



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 23, 2022 – 06:20 PM JST

PDB ID : 7YQ7
Title : Crystal structure of photosystem II expressing psbA3 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

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>.

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

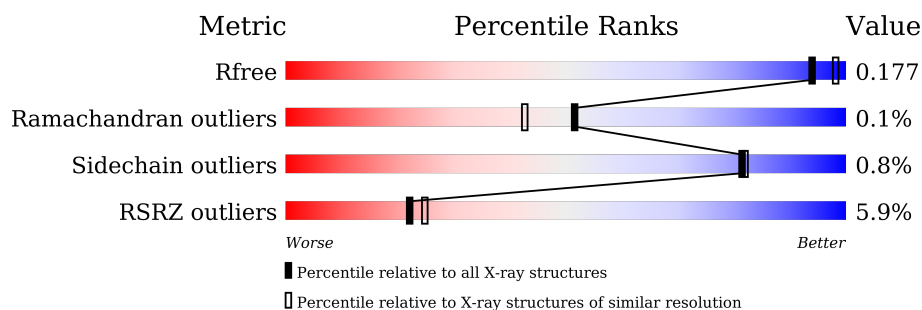
1 Overall quality at a glance

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 ≥ 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 92% • 7% </div> </div>
1	a	360	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 4% 94% • 5% </div> </div>
2	B	510	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 4% 98% •• </div> </div>
2	b	510	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 6% 98% • </div> </div>
3	C	461	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 97% •• </div> </div>
3	c	461	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 2% 98% •• </div> </div>
4	D	352	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 96% •• </div> </div>

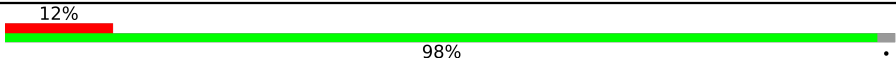
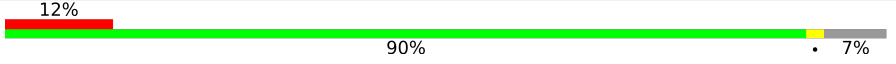
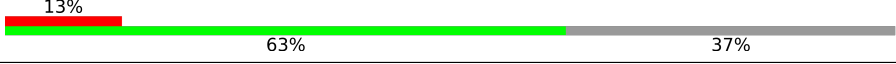
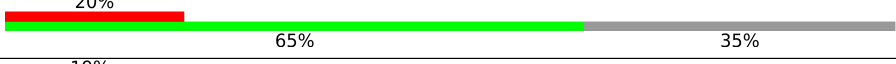
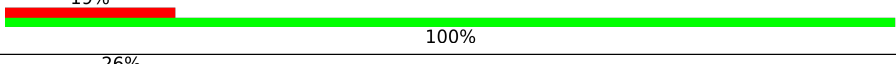
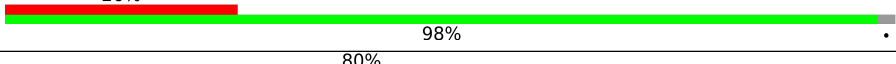
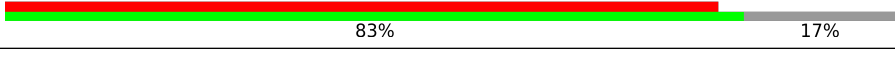
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Mol	Chain	Length	Quality of chain
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16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

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Mol	Chain	Length	Quality of chain
17	X	41	
17	x	41	
18	Y	46	
18	y	46	
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	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	609	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	B	618	X	-	-	-
24	CLA	C	503	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	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	514	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	D	406	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	410	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	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	503	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	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	d	406	X	-	-	-
34	DMS	C	501	-	-	-	X
34	DMS	O	308	-	-	-	X
34	DMS	o	305	-	-	-	X
34	DMS	u	203	-	-	-	X
36	HTG	B	626	-	-	-	X
36	HTG	u	201	-	-	-	X

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 55105 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2624	1720	429	461	14			
1	a	342	Total	C	N	O	S	0	0	0
			2658	1741	436	467	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	5	0
			3994	2618	668	695	13			
2	b	504	Total	C	N	O	S	0	6	0
			3978	2609	666	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	450	Total	C	N	O	S	0	2	0
			3492	2284	585	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3527	2311	586	617	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	1	0
			2714	1799	441	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

- 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
			647	424	103	120			
5	e	79	Total	C	N	O	0	2	0
			642	421	103	118			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	342	85	85	2			
7	h	65	Total	C	N	O	S	0	1	0
			519	344	86	87	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
			287	196	42	48	1			
8	i	37	Total	C	N	O	S	0	0	0
			304	206	47	50	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			256	174	38	43	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			305	205	48	51	1			
11	l	36	Total	C	N	O		0	1	0
			301	202	47	52				

- 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	0	0
			261	174	38	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	4	0
			1860	1165	310	380	5			
13	o	243	Total	C	N	O	S	0	3	0
			1848	1159	306	378	5			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			770	489	129	152			
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	1	0
			1070	678	178	210	4			
16	v	137	Total	C	N	O	S	0	1	0
			1065	677	175	209	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	40	Total	C	N	O	0	1	0
			295	198	47	50			
17	x	38	Total	C	N	O	0	0	0
			275	185	44	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			206	136	34	33	3			
18	y	30	Total	C	N	O	S	0	0	0
			215	140	38	34	3			

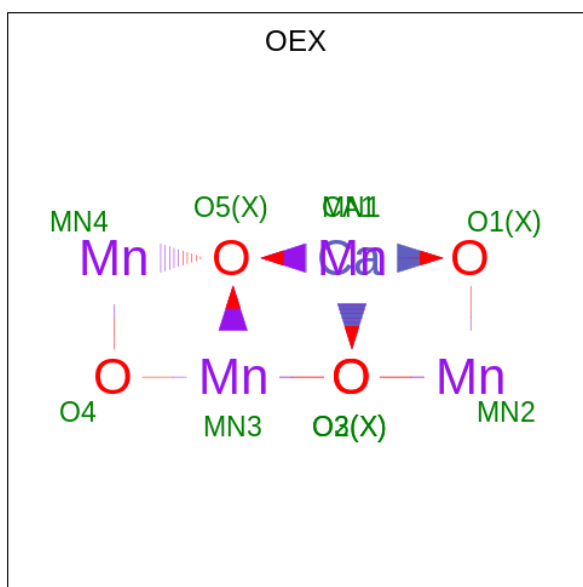
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	5	0
			495	341	74	78	2			
19	z	61	Total	C	N	O	S	0	0	0
			450	311	67	71	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			206	132	38	36			

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_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		

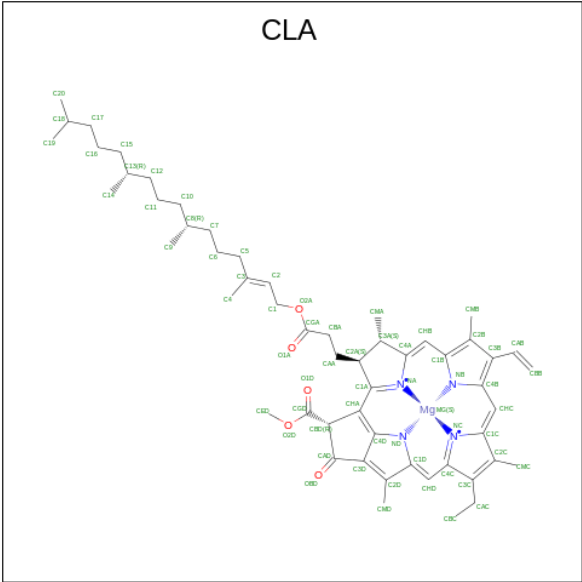
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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: C₅₅H₇₂MgN₄O₅).



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	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		
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	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
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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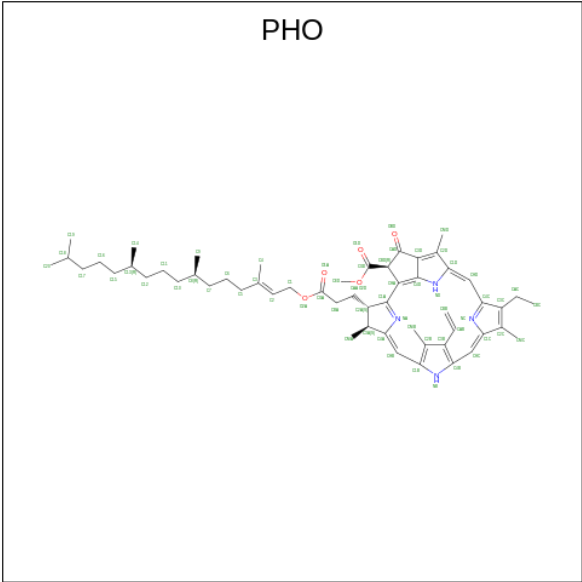
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24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	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

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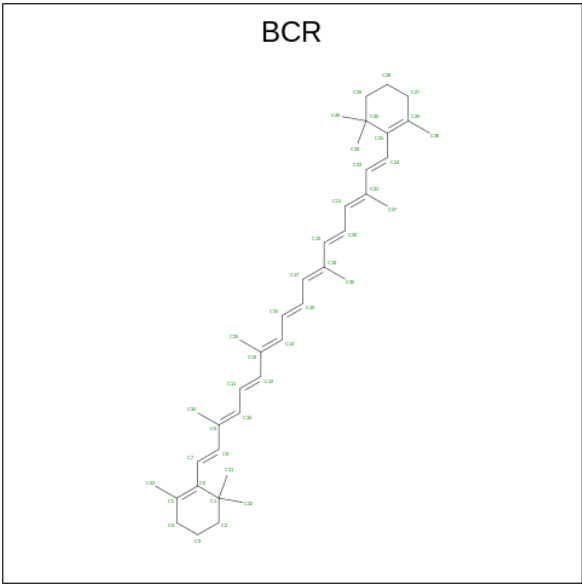
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



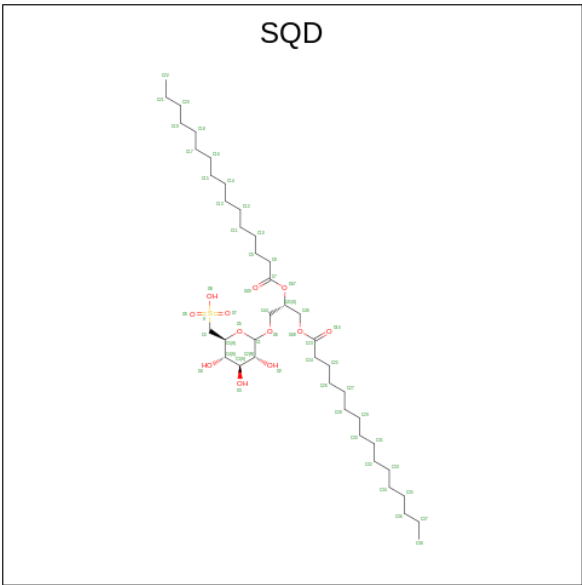
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



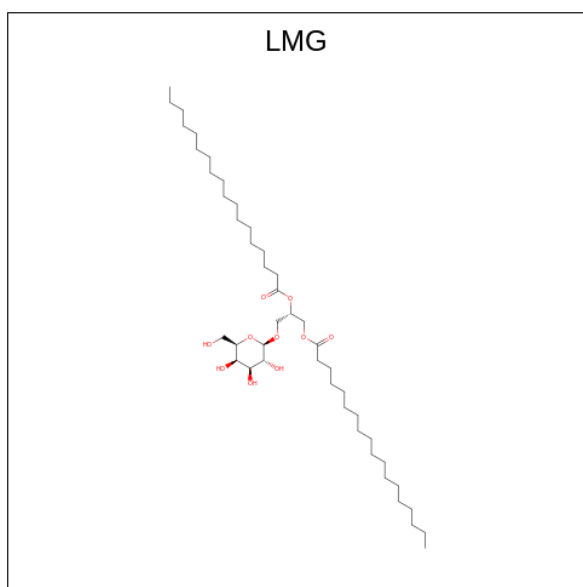
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total 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
26	t	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: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



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	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	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		

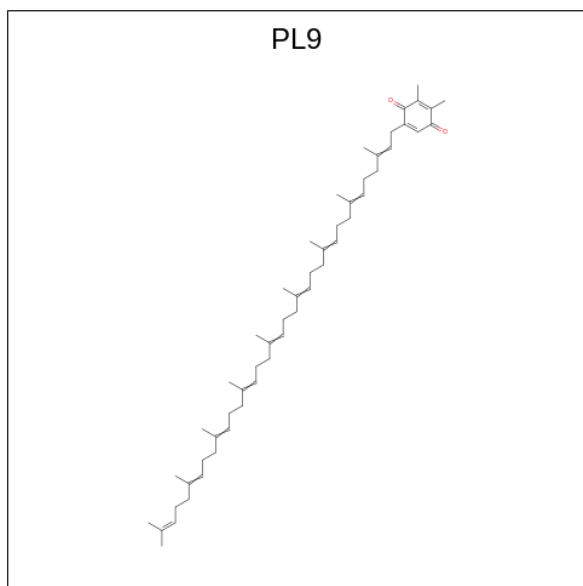
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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	Z	1	Total	C	O	0	0
			39	29	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	i	1	Total	C	O	0	0
			51	41	10		
28	z	1	Total	C	O	0	0
			37	27	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:

C₅₃H₈₀O₂) (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	5	Total	C		0	0
			39	39			
30	B	7	Total	C		0	0
			51	51			
30	C	9	Total	C	O	0	0
			85	80	5		
30	D	4	Total	C	O	0	0
			75	71	4		
30	E	2	Total	C		0	0
			22	22			
30	H	2	Total	C		0	0
			12	12			
30	I	6	Total	C		0	0
			81	81			

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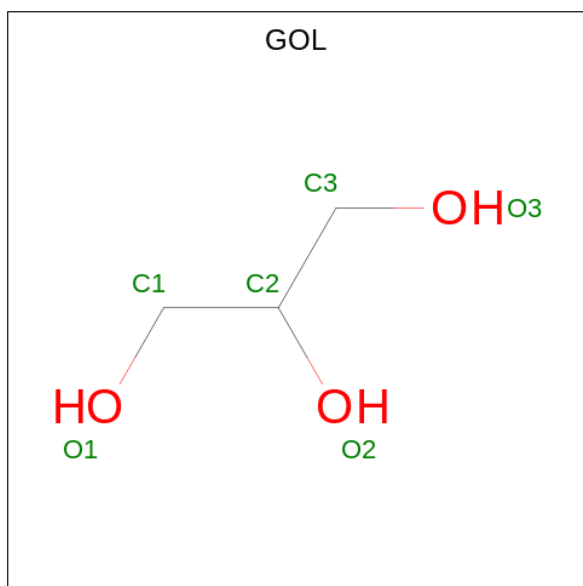
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	J	3	Total C 20 20	0	0
30	T	1	Total C 7 7	0	0
30	U	1	Total C 5 5	0	0
30	V	3	Total C 20 20	0	0
30	X	2	Total C O 44 39 5	0	0
30	Y	1	Total C 16 16	0	0
30	Z	3	Total C 15 15	0	0
30	a	2	Total C 17 17	0	0
30	b	6	Total C 53 53	0	0
30	c	5	Total C 36 36	0	0
30	d	3	Total C O 56 51 5	0	0
30	e	1	Total C 10 10	0	0
30	h	4	Total C 37 37	0	0
30	i	3	Total C 36 36	0	0
30	j	1	Total C 10 10	0	0
30	k	2	Total C O 38 33 5	0	0
30	l	1	Total C 13 13	0	0
30	m	1	Total C 8 8	0	0
30	t	1	Total C 8 8	0	0
30	x	1	Total C 11 11	0	0
30	y	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	z	1	Total C 6 6	0	0

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



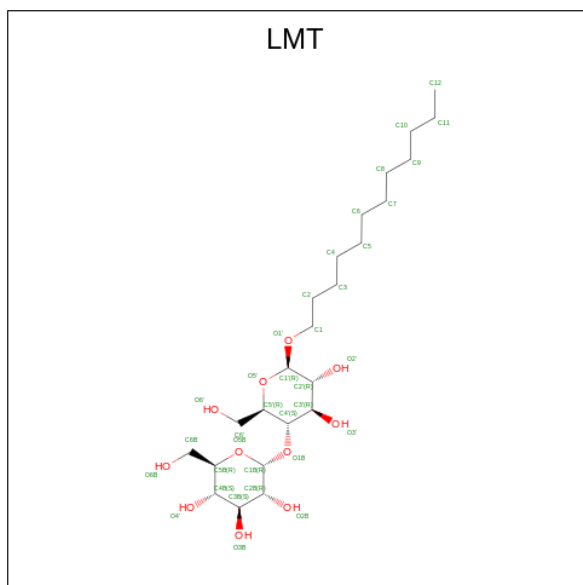
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 6 3 3	0	0
31	A	1	Total C O 6 3 3	0	0
31	C	1	Total C O 6 3 3	0	0
31	D	1	Total C O 6 3 3	0	0
31	O	1	Total C O 6 3 3	0	0
31	V	1	Total C O 6 3 3	0	0
31	a	1	Total C O 6 3 3	0	0
31	b	1	Total C O 6 3 3	0	0
31	b	1	Total C O 6 3 3	0	0
31	d	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



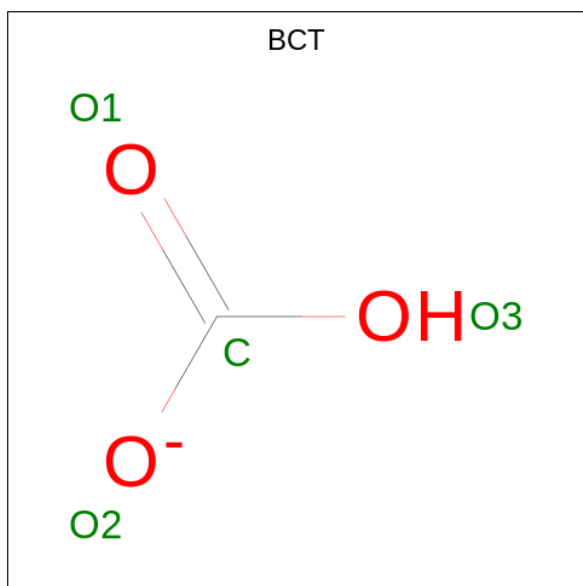
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total 35	C 24	O 11	0	0
32	B	1	Total 35	C 24	O 11	0	0
32	B	1	Total 35	C 24	O 11	0	0
32	D	1	Total 35	C 24	O 11	0	0
32	D	1	Total 35	C 24	O 11	0	0
32	F	1	Total 35	C 24	O 11	0	0
32	J	1	Total 24	C 18	O 6	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	a	1	Total 35	C 24	O 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 35 24 11	0	0
32	b	1	Total C O 35 24 11	0	0
32	b	1	Total C O 24 18 6	0	0
32	f	1	Total C O 25 19 6	0	0
32	j	1	Total C O 24 18 6	0	0
32	m	1	Total C O 35 24 11	0	0
32	m	1	Total C O 35 24 11	0	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



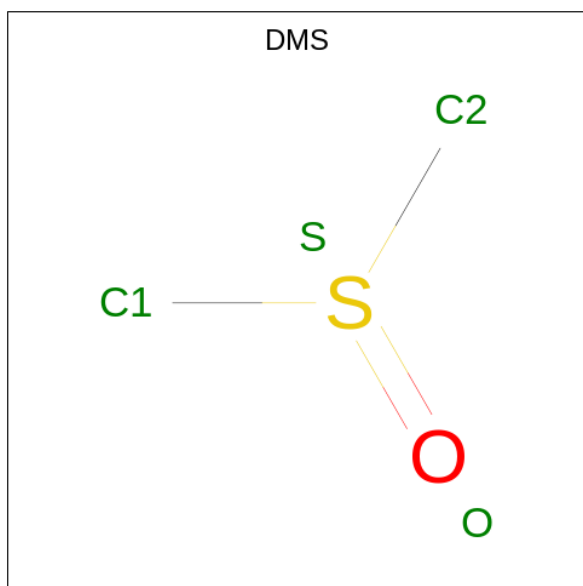
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 4 1 3	0	1
33	D	1	Total C O 4 1 3	0	1
33	a	1	Total C O 4 1 3	0	1

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

- Molecule 34 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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	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	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	E	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	T	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	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	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

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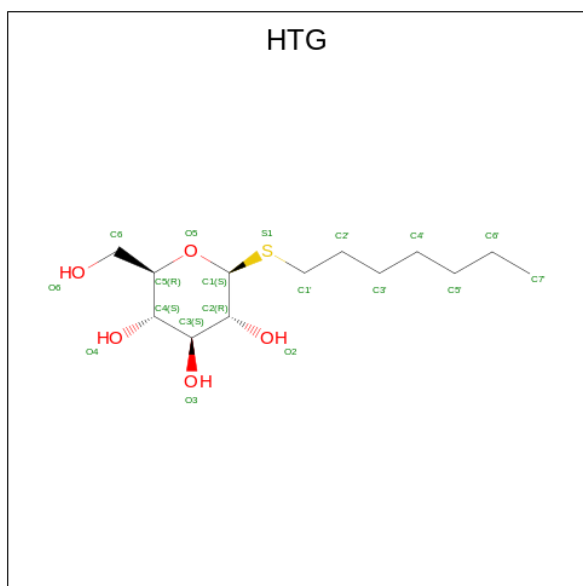
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2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

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

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

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



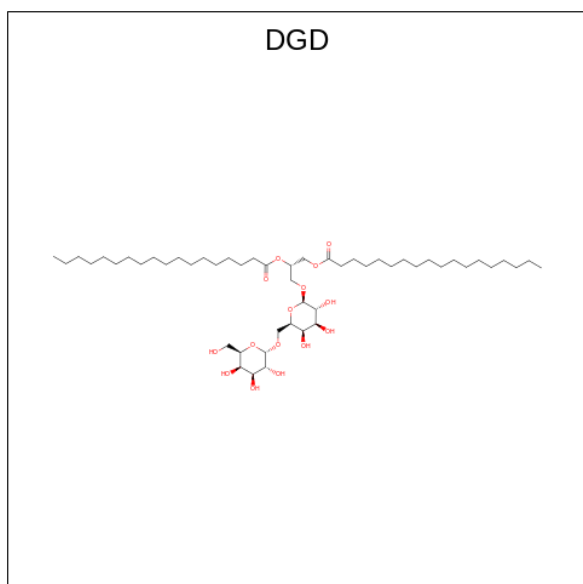
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0

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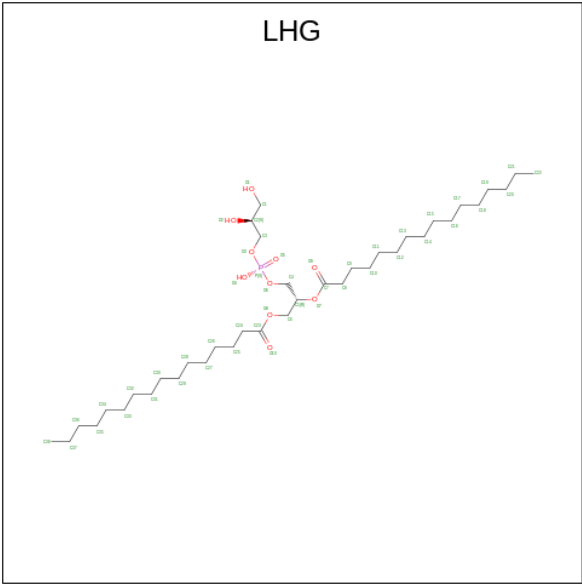
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	H	1	Total	C	O	S	0	0
			16	10	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			12	6	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	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	d	1	Total	C	O	S	0	0
			16	10	5	1		
36	o	1	Total	C	O	S	0	0
			19	13	5	1		
36	u	1	Total	C	O	S	0	0
			14	10	3	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	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
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: C₃₈H₇₅O₁₀P).



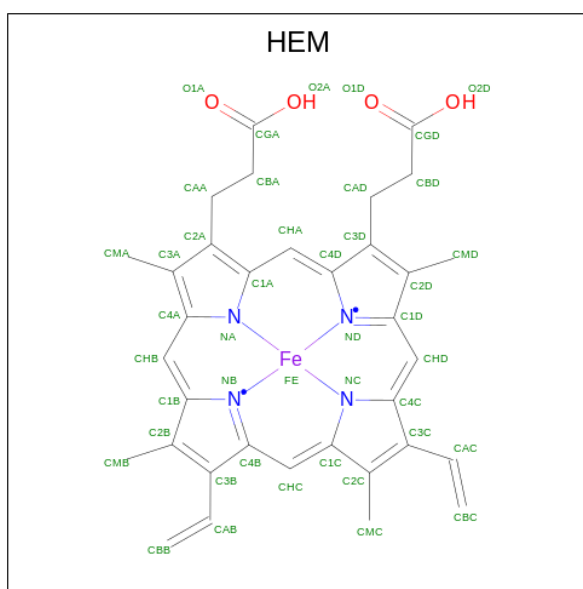
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		

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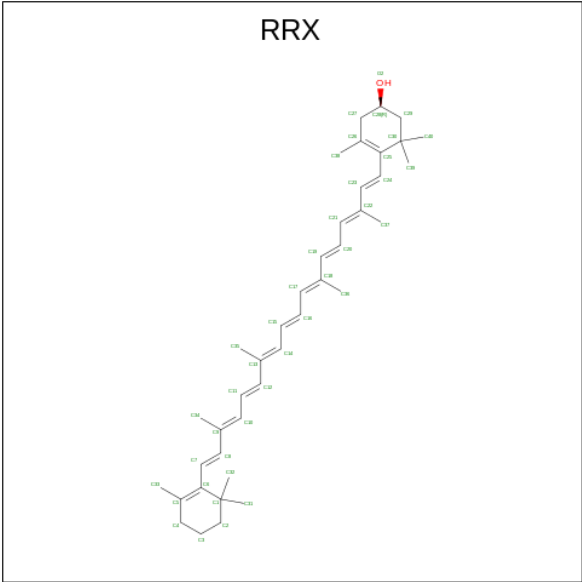
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			45	34	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		
38	L	1	Total	C	O	P	0	0
			49	38	10	1		
38	a	1	Total	C	O	P	0	0
			42	31	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			46	35	10	1		
38	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
			43	34	1	4	4	
39	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

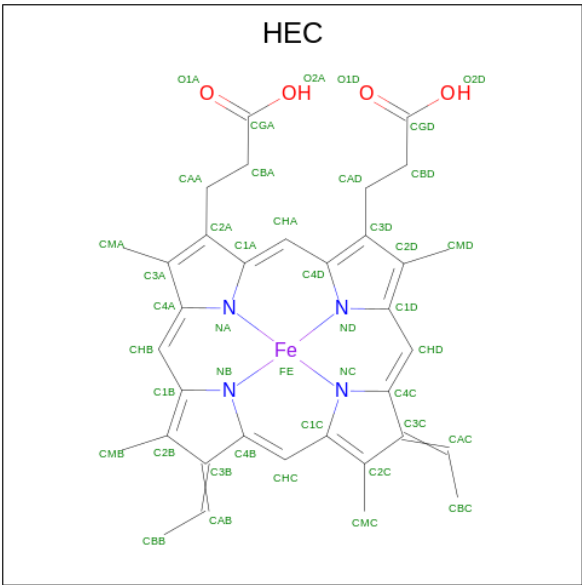


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	H	1	Total	C	O	0	0
			41	40	1		
40	h	1	Total	C	O	0	0
			41	40	1		

- 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: C₃₄H₃₄FeN₄O₄).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	164	Total	O	0	5
			169	169		
43	B	394	Total	O	0	15
			408	408		
43	C	274	Total	O	0	8
			282	282		
43	D	171	Total	O	0	5
			176	176		
43	E	31	Total	O	0	1
			32	32		
43	F	14	Total	O	0	0
			14	14		
43	H	56	Total	O	0	0
			56	56		
43	I	9	Total	O	0	0
			9	9		
43	J	16	Total	O	0	0
			16	16		
43	K	8	Total	O	0	1
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	L	20	Total 20	O 20	0	1
43	M	17	Total 19	O 19	0	2
43	O	197	Total 208	O 208	0	13
43	T	11	Total 11	O 11	0	0
43	U	99	Total 99	O 99	0	1
43	V	143	Total 146	O 146	0	3
43	X	16	Total 17	O 17	0	1
43	Y	7	Total 7	O 7	0	0
43	Z	1	Total 1	O 1	0	0
43	a	184	Total 192	O 192	0	9
43	b	381	Total 390	O 390	0	15
43	c	285	Total 298	O 298	0	12
43	d	170	Total 176	O 176	0	8
43	e	33	Total 34	O 34	0	1
43	f	8	Total 9	O 9	0	1
43	h	55	Total 57	O 57	0	2
43	i	19	Total 21	O 21	0	2
43	j	15	Total 16	O 16	0	2
43	k	11	Total 11	O 11	0	0
43	l	15	Total 17	O 17	0	3
43	m	23	Total 26	O 26	0	3

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	o	176	Total 188	O 188	0	12
43	t	18	Total 19	O 19	0	2
43	u	109	Total 114	O 114	0	6
43	v	112	Total 114	O 114	0	2
43	x	19	Total 19	O 19	0	0
43	y	5	Total 5	O 5	0	0
43	z	4	Total 4	O 4	0	0

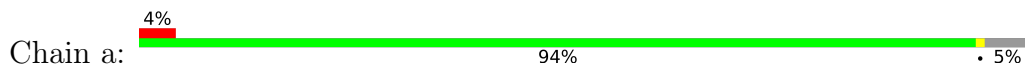
3 Residue-property plots [i](#)

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.

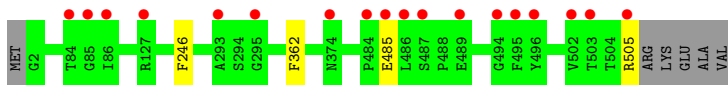
- Molecule 1: Photosystem II protein D1 3



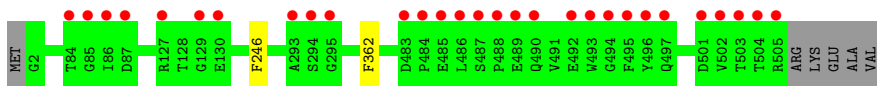
- Molecule 1: Photosystem II protein D1 3



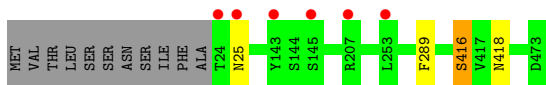
- Molecule 2: Photosystem II CP47 reaction center protein



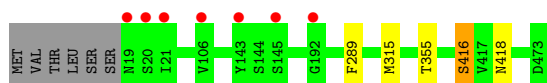
- Molecule 2: Photosystem II CP47 reaction center protein



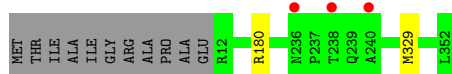
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



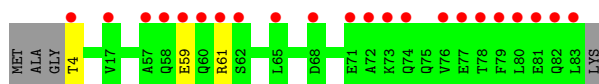
• Molecule 4: Photosystem II D2 protein



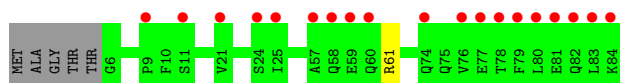
• Molecule 4: Photosystem II D2 protein



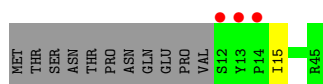
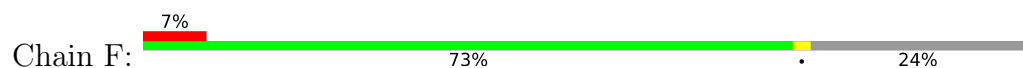
• Molecule 5: Cytochrome b559 subunit alpha



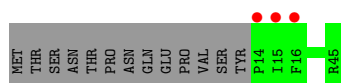
• Molecule 5: Cytochrome b559 subunit alpha



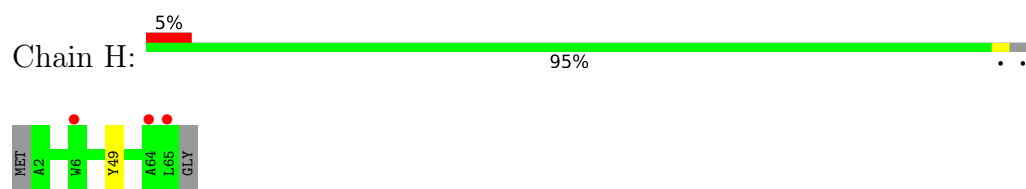
• Molecule 6: Cytochrome b559 subunit beta



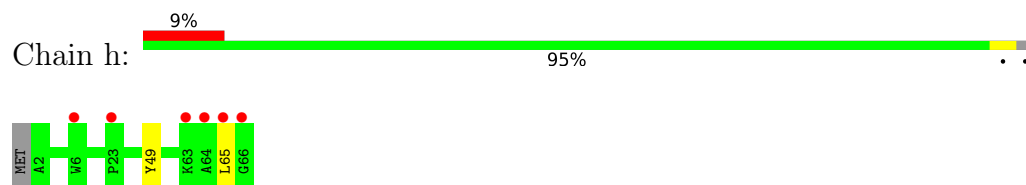
• Molecule 6: Cytochrome b559 subunit beta



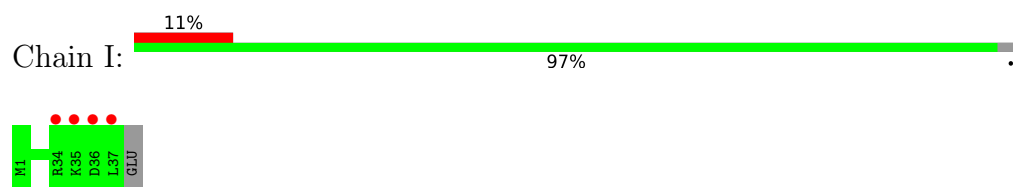
- Molecule 7: Photosystem II reaction center protein H



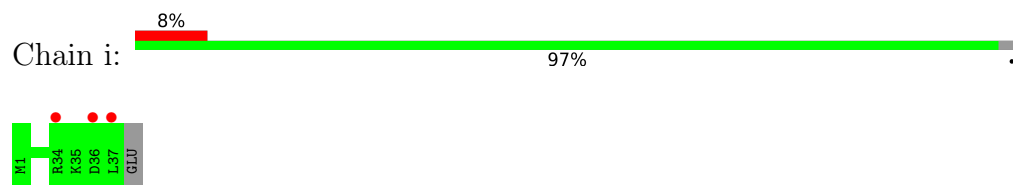
- Molecule 7: Photosystem II reaction center protein H



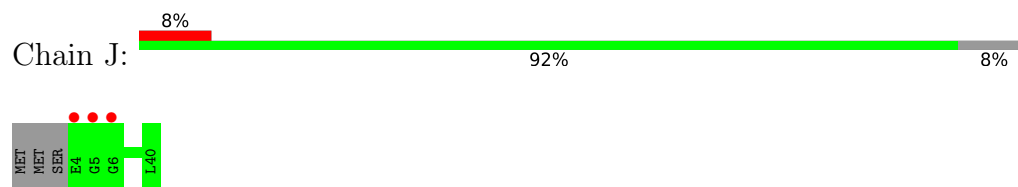
- Molecule 8: Photosystem II reaction center protein I



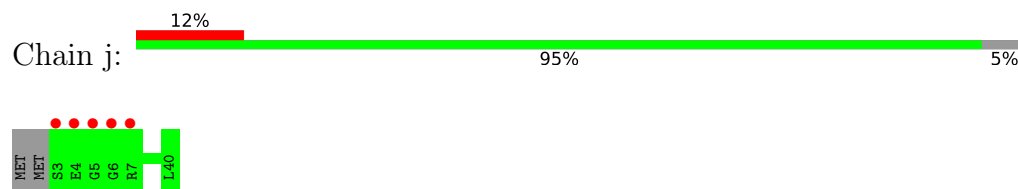
- Molecule 8: Photosystem II reaction center protein I



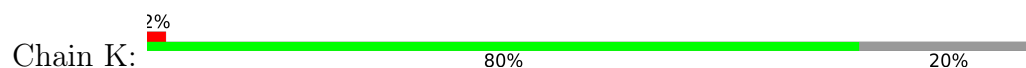
- Molecule 9: Photosystem II reaction center protein J

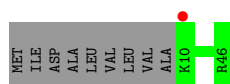


- Molecule 9: Photosystem II reaction center protein J

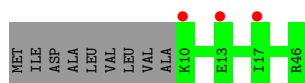
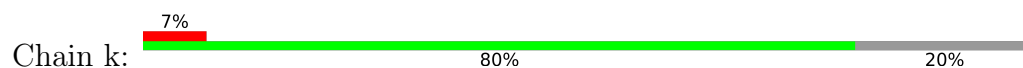


- Molecule 10: Photosystem II reaction center protein K

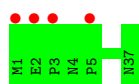




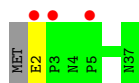
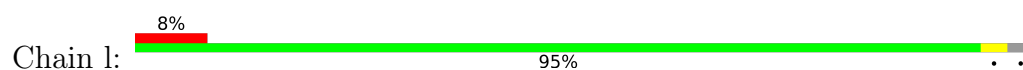
- Molecule 10: Photosystem II reaction center protein K



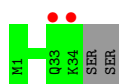
- Molecule 11: Photosystem II reaction center protein L



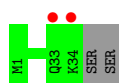
- Molecule 11: Photosystem II reaction center protein L



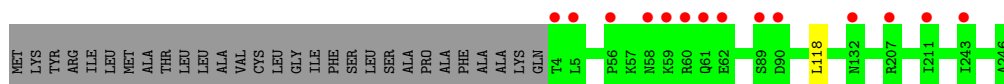
- Molecule 12: Photosystem II reaction center protein M



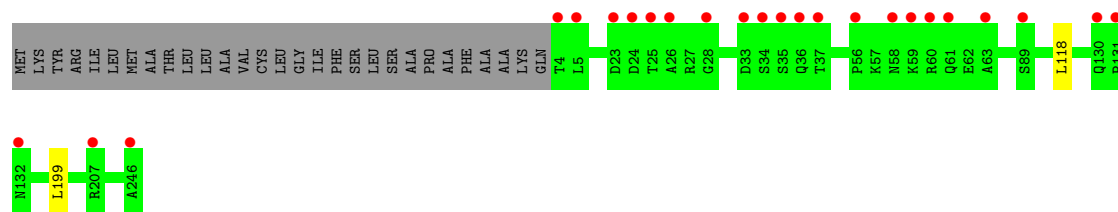
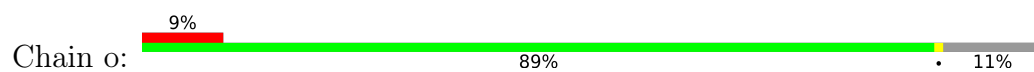
- Molecule 12: Photosystem II reaction center protein M



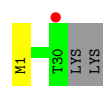
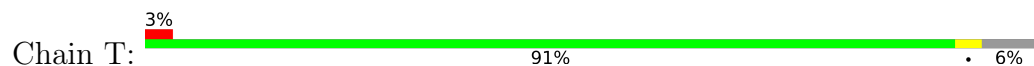
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



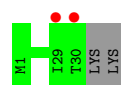
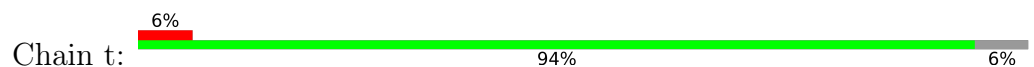
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



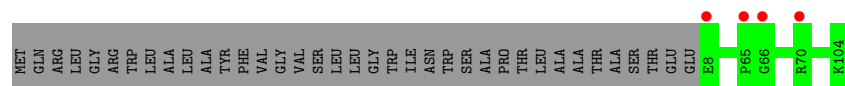
- Molecule 14: Photosystem II reaction center protein T



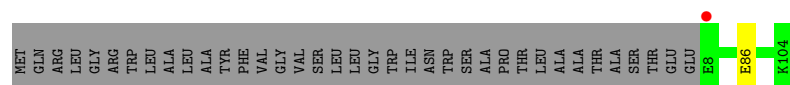
- Molecule 14: Photosystem II reaction center protein T



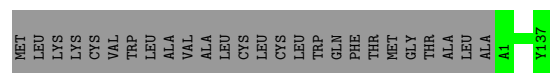
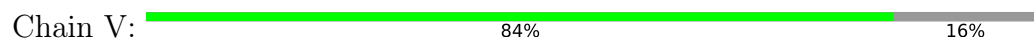
- Molecule 15: Photosystem II 12 kDa extrinsic protein



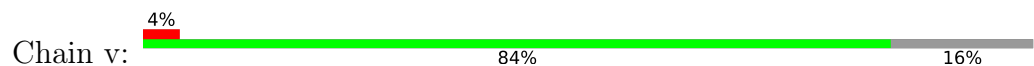
- Molecule 15: Photosystem II 12 kDa extrinsic protein

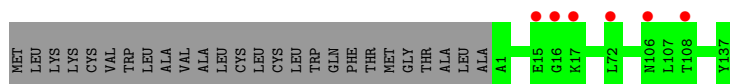


- Molecule 16: Cytochrome c-550

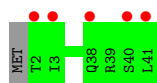


- Molecule 16: Cytochrome c-550





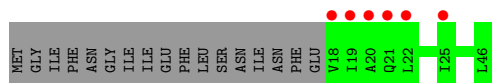
- Molecule 17: Photosystem II reaction center X protein



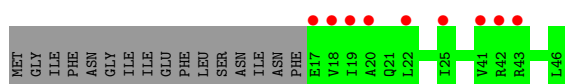
- Molecule 17: Photosystem II reaction center X protein



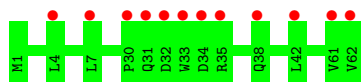
- Molecule 18: Photosystem II reaction center protein Ycf12



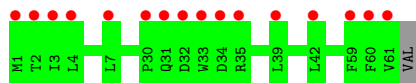
- Molecule 18: Photosystem II reaction center protein Ycf12



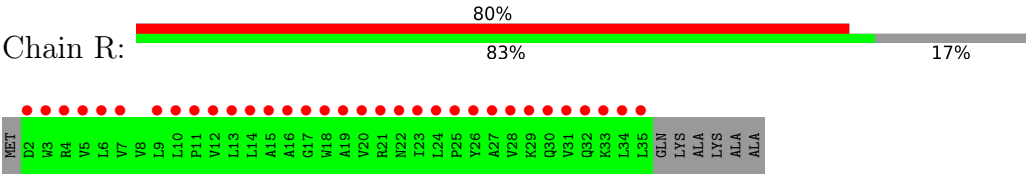
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.80Å 228.46Å 286.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.99-1.90) 99.6 (19.99-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, REFMAC 5.8.0103	Depositor
R, R_{free}	0.147 , 0.177 0.147 , 0.177	Depositor DCC
R_{free} test set	31327 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	55105	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.46	0/2709	0.56	0/3699
1	a	0.44	0/2743	0.54	0/3747
2	B	0.44	0/4145	0.53	0/5649
2	b	0.41	0/4134	0.53	0/5632
3	C	0.39	0/3608	0.51	0/4912
3	c	0.37	0/3653	0.50	0/4974
4	D	0.48	0/2812	0.56	0/3833
4	d	0.44	0/2817	0.53	0/3839
5	E	0.37	0/669	0.47	0/915
5	e	0.30	0/667	0.46	0/910
6	F	0.38	0/284	0.46	0/387
6	f	0.30	0/265	0.44	0/360
7	H	0.38	0/527	0.52	0/718
7	h	0.36	0/532	0.53	0/723
8	I	0.36	0/284	0.49	0/388
8	i	0.33	0/301	0.48	0/407
9	J	0.36	0/262	0.48	0/356
9	j	0.33	0/278	0.46	0/376
10	K	0.31	0/303	0.44	0/416
10	k	0.30	0/303	0.45	0/416
11	L	0.52	0/315	0.52	0/428
11	l	0.51	0/311	0.49	0/423
12	M	0.40	0/254	0.54	0/348
12	m	0.42	0/270	0.56	0/368
13	O	0.36	0/1903	0.57	0/2583
13	o	0.35	0/1888	0.57	0/2564
14	T	0.52	0/257	0.51	0/349
14	t	0.46	0/257	0.49	0/349
15	U	0.36	0/781	0.53	0/1059
15	u	0.36	0/785	0.52	0/1064
16	V	0.38	0/1091	0.52	0/1481

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1090	0.50	0/1483
17	X	0.29	0/301	0.40	0/407
17	x	0.29	0/278	0.42	0/376
18	Y	0.28	0/207	0.43	0/278
18	y	0.26	0/216	0.42	0/289
19	Z	0.28	0/509	0.40	0/699
19	z	0.27	0/461	0.37	0/633
20	R	0.23	0/208	0.39	0/289
All	All	0.40	0/42678	0.52	0/58127

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	328 (98%)	4 (1%)	1 (0%)	41	31
1	a	340/360 (94%)	335 (98%)	3 (1%)	2 (1%)	25	15
2	B	507/510 (99%)	501 (99%)	6 (1%)	0	100	100
2	b	508/510 (100%)	503 (99%)	5 (1%)	0	100	100
3	C	450/461 (98%)	440 (98%)	8 (2%)	2 (0%)	34	24
3	c	457/461 (99%)	448 (98%)	7 (2%)	2 (0%)	34	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/352 (97%)	334 (98%)	6 (2%)	0	100	100
4	d	340/352 (97%)	334 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	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	30/45 (67%)	30 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	9	2
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	35/40 (88%)	35 (100%)	0	0	100	100
9	j	36/40 (90%)	36 (100%)	0	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	36/37 (97%)	36 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	245/272 (90%)	239 (98%)	6 (2%)	0	100	100
13	o	244/272 (90%)	237 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
16	v	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
17	X	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
17	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
18	y	28/46 (61%)	28 (100%)	0	0	100	100
19	Z	65/62 (105%)	61 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
All	All	5262/5691 (92%)	5162 (98%)	92 (2%)	8 (0%)	51	38

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	4	VAL
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/291 (93%)	269 (100%)	1 (0%)	91	91
1	a	269/291 (92%)	269 (100%)	0	100	100
2	B	405/407 (100%)	401 (99%)	4 (1%)	76	76
2	b	401/407 (98%)	399 (100%)	2 (0%)	88	89
3	C	354/362 (98%)	349 (99%)	5 (1%)	67	65
3	c	359/362 (99%)	353 (98%)	6 (2%)	60	57
4	D	276/283 (98%)	274 (99%)	2 (1%)	84	84
4	d	276/283 (98%)	274 (99%)	2 (1%)	84	84
5	E	70/73 (96%)	67 (96%)	3 (4%)	29	19
5	e	69/73 (94%)	68 (99%)	1 (1%)	67	65
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	26
6	f	26/39 (67%)	26 (100%)	0	100	100
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	53
7	h	54/55 (98%)	53 (98%)	1 (2%)	57	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	29/34 (85%)	29 (100%)	0	100	100
8	i	33/34 (97%)	33 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	35
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	31/32 (97%)	31 (100%)	0	100	100
13	O	205/228 (90%)	204 (100%)	1 (0%)	88	89
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	76
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/112 (74%)	83 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	70
16	V	118/138 (86%)	118 (100%)	0	100	100
16	v	116/138 (84%)	116 (100%)	0	100	100
17	X	32/34 (94%)	32 (100%)	0	100	100
17	x	29/34 (85%)	28 (97%)	1 (3%)	37	28
18	Y	20/37 (54%)	20 (100%)	0	100	100
18	y	20/37 (54%)	20 (100%)	0	100	100
19	Z	49/52 (94%)	49 (100%)	0	100	100
19	z	45/52 (86%)	45 (100%)	0	100	100
20	R	11/33 (33%)	11 (100%)	0	100	100
All	All	4277/4643 (92%)	4242 (99%)	35 (1%)	81	82

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	61	ARG
7	h	49	TYR
13	o	199	LEU

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Mol	Chain	Res	Type
5	E	4	THR
4	D	329	MET

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	0.90	0	7,9,11	0.68	0
8	FME	i	1	8	8,9,10	0.88	0	7,9,11	0.98	0
14	FME	T	1	14	8,9,10	0.98	0	7,9,11	1.57	1 (14%)
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.68	0
14	FME	t	1	14	8,9,10	0.92	0	7,9,11	1.28	0
12	FME	m	1	12	8,9,10	1.04	0	7,9,11	0.50	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
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	3.12	115.37	109.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG

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 362 ligands modelled in this entry, 13 are monoatomic and 82 are unknown - leaving 267 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	F	103	-	36,36,36	0.46	0	47,47,47	0.79	1 (2%)
36	HTG	d	404	-	16,16,19	1.01	1 (6%)	20,21,24	1.55	1 (5%)
38	LHG	D	410	-	48,48,48	0.84	2 (4%)	51,54,54	1.21	8 (15%)
24	CLA	B	610	-	65,73,73	2.39	20 (30%)	76,113,113	2.37	24 (31%)
24	CLA	b	606	-	65,73,73	2.39	20 (30%)	76,113,113	2.44	26 (34%)
34	DMS	A	425	-	3,3,3	0.67	0	3,3,3	0.55	0
31	GOL	C	525	-	5,5,5	0.71	0	5,5,5	0.92	0
26	BCR	B	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.23	3 (5%)
29	PL9	a	417	-	55,55,55	0.63	1 (1%)	68,69,69	1.92	19 (27%)
31	GOL	O	304	-	5,5,5	0.90	0	5,5,5	0.96	0
34	DMS	c	539	-	3,3,3	0.69	0	3,3,3	0.53	0
27	SQD	B	622	-	53,54,54	1.03	3 (5%)	62,65,65	1.51	8 (12%)
24	CLA	b	609	-	65,73,73	2.37	18 (27%)	76,113,113	2.45	24 (31%)
40	RRX	h	101	-	42,42,42	3.99	15 (35%)	57,58,58	8.73	39 (68%)
36	HTG	B	629	-	19,19,19	0.95	2 (10%)	23,24,24	1.63	1 (4%)
34	DMS	b	633	-	3,3,3	0.66	0	3,3,3	0.66	0
39	HEM	e	102	6,5	41,50,50	1.34	8 (19%)	45,82,82	1.91	11 (24%)
24	CLA	b	610	-	65,73,73	2.43	19 (29%)	76,113,113	2.44	24 (31%)
31	GOL	b	638	-	5,5,5	0.97	0	5,5,5	0.98	0
34	DMS	C	538	-	3,3,3	0.65	0	3,3,3	0.59	0
34	DMS	B	641	-	3,3,3	0.66	0	3,3,3	0.57	0
34	DMS	C	535	-	3,3,3	0.58	0	3,3,3	0.53	0
36	HTG	H	101	-	16,16,19	1.03	1 (6%)	20,21,24	1.76	4 (20%)
34	DMS	e	103	-	3,3,3	0.67	0	3,3,3	0.49	0
36	HTG	V	202	-	11,12,19	0.29	0	15,17,24	1.73	3 (20%)
26	BCR	a	414	-	41,41,41	1.05	1 (2%)	56,56,56	1.08	2 (3%)
34	DMS	u	202	-	3,3,3	0.68	0	3,3,3	0.55	0
34	DMS	C	540	-	3,3,3	0.66	0	3,3,3	0.60	0
36	HTG	B	626	-	19,19,19	0.98	1 (5%)	23,24,24	1.93	3 (13%)
34	DMS	A	424	-	3,3,3	0.64	0	3,3,3	0.56	0
36	HTG	B	630	-	19,19,19	0.97	1 (5%)	23,24,24	1.37	1 (4%)
34	DMS	B	642	-	3,3,3	0.67	0	3,3,3	0.56	0
28	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.08	5 (8%)
27	SQD	A	411	-	53,54,54	0.94	3 (5%)	62,65,65	1.78	10 (16%)
24	CLA	B	616	-	65,73,73	2.27	21 (32%)	76,113,113	2.72	29 (38%)
34	DMS	c	529	-	3,3,3	0.67	0	3,3,3	0.61	0
34	DMS	c	531	-	3,3,3	0.67	0	3,3,3	0.39	0
28	LMG	D	413	41	51,51,55	0.83	2 (3%)	59,59,63	0.83	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	D	401	43	65,73,73	2.09	19 (29%)	76,113,113	2.56	28 (36%)
27	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.20	6 (9%)
34	DMS	c	537	-	3,3,3	0.67	0	3,3,3	0.58	0
37	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.95	5 (6%)
38	LHG	d	410	-	48,48,48	0.87	2 (4%)	51,54,54	0.89	2 (3%)
34	DMS	D	418	-	3,3,3	0.63	0	3,3,3	0.31	0
24	CLA	a	410	43	65,73,73	2.24	18 (27%)	76,113,113	2.81	30 (39%)
34	DMS	a	403	-	3,3,3	0.66	0	3,3,3	0.52	0
27	SQD	f	802	-	42,43,54	1.17	3 (7%)	51,54,65	1.55	8 (15%)
21	OEX	a	404	43,3,1	0,15,15	-	-	-	-	-
24	CLA	C	509	43	65,73,73	2.48	20 (30%)	76,113,113	2.56	25 (32%)
29	PL9	A	413	-	55,55,55	0.61	2 (3%)	68,69,69	1.89	20 (29%)
31	GOL	V	207	-	5,5,5	0.89	0	5,5,5	0.95	0
34	DMS	b	643	-	3,3,3	0.63	0	3,3,3	0.60	0
34	DMS	c	538	-	3,3,3	0.64	0	3,3,3	0.41	0
24	CLA	b	612	-	65,73,73	2.44	19 (29%)	76,113,113	2.35	27 (35%)
28	LMG	z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.31	6 (13%)
34	DMS	c	535	-	3,3,3	0.70	0	3,3,3	0.53	0
36	HTG	b	603	-	19,19,19	1.06	2 (10%)	23,24,24	0.99	1 (4%)
24	CLA	a	413	-	65,73,73	2.20	18 (27%)	76,113,113	2.60	28 (36%)
24	CLA	b	619	-	65,73,73	2.25	18 (27%)	76,113,113	2.52	26 (34%)
33	BCT	A	423[B]	22	2,3,3	0.65	0	2,3,3	0.56	0
24	CLA	c	506	43	65,73,73	2.32	19 (29%)	76,113,113	2.54	29 (38%)
28	LMG	b	624	-	51,51,55	0.92	2 (3%)	59,59,63	1.12	6 (10%)
31	GOL	A	418	-	5,5,5	1.01	0	5,5,5	1.00	0
37	DGD	d	416	-	50,50,67	0.98	2 (4%)	58,58,81	1.08	4 (6%)
28	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.13	5 (8%)
31	GOL	a	419	-	5,5,5	1.03	0	5,5,5	0.89	0
24	CLA	a	409	-	65,73,73	2.41	20 (30%)	76,113,113	2.43	25 (32%)
32	LMT	m	103	-	36,36,36	0.46	0	47,47,47	0.89	2 (4%)
27	SQD	A	415	-	53,54,54	1.00	3 (5%)	62,65,65	1.33	8 (12%)
34	DMS	h	107	-	3,3,3	0.66	0	3,3,3	0.50	0
38	LHG	D	412	-	44,44,48	0.87	2 (4%)	47,50,54	1.09	3 (6%)
24	CLA	b	607	-	65,73,73	2.44	19 (29%)	76,113,113	2.48	27 (35%)
34	DMS	O	310	-	3,3,3	0.67	0	3,3,3	0.73	0
34	DMS	c	530	-	3,3,3	0.61	0	3,3,3	0.64	0
34	DMS	B	643	-	3,3,3	0.68	0	3,3,3	0.53	0
34	DMS	V	208	-	3,3,3	0.65	0	3,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	614	43	65,73,73	2.40	19 (29%)	76,113,113	2.38	28 (36%)
24	CLA	A	405	-	65,73,73	2.36	18 (27%)	76,113,113	2.32	25 (32%)
24	CLA	B	612	43	65,73,73	2.35	20 (30%)	76,113,113	2.42	25 (32%)
32	LMT	b	629	-	24,24,36	0.49	0	29,29,47	1.25	5 (17%)
24	CLA	c	515	-	65,73,73	2.60	20 (30%)	76,113,113	2.39	24 (31%)
32	LMT	b	625	-	36,36,36	0.44	0	47,47,47	1.20	5 (10%)
34	DMS	T	103	-	3,3,3	0.66	0	3,3,3	0.65	0
34	DMS	a	422	-	3,3,3	0.74	0	3,3,3	0.28	0
34	DMS	b	644	-	3,3,3	0.66	0	3,3,3	0.67	0
24	CLA	c	504	-	65,73,73	2.53	20 (30%)	76,113,113	2.32	25 (32%)
34	DMS	c	534	-	3,3,3	0.67	0	3,3,3	0.52	0
34	DMS	v	205	-	3,3,3	0.68	0	3,3,3	0.52	0
36	HTG	b	628	-	19,19,19	1.03	2 (10%)	23,24,24	1.63	3 (13%)
24	CLA	c	508	-	65,73,73	2.62	20 (30%)	76,113,113	2.41	27 (35%)
34	DMS	C	536	-	3,3,3	0.69	0	3,3,3	0.46	0
24	CLA	B	607	-	65,73,73	2.45	18 (27%)	76,113,113	2.63	24 (31%)
34	DMS	V	210	-	3,3,3	0.66	0	3,3,3	0.51	0
37	DGD	H	104	-	63,63,67	0.88	3 (4%)	77,77,81	0.97	4 (5%)
34	DMS	d	418	-	3,3,3	0.66	0	3,3,3	0.65	0
24	CLA	B	605	-	65,73,73	2.34	19 (29%)	76,113,113	2.61	25 (32%)
34	DMS	E	104	-	3,3,3	0.67	0	3,3,3	0.52	0
34	DMS	O	305	-	3,3,3	0.64	0	3,3,3	0.43	0
34	DMS	B	634	-	3,3,3	0.65	0	3,3,3	0.75	0
32	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.86	0
24	CLA	B	614	-	65,73,73	2.21	18 (27%)	76,113,113	2.49	25 (32%)
34	DMS	O	307	-	3,3,3	0.68	0	3,3,3	0.58	0
42	HEC	V	201	16	32,50,50	1.50	4 (12%)	24,82,82	1.41	3 (12%)
37	DGD	C	520	-	63,63,67	0.81	2 (3%)	77,77,81	0.98	4 (5%)
24	CLA	C	505	-	65,73,73	2.81	19 (29%)	76,113,113	2.29	23 (30%)
34	DMS	a	426	-	3,3,3	0.65	0	3,3,3	0.45	0
32	LMT	j	102	-	24,24,36	0.49	0	29,29,47	0.76	0
24	CLA	B	606	-	65,73,73	2.36	19 (29%)	76,113,113	2.47	25 (32%)
34	DMS	c	536	-	3,3,3	0.65	0	3,3,3	0.57	0
34	DMS	d	417	-	3,3,3	0.64	0	3,3,3	0.33	0
34	DMS	d	419	-	3,3,3	0.68	0	3,3,3	0.56	0
36	HTG	b	602	-	19,19,19	0.99	2 (10%)	23,24,24	1.54	1 (4%)
29	PL9	D	408	-	55,55,55	0.72	2 (3%)	68,69,69	1.56	16 (23%)
29	PL9	d	408	-	55,55,55	0.77	2 (3%)	68,69,69	1.47	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	m	102	-	36,36,36	0.42	0	47,47,47	0.95	1 (2%)
25	PHO	A	407	-	51,69,69	1.70	7 (13%)	47,99,99	1.65	10 (21%)
33	BCT	D	404[A]	22	2,3,3	0.63	0	2,3,3	1.05	0
34	DMS	o	304	-	3,3,3	0.66	0	3,3,3	0.52	0
33	BCT	d	402[B]	22	2,3,3	0.61	0	2,3,3	1.15	0
24	CLA	B	611	-	65,73,73	2.47	18 (27%)	76,113,113	2.43	23 (30%)
26	BCR	d	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.56	13 (23%)
34	DMS	C	539	-	3,3,3	0.64	0	3,3,3	0.69	0
36	HTG	u	201	-	10,13,19	1.18	1 (10%)	13,14,24	1.79	1 (7%)
37	DGD	c	520	-	63,63,67	0.82	2 (3%)	77,77,81	0.94	5 (6%)
26	BCR	b	621	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	7 (12%)
24	CLA	B	603	43	65,73,73	2.49	21 (32%)	76,113,113	2.45	22 (28%)
33	BCT	a	408[A]	22	2,3,3	0.66	0	2,3,3	0.53	0
34	DMS	u	203	-	3,3,3	0.61	0	3,3,3	0.76	0
26	BCR	D	407	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	12 (21%)
34	DMS	o	303	-	3,3,3	0.63	0	3,3,3	0.58	0
24	CLA	A	406	43	65,73,73	2.18	19 (29%)	76,113,113	2.56	28 (36%)
24	CLA	b	618	-	65,73,73	2.21	18 (27%)	76,113,113	2.60	28 (36%)
34	DMS	a	424	-	3,3,3	0.66	0	3,3,3	0.60	0
24	CLA	b	613	-	65,73,73	2.67	19 (29%)	76,113,113	2.45	24 (31%)
26	BCR	k	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.38	9 (16%)
32	LMT	a	421	-	36,36,36	0.46	0	47,47,47	1.05	5 (10%)
37	DGD	C	518	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	5 (6%)
24	CLA	c	510	-	65,73,73	2.33	18 (27%)	76,113,113	2.57	24 (31%)
26	BCR	B	621	-	41,41,41	1.01	1 (2%)	56,56,56	1.24	4 (7%)
24	CLA	a	411	43	65,73,73	2.17	19 (29%)	76,113,113	2.51	26 (34%)
24	CLA	b	615	-	65,73,73	2.40	19 (29%)	76,113,113	2.57	28 (36%)
24	CLA	C	507	-	65,73,73	2.54	20 (30%)	76,113,113	2.29	21 (27%)
34	DMS	v	202	-	3,3,3	0.63	0	3,3,3	0.51	0
24	CLA	C	506	43	65,73,73	2.31	20 (30%)	76,113,113	2.61	30 (39%)
26	BCR	t	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.49	11 (19%)
32	LMT	b	626	-	36,36,36	0.39	0	47,47,47	0.97	3 (6%)
24	CLA	C	513	3	65,73,73	2.44	20 (30%)	76,113,113	2.36	26 (34%)
26	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	8 (14%)
26	BCR	b	622	-	41,41,41	1.05	1 (2%)	56,56,56	1.24	6 (10%)
34	DMS	V	211	-	3,3,3	0.66	0	3,3,3	0.57	0
24	CLA	b	617	-	65,73,73	2.32	20 (30%)	76,113,113	2.52	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	v	204	-	3,3,3	0.65	0	3,3,3	0.53	0
24	CLA	c	514	-	65,73,73	2.57	19 (29%)	76,113,113	2.44	29 (38%)
34	DMS	O	308	-	3,3,3	0.68	0	3,3,3	0.57	0
24	CLA	B	618	-	65,73,73	2.32	18 (27%)	76,113,113	2.55	23 (30%)
27	SQD	F	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.82	9 (17%)
28	LMG	B	623	-	51,51,55	0.95	2 (3%)	59,59,63	1.21	5 (8%)
28	LMG	d	412	41	51,51,55	0.87	2 (3%)	59,59,63	0.90	3 (5%)
24	CLA	C	515	-	65,73,73	2.57	19 (29%)	76,113,113	2.40	25 (32%)
24	CLA	c	509	43	65,73,73	2.60	20 (30%)	76,113,113	2.48	24 (31%)
34	DMS	C	534	-	3,3,3	0.70	0	3,3,3	0.31	0
31	GOL	A	421	-	5,5,5	0.90	0	5,5,5	1.00	0
28	LMG	C	533	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	6 (10%)
26	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.19	4 (7%)
31	GOL	d	415	-	5,5,5	0.91	0	5,5,5	0.79	0
28	LMG	i	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.14	5 (8%)
36	HTG	o	301	-	19,19,19	1.02	1 (5%)	23,24,24	1.50	2 (8%)
38	LHG	D	411	-	48,48,48	0.84	2 (4%)	51,54,54	0.93	3 (5%)
25	PHO	A	408	-	51,69,69	1.86	8 (15%)	47,99,99	1.73	7 (14%)
24	CLA	D	405	-	65,73,73	2.09	19 (29%)	76,113,113	2.63	27 (35%)
24	CLA	c	503	-	65,73,73	2.48	20 (30%)	76,113,113	2.60	24 (31%)
24	CLA	c	513	3	65,73,73	2.56	19 (29%)	76,113,113	2.26	28 (36%)
27	SQD	a	415	-	53,54,54	0.93	3 (5%)	62,65,65	1.92	11 (17%)
24	CLA	B	608	-	65,73,73	2.34	17 (26%)	76,113,113	2.79	26 (34%)
26	BCR	k	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	9 (16%)
24	CLA	b	611	43	65,73,73	2.34	20 (30%)	76,113,113	2.42	27 (35%)
34	DMS	b	631	-	3,3,3	0.66	0	3,3,3	0.31	0
34	DMS	b	632	-	3,3,3	0.64	0	3,3,3	0.37	0
34	DMS	b	642	-	3,3,3	0.67	0	3,3,3	0.58	0
38	LHG	L	101	-	48,48,48	0.88	2 (4%)	51,54,54	1.04	4 (7%)
24	CLA	C	514	-	65,73,73	2.39	20 (30%)	76,113,113	2.45	28 (36%)
34	DMS	O	309	-	3,3,3	0.68	0	3,3,3	0.74	0
38	LHG	d	411	-	45,45,48	0.93	2 (4%)	48,51,54	1.05	4 (8%)
38	LHG	a	416	-	41,41,48	1.02	2 (4%)	44,47,54	1.01	2 (4%)
34	DMS	T	104	-	3,3,3	0.67	0	3,3,3	0.46	0
34	DMS	O	306	-	3,3,3	0.67	0	3,3,3	0.60	0
28	LMG	A	412	-	51,51,55	0.94	2 (3%)	59,59,63	1.08	3 (5%)
32	LMT	A	422	-	36,36,36	0.46	0	47,47,47	0.96	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	T	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	12 (21%)
32	LMT	D	402	-	36,36,36	0.39	0	47,47,47	1.02	4 (8%)
25	PHO	d	401	-	51,69,69	1.82	8 (15%)	47,99,99	1.84	8 (17%)
24	CLA	D	406	-	65,73,73	2.27	19 (29%)	76,113,113	2.54	29 (38%)
31	GOL	v	203	-	5,5,5	0.91	0	5,5,5	1.09	0
34	DMS	B	632	-	3,3,3	0.67	0	3,3,3	0.40	0
24	CLA	C	503	-	65,73,73	2.40	20 (30%)	76,113,113	2.53	21 (27%)
24	CLA	b	620	-	65,73,73	2.45	18 (27%)	76,113,113	2.53	24 (31%)
34	DMS	b	641	-	3,3,3	0.68	0	3,3,3	0.32	0
34	DMS	O	302	-	3,3,3	0.62	0	3,3,3	0.46	0
36	HTG	c	523	-	19,19,19	0.97	2 (10%)	23,24,24	1.50	3 (13%)
34	DMS	a	425	-	3,3,3	0.65	0	3,3,3	0.58	0
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.16	4 (9%)
26	BCR	C	517	-	41,41,41	1.01	1 (2%)	56,56,56	1.45	10 (17%)
24	CLA	c	512	-	65,73,73	2.33	20 (30%)	76,113,113	2.40	27 (35%)
24	CLA	b	616	-	65,73,73	2.45	19 (29%)	76,113,113	2.54	25 (32%)
24	CLA	C	511	-	65,73,73	2.49	20 (30%)	76,113,113	2.46	29 (38%)
21	OEX	A	401	43,3,1	0,15,15	-	-	-	-	-
27	SQD	b	601	-	53,54,54	1.02	4 (7%)	62,65,65	1.37	9 (14%)
37	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.09	7 (9%)
24	CLA	C	510	-	65,73,73	2.36	19 (29%)	76,113,113	2.46	23 (30%)
24	CLA	A	409	-	65,73,73	2.26	21 (32%)	76,113,113	2.60	28 (36%)
24	CLA	C	504	-	65,73,73	2.52	20 (30%)	76,113,113	2.43	22 (28%)
34	DMS	C	501	-	3,3,3	0.68	0	3,3,3	0.58	0
36	HTG	O	303	-	19,19,19	1.01	1 (5%)	23,24,24	1.08	2 (8%)
24	CLA	B	604	-	65,73,73	2.35	20 (30%)	76,113,113	2.39	28 (36%)
24	CLA	C	508	-	65,73,73	2.49	21 (32%)	76,113,113	2.27	26 (34%)
32	LMT	B	624	-	36,36,36	0.40	0	47,47,47	1.23	5 (10%)
32	LMT	J	102	-	24,24,36	0.55	1 (4%)	29,29,47	0.93	1 (3%)
24	CLA	b	608	-	65,73,73	2.52	19 (29%)	76,113,113	2.36	23 (30%)
34	DMS	V	209	-	3,3,3	0.66	0	3,3,3	0.51	0
24	CLA	B	613	-	65,73,73	2.34	17 (26%)	76,113,113	2.45	28 (36%)
34	DMS	C	537	-	3,3,3	0.66	0	3,3,3	0.62	0
32	LMT	f	801	-	25,25,36	0.53	1 (4%)	30,30,47	0.57	0
32	LMT	D	409	-	36,36,36	0.48	0	47,47,47	1.08	4 (8%)
34	DMS	a	423	-	3,3,3	0.64	0	3,3,3	0.55	0
31	GOL	D	417	-	5,5,5	0.90	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	c	533	-	3,3,3	0.65	0	3,3,3	0.56	0
34	DMS	c	532	-	3,3,3	0.55	0	3,3,3	1.24	0
24	CLA	B	615	-	65,73,73	2.32	18 (27%)	76,113,113	2.51	24 (31%)
26	BCR	K	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.54	12 (21%)
24	CLA	c	507	-	65,73,73	2.45	19 (29%)	76,113,113	2.34	25 (32%)
36	HTG	B	625	-	19,19,19	0.78	1 (5%)	23,24,24	1.70	4 (17%)
36	HTG	C	523	-	19,19,19	1.00	2 (10%)	23,24,24	1.60	2 (8%)
24	CLA	B	609	43	65,73,73	2.30	19 (29%)	76,113,113	2.40	24 (31%)
26	BCR	c	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.34	8 (14%)
24	CLA	d	406	-	65,73,73	2.34	20 (30%)	76,113,113	2.46	27 (35%)
32	LMT	M	101	-	36,36,36	0.44	0	47,47,47	0.99	2 (4%)
32	LMT	B	638	-	36,36,36	0.41	0	47,47,47	1.09	4 (8%)
34	DMS	B	633	-	3,3,3	0.65	0	3,3,3	0.27	0
24	CLA	B	617	-	65,73,73	2.23	20 (30%)	76,113,113	2.43	26 (34%)
37	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.18	7 (9%)
34	DMS	B	640	-	3,3,3	0.64	0	3,3,3	0.47	0
28	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.20	6 (10%)
38	LHG	d	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
26	BCR	C	516	-	41,41,41	1.00	1 (2%)	56,56,56	1.27	5 (8%)
24	CLA	C	512	-	65,73,73	2.37	19 (29%)	76,113,113	2.40	26 (34%)
32	LMT	a	402	-	36,36,36	0.40	0	47,47,47	0.84	1 (2%)
34	DMS	V	203	-	3,3,3	0.67	0	3,3,3	0.57	0
24	CLA	c	505	-	65,73,73	2.47	19 (29%)	76,113,113	2.33	23 (30%)
31	GOL	b	639	-	5,5,5	1.15	0	5,5,5	1.00	0
26	BCR	A	410	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	13 (23%)
24	CLA	d	405	-	65,73,73	2.36	20 (30%)	76,113,113	2.41	26 (34%)
28	LMG	Z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.24	4 (8%)
39	HEM	F	102	6,5	41,50,50	1.35	5 (12%)	45,82,82	2.05	11 (24%)
38	LHG	l	102	-	48,48,48	0.86	2 (4%)	51,54,54	1.05	4 (7%)
36	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.61	3 (13%)
24	CLA	b	605	43	65,73,73	2.49	19 (29%)	76,113,113	2.47	24 (31%)
34	DMS	o	305	-	3,3,3	0.65	0	3,3,3	0.53	0
24	CLA	c	511	-	65,73,73	2.46	19 (29%)	76,113,113	2.43	27 (35%)
36	HTG	c	524	-	19,19,19	1.01	2 (10%)	23,24,24	1.57	4 (17%)
26	BCR	b	623	-	41,41,41	1.08	1 (2%)	56,56,56	1.39	10 (17%)
26	BCR	c	516	-	41,41,41	1.06	1 (2%)	56,56,56	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	RRX	H	103	-	42,42,42	4.02	15 (35%)	57,58,58	8.18	42 (73%)
42	HEC	v	201	16	32,50,50	1.51	4 (12%)	24,82,82	1.48	6 (25%)
37	DGD	h	102	-	63,63,67	0.92	4 (6%)	77,77,81	0.95	4 (5%)
34	DMS	B	639	-	3,3,3	0.66	0	3,3,3	0.51	0
25	PHO	a	412	-	51,69,69	1.73	7 (13%)	47,99,99	1.66	10 (21%)
36	HTG	b	627	-	19,19,19	0.88	1 (5%)	23,24,24	1.68	5 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	F	103	-	-	10/21/61/61	0/2/2/2
36	HTG	d	404	-	-	2/7/27/30	0/1/1/1
38	LHG	D	410	-	-	5/53/53/53	-
24	CLA	b	606	-	1/1/15/20	6/37/115/115	-
24	CLA	B	610	-	-	1/37/115/115	-
31	GOL	C	525	-	-	4/4/4/4	-
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2
29	PL9	a	417	-	-	12/53/73/73	0/1/1/1
31	GOL	O	304	-	-	0/4/4/4	-
27	SQD	B	622	-	-	20/49/69/69	0/1/1/1
24	CLA	b	609	-	1/1/15/20	7/37/115/115	-
40	RRX	h	101	-	-	6/29/65/65	0/2/2/2
36	HTG	B	629	-	-	3/10/30/30	0/1/1/1
39	HEM	e	102	6,5	-	6/12/54/54	-
24	CLA	b	610	-	1/1/15/20	4/37/115/115	-
31	GOL	b	638	-	-	0/4/4/4	-
36	HTG	H	101	-	-	1/7/27/30	0/1/1/1
36	HTG	V	202	-	-	0/2/22/30	0/1/1/1
26	BCR	a	414	-	-	0/29/63/63	0/2/2/2
36	HTG	B	630	-	-	0/10/30/30	0/1/1/1
36	HTG	B	626	-	-	5/10/30/30	0/1/1/1
28	LMG	c	522	-	-	13/46/66/70	0/1/1/1
27	SQD	A	411	-	-	10/49/69/69	0/1/1/1
24	CLA	B	616	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	D	413	41	-	6/46/66/70	0/1/1/1
24	CLA	D	401	43	-	3/37/115/115	-
27	SQD	a	401	-	-	18/49/69/69	0/1/1/1
37	DGD	c	519	-	-	12/51/91/95	0/2/2/2
38	LHG	d	410	-	-	8/53/53/53	-
24	CLA	a	410	43	1/1/15/20	6/37/115/115	-
27	SQD	f	802	-	-	15/38/58/69	0/1/1/1
24	CLA	C	509	43	1/1/15/20	7/37/115/115	-
29	PL9	A	413	-	-	8/53/73/73	0/1/1/1
31	GOL	V	207	-	-	2/4/4/4	-
36	HTG	b	603	-	-	1/10/30/30	0/1/1/1
24	CLA	b	612	-	-	1/37/115/115	-
28	LMG	z	101	-	-	8/31/51/70	0/1/1/1
24	CLA	b	619	-	1/1/15/20	4/37/115/115	-
24	CLA	a	413	-	-	10/37/115/115	-
24	CLA	c	506	43	1/1/15/20	10/37/115/115	-
28	LMG	b	624	-	-	10/46/66/70	0/1/1/1
31	GOL	A	418	-	-	4/4/4/4	-
37	DGD	d	416	-	-	14/44/64/95	0/1/1/2
28	LMG	C	521	-	-	7/46/66/70	0/1/1/1
31	GOL	a	419	-	-	2/4/4/4	-
24	CLA	a	409	-	1/1/15/20	3/37/115/115	-
32	LMT	m	103	-	-	5/21/61/61	0/2/2/2
27	SQD	A	415	-	-	15/49/69/69	0/1/1/1
38	LHG	D	412	-	-	13/49/49/53	-
24	CLA	b	607	-	1/1/15/20	5/37/115/115	-
24	CLA	b	614	43	1/1/15/20	6/37/115/115	-
24	CLA	A	405	-	1/1/15/20	4/37/115/115	-
24	CLA	B	612	43	1/1/15/20	4/37/115/115	-
32	LMT	b	629	-	-	7/15/35/61	0/1/1/2
24	CLA	c	515	-	-	4/37/115/115	-
32	LMT	b	625	-	-	7/21/61/61	0/2/2/2
36	HTG	b	628	-	-	5/10/30/30	0/1/1/1
24	CLA	c	504	-	-	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	508	-	1/1/15/20	4/37/115/115	-
24	CLA	B	607	-	1/1/15/20	5/37/115/115	-
37	DGD	H	104	-	-	13/51/91/95	0/2/2/2
24	CLA	B	605	-	1/1/15/20	6/37/115/115	-
32	LMT	M	102	-	-	1/21/61/61	0/2/2/2
24	CLA	B	614	-	1/1/15/20	0/37/115/115	-
42	HEC	V	201	16	-	2/10/54/54	-
37	DGD	C	520	-	-	6/51/91/95	0/2/2/2
24	CLA	C	505	-	1/1/15/20	3/37/115/115	-
32	LMT	j	102	-	-	2/15/35/61	0/1/1/2
24	CLA	B	606	-	1/1/15/20	3/37/115/115	-
36	HTG	b	602	-	-	2/10/30/30	0/1/1/1
29	PL9	D	408	-	-	1/53/73/73	0/1/1/1
29	PL9	d	408	-	-	1/53/73/73	0/1/1/1
32	LMT	m	102	-	-	0/21/61/61	0/2/2/2
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
24	CLA	B	611	-	1/1/15/20	4/37/115/115	-
26	BCR	d	407	-	-	4/29/63/63	0/2/2/2
36	HTG	u	201	-	-	8/12/14/30	-
37	DGD	c	520	-	-	14/51/91/95	0/2/2/2
26	BCR	b	621	-	-	1/29/63/63	0/2/2/2
24	CLA	B	603	43	1/1/15/20	16/37/115/115	-
26	BCR	D	407	-	-	4/29/63/63	0/2/2/2
24	CLA	b	618	-	1/1/15/20	13/37/115/115	-
24	CLA	A	406	43	-	3/37/115/115	-
24	CLA	b	613	-	1/1/15/20	3/37/115/115	-
26	BCR	k	103	-	-	0/29/63/63	0/2/2/2
32	LMT	a	421	-	-	6/21/61/61	0/2/2/2
37	DGD	C	518	-	-	14/51/91/95	0/2/2/2
24	CLA	c	510	-	-	2/37/115/115	-
26	BCR	B	621	-	-	0/29/63/63	0/2/2/2
24	CLA	a	411	43	-	7/37/115/115	-
24	CLA	b	615	-	-	0/37/115/115	-
24	CLA	C	507	-	1/1/15/20	0/37/115/115	-
24	CLA	C	506	43	1/1/15/20	6/37/115/115	-
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	b	626	-	-	5/21/61/61	0/2/2/2
24	CLA	C	513	3	1/1/15/20	0/37/115/115	-
26	BCR	K	102	-	-	0/29/63/63	0/2/2/2
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	CLA	b	617	-	1/1/15/20	5/37/115/115	-
24	CLA	c	514	-	1/1/15/20	4/37/115/115	-
24	CLA	B	618	-	1/1/15/20	8/37/115/115	-
27	SQD	F	101	-	-	7/38/58/69	0/1/1/1
28	LMG	B	623	-	-	15/46/66/70	0/1/1/1
28	LMG	d	412	41	-	6/46/66/70	0/1/1/1
24	CLA	C	515	-	-	4/37/115/115	-
24	CLA	c	509	43	1/1/15/20	4/37/115/115	-
31	GOL	A	421	-	-	0/4/4/4	-
28	LMG	C	533	-	-	5/46/66/70	0/1/1/1
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	GOL	d	415	-	-	2/4/4/4	-
28	LMG	i	101	-	-	17/46/66/70	0/1/1/1
36	HTG	o	301	-	-	2/10/30/30	0/1/1/1
38	LHG	D	411	-	-	7/53/53/53	-
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	D	405	-	1/1/15/20	2/37/115/115	-
24	CLA	c	503	-	1/1/15/20	3/37/115/115	-
24	CLA	c	513	3	1/1/15/20	3/37/115/115	-
27	SQD	a	415	-	-	8/49/69/69	0/1/1/1
24	CLA	B	608	-	1/1/15/20	8/37/115/115	-
26	BCR	k	102	-	-	3/29/63/63	0/2/2/2
24	CLA	b	611	43	1/1/15/20	1/37/115/115	-
38	LHG	L	101	-	-	11/53/53/53	-
24	CLA	C	514	-	1/1/15/20	10/37/115/115	-
38	LHG	d	411	-	-	8/50/50/53	-
38	LHG	a	416	-	-	18/46/46/53	-
28	LMG	A	412	-	-	15/46/66/70	0/1/1/1
32	LMT	A	422	-	-	7/21/61/61	0/2/2/2
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
32	LMT	D	402	-	-	6/21/61/61	0/2/2/2
25	PHO	d	401	-	-	1/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	406	-	1/1/15/20	5/37/115/115	-
31	GOL	v	203	-	-	2/4/4/4	-
24	CLA	C	503	-	1/1/15/20	2/37/115/115	-
24	CLA	b	620	-	1/1/15/20	11/37/115/115	-
36	HTG	c	523	-	-	2/10/30/30	0/1/1/1
38	LHG	E	101	-	-	22/46/46/53	-
26	BCR	C	517	-	-	2/29/63/63	0/2/2/2
24	CLA	c	512	-	1/1/15/20	6/37/115/115	-
24	CLA	b	616	-	1/1/15/20	3/37/115/115	-
24	CLA	C	511	-	1/1/15/20	6/37/115/115	-
37	DGD	C	519	-	-	17/51/91/95	0/2/2/2
27	SQD	b	601	-	-	18/49/69/69	0/1/1/1
24	CLA	C	510	-	-	2/37/115/115	-
24	CLA	A	409	-	-	7/37/115/115	-
24	CLA	C	504	-	-	5/37/115/115	-
36	HTG	O	303	-	-	1/10/30/30	0/1/1/1
24	CLA	B	604	-	1/1/15/20	4/37/115/115	-
24	CLA	C	508	-	1/1/15/20	5/37/115/115	-
32	LMT	B	624	-	-	5/21/61/61	0/2/2/2
32	LMT	J	102	-	-	4/15/35/61	0/1/1/2
24	CLA	b	608	-	1/1/15/20	5/37/115/115	-
24	CLA	B	613	-	1/1/15/20	6/37/115/115	-
32	LMT	f	801	-	-	7/17/37/61	0/1/1/2
32	LMT	D	409	-	-	9/21/61/61	0/2/2/2
31	GOL	D	417	-	-	1/4/4/4	-
24	CLA	B	615	-	1/1/15/20	2/37/115/115	-
26	BCR	K	101	-	-	4/29/63/63	0/2/2/2
24	CLA	c	507	-	1/1/15/20	4/37/115/115	-
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
36	HTG	C	523	-	-	2/10/30/30	0/1/1/1
24	CLA	B	609	43	1/1/15/20	1/37/115/115	-
26	BCR	c	517	-	-	1/29/63/63	0/2/2/2
24	CLA	d	406	-	1/1/15/20	3/37/115/115	-
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
32	LMT	B	638	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	617	-	1/1/15/20	4/37/115/115	-
37	DGD	c	518	-	-	9/51/91/95	0/2/2/2
28	LMG	c	521	-	-	19/46/66/70	0/1/1/1
38	LHG	d	409	-	-	4/53/53/53	-
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
24	CLA	C	512	-	1/1/15/20	7/37/115/115	-
32	LMT	a	402	-	-	4/21/61/61	0/2/2/2
24	CLA	c	505	-	1/1/15/20	3/37/115/115	-
31	GOL	b	639	-	-	4/4/4/4	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
24	CLA	d	405	-	1/1/15/20	1/37/115/115	-
28	LMG	Z	101	-	-	11/34/54/70	0/1/1/1
39	HEM	F	102	6,5	-	4/12/54/54	-
38	LHG	l	102	-	-	10/53/53/53	-
36	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	CLA	b	605	43	1/1/15/20	6/37/115/115	-
24	CLA	c	511	-	1/1/15/20	5/37/115/115	-
36	HTG	c	524	-	-	2/10/30/30	0/1/1/1
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
26	BCR	c	516	-	-	1/29/63/63	0/2/2/2
40	RRX	H	103	-	-	4/29/65/65	0/2/2/2
42	HEC	v	201	16	-	2/10/54/54	-
37	DGD	h	102	-	-	8/51/91/95	0/2/2/2
25	PHO	a	412	-	-	4/37/103/103	0/5/6/6
36	HTG	b	627	-	-	3/10/30/30	0/1/1/1

The worst 5 of 1571 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	MG-NA	12.55	2.36	2.06
24	c	513	CLA	MG-NA	10.20	2.30	2.06
24	c	509	CLA	MG-NA	9.90	2.29	2.06
24	b	613	CLA	MG-NA	9.82	2.29	2.06
24	b	620	CLA	MG-NA	9.81	2.29	2.06

The worst 5 of 2474 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	h	101	RRX	C20-C21-C22	21.81	158.43	127.31
40	h	101	RRX	C15-C16-C17	20.97	166.42	123.47
40	H	103	RRX	C16-C17-C18	20.52	156.60	127.31
40	h	101	RRX	C16-C17-C18	19.69	155.40	127.31
40	h	101	RRX	C15-C14-C13	19.68	155.39	127.31

5 of 56 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND

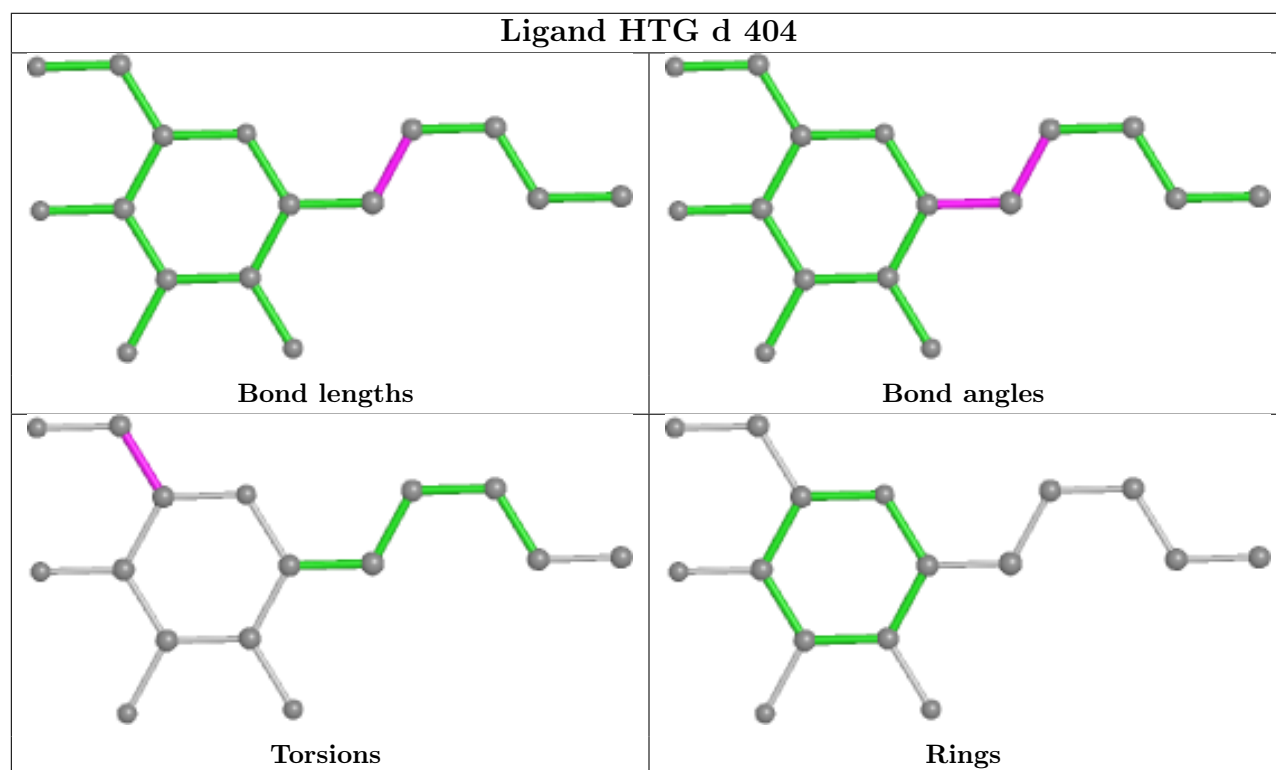
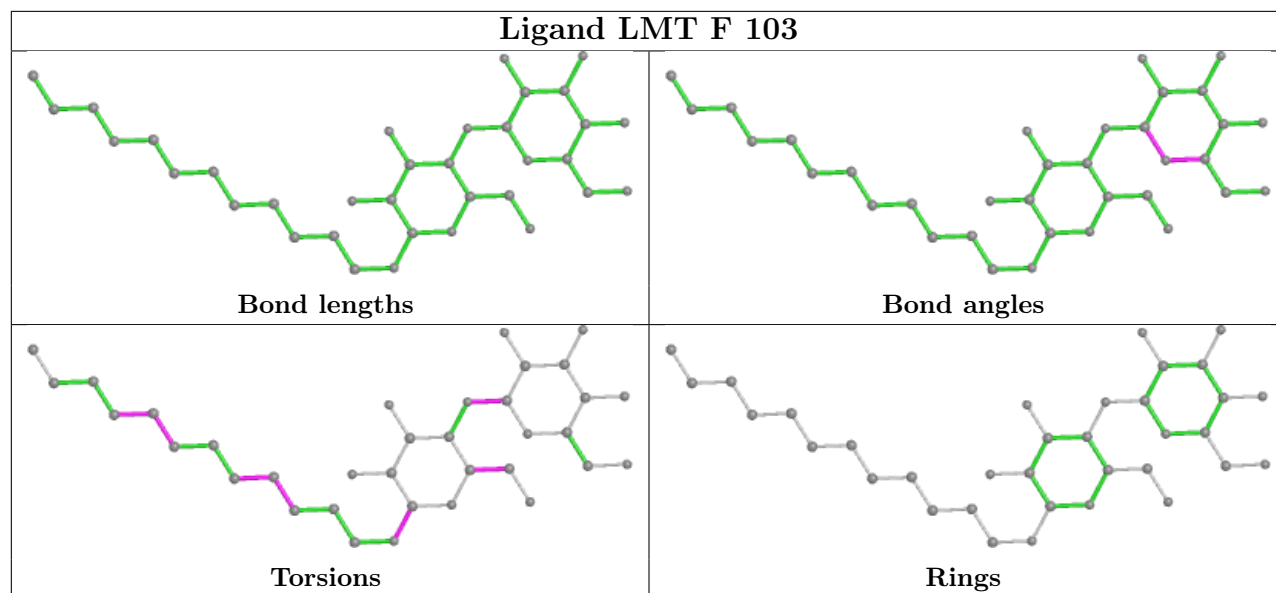
5 of 1021 torsion outliers are listed below:

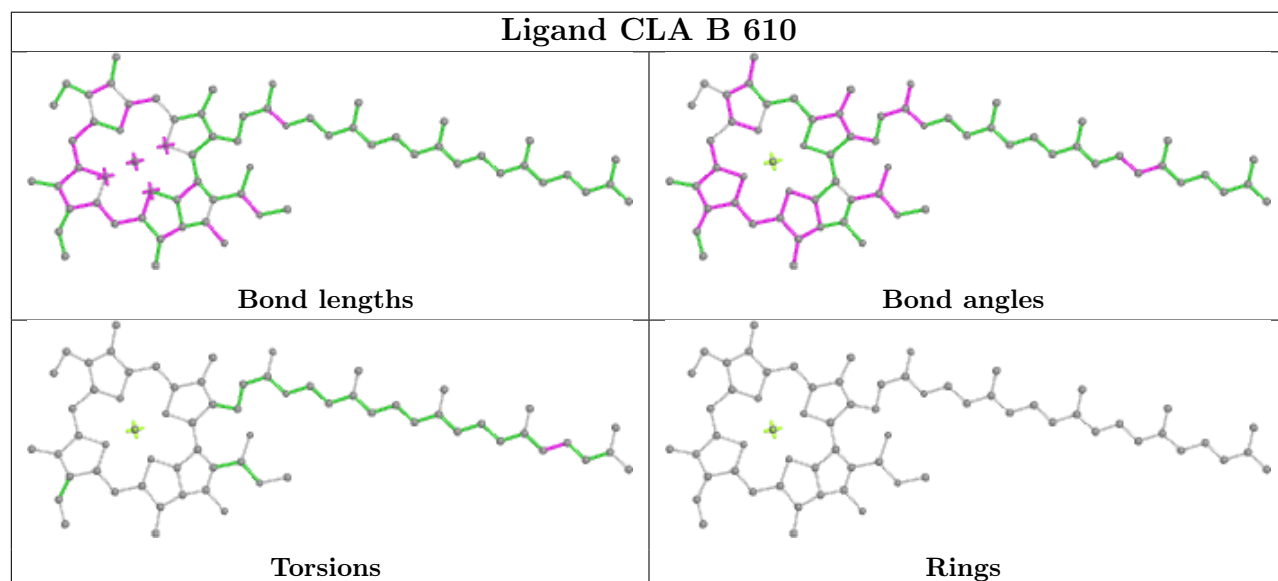
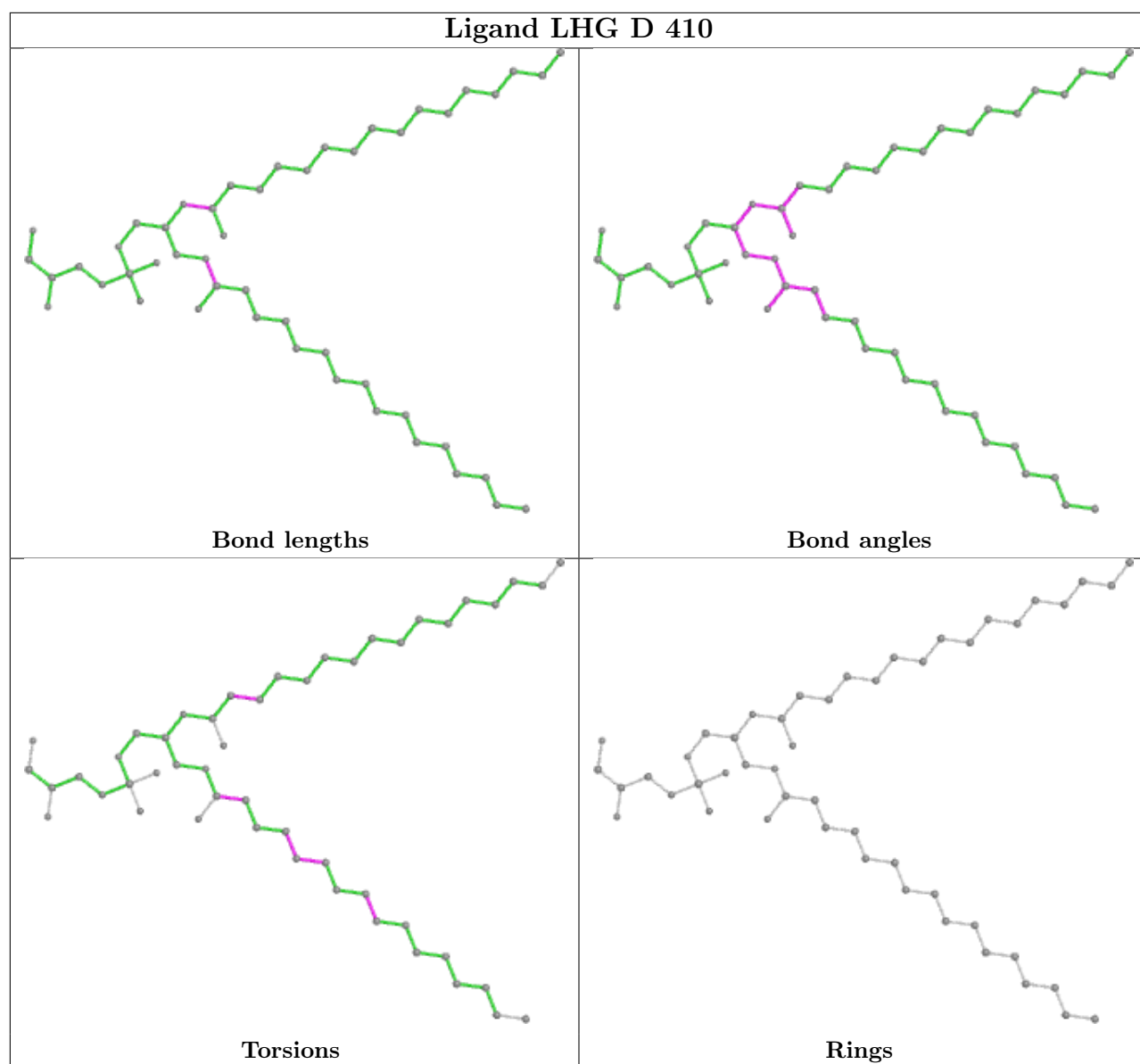
Mol	Chain	Res	Type	Atoms
24	B	607	CLA	C2-C3-C5-C6
24	B	608	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	616	CLA	CHA-CBD-CGD-O1D
24	B	616	CLA	CHA-CBD-CGD-O2D

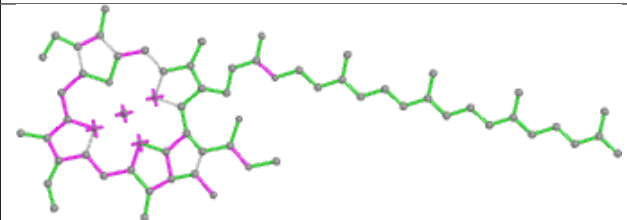
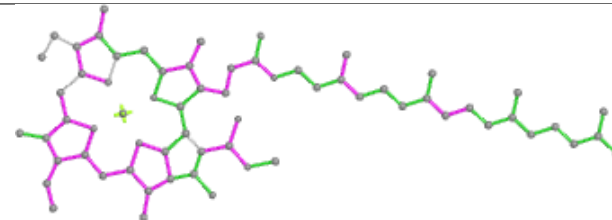
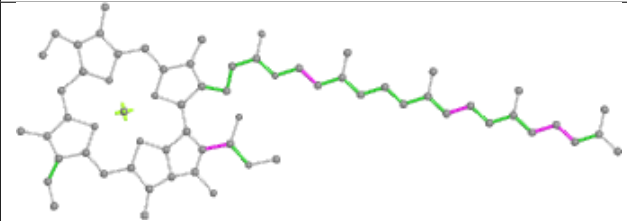
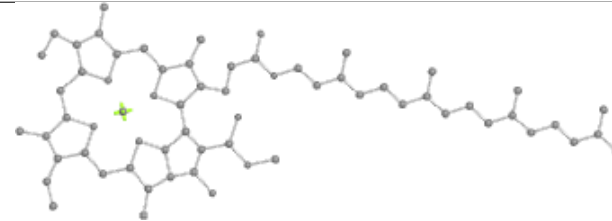
There are no ring outliers.

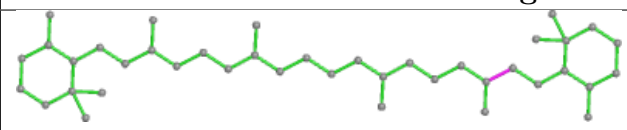
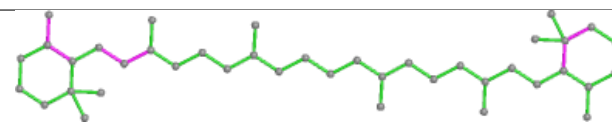
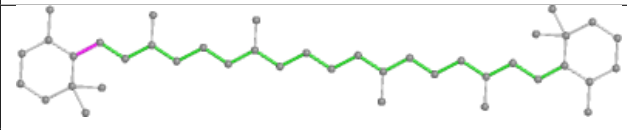
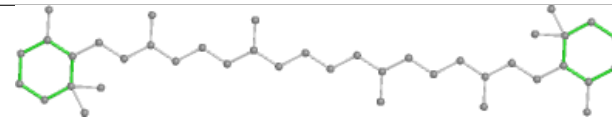
No monomer is involved in short contacts.

