



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 12:56 PM BST

PDB ID : 5ZZN
Title : Crystal structure of photosystem II from an SQDG-deficient mutant of *Thermosynechococcus elongatus*
Authors : Nakajima, Y.; Umena, Y.; Nagao, R.; Endo, K.; Kobayashi, K.; Akita, F.; Suga, M.; Wada, H.; Noguchi, T.; Shen, J.R.
Deposited on : 2018-06-03
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

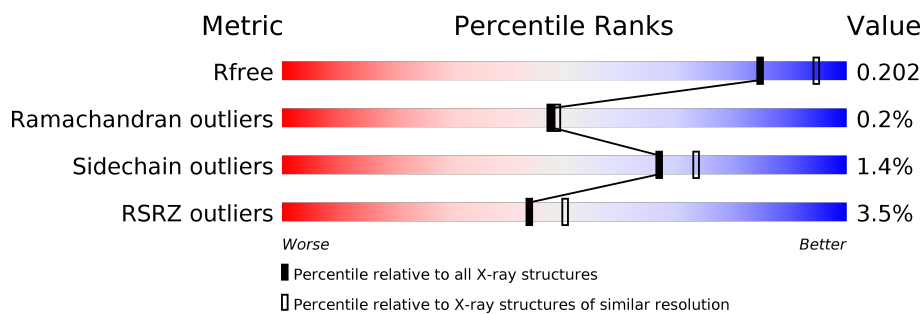
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



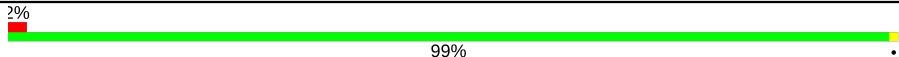
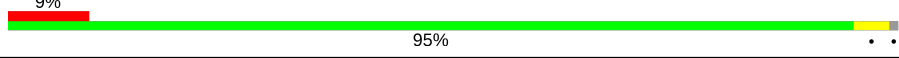
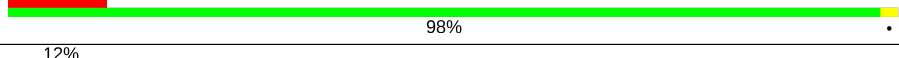
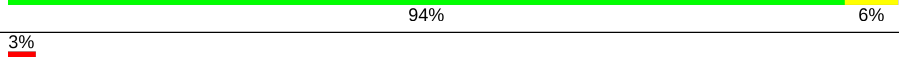
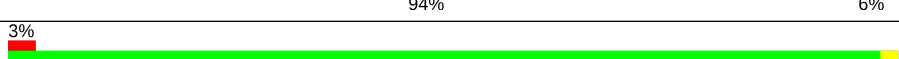
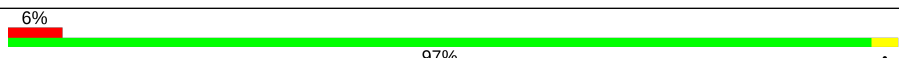
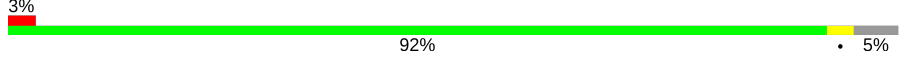
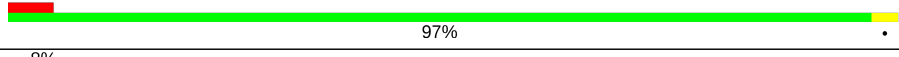
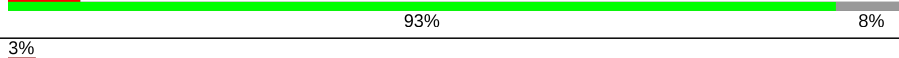

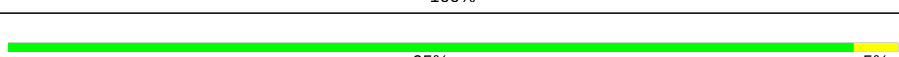
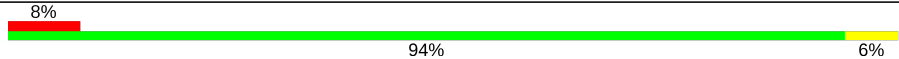
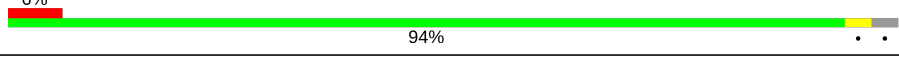
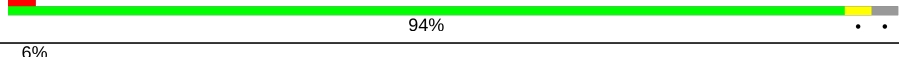
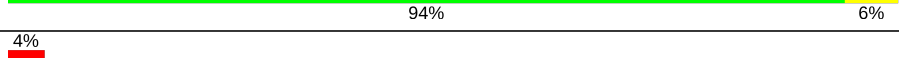
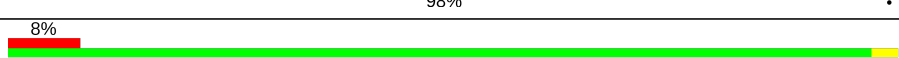
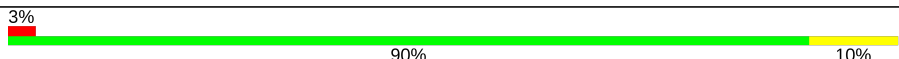
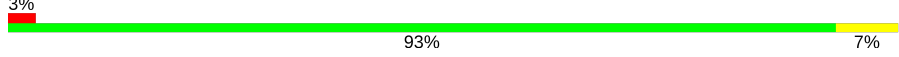
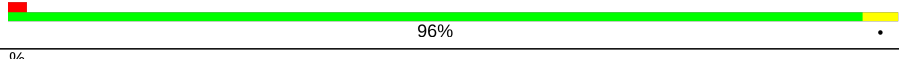
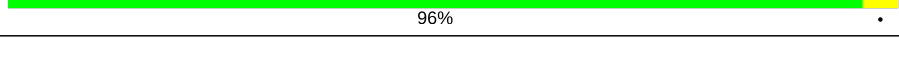
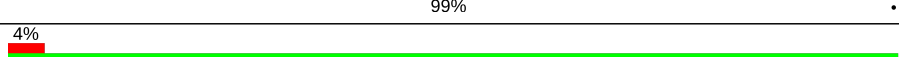
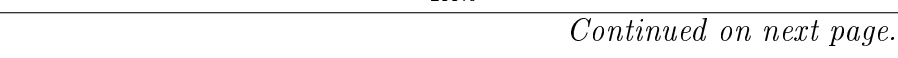


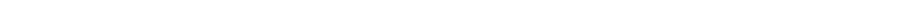
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 99% </div> </div>
1	a	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 98% </div> </div>
2	B	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 2% 99% </div> </div>
2	b	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 1%, green 93%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 5% 97% </div> </div>
3	C	455	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 97% </div> </div>
3	c	455	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 2% 97% </div> </div>
4	D	342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 98% </div> </div>

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	63	
7	h	63	
8	I	37	
8	i	37	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	36	
11	l	36	
12	M	34	
12	m	34	
13	O	243	
13	o	243	
14	T	30	
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	62	

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
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	a	409	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
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22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	-
22	CLA	b	620	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	d	405	X	-	-	-
28	LMT	C	520	X	-	-	-
28	LMT	z	101	X	-	-	-
32	HTG	B	624	-	-	-	X
32	HTG	U	203	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53800 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2626	1717	432	462	15			
1	a	334	Total	C	N	O	S	0	2	0
			2629	1721	433	460	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	5	0
			4009	2626	671	699	13			
2	b	504	Total	C	N	O	S	0	4	0
			3988	2616	661	698	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3526	2303	592	617	14			
3	c	455	Total	C	N	O	S	0	2	0
			3531	2311	591	615	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2746	1818	449	467	12			
4	d	342	Total	C	N	O	S	0	2	0
			2738	1813	448	464	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	2	0
			665	433	106	126			
5	e	81	Total	C	N	O	0	0	0
			649	425	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	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	63	Total	C	N	O	S	0	1	0
			509	339	84	84	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	337	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			284	193	44	46	1			
8	i	37	Total	C	N	O	S	0	0	1
			294	199	47	47	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
			262	177	41	43	1			
9	j	40	Total	C	N	O	S	0	0	0
			279	187	44	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	1	0
			296	206	43	47			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			285	199	42	44			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			292	196	45	51			
11	l	35	Total	C	N	O	0	2	0
			296	200	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			264	177	38	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			269	180	39	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
			1876	1172	315	385	4			
13	o	243	Total	C	N	O	S	0	6	0
			1876	1174	311	385	6			

- 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
			259	181	36	40	2			
14	t	30	Total	C	N	O	S	0	0	0
			259	181	36	40	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	1	0
			785	497	133	155			
15	u	97	Total	C	N	O	0	1	0
			783	496	130	157			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1083	685	183	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1063	672	178	209	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	1	0
			217	144	35	34	4			
17	y	29	Total	C	N	O	S	0	0	0
			209	136	37	33	3			

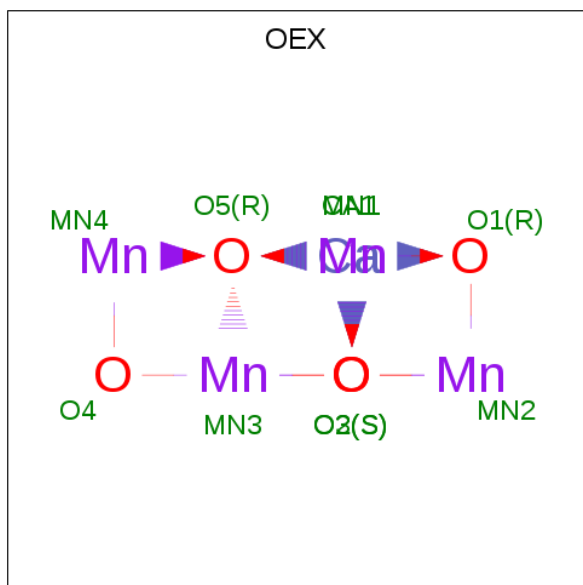
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	1	0
			292	196	47	49				
18	x	38	Total	C	N	O		0	1	0
			289	194	46	49				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			465	321	67	75	2			
19	z	62	Total	C	N	O	S	0	0	0
			459	318	67	72	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).

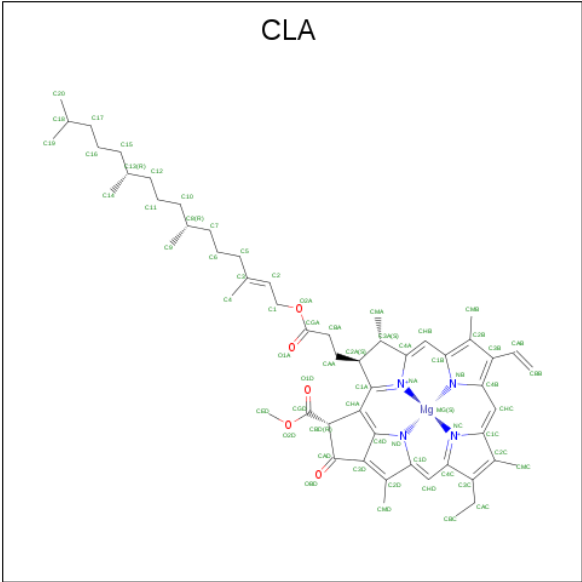


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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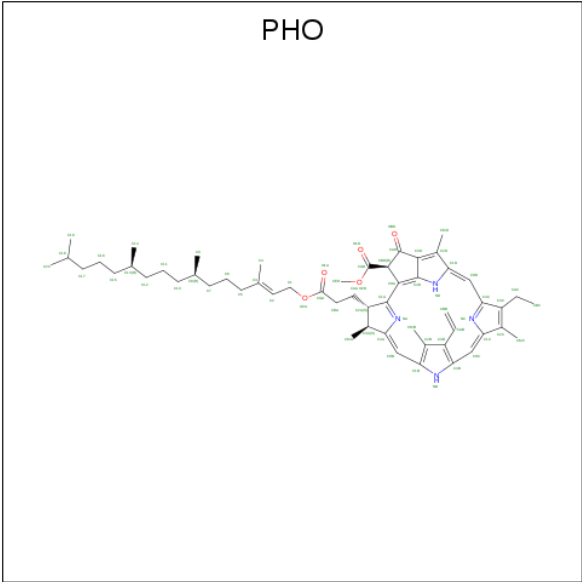
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N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

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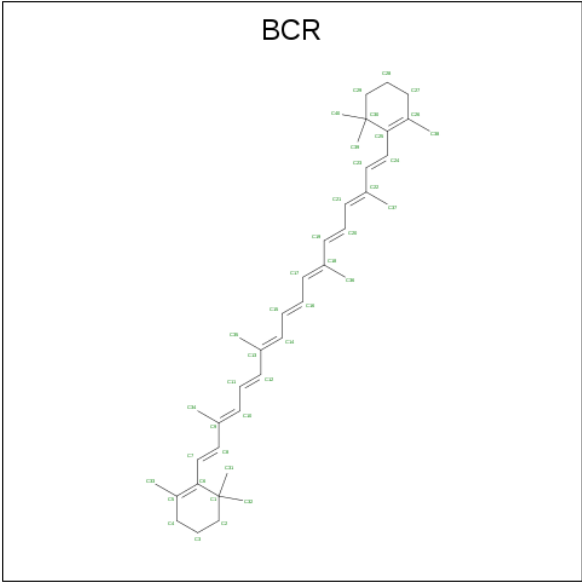
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



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

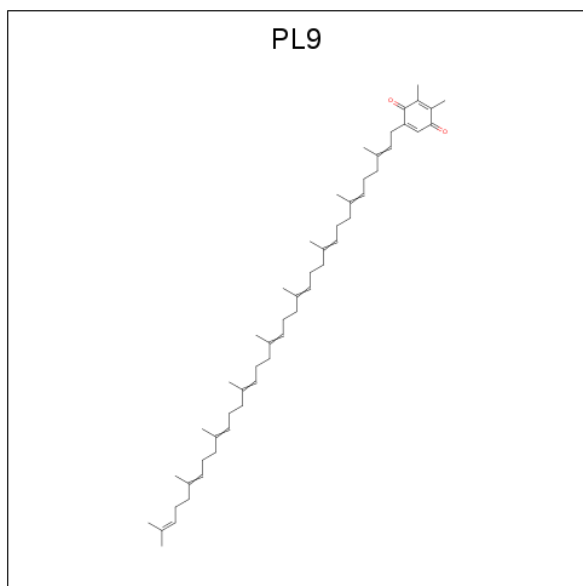
- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

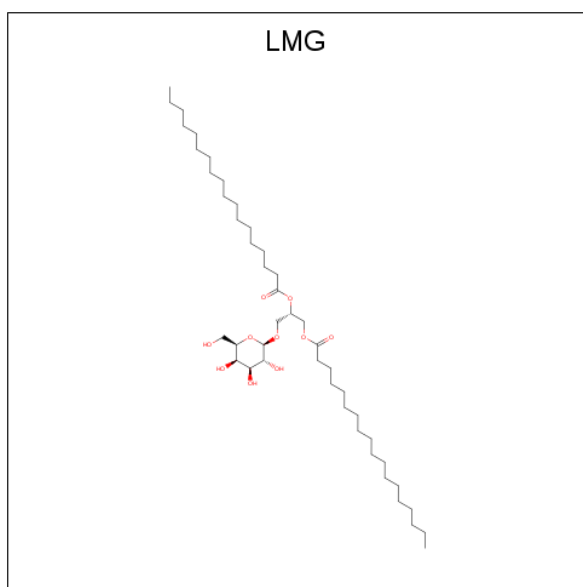
- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

C₅₃H₈₀O₂).



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

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			51	41	10		
26	B	1	Total	C	O	0	0
			51	41	10		
26	C	1	Total	C	O	0	0
			49	39	10		
26	C	1	Total	C	O	0	0
			48	38	10		
26	D	1	Total	C	O	0	0
			47	37	10		
26	a	1	Total	C	O	0	0
			51	41	10		
26	b	1	Total	C	O	0	0
			49	39	10		
26	c	1	Total	C	O	0	0
			38	28	10		
26	c	1	Total	C	O	0	0
			51	41	10		
26	d	1	Total	C	O	0	0
			47	37	10		

- Molecule 27 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	K	1	Total	C	0	0
			10	10		
27	h	1	Total	C	0	0
			8	8		

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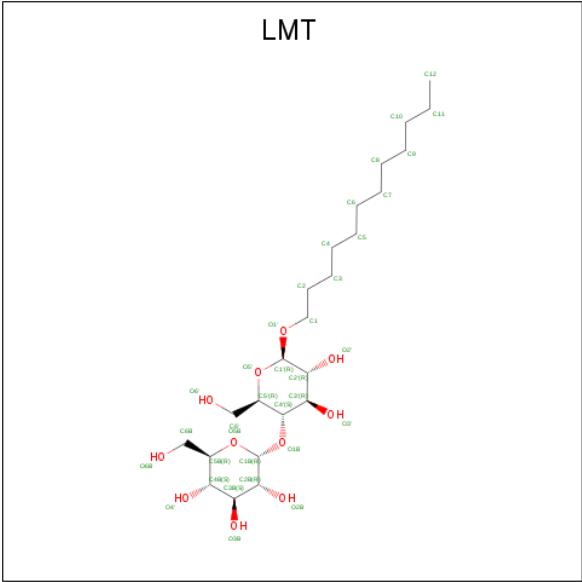
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	B	5	Total	C	O	0	0
			127	117	10		
27	c	3	Total	C	O	0	0
			53	48	5		
27	t	1	Total	C		0	0
			16	16			
27	X	1	Total	C		0	0
			16	16			
27	J	1	Total	C		0	0
			16	16			
27	E	2	Total	C		0	0
			29	29			
27	b	4	Total	C	O	0	0
			108	98	10		
27	A	5	Total	C	O	0	0
			119	104	15		
27	x	1	Total	C		0	0
			16	16			
27	j	2	Total	C	O	0	0
			49	44	5		
27	D	1	Total	C		0	0
			16	16			
27	e	2	Total	C		0	0
			19	19			
27	I	4	Total	C		0	0
			59	59			
27	Z	1	Total	C		0	0
			6	6			
27	a	4	Total	C	O	0	0
			96	86	10		
27	U	1	Total	C		0	0
			14	14			
27	d	2	Total	C	O	0	0
			52	47	5		
27	H	2	Total	C		0	0
			14	14			
27	i	4	Total	C		0	0
			60	60			
27	C	2	Total	C	O	0	0
			35	30	5		
27	T	1	Total	C		0	0
			13	13			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	u	1	Total	C		0	0
			13	13			

- Molecule 28 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



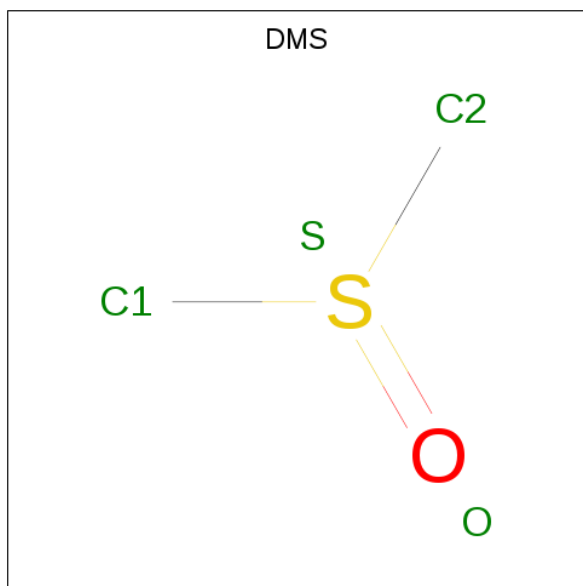
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			35	24	11		
28	B	1	Total	C	O	0	0
			35	24	11		
28	C	1	Total	C	O	0	0
			35	24	11		
28	F	1	Total	C	O	0	0
			24	18	6		
28	J	1	Total	C	O	0	0
			24	18	6		
28	M	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			24	18	6		
28	T	1	Total	C	O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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	b	1	Total	C	O	0	0
			25	19	6		
28	c	1	Total	C	O	0	0
			35	24	11		
28	j	1	Total	C	O	0	0
			23	18	5		
28	l	1	Total	C	O	0	0
			24	18	6		
28	m	1	Total	C	O	0	0
			35	24	11		
28	m	1	Total	C	O	0	0
			25	18	7		
28	m	1	Total	C	O	0	0
			23	18	5		
28	t	1	Total	C	O	0	0
			24	18	6		
28	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 29 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	C	1	Total 4	C 2	O 1	S 1	0	0
29	D	1	Total 4	C 2	O 1	S 1	0	0
29	D	1	Total 4	C 2	O 1	S 1	0	0
29	D	1	Total 4	C 2	O 1	S 1	0	0
29	D	1	Total 4	C 2	O 1	S 1	0	0
29	D	1	Total 4	C 2	O 1	S 1	0	0
29	E	1	Total 4	C 2	O 1	S 1	0	0
29	I	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	O	1	Total 4	C 2	O 1	S 1	0	0
29	U	1	Total 4	C 2	O 1	S 1	0	0
29	V	1	Total 4	C 2	O 1	S 1	0	0
29	V	1	Total 4	C 2	O 1	S 1	0	0

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

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

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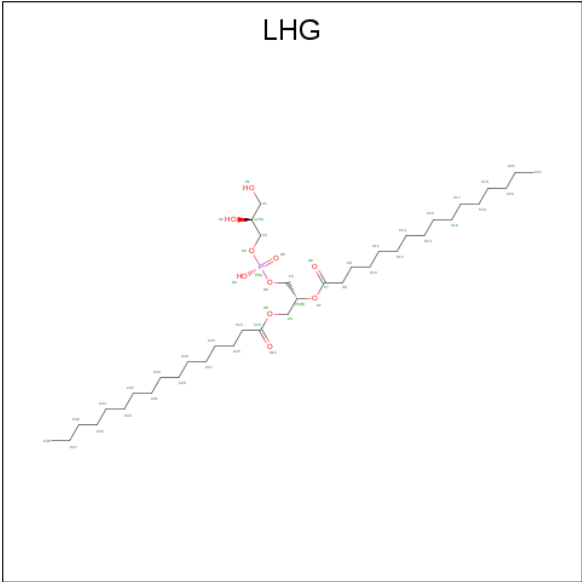
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	o	1	Total 4	C 2	O 1	S 1	0	0
29	u	1	Total 4	C 2	O 1	S 1	0	0
29	u	1	Total 4	C 2	O 1	S 1	0	0
29	u	1	Total 4	C 2	O 1	S 1	0	0
29	v	1	Total 4	C 2	O 1	S 1	0	0
29	v	1	Total 4	C 2	O 1	S 1	0	0
29	v	1	Total 4	C 2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

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

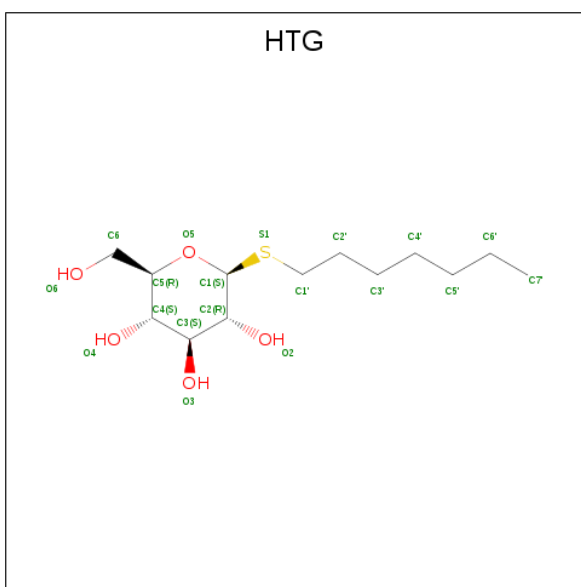
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total 1	Ca 1	0	0
30	c	1	Total 1	Ca 1	0	0
30	V	1	Total 1	Ca 1	0	0
30	v	1	Total 1	Ca 1	0	0
30	O	1	Total 1	Ca 1	0	0
30	o	1	Total 1	Ca 1	0	0
30	b	1	Total 1	Ca 1	0	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			44	33	10	1		
31	E	1	Total	C	O	P	0	0
			49	38	10	1		
31	F	1	Total	C	O	P	0	0
			38	27	10	1		
31	b	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			44	33	10	1		
31	e	1	Total	C	O	P	0	0
			38	29	8	1		
31	f	1	Total	C	O	P	0	0
			46	35	10	1		

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



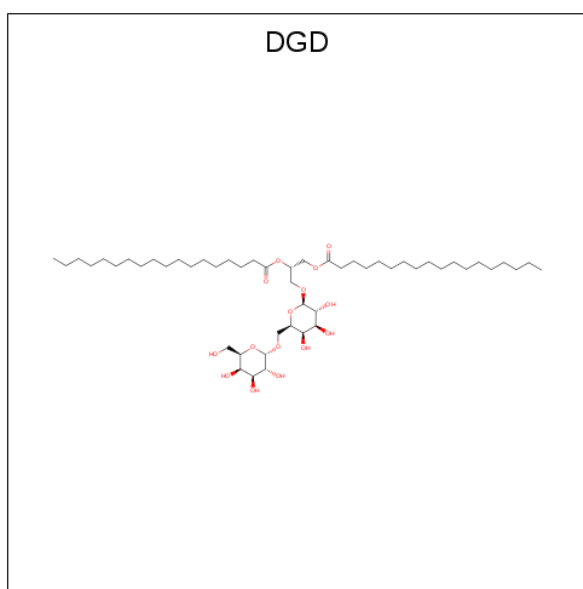
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total 19	C 13	O 5	S 1	0	0
32	B	1	Total 19	C 13	O 5	S 1	0	0
32	B	1	Total 19	C 13	O 5	S 1	0	0
32	B	1	Total 18	C 12	O 5	S 1	0	0
32	C	1	Total 19	C 13	O 5	S 1	0	0
32	C	1	Total 19	C 13	O 5	S 1	0	0
32	C	1	Total 9	C 8	O 1	S 1	0	0
32	C	1	Total 19	C 13	O 5	S 1	0	0
32	D	1	Total 16	C 10	O 5	S 1	0	0
32	O	1	Total 19	C 13	O 5	S 1	0	0
32	U	1	Total 14	C 8	O 5	S 1	0	0
32	V	1	Total 19	C 13	O 5	S 1	0	0
32	b	1	Total 19	C 13	O 5	S 1	0	0
32	b	1	Total 19	C 13	O 5	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 17 11 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C S 9 8 1	0	0
32	c	1	Total C O S 15 9 5 1	0	0
32	d	1	Total C O S 16 10 5 1	0	0
32	o	1	Total C O S 19 13 5 1	0	0
32	v	1	Total C O S 16 10 5 1	0	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			45	36	9		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			56	41	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	d	1	Total	C	O	0	0
			48	39	9		
33	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 34 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C	1	Total	C	O	0	0
			6	3	3		
34	D	1	Total	C	O	0	0
			6	3	3		
34	b	1	Total	C	O	0	0
			6	3	3		
34	c	1	Total	C	O	0	0
			6	3	3		

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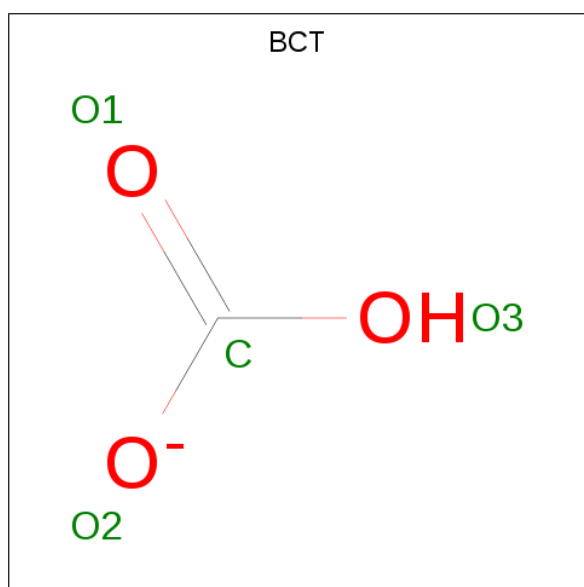
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	e	1	Total	C	O	0	0
			6	3	3		

- Molecule 35 is FE (II) ION (three-letter code: FE2) (formula: Fe).

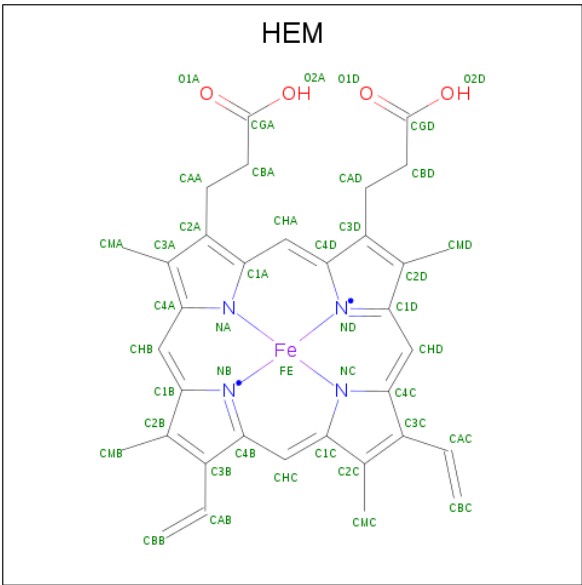
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	a	1	Total	Fe	0	0
			1	1		
35	D	1	Total	Fe	0	0
			1	1		

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



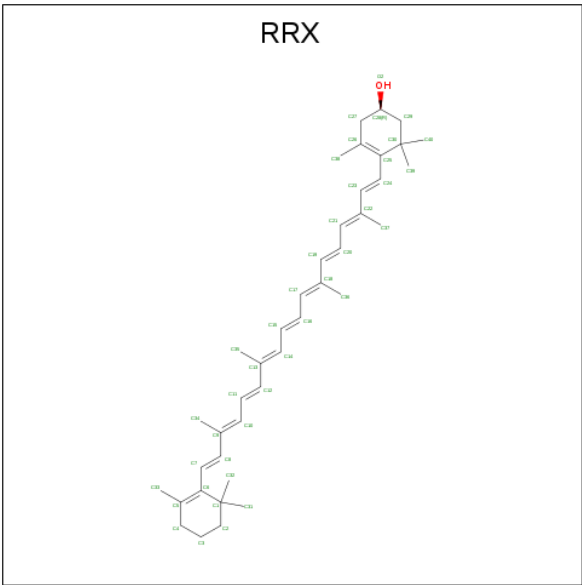
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D	1	Total	C	O	0	1
			8	2	6		
36	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 39 | J | 1 | Total Mg
1 1 | 0 | 0 |
| 39 | j | 1 | Total Mg
1 1 | 0 | 0 |
| 39 | K | 1 | Total Mg
1 1 | 0 | 0 |
| 39 | k | 1 | Total Mg
1 1 | 0 | 0 |

-
- ORTEP diagram of the HEC molecule. The structure shows a central iron atom (Fe) coordinated by four nitrogen atoms (N1, N2, N3, N4) in a porphyrin-like ring. The molecule is labeled with atom names (C1A, C2A, etc.) and includes thermal ellipsoids at the 50% probability level.

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41 | A | 139 | Total O
141 141 | 0 | 2 |
| 41 | B | 260 | Total O
263 263 | 0 | 3 |
| 41 | C | 216 | Total O
216 216 | 0 | 0 |



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	D	126	Total 130	O 130	0	4
41	E	20	Total 21	O 21	0	1
41	F	6	Total 6	O 6	0	0
41	H	43	Total 44	O 44	0	1
41	I	6	Total 6	O 6	0	0
41	J	11	Total 11	O 11	0	0
41	K	8	Total 8	O 8	0	0
41	L	11	Total 11	O 11	0	0
41	M	10	Total 11	O 11	0	1
41	O	148	Total 152	O 152	0	4
41	T	13	Total 13	O 13	0	0
41	U	71	Total 71	O 71	0	0
41	V	102	Total 103	O 103	0	1
41	Y	4	Total 5	O 5	0	1
41	X	12	Total 12	O 12	0	0
41	Z	3	Total 3	O 3	0	0
41	a	125	Total 126	O 126	0	1
41	b	255	Total 260	O 260	0	5
41	c	201	Total 203	O 203	0	2
41	d	133	Total 135	O 135	0	2
41	e	19	Total 20	O 20	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	f	11	Total 11	O 11	0	0
41	h	34	Total 35	O 35	0	1
41	i	6	Total 6	O 6	0	0
41	j	12	Total 12	O 12	0	0
41	k	5	Total 5	O 5	0	0
41	l	9	Total 9	O 9	0	0
41	m	8	Total 8	O 8	0	0
41	o	126	Total 129	O 129	0	3
41	t	9	Total 10	O 10	0	1
41	u	72	Total 72	O 72	0	0
41	v	75	Total 75	O 75	0	0
41	y	4	Total 4	O 4	0	0
41	x	7	Total 7	O 7	0	0
41	z	2	Total 2	O 2	0	0

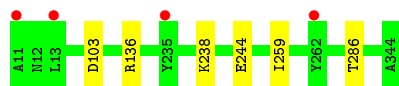
3 Residue-property plots [i](#)

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.

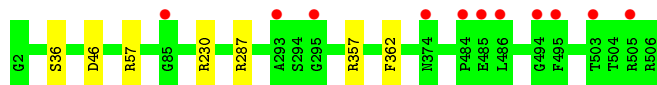
- Molecule 1: Photosystem II protein D1 1



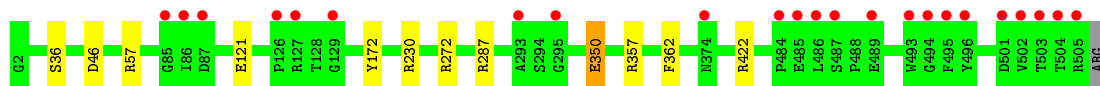
- Molecule 1: Photosystem II protein D1 1



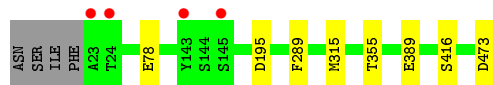
- Molecule 2: Photosystem II CP47 reaction center protein



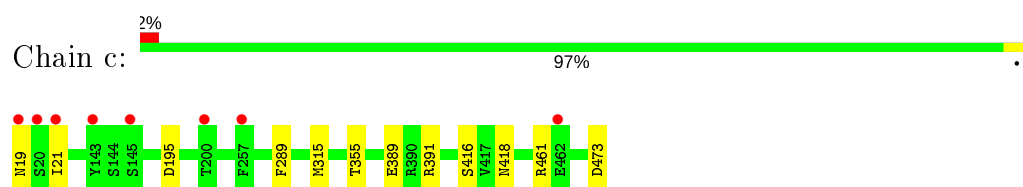
- Molecule 2: Photosystem II CP47 reaction center protein



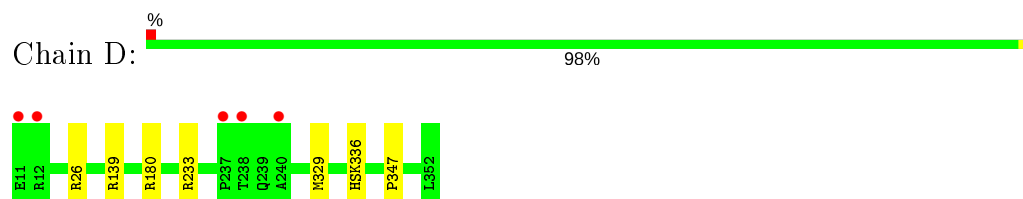
- Molecule 3: Photosystem II CP43 reaction center protein



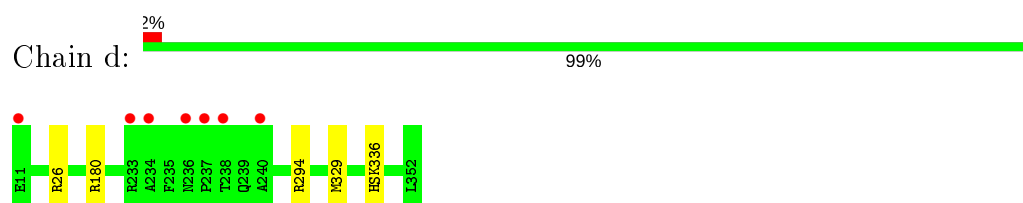
- Molecule 3: Photosystem II CP43 reaction center protein



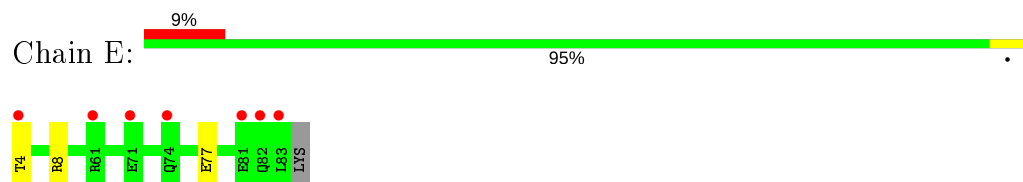
- Molecule 4: Photosystem II D2 protein



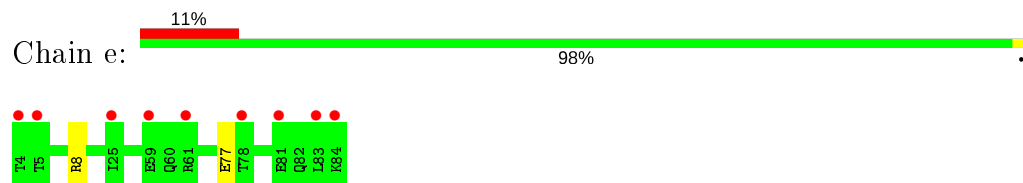
- Molecule 4: Photosystem II D2 protein



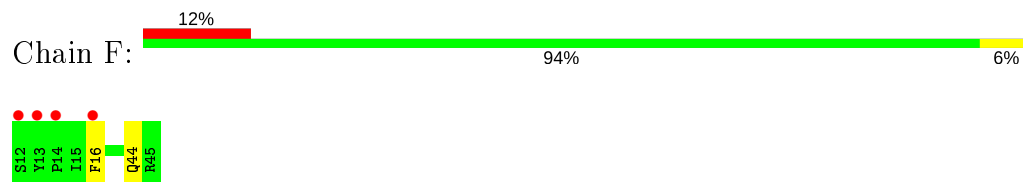
- Molecule 5: Cytochrome b559 subunit alpha



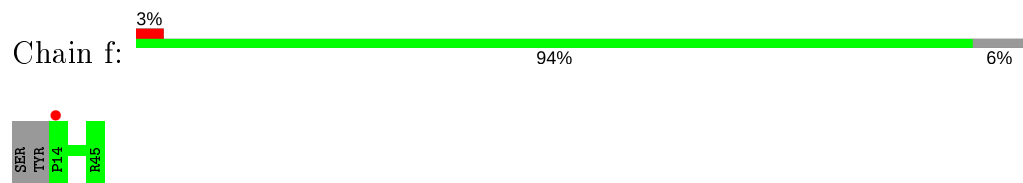
- Molecule 5: Cytochrome b559 subunit alpha



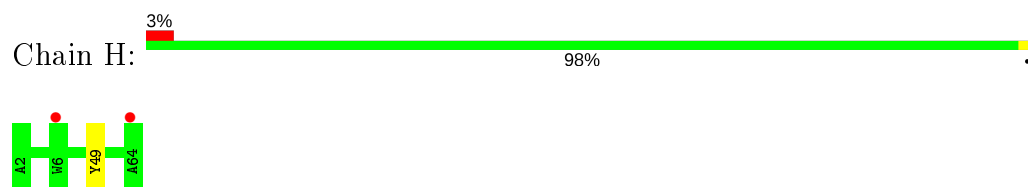
- Molecule 6: Cytochrome b559 subunit beta



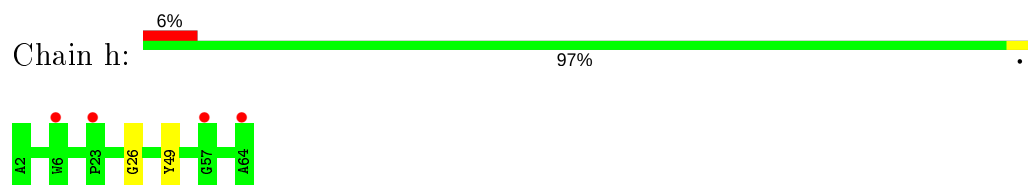
- Molecule 6: Cytochrome b559 subunit beta



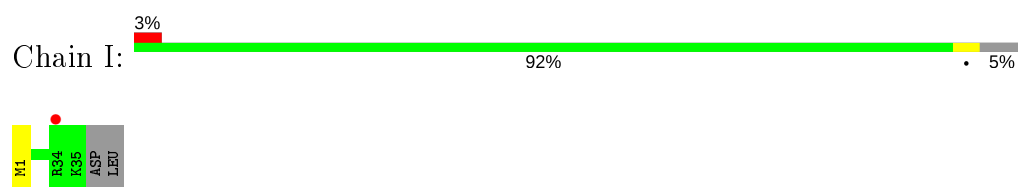
- Molecule 7: Photosystem II reaction center protein H



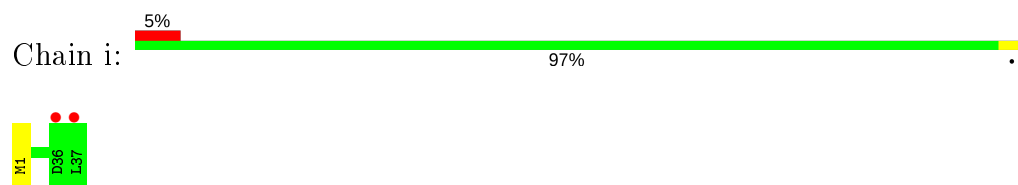
- Molecule 7: Photosystem II reaction center protein H



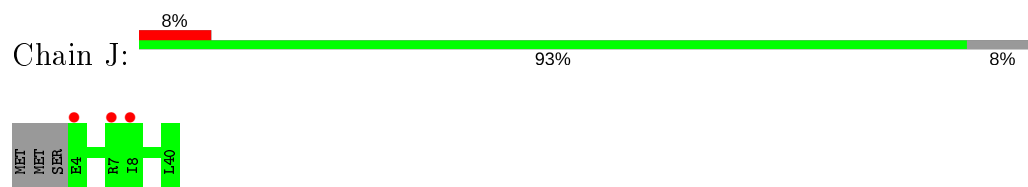
- Molecule 8: Photosystem II reaction center protein I



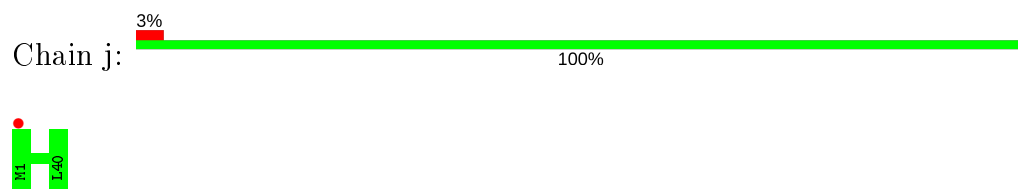
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



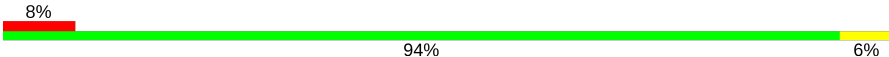
There are no outlier residues recorded for this chain.

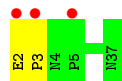
- Molecule 10: Photosystem II reaction center protein K

Chain k:  95% 5%



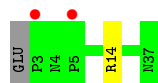
- Molecule 11: Photosystem II reaction center protein L

Chain L:  8% 94% 6%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  6% 94% . .



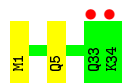
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 94% . .



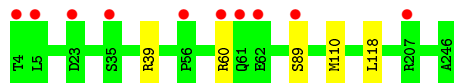
- Molecule 12: Photosystem II reaction center protein M

Chain m:  6% 94% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  4% 98% .

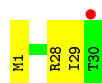
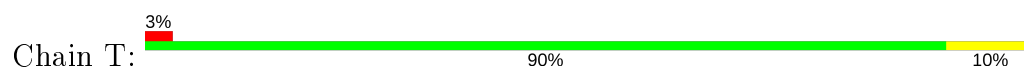


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

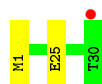
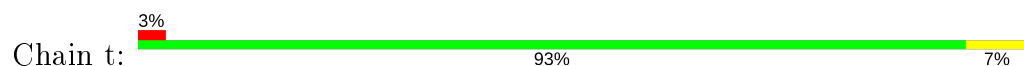
Chain o:  8% 97% .



- Molecule 14: Photosystem II reaction center protein T



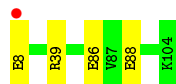
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



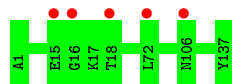
- Molecule 15: Photosystem II 12 kDa extrinsic protein



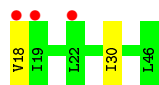
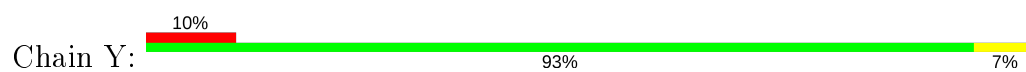
- Molecule 16: Cytochrome c-550



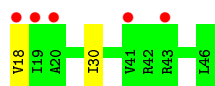
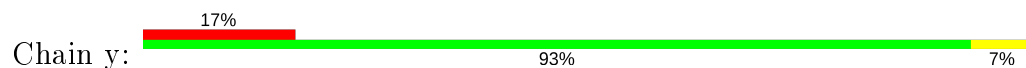
- Molecule 16: Cytochrome c-550



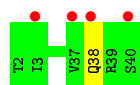
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



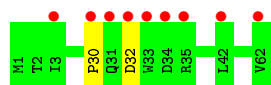
- Molecule 18: Photosystem II reaction center X protein



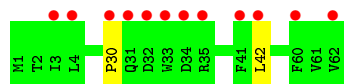
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.25Å 228.43Å 287.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 19.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-2.10) 99.5 (19.93-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.154 , 0.197 0.164 , 0.202	Depositor DCC
R_{free} test set	23043 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53800	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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: PL9, DMS, BCT, BCR, DGD, HSK, FE2, RRX, LHG, GOL, CL, CA, CLA, HEC, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, LMG

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	1.01	0/2711	0.84	2/3699 (0.1%)
1	a	0.97	0/2714	0.83	2/3702 (0.1%)
2	B	0.95	1/4149 (0.0%)	0.84	9/5655 (0.2%)
2	b	0.97	3/4128 (0.1%)	0.86	7/5628 (0.1%)
3	C	0.94	2/3639 (0.1%)	0.82	2/4953 (0.0%)
3	c	0.91	1/3645 (0.0%)	0.81	7/4962 (0.1%)
4	D	0.98	0/2821	0.84	2/3843 (0.1%)
4	d	0.95	0/2813	0.84	1/3831 (0.0%)
5	E	0.87	0/684	0.87	2/935 (0.2%)
5	e	0.86	0/668	0.89	1/913 (0.1%)
6	F	0.94	0/283	0.75	0/386
6	f	0.86	0/265	0.67	0/360
7	H	0.87	0/522	0.77	0/712
7	h	0.90	0/519	0.80	0/708
8	I	0.84	0/281	0.82	0/381
8	i	0.83	0/291	0.79	0/394
9	J	0.87	0/268	0.79	0/363
9	j	0.90	0/285	0.86	0/386
10	K	0.75	0/306	0.77	0/422
10	k	0.72	0/295	0.73	0/407
11	L	1.06	0/298	0.90	1/406 (0.2%)
11	l	1.01	0/303	0.86	1/413 (0.2%)
12	M	0.93	0/257	0.75	0/352
12	m	0.95	0/262	0.86	0/359
13	O	0.89	0/1907	0.91	1/2589 (0.0%)
13	o	0.86	1/1907 (0.1%)	0.88	2/2591 (0.1%)
14	T	1.03	0/258	0.94	1/349 (0.3%)
14	t	0.96	0/258	0.89	0/349
15	U	1.04	1/796 (0.1%)	1.00	2/1078 (0.2%)
15	u	1.05	1/794 (0.1%)	0.93	2/1076 (0.2%)
16	V	0.99	0/1104	0.92	1/1498 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.91	0/1084	0.84	0/1475
17	Y	0.69	0/218	0.81	0/292
17	y	0.63	0/210	0.80	0/281
18	X	0.80	0/295	0.73	0/399
18	x	0.77	0/292	0.74	0/395
19	Z	0.75	0/476	0.71	0/652
19	z	0.65	0/470	0.69	1/645 (0.2%)
All	All	0.94	10/42476 (0.0%)	0.84	47/57839 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	88	GLU	CD-OE2	7.36	1.33	1.25
2	B	36	SER	CB-OG	-6.90	1.33	1.42
3	c	389	GLU	CD-OE2	6.24	1.32	1.25
3	C	389[A]	GLU	CD-OE2	6.18	1.32	1.25
3	C	389[B]	GLU	CD-OE2	6.18	1.32	1.25

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	57	ARG	NE-CZ-NH1	7.50	124.05	120.30
13	O	39	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	c	391[A]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
3	c	391[B]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	B	57	ARG	NE-CZ-NH1	6.45	123.52	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/334 (100%)	328 (98%)	5 (2%)	1 (0%)	41	41
1	a	334/334 (100%)	327 (98%)	6 (2%)	1 (0%)	41	41
2	B	508/505 (101%)	501 (99%)	7 (1%)	0	100	100
2	b	506/505 (100%)	498 (98%)	8 (2%)	0	100	100
3	C	454/455 (100%)	444 (98%)	9 (2%)	1 (0%)	47	49
3	c	455/455 (100%)	446 (98%)	8 (2%)	1 (0%)	47	49
4	D	341/342 (100%)	336 (98%)	5 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	80/81 (99%)	78 (98%)	2 (2%)	0	100	100
5	e	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	56 (90%)	6 (10%)	0	100	100
7	h	62/63 (98%)	57 (92%)	4 (6%)	1 (2%)	9	5
8	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
8	i	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
9	J	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	35/36 (97%)	34 (97%)	0	1 (3%)	4	1
11	l	35/36 (97%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	239 (98%)	5 (2%)	1 (0%)	34	32
13	o	247/243 (102%)	240 (97%)	6 (2%)	1 (0%)	34	32
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
15	u	96/97 (99%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
17	Y	28/29 (97%)	27 (96%)	1 (4%)	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
All	All	5227/5270 (99%)	5106 (98%)	111 (2%)	10 (0%)	47	49

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	L	3	PRO
3	C	416	SER
3	c	416	SER
13	O	60	ARG
19	Z	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/270 (100%)	266 (99%)	3 (1%)	73	79
1	a	270/270 (100%)	267 (99%)	3 (1%)	73	79
2	B	404/403 (100%)	403 (100%)	1 (0%)	93	96
2	b	402/403 (100%)	399 (99%)	3 (1%)	84	88
3	C	356/356 (100%)	351 (99%)	5 (1%)	67	73
3	c	356/356 (100%)	349 (98%)	7 (2%)	55	60
4	D	277/276 (100%)	273 (99%)	4 (1%)	67	73
4	d	276/276 (100%)	273 (99%)	3 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/72 (100%)	69 (96%)	3 (4%)	30	30
5	e	68/72 (94%)	67 (98%)	1 (2%)	65	71
6	F	27/28 (96%)	25 (93%)	2 (7%)	13	10
6	f	26/28 (93%)	26 (100%)	0	100	100
7	H	54/53 (102%)	53 (98%)	1 (2%)	57	63
7	h	54/53 (102%)	53 (98%)	1 (2%)	57	63
8	I	30/33 (91%)	30 (100%)	0	100	100
8	i	31/33 (94%)	31 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	28/30 (93%)	26 (93%)	2 (7%)	14	11
11	L	32/34 (94%)	32 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	29/30 (97%)	29 (100%)	0	100	100
12	m	29/30 (97%)	28 (97%)	1 (3%)	37	39
13	O	205/206 (100%)	202 (98%)	3 (2%)	65	71
13	o	203/206 (98%)	199 (98%)	4 (2%)	55	60
14	T	26/26 (100%)	25 (96%)	1 (4%)	33	34
14	t	26/26 (100%)	25 (96%)	1 (4%)	33	34
15	U	85/84 (101%)	82 (96%)	3 (4%)	36	38
15	u	85/84 (101%)	83 (98%)	2 (2%)	49	53
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	115/117 (98%)	115 (100%)	0	100	100
17	Y	22/22 (100%)	20 (91%)	2 (9%)	9	6
17	y	20/22 (91%)	18 (90%)	2 (10%)	7	5
18	X	31/32 (97%)	30 (97%)	1 (3%)	39	41
18	x	32/32 (100%)	31 (97%)	1 (3%)	40	43
19	Z	49/52 (94%)	48 (98%)	1 (2%)	55	60
19	z	47/52 (90%)	47 (100%)	0	100	100
All	All	4268/4304 (99%)	4207 (99%)	61 (1%)	67	73

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Y	30	ILE
2	b	350	GLU
15	u	8	GLU
18	X	38	GLN
1	a	238	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	53	ASN
2	b	179	GLN
13	o	82	GLN
3	C	311	GLN
3	c	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	T	1	14	8,9,10	0.75	0	7,9,11	1.63	2 (28%)
4	HSK	D	336[A]	-	7,10,12	1.36	1 (14%)	3,12,16	1.89	1 (33%)
4	HSK	D	336[B]	-	7,11,12	2.26	1 (14%)	3,14,16	1.56	1 (33%)
12	FME	M	1	12	8,9,10	1.32	1 (12%)	7,9,11	1.19	0
4	HSK	d	336[B]	-	7,11,12	1.34	1 (14%)	3,14,16	1.22	0
14	FME	t	1	14	8,9,10	0.83	0	7,9,11	1.38	1 (14%)

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	0.35	0	7,9,11	1.72	2 (28%)
12	FME	m	1	12	8,9,10	1.09	1 (12%)	7,9,11	1.01	0
8	FME	I	1	8	8,9,10	0.72	0	7,9,11	1.81	3 (42%)
4	HSK	d	336[A]	-	7,10,12	1.30	1 (14%)	3,12,16	1.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
12	FME	M	1	12	-	1/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
14	FME	t	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[B]	HSK	CE1-ND1	-5.83	1.29	1.36
4	D	336[A]	HSK	CE1-ND1	-3.39	1.32	1.36
4	d	336[B]	HSK	CE1-ND1	-3.15	1.32	1.36
4	d	336[A]	HSK	CE1-ND1	-2.72	1.33	1.36
12	M	1	FME	CA-N	2.32	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	3.30	115.69	109.73
8	I	1	FME	C-CA-N	3.12	115.36	109.73
4	D	336[A]	HSK	CD2-NE2-CE1	2.67	109.94	105.78
4	D	336[B]	HSK	CD2-NE2-CE1	2.39	109.50	105.78
8	I	1	FME	O-C-CA	-2.30	118.74	124.78

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE

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 353 ligands modelled in this entry, 52 are unknown and 18 are monoatomic - leaving 283 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$
31	LHG	B	621	-	48,48,48	0.83	2 (4%)	51,54,54	1.31	6 (11%)
29	DMS	d	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.95	0
24	BCR	b	622	-	41,41,41	1.27	4 (9%)	56,56,56	1.15	4 (7%)
24	BCR	C	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	4 (7%)
31	LHG	e	101	-	37,37,48	1.12	2 (5%)	40,42,54	0.95	2 (5%)
28	LMT	J	102	-	24,24,36	0.80	1 (4%)	29,29,47	1.23	3 (10%)
29	DMS	a	420	-	3,3,3	2.81	1 (33%)	3,3,3	1.07	0
22	CLA	d	402	-	59,73,73	1.81	13 (22%)	67,113,113	1.98	21 (31%)
22	CLA	c	506	-	59,73,73	1.98	17 (28%)	67,113,113	1.93	18 (26%)
34	GOL	b	636	-	5,5,5	0.09	0	5,5,5	0.40	0
28	LMT	T	102	-	24,24,36	0.57	0	29,29,47	1.55	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	507	41	59,73,73	2.13	18 (30%)	67,113,113	2.16	14 (20%)
29	DMS	c	539	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
22	CLA	B	612	-	59,73,73	1.85	9 (15%)	67,113,113	2.07	17 (25%)
22	CLA	b	618	-	59,73,73	1.96	14 (23%)	67,113,113	2.28	21 (31%)
29	DMS	c	538	-	3,3,3	3.04	1 (33%)	3,3,3	1.05	0
22	CLA	b	615	-	59,73,73	1.79	11 (18%)	67,113,113	1.75	15 (22%)
31	LHG	d	410	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	5 (9%)
26	LMG	d	412	39	47,47,55	0.99	3 (6%)	55,55,63	1.30	5 (9%)
29	DMS	O	308	-	3,3,3	2.72	1 (33%)	3,3,3	1.60	1 (33%)
32	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.98	2 (8%)
29	DMS	c	537	-	3,3,3	2.64	1 (33%)	3,3,3	1.13	0
22	CLA	B	603	-	59,73,73	2.10	16 (27%)	67,113,113	2.26	21 (31%)
22	CLA	C	502	-	59,73,73	2.16	12 (20%)	67,113,113	1.98	17 (25%)
24	BCR	b	621	-	41,41,41	0.87	1 (2%)	56,56,56	1.47	9 (16%)
22	CLA	a	406	-	59,73,73	1.67	13 (22%)	67,113,113	2.13	17 (25%)
25	PL9	a	411	-	55,55,55	0.97	3 (5%)	68,69,69	2.26	20 (29%)
40	HEC	v	202	16	26,50,50	2.30	8 (30%)	18,82,82	2.05	7 (38%)
28	LMT	z	101	-	33,33,36	8.08	2 (6%)	44,44,47	2.76	11 (25%)
22	CLA	b	613	-	59,73,73	2.06	16 (27%)	67,113,113	1.89	16 (23%)
29	DMS	V	207	-	3,3,3	2.81	1 (33%)	3,3,3	0.56	0
29	DMS	c	535	-	3,3,3	2.61	1 (33%)	3,3,3	0.30	0
24	BCR	K	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	3 (5%)
22	CLA	B	605	-	59,73,73	1.87	16 (27%)	67,113,113	2.09	24 (35%)
31	LHG	D	410	-	48,48,48	0.79	3 (6%)	51,54,54	1.07	2 (3%)
29	DMS	b	634	-	3,3,3	2.71	1 (33%)	3,3,3	0.67	0
29	DMS	b	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.54	0
31	LHG	E	101	-	48,48,48	1.04	2 (4%)	51,54,54	0.94	2 (3%)
29	DMS	U	202	-	3,3,3	2.61	1 (33%)	3,3,3	1.60	1 (33%)
22	CLA	b	620	-	59,73,73	2.19	13 (22%)	67,113,113	2.11	23 (34%)
22	CLA	b	612	-	59,73,73	1.90	11 (18%)	67,113,113	2.16	20 (29%)
22	CLA	a	407	41	59,73,73	1.98	14 (23%)	67,113,113	2.25	17 (25%)
22	CLA	c	510	-	59,73,73	1.97	10 (16%)	67,113,113	2.29	21 (31%)
29	DMS	V	206	-	3,3,3	2.65	1 (33%)	3,3,3	0.79	0
24	BCR	D	406	-	41,41,41	1.40	7 (17%)	56,56,56	1.92	15 (26%)
23	PHO	A	407	-	67,69,69	1.77	12 (17%)	85,99,99	1.60	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	D	403	-	59,73,73	1.79	14 (23%)	67,113,113	2.13	18 (26%)
25	PL9	D	407	-	55,55,55	1.11	6 (10%)	68,69,69	1.47	7 (10%)
29	DMS	c	532	-	3,3,3	2.72	1 (33%)	3,3,3	0.89	0
31	LHG	D	409	-	48,48,48	0.90	3 (6%)	51,54,54	1.61	6 (11%)
29	DMS	V	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
28	LMT	m	101	-	36,36,36	0.74	0	47,47,47	1.53	10 (21%)
32	HTG	C	535	-	8,8,19	0.55	0	7,7,24	1.05	1 (14%)
22	CLA	C	501	-	59,73,73	1.84	13 (22%)	67,113,113	2.61	19 (28%)
37	HEM	f	101	5,6	27,50,50	2.17	8 (29%)	17,82,82	2.12	6 (35%)
29	DMS	b	639	-	3,3,3	2.57	1 (33%)	3,3,3	1.52	0
29	DMS	A	417	-	3,3,3	2.02	1 (33%)	3,3,3	0.55	0
22	CLA	B	602	41	59,73,73	2.41	15 (25%)	67,113,113	2.06	22 (32%)
29	DMS	O	311	-	3,3,3	2.64	1 (33%)	3,3,3	1.71	1 (33%)
31	LHG	D	411	-	43,43,48	1.12	3 (6%)	46,49,54	1.08	4 (8%)
22	CLA	B	610	-	59,73,73	1.66	12 (20%)	67,113,113	2.09	16 (23%)
22	CLA	C	510	-	59,73,73	2.02	15 (25%)	67,113,113	2.23	14 (20%)
29	DMS	o	309	-	3,3,3	2.65	1 (33%)	3,3,3	1.45	0
29	DMS	O	305	-	3,3,3	2.90	1 (33%)	3,3,3	1.17	0
28	LMT	B	623	-	36,36,36	0.80	1 (2%)	47,47,47	1.68	10 (21%)
22	CLA	A	404	-	59,73,73	1.91	12 (20%)	67,113,113	2.16	18 (26%)
29	DMS	C	532	-	3,3,3	3.06	1 (33%)	3,3,3	0.95	0
22	CLA	c	504	-	59,73,73	2.50	16 (27%)	67,113,113	2.29	14 (20%)
29	DMS	v	203	-	3,3,3	2.51	1 (33%)	3,3,3	0.76	0
26	LMG	A	411	-	51,51,55	1.04	2 (3%)	59,59,63	1.24	7 (11%)
29	DMS	b	630	-	3,3,3	1.99	1 (33%)	3,3,3	0.40	0
29	DMS	b	633	-	3,3,3	2.76	1 (33%)	3,3,3	1.10	0
29	DMS	h	104	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
33	DGD	c	519	-	63,63,67	1.04	4 (6%)	77,77,81	1.38	11 (14%)
24	BCR	T	101	-	41,41,41	0.95	0	56,56,56	1.79	14 (25%)
22	CLA	c	502	-	59,73,73	2.34	13 (22%)	67,113,113	2.26	14 (20%)
22	CLA	B	614	-	59,73,73	1.97	15 (25%)	67,113,113	1.85	16 (23%)
29	DMS	V	205	-	3,3,3	2.70	1 (33%)	3,3,3	0.96	0
24	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.37	8 (14%)
29	DMS	c	529	-	3,3,3	2.92	1 (33%)	3,3,3	0.89	0
22	CLA	b	609	-	59,73,73	1.51	9 (15%)	67,113,113	2.17	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DMS	o	305	-	3,3,3	2.67	1 (33%)	3,3,3	0.74	0
23	PHO	D	404	-	67,69,69	1.98	17 (25%)	85,99,99	1.74	15 (17%)
32	HTG	c	541	-	15,15,19	1.17	1 (6%)	18,20,24	3.42	6 (33%)
22	CLA	C	509	-	59,73,73	1.72	12 (20%)	67,113,113	2.30	24 (35%)
38	RRX	h	102	-	42,42,42	0.98	2 (4%)	57,58,58	1.61	11 (19%)
29	DMS	C	531	-	3,3,3	2.72	1 (33%)	3,3,3	0.72	0
22	CLA	C	504	41	59,73,73	2.17	13 (22%)	67,113,113	2.06	16 (23%)
29	DMS	B	640	-	3,3,3	3.00	1 (33%)	3,3,3	1.33	1 (33%)
22	CLA	C	512	-	59,73,73	2.21	14 (23%)	67,113,113	2.11	21 (31%)
28	LMT	l	101	-	24,24,36	0.83	1 (4%)	29,29,47	0.97	1 (3%)
26	LMG	C	519	-	48,48,55	1.29	3 (6%)	56,56,63	1.79	12 (21%)
32	HTG	U	203	-	14,14,19	0.99	1 (7%)	18,19,24	2.78	8 (44%)
33	DGD	c	517	-	63,63,67	1.05	3 (4%)	77,77,81	1.06	5 (6%)
32	HTG	B	624	-	19,19,19	1.01	1 (5%)	23,24,24	2.08	2 (8%)
22	CLA	C	506	-	59,73,73	2.02	11 (18%)	67,113,113	2.17	15 (22%)
28	LMT	m	103	-	23,23,36	0.88	0	27,27,47	1.70	2 (7%)
24	BCR	d	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.61	10 (17%)
22	CLA	d	403	41	59,73,73	1.91	12 (20%)	67,113,113	2.07	19 (28%)
25	PL9	d	407	-	55,55,55	1.17	9 (16%)	68,69,69	1.47	9 (13%)
28	LMT	C	520	-	36,36,36	0.92	1 (2%)	47,47,47	2.14	10 (21%)
31	LHG	f	102	-	45,45,48	1.08	2 (4%)	48,51,54	1.07	5 (10%)
31	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.62	4 (7%)
22	CLA	B	604	-	59,73,73	1.74	12 (20%)	67,113,113	2.32	22 (32%)
29	DMS	V	204	-	3,3,3	2.63	1 (33%)	3,3,3	1.40	1 (33%)
22	CLA	b	607	-	59,73,73	1.80	11 (18%)	67,113,113	2.16	16 (23%)
24	BCR	y	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.71	14 (25%)
22	CLA	b	611	41	59,73,73	1.79	12 (20%)	67,113,113	2.00	17 (25%)
29	DMS	o	310	-	3,3,3	2.89	1 (33%)	3,3,3	1.04	0
29	DMS	A	418	-	3,3,3	2.66	1 (33%)	3,3,3	1.18	0
29	DMS	B	632	-	3,3,3	2.43	1 (33%)	3,3,3	1.58	1 (33%)
29	DMS	D	419	-	3,3,3	2.73	1 (33%)	3,3,3	0.68	0
22	CLA	b	606	-	59,73,73	1.82	13 (22%)	67,113,113	2.22	24 (35%)
22	CLA	c	511	-	59,73,73	1.85	11 (18%)	67,113,113	1.95	20 (29%)
29	DMS	B	631	-	3,3,3	2.87	1 (33%)	3,3,3	0.91	0
22	CLA	B	608	41	59,73,73	1.72	12 (20%)	67,113,113	1.90	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DMS	c	540	-	3,3,3	2.84	1 (33%)	3,3,3	0.97	0
22	CLA	b	616	-	59,73,73	1.95	12 (20%)	67,113,113	2.36	20 (29%)
22	CLA	B	607	-	59,73,73	2.20	14 (23%)	67,113,113	1.88	16 (23%)
32	HTG	b	601	-	19,19,19	1.08	2 (10%)	23,24,24	1.44	4 (17%)
22	CLA	c	509	-	59,73,73	2.36	15 (25%)	67,113,113	1.88	12 (17%)
29	DMS	D	415	-	3,3,3	2.59	1 (33%)	3,3,3	1.23	0
32	HTG	c	523	-	19,19,19	0.70	0	23,24,24	1.49	3 (13%)
29	DMS	u	203	-	3,3,3	2.54	1 (33%)	3,3,3	1.25	0
29	DMS	O	307	-	3,3,3	2.72	1 (33%)	3,3,3	0.40	0
29	DMS	c	528	-	3,3,3	2.31	1 (33%)	3,3,3	1.49	1 (33%)
29	DMS	O	303	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
22	CLA	c	505	41	59,73,73	2.23	15 (25%)	67,113,113	2.05	19 (28%)
28	LMT	j	102	-	23,23,36	0.89	0	27,27,47	1.94	6 (22%)
22	CLA	b	608	-	59,73,73	1.91	14 (23%)	67,113,113	2.35	22 (32%)
29	DMS	u	202	-	3,3,3	2.76	1 (33%)	3,3,3	1.44	0
29	DMS	B	636	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
29	DMS	b	631	-	3,3,3	2.63	1 (33%)	3,3,3	0.57	0
26	LMG	b	625	-	49,49,55	1.23	3 (6%)	57,57,63	1.18	6 (10%)
29	DMS	B	635	-	3,3,3	2.80	1 (33%)	3,3,3	0.64	0
33	DGD	D	408	-	45,45,67	1.49	4 (8%)	53,53,81	1.70	10 (18%)
40	HEC	V	201	16	26,50,50	2.14	5 (19%)	18,82,82	1.75	4 (22%)
32	HTG	B	642	-	18,18,19	1.11	2 (11%)	22,23,24	2.72	10 (45%)
20	OEX	A	401	1,3,41	0,15,15	0.00	-	-	-	-
33	DGD	C	516	-	63,63,67	1.06	5 (7%)	77,77,81	1.00	4 (5%)
29	DMS	o	307	-	3,3,3	2.70	1 (33%)	3,3,3	1.24	0
32	HTG	O	302	-	19,19,19	1.64	4 (21%)	23,24,24	1.26	3 (13%)
29	DMS	d	415	-	3,3,3	2.34	1 (33%)	3,3,3	0.81	0
22	CLA	C	505	-	59,73,73	1.95	16 (27%)	67,113,113	2.08	14 (20%)
26	LMG	C	518	-	49,49,55	1.07	2 (4%)	57,57,63	1.25	7 (12%)
22	CLA	b	619	-	59,73,73	2.03	13 (22%)	67,113,113	2.47	24 (35%)
32	HTG	b	602	-	19,19,19	1.11	2 (10%)	23,24,24	1.64	3 (13%)
24	BCR	k	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	6 (10%)
22	CLA	B	617	-	59,73,73	1.96	14 (23%)	67,113,113	2.22	21 (31%)
29	DMS	o	306	-	3,3,3	2.55	1 (33%)	3,3,3	1.00	0
33	DGD	d	408	-	48,48,67	1.37	5 (10%)	56,56,81	1.58	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	508	-	59,73,73	2.11	13 (22%)	67,113,113	1.97	13 (19%)
28	LMT	m	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.03	3 (10%)
26	LMG	c	520	-	38,38,55	1.29	2 (5%)	46,46,63	1.33	5 (10%)
28	LMT	a	401	-	36,36,36	1.26	3 (8%)	47,47,47	2.27	16 (34%)
28	LMT	F	102	-	24,24,36	1.31	3 (12%)	29,29,47	1.44	6 (20%)
22	CLA	A	408	-	59,73,73	2.00	15 (25%)	67,113,113	1.97	18 (26%)
22	CLA	C	513	-	59,73,73	2.71	14 (23%)	67,113,113	1.98	18 (26%)
29	DMS	D	416	-	3,3,3	2.65	1 (33%)	3,3,3	0.10	0
29	DMS	O	310	-	3,3,3	2.71	1 (33%)	3,3,3	0.89	0
29	DMS	B	637	-	3,3,3	2.59	1 (33%)	3,3,3	1.10	0
29	DMS	O	304	-	3,3,3	2.65	1 (33%)	3,3,3	0.68	0
29	DMS	o	311	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
29	DMS	V	208	-	3,3,3	2.49	1 (33%)	3,3,3	1.17	1 (33%)
33	DGD	H	101	-	63,63,67	1.22	4 (6%)	77,77,81	1.63	13 (16%)
29	DMS	v	205	-	3,3,3	2.46	1 (33%)	3,3,3	0.84	0
29	DMS	v	206	-	3,3,3	2.65	1 (33%)	3,3,3	1.12	0
29	DMS	C	529	-	3,3,3	2.64	1 (33%)	3,3,3	0.81	0
24	BCR	B	619	-	41,41,41	1.30	5 (12%)	56,56,56	1.43	7 (12%)
28	LMT	Z	101	-	36,36,36	0.84	2 (5%)	47,47,47	1.46	7 (14%)
28	LMT	M	102	-	24,24,36	0.82	0	29,29,47	1.27	3 (10%)
29	DMS	O	306	-	3,3,3	2.80	1 (33%)	3,3,3	1.14	0
23	PHO	d	404	-	67,69,69	1.96	15 (22%)	85,99,99	1.82	15 (17%)
22	CLA	c	513	-	59,73,73	2.12	13 (22%)	67,113,113	2.06	20 (29%)
22	CLA	b	605	41	59,73,73	2.21	12 (20%)	67,113,113	2.44	22 (32%)
22	CLA	B	616	-	59,73,73	2.30	16 (27%)	67,113,113	2.27	16 (23%)
34	GOL	e	104	-	5,5,5	0.82	0	5,5,5	1.63	1 (20%)
29	DMS	B	633	-	3,3,3	2.55	1 (33%)	3,3,3	0.98	0
37	HEM	F	101	5,6	27,50,50	1.95	7 (25%)	17,82,82	2.46	7 (41%)
22	CLA	c	503	-	59,73,73	1.94	10 (16%)	67,113,113	2.13	21 (31%)
29	DMS	B	639	-	3,3,3	2.59	1 (33%)	3,3,3	0.95	0
29	DMS	o	304	-	3,3,3	2.57	1 (33%)	3,3,3	1.49	0
29	DMS	u	204	-	3,3,3	2.75	1 (33%)	3,3,3	1.02	0
22	CLA	c	514	-	59,73,73	2.07	12 (20%)	67,113,113	1.93	20 (29%)
34	GOL	c	533	-	5,5,5	0.52	0	5,5,5	0.97	0
22	CLA	A	406	41	59,73,73	1.57	12 (20%)	67,113,113	2.06	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OEX	a	402	1,3,41	0,15,15	0.00	-	-		
29	DMS	C	525	-	3,3,3	2.47	1 (33%)	3,3,3	1.10	0
32	HTG	b	627	-	19,19,19	0.98	1 (5%)	23,24,24	2.00	4 (17%)
28	LMT	c	522	-	36,36,36	0.98	1 (2%)	47,47,47	1.92	10 (21%)
32	HTG	D	413	-	16,16,19	1.08	2 (12%)	20,21,24	2.53	6 (30%)
22	CLA	c	507	-	59,73,73	1.78	11 (18%)	67,113,113	1.84	16 (23%)
26	LMG	c	521	-	51,51,55	1.15	3 (5%)	59,59,63	1.12	7 (11%)
29	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.44	0
29	DMS	a	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.73	0
32	HTG	V	202	-	19,19,19	1.02	2 (10%)	23,24,24	3.35	7 (30%)
29	DMS	b	632	-	3,3,3	2.62	1 (33%)	3,3,3	0.90	0
31	LHG	b	624	-	48,48,48	0.75	2 (4%)	51,54,54	1.10	5 (9%)
22	CLA	C	511	3	59,73,73	2.40	11 (18%)	67,113,113	2.14	15 (22%)
26	LMG	a	412	-	51,51,55	1.09	3 (5%)	59,59,63	1.05	3 (5%)
28	LMT	t	102	-	24,24,36	1.12	2 (8%)	29,29,47	1.45	5 (17%)
22	CLA	B	609	-	59,73,73	1.82	12 (20%)	67,113,113	2.13	17 (25%)
29	DMS	c	536	-	3,3,3	2.69	1 (33%)	3,3,3	1.07	0
24	BCR	b	623	-	41,41,41	1.17	4 (9%)	56,56,56	1.40	9 (16%)
32	HTG	d	413	-	16,16,19	0.98	1 (6%)	20,21,24	3.85	6 (30%)
23	PHO	a	408	-	67,69,69	1.95	14 (20%)	85,99,99	1.55	13 (15%)
29	DMS	c	531	-	3,3,3	2.64	1 (33%)	3,3,3	0.66	0
29	DMS	B	634	-	3,3,3	2.62	1 (33%)	3,3,3	0.54	0
22	CLA	B	615	-	59,73,73	1.93	11 (18%)	67,113,113	2.38	21 (31%)
26	LMG	D	412	39	47,47,55	1.05	3 (6%)	55,55,63	1.14	3 (5%)
29	DMS	C	528	-	3,3,3	2.55	1 (33%)	3,3,3	0.52	0
29	DMS	C	530	-	3,3,3	2.06	1 (33%)	3,3,3	0.70	0
28	LMT	A	415	-	36,36,36	1.33	4 (11%)	47,47,47	1.97	15 (31%)
28	LMT	b	626	-	25,25,36	0.96	1 (4%)	30,30,47	1.57	3 (10%)
32	HTG	B	629	-	19,19,19	0.97	2 (10%)	23,24,24	1.46	3 (13%)
33	DGD	C	517	-	63,63,67	0.95	4 (6%)	77,77,81	1.17	9 (11%)
29	DMS	A	419	-	3,3,3	2.96	1 (33%)	3,3,3	0.81	0
29	DMS	D	420	-	3,3,3	2.61	1 (33%)	3,3,3	0.95	0
22	CLA	b	610	-	59,73,73	2.39	13 (22%)	67,113,113	2.19	16 (23%)
22	CLA	c	508	41	59,73,73	2.12	16 (27%)	67,113,113	2.28	16 (23%)
29	DMS	C	526	-	3,3,3	2.76	1 (33%)	3,3,3	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DMS	b	635	-	3,3,3	2.89	1 (33%)	3,3,3	0.94	0
22	CLA	D	405	-	59,73,73	1.90	12 (20%)	67,113,113	1.74	16 (23%)
22	CLA	B	613	-	59,73,73	1.75	10 (16%)	67,113,113	2.19	20 (29%)
29	DMS	E	104	-	3,3,3	2.75	1 (33%)	3,3,3	1.00	0
36	BCT	d	401[B]	35	0,3,3	0.00	-	0,3,3	0.00	-
25	PL9	A	410	-	55,55,55	1.15	4 (7%)	68,69,69	2.12	17 (25%)
29	DMS	I	105	-	3,3,3	2.69	1 (33%)	3,3,3	1.03	0
26	LMG	B	622	-	51,51,55	1.01	3 (5%)	59,59,63	1.26	7 (11%)
29	DMS	D	418	-	3,3,3	2.59	1 (33%)	3,3,3	1.66	0
33	DGD	h	101	-	63,63,67	1.20	4 (6%)	77,77,81	1.43	15 (19%)
29	DMS	e	105	-	3,3,3	2.74	1 (33%)	3,3,3	1.02	0
29	DMS	O	312	-	3,3,3	2.72	1 (33%)	3,3,3	0.68	0
29	DMS	B	638	-	3,3,3	2.31	1 (33%)	3,3,3	1.19	0
22	CLA	d	405	-	59,73,73	2.13	15 (25%)	67,113,113	2.02	19 (28%)
29	DMS	a	418	-	3,3,3	2.79	1 (33%)	3,3,3	0.71	0
24	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.90	18 (32%)
22	CLA	B	606	-	59,73,73	2.01	13 (22%)	67,113,113	2.27	17 (25%)
22	CLA	C	503	-	59,73,73	2.01	14 (23%)	67,113,113	2.01	20 (29%)
32	HTG	o	301	-	19,19,19	1.94	3 (15%)	23,24,24	1.78	7 (30%)
32	HTG	B	628	-	19,19,19	0.49	0	23,24,24	1.76	2 (8%)
22	CLA	b	617	-	59,73,73	1.84	12 (20%)	67,113,113	1.83	18 (26%)
32	HTG	c	524	-	8,8,19	0.55	0	7,7,24	1.33	1 (14%)
36	BCT	D	402[B]	35	0,3,3	0.00	-	0,3,3	0.00	-
32	HTG	v	208	-	16,16,19	0.92	1 (6%)	20,21,24	3.35	6 (30%)
29	DMS	a	416	-	3,3,3	2.85	1 (33%)	3,3,3	1.15	0
22	CLA	b	614	41	59,73,73	1.71	13 (22%)	67,113,113	1.89	18 (26%)
36	BCT	d	401[A]	35	0,3,3	0.00	-	0,3,3	0.00	-
29	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	1.11	0
29	DMS	o	303	-	3,3,3	1.94	1 (33%)	3,3,3	0.78	0
29	DMS	o	308	-	3,3,3	2.81	1 (33%)	3,3,3	0.41	0
29	DMS	a	417	-	3,3,3	2.82	1 (33%)	3,3,3	1.16	0
31	LHG	d	411	-	43,43,48	1.03	3 (6%)	46,49,54	0.99	5 (10%)
24	BCR	a	410	-	41,41,41	1.05	4 (9%)	56,56,56	1.10	5 (8%)
24	BCR	B	618	-	41,41,41	0.91	0	56,56,56	1.34	9 (16%)
38	RRX	H	102	-	42,42,42	1.09	2 (4%)	57,58,58	1.51	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	611	41	59,73,73	2.18	14 (23%)	67,113,113	2.00	16 (23%)
33	DGD	C	515	-	63,63,67	1.01	4 (6%)	77,77,81	1.23	7 (9%)
29	DMS	O	309	-	3,3,3	2.76	1 (33%)	3,3,3	0.91	0
31	LHG	F	103	-	37,37,48	1.21	2 (5%)	40,43,54	1.58	4 (10%)
29	DMS	A	416	-	3,3,3	2.74	1 (33%)	3,3,3	1.01	0
29	DMS	v	207	-	3,3,3	2.99	1 (33%)	3,3,3	1.23	1 (33%)
33	DGD	c	518	-	57,57,67	0.95	4 (7%)	71,71,81	1.09	7 (9%)
28	LMT	M	101	-	36,36,36	0.66	0	47,47,47	1.37	6 (12%)
29	DMS	v	204	-	3,3,3	2.69	1 (33%)	3,3,3	1.08	0
22	CLA	c	512	3	59,73,73	2.57	14 (23%)	67,113,113	2.24	18 (26%)
24	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.37	11 (19%)
24	BCR	K	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.36	10 (17%)
29	DMS	c	530	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
29	DMS	b	638	-	3,3,3	3.10	1 (33%)	3,3,3	1.05	0
32	HTG	C	536	-	19,19,19	1.22	2 (10%)	23,24,24	1.82	1 (4%)
34	GOL	C	533	-	5,5,5	0.54	0	5,5,5	1.67	1 (20%)
29	DMS	B	641	-	3,3,3	2.83	1 (33%)	3,3,3	1.00	0
32	HTG	C	521	-	19,19,19	0.80	0	23,24,24	1.74	4 (17%)
22	CLA	A	405	41	59,73,73	2.11	11 (18%)	67,113,113	2.59	22 (32%)
24	BCR	B	620	-	41,41,41	1.24	3 (7%)	56,56,56	1.34	9 (16%)
24	BCR	c	516	-	41,41,41	1.11	3 (7%)	56,56,56	1.37	8 (14%)
32	HTG	b	640	-	17,17,19	2.71	5 (29%)	21,22,24	3.94	12 (57%)
22	CLA	a	409	-	59,73,73	1.66	11 (18%)	67,113,113	2.05	15 (22%)
34	GOL	D	417	-	5,5,5	0.48	0	5,5,5	0.47	0
24	BCR	A	409	-	41,41,41	1.44	8 (19%)	56,56,56	1.55	7 (12%)
36	BCT	D	402[A]	35	0,3,3	0.00	-	0,3,3	0.00	-
29	DMS	C	534	-	3,3,3	2.78	1 (33%)	3,3,3	1.01	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
31	LHG	B	621	-	-	14/53/53/53	-
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PL9	D	407	-	-	1/53/73/73	0/1/1/1
28	LMT	J	102	-	-	8/15/35/61	0/1/1/2
22	CLA	d	402	-	1/1/20/25	4/37/135/135	-
22	CLA	c	506	-	2/2/20/25	3/37/135/135	-
34	GOL	b	636	-	-	2/4/4/4	-
28	LMT	T	102	-	-	6/15/35/61	0/1/1/2
22	CLA	B	612	-	1/1/20/25	3/37/135/135	-
32	HTG	B	628	-	-	3/10/30/30	0/1/1/1
22	CLA	b	615	-	1/1/20/25	5/37/135/135	-
31	LHG	d	410	-	-	7/53/53/53	-
26	LMG	d	412	39	-	9/42/62/70	0/1/1/1
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
22	CLA	B	603	-	3/3/20/25	6/37/135/135	-
22	CLA	C	502	-	1/1/20/25	6/37/135/135	-
24	BCR	b	621	-	-	2/29/63/63	0/2/2/2
22	CLA	a	406	-	3/3/20/25	4/37/135/135	-
22	CLA	C	508	-	3/3/20/25	4/37/135/135	-
40	HEC	v	202	16	-	0/6/54/54	-
28	LMT	z	101	-	1/1/10/10	6/18/58/61	0/2/2/2
22	CLA	b	613	-	2/2/20/25	2/37/135/135	-
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
22	CLA	B	605	-	2/2/20/25	9/37/135/135	-
31	LHG	D	410	-	-	6/53/53/53	-
22	CLA	b	620	-	3/3/20/25	15/37/135/135	-
37	HEM	f	101	5,6	-	0/6/54/54	-
22	CLA	c	510	-	3/3/20/25	11/37/135/135	-
24	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
24	BCR	D	406	-	-	2/29/63/63	0/2/2/2
23	PHO	A	407	-	-	2/53/103/103	0/5/6/6
22	CLA	D	403	-	2/2/20/25	1/37/135/135	-
31	LHG	e	101	-	-	18/41/41/53	-
31	LHG	D	409	-	-	10/53/53/53	-
22	CLA	d	405	-	2/2/20/25	12/37/135/135	-
28	LMT	m	101	-	-	6/21/61/61	0/2/2/2
32	HTG	C	535	-	-	3/6/6/30	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	501	-	3/3/20/25	4/37/135/135	-
22	CLA	a	407	41	2/2/20/25	11/37/135/135	-
22	CLA	B	602	41	3/3/20/25	14/37/135/135	-
22	CLA	B	610	-	3/3/20/25	1/37/135/135	-
22	CLA	C	510	-	3/3/20/25	9/37/135/135	-
28	LMT	B	623	-	-	7/21/61/61	0/2/2/2
22	CLA	A	404	-	3/3/20/25	5/37/135/135	-
32	HTG	v	208	-	-	3/7/27/30	0/1/1/1
22	CLA	c	504	-	2/2/20/25	2/37/135/135	-
22	CLA	D	405	-	3/3/20/25	7/37/135/135	-
33	DGD	c	519	-	-	11/51/91/95	0/2/2/2
28	LMT	t	102	-	-	9/15/35/61	0/1/1/2
26	LMG	A	411	-	-	23/46/66/70	0/1/1/1
22	CLA	c	502	-	2/2/20/25	6/37/135/135	-
22	CLA	c	507	-	3/3/20/25	7/37/135/135	-
22	CLA	b	609	-	3/3/20/25	2/37/135/135	-
23	PHO	D	404	-	-	3/53/103/103	0/5/6/6
32	HTG	c	541	-	-	3/6/26/30	0/1/1/1
22	CLA	C	509	-	3/3/20/25	8/37/135/135	-
38	RRX	h	102	-	-	0/29/65/65	0/2/2/2
28	LMT	F	102	-	-	9/15/35/61	0/1/1/2
24	BCR	y	101	-	-	2/29/63/63	0/2/2/2
26	LMG	C	519	-	-	13/43/63/70	0/1/1/1
22	CLA	c	512	3	3/3/20/25	1/37/135/135	-
22	CLA	B	614	-	3/3/20/25	8/37/135/135	-
32	HTG	B	624	-	-	3/10/30/30	0/1/1/1
22	CLA	C	506	-	3/3/20/25	10/37/135/135	-
28	LMT	m	103	-	-	6/15/31/61	0/1/1/2
24	BCR	d	406	-	-	2/29/63/63	0/2/2/2
22	CLA	d	403	41	2/2/20/25	5/37/135/135	-
25	PL9	d	407	-	-	3/53/73/73	0/1/1/1
24	BCR	a	410	-	-	0/29/63/63	0/2/2/2
31	LHG	d	409	-	-	11/53/53/53	-
22	CLA	B	604	-	2/2/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	611	41	3/3/20/25	5/37/135/135	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
22	CLA	b	606	-	2/2/20/25	6/37/135/135	-
22	CLA	c	511	-	3/3/20/25	9/37/135/135	-
22	CLA	B	608	41	3/3/20/25	6/37/135/135	-
22	CLA	b	616	-	3/3/20/25	4/37/135/135	-
22	CLA	B	607	-	3/3/20/25	8/37/135/135	-
32	HTG	b	601	-	-	4/10/30/30	0/1/1/1
32	HTG	d	413	-	-	2/7/27/30	0/1/1/1
32	HTG	c	523	-	-	5/10/30/30	0/1/1/1
32	HTG	V	202	-	-	3/10/30/30	0/1/1/1
22	CLA	c	505	41	1/1/20/25	5/37/135/135	-
28	LMT	j	102	-	-	8/15/31/61	0/1/1/2
26	LMG	b	625	-	-	14/44/64/70	0/1/1/1
33	DGD	D	408	-	-	20/39/59/95	0/1/1/2
40	HEC	V	201	16	-	0/6/54/54	-
32	HTG	B	642	-	-	5/9/29/30	0/1/1/1
33	DGD	C	516	-	-	20/51/91/95	0/2/2/2
24	BCR	A	409	-	-	1/29/63/63	0/2/2/2
32	HTG	O	302	-	-	4/10/30/30	0/1/1/1
22	CLA	C	505	-	2/2/20/25	3/37/135/135	-
26	LMG	C	518	-	-	14/44/64/70	0/1/1/1
22	CLA	b	619	-	3/3/20/25	5/37/135/135	-
32	HTG	b	602	-	-	1/10/30/30	0/1/1/1
22	CLA	B	617	-	3/3/20/25	10/37/135/135	-
33	DGD	d	408	-	-	12/42/62/95	0/1/1/2
25	PL9	a	411	-	-	10/53/73/73	0/1/1/1
28	LMT	m	102	-	-	8/15/35/61	0/1/1/2
28	LMT	a	401	-	-	9/21/61/61	0/2/2/2
22	CLA	C	504	41	3/3/20/25	9/37/135/135	-
22	CLA	A	408	-	2/2/20/25	15/37/135/135	-
28	LMT	M	101	-	-	4/21/61/61	0/2/2/2
32	HTG	U	203	-	-	2/5/25/30	0/1/1/1
31	LHG	d	411	-	-	11/48/48/53	-
33	DGD	H	101	-	-	12/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
28	LMT	M	102	-	-	6/15/35/61	0/1/1/2
23	PHO	d	404	-	-	2/53/103/103	0/5/6/6
22	CLA	c	513	-	3/3/20/25	10/37/135/135	-
28	LMT	b	626	-	-	11/17/37/61	0/1/1/2
37	HEM	F	101	5,6	-	0/6/54/54	-
33	DGD	h	101	-	-	15/51/91/95	0/2/2/2
22	CLA	b	614	41	3/3/20/25	3/37/135/135	-
22	CLA	c	514	-	1/1/20/25	13/37/135/135	-
34	GOL	c	533	-	-	4/4/4/4	-
22	CLA	A	406	41	2/2/20/25	4/37/135/135	-
32	HTG	b	627	-	-	6/10/30/30	0/1/1/1
28	LMT	c	522	-	-	6/21/61/61	0/2/2/2
32	HTG	D	413	-	-	2/7/27/30	0/1/1/1
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	LHG	D	411	-	-	14/48/48/53	-
31	LHG	b	624	-	-	21/53/53/53	-
22	CLA	C	511	3	3/3/20/25	1/37/135/135	-
26	LMG	a	412	-	-	14/46/66/70	0/1/1/1
22	CLA	b	608	-	3/3/20/25	4/37/135/135	-
22	CLA	B	609	-	1/1/20/25	2/37/135/135	-
22	CLA	b	607	-	3/3/20/25	2/37/135/135	-
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
22	CLA	c	509	-	2/2/20/25	4/37/135/135	-
23	PHO	a	408	-	-	5/53/103/103	0/5/6/6
22	CLA	B	615	-	3/3/20/25	11/37/135/135	-
26	LMG	D	412	39	-	12/42/62/70	0/1/1/1
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
28	LMT	A	415	-	-	12/21/61/61	0/2/2/2
32	HTG	B	629	-	-	1/10/30/30	0/1/1/1
33	DGD	C	517	-	-	13/51/91/95	0/2/2/2
22	CLA	c	503	-	2/2/20/25	7/37/135/135	-
22	CLA	b	610	-	2/2/20/25	9/37/135/135	-
22	CLA	c	508	41	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	613	-	3/3/20/25	3/37/135/135	-
31	LHG	f	102	-	-	16/50/50/53	-
25	PL9	A	410	-	-	10/53/73/73	0/1/1/1
26	LMG	B	622	-	-	12/46/66/70	0/1/1/1
22	CLA	B	611	41	3/3/20/25	3/37/135/135	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
22	CLA	B	606	-	3/3/20/25	7/37/135/135	-
22	CLA	C	503	-	2/2/20/25	3/37/135/135	-
32	HTG	o	301	-	-	4/10/30/30	0/1/1/1
22	CLA	C	507	41	3/3/20/25	8/37/135/135	-
22	CLA	b	617	-	3/3/20/25	1/37/135/135	-
32	HTG	c	524	-	-	3/6/6/30	-
22	CLA	B	616	-	3/3/20/25	9/37/135/135	-
22	CLA	b	618	-	3/3/20/25	13/37/135/135	-
31	LHG	E	101	-	-	29/53/53/53	-
22	CLA	b	612	-	2/2/20/25	2/37/135/135	-
34	GOL	C	533	-	-	2/4/4/4	-
22	CLA	C	512	-	3/3/20/25	7/37/135/135	-
28	LMT	l	101	-	-	6/15/35/61	0/1/1/2
28	LMT	C	520	-	1/1/10/10	13/21/61/61	0/2/2/2
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	DGD	C	515	-	-	16/51/91/95	0/2/2/2
32	HTG	b	640	-	-	4/8/28/30	0/1/1/1
31	LHG	F	103	-	-	15/42/42/53	-
33	DGD	c	518	-	-	15/45/85/95	0/2/2/2
22	CLA	C	513	-	1/1/20/25	12/37/135/135	-
26	LMG	c	520	-	-	9/33/53/70	0/1/1/1
22	CLA	b	605	41	3/3/20/25	17/37/135/135	-
34	GOL	e	104	-	-	1/4/4/4	-
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
26	LMG	c	521	-	-	20/46/66/70	0/1/1/1
32	HTG	C	536	-	-	3/10/30/30	0/1/1/1
24	BCR	T	101	-	-	4/29/63/63	0/2/2/2
32	HTG	C	521	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	405	41	1/1/20/25	6/37/135/135	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	BCR	c	516	-	-	0/29/63/63	0/2/2/2
33	DGD	c	517	-	-	14/51/91/95	0/2/2/2
22	CLA	a	409	-	2/2/20/25	12/37/135/135	-
34	GOL	D	417	-	-	3/4/4/4	-

The worst 5 of 1330 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	z	101	LMT	C2-C1	46.12	3.47	1.51
22	C	513	CLA	MG-NA	14.53	2.40	2.06
22	c	512	CLA	MG-NA	13.25	2.37	2.06
22	c	504	CLA	MG-NA	12.94	2.37	2.06
22	C	511	CLA	MG-NA	12.29	2.35	2.06

The worst 5 of 2053 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	413	HTG	C1'-S1-C1	13.68	125.67	100.09
32	c	541	HTG	C1'-S1-C1	12.83	124.08	100.09
22	c	504	CLA	C4A-NA-C1A	11.98	112.09	106.71
22	B	616	CLA	C4A-NA-C1A	11.74	111.99	106.71
32	V	202	HTG	O5-C1-C2	-11.63	95.69	110.31

5 of 174 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	605	CLA	NC
22	B	605	CLA	NA
22	D	403	CLA	ND
22	D	403	CLA	NA
22	b	611	CLA	NC

5 of 1200 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	e	101	LHG	C3-O3-P-O4
31	e	101	LHG	C3-O3-P-O5
32	c	541	HTG	O5-C1-S1-C1'
32	B	624	HTG	O5-C1-S1-C1'

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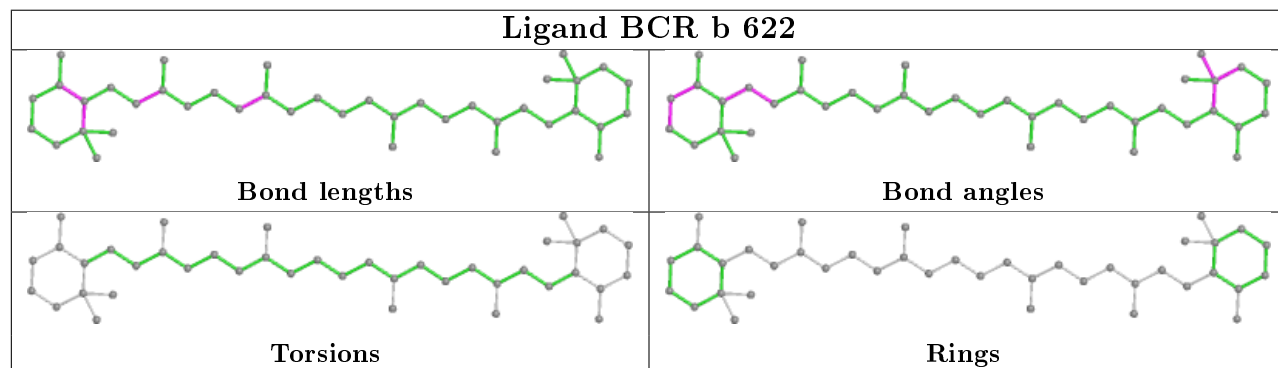
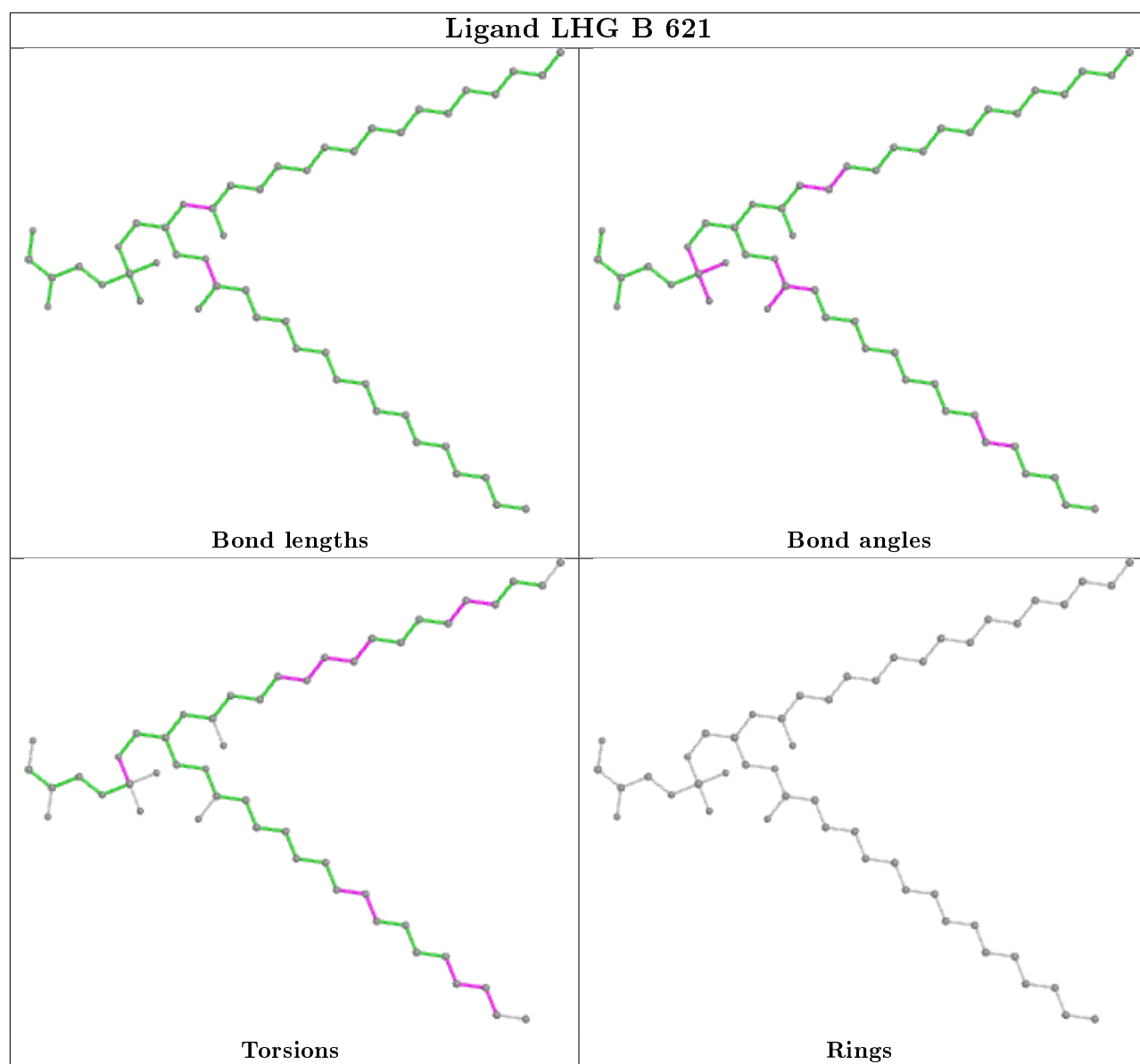
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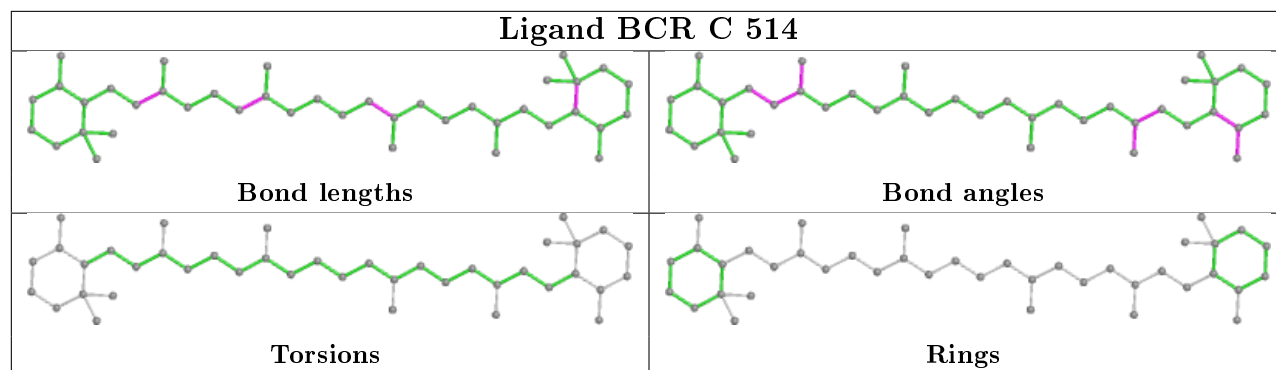
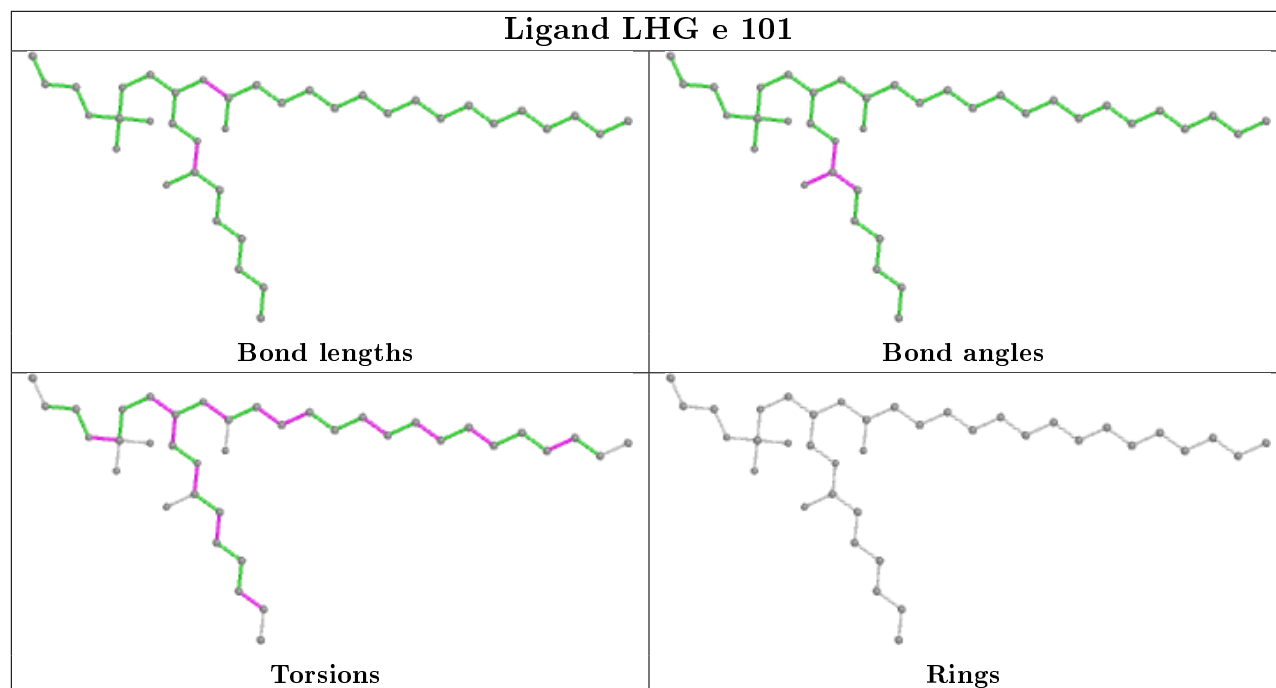
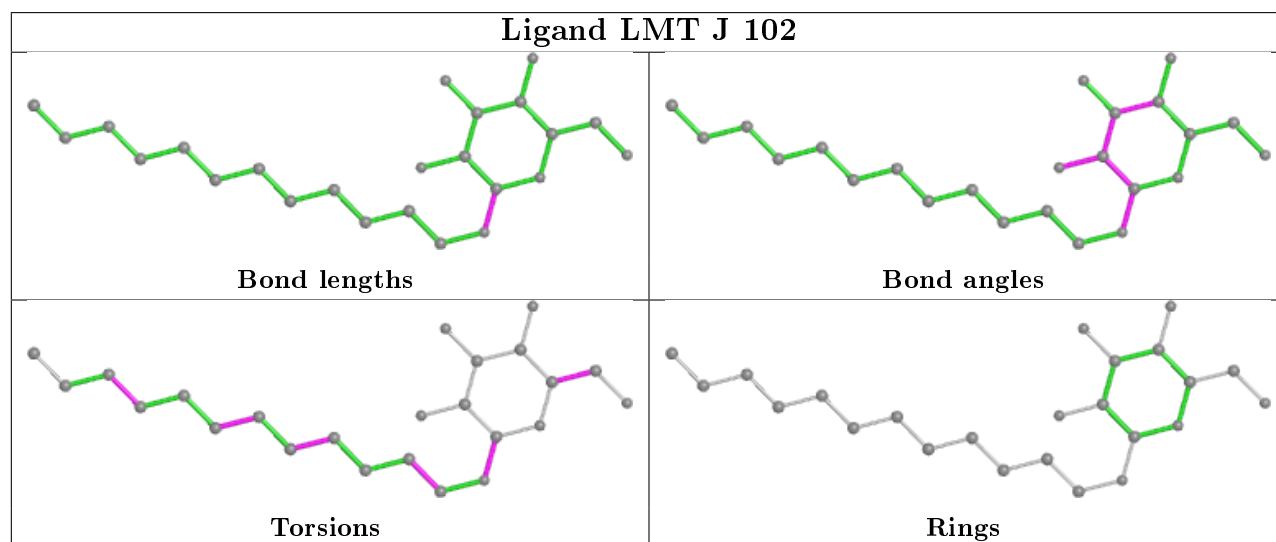
Mol	Chain	Res	Type	Atoms
32	B	642	HTG	C2'-C1'-S1-C1

There are no ring outliers.

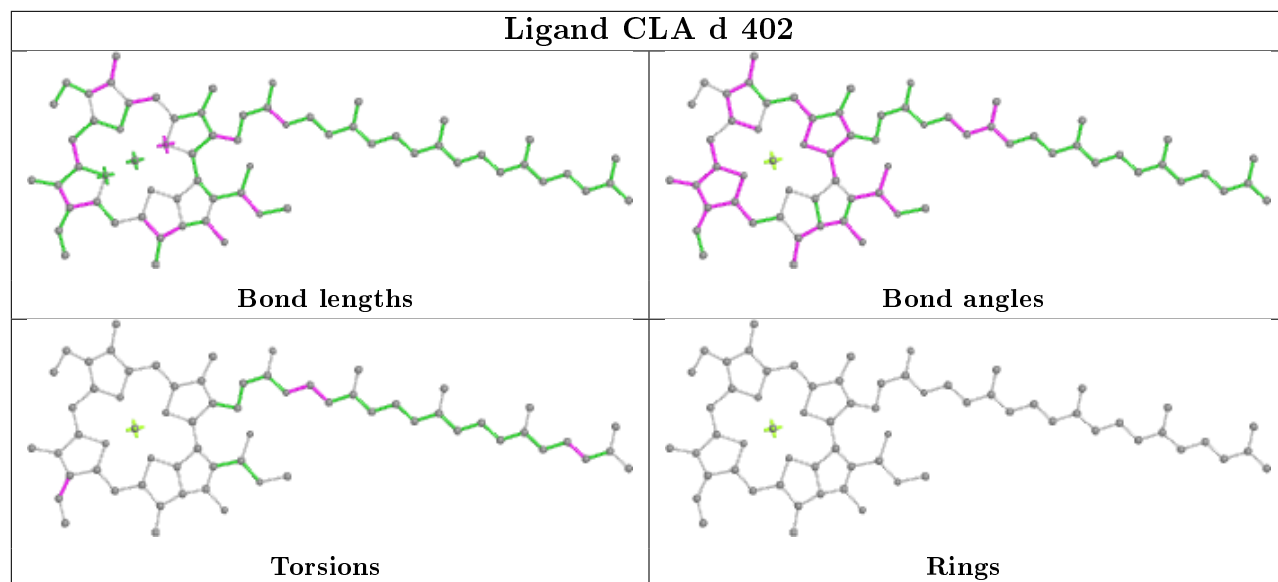
No monomer is involved in short contacts.

