



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:15 PM EDT

PDB ID : 3WU2 / pdb_00003wu2
Title : Crystal structure analysis of Photosystem II complex
Authors : Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.
Deposited on : 2014-04-21
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

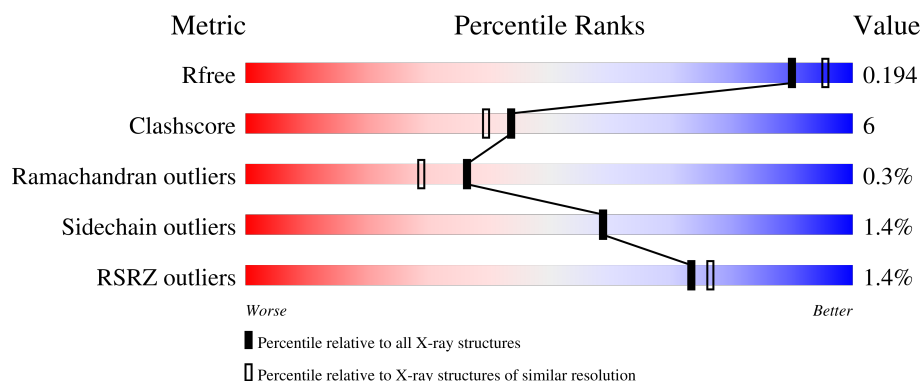
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



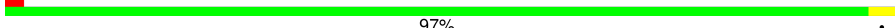
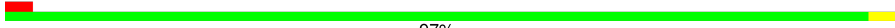
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	344	87% 9% . .
1	a	344	84% 13% .
2	B	504	2% 89% 11%
2	b	504	3% 90% 9% .
3	C	455	90% 9% .

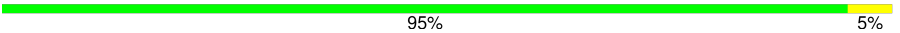
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	455	 91% 9%
4	D	342	 85% 14%
4	d	342	 88% 12%
5	E	83	 81% 17% 2%
5	e	83	 80% 14% 5%
6	F	44	 64% 14% 23%
6	f	44	 57% 14% 27%
7	H	63	 97% 2%
7	h	63	 86% 14% 2%
8	I	38	 84% 11% 5%
8	i	38	 84% 11% 5%
9	J	40	 80% 10% 10%
9	j	40	 85% 12% 5%
10	K	37	 84% 16%
10	k	37	 89% 11%
11	L	37	 86% 14%
11	l	37	 97% 3%
12	M	36	 72% 17% 8%
12	m	36	 81% 11% 6%
13	O	244	 85% 14% 2%
13	o	244	 87% 11% 2%
14	T	32	 84% 9% 6%
14	t	32	 81% 12% 6%
15	U	104	 87% 5% 7%
15	u	104	 88% 5% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
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
29	UNL	D	412	-	-	X	-
29	UNL	b	628	-	-	X	-
31	GOL	C	524	-	-	X	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 54036 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2633	1729	429	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2625	1722	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4009	2633	668	695	13			
2	b	501	Total	C	N	O	S	0	11	0
			3964	2605	658	688	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3502	2291	588	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			657	429	106	122				
5	e	79	Total	C	N	O		0	0	0
			639	419	103	117				

- 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	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	48	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
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	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
			261	176	37	47	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	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
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			770	489	129	152				
15	u	97	Total	C	N	O		0	1	0
			772	490	129	153				

- 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
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

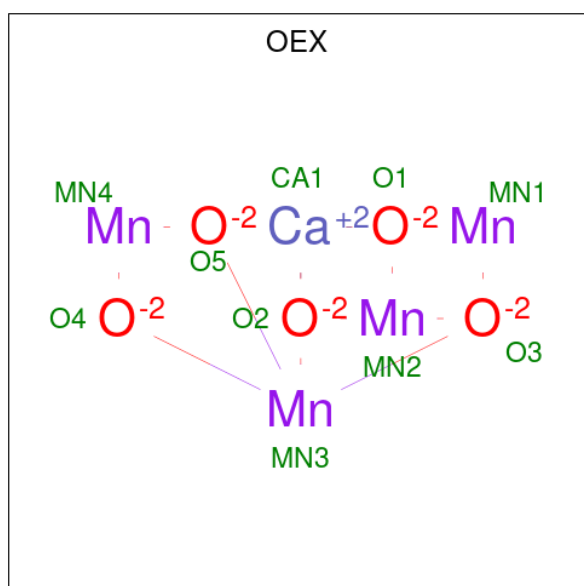
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O		0	1	0
			280	190	44	46				

- 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
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

Continued on next page...

Continued from previous page...

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

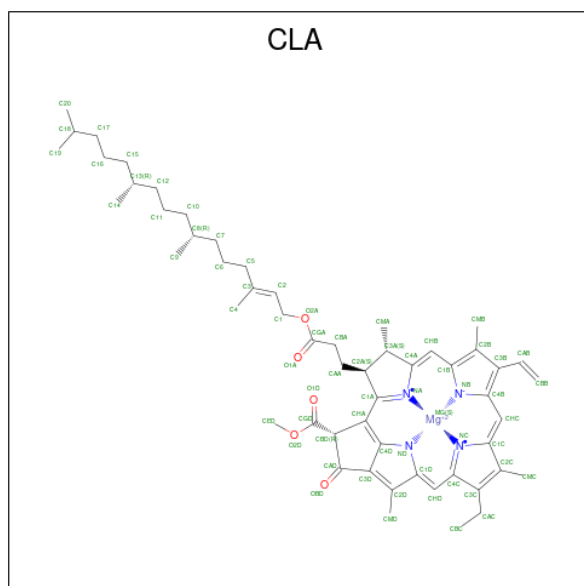
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

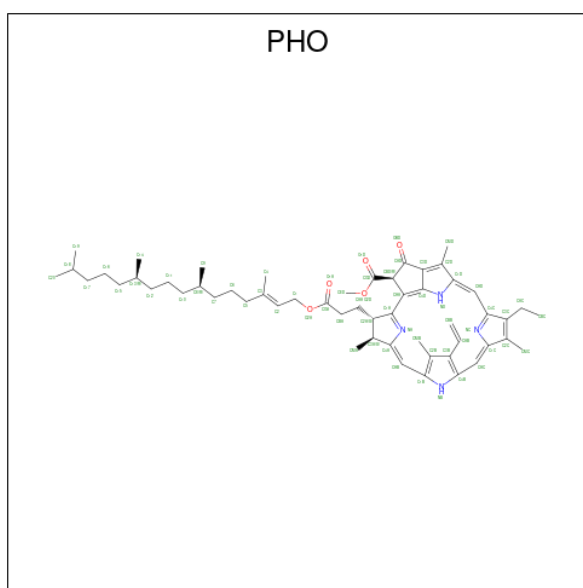
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

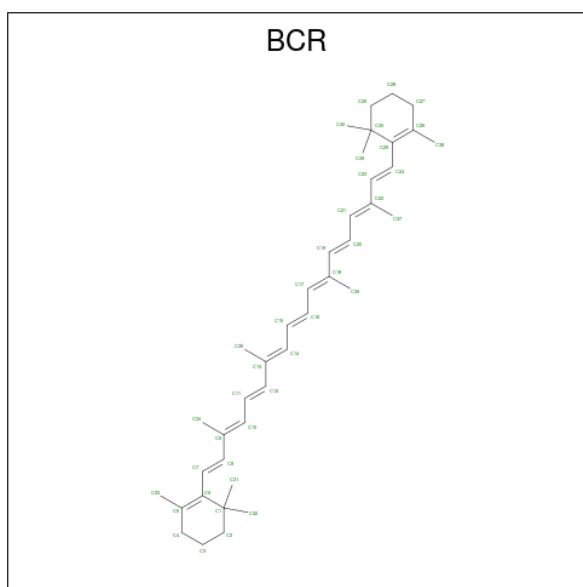
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



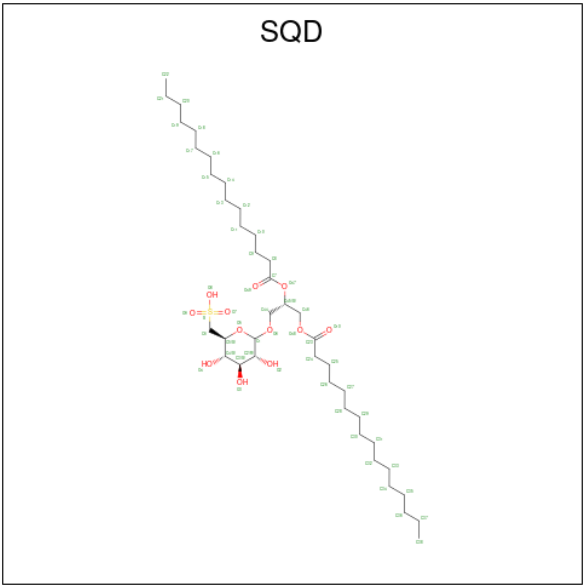
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



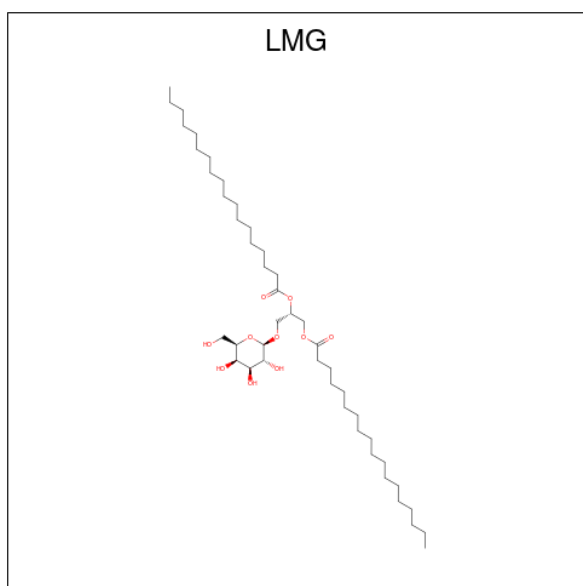
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			33	23	9	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



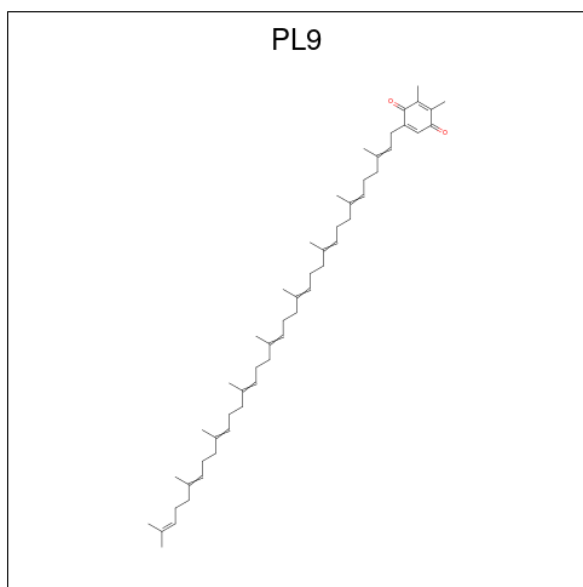
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O		0	0
			51	41	10			
27	B	1	Total	C	O		0	0
			51	41	10			
27	C	1	Total	C	O		0	0
			51	41	10			
27	D	1	Total	C	O		0	0
			51	41	10			
27	Z	1	Total	C	O		0	0
			51	41	10			
27	a	1	Total	C	O		0	0
			51	41	10			
27	b	1	Total	C	O		0	0
			51	41	10	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			51	41	10		
27	d	1	Total	C	O	0	0
			51	41	10		

- Molecule 28 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

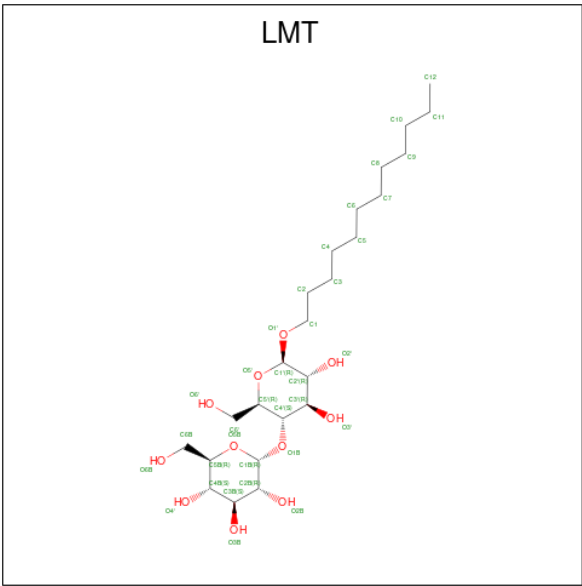
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	4	Total	C	O	0	0
			69	64	5		
29	B	4	Total	C		0	0
			56	56			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	1	Total C O 34 29 5	0	0
29	D	2	Total C O 56 51 5	0	0
29	E	2	Total C 27 27	0	0
29	H	1	Total C 10 10	0	0
29	I	2	Total C 24 24	0	0
29	J	2	Total C 26 26	0	0
29	L	1	Total C 14 14	0	0
29	M	1	Total C 16 16	0	0
29	T	1	Total C 13 13	0	0
29	X	1	Total C 16 16	0	0
29	Z	1	Total C 16 16	0	0
29	a	3	Total C O 56 51 5	0	0
29	b	4	Total C O 84 79 5	0	0
29	c	2	Total C O 40 35 5	0	0
29	d	1	Total C 16 16	0	0
29	e	1	Total C 11 11	0	0
29	i	4	Total C 55 55	0	0
29	j	2	Total C 28 28	0	0
29	t	1	Total C 16 16	0	0
29	x	1	Total C 16 16	0	0
29	z	1	Total C 16 16	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



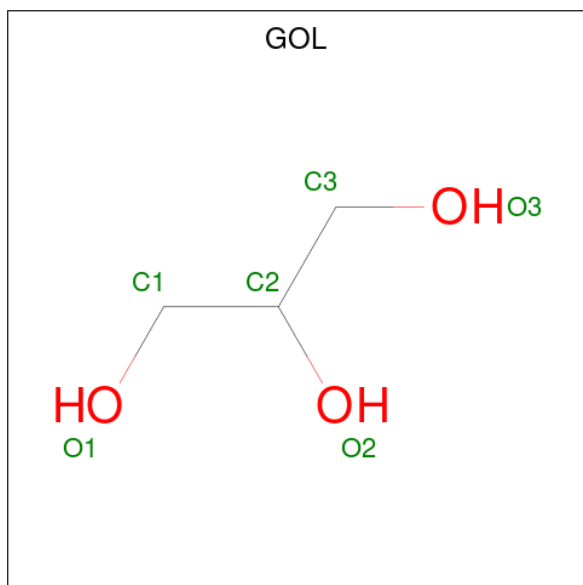
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	C	1	Total	C	O	0	0
			35	24	11		
30	F	1	Total	C	O	0	0
			35	24	11		
30	J	1	Total	C	O	0	0
			24	18	6		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	Z	1	Total	C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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	O	0	0
			35	24	11		
30	t	1	Total	C	O	0	0
			24	18	6		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	D	1	Total	C	O	0	0
			6	3	3		
31	L	1	Total	C	O	0	0
			6	3	3		
31	O	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

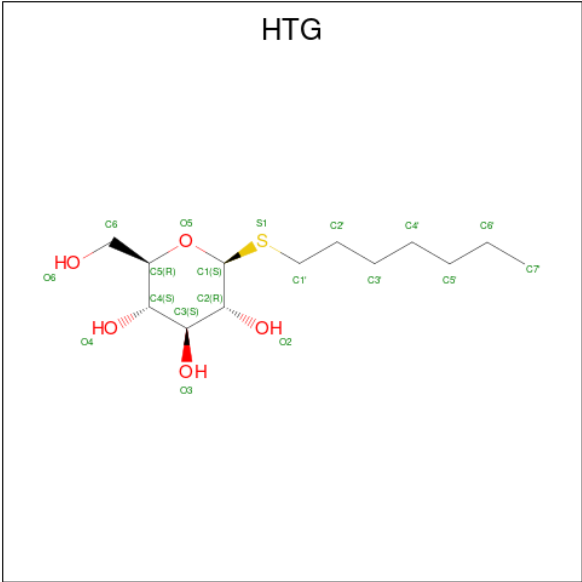
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 6 3 3	0	0
31	f	1	Total C O 6 3 3	0	0
31	h	1	Total C O 6 3 3	0	0
31	l	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



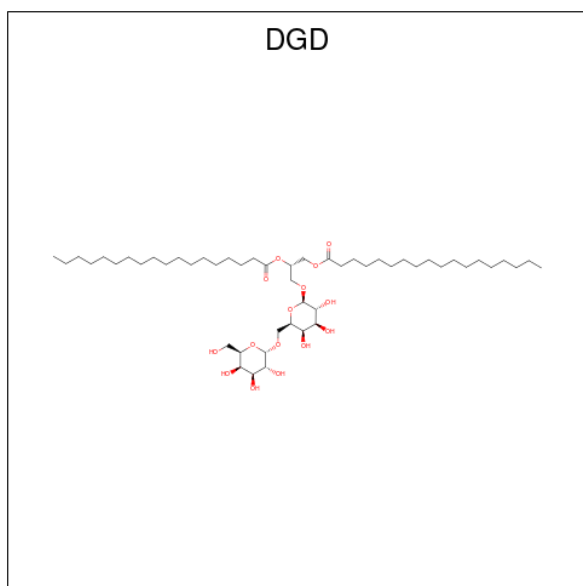
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			19	13	5	1		
33	O	1	Total	C	O	S	0	0
			19	13	5	1		
33	U	1	Total	C	S		0	0
			9	8	1			
33	V	1	Total	C	O	S	0	0
			13	7	5	1		
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	b	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	d	1	Total	C	O	S	0	0
			19	13	5	1		
33	u	1	Total	C	O	S	0	0
			14	10	3	1		

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



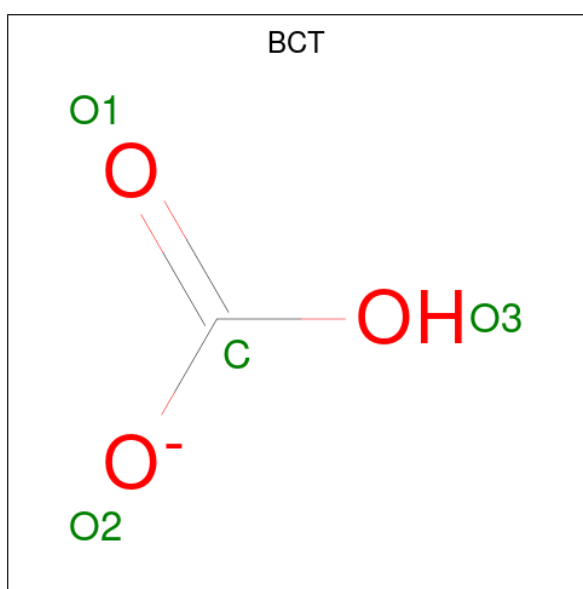
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C	1	Total	C	O	0	0
			62	47	15		
34	C	1	Total	C	O	0	0
			62	47	15		
34	C	1	Total	C	O	0	0
			62	47	15		
34	D	1	Total	C	O	0	0
			53	42	11		
34	H	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		

Continued on next page...

Continued from previous page...

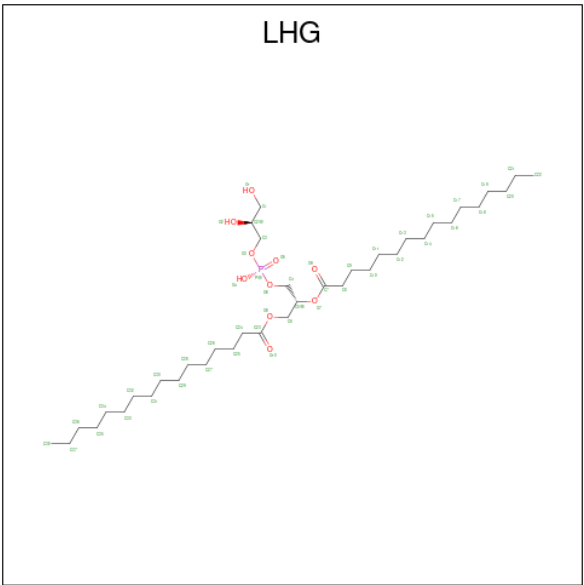
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	d	1	Total	C	O	0	0
			50	41	9		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



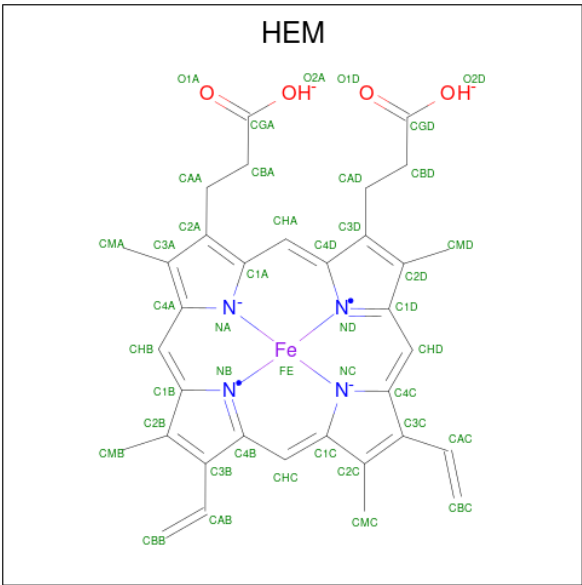
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	C	O	0	0
			4	1	3		
35	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



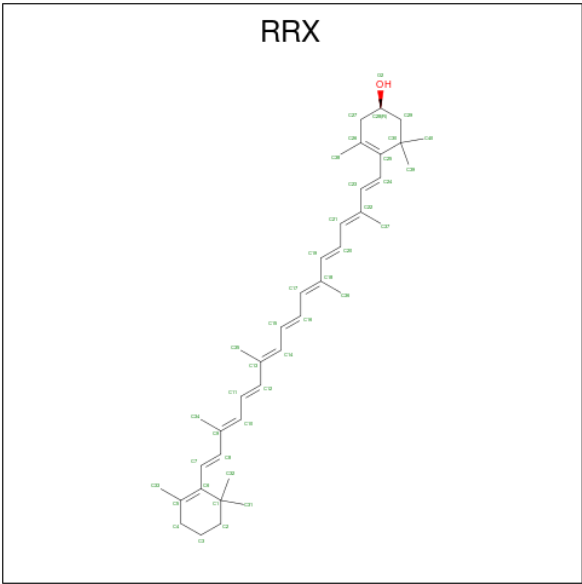
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			46	35	10	1		
36	E	1	Total	C	O	P	0	0
			49	38	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			40	29	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).

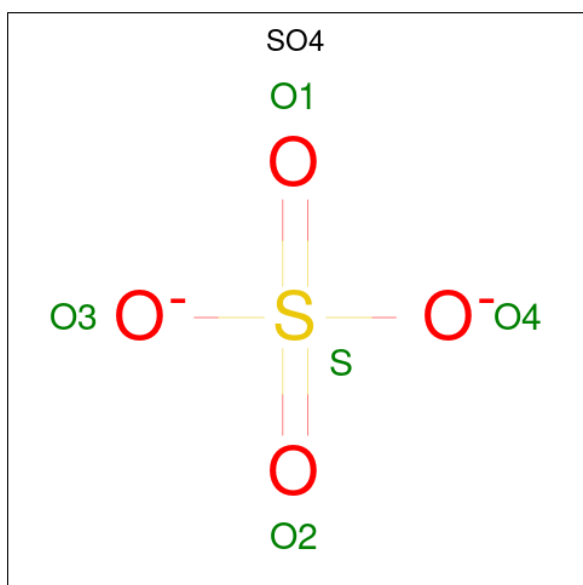


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	168	Total	O	0	2
			170	170		
41	B	311	Total	O	0	8
			319	319		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	253	Total 263	O 263	0	10
41	D	156	Total 161	O 161	0	5
41	E	32	Total 35	O 35	0	3
41	F	12	Total 12	O 12	0	0
41	H	50	Total 52	O 52	0	2
41	I	8	Total 8	O 8	0	0
41	J	9	Total 9	O 9	0	0
41	K	8	Total 8	O 8	0	0
41	L	23	Total 24	O 24	0	1
41	M	15	Total 16	O 16	0	1
41	O	193	Total 202	O 202	0	9
41	T	10	Total 10	O 10	0	0
41	U	98	Total 100	O 100	0	2
41	V	140	Total 144	O 144	0	4
41	Y	6	Total 6	O 6	0	0
41	X	13	Total 14	O 14	0	1
41	Z	1	Total 1	O 1	0	0
41	a	153	Total 155	O 155	0	2
41	b	295	Total 306	O 306	0	11
41	c	238	Total 245	O 245	0	7
41	d	156	Total 160	O 160	0	4

Continued on next page...

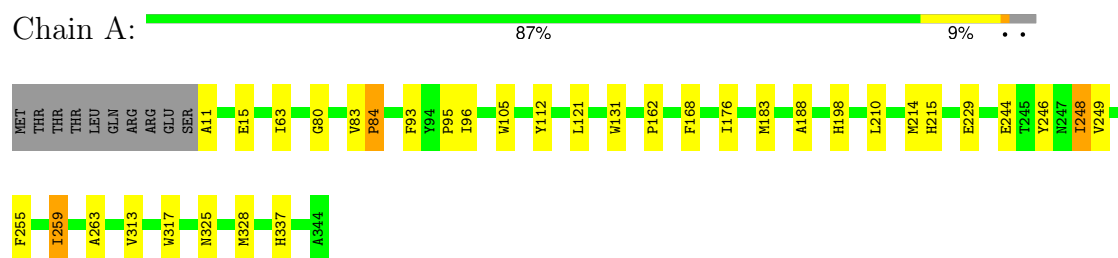
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	e	22	Total 22	O 22	0	0
41	f	13	Total 14	O 14	0	1
41	h	48	Total 53	O 53	0	5
41	i	13	Total 14	O 14	0	1
41	j	9	Total 9	O 9	0	0
41	k	5	Total 5	O 5	0	0
41	l	17	Total 18	O 18	0	1
41	m	15	Total 16	O 16	0	1
41	o	167	Total 175	O 175	0	8
41	t	12	Total 12	O 12	0	0
41	u	102	Total 106	O 106	0	4
41	v	98	Total 104	O 104	0	6
41	y	7	Total 7	O 7	0	0
41	x	6	Total 6	O 6	0	0
41	z	2	Total 2	O 2	0	0

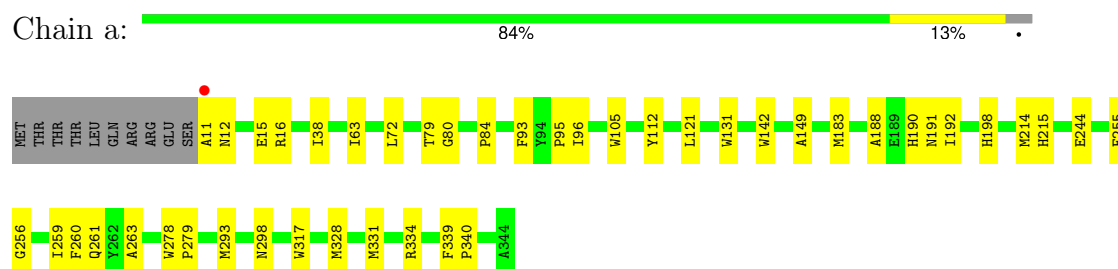
3 Residue-property plots [i](#)

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.

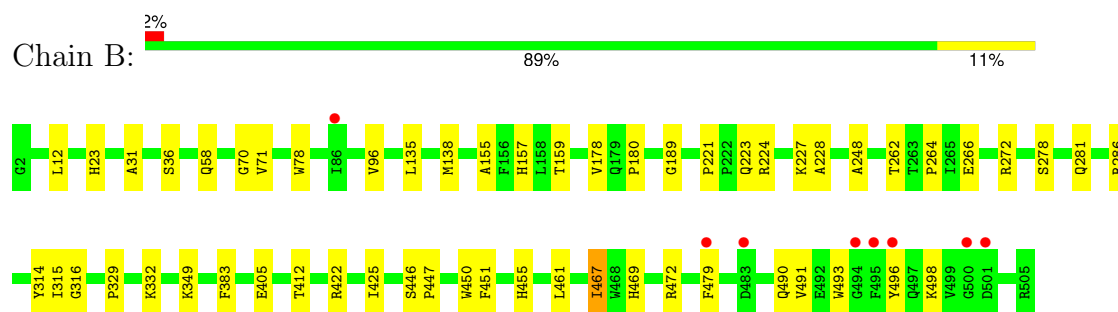
- Molecule 1: Photosystem Q(B) protein



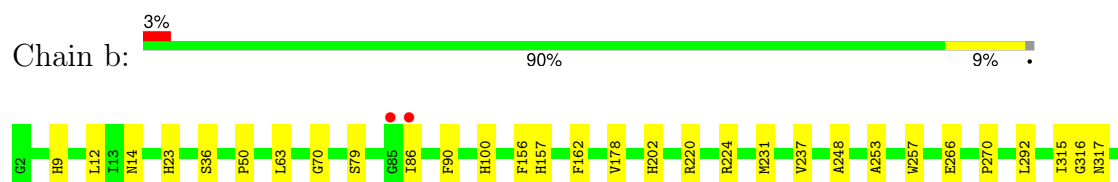
- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

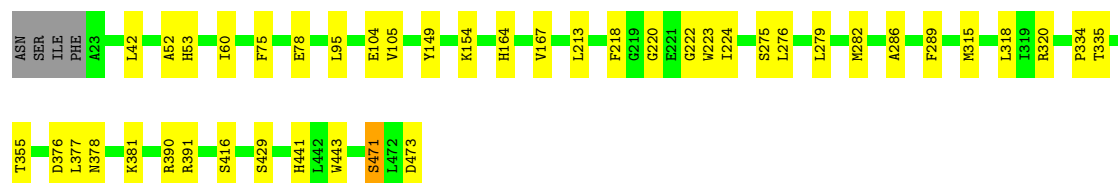
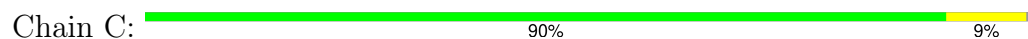


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

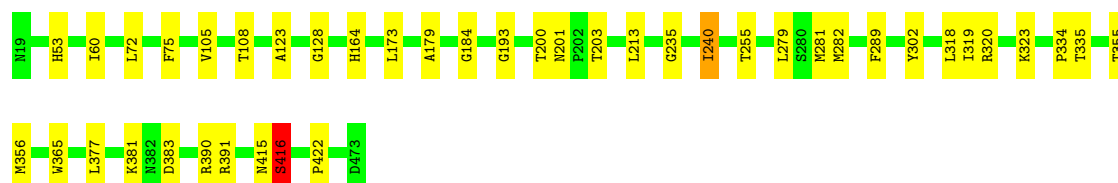




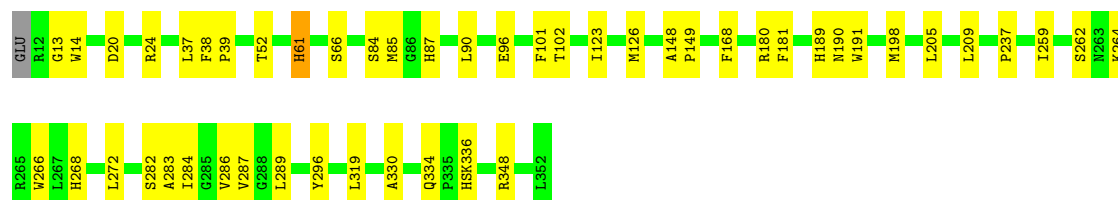
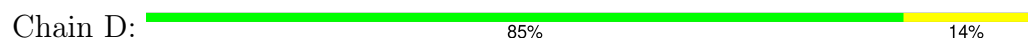
- Molecule 3: Photosystem II 44 kDa reaction center protein



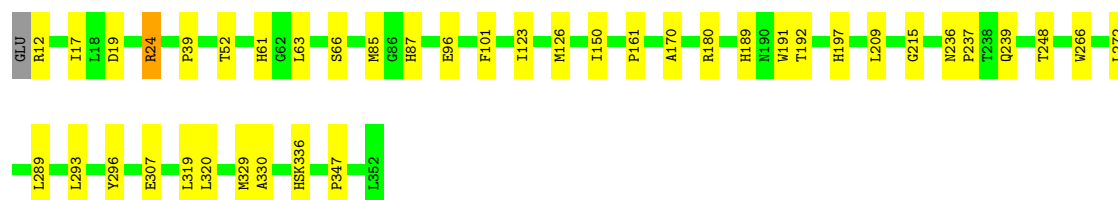
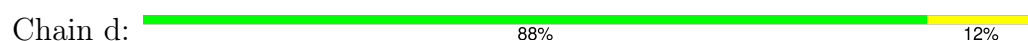
- Molecule 3: Photosystem II 44 kDa reaction center protein



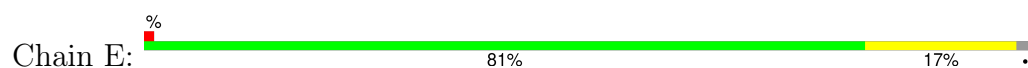
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha





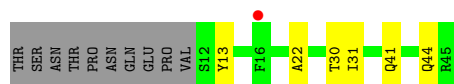
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 80% 14% 5%



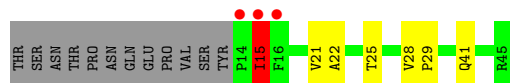
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 2% 64% 14% 23%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 7% 57% 14% 27%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 97% 1%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 86% 14%

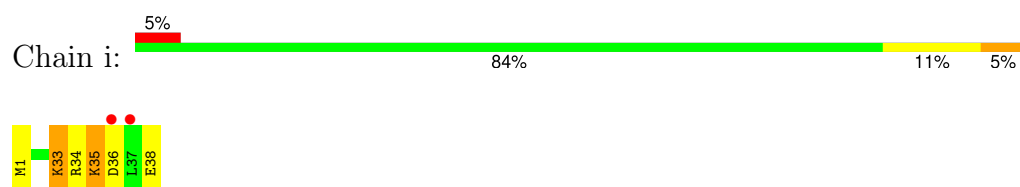


- Molecule 8: Photosystem II reaction center protein I

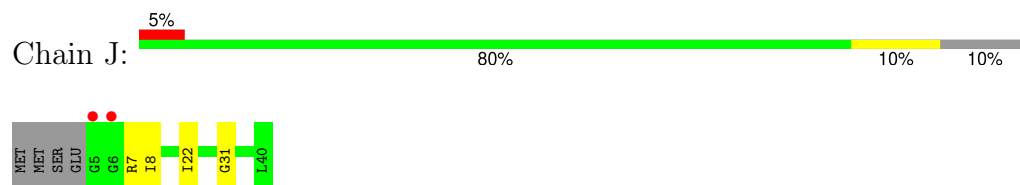
Chain I: 84% 11% 5%



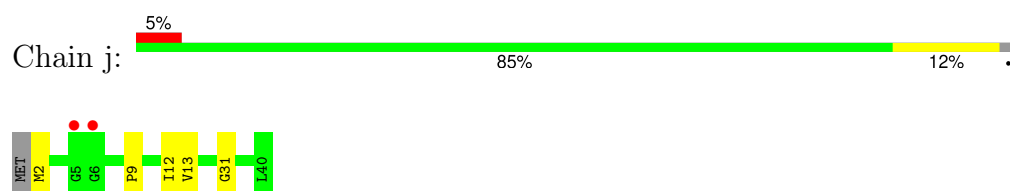
- Molecule 8: Photosystem II reaction center protein I



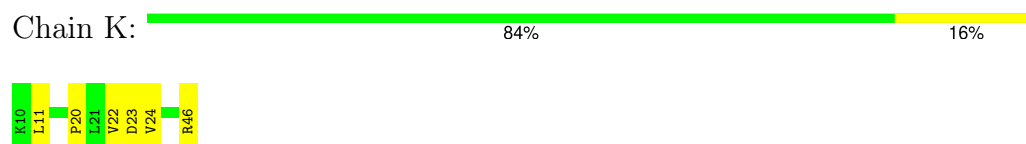
- Molecule 9: Photosystem II reaction center protein J



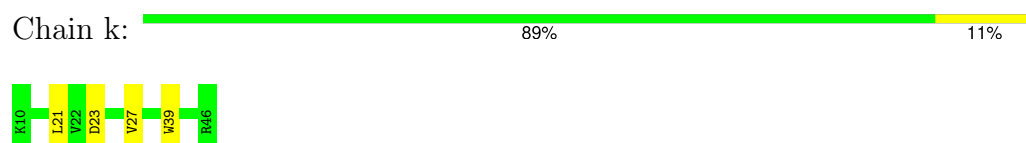
- Molecule 9: Photosystem II reaction center protein J



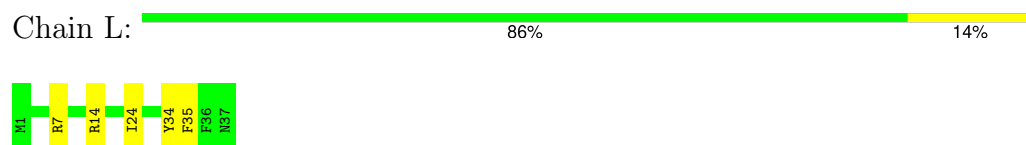
- Molecule 10: Photosystem II reaction center protein K



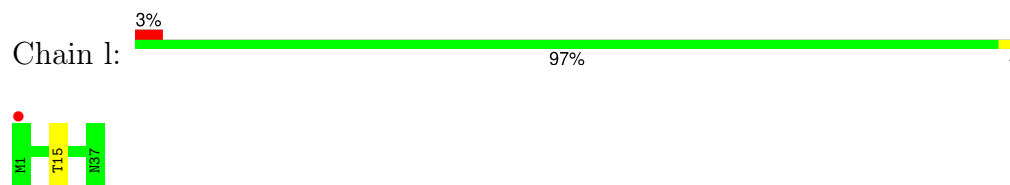
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  72% 17% 8%



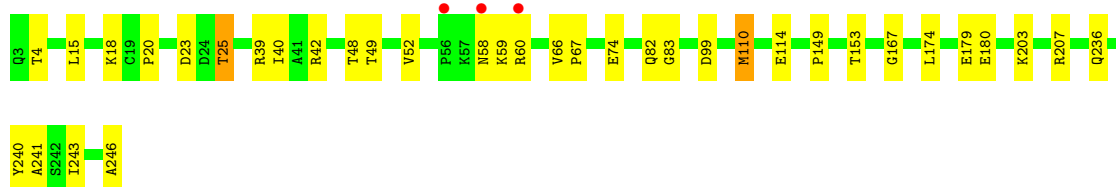
- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 81% 11% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  0% 85% 14%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  2% 87% 11%



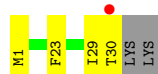
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 84% 9% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 81% 12% 6%

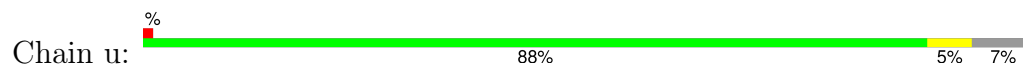


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  87% 5% 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



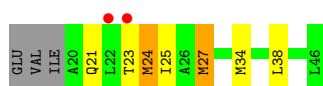
- Molecule 16: Cytochrome c-550



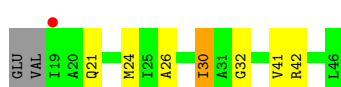
- Molecule 16: Cytochrome c-550



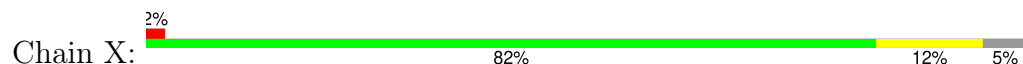
- Molecule 17: Photosystem II reaction center protein Ycf12



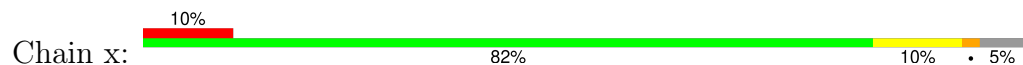
- Molecule 17: Photosystem II reaction center protein Ycf12

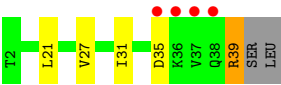


- Molecule 18: Photosystem II reaction center protein X

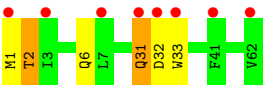
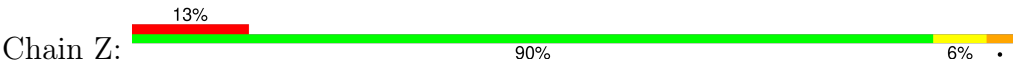


- Molecule 18: Photosystem II reaction center protein X

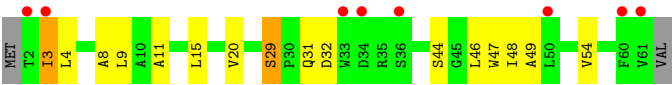




● Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.194 0.157 , 0.194	Depositor DCC
R_{free} test set	31215 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54036	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: MG, LHG, HEM, OEX, CL, DGD, SQD, FE2, BCR, BCT, LMT, GOL, LMG, PHO, PL9, CA, SO4, HSK, CLA, UNL, HTG, RRX, FME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.33	5/2730 (0.2%)	1.14	2/3723 (0.1%)
1	a	1.32	8/2721 (0.3%)	1.10	3/3711 (0.1%)
2	B	1.29	9/4179 (0.2%)	1.10	8/5693 (0.1%)
2	b	1.25	9/4134 (0.2%)	1.06	7/5633 (0.1%)
3	C	1.23	3/3624 (0.1%)	1.04	1/4933 (0.0%)
3	c	1.19	3/3662 (0.1%)	1.05	2/4986 (0.0%)
4	D	1.38	17/2804 (0.6%)	1.15	8/3820 (0.2%)
4	d	1.26	6/2825 (0.2%)	1.07	1/3847 (0.0%)
5	E	1.03	0/676	1.03	0/924
5	e	1.05	1/658 (0.2%)	1.09	1/899 (0.1%)
6	F	1.11	0/283	1.04	2/386 (0.5%)
6	f	1.12	0/265	0.93	1/360 (0.3%)
7	H	1.13	0/511	1.04	0/697
7	h	1.13	0/511	1.02	0/697
8	I	1.06	0/291	1.05	1/394 (0.3%)
8	i	1.03	1/308 (0.3%)	1.01	0/415
9	J	1.11	0/257	1.02	1/349 (0.3%)
9	j	0.96	0/277	1.04	0/376
10	K	0.94	0/303	1.11	0/418
10	k	0.99	0/296	1.09	0/408
11	L	1.17	1/312 (0.3%)	1.09	0/425
11	l	1.16	0/313	1.01	0/428
12	M	1.11	0/257	1.26	2/352 (0.6%)
12	m	1.08	0/270	1.03	0/370
13	O	1.09	0/1924	1.08	3/2610 (0.1%)
13	o	1.03	1/1900 (0.1%)	1.09	6/2577 (0.2%)
14	T	1.13	0/255	1.05	0/346
14	t	1.21	0/255	1.13	0/346
15	U	1.15	0/781	1.07	0/1059
15	u	1.18	0/786	1.07	1/1067 (0.1%)
16	V	1.28	3/1093 (0.3%)	1.13	2/1485 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	1.17	1/1084 (0.1%)	1.10	4/1475 (0.3%)
17	Y	0.79	0/197	0.98	0/263
17	y	0.76	0/197	1.27	2/264 (0.8%)
18	X	0.95	0/286	1.10	2/387 (0.5%)
18	x	0.95	0/286	1.06	0/387
19	Z	0.88	0/470	1.05	0/645
19	z	0.82	0/442	1.15	1/608 (0.2%)
All	All	1.21	68/42423 (0.2%)	1.08	61/57763 (0.1%)

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	33	LYS	N-CA	7.62	1.51	1.46
4	D	87	HIS	CE1-NE2	7.31	1.39	1.32
4	D	87	HIS	CG-CD2	7.20	1.43	1.35
4	D	319	LEU	N-CA	7.07	1.55	1.46
1	a	149	ALA	N-CA	-6.90	1.42	1.46

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	58	GLN	N-CA-C	8.24	121.30	111.33
16	V	85	GLU	N-CA-C	7.08	119.07	111.36
1	a	142	TRP	N-CA-C	6.95	121.46	112.92
16	v	105	ARG	N-CA-C	6.72	119.46	111.33
2	b	316	GLY	N-CA-C	-6.68	106.57	115.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2633	0	2544	28	0
1	a	2625	0	2538	31	0
2	B	4009	0	3879	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3964	0	3817	31	0
3	C	3502	0	3431	35	0
3	c	3536	0	3460	29	0
4	D	2726	0	2629	27	0
4	d	2741	0	2654	28	0
5	E	657	0	637	15	0
5	e	639	0	617	10	0
6	F	274	0	279	4	0
6	f	257	0	269	5	0
7	H	498	0	518	2	0
7	h	498	0	518	9	0
8	I	294	0	304	4	0
8	i	311	0	326	4	0
9	J	251	0	257	3	0
9	j	271	0	270	4	0
10	K	290	0	294	6	0
10	k	286	0	285	3	0
11	L	302	0	316	7	0
11	l	300	0	314	0	0
12	M	261	0	280	18	0
12	m	271	0	293	17	0
13	O	1878	0	1853	25	0
13	o	1855	0	1823	18	0
14	T	256	0	256	2	0
14	t	256	0	256	2	0
15	U	770	0	769	5	0
15	u	772	0	766	3	0
16	V	1066	0	1075	4	0
16	v	1060	0	1053	10	0
17	Y	196	0	219	8	0
17	y	196	0	208	4	0
18	X	280	0	312	5	0
18	x	280	0	312	5	0
19	Z	459	0	484	2	0
19	z	431	0	438	9	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	1040	0	1152	31	0
23	C	845	0	936	28	0
23	D	130	0	144	1	0
23	a	260	0	288	6	0
23	b	1040	0	1152	25	0
23	c	845	0	936	37	0
23	d	130	0	144	5	0
24	A	128	0	148	3	0
24	a	128	0	148	3	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0
25	C	80	0	112	4	0
25	D	40	0	56	2	0
25	K	80	0	112	6	0
25	T	40	0	56	5	0
25	a	40	0	56	2	0
25	b	120	0	168	3	0
25	c	80	0	112	6	0
25	d	40	0	56	5	0
25	k	80	0	112	5	0
25	t	40	0	56	7	0
26	A	108	0	155	5	0
26	B	54	0	78	5	0
26	D	45	0	57	3	0
26	L	54	0	78	5	0
26	a	108	0	156	10	0
26	f	33	0	39	2	0
27	A	51	0	72	3	0
27	B	51	0	72	4	0
27	C	51	0	72	2	0
27	D	51	0	72	2	0
27	Z	51	0	72	0	0
27	a	51	0	72	7	0
27	b	51	0	72	3	0
27	c	102	0	144	2	0
27	d	51	0	72	1	0
28	A	55	0	80	10	0
28	D	55	0	80	0	0
28	a	55	0	80	9	0
28	d	55	0	80	0	0
29	A	69	0	0	0	0
29	B	56	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	34	0	0	0	0
29	D	56	0	0	2	0
29	E	27	0	0	0	0
29	H	10	0	0	0	0
29	I	24	0	0	0	0
29	J	26	0	0	0	0
29	L	14	0	0	1	0
29	M	16	0	0	1	0
29	T	13	0	0	0	0
29	X	16	0	0	0	0
29	Z	16	0	0	0	0
29	a	56	0	0	1	0
29	b	84	0	0	2	0
29	c	40	0	0	1	0
29	d	16	0	0	0	0
29	e	11	0	0	0	0
29	i	55	0	0	0	0
29	j	28	0	0	0	0
29	t	16	0	0	0	0
29	x	16	0	0	1	0
29	z	16	0	0	0	0
30	A	35	0	46	0	0
30	B	35	0	46	4	0
30	C	35	0	46	4	0
30	F	35	0	46	0	0
30	J	24	0	35	1	0
30	M	70	0	92	2	0
30	Z	35	0	46	2	0
30	a	35	0	46	1	0
30	b	49	0	70	2	0
30	c	35	0	46	1	0
30	m	70	0	92	1	0
30	t	24	0	35	0	0
30	z	32	0	33	5	0
31	A	18	0	22	1	0
31	B	36	0	48	1	0
31	C	18	0	24	4	0
31	D	6	0	8	3	0
31	L	6	0	8	1	0
31	O	6	0	8	0	0
31	V	18	0	24	0	0
31	a	18	0	24	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	b	30	0	40	3	0
31	c	24	0	32	5	0
31	f	6	0	6	0	0
31	h	6	0	8	0	0
31	l	6	0	8	0	0
31	v	18	0	24	0	0
32	B	1	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	b	1	0	0	0	0
32	c	1	0	0	0	0
32	f	1	0	0	0	0
32	o	1	0	0	0	0
33	B	95	0	130	1	0
33	C	38	0	52	1	0
33	D	19	0	26	2	0
33	O	19	0	26	0	0
33	U	9	0	15	1	0
33	V	13	0	11	0	0
33	b	76	0	104	3	0
33	c	38	0	52	1	0
33	d	19	0	26	1	0
33	u	14	0	19	0	0
34	C	186	0	246	2	0
34	D	53	0	71	6	0
34	H	62	0	82	1	0
34	c	186	0	246	5	0
34	d	50	0	69	3	0
34	h	62	0	82	1	0
35	D	4	0	0	0	0
35	a	4	0	0	0	0
36	D	144	0	213	15	0
36	E	49	0	74	3	0
36	L	49	0	74	2	0
36	a	40	0	53	1	0
36	d	147	0	222	19	0
36	l	49	0	74	2	0
37	F	43	0	30	2	0
37	V	43	0	30	1	0
37	f	43	0	30	3	0
37	v	43	0	30	0	0
38	H	41	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	41	0	56	3	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	O	5	0	0	0	0
41	A	170	0	0	0	0
41	B	319	0	0	1	0
41	C	263	0	0	5	0
41	D	161	0	0	2	0
41	E	35	0	0	4	0
41	F	12	0	0	0	0
41	H	52	0	0	0	0
41	I	8	0	0	0	0
41	J	9	0	0	0	0
41	K	8	0	0	1	0
41	L	24	0	0	0	0
41	M	16	0	0	1	0
41	O	202	0	0	4	0
41	T	10	0	0	0	0
41	U	100	0	0	1	0
41	V	144	0	0	1	0
41	X	14	0	0	0	0
41	Y	6	0	0	0	0
41	Z	1	0	0	0	0
41	a	155	0	0	2	0
41	b	306	0	0	6	0
41	c	245	0	0	4	0
41	d	160	0	0	1	0
41	e	22	0	0	1	0
41	f	14	0	0	0	0
41	h	53	0	0	0	0
41	i	14	0	0	1	0
41	j	9	0	0	1	0
41	k	5	0	0	0	0
41	l	18	0	0	0	0
41	m	16	0	0	2	0
41	o	175	0	0	1	0
41	t	12	0	0	0	0
41	u	106	0	0	3	0
41	v	104	0	0	2	0
41	x	6	0	0	0	0
41	y	7	0	0	0	0
41	z	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	54036	0	51774	623	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 623 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16[A]:LEU:HD23	12:m:16[A]:LEU:CD2	1.41	1.49
12:M:16[A]:LEU:CD2	12:m:16[A]:LEU:HD23	1.63	1.27
12:M:16[A]:LEU:CD2	12:m:16[A]:LEU:CD2	2.16	1.21
36:d:409:LHG:C38	36:d:409:LHG:H112	1.72	1.17
26:L:103:SQD:H462	26:L:103:SQD:H1	1.28	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36	29
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100	100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	43	36
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	30	22
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	7	2
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	1	0
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	30	22
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	30	22
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	1	0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	1	0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	36	29

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	266 (98%)	6 (2%)	45	42
1	a	271/279 (97%)	269 (99%)	2 (1%)	76	78
2	B	407/402 (101%)	404 (99%)	3 (1%)	76	78
2	b	399/402 (99%)	395 (99%)	4 (1%)	68	70
3	C	355/356 (100%)	350 (99%)	5 (1%)	59	59
3	c	358/356 (101%)	352 (98%)	6 (2%)	53	52
4	D	275/276 (100%)	274 (100%)	1 (0%)	84	87
4	d	278/276 (101%)	275 (99%)	3 (1%)	65	67
5	E	71/72 (99%)	70 (99%)	1 (1%)	59	59
5	e	68/72 (94%)	66 (97%)	2 (3%)	37	31
6	F	27/38 (71%)	26 (96%)	1 (4%)	30	22
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	21
7	H	53/53 (100%)	52 (98%)	1 (2%)	50	47
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	33/34 (97%)	31 (94%)	2 (6%)	17	9
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/30 (97%)	29 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	31	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	31
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	207/207 (100%)	204 (99%)	3 (1%)	59	59
13	o	206/207 (100%)	201 (98%)	5 (2%)	43	38
14	T	25/28 (89%)	25 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	43	38
15	u	83/89 (93%)	83 (100%)	0	100	100
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	70	73
17	Y	19/23 (83%)	17 (90%)	2 (10%)	6	2
17	y	18/23 (78%)	16 (89%)	2 (11%)	6	2
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	29 (97%)	1 (3%)	33	26
19	Z	47/52 (90%)	46 (98%)	1 (2%)	47	44
19	z	40/52 (77%)	37 (92%)	3 (8%)	12	6
All	All	4253/4368 (97%)	4193 (99%)	60 (1%)	59	59

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	315	ILE
17	y	41	VAL
3	c	355	THR
17	y	30	ILE
19	z	29	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	332	GLN
6	f	44	GLN
13	o	104	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	74	GLN
4	D	332	GLN

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
4	HSK	D	336[A]	-	10,10,12	4.08	3 (30%)	5,12,16	2.44	2 (40%)
4	HSK	d	336[B]	-	10,11,12	2.28	3 (30%)	5,14,16	3.26	3 (60%)
14	FME	T	1	14	8,9,10	0.48	0	8,9,11	1.26	1 (12%)
14	FME	t	1	14	8,9,10	0.83	0	8,9,11	1.38	2 (25%)
12	FME	m	1	12	8,9,10	0.89	0	8,9,11	1.53	1 (12%)
8	FME	i	1	8	8,9,10	0.42	0	8,9,11	1.38	1 (12%)
12	FME	M	1	12	8,9,10	0.83	0	8,9,11	1.55	2 (25%)
4	HSK	D	336[B]	-	10,11,12	2.43	3 (30%)	5,14,16	3.23	3 (60%)
8	FME	I	1	8	8,9,10	0.62	0	8,9,11	1.05	0
4	HSK	d	336[A]	-	10,10,12	3.67	2 (20%)	5,12,16	1.85	2 (40%)

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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	5/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-11.73	1.16	1.38
4	d	336[A]	HSK	OM-ND1	-10.19	1.19	1.38
4	D	336[B]	HSK	OM-ND1	4.90	1.47	1.38
4	d	336[B]	HSK	CG-ND1	-4.63	1.34	1.40
4	D	336[B]	HSK	CG-ND1	-4.45	1.34	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336[B]	HSK	ND1-CE1-NE2	-5.23	105.50	111.54
4	d	336[B]	HSK	ND1-CE1-NE2	-5.21	105.53	111.54
4	D	336[A]	HSK	ND1-CE1-NE2	-3.56	107.44	111.54
4	D	336[B]	HSK	CD2-NE2-CE1	3.35	109.62	105.24
4	d	336[B]	HSK	CD2-NE2-CE1	3.32	109.58	105.24

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA
14	t	1	FME	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	0
12	M	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 15 are monoatomic and 43 are unknown - leaving 218 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	GOL	V	205	-	5,5,5	0.67	0	5,5,5	0.34	0
31	GOL	C	526	-	5,5,5	0.68	0	5,5,5	0.50	0
23	CLA	B	617	2	69,73,73	1.88	20 (28%)	82,113,113	2.33	25 (30%)
31	GOL	c	927	-	5,5,5	0.64	0	5,5,5	0.43	0
31	GOL	b	634	-	5,5,5	0.51	0	5,5,5	0.25	0
31	GOL	D	415	-	5,5,5	0.73	0	5,5,5	1.33	1 (20%)
31	GOL	f	104	32	5,5,5	0.55	0	5,5,5	0.45	0
34	DGD	d	406	-	50,50,67	1.20	3 (6%)	58,58,81	1.38	9 (15%)
26	SQD	D	407	-	43,45,54	1.26	3 (6%)	53,56,65	2.12	15 (28%)
23	CLA	B	613	2	69,73,73	2.25	20 (28%)	82,113,113	2.15	26 (31%)
23	CLA	C	505	3	69,73,73	2.19	20 (28%)	82,113,113	2.04	26 (31%)
27	LMG	D	411	39	51,51,55	0.87	2 (3%)	59,59,63	1.04	2 (3%)
33	HTG	c	924	-	19,19,19	0.94	1 (5%)	23,24,24	2.17	4 (17%)
25	BCR	C	514	-	41,41,41	0.91	0	56,56,56	1.33	9 (16%)
23	CLA	c	905	41	69,73,73	2.47	21 (30%)	82,113,113	2.48	27 (32%)
23	CLA	c	909	3	69,73,73	2.36	20 (28%)	82,113,113	2.33	29 (35%)
23	CLA	b	605	2	69,73,73	2.14	18 (26%)	82,113,113	2.17	29 (35%)
23	CLA	C	506	3	69,73,73	2.24	18 (26%)	82,113,113	2.31	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	604	2	69,73,73	2.03	18 (26%)	82,113,113	2.59	30 (36%)
23	CLA	d	403	4	69,73,73	2.16	21 (30%)	82,113,113	2.41	33 (40%)
25	BCR	k	101	-	41,41,41	0.86	0	56,56,56	1.49	12 (21%)
31	GOL	L	104	-	5,5,5	0.52	0	5,5,5	0.64	0
23	CLA	B	609	2	69,73,73	1.84	17 (24%)	82,113,113	2.53	29 (35%)
31	GOL	B	635	-	5,5,5	0.54	0	5,5,5	1.11	0
33	HTG	U	201	-	8,8,19	0.30	0	7,7,24	0.97	0
36	LHG	l	101	-	48,48,48	0.84	2 (4%)	51,54,54	1.12	5 (9%)
30	LMT	Z	102	-	36,36,36	0.68	1 (2%)	47,47,47	0.90	0
23	CLA	a	411	41	69,73,73	1.79	18 (26%)	82,113,113	2.38	36 (43%)
30	LMT	m	102	-	36,36,36	0.73	1 (2%)	47,47,47	1.09	3 (6%)
31	GOL	B	636	-	5,5,5	0.48	0	5,5,5	0.79	0
33	HTG	B	630	-	19,19,19	0.99	2 (10%)	23,24,24	1.42	3 (13%)
25	BCR	K	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.69	9 (16%)
31	GOL	c	930	-	5,5,5	0.47	0	5,5,5	0.71	0
23	CLA	B	606	2	69,73,73	2.08	19 (27%)	82,113,113	2.20	26 (31%)
23	CLA	b	614	2	69,73,73	2.06	16 (23%)	82,113,113	2.29	29 (35%)
36	LHG	L	101	-	48,48,48	0.83	2 (4%)	51,54,54	1.56	7 (13%)
31	GOL	C	524	-	5,5,5	0.36	0	5,5,5	1.69	1 (20%)
27	LMG	A	413	-	51,51,55	1.00	2 (3%)	59,59,63	1.22	4 (6%)
33	HTG	d	401	-	19,19,19	1.01	1 (5%)	23,24,24	1.25	1 (4%)
31	GOL	B	637	-	5,5,5	0.48	0	5,5,5	1.18	1 (20%)
27	LMG	Z	101	-	51,51,55	1.11	3 (5%)	59,59,63	1.37	7 (11%)
23	CLA	c	908	41	69,73,73	2.36	22 (31%)	82,113,113	2.44	30 (36%)
31	GOL	O	304	-	5,5,5	0.56	0	5,5,5	0.64	0
23	CLA	b	612	2	69,73,73	2.37	22 (31%)	82,113,113	1.98	25 (30%)
25	BCR	T	101	-	41,41,41	0.92	0	56,56,56	1.69	15 (26%)
23	CLA	c	913	3	69,73,73	2.55	21 (30%)	82,113,113	2.27	28 (34%)
31	GOL	B	638	-	5,5,5	0.53	0	5,5,5	0.92	0
33	HTG	C	521	-	19,19,19	0.85	1 (5%)	23,24,24	1.21	1 (4%)
23	CLA	A	405	1	69,73,73	2.00	17 (24%)	82,113,113	2.13	27 (32%)
25	BCR	K	101	-	41,41,41	0.91	0	56,56,56	1.70	12 (21%)
25	BCR	D	404	-	41,41,41	1.17	4 (9%)	56,56,56	2.10	18 (32%)
36	LHG	D	409	-	48,48,48	0.84	2 (4%)	51,54,54	1.14	5 (9%)
27	LMG	d	410	39	51,51,55	1.02	3 (5%)	59,59,63	1.15	7 (11%)
34	DGD	c	918	-	63,63,67	1.01	4 (6%)	77,77,81	1.23	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	610	2	69,73,73	2.02	20 (28%)	82,113,113	2.19	27 (32%)
25	BCR	c	916	-	41,41,41	0.99	1 (2%)	56,56,56	1.40	7 (12%)
23	CLA	b	610	41	69,73,73	2.32	18 (26%)	82,113,113	2.04	27 (32%)
23	CLA	b	613	41	69,73,73	2.15	18 (26%)	82,113,113	2.44	26 (31%)
26	SQD	a	416	-	52,54,54	0.89	2 (3%)	62,65,65	2.19	14 (22%)
31	GOL	A	423	32	5,5,5	0.33	0	5,5,5	0.83	0
33	HTG	u	201	-	10,13,19	0.76	0	13,14,24	1.69	2 (15%)
23	CLA	d	402	4	69,73,73	1.96	16 (23%)	82,113,113	2.32	29 (35%)
23	CLA	b	611	2	69,73,73	2.10	18 (26%)	82,113,113	2.10	24 (29%)
23	CLA	A	407	41	69,73,73	2.13	18 (26%)	82,113,113	2.33	30 (36%)
23	CLA	c	904	3	69,73,73	2.48	19 (27%)	82,113,113	2.26	26 (31%)
23	CLA	C	509	3	69,73,73	2.31	18 (26%)	82,113,113	2.33	28 (34%)
31	GOL	a	422	-	5,5,5	0.69	0	5,5,5	0.82	0
23	CLA	b	619	2	69,73,73	2.17	19 (27%)	82,113,113	2.33	28 (34%)
23	CLA	b	604	41	69,73,73	2.38	19 (27%)	82,113,113	2.32	26 (31%)
33	HTG	O	303	-	19,19,19	1.13	2 (10%)	23,24,24	1.22	1 (4%)
34	DGD	C	516	-	63,63,67	0.92	3 (4%)	77,77,81	1.36	12 (15%)
23	CLA	b	609	2	69,73,73	2.31	20 (28%)	82,113,113	2.43	30 (36%)
35	BCT	D	401	21	3,3,3	1.13	0	2,3,3	1.11	0
25	BCR	k	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.33	7 (12%)
23	CLA	c	911	3	69,73,73	2.13	20 (28%)	82,113,113	2.07	28 (34%)
25	BCR	d	404	-	41,41,41	1.03	3 (7%)	56,56,56	1.83	15 (26%)
24	PHO	A	409	-	58,69,69	2.57	11 (18%)	55,99,99	3.17	18 (32%)
33	HTG	C	522	-	19,19,19	0.95	2 (10%)	23,24,24	2.00	3 (13%)
23	CLA	a	410	41	69,73,73	1.99	21 (30%)	82,113,113	2.20	24 (29%)
25	BCR	B	620	-	41,41,41	1.03	1 (2%)	56,56,56	1.67	12 (21%)
23	CLA	B	615	2	69,73,73	2.19	20 (28%)	82,113,113	2.38	30 (36%)
23	CLA	c	907	3	69,73,73	2.24	18 (26%)	82,113,113	2.57	31 (37%)
31	GOL	C	525	-	5,5,5	0.82	0	5,5,5	0.93	0
31	GOL	b	636	-	5,5,5	0.59	0	5,5,5	1.05	0
31	GOL	A	421	-	5,5,5	0.91	0	5,5,5	0.53	0
37	HEM	F	101	6,5	50,50,50	2.01	9 (18%)	67,82,82	1.68	12 (17%)
34	DGD	h	102	-	63,63,67	1.00	3 (4%)	77,77,81	1.27	11 (14%)
34	DGD	H	102	-	63,63,67	1.13	3 (4%)	77,77,81	1.36	12 (15%)
25	BCR	b	622	-	41,41,41	0.96	2 (4%)	56,56,56	1.28	6 (10%)
38	RRX	H	101	-	42,42,42	1.10	3 (7%)	56,58,58	1.62	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	c	915	-	41,41,41	0.87	1 (2%)	56,56,56	1.26	6 (10%)
30	LMT	a	402	-	36,36,36	0.77	1 (2%)	47,47,47	1.60	10 (21%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.46	1 (20%)
23	CLA	B	607	2	69,73,73	2.16	14 (20%)	82,113,113	2.61	35 (42%)
23	CLA	B	603	2	69,73,73	2.36	21 (30%)	82,113,113	1.96	27 (32%)
26	SQD	A	412	-	52,54,54	0.86	2 (3%)	62,65,65	2.15	17 (27%)
34	DGD	C	518	-	63,63,67	0.79	3 (4%)	77,77,81	1.31	9 (11%)
25	BCR	b	621	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	7 (12%)
23	CLA	A	406	41	69,73,73	1.93	19 (27%)	82,113,113	2.50	34 (41%)
33	HTG	b	601	-	19,19,19	0.92	2 (10%)	23,24,24	1.24	3 (13%)
23	CLA	C	502	3	69,73,73	1.93	17 (24%)	82,113,113	2.33	29 (35%)
30	LMT	b	624	-	25,25,36	0.75	1 (4%)	30,30,47	1.39	5 (16%)
23	CLA	B	611	41	69,73,73	2.06	19 (27%)	82,113,113	2.50	31 (37%)
33	HTG	B	625	-	19,19,19	0.93	1 (5%)	23,24,24	1.38	4 (17%)
31	GOL	v	204	-	5,5,5	0.30	0	5,5,5	0.73	0
36	LHG	d	409	-	48,48,48	0.93	3 (6%)	51,54,54	1.09	4 (7%)
30	LMT	z	101	-	32,32,36	0.70	1 (3%)	42,42,47	1.01	4 (9%)
30	LMT	J	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.13	2 (6%)
25	BCR	t	101	-	41,41,41	1.04	3 (7%)	56,56,56	1.86	15 (26%)
23	CLA	B	616	2	69,73,73	2.32	16 (23%)	82,113,113	2.31	28 (34%)
30	LMT	F	102	-	36,36,36	0.75	1 (2%)	47,47,47	1.19	3 (6%)
33	HTG	B	626	-	19,19,19	0.87	1 (5%)	23,24,24	1.59	2 (8%)
31	GOL	h	103	-	5,5,5	0.37	0	5,5,5	0.29	0
23	CLA	C	508	3	69,73,73	2.52	19 (27%)	82,113,113	2.03	23 (28%)
23	CLA	b	617	2	69,73,73	1.91	16 (23%)	82,113,113	2.78	37 (45%)
31	GOL	A	422	-	5,5,5	0.44	0	5,5,5	0.52	0
28	PL9	d	405	-	55,55,55	1.27	9 (16%)	68,69,69	1.53	13 (19%)
31	GOL	c	928	-	5,5,5	0.23	0	5,5,5	0.86	0
38	RRX	h	101	-	42,42,42	0.96	1 (2%)	56,58,58	1.34	8 (14%)
23	CLA	c	903	3	69,73,73	2.20	18 (26%)	82,113,113	2.57	28 (34%)
23	CLA	c	912	3	69,73,73	2.26	19 (27%)	82,113,113	2.38	29 (35%)
36	LHG	D	408	-	48,48,48	0.80	1 (2%)	51,54,54	1.50	6 (11%)
30	LMT	M	101	-	36,36,36	0.87	1 (2%)	47,47,47	1.23	6 (12%)
23	CLA	c	902	3	69,73,73	2.08	19 (27%)	82,113,113	2.68	29 (35%)
31	GOL	a	424	-	5,5,5	0.68	0	5,5,5	0.79	0
23	CLA	b	607	2	69,73,73	2.12	18 (26%)	82,113,113	2.46	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GOL	c	929	-	5,5,5	0.56	0	5,5,5	0.90	0
23	CLA	C	501	3	69,73,73	1.99	19 (27%)	82,113,113	2.62	28 (34%)
23	CLA	c	906	3	69,73,73	2.10	20 (28%)	82,113,113	2.19	29 (35%)
31	GOL	b	632	-	5,5,5	0.54	0	5,5,5	1.38	0
23	CLA	D	402	4	69,73,73	1.97	19 (27%)	82,113,113	2.44	31 (37%)
34	DGD	c	919	-	63,63,67	1.06	5 (7%)	77,77,81	1.37	10 (12%)
34	DGD	D	406	-	53,53,67	1.20	3 (5%)	61,61,81	1.38	8 (13%)
40	SO4	O	302	-	4,4,4	0.60	0	6,6,6	0.40	0
36	LHG	d	407	-	48,48,48	0.81	2 (4%)	51,54,54	1.41	6 (11%)
31	GOL	V	203	-	5,5,5	1.03	0	5,5,5	0.84	0
31	GOL	v	203	-	5,5,5	0.75	0	5,5,5	0.51	0
25	BCR	C	515	-	41,41,41	0.95	1 (2%)	56,56,56	1.47	7 (12%)
27	LMG	a	418	-	51,51,55	0.94	2 (3%)	59,59,63	1.34	5 (8%)
34	DGD	c	917	-	63,63,67	0.91	4 (6%)	77,77,81	1.27	9 (11%)
24	PHO	A	408	-	58,69,69	2.26	11 (18%)	55,99,99	3.25	16 (29%)
25	BCR	b	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.76	15 (26%)
31	GOL	a	423	-	5,5,5	0.60	0	5,5,5	0.63	0
23	CLA	B	602	41	69,73,73	2.34	20 (28%)	82,113,113	2.62	30 (36%)
25	BCR	B	619	-	41,41,41	1.20	4 (9%)	56,56,56	1.25	8 (14%)
30	LMT	m	101	-	36,36,36	0.74	0	47,47,47	1.39	8 (17%)
30	LMT	c	922	-	36,36,36	0.75	1 (2%)	47,47,47	0.96	3 (6%)
31	GOL	B	634	-	5,5,5	0.85	0	5,5,5	0.71	0
37	HEM	v	201	16	50,50,50	1.98	9 (18%)	67,82,82	1.51	8 (11%)
23	CLA	B	605	2	69,73,73	2.00	16 (23%)	82,113,113	2.22	31 (37%)
30	LMT	b	625	-	24,24,36	0.54	0	29,29,47	1.25	4 (13%)
23	CLA	C	503	3	69,73,73	2.18	20 (28%)	82,113,113	2.13	24 (29%)
23	CLA	B	608	41	69,73,73	2.13	19 (27%)	82,113,113	2.19	27 (32%)
31	GOL	b	633	-	5,5,5	0.40	0	5,5,5	0.94	0
23	CLA	a	414	1	69,73,73	1.94	19 (27%)	82,113,113	2.45	33 (40%)
23	CLA	c	914	3	69,73,73	2.67	21 (30%)	82,113,113	2.01	26 (31%)
24	PHO	a	412	-	58,69,69	2.26	12 (20%)	55,99,99	2.74	14 (25%)
34	DGD	C	517	-	63,63,67	0.91	2 (3%)	77,77,81	1.06	3 (3%)
23	CLA	b	606	2	69,73,73	2.06	19 (27%)	82,113,113	2.45	30 (36%)
23	CLA	b	618	2	69,73,73	2.04	17 (24%)	82,113,113	2.39	28 (34%)
30	LMT	B	623	-	36,36,36	1.00	2 (5%)	47,47,47	1.39	8 (17%)
33	HTG	c	923	-	19,19,19	0.93	2 (10%)	23,24,24	1.37	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	a	401	-	52,54,54	1.13	2 (3%)	62,65,65	1.59	9 (14%)
25	BCR	a	415	-	41,41,41	1.22	5 (12%)	56,56,56	1.46	8 (14%)
23	CLA	b	616	2	69,73,73	1.93	18 (26%)	82,113,113	2.33	28 (34%)
30	LMT	C	520	-	36,36,36	0.62	1 (2%)	47,47,47	1.49	7 (14%)
33	HTG	b	626	-	19,19,19	0.97	1 (5%)	23,24,24	1.37	3 (13%)
26	SQD	A	418	-	52,54,54	1.09	2 (3%)	62,65,65	1.62	12 (19%)
30	LMT	M	102	-	36,36,36	0.62	0	47,47,47	1.35	7 (14%)
37	HEM	V	201	16	50,50,50	1.94	12 (24%)	67,82,82	1.30	7 (10%)
23	CLA	A	410	1	69,73,73	2.04	18 (26%)	82,113,113	2.52	31 (37%)
23	CLA	D	403	4	69,73,73	2.24	19 (27%)	82,113,113	2.28	29 (35%)
23	CLA	C	510	3	69,73,73	2.18	20 (28%)	82,113,113	2.32	26 (31%)
23	CLA	B	614	2	69,73,73	1.97	15 (21%)	82,113,113	2.10	27 (32%)
37	HEM	f	101	6,5	50,50,50	1.95	12 (24%)	67,82,82	1.43	9 (13%)
23	CLA	C	504	41	69,73,73	2.11	20 (28%)	82,113,113	2.19	26 (31%)
23	CLA	C	513	3	69,73,73	2.56	19 (27%)	82,113,113	2.21	24 (29%)
33	HTG	b	627	-	19,19,19	1.05	2 (10%)	23,24,24	1.42	1 (4%)
24	PHO	a	413	-	58,69,69	2.61	12 (20%)	55,99,99	3.10	18 (32%)
31	GOL	b	635	-	5,5,5	0.81	0	5,5,5	0.96	0
27	LMG	c	920	-	51,51,55	1.12	4 (7%)	59,59,63	1.28	9 (15%)
28	PL9	D	405	-	55,55,55	1.38	9 (16%)	68,69,69	1.53	12 (17%)
35	BCT	a	408	21	3,3,3	1.14	0	2,3,3	2.98	1 (50%)
36	LHG	d	408	-	48,48,48	0.79	2 (4%)	51,54,54	1.34	9 (17%)
36	LHG	a	417	-	39,39,48	1.17	2 (5%)	42,45,54	1.00	2 (4%)
20	OEX	A	401	1,41,3	0,14,14	-	-	-	-	-
30	LMT	A	419	-	36,36,36	0.84	1 (2%)	47,47,47	1.35	5 (10%)
33	HTG	V	202	-	12,13,19	0.73	0	17,18,24	3.30	7 (41%)
36	LHG	D	410	-	45,45,48	1.04	2 (4%)	48,51,54	1.06	3 (6%)
25	BCR	B	618	-	41,41,41	1.13	5 (12%)	56,56,56	1.60	9 (16%)
23	CLA	C	507	41	69,73,73	2.31	19 (27%)	82,113,113	2.29	24 (29%)
30	LMT	t	102	-	24,24,36	0.69	0	29,29,47	1.32	3 (10%)
33	HTG	b	602	-	19,19,19	0.74	0	23,24,24	1.09	2 (8%)
27	LMG	c	921	-	51,51,55	1.10	3 (5%)	59,59,63	1.23	6 (10%)
28	PL9	A	414	-	55,55,55	0.93	3 (5%)	68,69,69	1.51	11 (16%)
31	GOL	l	102	-	5,5,5	0.49	0	5,5,5	1.08	0
36	LHG	E	101	-	48,48,48	1.02	2 (4%)	51,54,54	0.94	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	A	411	-	41,41,41	1.05	0	56,56,56	1.50	11 (19%)
33	HTG	B	624	-	19,19,19	1.07	1 (5%)	23,24,24	1.40	6 (26%)
23	CLA	b	608	2	69,73,73	1.96	18 (26%)	82,113,113	2.43	28 (34%)
26	SQD	B	621	-	52,54,54	1.10	4 (7%)	62,65,65	1.84	12 (19%)
33	HTG	D	414	-	19,19,19	0.99	1 (5%)	23,24,24	1.04	1 (4%)
31	GOL	V	204	-	5,5,5	0.31	0	5,5,5	0.47	0
20	OEX	a	404	1,41,3	0,14,14	-	-	-	-	-
26	SQD	f	102	-	31,32,54	2.00	3 (9%)	33,36,65	1.61	5 (15%)
26	SQD	L	103	-	52,54,54	1.09	2 (3%)	62,65,65	1.66	12 (19%)
28	PL9	a	419	-	55,55,55	0.86	3 (5%)	68,69,69	1.76	18 (26%)
27	LMG	b	623	-	51,51,55	0.87	2 (3%)	59,59,63	1.47	7 (11%)
33	HTG	B	631	-	19,19,19	0.80	1 (5%)	23,24,24	1.68	3 (13%)
31	GOL	v	202	-	5,5,5	0.59	0	5,5,5	0.55	0
23	CLA	C	511	3	69,73,73	2.36	22 (31%)	82,113,113	2.58	29 (35%)
23	CLA	a	409	1	69,73,73	1.91	16 (23%)	82,113,113	2.28	28 (34%)
23	CLA	c	910	3	69,73,73	2.33	21 (30%)	82,113,113	2.47	35 (42%)
27	LMG	B	622	-	51,51,55	0.95	2 (3%)	59,59,63	1.63	9 (15%)
23	CLA	C	512	3	69,73,73	2.40	20 (28%)	82,113,113	2.24	27 (32%)
27	LMG	C	519	-	51,51,55	1.03	3 (5%)	59,59,63	1.48	9 (15%)
23	CLA	B	612	2	69,73,73	1.79	16 (23%)	82,113,113	2.46	30 (36%)
23	CLA	b	615	2	69,73,73	2.21	18 (26%)	82,113,113	2.50	28 (34%)

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	GOL	V	205	-	-	0/4/4/4	-
31	GOL	C	526	-	-	0/4/4/4	-
23	CLA	B	617	2	-	15/39/115/115	-
31	GOL	c	927	-	-	2/4/4/4	-
31	GOL	b	634	-	-	0/4/4/4	-
31	GOL	D	415	-	-	2/4/4/4	-
31	GOL	f	104	32	-	2/4/4/4	-
34	DGD	d	406	-	-	26/44/64/95	0/1/1/2
26	SQD	D	407	-	-	13/40/60/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	2	-	2/39/115/115	-
23	CLA	C	505	3	-	2/39/115/115	-
27	LMG	D	411	39	-	9/46/66/70	0/1/1/1
33	HTG	c	924	-	-	1/10/30/30	0/1/1/1
25	BCR	C	514	-	-	2/29/63/63	0/2/2/2
23	CLA	c	905	41	-	10/39/115/115	-
23	CLA	c	909	3	-	1/39/115/115	-
23	CLA	b	605	2	-	2/39/115/115	-
23	CLA	C	506	3	-	11/39/115/115	-
23	CLA	B	604	2	-	4/39/115/115	-
23	CLA	d	403	4	-	8/39/115/115	-
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
31	GOL	L	104	-	-	1/4/4/4	-
23	CLA	B	609	2	-	1/39/115/115	-
31	GOL	B	635	-	-	4/4/4/4	-
33	HTG	U	201	-	-	4/6/6/30	-
36	LHG	l	101	-	-	17/53/53/53	-
30	LMT	Z	102	-	-	13/21/61/61	0/2/2/2
23	CLA	a	411	41	-	8/39/115/115	-
30	LMT	m	102	-	-	6/21/61/61	0/2/2/2
31	GOL	B	636	-	-	0/4/4/4	-
33	HTG	B	630	-	-	4/10/30/30	0/1/1/1
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
31	GOL	c	930	-	-	4/4/4/4	-
23	CLA	B	606	2	-	6/39/115/115	-
23	CLA	b	614	2	-	5/39/115/115	-
36	LHG	L	101	-	-	10/53/53/53	-
31	GOL	C	524	-	-	2/4/4/4	-
27	LMG	A	413	-	-	25/46/66/70	0/1/1/1
33	HTG	d	401	-	-	5/10/30/30	0/1/1/1
31	GOL	B	637	-	-	0/4/4/4	-
27	LMG	Z	101	-	-	25/46/66/70	0/1/1/1
23	CLA	c	908	41	-	8/39/115/115	-
31	GOL	O	304	-	-	2/4/4/4	-
23	CLA	b	612	2	-	2/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	913	3	-	10/39/115/115	-
31	GOL	B	638	-	-	2/4/4/4	-
33	HTG	C	521	-	-	3/10/30/30	0/1/1/1
23	CLA	A	405	1	-	3/39/115/115	-
25	BCR	K	101	-	-	3/29/63/63	0/2/2/2
25	BCR	D	404	-	-	2/29/63/63	0/2/2/2
36	LHG	D	409	-	-	13/53/53/53	-
27	LMG	d	410	39	-	10/46/66/70	0/1/1/1
34	DGD	c	918	-	-	21/51/91/95	0/2/2/2
23	CLA	B	610	2	-	3/39/115/115	-
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	41	-	2/39/115/115	-
23	CLA	b	613	41	-	3/39/115/115	-
26	SQD	a	416	-	-	20/49/69/69	0/1/1/1
31	GOL	A	423	32	-	0/4/4/4	-
33	HTG	u	201	-	-	6/12/14/30	-
23	CLA	d	402	4	-	1/39/115/115	-
23	CLA	b	611	2	-	1/39/115/115	-
23	CLA	A	407	41	-	7/39/115/115	-
23	CLA	c	904	3	-	1/39/115/115	-
23	CLA	C	509	3	-	6/39/115/115	-
31	GOL	a	422	-	-	0/4/4/4	-
23	CLA	b	619	2	-	6/39/115/115	-
23	CLA	b	604	41	-	14/39/115/115	-
33	HTG	O	303	-	-	3/10/30/30	0/1/1/1
34	DGD	C	516	-	-	17/51/91/95	0/2/2/2
23	CLA	b	609	2	-	10/39/115/115	-
25	BCR	k	102	-	-	3/29/63/63	0/2/2/2
23	CLA	c	911	3	-	6/39/115/115	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	PHO	A	409	-	-	3/37/103/103	0/5/6/6
33	HTG	C	522	-	-	2/10/30/30	0/1/1/1
23	CLA	a	410	41	-	3/39/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
23	CLA	B	615	2	-	11/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	907	3	-	12/39/115/115	-
31	GOL	C	525	-	-	0/4/4/4	-
31	GOL	b	636	-	-	2/4/4/4	-
31	GOL	A	421	-	-	0/4/4/4	-
37	HEM	F	101	6,5	-	2/14/54/54	-
34	DGD	h	102	-	-	10/51/91/95	0/2/2/2
34	DGD	H	102	-	-	16/51/91/95	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
25	BCR	c	915	-	-	5/29/63/63	0/2/2/2
30	LMT	a	402	-	-	10/21/61/61	0/2/2/2
31	GOL	B	633	-	-	2/4/4/4	-
23	CLA	B	607	2	-	6/39/115/115	-
23	CLA	B	603	2	-	3/39/115/115	-
26	SQD	A	412	-	-	18/49/69/69	0/1/1/1
34	DGD	C	518	-	-	13/51/91/95	0/2/2/2
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	CLA	A	406	41	-	4/39/115/115	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
23	CLA	C	502	3	-	6/39/115/115	-
30	LMT	b	624	-	-	9/17/37/61	0/1/1/2
23	CLA	B	611	41	-	8/39/115/115	-
33	HTG	B	625	-	-	4/10/30/30	0/1/1/1
31	GOL	v	204	-	-	0/4/4/4	-
36	LHG	d	409	-	-	16/53/53/53	-
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
30	LMT	J	102	-	-	7/15/35/61	0/1/1/2
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	616	2	-	5/39/115/115	-
30	LMT	F	102	-	-	11/21/61/61	0/2/2/2
33	HTG	B	626	-	-	5/10/30/30	0/1/1/1
31	GOL	h	103	-	-	1/4/4/4	-
23	CLA	C	508	3	-	3/39/115/115	-
23	CLA	b	617	2	-	16/39/115/115	-
31	GOL	A	422	-	-	0/4/4/4	-
28	PL9	d	405	-	-	2/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	c	928	-	-	1/4/4/4	-
38	RRX	h	101	-	-	1/29/65/65	0/2/2/2
23	CLA	c	903	3	-	4/39/115/115	-
23	CLA	c	912	3	-	6/39/115/115	-
36	LHG	D	408	-	-	9/53/53/53	-
30	LMT	M	101	-	-	7/21/61/61	0/2/2/2
23	CLA	c	902	3	-	4/39/115/115	-
31	GOL	a	424	-	-	3/4/4/4	-
23	CLA	b	607	2	-	5/39/115/115	-
31	GOL	c	929	-	-	0/4/4/4	-
23	CLA	C	501	3	-	5/39/115/115	-
23	CLA	c	906	3	-	3/39/115/115	-
31	GOL	b	632	-	-	4/4/4/4	-
23	CLA	D	402	4	-	6/39/115/115	-
34	DGD	c	919	-	-	16/51/91/95	0/2/2/2
34	DGD	D	406	-	-	26/47/68/95	0/1/1/2
36	LHG	d	407	-	-	6/53/53/53	-
31	GOL	V	203	-	-	2/4/4/4	-
31	GOL	v	203	-	-	2/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	LMG	a	418	-	-	19/46/66/70	0/1/1/1
34	DGD	c	917	-	-	14/51/91/95	0/2/2/2
24	PHO	A	408	-	-	0/37/103/103	0/5/6/6
25	BCR	b	620	-	-	2/29/63/63	0/2/2/2
31	GOL	a	423	-	-	2/4/4/4	-
23	CLA	B	602	41	-	18/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	LMT	m	101	-	-	3/21/61/61	0/2/2/2
30	LMT	c	922	-	-	5/21/61/61	0/2/2/2
31	GOL	B	634	-	-	0/4/4/4	-
37	HEM	v	201	16	-	6/14/54/54	-
23	CLA	B	605	2	-	5/39/115/115	-
30	LMT	b	625	-	-	11/15/35/61	0/1/1/2
23	CLA	C	503	3	-	1/39/115/115	-
23	CLA	B	608	41	-	2/39/115/115	-
31	GOL	b	633	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	414	1	-	12/39/115/115	-
23	CLA	c	914	3	-	11/39/115/115	-
24	PHO	a	412	-	-	1/37/103/103	0/5/6/6
34	DGD	C	517	-	-	22/51/91/95	0/2/2/2
23	CLA	b	606	2	-	4/39/115/115	-
23	CLA	b	618	2	-	9/39/115/115	-
30	LMT	B	623	-	-	12/21/61/61	0/2/2/2
33	HTG	c	923	-	-	4/10/30/30	0/1/1/1
26	SQD	a	401	-	-	23/49/69/69	0/1/1/1
25	BCR	a	415	-	-	1/29/63/63	0/2/2/2
23	CLA	b	616	2	-	4/39/115/115	-
30	LMT	C	520	-	-	10/21/61/61	0/2/2/2
33	HTG	b	626	-	-	4/10/30/30	0/1/1/1
26	SQD	A	418	-	-	16/49/69/69	0/1/1/1
30	LMT	M	102	-	-	2/21/61/61	0/2/2/2
37	HEM	V	201	16	-	6/14/54/54	-
23	CLA	A	410	1	-	13/39/115/115	-
23	CLA	D	403	4	-	12/39/115/115	-
23	CLA	C	510	3	-	3/39/115/115	-
23	CLA	B	614	2	-	6/39/115/115	-
37	HEM	f	101	6,5	-	1/14/54/54	-
23	CLA	C	504	41	-	10/39/115/115	-
23	CLA	C	513	3	-	13/39/115/115	-
33	HTG	b	627	-	-	5/10/30/30	0/1/1/1
24	PHO	a	413	-	-	2/37/103/103	0/5/6/6
31	GOL	b	635	-	-	1/4/4/4	-
27	LMG	c	920	-	-	18/46/66/70	0/1/1/1
28	PL9	D	405	-	-	1/53/73/73	0/1/1/1
36	LHG	d	408	-	-	9/53/53/53	-
36	LHG	a	417	-	-	29/44/44/53	-
30	LMT	A	419	-	-	5/21/61/61	0/2/2/2
33	HTG	V	202	-	-	2/4/24/30	0/1/1/1
36	LHG	D	410	-	-	13/50/50/53	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
23	CLA	C	507	41	-	11/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	t	102	-	-	8/15/35/61	0/1/1/2
33	HTG	b	602	-	-	1/10/30/30	0/1/1/1
27	LMG	c	921	-	-	13/46/66/70	0/1/1/1
28	PL9	A	414	-	-	11/53/73/73	0/1/1/1
31	GOL	l	102	-	-	0/4/4/4	-
36	LHG	E	101	-	-	27/53/53/53	-
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
33	HTG	B	624	-	-	2/10/30/30	0/1/1/1
23	CLA	b	608	2	-	3/39/115/115	-
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
33	HTG	D	414	-	-	2/10/30/30	0/1/1/1
31	GOL	V	204	-	-	0/4/4/4	-
26	SQD	f	102	-	-	13/33/33/69	-
26	SQD	L	103	-	-	28/49/69/69	0/1/1/1
28	PL9	a	419	-	-	11/53/73/73	0/1/1/1
27	LMG	b	623	-	-	19/46/66/70	0/1/1/1
33	HTG	B	631	-	-	5/10/30/30	0/1/1/1
31	GOL	v	202	-	-	0/4/4/4	-
23	CLA	C	511	3	-	0/39/115/115	-
23	CLA	a	409	1	-	4/39/115/115	-
23	CLA	c	910	3	-	11/39/115/115	-
27	LMG	B	622	-	-	15/46/66/70	0/1/1/1
23	CLA	C	512	3	-	7/39/115/115	-
27	LMG	C	519	-	-	22/46/66/70	0/1/1/1
23	CLA	B	612	2	-	1/39/115/115	-
23	CLA	b	615	2	-	6/39/115/115	-

The worst 5 of 1598 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	MG-NA	12.57	2.36	2.06
23	c	914	CLA	MG-NC	11.74	2.34	2.06
23	C	512	CLA	MG-NA	11.26	2.33	2.06
23	C	511	CLA	MG-NA	11.02	2.32	2.06
23	B	616	CLA	MG-NA	10.89	2.32	2.06

The worst 5 of 2808 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	13.12	112.67	106.68
24	A	408	PHO	C2D-C1D-ND	12.68	118.60	109.43
23	b	609	CLA	C4A-NA-C1A	11.80	112.06	106.68
24	A	408	PHO	C3B-C4B-NB	11.40	114.89	107.46
23	C	501	CLA	O2D-CGD-O1D	-10.54	103.33	123.85

There are no chirality outliers.

5 of 1412 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	C11-C10-C8-C9
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

152 monomers are involved in 343 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	617	CLA	7	0
31	c	927	GOL	2	0
31	D	415	GOL	3	0
34	d	406	DGD	3	0
26	D	407	SQD	3	0
23	B	613	CLA	1	0
27	D	411	LMG	2	0
25	C	514	BCR	1	0
23	c	905	CLA	3	0
23	c	909	CLA	3	0
23	C	506	CLA	3	0
23	B	604	CLA	2	0
23	d	403	CLA	4	0
25	k	101	BCR	3	0
31	L	104	GOL	1	0
23	B	609	CLA	1	0
31	B	635	GOL	1	0
33	U	201	HTG	1	0
36	l	101	LHG	2	0
30	Z	102	LMT	2	0
23	a	411	CLA	1	0
25	K	102	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	606	CLA	4	0
36	L	101	LHG	2	0
31	C	524	GOL	4	0
27	A	413	LMG	3	0
33	d	401	HTG	1	0
23	c	908	CLA	2	0
23	b	612	CLA	1	0
25	T	101	BCR	5	0
23	c	913	CLA	3	0
33	C	521	HTG	1	0
23	A	405	CLA	4	0
25	K	101	BCR	3	0
25	D	404	BCR	2	0
36	D	409	LHG	1	0
27	d	410	LMG	1	0
34	c	918	DGD	3	0
23	B	610	CLA	1	0
25	c	916	BCR	6	0
23	b	610	CLA	1	0
23	b	613	CLA	5	0
26	a	416	SQD	7	0
23	d	402	CLA	1	0
23	c	904	CLA	4	0
23	C	509	CLA	5	0
23	b	619	CLA	2	0
23	b	604	CLA	1	0
23	b	609	CLA	2	0
25	k	102	BCR	2	0
23	c	911	CLA	2	0
25	d	404	BCR	5	0
24	A	409	PHO	2	0
25	B	620	BCR	2	0
23	B	615	CLA	3	0
23	c	907	CLA	5	0
31	b	636	GOL	1	0
37	F	101	HEM	2	0
34	h	102	DGD	1	0
34	H	102	DGD	1	0
25	b	622	BCR	2	0
38	H	101	RRX	2	0
30	a	402	LMT	1	0
23	B	607	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	412	SQD	4	0
25	b	621	BCR	1	0
23	A	406	CLA	4	0
23	C	502	CLA	2	0
30	b	624	LMT	2	0
23	B	611	CLA	5	0
36	d	409	LHG	17	0
30	z	101	LMT	5	0
30	J	102	LMT	1	0
25	t	101	BCR	7	0
23	B	616	CLA	1	0
23	C	508	CLA	2	0
23	b	617	CLA	3	0
31	A	422	GOL	1	0
31	c	928	GOL	3	0
38	h	101	RRX	3	0
23	c	903	CLA	2	0
23	c	912	CLA	3	0
36	D	408	LHG	1	0
30	M	101	LMT	2	0
23	c	902	CLA	3	0
23	b	607	CLA	1	0
23	C	501	CLA	3	0
23	c	906	CLA	7	0
34	c	919	DGD	2	0
34	D	406	DGD	6	0
36	d	407	LHG	1	0
25	C	515	BCR	3	0
27	a	418	LMG	7	0
34	c	917	DGD	1	0
24	A	408	PHO	1	0
31	a	423	GOL	3	0
23	B	602	CLA	1	0
25	B	619	BCR	3	0
30	m	101	LMT	1	0
30	c	922	LMT	1	0
23	B	605	CLA	3	0
23	C	503	CLA	2	0
31	b	633	GOL	2	0
23	a	414	CLA	3	0
23	c	914	CLA	5	0
24	a	412	PHO	1	0

Continued on next page...

Continued from previous page...