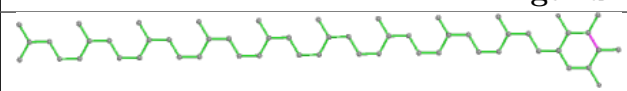
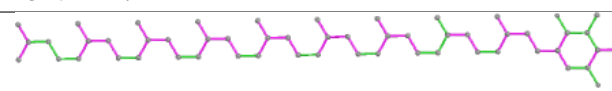
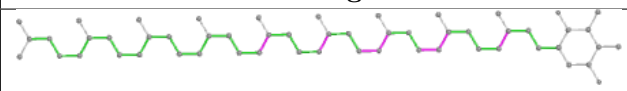
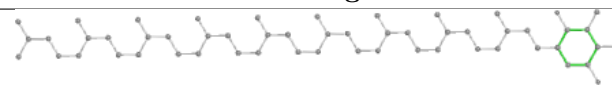
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

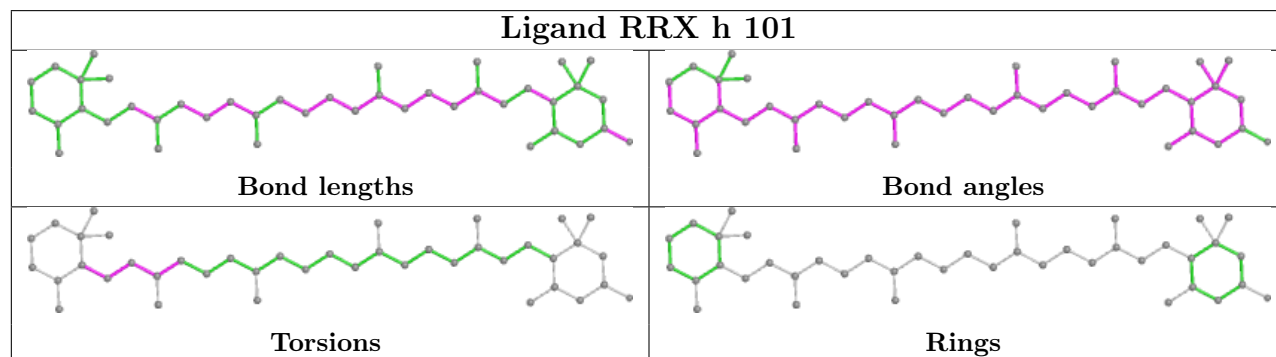
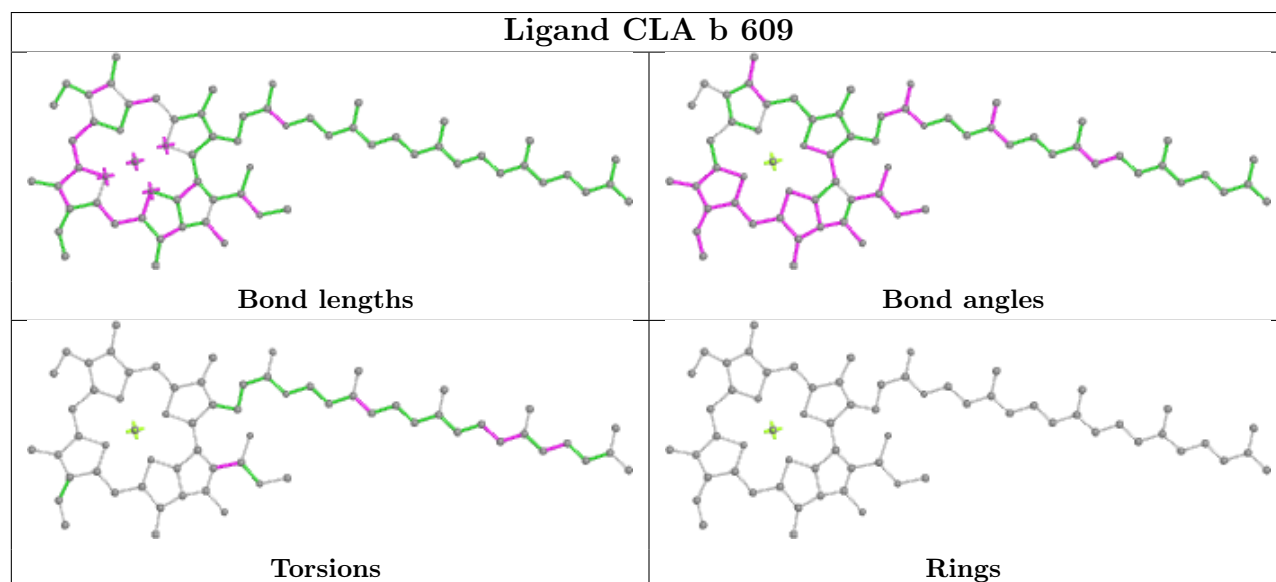
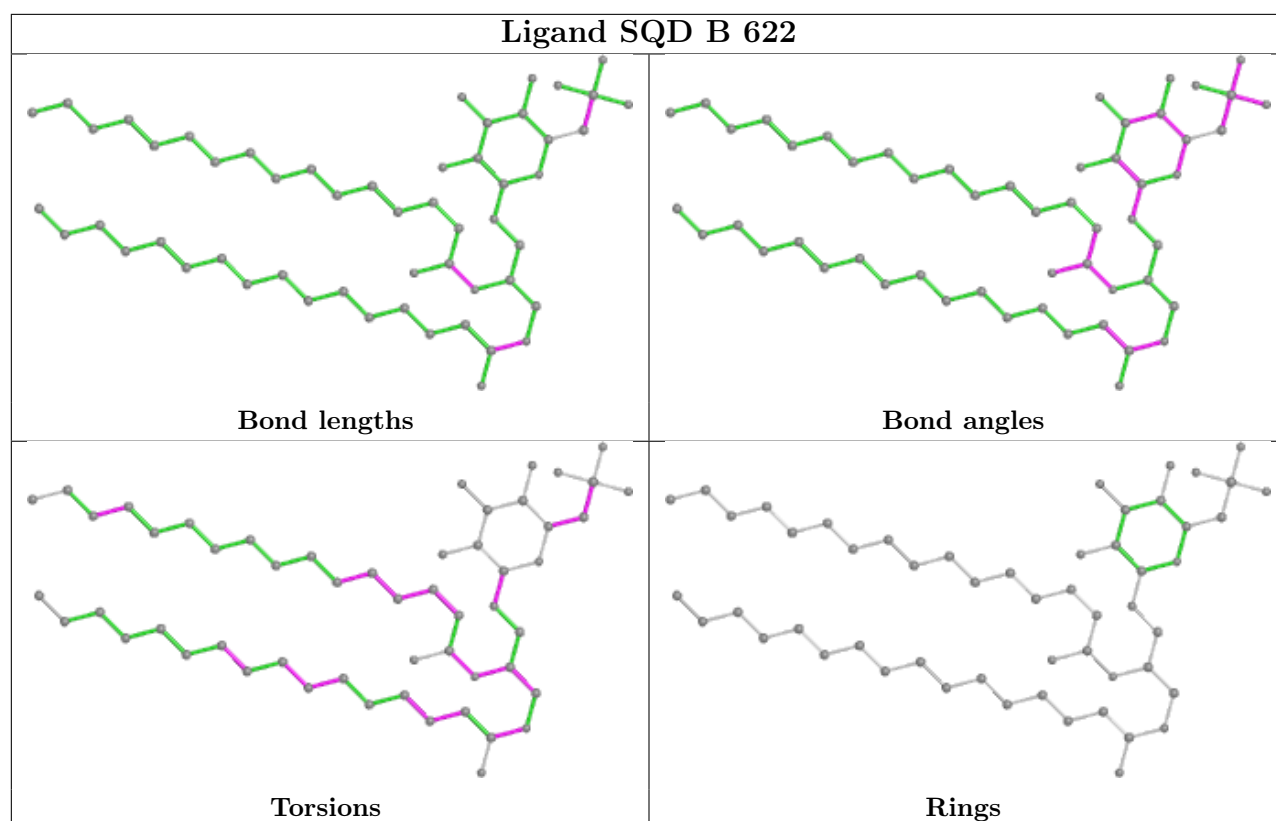


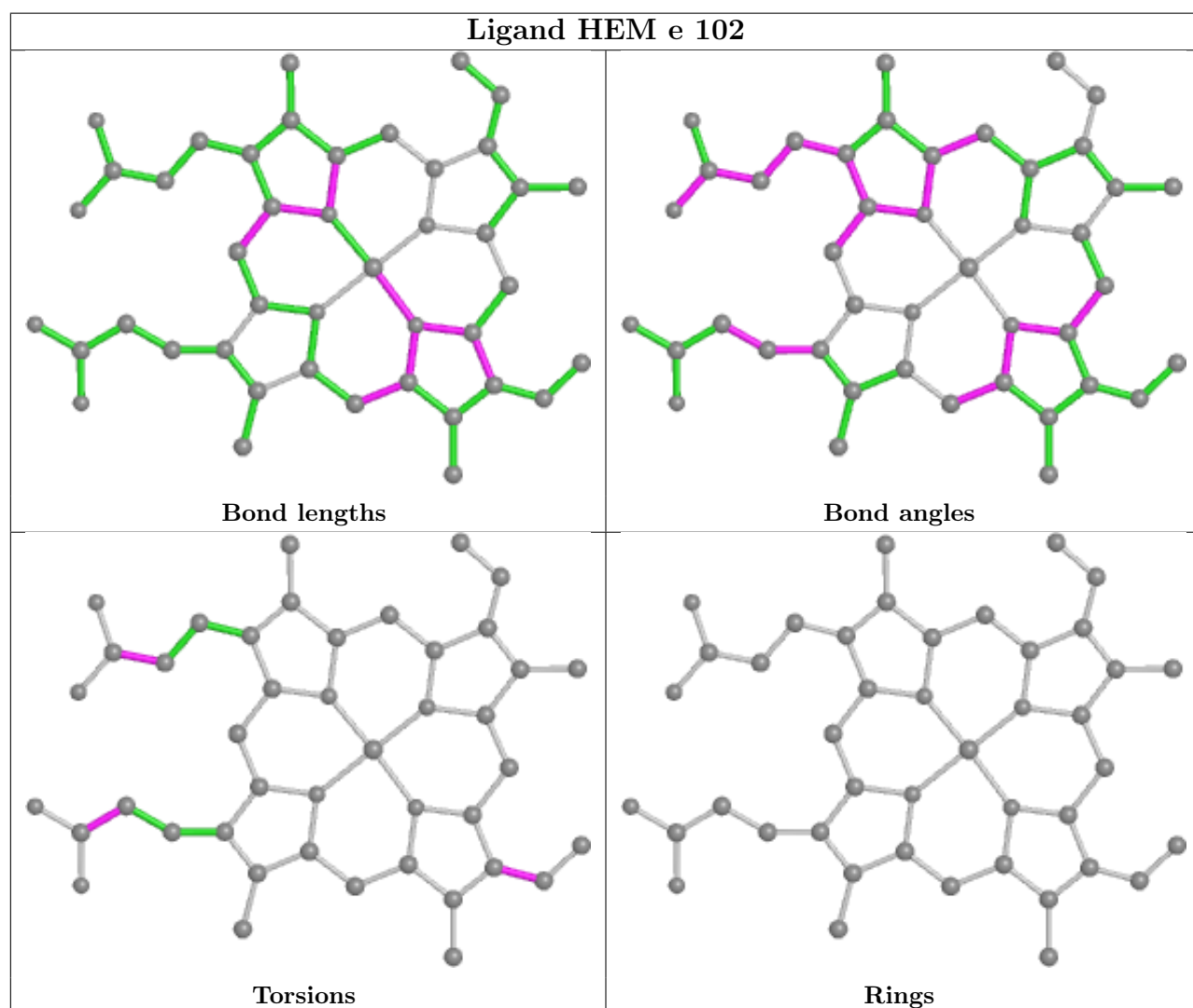
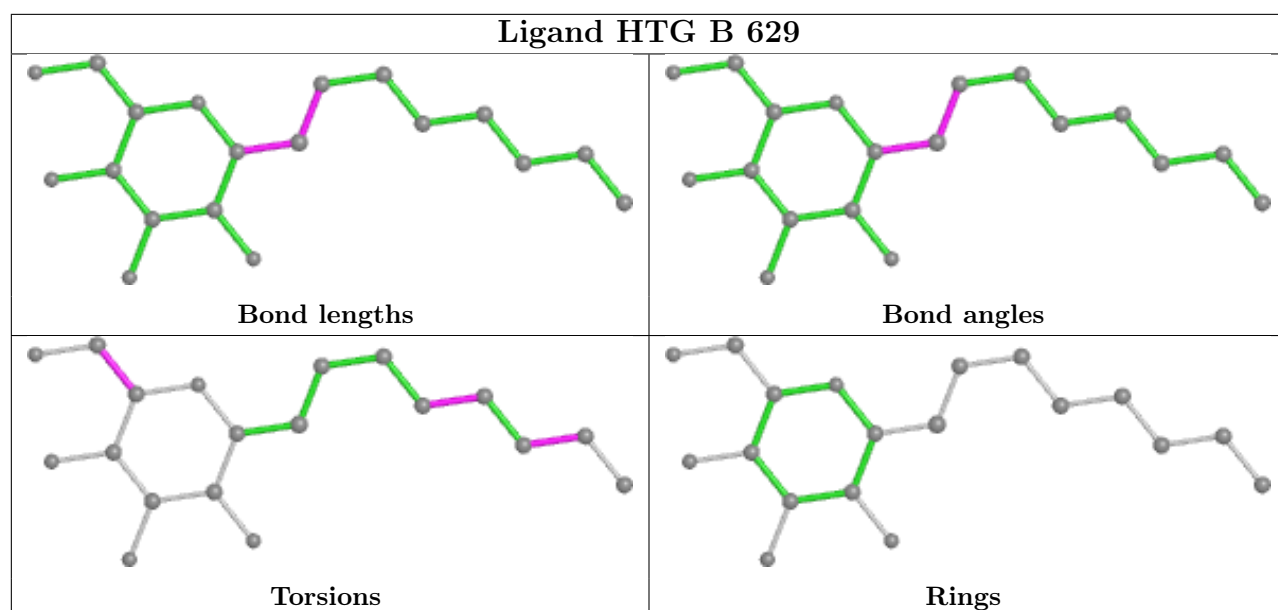


Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

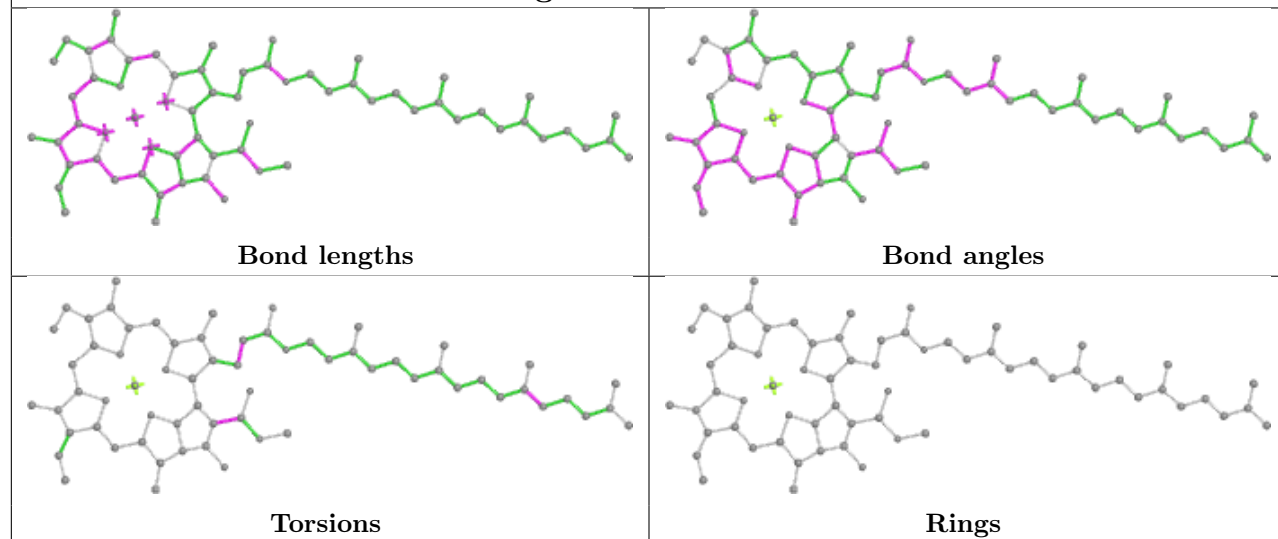
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

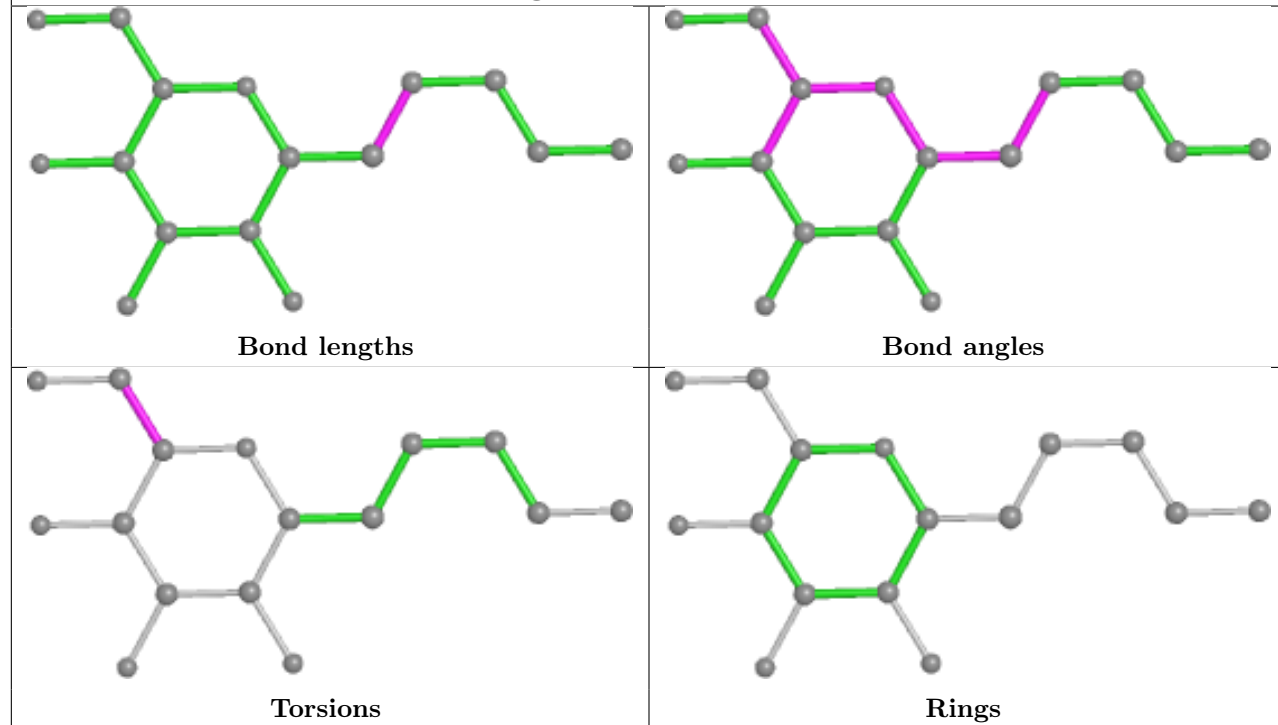


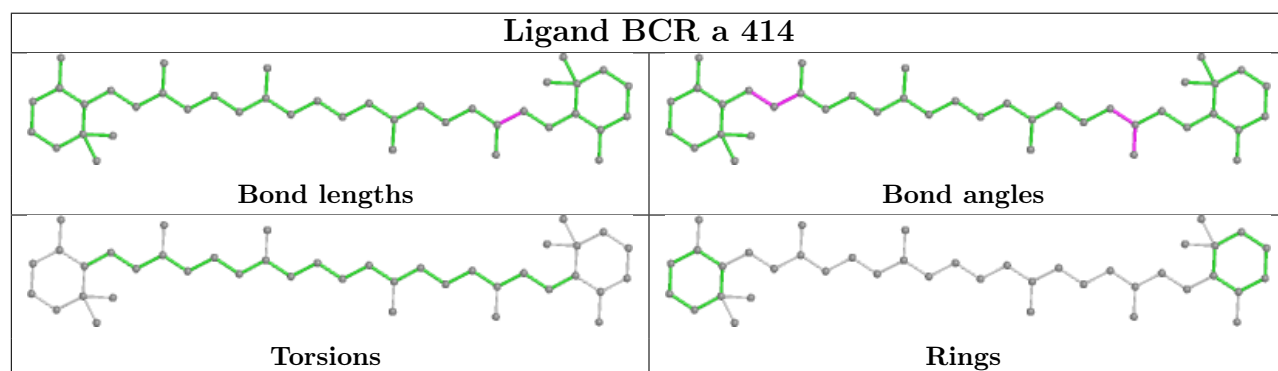
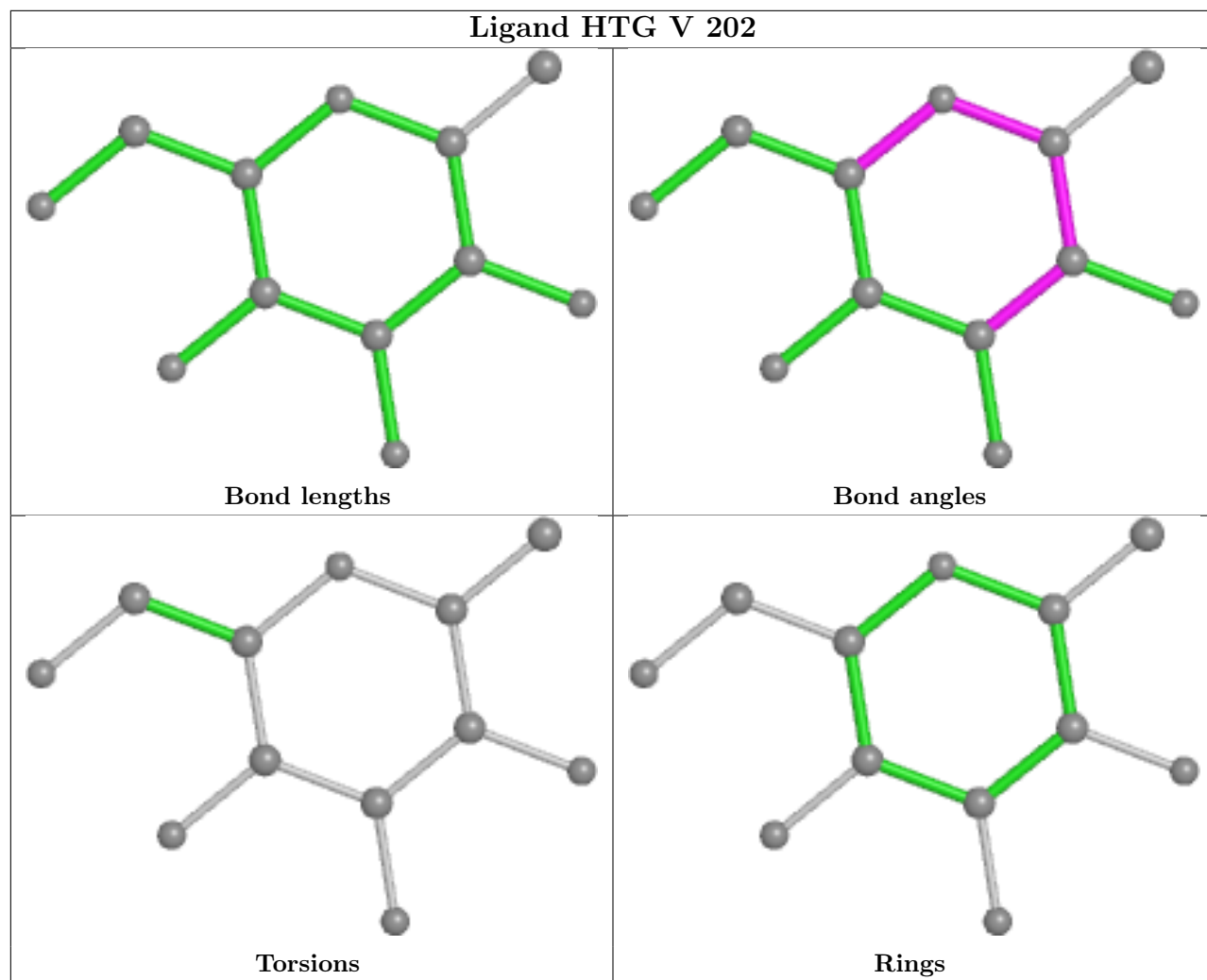


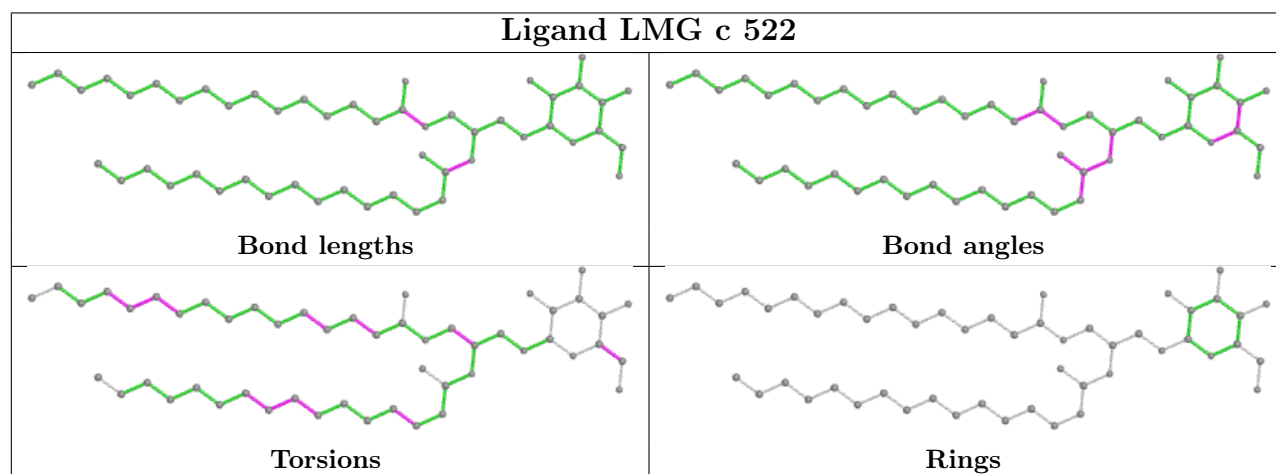
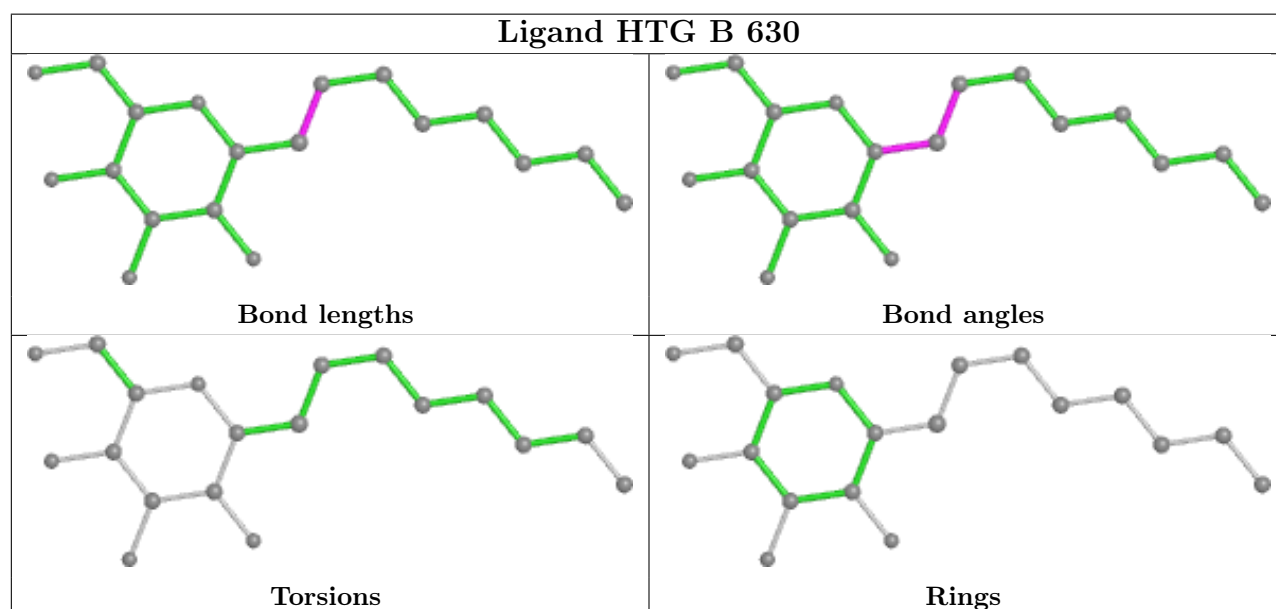
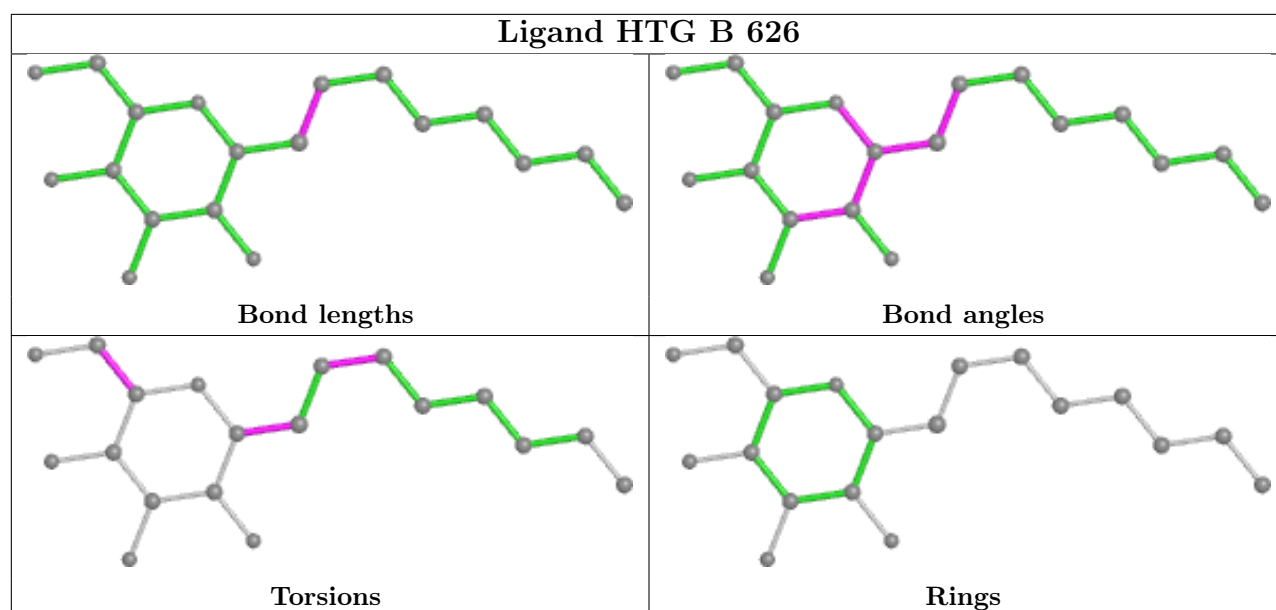
Ligand CLA b 610

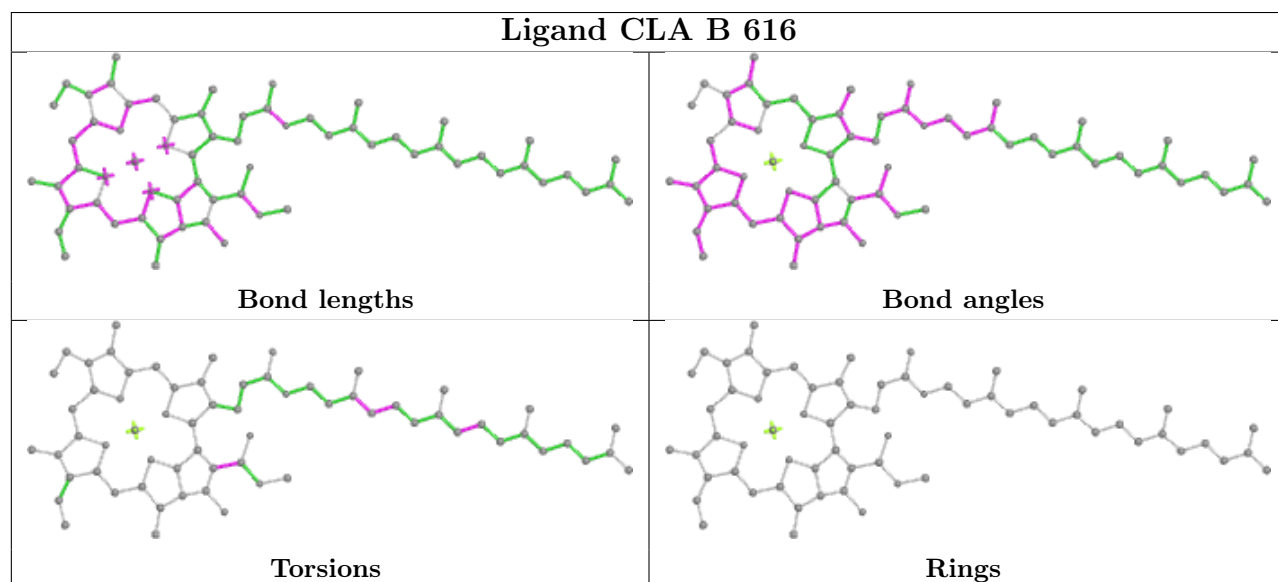
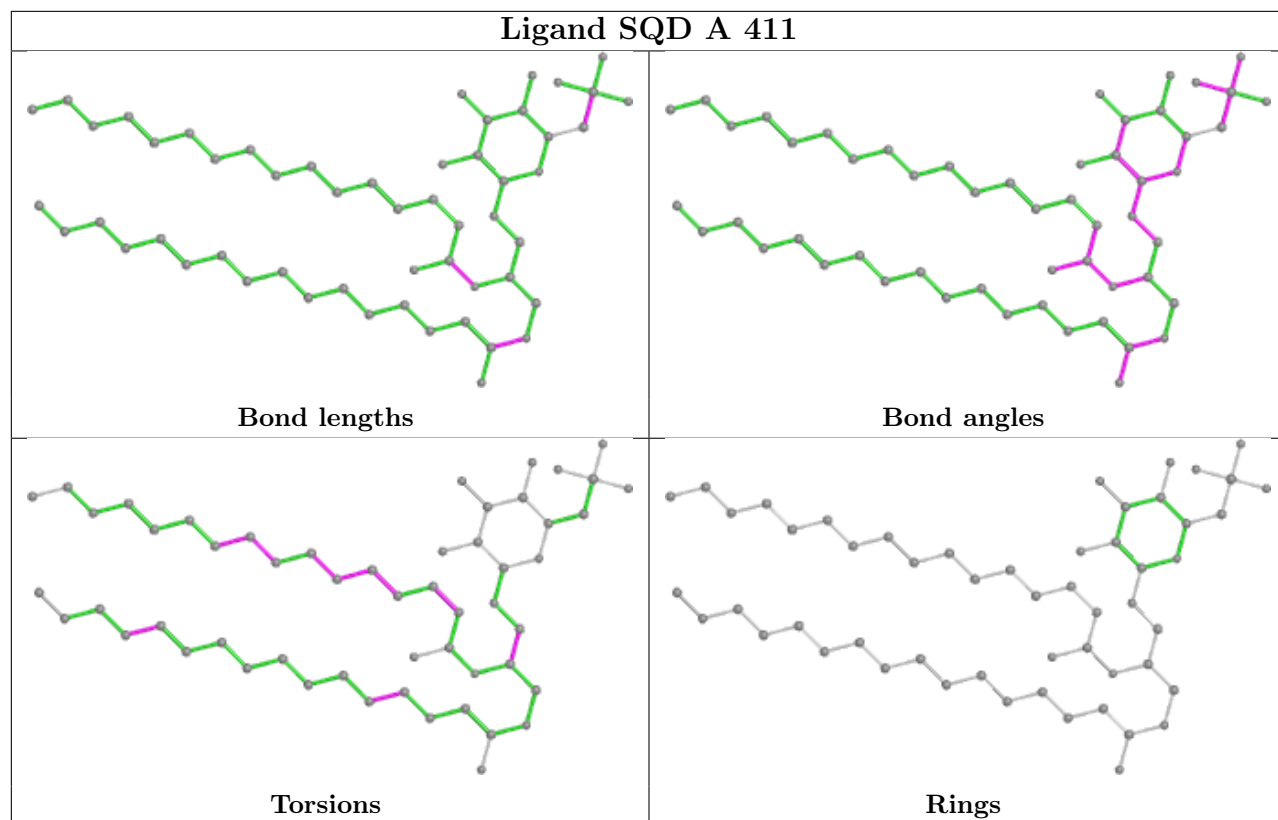


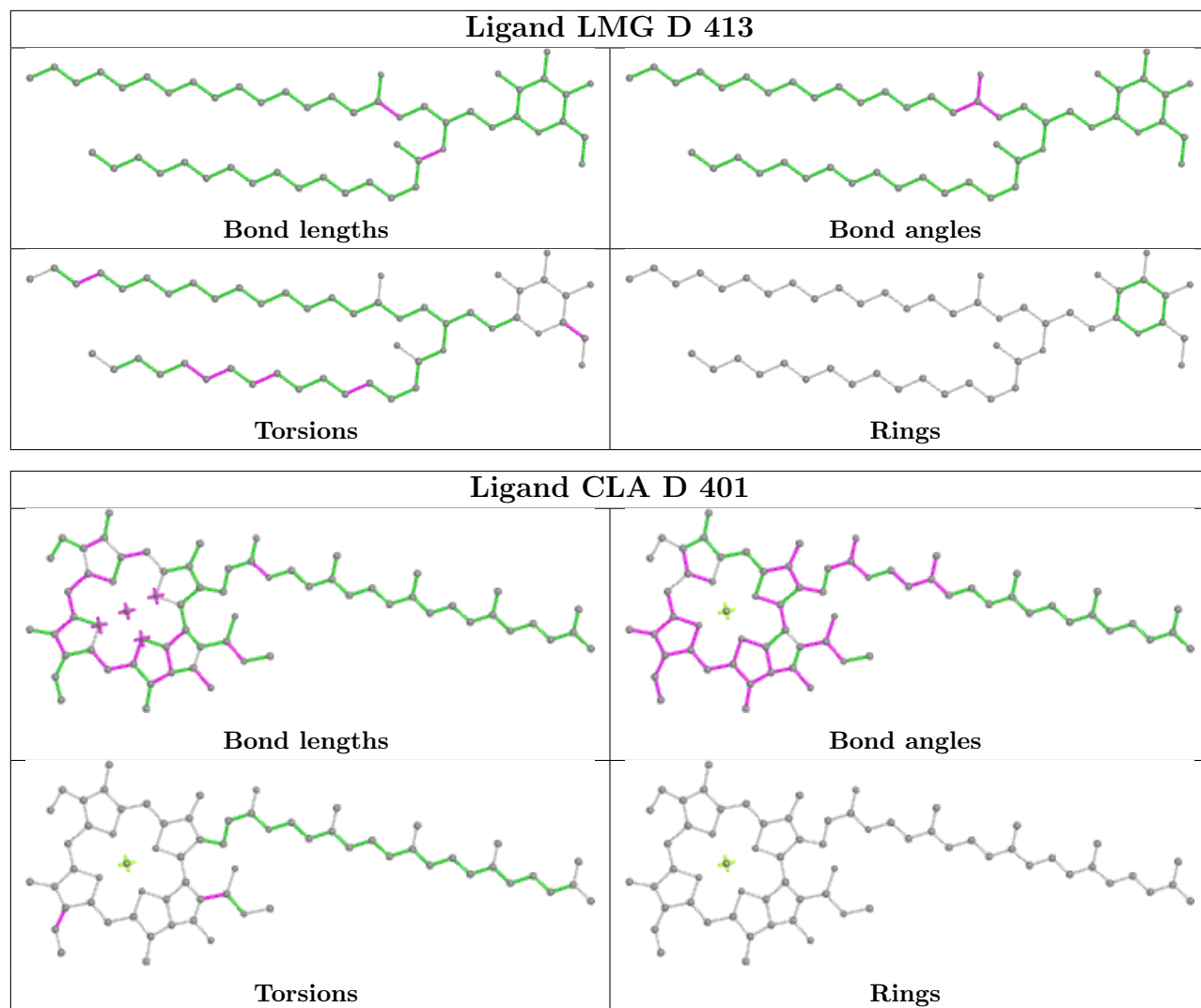
Ligand HTG H 101

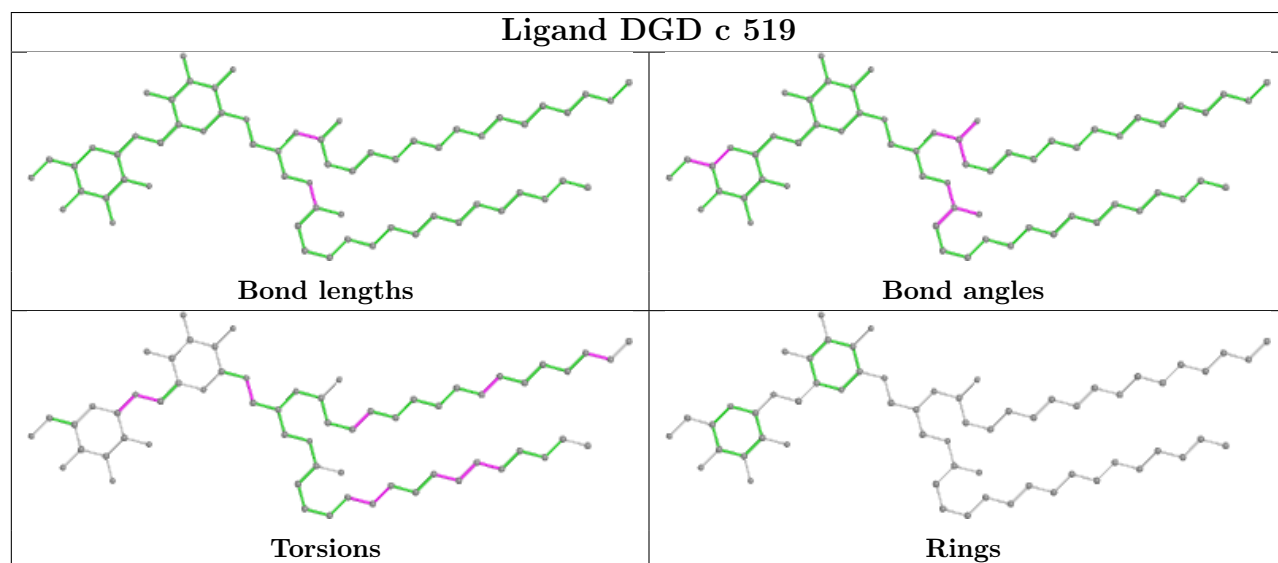
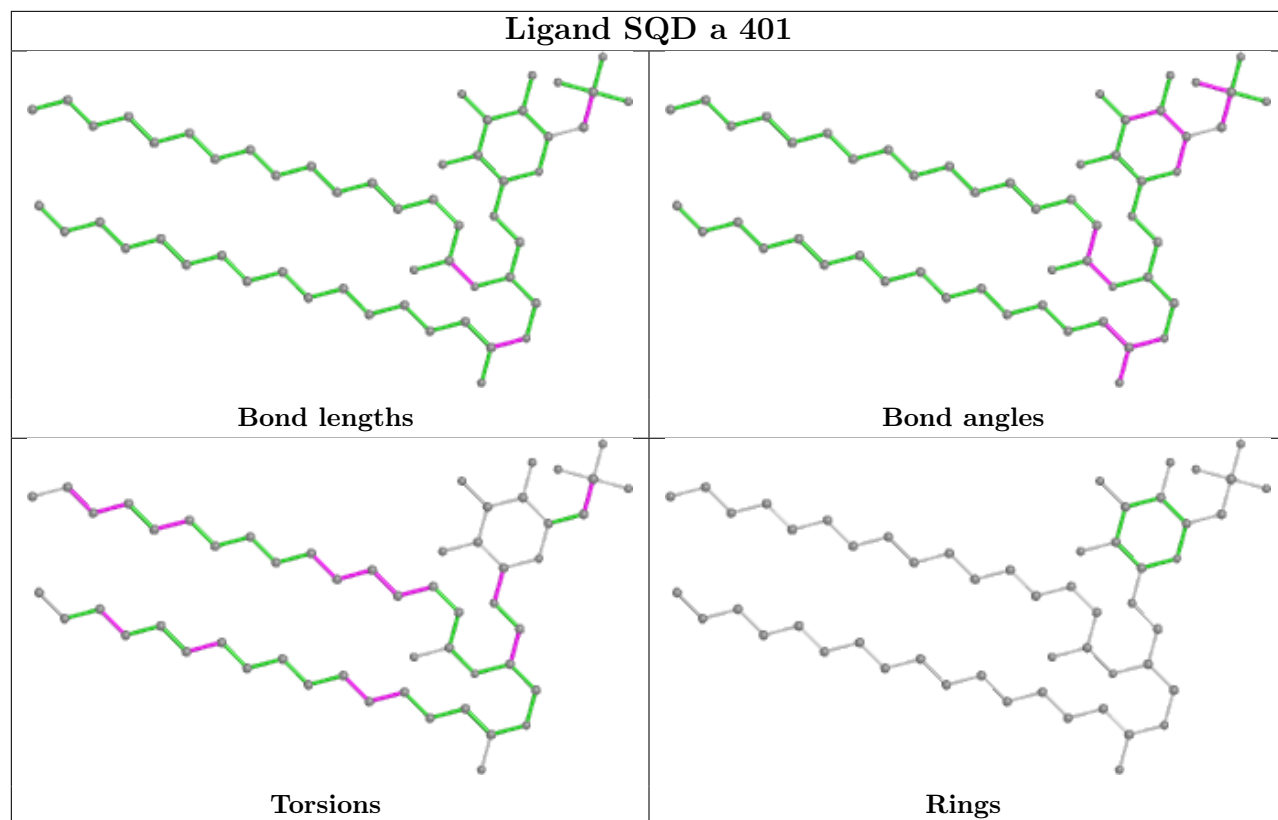


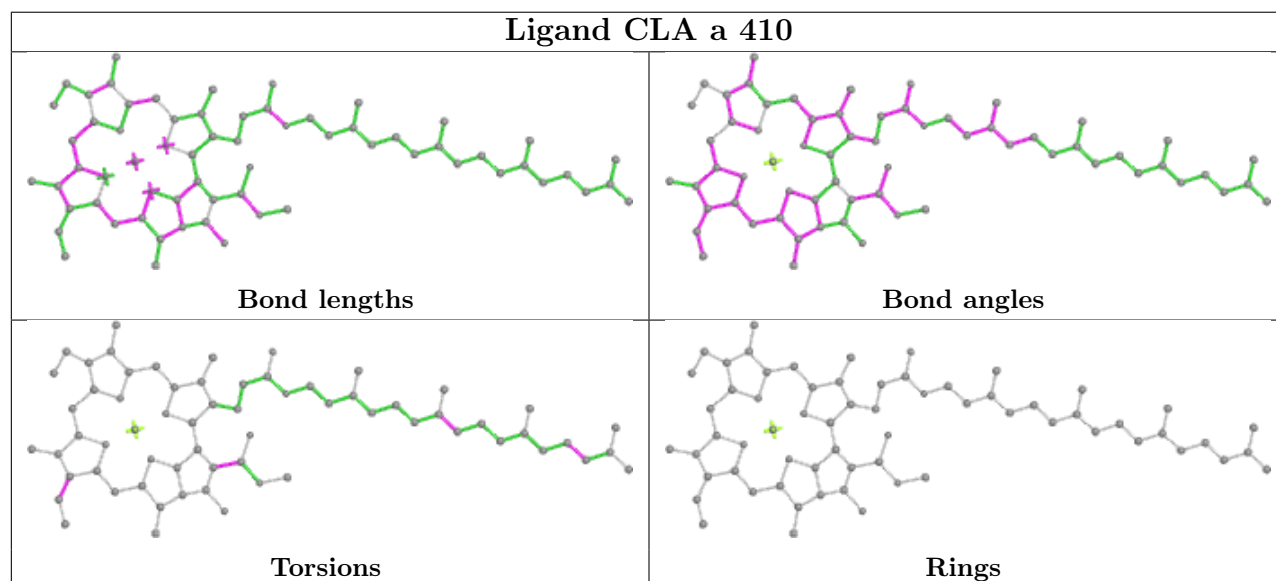
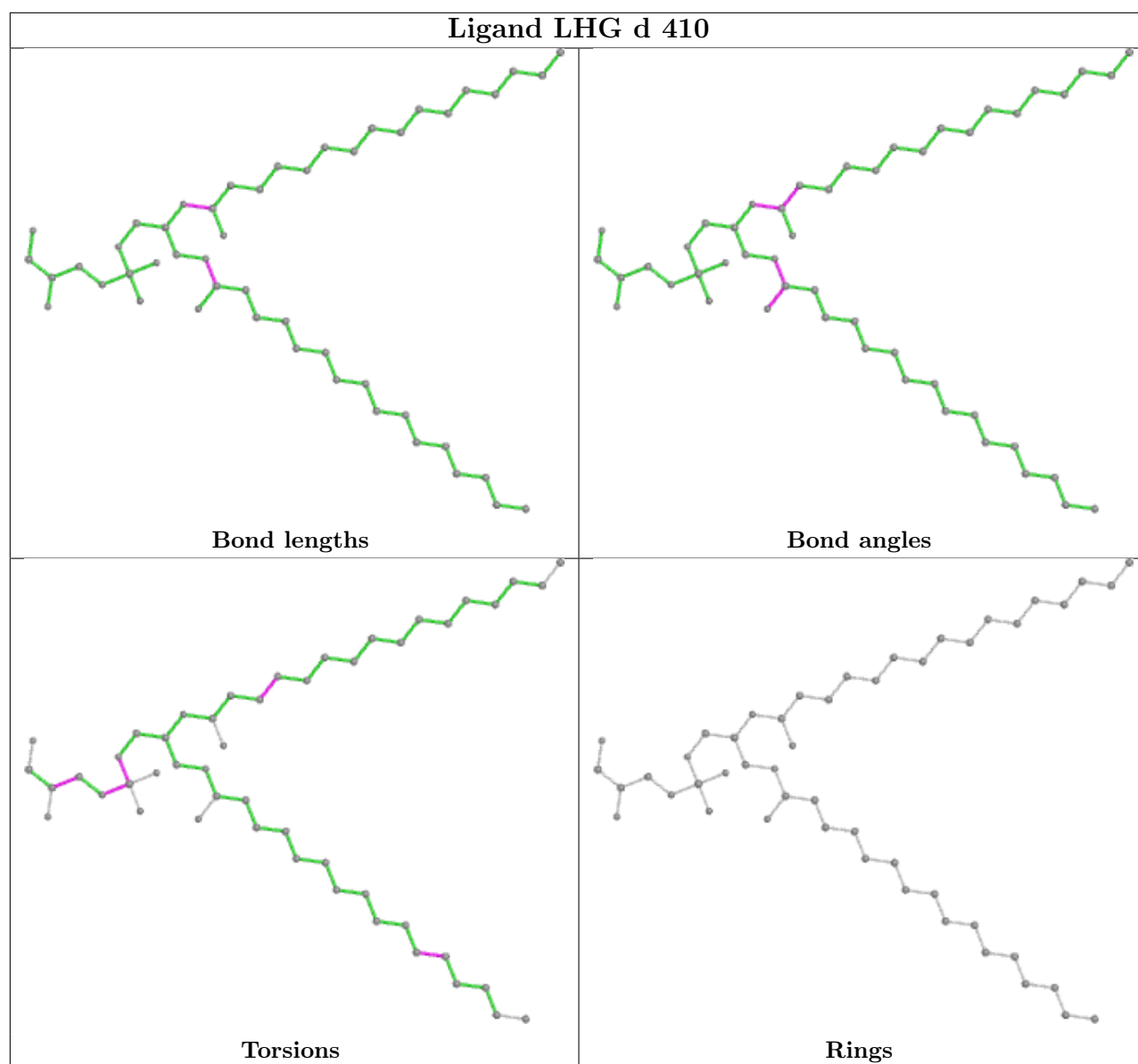


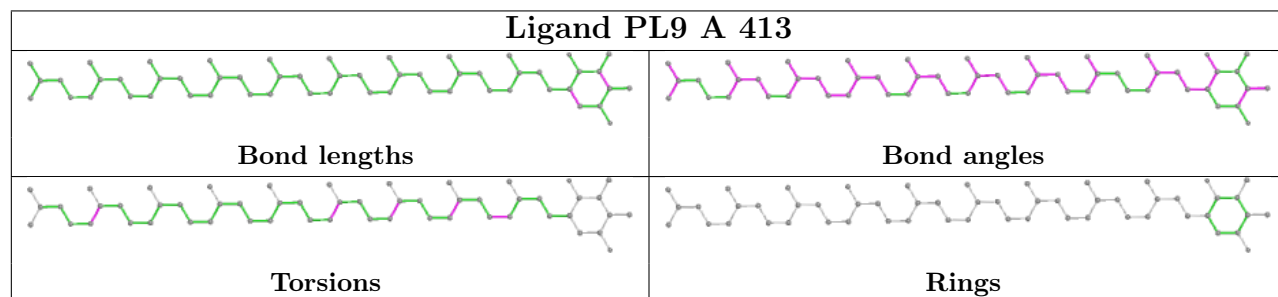
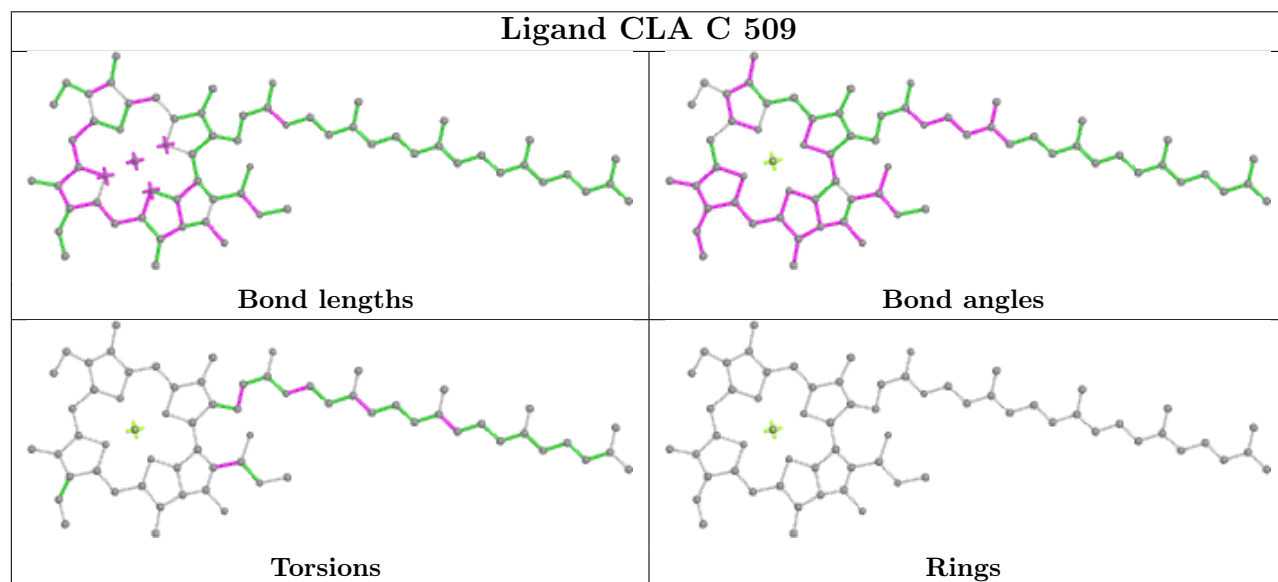
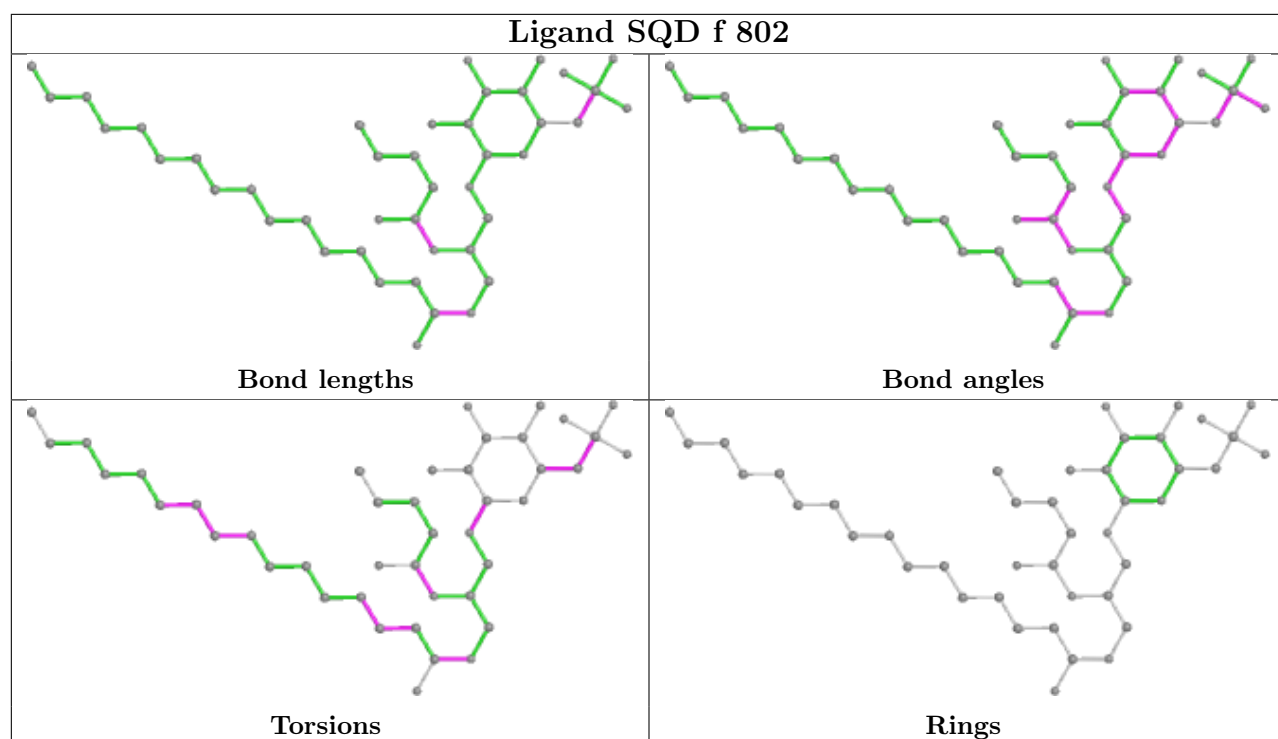




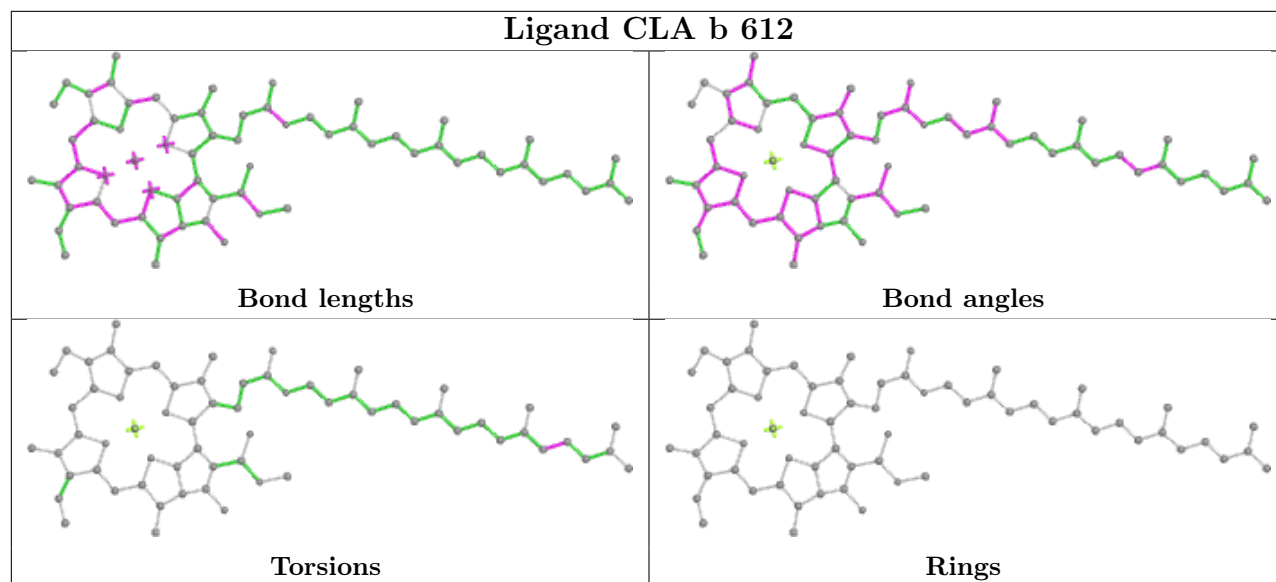




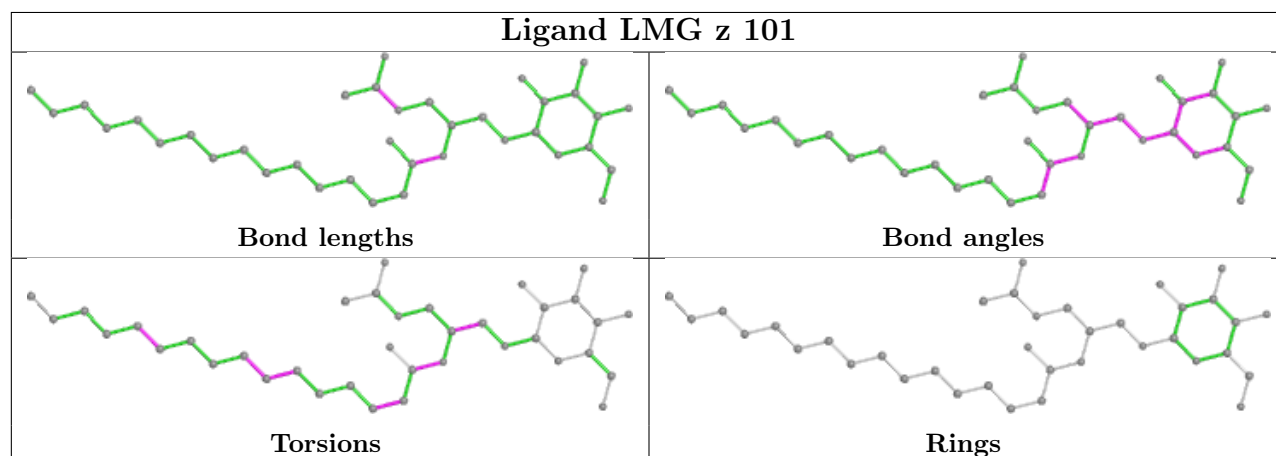




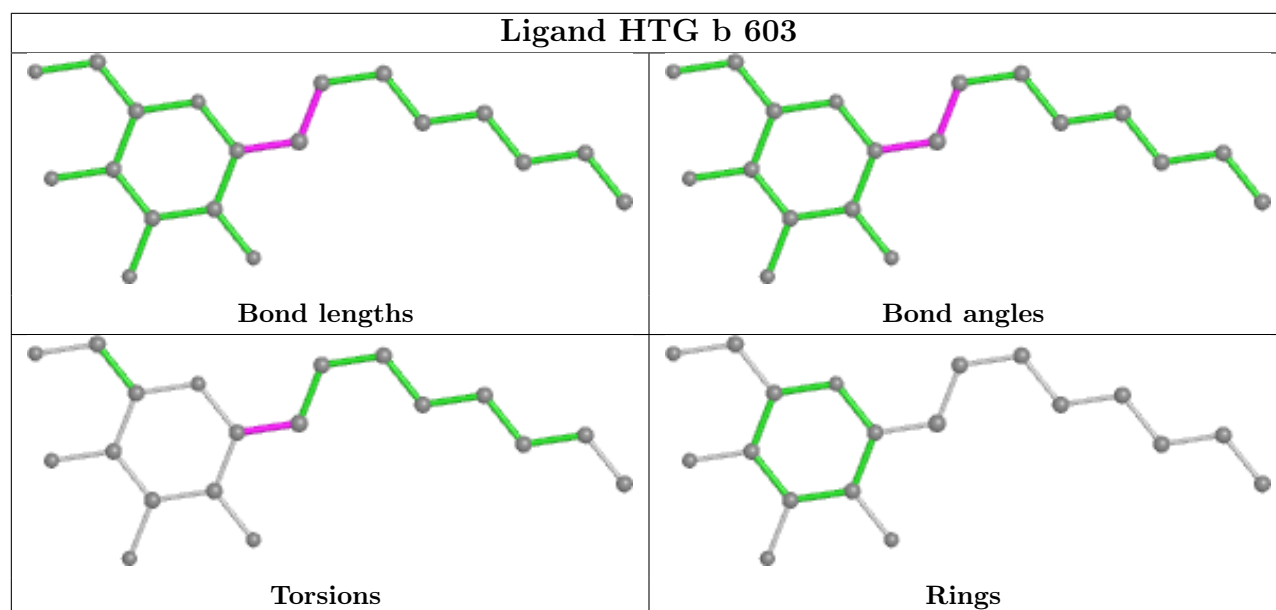
Ligand CLA b 612



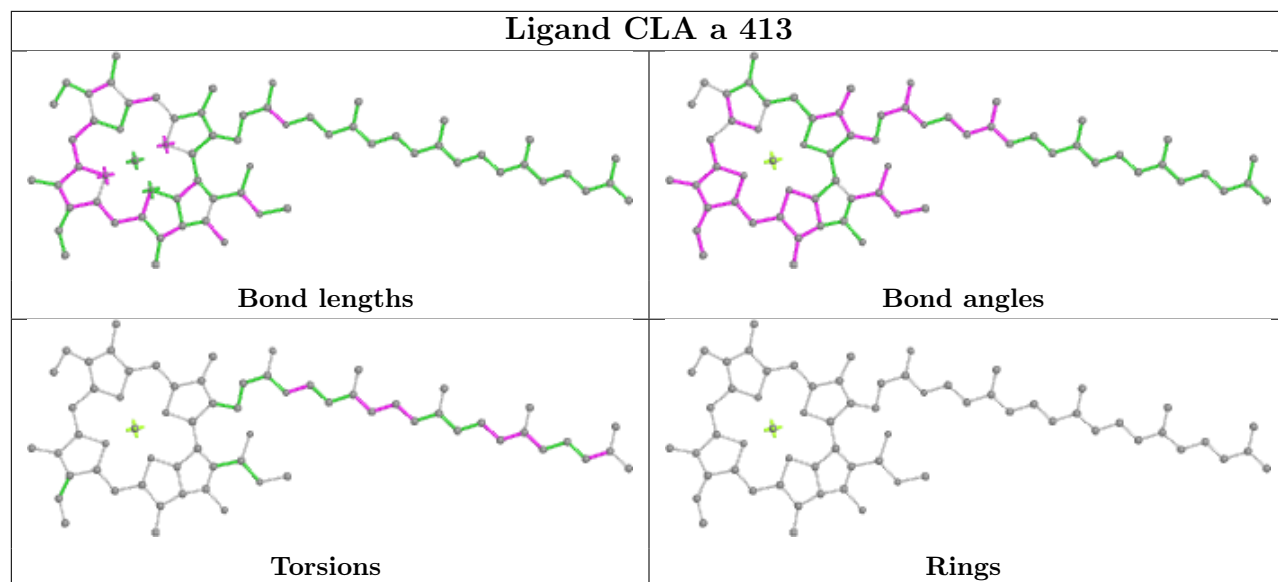
Ligand LMG z 101



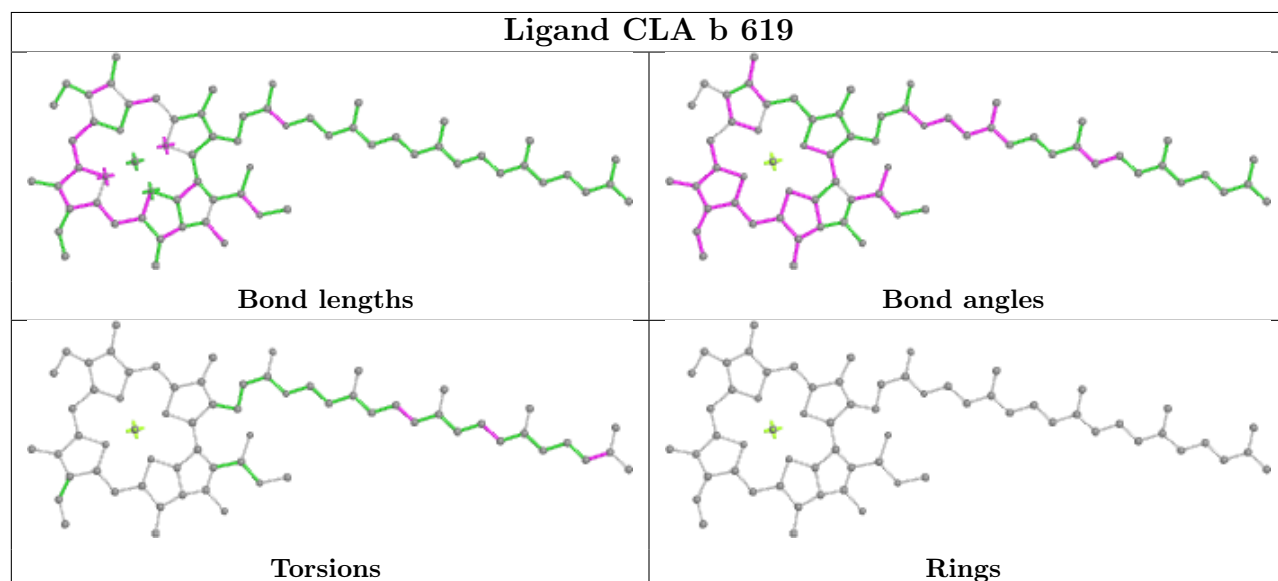
Ligand HTG b 603



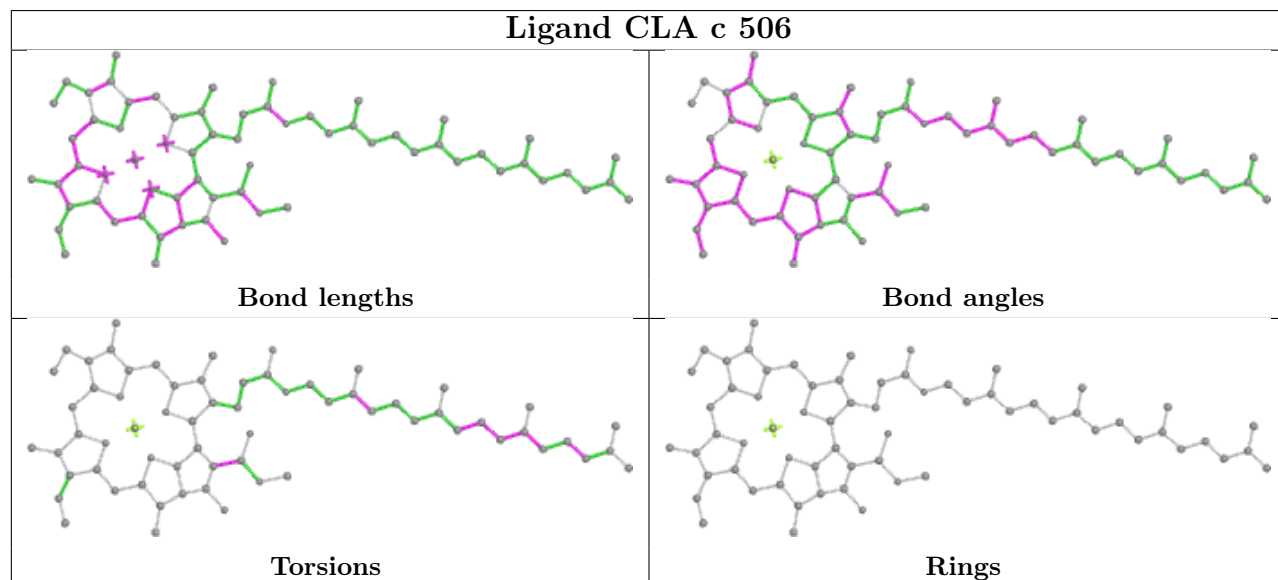
Ligand CLA a 413

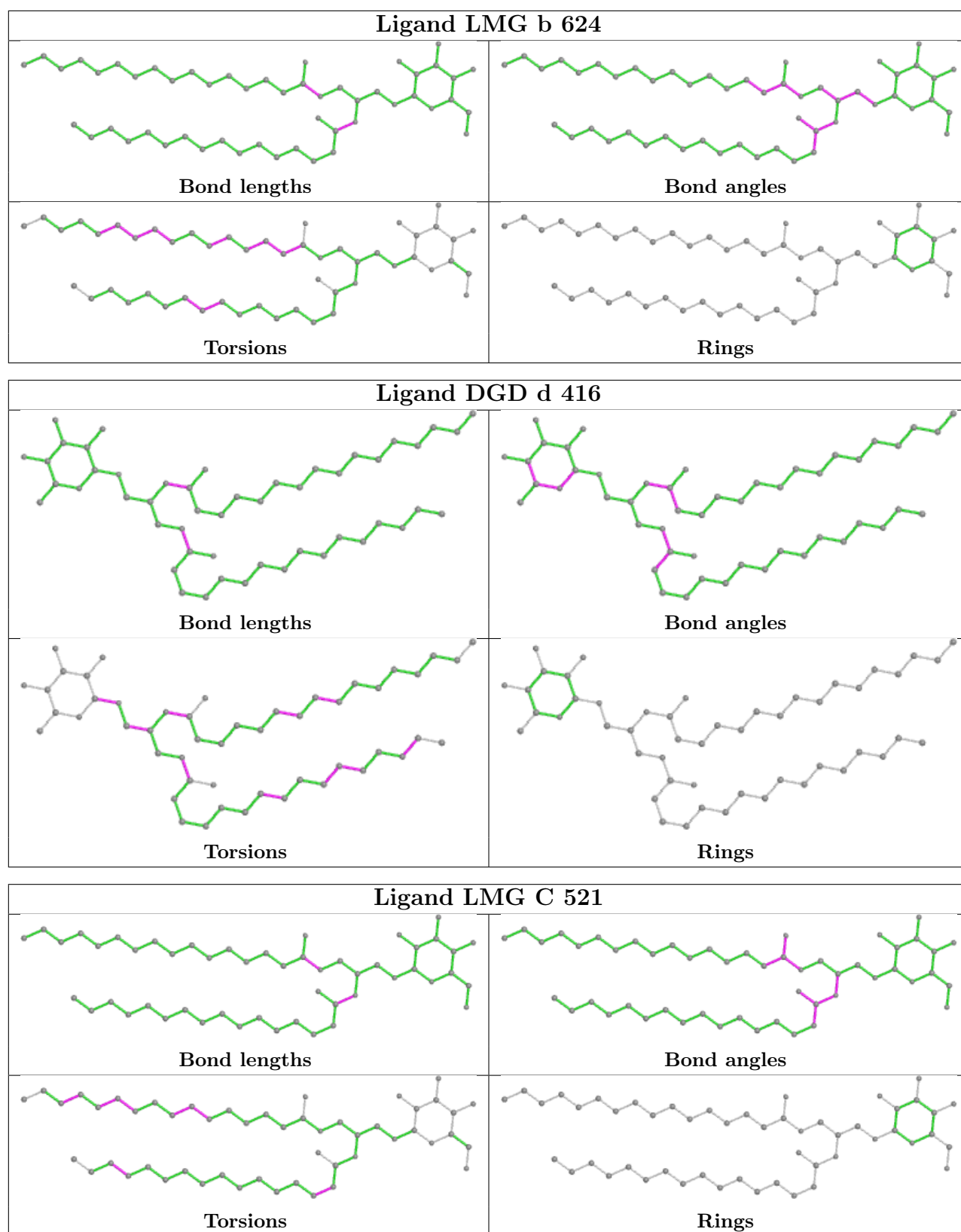


Ligand CLA b 619

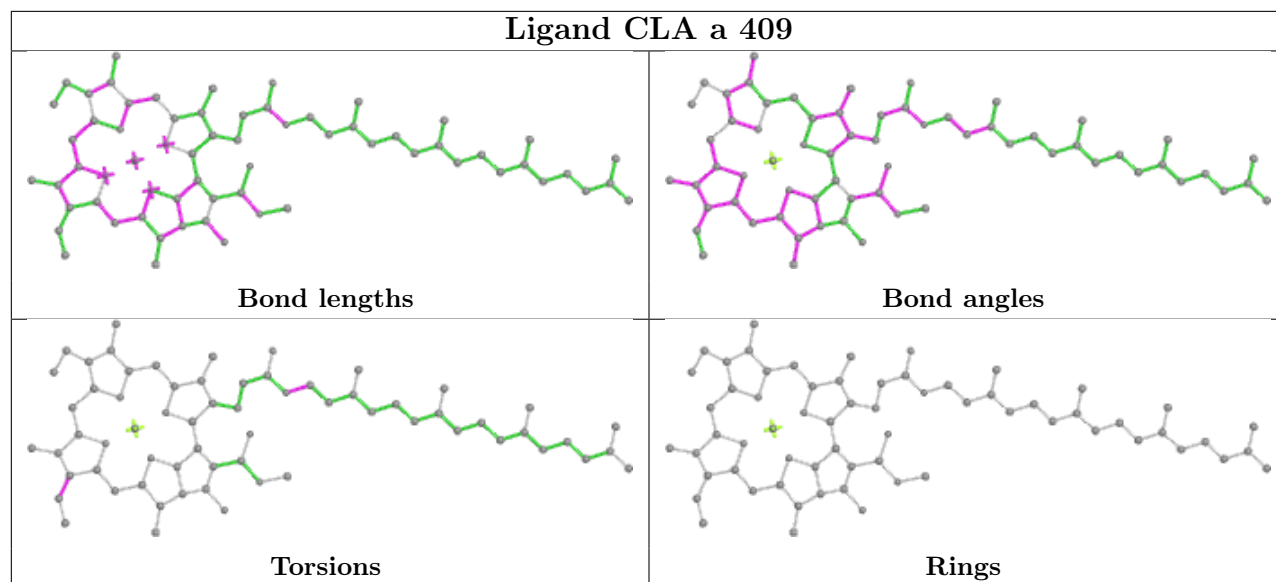


Ligand CLA c 506

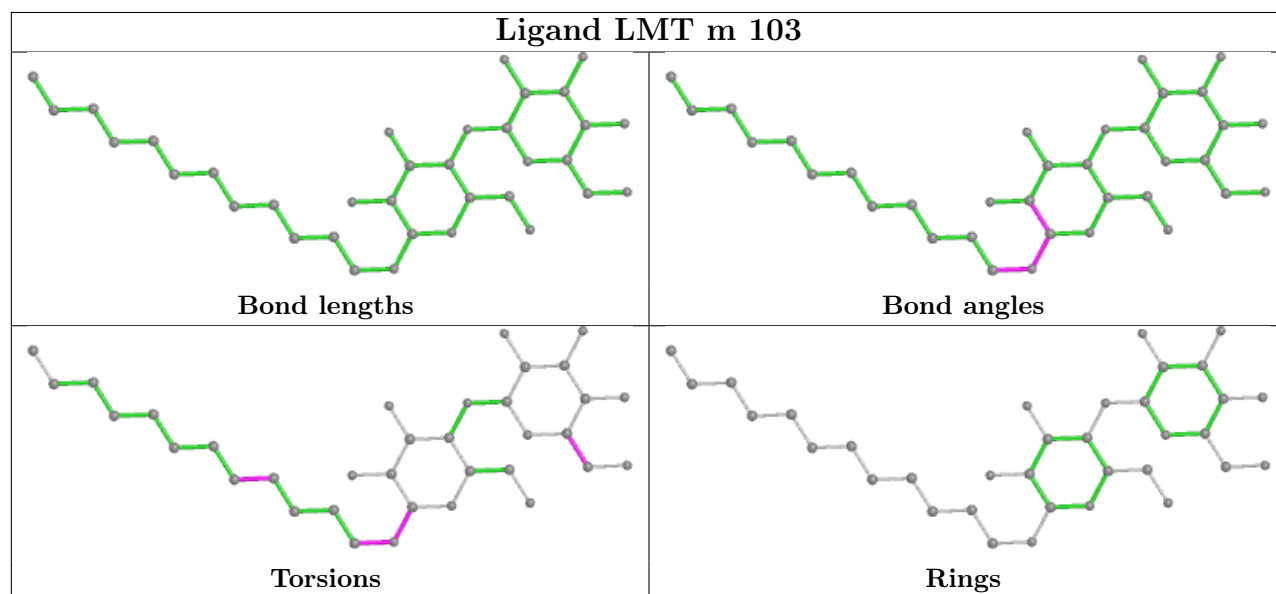


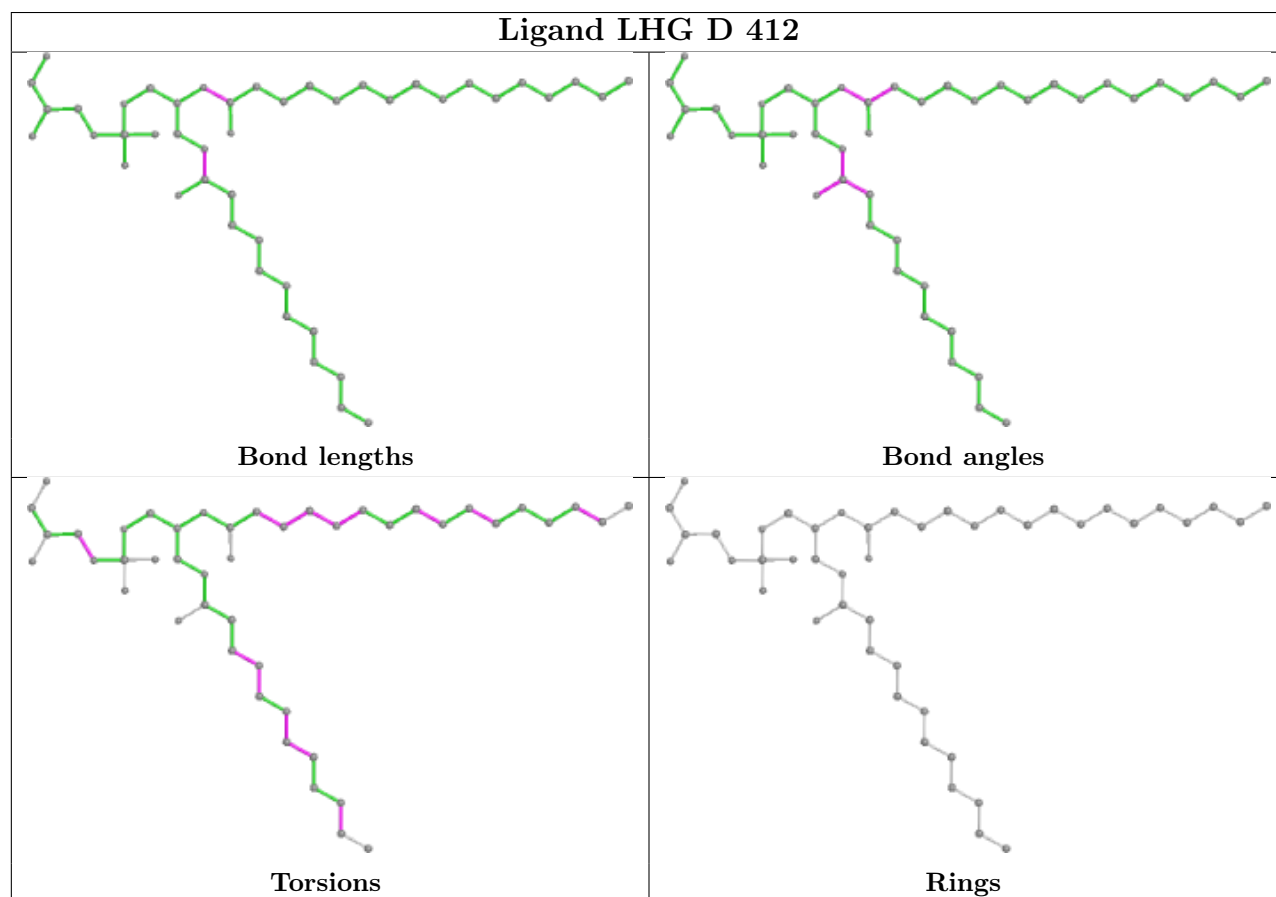
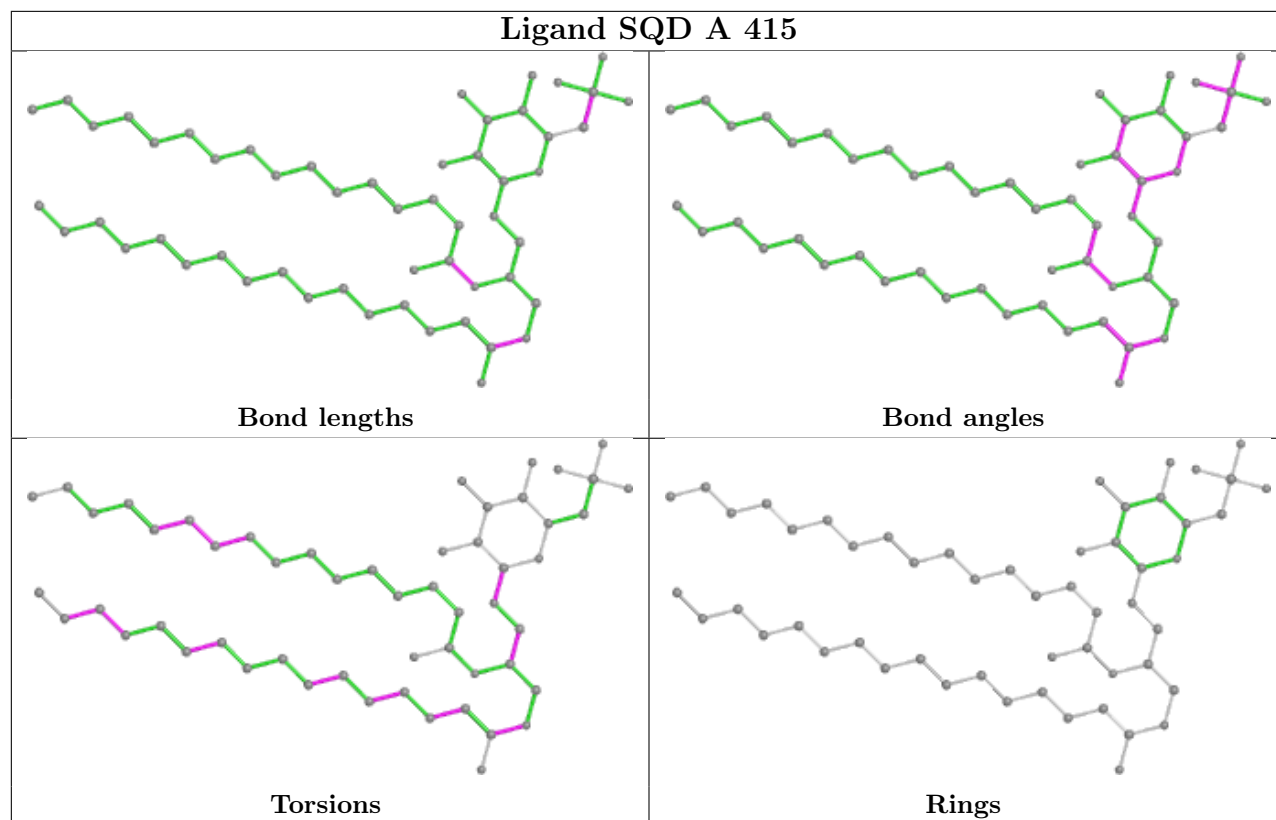


Ligand CLA a 409

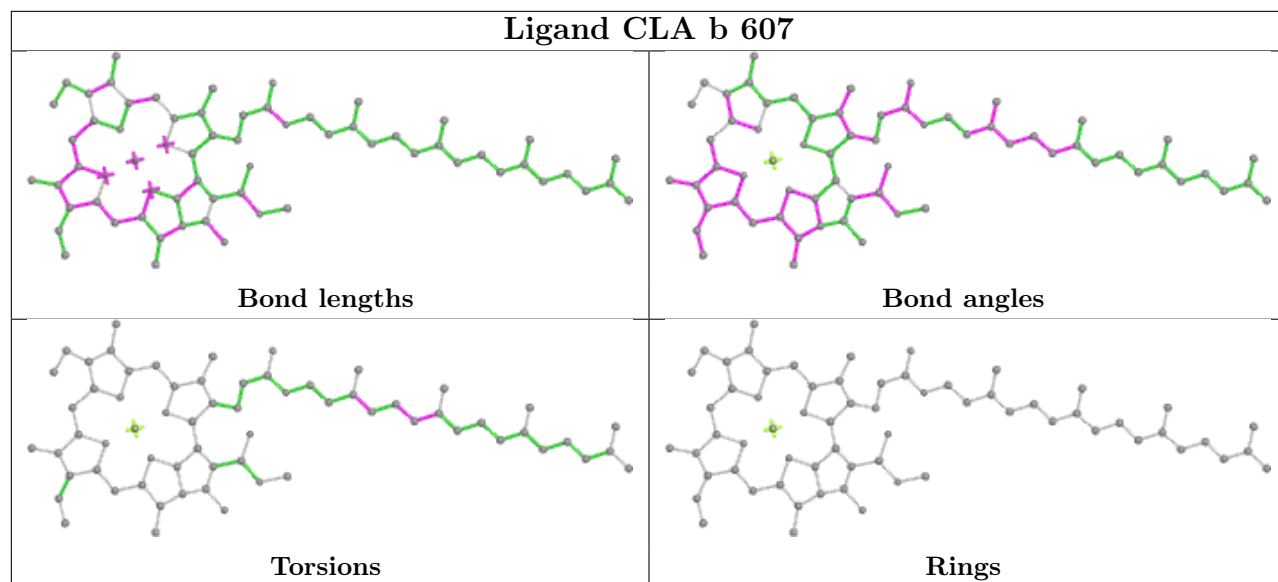


Ligand LMT m 103

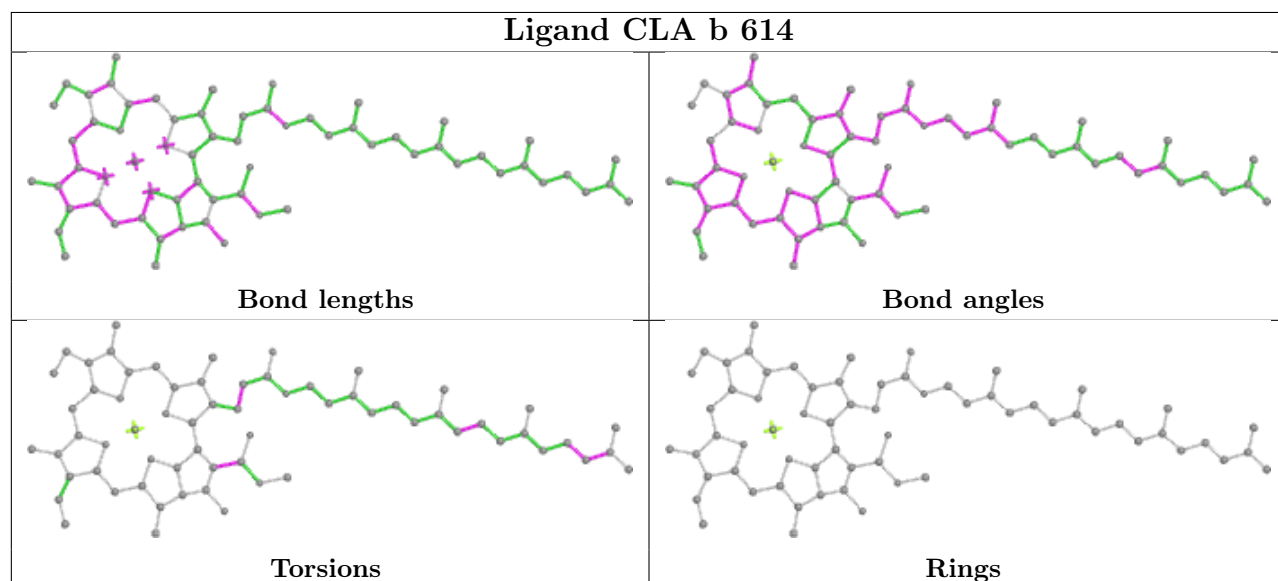




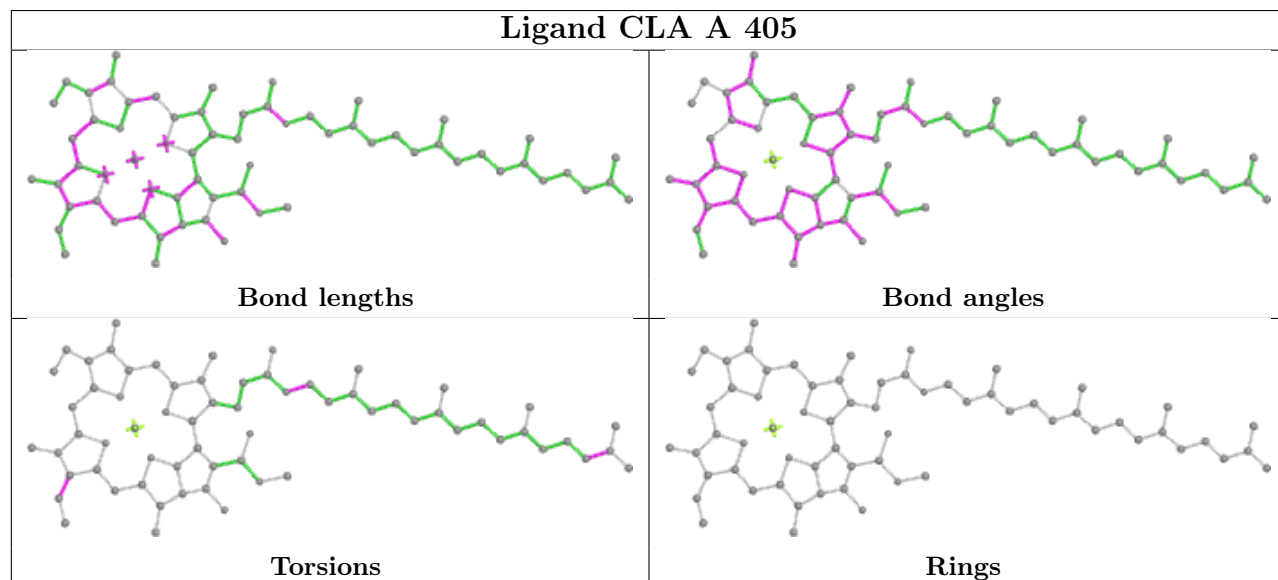
Ligand CLA b 607

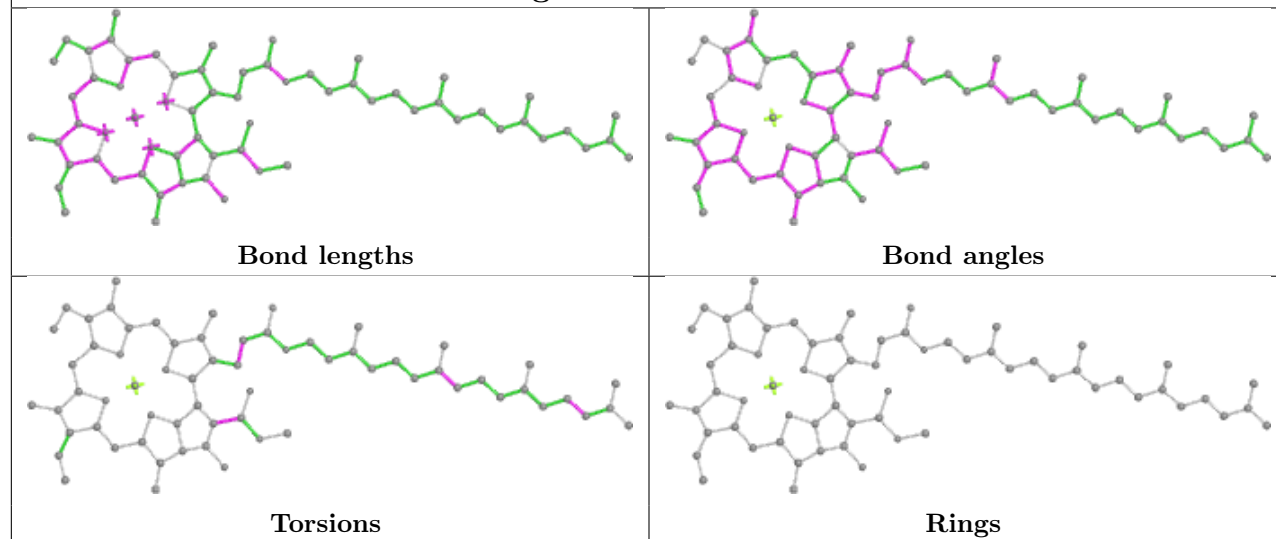
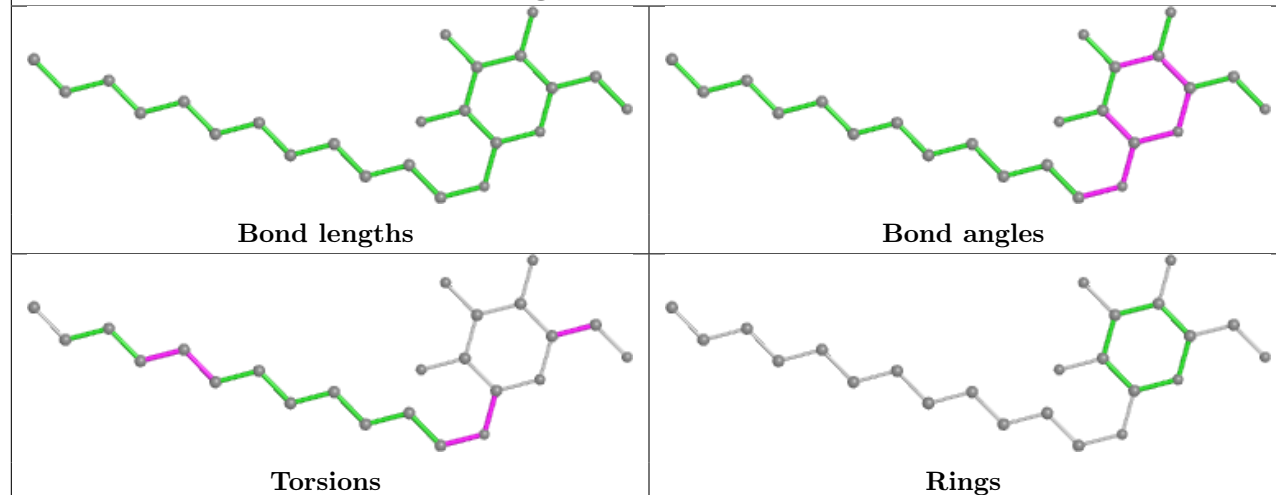
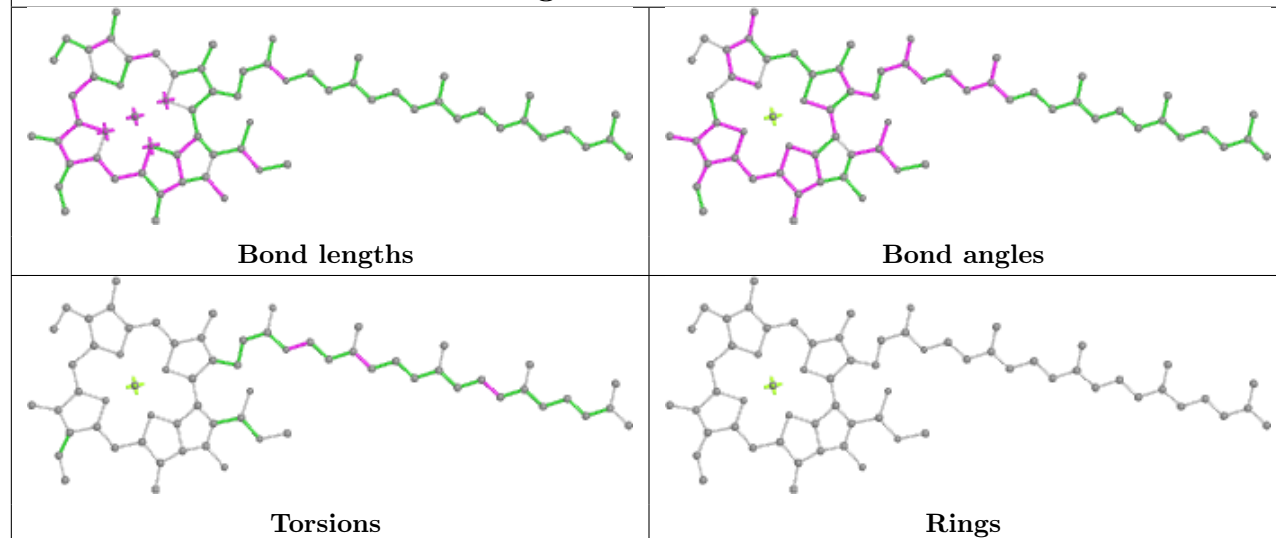


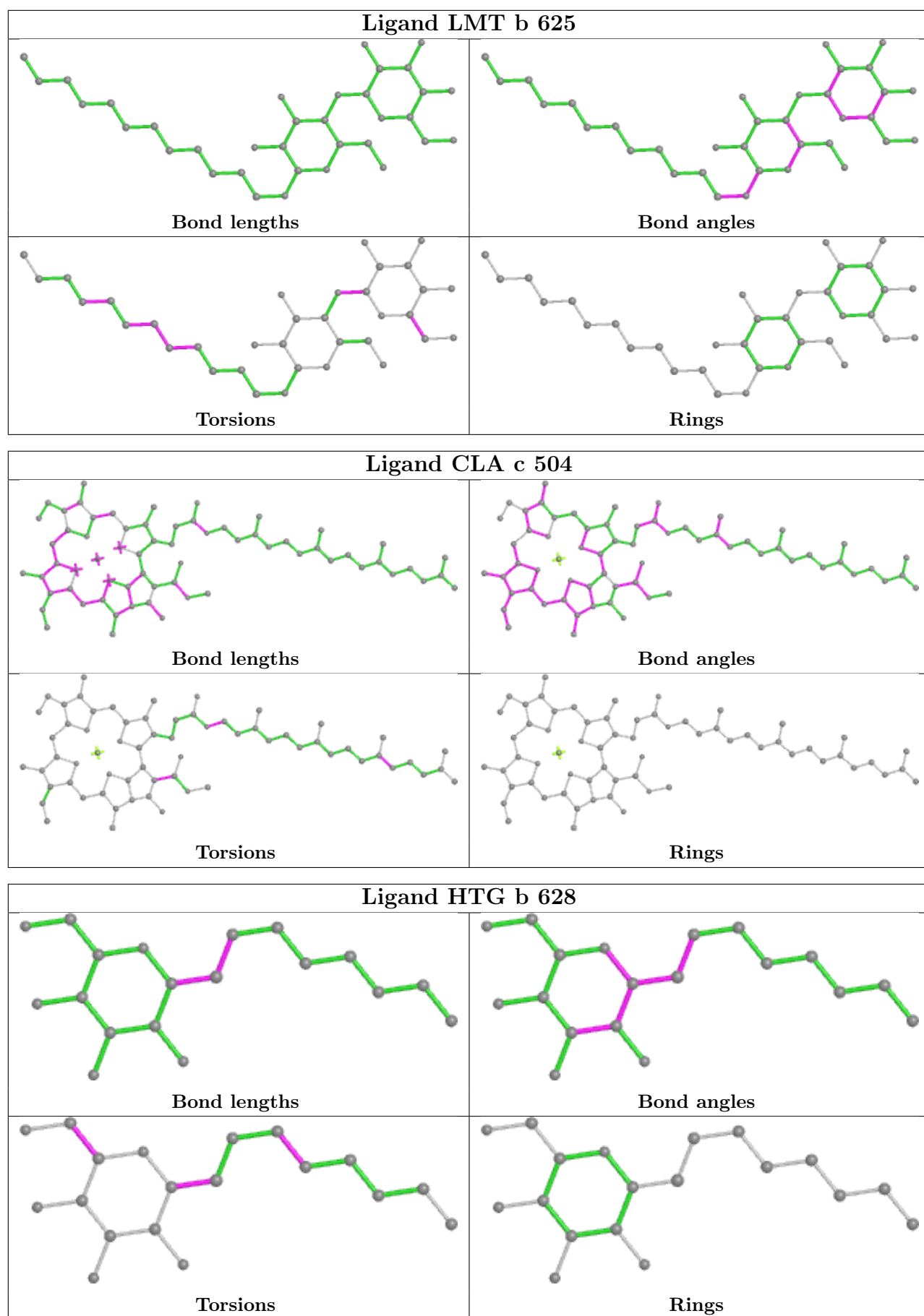
Ligand CLA b 614



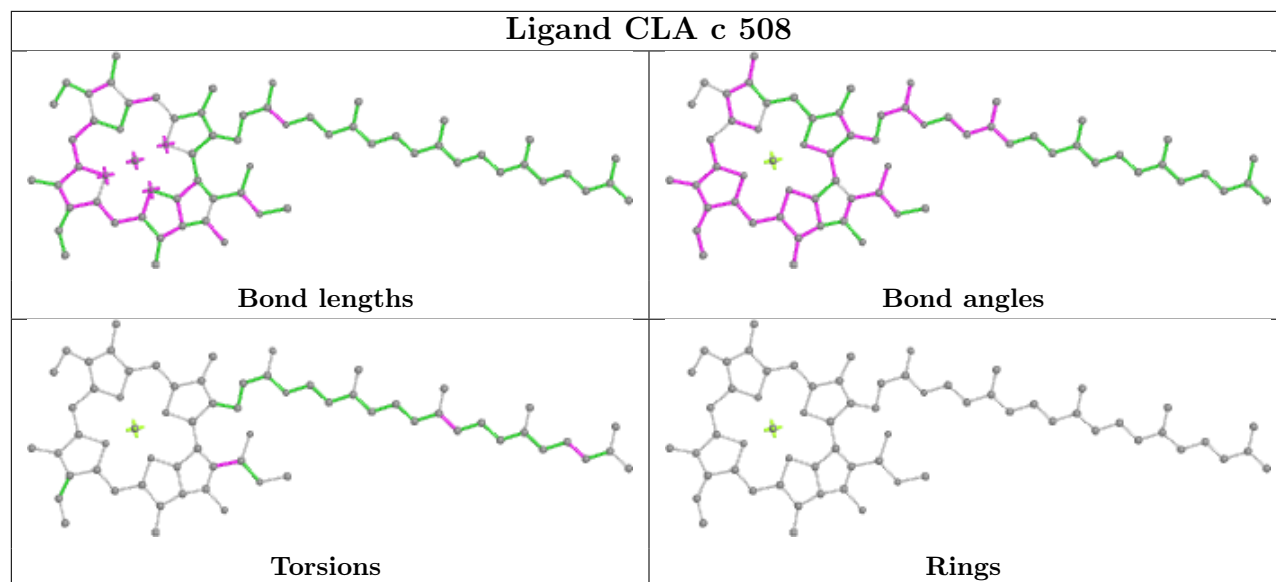
Ligand CLA A 405



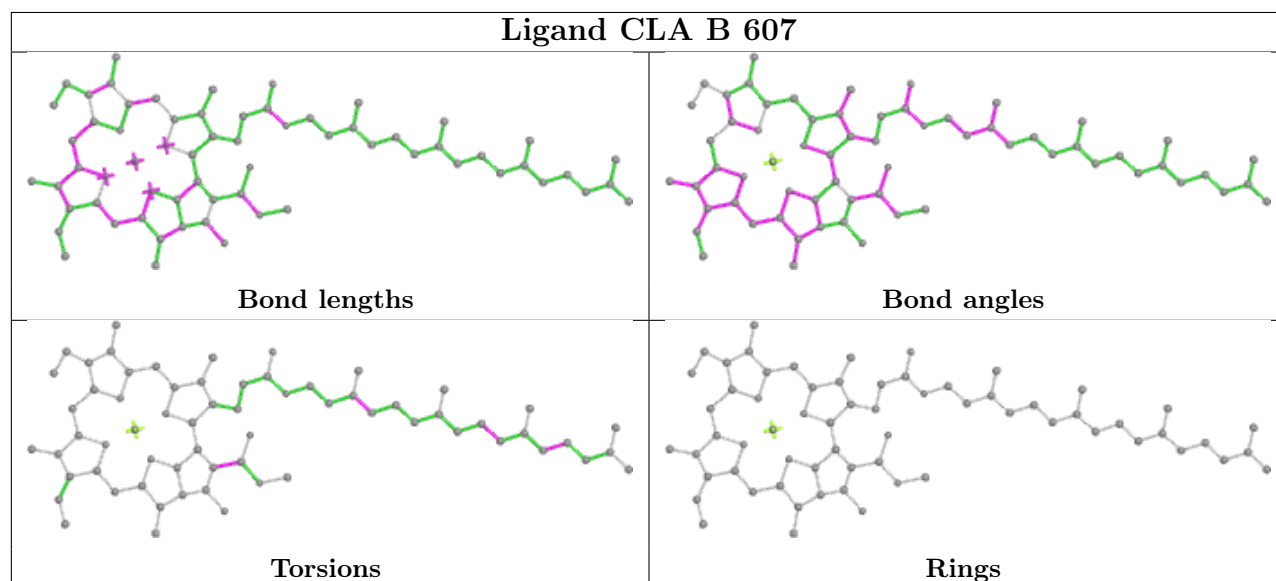
Ligand CLA B 612**Ligand LMT b 629****Ligand CLA c 515**