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

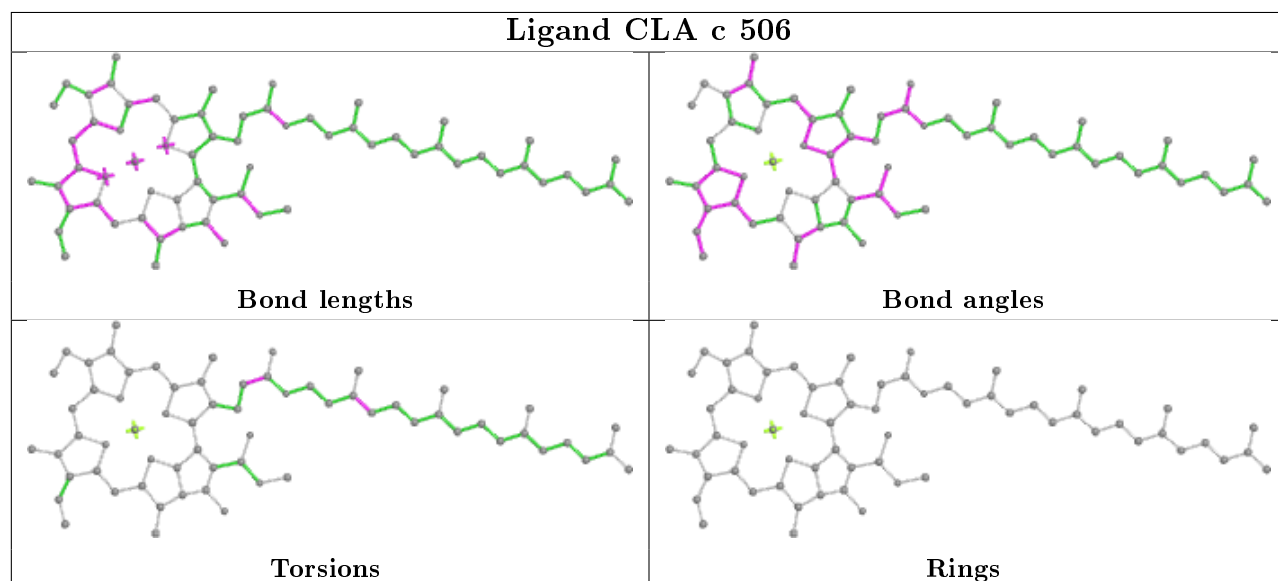


Ligand BCR C 514**Ligand LHG e 101****Ligand LMT J 102**

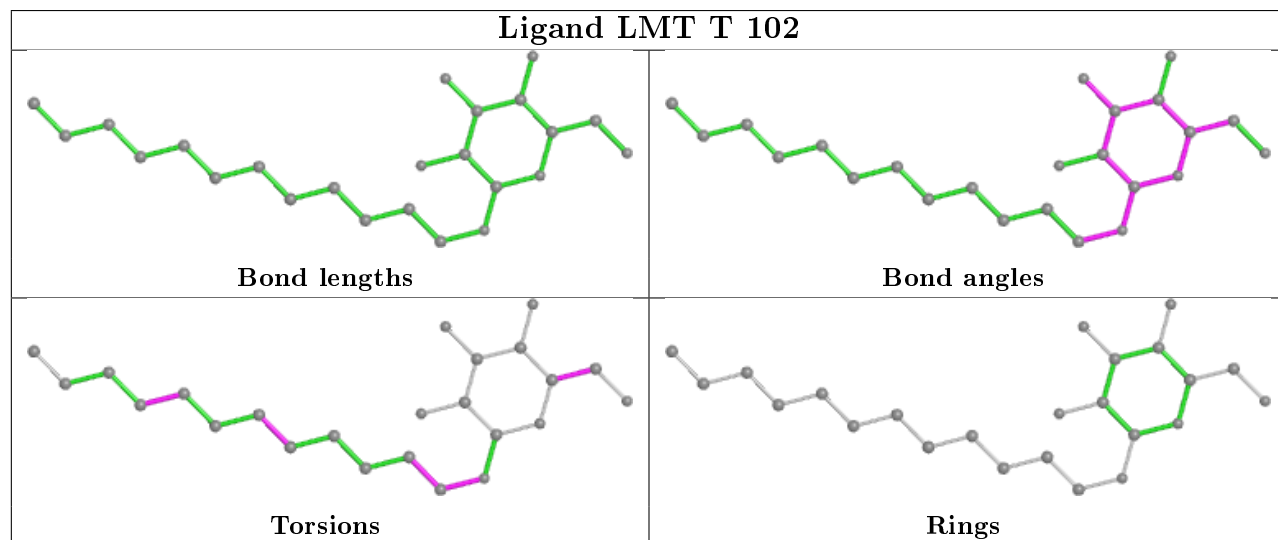
Ligand CLA d 402

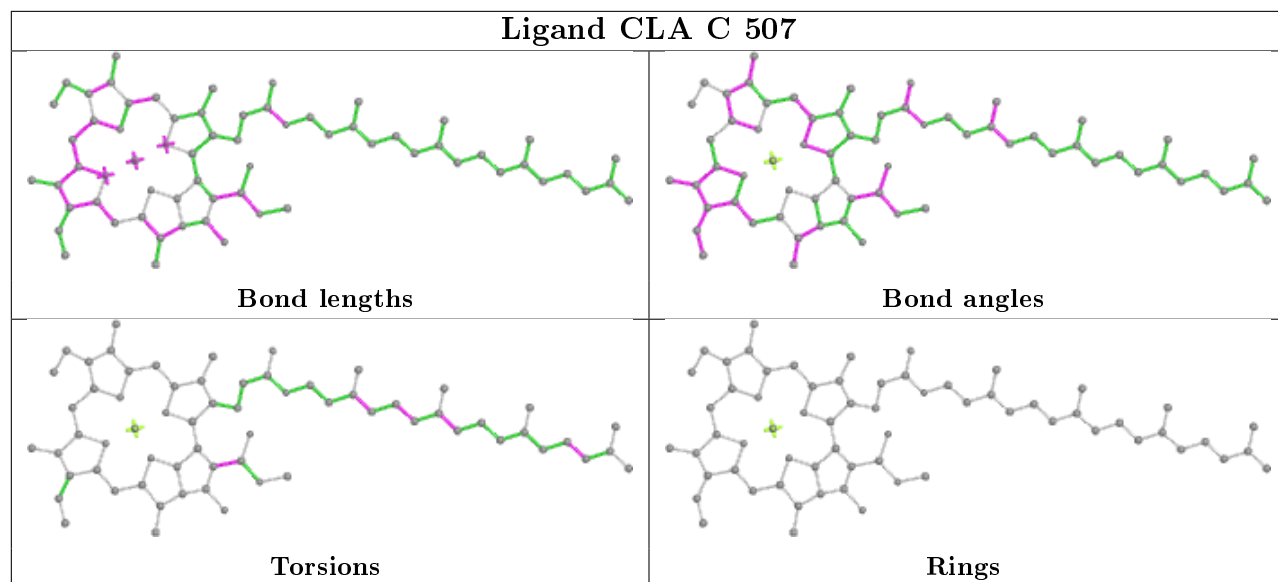
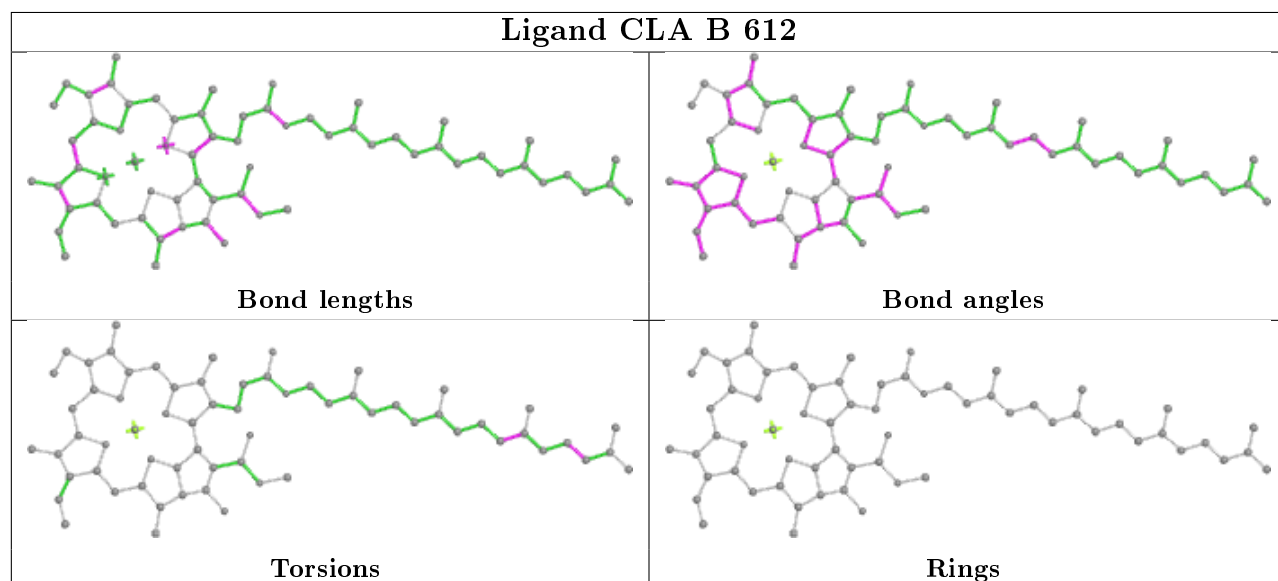
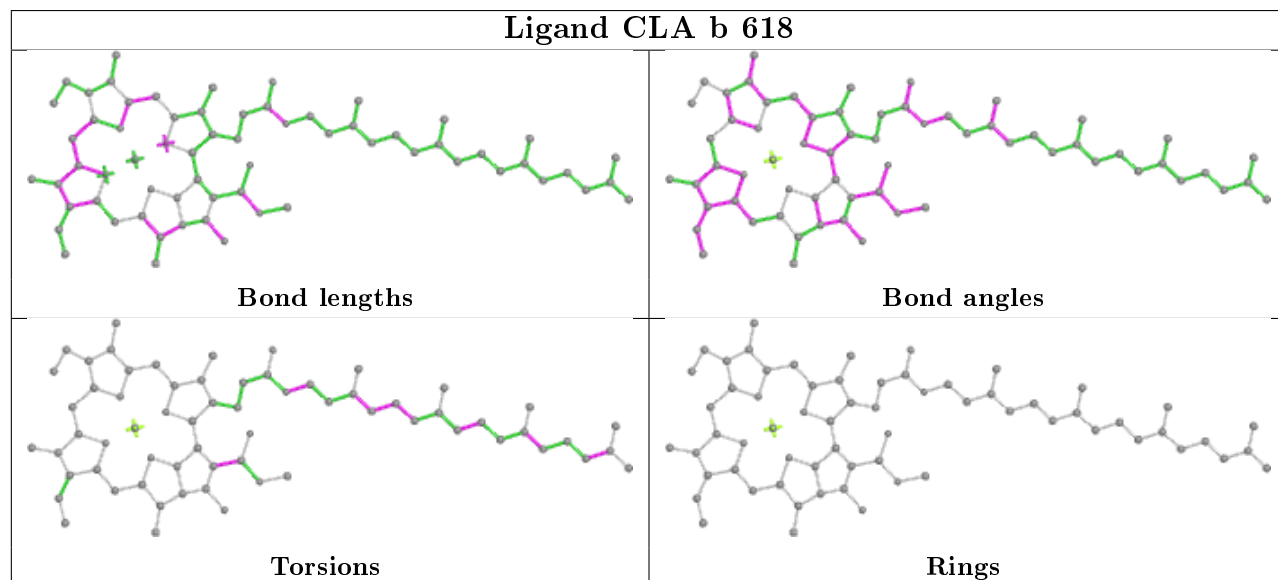


Ligand CLA c 506

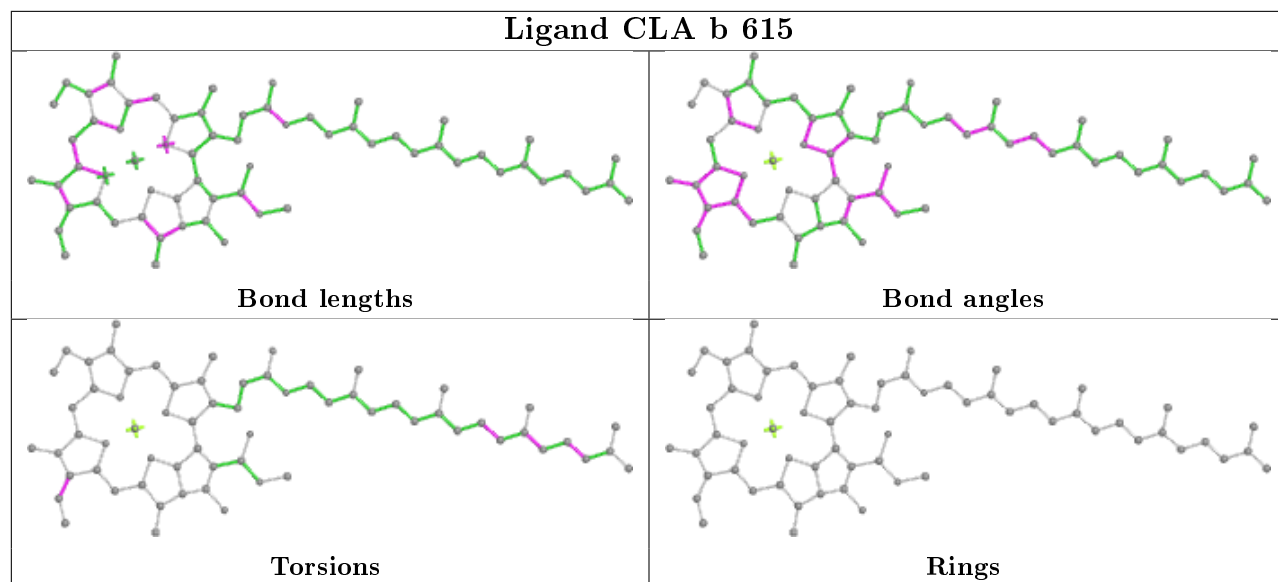


Ligand LMT T 102

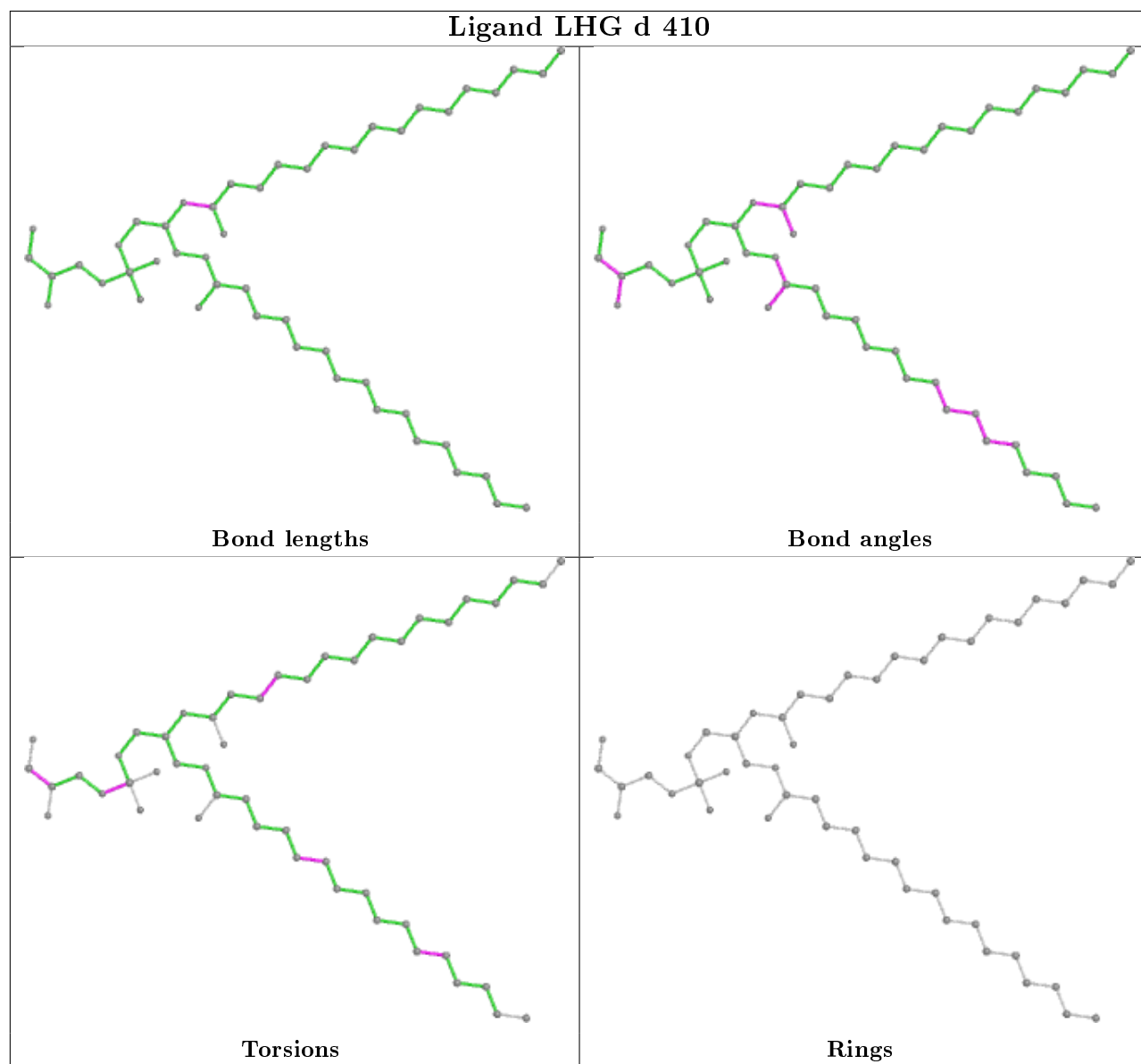


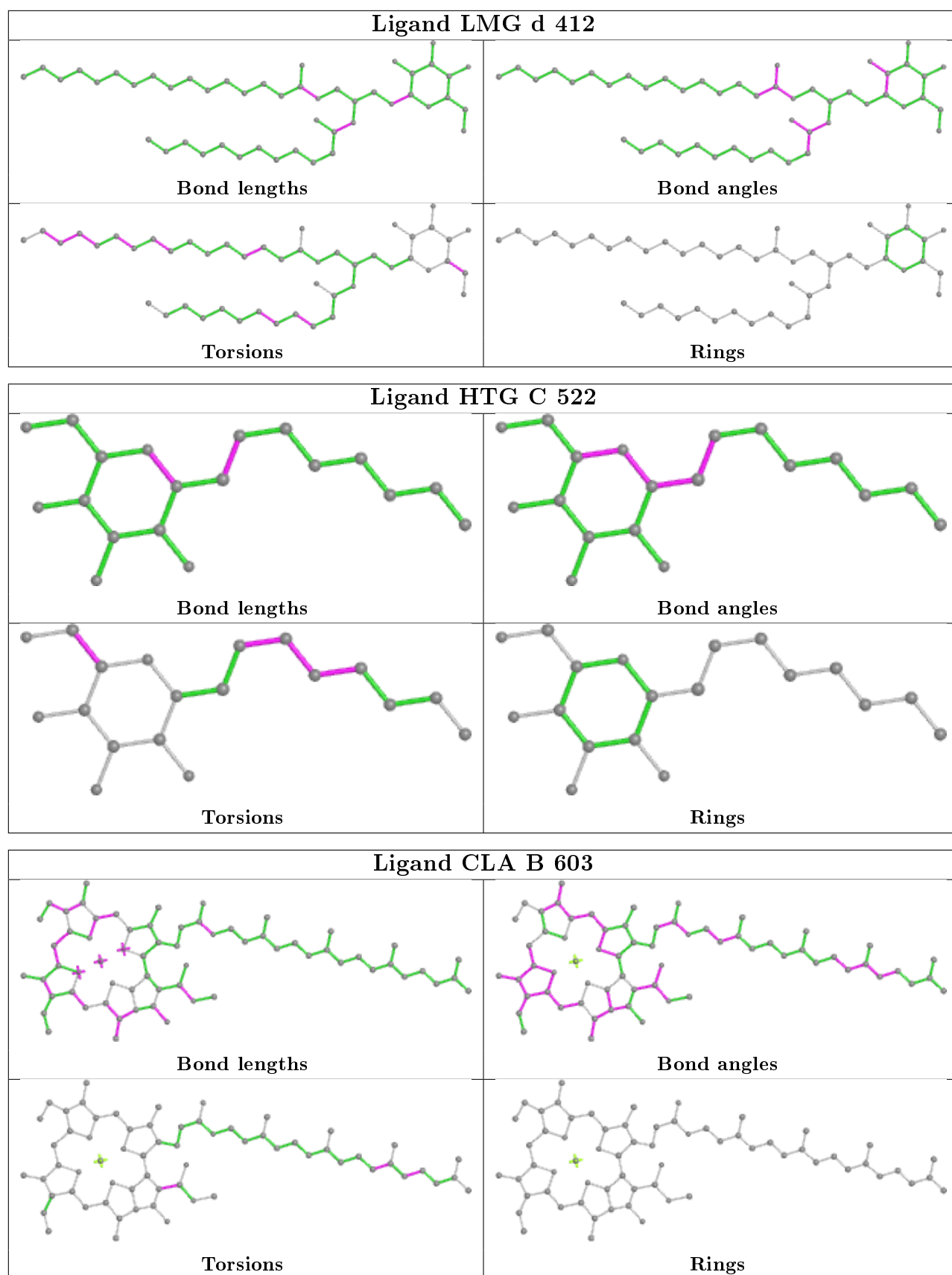
Ligand CLA C 507**Ligand CLA B 612****Ligand CLA b 618**

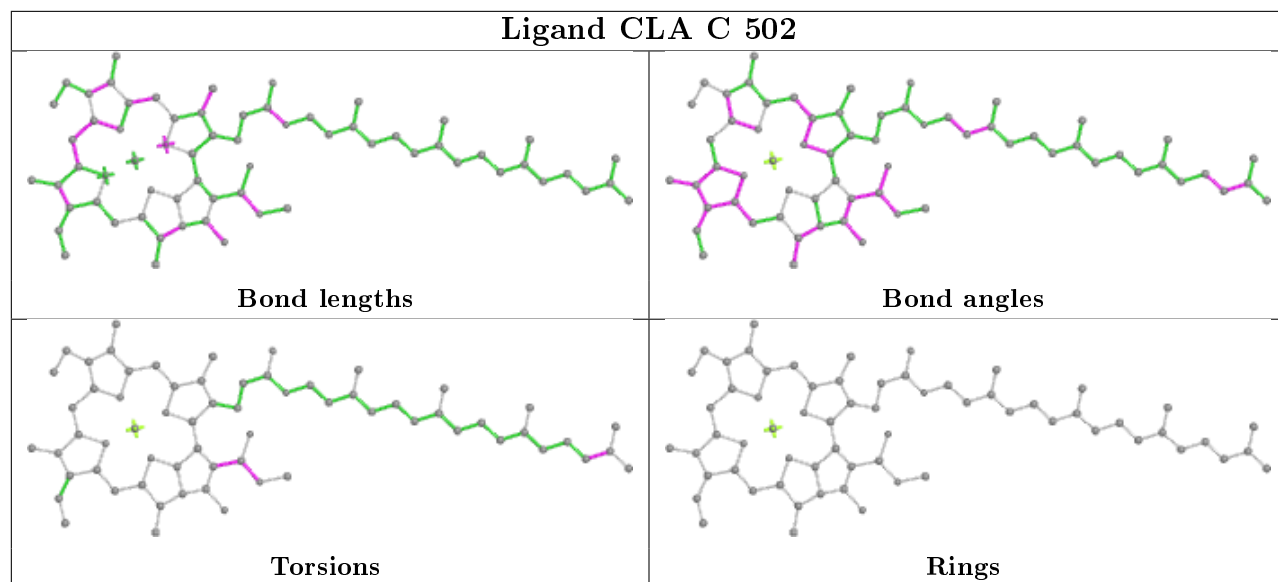
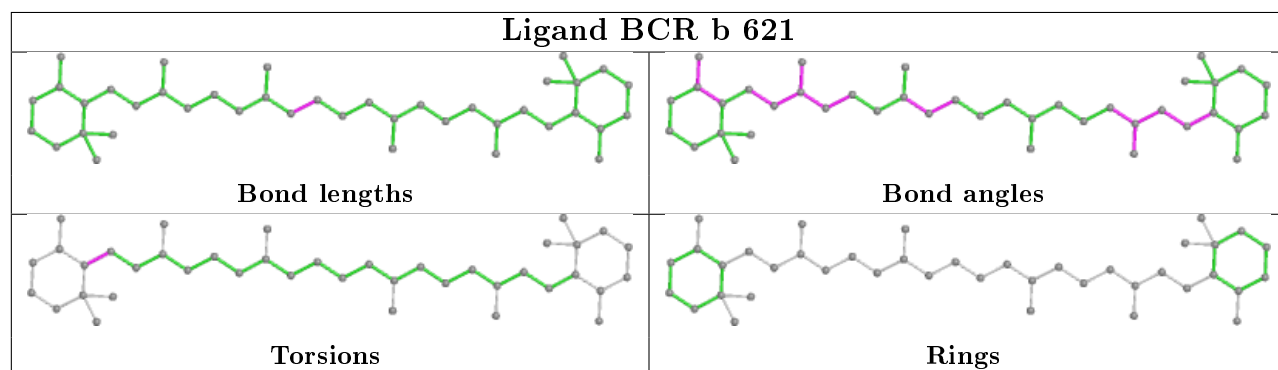
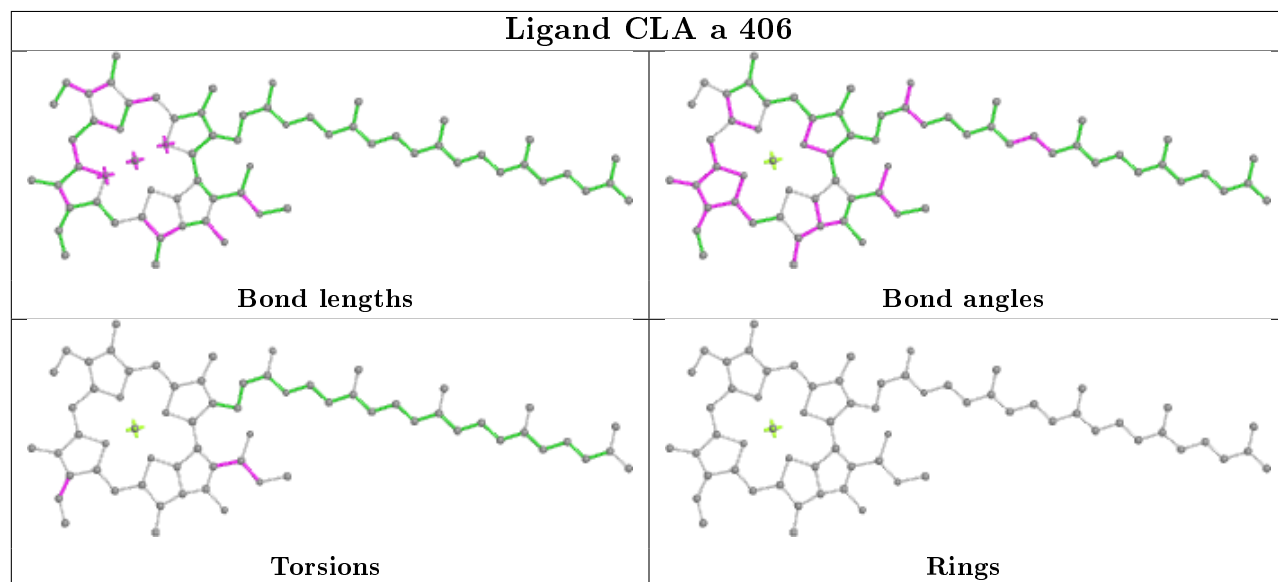
Ligand CLA b 615

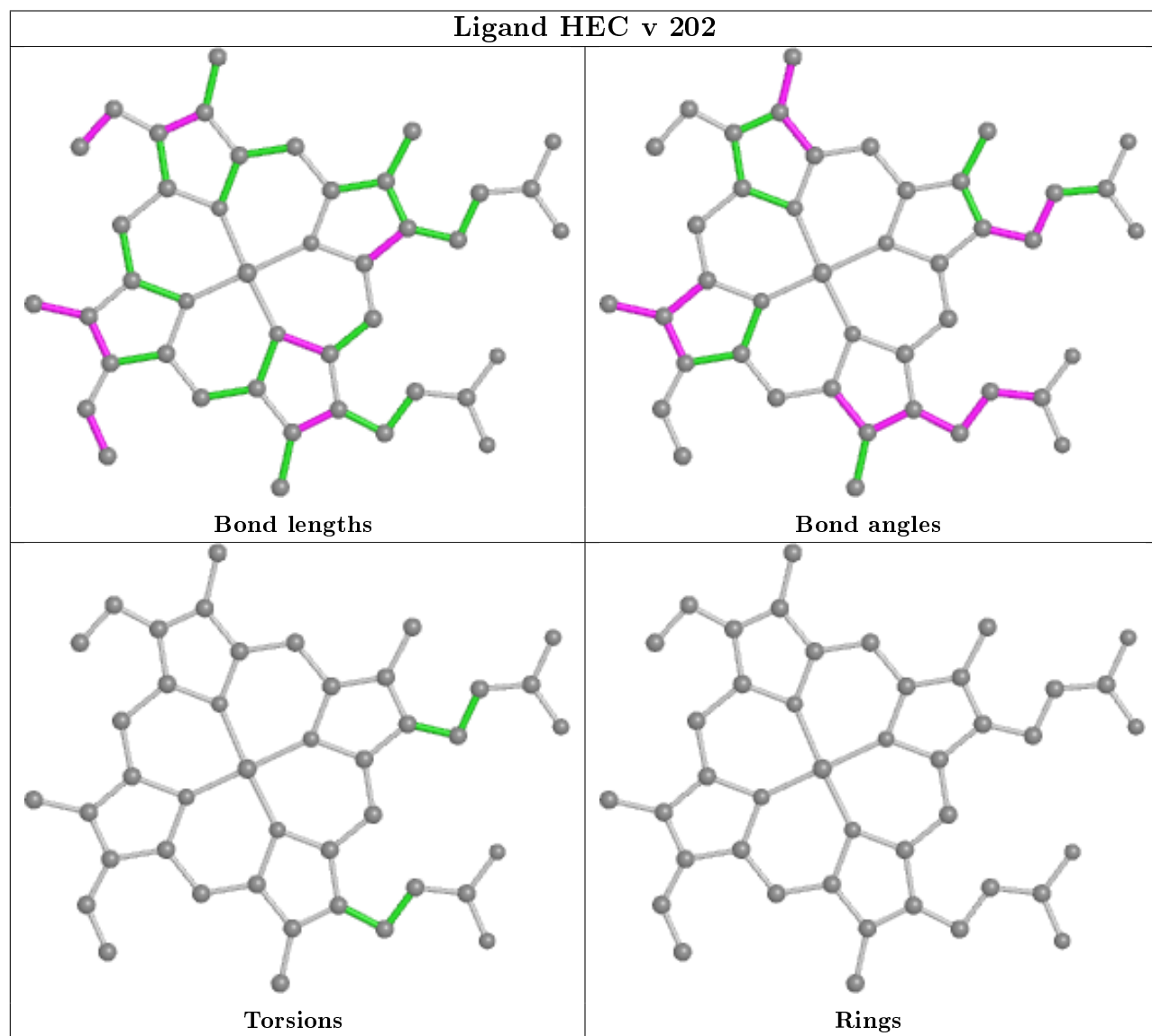
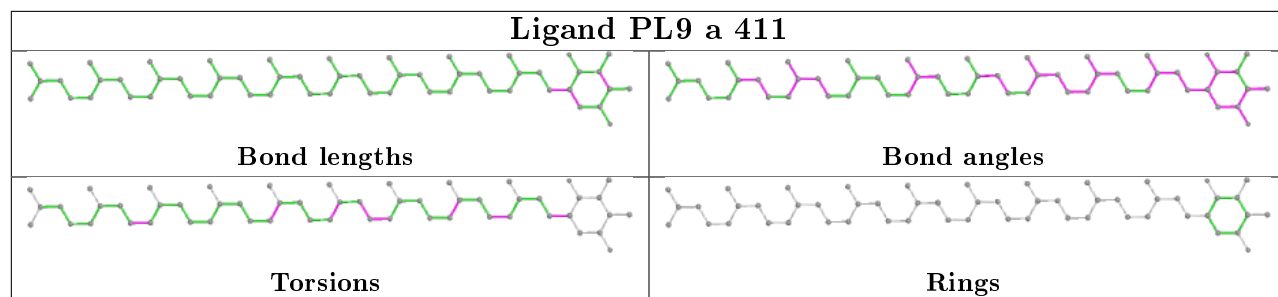


Ligand LHG d 410

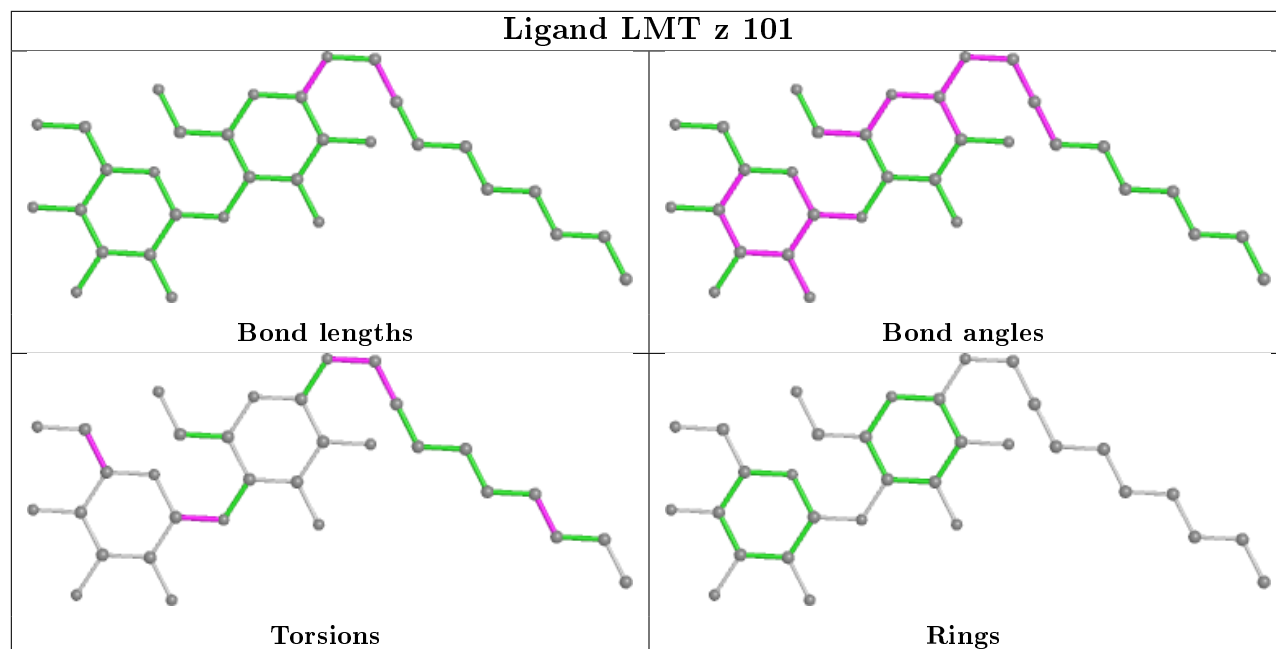




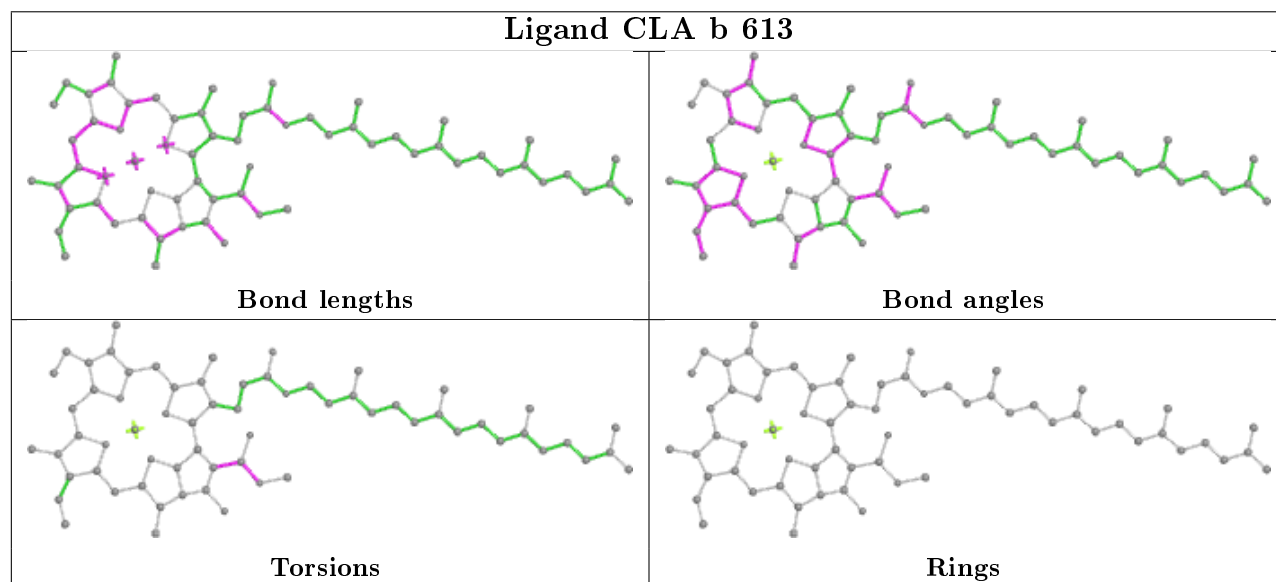
Ligand CLA C 502**Ligand BCR b 621****Ligand CLA a 406**



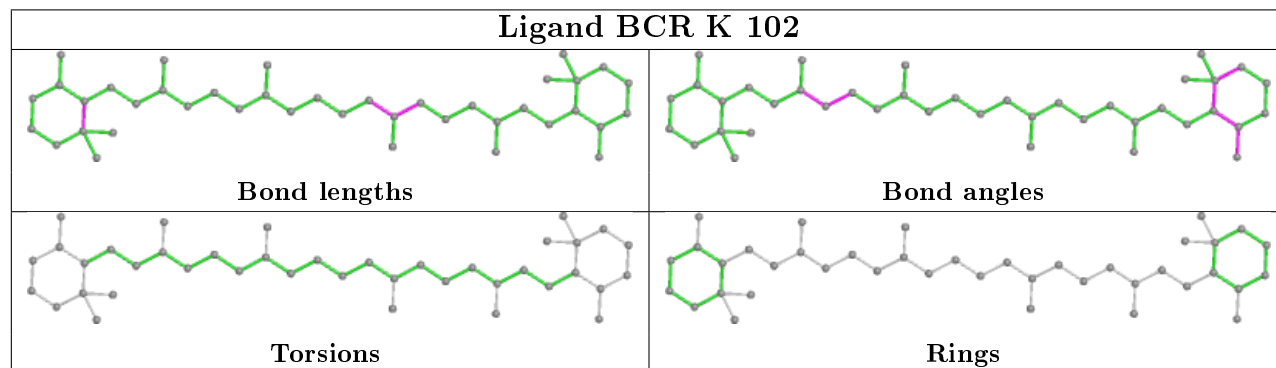
Ligand LMT z 101

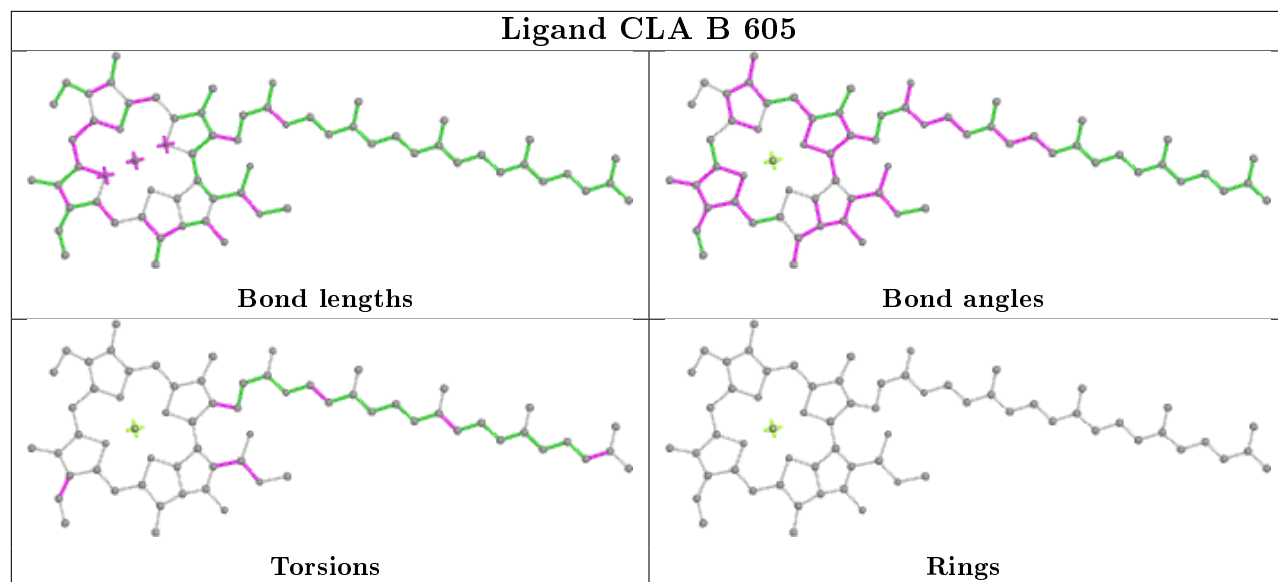
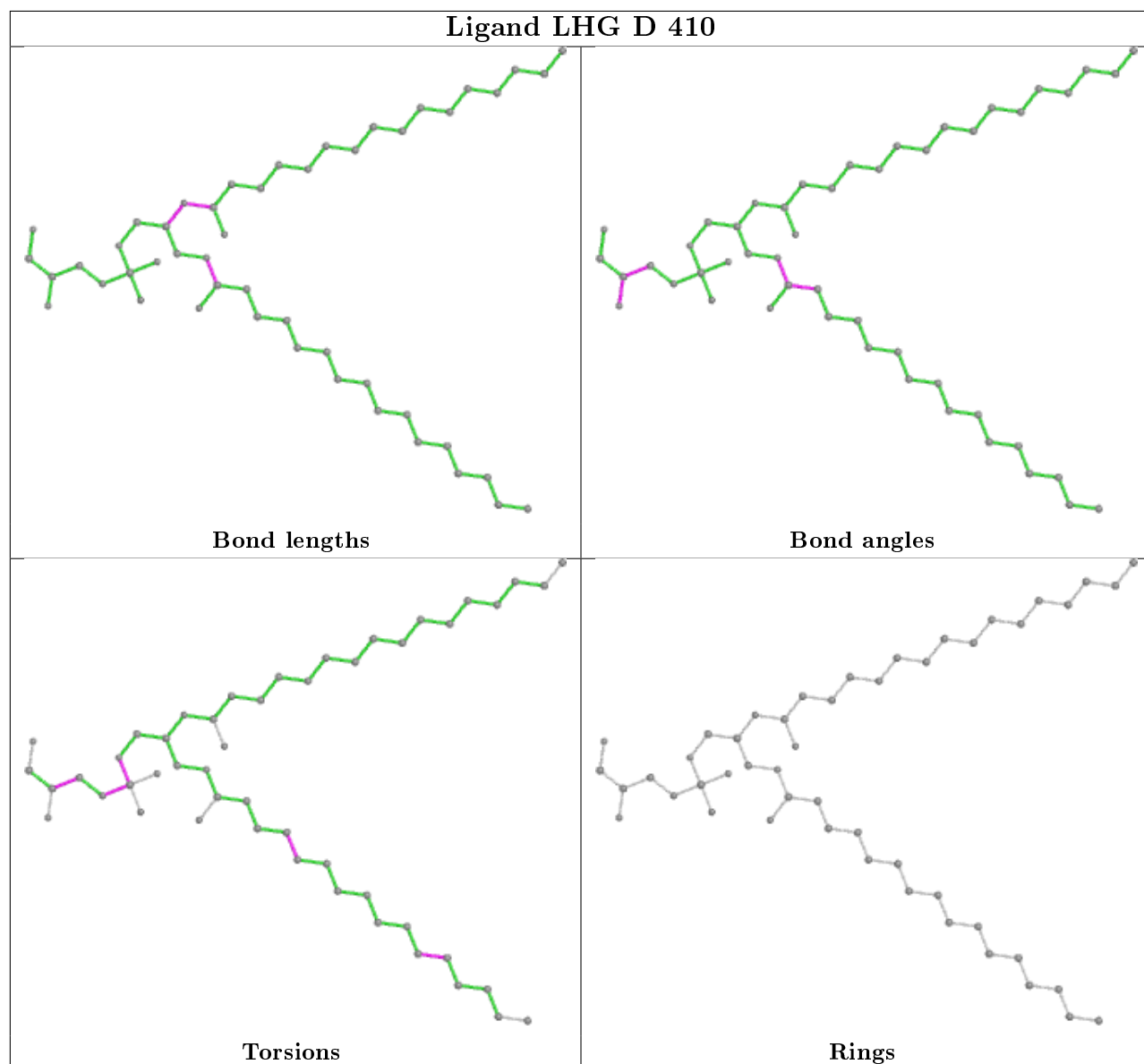


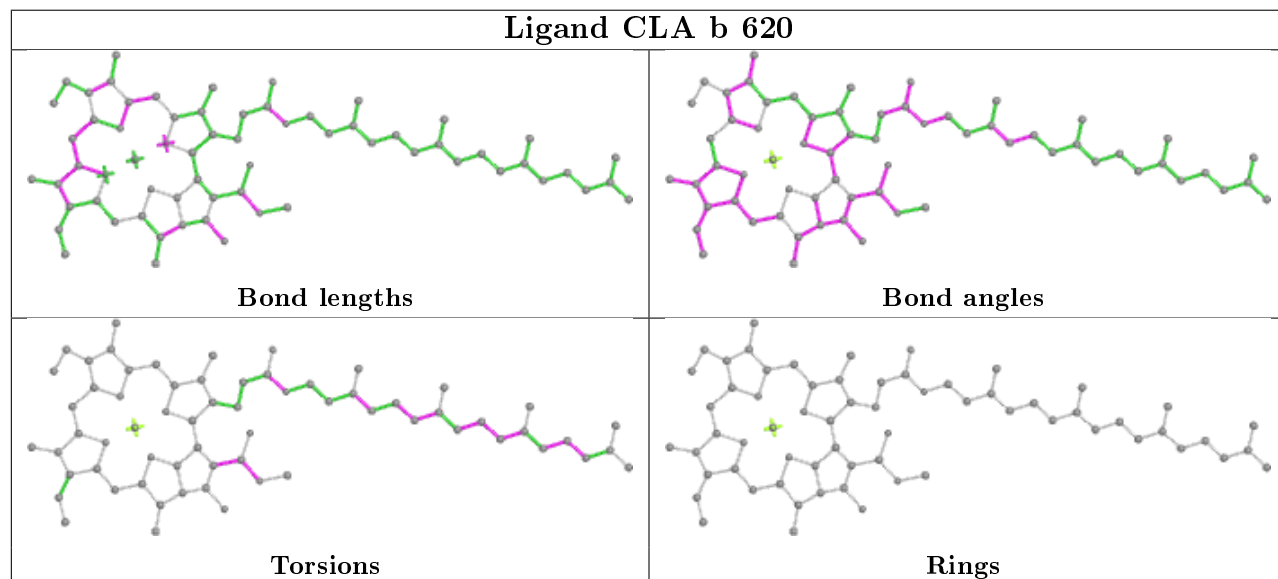
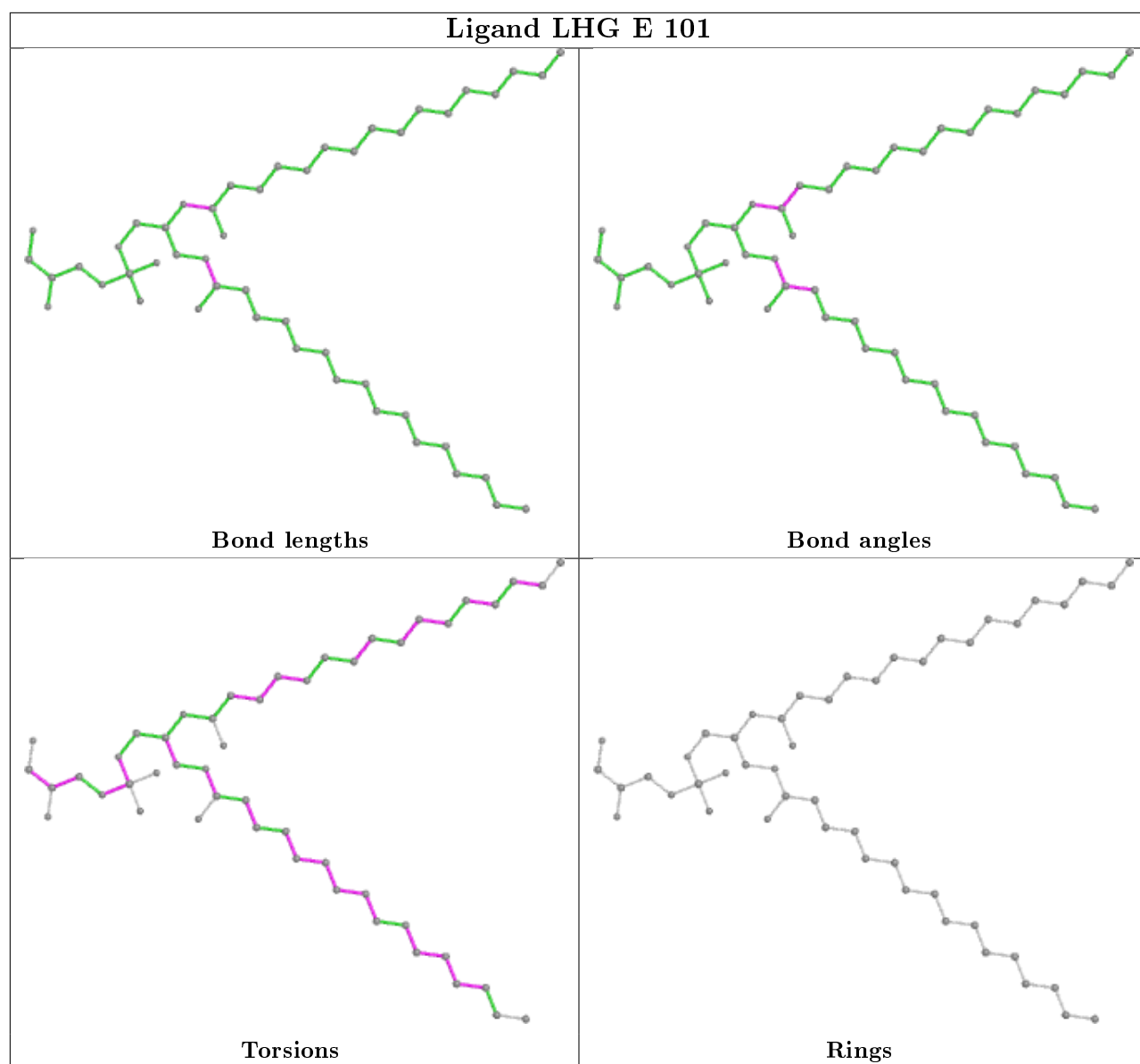
Ligand CLA b 613

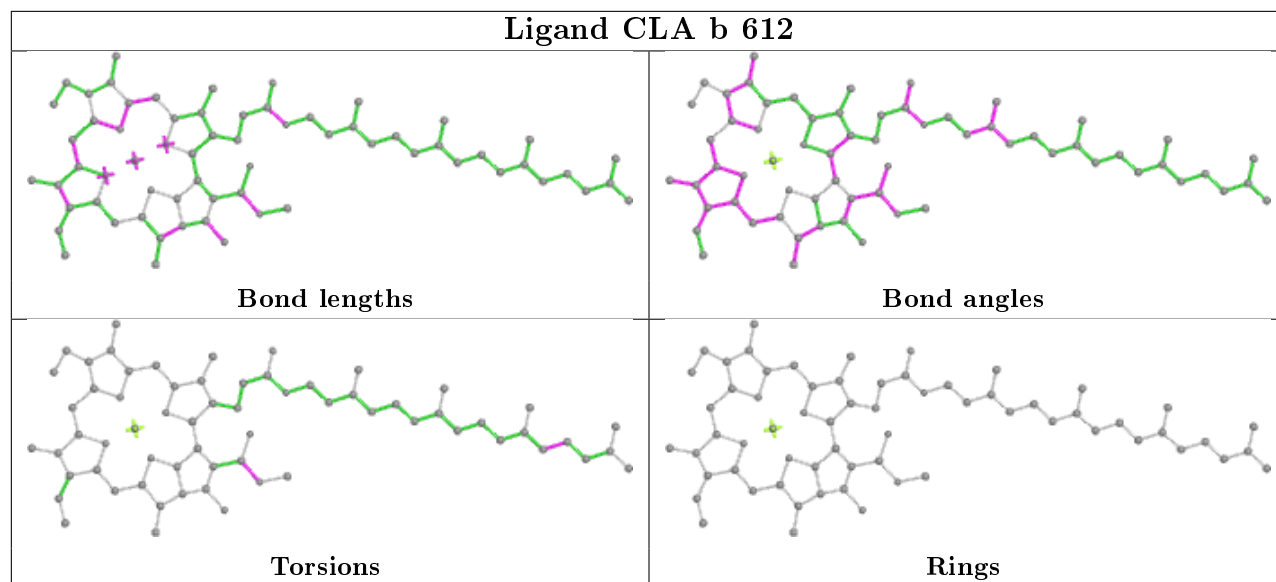
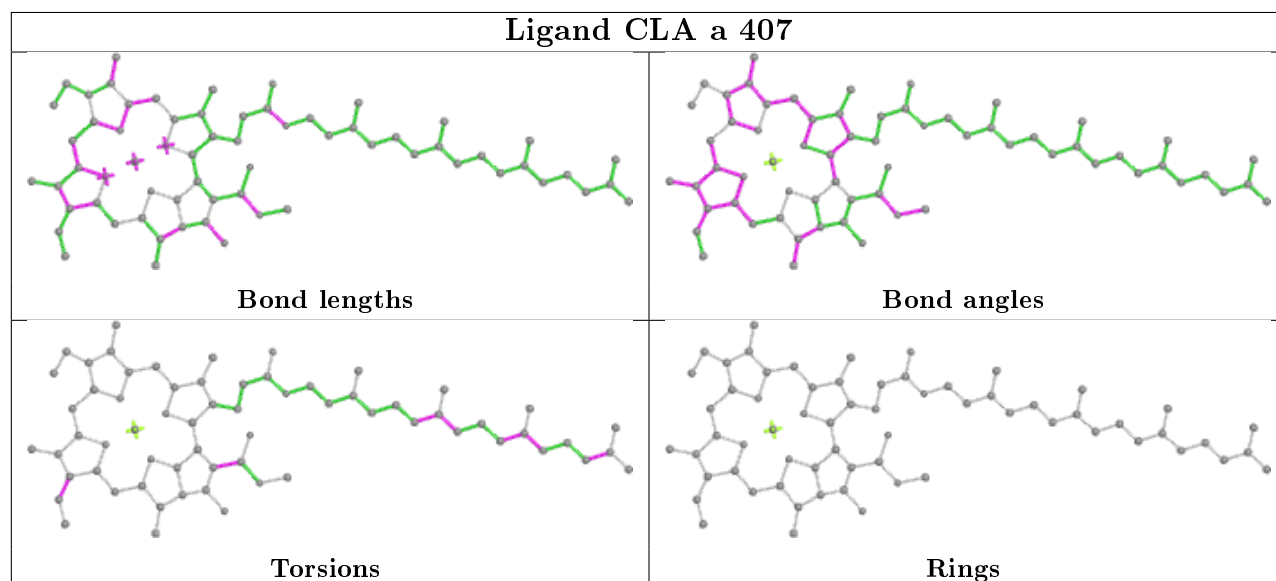
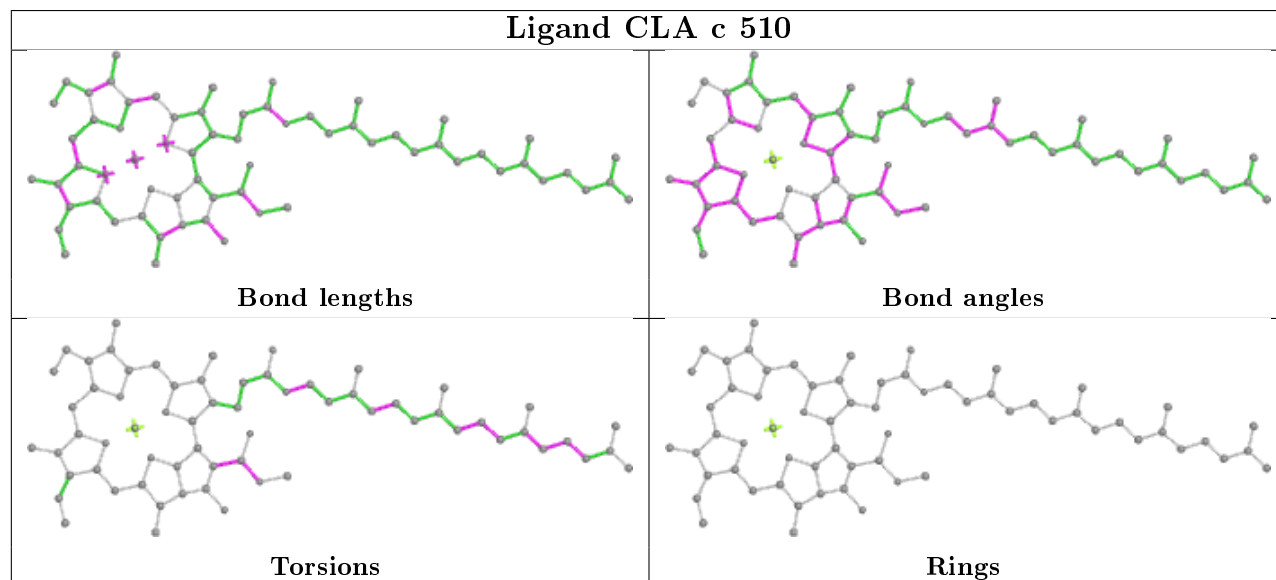


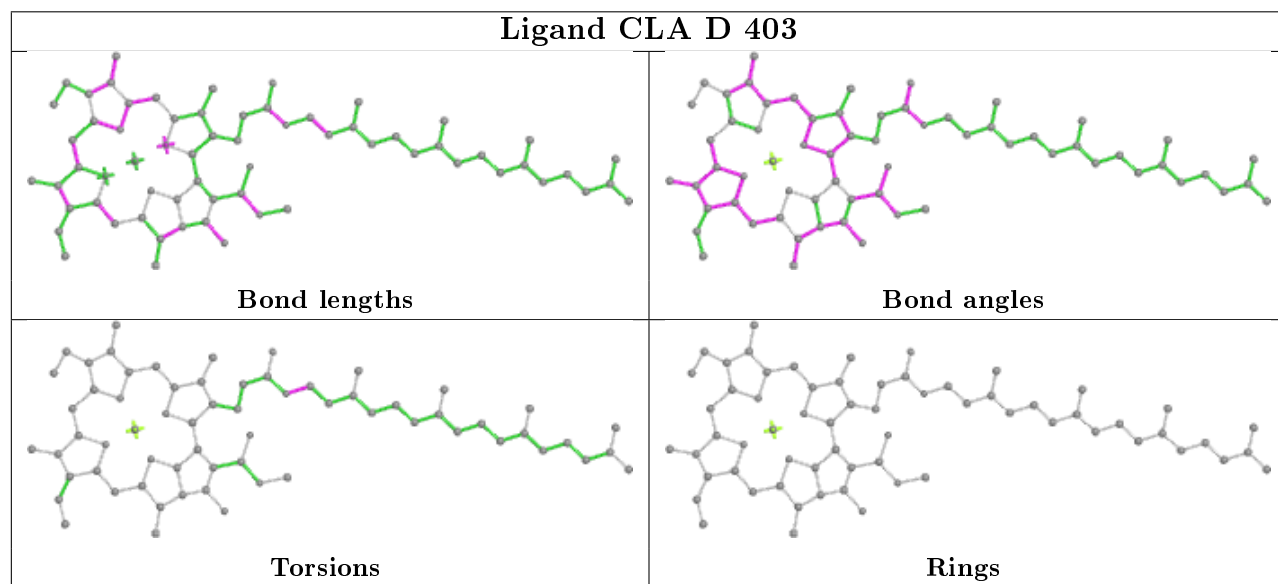
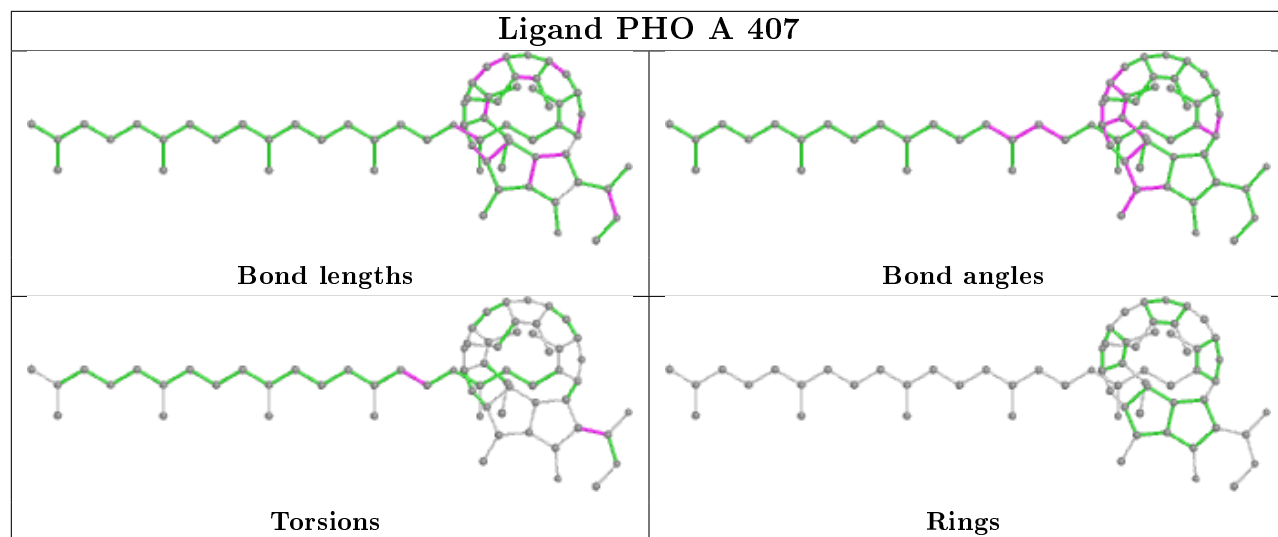
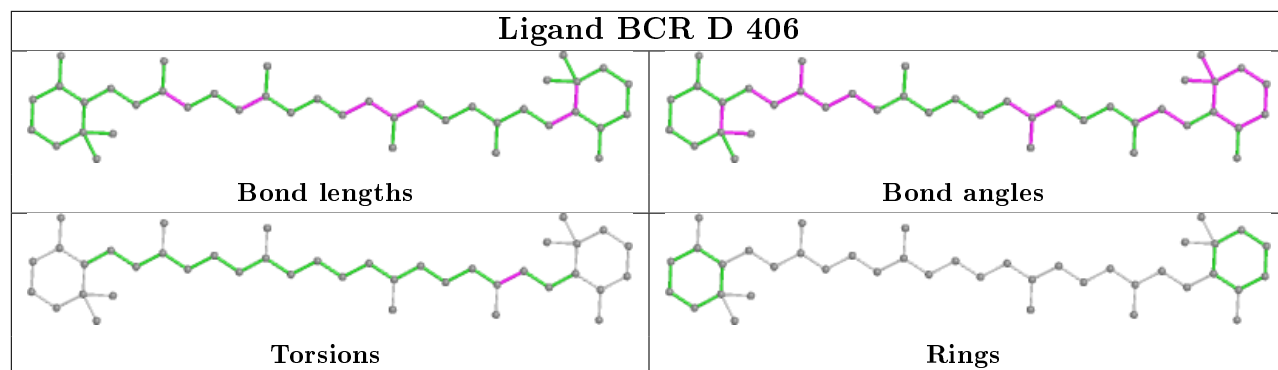
Ligand BCR K 102

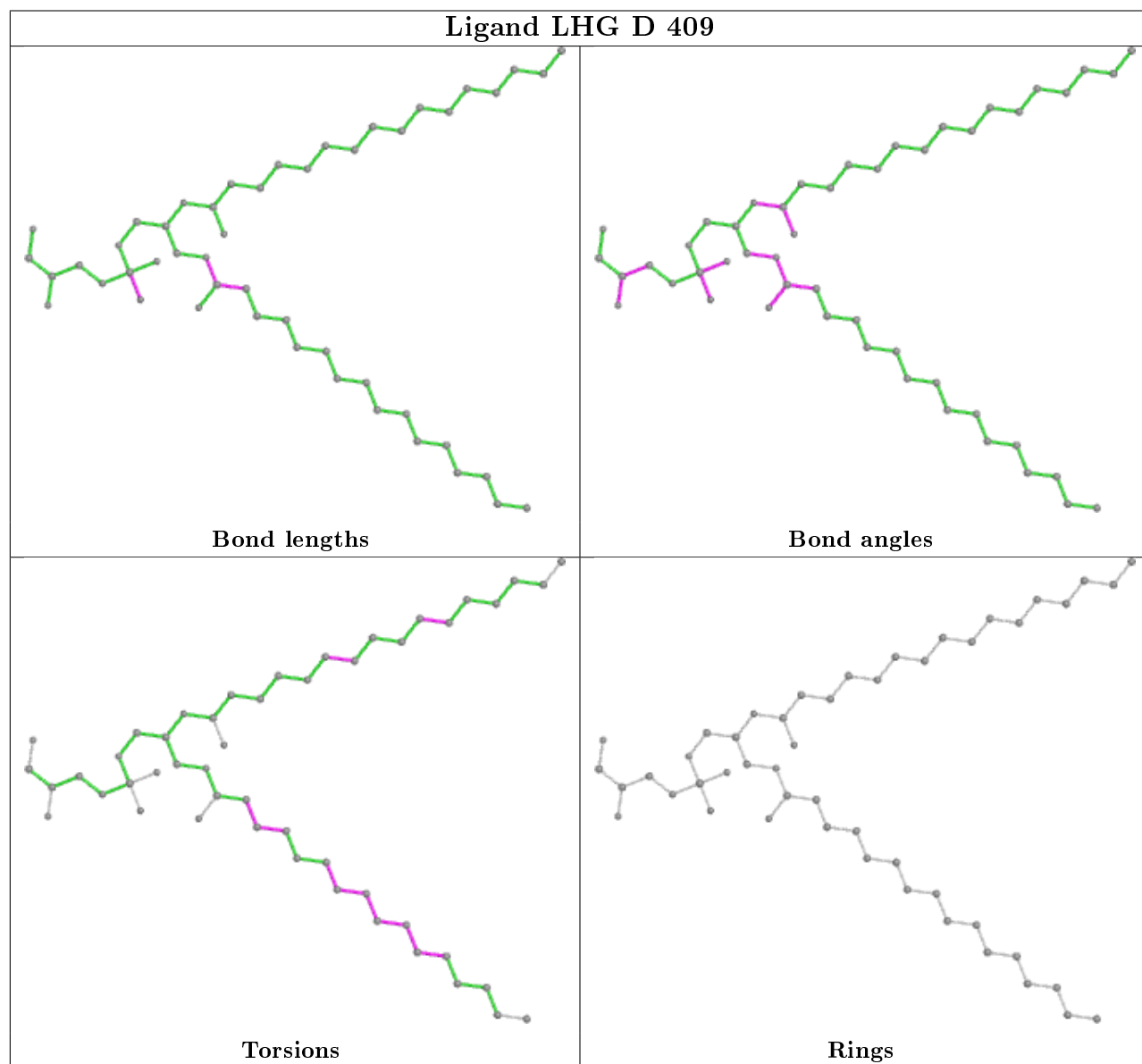
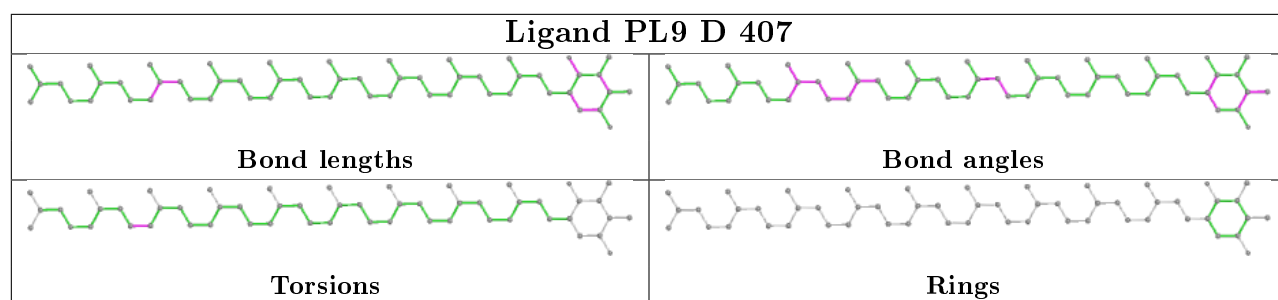


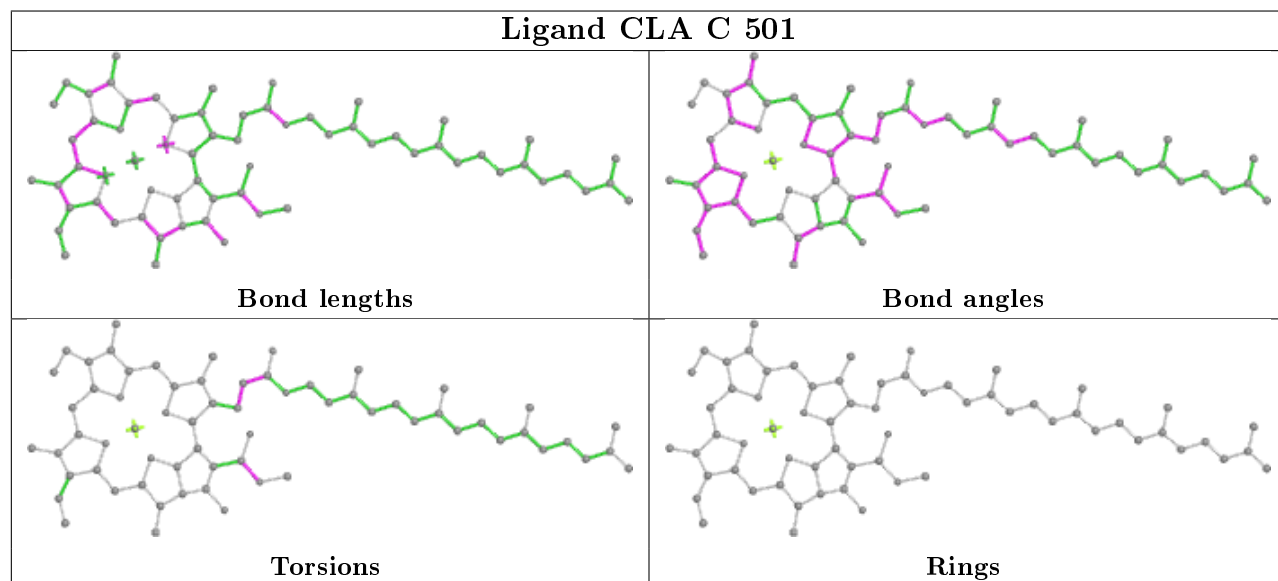
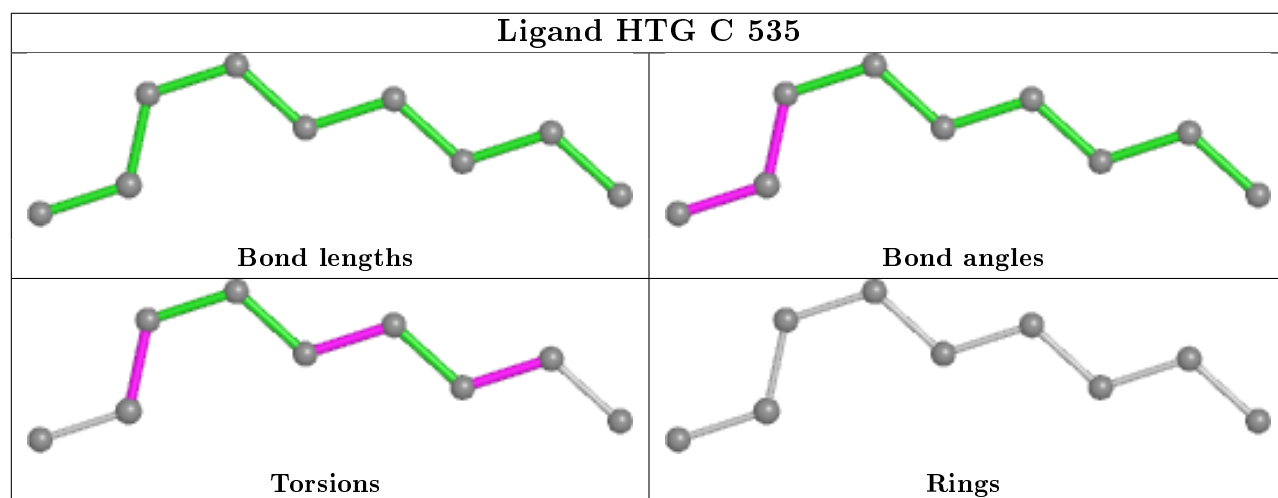
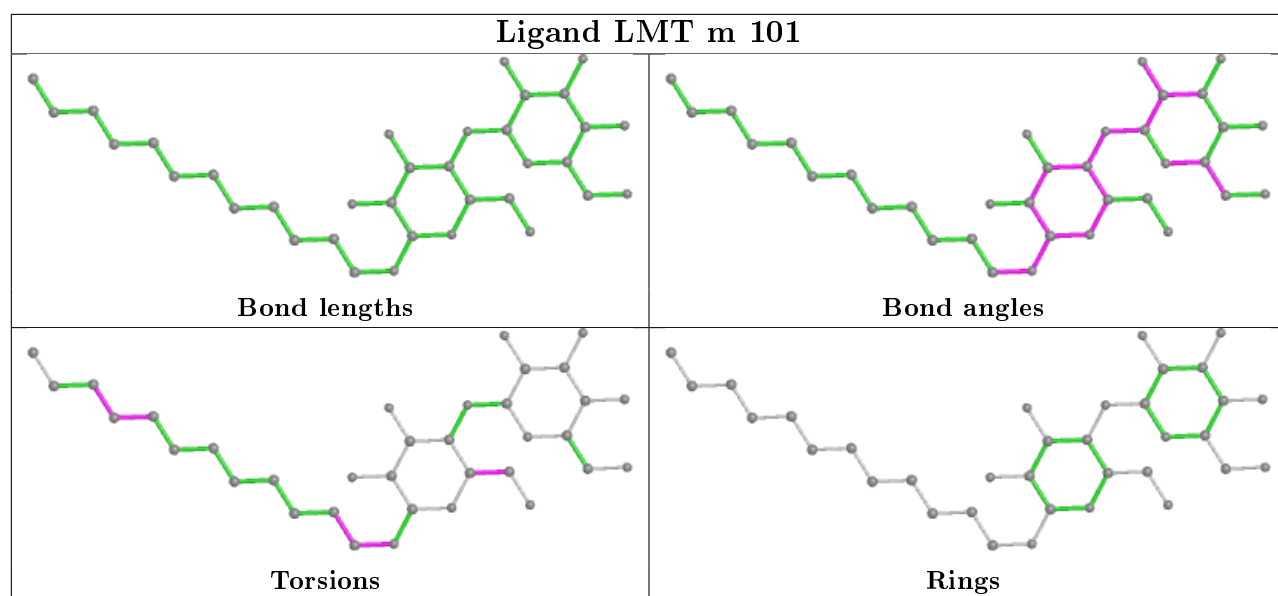
Ligand CLA B 605**Ligand LHG D 410**



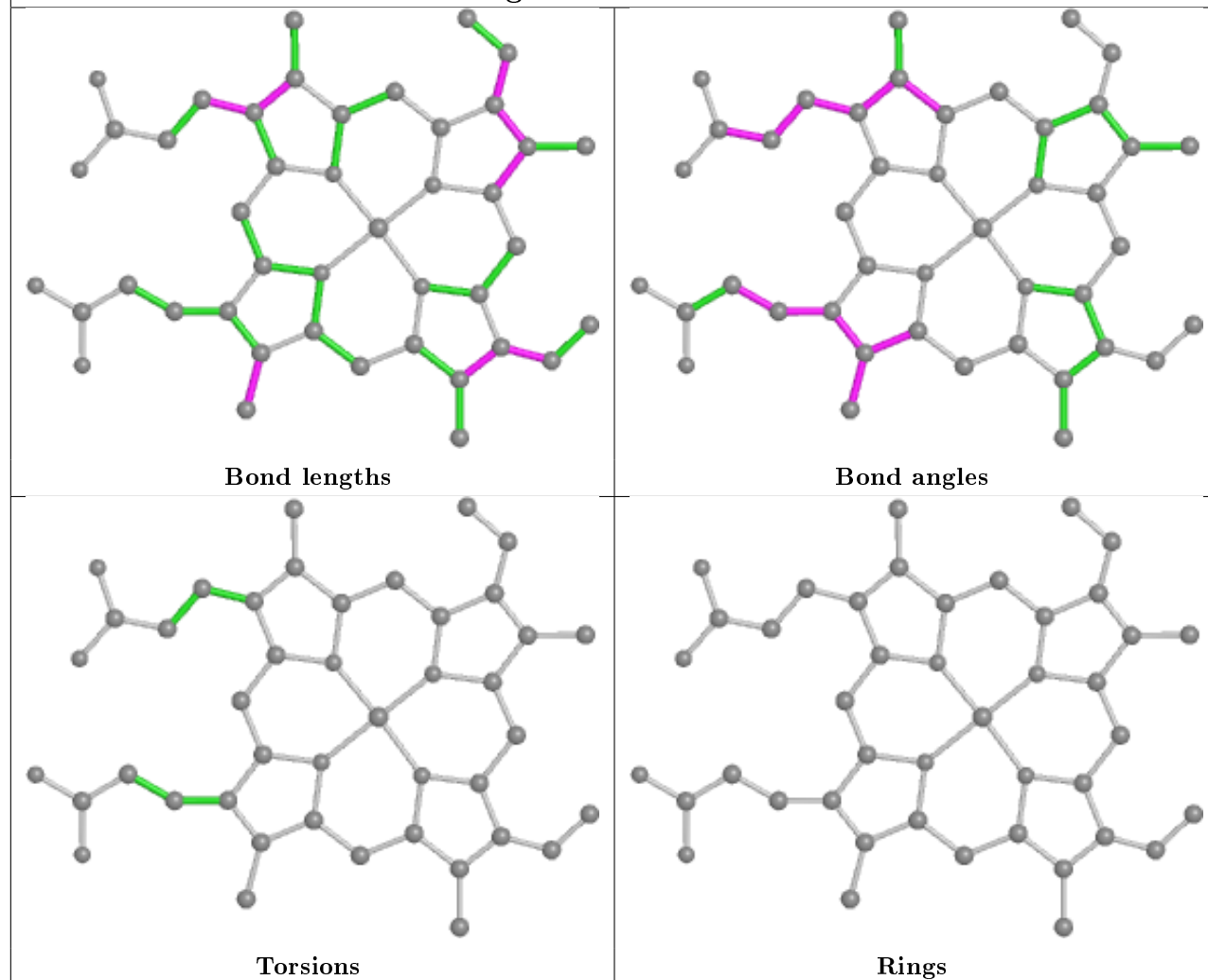
Ligand CLA b 612**Ligand CLA a 407****Ligand CLA c 510**



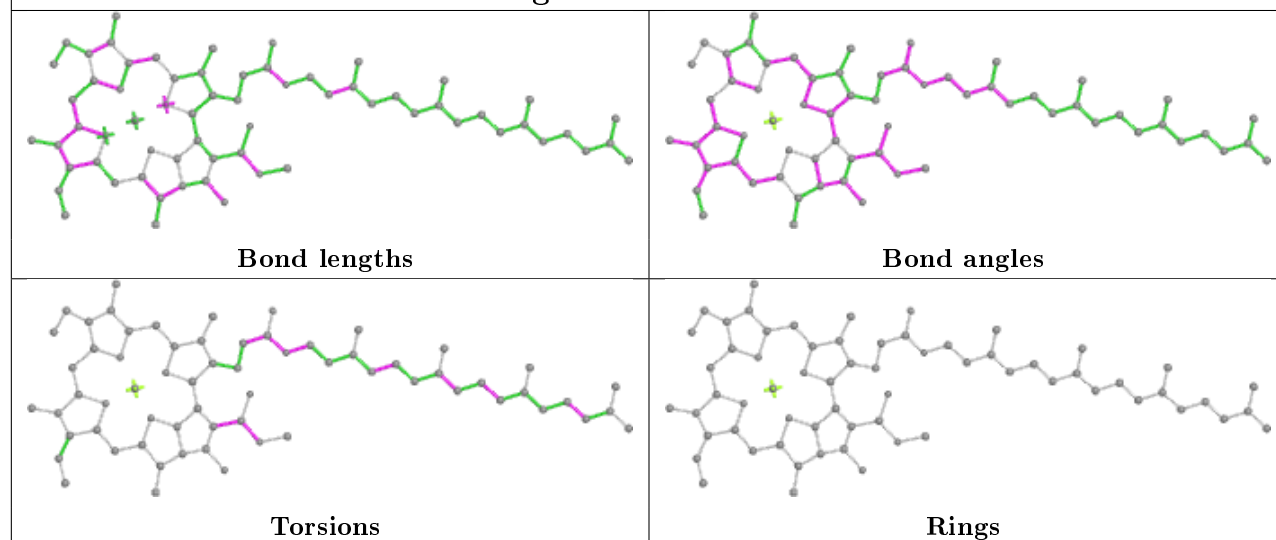


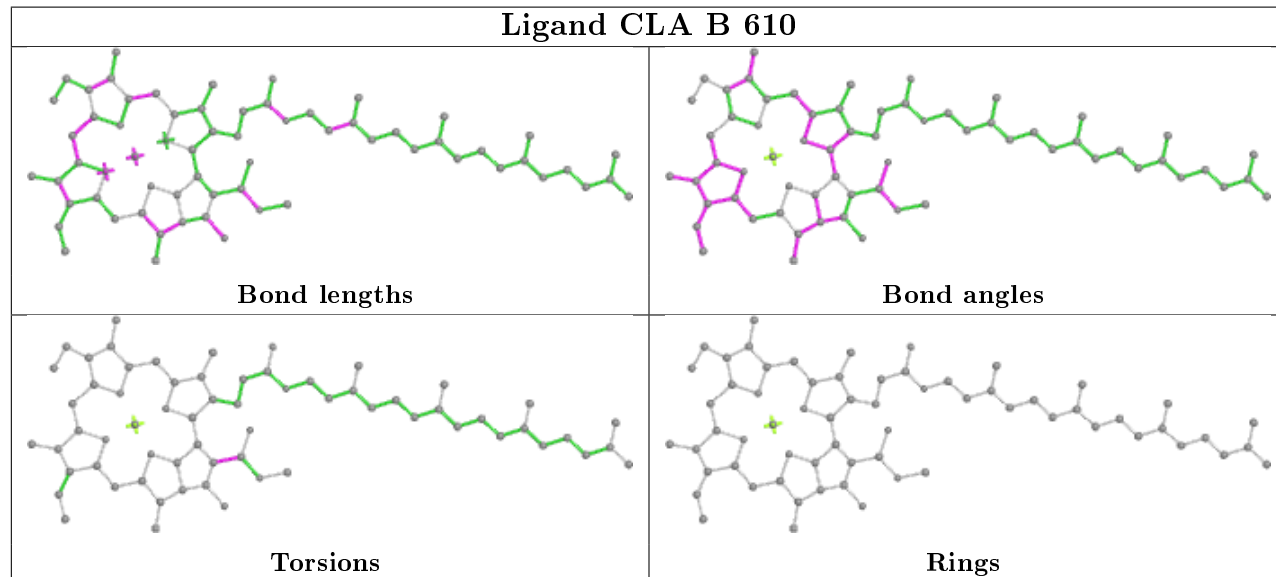
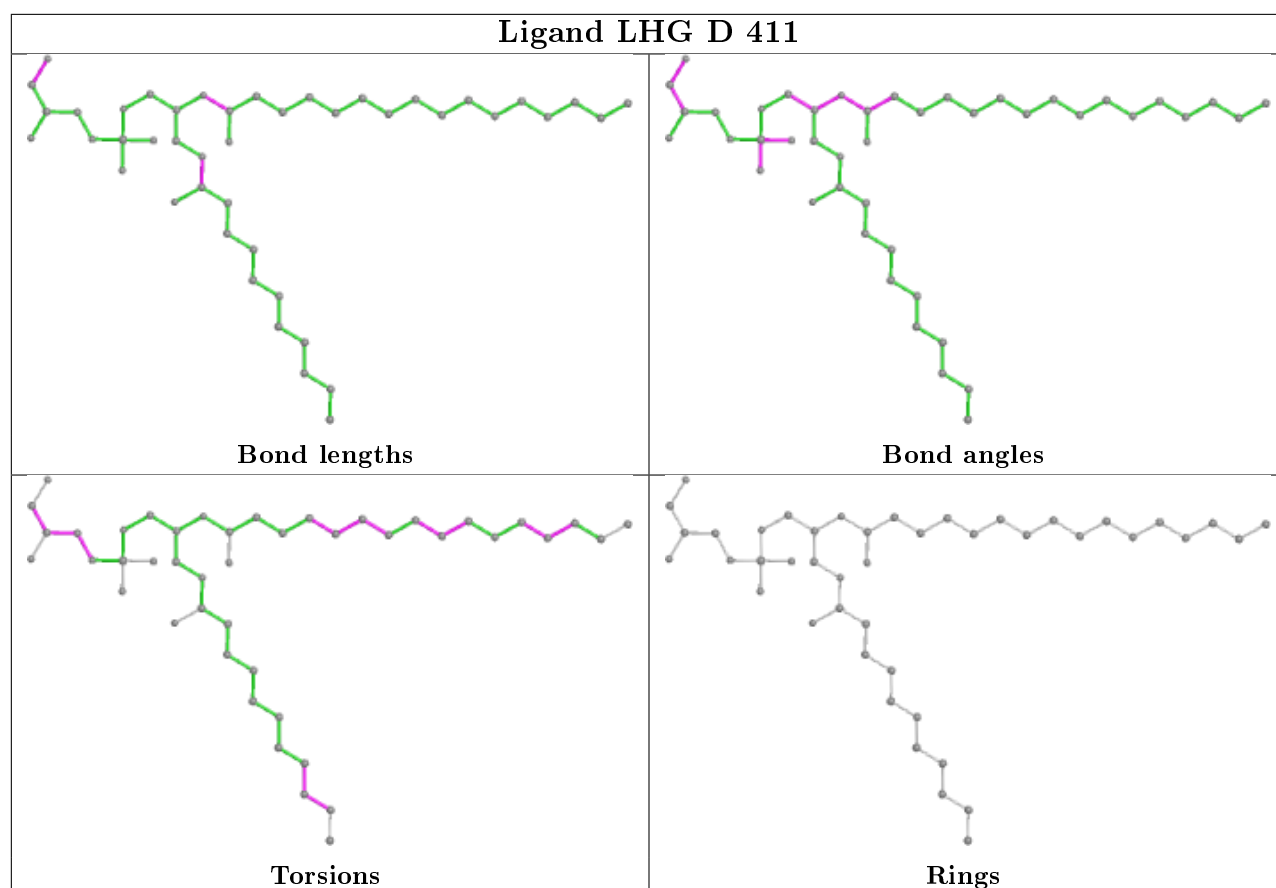


Ligand HEM f 101

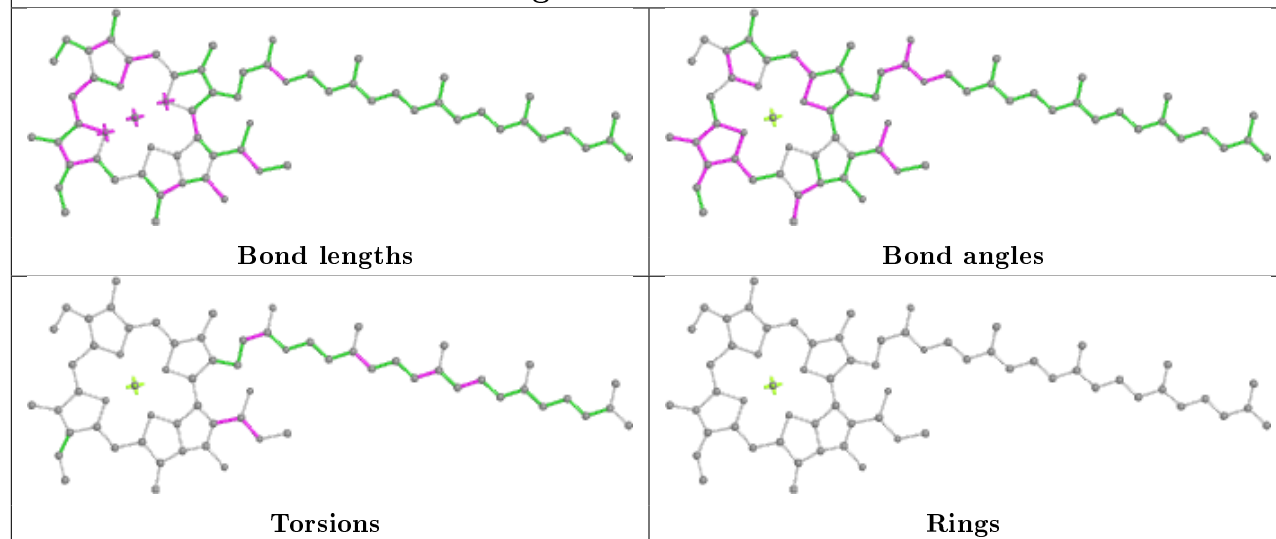


Ligand CLA B 602

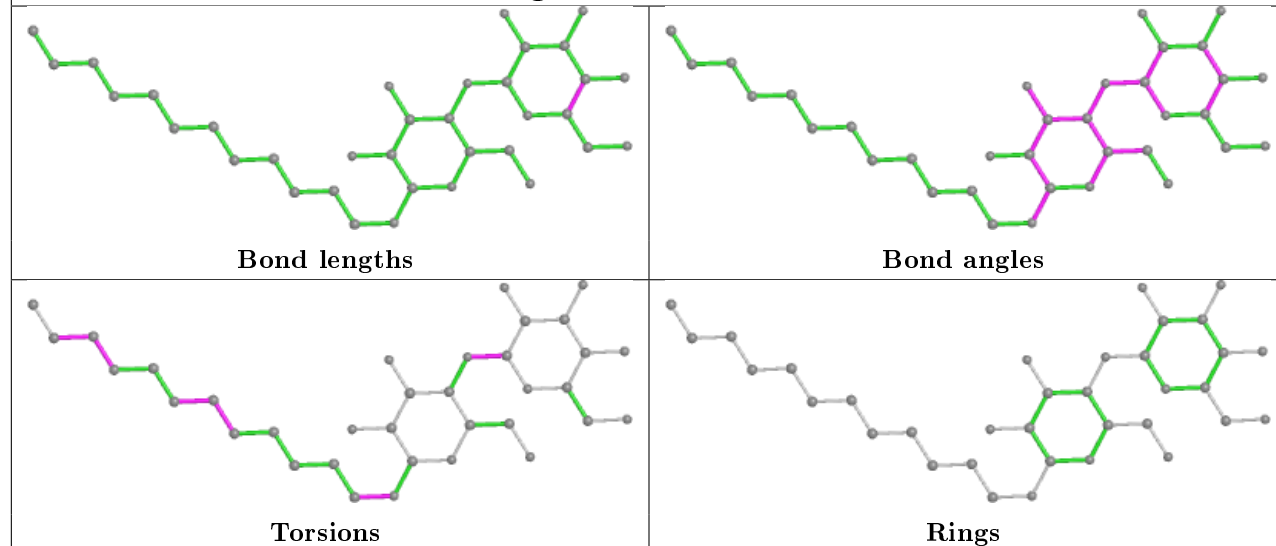




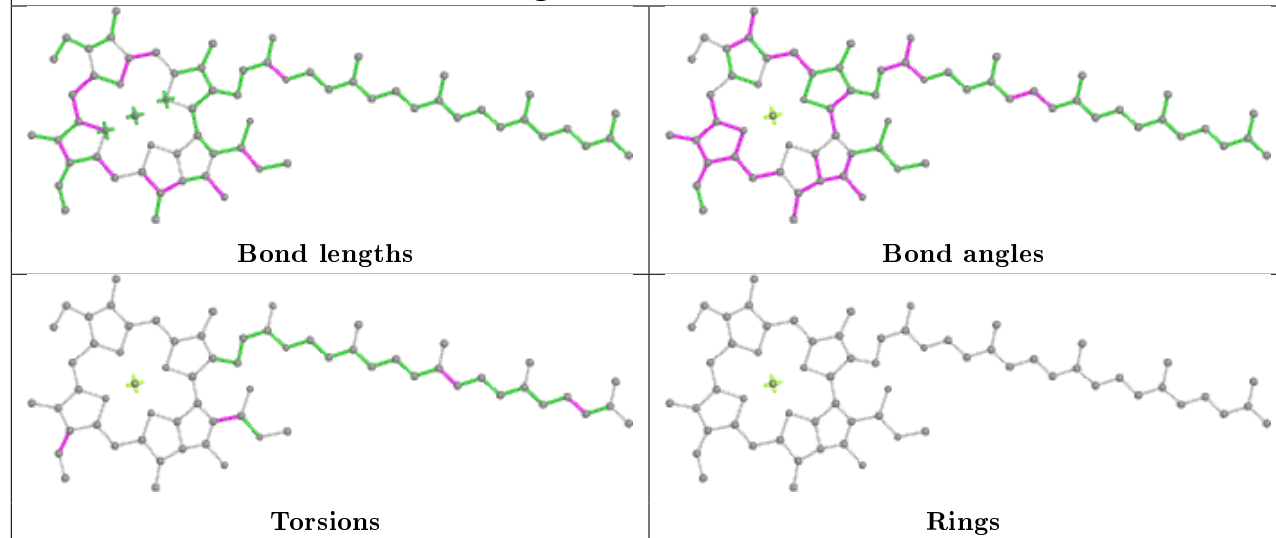
Ligand CLA C 510



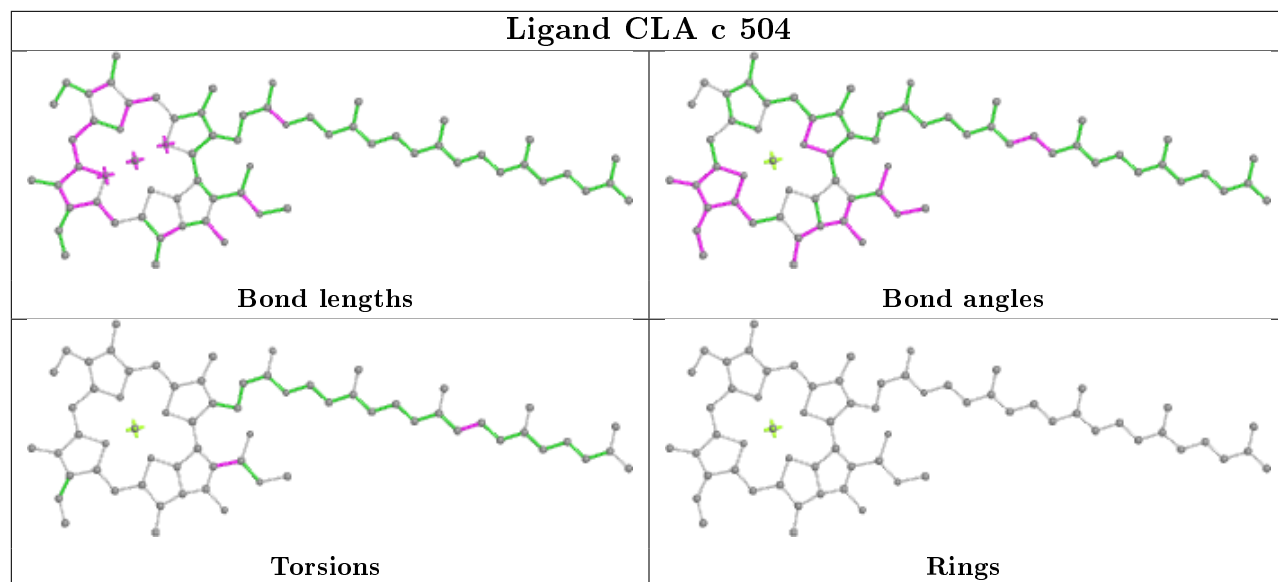
Ligand LMT B 623



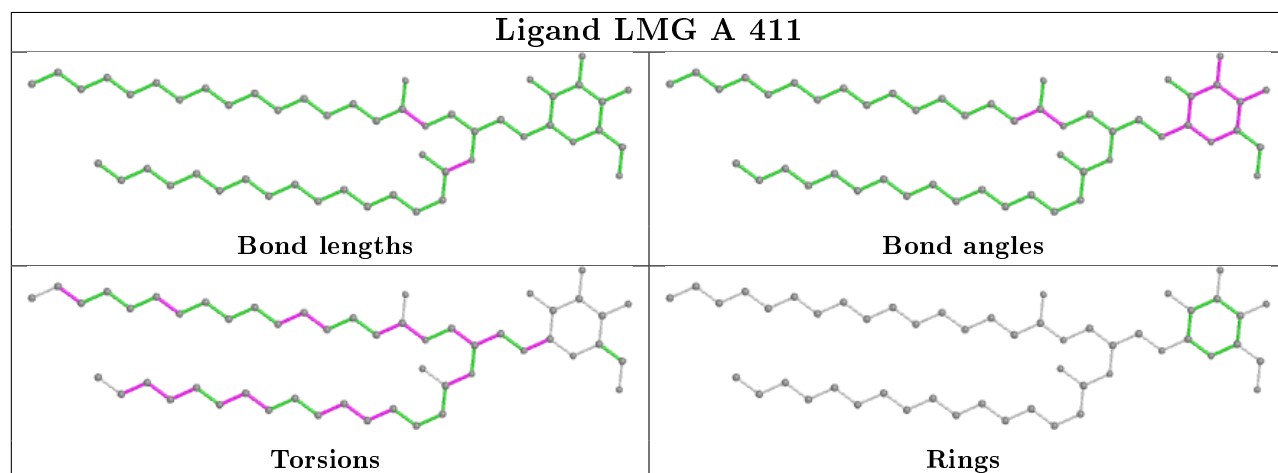
Ligand CLA A 404



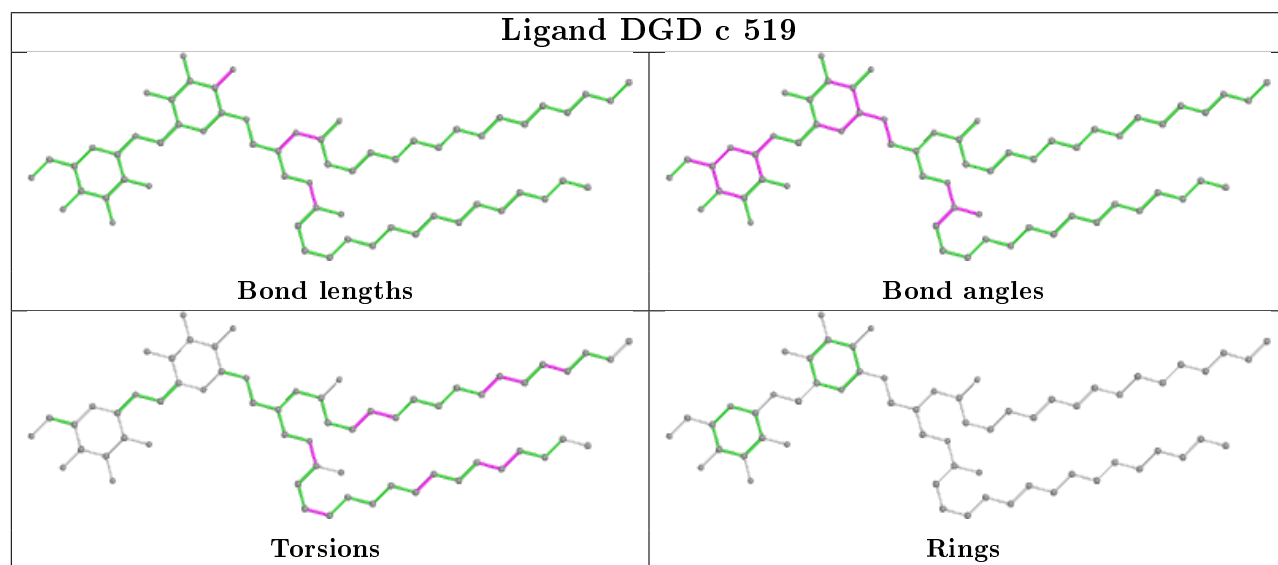
Ligand CLA c 504

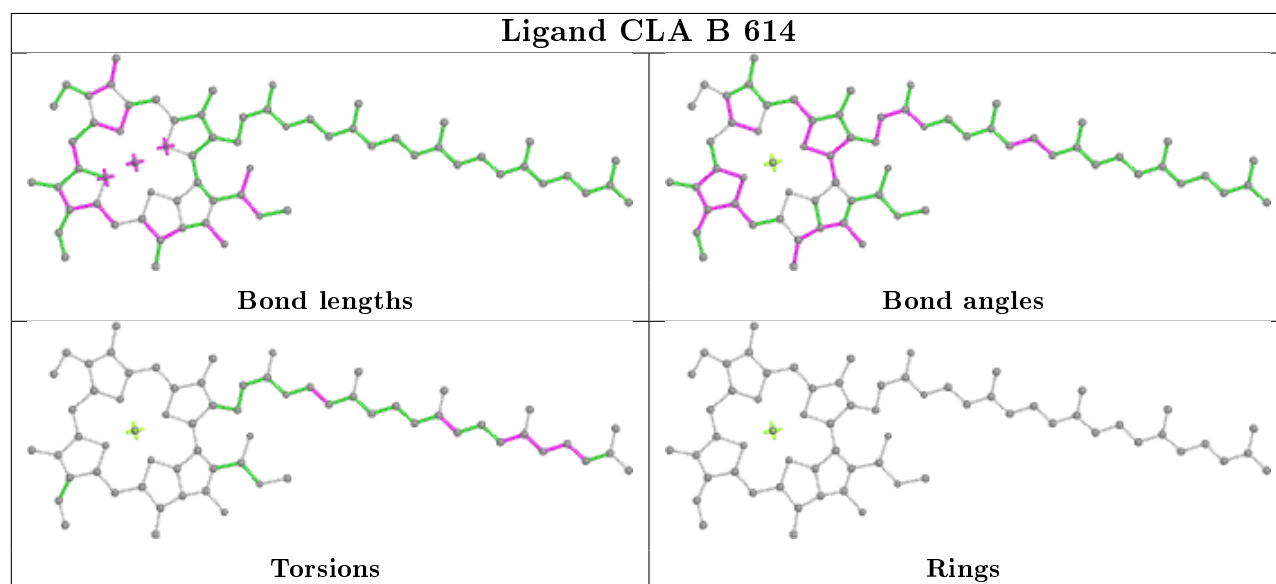
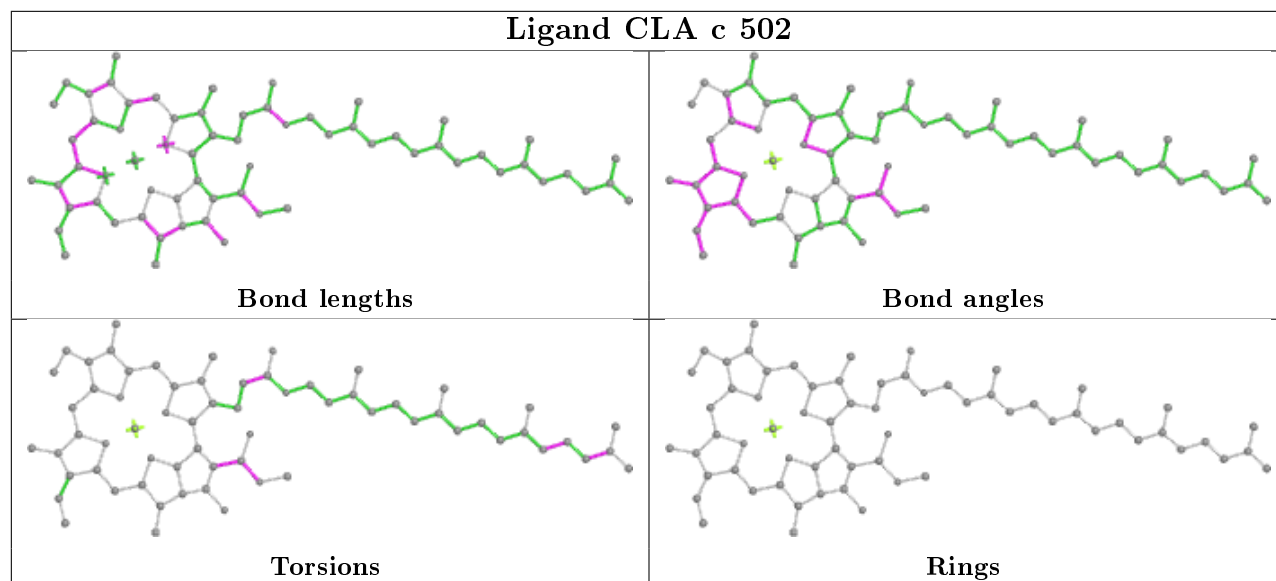
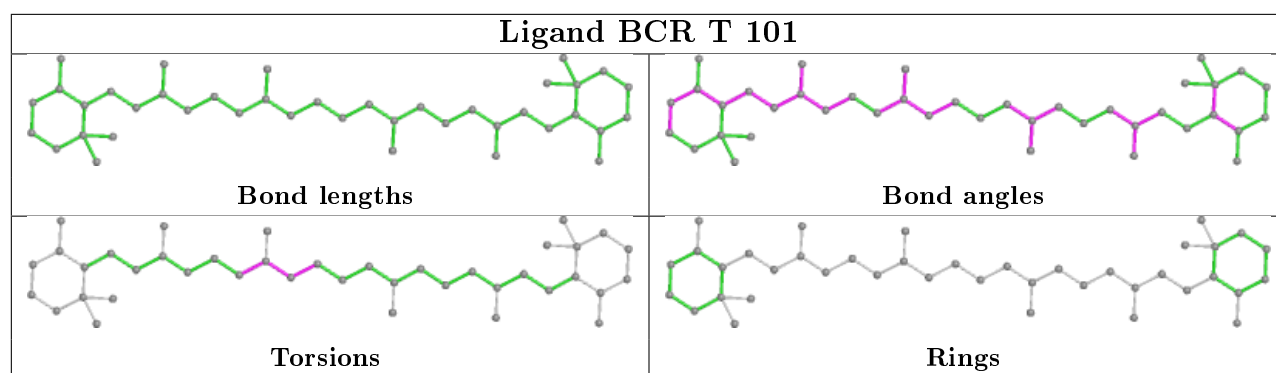


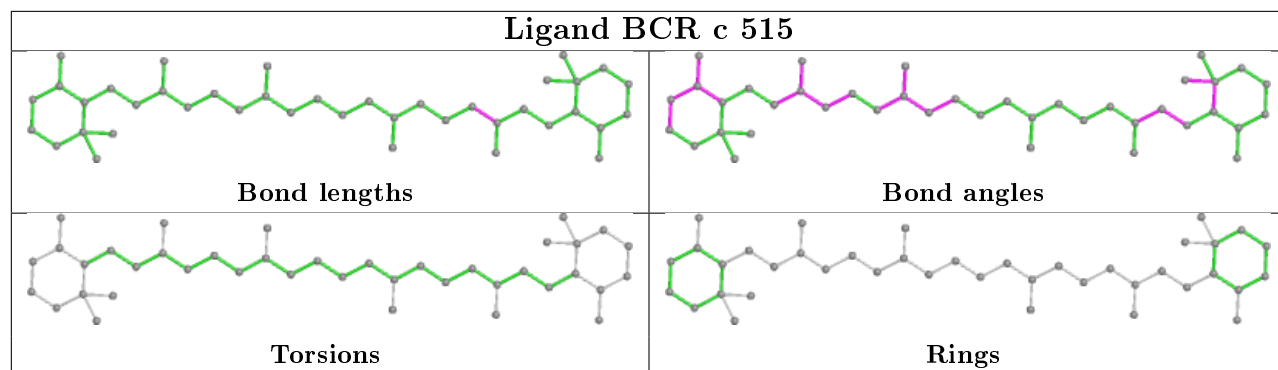
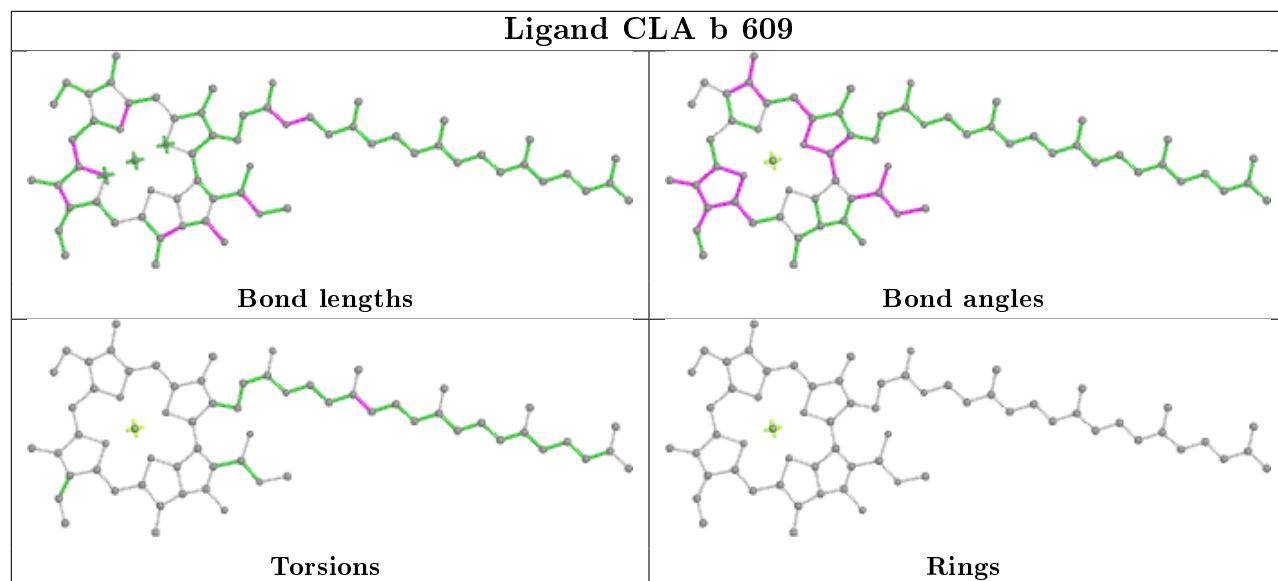
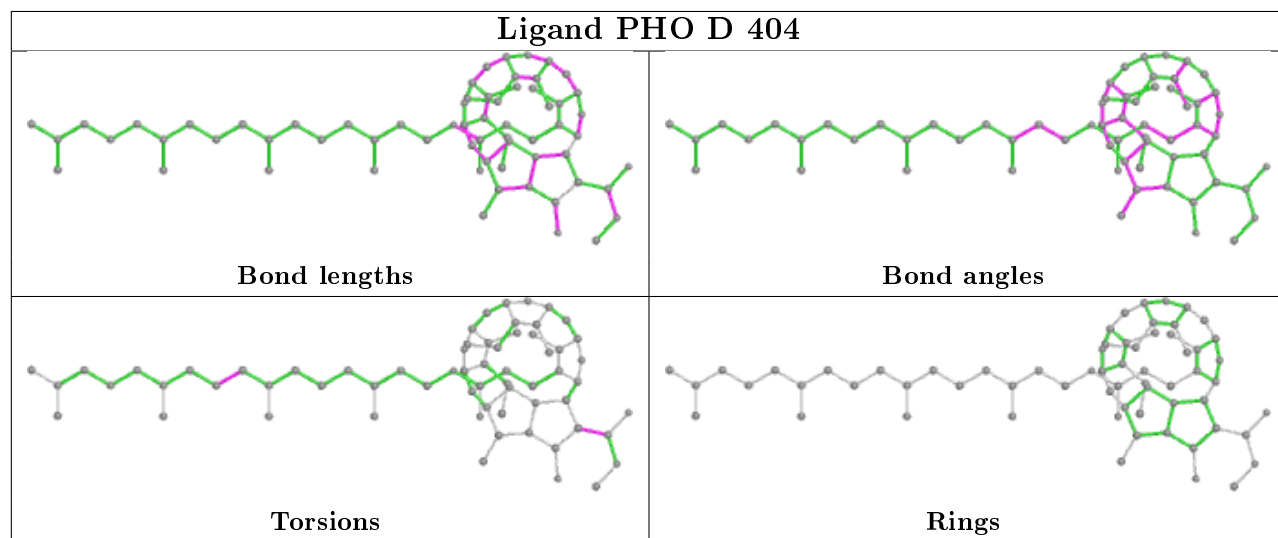
Ligand LMG A 411

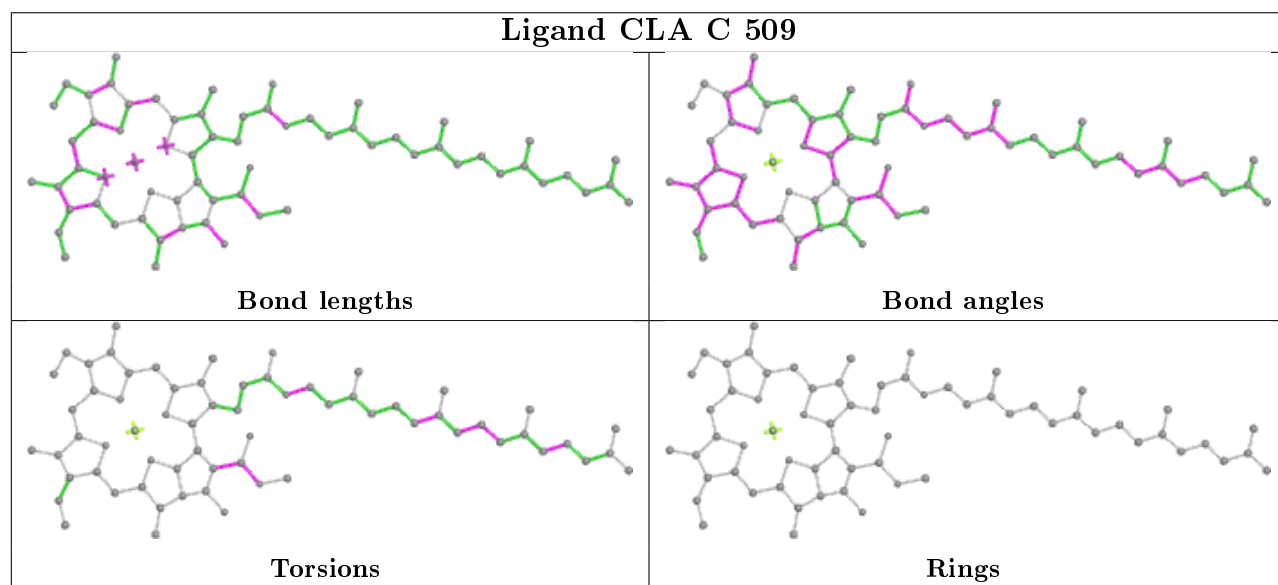
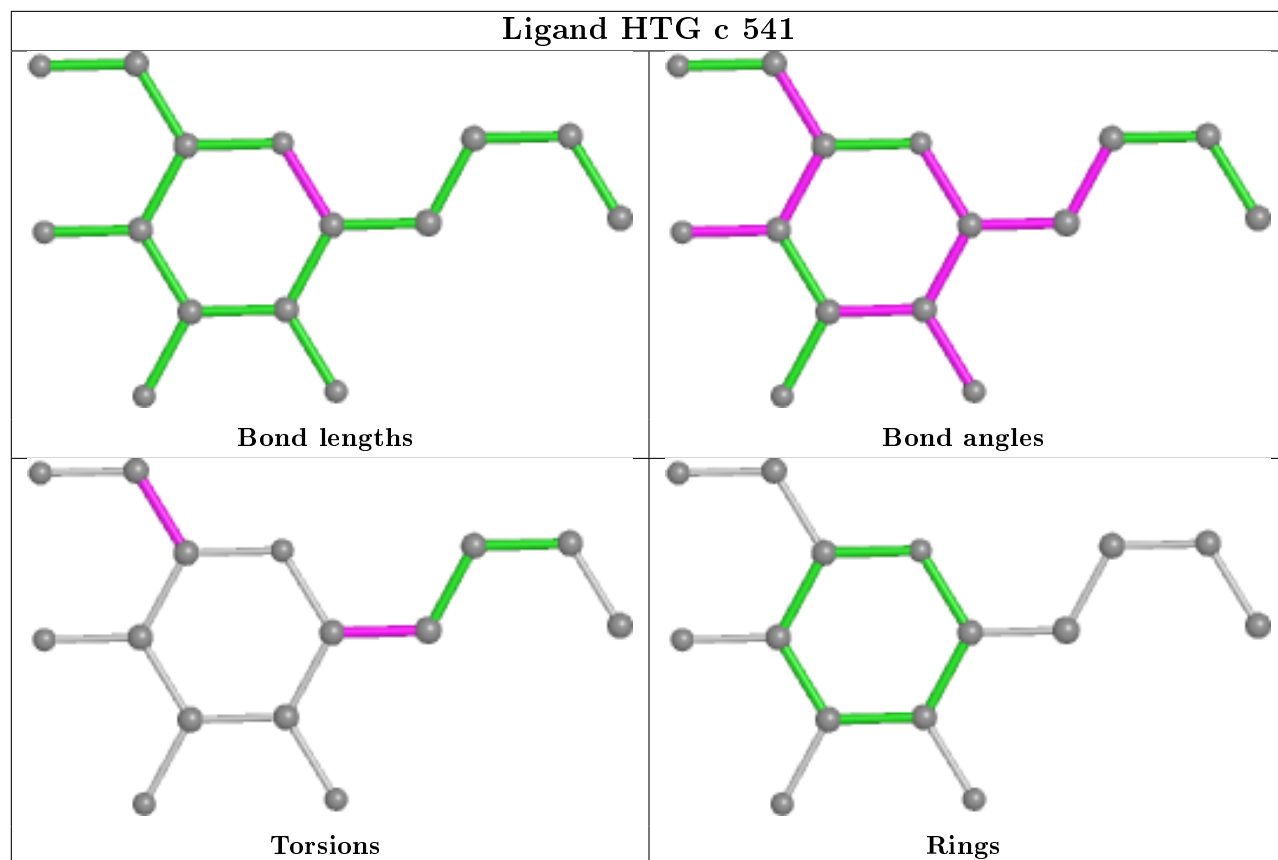