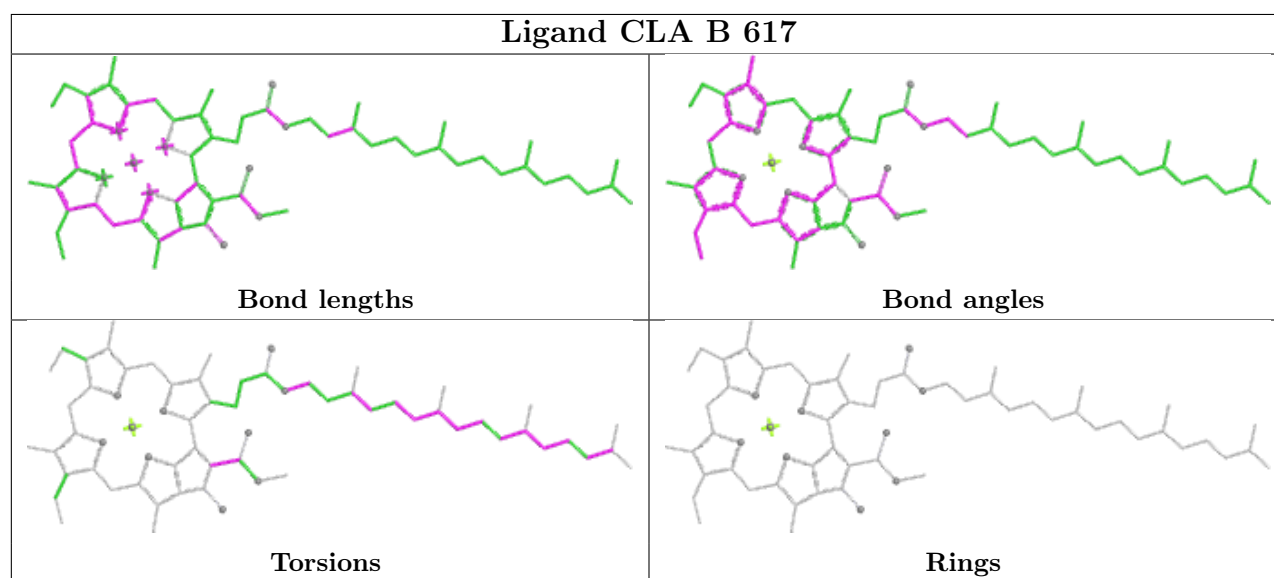
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	517	DGD	2	0
23	b	606	CLA	2	0
23	b	618	CLA	4	0
30	B	623	LMT	4	0
33	c	923	HTG	1	0
26	a	401	SQD	3	0
25	a	415	BCR	2	0
23	b	616	CLA	5	0
30	C	520	LMT	4	0
33	b	626	HTG	2	0
26	A	418	SQD	1	0
37	V	201	HEM	1	0
23	A	410	CLA	1	0
23	D	403	CLA	1	0
23	C	510	CLA	1	0
23	B	614	CLA	2	0
37	f	101	HEM	3	0
23	C	504	CLA	4	0
23	C	513	CLA	2	0
33	b	627	HTG	1	0
24	a	413	PHO	2	0
27	c	920	LMG	1	0
36	d	408	LHG	1	0
36	a	417	LHG	1	0
36	D	410	LHG	13	0
23	C	507	CLA	1	0
27	c	921	LMG	1	0
28	A	414	PL9	10	0
36	E	101	LHG	3	0
25	A	411	BCR	2	0
23	b	608	CLA	2	0
26	B	621	SQD	5	0
33	D	414	HTG	2	0
26	f	102	SQD	2	0
26	L	103	SQD	5	0
28	a	419	PL9	9	0
27	b	623	LMG	3	0
33	B	631	HTG	1	0
23	C	511	CLA	4	0
23	a	409	CLA	2	0
23	c	910	CLA	2	0
27	B	622	LMG	4	0

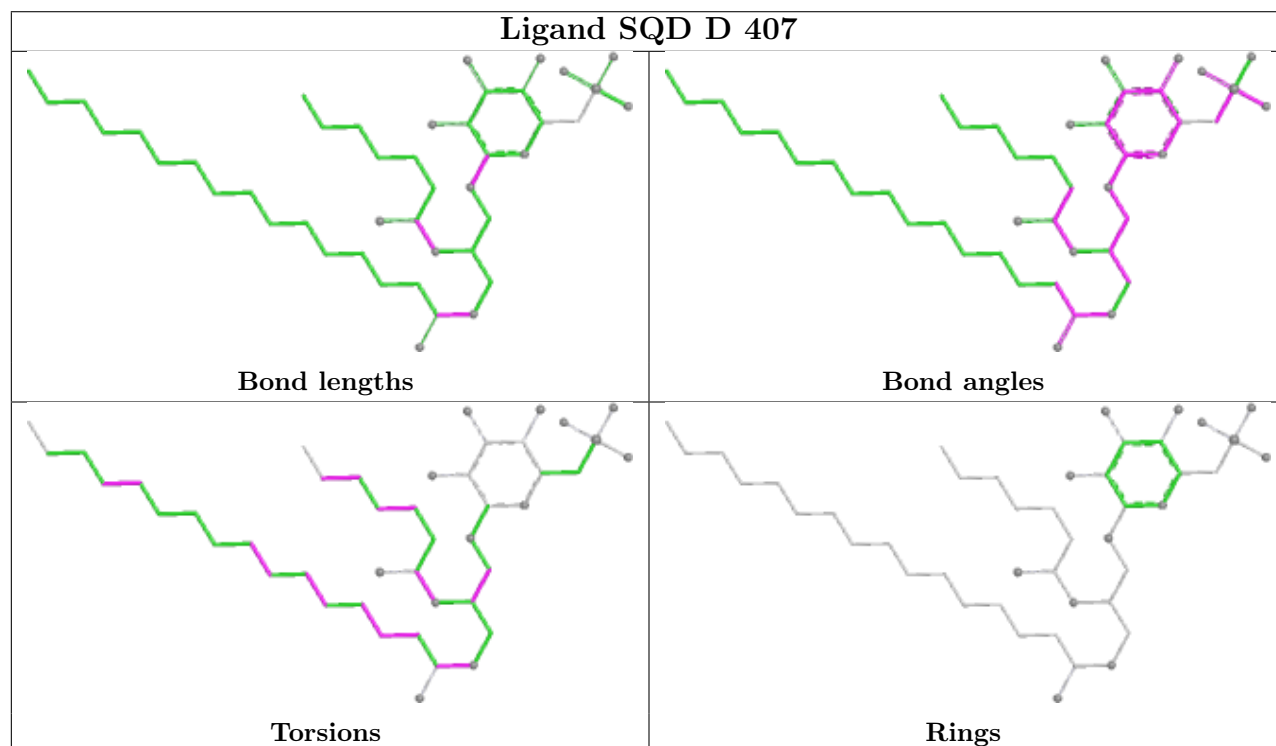
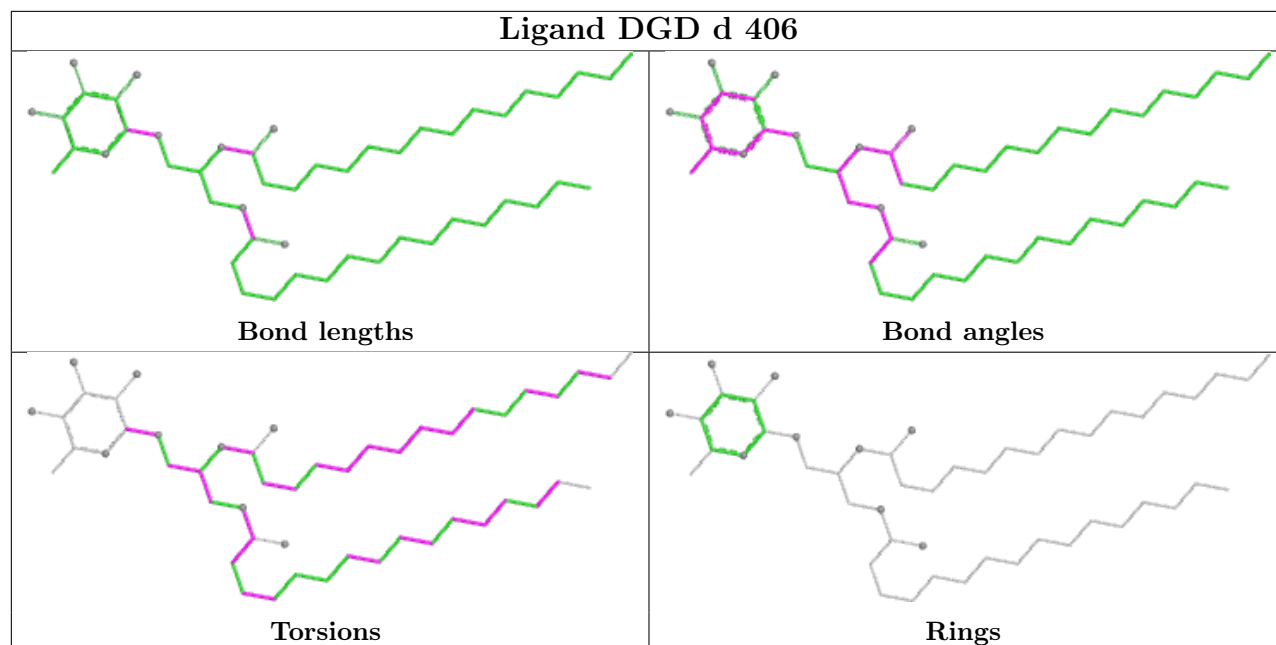
Continued on next page...

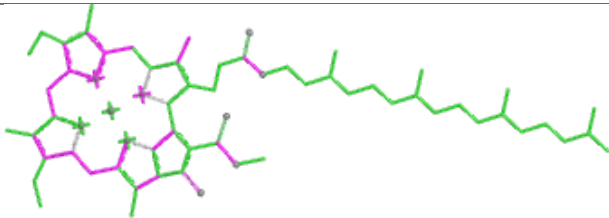
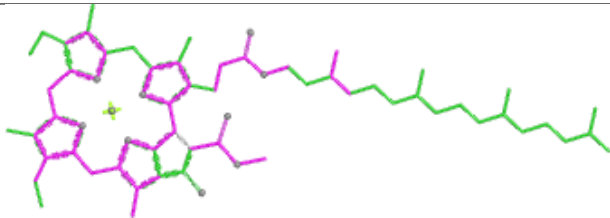
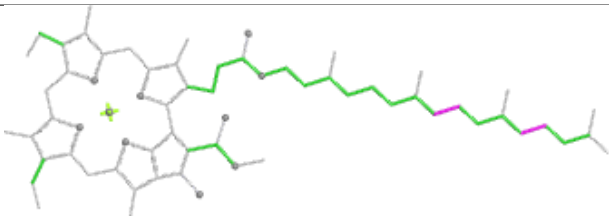
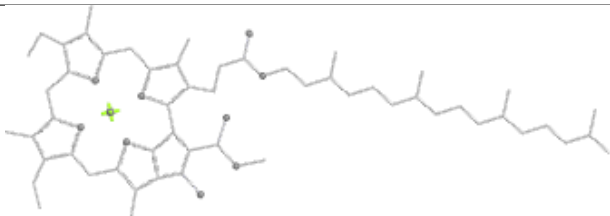
Continued from previous page...

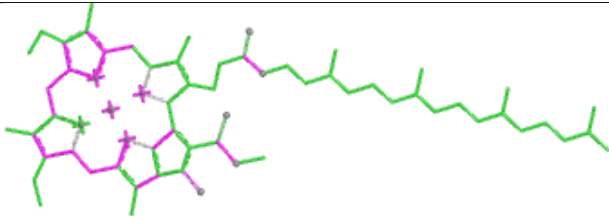
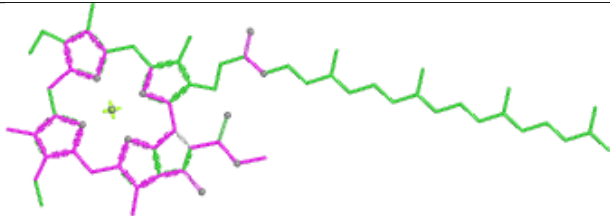
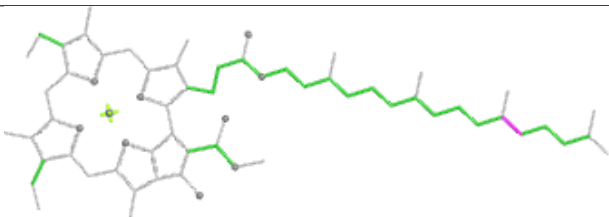
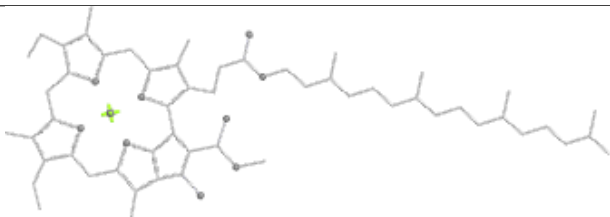
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	512	CLA	3	0
27	C	519	LMG	2	0
23	B	612	CLA	3	0
23	b	615	CLA	1	0

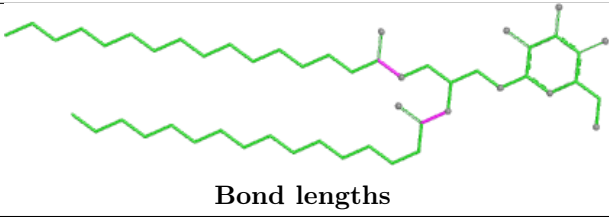
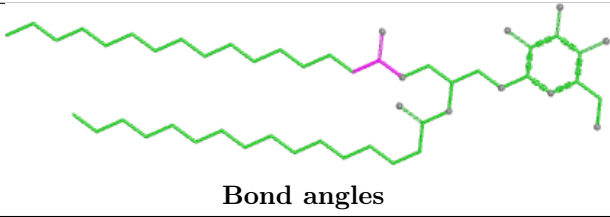
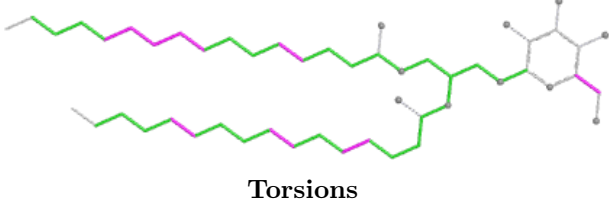
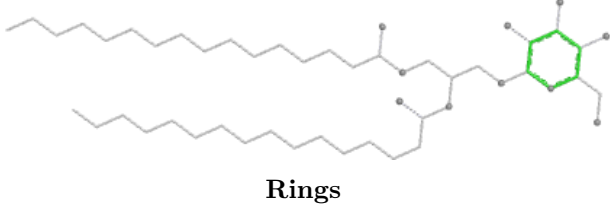
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

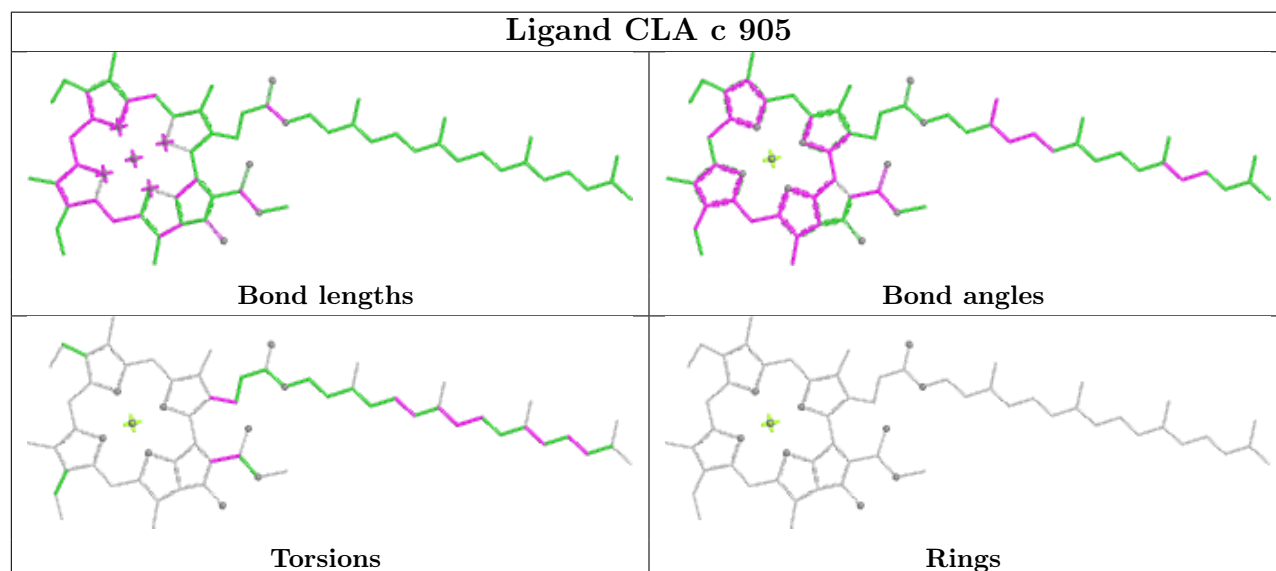
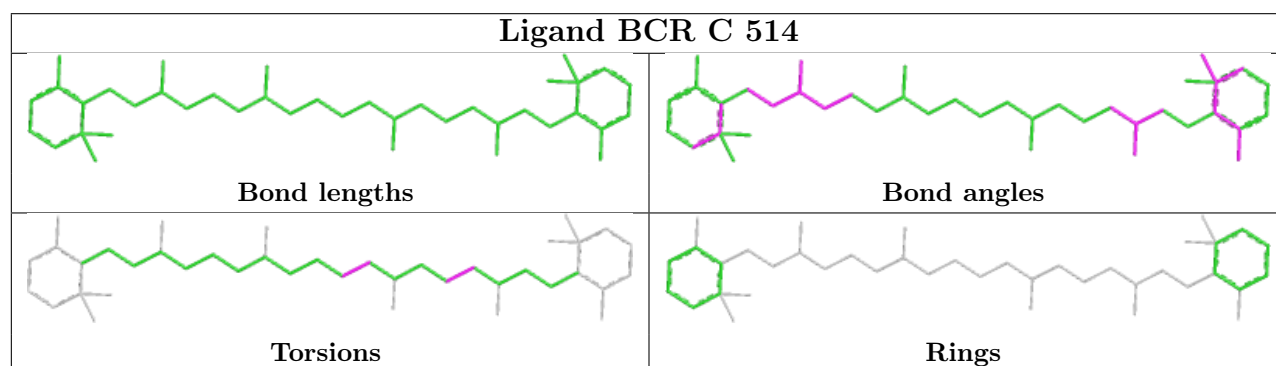
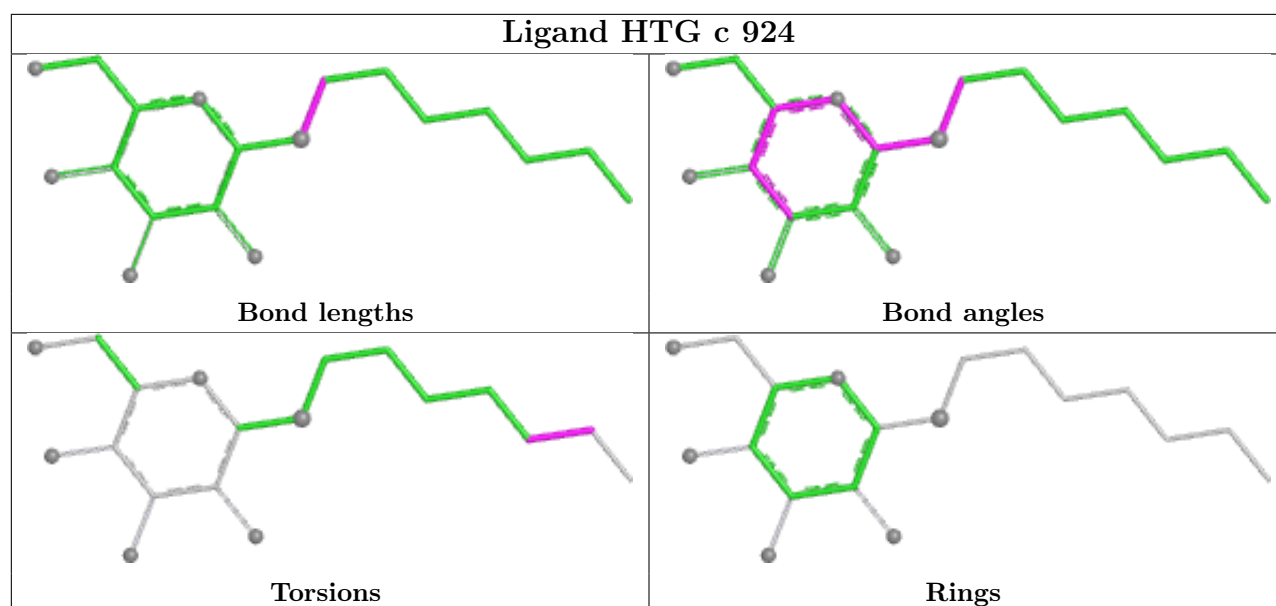


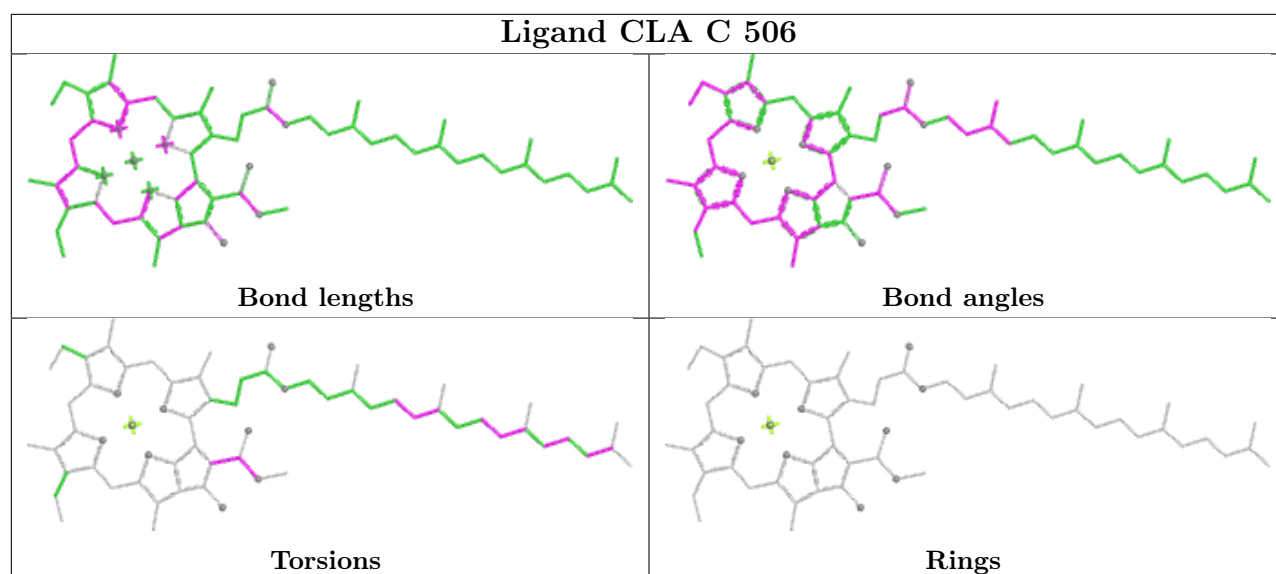
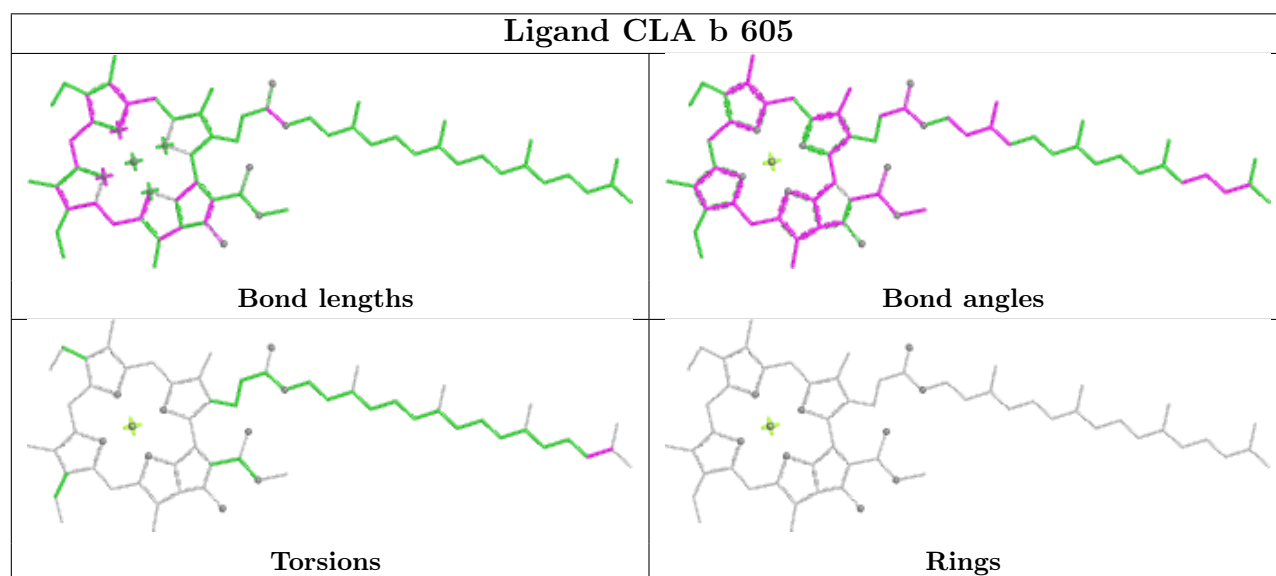
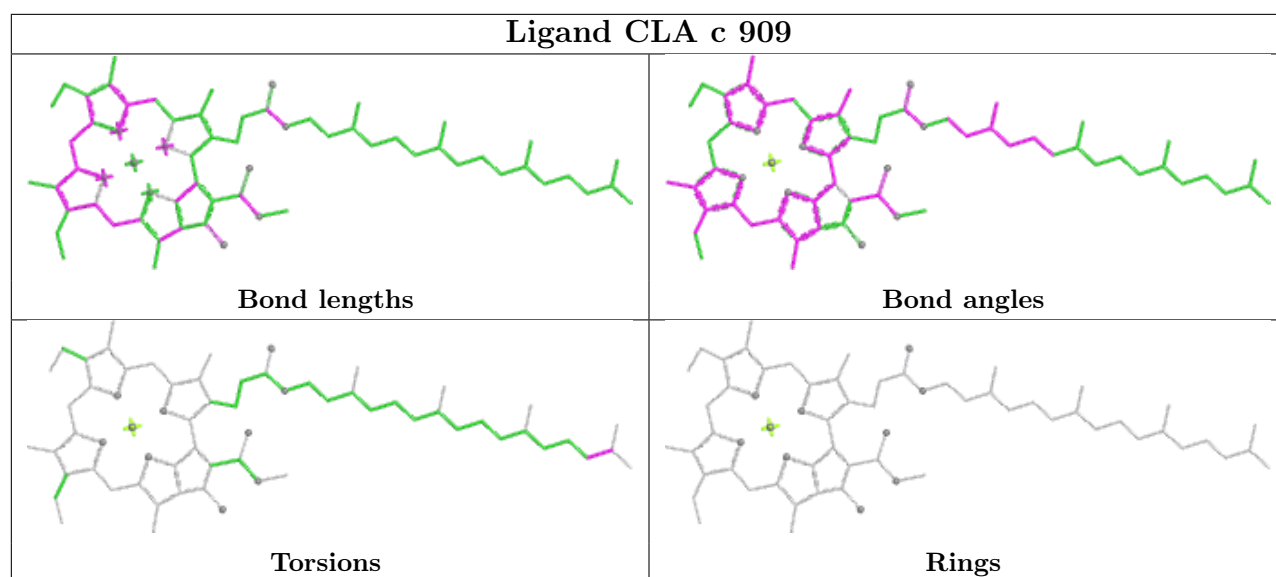


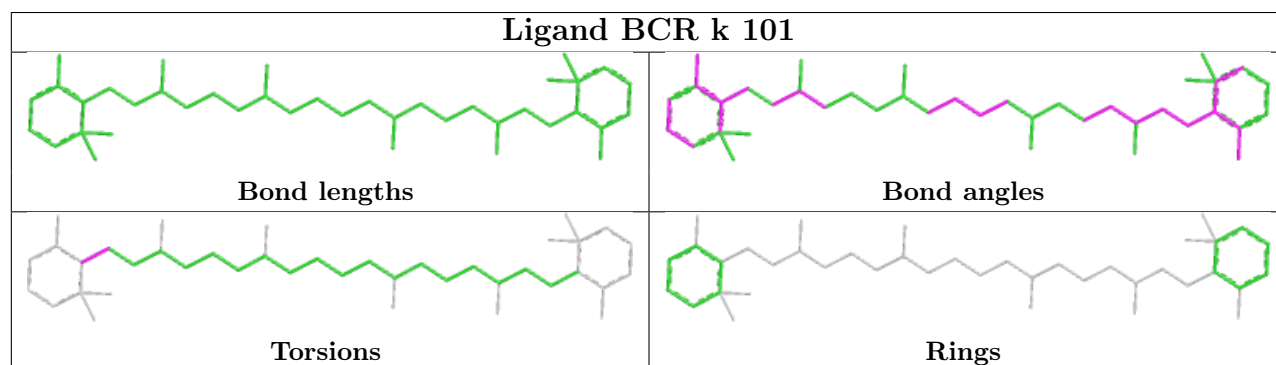
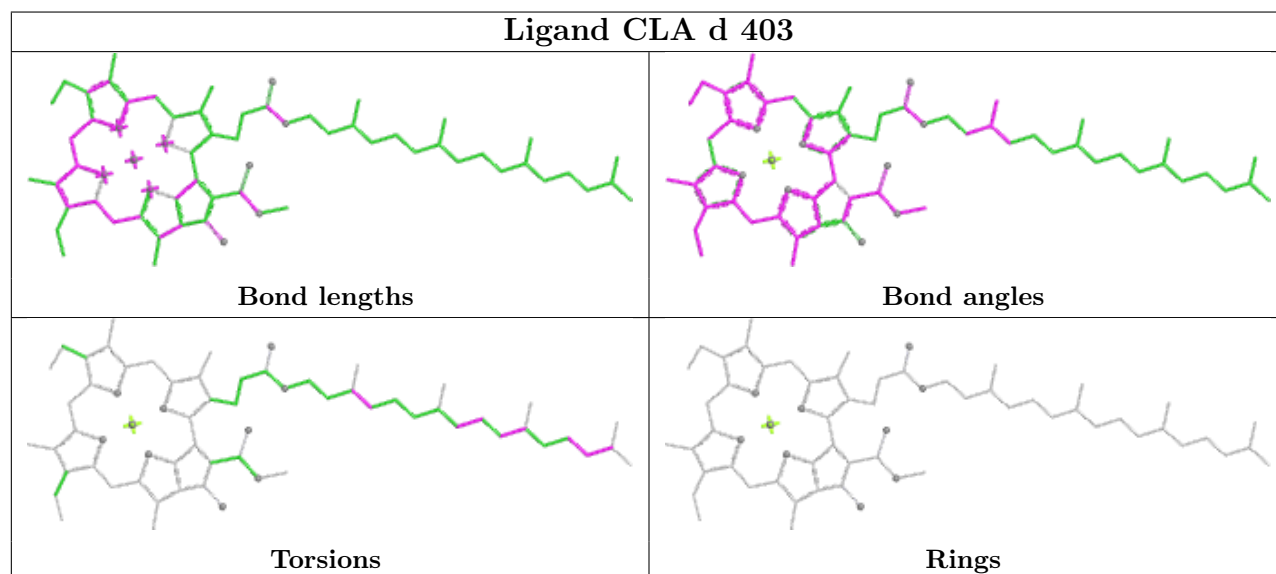
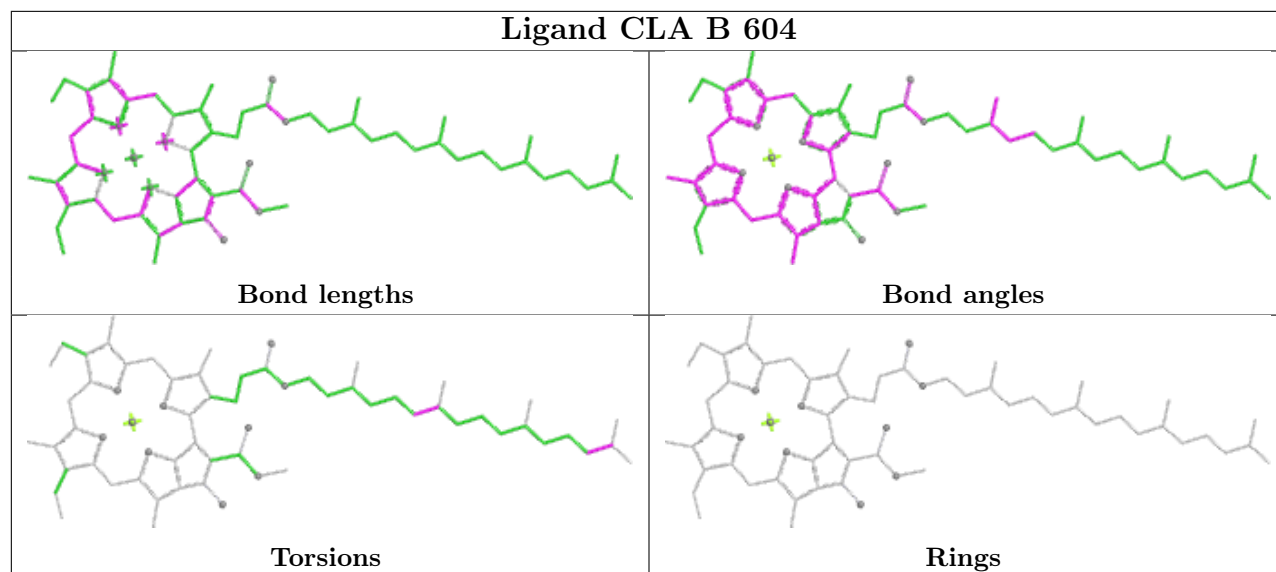
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

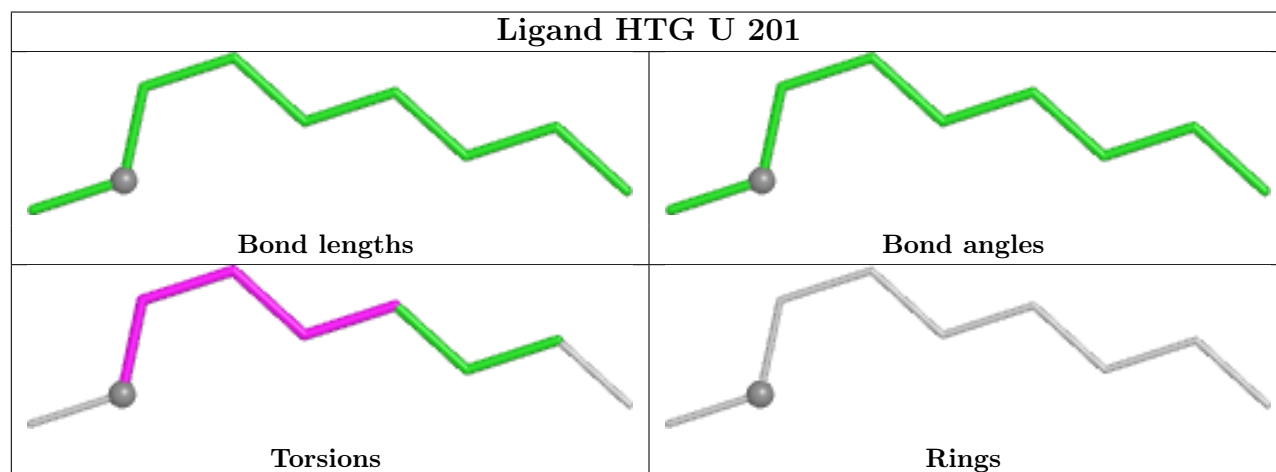
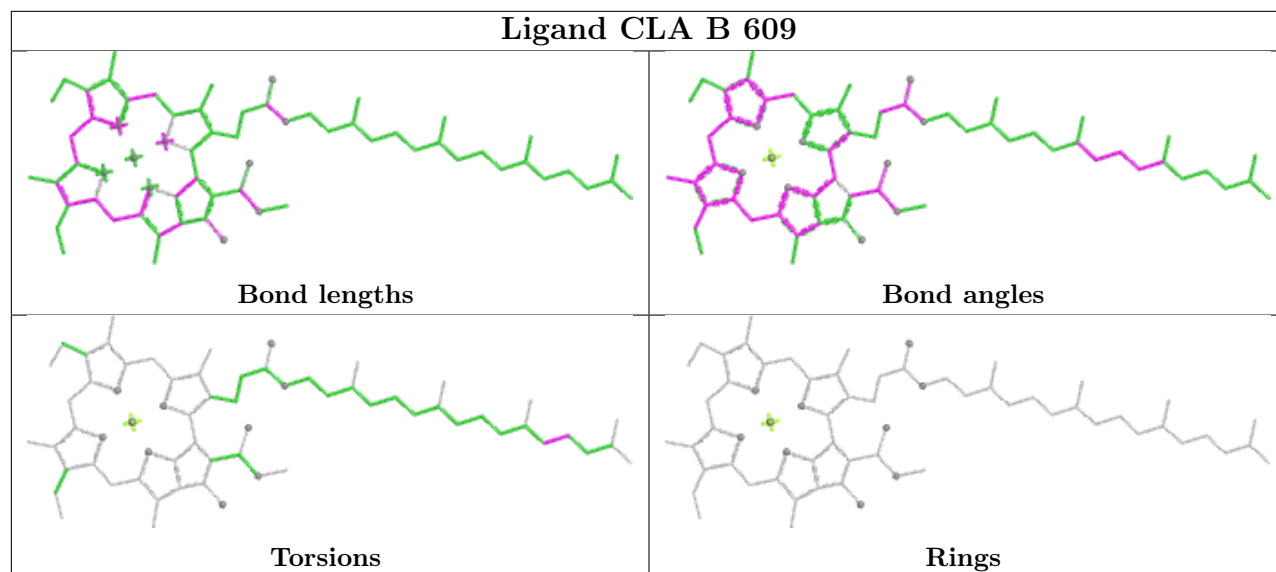
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

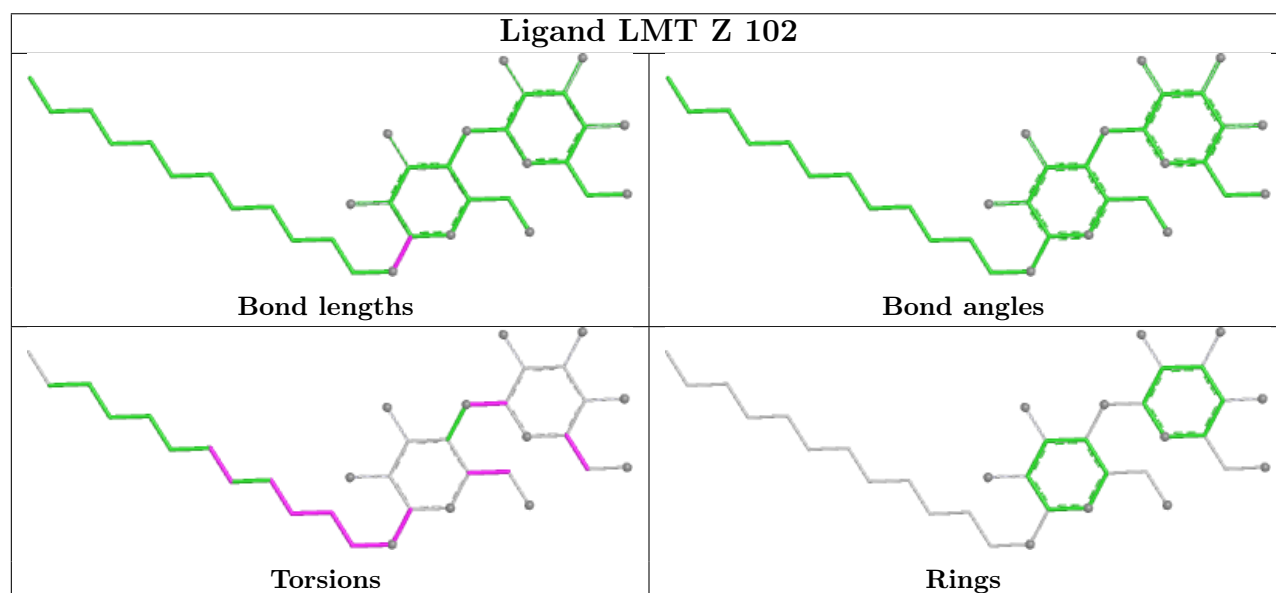
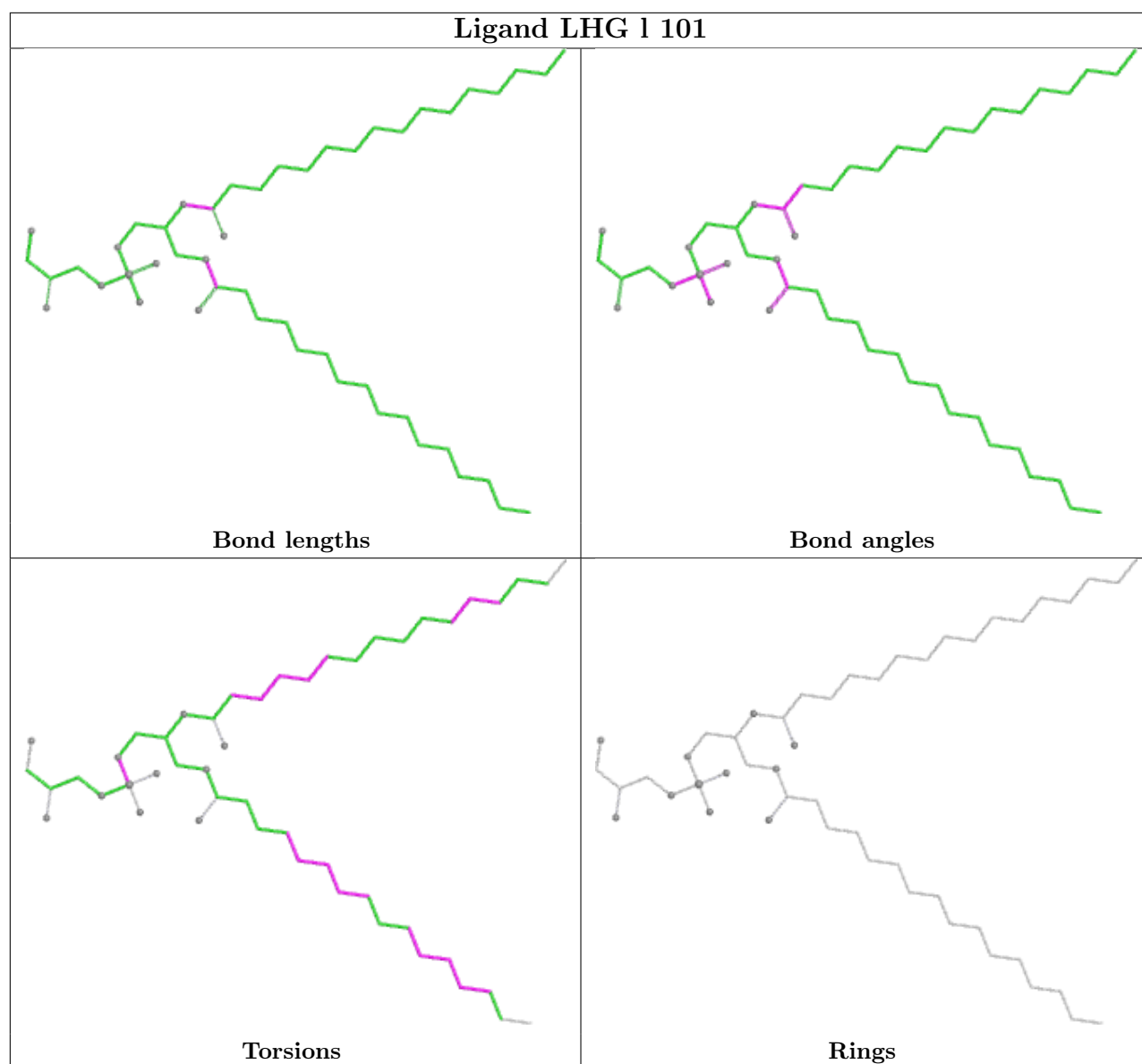
Ligand LMG D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

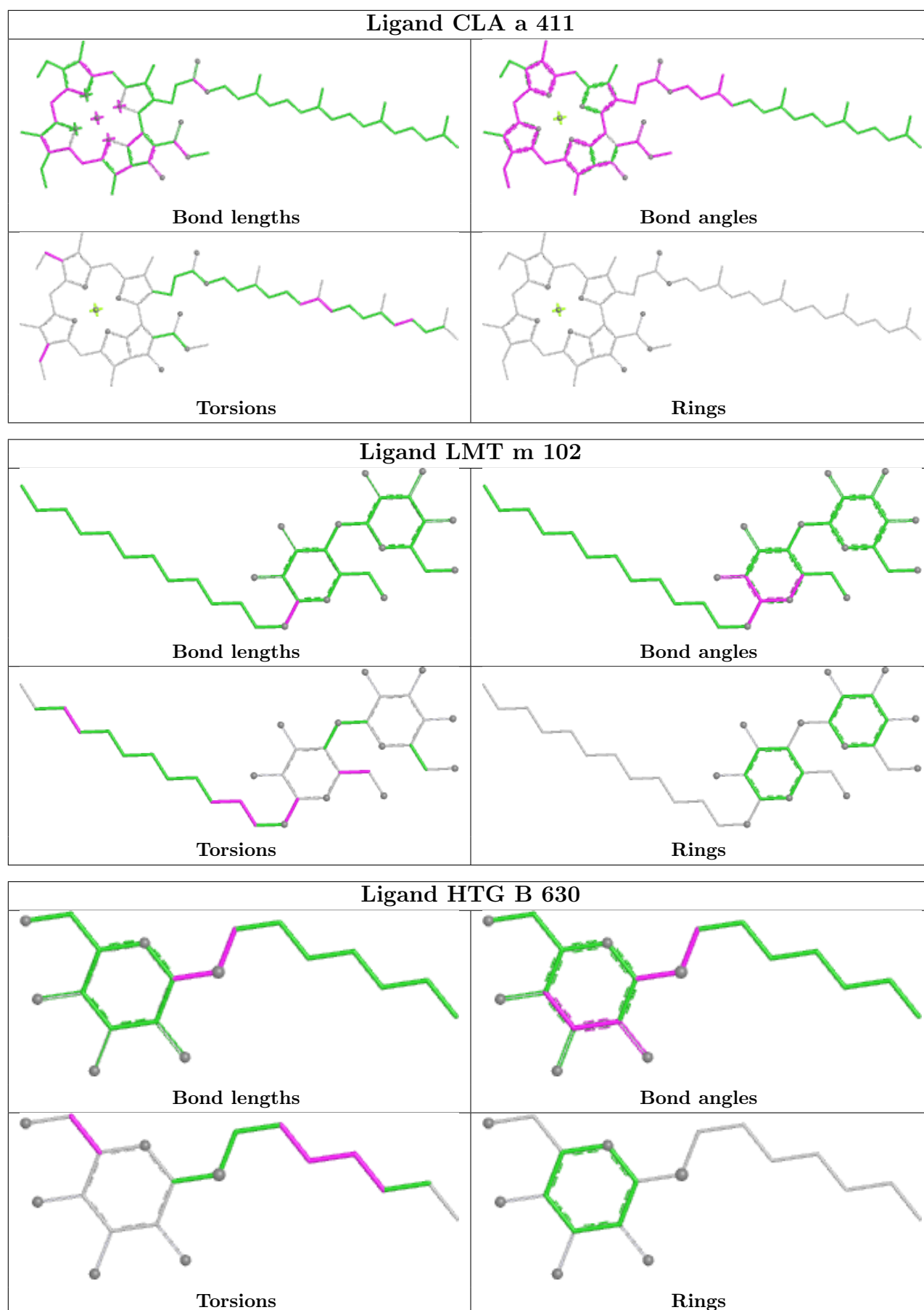


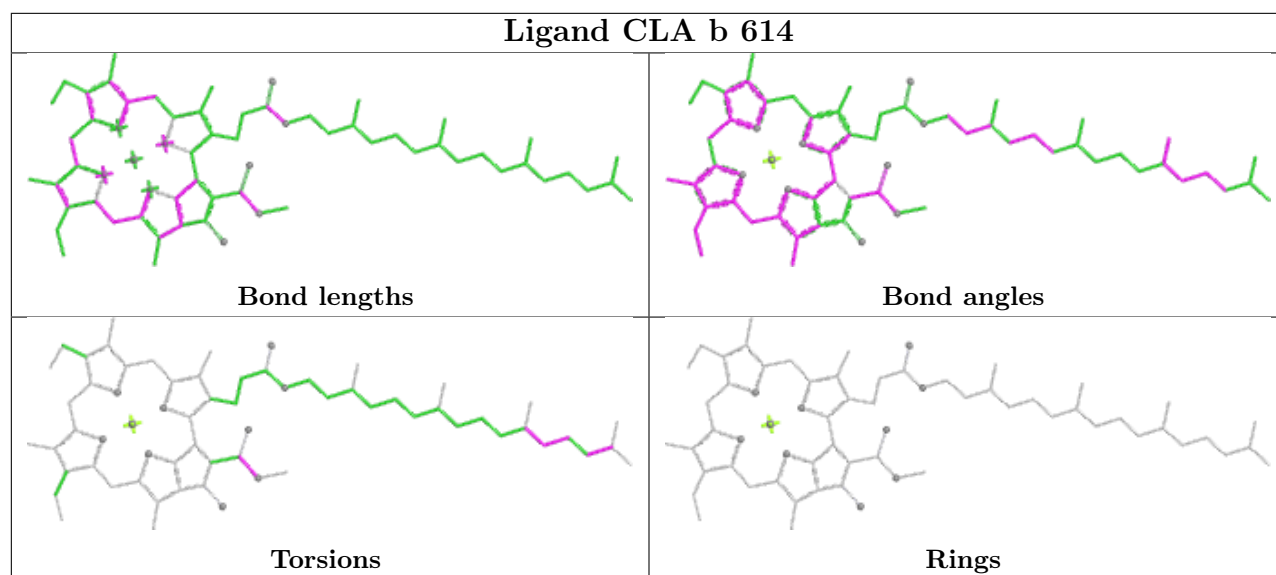
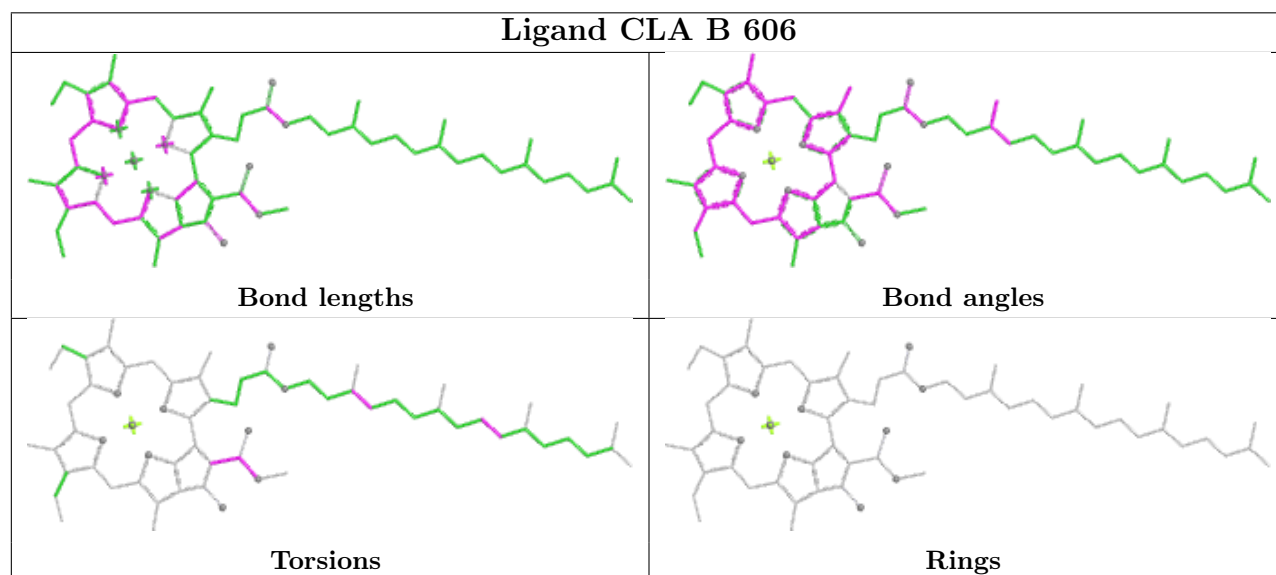
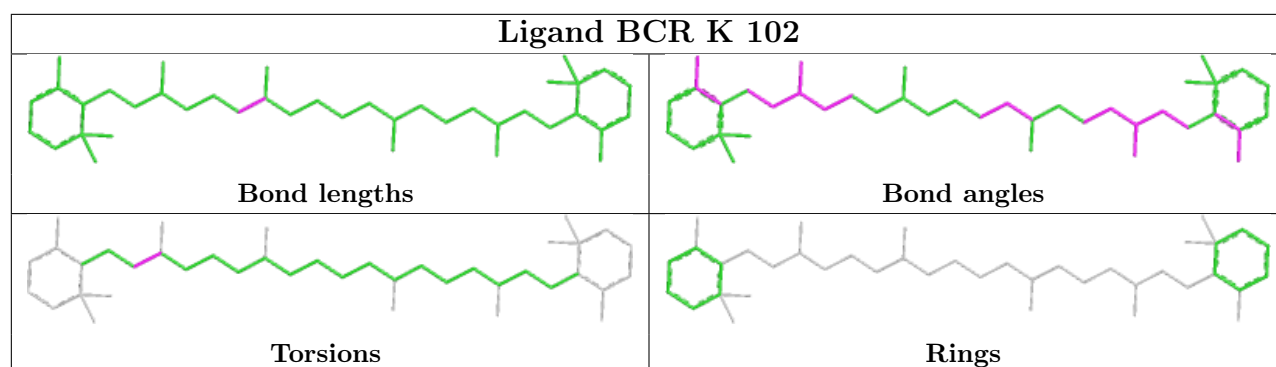


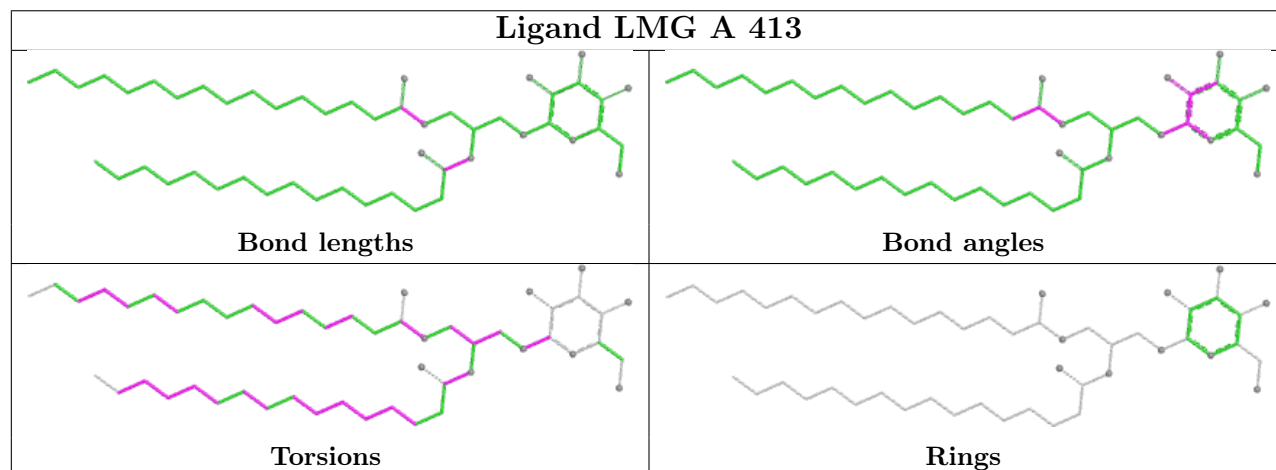
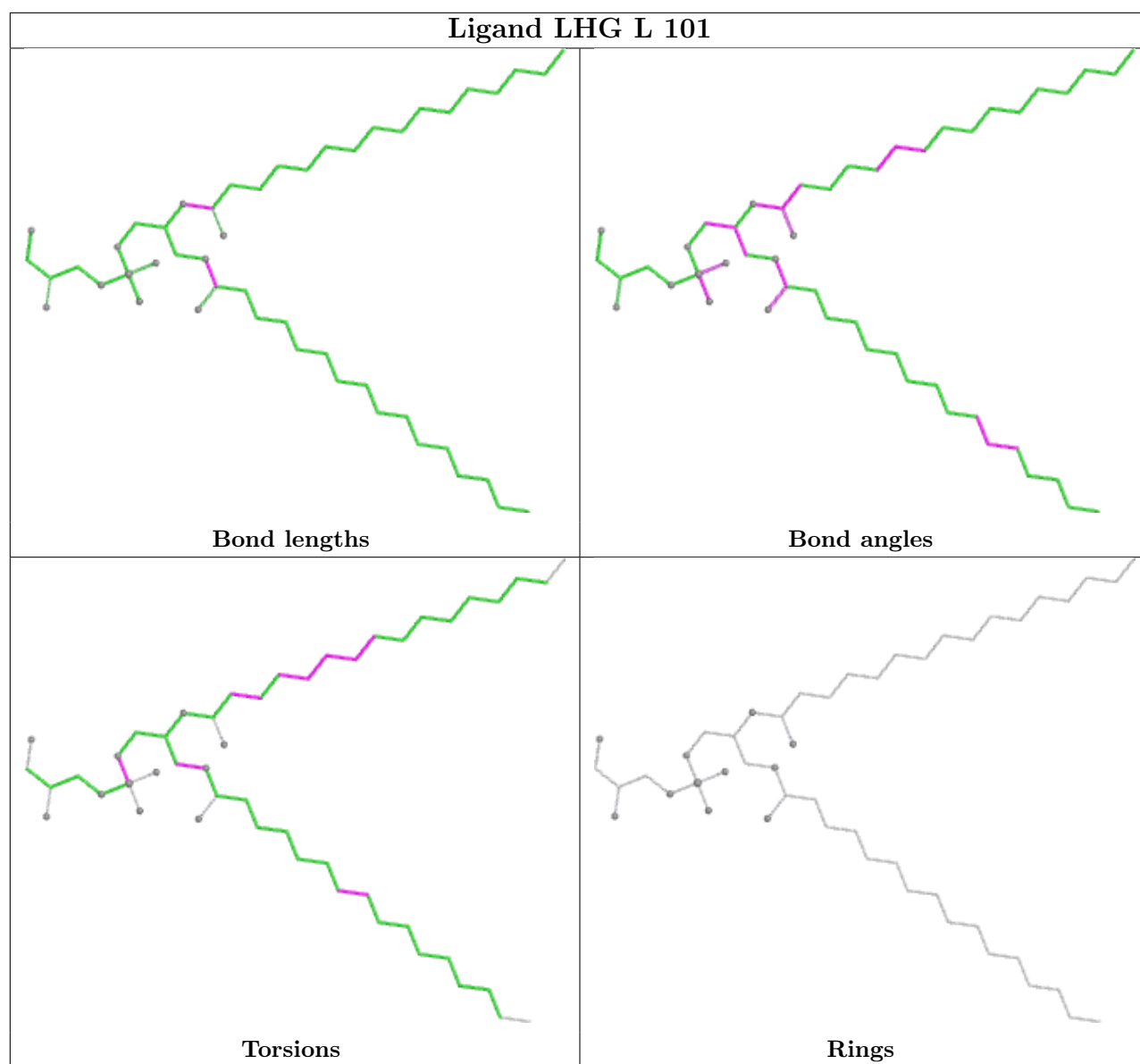


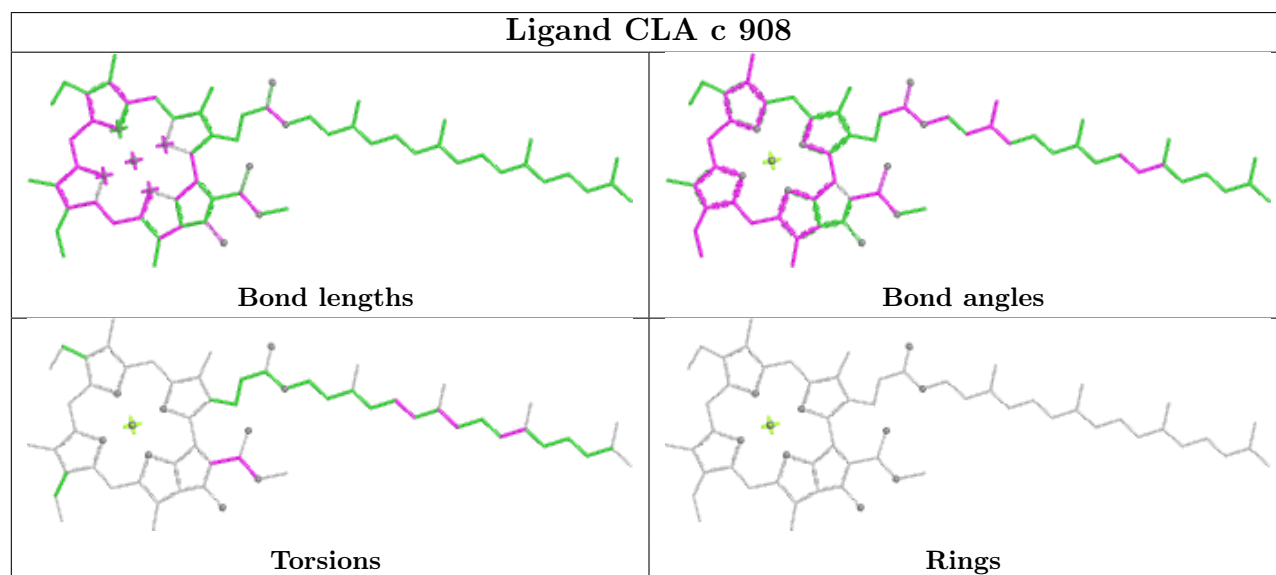
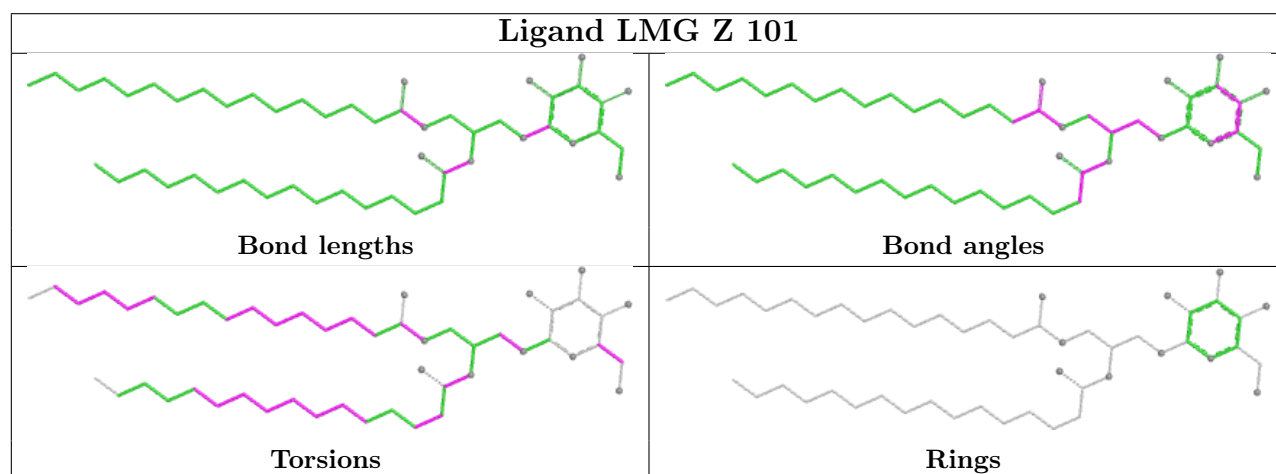
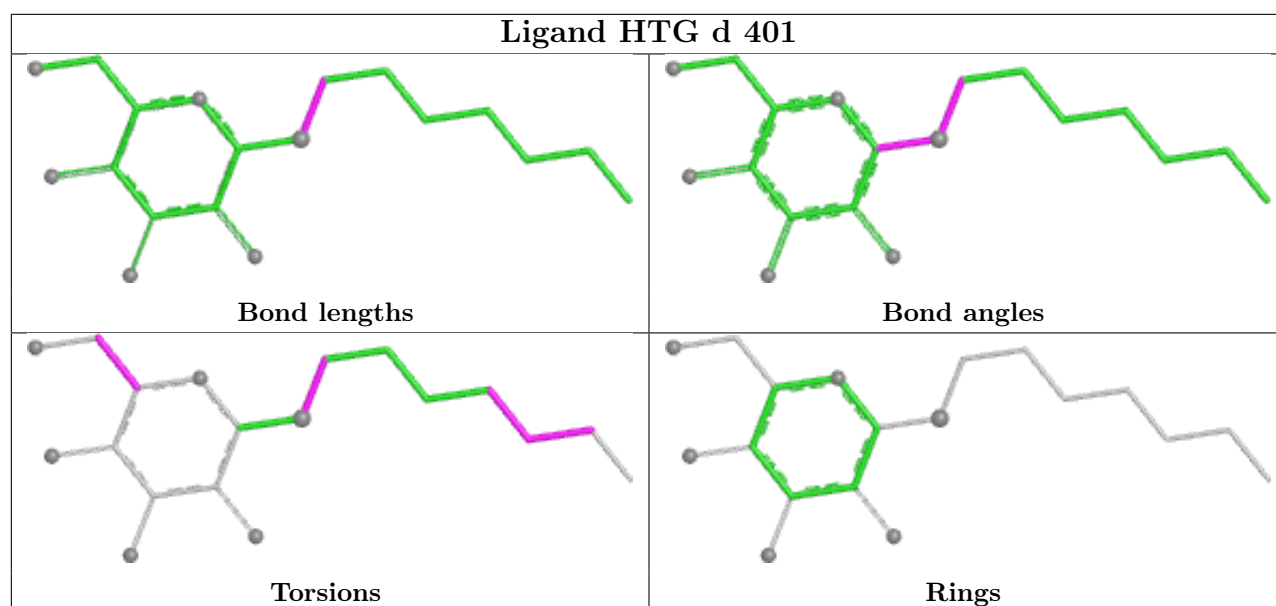


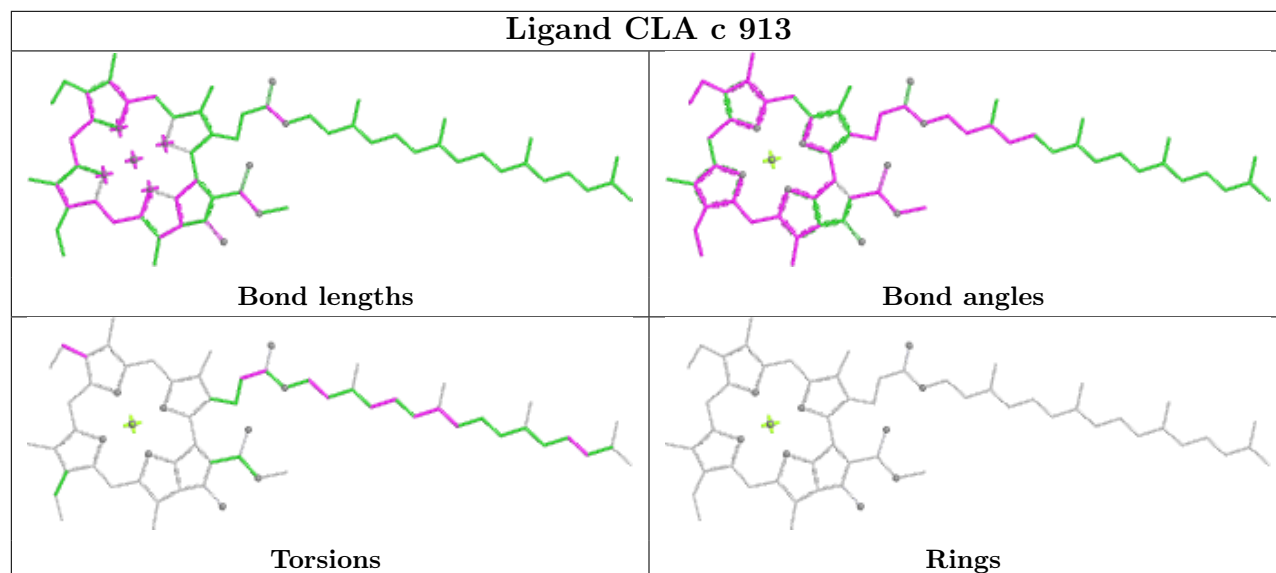
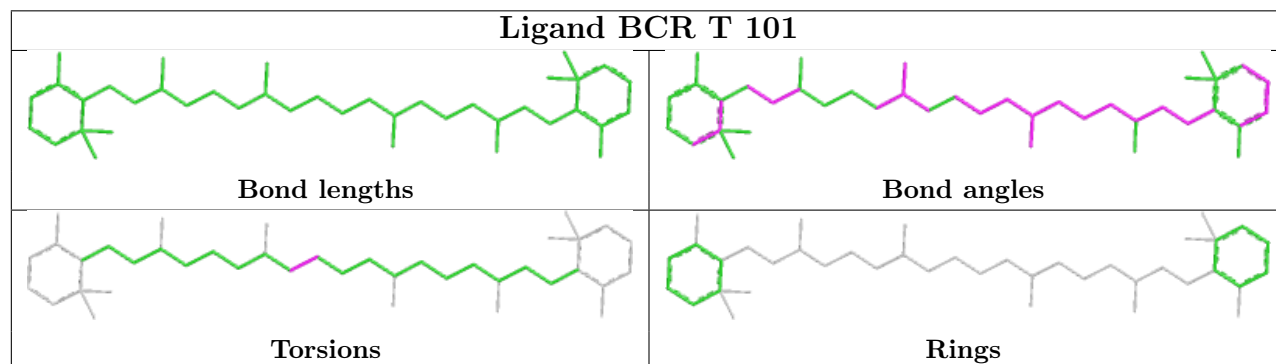
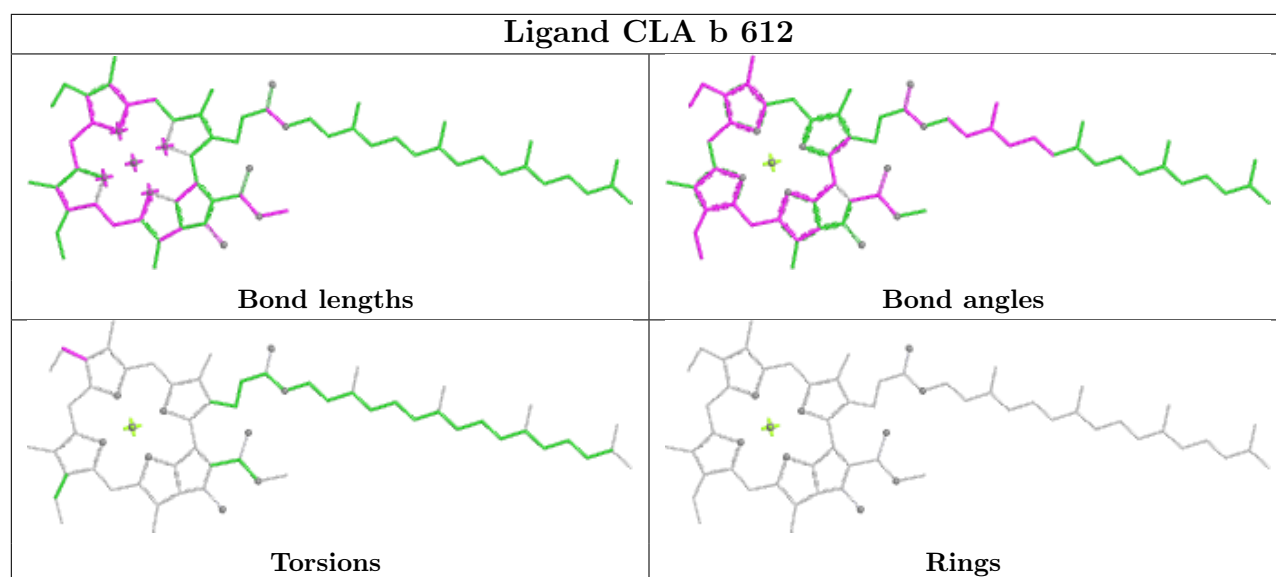


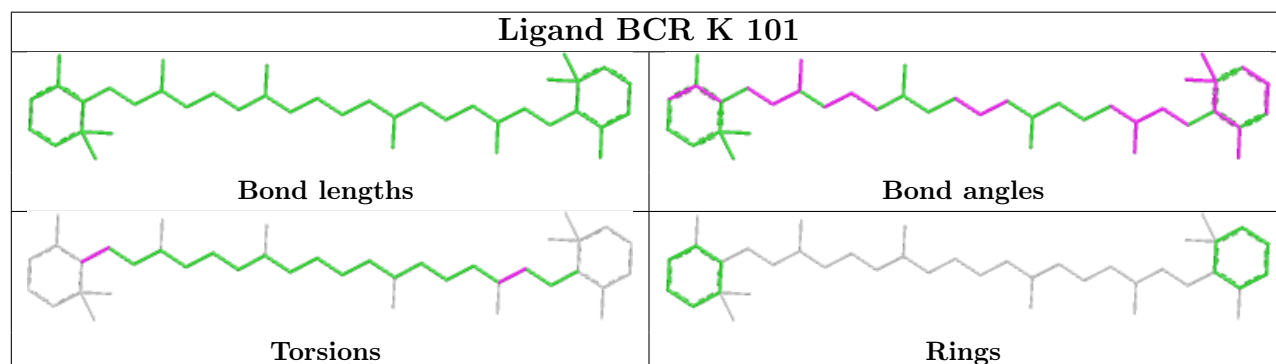
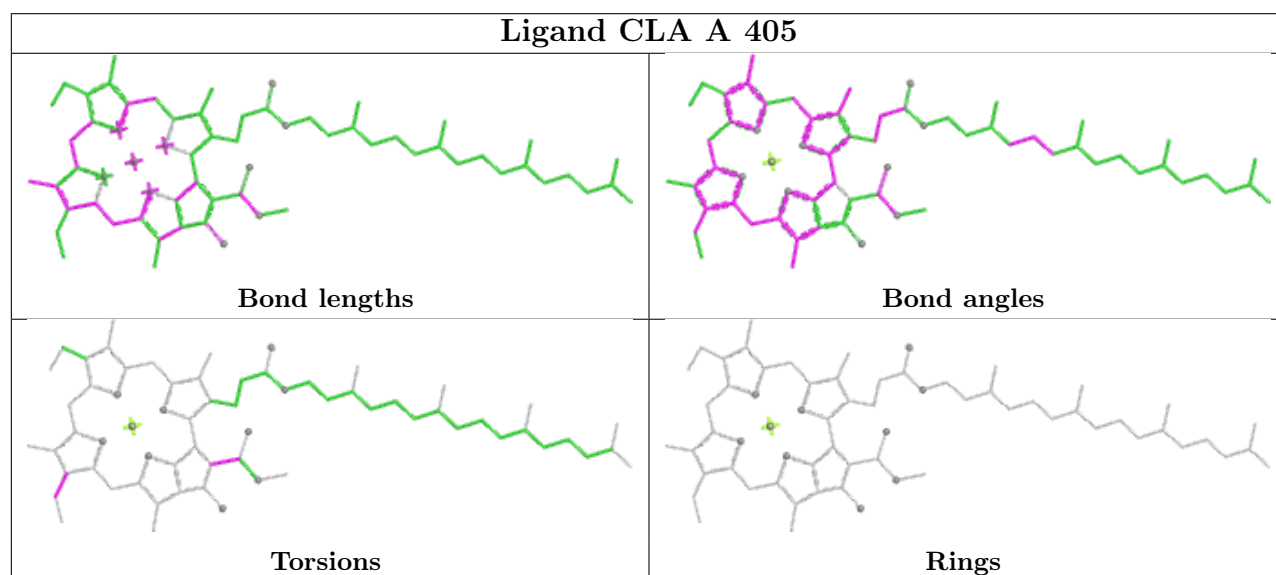
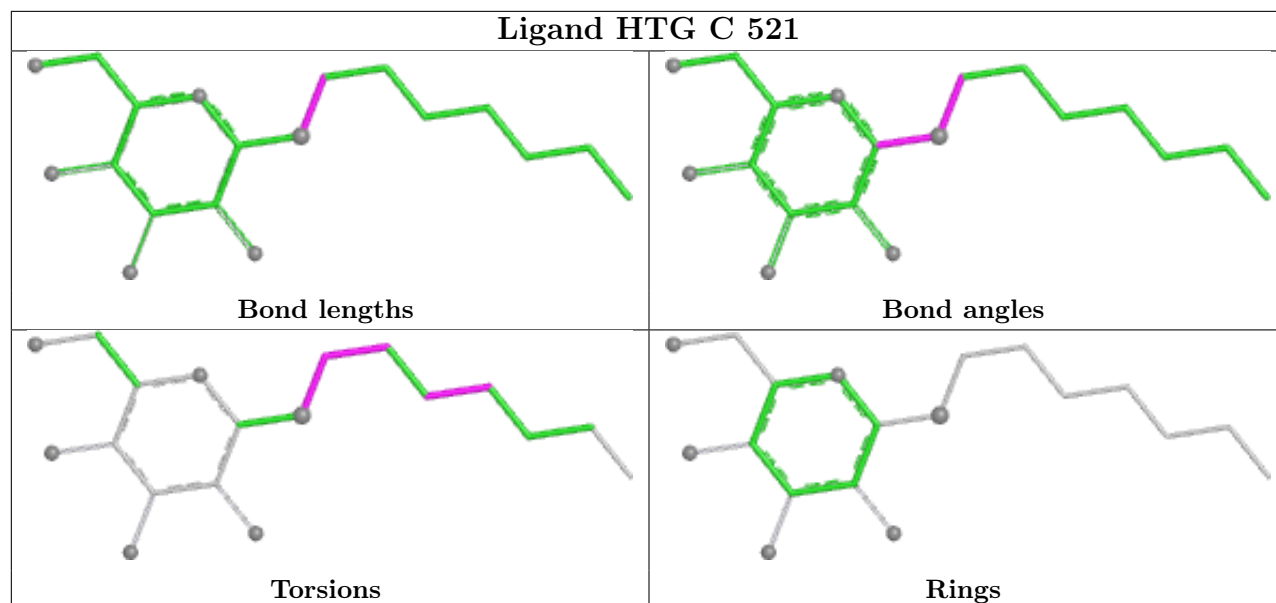


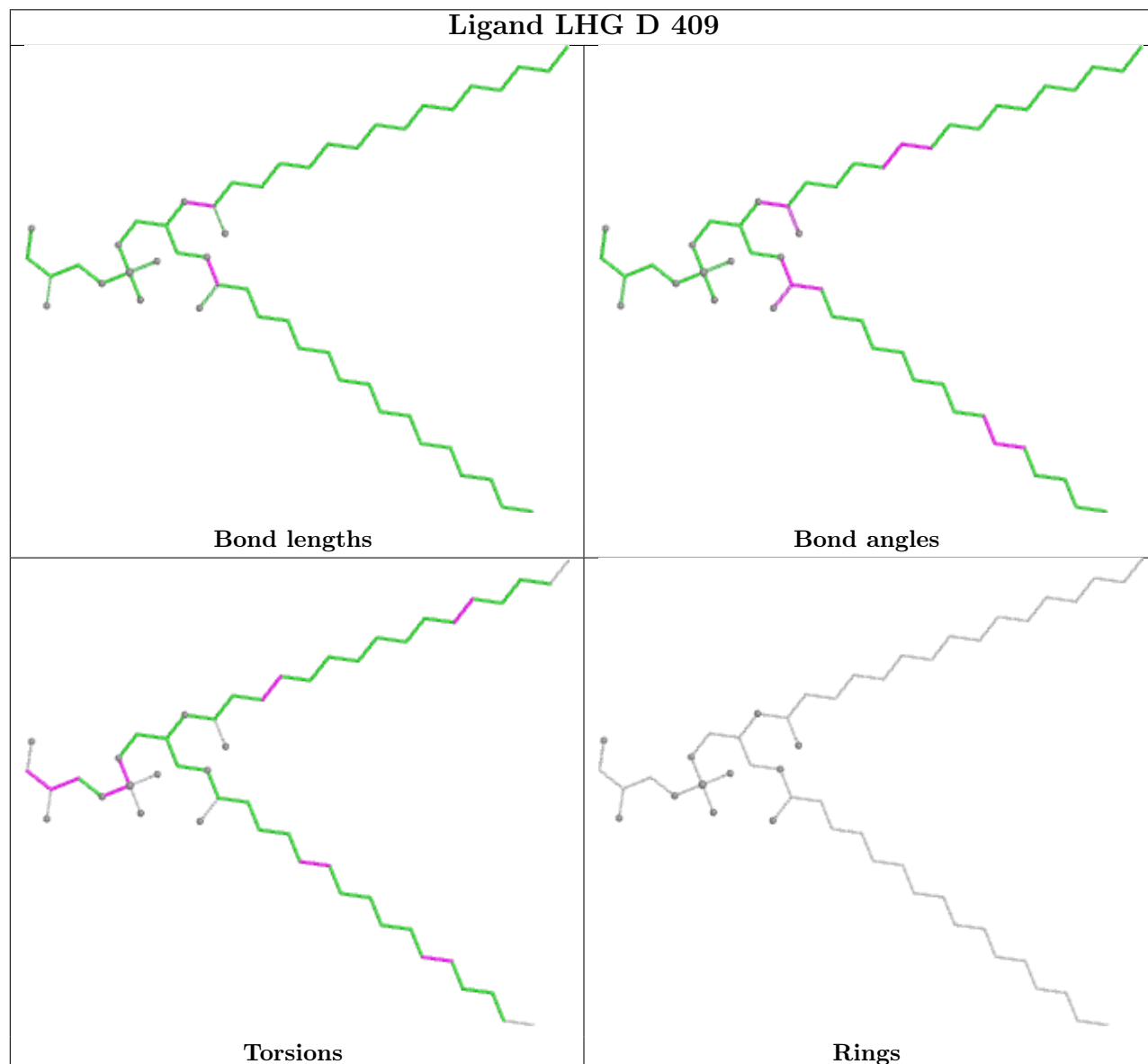
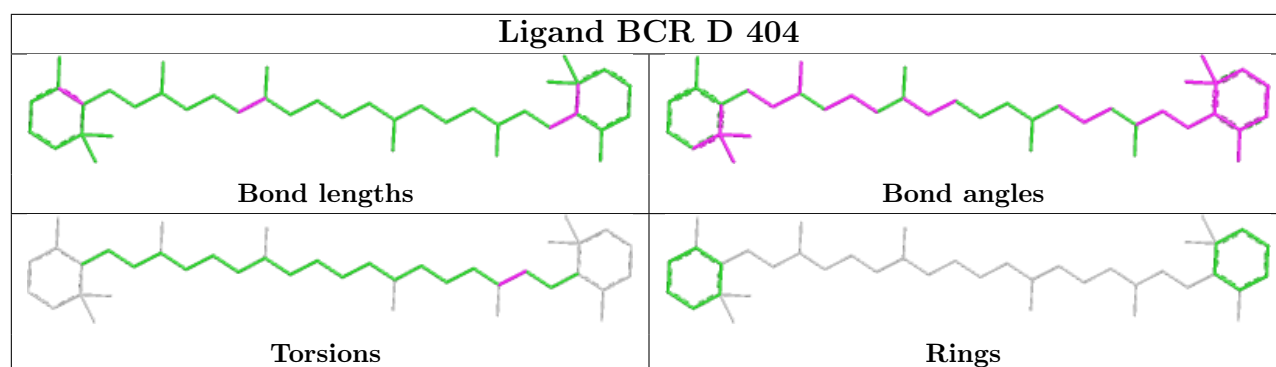


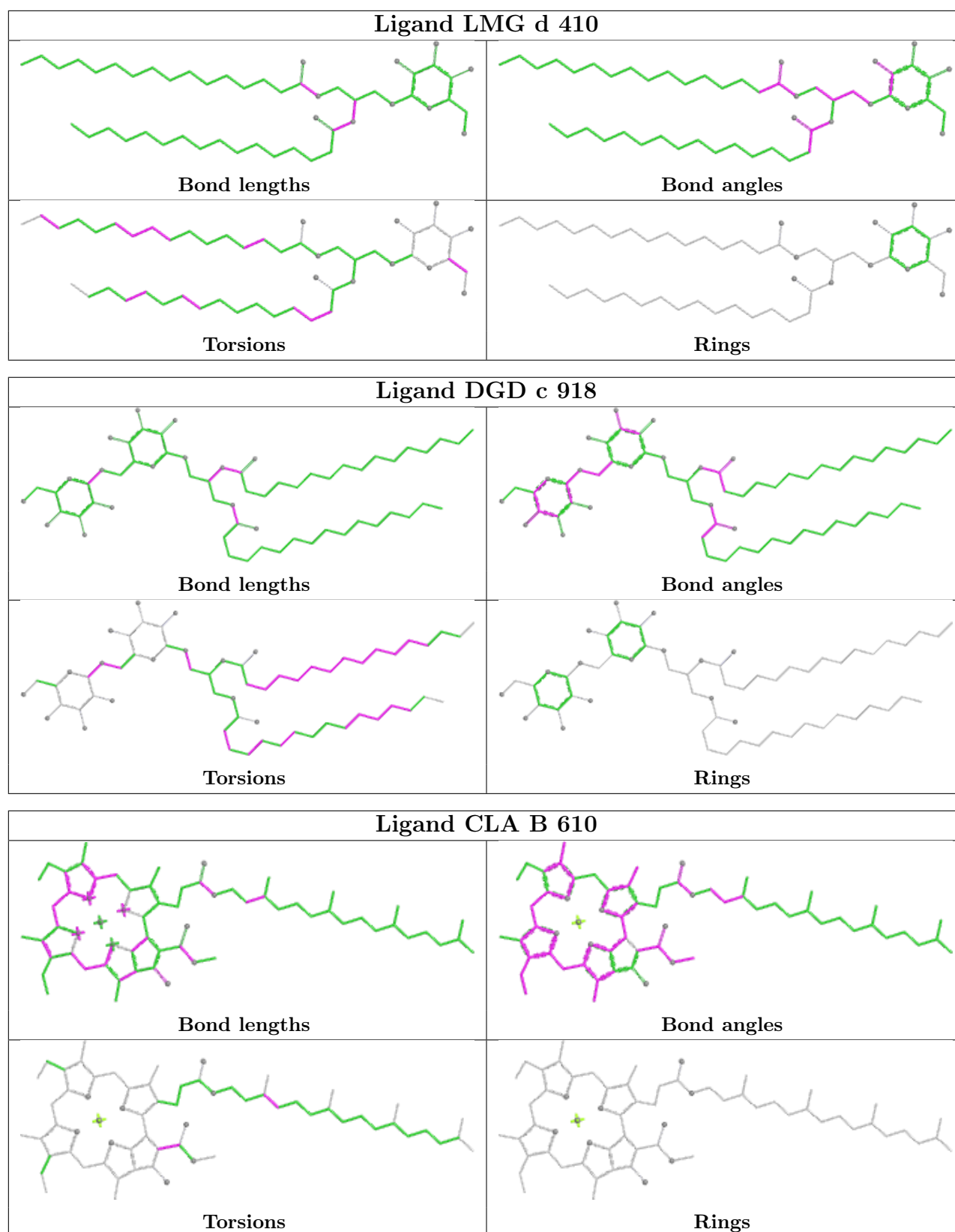


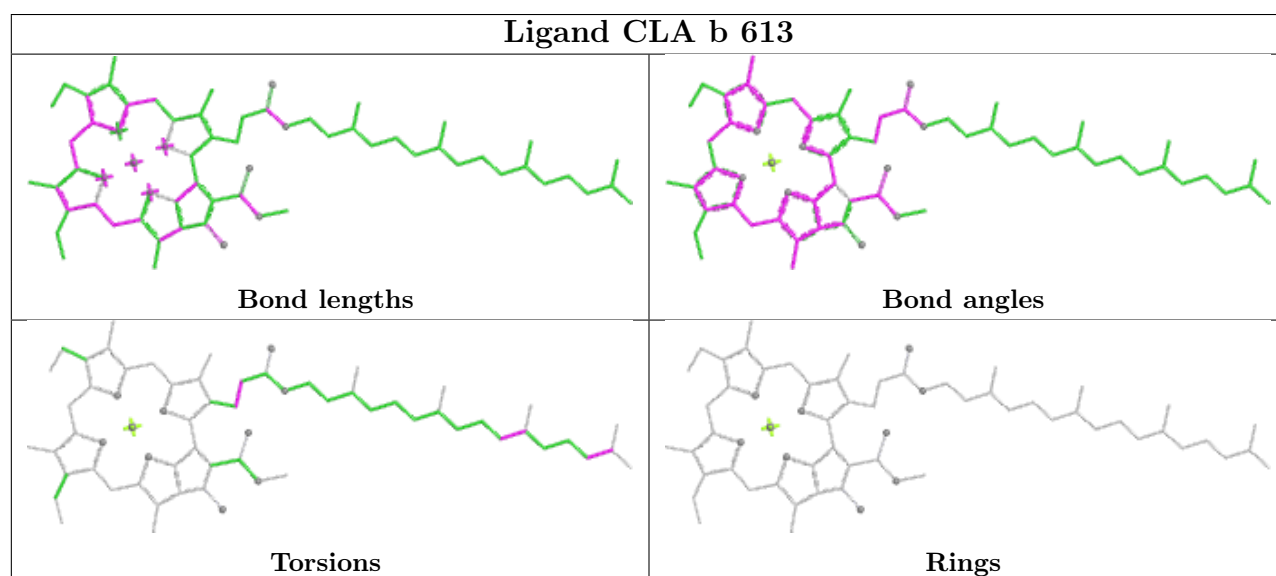
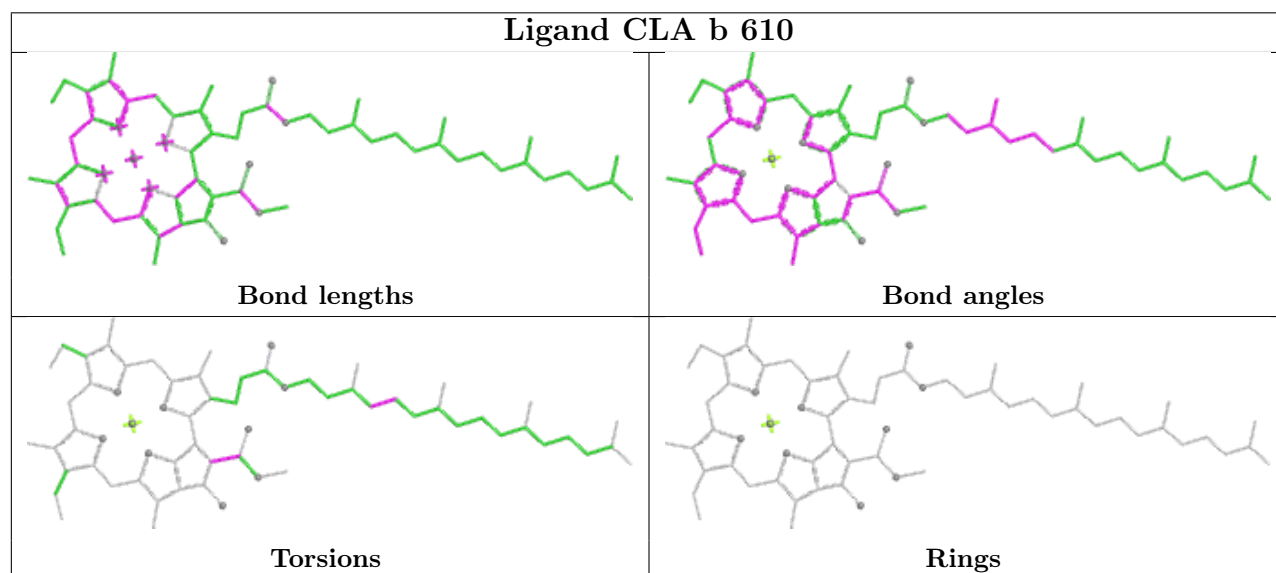
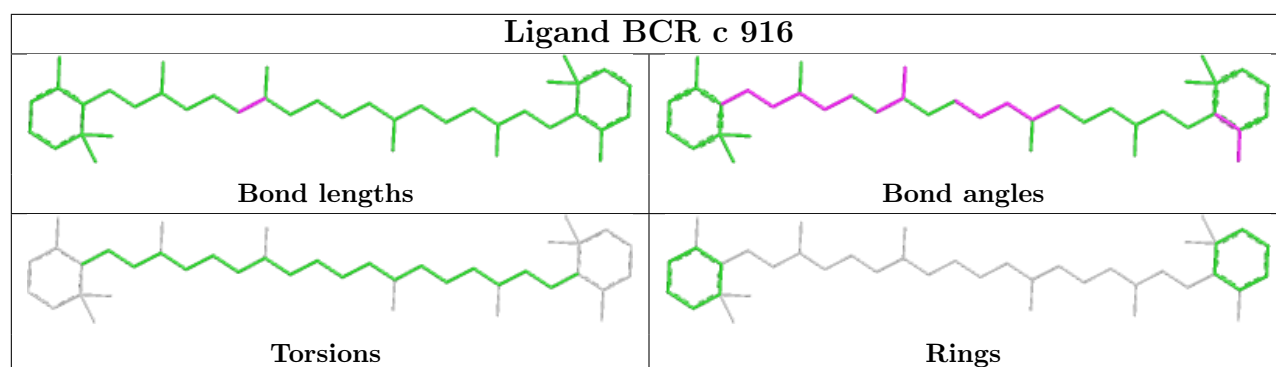


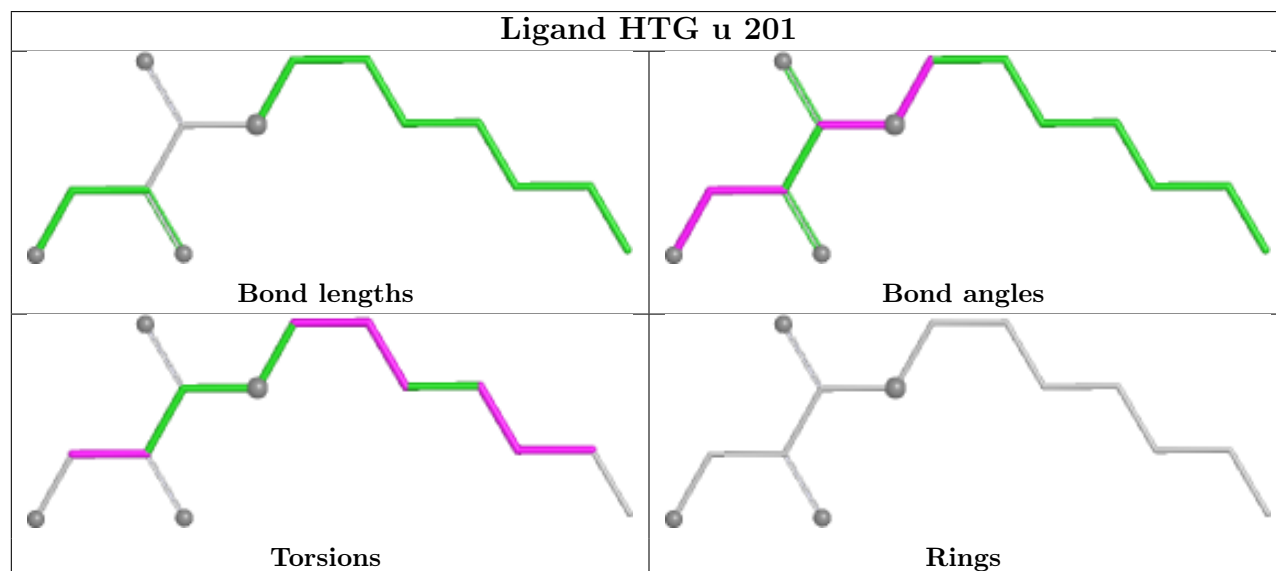
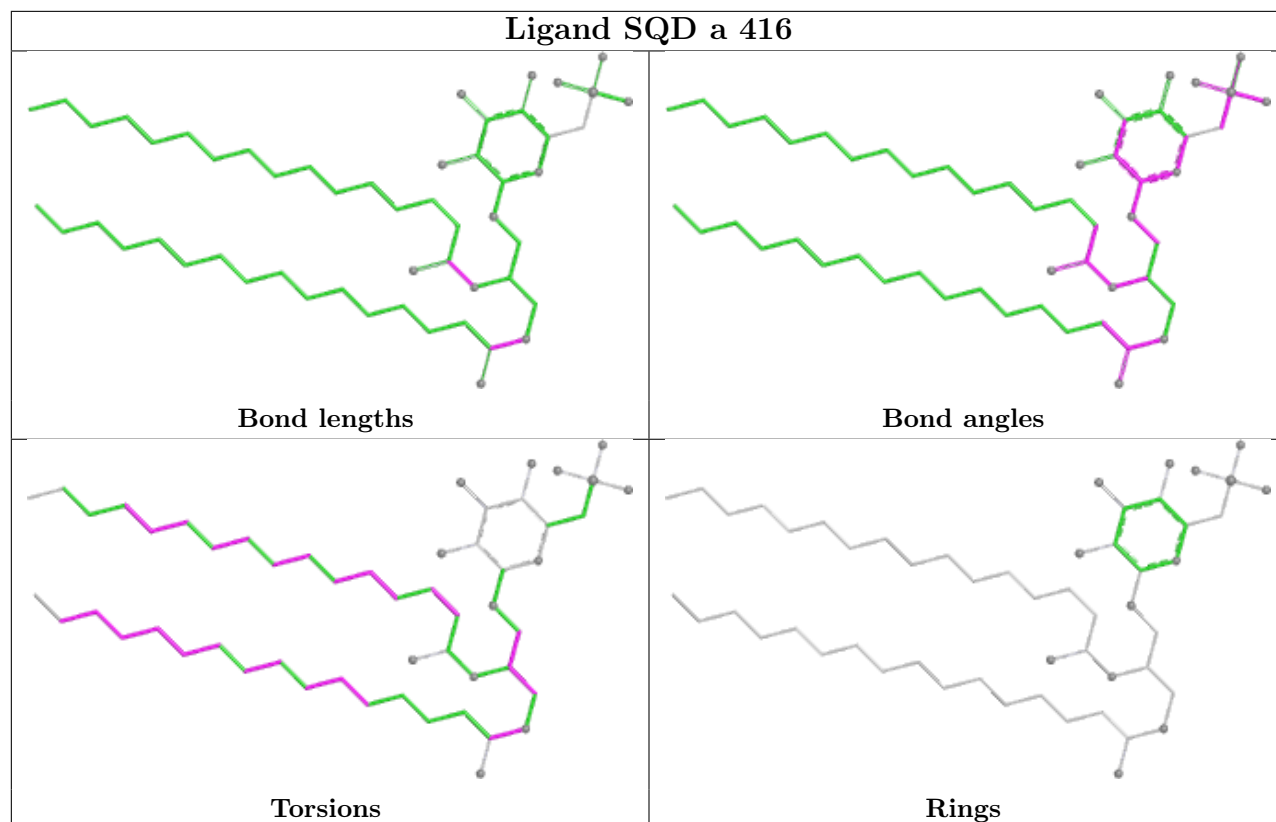


