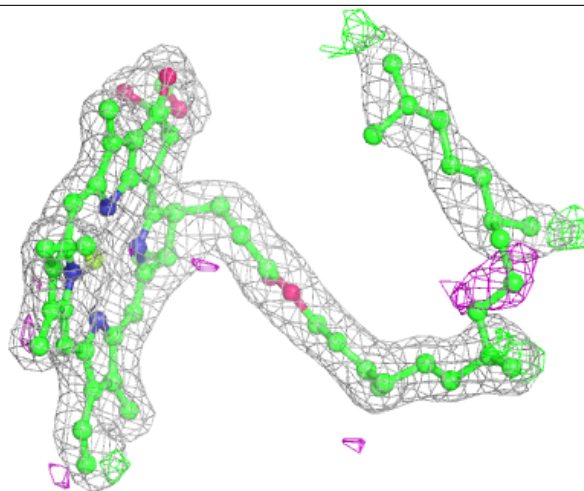
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





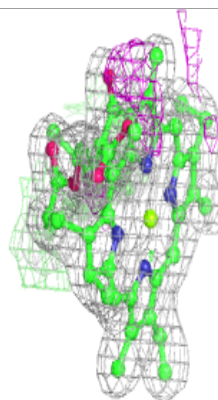
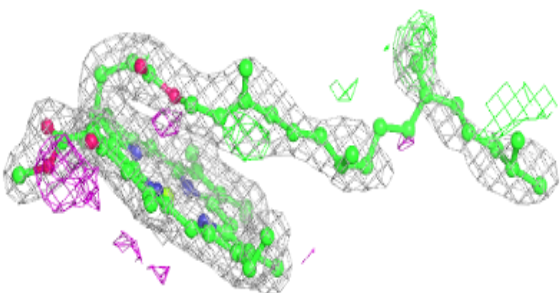
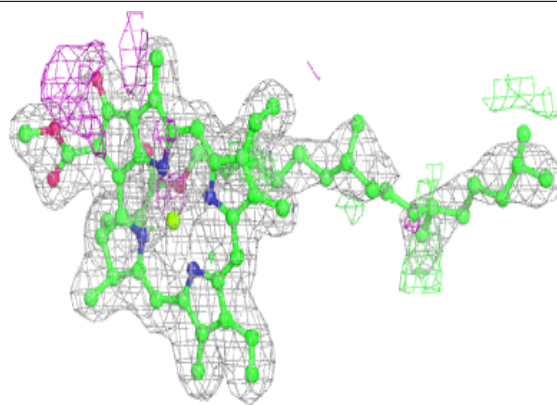
**Electron density around CLA b 610:**

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

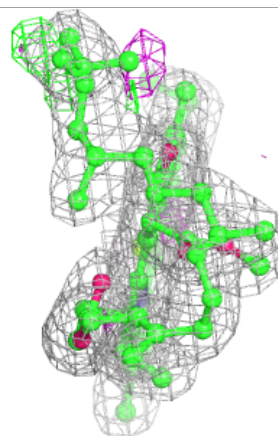
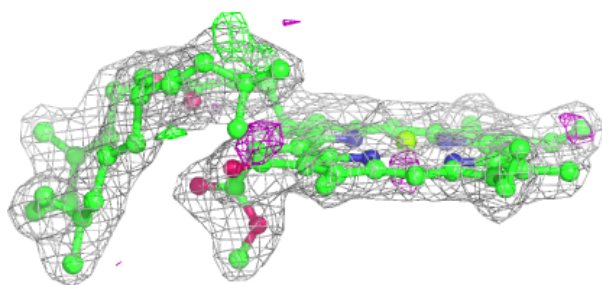
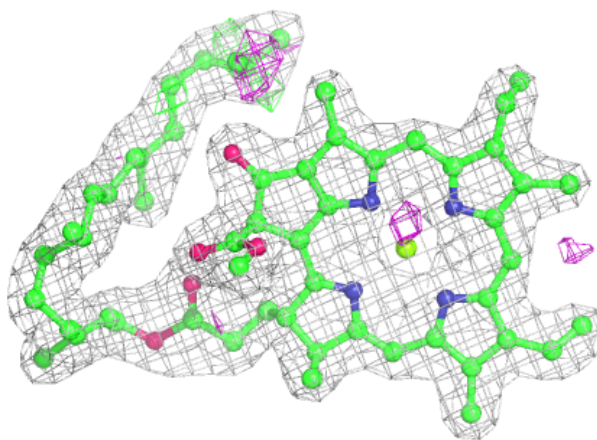


**Electron density around CLA B 615:**

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

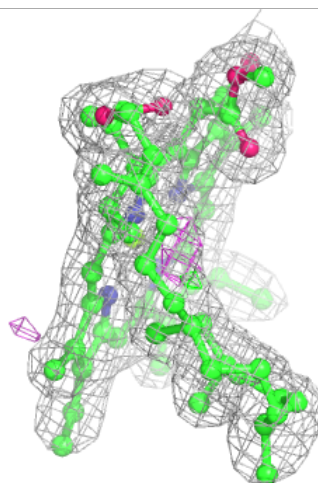
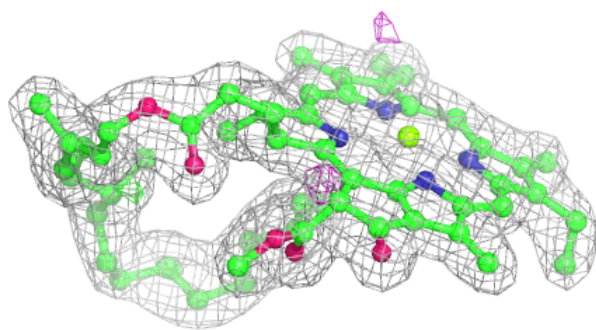
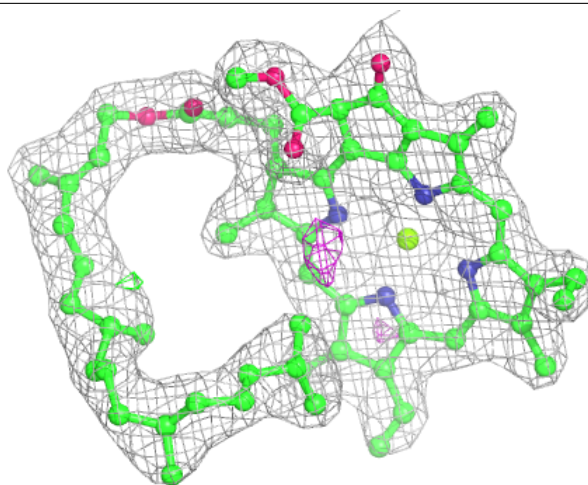
**Electron density around CLA b 614:**

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



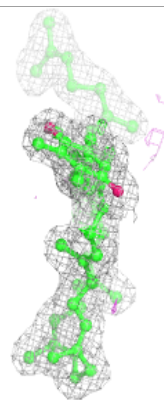
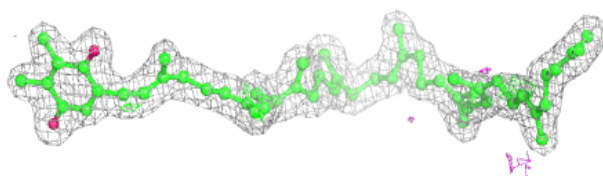
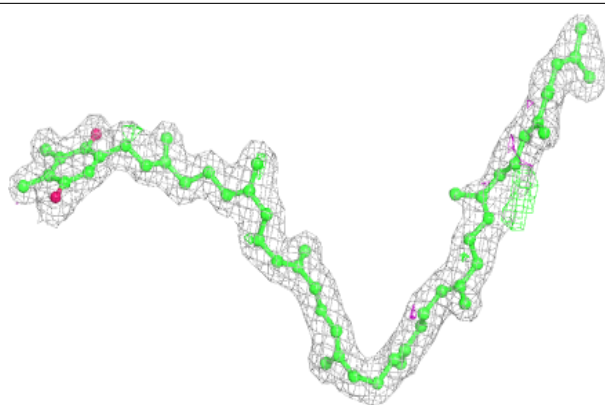
**Electron density around CLA b 619:**

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

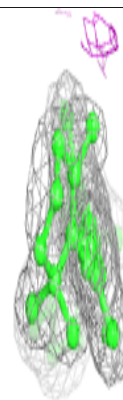
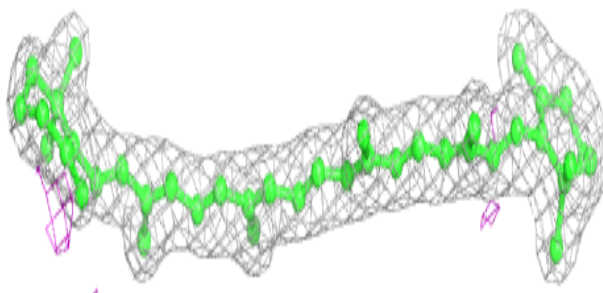
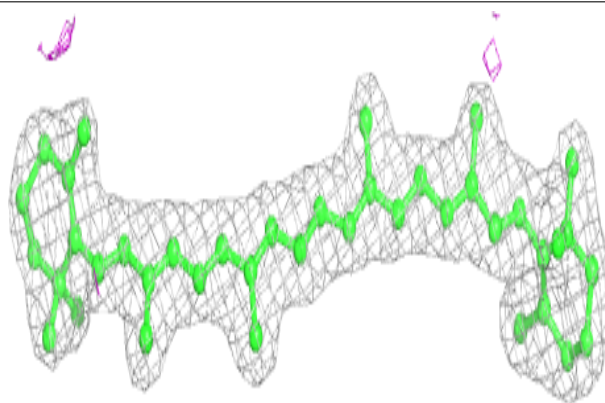


**Electron density around PL9 d 407:**

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

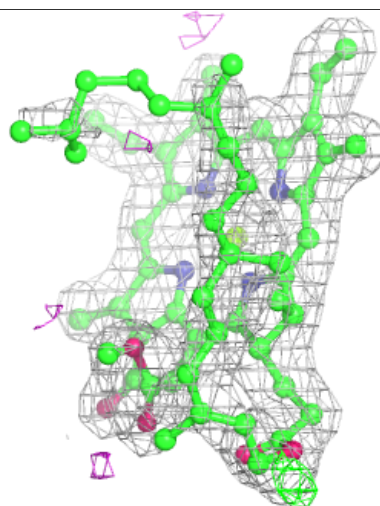
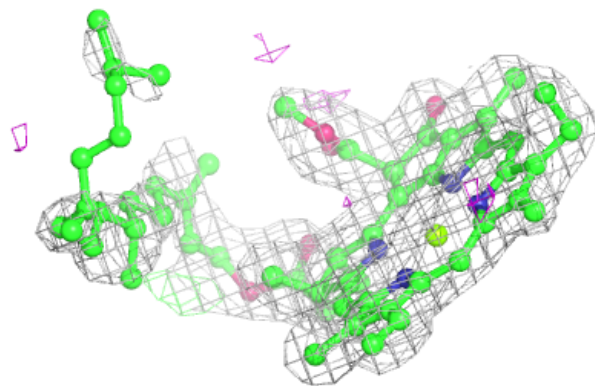
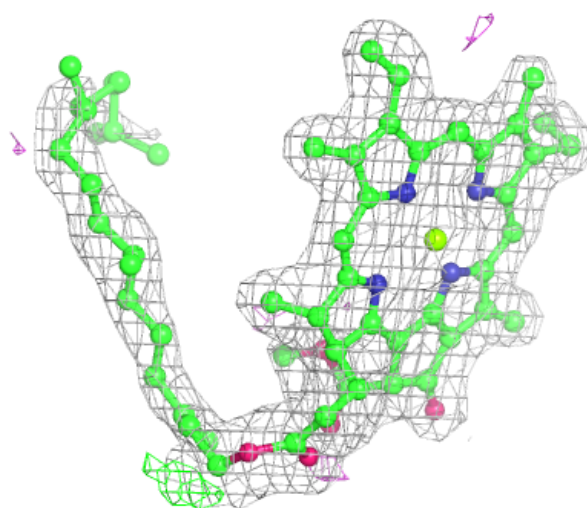
**Electron density around BCR b 623:**

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



**Electron density around CLA b 620:**

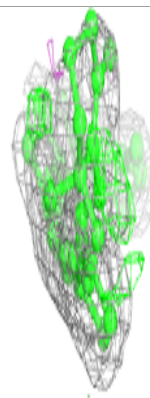
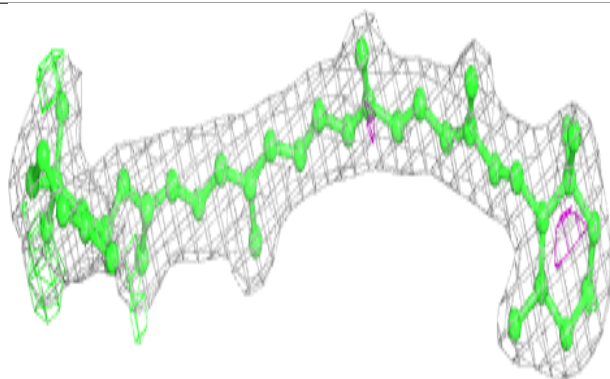
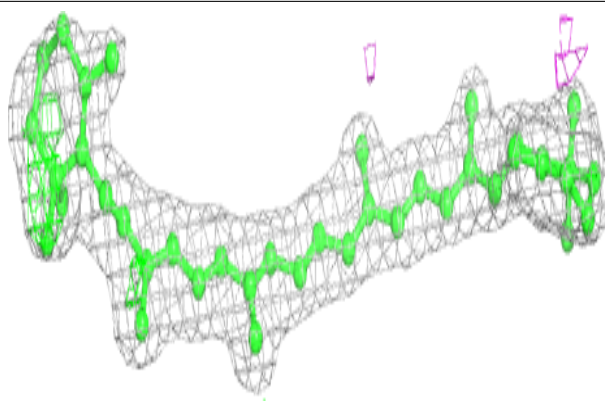
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



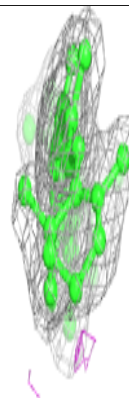
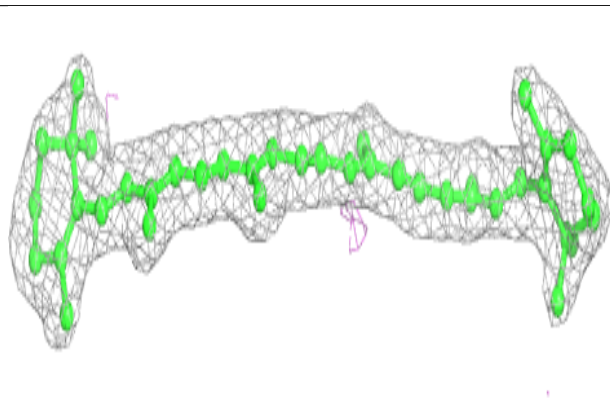
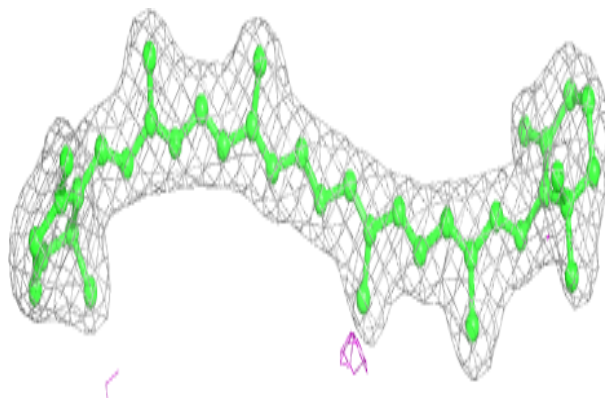


**Electron density around BCR d 406:**

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

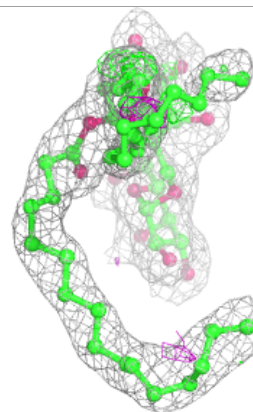
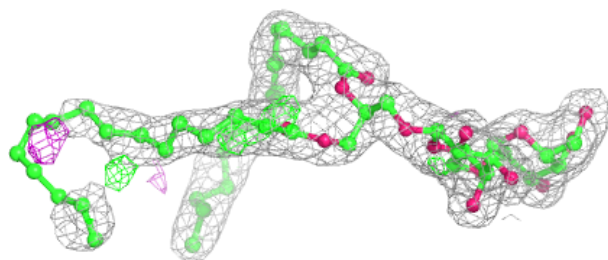
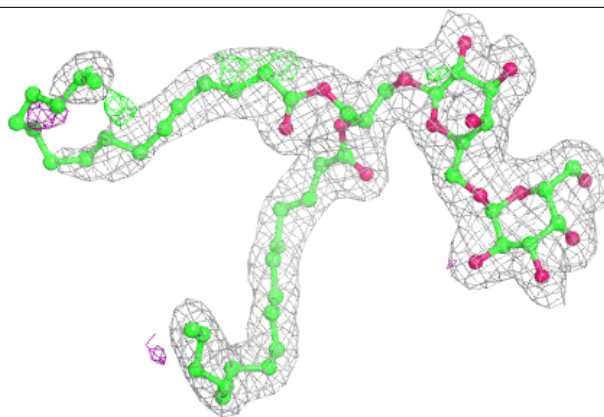
**Electron density around BCR k 102:**

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

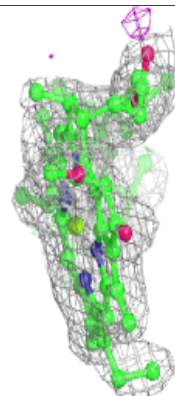
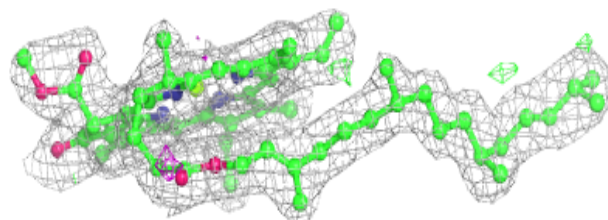
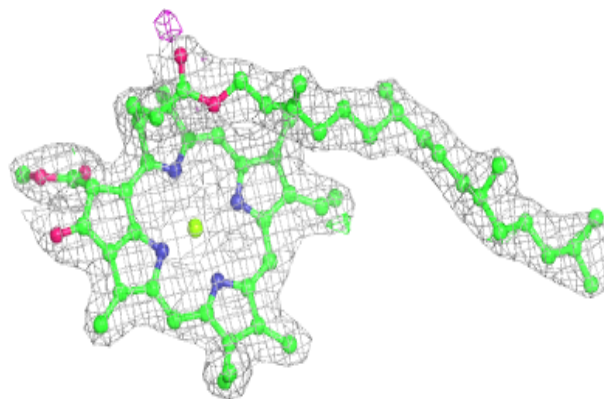


**Electron density around DGD c 918:**

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

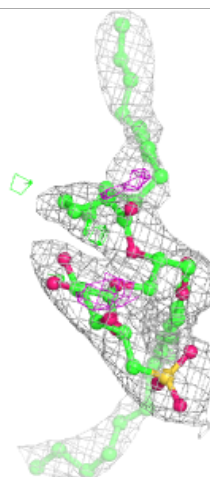
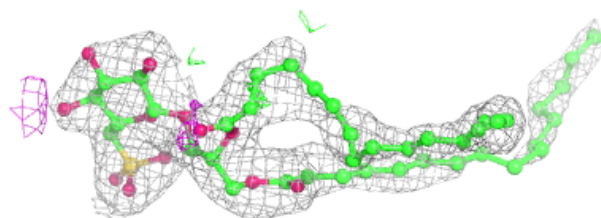
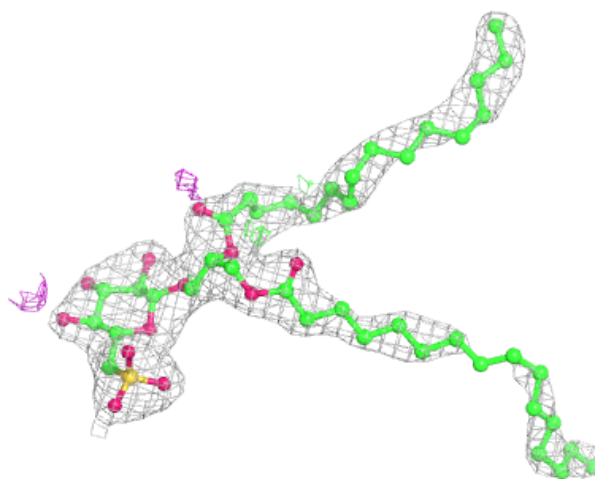
**Electron density around CLA c 902:**

