



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 01:52 PM JST

PDB ID : 5ZZN / pdb_00005zzn
Title : Crystal structure of photosystem II from an SQDG-deficient mutant of *Thermosynechococcus elongatus*
Authors : Nakajima, Y.; Umena, Y.; Nagao, R.; Endo, K.; Kobayashi, K.; Akita, F.; Suga, M.; Wada, H.; Noguchi, T.; Shen, J.R.
Deposited on : 2018-06-03
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	1.8.5 (274361), CSD as541be (2020)
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

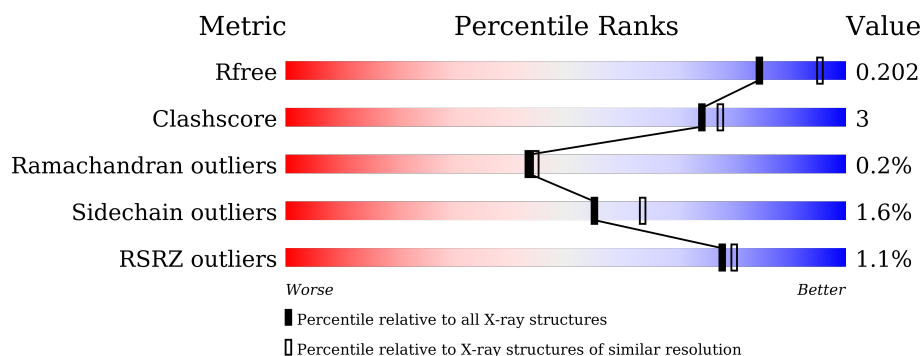
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



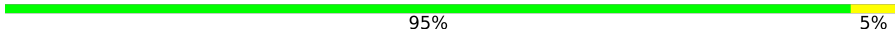
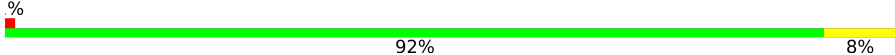
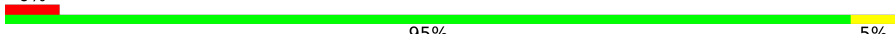
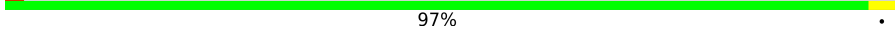
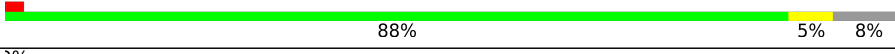
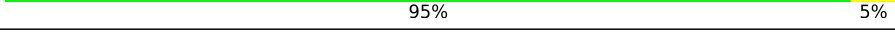
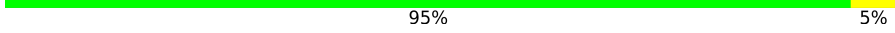
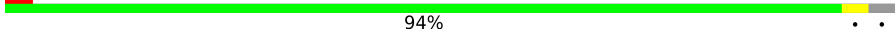
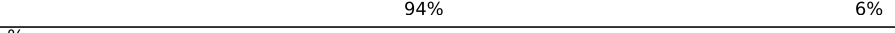
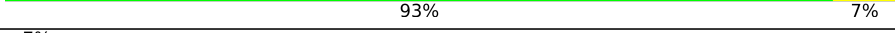
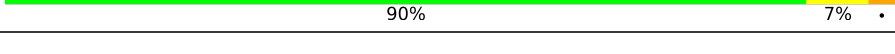
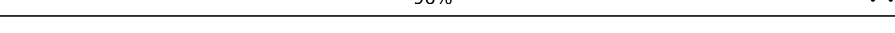
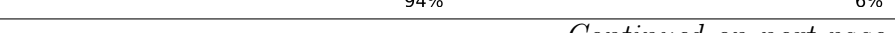
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	334	 90% 10%
1	a	334	 93% 7%
2	B	505	 95% .
2	b	505	 94% 6%
3	C	455	 94% 5% .

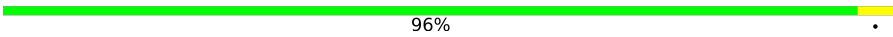
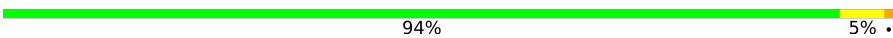
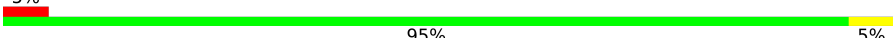
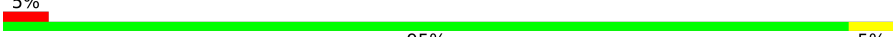
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Mol	Chain	Length	Quality of chain
3	c	455	 95% 5%
4	D	342	 92% 8%
4	d	342	 91% 9%
5	E	81	 90% 9%
5	e	81	 95% 5%
6	F	34	 88% 12%
6	f	34	 82% 12% 6%
7	H	63	 97%
7	h	63	 86% 14%
8	I	37	 89% 5% 5%
8	i	37	 89% 11%
9	J	40	 88% 5% 8%
9	j	40	 95% 5%
10	K	37	 92% 8%
10	k	37	 95% 5%
11	L	36	 86% 14%
11	l	36	 94%
12	M	34	 82% 15%
12	m	34	 85% 15%
13	O	243	 94% 6%
13	o	243	 93% 7%
14	T	30	 90% 7%
14	t	30	 90% 7%
15	U	97	 96%
15	u	97	 94% 6%

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Mol	Chain	Length	Quality of chain
16	V	137	 96% .
16	v	137	 94% 5% .
17	Y	29	 7% 86% 10% .
17	y	29	 3% 90% 10%
18	X	39	 5% 95% 5%
18	x	39	 5% 92% 5% .
19	Z	62	 5% 95% 5%
19	z	62	 10% 94% 6%

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
28	LMT	C	520	X	-	-	-
28	LMT	z	101	X	-	-	-
29	DMS	B	631	-	-	X	-
29	DMS	C	525	-	-	X	-
29	DMS	c	529	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	1	0
			509	339	84	84	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	337	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			284	193	44	46	1			
8	i	37	Total	C	N	O	S	0	0	1
			294	199	47	47	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			262	177	41	43	1			
9	j	40	Total	C	N	O	S	0	0	0
			279	187	44	47	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			296	206	43	47			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			264	177	38	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			269	180	39	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	4	0
			1876	1172	315	385	4			
13	o	243	Total	C	N	O	S	0	6	0
			1876	1174	311	385	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			259	181	36	40	2			
14	t	30	Total	C	N	O	S	0	0	0
			259	181	36	40	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			785	497	133	155			
15	u	97	Total	C	N	O	0	1	0
			783	496	130	157			

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

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

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

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

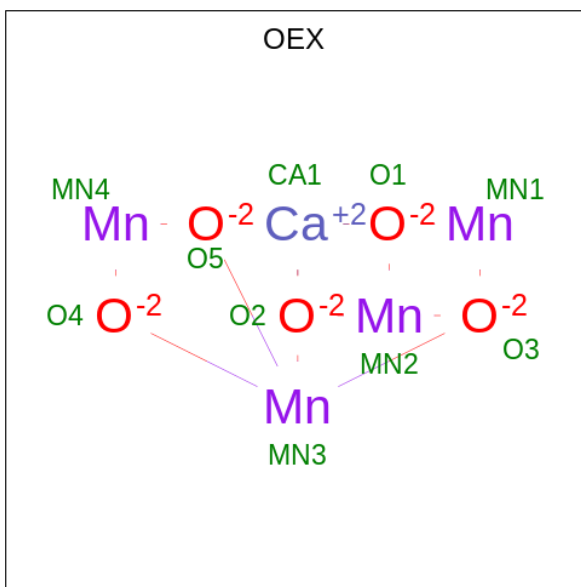
- Molecule 18 is a protein called Photosystem II reaction center X protein.

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

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

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

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

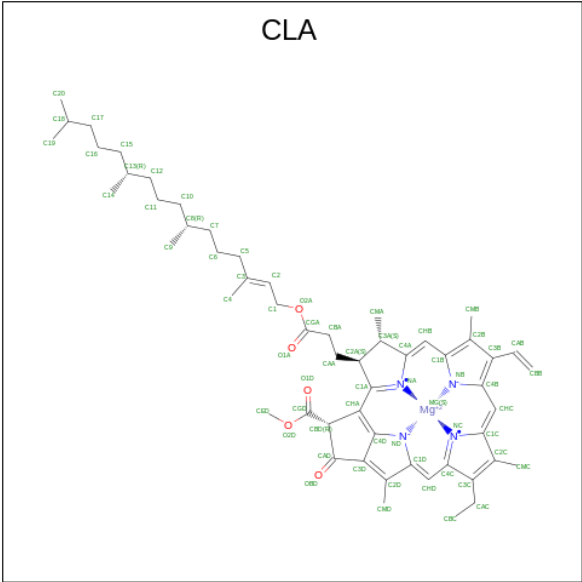


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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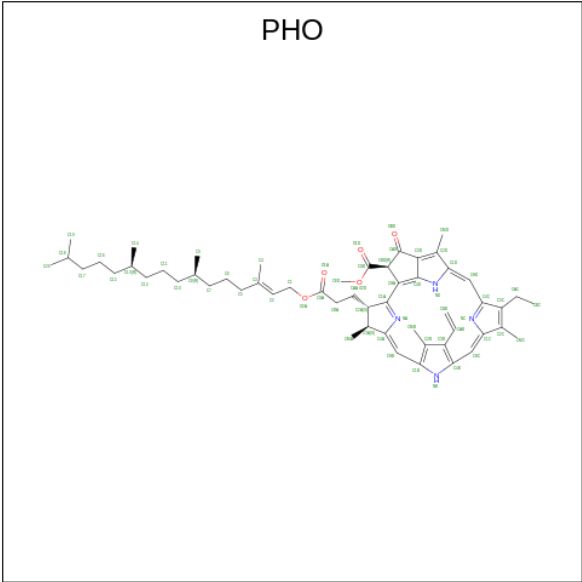
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total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

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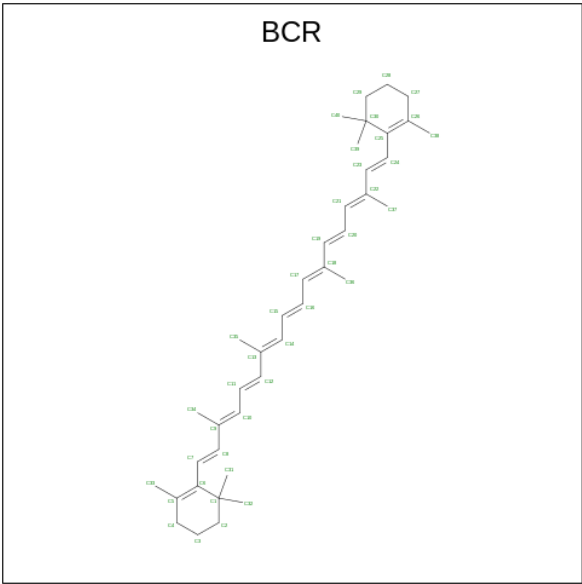
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total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

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



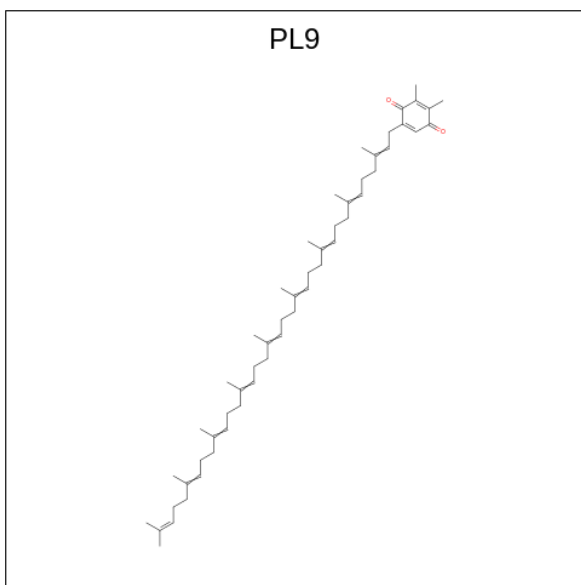
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



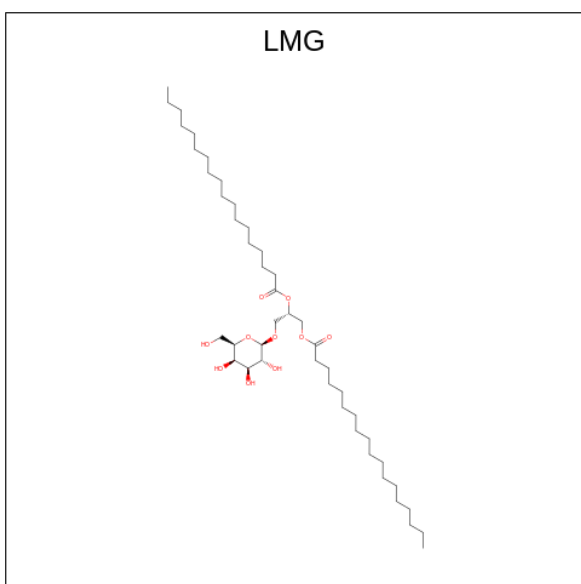
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total C 40 40	0	0
24	a	1	Total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

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 27 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

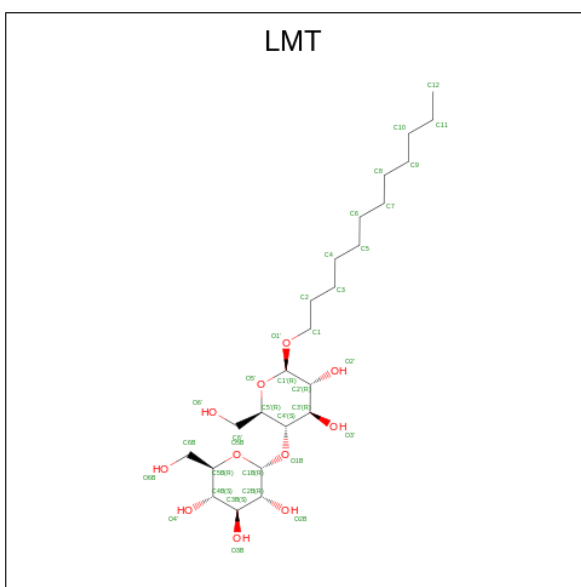
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	5	Total C O 119 104 15	0	0
27	B	5	Total C O 127 117 10	0	0
27	C	2	Total C O 35 30 5	0	0
27	D	1	Total C 16 16	0	0
27	E	2	Total C 29 29	0	0
27	H	2	Total C 14 14	0	0
27	I	4	Total C 59 59	0	0
27	J	1	Total C 16 16	0	0
27	K	1	Total C 10 10	0	0
27	T	1	Total C 13 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	U	1	Total C 14 14	0	0
27	X	1	Total C 16 16	0	0
27	Z	1	Total C 6 6	0	0
27	a	4	Total C O 96 86 10	0	0
27	b	4	Total C O 108 98 10	0	0
27	c	3	Total C O 53 48 5	0	0
27	d	2	Total C O 52 47 5	0	0
27	e	2	Total C 19 19	0	0
27	h	1	Total C 8 8	0	0
27	i	4	Total C 60 60	0	0
27	j	2	Total C O 49 44 5	0	0
27	t	1	Total C 16 16	0	0
27	u	1	Total C 13 13	0	0
27	x	1	Total C 16 16	0	0

- Molecule 28 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



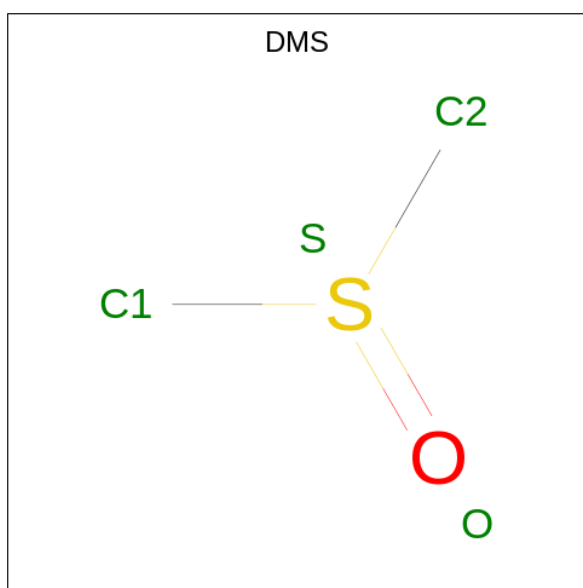
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total 35	C 24	O 11	0	0
28	B	1	Total 35	C 24	O 11	0	0
28	C	1	Total 35	C 24	O 11	0	0
28	F	1	Total 24	C 18	O 6	0	0
28	J	1	Total 24	C 18	O 6	0	0
28	M	1	Total 35	C 24	O 11	0	0
28	M	1	Total 24	C 18	O 6	0	0
28	T	1	Total 24	C 18	O 6	0	0
28	Z	1	Total 35	C 24	O 11	0	0
28	a	1	Total 35	C 24	O 11	0	0
28	b	1	Total 25	C 19	O 6	0	0
28	c	1	Total 35	C 24	O 11	0	0
28	j	1	Total 23	C 18	O 5	0	0
28	l	1	Total 24	C 18	O 6	0	0

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

- Molecule 29 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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

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

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

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

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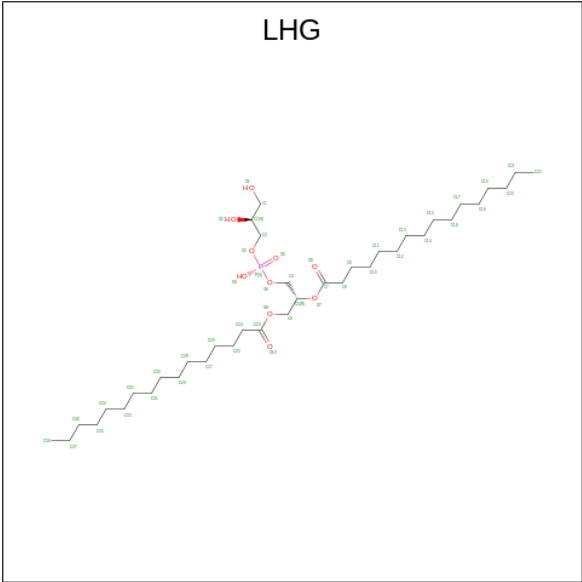
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	v	1	Total 4	C 2	O 1	S 1	0	0
29	v	1	Total 4	C 2	O 1	S 1	0	0
29	v	1	Total 4	C 2	O 1	S 1	0	0
29	v	1	Total 4	C 2	O 1	S 1	0	0
29	v	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

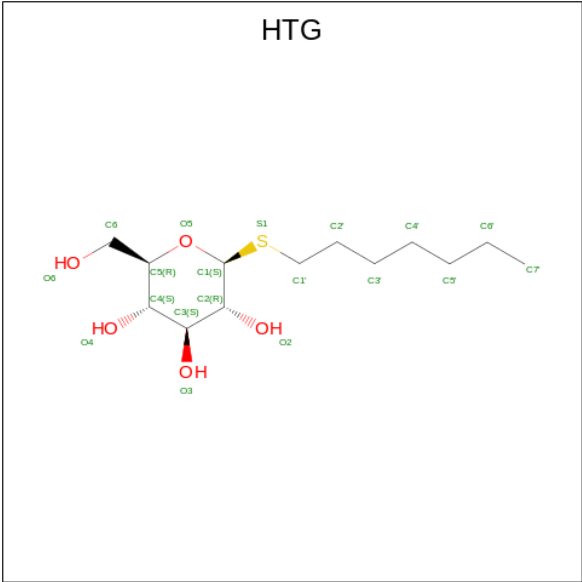
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total 1	Ca 1	0	0
30	O	1	Total 1	Ca 1	0	0
30	V	1	Total 1	Ca 1	0	0
30	b	1	Total 1	Ca 1	0	0
30	c	1	Total 1	Ca 1	0	0
30	o	1	Total 1	Ca 1	0	0
30	v	1	Total 1	Ca 1	0	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



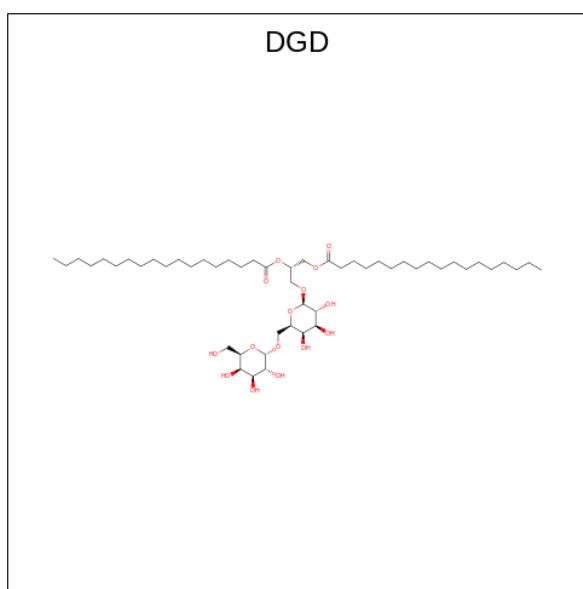
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			18	12	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	S		0	0
			9	8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

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

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



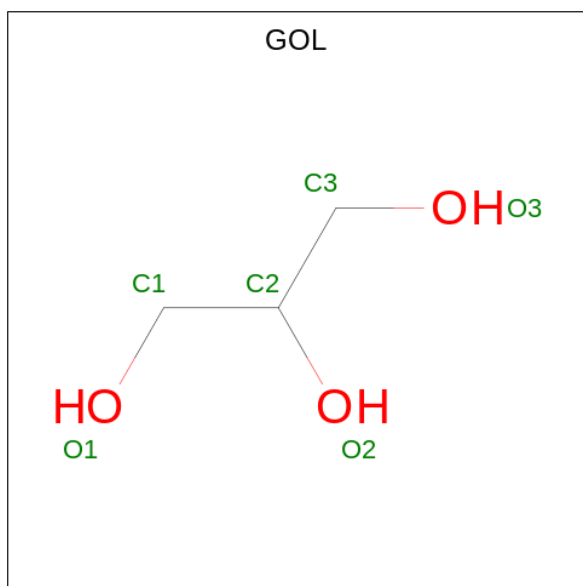
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		

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

- Molecule 34 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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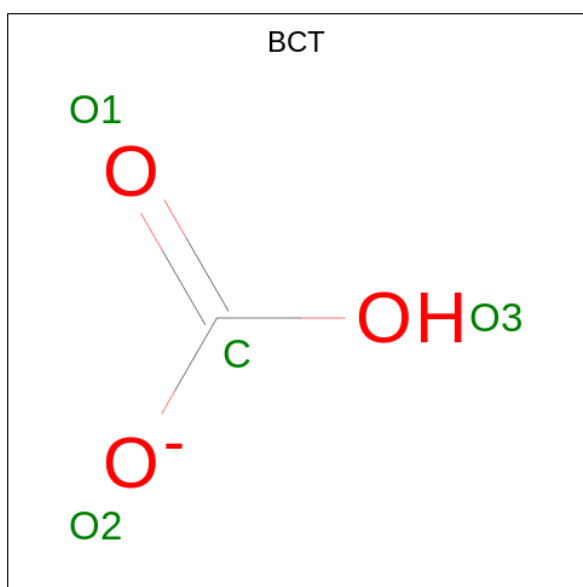
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	e	1	Total	C	O	0	0
			6	3	3		

- Molecule 35 is FE (II) ION (CCD ID: FE2) (formula: Fe).

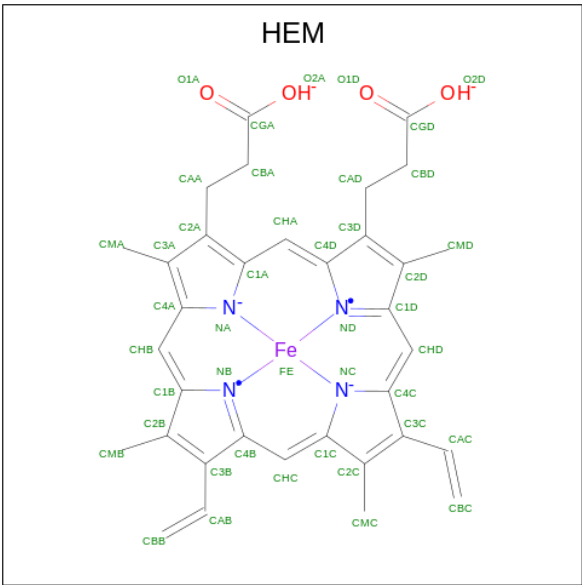
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	Fe		0	0
			1	1			
35	a	1	Total	Fe		0	0
			1	1			

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



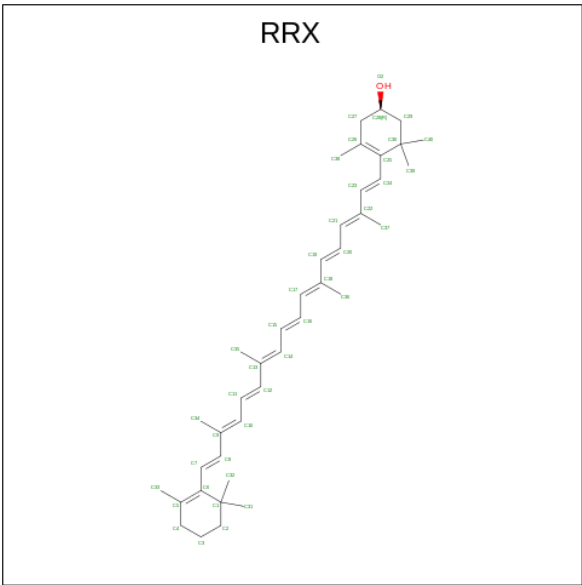
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D	1	Total	C	O	0	1
			8	2	6		
36	d	1	Total	C	O	0	1
			8	2	6		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	F	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

- 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		

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

- # HEC
-
- The chemical structure of HEC (Hexaethylcobalamin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including ethyl groups (C2C, C3C, C4C, C1C, C2B, C3B, C4B, C1B), methyl groups (C2D, C3D, C4D, C1D, C2A, C3A, C4A, C1A), and a central iron atom (Fe). The structure is labeled with various carbon and nitrogen atoms, and the central iron atom is labeled Fe.

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

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



WORLD WIDE
PDB
PROTEIN DATA BANK

Continued from previous page...

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

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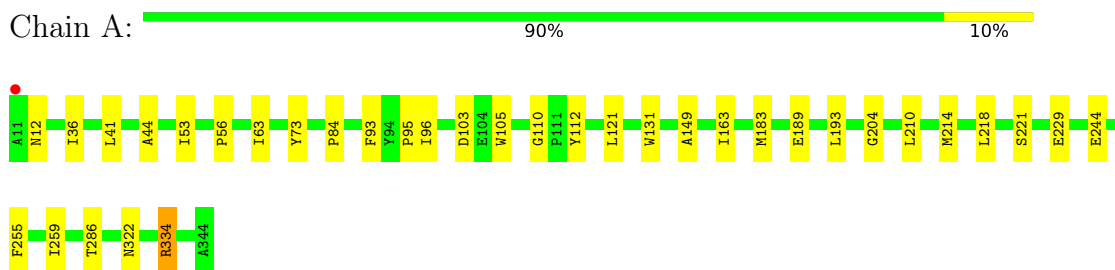
Continued from previous page...

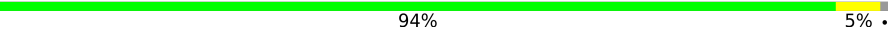
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	f	11	Total 11	O 11	0	0
41	h	34	Total 35	O 35	0	1
41	i	6	Total 6	O 6	0	0
41	j	12	Total 12	O 12	0	0
41	k	5	Total 5	O 5	0	0
41	l	9	Total 9	O 9	0	0
41	m	8	Total 8	O 8	0	0
41	o	126	Total 129	O 129	0	3
41	t	9	Total 10	O 10	0	1
41	u	72	Total 72	O 72	0	0
41	v	75	Total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

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



Chain C:  94% 5%

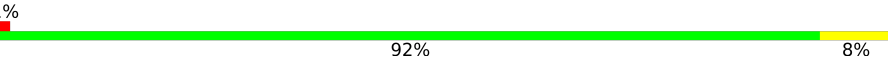


- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  95% 5%



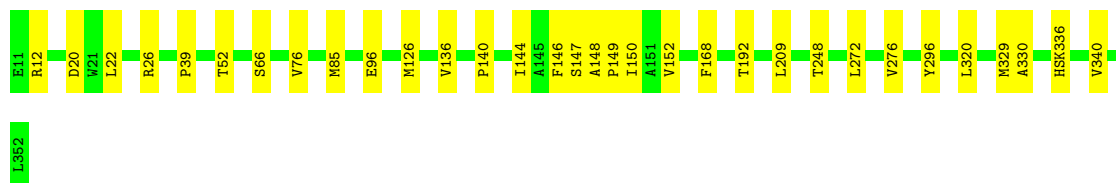
- Molecule 4: Photosystem II D2 protein

Chain D:  92% 8%

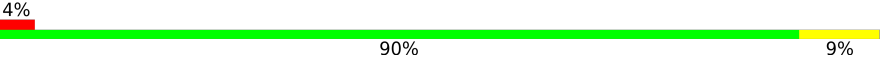


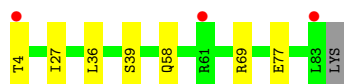
- Molecule 4: Photosystem II D2 protein

Chain d:  91% 9%

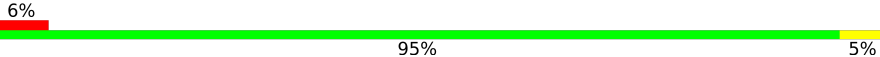


- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  90% 9%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  95% 5%

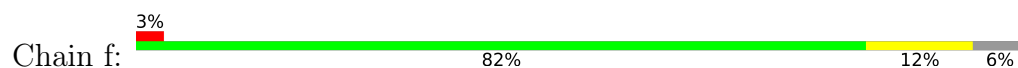


- Molecule 6: Cytochrome b559 subunit beta

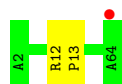
Chain F:  88% 12%



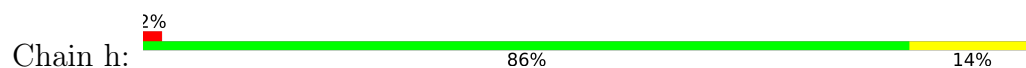
- Molecule 6: Cytochrome b559 subunit beta



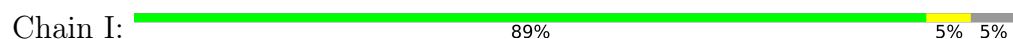
- Molecule 7: Photosystem II reaction center protein H



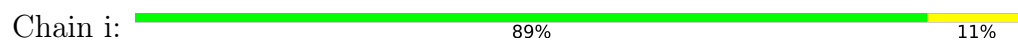
- Molecule 7: Photosystem II reaction center protein H



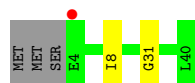
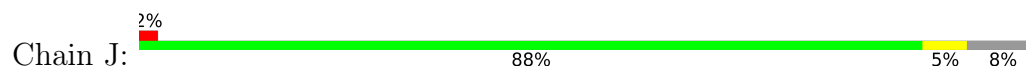
- Molecule 8: Photosystem II reaction center protein I



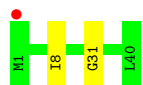
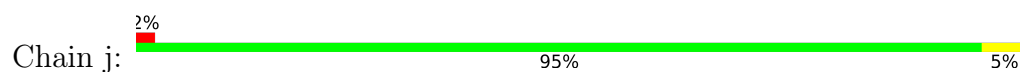
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



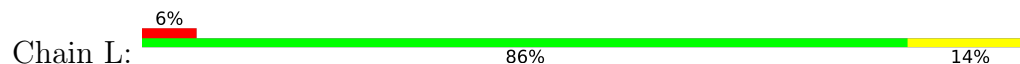
- Molecule 10: Photosystem II reaction center protein K



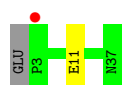
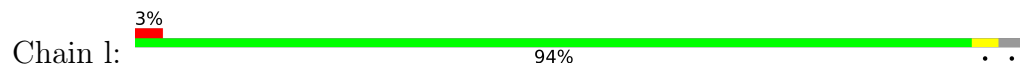
- Molecule 10: Photosystem II reaction center protein K



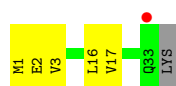
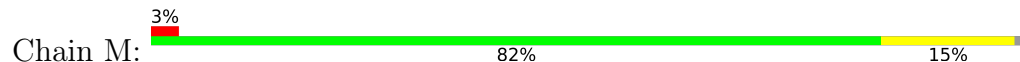
- Molecule 11: Photosystem II reaction center protein L



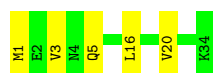
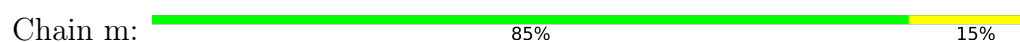
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



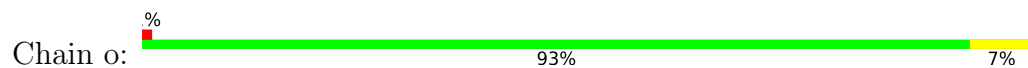
- Molecule 12: Photosystem II reaction center protein M



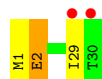
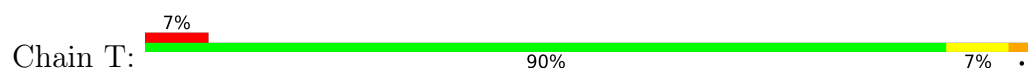
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



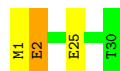
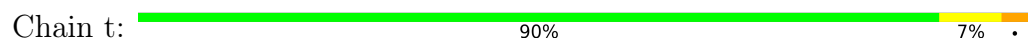
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



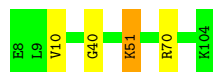
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T



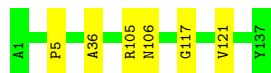
- Molecule 15: Photosystem II 12 kDa extrinsic protein



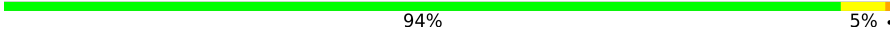
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



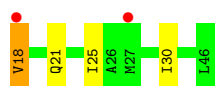
- Molecule 16: Cytochrome c-550

Chain v:  94% 5%

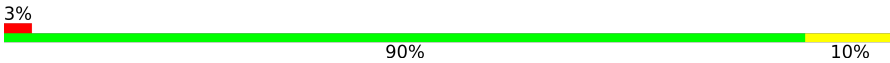


- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  7% 86% 10%

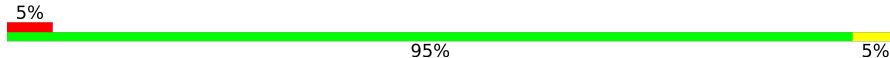


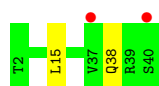
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  3% 90% 10%

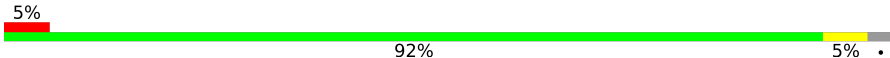


- Molecule 18: Photosystem II reaction center X protein

Chain X:  5% 95% 5%

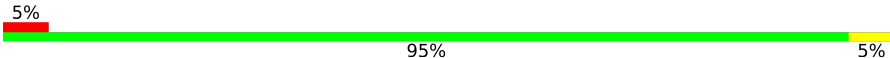


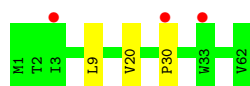
- Molecule 18: Photosystem II reaction center X protein

Chain x:  5% 92% 5%

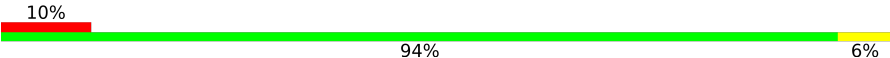


- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  5% 95% 5%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  10% 94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.25Å 228.43Å 287.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-2.10) 99.3 (19.99-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.154 , 0.197 0.164 , 0.202	Depositor DCC
R_{free} test set	23043 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53800	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.32	7/2711 (0.3%)	1.06	7/3699 (0.2%)
1	a	1.27	4/2714 (0.1%)	1.06	4/3702 (0.1%)
2	B	1.25	4/4149 (0.1%)	1.02	3/5655 (0.1%)
2	b	1.24	7/4128 (0.2%)	1.03	5/5628 (0.1%)
3	C	1.21	6/3639 (0.2%)	1.00	1/4953 (0.0%)
3	c	1.19	4/3645 (0.1%)	1.01	2/4962 (0.0%)
4	D	1.31	5/2821 (0.2%)	1.00	3/3843 (0.1%)
4	d	1.24	7/2813 (0.2%)	1.01	2/3831 (0.1%)
5	E	1.12	0/684	1.08	1/935 (0.1%)
5	e	1.15	0/668	1.11	1/913 (0.1%)
6	F	1.20	0/283	1.02	0/386
6	f	1.09	0/265	0.88	0/360
7	H	1.23	0/522	0.95	0/712
7	h	1.19	0/519	0.93	0/708
8	I	1.11	1/281 (0.4%)	0.92	0/381
8	i	1.18	1/291 (0.3%)	0.97	0/394
9	J	1.13	0/268	1.06	0/363
9	j	1.22	0/285	1.08	0/386
10	K	1.03	0/306	1.05	0/422
10	k	0.99	0/295	1.03	0/407
11	L	1.32	1/298 (0.3%)	1.70	4/406 (1.0%)
11	l	1.30	1/303 (0.3%)	1.00	0/413
12	M	1.32	1/257 (0.4%)	1.04	0/352
12	m	1.27	0/262	1.11	0/359
13	O	1.20	0/1907	1.00	1/2589 (0.0%)
13	o	1.15	2/1907 (0.1%)	1.00	2/2591 (0.1%)
14	T	1.32	0/258	1.02	0/349
14	t	1.22	0/258	1.01	0/349
15	U	1.24	0/796	1.08	1/1078 (0.1%)
15	u	1.30	1/794 (0.1%)	1.06	0/1076
16	V	1.29	1/1104 (0.1%)	1.09	1/1498 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	1.24	2/1084 (0.2%)	1.05	0/1475
17	Y	1.00	0/218	1.04	0/292
17	y	0.96	0/210	1.06	0/281
18	X	1.06	0/295	0.97	0/399
18	x	1.07	0/292	0.95	0/395
19	Z	1.08	0/476	1.04	0/652
19	z	0.94	0/470	0.99	0/645
All	All	1.23	55/42476 (0.1%)	1.03	38/57839 (0.1%)

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	205	LEU	N-CA	7.26	1.55	1.46
12	M	17	VAL	CA-C	7.25	1.59	1.52
4	D	287	VAL	N-CA	6.97	1.54	1.46
2	b	297	THR	CA-C	6.96	1.62	1.53
2	B	414	PRO	CA-C	6.89	1.58	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	2	GLU	CA-C-N	18.80	143.34	119.84
11	L	2	GLU	C-N-CA	18.80	143.34	119.84
1	a	142	TRP	N-CA-C	6.66	121.11	112.92
4	D	344	GLU	N-CA-C	6.30	118.95	111.71
3	c	134	ILE	CB-CA-C	-6.15	105.65	111.06

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2626	0	2504	16	0
1	a	2629	0	2520	11	0
2	B	4009	0	3844	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3988	0	3820	13	0
3	C	3526	0	3434	14	0
3	c	3531	0	3443	16	0
4	D	2746	0	2640	18	0
4	d	2738	0	2635	18	0
5	E	665	0	637	3	0
5	e	649	0	621	1	0
6	F	274	0	279	2	0
6	f	257	0	269	3	0
7	H	509	0	531	2	0
7	h	506	0	521	6	0
8	I	284	0	296	0	0
8	i	294	0	309	1	0
9	J	262	0	270	1	0
9	j	279	0	284	1	0
10	K	296	0	302	4	0
10	k	285	0	290	0	0
11	L	292	0	293	1	0
11	l	296	0	306	0	0
12	M	264	0	279	9	0
12	m	269	0	281	8	0
13	O	1876	0	1829	10	0
13	o	1876	0	1813	7	0
14	T	259	0	261	1	0
14	t	259	0	261	1	0
15	U	785	0	785	1	0
15	u	783	0	778	3	0
16	V	1083	0	1090	4	0
16	v	1063	0	1052	6	0
17	Y	217	0	243	4	0
17	y	209	0	228	1	0
18	X	292	0	319	1	0
18	x	289	0	322	4	0
19	Z	465	0	493	1	0
19	z	459	0	484	1	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
21	v	1	0	0	0	0
22	A	260	0	288	8	0
22	B	1040	0	1152	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	845	0	936	16	0
22	D	130	0	144	2	0
22	a	195	0	216	3	0
22	b	1040	0	1152	18	0
22	c	845	0	936	11	0
22	d	195	0	216	8	0
23	A	64	0	74	0	0
23	D	64	0	74	1	0
23	a	64	0	74	0	0
23	d	64	0	74	1	0
24	A	40	0	56	1	0
24	B	120	0	168	7	0
24	C	40	0	56	1	0
24	D	40	0	56	2	0
24	K	80	0	112	2	0
24	T	40	0	56	2	0
24	Y	40	0	56	0	0
24	a	40	0	56	0	0
24	b	120	0	168	6	0
24	c	80	0	112	6	0
24	d	40	0	56	4	0
24	k	40	0	56	2	0
24	t	40	0	56	4	0
24	y	40	0	56	1	0
25	A	55	0	80	5	0
25	D	55	0	80	1	0
25	a	55	0	80	6	0
25	d	55	0	80	0	0
26	A	51	0	72	0	0
26	B	51	0	72	1	0
26	C	97	0	134	0	0
26	D	47	0	64	0	0
26	a	51	0	72	2	0
26	b	49	0	68	1	0
26	c	89	0	118	1	0
26	d	47	0	64	0	0
27	A	119	0	0	0	0
27	B	127	0	0	0	0
27	C	35	0	0	0	0
27	D	16	0	0	0	0
27	E	29	0	0	0	0
27	H	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	I	59	0	0	0	0
27	J	16	0	0	0	0
27	K	10	0	0	0	0
27	T	13	0	0	0	0
27	U	14	0	0	0	0
27	X	16	0	0	0	0
27	Z	6	0	0	0	0
27	a	96	0	0	1	0
27	b	108	0	0	1	0
27	c	53	0	0	0	0
27	d	52	0	0	0	0
27	e	19	0	0	0	0
27	h	8	0	0	0	0
27	i	60	0	0	0	0
27	j	49	0	0	0	0
27	t	16	0	0	0	0
27	u	13	0	0	0	0
27	x	16	0	0	0	0
28	A	35	0	46	4	0
28	B	35	0	46	0	0
28	C	35	0	45	1	0
28	F	24	0	35	0	0
28	J	24	0	35	0	0
28	M	59	0	81	0	0
28	T	24	0	35	0	0
28	Z	35	0	46	0	0
28	a	35	0	46	2	0
28	b	25	0	35	0	0
28	c	35	0	46	0	0
28	j	23	0	33	1	0
28	l	24	0	35	0	0
28	m	83	0	114	3	0
28	t	24	0	35	0	0
28	z	32	0	36	0	0
29	A	16	0	24	1	0
29	B	44	0	66	13	0
29	C	36	0	54	7	0
29	D	20	0	30	6	0
29	E	4	0	6	0	0
29	I	4	0	6	0	0
29	O	40	0	60	5	0
29	U	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	V	24	0	36	3	0
29	a	20	0	30	0	0
29	b	36	0	54	4	0
29	c	48	0	72	13	0
29	d	8	0	12	0	0
29	e	4	0	6	1	0
29	h	4	0	6	0	0
29	o	36	0	54	5	0
29	u	12	0	18	3	0
29	v	20	0	30	8	0
30	B	1	0	0	0	0
30	O	1	0	0	0	0
30	V	1	0	0	0	0
30	b	1	0	0	0	0
30	c	1	0	0	0	0
30	o	1	0	0	0	0
30	v	1	0	0	0	0
31	B	49	0	74	0	0
31	D	142	0	208	0	0
31	E	49	0	74	0	0
31	F	38	0	46	0	0
31	b	49	0	74	0	0
31	d	142	0	209	1	0
31	e	38	0	48	0	0
31	f	46	0	62	0	0
32	B	75	0	99	2	0
32	C	66	0	93	1	0
32	D	16	0	17	1	0
32	O	19	0	26	0	0
32	U	14	0	13	0	0
32	V	19	0	26	0	0
32	b	74	0	97	3	0
32	c	43	0	56	0	0
32	d	16	0	17	0	0
32	o	19	0	26	2	0
32	v	16	0	17	0	0
33	C	186	0	246	2	0
33	D	45	0	59	0	0
33	H	62	0	82	0	0
33	c	180	0	234	2	0
33	d	48	0	65	0	0
33	h	62	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	6	0	8	1	0
34	D	6	0	8	0	0
34	b	6	0	8	0	0
34	c	6	0	8	1	0
34	e	6	0	8	0	0
35	D	1	0	0	0	0
35	a	1	0	0	0	0
36	D	8	0	0	0	0
36	d	8	0	0	0	0
37	F	43	0	30	1	0
37	f	43	0	30	0	0
38	H	41	0	56	2	0
38	h	41	0	56	5	0
39	J	1	0	0	0	0
39	K	1	0	0	0	0
39	j	1	0	0	0	0
39	k	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	141	0	0	2	0
41	B	263	0	0	2	0
41	C	216	0	0	2	0
41	D	130	0	0	2	0
41	E	21	0	0	0	0
41	F	6	0	0	0	0
41	H	44	0	0	0	0
41	I	6	0	0	0	0
41	J	11	0	0	0	0
41	K	8	0	0	0	0
41	L	11	0	0	0	0
41	M	11	0	0	0	0
41	O	152	0	0	0	0
41	T	13	0	0	0	0
41	U	71	0	0	0	0
41	V	103	0	0	1	0
41	X	12	0	0	0	0
41	Y	5	0	0	1	0
41	Z	3	0	0	0	0
41	a	126	0	0	0	0
41	b	260	0	0	2	0
41	c	203	0	0	2	0
41	d	135	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	e	20	0	0	0	0
41	f	11	0	0	0	0
41	h	35	0	0	1	0
41	i	6	0	0	0	0
41	j	12	0	0	0	0
41	k	5	0	0	0	0
41	l	9	0	0	0	0
41	m	8	0	0	0	0
41	o	129	0	0	1	0
41	t	10	0	0	0	0
41	u	72	0	0	4	0
41	v	75	0	0	0	0
41	x	7	0	0	0	0
41	y	4	0	0	0	0
41	z	2	0	0	0	0
All	All	53800	0	51647	318	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 3.

The worst 5 of 318 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[B]:LEU:HD23	12:m:16[B]:LEU:CD2	1.38	1.51
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD23	1.46	1.44
3:C:228:ASN:HD22	29:C:525:DMS:H23	1.15	1.08
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CD2	2.18	1.00
3:c:228:ASN:HD22	29:c:528:DMS:H23	1.24	0.97

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	334/334 (100%)	328 (98%)	5 (2%)	1 (0%)	36	36
1	a	334/334 (100%)	327 (98%)	6 (2%)	1 (0%)	36	36
2	B	508/505 (101%)	501 (99%)	7 (1%)	0	100	100
2	b	506/505 (100%)	498 (98%)	8 (2%)	0	100	100
3	C	454/455 (100%)	444 (98%)	9 (2%)	1 (0%)	43	44
3	c	455/455 (100%)	446 (98%)	8 (2%)	1 (0%)	43	44
4	D	341/342 (100%)	336 (98%)	5 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	80/81 (99%)	78 (98%)	2 (2%)	0	100	100
5	e	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	56 (90%)	6 (10%)	0	100	100
7	h	62/63 (98%)	57 (92%)	4 (6%)	1 (2%)	7	4
8	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
8	i	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
9	J	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	35/36 (97%)	34 (97%)	0	1 (3%)	3	1
11	l	35/36 (97%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	239 (98%)	5 (2%)	1 (0%)	30	28
13	o	247/243 (102%)	240 (97%)	6 (2%)	1 (0%)	30	28
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
15	u	96/97 (99%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	28/29 (97%)	27 (96%)	1 (4%)	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
All	All	5227/5270 (99%)	5106 (98%)	111 (2%)	10 (0%)	43	44

5 of 10 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/270 (100%)	265 (98%)	4 (2%)	57	65
1	a	270/270 (100%)	267 (99%)	3 (1%)	65	74
2	B	404/403 (100%)	403 (100%)	1 (0%)	87	93
2	b	402/403 (100%)	397 (99%)	5 (1%)	63	72
3	C	356/356 (100%)	351 (99%)	5 (1%)	59	67
3	c	356/356 (100%)	349 (98%)	7 (2%)	48	56
4	D	277/276 (100%)	274 (99%)	3 (1%)	65	74
4	d	276/276 (100%)	273 (99%)	3 (1%)	65	74
5	E	72/72 (100%)	69 (96%)	3 (4%)	26	28
5	e	68/72 (94%)	66 (97%)	2 (3%)	37	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	27/28 (96%)	26 (96%)	1 (4%)	30	33
6	f	26/28 (93%)	26 (100%)	0	100	100
7	H	54/53 (102%)	54 (100%)	0	100	100
7	h	54/53 (102%)	54 (100%)	0	100	100
8	I	30/33 (91%)	30 (100%)	0	100	100
8	i	31/33 (94%)	31 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	28
9	j	25/28 (89%)	24 (96%)	1 (4%)	28	29
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	28/30 (93%)	26 (93%)	2 (7%)	13	11
11	L	32/34 (94%)	32 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	29/30 (97%)	29 (100%)	0	100	100
12	m	29/30 (97%)	27 (93%)	2 (7%)	14	12
13	O	205/206 (100%)	202 (98%)	3 (2%)	57	65
13	o	203/206 (98%)	199 (98%)	4 (2%)	48	56
14	T	26/26 (100%)	24 (92%)	2 (8%)	12	9
14	t	26/26 (100%)	24 (92%)	2 (8%)	12	9
15	U	85/84 (101%)	81 (95%)	4 (5%)	23	24
15	u	85/84 (101%)	82 (96%)	3 (4%)	32	35
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	70	78
17	Y	22/22 (100%)	20 (91%)	2 (9%)	9	6
17	y	20/22 (91%)	18 (90%)	2 (10%)	7	5
18	X	31/32 (97%)	30 (97%)	1 (3%)	34	38
18	x	32/32 (100%)	31 (97%)	1 (3%)	35	39
19	Z	49/52 (94%)	48 (98%)	1 (2%)	48	56
19	z	47/52 (90%)	45 (96%)	2 (4%)	26	27
All	All	4268/4304 (99%)	4197 (98%)	71 (2%)	55	62

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	118	LEU
13	o	181	GLU
16	v	57	GLU
15	U	51	LYS
15	U	10	VAL

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

Mol	Chain	Res	Type
13	o	104	GLN
13	o	132	ASN
15	u	81	HIS
13	O	88	ASN
13	O	80	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	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.09	1 (12%)	7,9,11	1.01	0
4	HSK	d	336[A]	-	9,10,12	3.86	4 (44%)	6,12,16	1.63	1 (16%)
14	FME	T	1	14	8,9,10	0.75	0	7,9,11	1.63	2 (28%)
8	FME	I	1	8	8,9,10	0.72	0	7,9,11	1.81	3 (42%)
4	HSK	D	336[A]	-	9,10,12	4.30	3 (33%)	6,12,16	2.39	3 (50%)
8	FME	i	1	8	8,9,10	0.35	0	7,9,11	1.72	2 (28%)
12	FME	M	1	12	8,9,10	1.32	1 (12%)	7,9,11	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	t	1	14	8,9,10	0.83	0	7,9,11	1.38	1 (14%)
4	HSK	d	336[B]	-	9,11,12	2.34	4 (44%)	6,14,16	2.59	3 (50%)
4	HSK	D	336[B]	-	9,11,12	1.73	1 (11%)	6,14,16	4.52	4 (66%)

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

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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-12.26	1.22	1.38
4	d	336[A]	HSK	OM-ND1	-10.64	1.24	1.38
4	d	336[B]	HSK	OM-ND1	5.18	1.45	1.38
4	D	336[B]	HSK	CE1-ND1	-4.24	1.29	1.37
4	d	336[B]	HSK	CD2-CG	2.83	1.40	1.36

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336[B]	HSK	CE1-ND1-CG	7.35	116.78	107.37
4	D	336[B]	HSK	ND1-CE1-NE2	-6.58	103.53	111.75
4	D	336[A]	HSK	CD2-NE2-CE1	3.87	109.94	105.22
4	d	336[B]	HSK	ND1-CE1-NE2	-3.85	106.93	111.75
4	d	336[B]	HSK	CE1-ND1-CG	3.70	112.10	107.37