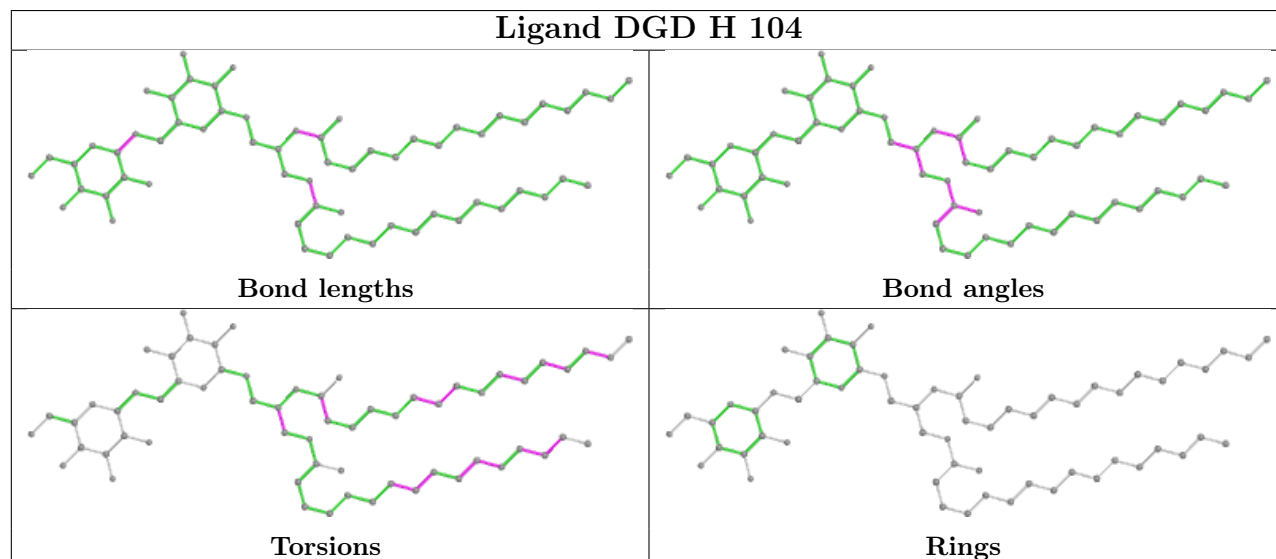
Ligand CLA c 508



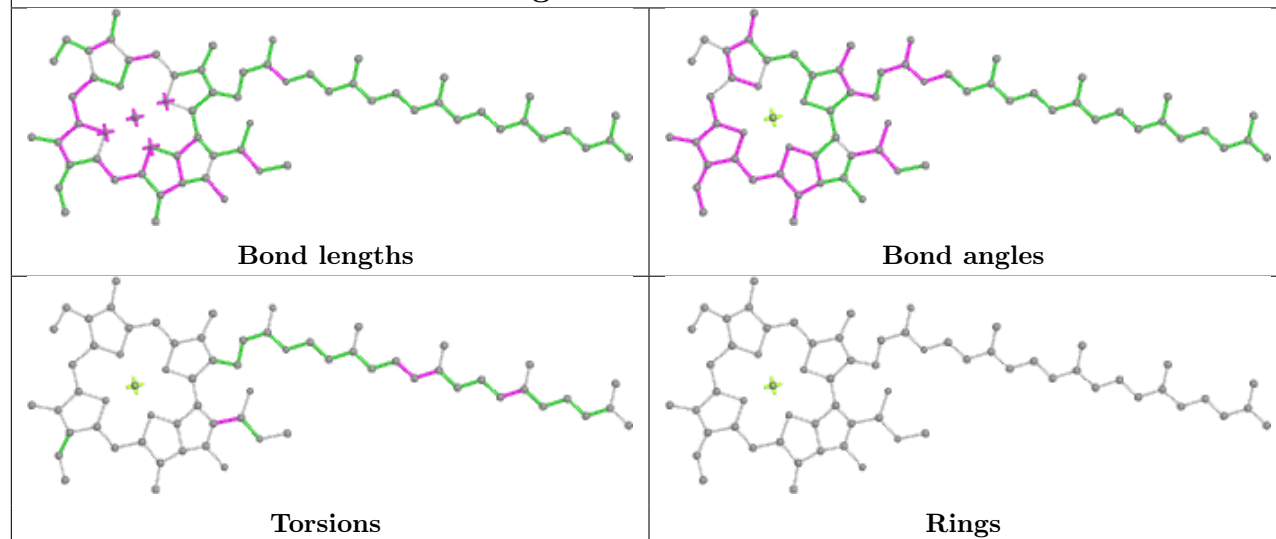
Ligand CLA B 607



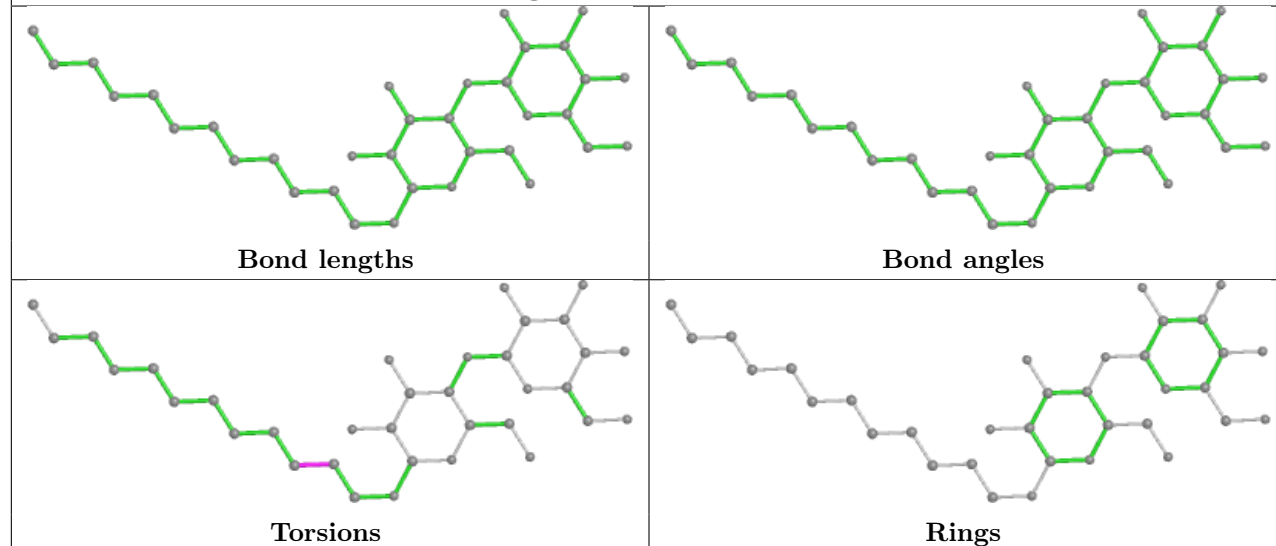
Ligand DGD H 104



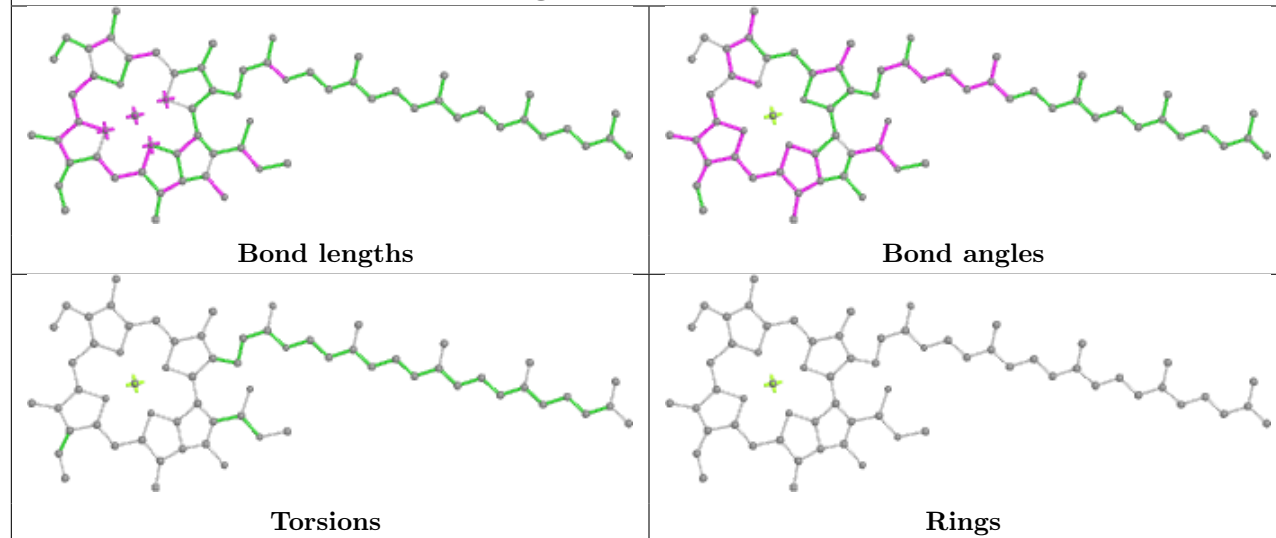
Ligand CLA B 605



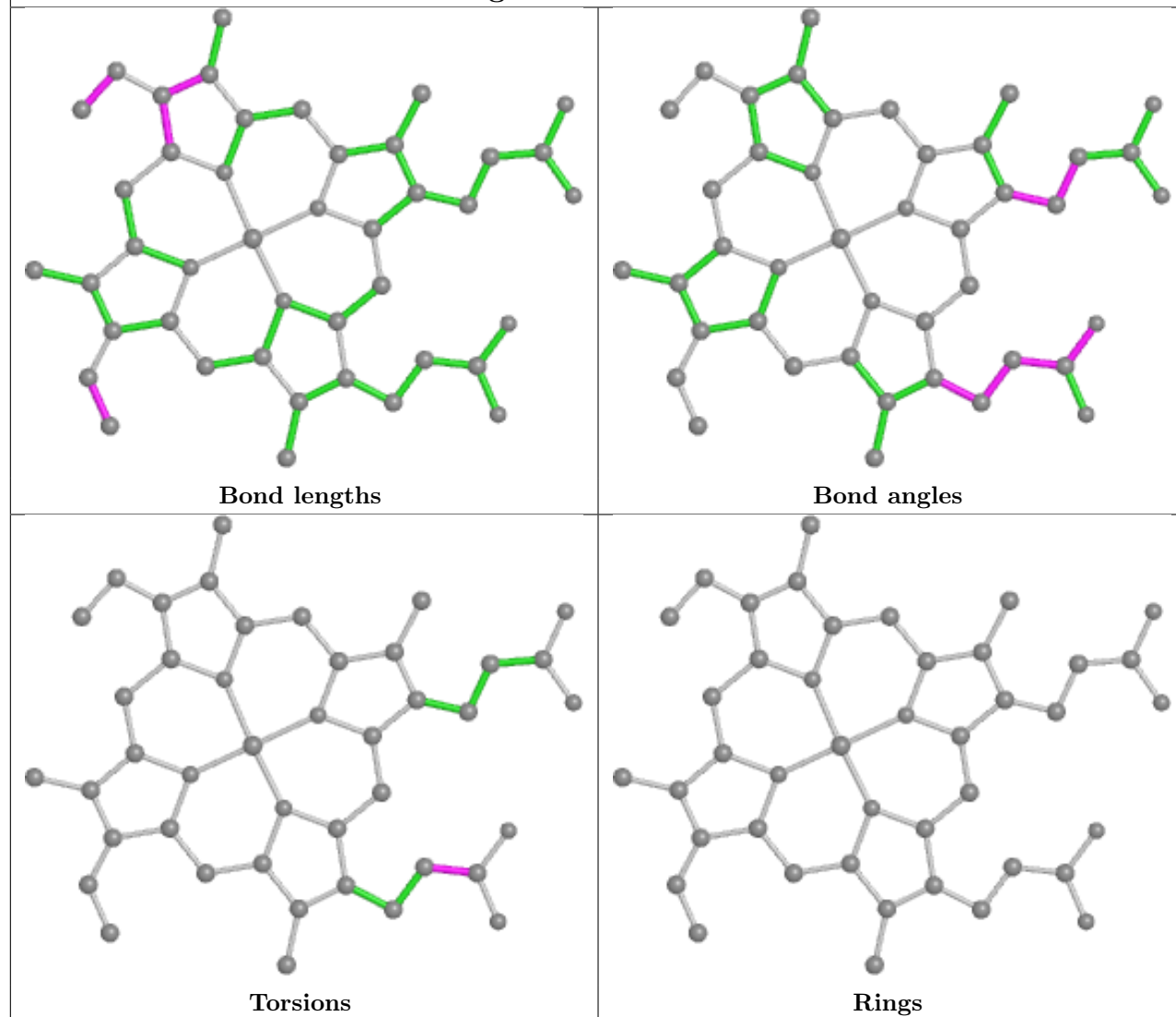
Ligand LMT M 102



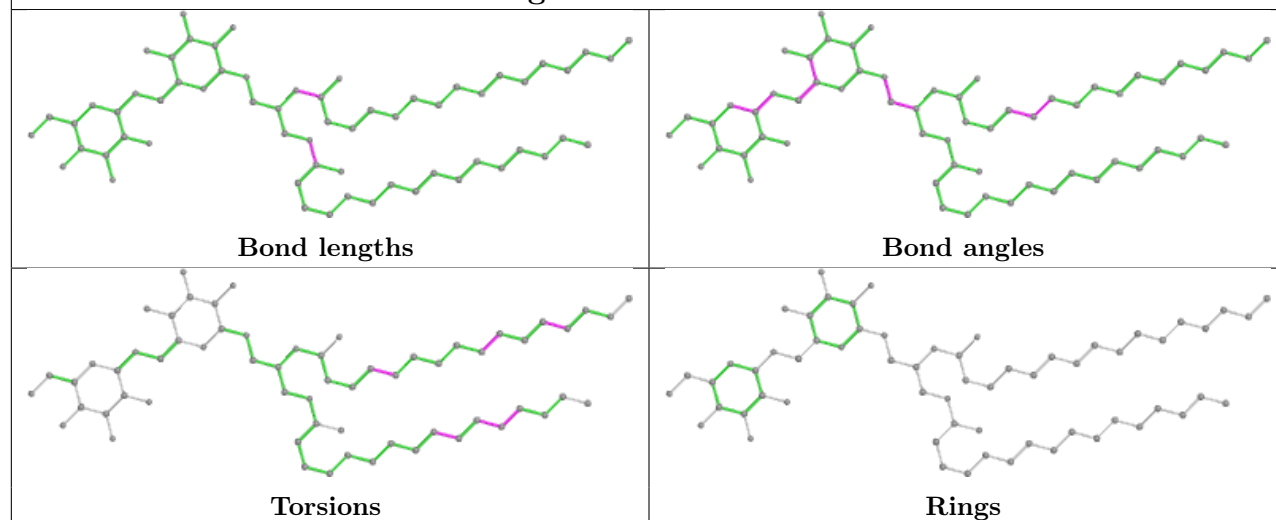
Ligand CLA B 614



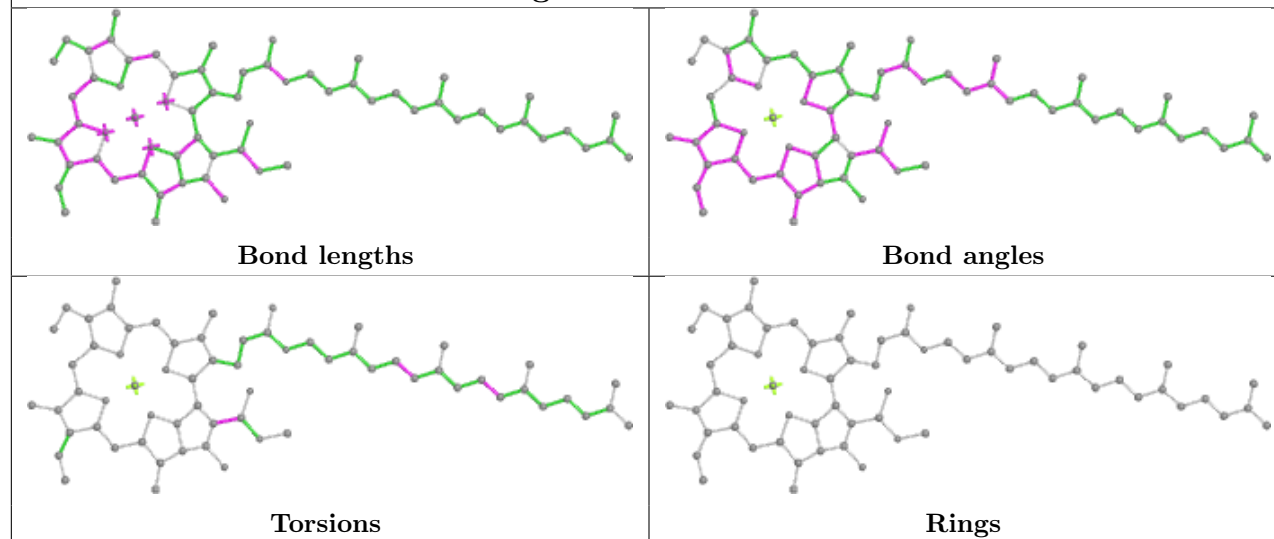
Ligand HEC V 201



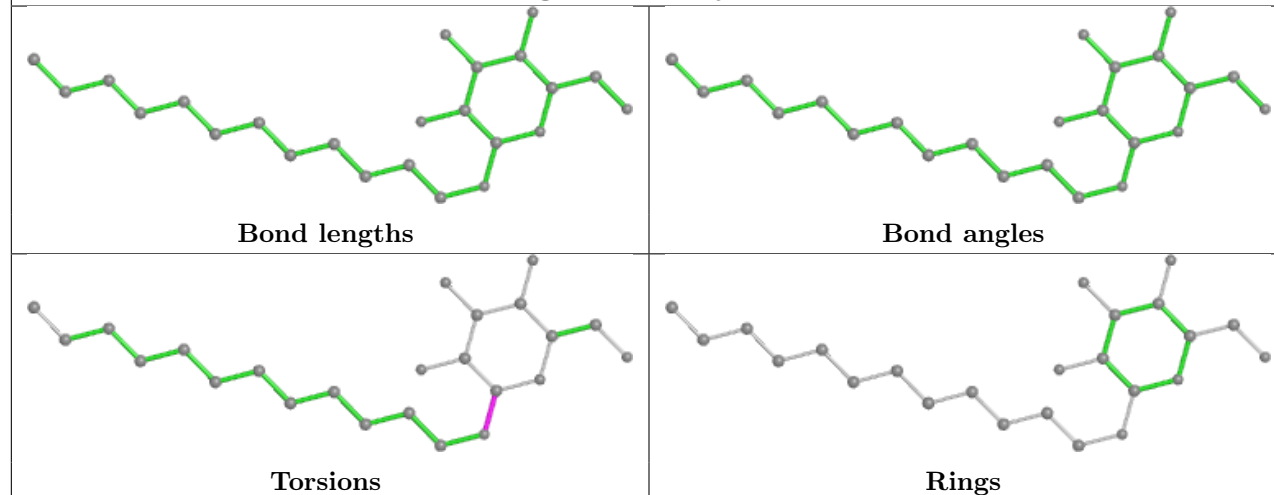
Ligand DGD C 520



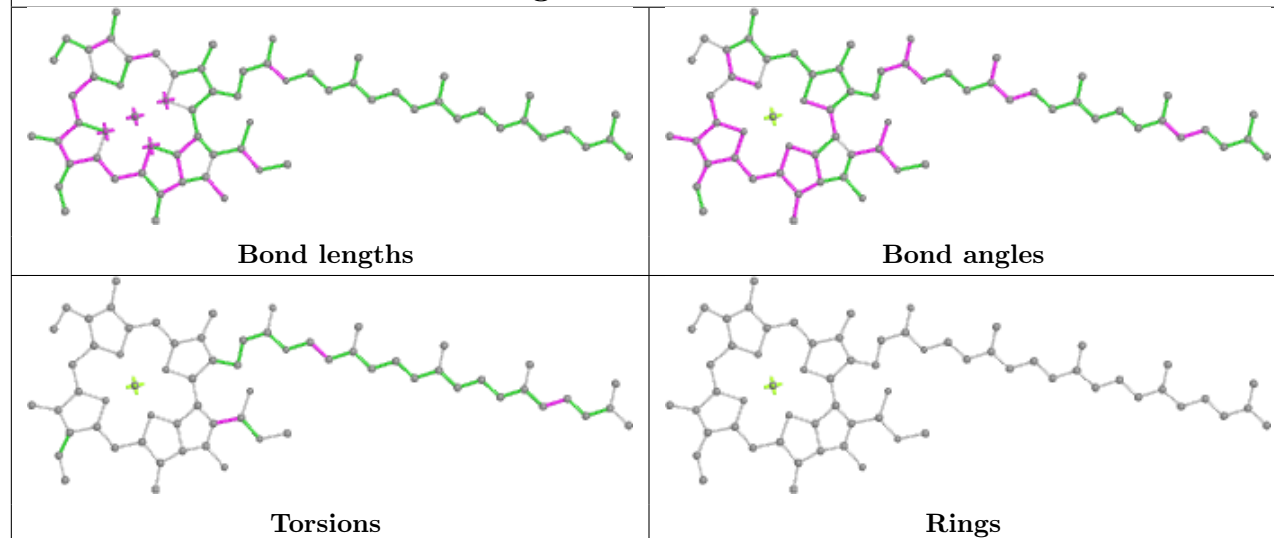
Ligand CLA C 505

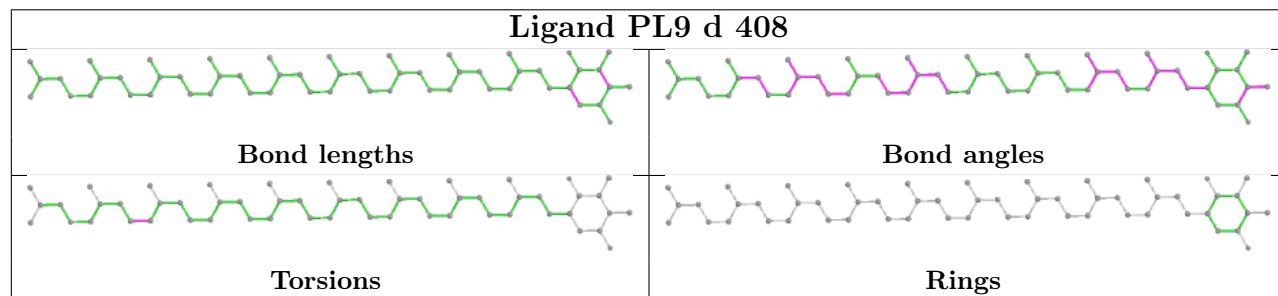
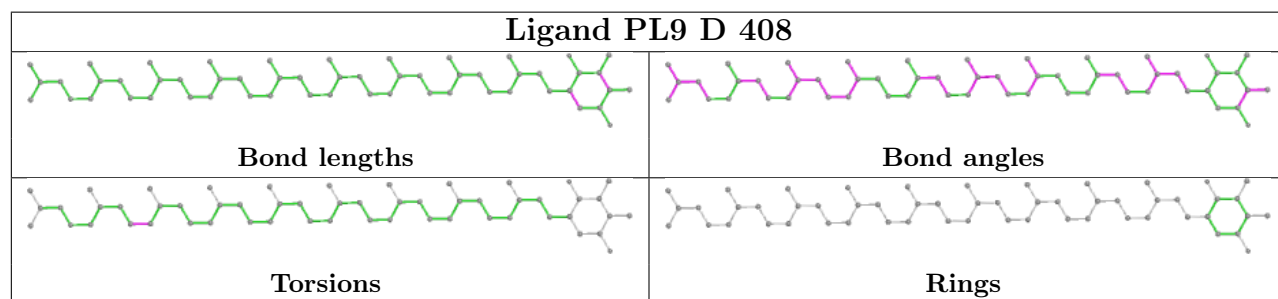
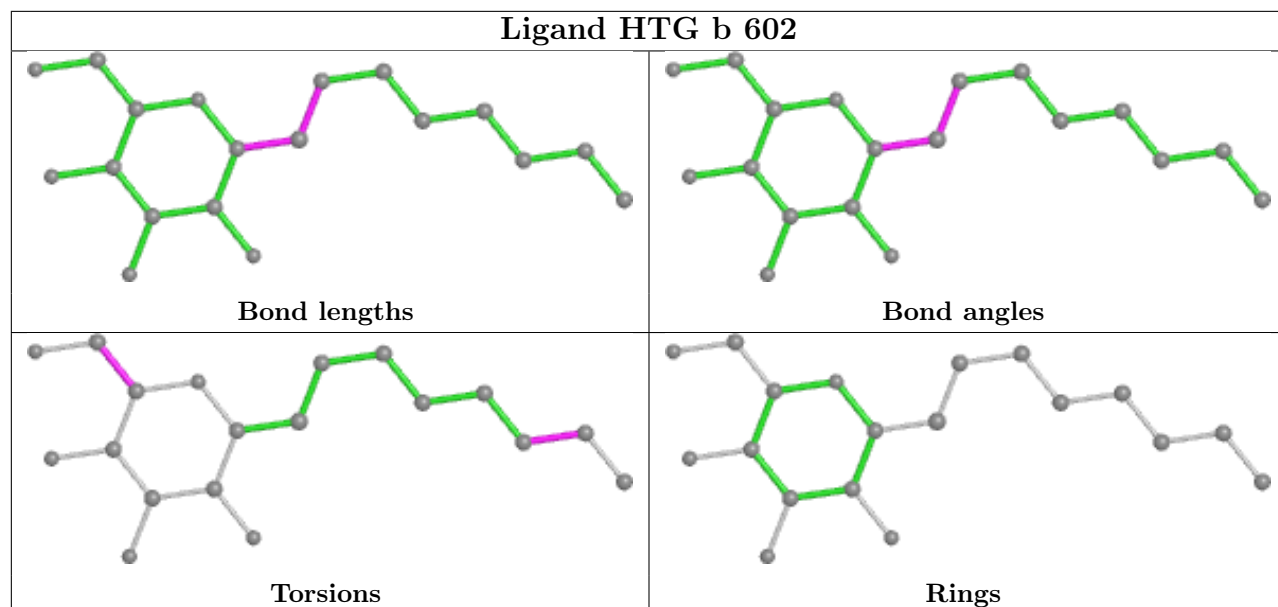


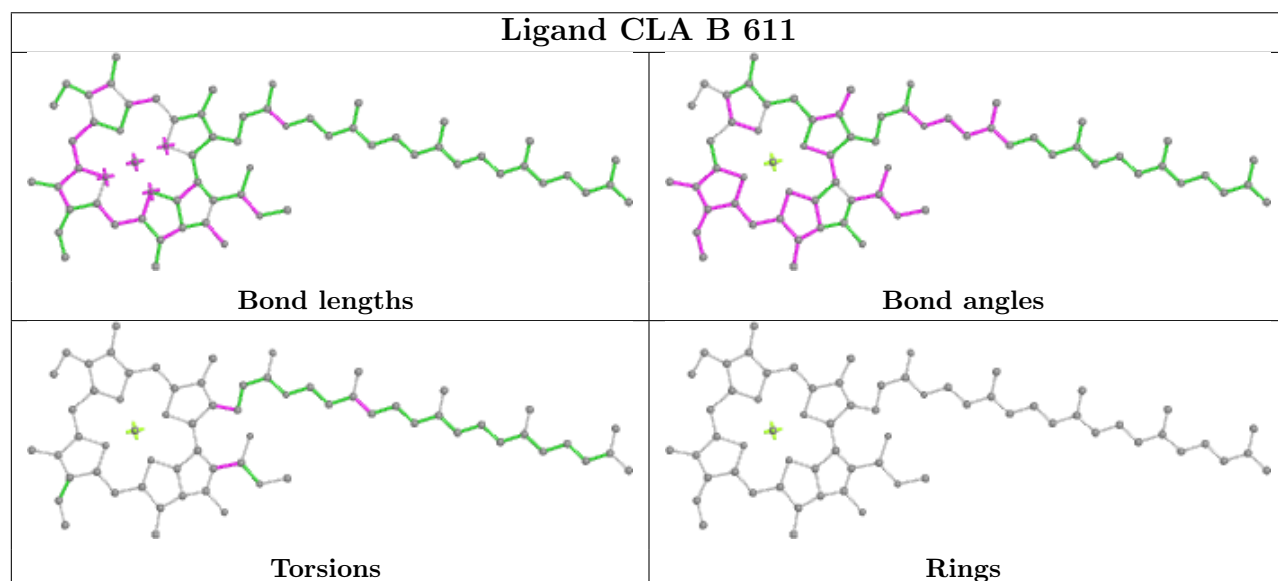
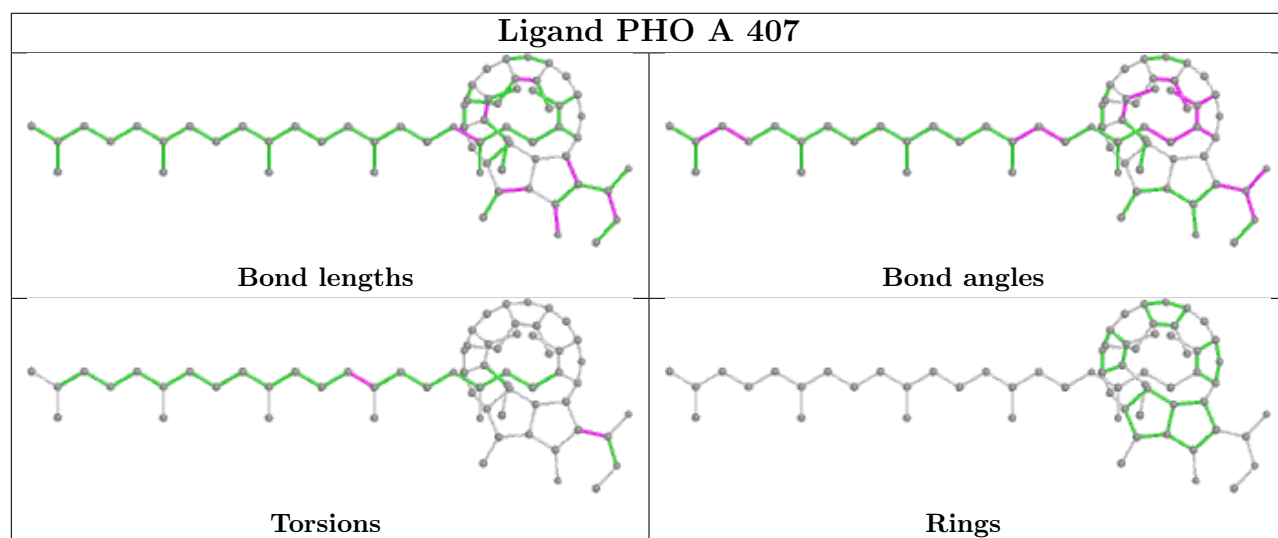
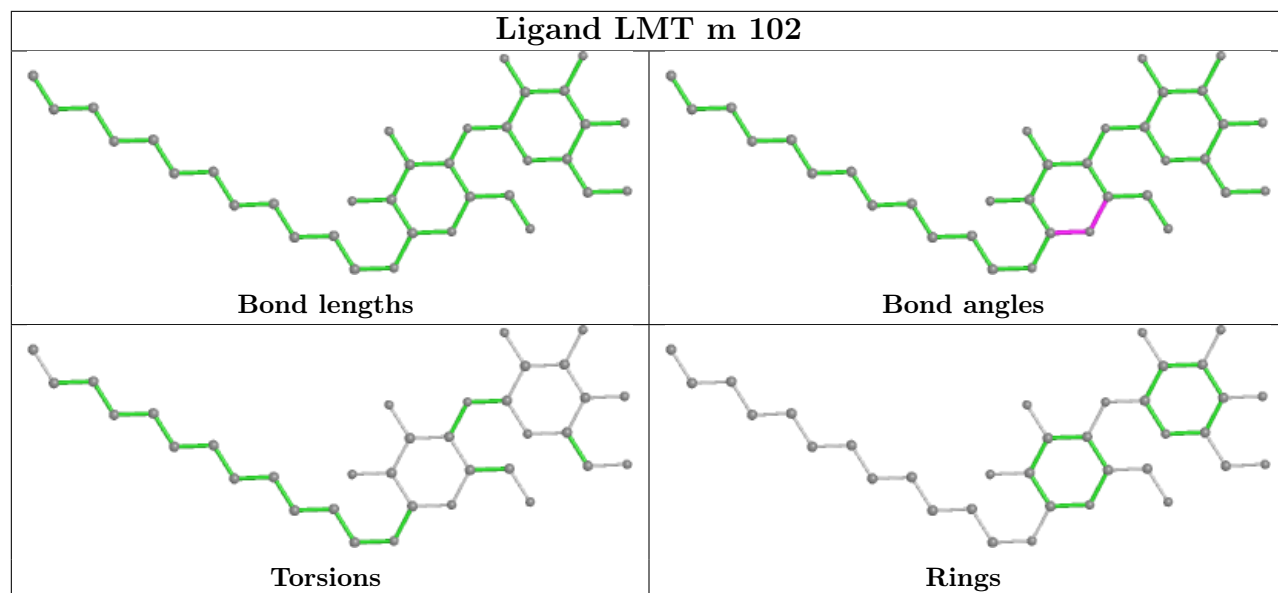
Ligand LMT j 102

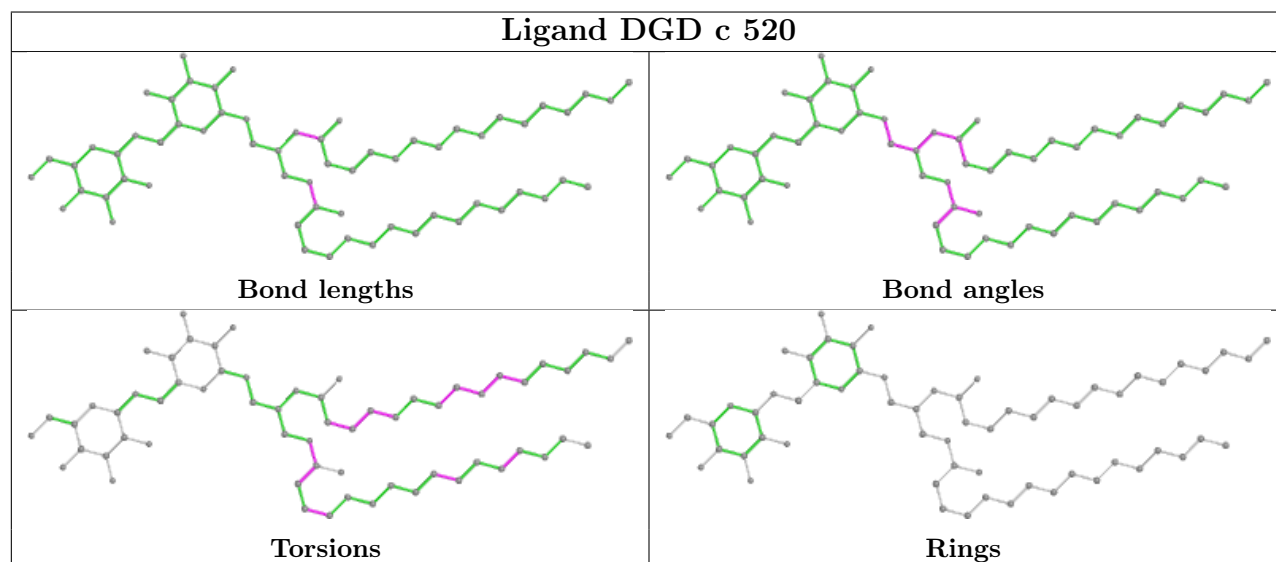
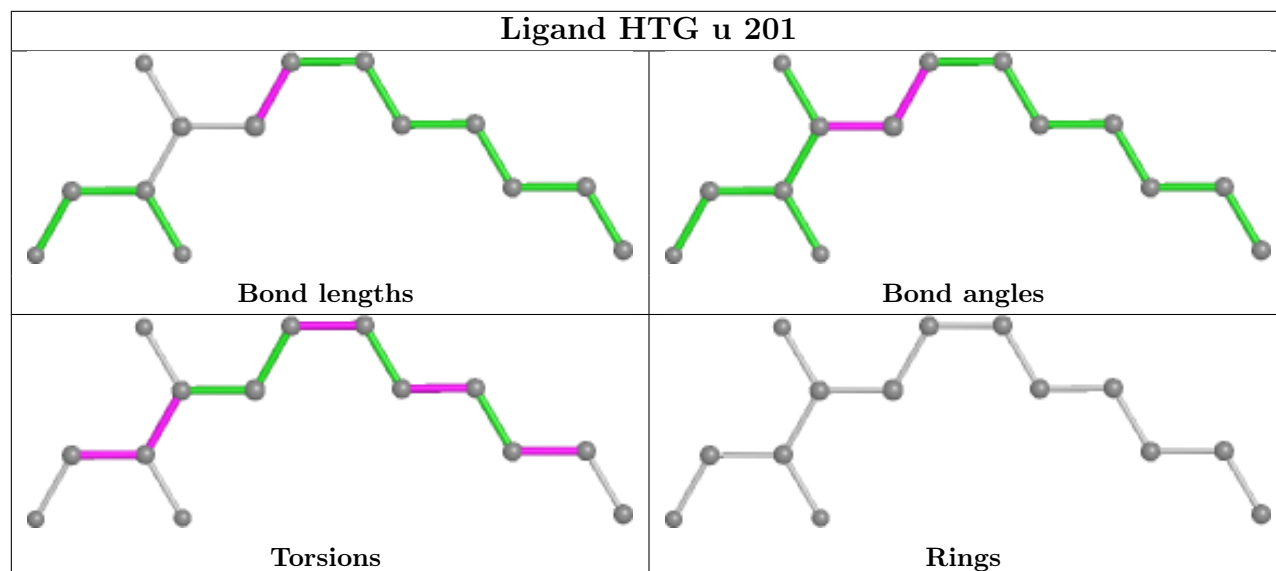
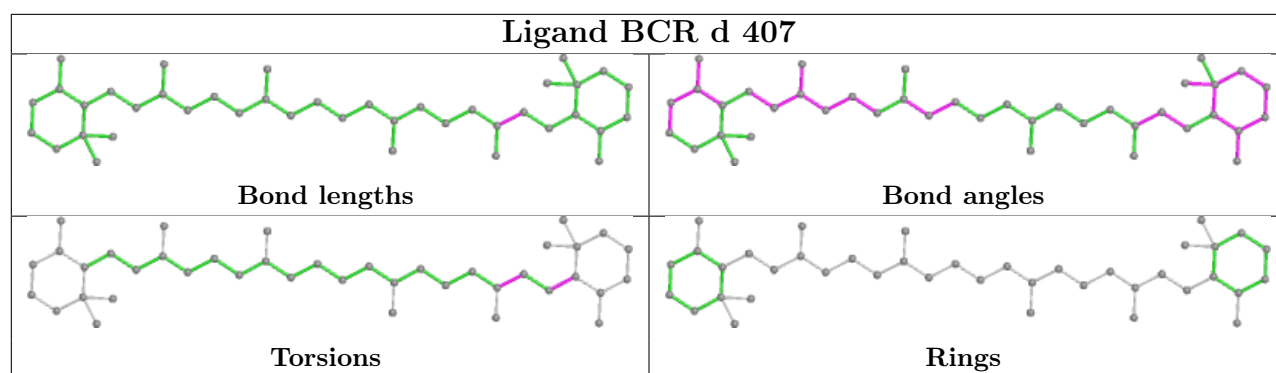


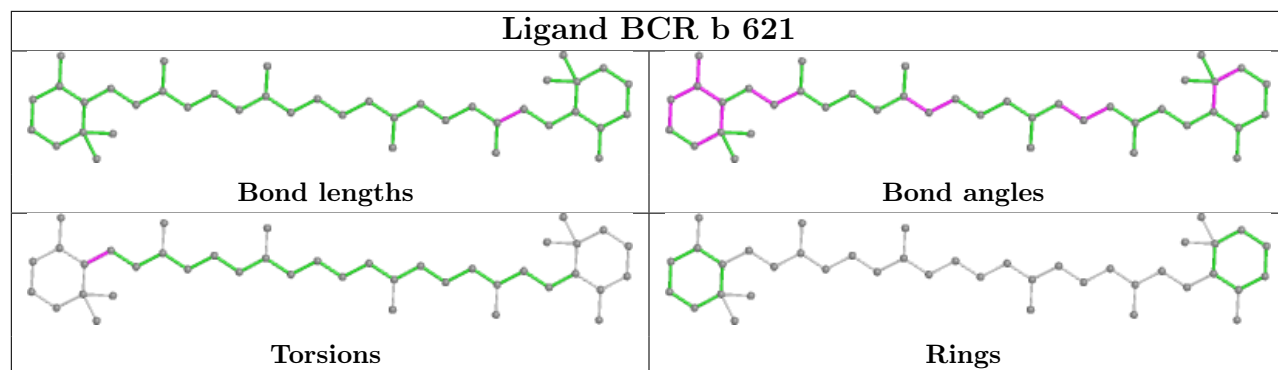
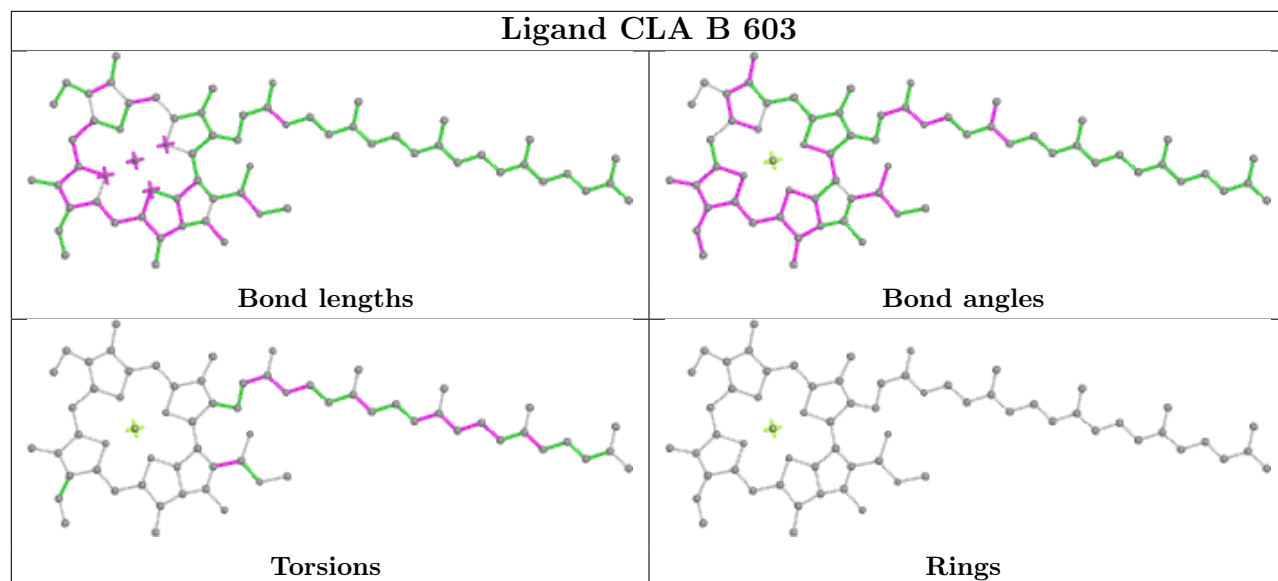
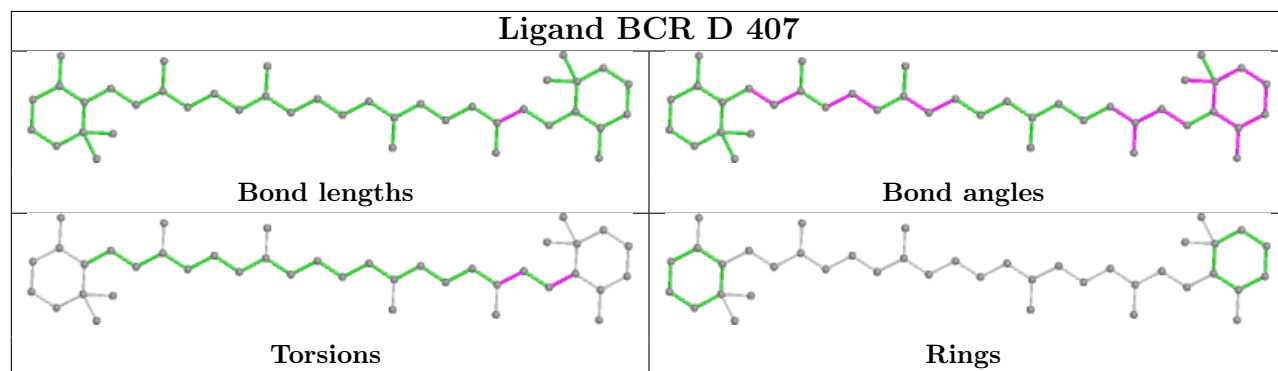
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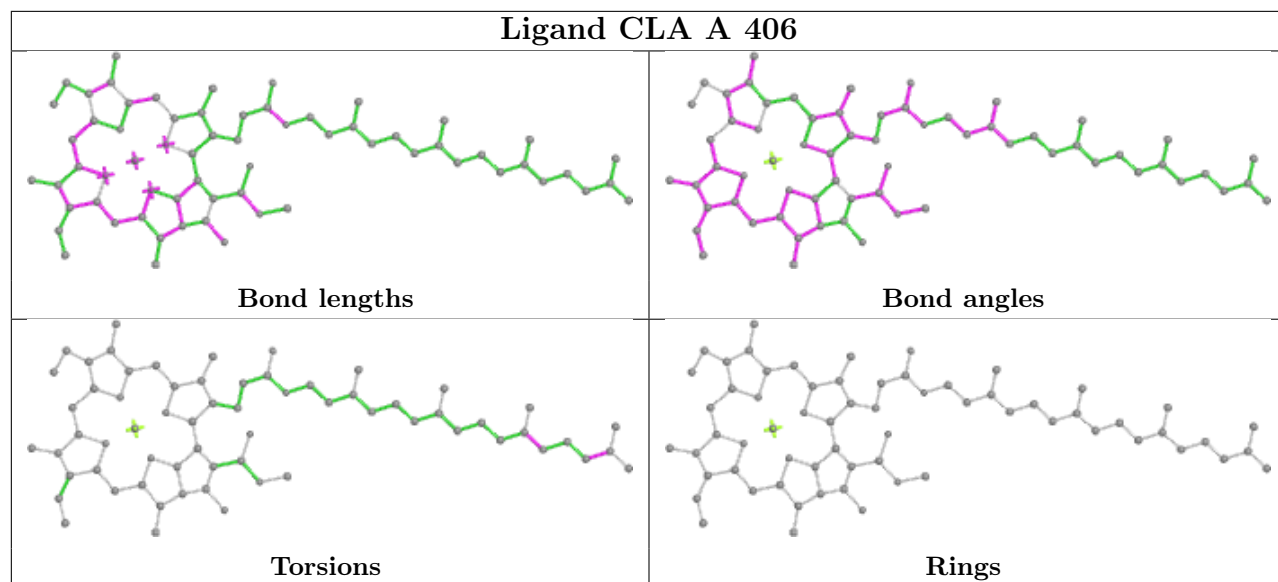
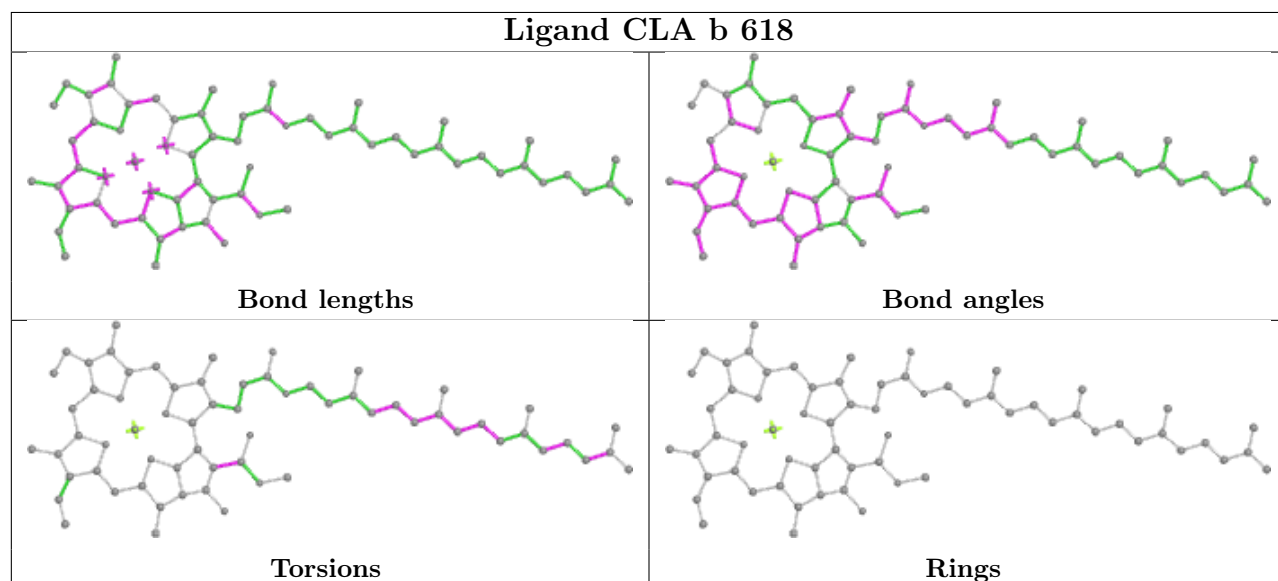
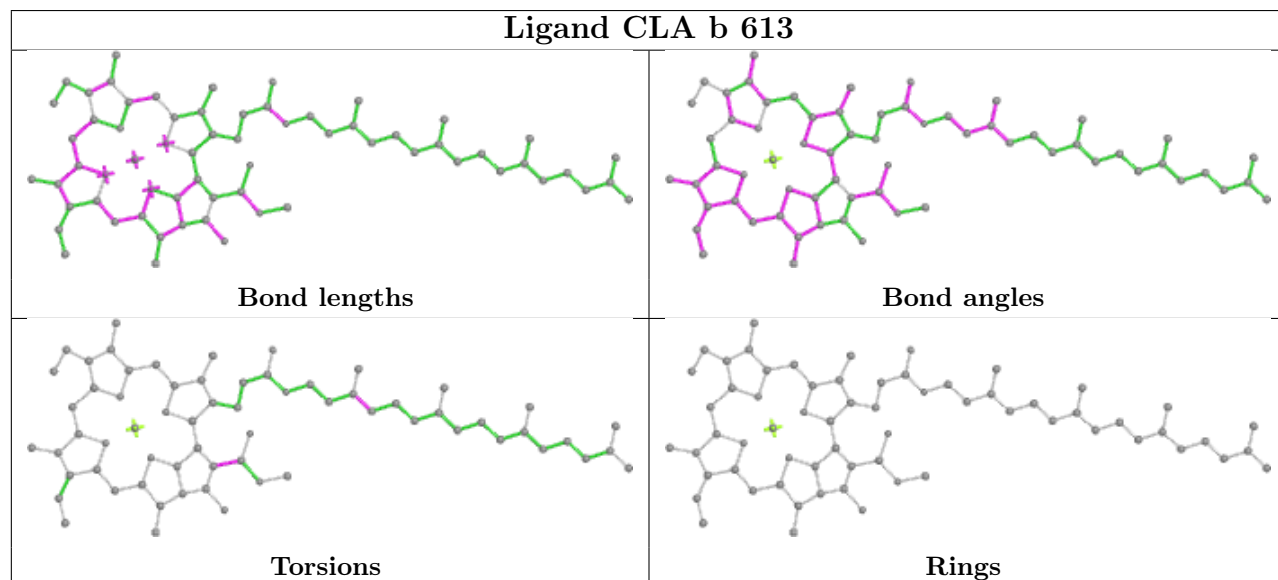


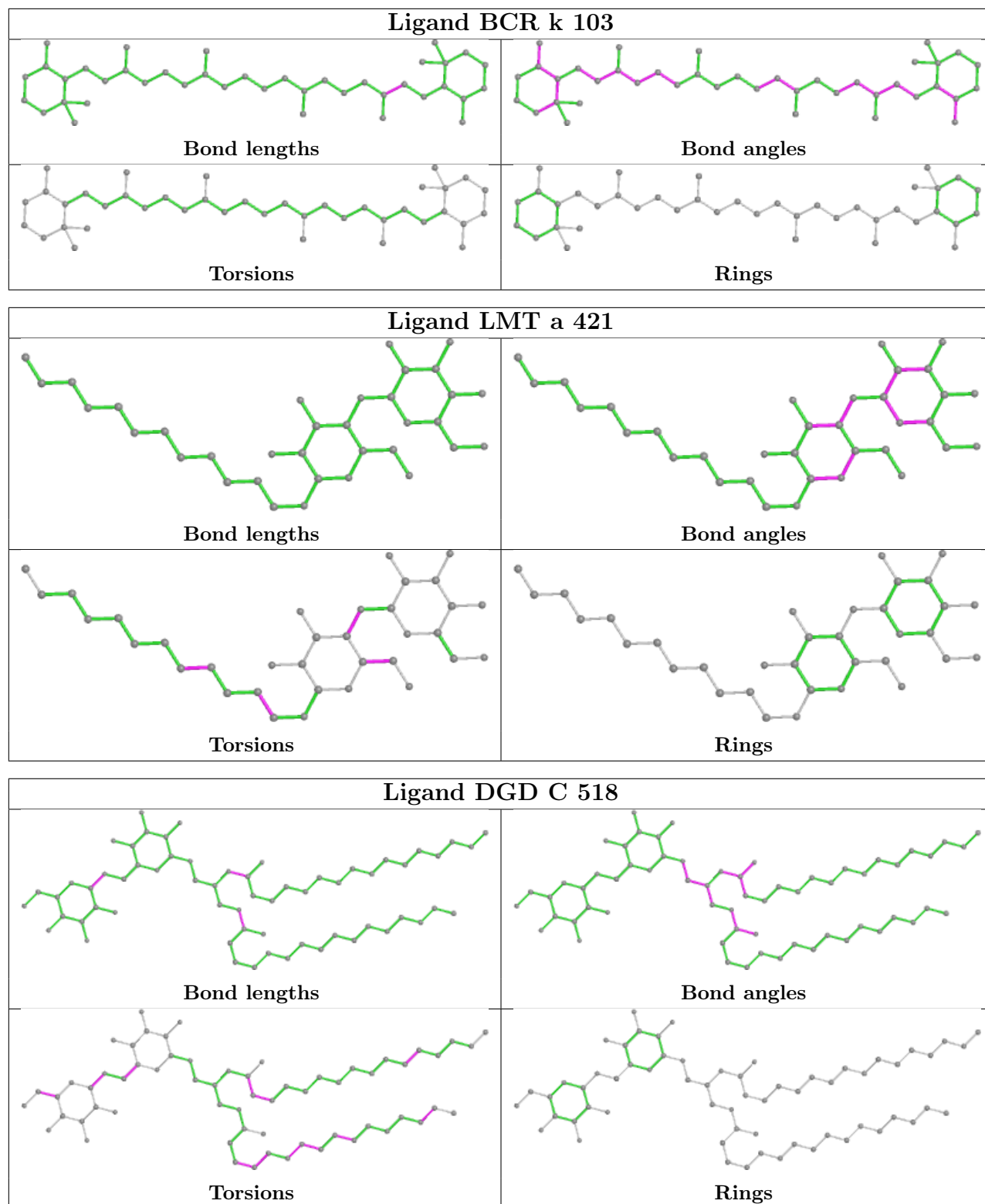




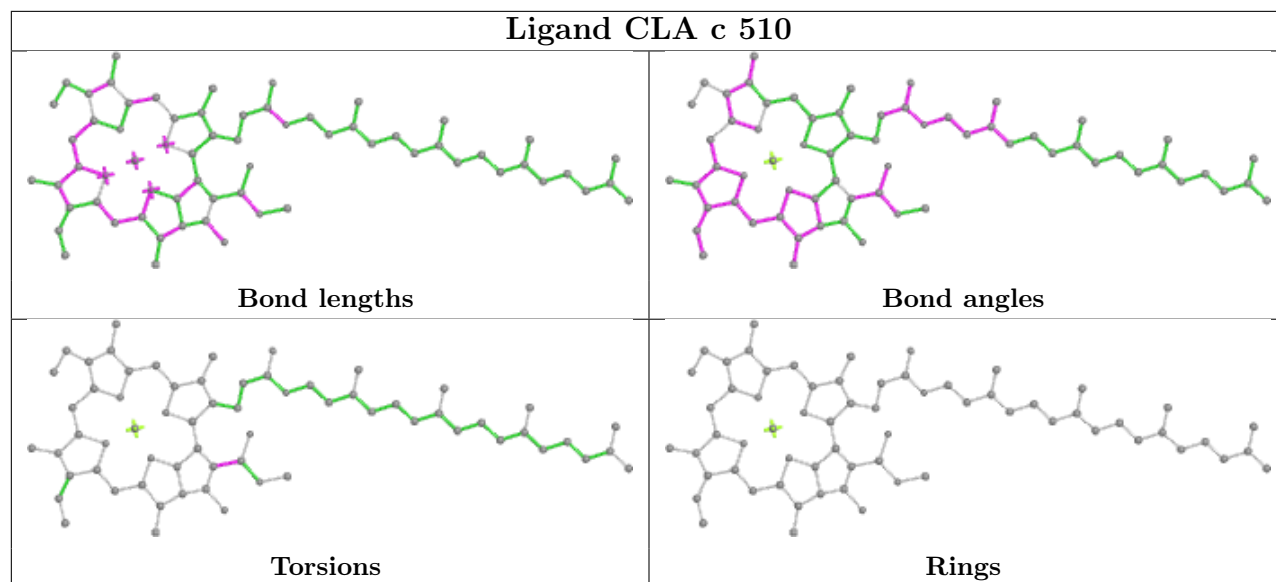


Ligand BCR b 621**Ligand CLA B 603****Ligand BCR D 407**

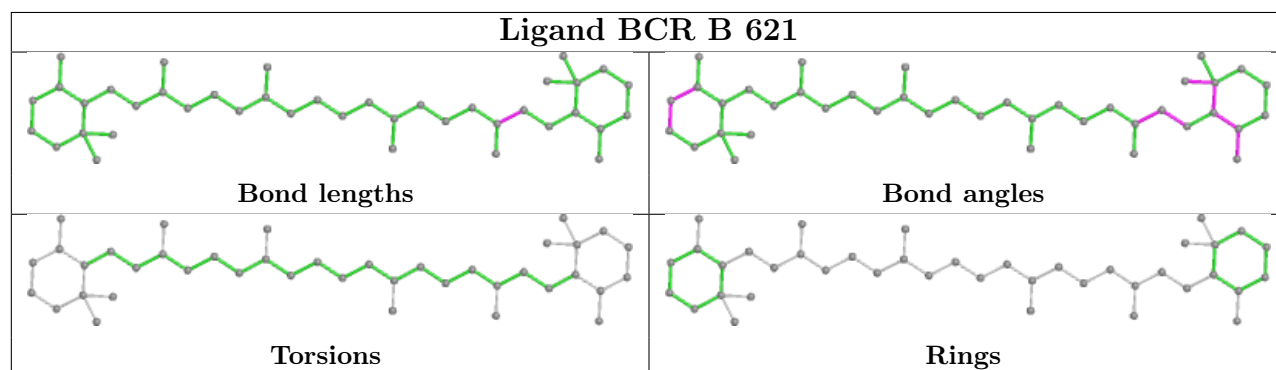
Ligand CLA A 406**Ligand CLA b 618****Ligand CLA b 613**



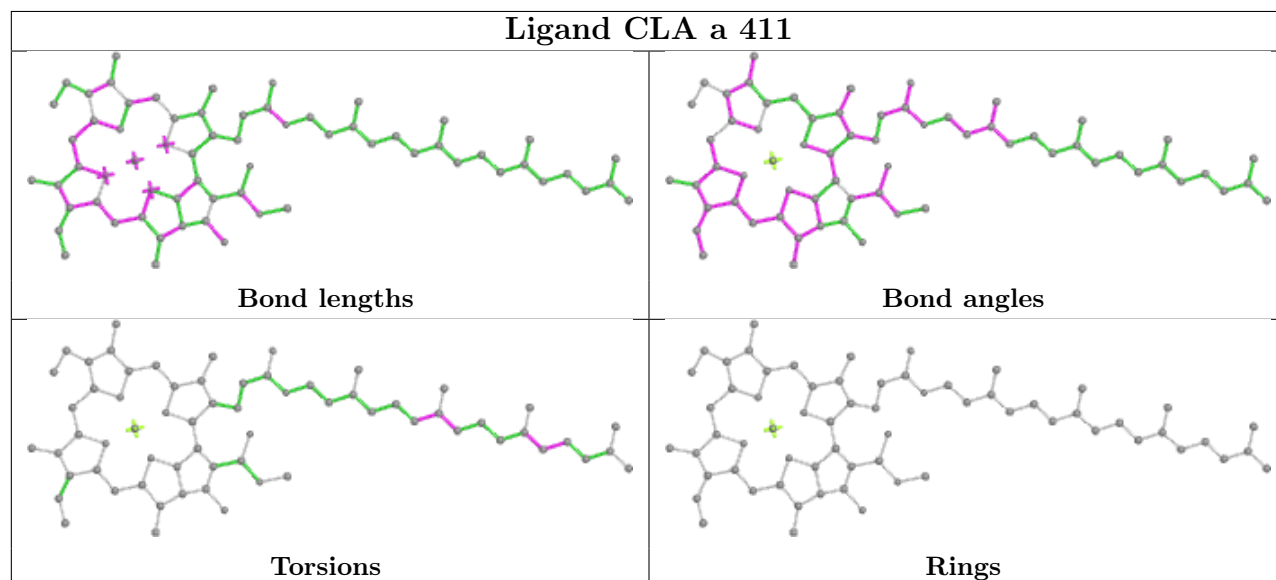
Ligand CLA c 510



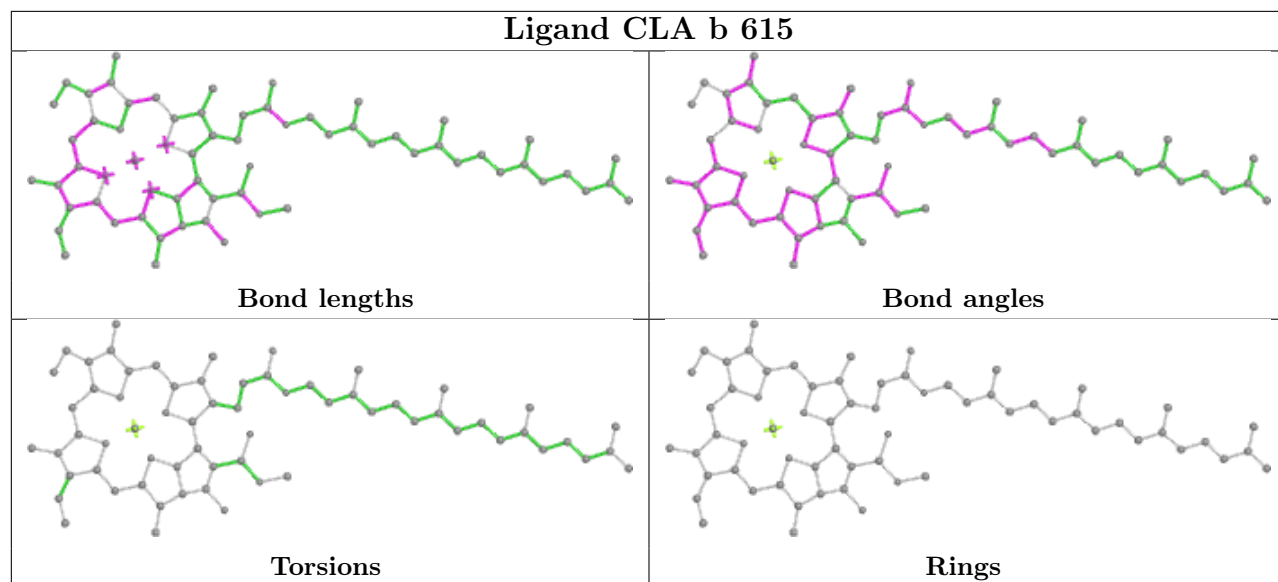
Ligand BCR B 621



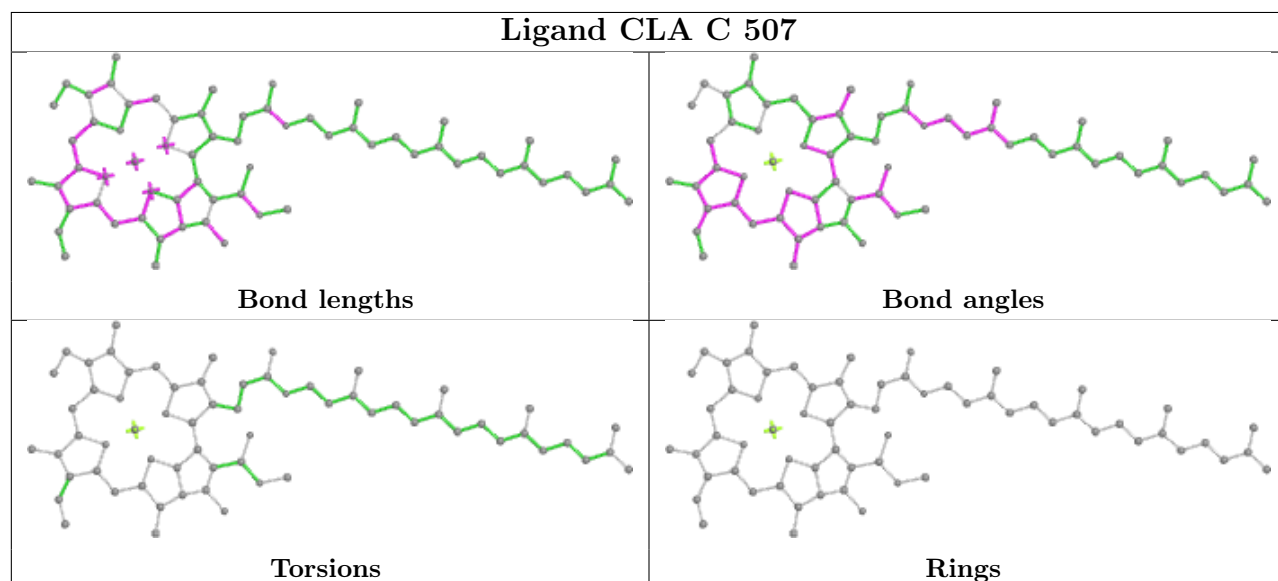
Ligand CLA a 411



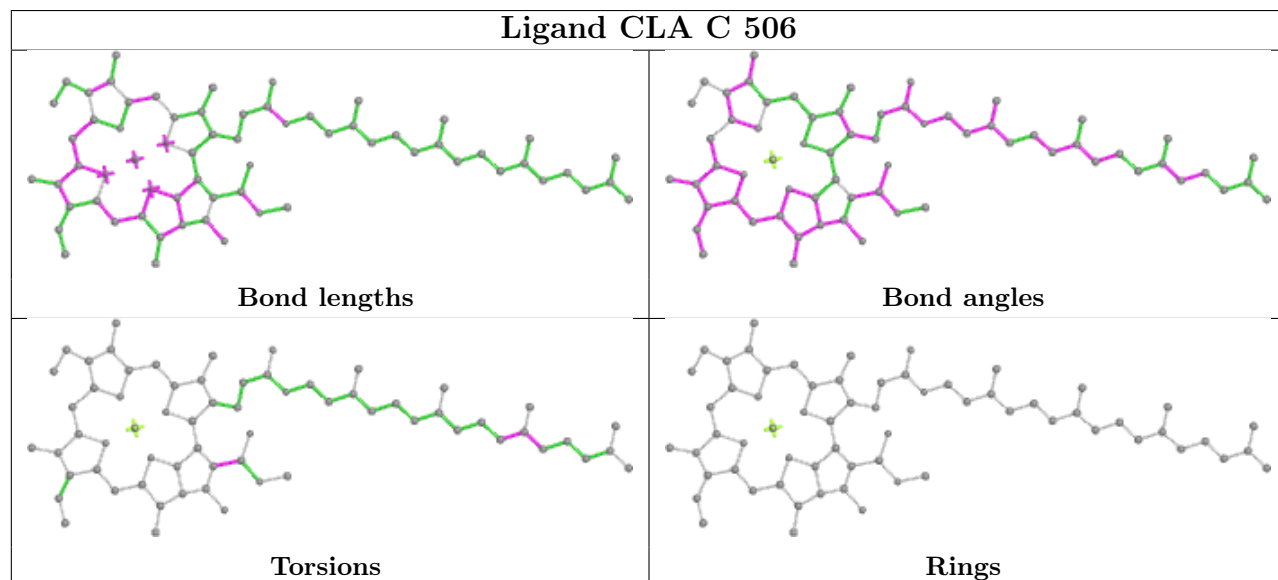
Ligand CLA b 615



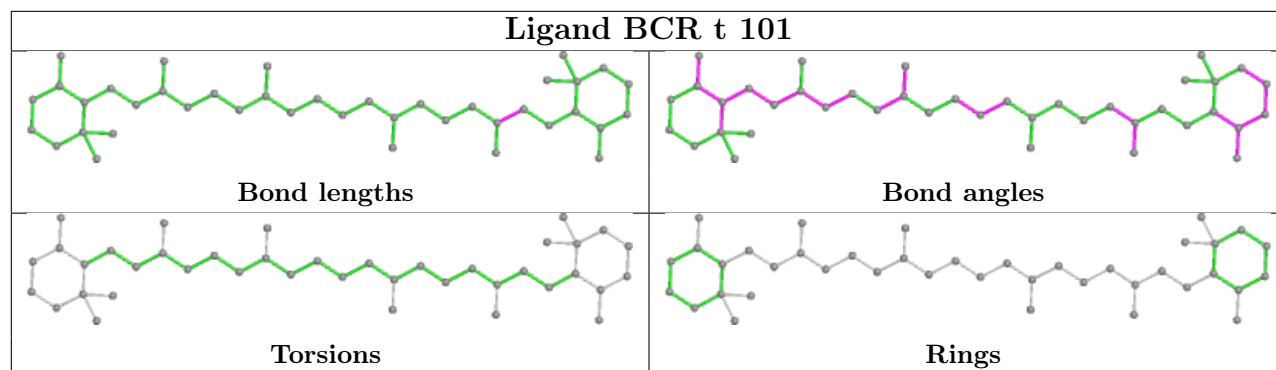
Ligand CLA C 507



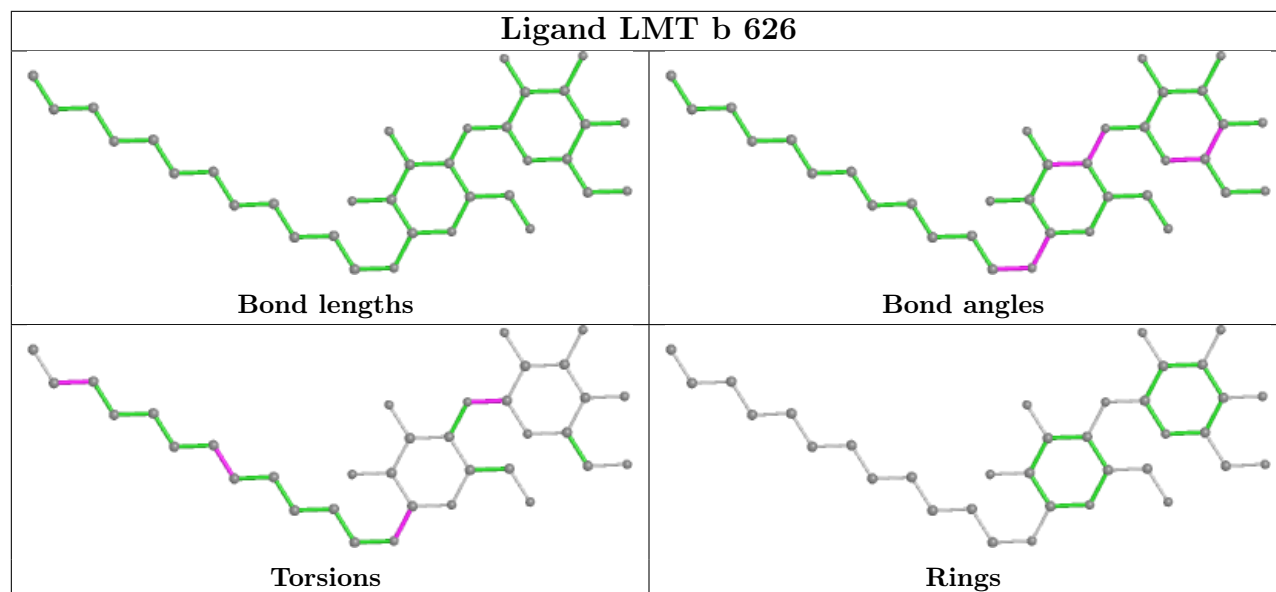
Ligand CLA C 506



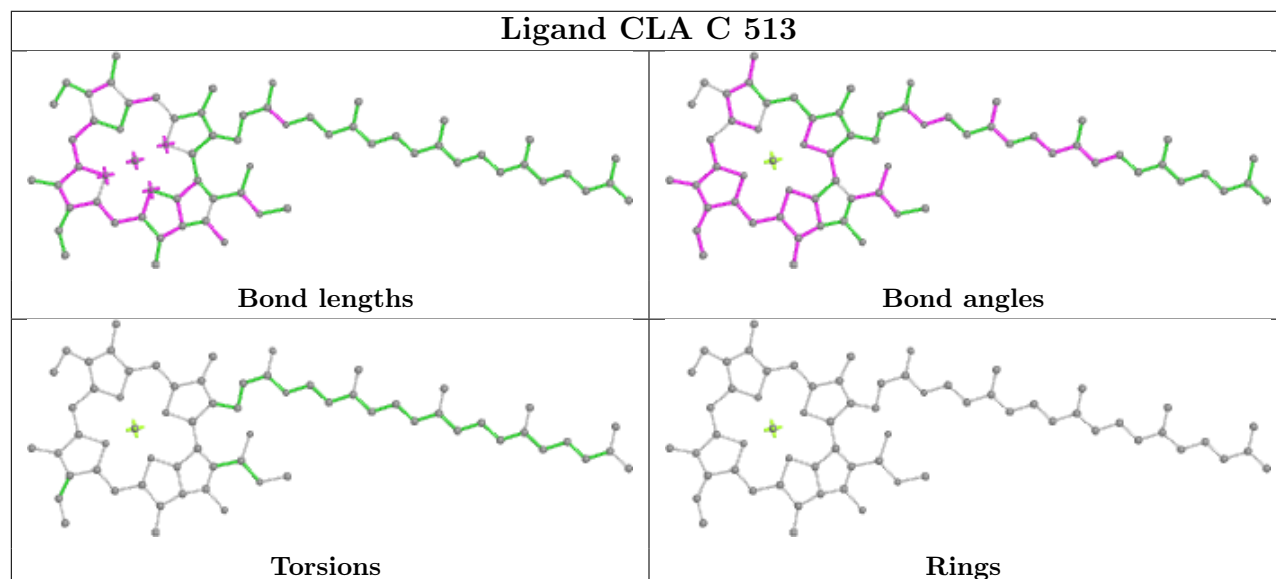
Ligand BCR t 101

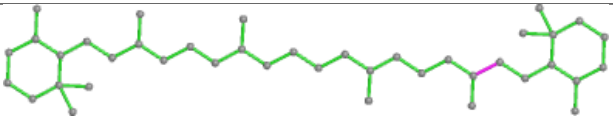
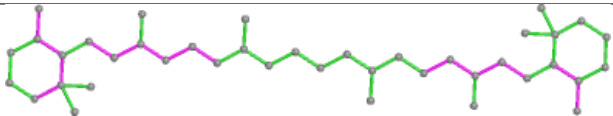
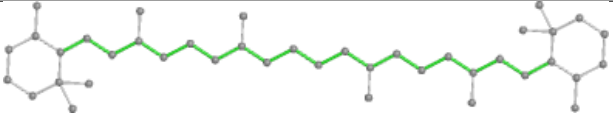
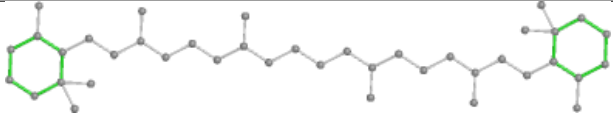


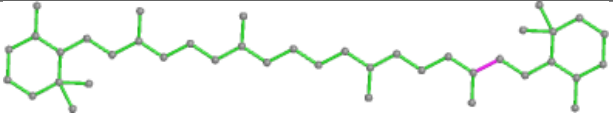
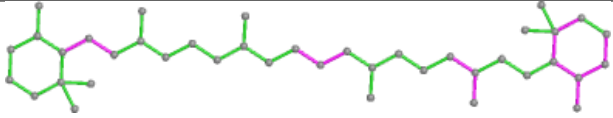
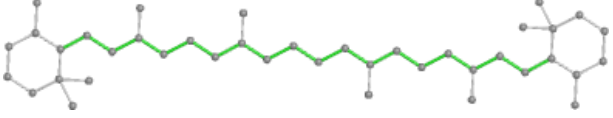
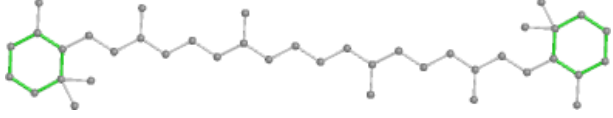
Ligand LMT b 626

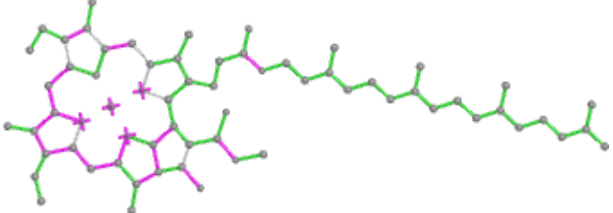
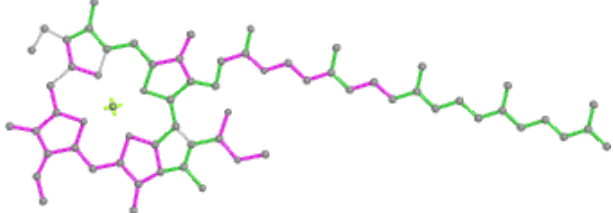
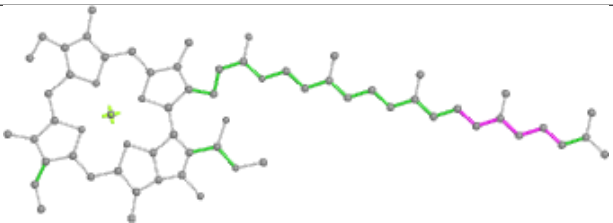
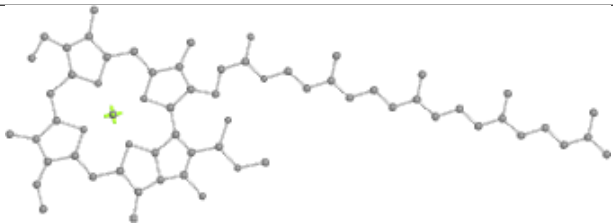


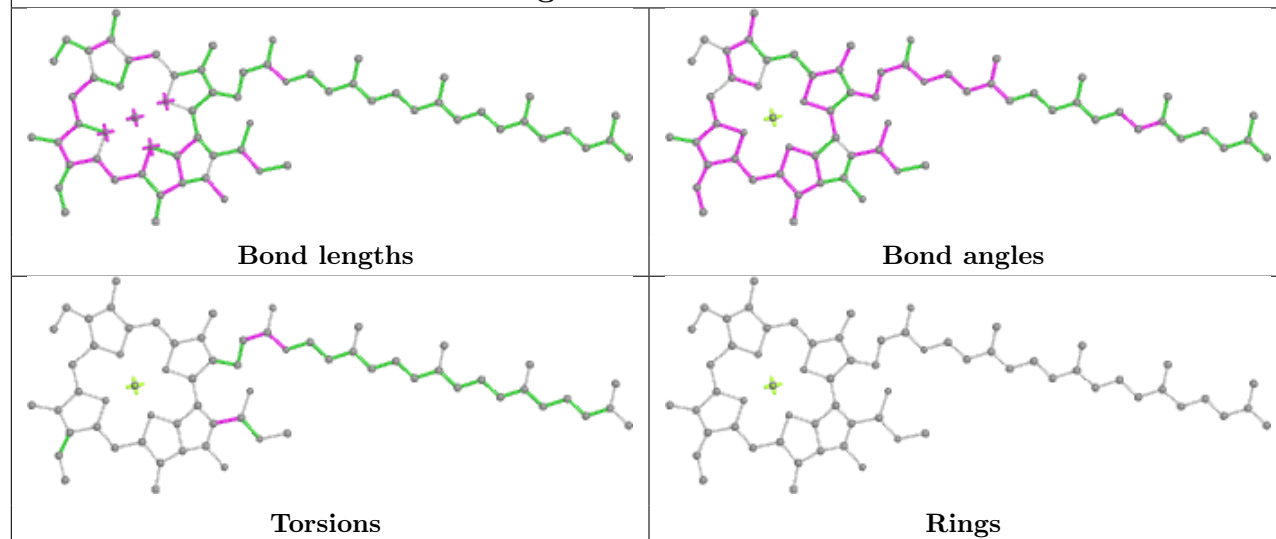
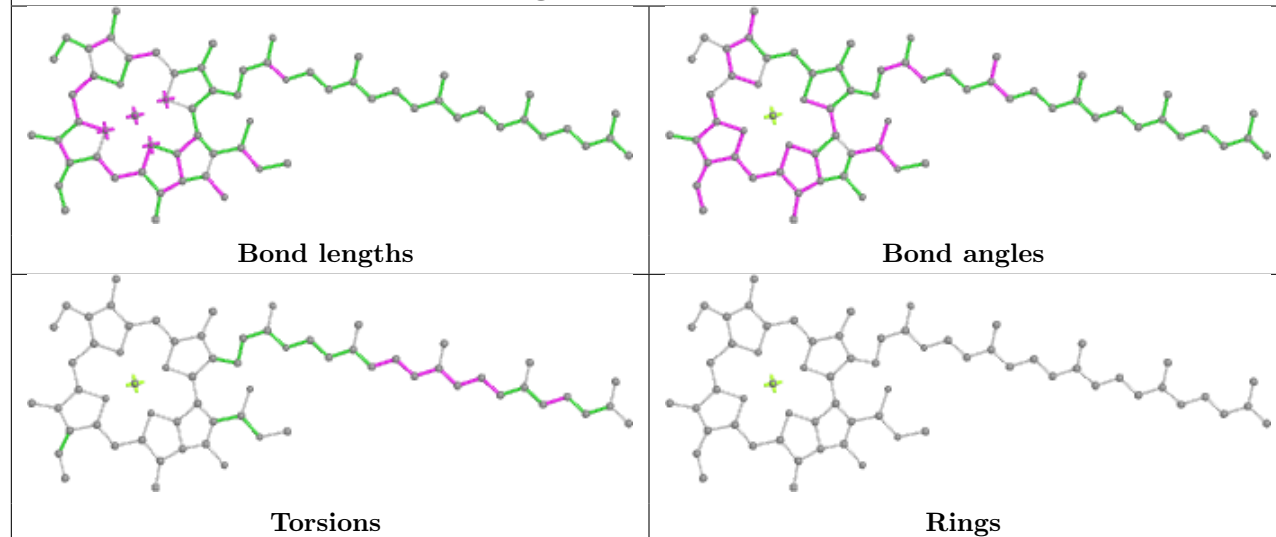
Ligand CLA C 513

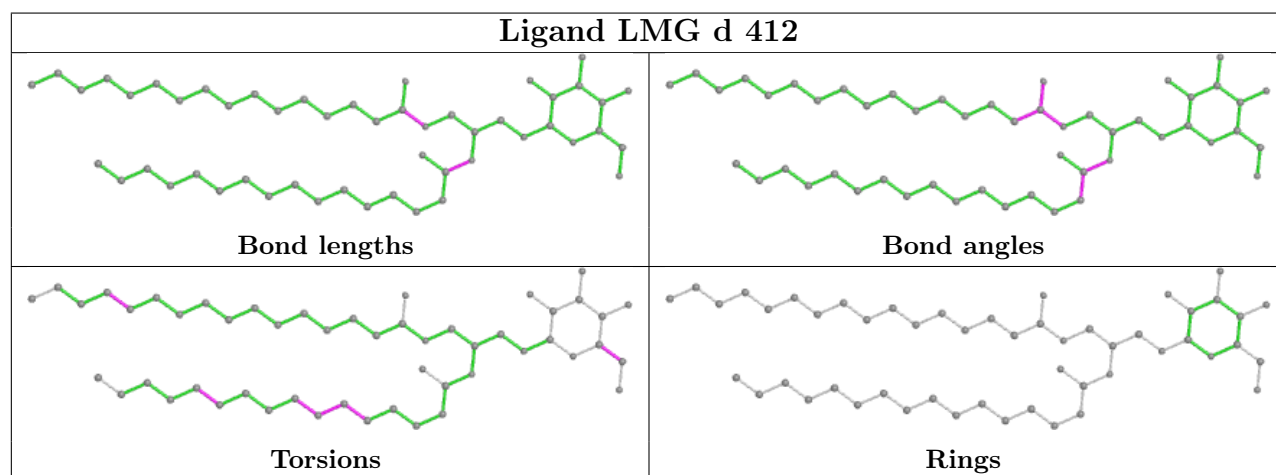
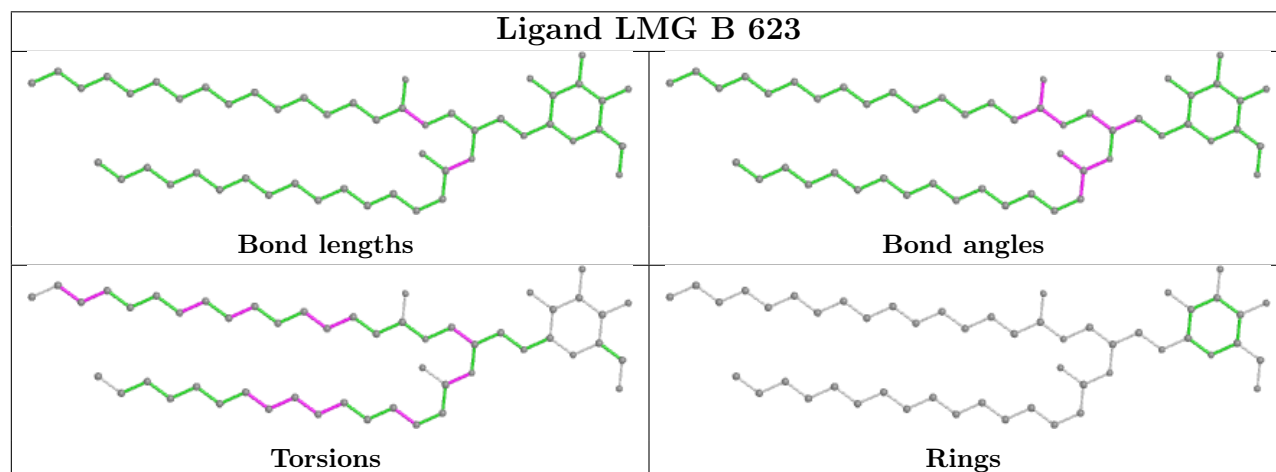
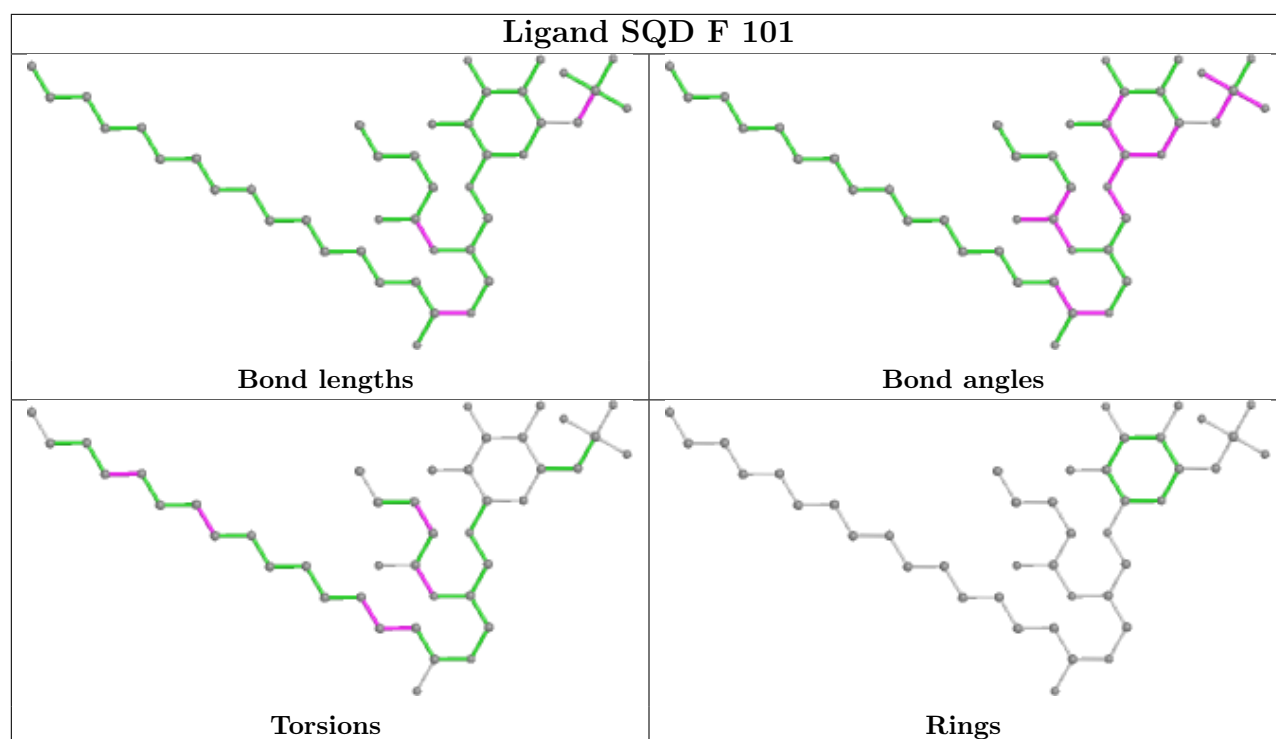


Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

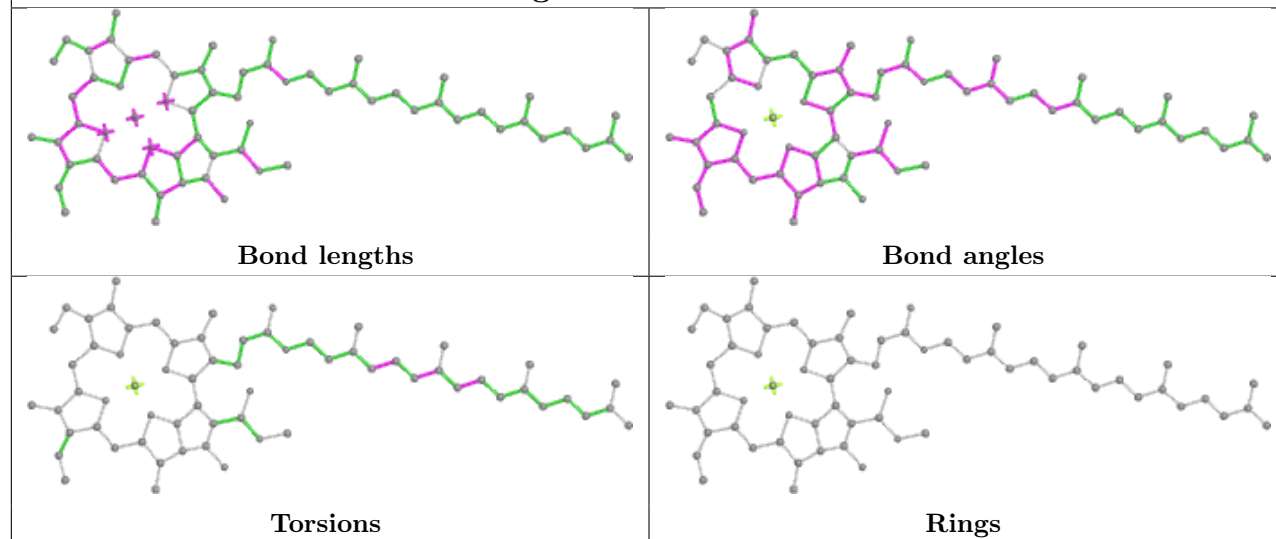
Ligand BCR b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

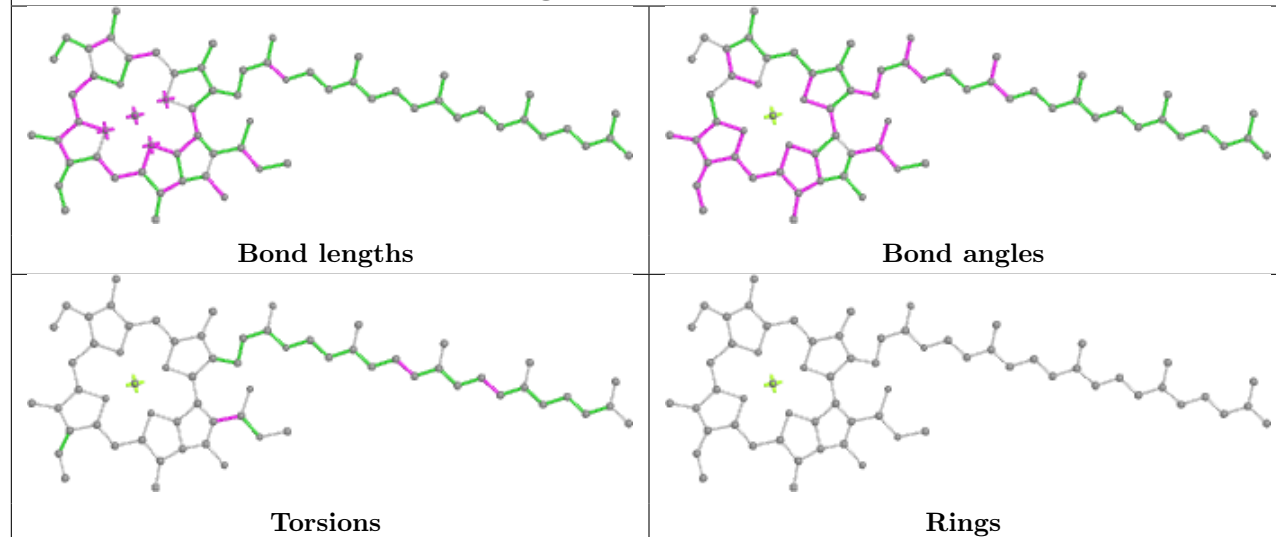
Ligand CLA c 514**Ligand CLA B 618**



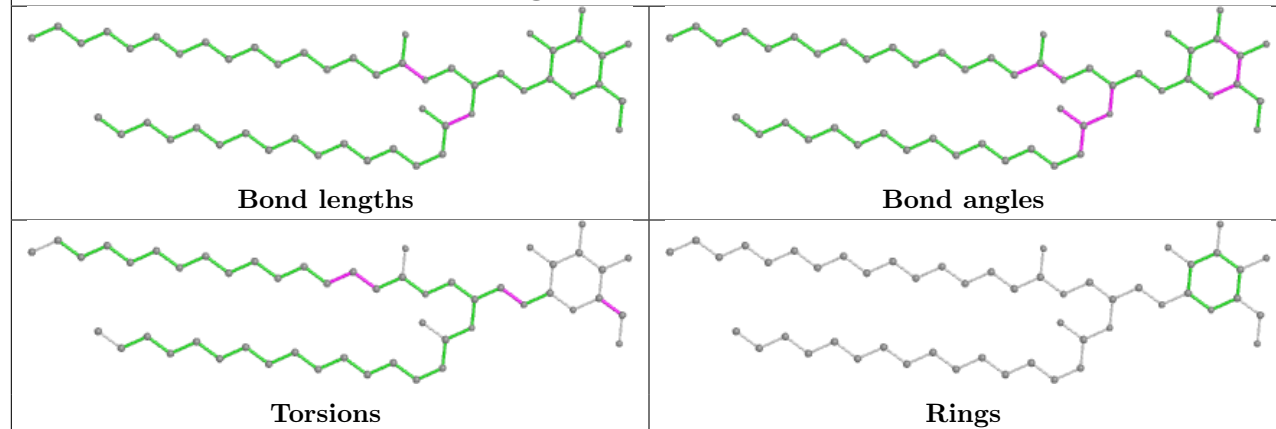
Ligand CLA C 515

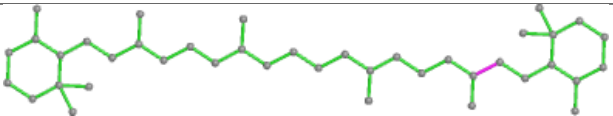
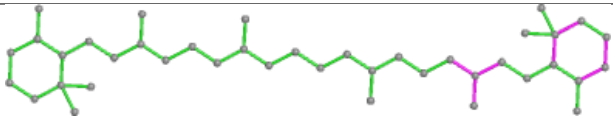
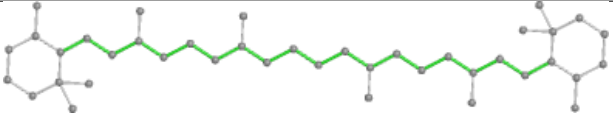
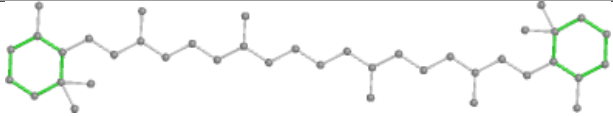


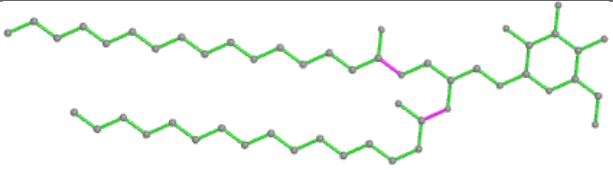
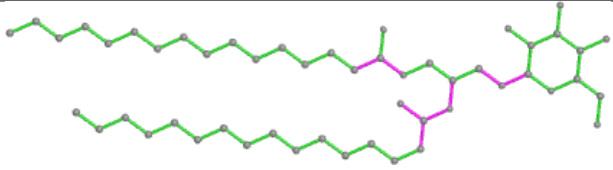
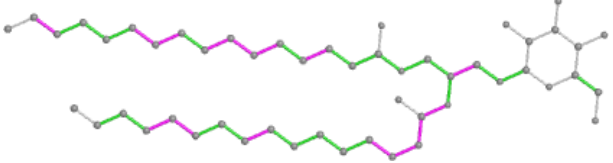
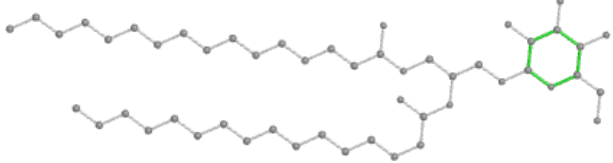
Ligand CLA c 509

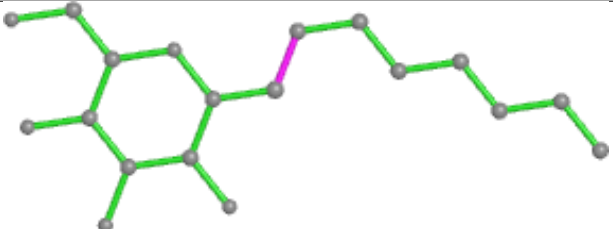
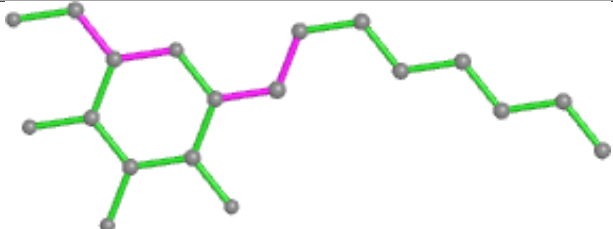
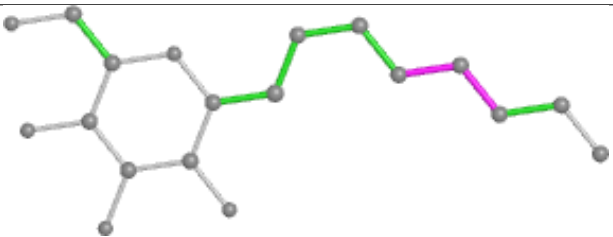
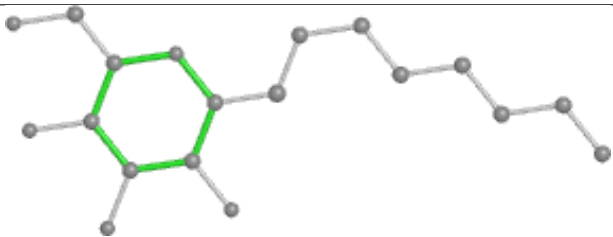


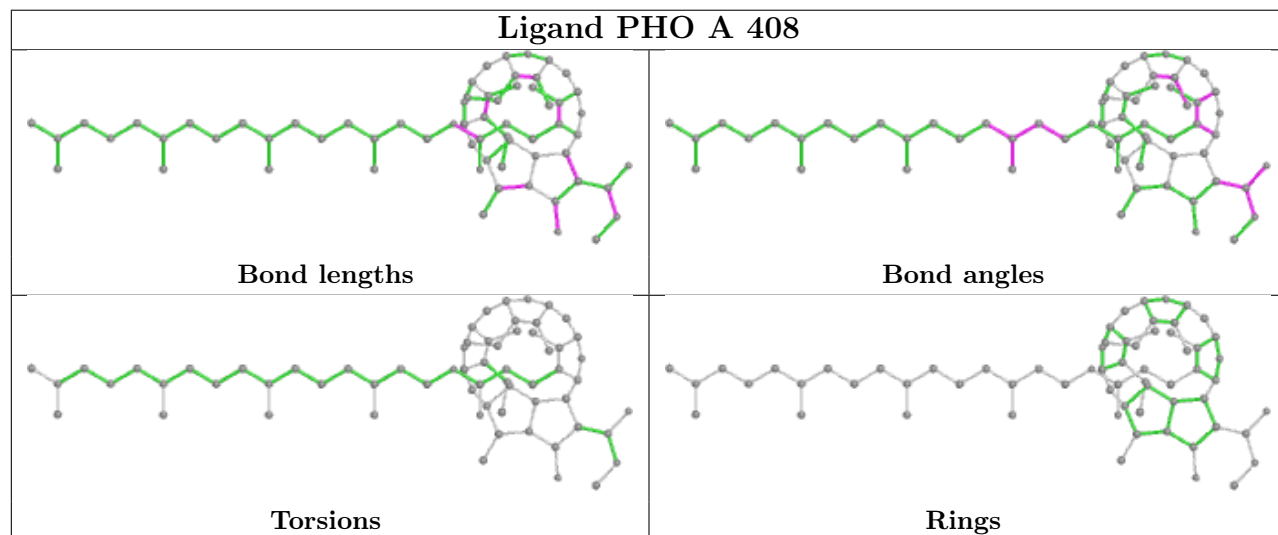
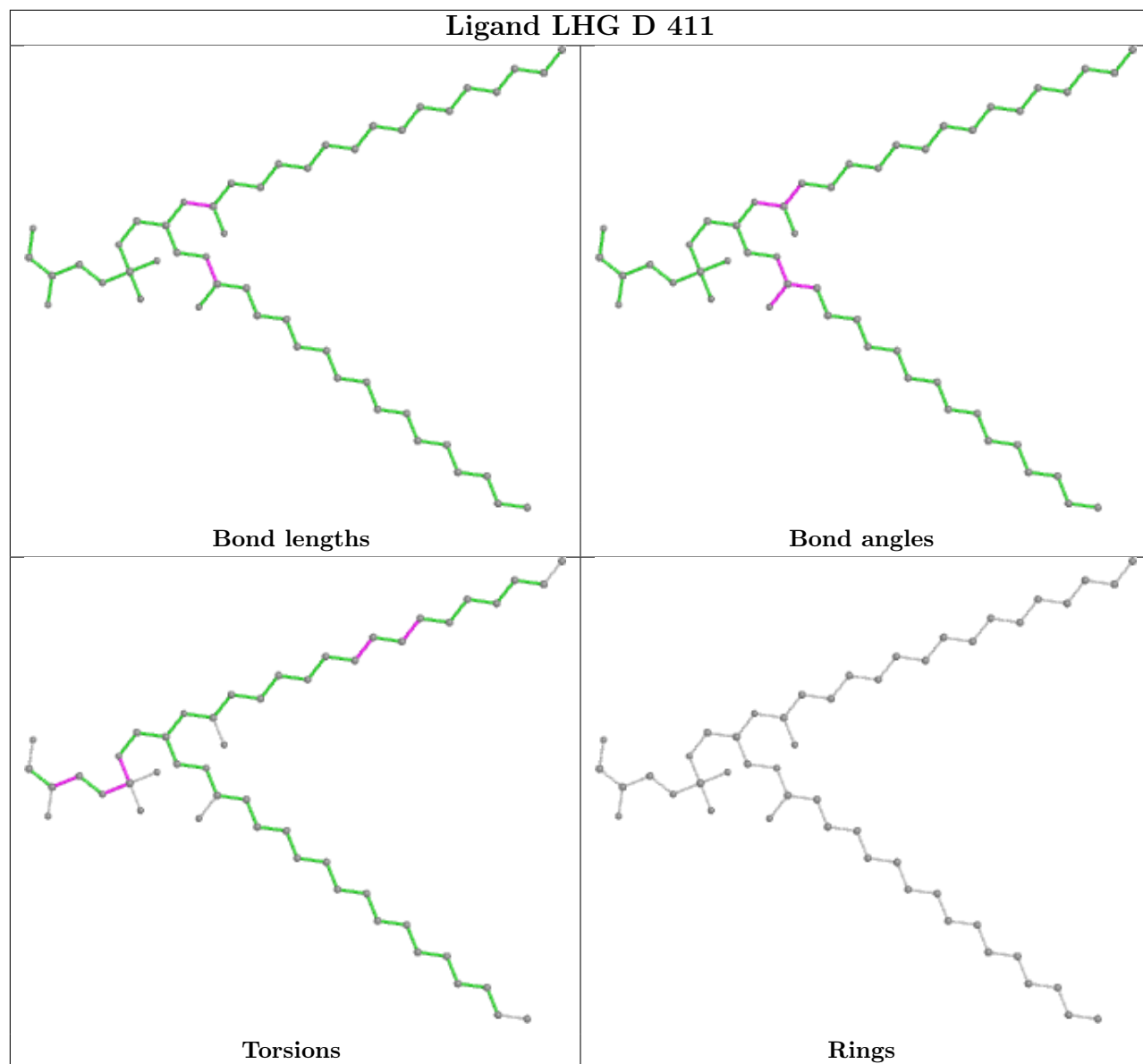
Ligand LMG C 533