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



**Electron density around SQD A 412:**

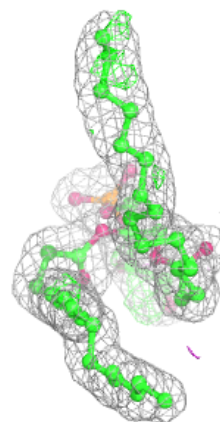
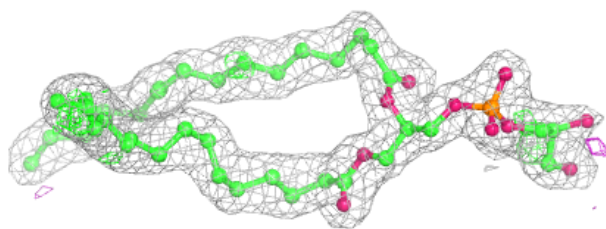
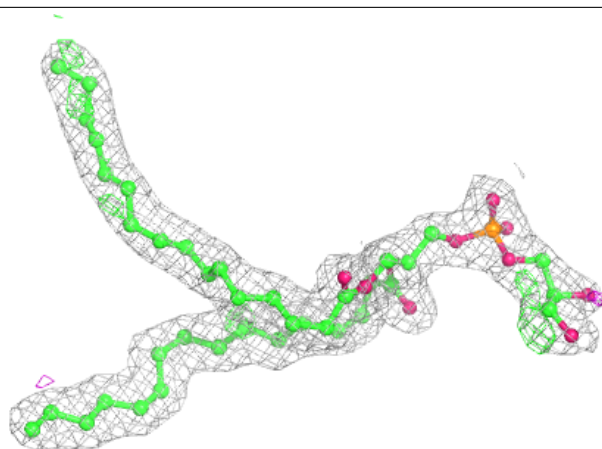
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





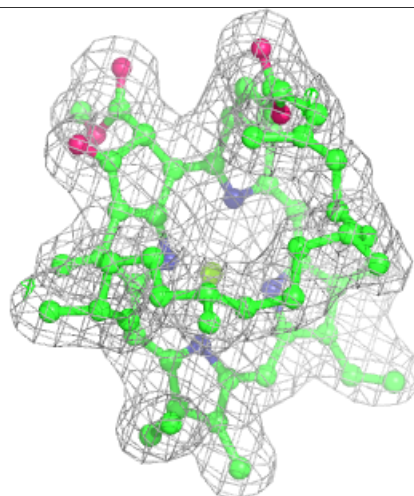
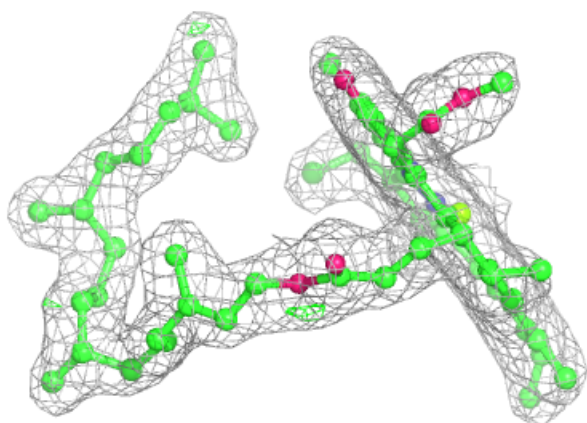
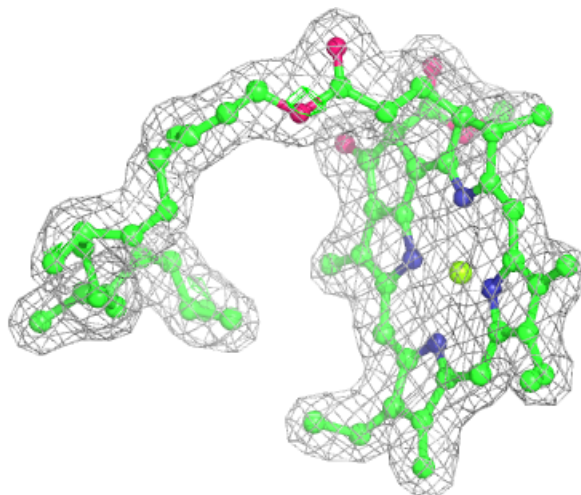
**Electron density around LHG d 410:**

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



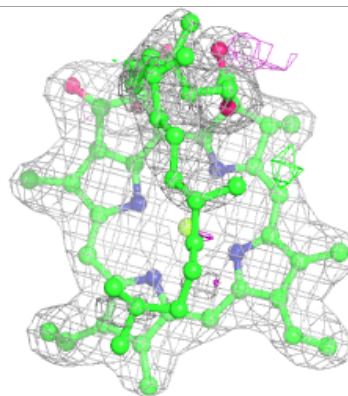
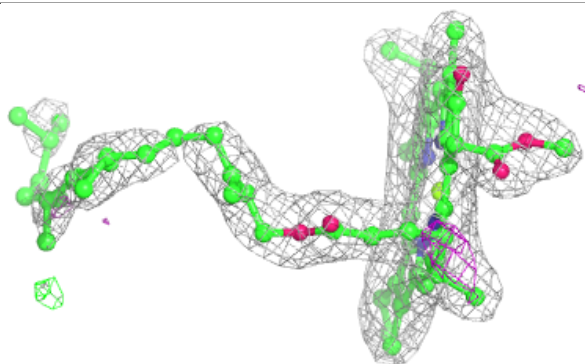
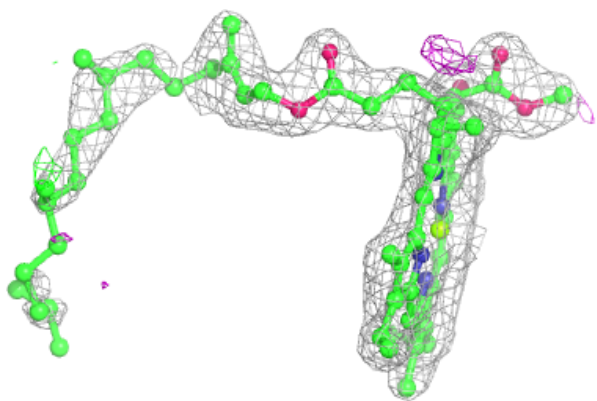
**Electron density around CLA C 503:**

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



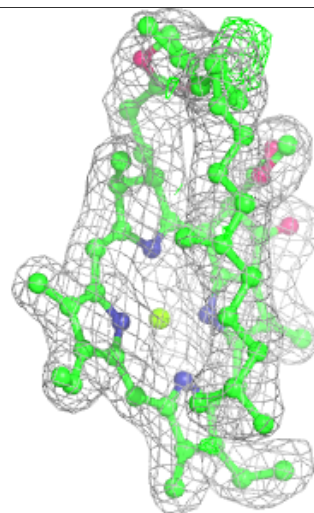
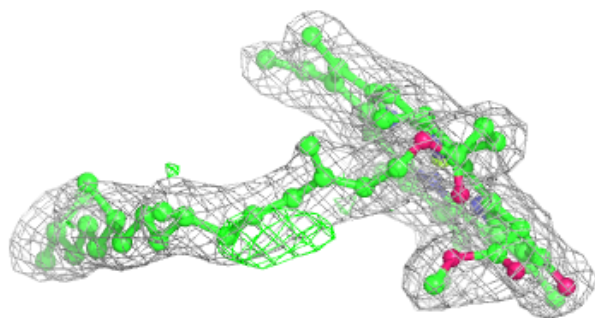
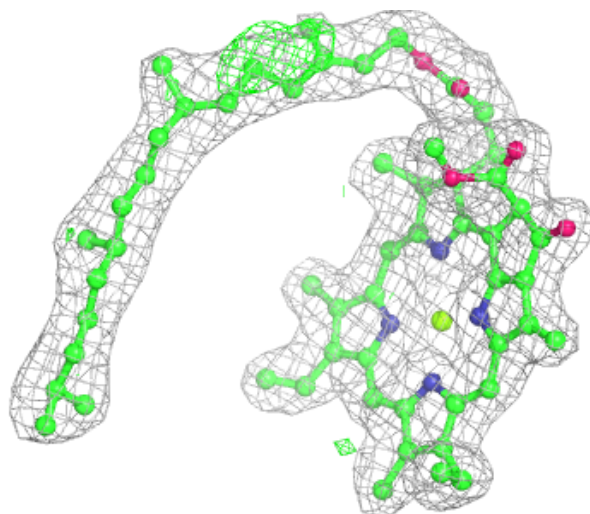
**Electron density around CLA C 506:**

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



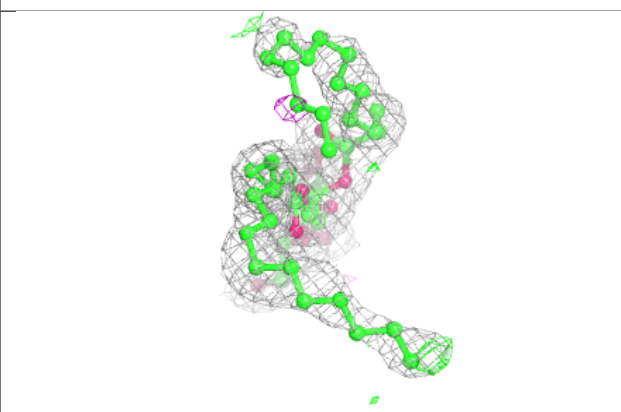
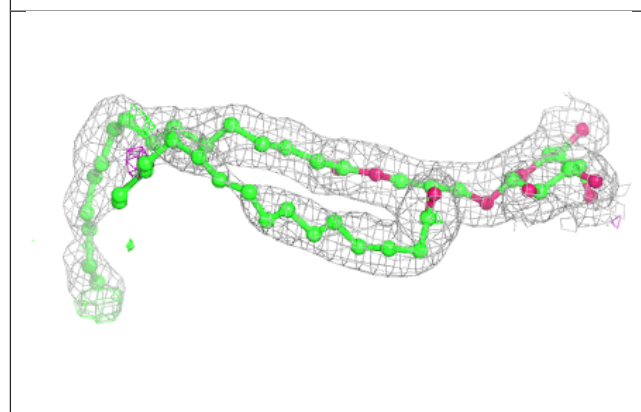
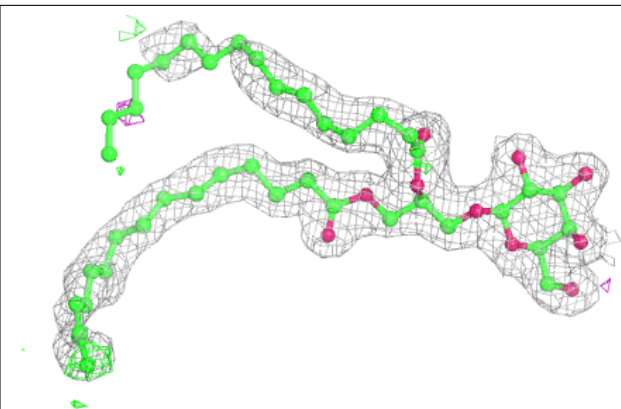
**Electron density around CLA c 908:**

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

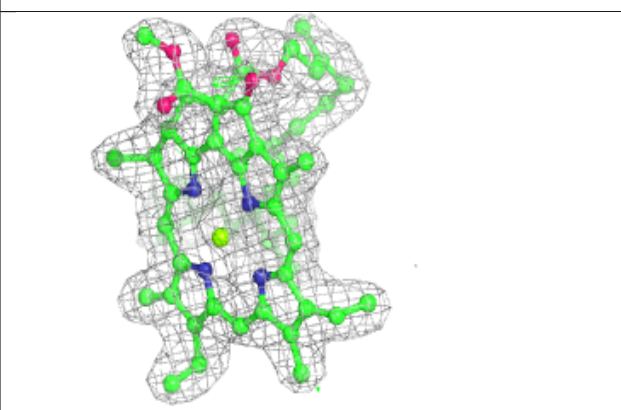
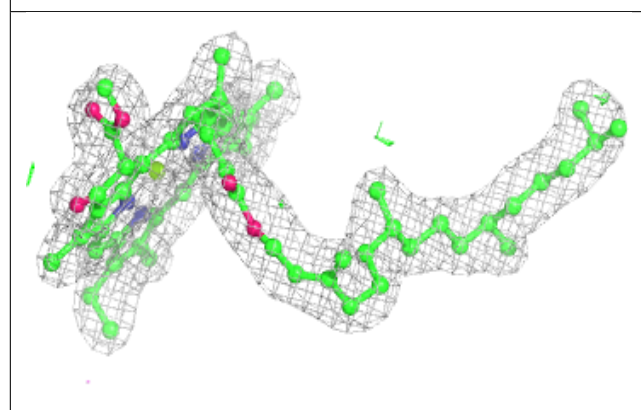
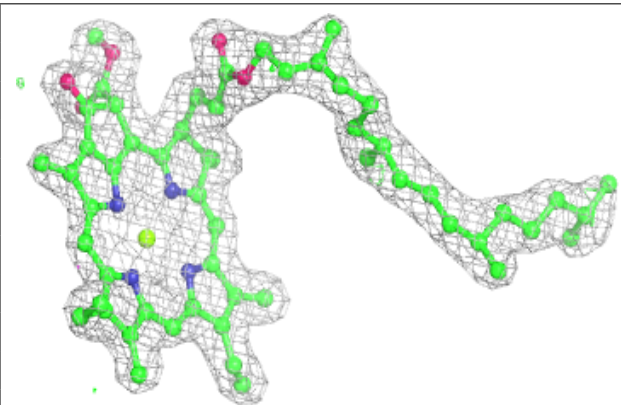


**Electron density around LMG D 409:**

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

**Electron density around CLA c 912:**

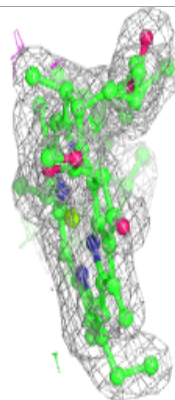
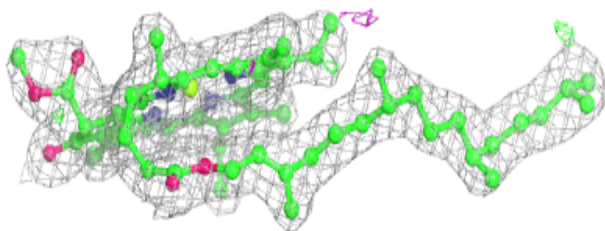
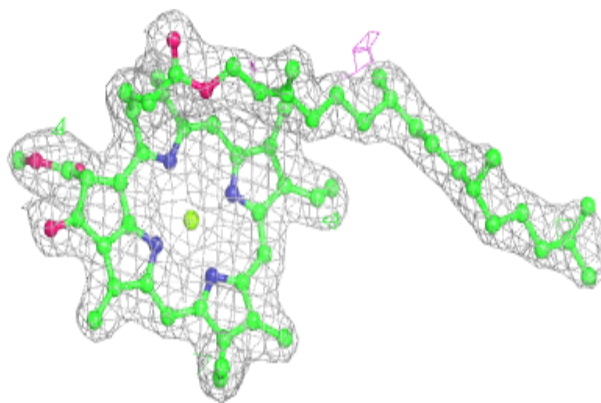
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



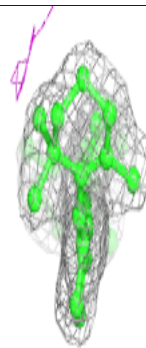
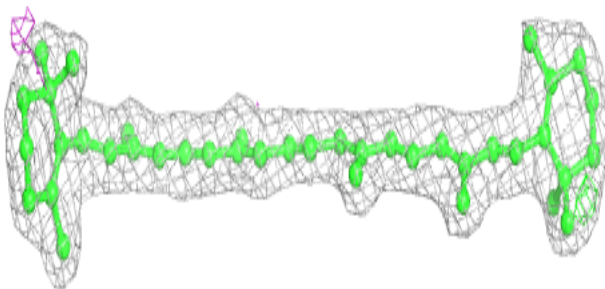
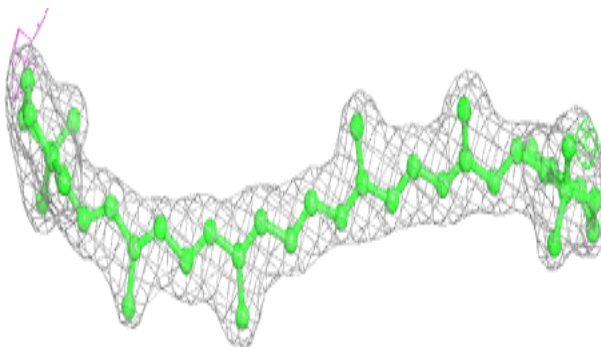


**Electron density around CLA C 501:**

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

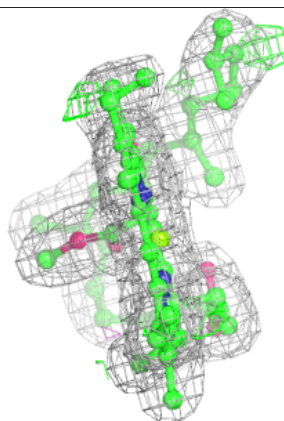
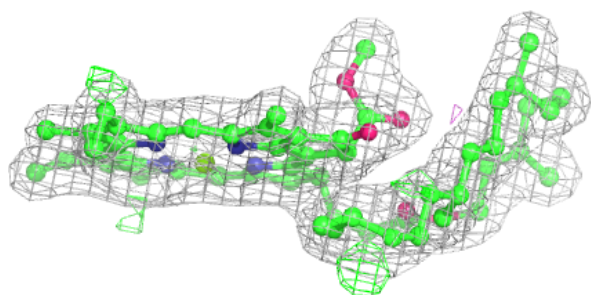
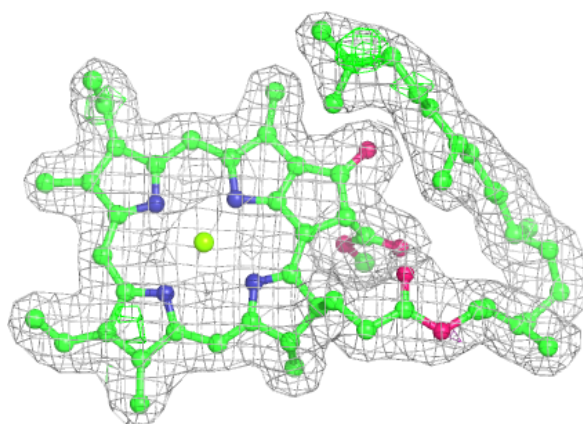
**Electron density around BCR c 916:**

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

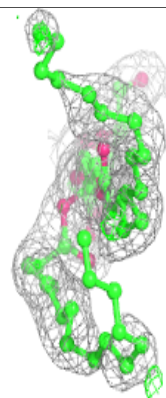
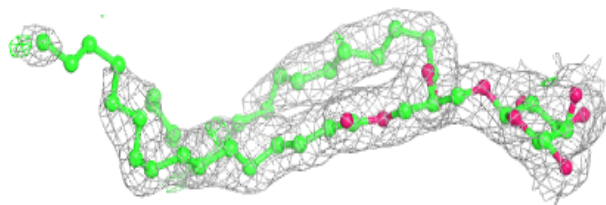
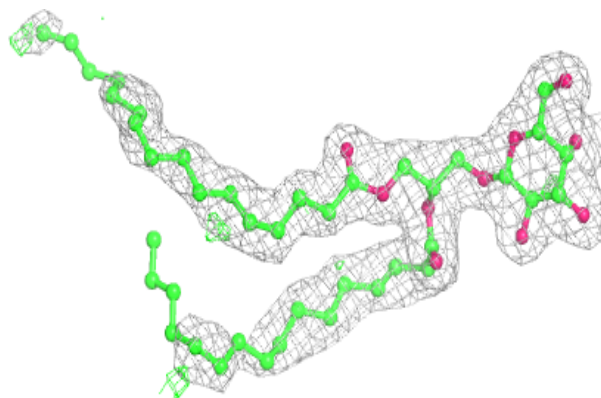