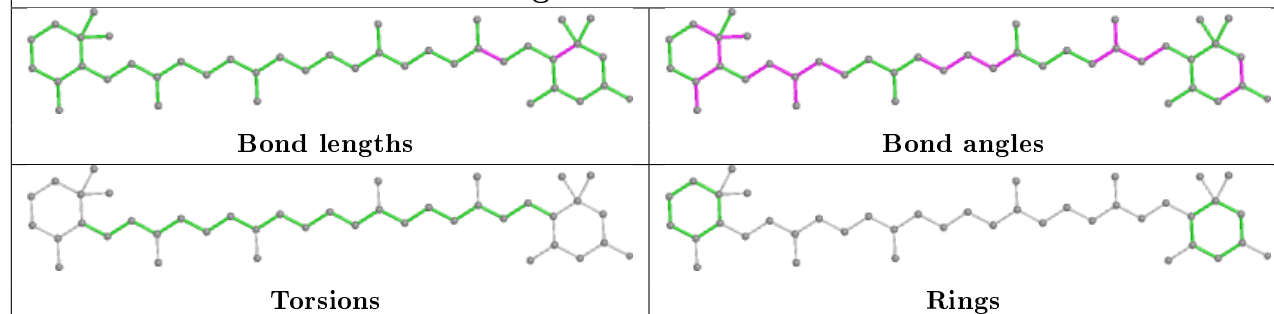
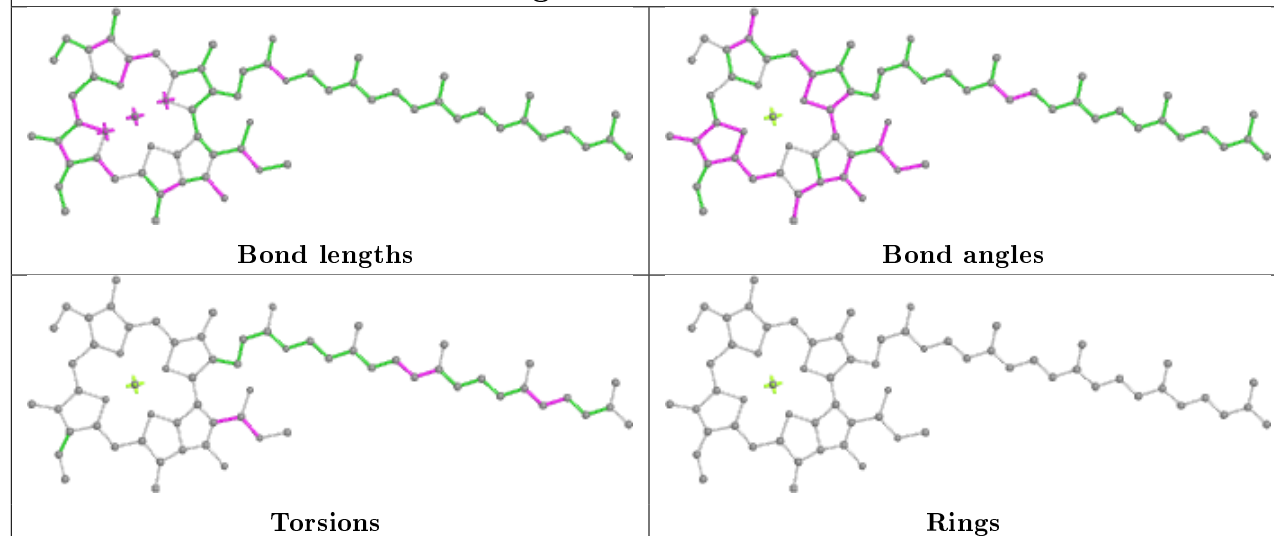
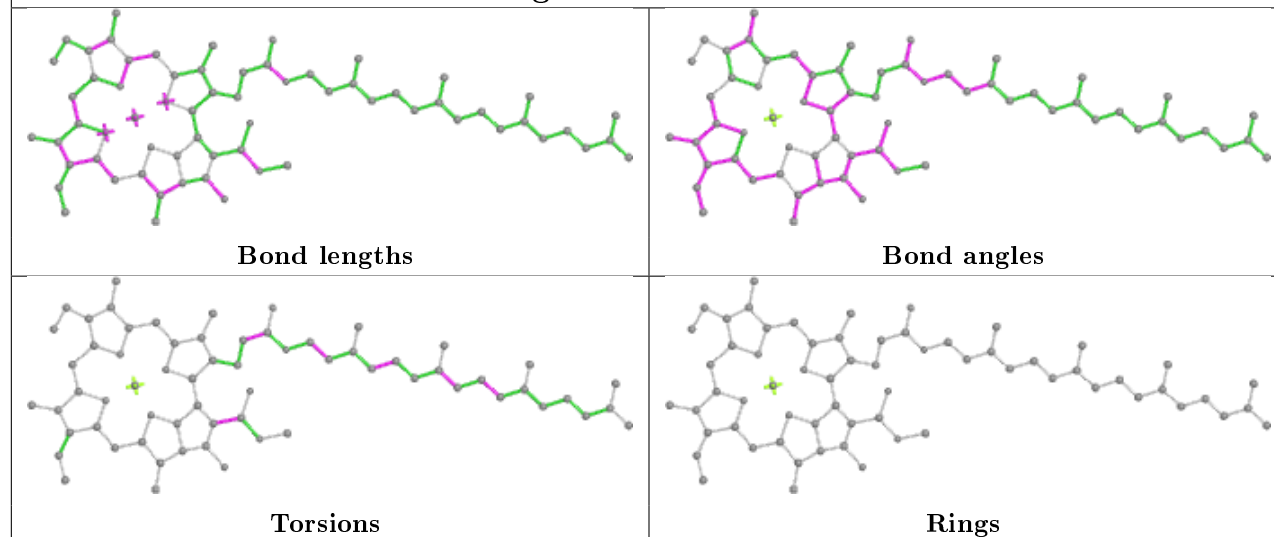
Ligand DGD c 519

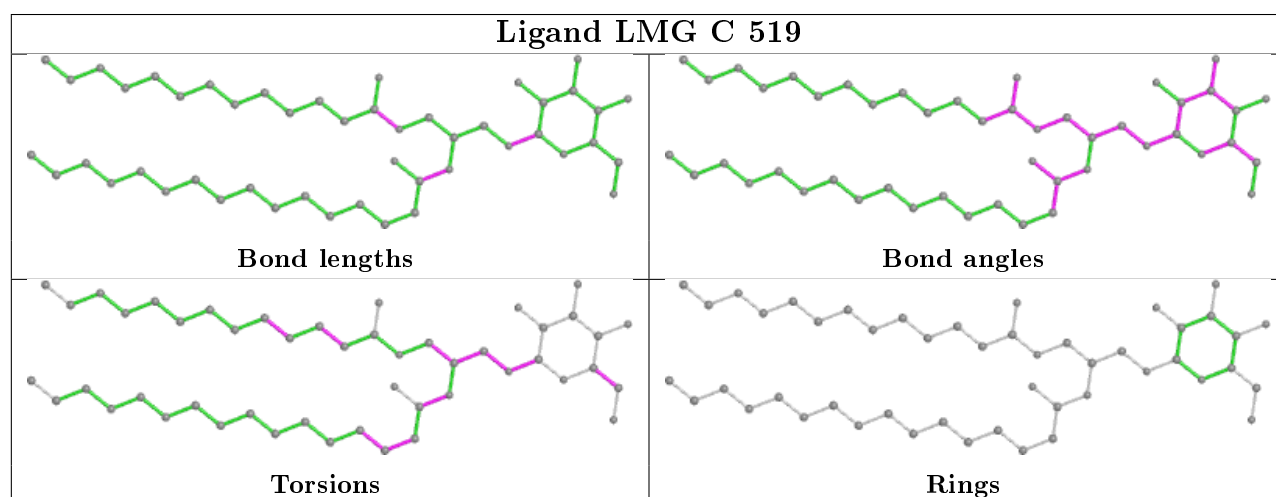
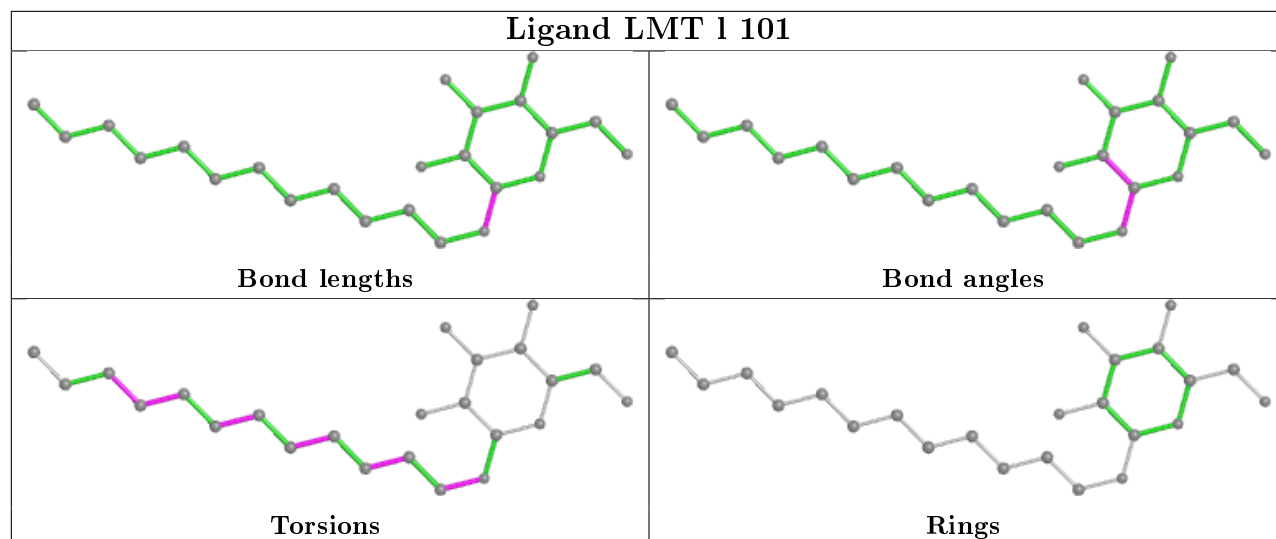


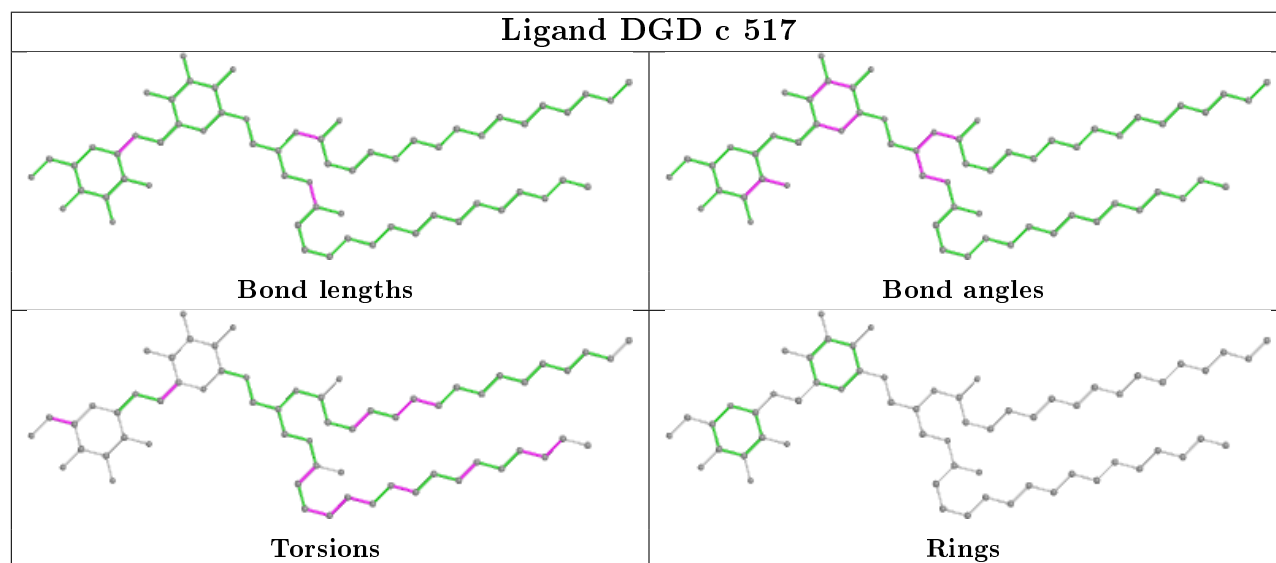
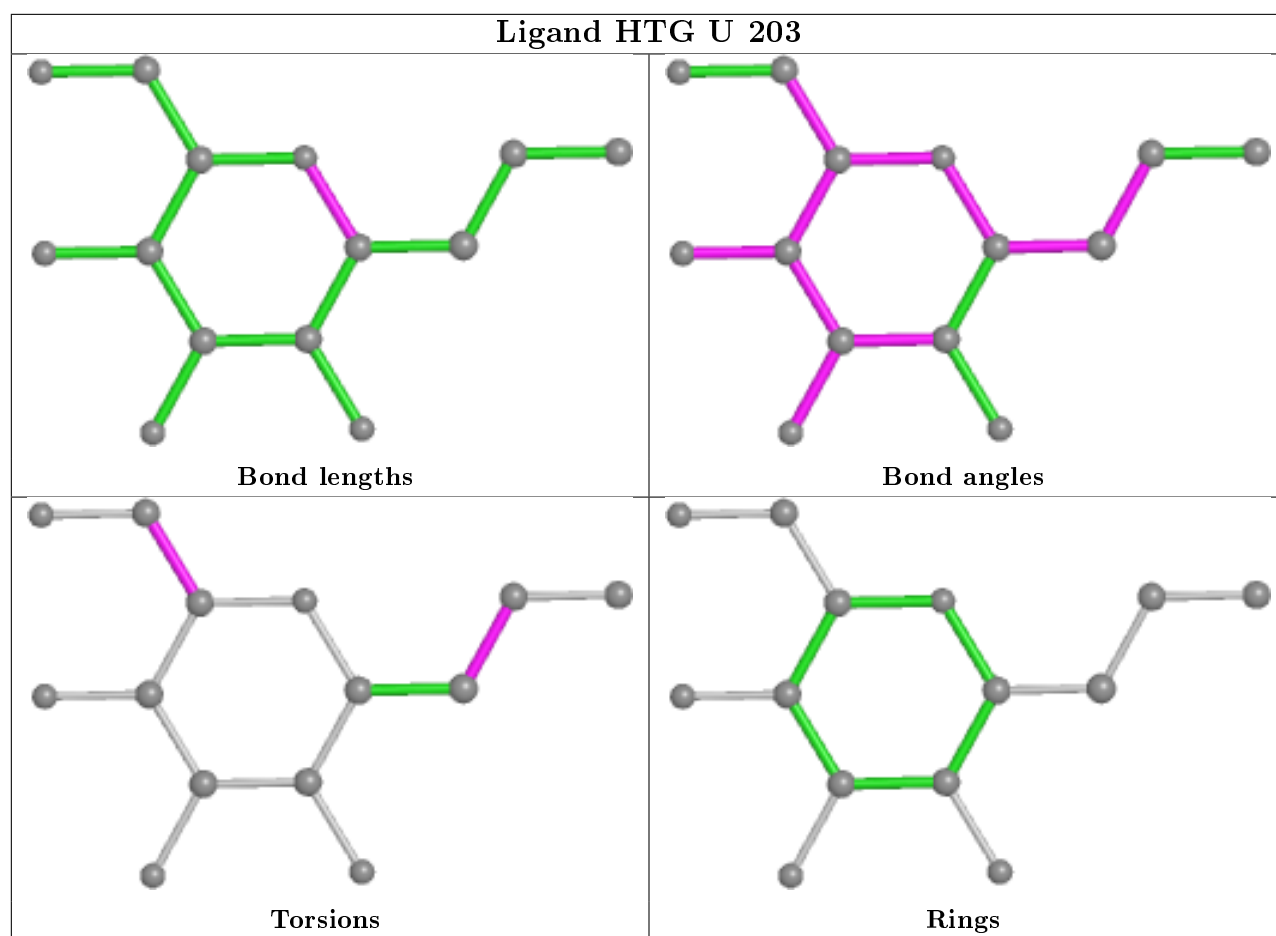


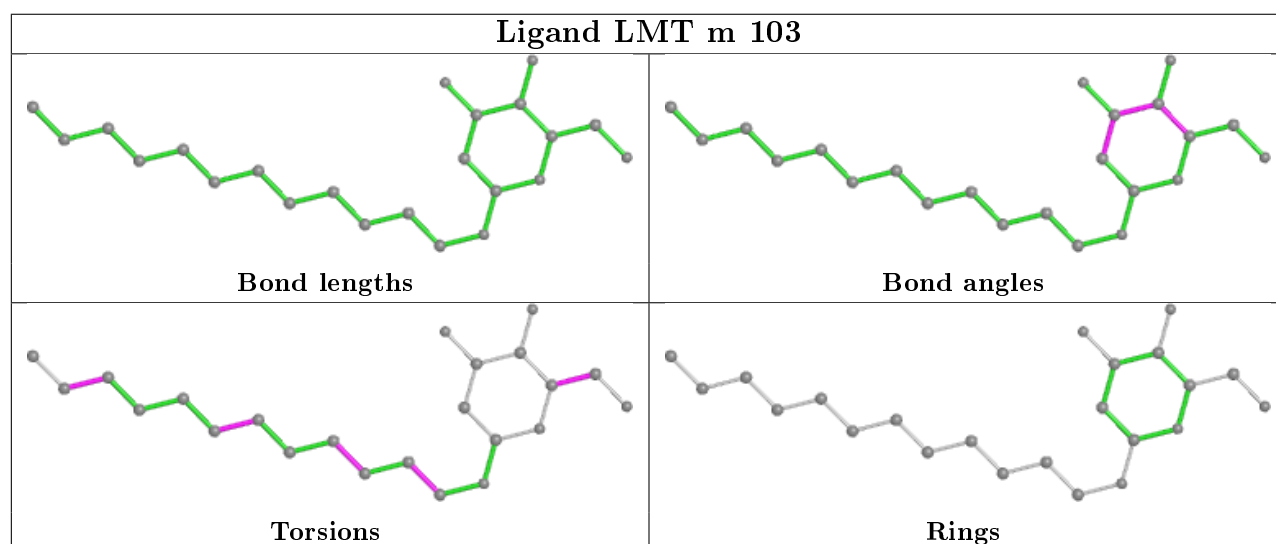
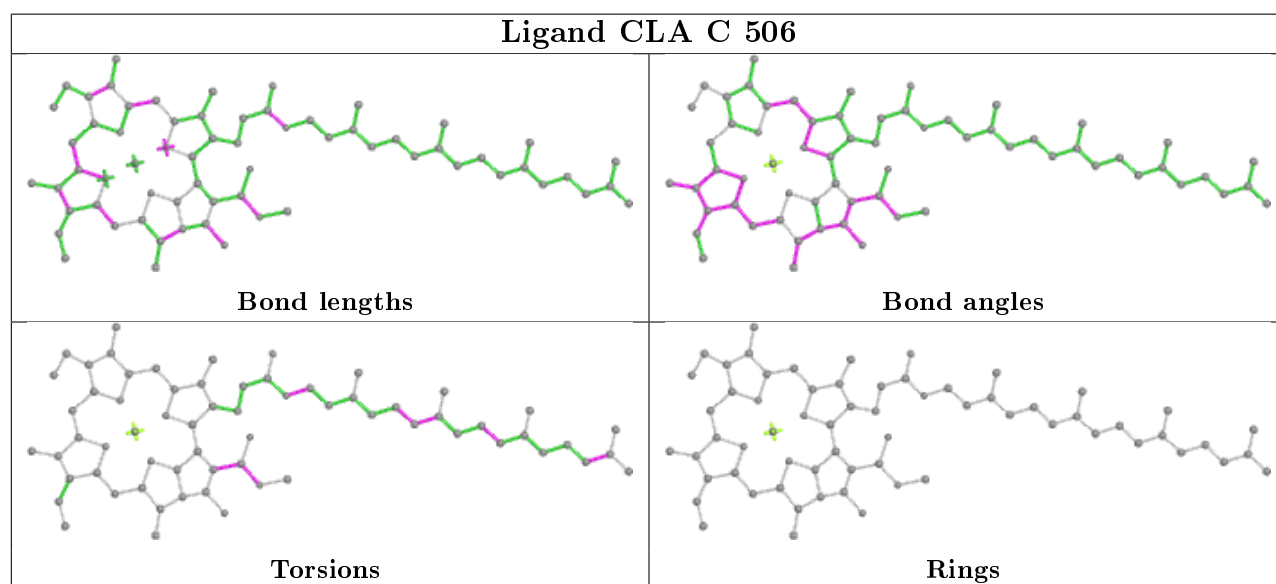
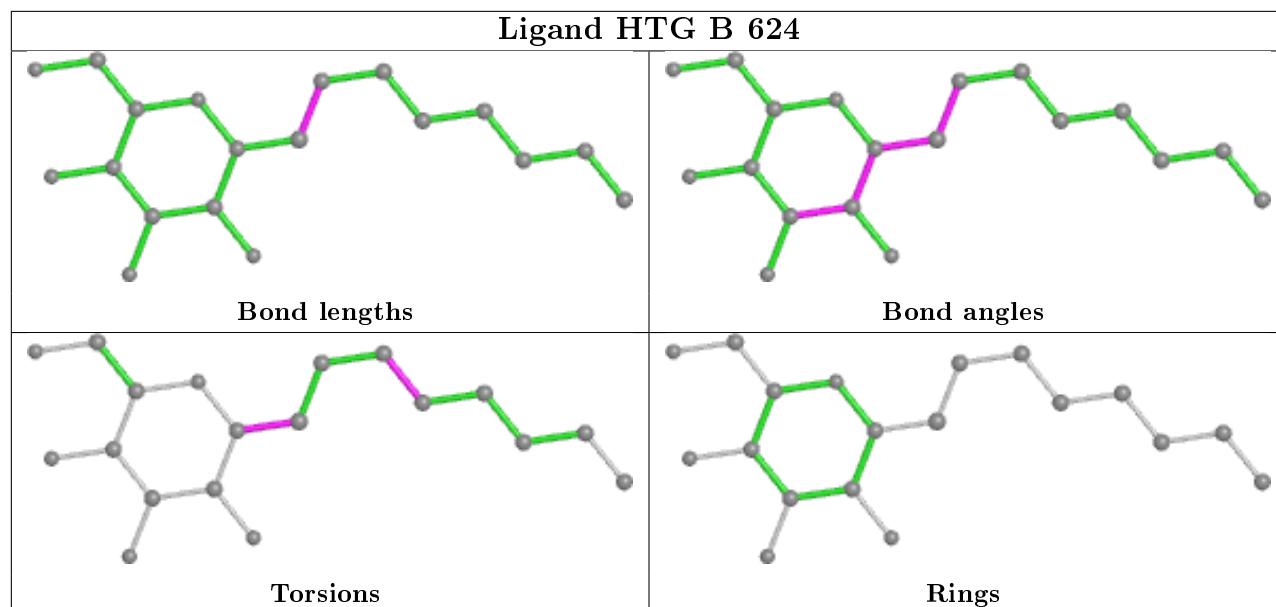
Ligand BCR c 515**Ligand CLA b 609****Ligand PHO D 404**

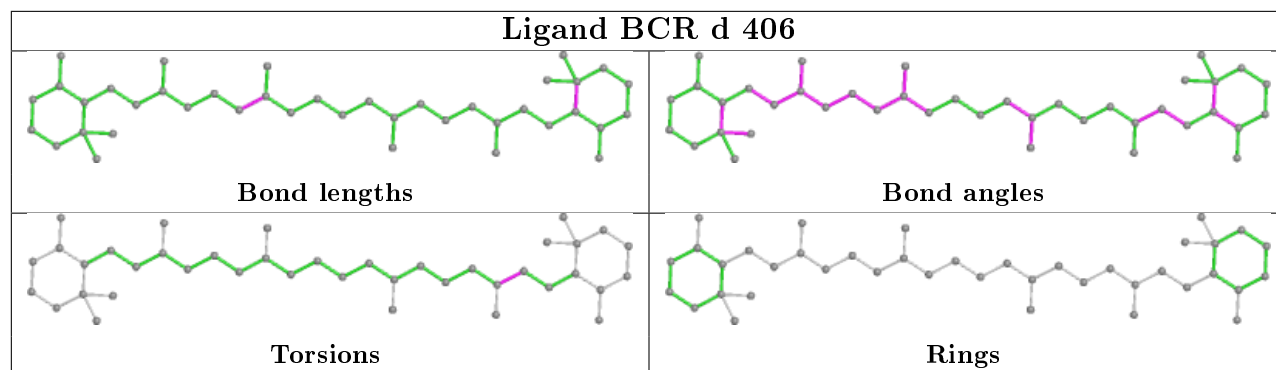
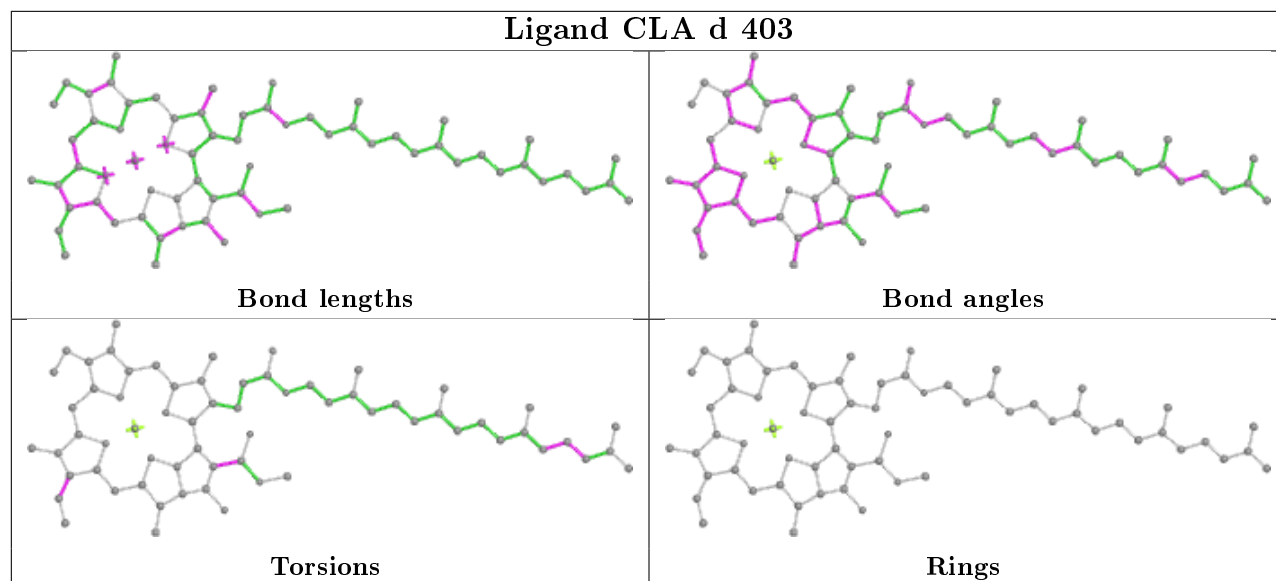
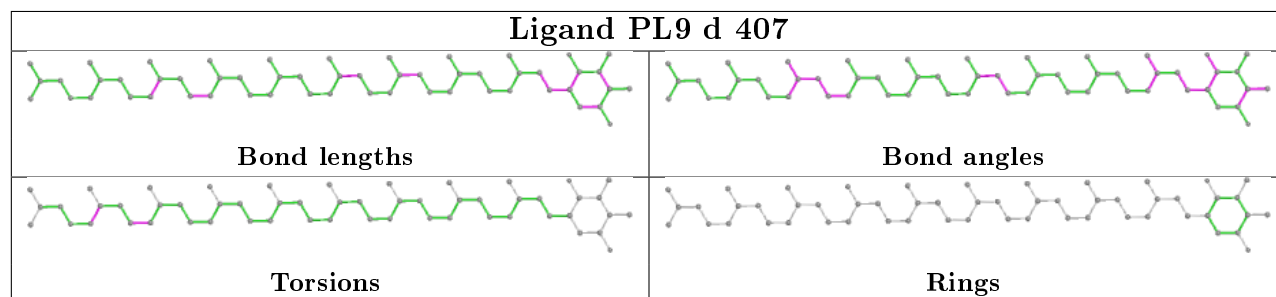


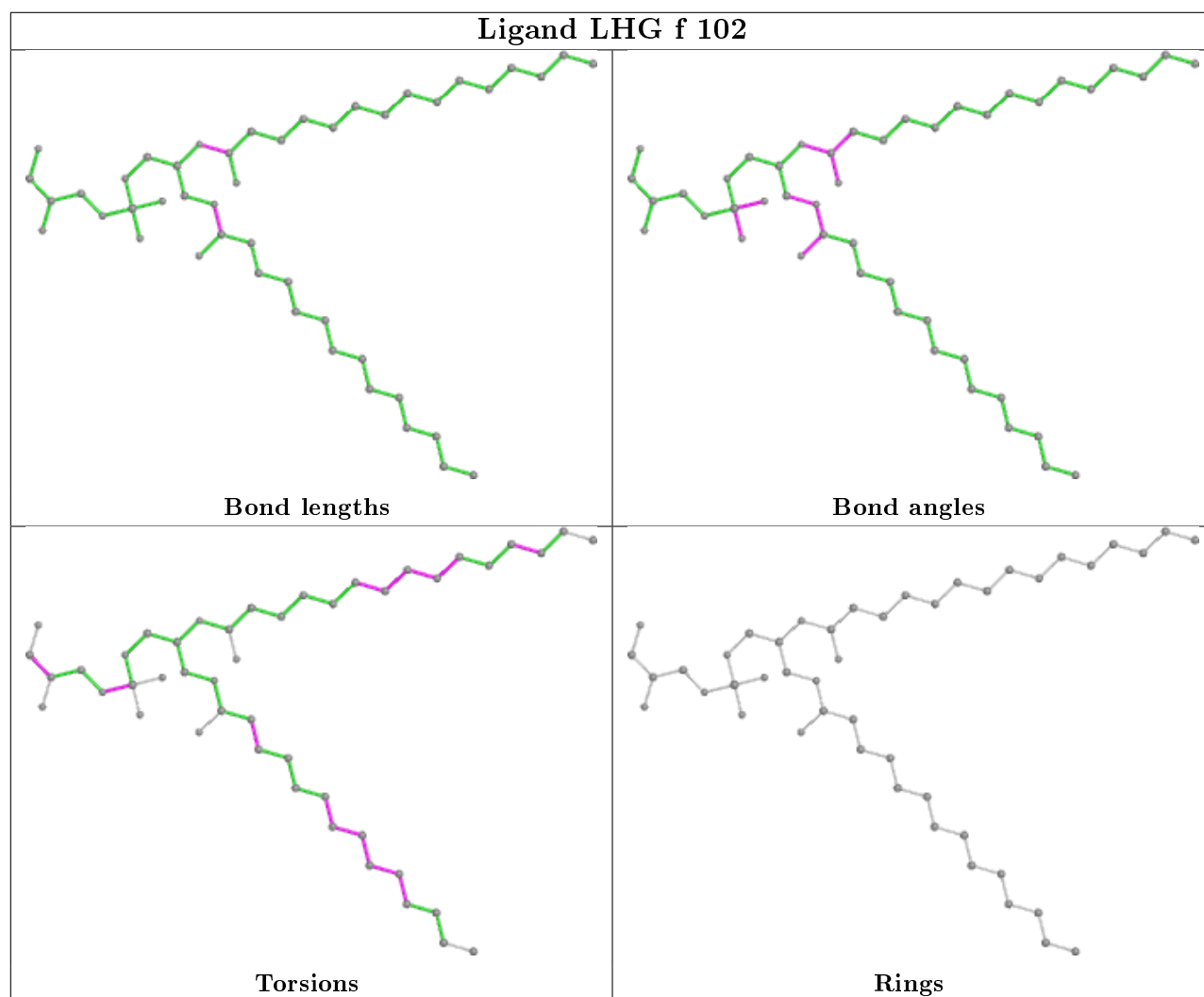
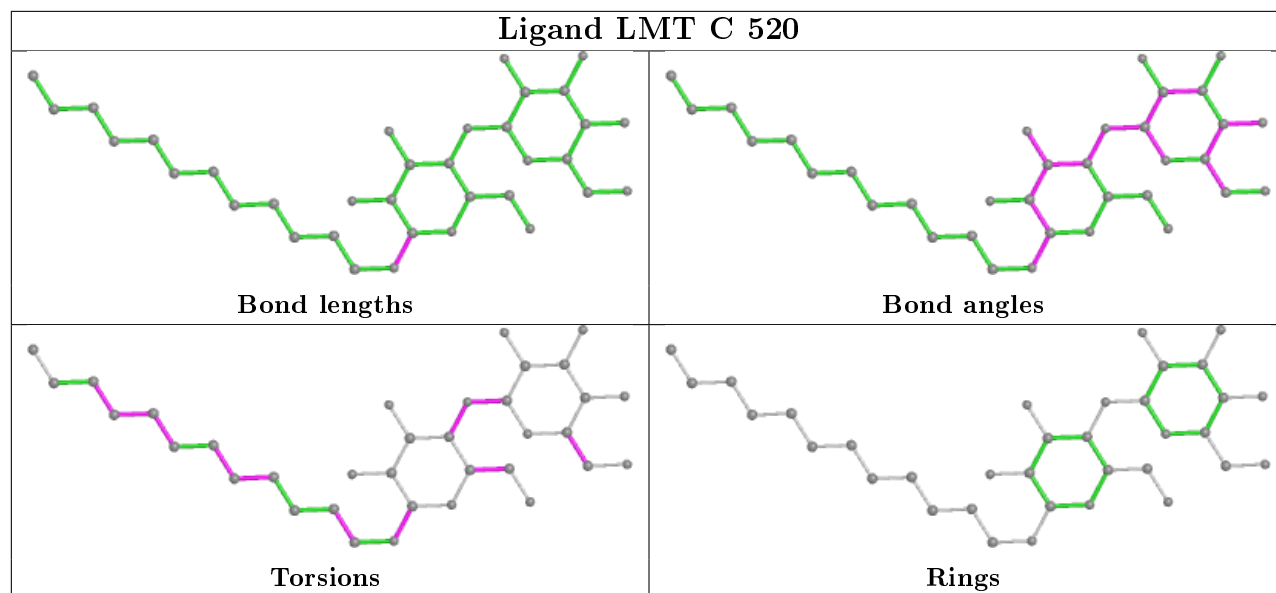
Ligand RRX h 102**Ligand CLA C 504****Ligand CLA C 512**



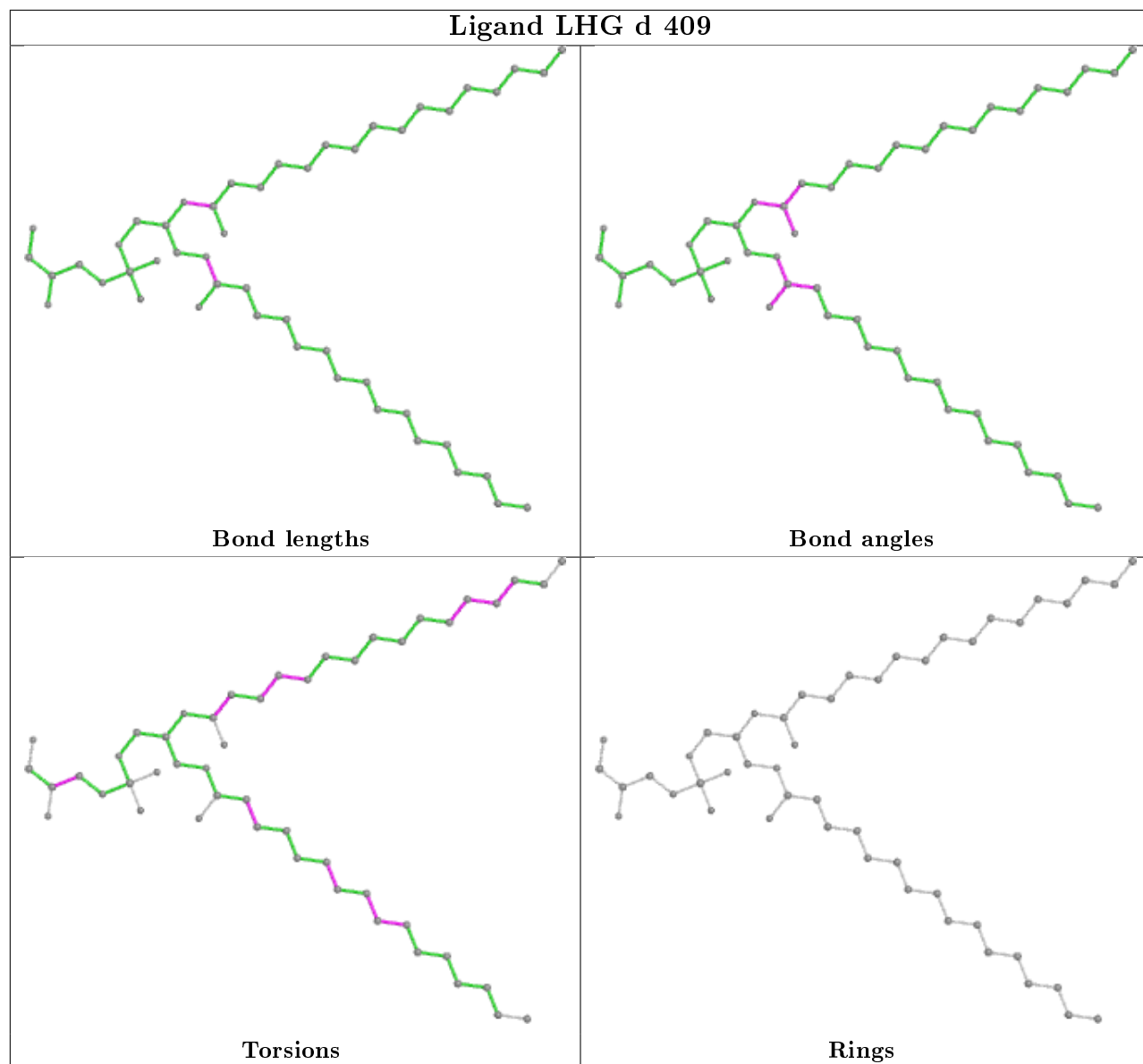




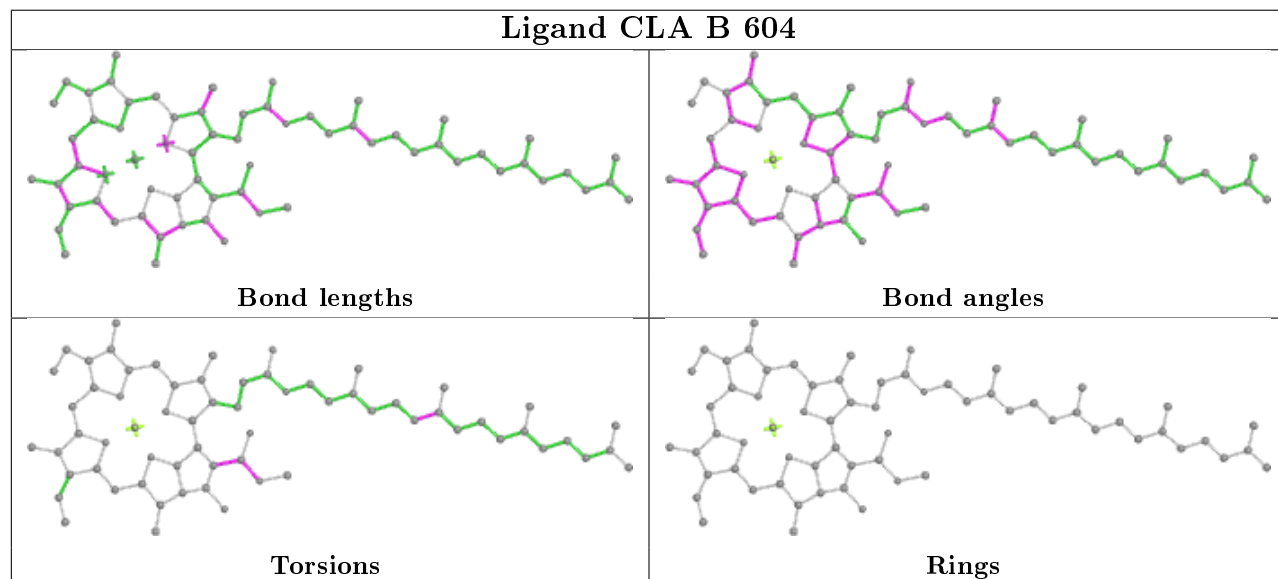
Ligand BCR d 406**Ligand CLA d 403****Ligand PL9 d 407**



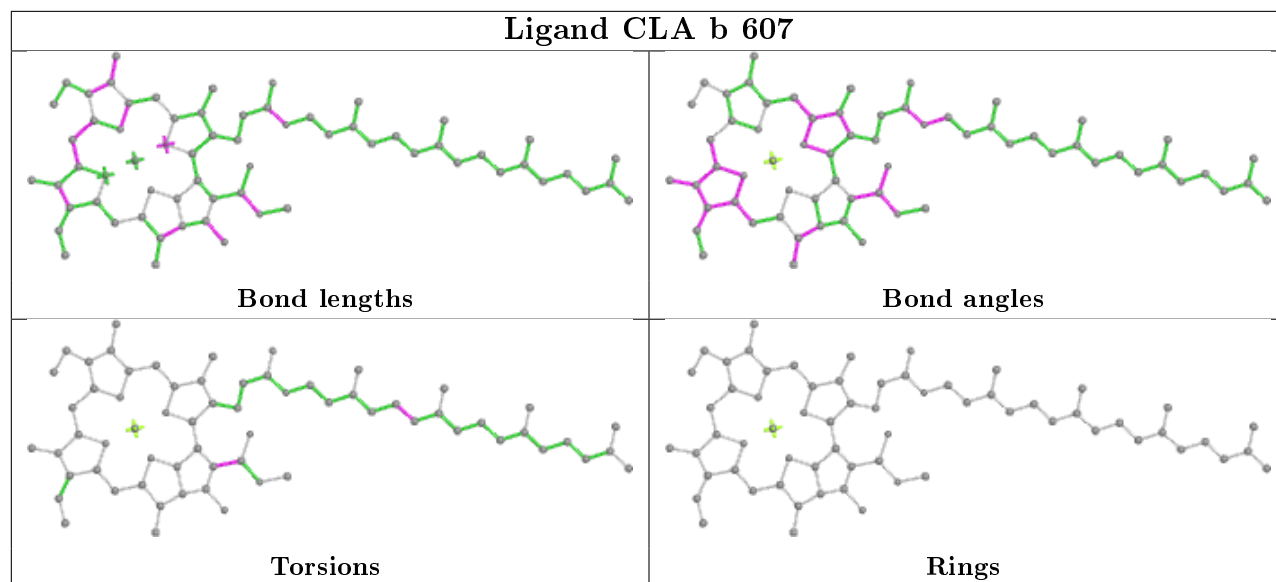
Ligand LHG d 409



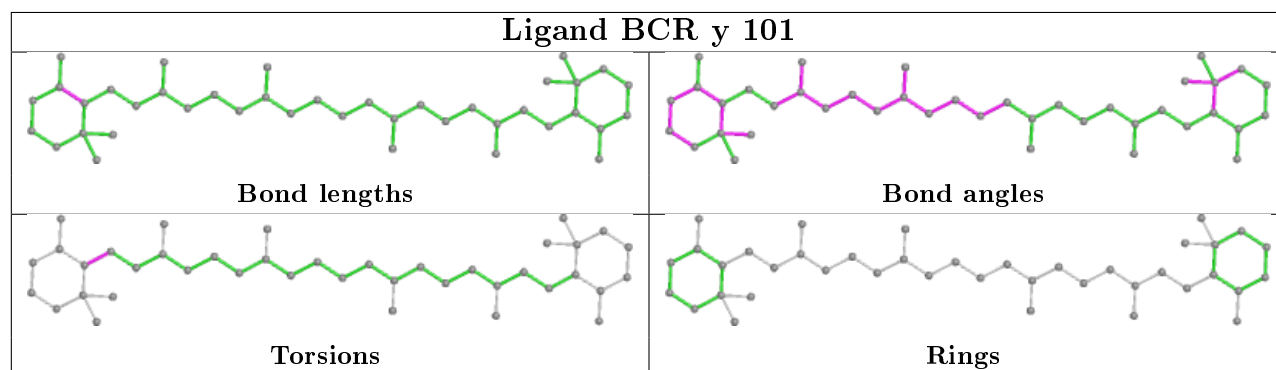
Ligand CLA B 604



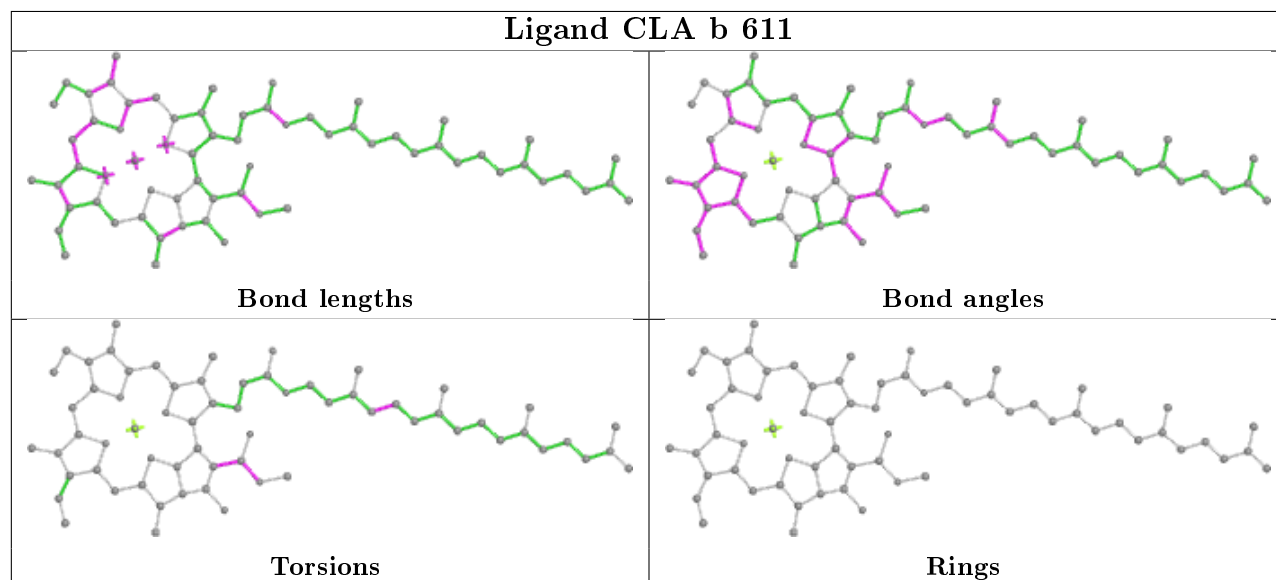
Ligand CLA b 607



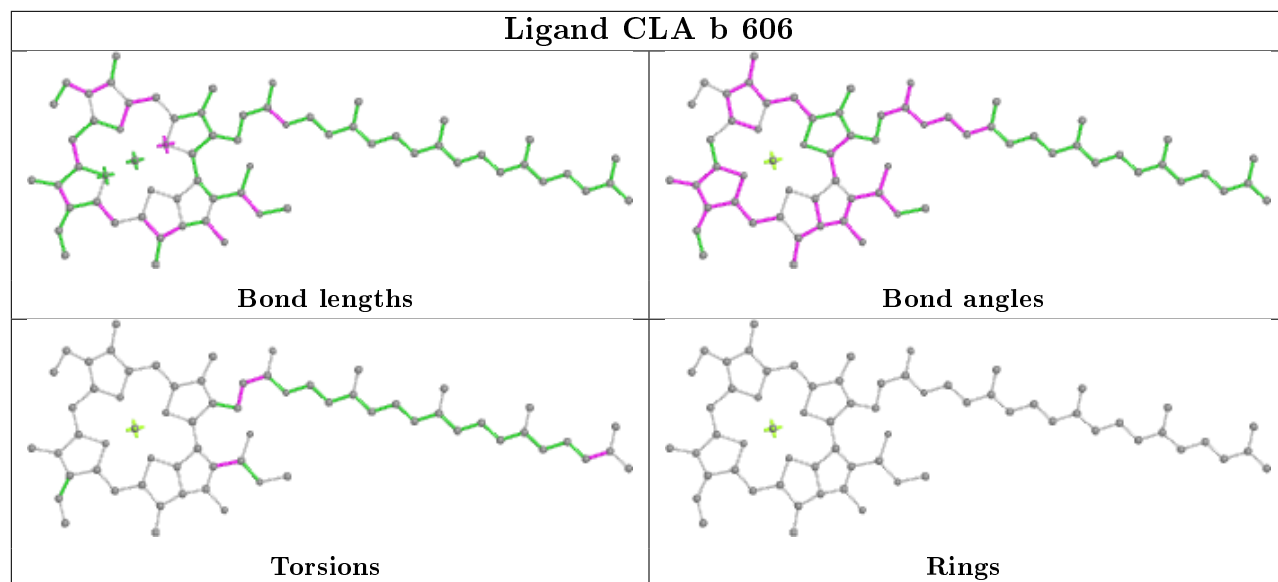
Ligand BCR y 101



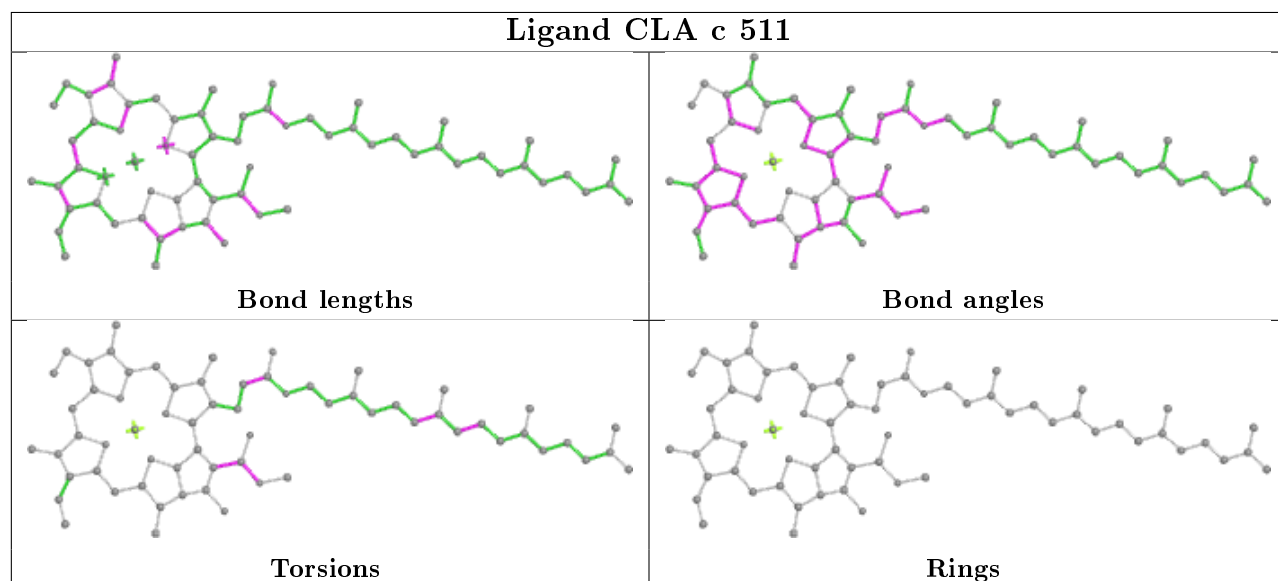
Ligand CLA b 611



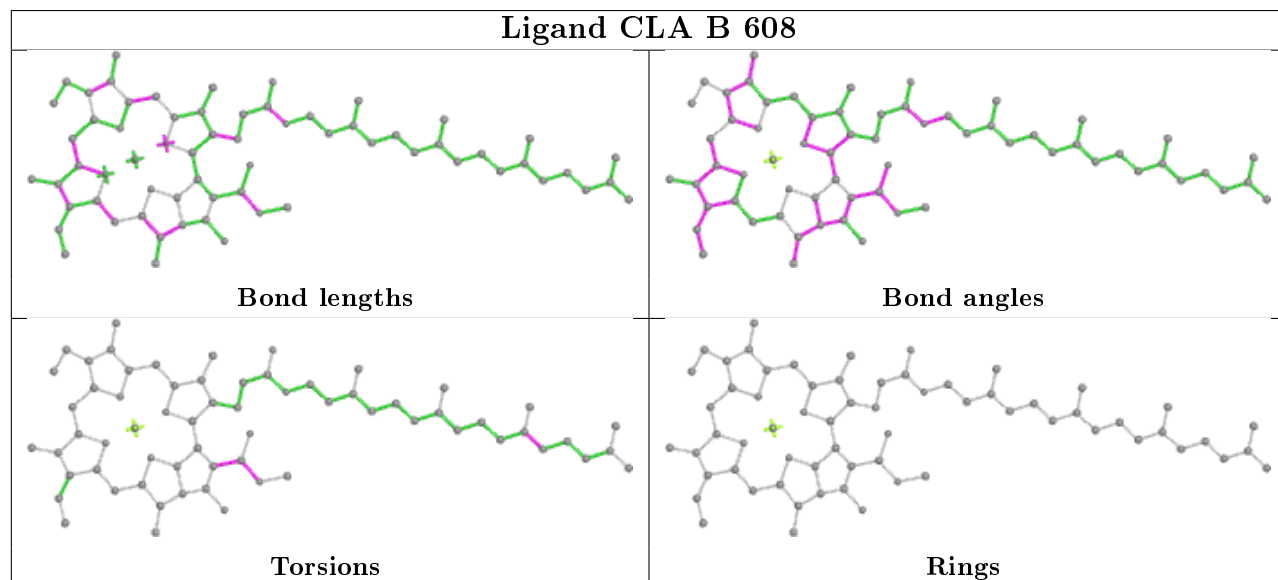
Ligand CLA b 606



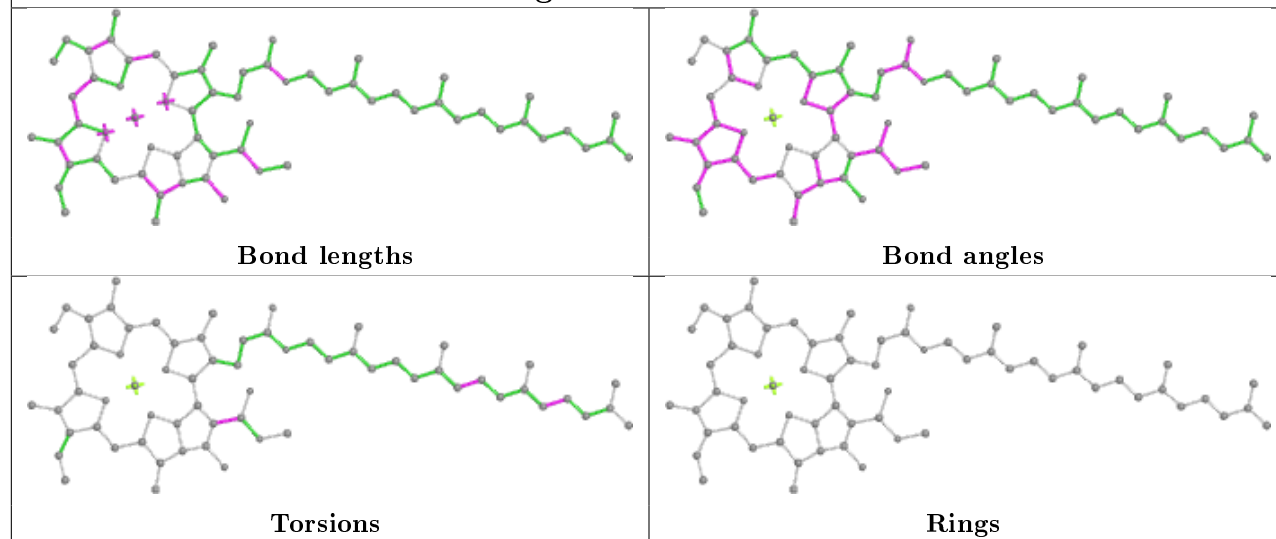
Ligand CLA c 511



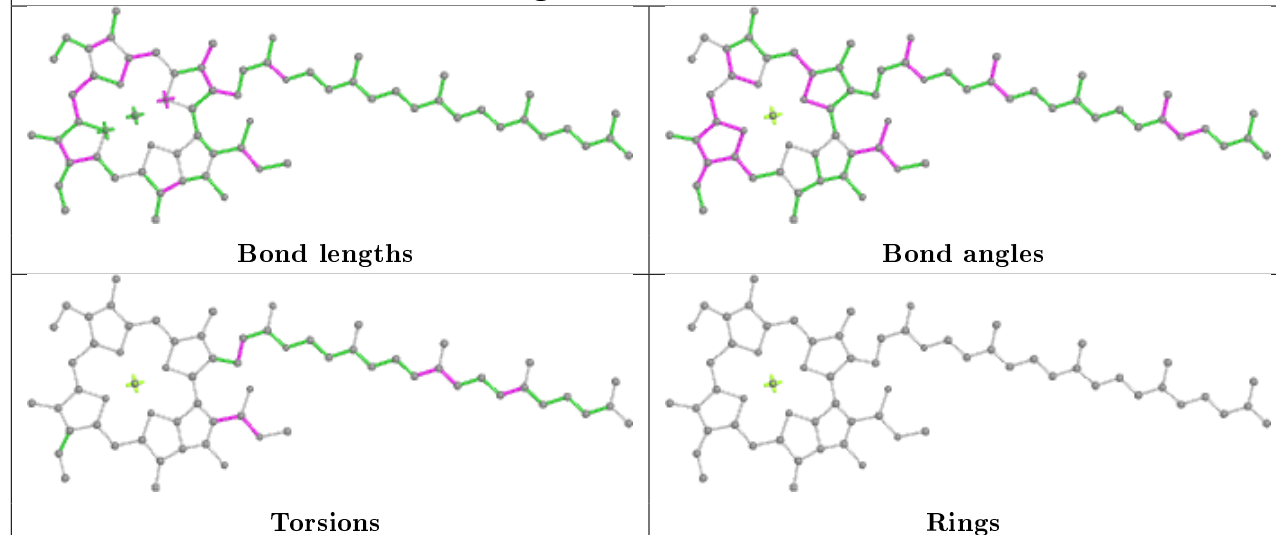
Ligand CLA B 608



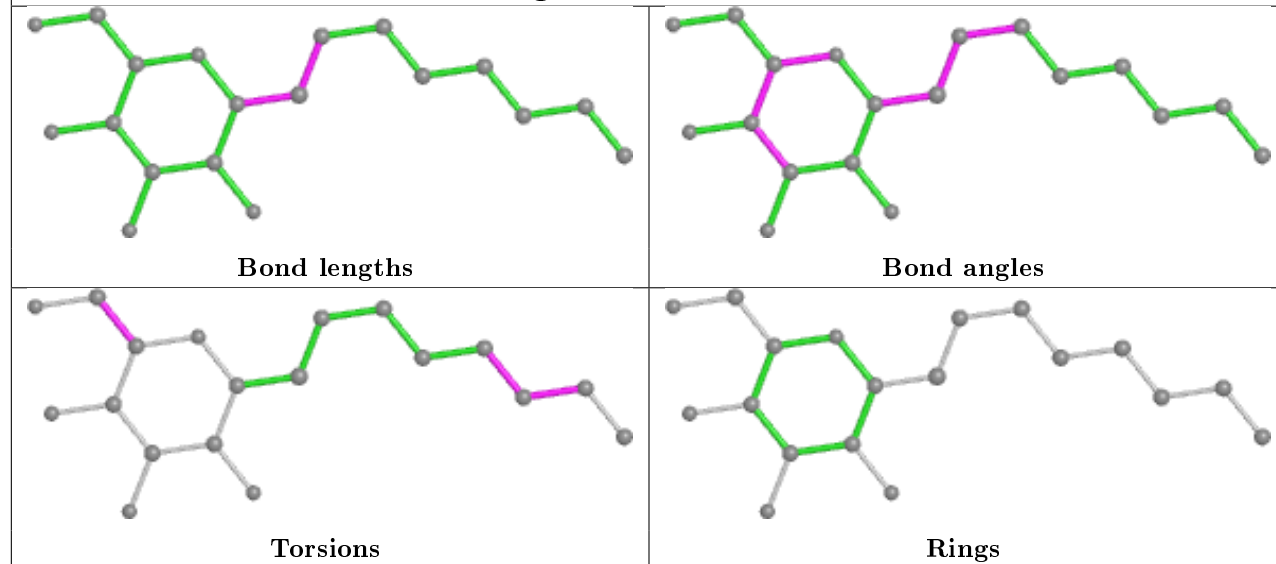
Ligand CLA b 616



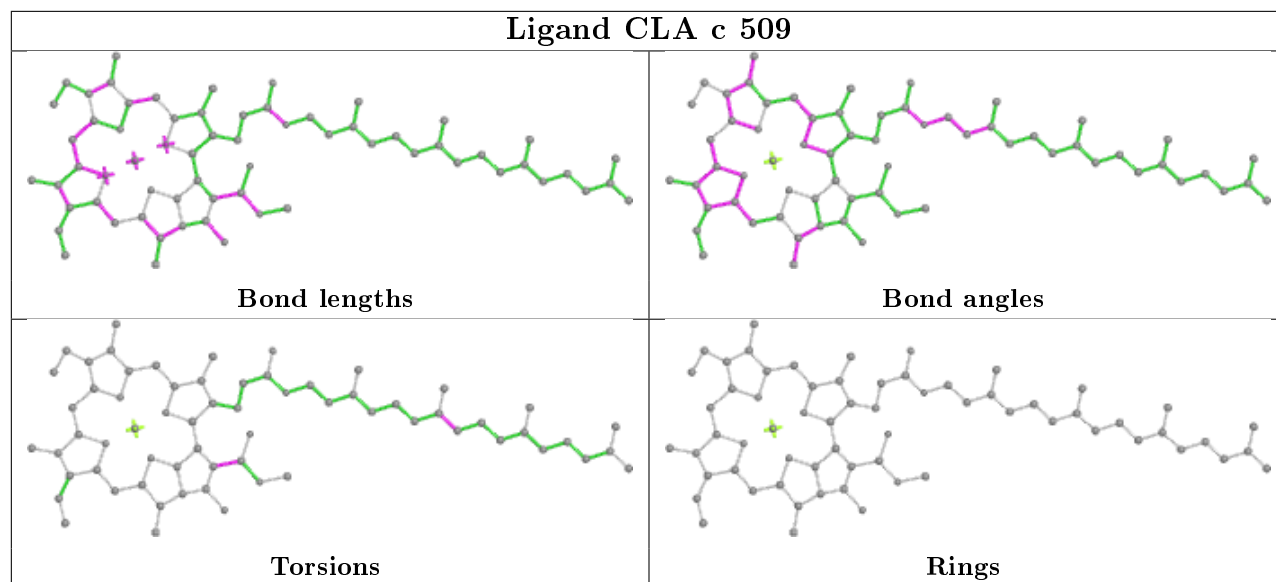
Ligand CLA B 607



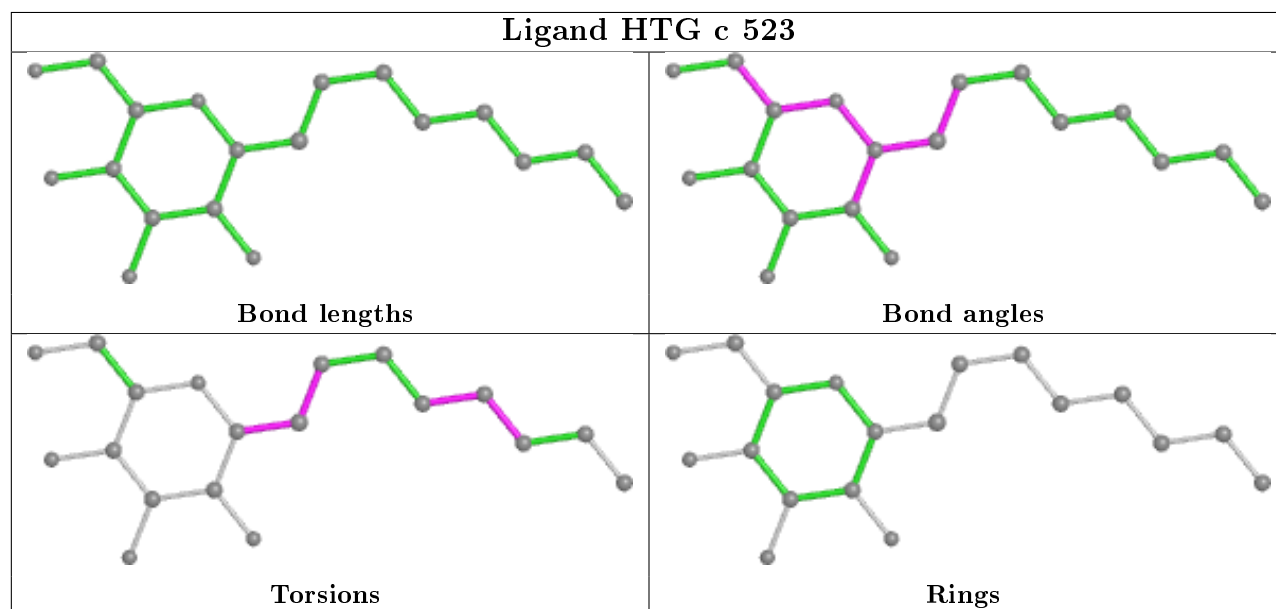
Ligand HTG b 601



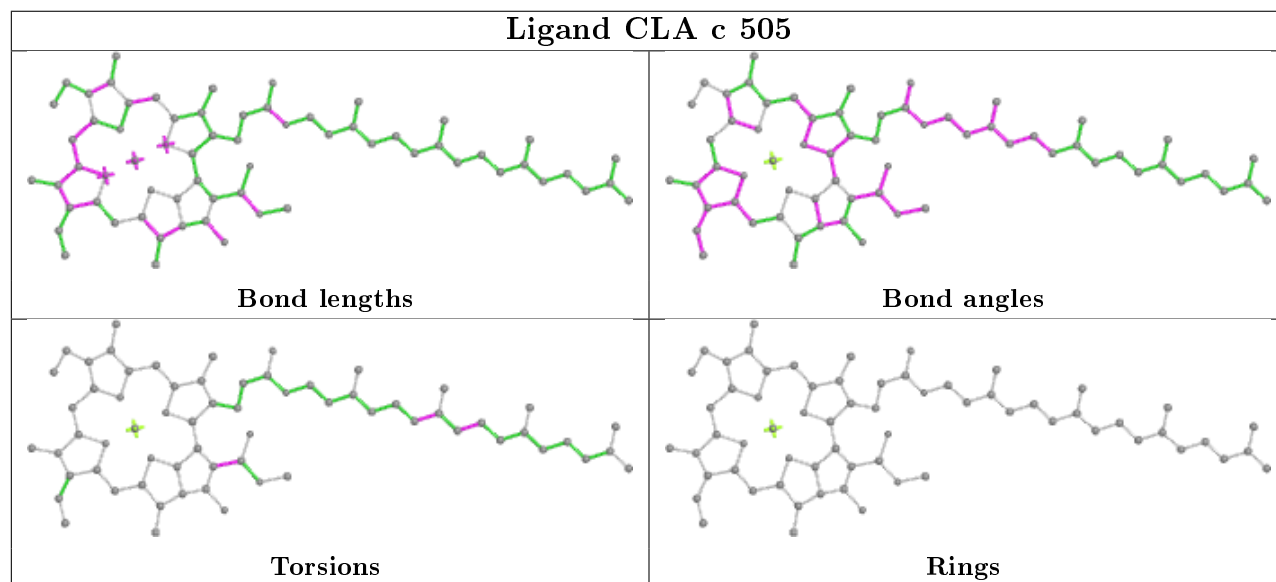
Ligand CLA c 509

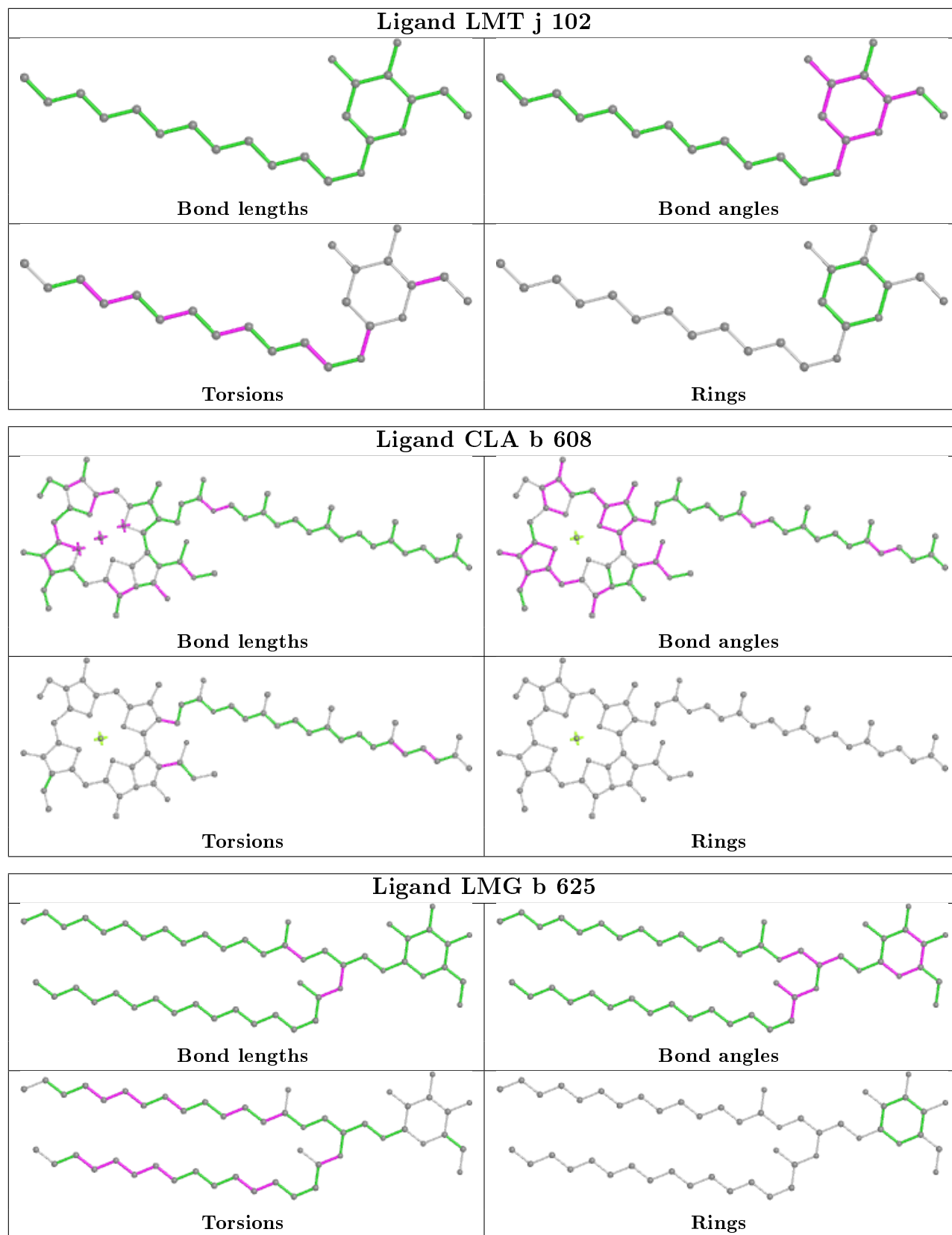


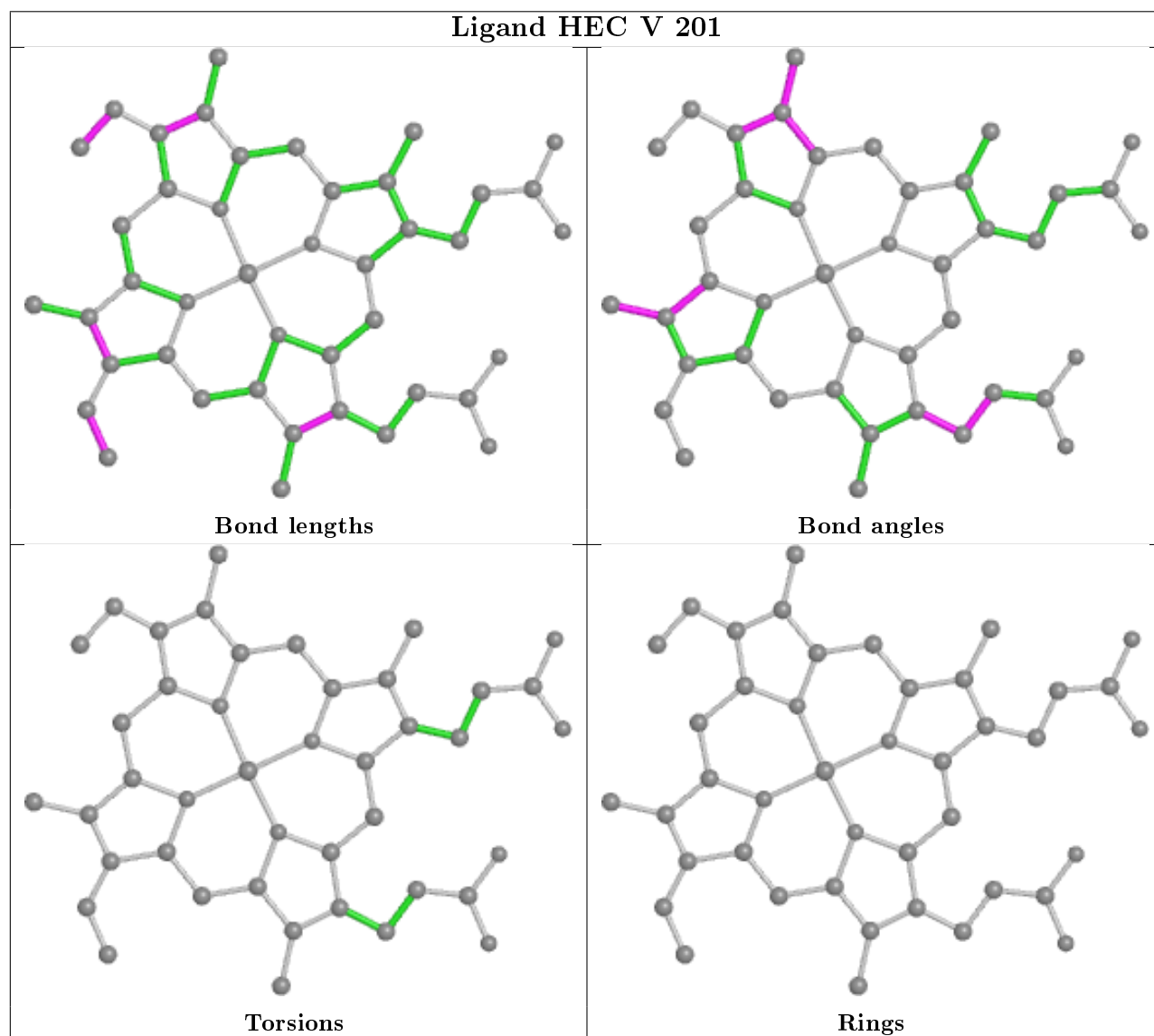
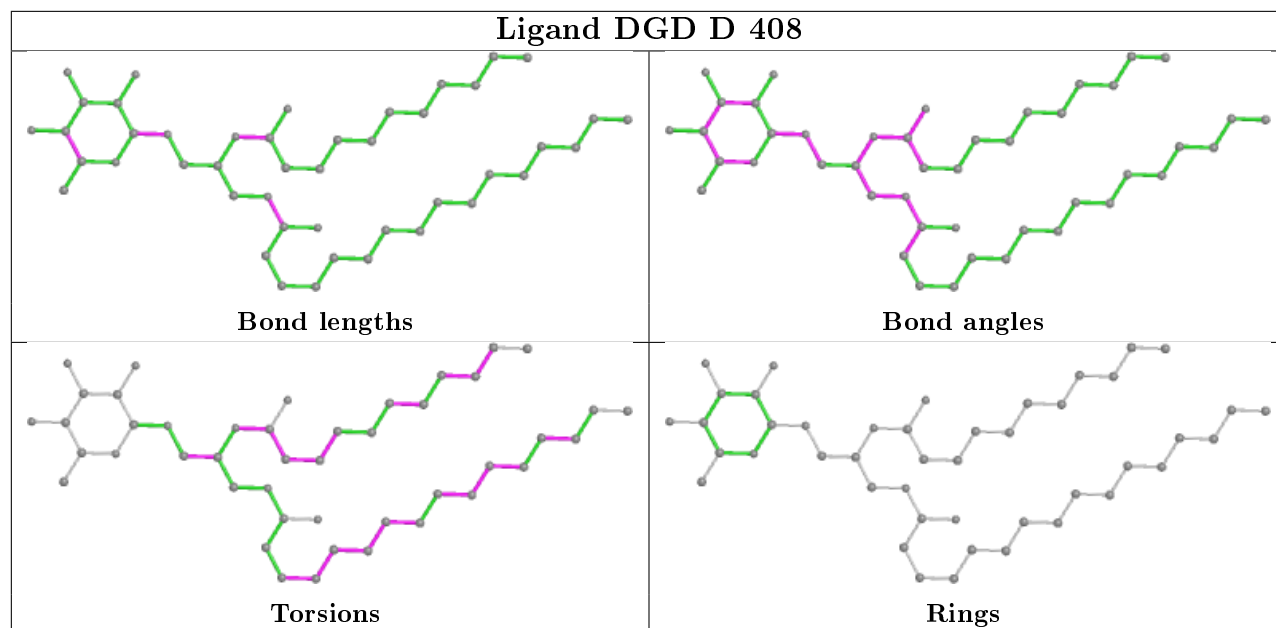
Ligand HTG c 523

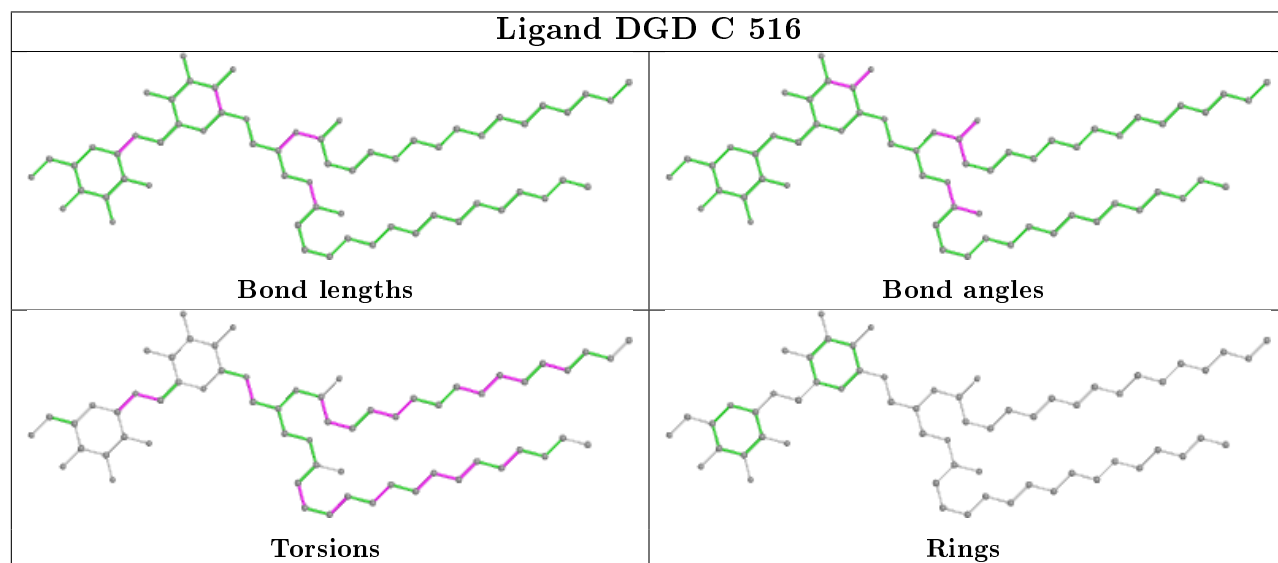
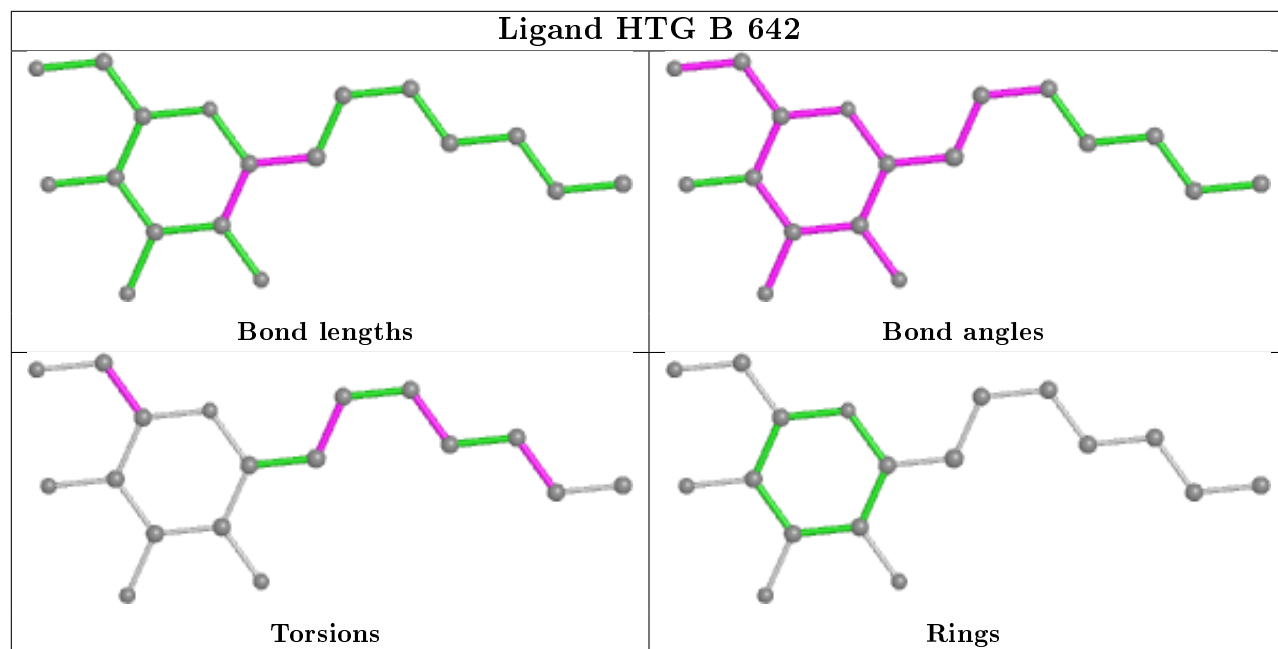


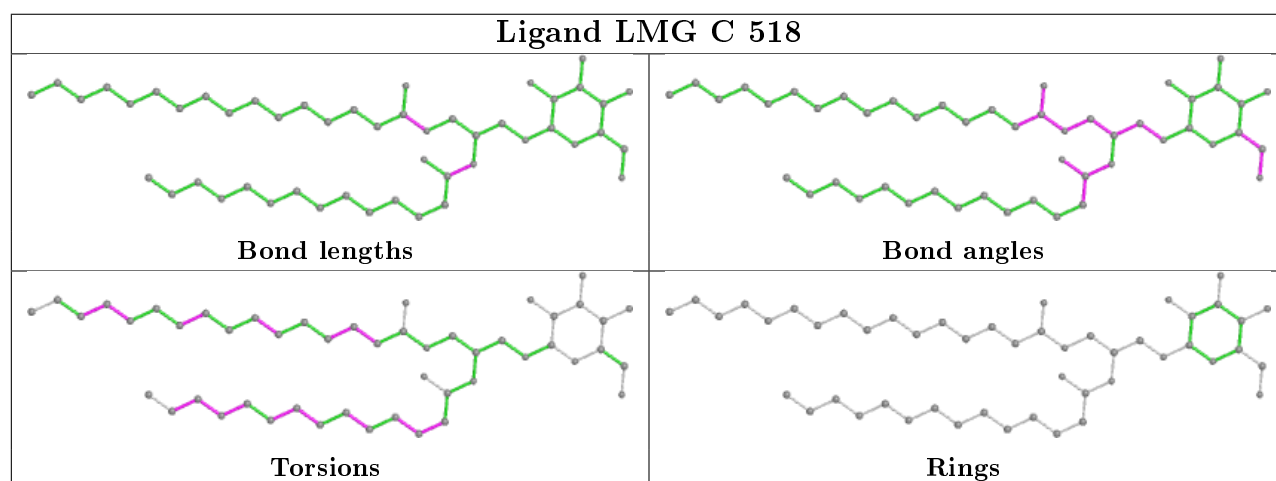
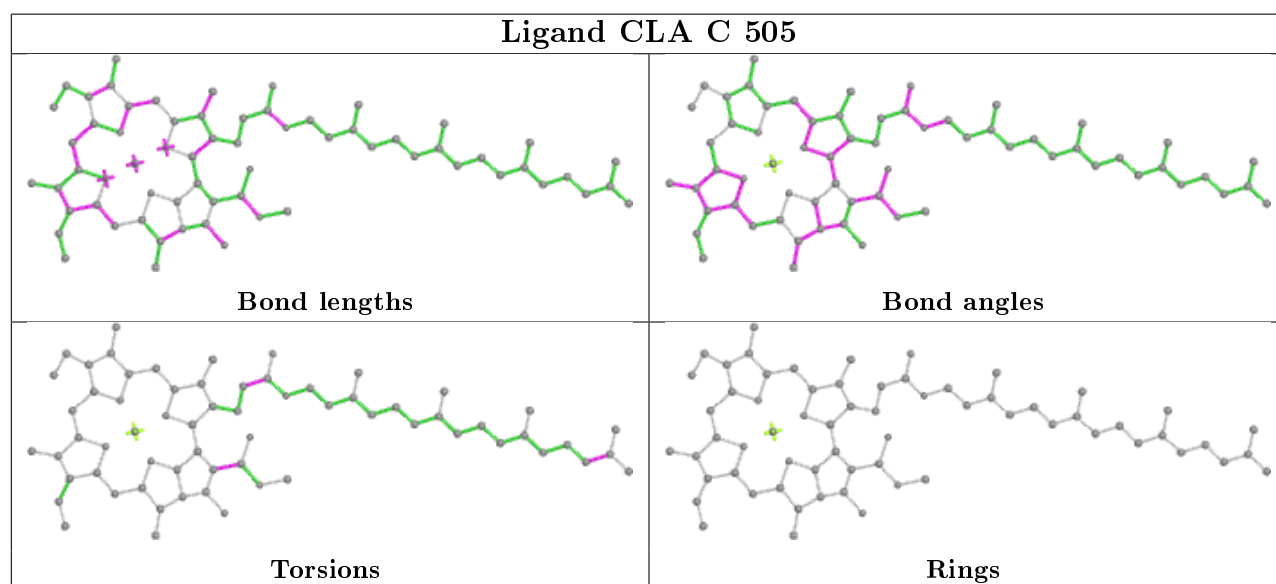
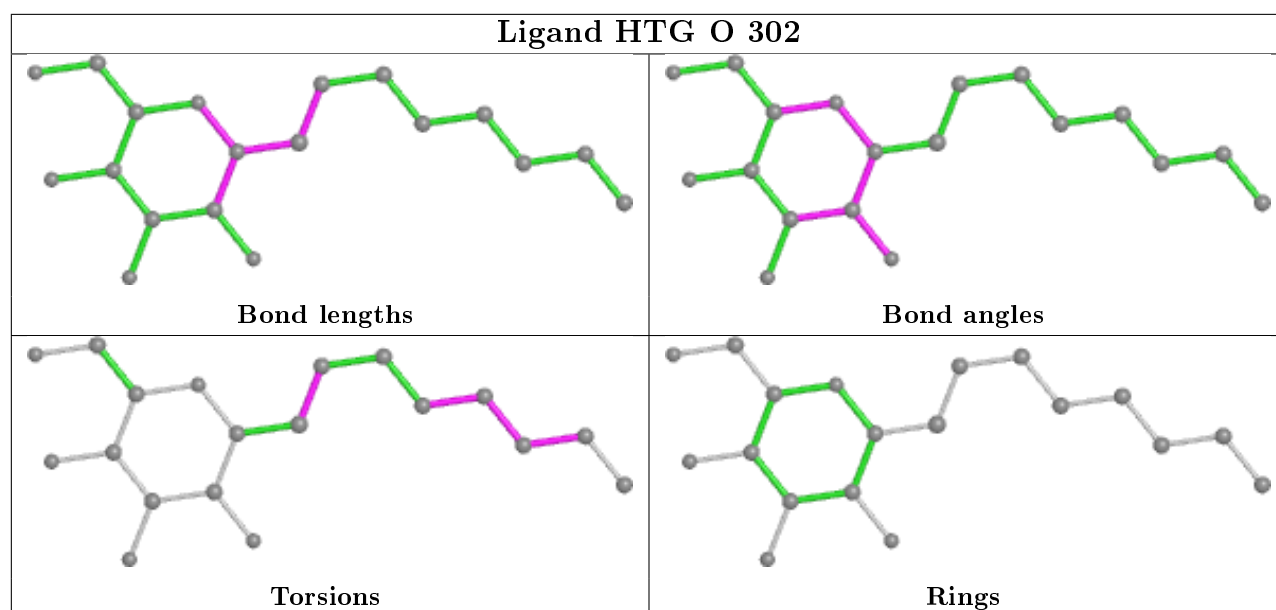
Ligand CLA c 505



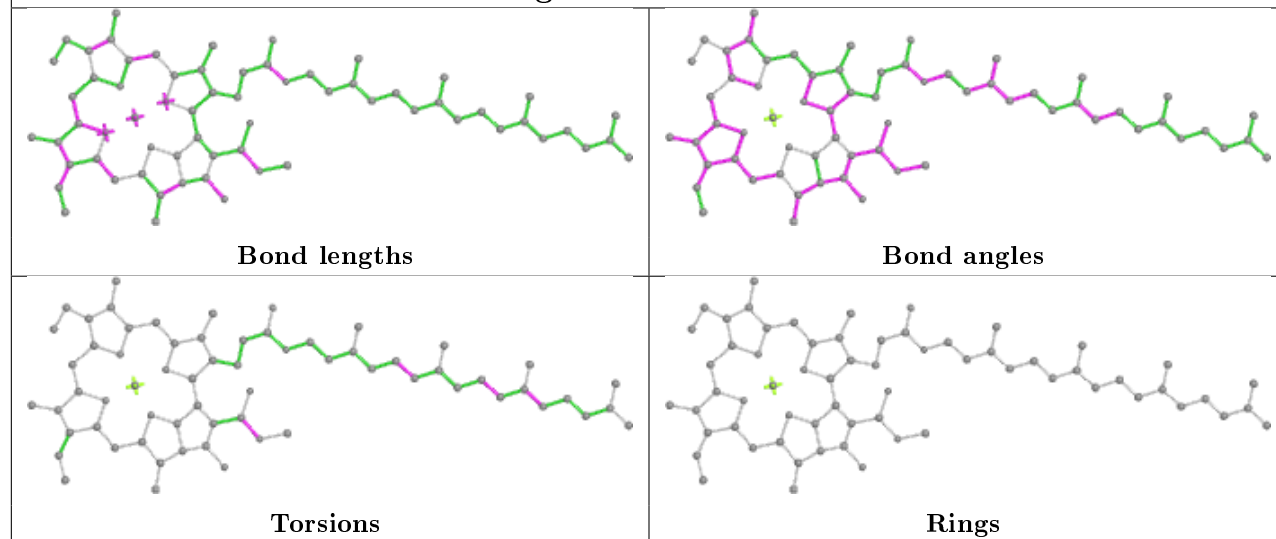




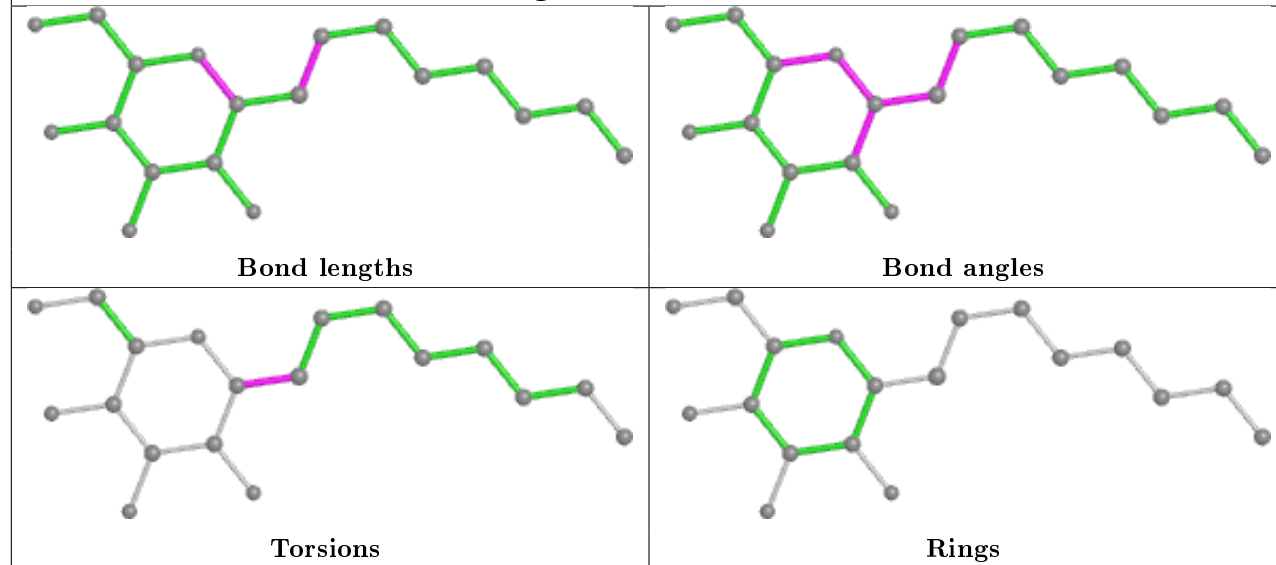




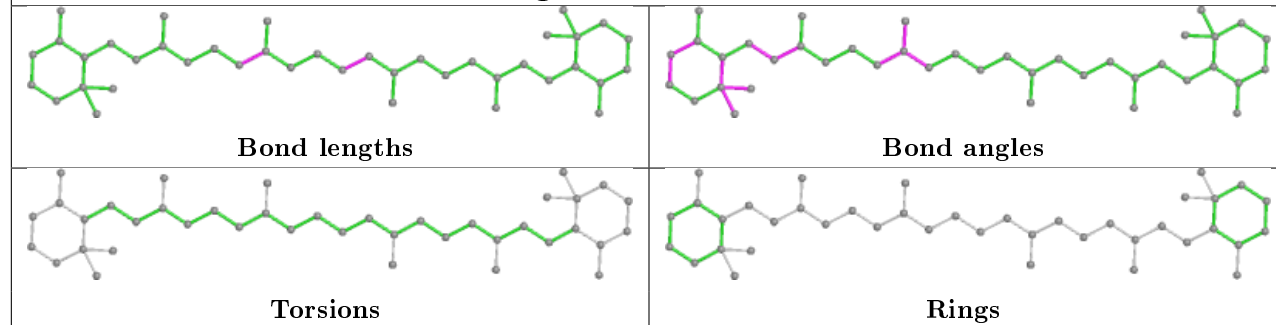
Ligand CLA b 619



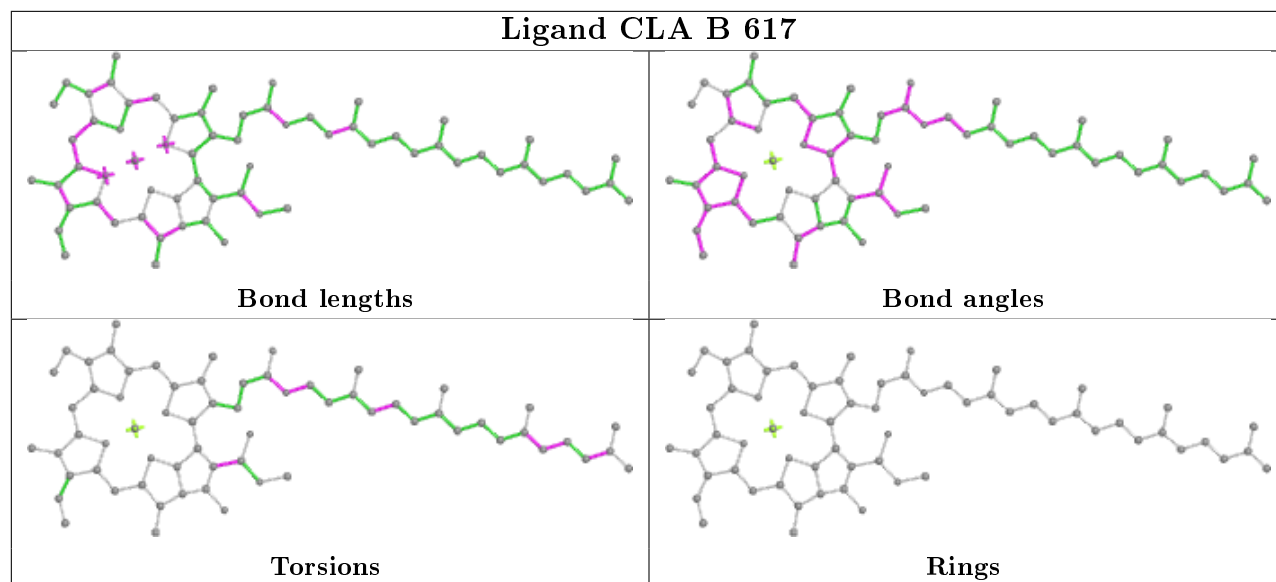
Ligand HTG b 602



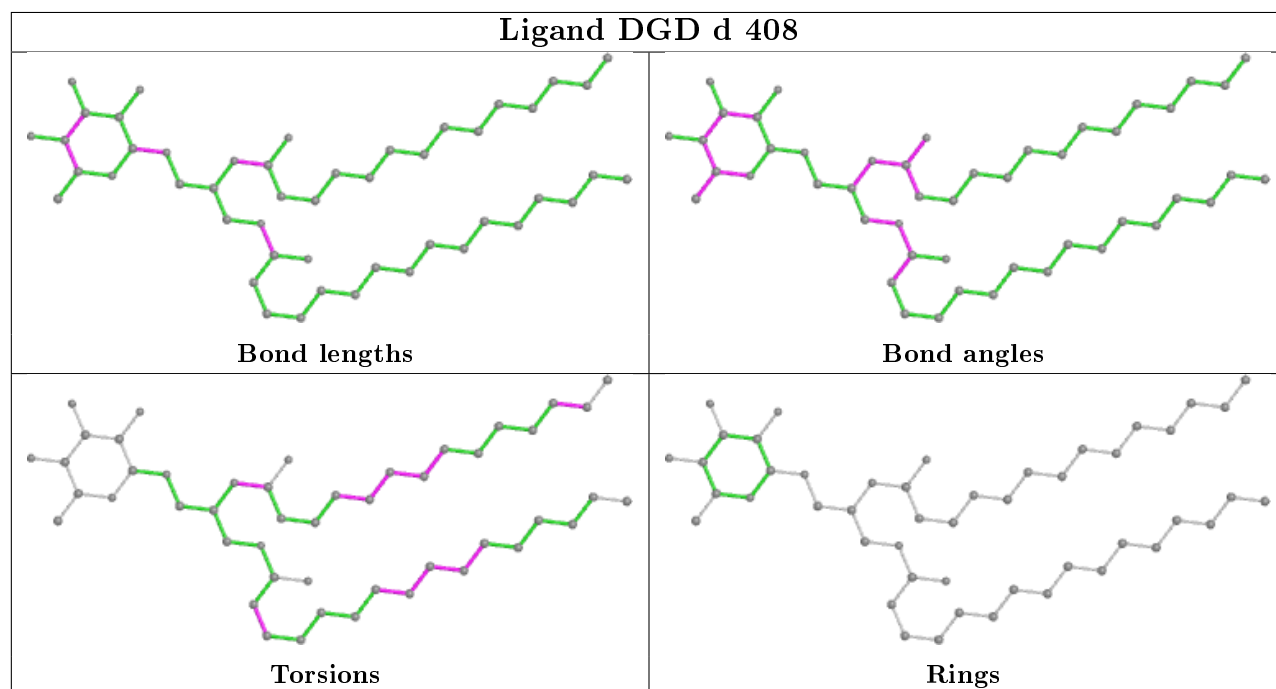
Ligand BCR k 101

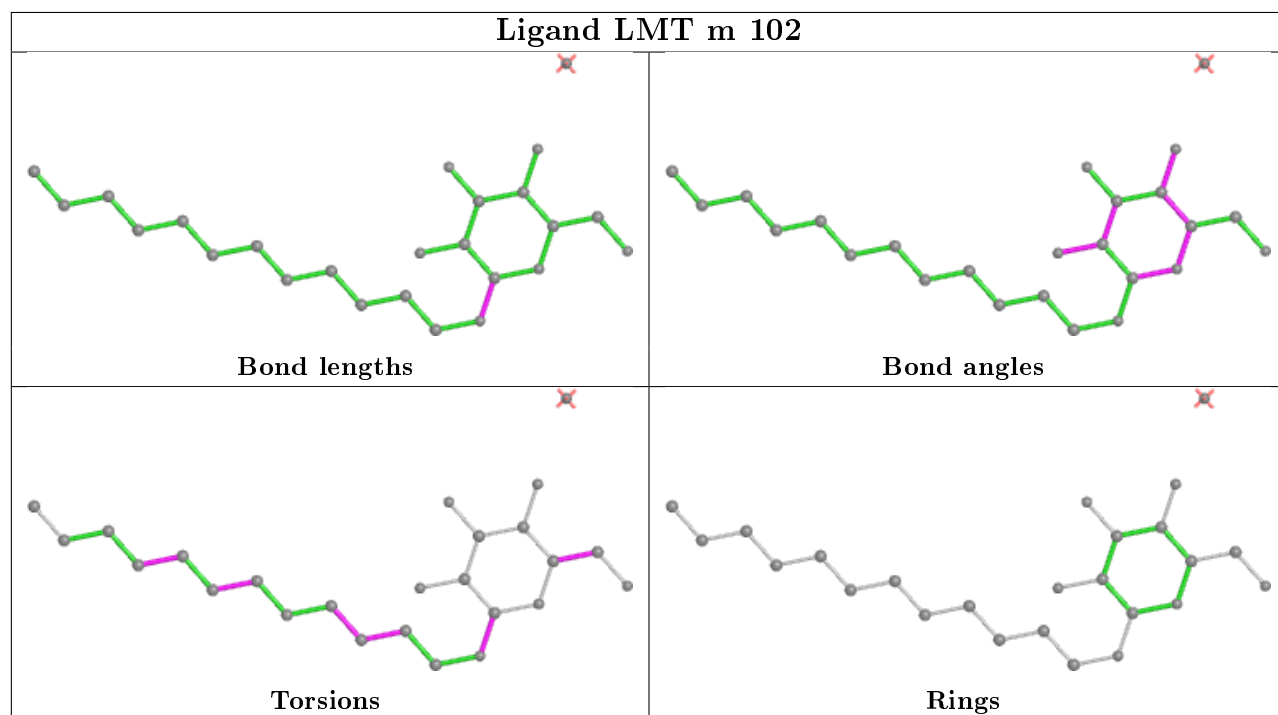
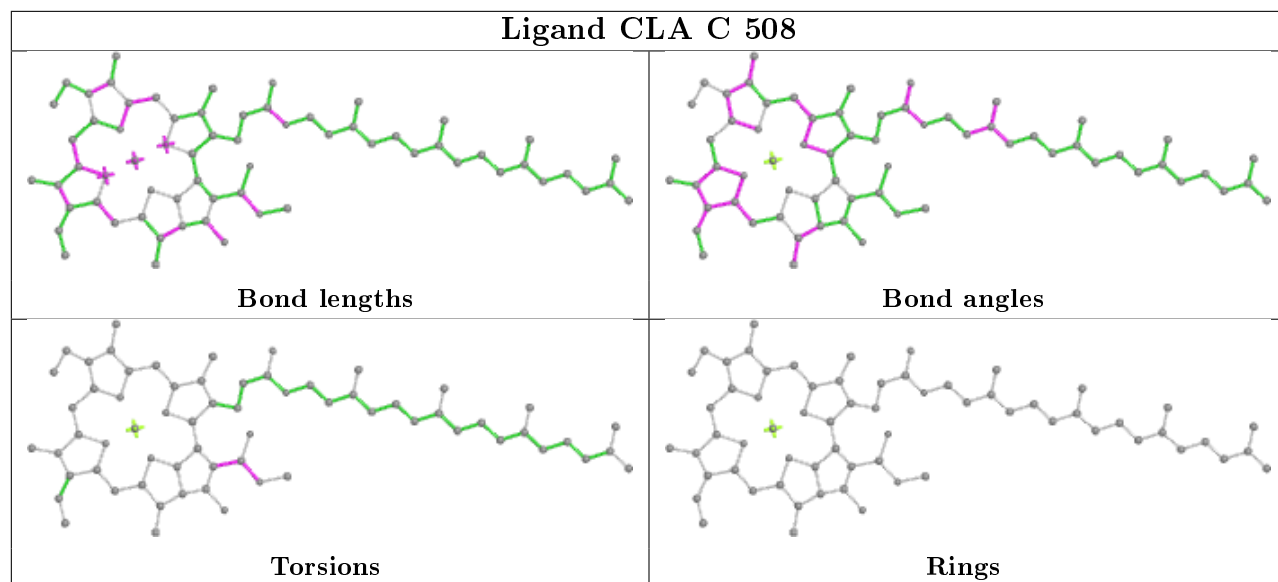


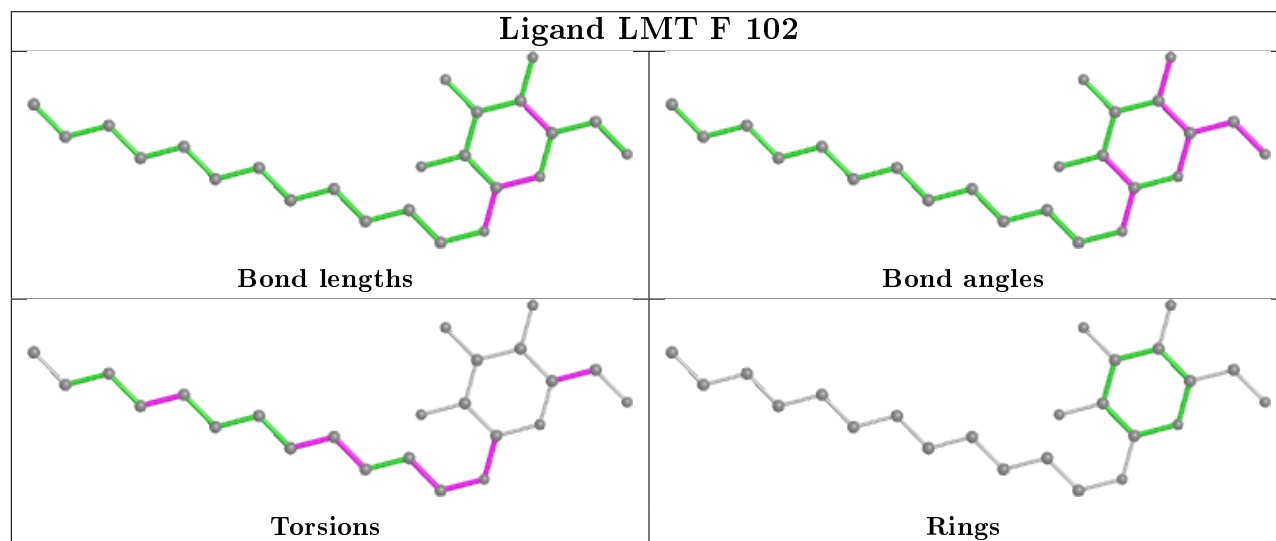
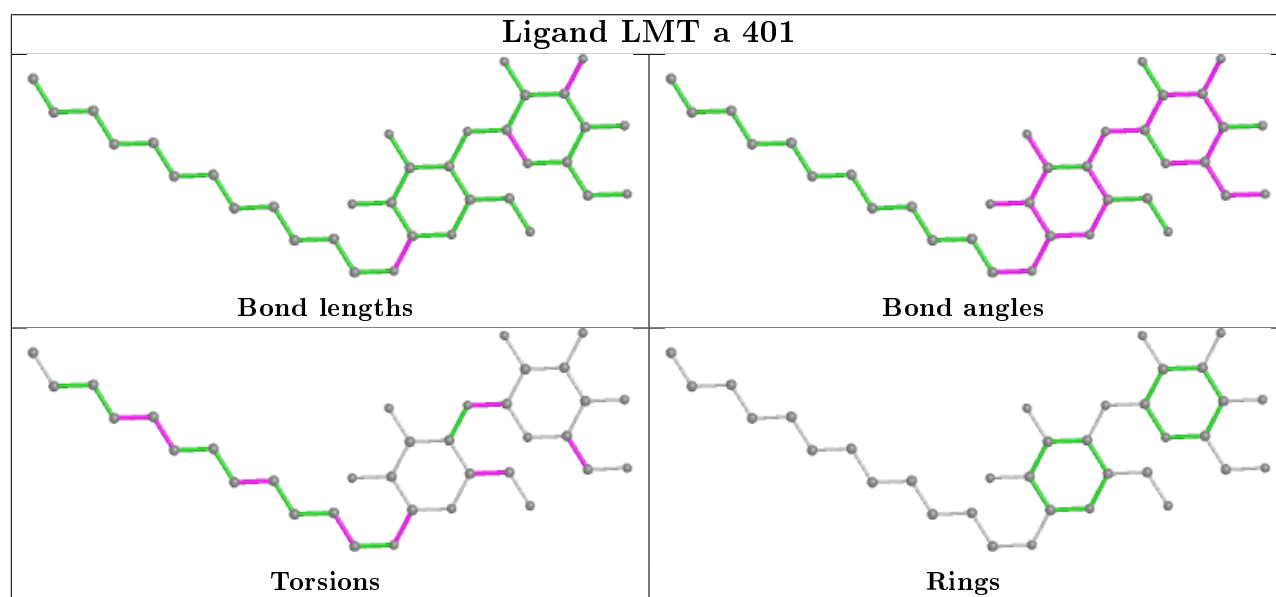
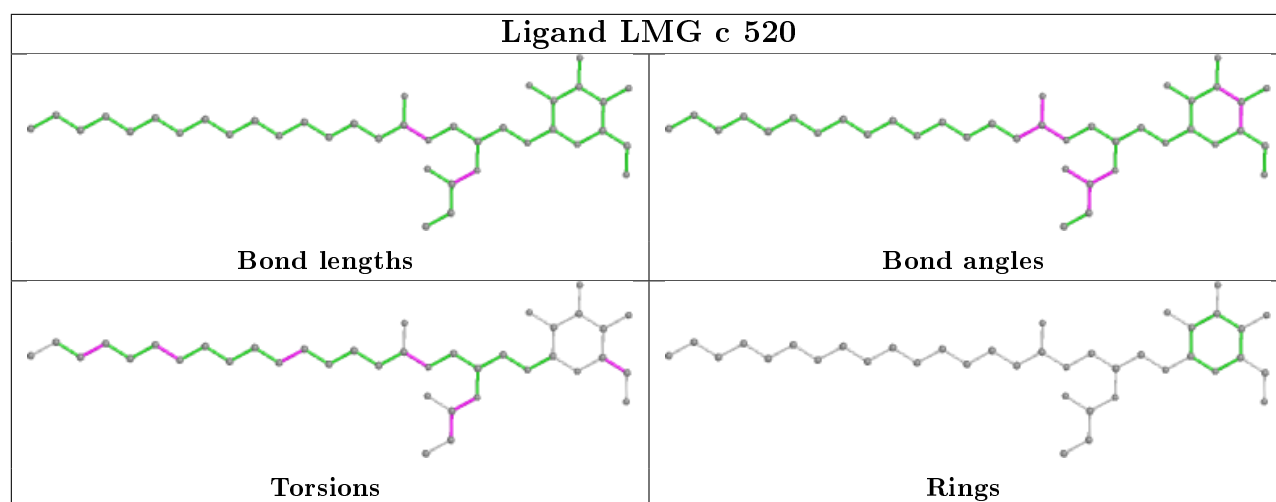
Ligand CLA B 617