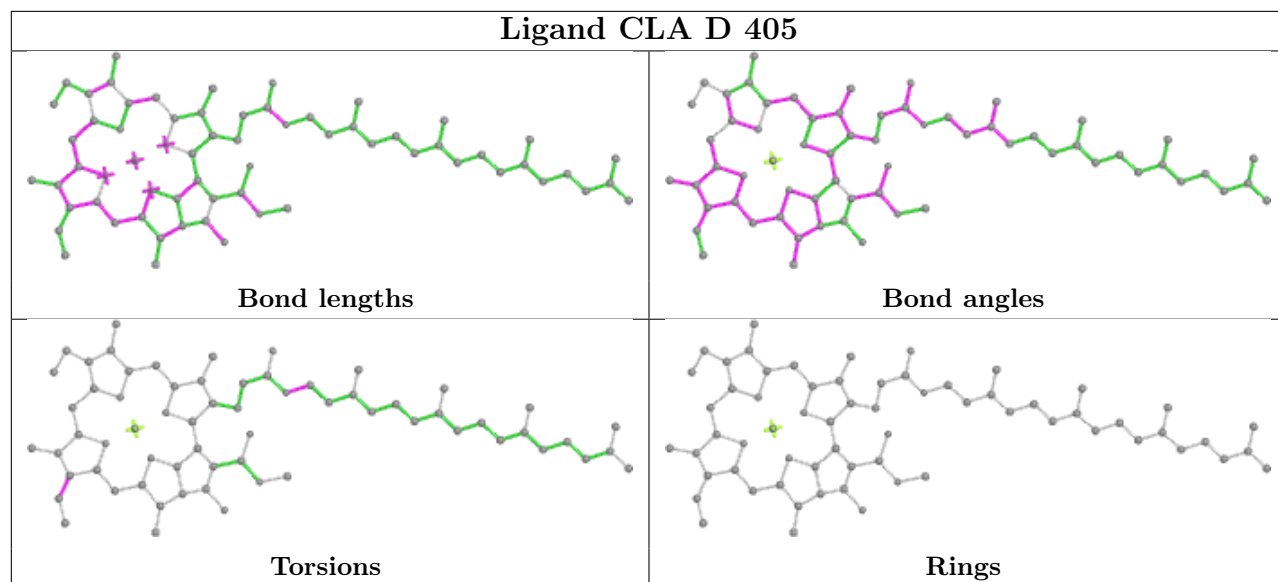
Ligand BCR B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG i 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

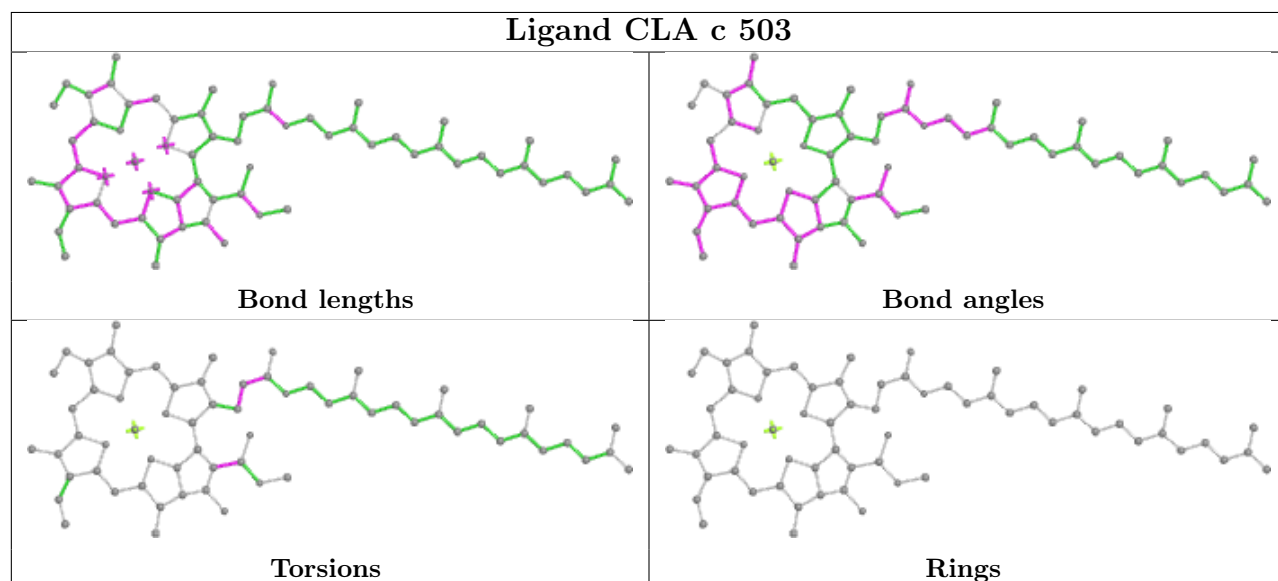
Ligand HTG o 301	
	
Bond lengths	Bond angles
	
Torsions	Rings



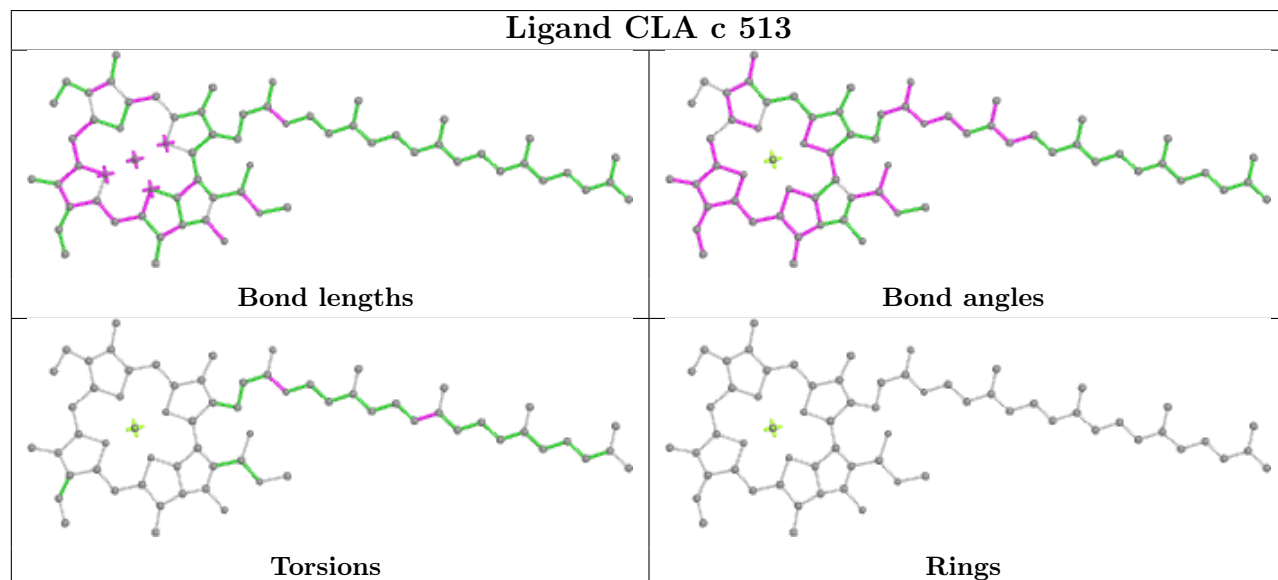
Ligand CLA D 405

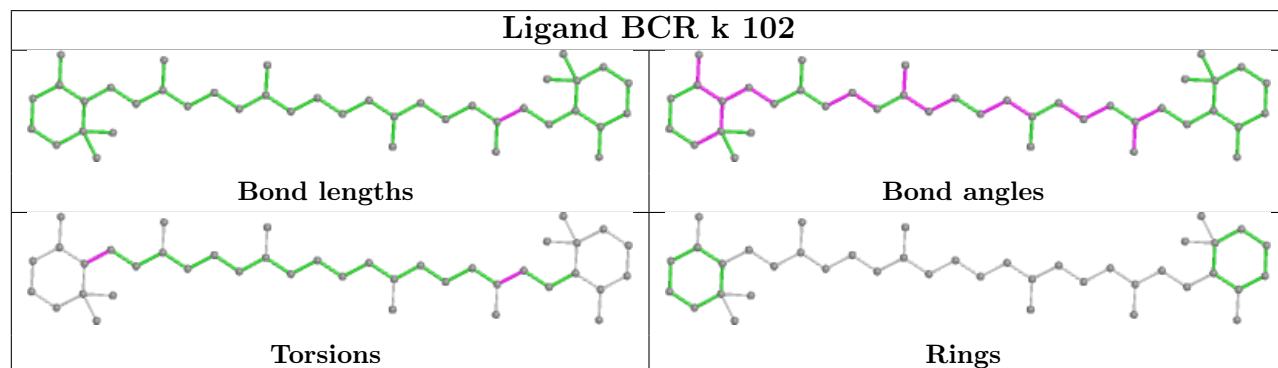
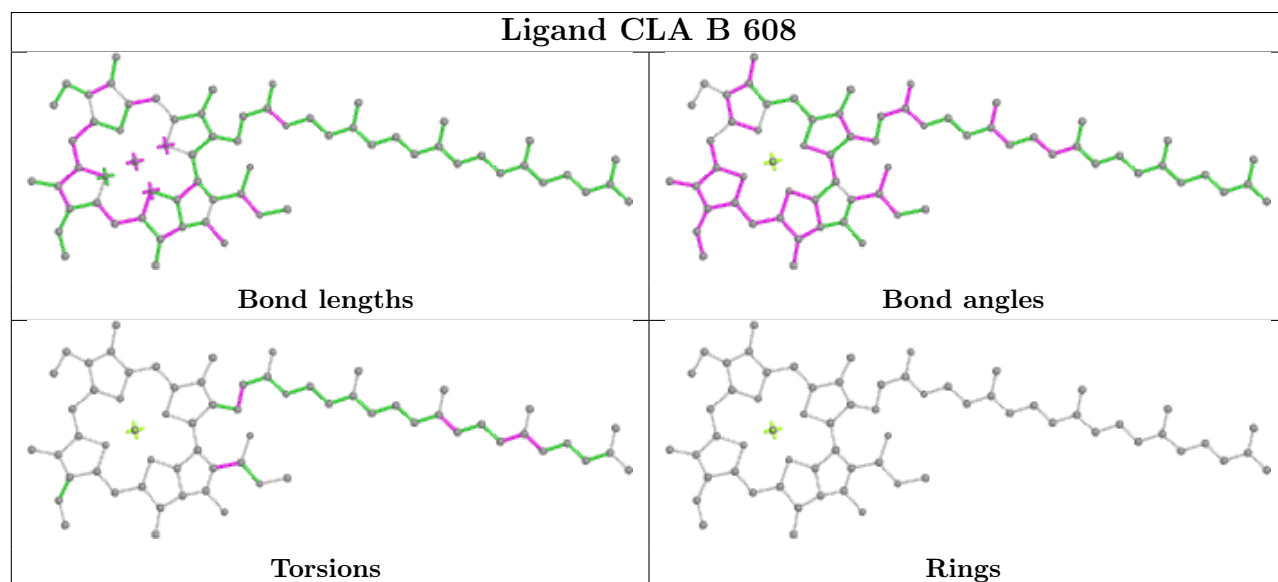
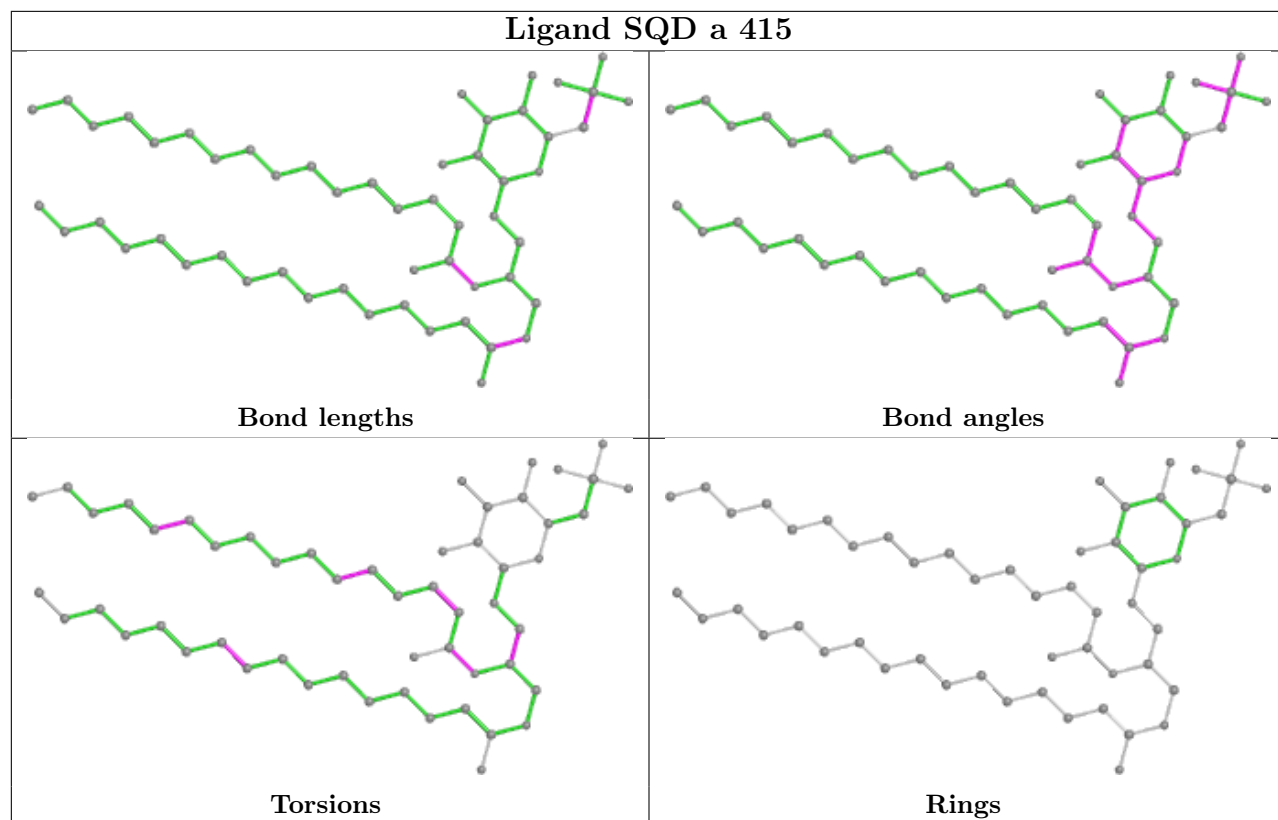


Ligand CLA c 503

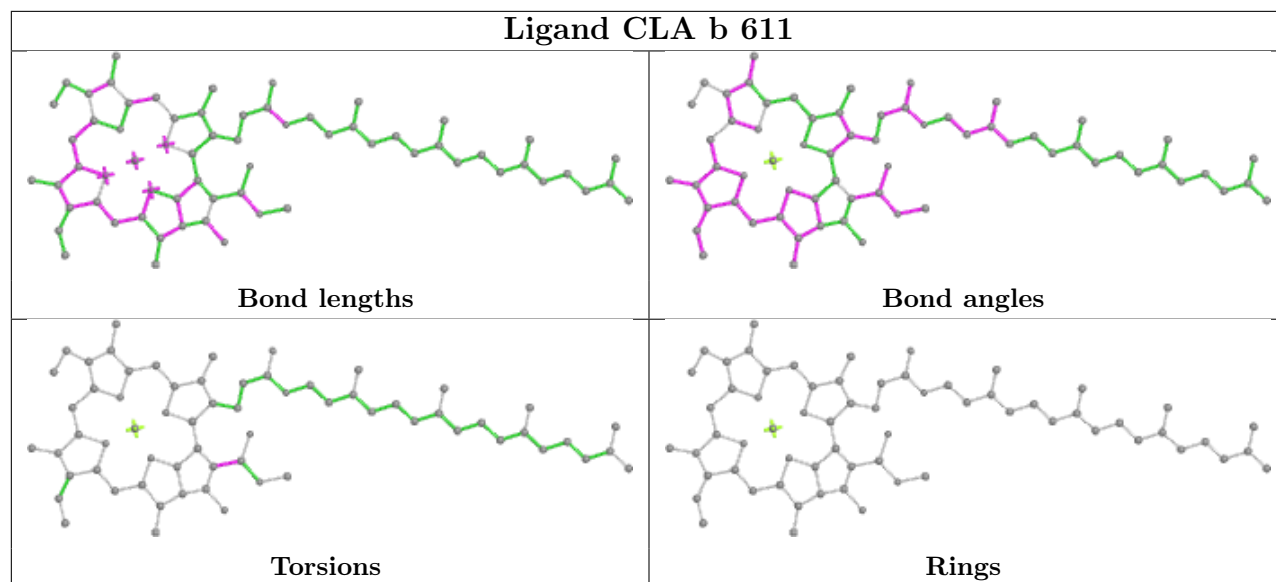


Ligand CLA c 513

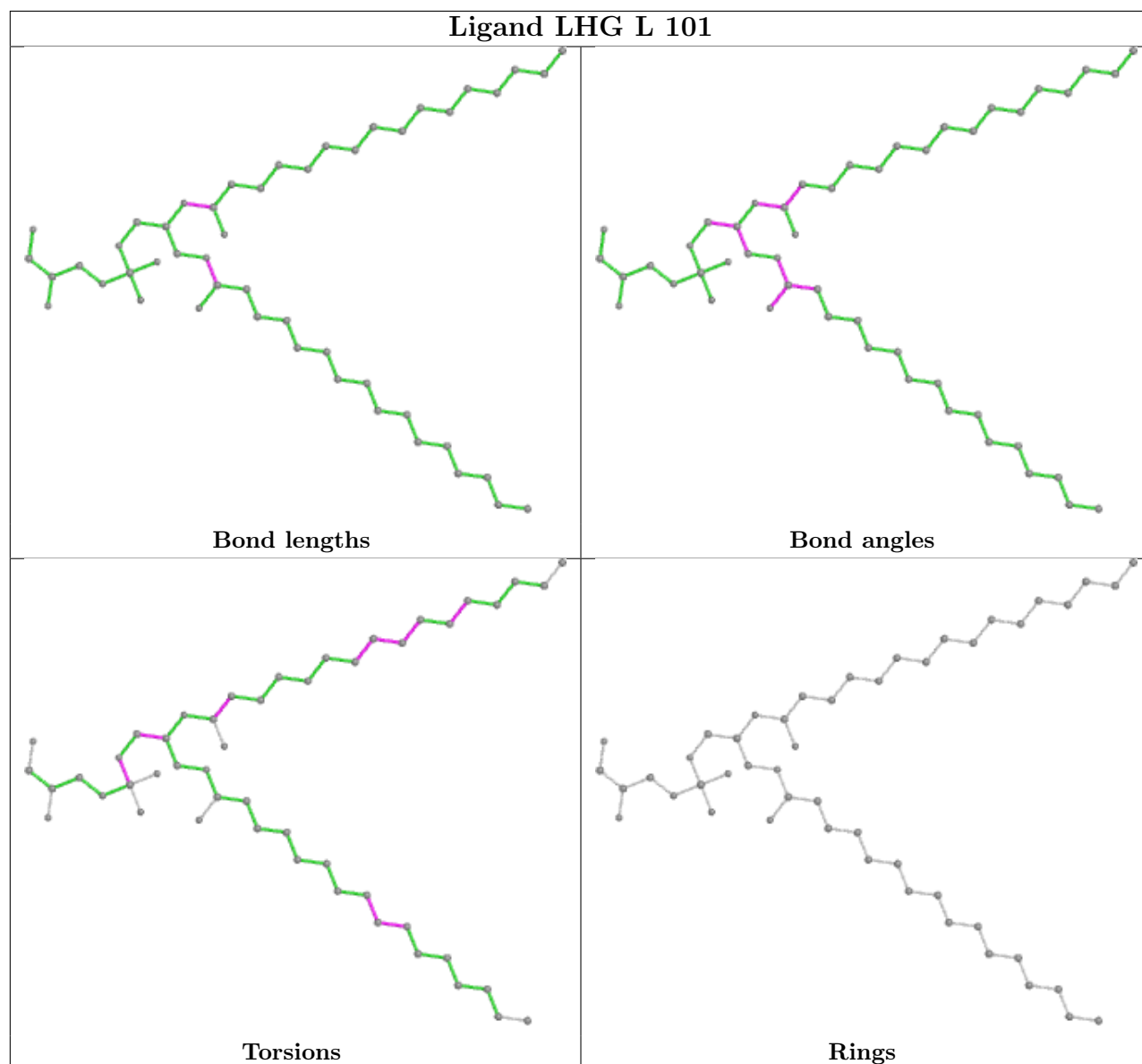


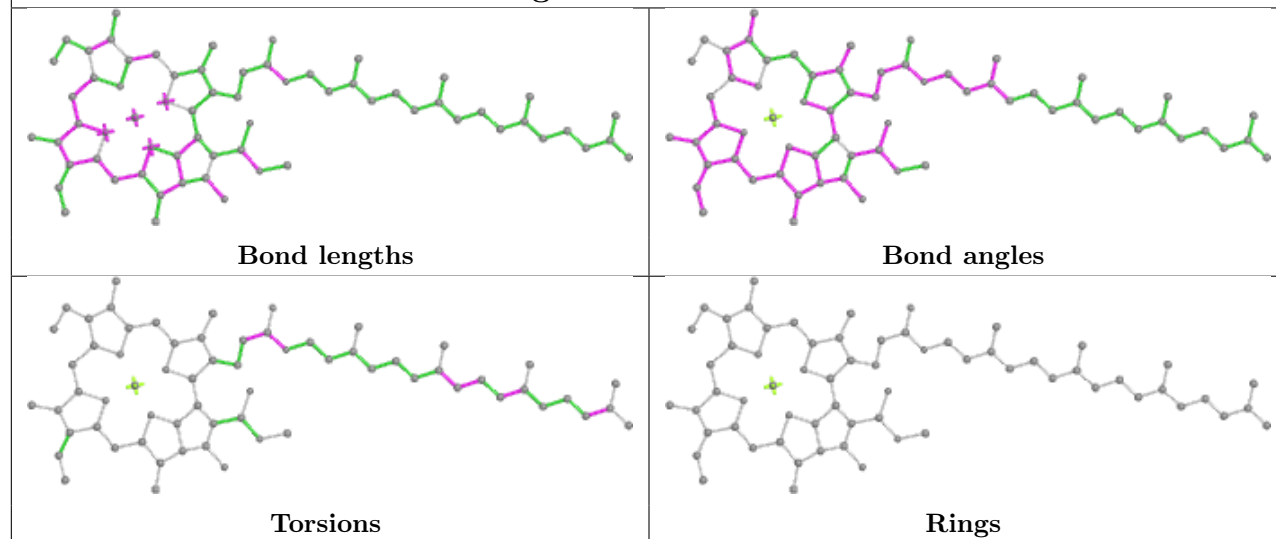
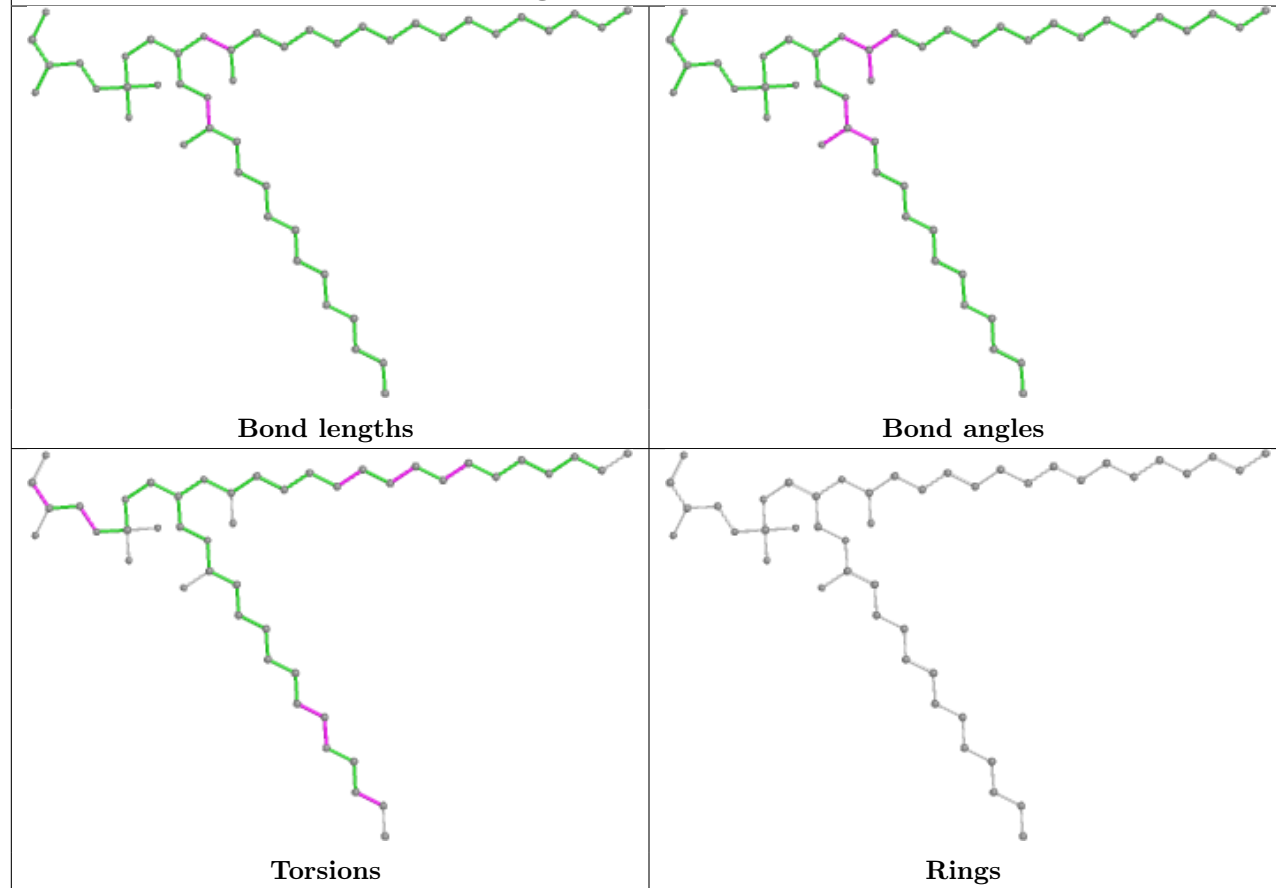


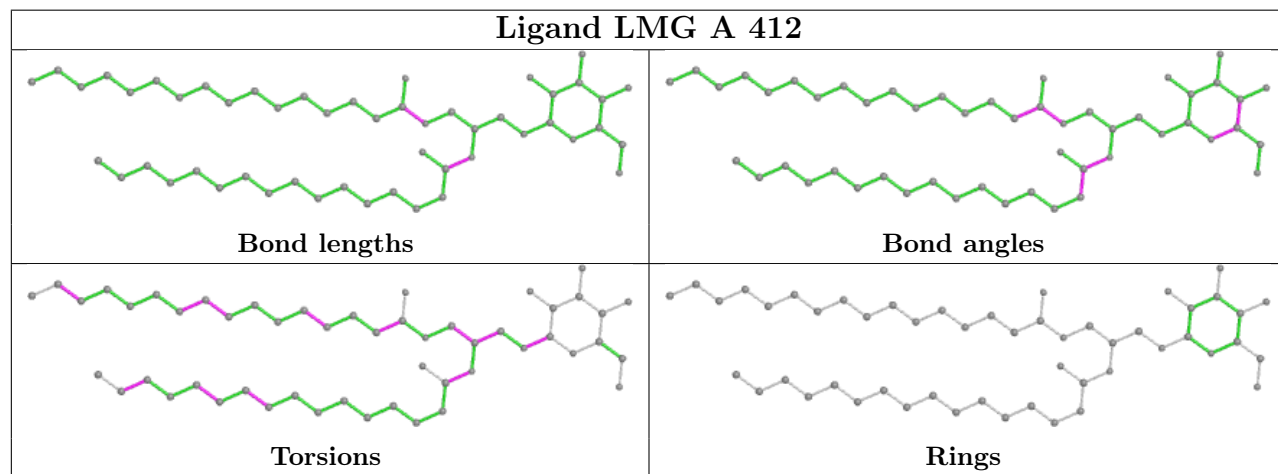
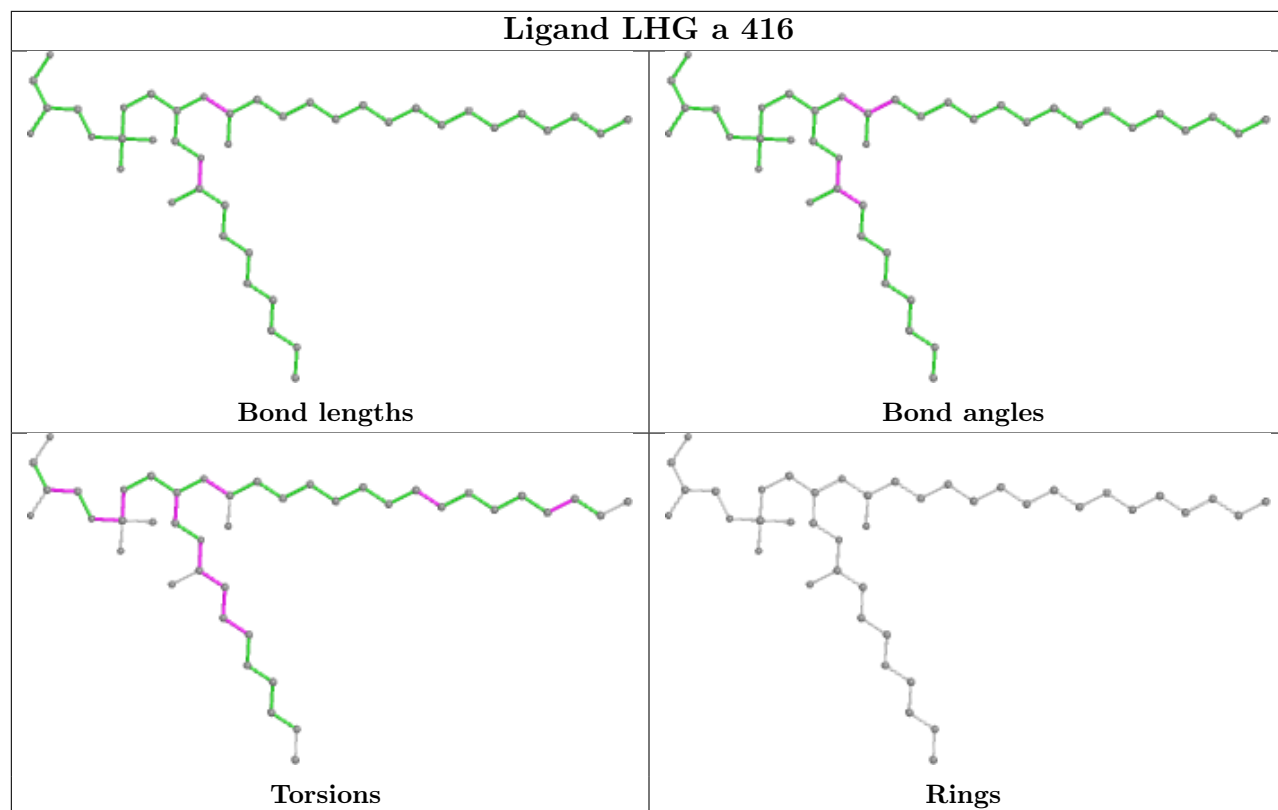
Ligand CLA b 611

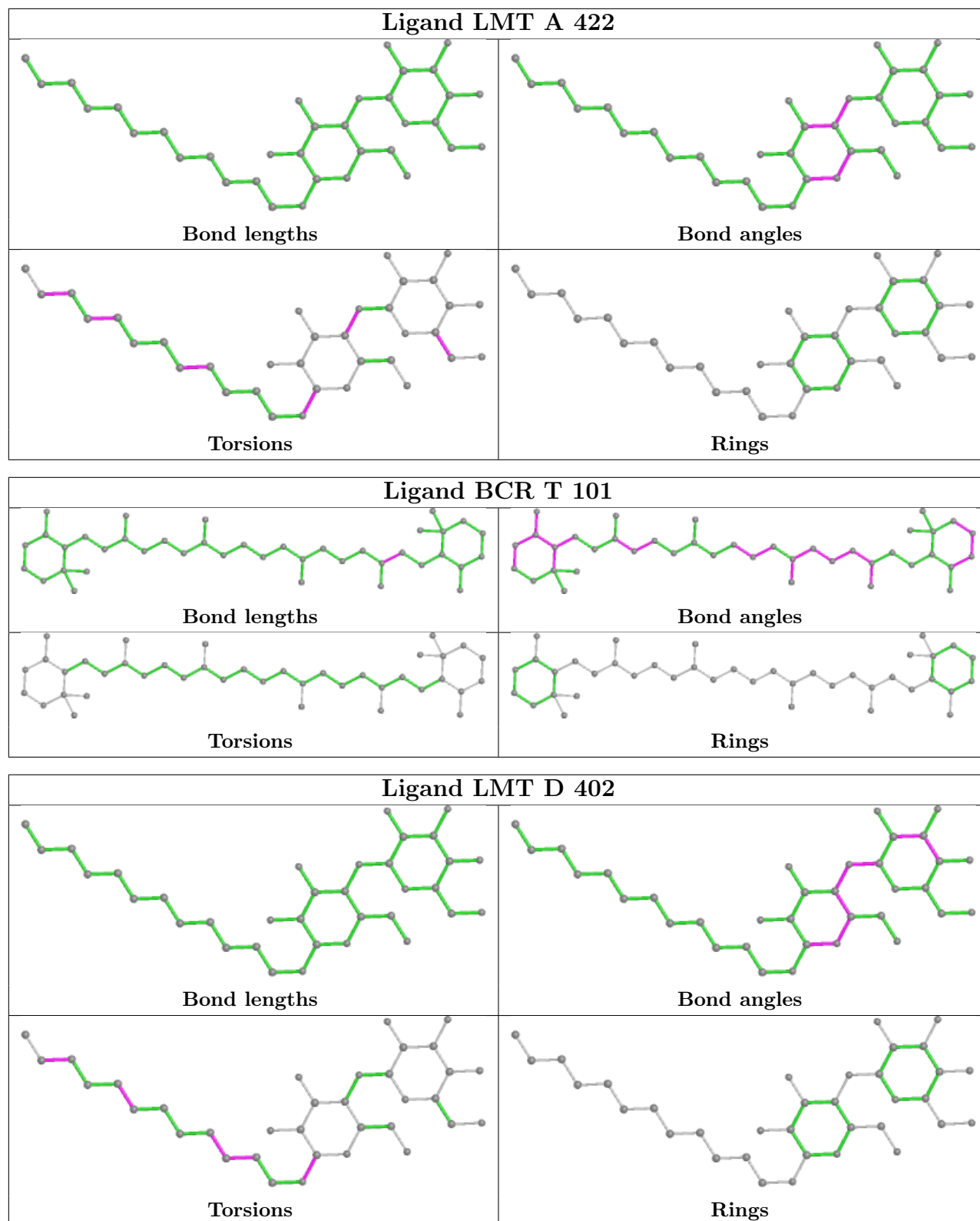


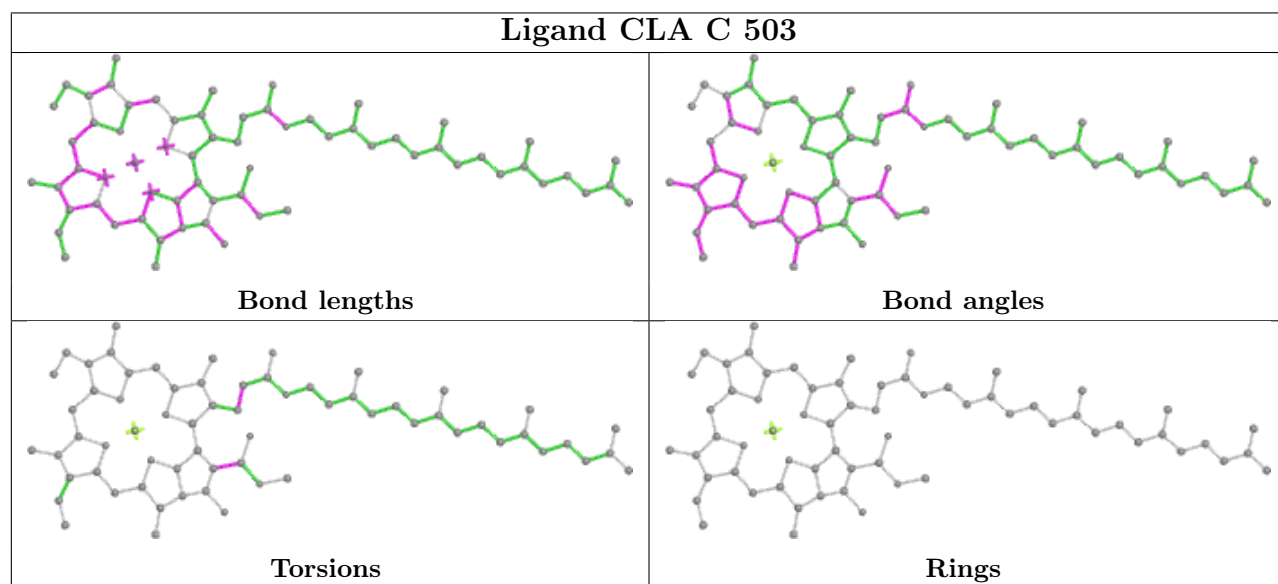
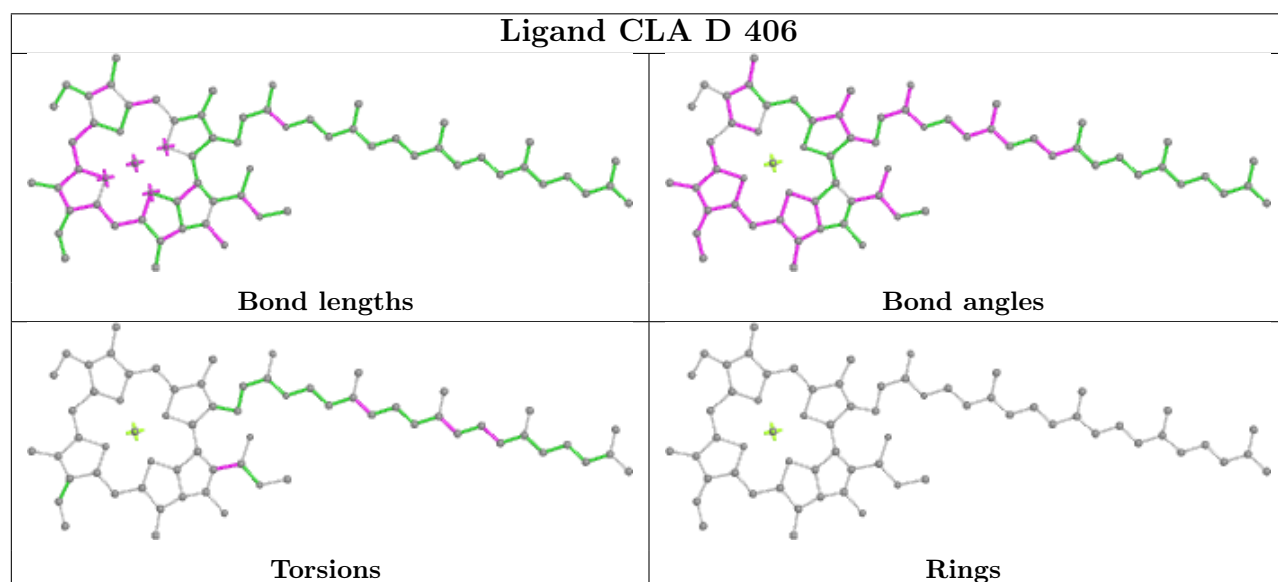
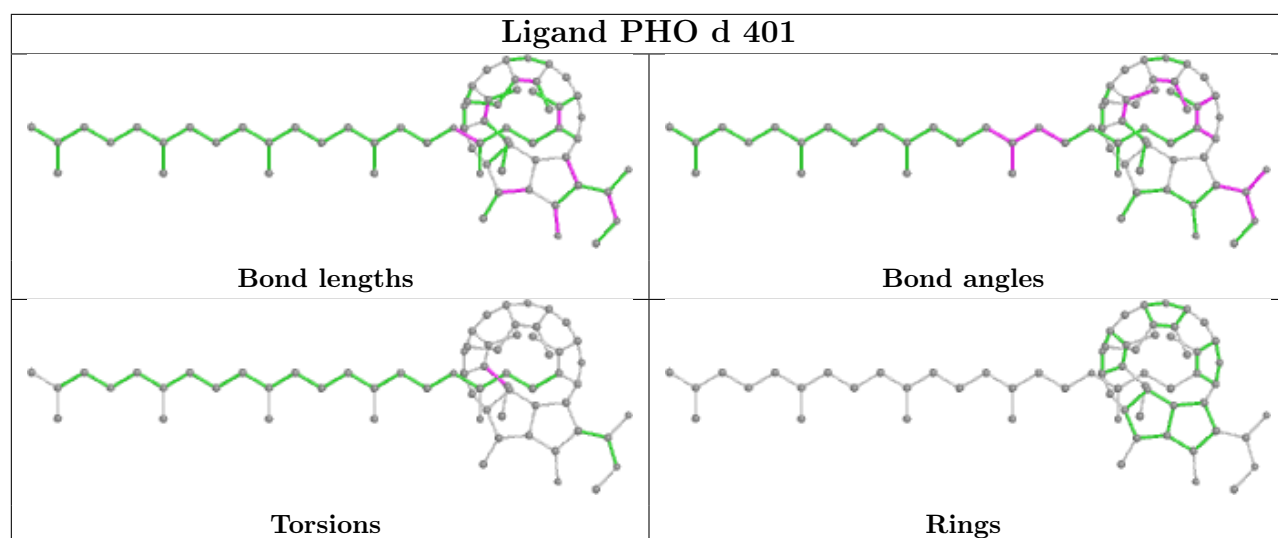
Ligand LHG L 101



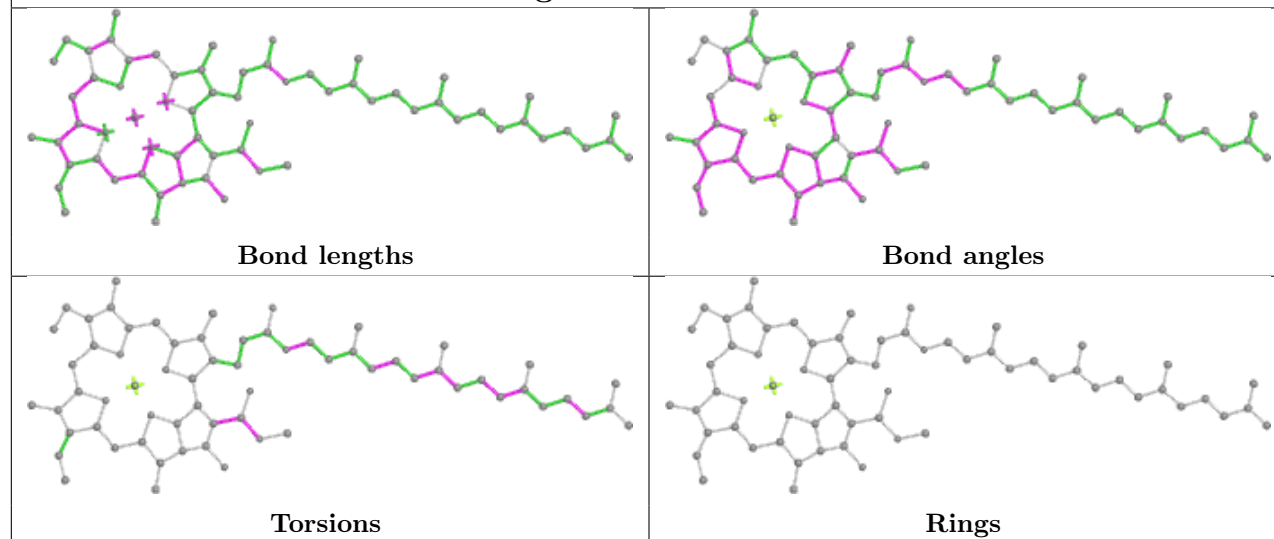
Ligand CLA C 514**Ligand LHG d 411**



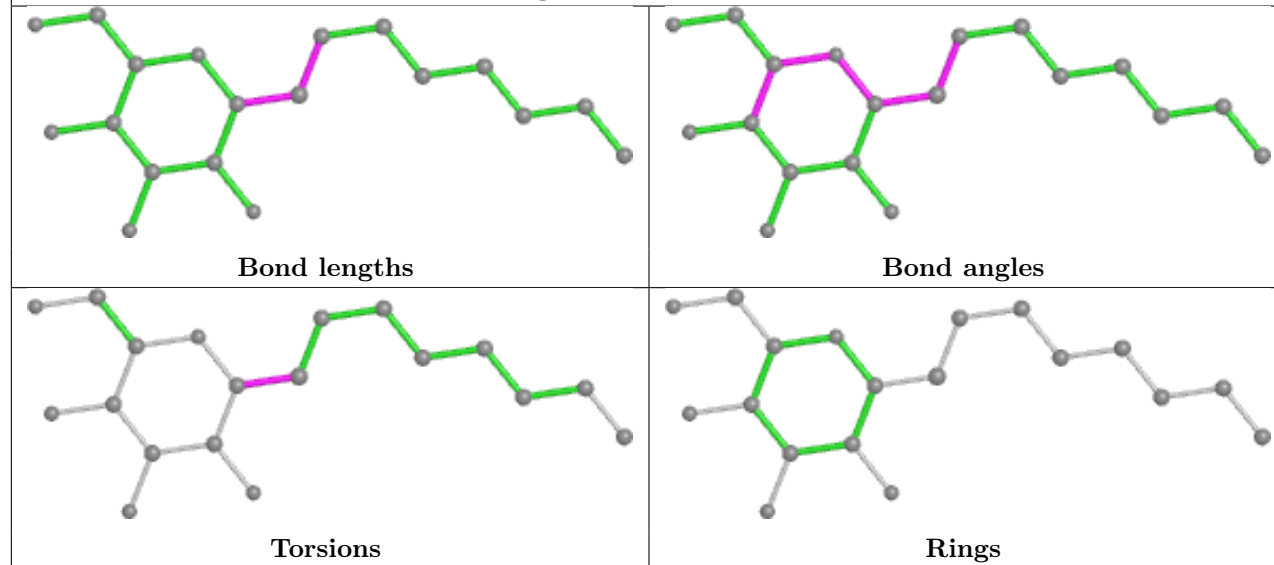


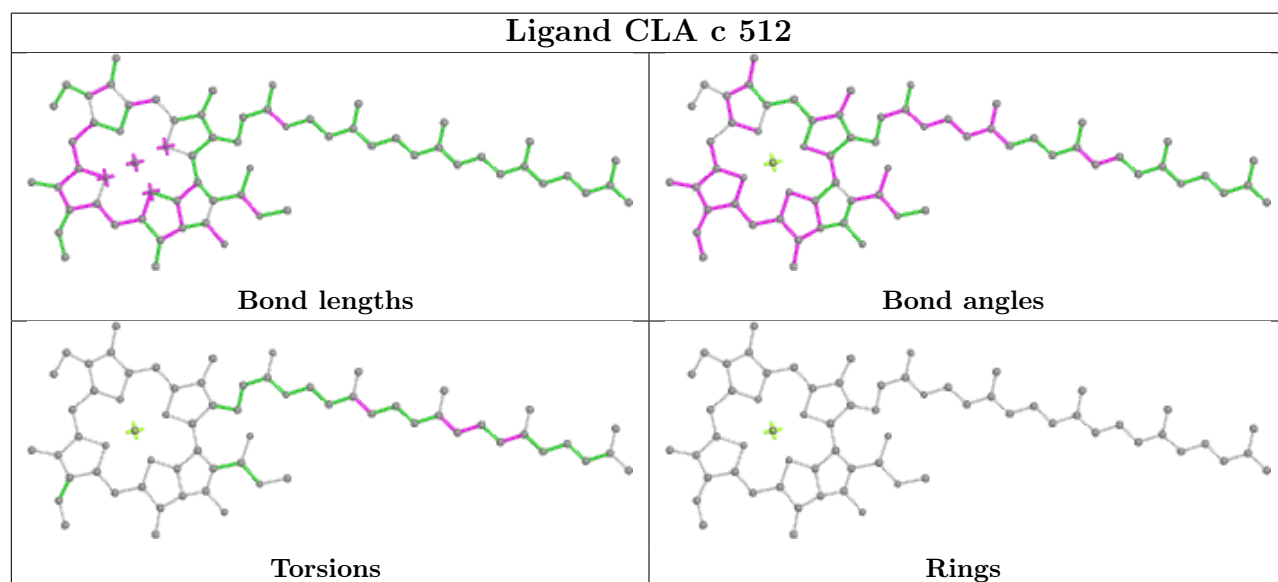
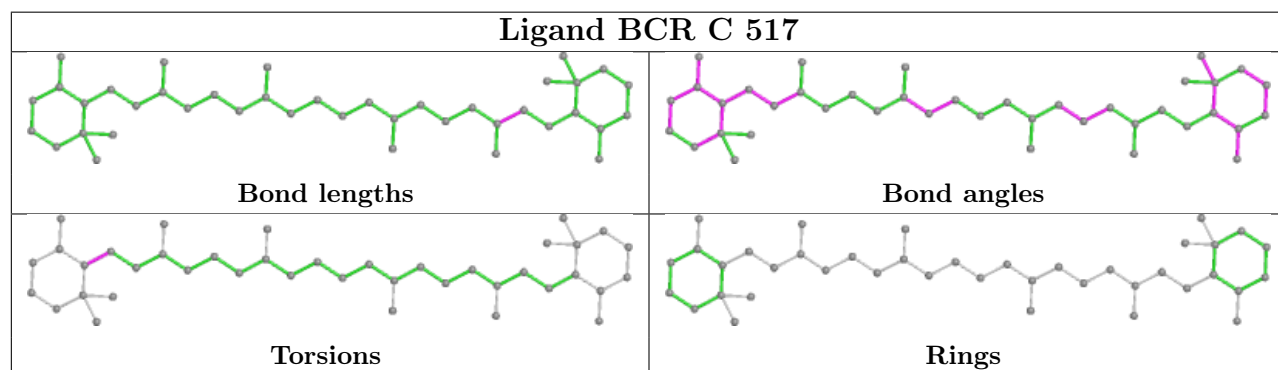
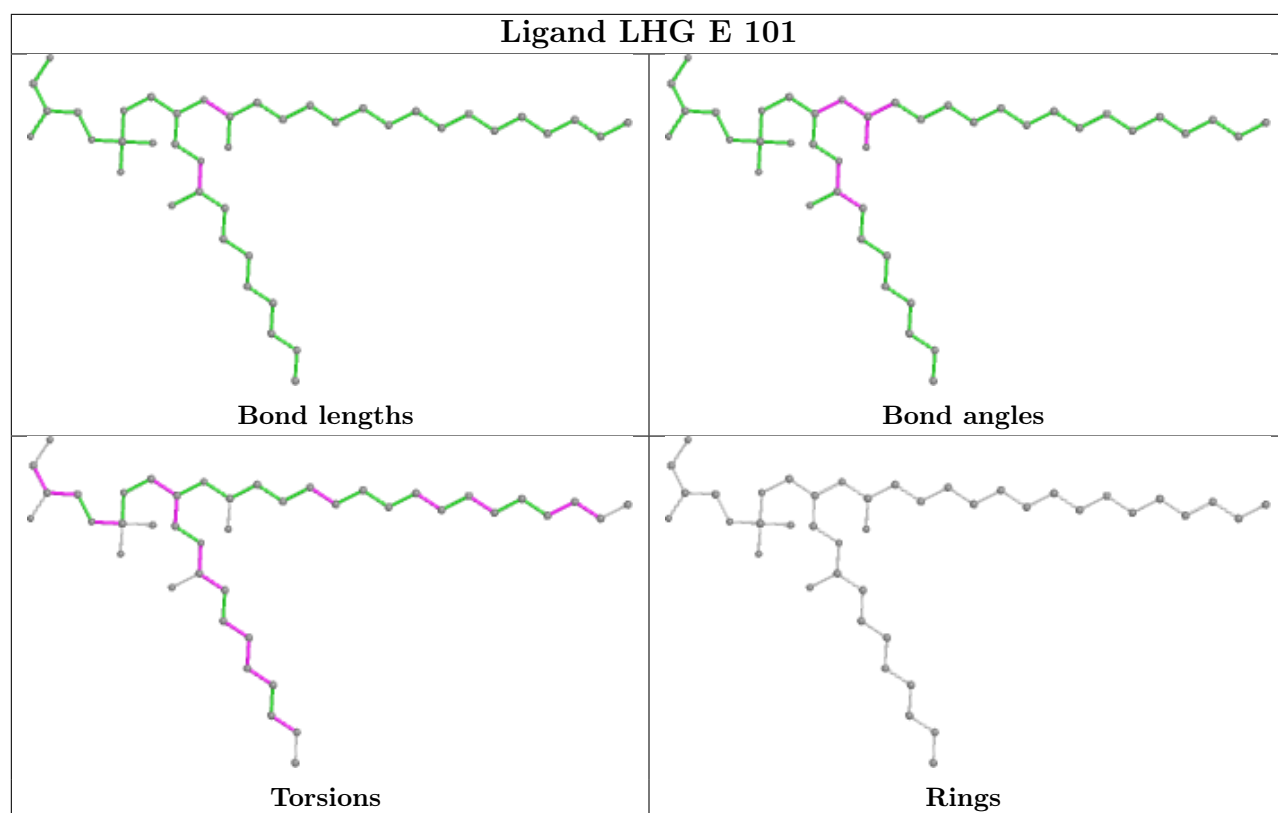


Ligand CLA b 620

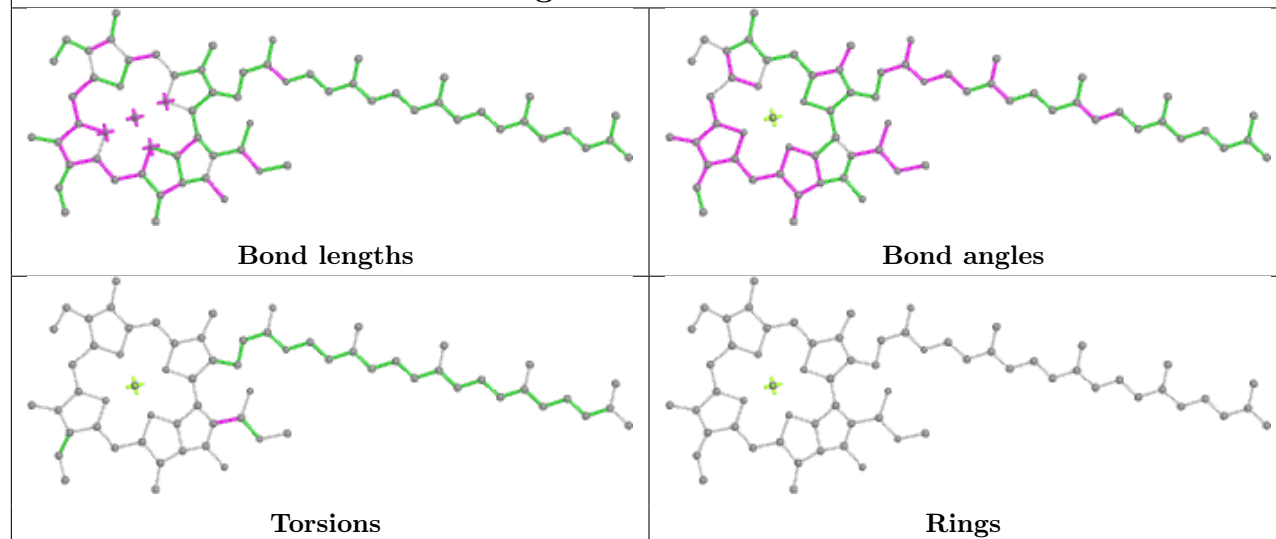


Ligand HTG c 523

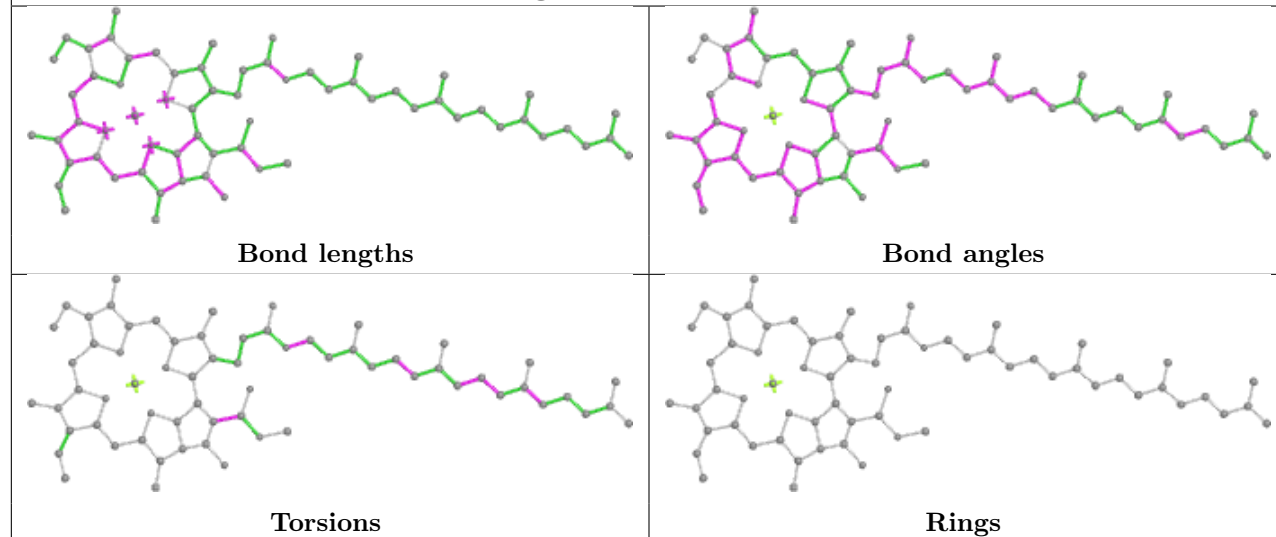


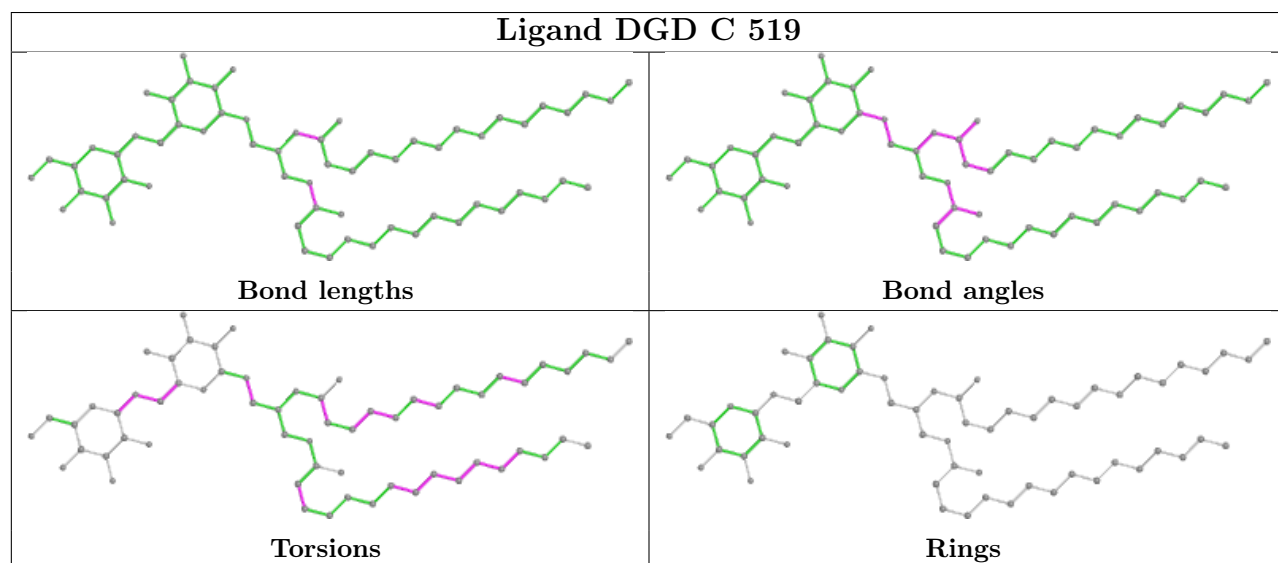
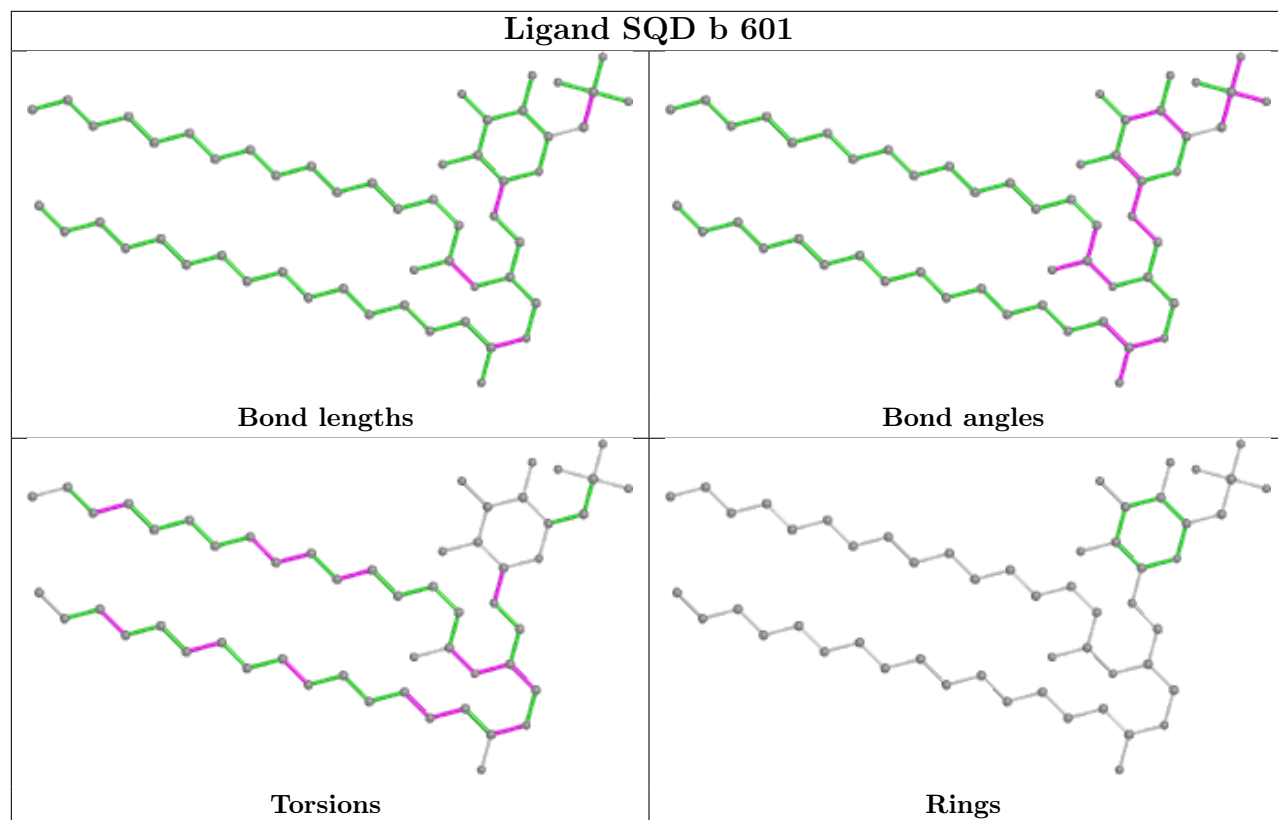


Ligand CLA b 616

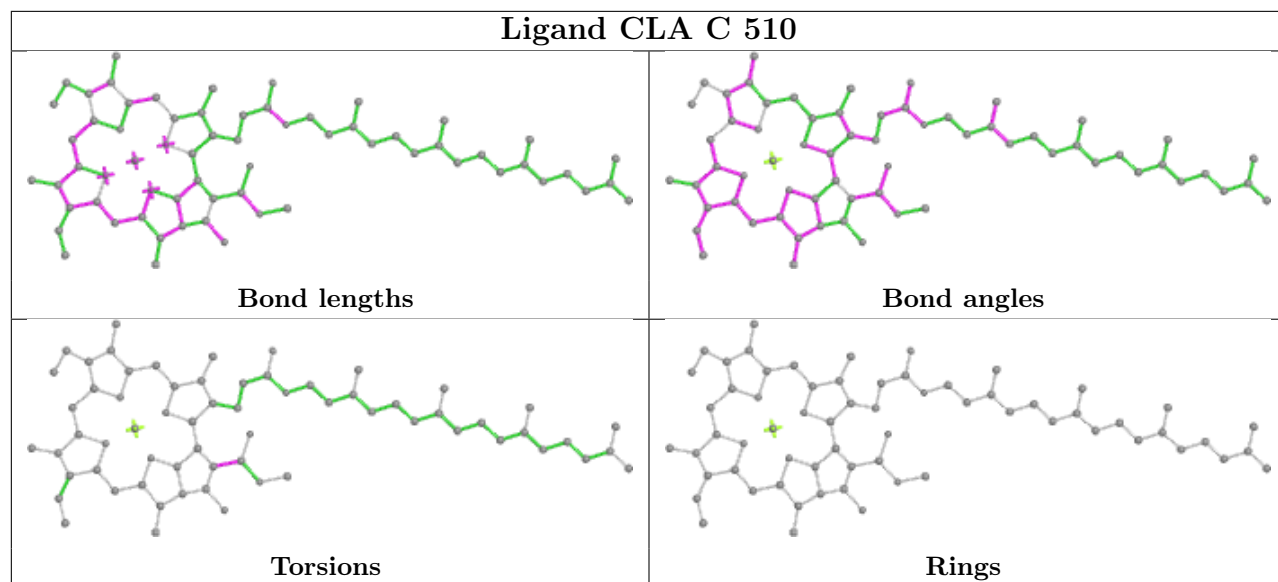


Ligand CLA C 511

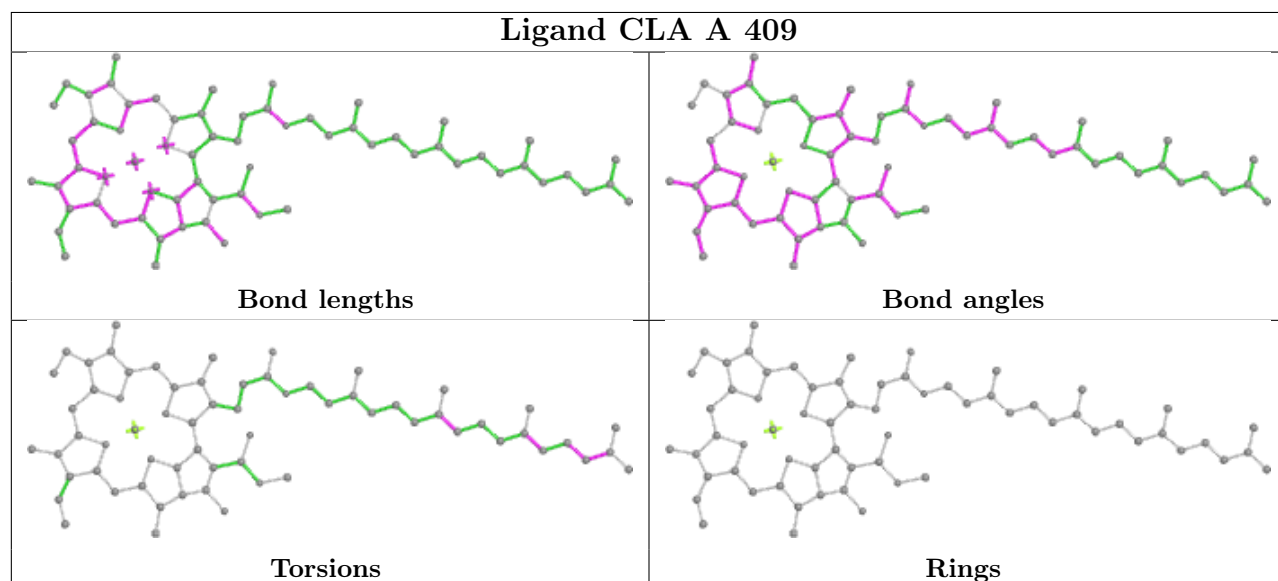




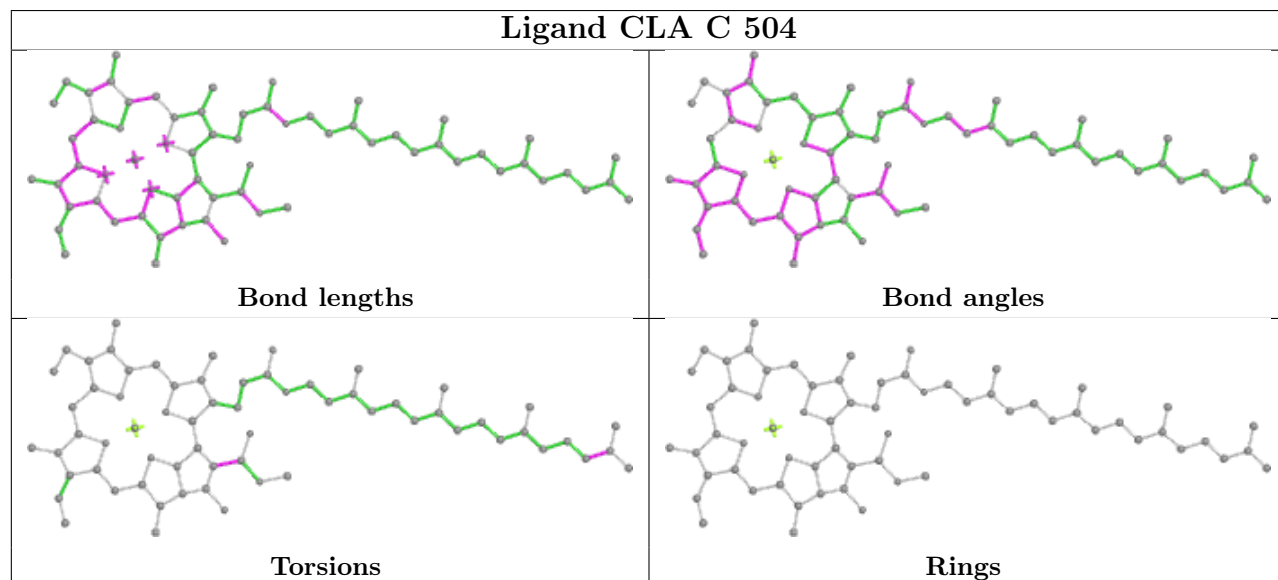
Ligand CLA C 510

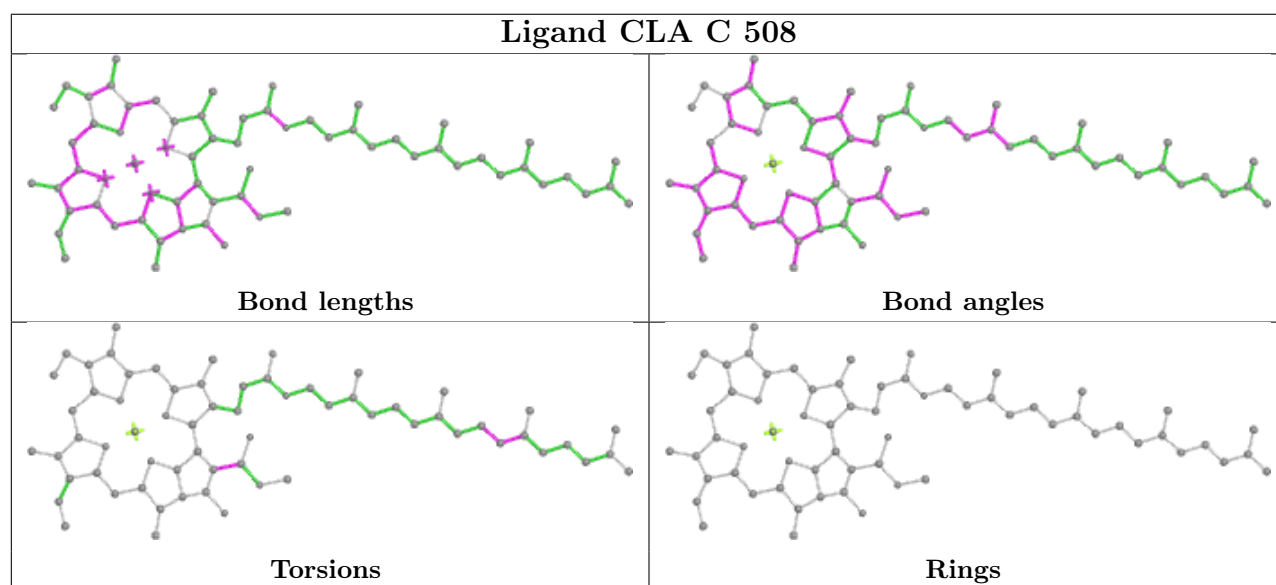
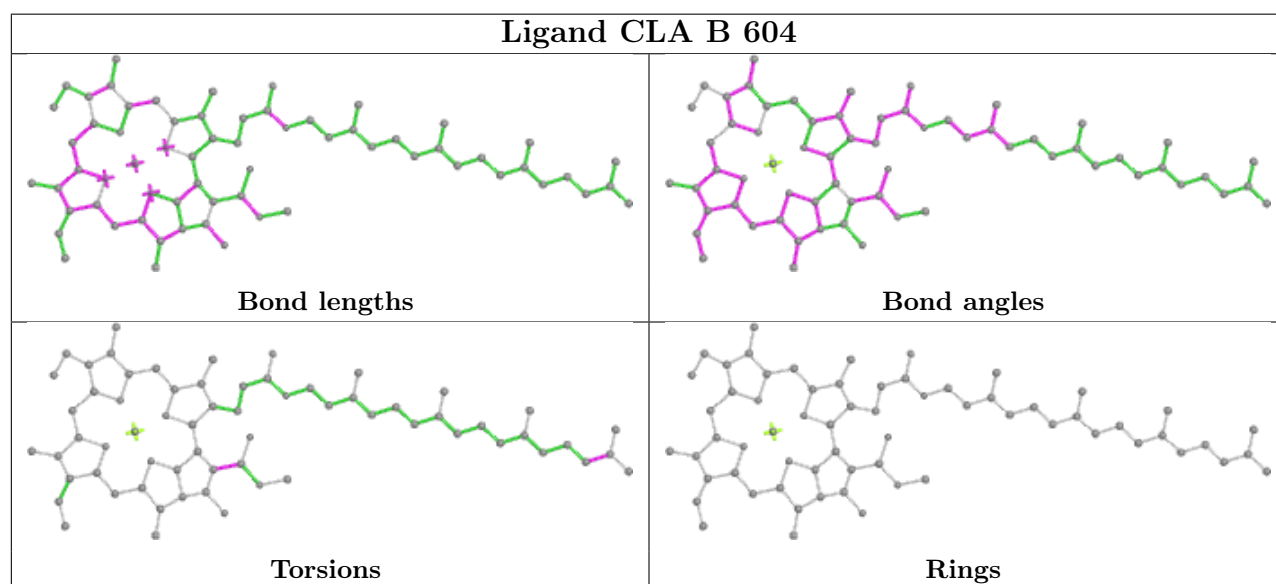
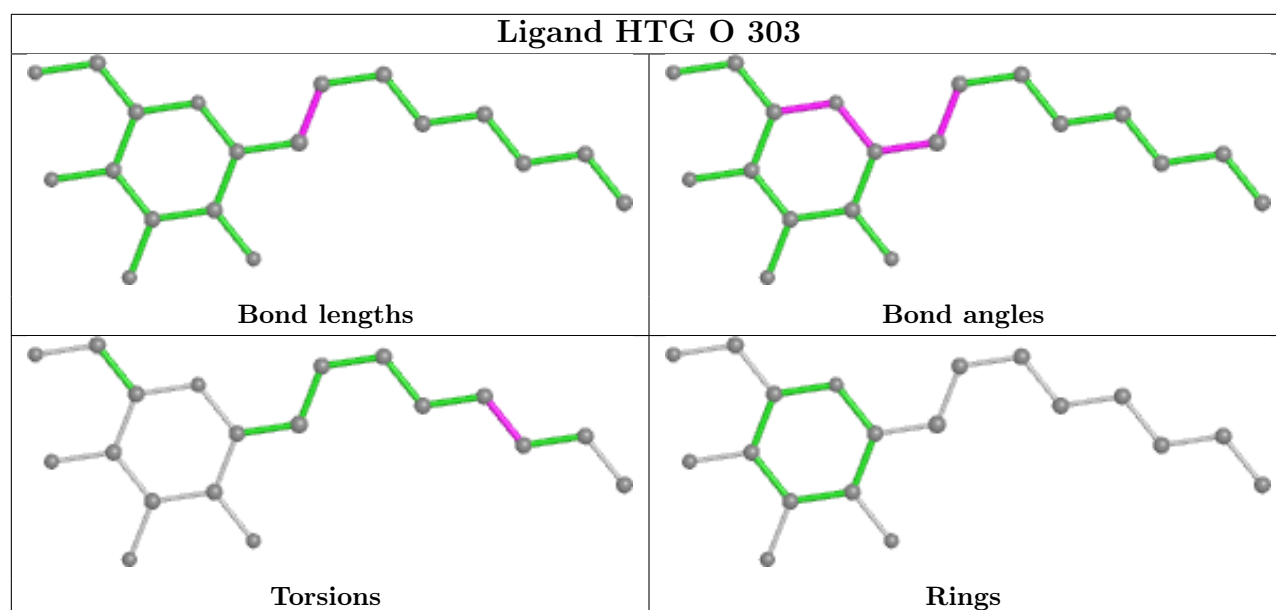


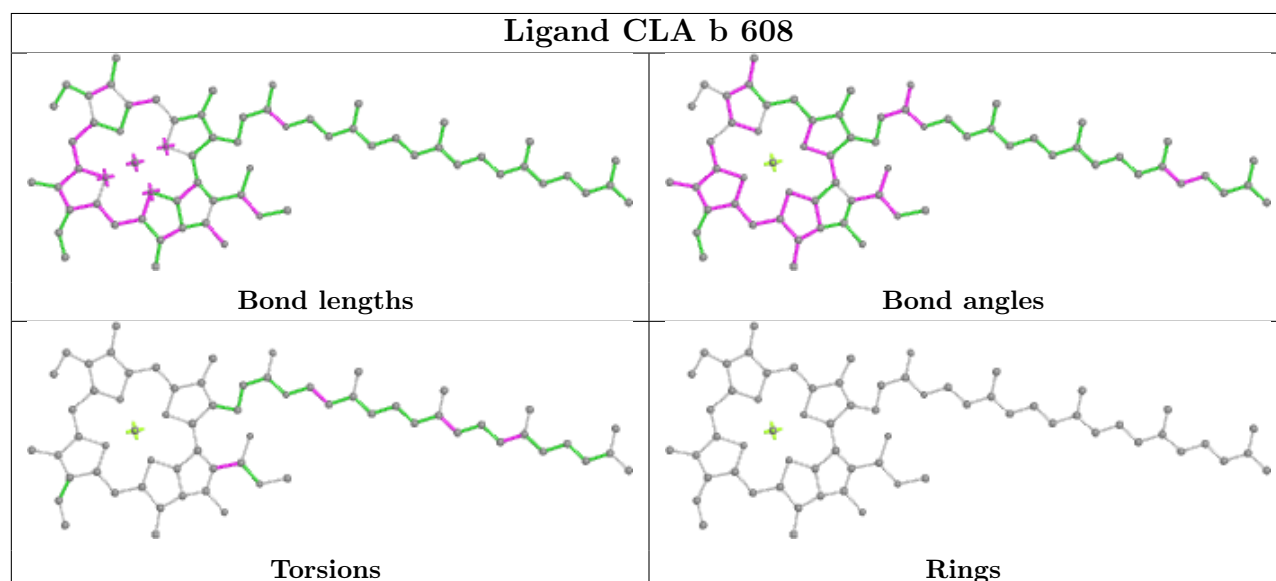
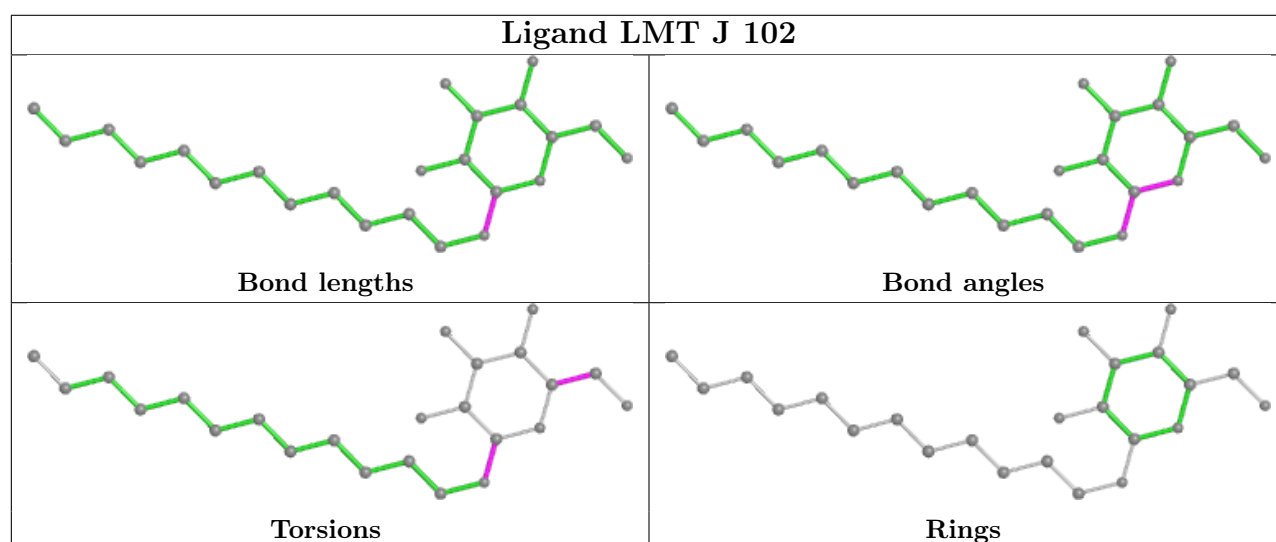
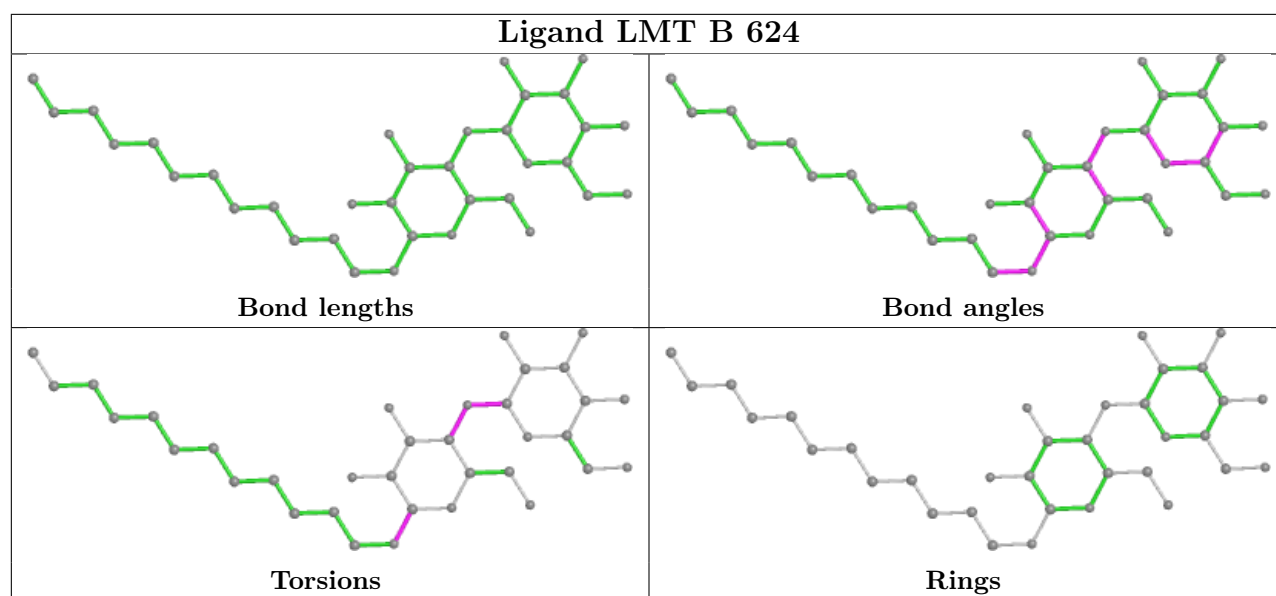
Ligand CLA A 409



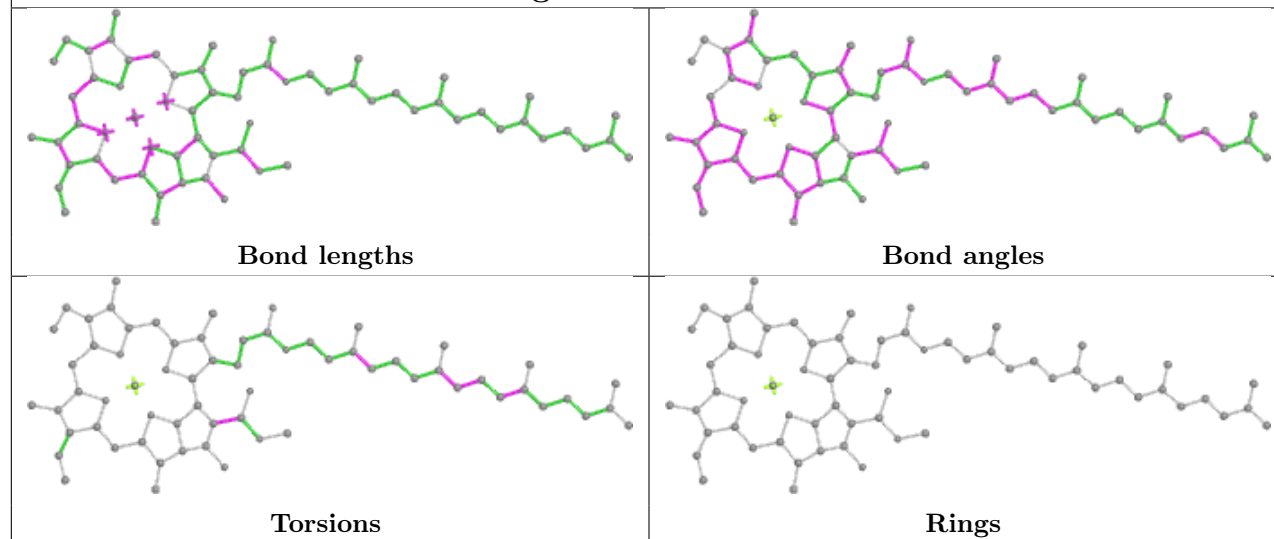
Ligand CLA C 504



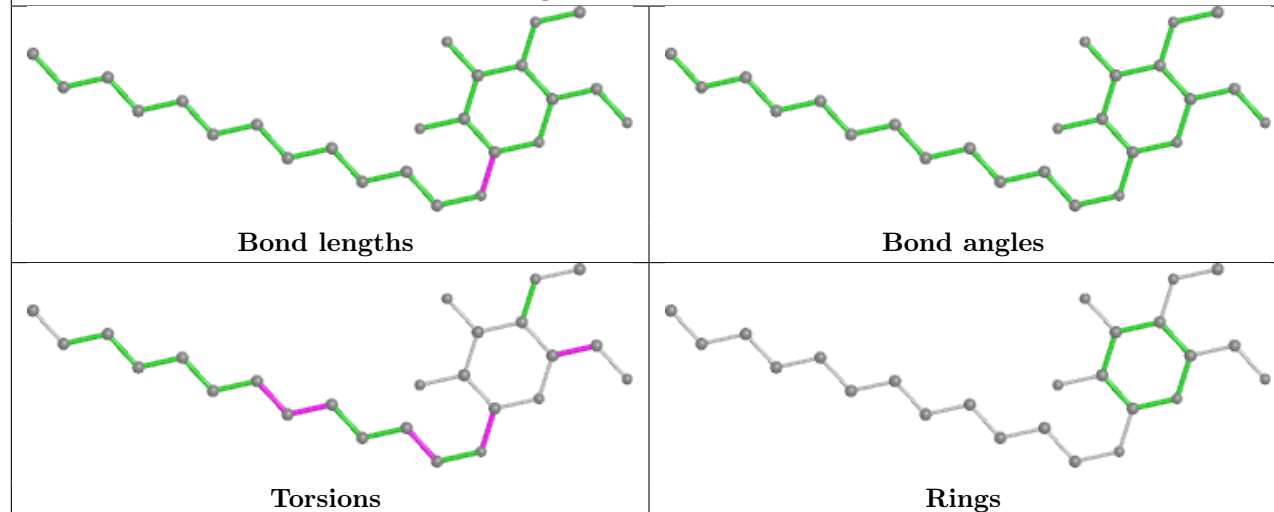




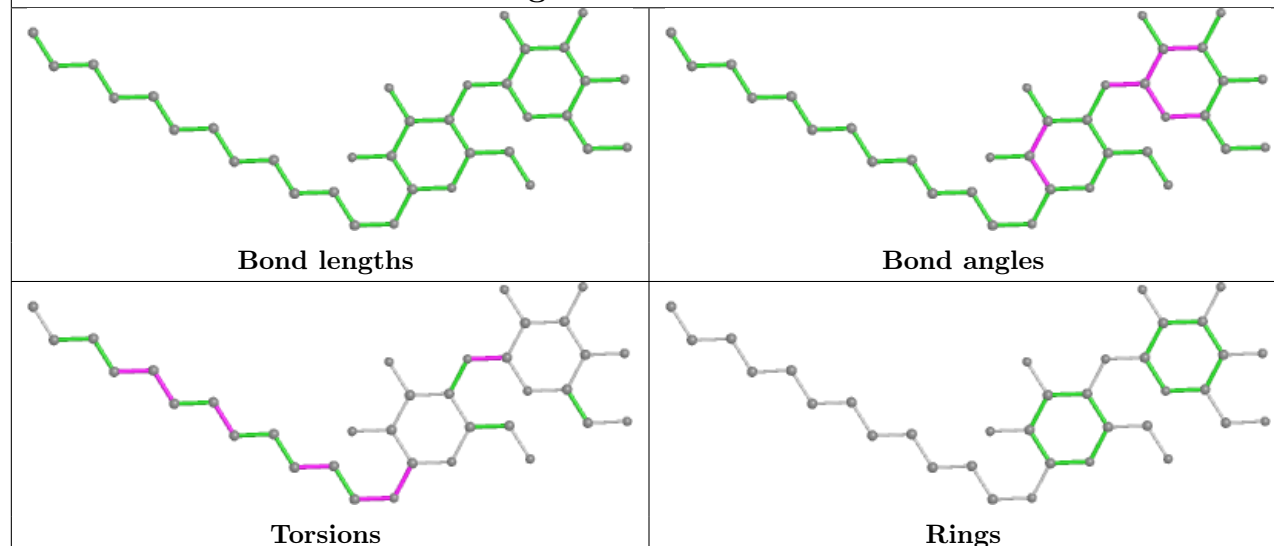
Ligand CLA B 613

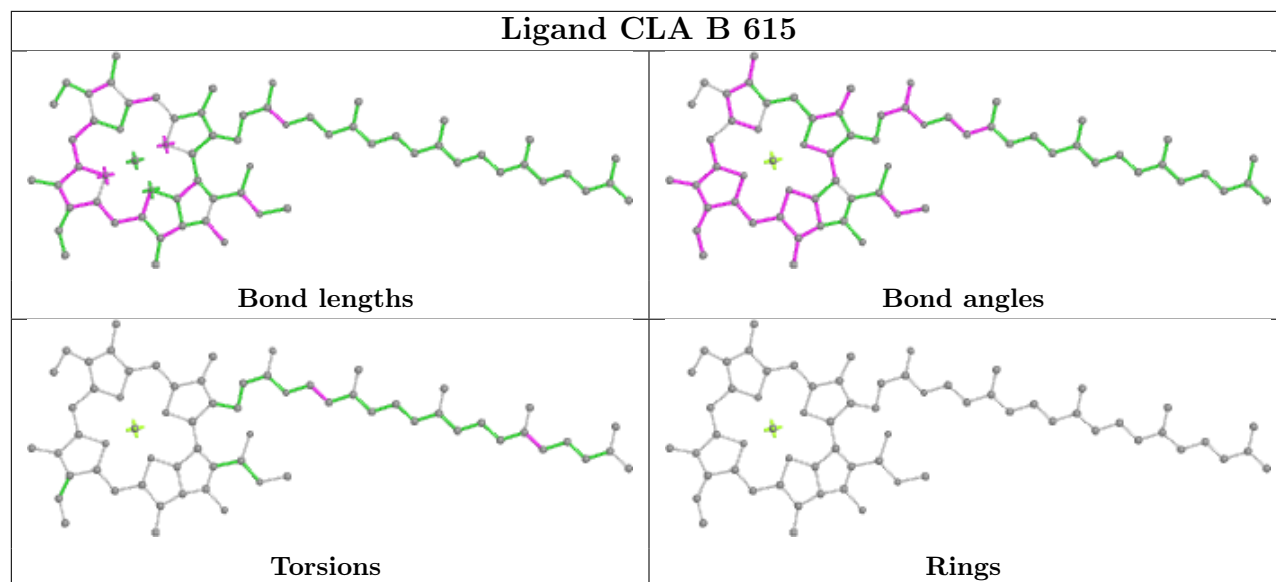
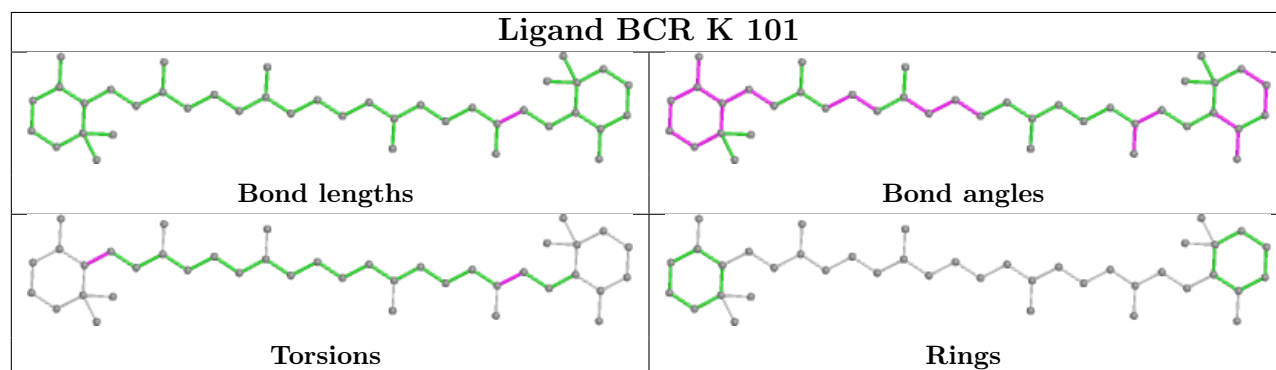
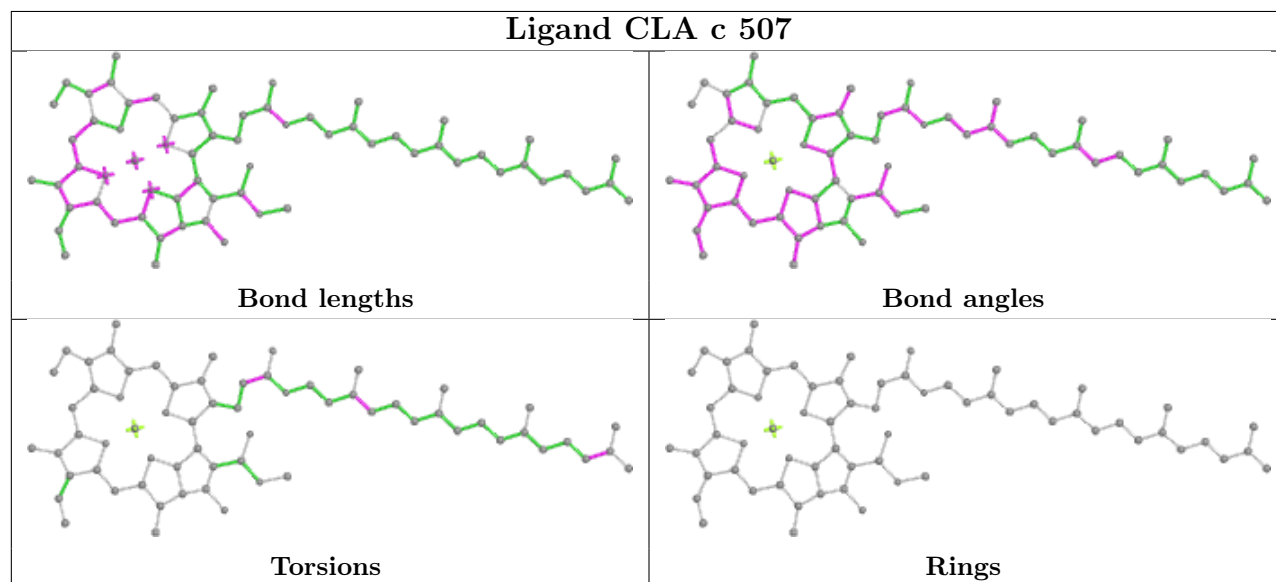


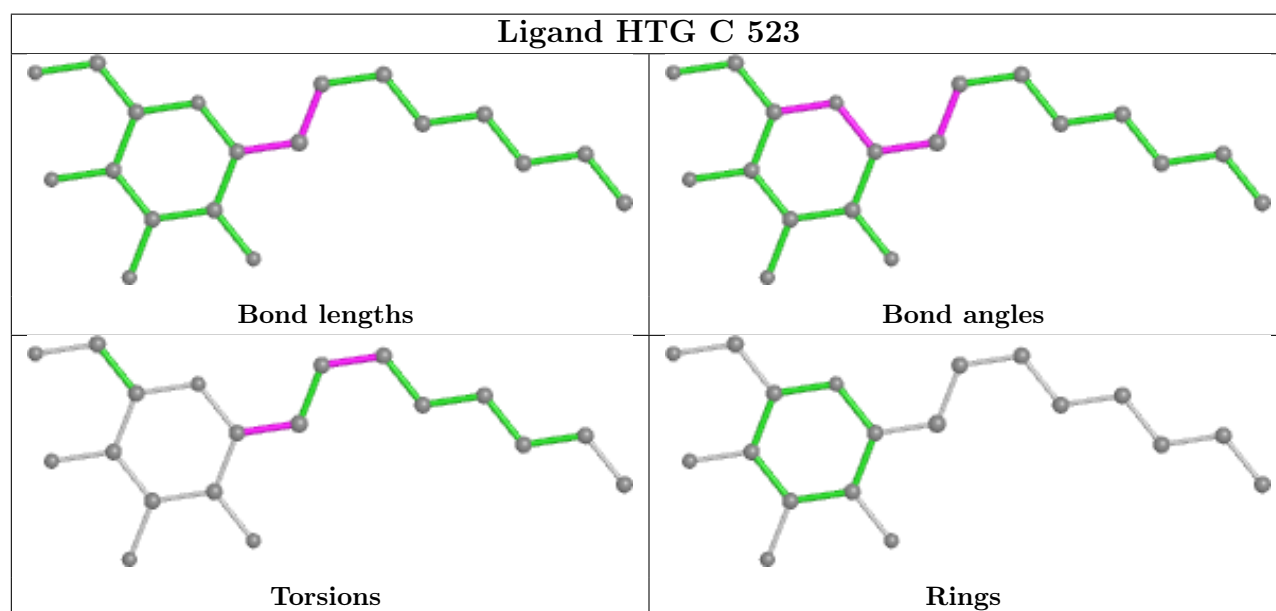
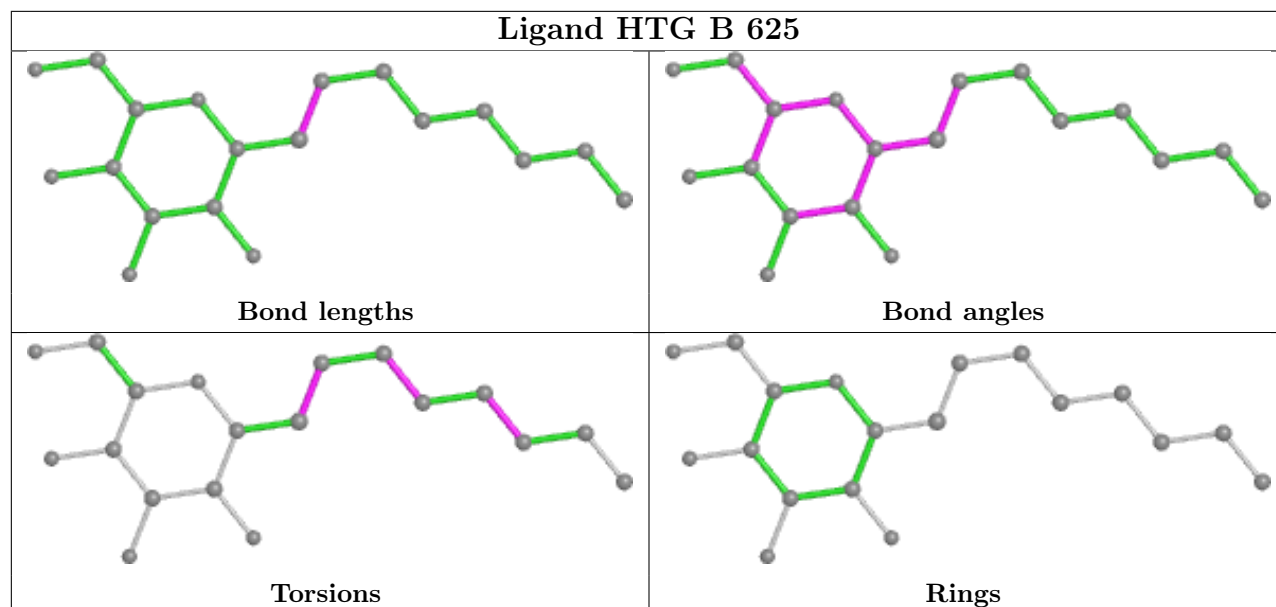
Ligand LMT f 801