**Electron density around CLA B 611:**

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

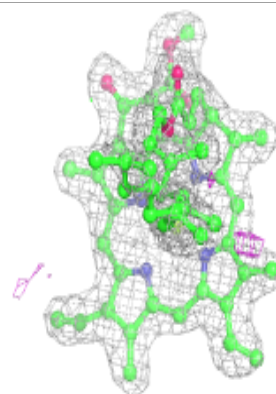
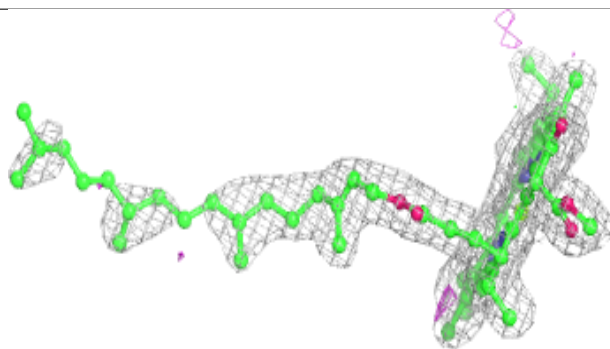
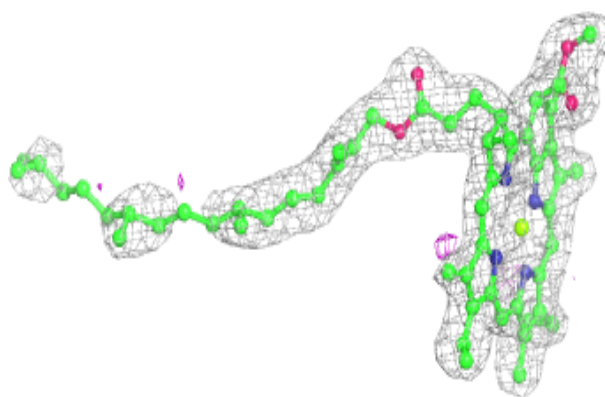
**Electron density around LMG d 412:**

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

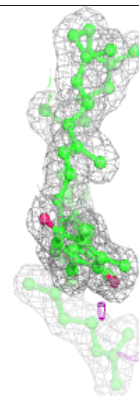
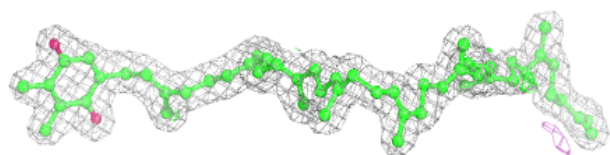
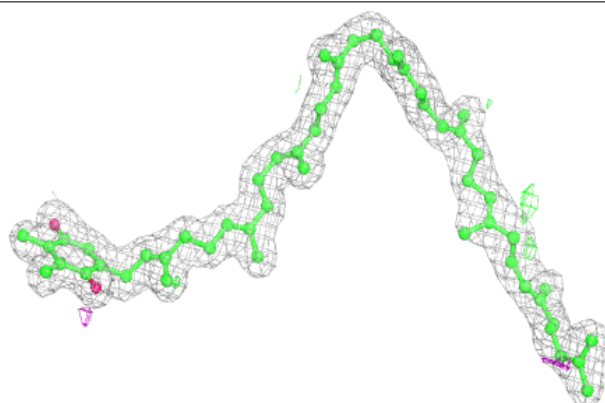


**Electron density around CLA d 405:**

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

**Electron density around PL9 D 404:**

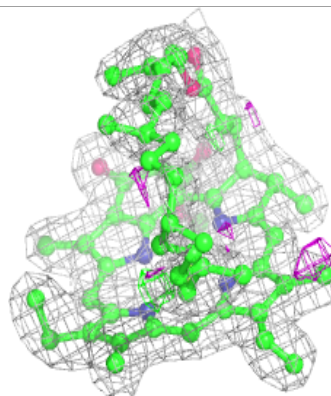
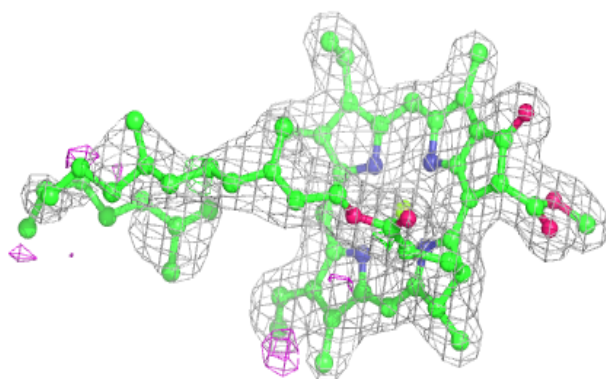
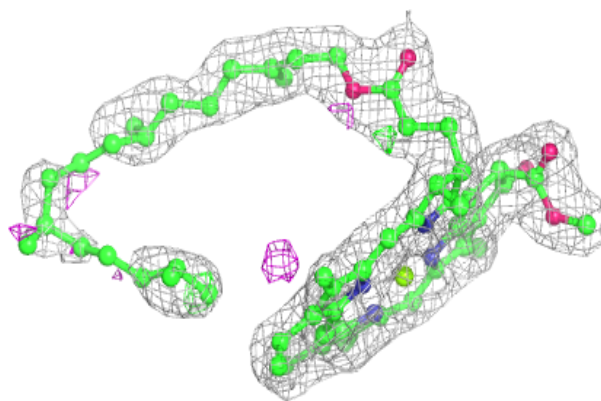
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





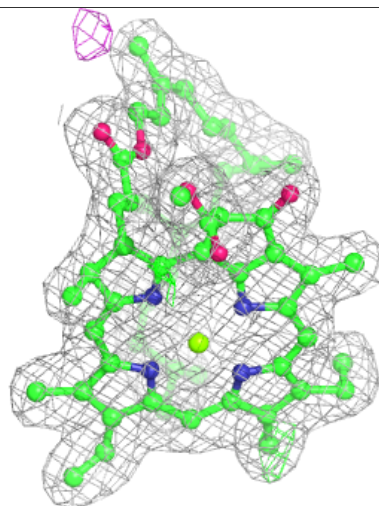
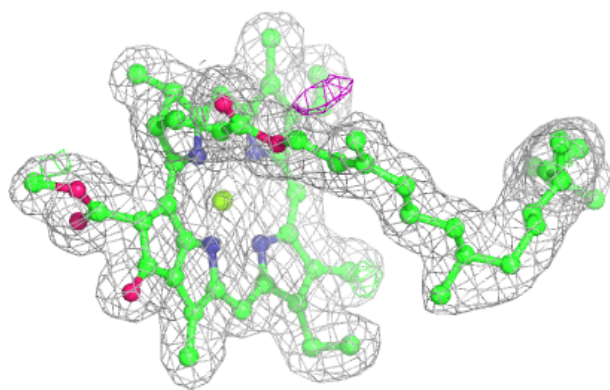
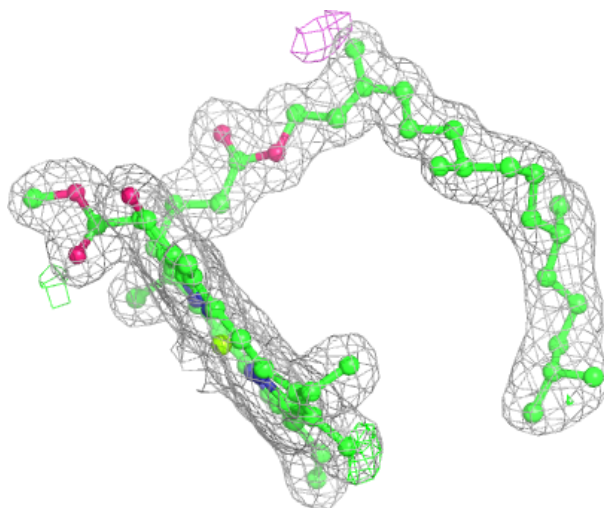
**Electron density around CLA C 504:**

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



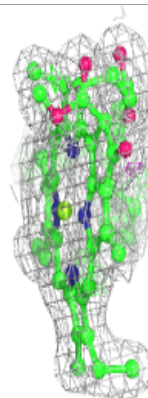
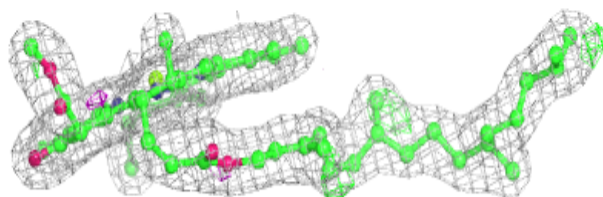
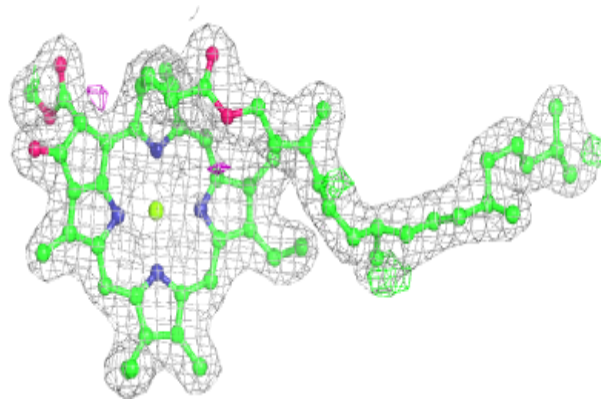
**Electron density around CLA B 612:**

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

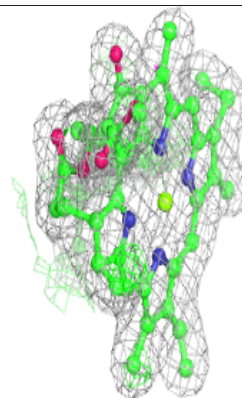
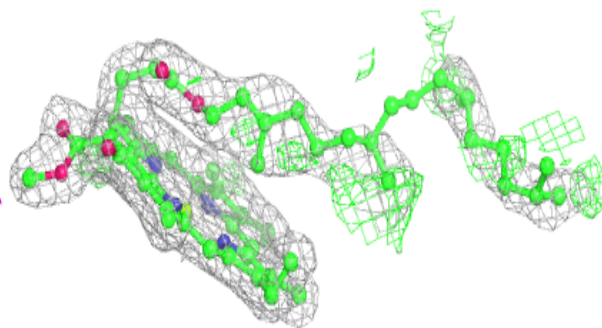
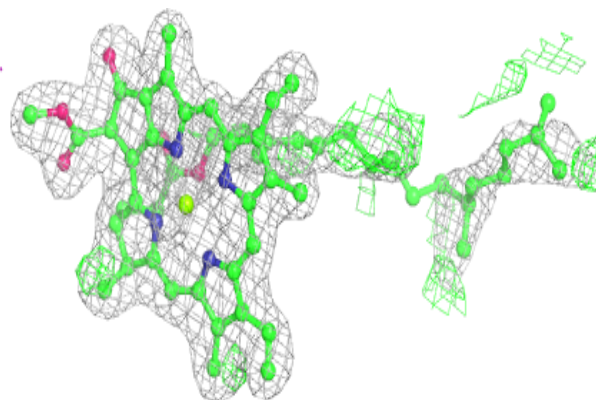


**Electron density around CLA B 604:**

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

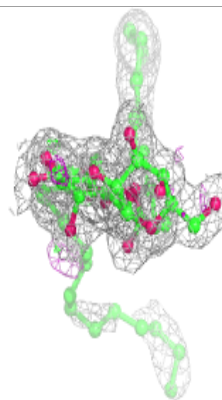
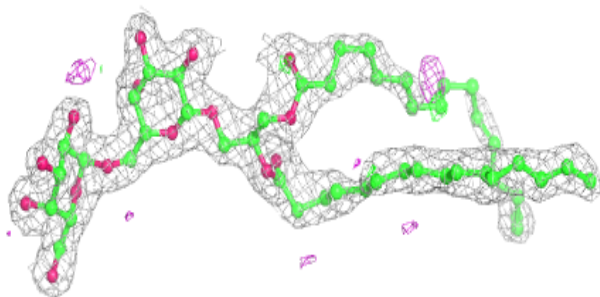
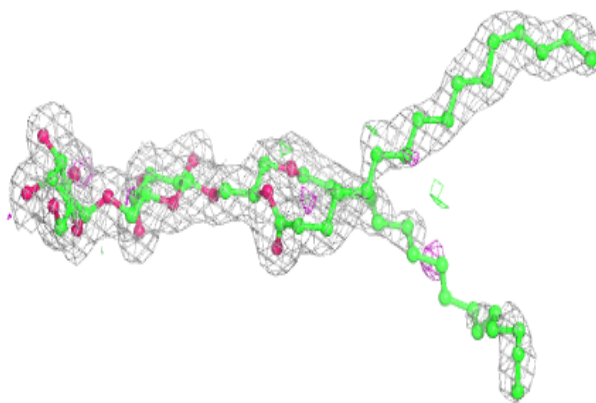
**Electron density around CLA b 618:**

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

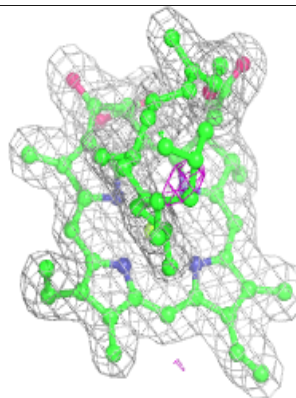
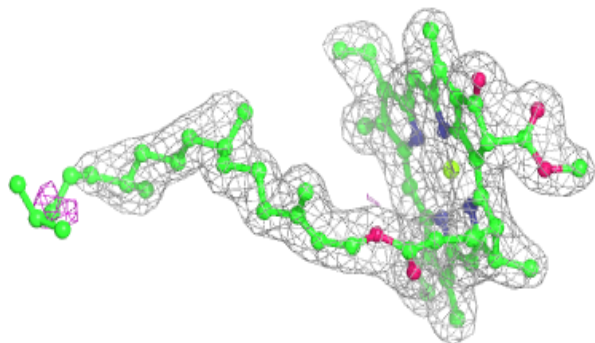
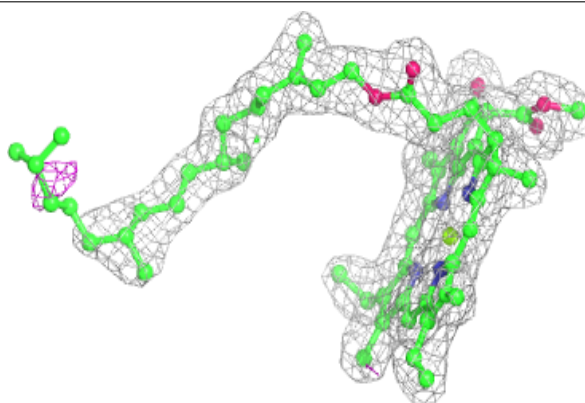


**Electron density around DGD c 917:**

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

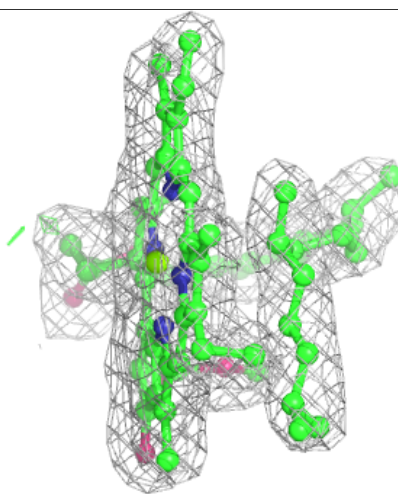
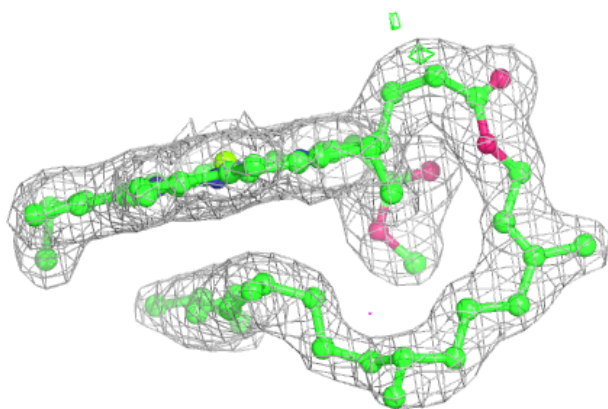
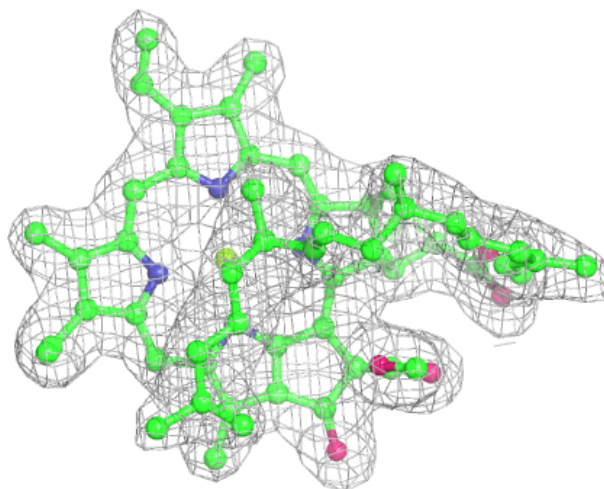
**Electron density around CLA C 508:**

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



**Electron density around CLA C 510:**

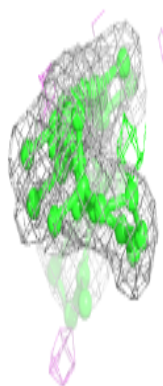
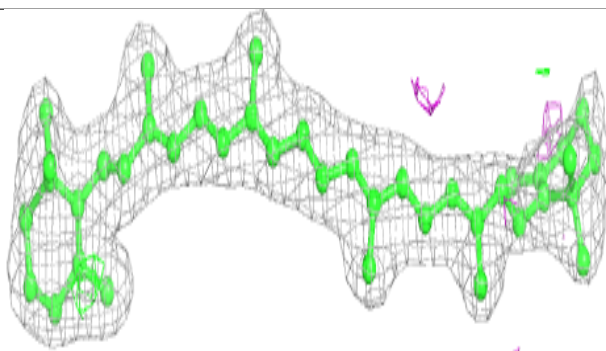
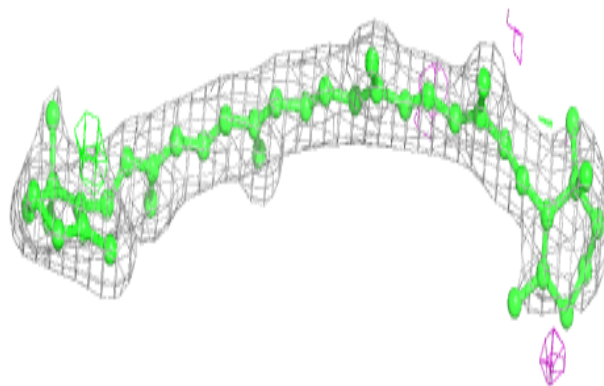
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



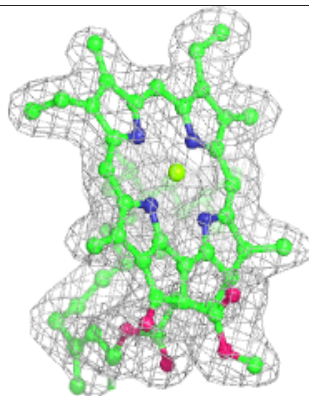
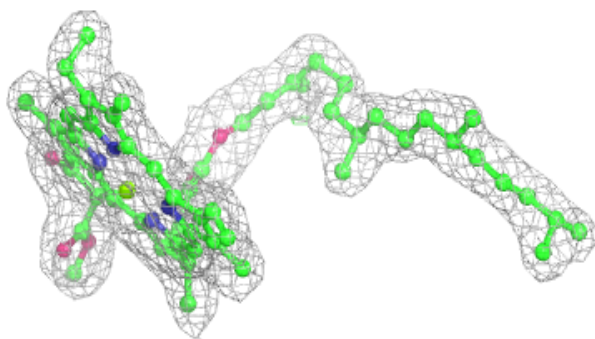
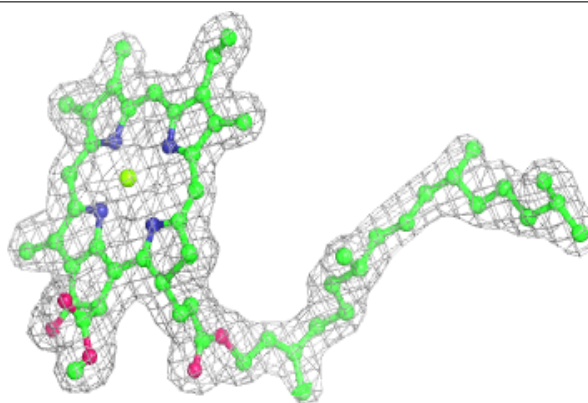