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 353 ligands modelled in this entry, 18 are monoatomic and 52 are unknown - leaving 283 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	B	615	2	69,73,73	2.15	17 (24%)	83,113,113	2.70	32 (38%)
22	CLA	b	614	41	69,73,73	1.81	20 (28%)	83,113,113	2.13	25 (30%)
22	CLA	c	506	3	69,73,73	2.09	22 (31%)	83,113,113	2.24	27 (32%)
29	DMS	O	312	-	3,3,3	2.72	1 (33%)	3,3,3	0.68	0
24	BCR	T	101	-	41,41,41	0.95	0	56,56,56	1.79	14 (25%)
32	HTG	B	629	-	19,19,19	0.97	2 (10%)	23,24,24	1.46	3 (13%)
29	DMS	v	204	-	3,3,3	2.69	1 (33%)	3,3,3	1.08	0
25	PL9	A	410	-	55,55,55	1.15	4 (7%)	68,69,69	2.12	17 (25%)
29	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	1.11	0
26	LMG	D	412	39	47,47,55	1.05	3 (6%)	55,55,63	1.14	3 (5%)
29	DMS	U	202	-	3,3,3	2.61	1 (33%)	3,3,3	1.60	1 (33%)
38	RRX	h	102	-	42,42,42	0.98	2 (4%)	57,58,58	1.61	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMG	B	622	-	51,51,55	1.01	3 (5%)	59,59,63	1.26	7 (11%)
22	CLA	b	613	2	69,73,73	2.27	21 (30%)	83,113,113	2.12	23 (27%)
29	DMS	O	306	-	3,3,3	2.80	1 (33%)	3,3,3	1.14	0
38	RRX	H	102	-	42,42,42	1.09	2 (4%)	57,58,58	1.51	9 (15%)
29	DMS	V	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
22	CLA	A	408	1	69,73,73	2.02	18 (26%)	83,113,113	2.43	27 (32%)
26	LMG	d	412	39	47,47,55	0.99	3 (6%)	55,55,63	1.30	5 (9%)
32	HTG	b	640	-	17,17,19	2.71	5 (29%)	21,22,24	3.94	12 (57%)
22	CLA	c	513	3	69,73,73	2.27	21 (30%)	83,113,113	2.28	25 (30%)
29	DMS	h	104	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
29	DMS	b	634	-	3,3,3	2.71	1 (33%)	3,3,3	0.67	0
31	LHG	F	103	-	37,37,48	1.21	2 (5%)	40,43,54	1.58	4 (10%)
31	LHG	D	409	-	48,48,48	0.90	3 (6%)	51,54,54	1.61	6 (11%)
29	DMS	o	306	-	3,3,3	2.55	1 (33%)	3,3,3	1.00	0
26	LMG	A	411	-	51,51,55	1.04	2 (3%)	59,59,63	1.24	7 (11%)
22	CLA	b	611	41	69,73,73	1.93	17 (24%)	83,113,113	2.29	27 (32%)
24	BCR	b	622	-	41,41,41	1.27	4 (9%)	56,56,56	1.15	4 (7%)
22	CLA	b	620	2	69,73,73	2.27	19 (27%)	83,113,113	2.42	30 (36%)
22	CLA	b	605	41	69,73,73	2.31	18 (26%)	83,113,113	2.63	30 (36%)
22	CLA	c	503	3	69,73,73	2.03	19 (27%)	83,113,113	2.40	29 (34%)
36	BCT	d	401[B]	35	2,3,3	0.78	0	2,3,3	0.66	0
22	CLA	a	406	1	69,73,73	1.75	17 (24%)	83,113,113	2.44	28 (33%)
24	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.37	8 (14%)
29	DMS	B	635	-	3,3,3	2.80	1 (33%)	3,3,3	0.64	0
22	CLA	B	610	2	69,73,73	2.03	17 (24%)	83,113,113	2.24	24 (28%)
22	CLA	c	509	3	69,73,73	2.31	21 (30%)	83,113,113	2.24	21 (25%)
22	CLA	c	502	3	69,73,73	2.59	20 (28%)	83,113,113	2.73	27 (32%)
29	DMS	b	638	-	3,3,3	3.10	1 (33%)	3,3,3	1.05	0
32	HTG	v	208	-	16,16,19	0.92	1 (6%)	20,21,24	3.35	6 (30%)
29	DMS	u	202	-	3,3,3	2.76	1 (33%)	3,3,3	1.44	0
29	DMS	c	529	-	3,3,3	2.92	1 (33%)	3,3,3	0.89	0
29	DMS	O	310	-	3,3,3	2.71	1 (33%)	3,3,3	0.89	0
23	PHO	d	404	-	58,69,69	2.46	14 (24%)	56,99,99	2.17	12 (21%)
22	CLA	C	510	3	69,73,73	2.37	22 (31%)	83,113,113	2.17	20 (24%)
24	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.90	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DGD	D	408	-	45,45,67	1.49	4 (8%)	53,53,81	1.70	10 (18%)
40	HEC	V	201	16	50,50,50	1.80	9 (18%)	68,82,82	1.65	11 (16%)
28	LMT	M	102	-	24,24,36	0.82	0	29,29,47	1.27	3 (10%)
29	DMS	c	537	-	3,3,3	2.64	1 (33%)	3,3,3	1.13	0
22	CLA	B	605	2	69,73,73	1.97	18 (26%)	83,113,113	2.36	30 (36%)
29	DMS	I	105	-	3,3,3	2.69	1 (33%)	3,3,3	1.03	0
32	HTG	o	301	-	19,19,19	1.94	3 (15%)	23,24,24	1.78	7 (30%)
22	CLA	D	405	4	69,73,73	1.97	17 (24%)	83,113,113	2.00	22 (26%)
22	CLA	C	512	3	69,73,73	2.26	21 (30%)	83,113,113	2.31	28 (33%)
24	BCR	k	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	6 (10%)
28	LMT	A	415	-	36,36,36	1.33	4 (11%)	47,47,47	1.97	15 (31%)
29	DMS	D	415	-	3,3,3	2.59	1 (33%)	3,3,3	1.23	0
22	CLA	C	509	3	69,73,73	1.82	19 (27%)	83,113,113	2.88	37 (44%)
22	CLA	b	619	2	69,73,73	2.27	21 (30%)	83,113,113	2.56	33 (39%)
22	CLA	B	612	2	69,73,73	2.10	19 (27%)	83,113,113	2.54	28 (33%)
22	CLA	C	501	3	69,73,73	2.03	19 (27%)	83,113,113	2.83	29 (34%)
29	DMS	A	419	-	3,3,3	2.96	1 (33%)	3,3,3	0.81	0
29	DMS	c	538	-	3,3,3	3.04	1 (33%)	3,3,3	1.05	0
29	DMS	d	415	-	3,3,3	2.34	1 (33%)	3,3,3	0.81	0
31	LHG	d	411	-	43,43,48	1.03	3 (6%)	46,49,54	0.99	5 (10%)
29	DMS	c	540	-	3,3,3	2.84	1 (33%)	3,3,3	0.97	0
22	CLA	b	618	2	69,73,73	2.12	21 (30%)	83,113,113	2.50	32 (38%)
26	LMG	C	519	-	48,48,55	1.29	3 (6%)	56,56,63	1.79	12 (21%)
34	GOL	e	104	-	5,5,5	0.82	0	5,5,5	1.63	1 (20%)
37	HEM	f	101	5,6	50,50,50	1.96	8 (16%)	66,82,82	1.27	7 (10%)
22	CLA	c	505	41	69,73,73	2.26	21 (30%)	83,113,113	2.48	33 (39%)
29	DMS	C	532	-	3,3,3	3.06	1 (33%)	3,3,3	0.95	0
29	DMS	O	308	-	3,3,3	2.72	1 (33%)	3,3,3	1.60	1 (33%)
22	CLA	B	617	2	69,73,73	2.04	19 (27%)	83,113,113	2.56	32 (38%)
29	DMS	c	532	-	3,3,3	2.72	1 (33%)	3,3,3	0.89	0
31	LHG	D	411	-	43,43,48	1.12	3 (6%)	46,49,54	1.08	4 (8%)
22	CLA	B	608	41	69,73,73	2.07	18 (26%)	83,113,113	2.27	25 (30%)
29	DMS	E	104	-	3,3,3	2.75	1 (33%)	3,3,3	1.00	0
29	DMS	O	309	-	3,3,3	2.76	1 (33%)	3,3,3	0.91	0
22	CLA	c	511	3	69,73,73	2.01	16 (23%)	83,113,113	2.64	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	HTG	V	202	-	19,19,19	1.02	2 (10%)	23,24,24	3.35	7 (30%)
33	DGD	C	516	-	63,63,67	1.06	5 (7%)	77,77,81	1.00	4 (5%)
33	DGD	H	101	-	63,63,67	1.22	4 (6%)	77,77,81	1.63	13 (16%)
22	CLA	b	612	2	69,73,73	2.04	19 (27%)	83,113,113	2.23	26 (31%)
29	DMS	o	307	-	3,3,3	2.70	1 (33%)	3,3,3	1.24	0
28	LMT	B	623	-	36,36,36	0.80	1 (2%)	47,47,47	1.68	10 (21%)
29	DMS	a	418	-	3,3,3	2.79	1 (33%)	3,3,3	0.71	0
28	LMT	F	102	-	24,24,36	1.31	3 (12%)	29,29,47	1.44	6 (20%)
32	HTG	C	521	-	19,19,19	0.80	0	23,24,24	1.74	4 (17%)
32	HTG	D	413	-	16,16,19	1.08	2 (12%)	20,21,24	2.53	6 (30%)
22	CLA	B	611	41	69,73,73	2.27	21 (30%)	83,113,113	2.16	24 (28%)
22	CLA	c	514	3	69,73,73	2.09	21 (30%)	83,113,113	2.28	28 (33%)
24	BCR	C	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	4 (7%)
26	LMG	b	625	-	49,49,55	1.23	3 (6%)	57,57,63	1.18	6 (10%)
22	CLA	A	405	41	69,73,73	2.19	18 (26%)	83,113,113	2.56	29 (34%)
24	BCR	K	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	3 (5%)
29	DMS	c	539	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
28	LMT	a	401	-	36,36,36	1.26	3 (8%)	47,47,47	2.27	16 (34%)
22	CLA	b	606	2	69,73,73	2.08	18 (26%)	83,113,113	2.32	31 (37%)
22	CLA	b	617	2	69,73,73	1.99	18 (26%)	83,113,113	2.02	26 (31%)
22	CLA	c	507	3	69,73,73	2.14	19 (27%)	83,113,113	2.43	27 (32%)
22	CLA	d	405	4	69,73,73	2.14	20 (28%)	83,113,113	2.32	30 (36%)
22	CLA	C	507	41	69,73,73	2.38	24 (34%)	83,113,113	2.45	19 (22%)
24	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.37	11 (19%)
24	BCR	d	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.61	10 (17%)
29	DMS	c	536	-	3,3,3	2.69	1 (33%)	3,3,3	1.07	0
29	DMS	o	311	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
29	DMS	b	633	-	3,3,3	2.76	1 (33%)	3,3,3	1.10	0
22	CLA	c	510	3	69,73,73	2.13	19 (27%)	83,113,113	2.56	32 (38%)
29	DMS	v	205	-	3,3,3	2.46	1 (33%)	3,3,3	0.84	0
23	PHO	a	408	-	58,69,69	2.42	15 (25%)	56,99,99	1.66	9 (16%)
24	BCR	c	516	-	41,41,41	1.11	3 (7%)	56,56,56	1.37	8 (14%)
29	DMS	O	311	-	3,3,3	2.64	1 (33%)	3,3,3	1.71	1 (33%)
29	DMS	v	206	-	3,3,3	2.65	1 (33%)	3,3,3	1.12	0
32	HTG	b	627	-	19,19,19	0.98	1 (5%)	23,24,24	2.00	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	409	1	69,73,73	1.85	16 (23%)	83,113,113	2.40	25 (30%)
24	BCR	K	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.36	10 (17%)
31	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.62	4 (7%)
28	LMT	T	102	-	24,24,36	0.57	0	29,29,47	1.55	7 (24%)
29	DMS	b	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.54	0
29	DMS	b	639	-	3,3,3	2.57	1 (33%)	3,3,3	1.52	0
29	DMS	A	417	-	3,3,3	2.02	1 (33%)	3,3,3	0.55	0
29	DMS	B	636	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
29	DMS	V	207	-	3,3,3	2.81	1 (33%)	3,3,3	0.56	0
29	DMS	B	641	-	3,3,3	2.83	1 (33%)	3,3,3	1.00	0
29	DMS	a	420	-	3,3,3	2.81	1 (33%)	3,3,3	1.07	0
22	CLA	b	615	2	69,73,73	1.76	16 (23%)	83,113,113	2.07	29 (34%)
22	CLA	B	609	2	69,73,73	2.06	20 (28%)	83,113,113	2.51	27 (32%)
25	PL9	d	407	-	55,55,55	1.17	9 (16%)	68,69,69	1.47	9 (13%)
22	CLA	C	502	3	69,73,73	2.16	18 (26%)	83,113,113	2.45	27 (32%)
33	DGD	C	517	-	63,63,67	0.95	4 (6%)	77,77,81	1.17	9 (11%)
29	DMS	B	633	-	3,3,3	2.55	1 (33%)	3,3,3	0.98	0
29	DMS	D	418	-	3,3,3	2.59	1 (33%)	3,3,3	1.66	0
29	DMS	C	525	-	3,3,3	2.47	1 (33%)	3,3,3	1.10	0
29	DMS	C	534	-	3,3,3	2.78	1 (33%)	3,3,3	1.01	0
32	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.98	2 (8%)
29	DMS	b	630	-	3,3,3	1.99	1 (33%)	3,3,3	0.40	0
32	HTG	b	601	-	19,19,19	1.08	2 (10%)	23,24,24	1.44	4 (17%)
22	CLA	c	504	3	69,73,73	2.79	21 (30%)	83,113,113	2.33	21 (25%)
28	LMT	m	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.03	3 (10%)
28	LMT	t	102	-	24,24,36	1.12	2 (8%)	29,29,47	1.45	5 (17%)
29	DMS	C	530	-	3,3,3	2.06	1 (33%)	3,3,3	0.70	0
29	DMS	a	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.73	0
34	GOL	c	533	-	5,5,5	0.52	0	5,5,5	0.97	0
29	DMS	V	204	-	3,3,3	2.63	1 (33%)	3,3,3	1.40	1 (33%)
32	HTG	b	602	-	19,19,19	1.11	2 (10%)	23,24,24	1.64	3 (13%)
33	DGD	c	518	-	57,57,67	0.95	4 (7%)	71,71,81	1.09	7 (9%)
29	DMS	A	418	-	3,3,3	2.66	1 (33%)	3,3,3	1.18	0
32	HTG	U	203	-	14,14,19	0.99	1 (7%)	18,19,24	2.78	8 (44%)
22	CLA	b	609	2	69,73,73	1.80	15 (21%)	83,113,113	2.39	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	BCT	D	402[A]	35	2,3,3	0.45	0	2,3,3	0.63	0
24	BCR	y	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.71	14 (25%)
32	HTG	O	302	-	19,19,19	1.64	4 (21%)	23,24,24	1.26	3 (13%)
22	CLA	B	616	2	69,73,73	2.48	22 (31%)	83,113,113	2.40	25 (30%)
29	DMS	C	528	-	3,3,3	2.55	1 (33%)	3,3,3	0.52	0
29	DMS	o	304	-	3,3,3	2.57	1 (33%)	3,3,3	1.49	0
28	LMT	j	102	-	23,23,36	0.89	0	27,27,47	1.94	6 (22%)
31	LHG	d	410	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	5 (9%)
24	BCR	A	409	-	41,41,41	1.44	8 (19%)	56,56,56	1.55	7 (12%)
28	LMT	m	101	-	36,36,36	0.74	0	47,47,47	1.53	10 (21%)
33	DGD	h	101	-	63,63,67	1.20	4 (6%)	77,77,81	1.43	15 (19%)
28	LMT	J	102	-	24,24,36	0.80	1 (4%)	29,29,47	1.23	3 (10%)
22	CLA	D	403	4	69,73,73	1.98	21 (30%)	83,113,113	2.16	22 (26%)
26	LMG	c	520	-	38,38,55	1.29	2 (5%)	46,46,63	1.33	5 (10%)
29	DMS	V	206	-	3,3,3	2.65	1 (33%)	3,3,3	0.79	0
29	DMS	c	535	-	3,3,3	2.61	1 (33%)	3,3,3	0.30	0
29	DMS	O	303	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
22	CLA	a	407	41	69,73,73	2.09	21 (30%)	83,113,113	2.53	24 (28%)
25	PL9	a	411	-	55,55,55	0.97	3 (5%)	68,69,69	2.26	20 (29%)
31	LHG	D	410	-	48,48,48	0.79	3 (6%)	51,54,54	1.07	2 (3%)
29	DMS	V	208	-	3,3,3	2.49	1 (33%)	3,3,3	1.17	1 (33%)
32	HTG	c	523	-	19,19,19	0.70	0	23,24,24	1.49	3 (13%)
22	CLA	b	607	2	69,73,73	1.94	16 (23%)	83,113,113	2.25	24 (28%)
29	DMS	u	203	-	3,3,3	2.54	1 (33%)	3,3,3	1.25	0
28	LMT	M	101	-	36,36,36	0.66	0	47,47,47	1.37	6 (12%)
29	DMS	C	531	-	3,3,3	2.72	1 (33%)	3,3,3	0.72	0
31	LHG	B	621	-	48,48,48	0.83	2 (4%)	51,54,54	1.31	6 (11%)
32	HTG	C	536	-	19,19,19	1.22	2 (10%)	23,24,24	1.82	1 (4%)
32	HTG	B	624	-	19,19,19	1.01	1 (5%)	23,24,24	2.08	2 (8%)
22	CLA	B	614	2	69,73,73	2.03	16 (23%)	83,113,113	2.12	22 (26%)
26	LMG	a	412	-	51,51,55	1.09	3 (5%)	59,59,63	1.05	3 (5%)
22	CLA	B	606	2	69,73,73	2.20	20 (28%)	83,113,113	2.50	23 (27%)
29	DMS	v	207	-	3,3,3	2.99	1 (33%)	3,3,3	1.23	1 (33%)
29	DMS	B	637	-	3,3,3	2.59	1 (33%)	3,3,3	1.10	0
28	LMT	Z	101	-	36,36,36	0.84	2 (5%)	47,47,47	1.46	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DMS	D	419	-	3,3,3	2.73	1 (33%)	3,3,3	0.68	0
29	DMS	u	204	-	3,3,3	2.75	1 (33%)	3,3,3	1.02	0
20	OEX	a	402	41,1,3	0,14,14	-	-	-	-	-
29	DMS	a	417	-	3,3,3	2.82	1 (33%)	3,3,3	1.16	0
32	HTG	B	642	-	18,18,19	1.11	2 (11%)	22,23,24	2.72	10 (45%)
32	HTG	B	628	-	19,19,19	0.49	0	23,24,24	1.76	2 (8%)
33	DGD	C	515	-	63,63,67	1.01	4 (6%)	77,77,81	1.23	7 (9%)
29	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.44	0
24	BCR	b	623	-	41,41,41	1.17	4 (9%)	56,56,56	1.40	9 (16%)
29	DMS	D	416	-	3,3,3	2.65	1 (33%)	3,3,3	0.10	0
22	CLA	A	404	1	69,73,73	1.89	16 (23%)	83,113,113	2.32	25 (30%)
29	DMS	c	530	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
29	DMS	o	305	-	3,3,3	2.67	1 (33%)	3,3,3	0.74	0
34	GOL	D	417	-	5,5,5	0.48	0	5,5,5	0.47	0
32	HTG	c	541	-	15,15,19	1.17	1 (6%)	18,20,24	3.42	6 (33%)
29	DMS	B	638	-	3,3,3	2.31	1 (33%)	3,3,3	1.19	0
22	CLA	c	512	3	69,73,73	2.71	22 (31%)	83,113,113	2.34	23 (27%)
29	DMS	O	304	-	3,3,3	2.65	1 (33%)	3,3,3	0.68	0
28	LMT	b	626	-	25,25,36	0.96	1 (4%)	30,30,47	1.57	3 (10%)
22	CLA	C	511	3	69,73,73	2.43	20 (28%)	83,113,113	2.62	29 (34%)
36	BCT	d	401[A]	35	2,3,3	0.58	0	2,3,3	1.26	0
22	CLA	B	603	2	69,73,73	2.22	16 (23%)	83,113,113	2.22	25 (30%)
22	CLA	B	607	2	69,73,73	2.22	20 (28%)	83,113,113	2.16	26 (31%)
28	LMT	m	103	-	23,23,36	0.88	0	27,27,47	1.70	2 (7%)
28	LMT	C	520	-	36,36,36	0.92	1 (2%)	47,47,47	2.14	10 (21%)
22	CLA	C	504	41	69,73,73	2.27	19 (27%)	83,113,113	2.20	19 (22%)
37	HEM	F	101	5,6	50,50,50	1.93	9 (18%)	66,82,82	1.67	10 (15%)
23	PHO	D	404	-	58,69,69	2.69	17 (29%)	56,99,99	1.61	12 (21%)
23	PHO	A	407	-	58,69,69	2.36	16 (27%)	56,99,99	2.01	14 (25%)
24	BCR	B	620	-	41,41,41	1.24	3 (7%)	56,56,56	1.34	9 (16%)
29	DMS	B	632	-	3,3,3	2.43	1 (33%)	3,3,3	1.58	1 (33%)
32	HTG	C	535	-	8,8,19	0.55	0	7,7,24	1.05	1 (14%)
29	DMS	o	309	-	3,3,3	2.65	1 (33%)	3,3,3	1.45	0
22	CLA	C	508	3	69,73,73	2.13	20 (28%)	83,113,113	2.19	22 (26%)
22	CLA	d	403	41	69,73,73	1.92	19 (27%)	83,113,113	2.41	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PL9	D	407	-	55,55,55	1.11	6 (10%)	68,69,69	1.47	7 (10%)
28	LMT	l	101	-	24,24,36	0.83	1 (4%)	29,29,47	0.97	1 (3%)
29	DMS	B	639	-	3,3,3	2.59	1 (33%)	3,3,3	0.95	0
29	DMS	e	105	-	3,3,3	2.74	1 (33%)	3,3,3	1.02	0
22	CLA	B	613	2	69,73,73	2.03	16 (23%)	83,113,113	2.20	23 (27%)
22	CLA	d	402	4	69,73,73	1.85	19 (27%)	83,113,113	1.99	25 (30%)
24	BCR	b	621	-	41,41,41	0.87	1 (2%)	56,56,56	1.47	9 (16%)
29	DMS	o	303	-	3,3,3	1.94	1 (33%)	3,3,3	0.78	0
33	DGD	c	519	-	63,63,67	1.04	4 (6%)	77,77,81	1.38	11 (14%)
22	CLA	B	604	2	69,73,73	1.90	18 (26%)	83,113,113	2.75	32 (38%)
24	BCR	a	410	-	41,41,41	1.05	4 (9%)	56,56,56	1.10	5 (8%)
29	DMS	C	529	-	3,3,3	2.64	1 (33%)	3,3,3	0.81	0
31	LHG	b	624	-	48,48,48	0.75	2 (4%)	51,54,54	1.10	5 (9%)
29	DMS	c	531	-	3,3,3	2.64	1 (33%)	3,3,3	0.66	0
34	GOL	b	636	-	5,5,5	0.09	0	5,5,5	0.40	0
22	CLA	b	616	2	69,73,73	2.13	21 (30%)	83,113,113	2.56	27 (32%)
29	DMS	A	416	-	3,3,3	2.74	1 (33%)	3,3,3	1.01	0
31	LHG	f	102	-	45,45,48	1.08	2 (4%)	48,51,54	1.07	5 (10%)
22	CLA	b	610	2	69,73,73	2.55	19 (27%)	83,113,113	2.40	25 (30%)
29	DMS	b	632	-	3,3,3	2.62	1 (33%)	3,3,3	0.90	0
22	CLA	C	505	3	69,73,73	2.16	22 (31%)	83,113,113	2.17	22 (26%)
26	LMG	c	521	-	51,51,55	1.15	3 (5%)	59,59,63	1.12	7 (11%)
29	DMS	B	634	-	3,3,3	2.62	1 (33%)	3,3,3	0.54	0
24	BCR	B	618	-	41,41,41	0.91	0	56,56,56	1.34	9 (16%)
29	DMS	B	640	-	3,3,3	3.00	1 (33%)	3,3,3	1.33	1 (33%)
29	DMS	c	528	-	3,3,3	2.31	1 (33%)	3,3,3	1.49	1 (33%)
24	BCR	D	406	-	41,41,41	1.40	7 (17%)	56,56,56	1.92	15 (26%)
29	DMS	v	203	-	3,3,3	2.51	1 (33%)	3,3,3	0.76	0
32	HTG	c	524	-	8,8,19	0.55	0	7,7,24	1.33	1 (14%)
36	BCT	D	402[B]	35	2,3,3	0.63	0	2,3,3	0.78	0
28	LMT	z	101	-	33,33,36	8.08	2 (6%)	44,44,47	2.76	11 (25%)
29	DMS	O	307	-	3,3,3	2.72	1 (33%)	3,3,3	0.40	0
29	DMS	B	631	-	3,3,3	2.87	1 (33%)	3,3,3	0.91	0
33	DGD	d	408	-	48,48,67	1.37	5 (10%)	56,56,81	1.58	8 (14%)
20	OEX	A	401	41,1,3	0,14,14	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	513	3	69,73,73	2.71	20 (28%)	83,113,113	2.23	26 (31%)
24	BCR	B	619	-	41,41,41	1.30	5 (12%)	56,56,56	1.43	7 (12%)
34	GOL	C	533	-	5,5,5	0.54	0	5,5,5	1.67	1 (20%)
29	DMS	o	308	-	3,3,3	2.81	1 (33%)	3,3,3	0.41	0
22	CLA	B	602	41	69,73,73	2.41	23 (33%)	83,113,113	2.27	30 (36%)
29	DMS	o	310	-	3,3,3	2.89	1 (33%)	3,3,3	1.04	0
22	CLA	C	506	3	69,73,73	2.20	18 (26%)	83,113,113	2.46	24 (28%)
29	DMS	V	205	-	3,3,3	2.70	1 (33%)	3,3,3	0.96	0
29	DMS	a	416	-	3,3,3	2.85	1 (33%)	3,3,3	1.15	0
29	DMS	b	635	-	3,3,3	2.89	1 (33%)	3,3,3	0.94	0
22	CLA	A	406	41	69,73,73	1.75	20 (28%)	83,113,113	2.26	27 (32%)
22	CLA	b	608	2	69,73,73	2.18	20 (28%)	83,113,113	2.51	29 (34%)
29	DMS	D	420	-	3,3,3	2.61	1 (33%)	3,3,3	0.95	0
29	DMS	b	631	-	3,3,3	2.63	1 (33%)	3,3,3	0.57	0
40	HEC	v	202	16	50,50,50	1.88	11 (22%)	68,82,82	1.67	11 (16%)
22	CLA	C	503	3	69,73,73	2.11	19 (27%)	83,113,113	2.34	27 (32%)
28	LMT	c	522	-	36,36,36	0.98	1 (2%)	47,47,47	1.92	10 (21%)
32	HTG	d	413	-	16,16,19	0.98	1 (6%)	20,21,24	3.85	6 (30%)
33	DGD	c	517	-	63,63,67	1.05	3 (4%)	77,77,81	1.06	5 (6%)
29	DMS	C	526	-	3,3,3	2.76	1 (33%)	3,3,3	1.19	0
26	LMG	C	518	-	49,49,55	1.07	2 (4%)	57,57,63	1.25	7 (12%)
22	CLA	c	508	41	69,73,73	2.16	20 (28%)	83,113,113	2.46	26 (31%)
29	DMS	d	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.95	0
31	LHG	E	101	-	48,48,48	1.04	2 (4%)	51,54,54	0.94	2 (3%)
31	LHG	e	101	-	37,37,48	1.12	2 (5%)	40,42,54	0.95	2 (5%)
29	DMS	O	305	-	3,3,3	2.90	1 (33%)	3,3,3	1.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	615	2	-	11/39/115/115	-
22	CLA	b	614	41	-	3/39/115/115	-
22	CLA	c	506	3	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	T	101	-	-	4/29/63/63	0/2/2/2
32	HTG	B	629	-	-	1/10/30/30	0/1/1/1
25	PL9	A	410	-	-	10/53/73/73	0/1/1/1
26	LMG	D	412	39	-	12/42/62/70	0/1/1/1
38	RRX	h	102	-	-	0/29/65/65	0/2/2/2
26	LMG	B	622	-	-	12/46/66/70	0/1/1/1
22	CLA	b	613	2	-	2/39/115/115	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
22	CLA	A	408	1	-	15/39/115/115	-
26	LMG	d	412	39	-	9/42/62/70	0/1/1/1
32	HTG	b	640	-	-	4/8/28/30	0/1/1/1
22	CLA	c	513	3	-	10/39/115/115	-
31	LHG	F	103	-	-	15/42/42/53	-
31	LHG	D	409	-	-	10/53/53/53	-
26	LMG	A	411	-	-	23/46/66/70	0/1/1/1
22	CLA	b	611	41	-	5/39/115/115	-
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
22	CLA	b	620	2	-	15/39/115/115	-
22	CLA	b	605	41	-	17/39/115/115	-
22	CLA	c	503	3	-	7/39/115/115	-
22	CLA	a	406	1	-	4/39/115/115	-
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
22	CLA	B	610	2	-	1/39/115/115	-
22	CLA	c	509	3	-	4/39/115/115	-
22	CLA	c	502	3	-	6/39/115/115	-
32	HTG	v	208	-	-	3/7/27/30	0/1/1/1
23	PHO	d	404	-	-	1/37/103/103	0/5/6/6
22	CLA	C	510	3	-	9/39/115/115	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
33	DGD	D	408	-	-	20/39/59/95	0/1/1/2
28	LMT	M	102	-	-	6/15/35/61	0/1/1/2
22	CLA	B	605	2	-	9/39/115/115	-
32	HTG	o	301	-	-	4/10/30/30	0/1/1/1
22	CLA	D	405	4	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	512	3	-	7/39/115/115	-
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
28	LMT	A	415	-	-	12/21/61/61	0/2/2/2
22	CLA	C	509	3	-	8/39/115/115	-
22	CLA	b	619	2	-	5/39/115/115	-
22	CLA	B	612	2	-	3/39/115/115	-
22	CLA	C	501	3	-	4/39/115/115	-
31	LHG	d	411	-	-	11/48/48/53	-
34	GOL	e	104	-	-	1/4/4/4	-
22	CLA	b	618	2	-	13/39/115/115	-
26	LMG	C	519	-	-	13/43/63/70	0/1/1/1
37	HEM	f	101	5,6	-	4/14/54/54	-
22	CLA	c	505	41	-	5/39/115/115	-
31	LHG	D	411	-	-	14/48/48/53	-
22	CLA	B	617	2	-	10/39/115/115	-
33	DGD	H	101	-	-	12/51/91/95	0/2/2/2
22	CLA	B	608	41	-	6/39/115/115	-
32	HTG	V	202	-	-	3/10/30/30	0/1/1/1
33	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	c	511	3	-	9/39/115/115	-
22	CLA	b	612	2	-	2/39/115/115	-
28	LMT	B	623	-	-	7/21/61/61	0/2/2/2
28	LMT	F	102	-	-	9/15/35/61	0/1/1/2
32	HTG	C	521	-	-	3/10/30/30	0/1/1/1
32	HTG	D	413	-	-	2/7/27/30	0/1/1/1
22	CLA	B	611	41	-	3/39/115/115	-
22	CLA	c	514	3	-	14/39/115/115	-
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
26	LMG	b	625	-	-	14/44/64/70	0/1/1/1
22	CLA	A	405	41	-	6/39/115/115	-
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
32	HTG	B	624	-	-	3/10/30/30	0/1/1/1
28	LMT	a	401	-	-	9/21/61/61	0/2/2/2
22	CLA	b	606	2	-	6/39/115/115	-
22	CLA	b	617	2	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	3	-	7/39/115/115	-
22	CLA	d	405	4	-	12/39/115/115	-
22	CLA	C	507	41	-	8/39/115/115	-
24	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
24	BCR	d	406	-	-	2/29/63/63	0/2/2/2
22	CLA	c	510	3	-	11/39/115/115	-
23	PHO	a	408	-	-	5/37/103/103	0/5/6/6
24	BCR	c	516	-	-	0/29/63/63	0/2/2/2
32	HTG	b	627	-	-	6/10/30/30	0/1/1/1
22	CLA	a	409	1	-	12/39/115/115	-
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
31	LHG	d	409	-	-	11/53/53/53	-
28	LMT	T	102	-	-	6/15/35/61	0/1/1/2
22	CLA	b	615	2	-	5/39/115/115	-
22	CLA	B	609	2	-	2/39/115/115	-
25	PL9	d	407	-	-	3/53/73/73	0/1/1/1
22	CLA	C	502	3	-	6/39/115/115	-
33	DGD	C	517	-	-	13/51/91/95	0/2/2/2
32	HTG	b	601	-	-	4/10/30/30	0/1/1/1
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
34	GOL	c	533	-	-	4/4/4/4	-
22	CLA	c	504	3	-	2/39/115/115	-
28	LMT	m	102	-	-	8/15/35/61	0/1/1/2
28	LMT	t	102	-	-	9/15/35/61	0/1/1/2
32	HTG	b	602	-	-	1/10/30/30	0/1/1/1
33	DGD	c	518	-	-	15/45/85/95	0/2/2/2
32	HTG	U	203	-	-	2/5/25/30	0/1/1/1
22	CLA	b	609	2	-	2/39/115/115	-
24	BCR	y	101	-	-	2/29/63/63	0/2/2/2
32	HTG	O	302	-	-	4/10/30/30	0/1/1/1
22	CLA	B	616	2	-	9/39/115/115	-
31	LHG	d	410	-	-	7/53/53/53	-
28	LMT	j	102	-	-	8/15/31/61	0/1/1/2
24	BCR	A	409	-	-	1/29/63/63	0/2/2/2
28	LMT	m	101	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	h	101	-	-	15/51/91/95	0/2/2/2
28	LMT	J	102	-	-	8/15/35/61	0/1/1/2
22	CLA	D	403	4	-	1/39/115/115	-
26	LMG	c	520	-	-	9/33/53/70	0/1/1/1
22	CLA	a	407	41	-	11/39/115/115	-
25	PL9	a	411	-	-	10/53/73/73	0/1/1/1
31	LHG	D	410	-	-	6/53/53/53	-
32	HTG	c	523	-	-	5/10/30/30	0/1/1/1
22	CLA	b	607	2	-	2/39/115/115	-
28	LMT	M	101	-	-	4/21/61/61	0/2/2/2
31	LHG	B	621	-	-	14/53/53/53	-
32	HTG	C	536	-	-	3/10/30/30	0/1/1/1
22	CLA	B	614	2	-	8/39/115/115	-
26	LMG	a	412	-	-	14/46/66/70	0/1/1/1
22	CLA	B	606	2	-	7/39/115/115	-
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
32	HTG	B	642	-	-	5/9/29/30	0/1/1/1
32	HTG	B	628	-	-	3/10/30/30	0/1/1/1
33	DGD	C	515	-	-	16/51/91/95	0/2/2/2
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
22	CLA	A	404	1	-	5/39/115/115	-
34	GOL	D	417	-	-	3/4/4/4	-
32	HTG	c	541	-	-	3/6/26/30	0/1/1/1
22	CLA	c	512	3	-	1/39/115/115	-
28	LMT	b	626	-	-	11/17/37/61	0/1/1/2
22	CLA	C	511	3	-	1/39/115/115	-
22	CLA	B	607	2	-	8/39/115/115	-
22	CLA	B	603	2	-	6/39/115/115	-
28	LMT	m	103	-	-	6/15/31/61	0/1/1/2
28	LMT	C	520	-	1/1/10/10	13/21/61/61	0/2/2/2
22	CLA	C	504	41	-	9/39/115/115	-
37	HEM	F	101	5,6	-	3/14/54/54	-
23	PHO	D	404	-	-	2/37/103/103	0/5/6/6
23	PHO	A	407	-	-	2/37/103/103	0/5/6/6
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	C	535	-	-	3/6/6/30	-
22	CLA	C	508	3	-	4/39/115/115	-
22	CLA	d	403	41	-	5/39/115/115	-
25	PL9	D	407	-	-	1/53/73/73	0/1/1/1
28	LMT	l	101	-	-	6/15/35/61	0/1/1/2
33	DGD	c	519	-	-	11/51/91/95	0/2/2/2
22	CLA	B	613	2	-	3/39/115/115	-
22	CLA	d	402	4	-	4/39/115/115	-
24	BCR	b	621	-	-	2/29/63/63	0/2/2/2
22	CLA	B	604	2	-	4/39/115/115	-
24	BCR	a	410	-	-	0/29/63/63	0/2/2/2
34	GOL	b	636	-	-	2/4/4/4	-
31	LHG	b	624	-	-	21/53/53/53	-
22	CLA	b	616	2	-	4/39/115/115	-
31	LHG	f	102	-	-	16/50/50/53	-
22	CLA	b	610	2	-	9/39/115/115	-
22	CLA	C	505	3	-	3/39/115/115	-
26	LMG	c	521	-	-	20/46/66/70	0/1/1/1
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	BCR	D	406	-	-	2/29/63/63	0/2/2/2
32	HTG	c	524	-	-	3/6/6/30	-
28	LMT	z	101	-	1/1/10/10	6/18/58/61	0/2/2/2
33	DGD	d	408	-	-	12/42/62/95	0/1/1/2
22	CLA	C	513	3	-	12/39/115/115	-
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
34	GOL	C	533	-	-	2/4/4/4	-
22	CLA	B	602	41	-	14/39/115/115	-
22	CLA	C	506	3	-	10/39/115/115	-
22	CLA	A	406	41	-	4/39/115/115	-
22	CLA	b	608	2	-	4/39/115/115	-
40	HEC	v	202	16	1/1/3/7	6/14/54/54	-
22	CLA	C	503	3	-	3/39/115/115	-
28	LMT	c	522	-	-	6/21/61/61	0/2/2/2
32	HTG	d	413	-	-	2/7/27/30	0/1/1/1
33	DGD	c	517	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	C	518	-	-	14/44/64/70	0/1/1/1
22	CLA	c	508	41	-	6/39/115/115	-
31	LHG	E	101	-	-	29/53/53/53	-
31	LHG	e	101	-	-	18/41/41/53	-

The worst 5 of 1774 bond length outliers are listed below:

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

The worst 5 of 2646 bond angle outliers are listed below:

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

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	C	520	LMT	C1B
28	z	101	LMT	C1B
40	V	201	HEC	NA
40	v	202	HEC	NA

5 of 1218 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	CHA-CBD-CGD-O1D
22	A	408	CLA	C4-C3-C5-C6
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	C11-C10-C8-C9
22	B	606	CLA	C4-C3-C5-C6

There are no ring outliers.

137 monomers are involved in 222 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	615	CLA	2	0
22	b	614	CLA	3	0
24	T	101	BCR	2	0
29	v	204	DMS	1	0
25	A	410	PL9	5	0
38	h	102	RRX	5	0
26	B	622	LMG	1	0
22	b	613	CLA	2	0
29	O	306	DMS	1	0
38	H	102	RRX	2	0
22	A	408	CLA	1	0
32	b	640	HTG	1	0
22	c	513	CLA	1	0
29	b	634	DMS	1	0
29	o	306	DMS	2	0
22	b	611	CLA	2	0
24	b	622	BCR	2	0
22	b	605	CLA	2	0
22	c	503	CLA	1	0
22	a	406	CLA	3	0
24	c	515	BCR	5	0
22	B	610	CLA	1	0
29	b	638	DMS	1	0
29	c	529	DMS	4	0
29	O	310	DMS	1	0
23	d	404	PHO	1	0
22	C	510	CLA	1	0
24	t	101	BCR	4	0
22	B	605	CLA	1	0
32	o	301	HTG	2	0
22	D	405	CLA	1	0
22	C	512	CLA	2	0
24	k	101	BCR	2	0
28	A	415	LMT	4	0
29	D	415	DMS	3	0
22	C	509	CLA	3	0
22	B	612	CLA	2	0
29	c	538	DMS	1	0
22	b	618	CLA	1	0
22	c	505	CLA	1	0
22	B	617	CLA	3	0
22	B	608	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	413	HTG	1	0
22	B	611	CLA	2	0
22	c	514	CLA	2	0
24	C	514	BCR	1	0
26	b	625	LMG	1	0
22	A	405	CLA	2	0
28	a	401	LMT	2	0
22	b	617	CLA	2	0
22	d	405	CLA	4	0
22	C	507	CLA	1	0
24	d	406	BCR	4	0
22	c	510	CLA	3	0
29	v	205	DMS	2	0
24	c	516	BCR	1	0
29	v	206	DMS	2	0
24	K	101	BCR	2	0
31	d	409	LHG	1	0
29	b	639	DMS	1	0
29	B	636	DMS	1	0
29	B	641	DMS	1	0
22	C	502	CLA	2	0
29	B	633	DMS	3	0
29	D	418	DMS	1	0
29	C	525	DMS	4	0
29	C	534	DMS	1	0
29	b	630	DMS	1	0
32	b	601	HTG	1	0
22	c	504	CLA	2	0
34	c	533	GOL	1	0
32	b	602	HTG	2	0
33	c	518	DGD	1	0
22	b	609	CLA	3	0
24	y	101	BCR	1	0
22	B	616	CLA	2	0
29	o	304	DMS	1	0
28	j	102	LMT	1	0
24	A	409	BCR	1	0
28	m	101	LMT	3	0
22	D	403	CLA	1	0
25	a	411	PL9	6	0
29	V	208	DMS	2	0
22	b	607	CLA	1	0

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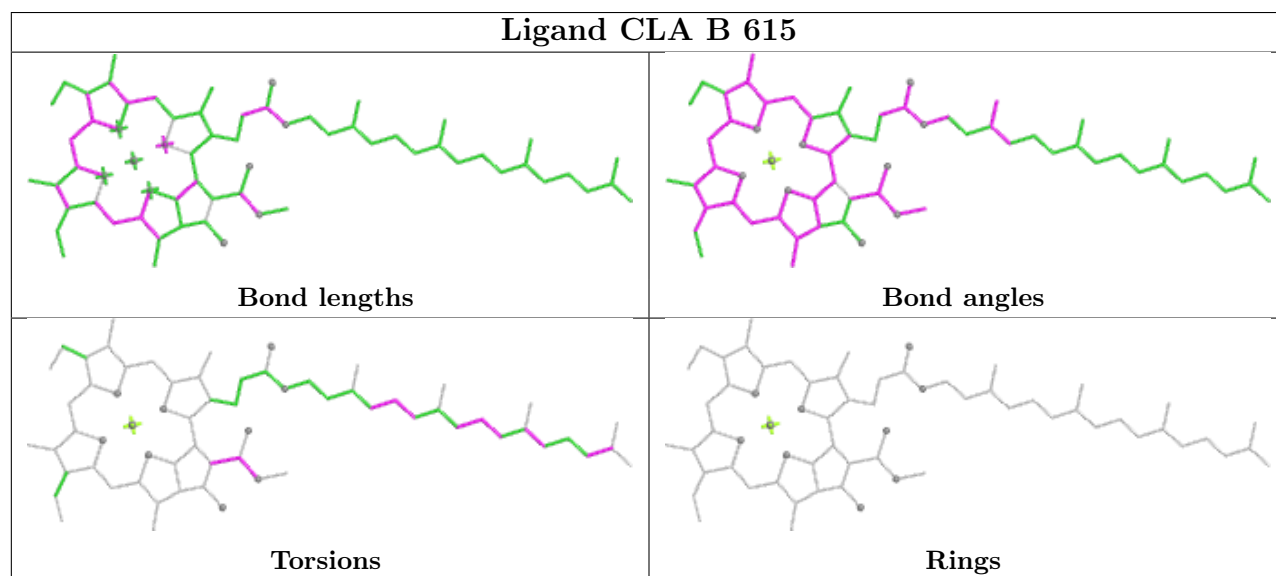
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32	C	536	HTG	1	0
22	B	614	CLA	4	0
26	a	412	LMG	2	0
22	B	606	CLA	2	0
29	v	207	DMS	2	0
29	B	637	DMS	1	0
29	u	204	DMS	1	0
32	B	642	HTG	2	0
33	C	515	DGD	2	0
29	c	534	DMS	2	0
24	b	623	BCR	3	0
29	D	416	DMS	2	0
22	A	404	CLA	3	0
22	c	512	CLA	1	0
29	O	304	DMS	2	0
28	C	520	LMT	1	0
37	F	101	HEM	1	0
23	D	404	PHO	1	0
24	B	620	BCR	1	0
29	B	632	DMS	1	0
29	o	309	DMS	1	0
22	d	403	CLA	3	0
25	D	407	PL9	1	0
29	B	639	DMS	2	0
29	e	105	DMS	1	0
22	d	402	CLA	1	0
24	b	621	BCR	1	0
22	B	604	CLA	1	0
29	c	531	DMS	3	0
29	A	416	DMS	1	0
22	b	610	CLA	1	0
22	C	505	CLA	2	0
26	c	521	LMG	1	0
24	B	618	BCR	1	0
29	c	528	DMS	3	0
24	D	406	BCR	2	0
29	v	203	DMS	1	0
29	O	307	DMS	1	0
29	B	631	DMS	4	0
22	C	513	CLA	2	0
24	B	619	BCR	5	0

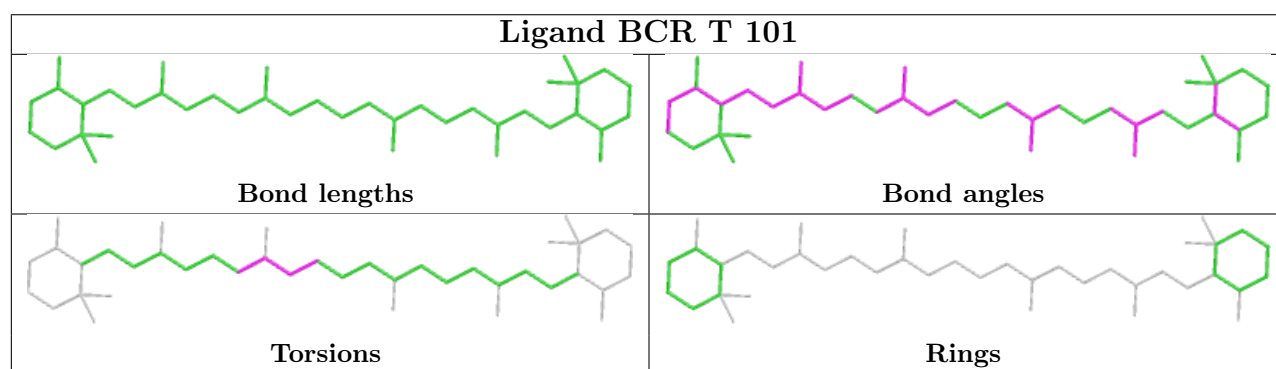
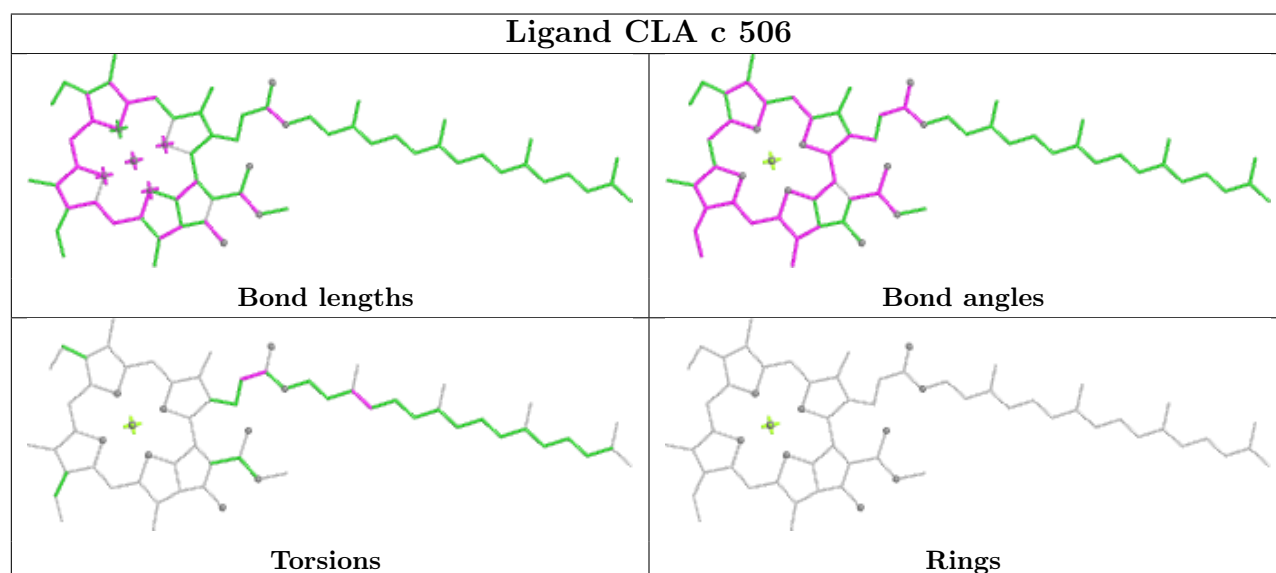
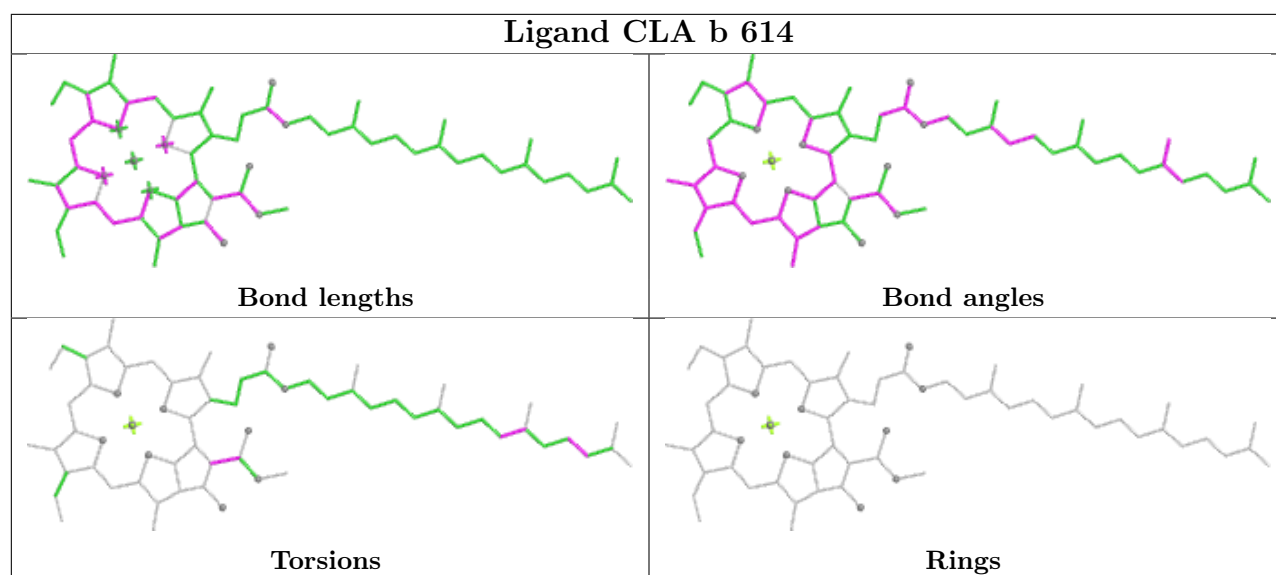
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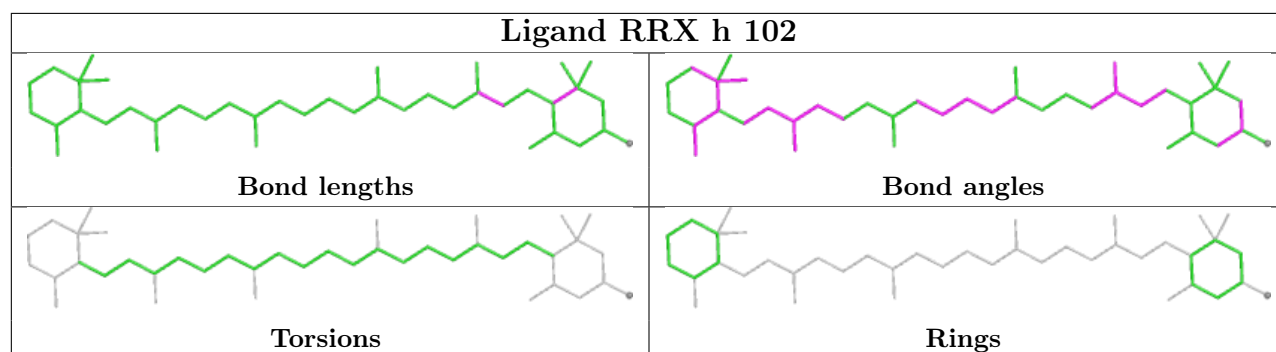
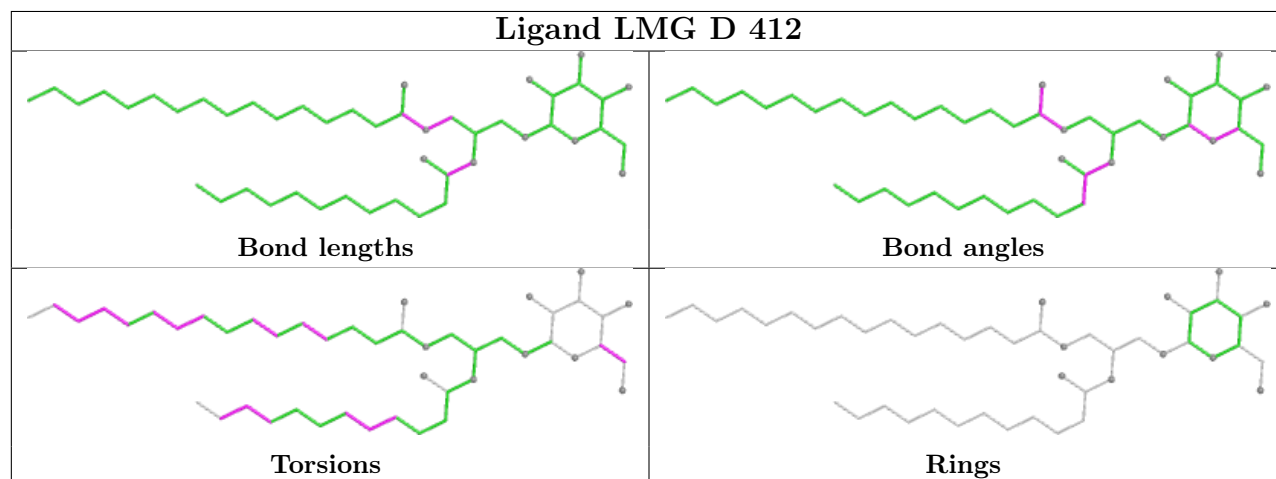
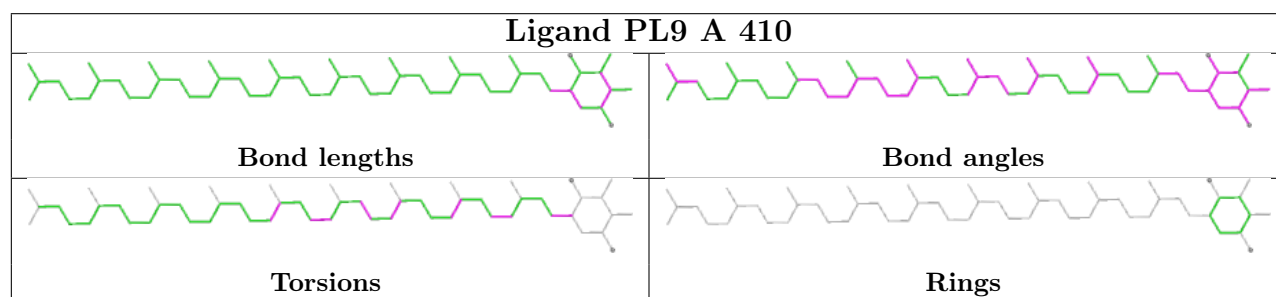
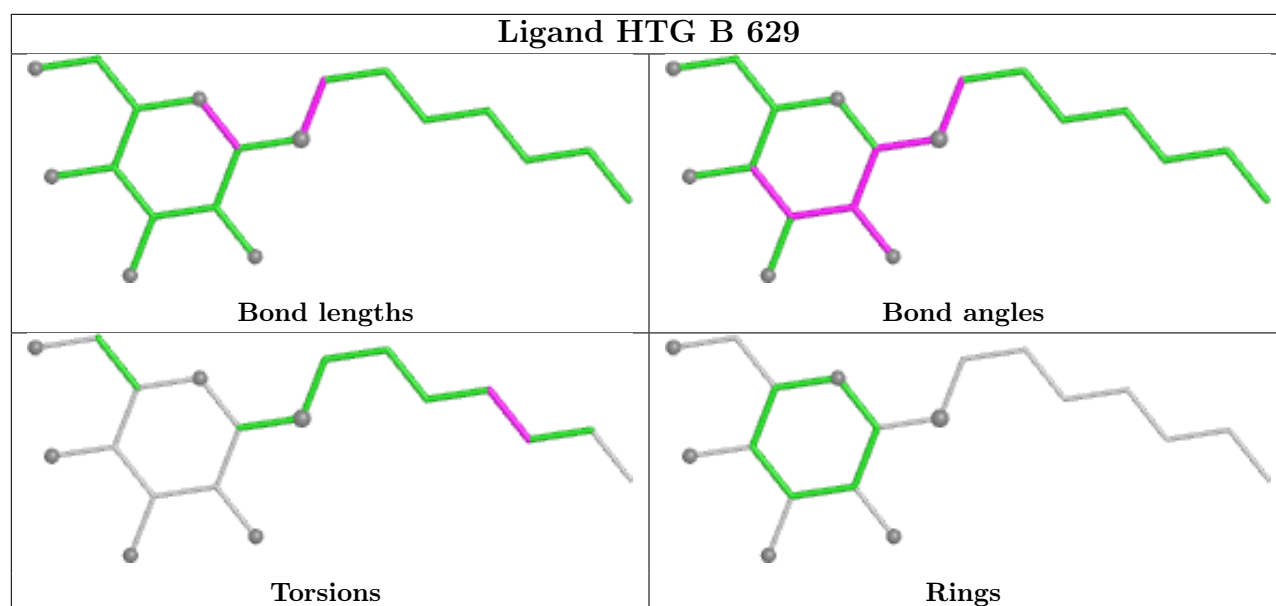
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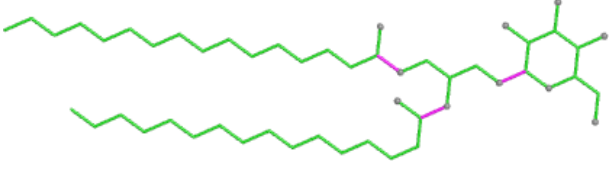
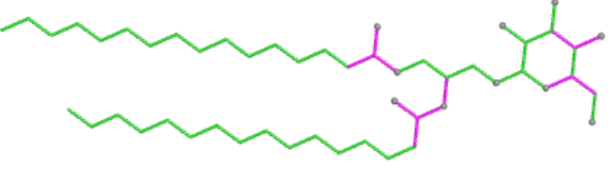
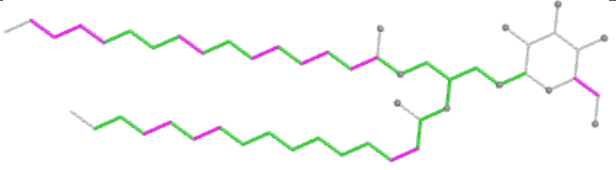
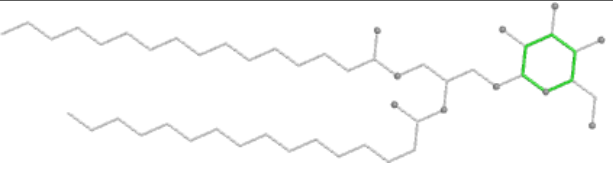
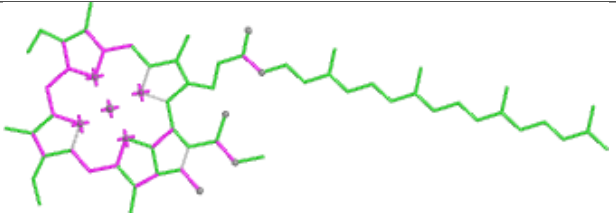
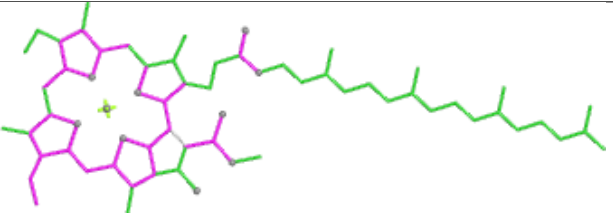
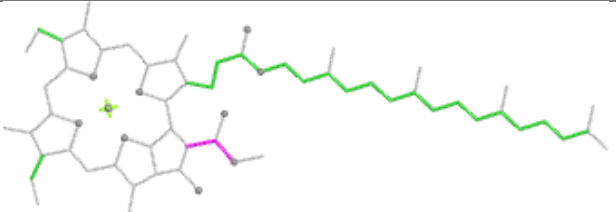
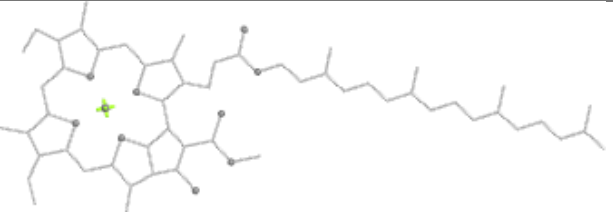
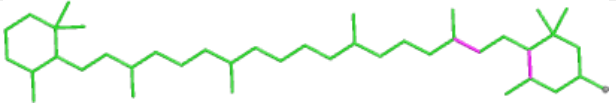
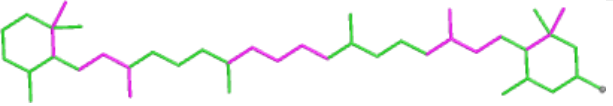
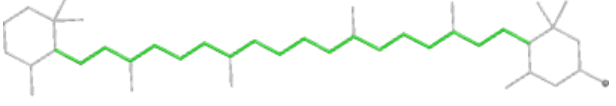
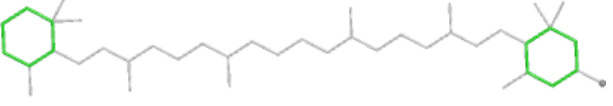
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	533	GOL	1	0
22	B	602	CLA	1	0
29	o	310	DMS	1	0
22	C	506	CLA	3	0
29	V	205	DMS	1	0
22	A	406	CLA	2	0
22	b	608	CLA	2	0
22	C	503	CLA	1	0
33	c	517	DGD	1	0
29	C	526	DMS	2	0
22	c	508	CLA	1	0

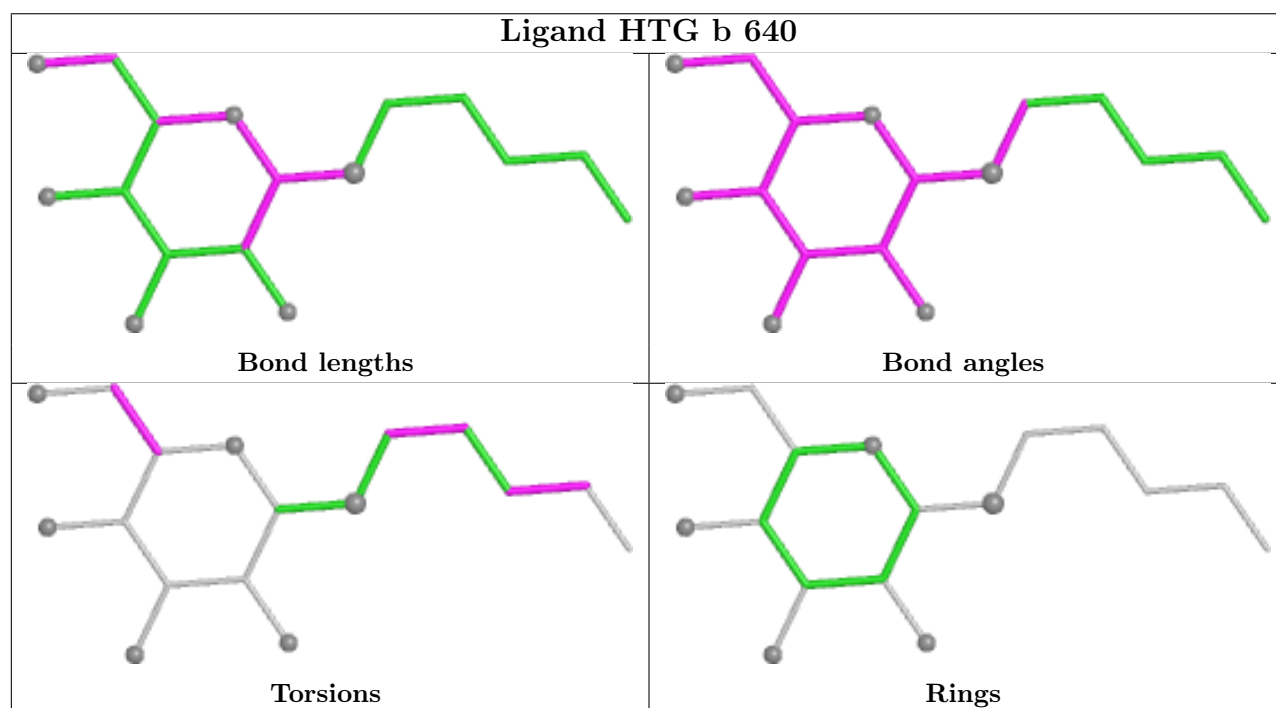
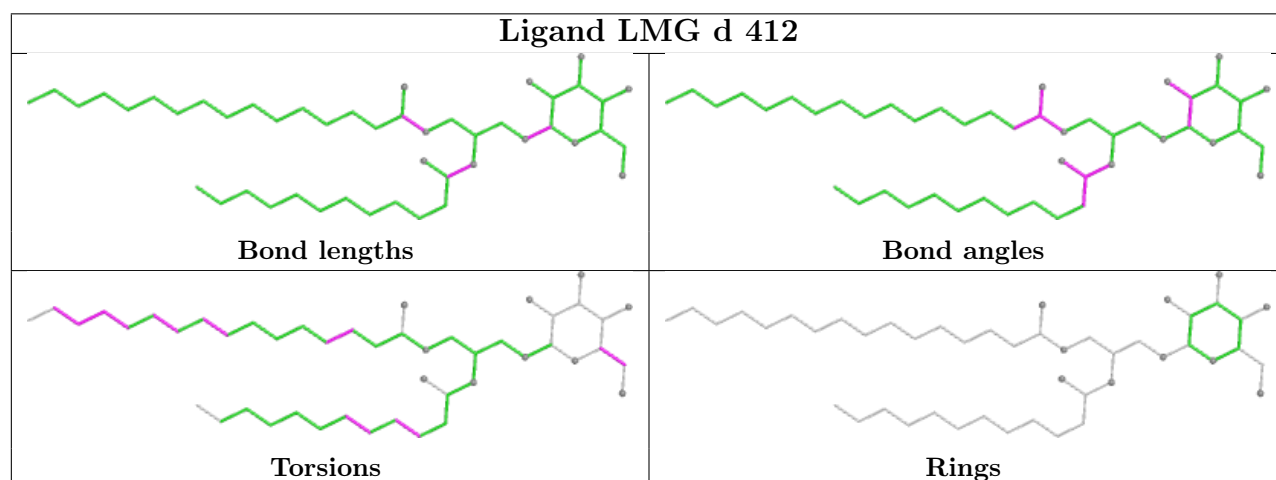
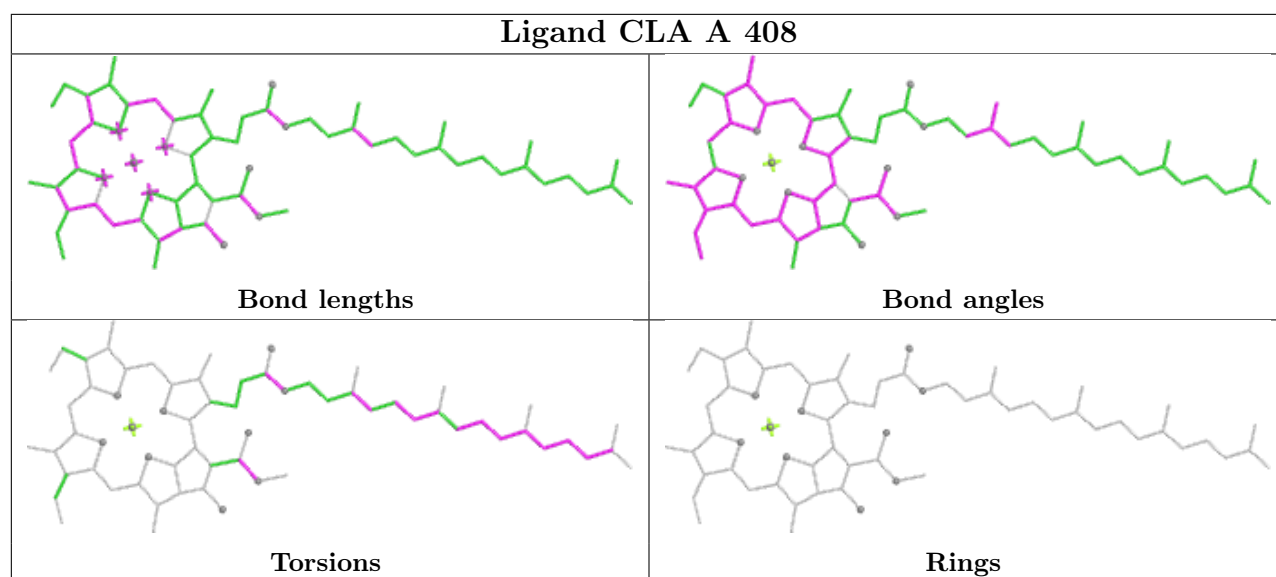
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



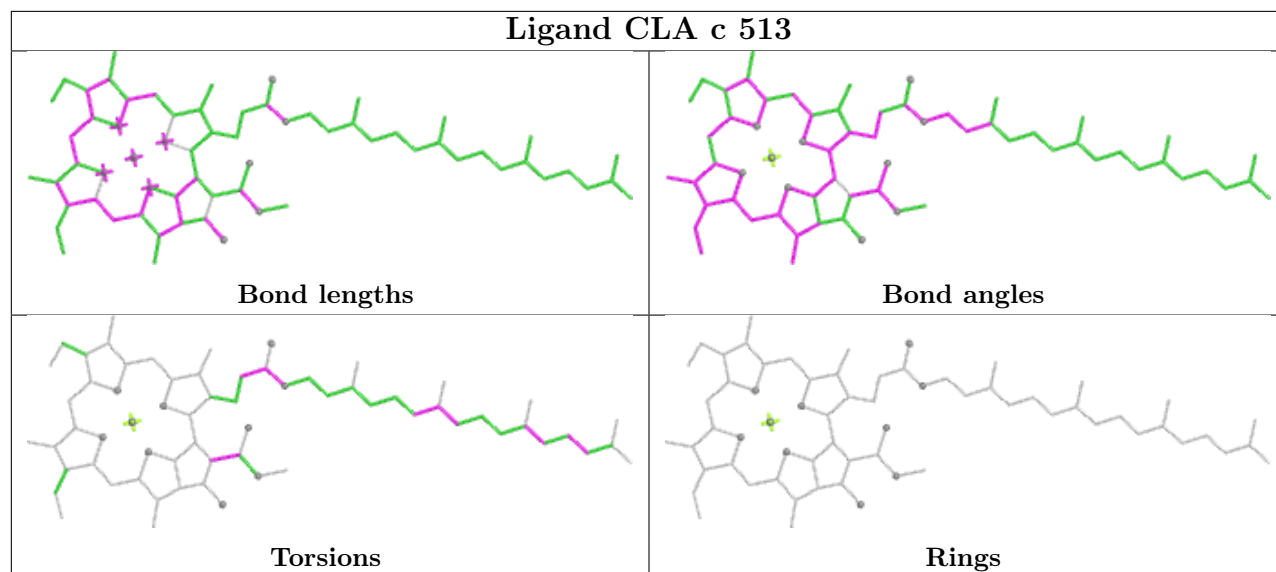




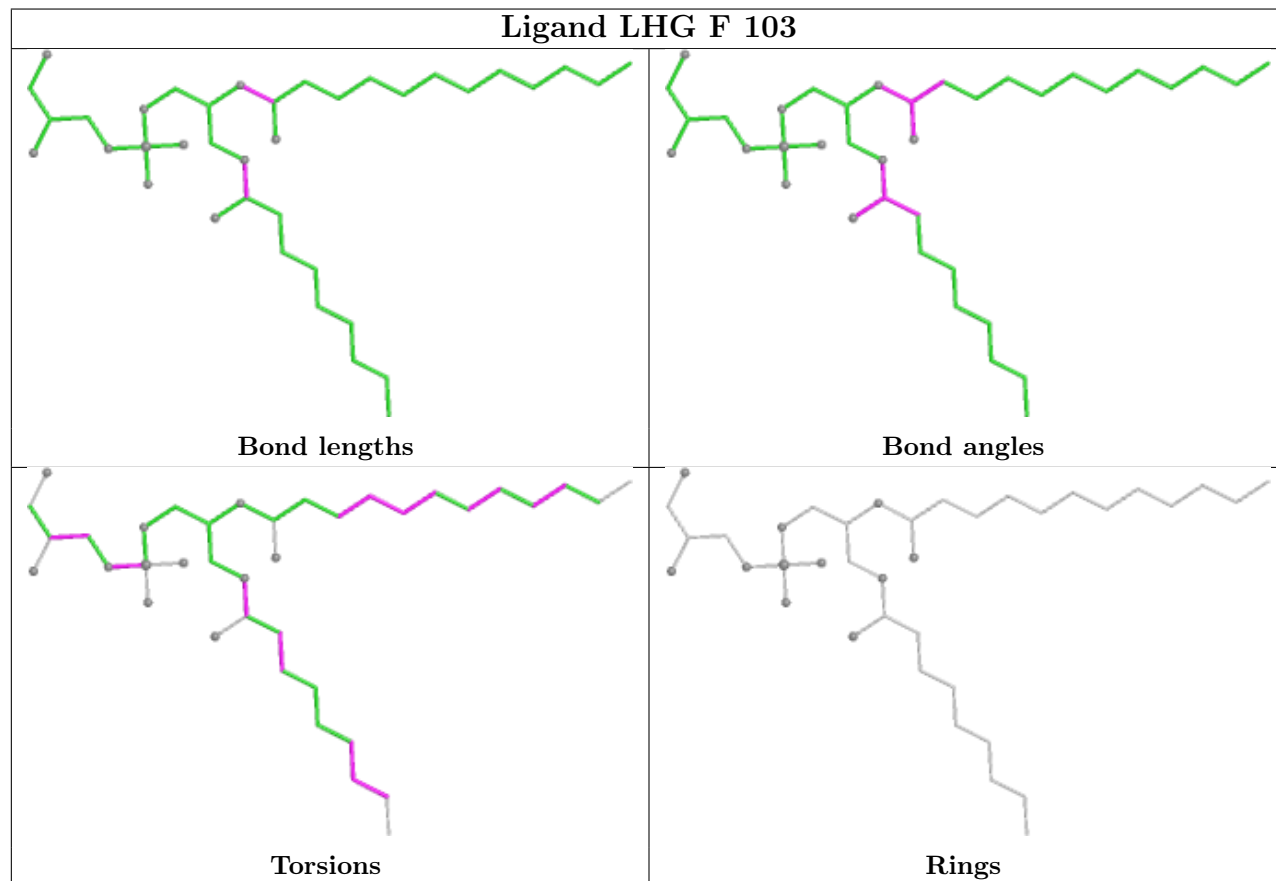
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