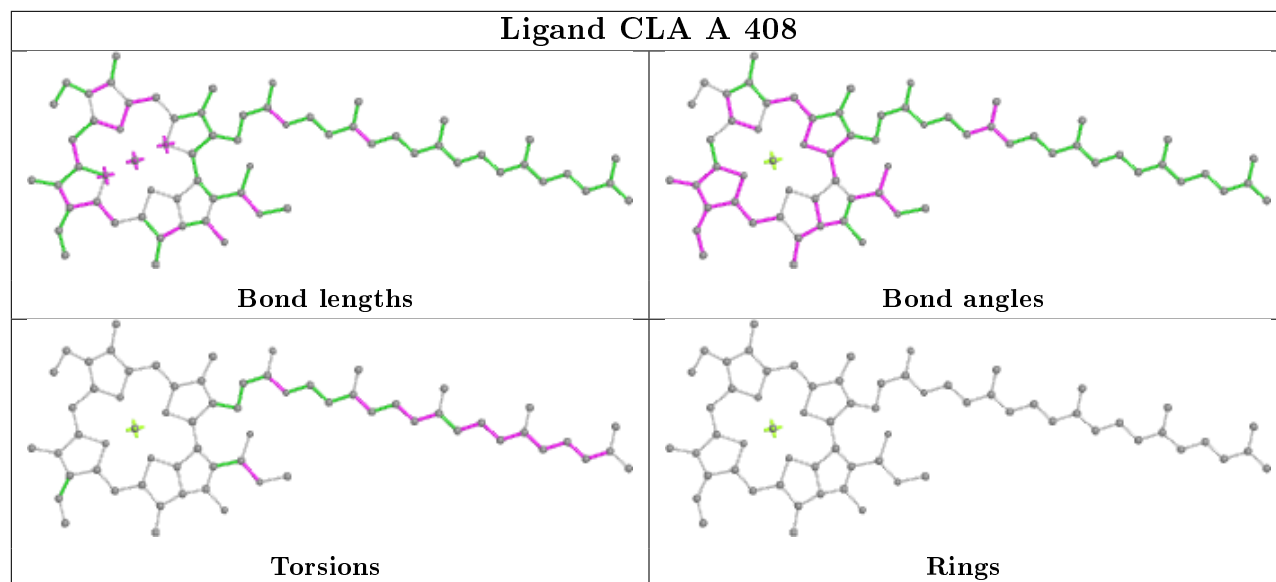
Ligand DGD d 408



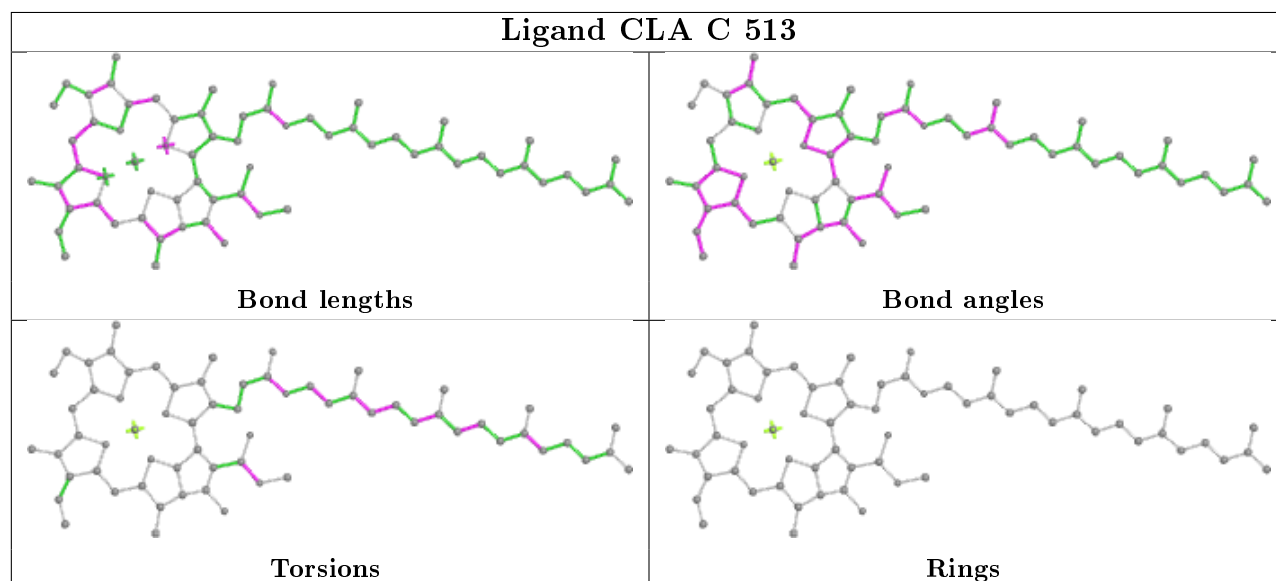




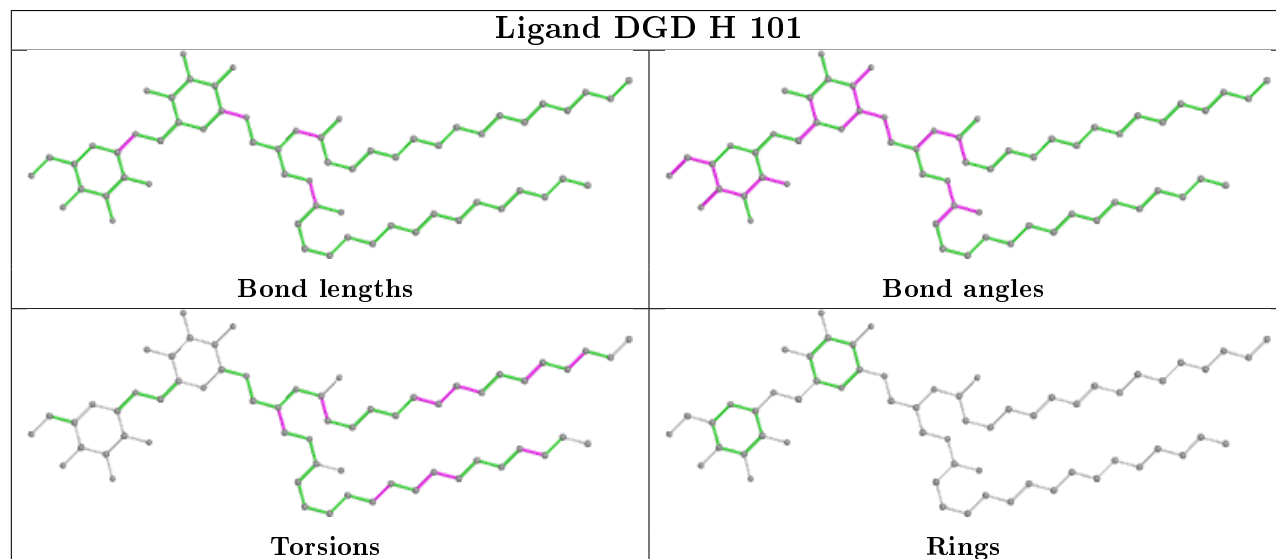
Ligand CLA A 408

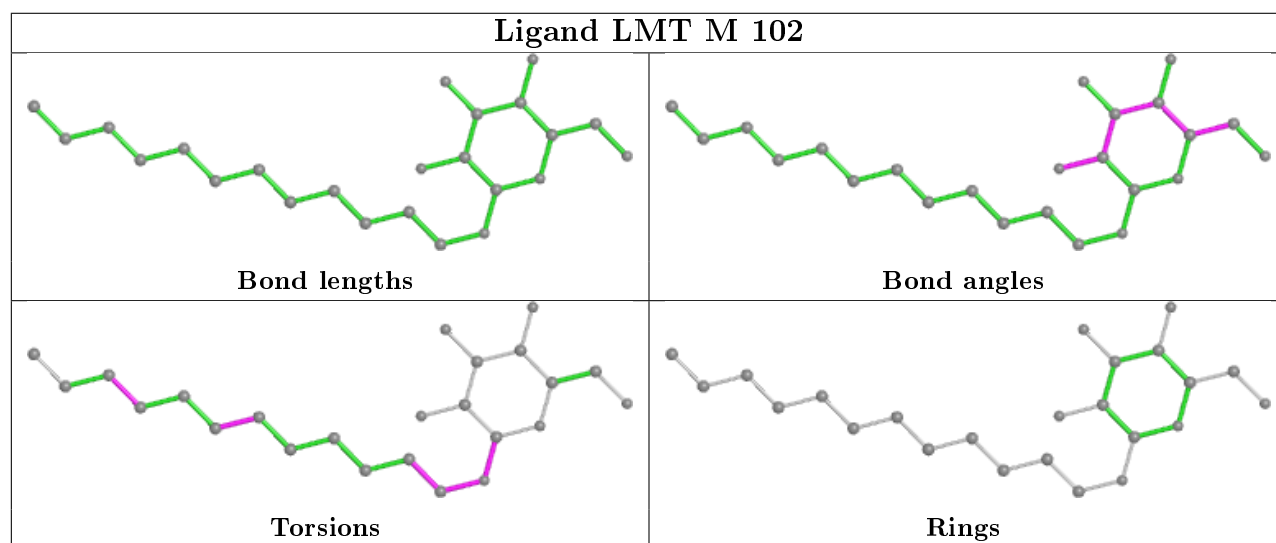
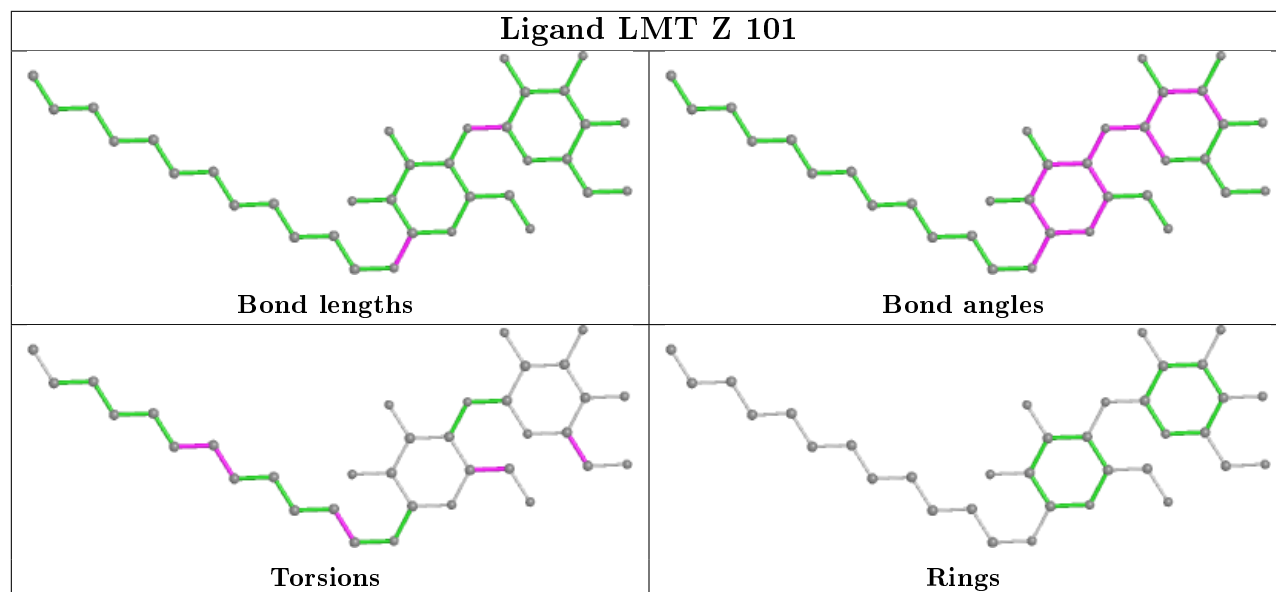
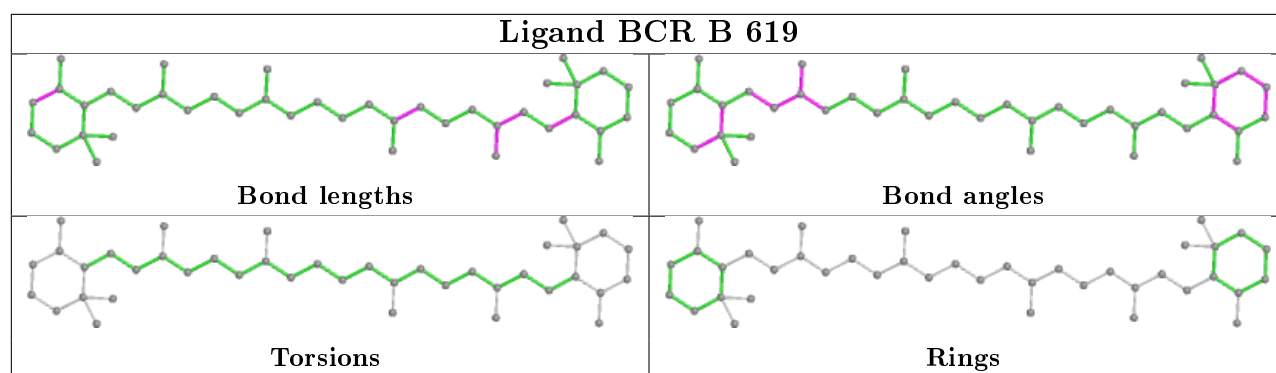


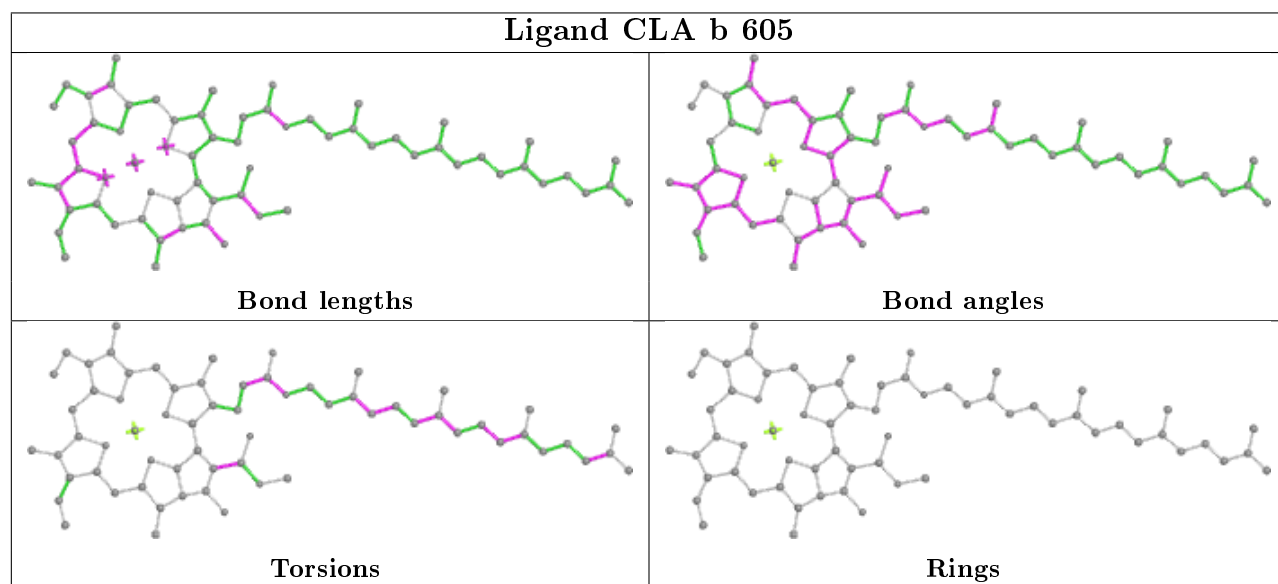
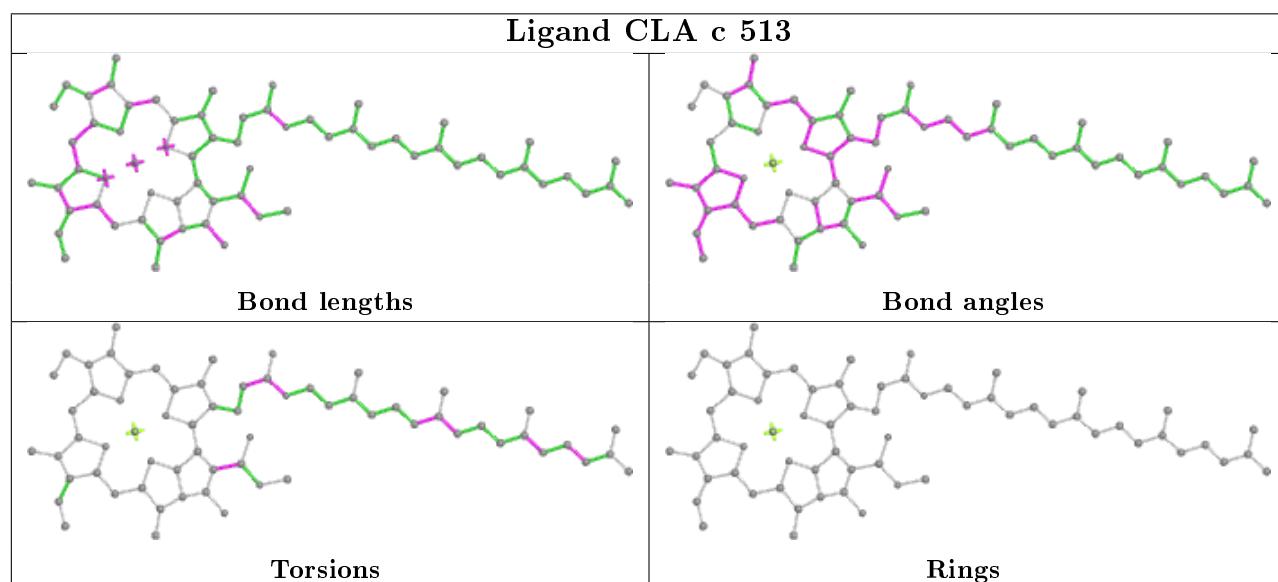
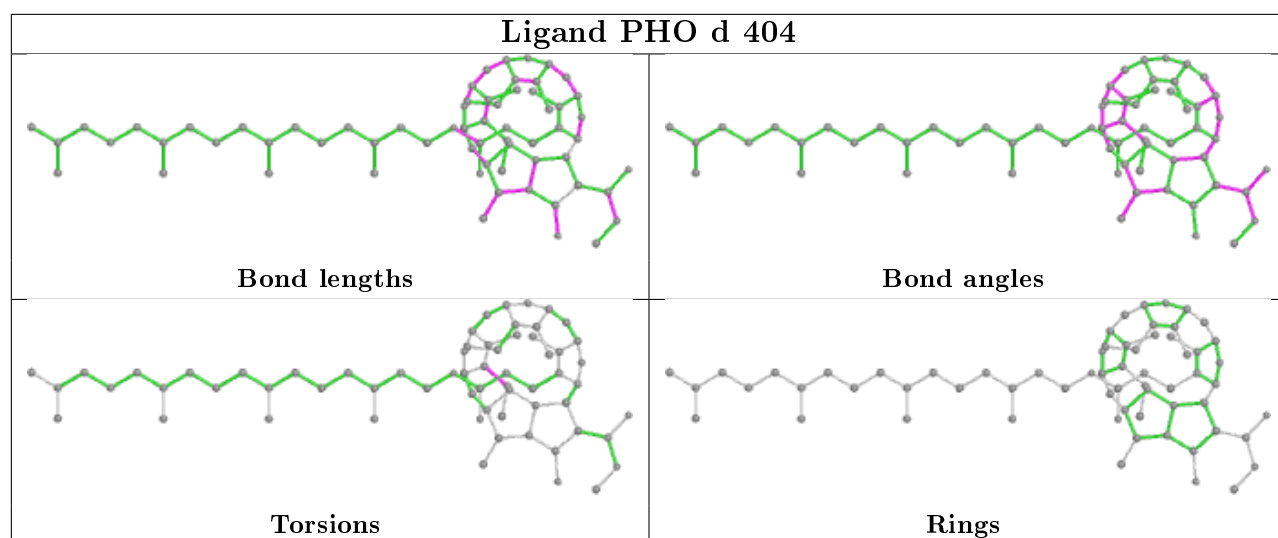
Ligand CLA C 513



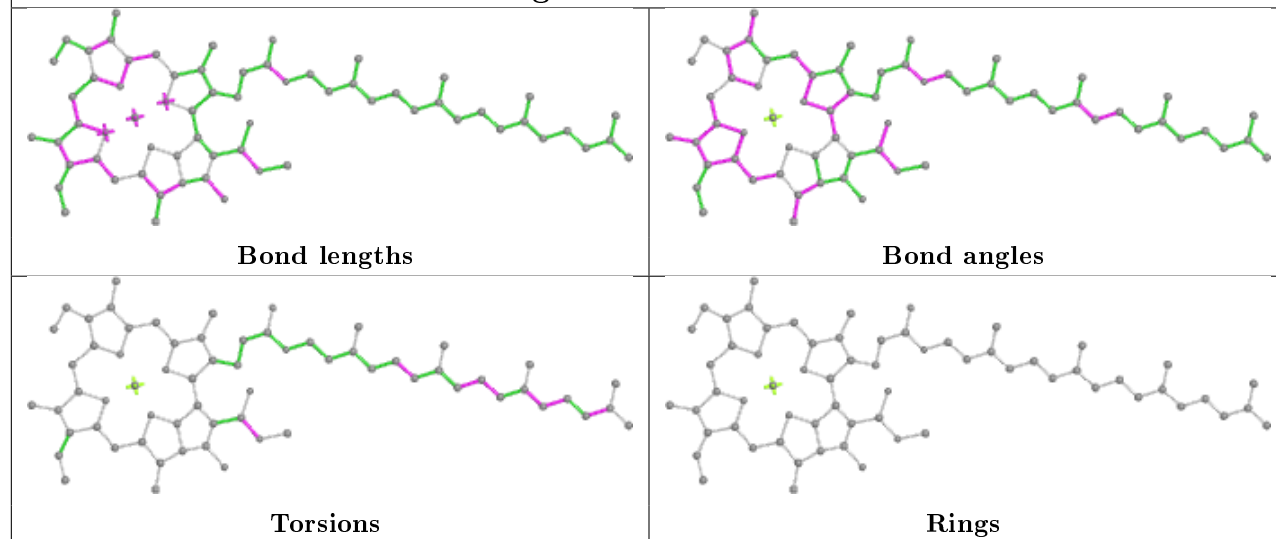
Ligand DGD H 101



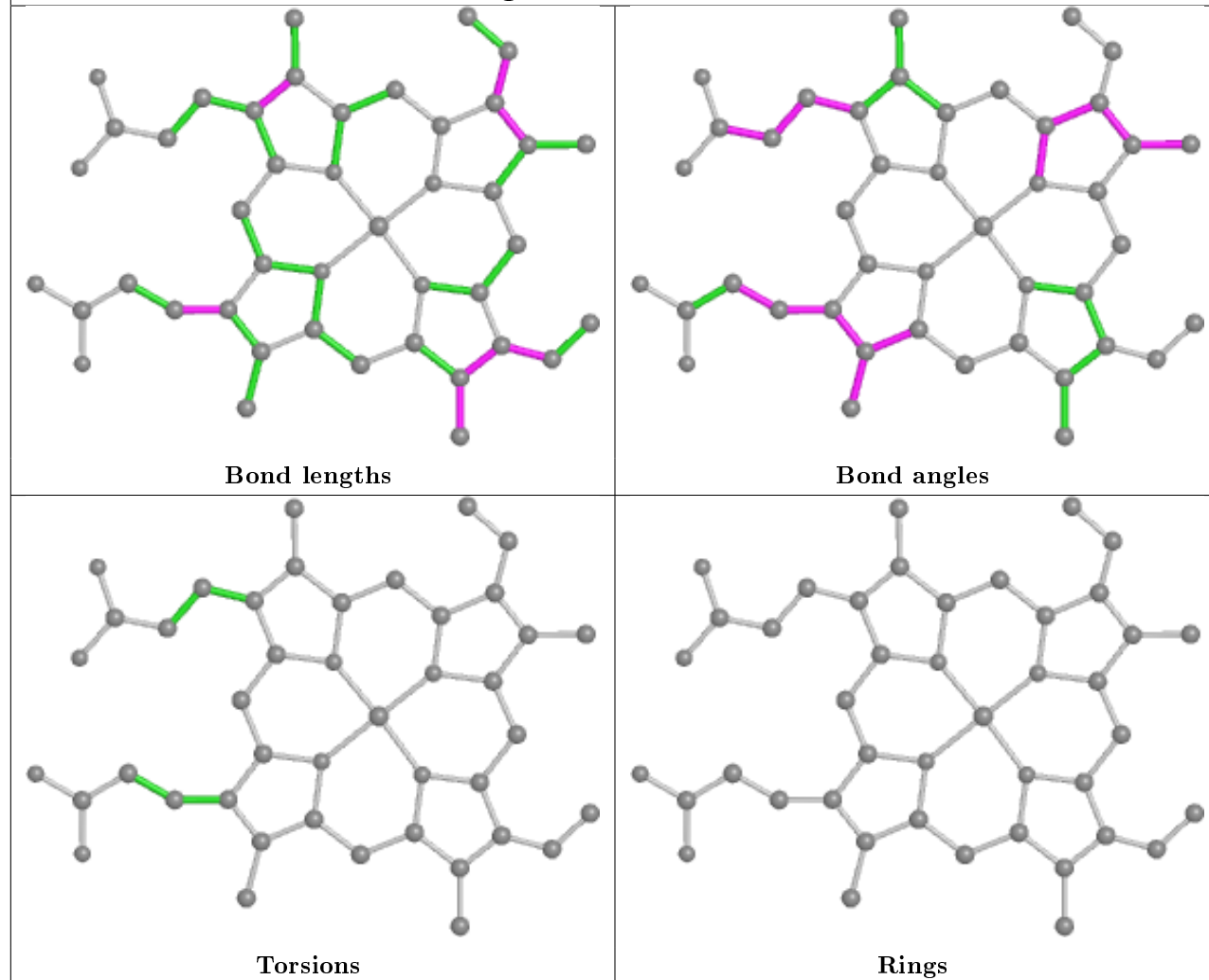




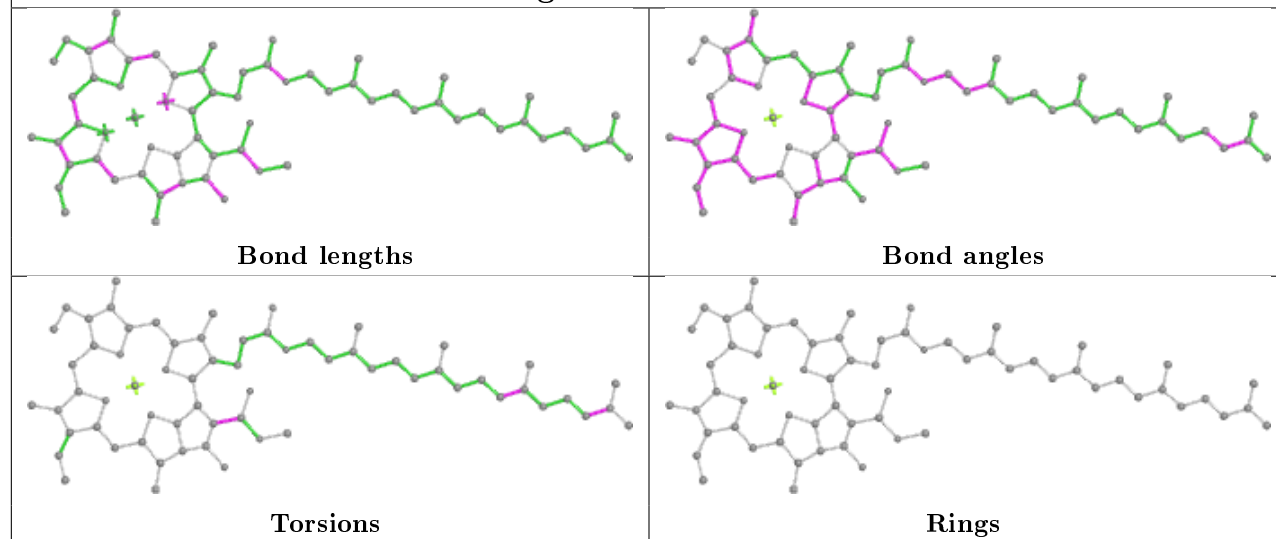
Ligand CLA B 616



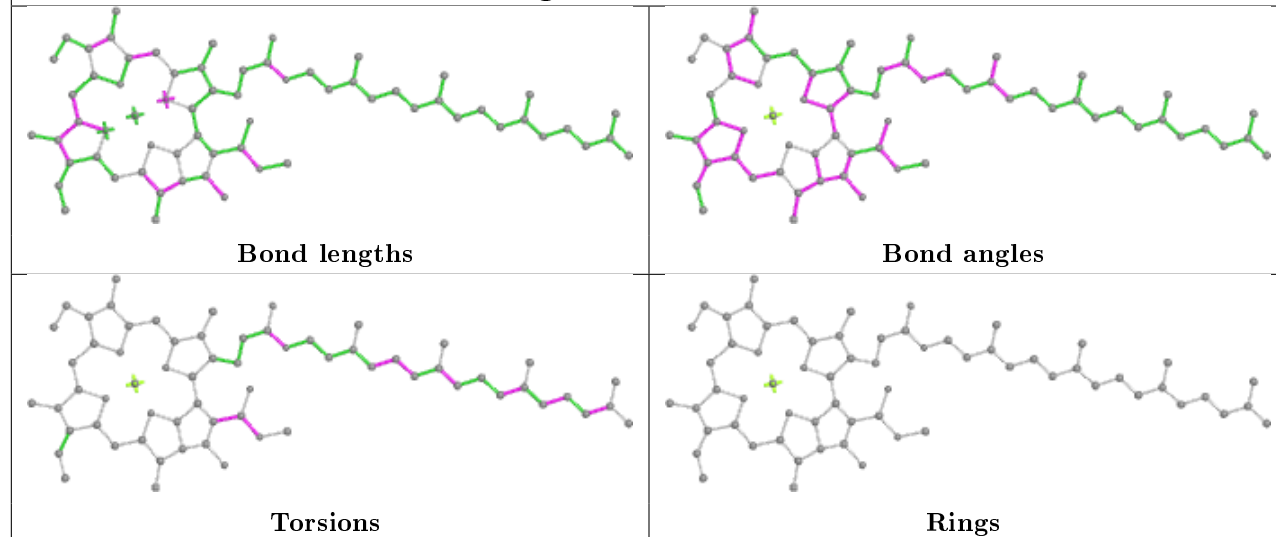
Ligand HEM F 101



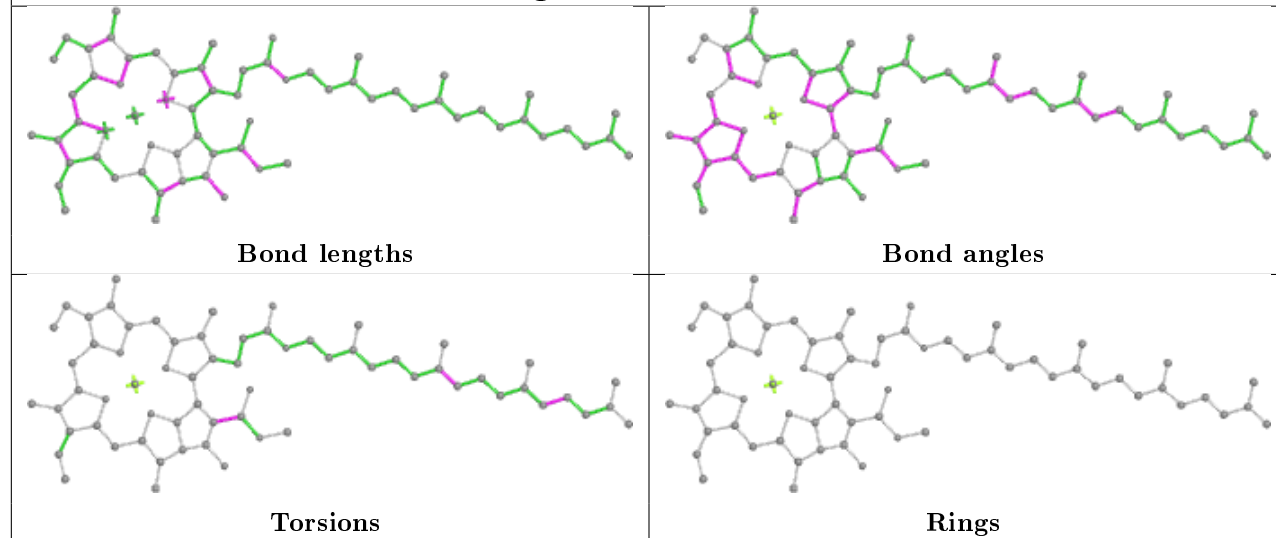
Ligand CLA c 503

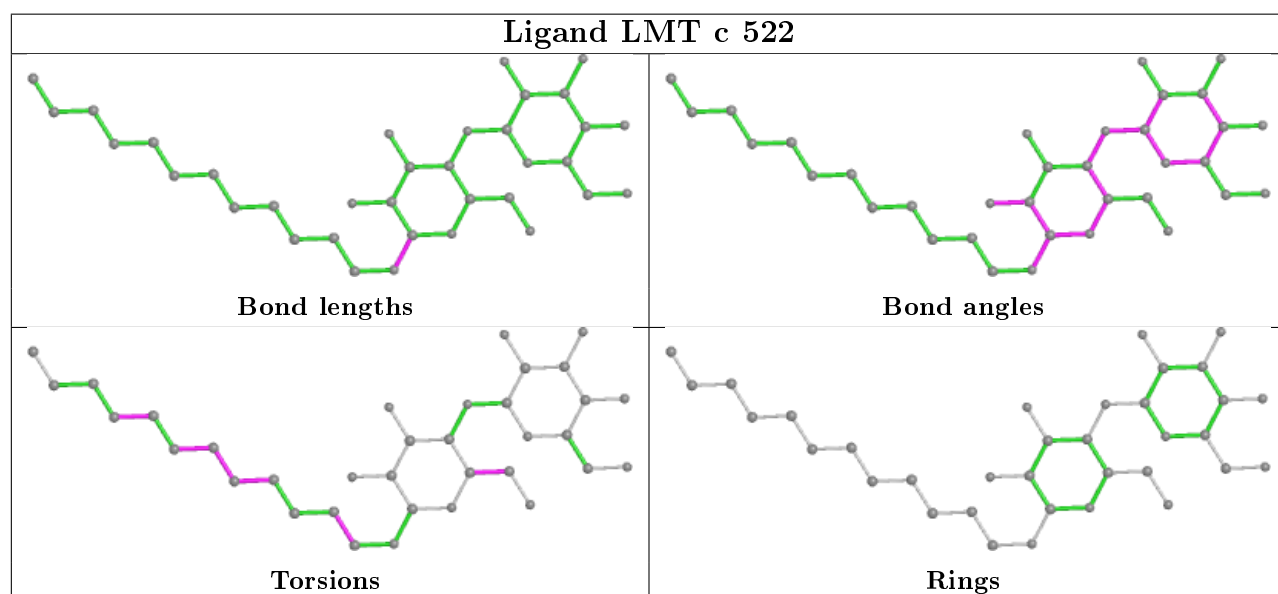
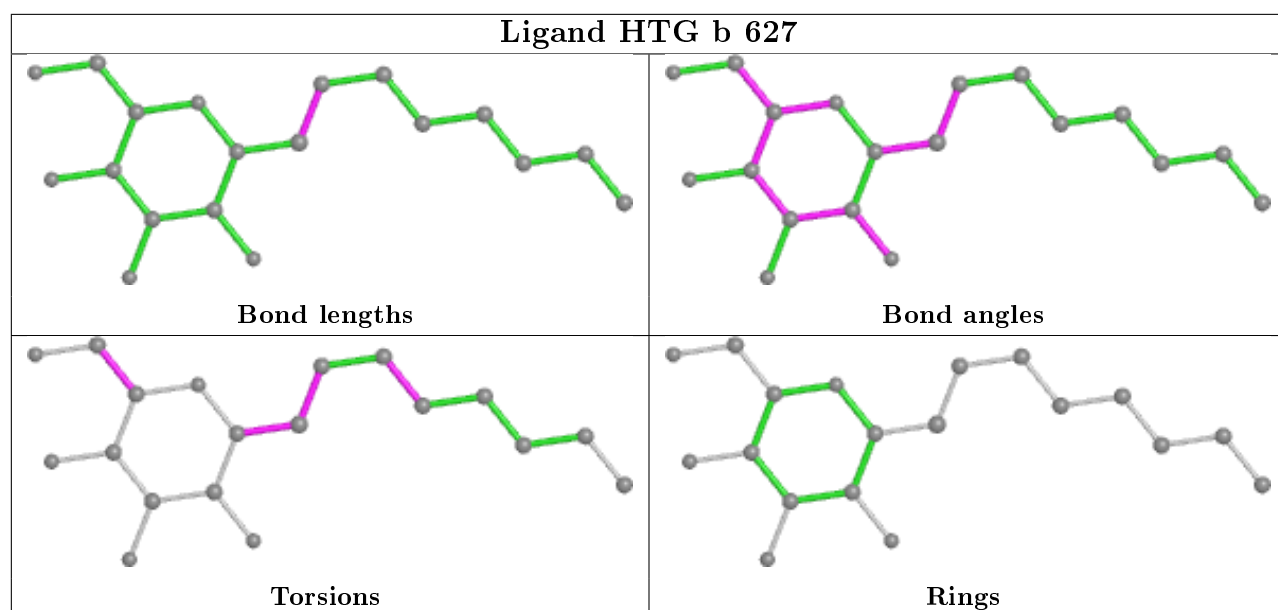


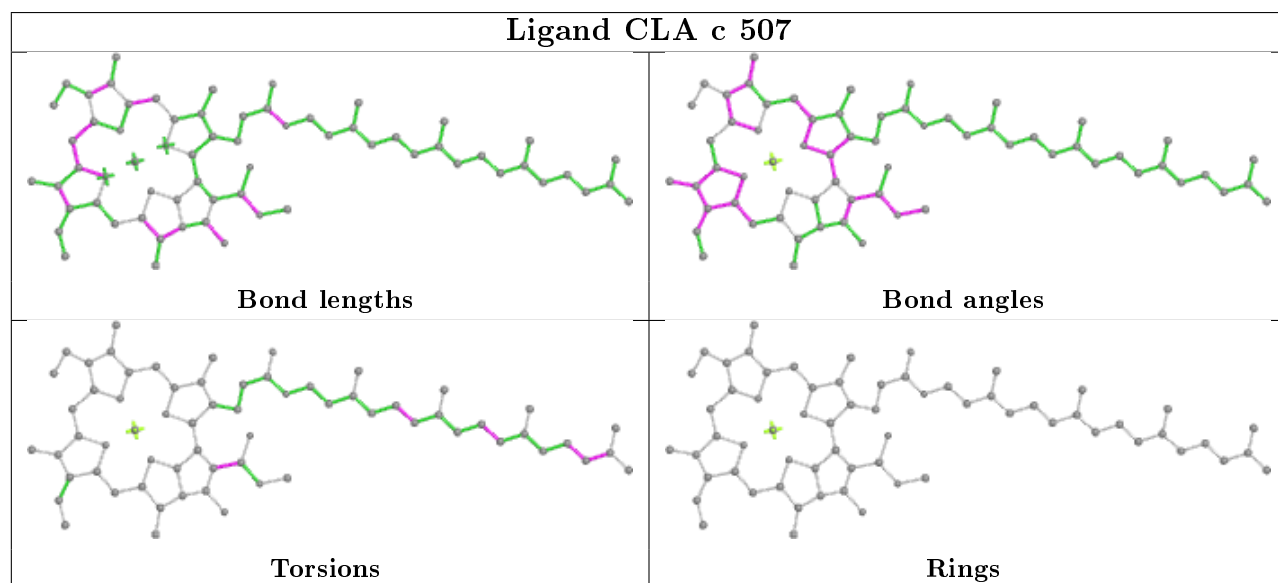
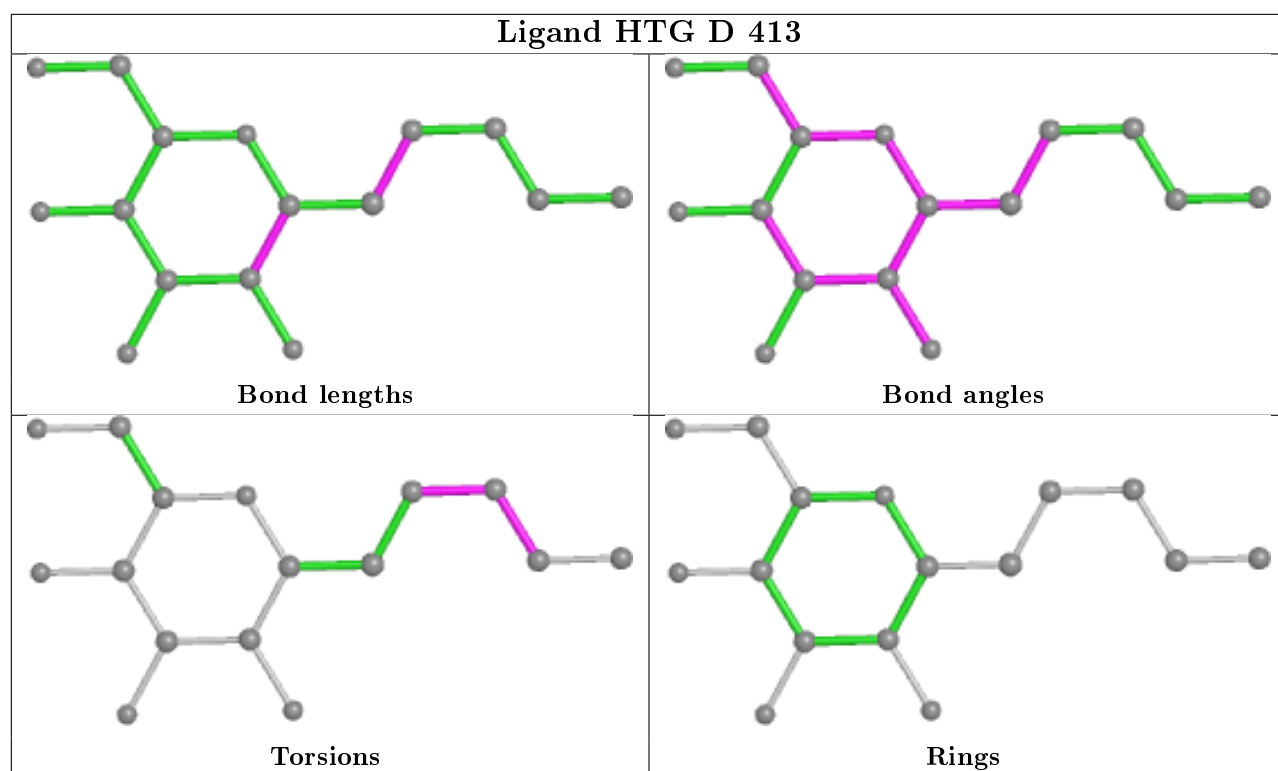
Ligand CLA c 514

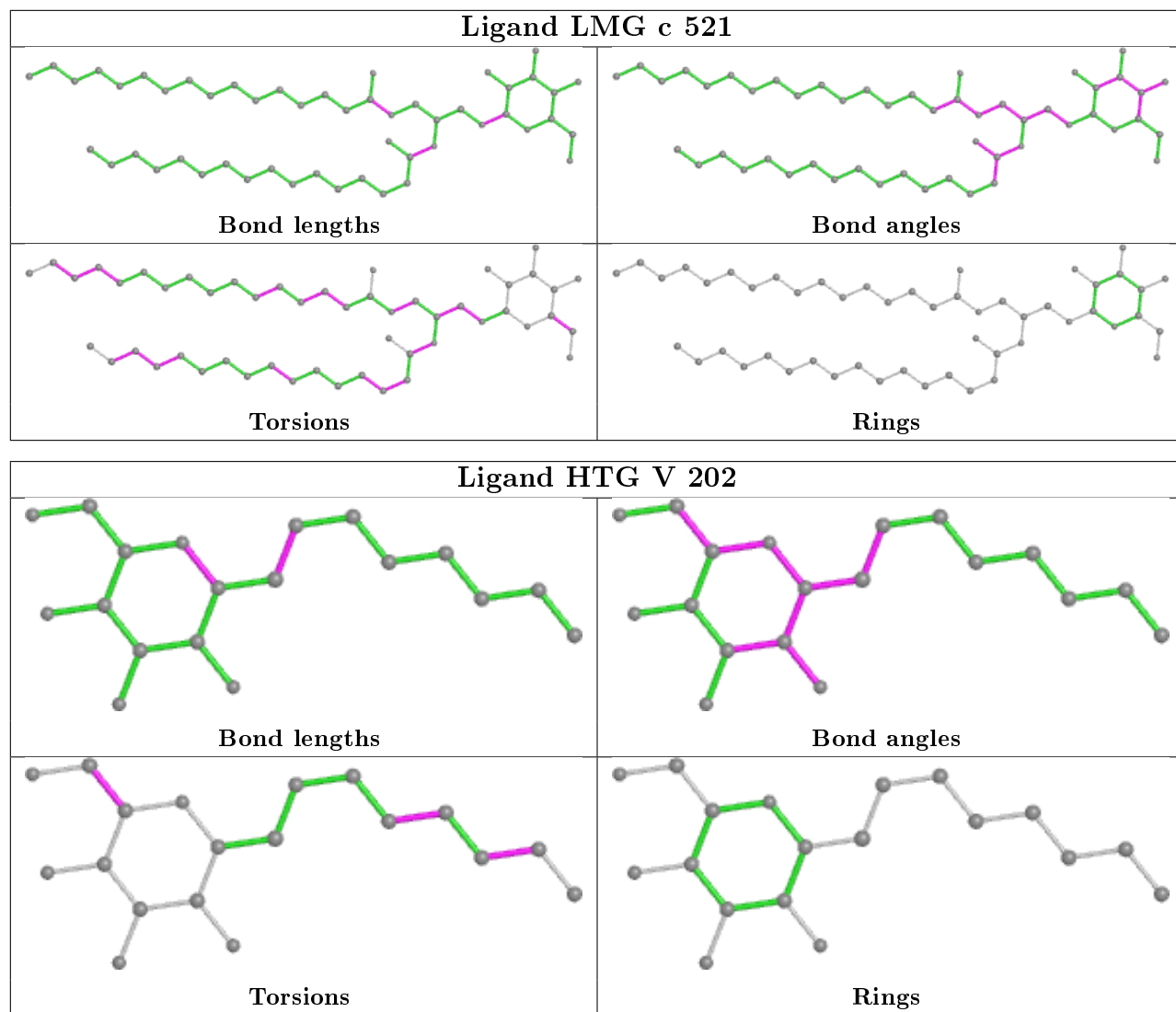


Ligand CLA A 406

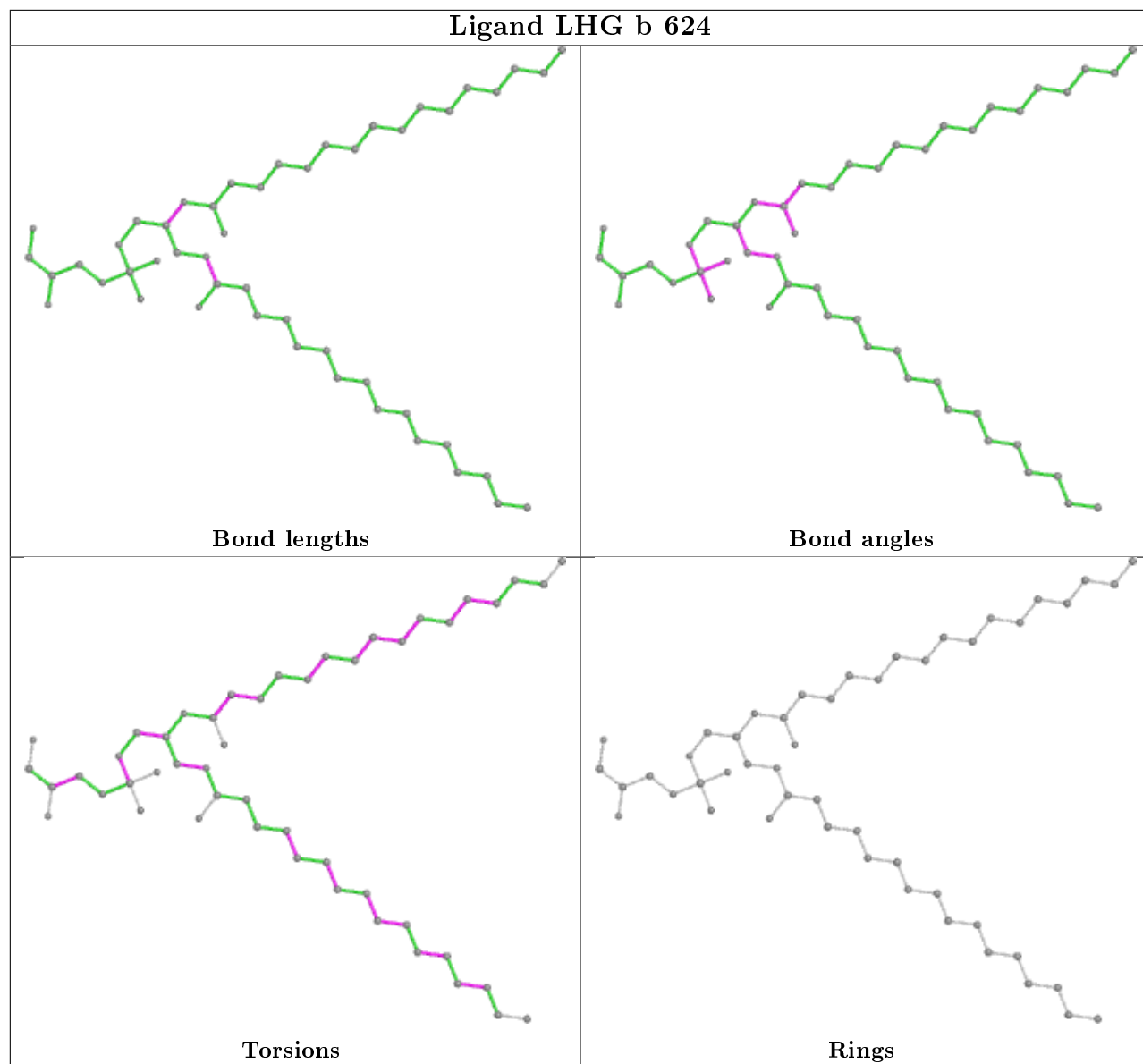




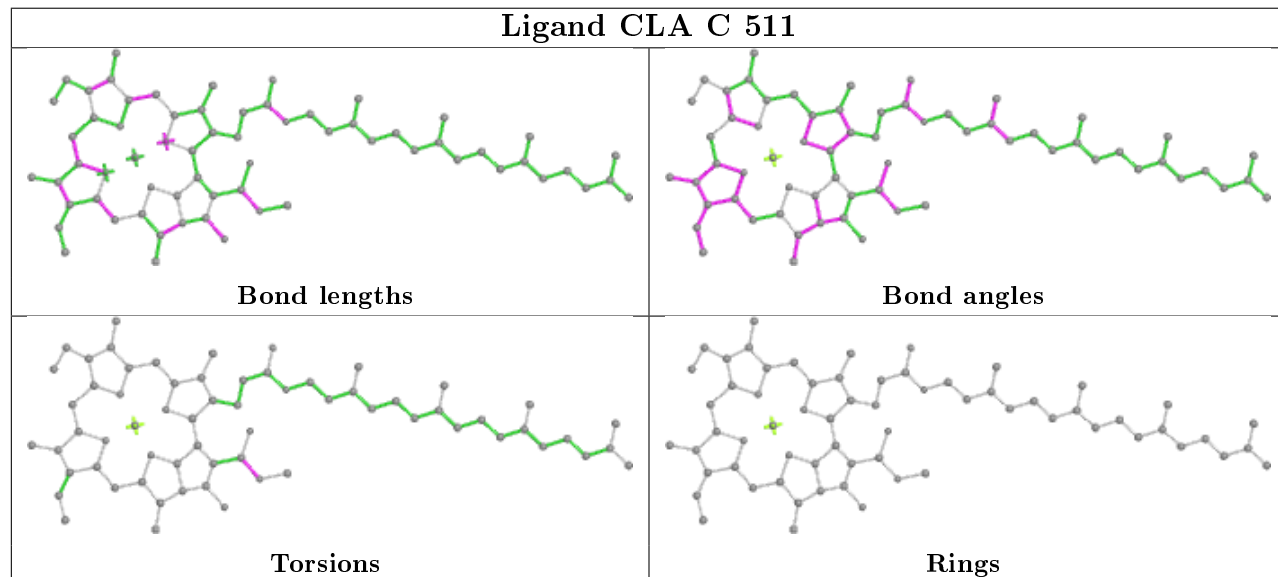


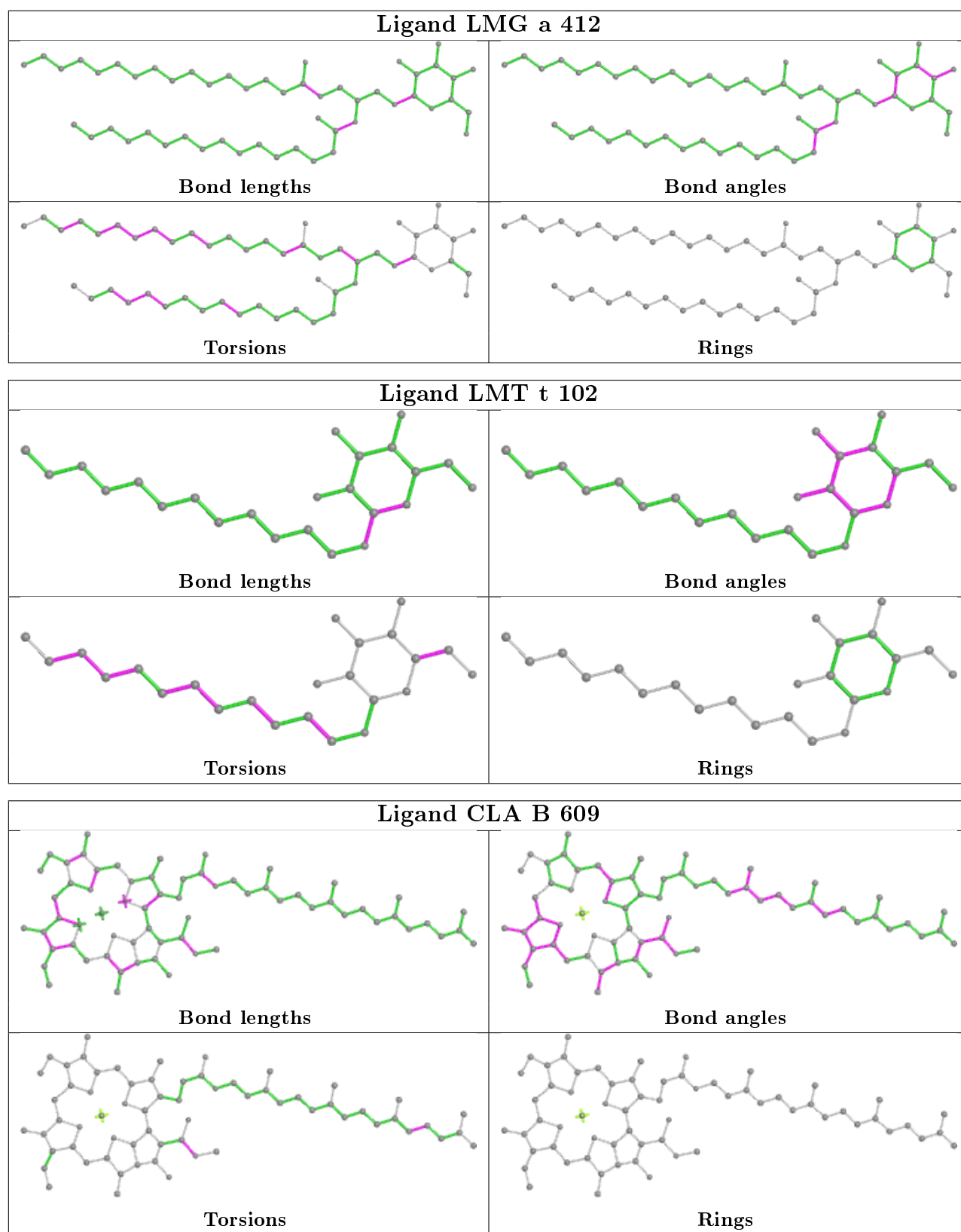


Ligand LHG b 624

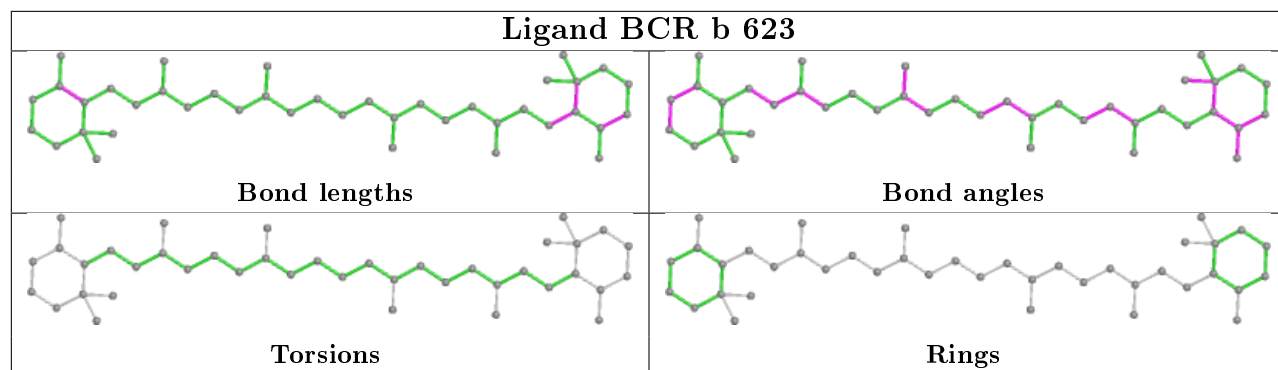


Ligand CLA C 511

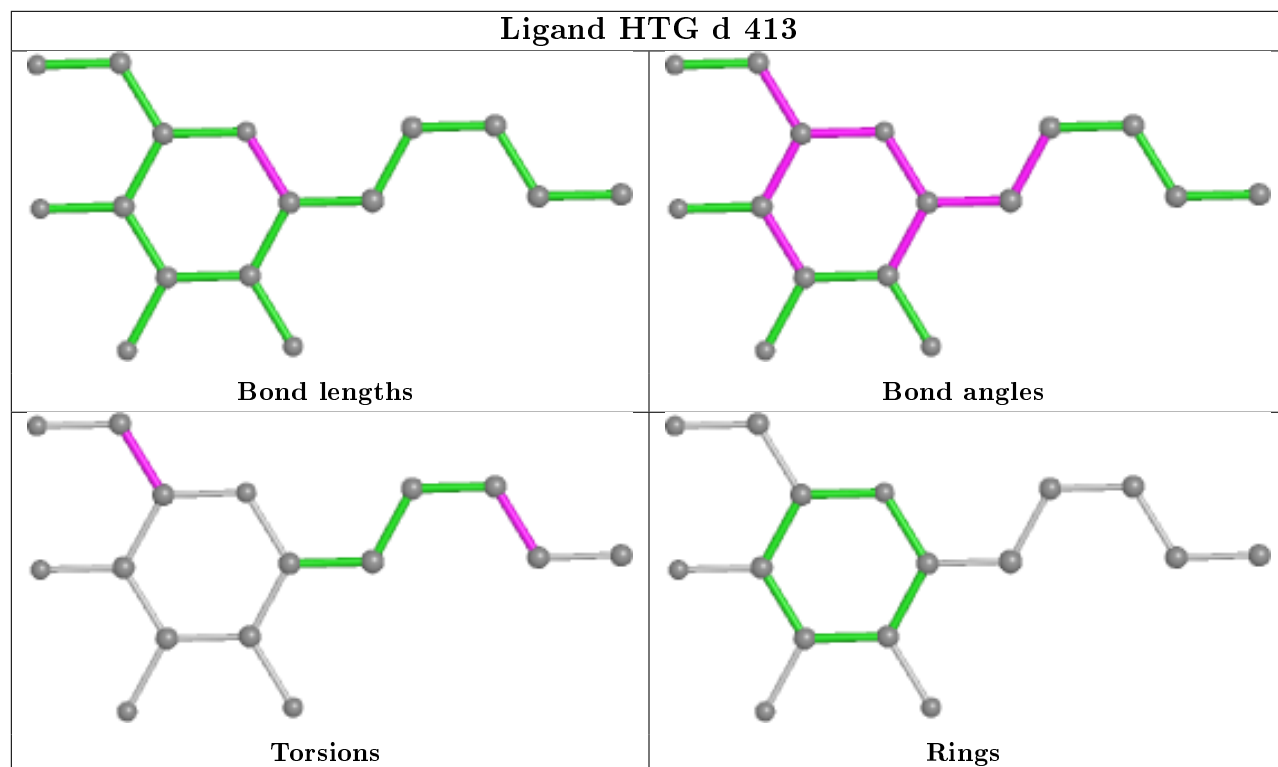




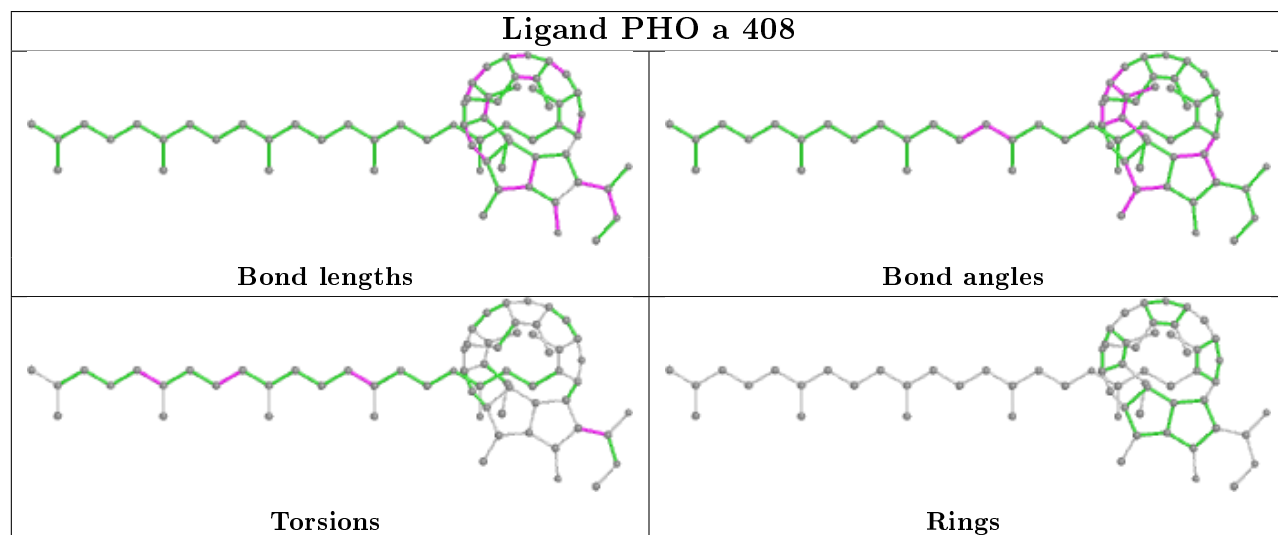
Ligand BCR b 623



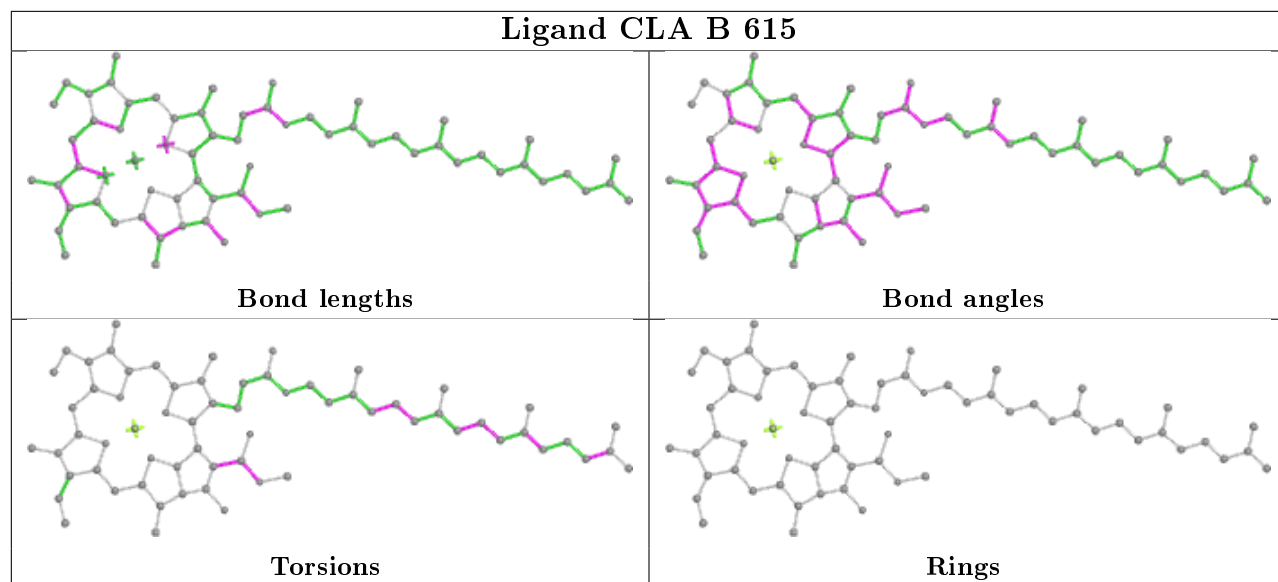
Ligand HTG d 413



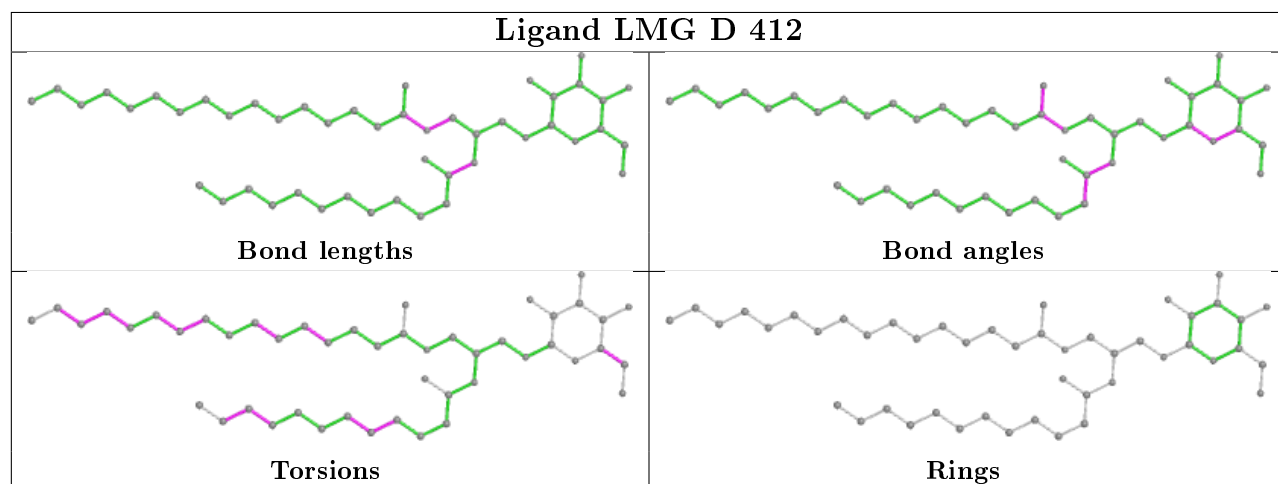
Ligand PHO a 408



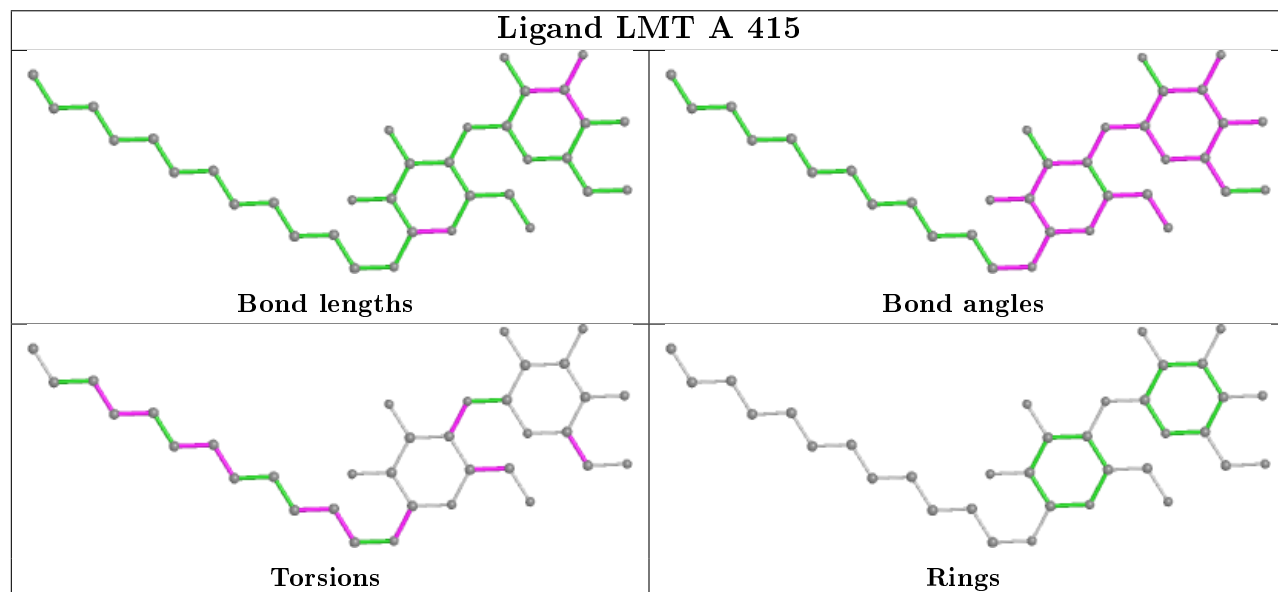
Ligand CLA B 615



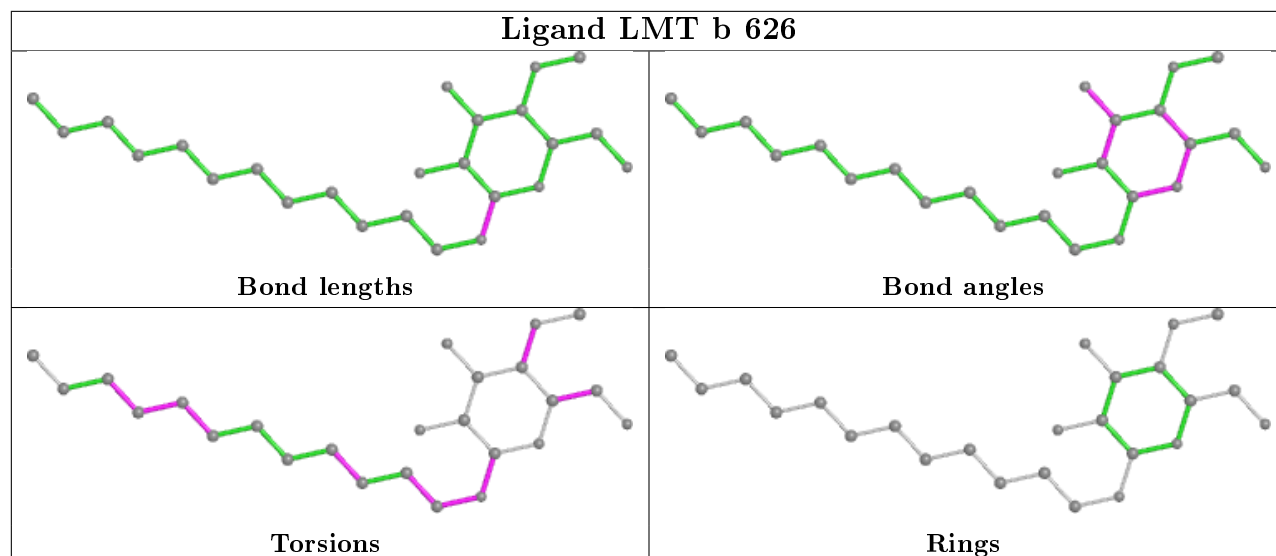
Ligand LMG D 412



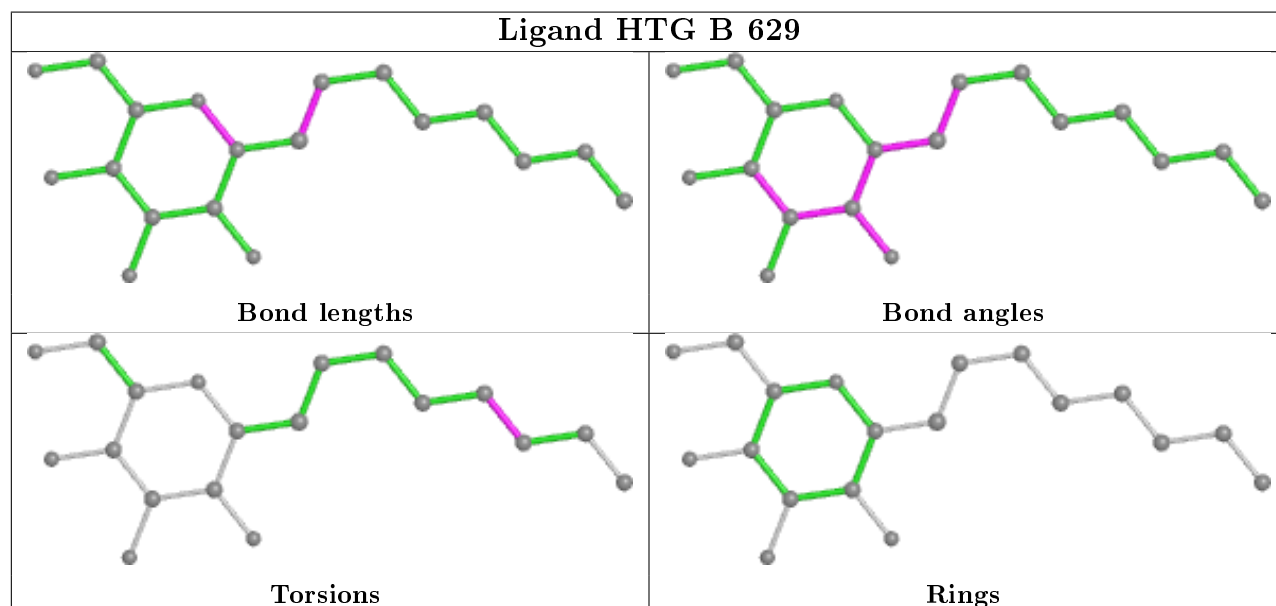
Ligand LMT A 415



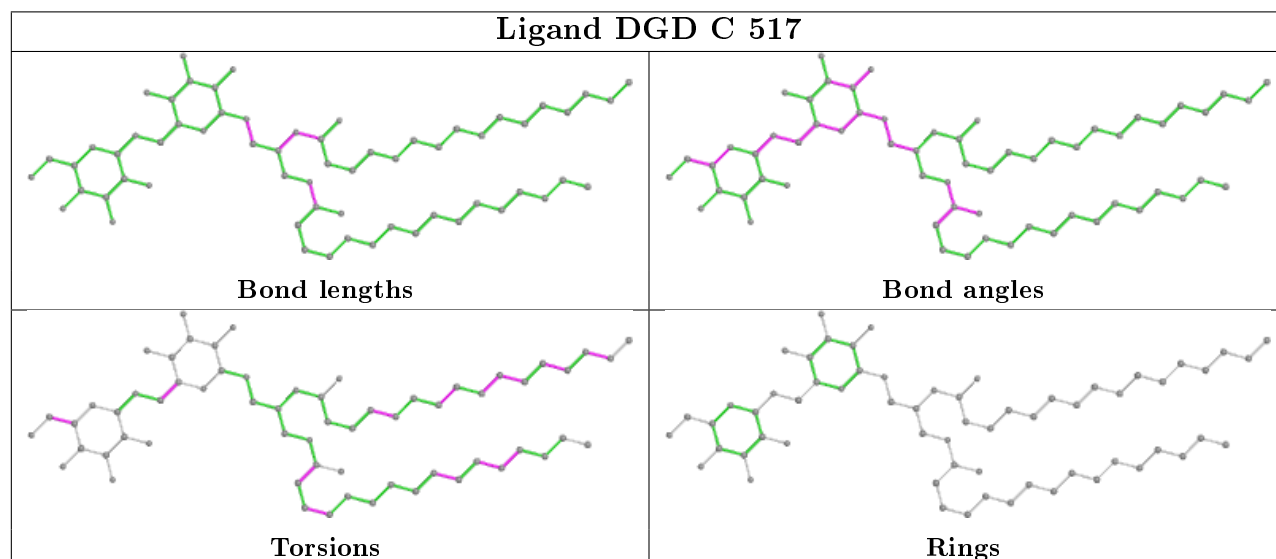
Ligand LMT b 626



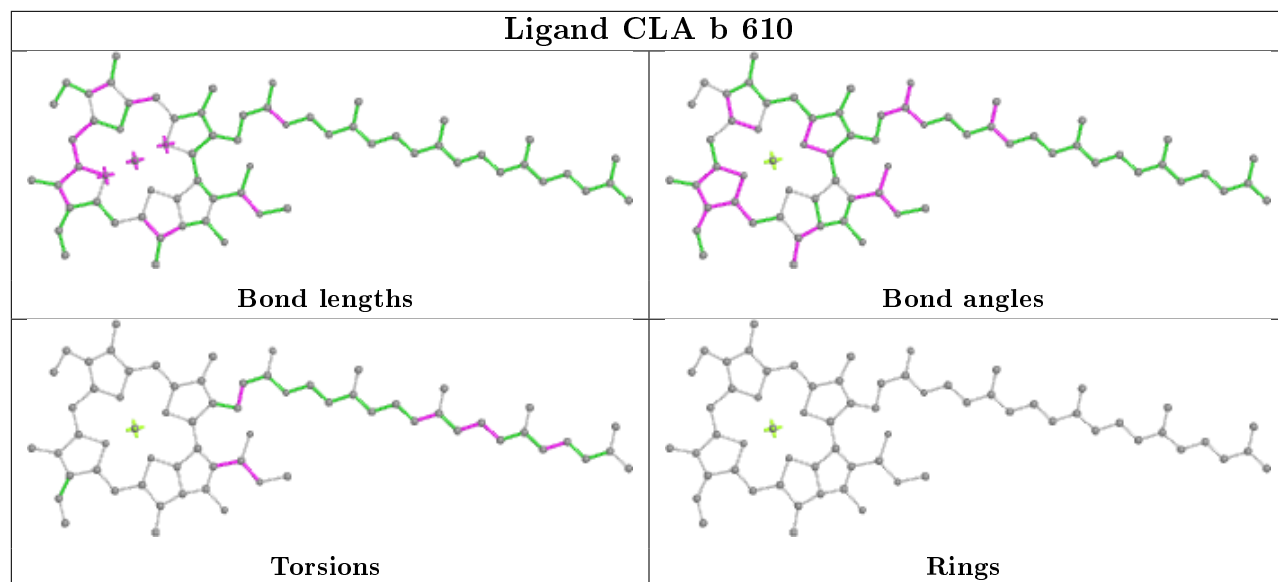
Ligand HTG B 629



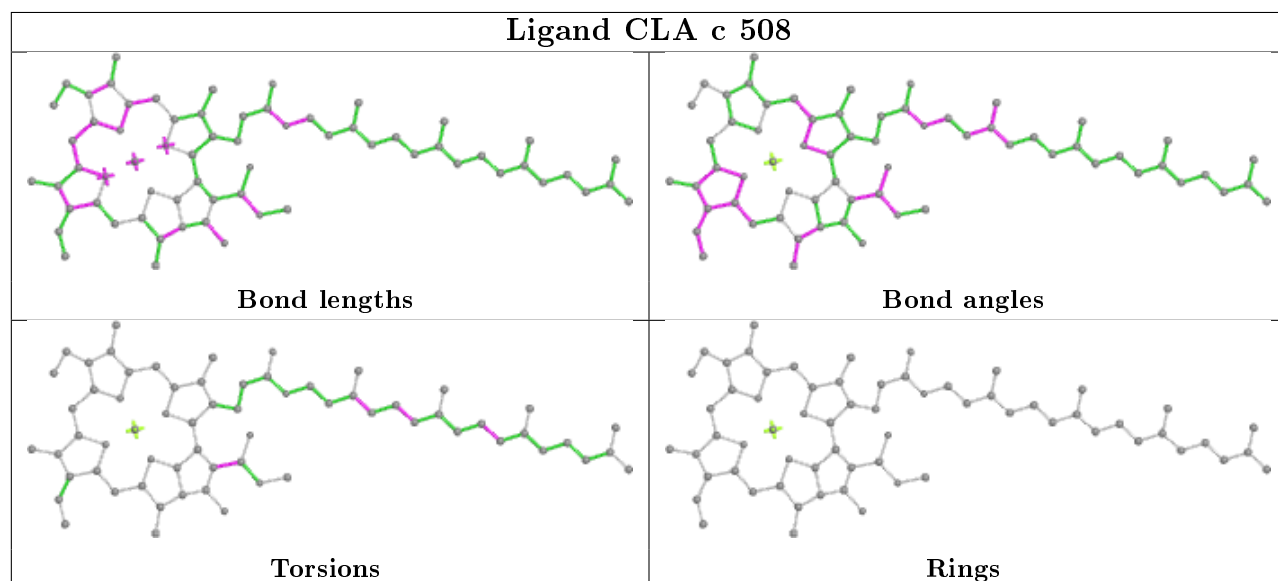
Ligand DGD C 517



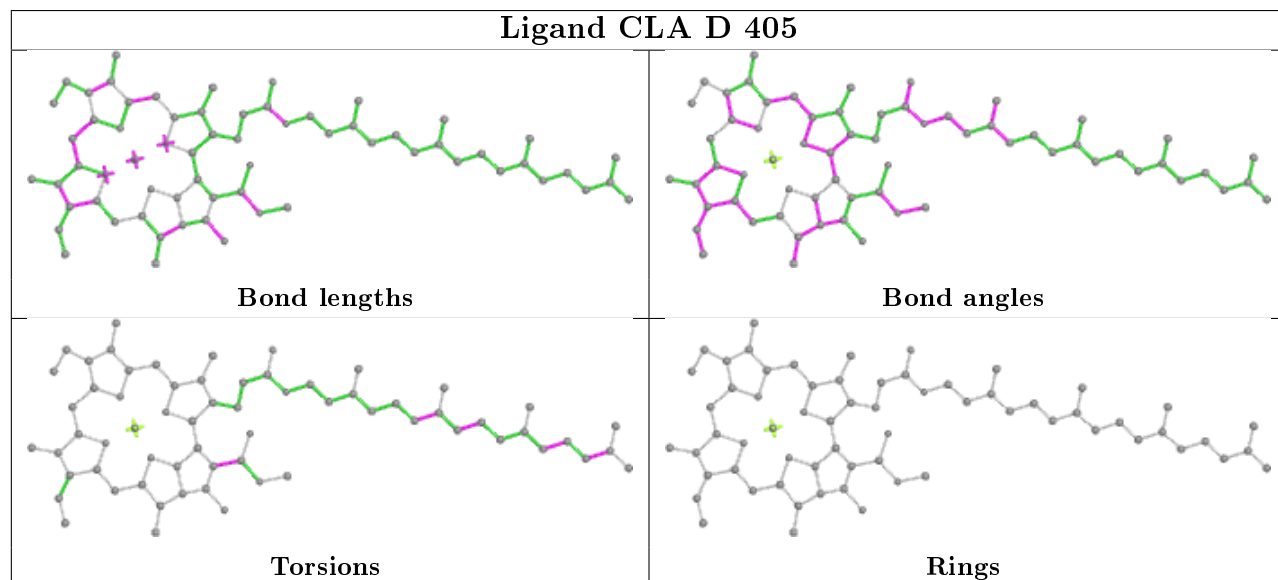
Ligand CLA b 610

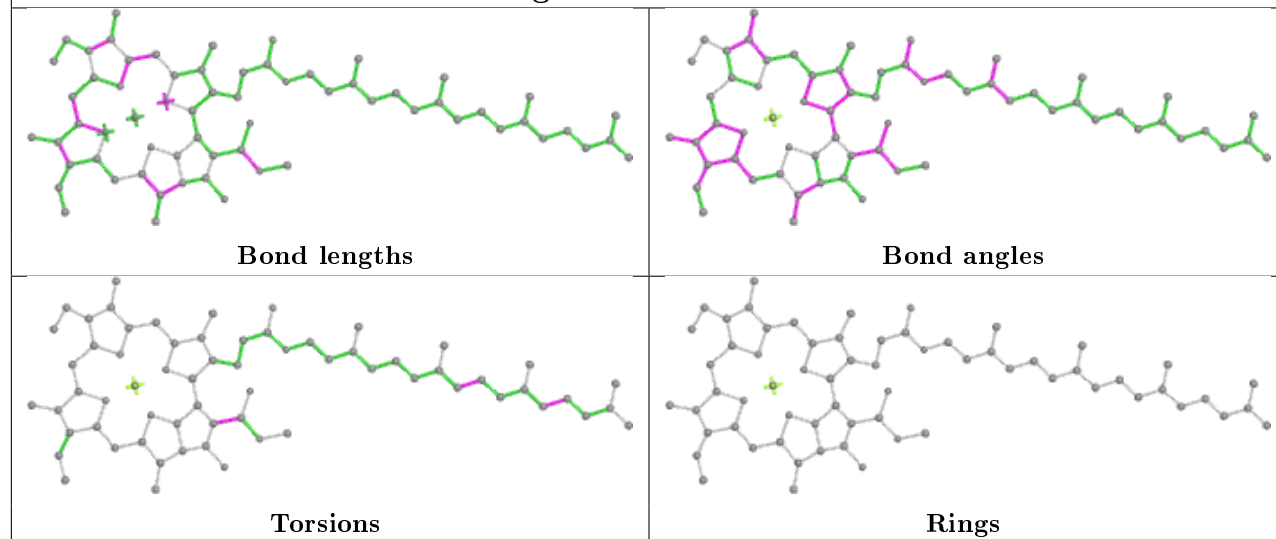
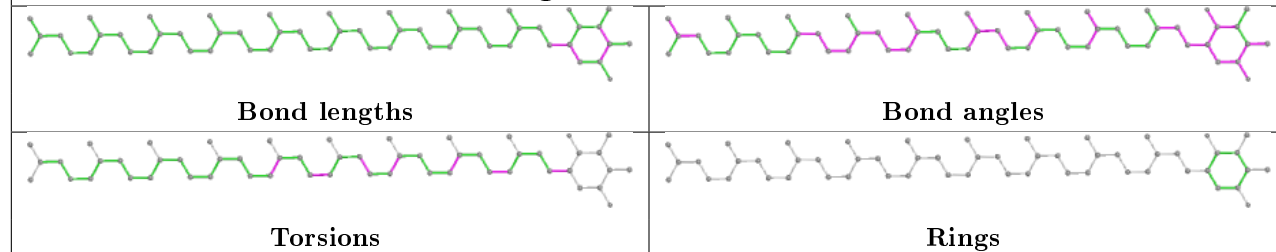
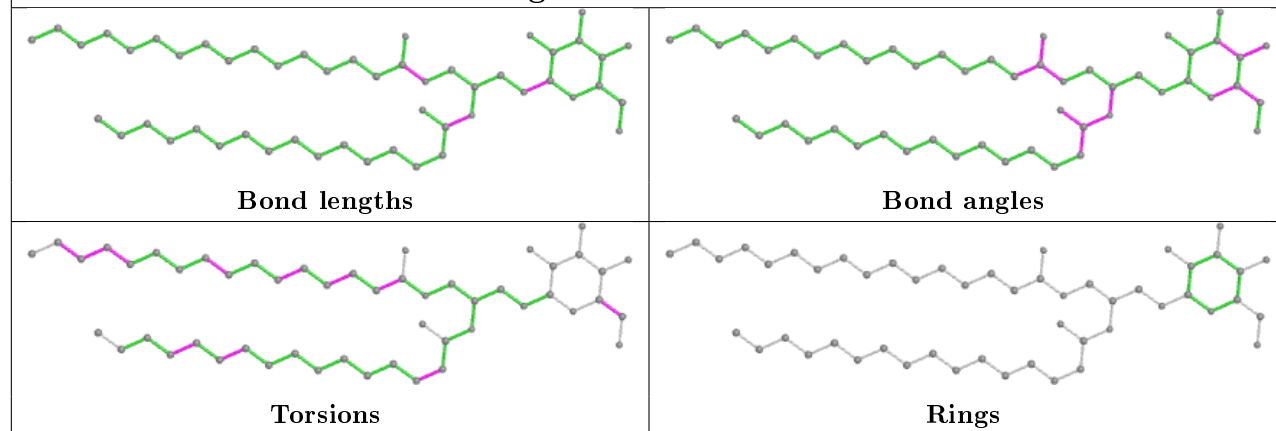


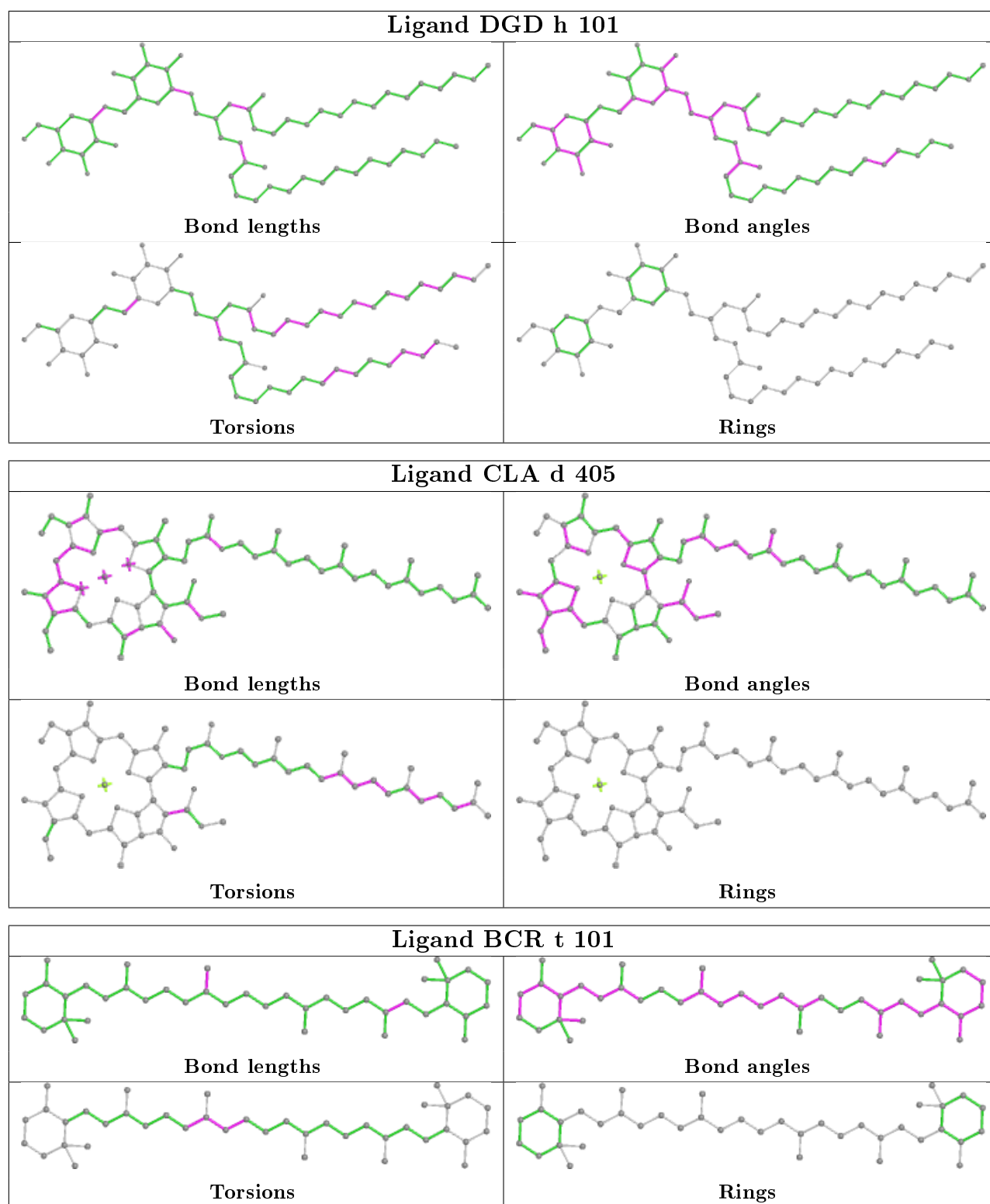
Ligand CLA c 508



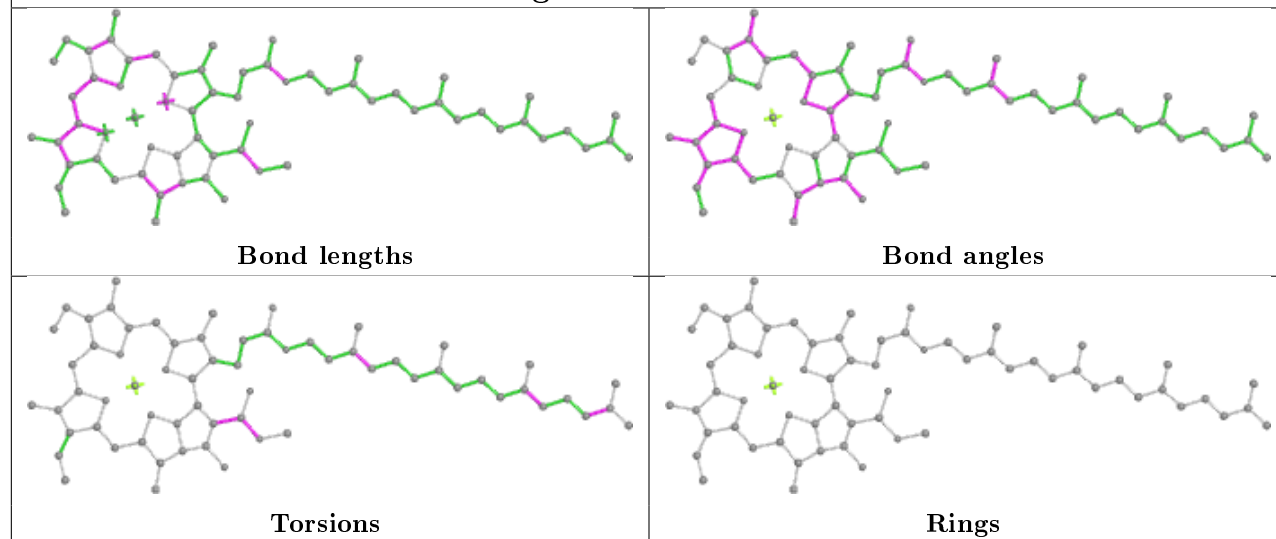
Ligand CLA D 405



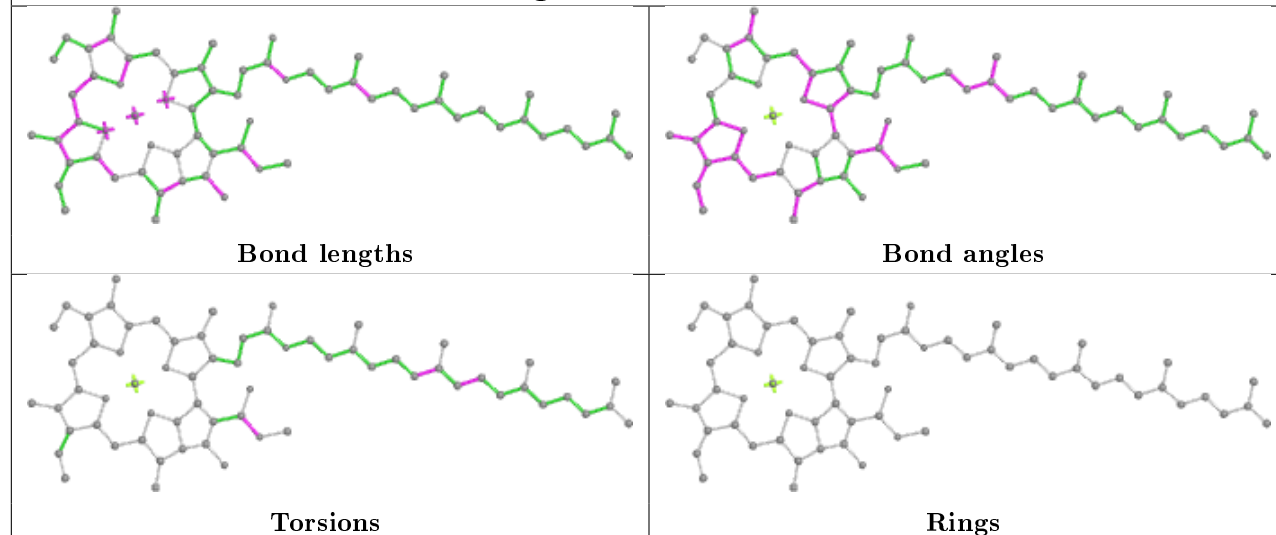
Ligand CLA B 613**Ligand PL9 A 410****Ligand LMG B 622**



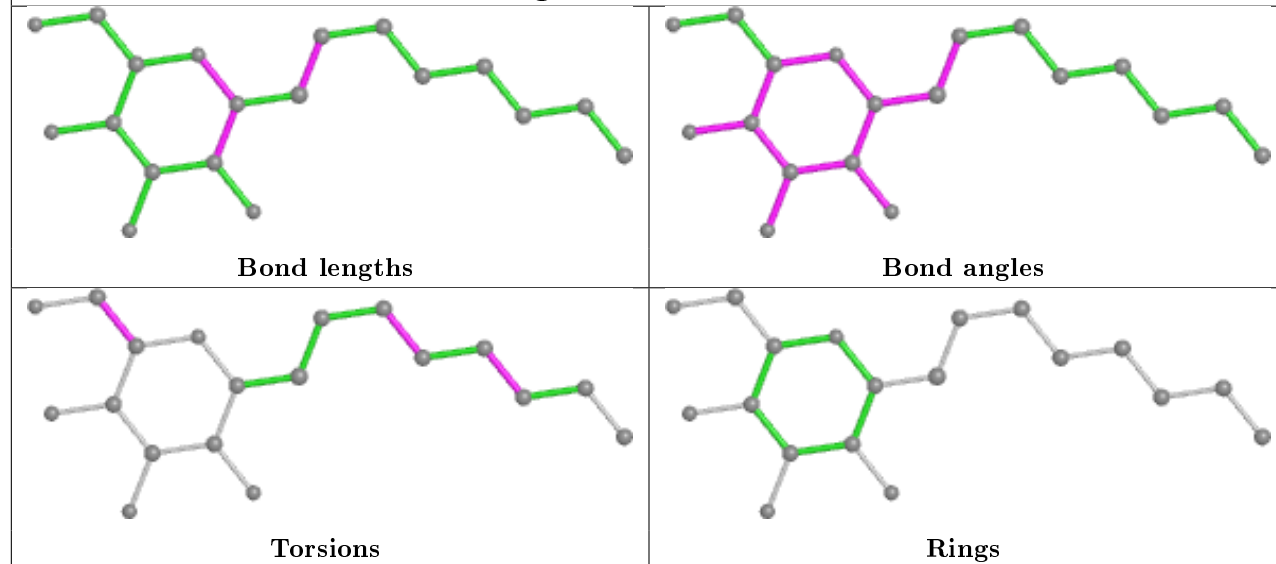
Ligand CLA B 606

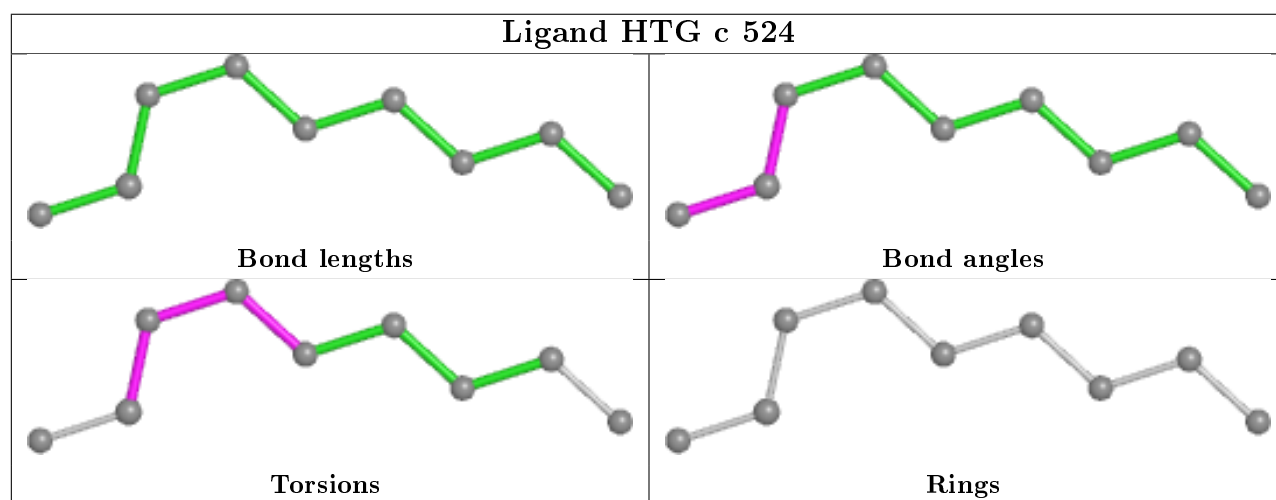
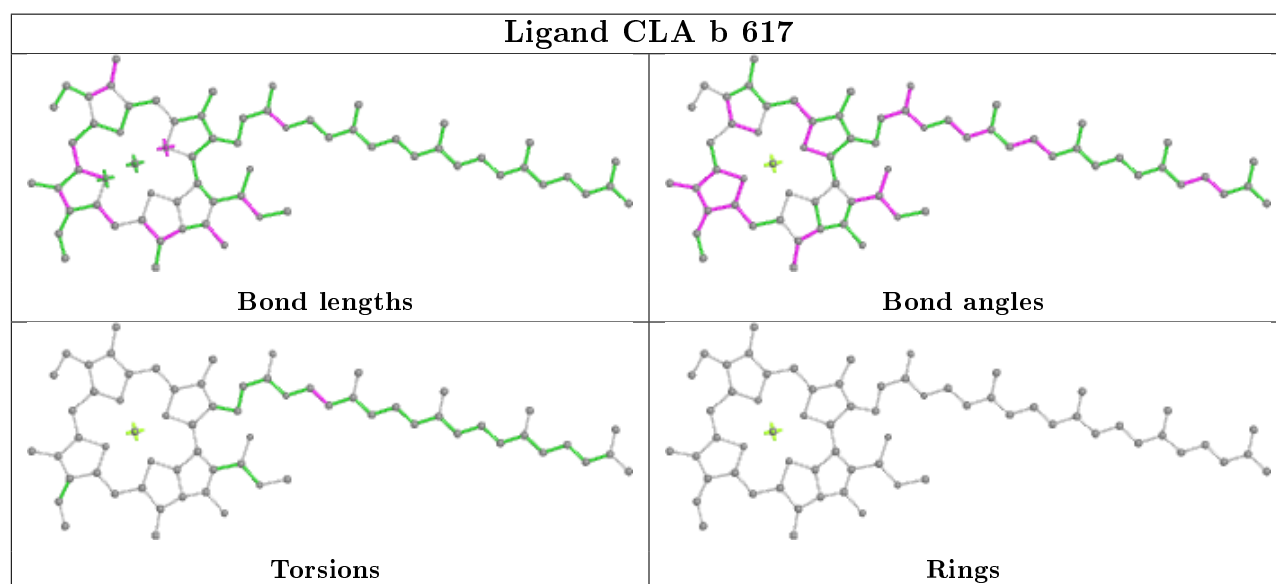
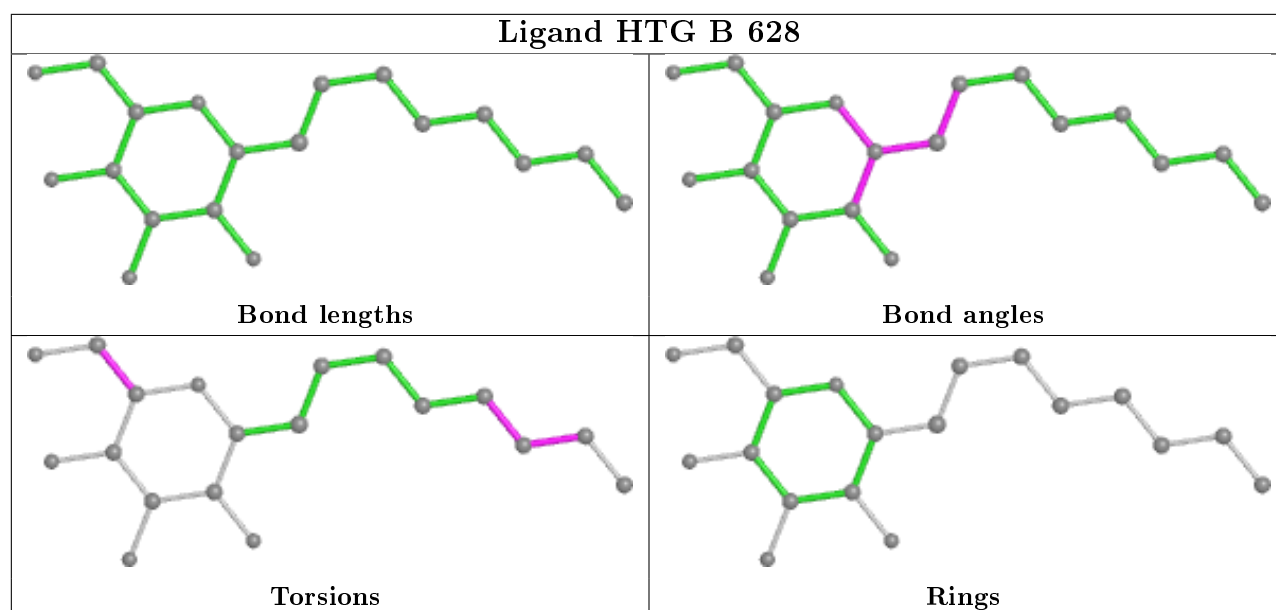


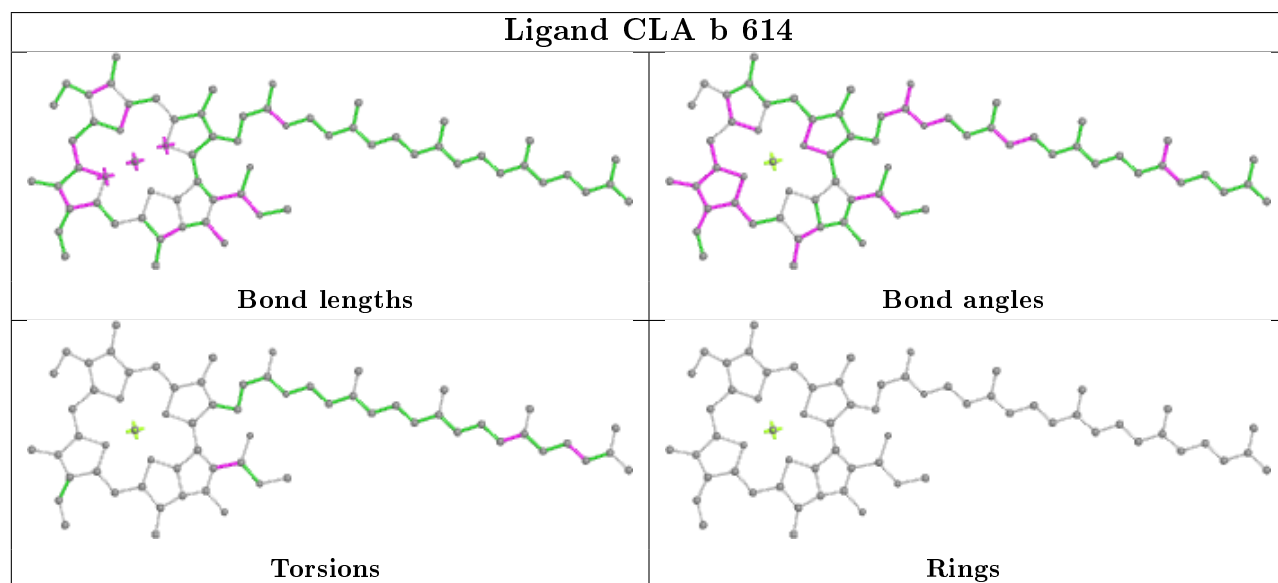
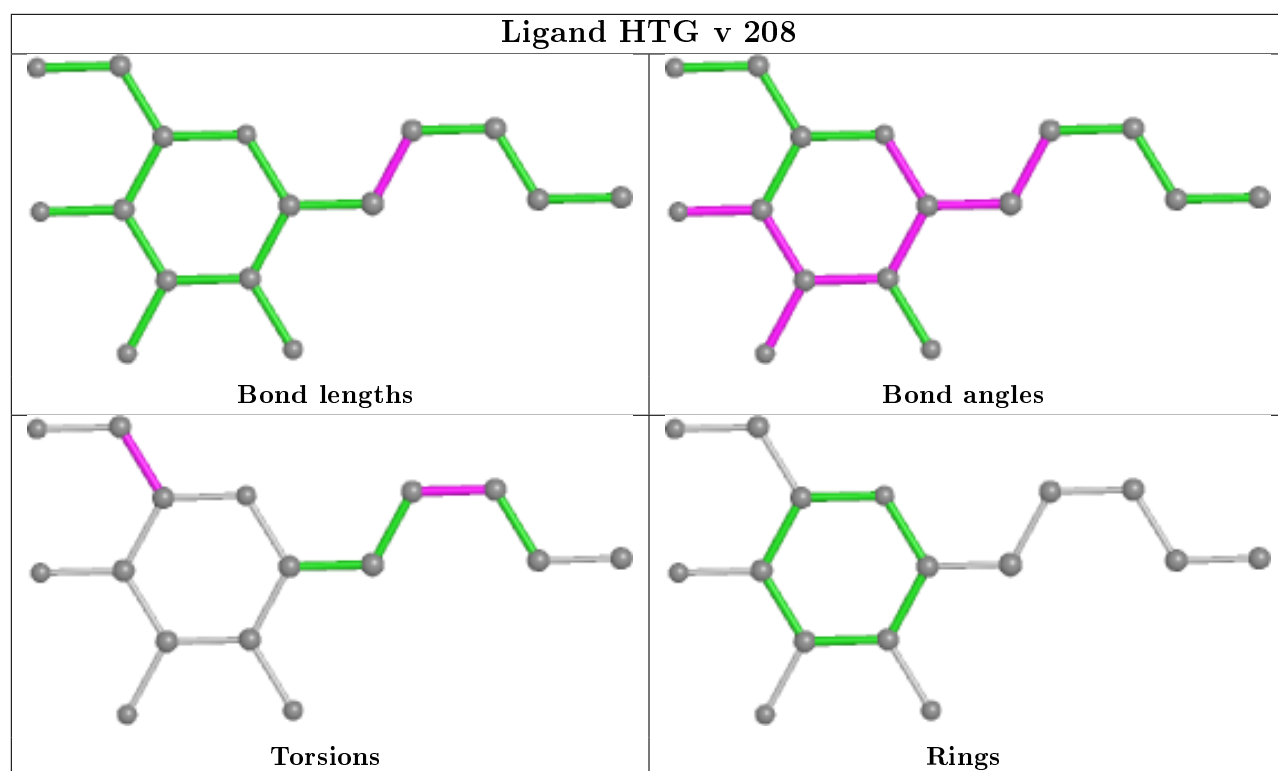
Ligand CLA C 503