**Electron density around BCR D 403:**

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

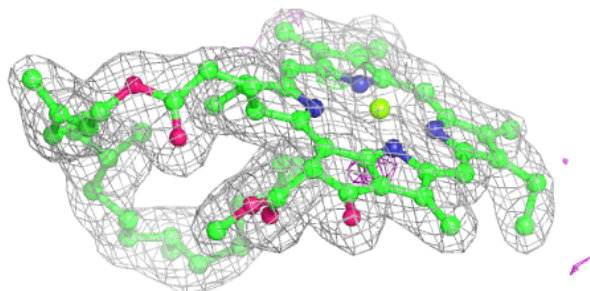
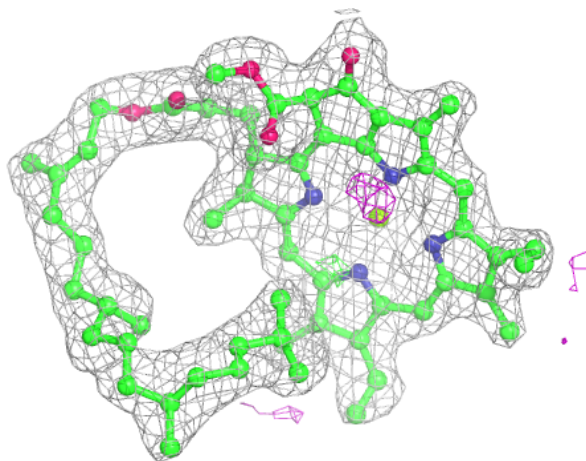
**Electron density around CLA C 511:**

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



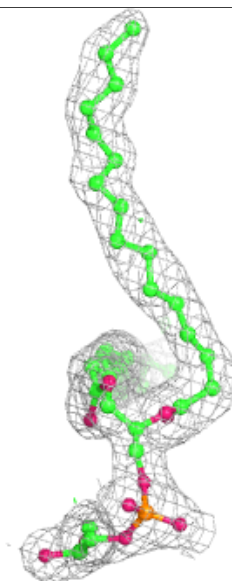
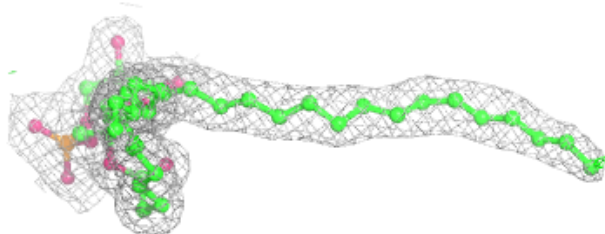
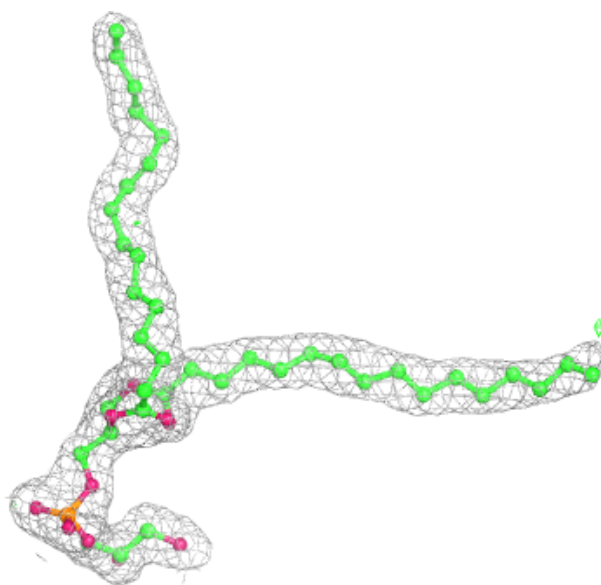
**Electron density around CLA B 616:**

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



**Electron density around LHG L 101:**

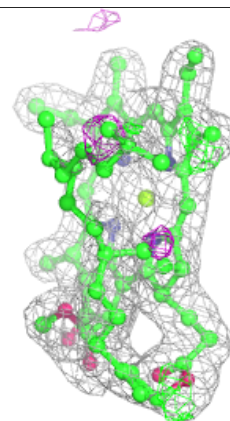
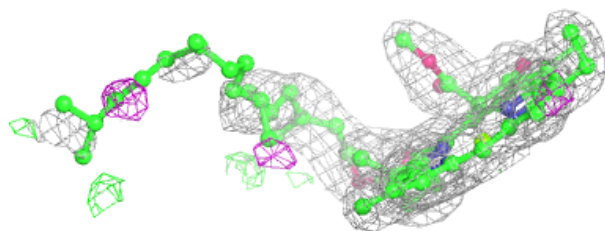
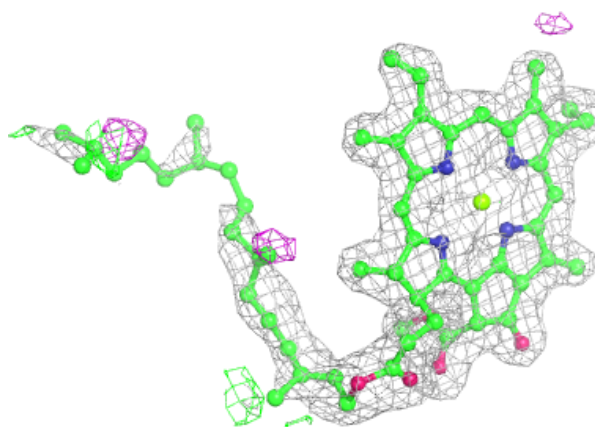
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



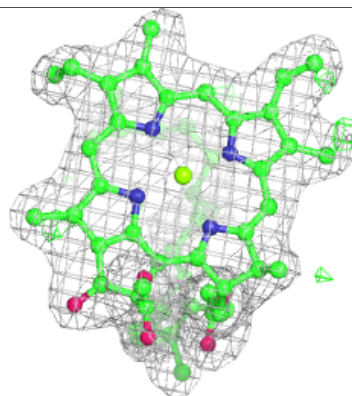
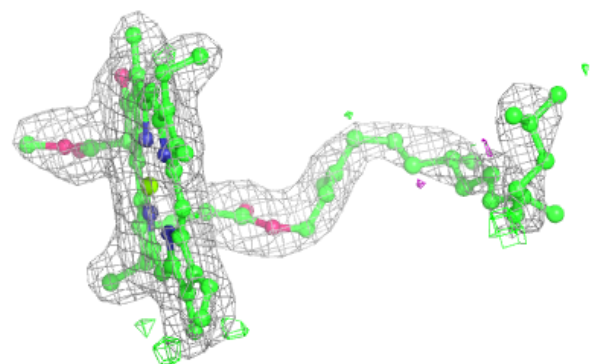
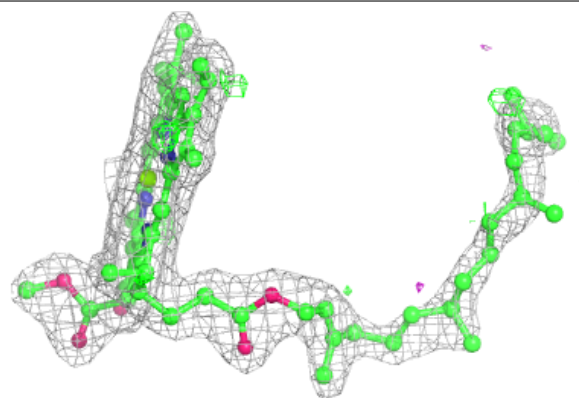


**Electron density around CLA B 617:**

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

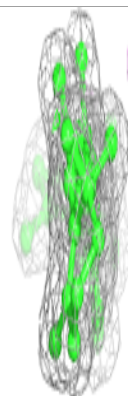
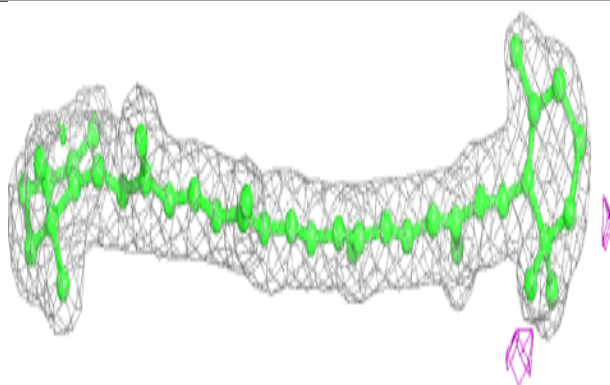
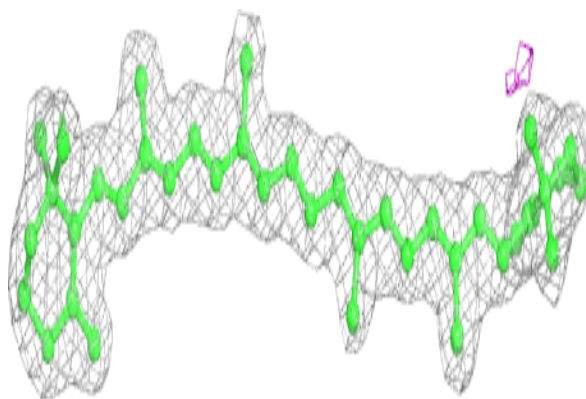
**Electron density around CLA c 907:**

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

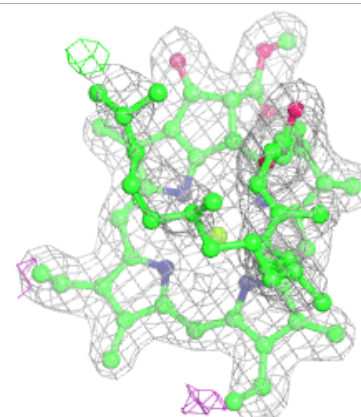
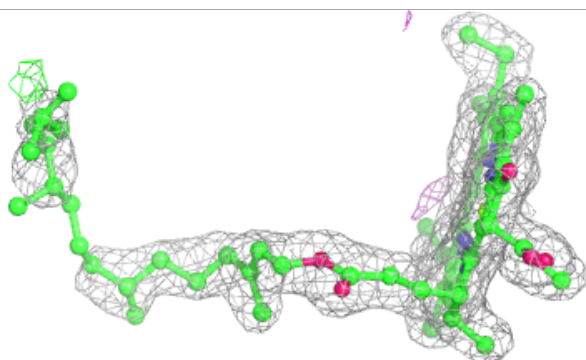
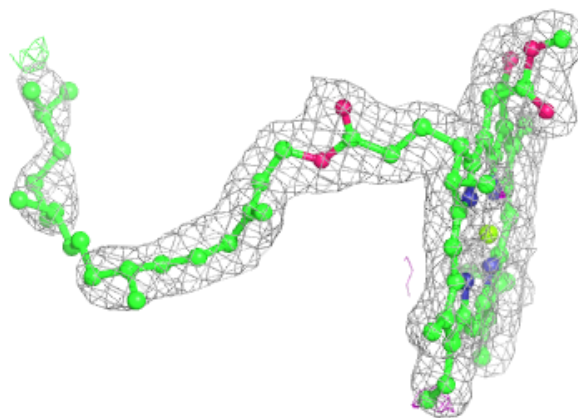


**Electron density around BCR b 621:**

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

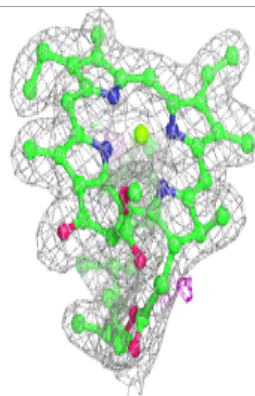
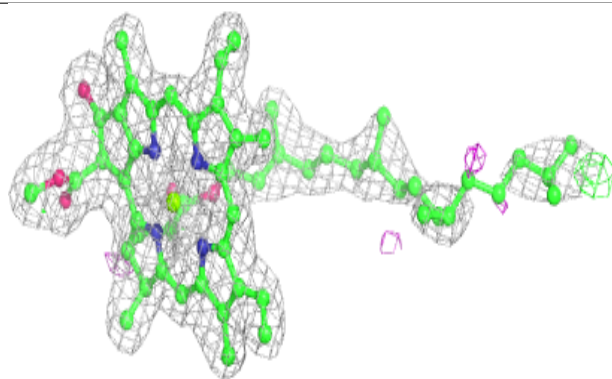
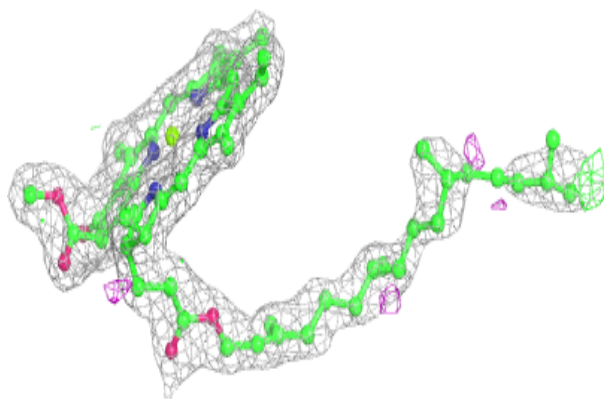
**Electron density around CLA D 402:**

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

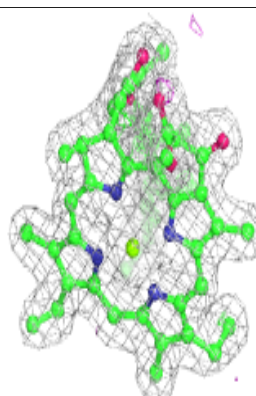
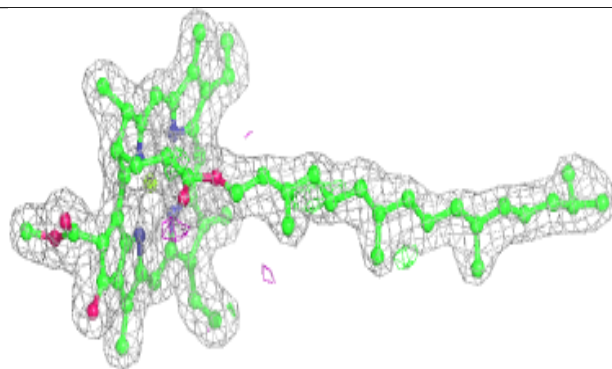
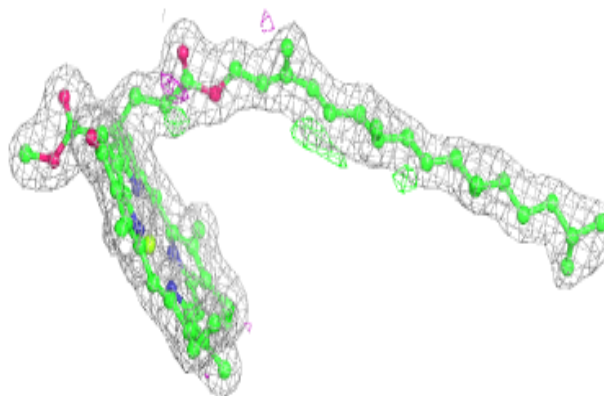


**Electron density around CLA c 905:**

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

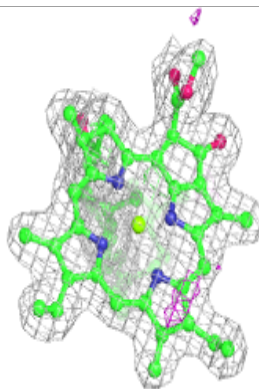
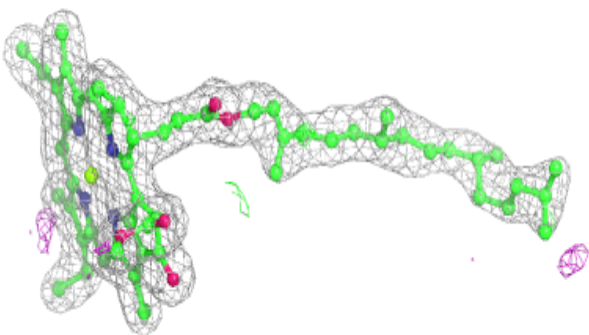
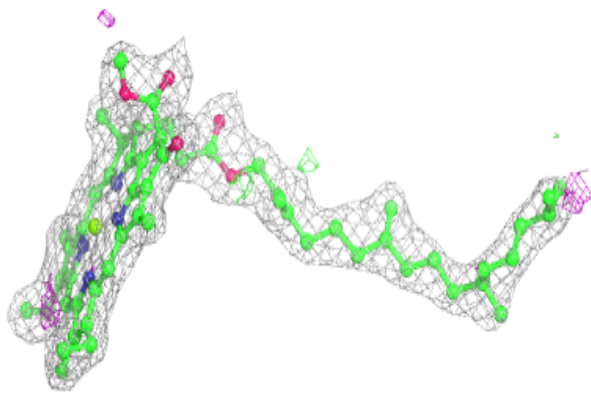
**Electron density around CLA b 611:**

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

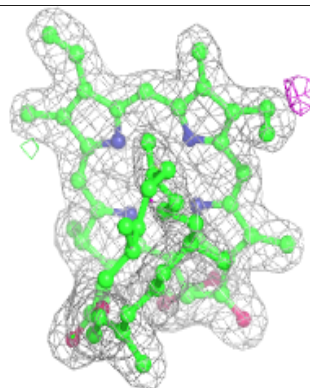
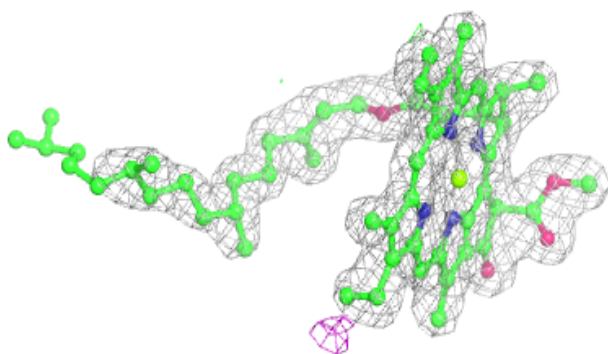
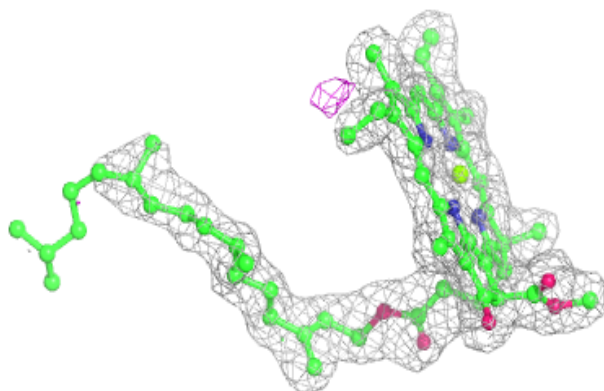


**Electron density around CLA B 605:**

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

**Electron density around CLA c 909:**

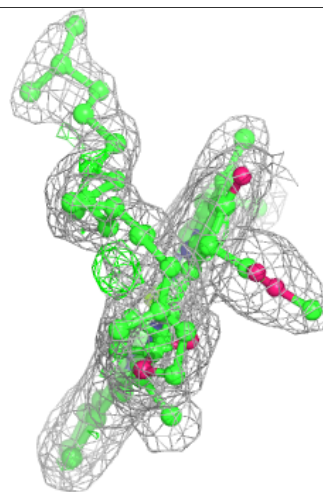
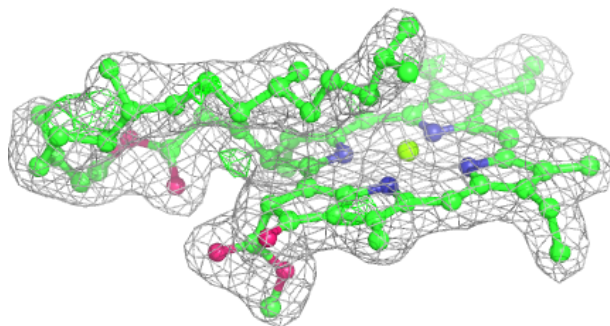
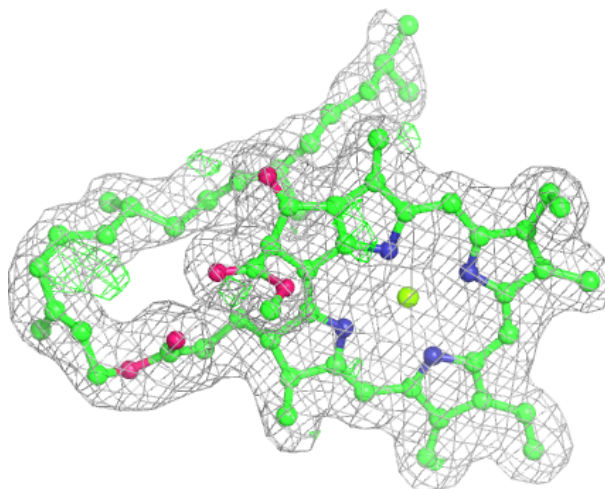
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