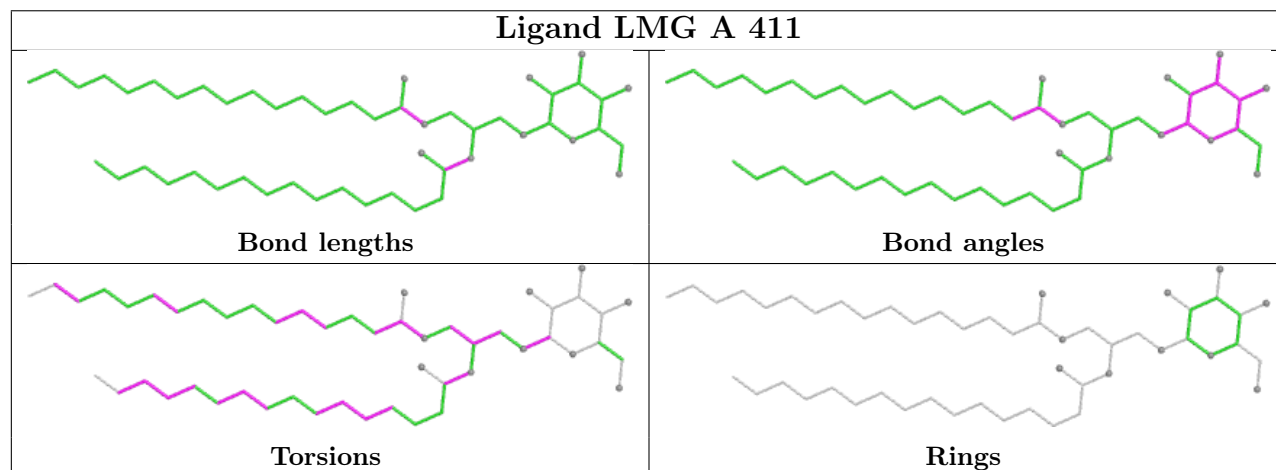
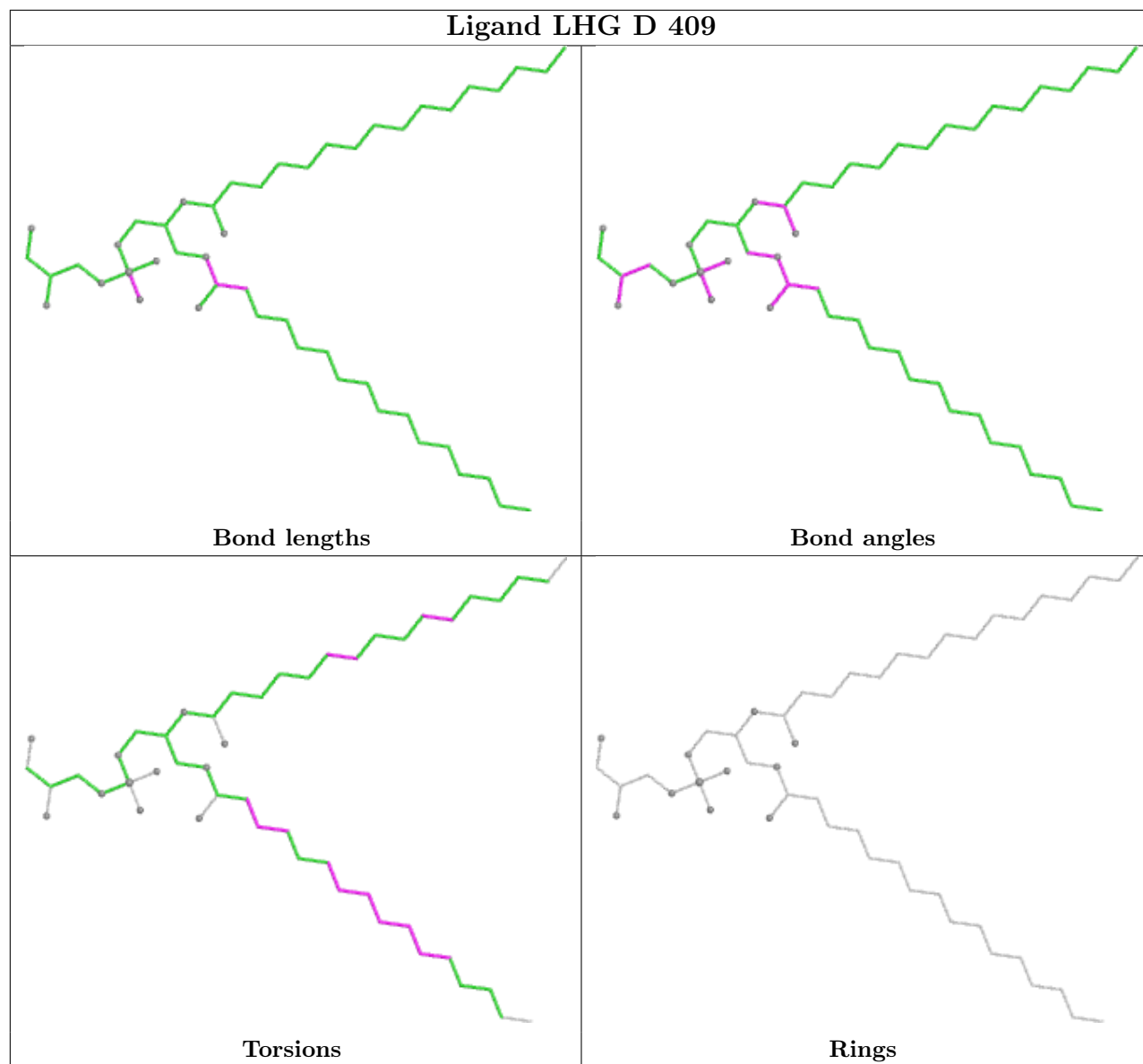


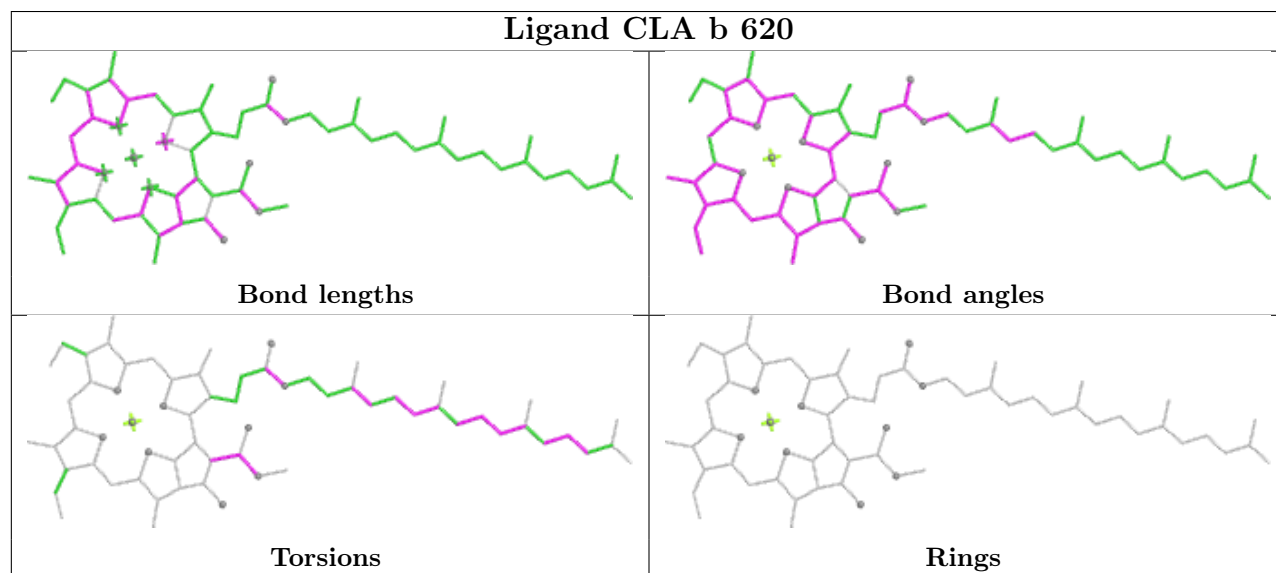
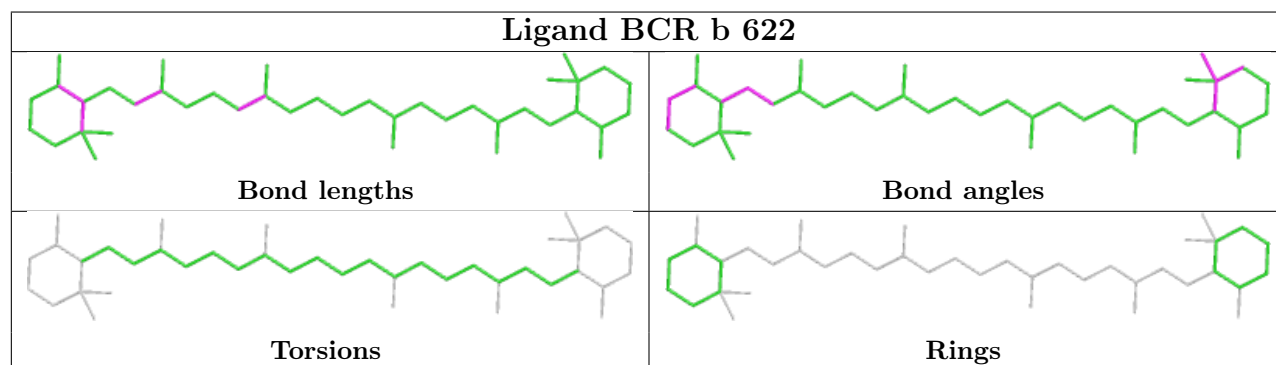
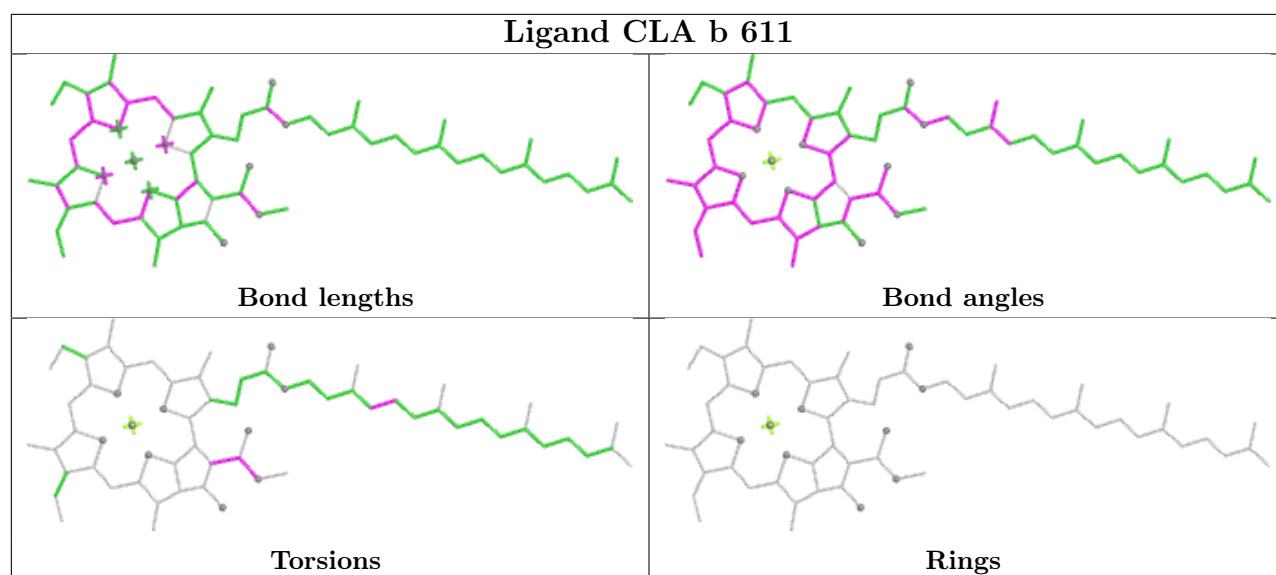
Ligand CLA c 513

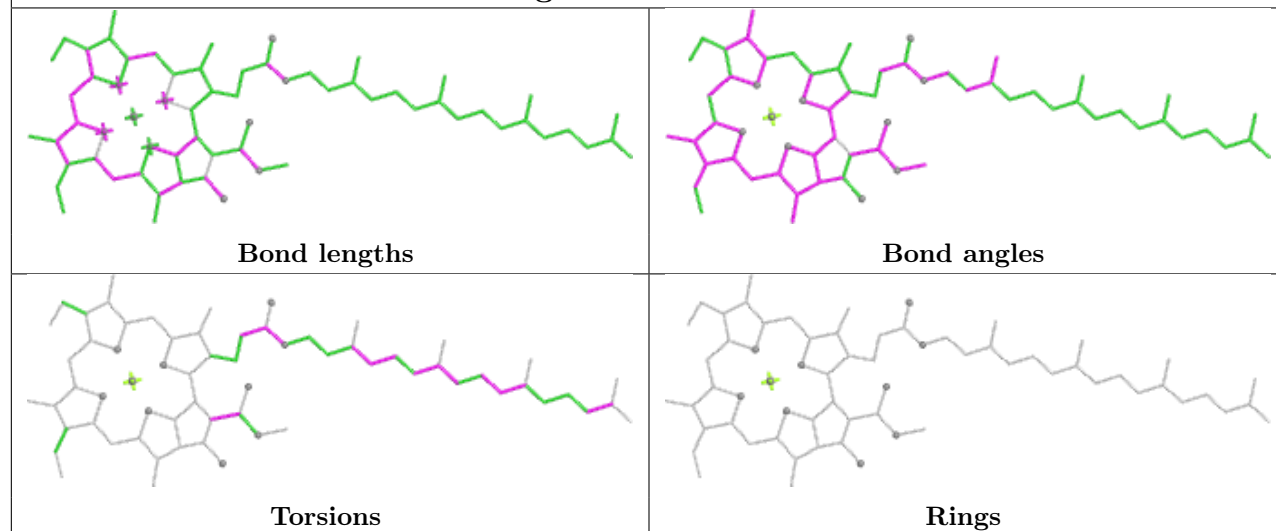
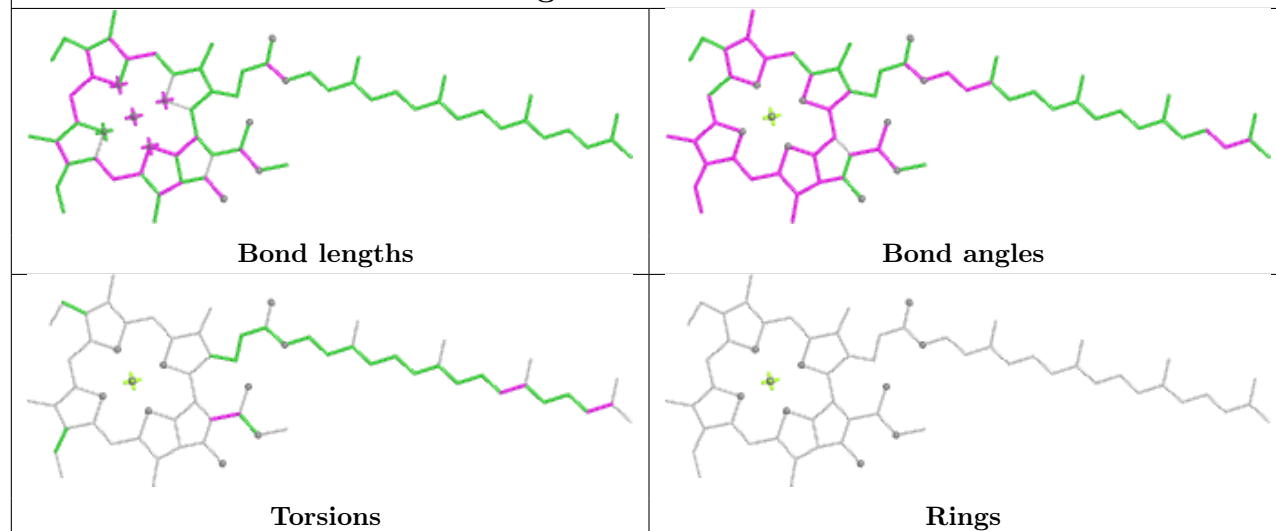
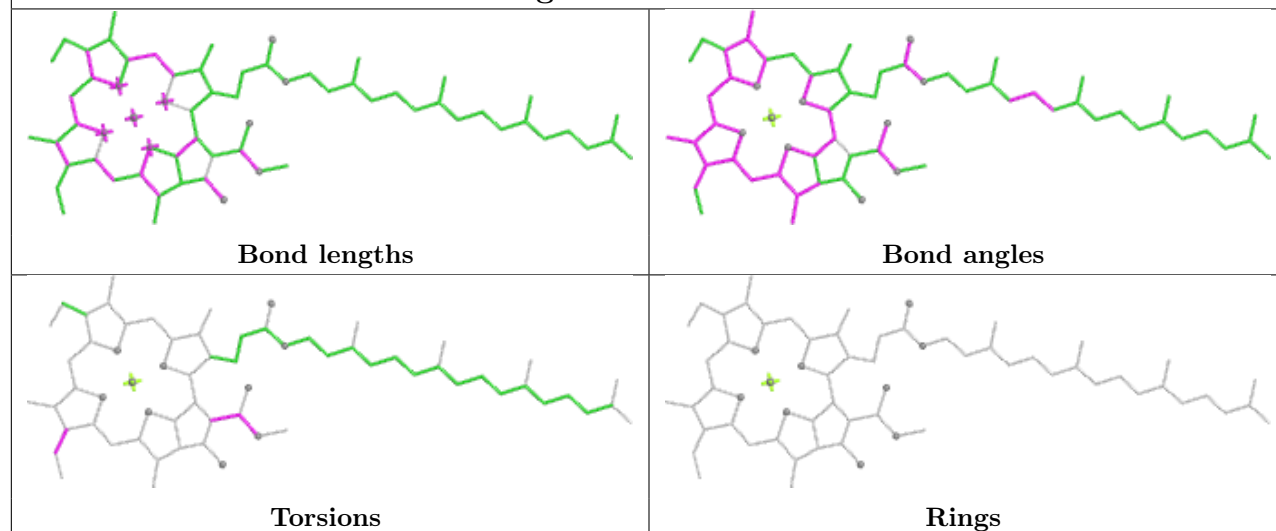


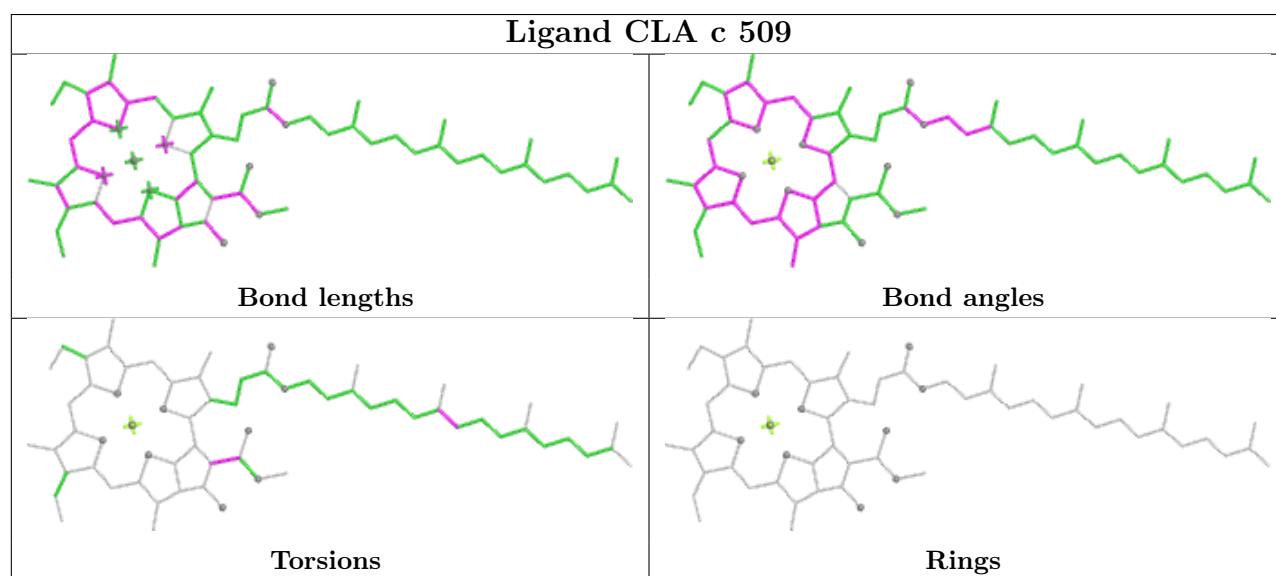
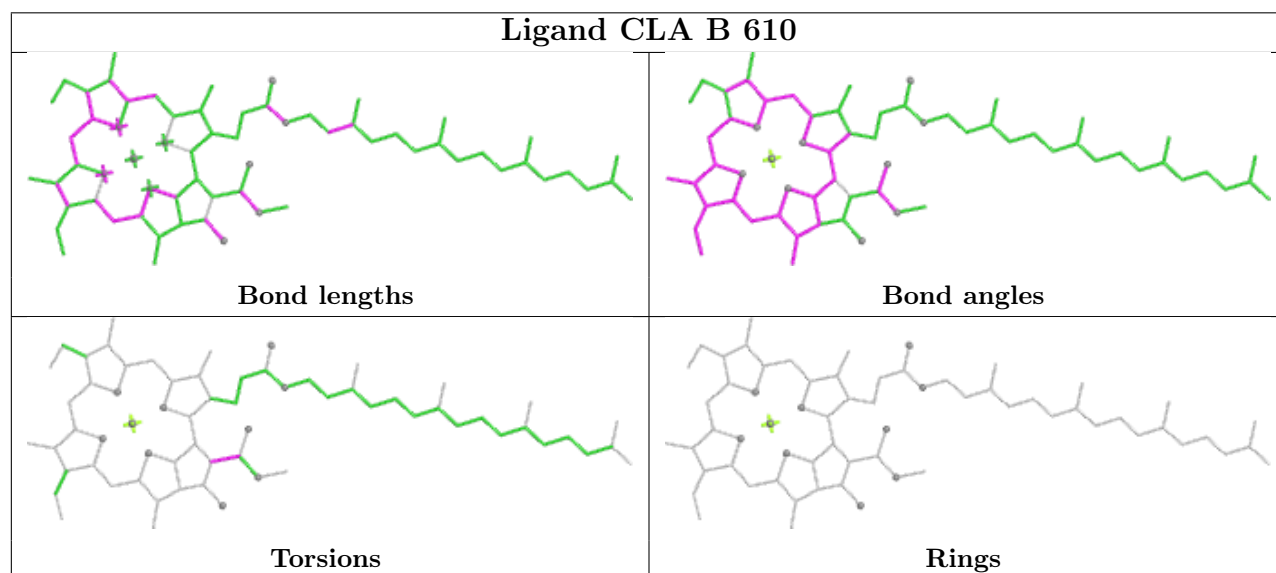
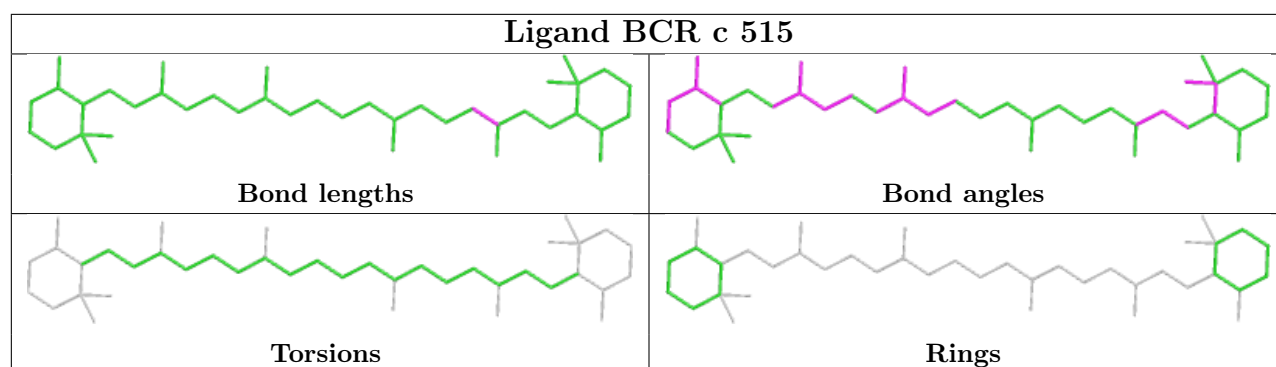
Ligand LHG F 103

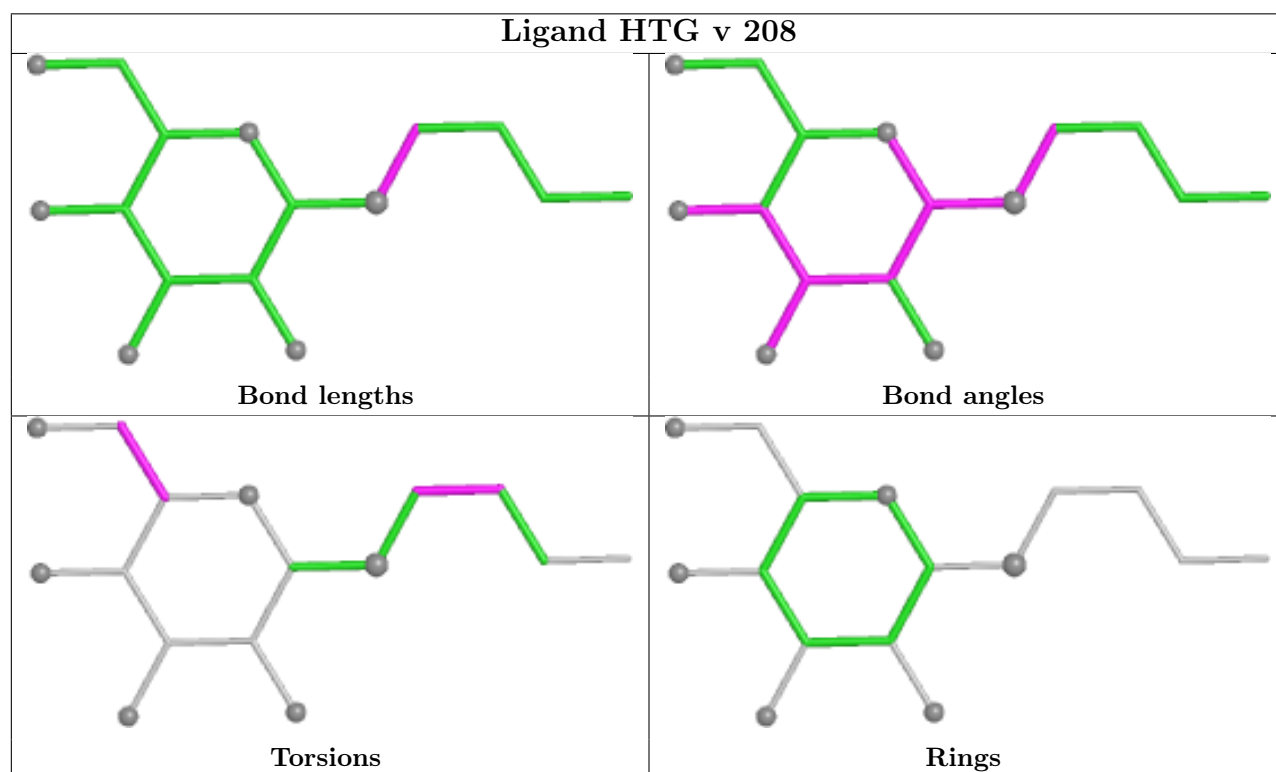
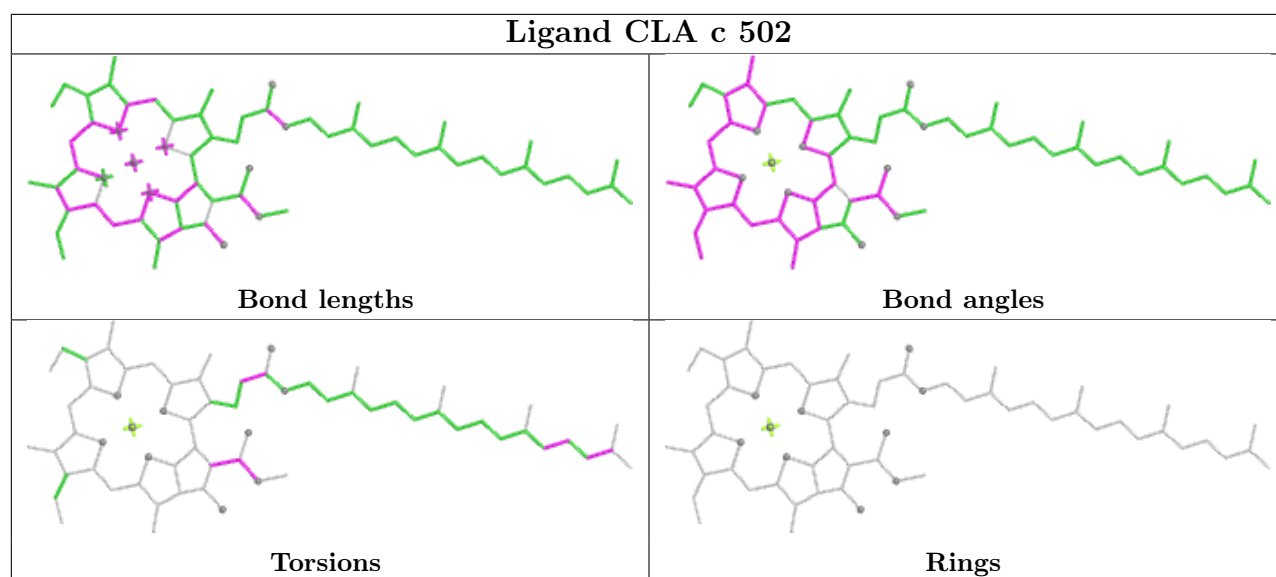


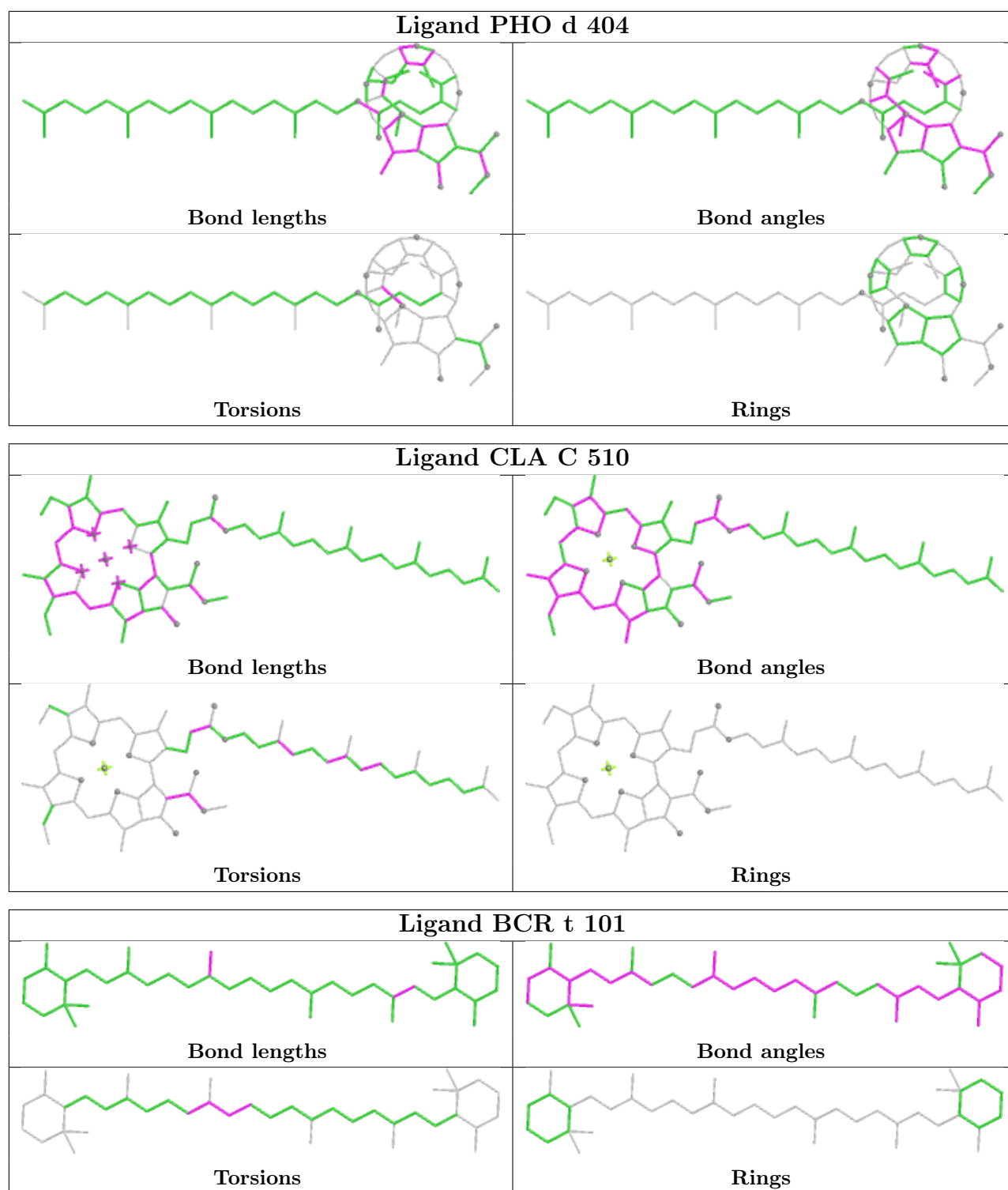


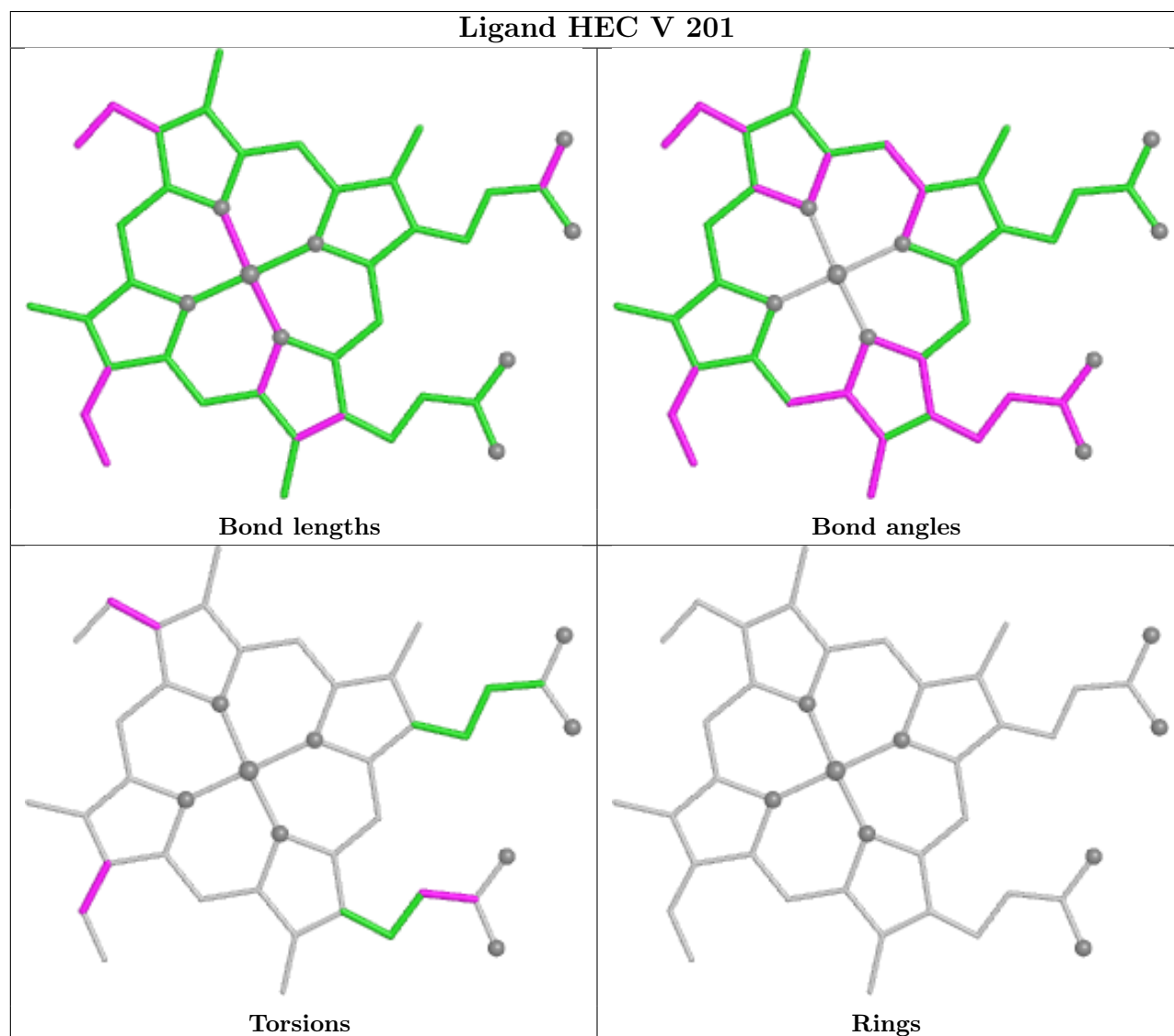
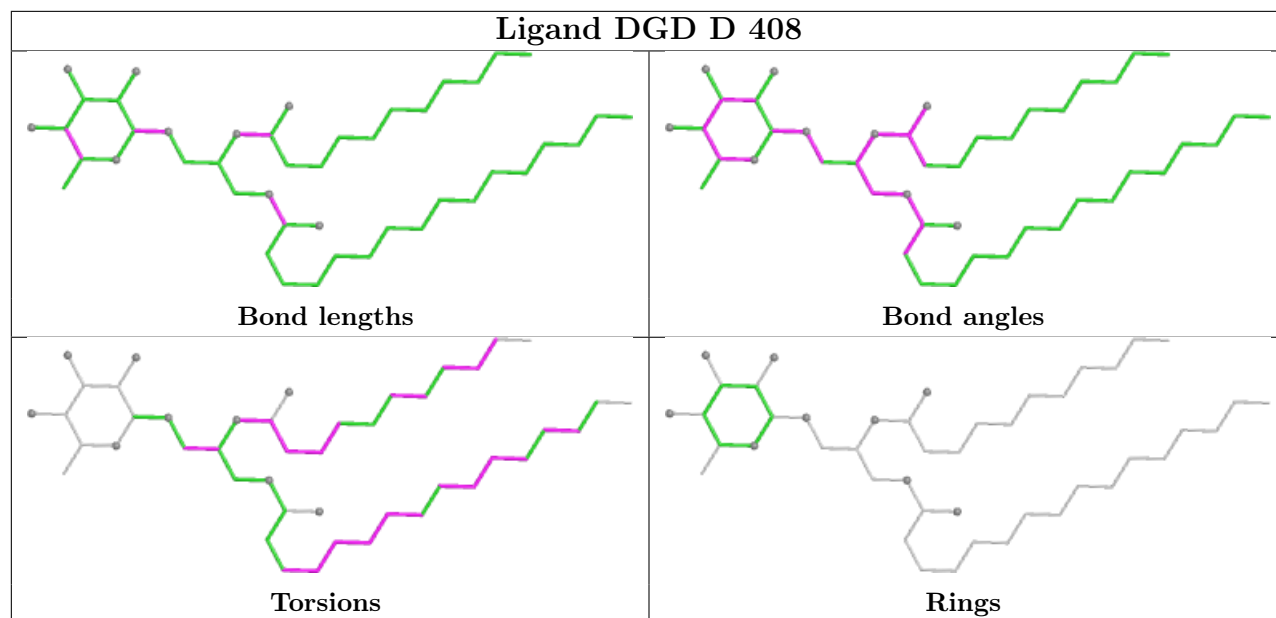


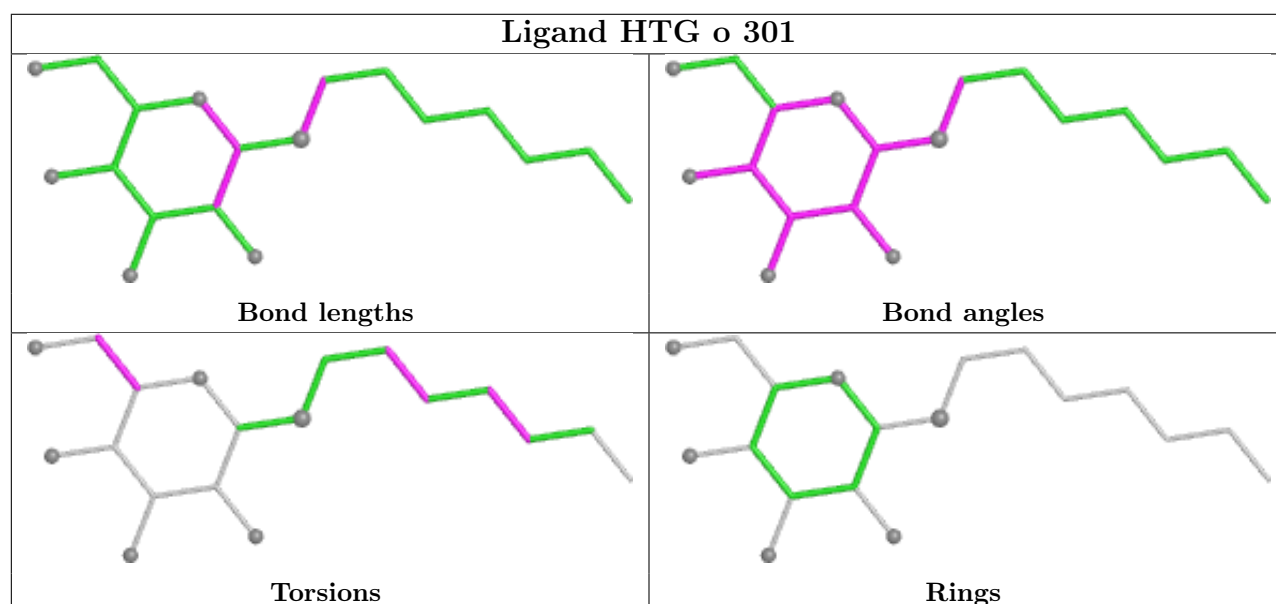
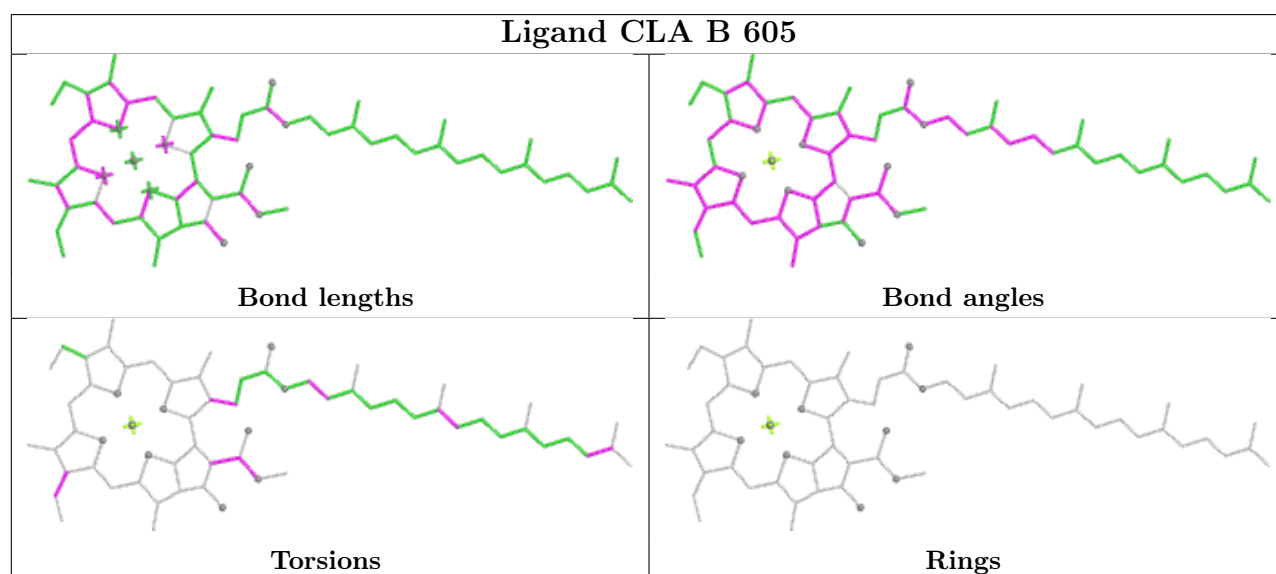
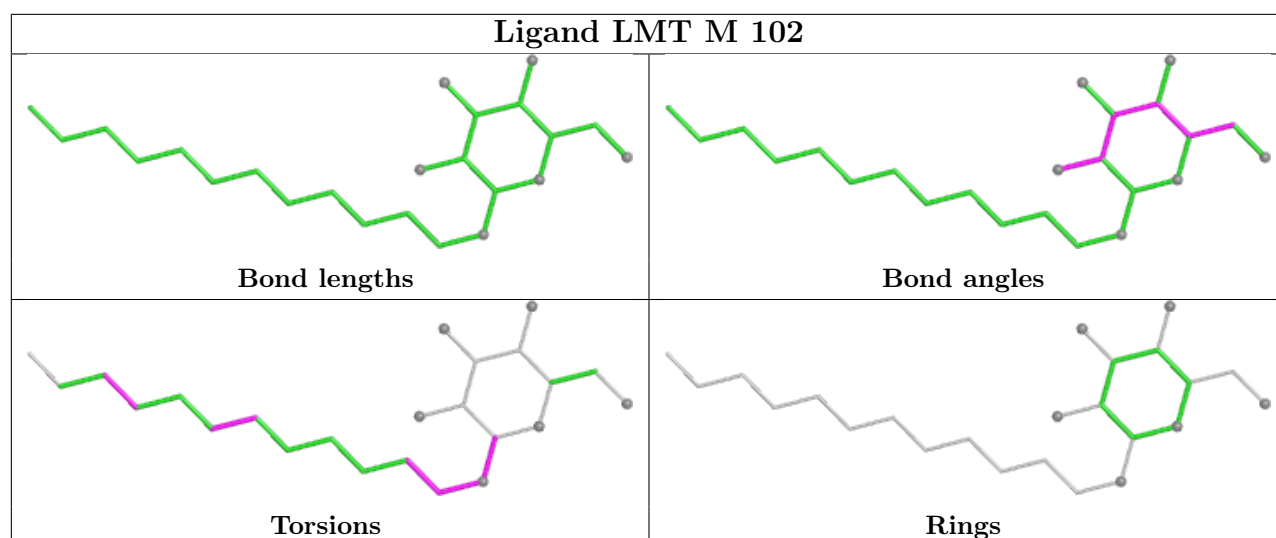
Ligand CLA b 605**Ligand CLA c 503****Ligand CLA a 406**

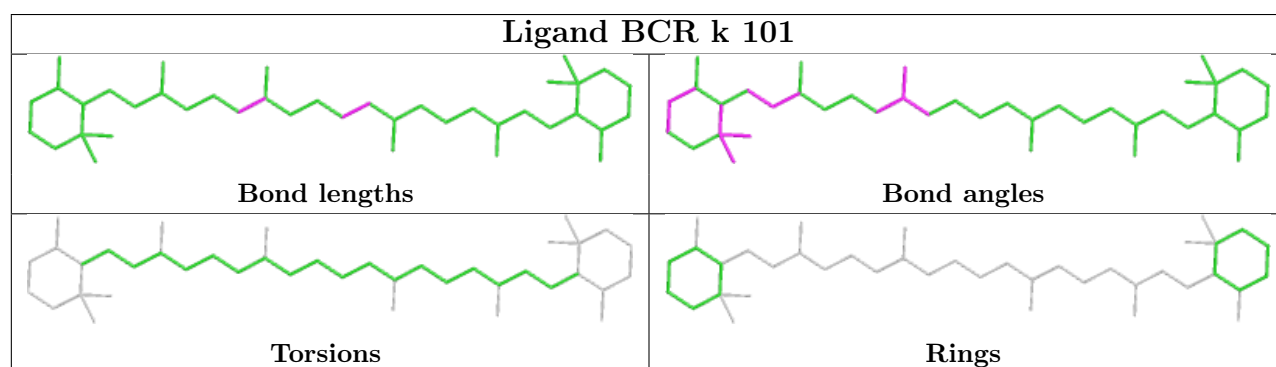
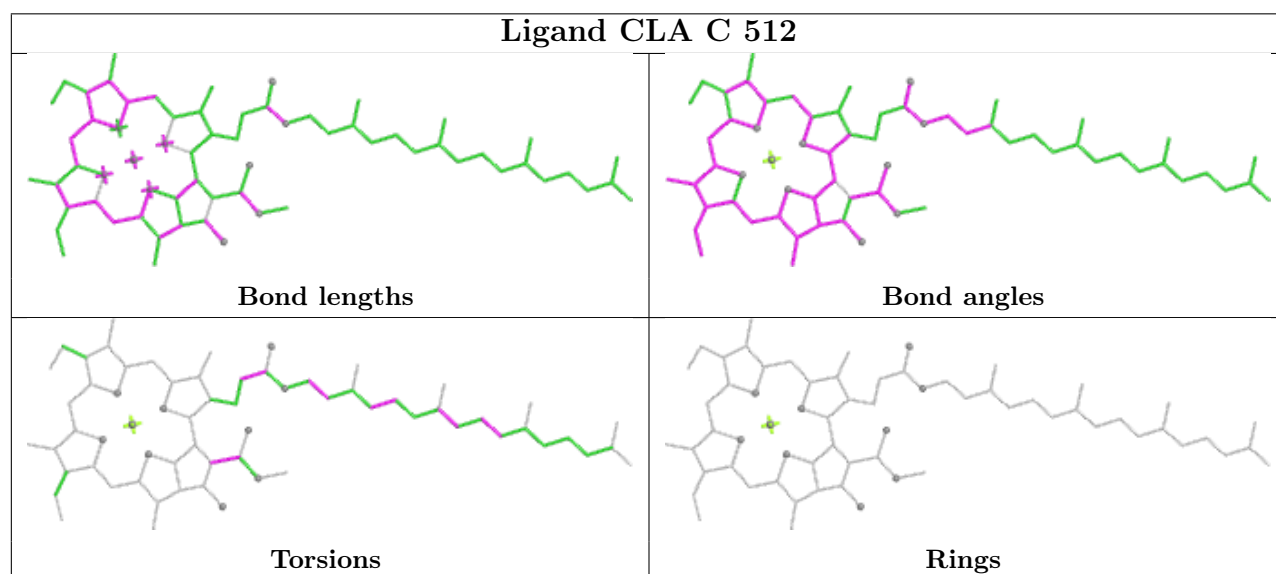
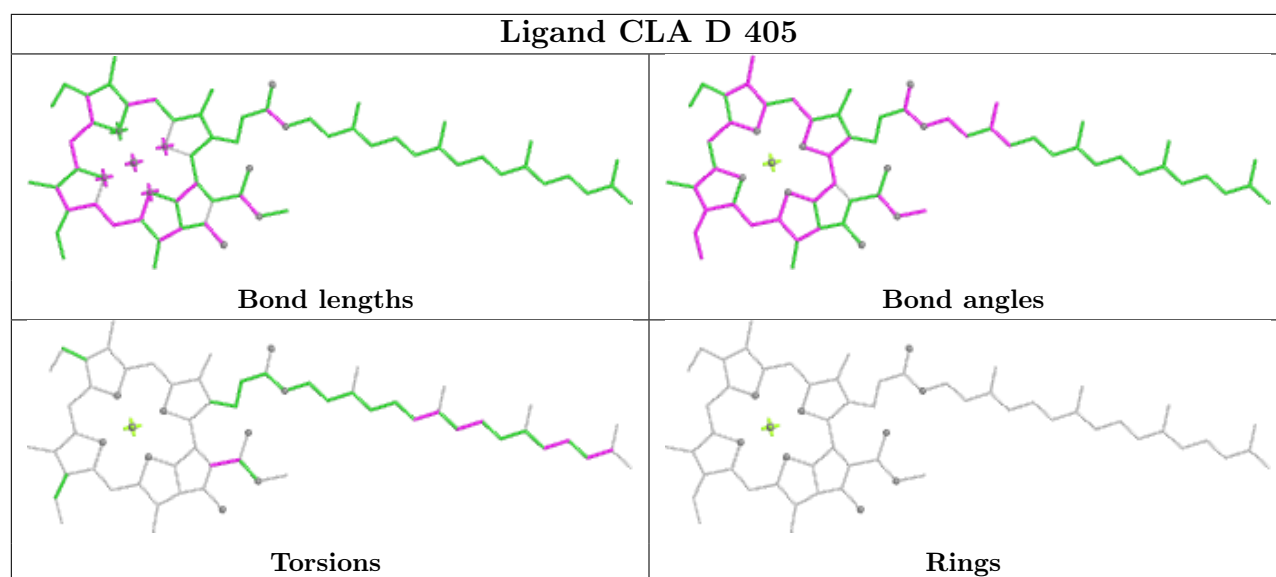


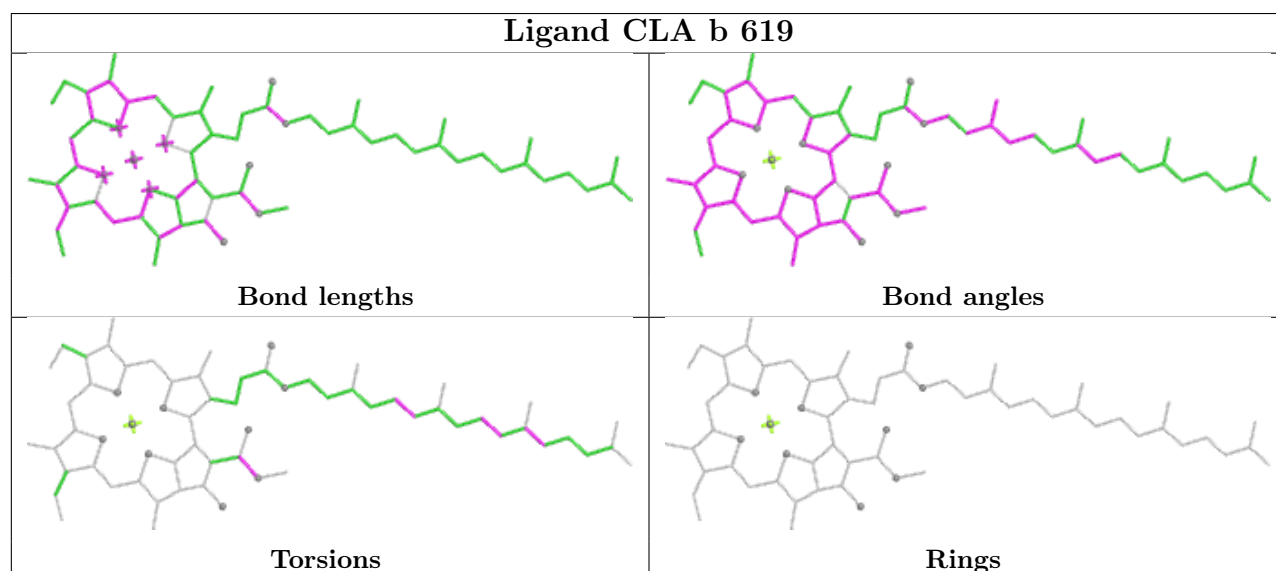
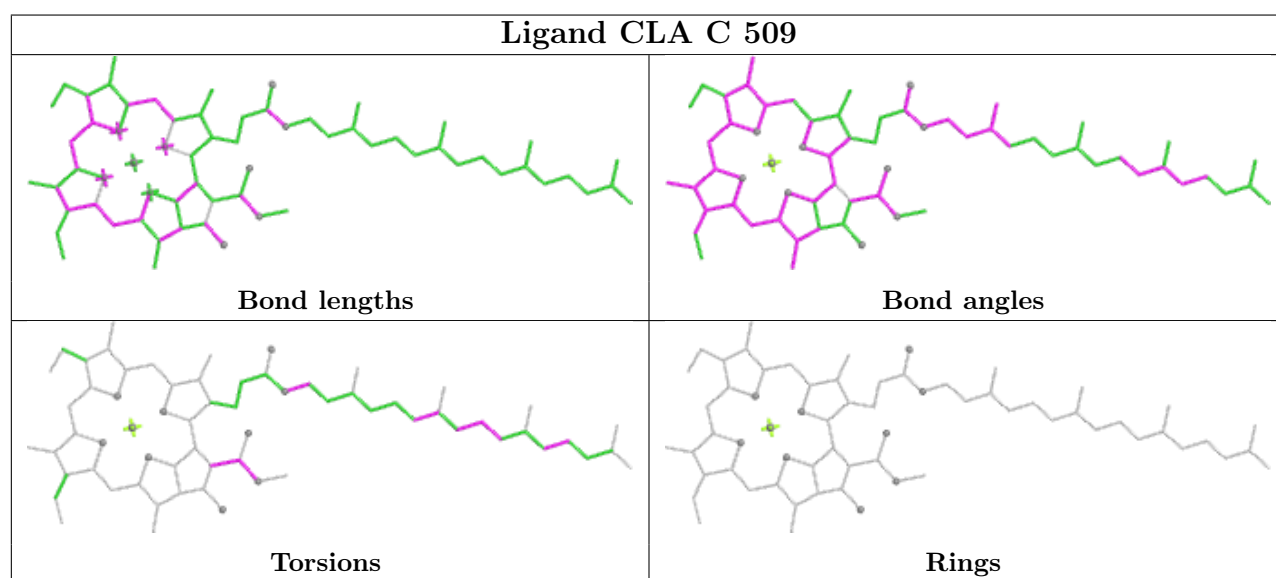
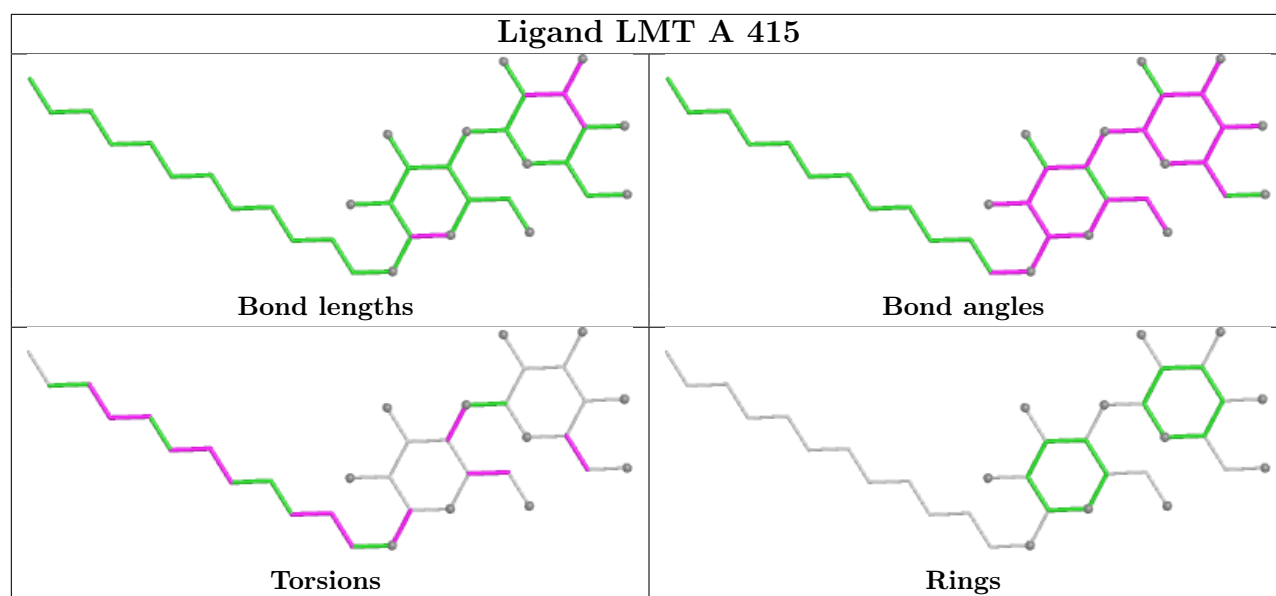


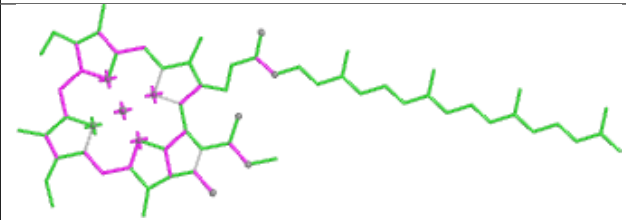
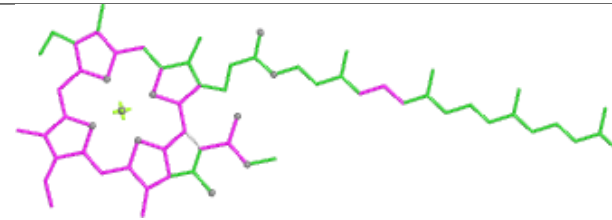
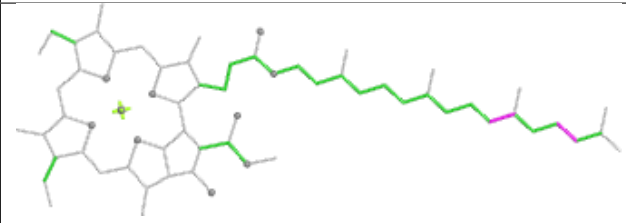
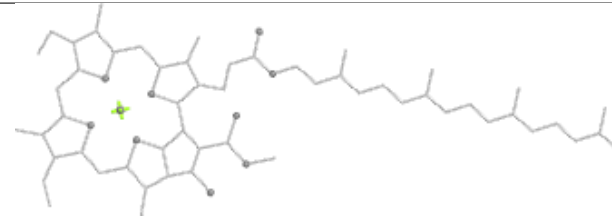


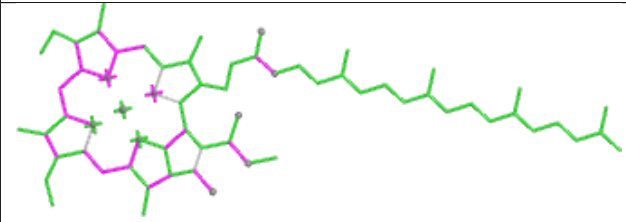
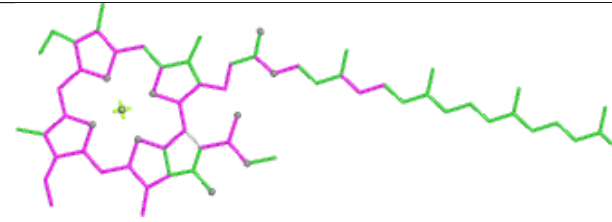
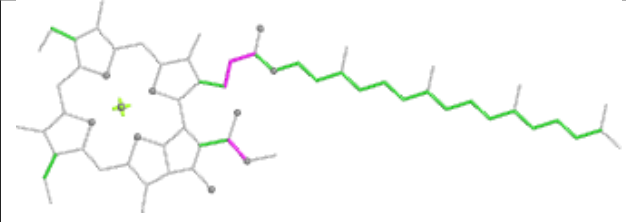
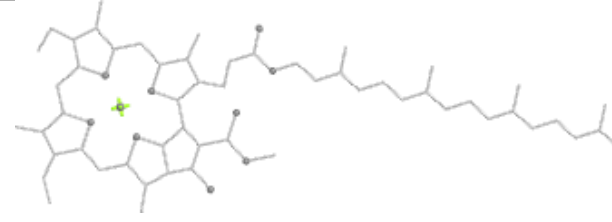