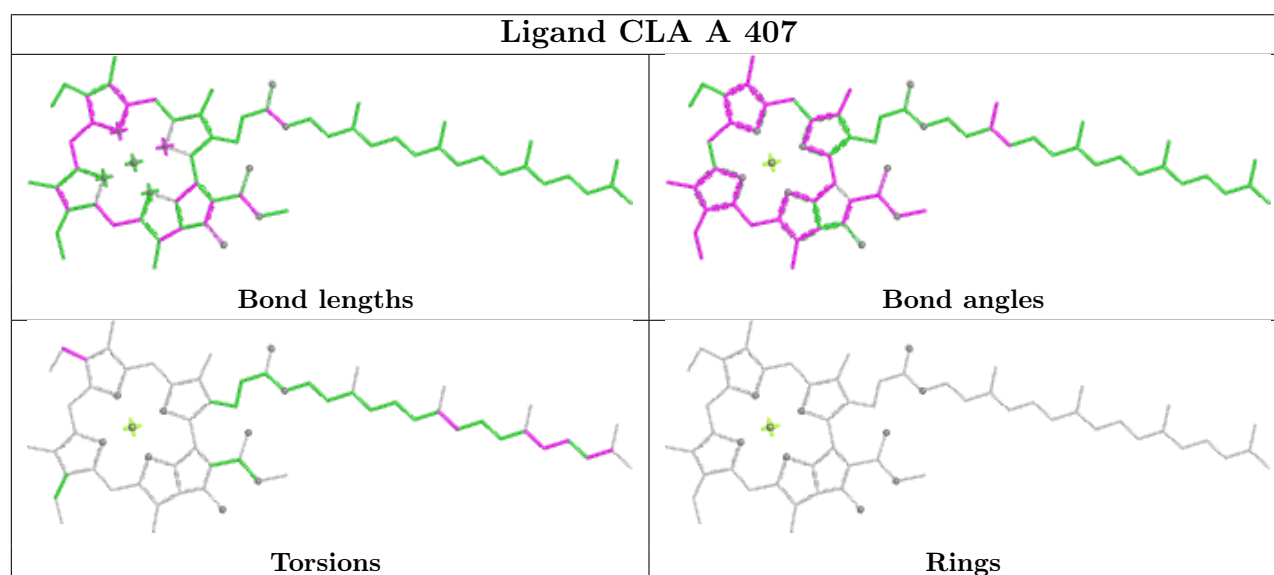
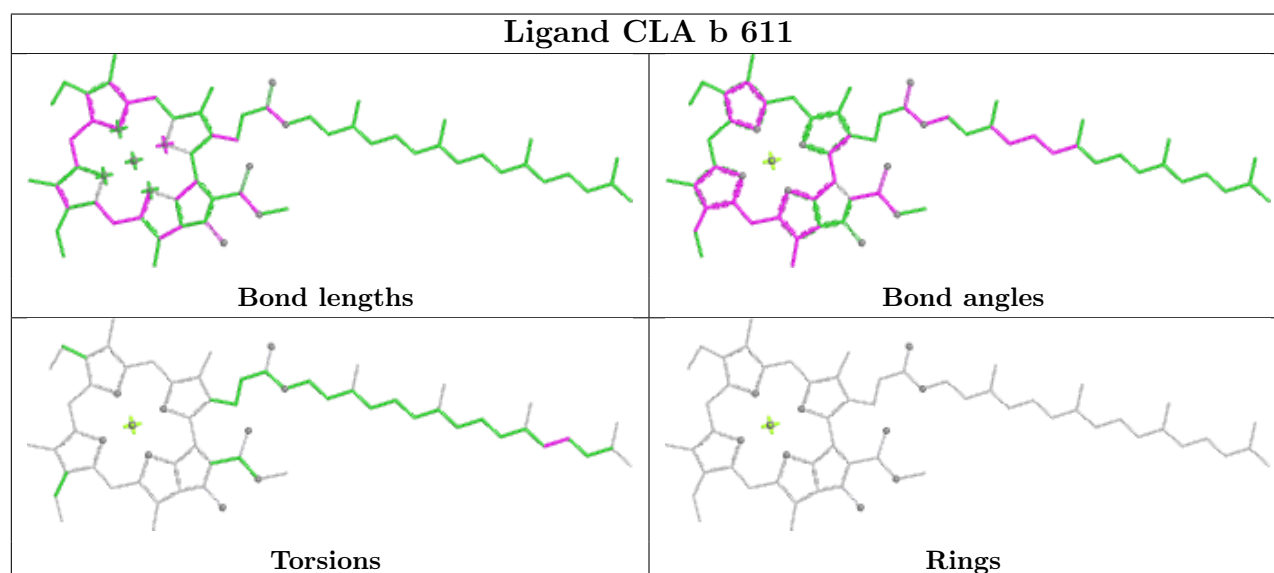
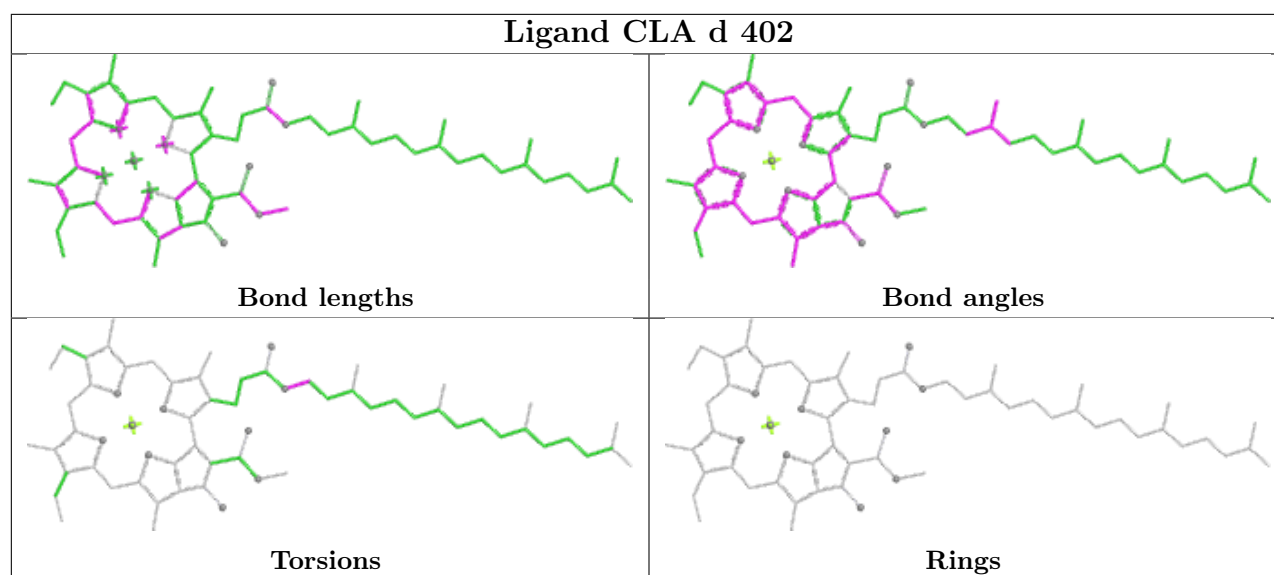


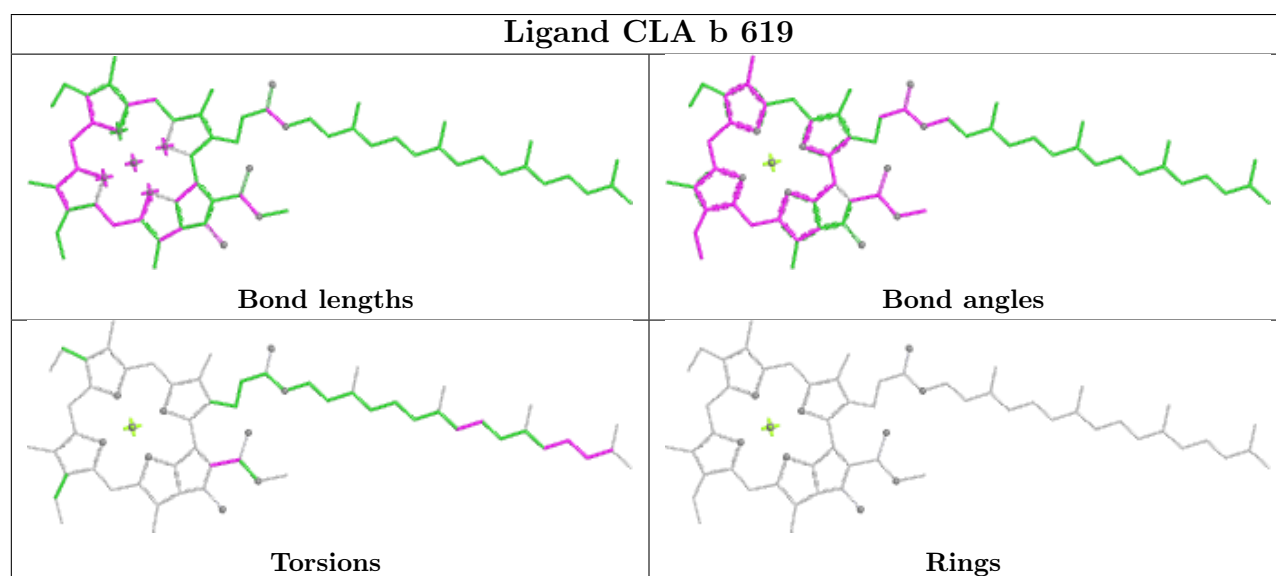
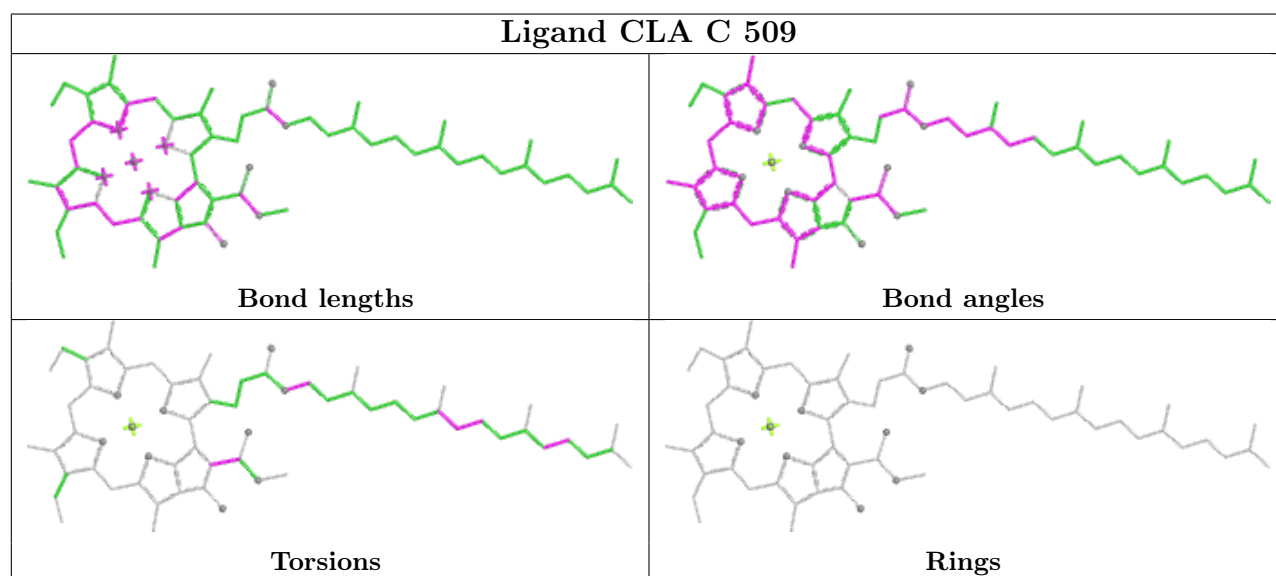
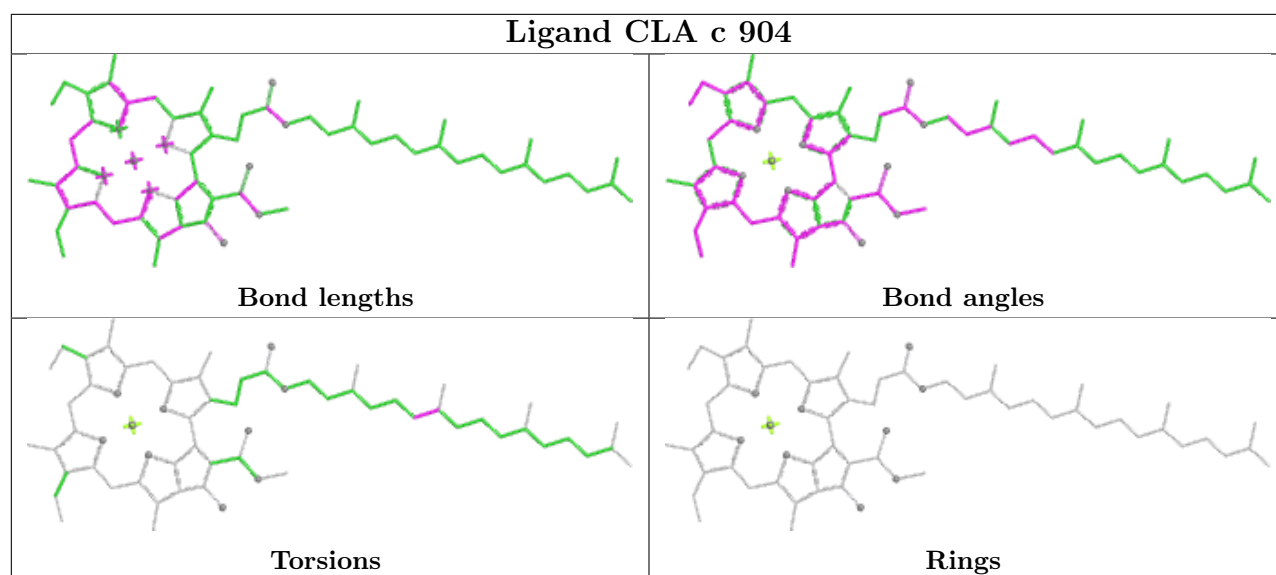


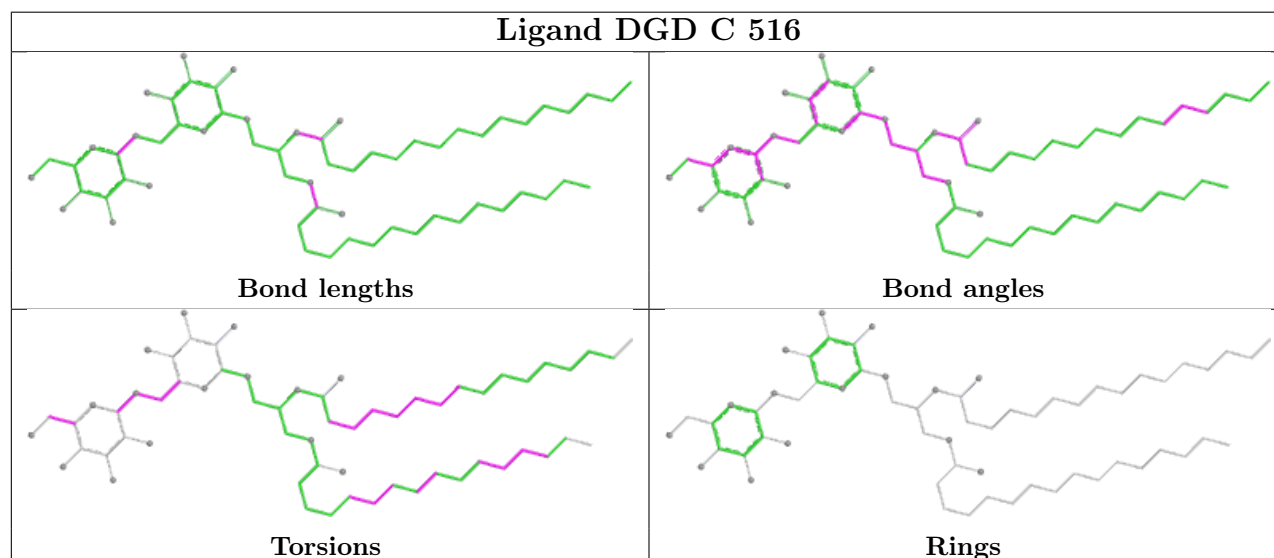
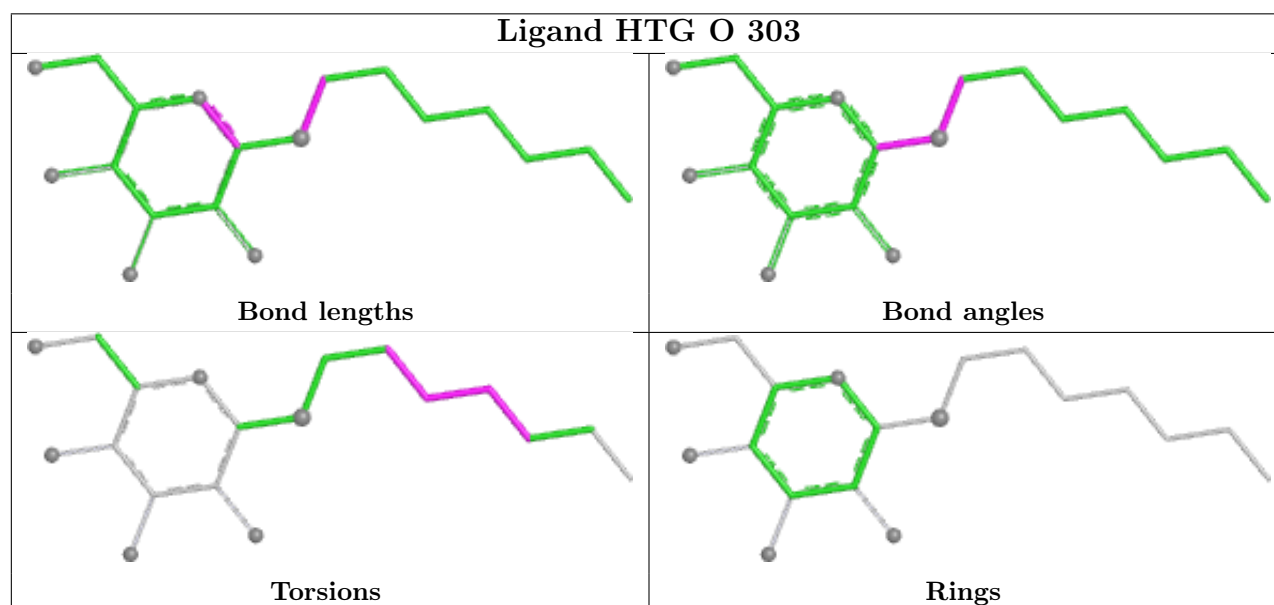
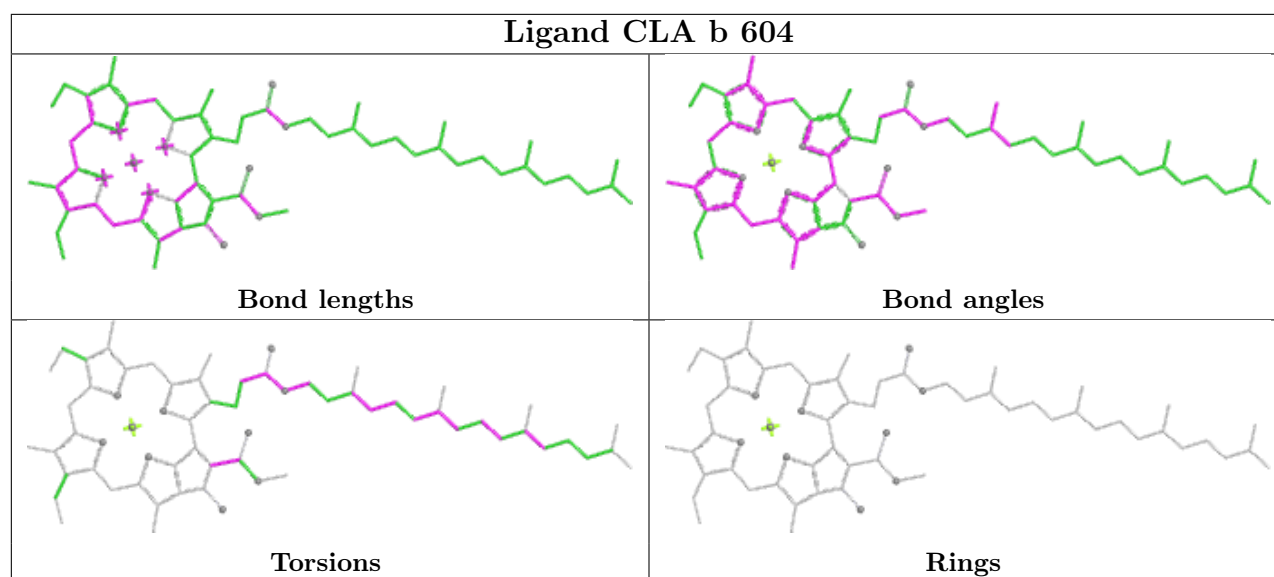


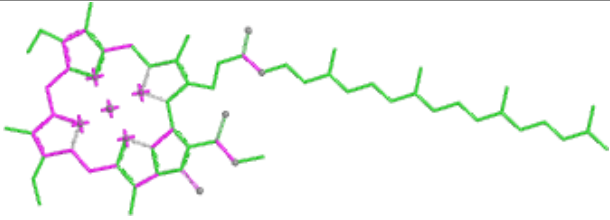
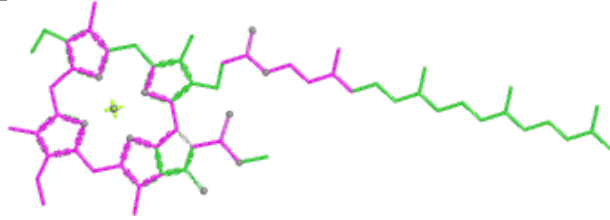
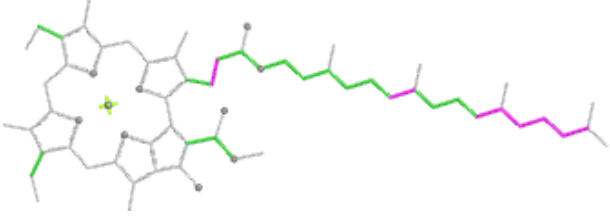
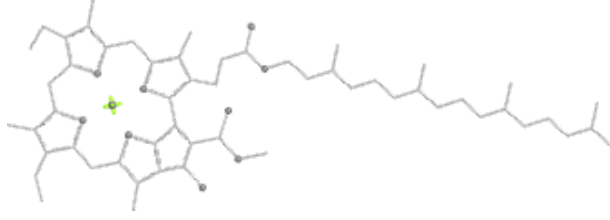
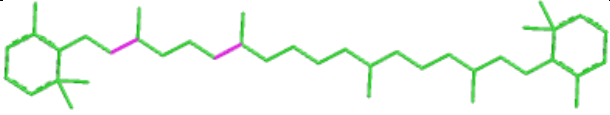
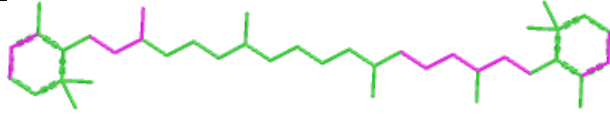
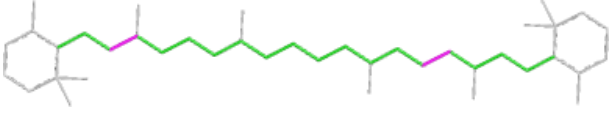
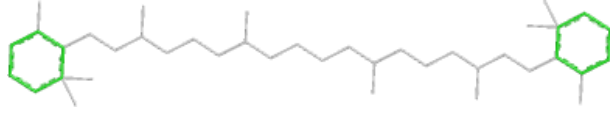
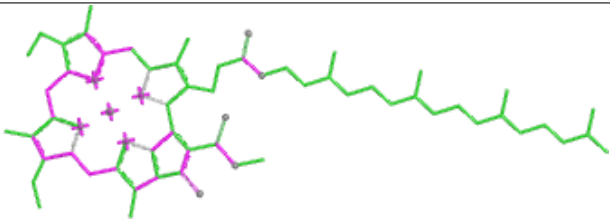
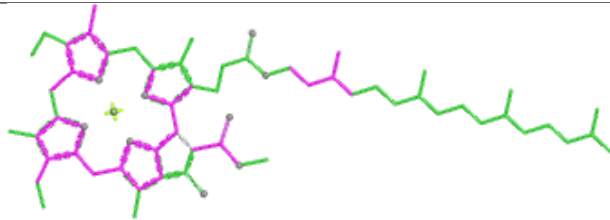
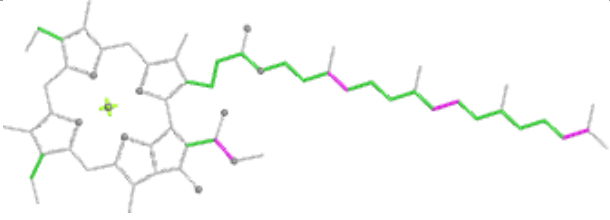
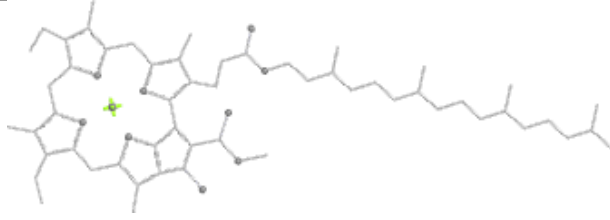


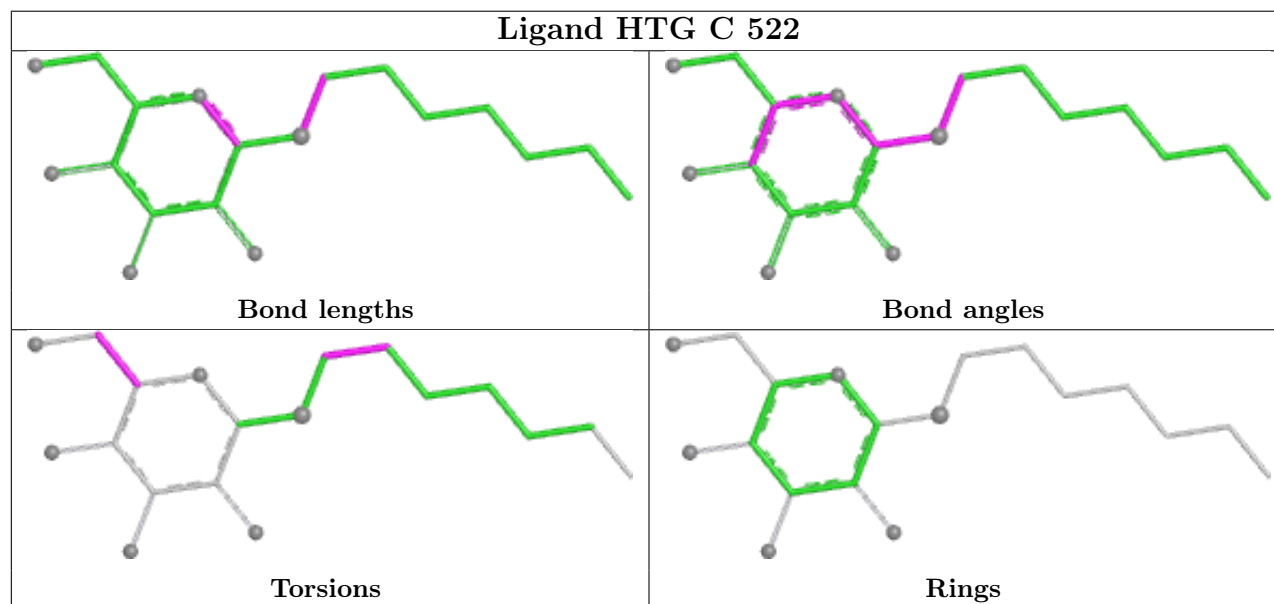
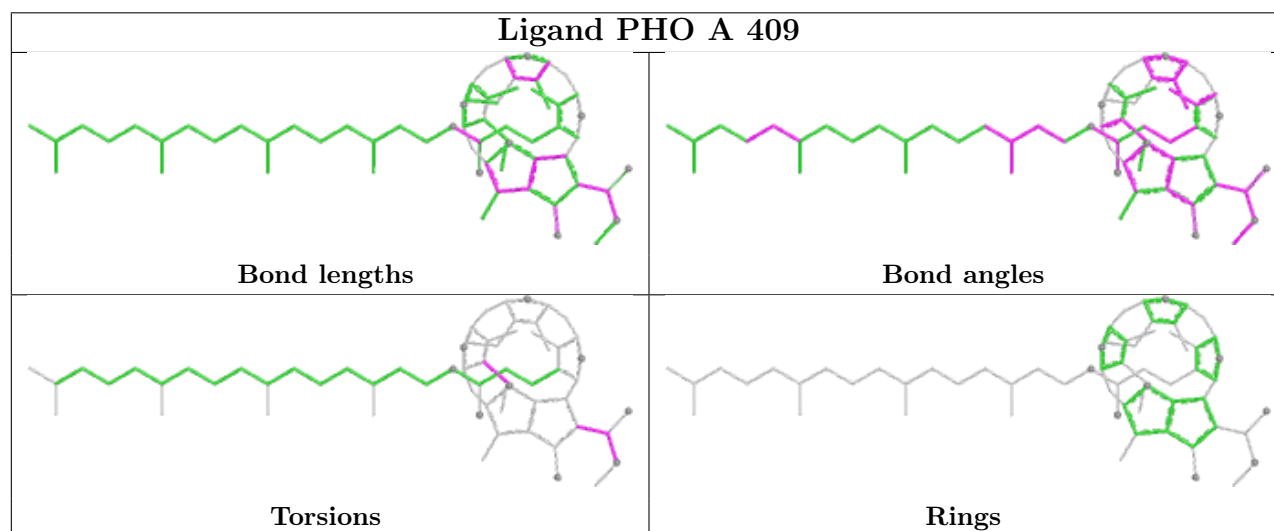
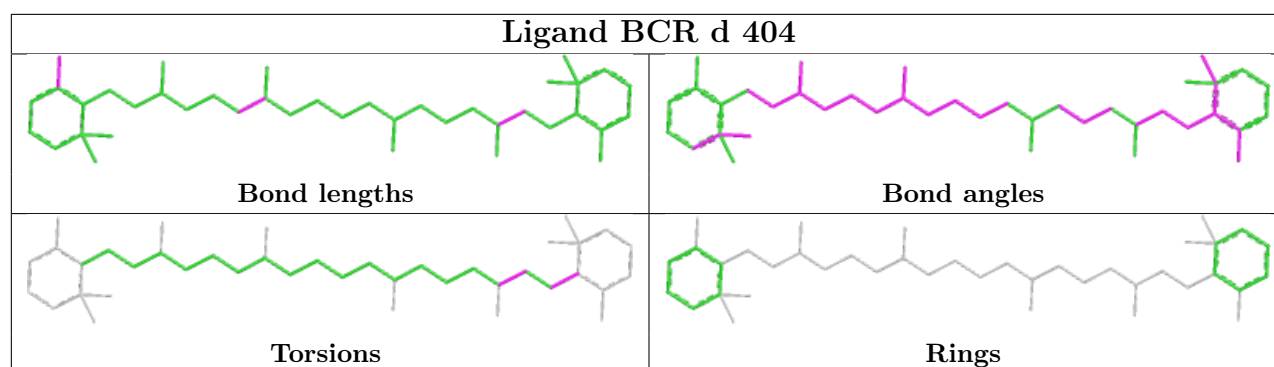


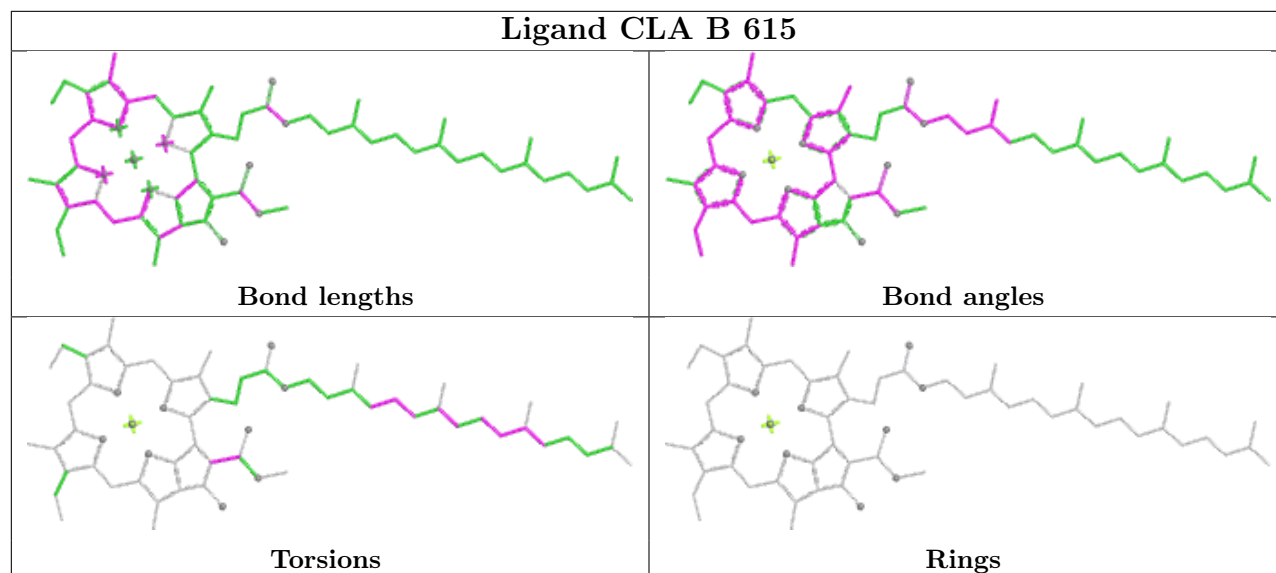
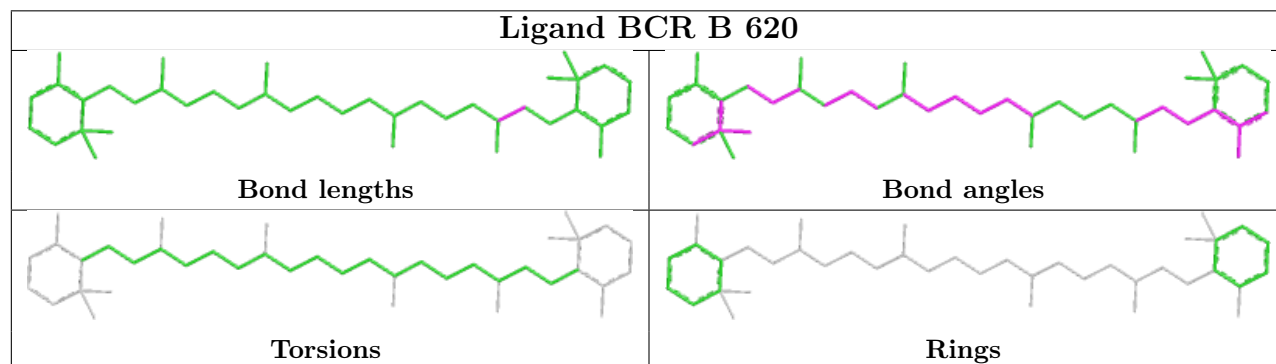
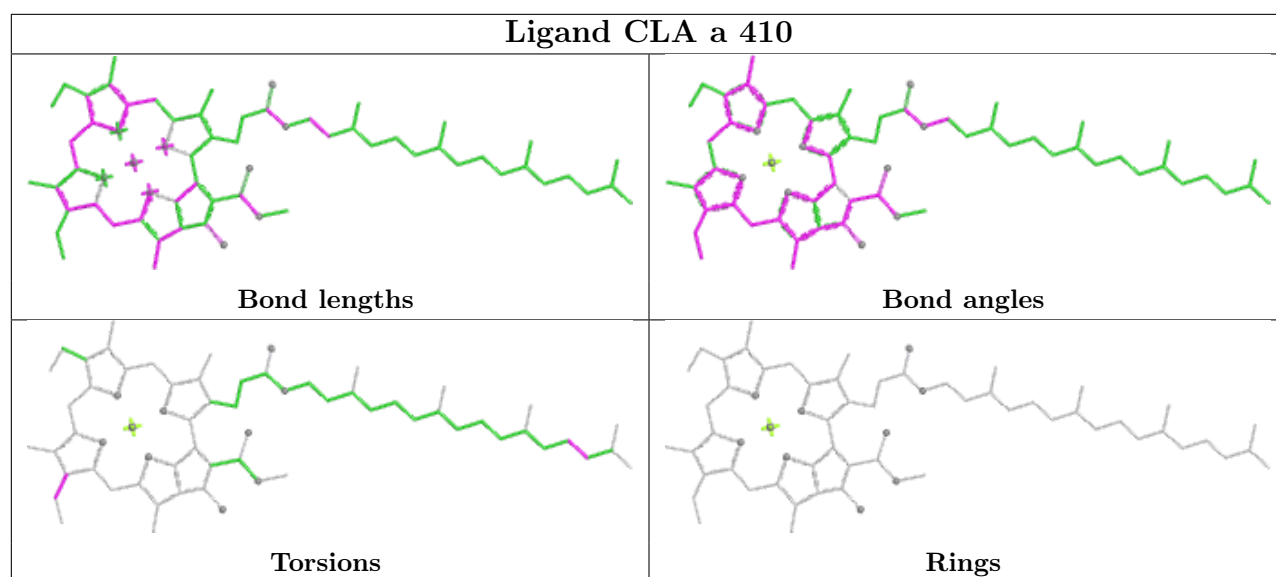




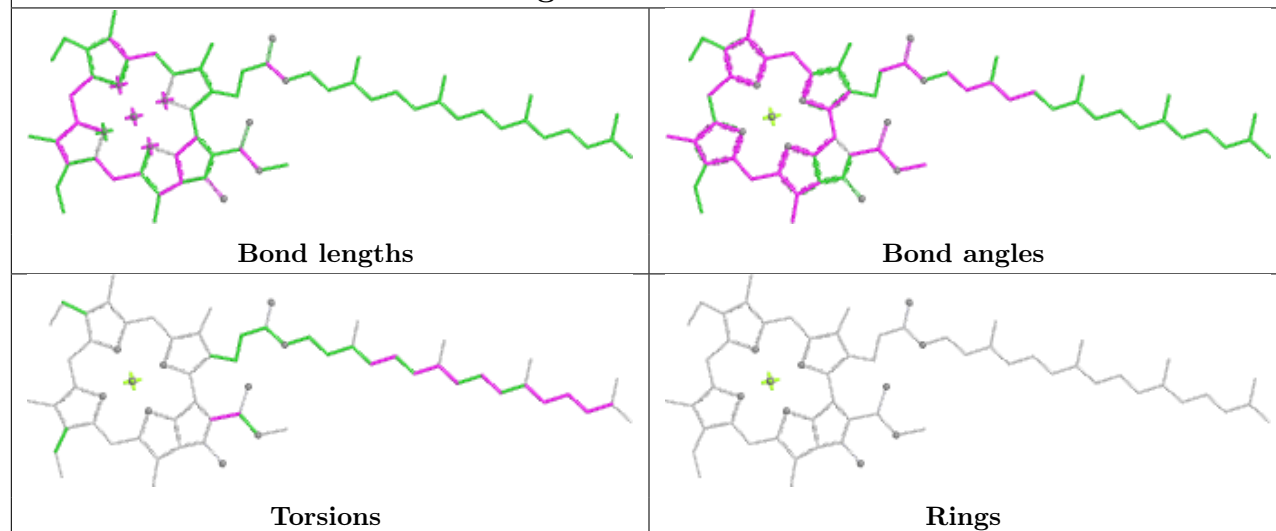


Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 911	
 Bond lengths	 Bond angles
 Torsions	 Rings

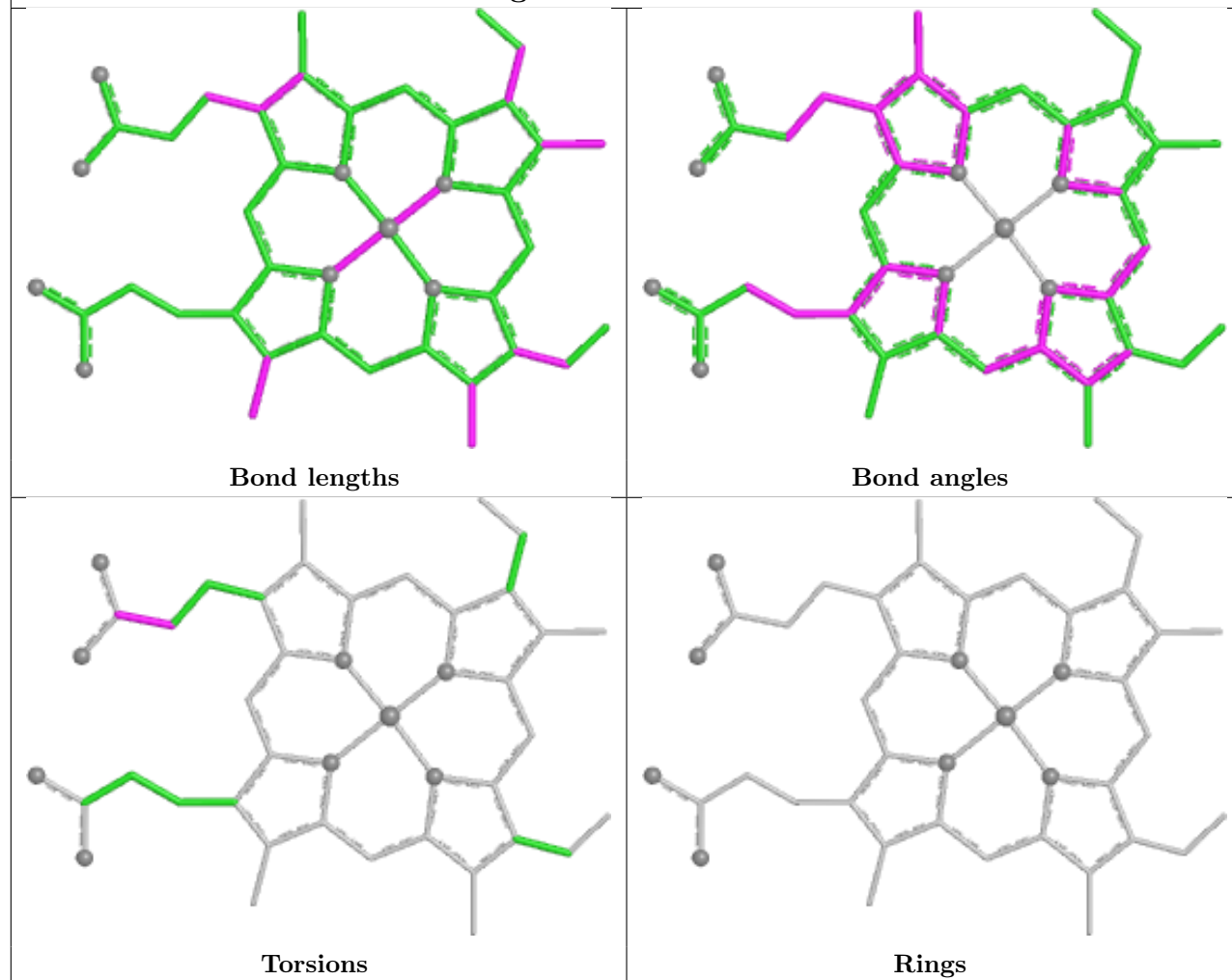


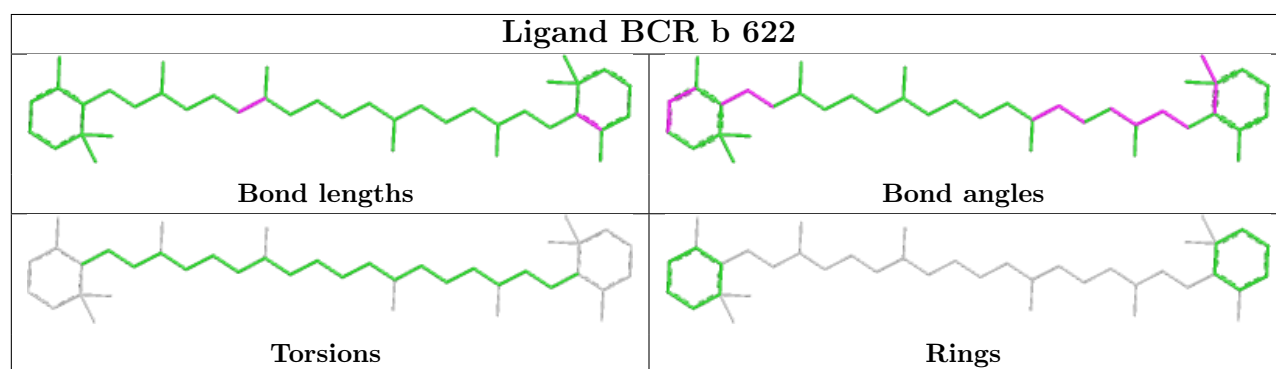
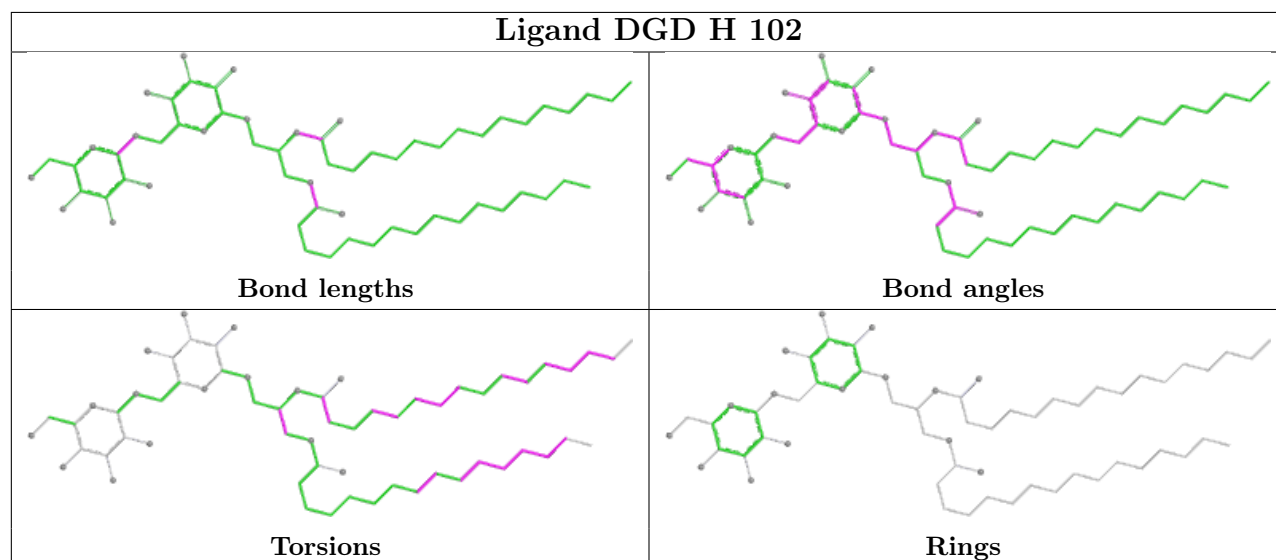
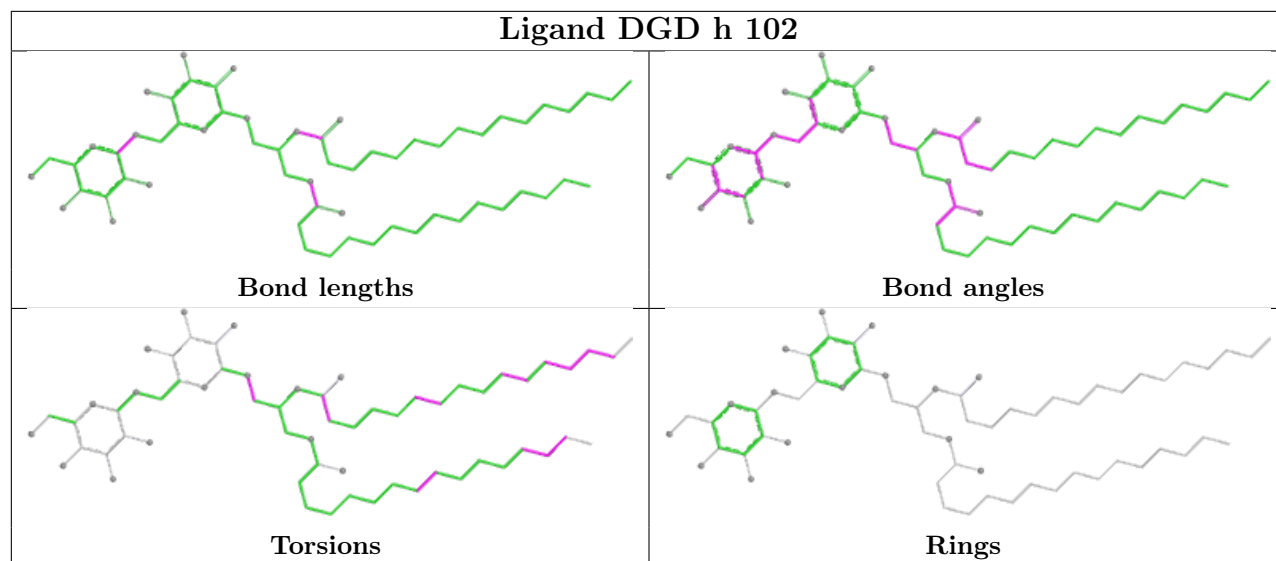


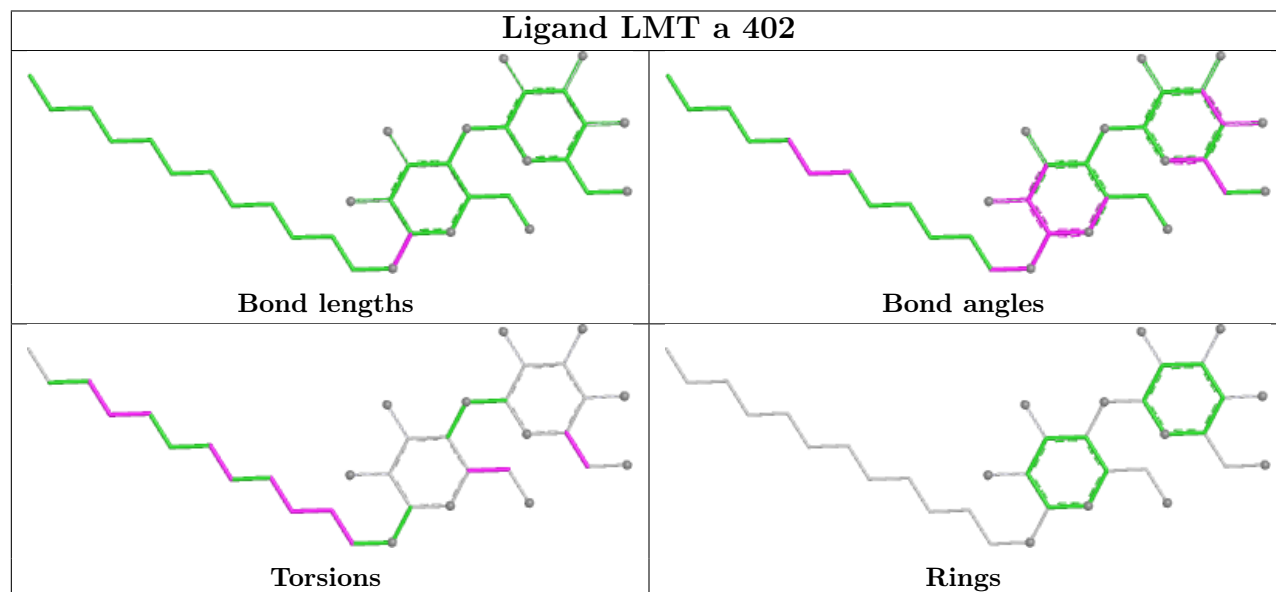
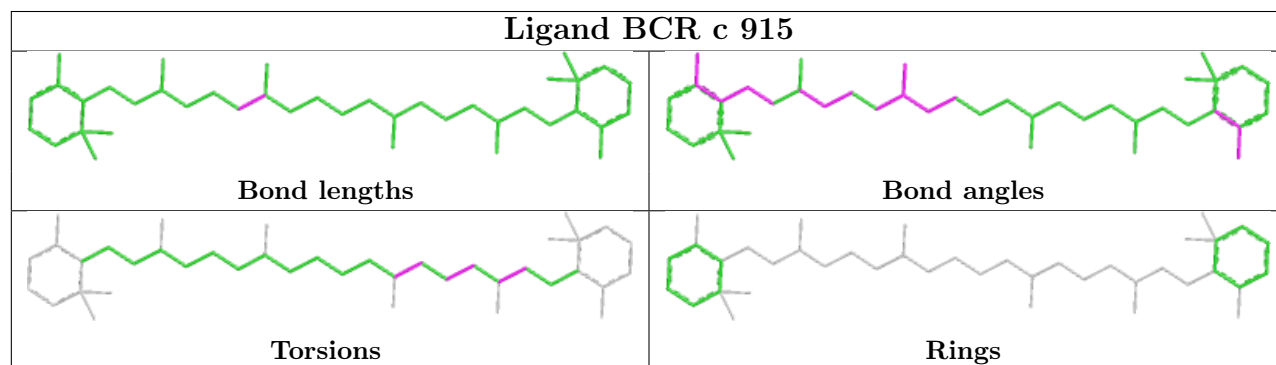
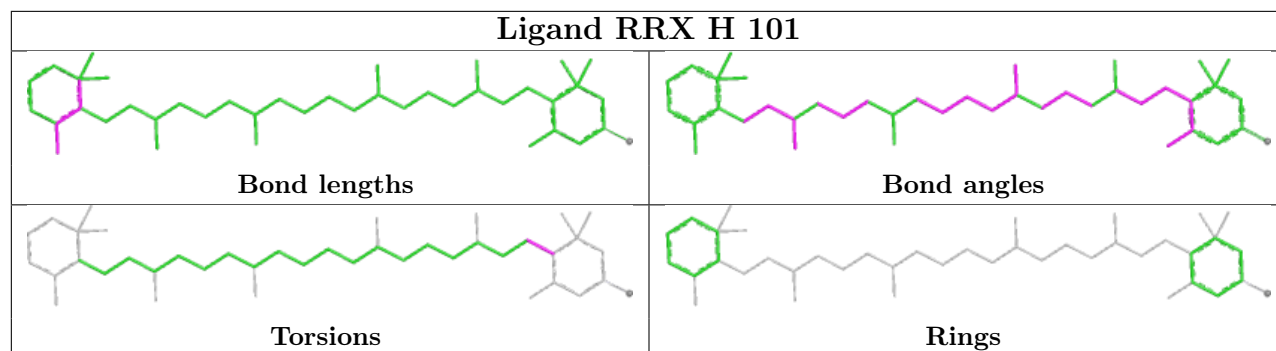
Ligand CLA c 907

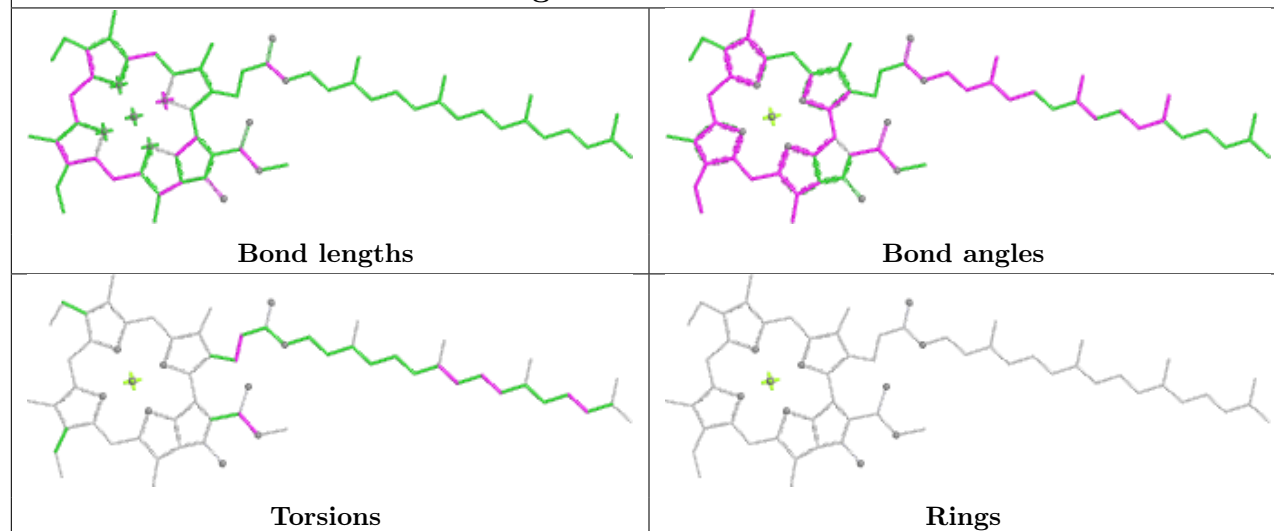
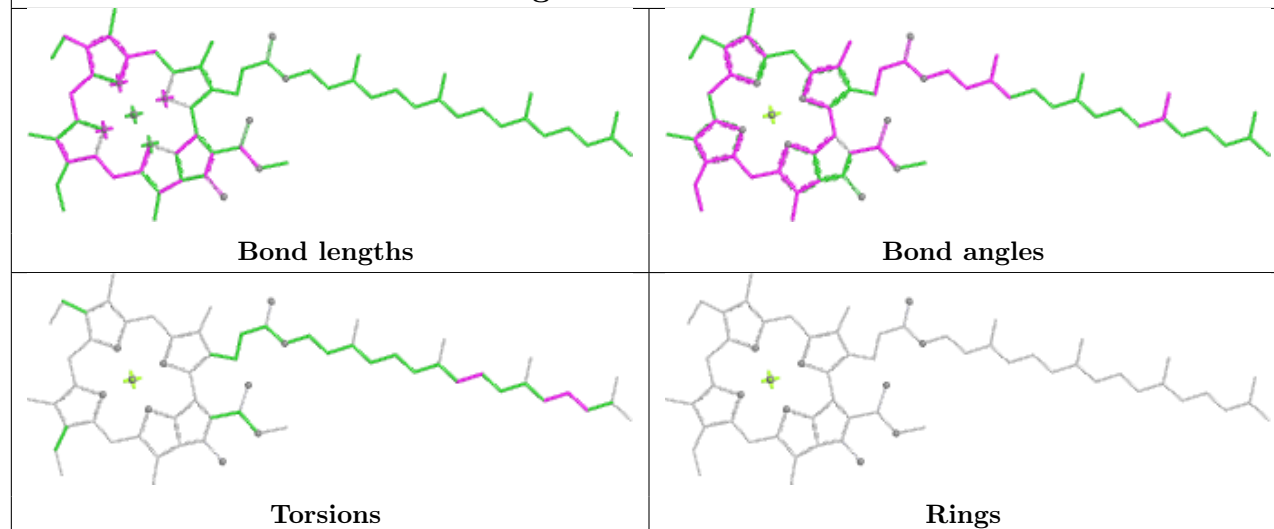


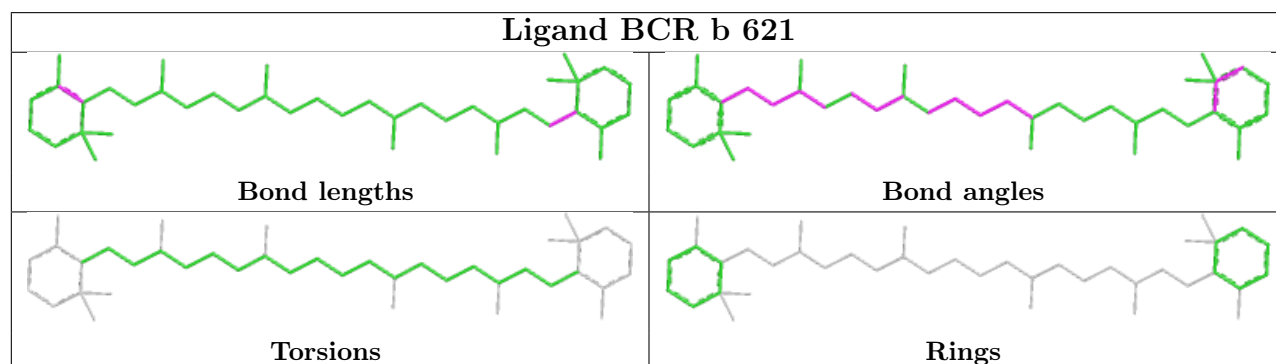
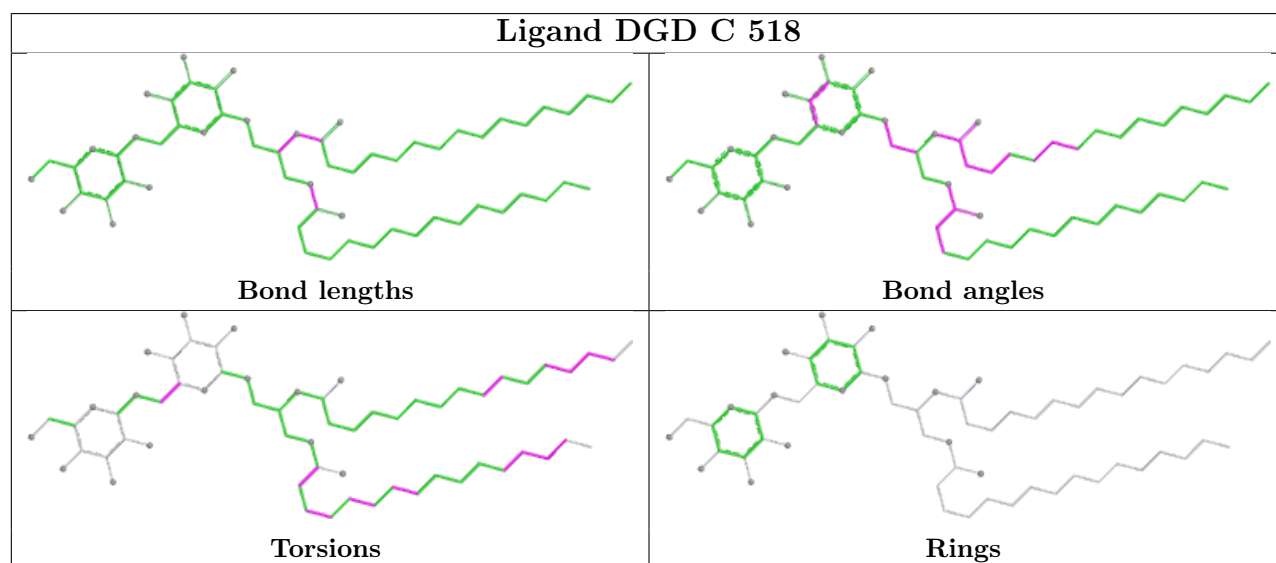
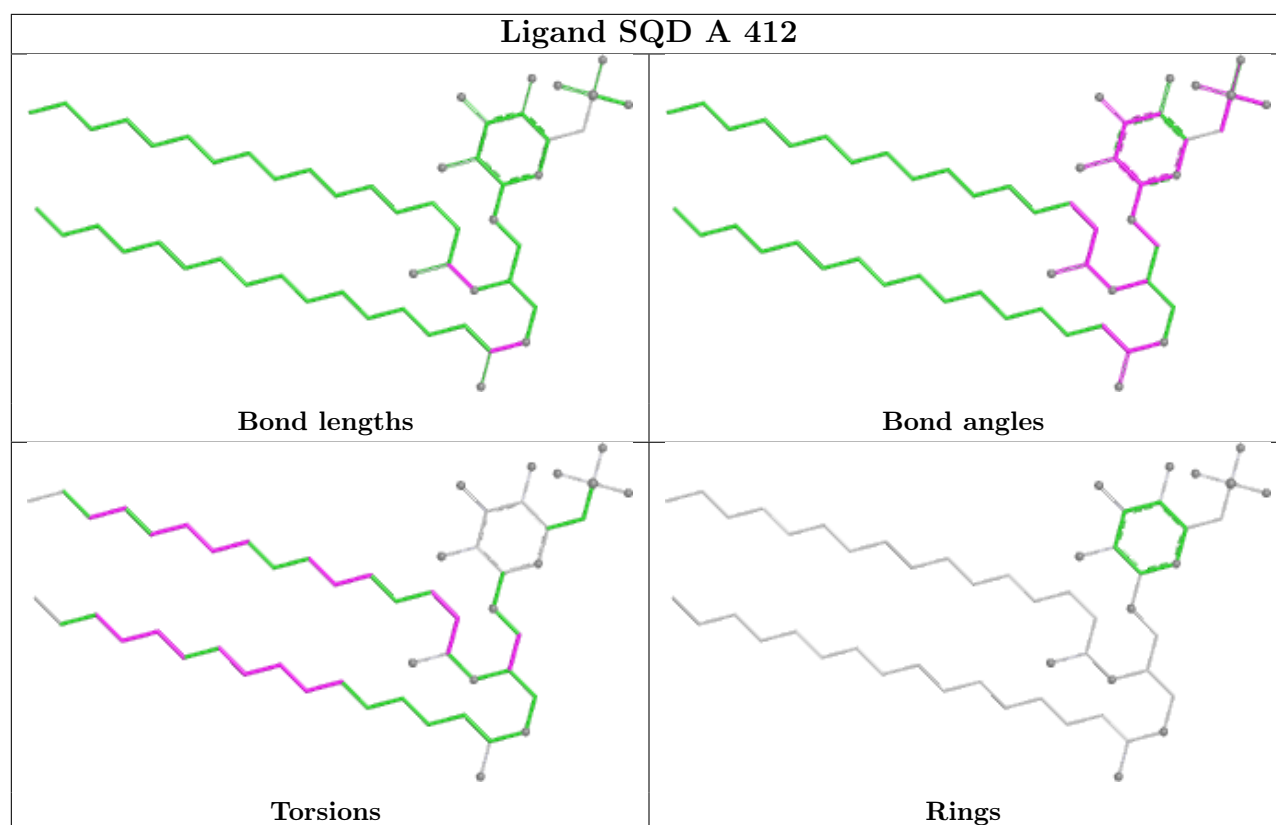
Ligand HEM F 101



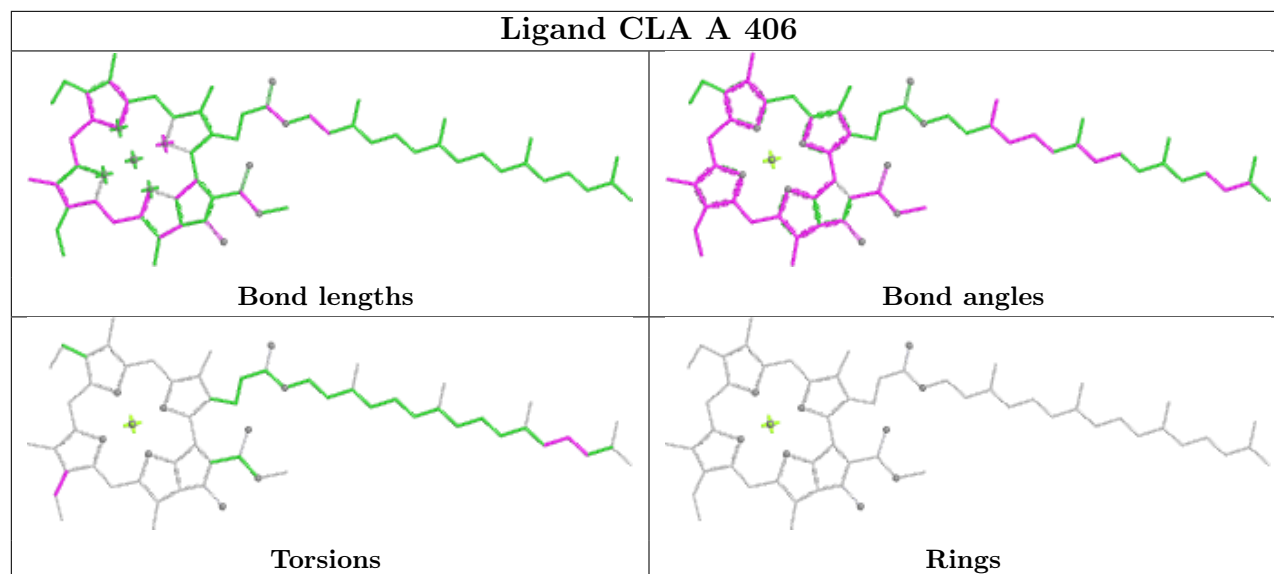




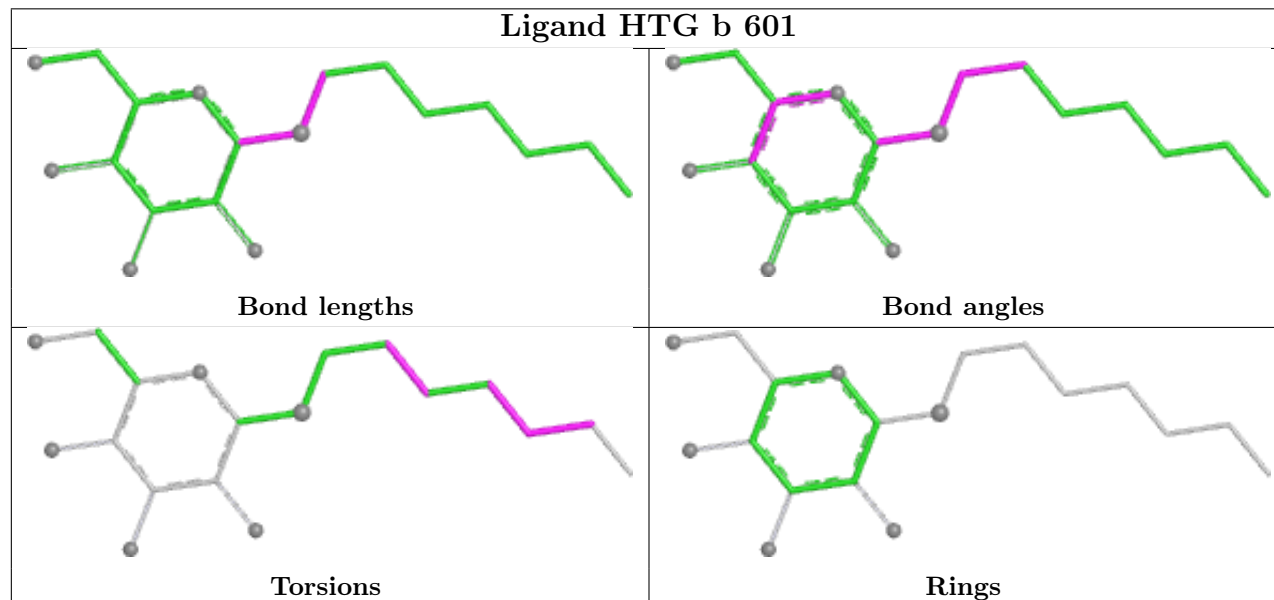
Ligand CLA B 607**Ligand CLA B 603**



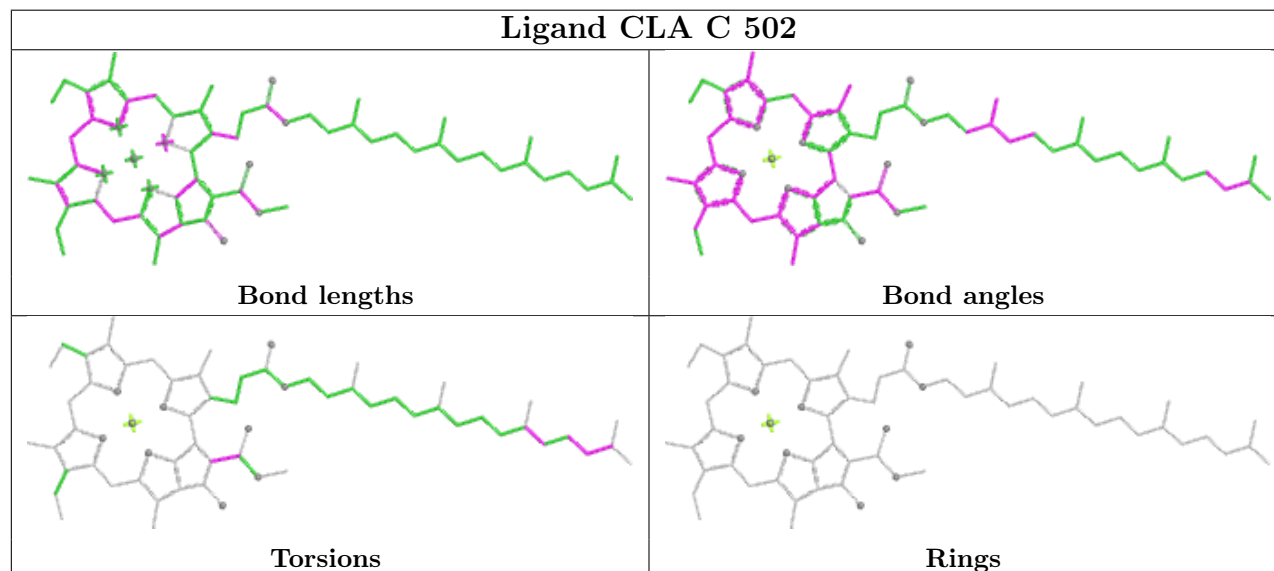
Ligand CLA A 406

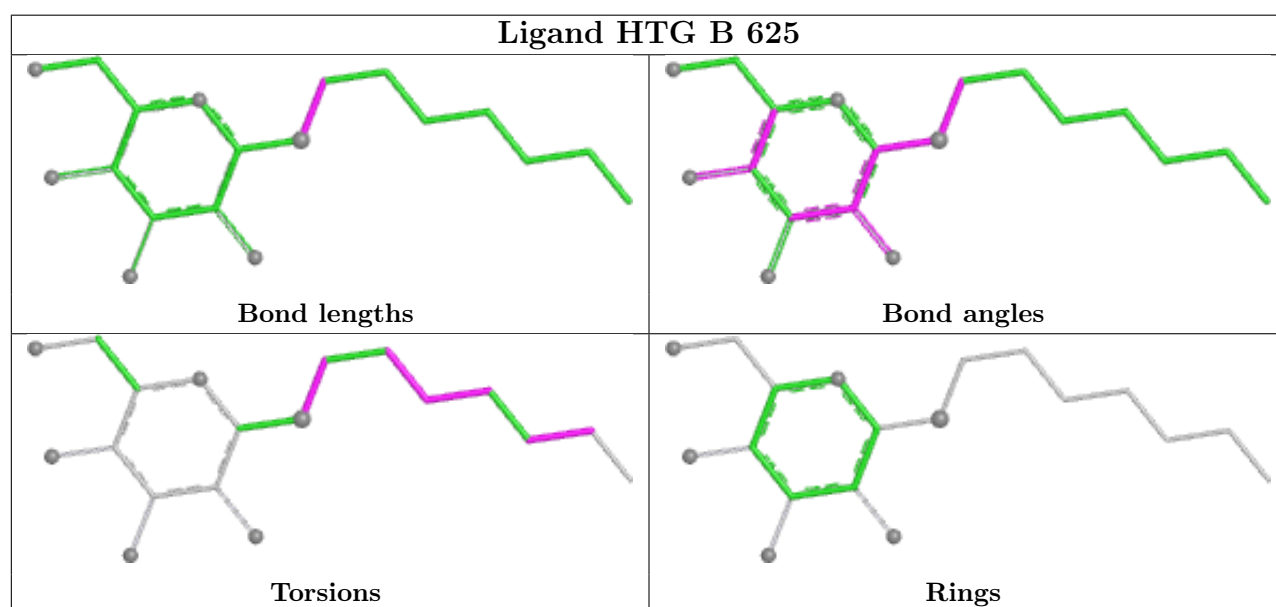
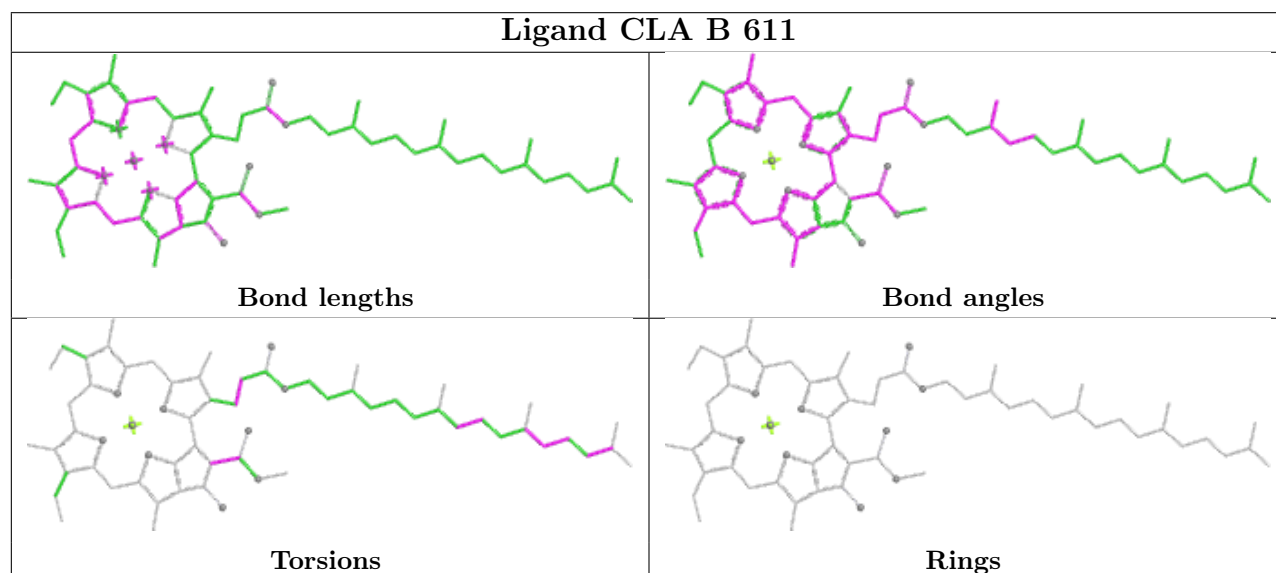
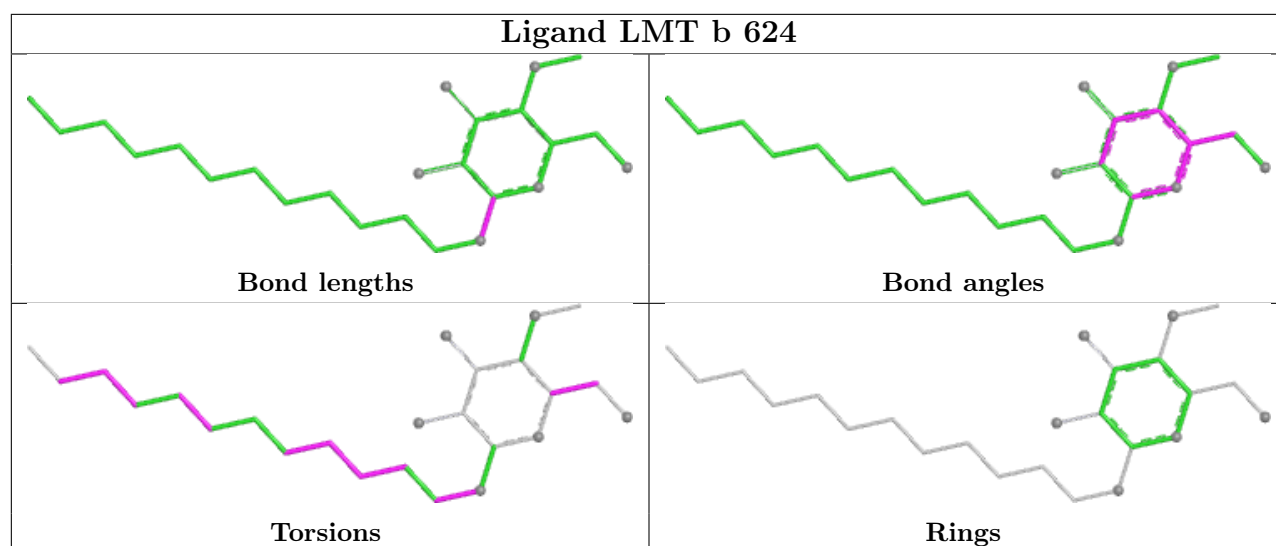


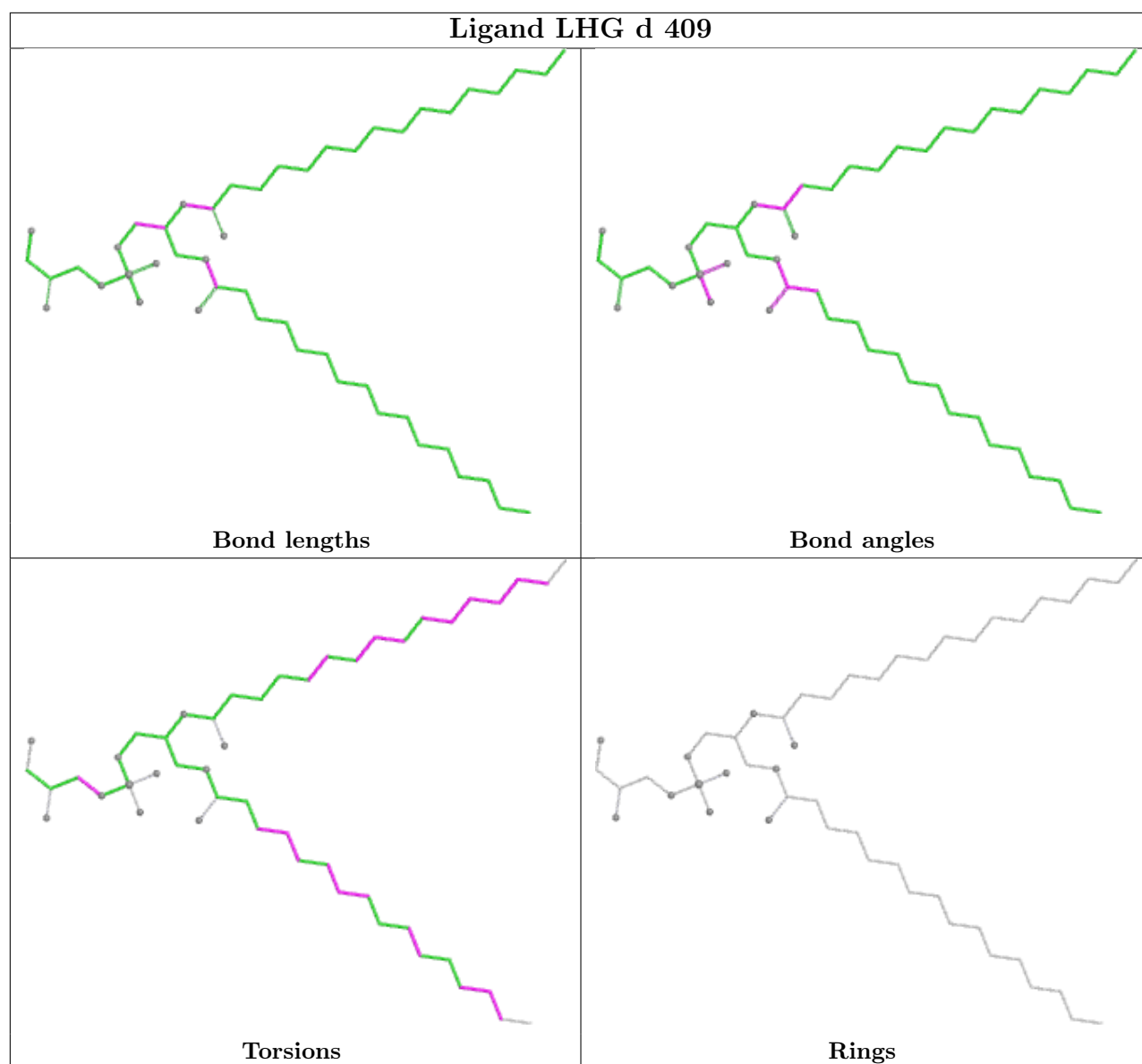
Ligand HTG b 601

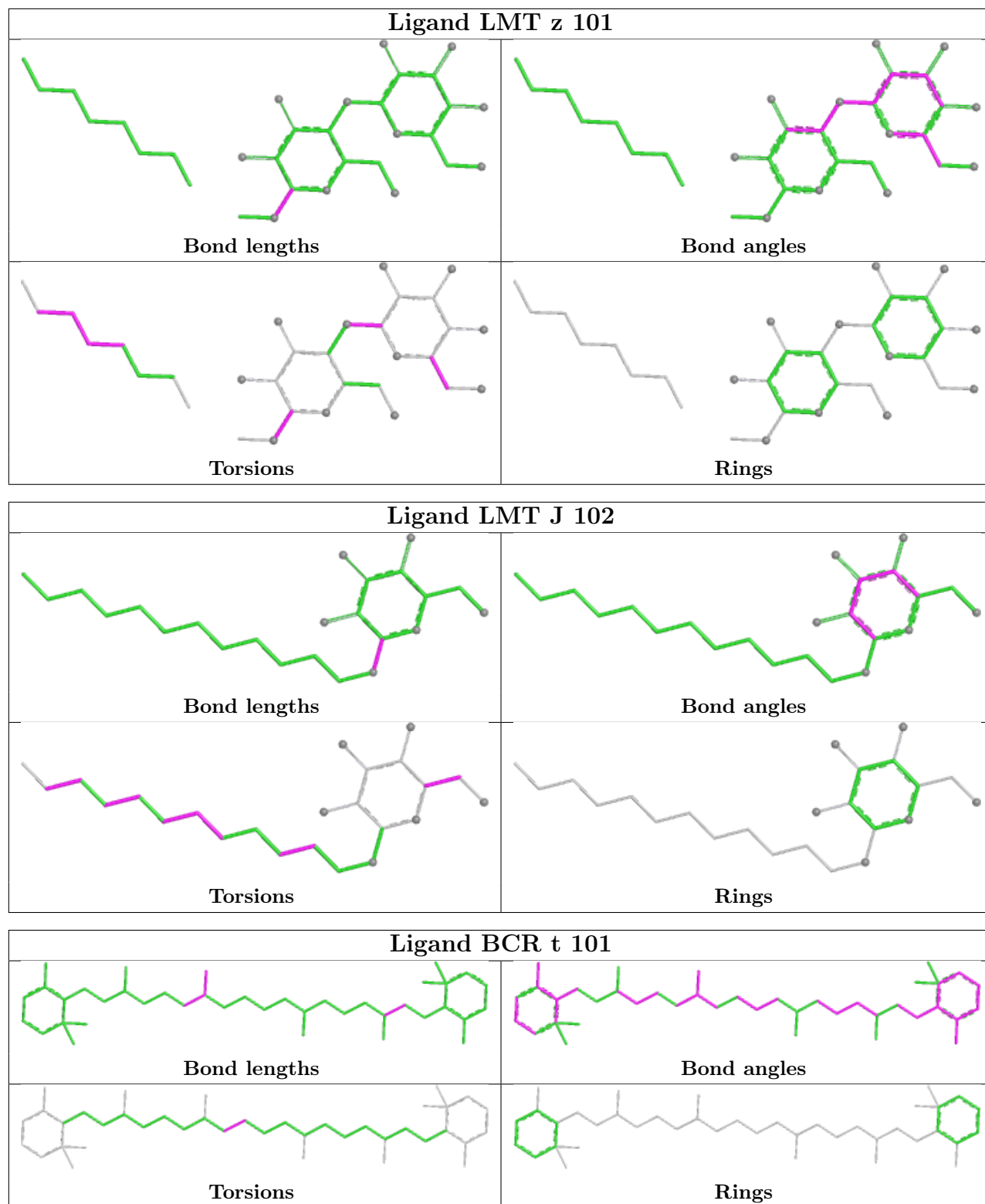


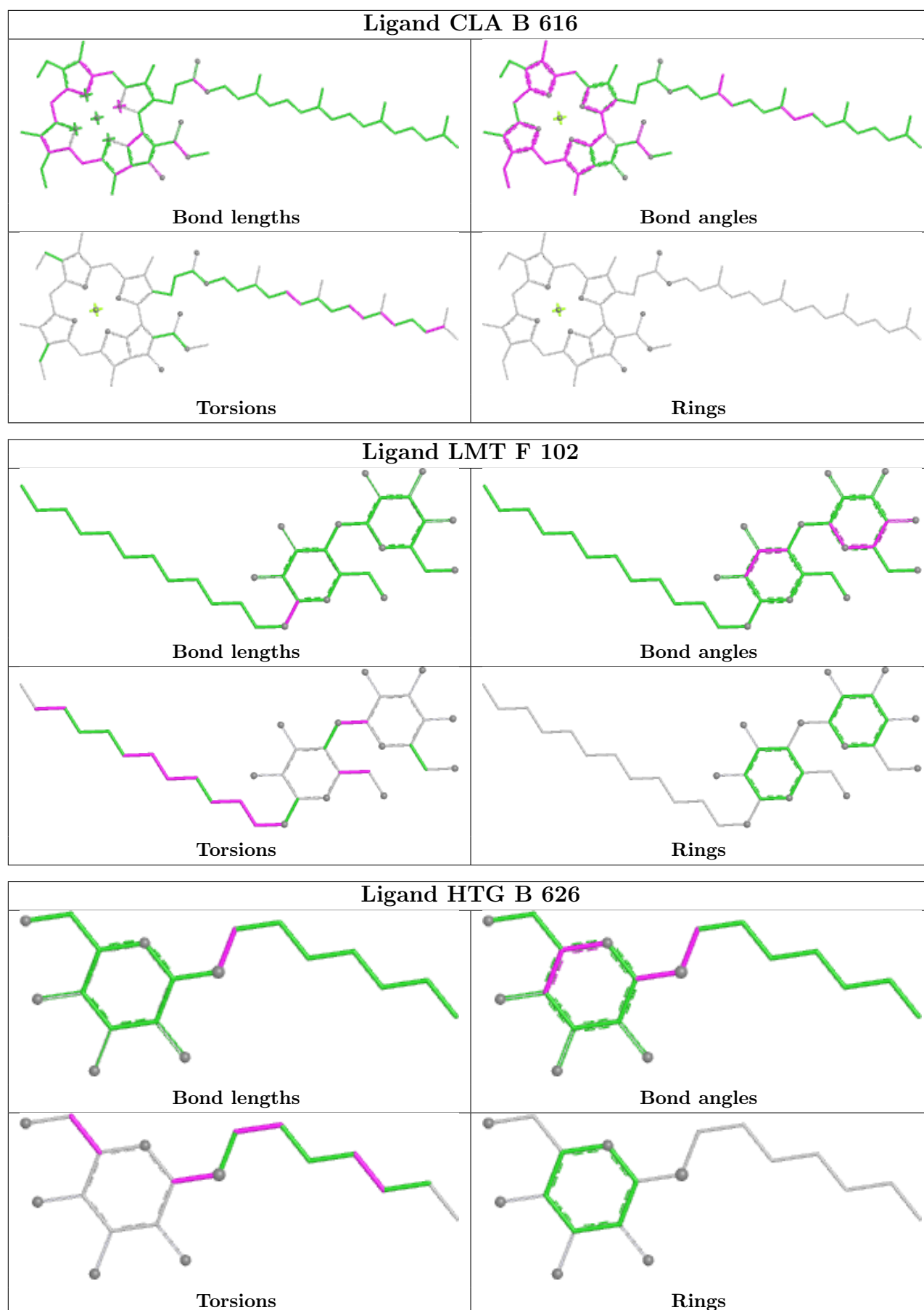
Ligand CLA C 502

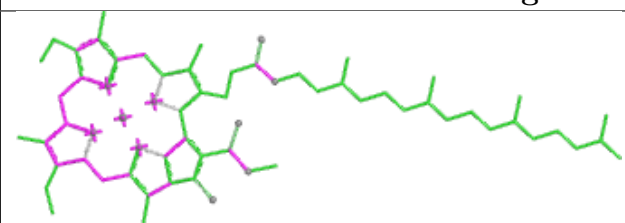
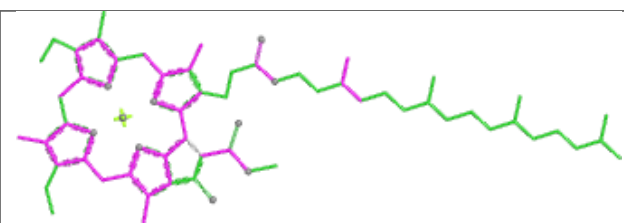
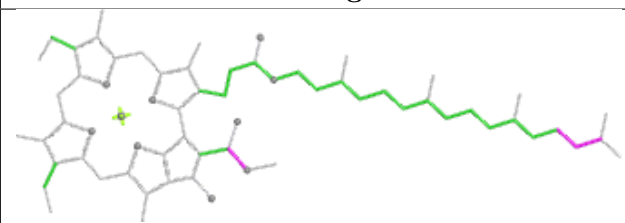
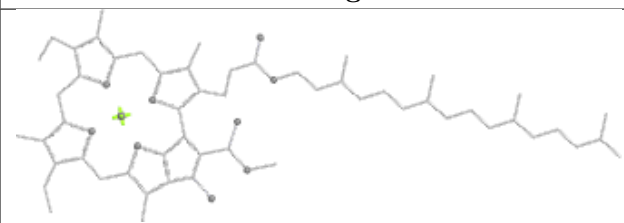


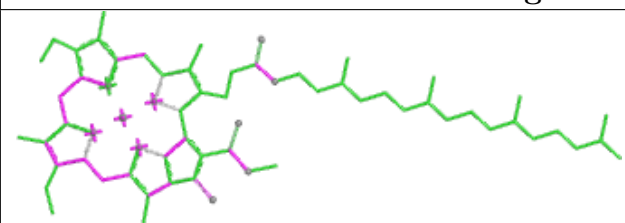
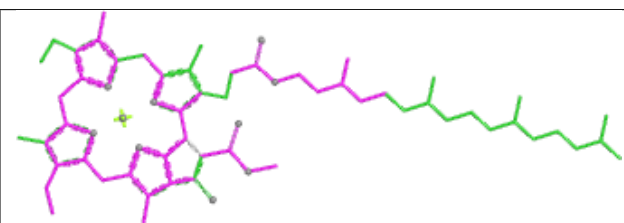
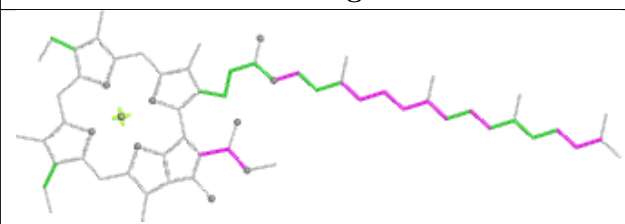
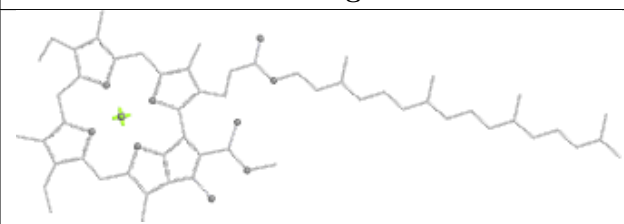