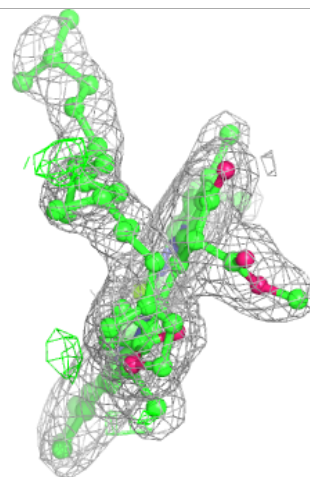
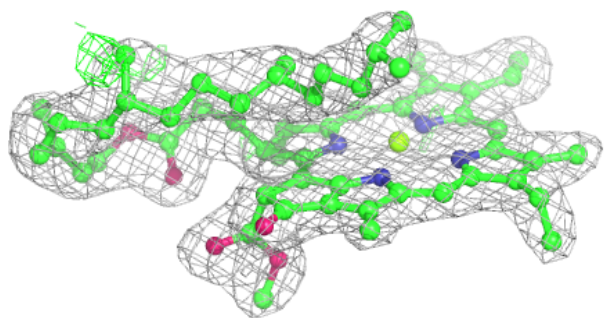
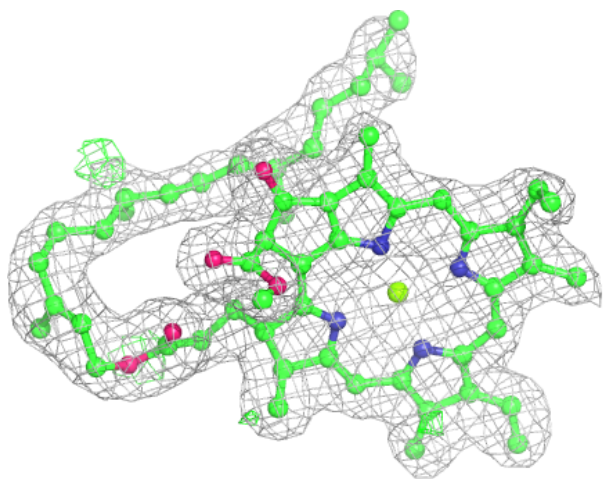
**Electron density around CLA c 910:**

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



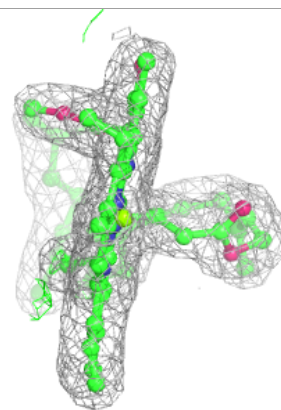
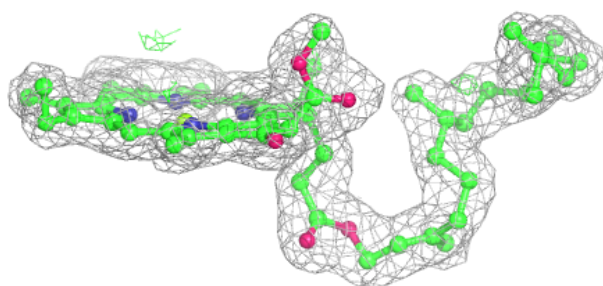
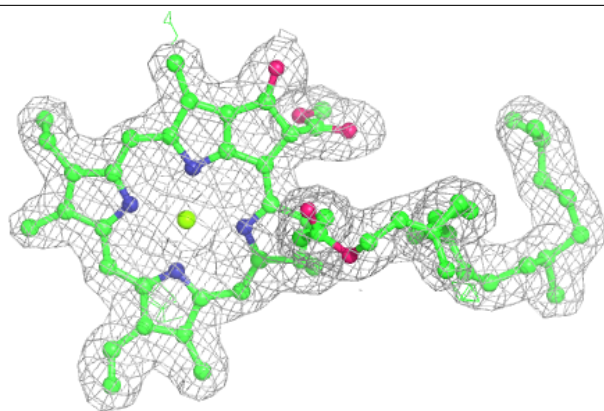
**Electron density around CLA C 509:**

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

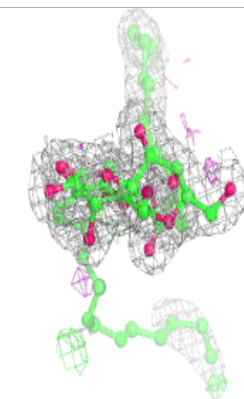
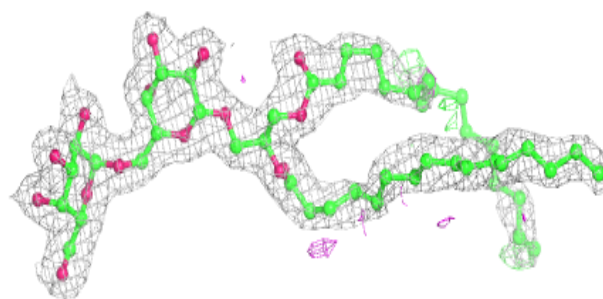
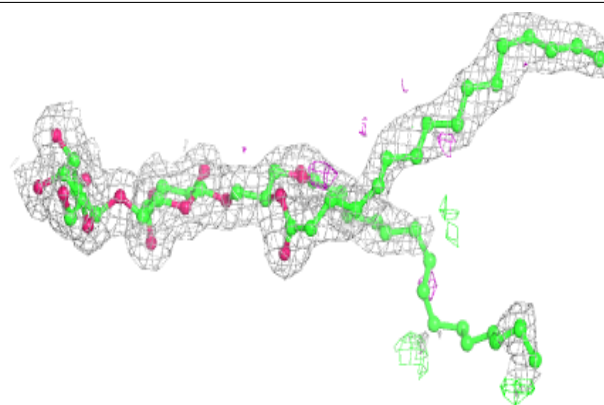


**Electron density around CLA b 616:**

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

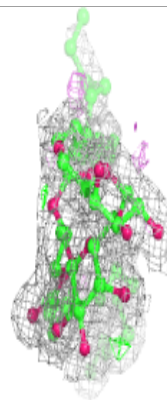
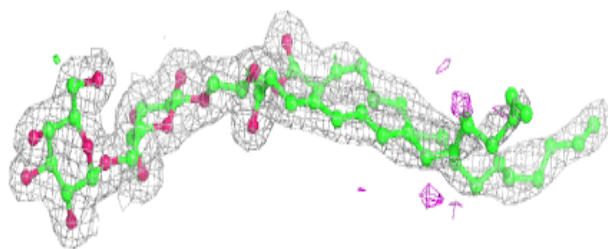
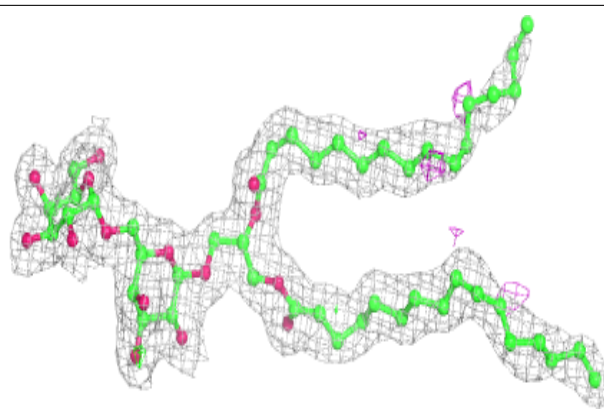
**Electron density around DGD C 516:**

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



**Electron density around DGD C 518:**

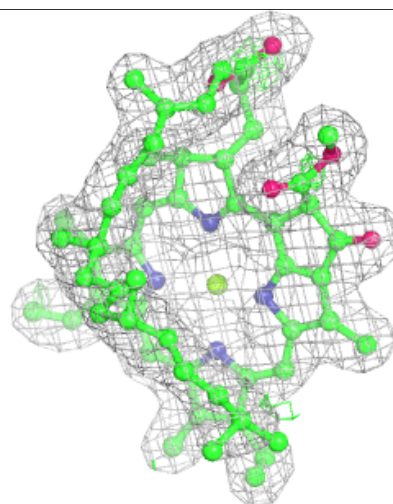
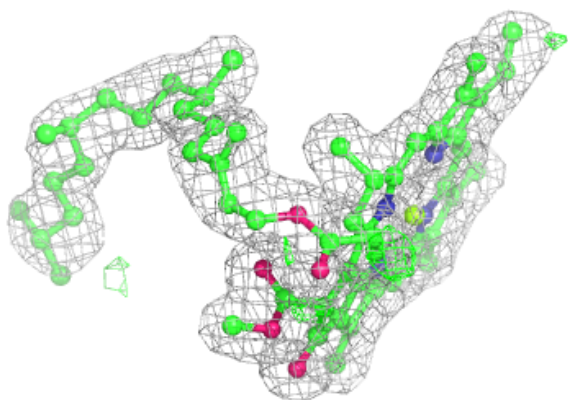
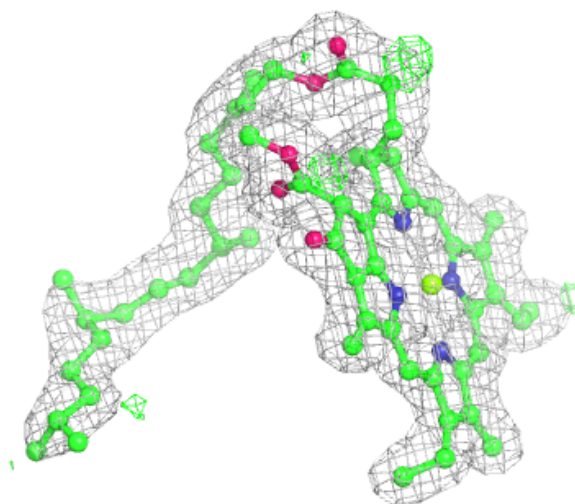
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





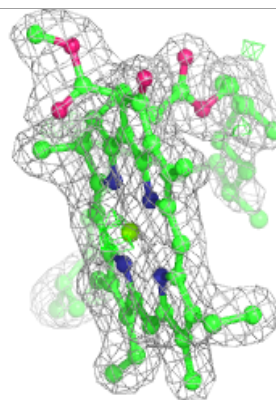
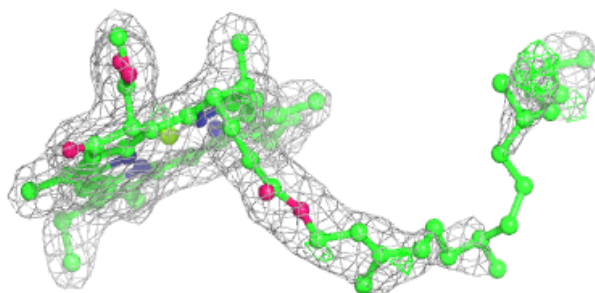
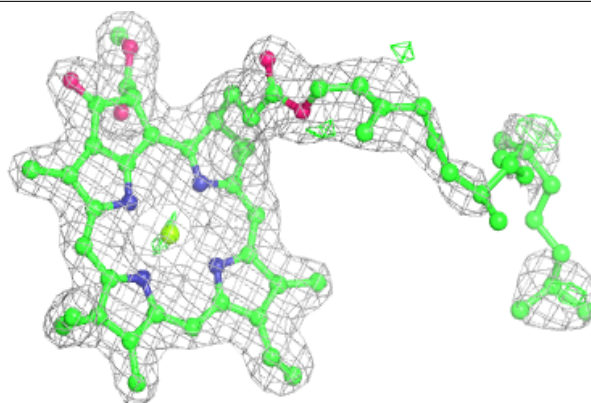
**Electron density around CLA b 617:**

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

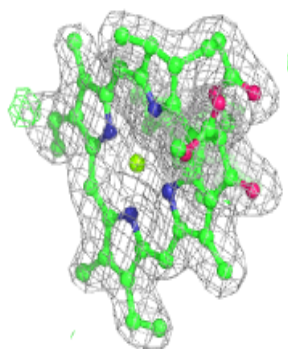
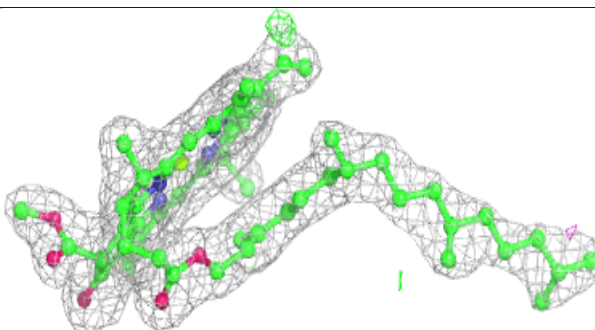
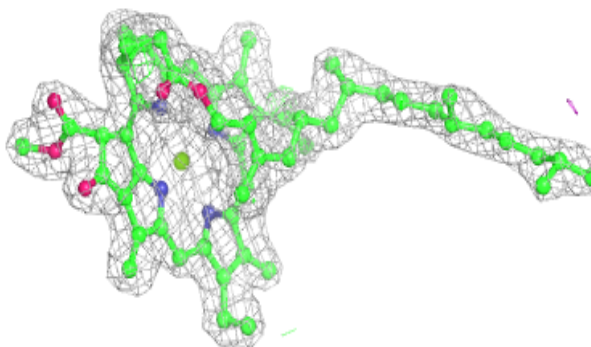


**Electron density around CLA a 413:**

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

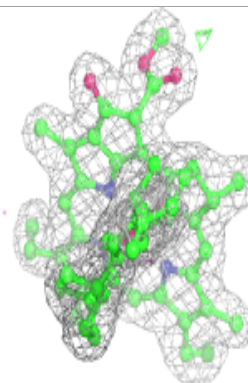
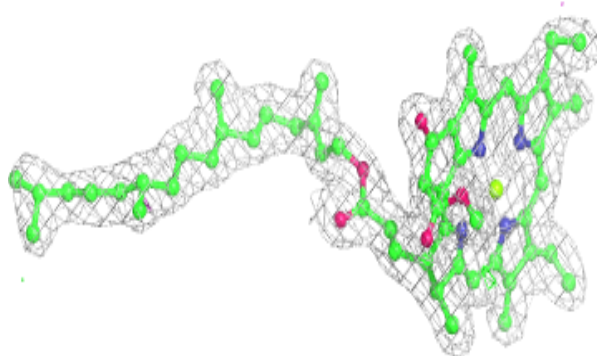
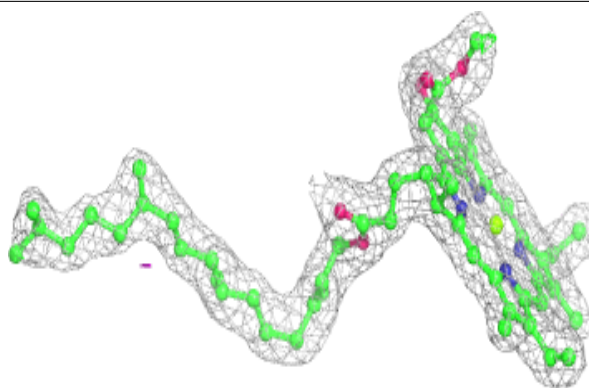
**Electron density around CLA C 505:**

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

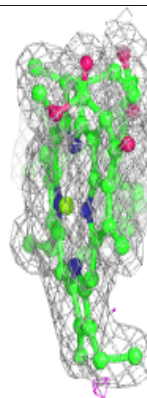
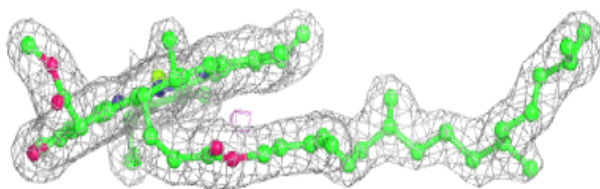
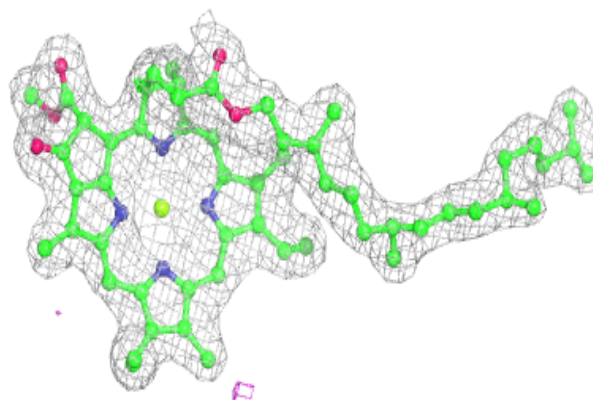


**Electron density around CLA C 502:**

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

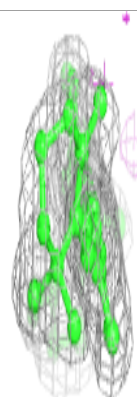
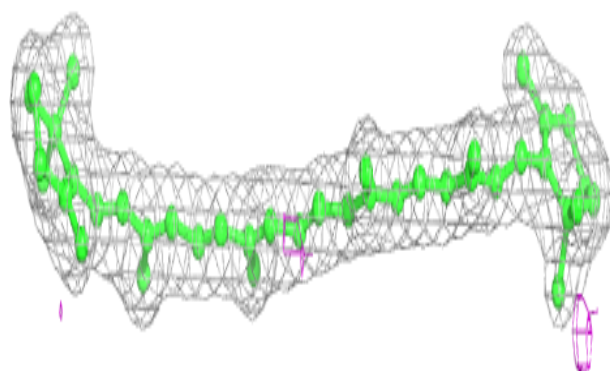
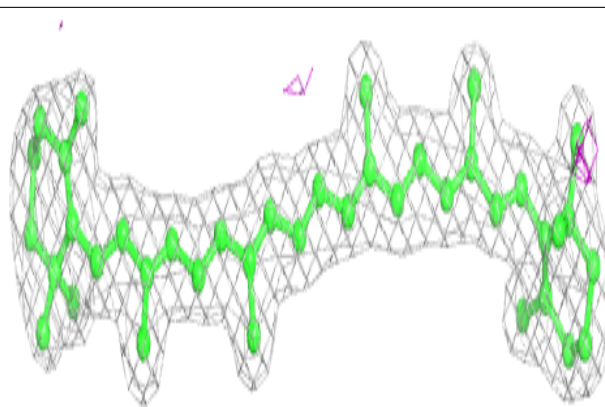
**Electron density around CLA b 607:**

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

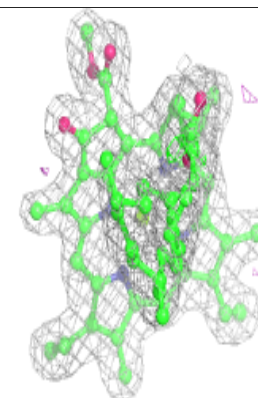
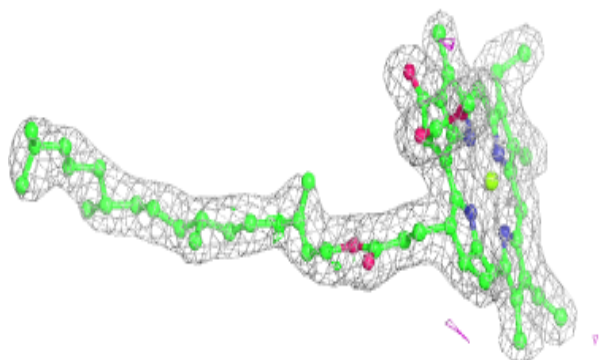
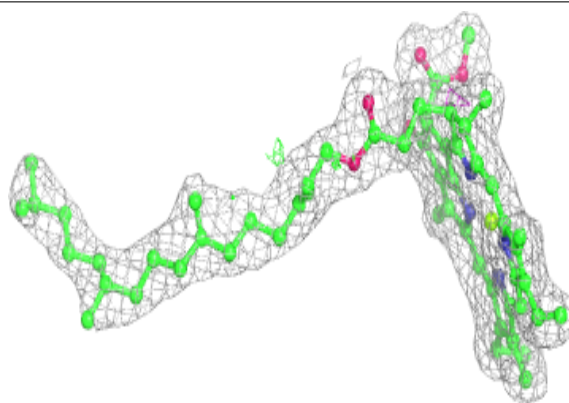