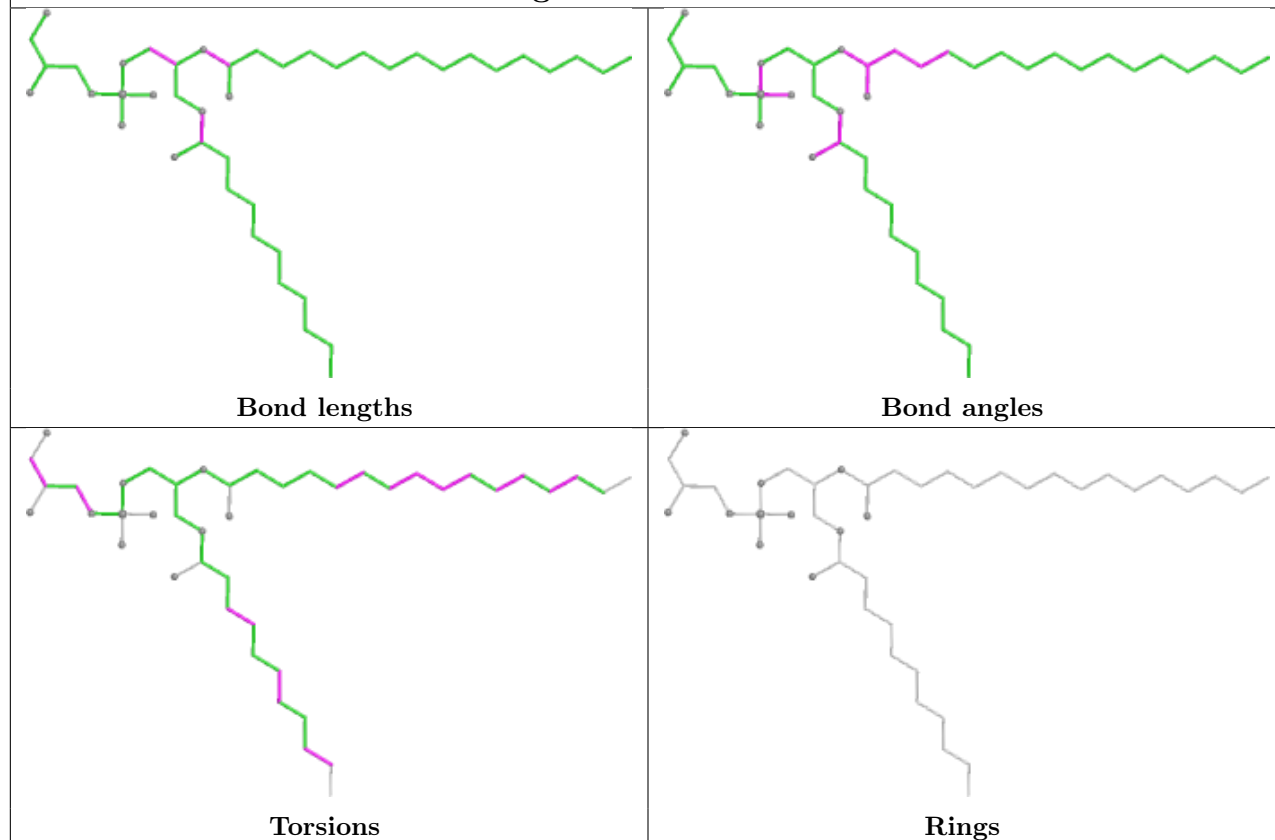




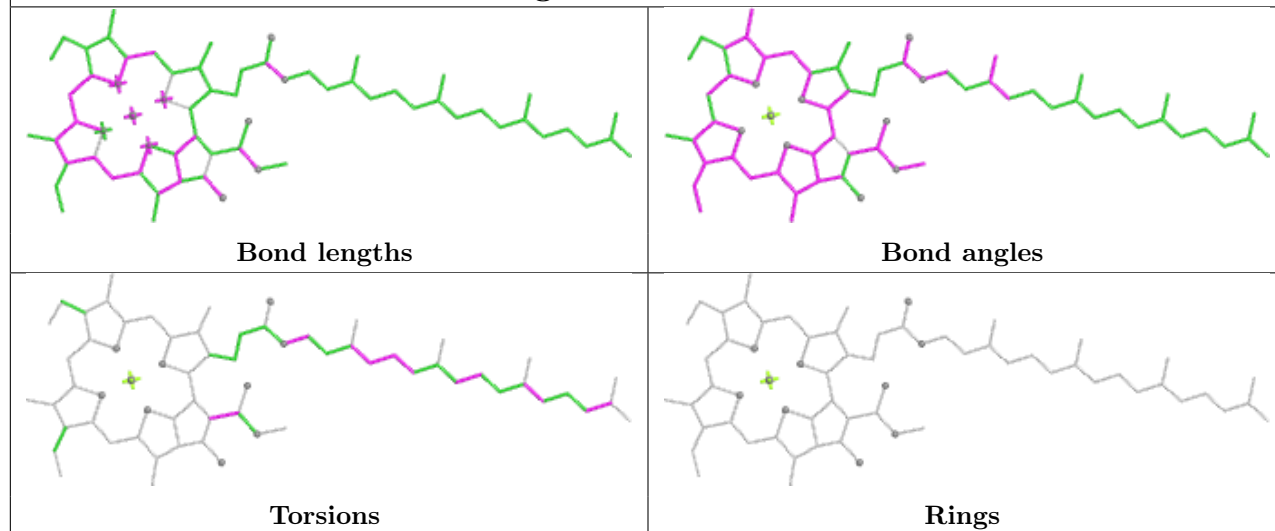
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

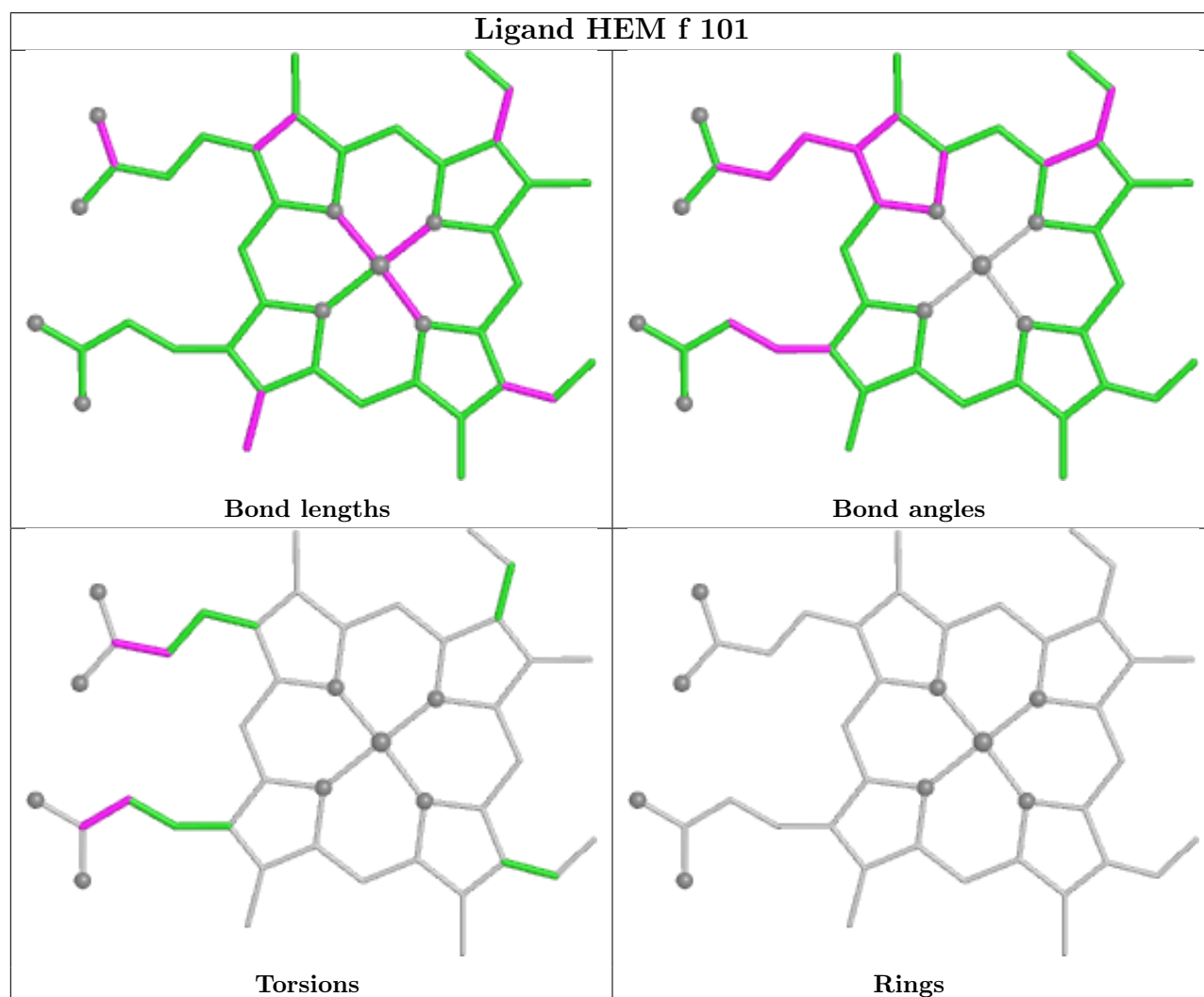
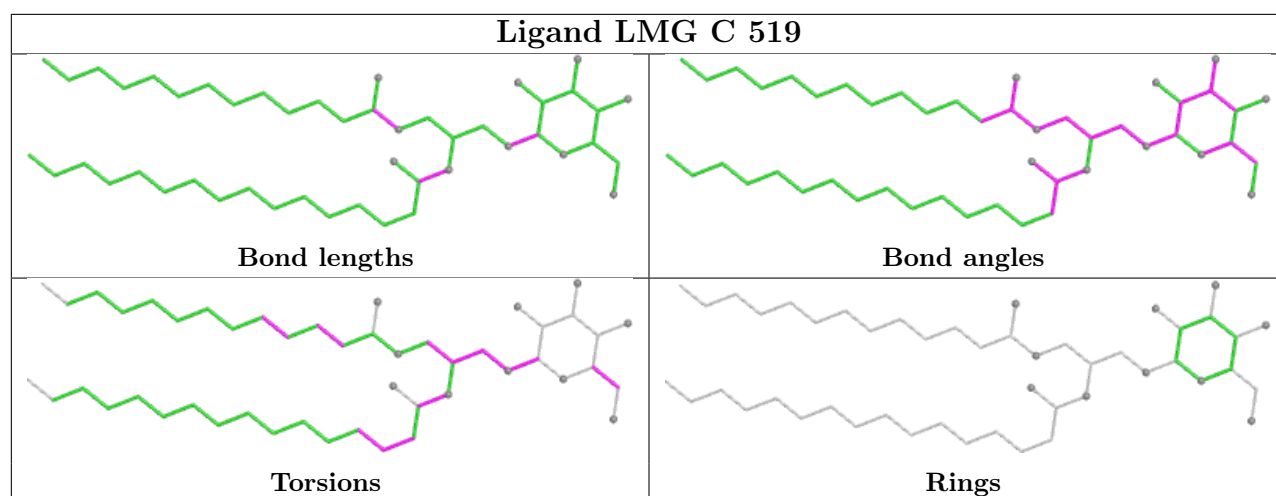
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

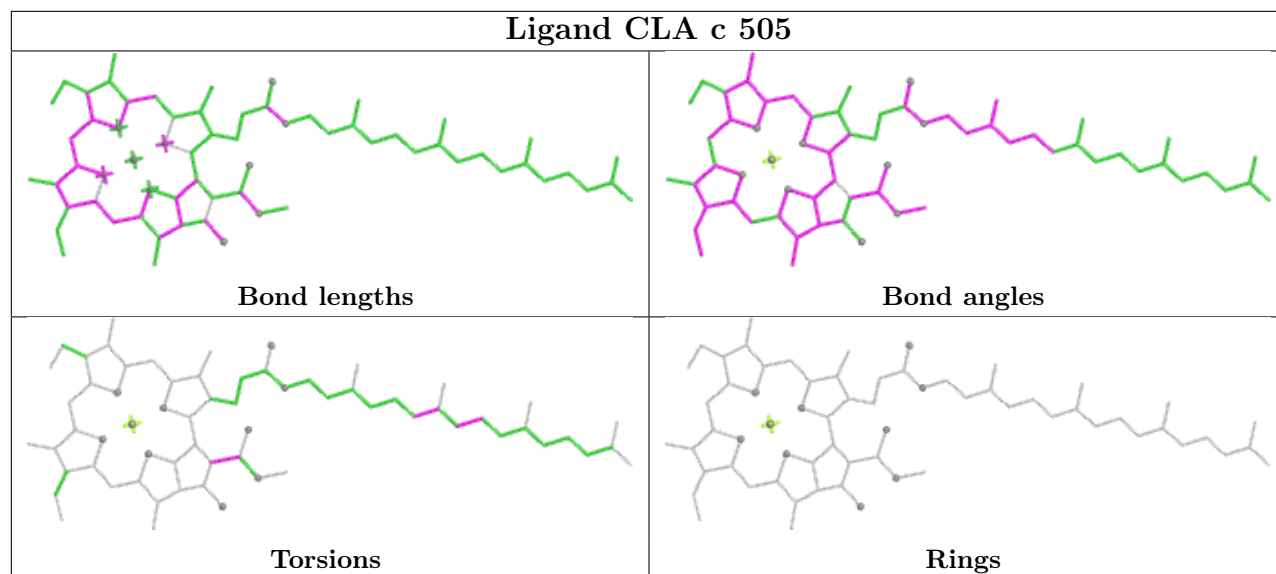
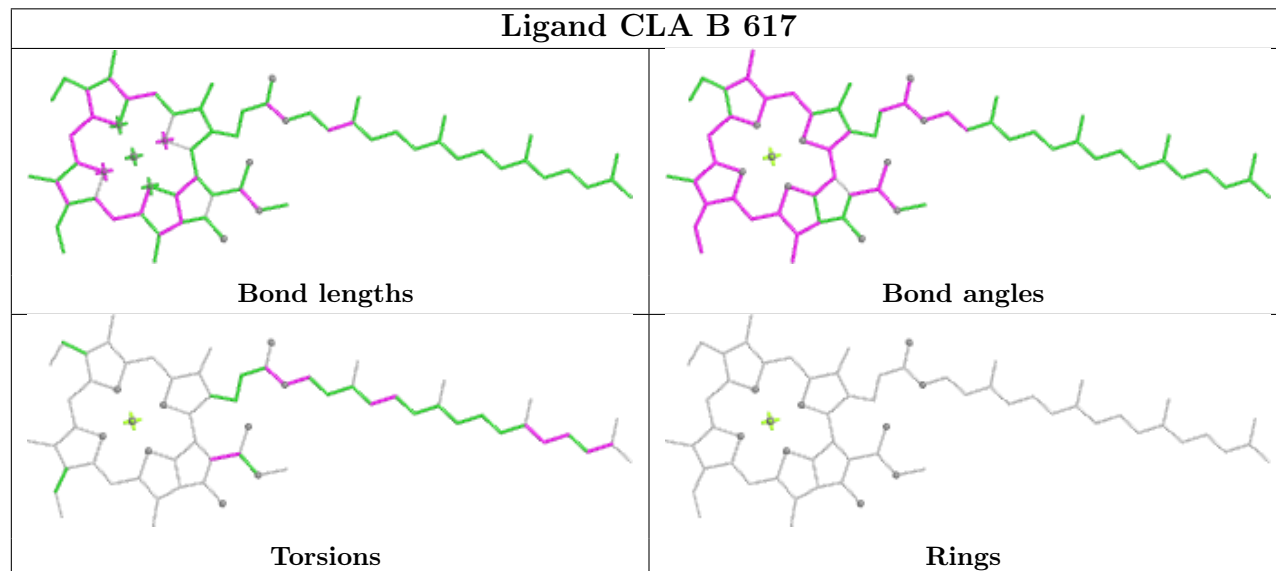
Ligand LHG d 411

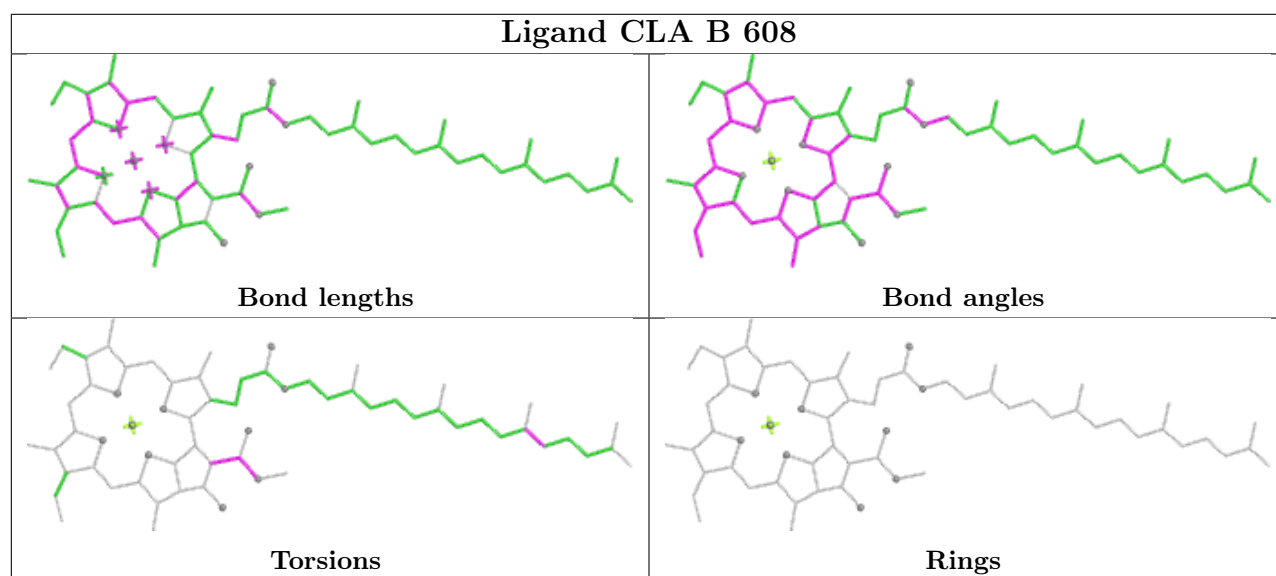
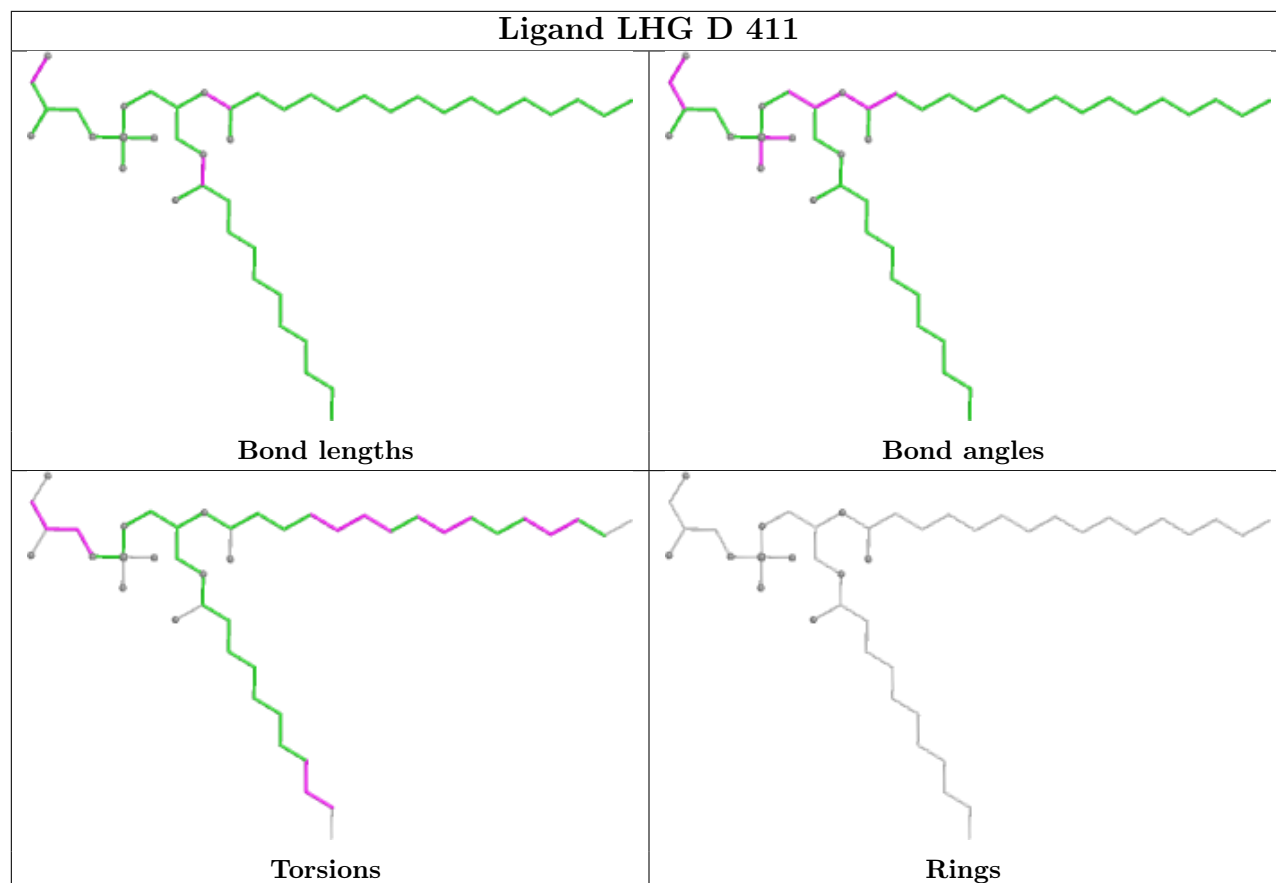


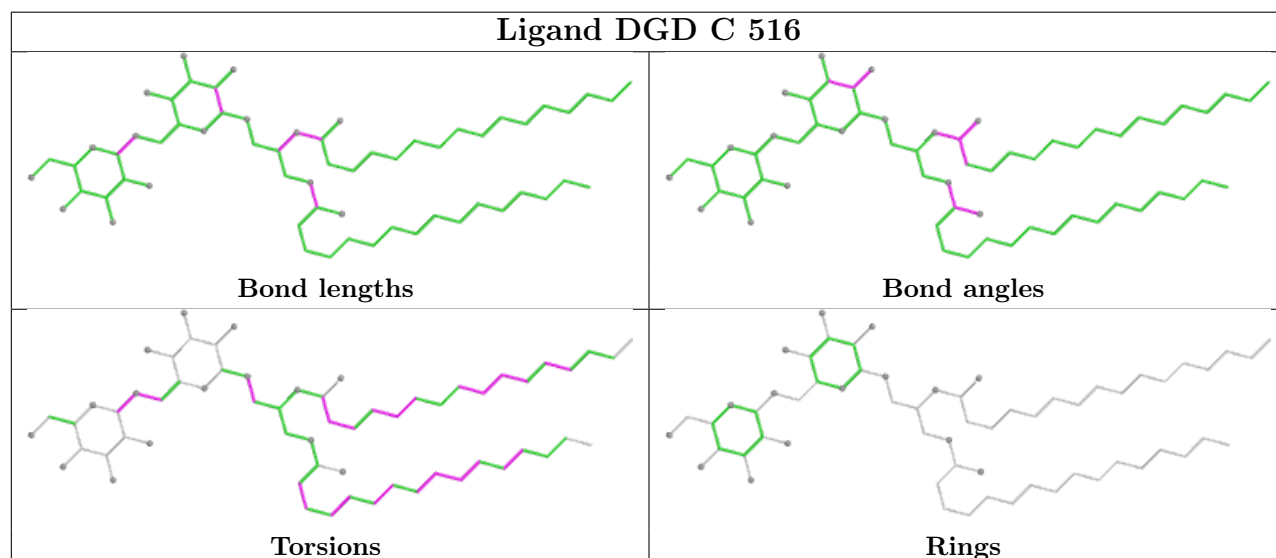
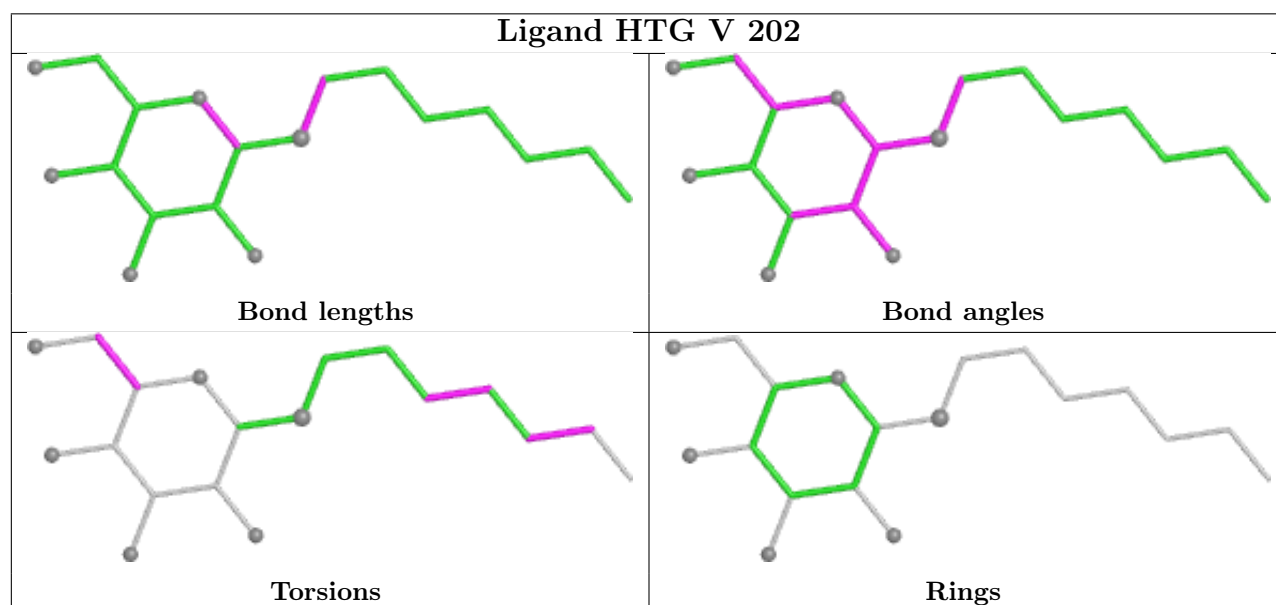
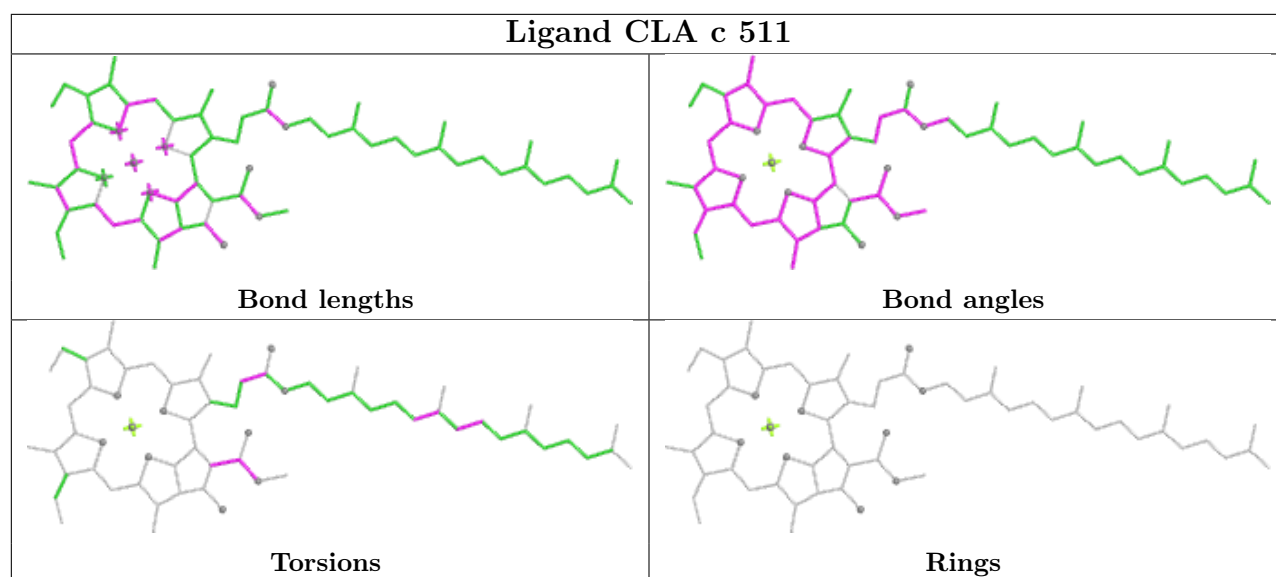
Ligand CLA b 618

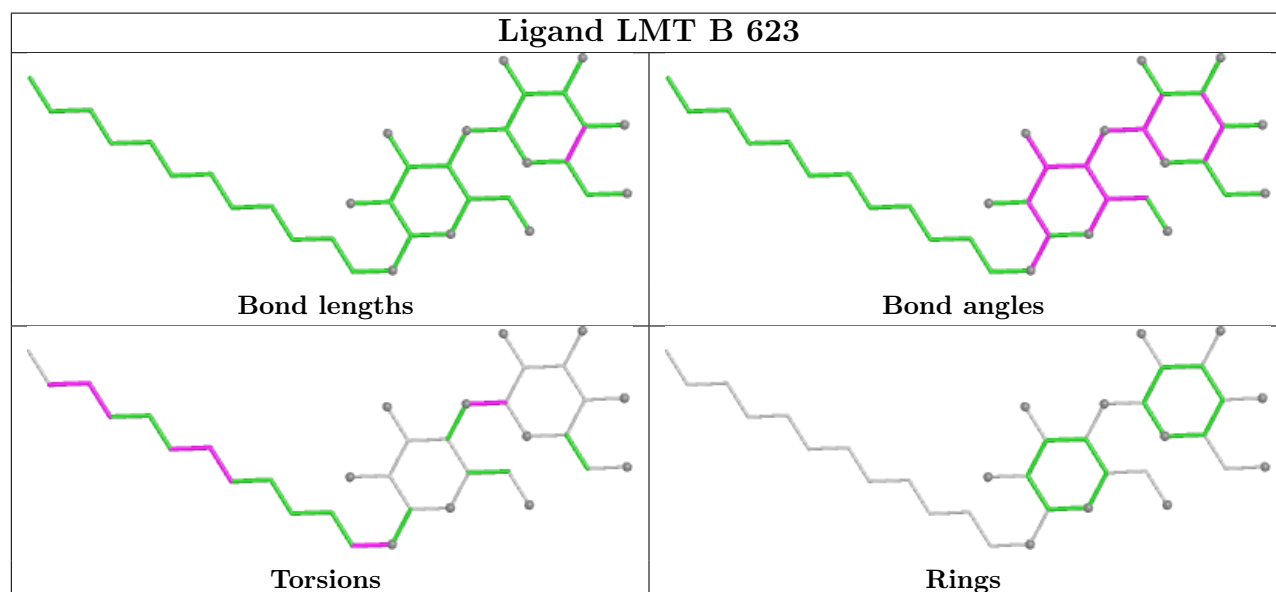
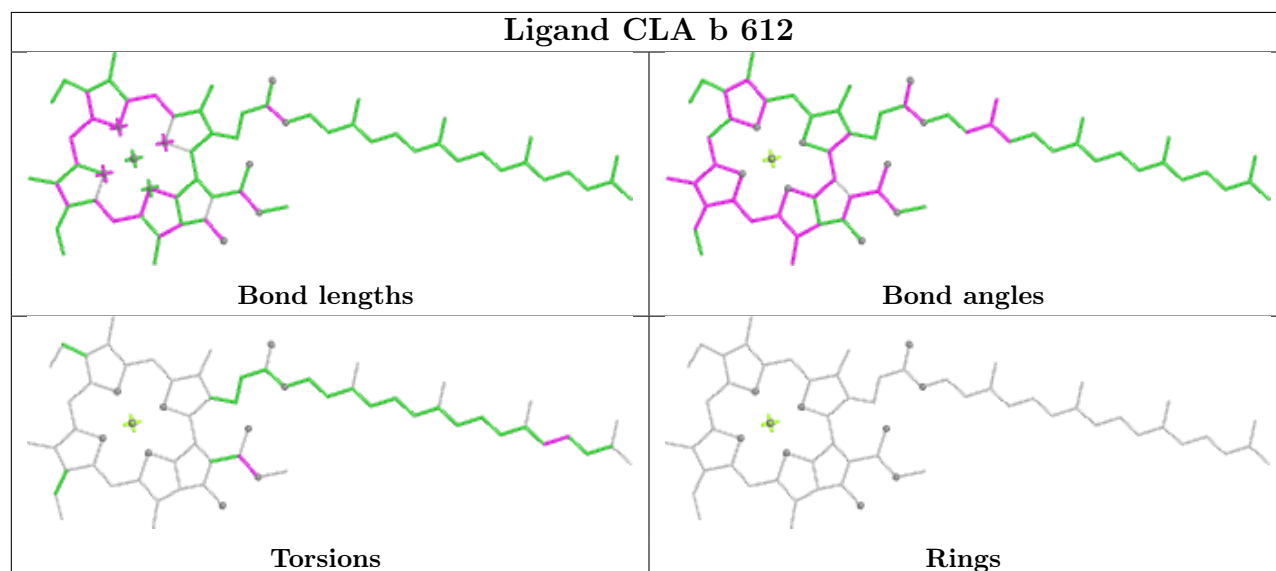
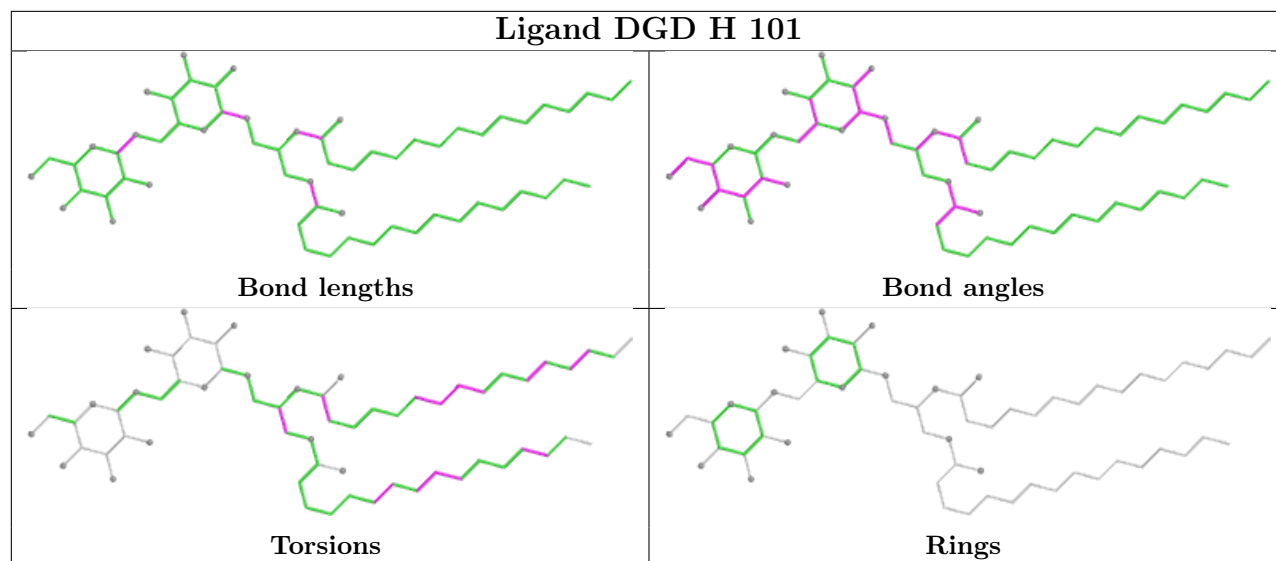


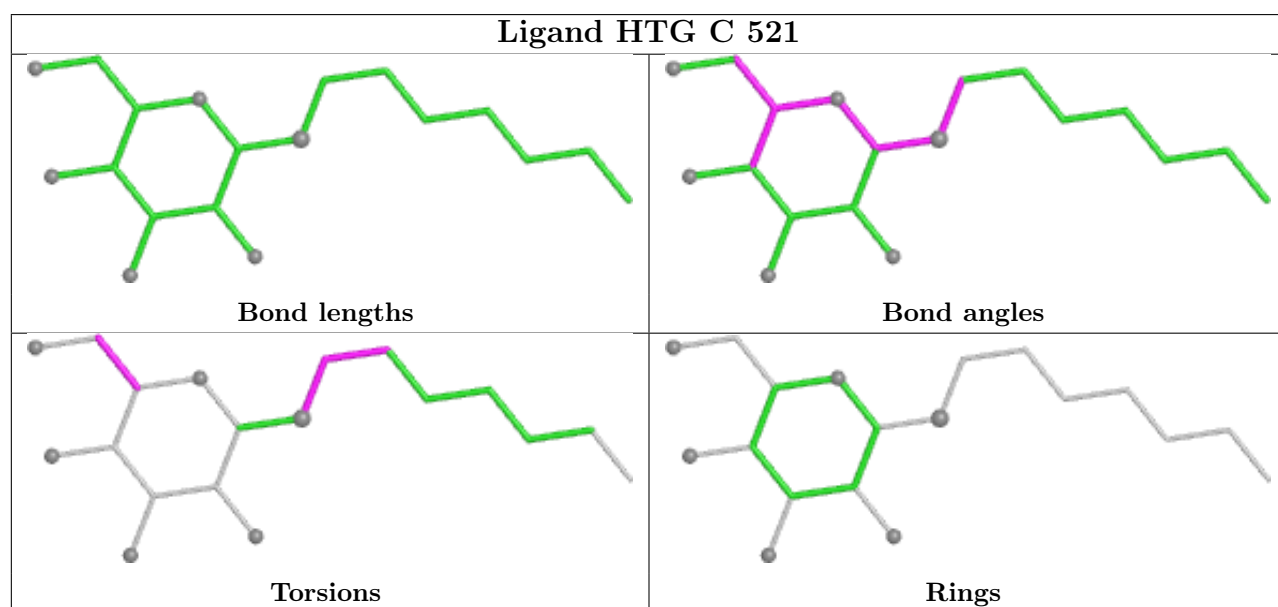
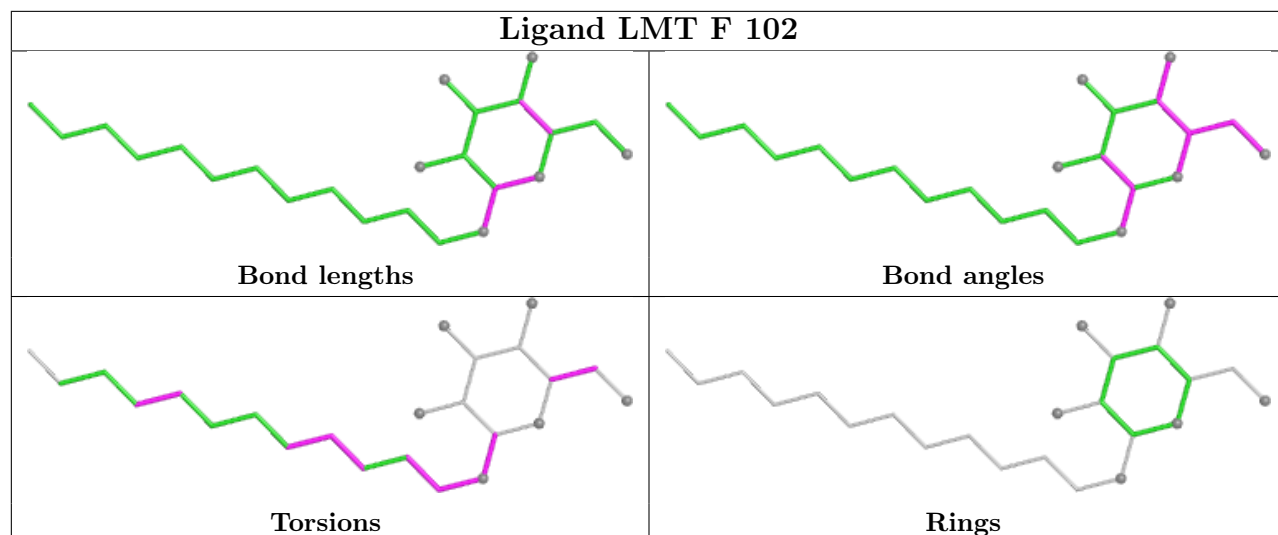


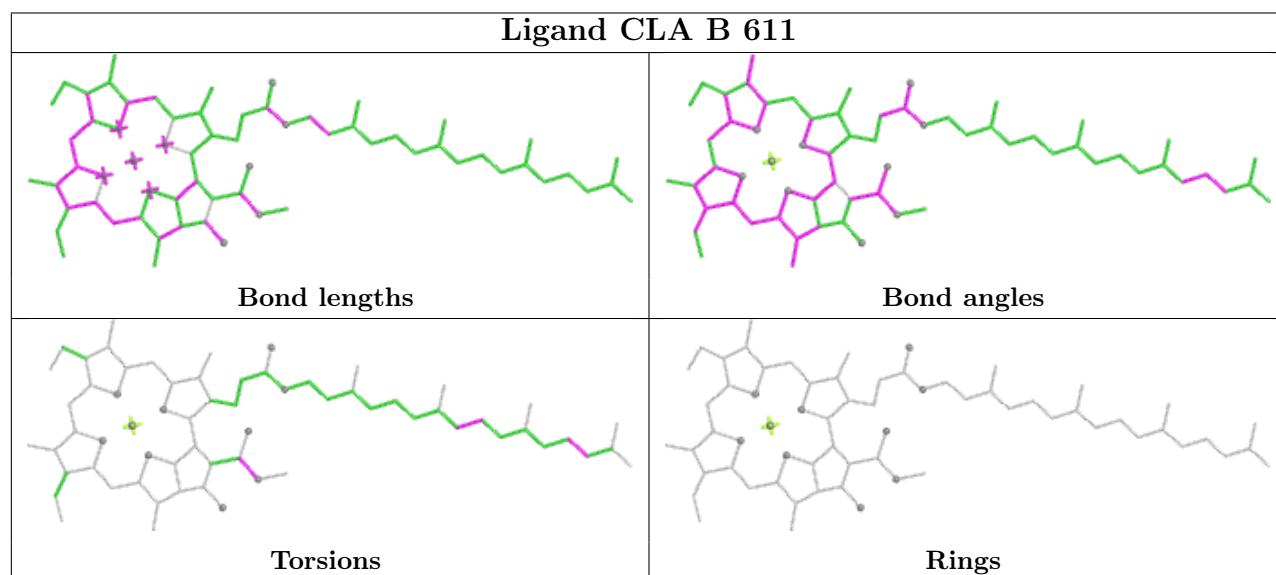
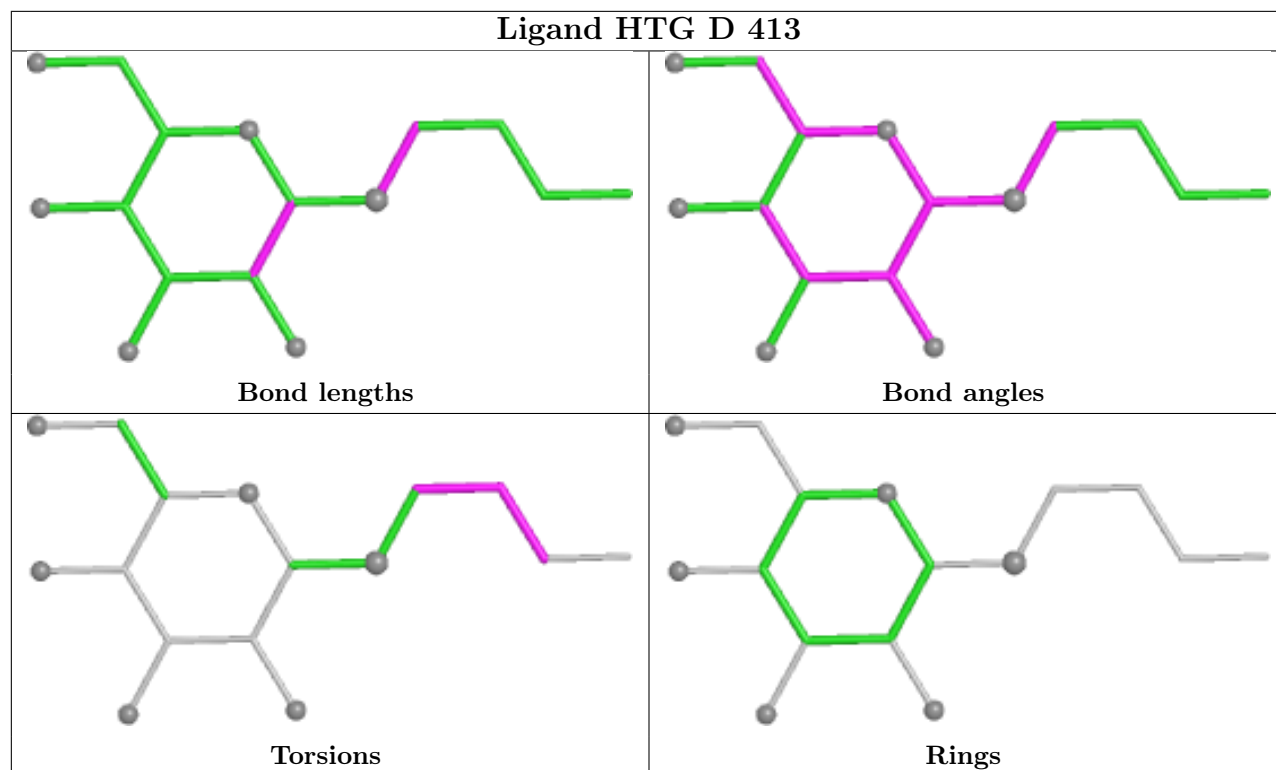
Ligand CLA c 505**Ligand CLA B 617**

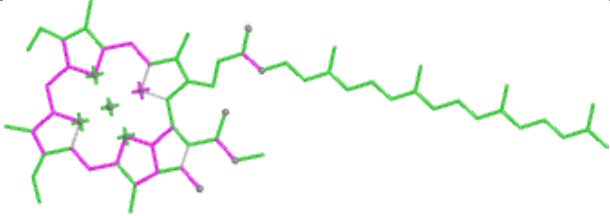
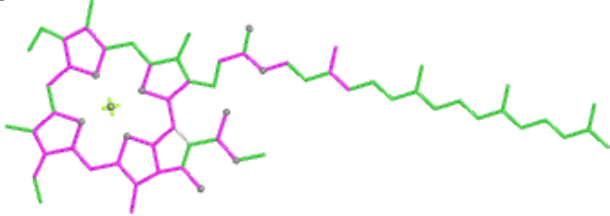
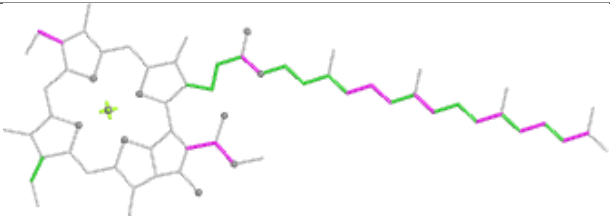
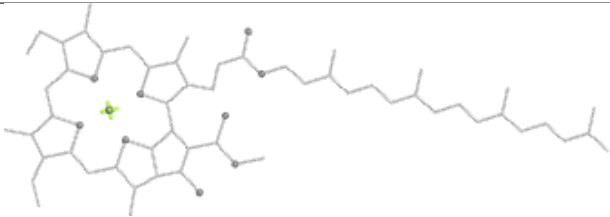
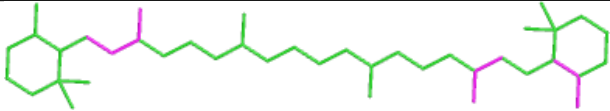
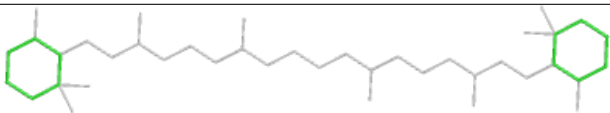
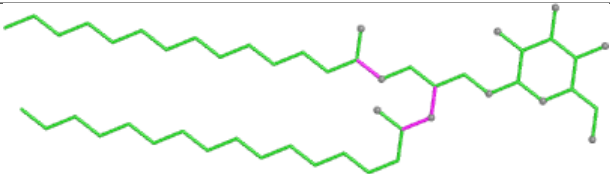
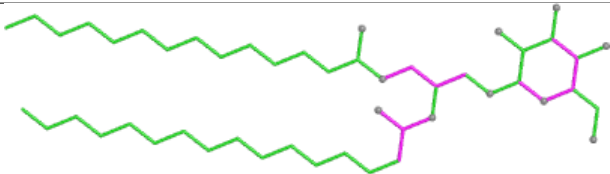
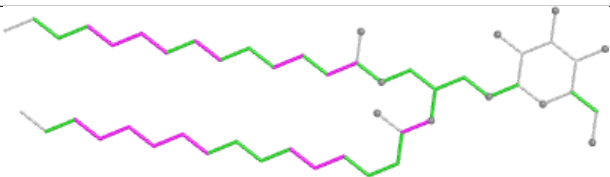
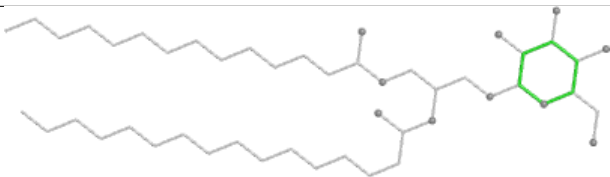


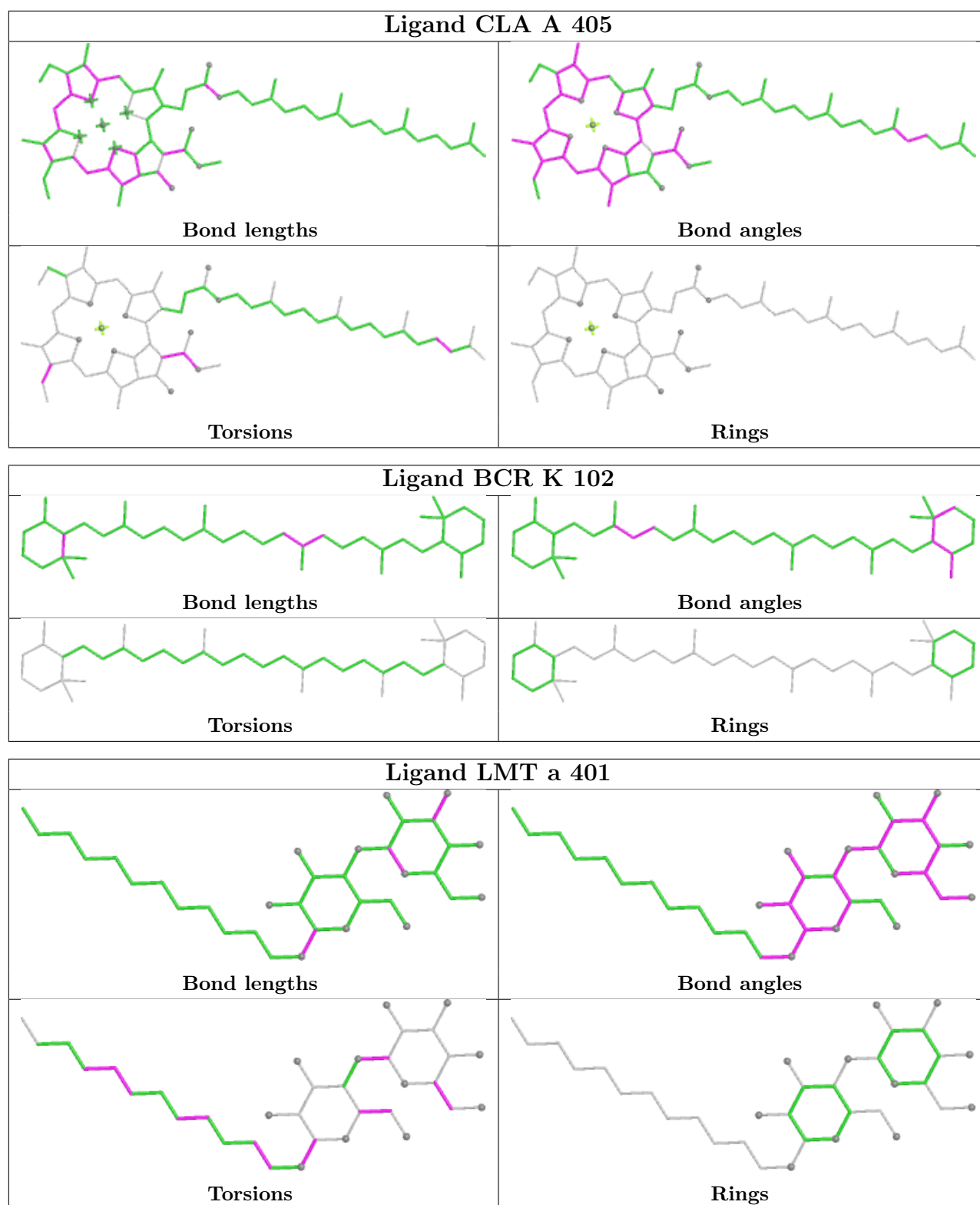




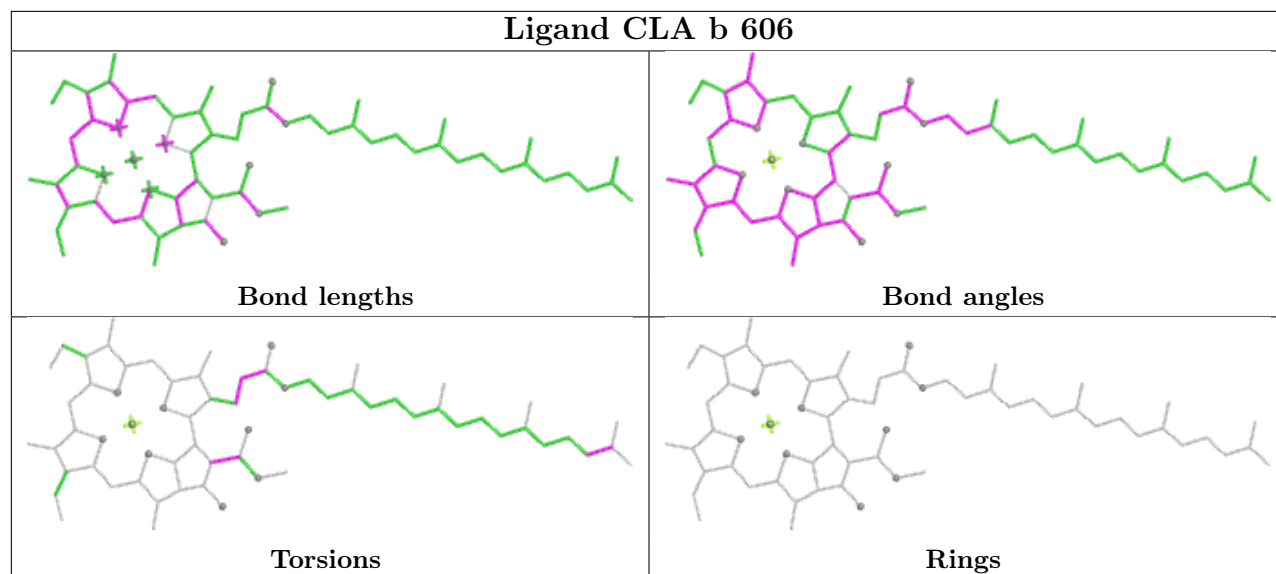




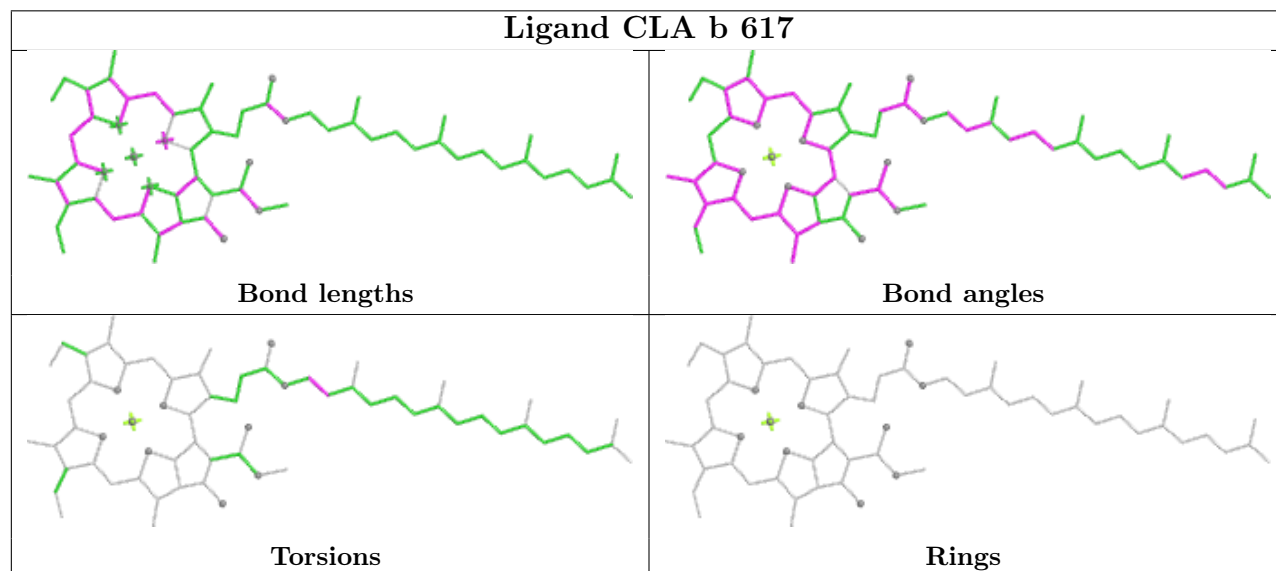
Ligand CLA c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings



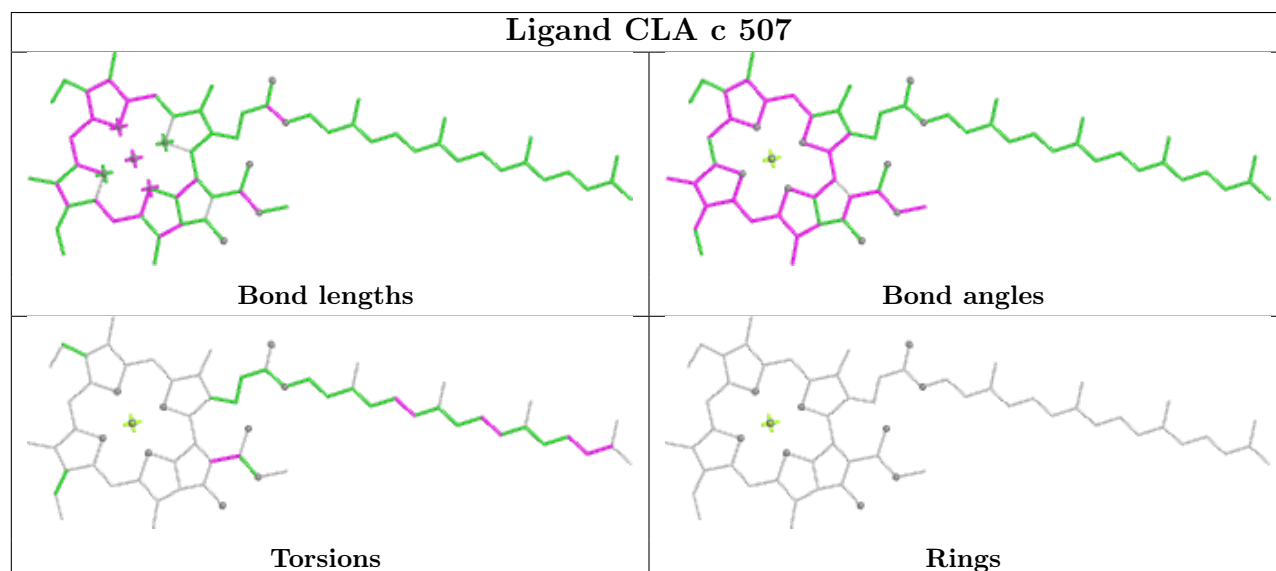
Ligand CLA b 606



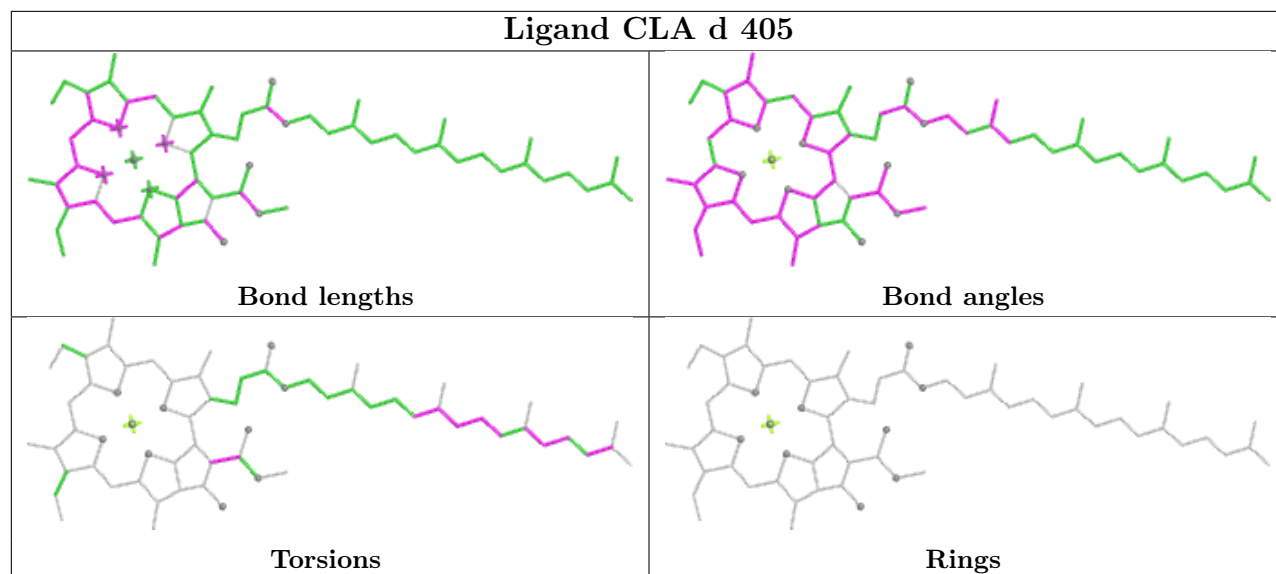
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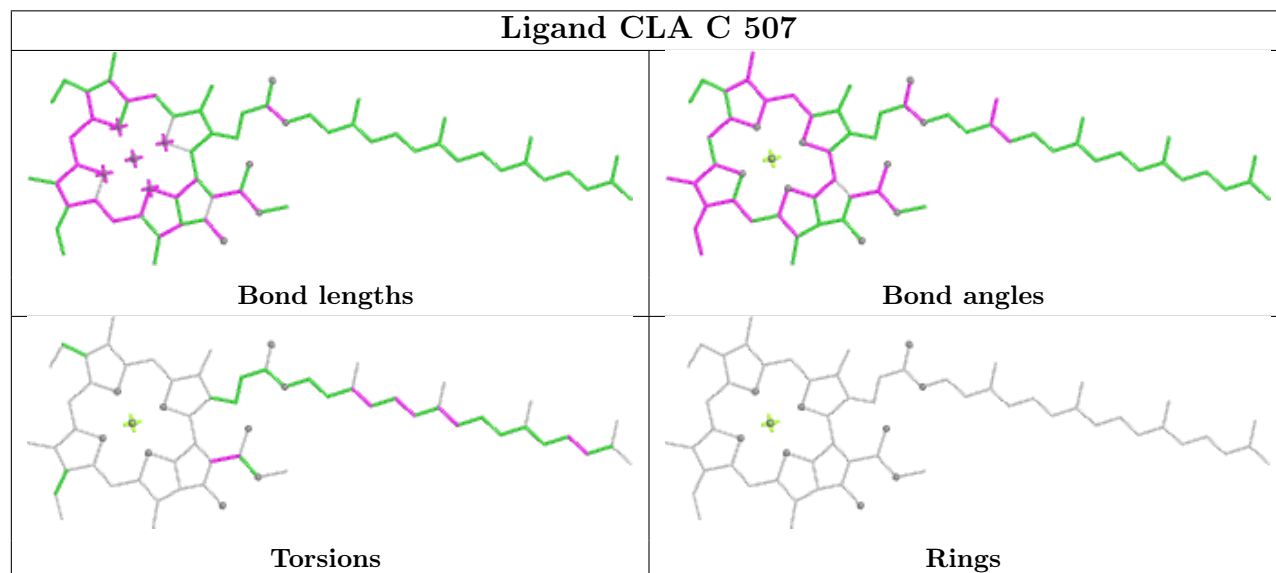
Ligand CLA c 507