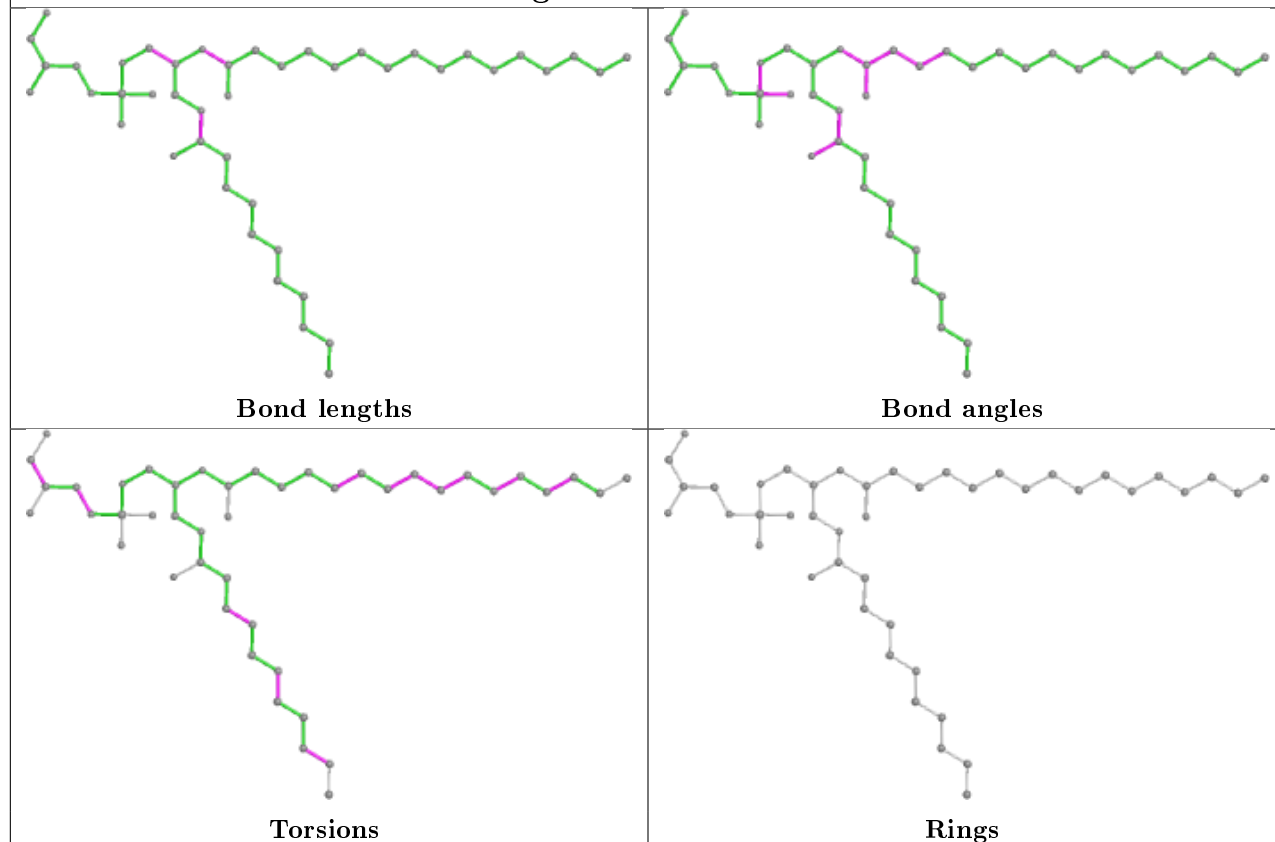
Ligand HTG o 301



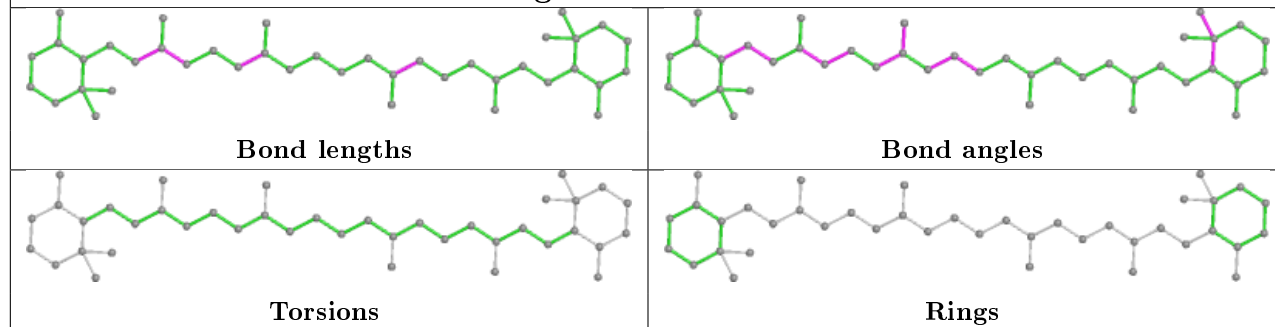




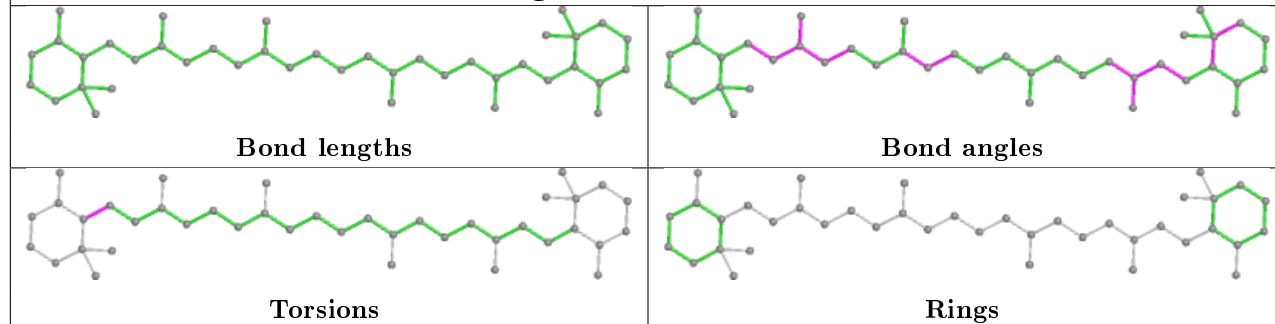
Ligand LHG d 411

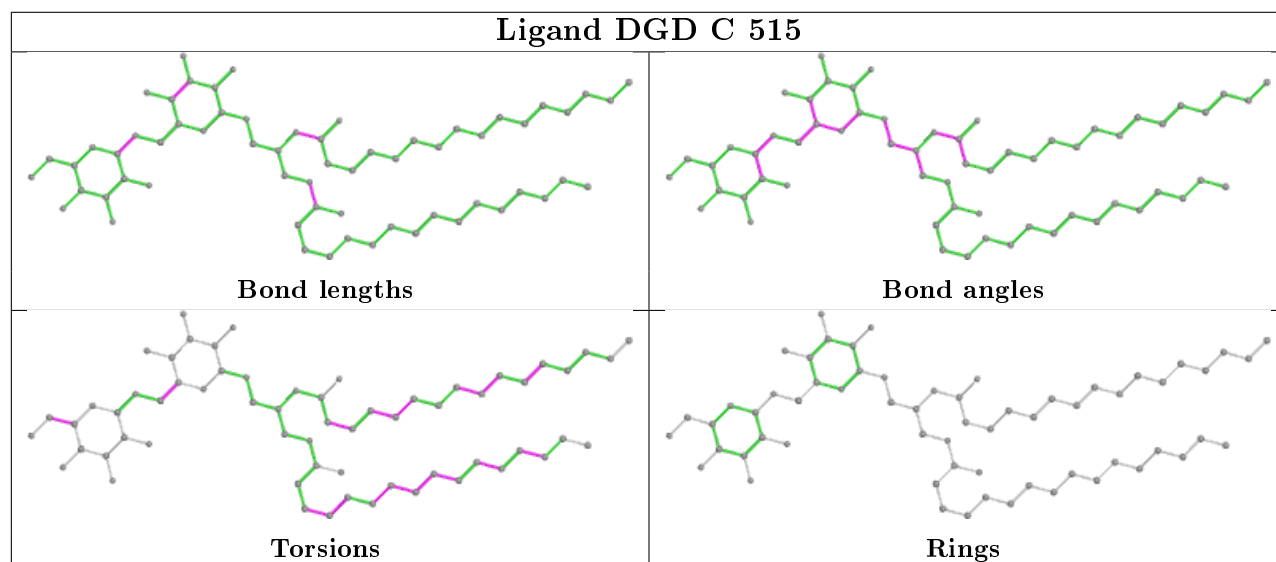
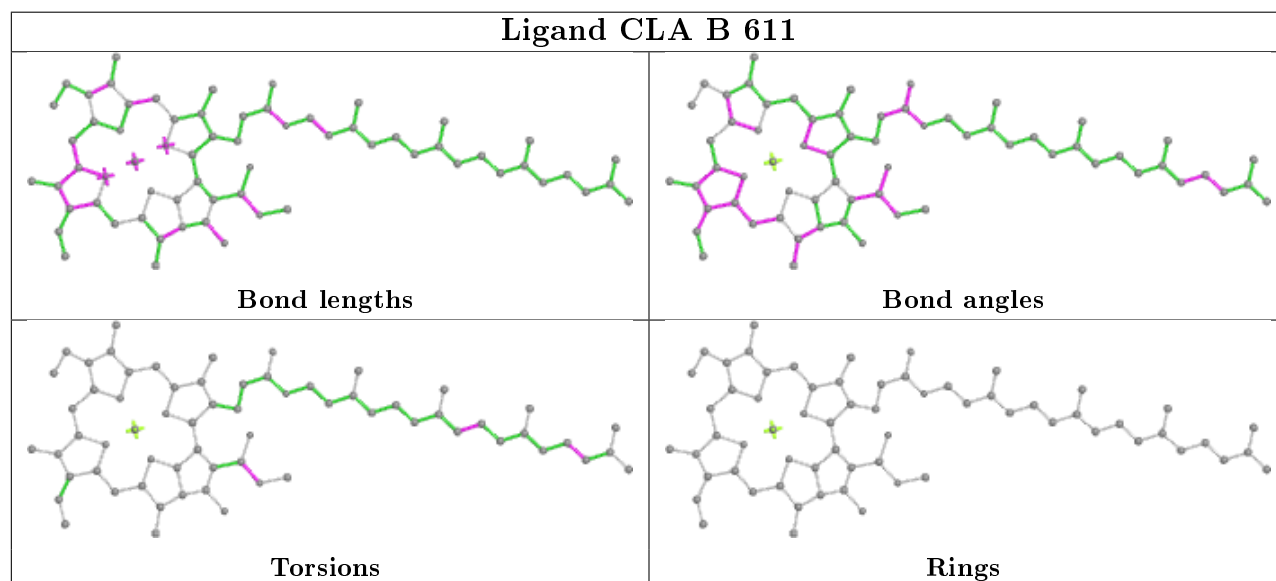
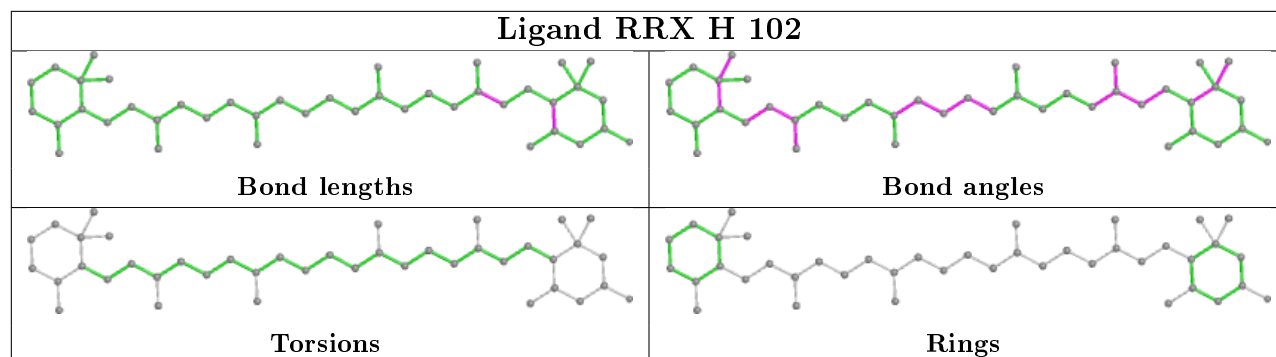


Ligand BCR a 410

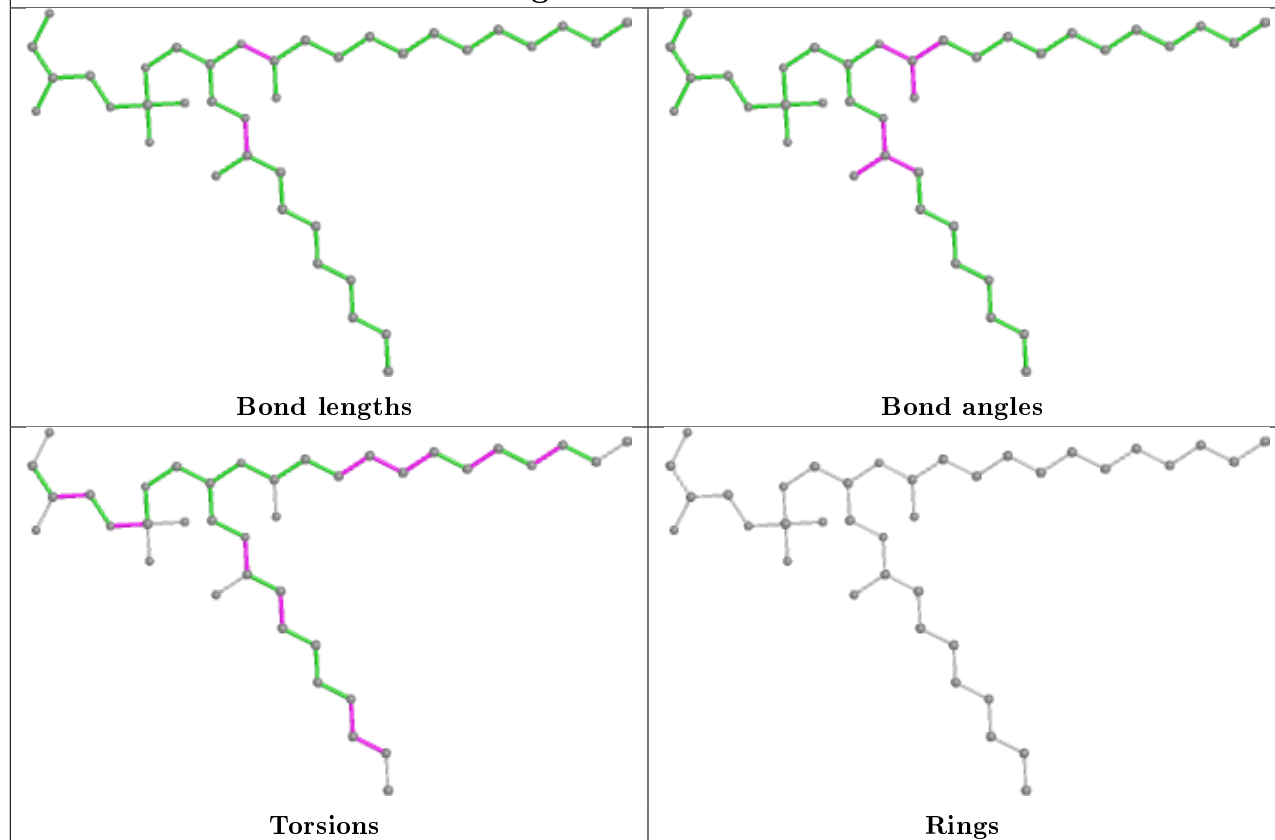


Ligand BCR B 618

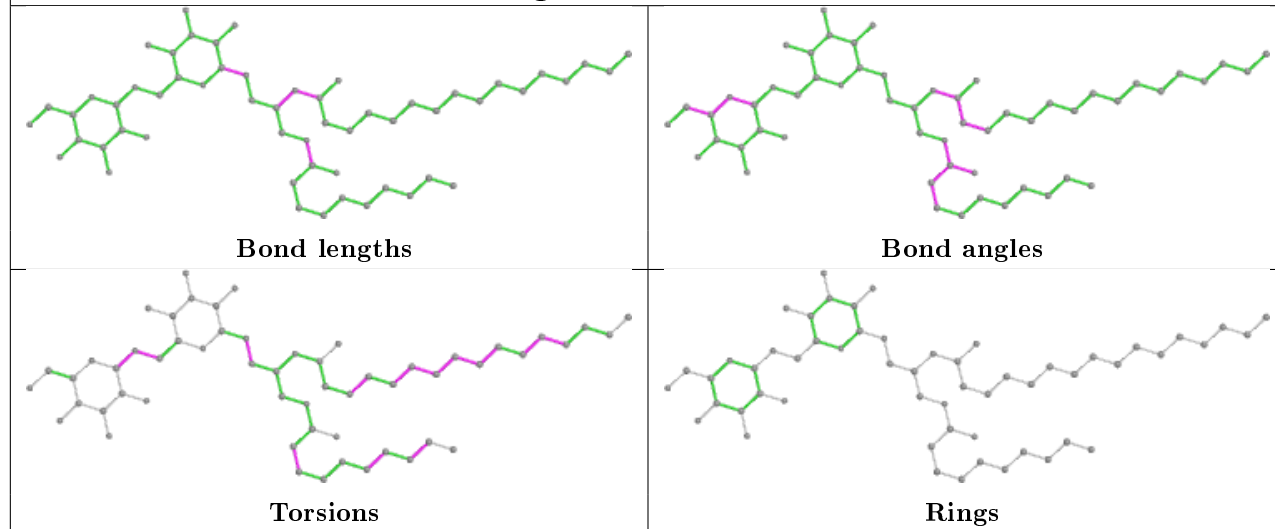


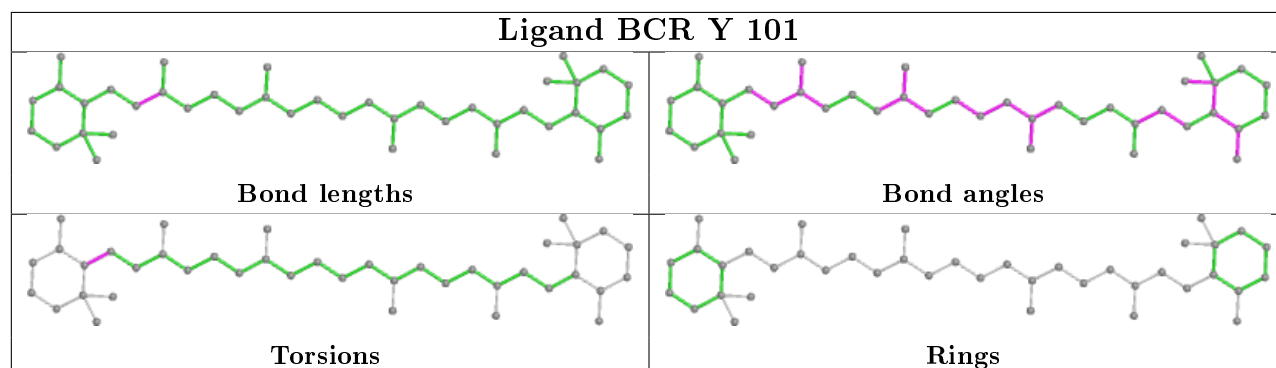
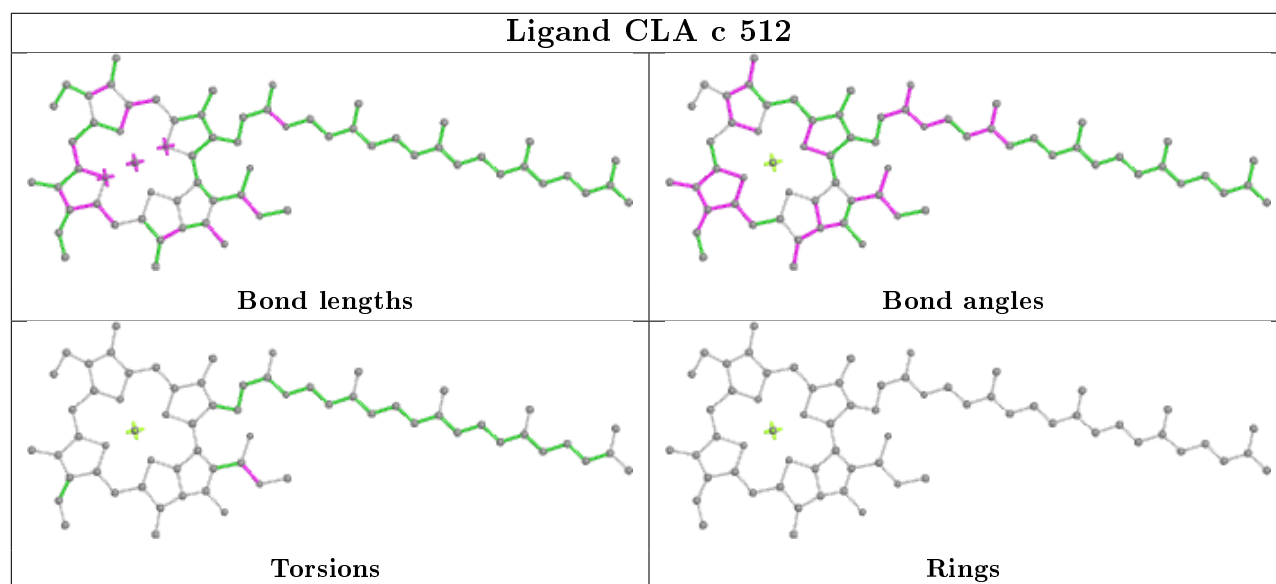
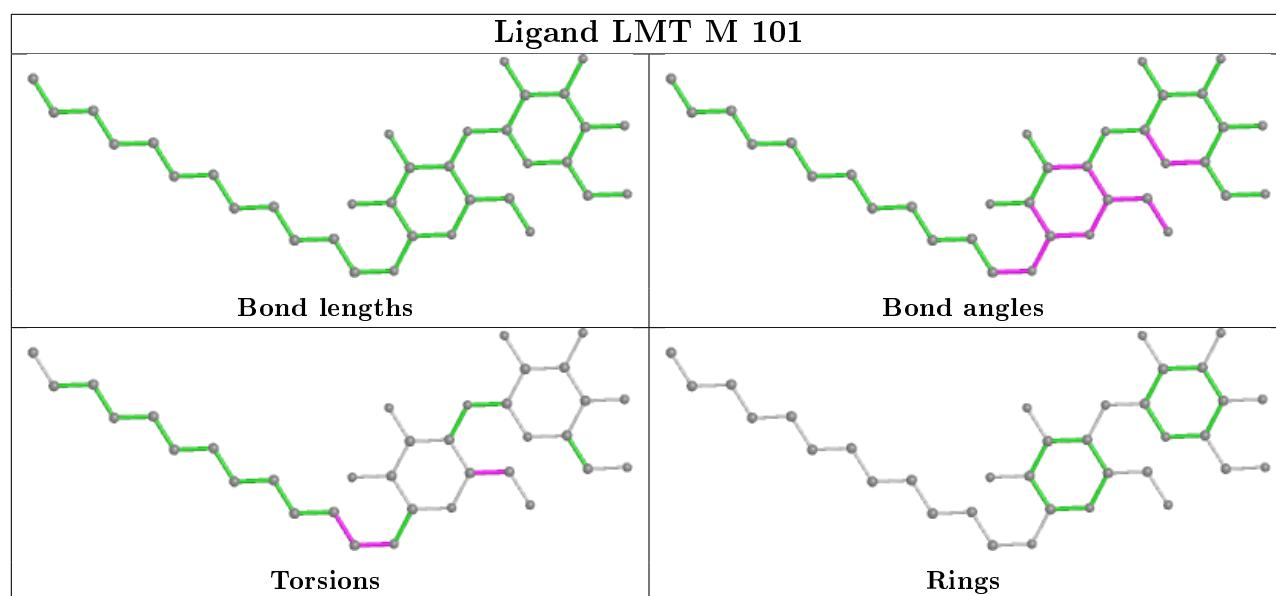


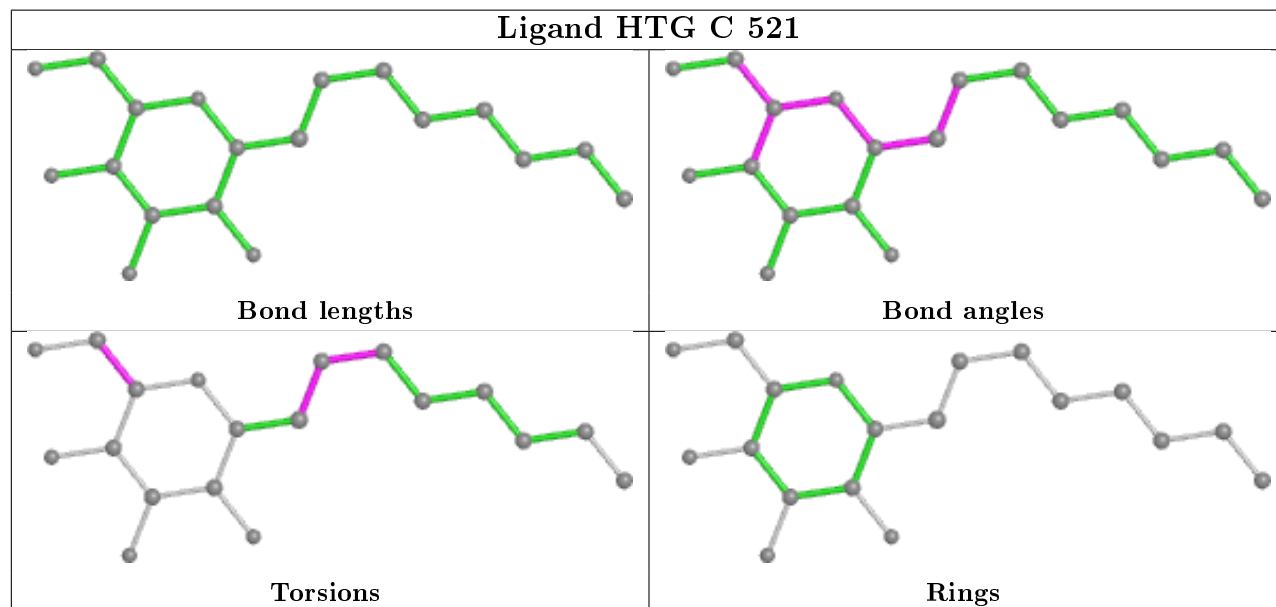
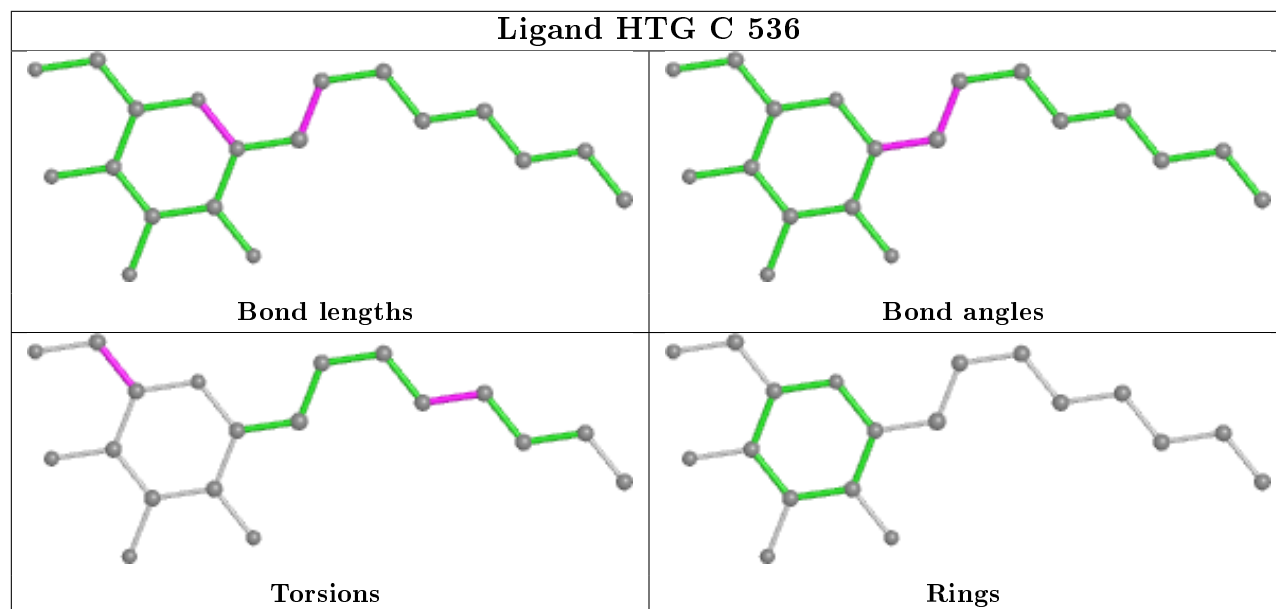
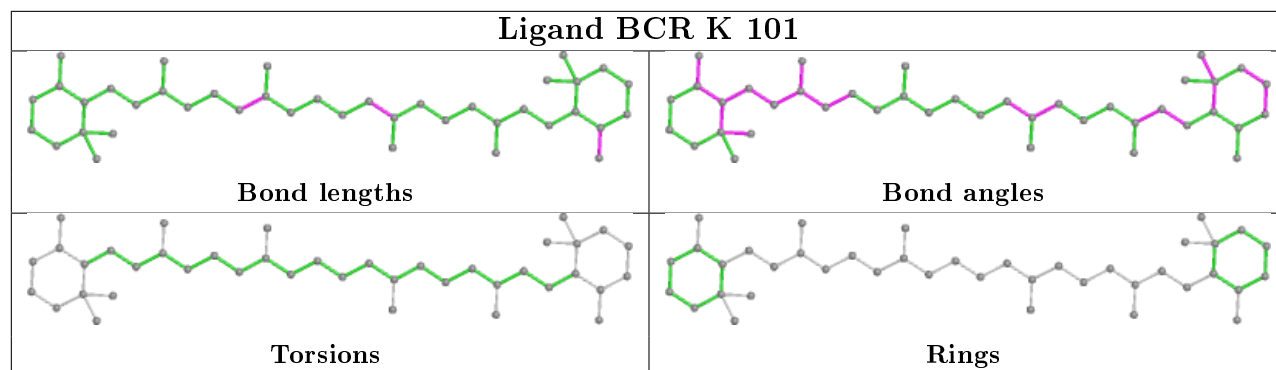
Ligand LHG F 103

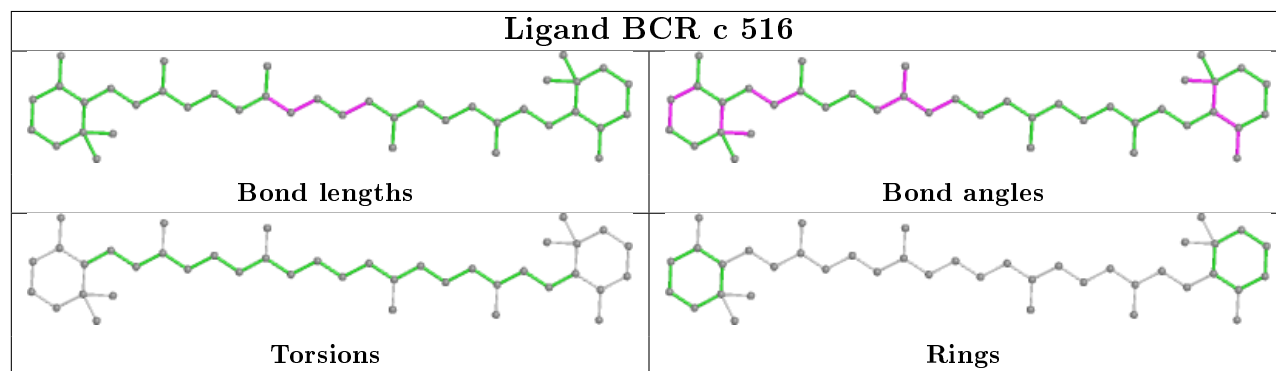
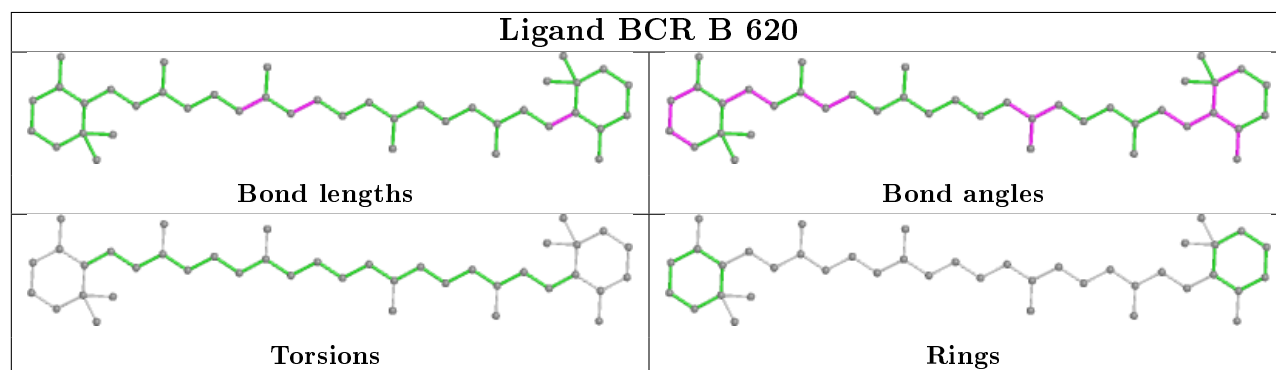
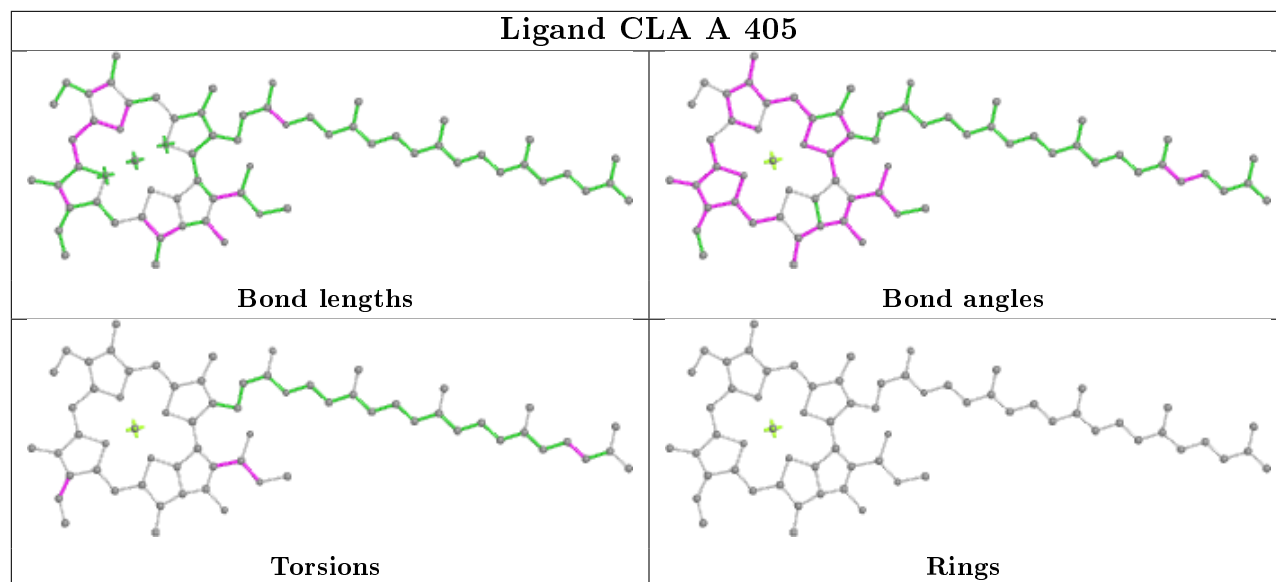


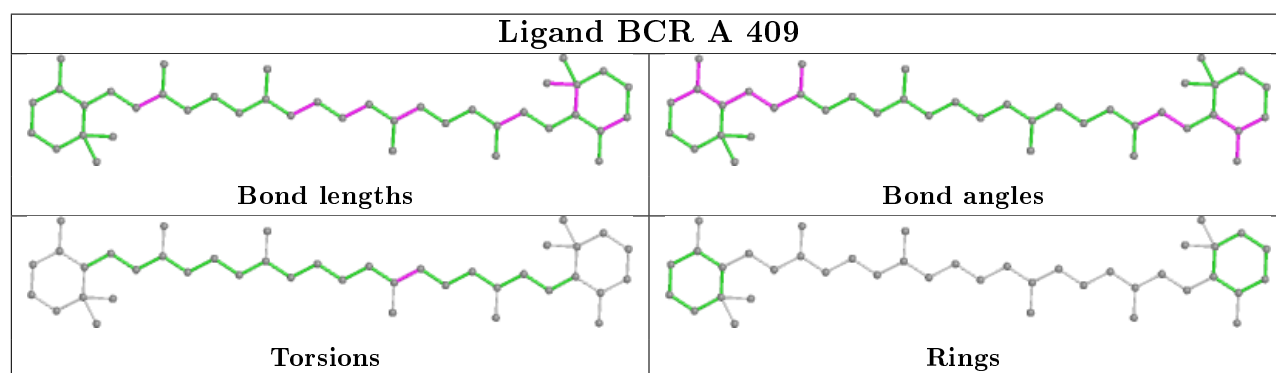
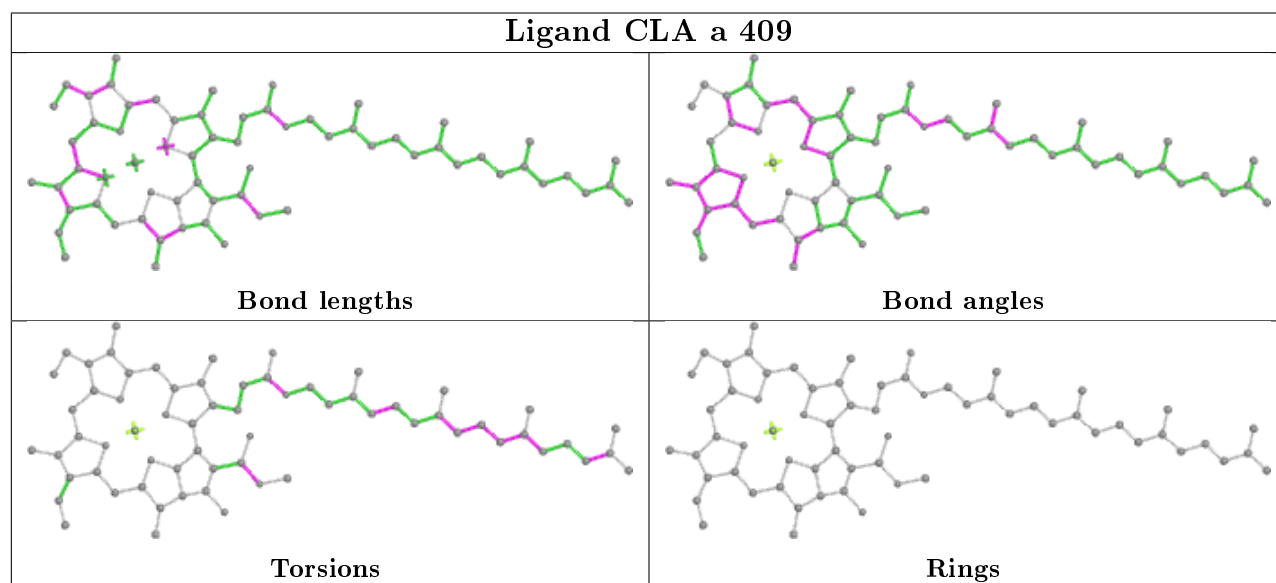
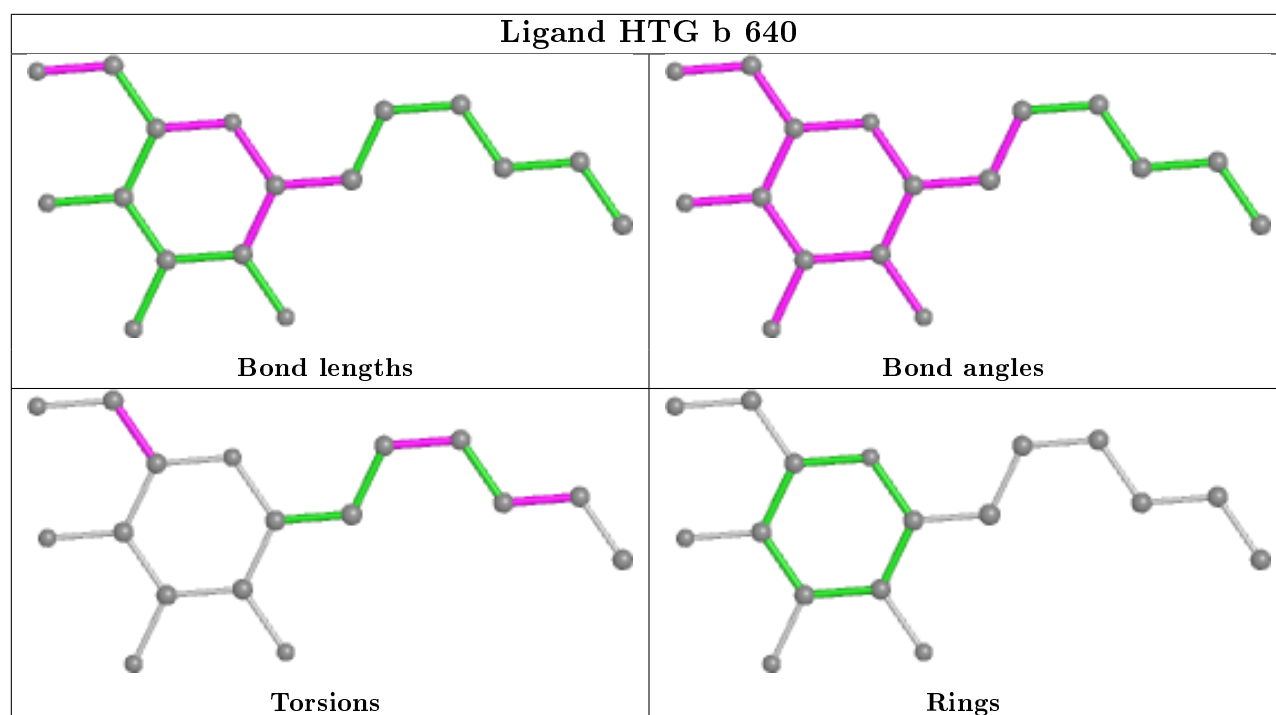
Ligand DGD c 518

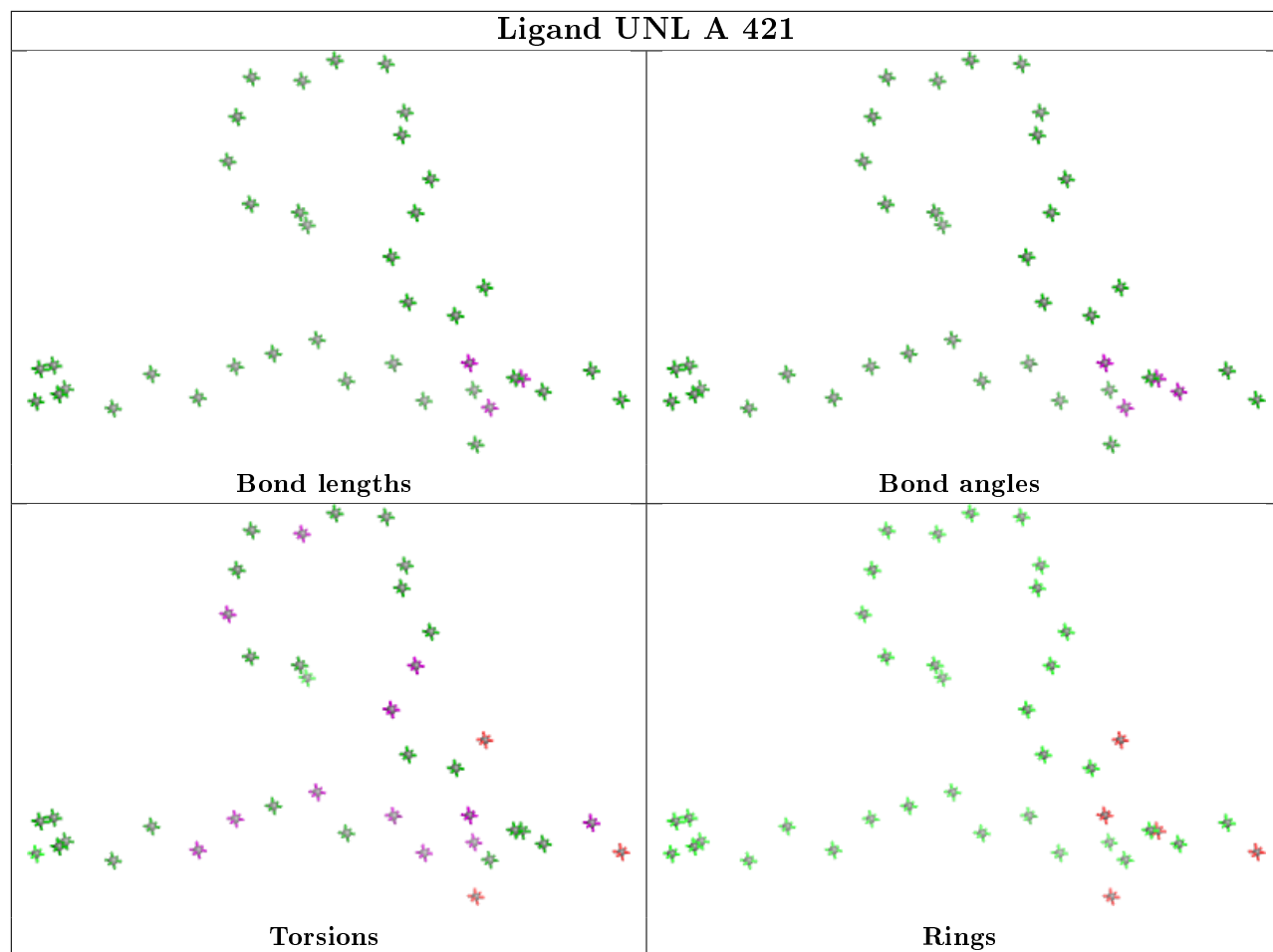


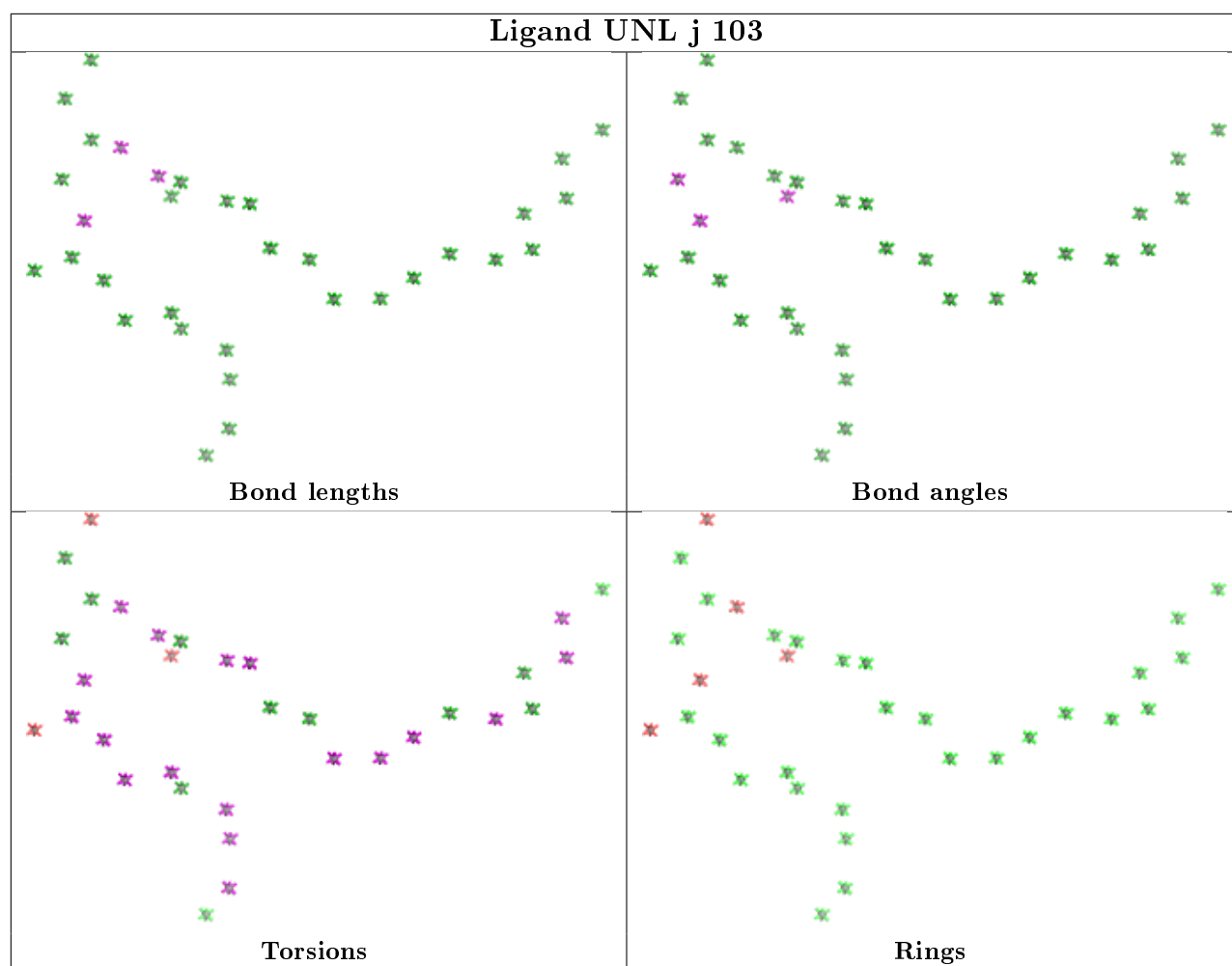


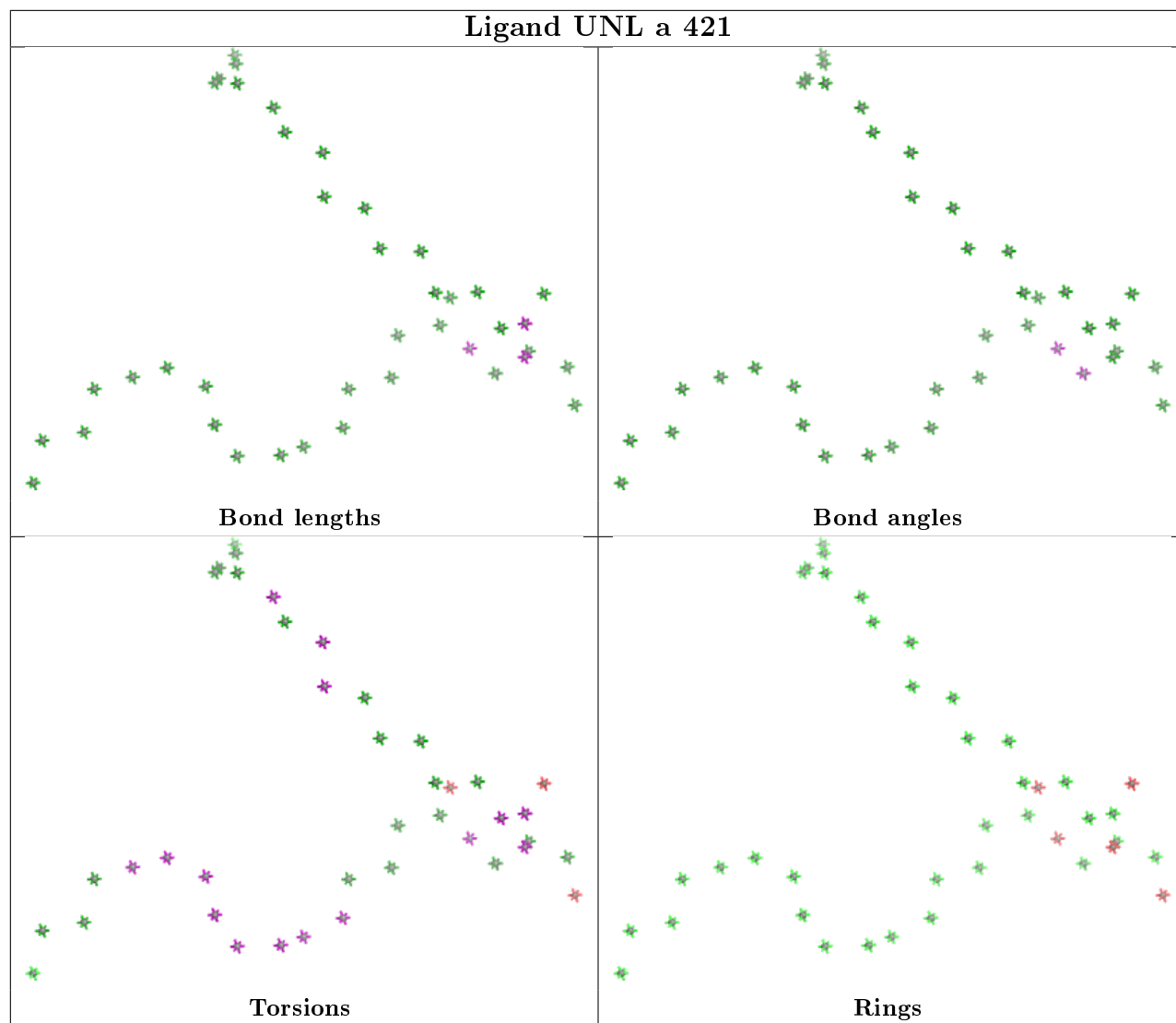


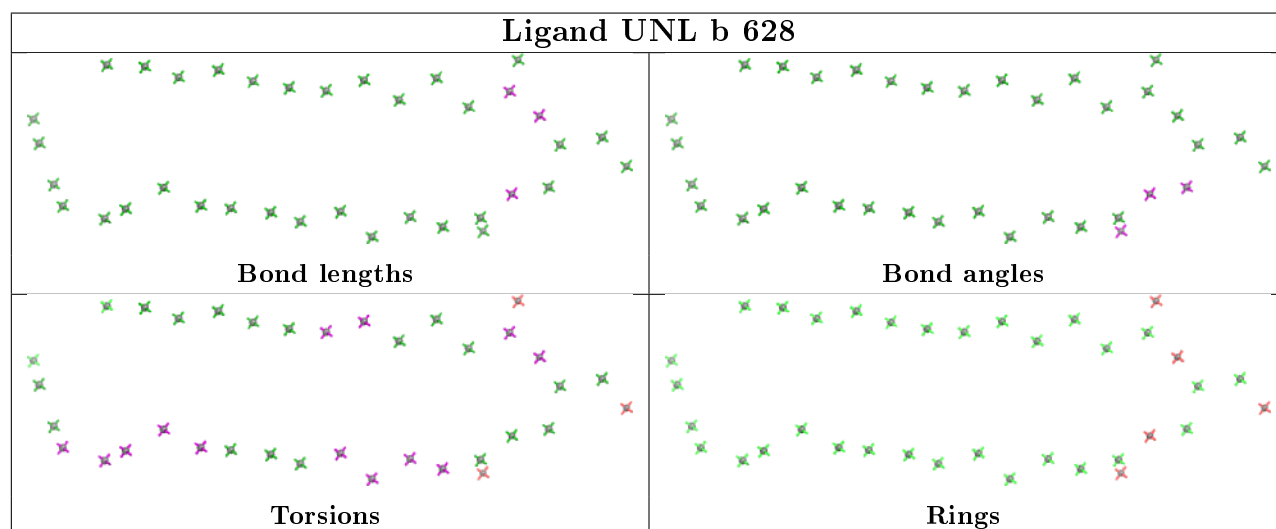
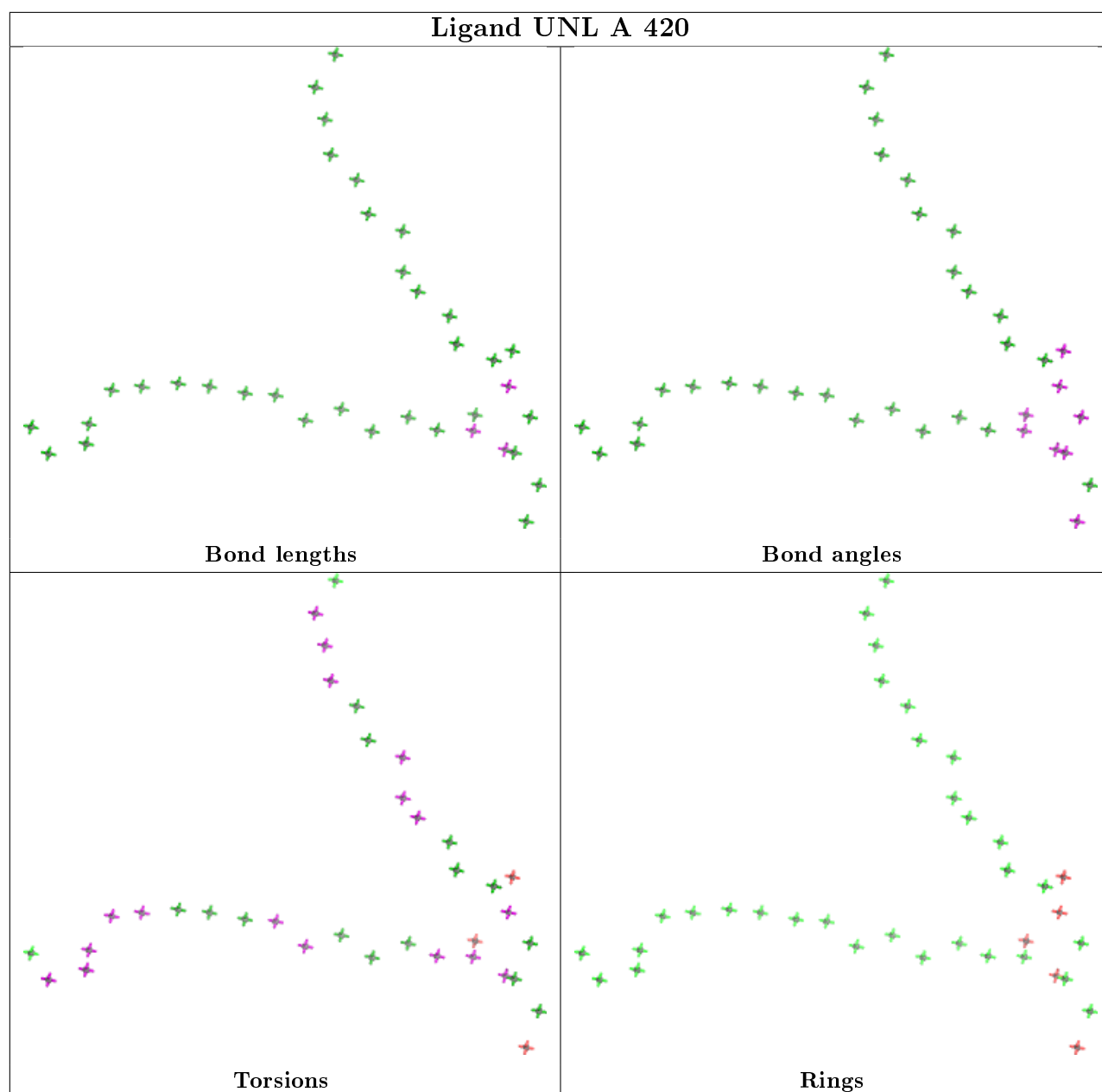


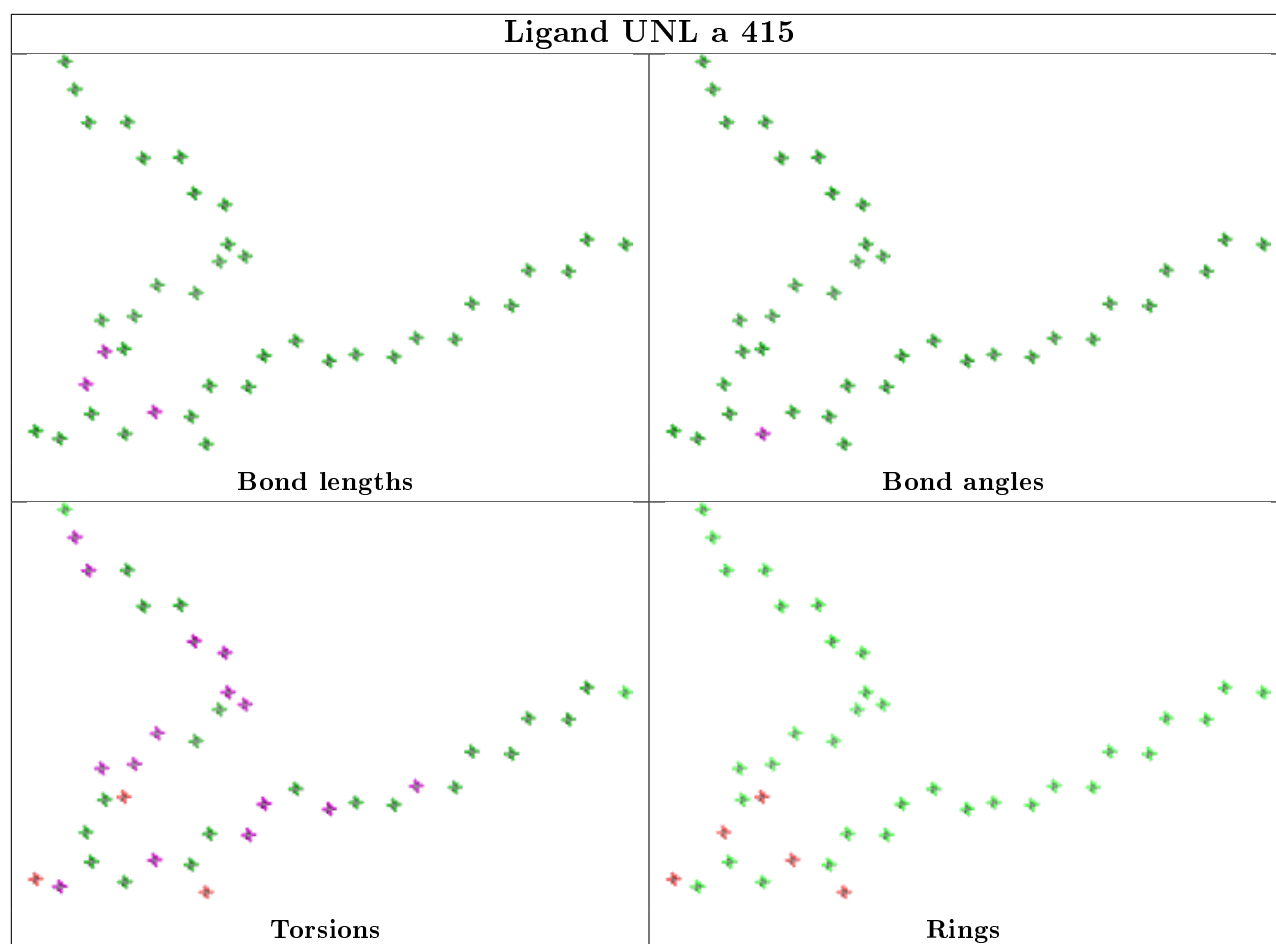


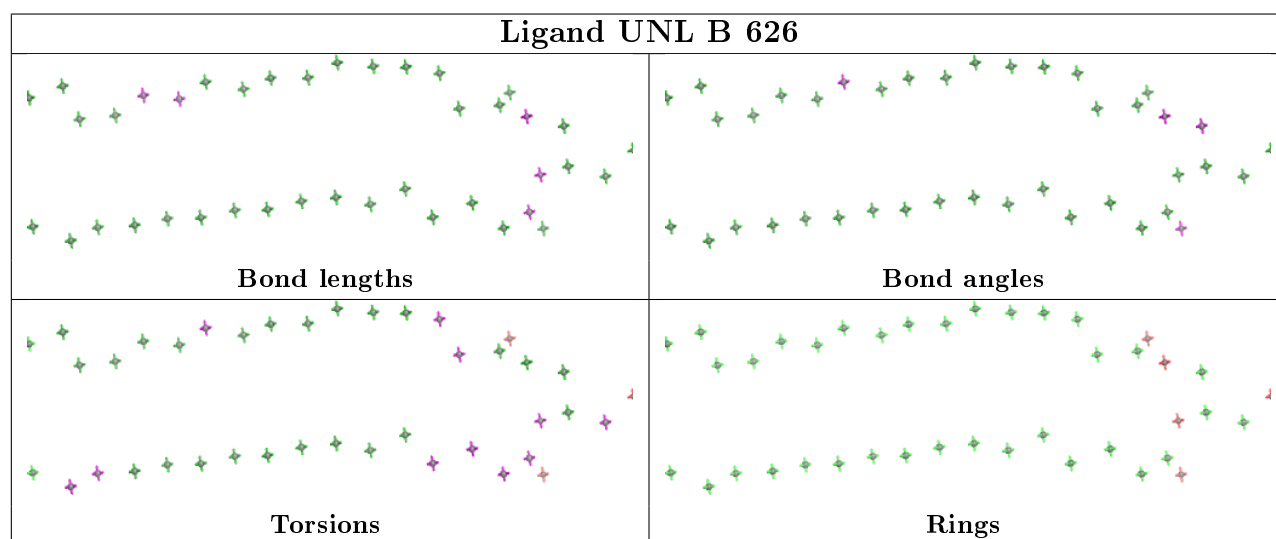
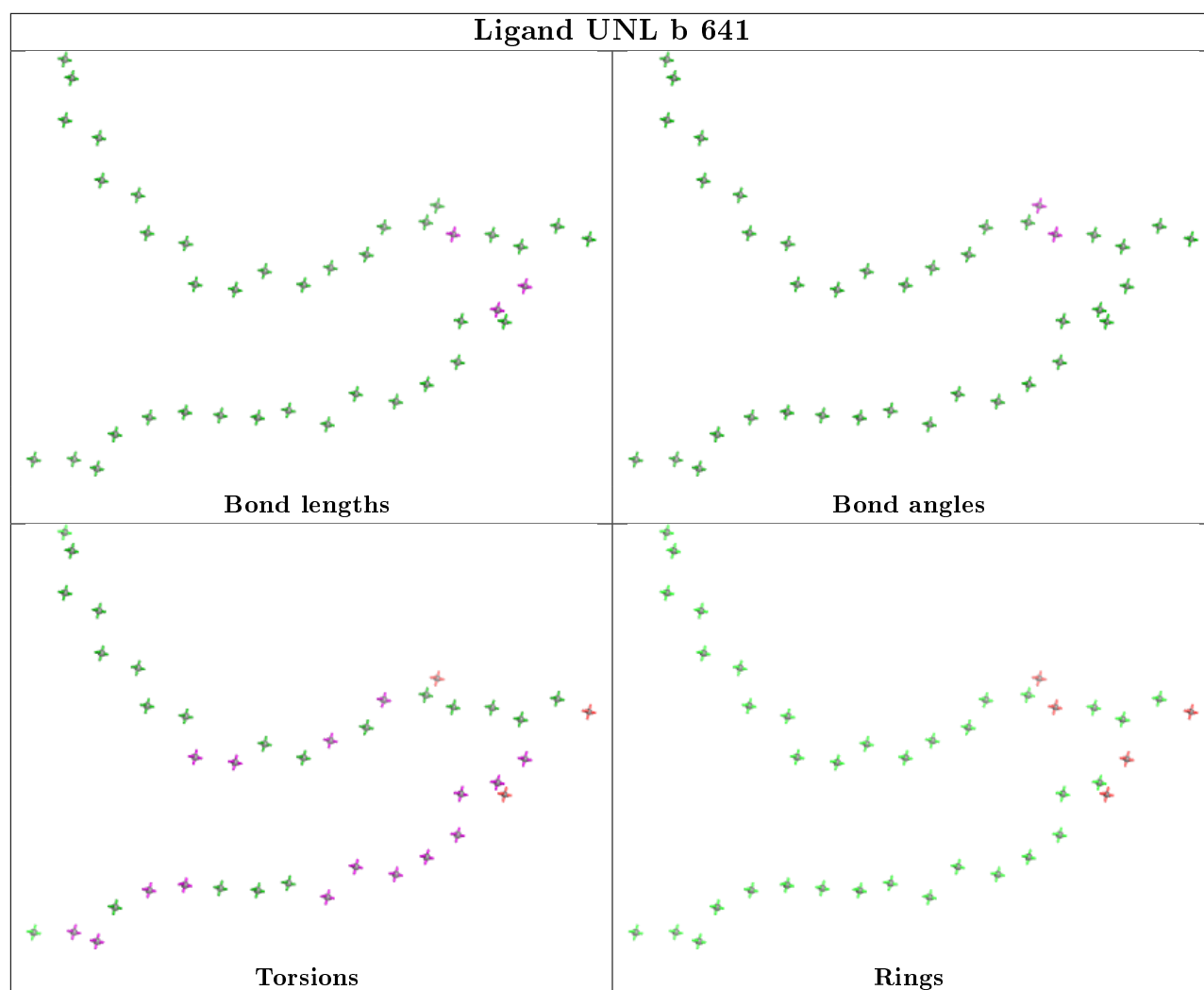


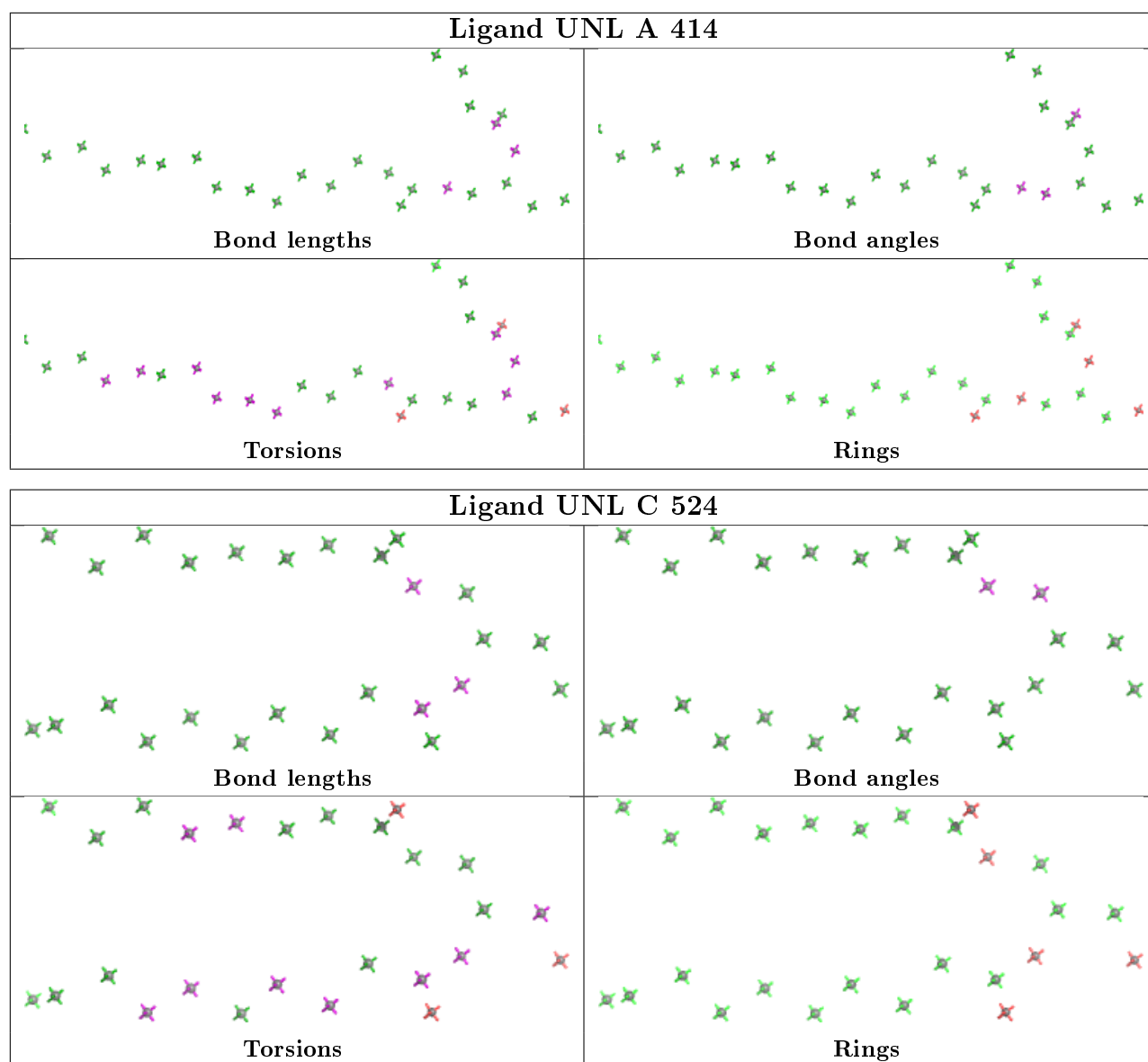


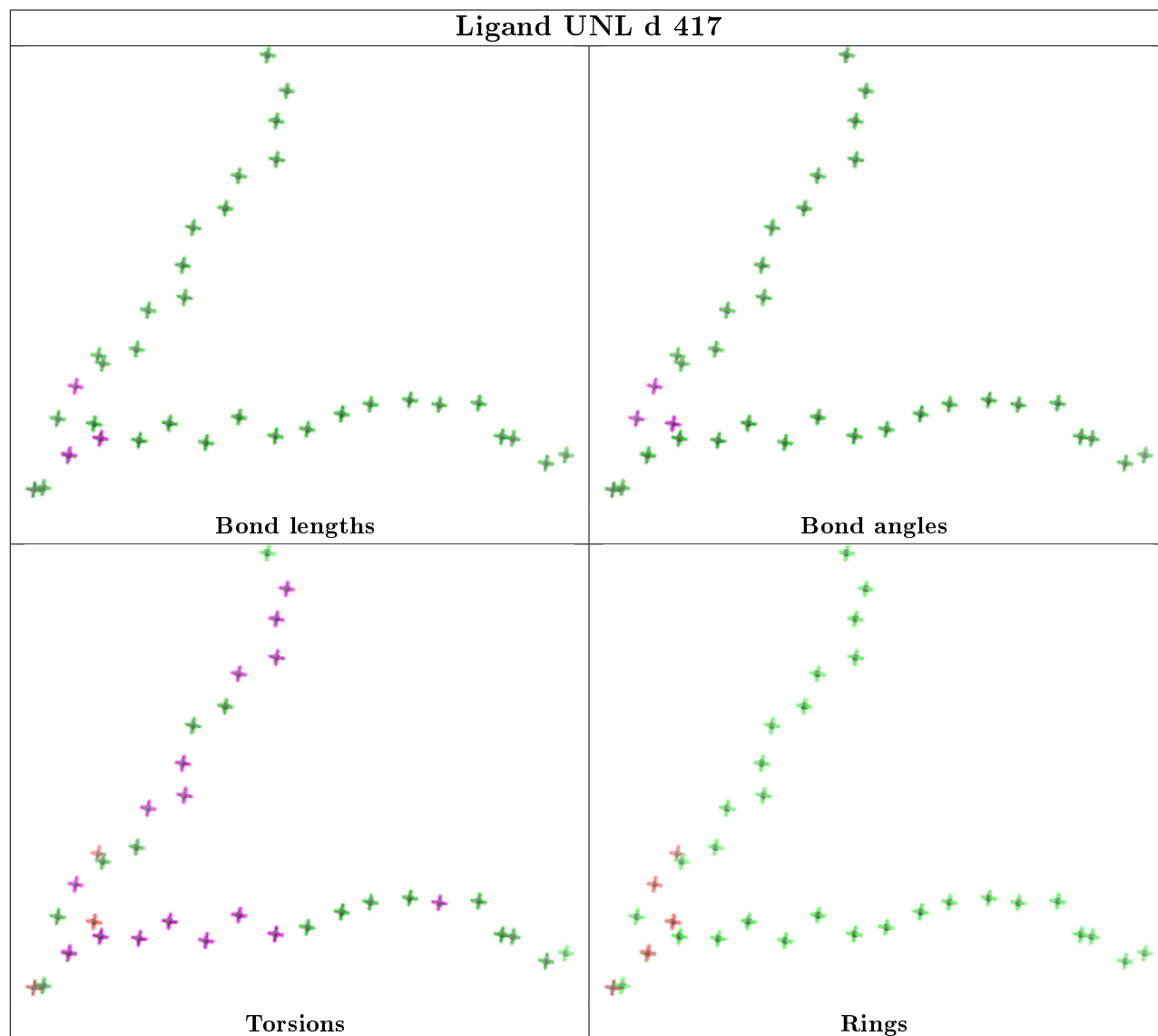
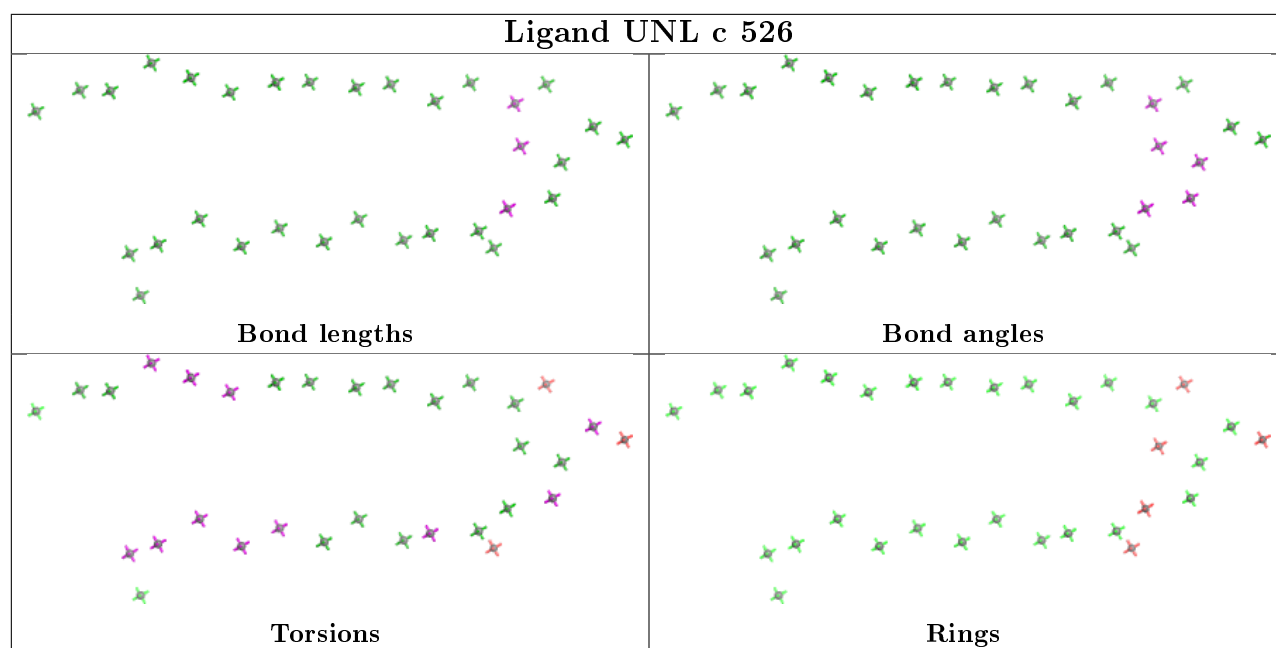


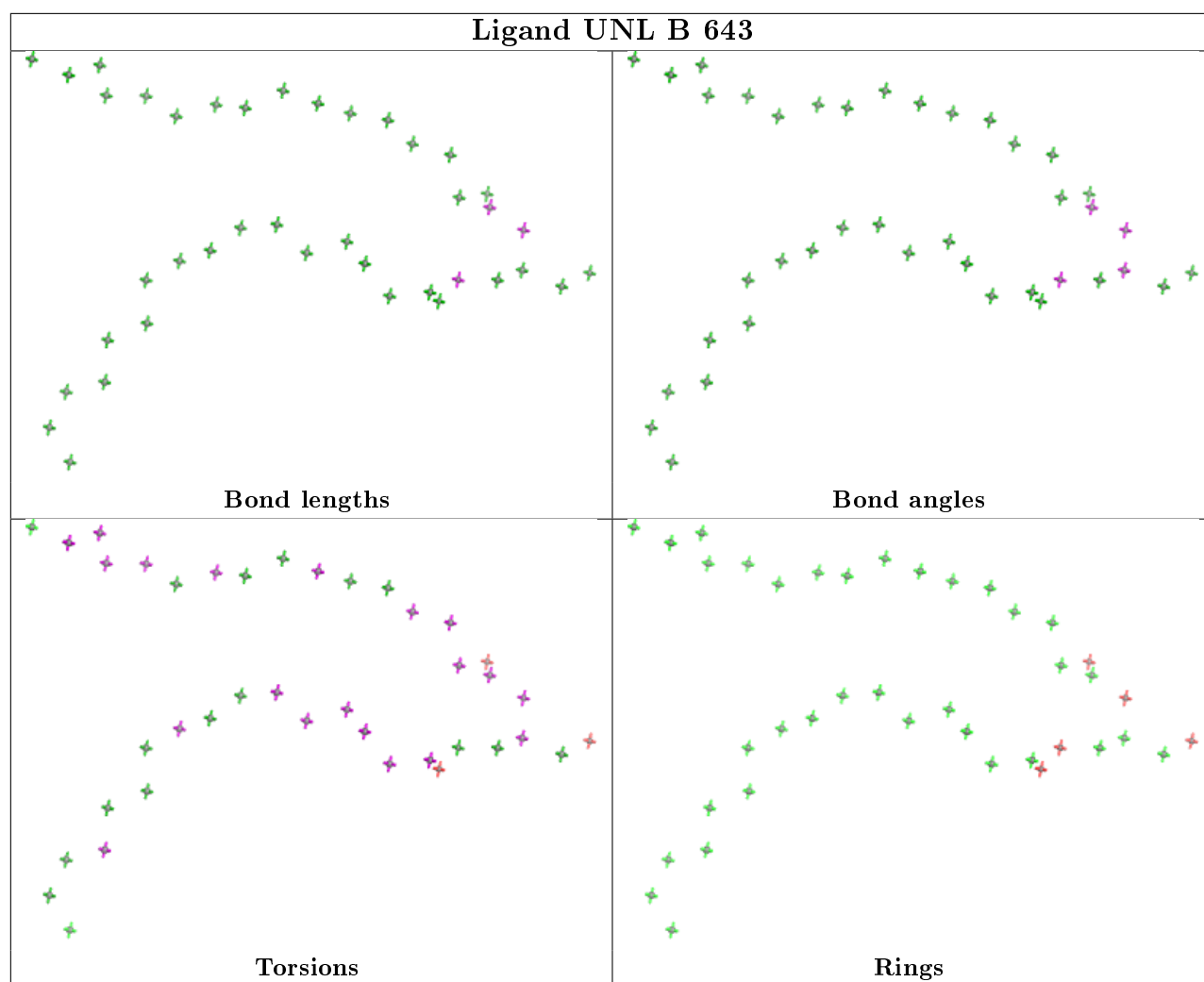












5.7 Other polymers [i](#)

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	334/334 (100%)	-0.79	3 (0%) 84 86	24, 33, 56, 90	0
1	a	334/334 (100%)	-0.78	4 (1%) 79 82	27, 35, 59, 92	0
2	B	505/505 (100%)	-0.58	11 (2%) 62 66	23, 38, 68, 90	0
2	b	504/505 (99%)	-0.47	23 (4%) 32 38	29, 39, 71, 131	0
3	C	451/455 (99%)	-0.64	4 (0%) 84 86	28, 41, 60, 115	0
3	c	455/455 (100%)	-0.53	8 (1%) 68 72	32, 45, 62, 110	0
4	D	341/342 (99%)	-0.76	5 (1%) 73 77	25, 34, 52, 118	0
4	d	341/342 (99%)	-0.78	7 (2%) 63 68	27, 35, 56, 98	0
5	E	80/81 (98%)	0.21	7 (8%) 10 12	37, 58, 90, 102	0
5	e	81/81 (100%)	0.27	9 (11%) 5 7	40, 54, 83, 105	0
6	F	34/34 (100%)	0.07	4 (11%) 4 5	36, 46, 86, 115	0
6	f	32/34 (94%)	-0.39	1 (3%) 49 55	38, 46, 70, 77	0
7	H	63/63 (100%)	-0.34	2 (3%) 47 54	34, 46, 59, 106	0
7	h	63/63 (100%)	-0.24	4 (6%) 20 24	35, 49, 66, 85	0
8	I	34/37 (91%)	-0.41	1 (2%) 51 57	36, 47, 67, 90	0
8	i	36/37 (97%)	-0.26	2 (5%) 24 29	38, 49, 90, 96	0
9	J	37/40 (92%)	-0.28	3 (8%) 12 15	32, 50, 104, 120	0
9	j	40/40 (100%)	-0.42	1 (2%) 57 62	39, 52, 67, 90	0
10	K	37/37 (100%)	-0.48	0 100 100	41, 49, 62, 73	0
10	k	37/37 (100%)	-0.44	0 100 100	44, 52, 74, 77	0
11	L	36/36 (100%)	-0.46	3 (8%) 11 14	26, 32, 77, 105	0
11	l	35/36 (97%)	-0.51	2 (5%) 23 29	29, 33, 69, 106	0
12	M	32/34 (94%)	-0.81	1 (3%) 49 55	31, 35, 55, 89	0
12	m	33/34 (97%)	-0.52	2 (6%) 21 26	32, 37, 76, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.24	10 (4%) 37 43	28, 45, 73, 129	0
13	o	243/243 (100%)	-0.13	19 (7%) 13 17	29, 47, 80, 114	0
14	T	29/30 (96%)	-0.58	1 (3%) 45 51	28, 35, 58, 126	0
14	t	29/30 (96%)	-0.65	1 (3%) 45 51	29, 34, 61, 103	0
15	U	97/97 (100%)	-0.45	2 (2%) 63 68	30, 40, 61, 89	0
15	u	97/97 (100%)	-0.43	1 (1%) 82 85	34, 42, 63, 108	0
16	V	137/137 (100%)	-0.66	0 100 100	29, 39, 58, 77	0
16	v	137/137 (100%)	-0.28	5 (3%) 42 49	36, 49, 70, 90	0
17	Y	29/29 (100%)	0.56	3 (10%) 6 8	48, 62, 85, 111	0
17	y	29/29 (100%)	0.57	5 (17%) 1 1	53, 69, 83, 94	0
18	X	39/39 (100%)	0.07	4 (10%) 6 8	41, 51, 80, 108	0
18	x	38/39 (97%)	-0.09	4 (10%) 6 8	42, 52, 97, 107	0
19	Z	62/62 (100%)	0.11	9 (14%) 2 3	46, 59, 102, 129	0
19	z	62/62 (100%)	0.47	12 (19%) 1 1	57, 73, 113, 130	0
All	All	5246/5270 (99%)	-0.49	183 (3%) 44 50	23, 41, 73, 131	0

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	12	SER	9.3
18	X	40	SER	8.9
14	T	30	THR	7.0
2	b	486	LEU	7.0
7	H	64	ALA	6.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
12	FME	M	1	10/11	0.93	0.13	39,42,73,78	0
12	FME	m	1	10/11	0.94	0.13	40,46,74,76	0
8	FME	I	1	10/11	0.95	0.08	36,43,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	FME	t	1	10/11	0.96	0.08	31,41,67,75	0
8	FME	i	1	10/11	0.97	0.08	40,45,49,51	0
14	FME	T	1	10/11	0.98	0.06	35,40,67,76	0
4	HSK	D	336[A]	10/12	0.99	0.07	32,36,37,37	7
4	HSK	d	336[B]	11/12	0.99	0.06	35,42,52,56	8
4	HSK	D	336[B]	11/12	0.99	0.07	35,37,42,45	8
4	HSK	d	336[A]	10/12	0.99	0.06	35,38,42,42	7

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	UNL	J	103	16/-	0.42	0.27	74,97,111,112	0
27	UNL	b	603	16/-	0.47	0.26	73,94,114,115	0
27	UNL	j	104	16/-	0.52	0.27	77,91,113,115	0
32	HTG	D	413	16/19	0.52	0.33	80,99,115,116	0
27	UNL	I	102	14/-	0.52	0.22	82,96,101,101	0
28	LMT	J	102	24/35	0.53	0.26	62,83,124,131	0
28	LMT	m	103	23/35	0.53	0.23	59,80,125,127	0
32	HTG	C	536	19/19	0.53	0.32	79,117,138,138	0
27	UNL	B	625	15/-	0.54	0.23	83,93,115,120	0
32	HTG	b	602	19/19	0.56	0.20	71,113,132,135	0
27	UNL	c	525	5/-	0.56	0.16	72,83,84,84	0
33	DGD	d	408	48/66	0.56	0.30	70,100,122,132	0
32	HTG	B	624	19/19	0.56	0.40	65,99,109,114	0
27	UNL	C	524	26/-	0.58	0.24	76,97,109,120	0
32	HTG	C	522	19/19	0.58	0.33	61,92,117,117	0
28	LMT	a	401	35/35	0.59	0.33	38,67,86,100	35
28	LMT	A	415	35/35	0.59	0.27	54,88,106,116	0
27	UNL	e	103	11/-	0.60	0.33	67,81,102,104	0
27	UNL	i	101	16/-	0.61	0.23	82,85,100,101	0
28	LMT	l	101	24/35	0.61	0.23	59,76,130,142	0
27	UNL	E	103	16/-	0.62	0.25	78,88,108,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	DGD	D	408	45/66	0.63	0.25	70,93,120,129	0
32	HTG	d	413	16/19	0.63	0.32	66,100,118,131	0
27	UNL	K	103	10/-	0.63	0.23	78,89,97,98	0
32	HTG	U	203	14/19	0.64	0.48	76,107,133,154	0
32	HTG	c	541	15/19	0.64	0.37	74,104,117,120	0
27	UNL	I	101	16/-	0.65	0.21	78,88,102,110	0
27	UNL	H	104	7/-	0.65	0.18	78,82,85,88	0
28	LMT	j	102	23/35	0.67	0.21	71,81,105,108	0
28	LMT	m	101	35/35	0.68	0.23	38,70,81,85	0
27	UNL	u	201	13/-	0.68	0.26	57,67,80,84	0
28	LMT	m	102	25/35	0.68	0.26	45,72,116,124	0
28	LMT	F	102	24/35	0.68	0.25	60,97,113,121	0
28	LMT	M	101	35/35	0.68	0.21	43,73,83,90	0
28	LMT	t	102	24/35	0.69	0.20	67,87,121,126	0
27	UNL	a	415	40/-	0.69	0.24	75,97,121,124	0
32	HTG	B	629	19/19	0.70	0.20	59,118,133,135	0
27	UNL	j	103	33/-	0.70	0.24	67,112,139,141	0
32	HTG	b	627	19/19	0.70	0.25	69,91,106,109	0
34	GOL	e	104	6/6	0.70	0.23	72,77,81,84	0
32	HTG	c	524	9/19	0.70	0.19	73,79,97,114	0
27	UNL	A	414	28/-	0.70	0.23	76,94,110,114	0
29	DMS	c	540	4/4	0.71	0.33	99,101,109,120	0
26	LMG	C	519	48/55	0.71	0.23	52,89,111,119	0
26	LMG	c	521	51/55	0.71	0.23	51,93,114,122	0
27	UNL	i	102	14/-	0.71	0.23	91,101,109,109	0
27	UNL	c	526	32/-	0.72	0.24	67,94,116,119	0
28	LMT	b	626	25/35	0.72	0.20	62,76,105,114	0
29	DMS	O	312	4/4	0.72	0.29	78,88,109,113	0
27	UNL	c	527	16/-	0.72	0.24	73,83,115,120	0
27	UNL	Z	102	6/-	0.73	0.19	71,83,89,90	0
27	UNL	A	413	7/-	0.74	0.21	84,90,95,96	0
31	LHG	E	101	49/49	0.74	0.25	60,95,130,135	0
27	UNL	E	102	13/-	0.75	0.18	81,91,100,100	0
29	DMS	c	538	4/4	0.75	0.19	70,106,108,128	0
27	UNL	U	201	14/-	0.76	0.23	54,74,82,82	0
32	HTG	c	523	19/19	0.76	0.23	86,101,115,118	0
28	LMT	T	102	24/35	0.76	0.20	43,78,107,110	0
28	LMT	z	101	32/35	0.77	0.18	53,88,118,138	0
27	UNL	e	102	8/-	0.77	0.18	77,82,84,84	0
28	LMT	M	102	24/35	0.77	0.15	51,70,94,108	0
29	DMS	a	418	4/4	0.78	0.19	97,107,116,118	0
27	UNL	T	103	13/-	0.78	0.28	80,89,96,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	UNL	a	414	8/-	0.78	0.16	77,81,86,90	0
29	DMS	O	309	4/4	0.79	0.33	80,106,109,118	0
27	UNL	b	641	40/-	0.80	0.18	60,77,94,97	0
27	UNL	A	412	8/-	0.80	0.16	64,74,78,79	0
27	UNL	B	630	16/-	0.80	0.18	69,81,89,89	0
27	UNL	B	643	40/-	0.80	0.20	60,76,101,112	0
27	UNL	A	421	40/-	0.81	0.16	56,78,120,123	0
27	UNL	i	104	14/-	0.81	0.18	69,80,99,101	0
27	UNL	a	413	8/-	0.81	0.15	76,83,90,95	0
28	LMT	Z	101	35/35	0.81	0.19	48,88,101,103	0
31	LHG	e	101	38/49	0.81	0.23	63,94,111,113	0
29	DMS	d	416	4/4	0.81	0.24	99,114,115,118	0
34	GOL	D	417	6/6	0.81	0.21	63,70,73,74	0
29	DMS	a	419	4/4	0.82	0.27	96,109,116,119	0
27	UNL	A	420	36/-	0.82	0.15	41,86,102,108	0
29	DMS	v	207	4/4	0.82	0.20	75,78,83,99	0
27	UNL	C	523	9/-	0.82	0.13	75,77,85,87	0
29	DMS	D	419	4/4	0.82	0.22	96,114,118,120	0
27	UNL	d	417	36/-	0.82	0.15	49,87,101,107	0
27	UNL	B	627	16/-	0.83	0.17	53,64,87,88	0
34	GOL	b	636	6/6	0.83	0.31	61,76,83,103	0
28	LMT	C	520	35/35	0.83	0.23	71,97,104,104	0
32	HTG	B	642	18/19	0.83	0.22	25,38,48,49	18
29	DMS	c	532	4/4	0.83	0.22	64,81,98,107	0
27	UNL	X	101	16/-	0.83	0.16	47,53,78,80	0
29	DMS	B	640	4/4	0.83	0.31	70,86,87,96	0
25	PL9	A	410	55/55	0.84	0.19	51,77,105,110	0
29	DMS	V	207	4/4	0.84	0.29	85,97,101,104	0
26	LMG	a	412	51/55	0.84	0.14	51,69,85,98	0
29	DMS	c	534	4/4	0.84	0.26	80,90,95,100	0
32	HTG	b	640	17/19	0.84	0.20	27,44,57,61	17
29	DMS	A	419	4/4	0.84	0.22	94,96,101,109	0
27	UNL	b	628	36/-	0.84	0.17	50,73,110,135	0
26	LMG	A	411	51/55	0.85	0.15	54,68,92,105	0
29	DMS	O	306	4/4	0.85	0.25	76,88,93,106	0
29	DMS	O	308	4/4	0.85	0.24	67,71,84,97	0
27	UNL	t	103	16/-	0.85	0.19	71,86,109,110	0
29	DMS	I	105	4/4	0.85	0.41	76,86,99,99	0
28	LMT	c	522	35/35	0.85	0.26	65,89,117,127	0
28	LMT	B	623	35/35	0.85	0.16	56,68,85,93	0
25	PL9	a	411	55/55	0.85	0.18	54,73,105,110	0
27	UNL	B	626	40/-	0.85	0.15	46,68,109,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	HTG	b	601	19/19	0.85	0.15	57,66,80,92	0
27	UNL	h	103	8/-	0.85	0.17	66,79,89,91	0
27	UNL	H	103	7/-	0.85	0.11	69,72,89,93	0
29	DMS	c	539	4/4	0.86	0.16	106,108,113,115	0
29	DMS	c	536	4/4	0.86	0.37	97,97,105,115	0
26	LMG	c	520	38/55	0.86	0.14	43,70,87,91	0
29	DMS	O	310	4/4	0.86	0.29	70,98,98,109	0
26	LMG	C	518	49/55	0.86	0.18	42,73,104,111	0
29	DMS	u	203	4/4	0.87	0.31	48,83,83,92	0
27	UNL	a	421	40/-	0.87	0.12	55,75,110,112	0
26	LMG	B	622	51/55	0.87	0.13	48,60,79,84	0
32	HTG	B	628	19/19	0.87	0.14	47,69,90,102	0
32	HTG	v	208	16/19	0.87	0.23	60,80,108,119	0
29	DMS	O	304	4/4	0.87	0.44	85,104,105,105	0
27	UNL	I	104	13/-	0.88	0.16	57,66,93,95	0
27	UNL	x	101	16/-	0.88	0.20	56,65,93,94	0
32	HTG	C	535	9/19	0.88	0.15	72,80,85,97	0
32	HTG	C	521	19/19	0.88	0.19	70,88,102,103	0
29	DMS	o	310	4/4	0.89	0.25	73,80,91,101	0
29	DMS	a	416	4/4	0.89	0.19	75,83,103,104	0
22	CLA	B	602	65/65	0.89	0.13	39,52,116,127	0
29	DMS	o	307	4/4	0.89	0.31	63,84,93,93	0
27	UNL	i	103	16/-	0.89	0.21	50,59,84,85	0
33	DGD	h	101	62/66	0.89	0.14	35,47,64,65	0
27	UNL	I	103	16/-	0.89	0.22	47,62,98,98	0
29	DMS	b	633	4/4	0.89	0.17	77,78,82,98	0
27	UNL	b	629	16/-	0.89	0.13	48,62,81,82	0
38	RRX	h	102	41/41	0.90	0.12	38,46,63,72	0
29	DMS	o	306	4/4	0.90	0.35	87,88,103,119	0
24	BCR	d	406	40/40	0.90	0.11	30,42,75,76	0
31	LHG	f	102	46/49	0.90	0.14	52,78,107,120	0
26	LMG	b	625	49/55	0.90	0.12	47,57,79,86	0
22	CLA	C	513	65/65	0.90	0.11	46,58,99,105	0
29	DMS	V	206	4/4	0.90	0.39	61,85,90,90	0
29	DMS	C	529	4/4	0.90	0.33	90,90,93,97	0
29	DMS	O	307	4/4	0.91	0.25	87,92,93,94	0
24	BCR	T	101	40/40	0.91	0.11	40,52,78,83	0
29	DMS	v	204	4/4	0.91	0.27	89,92,96,99	0
24	BCR	K	101	40/40	0.91	0.16	36,47,54,58	0
24	BCR	D	406	40/40	0.91	0.10	32,40,73,76	0
32	HTG	O	302	19/19	0.91	0.12	41,57,74,75	0
22	CLA	b	620	65/65	0.91	0.11	32,44,112,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	DGD	H	101	62/66	0.91	0.13	34,46,55,59	0
27	UNL	D	414	16/-	0.91	0.17	44,53,66,73	0
29	DMS	v	206	4/4	0.91	0.20	63,73,80,85	0
29	DMS	B	639	4/4	0.91	0.27	75,84,91,94	0
24	BCR	c	515	40/40	0.91	0.11	50,62,69,70	0
22	CLA	b	605	65/65	0.91	0.14	41,60,107,122	0
30	CA	v	209	1/1	0.91	0.19	90,90,90,90	0
24	BCR	K	102	40/40	0.91	0.10	42,53,57,60	0
29	DMS	C	527	4/4	0.91	0.15	75,76,79,93	0
29	DMS	U	202	4/4	0.91	0.15	40,61,69,82	0
29	DMS	C	534	4/4	0.91	0.30	67,81,87,87	0
27	UNL	d	414	16/-	0.92	0.17	44,56,84,88	0
31	LHG	F	103	38/49	0.92	0.15	56,82,111,112	0
29	DMS	O	311	4/4	0.92	0.15	80,88,88,91	0
22	CLA	B	617	65/65	0.92	0.12	31,43,129,145	0
29	DMS	B	634	4/4	0.92	0.35	83,86,86,94	0
29	DMS	h	104	4/4	0.92	0.19	103,104,106,109	0
33	DGD	C	516	62/66	0.92	0.11	31,45,103,116	0
29	DMS	C	532	4/4	0.92	0.25	58,72,80,81	0
38	RRX	H	102	41/41	0.92	0.11	36,42,56,60	0
29	DMS	a	417	4/4	0.92	0.35	69,78,88,92	0
29	DMS	u	202	4/4	0.92	0.17	48,69,70,82	0
24	BCR	t	101	40/40	0.92	0.10	36,52,72,74	0
32	HTG	o	301	19/19	0.92	0.11	49,58,70,73	0
29	DMS	D	420	4/4	0.92	0.33	93,98,108,110	0
29	DMS	B	633	4/4	0.93	0.15	94,98,98,100	0
29	DMS	E	104	4/4	0.93	0.28	91,95,98,105	0
34	GOL	c	533	6/6	0.93	0.25	58,62,76,81	0
29	DMS	B	635	4/4	0.93	0.21	90,94,95,106	0
29	DMS	o	309	4/4	0.93	0.26	70,78,79,91	0
24	BCR	y	101	40/40	0.93	0.09	40,47,57,59	0
26	LMG	d	412	47/55	0.93	0.12	37,47,99,103	0
29	DMS	e	105	4/4	0.93	0.33	80,93,97,97	0
22	CLA	c	507	65/65	0.93	0.10	42,51,109,121	0
32	HTG	V	202	19/19	0.93	0.27	50,62,107,107	0
29	DMS	u	204	4/4	0.94	0.09	70,83,95,98	0
22	CLA	C	506	65/65	0.94	0.10	39,55,121,136	0
22	CLA	c	513	65/65	0.94	0.10	43,56,94,107	0
24	BCR	Y	101	40/40	0.94	0.10	37,43,55,57	0
24	BCR	c	516	40/40	0.94	0.09	37,46,57,58	0
29	DMS	V	204	4/4	0.94	0.13	68,73,75,90	0
29	DMS	B	638	4/4	0.94	0.27	43,55,65,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
29	DMS	A	418	4/4	0.94	0.23	82,92,94,95	0
24	BCR	b	623	40/40	0.94	0.09	33,44,60,61	0
22	CLA	C	512	65/65	0.94	0.09	39,51,96,105	0
22	CLA	b	610	65/65	0.94	0.09	31,42,81,83	0
29	DMS	b	638	4/4	0.94	0.23	80,89,92,92	0
29	DMS	b	637	4/4	0.94	0.18	71,82,87,95	0
22	CLA	c	514	65/65	0.94	0.11	44,66,111,118	0
29	DMS	O	305	4/4	0.94	0.17	77,88,91,93	0
33	DGD	c	518	56/66	0.94	0.09	37,45,80,86	0
29	DMS	O	303	4/4	0.94	0.19	72,84,93,96	0
29	DMS	V	208	4/4	0.94	0.11	83,84,90,91	0
31	LHG	d	411	44/49	0.95	0.13	37,47,109,121	0
29	DMS	b	634	4/4	0.95	0.20	73,77,82,89	0
29	DMS	A	416	4/4	0.95	0.21	71,73,77,85	0
31	LHG	D	411	44/49	0.95	0.11	35,44,110,117	0
24	BCR	B	619	40/40	0.95	0.08	30,40,55,70	0
33	DGD	C	517	62/66	0.95	0.08	27,42,77,83	0
22	CLA	D	405	65/65	0.95	0.09	31,39,114,126	0
31	LHG	D	409	49/49	0.95	0.10	37,48,64,69	0
29	DMS	V	205	4/4	0.95	0.25	77,79,80,89	0
22	CLA	C	508	65/65	0.95	0.09	33,39,105,122	0
29	DMS	c	535	4/4	0.95	0.21	84,92,99,112	0
29	DMS	D	418	4/4	0.95	0.24	83,92,96,114	0
29	DMS	v	205	4/4	0.95	0.16	61,68,69,70	0
21	CL	v	201	1/1	0.95	0.26	93,93,93,93	0
29	DMS	b	639	4/4	0.95	0.27	87,93,94,106	0
34	GOL	C	533	6/6	0.95	0.17	46,53,57,61	0
29	DMS	B	641	4/4	0.95	0.25	65,66,71,83	0
29	DMS	a	420	4/4	0.95	0.17	87,90,91,93	0
33	DGD	c	519	62/66	0.95	0.09	32,45,73,87	0
29	DMS	b	635	4/4	0.95	0.22	70,71,71,73	0
26	LMG	D	412	47/55	0.95	0.10	34,44,84,95	0
29	DMS	v	203	4/4	0.95	0.18	76,78,80,82	0
29	DMS	B	636	4/4	0.95	0.25	65,83,88,91	0
29	DMS	c	537	4/4	0.95	0.31	85,94,103,106	0
29	DMS	C	531	4/4	0.95	0.12	86,87,90,92	0
22	CLA	C	507	65/65	0.95	0.10	37,44,68,75	0
22	CLA	c	508	65/65	0.95	0.09	34,44,68,76	0
39	MG	K	104	1/1	0.95	0.09	56,56,56,56	0
24	BCR	B	618	40/40	0.95	0.08	31,39,51,54	0
22	CLA	c	512	65/65	0.96	0.10	40,49,56,65	0
22	CLA	a	409	65/65	0.96	0.11	29,37,126,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	607	65/65	0.96	0.09	32,39,71,87	0
29	DMS	V	203	4/4	0.96	0.15	74,84,87,92	0
30	CA	c	501	1/1	0.96	0.10	62,62,62,62	0
22	CLA	B	603	65/65	0.96	0.08	30,38,46,50	0
22	CLA	C	503	65/65	0.96	0.08	33,41,47,58	0
22	CLA	c	505	65/65	0.96	0.07	35,40,74,82	0
22	CLA	b	606	65/65	0.96	0.09	32,37,48,59	0
22	CLA	b	611	65/65	0.96	0.07	26,32,50,58	0
22	CLA	A	408	65/65	0.96	0.09	25,34,110,115	0
24	BCR	A	409	40/40	0.96	0.08	28,35,42,44	0
29	DMS	B	637	4/4	0.96	0.12	69,73,81,82	0
22	CLA	b	616	65/65	0.96	0.08	29,36,44,50	0
22	CLA	b	619	65/65	0.96	0.08	32,42,59,67	0
22	CLA	C	510	65/65	0.96	0.08	33,40,52,66	0
22	CLA	c	509	65/65	0.96	0.08	34,41,100,113	0
29	DMS	b	631	4/4	0.96	0.08	66,78,80,82	0
22	CLA	b	614	65/65	0.96	0.07	30,40,46,51	0
30	CA	V	209	1/1	0.96	0.15	93,93,93,93	0
22	CLA	c	510	65/65	0.96	0.10	30,42,76,81	0
29	DMS	b	632	4/4	0.96	0.12	63,72,72,73	0
22	CLA	C	509	65/65	0.96	0.10	33,42,68,76	0
22	CLA	d	405	65/65	0.96	0.08	31,43,111,120	0
33	DGD	C	515	62/66	0.96	0.11	30,41,105,109	0
25	PL9	d	407	55/55	0.96	0.08	27,34,46,55	0
22	CLA	c	504	65/65	0.96	0.08	34,47,56,58	0
24	BCR	B	620	40/40	0.96	0.08	31,41,57,60	0
29	DMS	C	528	4/4	0.96	0.25	74,81,82,82	0
24	BCR	b	622	40/40	0.96	0.08	29,44,58,67	0
24	BCR	a	410	40/40	0.96	0.07	32,39,45,46	0
24	BCR	C	514	40/40	0.96	0.09	35,46,60,63	0
29	DMS	c	530	4/4	0.96	0.17	70,88,95,104	0
22	CLA	B	611	65/65	0.96	0.09	30,37,44,57	0
24	BCR	b	621	40/40	0.96	0.07	36,42,55,58	0
22	CLA	a	407	65/65	0.97	0.08	25,33,104,120	0
22	CLA	B	610	65/65	0.97	0.10	33,41,49,54	0
25	PL9	D	407	55/55	0.97	0.08	26,35,43,54	0
22	CLA	c	502	65/65	0.97	0.07	38,43,56,64	0
29	DMS	d	415	4/4	0.97	0.18	64,70,75,87	0
29	DMS	C	526	4/4	0.97	0.20	60,61,66,69	0
22	CLA	C	511	65/65	0.97	0.09	36,44,50,53	0
31	LHG	b	624	49/49	0.97	0.09	33,42,65,76	0
22	CLA	c	506	65/65	0.97	0.07	34,43,57,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	DMS	o	305	4/4	0.97	0.31	88,91,92,102	0
23	PHO	a	408	64/64	0.97	0.07	27,33,38,42	0
39	MG	J	101	1/1	0.97	0.04	45,45,45,45	0
22	CLA	B	615	65/65	0.97	0.07	27,36,115,119	0
31	LHG	d	409	49/49	0.97	0.12	40,47,64,70	0
39	MG	k	102	1/1	0.97	0.13	61,61,61,61	0
23	PHO	D	404	64/64	0.97	0.08	25,34,41,45	0
22	CLA	b	607	65/65	0.97	0.07	29,36,47,51	0
22	CLA	A	404	65/65	0.97	0.09	22,28,40,59	0
22	CLA	B	608	65/65	0.97	0.08	24,31,47,62	0
22	CLA	C	502	65/65	0.97	0.07	30,36,52,61	0
29	DMS	c	531	4/4	0.97	0.27	90,91,96,98	0
22	CLA	B	604	65/65	0.97	0.07	26,34,44,55	0
29	DMS	B	632	4/4	0.97	0.09	53,54,55,69	0
22	CLA	b	613	65/65	0.97	0.10	35,40,50,54	0
29	DMS	o	308	4/4	0.97	0.26	71,77,85,85	0
22	CLA	b	608	65/65	0.97	0.08	29,35,75,79	0
22	CLA	C	505	65/65	0.97	0.07	34,41,54,60	0
22	CLA	B	614	65/65	0.97	0.07	26,32,69,94	0
22	CLA	c	511	65/65	0.97	0.08	30,40,54,58	0
29	DMS	C	530	4/4	0.97	0.16	40,54,55,58	0
31	LHG	B	621	49/49	0.97	0.10	33,41,61,65	0
22	CLA	b	617	65/65	0.97	0.08	30,35,74,80	0
22	CLA	D	403	65/65	0.97	0.08	23,28,49,53	0
29	DMS	C	525	4/4	0.97	0.10	42,51,52,58	0
22	CLA	c	503	65/65	0.97	0.07	31,38,55,64	0
31	LHG	d	410	49/49	0.97	0.11	27,38,58,73	0
33	DGD	c	517	62/66	0.97	0.09	32,46,93,108	0
22	CLA	C	504	65/65	0.97	0.07	32,38,72,74	0
22	CLA	a	406	65/65	0.97	0.10	25,31,40,56	0
36	BCT	d	401[A]	4/4	0.97	0.12	50,52,55,67	4
22	CLA	B	616	65/65	0.97	0.07	32,39,61,67	0
24	BCR	k	101	40/40	0.97	0.12	41,48,56,58	0
29	DMS	o	311	4/4	0.97	0.20	80,91,94,116	0
23	PHO	A	407	64/64	0.97	0.07	25,30,33,38	0
22	CLA	b	618	65/65	0.97	0.09	29,36,123,128	0
22	CLA	B	605	65/65	0.97	0.08	26,33,65,73	0
22	CLA	b	612	65/65	0.97	0.07	26,35,44,49	0
37	HEM	F	101	43/43	0.97	0.09	43,52,63,69	0
36	BCT	d	401[B]	4/4	0.97	0.12	21,31,31,38	4
22	CLA	C	501	65/65	0.97	0.08	32,41,55,66	0
29	DMS	o	304	4/4	0.97	0.14	85,86,87,87	0

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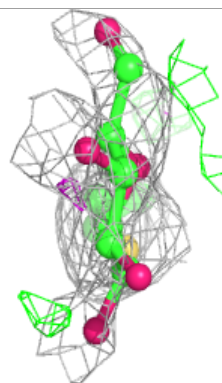
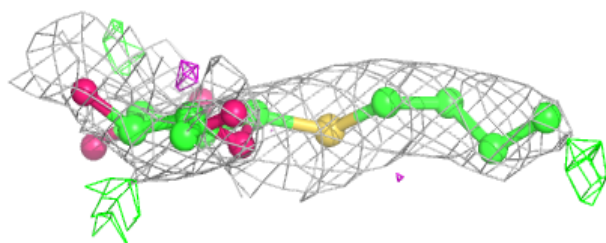
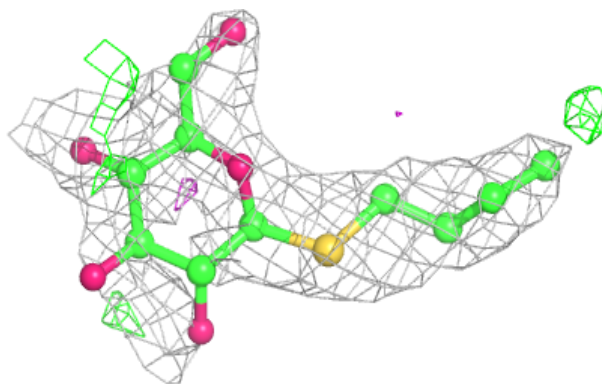
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	609	65/65	0.98	0.07	28,35,44,47	0
22	CLA	b	609	65/65	0.98	0.09	28,33,47,48	0
29	DMS	D	415	4/4	0.98	0.11	65,68,77,91	0
30	CA	b	604	1/1	0.98	0.07	63,63,63,63	0
40	HEC	v	202	43/43	0.98	0.09	37,44,49,57	0
39	MG	j	101	1/1	0.98	0.06	50,50,50,50	0
22	CLA	B	613	65/65	0.98	0.07	28,33,40,43	0
22	CLA	A	406	65/65	0.98	0.06	24,33,95,113	0
36	BCT	D	402[A]	4/4	0.98	0.16	24,36,36,40	4
29	DMS	b	630	4/4	0.98	0.10	37,40,40,42	0
31	LHG	D	410	49/49	0.98	0.12	30,38,53,67	0
22	CLA	d	403	65/65	0.98	0.07	26,29,43,53	0
29	DMS	B	631	4/4	0.98	0.09	31,35,36,42	0
40	HEC	V	201	43/43	0.98	0.10	28,32,39,44	0
22	CLA	d	402	65/65	0.98	0.09	25,30,48,56	0
29	DMS	D	416	4/4	0.98	0.17	68,80,85,89	0
37	HEM	f	101	43/43	0.98	0.07	42,50,58,63	0
22	CLA	b	615	65/65	0.98	0.08	25,33,52,55	0
29	DMS	c	529	4/4	0.98	0.16	52,56,57,67	0
36	BCT	D	402[B]	4/4	0.98	0.16	36,44,46,50	4
29	DMS	c	528	4/4	0.98	0.10	41,54,55,56	0
22	CLA	A	405	65/65	0.98	0.07	22,27,39,48	0
30	CA	o	302	1/1	0.98	0.07	58,58,58,58	0
22	CLA	B	606	65/65	0.98	0.09	28,34,51,56	0
23	PHO	d	404	64/64	0.98	0.09	27,34,41,48	0
30	CA	O	301	1/1	0.98	0.05	57,57,57,57	0
22	CLA	B	612	65/65	0.98	0.07	25,32,48,55	0
21	CL	A	402	1/1	0.99	0.04	31,31,31,31	0
21	CL	a	404	1/1	0.99	0.02	35,35,35,35	0
29	DMS	A	417	4/4	0.99	0.07	32,36,37,38	0
21	CL	a	405	1/1	0.99	0.06	34,34,34,34	0
29	DMS	o	303	4/4	0.99	0.05	31,40,41,44	0
20	OEX	a	402	10/10	0.99	0.04	28,33,39,41	0
30	CA	B	601	1/1	0.99	0.10	60,60,60,60	0
20	OEX	A	401	10/10	1.00	0.04	28,31,39,40	0
35	FE2	D	401	1/1	1.00	0.06	41,41,41,41	0
35	FE2	a	403	1/1	1.00	0.07	40,40,40,40	0
21	CL	A	403	1/1	1.00	0.04	29,29,29,29	0