**Electron density around BCR B 620:**

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

**Electron density around CLA b 608:**

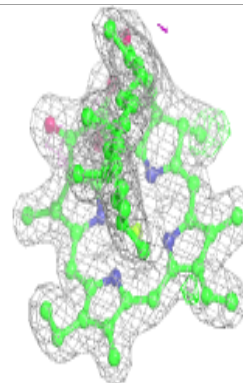
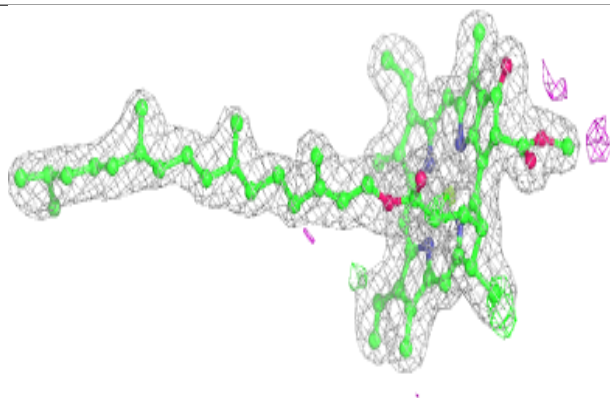
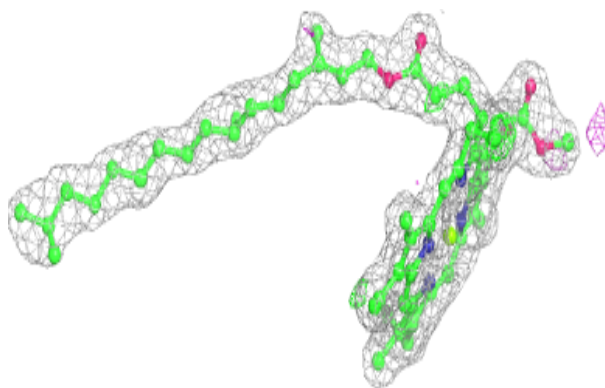
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



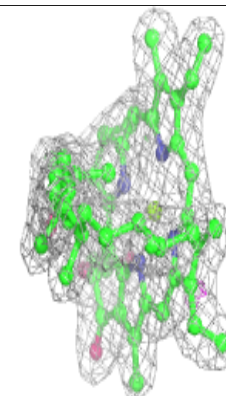
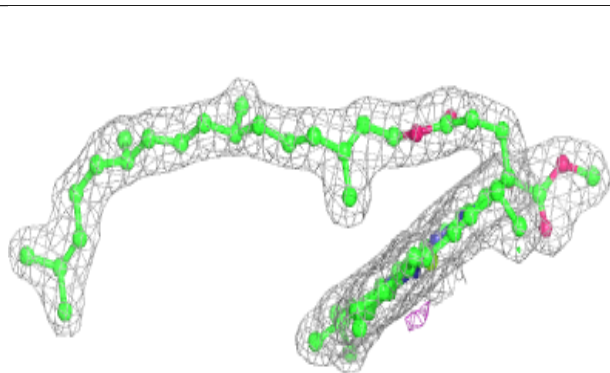
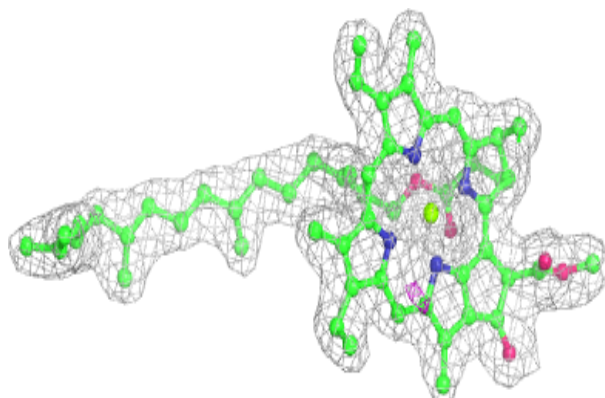


**Electron density around CLA B 608:**

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

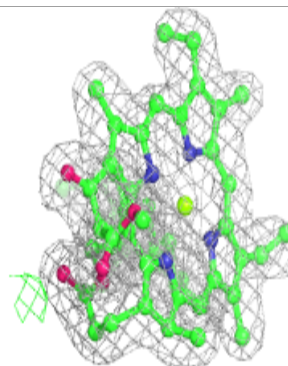
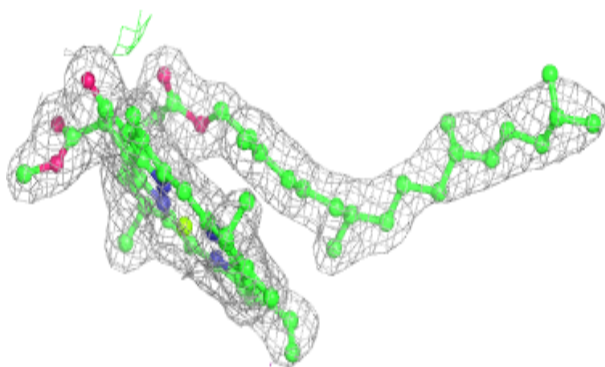
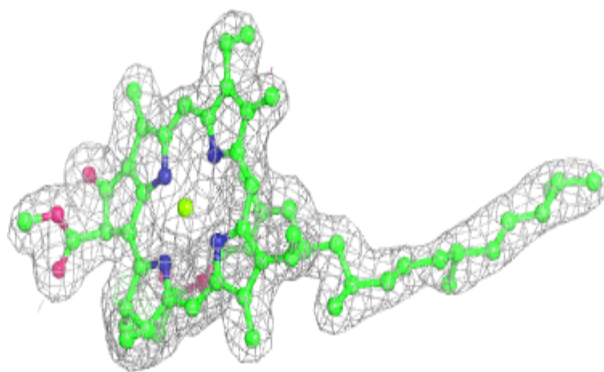
**Electron density around CLA b 612:**

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

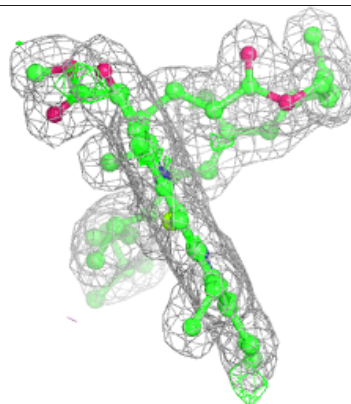
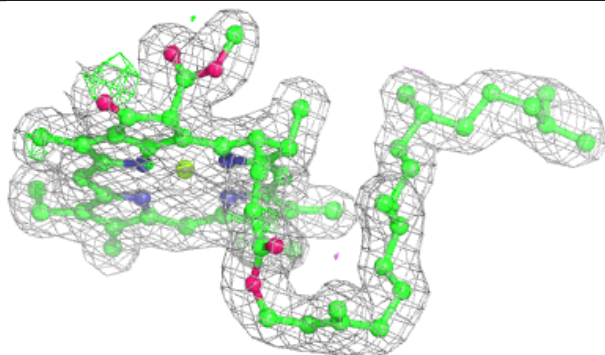
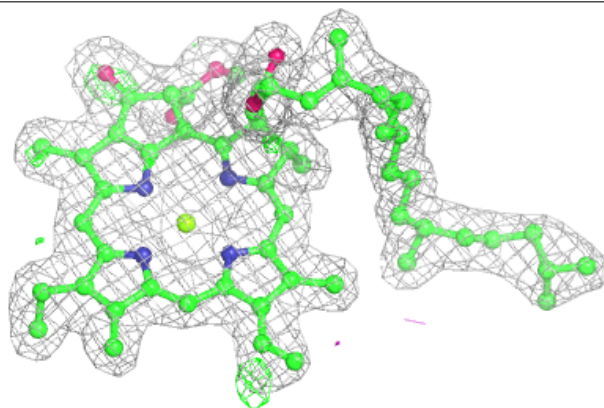


**Electron density around CLA c 906:**

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

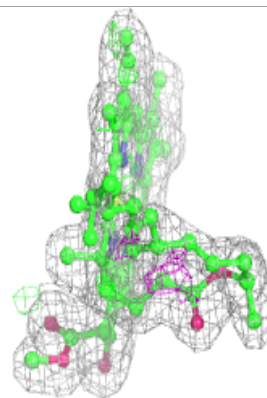
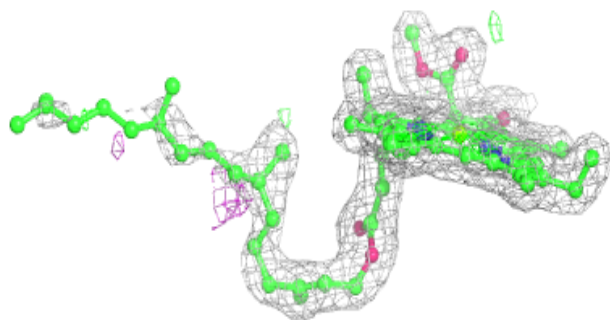
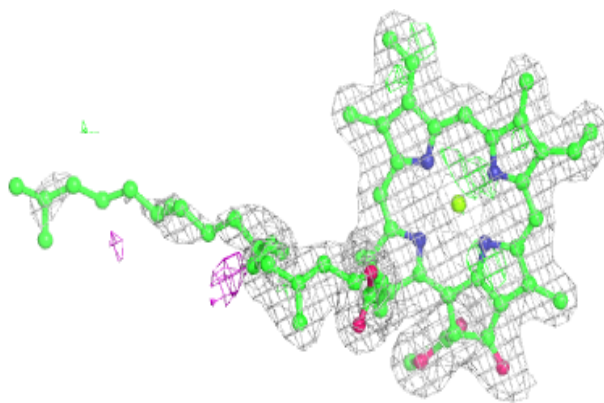
**Electron density around CLA A 406:**

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



**Electron density around CLA a 410:**

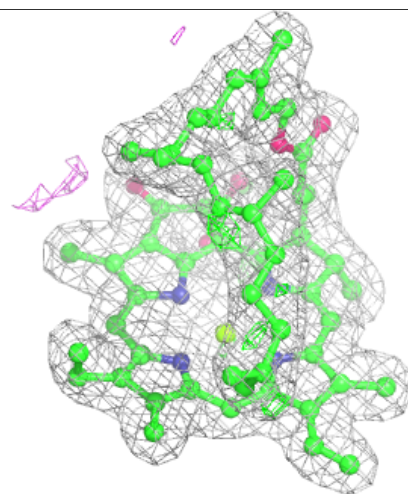
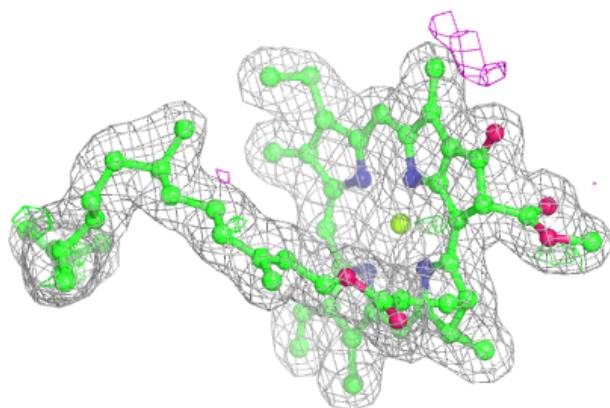
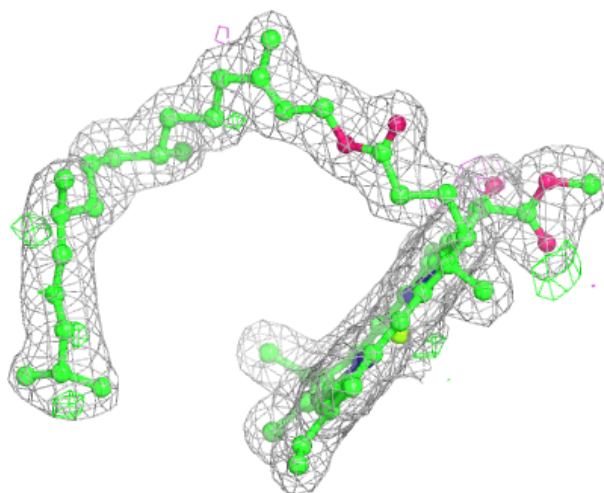
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





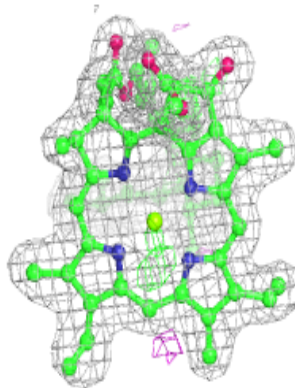
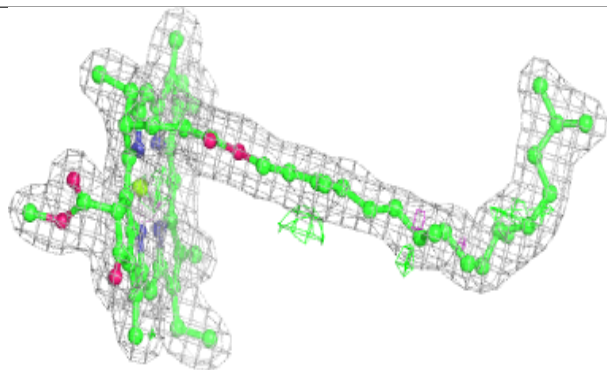
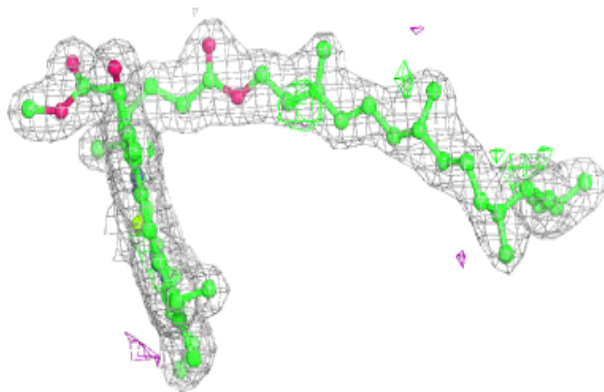
**Electron density around CLA b 615:**

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



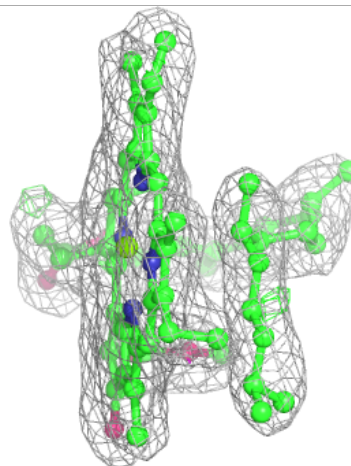
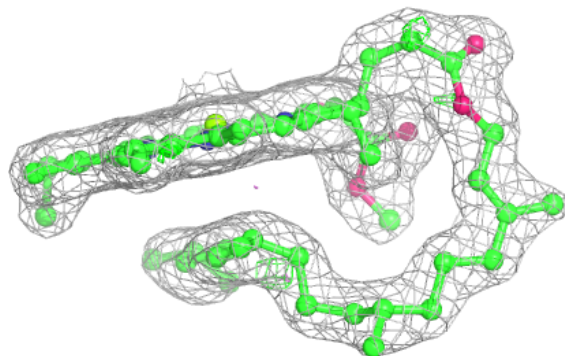
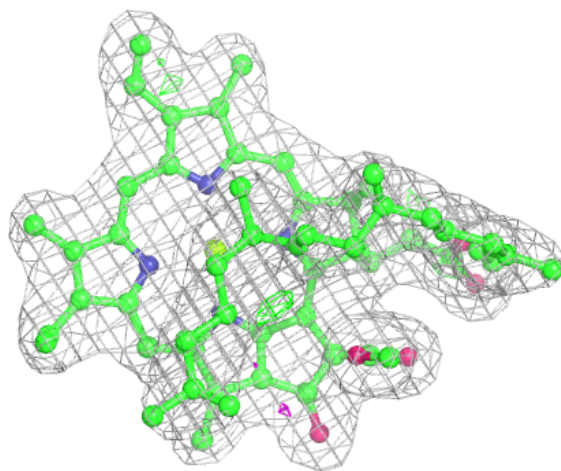
**Electron density around CLA B 606:**

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



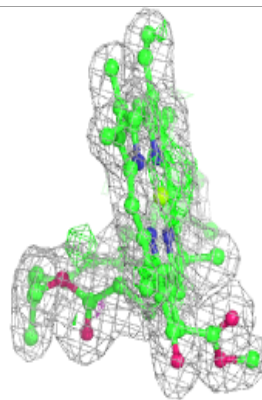
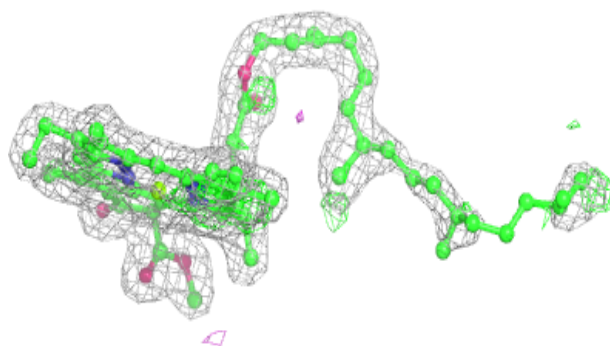
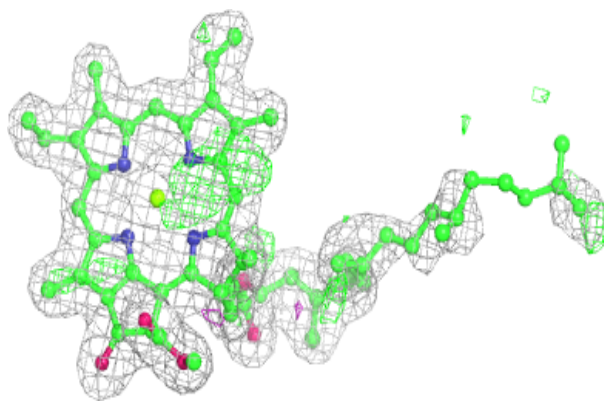
**Electron density around CLA c 911:**

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

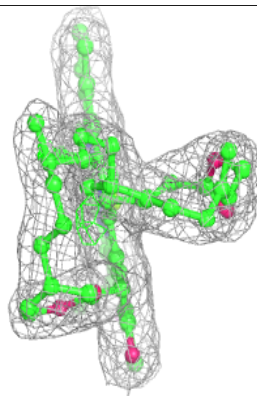
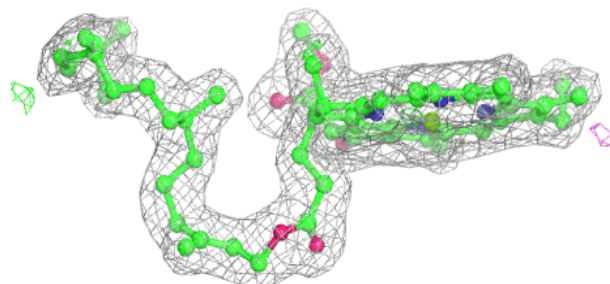
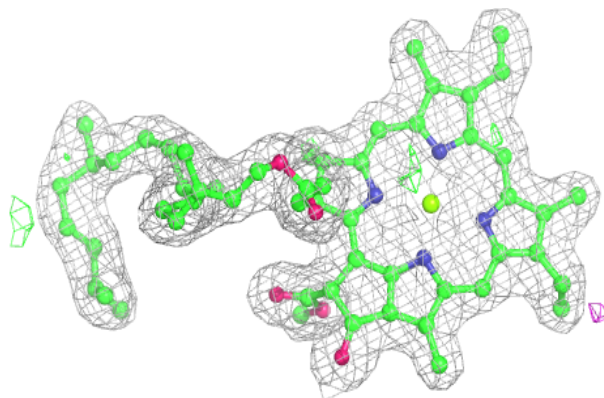