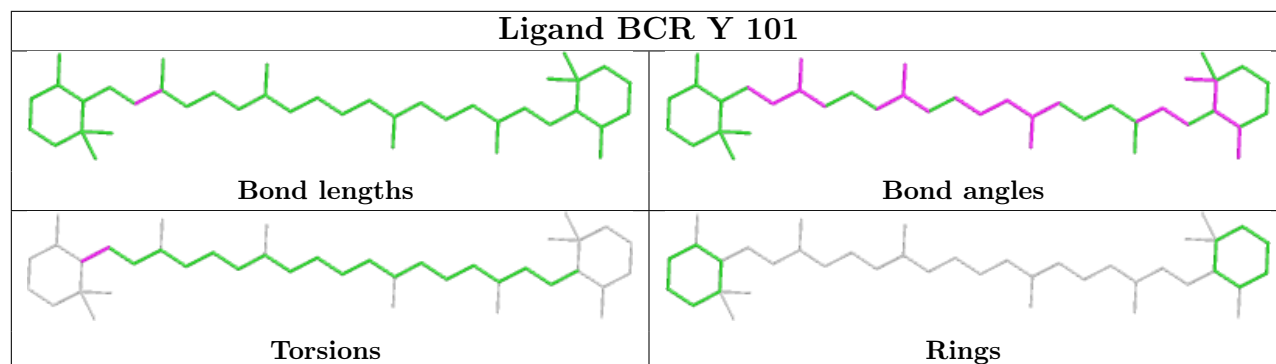
Ligand CLA d 405

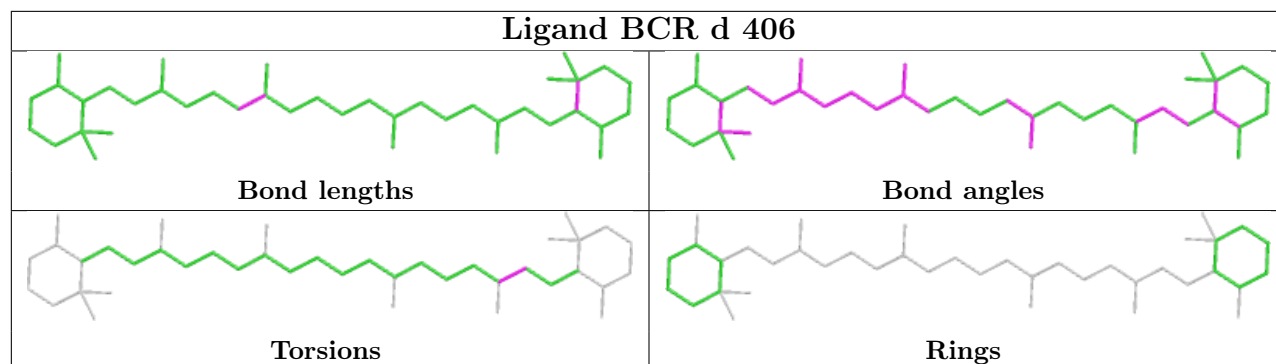
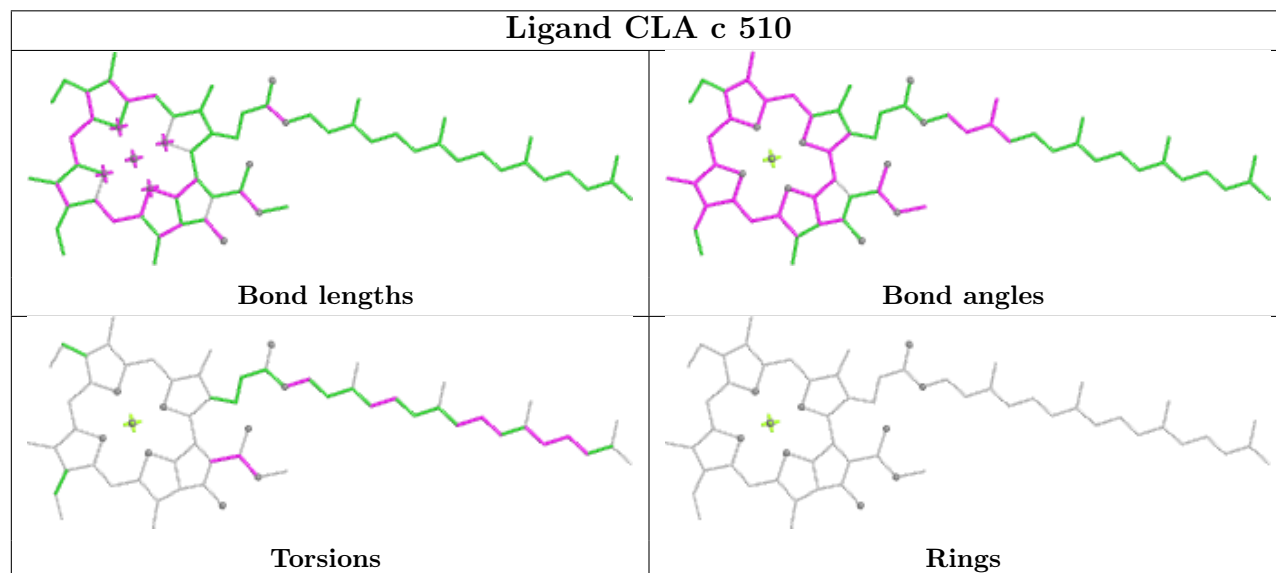
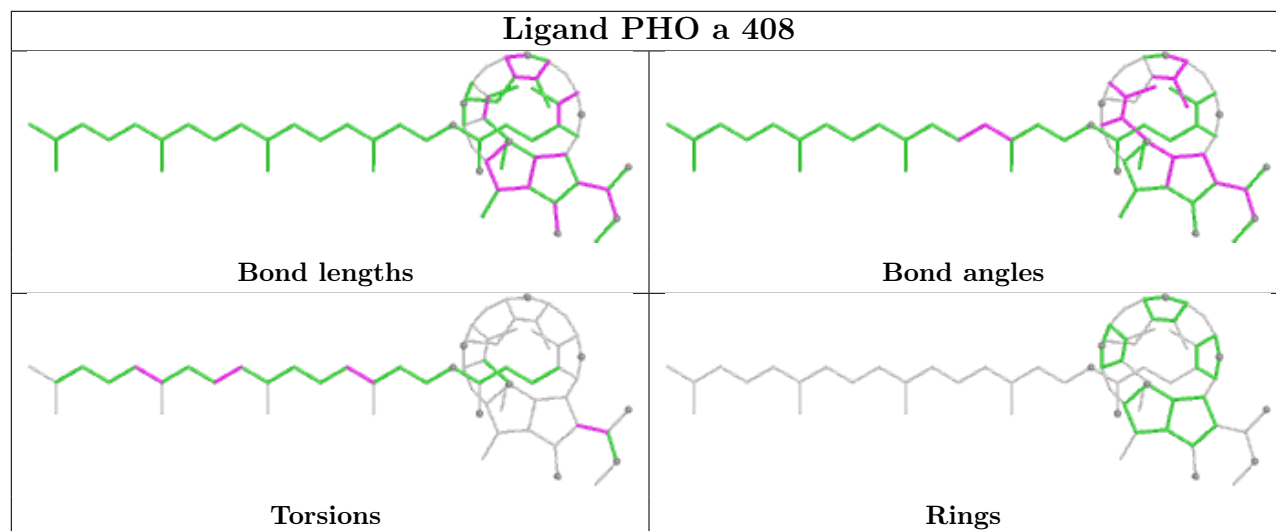


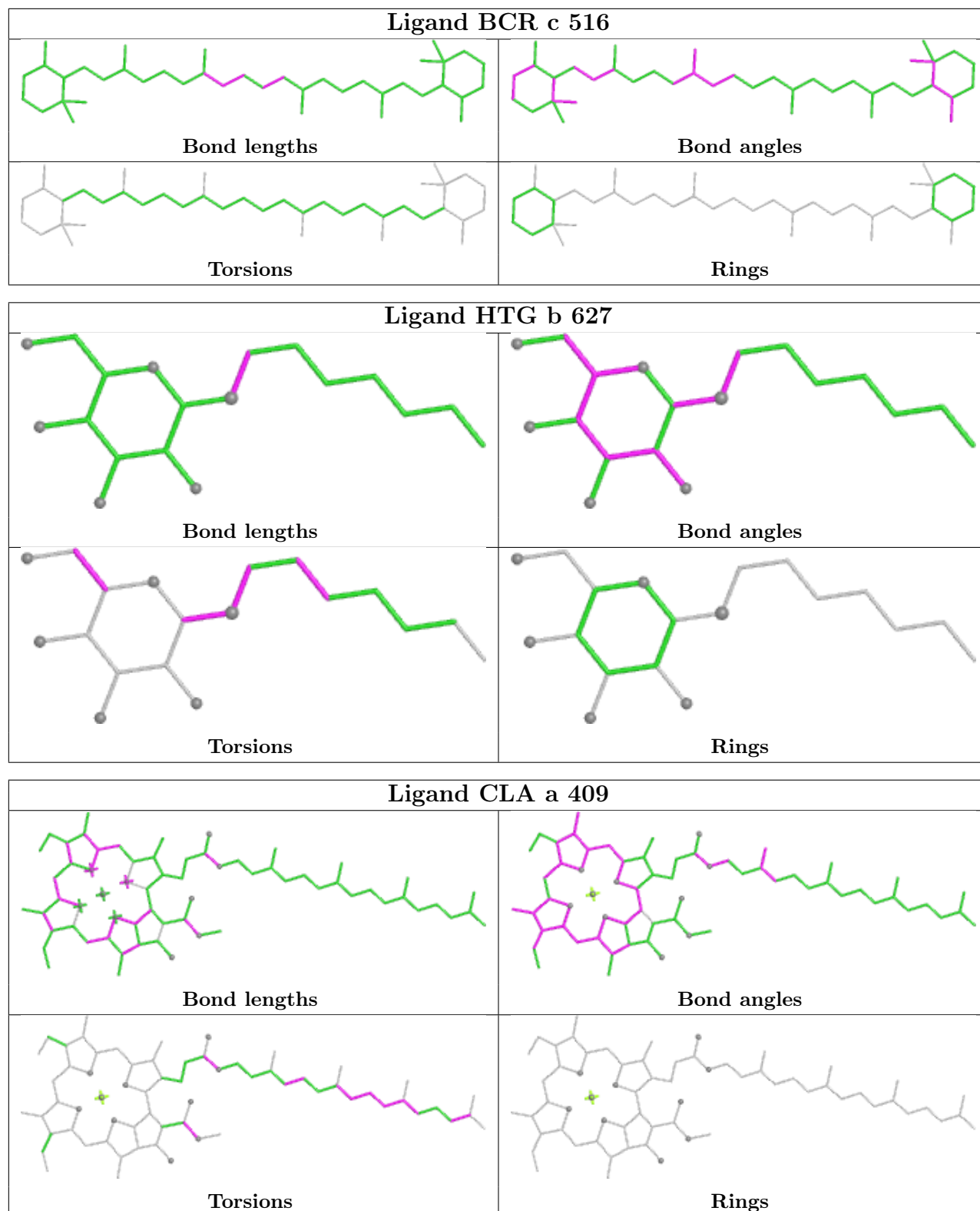
Ligand CLA C 507

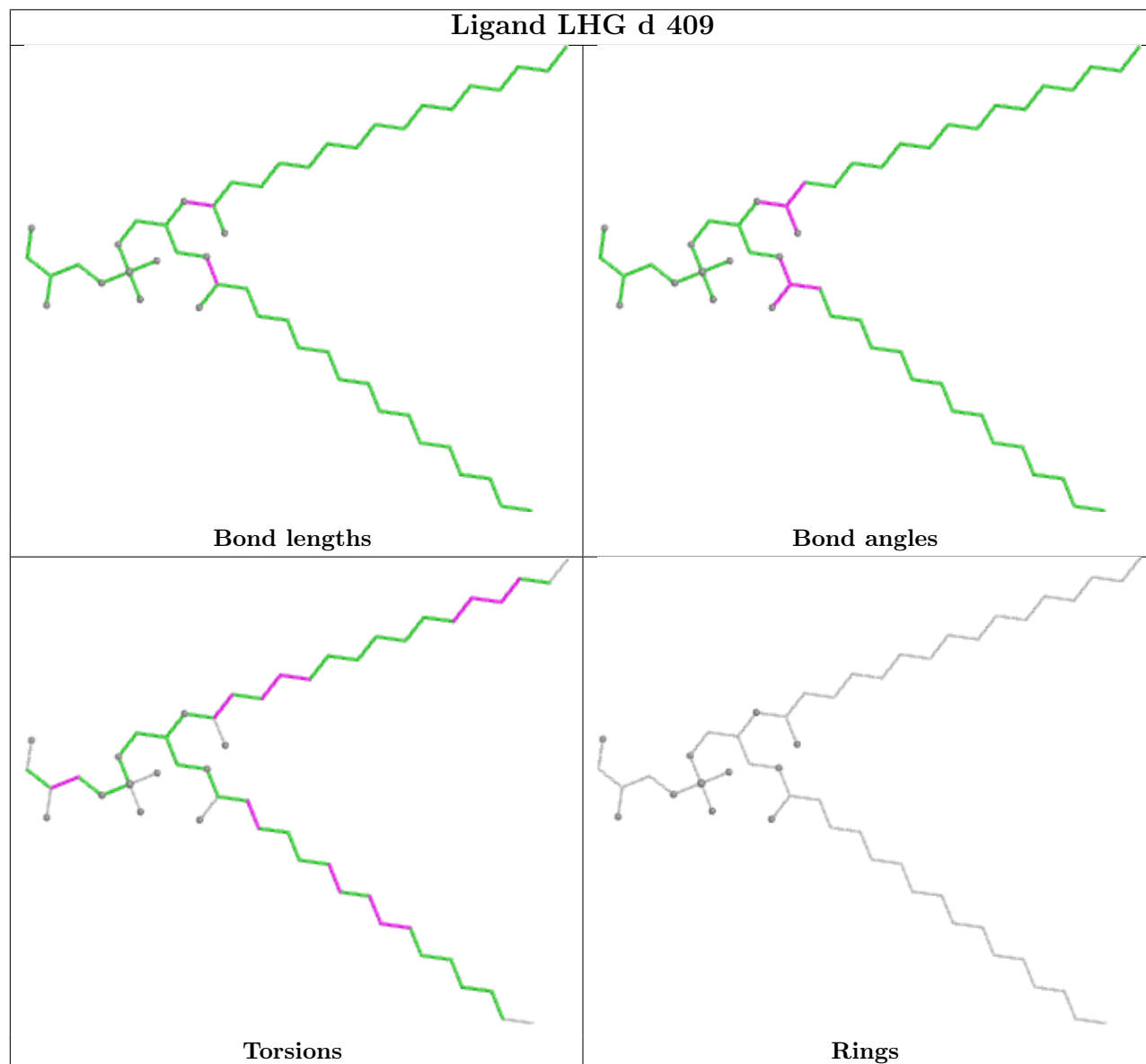
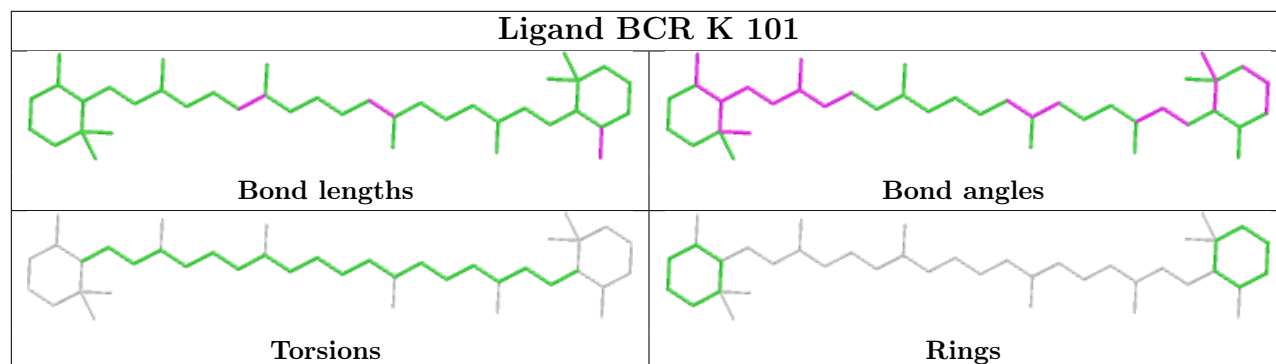


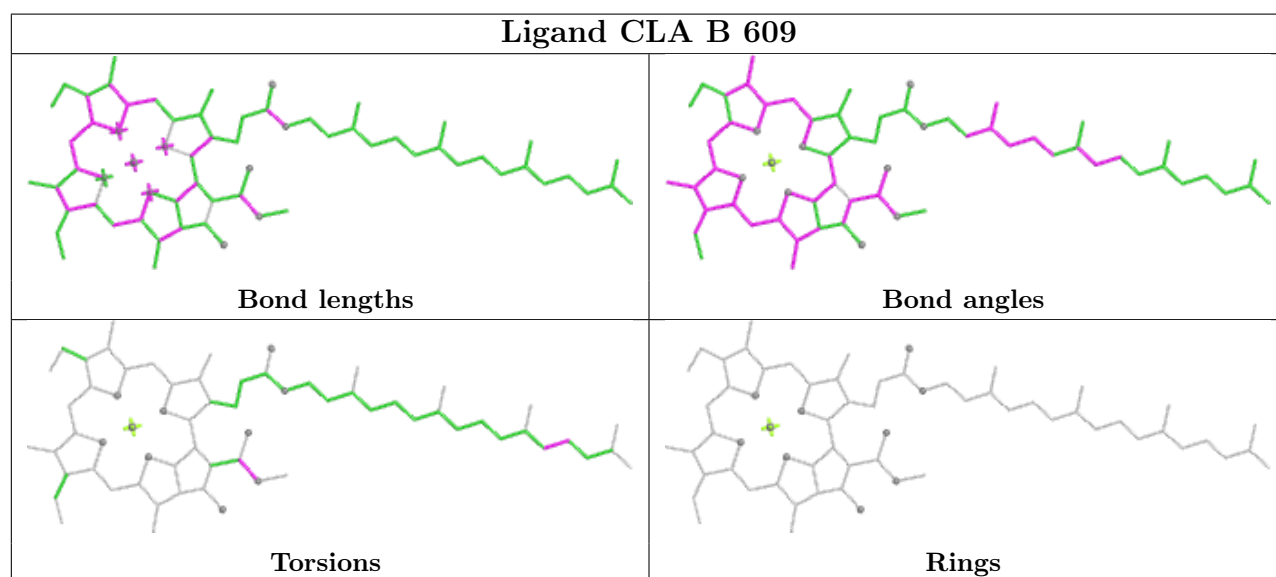
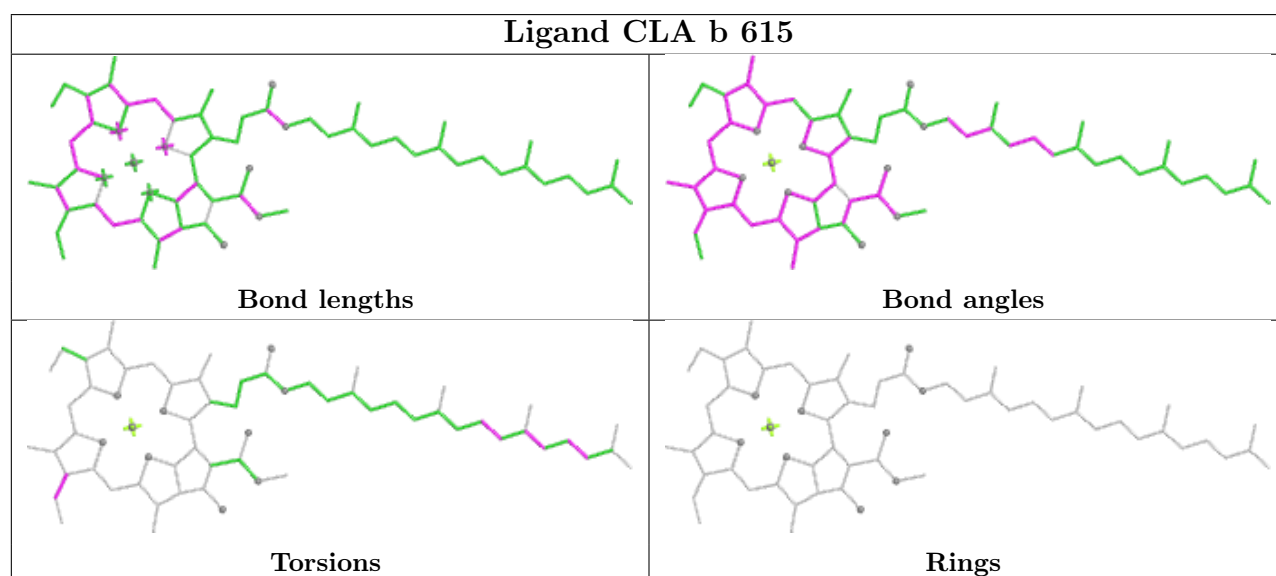
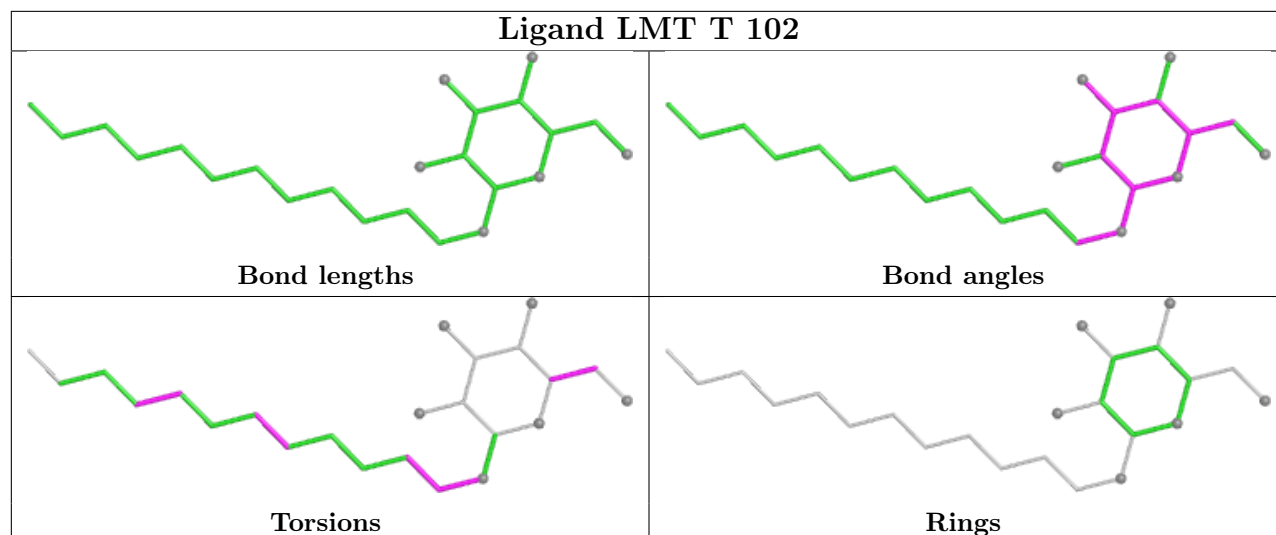
Ligand BCR Y 101

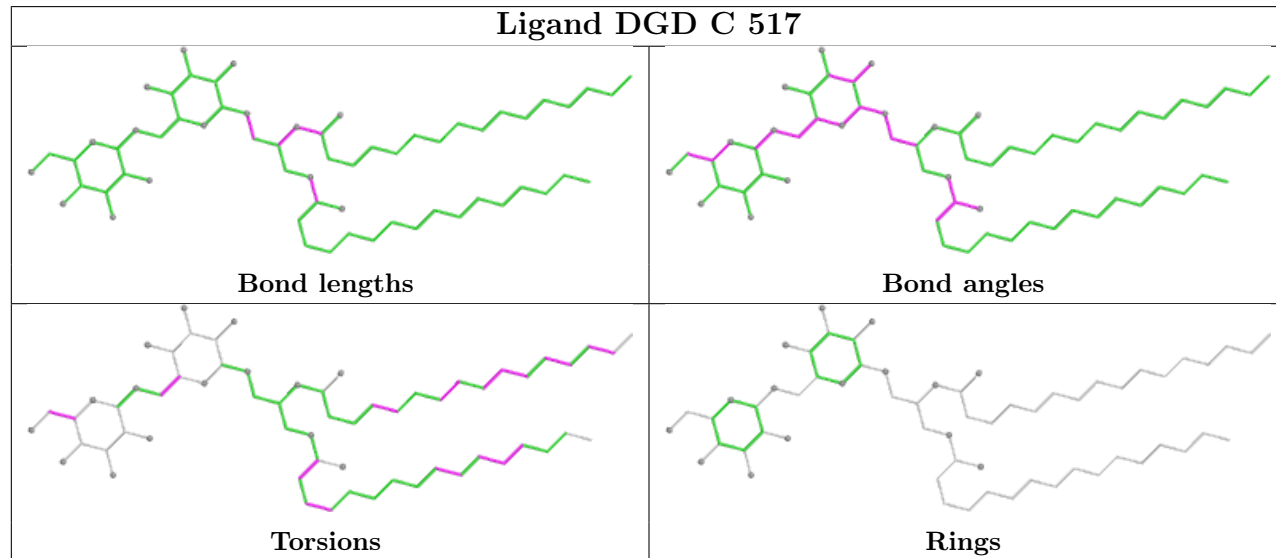
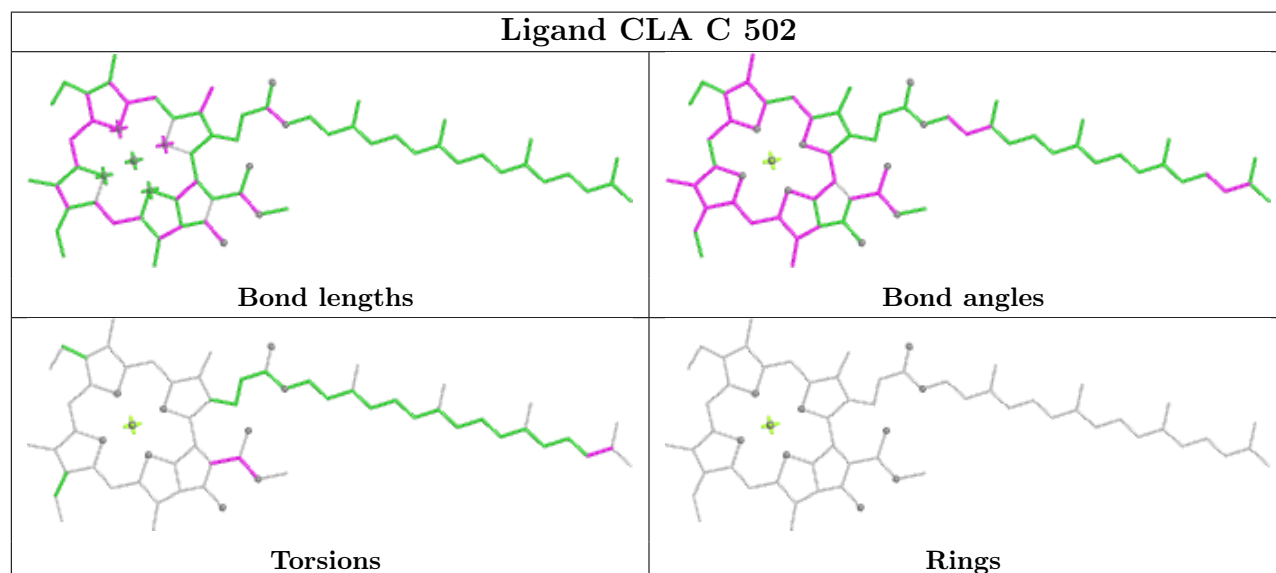
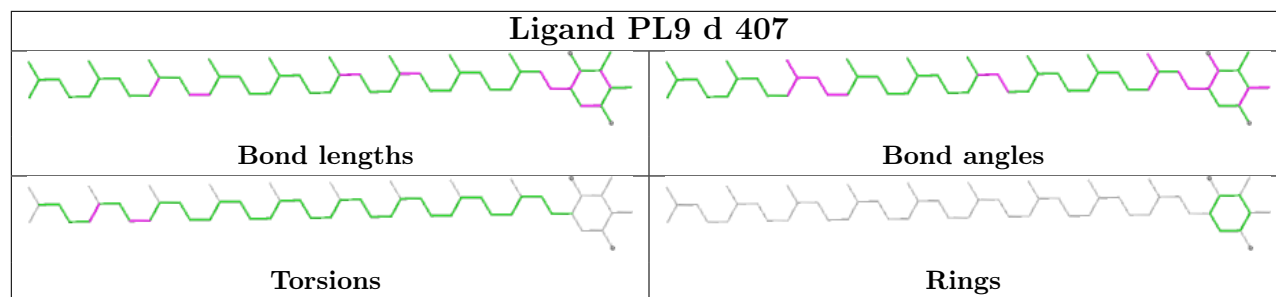


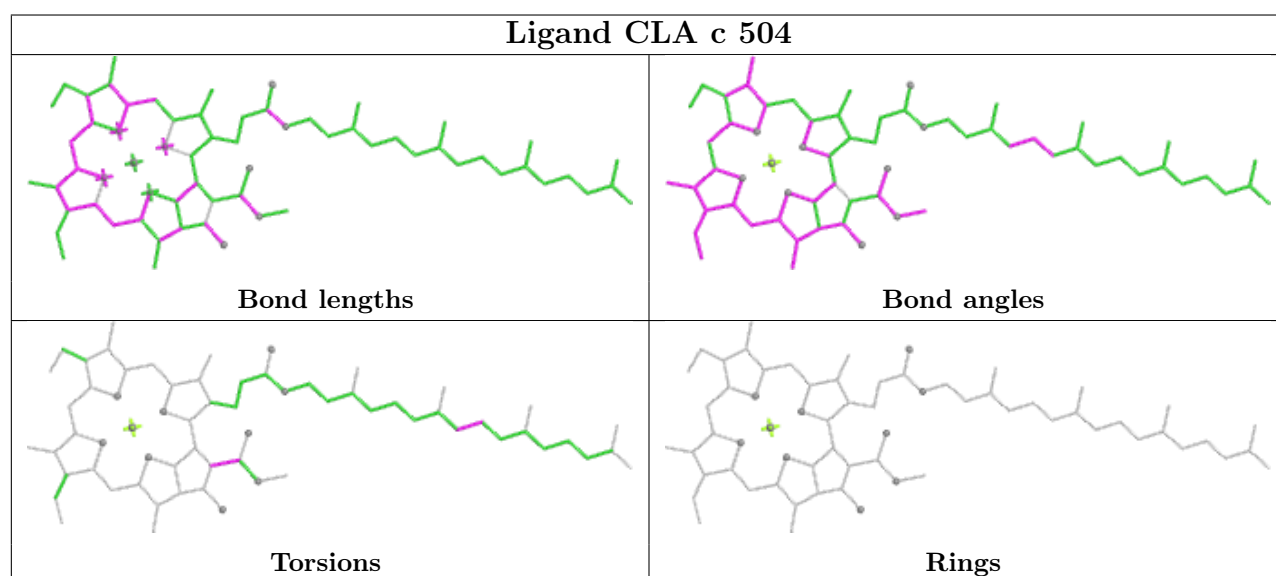
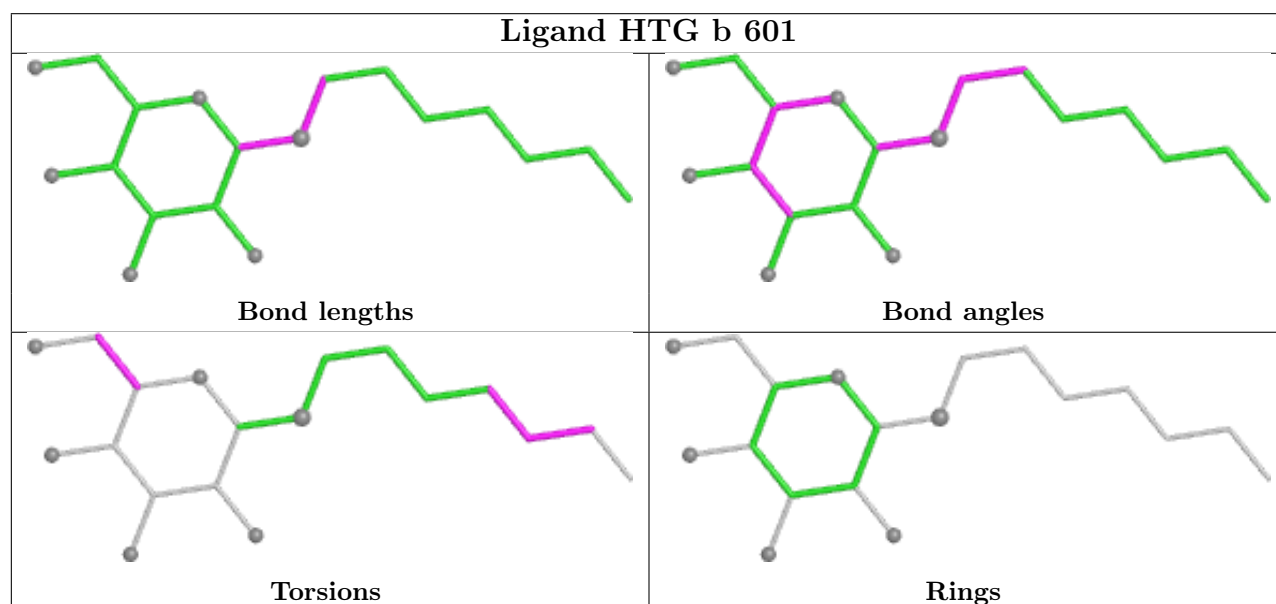
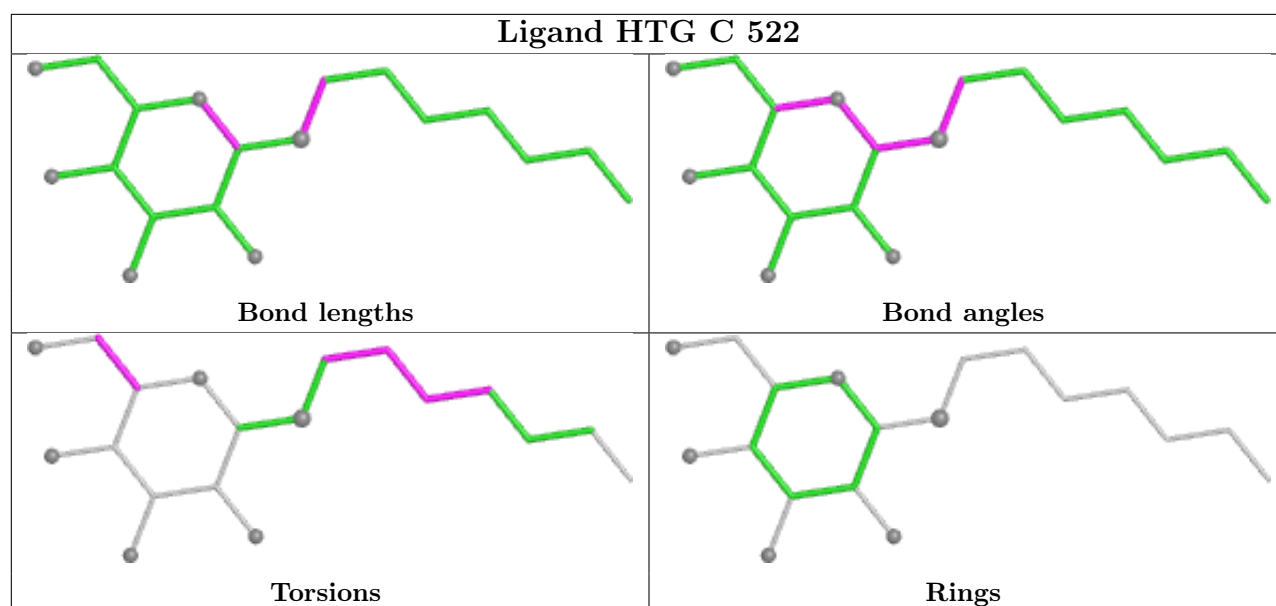
Ligand BCR d 406**Ligand CLA c 510****Ligand PHO a 408**

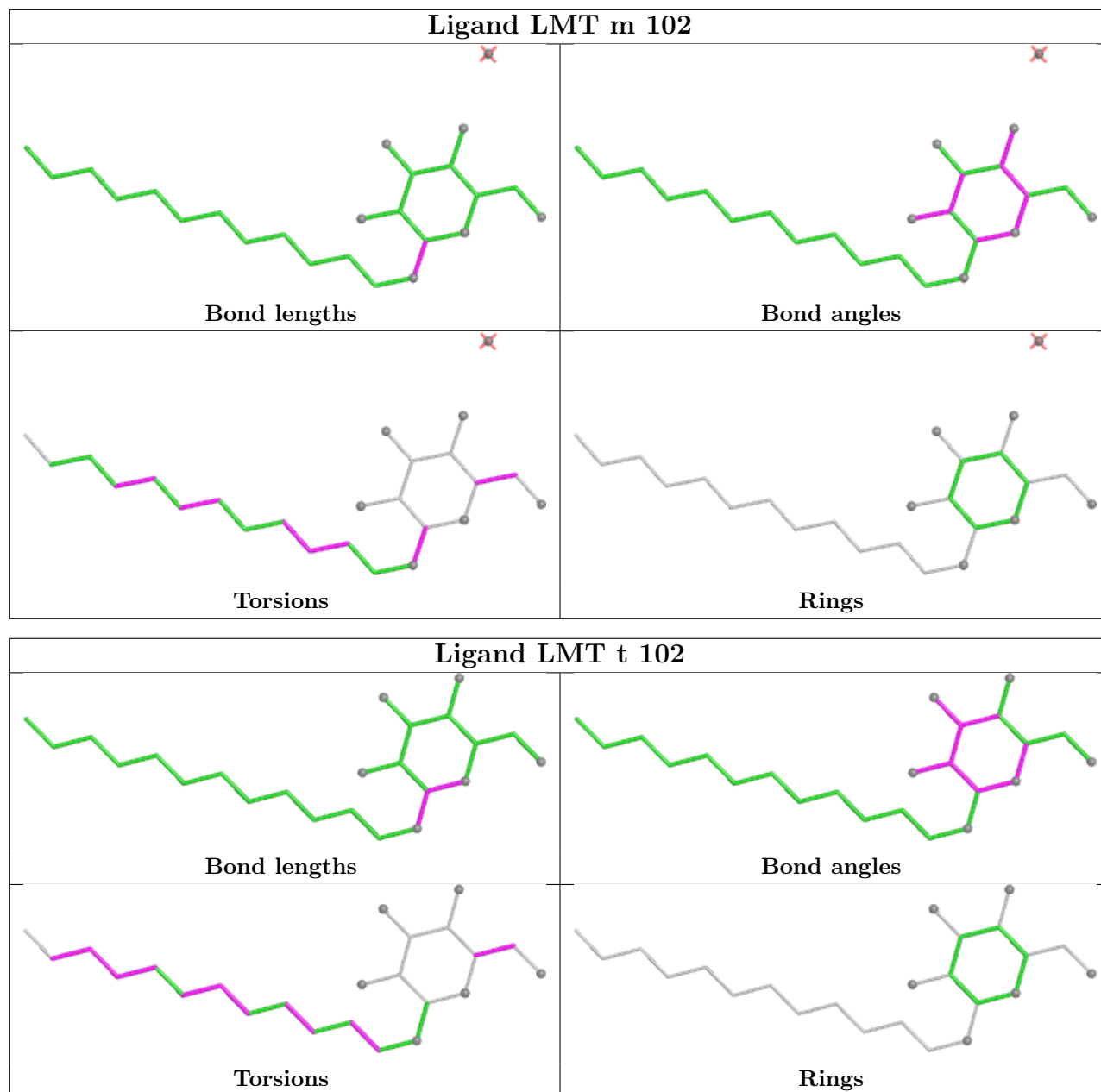


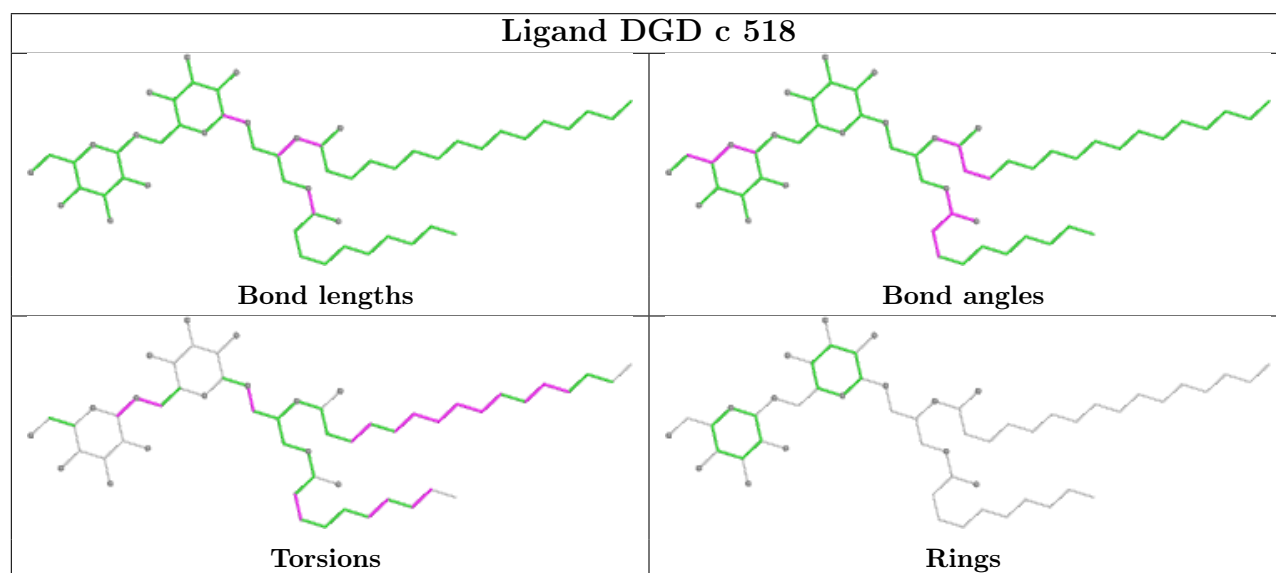
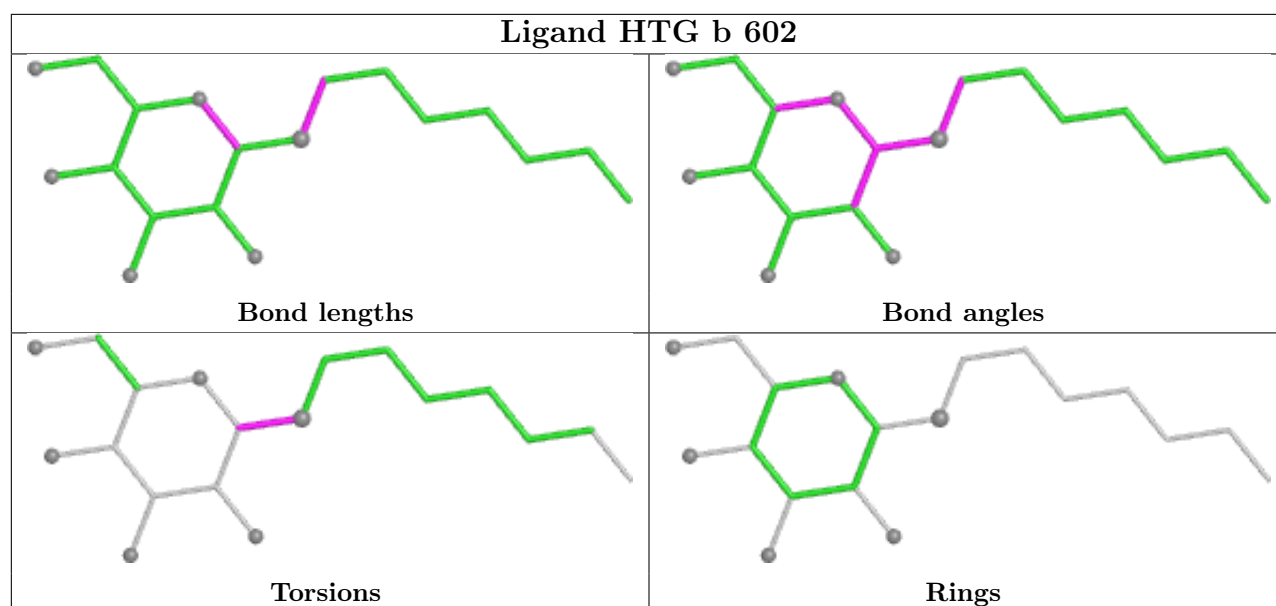


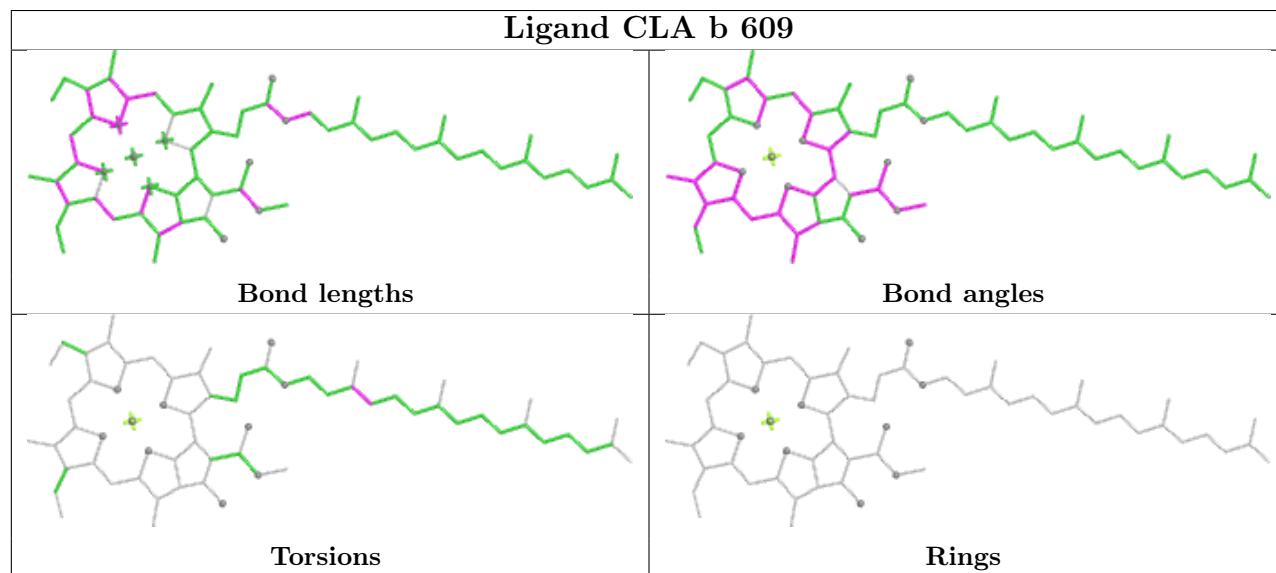
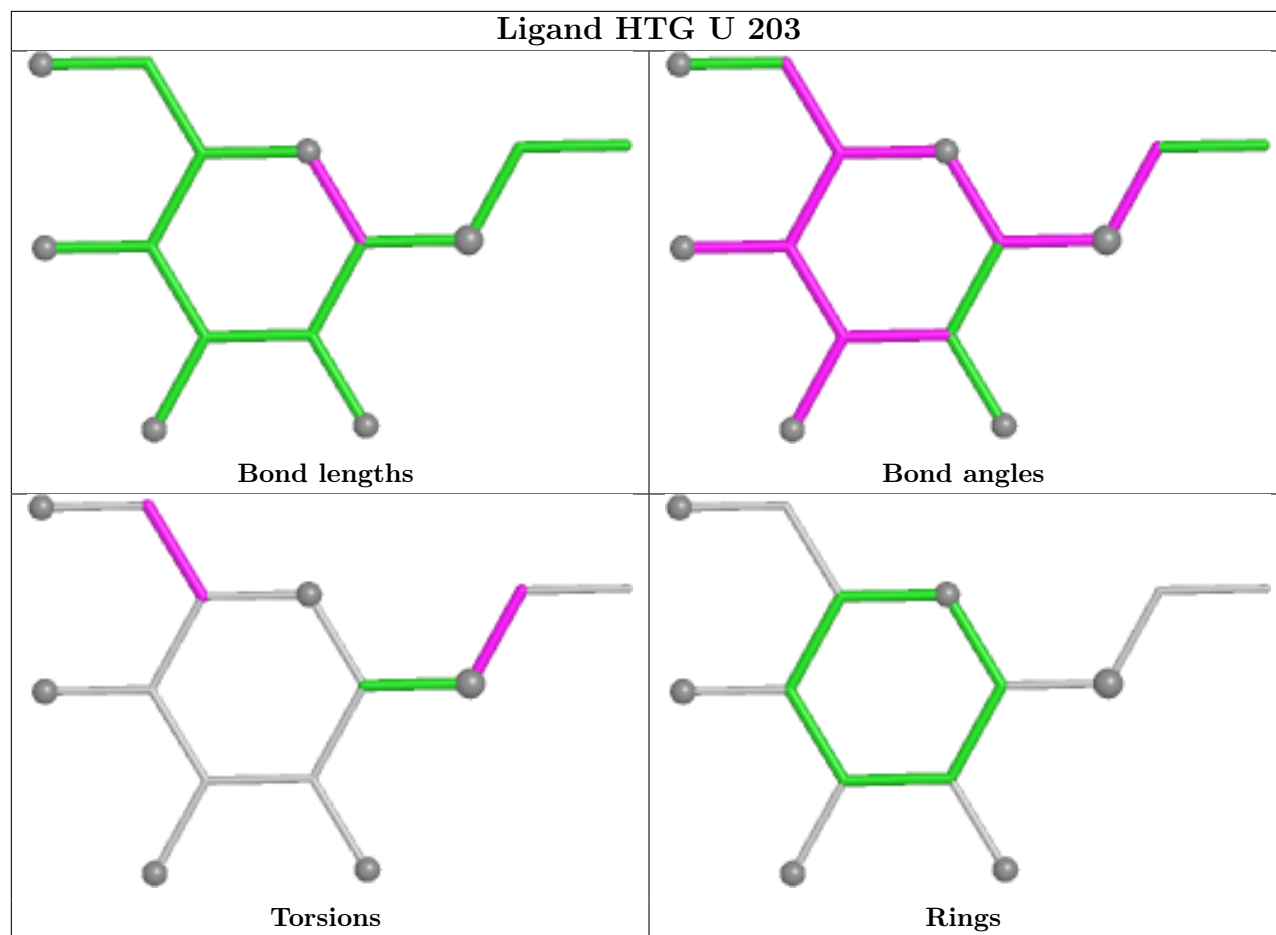


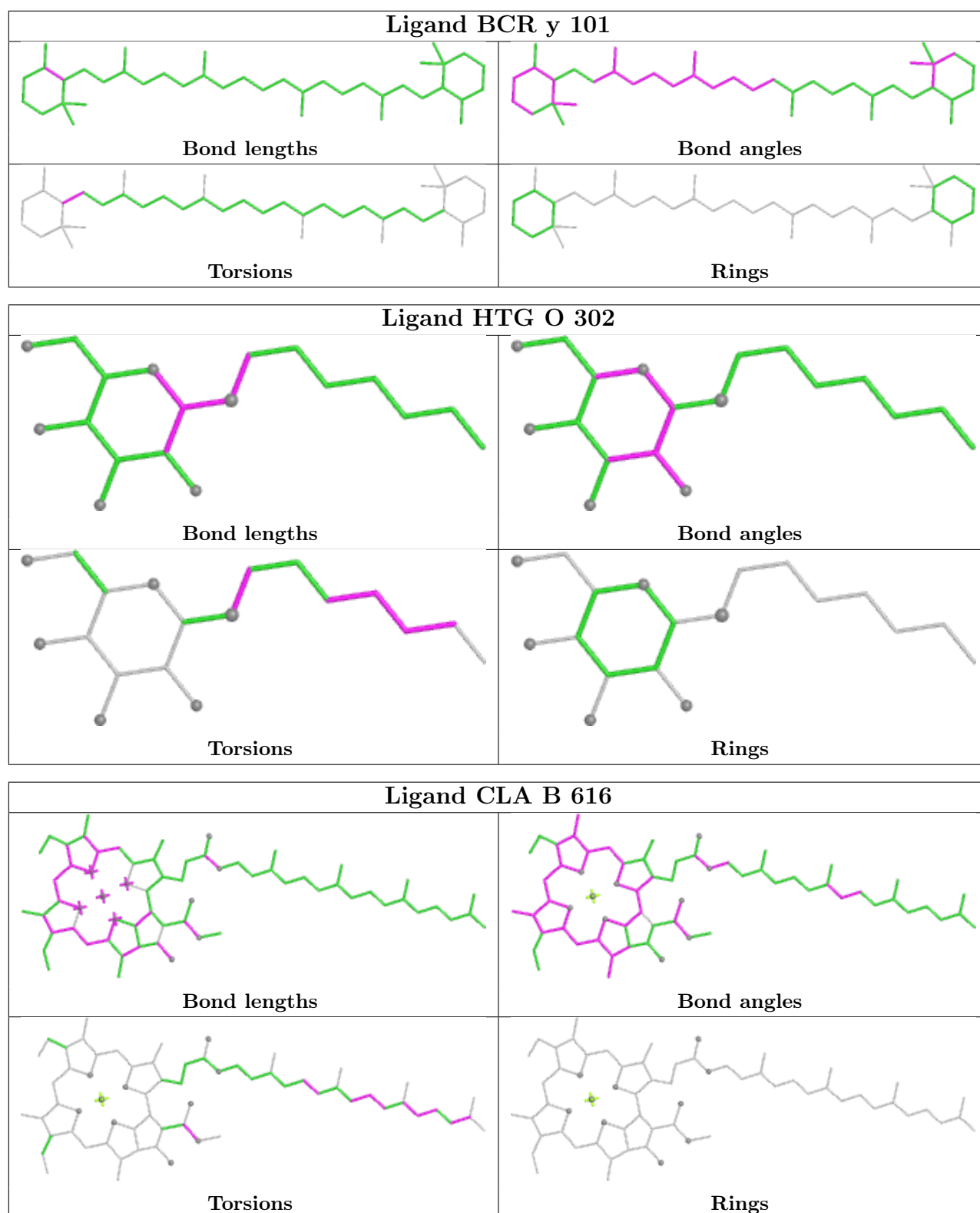


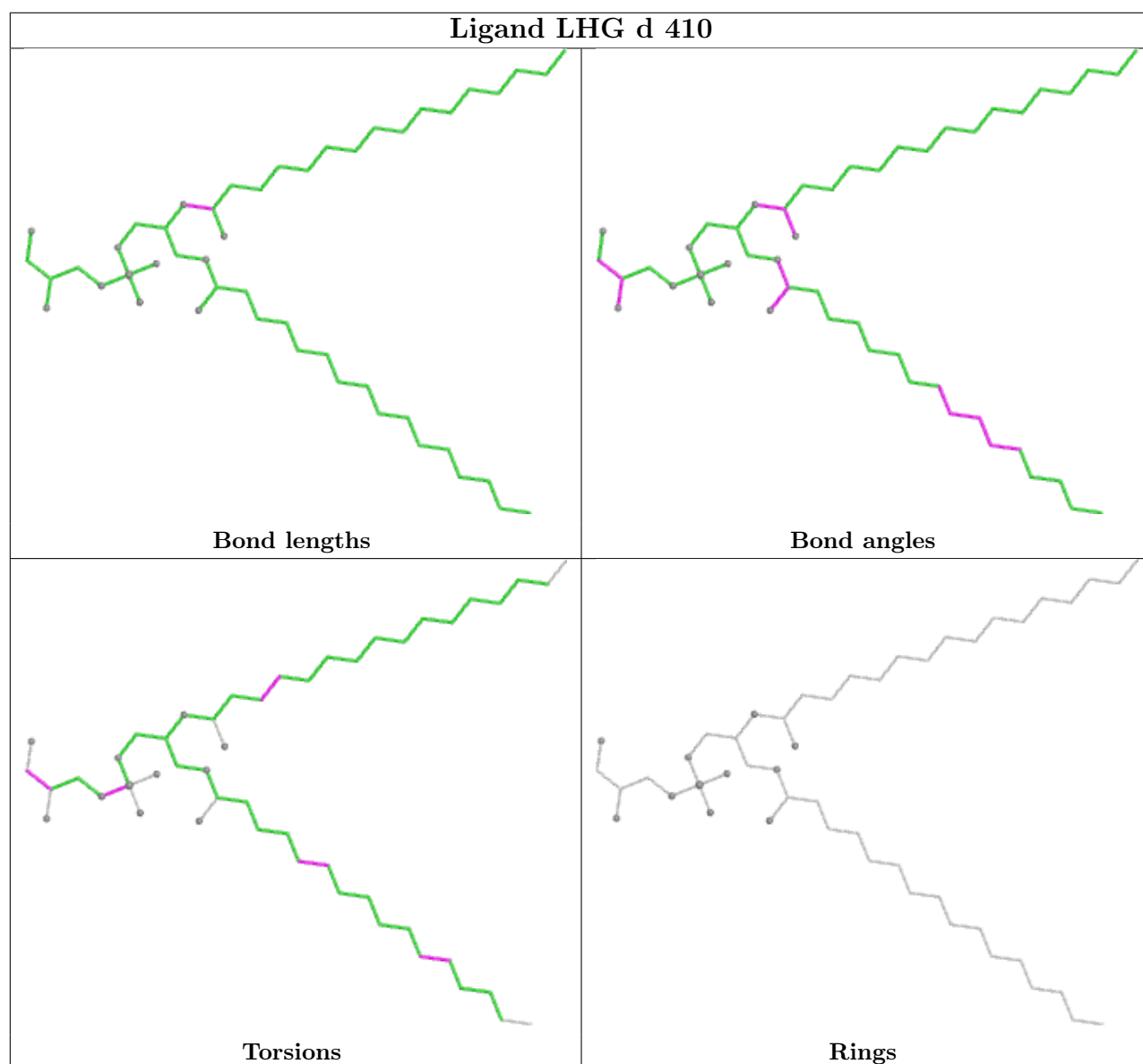
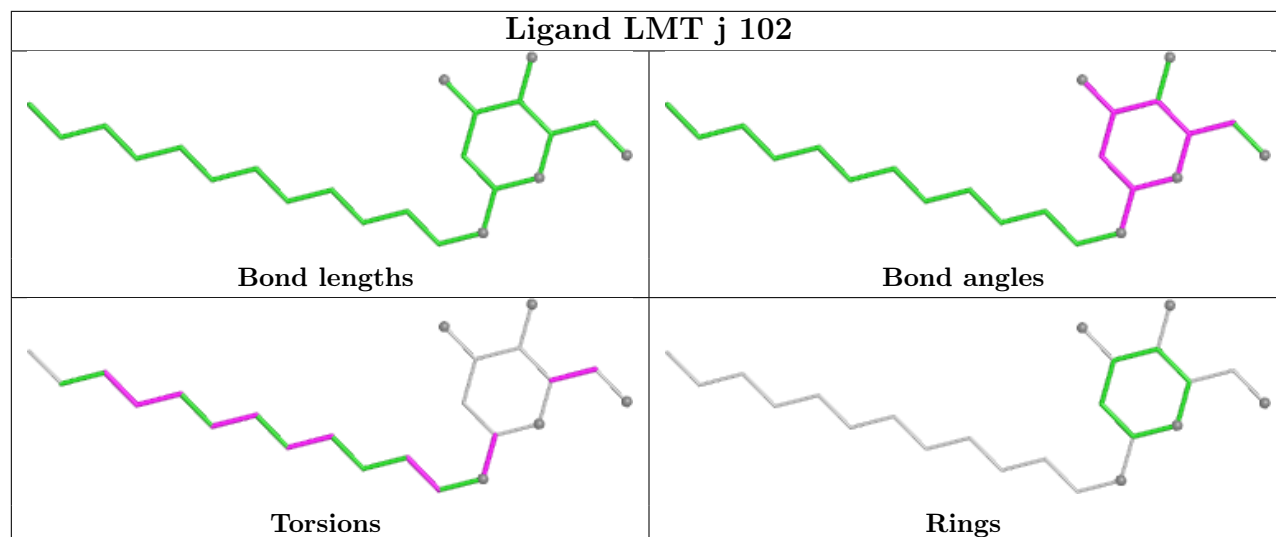