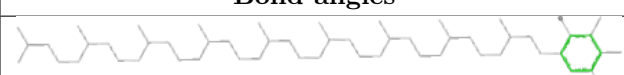


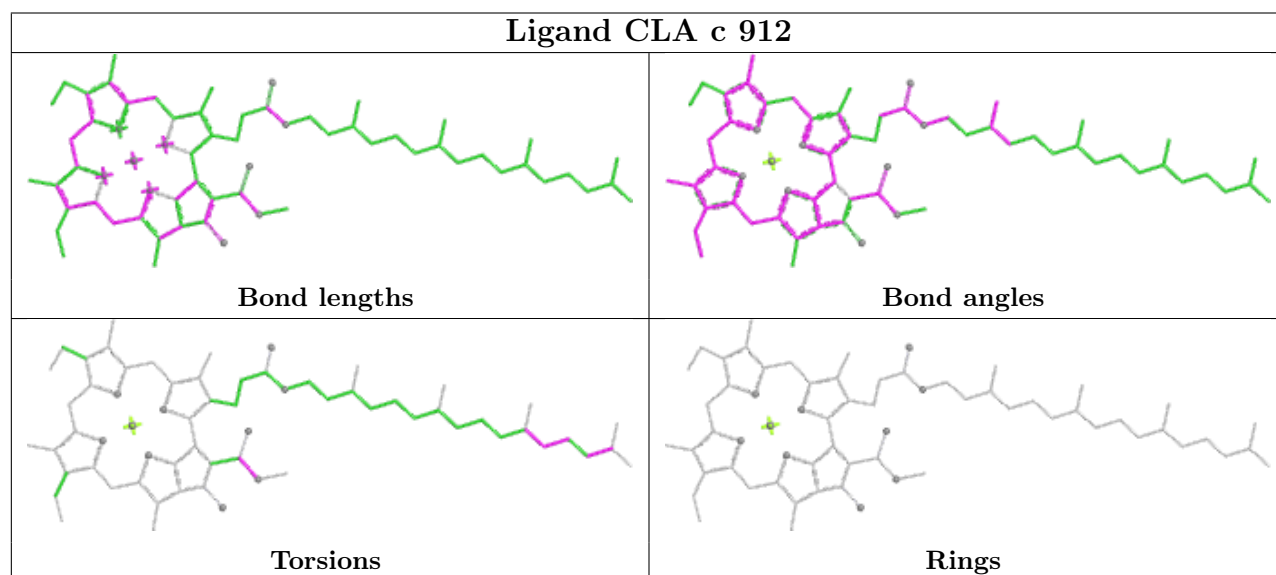
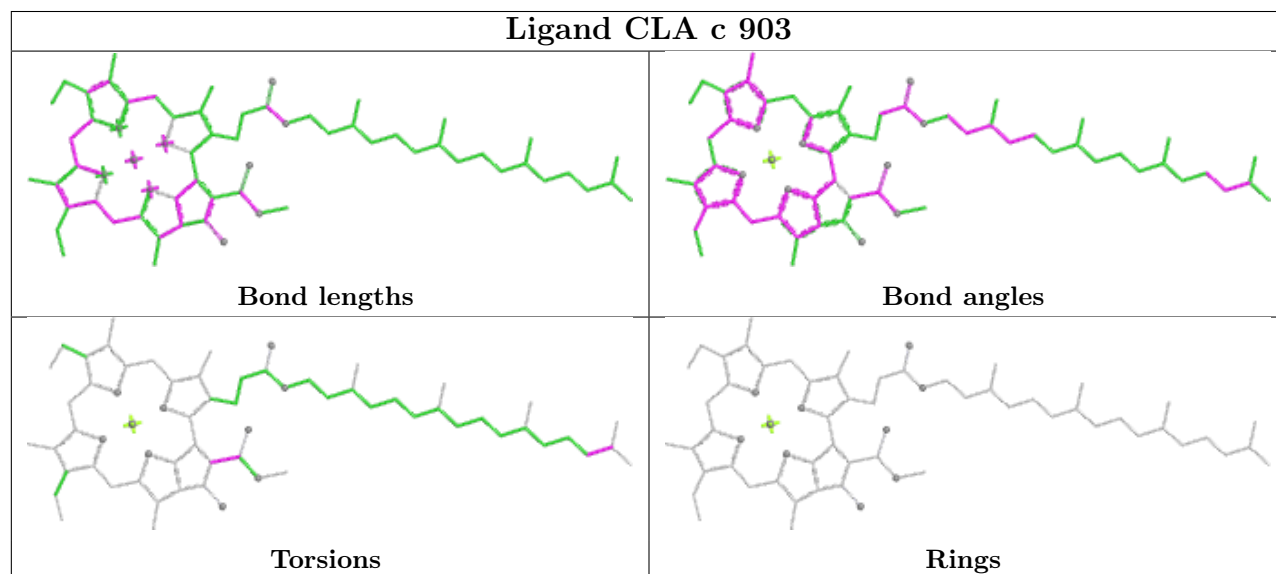
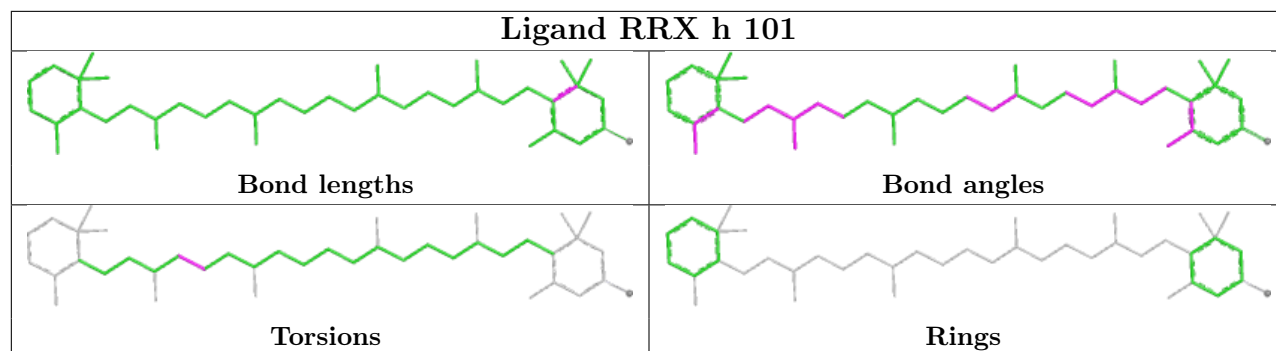


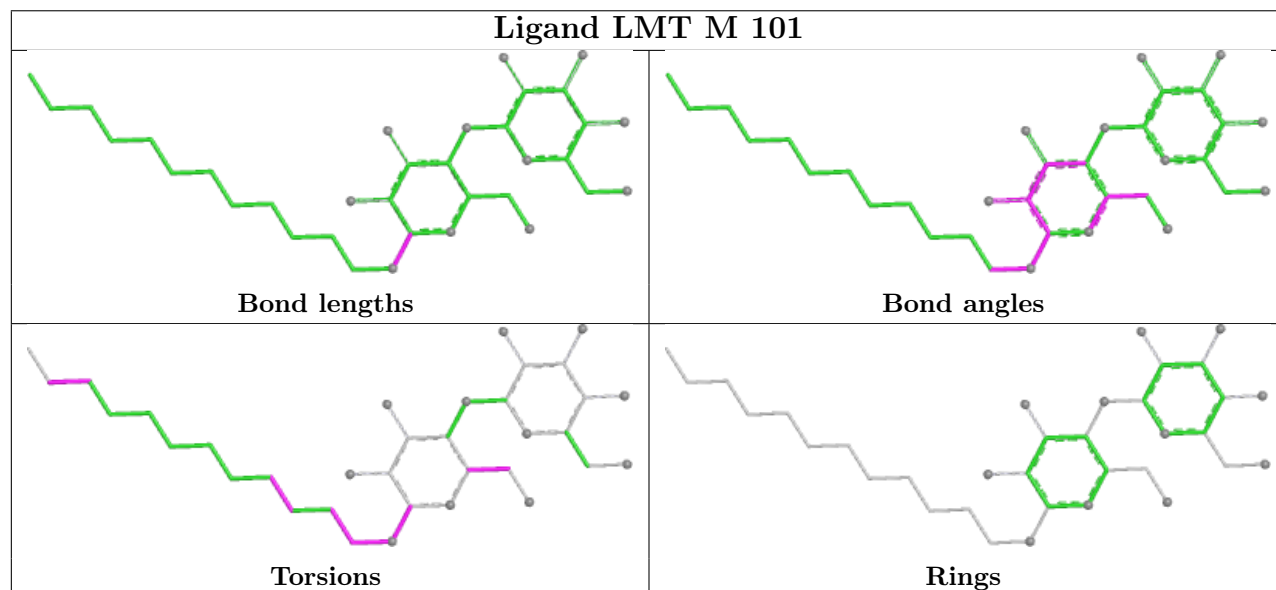
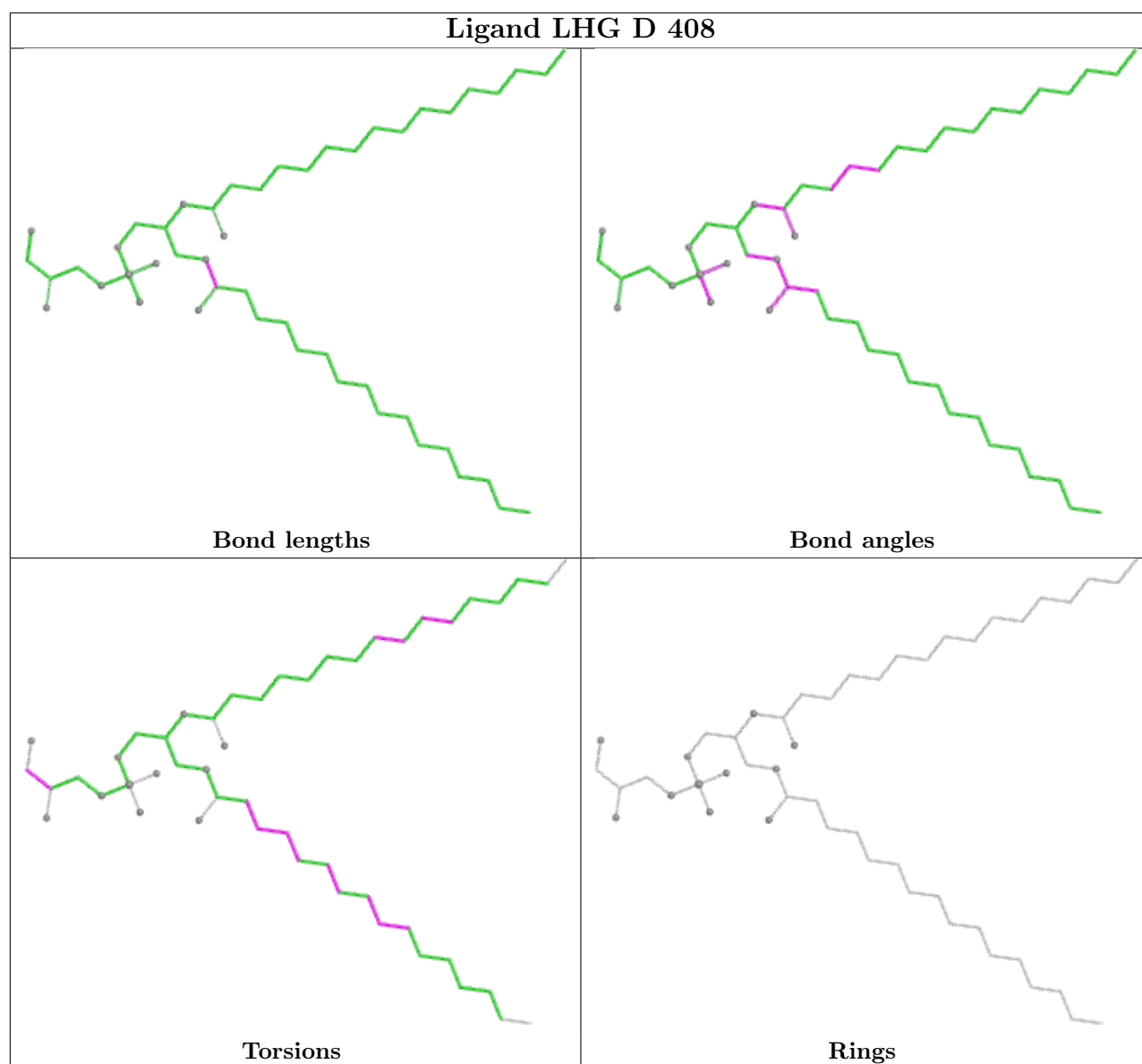


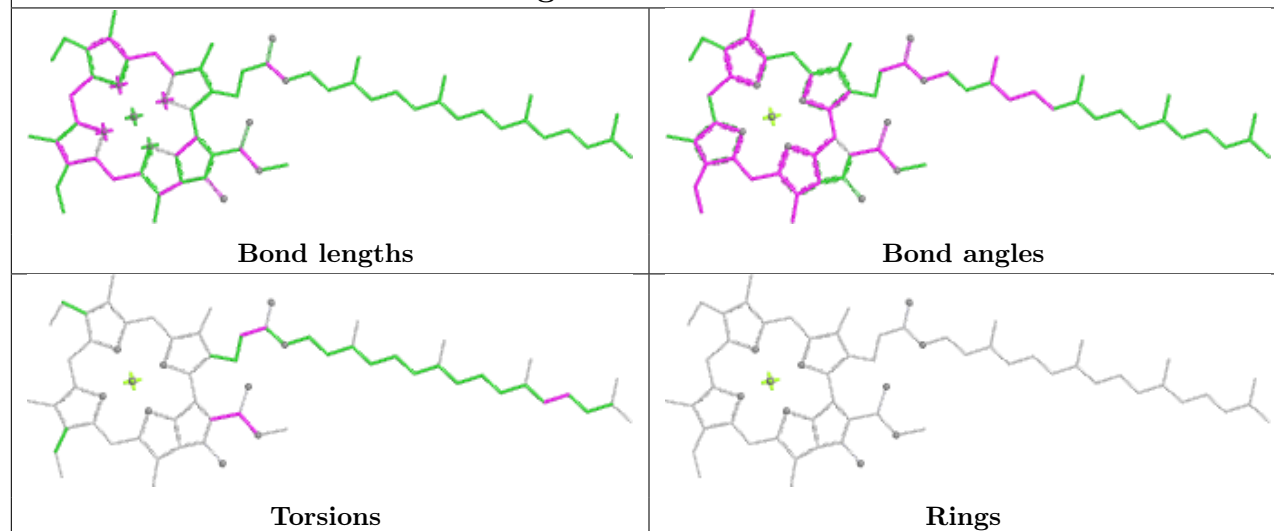
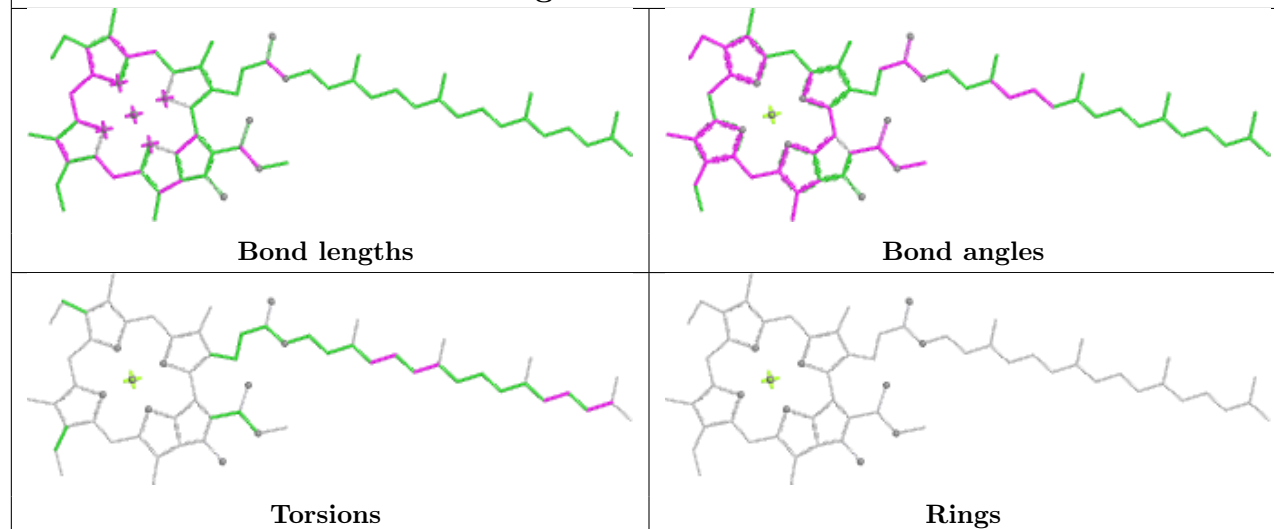
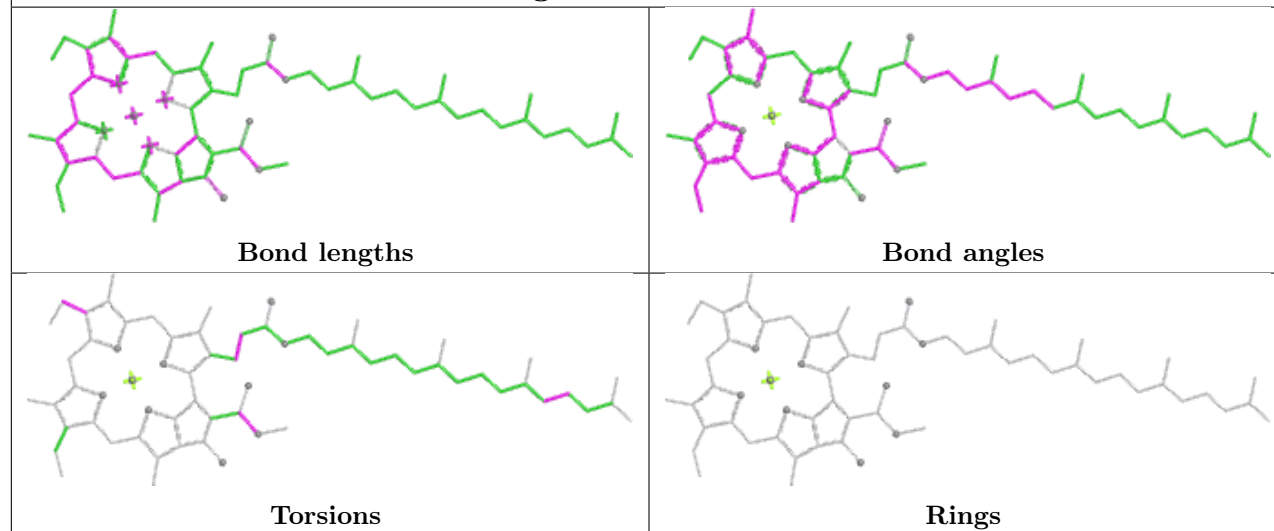
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

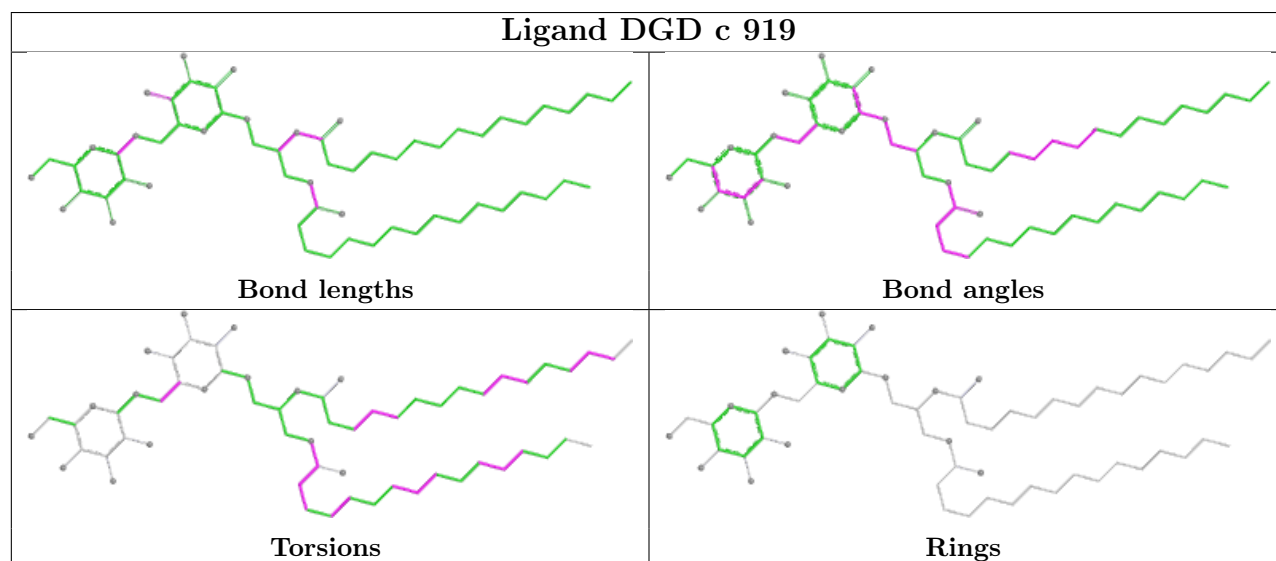
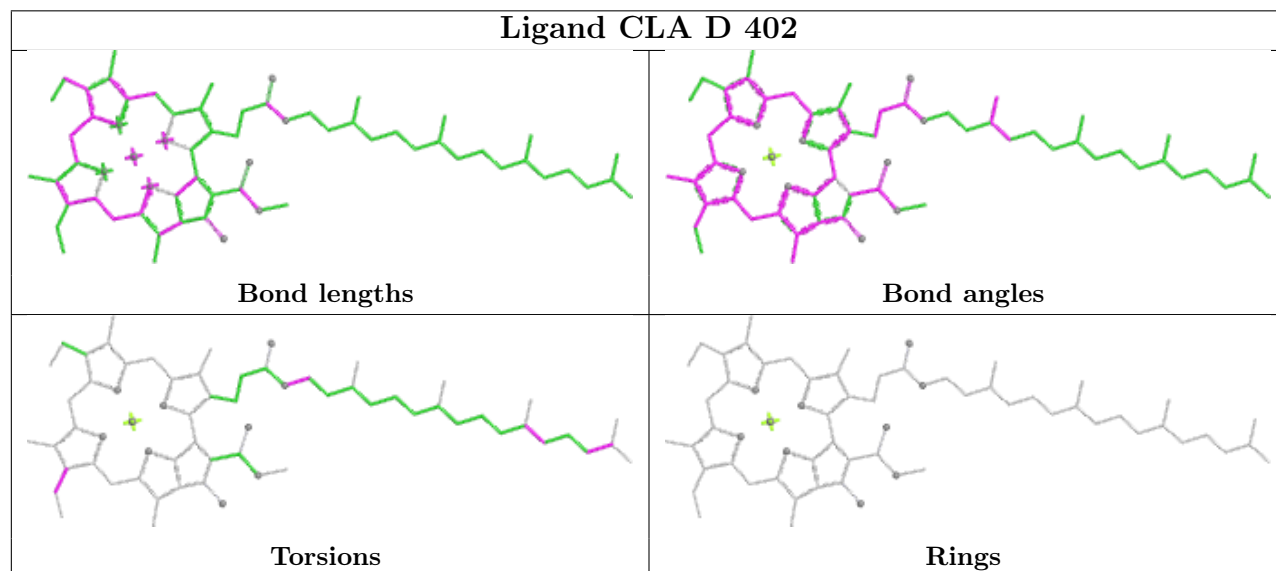
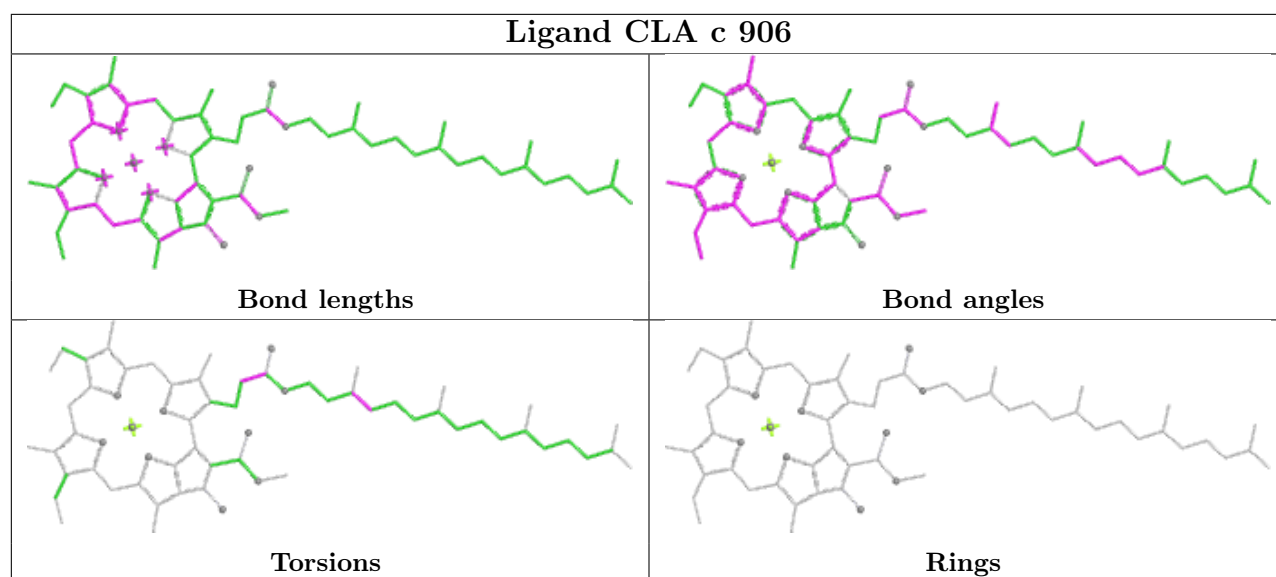
Ligand CLA b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

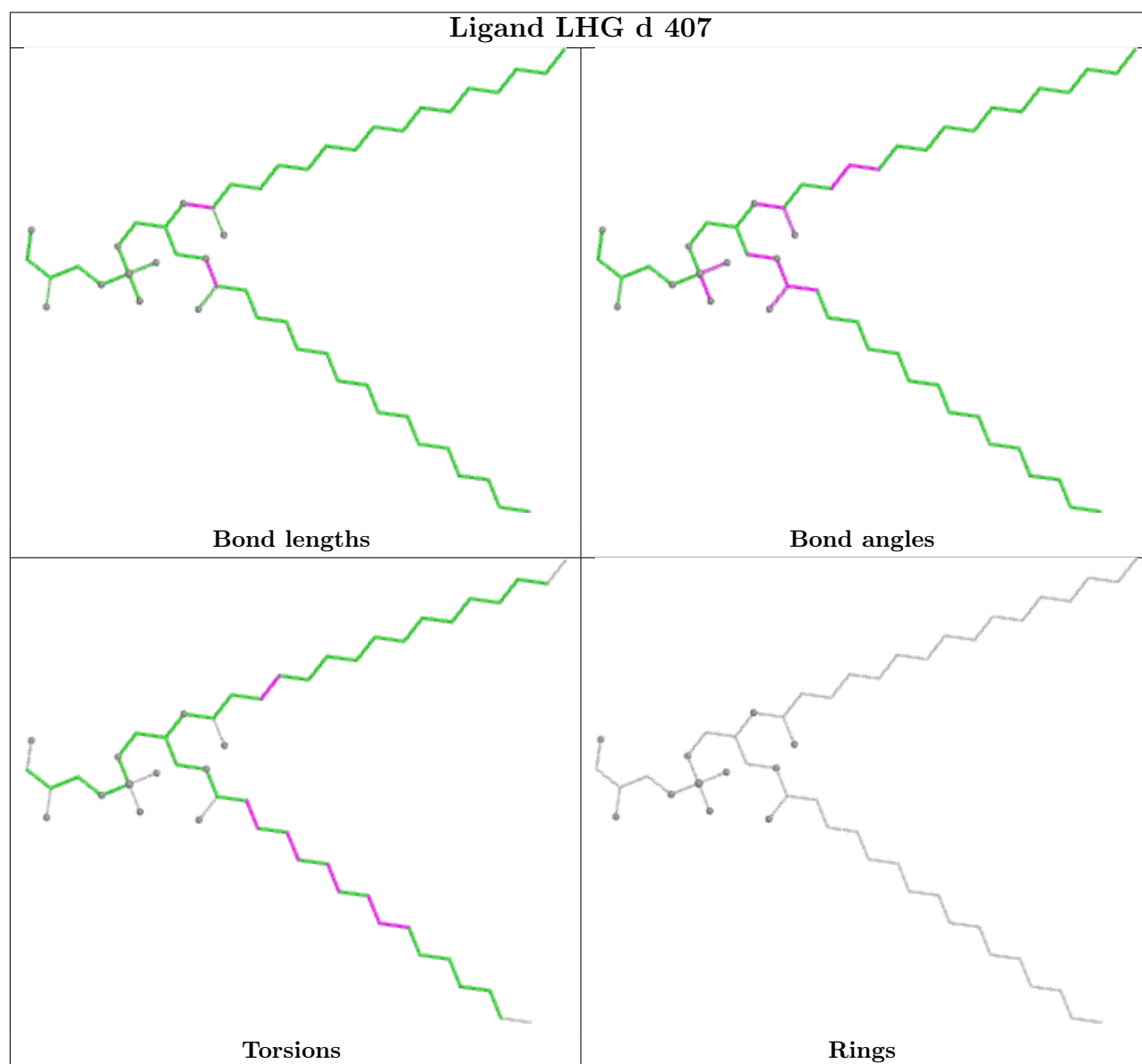
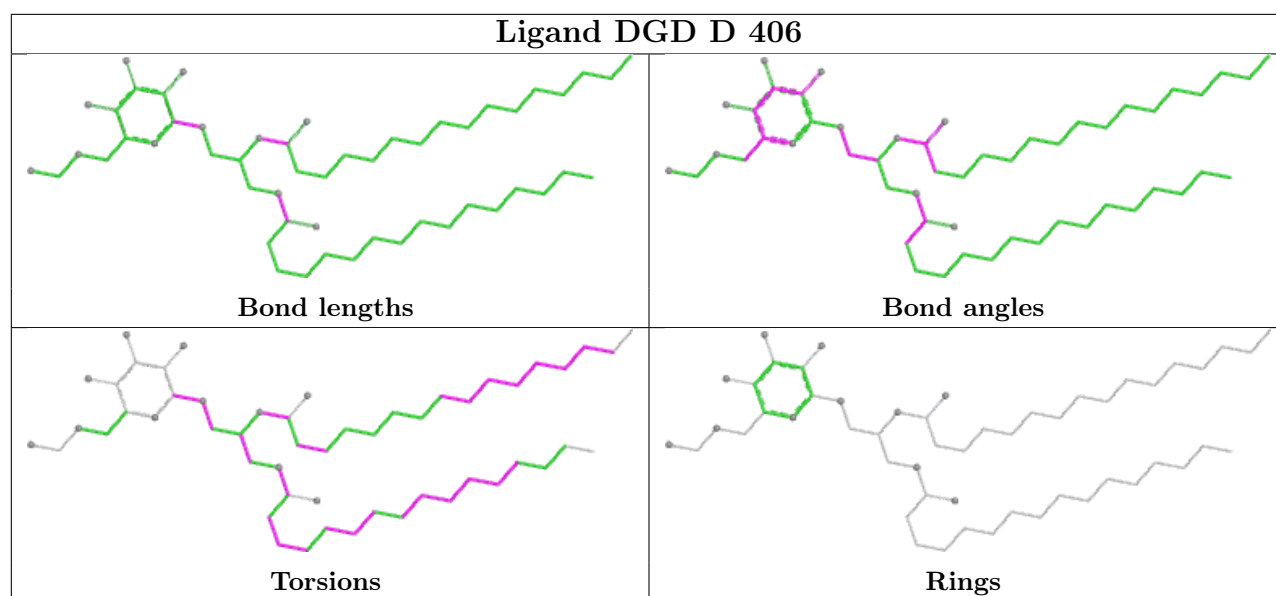
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

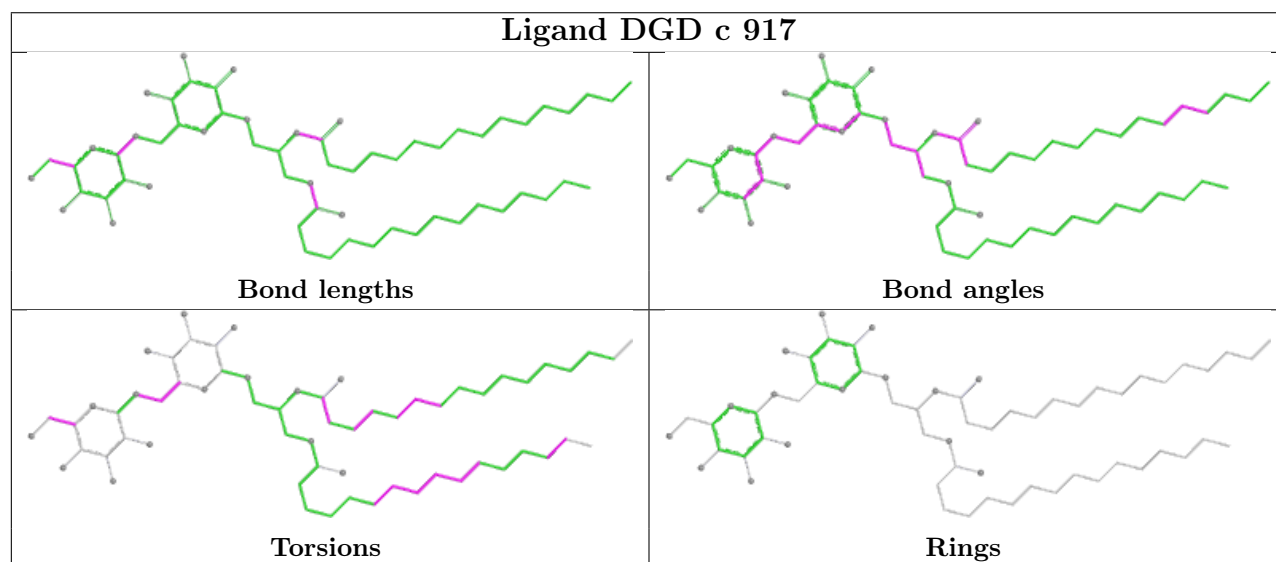
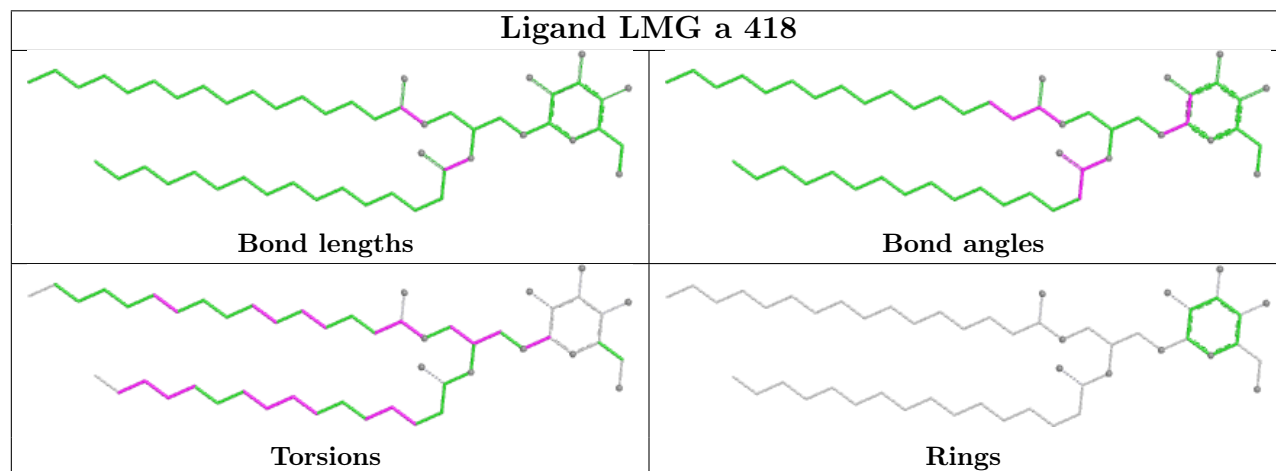
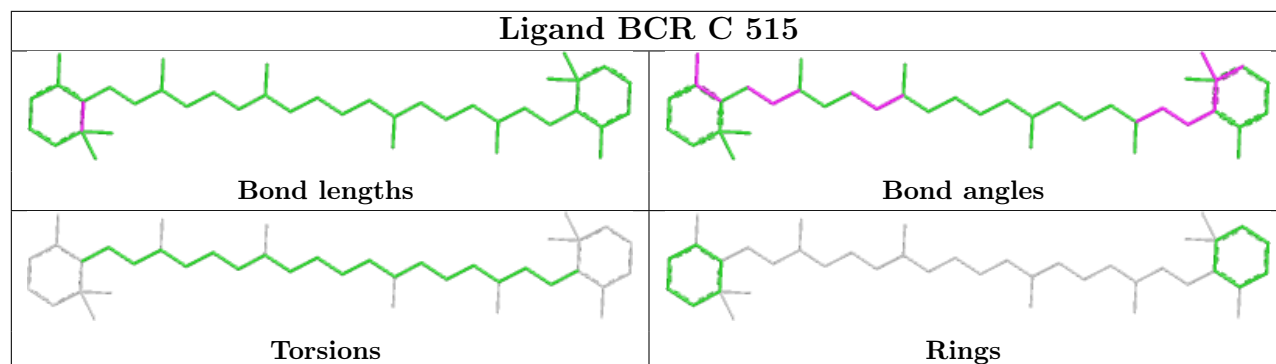


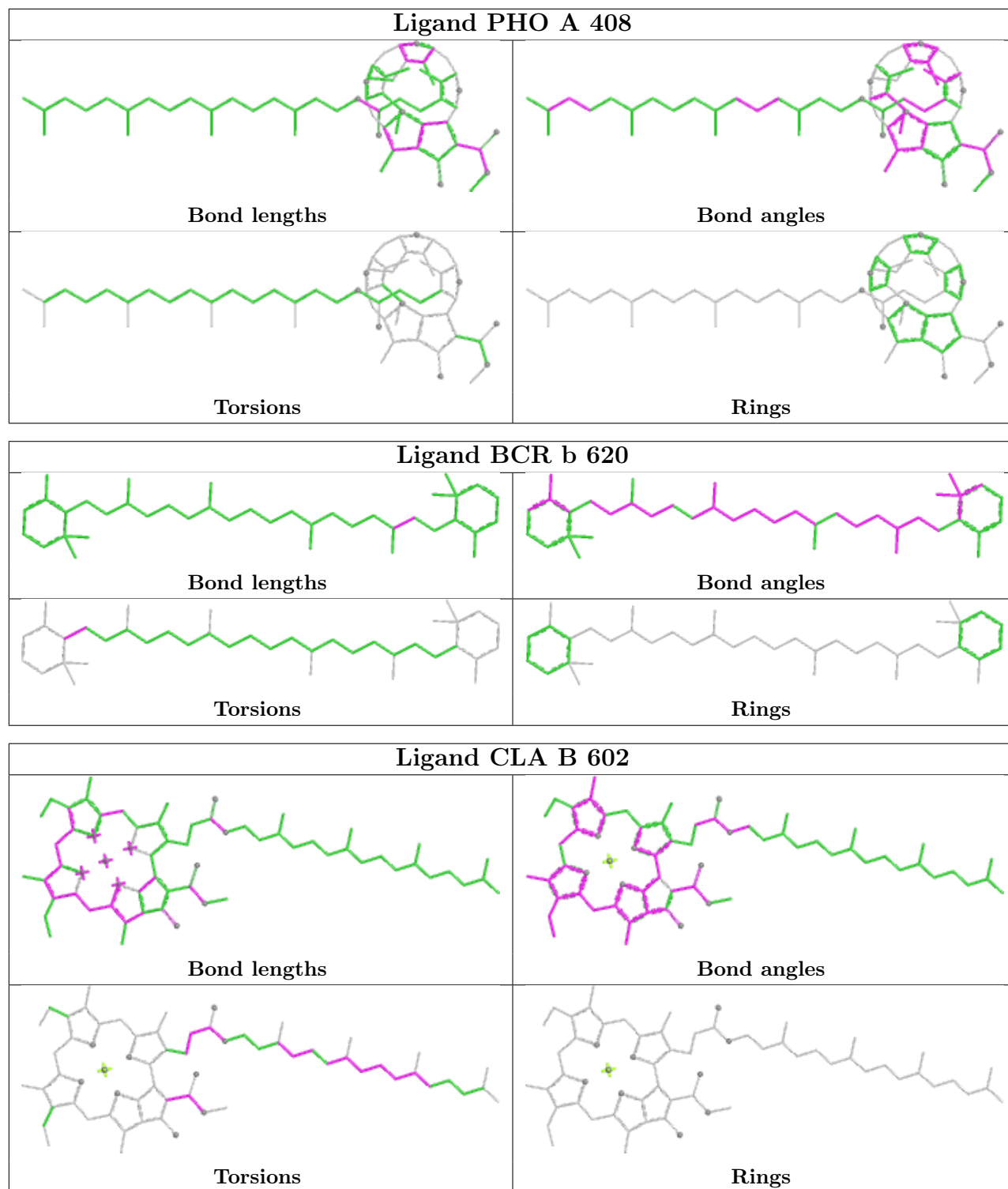


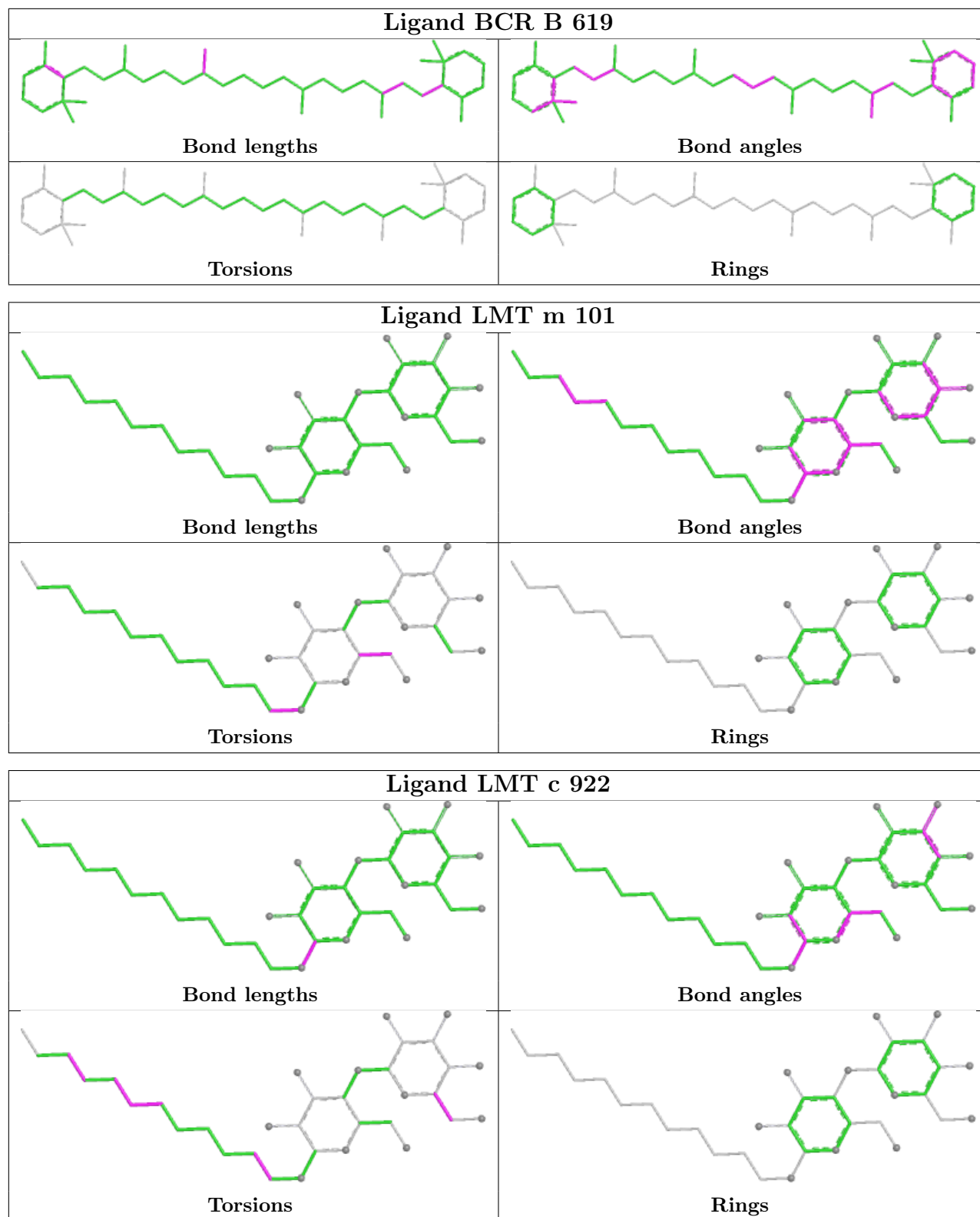
Ligand CLA c 902**Ligand CLA b 607****Ligand CLA C 501**

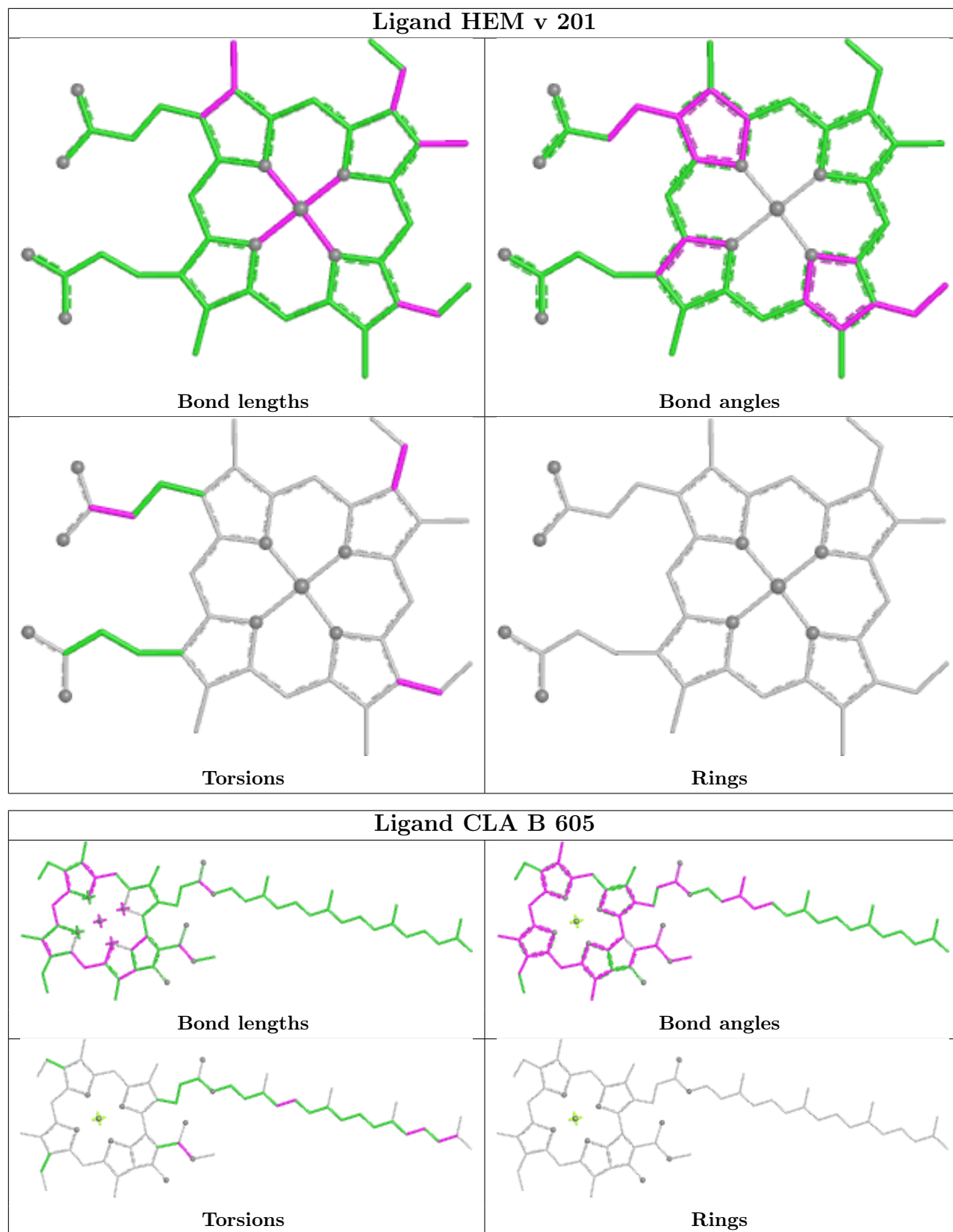


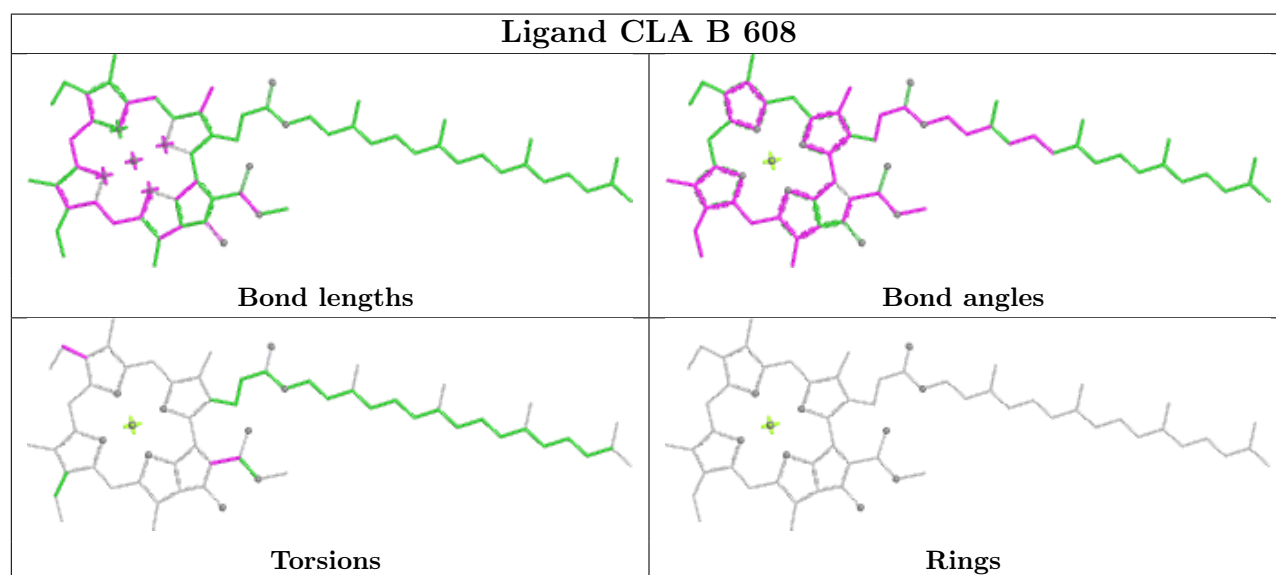
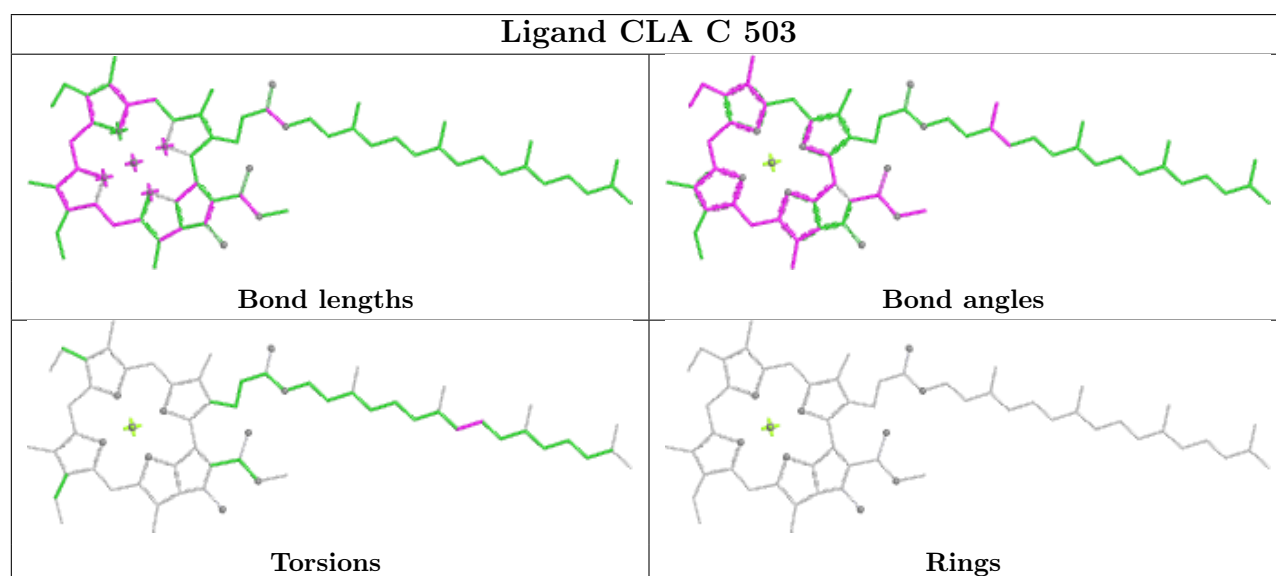
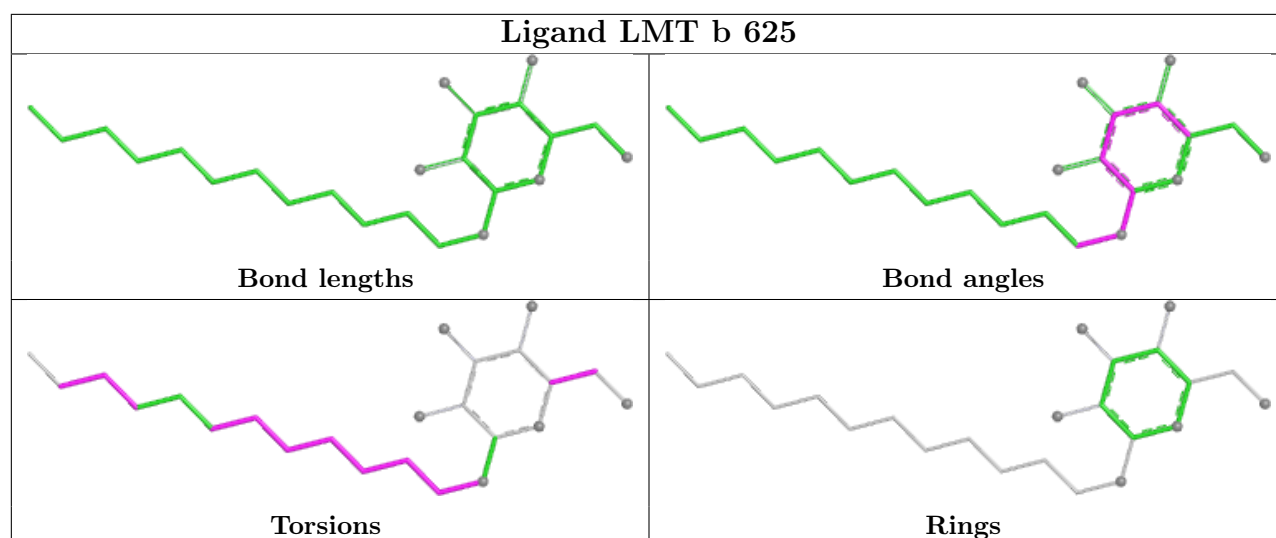


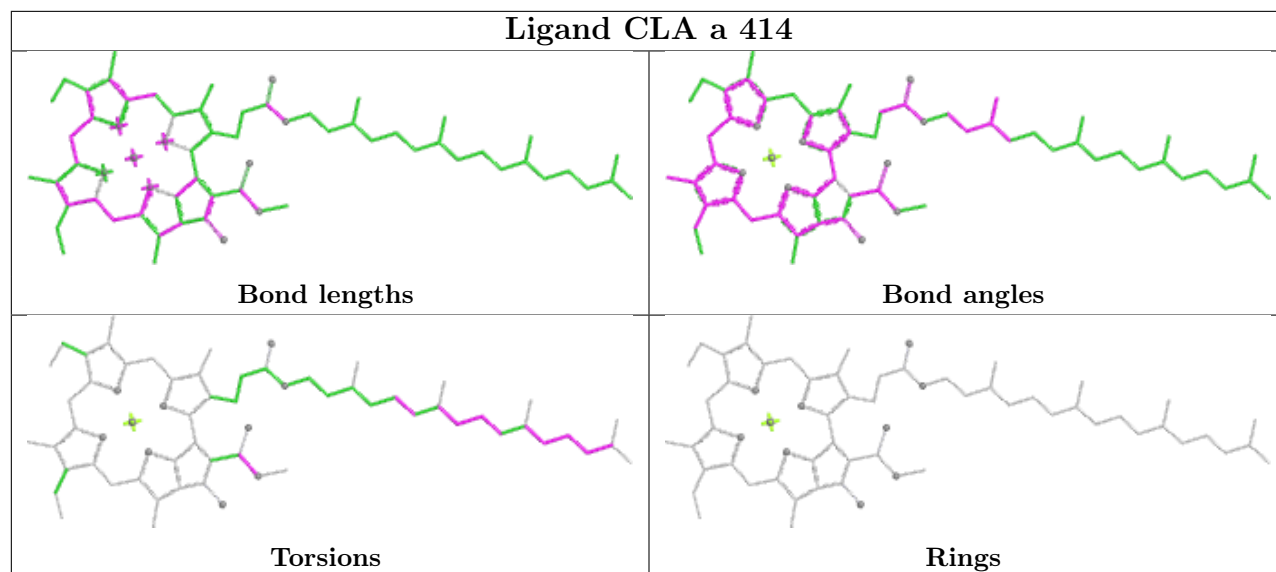
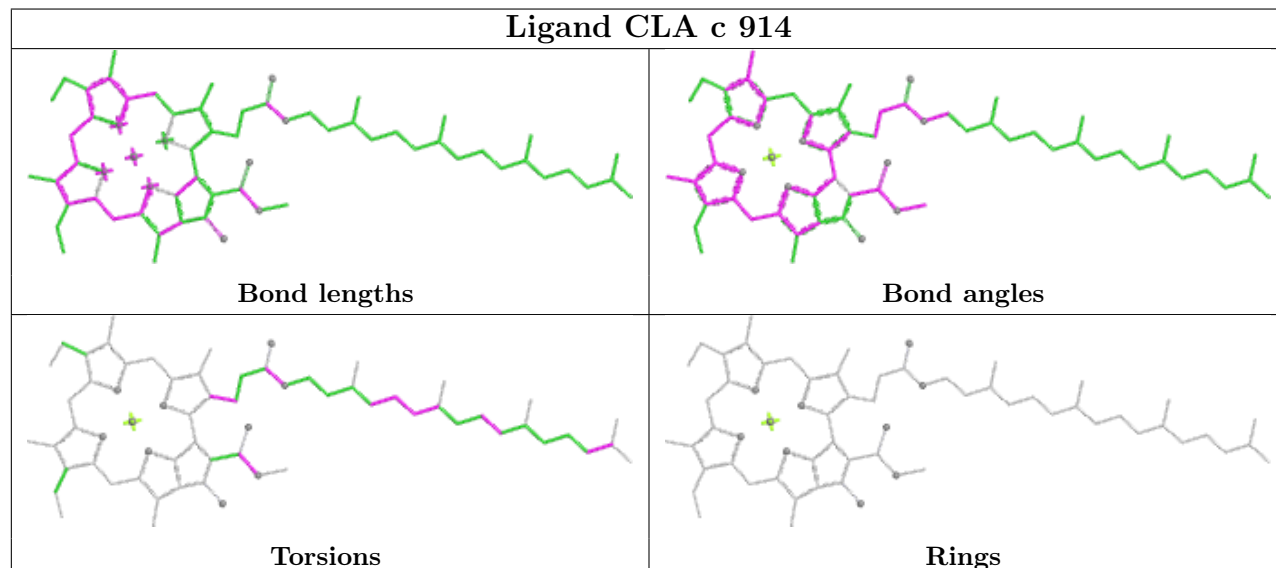
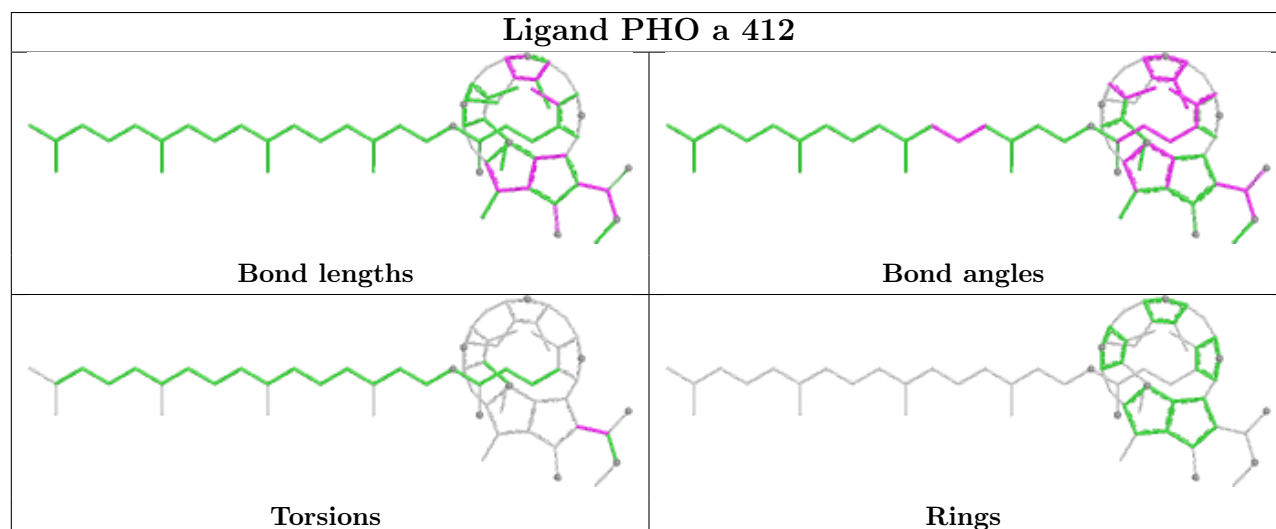


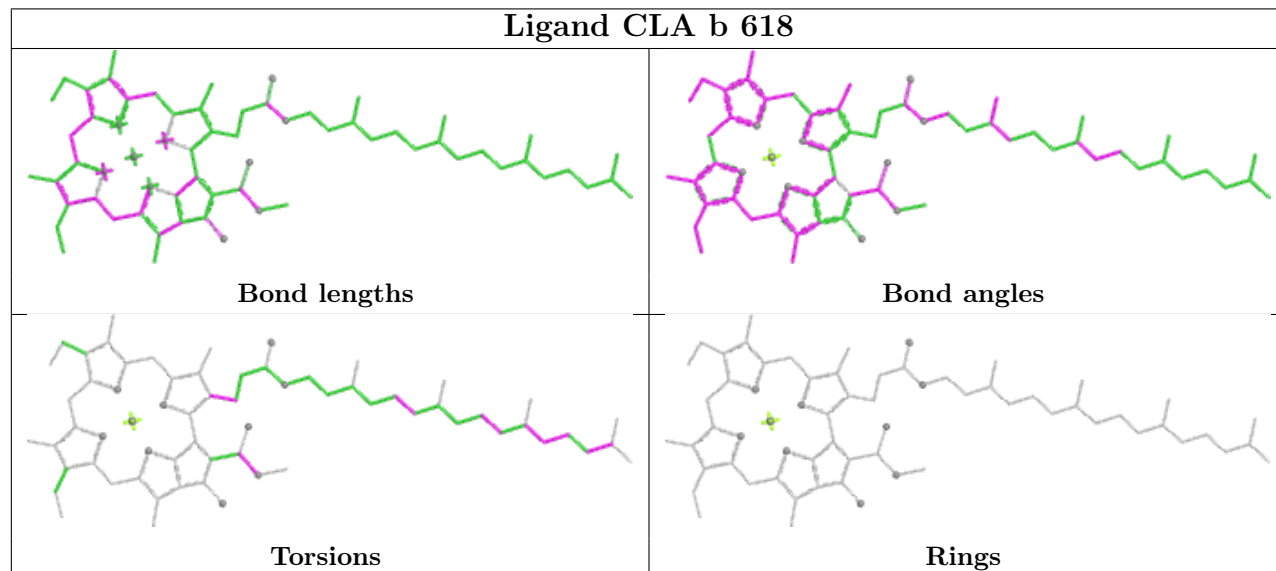
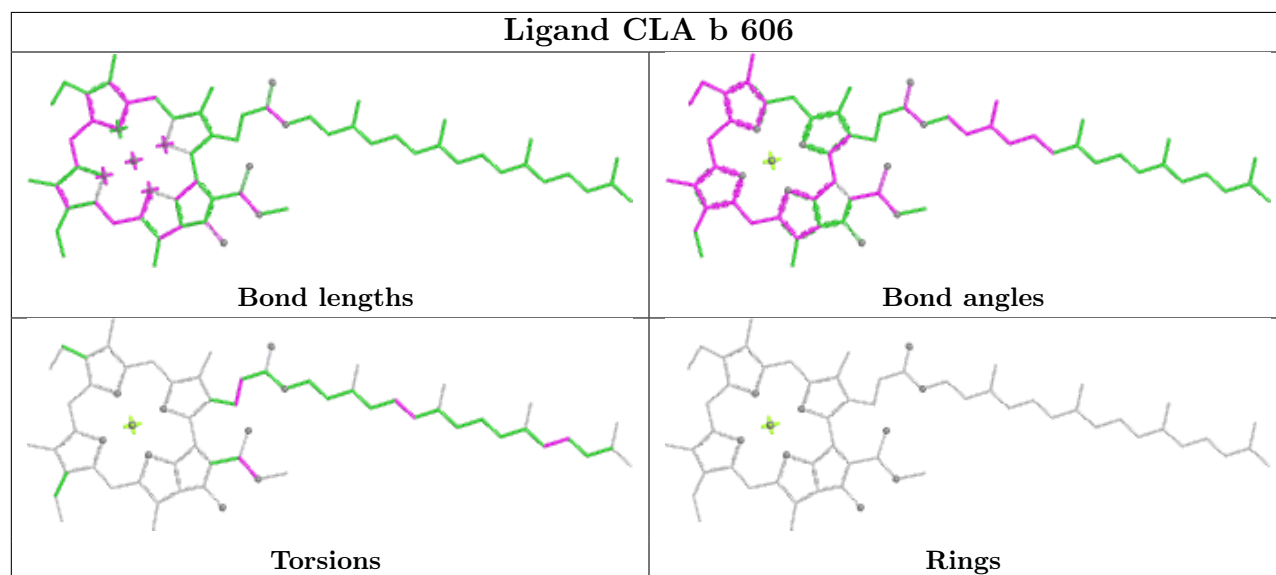
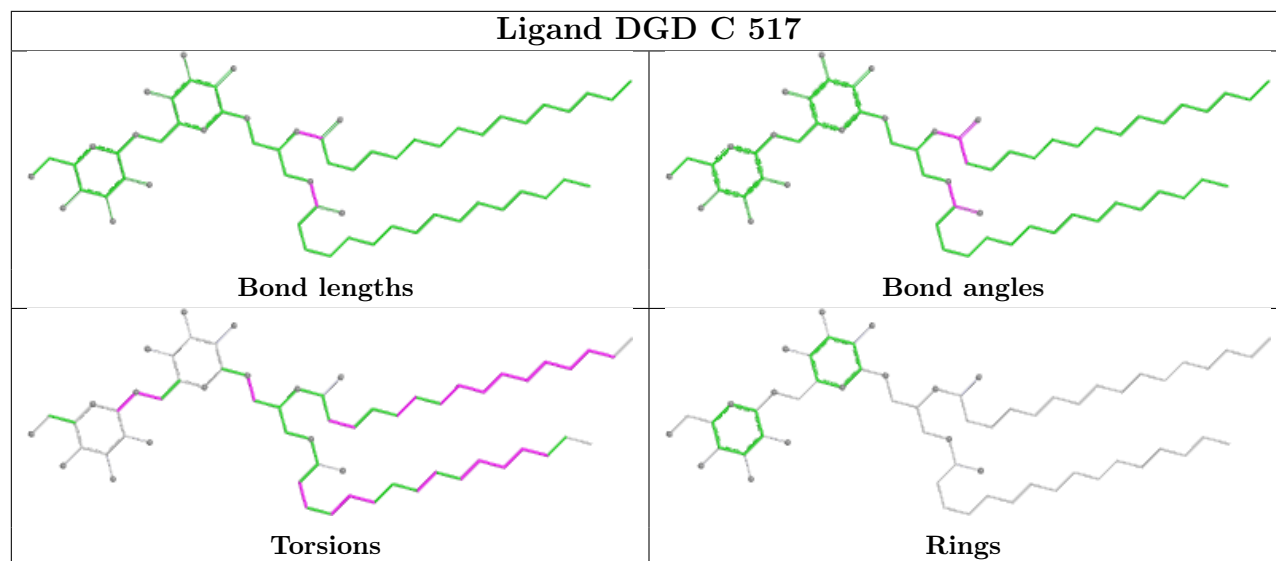


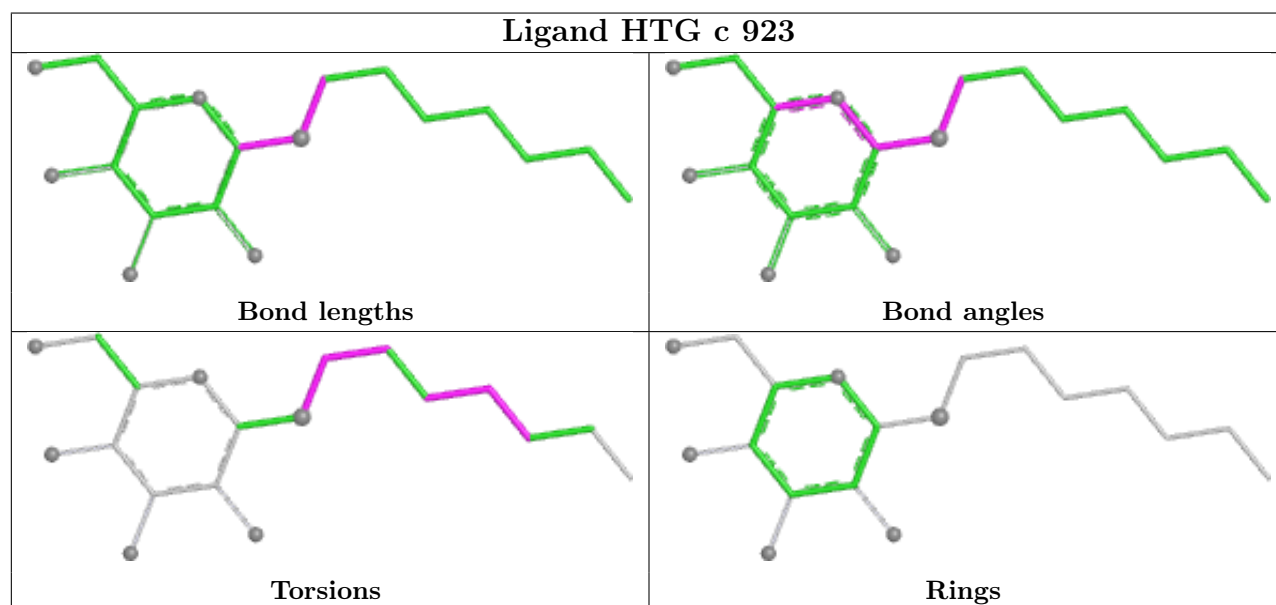
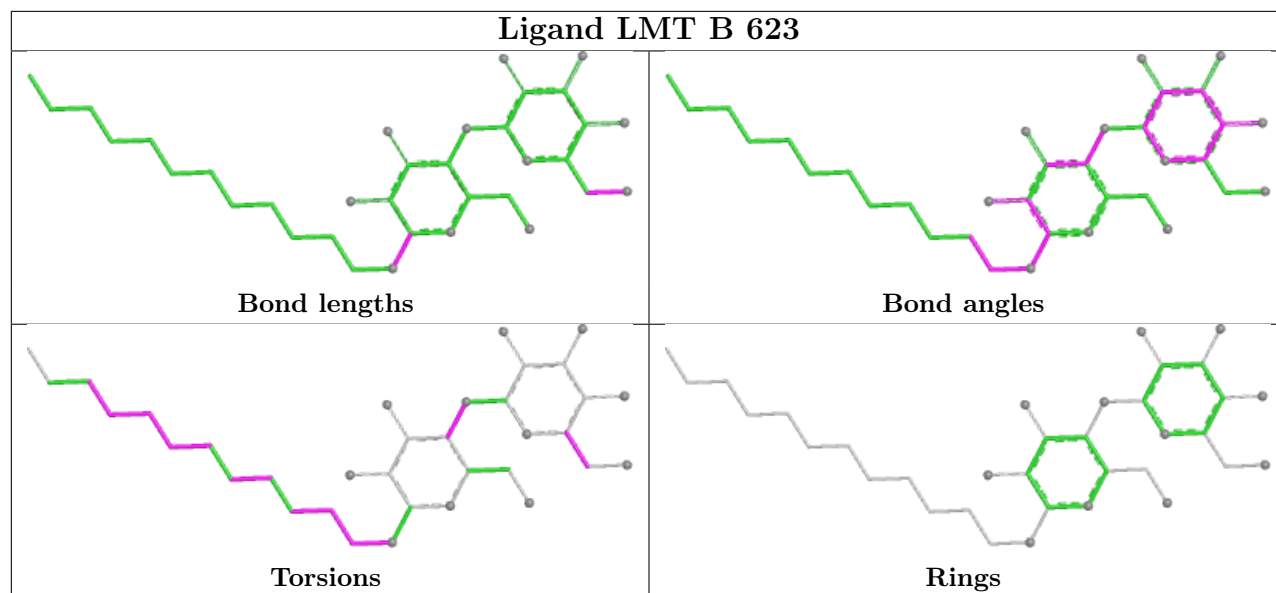


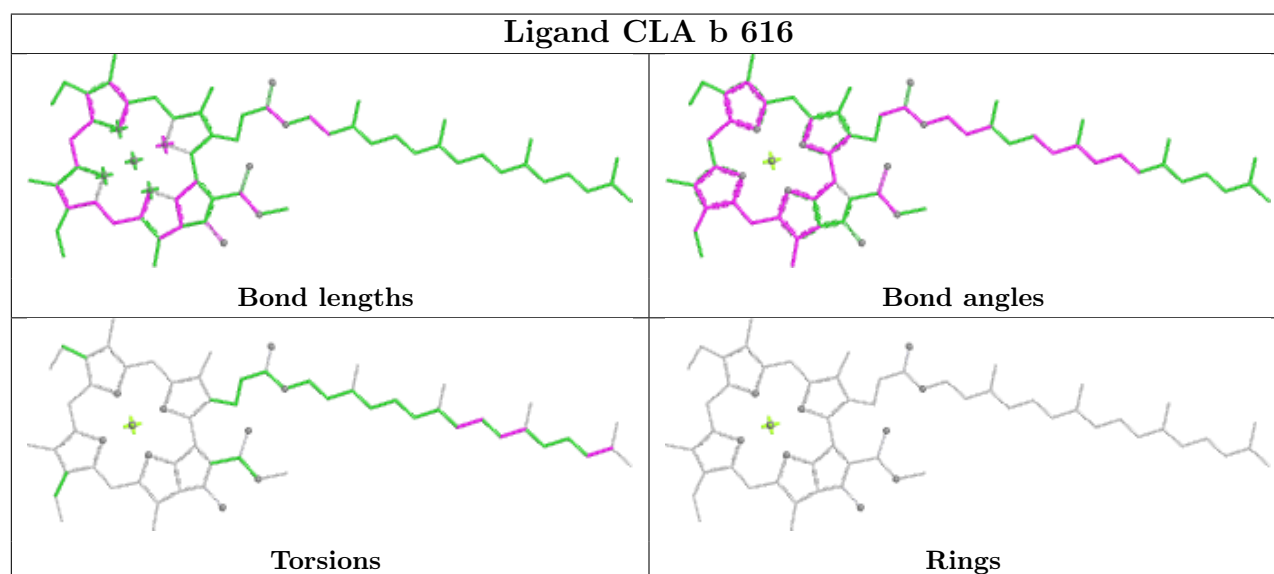
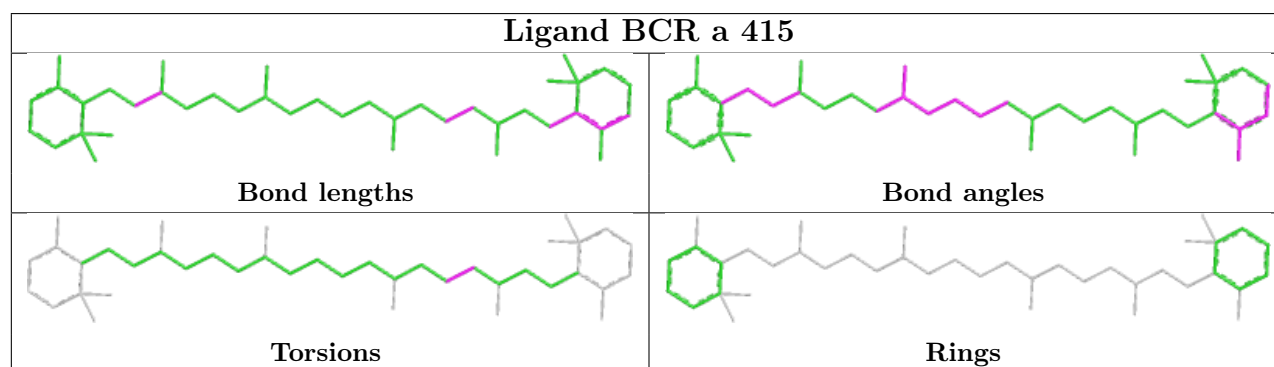
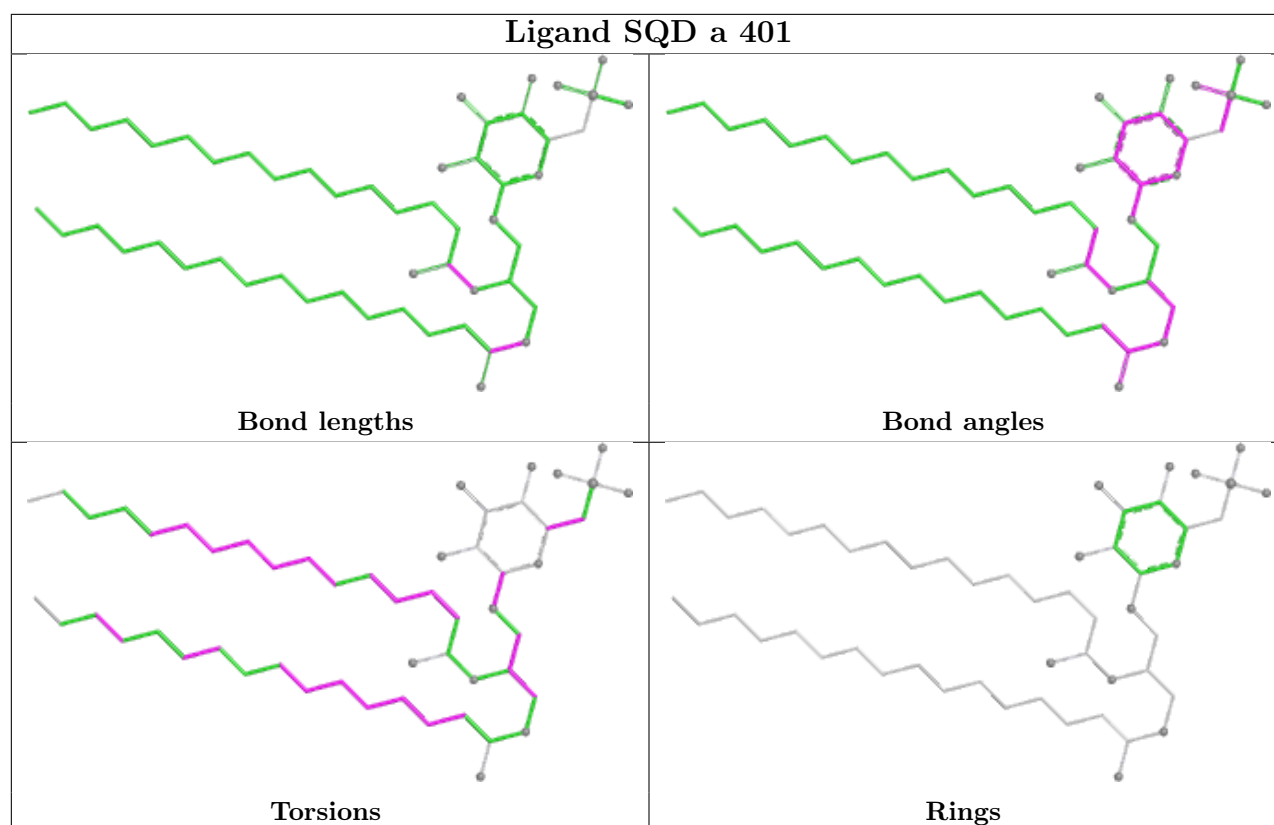


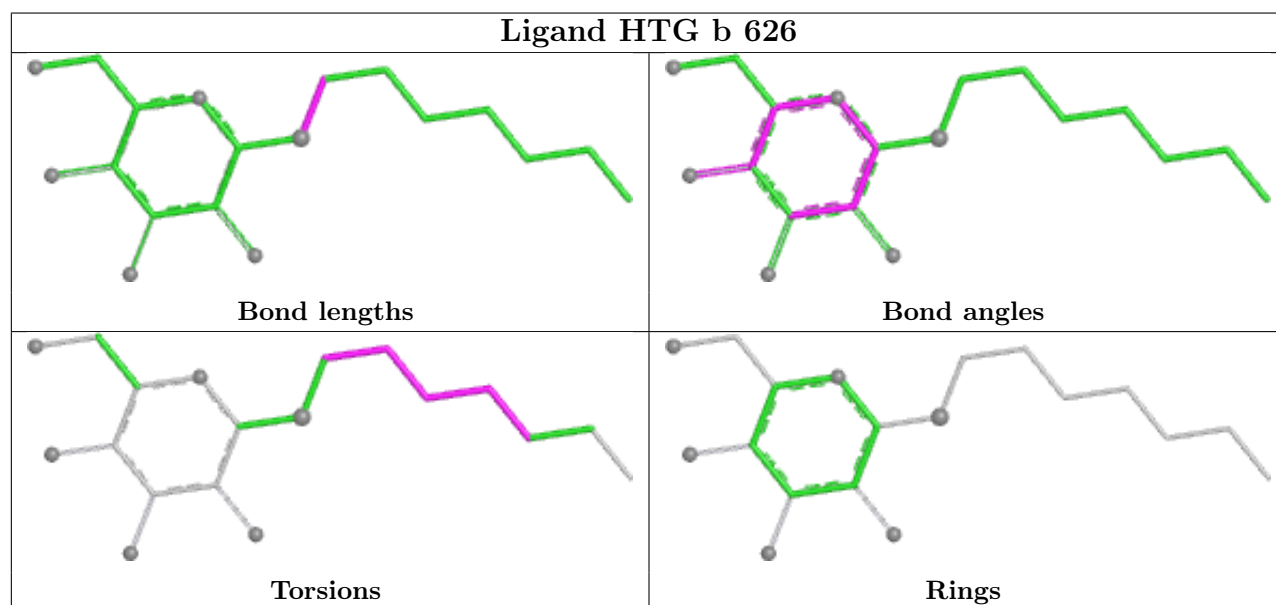
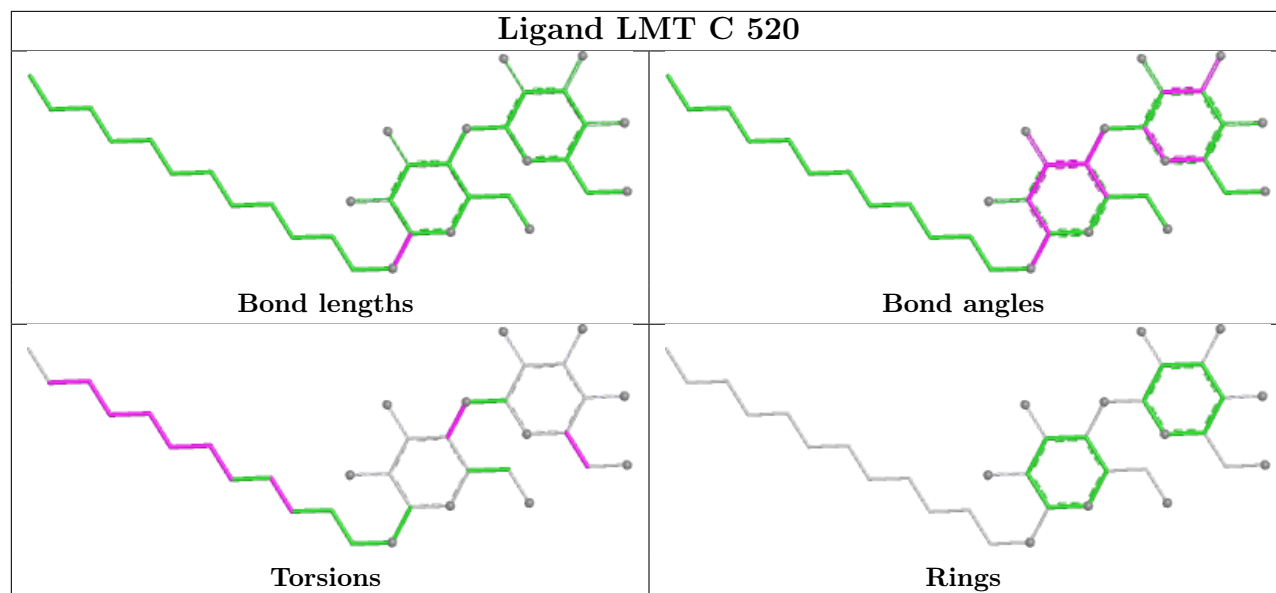


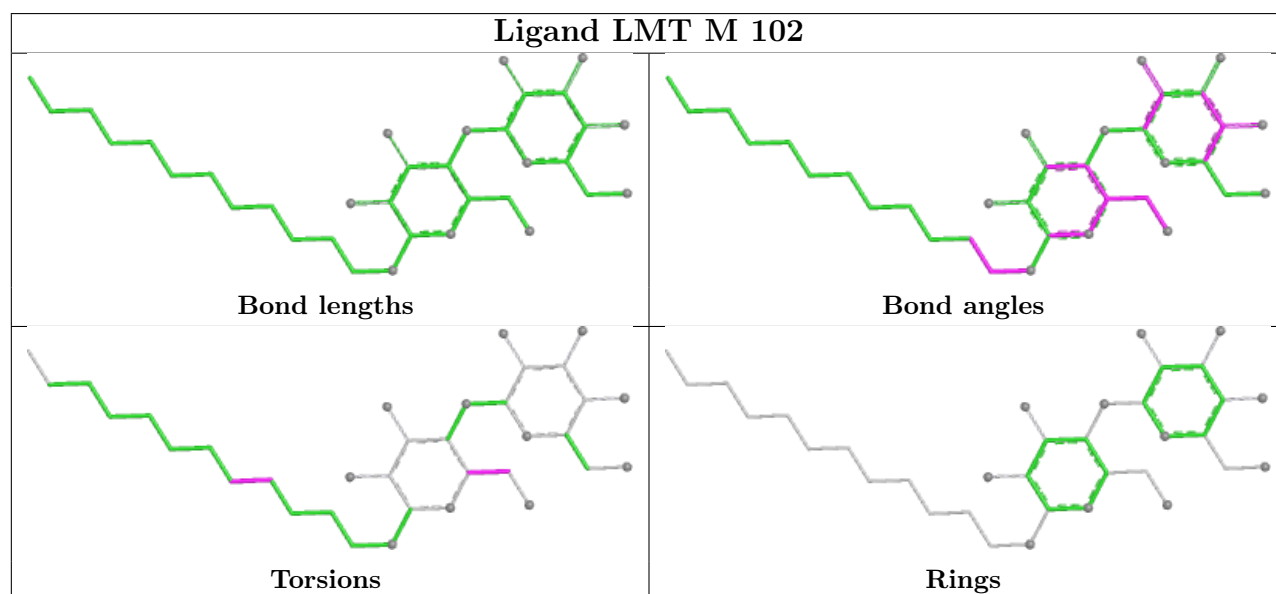
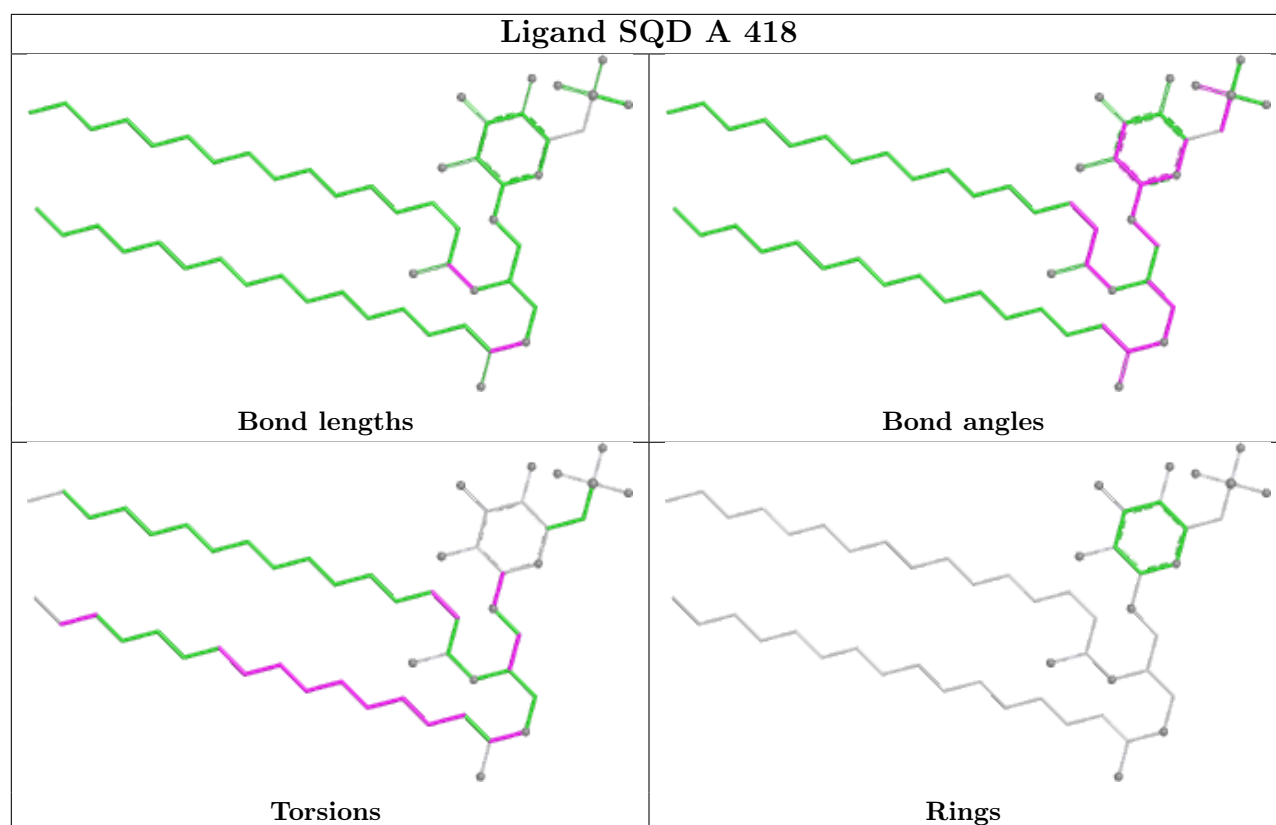
Ligand CLA a 414**Ligand CLA c 914****Ligand PHO a 412**