**Electron density around CLA A 407:**

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

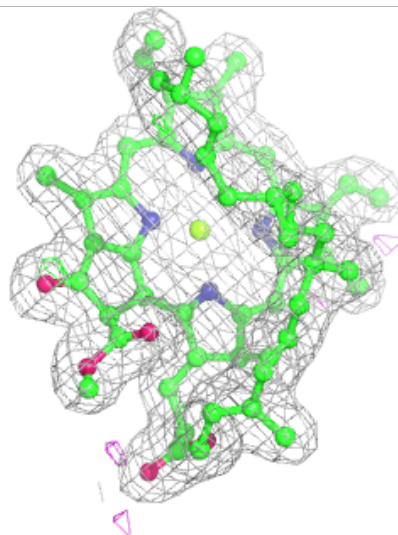
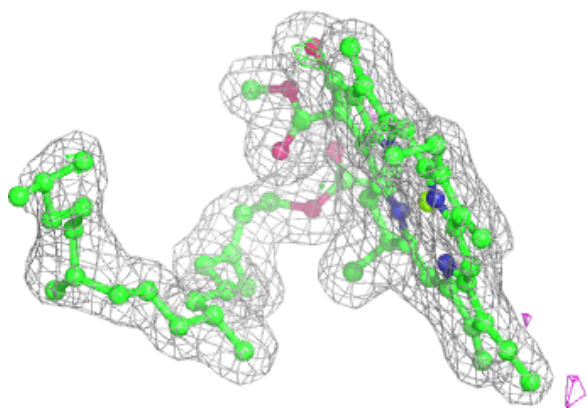
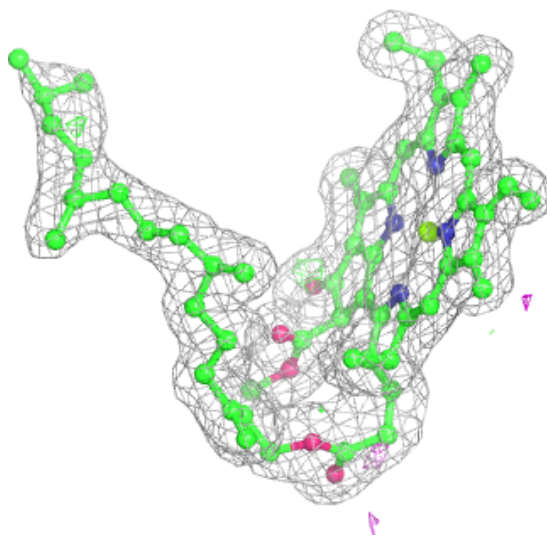
**Electron density around CLA B 613:**

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



**Electron density around CLA B 614:**

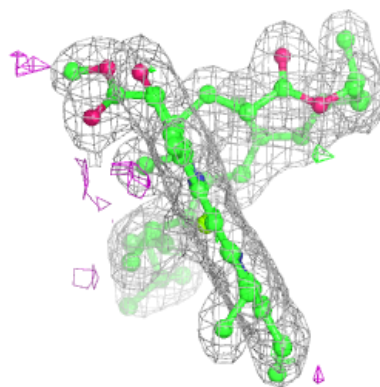
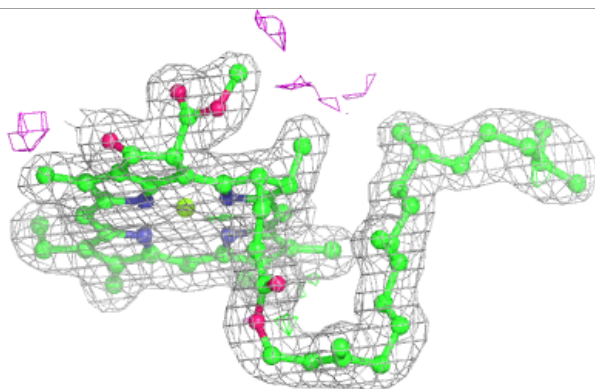
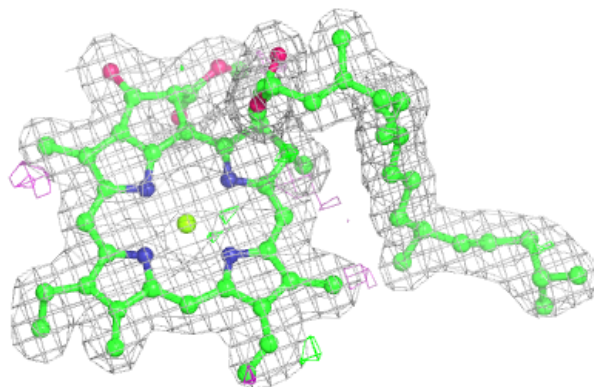
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



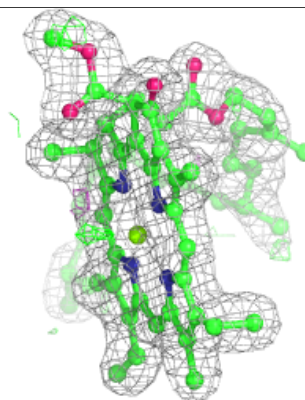
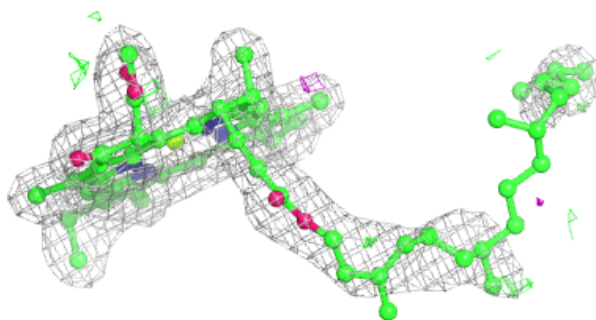
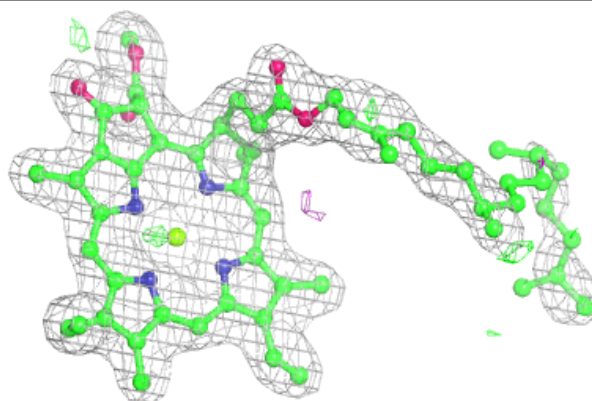


**Electron density around CLA d 401:**

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

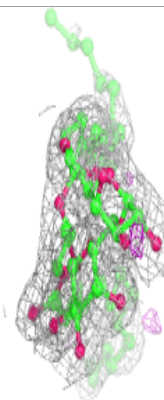
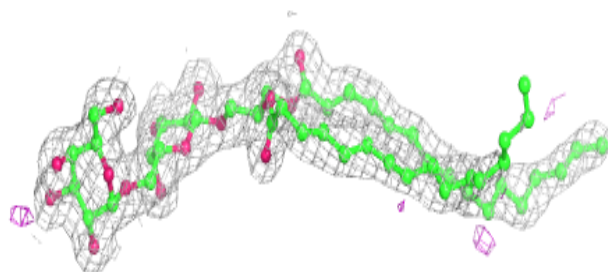
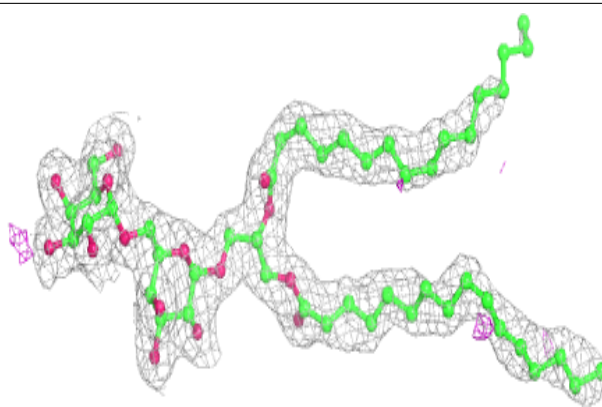
**Electron density around CLA A 410:**

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



**Electron density around DGD c 919:**

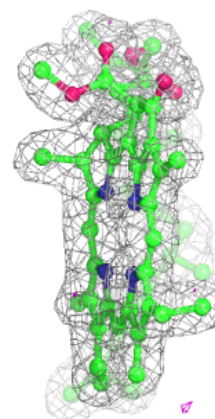
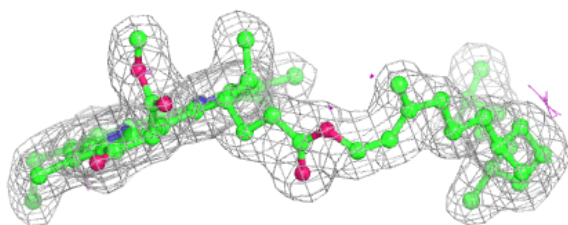
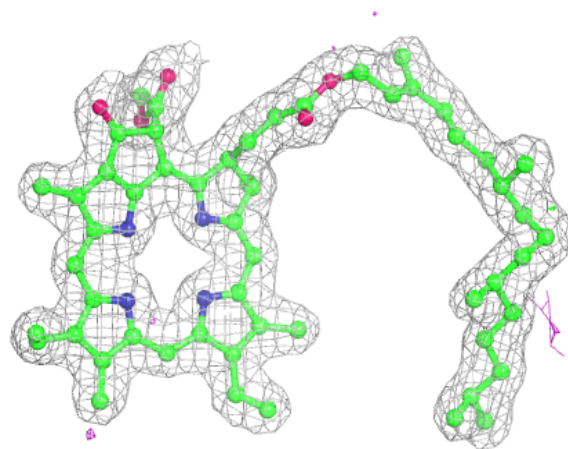
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





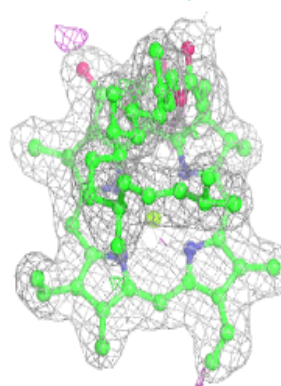
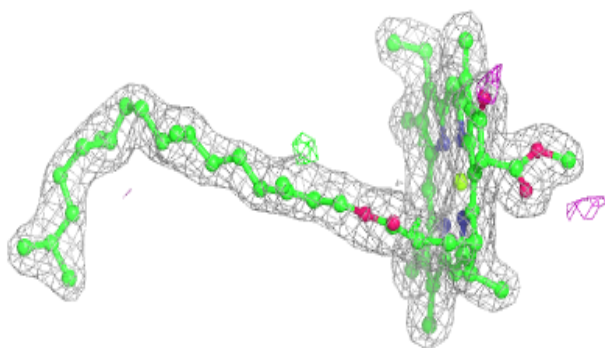
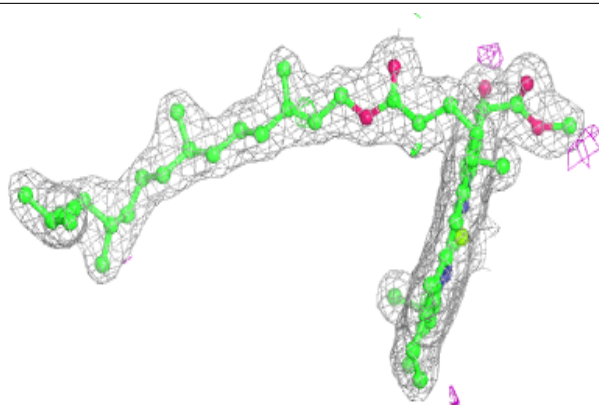
**Electron density around PHO A 408:**

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

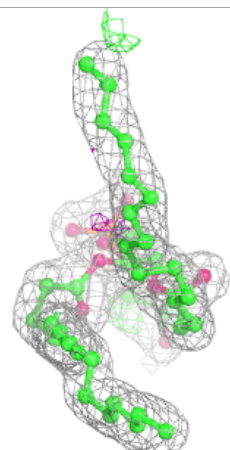
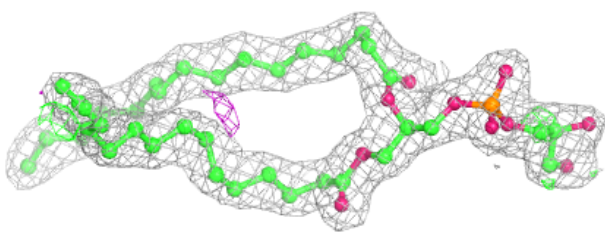
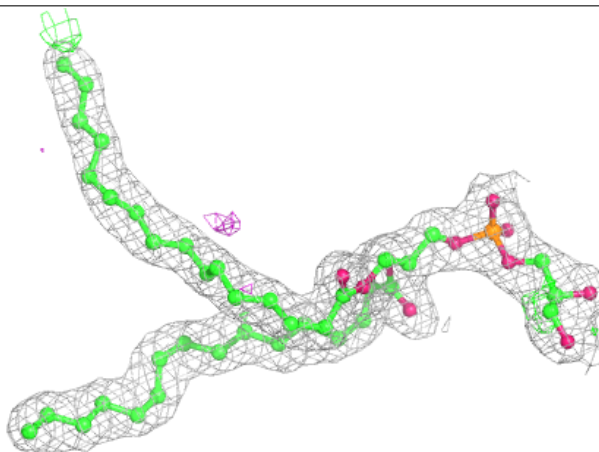


**Electron density around CLA b 609:**

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

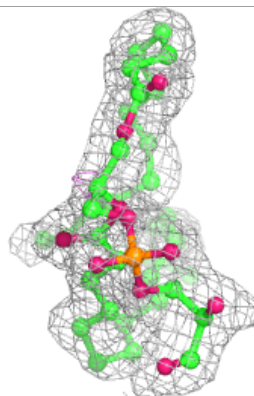
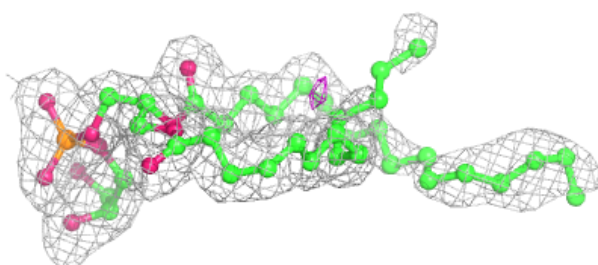
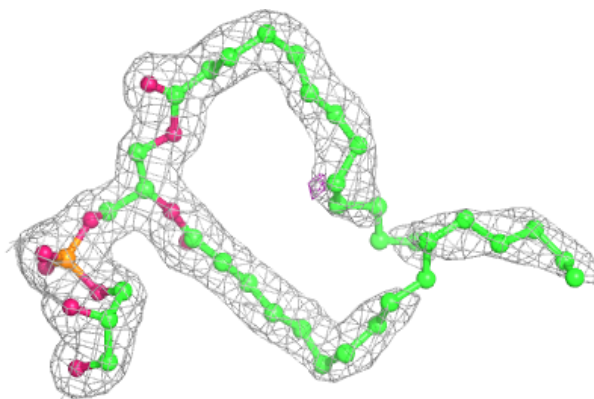
**Electron density around LHG D 407:**

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

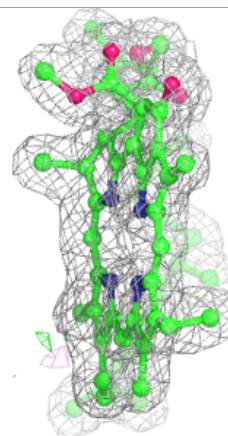
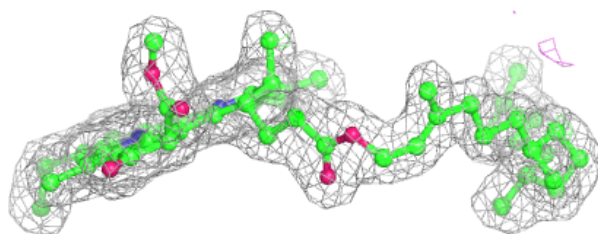
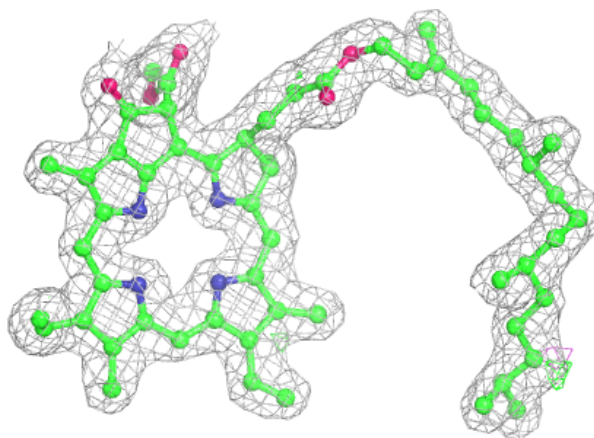


**Electron density around LHG D 408:**

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

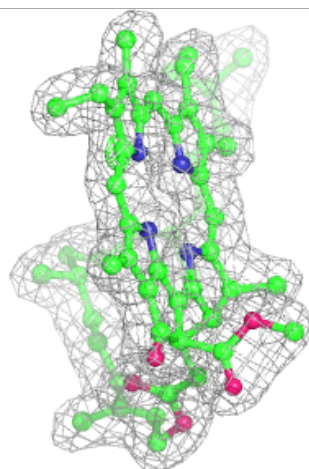
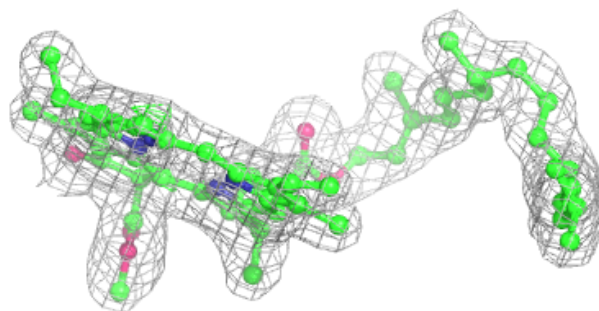
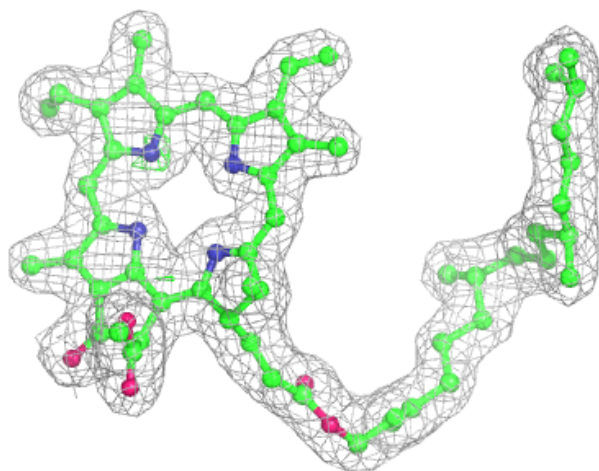
**Electron density around PHO a 411:**

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



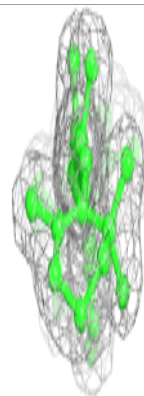
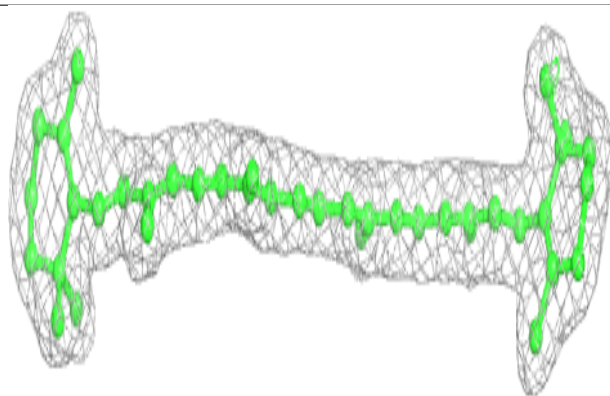
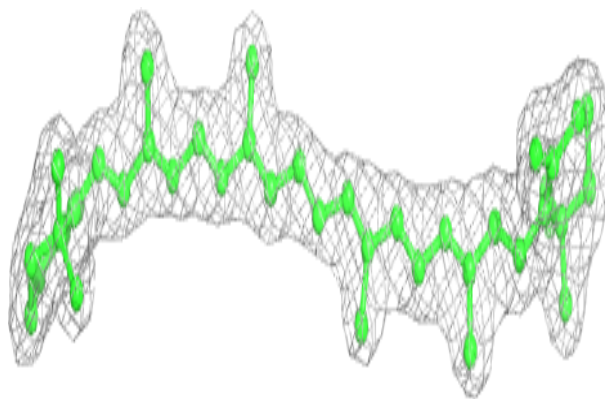
**Electron density around PHO a 412:**