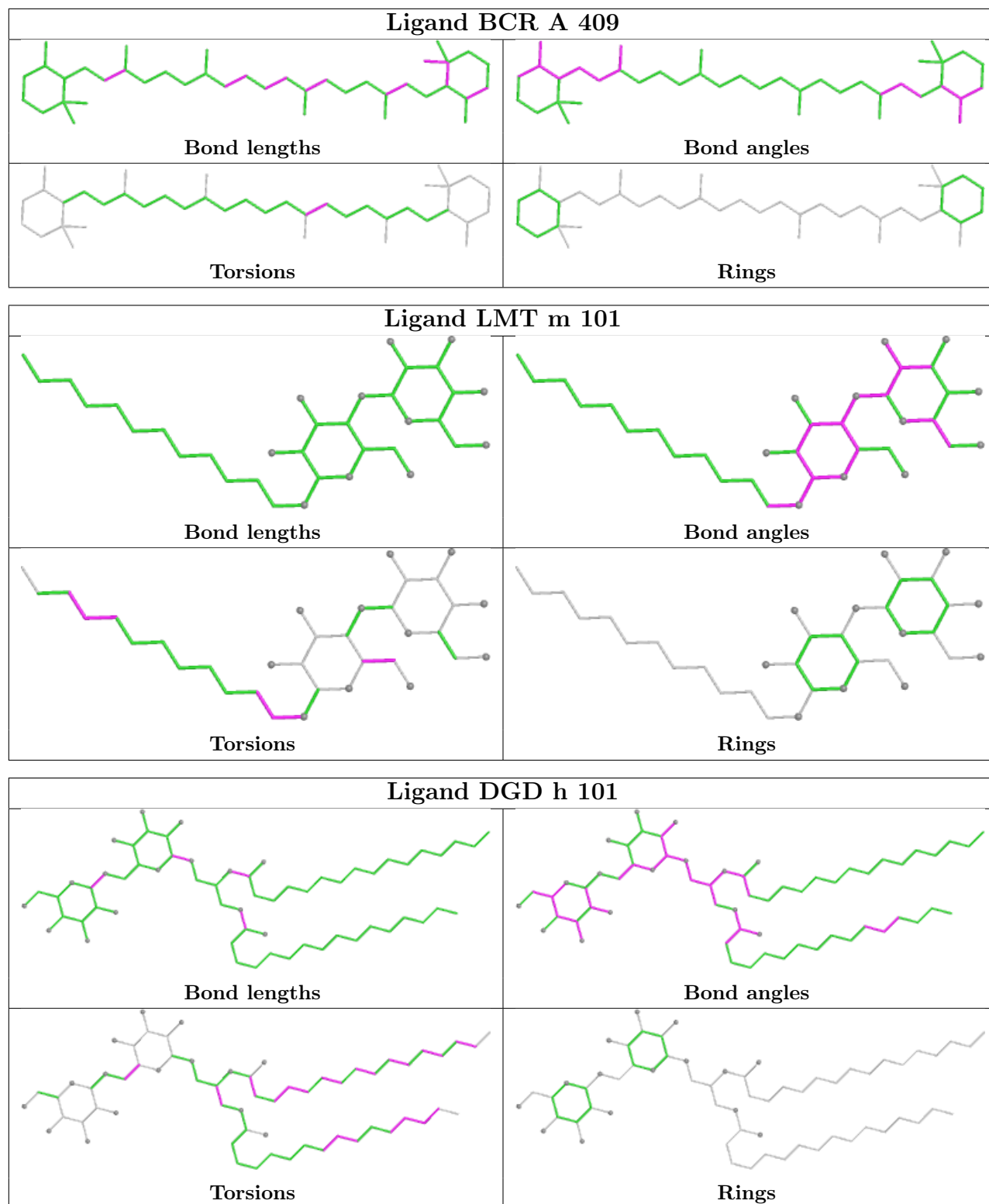


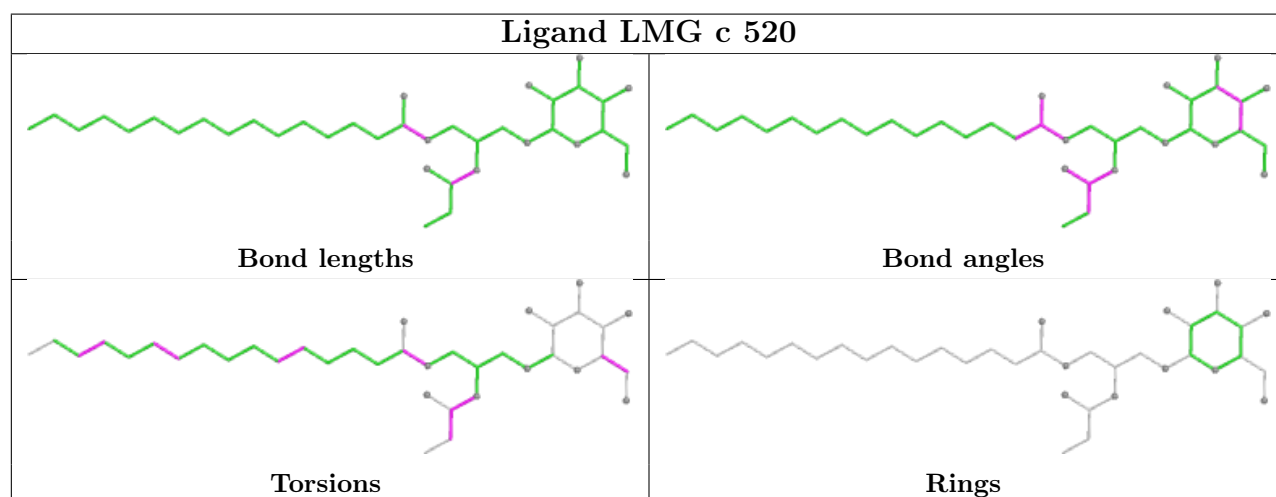
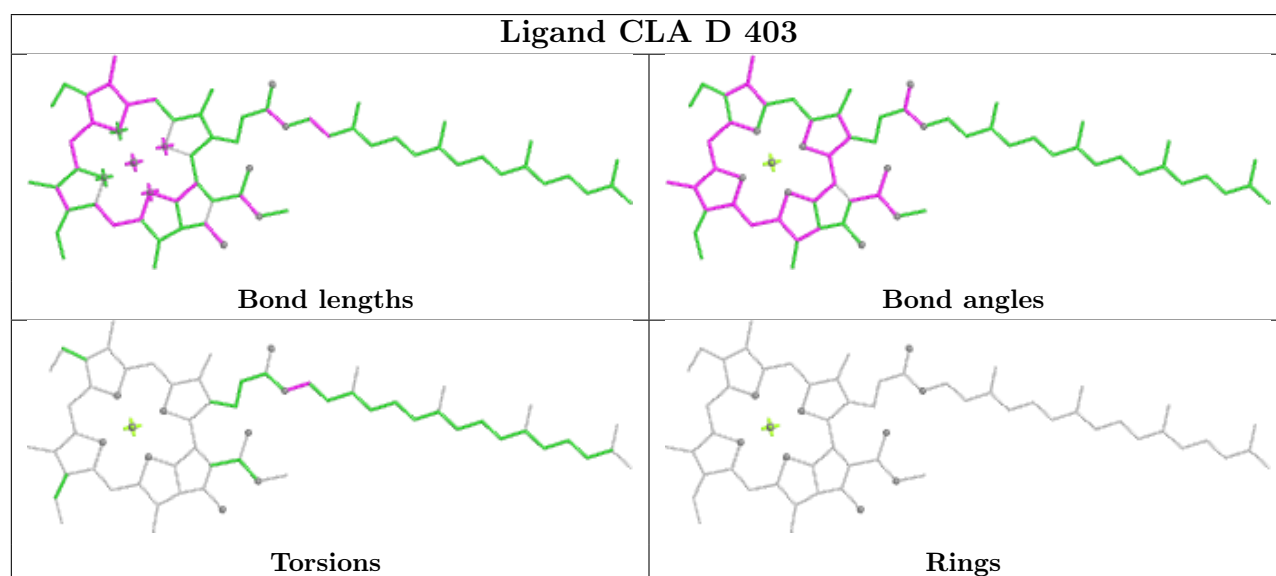
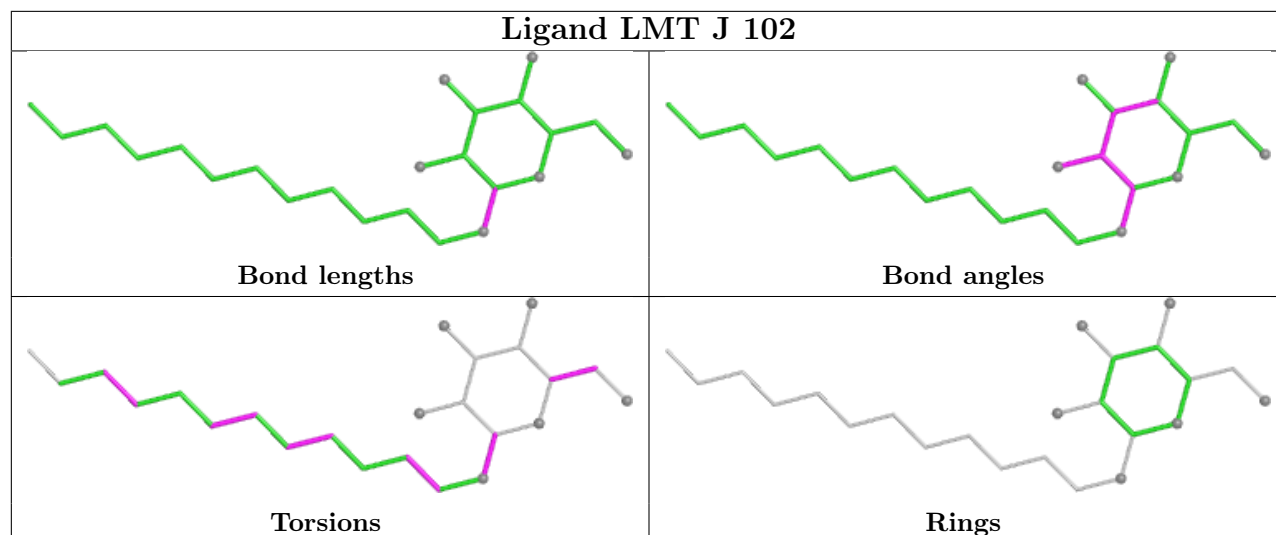


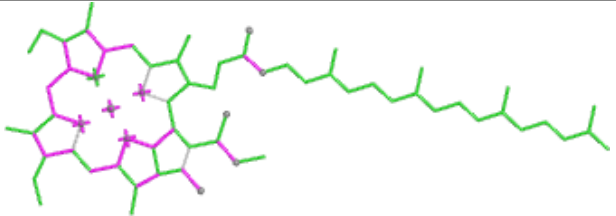
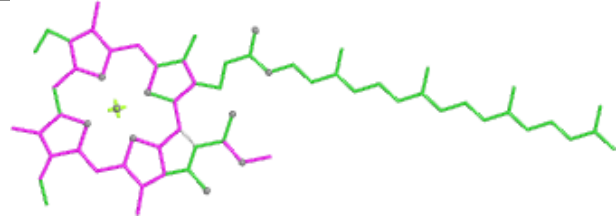
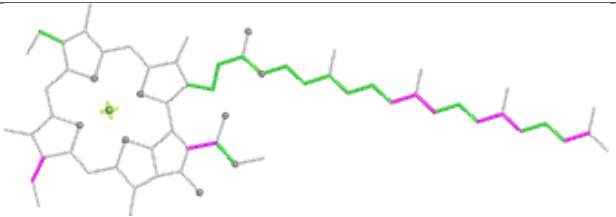
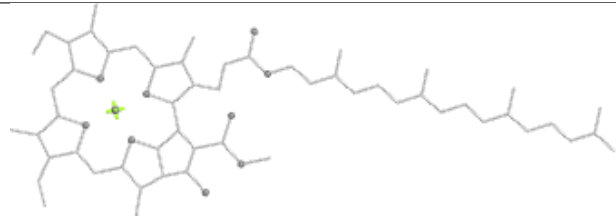


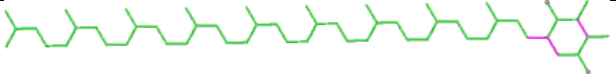
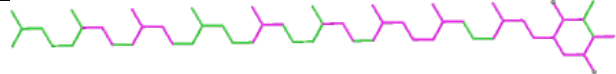
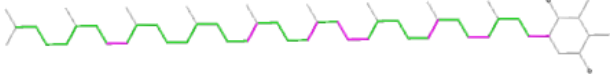
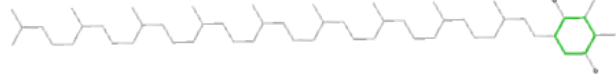


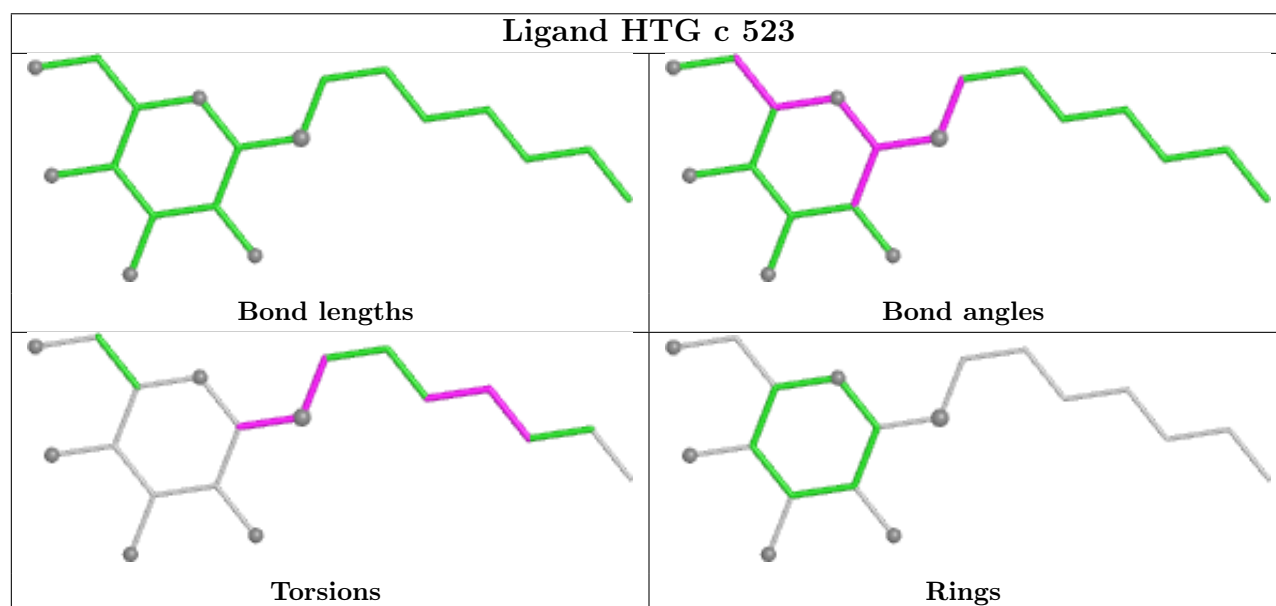
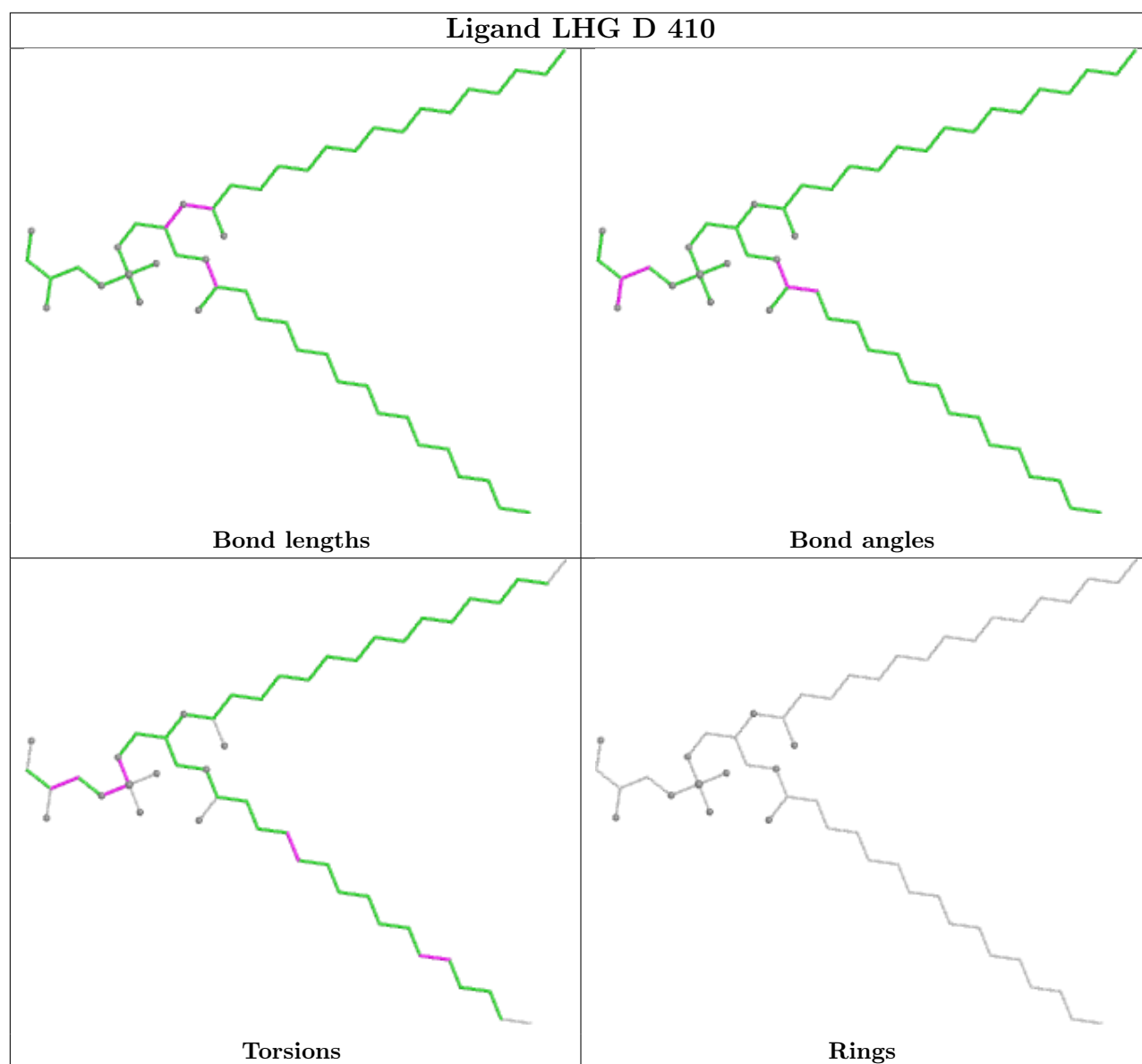


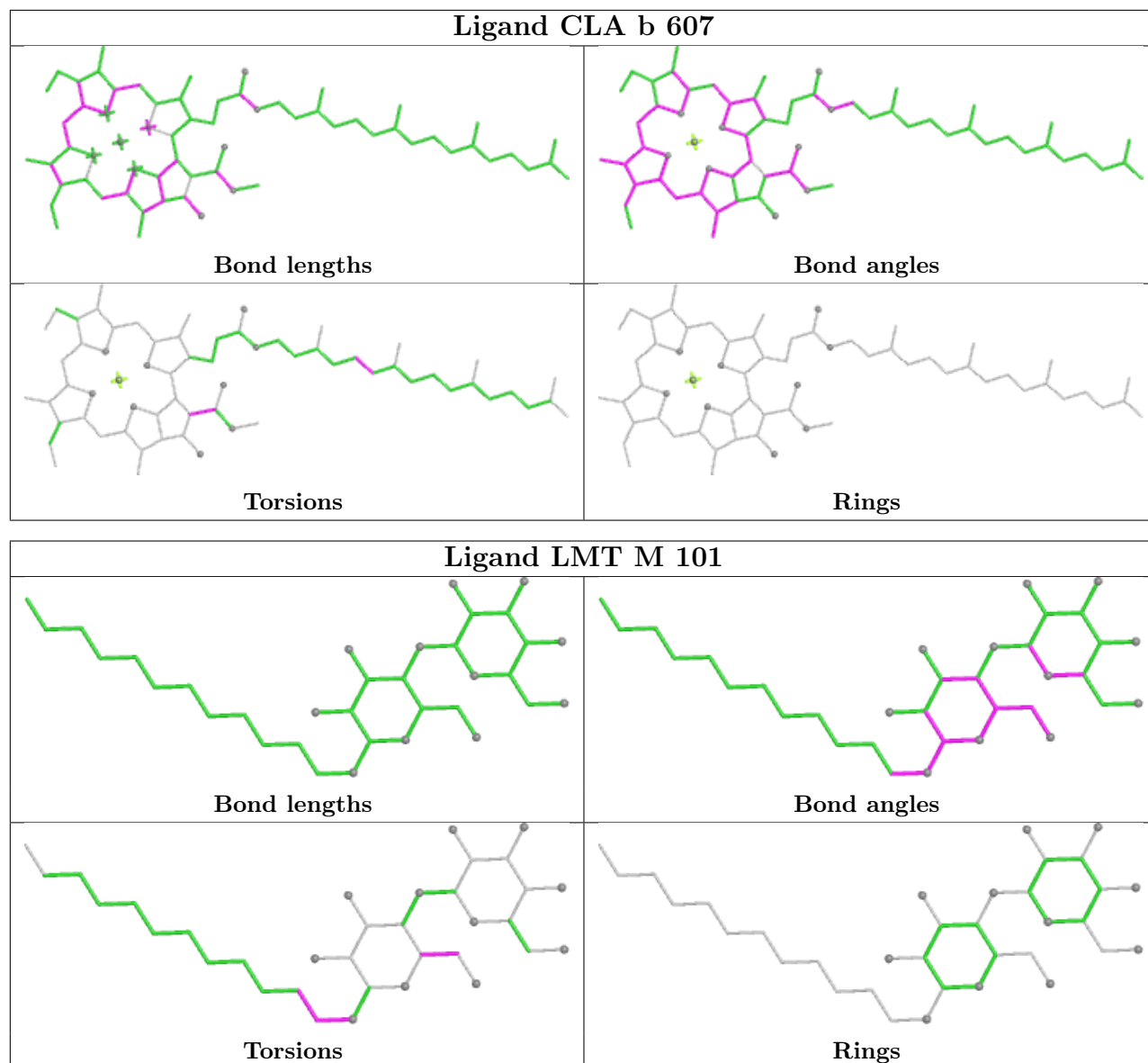


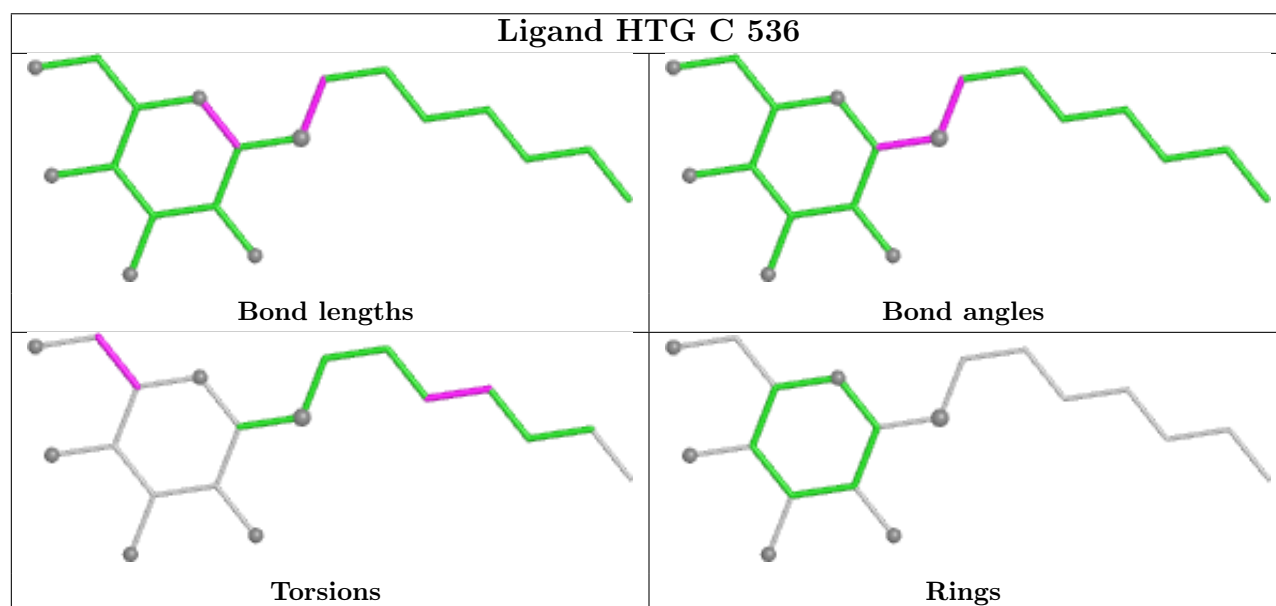
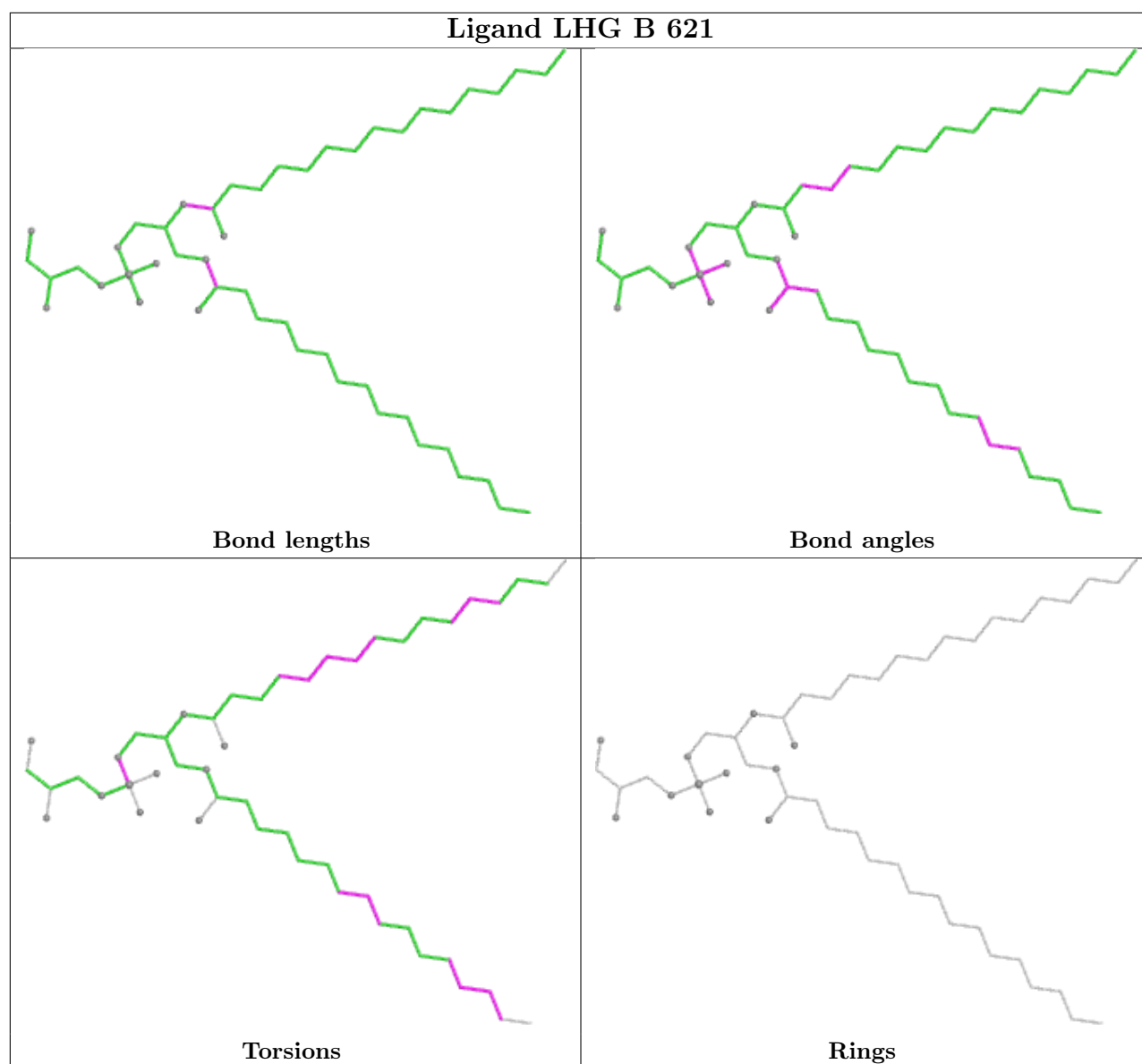


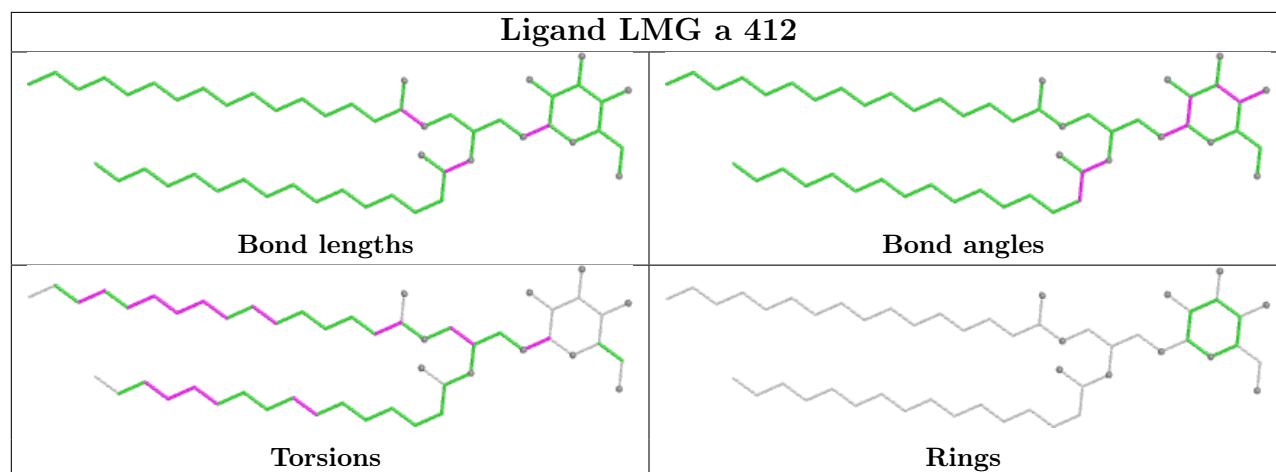
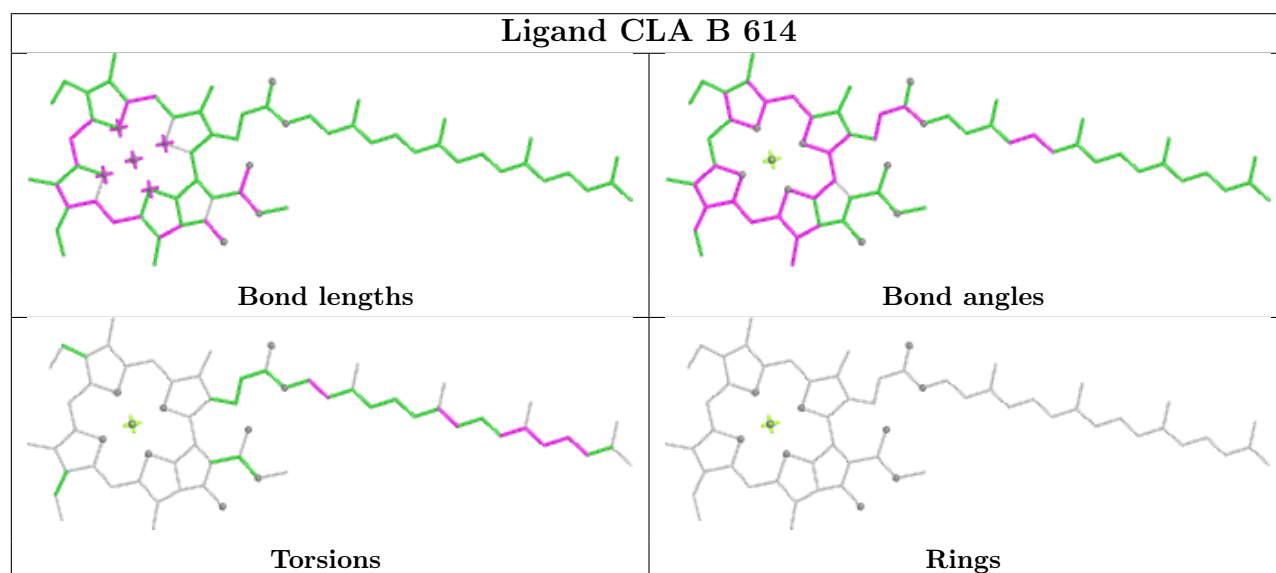
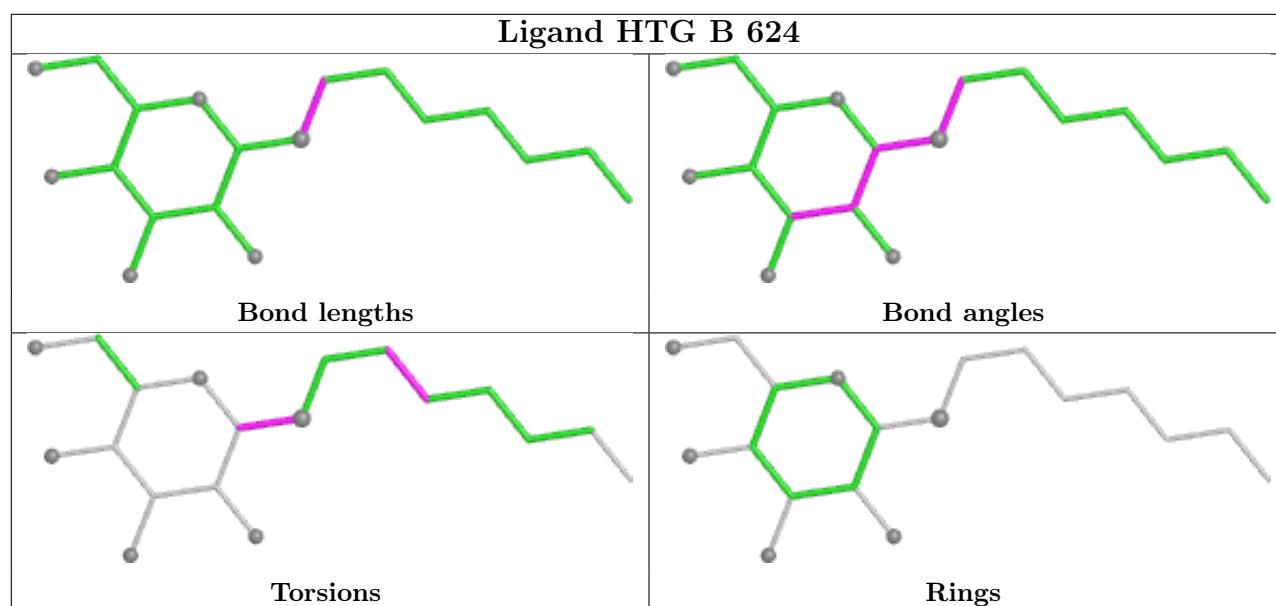
Ligand CLA a 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

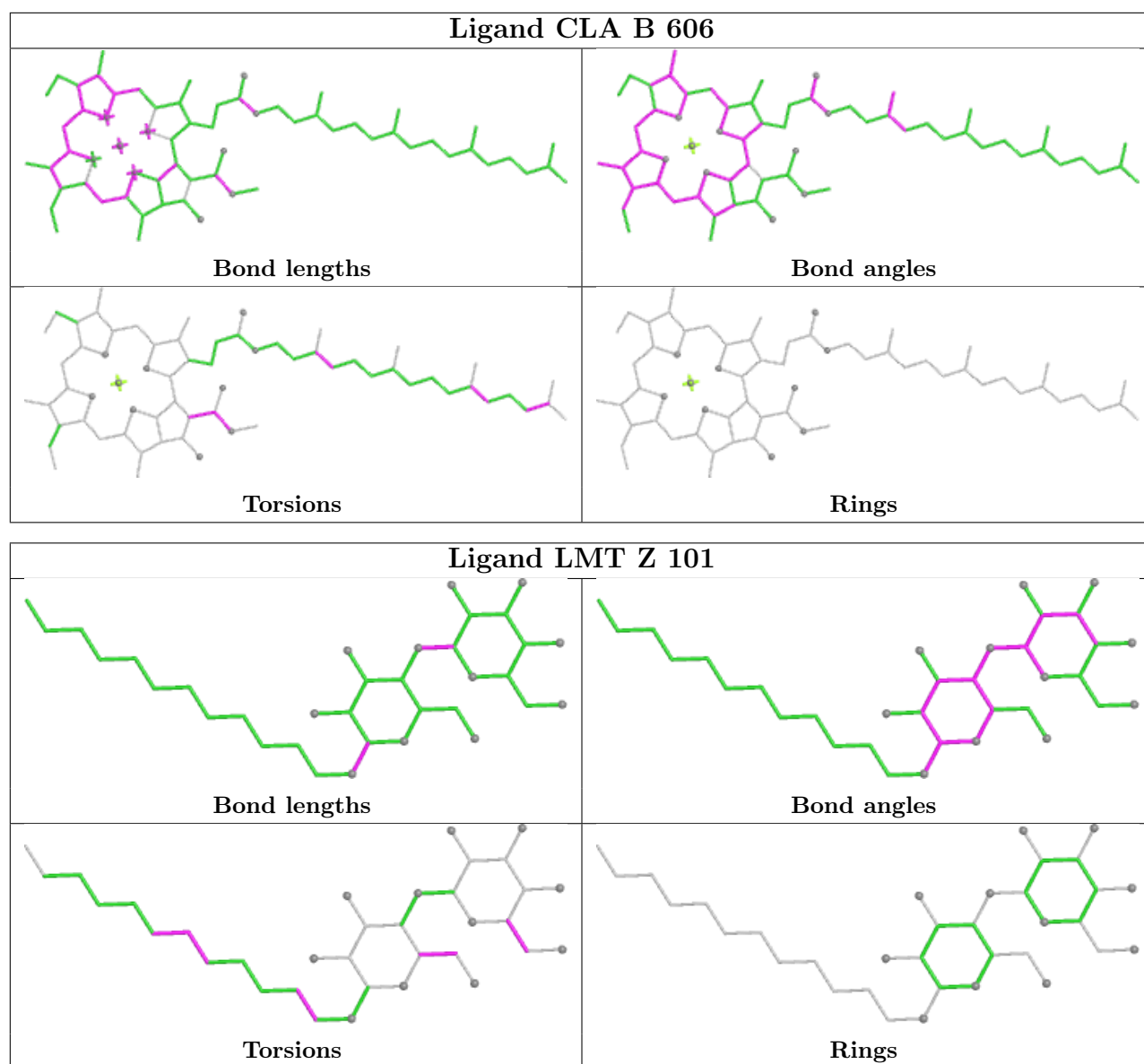
Ligand PL9 a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

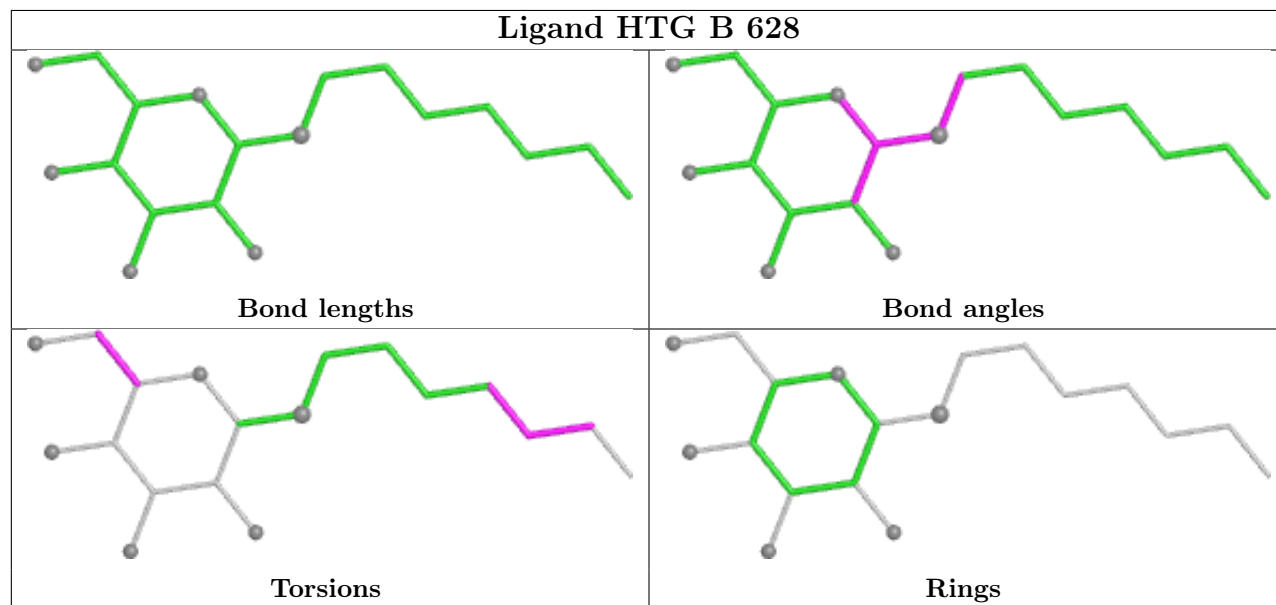
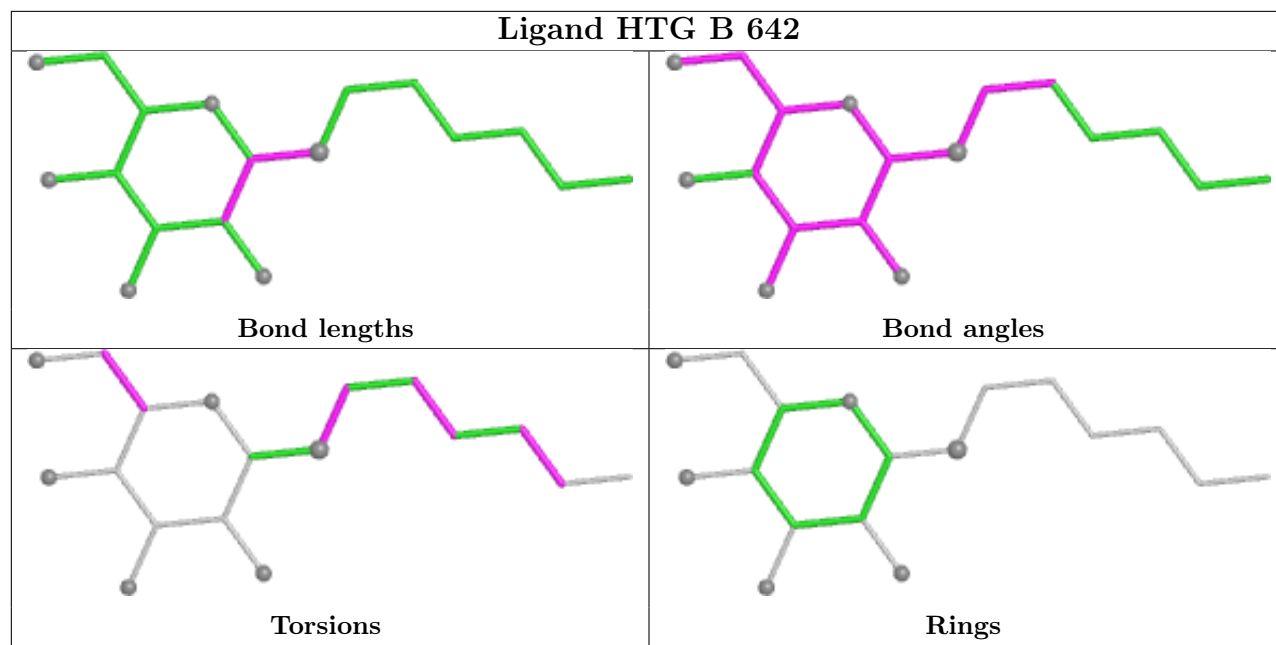


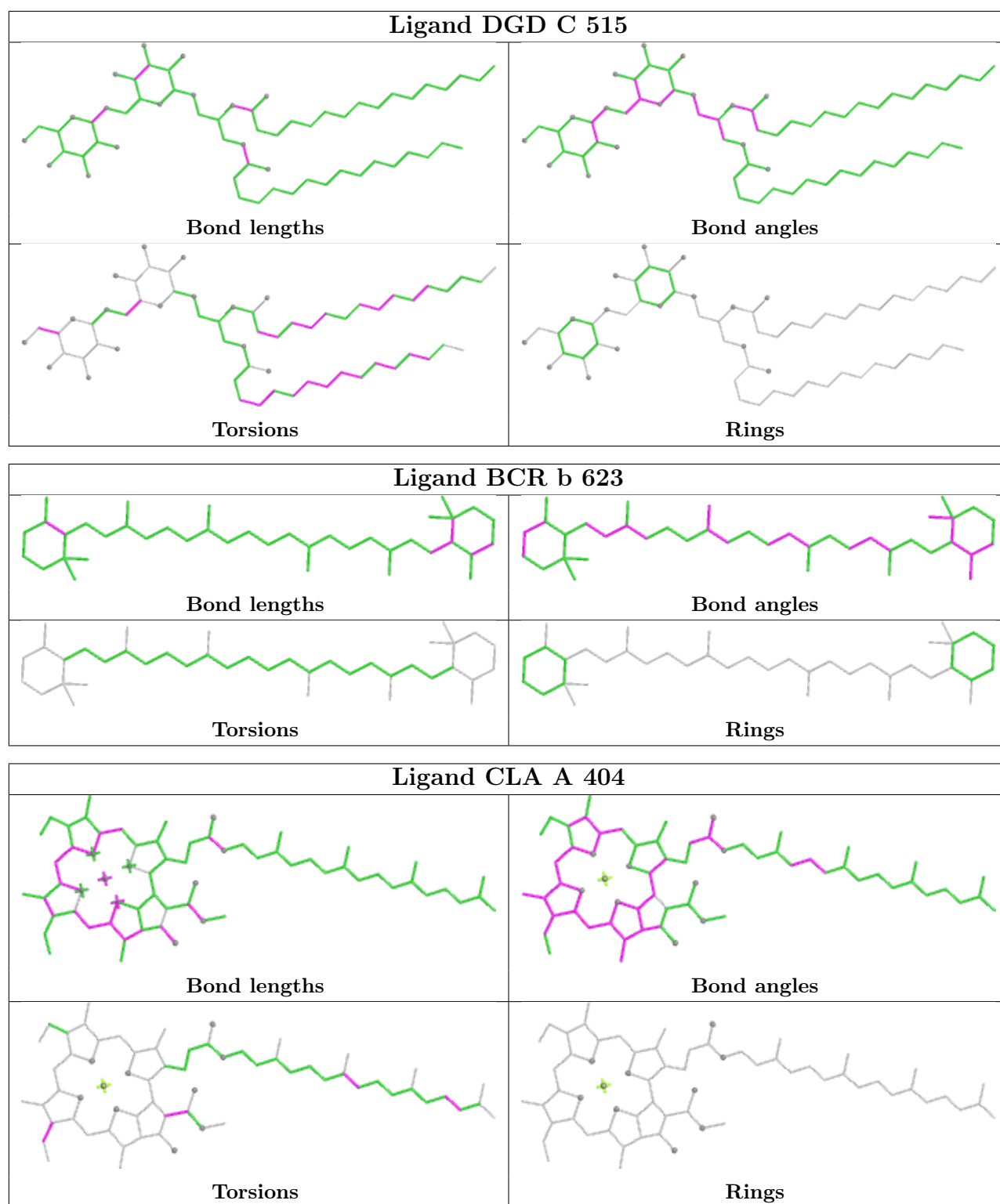




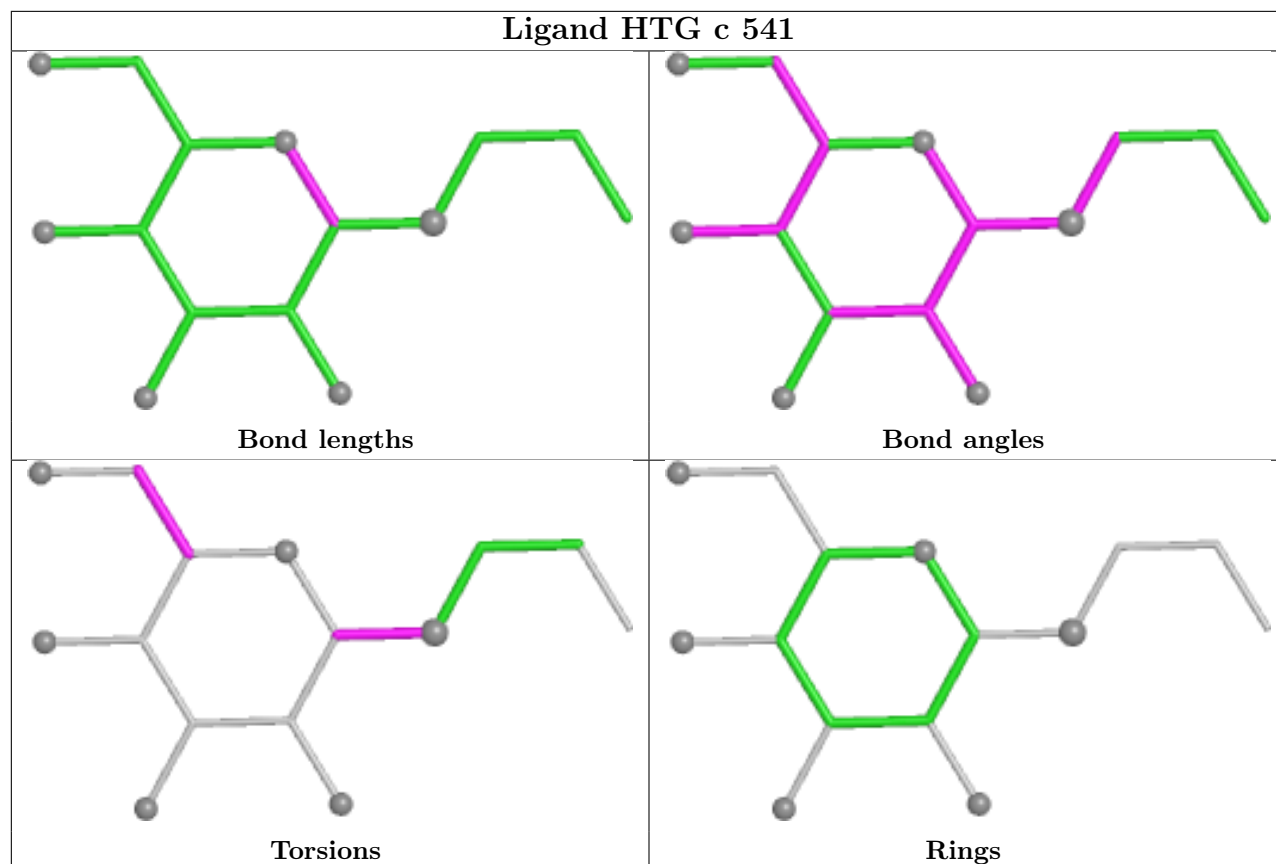




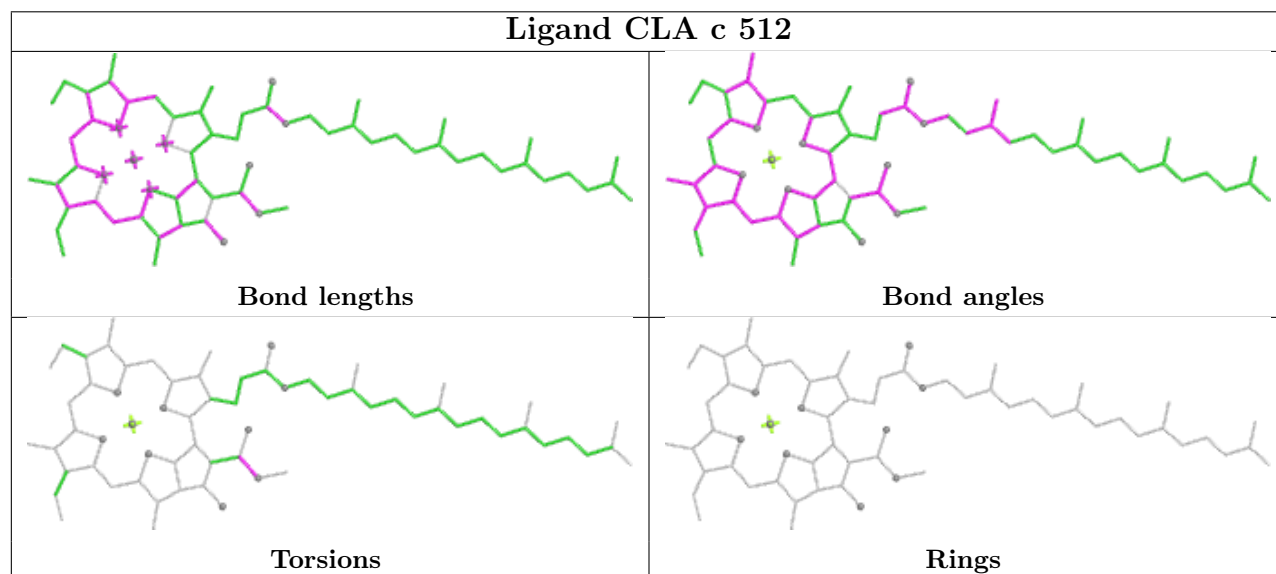


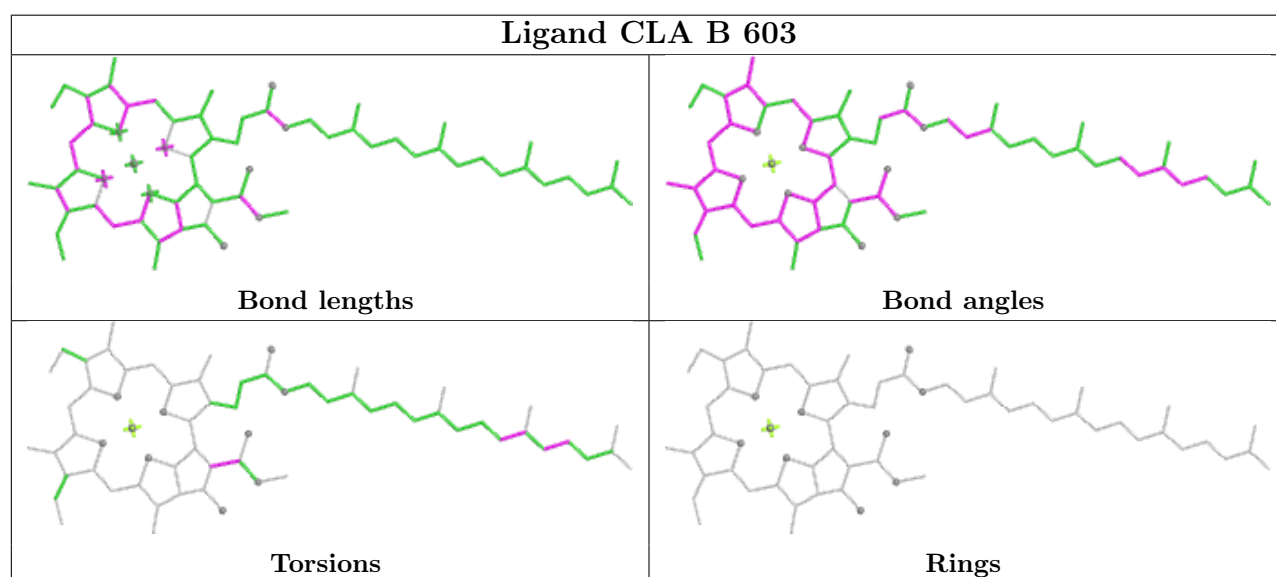
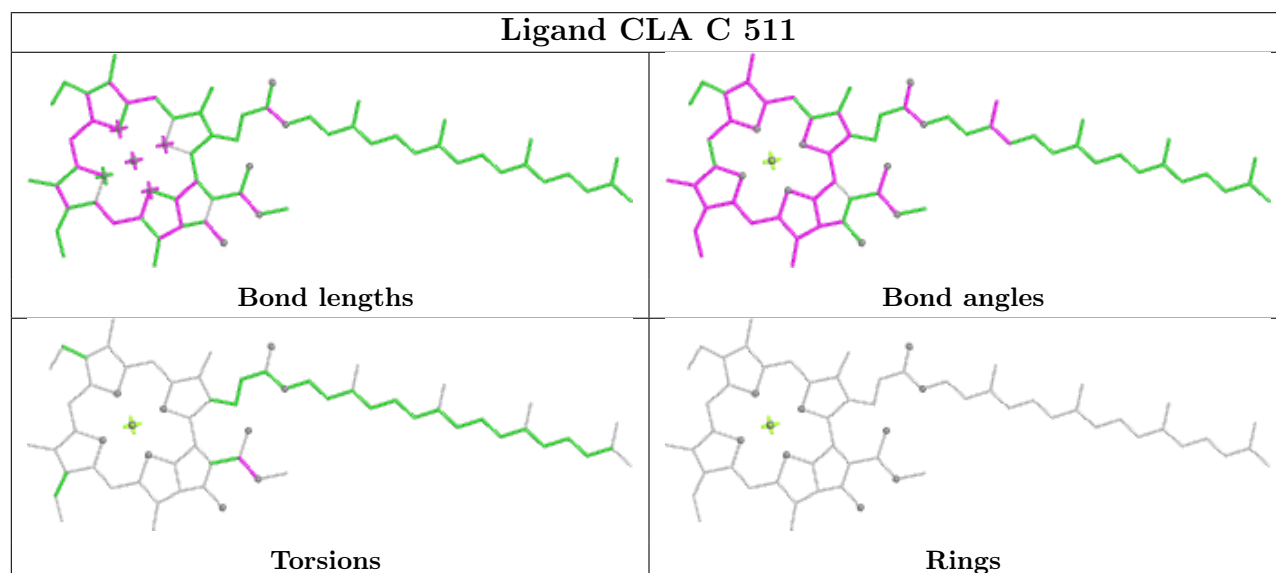
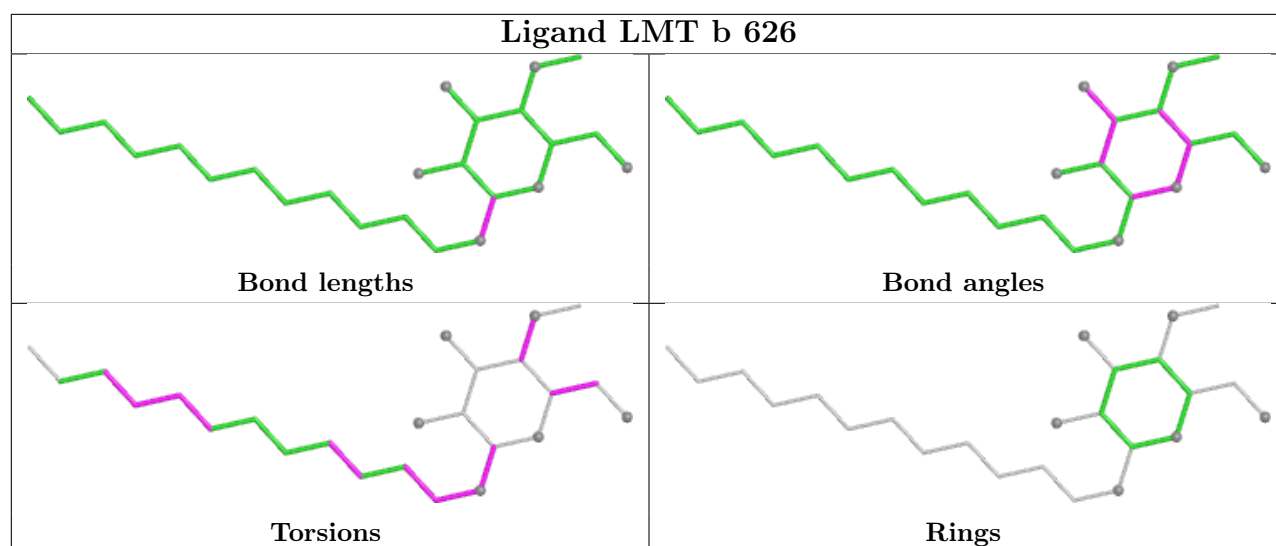


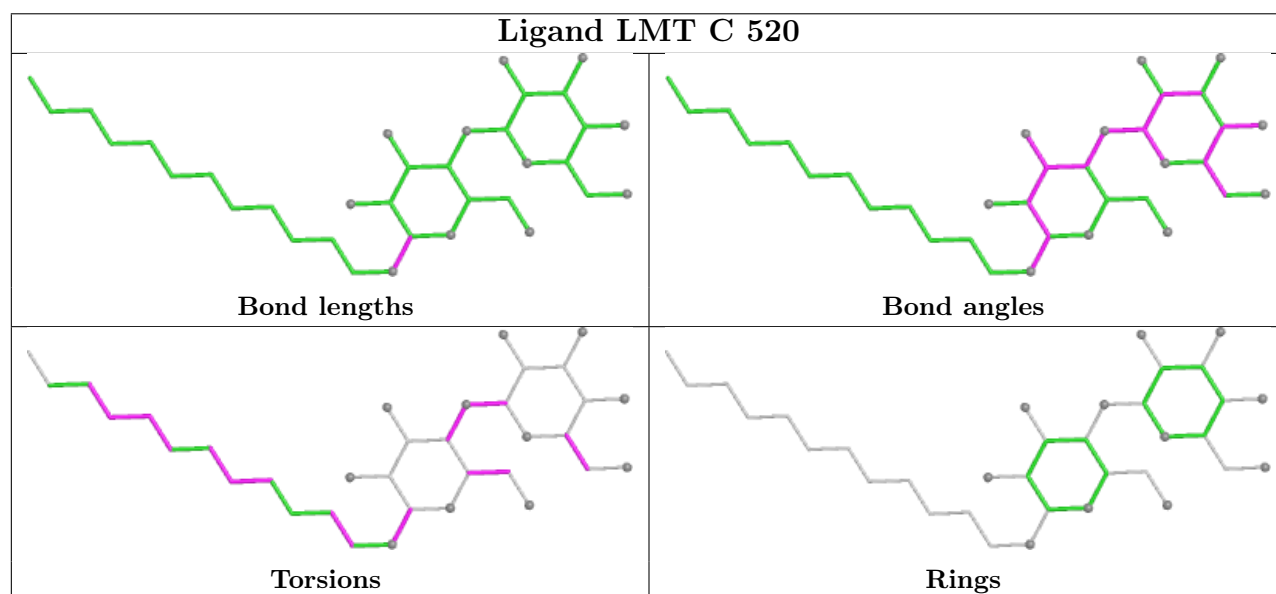
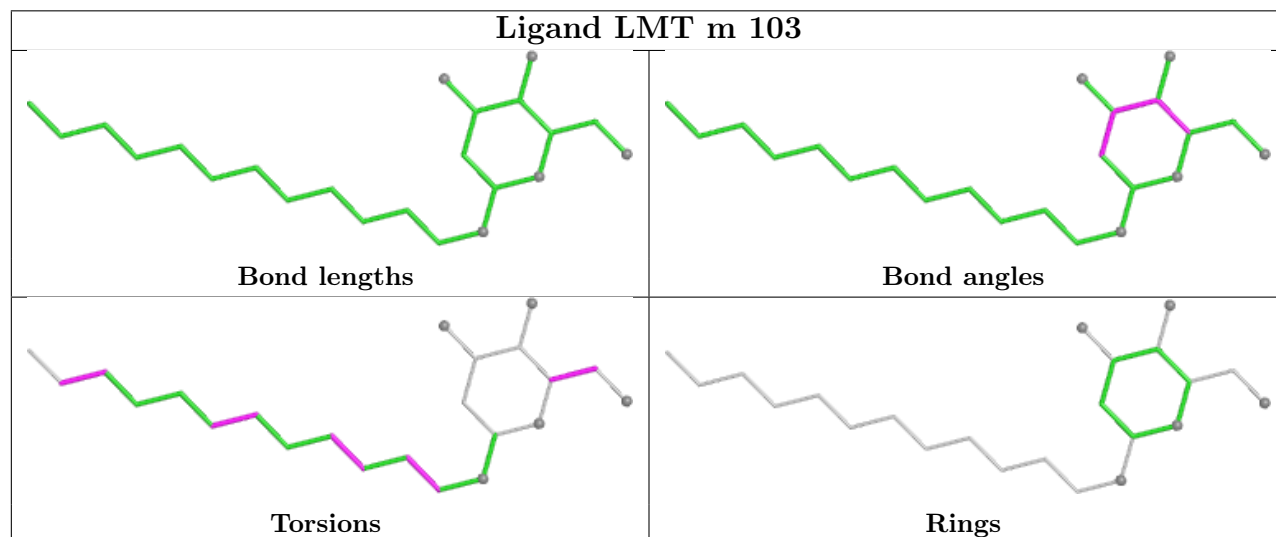
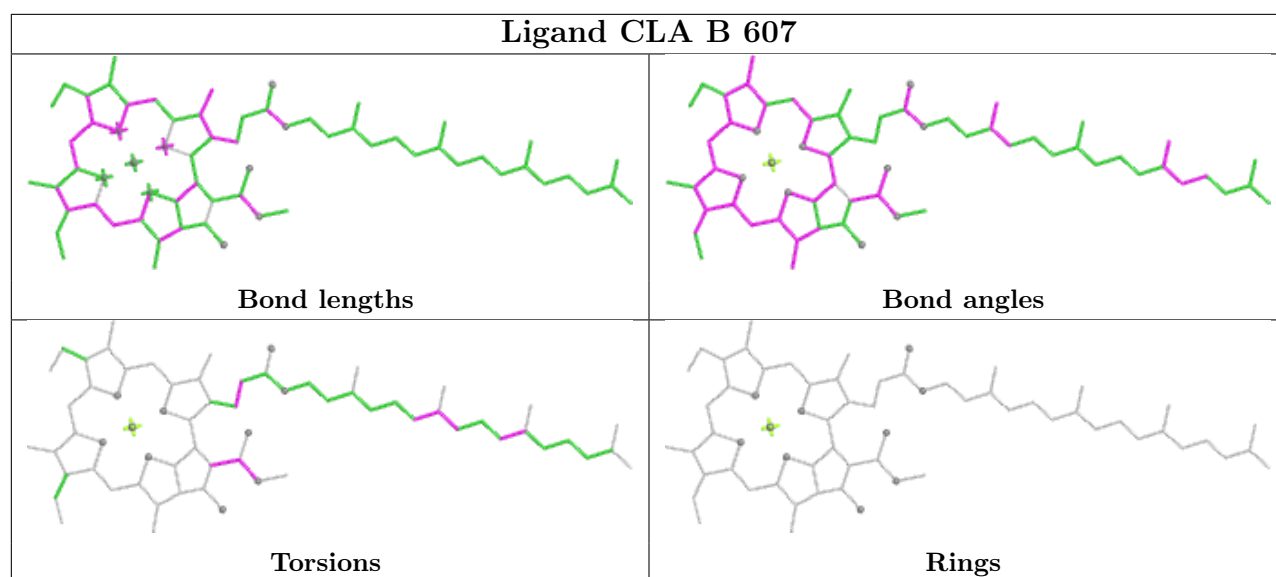
Ligand HTG c 541