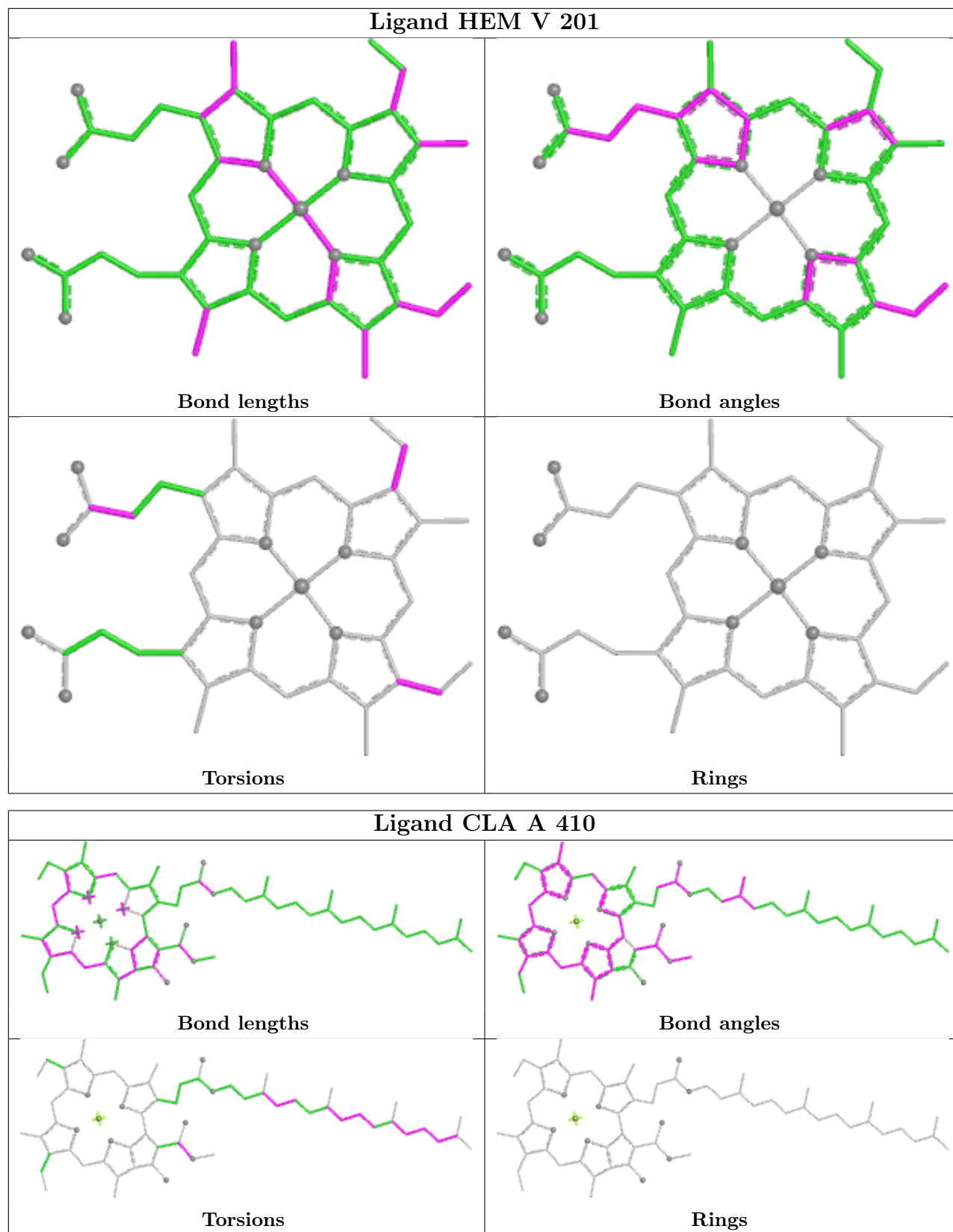




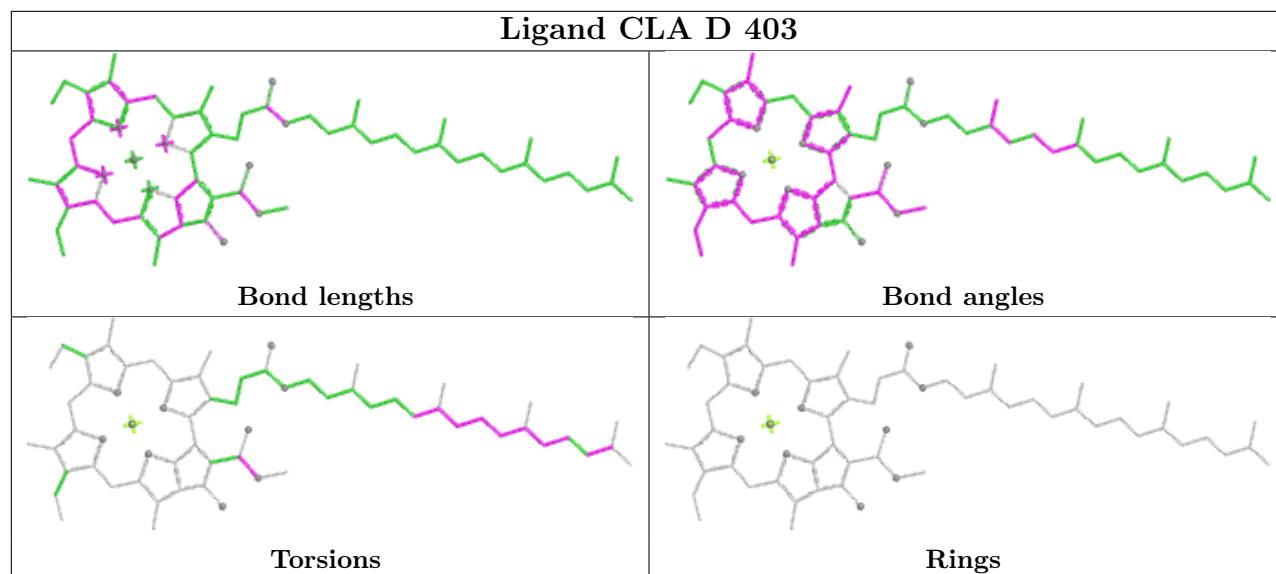




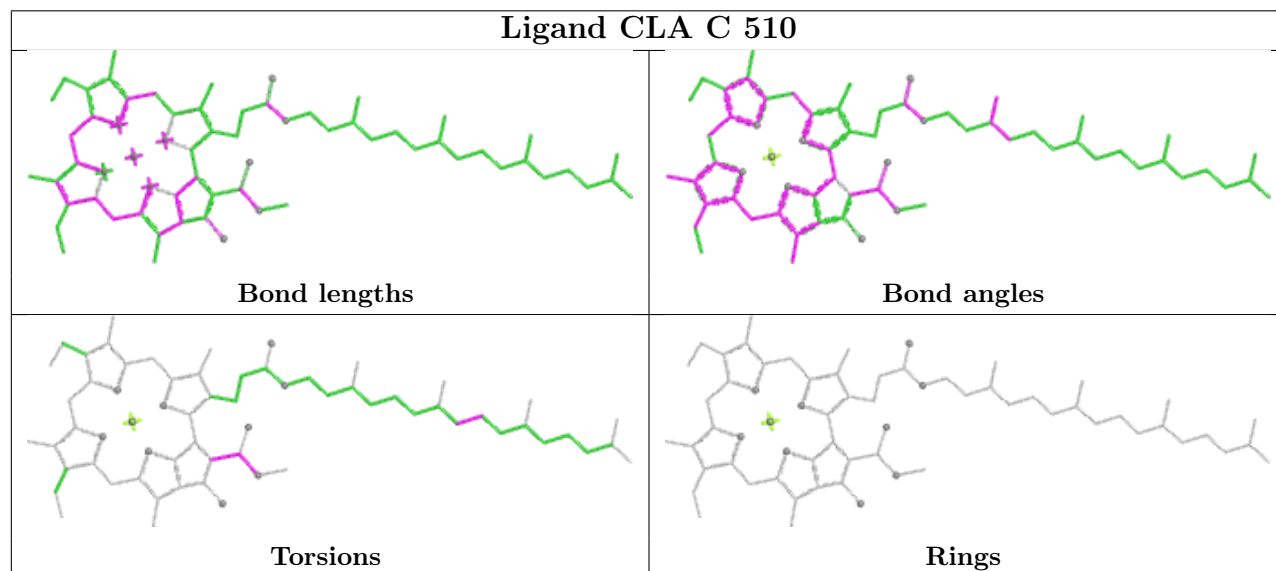




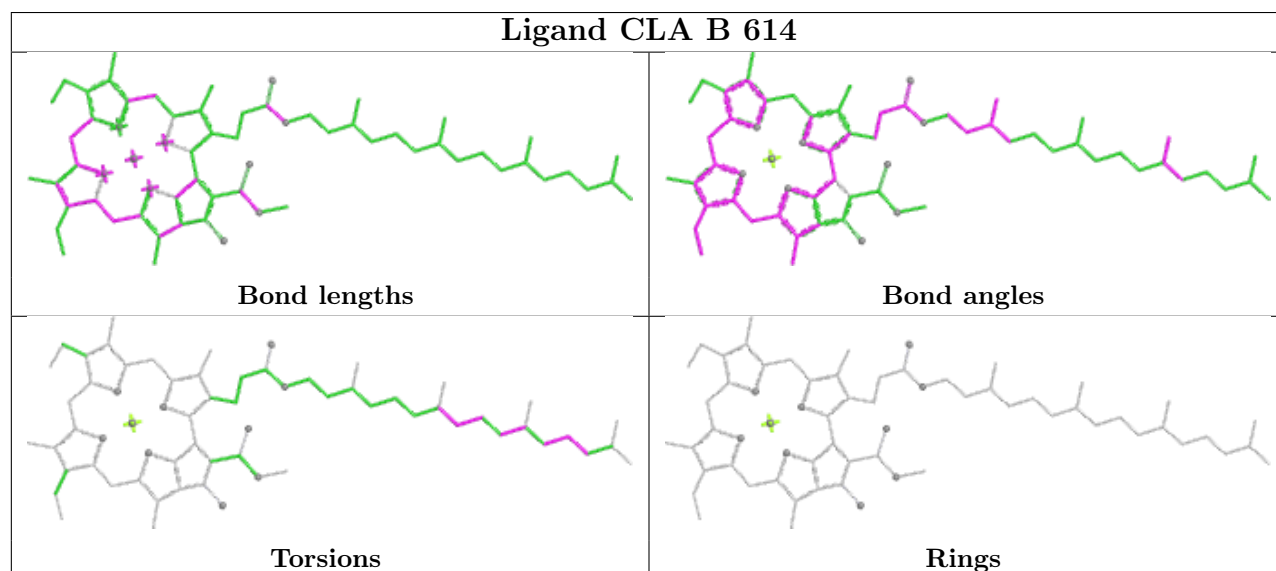
Ligand CLA D 403



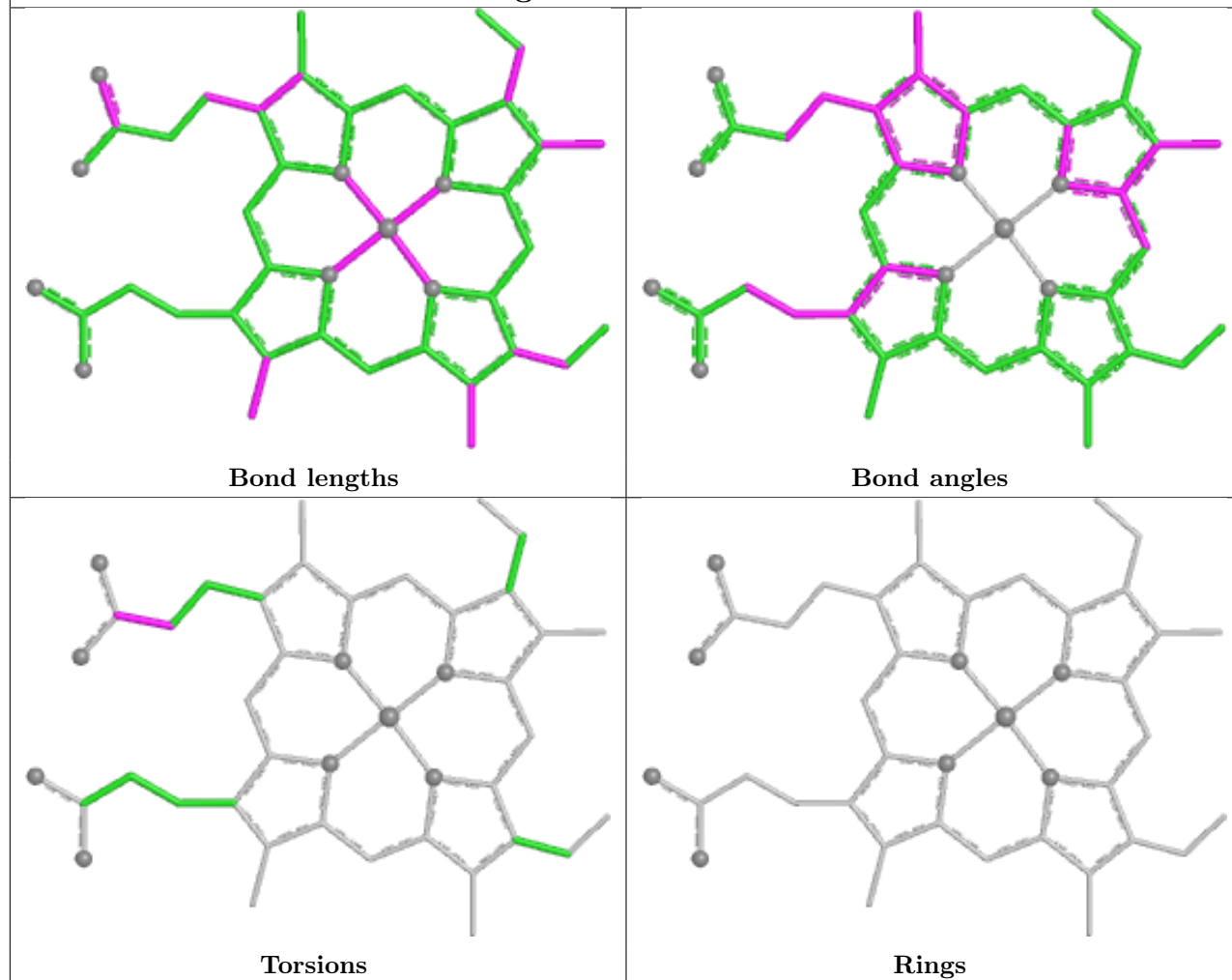
Ligand CLA C 510



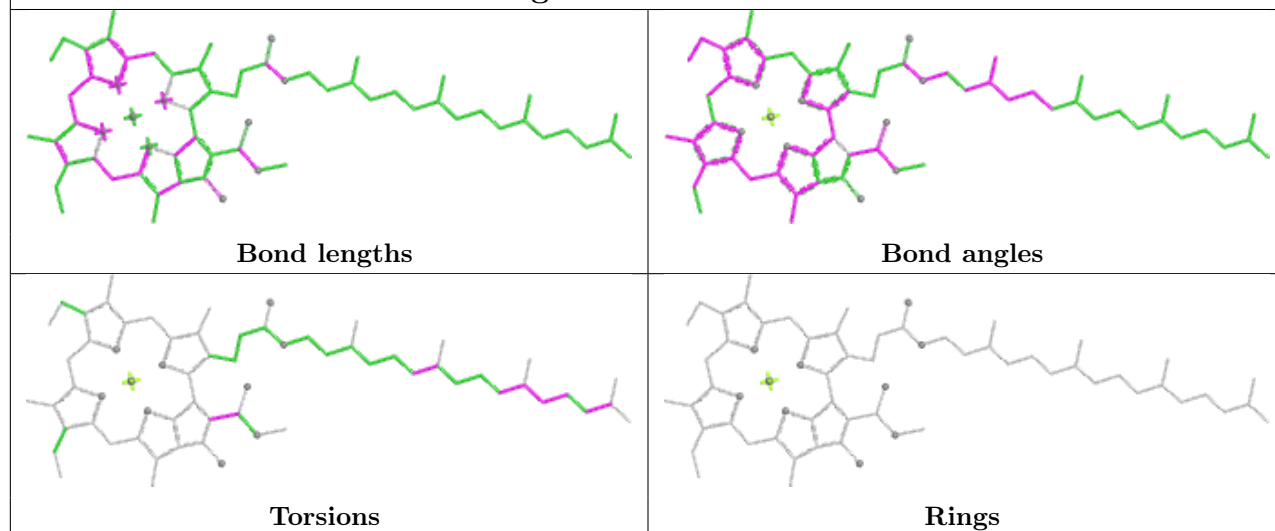
Ligand CLA B 614

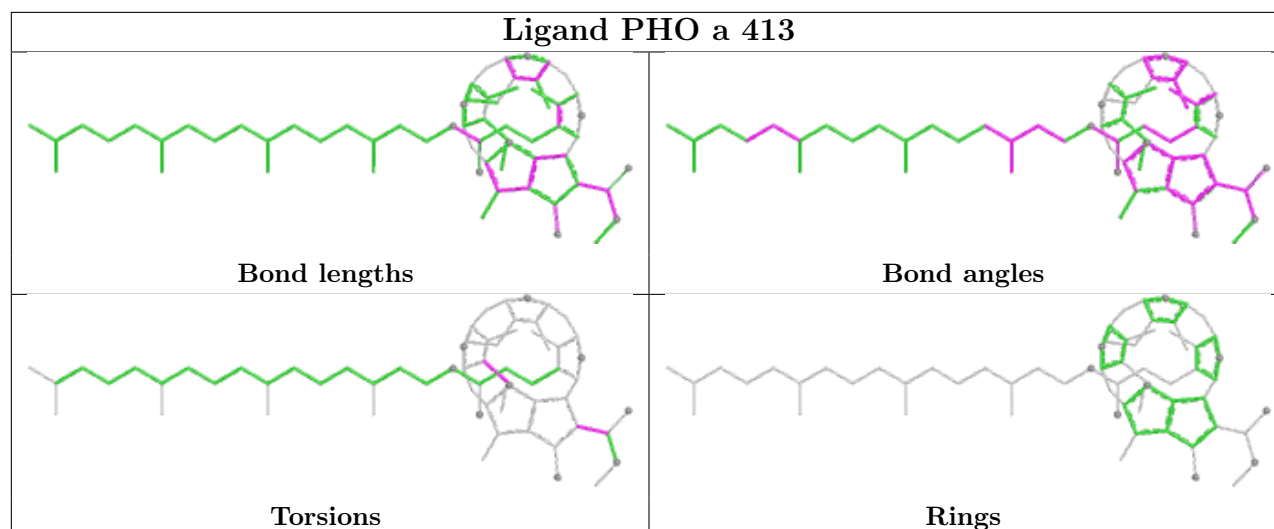
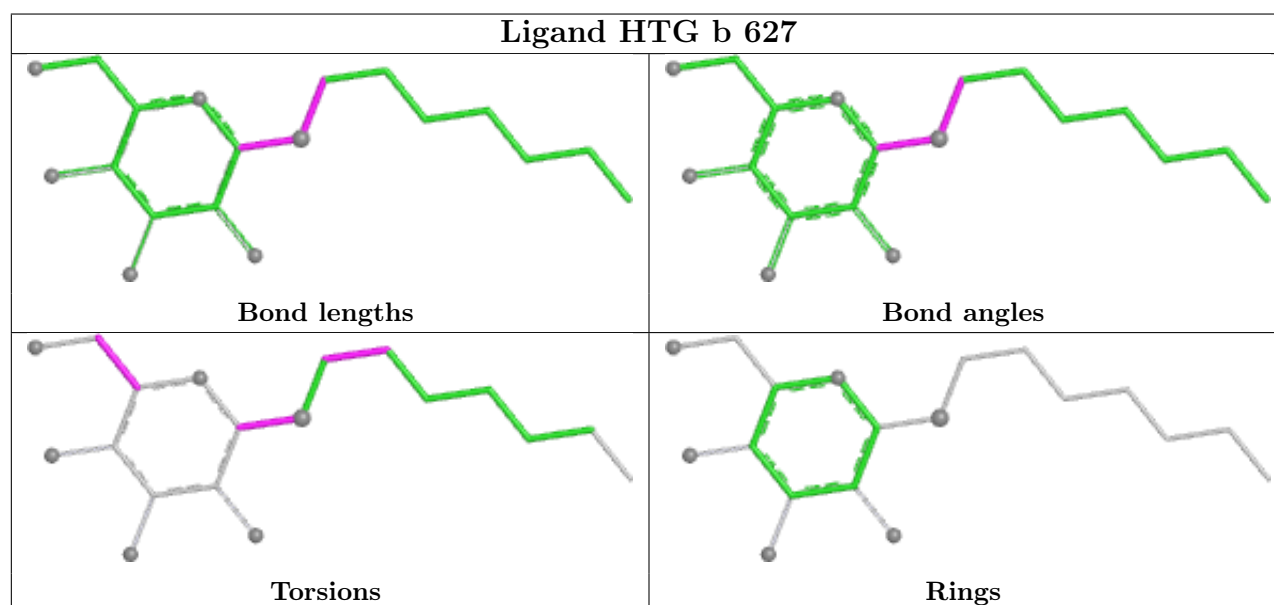
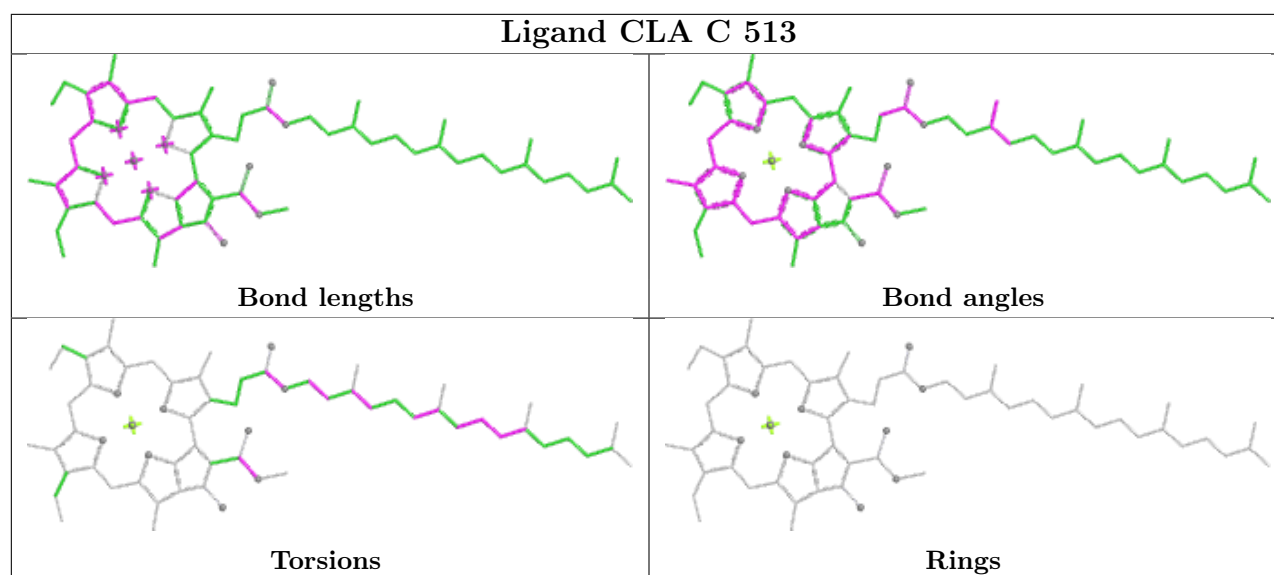


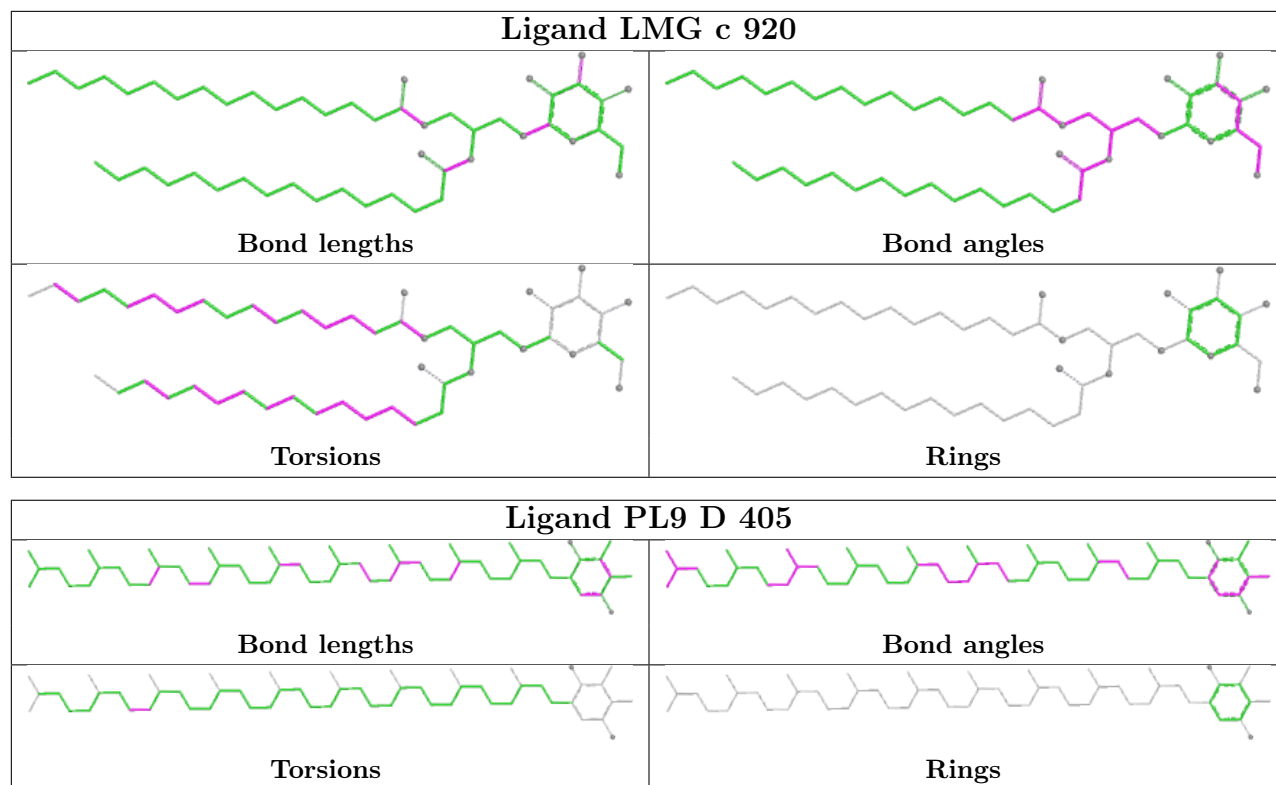
Ligand HEM f 101

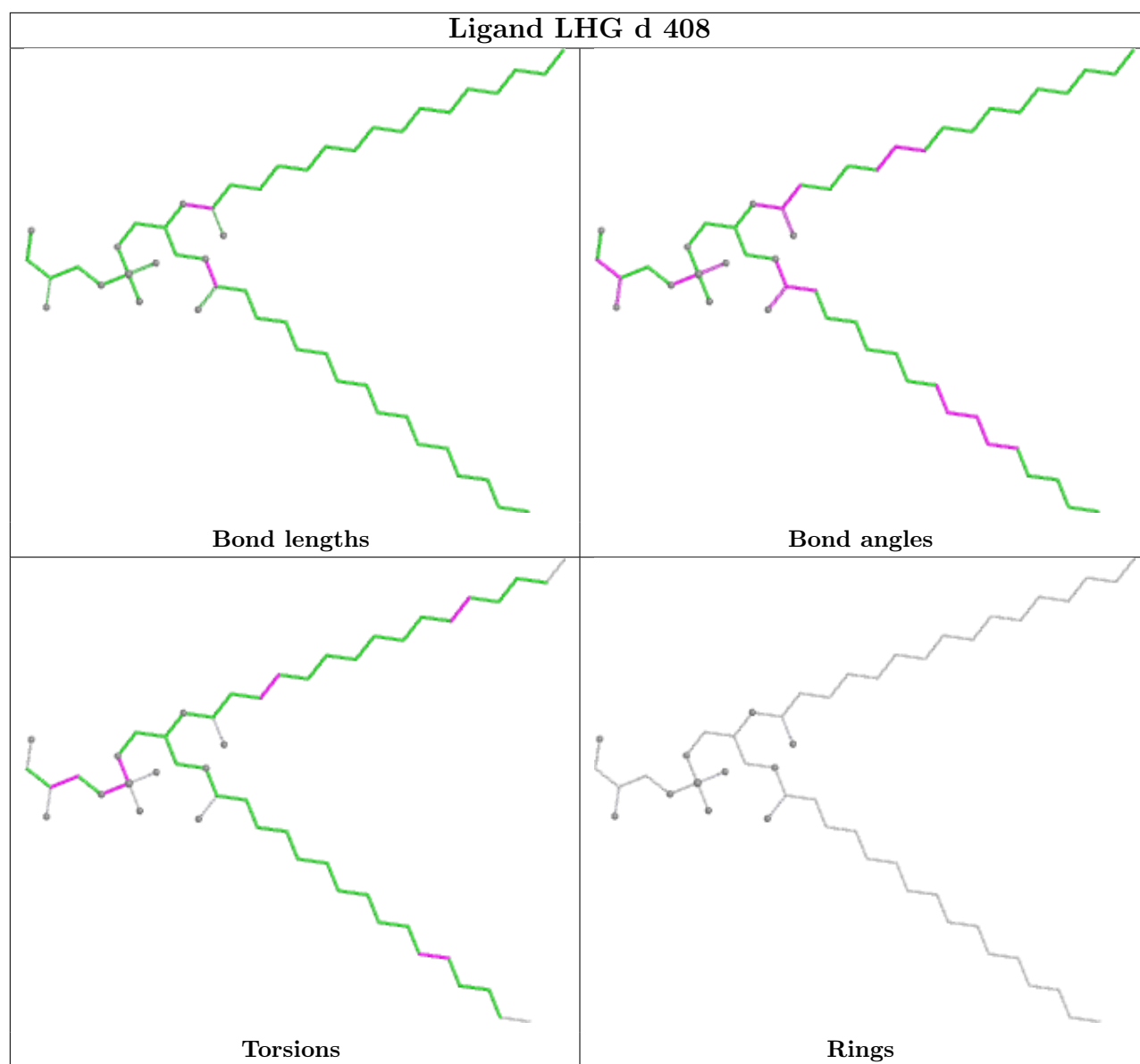


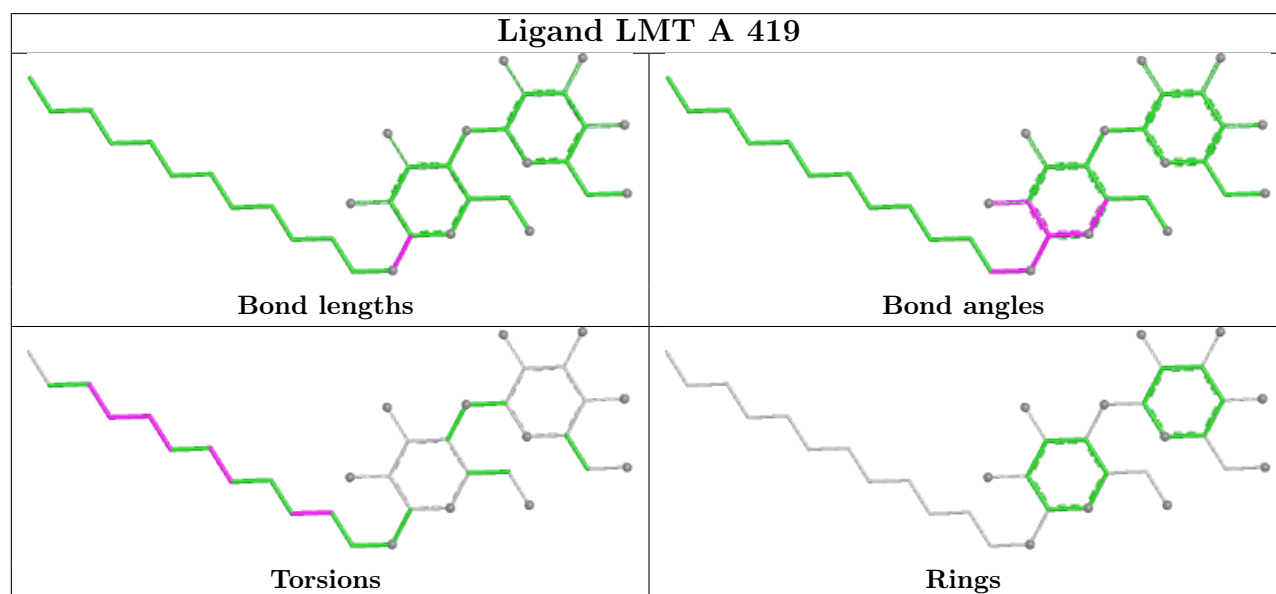
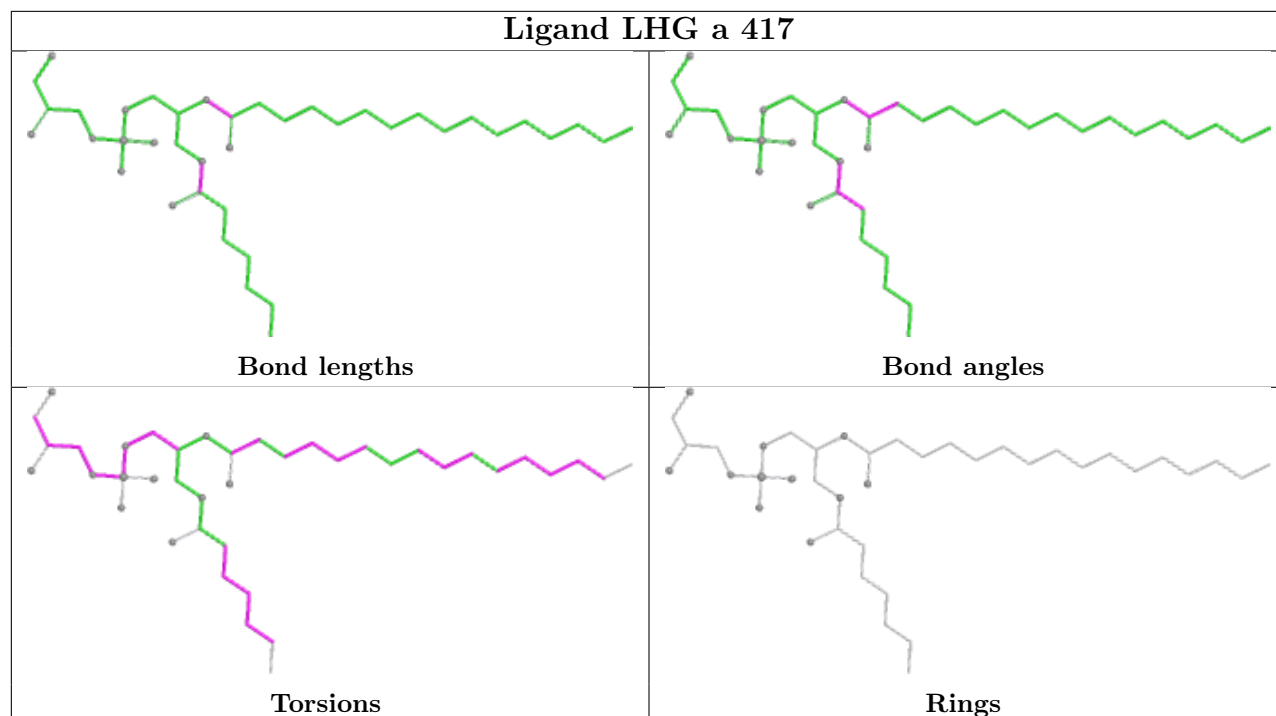
Ligand CLA C 504

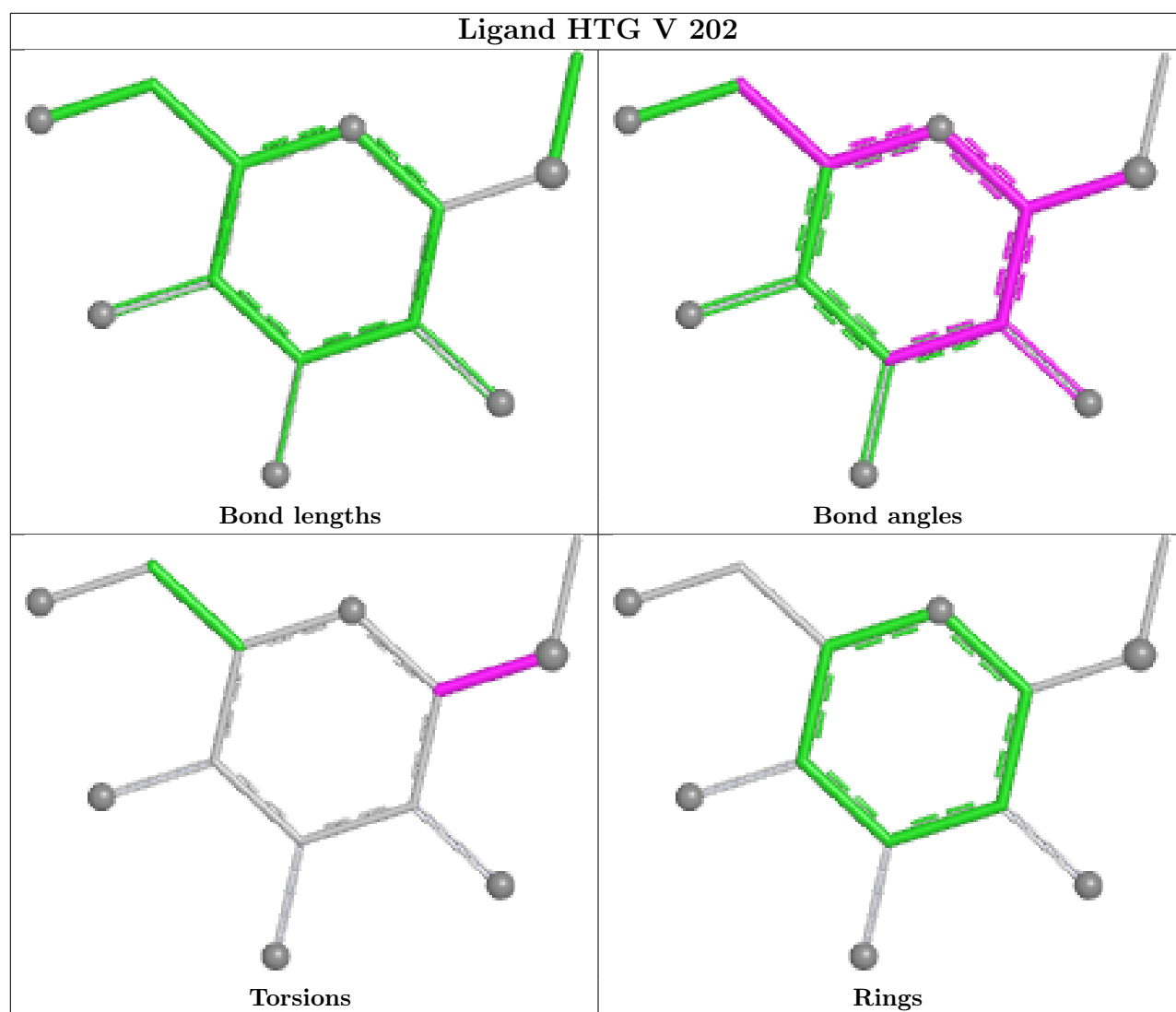


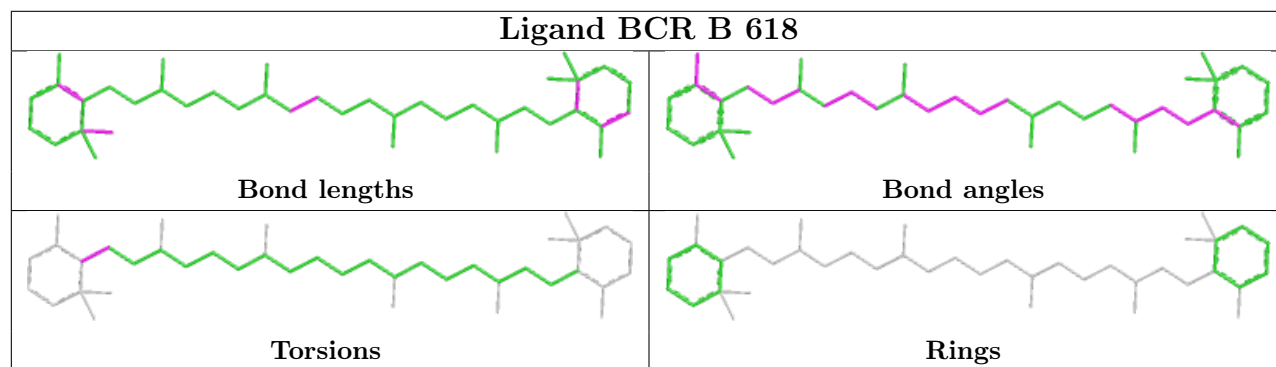
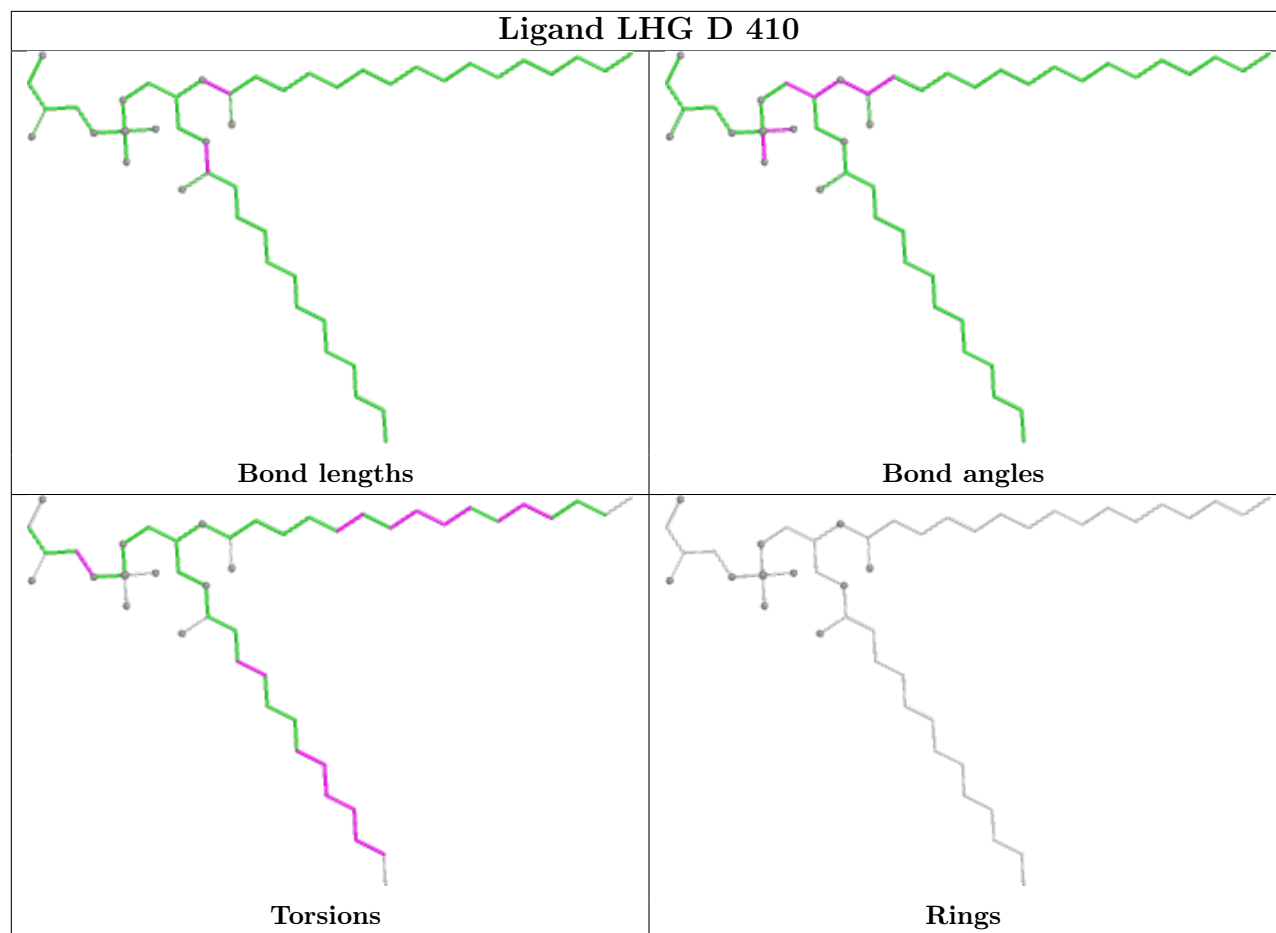


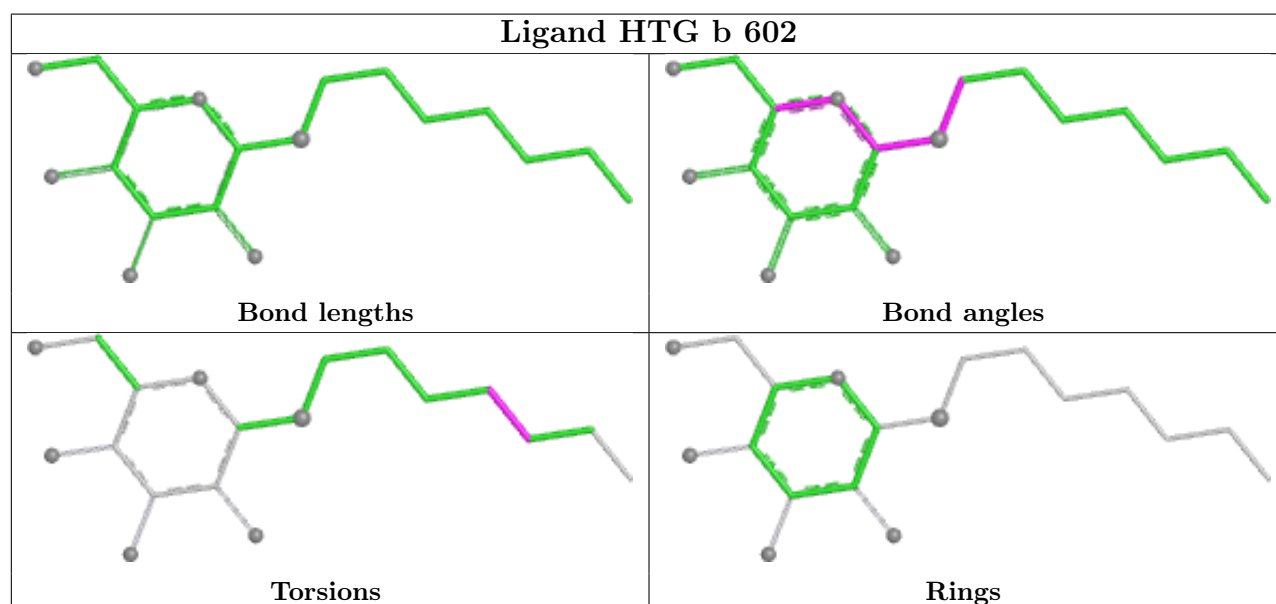
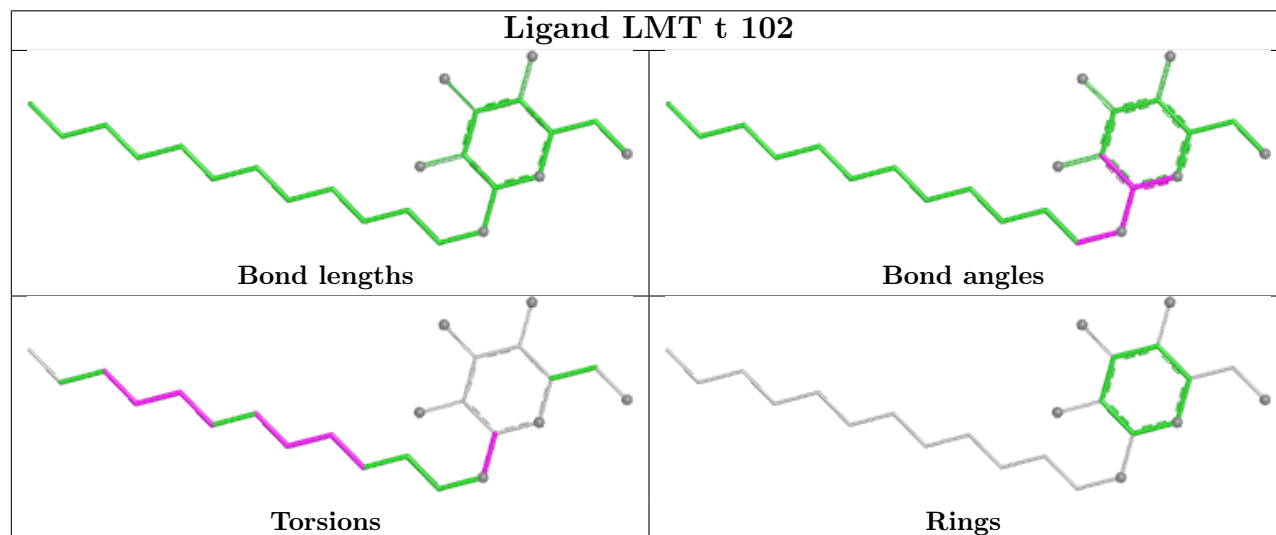
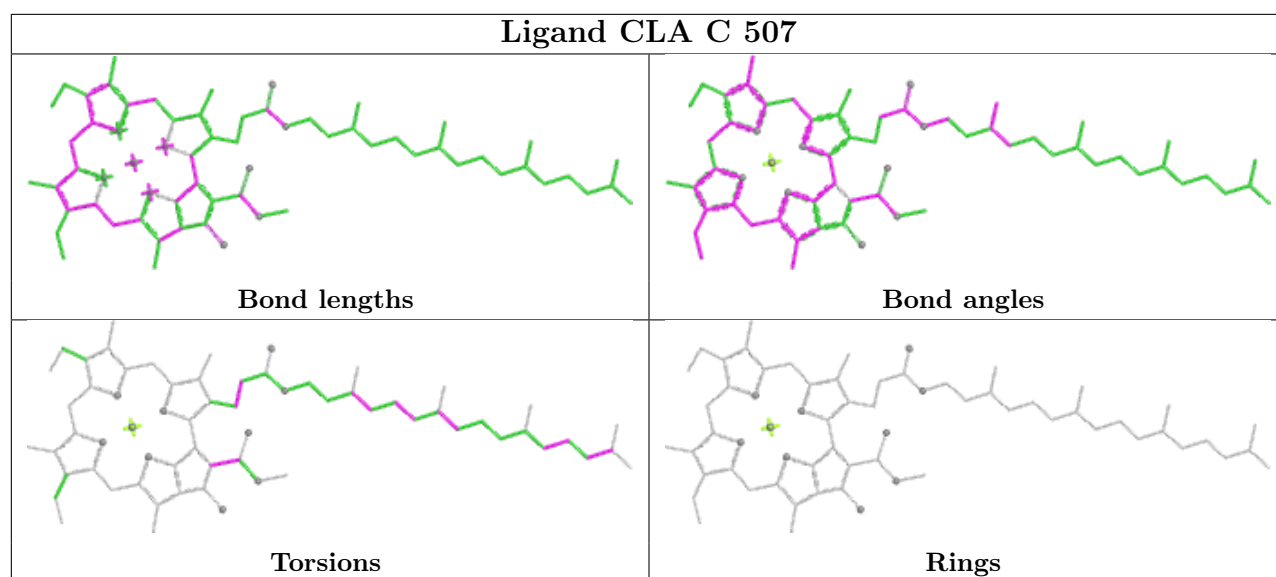


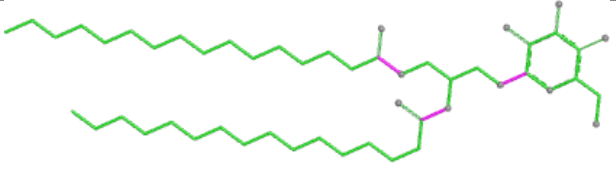
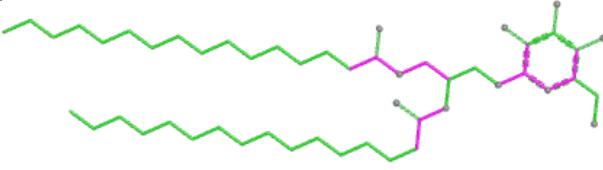
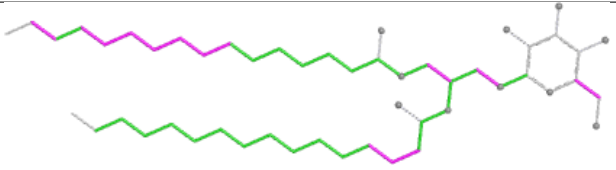
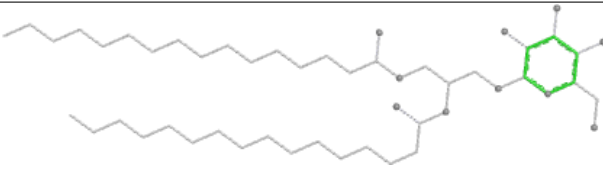
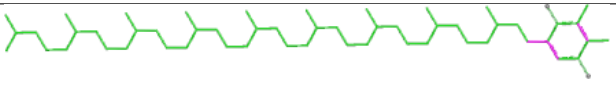
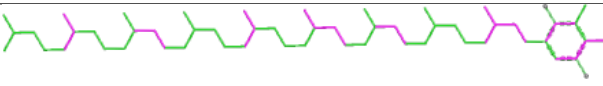
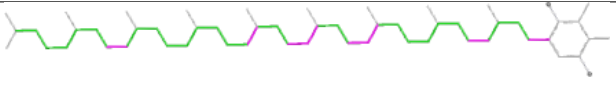
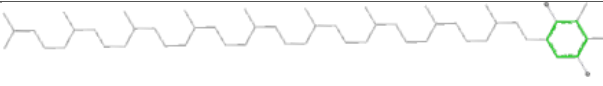




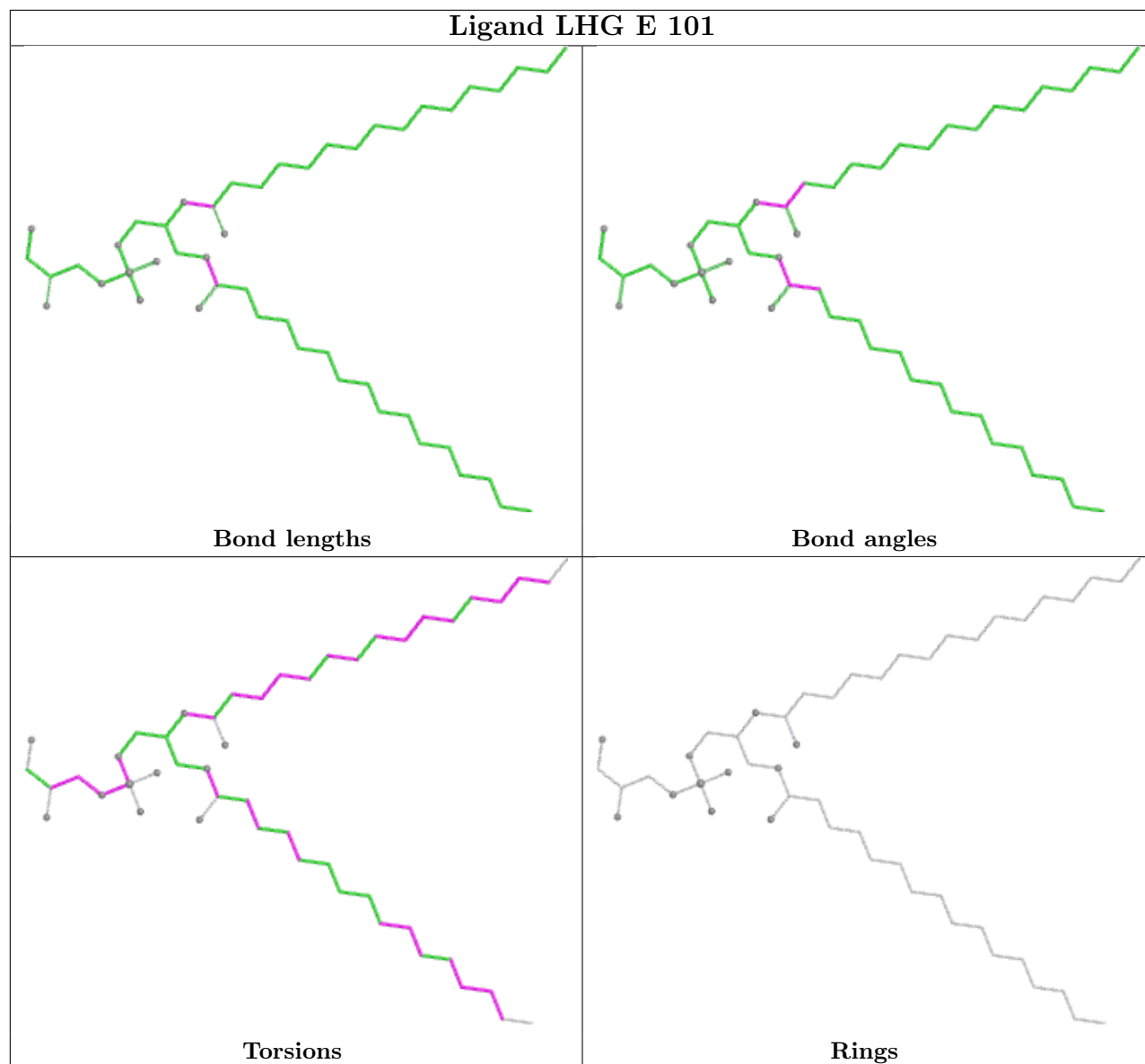




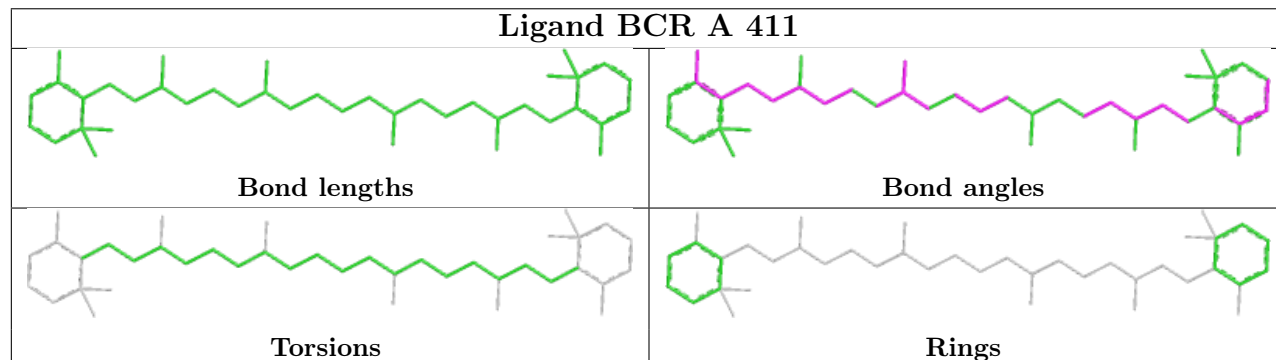


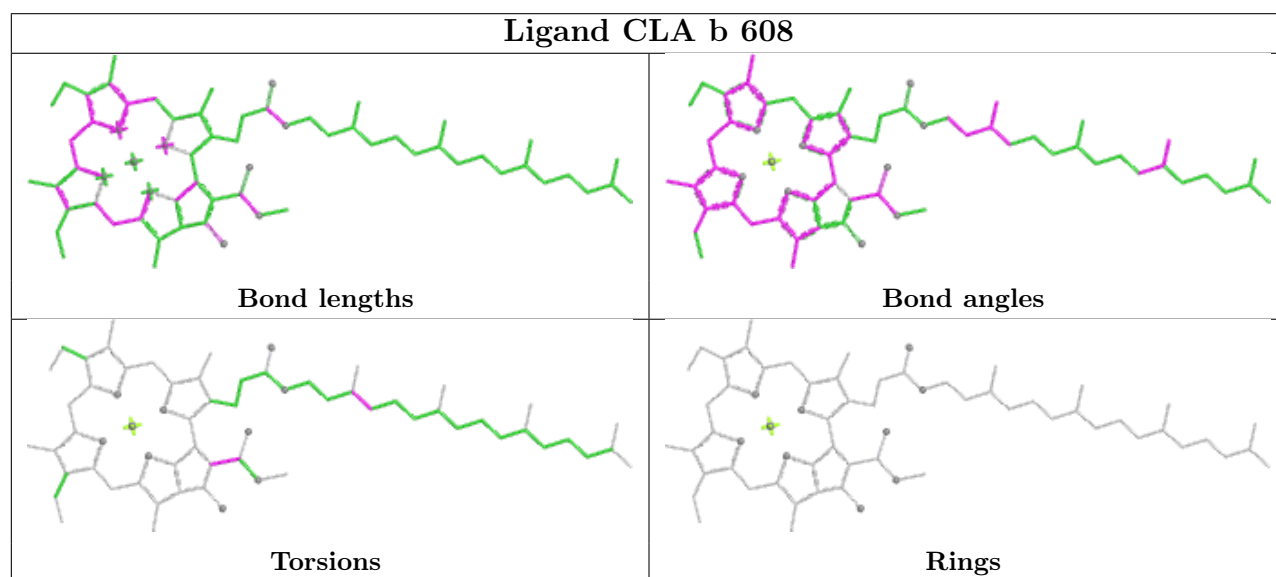
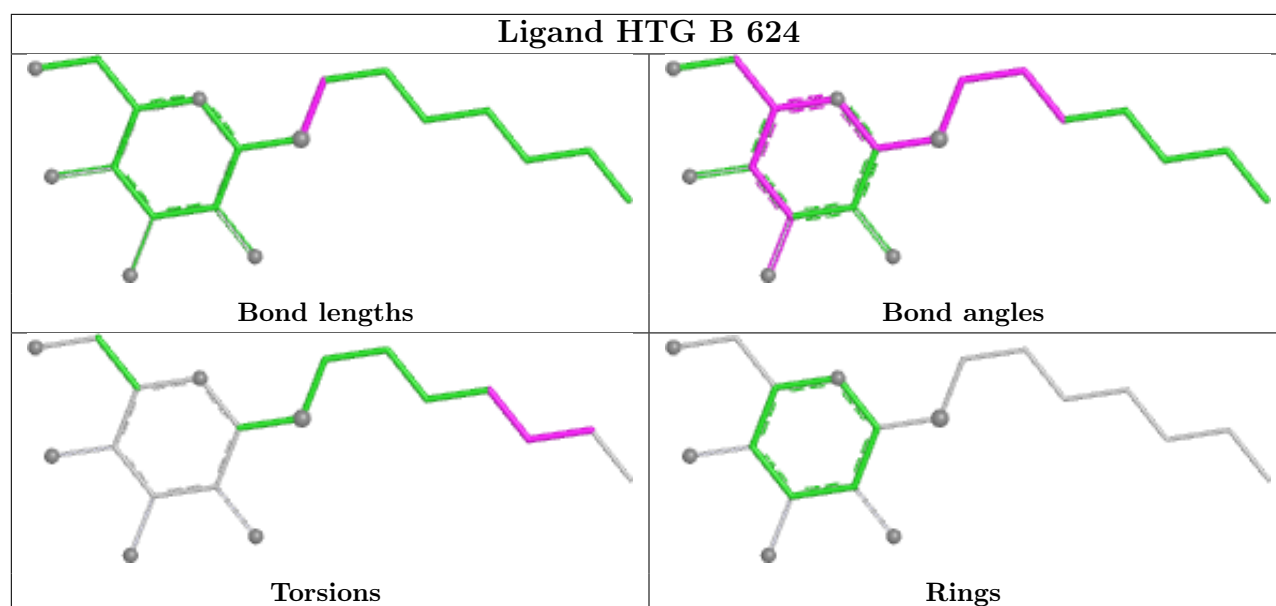
Ligand LMG c 921	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 414	
 Bond lengths	 Bond angles
 Torsions	 Rings

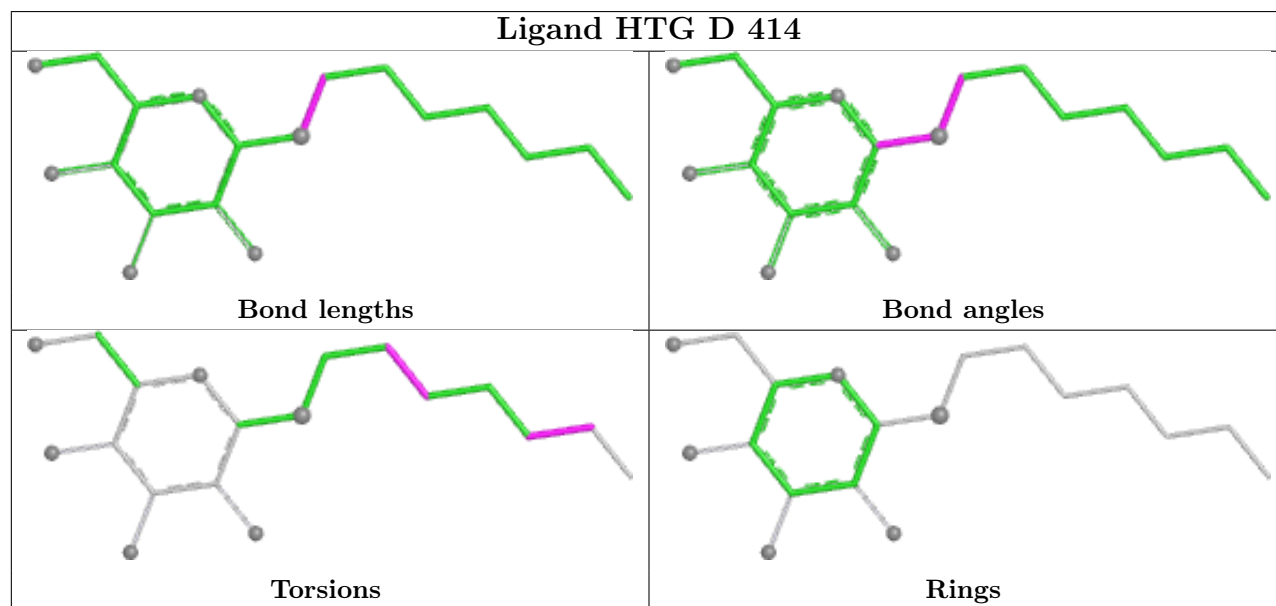
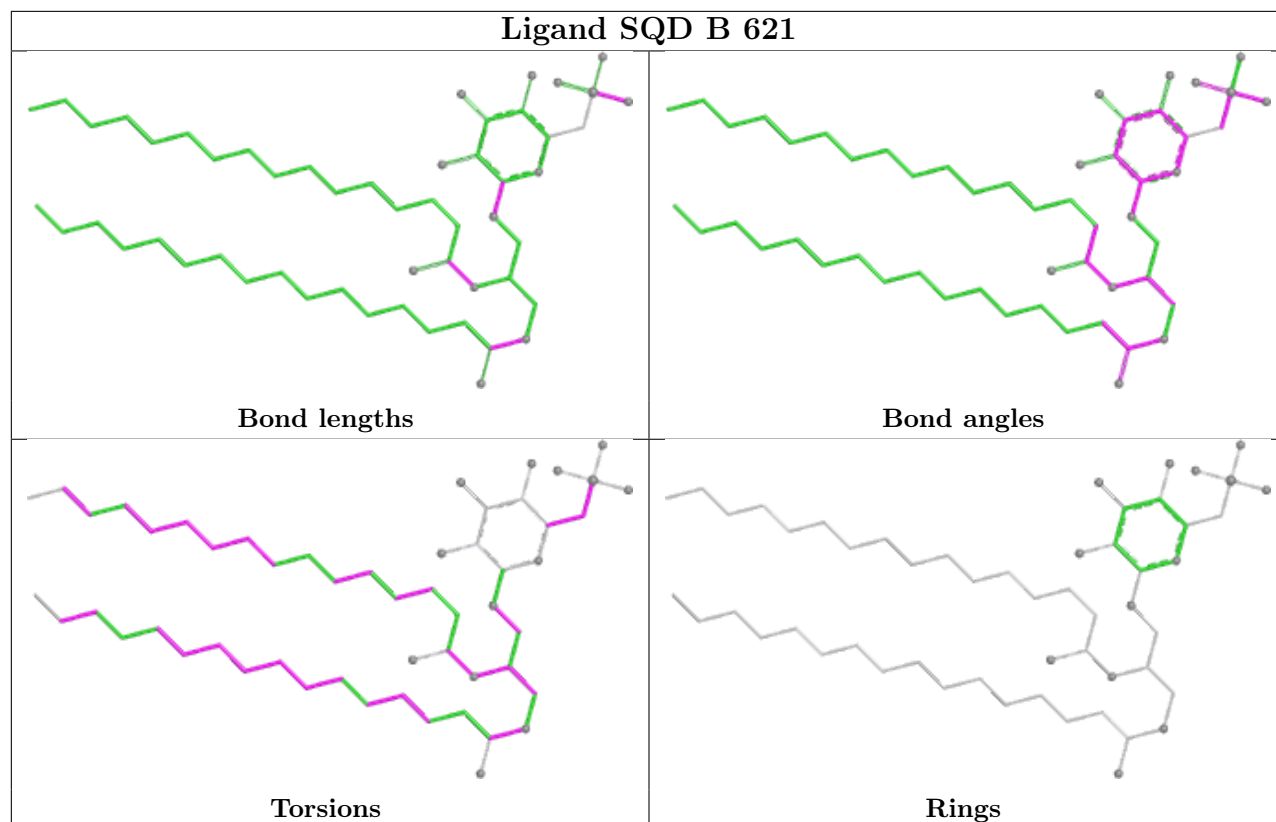
Ligand LHG E 101

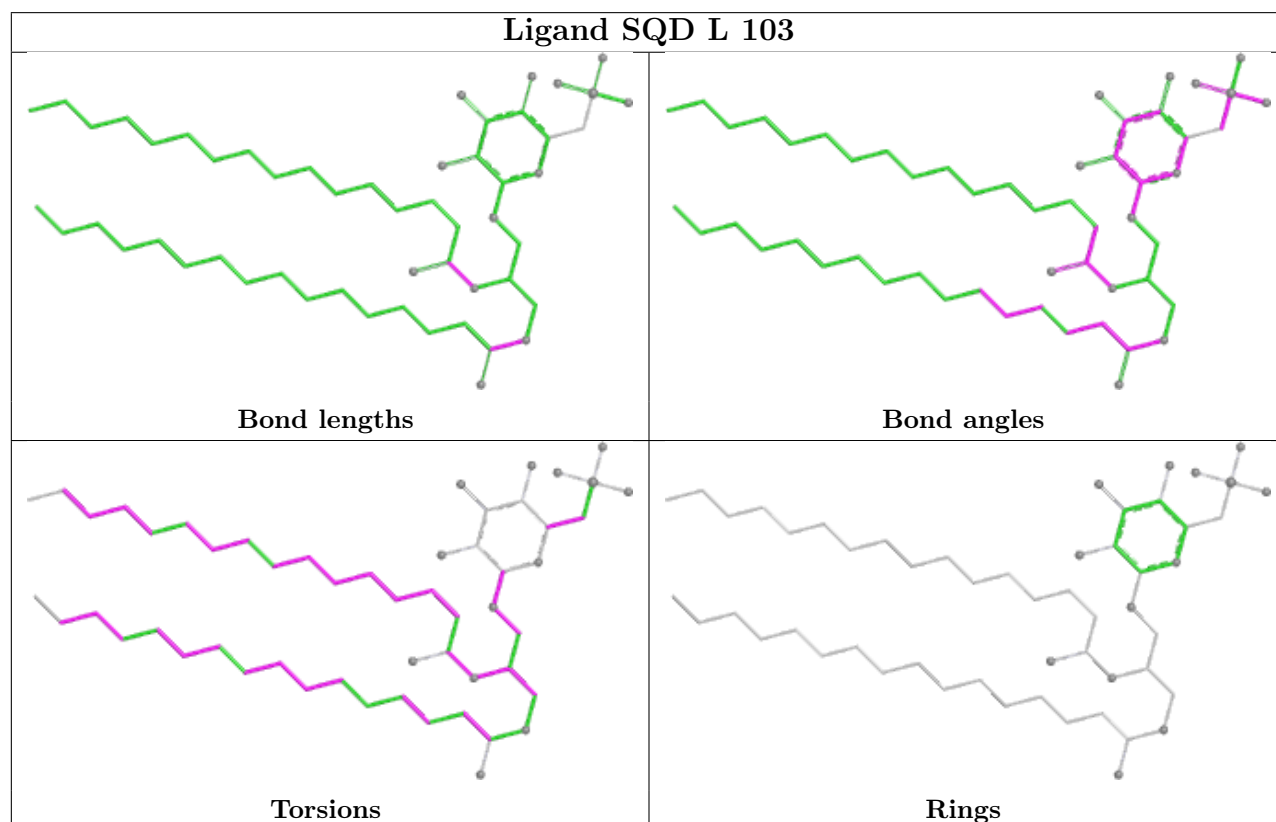
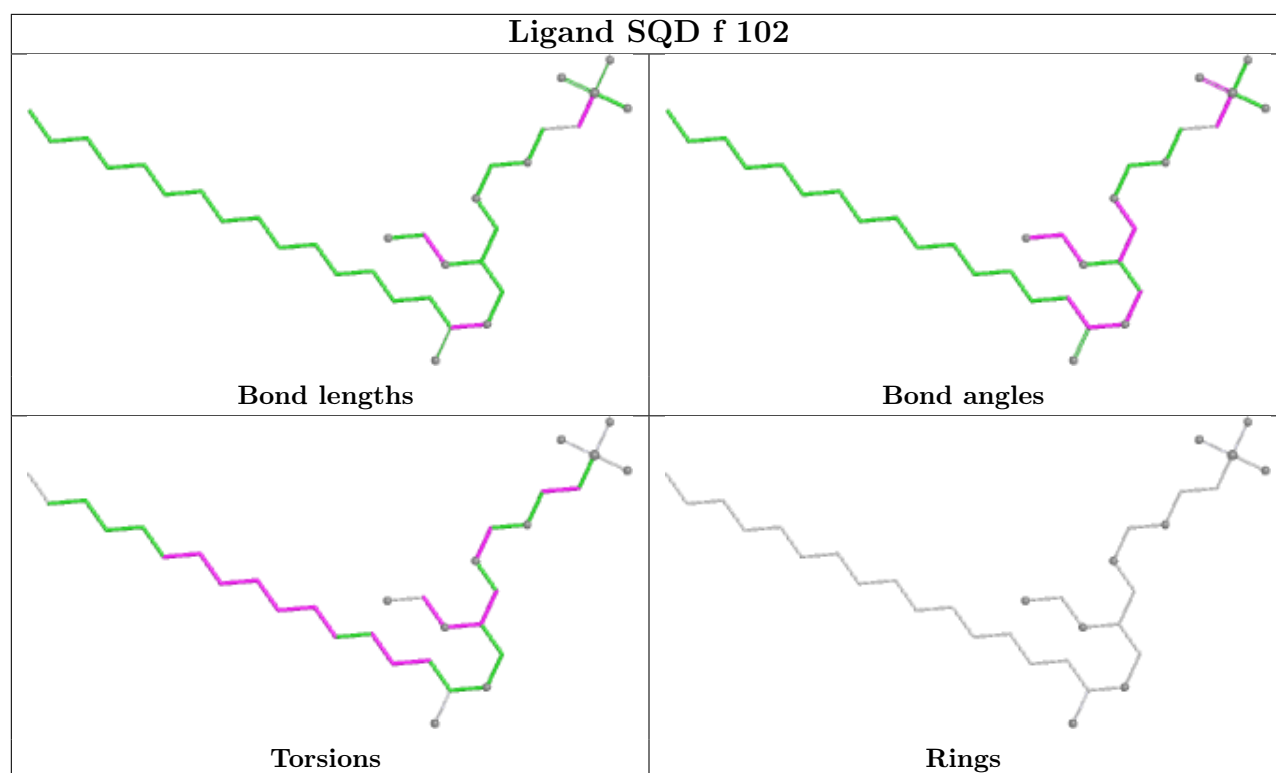


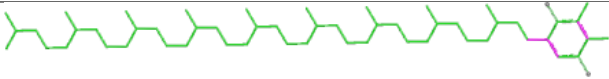
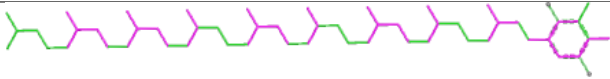
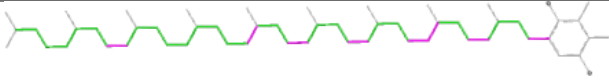
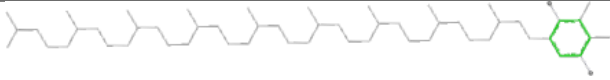
Ligand BCR A 411

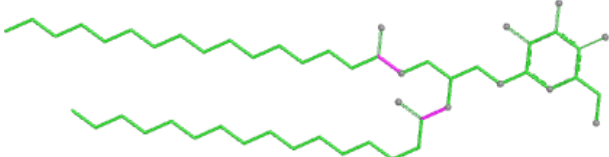
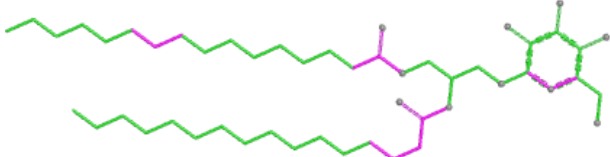
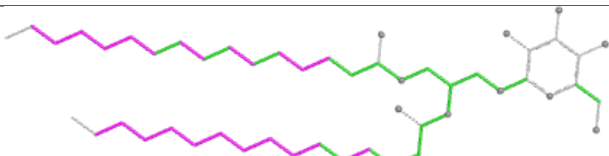
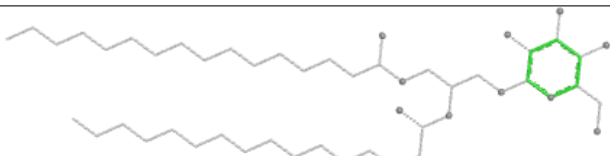


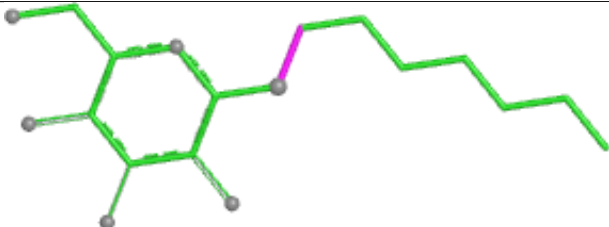
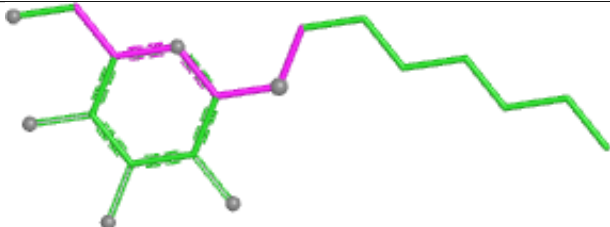
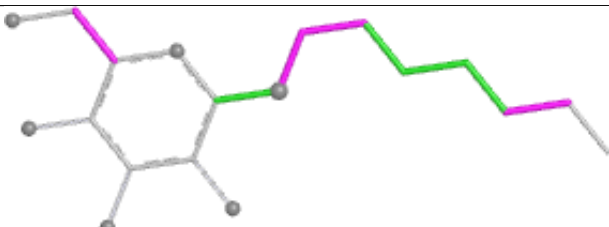
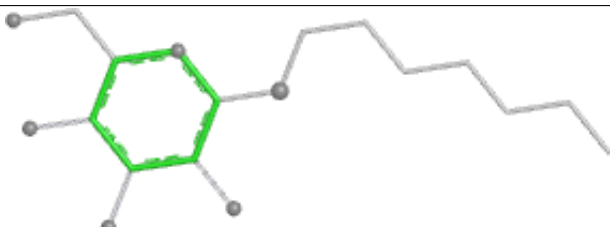




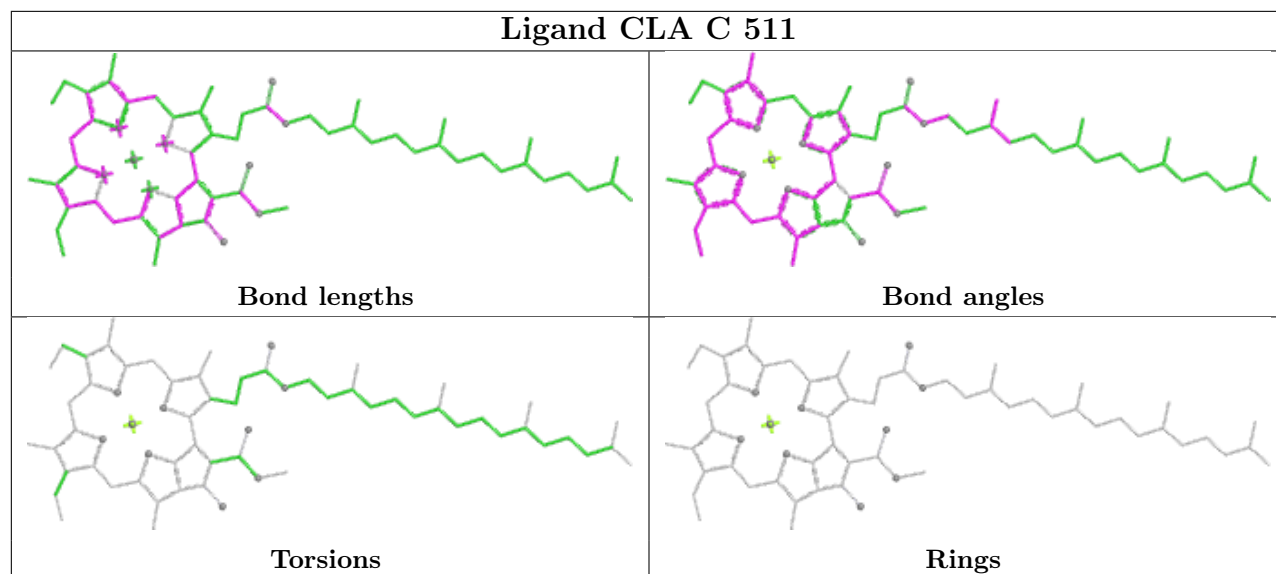


Ligand PL9 a 419	
 Bond lengths	 Bond angles
 Torsions	 Rings

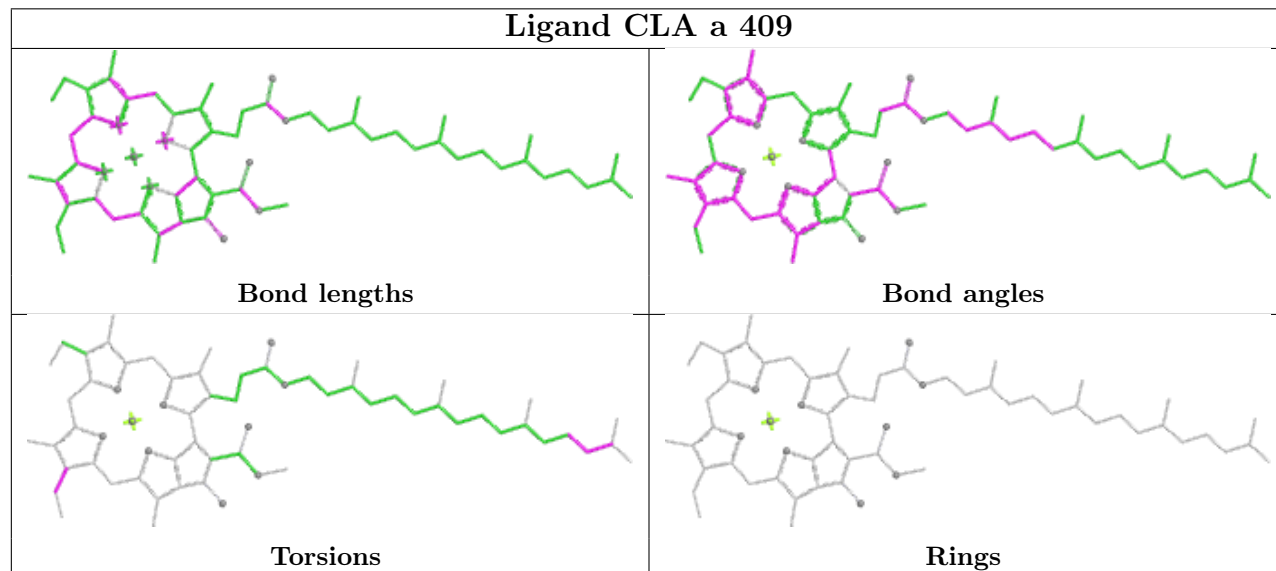
Ligand LMG b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG B 631	
 Bond lengths	 Bond angles
 Torsions	 Rings

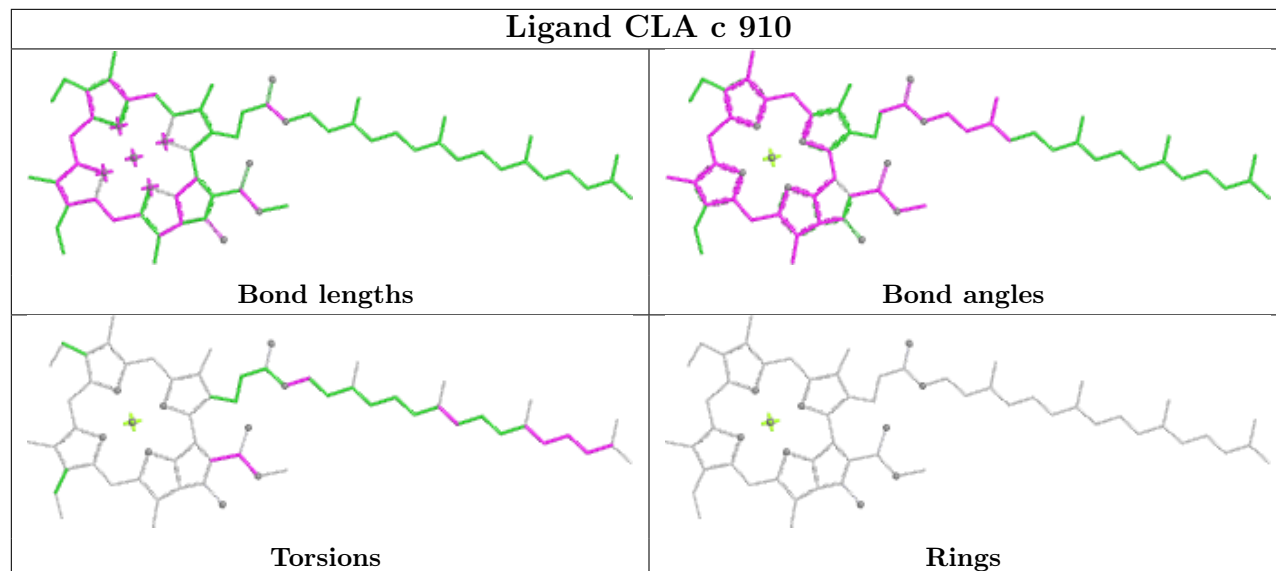
Ligand CLA C 511

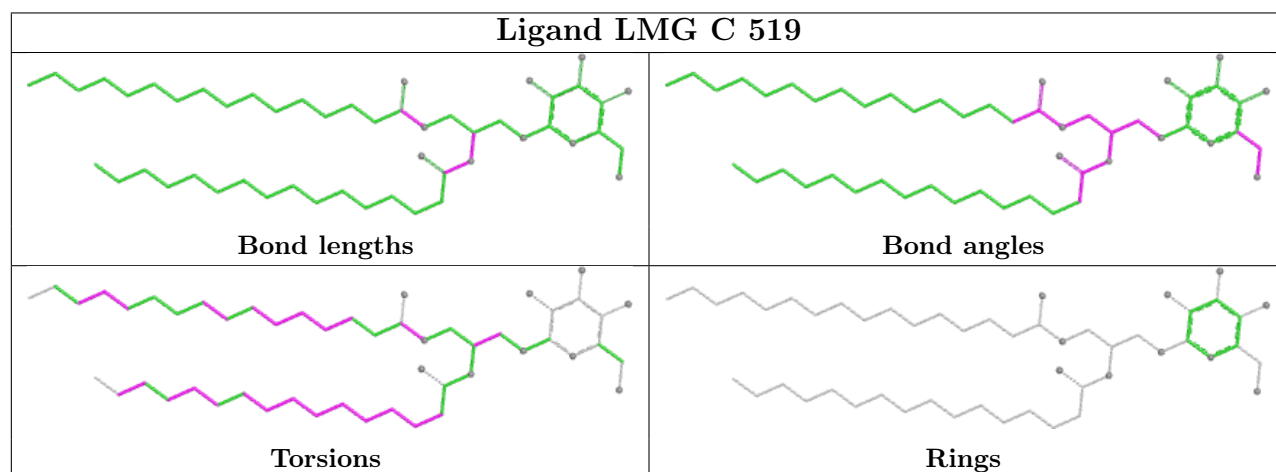
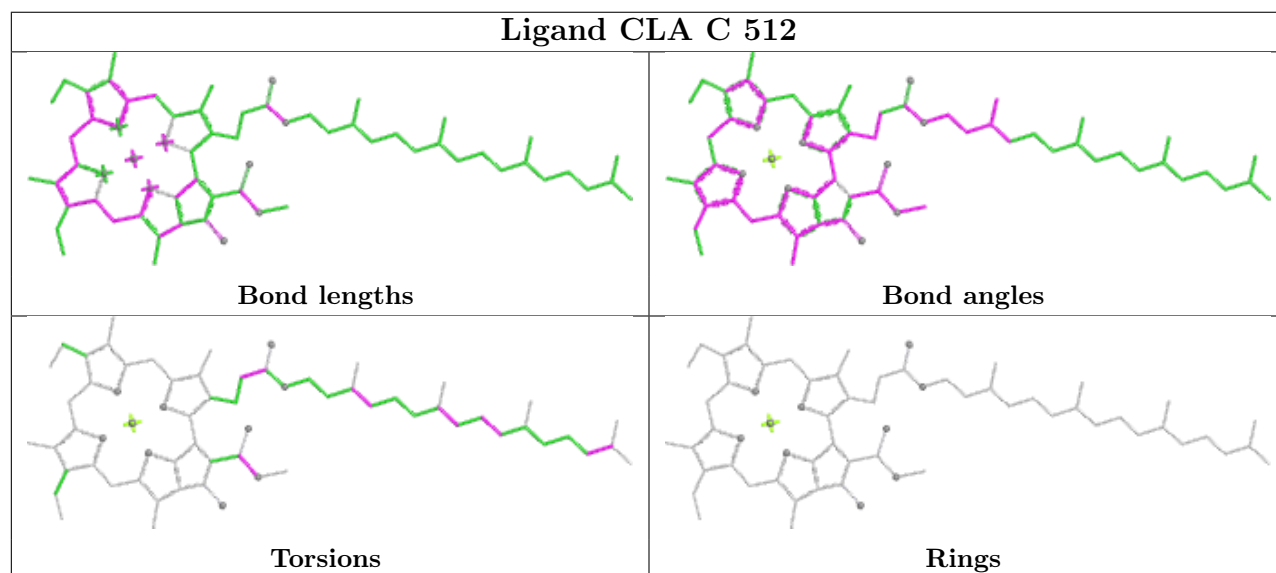
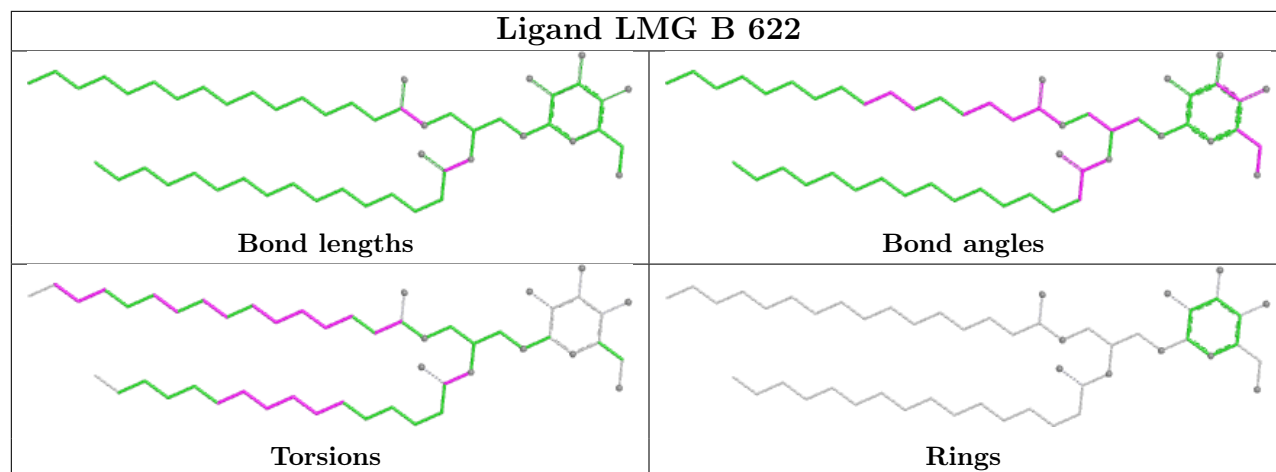


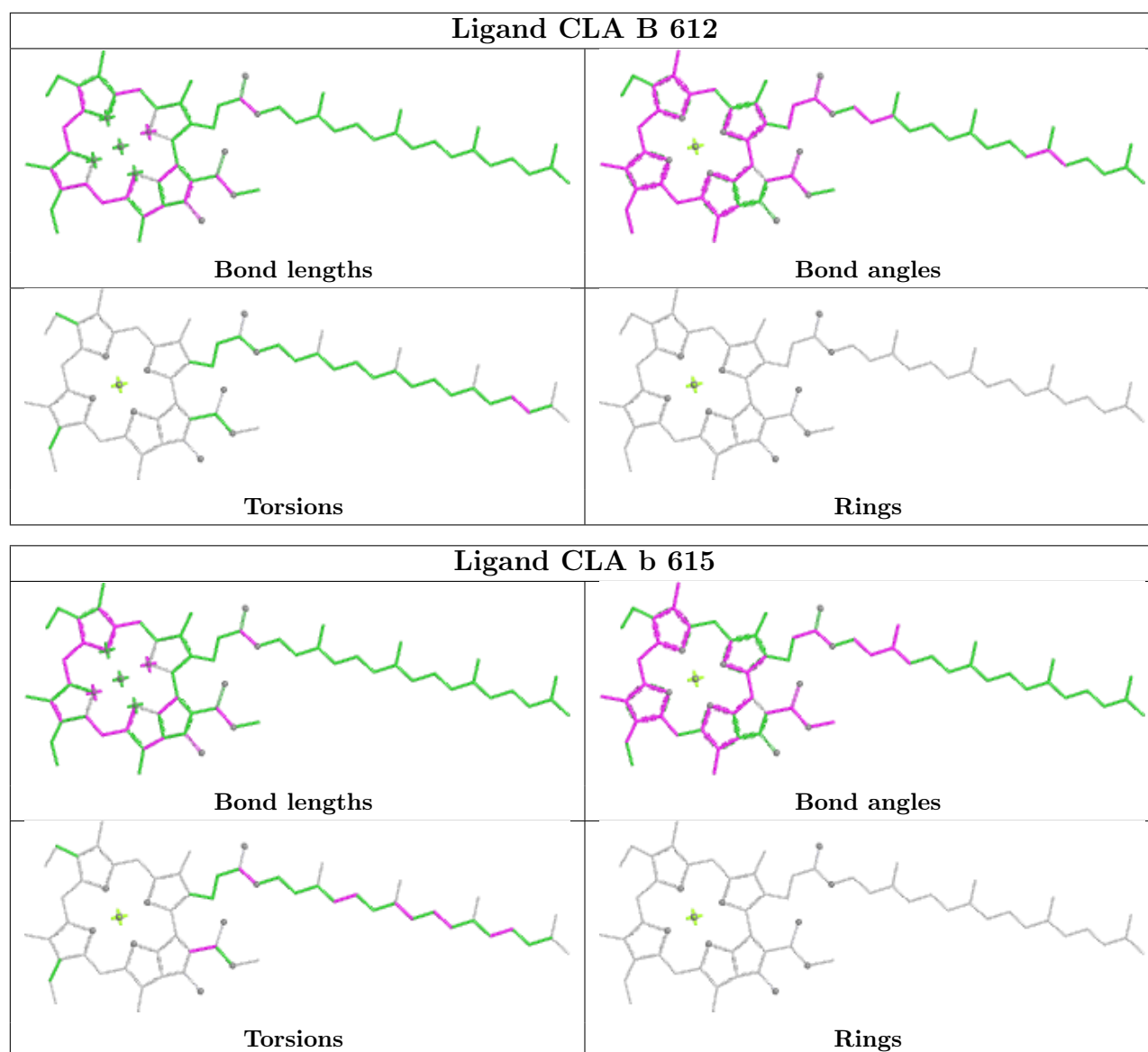
Ligand CLA a 409



Ligand CLA c 910







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.68	0 100 100	15, 23, 46, 69	4 (1%)
1	a	334/344 (97%)	-0.62	1 (0%) 90 91	17, 24, 50, 76	4 (1%)
2	B	504/504 (100%)	-0.48	8 (1%) 70 74	14, 27, 54, 88	10 (1%)
2	b	501/504 (99%)	-0.35	17 (3%) 48 51	16, 29, 58, 119	11 (2%)
3	C	451/455 (99%)	-0.42	0 100 100	17, 31, 46, 81	3 (0%)
3	c	455/455 (100%)	-0.27	0 100 100	21, 34, 48, 79	4 (0%)
4	D	340/342 (99%)	-0.74	0 100 100	13, 24, 40, 70	1 (0%)
4	d	340/342 (99%)	-0.67	0 100 100	13, 26, 45, 80	3 (0%)
5	E	81/83 (97%)	0.10	1 (1%) 76 79	27, 40, 62, 82	0
5	e	79/83 (95%)	0.30	0 100 100	32, 44, 72, 82	0
6	F	34/44 (77%)	-0.09	1 (2%) 53 57	26, 34, 63, 74	0
6	f	32/44 (72%)	0.05	3 (9%) 14 14	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.19	1 (1%) 70 74	24, 33, 43, 70	0
7	h	63/63 (100%)	0.03	1 (1%) 70 74	27, 37, 51, 81	0
8	I	35/38 (92%)	-0.05	0 100 100	27, 34, 64, 86	0
8	i	37/38 (97%)	-0.03	2 (5%) 31 33	26, 34, 71, 83	0
9	J	36/40 (90%)	-0.13	2 (5%) 30 32	26, 38, 65, 79	0
9	j	39/40 (97%)	0.28	2 (5%) 33 36	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.30	0 100 100	24, 38, 47, 63	1 (2%)
10	k	37/37 (100%)	0.06	0 100 100	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.63	0 100 100	11, 22, 65, 75	1 (2%)
11	l	37/37 (100%)	-0.65	1 (2%) 56 60	13, 23, 64, 95	2 (5%)
12	M	32/36 (88%)	-0.68	0 100 100	13, 24, 40, 56	1 (3%)
12	m	33/36 (91%)	-0.55	1 (3%) 52 56	13, 25, 48, 68	2 (6%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.30	3 (1%) 76 79	17, 33, 66, 120	5 (2%)
13	o	241/244 (98%)	-0.15	4 (1%) 69 72	17, 34, 71, 87	5 (2%)
14	T	29/32 (90%)	-0.61	1 (3%) 48 51	19, 23, 49, 85	0
14	t	29/32 (90%)	-0.59	1 (3%) 48 51	20, 23, 47, 72	0
15	U	97/104 (93%)	-0.39	0 100 100	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.47	1 (1%) 79 82	20, 30, 40, 66	1 (1%)
16	V	137/137 (100%)	-0.62	0 100 100	16, 28, 42, 51	2 (1%)
16	v	137/137 (100%)	-0.10	0 100 100	19, 37, 52, 72	1 (0%)
17	Y	27/30 (90%)	0.59	2 (7%) 20 22	37, 47, 70, 77	0
17	y	28/30 (93%)	0.79	1 (3%) 46 49	45, 55, 73, 77	0
18	X	38/40 (95%)	0.30	1 (2%) 57 61	23, 39, 65, 69	1 (2%)
18	x	38/40 (95%)	0.53	4 (10%) 11 12	26, 42, 83, 94	1 (2%)
19	Z	62/62 (100%)	0.64	8 (12%) 7 7	37, 46, 75, 92	0
19	z	60/62 (96%)	1.24	8 (13%) 7 7	47, 57, 88, 95	0
All	All	5235/5344 (97%)	-0.36	75 (1%) 73 76	11, 30, 59, 120	63 (1%)