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

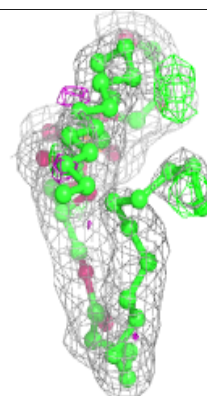
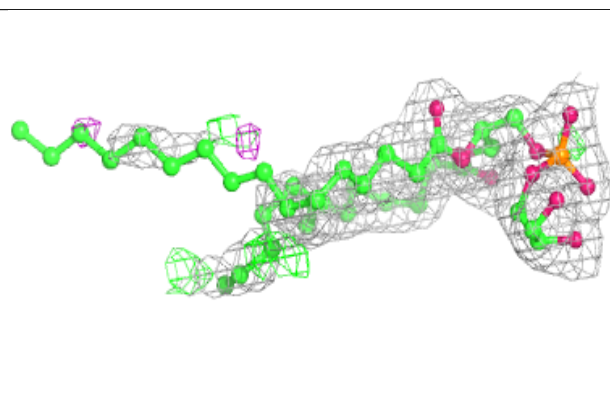
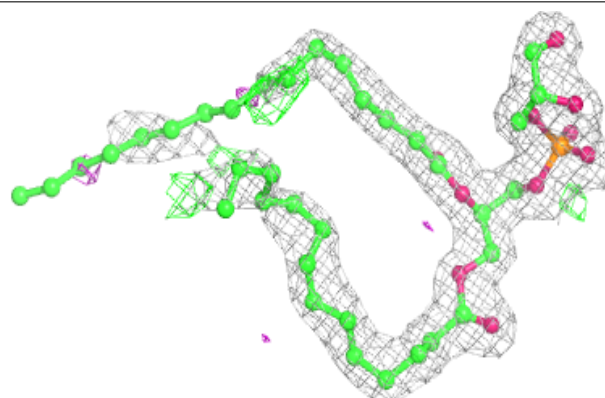


**Electron density around BCR A 411:**

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

**Electron density around LHG d 411:**

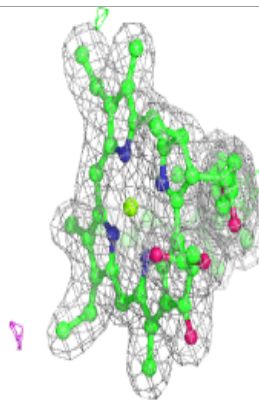
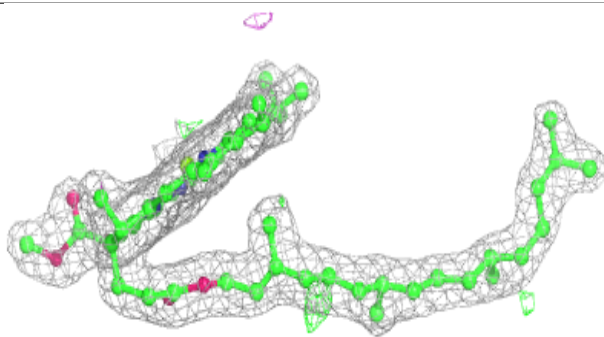
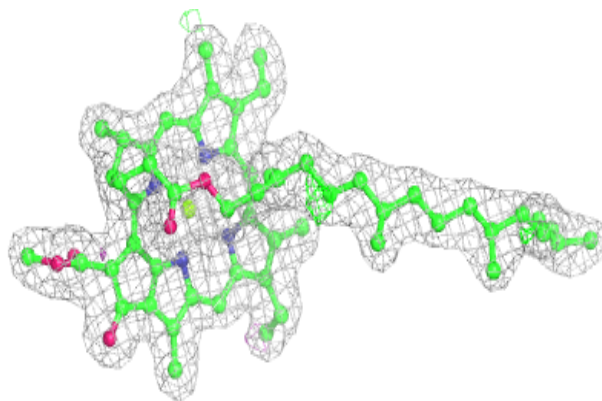
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





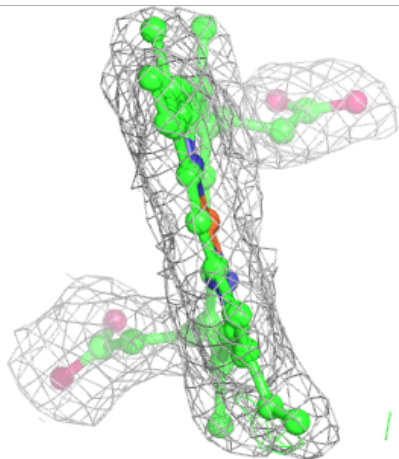
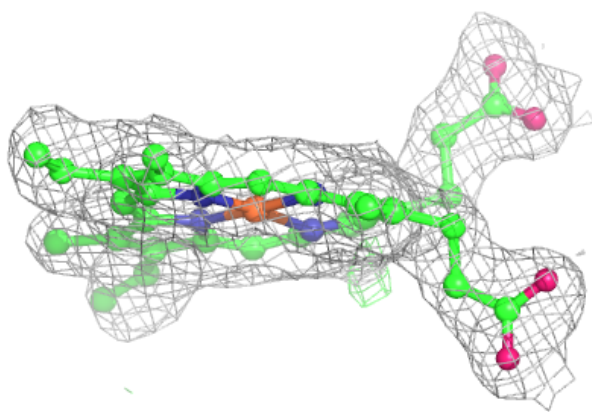
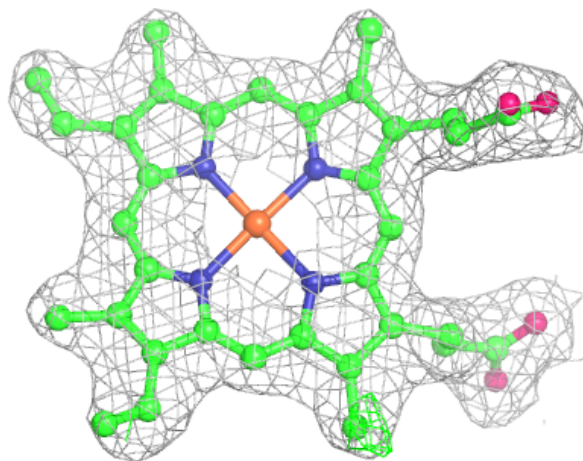
**Electron density around CLA B 609:**

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



**Electron density around HEM F 102:**

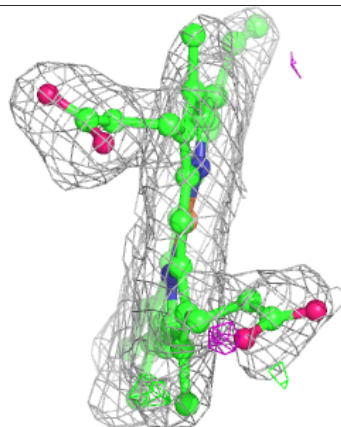
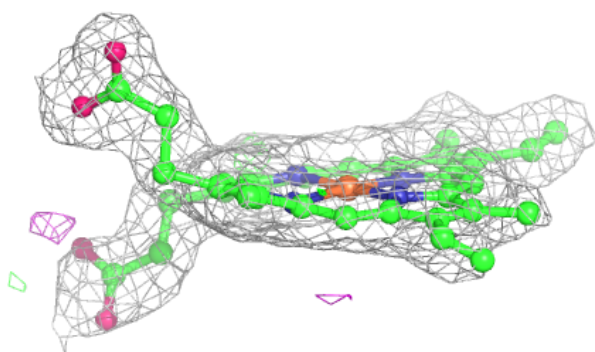
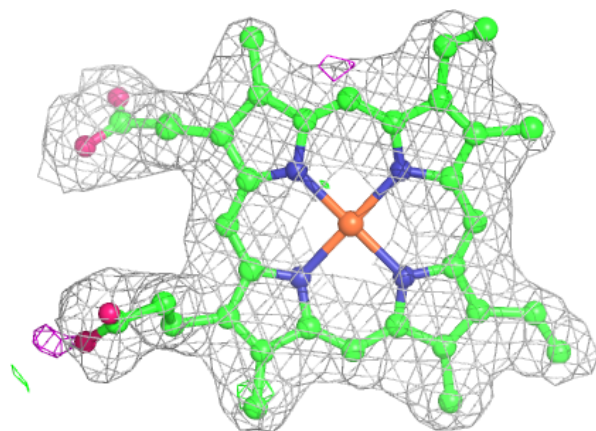
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



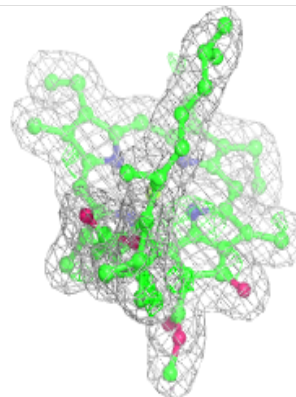
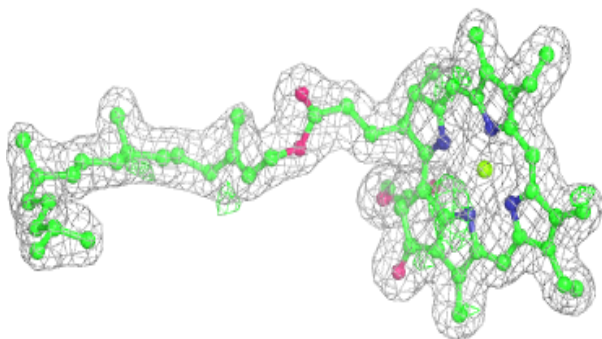
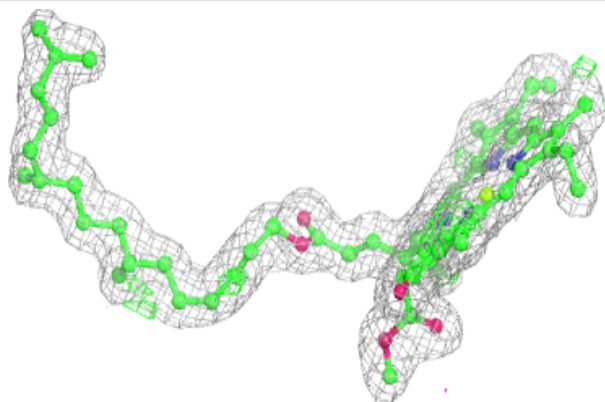


**Electron density around HEM f 101:**

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

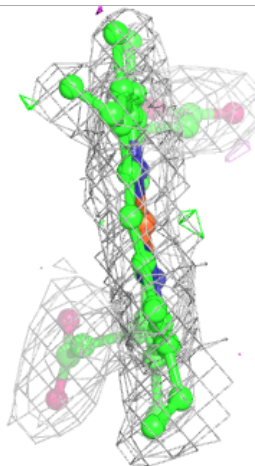
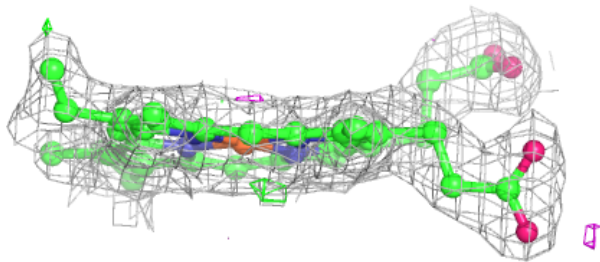
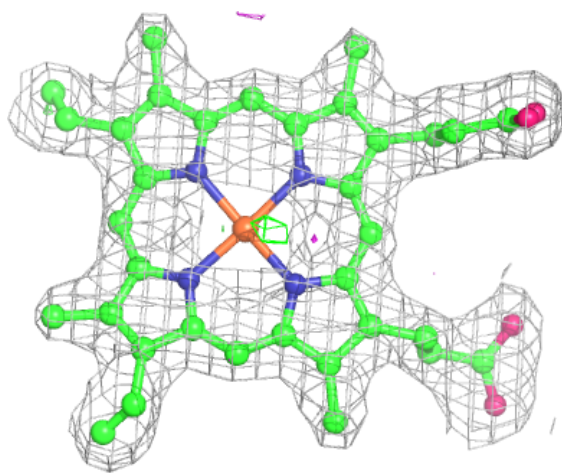
**Electron density around CLA D 401:**

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



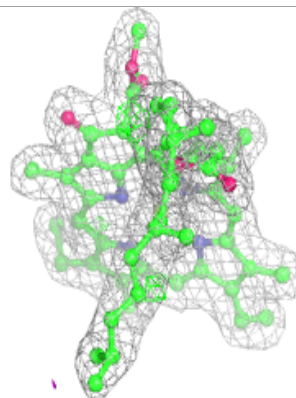
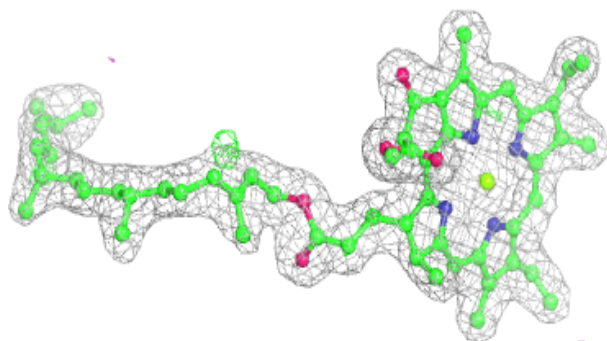
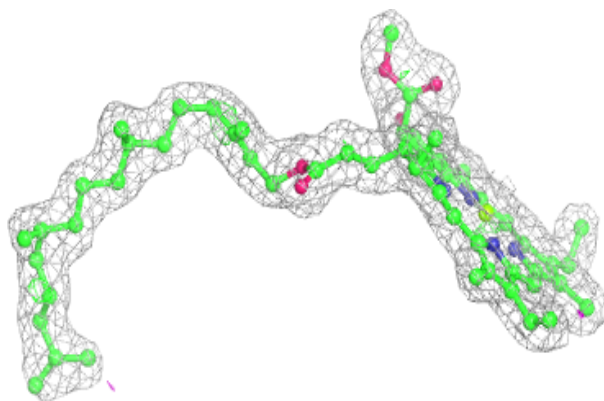
**Electron density around HEC v 202:**

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

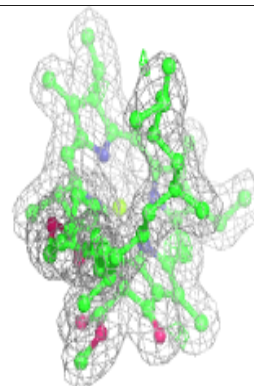
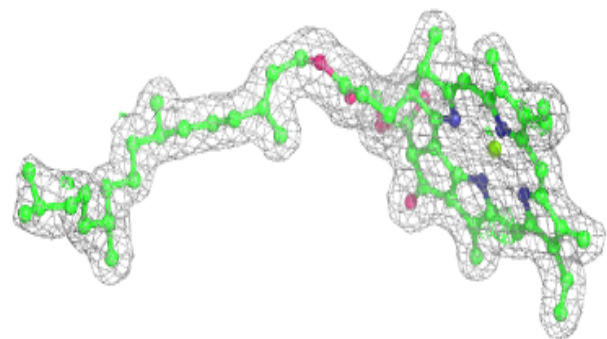
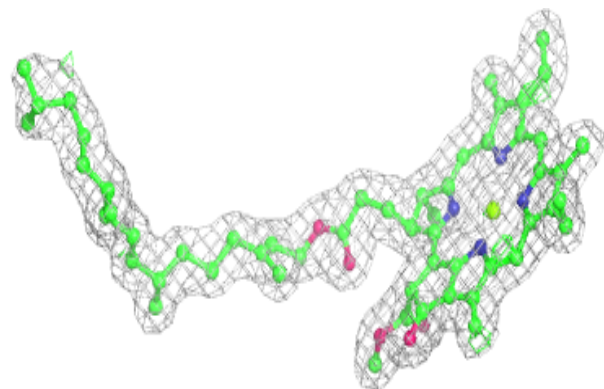


**Electron density around CLA d 404:**

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

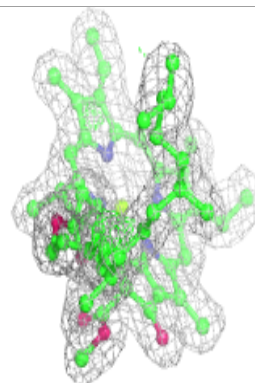
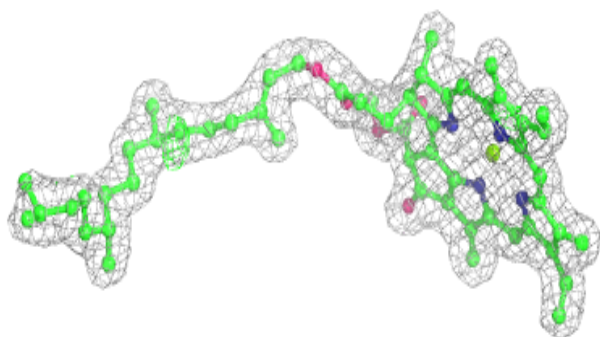
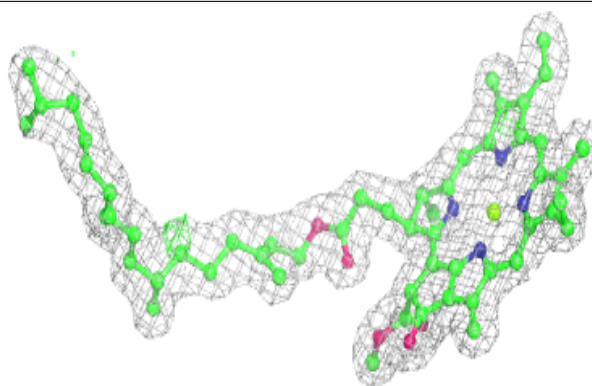
**Electron density around CLA A 405:**

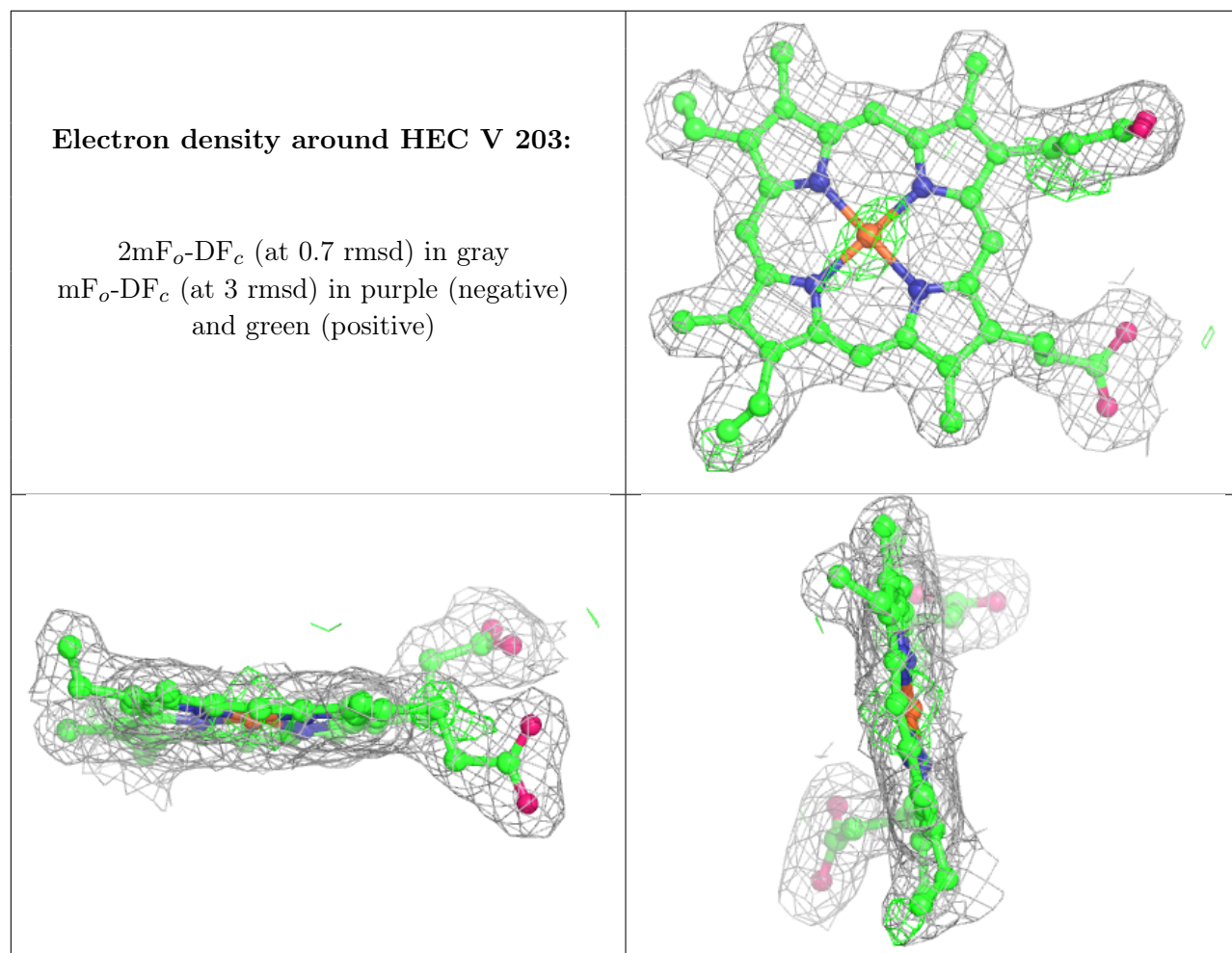
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 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.