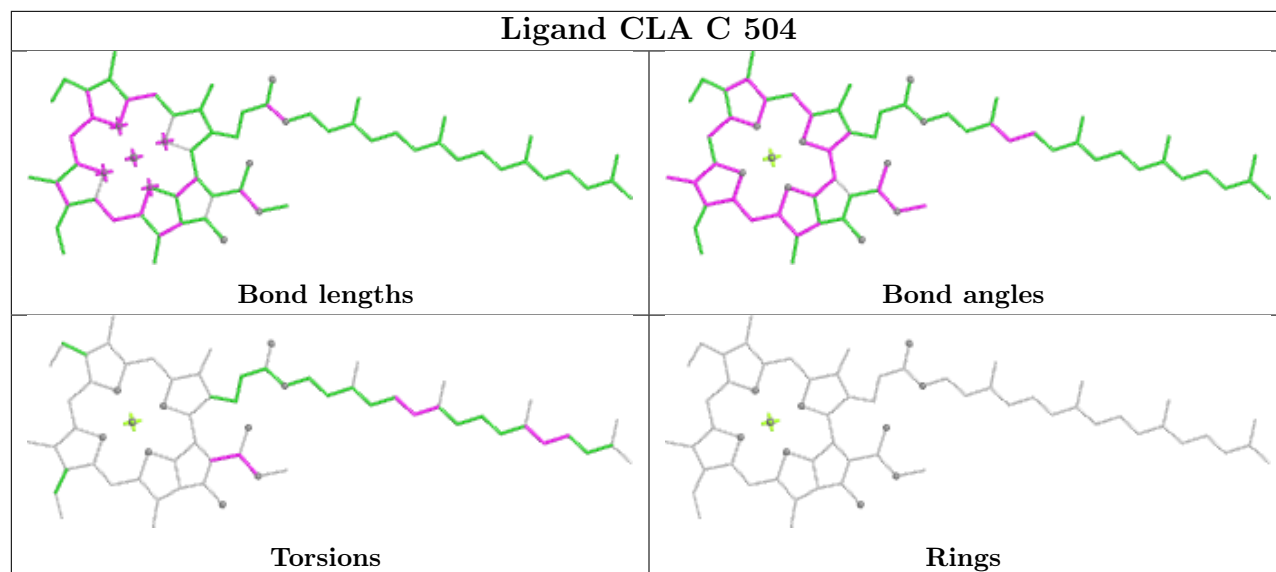
Ligand CLA c 512



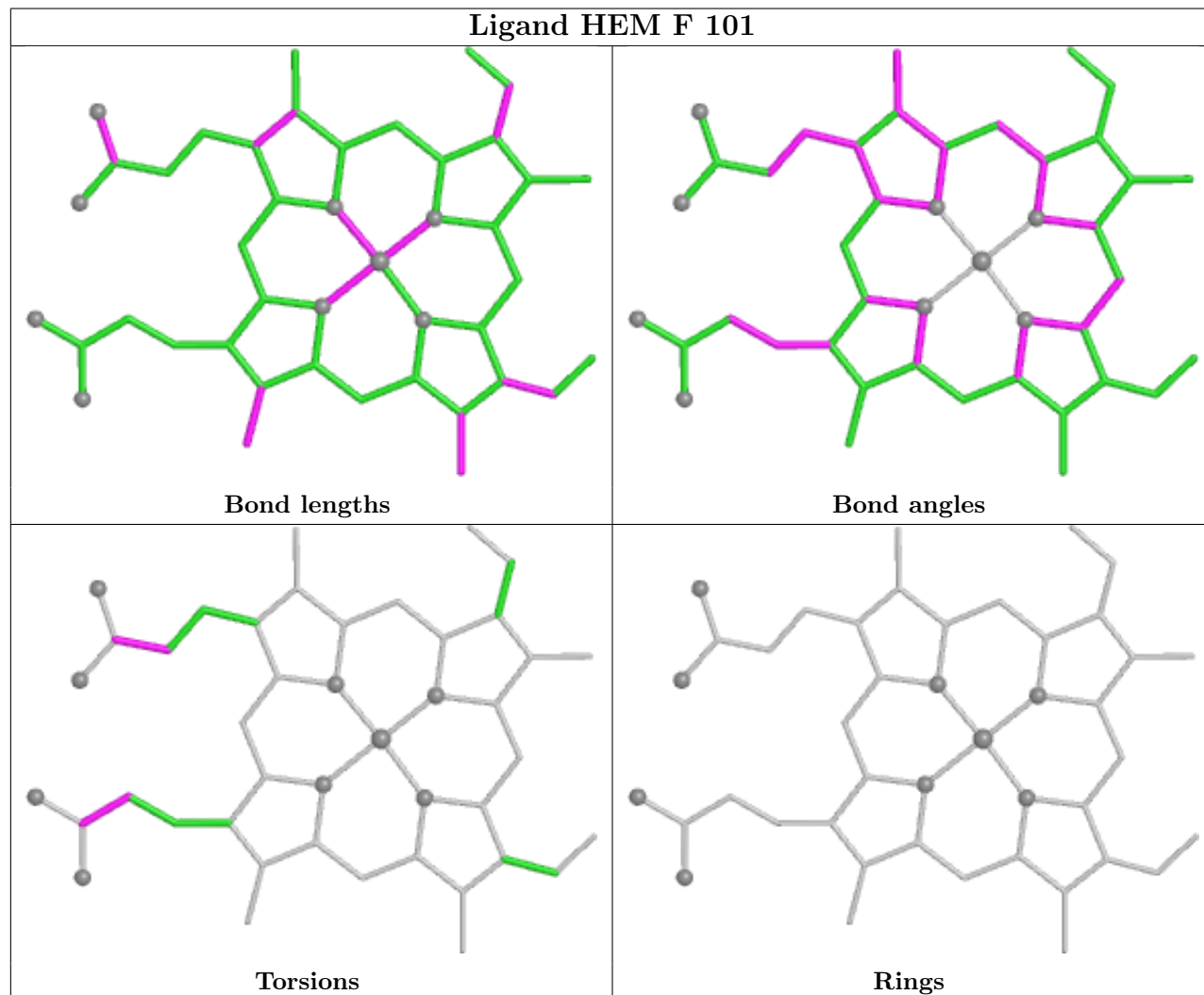


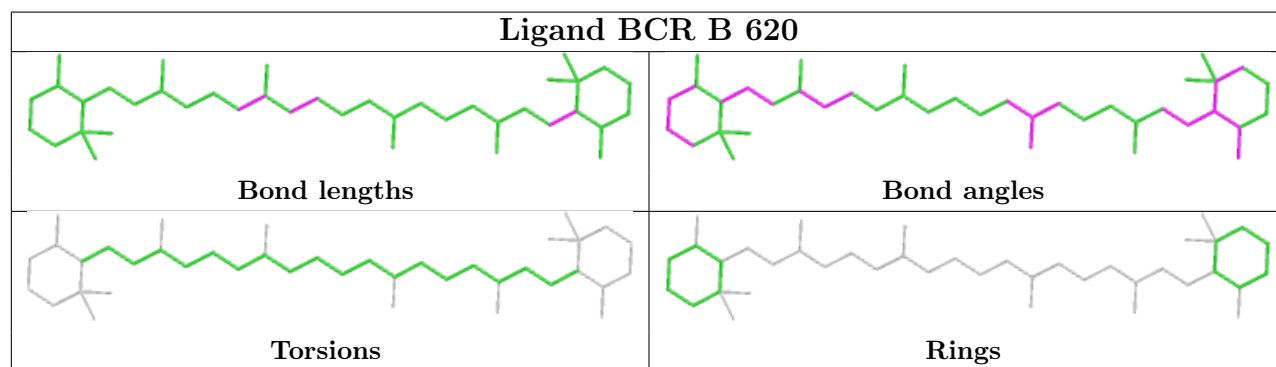
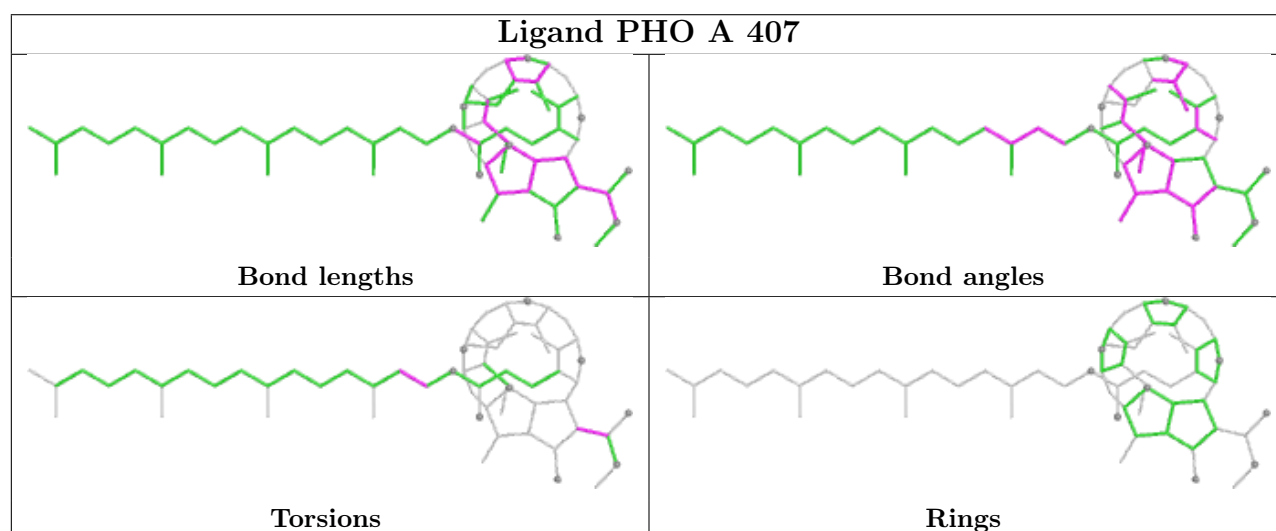
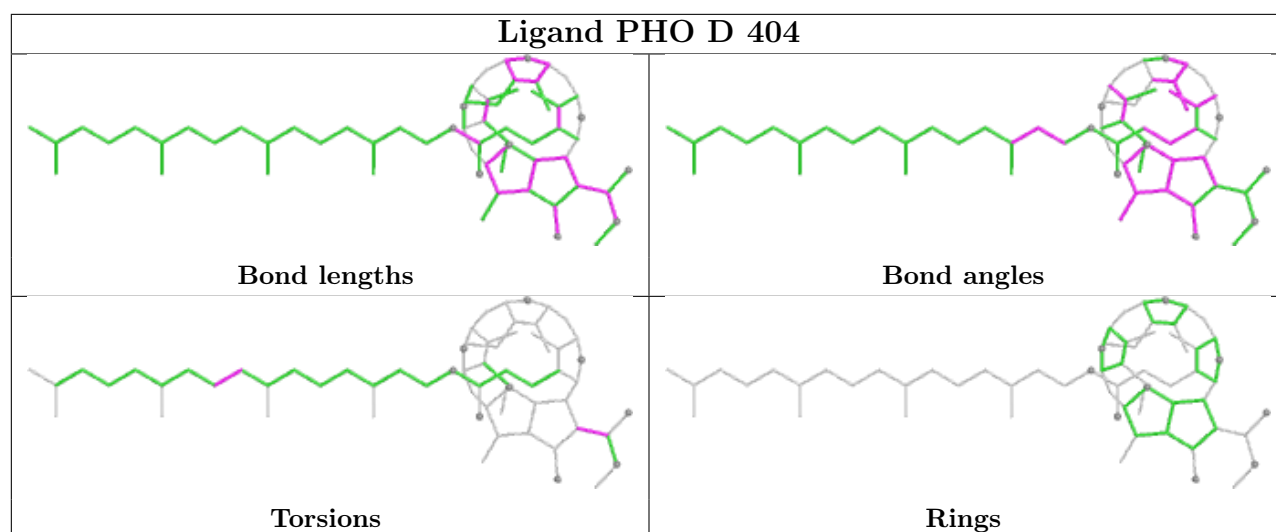


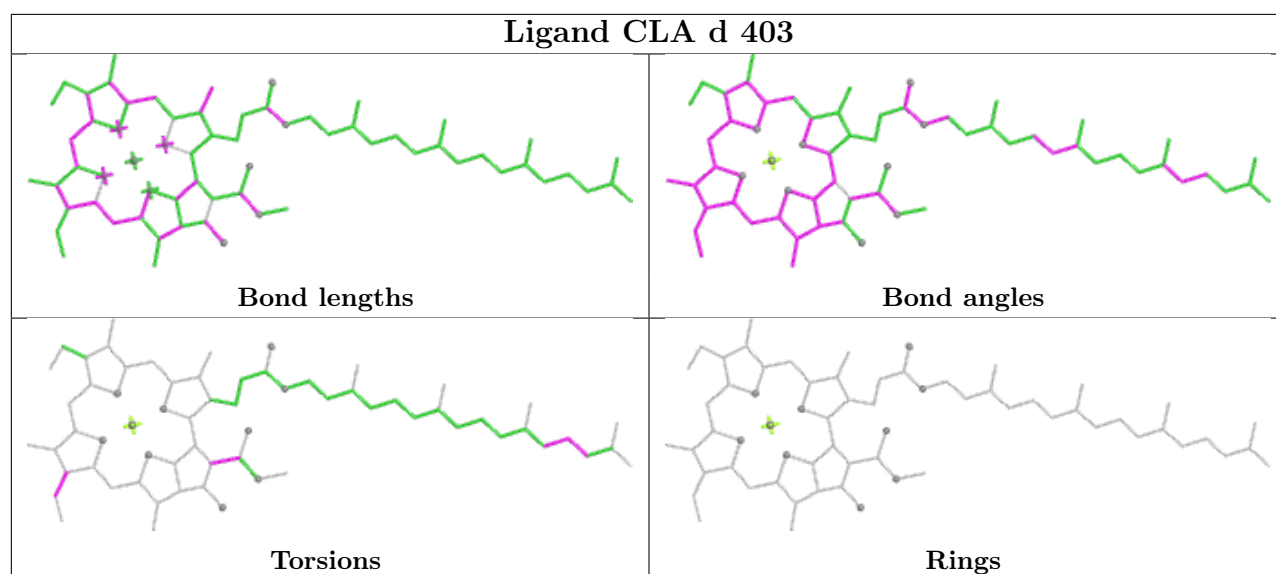
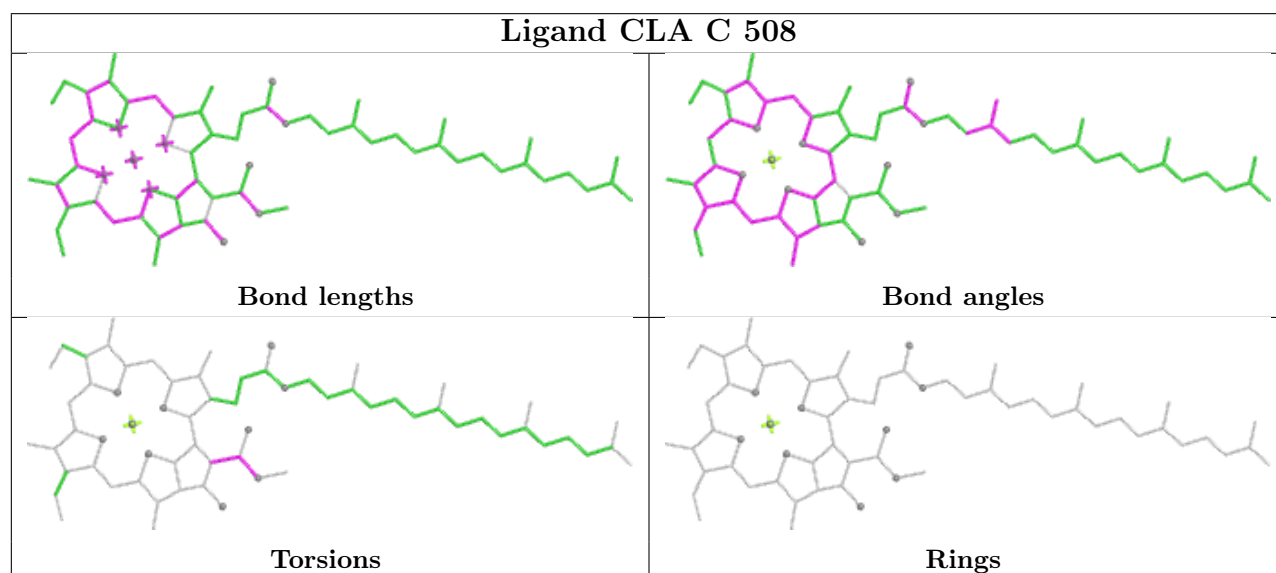
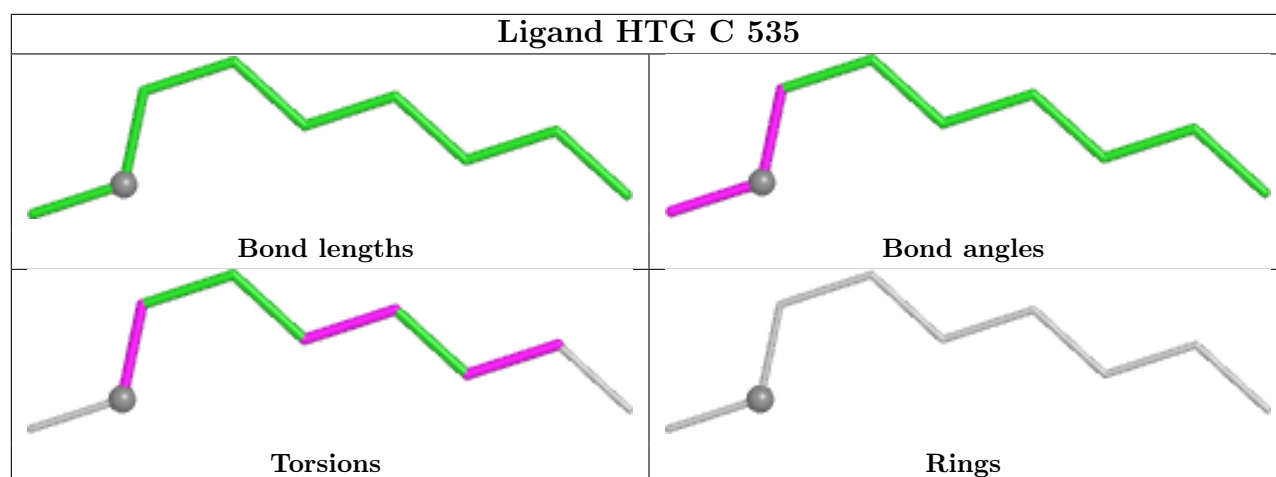
Ligand CLA C 504

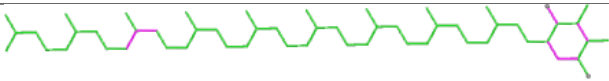
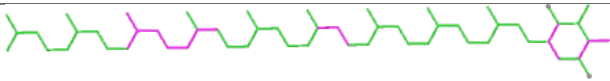
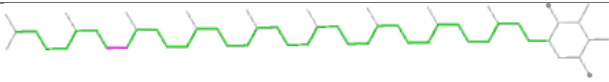
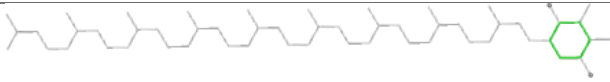


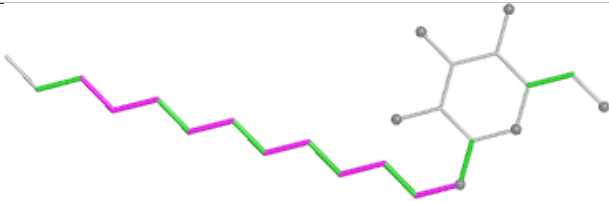
Ligand HEM F 101

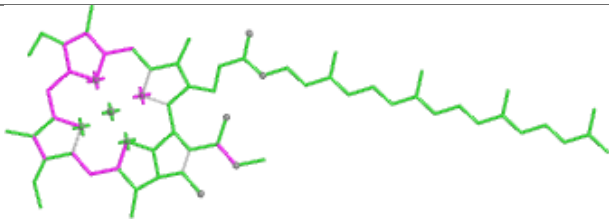
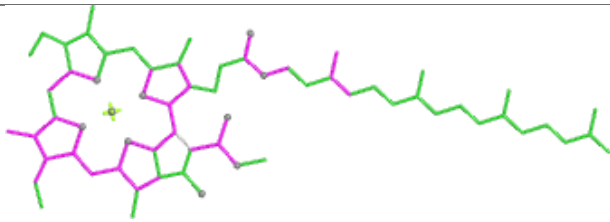
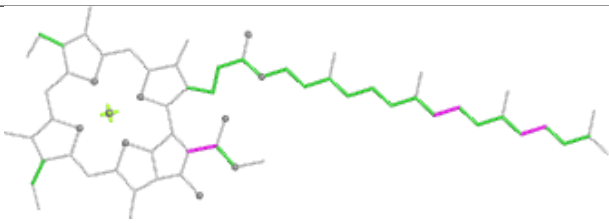
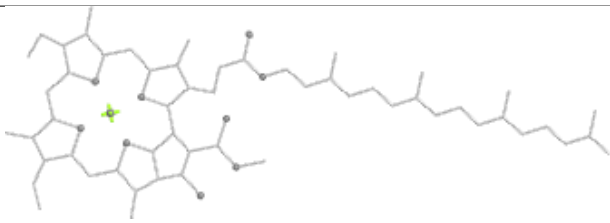


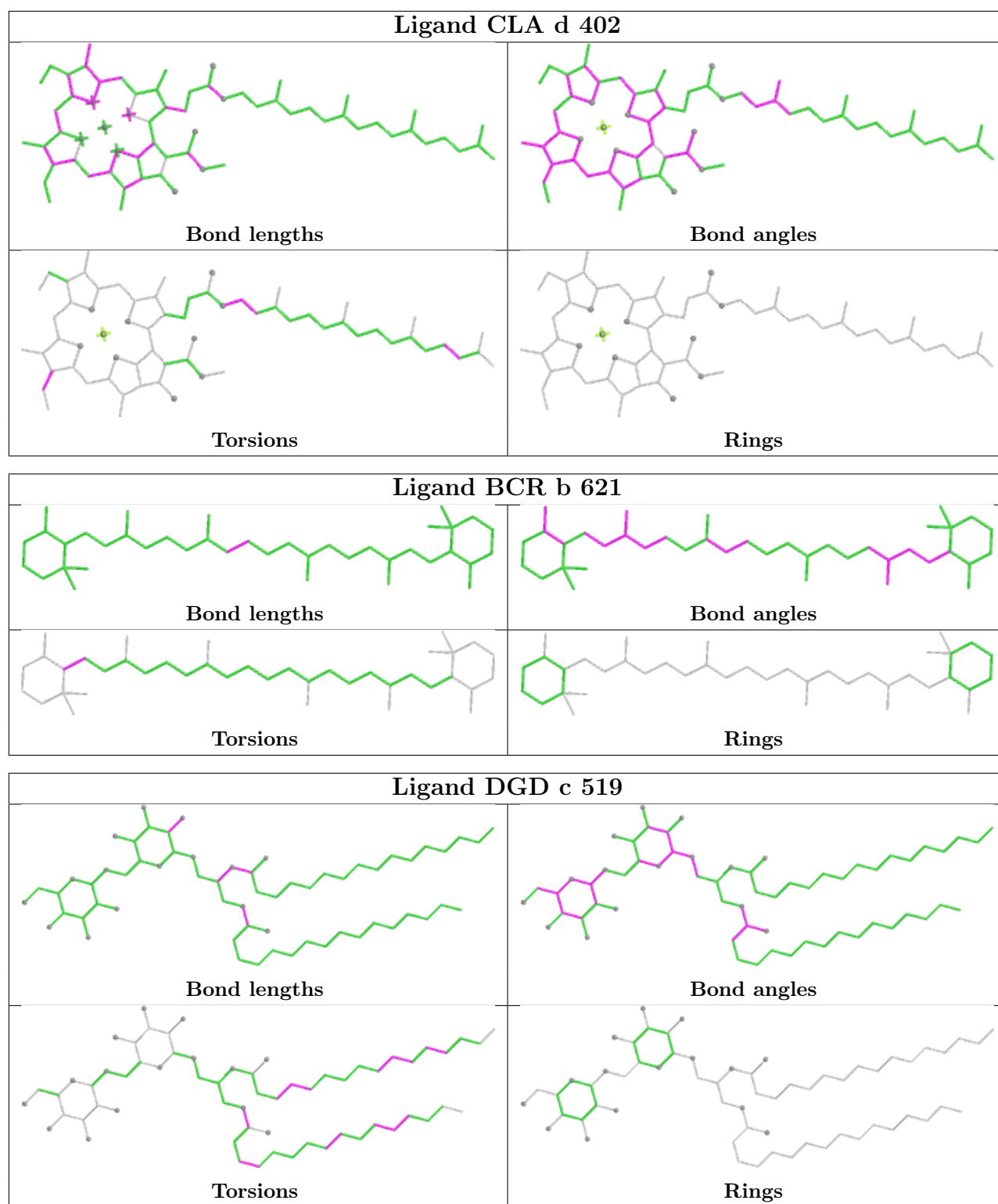


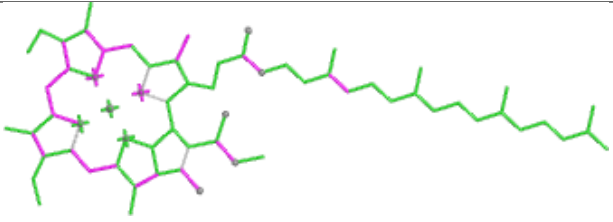
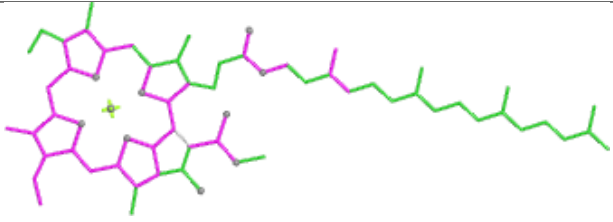
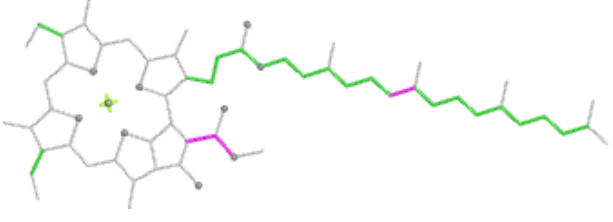
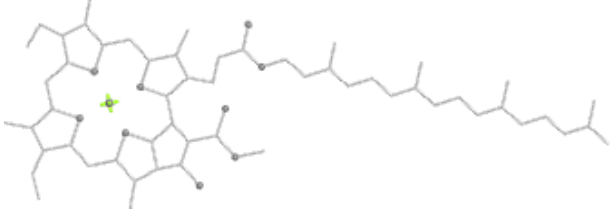
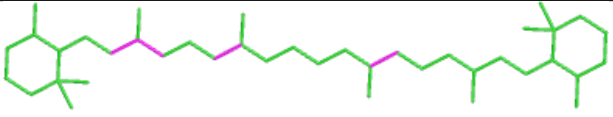
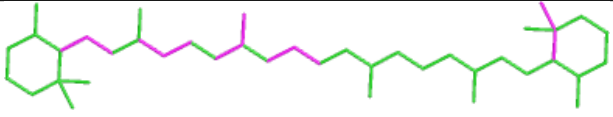
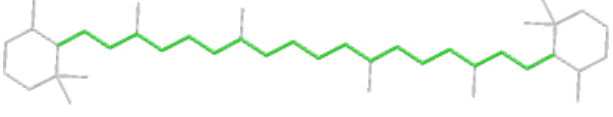
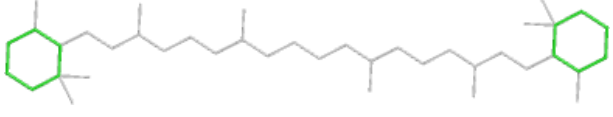


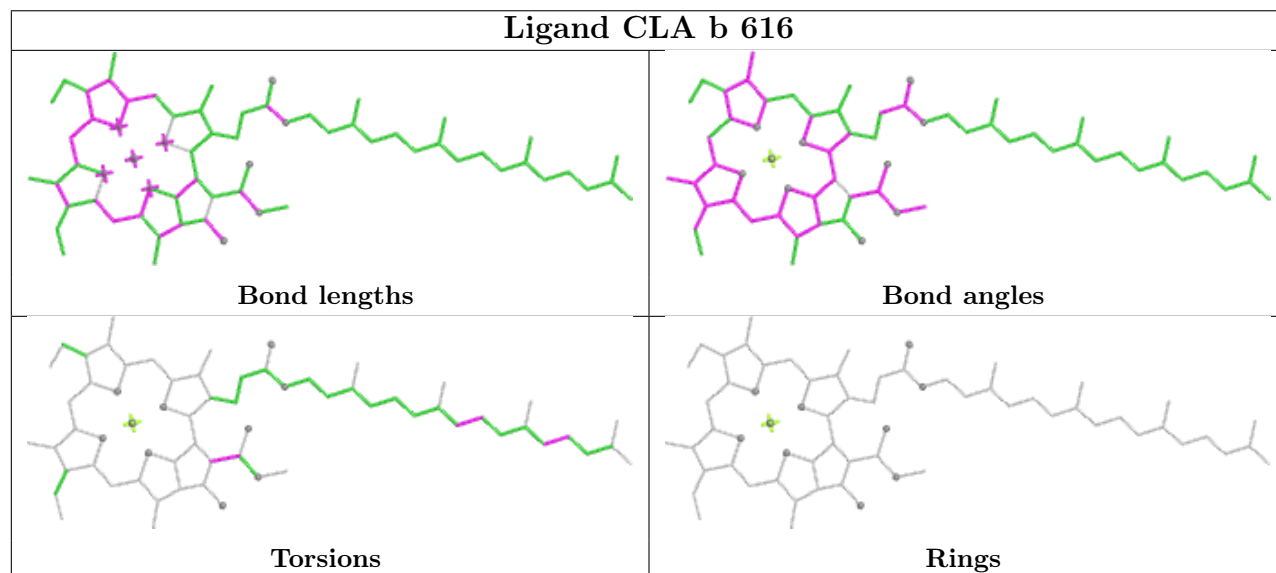
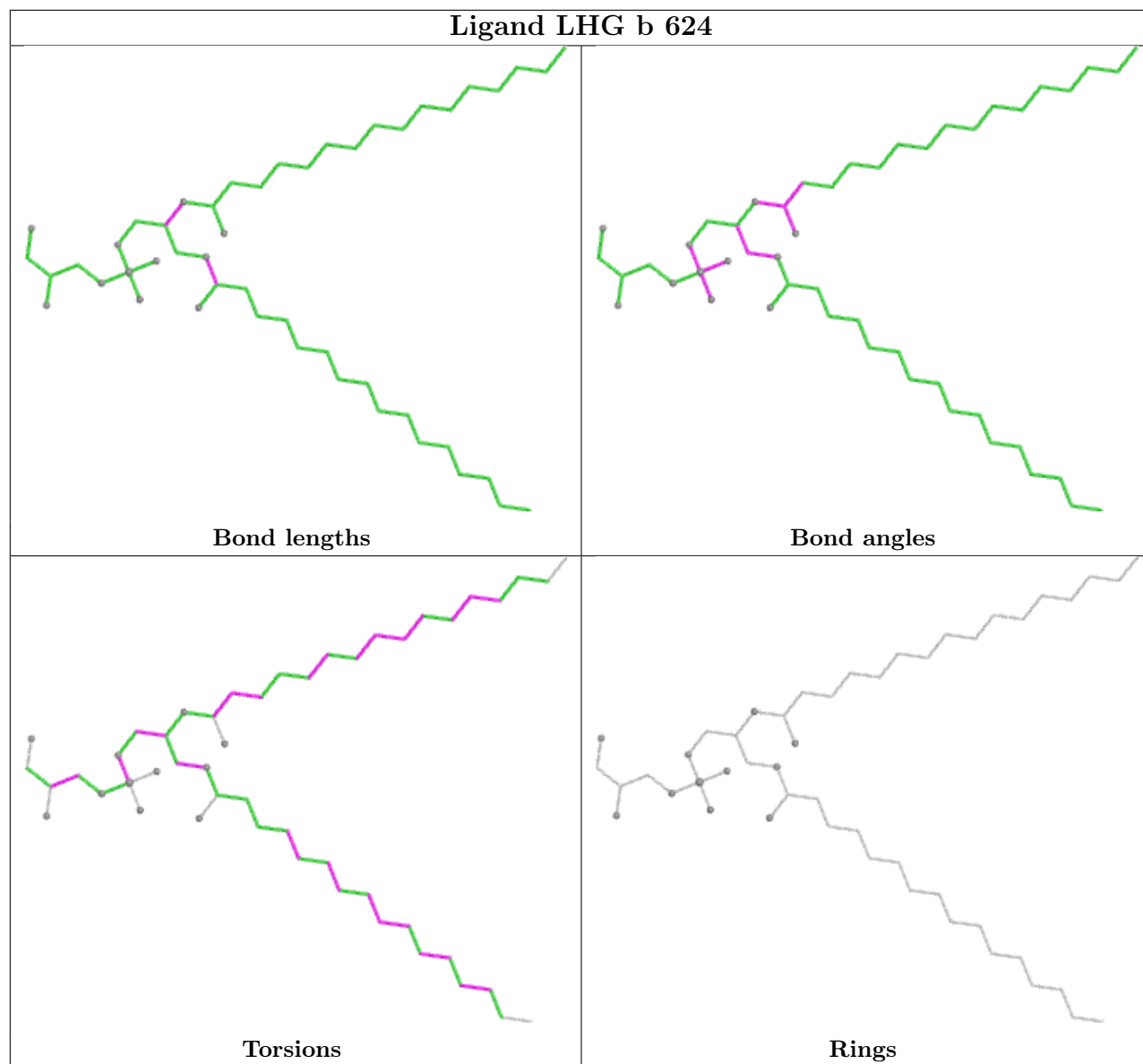
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT l 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

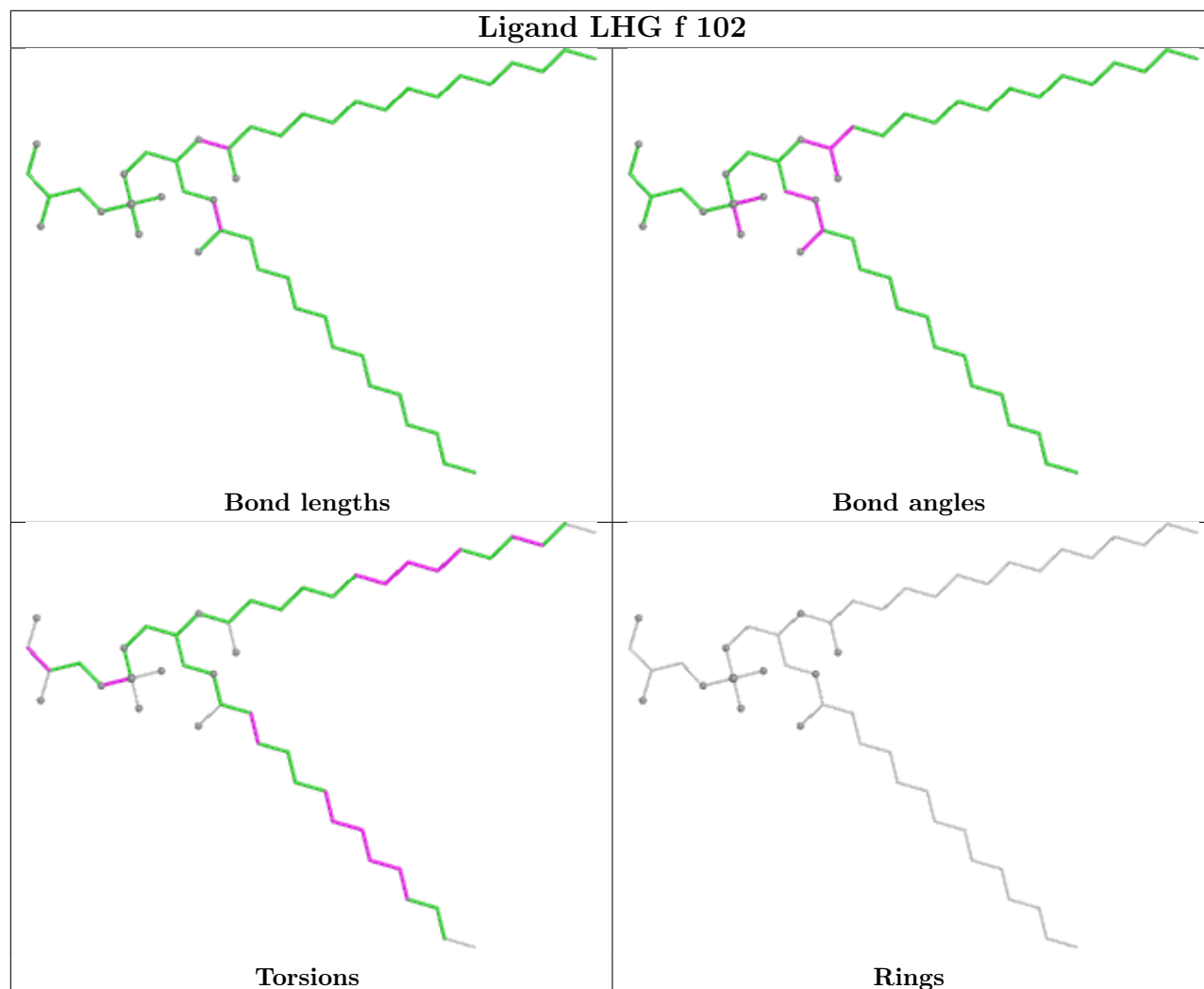
Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings



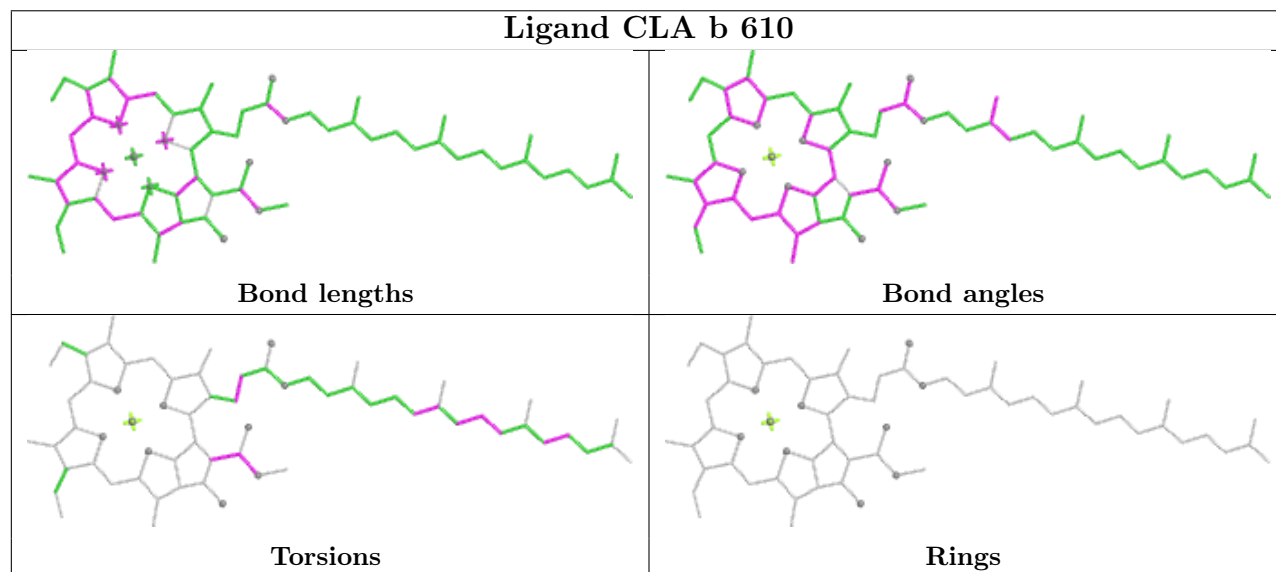
Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

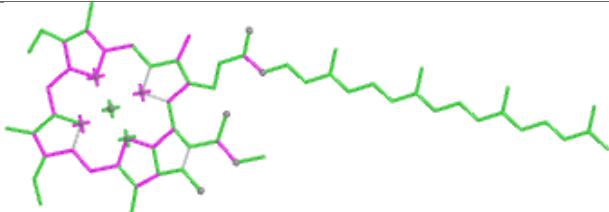
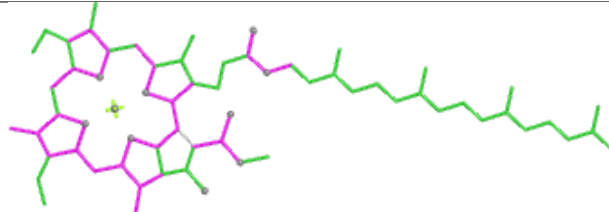
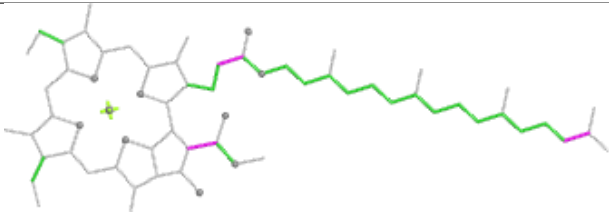
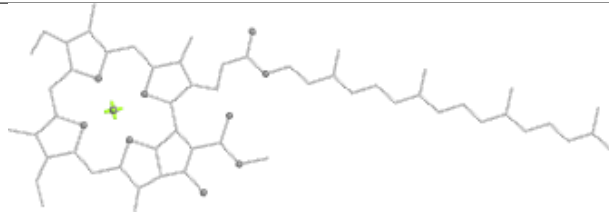


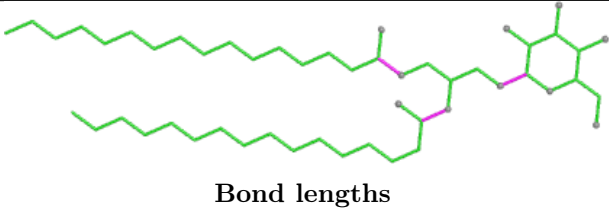
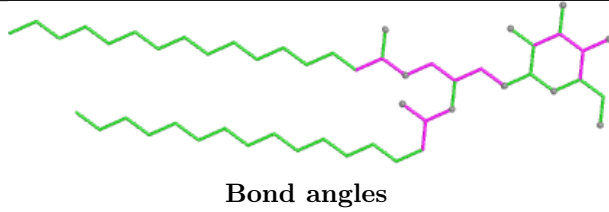
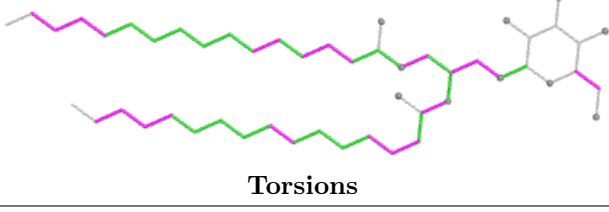
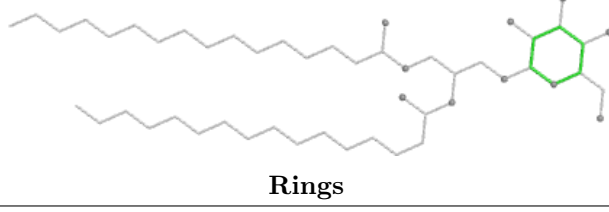
Ligand LHG f 102

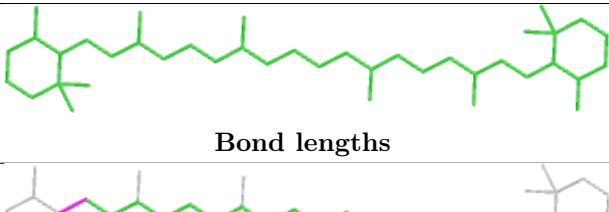
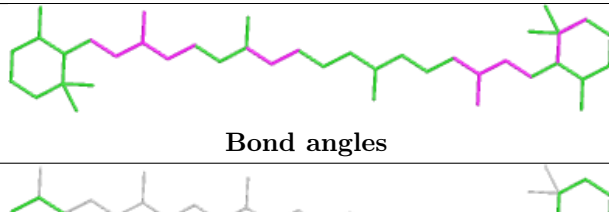


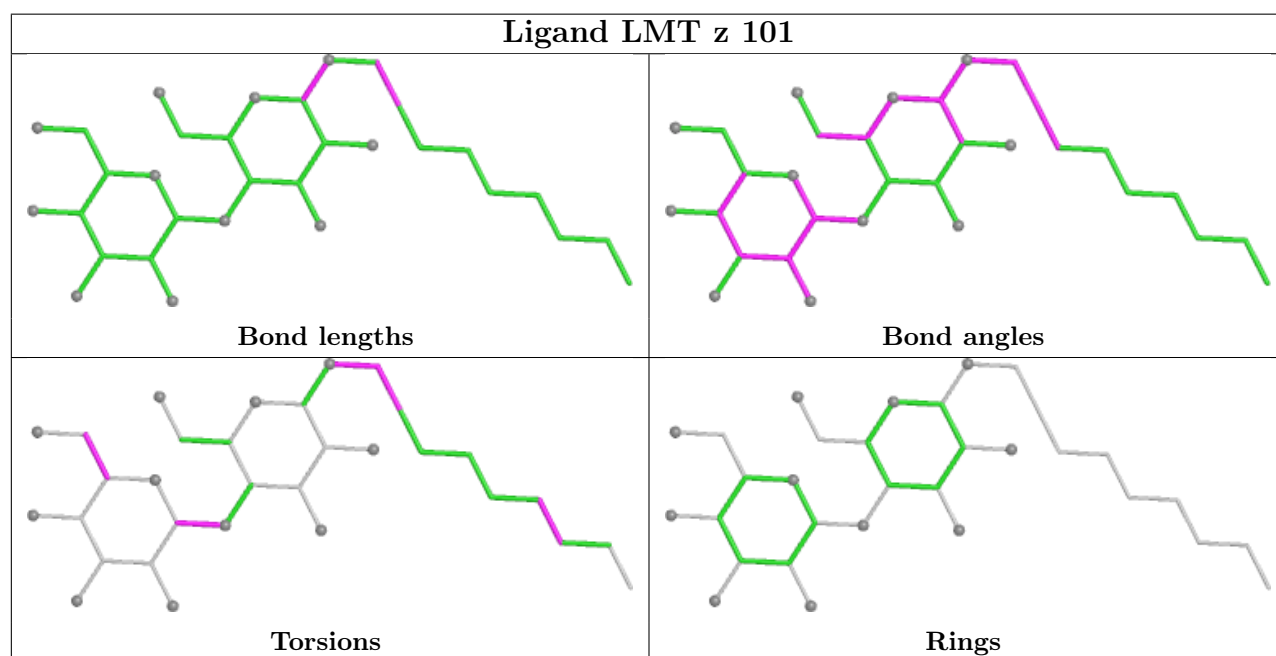
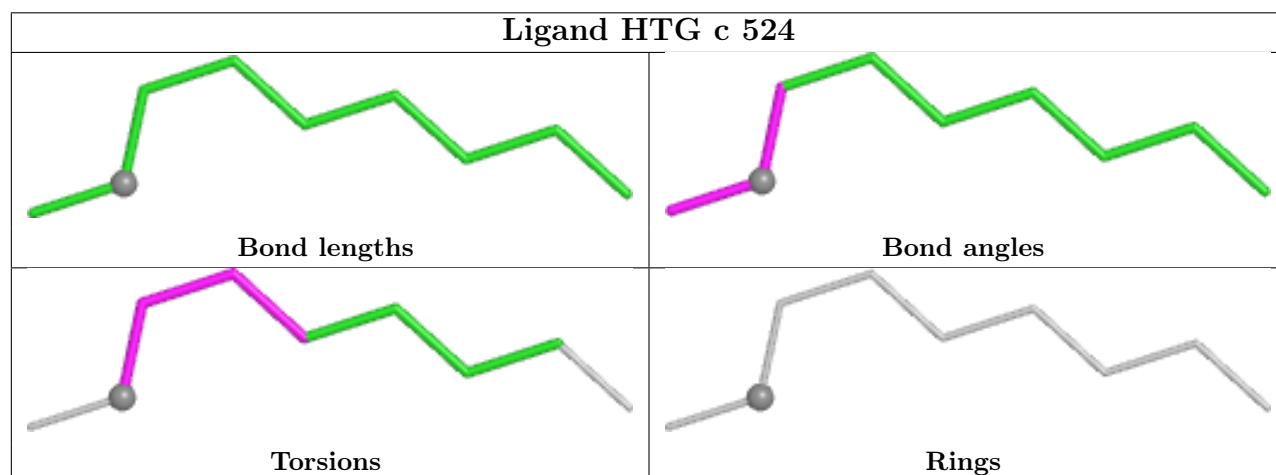
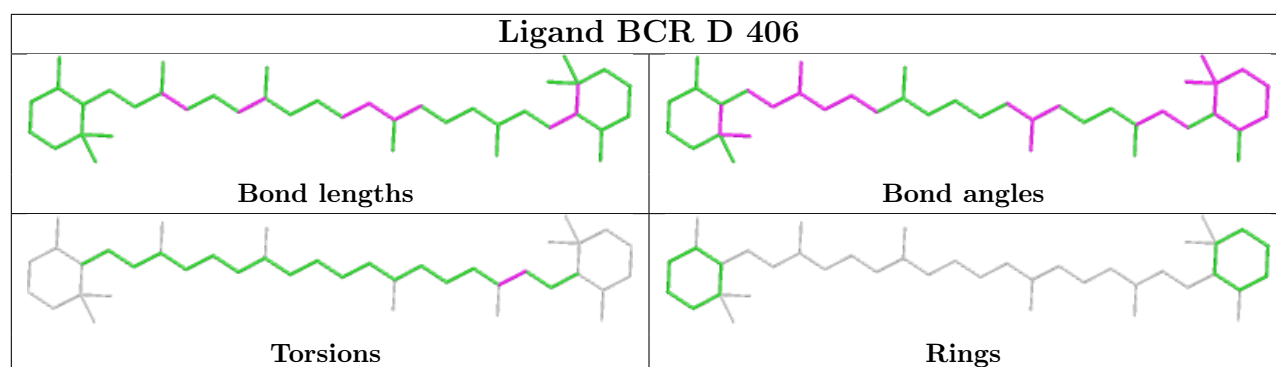
Ligand CLA b 610

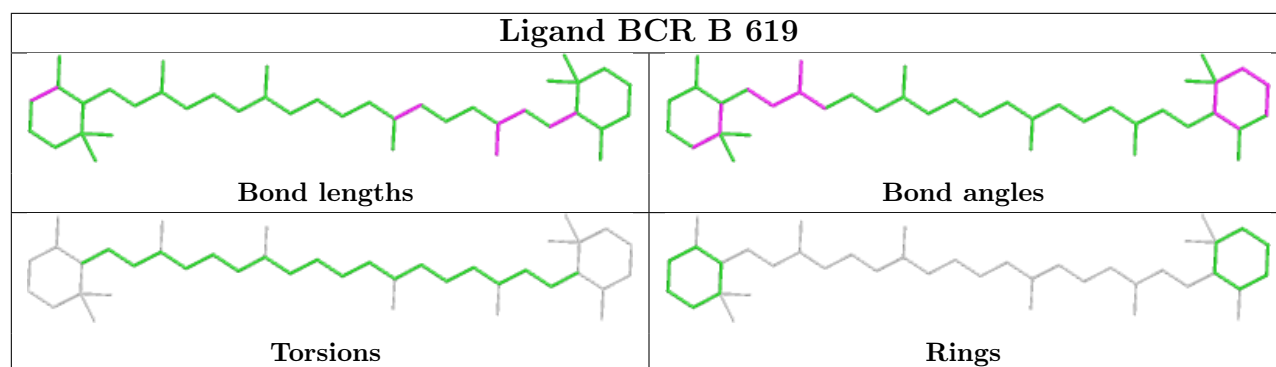
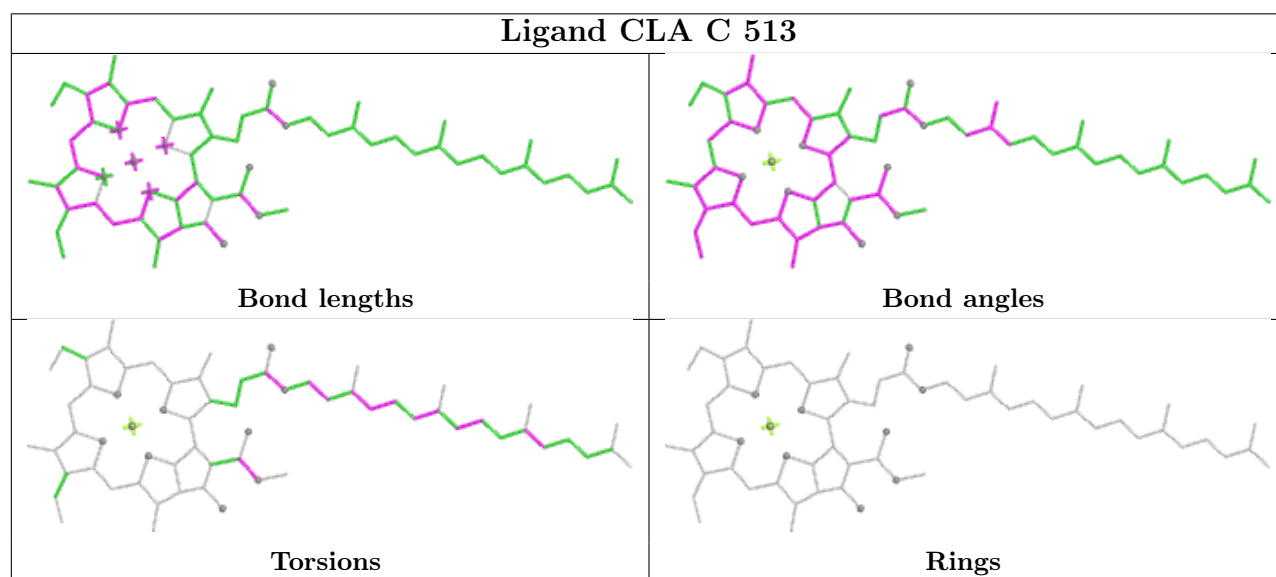
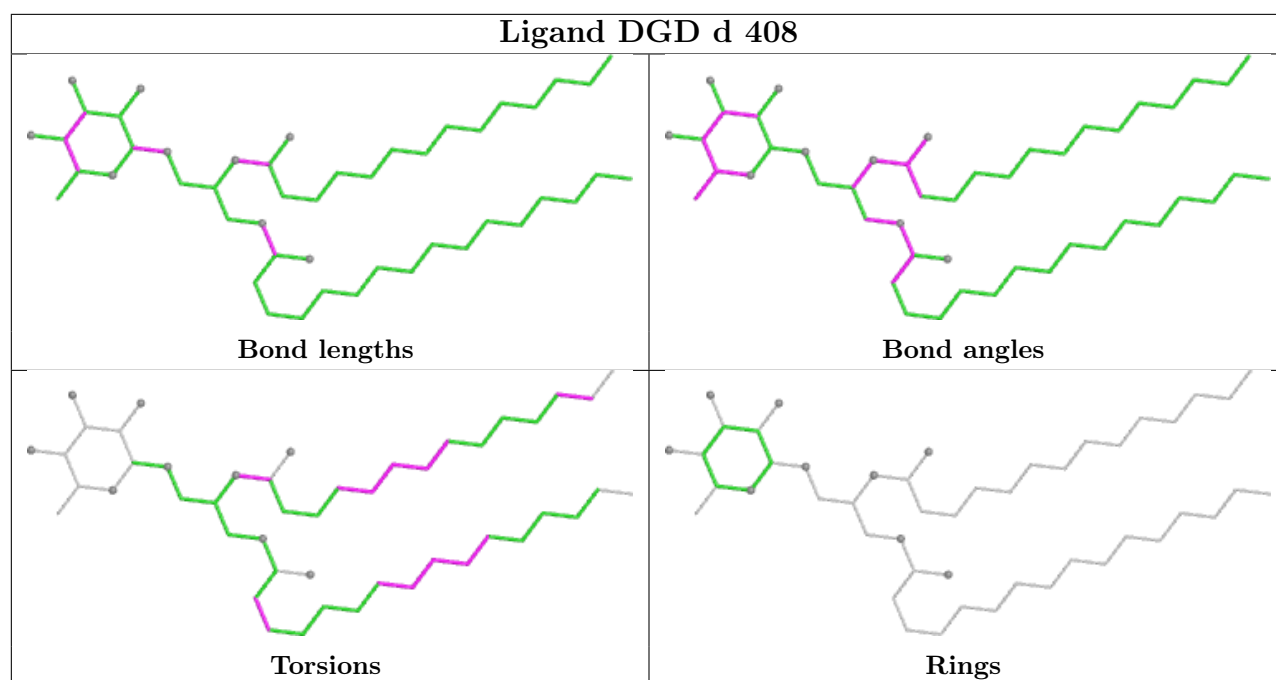


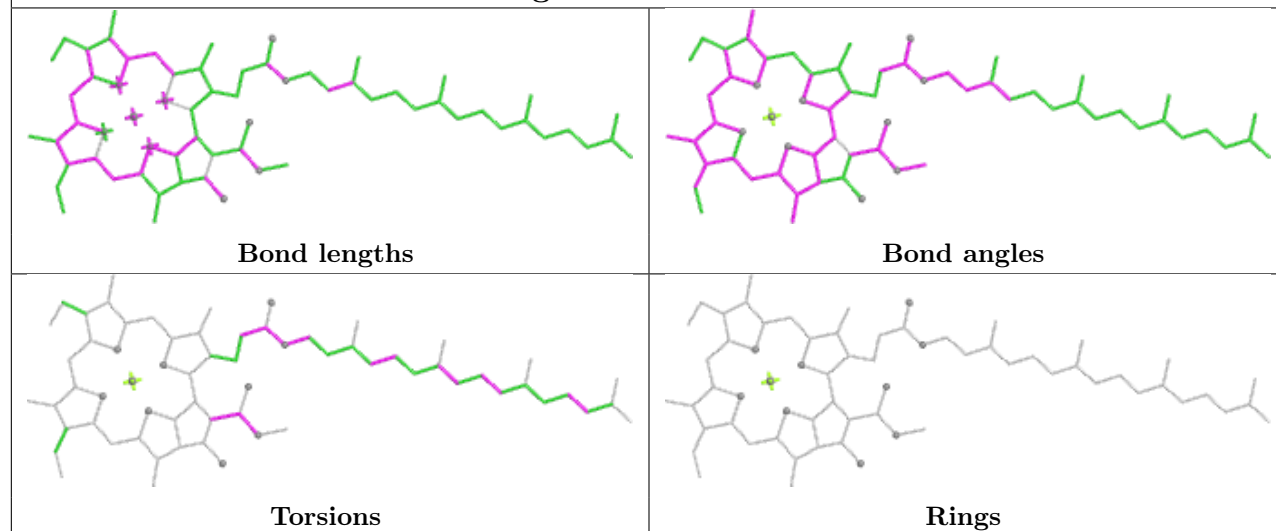
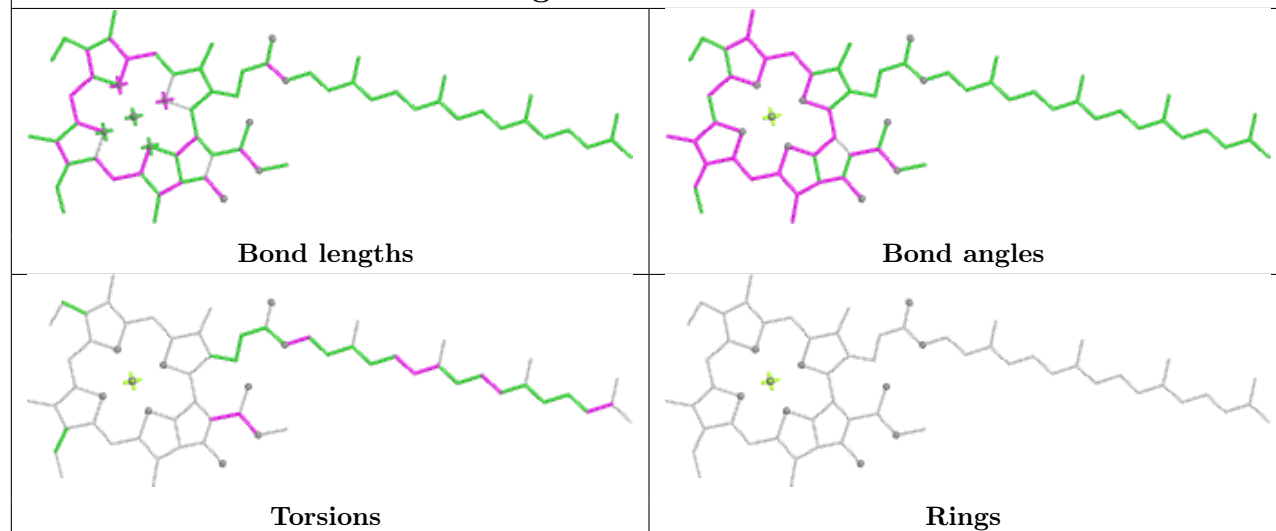
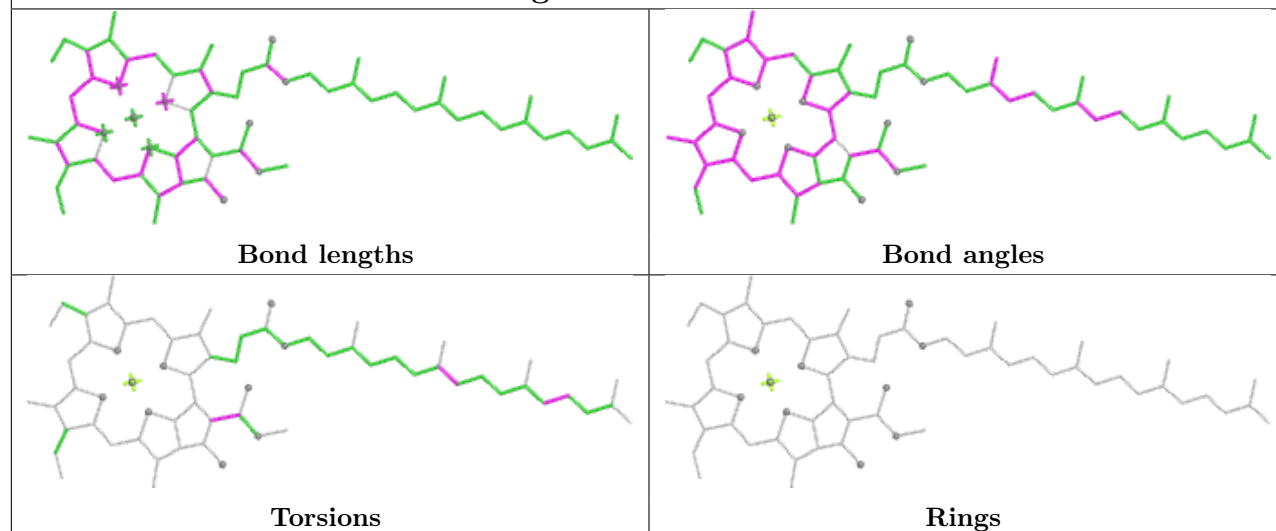
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