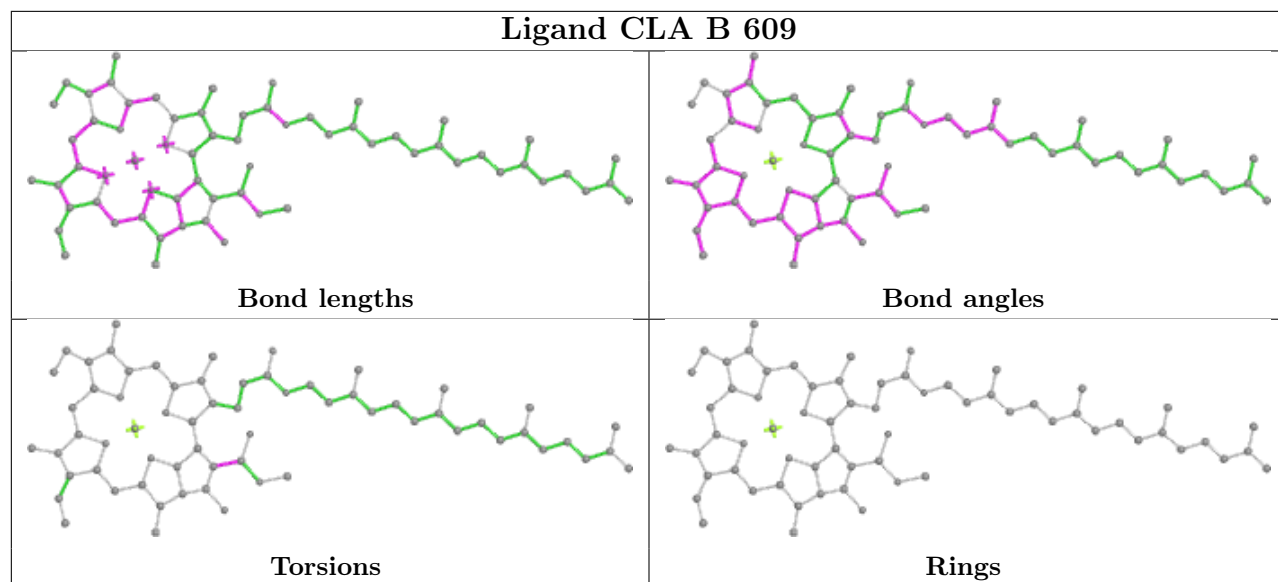
Ligand LMT D 409



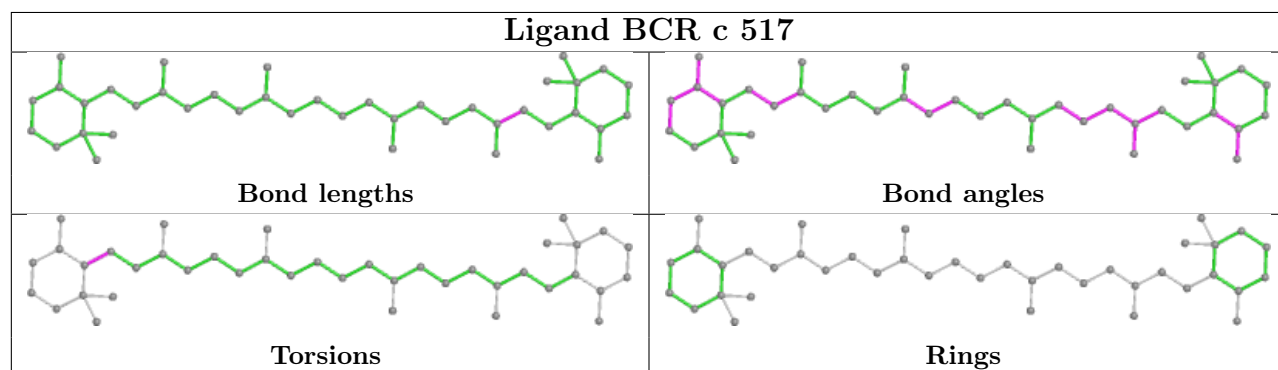
Ligand CLA B 615**Ligand BCR K 101****Ligand CLA c 507**



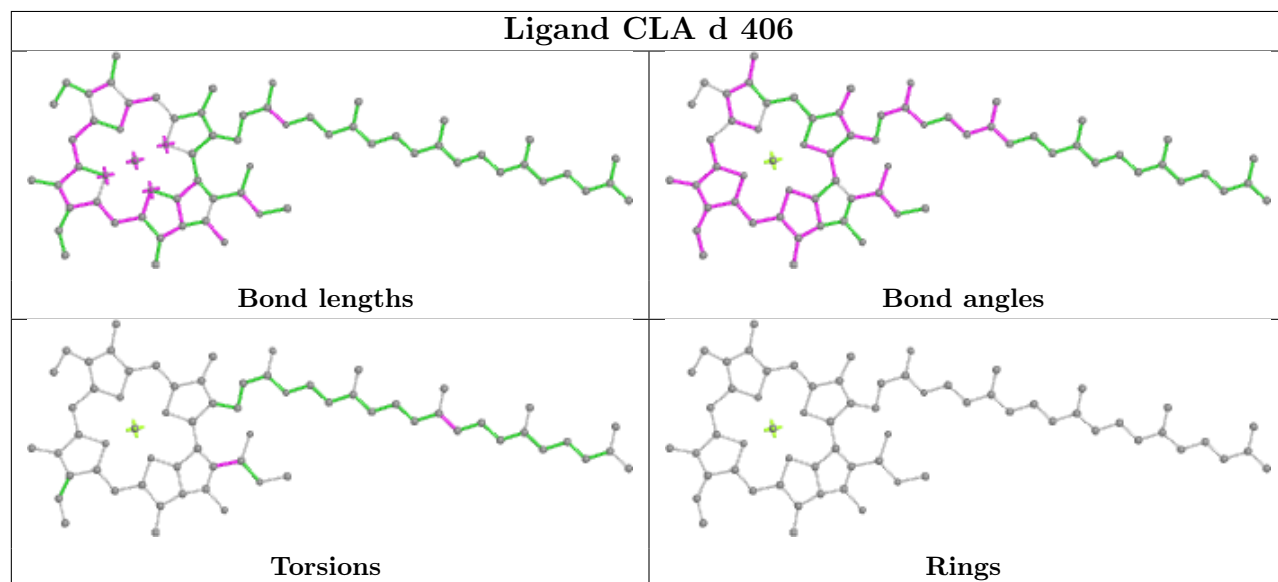
Ligand CLA B 609

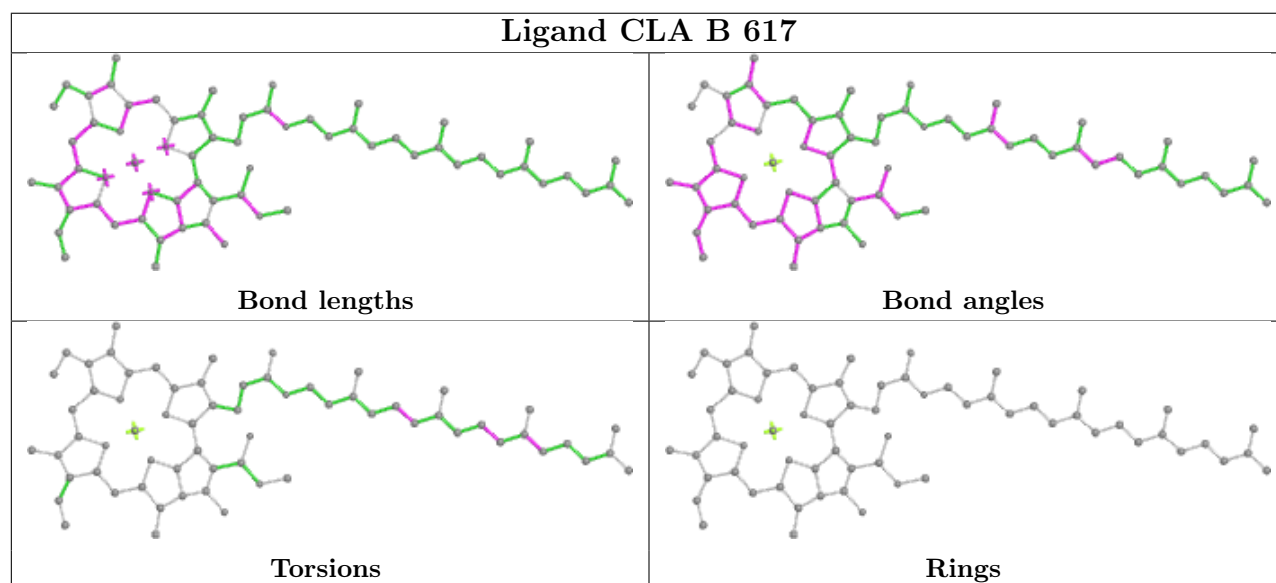
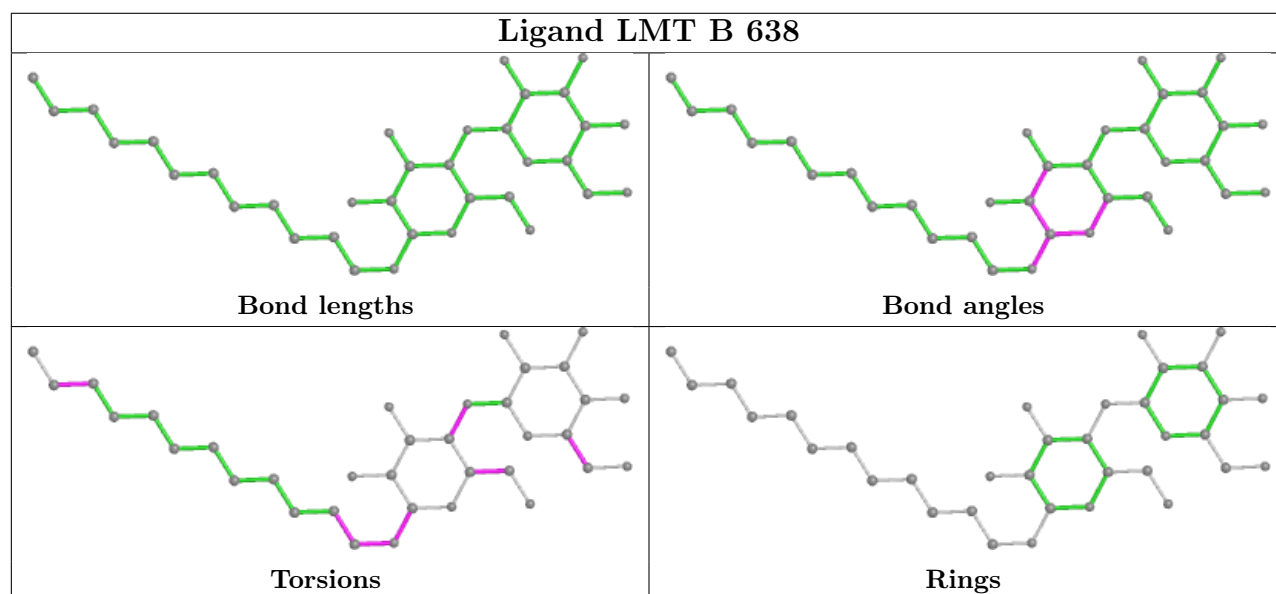
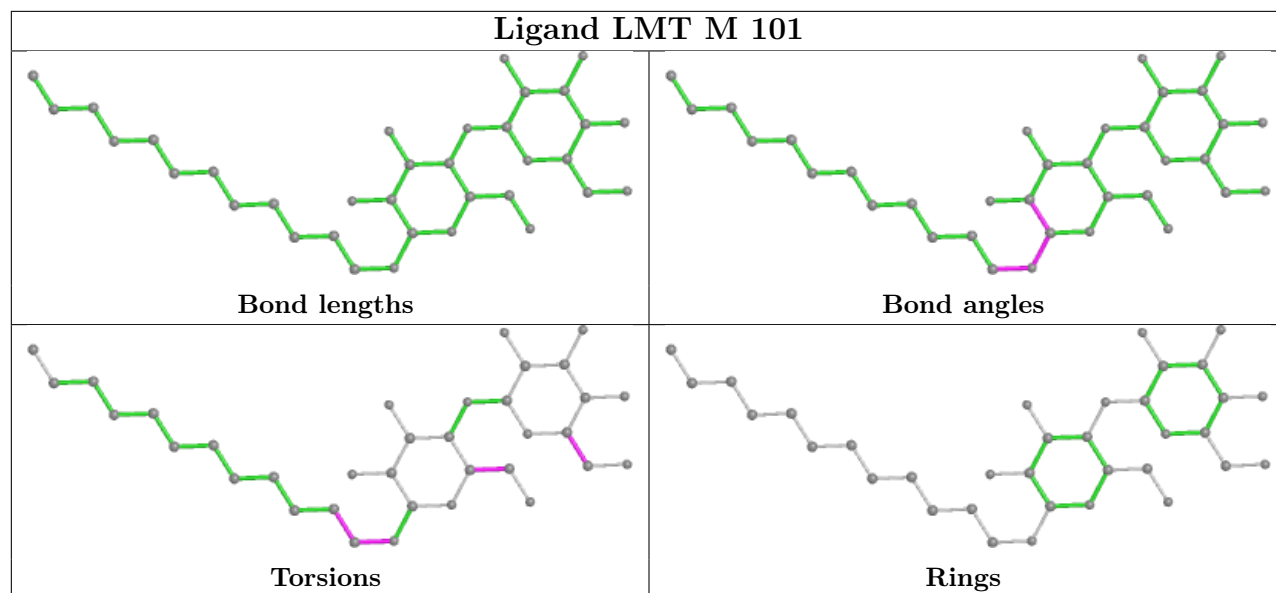


Ligand BCR c 517

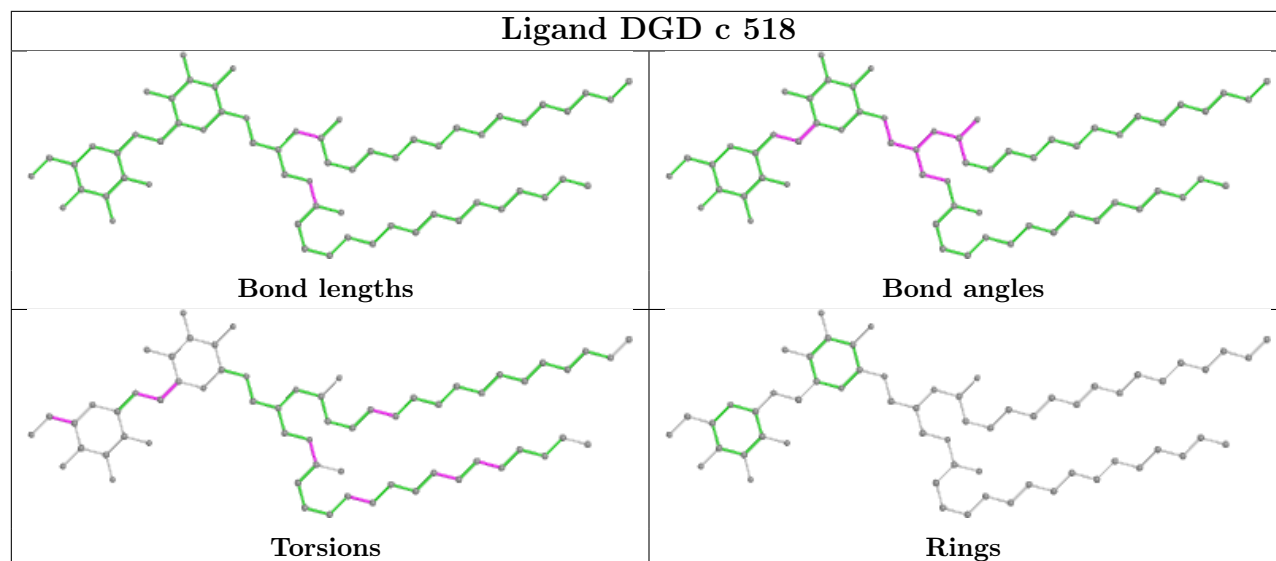


Ligand CLA d 406

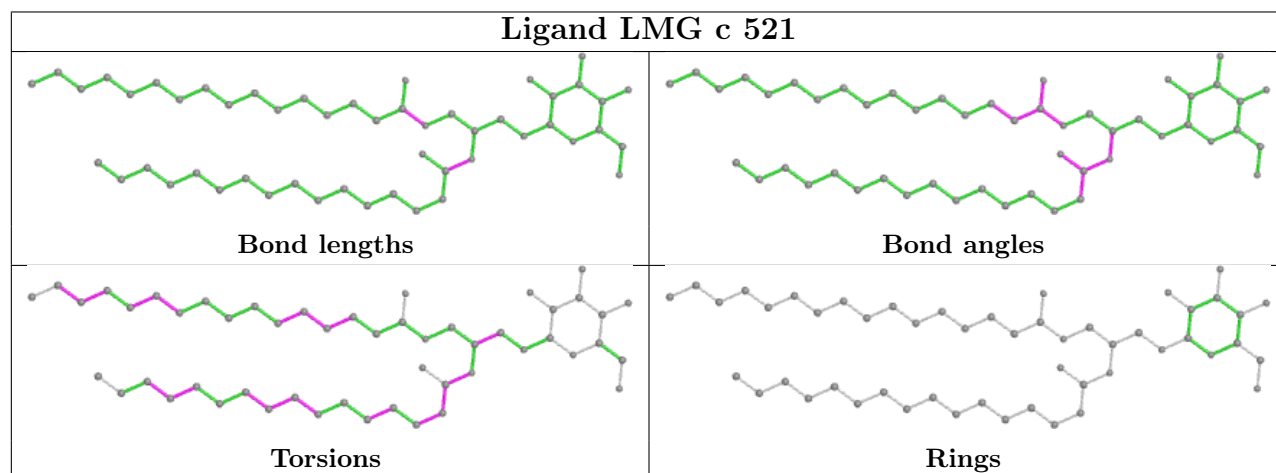




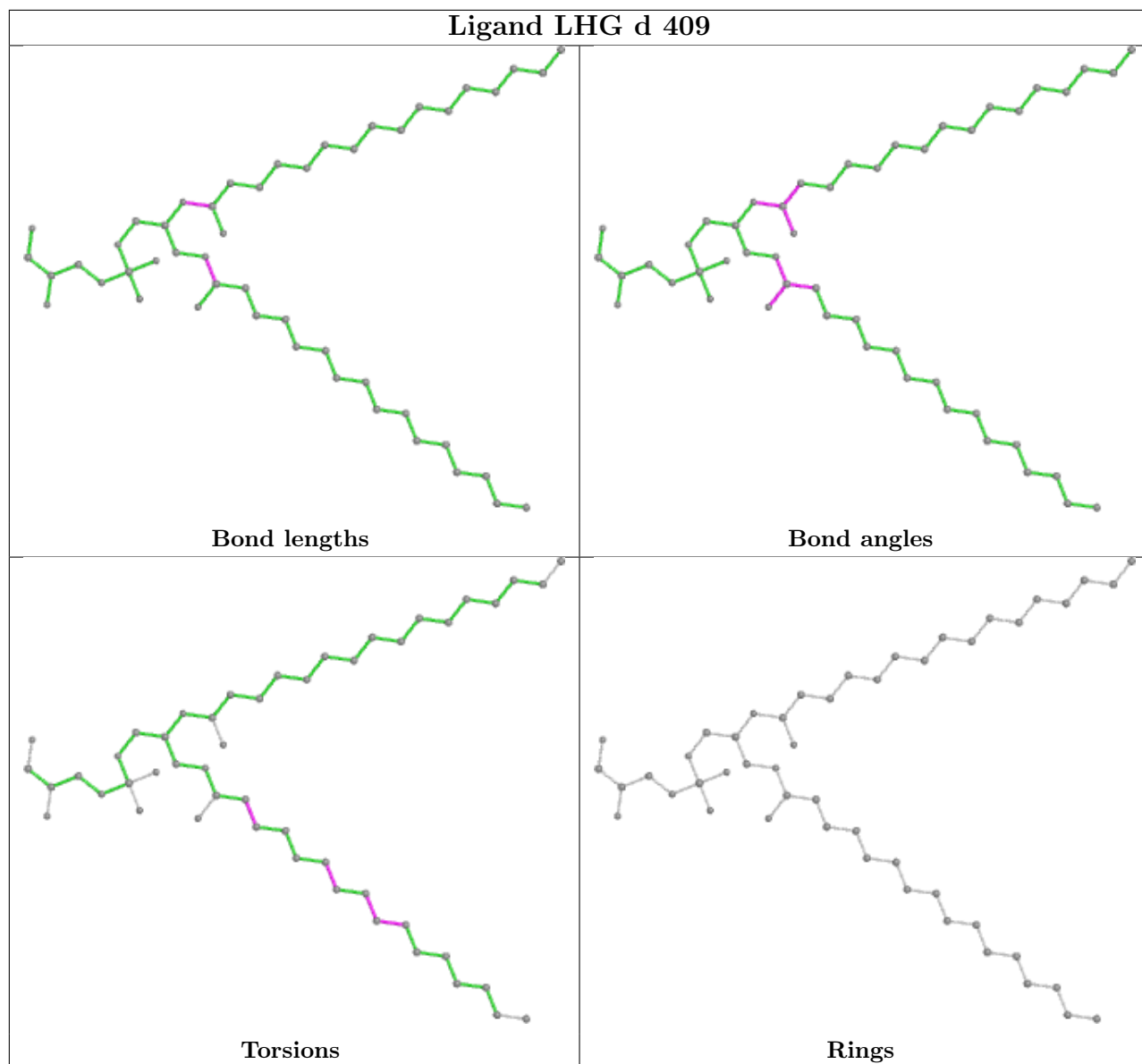
Ligand DGD c 518



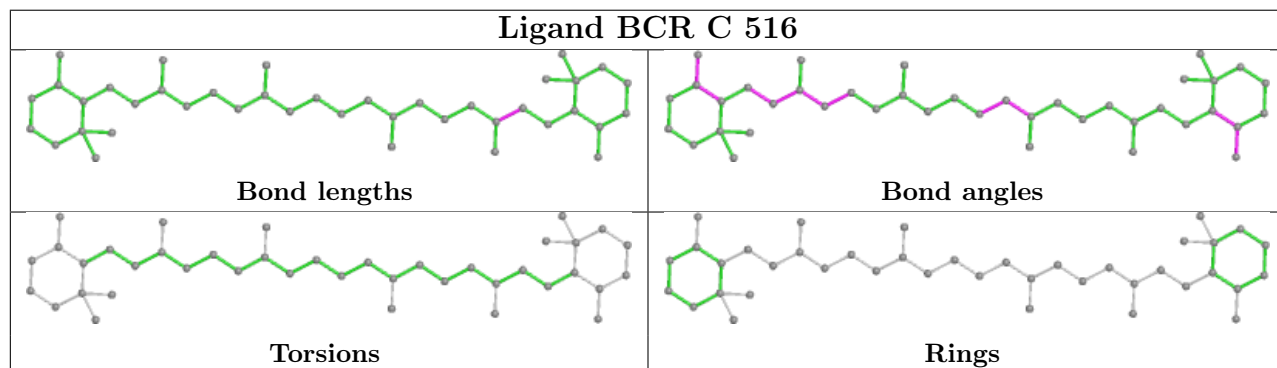
Ligand LMG c 521



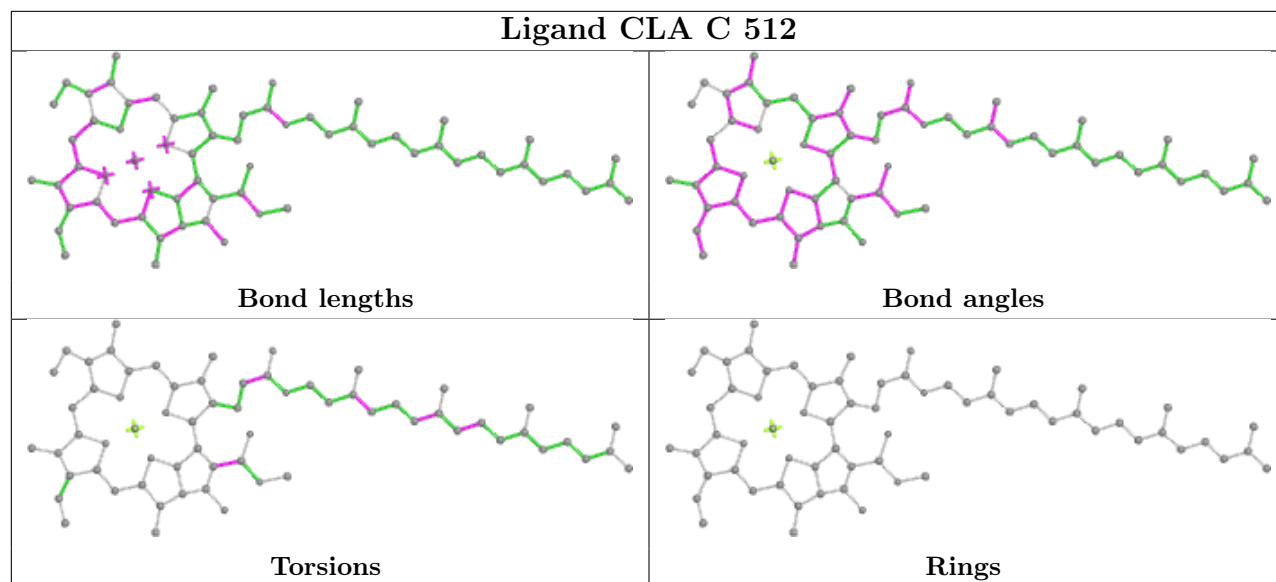
Ligand LHG d 409



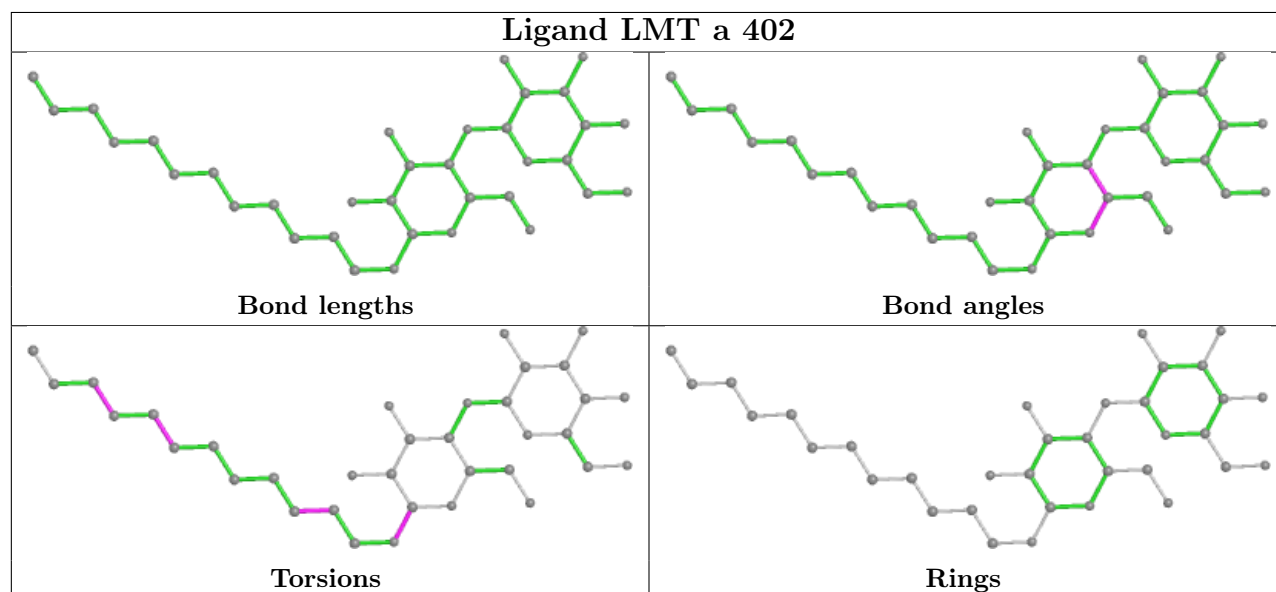
Ligand BCR C 516



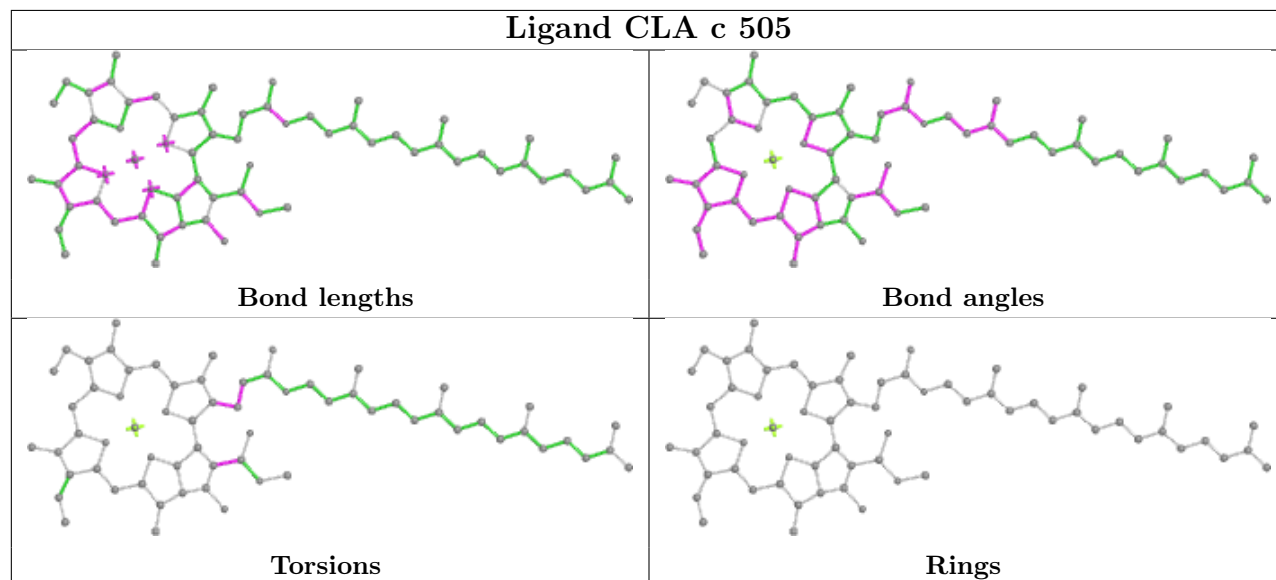
Ligand CLA C 512

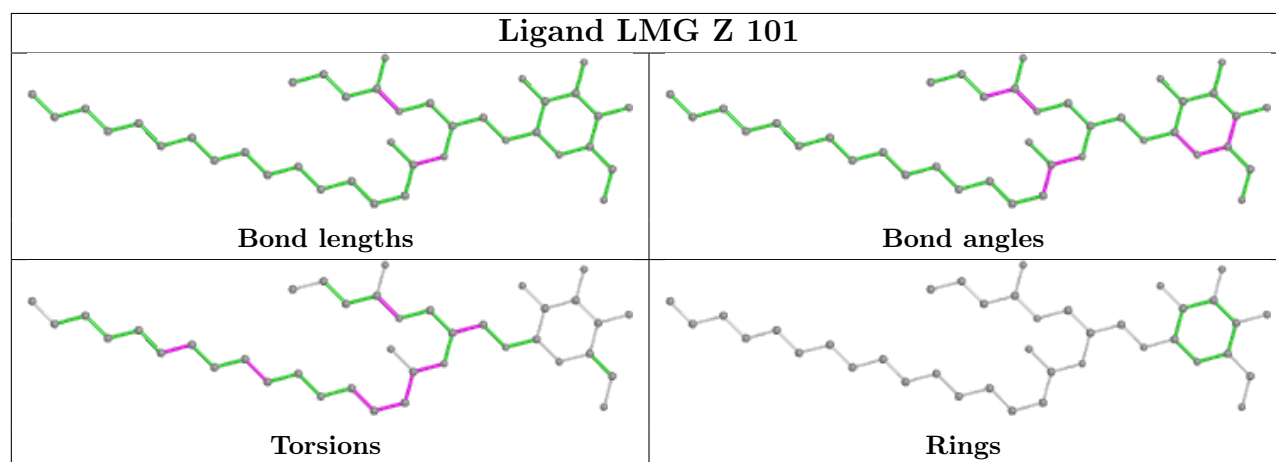
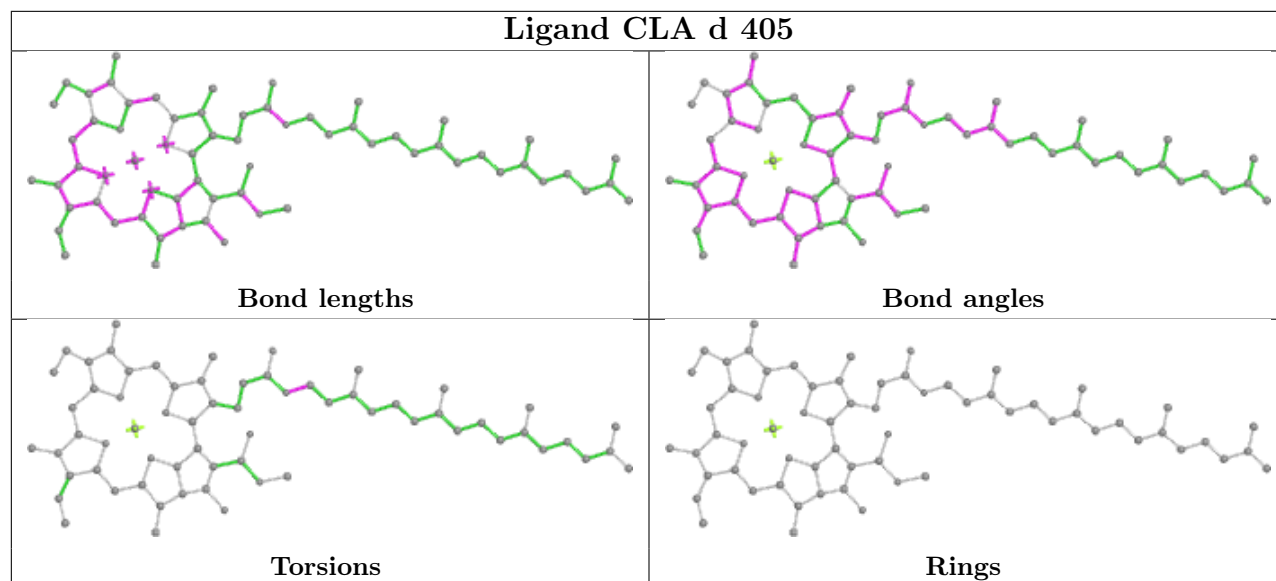
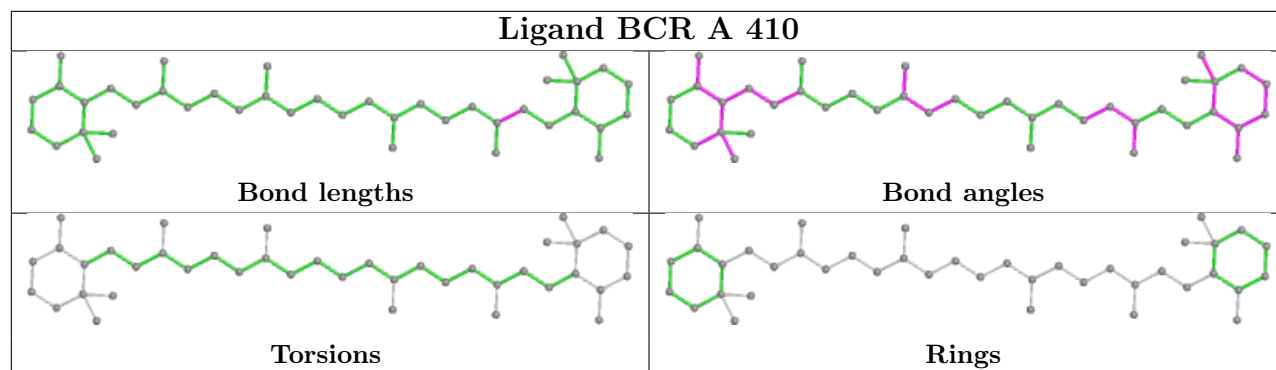


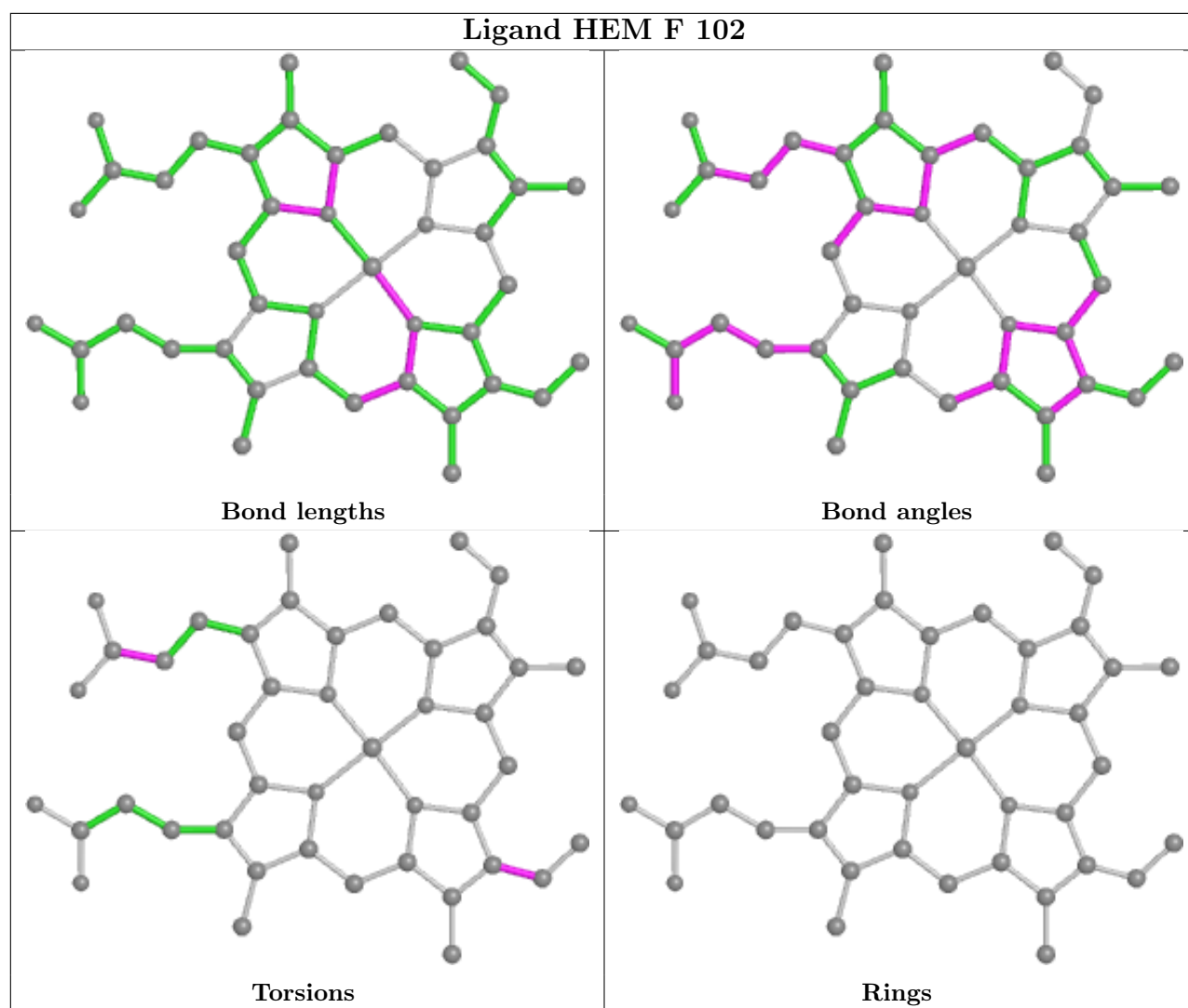
Ligand LMT a 402



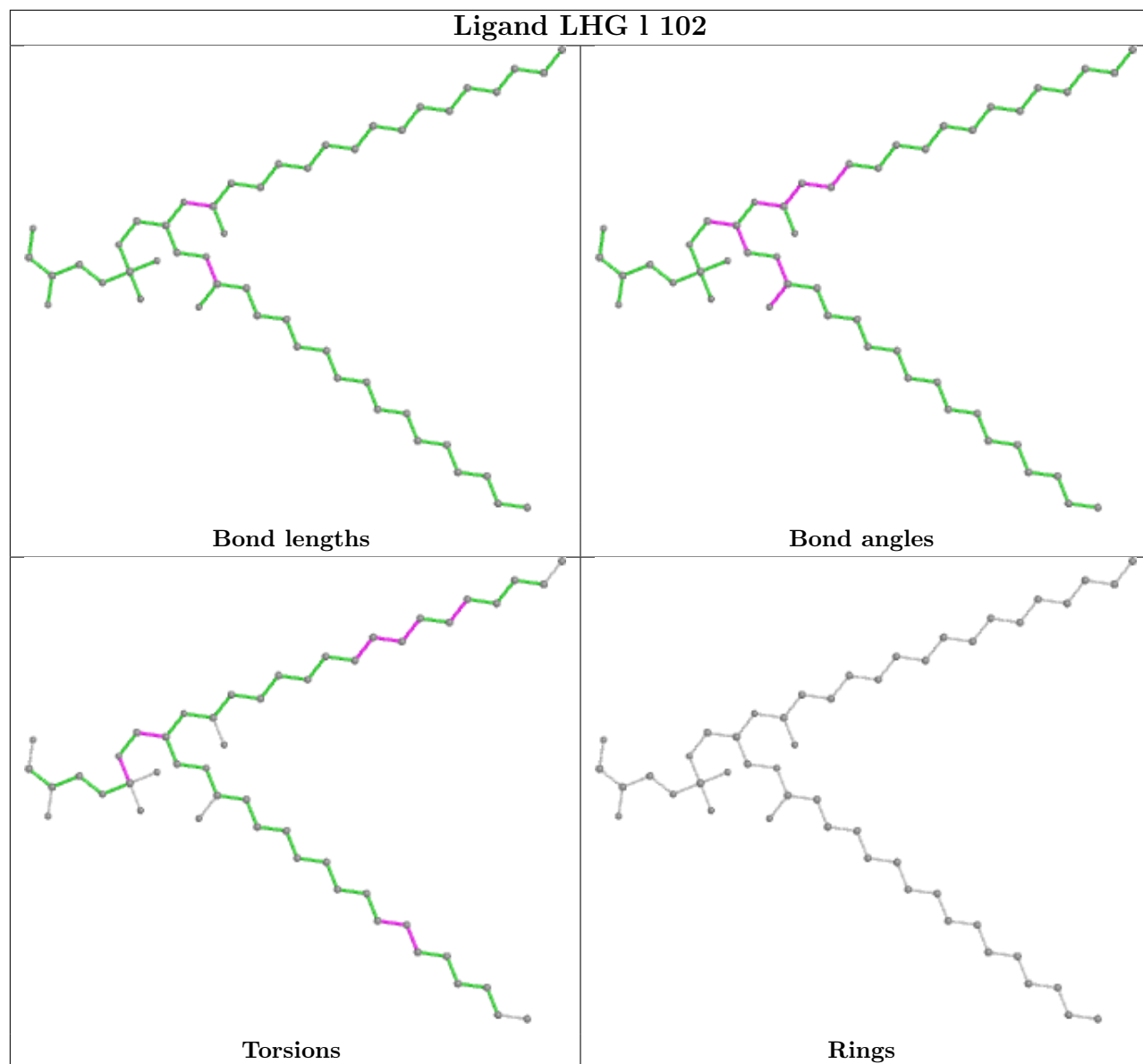
Ligand CLA c 505



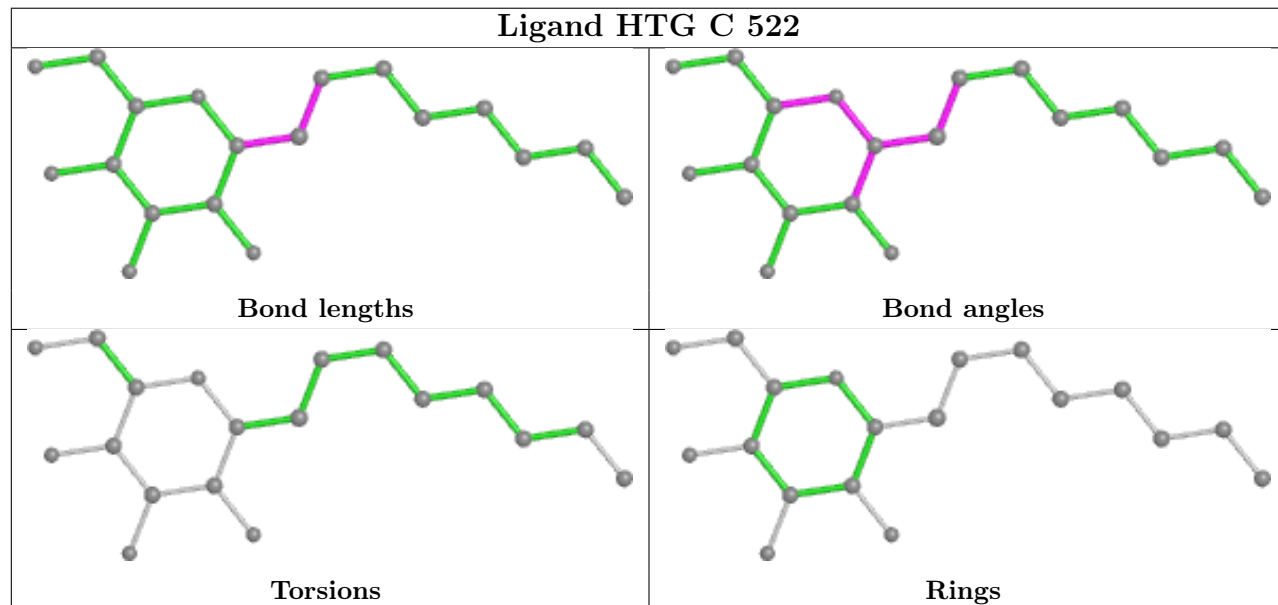




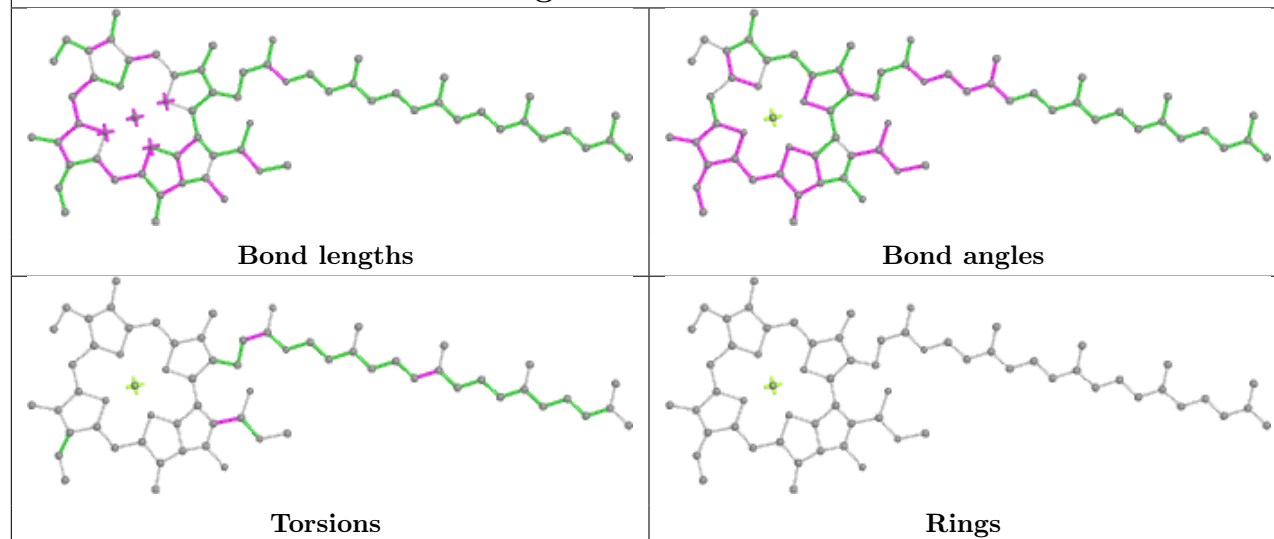
Ligand LHG 1 102



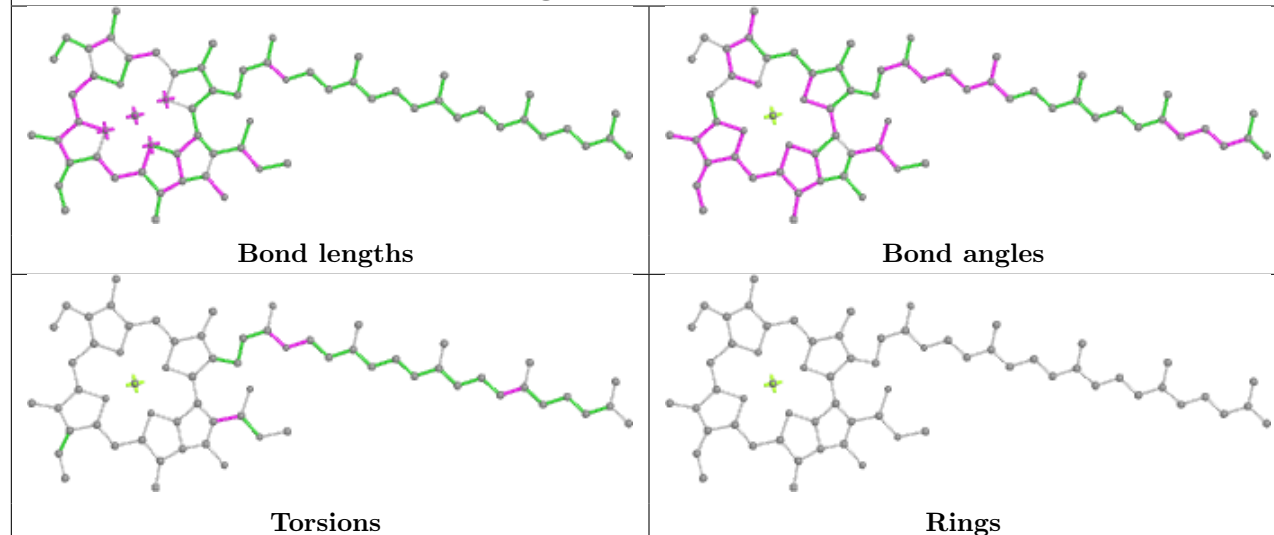
Ligand HTG C 522



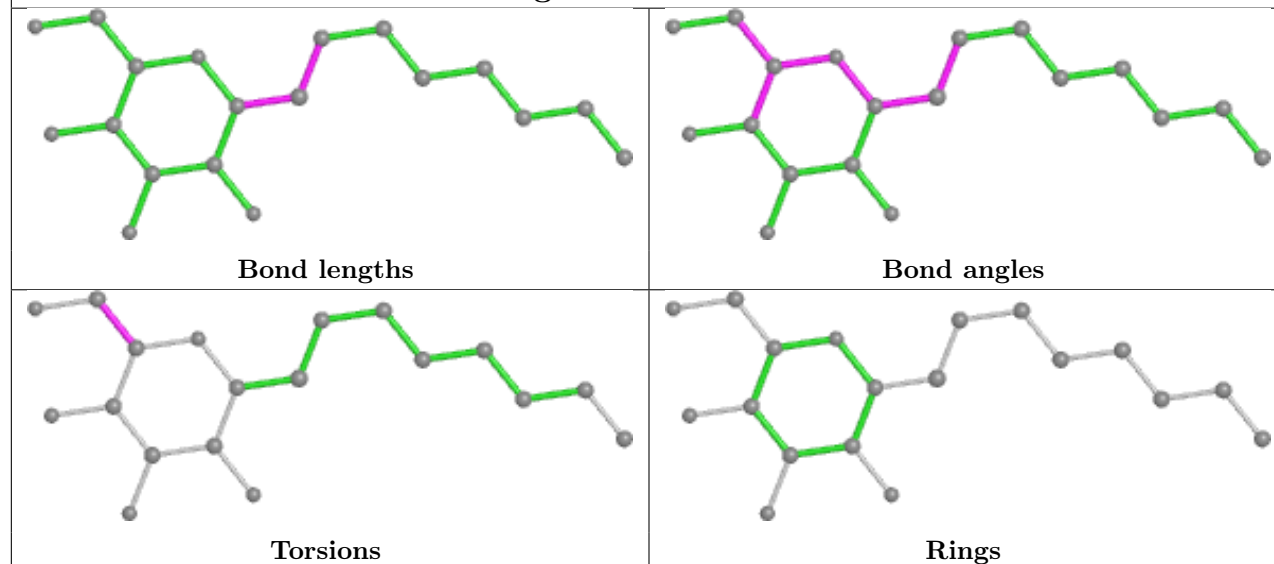
Ligand CLA b 605

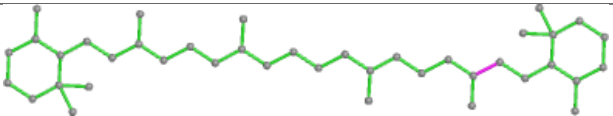
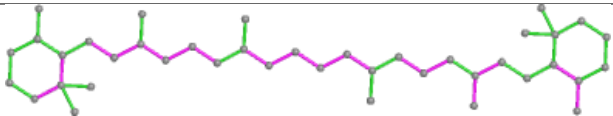
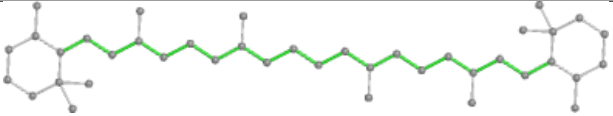
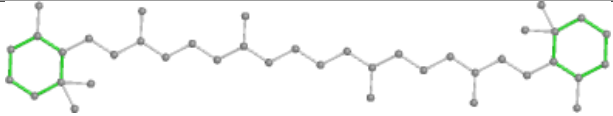


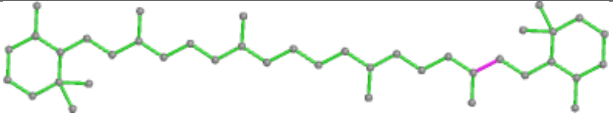
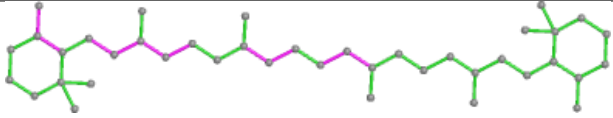
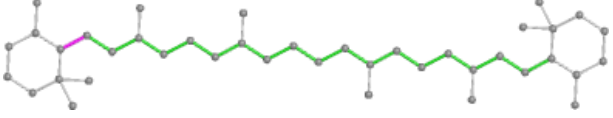
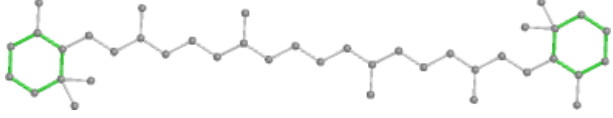
Ligand CLA c 511

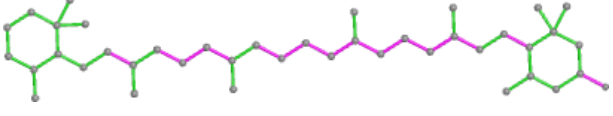
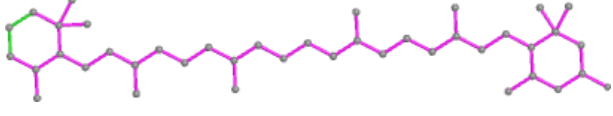
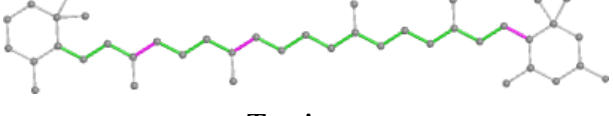
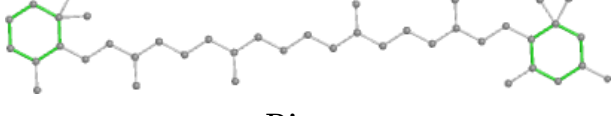


Ligand HTG c 524

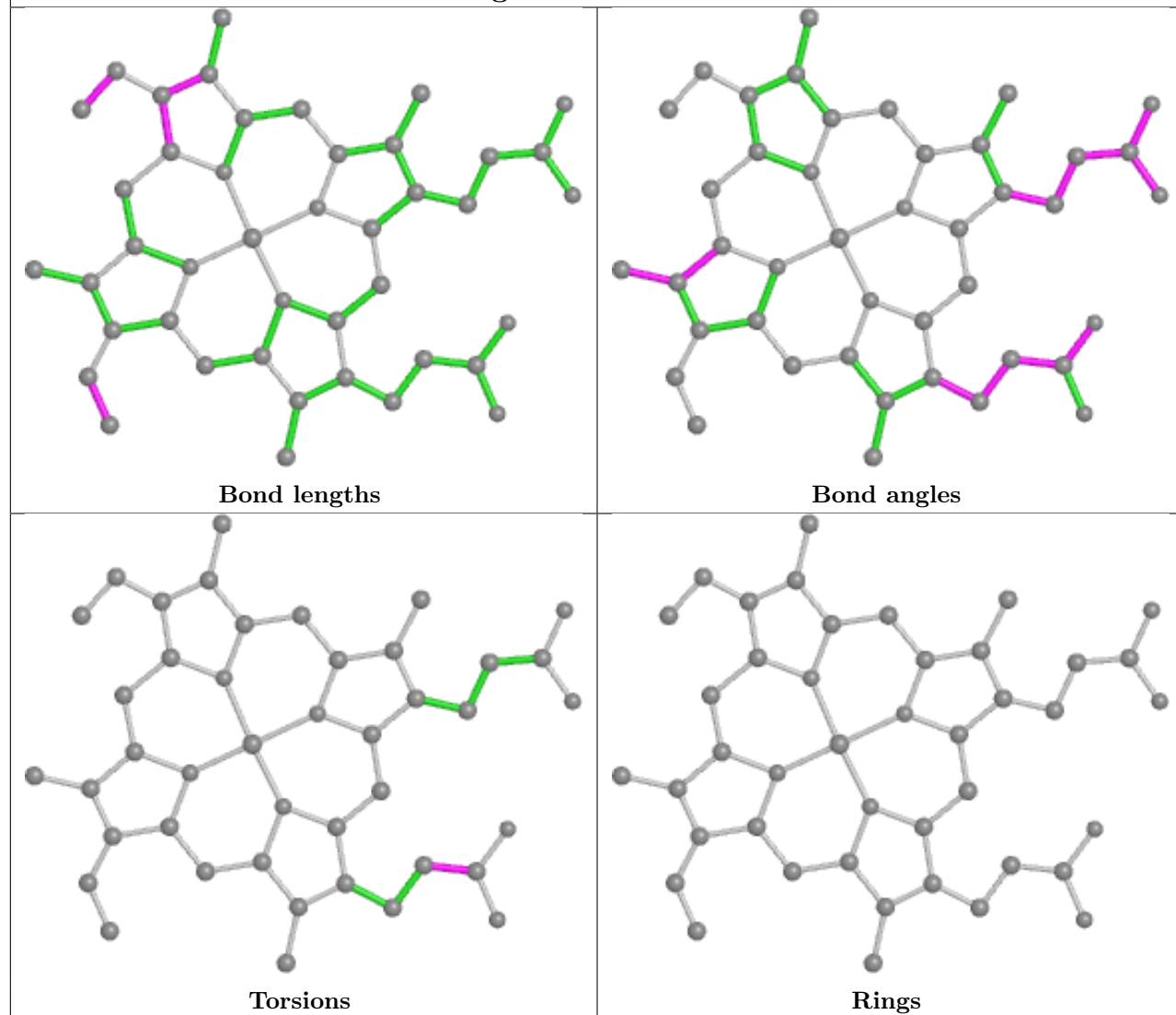


Ligand BCR b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

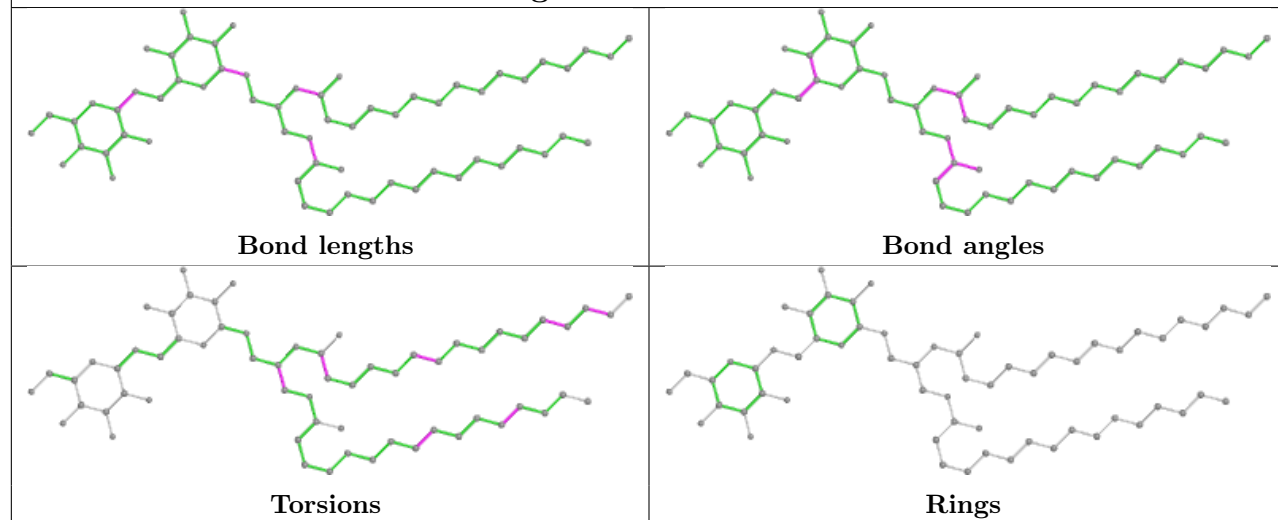
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

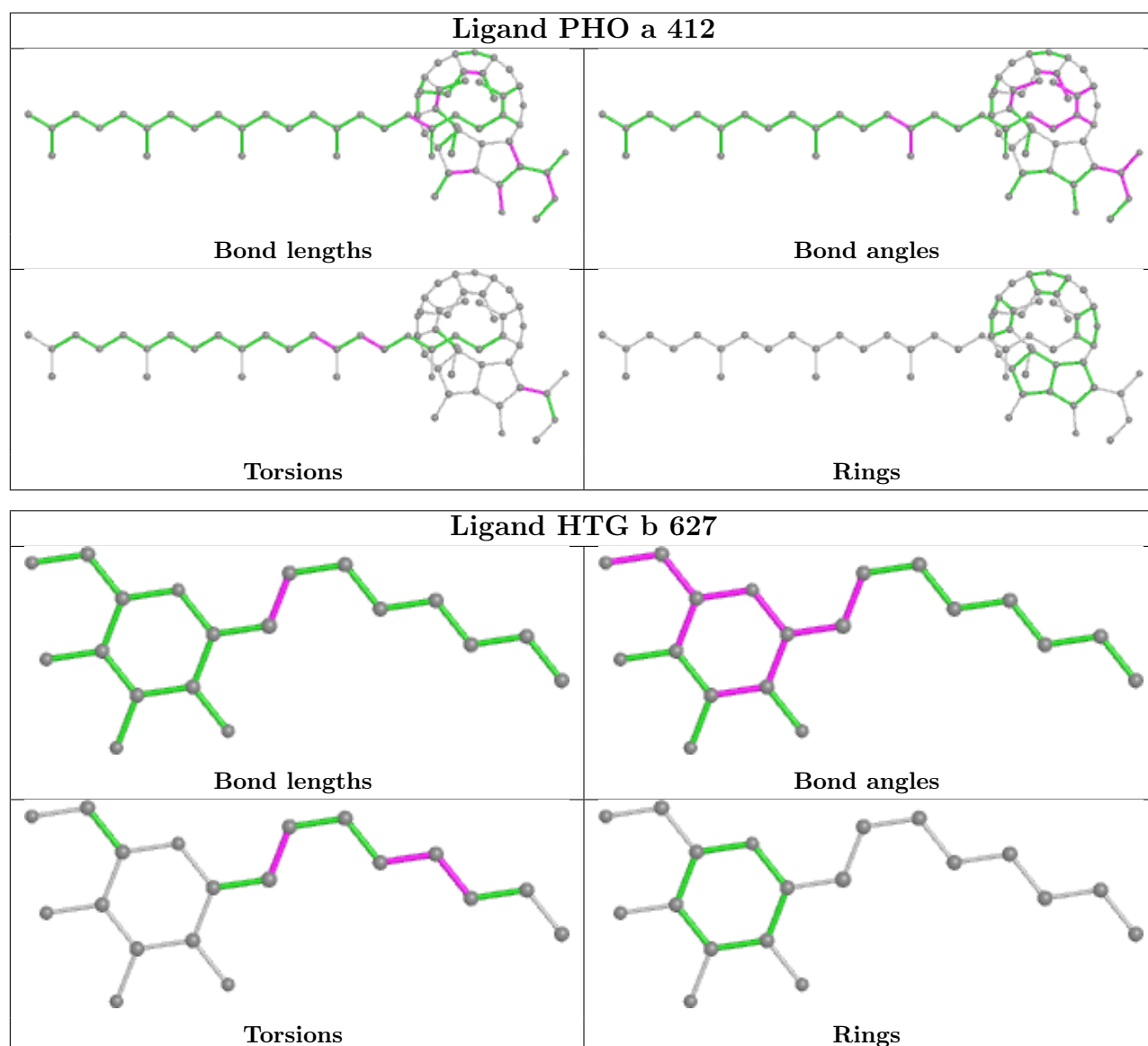
Ligand RRX H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HEC v 201



Ligand DGD h 102





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/360 (92%)	-0.71	5 (1%) 73 76	21, 28, 47, 90	0
1	a	342/360 (95%)	-0.51	13 (3%) 40 43	22, 30, 62, 142	0
2	B	504/510 (98%)	-0.50	18 (3%) 42 45	23, 33, 57, 122	0
2	b	504/510 (98%)	-0.34	29 (5%) 23 25	24, 35, 67, 147	0
3	C	450/461 (97%)	-0.55	6 (1%) 77 79	26, 37, 55, 93	0
3	c	455/461 (98%)	-0.46	7 (1%) 73 76	30, 41, 57, 114	0
4	D	341/352 (96%)	-0.75	3 (0%) 84 85	21, 28, 45, 92	0
4	d	342/352 (97%)	-0.66	7 (2%) 65 68	23, 32, 53, 119	0
5	E	80/84 (95%)	0.80	22 (27%) 0 0	33, 49, 106, 133	0
5	e	79/84 (94%)	0.84	19 (24%) 0 0	39, 54, 96, 126	0
6	F	34/45 (75%)	-0.16	3 (8%) 10 11	32, 41, 64, 96	0
6	f	32/45 (71%)	-0.11	3 (9%) 8 9	36, 43, 91, 120	0
7	H	64/66 (96%)	-0.06	3 (4%) 31 34	29, 40, 53, 136	0
7	h	65/66 (98%)	0.14	6 (9%) 9 10	34, 43, 58, 147	0
8	I	36/38 (94%)	0.14	4 (11%) 5 6	32, 42, 98, 126	0
8	i	36/38 (94%)	-0.09	3 (8%) 11 13	32, 40, 85, 116	0
9	J	37/40 (92%)	-0.26	3 (8%) 12 13	31, 41, 106, 122	0
9	j	38/40 (95%)	0.14	5 (13%) 3 3	36, 47, 85, 104	0
10	K	37/46 (80%)	-0.42	1 (2%) 54 57	35, 42, 67, 71	0
10	k	37/46 (80%)	-0.09	3 (8%) 12 13	39, 48, 72, 87	0
11	L	37/37 (100%)	-0.21	4 (10%) 5 6	21, 26, 78, 100	0
11	l	36/37 (97%)	-0.34	3 (8%) 11 13	23, 26, 79, 112	0
12	M	33/36 (91%)	-0.55	2 (6%) 21 24	24, 29, 59, 110	0
12	m	33/36 (91%)	-0.58	2 (6%) 21 24	24, 29, 59, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	-0.18	14 (5%) 23 25	23, 41, 72, 114	0
13	o	243/272 (89%)	0.09	24 (9%) 7 8	26, 44, 78, 127	0
14	T	29/32 (90%)	-0.53	1 (3%) 45 48	23, 26, 49, 117	0
14	t	29/32 (90%)	-0.32	2 (6%) 16 19	25, 28, 55, 85	0
15	U	97/134 (72%)	-0.20	4 (4%) 37 40	29, 40, 68, 107	0
15	u	97/134 (72%)	-0.24	1 (1%) 82 84	33, 43, 62, 126	0
16	V	137/163 (84%)	-0.48	0 100 100	27, 36, 57, 84	0
16	v	137/163 (84%)	-0.20	6 (4%) 34 37	34, 49, 77, 99	0
17	X	40/41 (97%)	0.07	5 (12%) 3 4	36, 46, 80, 99	0
17	x	38/41 (92%)	0.26	5 (13%) 3 3	41, 50, 98, 113	0
18	Y	29/46 (63%)	1.30	6 (20%) 1 1	43, 54, 91, 119	0
18	y	30/46 (65%)	1.17	9 (30%) 0 0	51, 63, 102, 111	0
19	Z	62/62 (100%)	0.41	12 (19%) 1 1	44, 55, 90, 101	0
19	z	61/62 (98%)	0.94	16 (26%) 0 0	52, 65, 107, 126	0
20	R	34/41 (82%)	5.30	33 (97%) 0 0	70, 121, 137, 141	0
All	All	5292/5691 (92%)	-0.29	312 (5%) 22 25	21, 37, 75, 147	0

The worst 5 of 312 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	66	GLY	11.3
7	h	64	ALA	10.5
20	R	18	TRP	9.2
2	b	486	LEU	8.8
2	b	494	GLY	8.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.95	0.08	27,32,61,65	0
14	FME	T	1	10/11	0.96	0.08	25,32,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	FME	M	1	10/11	0.96	0.12	28,38,66,77	0
12	FME	m	1	10/11	0.97	0.10	29,37,67,73	0
8	FME	i	1	10/11	0.97	0.12	31,39,45,51	0
8	FME	I	1	10/11	0.98	0.07	32,39,44,49	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	UNL	I	106	10/-	0.29	0.40	63,88,93,94	0
36	HTG	d	404	16/19	0.47	0.34	63,100,108,111	0
36	HTG	H	101	16/19	0.48	0.30	63,123,128,130	0
34	DMS	v	205	4/4	0.48	0.37	129,131,133,136	0
32	LMT	j	102	24/35	0.51	0.27	64,83,130,132	0
34	DMS	u	203	4/4	0.52	0.40	60,81,82,87	0
30	UNL	V	206	7/-	0.55	0.24	75,86,100,101	0
31	GOL	O	304	6/6	0.56	0.26	80,88,90,92	0
30	UNL	C	527	8/-	0.56	0.24	87,99,102,102	0
37	DGD	d	416	50/66	0.56	0.32	81,99,118,119	0
36	HTG	u	201	14/19	0.57	0.42	63,93,113,120	0
36	HTG	B	630	19/19	0.57	0.25	53,112,124,125	0
32	LMT	M	101	35/35	0.58	0.28	50,115,142,145	0
32	LMT	F	103	35/35	0.59	0.37	74,113,128,129	0
30	UNL	X	102	10/-	0.59	0.28	70,77,82,84	0
36	HTG	b	603	19/19	0.60	0.22	56,104,122,125	0
30	UNL	E	102	12/-	0.60	0.31	66,75,95,97	0
30	UNL	D	416	16/-	0.60	0.26	78,82,87,88	0
32	LMT	J	102	24/35	0.60	0.24	56,70,106,110	0
30	UNL	h	104	16/-	0.61	0.29	65,75,101,101	0
34	DMS	B	641	4/4	0.61	0.33	123,126,128,129	0
36	HTG	B	626	19/19	0.61	0.41	56,115,122,124	0
34	DMS	C	539	4/4	0.62	0.35	99,100,102,106	0
30	UNL	C	528	7/-	0.62	0.39	54,74,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	UNL	b	640	13/-	0.63	0.36	73,90,108,109	0
30	UNL	C	524	28/-	0.63	0.20	55,73,107,110	0
30	UNL	V	204	8/-	0.63	0.30	49,66,70,71	0
30	UNL	h	105	10/-	0.64	0.21	70,85,94,97	0
30	UNL	h	103	7/-	0.64	0.25	78,80,84,85	0
34	DMS	O	308	4/4	0.64	0.44	107,116,120,120	0
36	HTG	b	628	19/19	0.65	0.26	60,120,129,130	0
28	LMG	Z	101	39/55	0.65	0.27	52,91,115,120	0
32	LMT	a	421	35/35	0.65	0.37	89,107,136,139	0
30	UNL	X	101	34/-	0.65	0.25	37,74,119,123	0
30	UNL	k	101	30/-	0.66	0.20	59,87,110,113	0
30	UNL	J	103	8/-	0.66	0.22	70,72,74,75	0
32	LMT	B	638	35/35	0.66	0.25	42,110,127,128	0
34	DMS	C	501	4/4	0.66	0.48	129,130,133,134	0
36	HTG	c	524	19/19	0.67	0.37	70,95,108,112	0
34	DMS	o	305	4/4	0.67	0.41	123,128,128,131	0
38	LHG	a	416	42/49	0.67	0.28	64,113,146,149	0
30	UNL	I	105	16/-	0.68	0.23	70,80,84,88	0
30	UNL	j	103	10/-	0.68	0.20	63,68,76,77	0
30	UNL	c	526	4/-	0.68	0.26	67,72,73,74	0
30	UNL	c	528	8/-	0.69	0.33	61,79,81,84	0
30	UNL	Z	102	5/-	0.69	0.20	61,63,66,69	0
30	UNL	C	532	10/-	0.69	0.32	82,86,88,89	0
34	DMS	O	306	4/4	0.69	0.26	106,111,111,112	0
28	LMG	c	522	51/55	0.69	0.26	46,91,109,123	0
32	LMT	D	409	35/35	0.69	0.34	73,105,130,134	0
30	UNL	J	105	6/-	0.70	0.20	78,83,85,85	0
32	LMT	m	103	35/35	0.70	0.22	51,107,122,129	0
32	LMT	B	624	35/35	0.70	0.22	55,82,98,101	0
32	LMT	b	629	24/35	0.70	0.23	47,74,124,126	0
30	UNL	c	501	8/-	0.71	0.15	63,73,83,84	0
30	UNL	b	630	10/-	0.71	0.22	80,85,90,91	0
34	DMS	a	424	4/4	0.71	0.23	110,112,113,114	0
32	LMT	b	626	35/35	0.71	0.25	38,102,128,130	0
32	LMT	b	625	35/35	0.72	0.23	55,102,123,127	0
34	DMS	b	644	4/4	0.72	0.33	119,122,123,124	0
32	LMT	a	402	35/35	0.72	0.27	43,84,103,110	0
34	DMS	B	639	4/4	0.72	0.34	111,114,115,115	0
30	UNL	B	628	6/-	0.72	0.30	55,60,66,69	0
31	GOL	b	638	6/6	0.73	0.21	88,94,100,100	0
30	UNL	h	106	4/-	0.73	0.19	69,70,72,74	0
32	LMT	f	801	25/35	0.73	0.31	73,101,111,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	DMS	O	302	4/4	0.73	0.32	104,111,113,118	0
30	UNL	I	103	16/-	0.73	0.20	53,72,92,94	0
27	SQD	B	622	54/54	0.73	0.20	43,72,113,116	0
30	UNL	B	635	4/-	0.73	0.20	67,72,73,78	0
30	UNL	A	417	12/-	0.74	0.20	77,79,82,83	0
30	UNL	y	101	10/-	0.74	0.15	83,85,87,88	0
30	UNL	B	601	4/-	0.74	0.27	70,71,72,74	0
34	DMS	c	537	4/4	0.74	0.37	115,117,119,122	0
34	DMS	d	419	4/4	0.74	0.23	106,112,113,114	0
28	LMG	C	533	51/55	0.74	0.22	43,88,98,101	0
36	HTG	c	523	19/19	0.75	0.23	87,103,110,114	0
36	HTG	B	625	19/19	0.75	0.24	34,61,77,79	0
34	DMS	O	310	4/4	0.75	0.30	89,93,96,97	0
32	LMT	A	422	35/35	0.76	0.31	76,95,118,119	0
28	LMG	z	101	37/55	0.76	0.21	50,105,120,121	0
30	UNL	a	420	7/-	0.76	0.24	61,67,71,74	0
30	UNL	B	631	11/-	0.77	0.27	63,70,103,106	0
30	UNL	C	529	8/-	0.77	0.20	75,78,82,84	0
30	UNL	i	103	10/-	0.77	0.14	54,64,75,76	0
30	UNL	I	104	16/-	0.77	0.24	69,82,85,85	0
30	UNL	Z	104	5/-	0.77	0.20	67,70,78,78	0
30	UNL	i	104	10/-	0.78	0.22	69,72,77,81	0
30	UNL	A	414	10/-	0.78	0.25	67,79,83,83	0
34	DMS	v	204	4/4	0.78	0.20	127,130,131,132	0
38	LHG	E	101	42/49	0.78	0.25	58,83,103,104	0
34	DMS	b	643	4/4	0.78	0.33	113,115,117,117	0
34	DMS	T	103	4/4	0.79	0.21	89,96,101,104	0
36	HTG	C	523	19/19	0.79	0.26	59,93,111,113	0
27	SQD	b	601	54/54	0.79	0.19	46,64,119,123	0
32	LMT	D	402	35/35	0.79	0.22	50,91,100,105	0
34	DMS	a	403	4/4	0.80	0.18	101,106,108,108	0
30	UNL	b	637	7/-	0.80	0.15	59,63,77,83	0
30	UNL	C	530	4/-	0.80	0.14	69,73,78,80	0
30	UNL	Y	101	16/-	0.80	0.25	75,81,88,88	0
30	UNL	c	525	10/-	0.80	0.27	65,70,85,89	0
32	LMT	m	102	35/35	0.80	0.19	33,59,77,79	0
30	UNL	I	102	7/-	0.81	0.15	66,69,73,74	0
30	UNL	E	103	10/-	0.81	0.19	70,73,77,78	0
34	DMS	A	425	4/4	0.81	0.25	113,114,116,117	0
30	UNL	m	101	8/-	0.81	0.22	48,50,54,58	0
30	UNL	B	637	6/-	0.82	0.20	69,71,75,79	0
34	DMS	V	210	4/4	0.82	0.18	123,123,125,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LMT	M	102	35/35	0.82	0.16	36,58,72,75	0
36	HTG	b	627	19/19	0.82	0.30	39,62,87,91	0
27	SQD	a	401	54/54	0.82	0.17	44,67,92,99	0
29	PL9	a	417	55/55	0.82	0.18	55,70,98,100	0
34	DMS	E	104	4/4	0.83	0.19	122,125,125,126	0
34	DMS	b	641	4/4	0.83	0.29	85,91,95,97	0
30	UNL	d	414	10/-	0.83	0.21	67,74,78,80	0
29	PL9	A	413	55/55	0.83	0.18	45,65,92,96	0
30	UNL	b	634	12/-	0.83	0.22	58,68,84,85	0
28	LMG	i	101	51/55	0.84	0.18	53,68,86,93	0
34	DMS	O	309	4/4	0.84	0.25	97,101,102,103	0
30	UNL	a	418	10/-	0.84	0.20	73,77,86,90	0
34	DMS	C	540	4/4	0.84	0.27	123,124,124,124	0
34	DMS	c	538	4/4	0.84	0.22	122,123,123,124	0
30	UNL	H	102	4/-	0.84	0.18	67,67,72,76	0
30	UNL	H	105	8/-	0.84	0.12	64,69,75,75	0
36	HTG	b	602	19/19	0.84	0.16	46,71,81,82	0
30	UNL	D	414	39/-	0.84	0.17	42,64,108,112	0
30	UNL	i	102	16/-	0.85	0.18	45,52,86,88	0
34	DMS	C	535	4/4	0.85	0.24	46,62,66,70	0
34	DMS	T	104	4/4	0.85	0.23	119,119,120,122	0
34	DMS	V	203	4/4	0.85	0.18	110,111,113,115	0
31	GOL	D	417	6/6	0.85	0.23	75,77,79,85	0
30	UNL	D	403	5/-	0.85	0.17	61,66,69,72	0
31	GOL	V	207	6/6	0.85	0.15	67,71,73,75	0
34	DMS	A	424	4/4	0.85	0.24	109,112,114,115	0
30	UNL	Z	103	5/-	0.85	0.19	58,67,76,78	0
31	GOL	b	639	6/6	0.85	0.36	41,60,66,74	0
31	GOL	v	203	6/6	0.85	0.16	65,73,75,85	0
27	SQD	A	415	54/54	0.86	0.15	39,58,89,92	0
34	DMS	C	538	4/4	0.86	0.34	96,97,101,107	0
27	SQD	f	802	43/54	0.86	0.24	59,85,114,121	0
28	LMG	B	623	51/55	0.86	0.14	34,50,66,71	0
30	UNL	A	419	8/-	0.86	0.15	62,71,73,74	0
30	UNL	J	104	6/-	0.86	0.12	57,58,60,62	0
30	UNL	C	502	4/-	0.87	0.16	67,67,68,69	0
30	UNL	b	635	7/-	0.87	0.14	49,51,57,57	0
34	DMS	c	529	4/4	0.87	0.24	87,99,100,101	0
30	UNL	B	636	6/-	0.87	0.21	67,69,69,71	0
36	HTG	B	629	19/19	0.87	0.14	44,80,103,108	0
30	UNL	c	527	6/-	0.87	0.15	76,77,78,78	0
36	HTG	C	522	19/19	0.87	0.20	75,88,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	LMG	A	412	51/55	0.87	0.15	51,66,85,92	0
34	DMS	b	633	4/4	0.87	0.14	78,79,87,91	0
30	UNL	k	104	8/-	0.87	0.15	63,67,77,81	0
28	LMG	C	521	51/55	0.88	0.18	34,66,96,101	0
30	UNL	A	416	3/-	0.88	0.09	68,68,72,74	0
30	UNL	z	102	6/-	0.88	0.18	77,79,79,80	0
34	DMS	O	307	4/4	0.88	0.30	93,98,99,102	0
34	DMS	C	537	4/4	0.88	0.18	91,93,94,95	0
34	DMS	a	425	4/4	0.88	0.18	79,91,92,99	0
26	BCR	d	407	40/40	0.88	0.12	32,40,69,72	0
30	UNL	b	636	4/-	0.88	0.09	61,63,66,66	0
30	UNL	e	101	10/-	0.88	0.12	64,67,69,70	0
28	LMG	c	521	51/55	0.89	0.15	39,69,95,97	0
34	DMS	c	534	4/4	0.89	0.31	108,111,112,114	0
34	DMS	c	536	4/4	0.89	0.27	105,108,108,109	0
30	UNL	B	627	14/-	0.89	0.16	50,56,68,70	0
30	UNL	U	201	5/-	0.89	0.14	52,55,68,73	0
28	LMG	d	412	51/55	0.89	0.13	33,45,84,94	0
30	UNL	l	101	13/-	0.89	0.17	42,51,74,75	0
30	UNL	I	101	16/-	0.90	0.15	39,54,68,70	0
31	GOL	a	419	6/6	0.90	0.15	53,57,60,64	0
36	HTG	V	202	12/19	0.90	0.23	51,59,78,102	0
34	DMS	B	643	4/4	0.90	0.22	87,92,94,95	0
30	UNL	d	403	32/-	0.90	0.15	45,62,113,118	0
30	UNL	A	420	6/-	0.90	0.16	31,50,66,74	0
24	CLA	B	603	65/65	0.90	0.12	33,47,99,108	0
40	RRX	h	101	41/41	0.90	0.10	29,46,55,66	0
28	LMG	b	624	51/55	0.91	0.12	35,50,61,74	0
27	SQD	F	101	43/54	0.91	0.19	47,81,103,107	0
36	HTG	O	303	19/19	0.91	0.12	36,44,56,60	0
30	UNL	d	413	14/-	0.91	0.12	40,50,58,63	0
34	DMS	b	642	4/4	0.91	0.16	101,102,104,105	0
34	DMS	B	642	4/4	0.91	0.36	95,96,98,101	0
24	CLA	b	620	65/65	0.91	0.13	28,38,101,102	0
24	CLA	b	605	65/65	0.91	0.14	39,50,99,105	0
30	UNL	C	526	6/-	0.92	0.09	64,68,77,79	0
34	DMS	u	202	4/4	0.92	0.16	86,88,88,90	0
31	GOL	d	415	6/6	0.92	0.20	47,58,64,67	0
31	GOL	A	421	6/6	0.92	0.18	62,81,86,87	0
24	CLA	B	618	65/65	0.92	0.14	24,34,96,96	0
34	DMS	V	211	4/4	0.92	0.16	102,102,102,102	0
24	CLA	C	515	65/65	0.92	0.12	38,50,90,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	DMS	a	423	4/4	0.92	0.21	91,92,95,102	0
36	HTG	o	301	19/19	0.92	0.13	39,48,52,59	0
27	SQD	a	415	54/54	0.92	0.14	38,53,94,97	0
30	UNL	V	205	5/-	0.92	0.30	57,62,63,74	0
34	DMS	d	418	4/4	0.92	0.20	80,89,93,93	0
26	BCR	D	407	40/40	0.92	0.11	28,36,67,69	0
34	DMS	o	303	4/4	0.92	0.28	105,109,109,110	0
24	CLA	C	514	65/65	0.93	0.10	37,47,79,81	0
28	LMG	D	413	51/55	0.93	0.12	29,39,100,108	0
34	DMS	e	103	4/4	0.93	0.27	96,98,98,100	0
34	DMS	h	107	4/4	0.93	0.31	125,127,128,129	0
24	CLA	c	514	65/65	0.93	0.10	39,47,78,82	0
30	UNL	T	102	7/-	0.93	0.22	52,60,79,80	0
34	DMS	B	634	4/4	0.93	0.14	78,80,81,83	0
26	BCR	C	516	40/40	0.93	0.09	40,46,51,52	0
34	DMS	v	202	4/4	0.93	0.20	97,97,103,108	0
34	DMS	B	640	4/4	0.93	0.18	107,110,112,114	0
34	DMS	c	539	4/4	0.93	0.25	77,79,80,89	0
24	CLA	D	406	65/65	0.94	0.10	26,34,98,102	0
34	DMS	c	531	4/4	0.94	0.28	92,93,94,97	0
24	CLA	c	515	65/65	0.94	0.11	42,54,86,92	0
26	BCR	B	621	40/40	0.94	0.08	29,35,46,50	0
24	CLA	B	608	65/65	0.94	0.09	23,32,67,71	0
26	BCR	C	517	40/40	0.94	0.10	31,42,53,56	0
24	CLA	b	610	65/65	0.94	0.09	26,35,83,91	0
34	DMS	V	208	4/4	0.94	0.31	76,81,83,84	0
31	GOL	C	525	6/6	0.94	0.15	38,43,58,63	0
26	BCR	K	101	40/40	0.94	0.09	35,41,47,49	0
26	BCR	K	102	40/40	0.94	0.12	32,39,47,51	0
26	BCR	a	414	40/40	0.94	0.08	23,31,38,41	0
30	UNL	C	531	10/-	0.94	0.24	70,73,94,97	0
26	BCR	c	516	40/40	0.94	0.09	47,54,64,65	0
34	DMS	a	426	4/4	0.94	0.13	105,106,106,107	0
26	BCR	c	517	40/40	0.94	0.10	32,41,49,50	0
37	DGD	C	519	62/66	0.94	0.11	29,38,88,97	0
37	DGD	H	104	62/66	0.94	0.11	26,37,47,57	0
37	DGD	c	519	62/66	0.94	0.10	34,43,90,100	0
24	CLA	C	508	65/65	0.94	0.09	38,47,94,101	0
37	DGD	h	102	62/66	0.94	0.10	30,38,51,59	0
26	BCR	t	101	40/40	0.94	0.09	23,34,47,52	0
27	SQD	A	411	54/54	0.94	0.12	40,53,86,87	0
40	RRX	H	103	41/41	0.94	0.08	27,41,53,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	c	508	65/65	0.94	0.09	36,47,88,92	0
33	BCT	d	402[B]	4/4	0.95	0.11	28,31,36,38	4
37	DGD	c	518	62/66	0.95	0.09	29,37,85,91	0
26	BCR	B	620	40/40	0.95	0.08	24,32,56,63	0
34	DMS	o	304	4/4	0.95	0.18	98,102,102,102	0
24	CLA	a	411	65/65	0.95	0.10	23,30,89,94	0
38	LHG	D	410	49/49	0.95	0.10	24,38,53,61	0
26	BCR	b	622	40/40	0.95	0.08	23,32,49,52	0
26	BCR	k	102	40/40	0.95	0.08	36,43,54,57	0
38	LHG	d	409	49/49	0.95	0.11	30,42,52,55	0
30	UNL	x	101	11/-	0.95	0.20	40,44,63,64	0
37	DGD	C	520	62/66	0.95	0.10	25,36,71,82	0
34	DMS	D	418	4/4	0.96	0.19	71,78,84,86	0
26	BCR	T	101	40/40	0.96	0.07	23,33,46,49	0
24	CLA	b	614	65/65	0.96	0.07	25,33,40,51	0
29	PL9	D	408	55/55	0.96	0.09	19,27,35,39	0
24	CLA	b	616	65/65	0.96	0.08	24,29,40,44	0
29	PL9	d	408	55/55	0.96	0.08	21,27,36,45	0
26	BCR	b	623	40/40	0.96	0.08	28,37,51,53	0
24	CLA	b	618	65/65	0.96	0.08	20,29,78,85	0
24	CLA	b	619	65/65	0.96	0.08	26,35,53,57	0
24	CLA	C	511	65/65	0.96	0.09	30,38,58,63	0
24	CLA	c	503	65/65	0.96	0.08	31,41,53,61	0
26	BCR	k	103	40/40	0.96	0.10	35,46,55,59	0
34	DMS	V	209	4/4	0.96	0.21	95,97,98,103	0
24	CLA	c	505	65/65	0.96	0.08	34,41,49,67	0
24	CLA	c	506	65/65	0.96	0.08	30,37,84,89	0
24	CLA	C	513	65/65	0.96	0.09	29,40,46,50	0
24	CLA	c	509	65/65	0.96	0.09	31,38,59,65	0
24	CLA	c	510	65/65	0.96	0.09	27,35,96,109	0
24	CLA	c	512	65/65	0.96	0.08	28,37,50,58	0
24	CLA	c	513	65/65	0.96	0.08	33,41,52,54	0
34	DMS	b	632	4/4	0.96	0.11	70,74,76,84	0
24	CLA	B	616	65/65	0.96	0.09	21,29,80,89	0
30	UNL	t	102	8/-	0.96	0.16	50,57,68,71	0
24	CLA	A	409	65/65	0.96	0.09	23,31,98,103	0
24	CLA	d	406	65/65	0.96	0.09	31,38,92,94	0
25	PHO	A	408	64/64	0.96	0.09	21,27,35,41	0
26	BCR	A	410	40/40	0.96	0.08	24,30,37,38	0
34	DMS	c	530	4/4	0.96	0.27	73,76,80,83	0
26	BCR	B	619	40/40	0.96	0.07	21,30,37,39	0
34	DMS	c	533	4/4	0.96	0.15	96,97,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	C	505	65/65	0.96	0.07	29,36,44,51	0
37	DGD	c	520	62/66	0.96	0.08	31,40,68,76	0
24	CLA	C	506	65/65	0.96	0.08	26,32,71,77	0
24	CLA	a	413	65/65	0.96	0.10	25,32,90,93	0
24	CLA	B	611	65/65	0.96	0.10	26,33,40,44	0
38	LHG	D	412	45/49	0.96	0.09	29,34,56,60	0
34	DMS	C	536	4/4	0.96	0.24	58,60,65,69	0
30	UNL	D	415	15/-	0.96	0.11	41,45,53,59	0
24	CLA	b	606	65/65	0.96	0.08	27,35,45,51	0
24	CLA	C	510	65/65	0.96	0.08	25,33,94,111	0
24	CLA	b	613	65/65	0.96	0.10	30,36,43,60	0
24	CLA	C	503	65/65	0.97	0.07	29,37,51,59	0
24	CLA	c	511	65/65	0.97	0.09	30,40,59,62	0
24	CLA	C	504	65/65	0.97	0.07	26,33,45,50	0
24	CLA	B	606	65/65	0.97	0.08	19,27,64,70	0
24	CLA	B	607	65/65	0.97	0.08	22,28,39,45	0
24	CLA	b	607	65/65	0.97	0.07	25,33,42,44	0
24	CLA	b	608	65/65	0.97	0.08	21,28,64,70	0
24	CLA	b	609	65/65	0.97	0.08	22,29,40,45	0
25	PHO	a	412	64/64	0.97	0.08	20,26,30,31	0
34	DMS	c	532	4/4	0.97	0.14	43,53,53,63	0
24	CLA	C	507	65/65	0.97	0.07	27,36,61,65	0
24	CLA	b	611	65/65	0.97	0.07	21,27,39,44	0
34	DMS	c	535	4/4	0.97	0.18	63,65,67,68	0
24	CLA	A	405	65/65	0.97	0.08	18,24,33,45	0
24	CLA	C	509	65/65	0.97	0.07	31,38,57,61	0
24	CLA	b	615	65/65	0.97	0.07	21,27,47,51	0
37	DGD	C	518	62/66	0.97	0.08	26,32,87,94	0
31	GOL	A	418	6/6	0.97	0.17	56,62,66,76	0
24	CLA	B	609	65/65	0.97	0.07	17,27,40,50	0
24	CLA	A	406	65/65	0.97	0.08	20,26,97,101	0
24	CLA	C	512	65/65	0.97	0.07	28,34,45,51	0
33	BCT	A	423[B]	4/4	0.97	0.10	23,31,38,38	4
33	BCT	D	404[A]	4/4	0.97	0.10	27,35,36,41	4
33	BCT	a	408[A]	4/4	0.97	0.10	25,35,36,36	4
24	CLA	B	612	65/65	0.97	0.08	24,29,45,53	0
24	CLA	B	604	65/65	0.97	0.07	24,32,37,44	0
24	CLA	B	617	65/65	0.97	0.07	25,32,53,59	0
34	DMS	B	633	4/4	0.97	0.11	58,61,66,68	0
38	LHG	L	101	49/49	0.97	0.10	27,34,55,59	0
24	CLA	D	405	65/65	0.97	0.08	17,23,44,47	0
24	CLA	c	507	65/65	0.97	0.07	29,35,61,73	0

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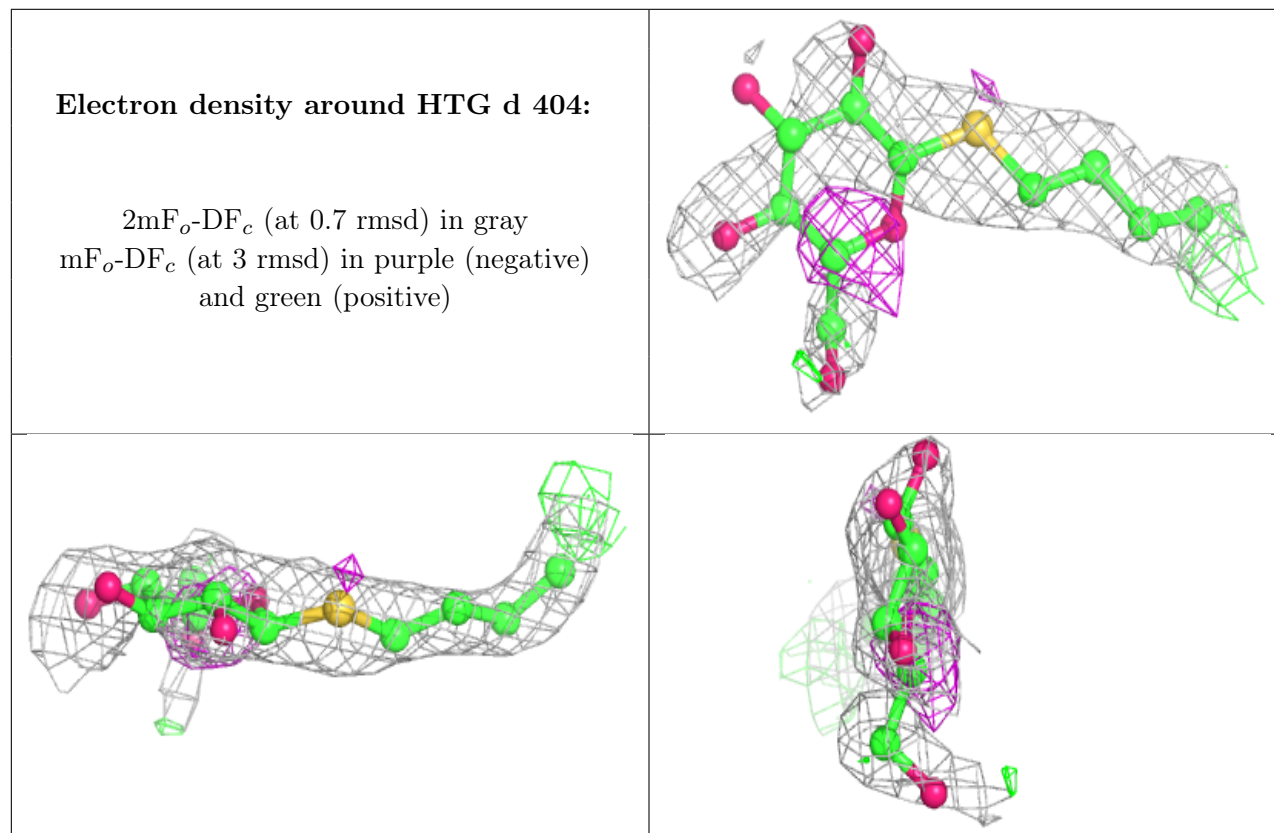
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	LHG	d	410	49/49	0.97	0.10	26,32,59,68	0
38	LHG	d	411	46/49	0.97	0.10	32,36,67,74	0
38	LHG	l	102	49/49	0.97	0.09	25,35,56,64	0
39	HEM	e	102	43/43	0.97	0.09	39,50,74,89	0
24	CLA	B	605	65/65	0.97	0.07	24,30,39,42	0
24	CLA	a	409	65/65	0.97	0.09	21,26,40,51	0
41	MG	j	101	1/1	0.97	0.14	43,43,43,43	0
42	HEC	v	201	43/43	0.97	0.09	35,40,45,49	0
24	CLA	B	615	65/65	0.98	0.06	19,26,56,63	0
25	PHO	A	407	64/64	0.98	0.07	19,25,28,31	0
24	CLA	b	617	65/65	0.98	0.07	21,27,64,71	0
24	CLA	D	401	65/65	0.98	0.06	16,22,30,43	0
26	BCR	b	621	40/40	0.98	0.06	22,31,40,42	0
38	LHG	D	411	49/49	0.98	0.10	22,32,48,55	0
25	PHO	d	401	64/64	0.98	0.09	24,31,37,40	0
24	CLA	B	610	65/65	0.98	0.07	23,30,38,45	0
24	CLA	b	612	65/65	0.98	0.06	25,31,42,48	0
24	CLA	B	613	65/65	0.98	0.07	18,26,43,50	0
35	CA	O	301	1/1	0.98	0.04	58,58,58,58	0
35	CA	b	604	1/1	0.98	0.15	52,52,52,52	0
35	CA	c	502	1/1	0.98	0.06	49,49,49,49	0
35	CA	o	302	1/1	0.98	0.06	57,57,57,57	0
39	HEM	F	102	43/43	0.98	0.08	37,44,54,60	0
24	CLA	c	504	65/65	0.98	0.07	27,36,48,55	0
34	DMS	d	417	4/4	0.98	0.11	69,74,75,78	0
24	CLA	B	614	65/65	0.98	0.07	21,28,35,41	0
24	CLA	a	410	65/65	0.98	0.06	20,25,38,45	0
42	HEC	V	201	43/43	0.98	0.07	27,31,36,40	0
24	CLA	d	405	65/65	0.98	0.08	20,26,48,57	0
34	DMS	B	632	4/4	0.99	0.05	25,28,32,37	0
34	DMS	O	305	4/4	0.99	0.05	29,35,37,44	0
34	DMS	C	534	4/4	0.99	0.06	45,45,48,51	0
41	MG	J	101	1/1	0.99	0.02	34,34,34,34	0
34	DMS	a	422	4/4	0.99	0.06	29,35,39,45	0
34	DMS	b	631	4/4	0.99	0.06	29,34,36,40	0
35	CA	B	602	1/1	0.99	0.20	53,53,53,53	0
22	FE2	A	402	1/1	1.00	0.03	30,30,30,30	0
22	FE2	a	405	1/1	1.00	0.04	31,31,31,31	0
23	CL	A	403	1/1	1.00	0.04	27,27,27,27	0
23	CL	A	404	1/1	1.00	0.05	28,28,28,28	0
23	CL	a	406	1/1	1.00	0.03	31,31,31,31	0
23	CL	a	407	1/1	1.00	0.05	33,33,33,33	0

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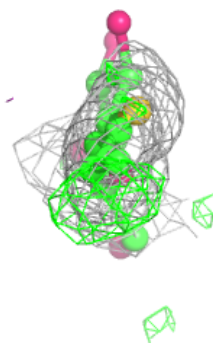
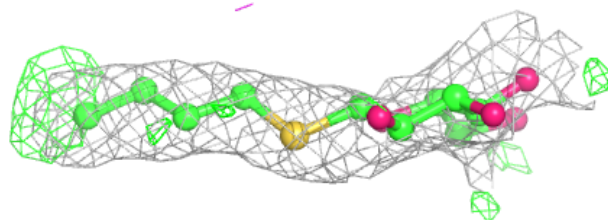
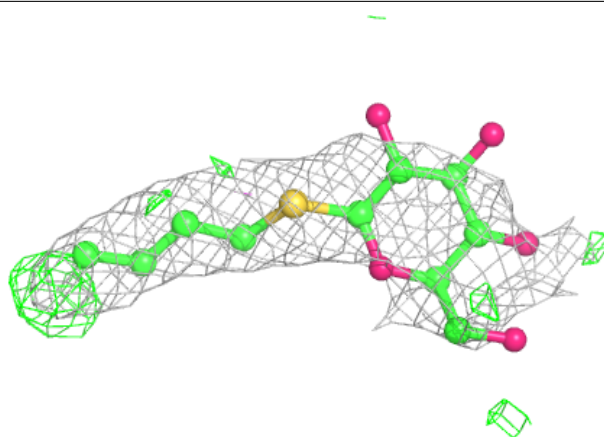
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	OEX	A	401	10/10	1.00	0.04	24,27,29,31	0
21	OEX	a	404	10/10	1.00	0.03	27,30,31,32	0

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.