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	64	ALA	5.7
2	B	494	GLY	4.3
2	b	502	VAL	4.2
2	b	499	VAL	4.2
19	z	3	ILE	4.0

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	0.11	31,38,54,60	0
14	FME	t	1	10/11	0.93	0.08	20,23,41,50	0
12	FME	M	1	10/11	0.95	0.08	27,34,51,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HSK	d	336[B]	11/12	0.96	0.08	30,31,37,38	8
14	FME	T	1	10/11	0.96	0.06	24,27,43,50	0
4	HSK	d	336[A]	10/12	0.96	0.08	30,33,40,44	7
4	HSK	D	336[A]	10/12	0.97	0.06	26,28,31,34	7
4	HSK	D	336[B]	11/12	0.97	0.06	23,26,27,29	8
8	FME	I	1	10/11	0.97	0.07	27,34,38,39	0
8	FME	i	1	10/11	0.98	0.06	30,32,37,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
34	DGD	d	406	50/66	0.60	0.17	56,75,94,97	0
29	UNL	b	630	16/-	0.66	0.15	51,62,73,74	0
34	DGD	D	406	53/66	0.67	0.15	53,77,92,103	0
29	UNL	b	631	16/-	0.69	0.17	59,66,77,79	0
29	UNL	E	103	12/-	0.70	0.16	65,73,83,88	0
29	UNL	B	629	14/-	0.71	0.17	61,70,89,90	0
36	LHG	a	417	40/49	0.71	0.14	60,109,148,151	0
29	UNL	i	103	13/-	0.72	0.16	58,65,76,78	0
29	UNL	a	420	40/-	0.72	0.16	53,72,88,94	0
29	UNL	j	103	12/-	0.73	0.14	55,65,70,71	0
29	UNL	E	102	15/-	0.74	0.20	57,64,83,83	0
29	UNL	c	926	10/-	0.74	0.14	65,67,71,72	0
29	UNL	Z	103	16/-	0.74	0.16	48,63,81,81	0
29	UNL	j	102	16/-	0.74	0.17	52,61,69,69	0
29	UNL	A	415	36/-	0.75	0.15	58,67,75,79	0
29	UNL	i	104	10/-	0.75	0.12	67,72,77,78	0
30	LMT	F	102	35/35	0.75	0.13	53,84,91,96	0
33	HTG	d	401	19/19	0.76	0.14	55,101,111,114	0
29	UNL	z	102	16/-	0.77	0.17	51,70,89,92	0
29	UNL	C	523	34/-	0.77	0.14	52,77,88,93	0
29	UNL	H	103	10/-	0.77	0.16	60,69,74,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	UNL	T	102	13/-	0.77	0.14	66,70,83,87	0
29	UNL	B	628	10/-	0.77	0.15	52,56,70,74	0
29	UNL	t	103	16/-	0.77	0.14	63,74,94,95	0
29	UNL	e	800	11/-	0.78	0.16	53,60,68,68	0
33	HTG	B	631	19/19	0.78	0.14	49,111,120,125	0
29	UNL	J	103	14/-	0.79	0.14	61,66,73,76	0
33	HTG	C	522	19/19	0.79	0.12	50,79,92,94	0
33	HTG	U	201	9/19	0.79	0.17	54,59,82,98	0
26	SQD	f	102	33/54	0.79	0.15	63,73,113,114	0
29	UNL	B	632	16/-	0.79	0.15	50,59,73,73	0
30	LMT	c	922	35/35	0.79	0.12	61,73,85,90	0
31	GOL	h	103	6/6	0.79	0.12	78,83,83,84	0
40	SO4	O	302	5/5	0.79	0.12	78,87,95,105	0
30	LMT	M	101	35/35	0.80	0.12	43,61,77,90	0
33	HTG	b	627	19/19	0.80	0.14	53,94,104,105	0
33	HTG	c	924	19/19	0.80	0.12	53,85,97,100	0
28	PL9	a	419	55/55	0.80	0.15	52,74,98,109	0
30	LMT	z	101	32/35	0.80	0.12	46,85,90,100	0
29	UNL	A	417	13/-	0.80	0.15	56,59,66,66	0
29	UNL	c	925	30/-	0.80	0.14	59,72,89,95	0
29	UNL	L	102	14/-	0.80	0.15	52,58,66,69	0
33	HTG	b	602	19/19	0.81	0.13	50,93,111,117	0
27	LMG	c	921	51/55	0.81	0.13	38,80,95,111	0
33	HTG	c	923	19/19	0.81	0.11	64,75,82,83	0
31	GOL	O	304	6/6	0.81	0.10	52,60,61,63	0
30	LMT	B	623	35/35	0.81	0.14	43,79,117,129	0
29	UNL	b	629	16/-	0.81	0.15	43,48,56,60	0
26	SQD	B	621	54/54	0.81	0.14	48,65,108,109	0
33	HTG	D	414	19/19	0.81	0.12	66,93,106,107	0
29	UNL	J	104	12/-	0.81	0.15	53,65,72,74	0
29	UNL	A	420	4/-	0.82	0.13	64,66,66,66	0
28	PL9	A	414	55/55	0.82	0.14	47,66,93,96	0
29	UNL	D	412	40/-	0.82	0.13	39,60,96,99	0
36	LHG	E	101	49/49	0.82	0.13	50,80,94,97	0
29	UNL	x	101	16/-	0.82	0.16	36,45,70,73	0
26	SQD	D	407	45/54	0.82	0.14	50,78,94,101	0
29	UNL	a	421	10/-	0.83	0.13	53,57,61,64	0
33	HTG	u	201	14/19	0.83	0.14	46,64,90,96	0
26	SQD	L	103	54/54	0.83	0.12	43,64,89,96	0
30	LMT	J	102	24/35	0.83	0.12	45,55,79,83	0
33	HTG	B	626	19/19	0.83	0.10	48,87,92,93	0
27	LMG	Z	101	51/55	0.83	0.14	41,76,102,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	UNL	d	411	16/-	0.83	0.12	39,49,63,66	0
29	UNL	M	103	16/-	0.84	0.13	49,58,77,79	0
32	CA	B	601	1/1	0.84	0.08	81,81,81,81	0
29	UNL	i	101	16/-	0.84	0.13	40,46,56,62	0
29	UNL	b	628	36/-	0.84	0.13	44,65,101,106	0
30	LMT	Z	102	35/35	0.84	0.14	41,87,102,107	0
29	UNL	a	403	6/-	0.84	0.09	57,62,66,66	0
29	UNL	I	102	11/-	0.84	0.12	62,65,66,68	0
30	LMT	C	520	35/35	0.84	0.11	52,71,83,89	0
31	GOL	b	636	6/6	0.84	0.12	45,56,58,60	0
31	GOL	b	635	6/6	0.85	0.12	40,43,46,48	0
30	LMT	b	624	25/35	0.85	0.11	51,71,94,98	0
31	GOL	c	928	6/6	0.85	0.10	42,51,54,54	0
29	UNL	I	101	13/-	0.85	0.10	44,53,61,63	0
29	UNL	D	413	16/-	0.85	0.12	39,47,65,65	0
31	GOL	C	524	6/6	0.85	0.19	36,45,47,53	0
26	SQD	A	418	54/54	0.85	0.11	42,59,81,86	0
31	GOL	c	927	6/6	0.86	0.12	43,53,60,68	0
30	LMT	b	625	24/35	0.86	0.14	35,61,99,100	0
26	SQD	a	401	54/54	0.86	0.11	45,59,85,90	0
30	LMT	t	102	24/35	0.86	0.12	33,55,94,95	0
29	UNL	i	102	16/-	0.86	0.11	54,65,83,84	0
30	LMT	m	102	35/35	0.87	0.10	41,54,72,84	0
29	UNL	A	416	16/-	0.87	0.12	41,46,73,73	0
29	UNL	X	101	16/-	0.87	0.12	34,39,58,60	0
31	GOL	A	422	6/6	0.87	0.11	42,55,58,67	0
30	LMT	A	419	35/35	0.88	0.10	37,56,73,94	0
31	GOL	l	102	6/6	0.88	0.13	37,55,57,57	0
33	HTG	V	202	13/19	0.88	0.09	43,48,76,84	0
30	LMT	a	402	35/35	0.88	0.10	37,54,69,80	0
27	LMG	A	413	51/55	0.88	0.10	42,57,76,78	0
29	UNL	B	627	16/-	0.88	0.12	43,47,69,69	0
30	LMT	M	102	35/35	0.88	0.10	35,52,60,63	0
31	GOL	b	633	6/6	0.90	0.10	41,46,49,52	0
31	GOL	B	638	6/6	0.90	0.10	35,47,49,53	0
27	LMG	a	418	51/55	0.90	0.09	43,60,68,73	0
31	GOL	L	104	6/6	0.90	0.11	44,52,54,55	0
30	LMT	m	101	35/35	0.90	0.09	32,51,61,62	0
32	CA	b	603	1/1	0.91	0.06	82,82,82,82	0
27	LMG	C	519	51/55	0.91	0.11	29,59,97,105	0
33	HTG	B	630	19/19	0.91	0.10	39,52,66,79	0
31	GOL	C	526	6/6	0.91	0.09	38,43,51,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	HTG	C	521	19/19	0.91	0.09	56,63,76,80	0
27	LMG	c	920	51/55	0.91	0.10	30,65,100,104	0
31	GOL	B	633	6/6	0.91	0.10	34,39,47,52	0
31	GOL	B	637	6/6	0.91	0.10	36,38,45,54	0
31	GOL	v	204	6/6	0.91	0.09	46,50,61,62	0
23	CLA	c	914	65/65	0.91	0.10	38,53,90,98	0
31	GOL	b	632	6/6	0.92	0.09	35,42,46,47	0
23	CLA	B	602	65/65	0.92	0.10	29,41,78,95	0
33	HTG	B	625	19/19	0.92	0.12	31,38,71,75	0
27	LMG	B	622	51/55	0.92	0.08	28,37,53,63	0
25	BCR	c	915	40/40	0.92	0.08	44,51,59,60	0
23	CLA	C	506	65/65	0.92	0.09	25,38,94,97	0
23	CLA	b	604	65/65	0.92	0.09	34,47,73,81	0
31	GOL	f	104	6/6	0.92	0.08	46,51,51,54	0
31	GOL	B	635	6/6	0.92	0.08	38,47,49,50	0
31	GOL	a	422	6/6	0.92	0.09	30,38,44,45	0
31	GOL	a	424	6/6	0.92	0.10	42,56,59,74	0
25	BCR	d	404	40/40	0.93	0.07	25,33,56,58	0
25	BCR	k	101	40/40	0.93	0.07	33,39,47,49	0
25	BCR	k	102	40/40	0.93	0.07	29,41,48,50	0
26	SQD	A	412	54/54	0.93	0.09	35,54,71,74	0
26	SQD	a	416	54/54	0.93	0.09	37,55,88,90	0
27	LMG	b	623	51/55	0.93	0.08	30,39,52,63	0
31	GOL	A	421	6/6	0.93	0.09	30,37,38,41	0
33	HTG	b	601	19/19	0.93	0.08	43,51,62,68	0
25	BCR	C	514	40/40	0.93	0.07	33,42,46,46	0
38	RRX	H	101	41/41	0.93	0.07	25,30,44,47	0
38	RRX	h	101	41/41	0.93	0.07	27,35,49,54	0
33	HTG	b	626	19/19	0.93	0.12	29,40,73,75	0
31	GOL	A	423	6/6	0.94	0.10	39,43,45,53	0
23	CLA	C	512	65/65	0.94	0.07	34,41,69,74	0
25	BCR	D	404	40/40	0.94	0.07	24,29,55,57	0
25	BCR	T	101	40/40	0.94	0.06	24,32,47,53	0
23	CLA	b	609	65/65	0.94	0.08	23,31,57,63	0
23	CLA	c	907	65/65	0.94	0.07	28,36,76,80	0
23	CLA	c	913	65/65	0.94	0.07	33,45,67,72	0
34	DGD	c	918	62/66	0.94	0.08	27,35,79,91	0
31	GOL	c	930	6/6	0.94	0.07	49,54,57,59	0
35	BCT	D	401	4/4	0.94	0.08	32,35,41,51	0
31	GOL	D	415	6/6	0.94	0.12	35,36,42,46	0
23	CLA	C	513	65/65	0.94	0.08	35,46,78,83	0
25	BCR	t	101	40/40	0.94	0.06	23,30,42,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	GOL	v	203	6/6	0.94	0.10	31,35,41,43	0
27	LMG	d	410	51/55	0.94	0.09	29,36,80,91	0
25	BCR	K	101	40/40	0.95	0.06	30,35,40,43	0
31	GOL	V	203	6/6	0.95	0.08	26,32,36,38	0
31	GOL	V	204	6/6	0.95	0.07	39,52,59,59	0
31	GOL	V	205	6/6	0.95	0.09	33,36,37,41	0
27	LMG	D	411	51/55	0.95	0.09	23,35,91,99	0
31	GOL	a	423	6/6	0.95	0.09	33,34,35,45	0
25	BCR	K	102	40/40	0.95	0.07	28,31,39,42	0
23	CLA	b	612	65/65	0.95	0.06	26,30,36,38	0
34	DGD	H	102	62/66	0.95	0.07	24,31,40,45	0
31	GOL	B	636	6/6	0.95	0.09	33,43,47,56	0
34	DGD	c	919	62/66	0.95	0.07	25,35,60,71	0
31	GOL	b	634	6/6	0.95	0.08	32,39,44,46	0
34	DGD	h	102	62/66	0.95	0.07	27,35,45,52	0
23	CLA	c	908	65/65	0.95	0.07	26,32,52,55	0
35	BCT	a	408	4/4	0.95	0.07	30,32,37,46	0
36	LHG	D	408	49/49	0.95	0.07	26,35,45,45	0
23	CLA	c	912	65/65	0.95	0.07	29,37,45,50	0
23	CLA	b	617	65/65	0.95	0.07	20,25,71,83	0
36	LHG	d	409	49/49	0.95	0.09	27,32,85,91	0
23	CLA	c	902	65/65	0.95	0.07	27,34,46,50	0
23	CLA	c	904	65/65	0.95	0.06	24,37,42,42	0
23	CLA	c	905	65/65	0.95	0.06	24,31,64,66	0
23	CLA	c	909	65/65	0.96	0.06	25,30,82,98	0
23	CLA	c	911	65/65	0.96	0.06	24,30,41,45	0
23	CLA	B	615	65/65	0.96	0.07	19,24,67,74	0
23	CLA	D	403	65/65	0.96	0.07	22,28,73,79	0
23	CLA	B	616	65/65	0.96	0.06	23,28,48,50	0
23	CLA	d	403	65/65	0.96	0.07	25,32,83,90	0
25	BCR	A	411	40/40	0.96	0.05	21,26,33,36	0
25	BCR	B	619	40/40	0.96	0.06	19,26,42,45	0
25	BCR	B	620	40/40	0.96	0.06	22,31,41,44	0
23	CLA	b	605	65/65	0.96	0.06	24,29,36,39	0
25	BCR	C	515	40/40	0.96	0.06	28,34,41,44	0
23	CLA	C	503	65/65	0.96	0.06	26,31,38,39	0
23	CLA	C	505	65/65	0.96	0.06	26,31,47,51	0
23	CLA	b	613	65/65	0.96	0.06	24,28,35,40	0
23	CLA	b	615	65/65	0.96	0.06	19,27,33,38	0
25	BCR	a	415	40/40	0.96	0.05	21,25,30,31	0
34	DGD	C	516	62/66	0.96	0.07	22,32,85,87	0
34	DGD	C	517	62/66	0.96	0.07	22,31,78,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	DGD	C	518	62/66	0.96	0.06	20,30,68,75	0
28	PL9	D	405	55/55	0.96	0.05	18,23,31,38	0
25	BCR	b	621	40/40	0.96	0.06	21,28,43,46	0
34	DGD	c	917	62/66	0.96	0.07	24,33,77,80	0
25	BCR	b	622	40/40	0.96	0.06	25,33,43,45	0
23	CLA	B	607	65/65	0.96	0.07	21,27,55,61	0
25	BCR	c	916	40/40	0.96	0.06	28,36,45,47	0
23	CLA	b	618	65/65	0.96	0.06	24,30,49,53	0
23	CLA	b	619	65/65	0.96	0.08	25,32,89,97	0
31	GOL	v	202	6/6	0.96	0.08	35,36,40,41	0
23	CLA	C	507	65/65	0.96	0.06	26,33,56,61	0
36	LHG	D	410	46/49	0.96	0.07	24,32,82,87	0
23	CLA	C	508	65/65	0.96	0.06	24,29,73,81	0
36	LHG	L	101	49/49	0.96	0.06	22,31,44,49	0
23	CLA	C	509	65/65	0.96	0.06	27,31,47,51	0
36	LHG	d	407	49/49	0.96	0.06	27,36,46,49	0
32	CA	O	301	1/1	0.96	0.07	49,49,49,49	0
36	LHG	l	101	49/49	0.96	0.07	22,31,47,57	0
23	CLA	C	511	65/65	0.96	0.06	27,34,40,42	0
32	CA	o	301	1/1	0.96	0.06	51,51,51,51	0
23	CLA	B	610	65/65	0.96	0.06	23,28,33,35	0
23	CLA	C	501	65/65	0.97	0.05	25,32,46,53	0
23	CLA	C	502	65/65	0.97	0.05	21,26,39,48	0
23	CLA	b	606	65/65	0.97	0.05	20,26,37,42	0
23	CLA	b	607	65/65	0.97	0.06	20,25,54,59	0
24	PHO	A	408	64/64	0.97	0.04	16,21,25,27	0
24	PHO	A	409	64/64	0.97	0.04	19,22,29,37	0
24	PHO	a	413	64/64	0.97	0.05	19,25,30,35	0
23	CLA	b	608	65/65	0.97	0.05	20,24,33,34	0
25	BCR	B	618	40/40	0.97	0.05	20,26,29,30	0
23	CLA	A	410	65/65	0.97	0.08	20,24,99,105	0
23	CLA	b	611	65/65	0.97	0.04	22,27,39,43	0
23	CLA	C	504	65/65	0.97	0.06	23,28,62,68	0
23	CLA	B	608	65/65	0.97	0.05	17,20,34,37	0
23	CLA	B	603	65/65	0.97	0.05	23,26,34,37	0
23	CLA	b	616	65/65	0.97	0.05	20,24,46,50	0
23	CLA	B	611	65/65	0.97	0.05	19,25,34,39	0
23	CLA	B	612	65/65	0.97	0.05	18,21,34,37	0
23	CLA	B	613	65/65	0.97	0.05	19,24,31,34	0
25	BCR	b	620	40/40	0.97	0.04	23,27,33,33	0
28	PL9	d	405	55/55	0.97	0.05	19,25,30,34	0
23	CLA	C	510	65/65	0.97	0.05	22,28,38,41	0

Continued on next page...

Continued from previous page...

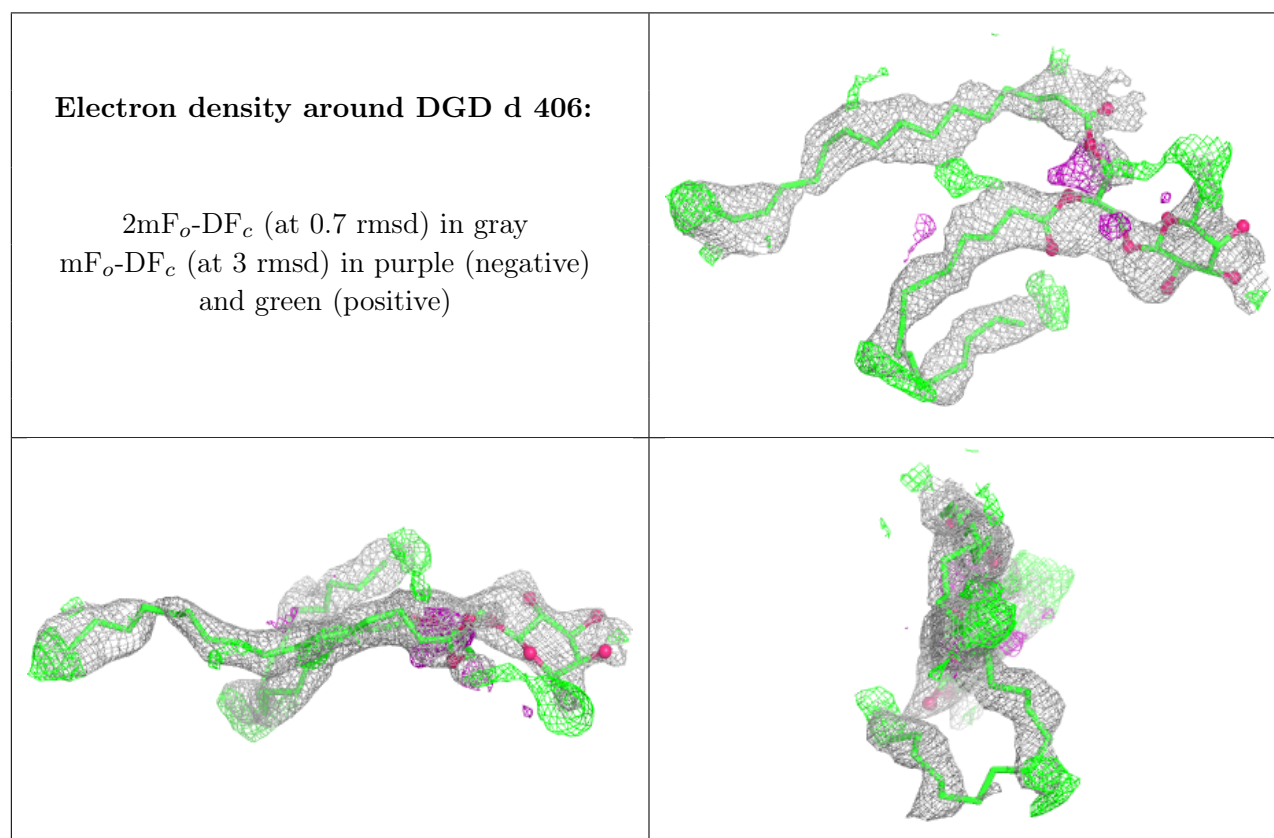
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	903	65/65	0.97	0.06	22,29,42,55	0
23	CLA	B	614	65/65	0.97	0.05	18,23,48,54	0
32	CA	F	103	1/1	0.97	0.10	55,55,55,55	0
31	GOL	B	634	6/6	0.97	0.08	29,29,34,37	0
23	CLA	B	604	65/65	0.97	0.05	17,22,34,41	0
32	CA	c	901	1/1	0.97	0.06	46,46,46,46	0
32	CA	f	103	1/1	0.97	0.11	56,56,56,56	0
23	CLA	c	906	65/65	0.97	0.05	26,31,46,50	0
33	HTG	B	624	19/19	0.97	0.06	27,33,41,51	0
36	LHG	d	408	49/49	0.97	0.06	22,27,42,47	0
23	CLA	B	606	65/65	0.97	0.05	17,23,35,40	0
23	CLA	B	617	65/65	0.97	0.08	20,28,79,83	0
37	HEM	f	101	43/43	0.97	0.08	39,47,61,77	0
23	CLA	a	411	65/65	0.97	0.07	18,23,106,117	0
23	CLA	c	910	65/65	0.97	0.06	25,31,49,52	0
23	CLA	a	414	65/65	0.97	0.08	19,25,99,104	0
31	GOL	c	929	6/6	0.98	0.04	25,27,30,30	0
23	CLA	B	609	65/65	0.98	0.04	18,24,31,34	0
23	CLA	b	614	65/65	0.98	0.05	20,24,36,45	0
36	LHG	D	409	49/49	0.98	0.05	22,28,40,44	0
23	CLA	B	605	65/65	0.98	0.05	19,22,53,55	0
24	PHO	a	412	64/64	0.98	0.04	17,22,26,27	0
23	CLA	D	402	65/65	0.98	0.04	13,18,36,39	0
23	CLA	A	406	65/65	0.98	0.04	13,18,29,39	0
23	CLA	a	409	65/65	0.98	0.04	18,21,31,43	0
23	CLA	a	410	65/65	0.98	0.04	17,20,28,34	0
33	HTG	O	303	19/19	0.98	0.06	27,32,50,52	0
31	GOL	C	525	6/6	0.98	0.04	26,26,27,29	0
37	HEM	F	101	43/43	0.98	0.07	36,42,49,52	0
23	CLA	b	610	65/65	0.98	0.04	18,23,32,35	0
37	HEM	v	201	43/43	0.98	0.06	25,31,35,38	0
23	CLA	A	407	65/65	0.98	0.06	18,21,80,92	0
23	CLA	A	405	65/65	0.98	0.04	14,19,25,42	0
39	MG	J	101	1/1	0.98	0.05	28,28,28,28	0
39	MG	j	101	1/1	0.98	0.09	35,35,35,35	0
23	CLA	d	402	65/65	0.98	0.04	18,21,39,44	0
37	HEM	V	201	43/43	0.99	0.04	22,24,28,33	0
22	CL	a	406	1/1	0.99	0.06	29,29,29,29	0
22	CL	A	403	1/1	0.99	0.04	25,25,25,25	0
22	CL	A	404	1/1	0.99	0.02	22,22,22,22	0
21	FE2	A	402	1/1	1.00	0.01	26,26,26,26	0
22	CL	a	407	1/1	1.00	0.02	27,27,27,27	0

Continued on next page...

Continued from previous page...

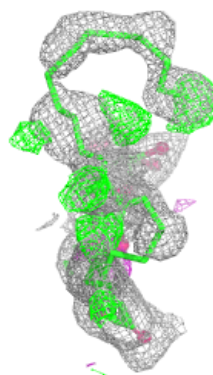
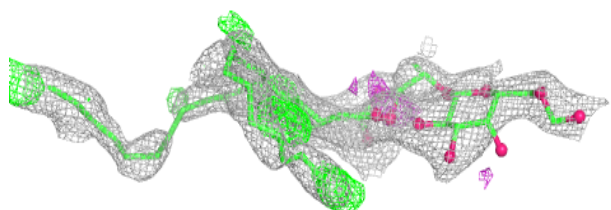
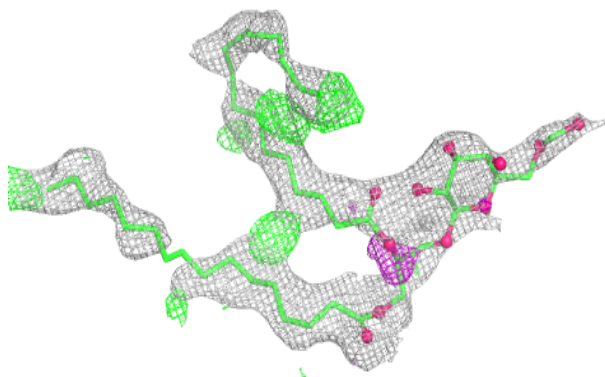
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	FE2	a	405	1/1	1.00	0.01	27,27,27,27	0
20	OEX	A	401	10/10	1.00	0.03	21,23,27,28	0
20	OEX	a	404	10/10	1.00	0.02	22,26,28,29	0

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.

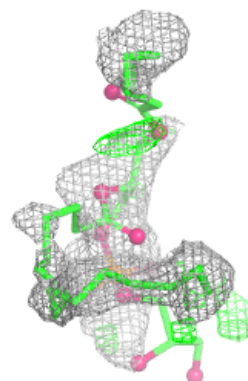
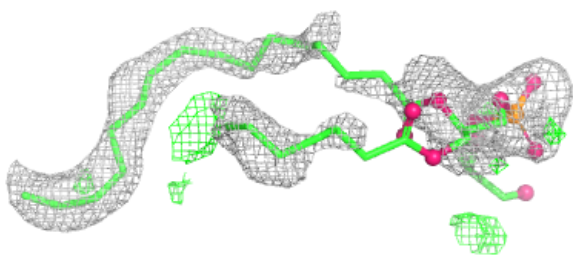
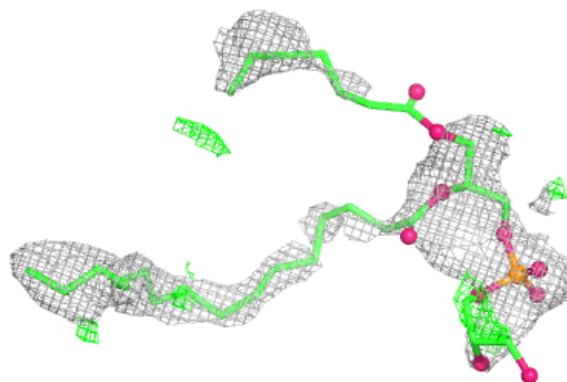


Electron density around DGD D 406:

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

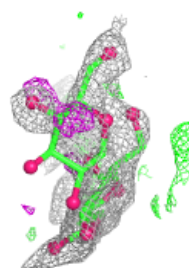
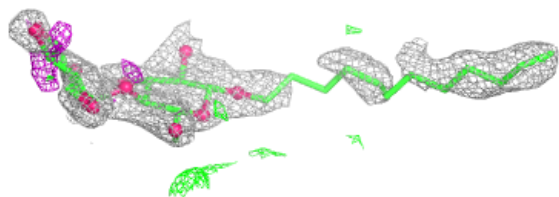
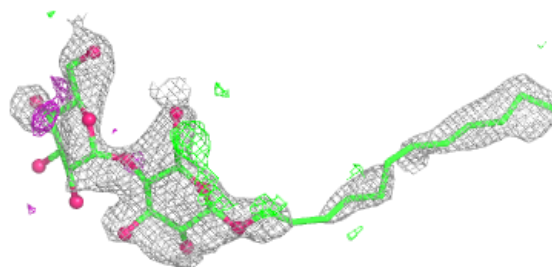
**Electron density around LHG a 417:**

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

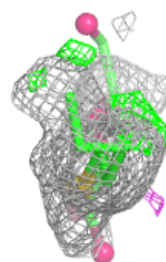
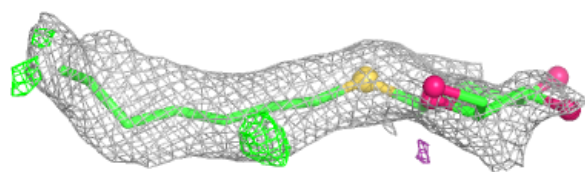
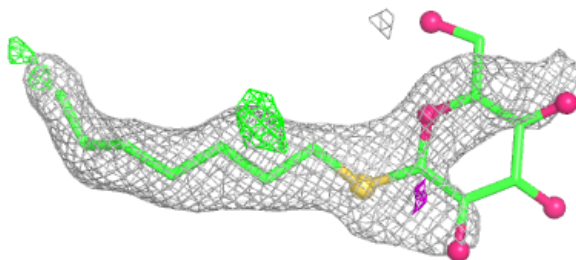


Electron density around LMT F 102:

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

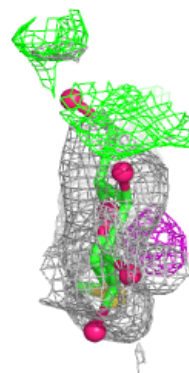
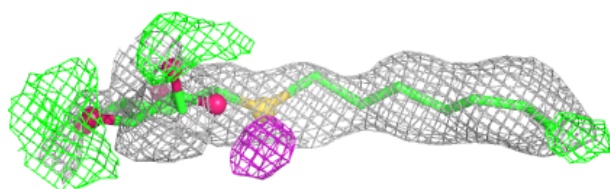
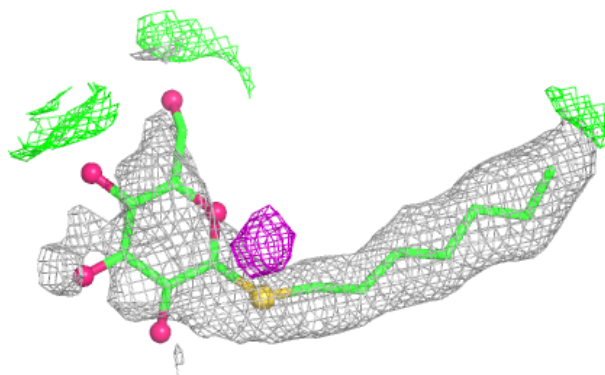
**Electron density around HTG d 401:**

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

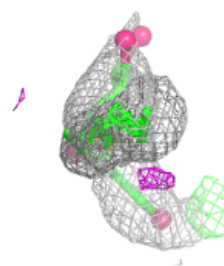
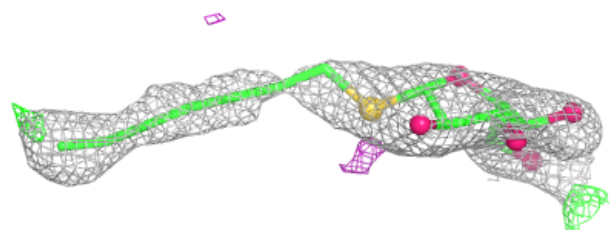
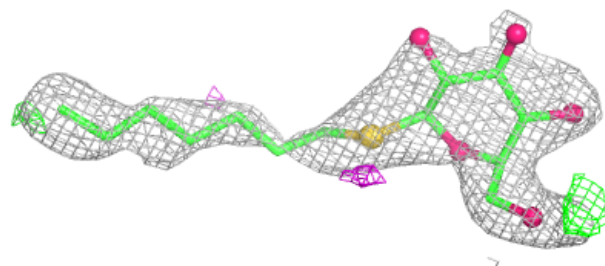


Electron density around HTG B 631:

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

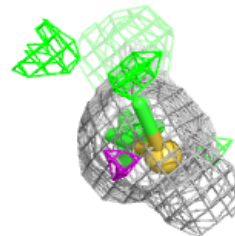
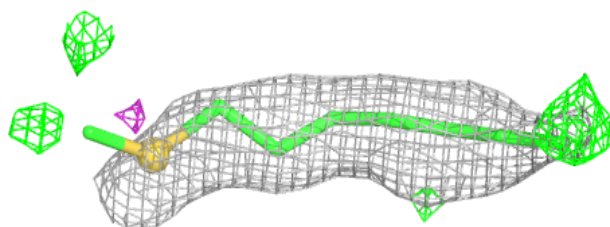
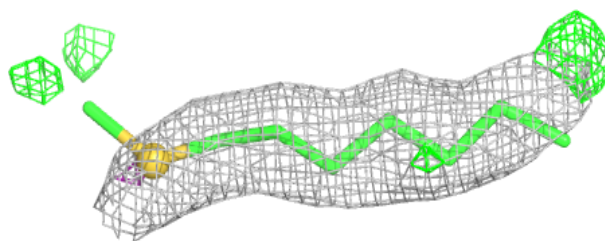
**Electron density around HTG C 522:**

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

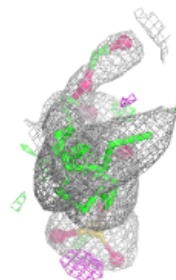
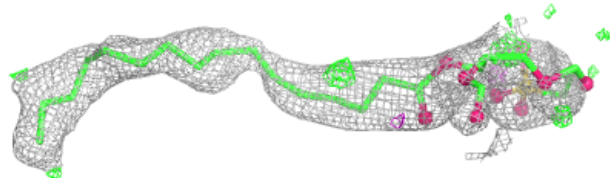
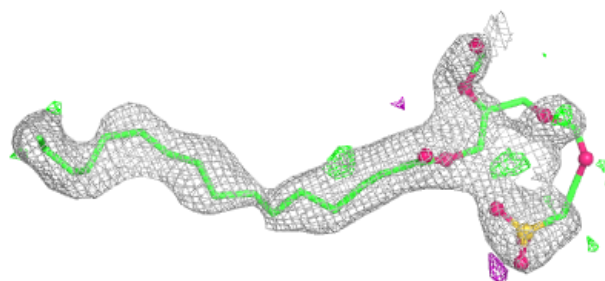


Electron density around HTG U 201:

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

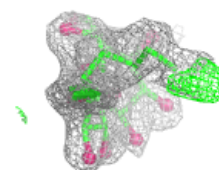
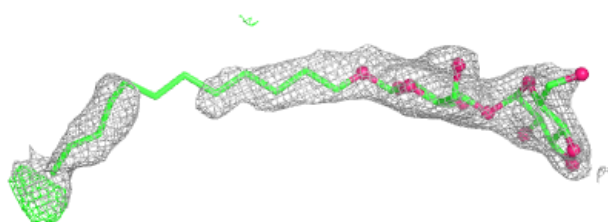
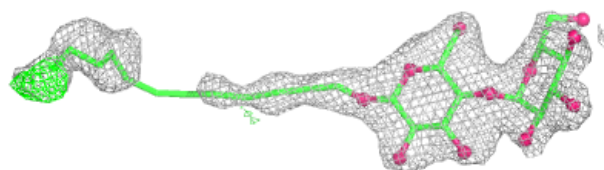
**Electron density around SQD f 102:**

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

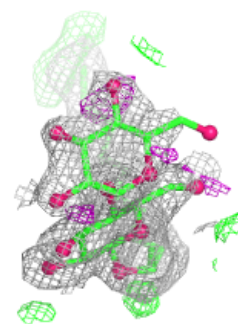
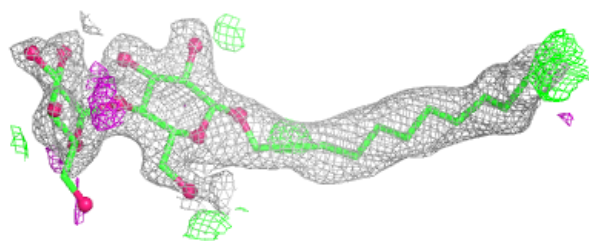
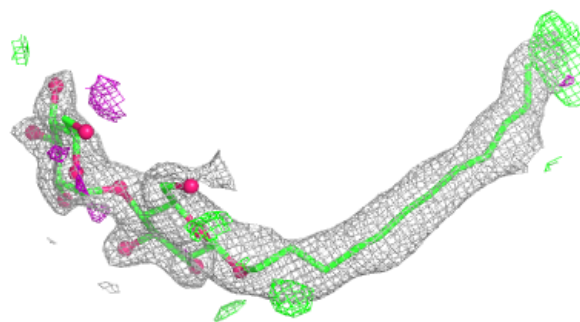


Electron density around LMT c 922:

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

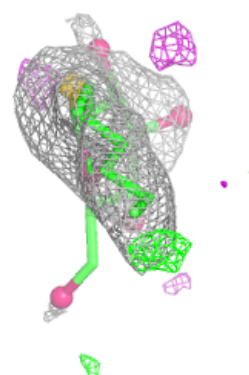
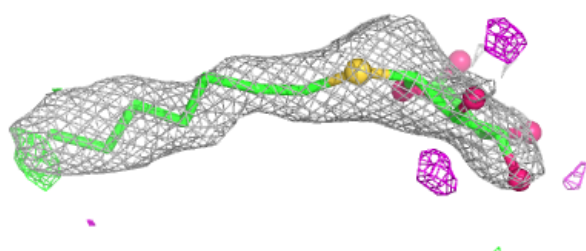
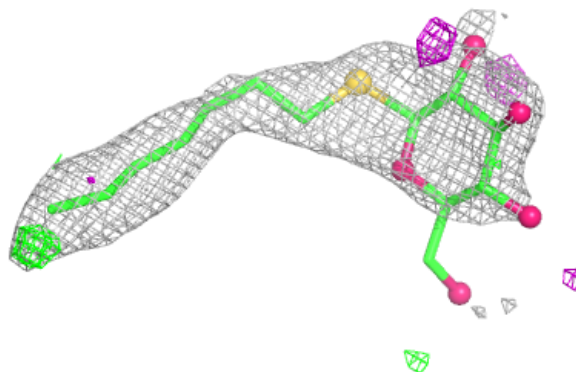
**Electron density around LMT M 101:**

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

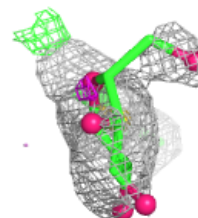
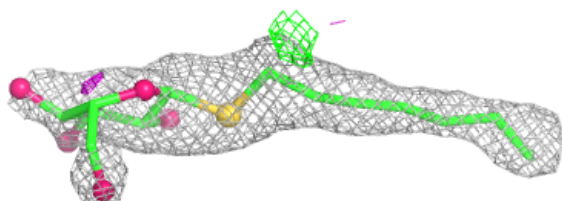
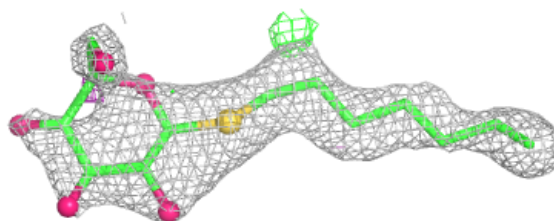


Electron density around HTG b 627:

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

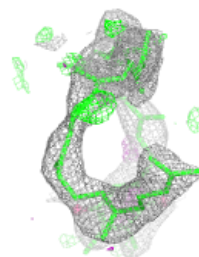
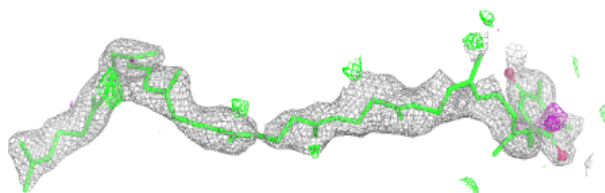
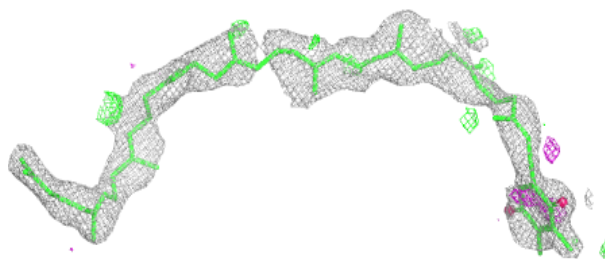
**Electron density around HTG c 924:**

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

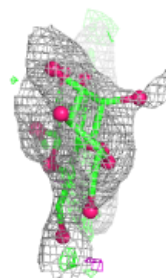
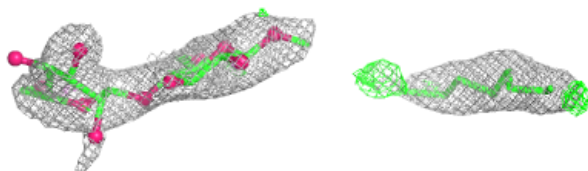
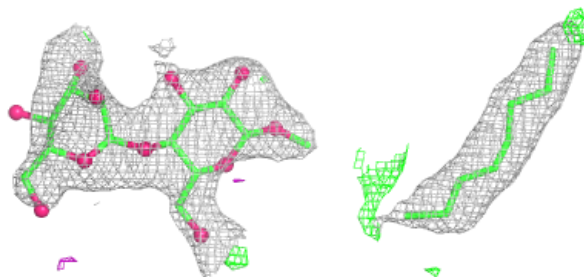


Electron density around PL9 a 419:

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

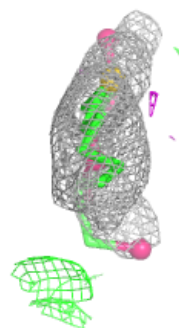
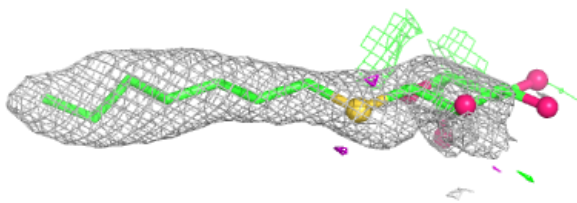
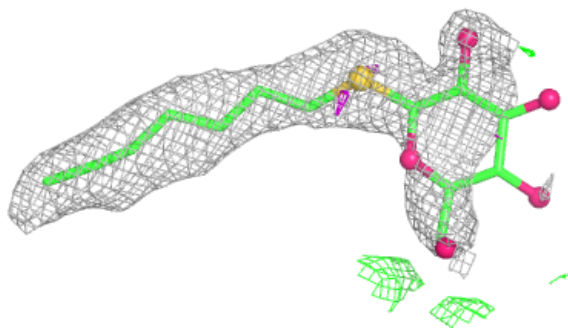
**Electron density around LMT z 101:**

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

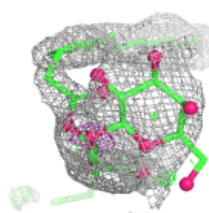
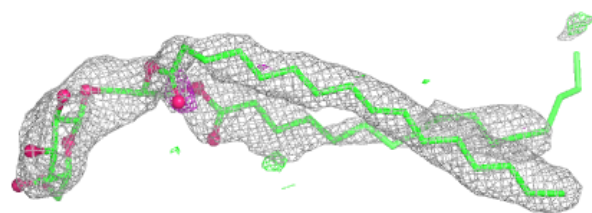
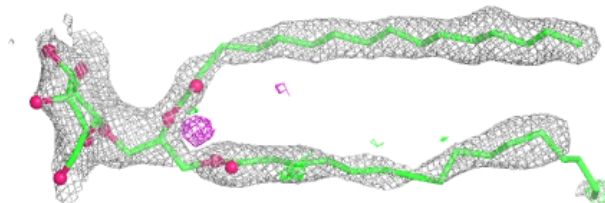


Electron density around HTG b 602:

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

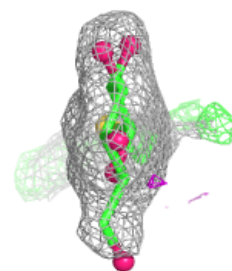
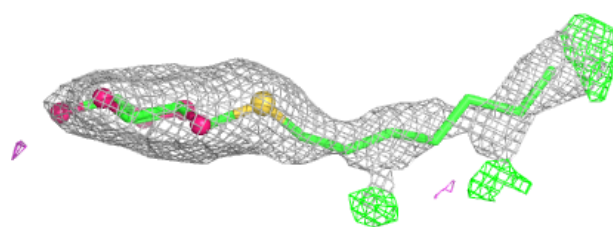
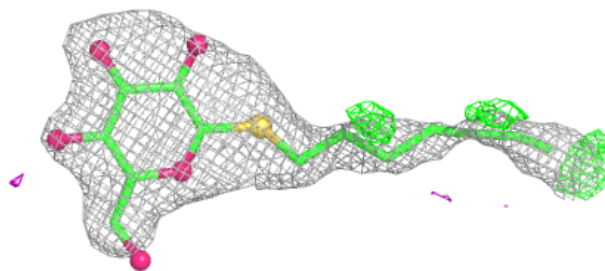
**Electron density around LMG c 921:**

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

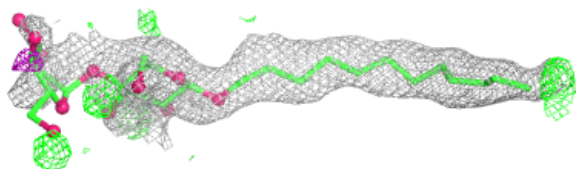
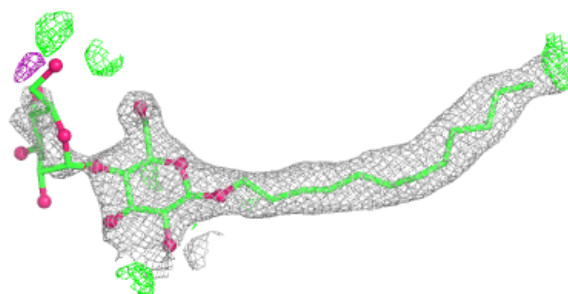


Electron density around HTG c 923:

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

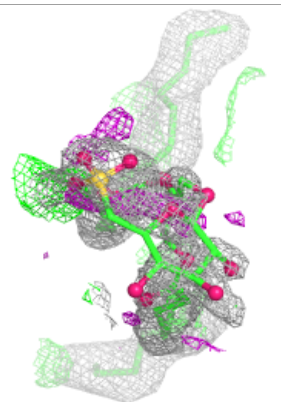
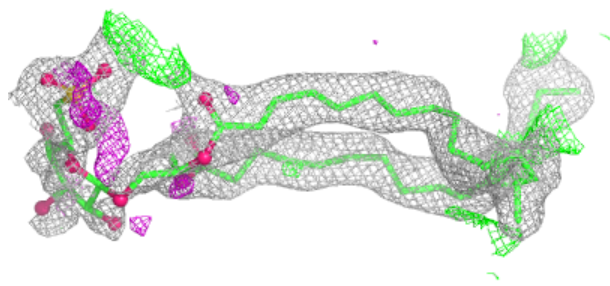
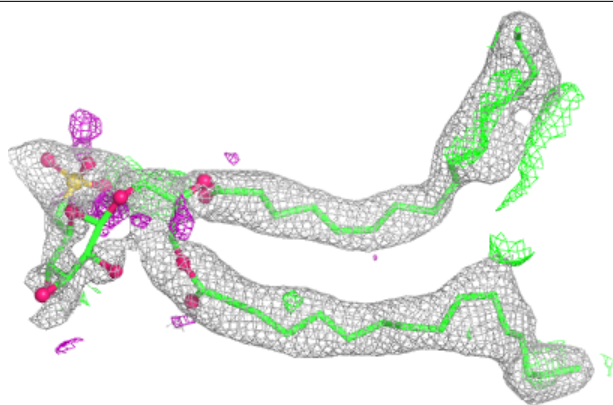
**Electron density around LMT B 623:**

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

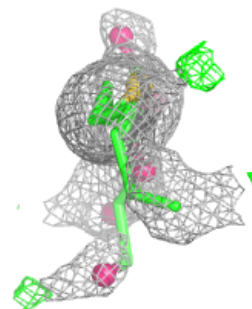
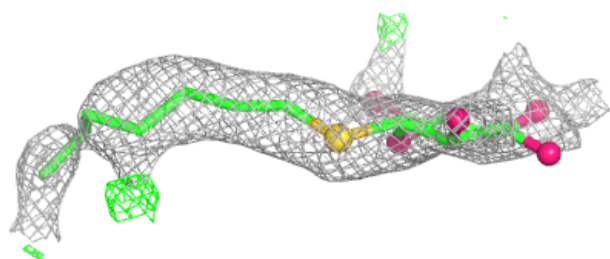
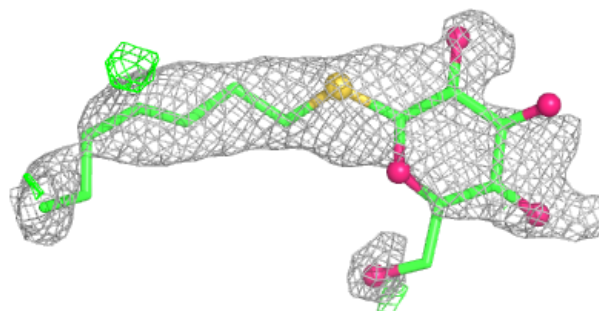


Electron density around SQD B 621:

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

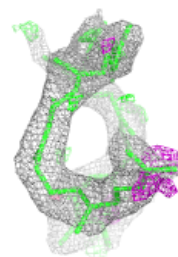
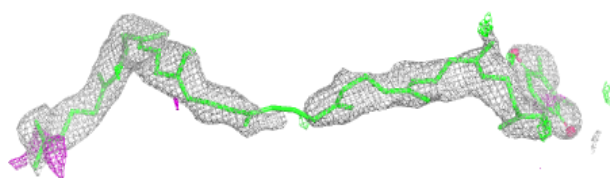
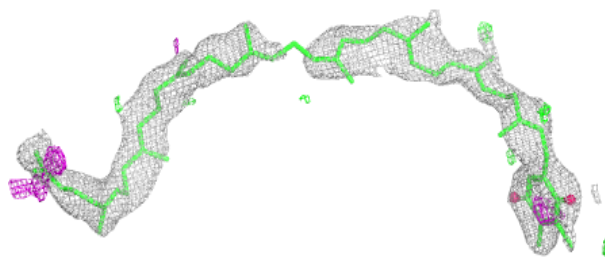
**Electron density around HTG D 414:**

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

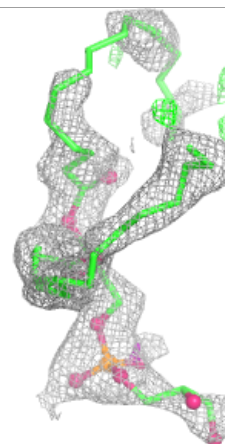
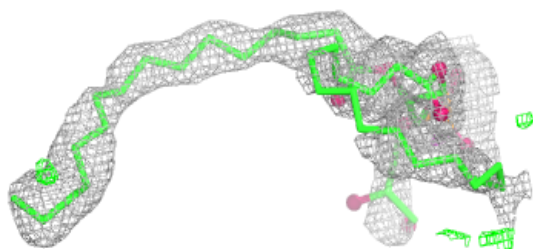
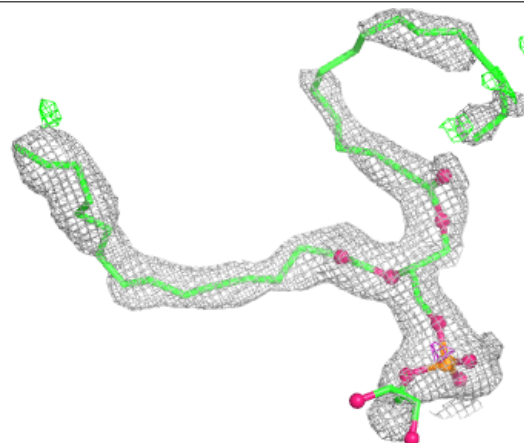


Electron density around PL9 A 414:

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

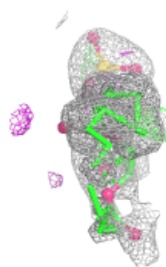
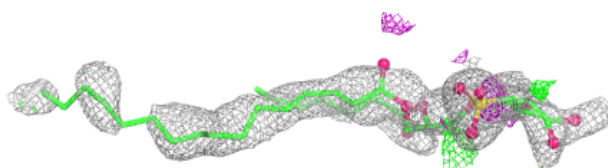
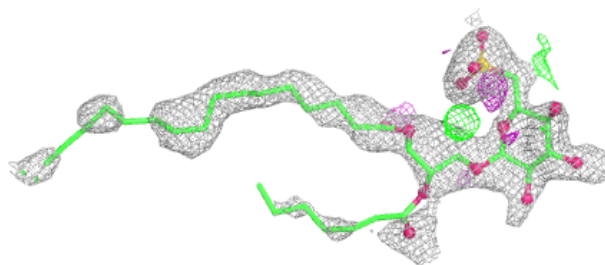
**Electron density around LHG E 101:**

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

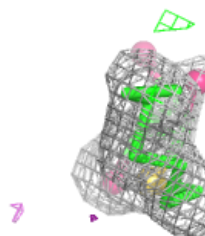
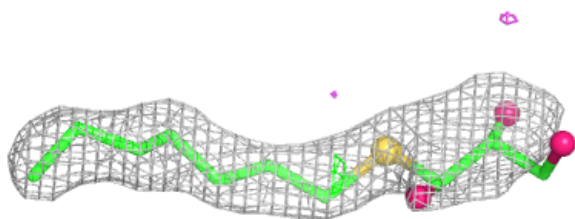
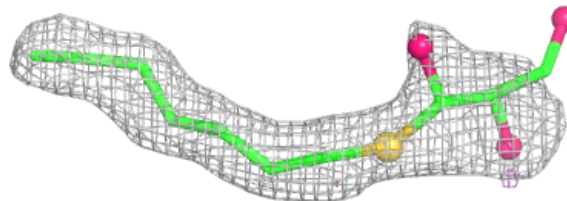


Electron density around SQD D 407:

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

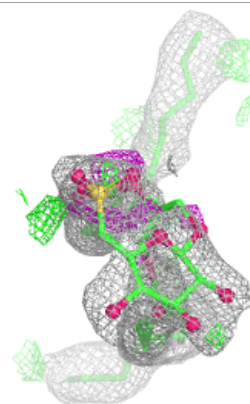
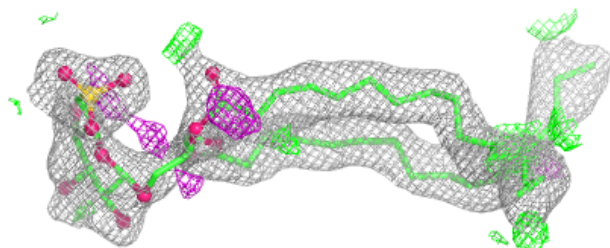
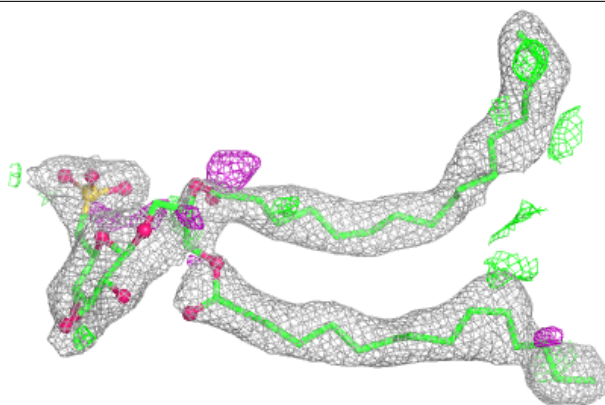
**Electron density around HTG u 201:**

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

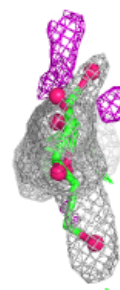
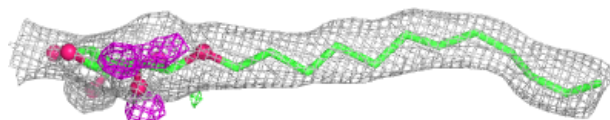
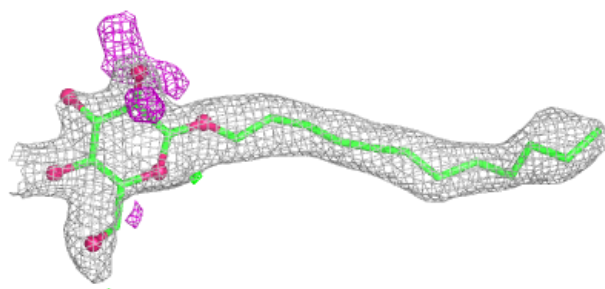


Electron density around SQD L 103:

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

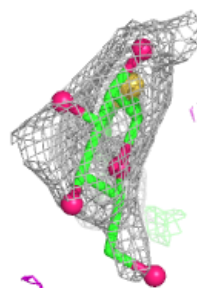
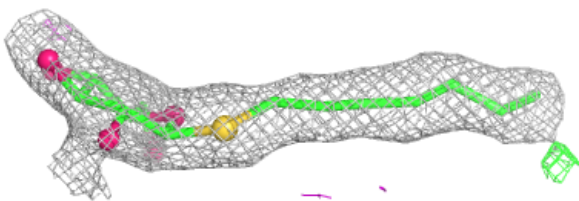
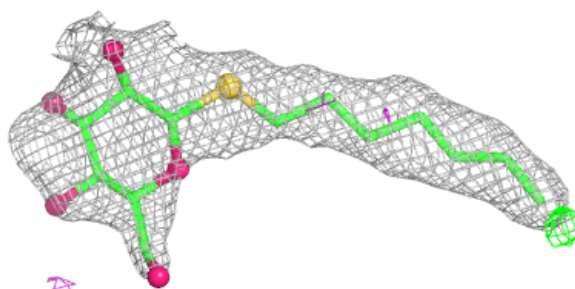
**Electron density around LMT J 102:**

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

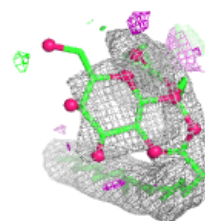
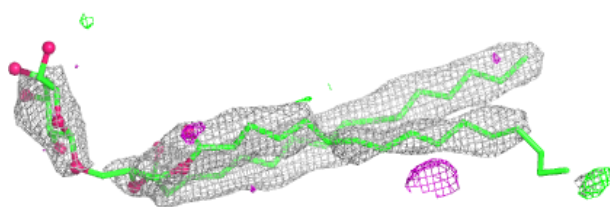
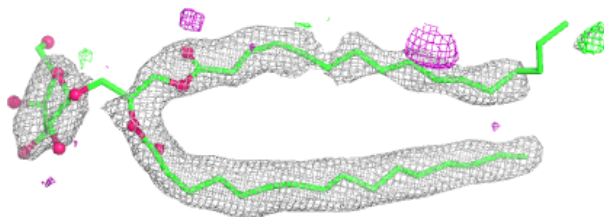


Electron density around HTG B 626:

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

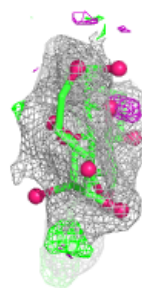
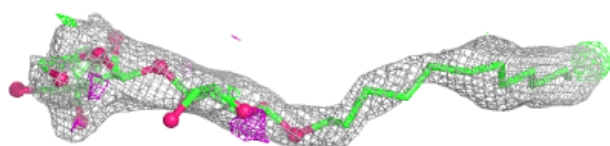
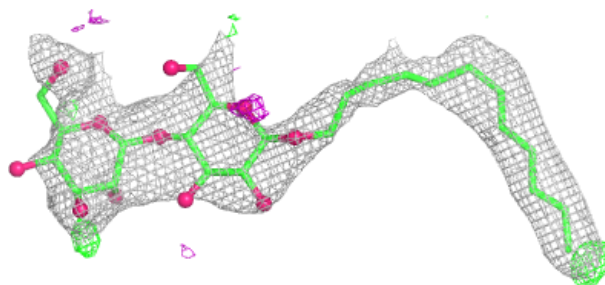
**Electron density around LMG Z 101:**

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

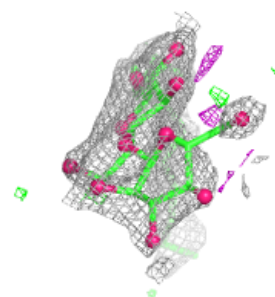
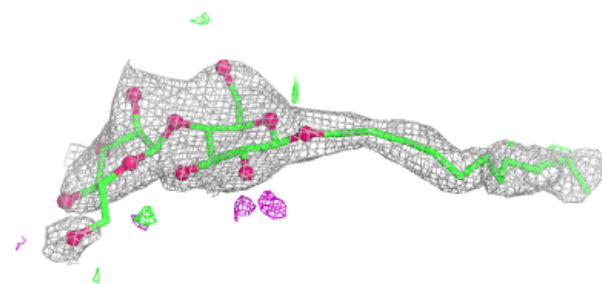
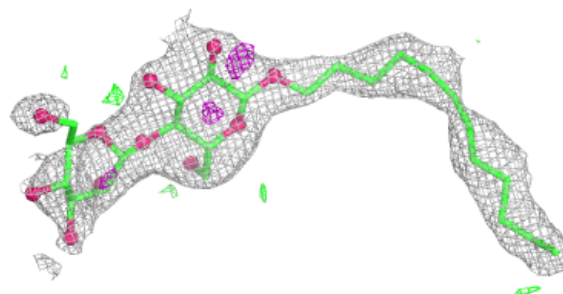


Electron density around LMT Z 102:

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

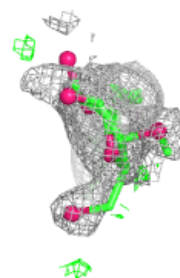
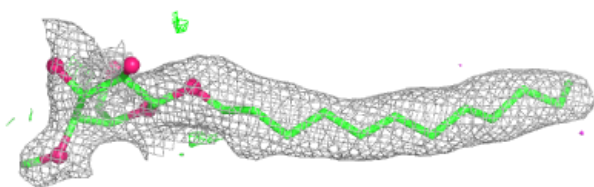
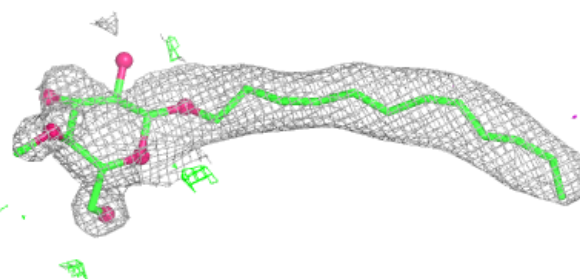
**Electron density around LMT C 520:**

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

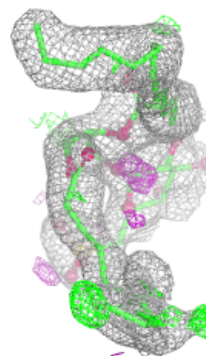
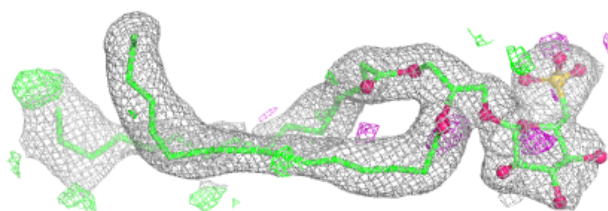
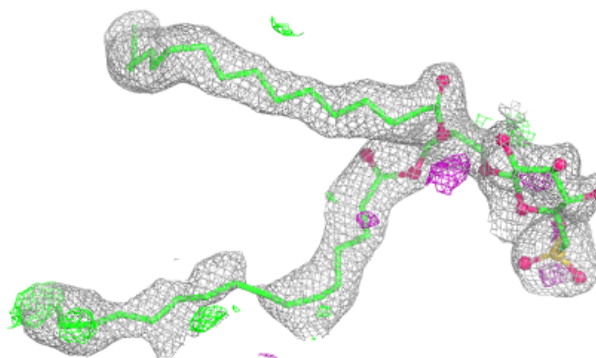


Electron density around LMT b 624:

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

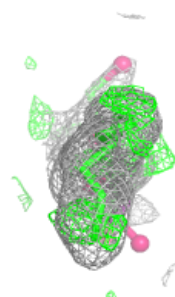
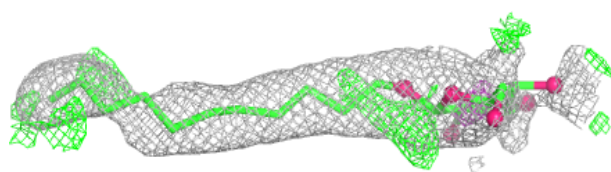
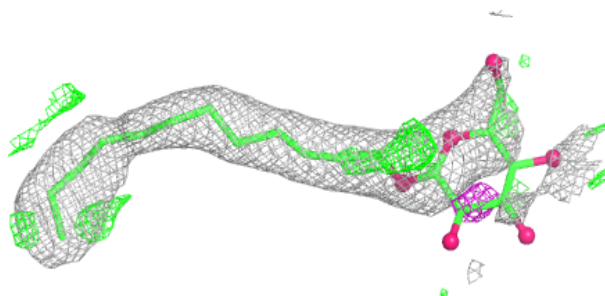
**Electron density around SQD A 418:**

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

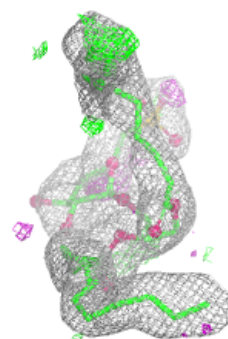
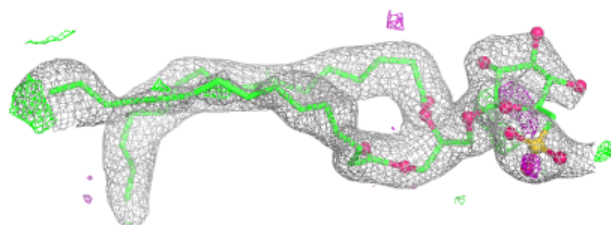
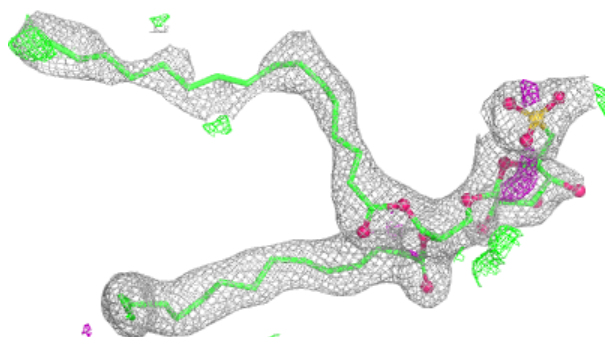


Electron density around LMT b 625:

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

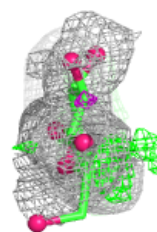
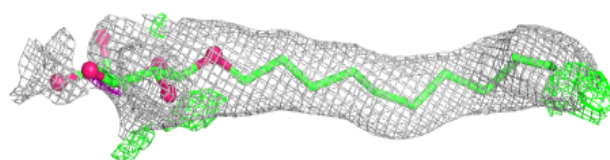
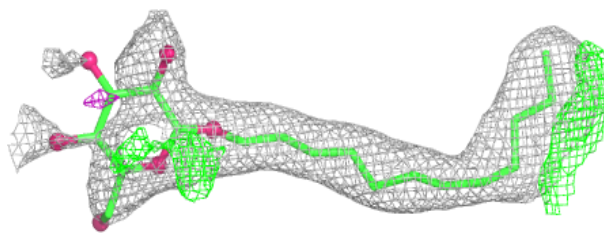
**Electron density around SQD a 401:**

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

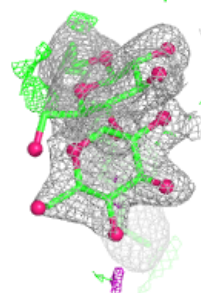
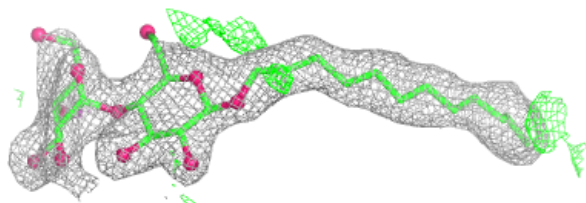
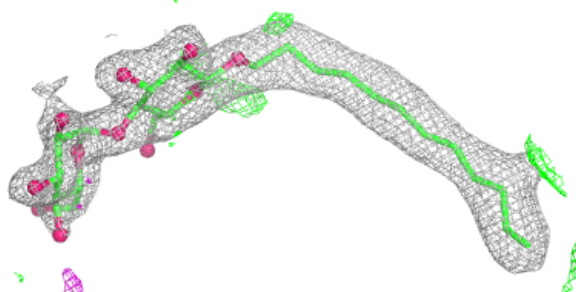


Electron density around LMT t 102:

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

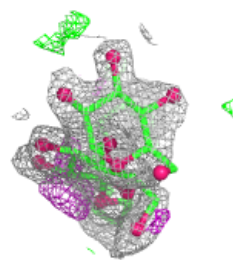
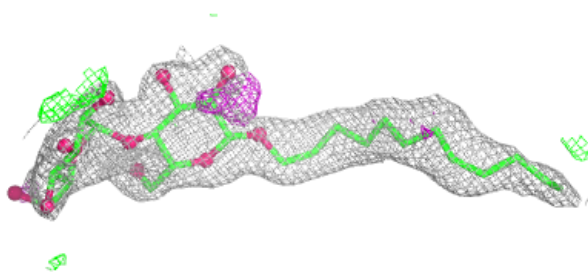
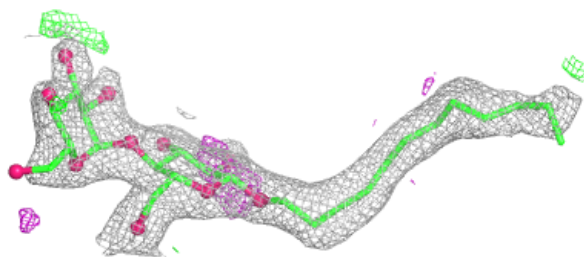
**Electron density around LMT m 102:**

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



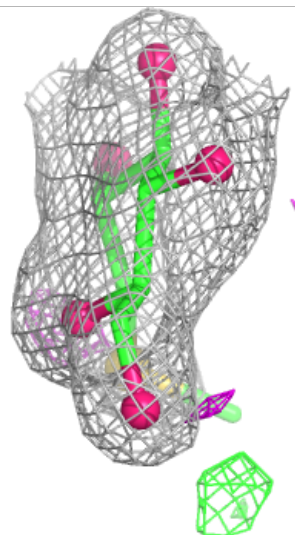
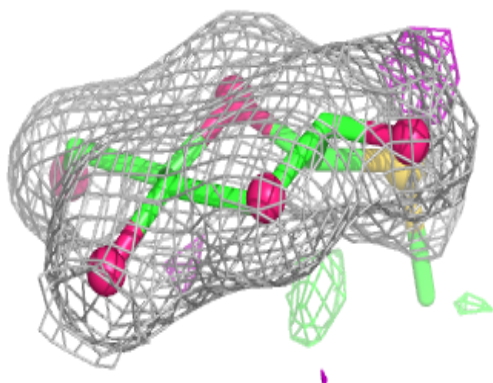
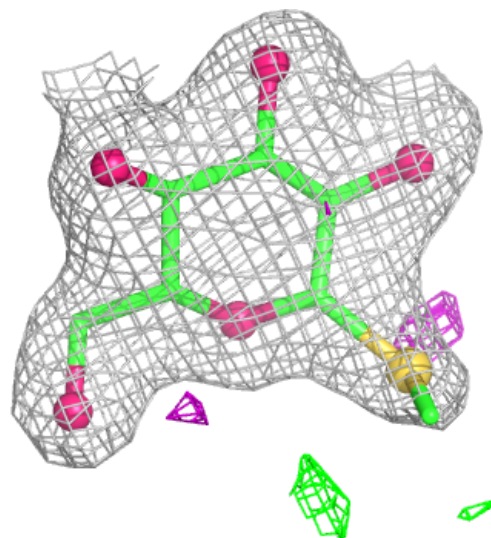
Electron density around LMT A 419:

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



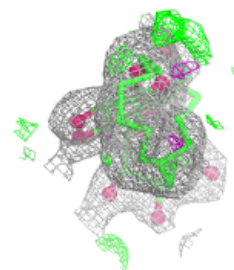
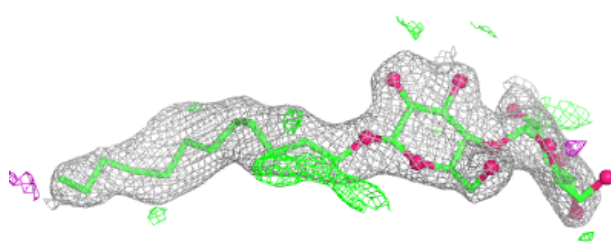
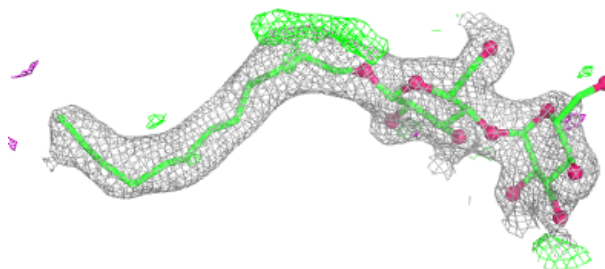
Electron density around HTG V 202:

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

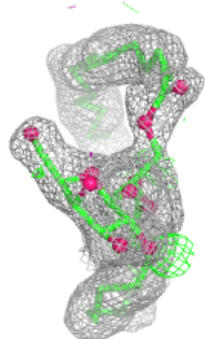
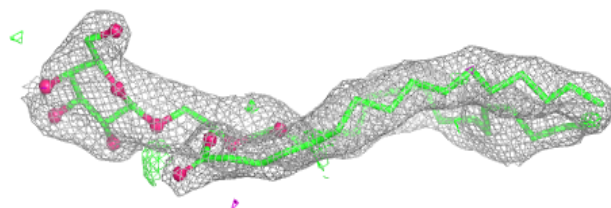
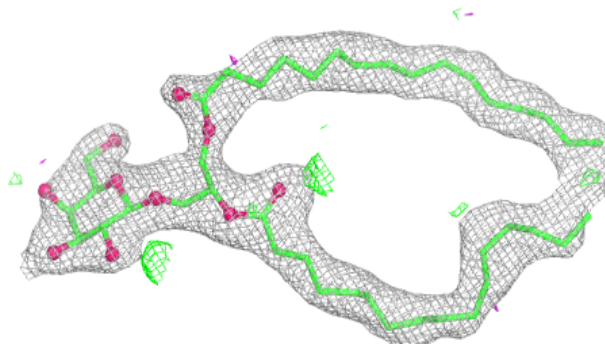


Electron density around LMT a 402:

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

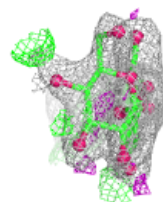
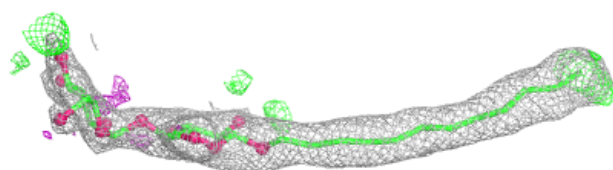
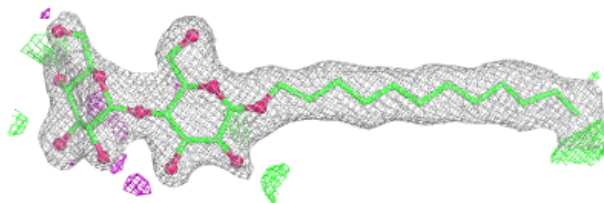
**Electron density around LMG A 413:**

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

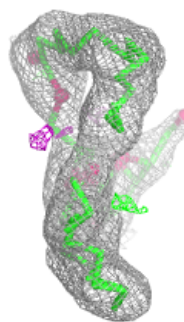
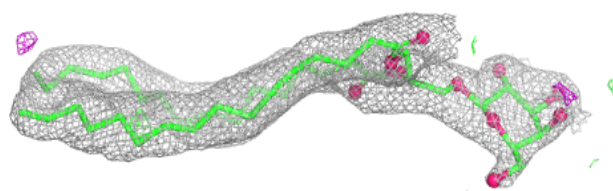
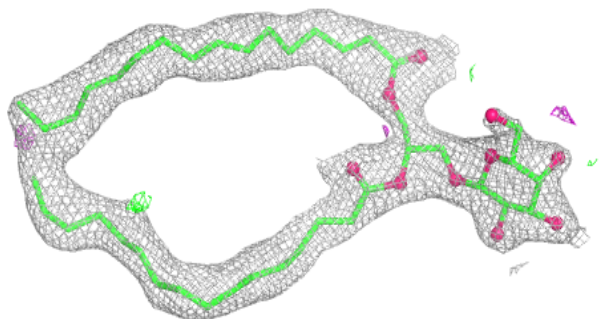


Electron density around LMT M 102:

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

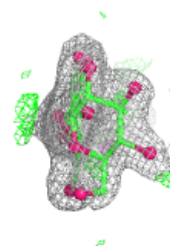
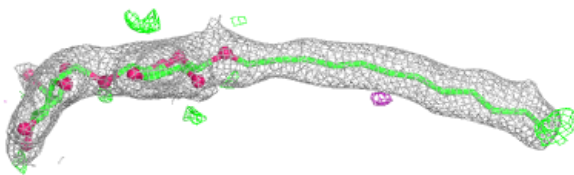
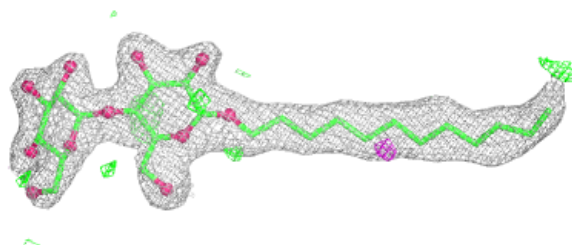
**Electron density around LMG a 418:**

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



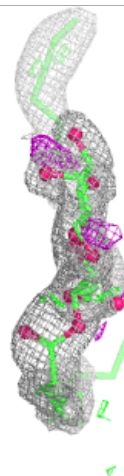
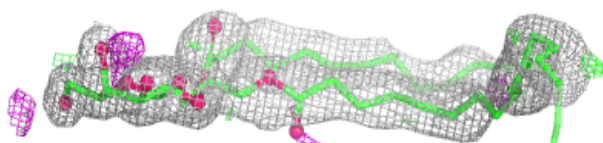
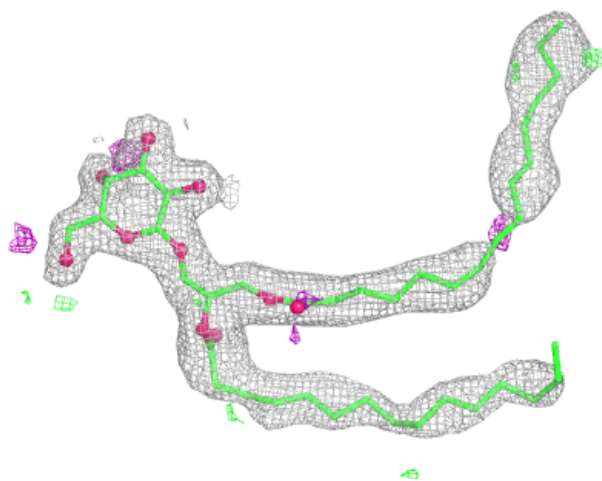
Electron density around LMT m 101:

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



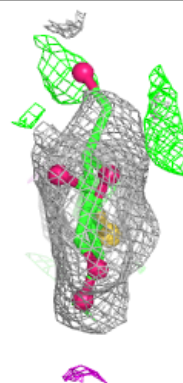
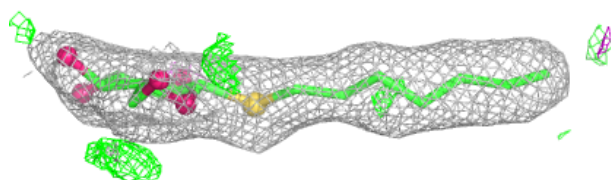
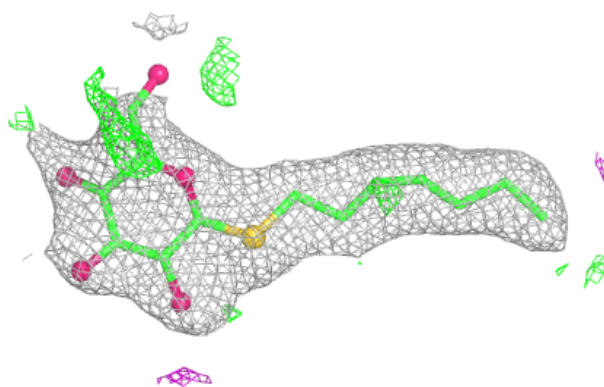
Electron density around LMG C 519:

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

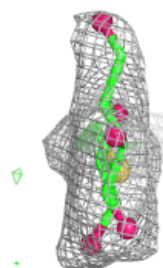
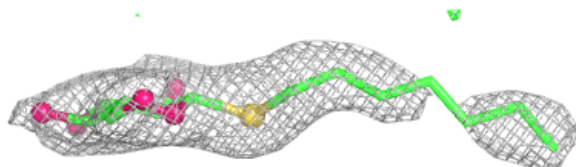
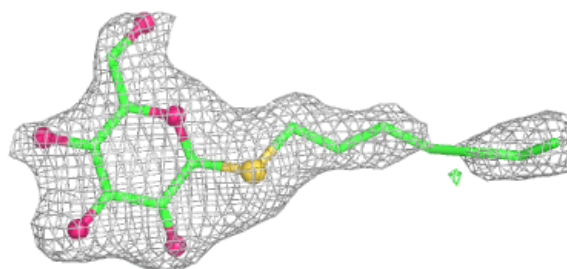


Electron density around HTG B 630:

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

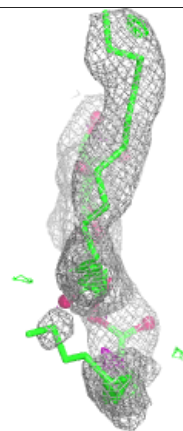
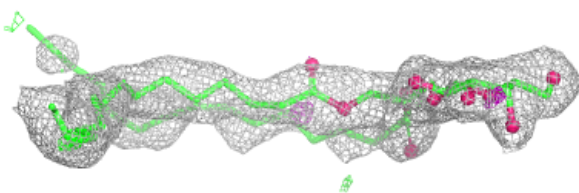
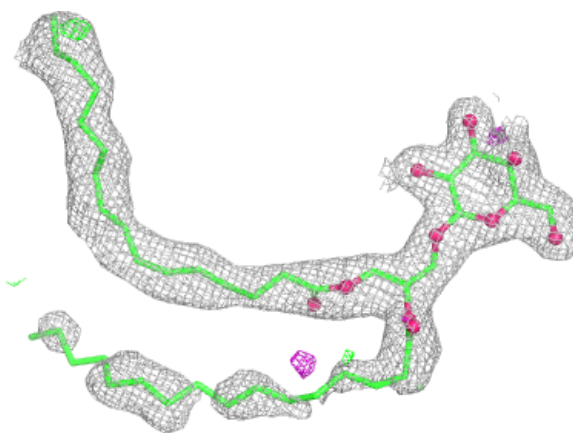
**Electron density around HTG C 521:**

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

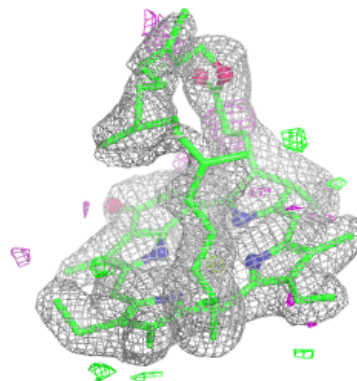
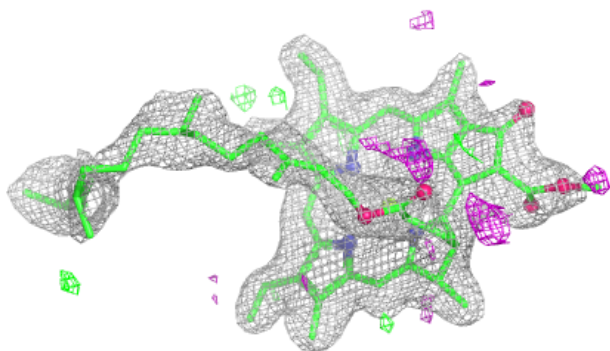
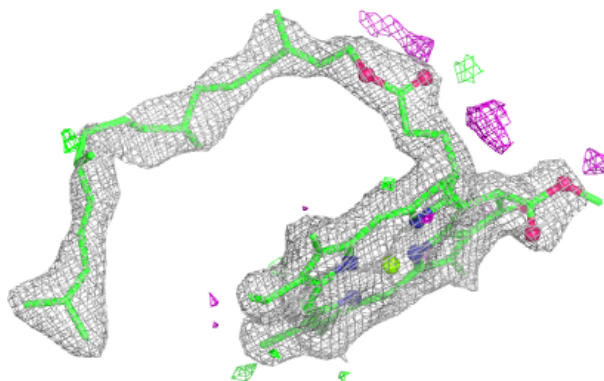


Electron density around LMG c 920:

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

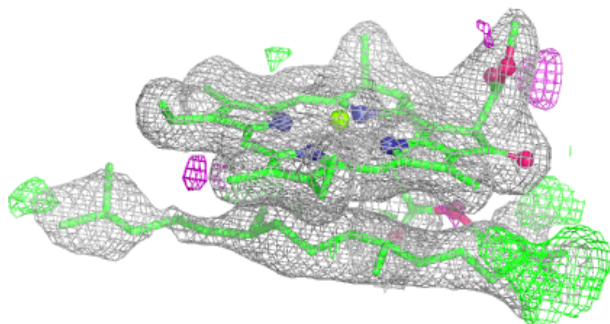
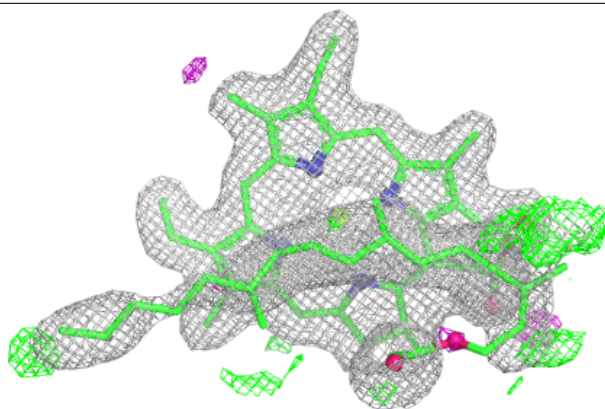
**Electron density around CLA c 914:**

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

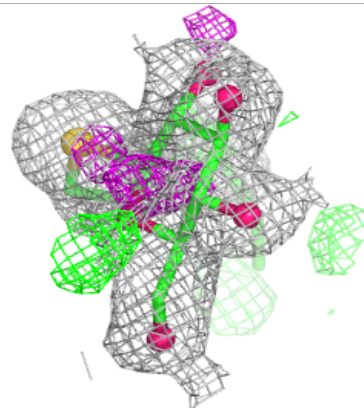
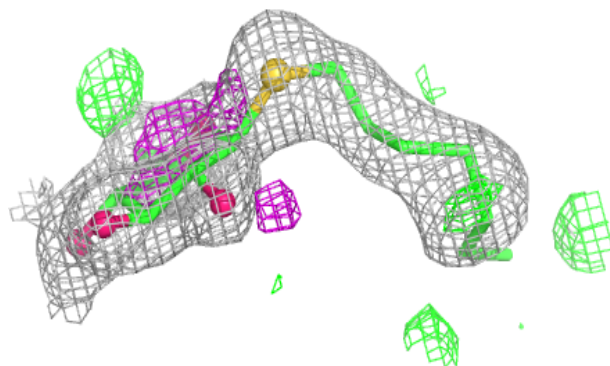
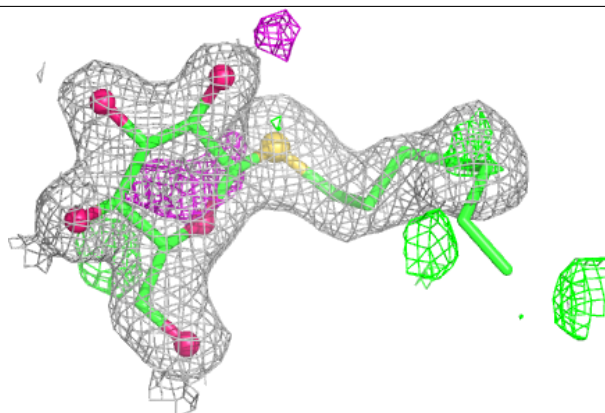


Electron density around CLA B 602:

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

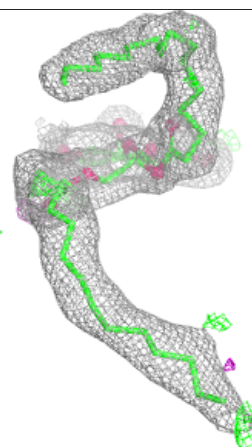
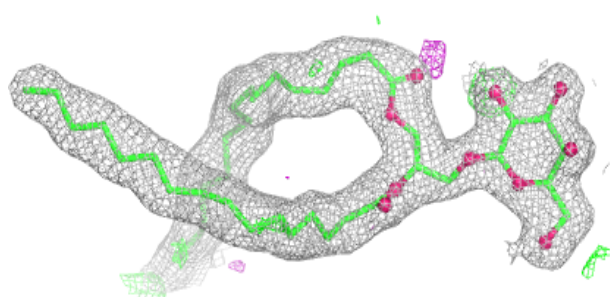
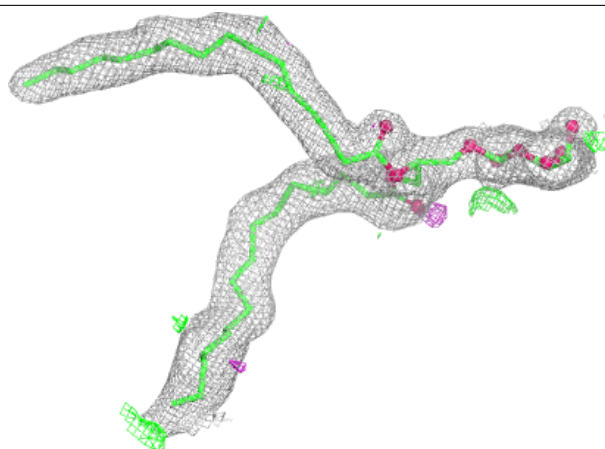
**Electron density around HTG B 625:**

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

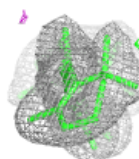
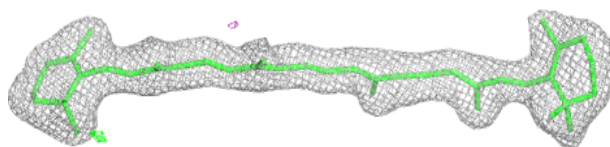
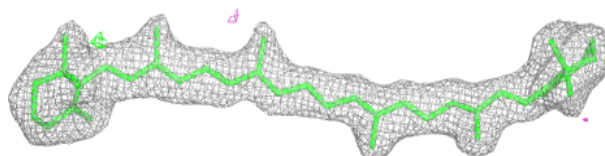


Electron density around LMG B 622:

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

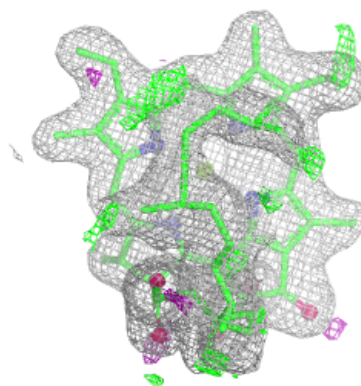
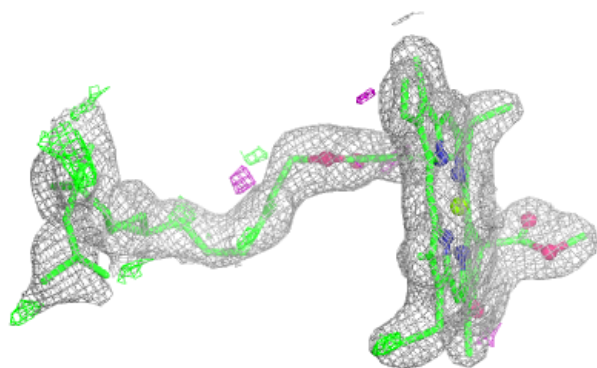
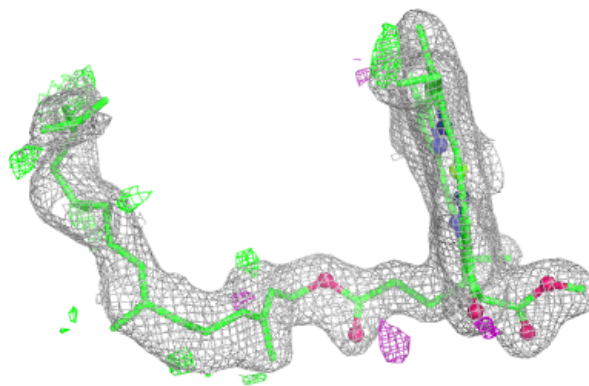
**Electron density around BCR c 915:**

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



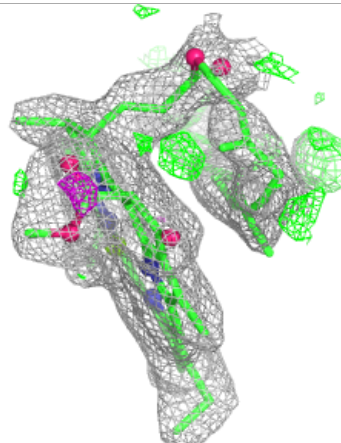
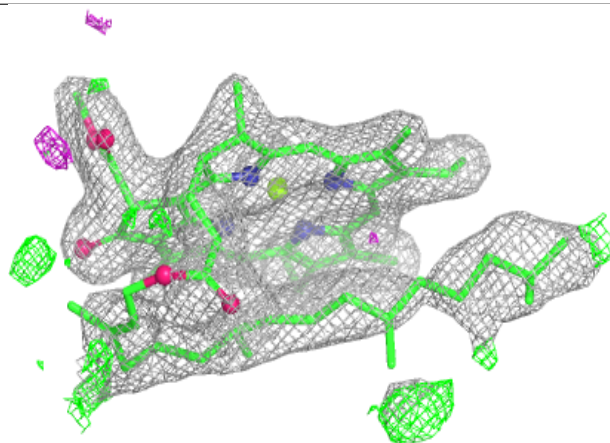
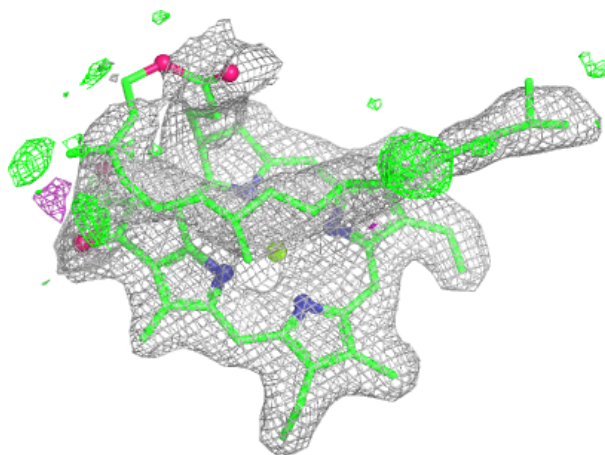
Electron density around CLA C 506:

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



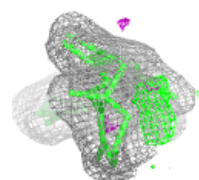
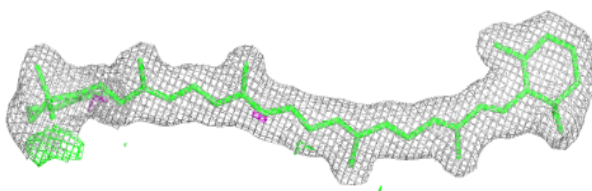
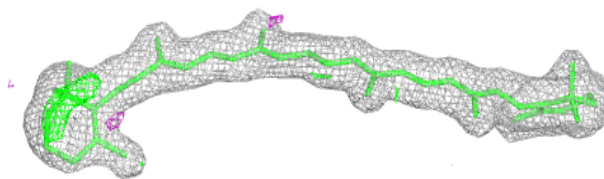
Electron density around CLA b 604:

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

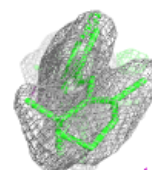
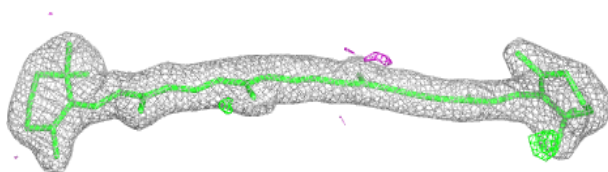
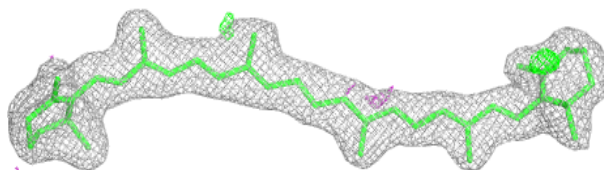


Electron density around BCR d 404:

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

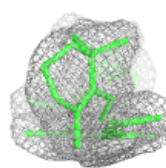
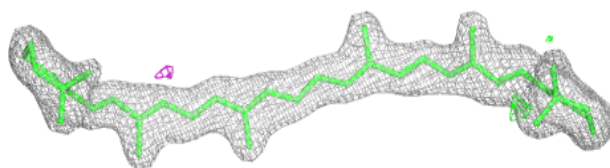
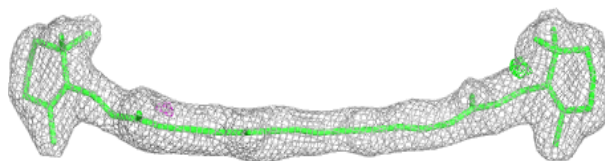
**Electron density around BCR k 101:**

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



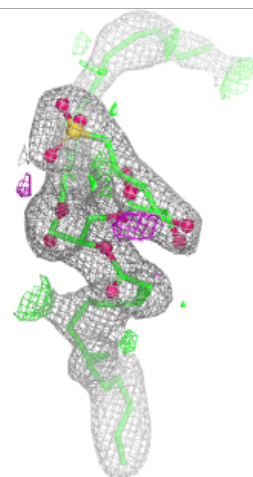
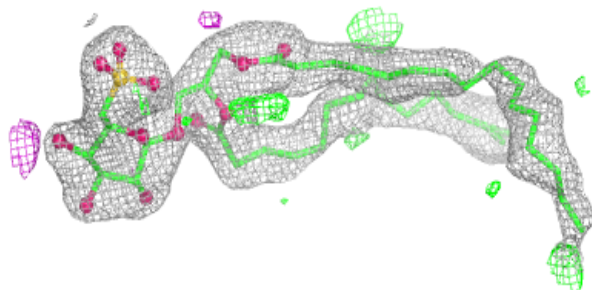
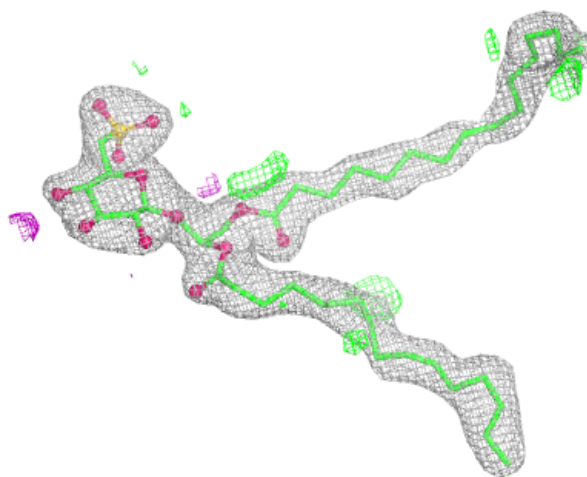
Electron density around BCR k 102:

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



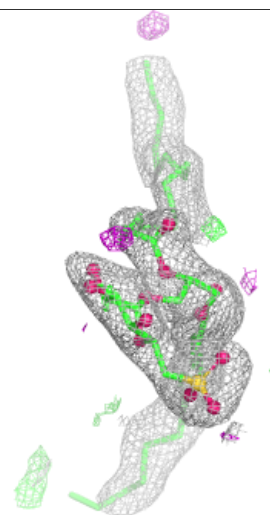
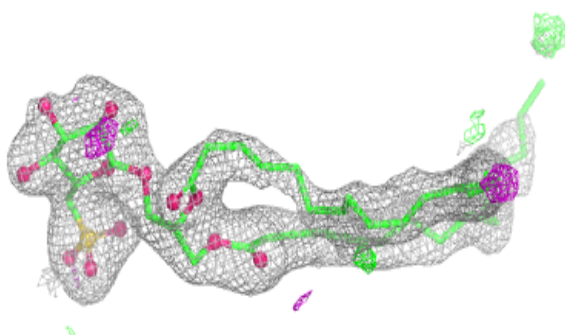
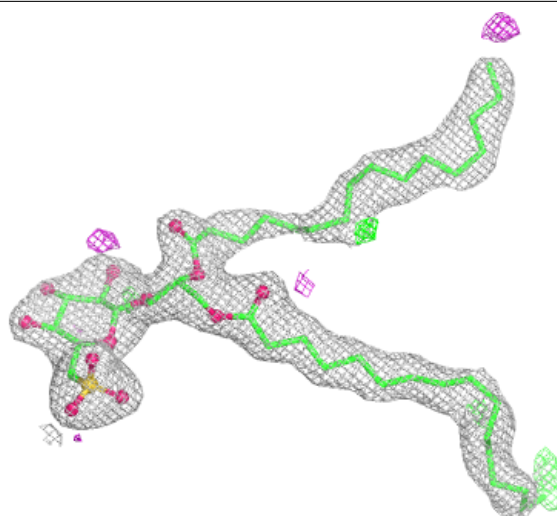
Electron density around SQD A 412:

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



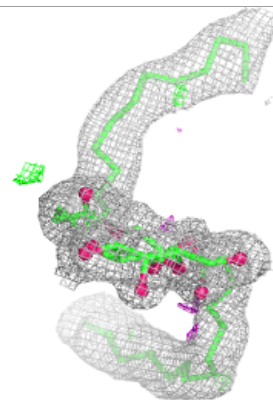
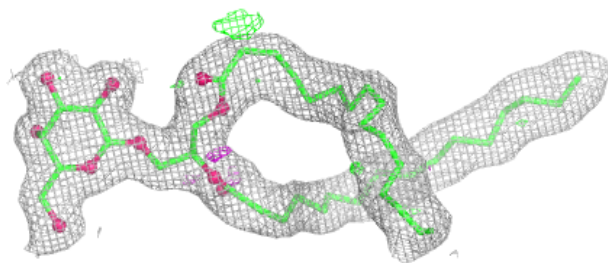
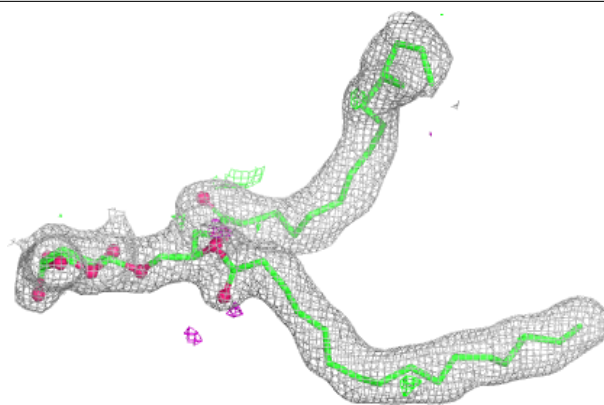
Electron density around SQD a 416:

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

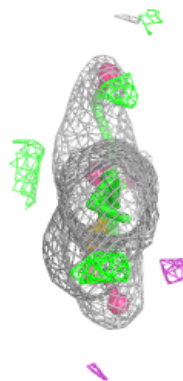
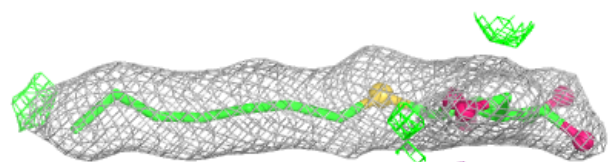
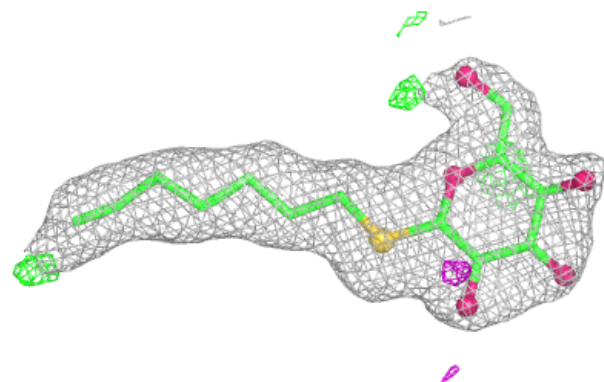


Electron density around LMG b 623:

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

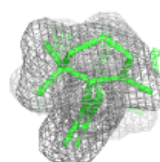
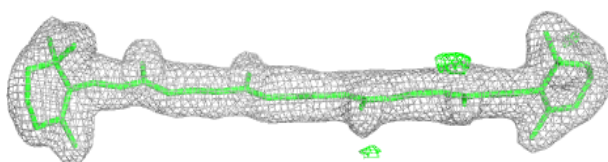
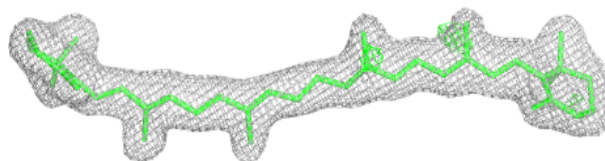
**Electron density around HTG b 601:**

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

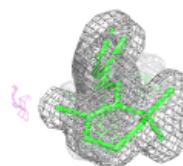
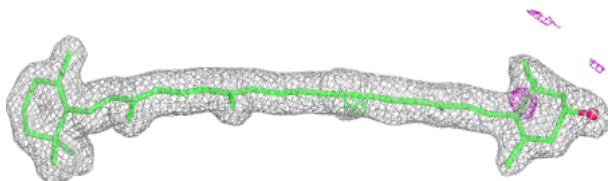
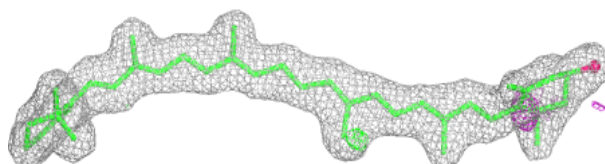


Electron density around BCR C 514:

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

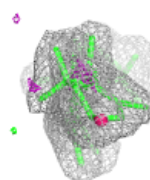
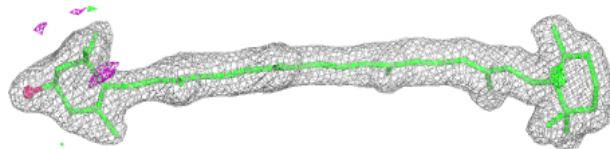
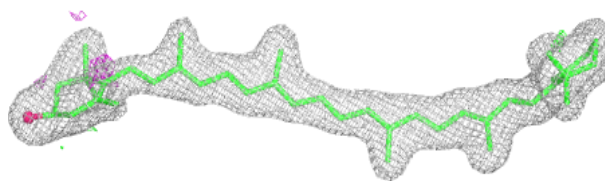
**Electron density around RRX H 101:**

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

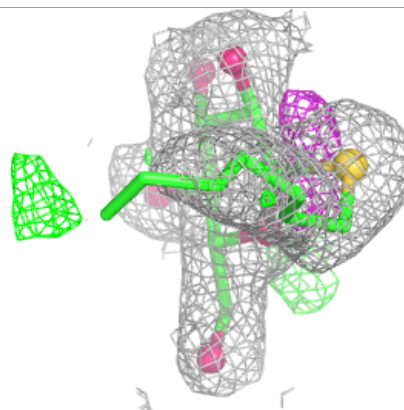
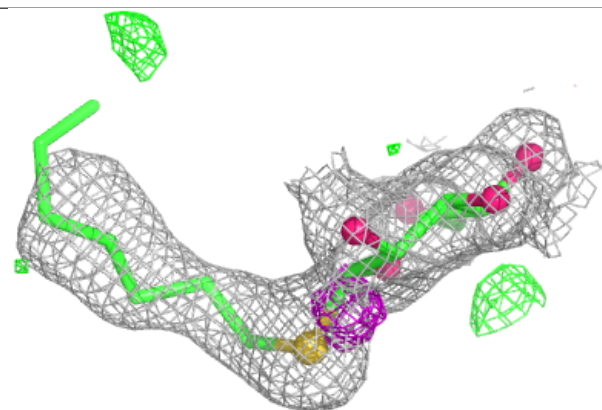
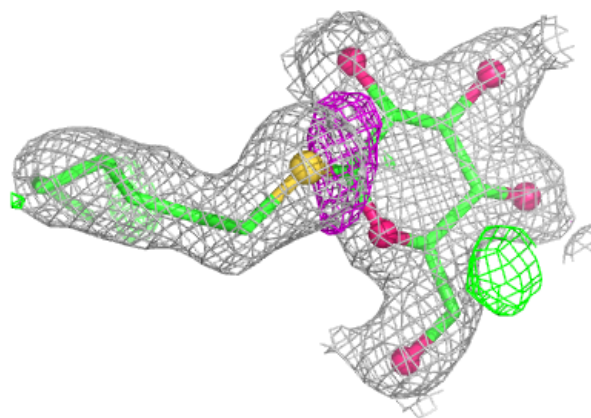


Electron density around RRX h 101:

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

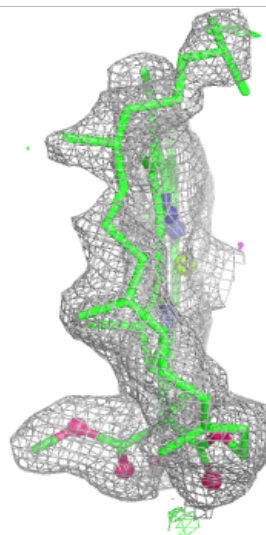
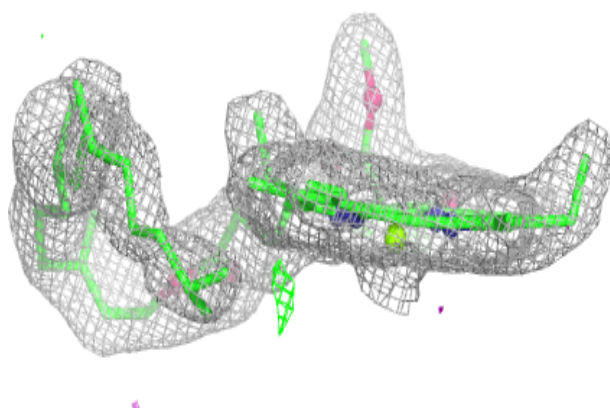
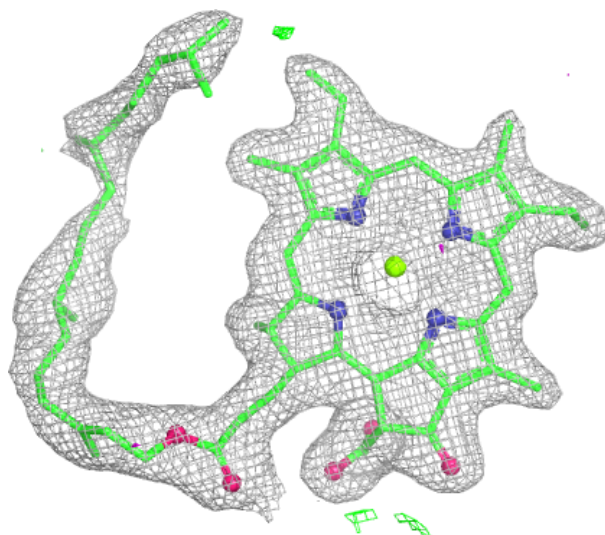
**Electron density around HTG b 626:**

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



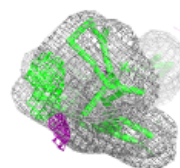
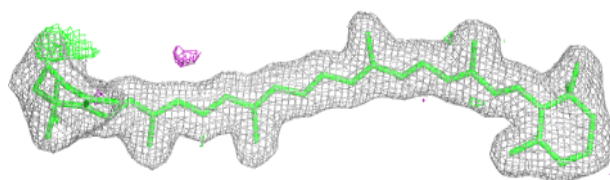
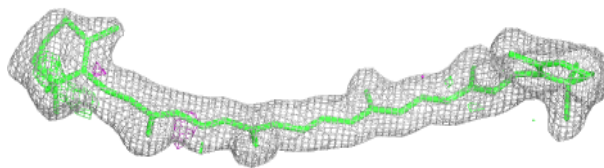
Electron density around CLA C 512:

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

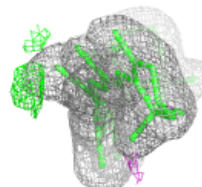
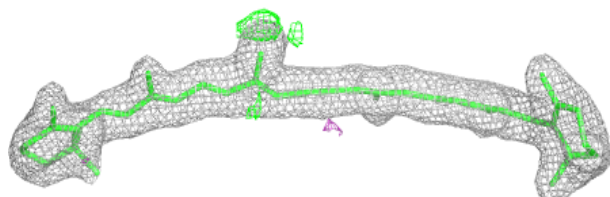
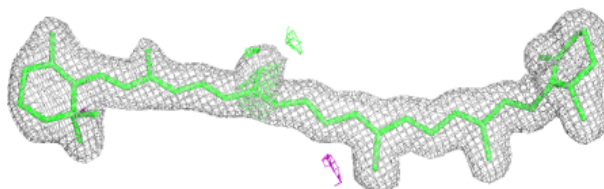


Electron density around BCR D 404:

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

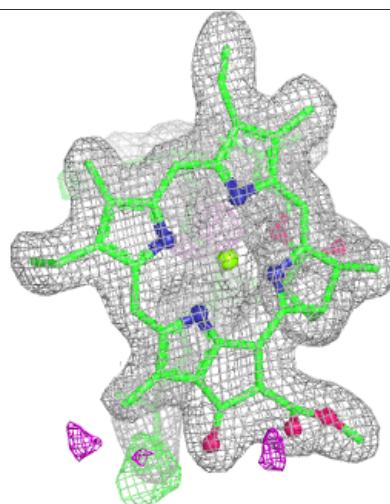
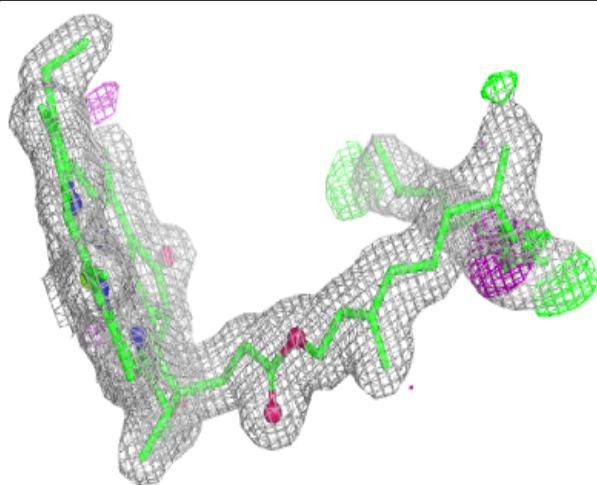
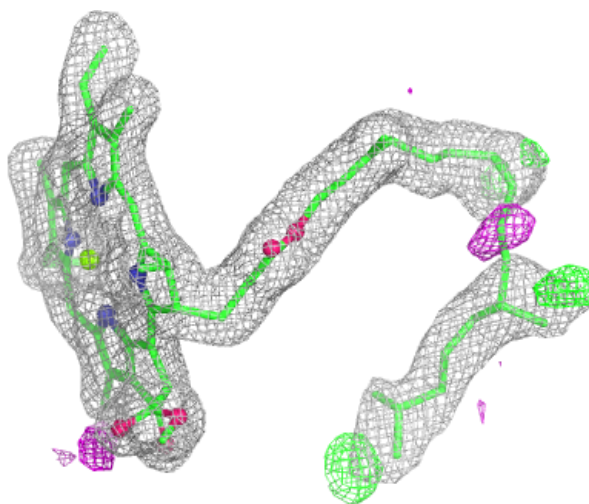
**Electron density around BCR T 101:**

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



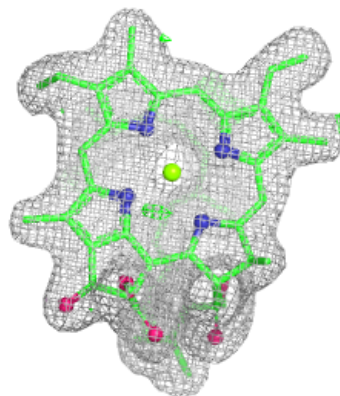
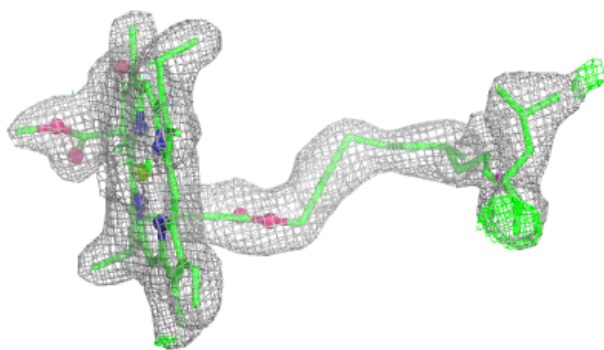
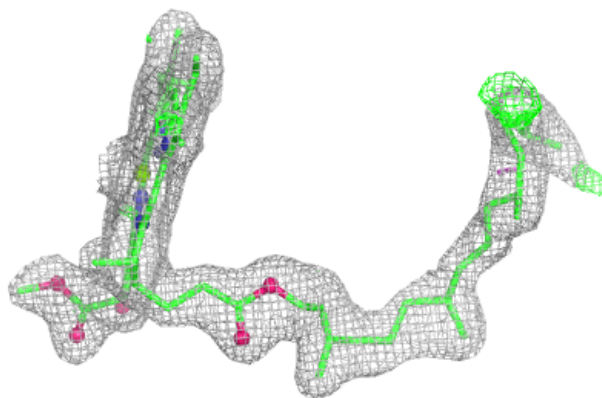
Electron density around CLA b 609:

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



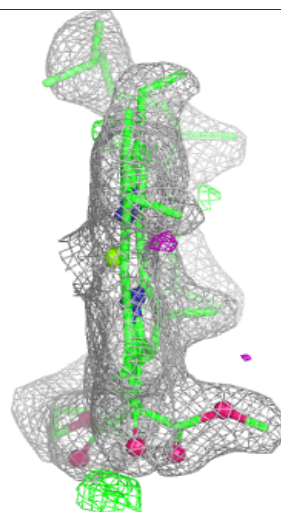
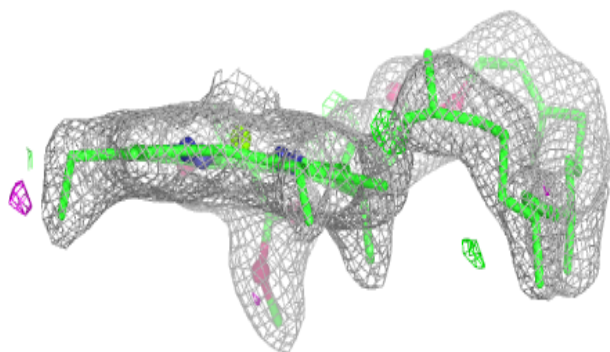
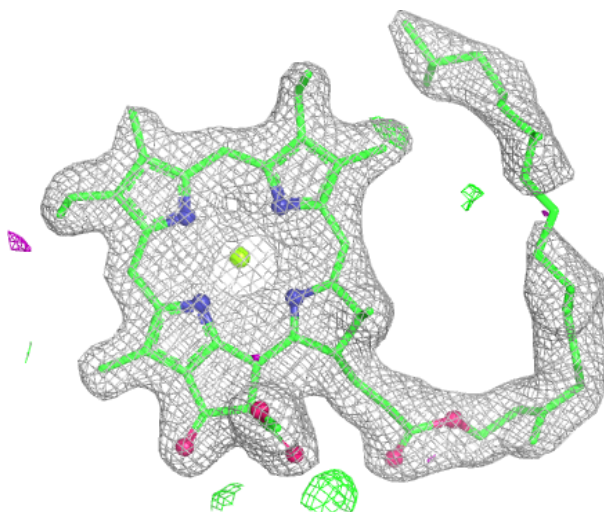
Electron density around CLA c 907:

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



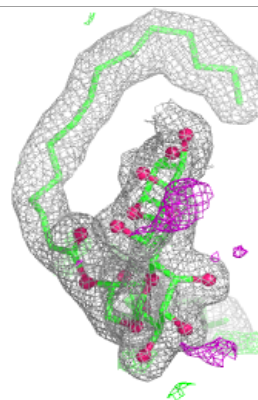
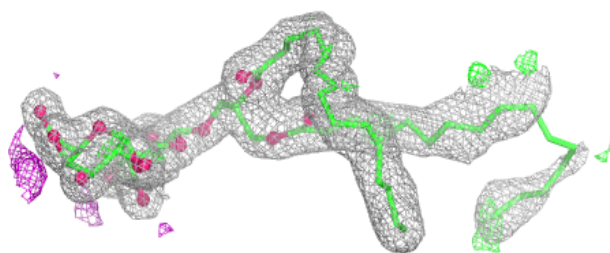
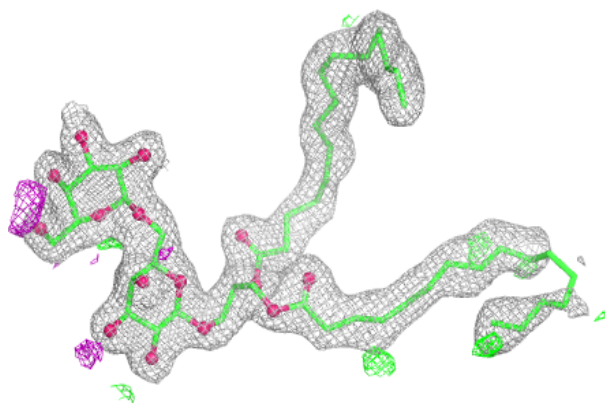
Electron density around CLA c 913:

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

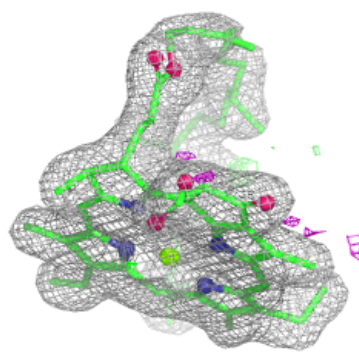
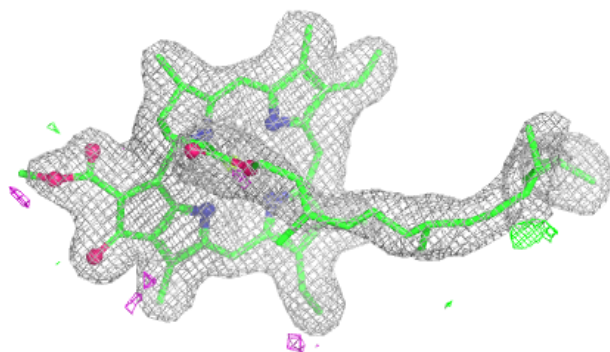
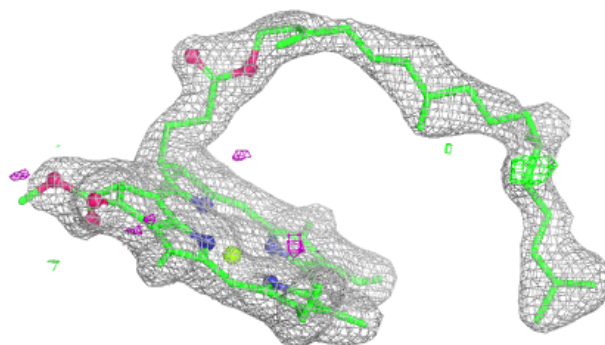


Electron density around DGD c 918:

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

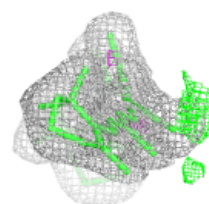
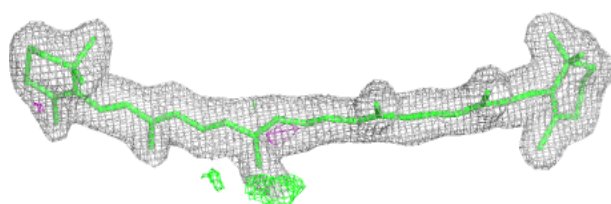
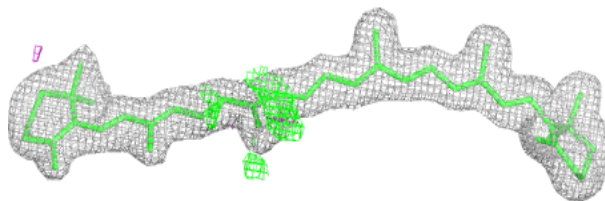
**Electron density around CLA C 513:**

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

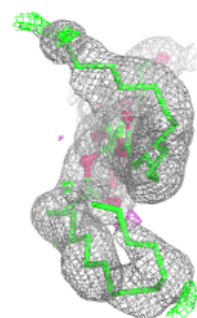
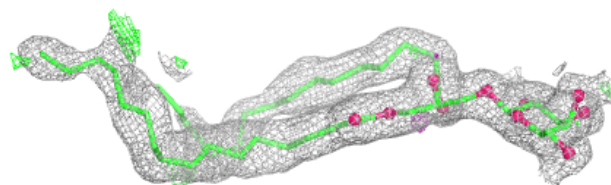
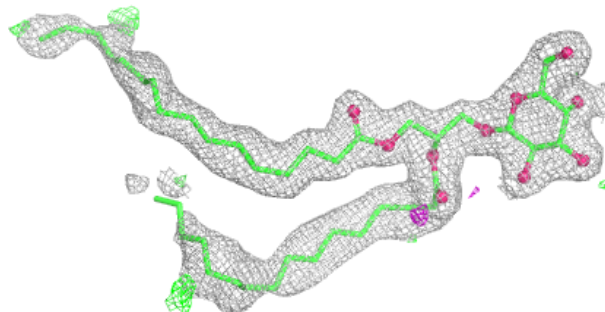


Electron density around BCR t 101:

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

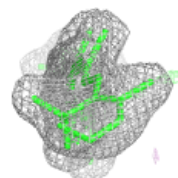
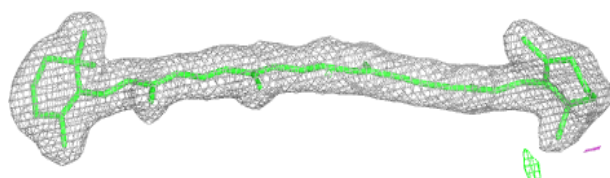
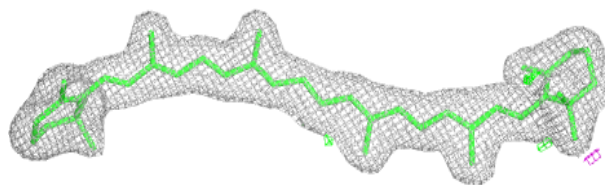
**Electron density around LMG d 410:**

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

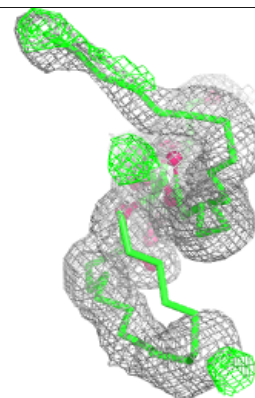
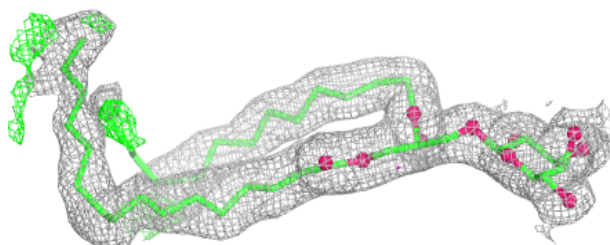
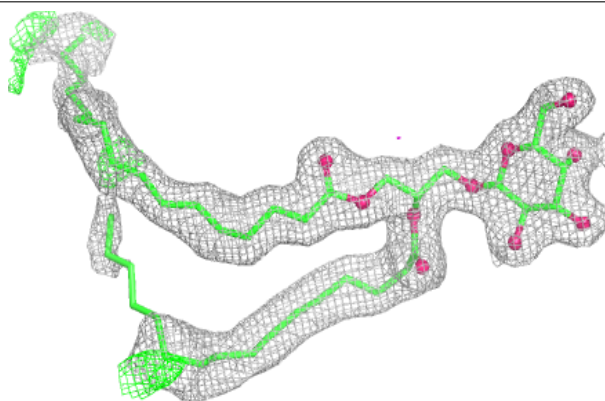


Electron density around BCR K 101:

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

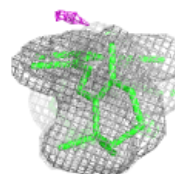
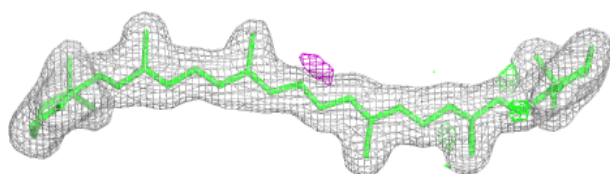
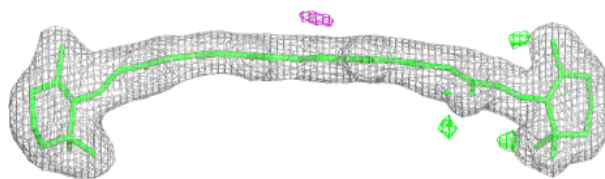
**Electron density around LMG D 411:**

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

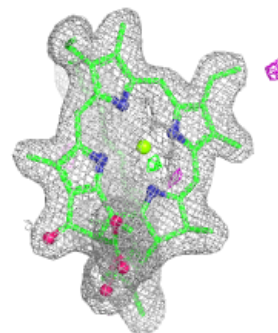
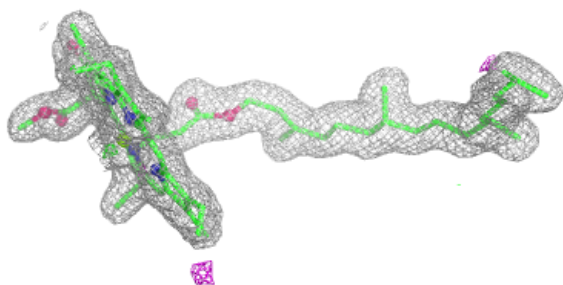
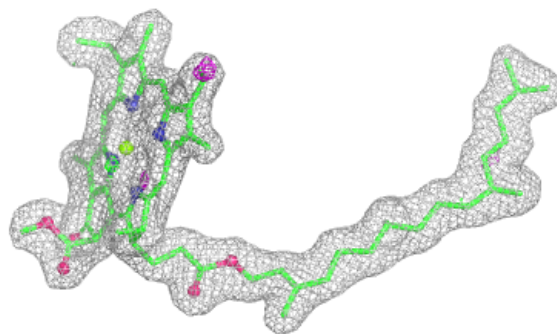


Electron density around BCR K 102:

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

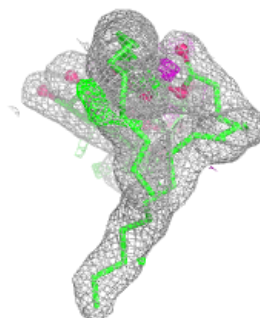
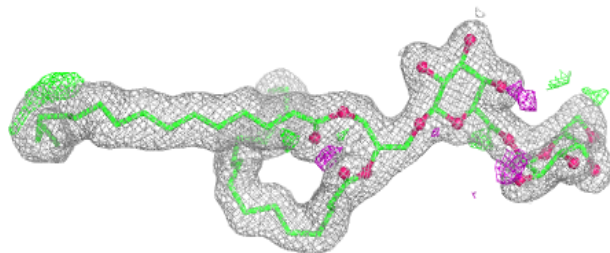
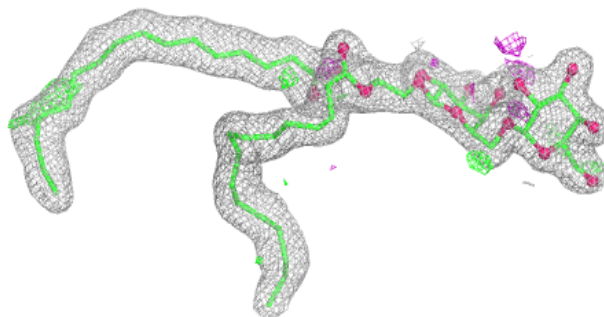
**Electron density around CLA b 612:**

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

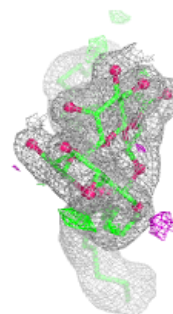
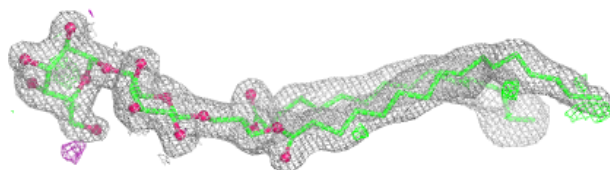
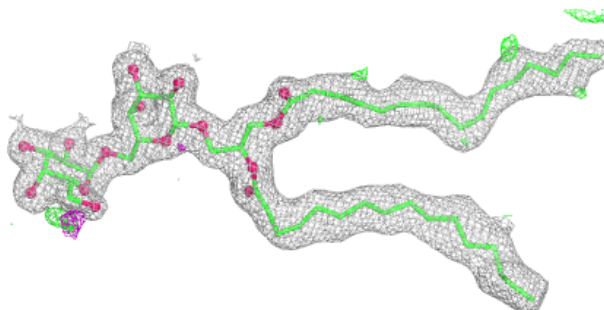


Electron density around DGD H 102:

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

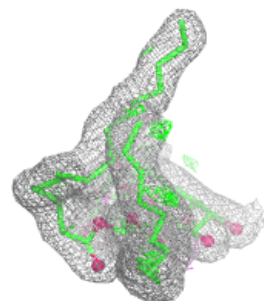
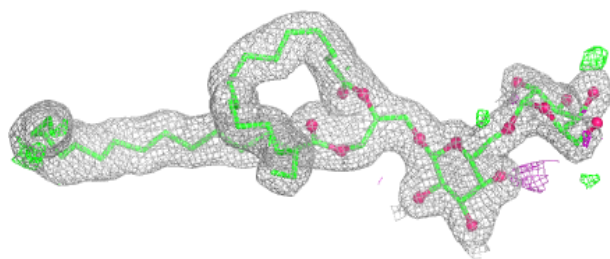
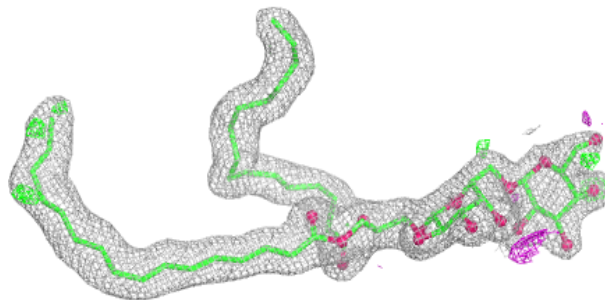
**Electron density around DGD c 919:**

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



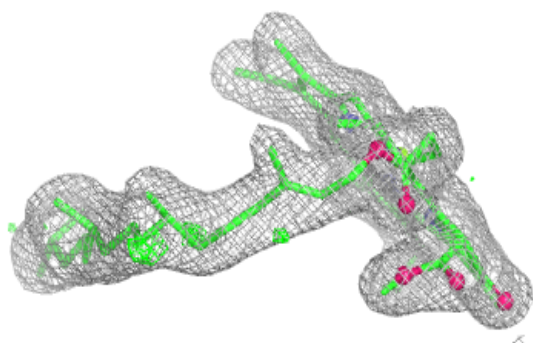
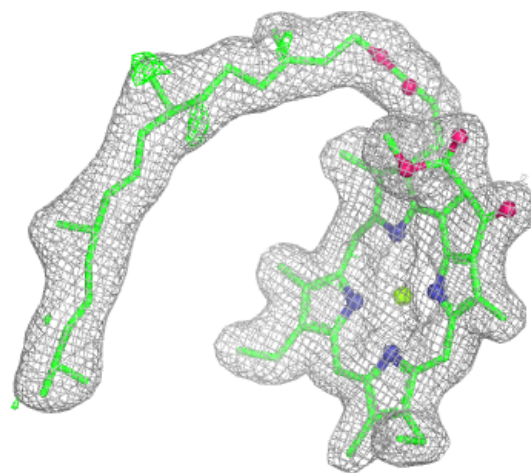
Electron density around DGD h 102:

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



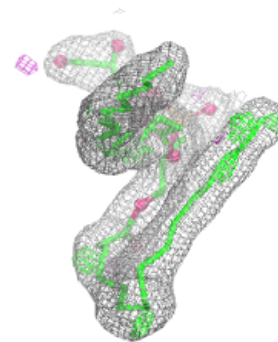
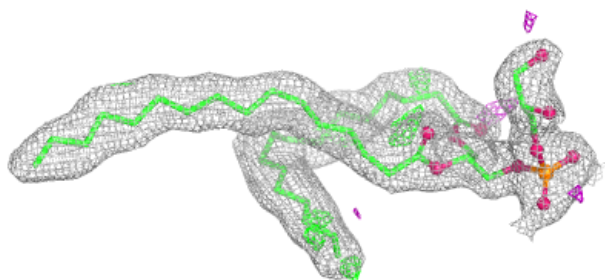
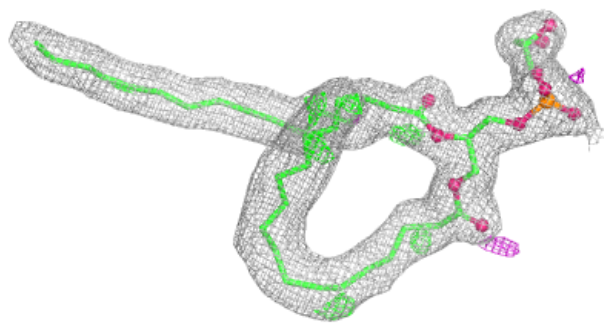
Electron density around CLA c 908:

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

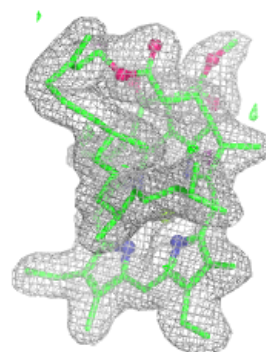
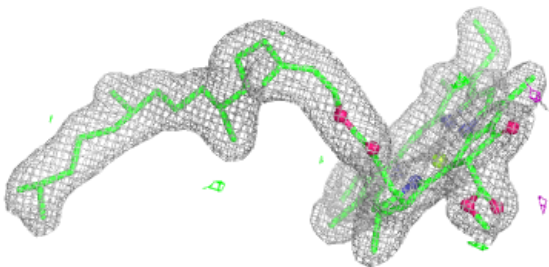
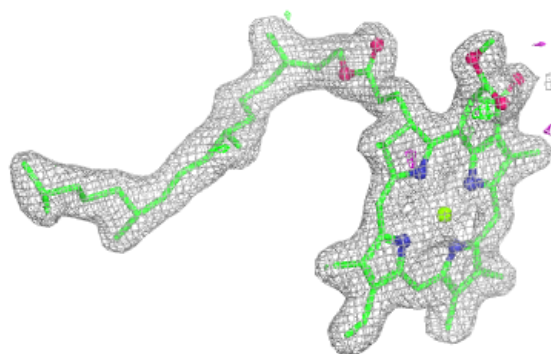


Electron density around LHG D 408:

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

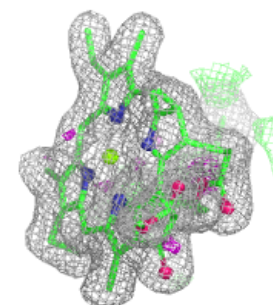
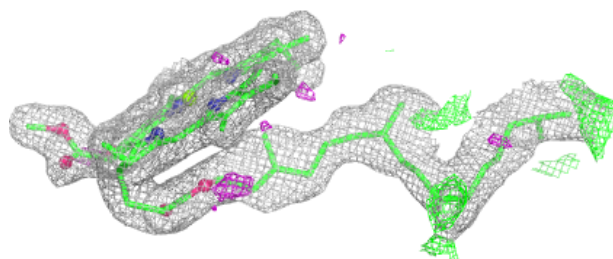
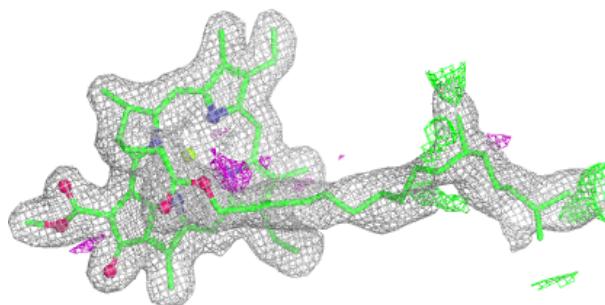
**Electron density around CLA c 912:**

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

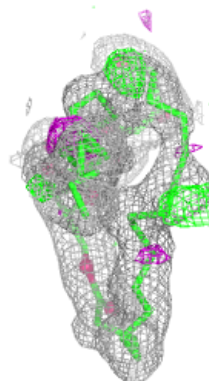
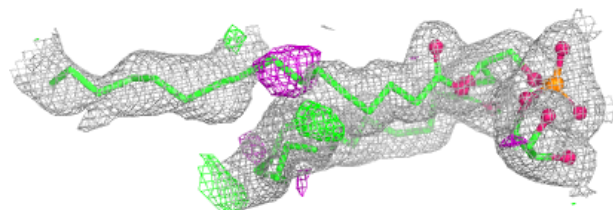
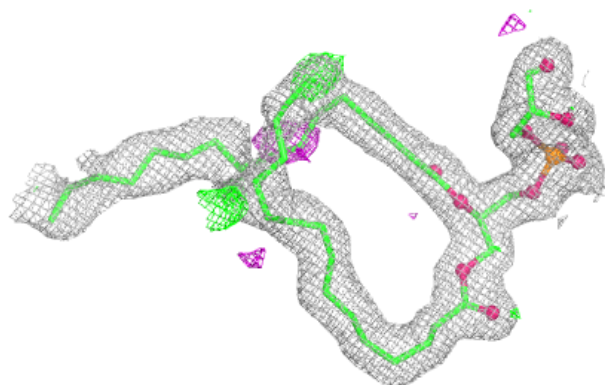


Electron density around CLA b 617:

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

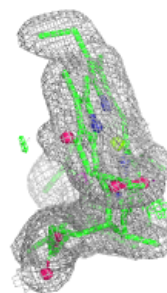
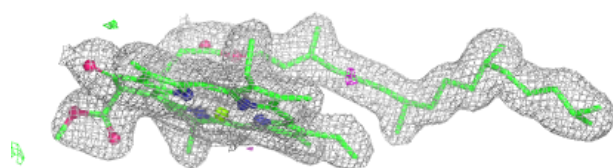
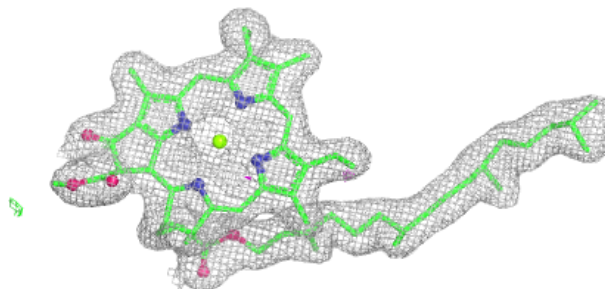
**Electron density around LHG d 409:**

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

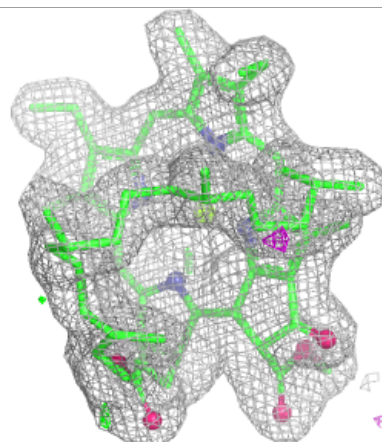
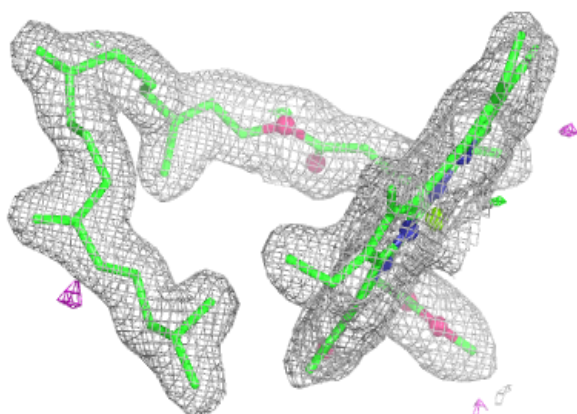
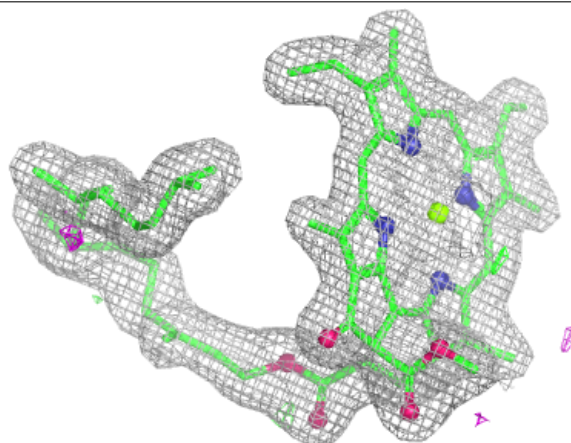


Electron density around CLA c 902:

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

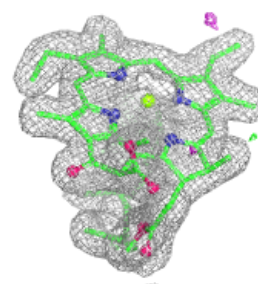
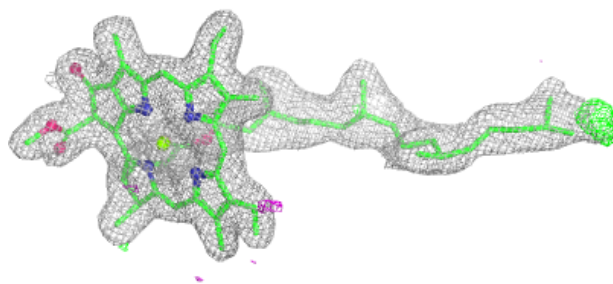
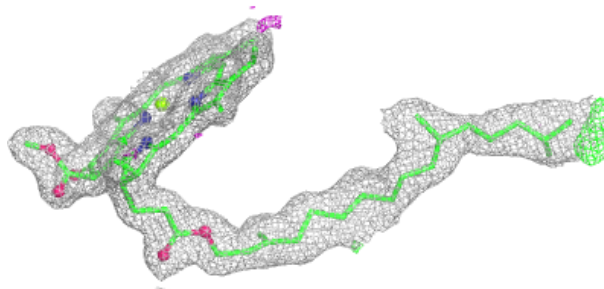
**Electron density around CLA c 904:**

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

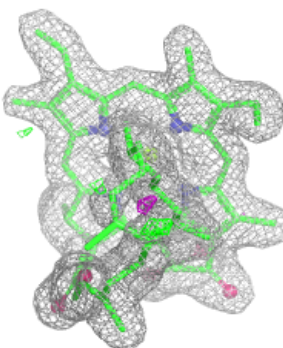
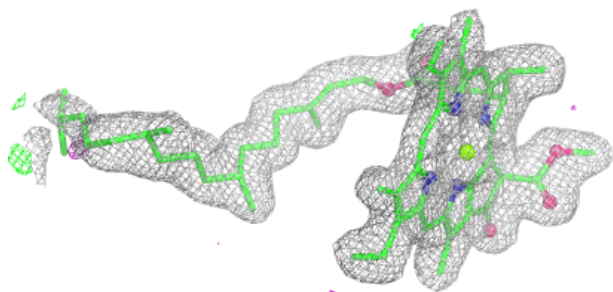
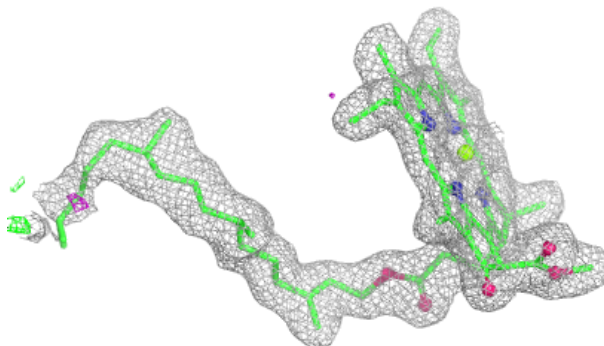


Electron density around CLA c 905:

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

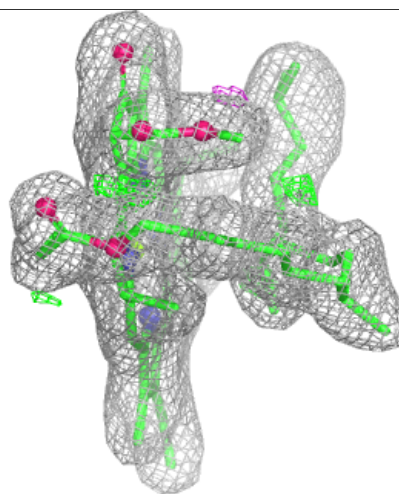
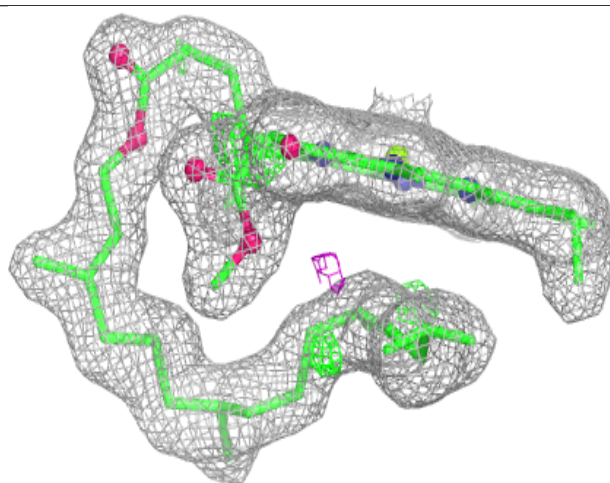
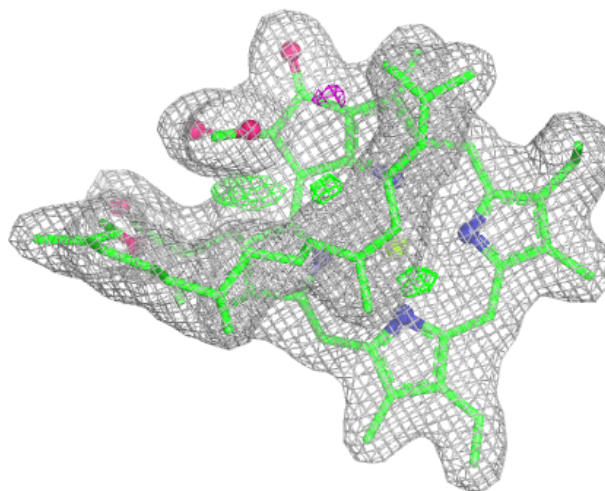
**Electron density around CLA c 909:**

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



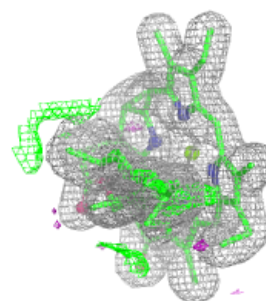
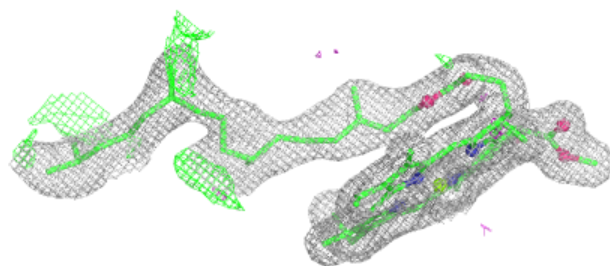
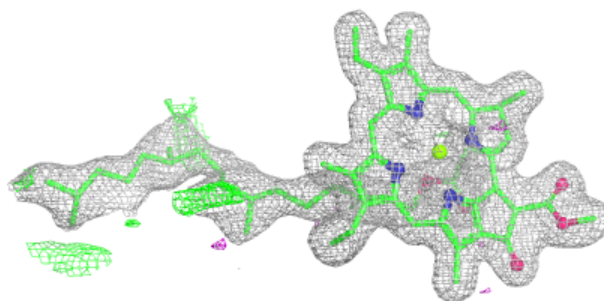
Electron density around CLA c 911:

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

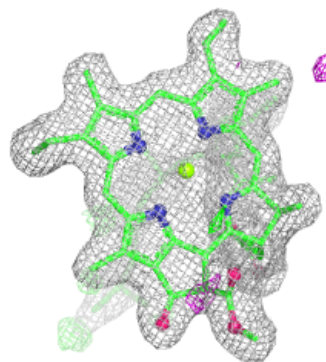
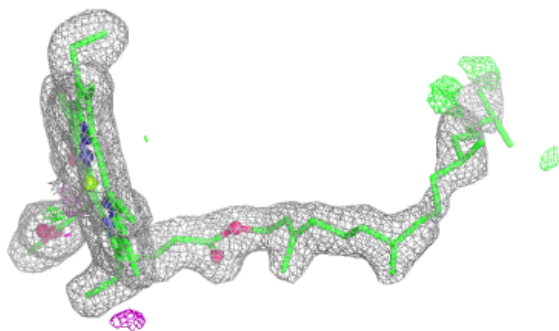
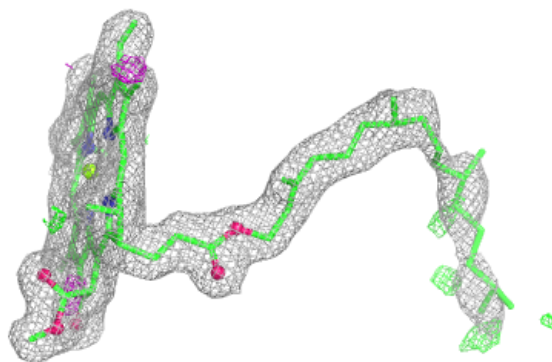


Electron density around CLA B 615:

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

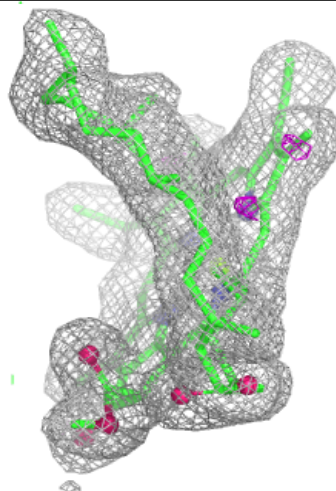
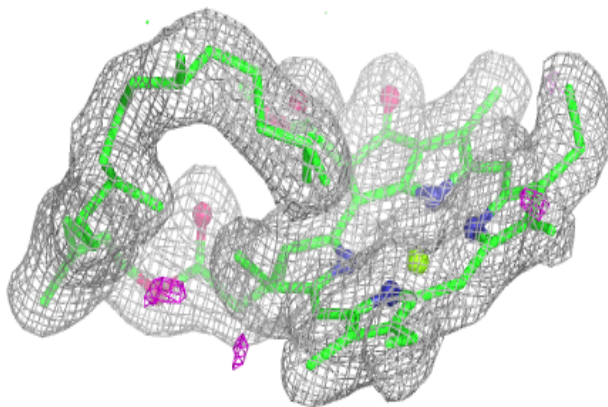
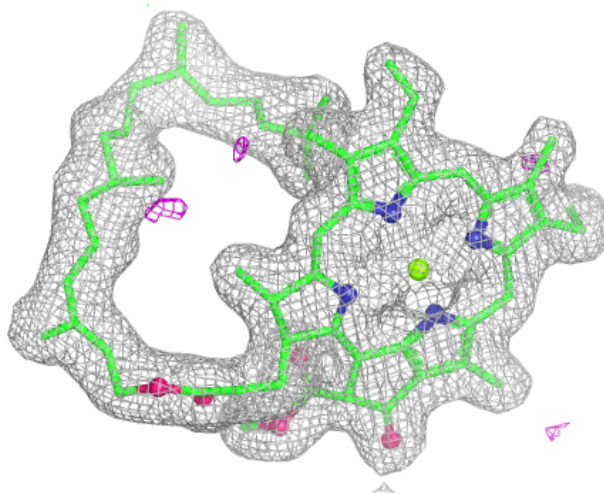
**Electron density around CLA D 403:**

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



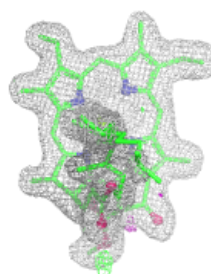
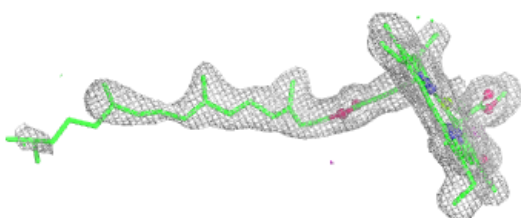
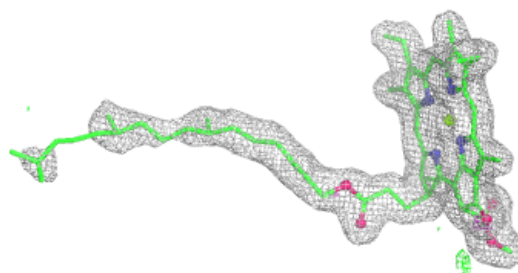
Electron density around CLA B 616:

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

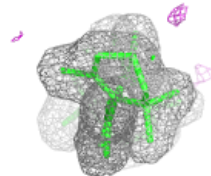
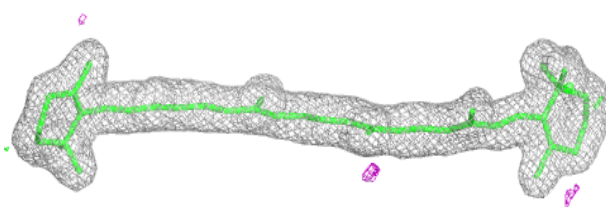
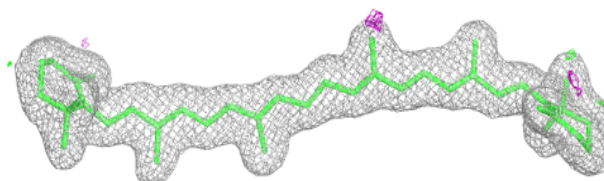


Electron density around CLA d 403:

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

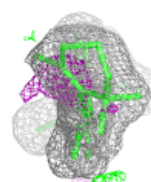
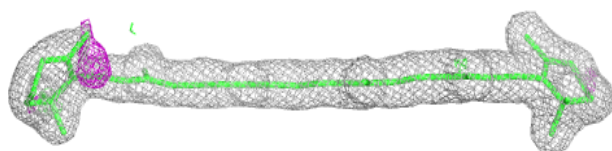
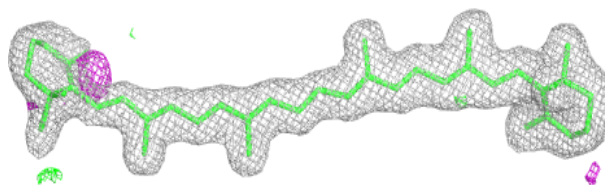
**Electron density around BCR A 411:**

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

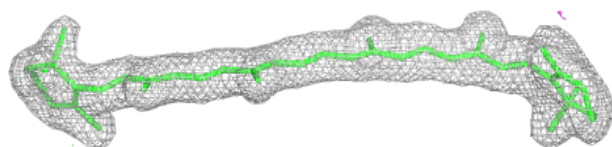
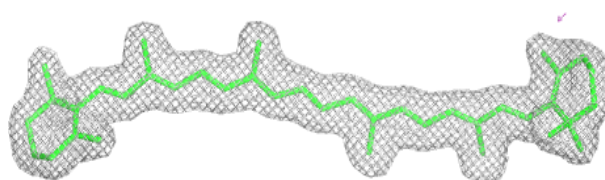


Electron density around BCR B 619:

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

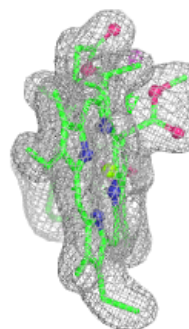
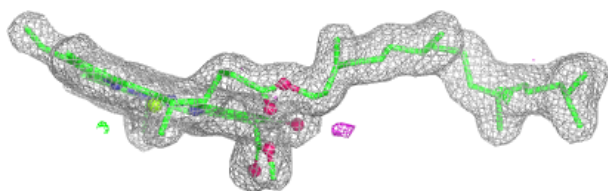
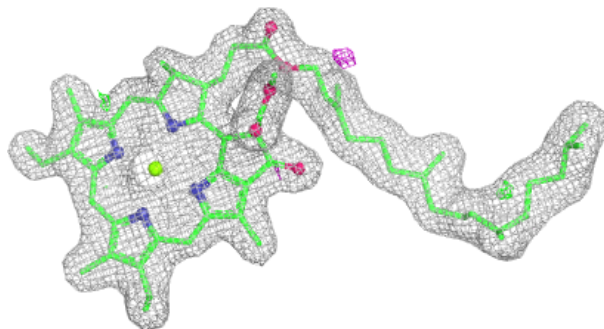
**Electron density around BCR B 620:**

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

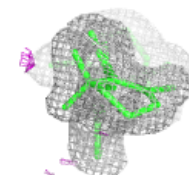
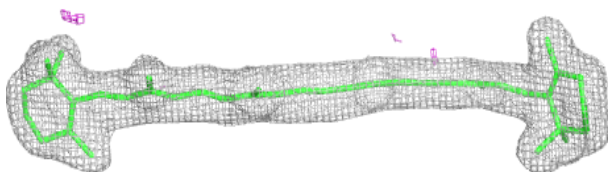
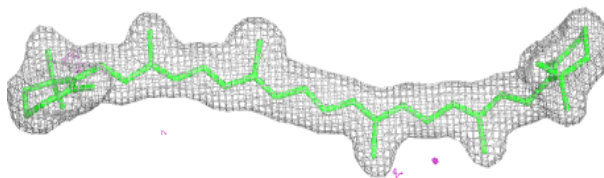


Electron density around CLA b 605:

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

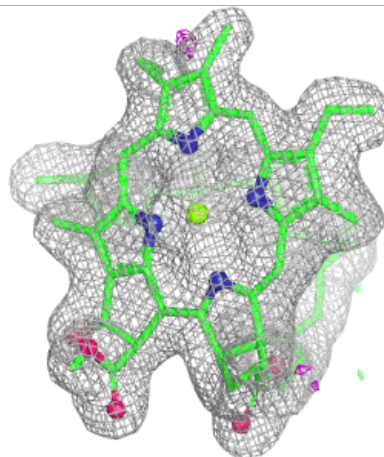
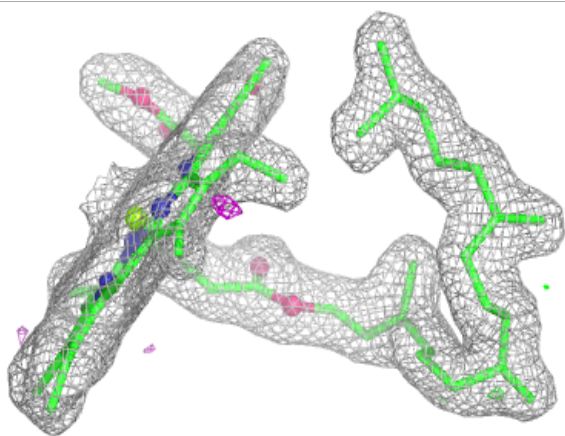
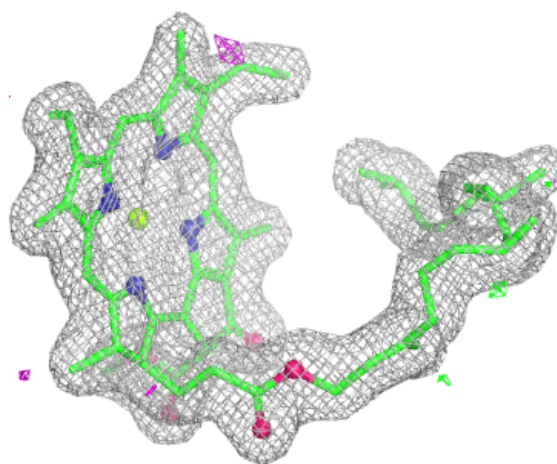
**Electron density around BCR C 515:**

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



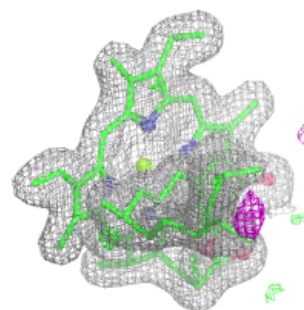
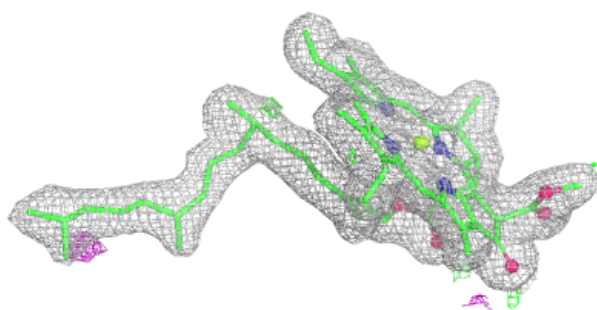
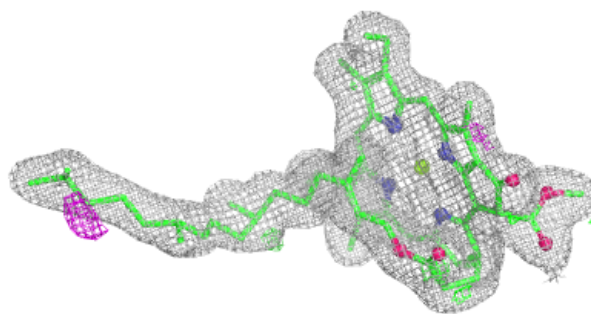
Electron density around CLA C 503:

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



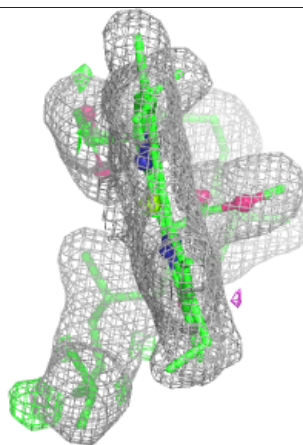
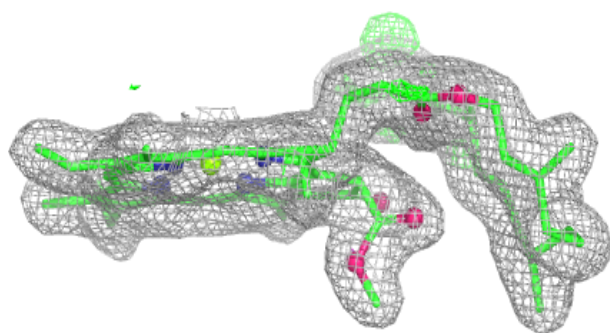
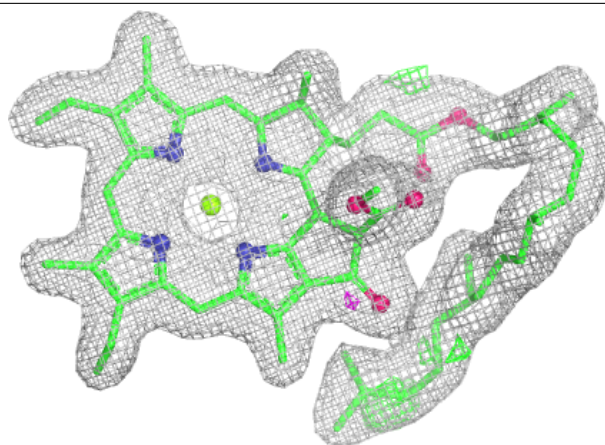
Electron density around CLA C 505:

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

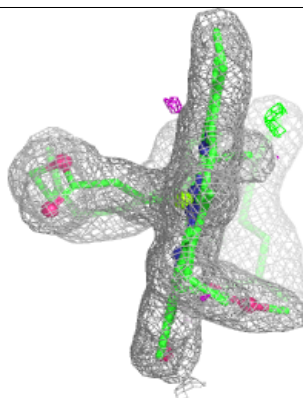
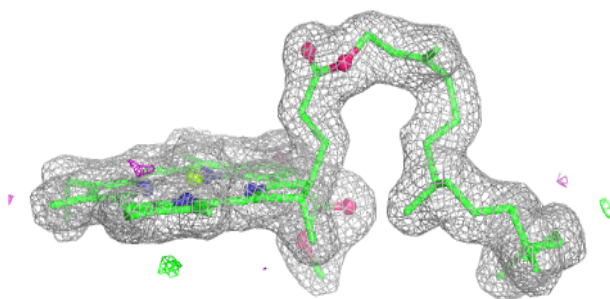
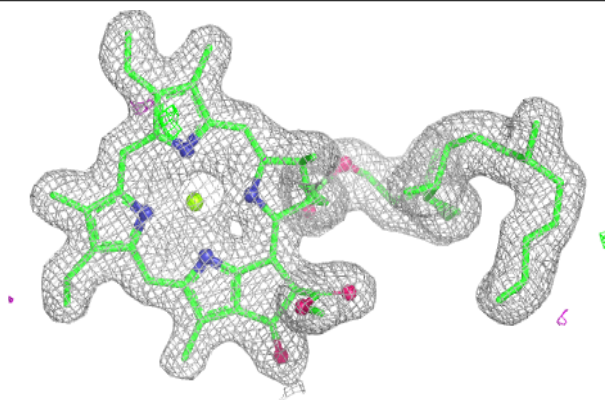


Electron density around CLA b 613:

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

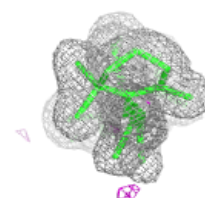
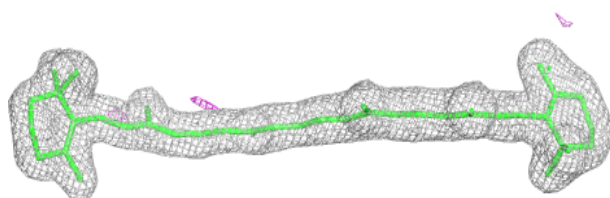
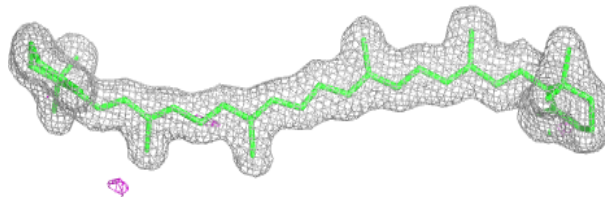
**Electron density around CLA b 615:**

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

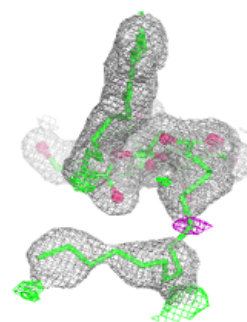
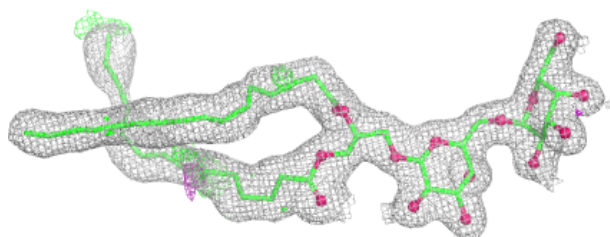
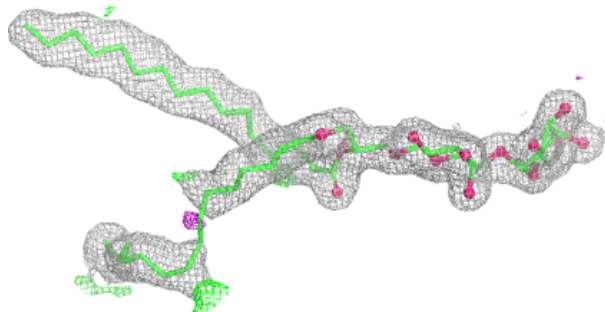


Electron density around BCR a 415:

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

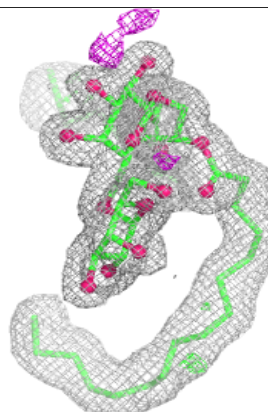
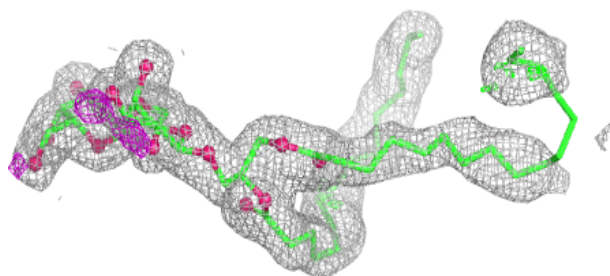
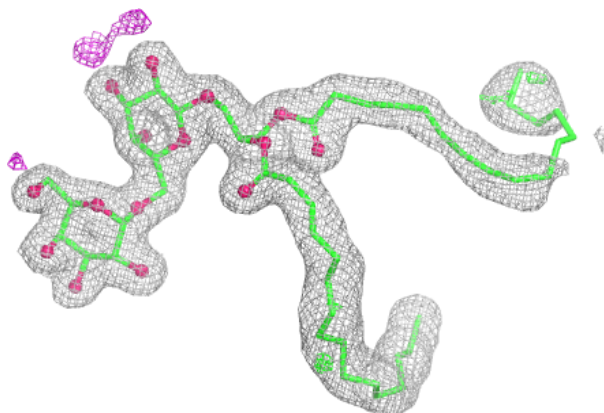
**Electron density around DGD C 516:**

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

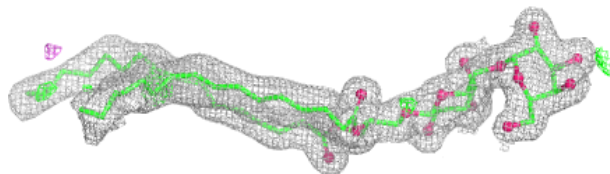
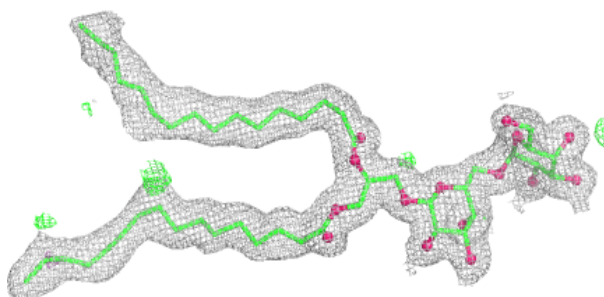


Electron density around DGD C 517:

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

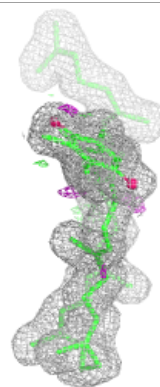
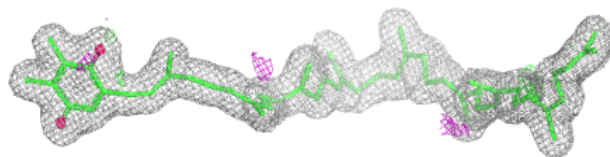
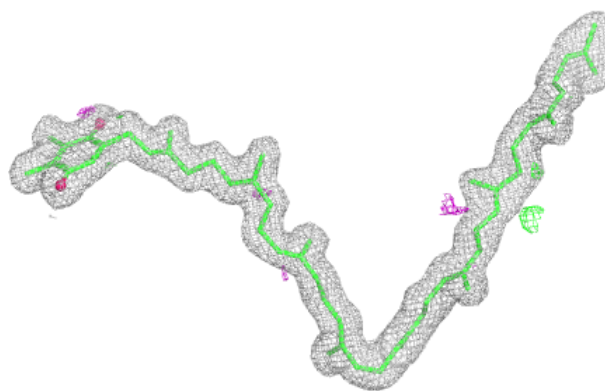
**Electron density around DGD C 518:**

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

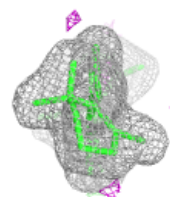
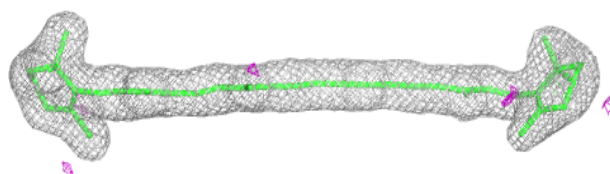
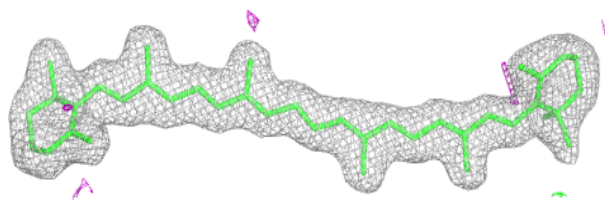


Electron density around PL9 D 405:

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

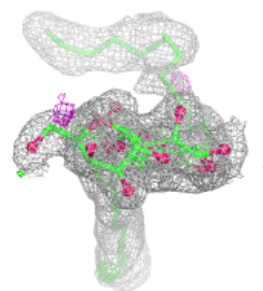
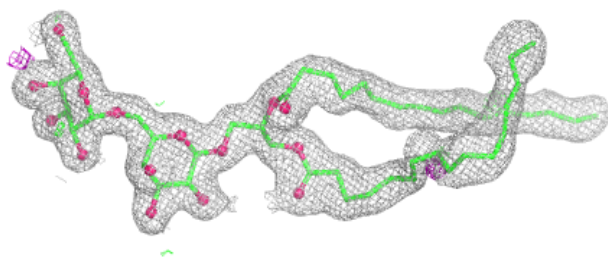
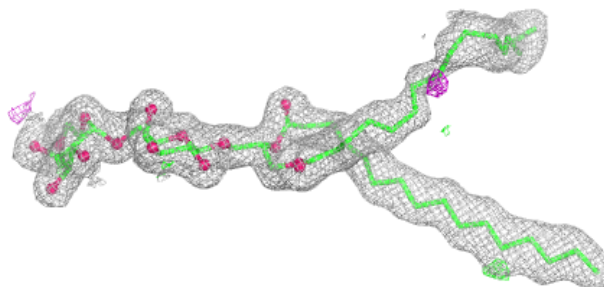
**Electron density around BCR b 621:**

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

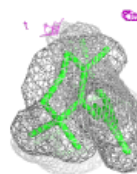
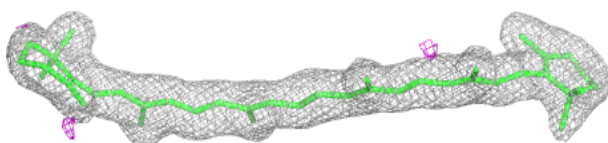
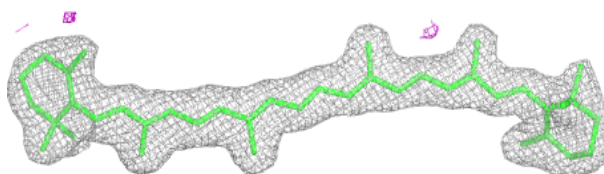


Electron density around DGD c 917:

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

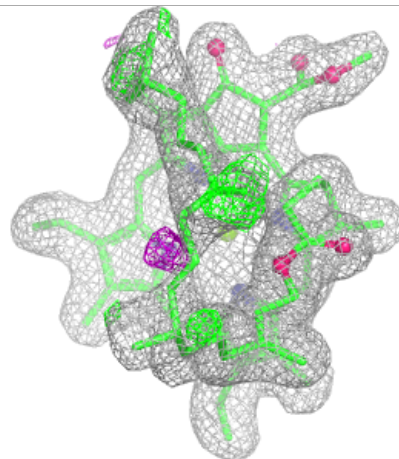
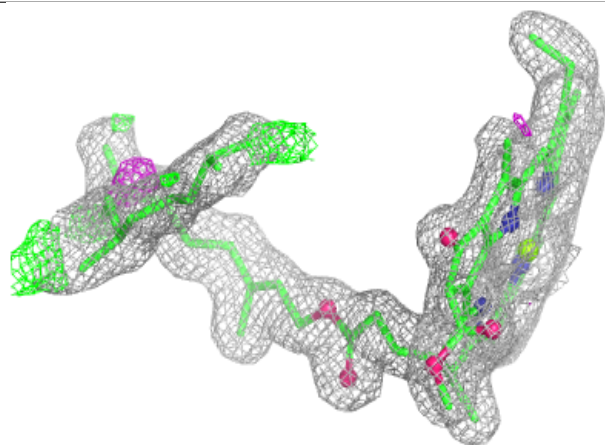
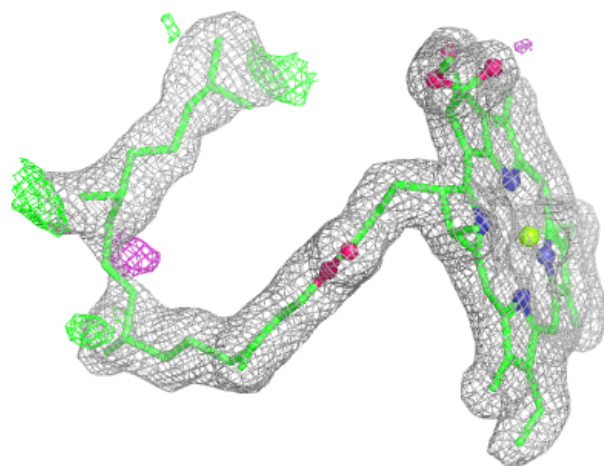
**Electron density around BCR b 622:**

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



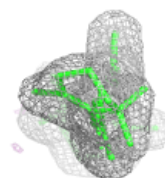
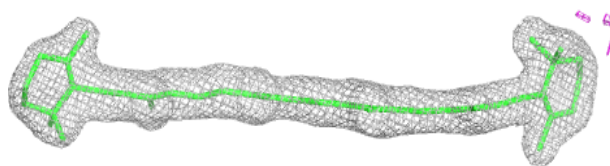
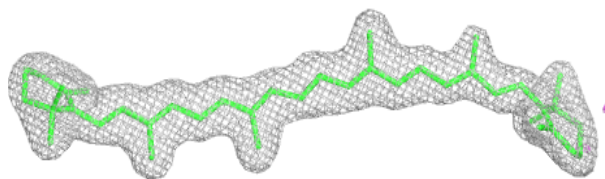
Electron density around CLA B 607:

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



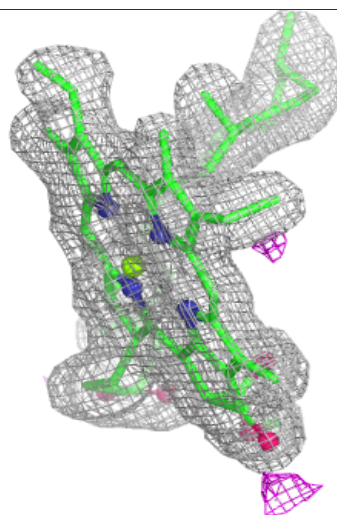
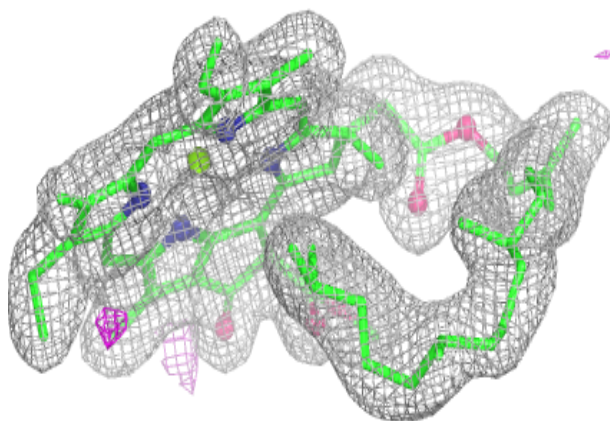
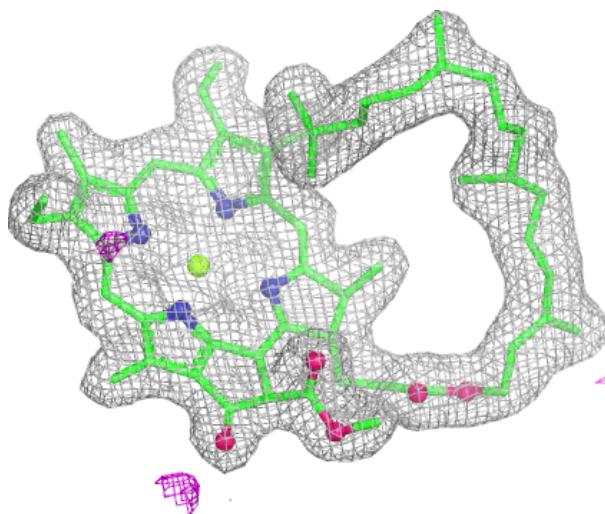
Electron density around BCR c 916:

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



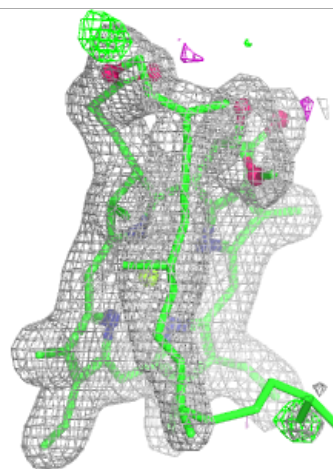
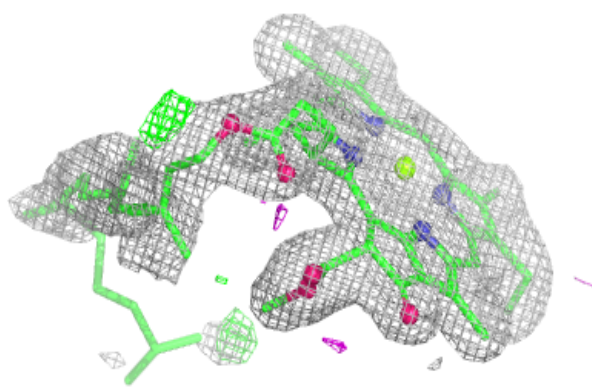
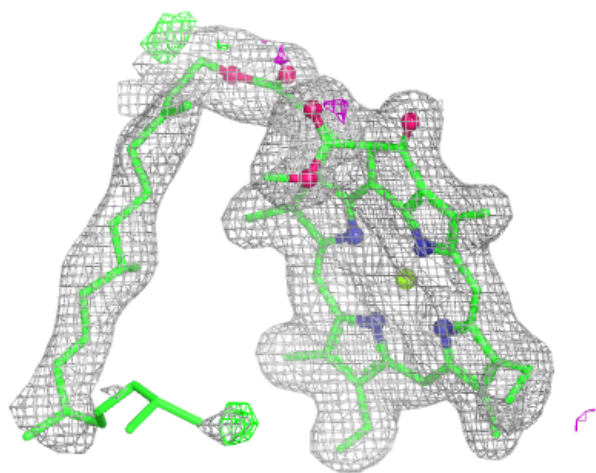
Electron density around CLA b 618:

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



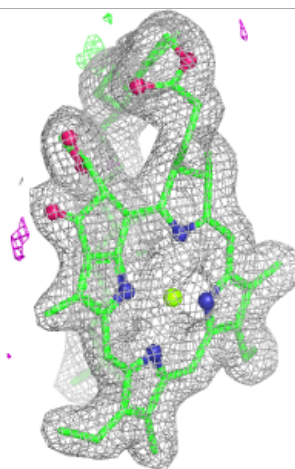
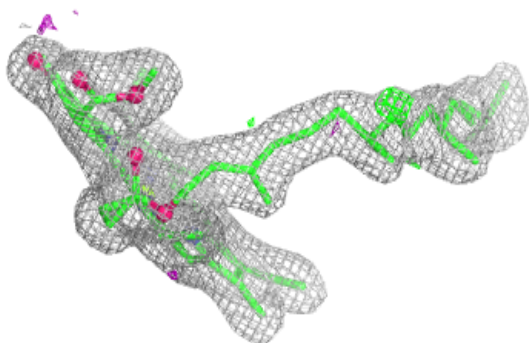
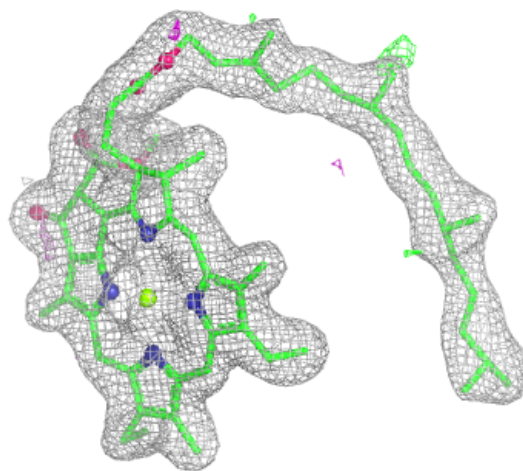
Electron density around CLA b 619:

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



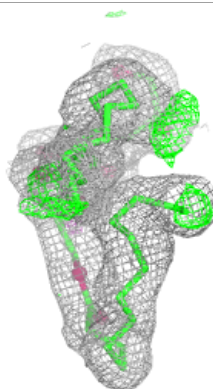
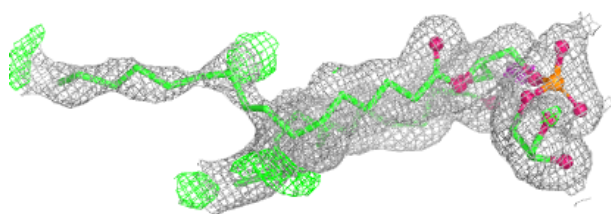
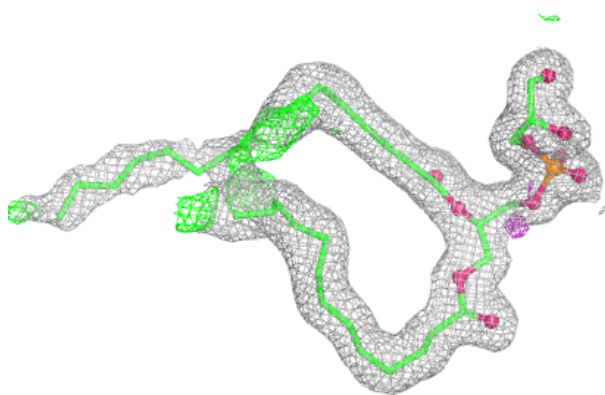
Electron density around CLA C 507:

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

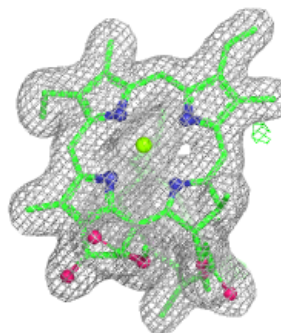
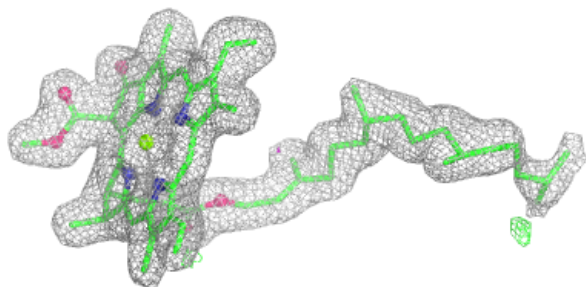
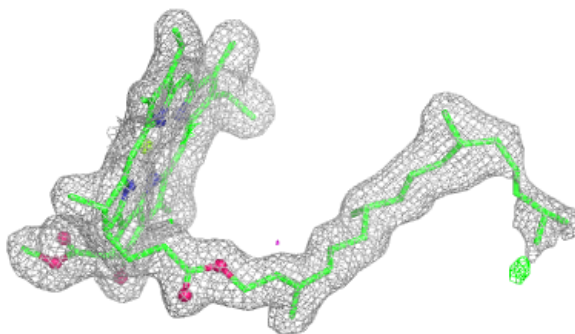


Electron density around LHG D 410:

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

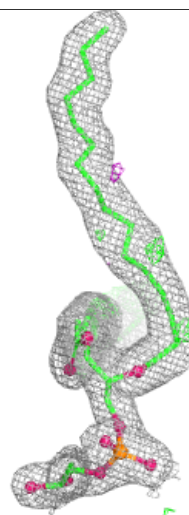
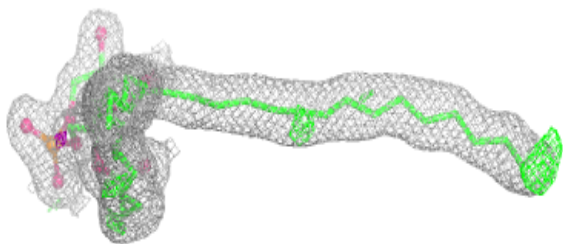
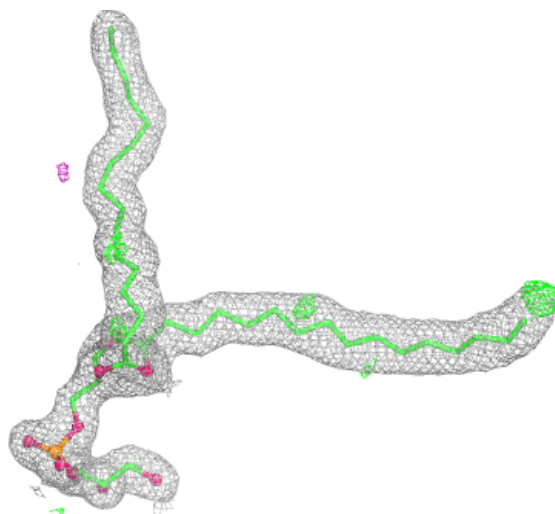
**Electron density around CLA C 508:**

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



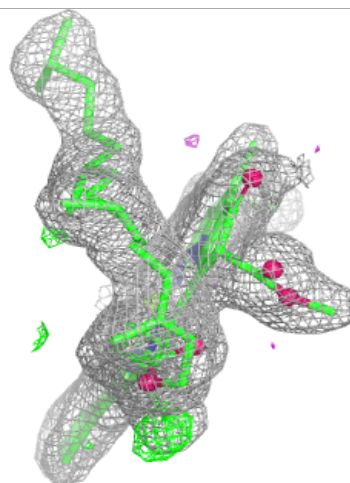
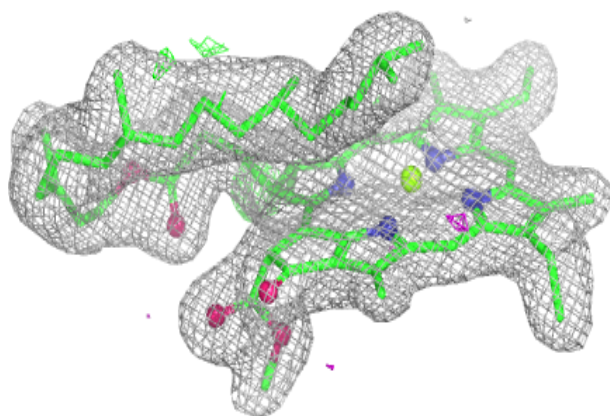
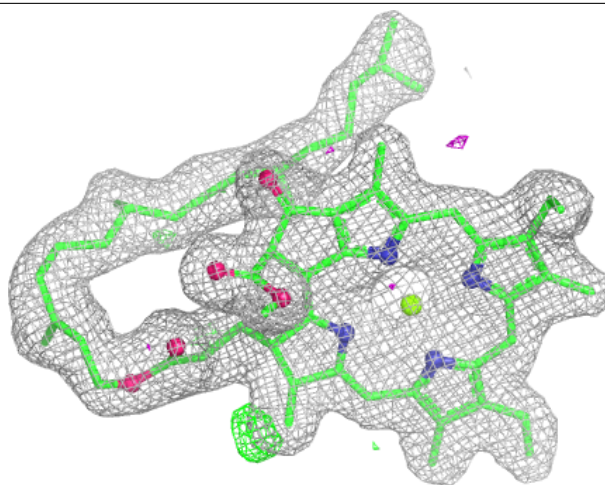
Electron density around LHG L 101:

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



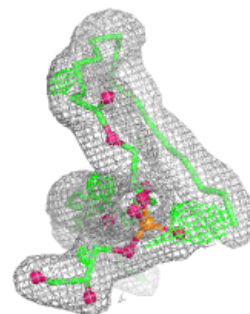
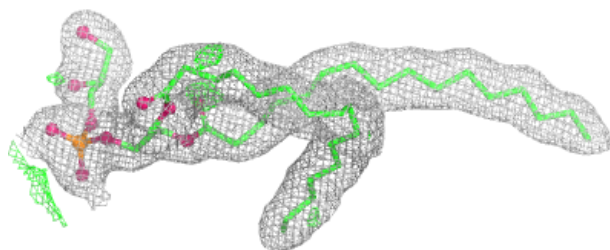
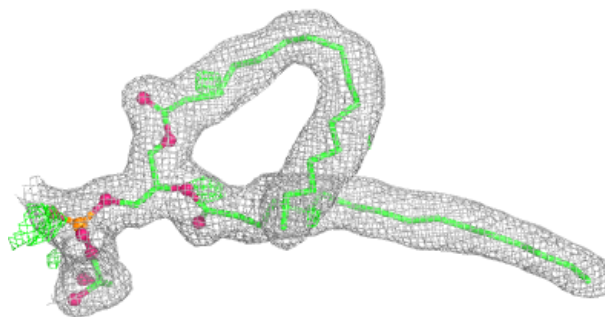
Electron density around CLA C 509:

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



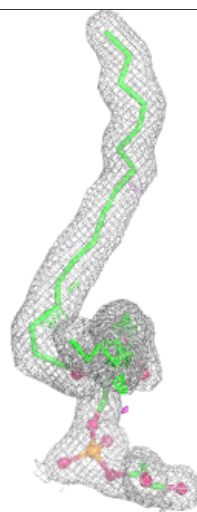
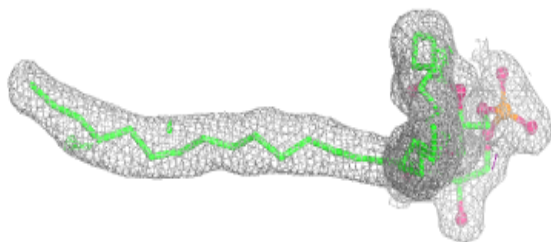
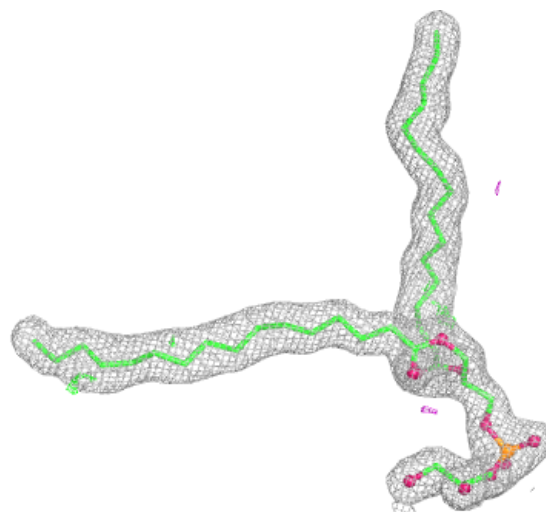
Electron density around LHG d 407:

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



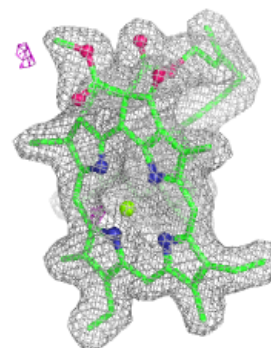
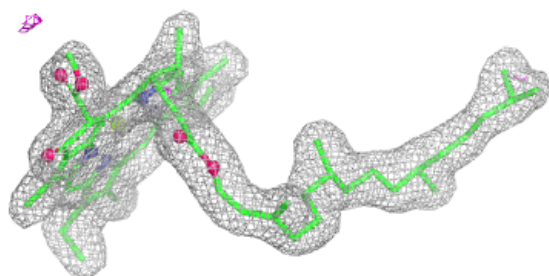
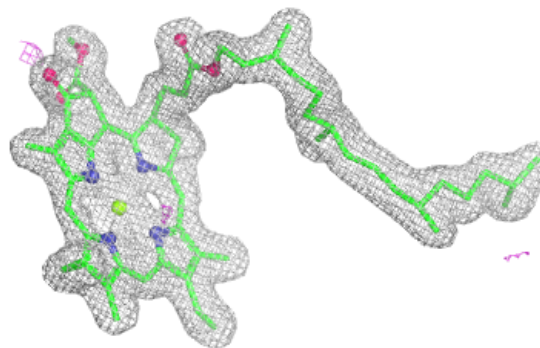
Electron density around LHG 1 101:

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

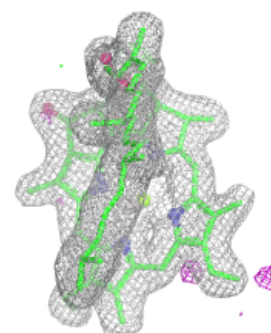
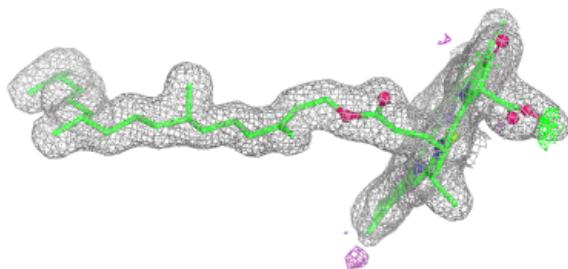
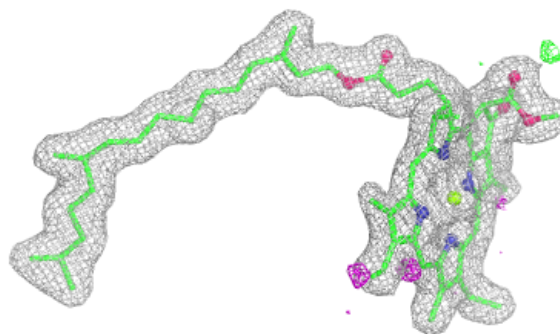


Electron density around CLA C 511:

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

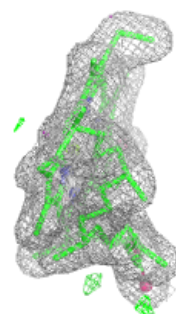
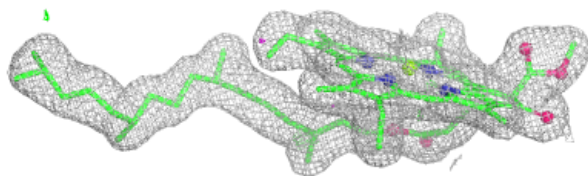
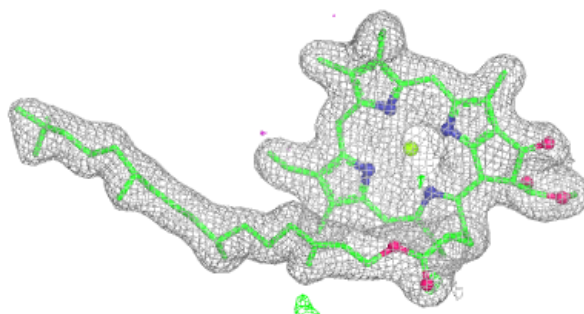
**Electron density around CLA B 610:**

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

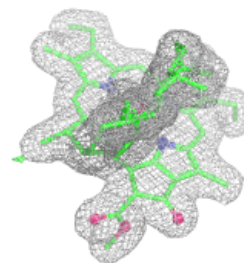
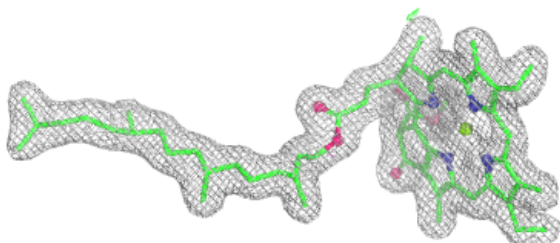
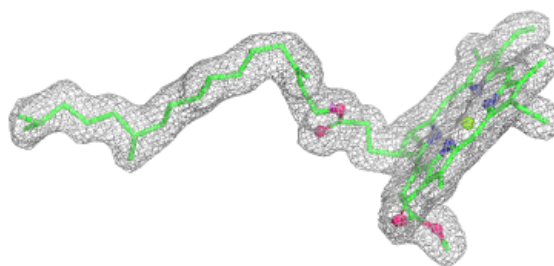


Electron density around CLA C 501:

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

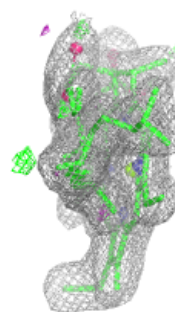
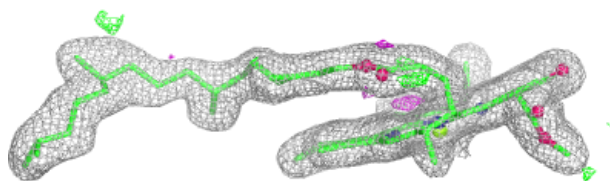
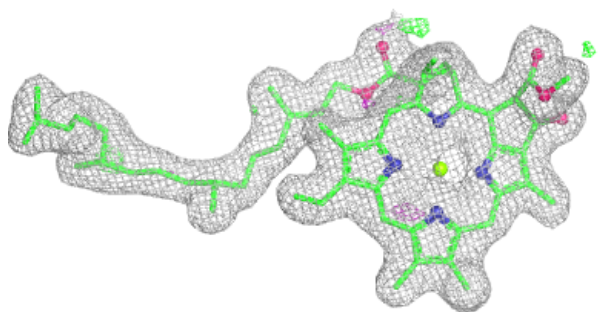
**Electron density around CLA C 502:**

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

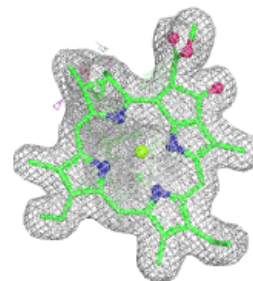
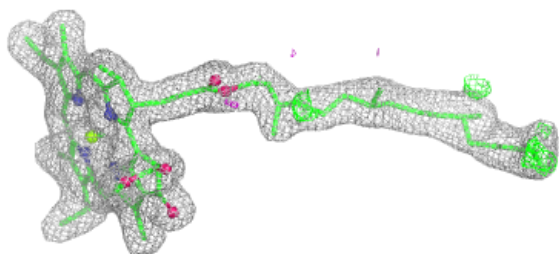
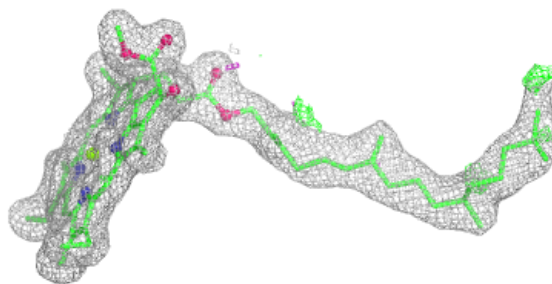


Electron density around CLA b 606:

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

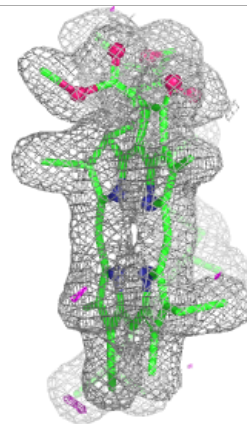
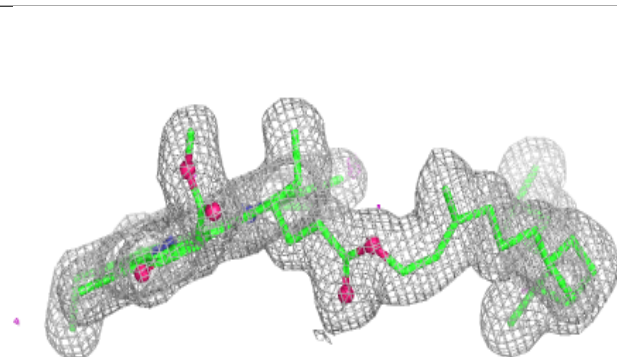
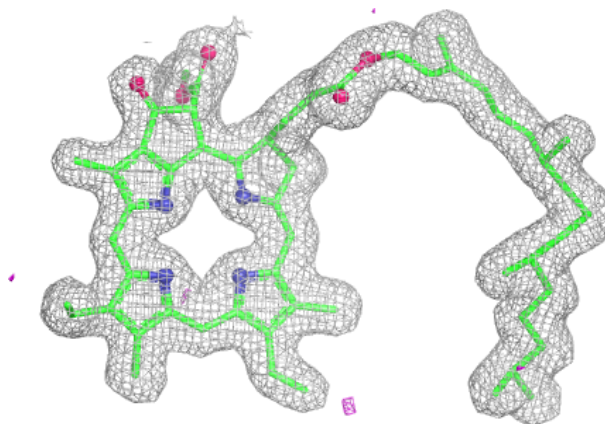
**Electron density around CLA b 607:**

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



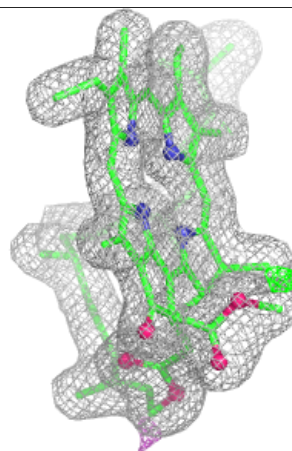
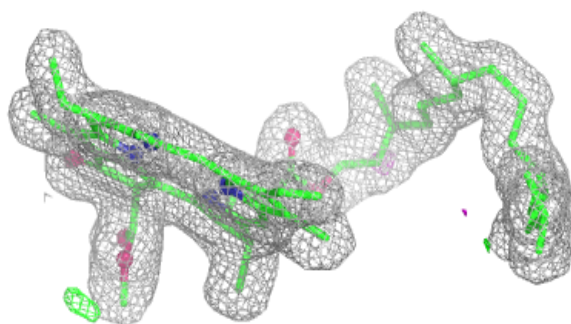
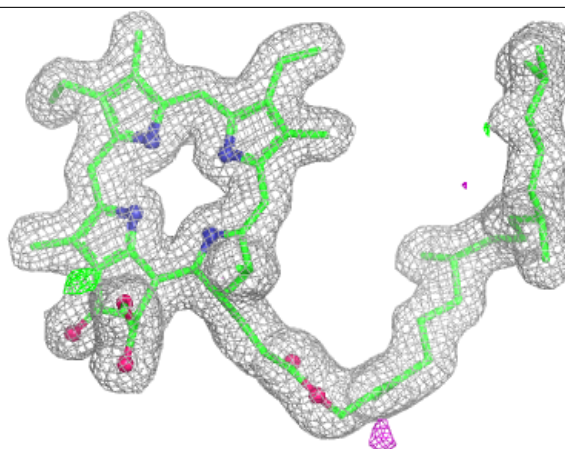
Electron density around PHO A 408:

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



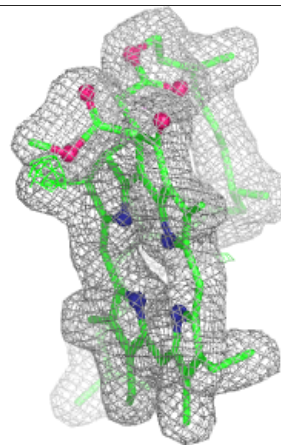
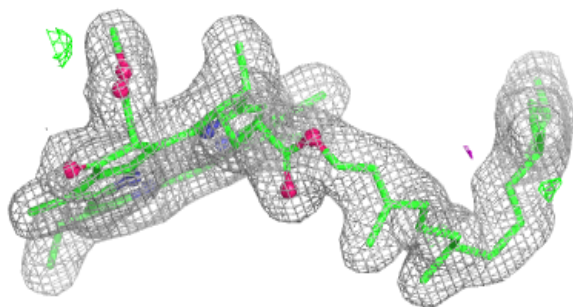
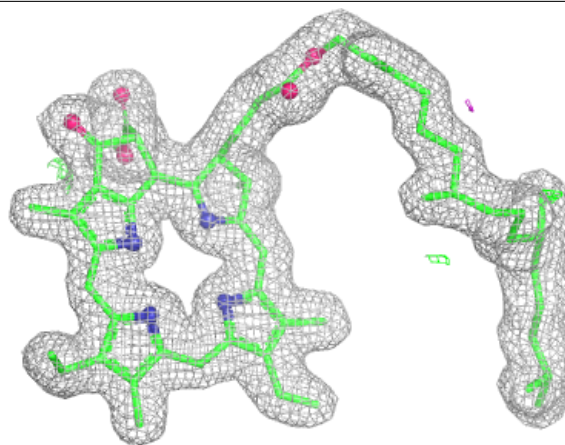
Electron density around PHO A 409:

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



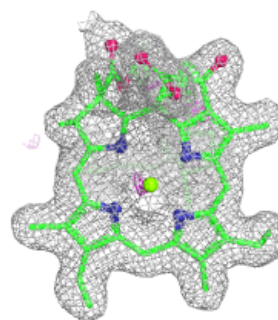
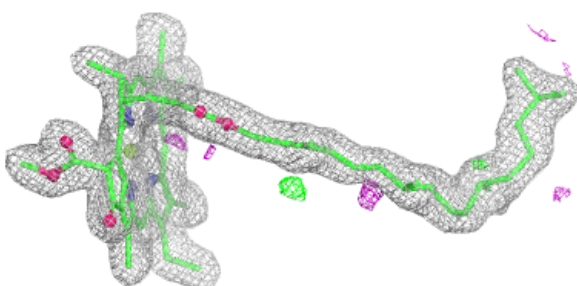
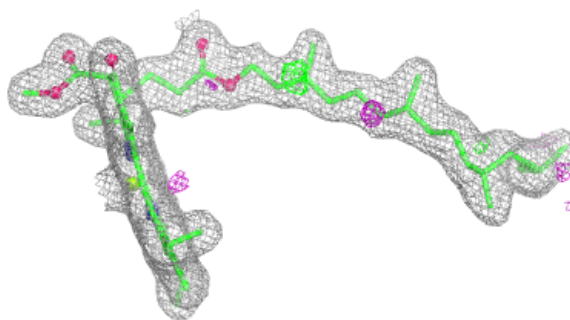
Electron density around PHO a 413:

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

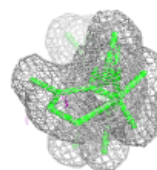
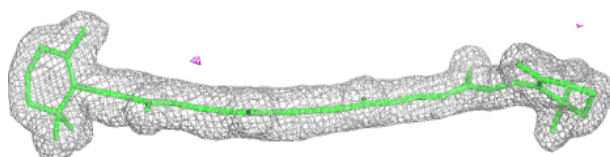
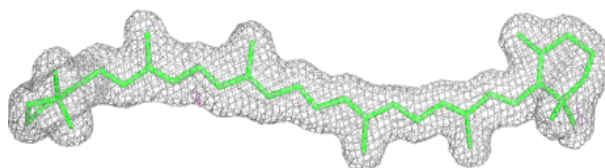


Electron density around CLA b 608:

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

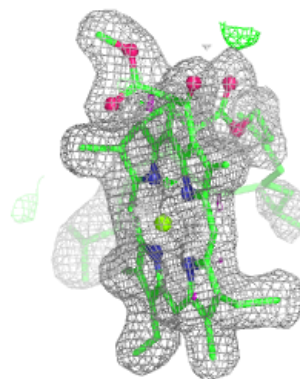
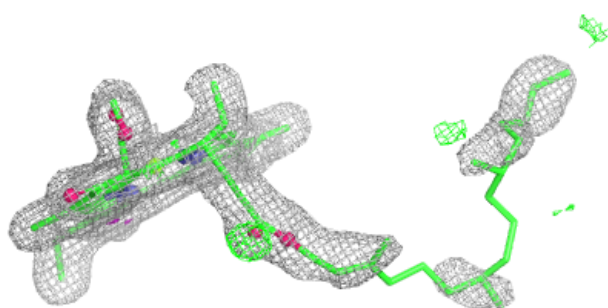
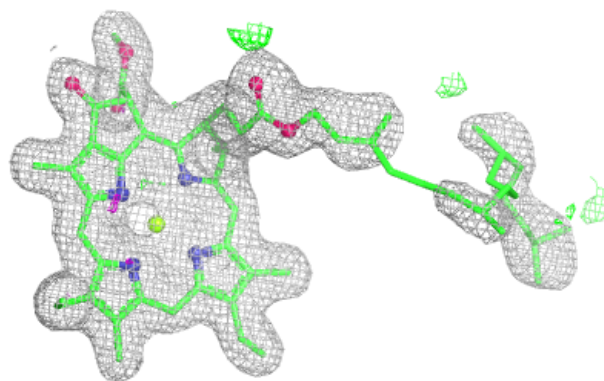
**Electron density around BCR B 618:**

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

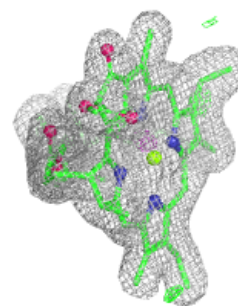
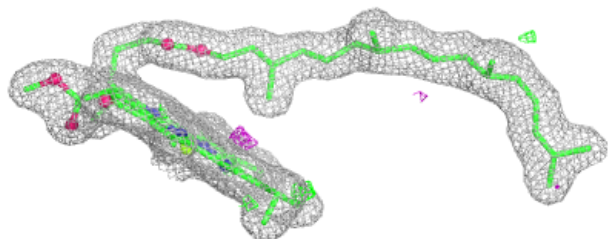
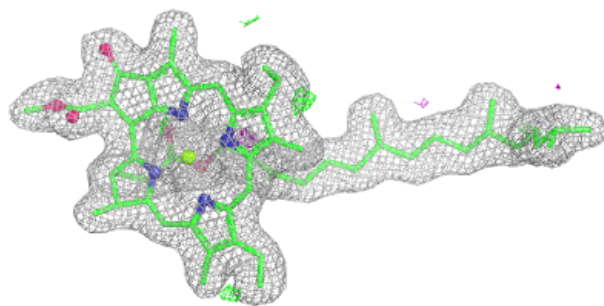


Electron density around CLA A 410:

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

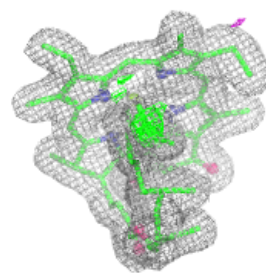
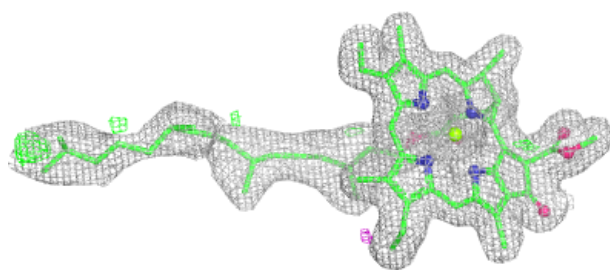
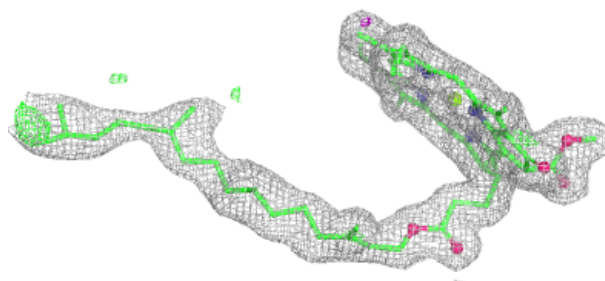
**Electron density around CLA b 611:**

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

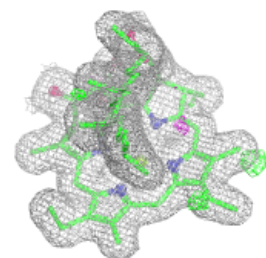
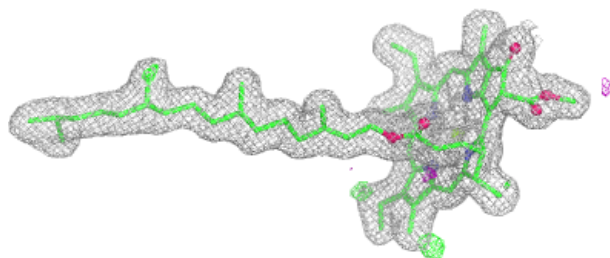
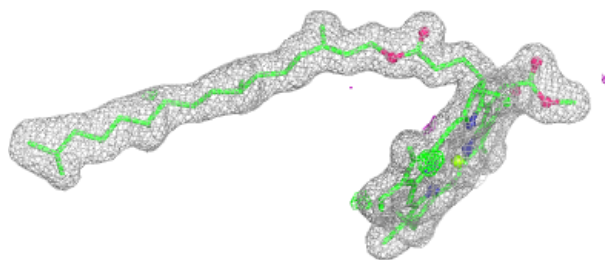


Electron density around CLA C 504:

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

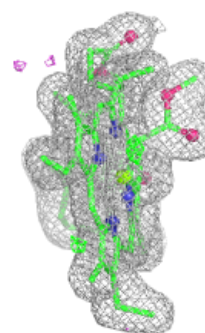
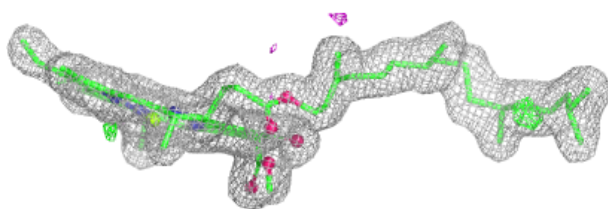
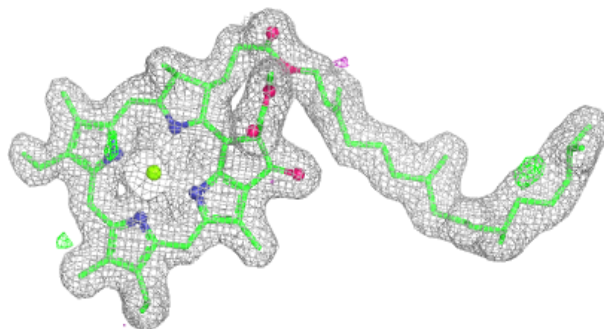
**Electron density around CLA B 608:**

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



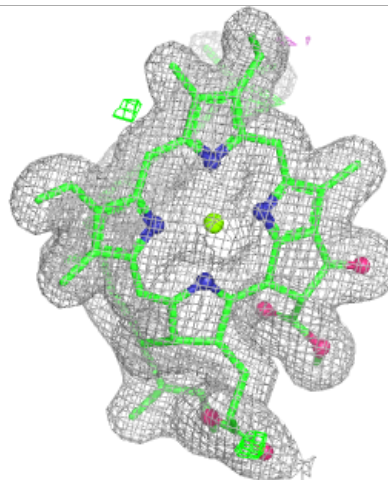
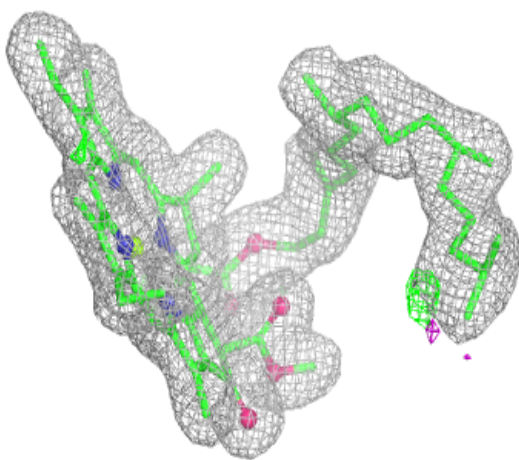
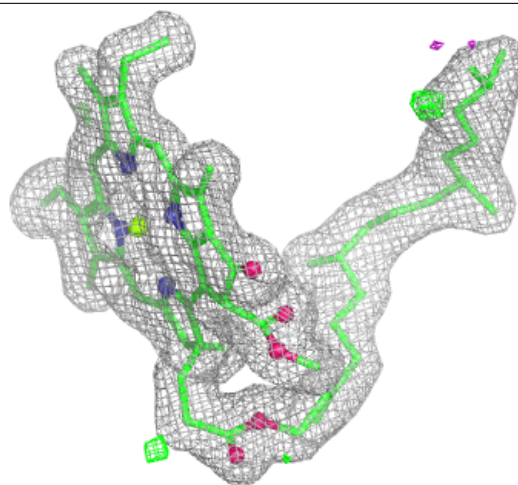
Electron density around CLA B 603:

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



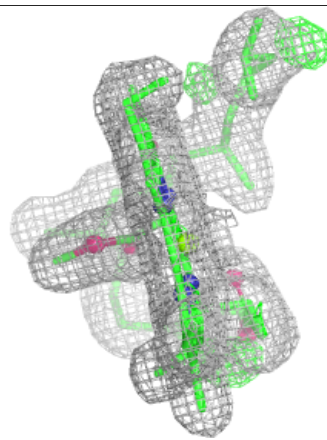
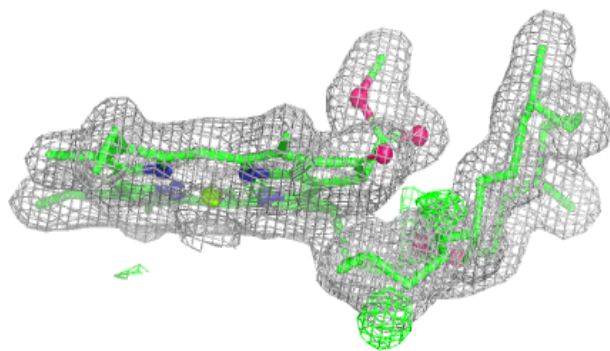
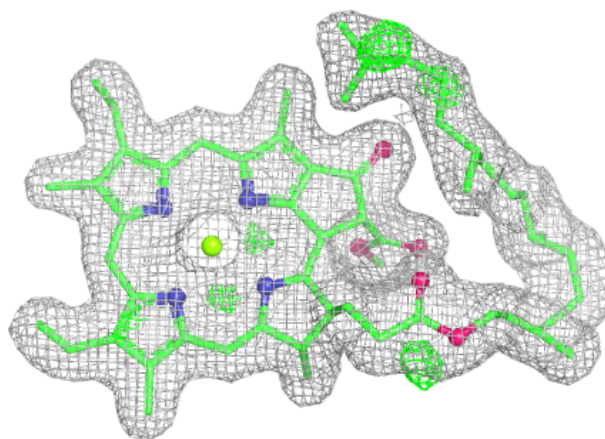
Electron density around CLA b 616:

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



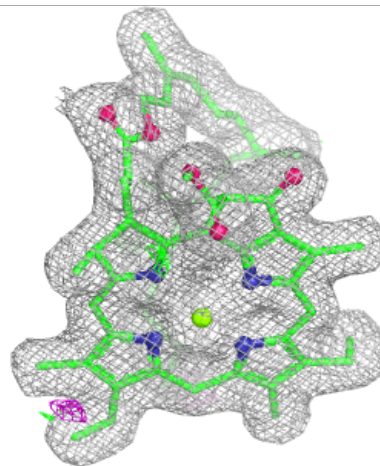
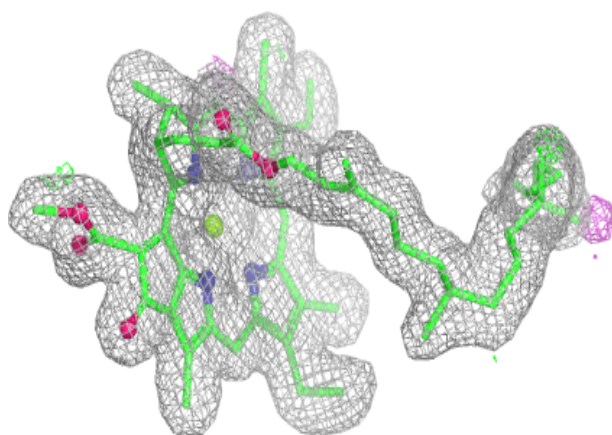
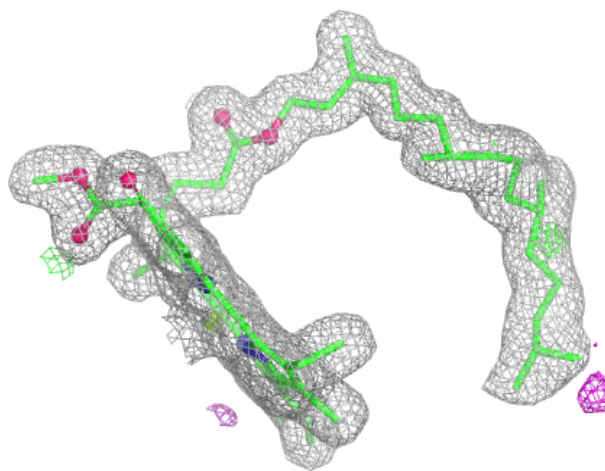
Electron density around CLA B 611:

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



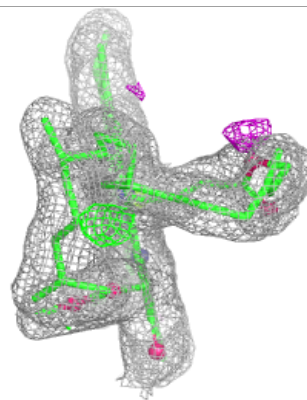
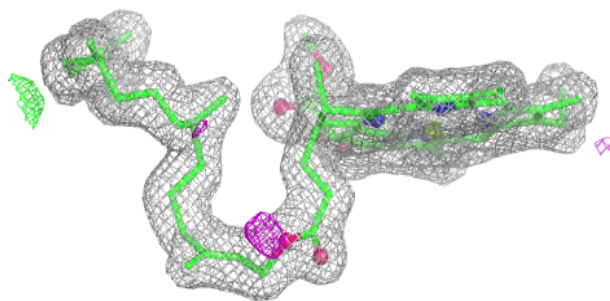
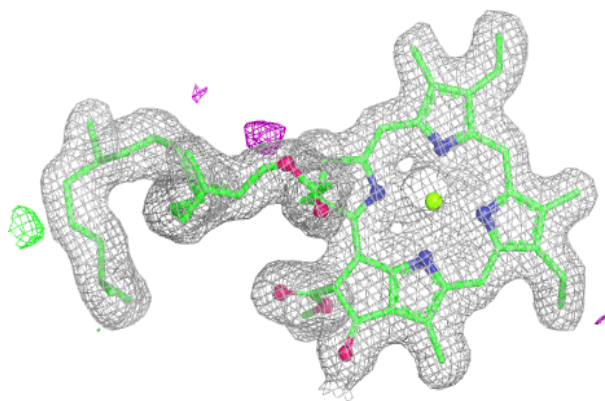
Electron density around CLA B 612:

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

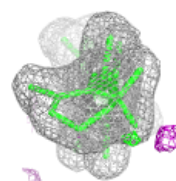
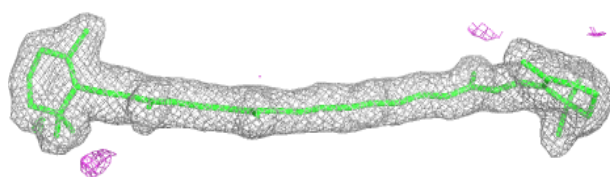
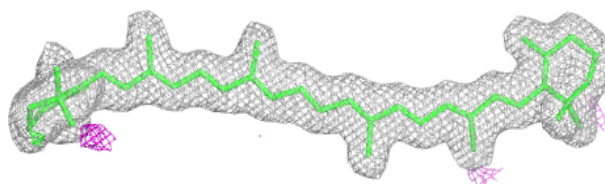


Electron density around CLA B 613:

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

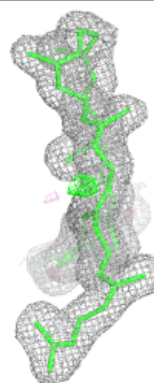
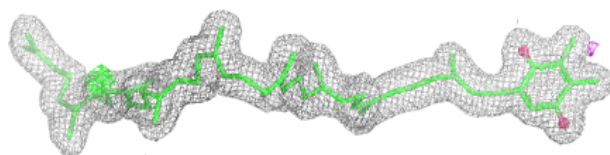
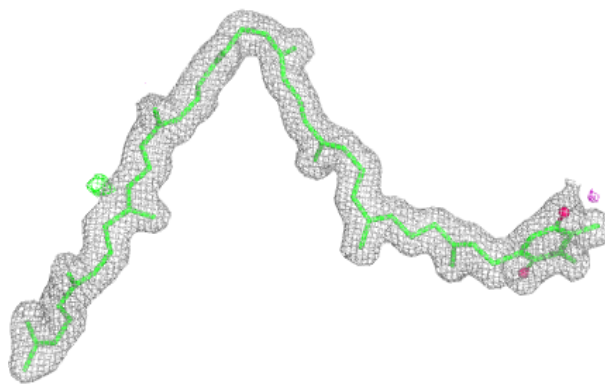
**Electron density around BCR b 620:**

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



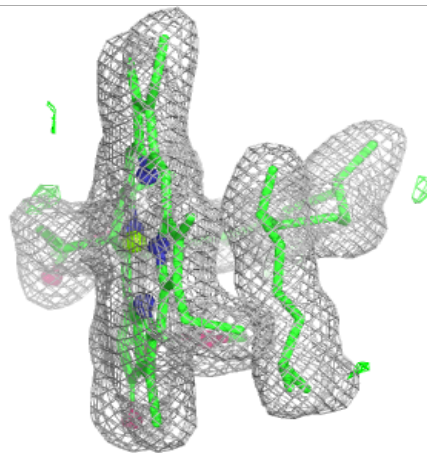
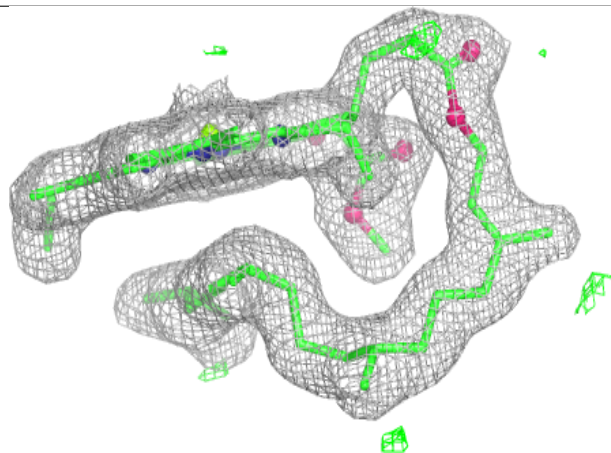
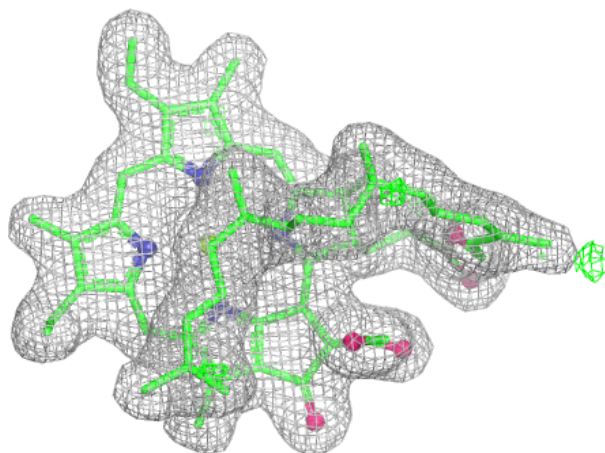
Electron density around PL9 d 405:

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



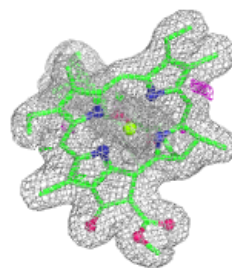
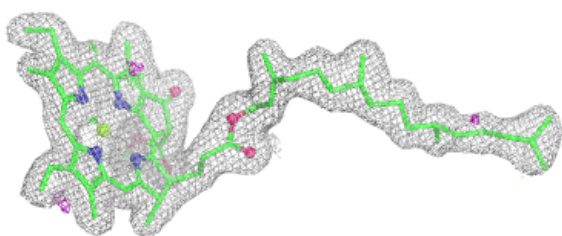
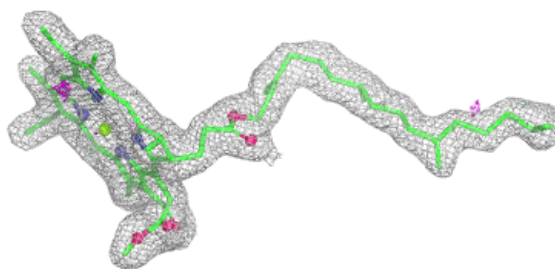
Electron density around CLA C 510:

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



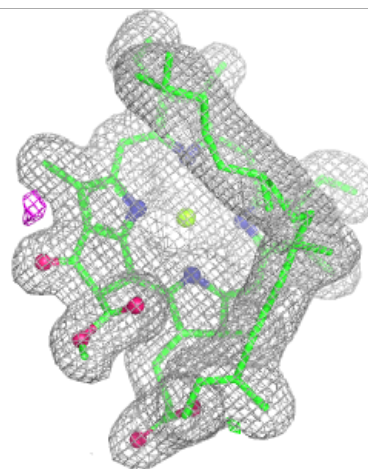
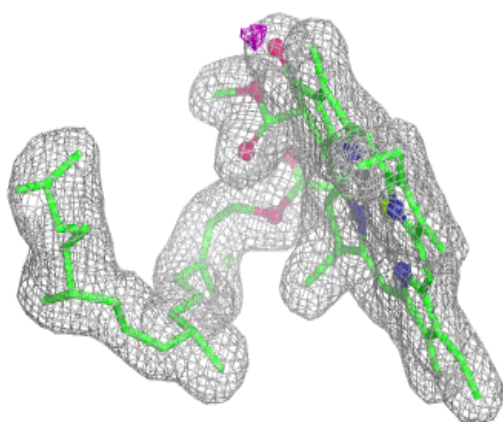
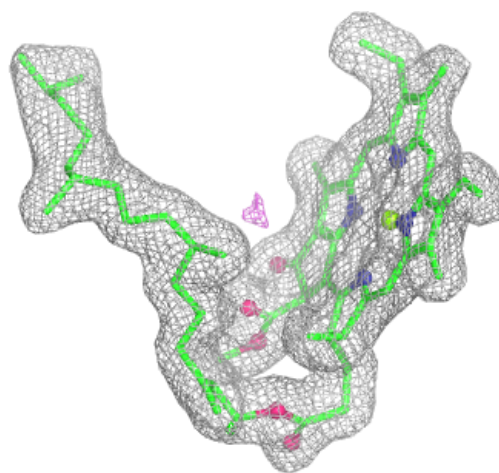
Electron density around CLA c 903:

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



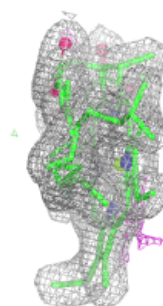
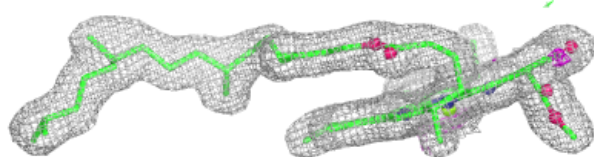
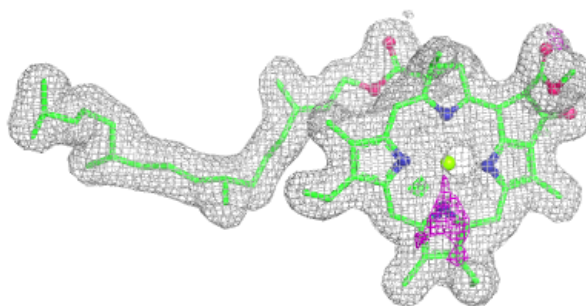
Electron density around CLA B 614:

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

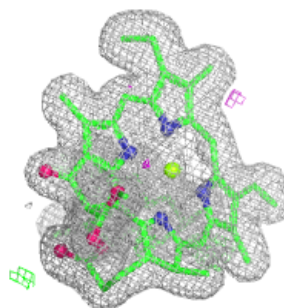
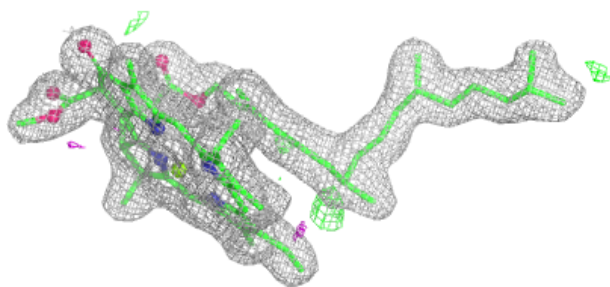
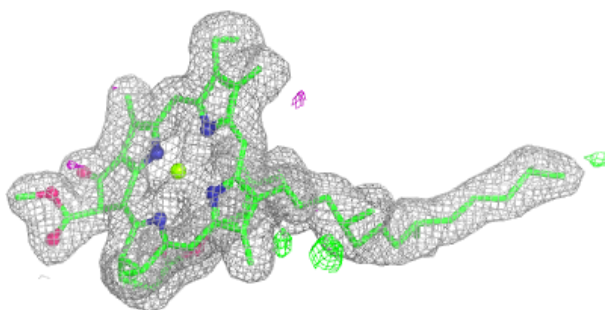


Electron density around CLA B 604:

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

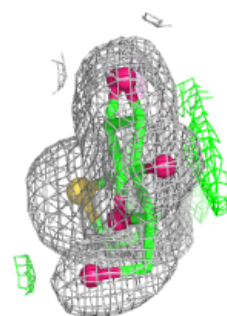
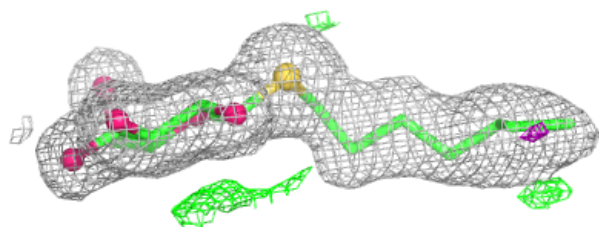
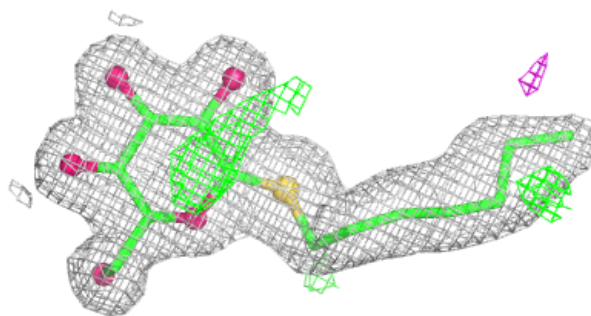
**Electron density around CLA c 906:**

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



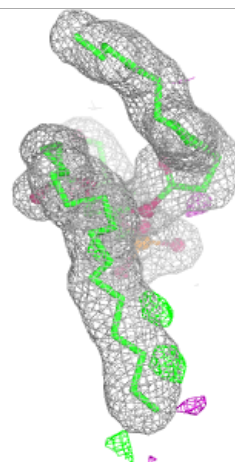
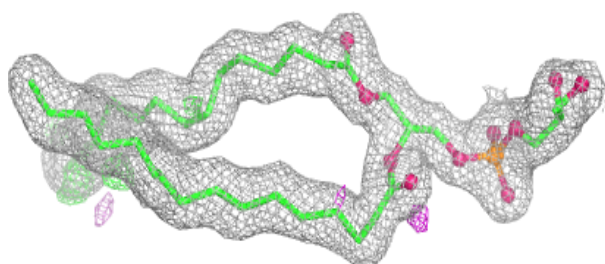
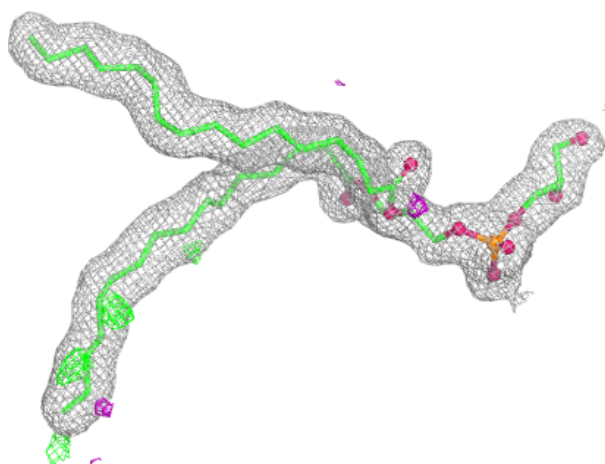
Electron density around HTG B 624:

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



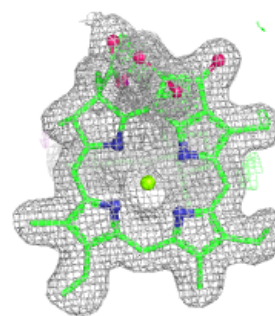
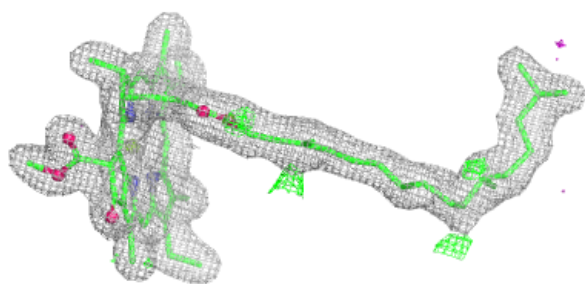
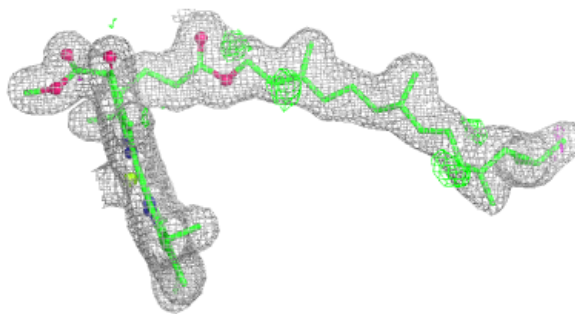
Electron density around LHG d 408:

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



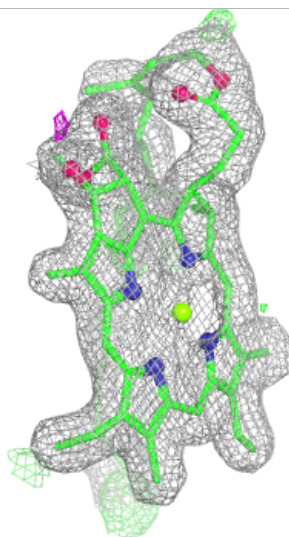
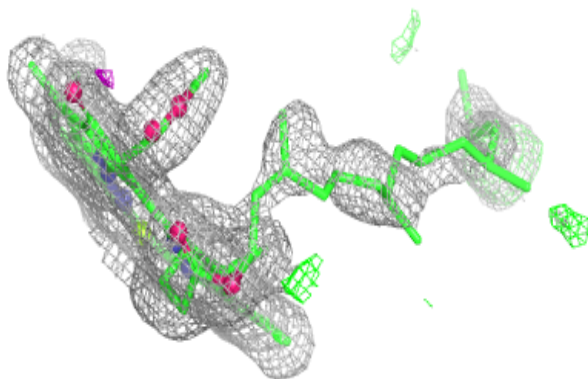
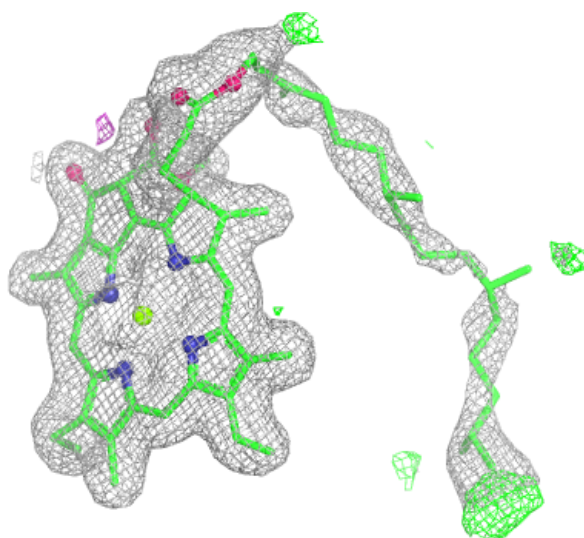
Electron density around CLA B 606:

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



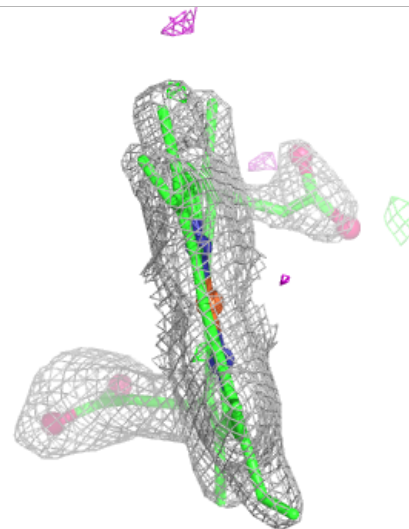
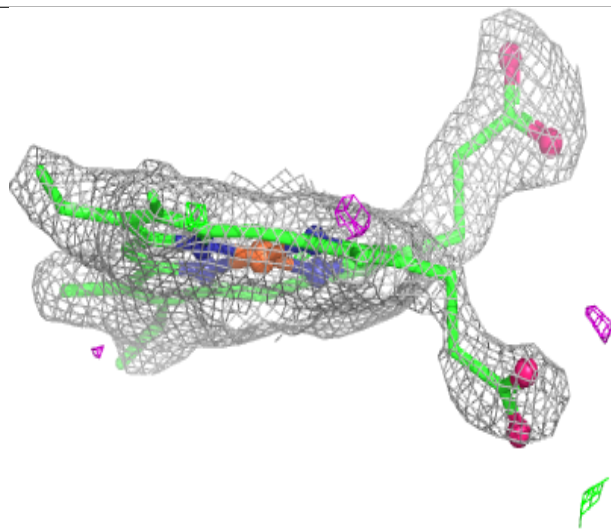
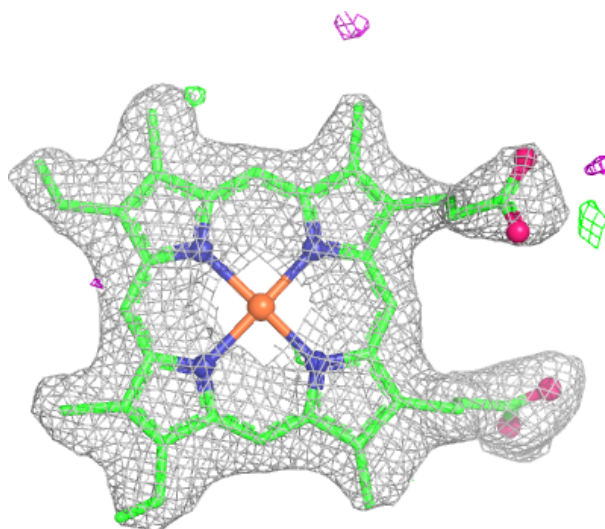
Electron density around CLA B 617:

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



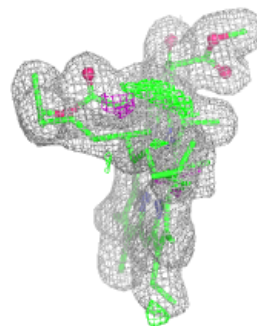
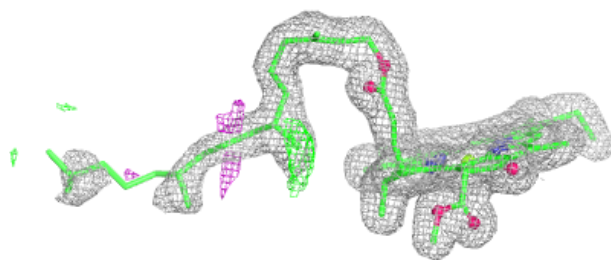
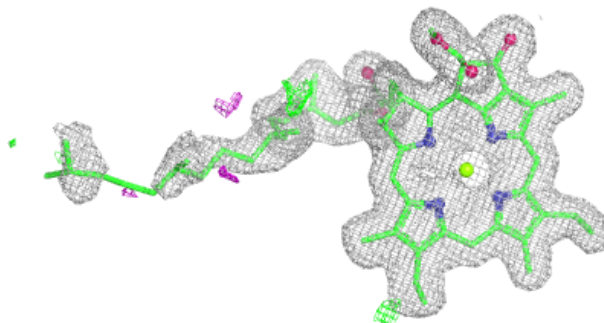
Electron density around HEM f 101:

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



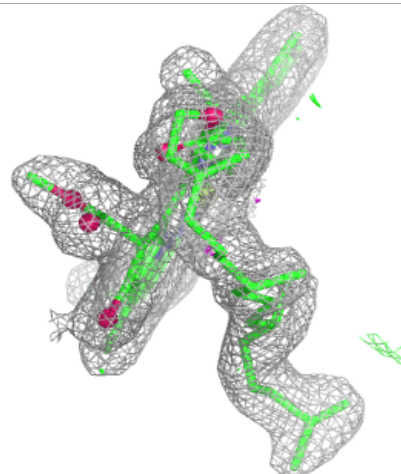
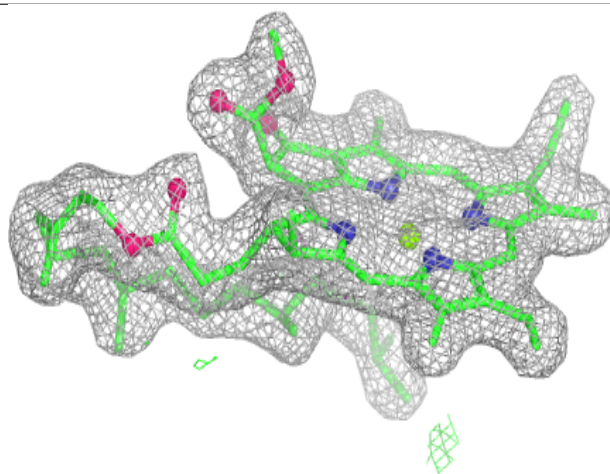
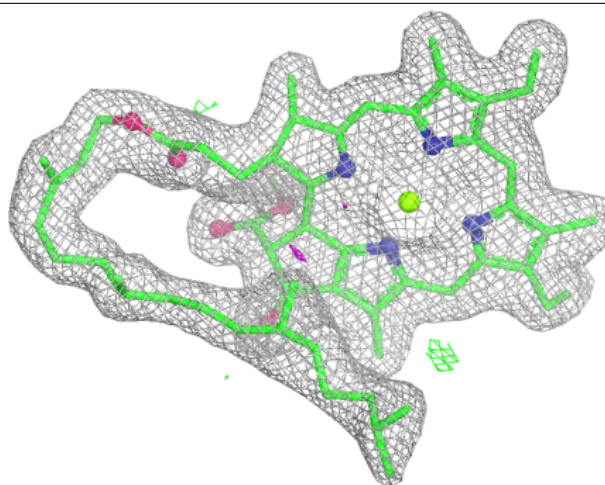
Electron density around CLA a 411:

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



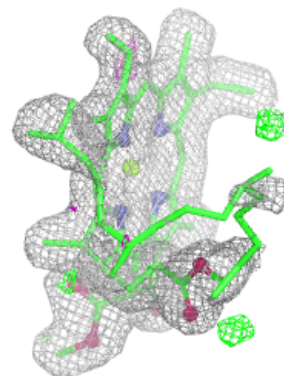
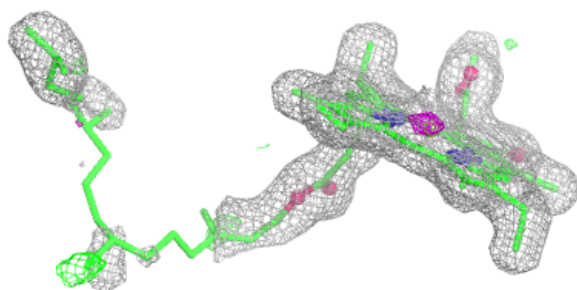
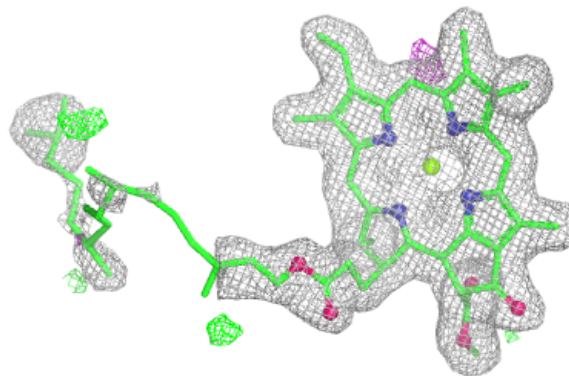
Electron density around CLA c 910:

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

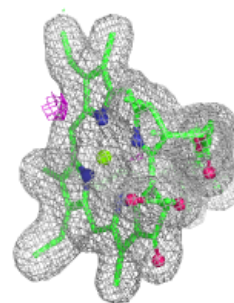
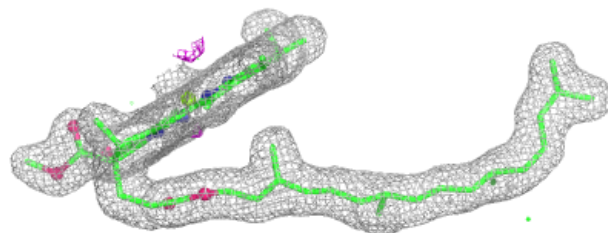
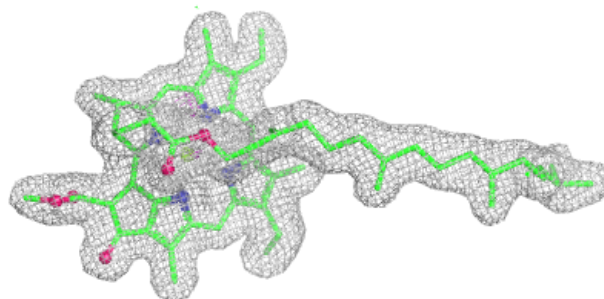


Electron density around CLA a 414:

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

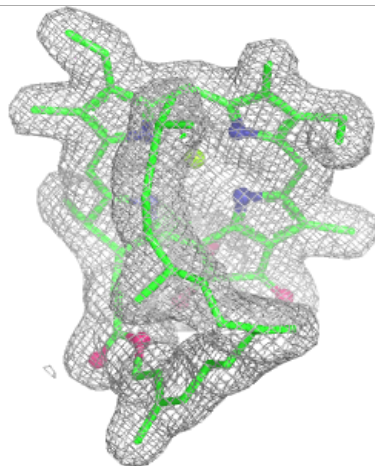
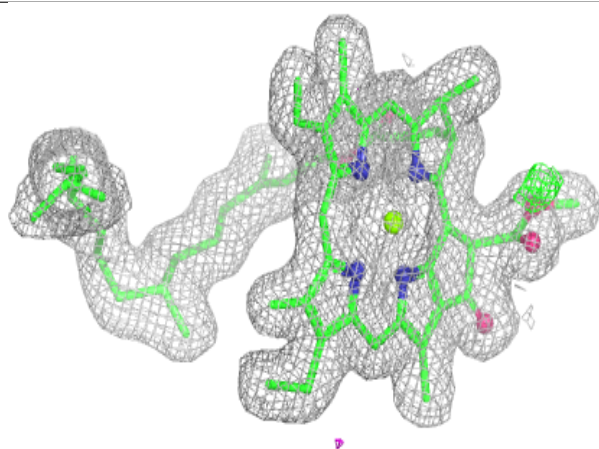
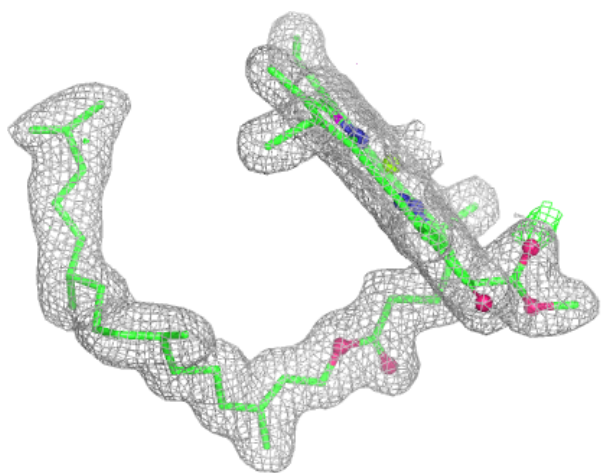
**Electron density around CLA B 609:**

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



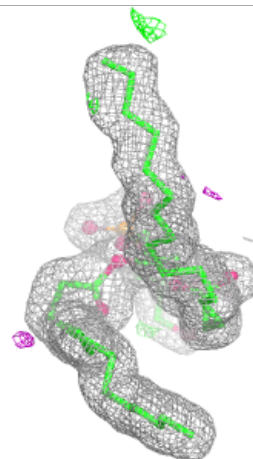
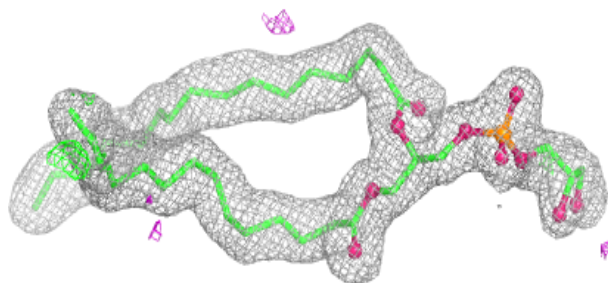
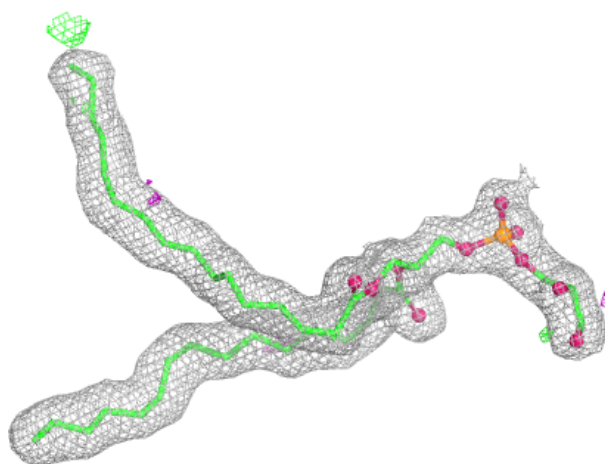
Electron density around CLA b 614:

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



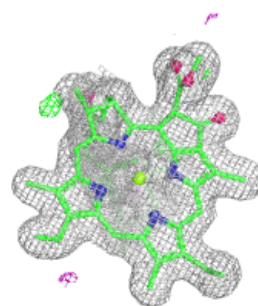
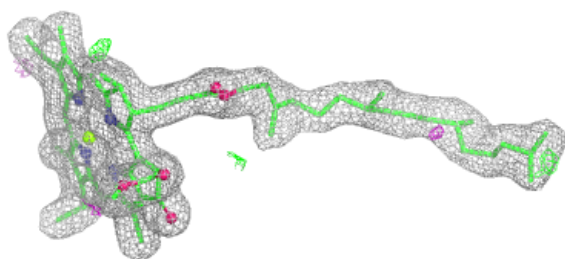
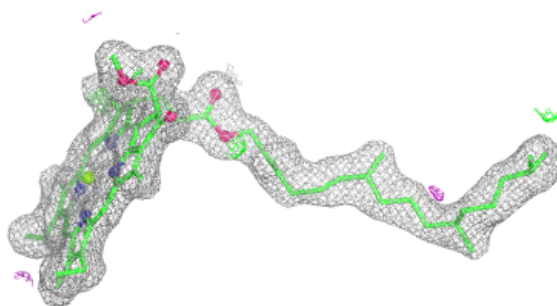
Electron density around LHG D 409:

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



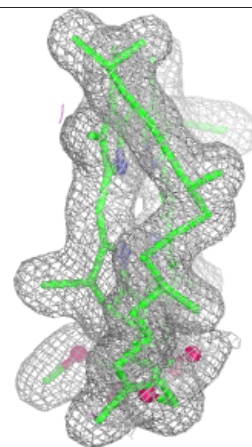
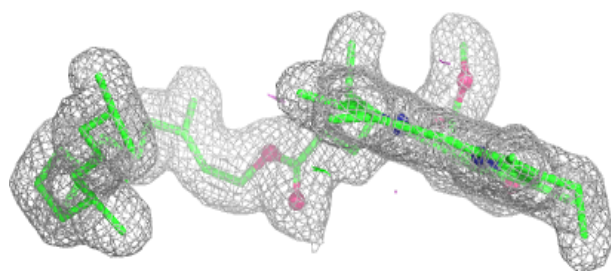
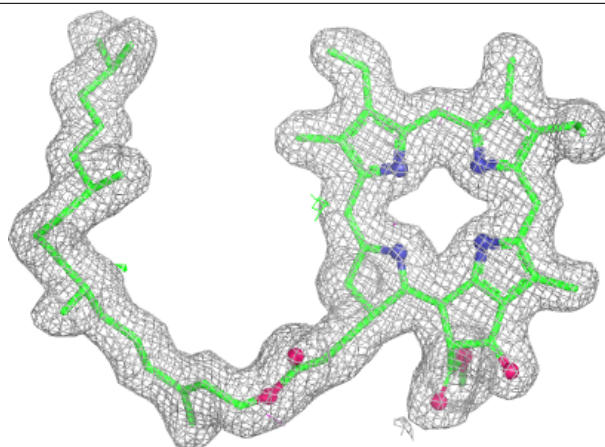
Electron density around CLA B 605:

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



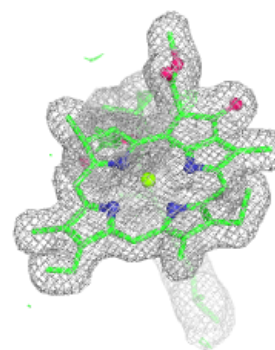
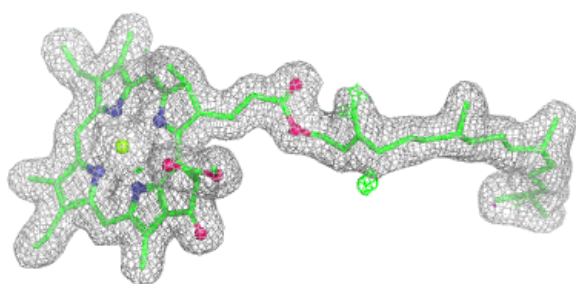
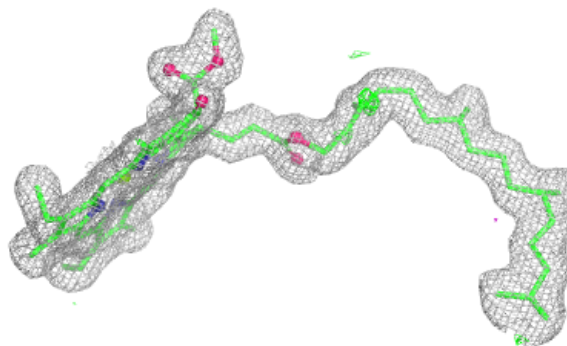
Electron density around PHO a 412:

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

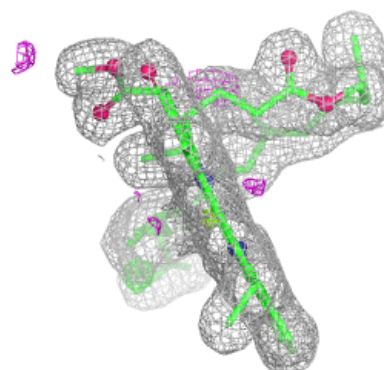
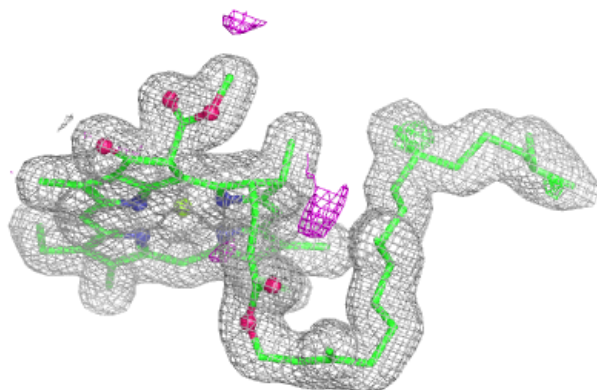
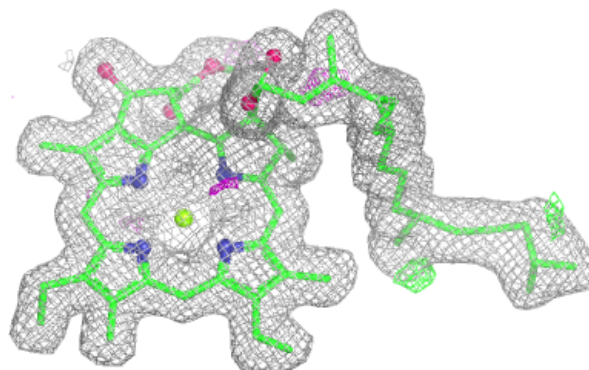


Electron density around CLA D 402:

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

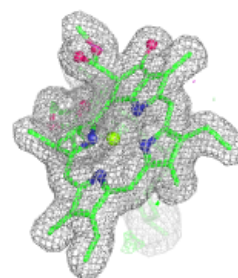
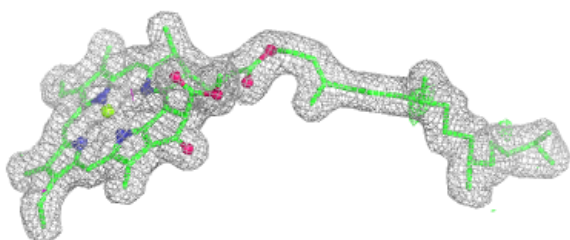
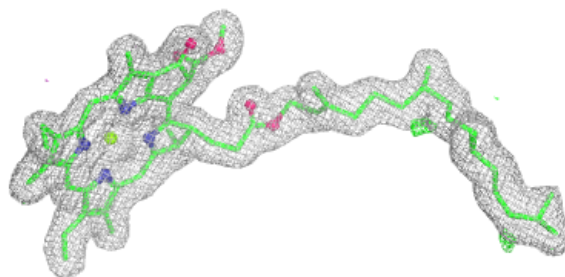
**Electron density around CLA A 406:**

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

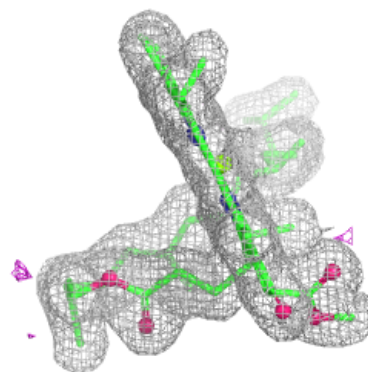
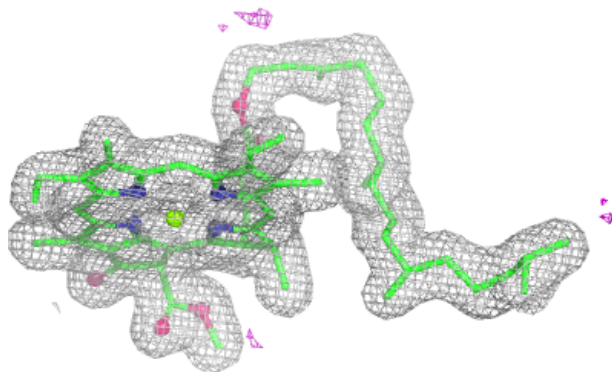
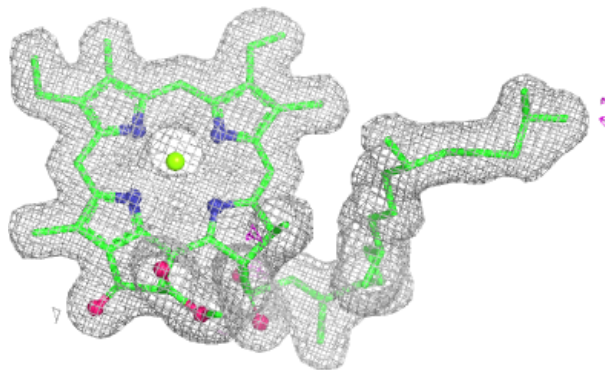


Electron density around CLA a 409:

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

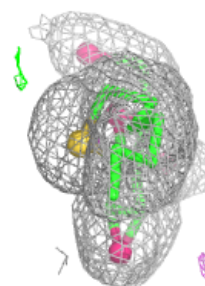
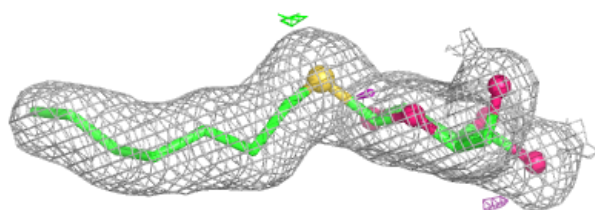
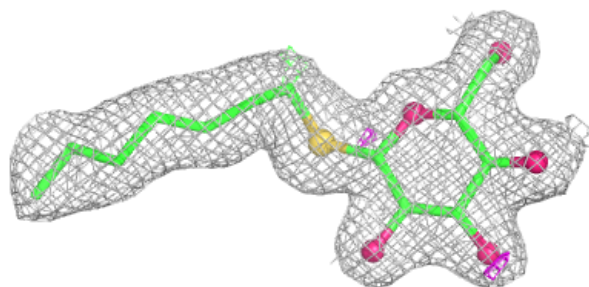
**Electron density around CLA a 410:**

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



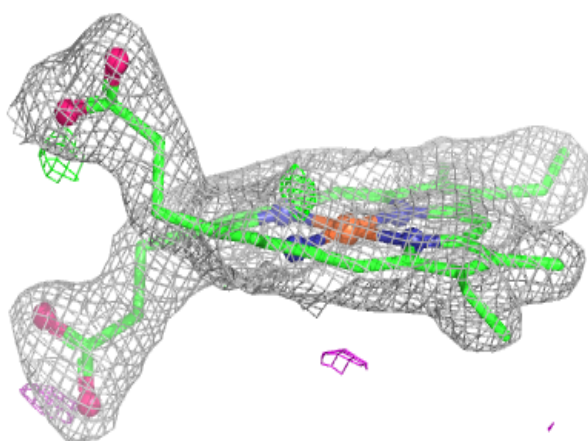
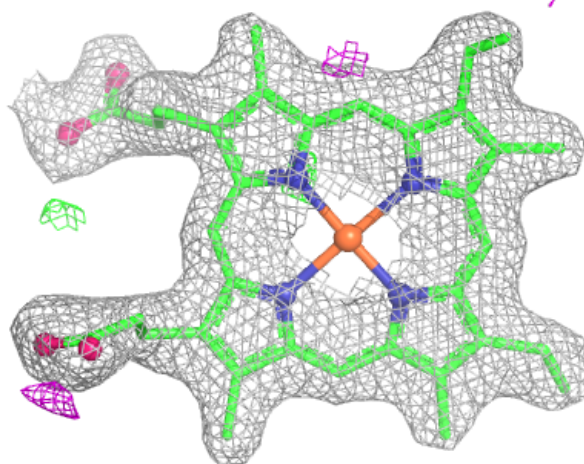
Electron density around HTG O 303:

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



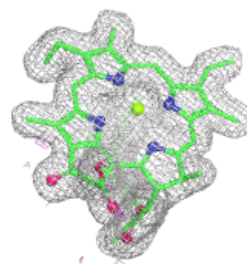
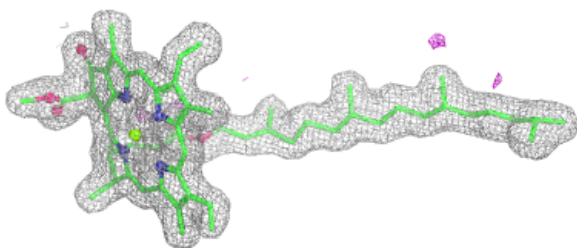
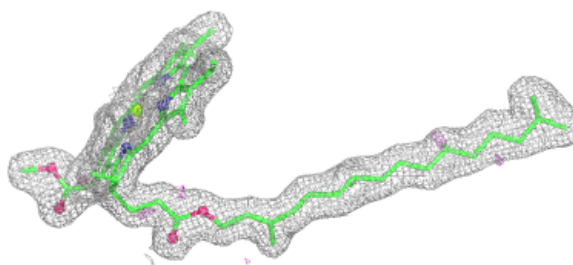
Electron density around HEM F 101:

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



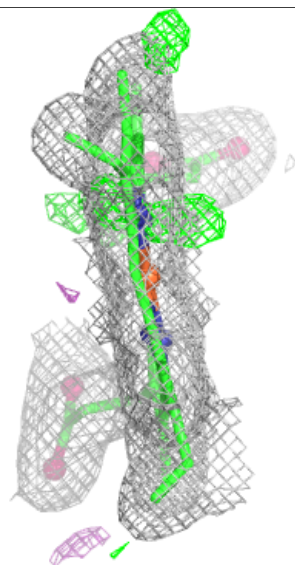
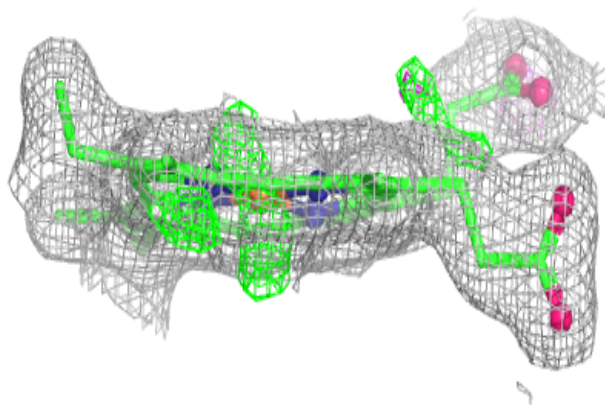
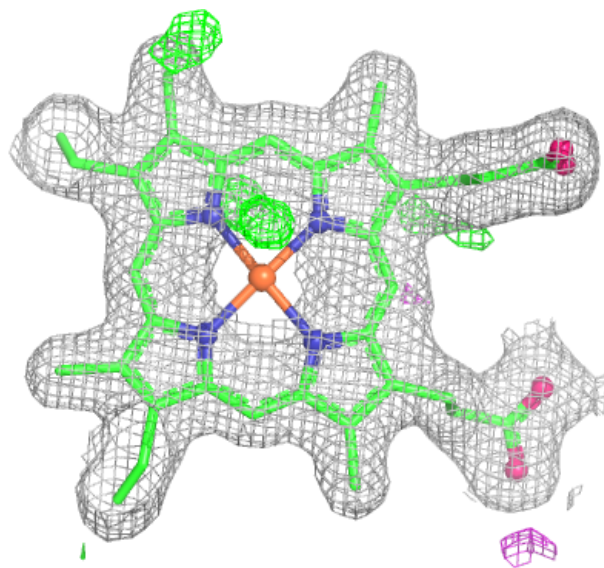
Electron density around CLA b 610:

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



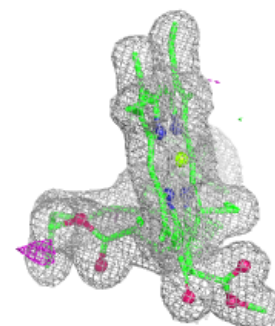
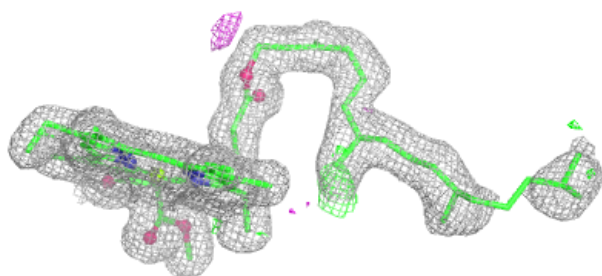
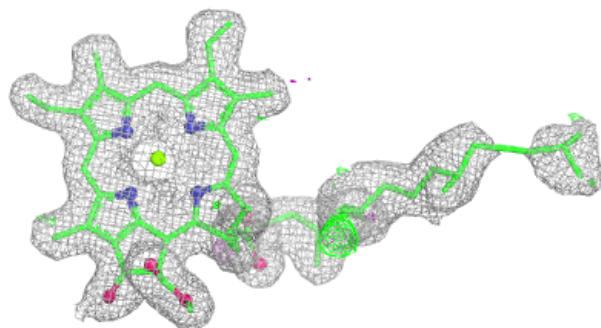
Electron density around HEM v 201:

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

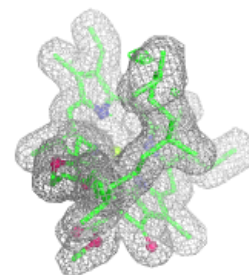
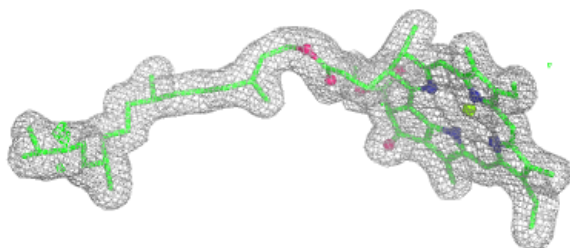
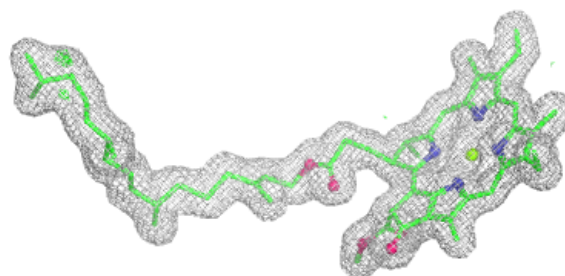


Electron density around CLA A 407:

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

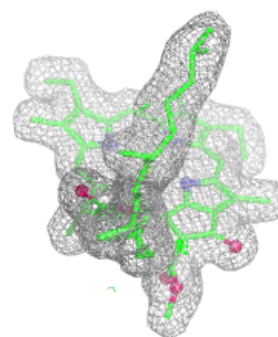
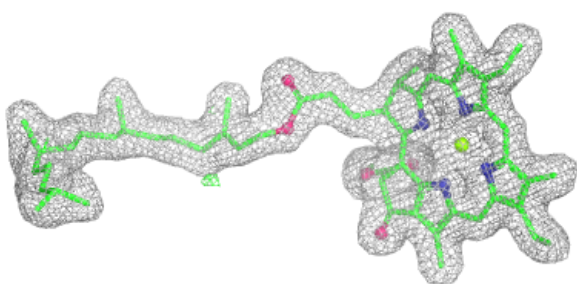
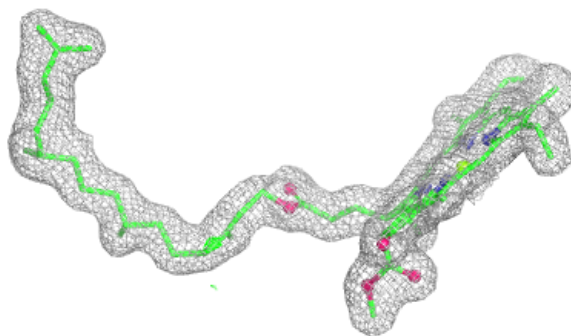
**Electron density around CLA A 405:**

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



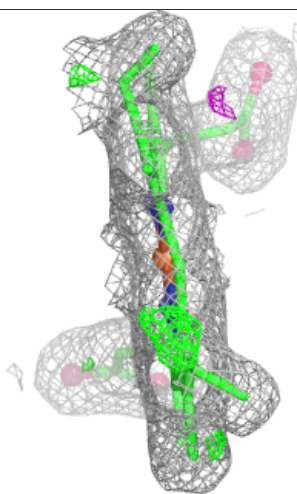
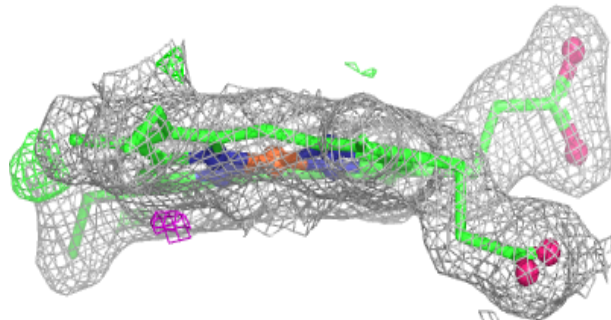
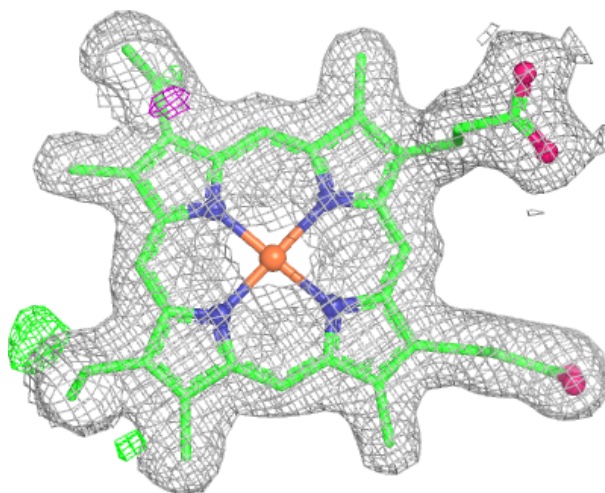
Electron density around CLA d 402:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.