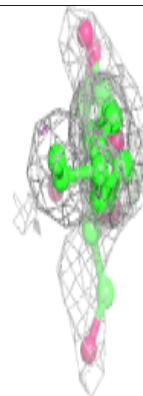
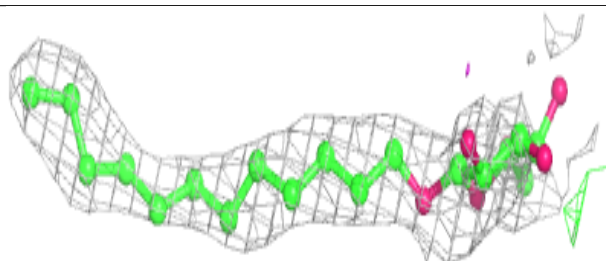
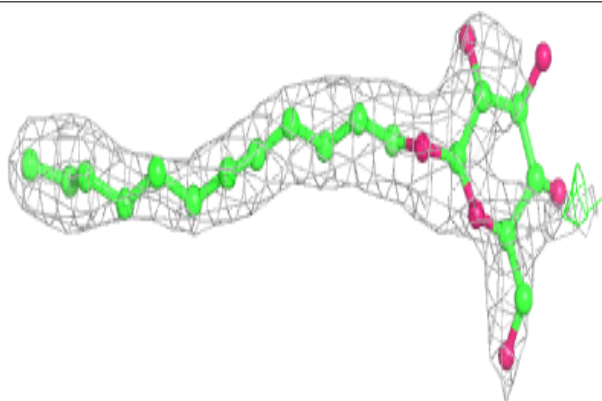
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG 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)

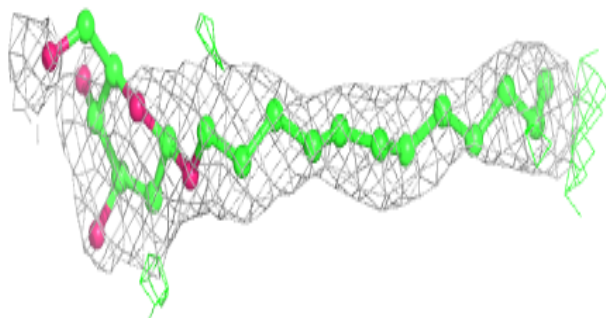
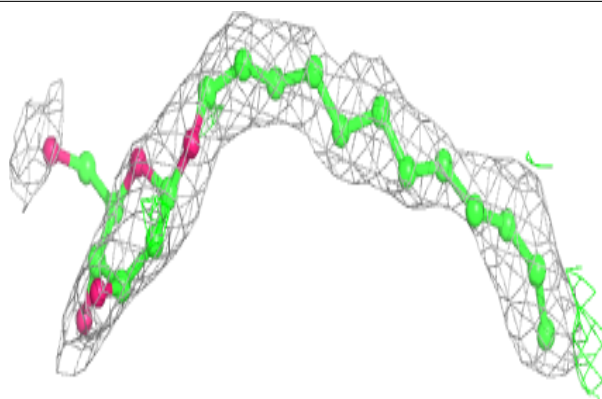
**Electron density around LMT J 102:**

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

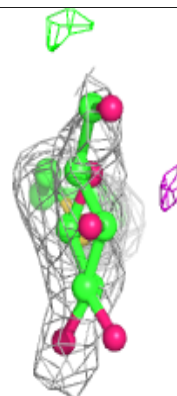
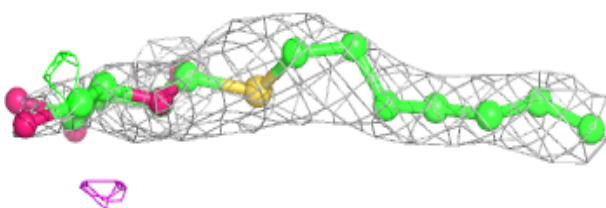
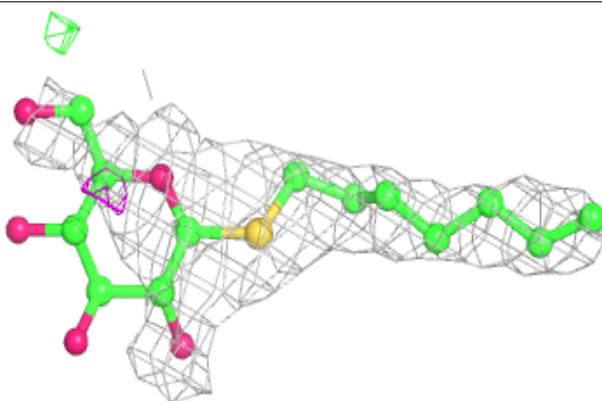


Electron density around LMT m 103:

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

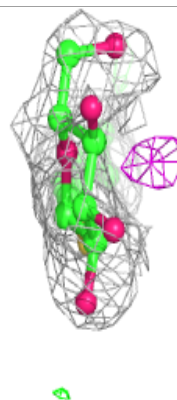
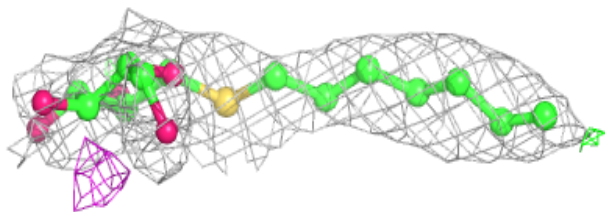
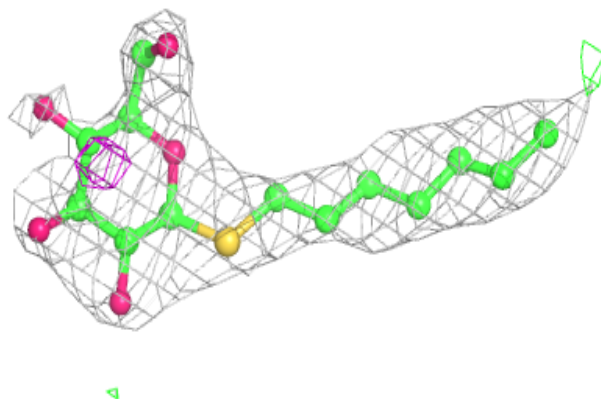
**Electron density around HTG C 536:**

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



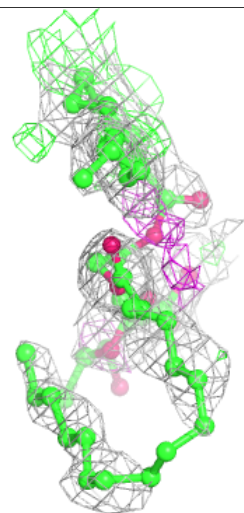
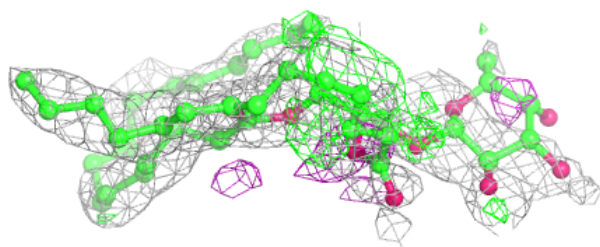
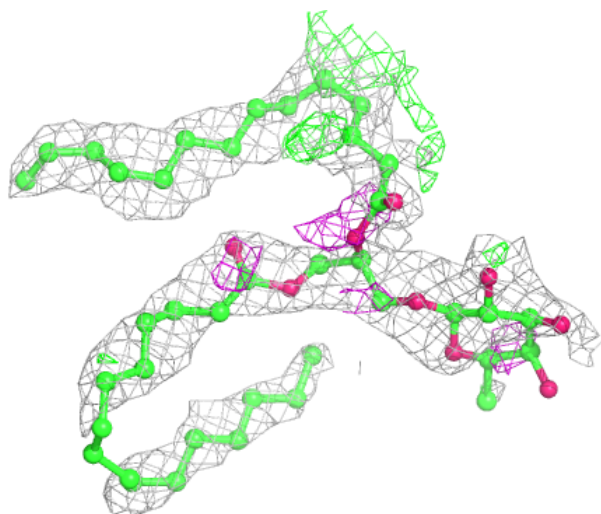
Electron density around HTG b 602:

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



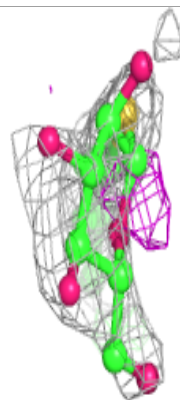
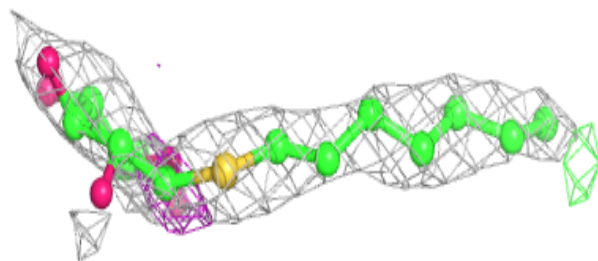
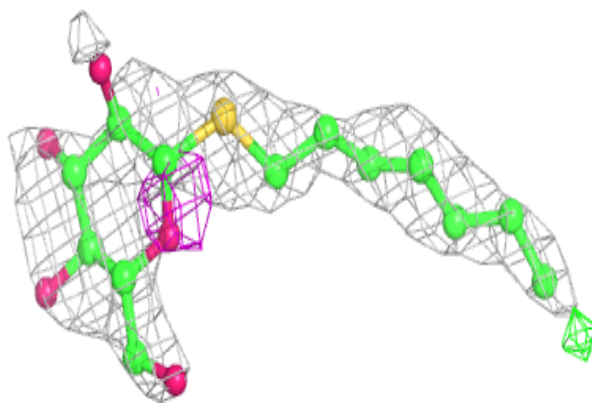
Electron density around DGD d 408:

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

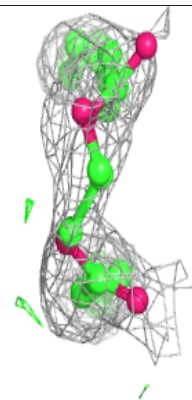
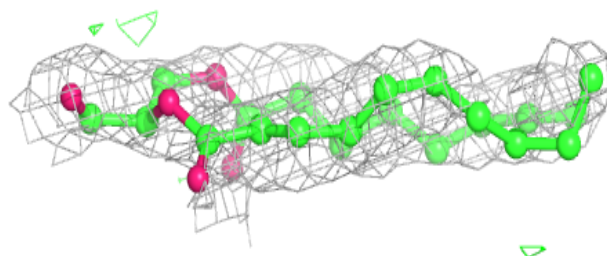
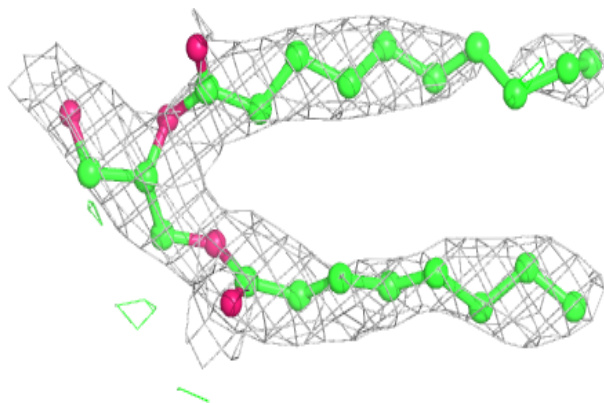


Electron density around HTG B 624:

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

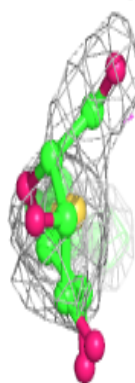
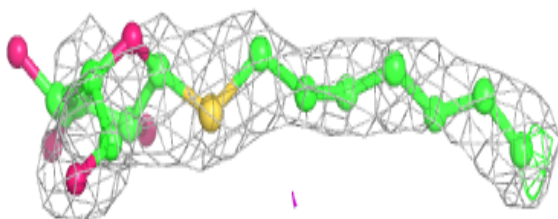
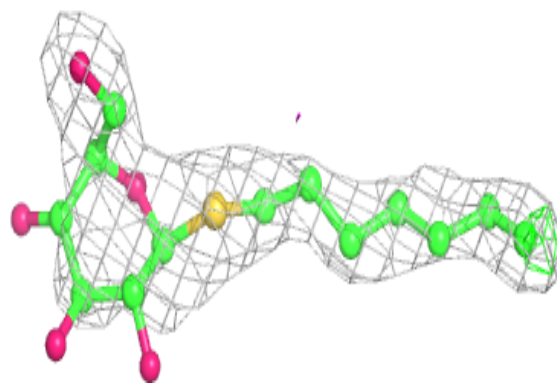
**Electron density around UNL C 524:**

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

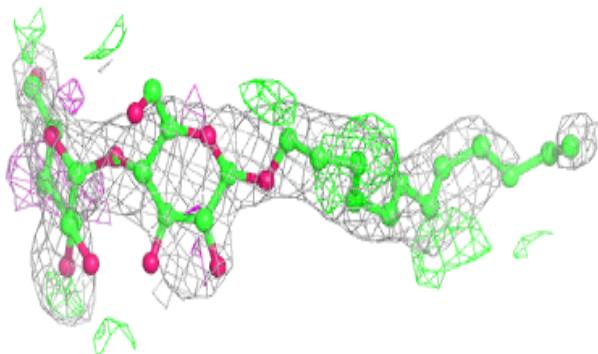
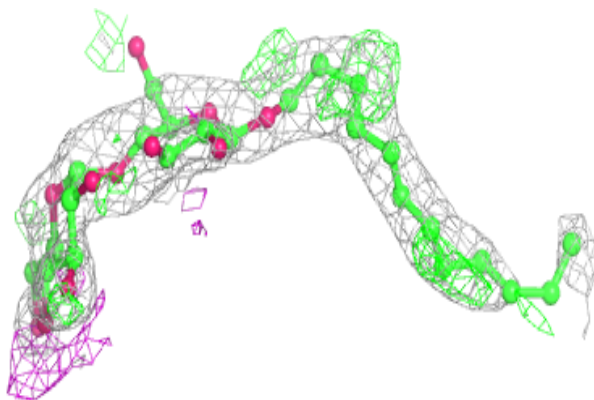


Electron density around HTG C 522:

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

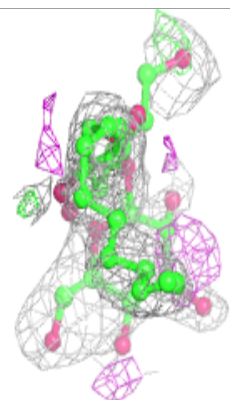
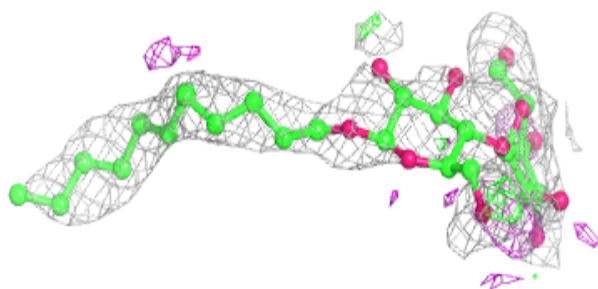
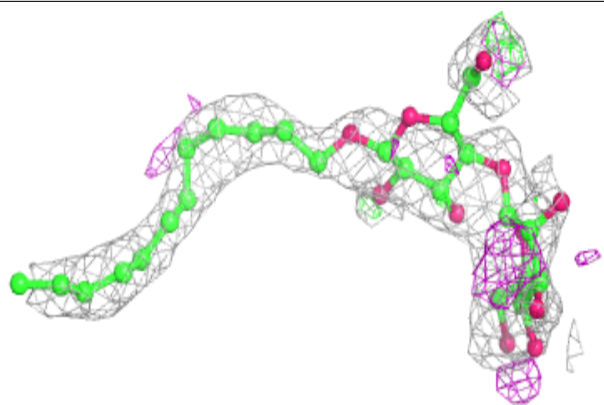
**Electron density around LMT a 401:**

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

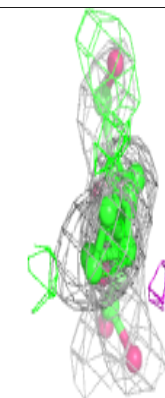
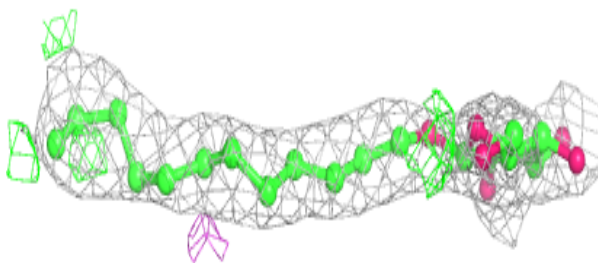
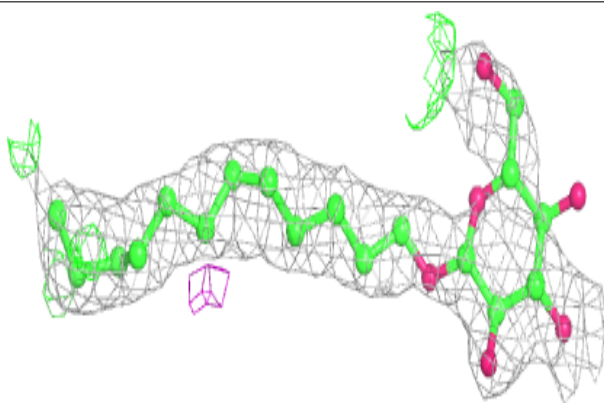


Electron density around LMT A 415:

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

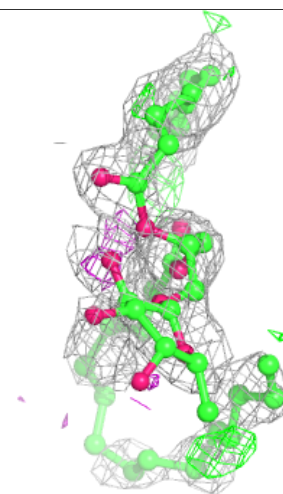
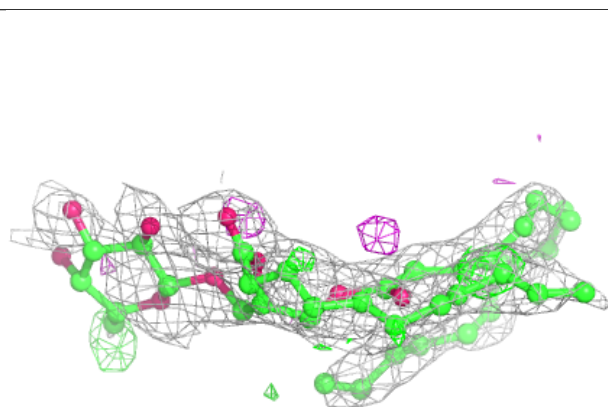
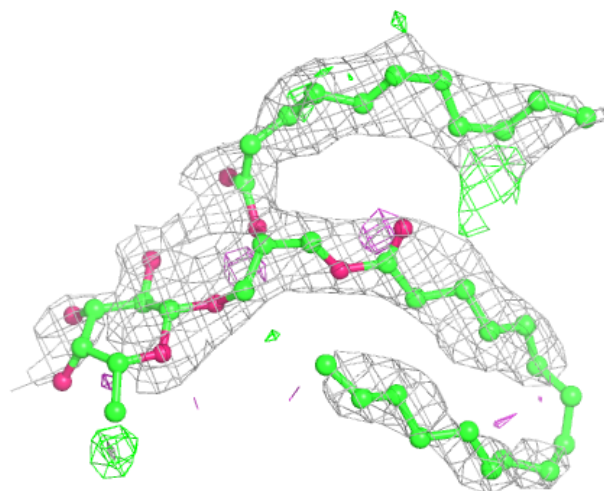
**Electron density around LMT I 101:**

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



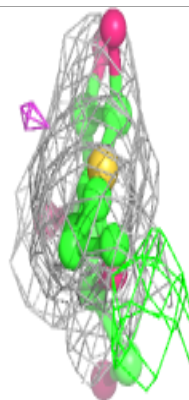
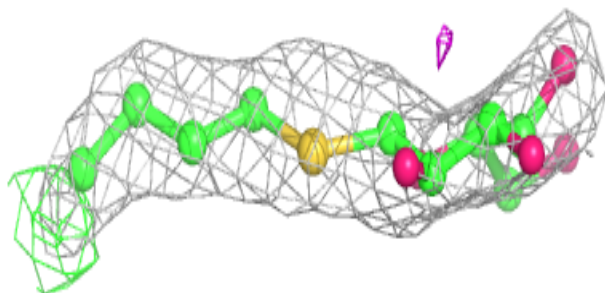
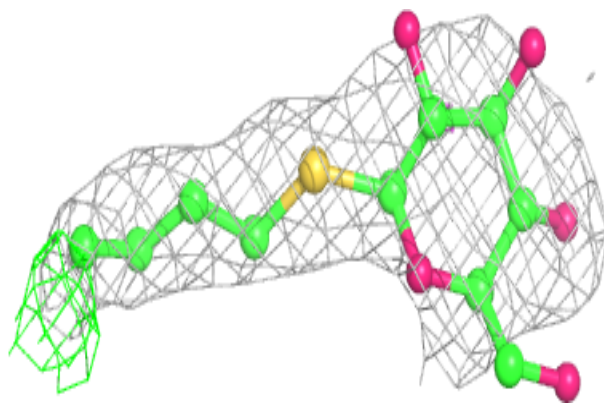
Electron density around DGD D 408:

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



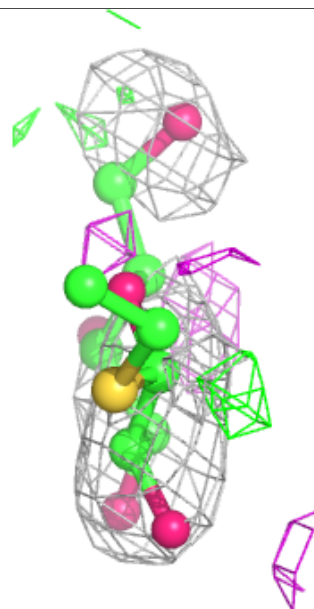
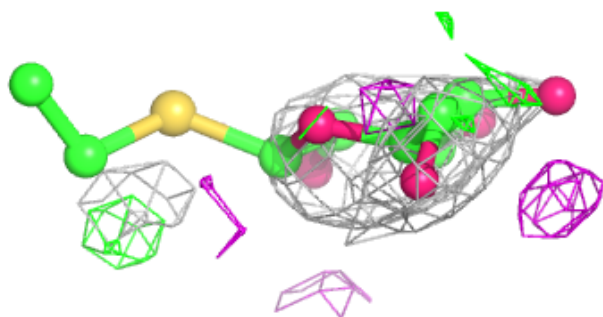
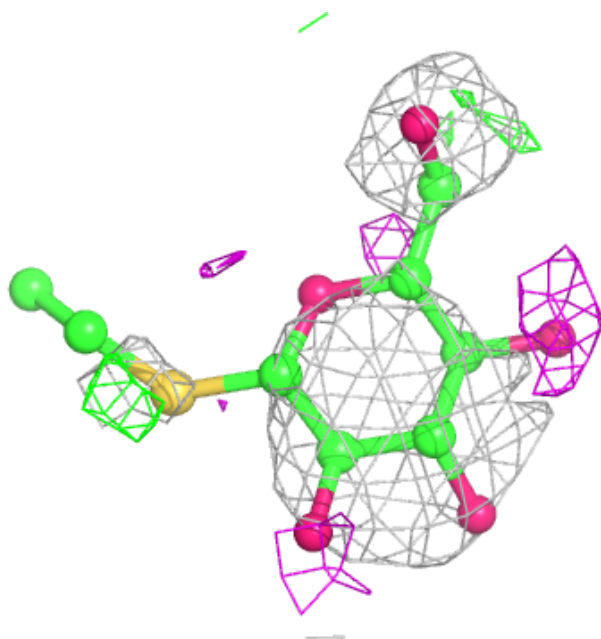
Electron density around HTG d 413:

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



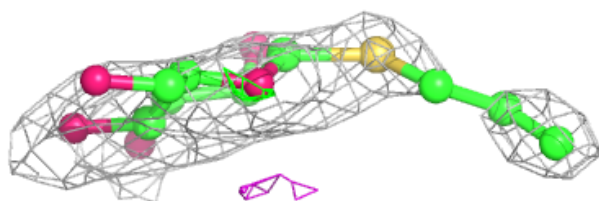
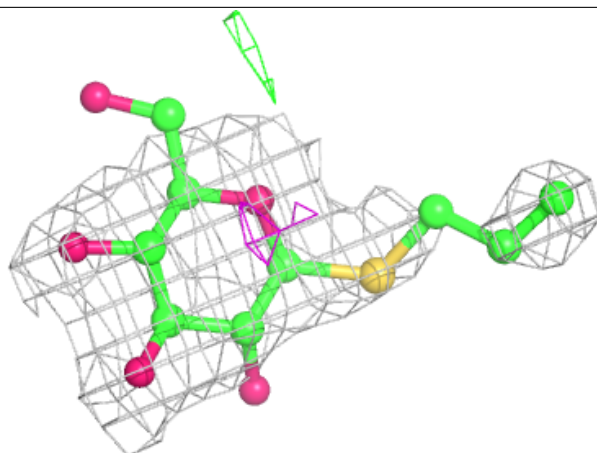
Electron density around HTG U 203:

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

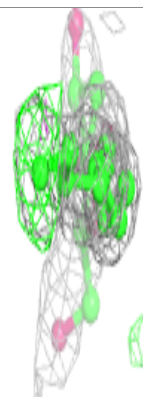
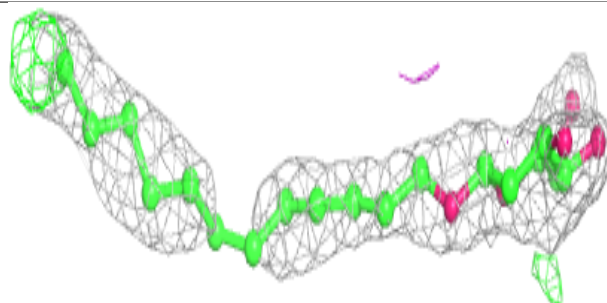
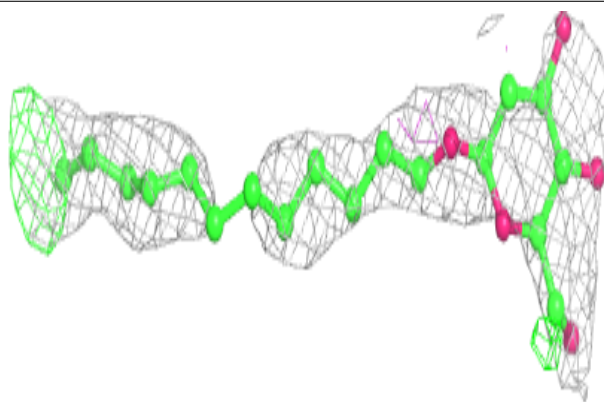


Electron density around HTG c 541:

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

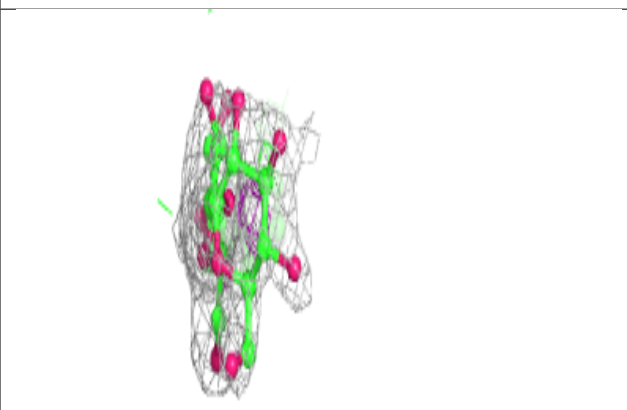
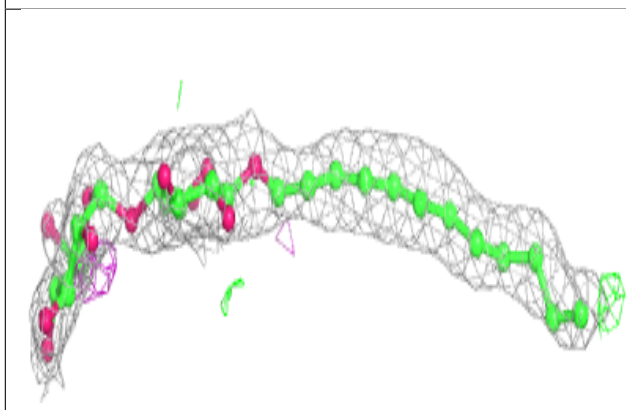
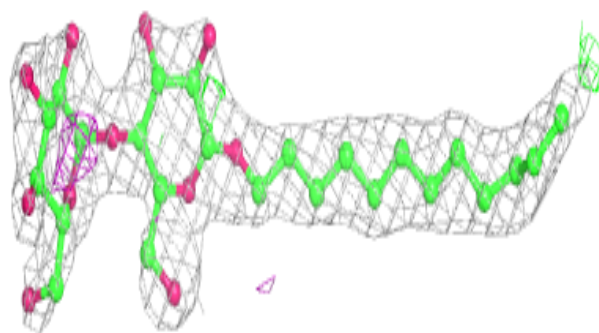
**Electron density around LMT j 102:**

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

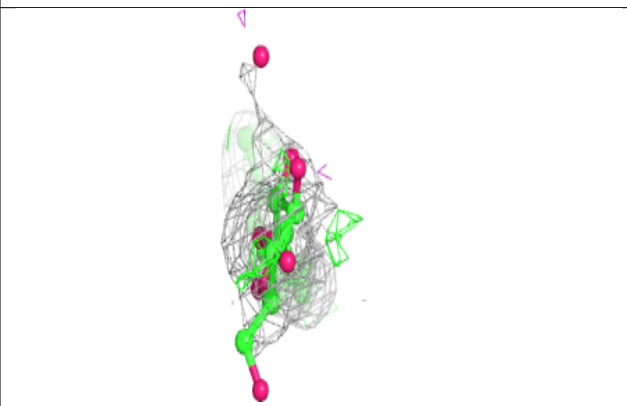
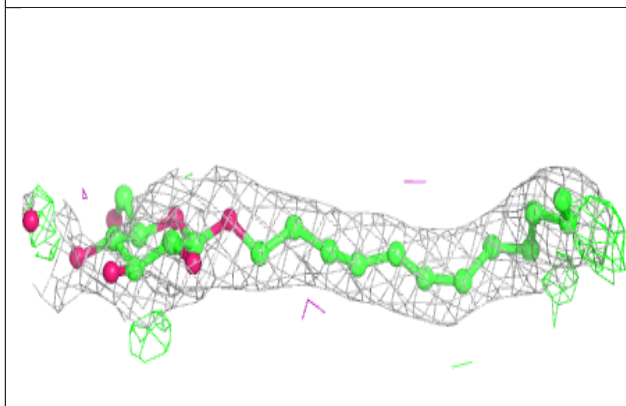
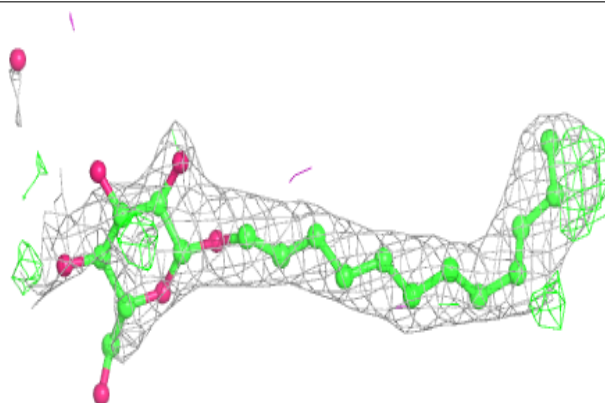


Electron density around LMT m 101:

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

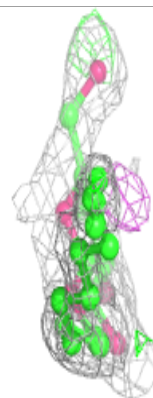
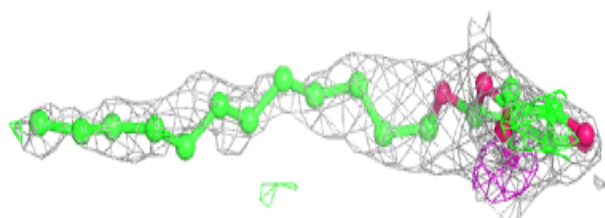
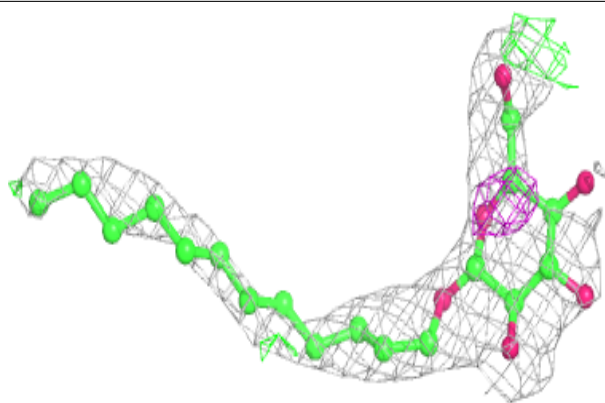
**Electron density around LMT m 102:**

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

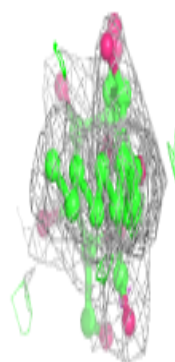
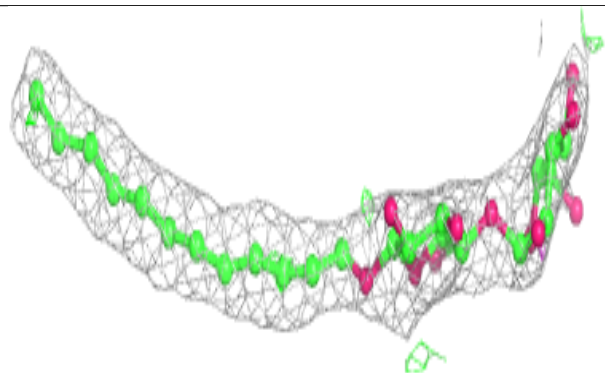
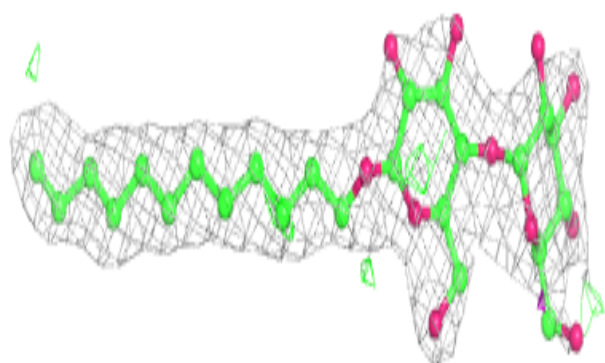


Electron density around LMT F 102:

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

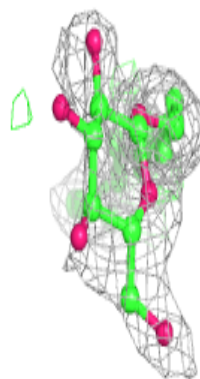
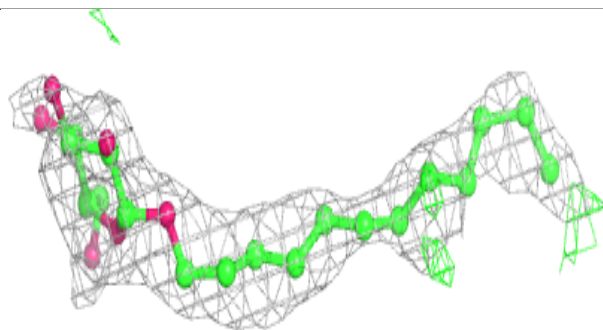
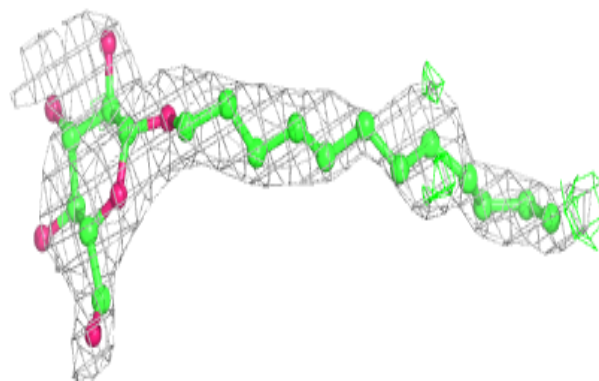
**Electron density around LMT M 101:**

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

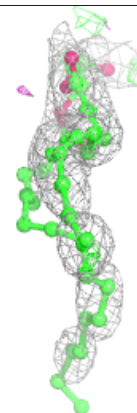
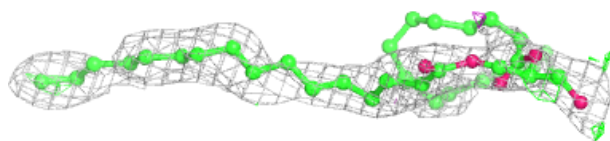


Electron density around LMT t 102:

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

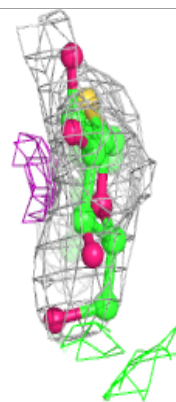
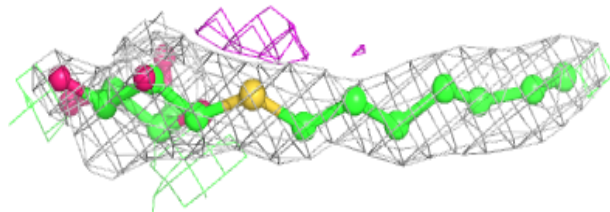
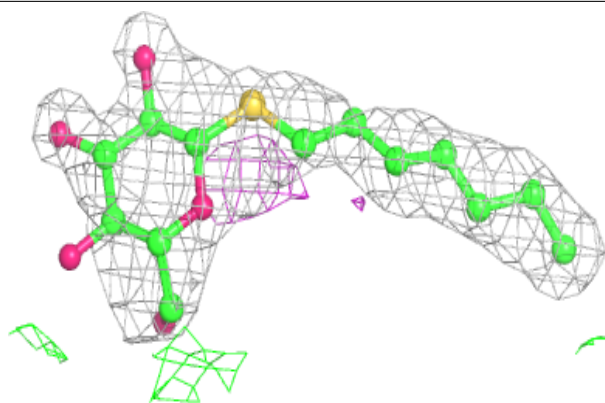
**Electron density around UNL a 415:**

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



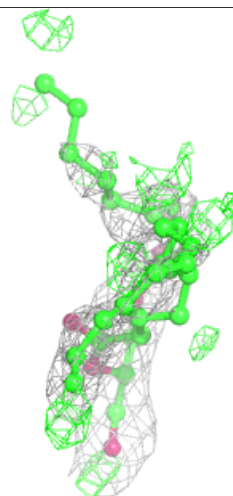
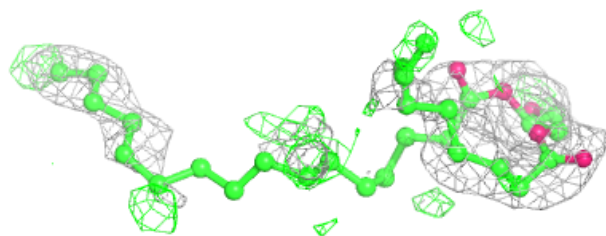
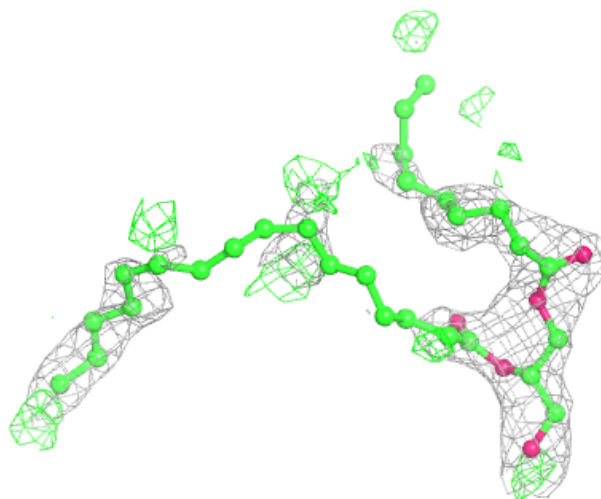
Electron density around HTG B 629:

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



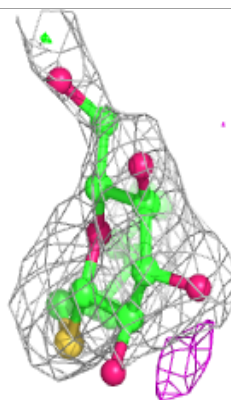
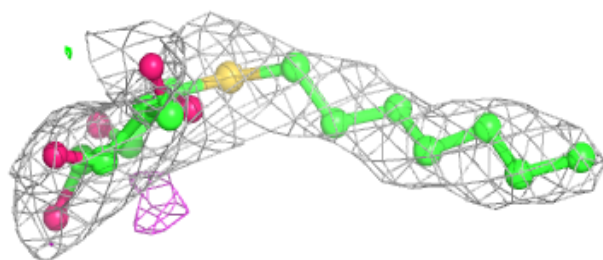
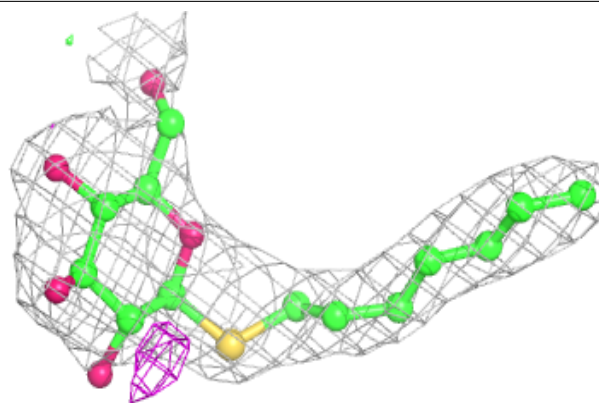
Electron density around UNL j 103:

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

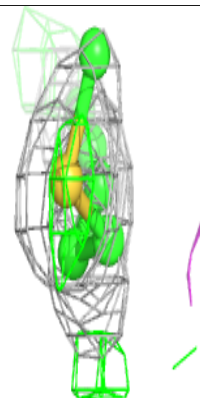
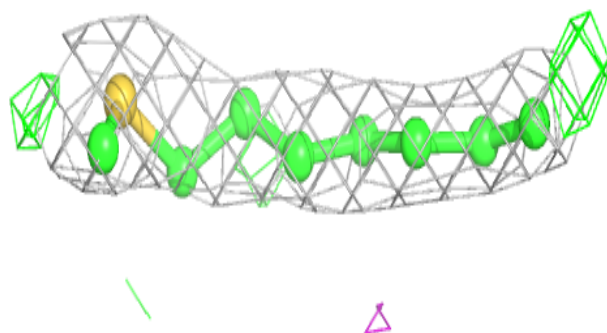
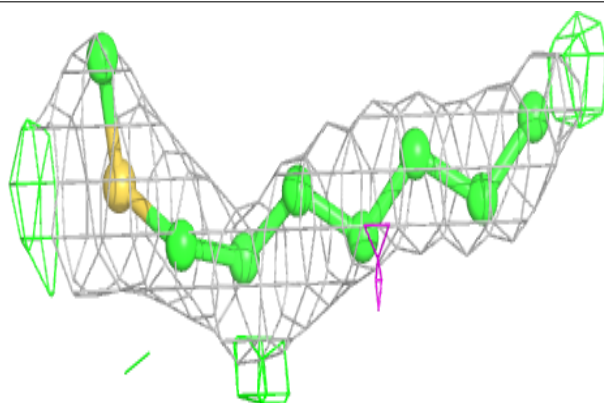


Electron density around HTG b 627:

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

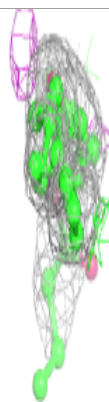
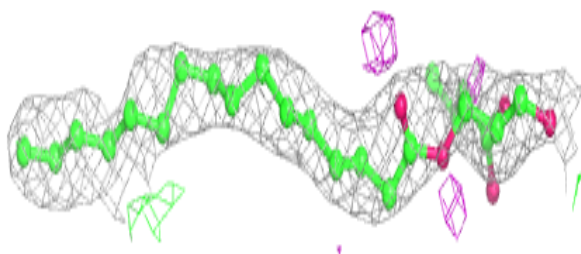
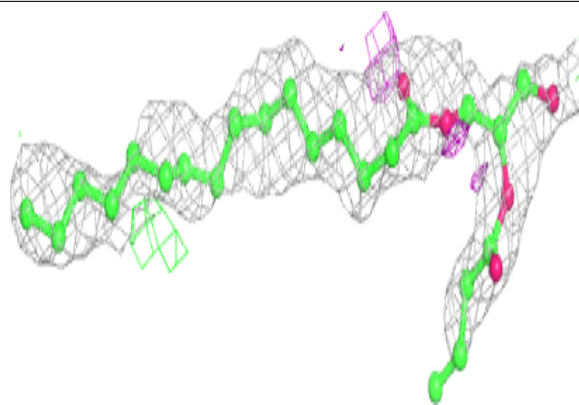
**Electron density around HTG c 524:**

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

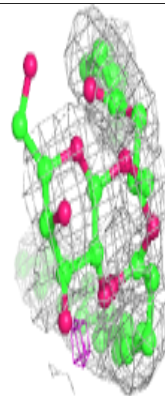
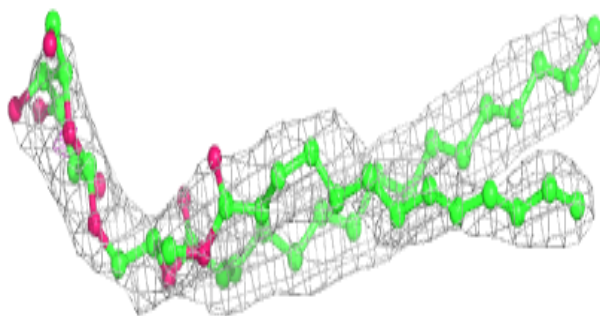
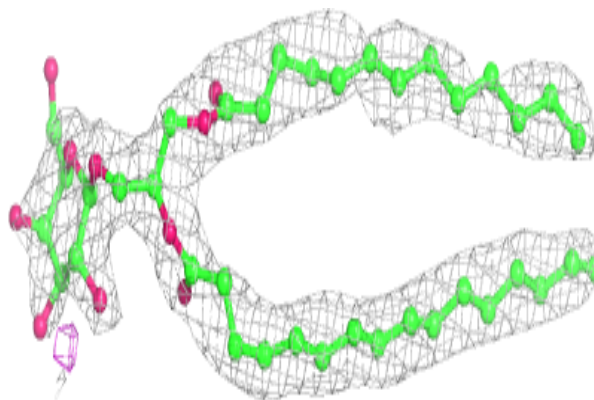


Electron density around UNL A 414:

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

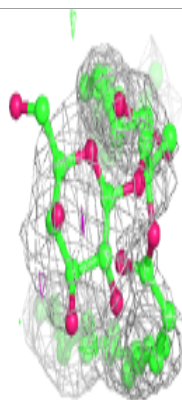
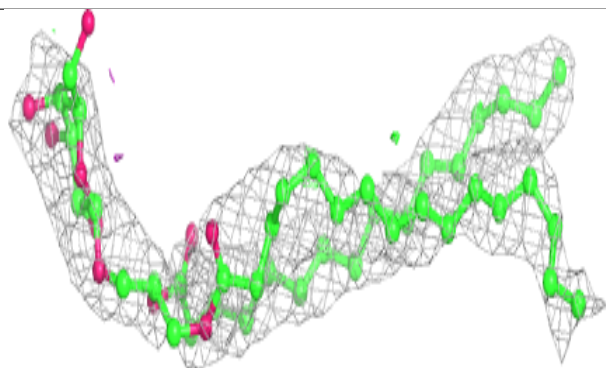
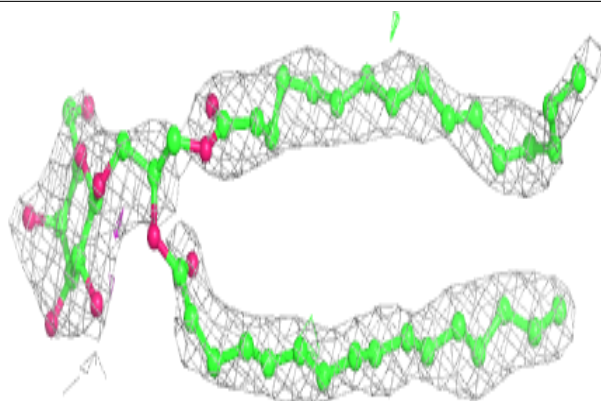
**Electron density around LMG C 519:**

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

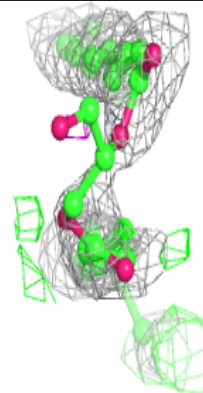
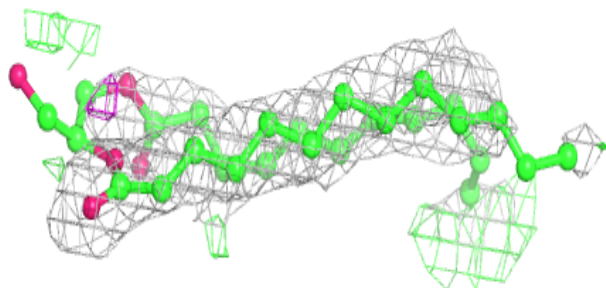
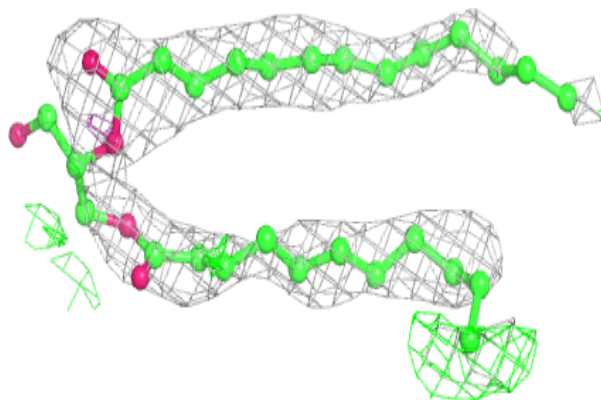


Electron density around LMG c 521:

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

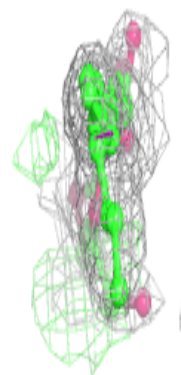
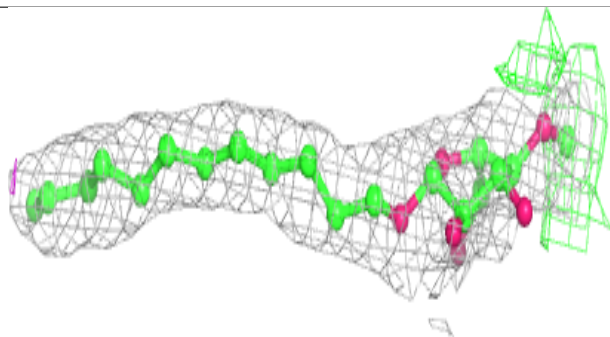
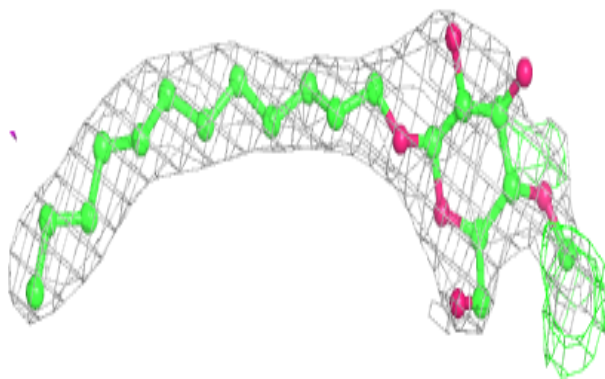
**Electron density around UNL c 526:**

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



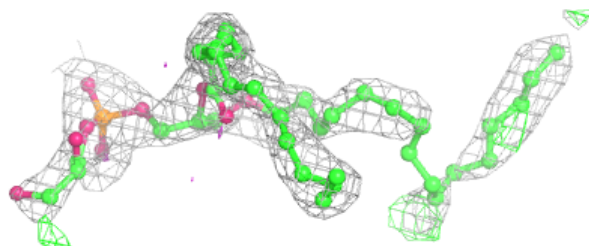
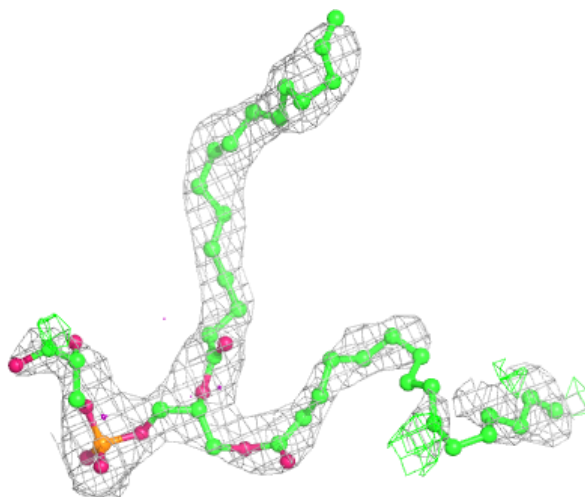
Electron density around LMT b 626:

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



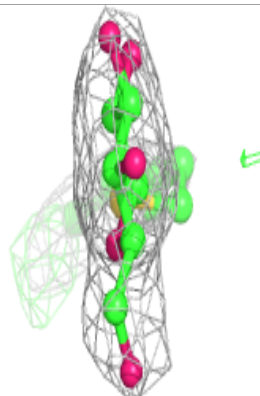
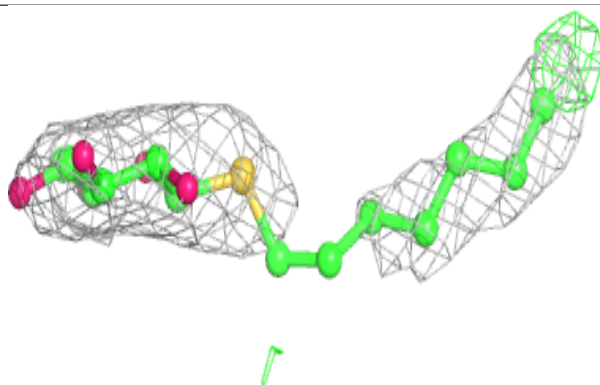
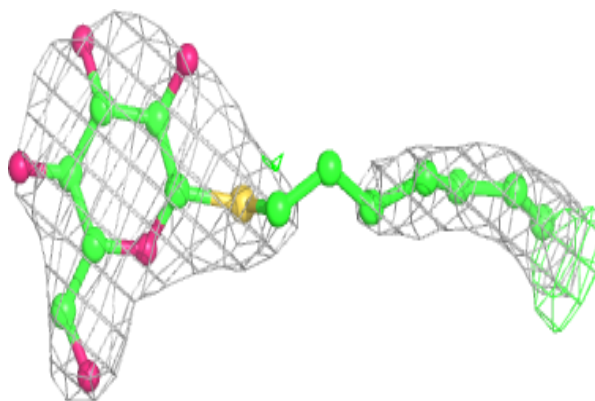
Electron density around LHG E 101:

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

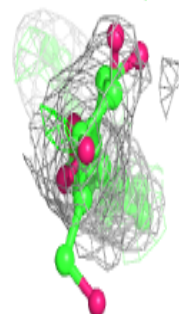
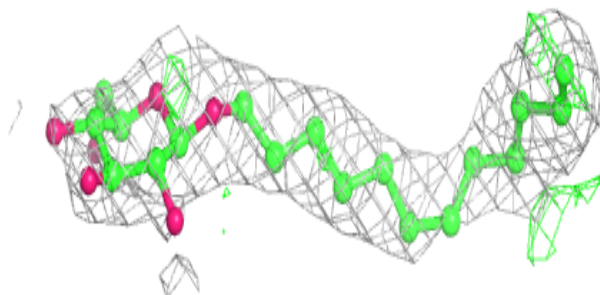
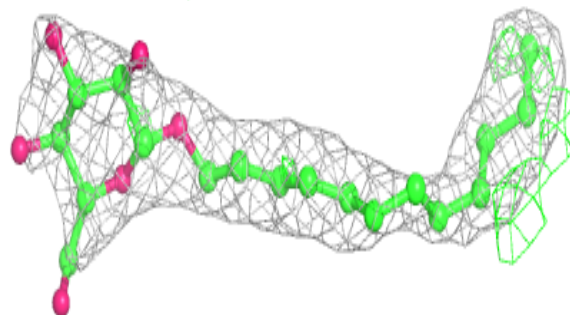


Electron density around HTG c 523:

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

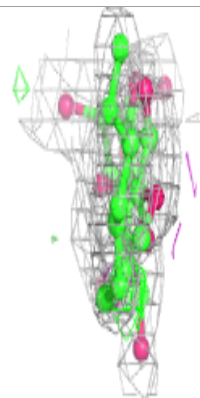
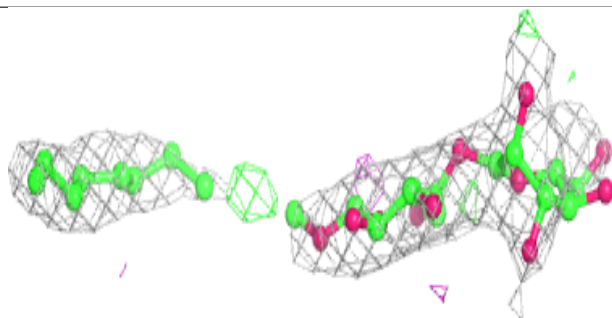
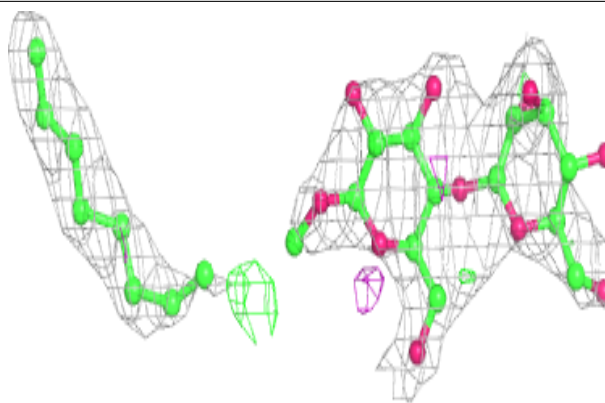
**Electron density around LMT T 102:**

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

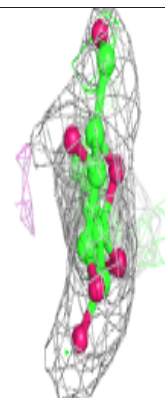
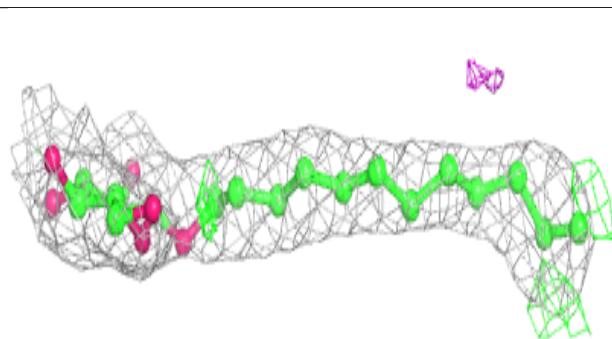
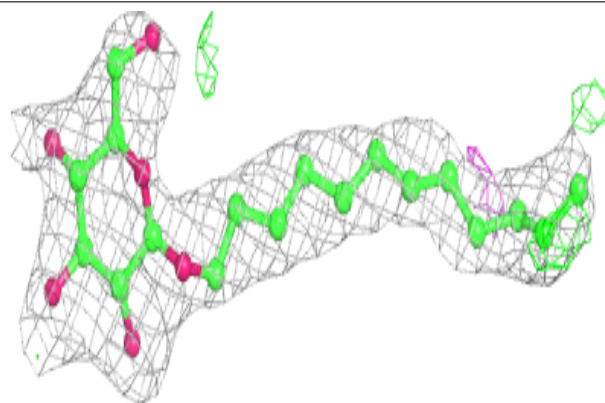


Electron density around LMT z 101:

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

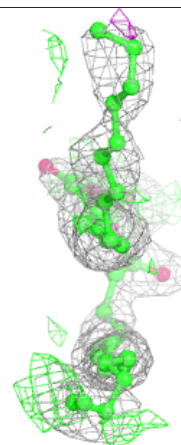
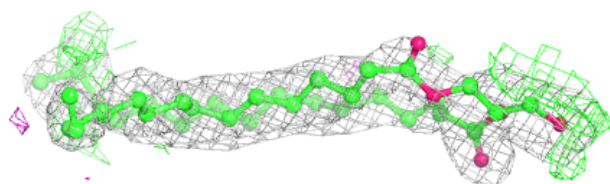
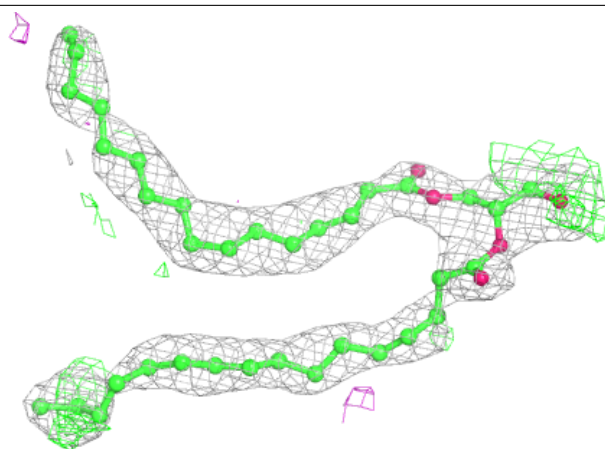
**Electron density around LMT M 102:**

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



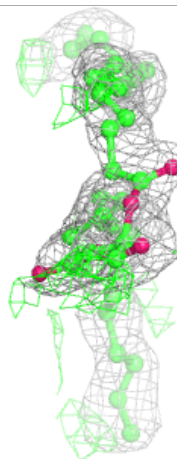
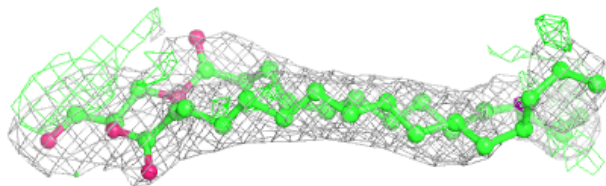
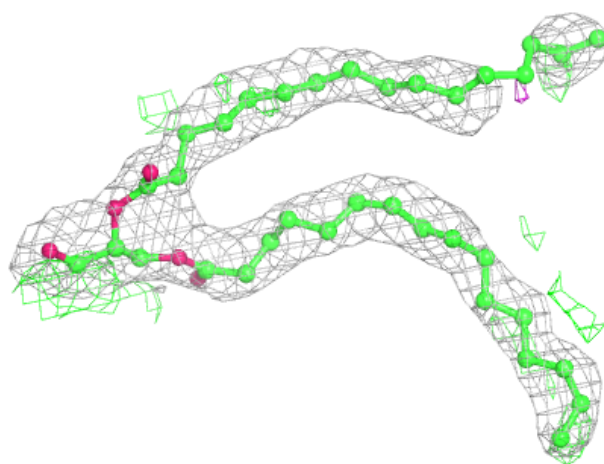
Electron density around UNL b 641:

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



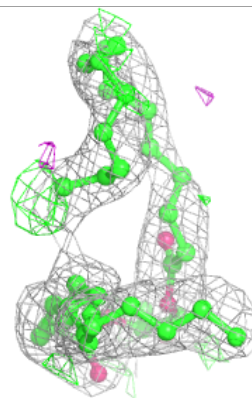
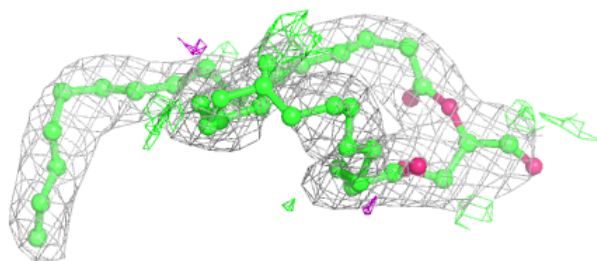
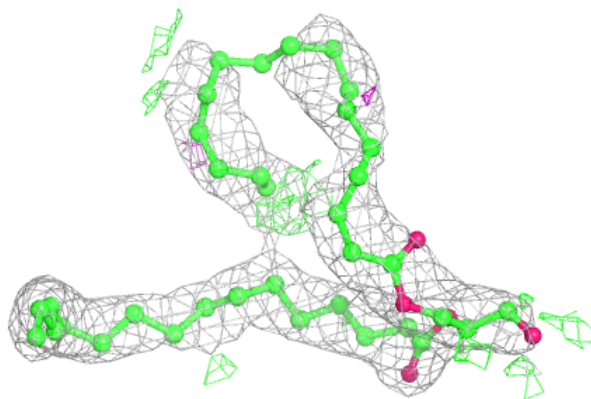
Electron density around UNL B 643:

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

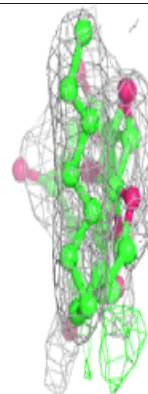
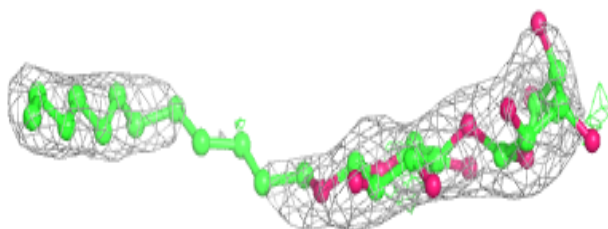
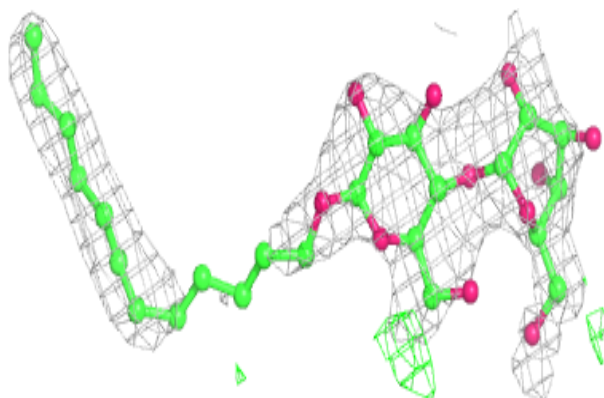


Electron density around UNL A 421:

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

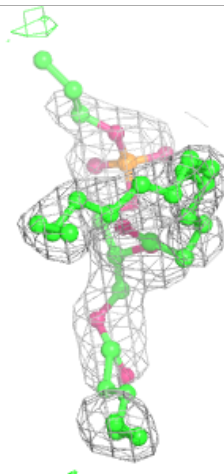
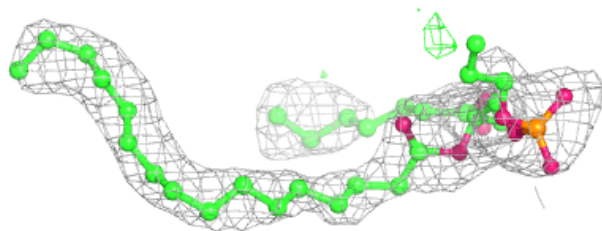
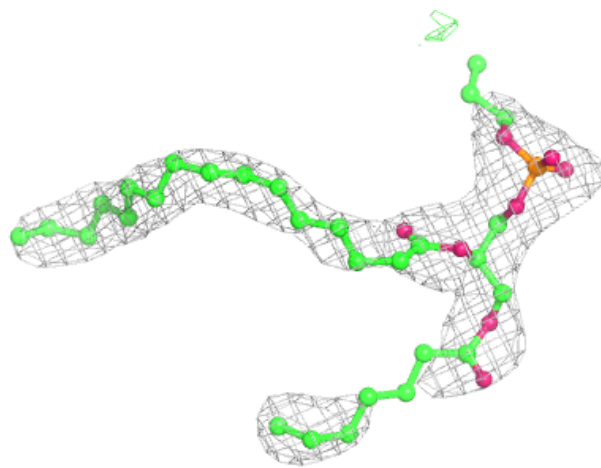
**Electron density around LMT Z 101:**

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



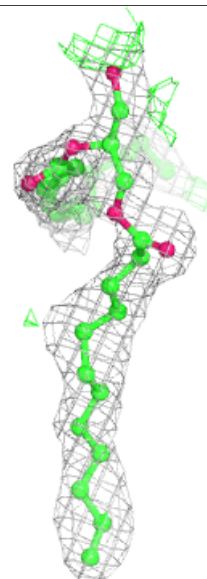
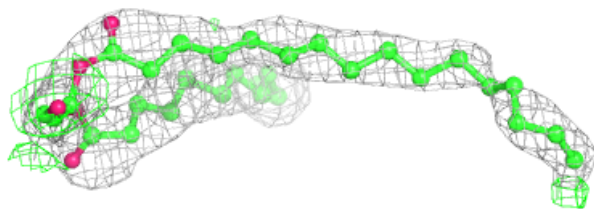
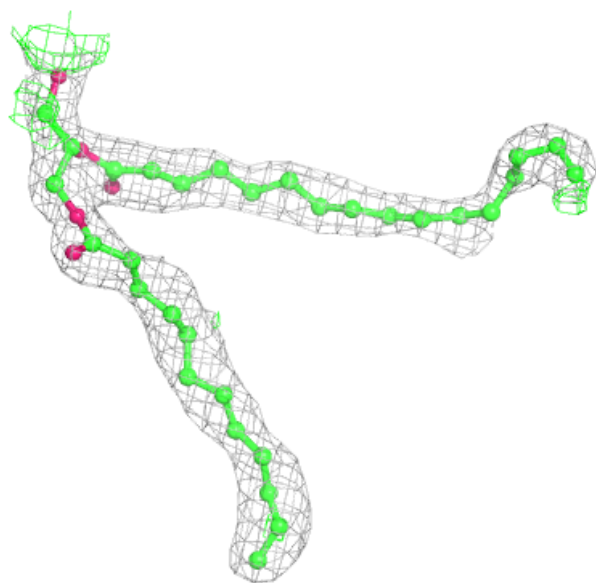
Electron density around LHG e 101:

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



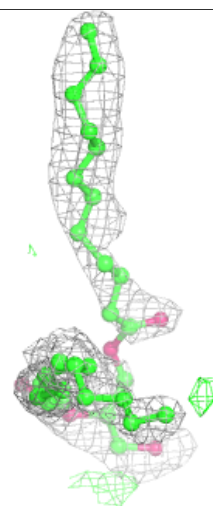
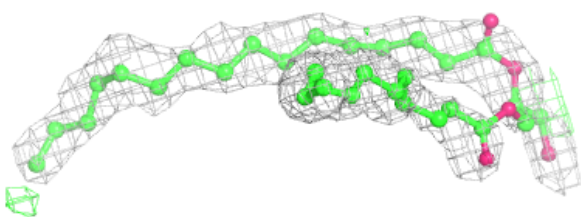
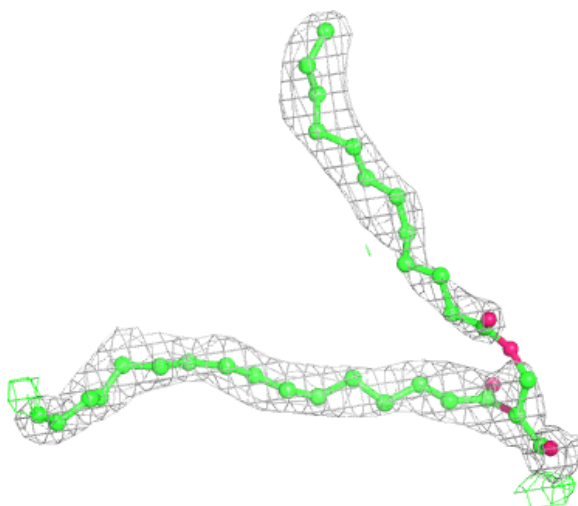
Electron density around UNL A 420:

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



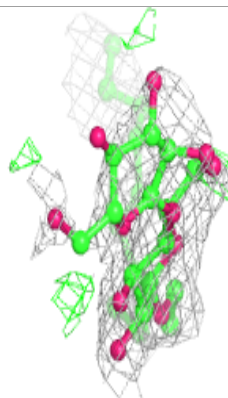
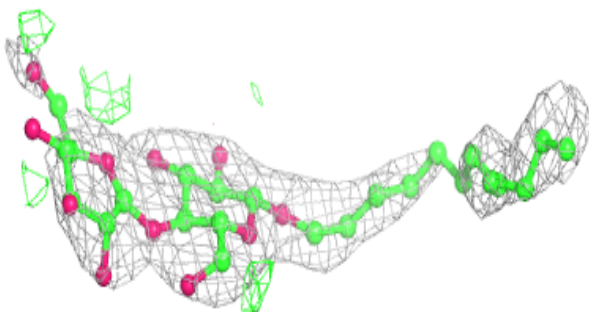
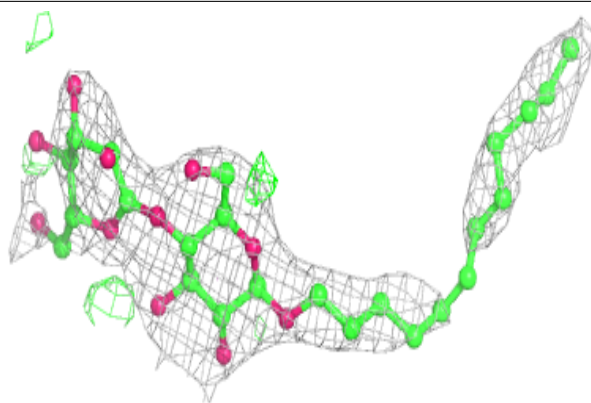
Electron density around UNL d 417:

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

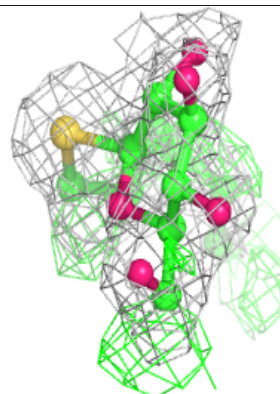
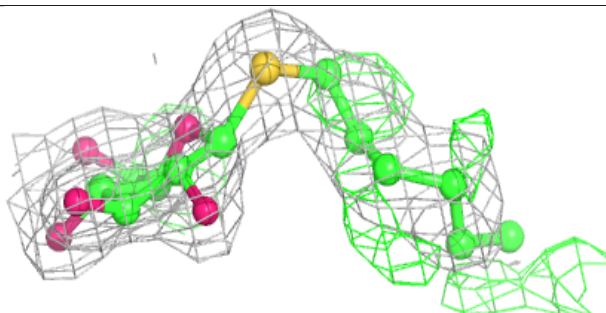
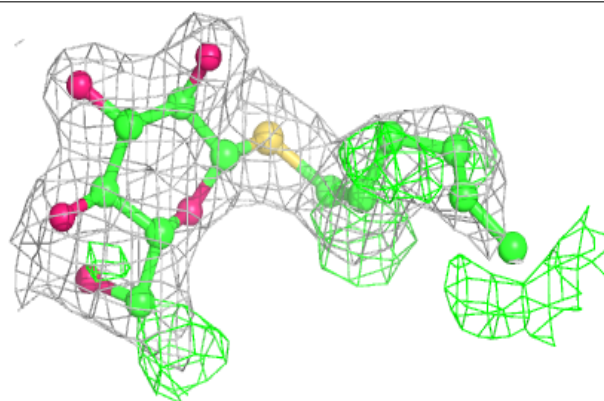


Electron density around LMT C 520:

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

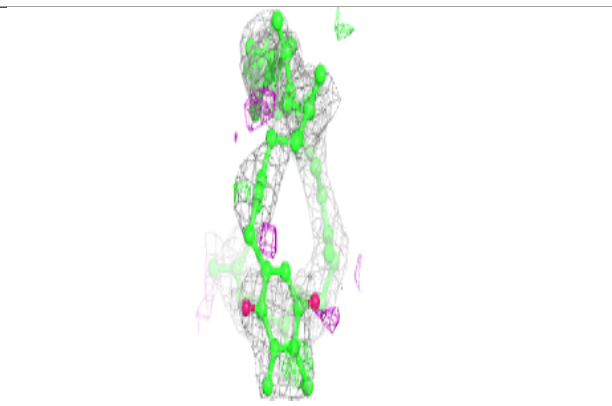
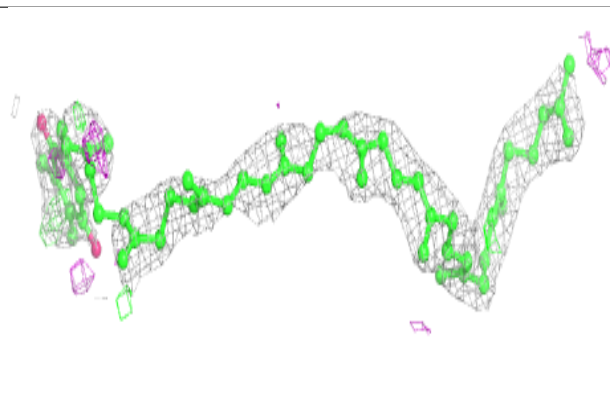
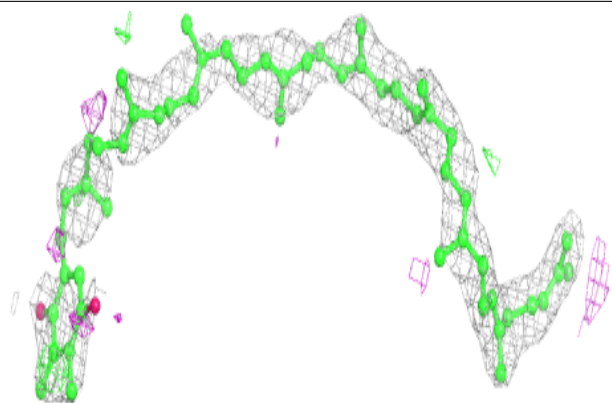
**Electron density around HTG B 642:**

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

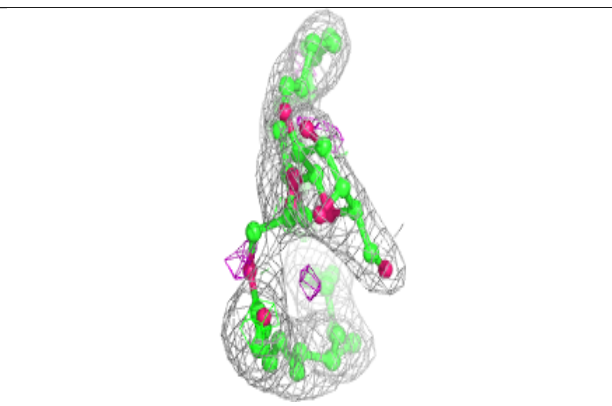
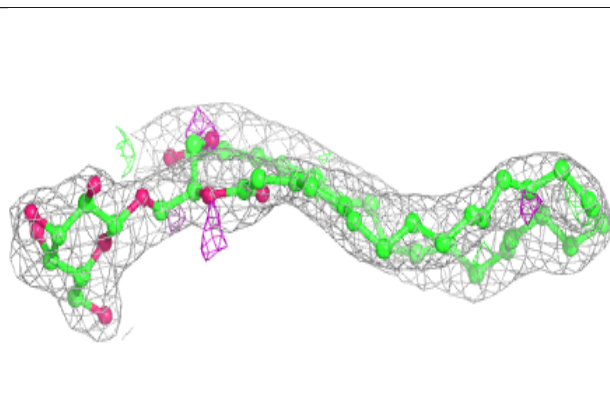
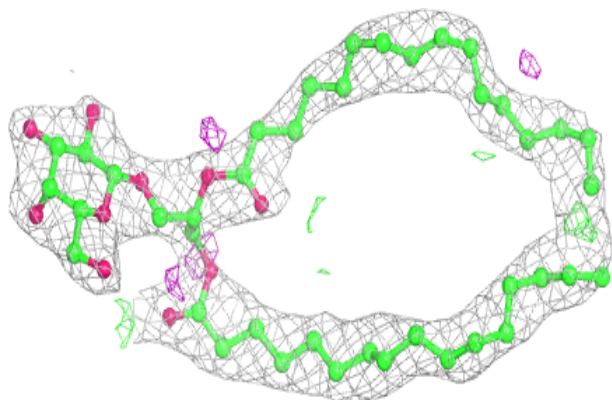


Electron density around PL9 A 410:

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

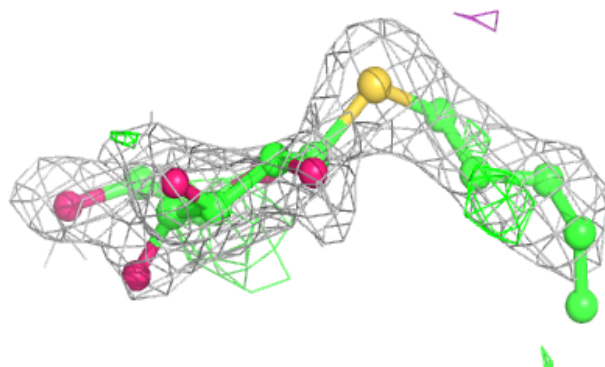
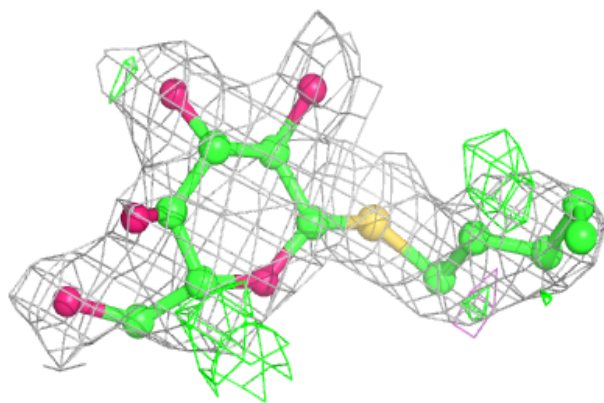
**Electron density around LMG a 412:**

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

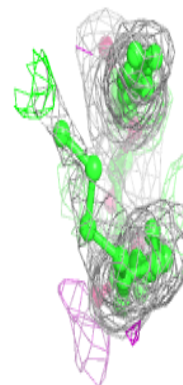
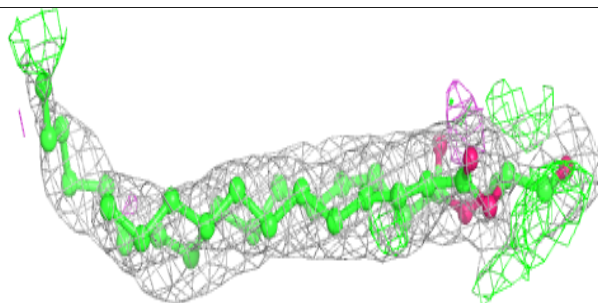
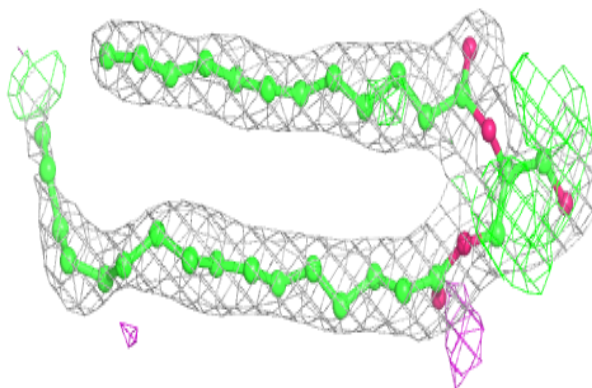


Electron density around HTG b 640:

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

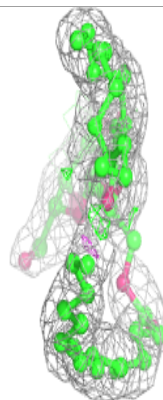
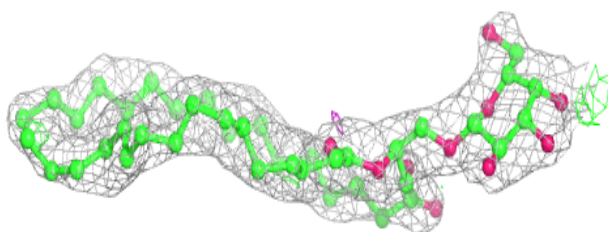
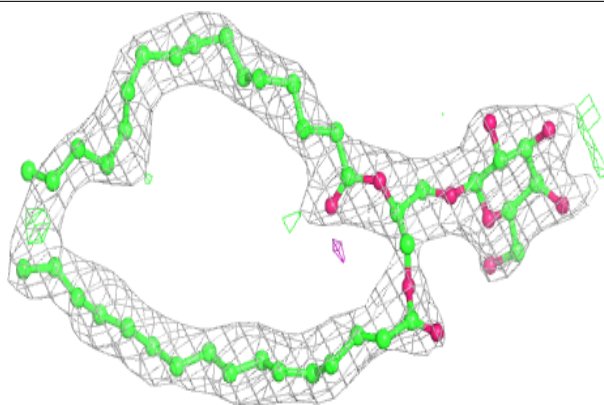
**Electron density around UNL b 628:**

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

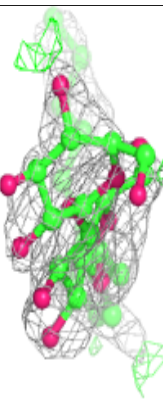
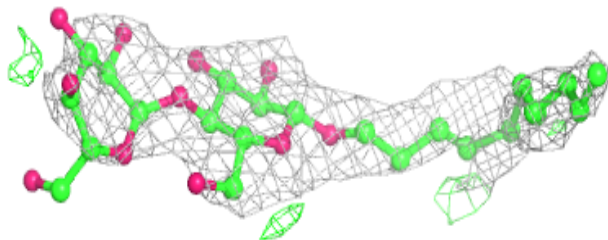
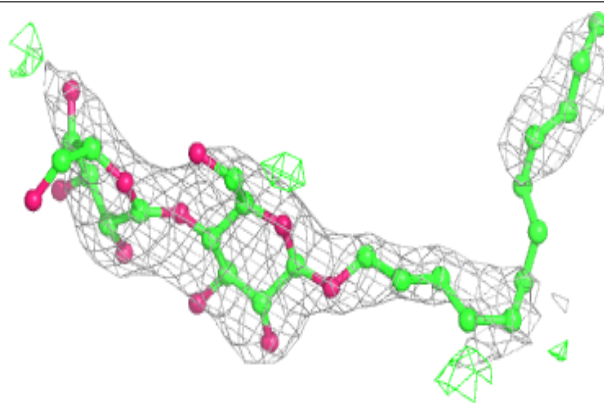


Electron density around LMG A 411:

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

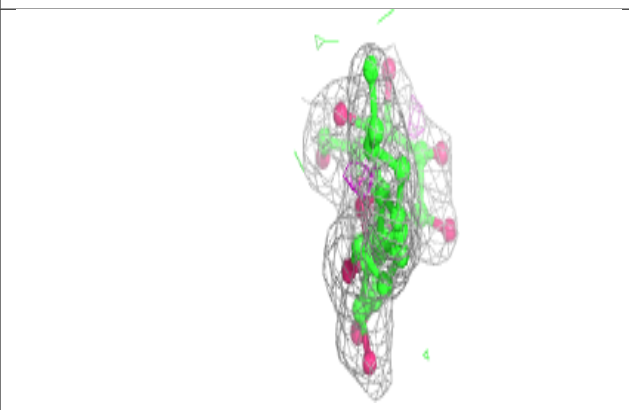
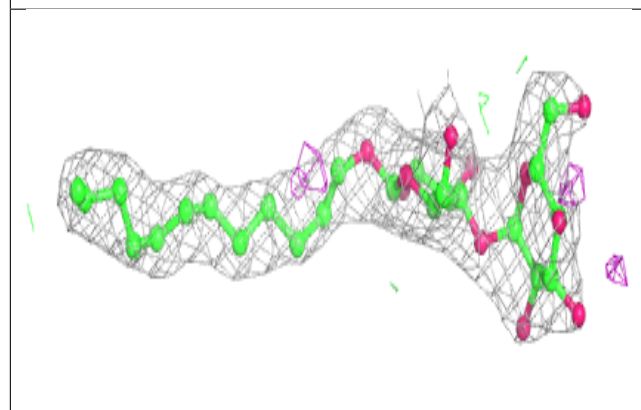
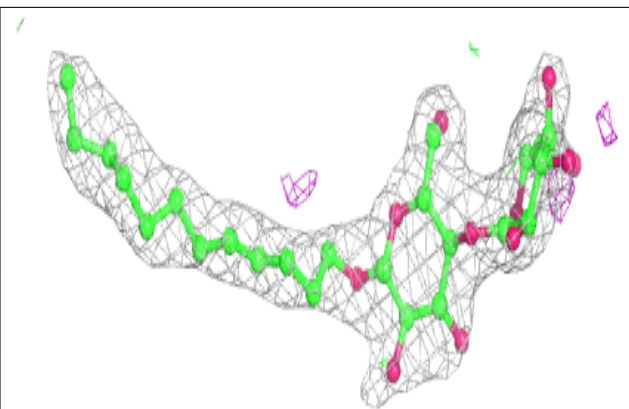
**Electron density around LMT c 522:**

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

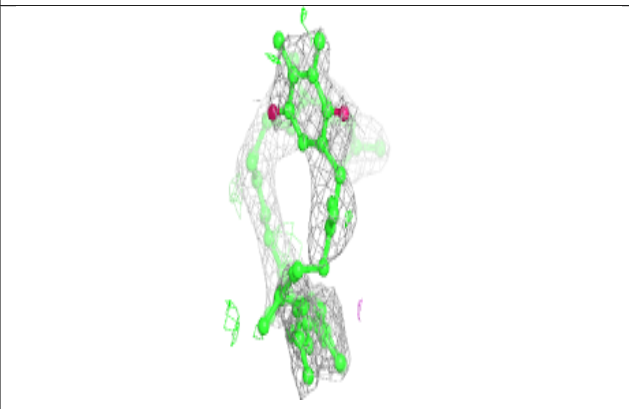
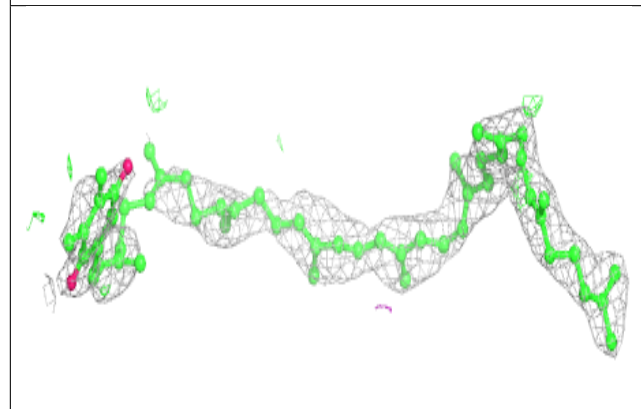
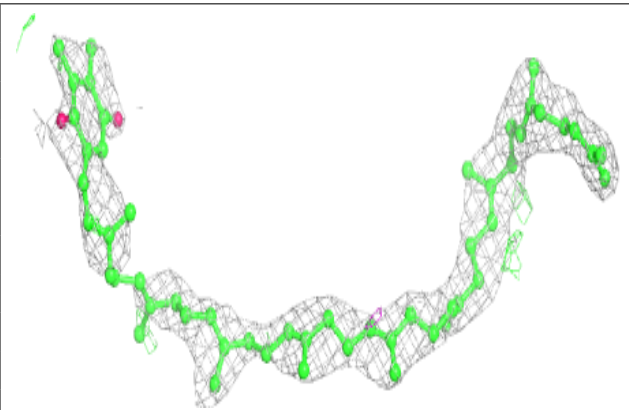


Electron density around LMT B 623:

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

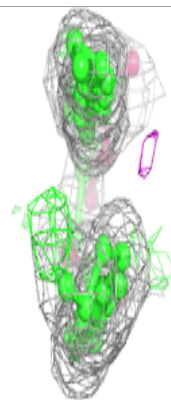
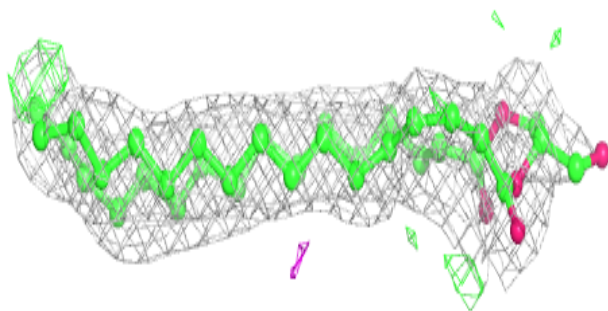
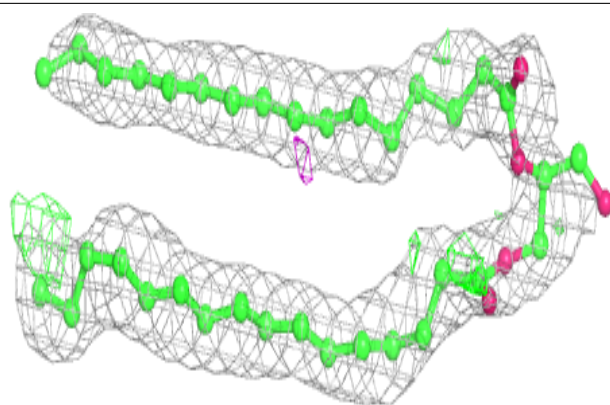
**Electron density around PL9 a 411:**

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

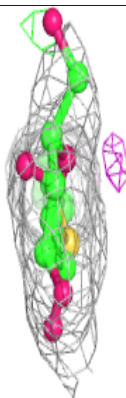
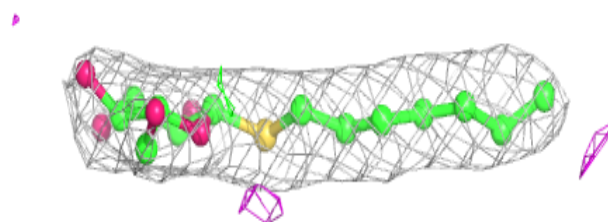
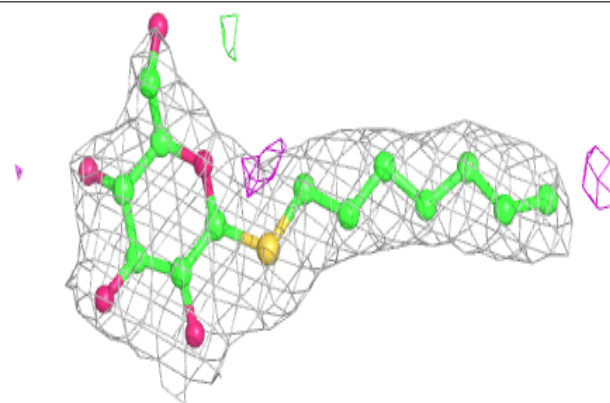


Electron density around UNL B 626:

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

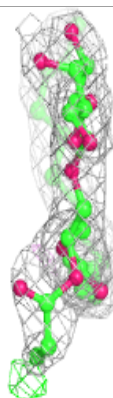
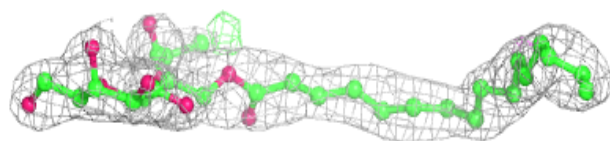
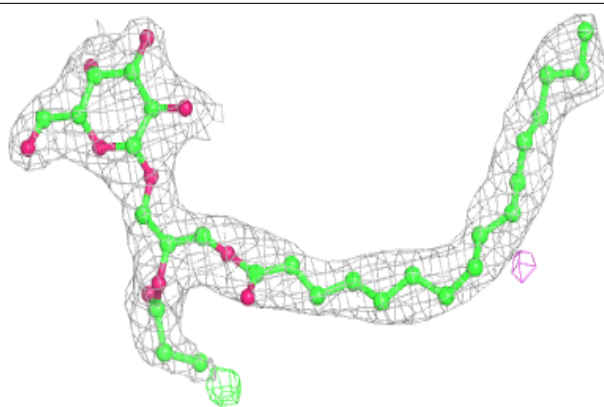
**Electron density around HTG b 601:**

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



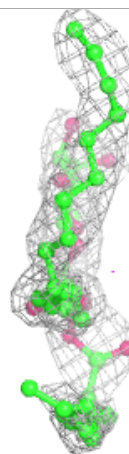
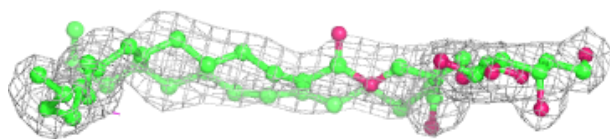
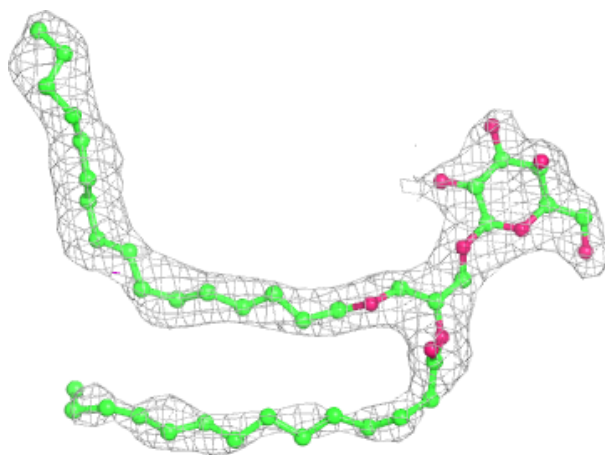
Electron density around LMG c 520:

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



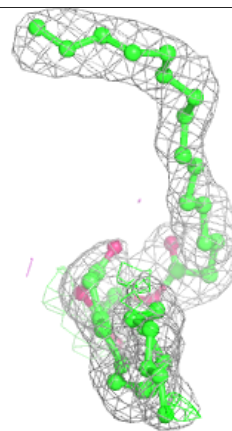
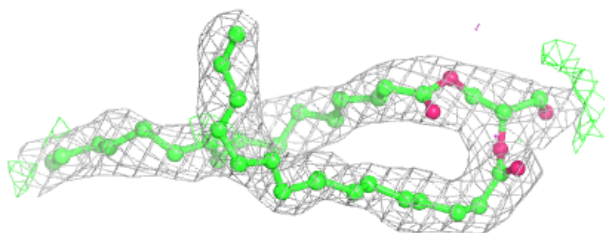
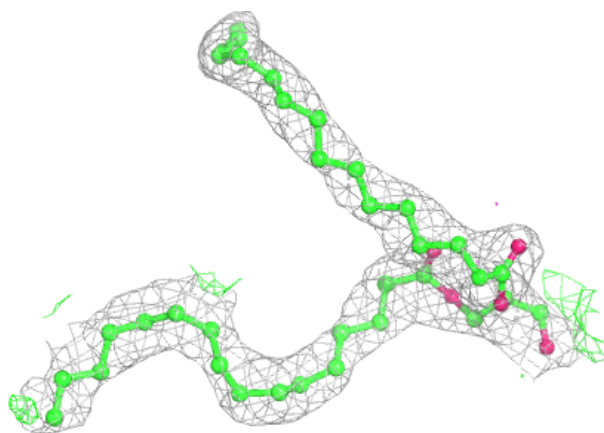
Electron density around LMG C 518:

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

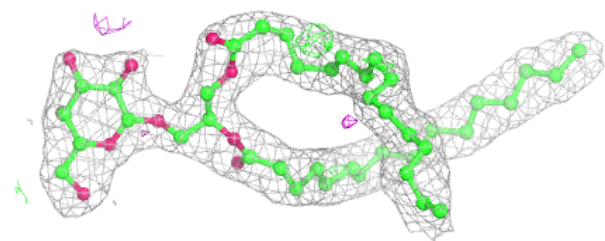
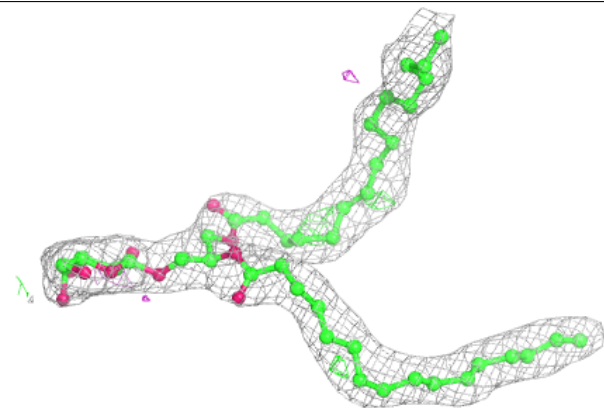


Electron density around UNL a 421:

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

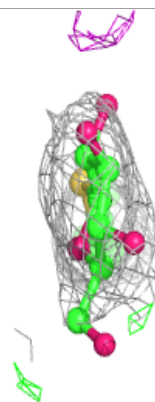
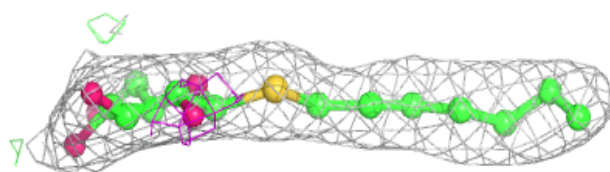
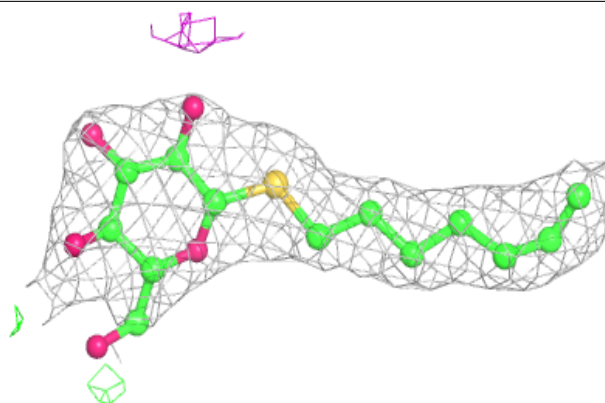
**Electron density around LMG B 622:**

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



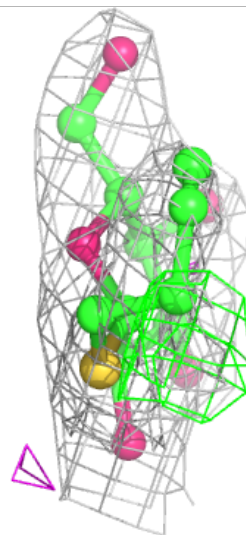
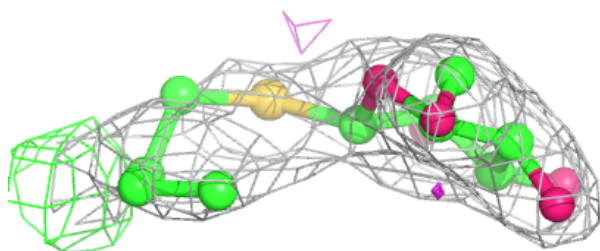
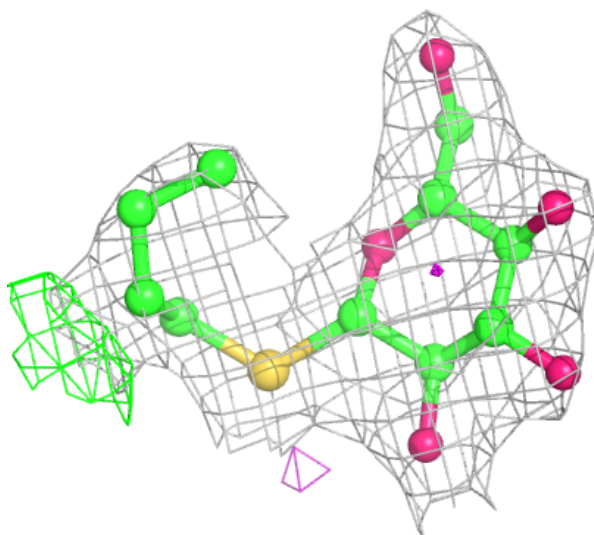
Electron density around HTG B 628:

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



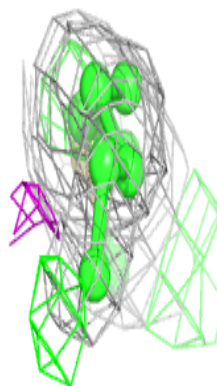
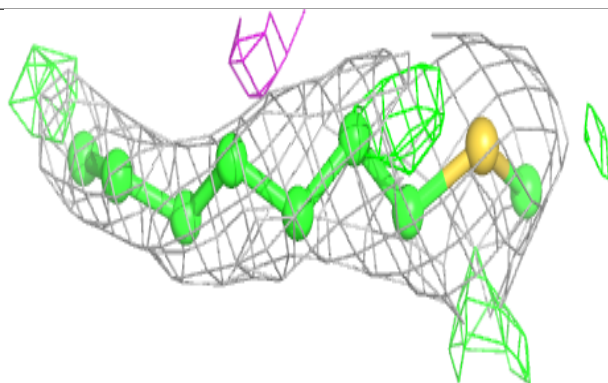
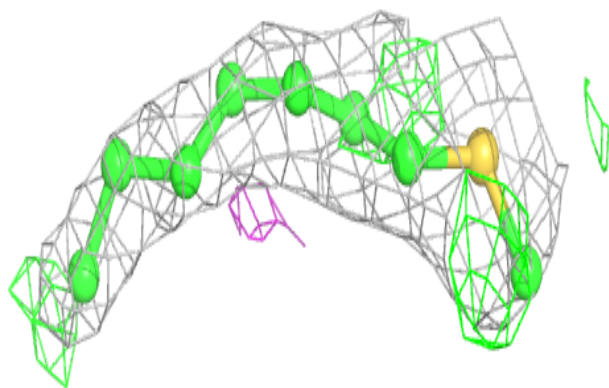
Electron density around HTG v 208:

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

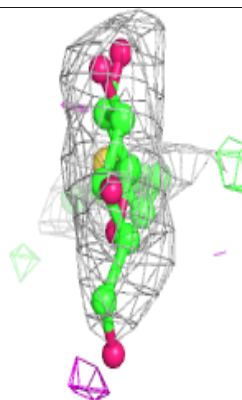
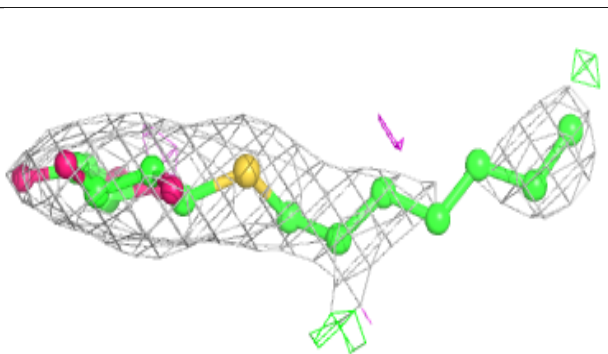
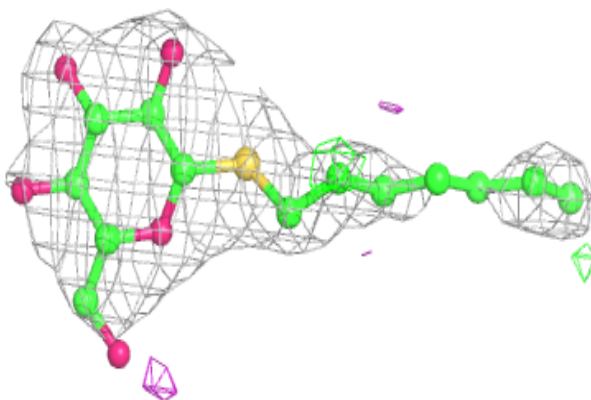


Electron density around HTG C 535:

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

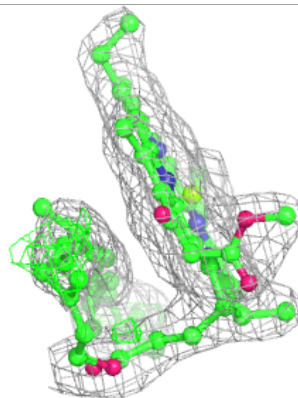
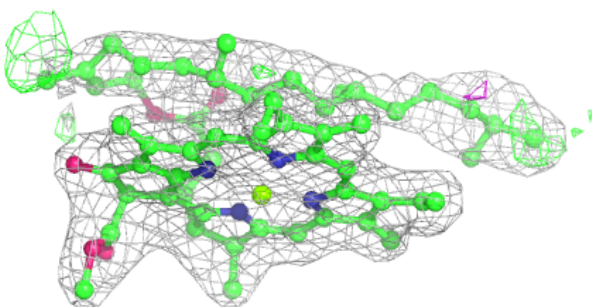
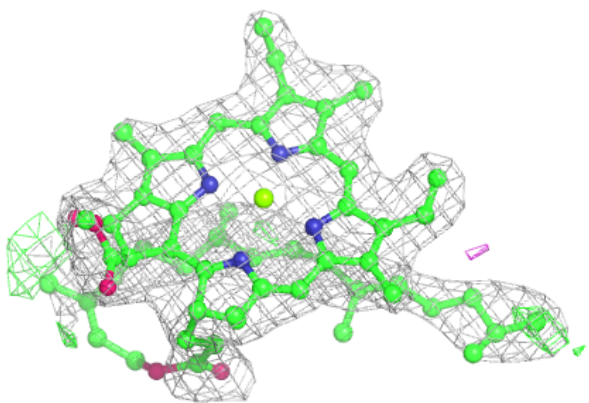
**Electron density around HTG C 521:**

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

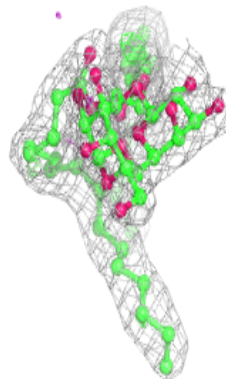
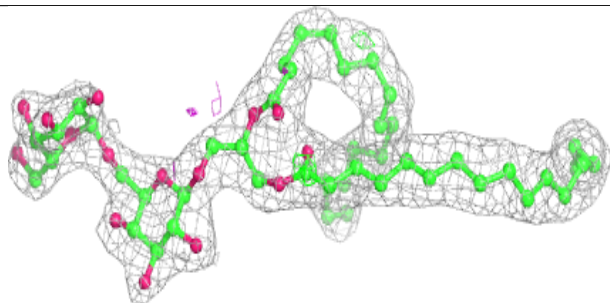
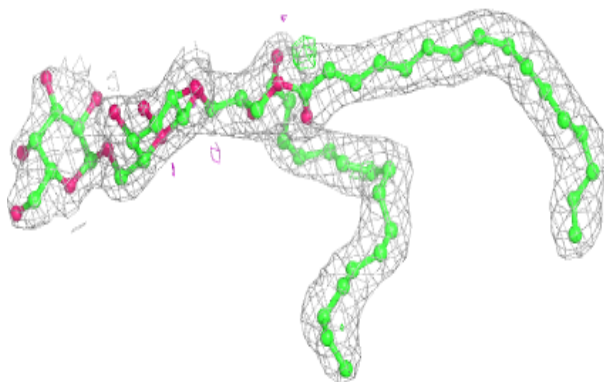


Electron density around CLA B 602:

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

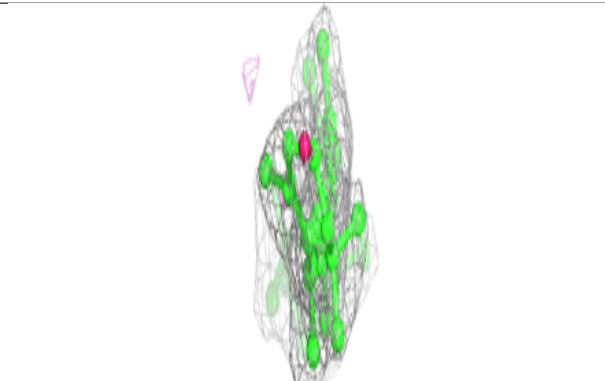
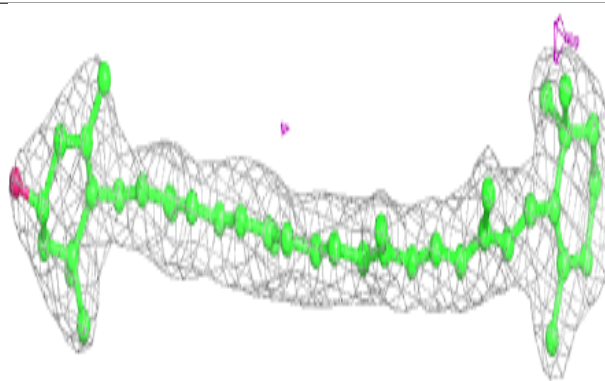
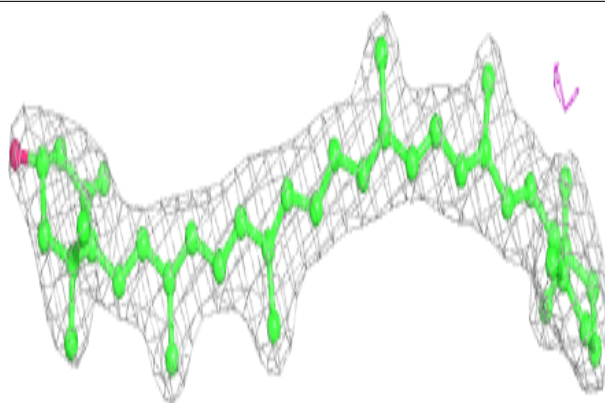
**Electron density around DGD h 101:**