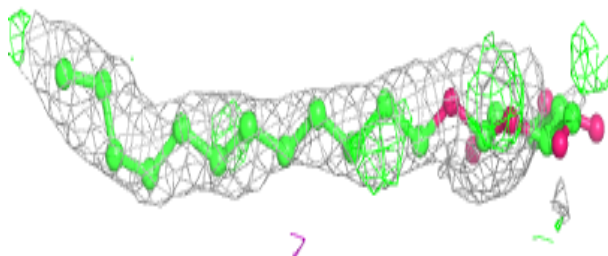
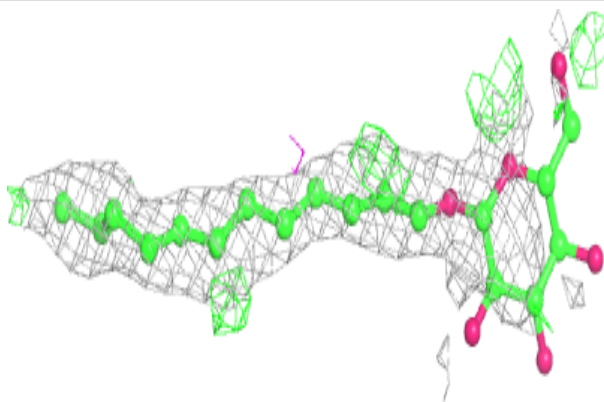


Electron density around HTG H 101:

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

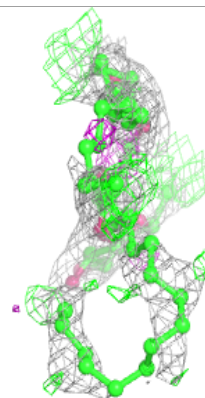
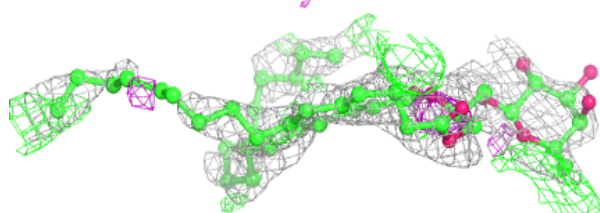
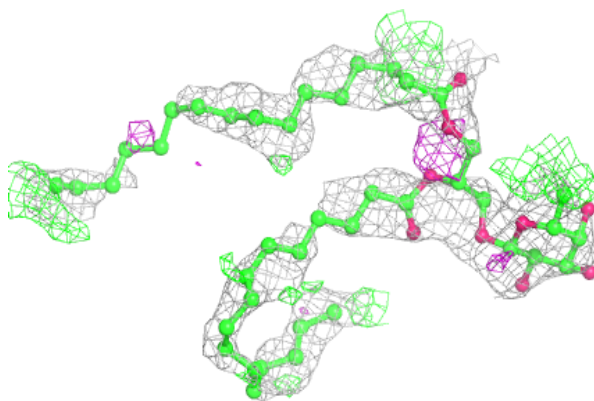
**Electron density around LMT j 102:**

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

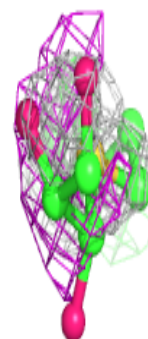
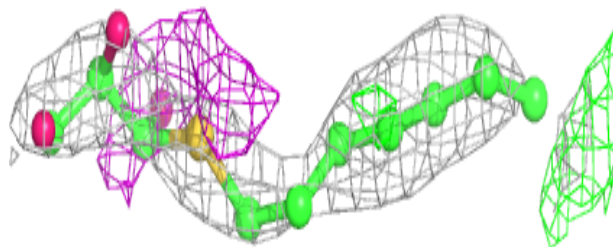
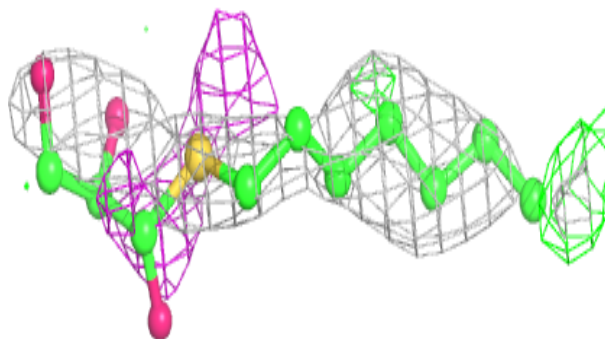


Electron density around DGD d 416:

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

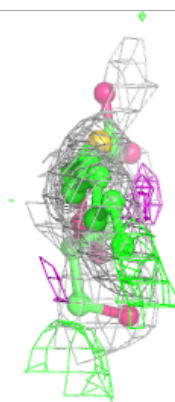
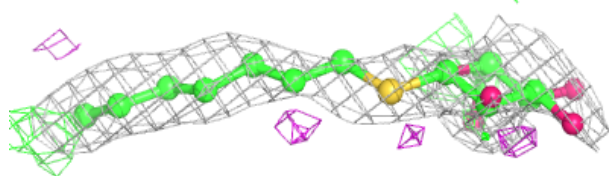
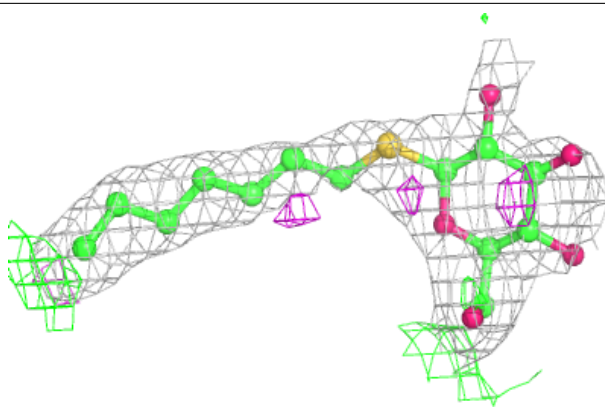
**Electron density around HTG u 201:**

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

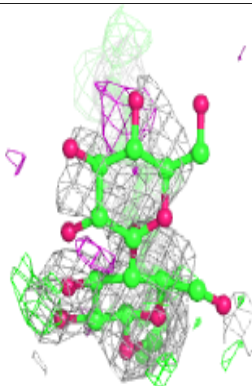
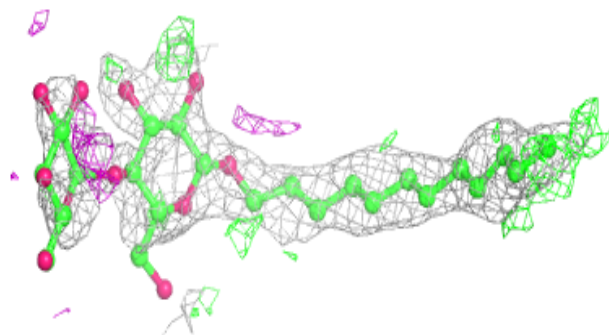
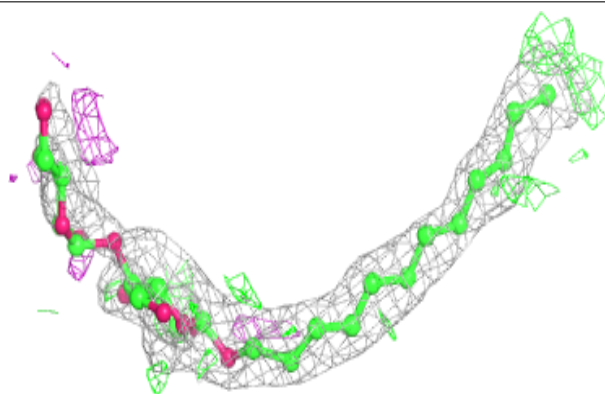


Electron density around HTG B 630:

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

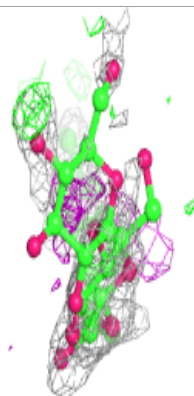
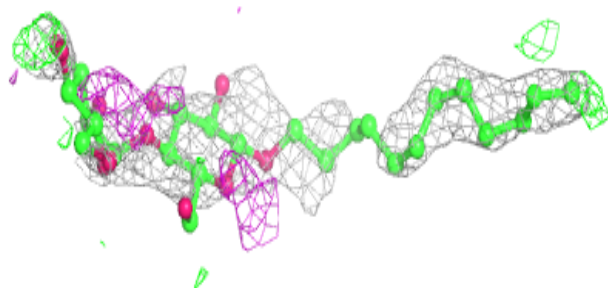
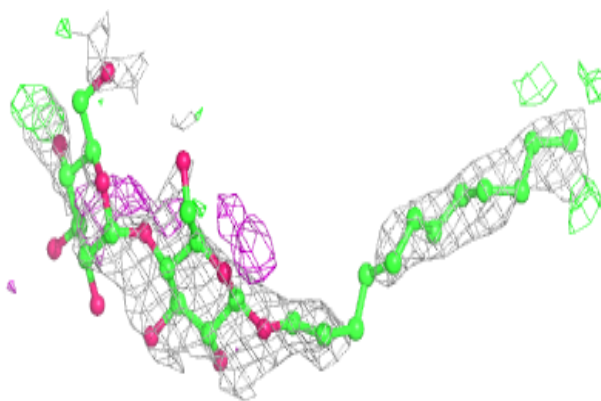
**Electron density around LMT M 101:**

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

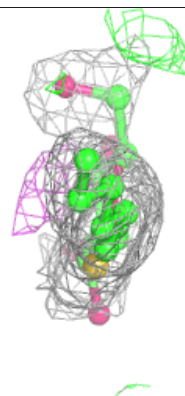
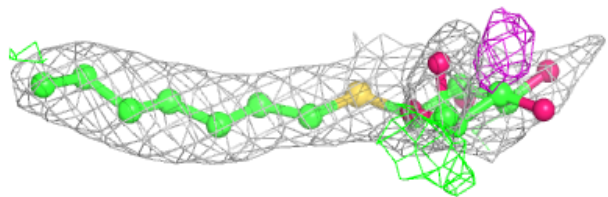
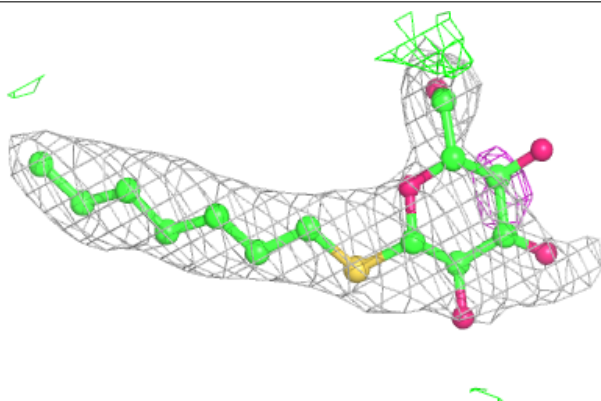


Electron density around LMT F 103:

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

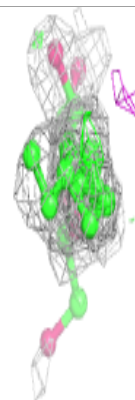
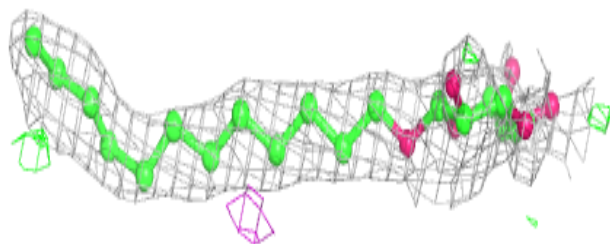
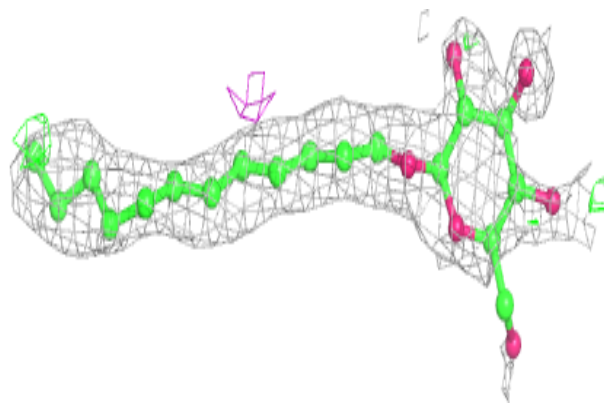
**Electron density around HTG b 603:**

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

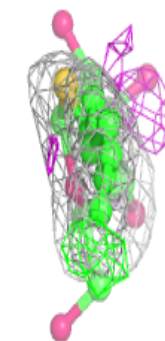
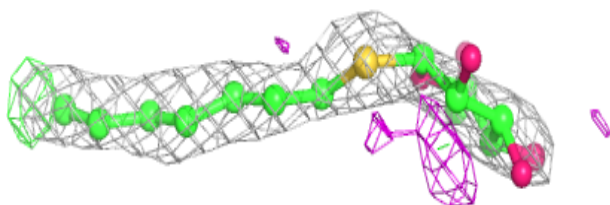
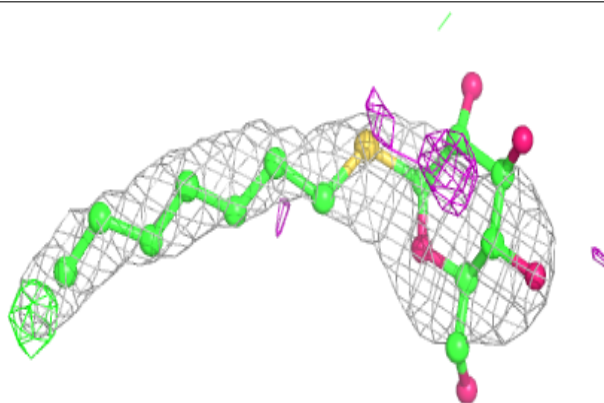


Electron density around LMT J 102:

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

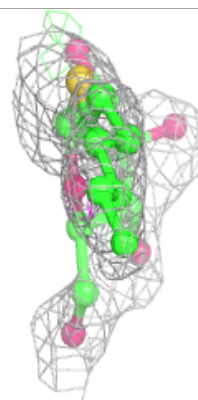
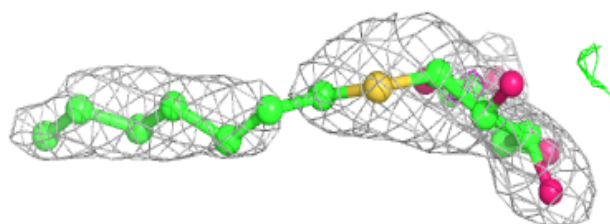
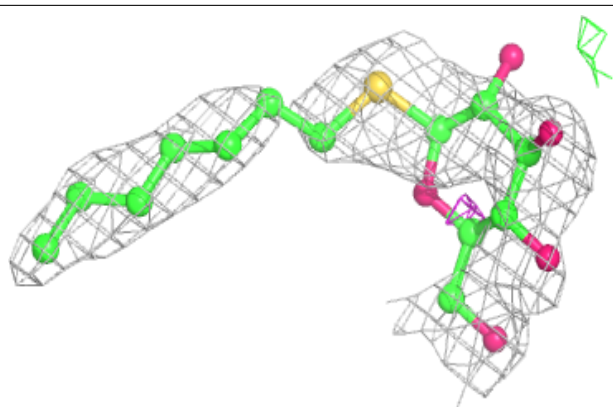
**Electron density around HTG B 626:**

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

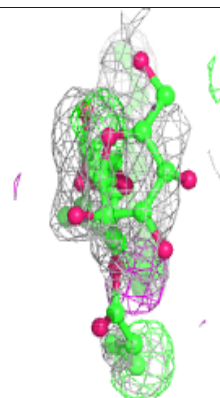
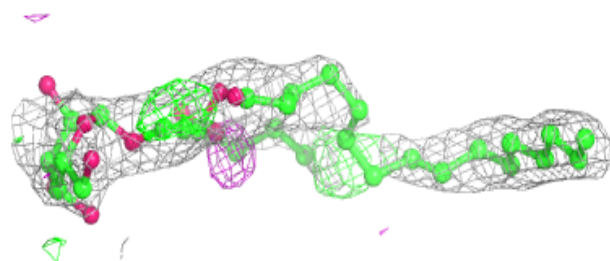
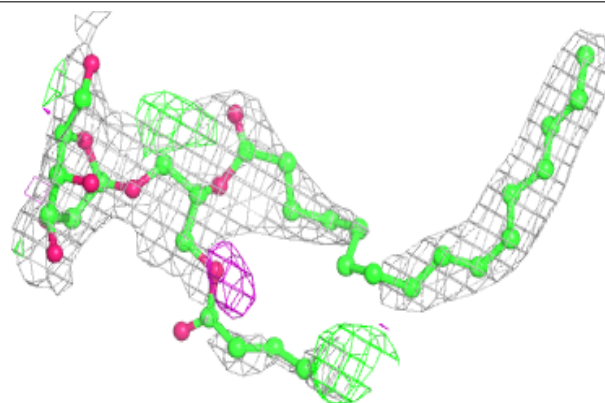


Electron density around HTG b 628:

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

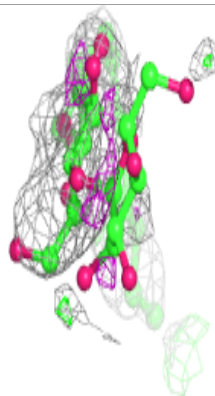
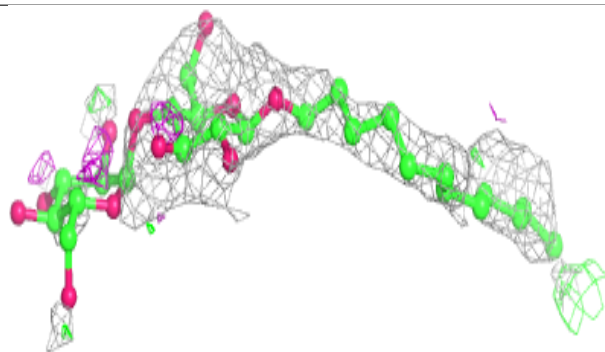
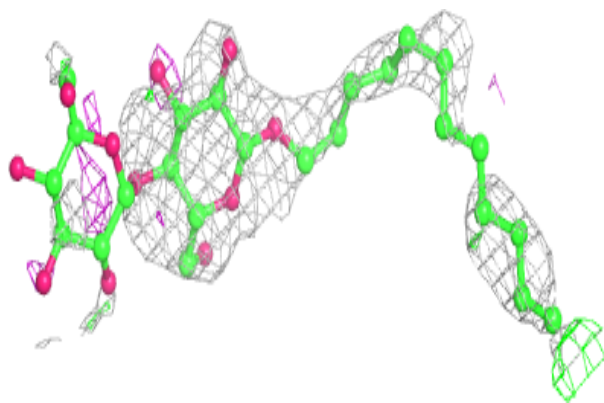
**Electron density around LMG Z 101:**

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

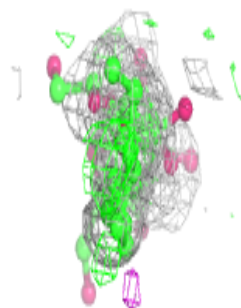
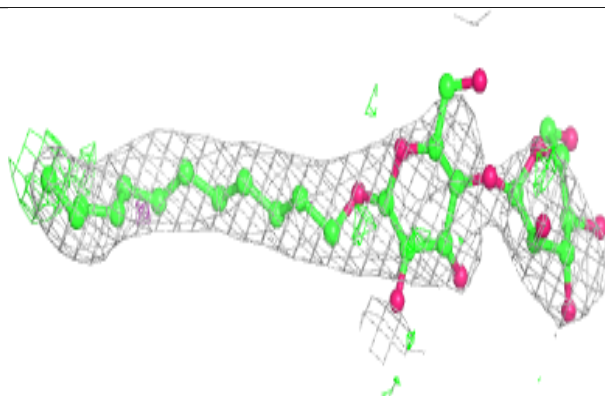
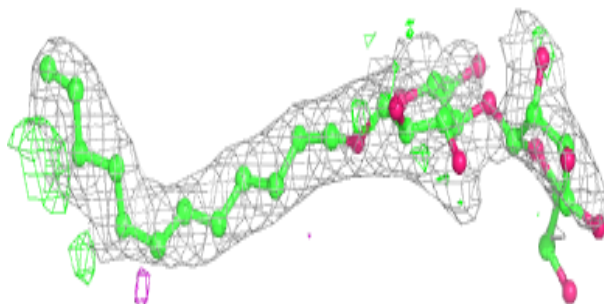


Electron density around LMT a 421:

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

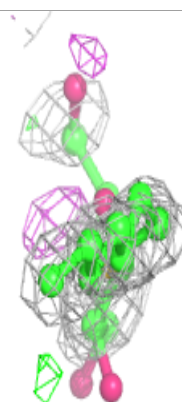
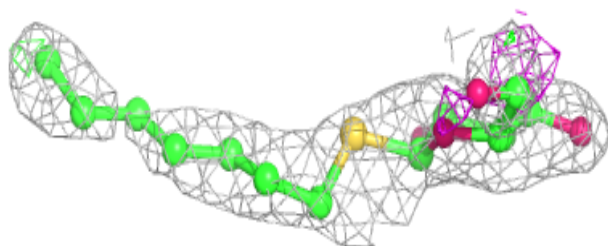
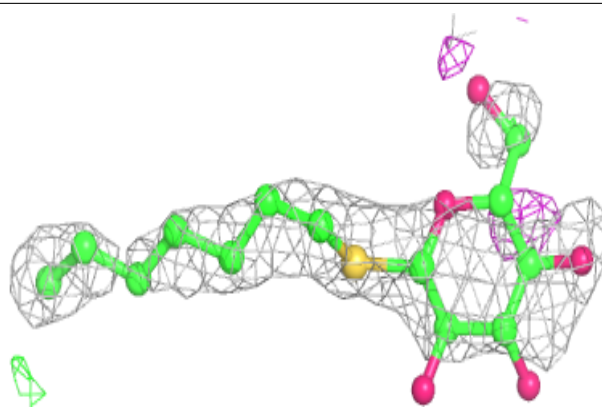
**Electron density around LMT B 638:**

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

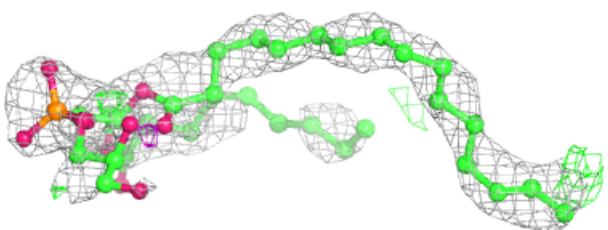
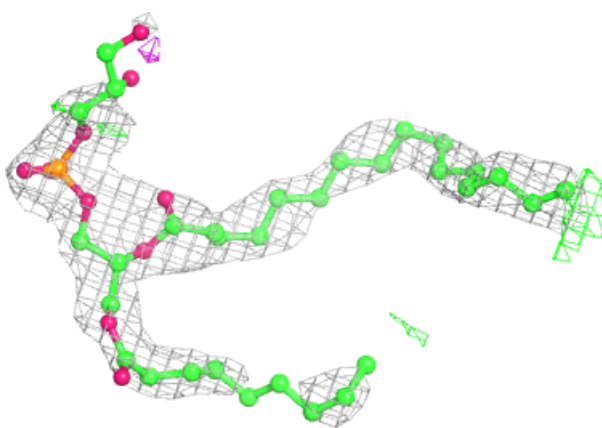


Electron density around HTG c 524:

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

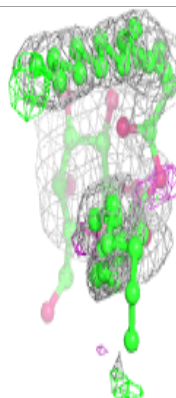
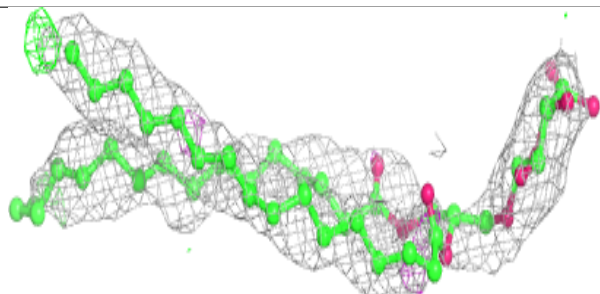
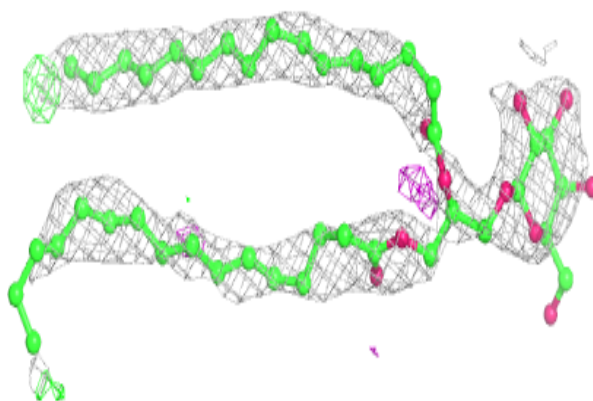
**Electron density around LHG a 416:**

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

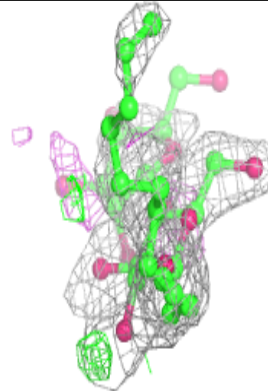
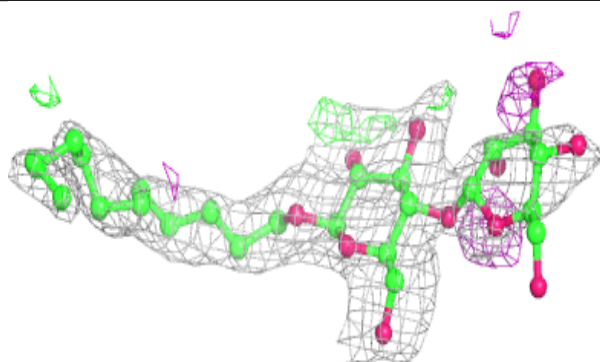
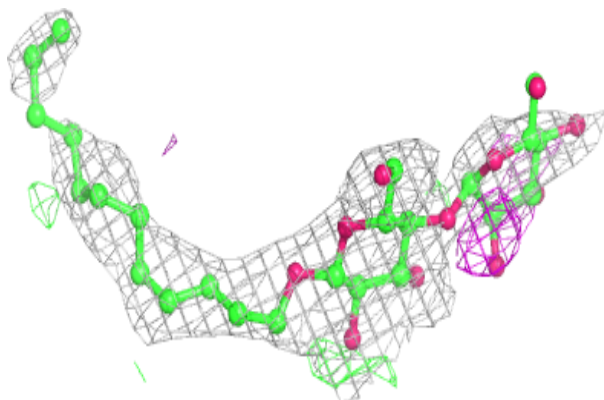


Electron density around LMG c 522:

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

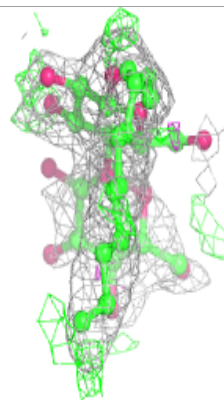
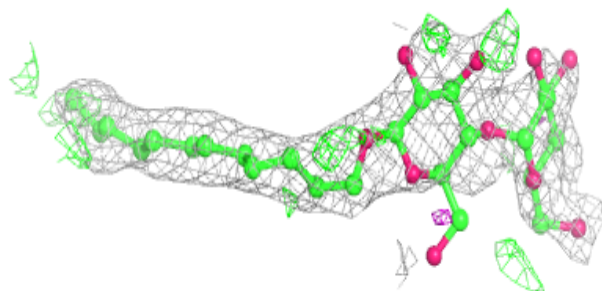
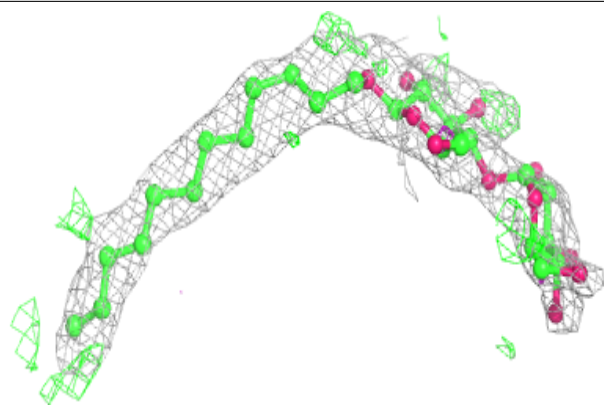
**Electron density around LMT D 409:**

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

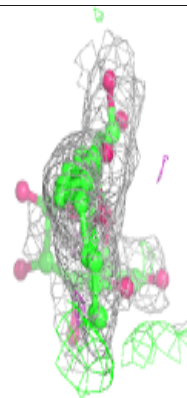
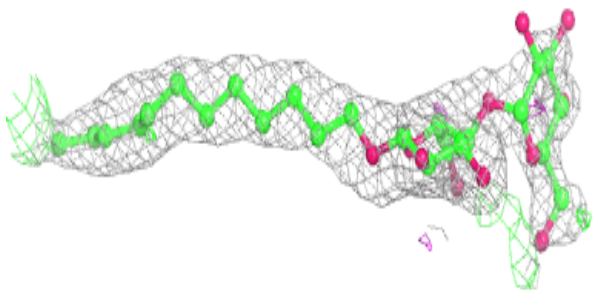
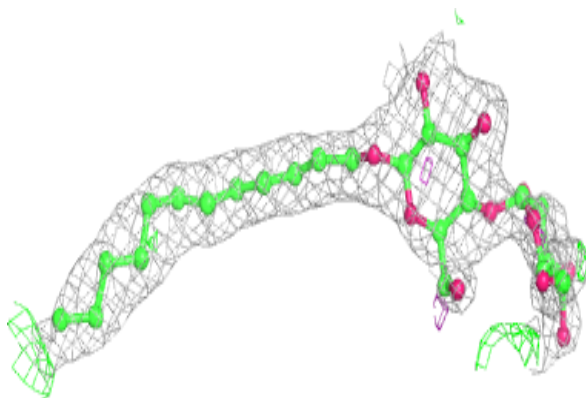


Electron density around LMT m 103:

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

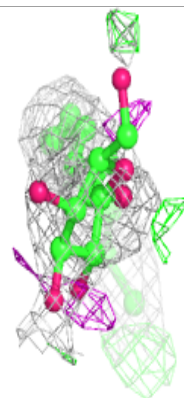
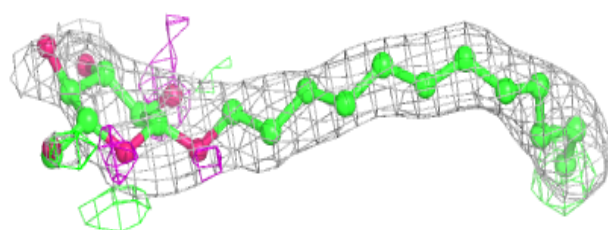
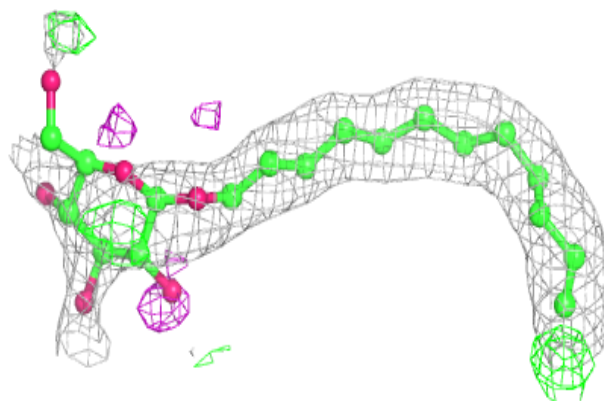
**Electron density around LMT B 624:**

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

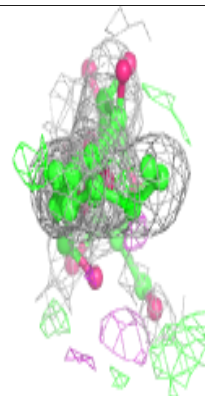
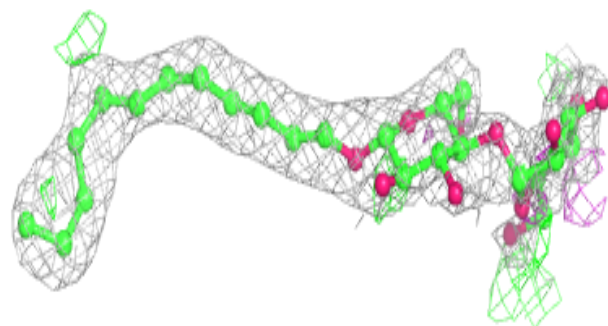
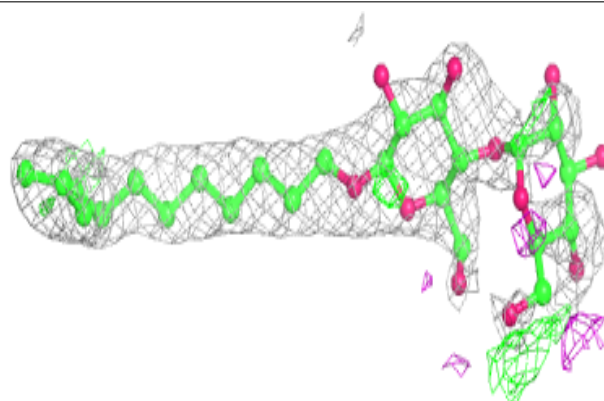


Electron density around LMT b 629:

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

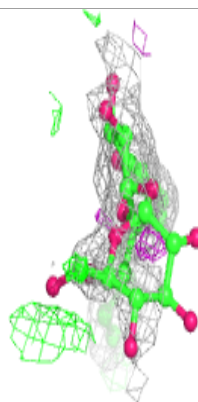
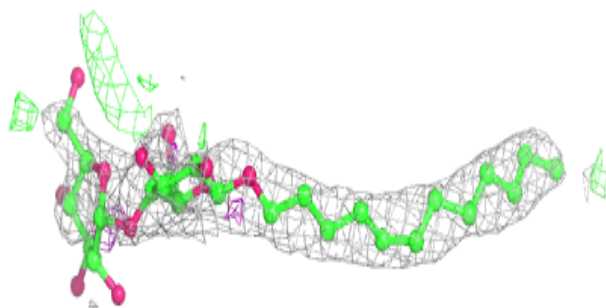
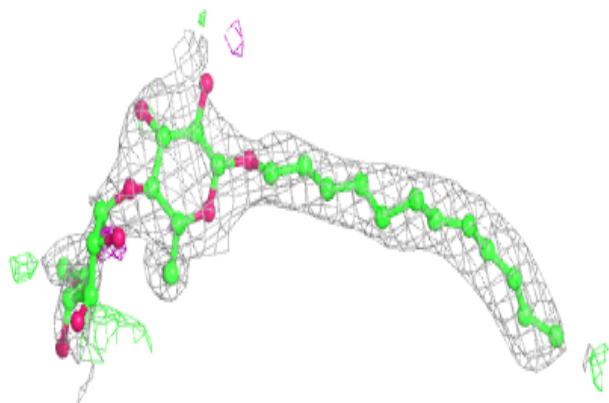
**Electron density around LMT b 626:**

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

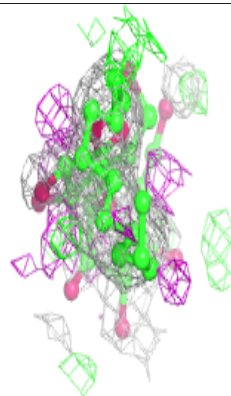
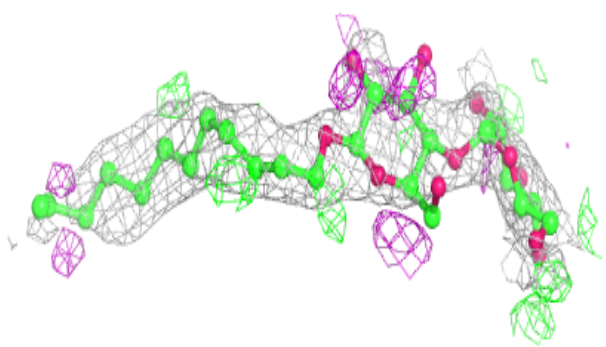
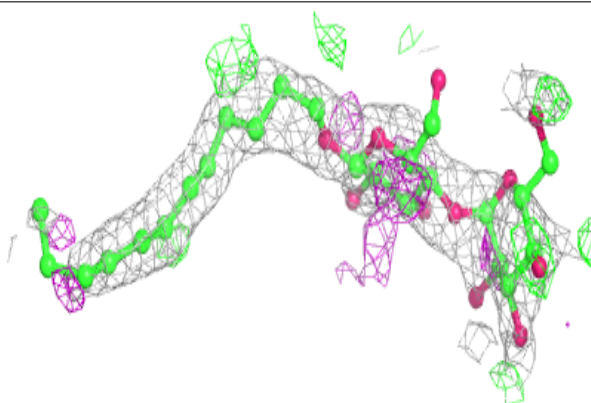


Electron density around LMT b 625:

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

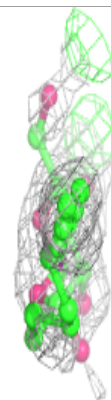
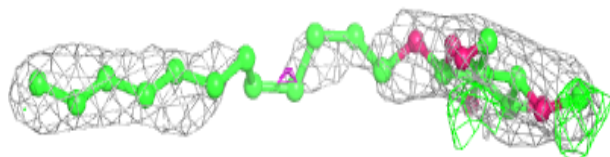
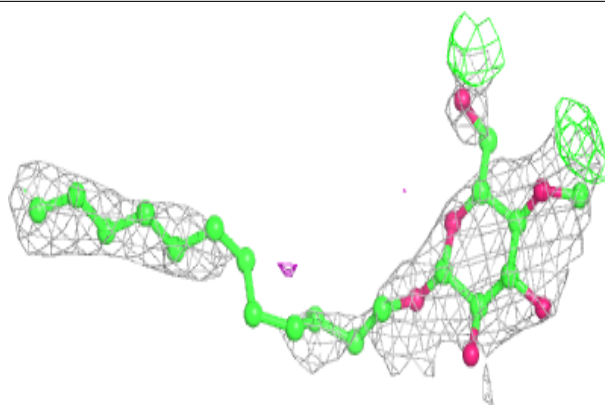
**Electron density around LMT a 402:**

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

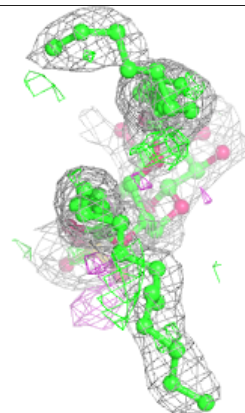
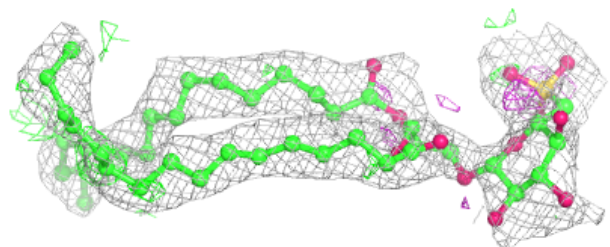
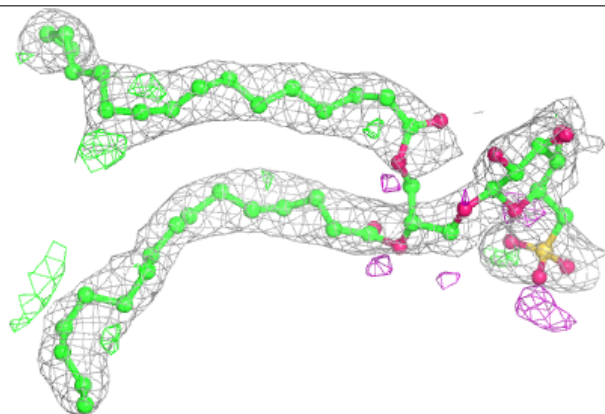


Electron density around LMT f 801:

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

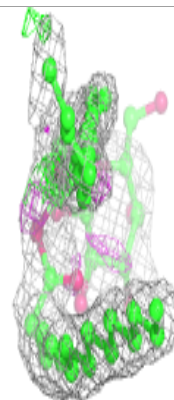
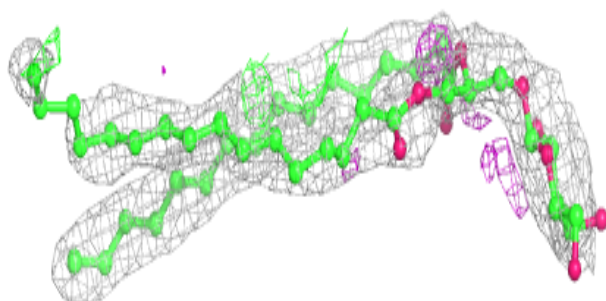
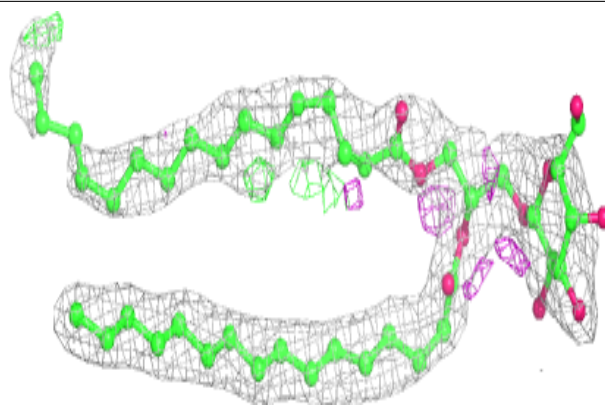
**Electron density around SQD B 622:**

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

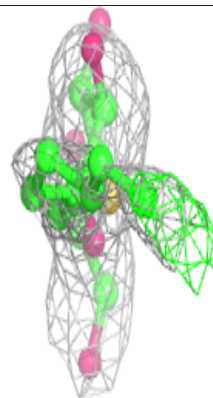
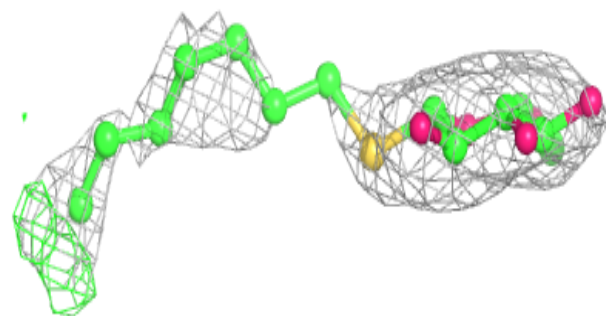
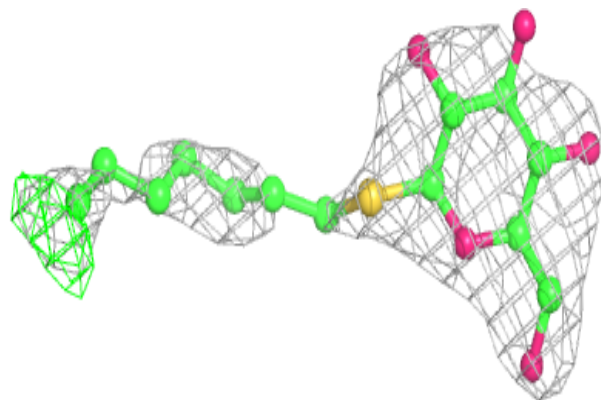


Electron density around LMG C 533:

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

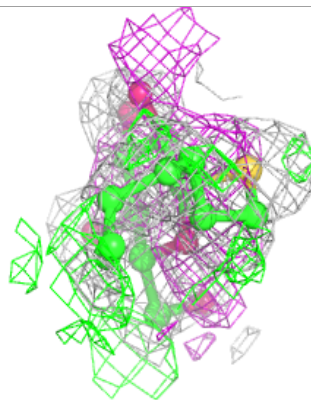
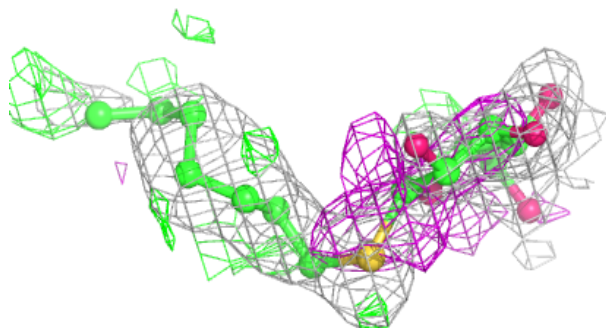
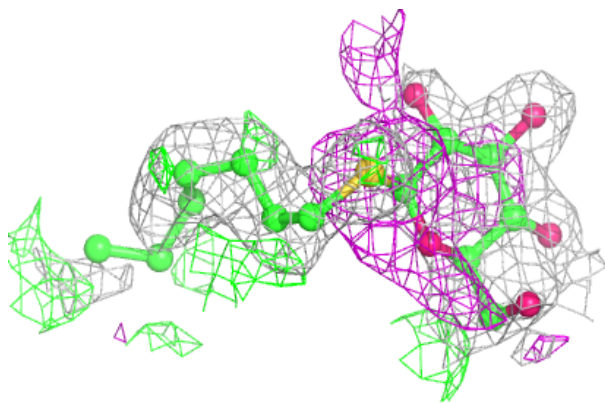
**Electron density around HTG c 523:**

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

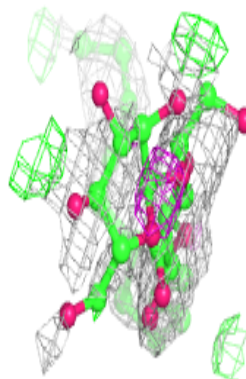
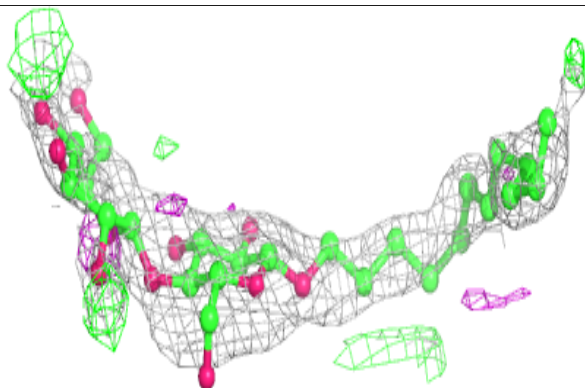
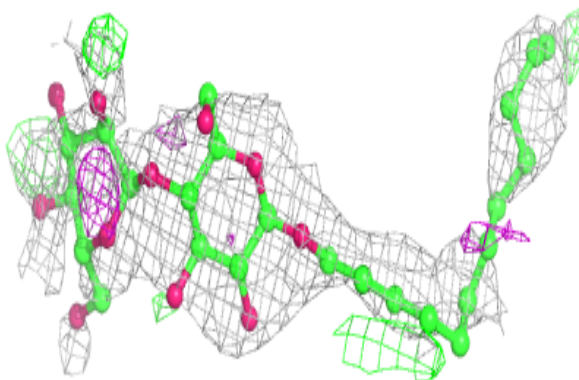


Electron density around HTG B 625:

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

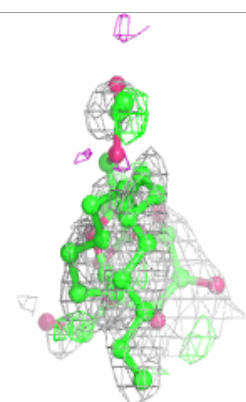
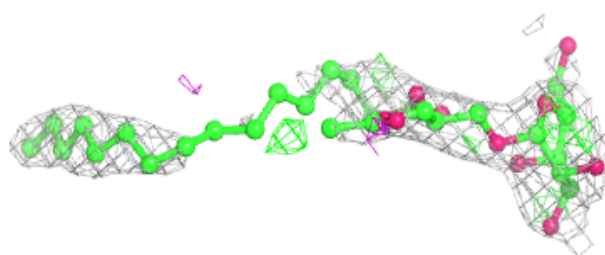
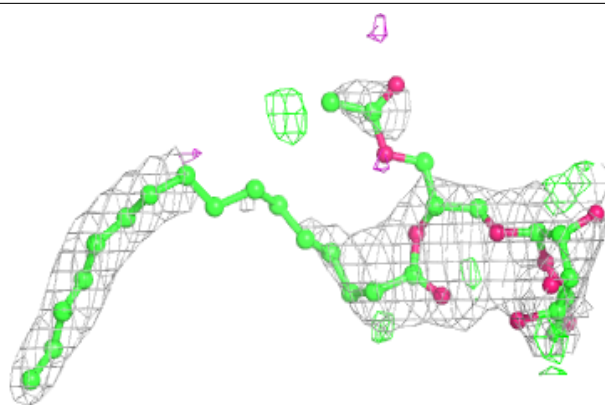
**Electron density around LMT A 422:**

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

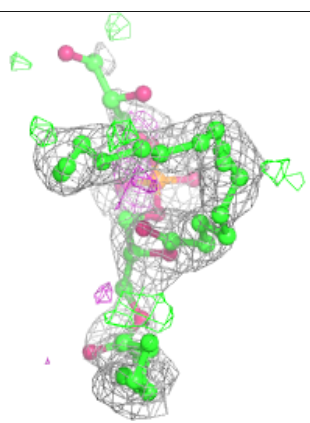
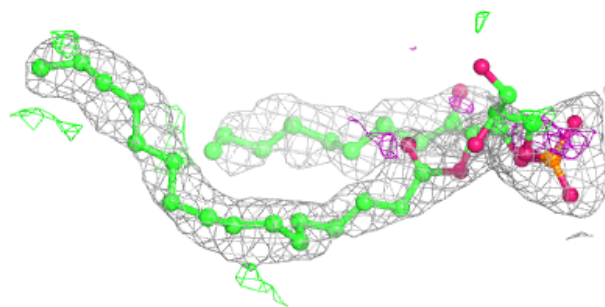
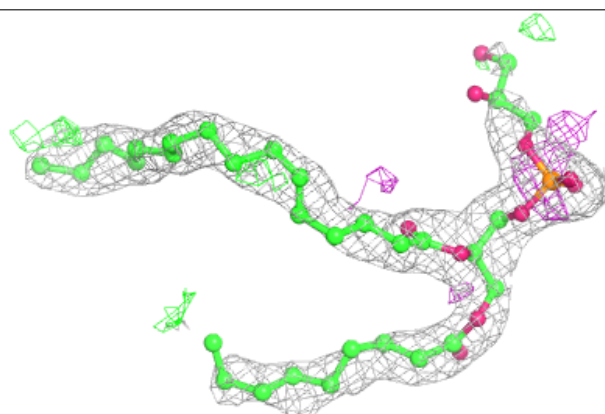


Electron density around LMG z 101:

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

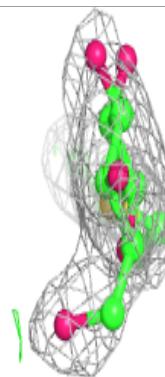
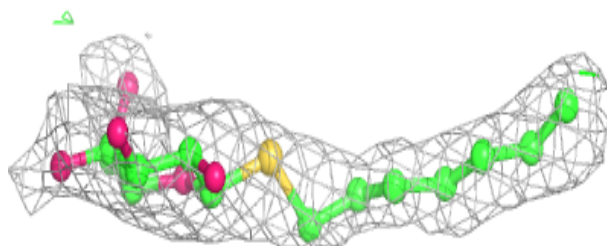
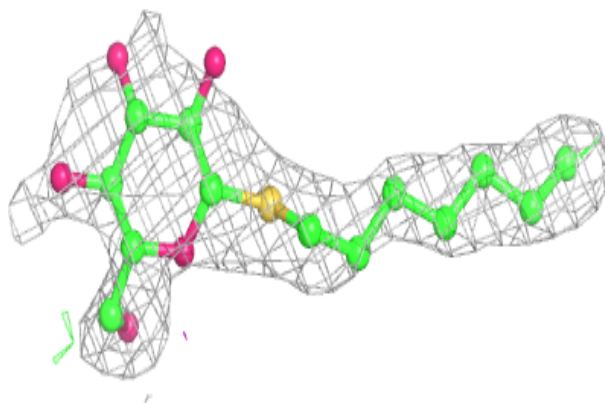
**Electron density around LHG E 101:**

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

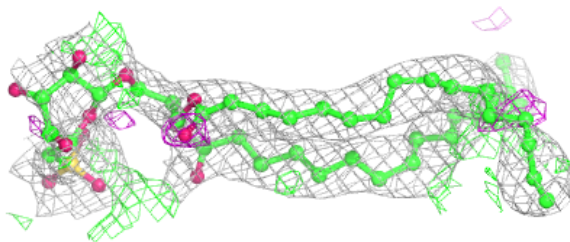
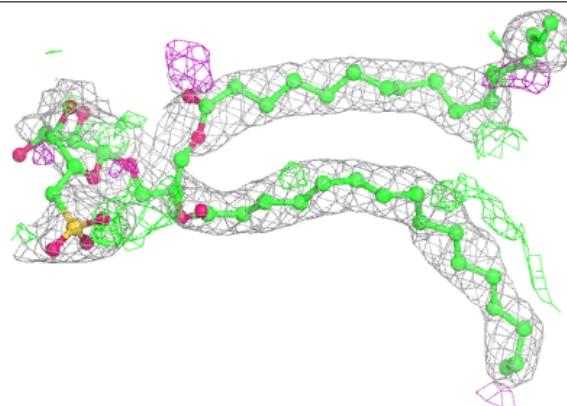


Electron density around HTG C 523:

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

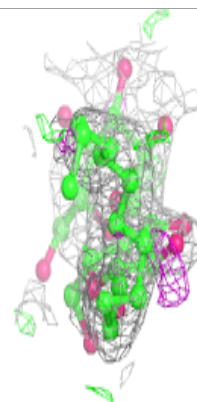
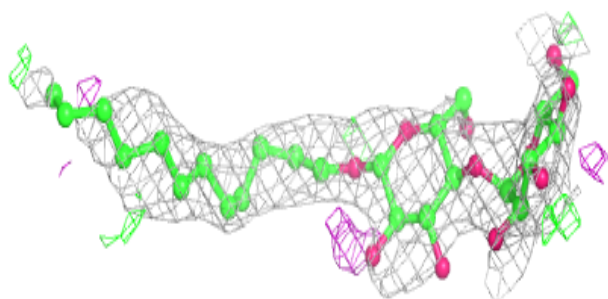
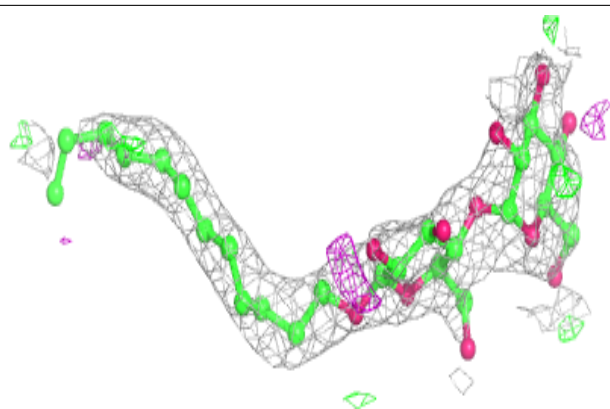
**Electron density around SQD b 601:**

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

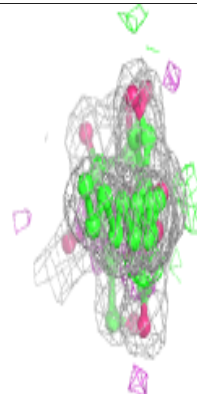
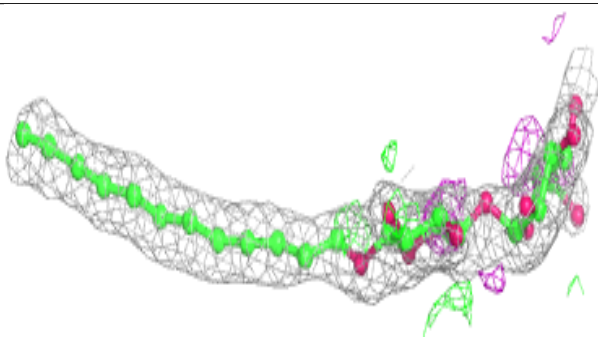
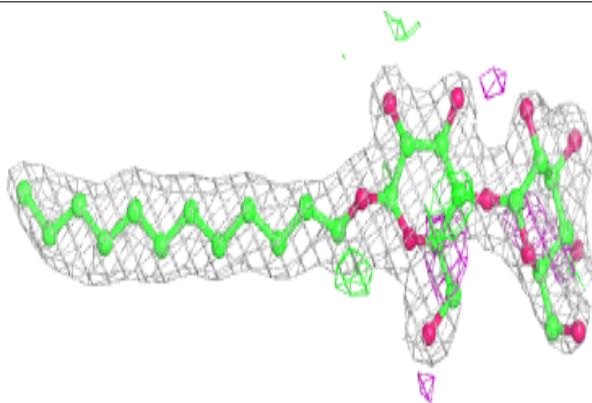


Electron density around LMT D 402:

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

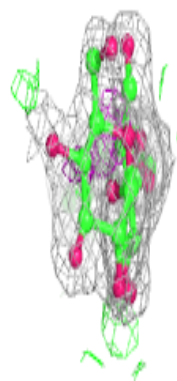
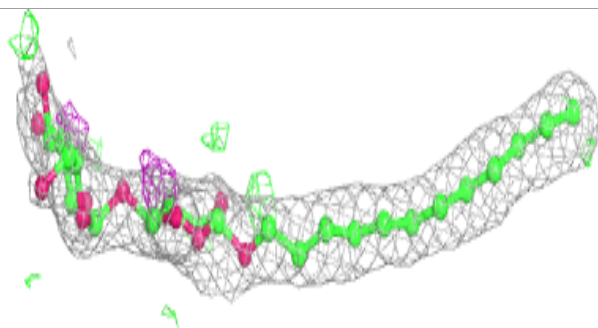
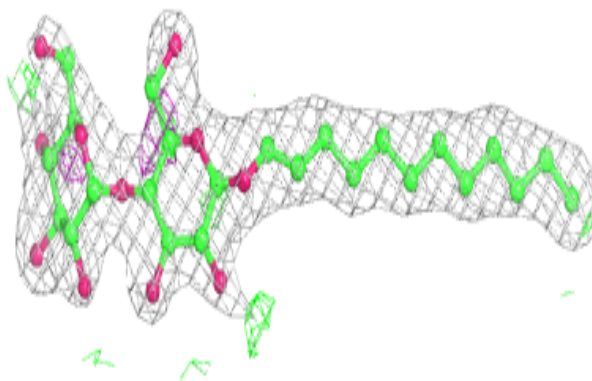
**Electron density around LMT m 102:**

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

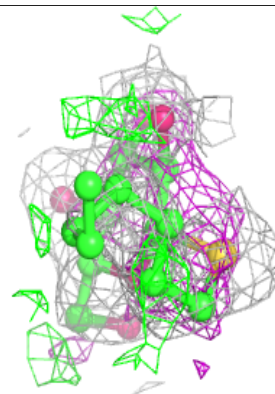
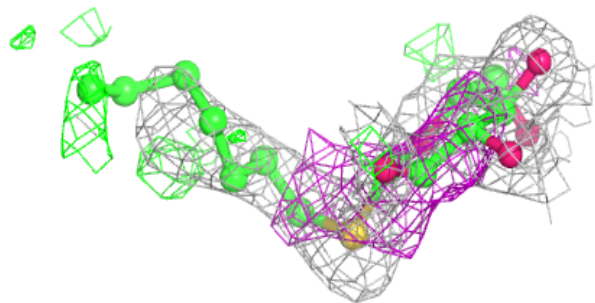
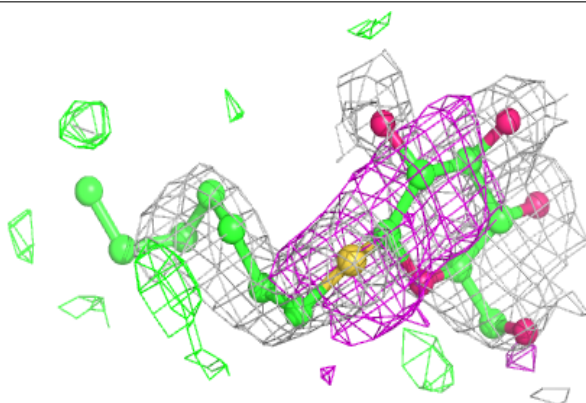


Electron density around LMT M 102:

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

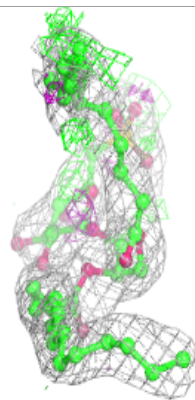
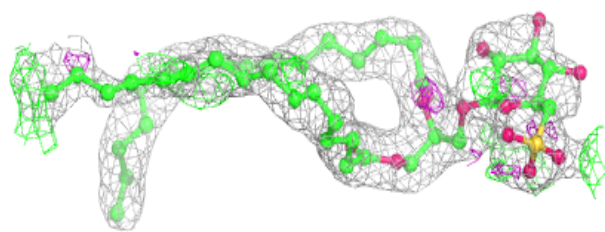
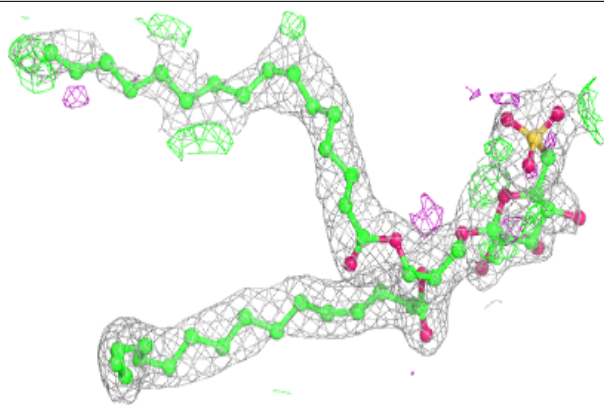
**Electron density around HTG b 627:**

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

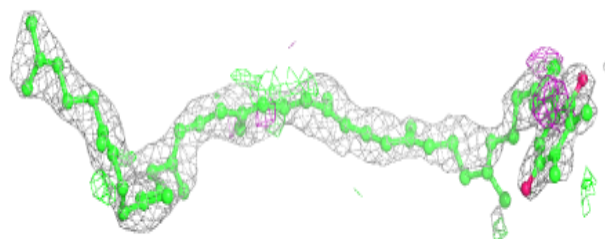
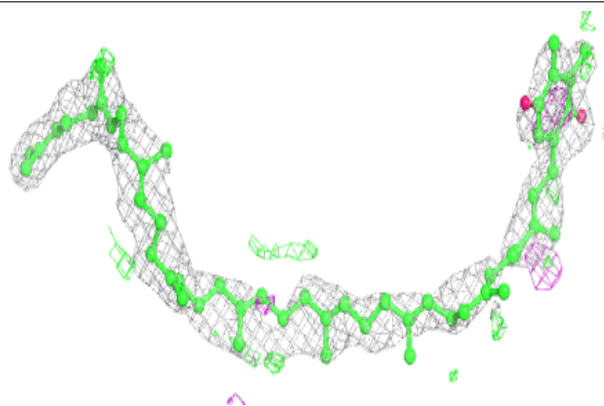


Electron density around SQD a 401:

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

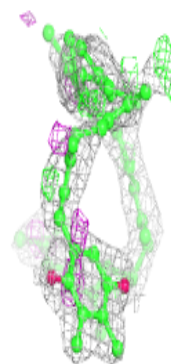
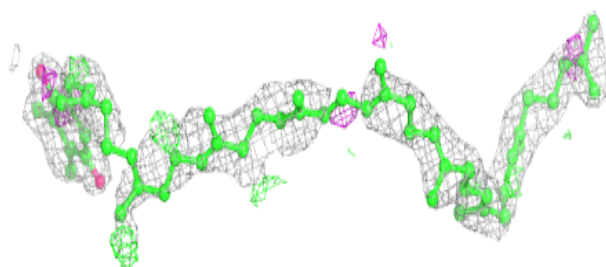
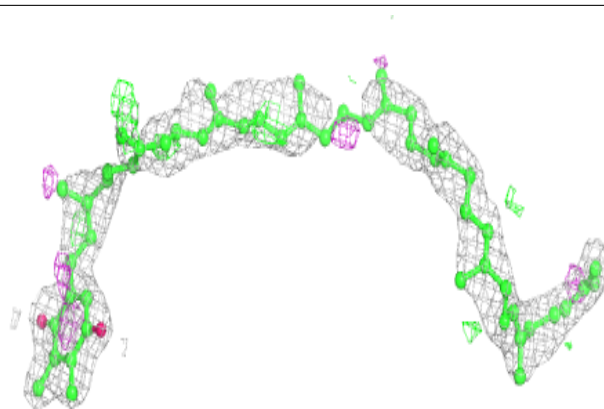
**Electron density around PL9 a 417:**

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

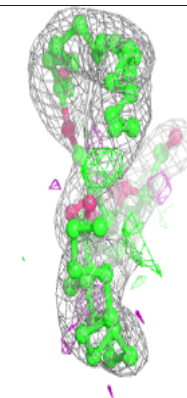
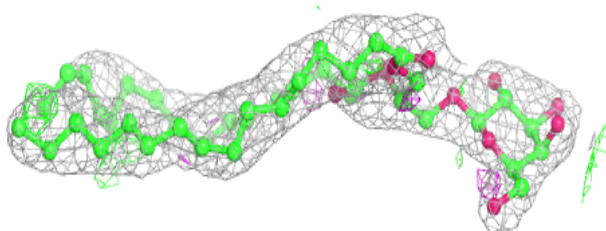
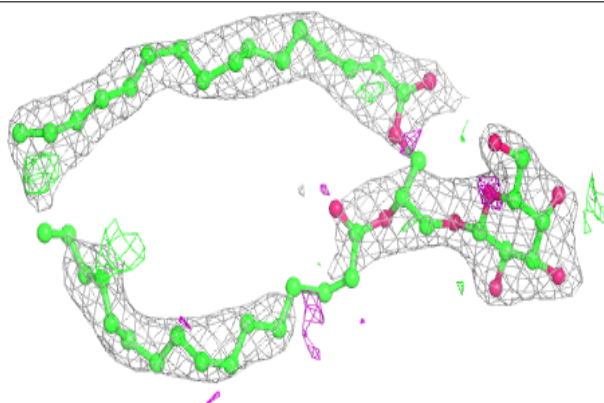


Electron density around PL9 A 413:

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

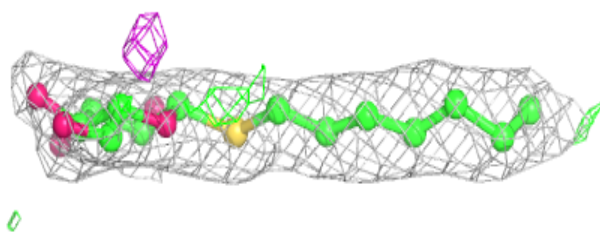
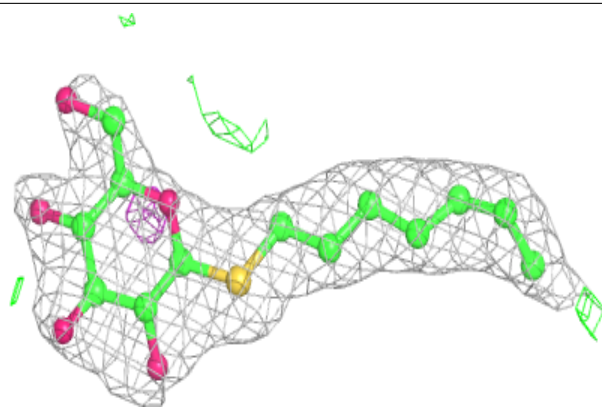
**Electron density around LMG i 101:**

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

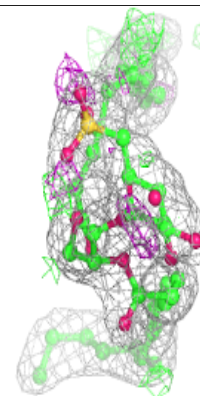
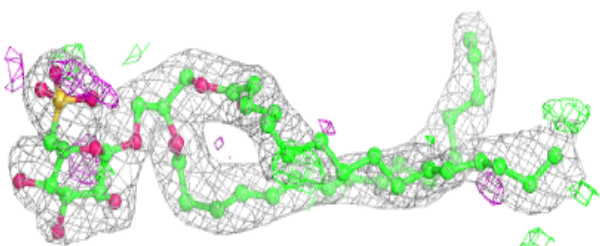
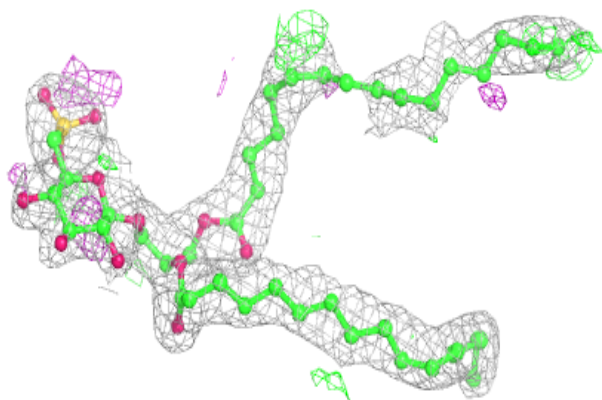


Electron density around HTG b 602:

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

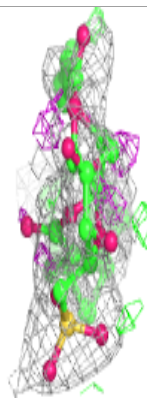
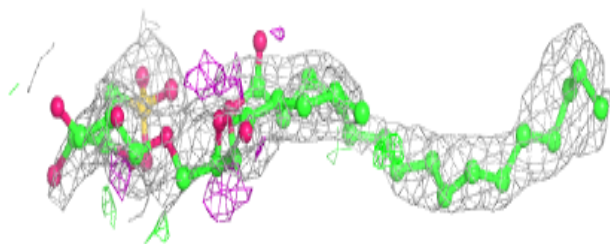
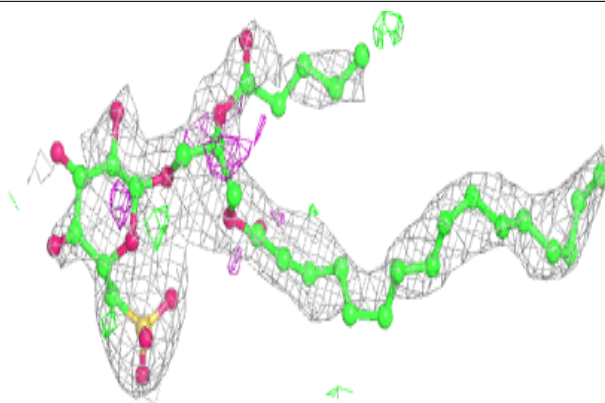
**Electron density around SQD A 415:**

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

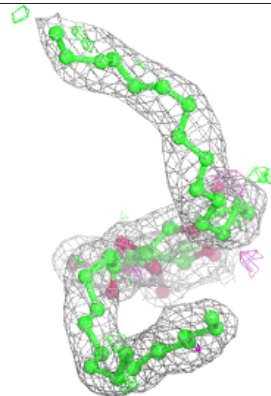
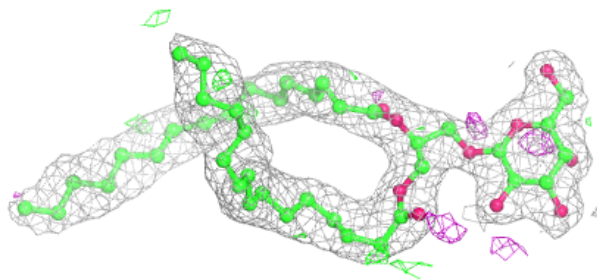
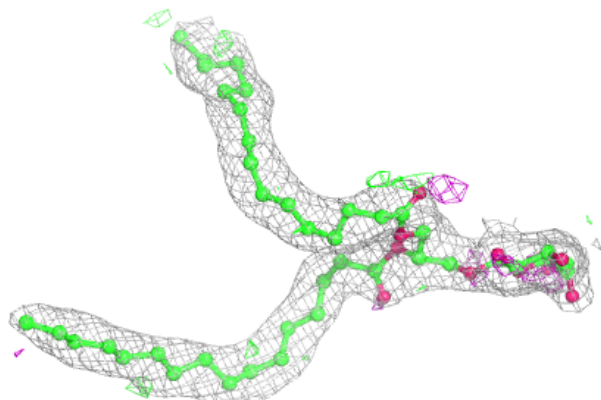


Electron density around SQD f 802:

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

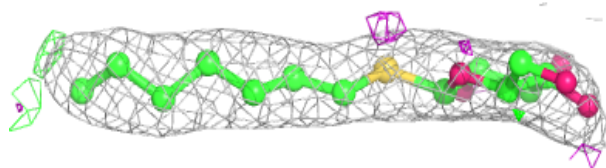
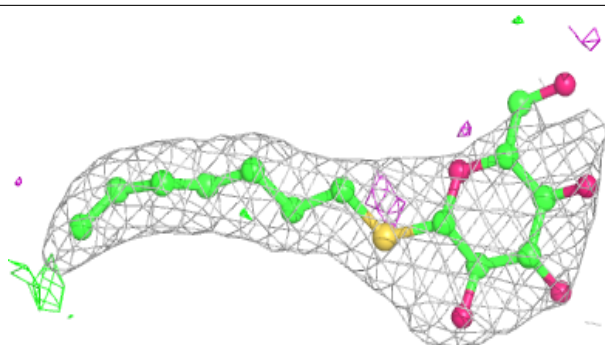
**Electron density around LMG B 623:**

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

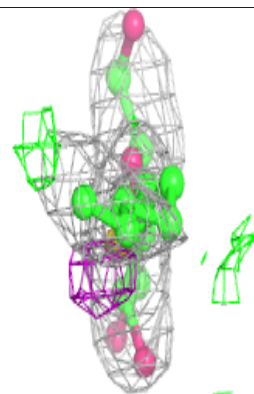
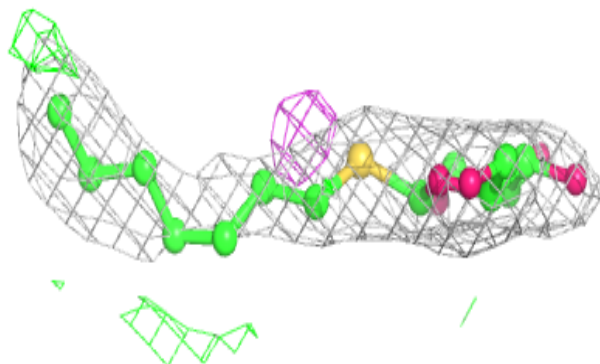
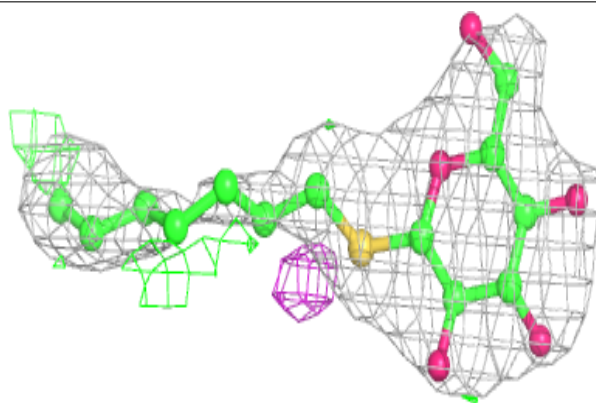


Electron density around HTG B 629:

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

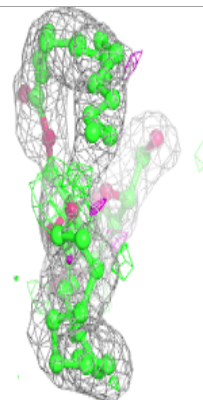
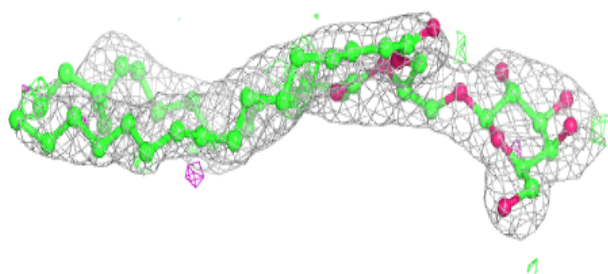
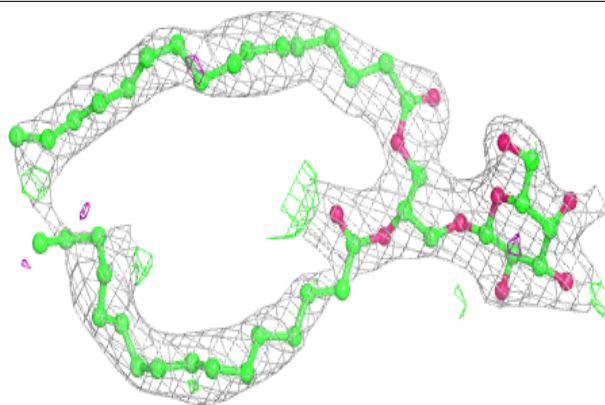
**Electron density around HTG C 522:**

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

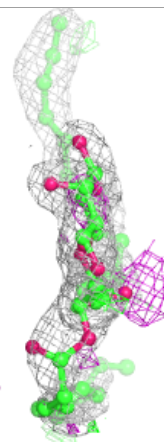
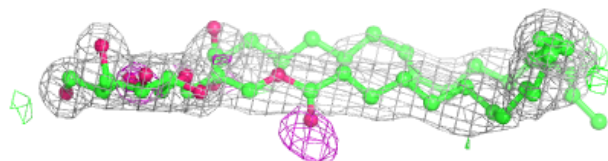
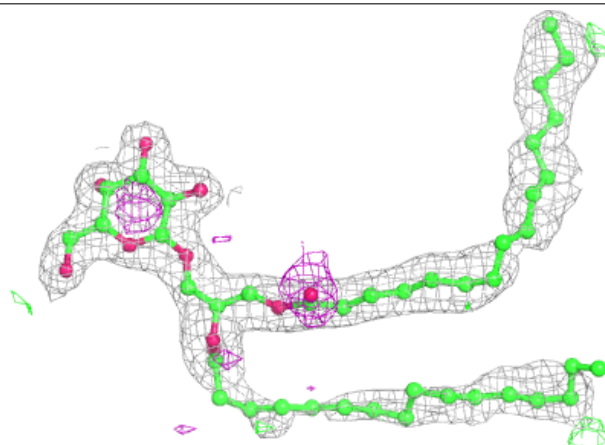


Electron density around LMG A 412:

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

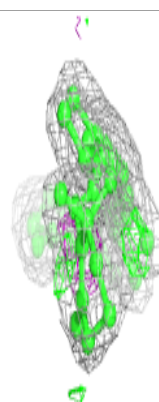
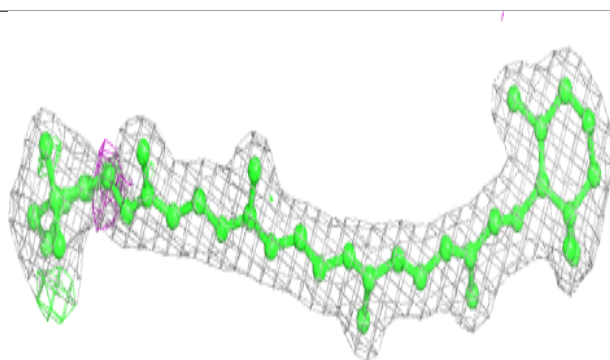
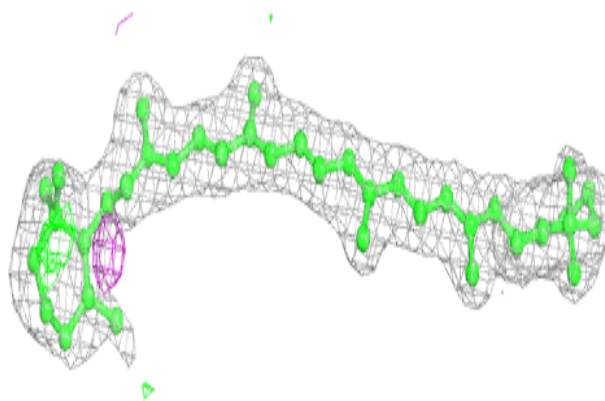
**Electron density around LMG C 521:**

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

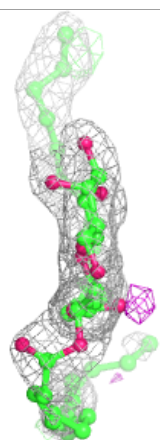
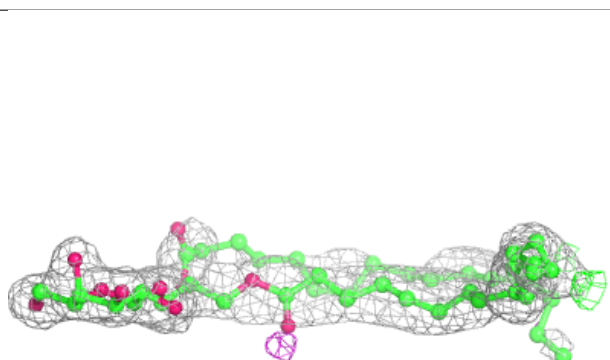
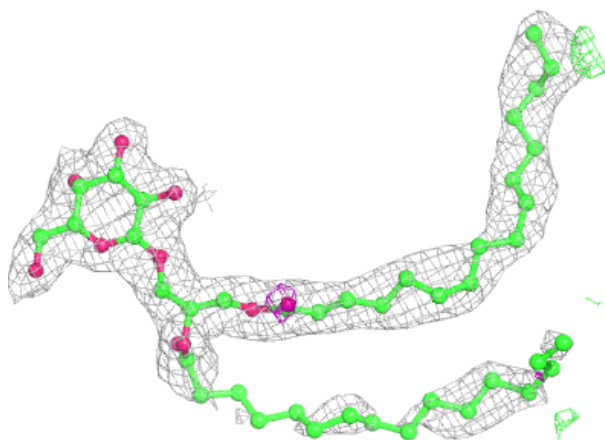


Electron density around BCR d 407:

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

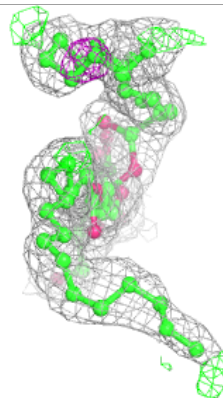
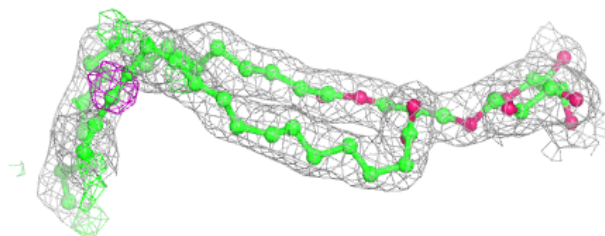
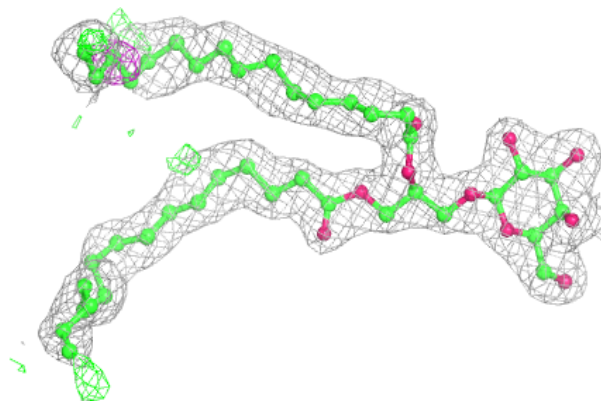
**Electron density around LMG c 521:**

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



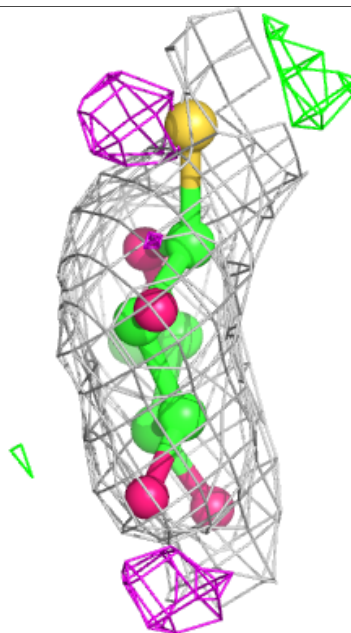
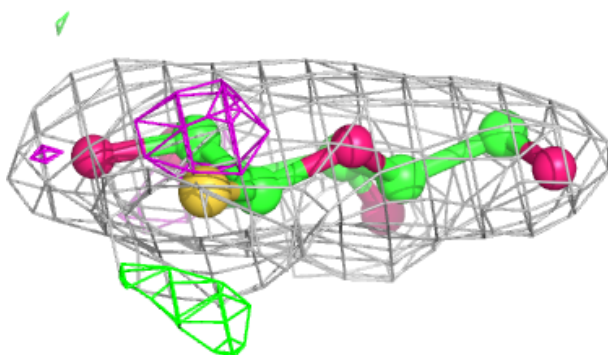
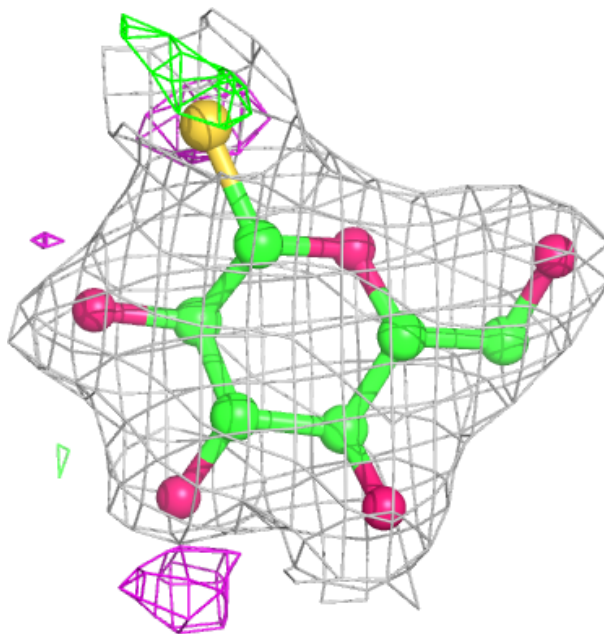
Electron density around LMG d 412:

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



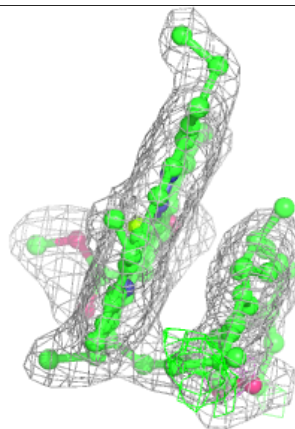
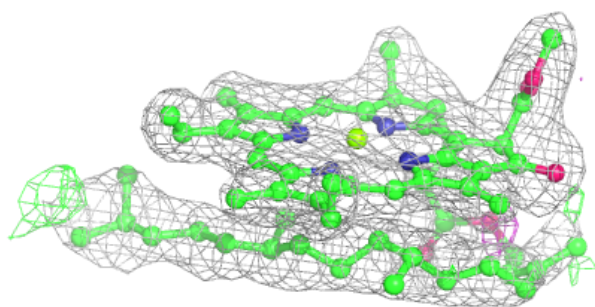
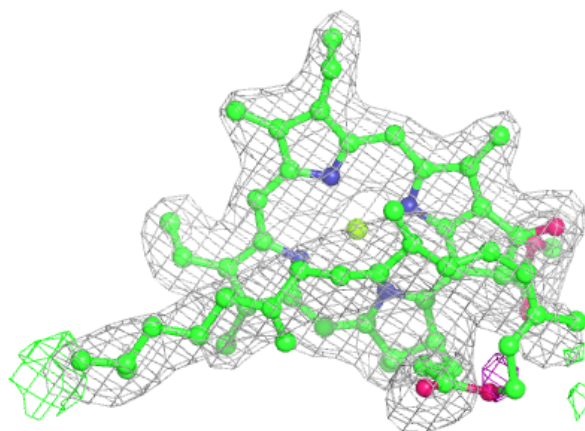
Electron density around HTG V 202:

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

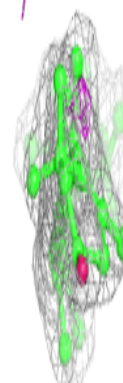
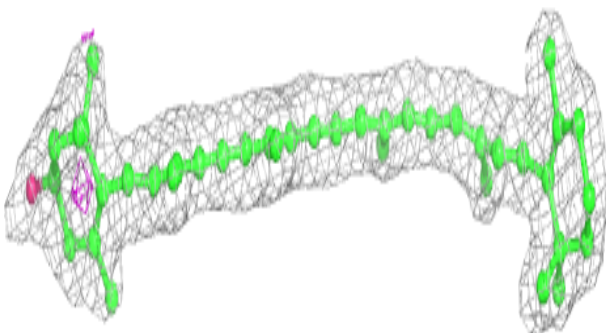
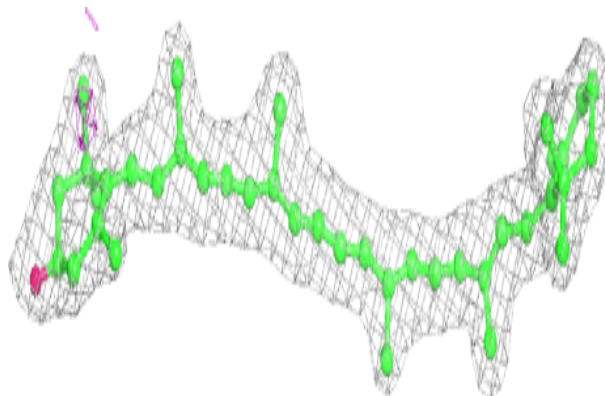


Electron density around CLA B 603:

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

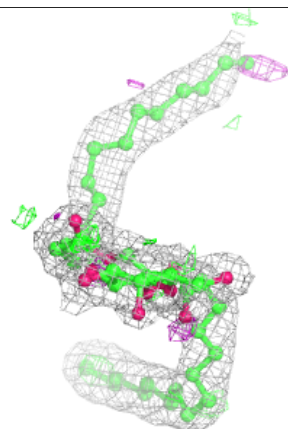
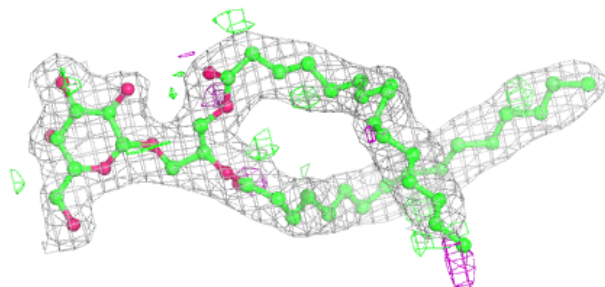
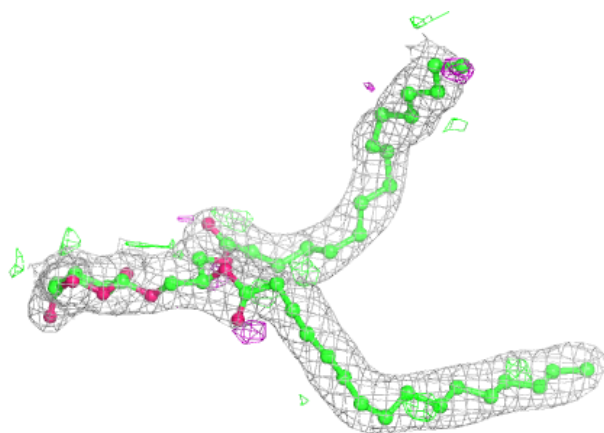
**Electron density around RRX h 101:**

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

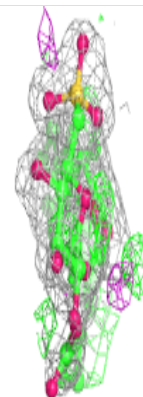
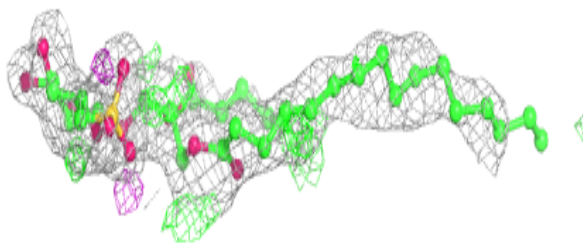
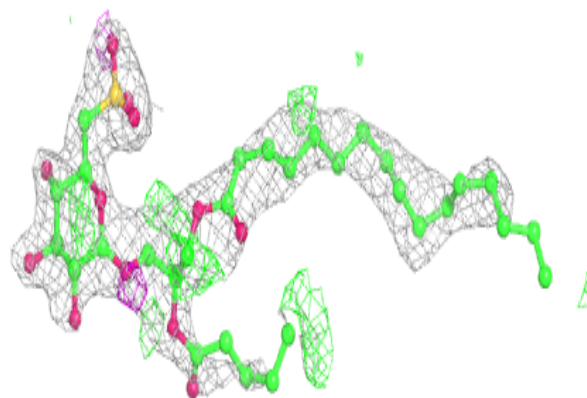


Electron density around LMG b 624:

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

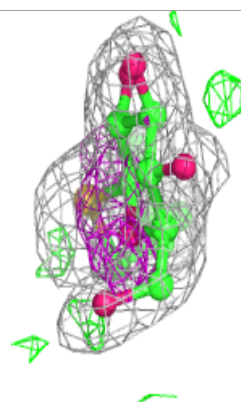
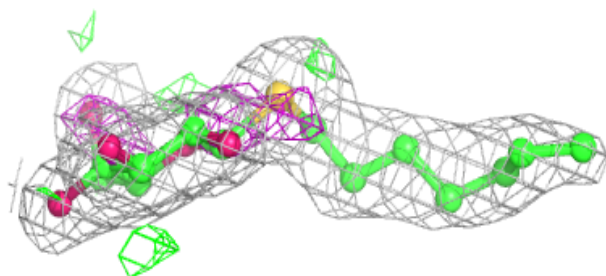
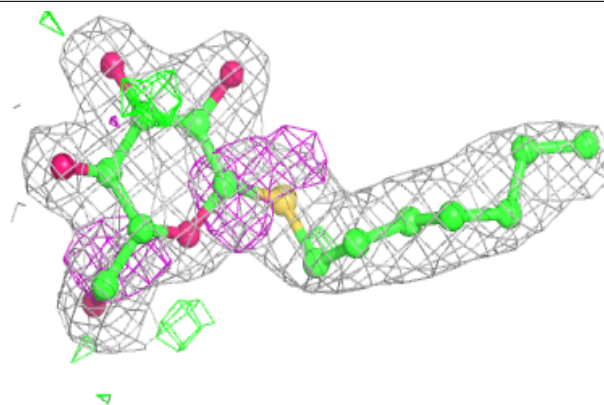
**Electron density around SQD F 101:**

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



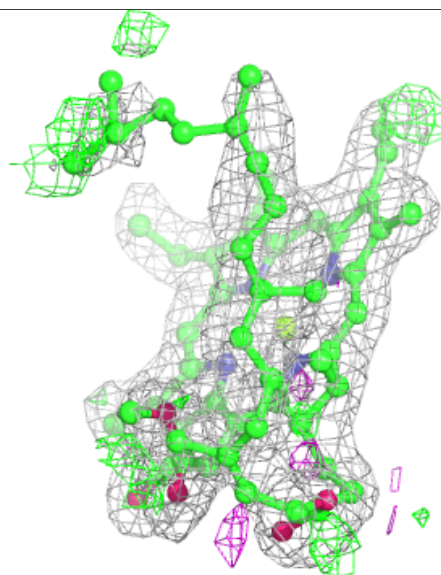
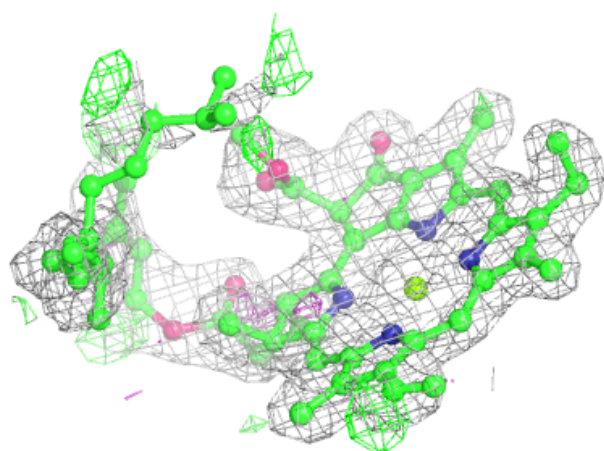
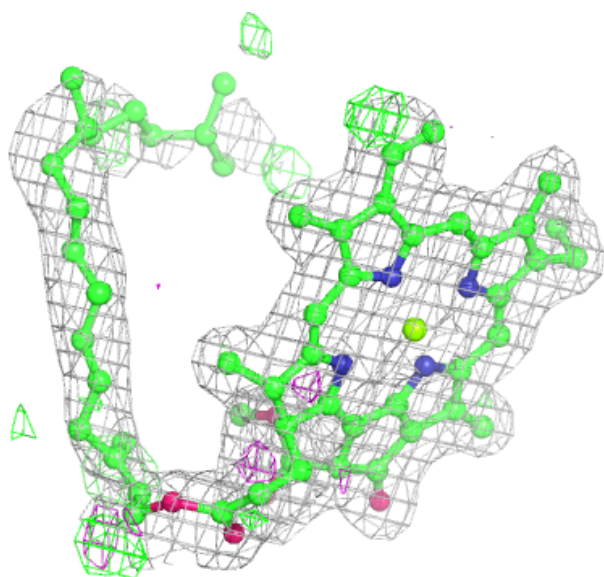
Electron density around HTG O 303:

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



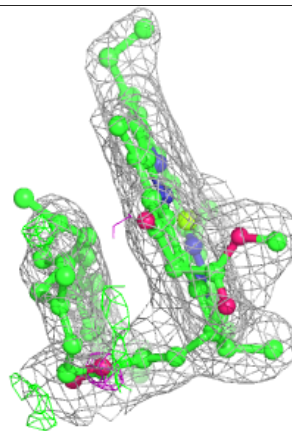
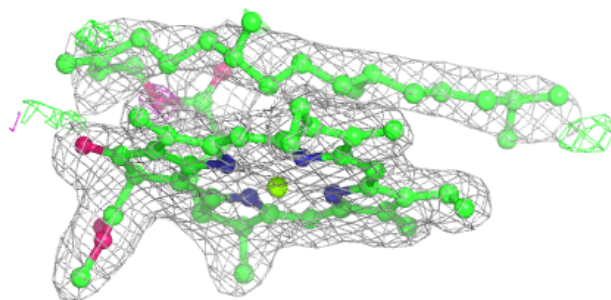
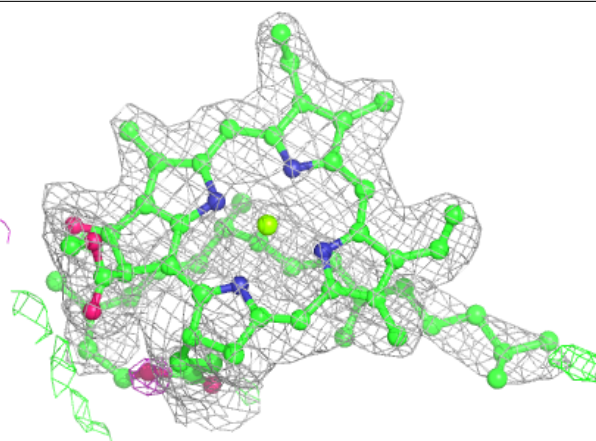
Electron density around CLA b 620:

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



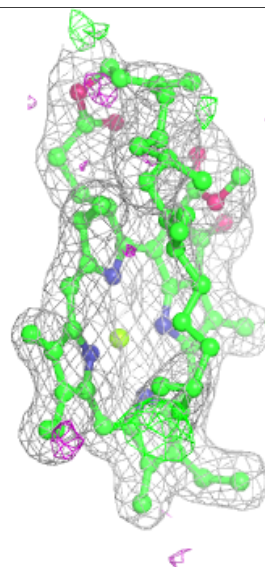
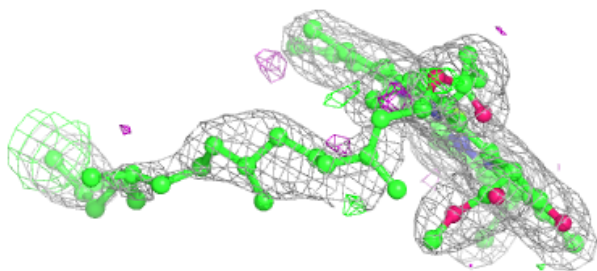
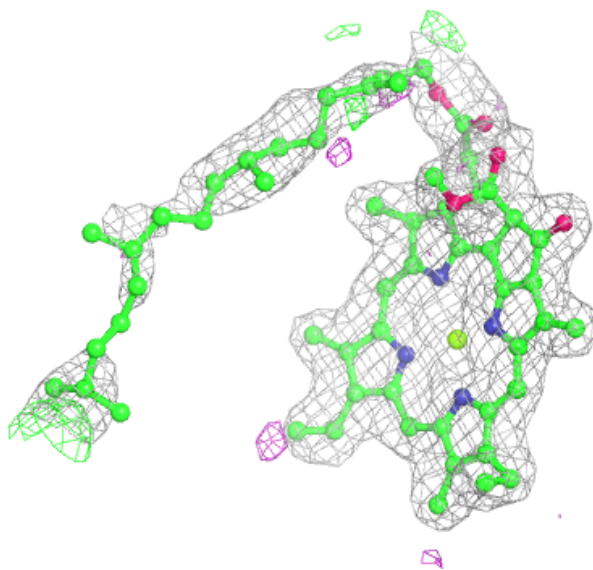
Electron density around CLA b 605:

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



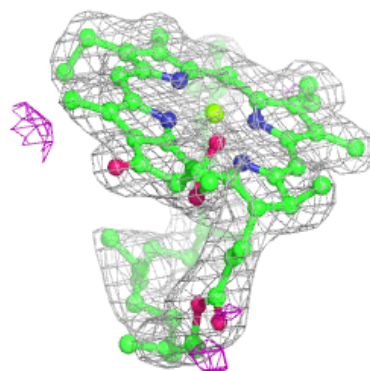
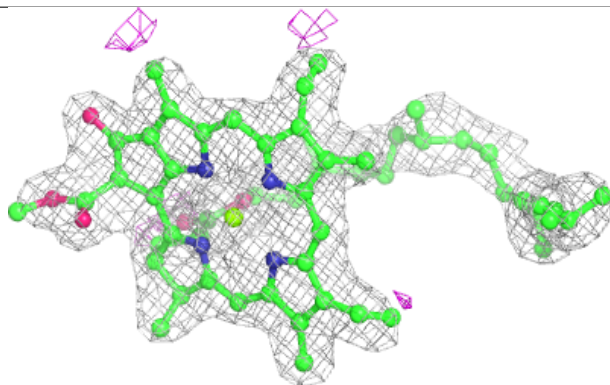
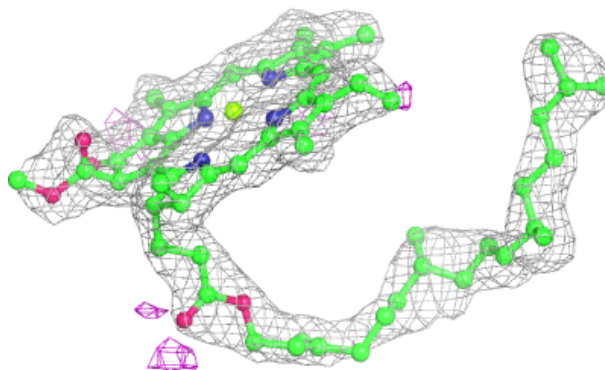
Electron density around CLA B 618:

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

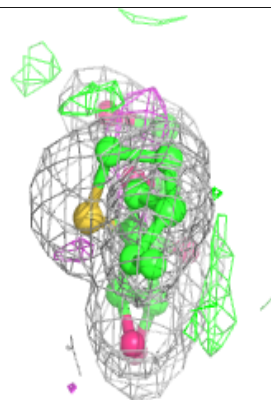
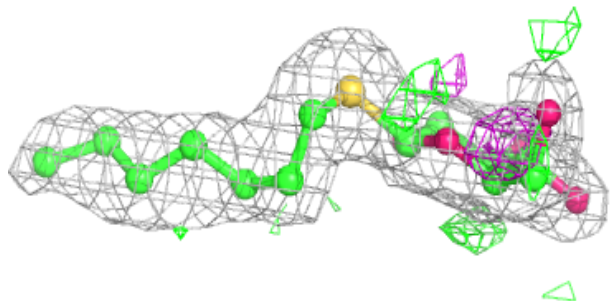
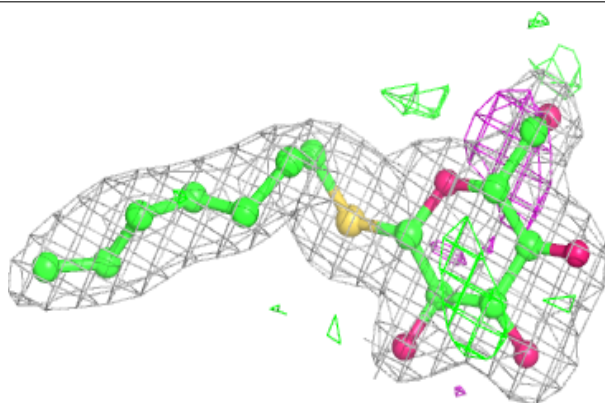


Electron density around CLA C 515:

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

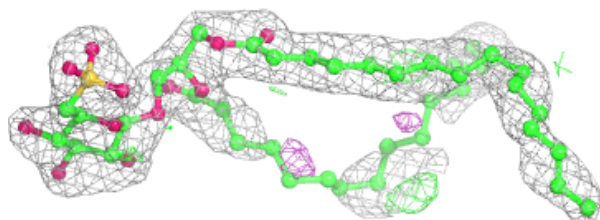
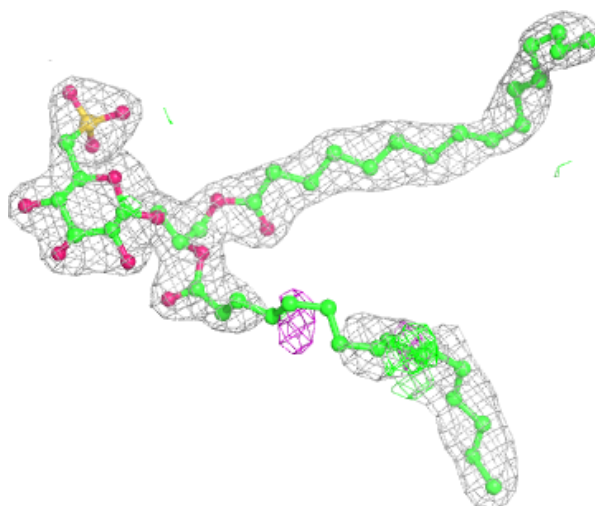
**Electron density around HTG o 301:**

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



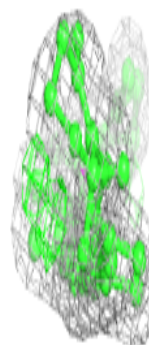
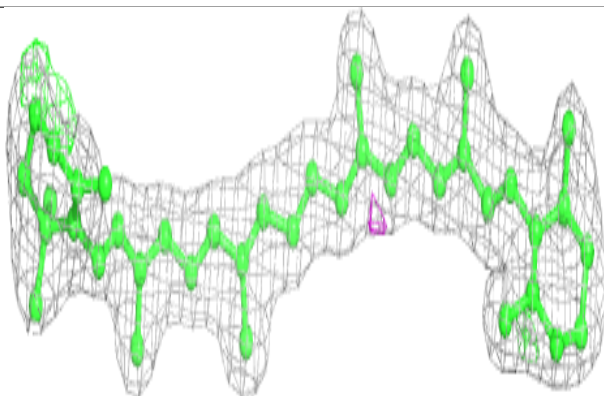
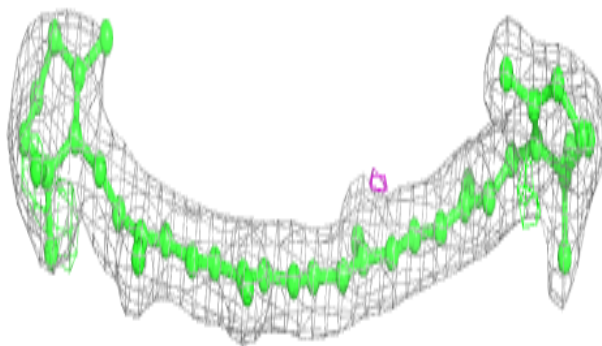
Electron density around SQD a 415:

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



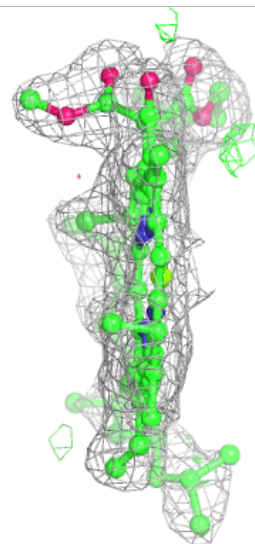
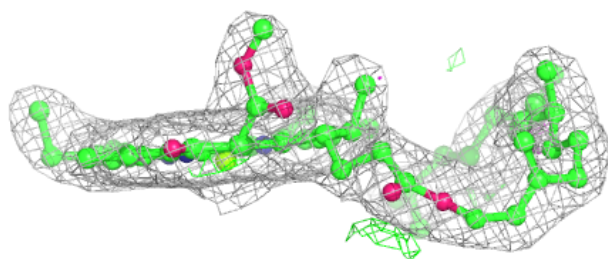
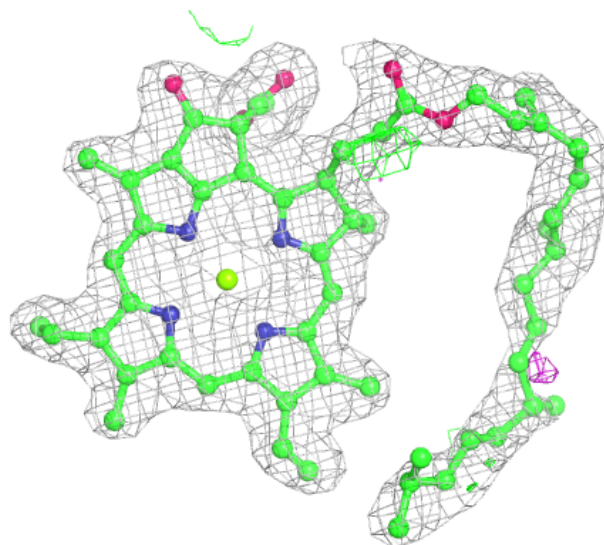
Electron density around BCR D 407:

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



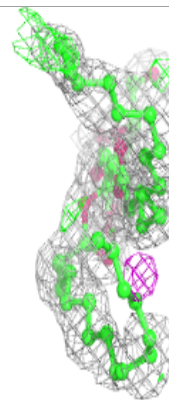
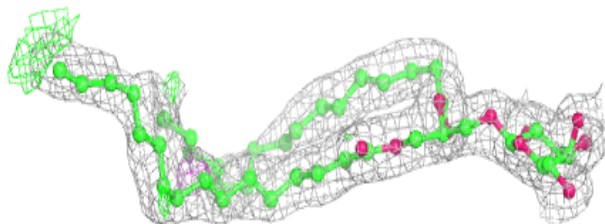
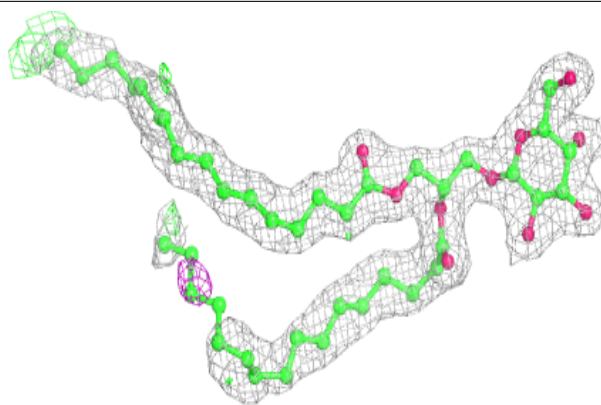
Electron density around CLA C 514:

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



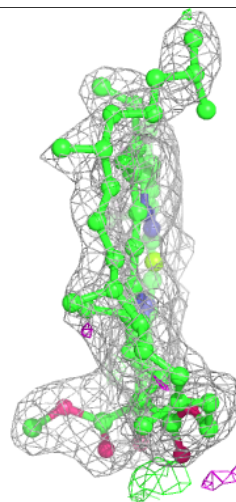
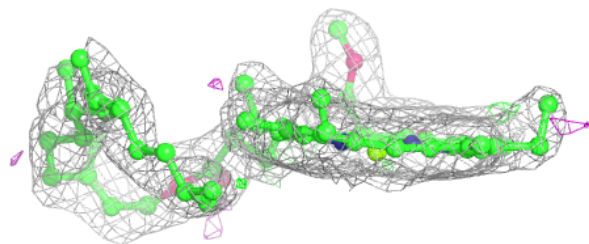
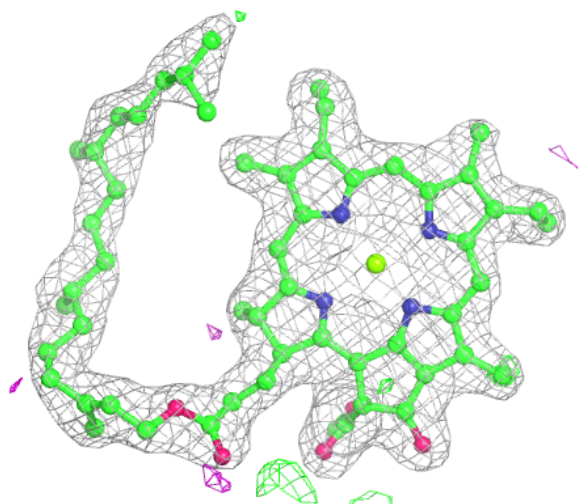
Electron density around LMG D 413:

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



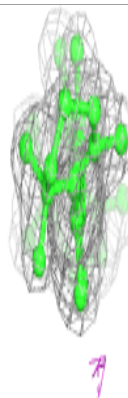
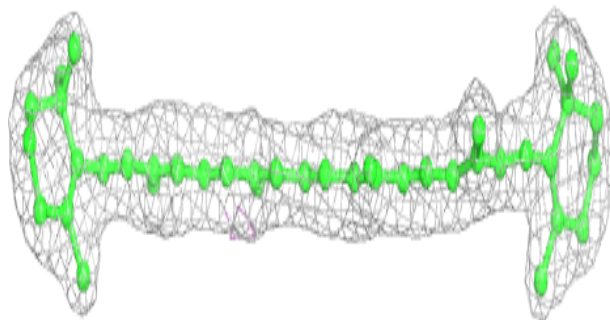
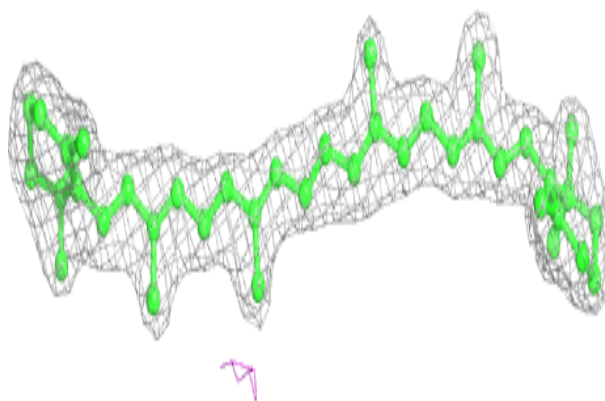
Electron density around CLA c 514:

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

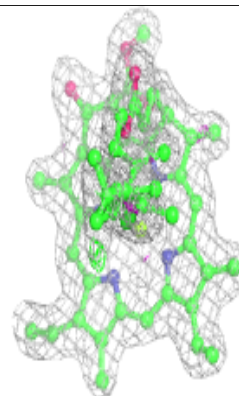
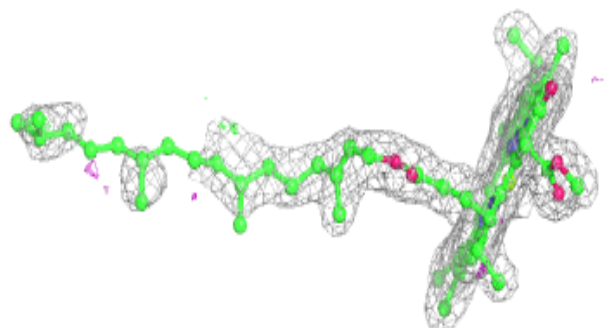
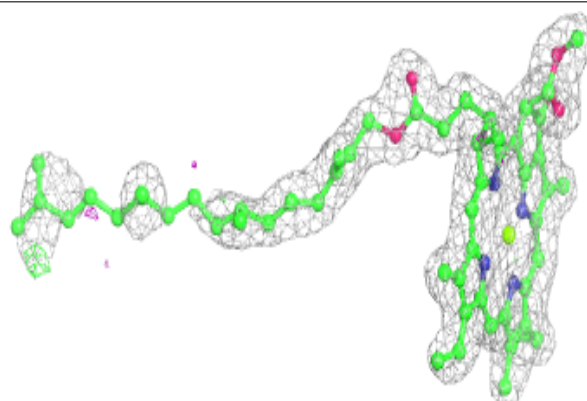


Electron density around BCR C 516:

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

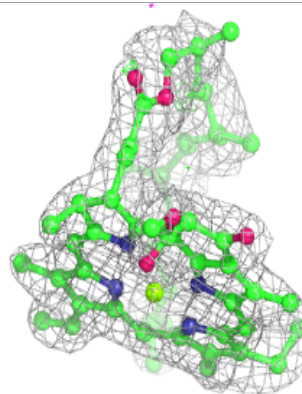
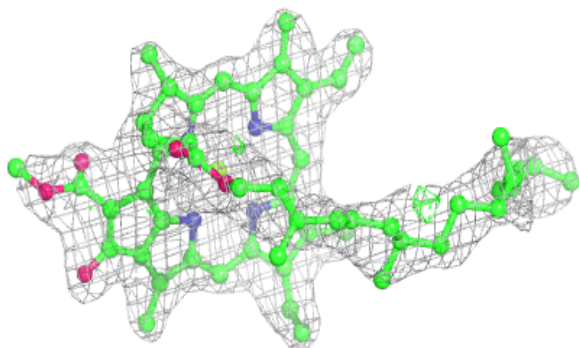
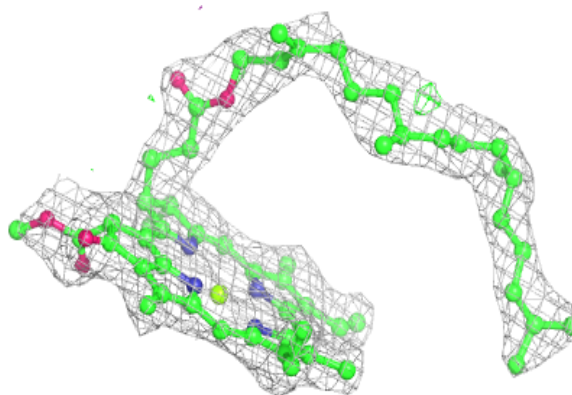
**Electron density around CLA D 406:**

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

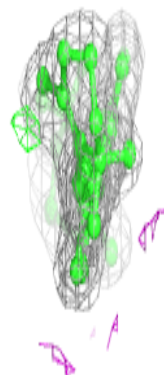
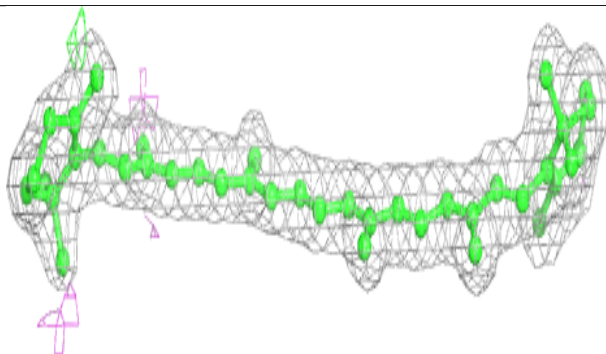
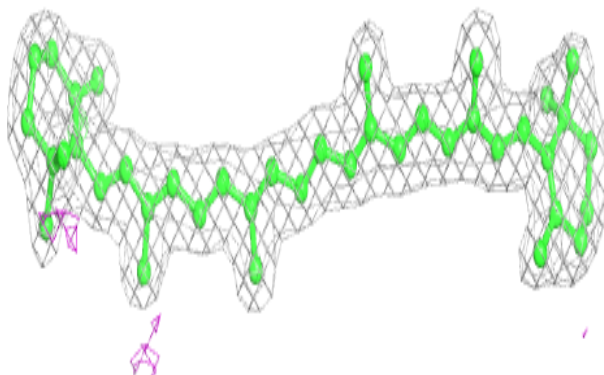


Electron density around CLA c 515:

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

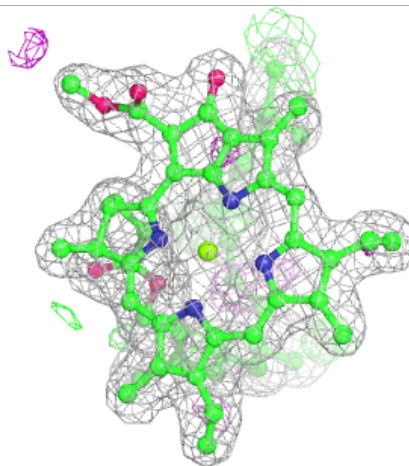
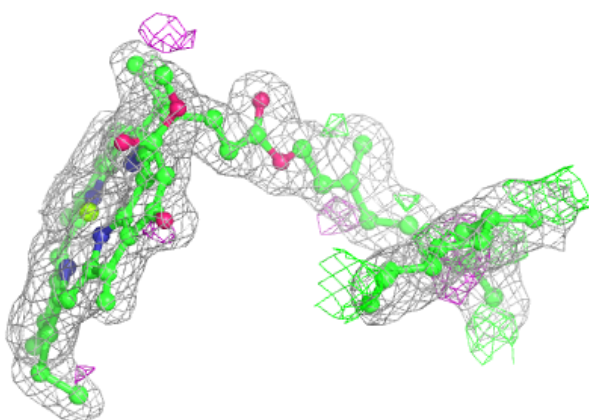
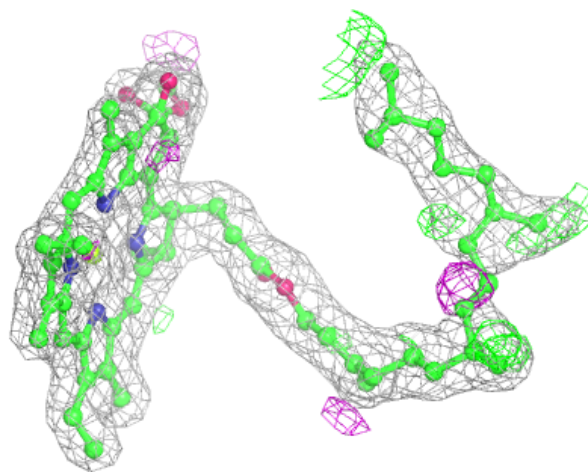
**Electron density around BCR B 621:**

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



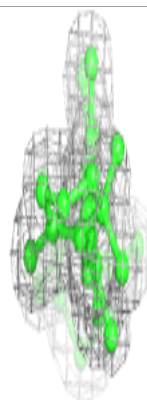
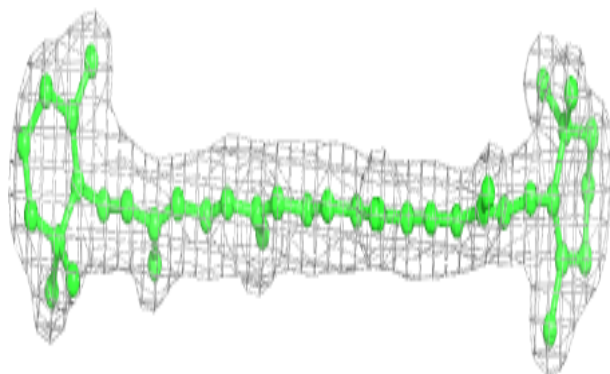
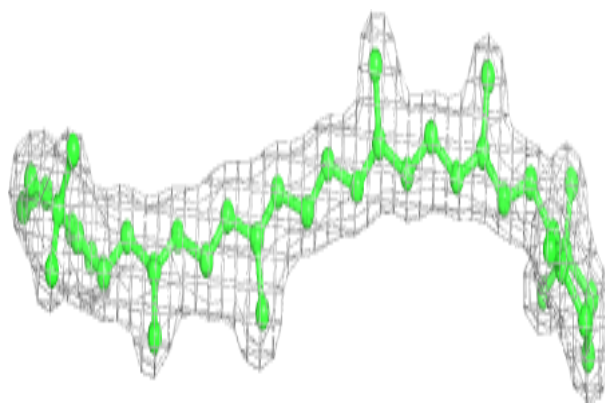
Electron density around CLA B 608:

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

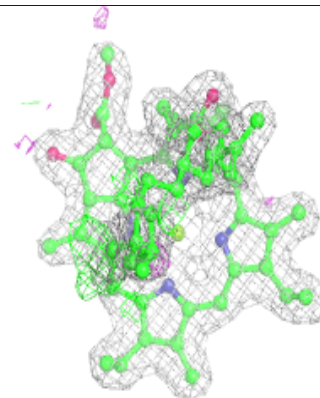
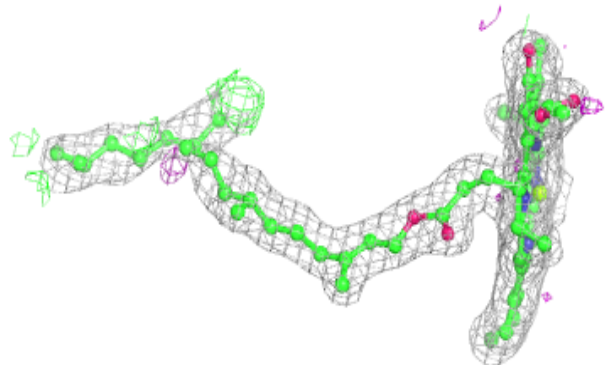
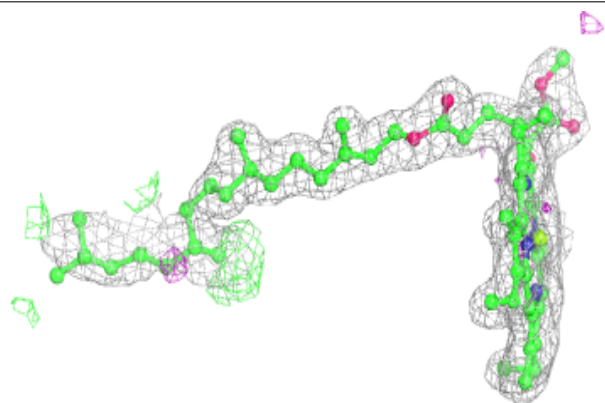


Electron density around BCR C 517:

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

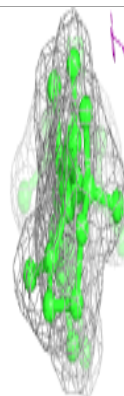
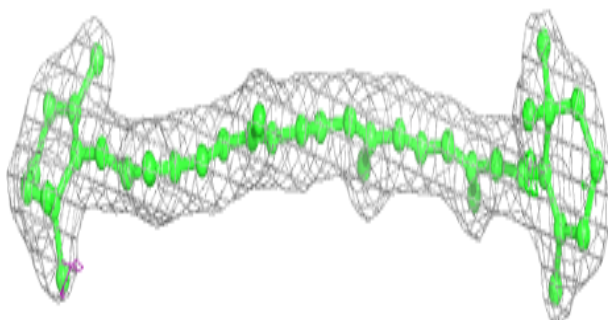
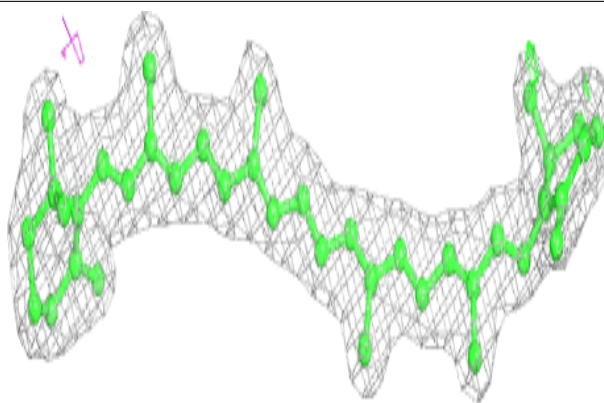
**Electron density around CLA b 610:**

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

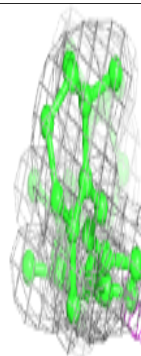
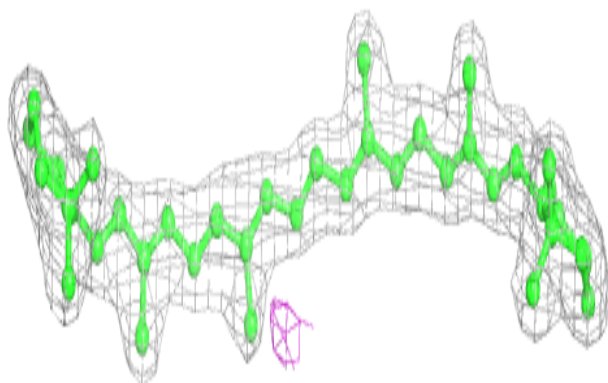
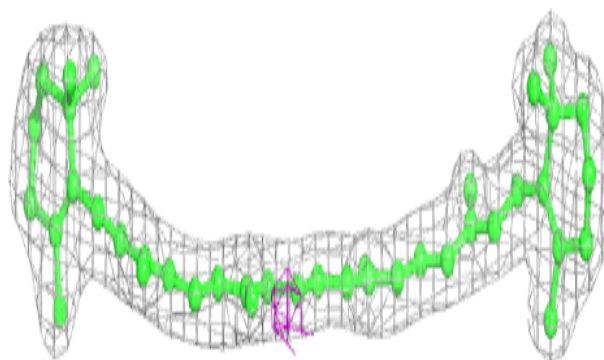


Electron density around BCR K 101:

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

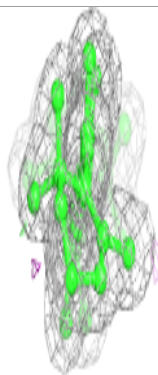
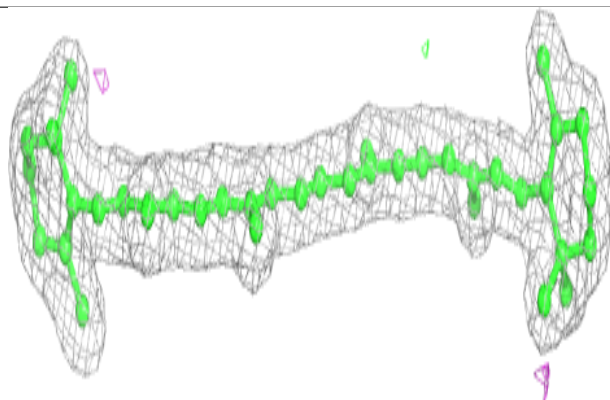
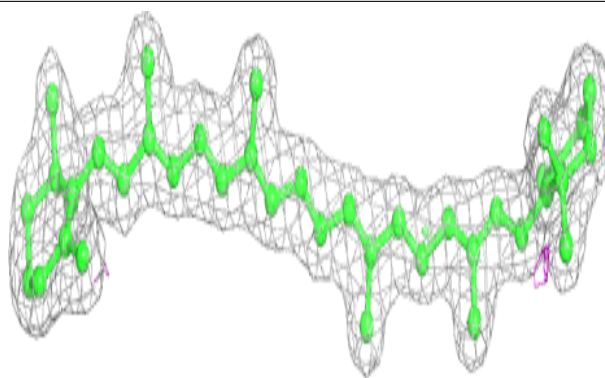
**Electron density around BCR K 102:**

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

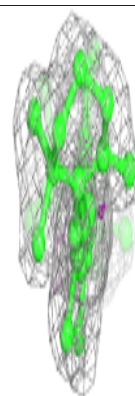
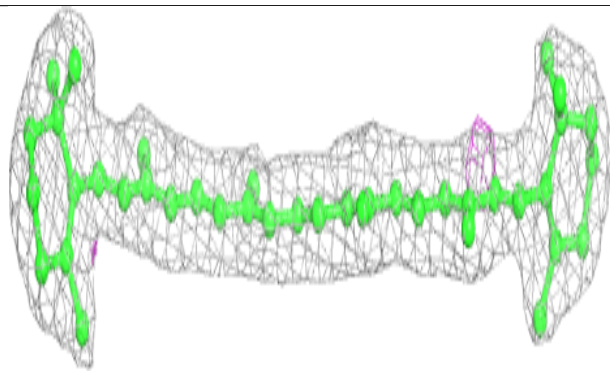
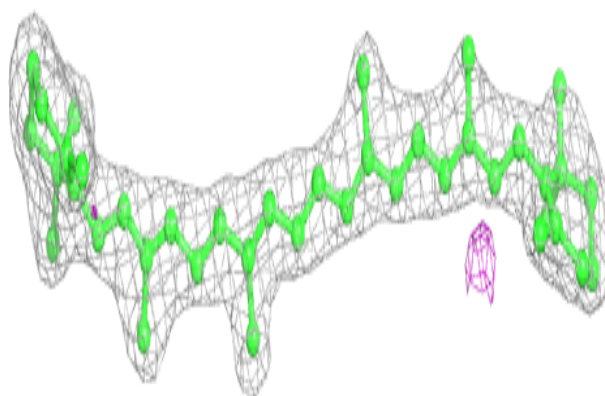


Electron density around BCR a 414:

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

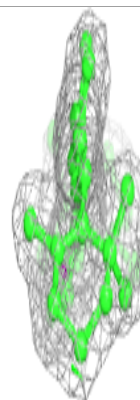
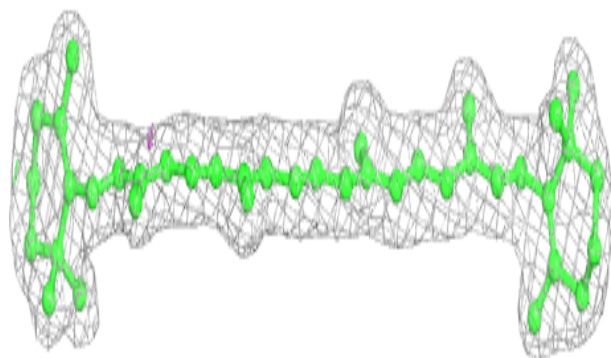
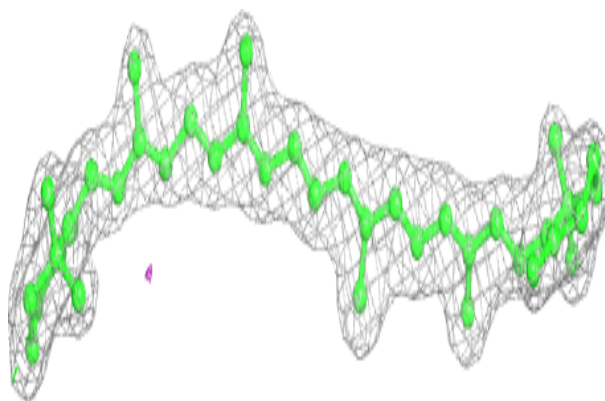
**Electron density around BCR c 516:**

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

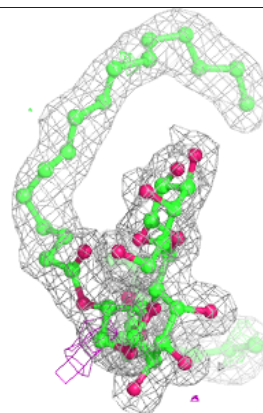
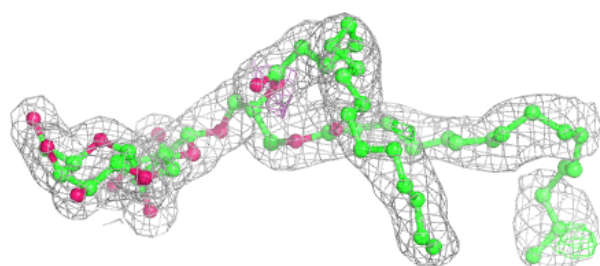
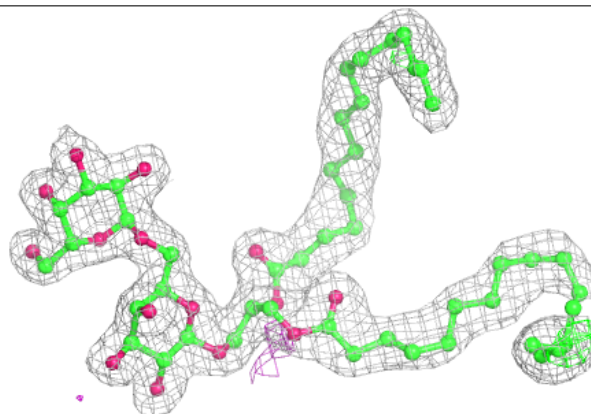


Electron density around BCR c 517:

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

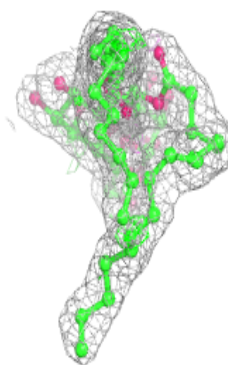
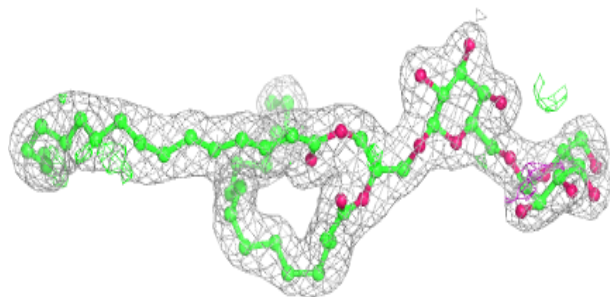
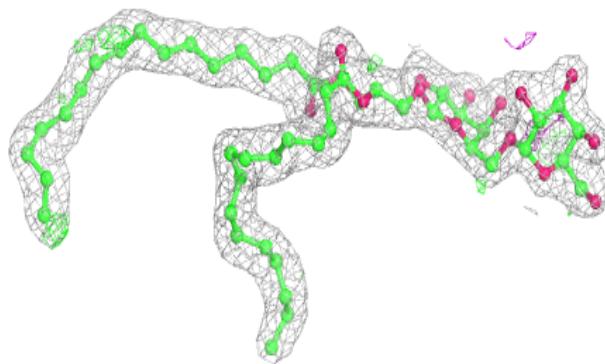
**Electron density around DGD C 519:**

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

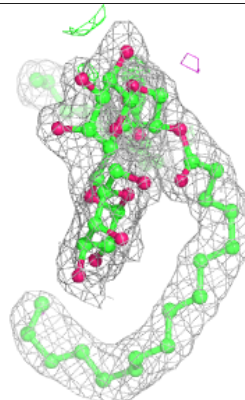
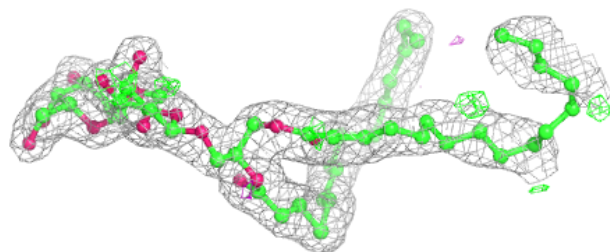
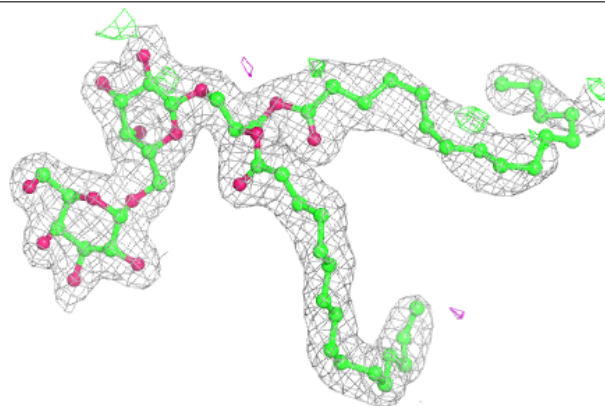


Electron density around DGD H 104:

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

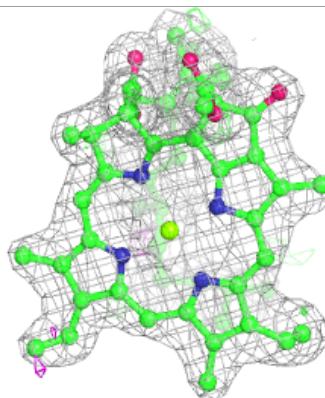
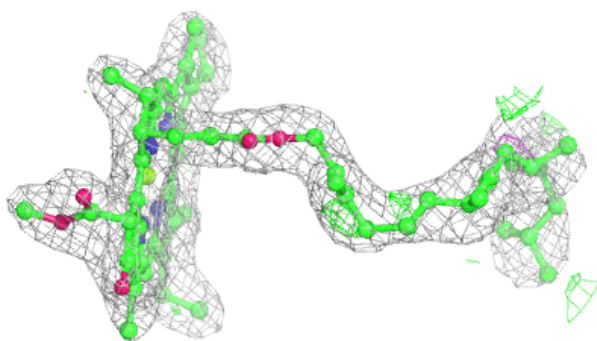
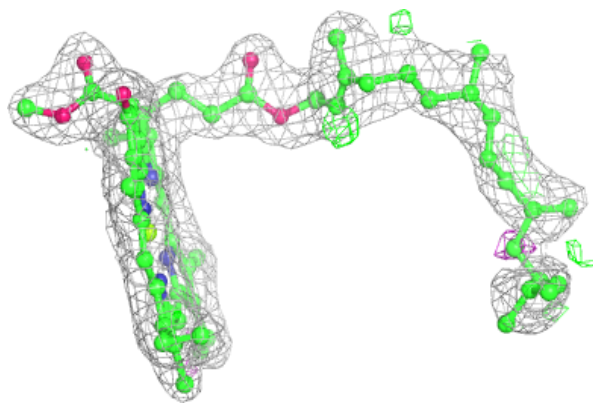
**Electron density around DGD c 519:**

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

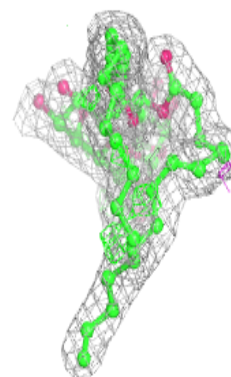
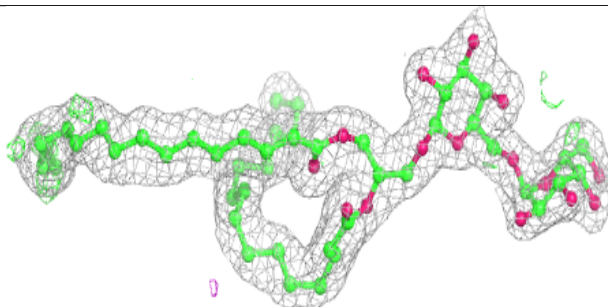
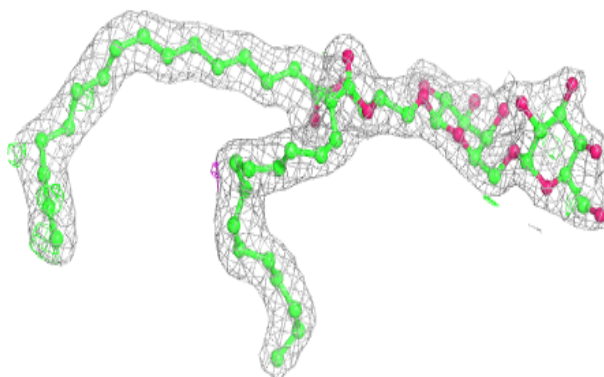


Electron density around CLA C 508:

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

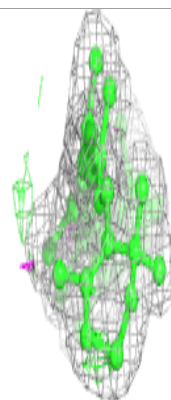
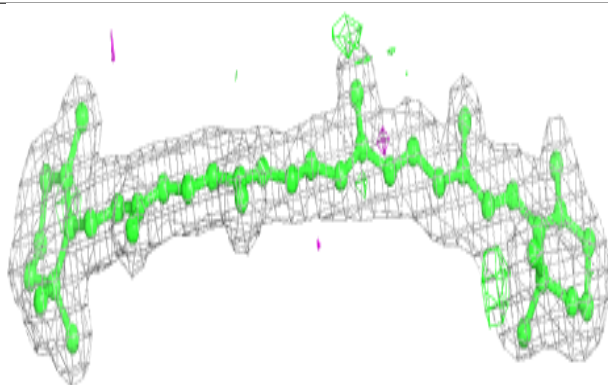
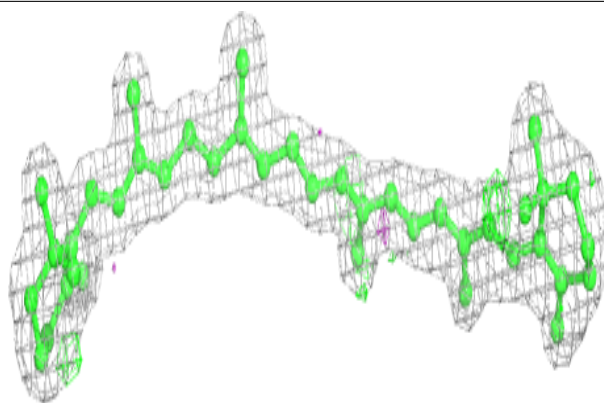
**Electron density around DGD h 102:**

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

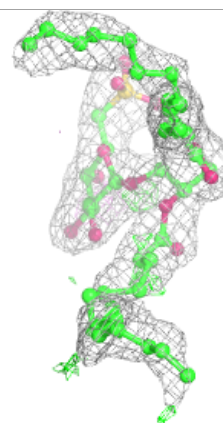
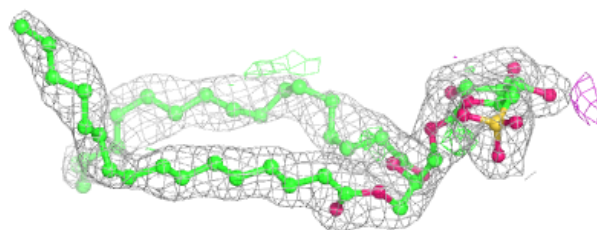
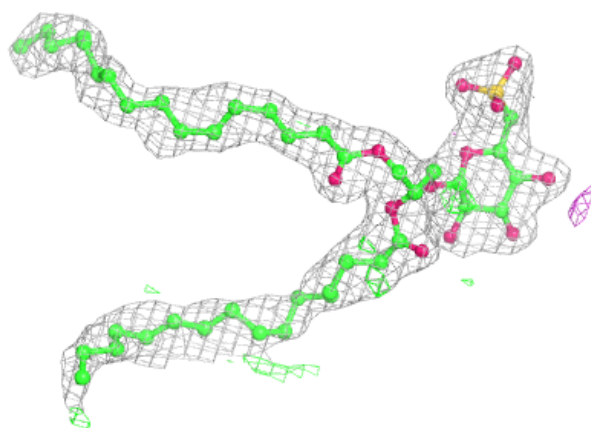


Electron density around BCR t 101:

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

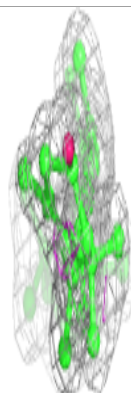
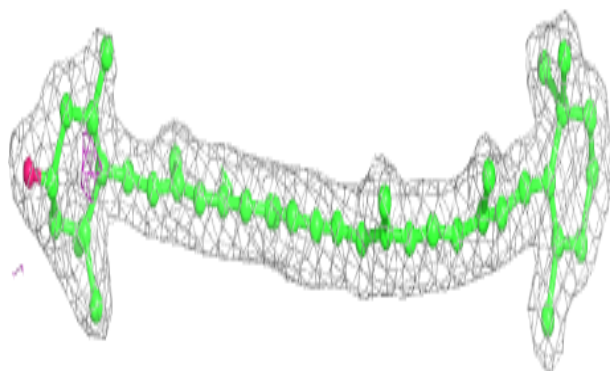
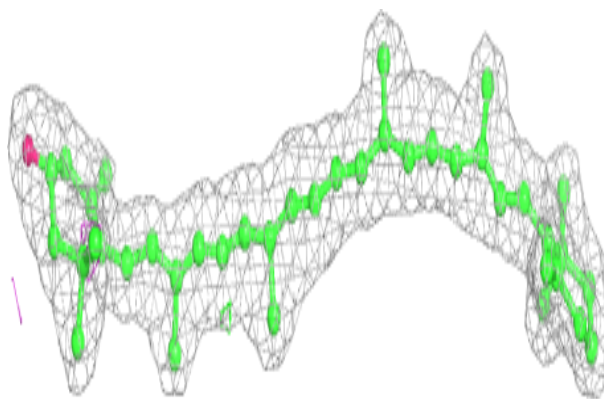
**Electron density around SQD A 411:**

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

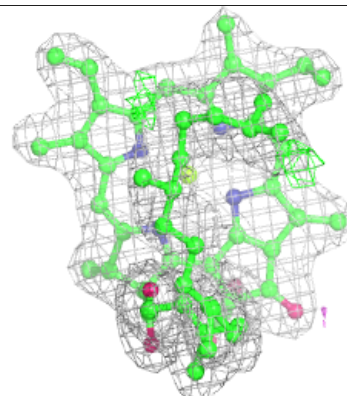
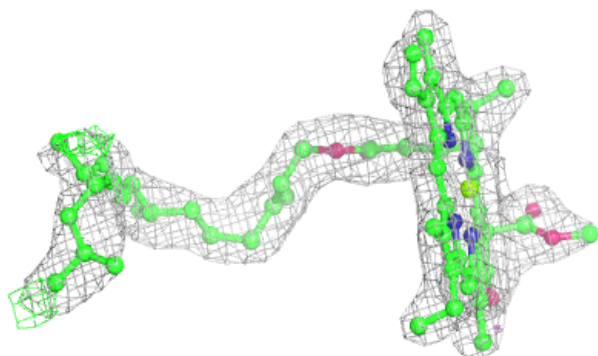
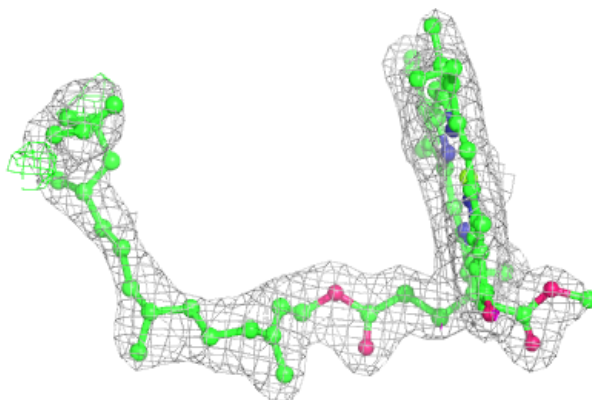


Electron density around RRX H 103:

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

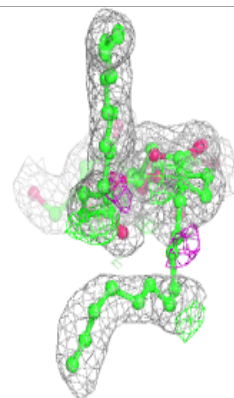
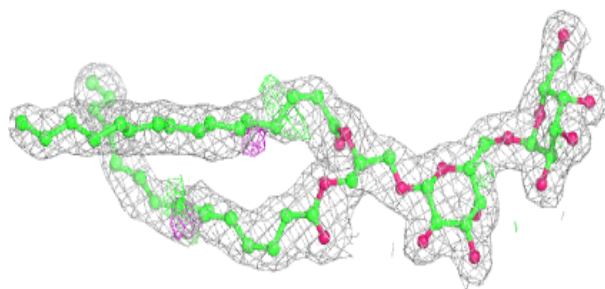
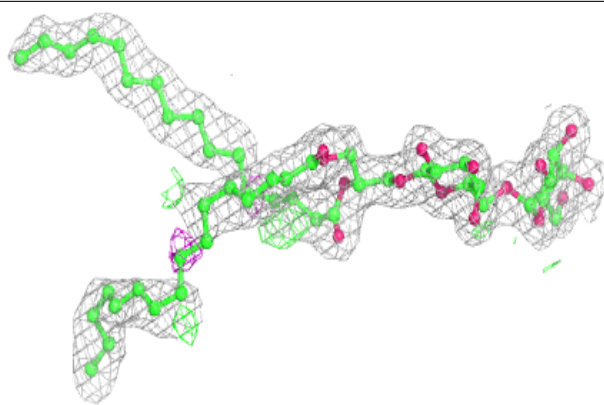
**Electron density around CLA c 508:**

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

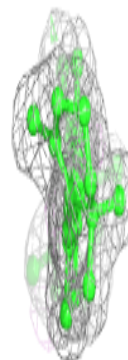
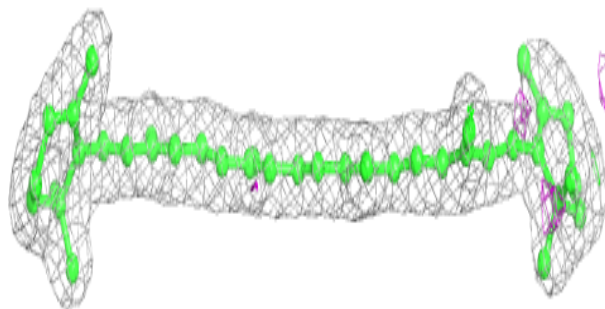
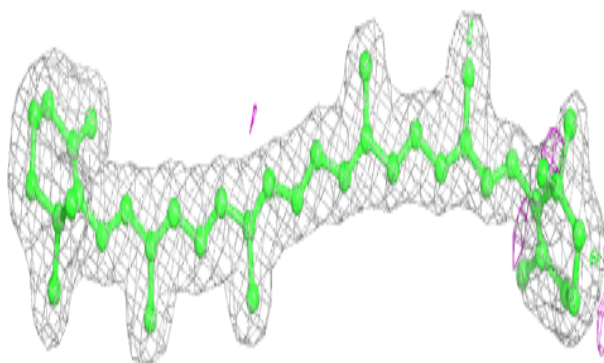


Electron density around DGD c 518:

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

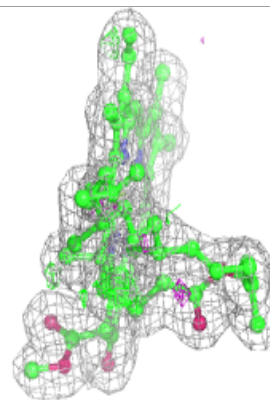
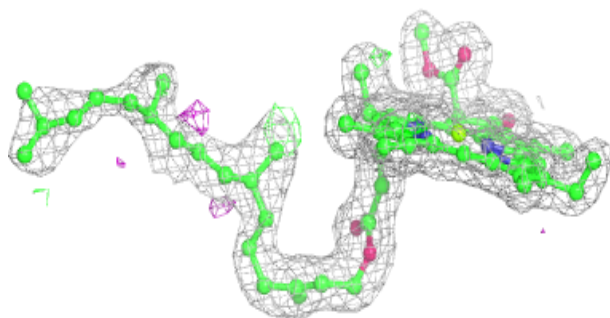
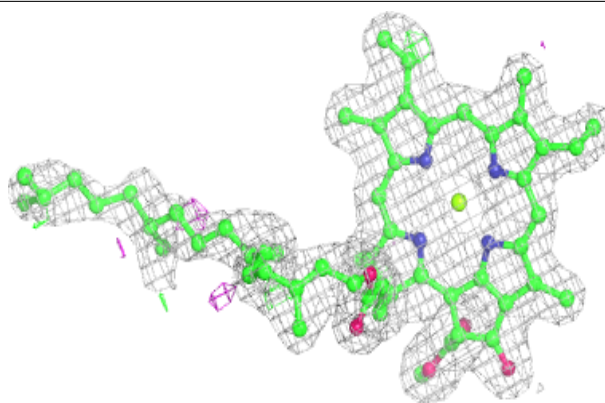
**Electron density around BCR B 620:**

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

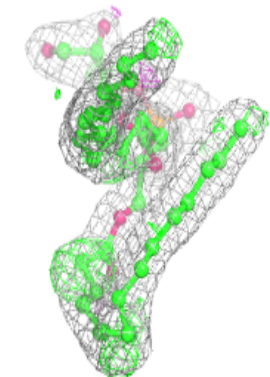
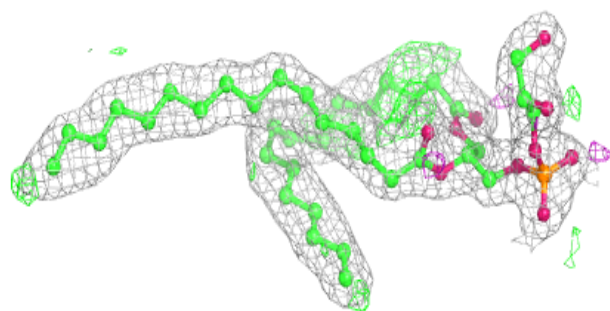
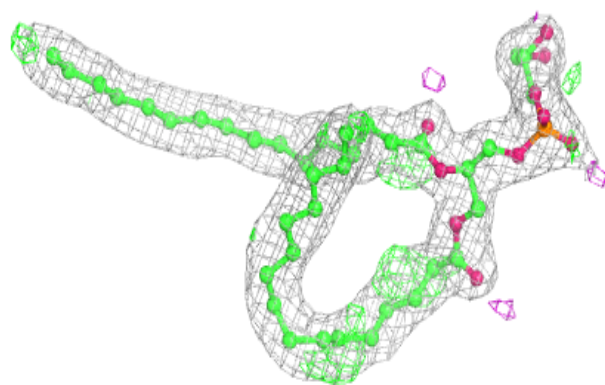


Electron density around CLA a 411:

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

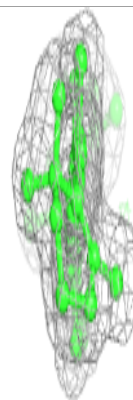
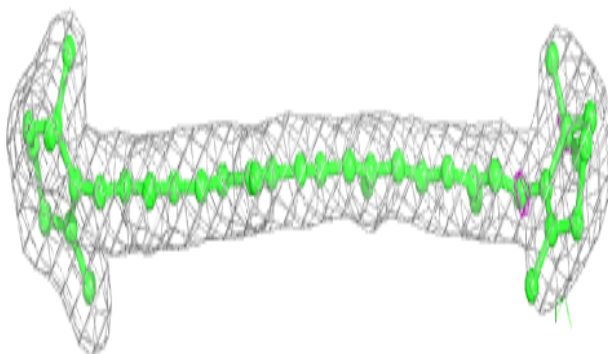
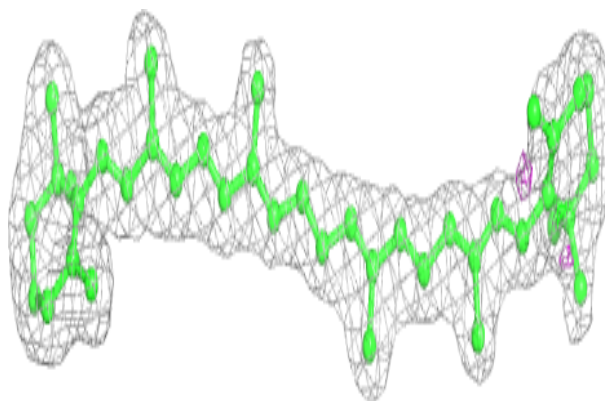
**Electron density around LHG D 410:**

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

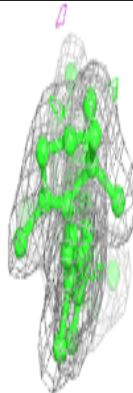
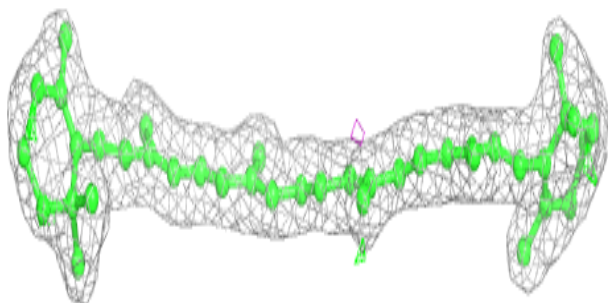
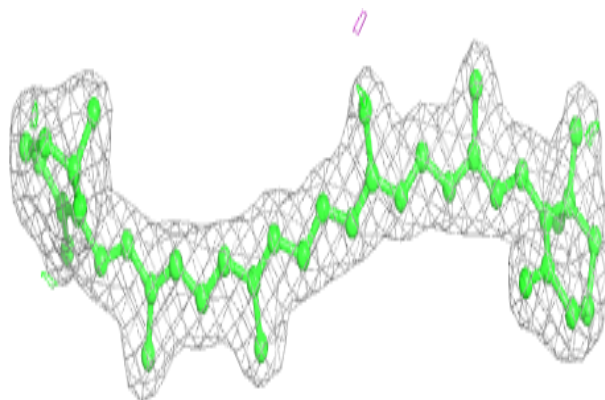


Electron density around BCR b 622:

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

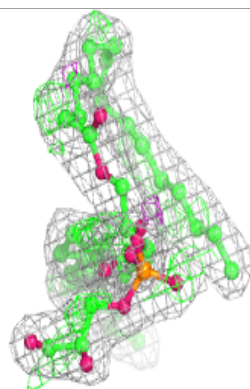
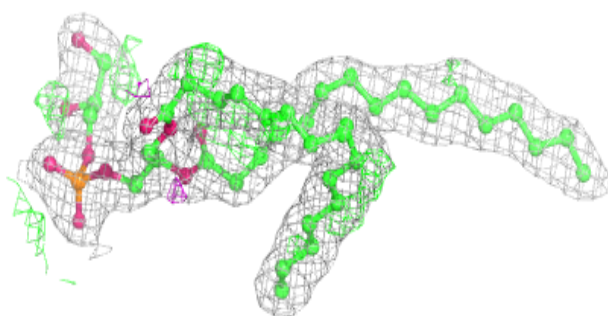
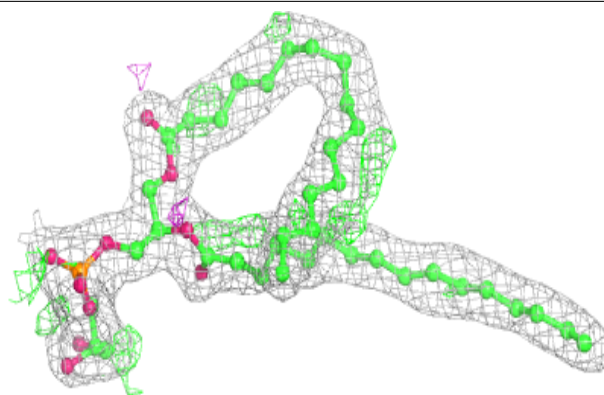
**Electron density around BCR k 102:**

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

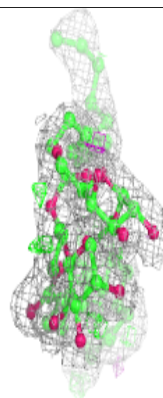
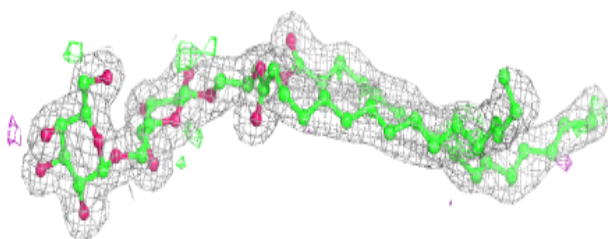
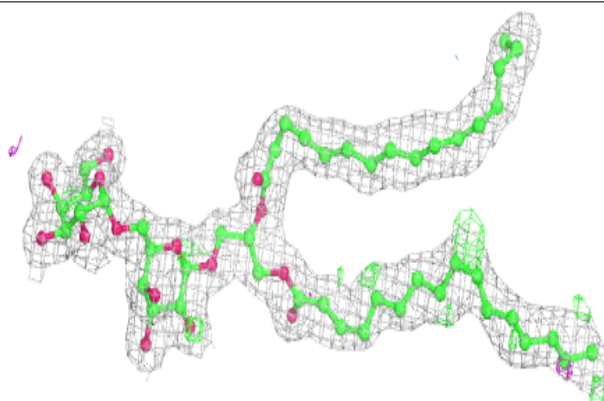


Electron density around LHG d 409:

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

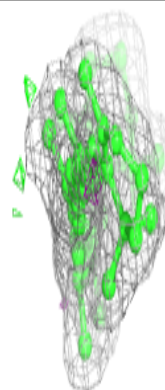
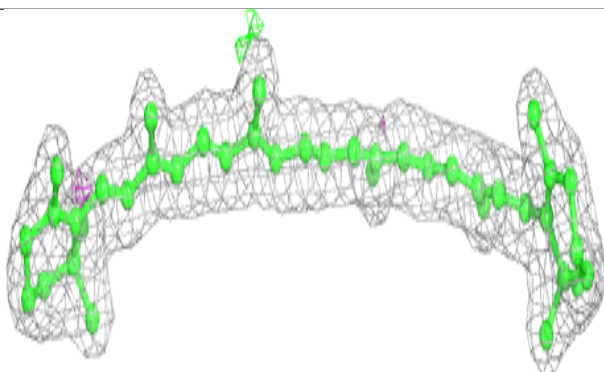
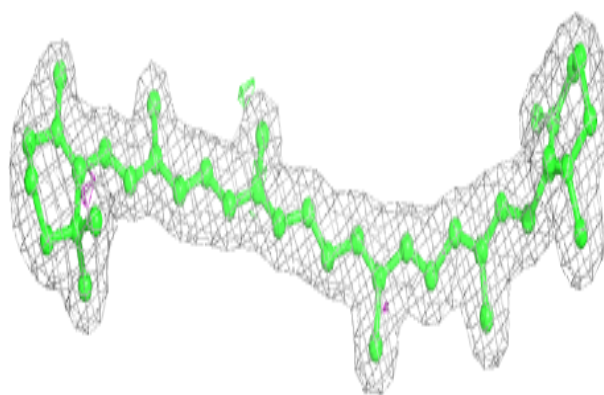
**Electron density around DGD C 520:**

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

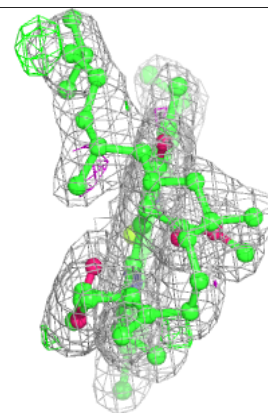
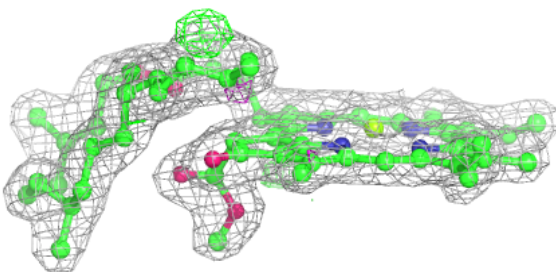
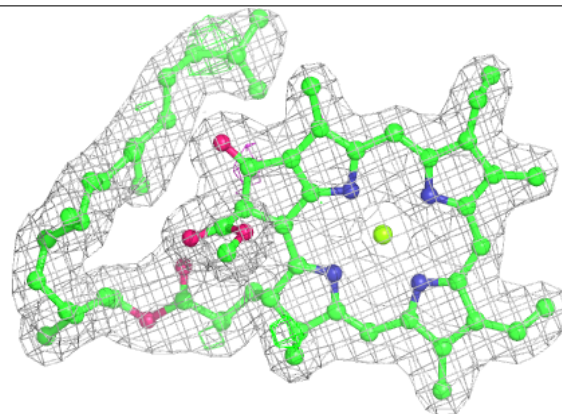


Electron density around BCR T 101:

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

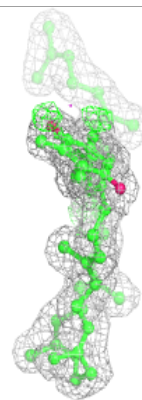
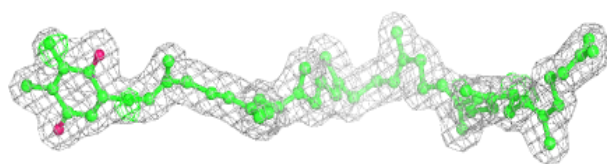
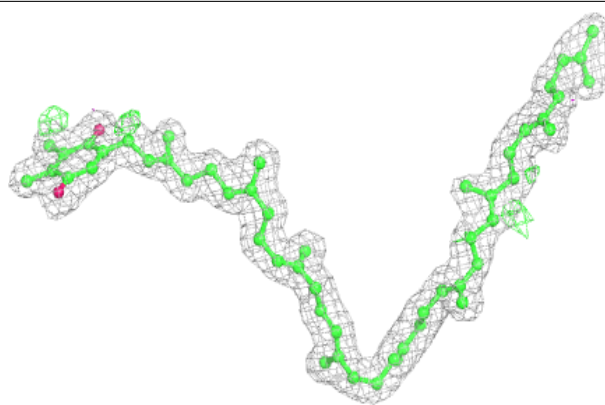
**Electron density around CLA b 614:**

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

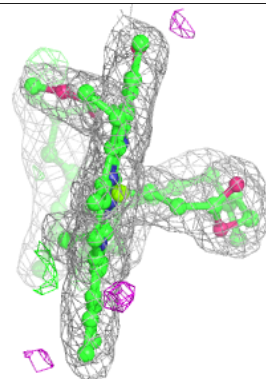
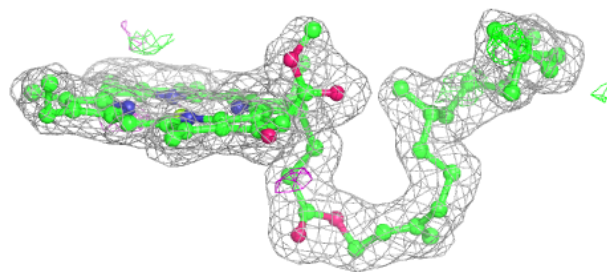
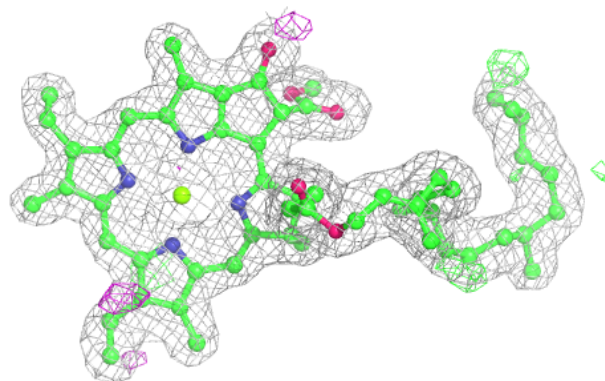


Electron density around PL9 D 408:

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

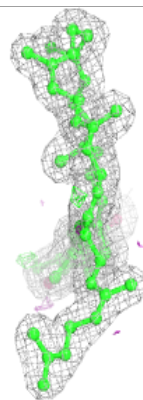
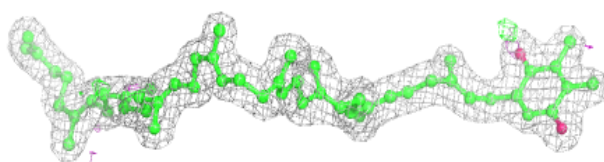
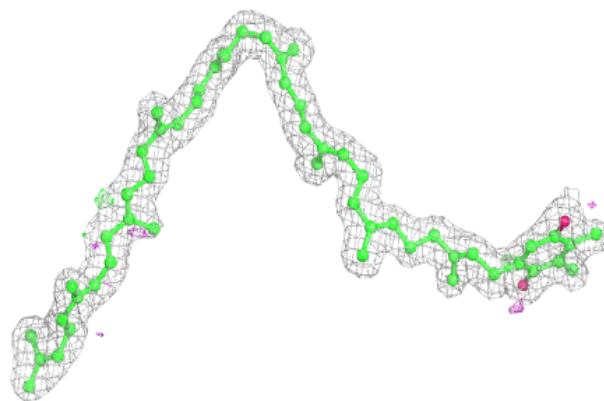
**Electron density around CLA b 616:**

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

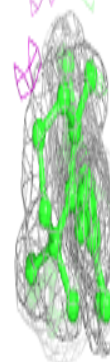
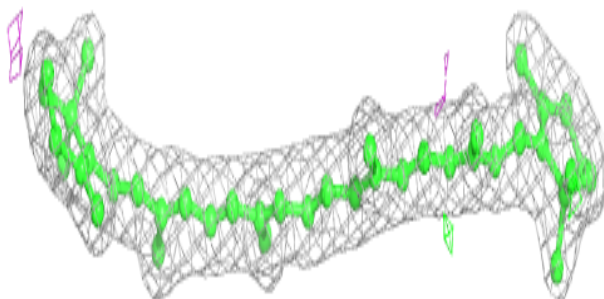
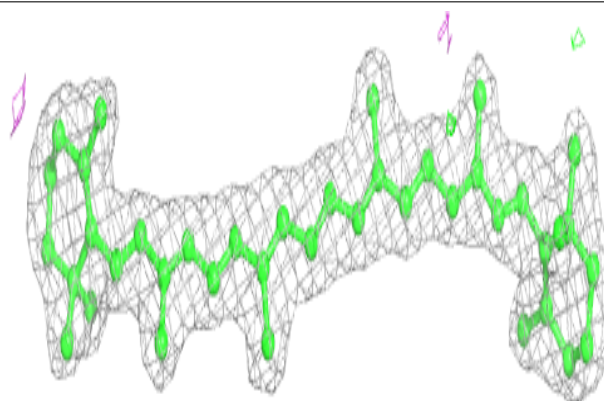


Electron density around PL9 d 408:

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

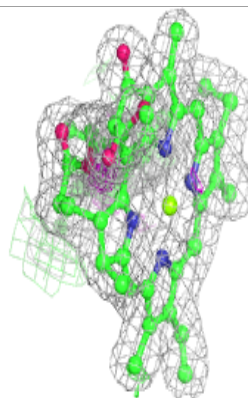
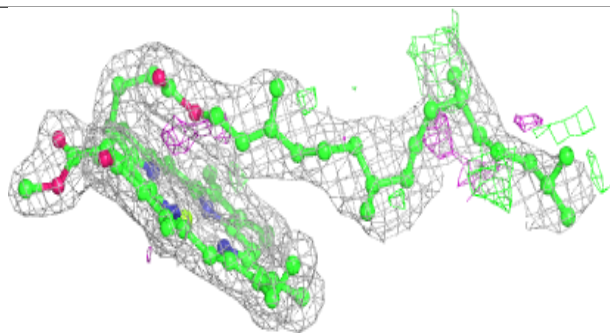
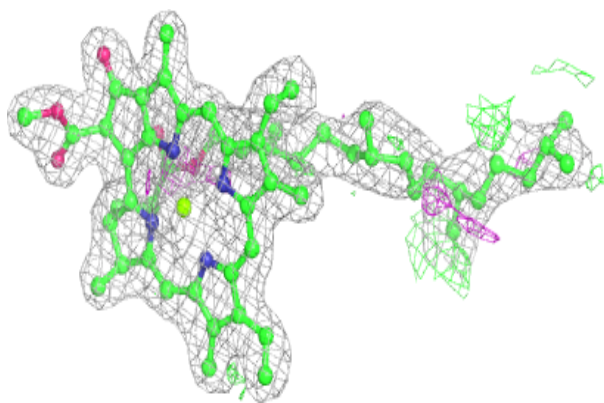
**Electron density around BCR b 623:**

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



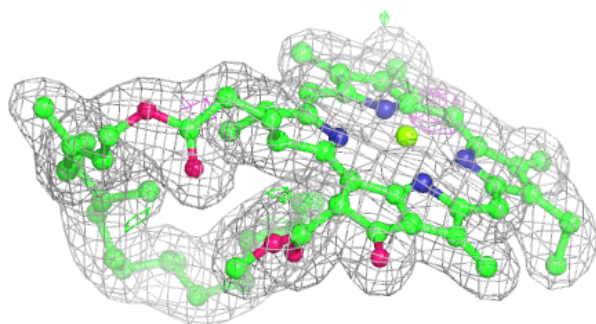
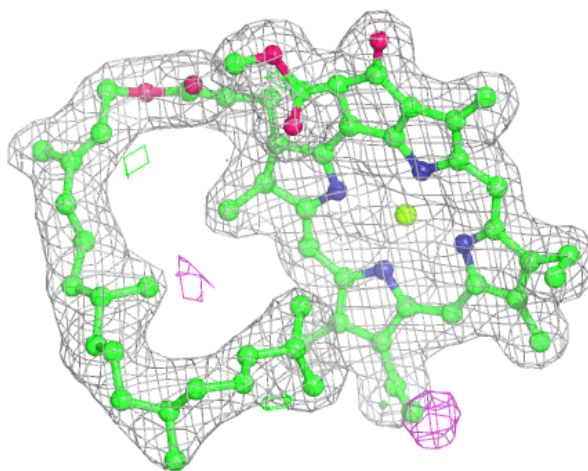
Electron density around CLA b 618:

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



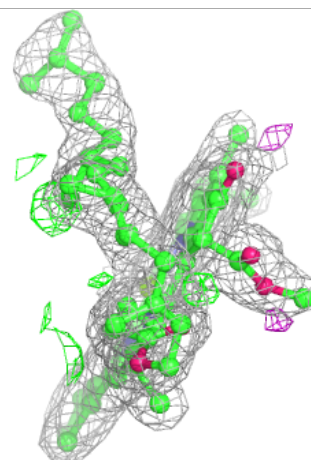
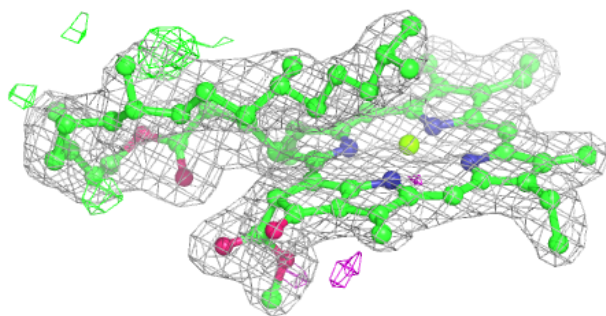
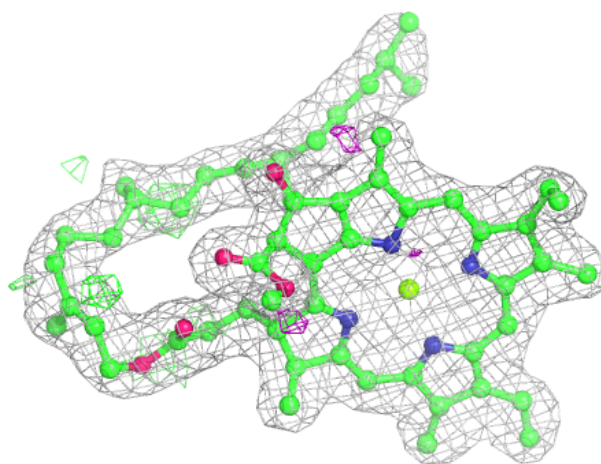
Electron density around CLA b 619:

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



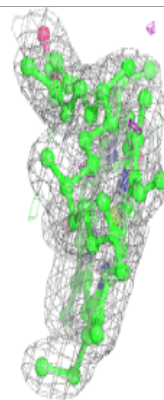
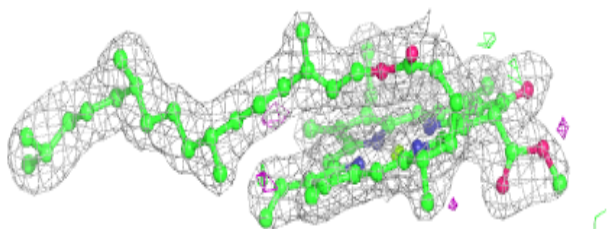
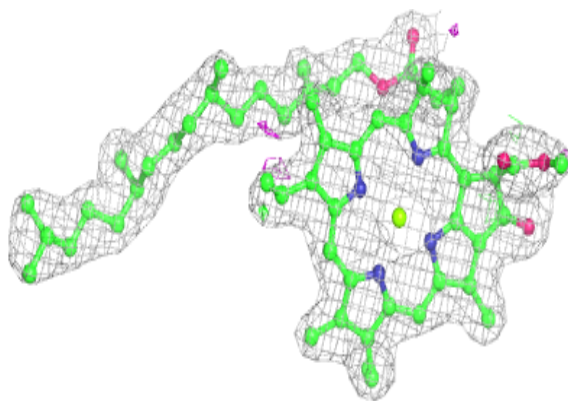
Electron density around CLA C 511:

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

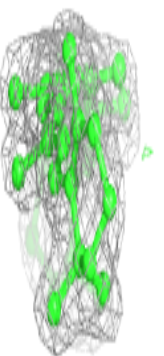
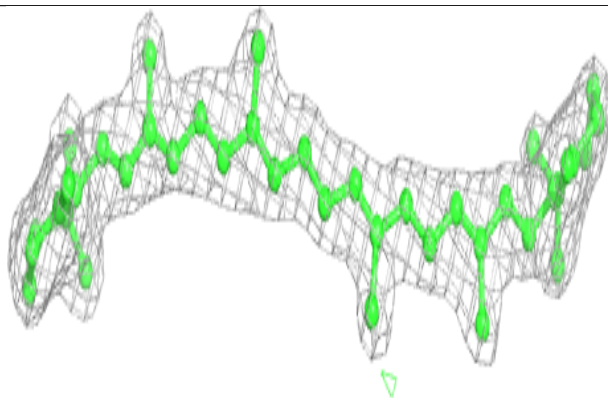
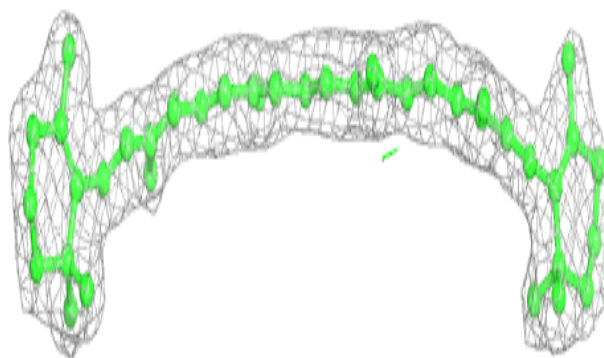


Electron density around CLA c 503:

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

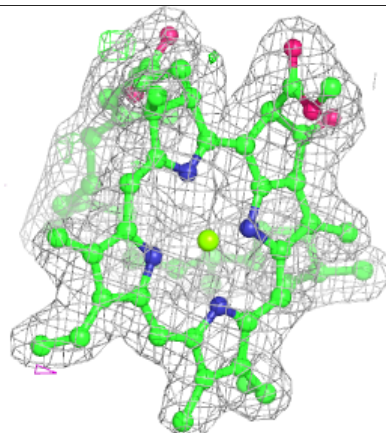
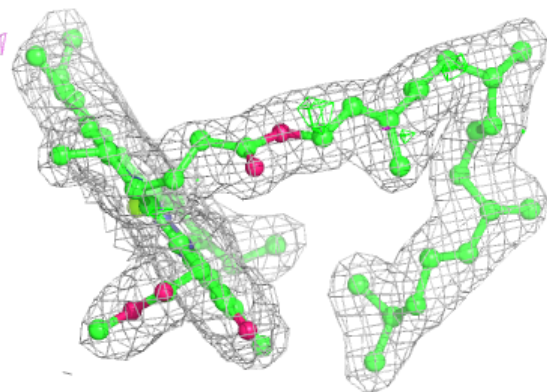
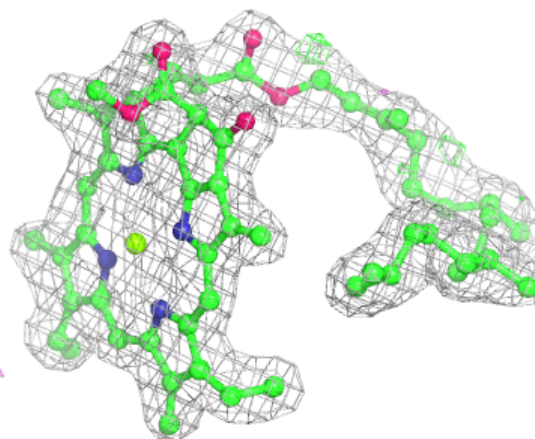
**Electron density around BCR k 103:**

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

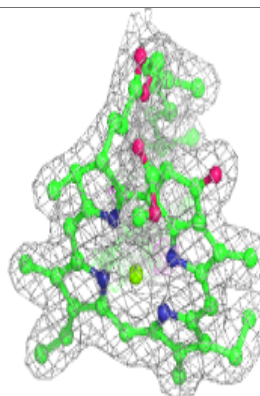
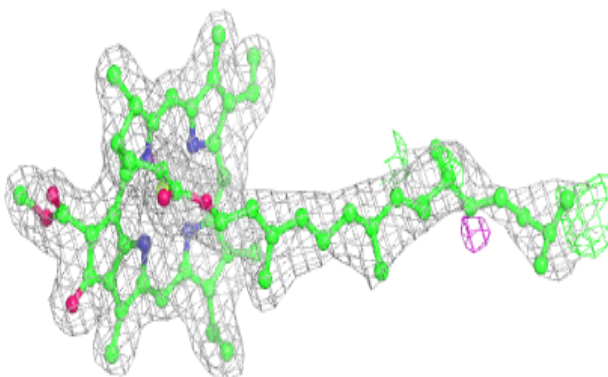
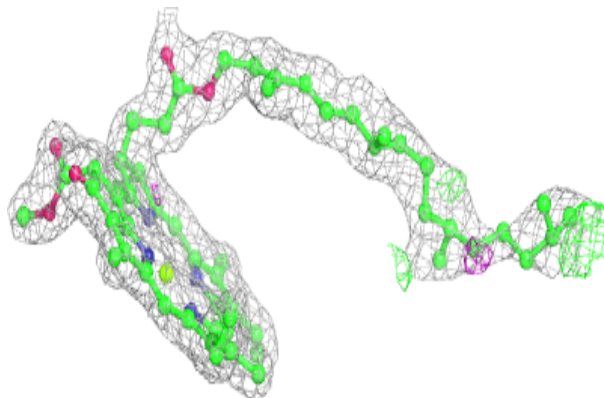


Electron density around CLA c 505:

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

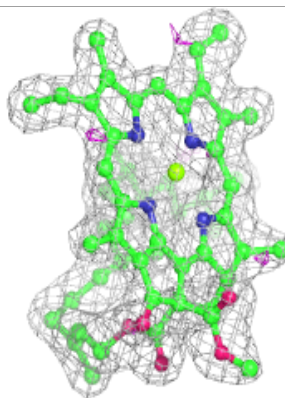
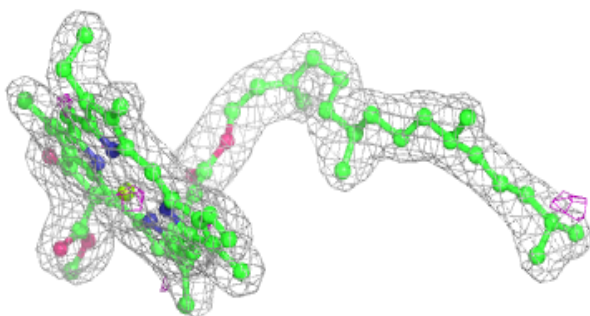
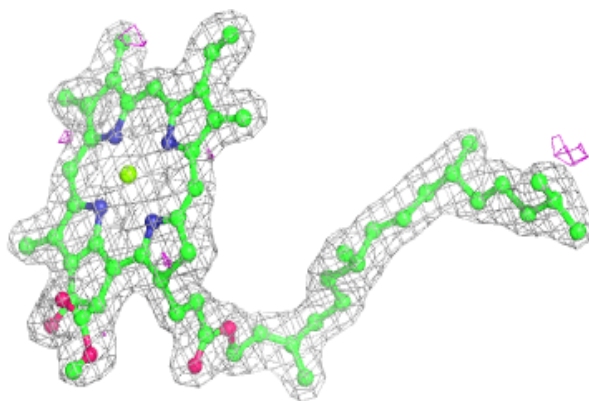
**Electron density around CLA c 506:**

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



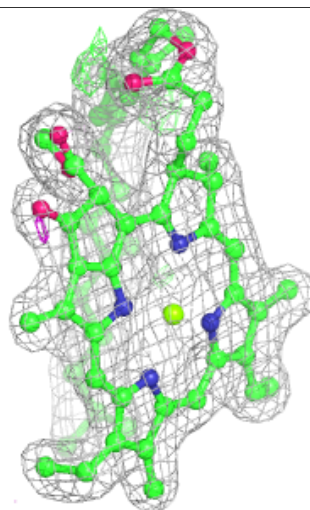
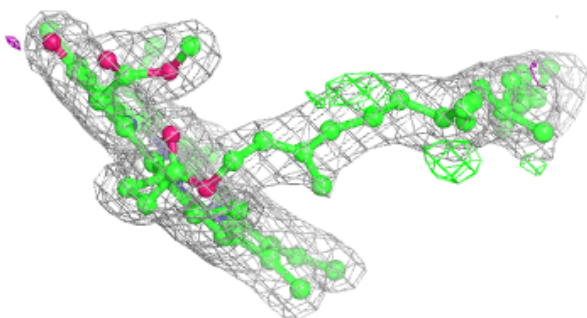
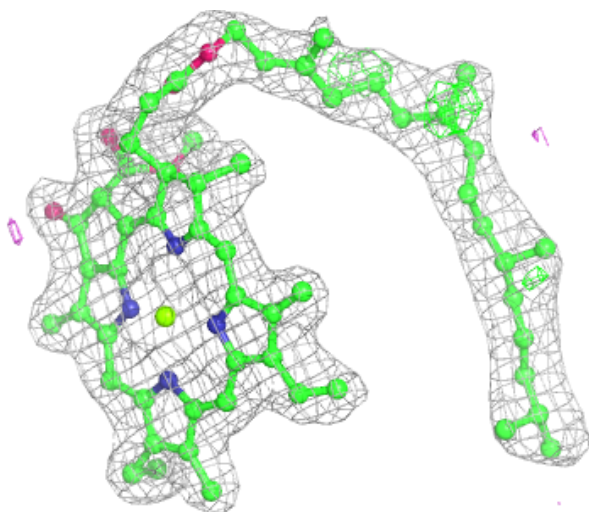
Electron density around CLA C 513:

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



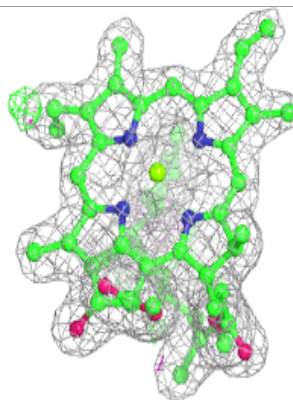
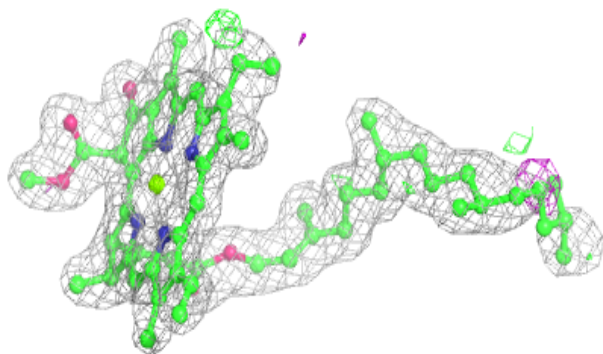
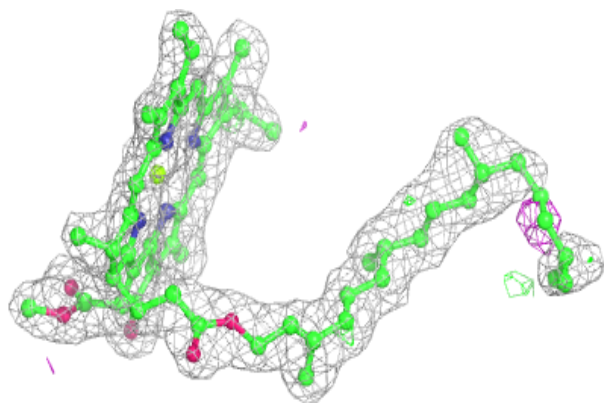
Electron density around CLA c 509:

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



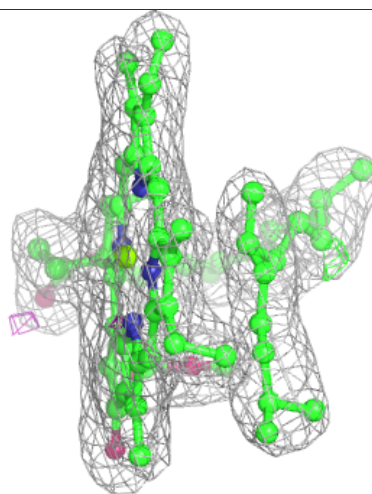
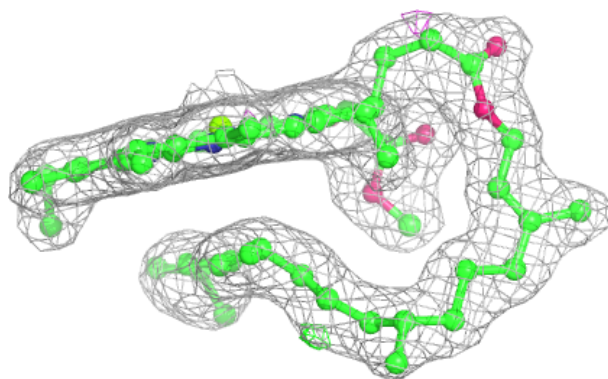
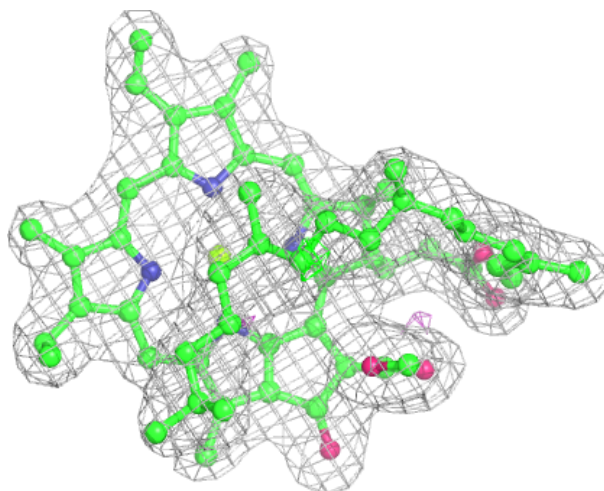
Electron density around CLA c 510:

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



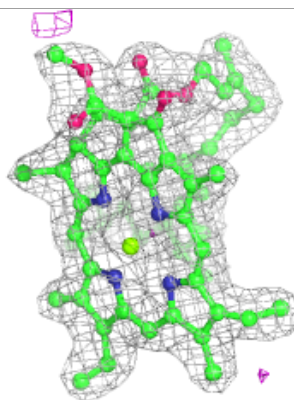
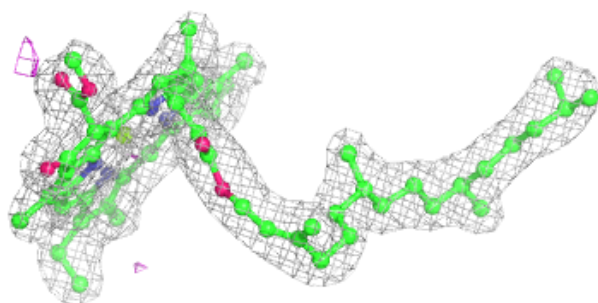
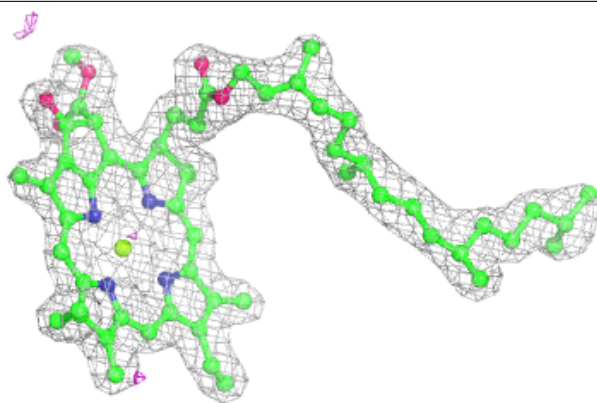
Electron density around CLA c 512:

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

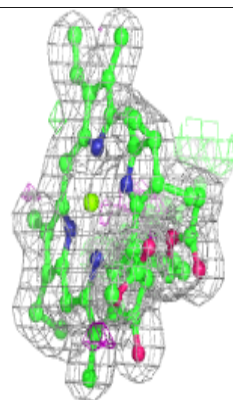
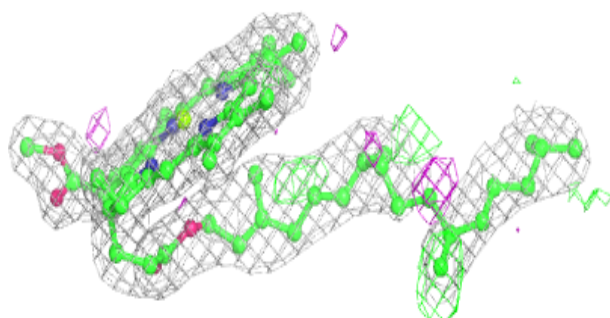
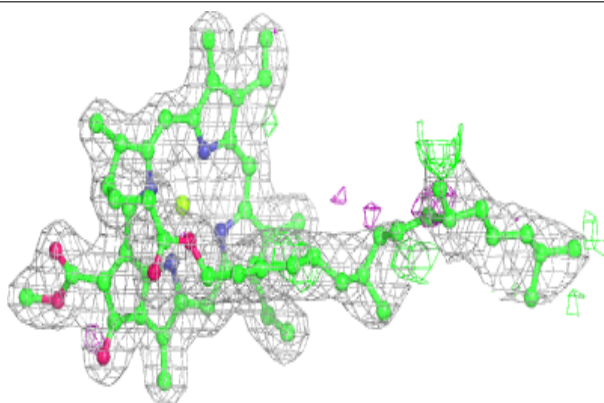


Electron density around CLA c 513:

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

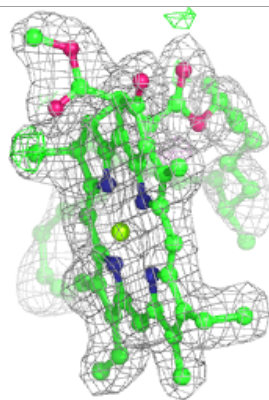
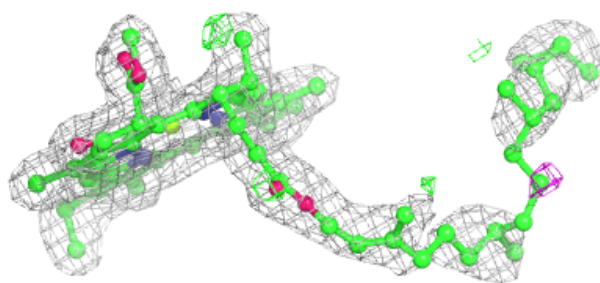
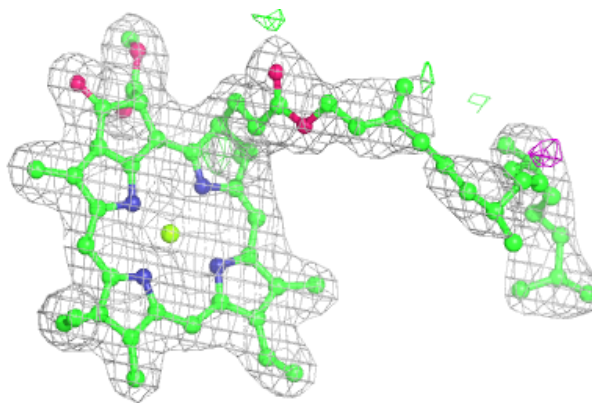
**Electron density around CLA B 616:**

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

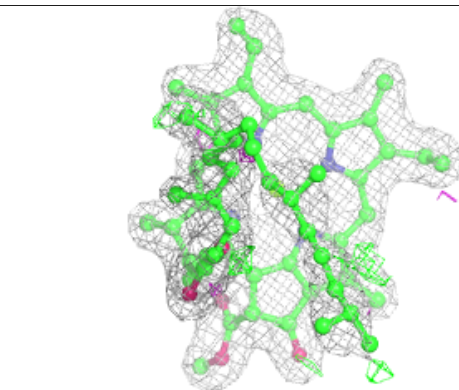
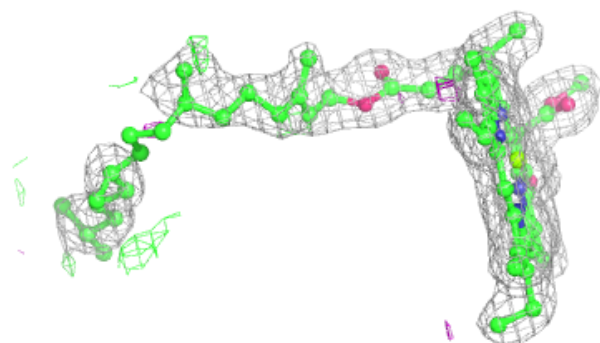
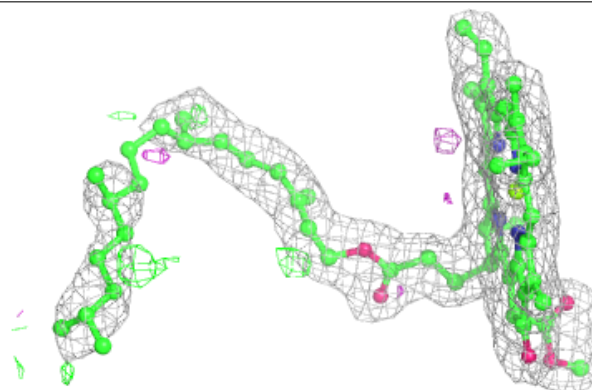


Electron density around CLA A 409:

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

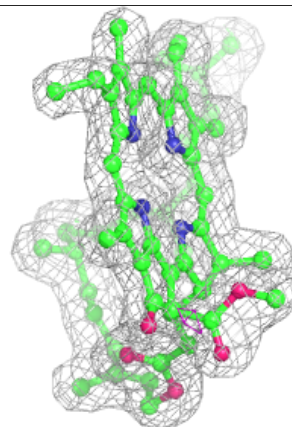
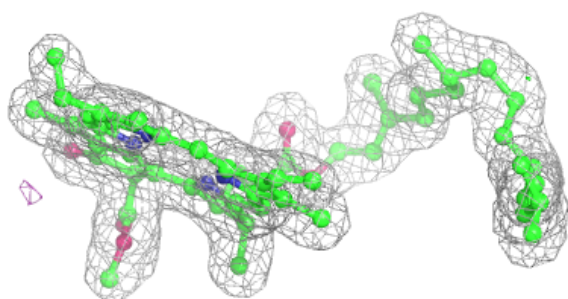
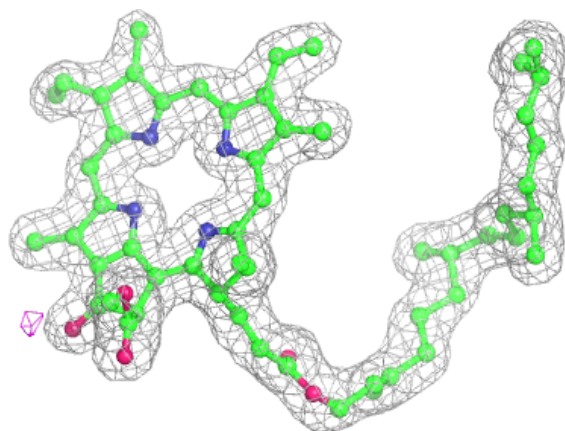
**Electron density around CLA d 406:**

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

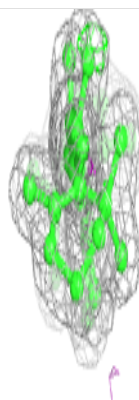
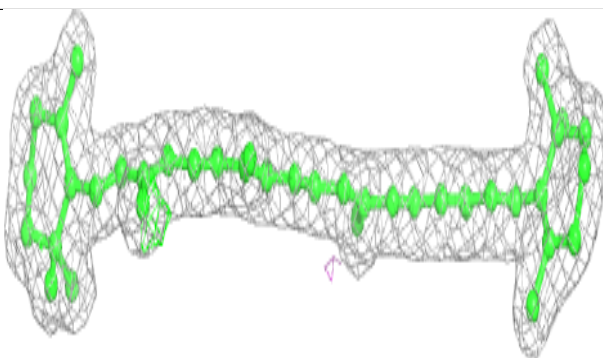
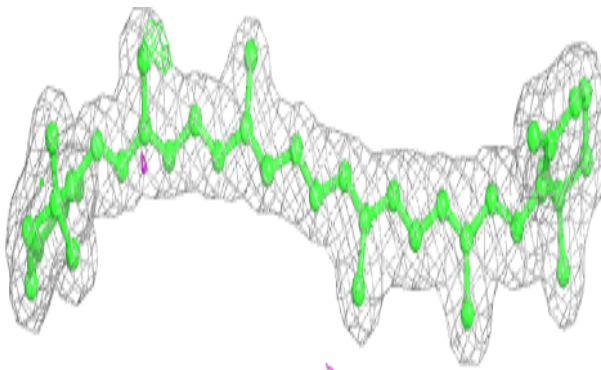


Electron density around PHO A 408:

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

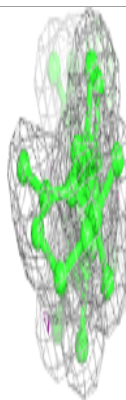
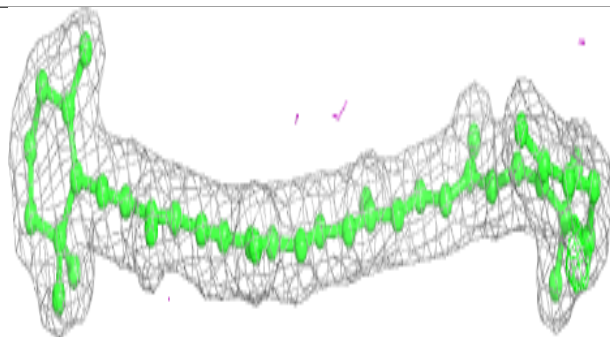
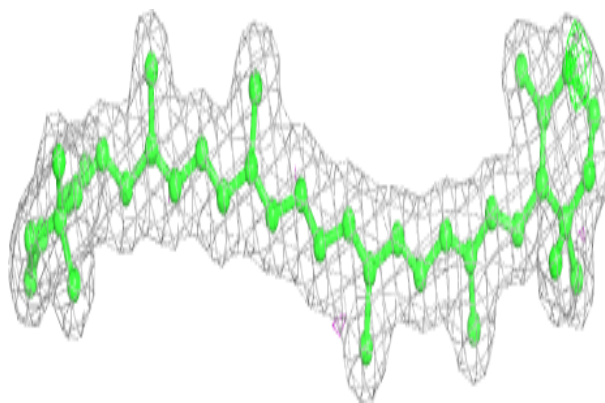
**Electron density around BCR A 410:**

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



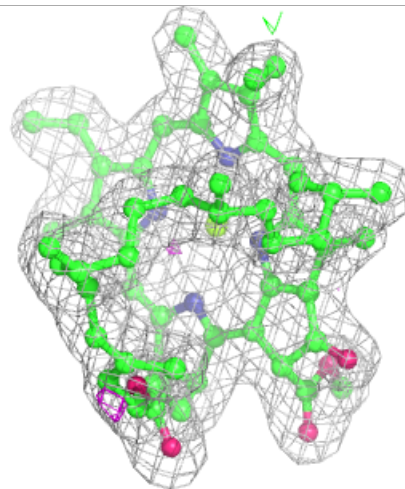
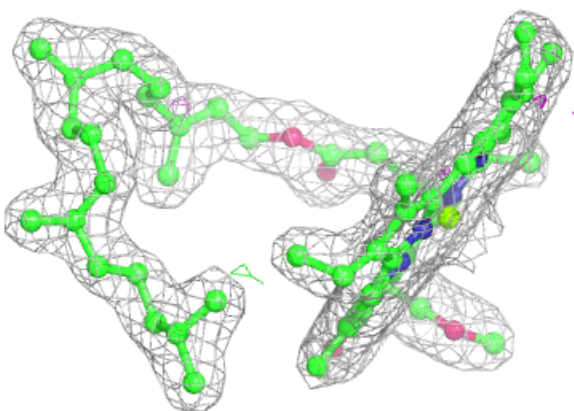
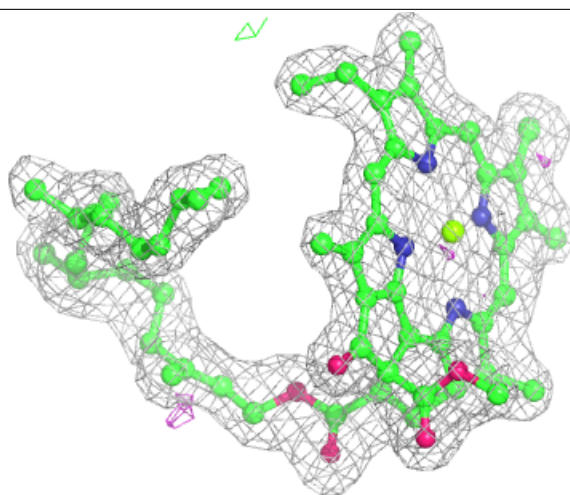
Electron density around BCR B 619:

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



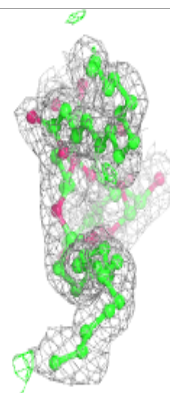
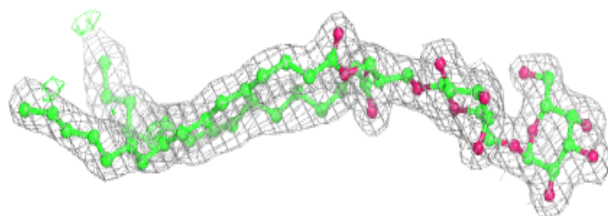
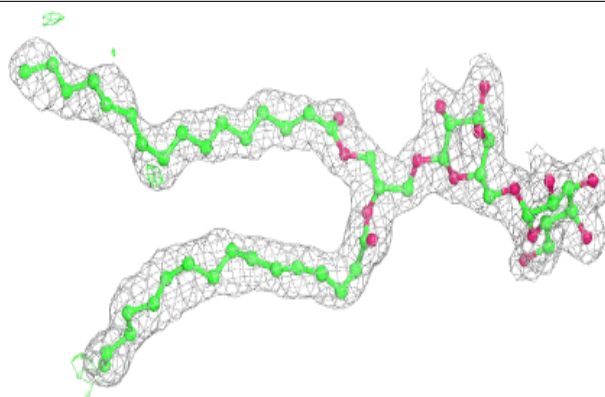
Electron density around CLA C 505:

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

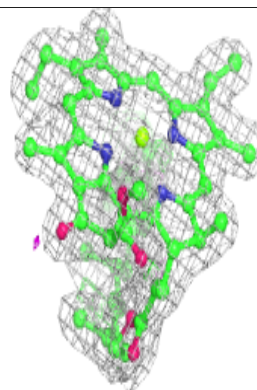
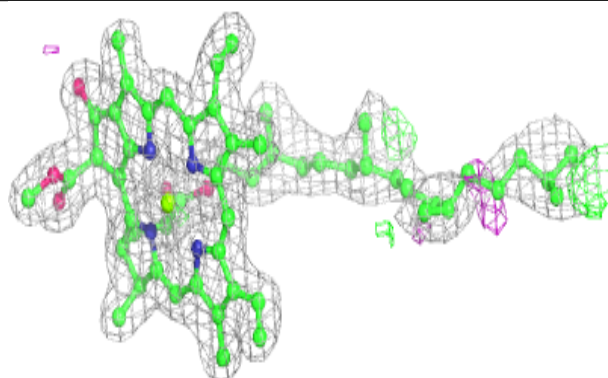
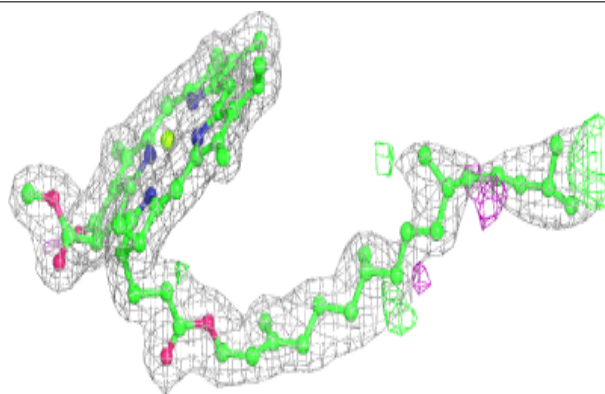


Electron density around DGD c 520:

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

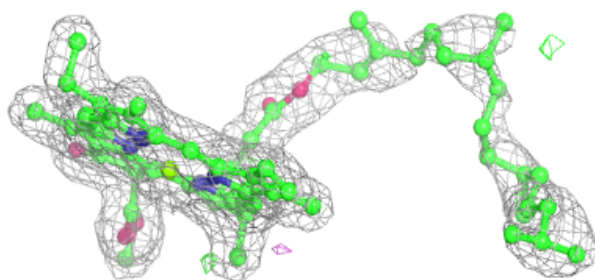
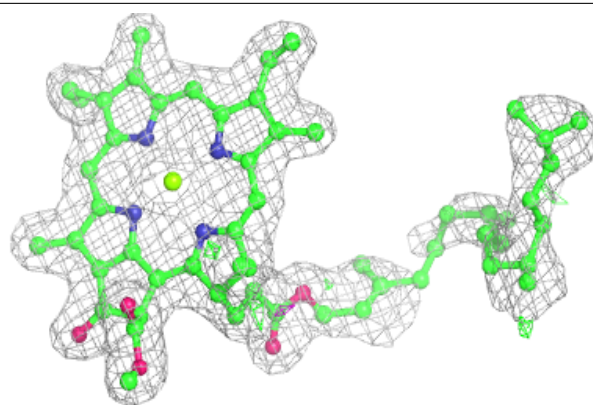
**Electron density around CLA C 506:**

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

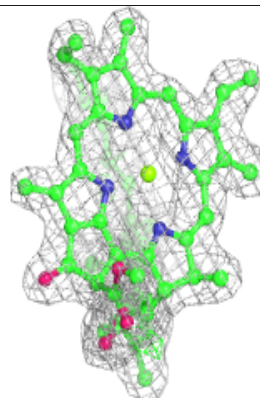
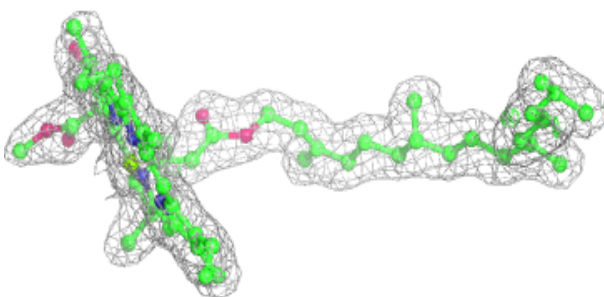
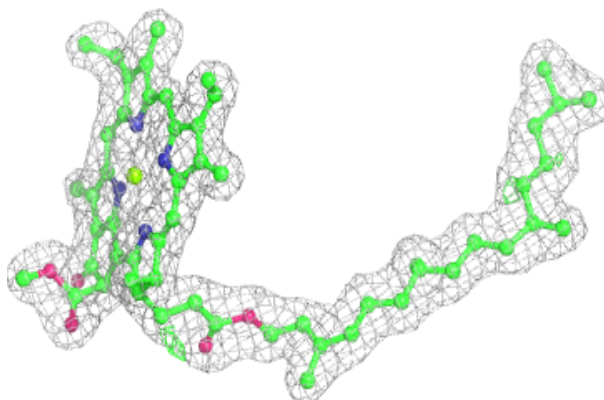


Electron density around CLA a 413:

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

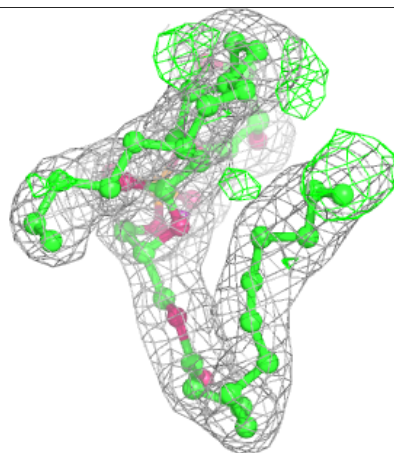
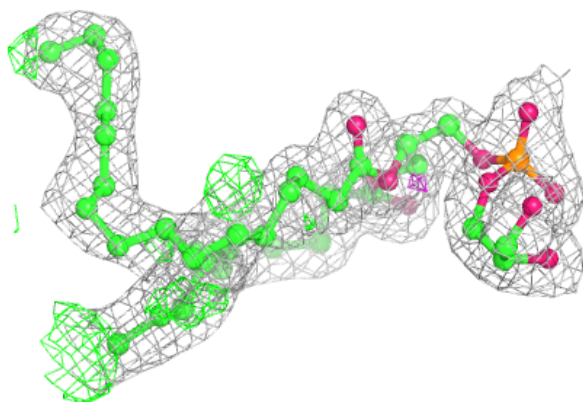
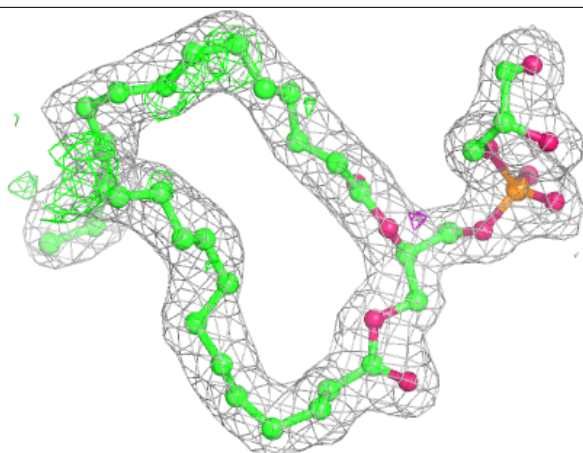
**Electron density around CLA B 611:**

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

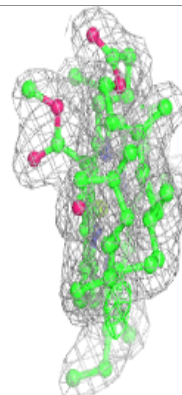
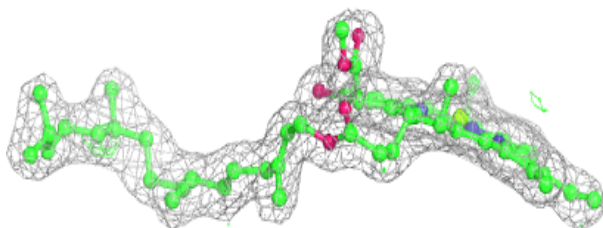
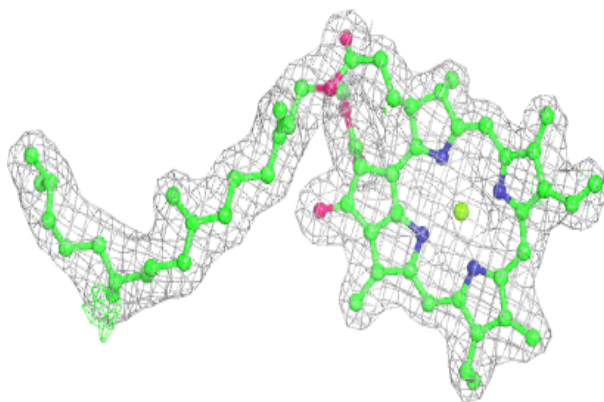


Electron density around LHG D 412:

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

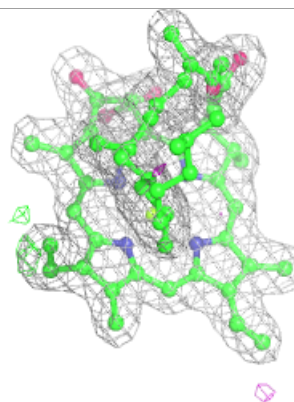
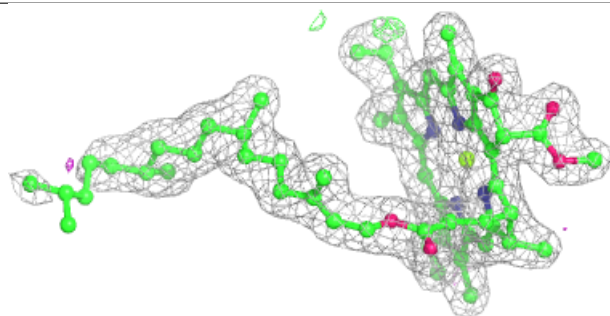
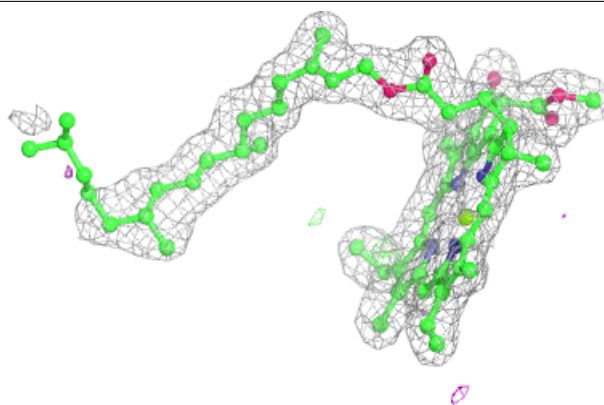
**Electron density around CLA b 606:**

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

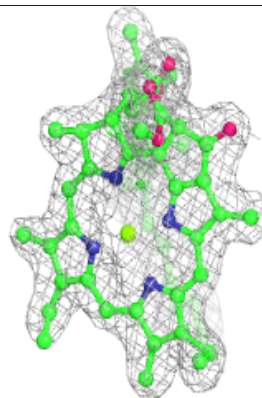
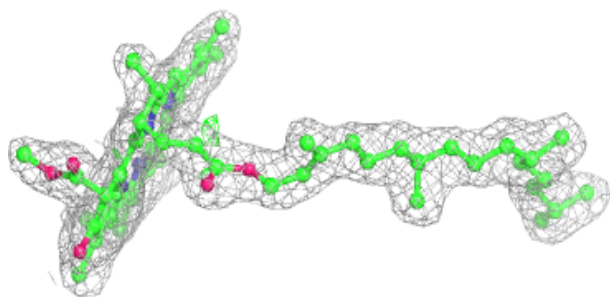
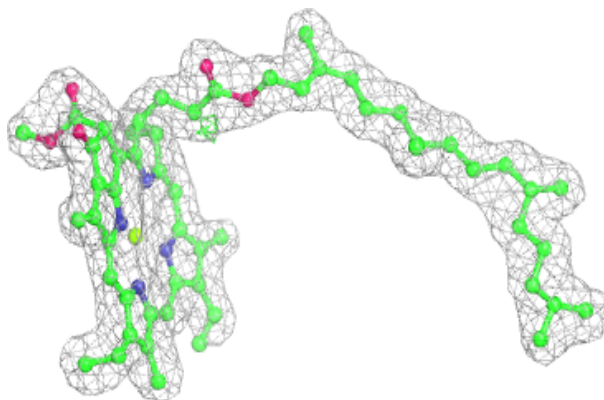


Electron density around CLA C 510:

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

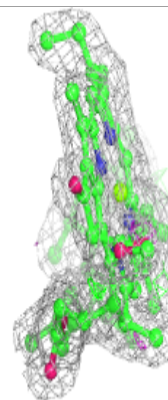
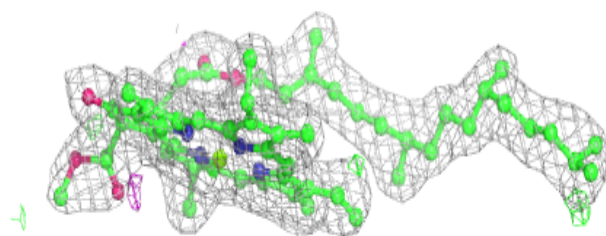
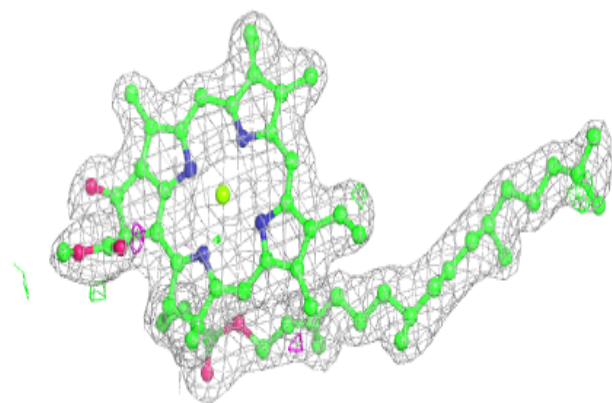
**Electron density around CLA b 613:**

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



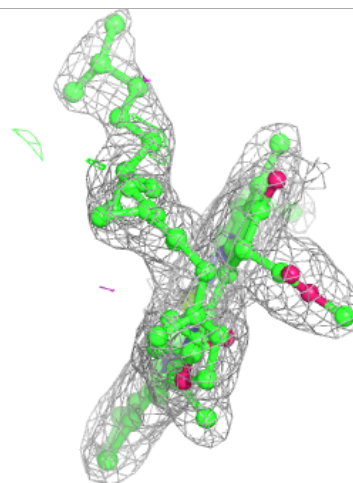
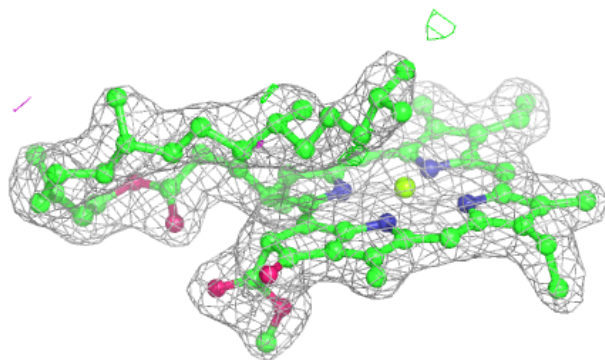
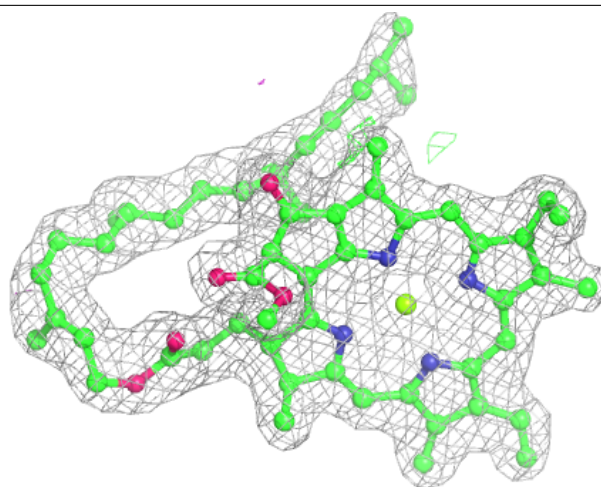
Electron density around CLA C 503:

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



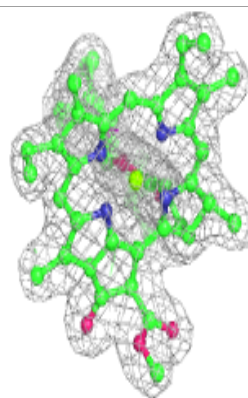
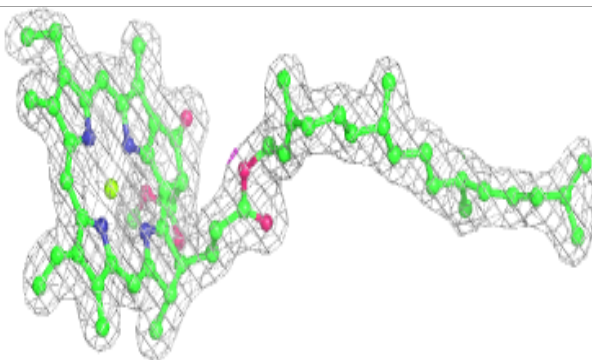
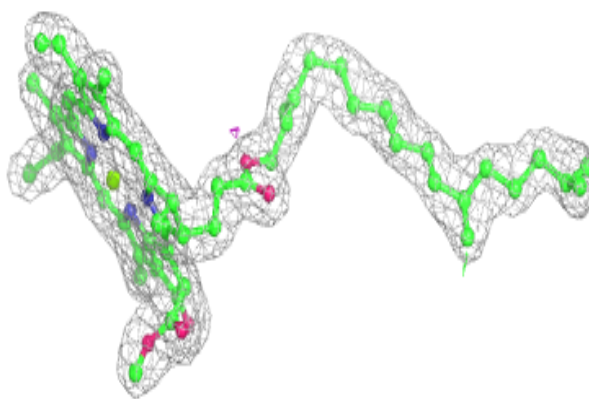
Electron density around CLA c 511:

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

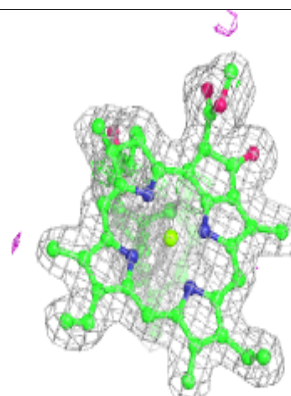
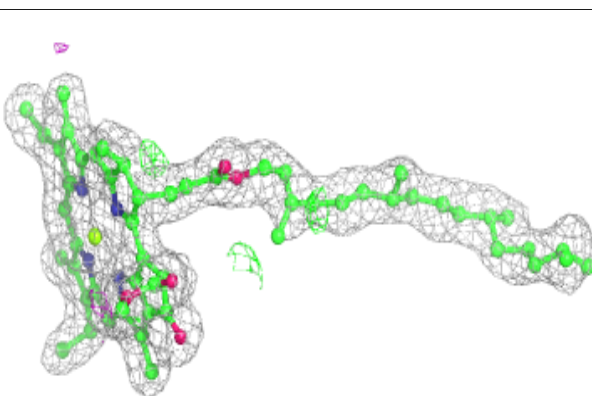
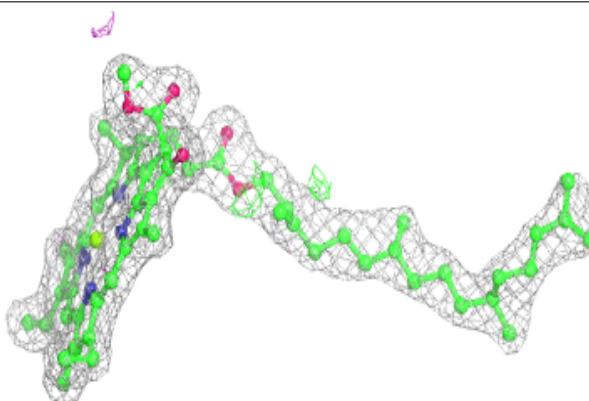


Electron density around CLA C 504:

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

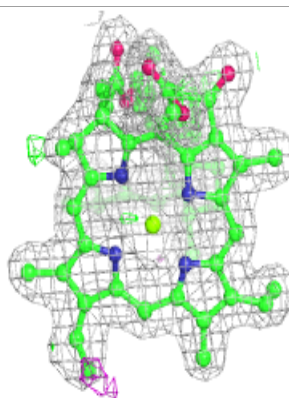
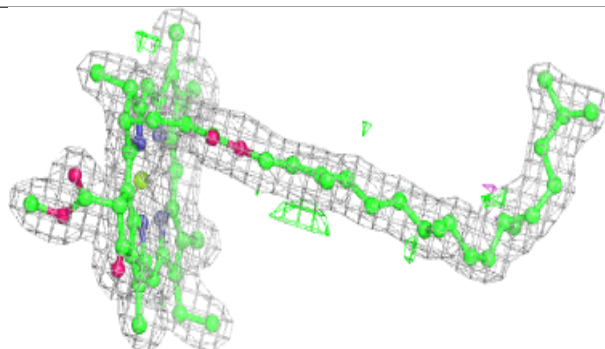
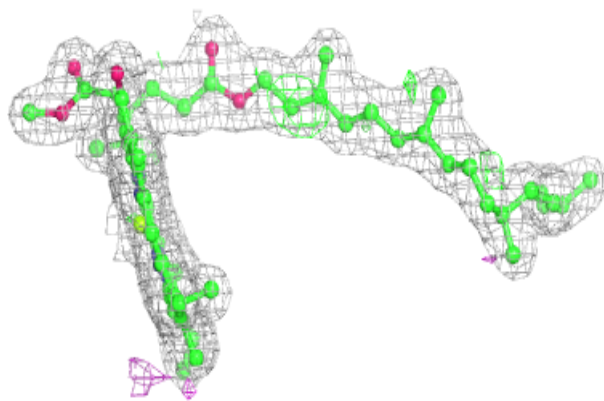
**Electron density around CLA B 606:**

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

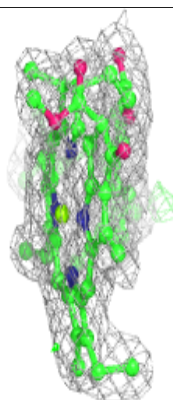
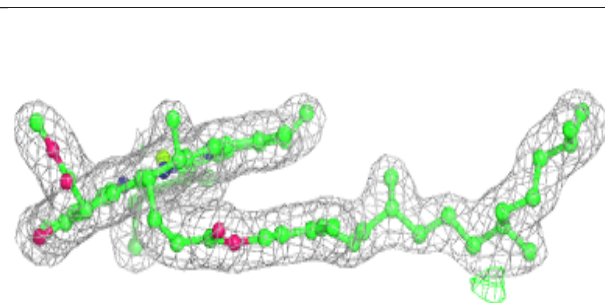
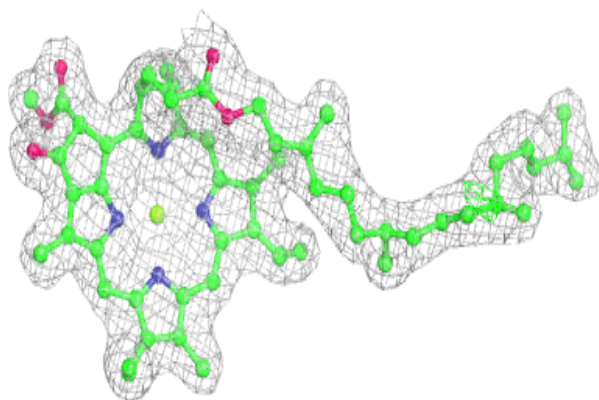


Electron density around CLA B 607:

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

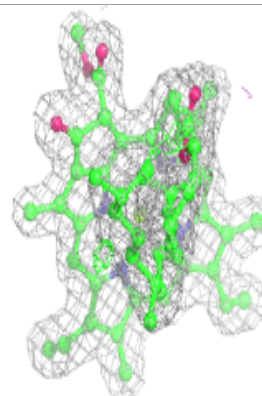
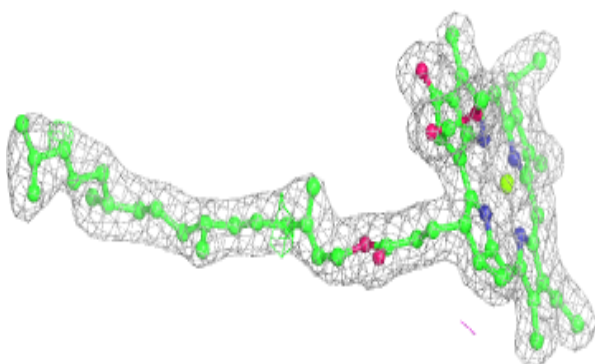
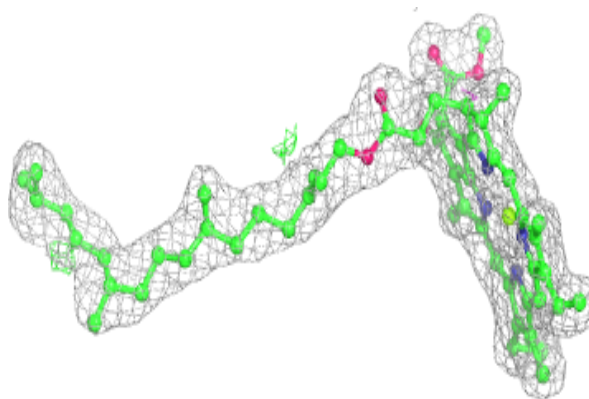
**Electron density around CLA b 607:**

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

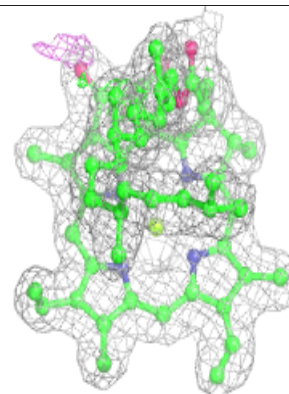
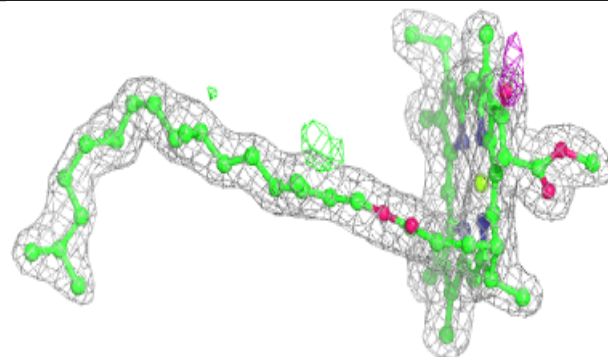
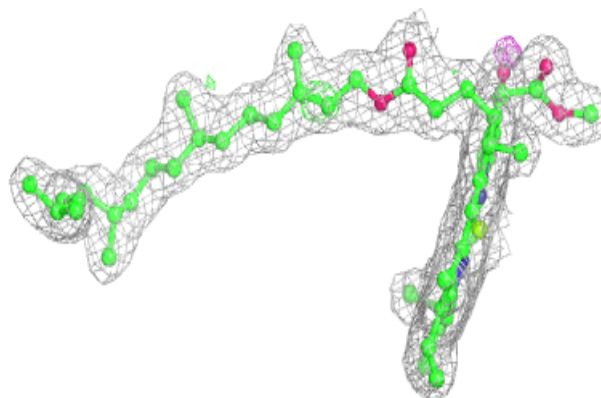


Electron density around CLA b 608:

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

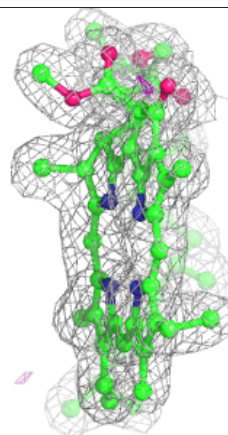
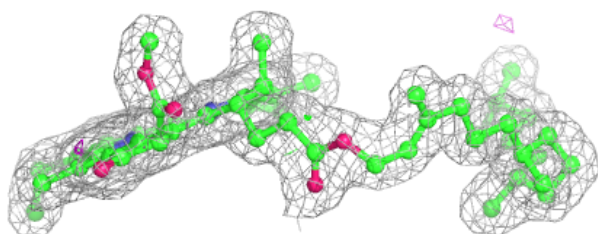
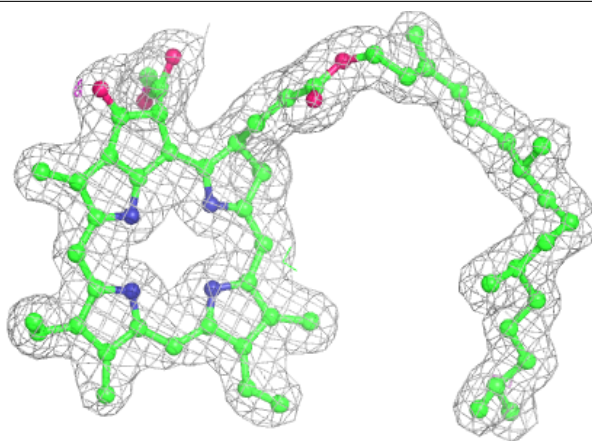
**Electron density around CLA b 609:**

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

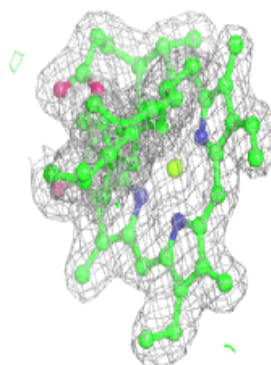
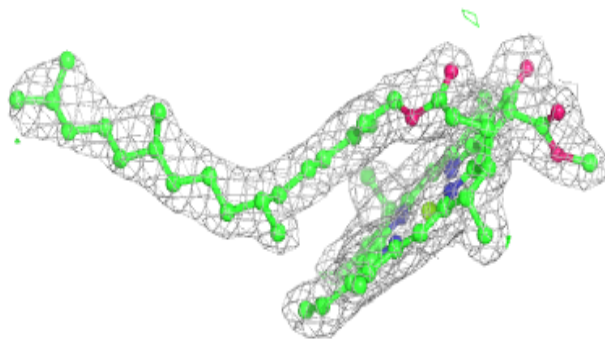
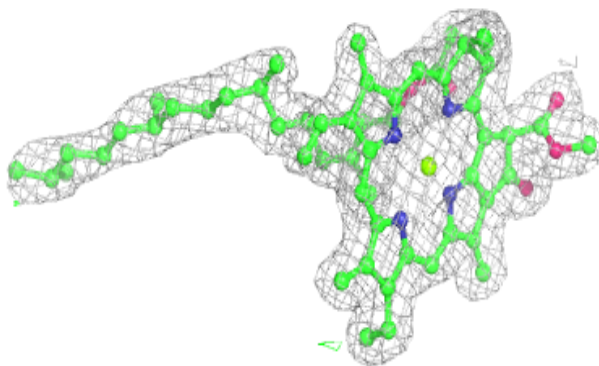


Electron density around PHO a 412:

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

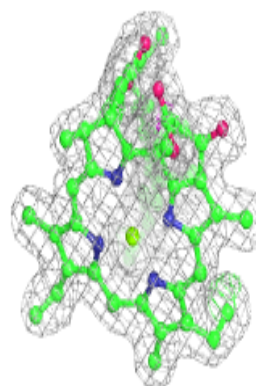
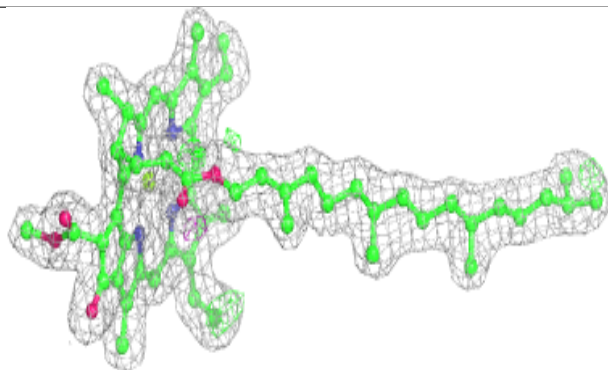
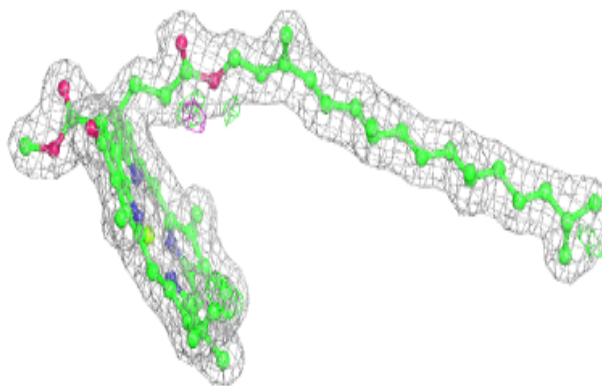
**Electron density around CLA C 507:**

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

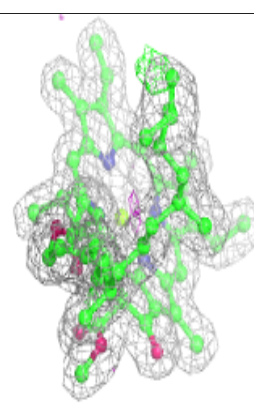
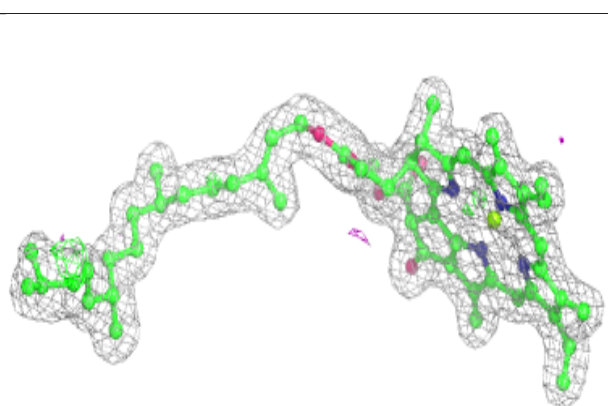
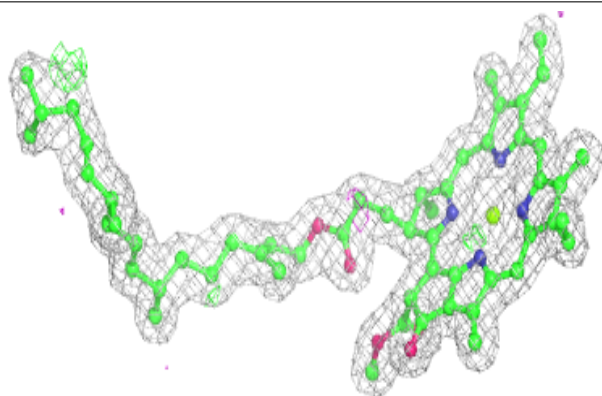


Electron density around CLA b 611:

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

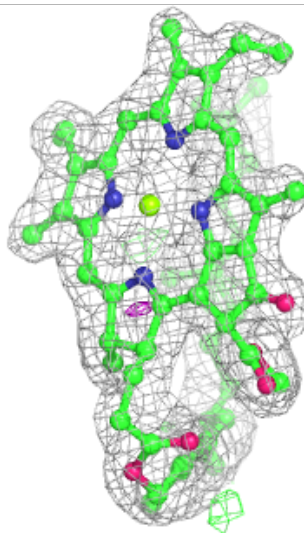
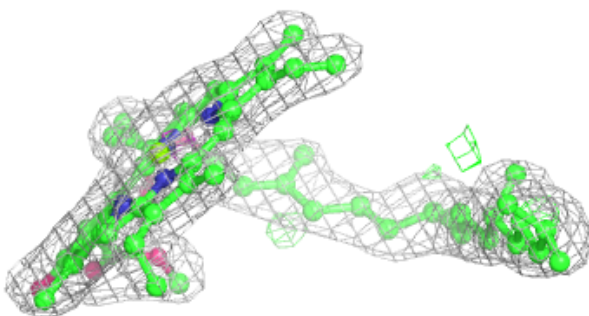
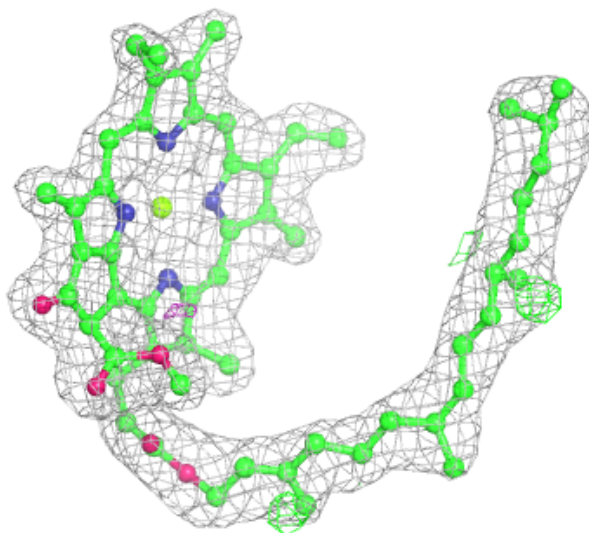
**Electron density around CLA A 405:**

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



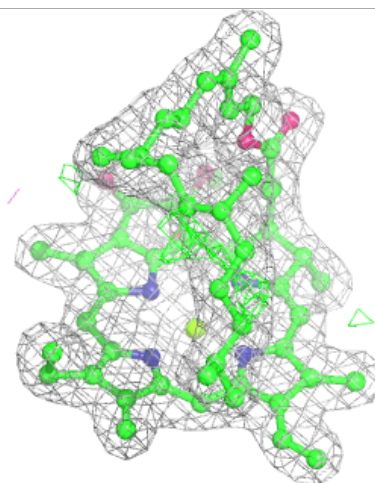
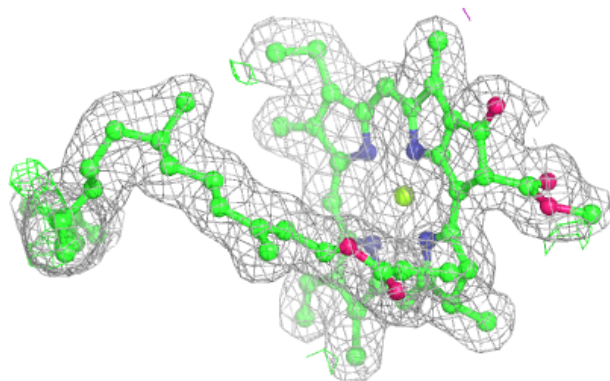
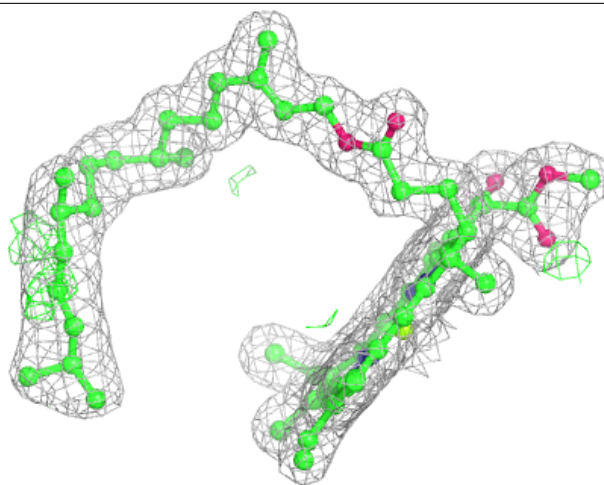
Electron density around CLA C 509:

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



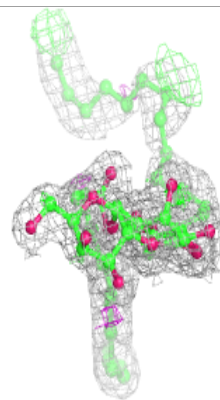
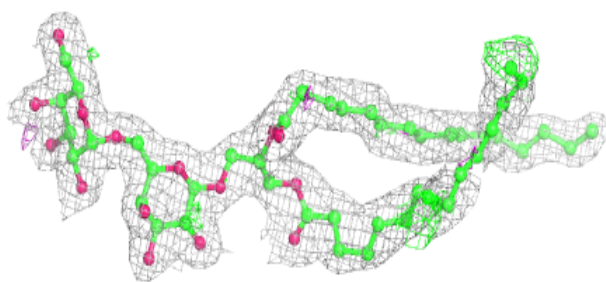
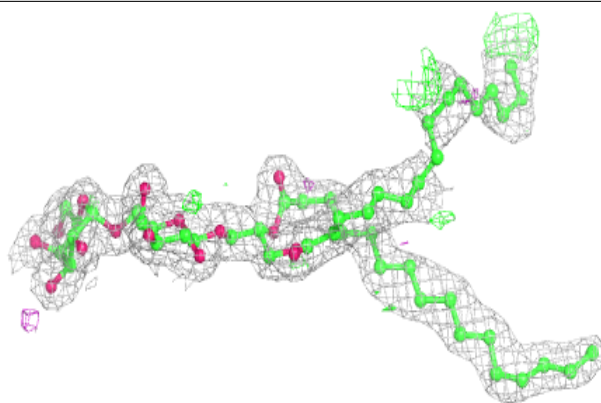
Electron density around CLA b 615:

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

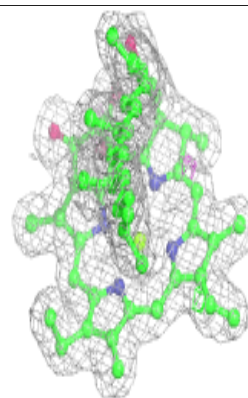
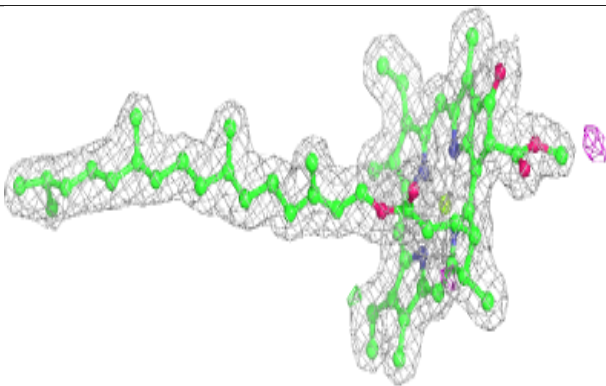
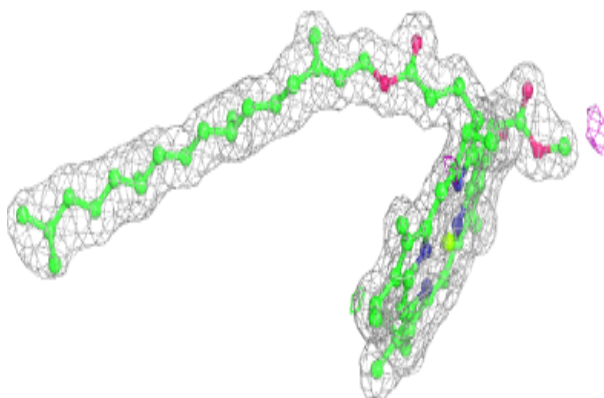


Electron density around DGD C 518:

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

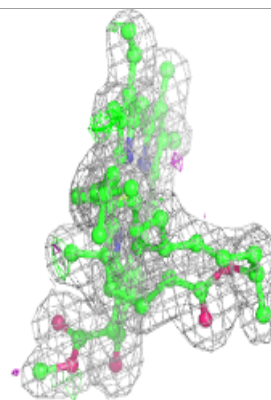
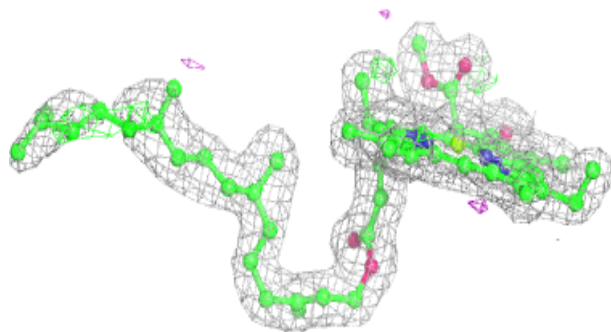
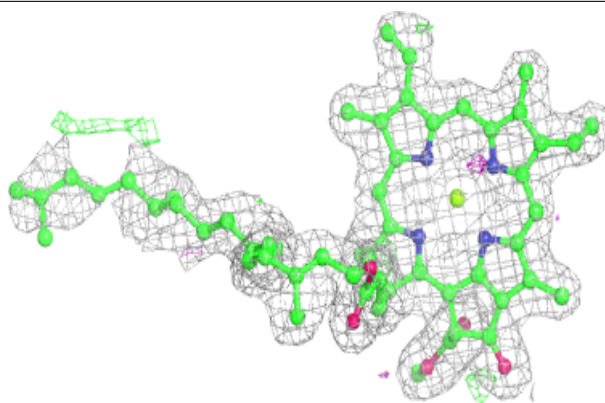
**Electron density around CLA B 609:**

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



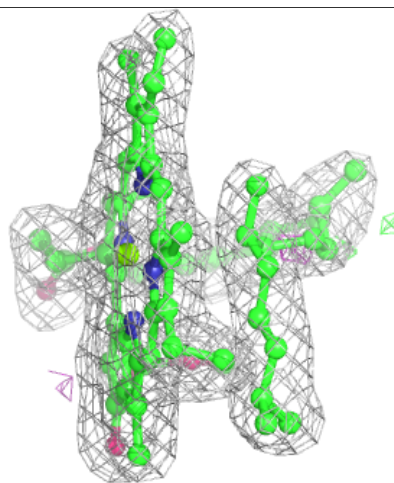
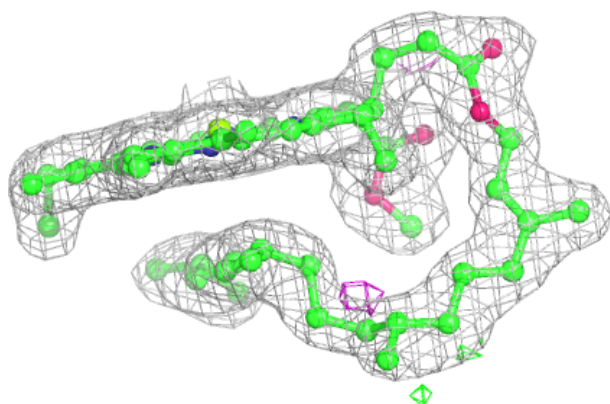
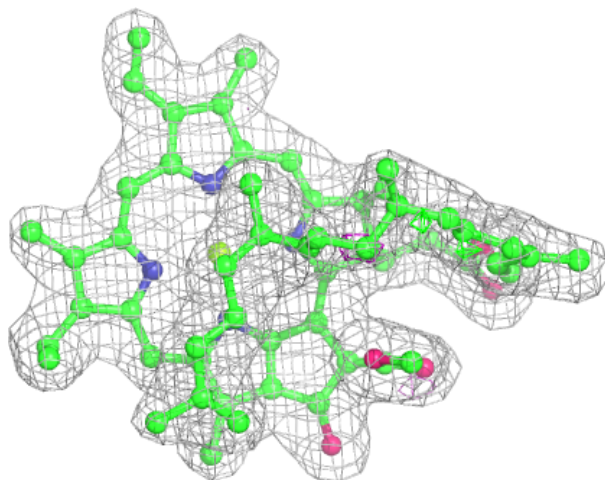
Electron density around CLA A 406:

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



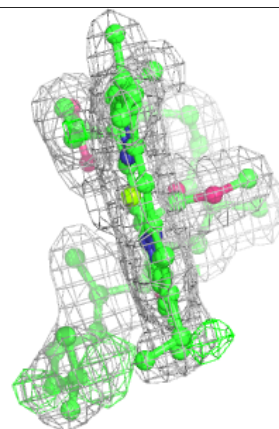
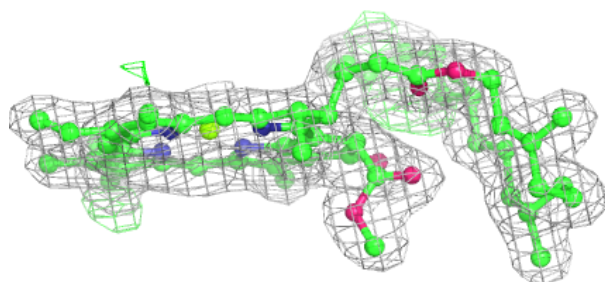
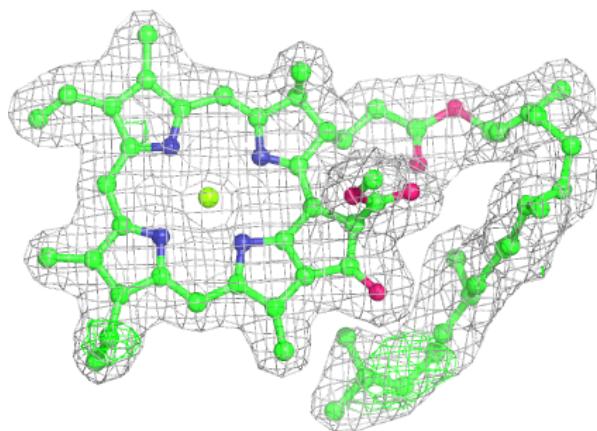
Electron density around CLA C 512:

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

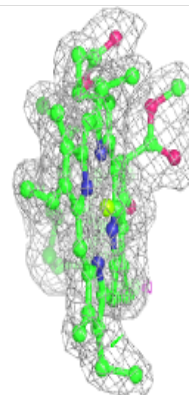
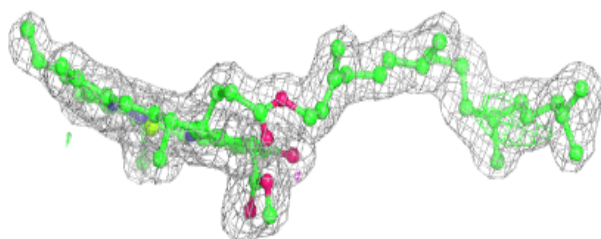
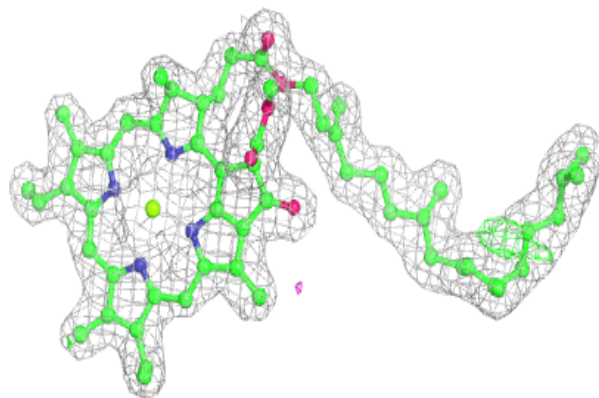


Electron density around CLA B 612:

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

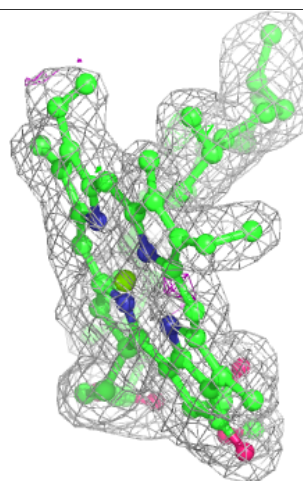
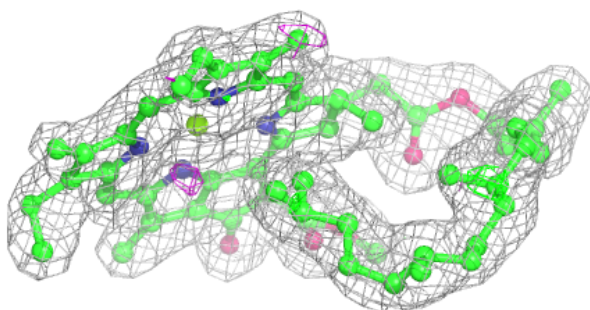
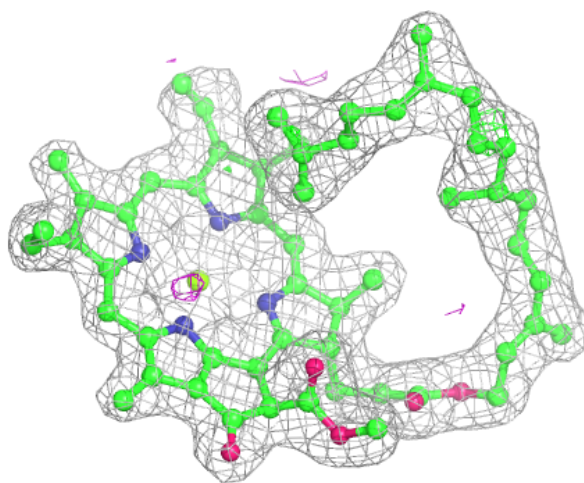
**Electron density around CLA B 604:**

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



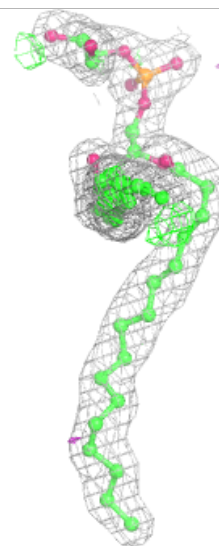
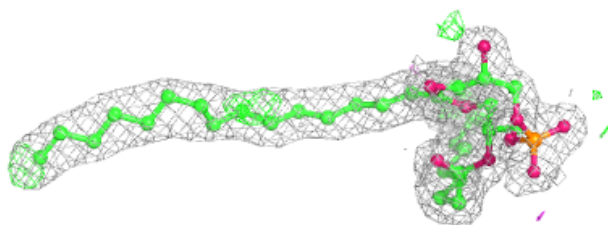
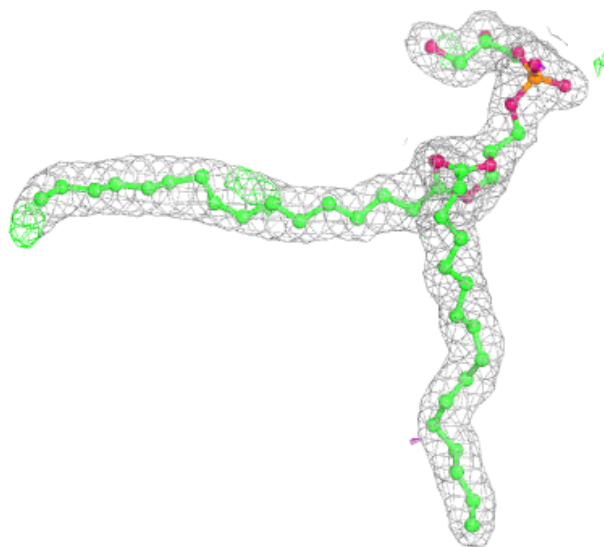
Electron density around CLA B 617:

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



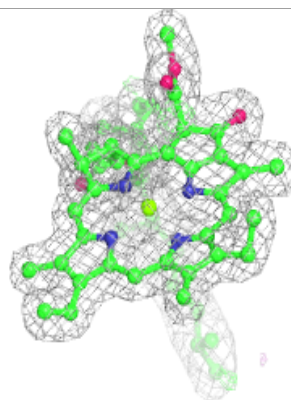
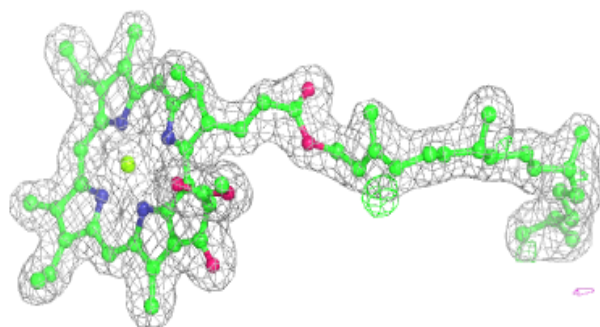
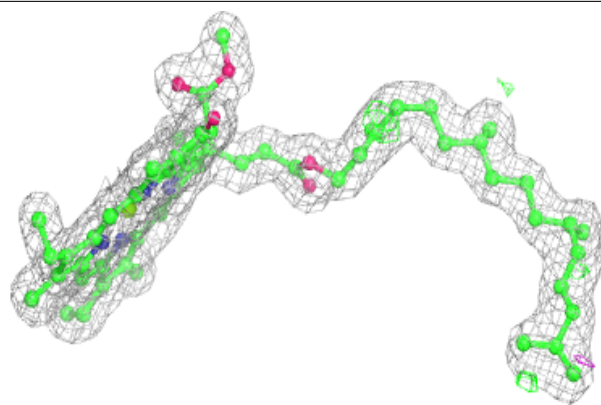
Electron density around LHG L 101:

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

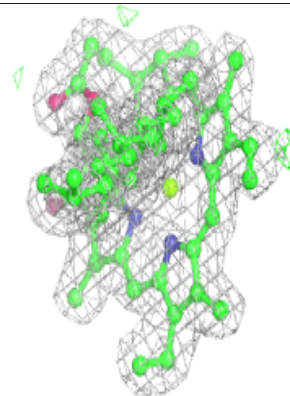
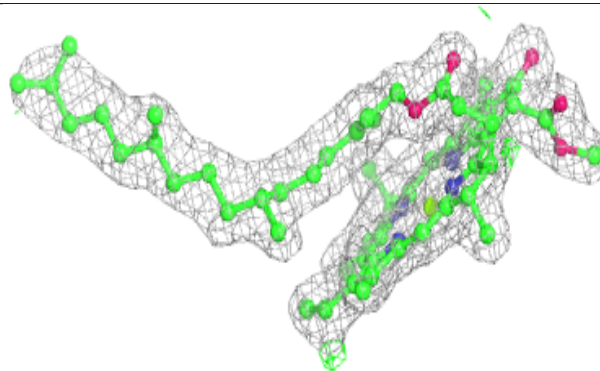
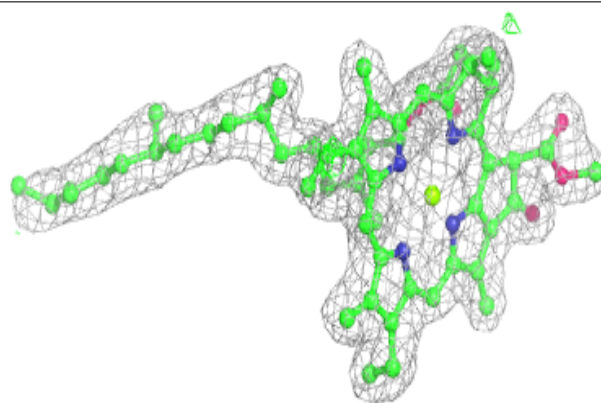


Electron density around CLA D 405:

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

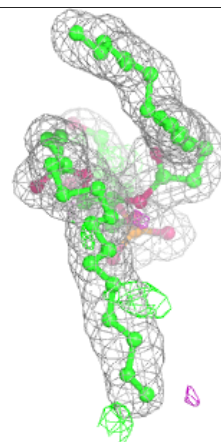
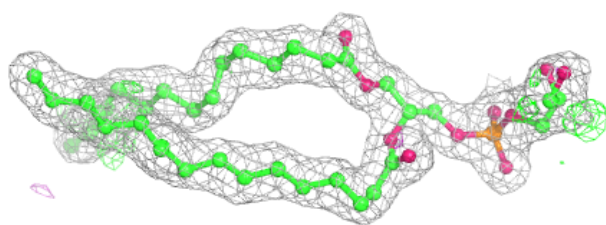
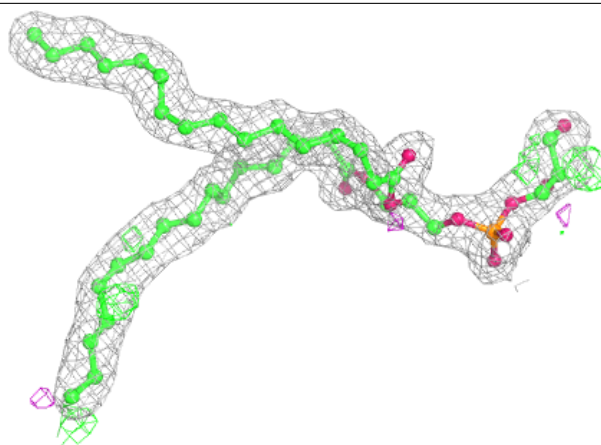
**Electron density around CLA c 507:**

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



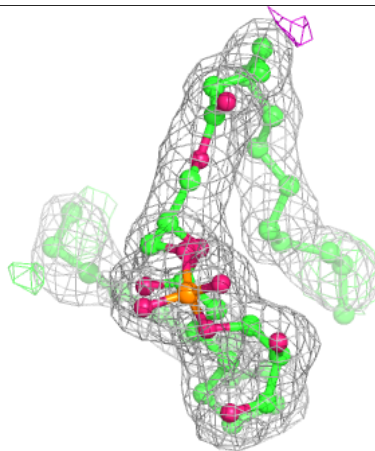
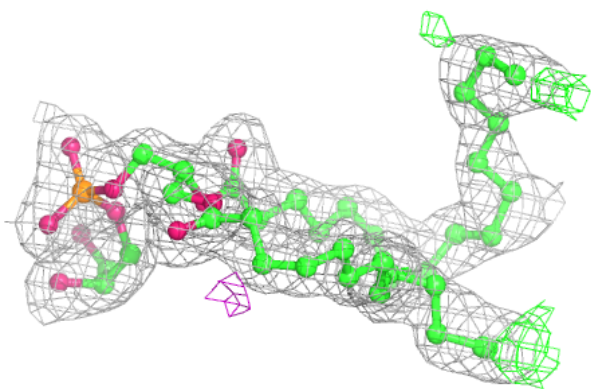
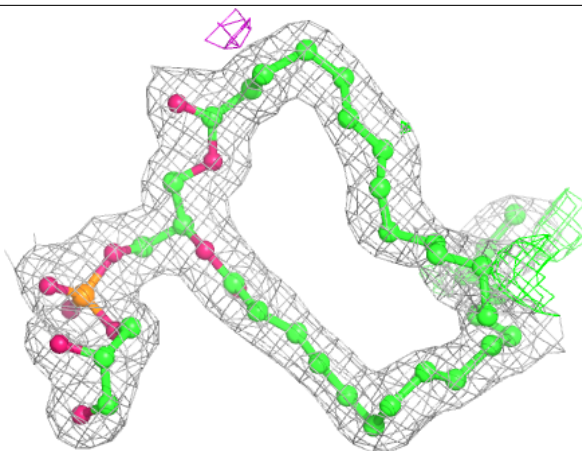
Electron density around LHG d 410:

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



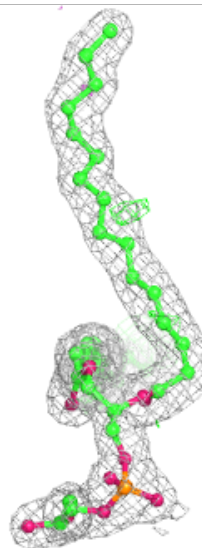
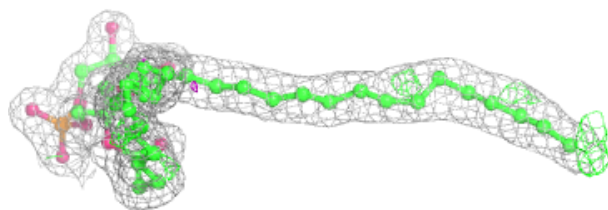
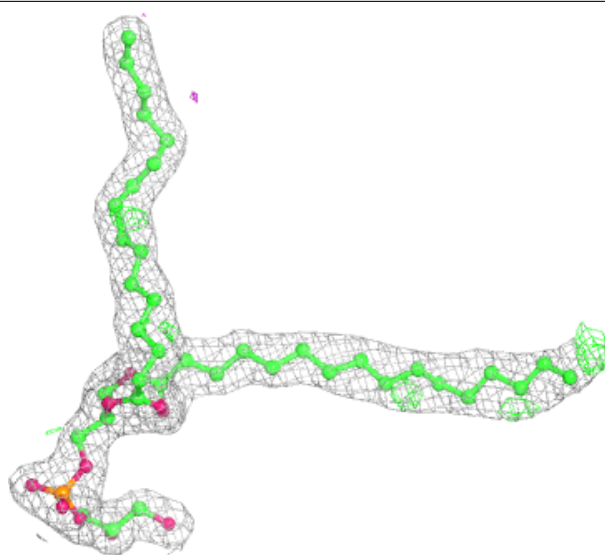
Electron density around LHG d 411:

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



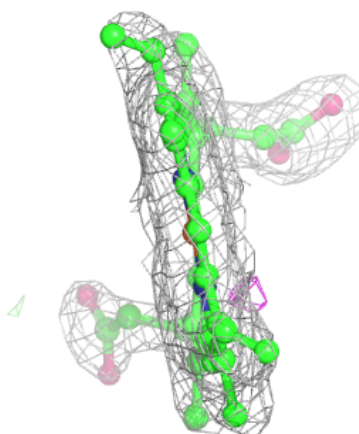
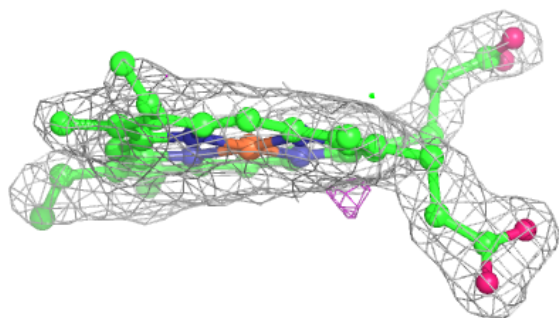
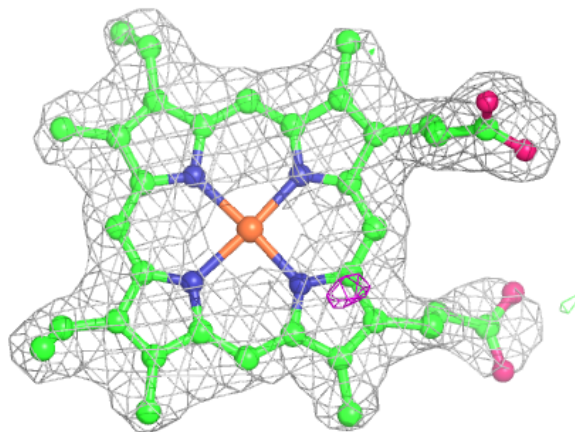
Electron density around LHG 1 102:

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



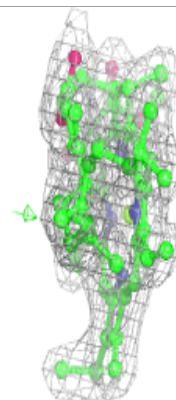
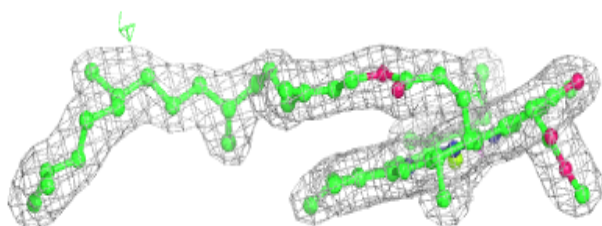
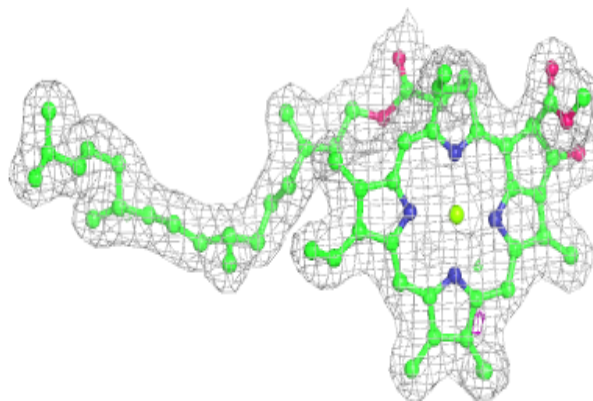
Electron density around HEM e 102:

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

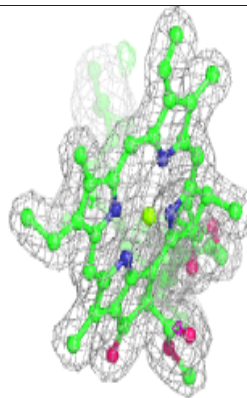
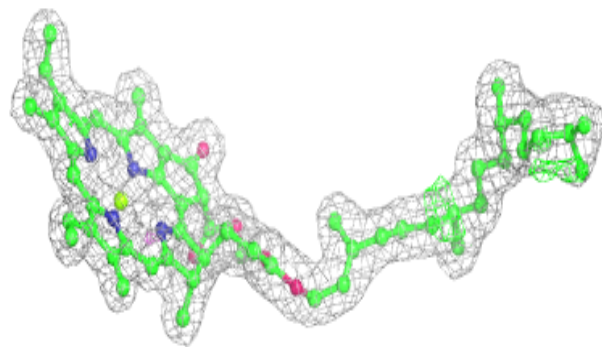
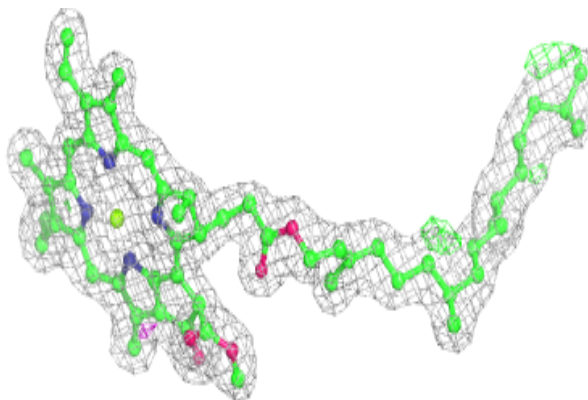


Electron density around CLA B 605:

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

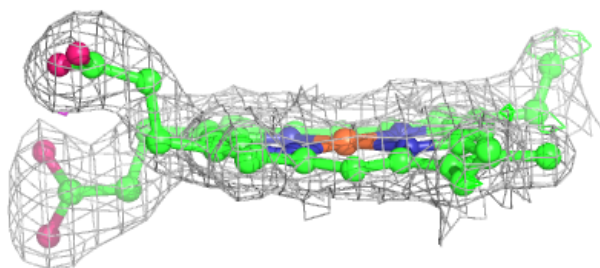
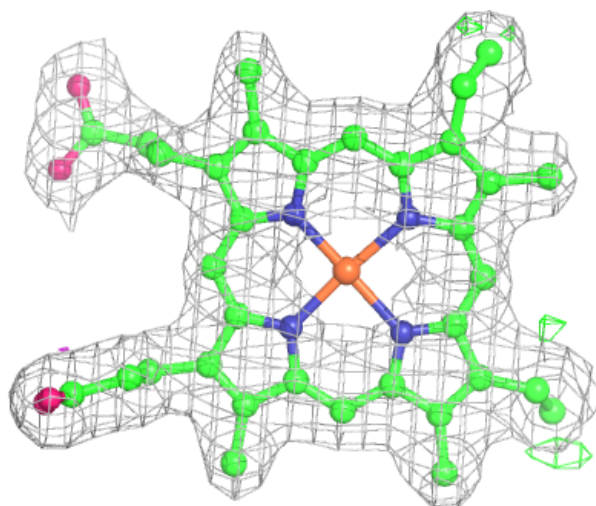
**Electron density around CLA a 409:**

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



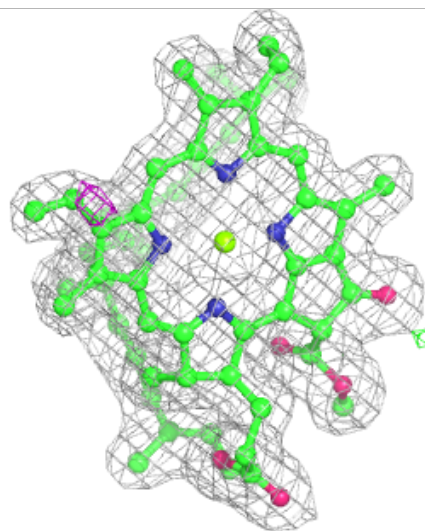
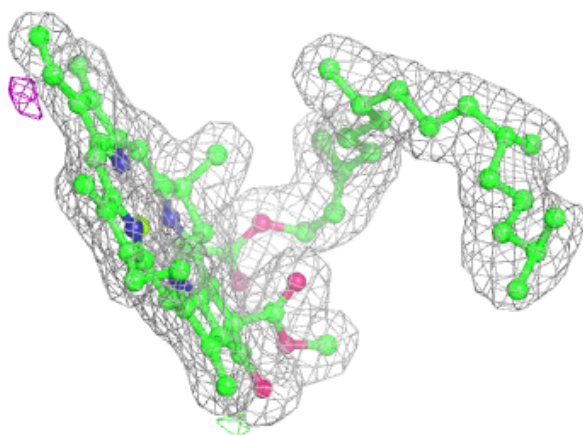
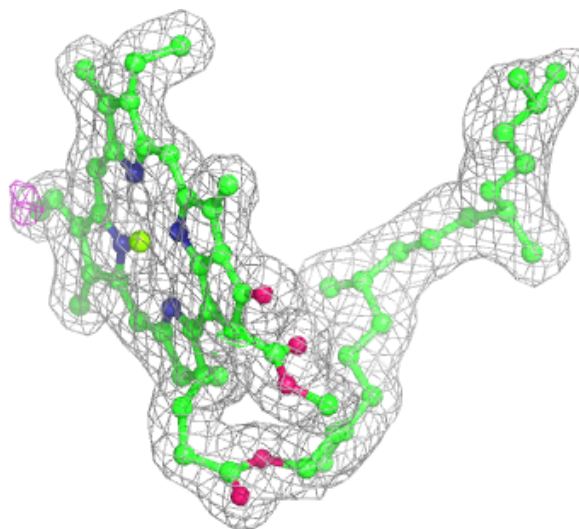
Electron density around HEC v 201:

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



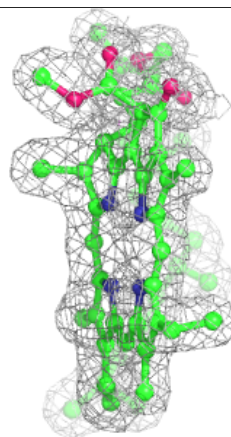
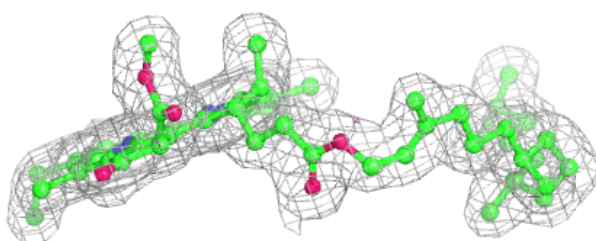
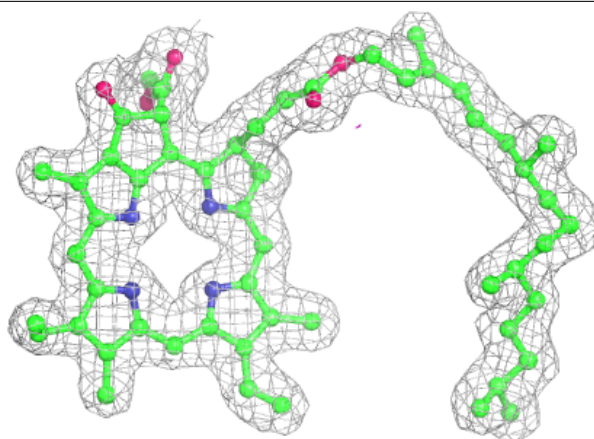
Electron density around CLA B 615:

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



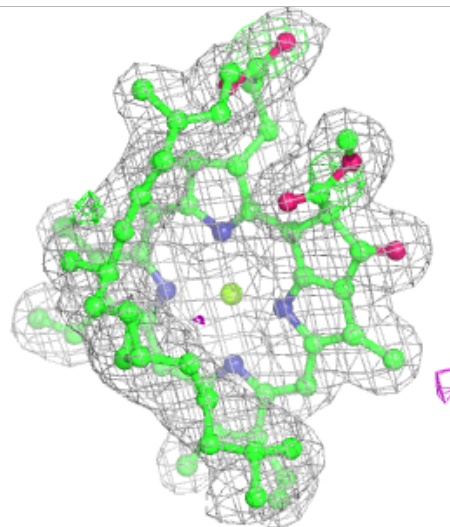
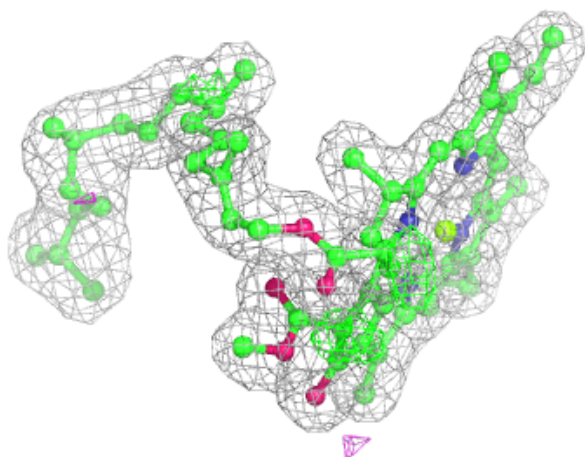
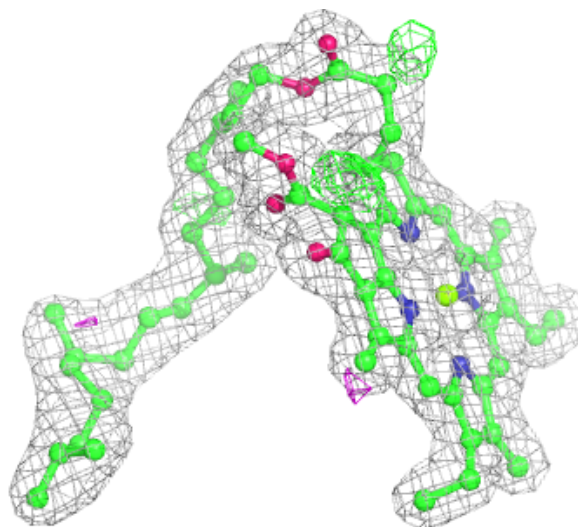
Electron density around PHO A 407:

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



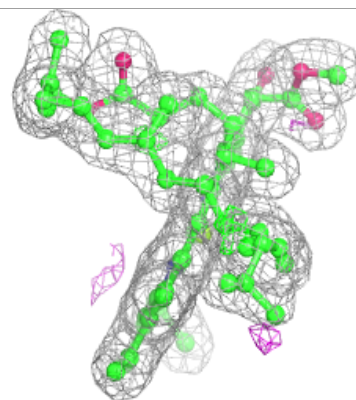
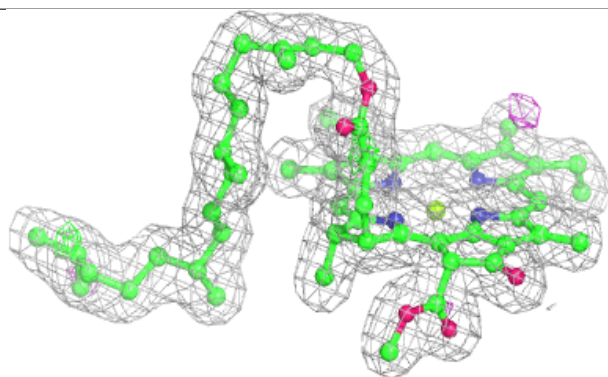
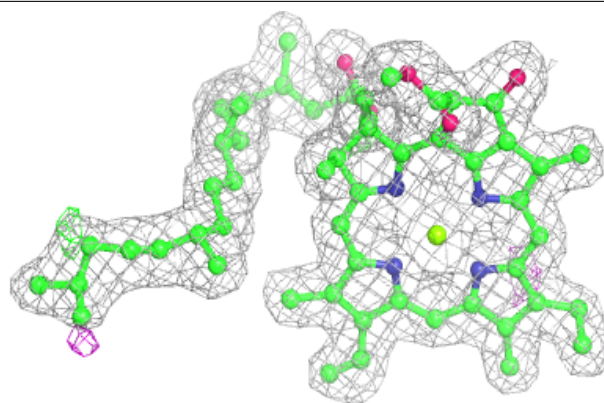
Electron density around CLA b 617:

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

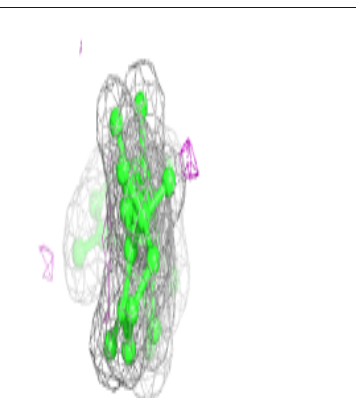
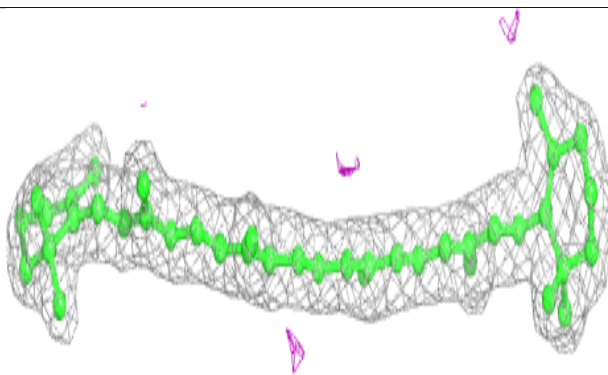
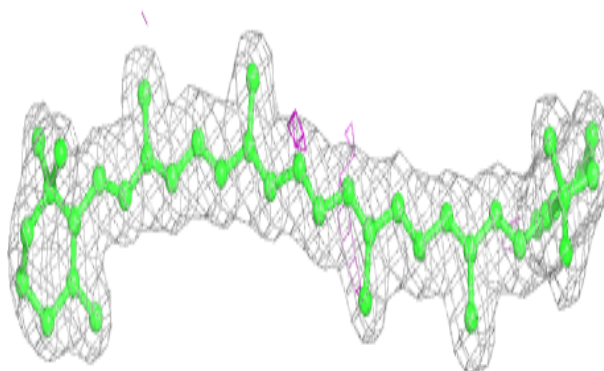


Electron density around CLA D 401:

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

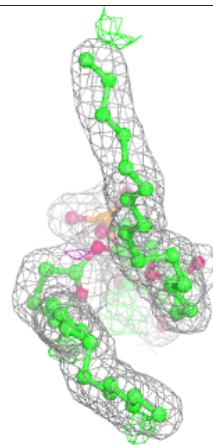
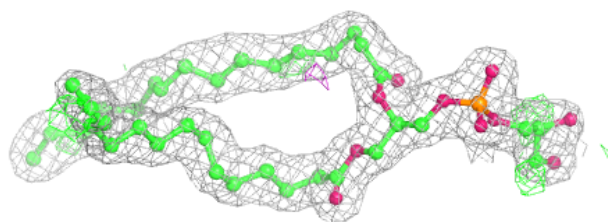
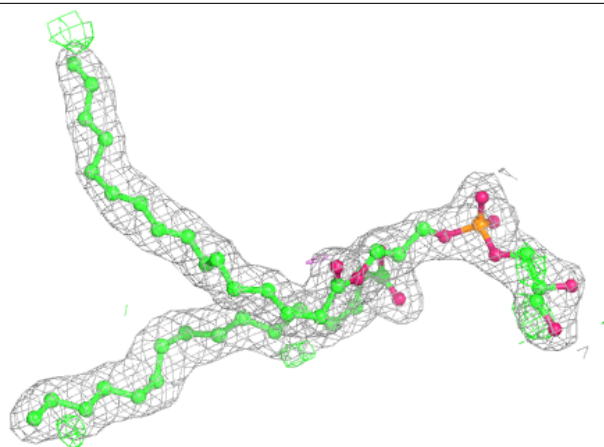
**Electron density around BCR b 621:**

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



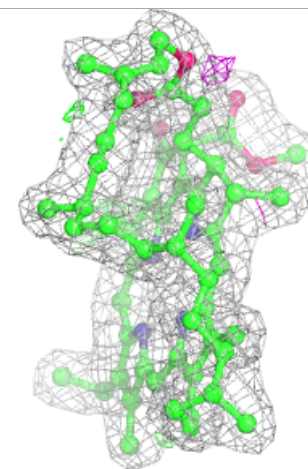
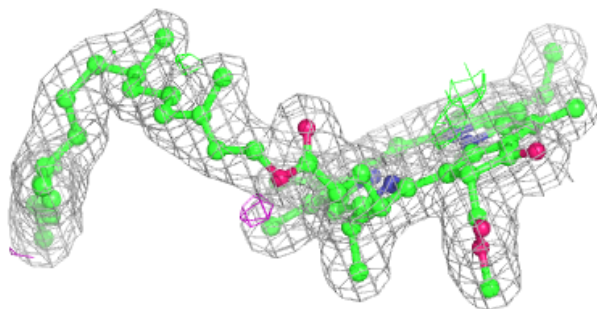
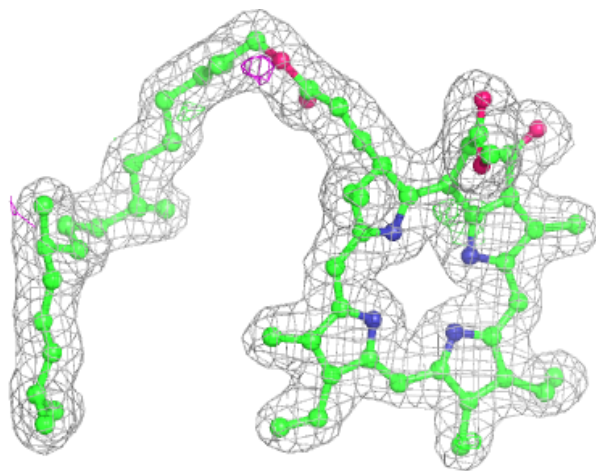
Electron density around LHG D 411:

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



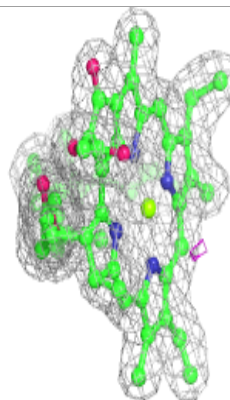
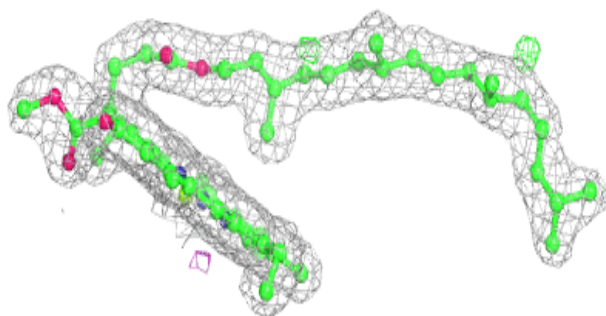
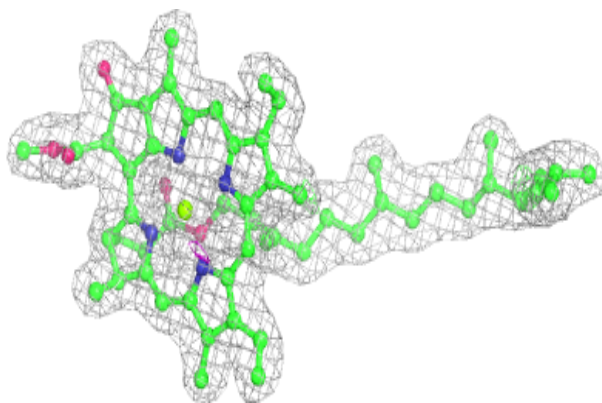
Electron density around PHO d 401:

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

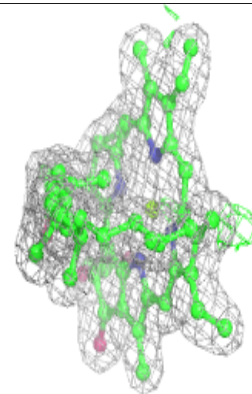
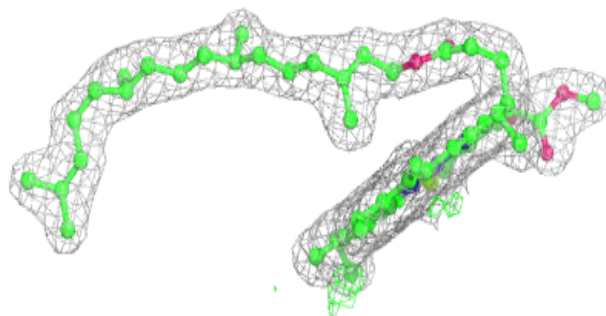
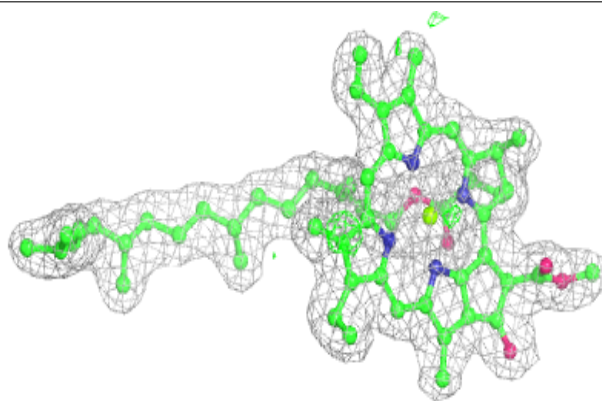


Electron density around CLA B 610:

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

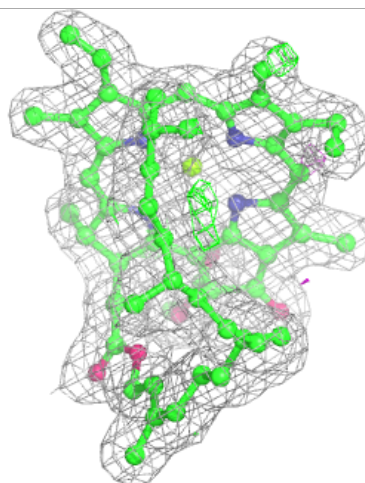
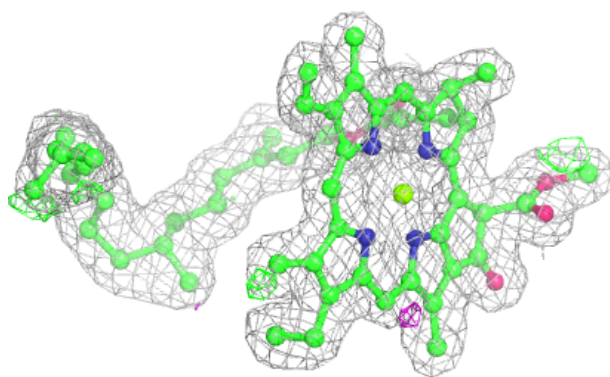
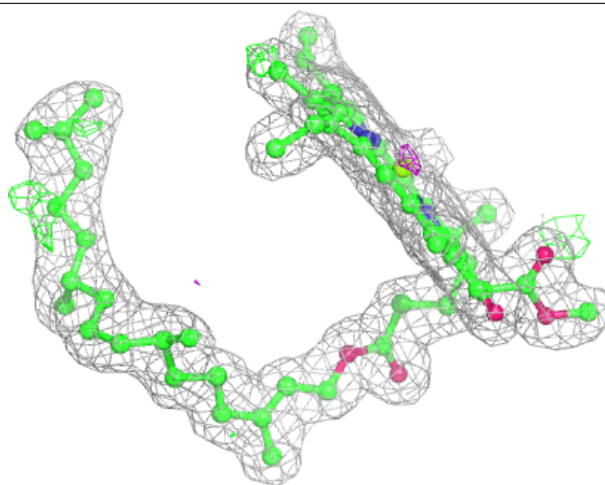
**Electron density around CLA b 612:**

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



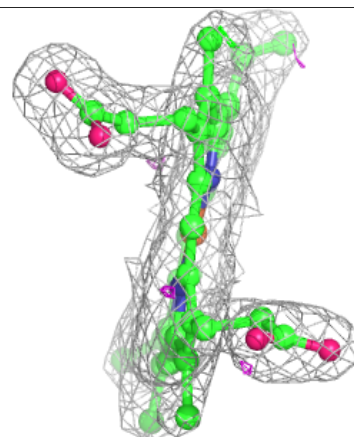
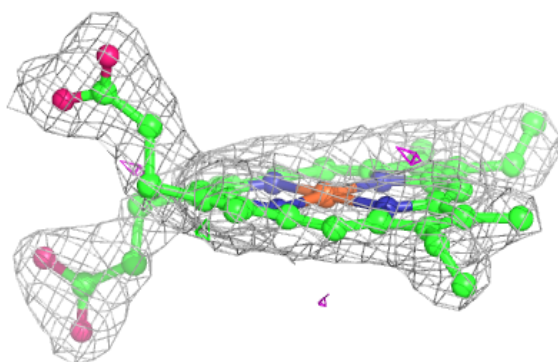
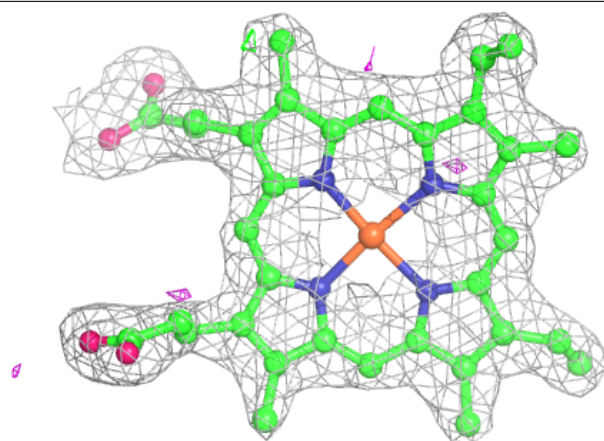
Electron density around CLA B 613:

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

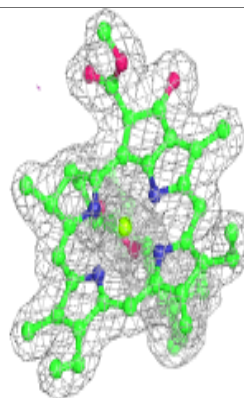
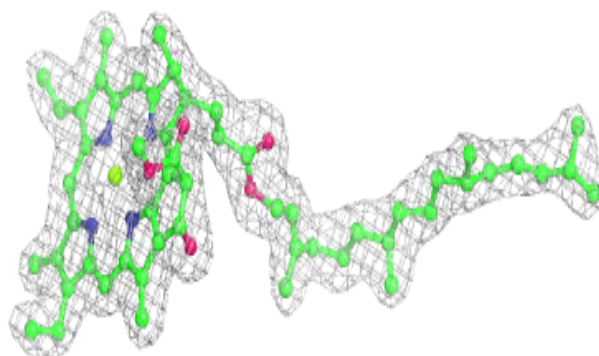
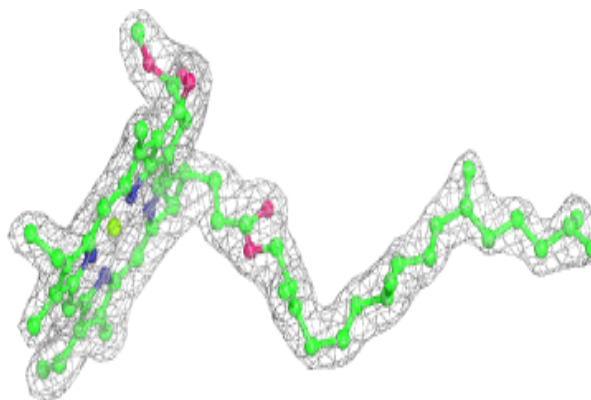


Electron density around HEM F 102:

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

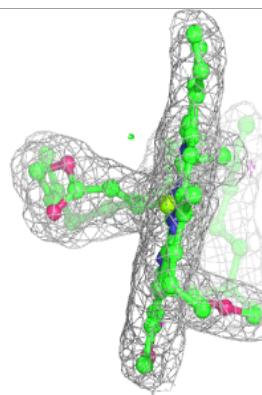
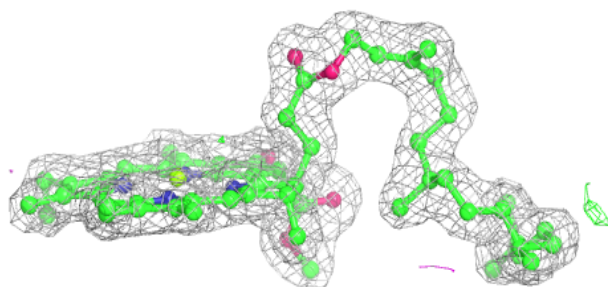
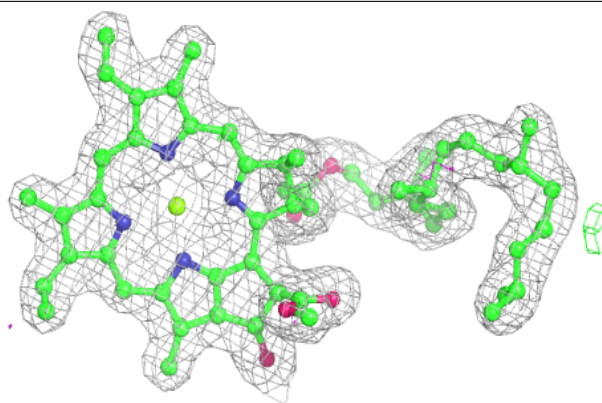
**Electron density around CLA c 504:**

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

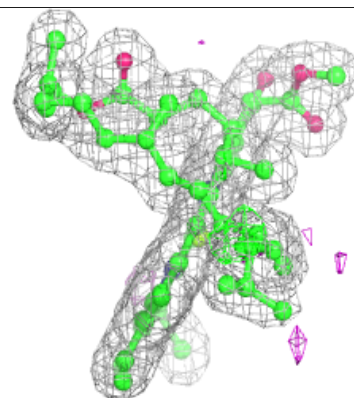
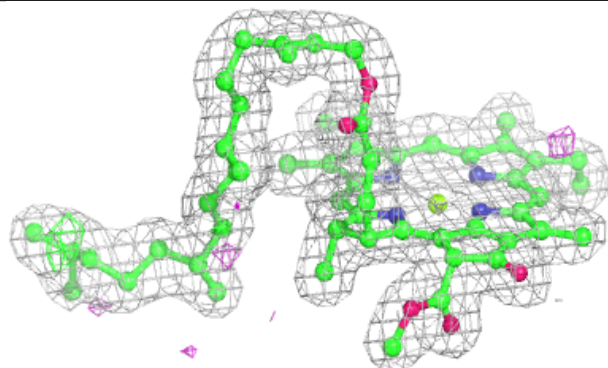
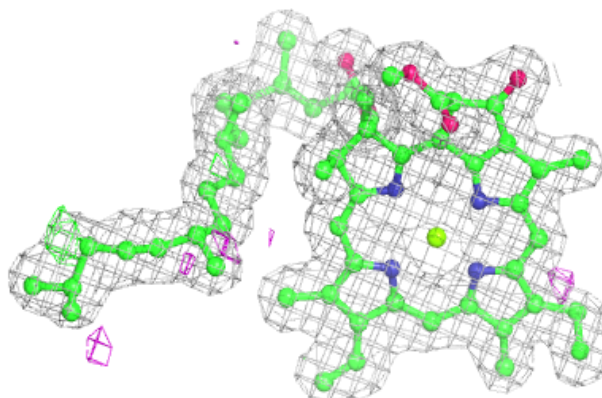


Electron density around CLA B 614:

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

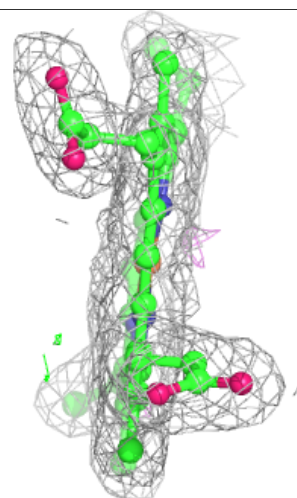
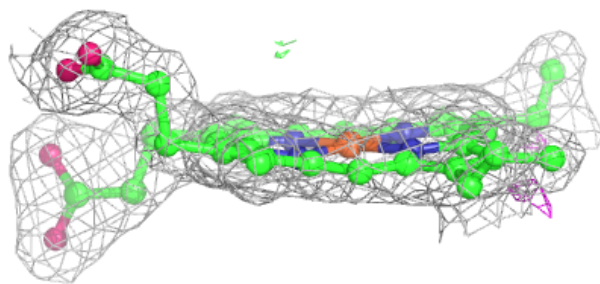
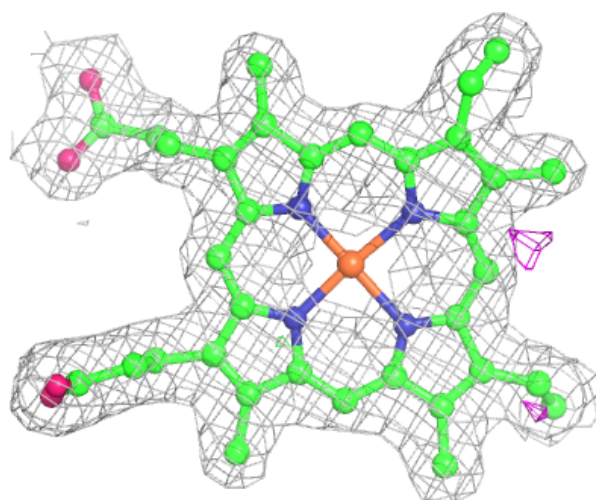
**Electron density around CLA a 410:**

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



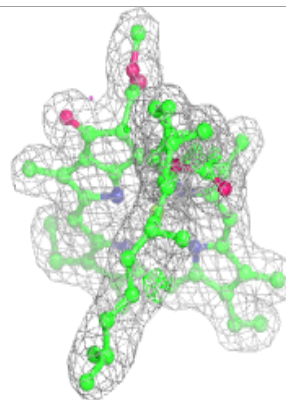
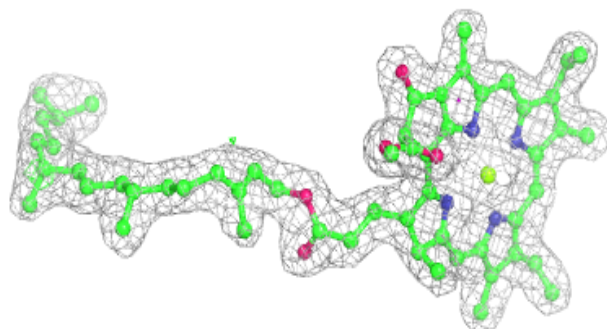
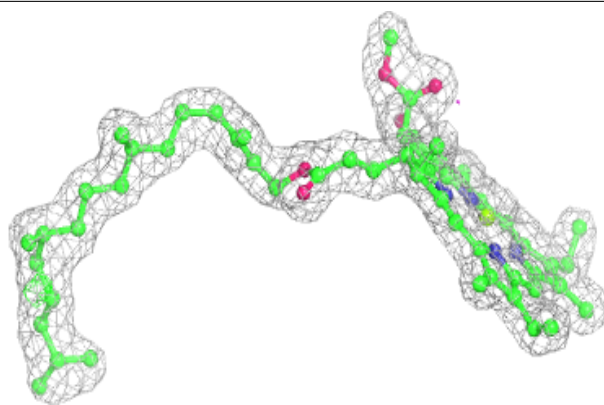
Electron density around HEC V 201:

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



Electron density around CLA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.