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

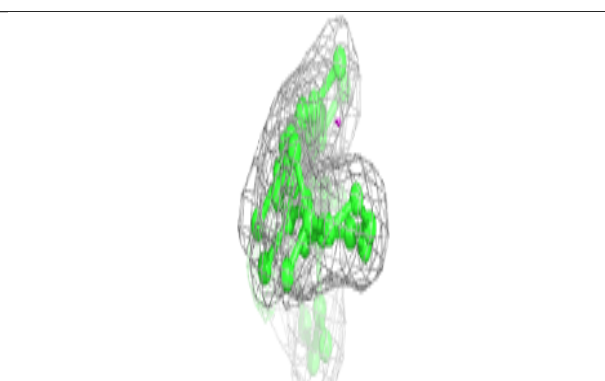
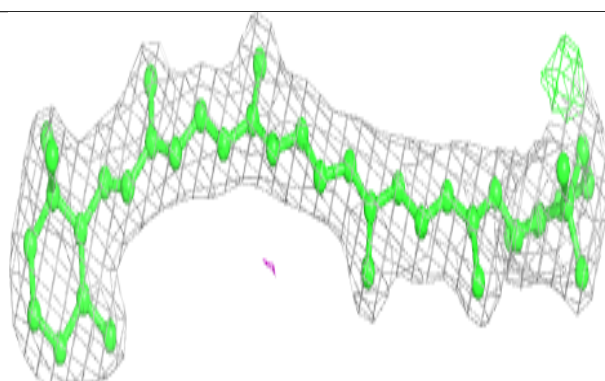
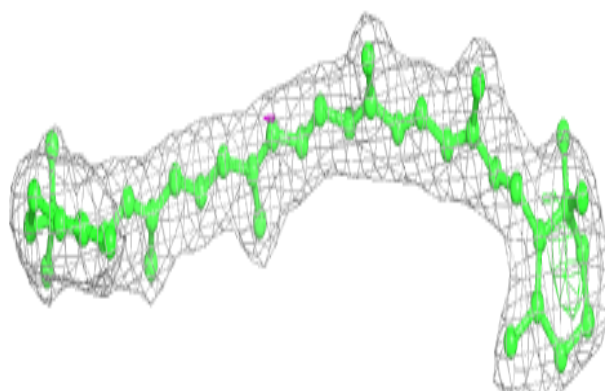


Electron density around RRX h 102:

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

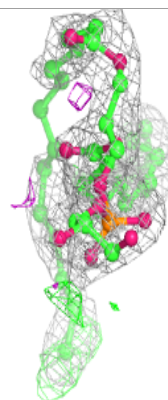
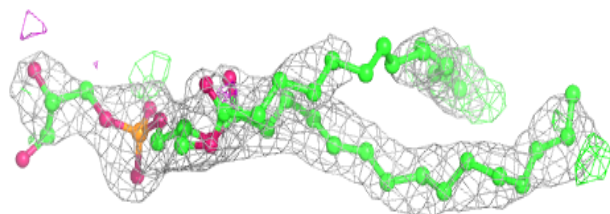
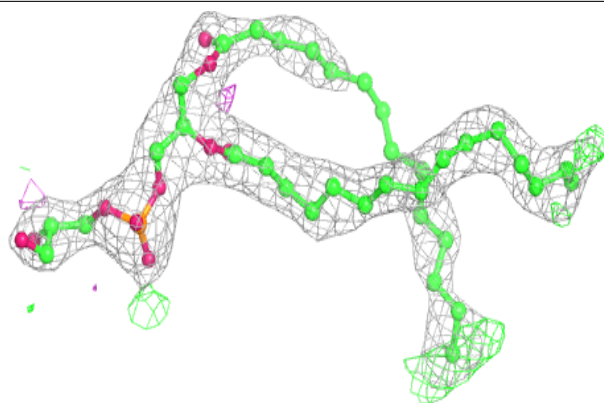
**Electron density around BCR d 406:**

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

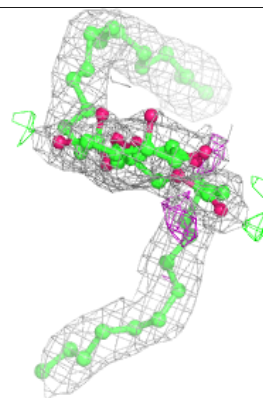
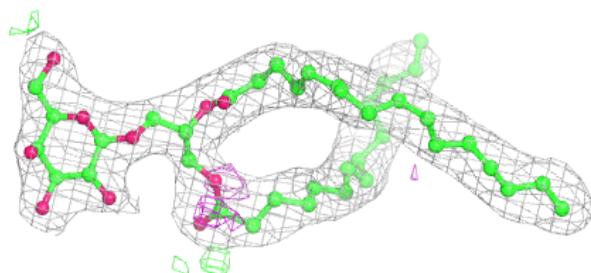
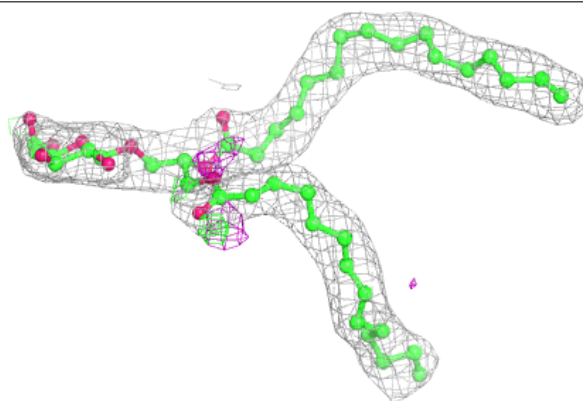


Electron density around LHG f 102:

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

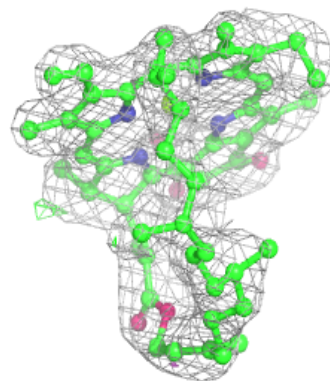
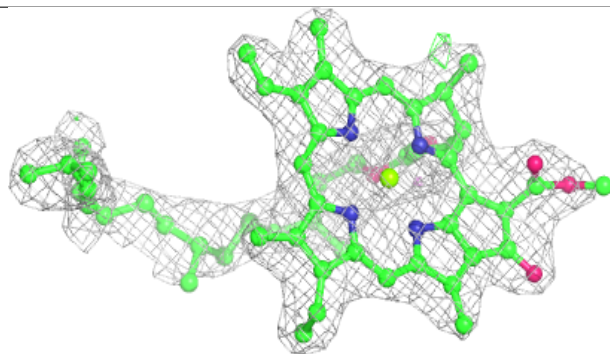
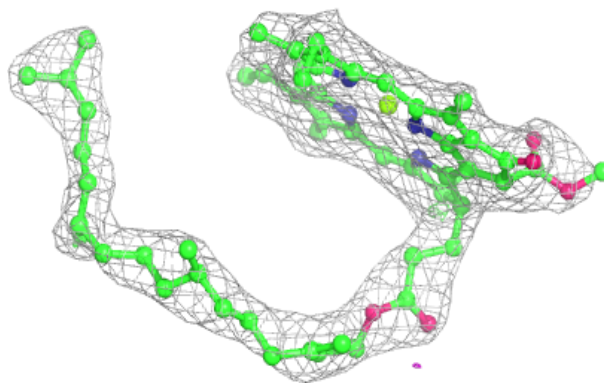
**Electron density around LMG b 625:**

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

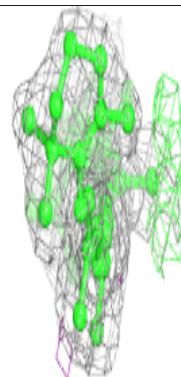
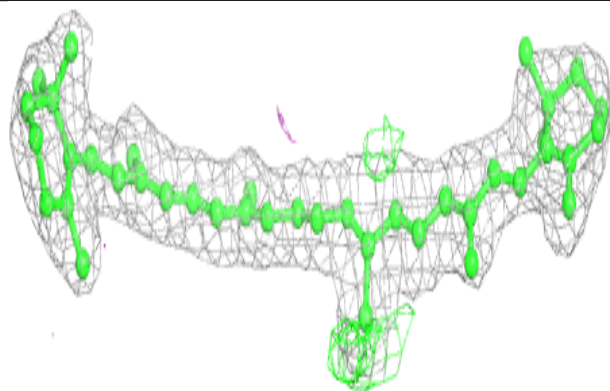
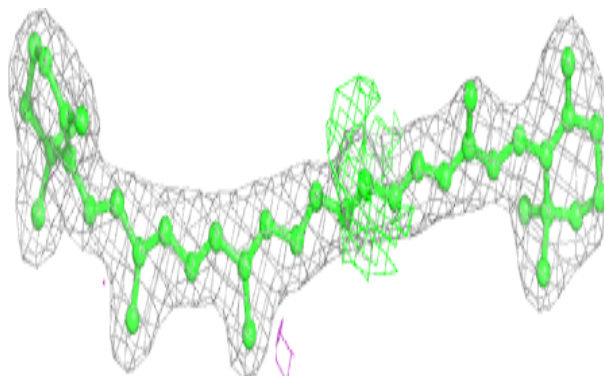


Electron density around CLA C 513:

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

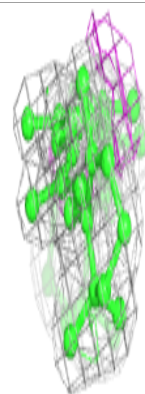
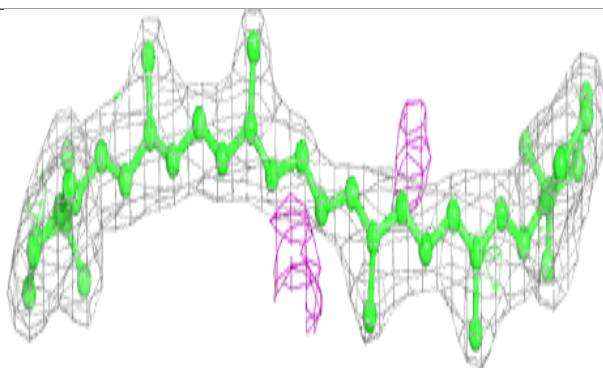
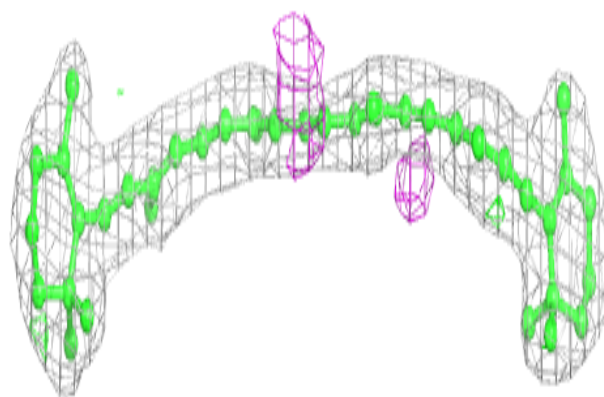
**Electron density around BCR T 101:**

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

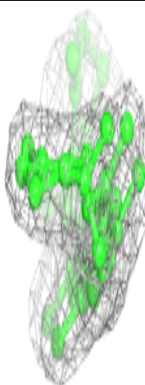
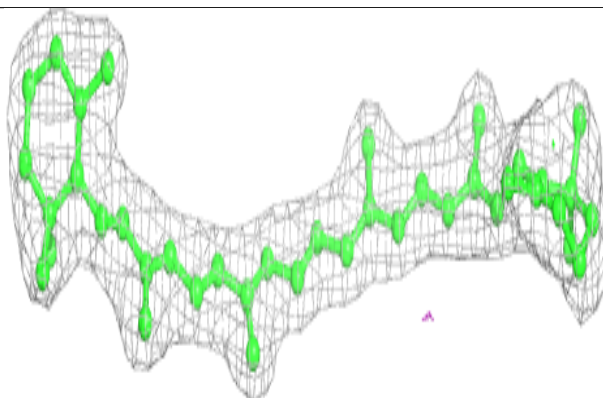
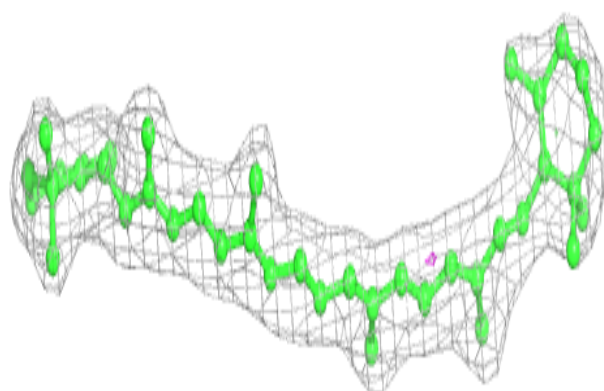


Electron density around BCR K 101:

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

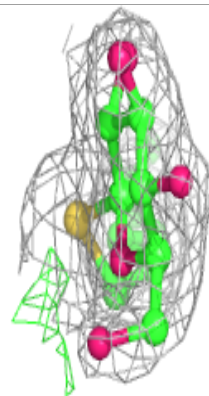
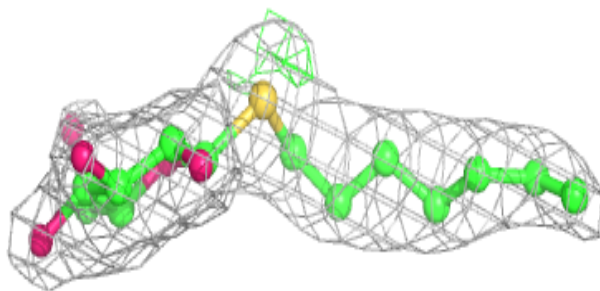
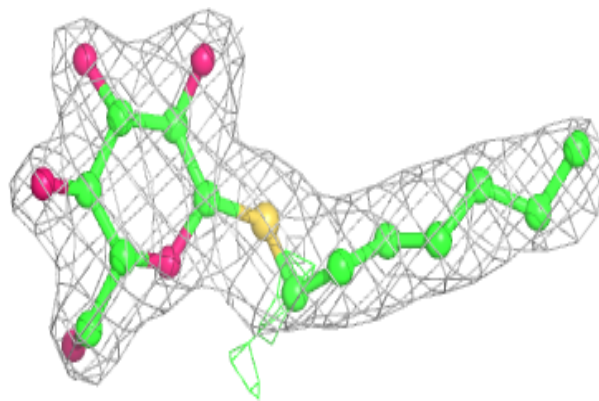
**Electron density around BCR D 406:**

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



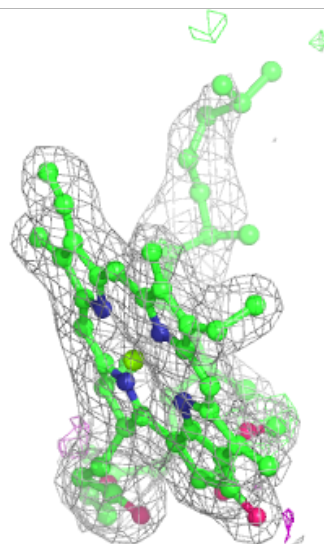
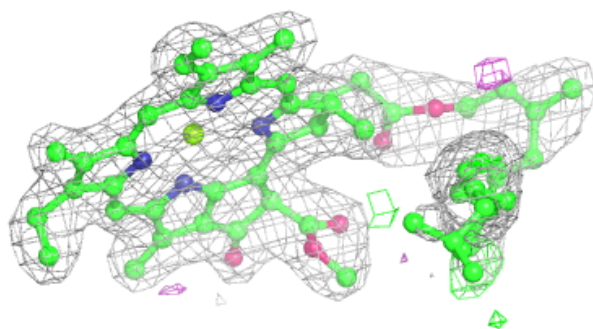
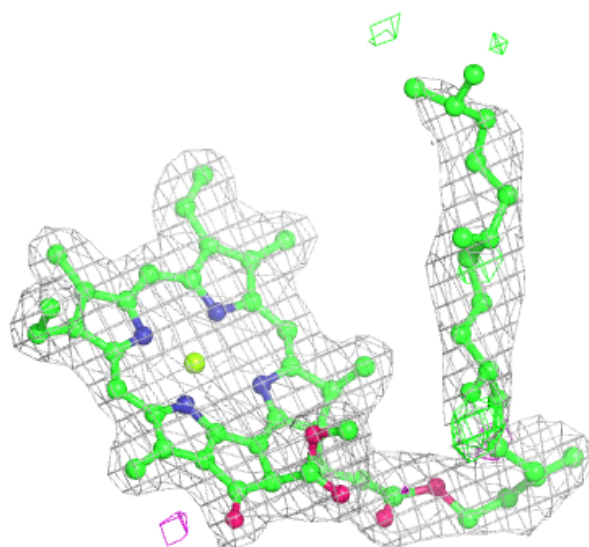
Electron density around HTG O 302:

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



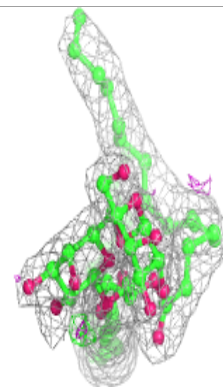
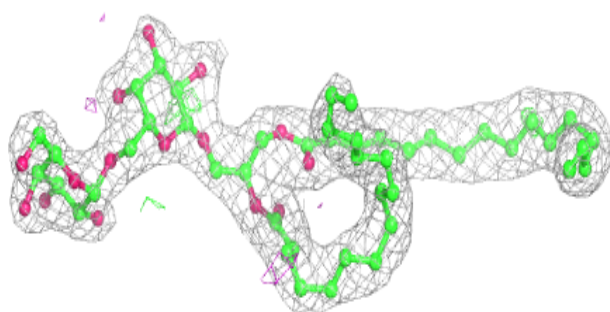
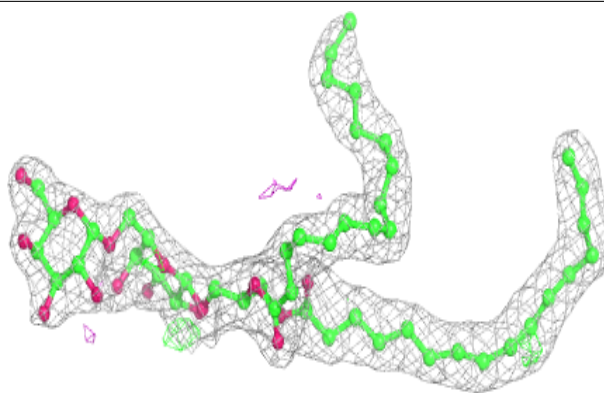
Electron density around CLA b 620:

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

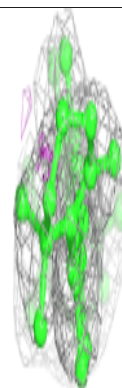
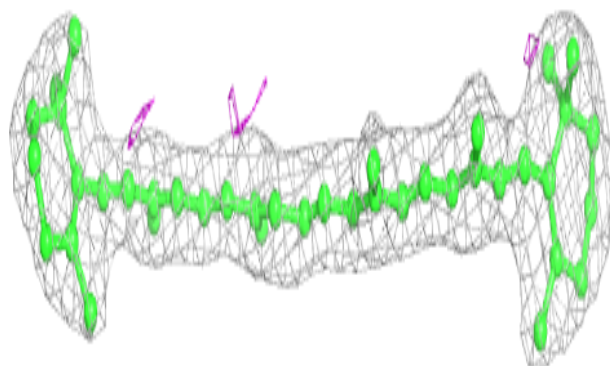
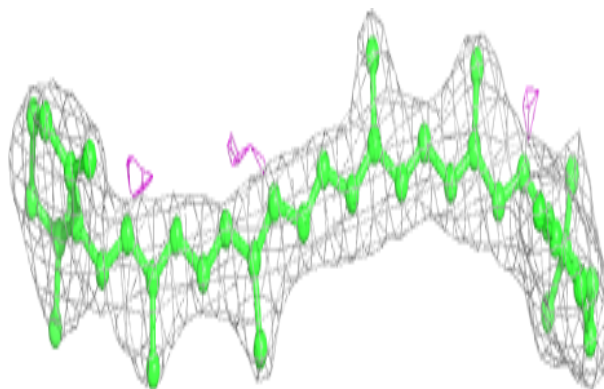


Electron density around DGD H 101:

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

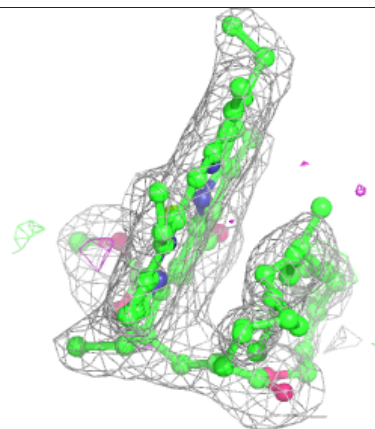
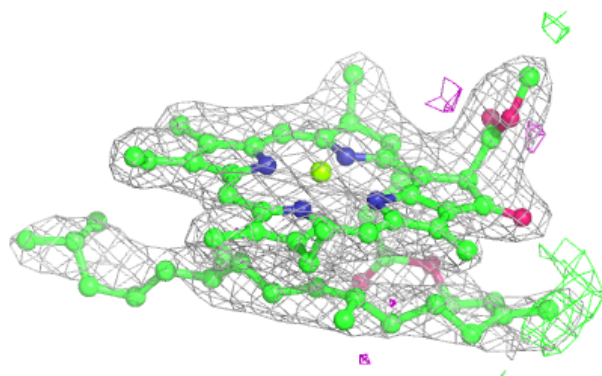
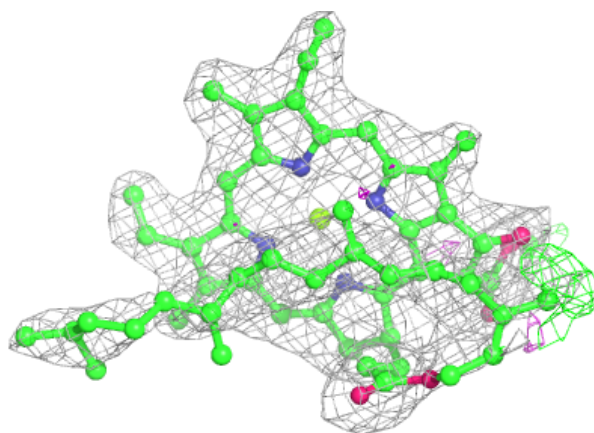
**Electron density around BCR c 515:**

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

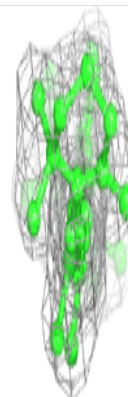
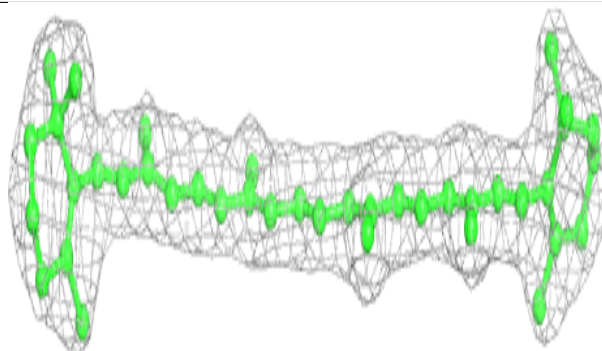
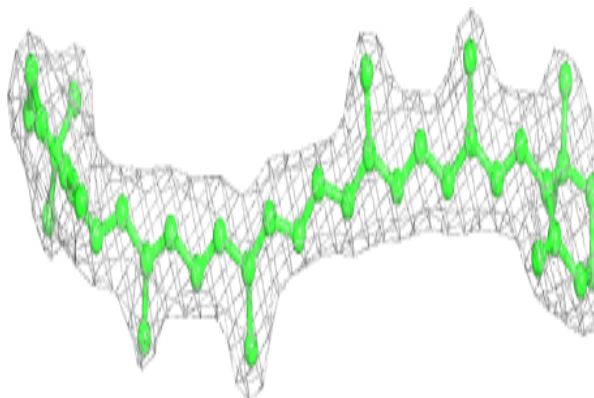


Electron density around CLA b 605:

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

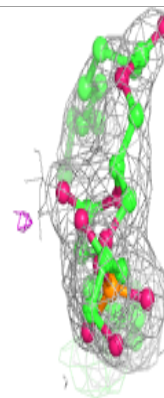
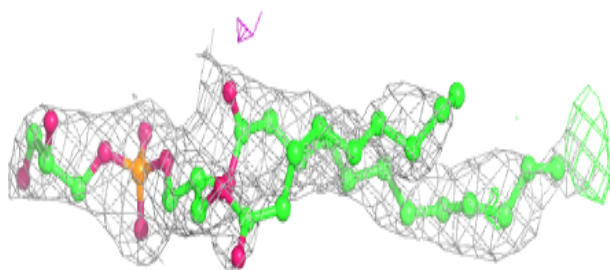
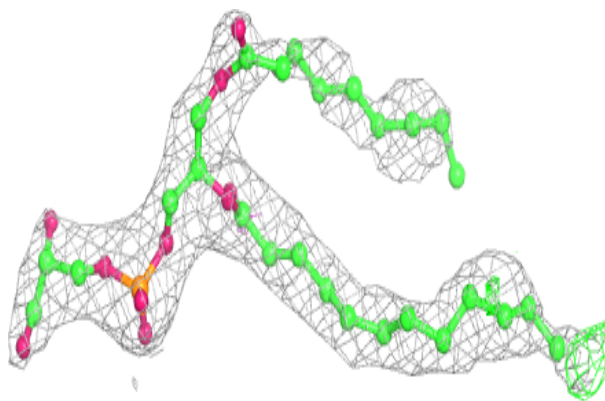
**Electron density around BCR K 102:**

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



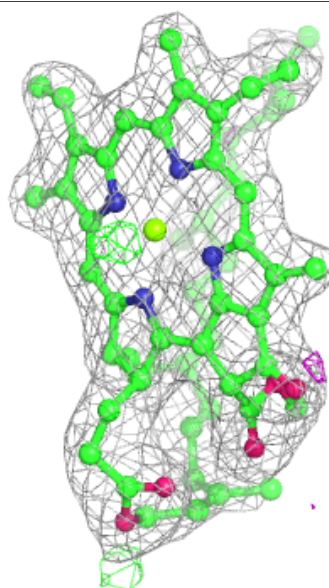
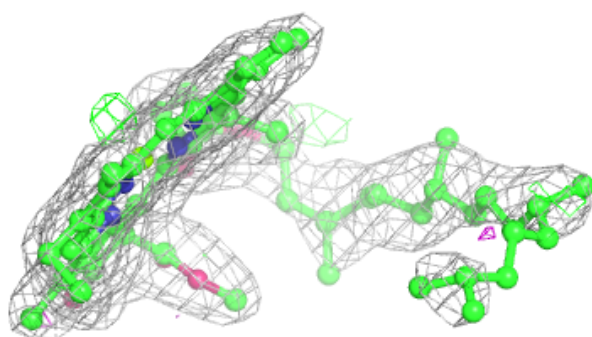
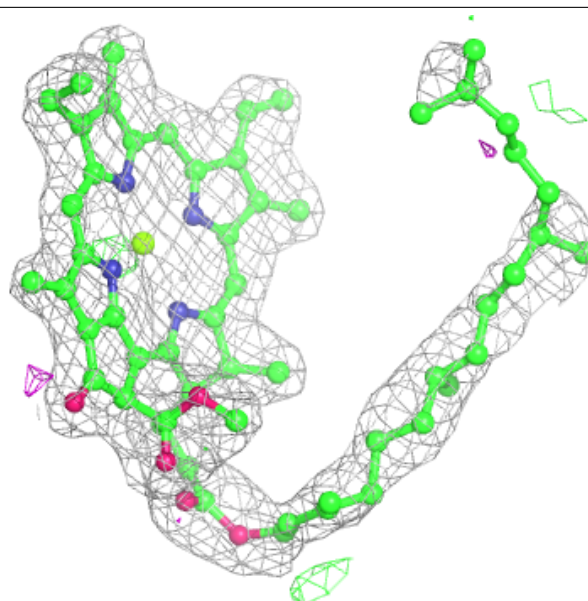
Electron density around LHG F 103:

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



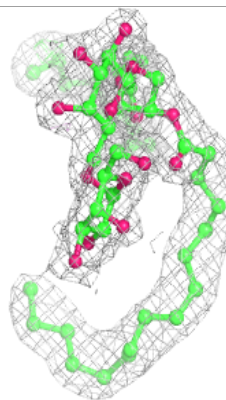
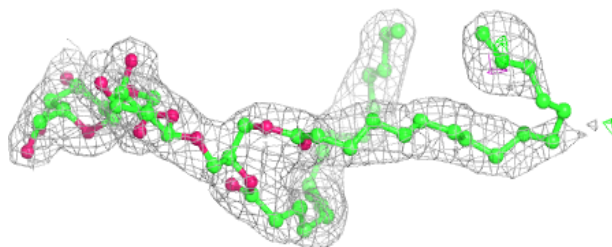
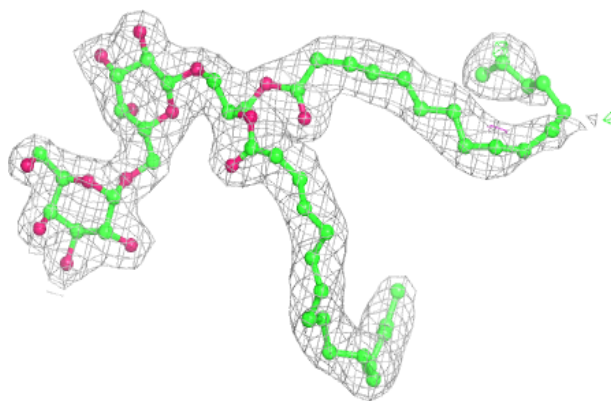
Electron density around CLA B 617:

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

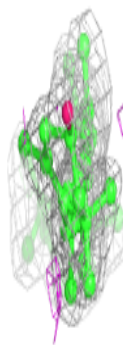
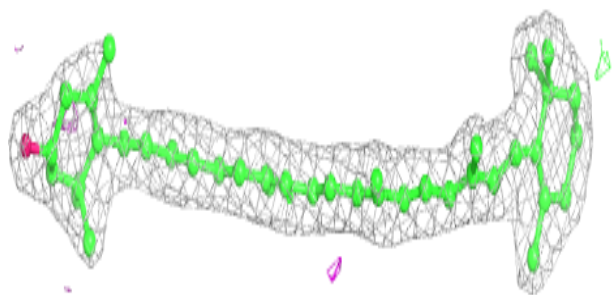
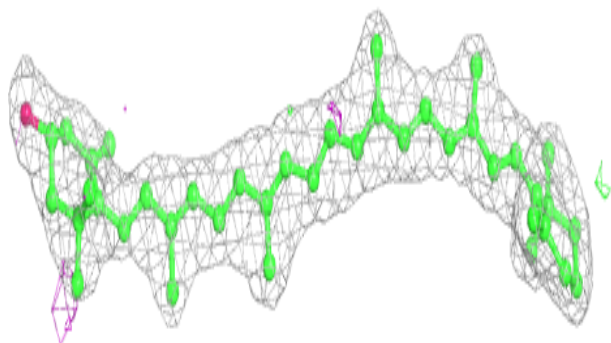


Electron density around DGD C 516:

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

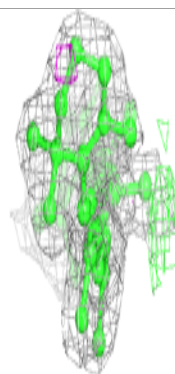
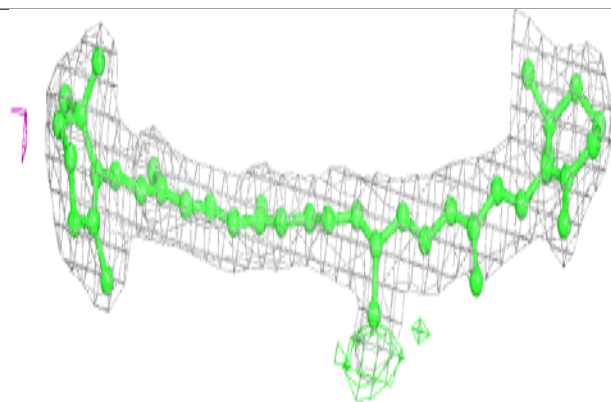
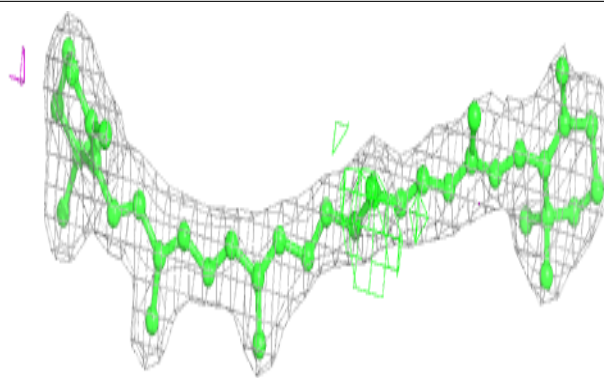
**Electron density around RRX H 102:**

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

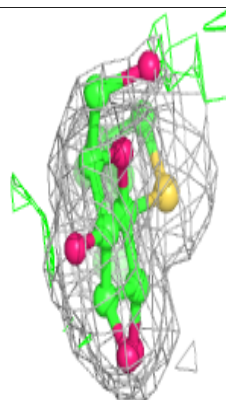
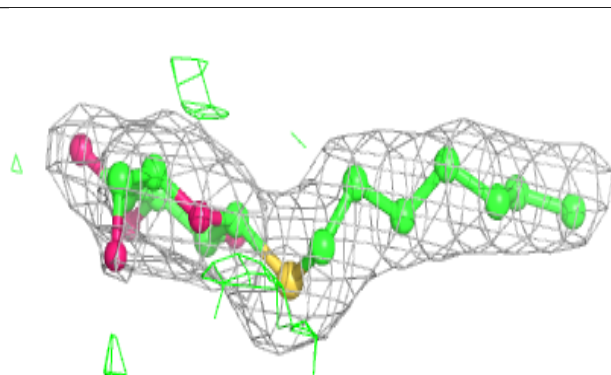
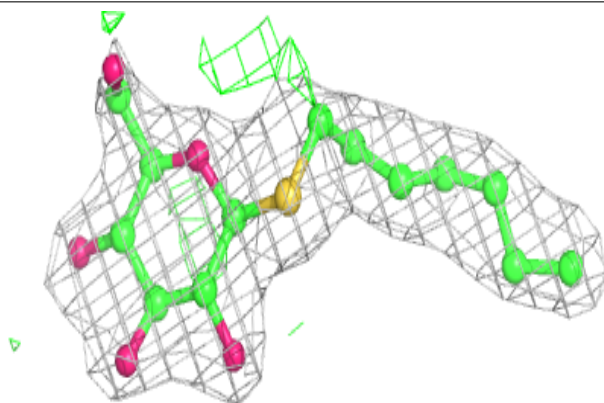


Electron density around BCR t 101:

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

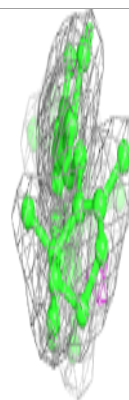
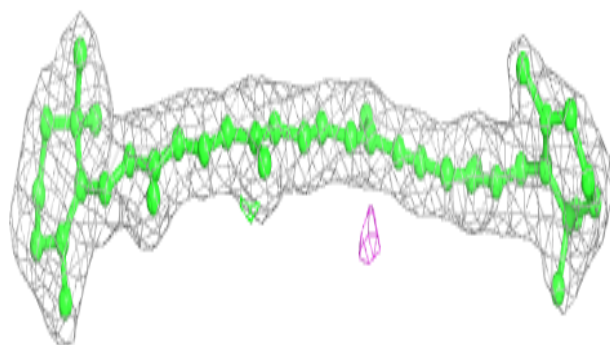
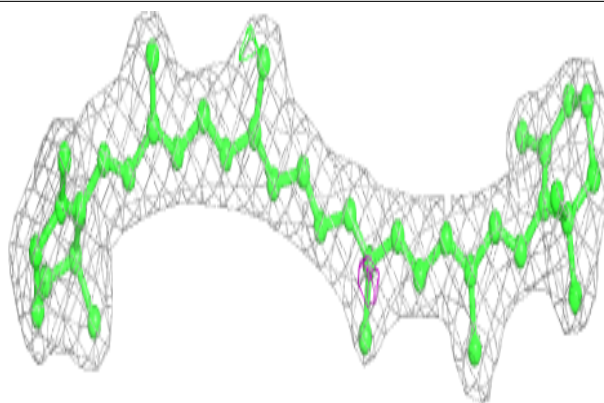
**Electron density around HTG o 301:**

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

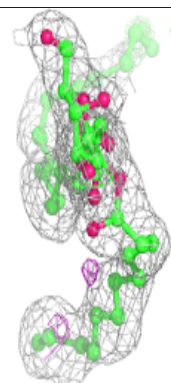
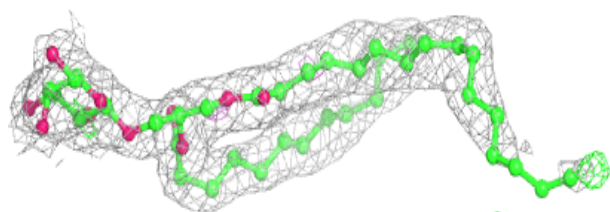
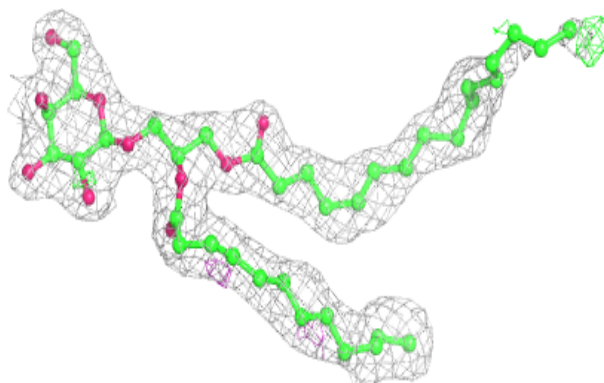


Electron density around BCR y 101:

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

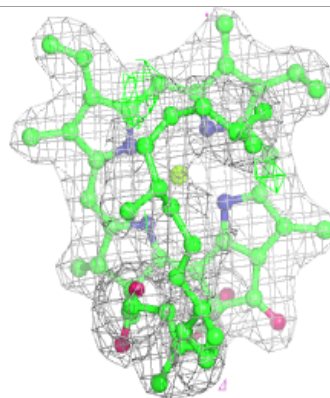
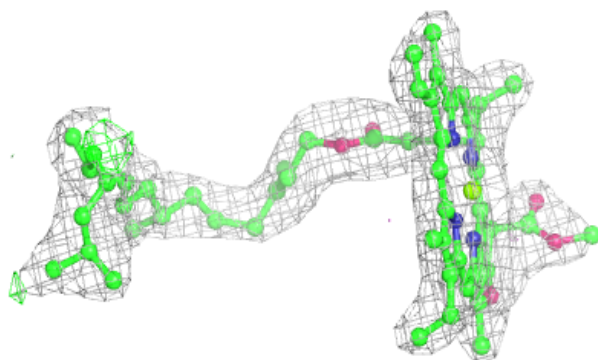
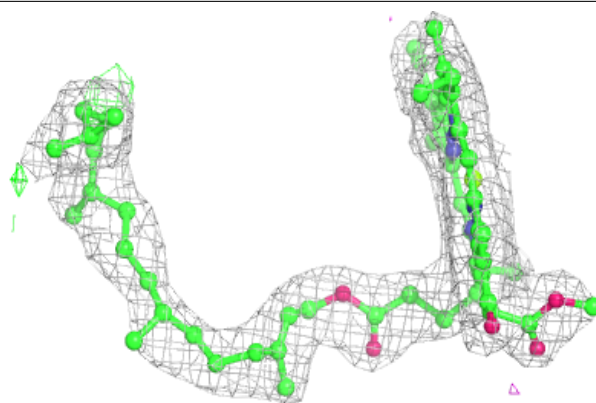
**Electron density around LMG d 412:**

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

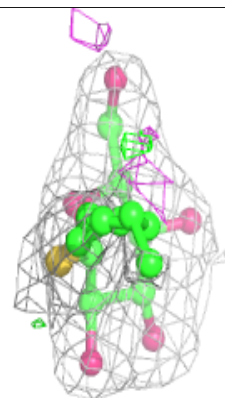
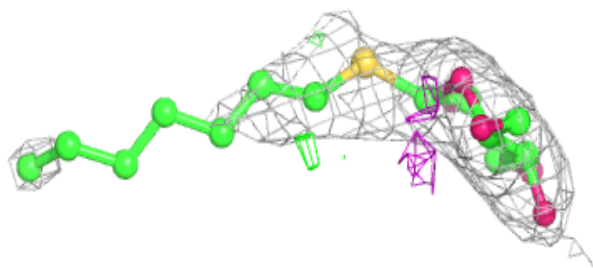
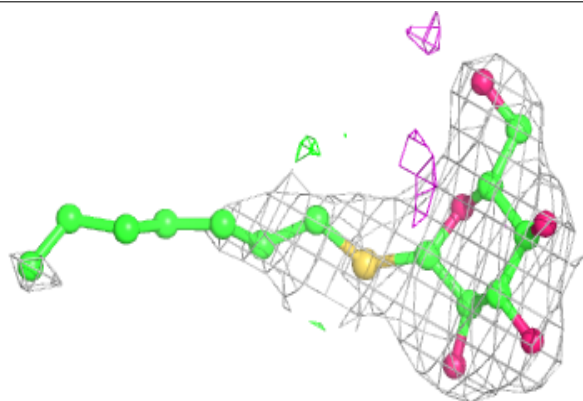


Electron density around CLA c 507:

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

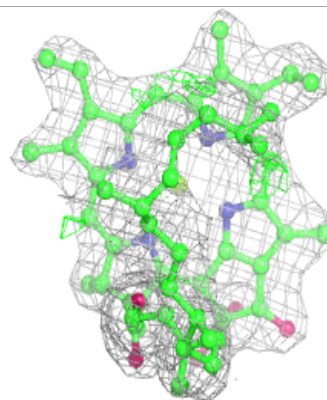
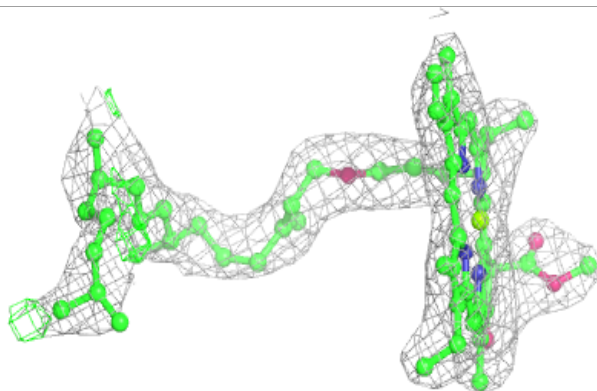
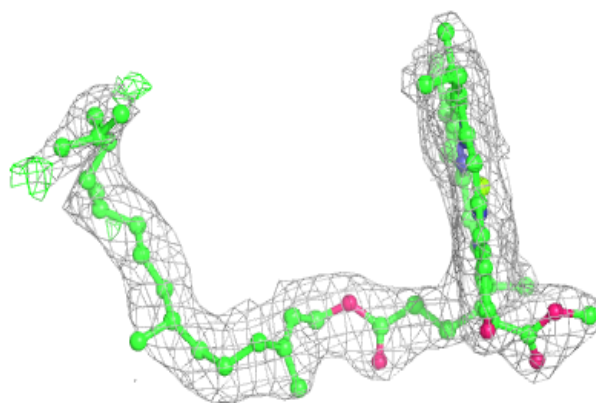
**Electron density around HTG V 202:**

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



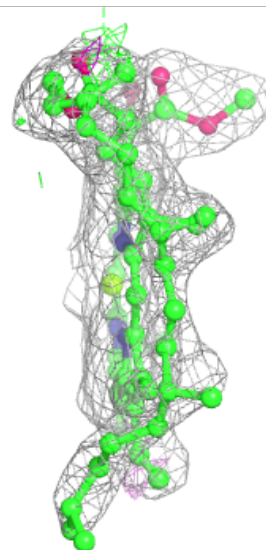
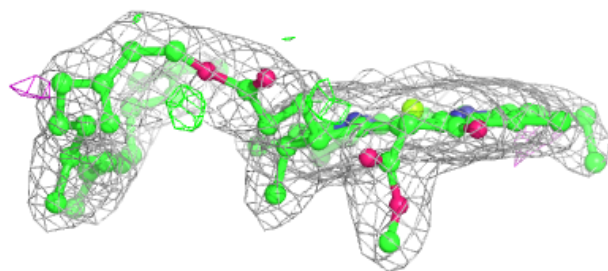
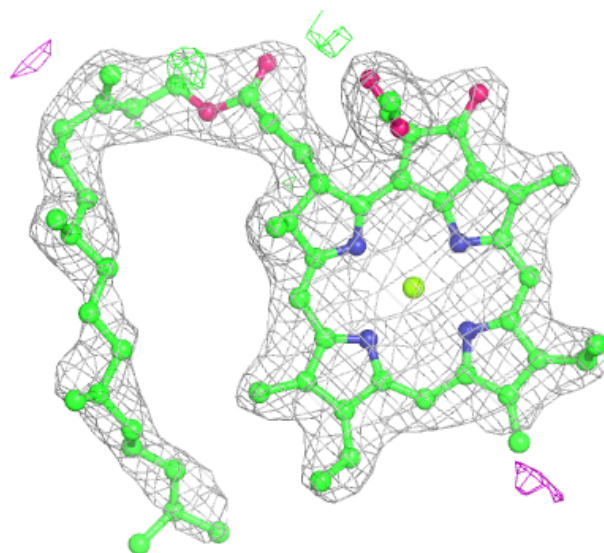
Electron density around CLA C 506:

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



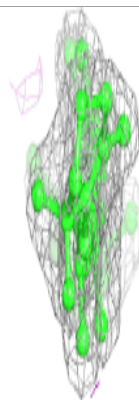
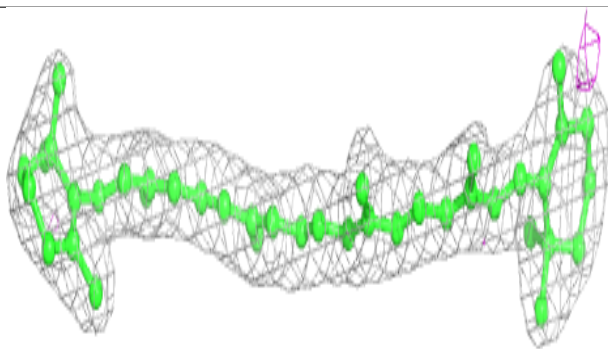
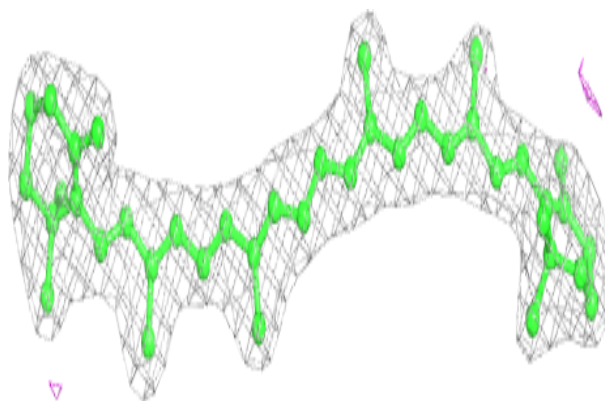
Electron density around CLA c 513:

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

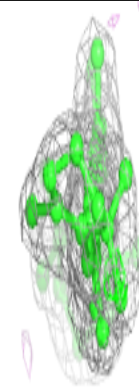
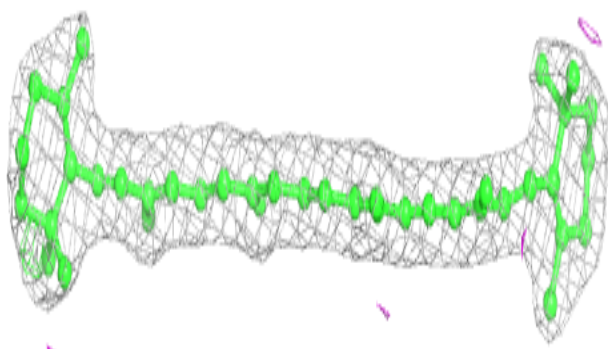
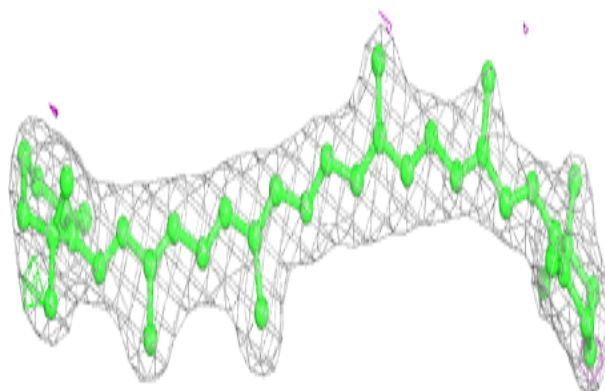


Electron density around BCR Y 101:

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

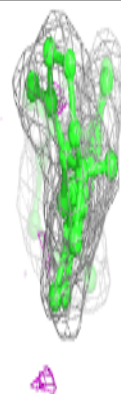
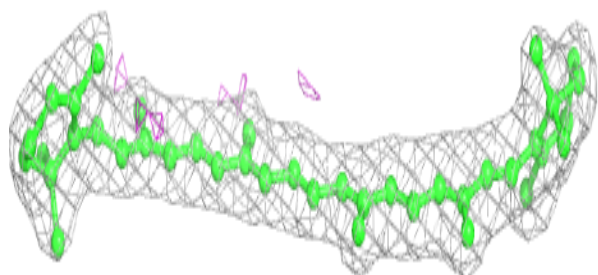
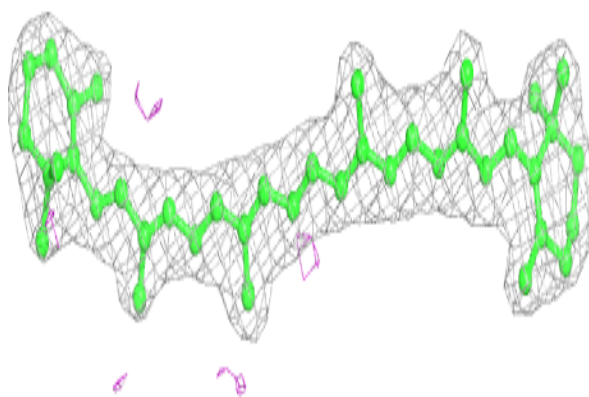
**Electron density around BCR c 516:**

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



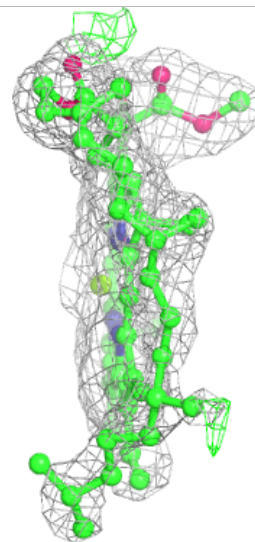
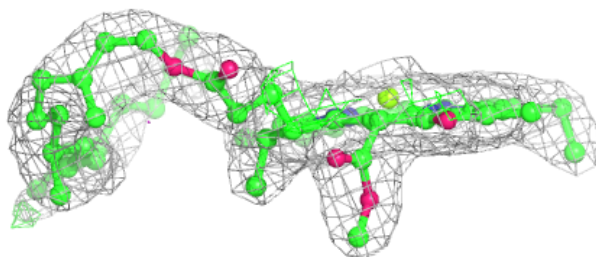
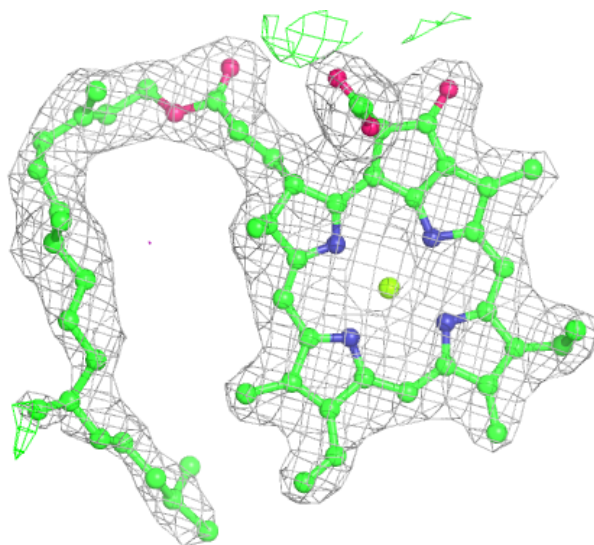
Electron density around BCR b 623:

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



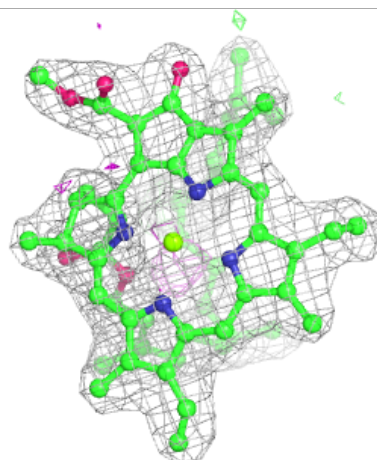
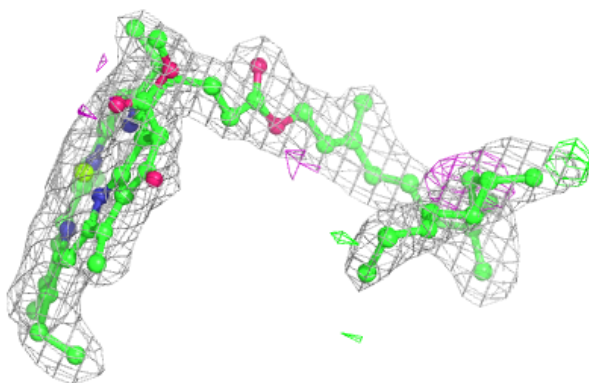
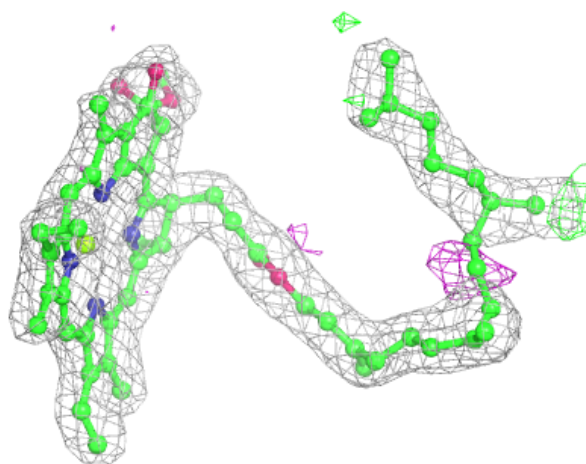
Electron density around CLA C 512:

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



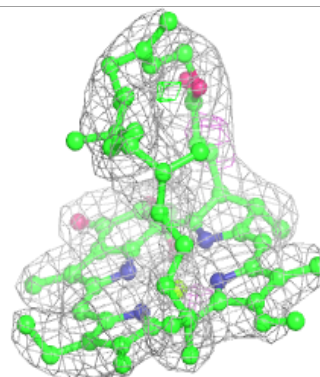
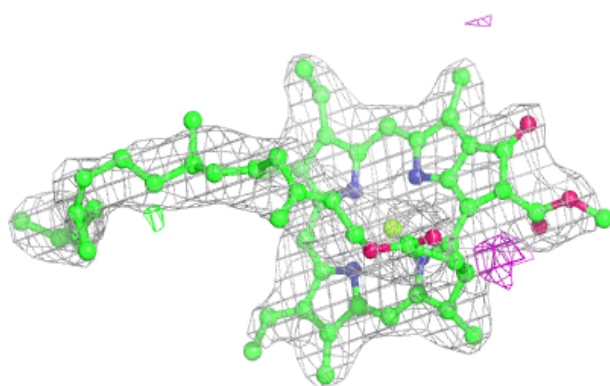
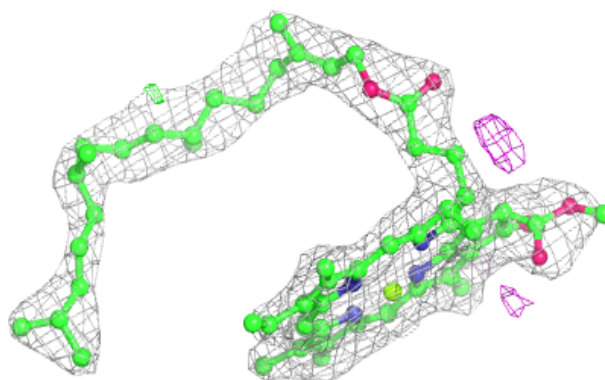
Electron density around CLA b 610:

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

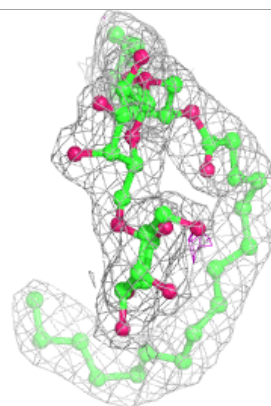
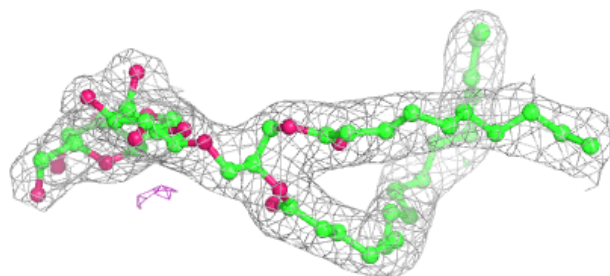
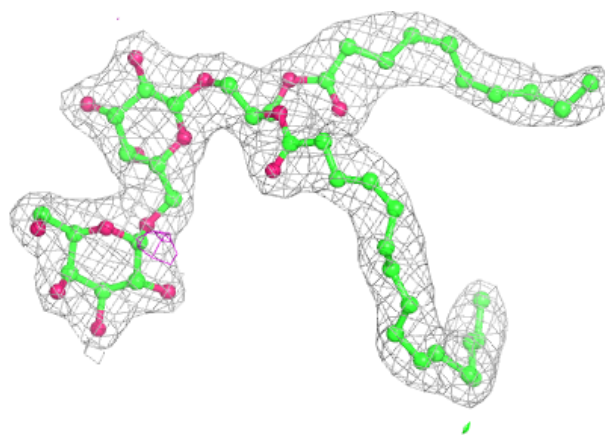


Electron density around CLA c 514:

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

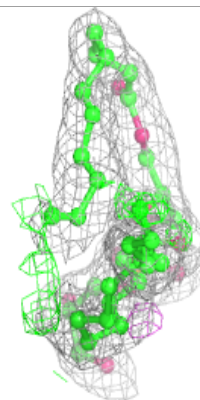
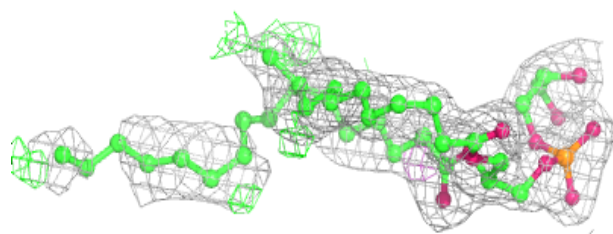
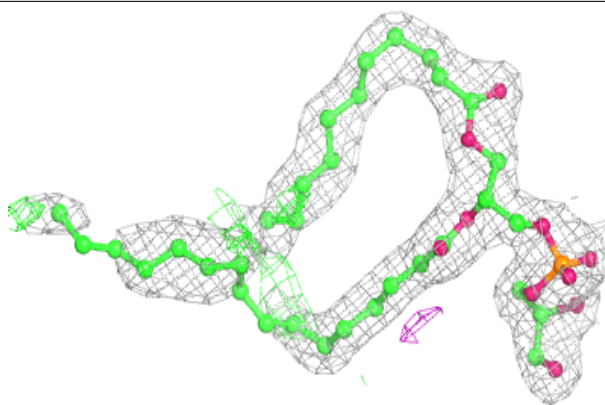
**Electron density around DGD c 518:**

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

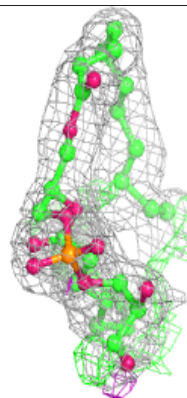
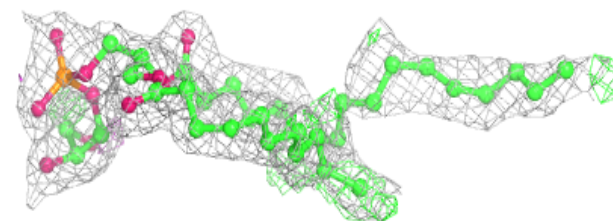
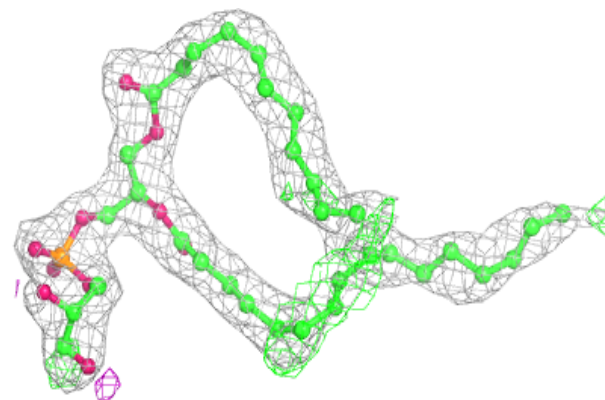


Electron density around LHG d 411:

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

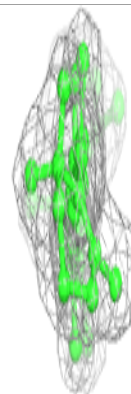
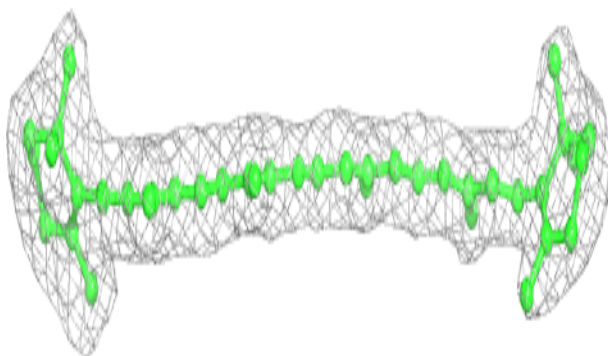
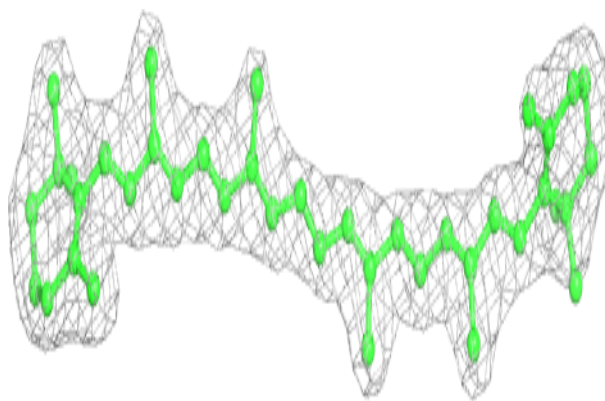
**Electron density around LHG D 411:**

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

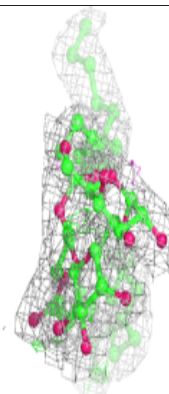
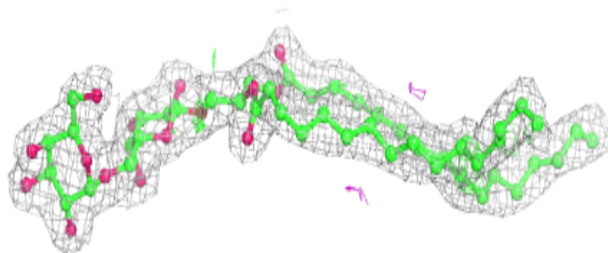
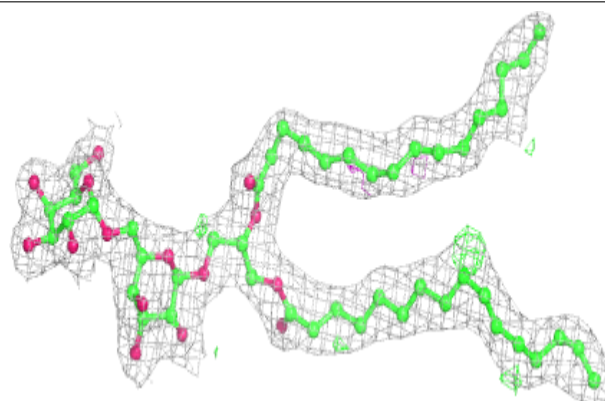


Electron density around BCR B 619:

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

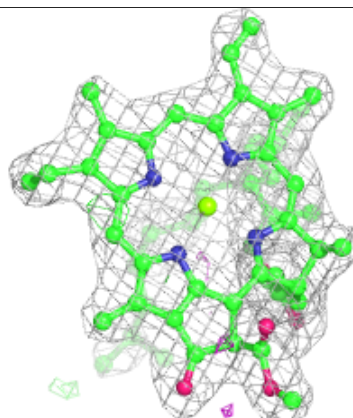
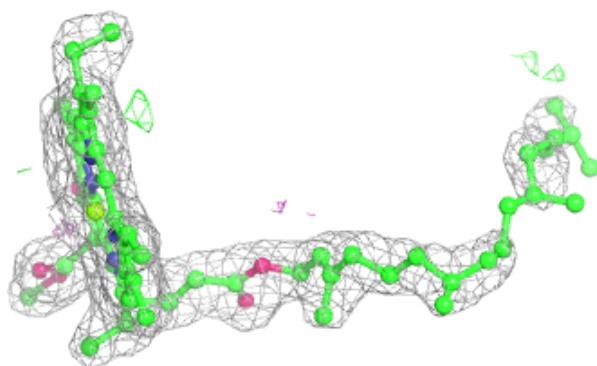
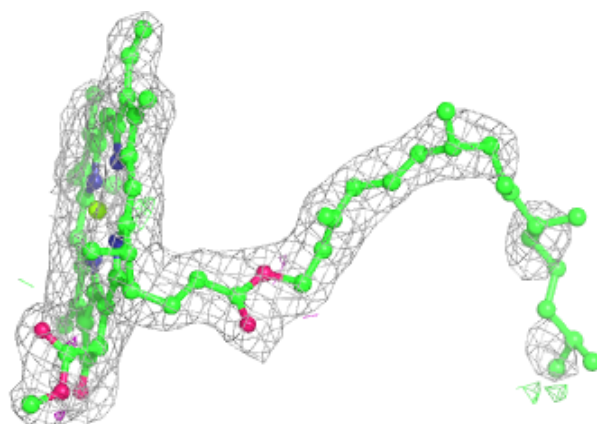
**Electron density around DGD C 517:**

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

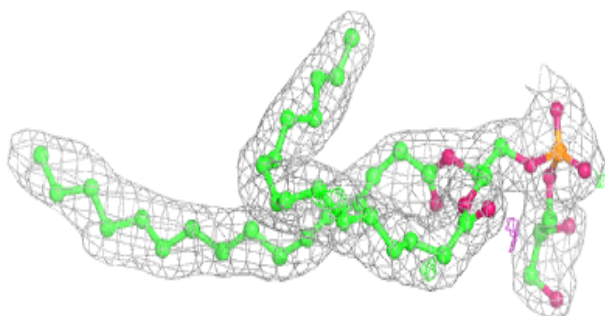
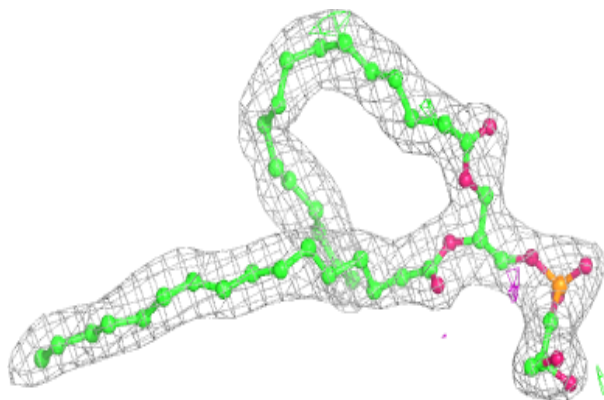


Electron density around CLA D 405:

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

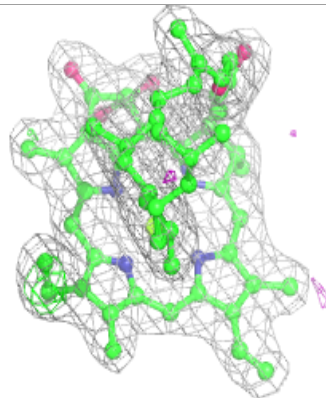
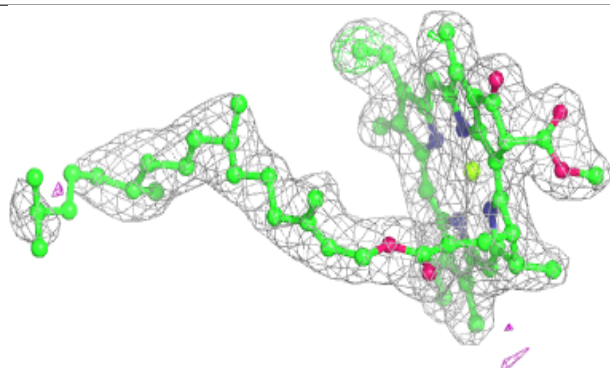
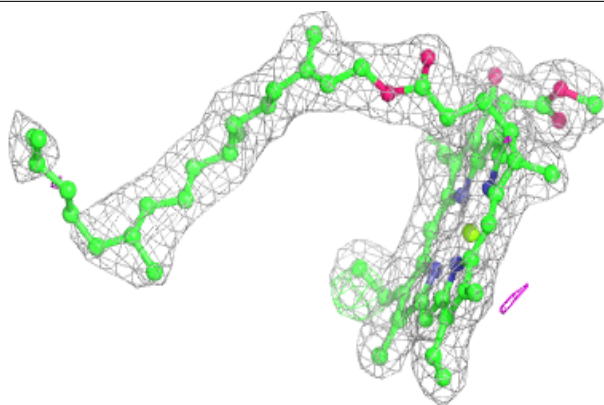
**Electron density around LHG D 409:**

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

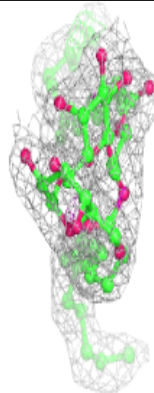
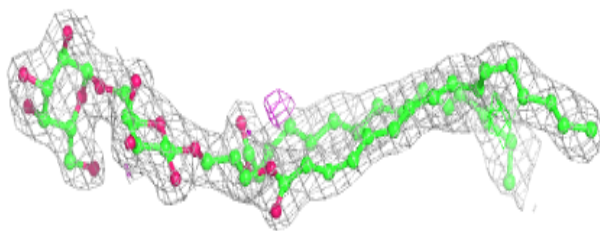
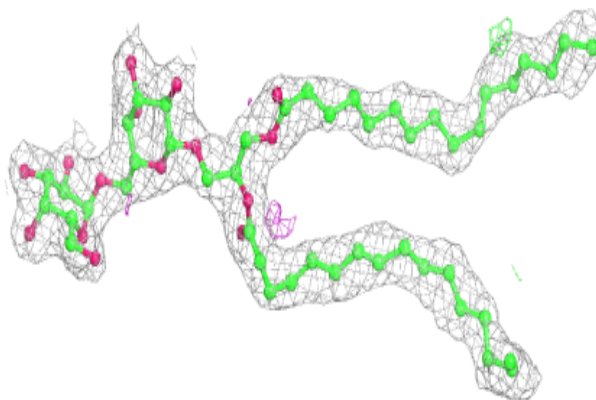


Electron density around CLA C 508:

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

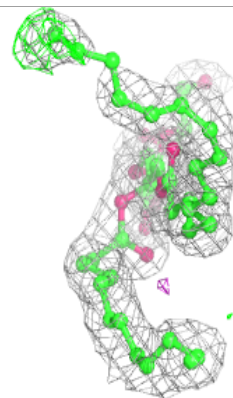
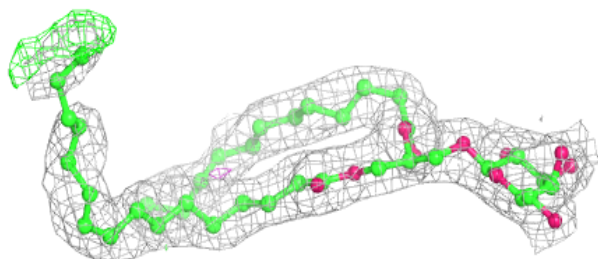
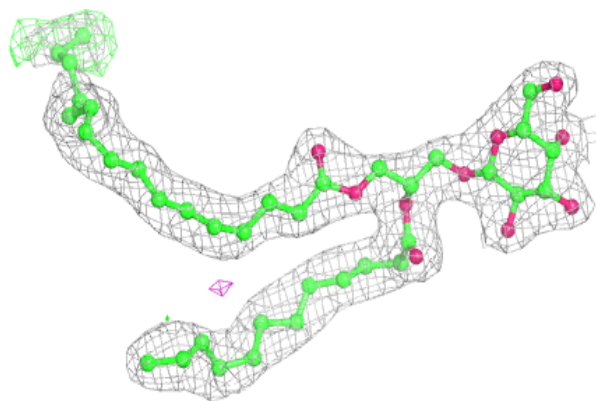
**Electron density around DGD c 519:**

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



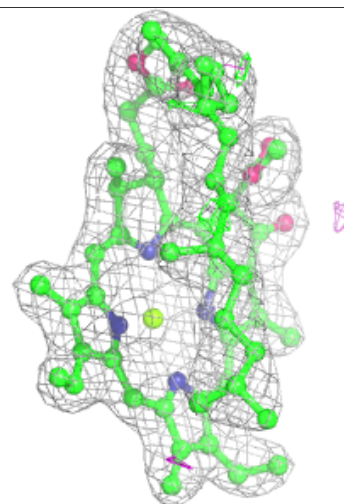
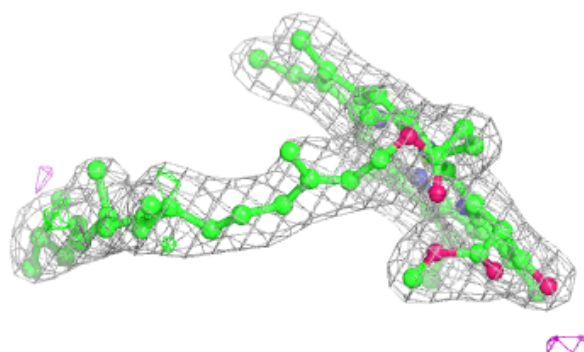
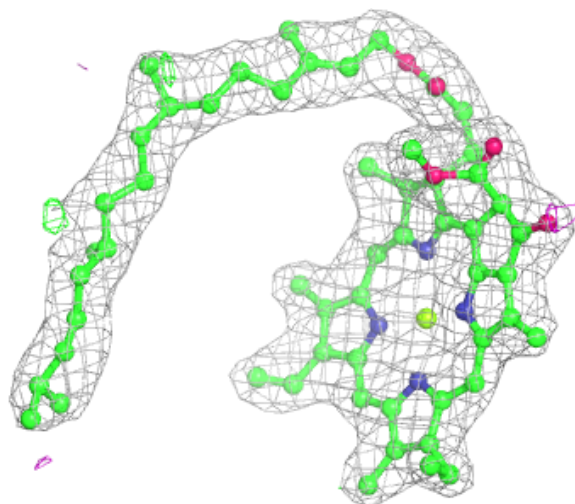
Electron density around LMG D 412:

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



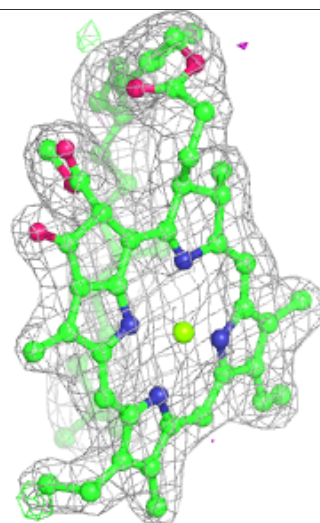
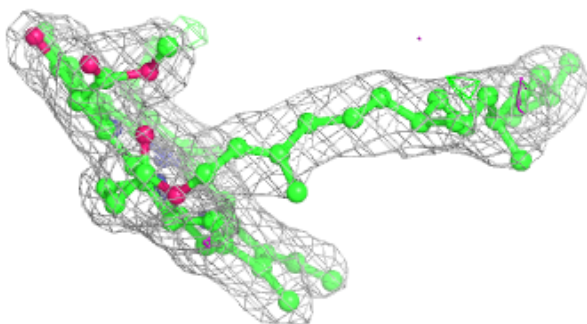
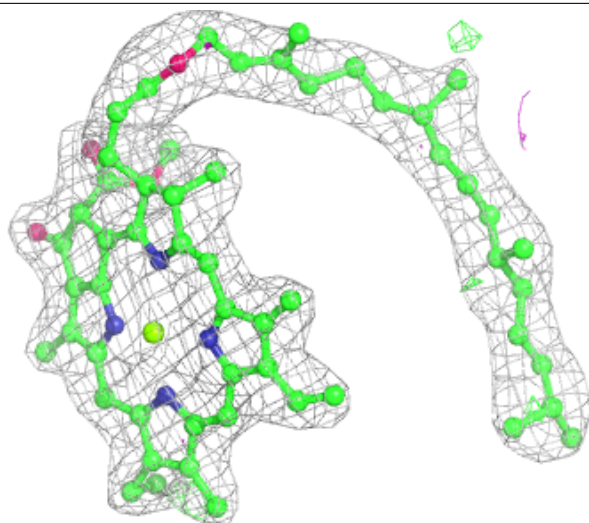
Electron density around CLA C 507:

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



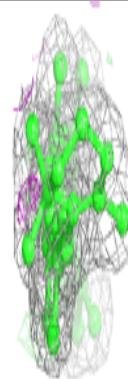
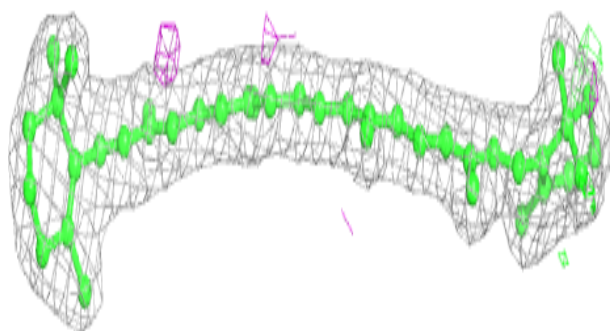
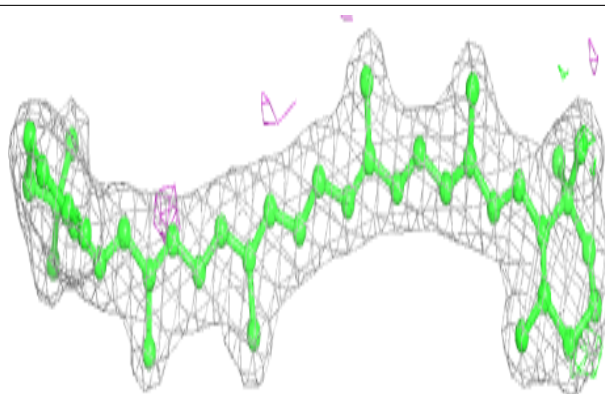
Electron density around CLA c 508:

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

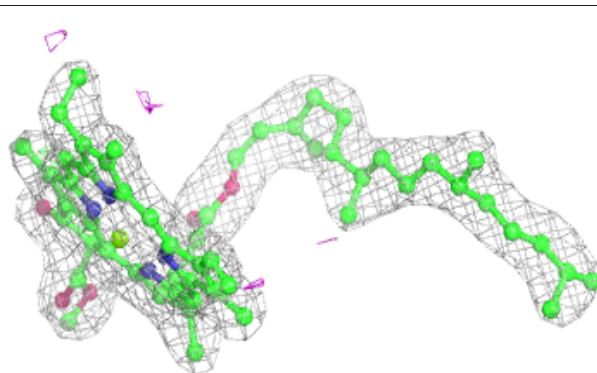
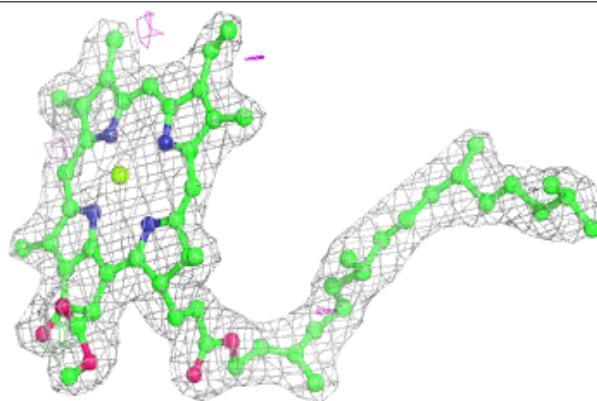


Electron density around BCR B 618:

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

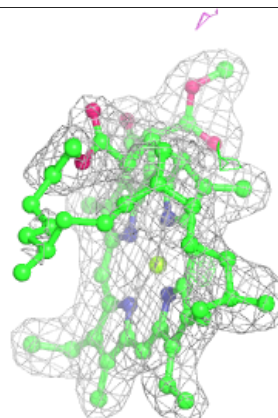
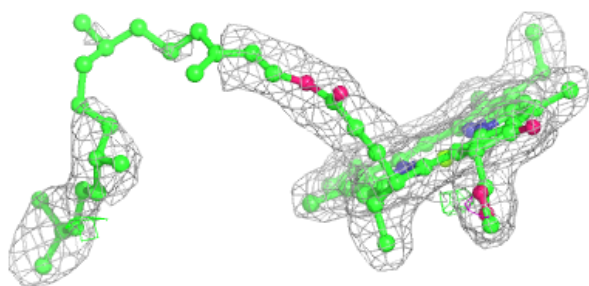
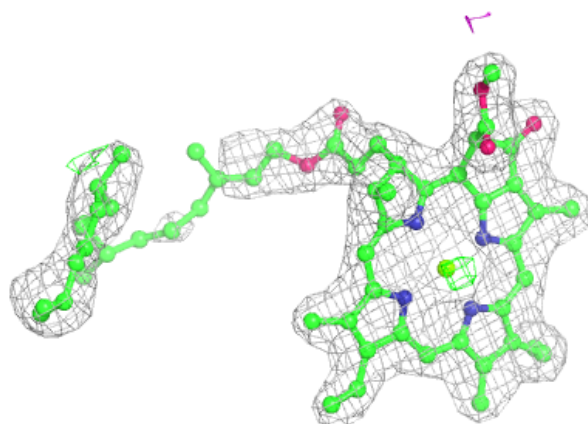
**Electron density around CLA c 512:**

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



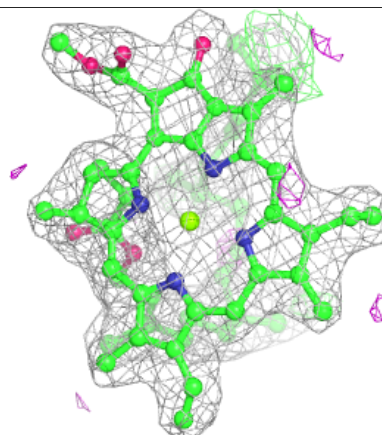
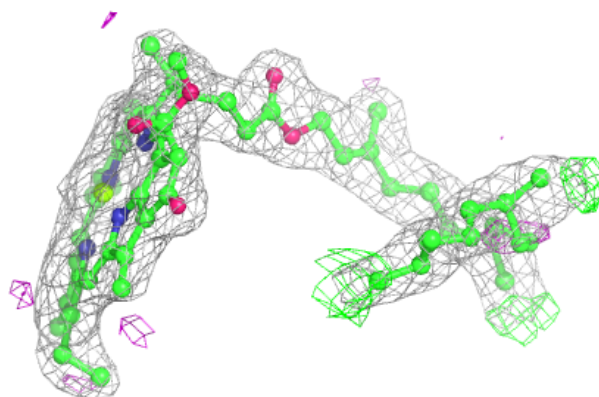
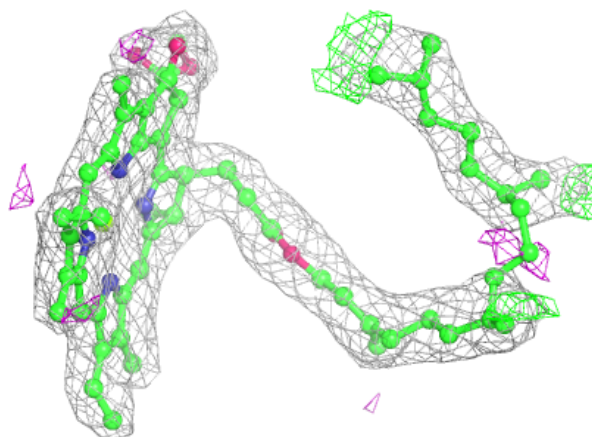
Electron density around CLA a 409:

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

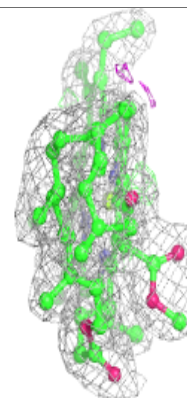
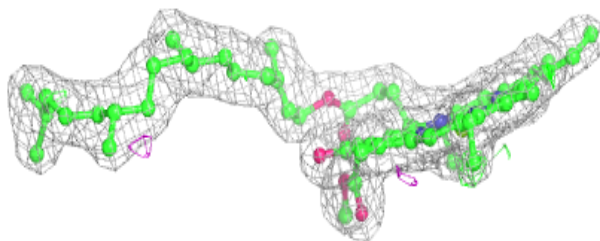
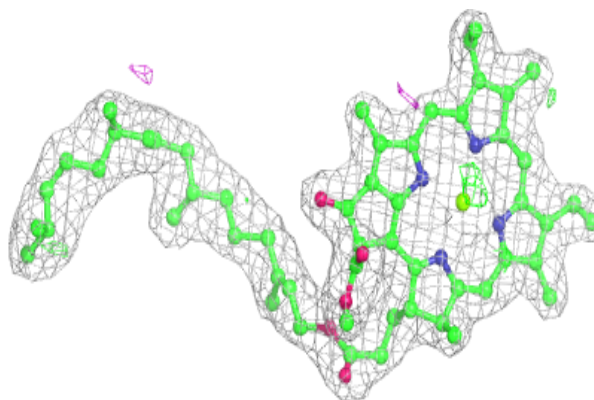


Electron density around CLA B 607:

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

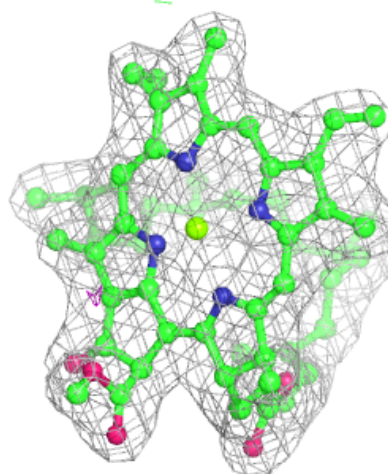
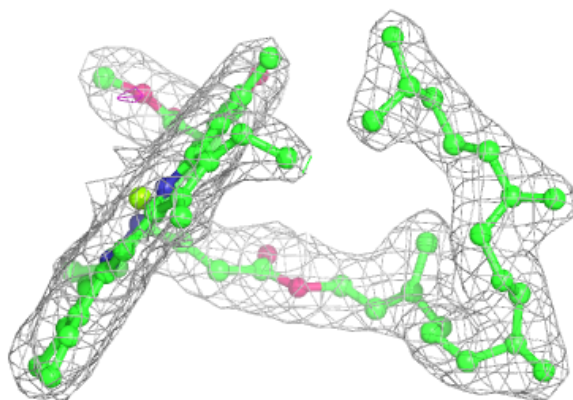
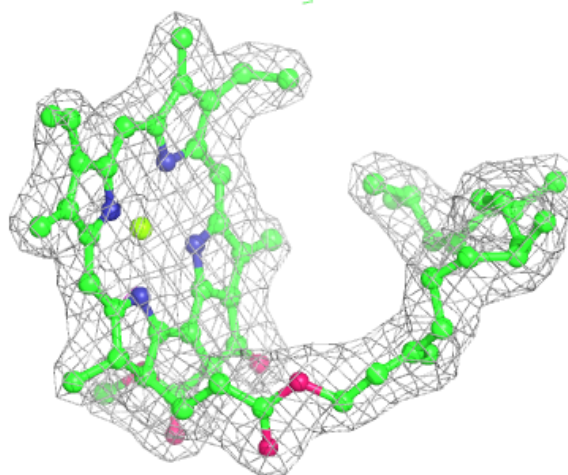
**Electron density around CLA B 603:**

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



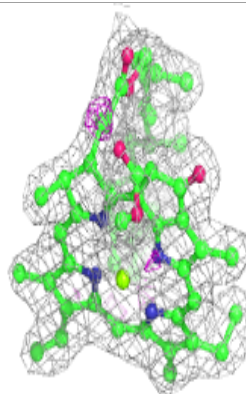
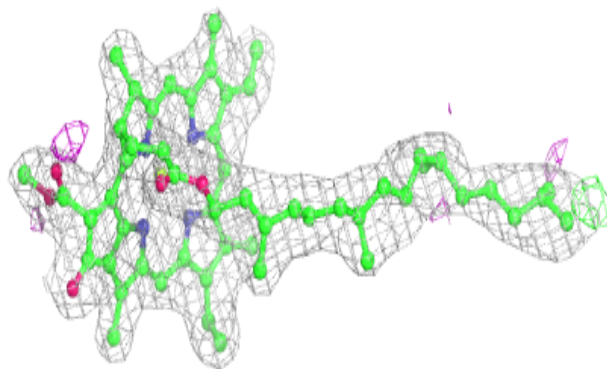
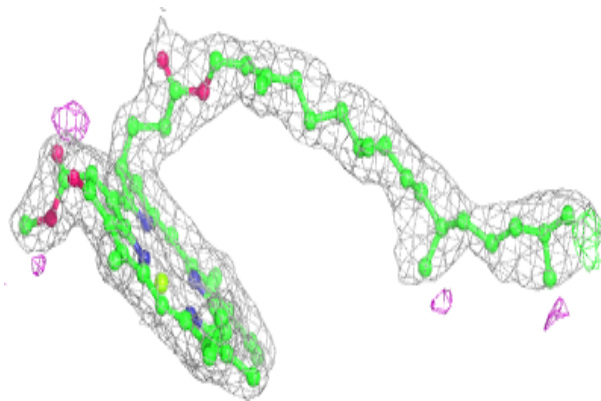
Electron density around CLA C 503:

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

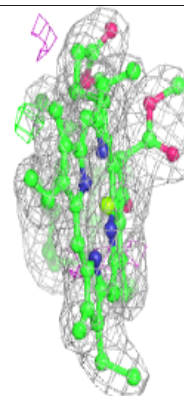
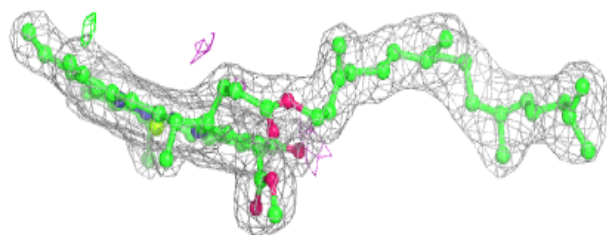
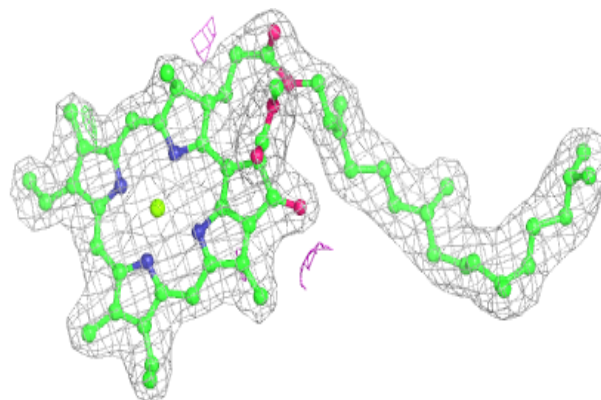


Electron density around CLA c 505:

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

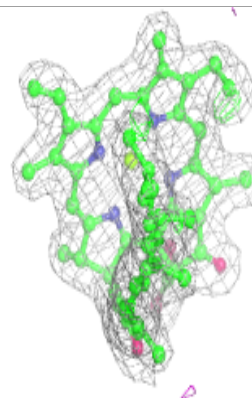
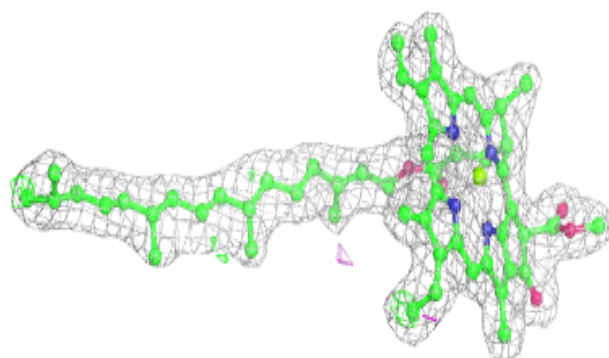
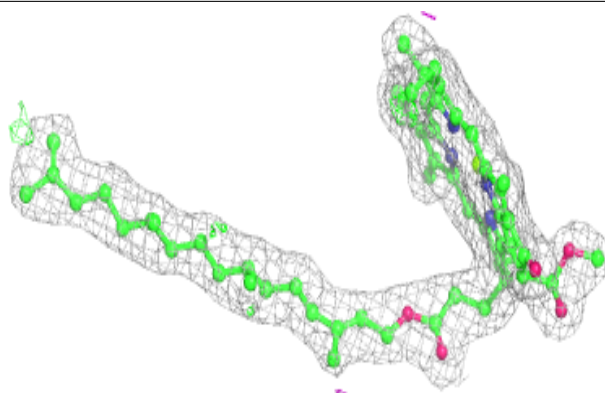
**Electron density around CLA b 606:**

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

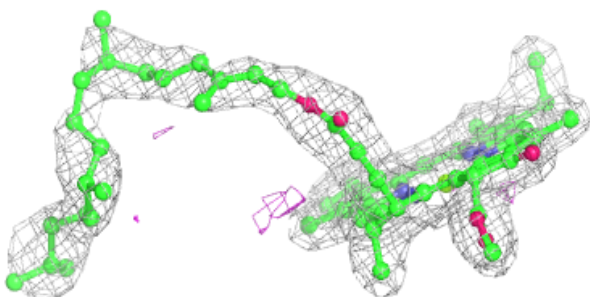
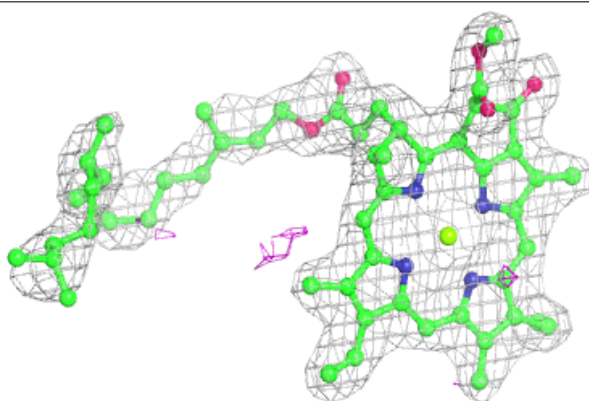


Electron density around CLA b 611:

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

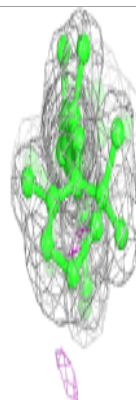
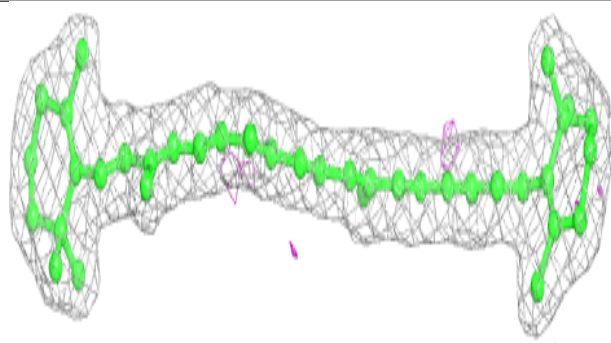
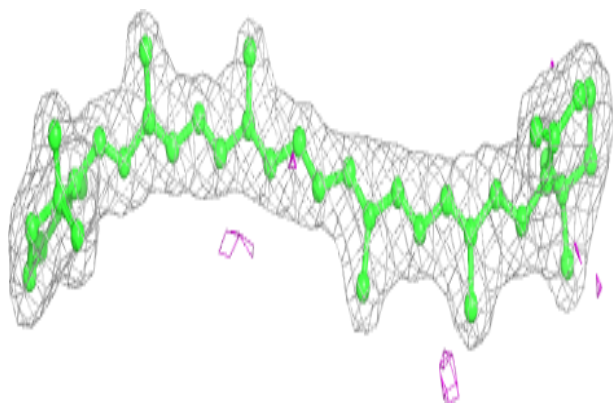
**Electron density around CLA A 408:**

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

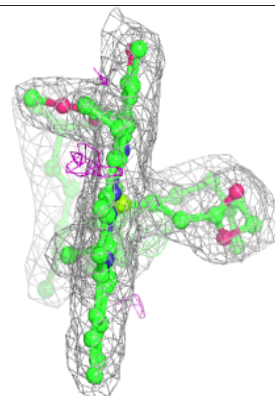
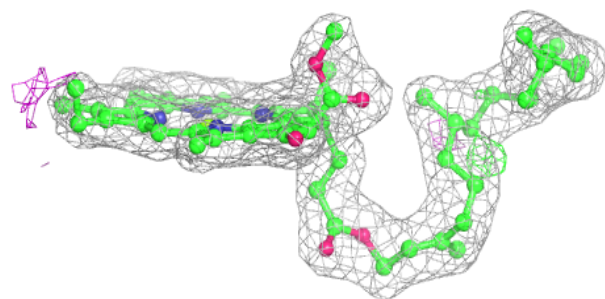
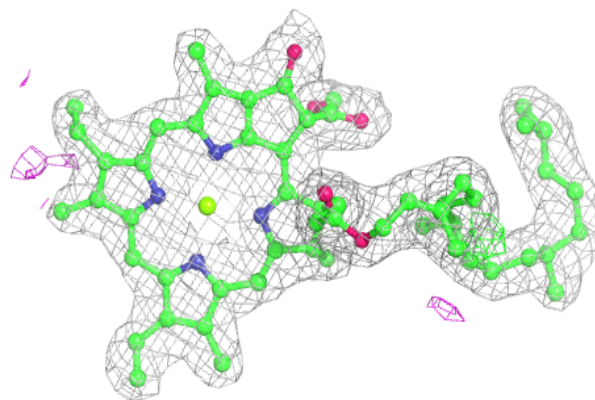


Electron density around BCR A 409:

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

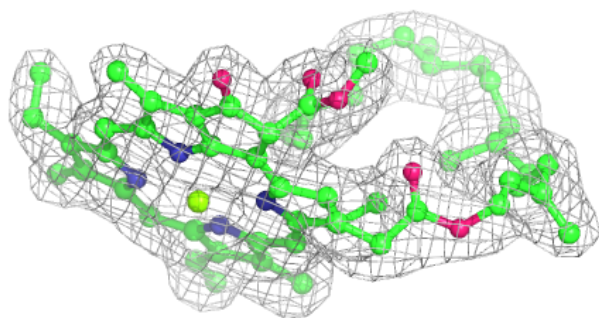
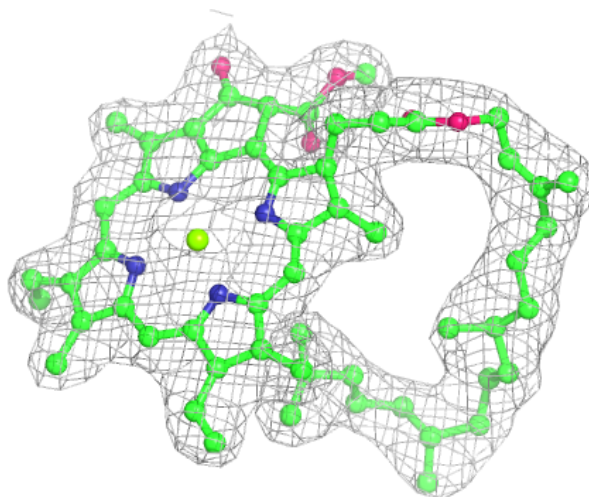
**Electron density around CLA b 616:**

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



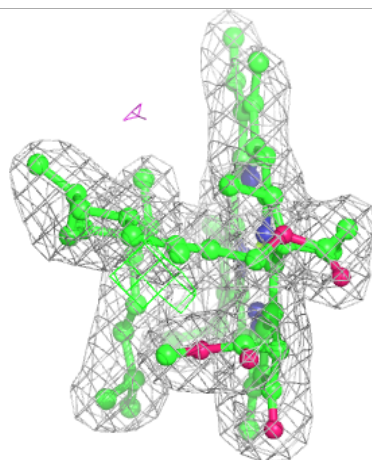
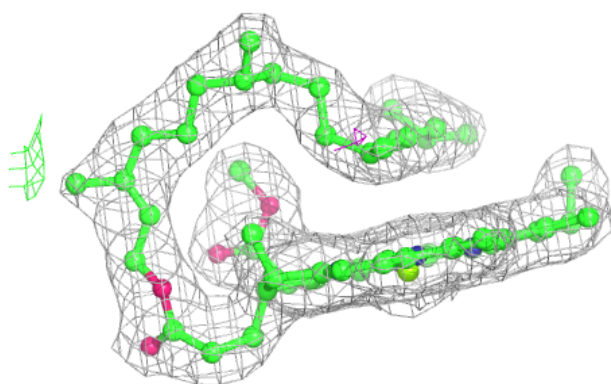
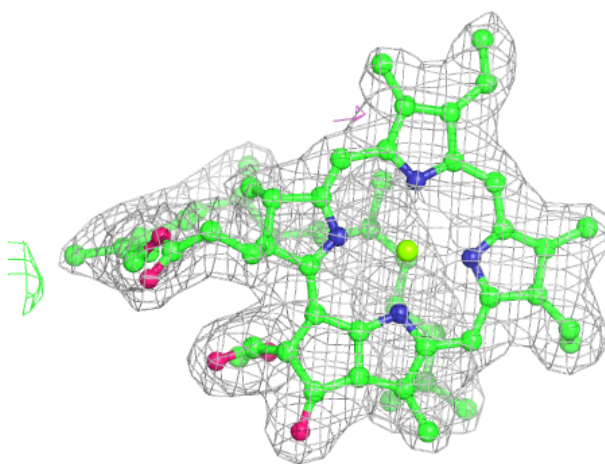
Electron density around CLA b 619:

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



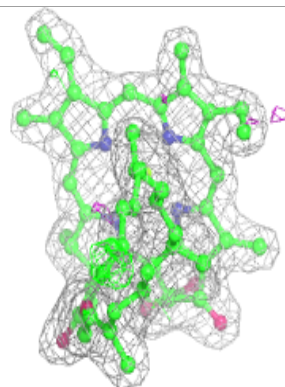
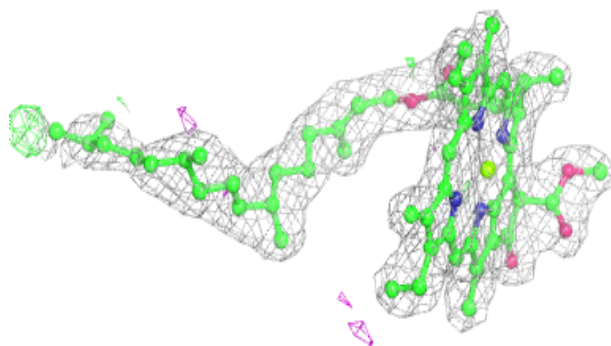
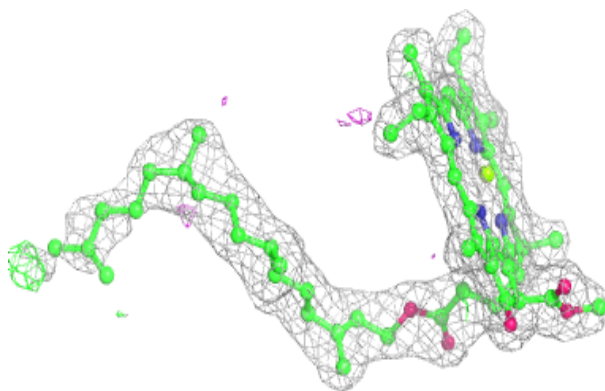
Electron density around CLA C 510:

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

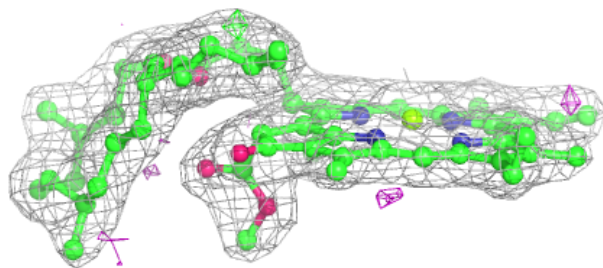
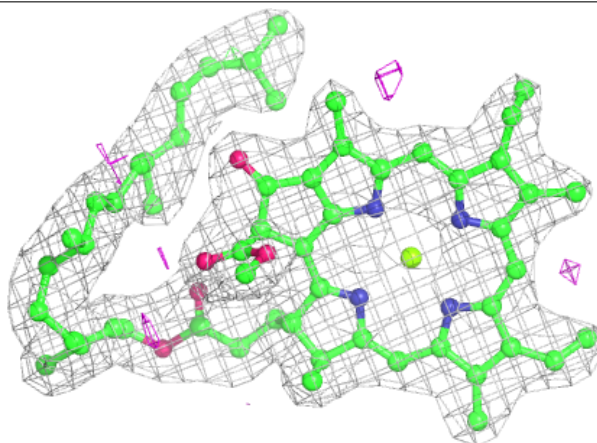


Electron density around CLA c 509:

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

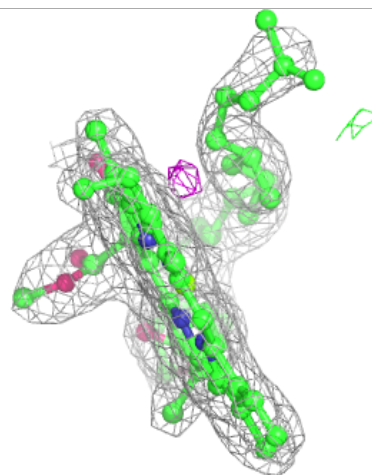
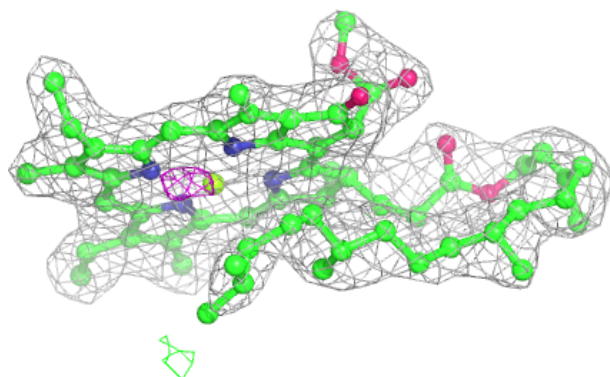
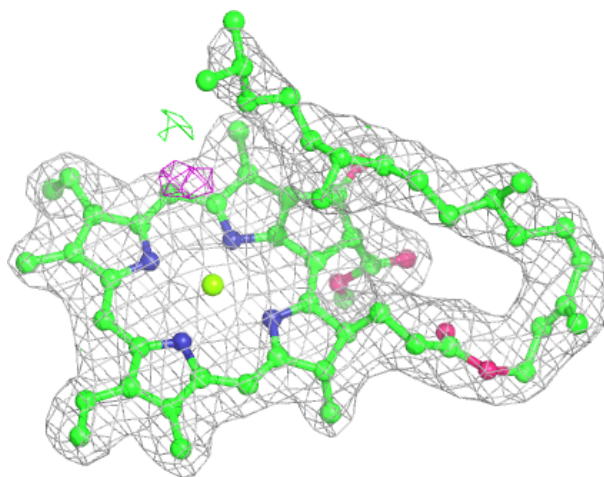
**Electron density around CLA b 614:**

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



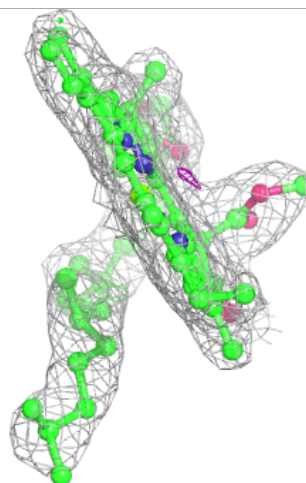
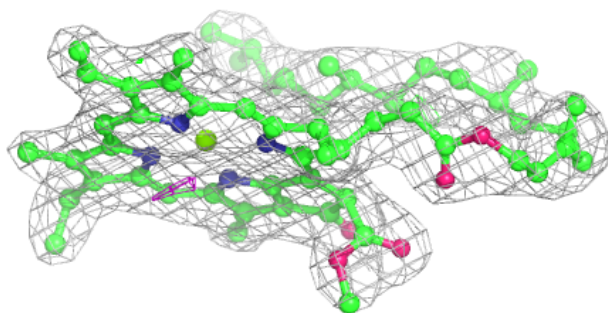
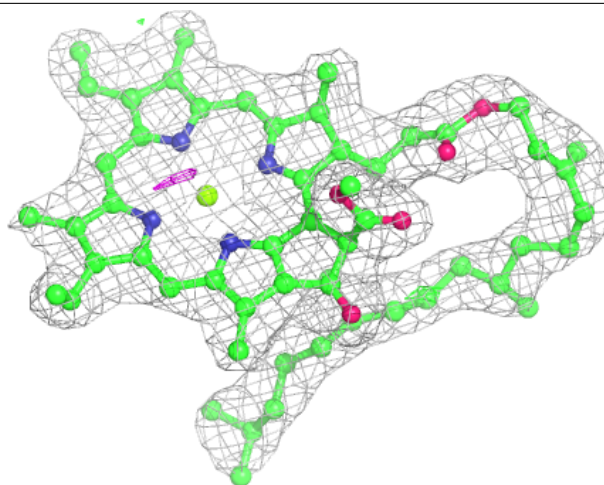
Electron density around CLA c 510:

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



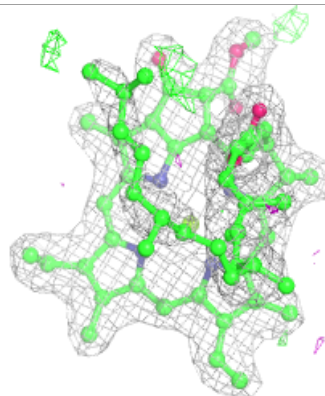
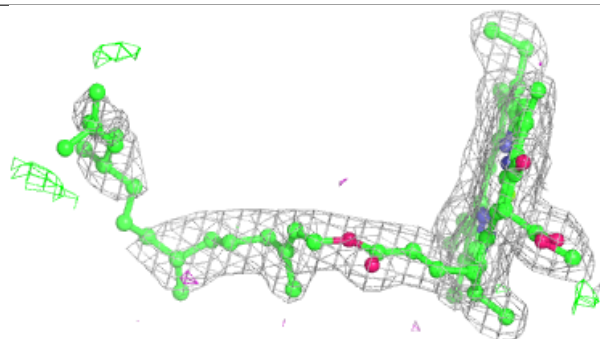
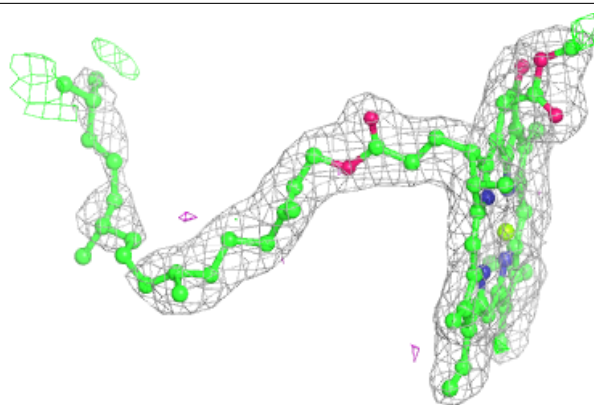
Electron density around CLA C 509:

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

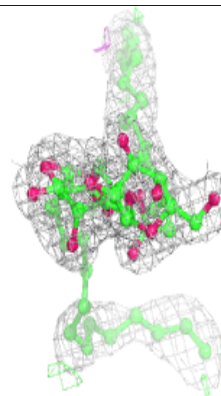
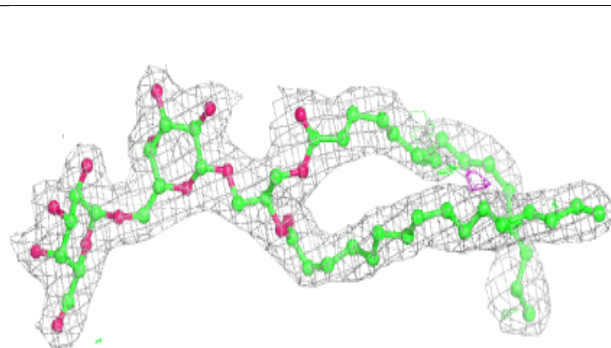
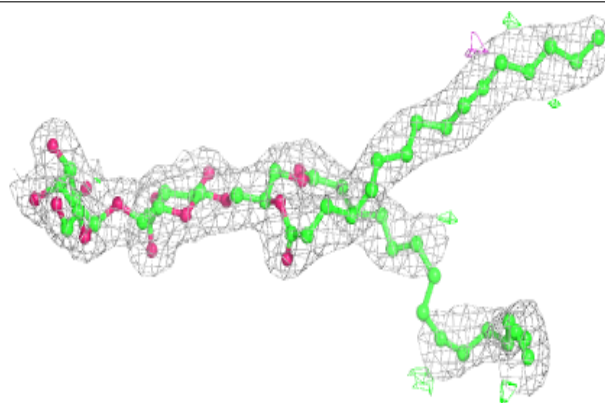


Electron density around CLA d 405:

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

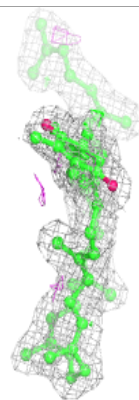
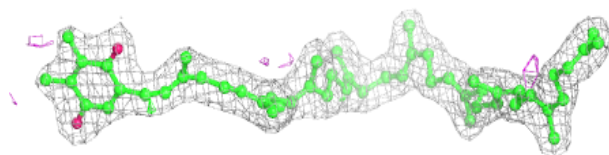
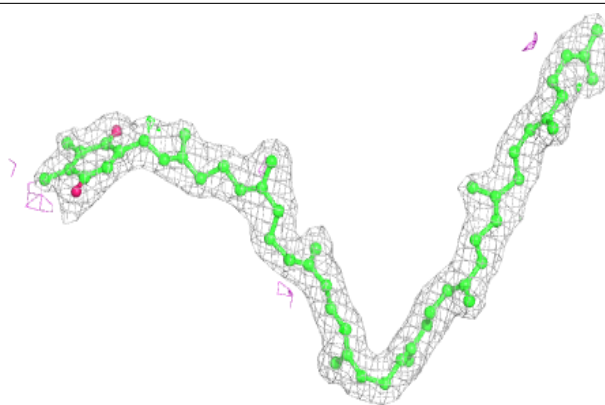
**Electron density around DGD C 515:**

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

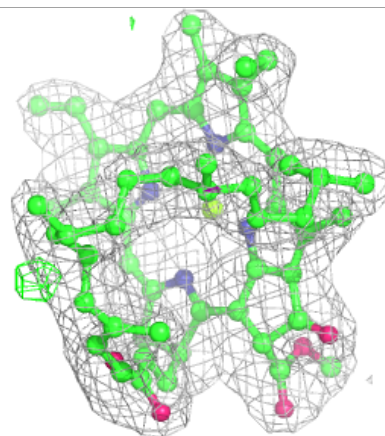
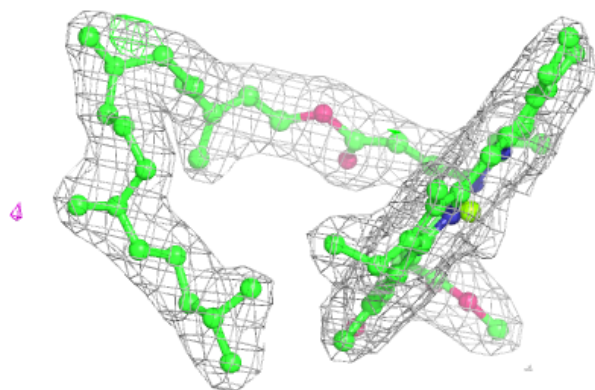
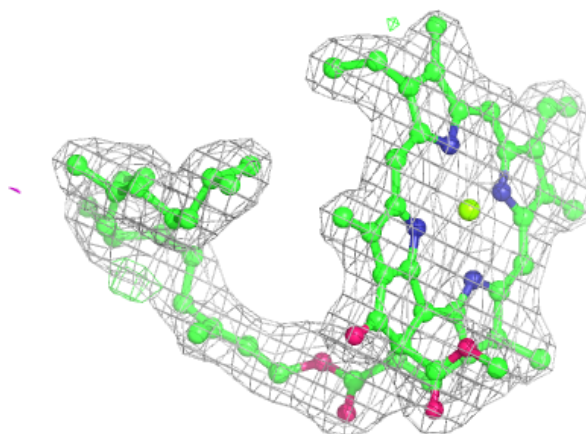


Electron density around PL9 d 407:

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

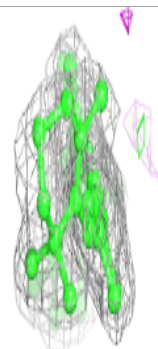
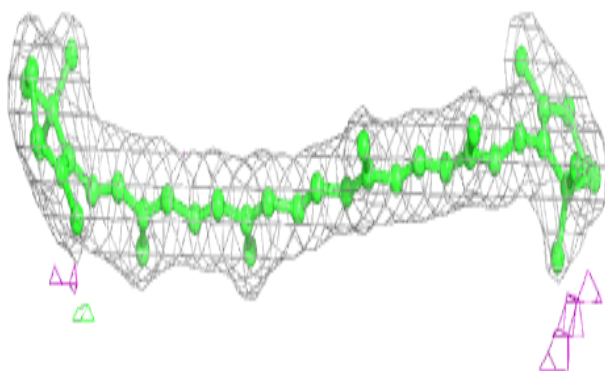
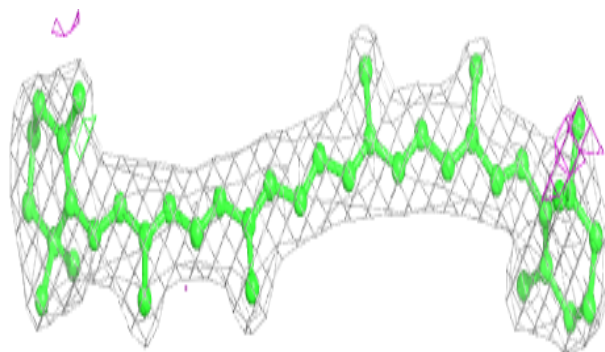
**Electron density around CLA c 504:**

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

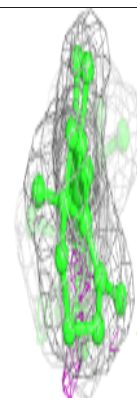
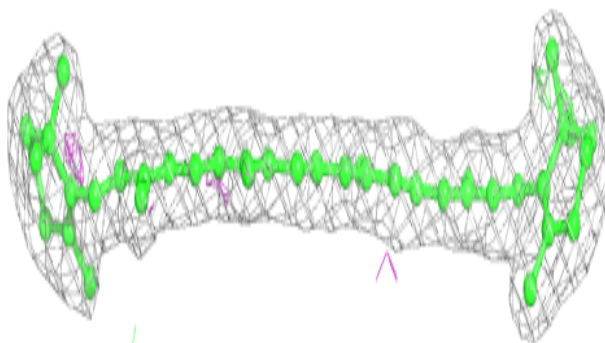
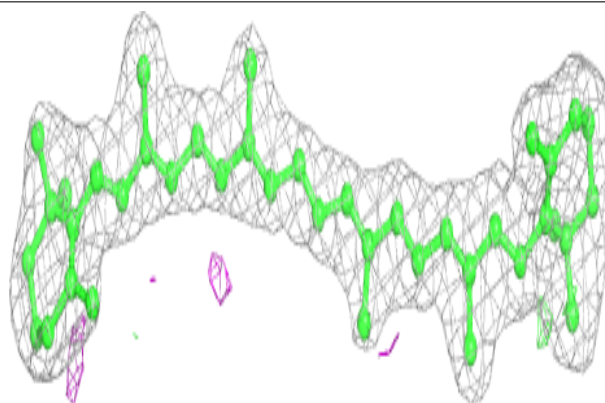


Electron density around BCR B 620:

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

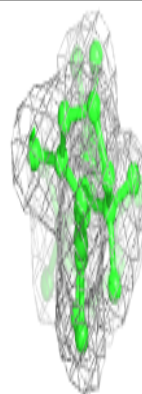
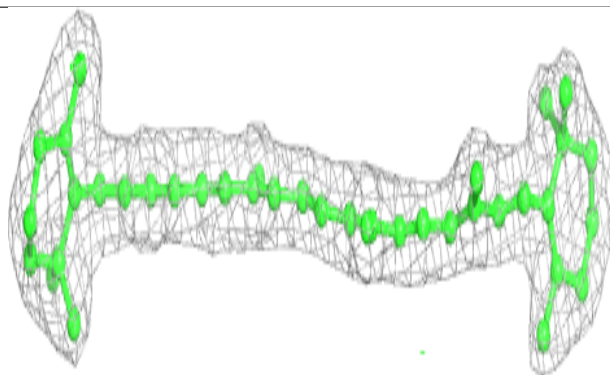
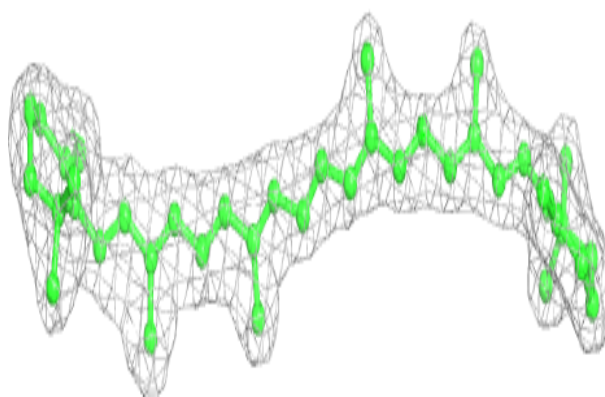
**Electron density around BCR b 622:**

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

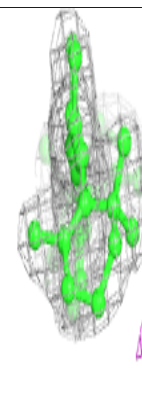
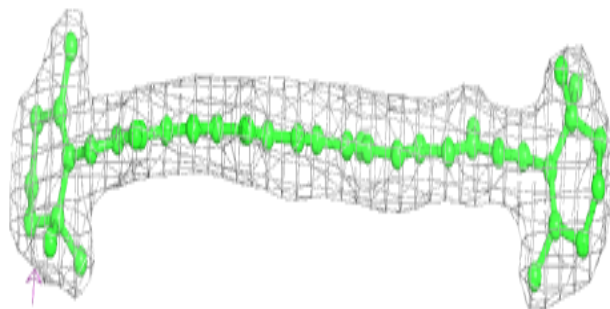
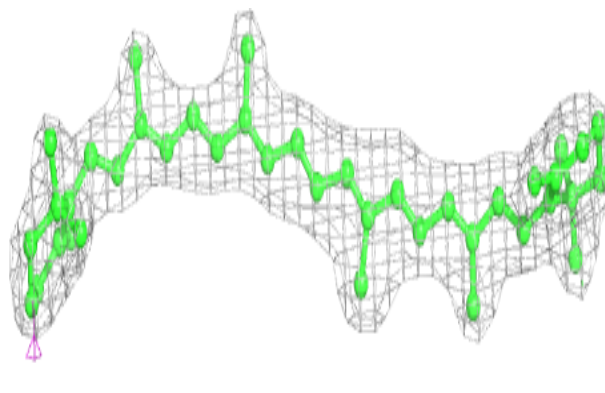


Electron density around BCR a 410:

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

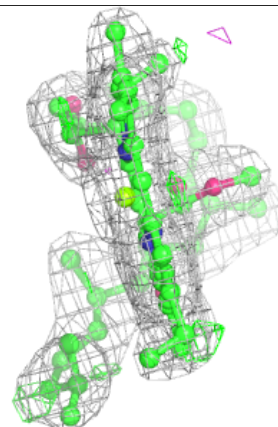
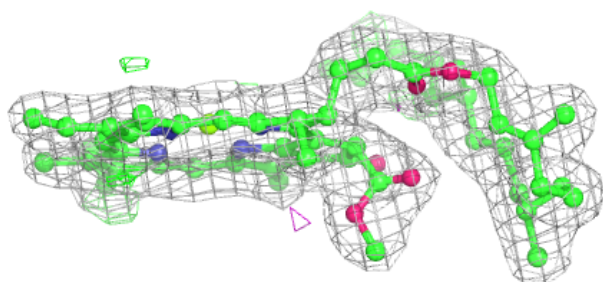
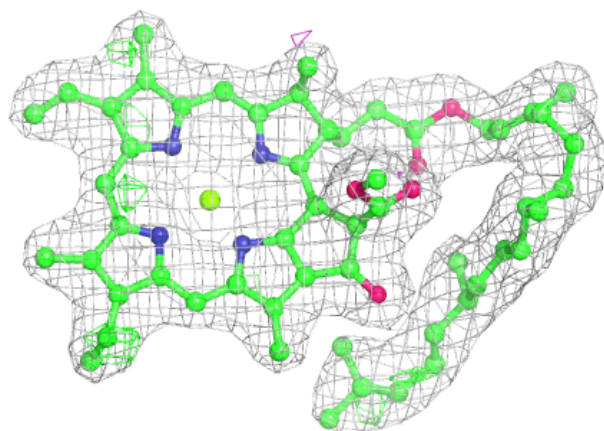
**Electron density around BCR C 514:**

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

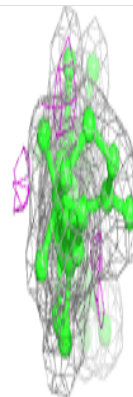
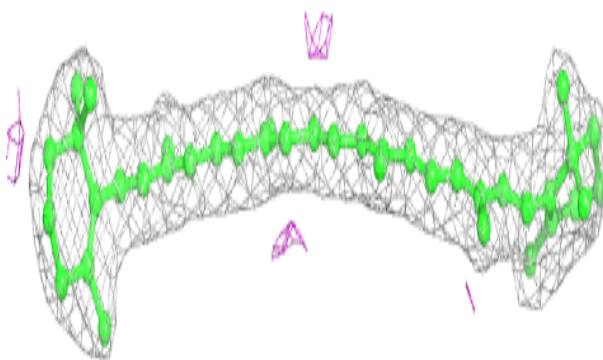
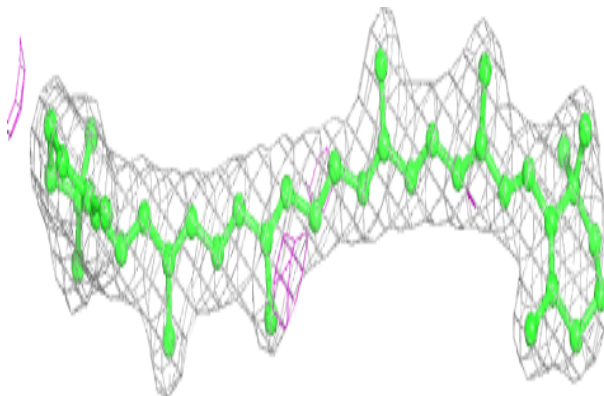


Electron density around CLA B 611:

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

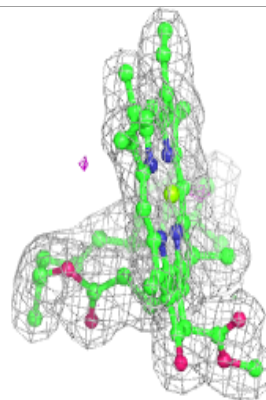
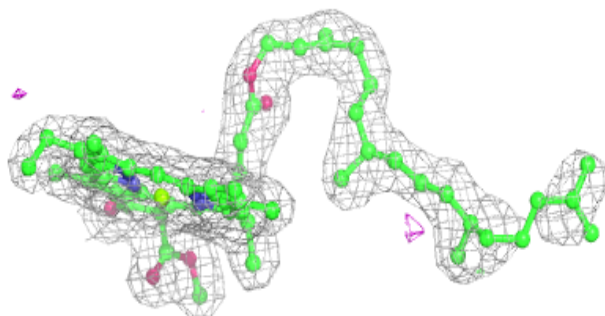
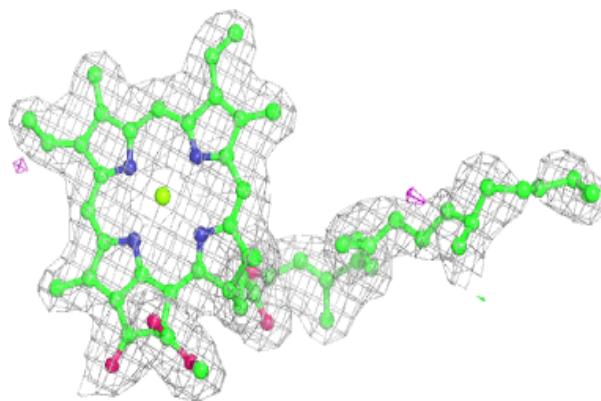
**Electron density around BCR b 621:**

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

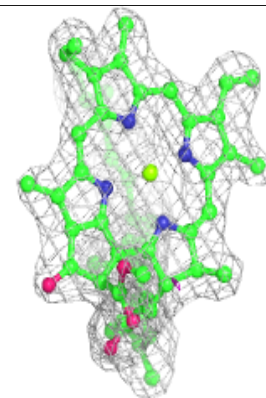
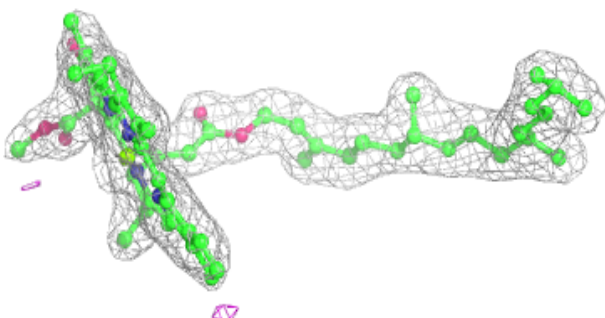
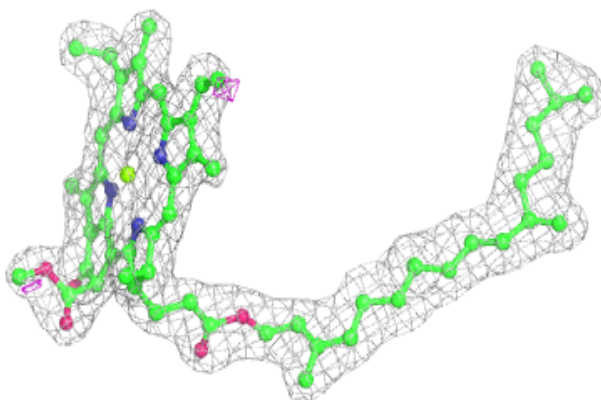


Electron density around CLA a 407:

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

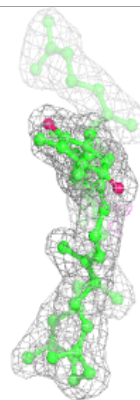
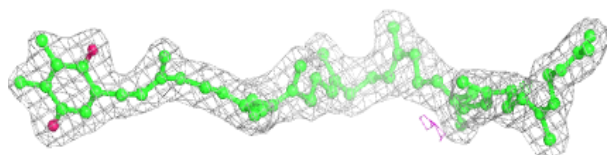
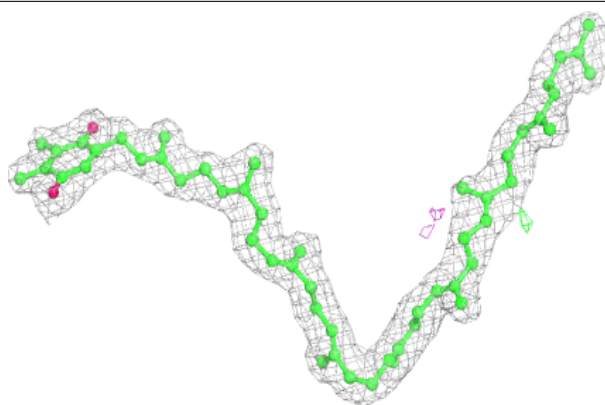
**Electron density around CLA B 610:**

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

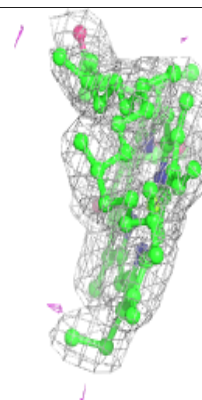
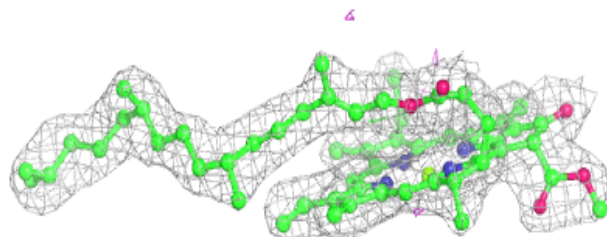
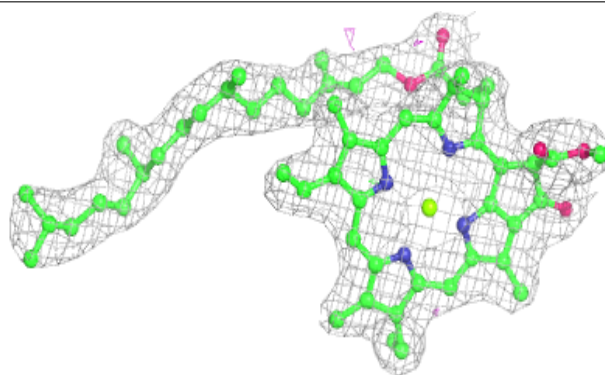


Electron density around PL9 D 407:

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

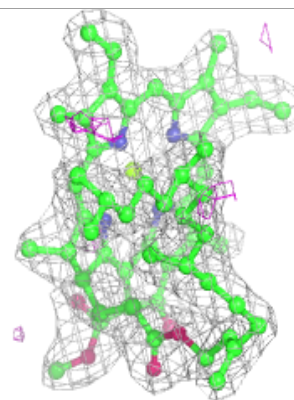
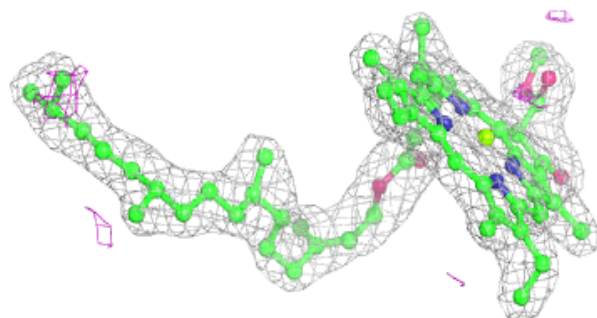
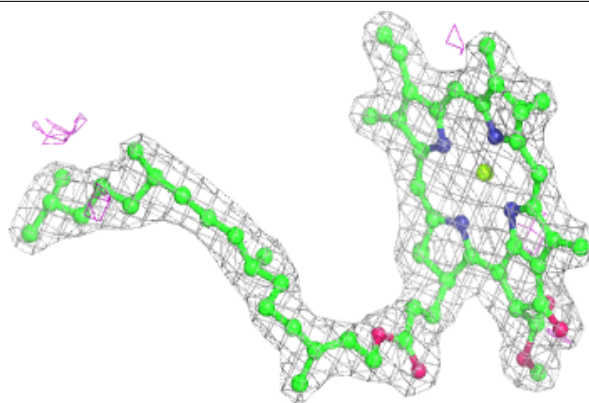
**Electron density around CLA c 502:**

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



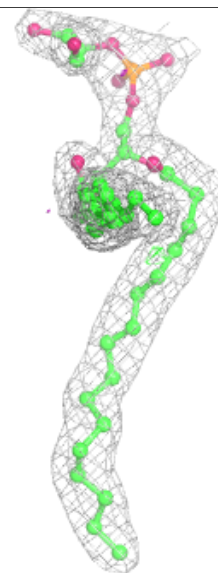
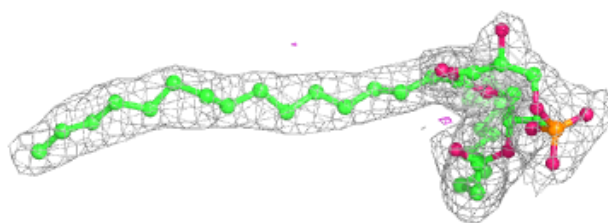
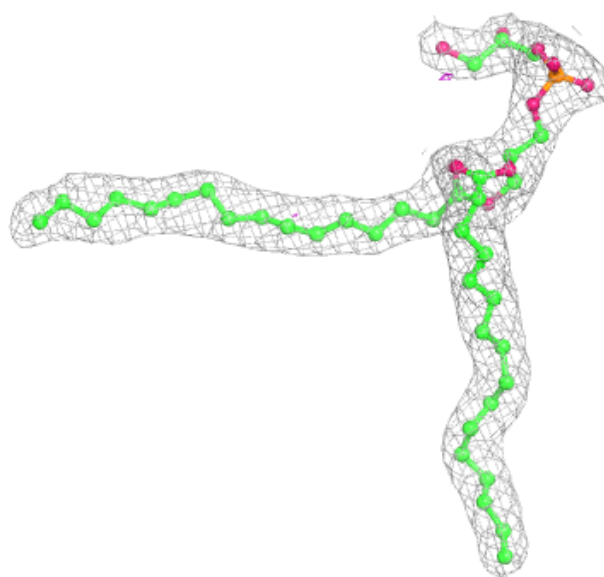
Electron density around CLA C 511:

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



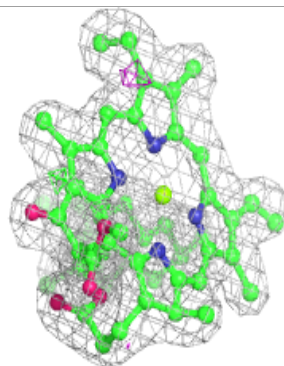
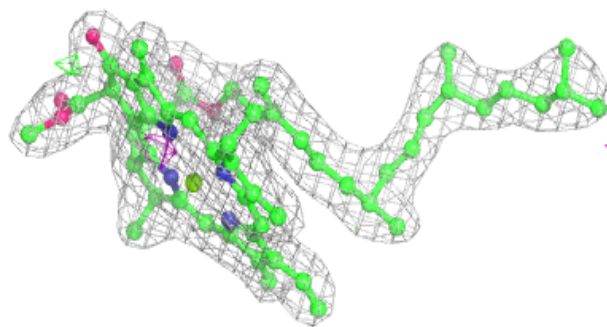
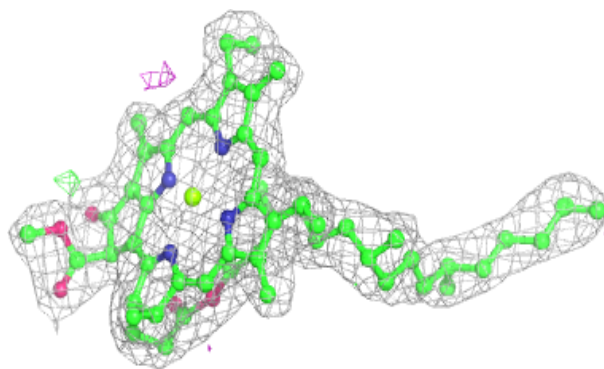
Electron density around LHG b 624:

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



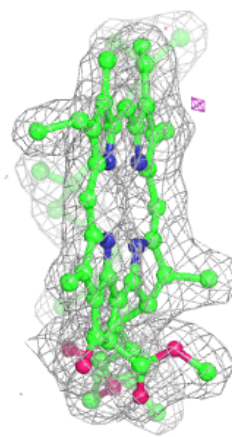
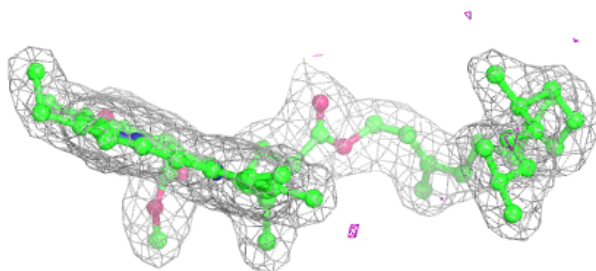
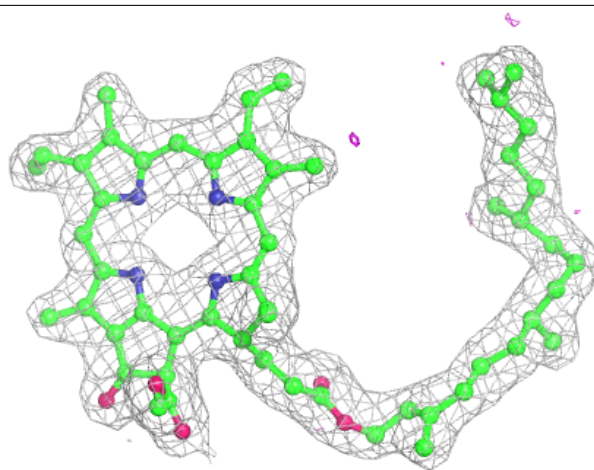
Electron density around CLA c 506:

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



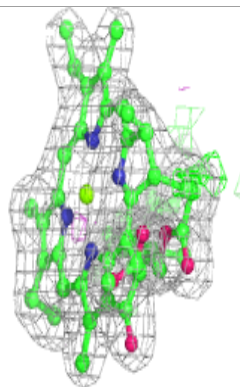
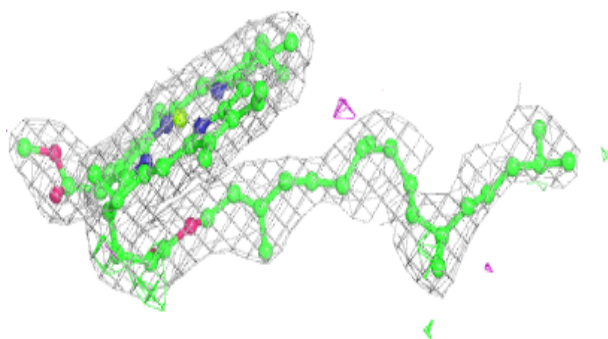
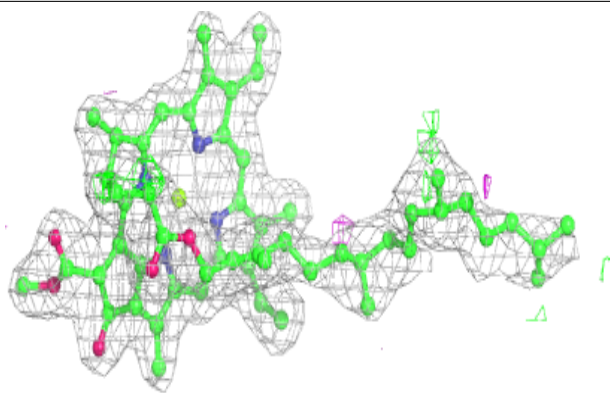
Electron density around PHO a 408:

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

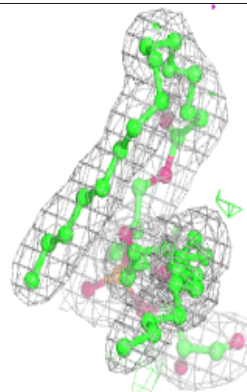
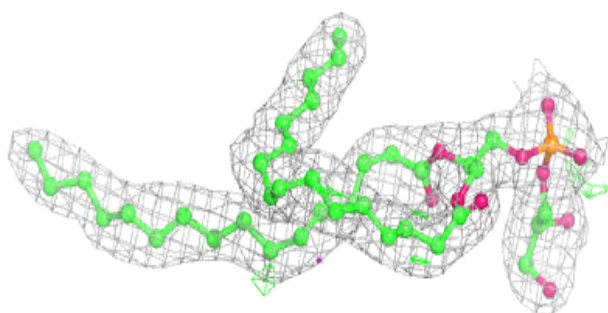
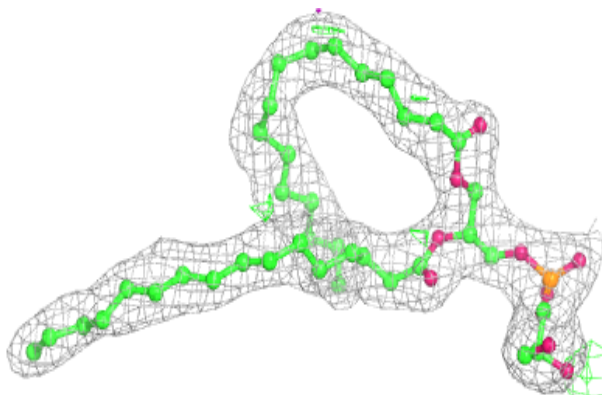


Electron density around CLA B 615:

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

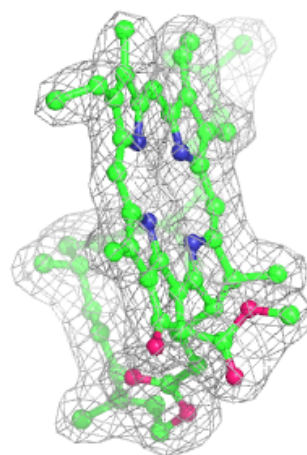
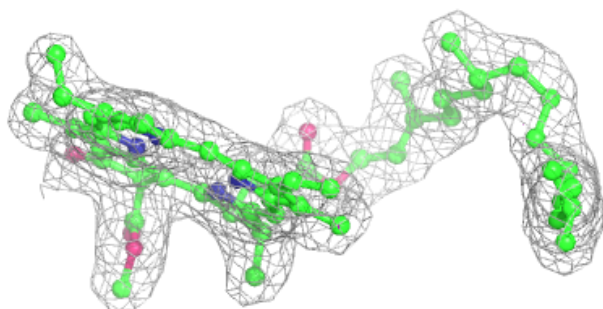
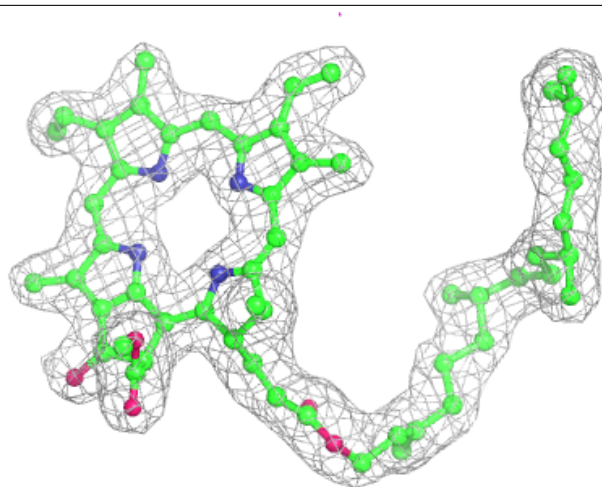
**Electron density around LHG d 409:**

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



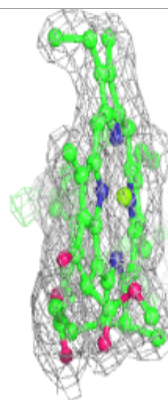
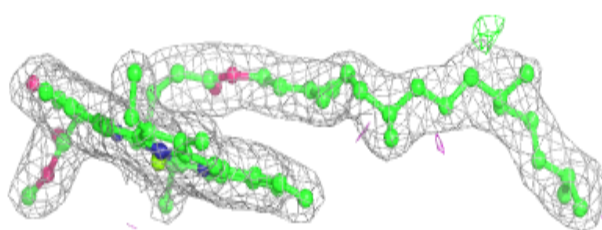
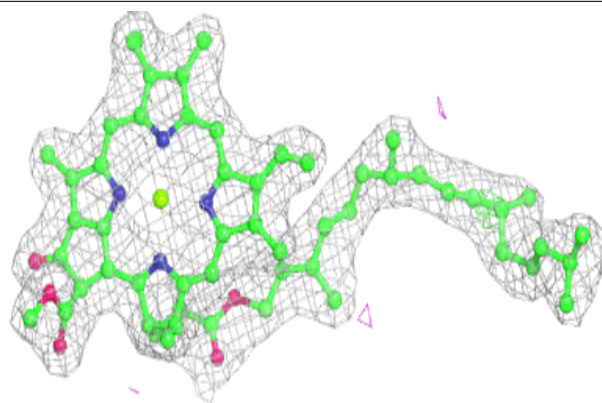
Electron density around PHO D 404:

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

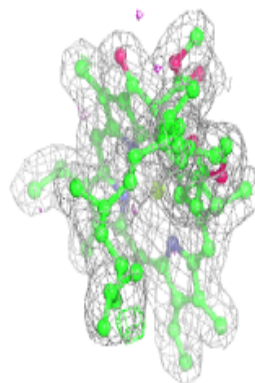
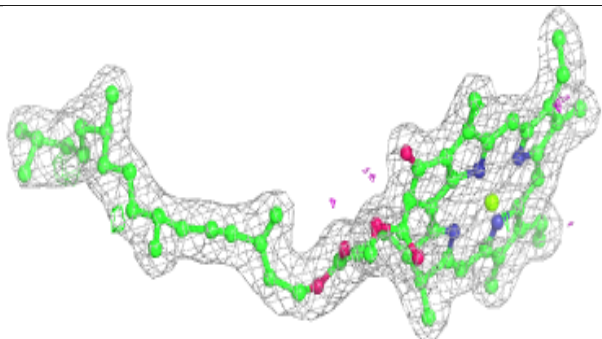
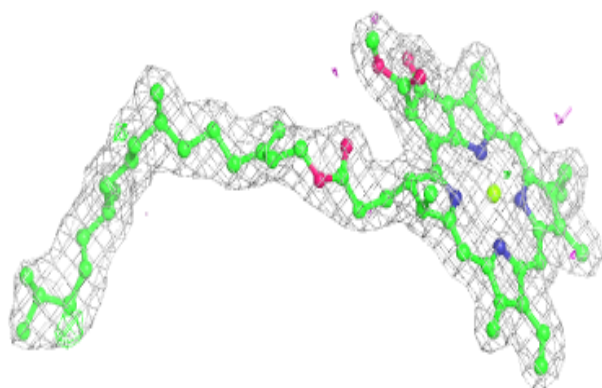


Electron density around CLA b 607:

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

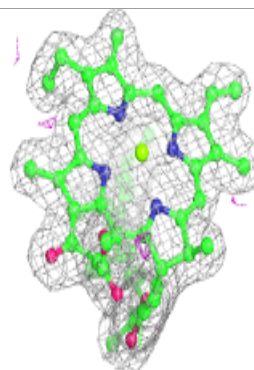
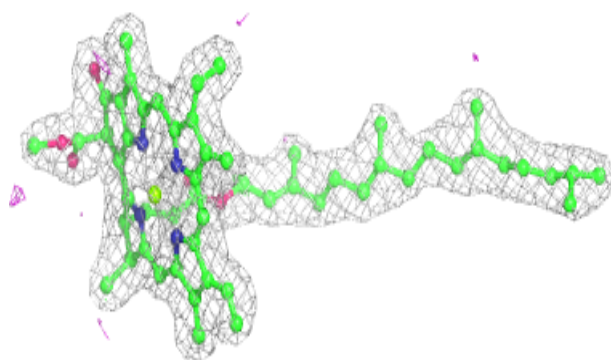
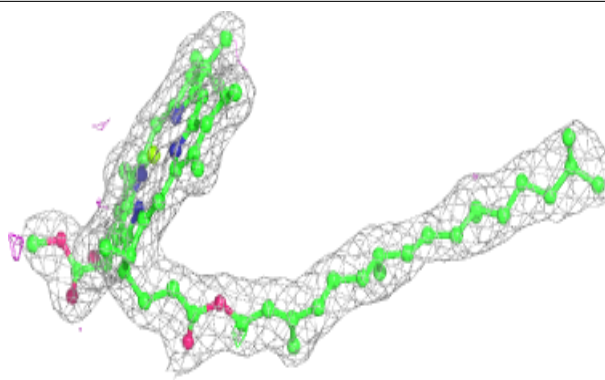
**Electron density around CLA A 404:**

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

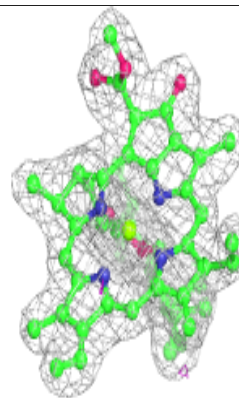
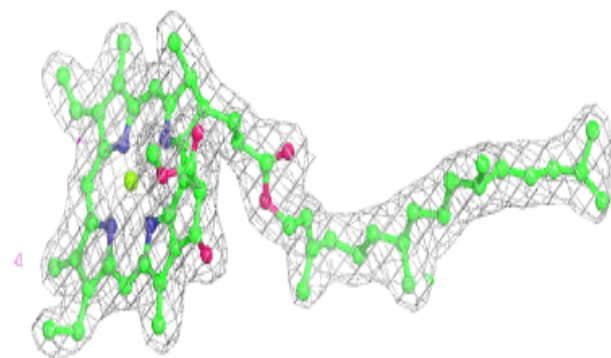
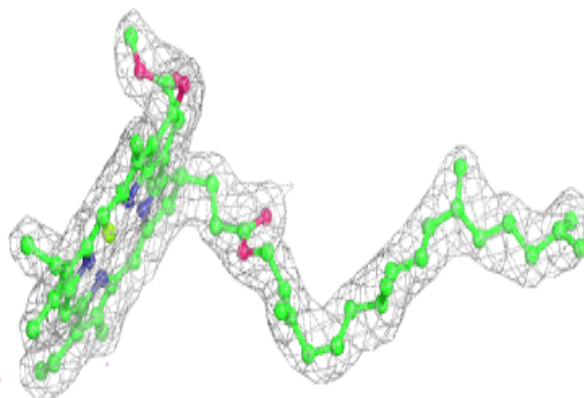


Electron density around CLA B 608:

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

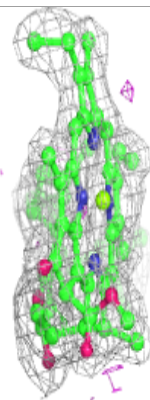
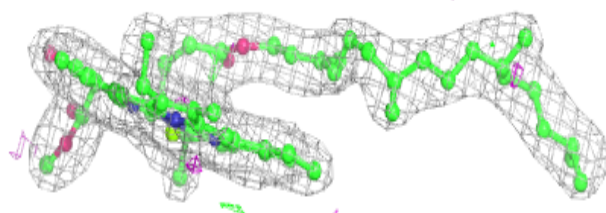
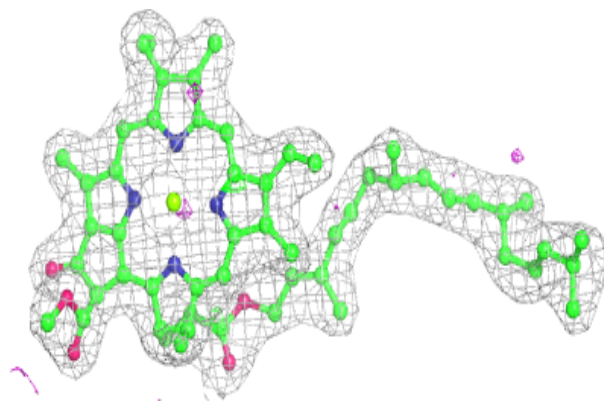
**Electron density around CLA C 502:**

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

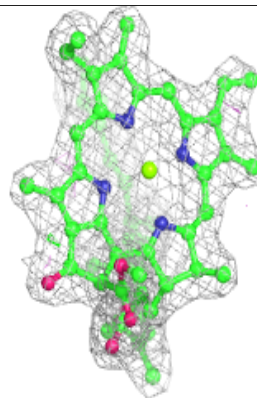
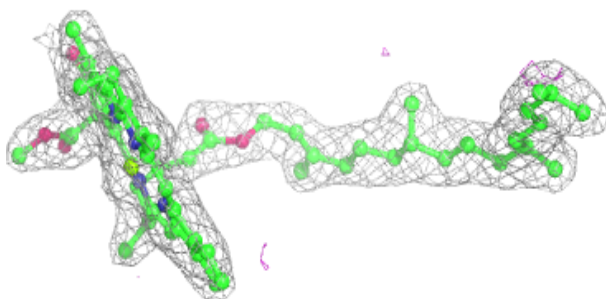
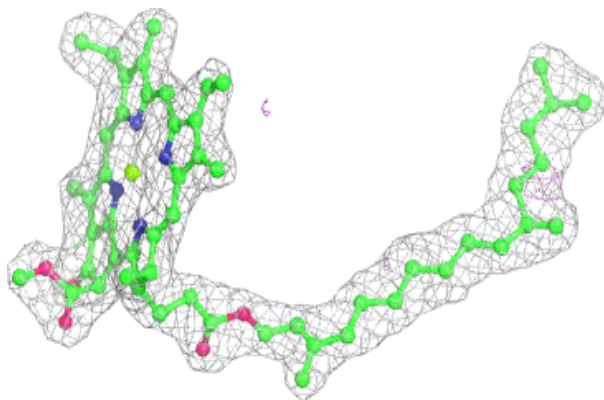


Electron density around CLA B 604:

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

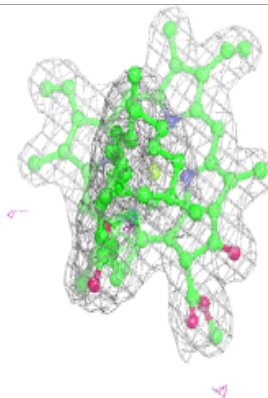
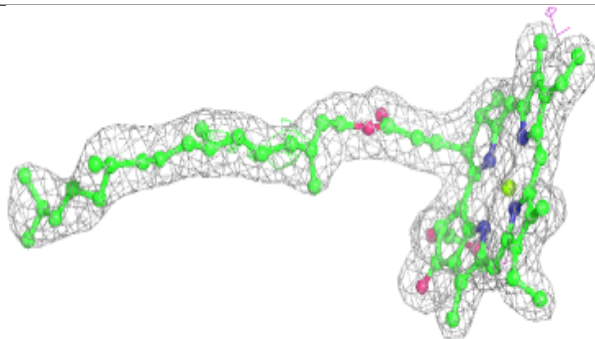
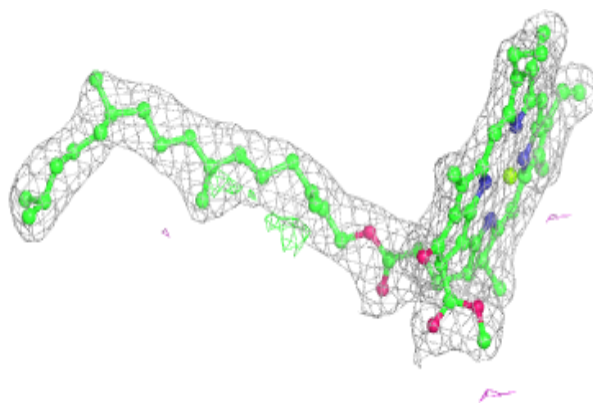
**Electron density around CLA b 613:**

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

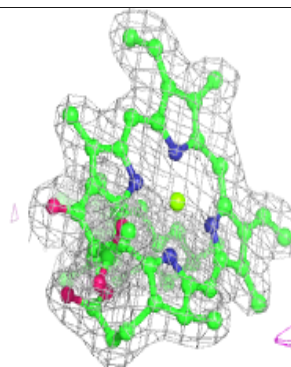
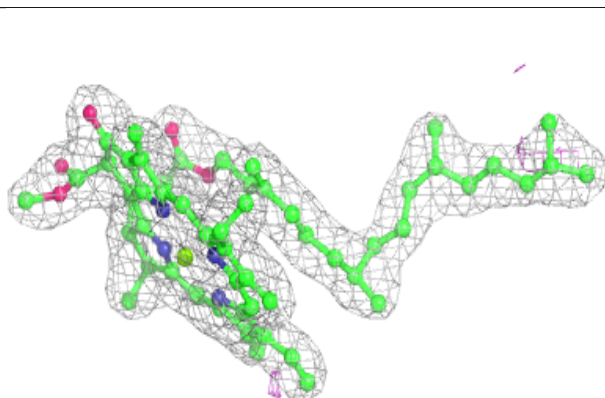
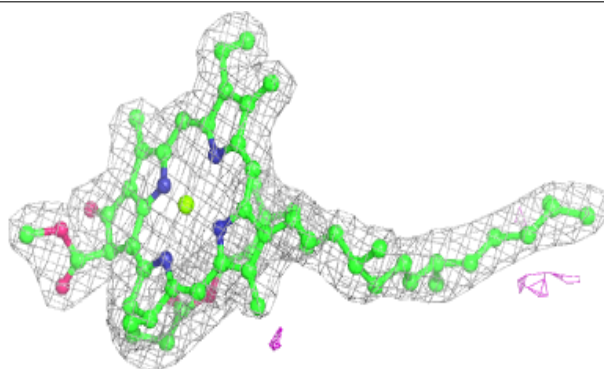


Electron density around CLA b 608:

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

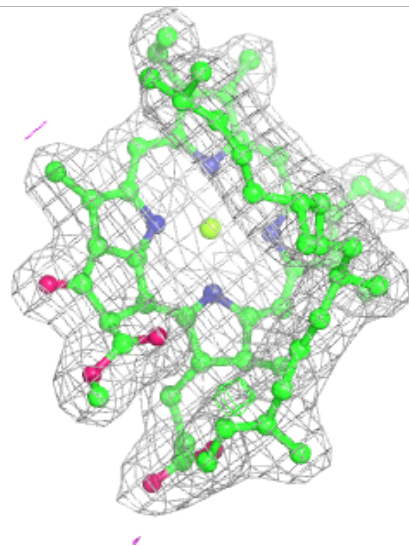
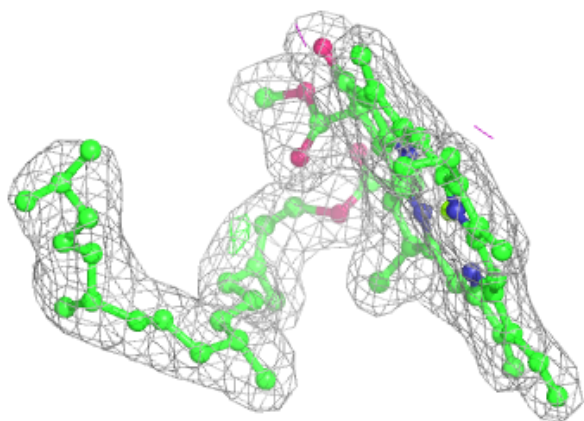
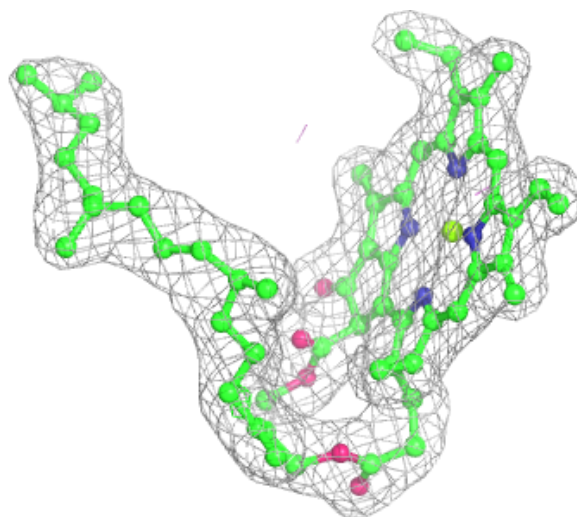
**Electron density around CLA C 505:**

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



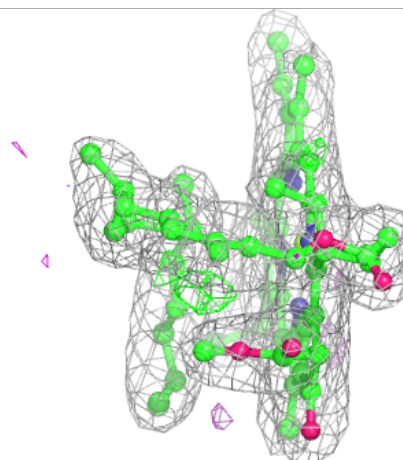
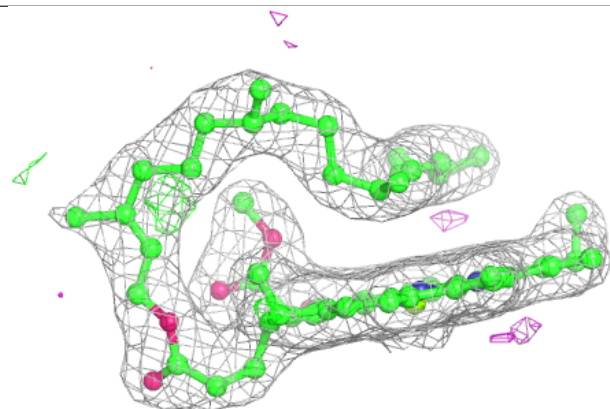
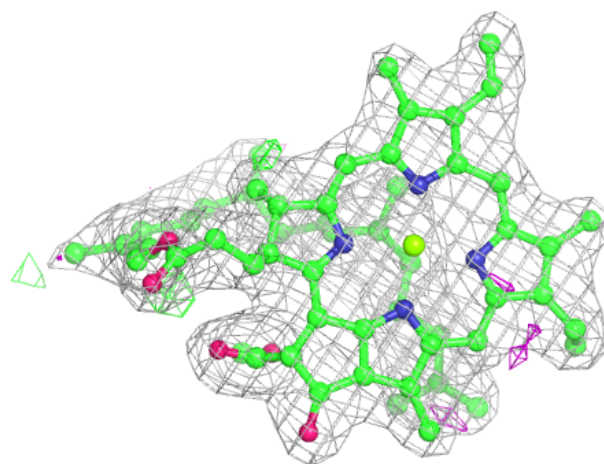
Electron density around CLA B 614:

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



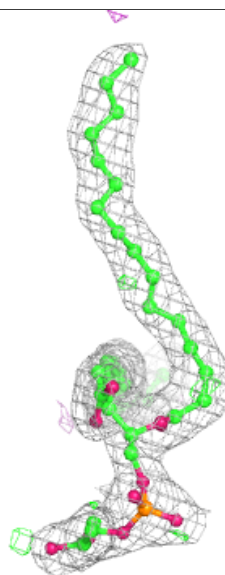
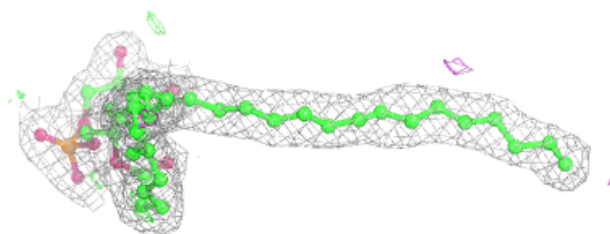
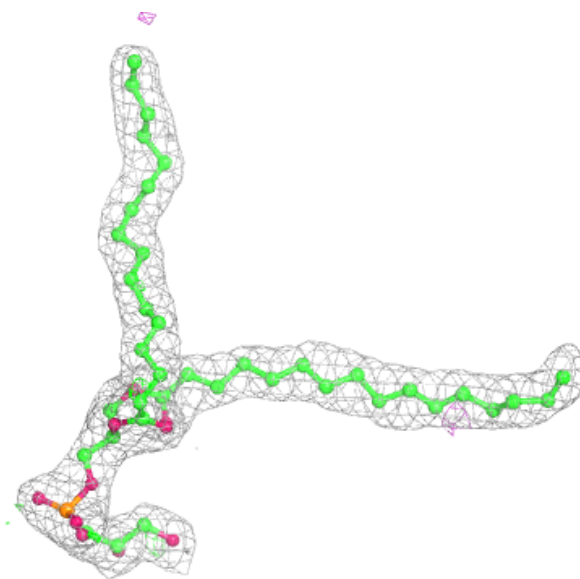
Electron density around CLA c 511:

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



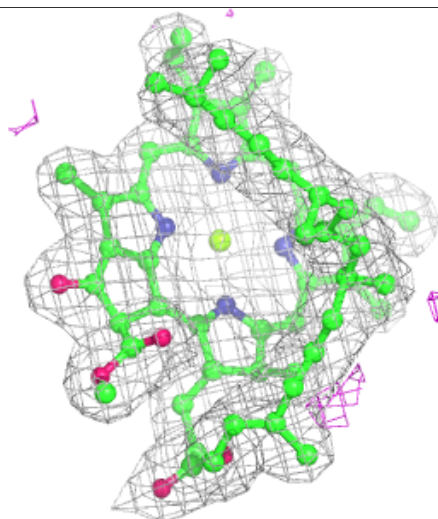
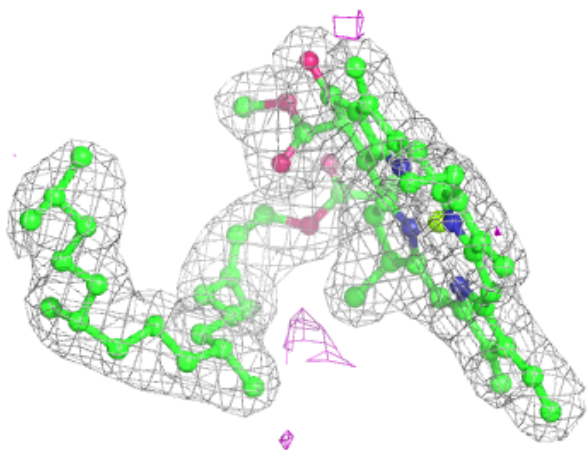
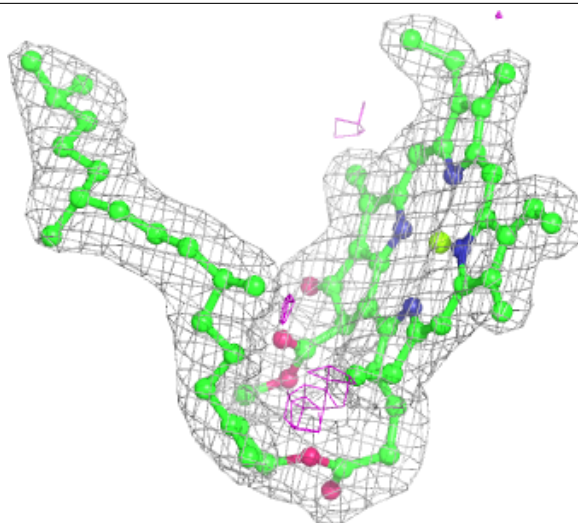
Electron density around LHG B 621:

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



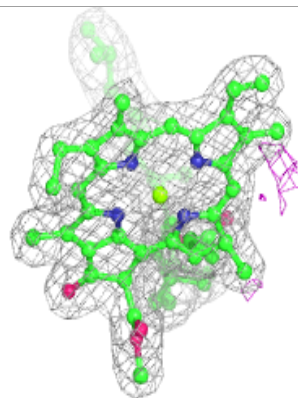
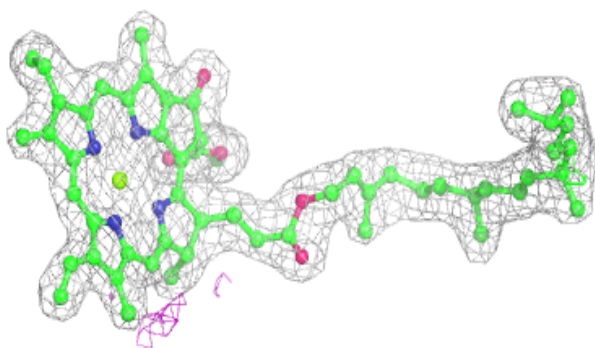
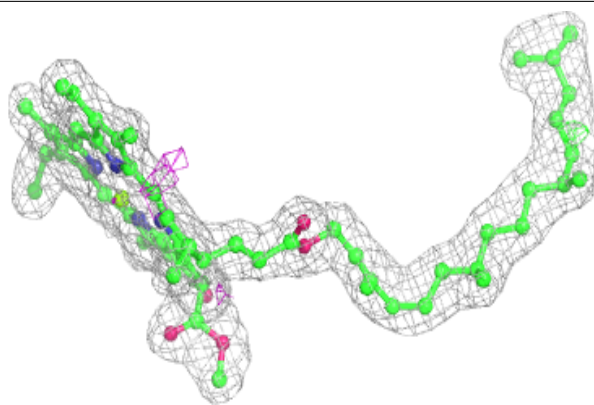
Electron density around CLA b 617:

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

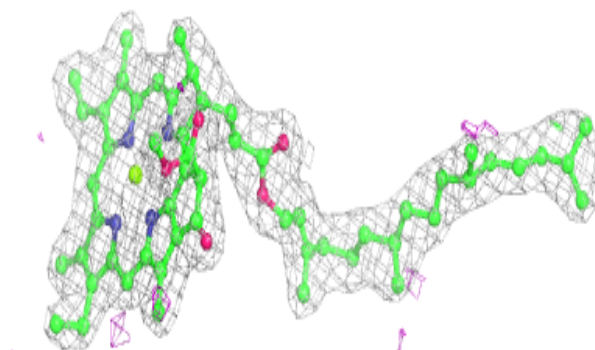
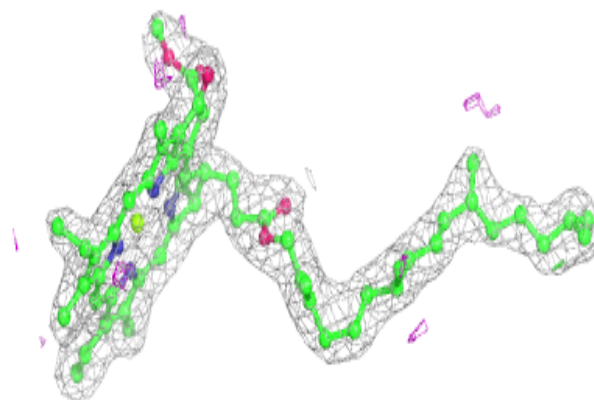


Electron density around CLA D 403:

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

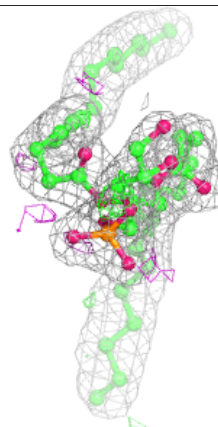
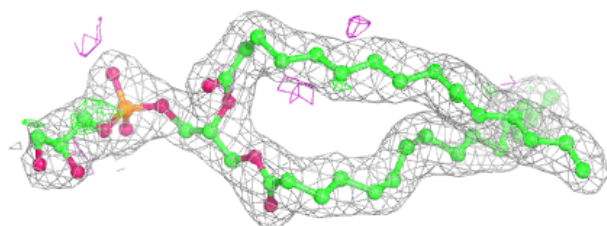
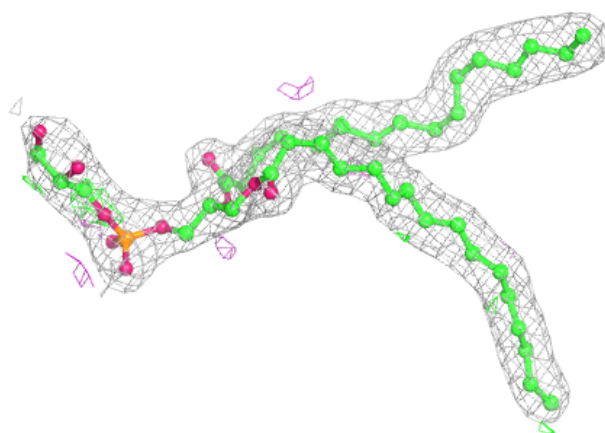
**Electron density around CLA c 503:**

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

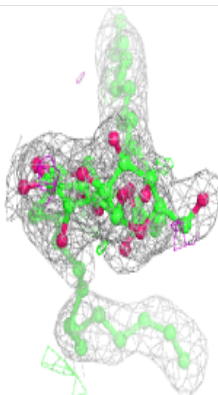
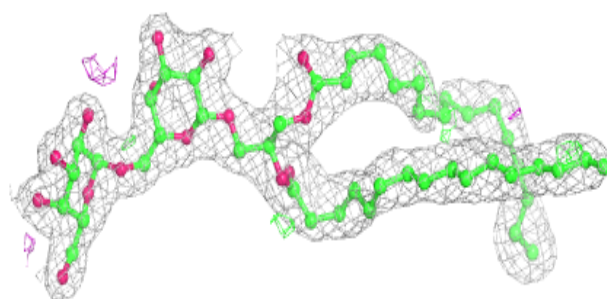
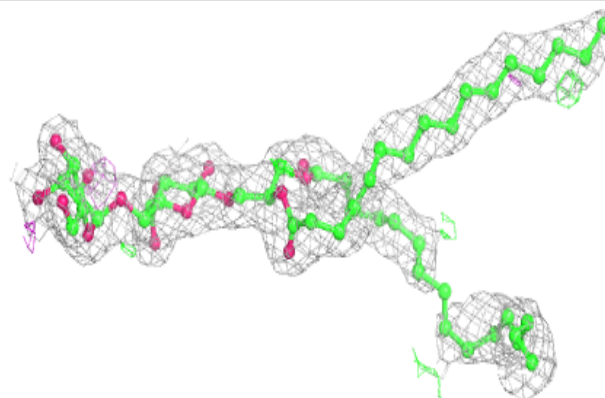


Electron density around LHG d 410:

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

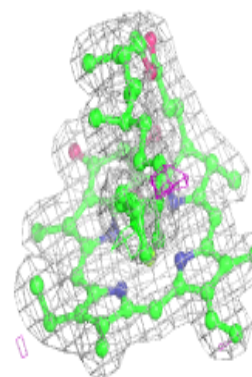
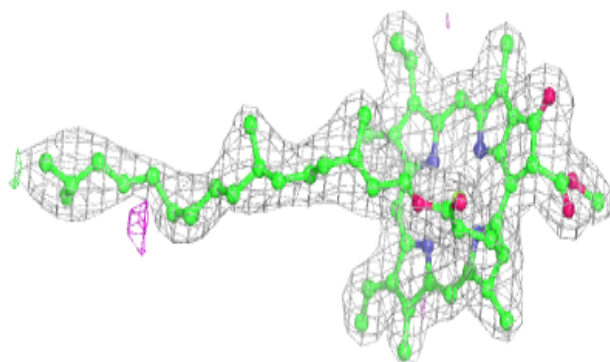
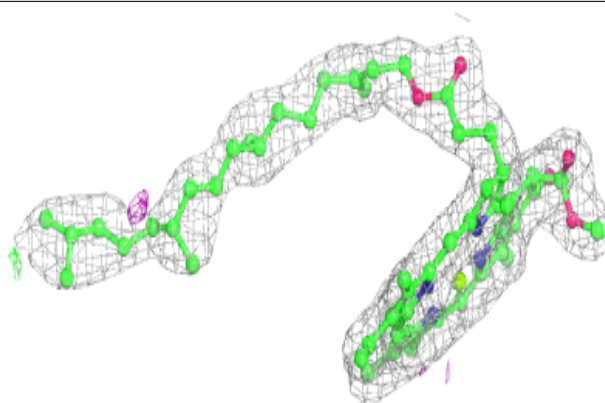
**Electron density around DGD c 517:**

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

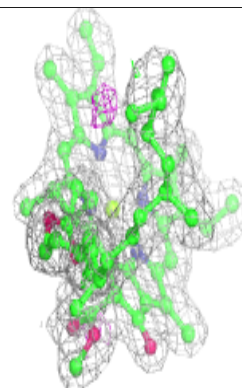
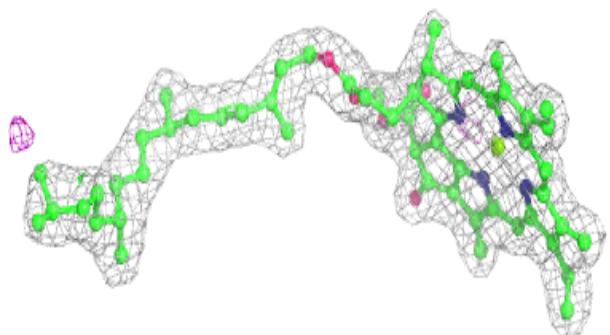
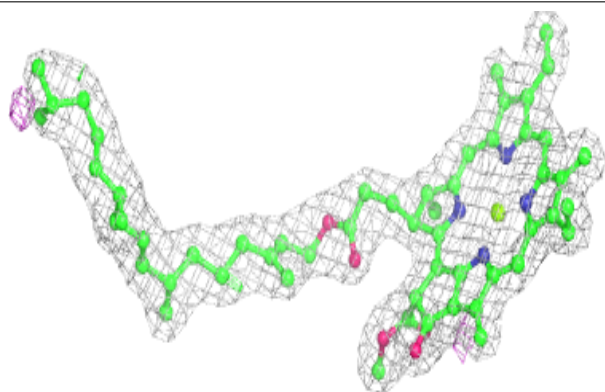


Electron density around CLA C 504:

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

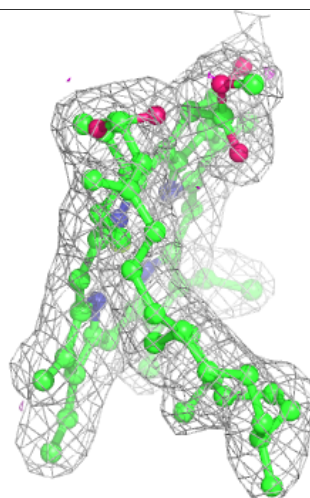
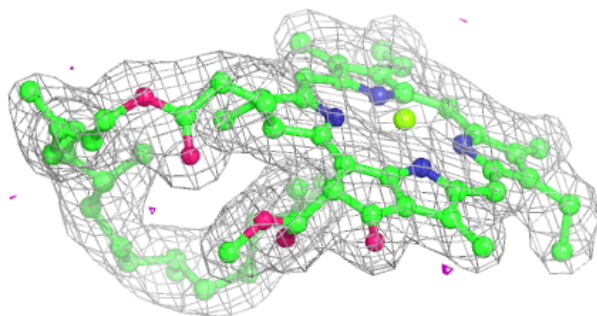
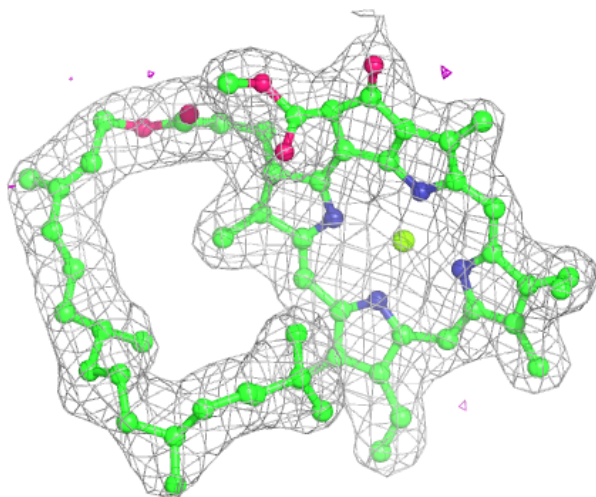
**Electron density around CLA a 406:**

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



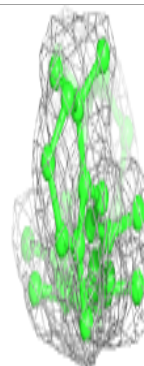
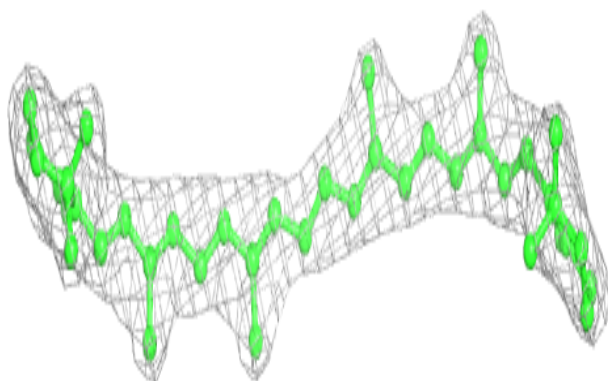
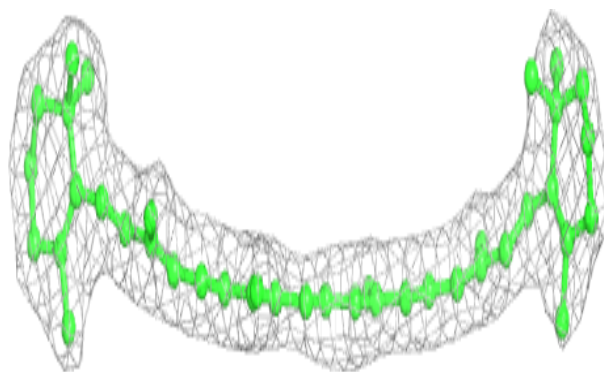
Electron density around CLA B 616:

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



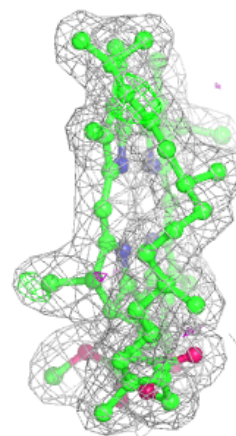
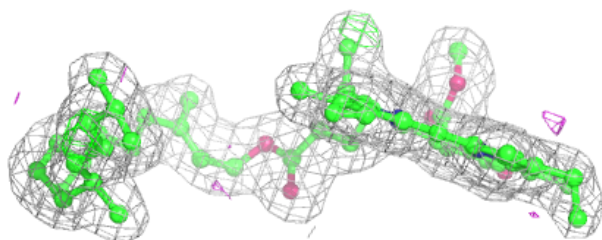
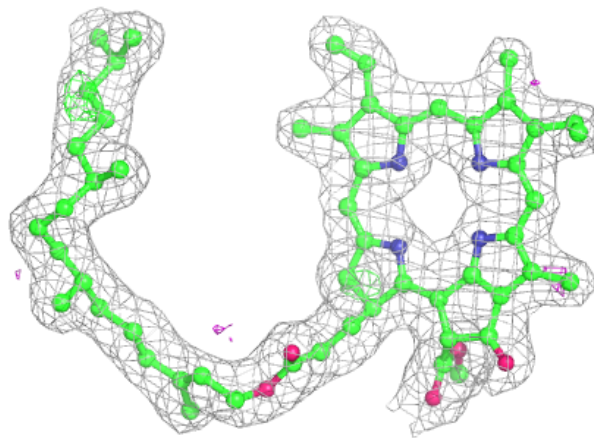
Electron density around BCR k 101:

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



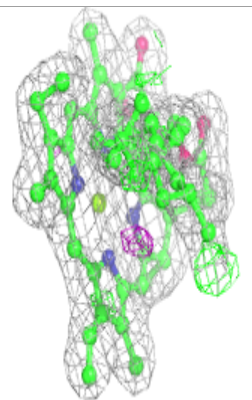
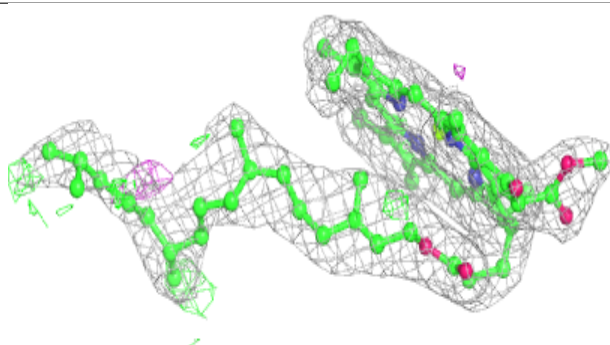
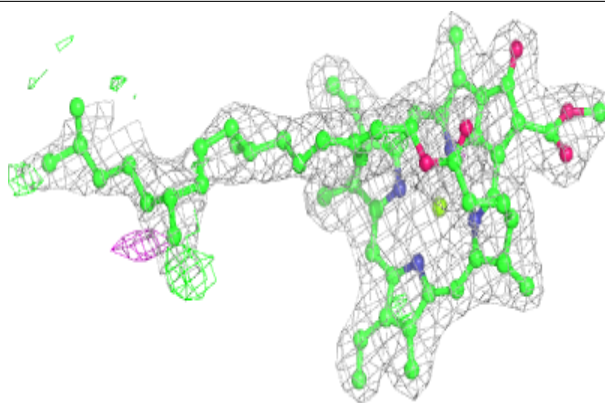
Electron density around PHO A 407:

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

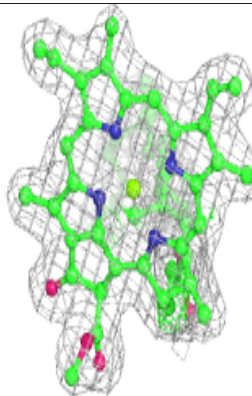
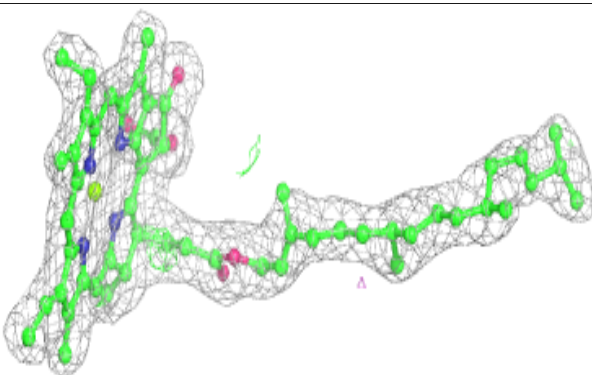
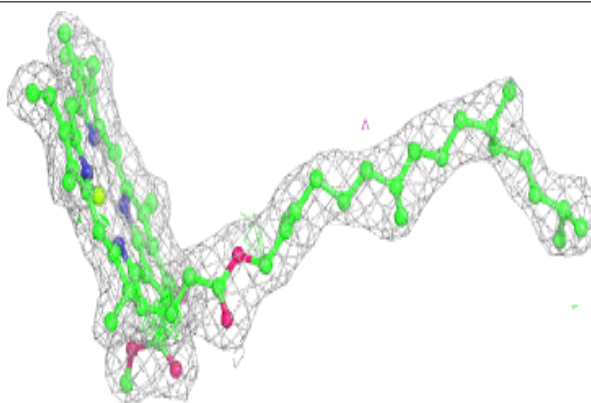


Electron density around CLA b 618:

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

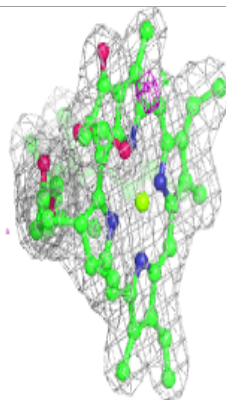
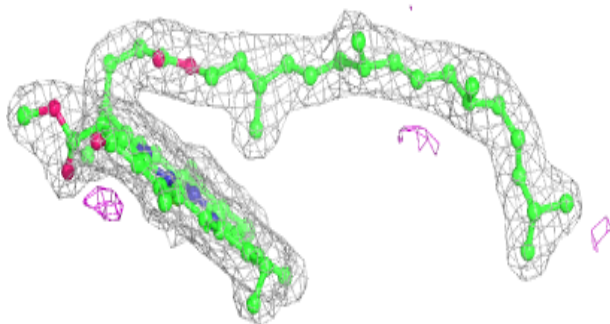
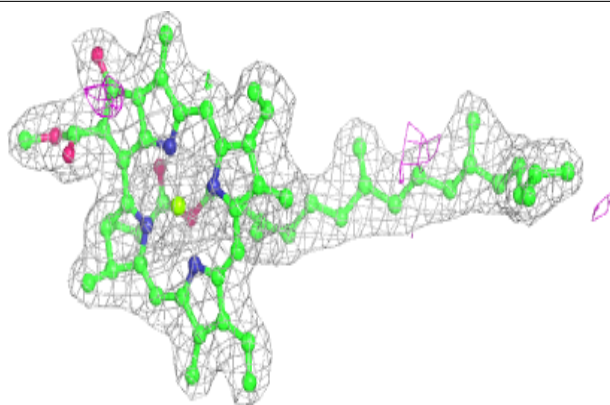
**Electron density around CLA B 605:**

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



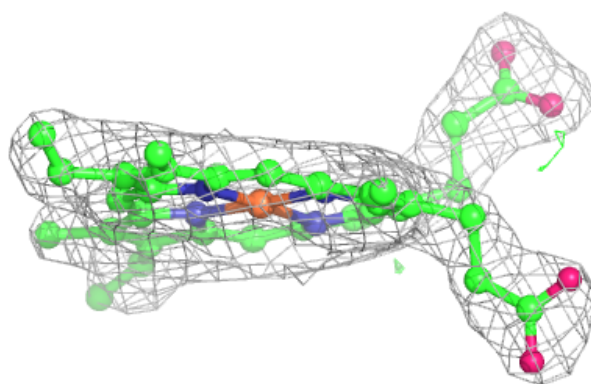
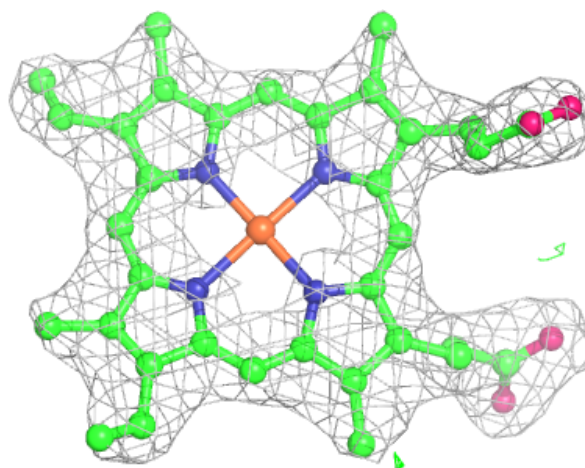
Electron density around CLA b 612:

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



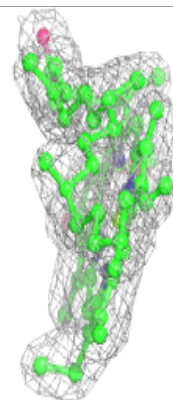
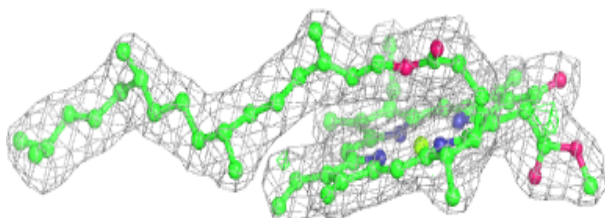
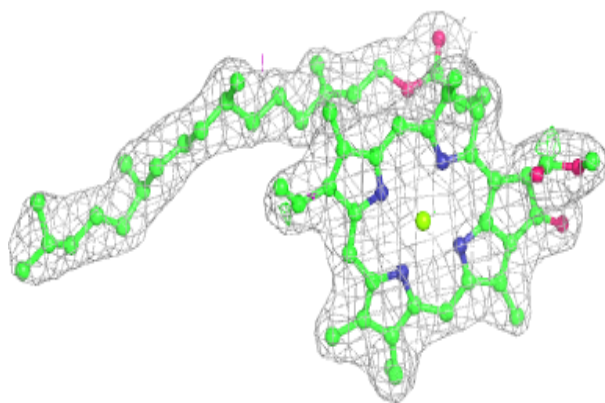
Electron density around HEM F 101:

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

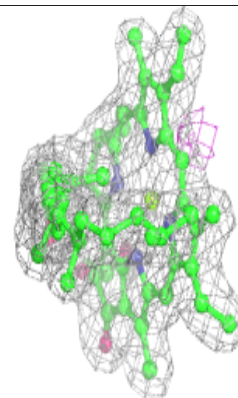
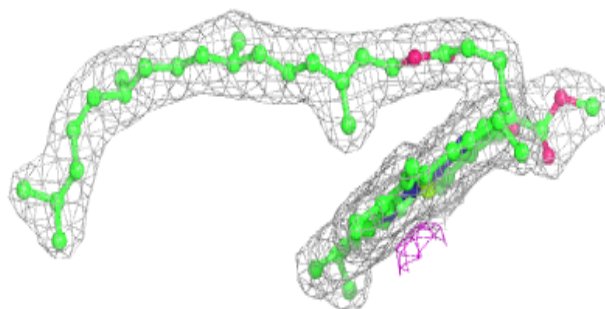
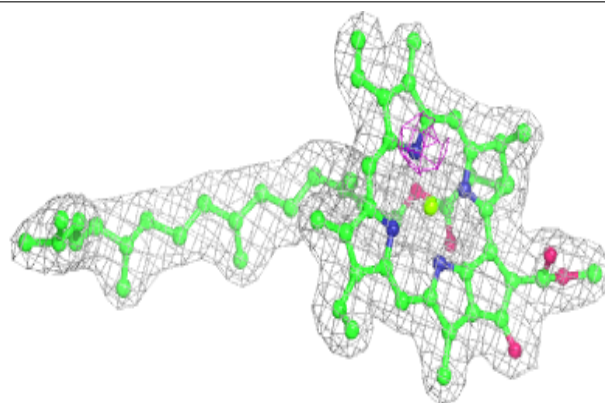


Electron density around CLA C 501:

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

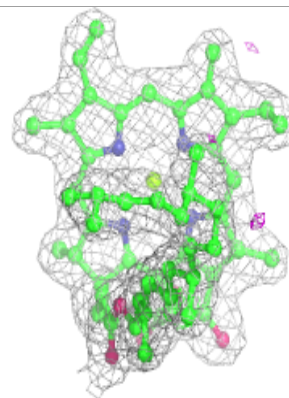
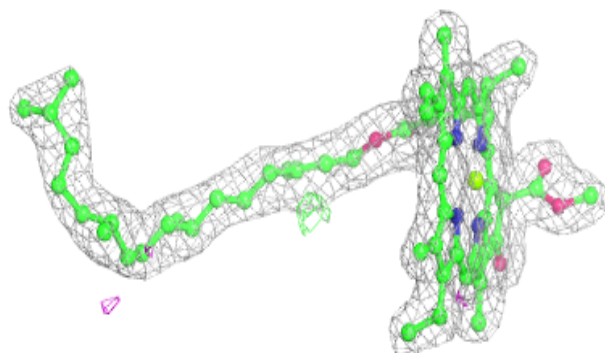
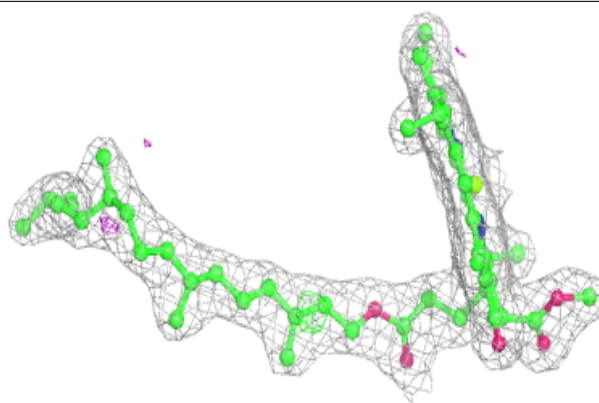
**Electron density around CLA B 609:**

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



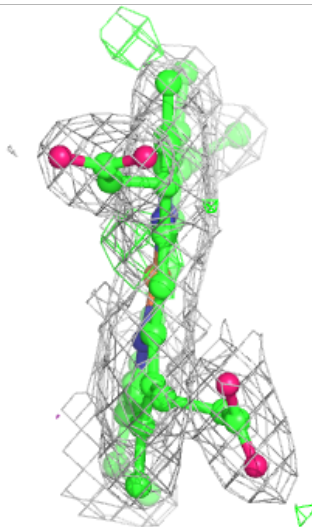
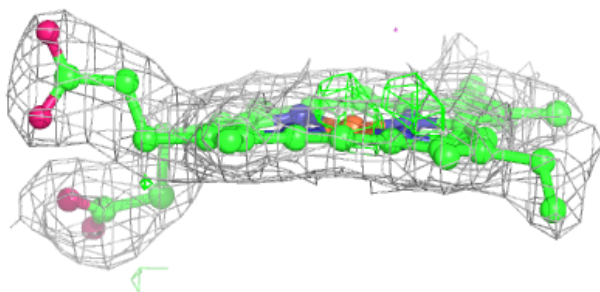
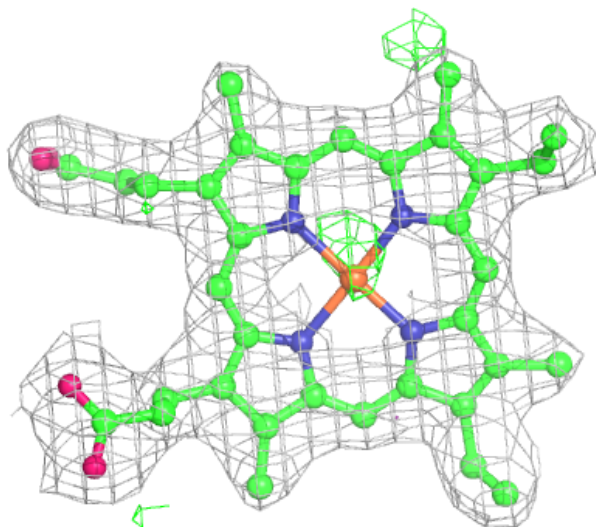
Electron density around CLA b 609:

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



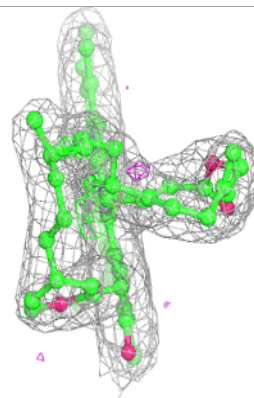
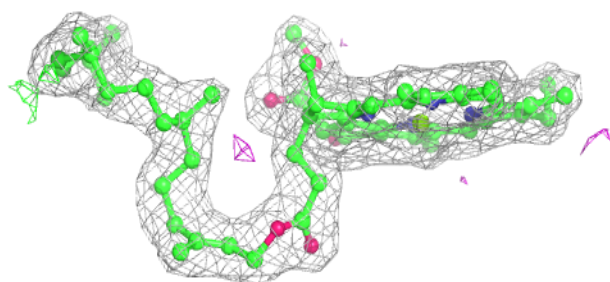
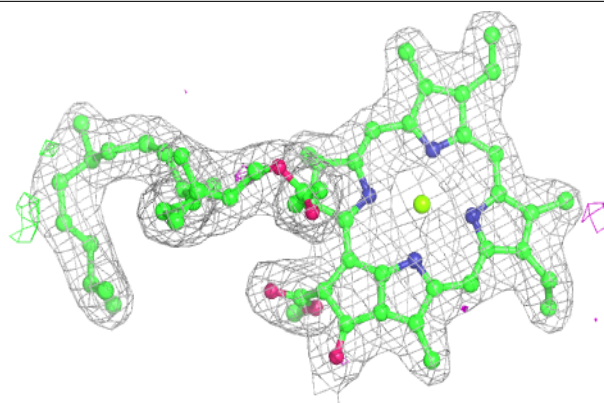
Electron density around HEC v 202:

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

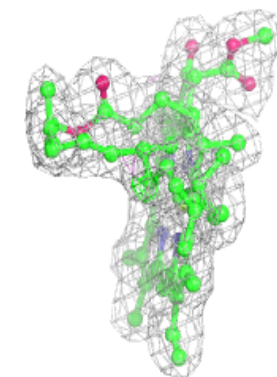
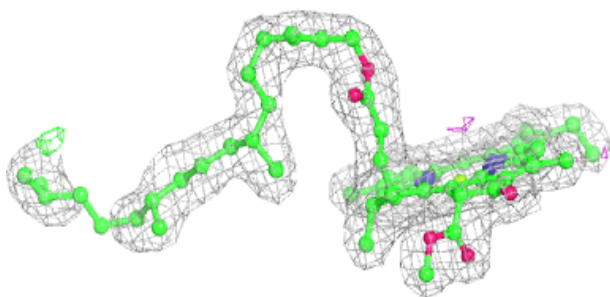
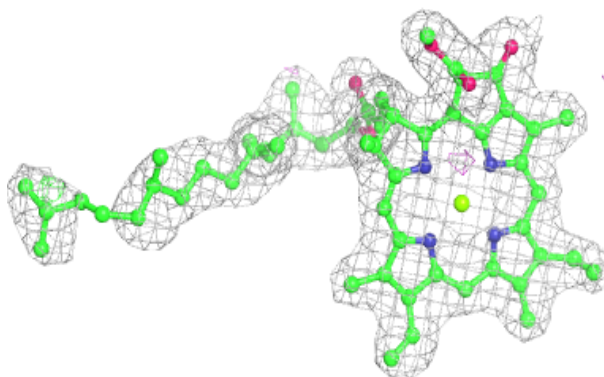


Electron density around CLA B 613:

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

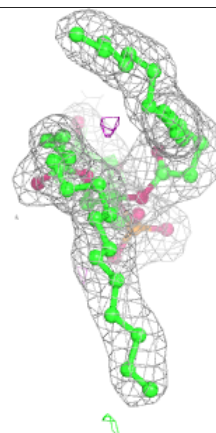
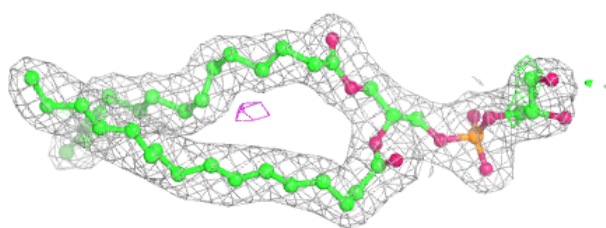
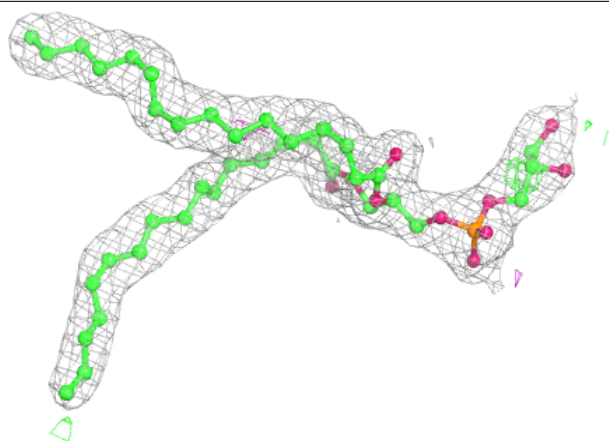
**Electron density around CLA A 406:**

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

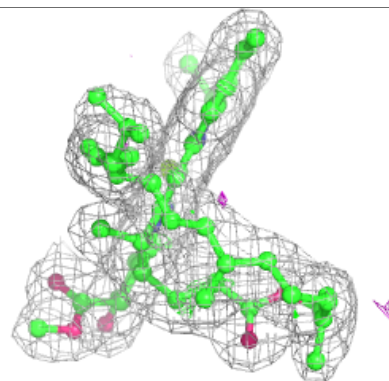
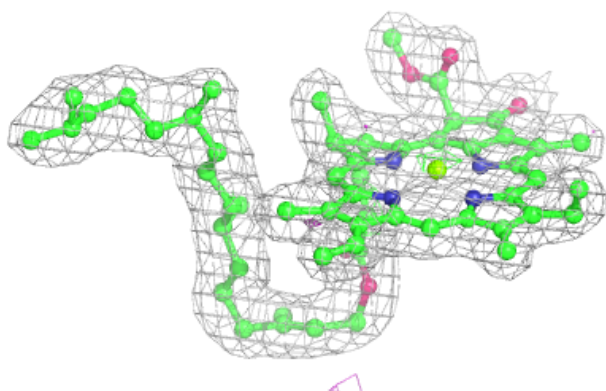
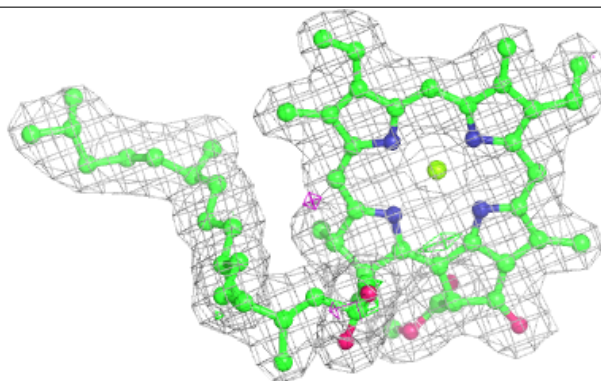


Electron density around LHG D 410:

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

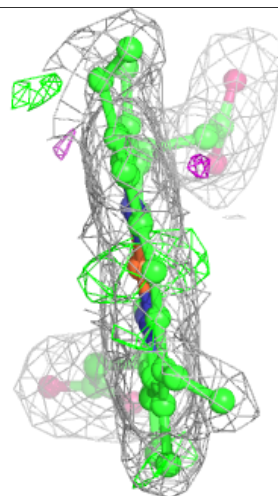
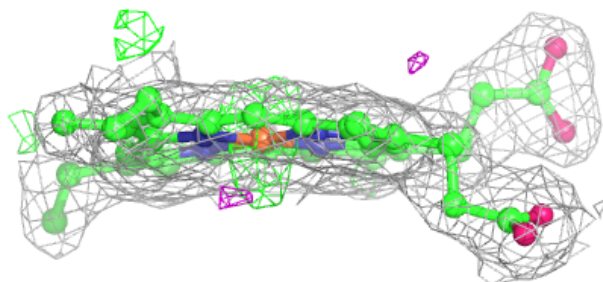
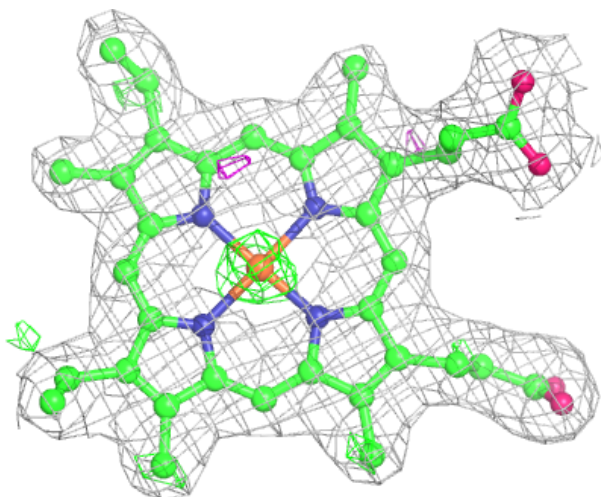
**Electron density around CLA d 403:**

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



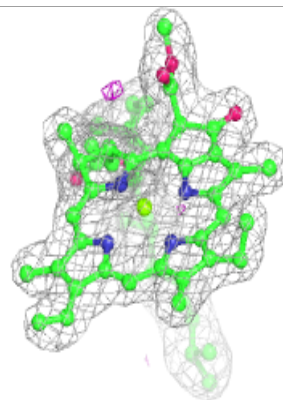
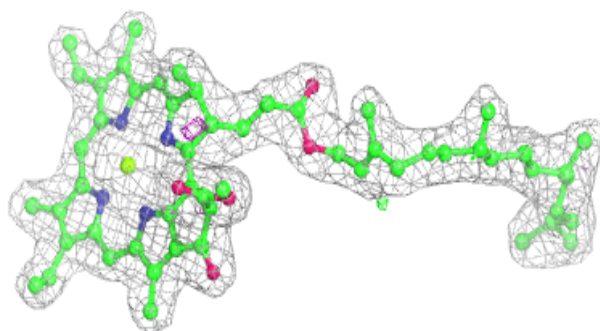
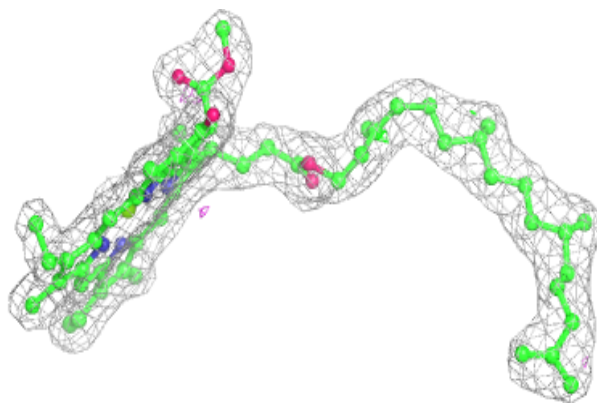
Electron density around HEC V 201:

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

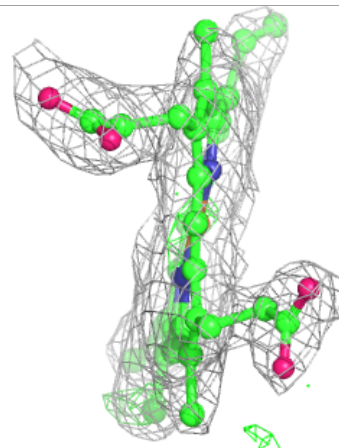
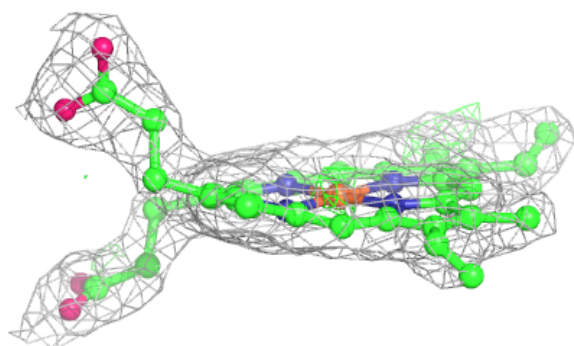
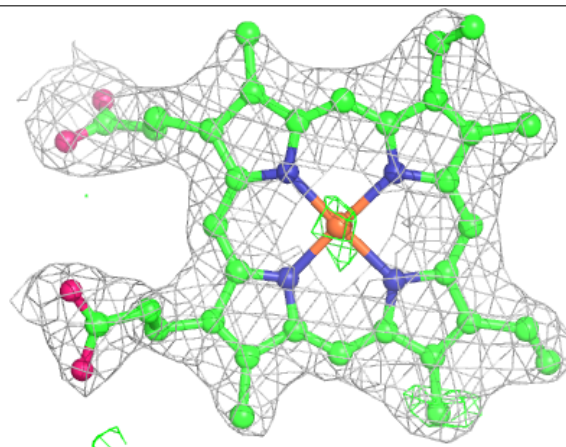


Electron density around CLA d 402:

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

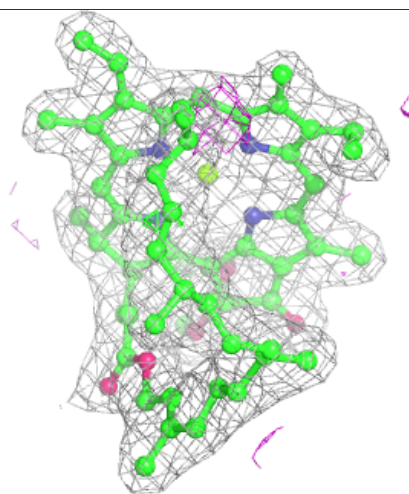
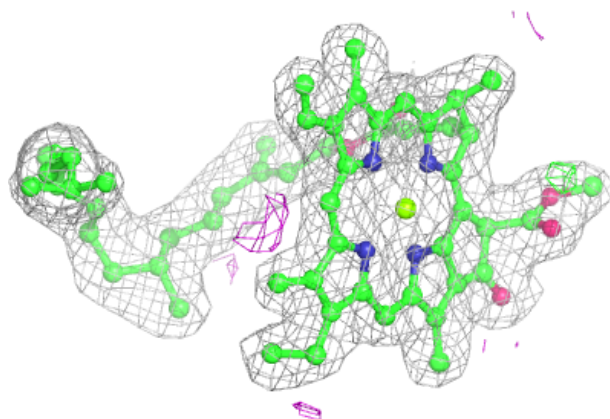
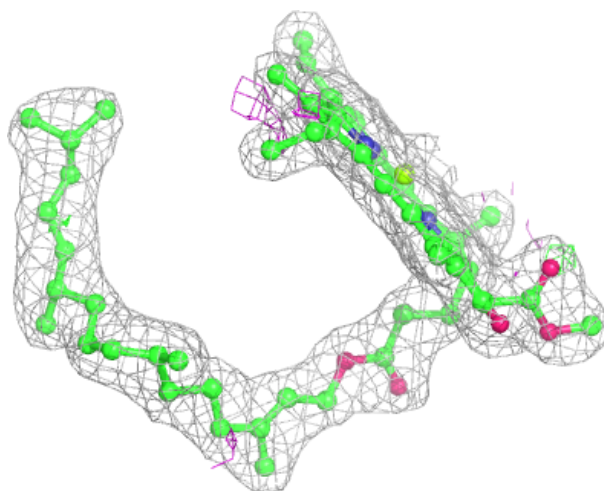
**Electron density around HEM f 101:**

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



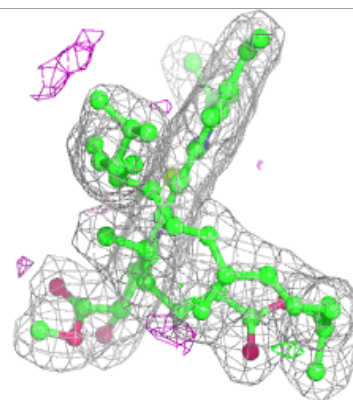
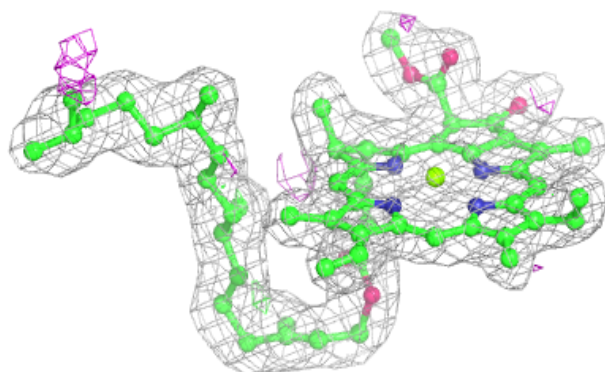
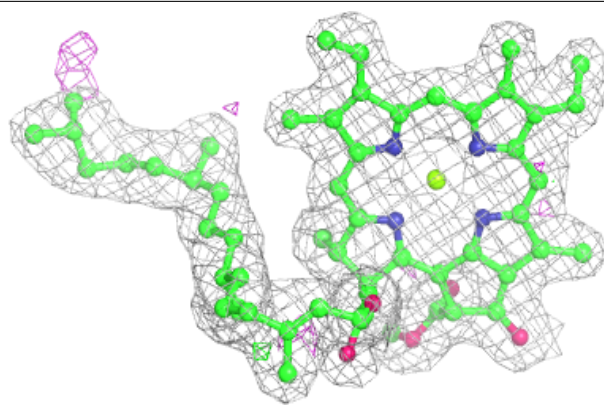
Electron density around CLA b 615:

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

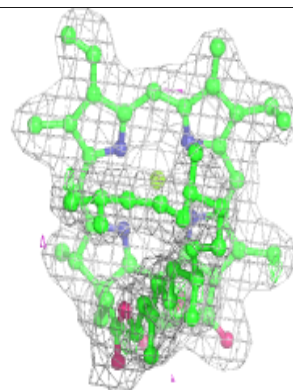
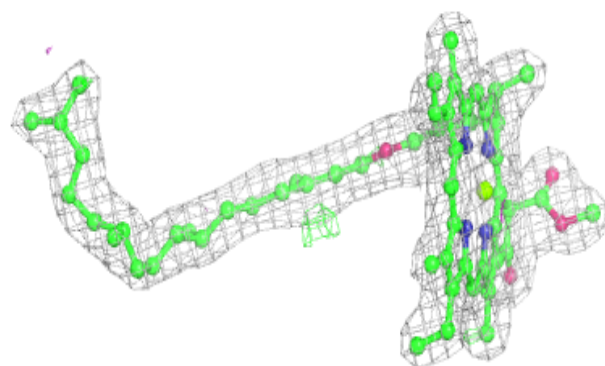
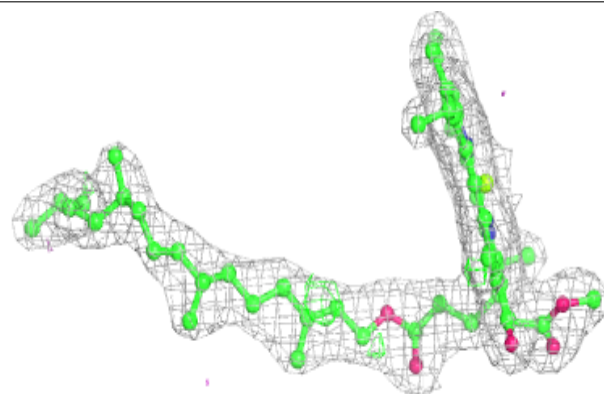


Electron density around CLA A 405:

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

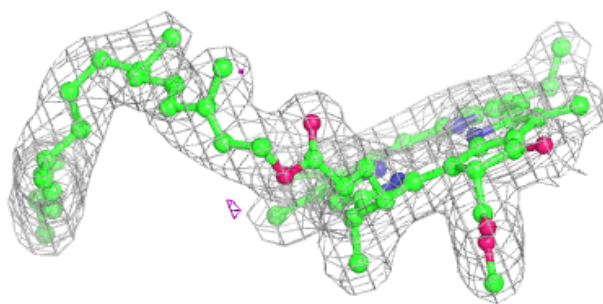
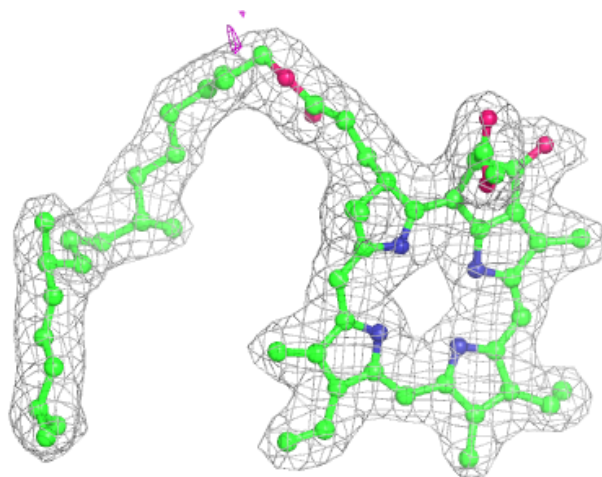
**Electron density around CLA B 606:**

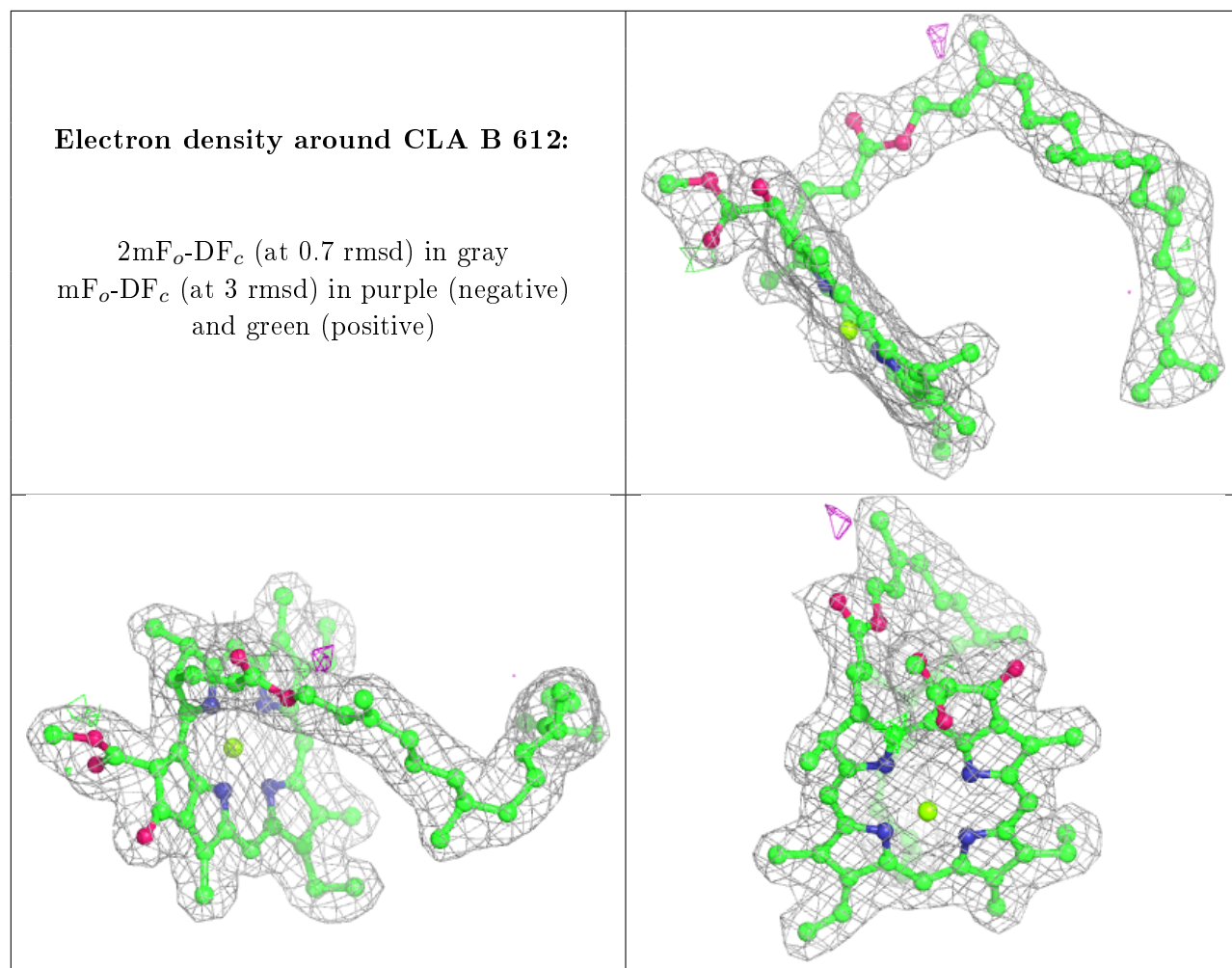
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO d 404:

$2mF_o-DF_c$ (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.