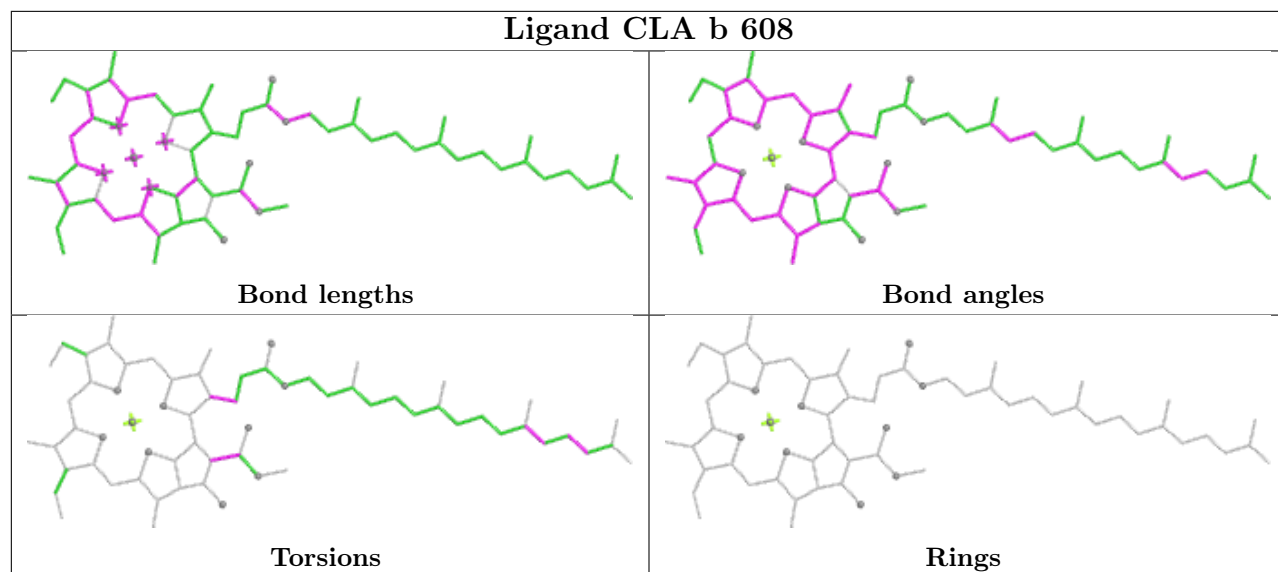
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



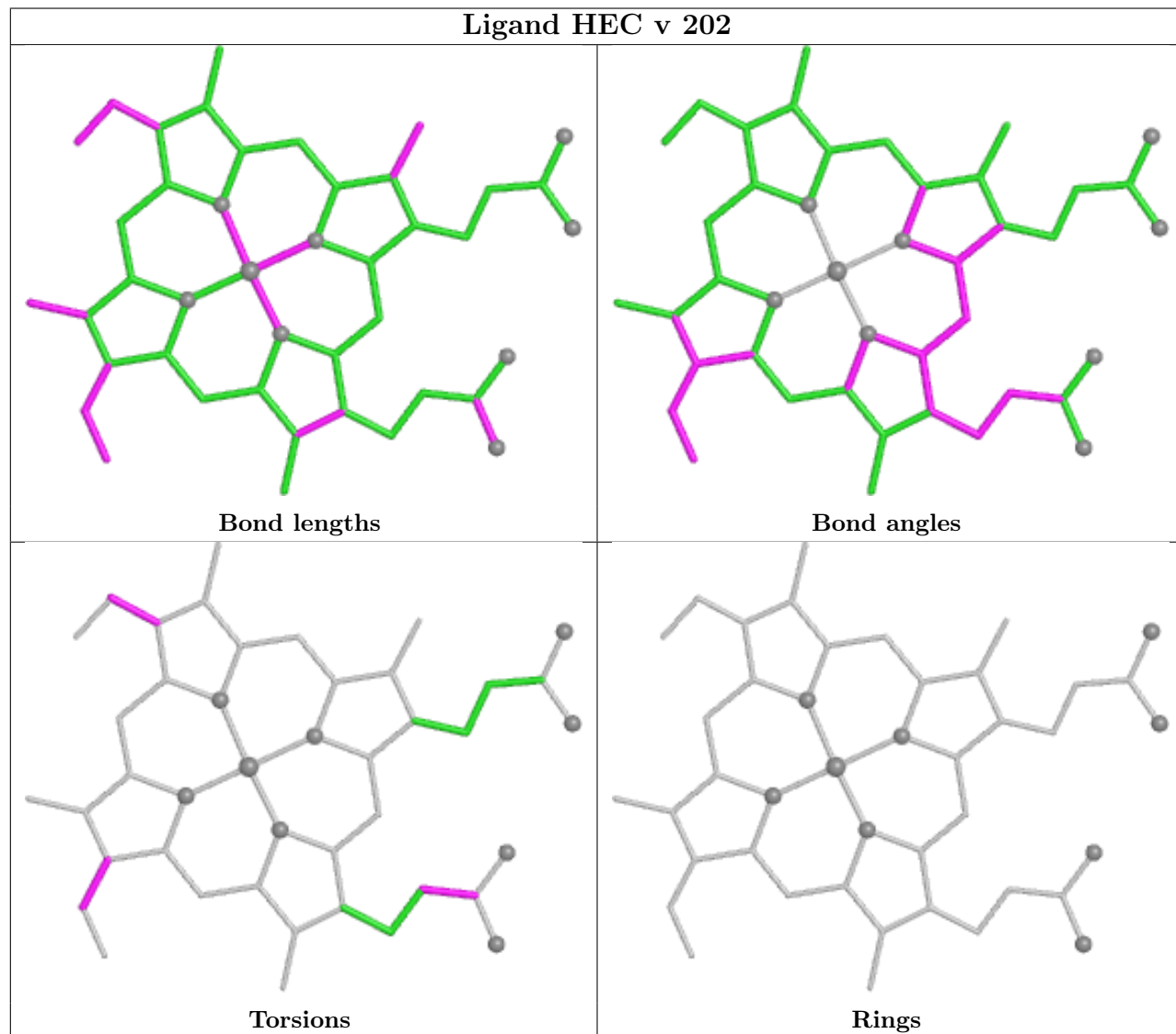


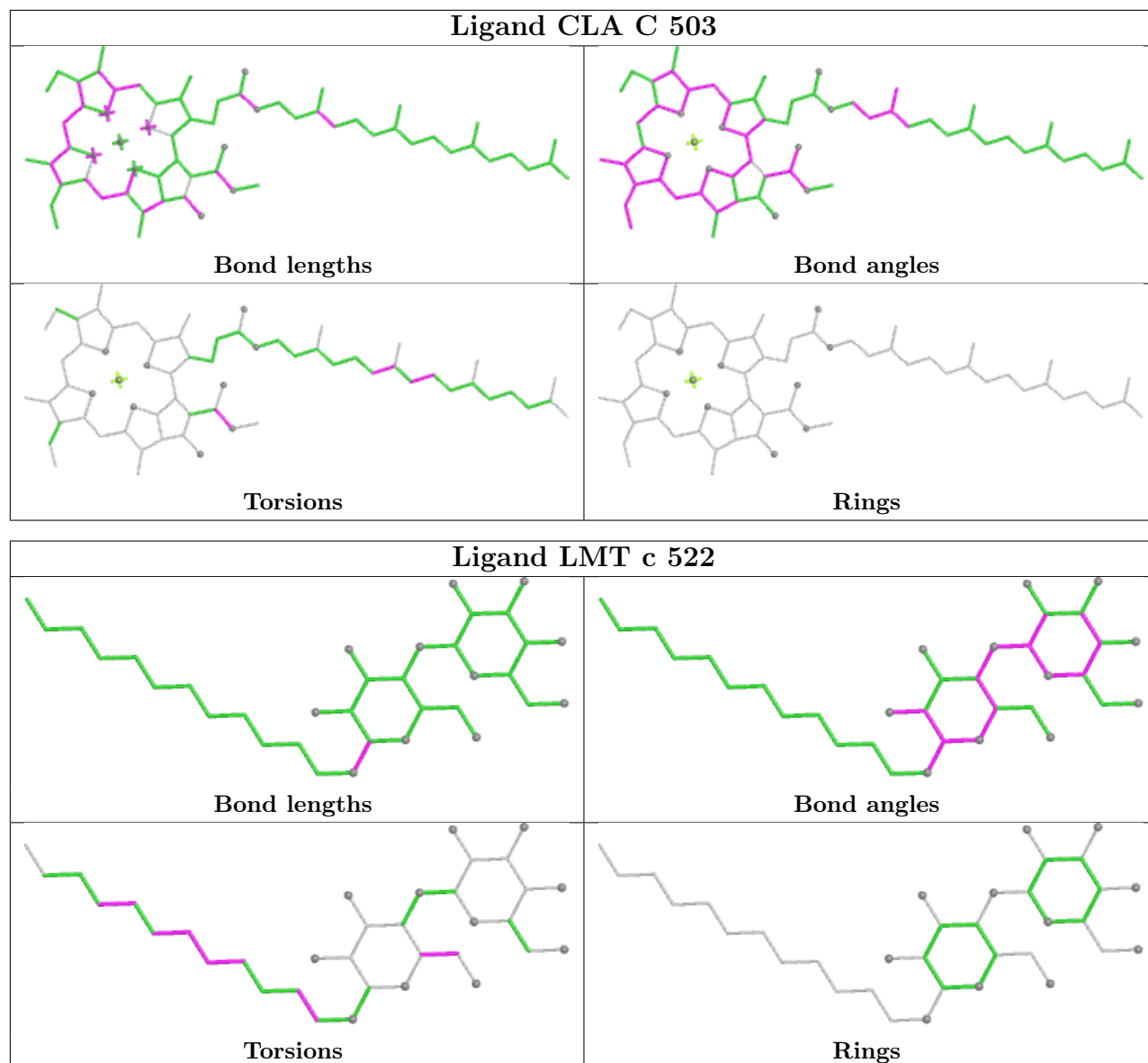
Ligand CLA B 602**Ligand CLA C 506****Ligand CLA A 406**

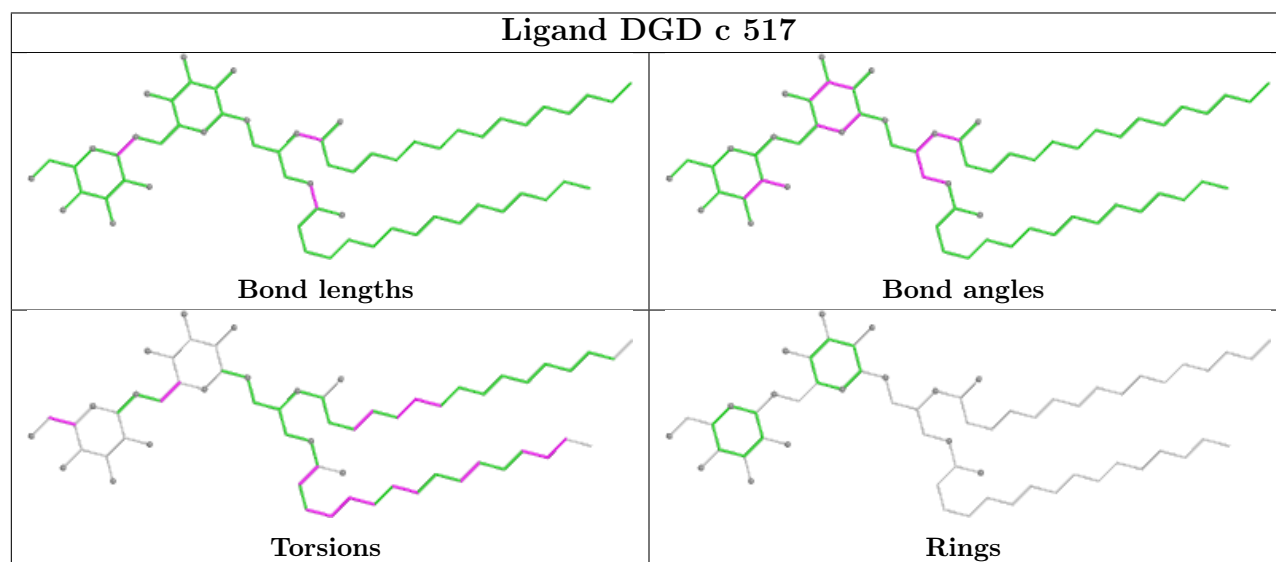
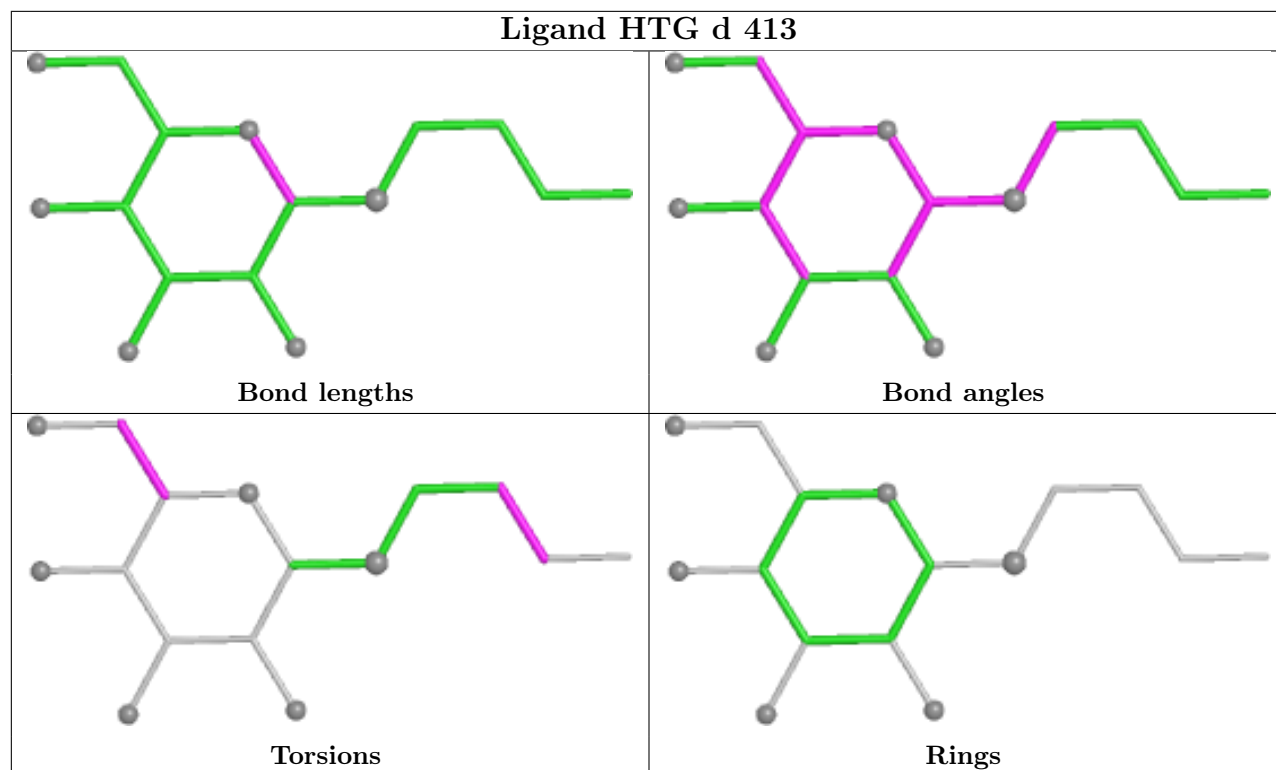
Ligand CLA b 608

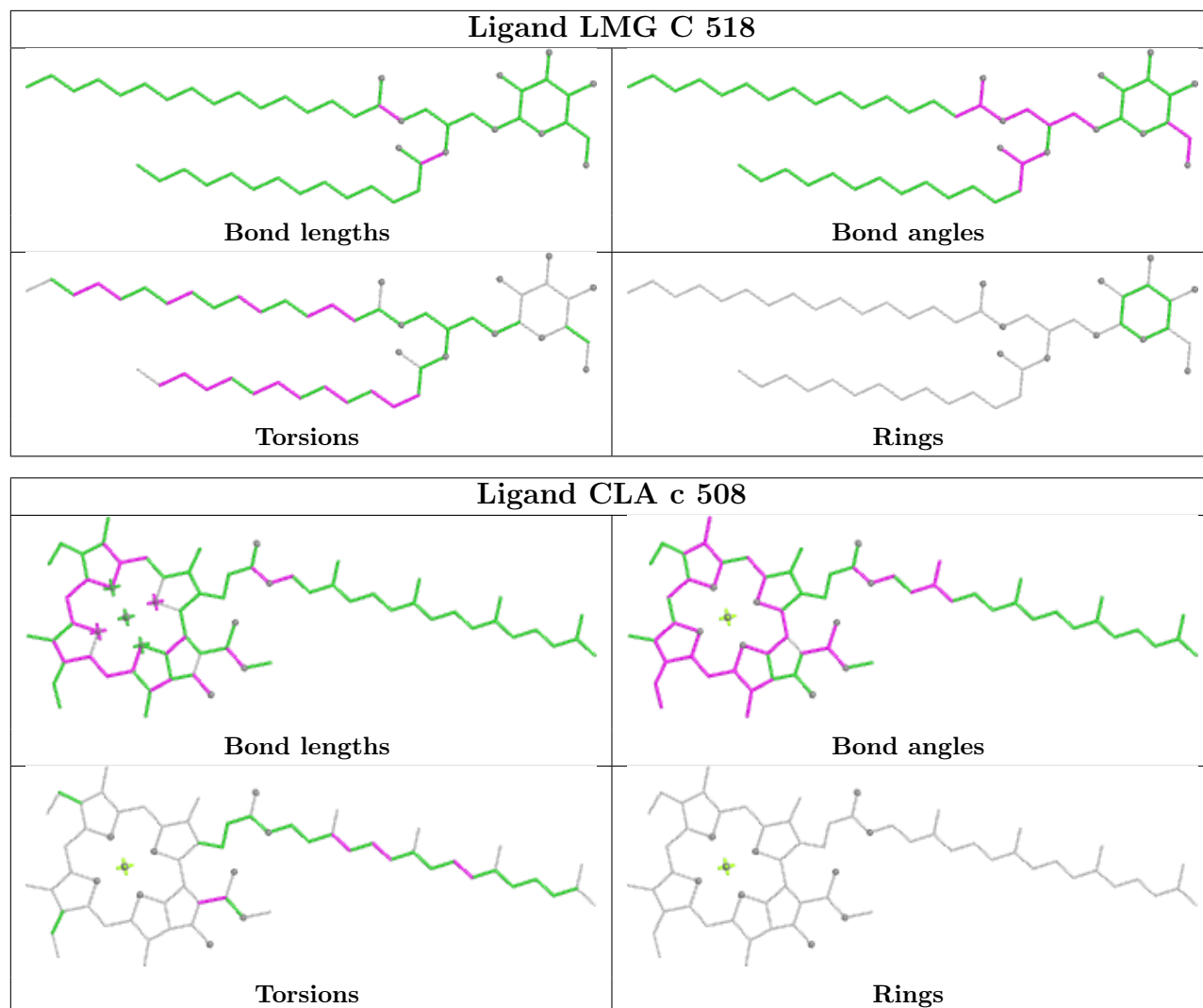


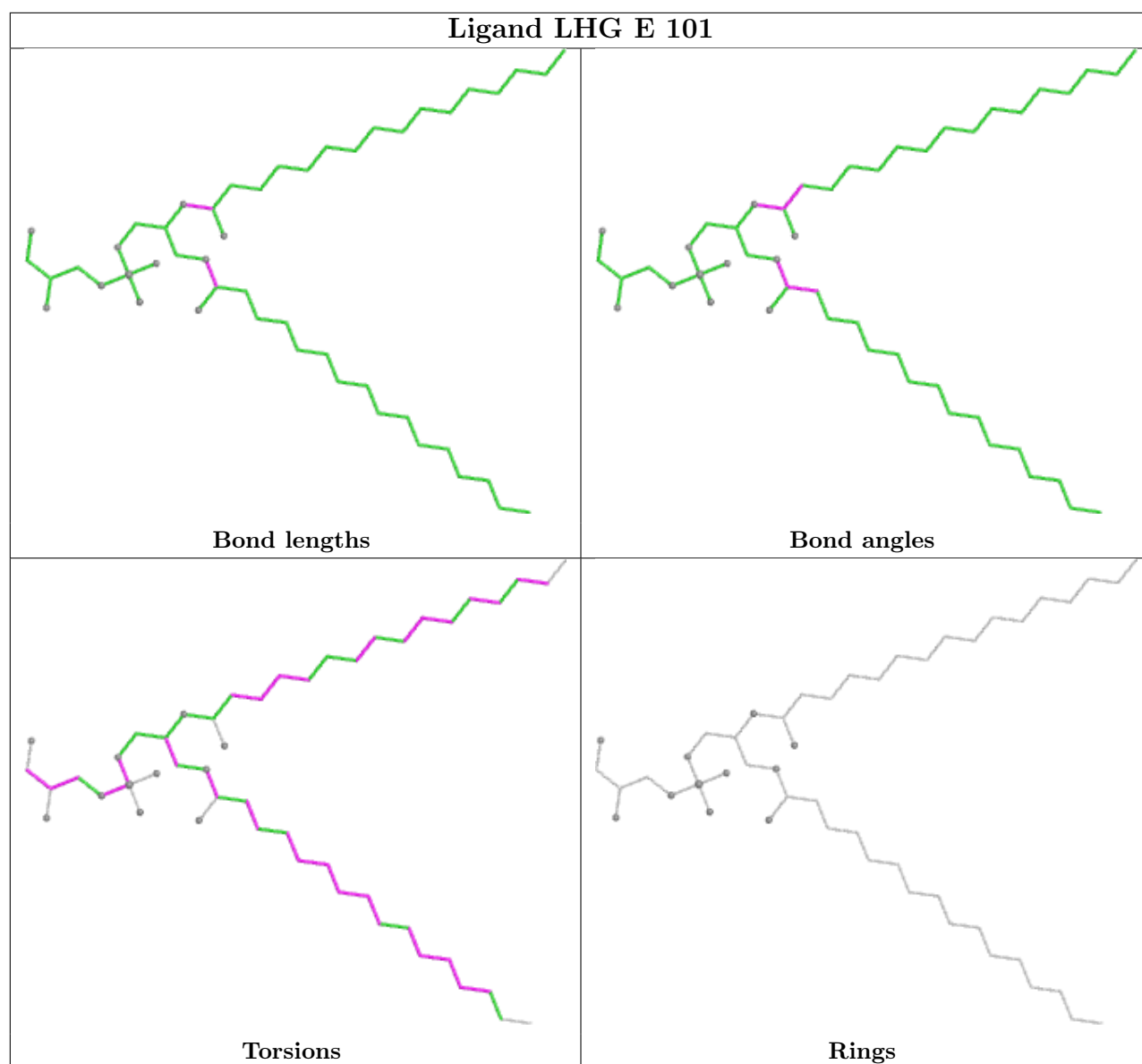
Ligand HEC v 202

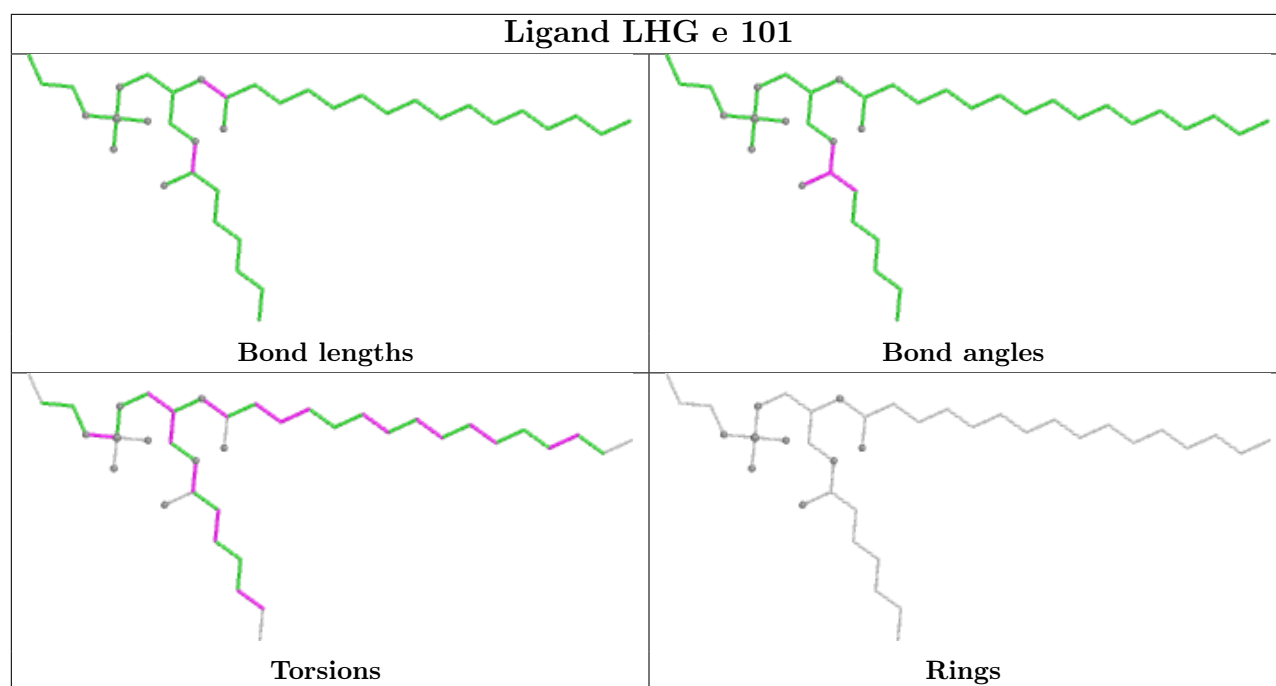












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.61	1 (0%) 90 91	21, 33, 56, 90	2 (0%)
1	a	334/334 (100%)	-0.52	1 (0%) 90 91	19, 35, 59, 92	2 (0%)
2	B	505/505 (100%)	-0.46	3 (0%) 85 87	17, 38, 68, 90	5 (0%)
2	b	504/505 (99%)	-0.35	7 (1%) 73 75	19, 39, 71, 131	4 (0%)
3	C	451/455 (99%)	-0.40	2 (0%) 88 90	17, 41, 60, 115	5 (1%)
3	c	455/455 (100%)	-0.28	0 100 100	21, 45, 62, 110	2 (0%)
4	D	341/342 (99%)	-0.60	2 (0%) 85 87	18, 34, 52, 118	2 (0%)
4	d	341/342 (99%)	-0.58	0 100 100	19, 35, 56, 98	1 (0%)
5	E	80/81 (98%)	0.16	3 (3%) 44 46	30, 55, 90, 102	2 (2%)
5	e	81/81 (100%)	0.24	5 (6%) 26 28	40, 54, 83, 105	0
6	F	34/34 (100%)	-0.04	2 (5%) 28 30	36, 46, 86, 115	0
6	f	32/34 (94%)	-0.20	1 (3%) 51 54	38, 46, 70, 77	0
7	H	63/63 (100%)	-0.13	1 (1%) 70 73	24, 45, 59, 106	1 (1%)
7	h	63/63 (100%)	-0.07	1 (1%) 70 73	26, 48, 66, 85	1 (1%)
8	I	34/37 (91%)	-0.08	0 100 100	36, 47, 67, 90	0
8	i	36/37 (97%)	-0.19	0 100 100	38, 49, 90, 96	0
9	J	37/40 (92%)	-0.02	1 (2%) 56 59	32, 50, 104, 120	0
9	j	40/40 (100%)	-0.11	1 (2%) 58 61	39, 52, 67, 90	0
10	K	37/37 (100%)	-0.18	0 100 100	25, 49, 62, 73	1 (2%)
10	k	37/37 (100%)	-0.05	0 100 100	44, 52, 74, 77	0
11	L	36/36 (100%)	-0.48	2 (5%) 30 32	15, 32, 77, 105	1 (2%)
11	l	35/36 (97%)	-0.47	1 (2%) 53 56	15, 33, 69, 106	2 (5%)
12	M	32/34 (94%)	-0.59	1 (3%) 51 54	17, 35, 55, 89	1 (3%)
12	m	33/34 (97%)	-0.53	0 100 100	18, 37, 76, 89	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.24	2 (0%) 82 84	18, 44, 73, 129	4 (1%)
13	o	243/243 (100%)	-0.23	2 (0%) 82 84	20, 47, 80, 114	6 (2%)
14	T	29/30 (96%)	-0.52	2 (6%) 23 24	28, 35, 58, 126	0
14	t	29/30 (96%)	-0.49	0 100 100	29, 34, 61, 103	0
15	U	97/97 (100%)	-0.41	0 100 100	24, 40, 60, 89	1 (1%)
15	u	97/97 (100%)	-0.37	0 100 100	22, 42, 63, 108	1 (1%)
16	V	137/137 (100%)	-0.50	0 100 100	19, 39, 58, 77	2 (1%)
16	v	137/137 (100%)	-0.15	0 100 100	22, 49, 70, 90	1 (0%)
17	Y	29/29 (100%)	0.37	2 (6%) 23 24	36, 60, 85, 111	1 (3%)
17	y	29/29 (100%)	0.39	1 (3%) 48 50	53, 69, 83, 94	0
18	X	39/39 (100%)	0.27	2 (5%) 33 35	25, 51, 80, 108	1 (2%)
18	x	38/39 (97%)	0.27	2 (5%) 32 34	26, 52, 97, 107	1 (2%)
19	Z	62/62 (100%)	0.44	3 (4%) 35 38	46, 59, 102, 129	0
19	z	62/62 (100%)	0.82	6 (9%) 13 14	57, 73, 113, 130	0
All	All	5246/5270 (99%)	-0.34	57 (1%) 78 80	15, 41, 73, 131	51 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	5.9
9	J	4	GLU	5.4
2	b	486	LEU	4.8
11	l	3	PRO	4.4
7	H	64	ALA	4.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.94	0.09	31,41,67,75	0
8	FME	I	1	10/11	0.95	0.09	36,43,47,48	0
14	FME	T	1	10/11	0.96	0.08	35,40,67,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.96	0.09	39,42,73,78	0
4	HSK	D	336[A]	10/12	0.97	0.06	32,36,37,37	7
8	FME	i	1	10/11	0.97	0.06	40,45,49,51	0
12	FME	m	1	10/11	0.97	0.08	40,46,74,76	0
4	HSK	D	336[B]	11/12	0.97	0.06	35,37,42,45	8
4	HSK	d	336[B]	11/12	0.98	0.07	35,42,52,56	8
4	HSK	d	336[A]	10/12	0.98	0.07	35,38,42,42	7

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
32	HTG	U	203	14/19	0.58	0.19	76,107,133,154	0
27	UNL	I	102	14/-	0.60	0.20	82,96,101,101	0
33	DGD	d	408	48/66	0.62	0.17	70,100,122,132	0
27	UNL	A	413	7/-	0.64	0.15	84,90,95,96	0
29	DMS	O	304	4/4	0.65	0.19	85,104,105,105	0
32	HTG	c	541	15/19	0.66	0.14	74,104,117,120	0
29	DMS	B	640	4/4	0.66	0.24	70,86,87,96	0
27	UNL	I	101	16/-	0.67	0.20	78,88,102,110	0
27	UNL	K	103	10/-	0.68	0.25	78,89,97,98	0
27	UNL	c	527	16/-	0.69	0.22	73,83,115,120	0
29	DMS	c	540	4/4	0.70	0.27	99,101,109,120	0
27	UNL	c	525	5/-	0.70	0.21	72,83,84,84	0
27	UNL	c	526	32/-	0.71	0.14	67,94,116,119	0
27	UNL	E	103	16/-	0.71	0.23	78,88,108,109	0
27	UNL	e	103	11/-	0.71	0.22	67,81,102,104	0
27	UNL	i	101	16/-	0.72	0.17	82,85,100,101	0
29	DMS	O	306	4/4	0.72	0.22	76,88,93,106	0
27	UNL	j	103	33/-	0.72	0.20	67,112,139,141	0
32	HTG	B	629	19/19	0.72	0.12	59,118,133,135	0
32	HTG	D	413	16/19	0.72	0.16	80,99,115,116	0
27	UNL	j	104	16/-	0.72	0.18	77,91,113,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	LMT	F	102	24/35	0.72	0.17	60,97,113,121	0
33	DGD	D	408	45/66	0.72	0.16	70,93,120,129	0
27	UNL	h	103	8/-	0.72	0.18	66,79,89,91	0
27	UNL	A	412	8/-	0.73	0.14	64,74,78,79	0
27	UNL	e	102	8/-	0.73	0.17	77,82,84,84	0
29	DMS	c	536	4/4	0.73	0.20	97,97,105,115	0
29	DMS	c	538	4/4	0.73	0.21	70,106,108,128	0
27	UNL	B	625	15/-	0.73	0.20	83,93,115,120	0
32	HTG	B	624	19/19	0.73	0.14	65,99,109,114	0
32	HTG	b	602	19/19	0.74	0.13	71,113,132,135	0
27	UNL	u	201	13/-	0.74	0.23	57,67,80,84	0
29	DMS	O	309	4/4	0.74	0.21	80,106,109,118	0
27	UNL	a	415	40/-	0.74	0.15	75,97,121,124	0
34	GOL	e	104	6/6	0.74	0.13	72,77,81,84	0
27	UNL	B	630	16/-	0.75	0.17	69,81,89,89	0
27	UNL	T	103	13/-	0.75	0.15	80,89,96,101	0
27	UNL	i	102	14/-	0.75	0.15	91,101,109,109	0
29	DMS	a	419	4/4	0.75	0.18	96,109,116,119	0
28	LMT	a	401	35/35	0.75	0.18	38,67,86,100	35
29	DMS	c	537	4/4	0.75	0.17	85,94,103,106	0
28	LMT	b	626	25/35	0.75	0.12	62,76,105,114	0
27	UNL	a	413	8/-	0.75	0.14	76,83,90,95	0
29	DMS	o	307	4/4	0.75	0.19	63,84,93,93	0
29	DMS	d	416	4/4	0.76	0.17	99,114,115,118	0
29	DMS	D	419	4/4	0.76	0.20	96,114,118,120	0
29	DMS	v	204	4/4	0.76	0.20	89,92,96,99	0
31	LHG	E	101	49/49	0.76	0.15	60,95,130,135	0
27	UNL	b	603	16/-	0.76	0.17	73,94,114,115	0
28	LMT	A	415	35/35	0.76	0.16	54,88,106,116	0
32	HTG	C	522	19/19	0.76	0.11	61,92,117,117	0
29	DMS	A	419	4/4	0.77	0.20	94,96,101,109	0
27	UNL	A	414	28/-	0.77	0.13	76,94,110,114	0
27	UNL	C	524	26/-	0.77	0.14	76,97,109,120	0
27	UNL	b	629	16/-	0.77	0.19	48,62,81,82	0
28	LMT	c	522	35/35	0.77	0.14	65,89,117,127	0
28	LMT	j	102	23/35	0.77	0.14	71,81,105,108	0
32	HTG	C	536	19/19	0.77	0.13	79,117,138,138	0
27	UNL	C	523	9/-	0.78	0.17	75,77,85,87	0
32	HTG	c	524	9/19	0.78	0.18	73,79,97,114	0
29	DMS	o	310	4/4	0.78	0.20	73,80,91,101	0
32	HTG	d	413	16/19	0.78	0.13	66,100,118,131	0
29	DMS	O	312	4/4	0.78	0.18	78,88,109,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	DMS	C	529	4/4	0.78	0.17	90,90,93,97	0
29	DMS	C	532	4/4	0.78	0.23	58,72,80,81	0
28	LMT	m	103	23/35	0.79	0.14	59,80,125,127	0
28	LMT	C	520	35/35	0.79	0.12	71,97,104,104	0
27	UNL	t	103	16/-	0.79	0.14	71,86,109,110	0
32	HTG	c	523	19/19	0.80	0.12	86,101,115,118	0
29	DMS	V	207	4/4	0.80	0.16	85,97,101,104	0
27	UNL	B	627	16/-	0.80	0.16	53,64,87,88	0
27	UNL	b	628	36/-	0.80	0.14	50,73,110,135	0
32	HTG	v	208	16/19	0.80	0.13	60,80,108,119	0
27	UNL	J	103	16/-	0.80	0.14	74,97,111,112	0
28	LMT	J	102	24/35	0.80	0.14	62,83,124,131	0
28	LMT	l	101	24/35	0.80	0.13	59,76,130,142	0
29	DMS	e	105	4/4	0.81	0.16	80,93,97,97	0
29	DMS	o	306	4/4	0.81	0.19	87,88,103,119	0
27	UNL	H	103	7/-	0.81	0.17	69,72,89,93	0
32	HTG	b	627	19/19	0.81	0.12	69,91,106,109	0
29	DMS	a	418	4/4	0.81	0.18	97,107,116,118	0
27	UNL	a	414	8/-	0.81	0.17	77,81,86,90	0
29	DMS	v	207	4/4	0.81	0.18	75,78,83,99	0
28	LMT	t	102	24/35	0.81	0.14	67,87,121,126	0
28	LMT	z	101	32/35	0.81	0.12	53,88,118,138	0
27	UNL	B	643	40/-	0.81	0.14	60,76,101,112	0
29	DMS	B	639	4/4	0.81	0.20	75,84,91,94	0
27	UNL	b	641	40/-	0.81	0.14	60,77,94,97	0
27	UNL	d	417	36/-	0.82	0.14	49,87,101,107	0
29	DMS	b	633	4/4	0.82	0.17	77,78,82,98	0
27	UNL	i	104	14/-	0.82	0.15	69,80,99,101	0
27	UNL	E	102	13/-	0.82	0.18	81,91,100,100	0
29	DMS	u	203	4/4	0.82	0.22	48,83,83,92	0
27	UNL	U	201	14/-	0.82	0.17	54,74,82,82	0
27	UNL	H	104	7/-	0.82	0.15	78,82,85,88	0
34	GOL	D	417	6/6	0.82	0.15	63,70,73,74	0
34	GOL	b	636	6/6	0.82	0.13	61,76,83,103	0
26	LMG	c	521	51/55	0.82	0.12	51,93,114,122	0
27	UNL	A	420	36/-	0.83	0.13	41,86,102,108	0
29	DMS	V	208	4/4	0.83	0.17	83,84,90,91	0
29	DMS	h	104	4/4	0.83	0.16	103,104,106,109	0
29	DMS	a	416	4/4	0.83	0.19	75,83,103,104	0
28	LMT	M	102	24/35	0.83	0.12	51,70,94,108	0
29	DMS	O	305	4/4	0.83	0.17	77,88,91,93	0
29	DMS	a	420	4/4	0.83	0.23	87,90,91,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	UNL	a	421	40/-	0.83	0.11	55,75,110,112	0
29	DMS	b	635	4/4	0.83	0.20	70,71,71,73	0
29	DMS	b	638	4/4	0.83	0.21	80,89,92,92	0
27	UNL	A	421	40/-	0.83	0.12	56,78,120,123	0
29	DMS	O	311	4/4	0.83	0.19	80,88,88,91	0
27	UNL	i	103	16/-	0.83	0.14	50,59,84,85	0
29	DMS	V	203	4/4	0.83	0.18	74,84,87,92	0
29	DMS	C	534	4/4	0.84	0.20	67,81,87,87	0
28	LMT	Z	101	35/35	0.84	0.12	48,88,101,103	0
29	DMS	u	204	4/4	0.84	0.18	70,83,95,98	0
26	LMG	C	519	48/55	0.84	0.12	52,89,111,119	0
29	DMS	O	307	4/4	0.85	0.15	87,92,93,94	0
32	HTG	C	535	9/19	0.85	0.16	72,80,85,97	0
29	DMS	D	420	4/4	0.85	0.14	93,98,108,110	0
29	DMS	O	310	4/4	0.85	0.19	70,98,98,109	0
29	DMS	c	532	4/4	0.85	0.17	64,81,98,107	0
25	PL9	A	410	55/55	0.85	0.15	51,77,105,110	0
29	DMS	C	527	4/4	0.85	0.17	75,76,79,93	0
32	HTG	b	640	17/19	0.85	0.16	27,44,57,61	17
28	LMT	M	101	35/35	0.85	0.11	43,73,83,90	0
25	PL9	a	411	55/55	0.86	0.14	54,73,105,110	0
31	LHG	e	101	38/49	0.86	0.10	63,94,111,113	0
29	DMS	B	633	4/4	0.86	0.15	94,98,98,100	0
29	DMS	O	308	4/4	0.86	0.15	67,71,84,97	0
32	HTG	B	642	18/19	0.86	0.15	25,38,48,49	18
28	LMT	m	102	25/35	0.86	0.12	45,72,116,124	0
27	UNL	d	414	16/-	0.86	0.13	44,56,84,88	0
29	DMS	E	104	4/4	0.86	0.16	91,95,98,105	0
28	LMT	T	102	24/35	0.86	0.12	43,78,107,110	0
29	DMS	v	206	4/4	0.86	0.16	63,73,80,85	0
32	HTG	V	202	19/19	0.86	0.11	50,62,107,107	0
27	UNL	D	414	16/-	0.86	0.12	44,53,66,73	0
27	UNL	x	101	16/-	0.87	0.16	56,65,93,94	0
29	DMS	I	105	4/4	0.87	0.21	76,86,99,99	0
29	DMS	c	535	4/4	0.87	0.16	84,92,99,112	0
24	BCR	t	101	40/40	0.87	0.09	36,52,72,74	0
32	HTG	C	521	19/19	0.87	0.12	70,88,102,103	0
27	UNL	I	104	13/-	0.87	0.12	57,66,93,95	0
24	BCR	T	101	40/40	0.87	0.09	40,52,78,83	0
29	DMS	o	309	4/4	0.87	0.15	70,78,79,91	0
26	LMG	a	412	51/55	0.88	0.10	51,69,85,98	0
29	DMS	o	305	4/4	0.88	0.13	88,91,92,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	LMT	B	623	35/35	0.88	0.09	56,68,85,93	0
29	DMS	A	418	4/4	0.88	0.17	82,92,94,95	0
31	LHG	F	103	38/49	0.88	0.13	56,82,111,112	0
29	DMS	c	539	4/4	0.88	0.15	106,108,113,115	0
31	LHG	f	102	46/49	0.88	0.13	52,78,107,120	0
28	LMT	m	101	35/35	0.88	0.10	38,70,81,85	0
27	UNL	B	626	40/-	0.88	0.11	46,68,109,118	0
27	UNL	I	103	16/-	0.88	0.13	47,62,98,98	0
26	LMG	c	520	38/55	0.89	0.10	43,70,87,91	0
27	UNL	X	101	16/-	0.89	0.11	47,53,78,80	0
29	DMS	a	417	4/4	0.89	0.15	69,78,88,92	0
29	DMS	u	202	4/4	0.89	0.19	48,69,70,82	0
29	DMS	U	202	4/4	0.89	0.16	40,61,69,82	0
29	DMS	B	635	4/4	0.89	0.14	90,94,95,106	0
29	DMS	o	304	4/4	0.89	0.17	85,86,87,87	0
29	DMS	V	206	4/4	0.89	0.15	61,85,90,90	0
34	GOL	c	533	6/6	0.89	0.14	58,62,76,81	0
27	UNL	Z	102	6/-	0.89	0.15	71,83,89,90	0
24	BCR	c	515	40/40	0.90	0.09	50,62,69,70	0
26	LMG	B	622	51/55	0.90	0.09	48,60,79,84	0
29	DMS	B	641	4/4	0.90	0.15	65,66,71,83	0
29	DMS	c	530	4/4	0.90	0.15	70,88,95,104	0
26	LMG	b	625	49/55	0.90	0.10	47,57,79,86	0
26	LMG	C	518	49/55	0.90	0.11	42,73,104,111	0
29	DMS	V	205	4/4	0.90	0.13	77,79,80,89	0
29	DMS	C	531	4/4	0.90	0.16	86,87,90,92	0
29	DMS	b	631	4/4	0.90	0.13	66,78,80,82	0
36	BCT	D	402[A]	4/4	0.90	0.13	24,36,36,40	4
36	BCT	D	402[B]	4/4	0.90	0.13	36,44,46,50	4
29	DMS	V	204	4/4	0.91	0.15	68,73,75,90	0
29	DMS	c	534	4/4	0.91	0.16	80,90,95,100	0
34	GOL	C	533	6/6	0.91	0.17	46,53,57,61	0
29	DMS	O	303	4/4	0.91	0.13	72,84,93,96	0
29	DMS	o	311	4/4	0.91	0.14	80,91,94,116	0
22	CLA	C	506	65/65	0.91	0.10	39,55,121,136	0
22	CLA	b	605	65/65	0.91	0.10	41,60,107,122	0
29	DMS	b	639	4/4	0.91	0.15	87,93,94,106	0
22	CLA	c	514	65/65	0.91	0.09	44,66,111,118	0
32	HTG	B	628	19/19	0.92	0.09	47,69,90,102	0
26	LMG	A	411	51/55	0.92	0.09	54,68,92,105	0
29	DMS	A	416	4/4	0.92	0.15	71,73,77,85	0
29	DMS	v	203	4/4	0.92	0.13	76,78,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	HTG	o	301	19/19	0.92	0.09	49,58,70,73	0
29	DMS	b	632	4/4	0.92	0.15	63,72,72,73	0
22	CLA	c	507	65/65	0.92	0.09	42,51,109,121	0
21	CL	v	201	1/1	0.92	0.08	93,93,93,93	0
33	DGD	h	101	62/66	0.92	0.09	35,47,64,65	0
31	LHG	D	411	44/49	0.92	0.10	35,44,110,117	0
29	DMS	o	308	4/4	0.92	0.11	71,77,85,85	0
24	BCR	y	101	40/40	0.92	0.07	40,47,57,59	0
32	HTG	b	601	19/19	0.92	0.09	57,66,80,92	0
24	BCR	K	101	40/40	0.92	0.09	36,47,54,58	0
29	DMS	B	638	4/4	0.92	0.15	43,55,65,71	0
22	CLA	B	602	65/65	0.92	0.10	39,52,116,127	0
29	DMS	c	531	4/4	0.93	0.14	90,91,96,98	0
24	BCR	K	102	40/40	0.93	0.07	42,53,57,60	0
26	LMG	d	412	47/55	0.93	0.09	37,47,99,103	0
29	DMS	v	205	4/4	0.93	0.13	61,68,69,70	0
29	DMS	D	415	4/4	0.93	0.13	65,68,77,91	0
22	CLA	c	513	65/65	0.93	0.08	43,56,94,107	0
30	CA	v	209	1/1	0.93	0.09	90,90,90,90	0
31	LHG	D	409	49/49	0.93	0.09	37,48,64,69	0
22	CLA	b	620	65/65	0.93	0.09	32,44,112,139	0
29	DMS	b	634	4/4	0.93	0.16	73,77,82,89	0
24	BCR	k	101	40/40	0.93	0.09	41,48,56,58	0
31	LHG	d	411	44/49	0.93	0.10	37,47,109,121	0
29	DMS	B	634	4/4	0.93	0.13	83,86,86,94	0
29	DMS	C	530	4/4	0.93	0.20	40,54,55,58	0
22	CLA	C	513	65/65	0.93	0.08	46,58,99,105	0
38	RRX	H	102	41/41	0.93	0.07	36,42,56,60	0
39	MG	K	104	1/1	0.93	0.06	56,56,56,56	0
24	BCR	d	406	40/40	0.94	0.07	30,42,75,76	0
22	CLA	c	509	65/65	0.94	0.07	34,41,100,113	0
26	LMG	D	412	47/55	0.94	0.08	34,44,84,95	0
22	CLA	C	512	65/65	0.94	0.07	39,51,96,105	0
33	DGD	H	101	62/66	0.94	0.09	34,46,55,59	0
29	DMS	B	636	4/4	0.94	0.16	65,83,88,91	0
32	HTG	O	302	19/19	0.94	0.09	41,57,74,75	0
29	DMS	B	637	4/4	0.94	0.14	69,73,81,82	0
29	DMS	D	418	4/4	0.94	0.14	83,92,96,114	0
22	CLA	b	610	65/65	0.94	0.08	31,42,81,83	0
24	BCR	Y	101	40/40	0.94	0.07	37,43,55,57	0
24	BCR	a	410	40/40	0.94	0.06	32,39,45,46	0
24	BCR	B	618	40/40	0.94	0.06	31,39,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	c	516	40/40	0.94	0.07	37,46,57,58	0
29	DMS	b	637	4/4	0.94	0.14	71,82,87,95	0
38	RRX	h	102	41/41	0.94	0.08	38,46,63,72	0
29	DMS	C	528	4/4	0.94	0.13	74,81,82,82	0
22	CLA	d	405	65/65	0.95	0.08	31,43,111,120	0
24	BCR	A	409	40/40	0.95	0.06	28,35,42,44	0
22	CLA	B	607	65/65	0.95	0.07	32,39,71,87	0
24	BCR	B	619	40/40	0.95	0.06	30,40,55,70	0
24	BCR	B	620	40/40	0.95	0.06	31,41,57,60	0
29	DMS	c	529	4/4	0.95	0.18	52,56,57,67	0
33	DGD	C	516	62/66	0.95	0.07	31,45,103,116	0
33	DGD	C	517	62/66	0.95	0.07	27,42,77,83	0
29	DMS	D	416	4/4	0.95	0.14	68,80,85,89	0
24	BCR	C	514	40/40	0.95	0.06	35,46,60,63	0
33	DGD	c	517	62/66	0.95	0.07	32,46,93,108	0
33	DGD	c	518	56/66	0.95	0.07	37,45,80,86	0
33	DGD	c	519	62/66	0.95	0.07	32,45,73,87	0
24	BCR	D	406	40/40	0.95	0.07	32,40,73,76	0
22	CLA	c	504	65/65	0.95	0.06	34,47,56,58	0
22	CLA	c	505	65/65	0.95	0.06	35,40,74,82	0
22	CLA	B	610	65/65	0.95	0.07	33,41,49,54	0
22	CLA	c	508	65/65	0.95	0.08	34,44,68,76	0
22	CLA	B	617	65/65	0.95	0.09	31,43,129,145	0
24	BCR	b	621	40/40	0.95	0.06	36,42,55,58	0
24	BCR	b	622	40/40	0.95	0.06	29,44,58,67	0
29	DMS	d	415	4/4	0.95	0.11	64,70,75,87	0
24	BCR	b	623	40/40	0.95	0.06	33,44,60,61	0
22	CLA	B	603	65/65	0.95	0.06	30,38,46,50	0
22	CLA	b	618	65/65	0.95	0.08	29,36,123,128	0
22	CLA	a	406	65/65	0.96	0.06	25,31,40,56	0
22	CLA	a	409	65/65	0.96	0.09	29,37,126,135	0
22	CLA	A	408	65/65	0.96	0.08	25,34,110,115	0
22	CLA	b	606	65/65	0.96	0.06	32,37,48,59	0
29	DMS	C	525	4/4	0.96	0.09	42,51,52,58	0
29	DMS	C	526	4/4	0.96	0.13	60,61,66,69	0
22	CLA	C	503	65/65	0.96	0.06	33,41,47,58	0
22	CLA	b	611	65/65	0.96	0.06	26,32,50,58	0
22	CLA	b	613	65/65	0.96	0.06	35,40,50,54	0
22	CLA	b	614	65/65	0.96	0.06	30,40,46,51	0
22	CLA	b	616	65/65	0.96	0.06	29,36,44,50	0
22	CLA	C	504	65/65	0.96	0.06	32,38,72,74	0
22	CLA	b	619	65/65	0.96	0.06	32,42,59,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	505	65/65	0.96	0.06	34,41,54,60	0
22	CLA	c	502	65/65	0.96	0.06	38,43,56,64	0
22	CLA	B	604	65/65	0.96	0.06	26,34,44,55	0
22	CLA	C	507	65/65	0.96	0.07	37,44,68,75	0
33	DGD	C	515	62/66	0.96	0.07	30,41,105,109	0
22	CLA	c	506	65/65	0.96	0.06	34,43,57,71	0
22	CLA	C	508	65/65	0.96	0.06	33,39,105,122	0
30	CA	V	209	1/1	0.96	0.06	93,93,93,93	0
29	DMS	c	528	4/4	0.96	0.09	41,54,55,56	0
22	CLA	C	509	65/65	0.96	0.07	33,42,68,76	0
22	CLA	C	510	65/65	0.96	0.06	33,40,52,66	0
22	CLA	c	511	65/65	0.96	0.06	30,40,54,58	0
25	PL9	D	407	55/55	0.96	0.05	26,35,43,54	0
31	LHG	b	624	49/49	0.96	0.06	33,42,65,76	0
31	LHG	d	409	49/49	0.96	0.07	40,47,64,70	0
31	LHG	d	410	49/49	0.96	0.07	27,38,58,73	0
22	CLA	c	512	65/65	0.96	0.07	40,49,56,65	0
25	PL9	d	407	55/55	0.96	0.06	27,34,46,55	0
29	DMS	B	632	4/4	0.96	0.10	53,54,55,69	0
22	CLA	C	511	65/65	0.96	0.06	36,44,50,53	0
22	CLA	B	611	65/65	0.96	0.06	30,37,44,57	0
36	BCT	d	401[A]	4/4	0.96	0.09	50,52,55,67	4
36	BCT	d	401[B]	4/4	0.96	0.09	21,31,31,38	4
22	CLA	B	615	65/65	0.96	0.07	27,36,115,119	0
23	PHO	D	404	64/64	0.96	0.05	25,34,41,45	0
22	CLA	D	405	65/65	0.96	0.08	31,39,114,126	0
29	DMS	B	631	4/4	0.97	0.08	31,35,36,42	0
22	CLA	B	606	65/65	0.97	0.05	28,34,51,56	0
22	CLA	b	615	65/65	0.97	0.05	25,33,52,55	0
22	CLA	B	616	65/65	0.97	0.06	32,39,61,67	0
30	CA	B	601	1/1	0.97	0.05	60,60,60,60	0
22	CLA	b	617	65/65	0.97	0.05	30,35,74,80	0
22	CLA	A	404	65/65	0.97	0.05	22,28,40,59	0
31	LHG	B	621	49/49	0.97	0.06	33,41,61,65	0
22	CLA	C	501	65/65	0.97	0.06	32,41,55,66	0
22	CLA	D	403	65/65	0.97	0.05	23,28,49,53	0
22	CLA	C	502	65/65	0.97	0.05	30,36,52,61	0
22	CLA	c	503	65/65	0.97	0.06	31,38,55,64	0
22	CLA	B	608	65/65	0.97	0.05	24,31,47,62	0
22	CLA	a	407	65/65	0.97	0.06	25,33,104,120	0
22	CLA	B	609	65/65	0.97	0.04	28,35,44,47	0
22	CLA	A	405	65/65	0.97	0.05	22,27,39,48	0

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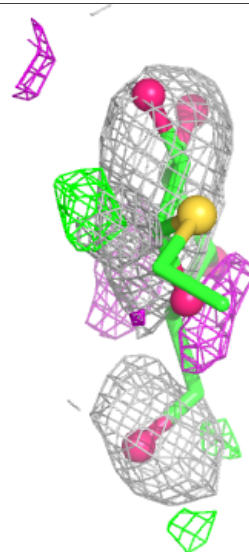
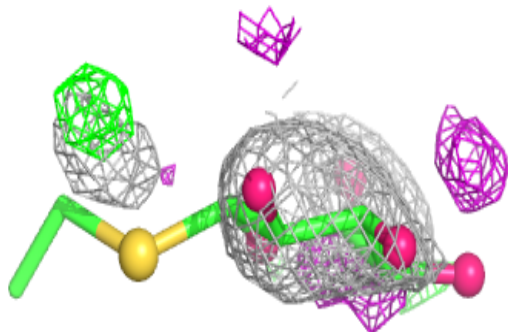
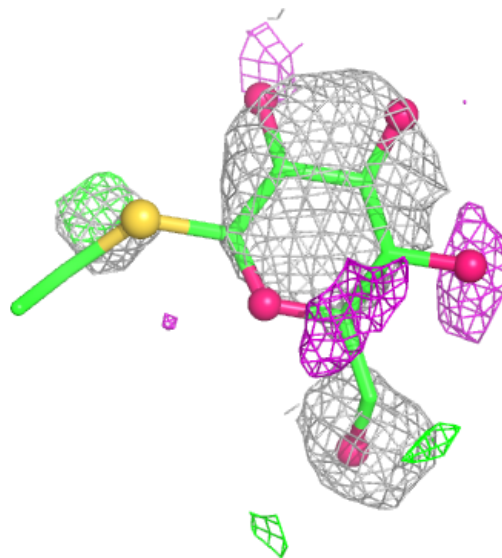
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	B	605	65/65	0.97	0.06	26,33,65,73	0
22	CLA	b	607	65/65	0.97	0.05	29,36,47,51	0
22	CLA	c	510	65/65	0.97	0.08	30,42,76,81	0
22	CLA	b	608	65/65	0.97	0.06	29,35,75,79	0
22	CLA	b	609	65/65	0.97	0.05	28,33,47,48	0
22	CLA	B	612	65/65	0.97	0.05	25,32,48,55	0
22	CLA	B	613	65/65	0.97	0.05	28,33,40,43	0
29	DMS	b	630	4/4	0.97	0.08	37,40,40,42	0
22	CLA	d	402	65/65	0.97	0.05	25,30,48,56	0
22	CLA	d	403	65/65	0.97	0.04	26,29,43,53	0
22	CLA	b	612	65/65	0.97	0.05	26,35,44,49	0
23	PHO	A	407	64/64	0.97	0.05	25,30,33,38	0
22	CLA	B	614	65/65	0.97	0.05	26,32,69,94	0
23	PHO	a	408	64/64	0.97	0.04	27,33,38,42	0
23	PHO	d	404	64/64	0.97	0.04	27,34,41,48	0
39	MG	k	102	1/1	0.97	0.04	61,61,61,61	0
37	HEM	f	101	43/43	0.98	0.07	42,50,58,63	0
31	LHG	D	410	49/49	0.98	0.05	30,38,53,67	0
30	CA	c	501	1/1	0.98	0.07	62,62,62,62	0
39	MG	J	101	1/1	0.98	0.04	45,45,45,45	0
22	CLA	A	406	65/65	0.98	0.05	24,33,95,113	0
39	MG	j	101	1/1	0.98	0.06	50,50,50,50	0
37	HEM	F	101	43/43	0.98	0.06	43,52,63,69	0
40	HEC	V	201	43/43	0.98	0.05	28,32,39,44	0
40	HEC	v	202	43/43	0.98	0.06	37,44,49,57	0
21	CL	A	402	1/1	0.99	0.05	31,31,31,31	0
29	DMS	A	417	4/4	0.99	0.05	32,36,37,38	0
21	CL	A	403	1/1	0.99	0.05	29,29,29,29	0
30	CA	O	301	1/1	0.99	0.03	57,57,57,57	0
29	DMS	o	303	4/4	0.99	0.05	31,40,41,44	0
30	CA	b	604	1/1	0.99	0.03	63,63,63,63	0
21	CL	a	404	1/1	0.99	0.09	35,35,35,35	0
30	CA	o	302	1/1	0.99	0.03	58,58,58,58	0
21	CL	a	405	1/1	0.99	0.03	34,34,34,34	0
35	FE2	D	401	1/1	1.00	0.02	41,41,41,41	0
35	FE2	a	403	1/1	1.00	0.03	40,40,40,40	0
20	OEX	a	402	10/10	1.00	0.03	28,33,39,41	0
20	OEX	A	401	10/10	1.00	0.03	28,31,39,40	0

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

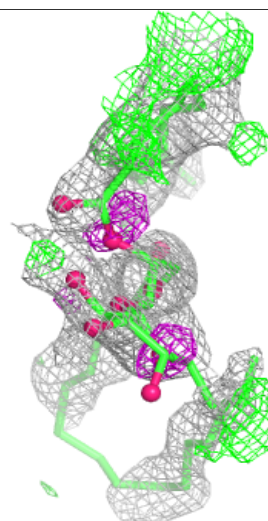
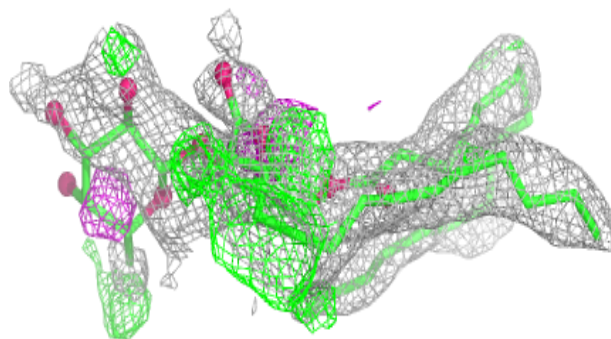
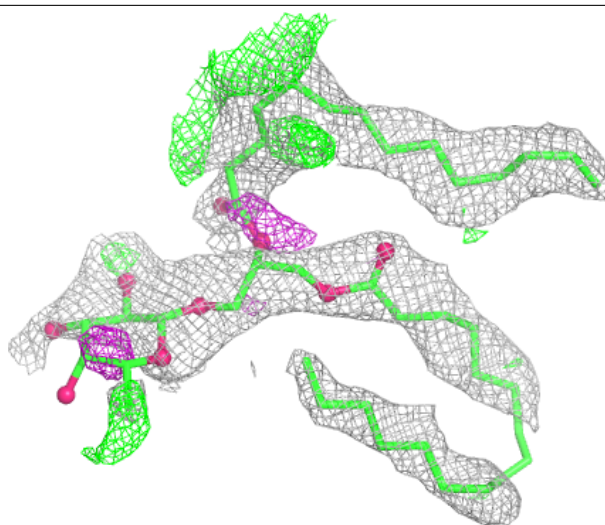
Electron density around HTG U 203:

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



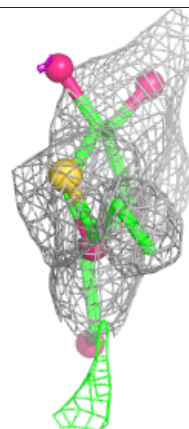
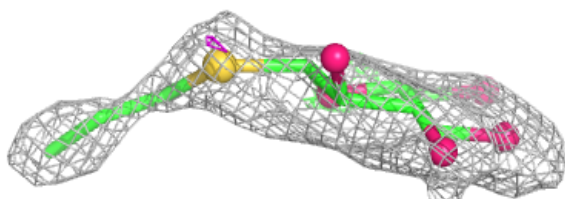
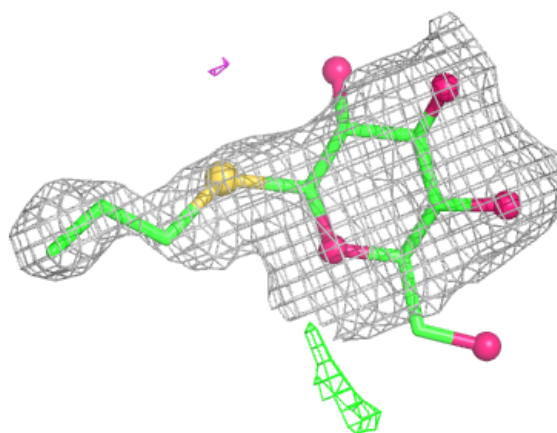
Electron density around DGD d 408:

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

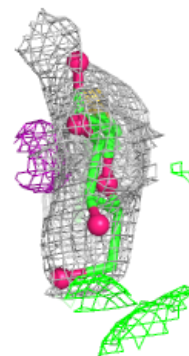
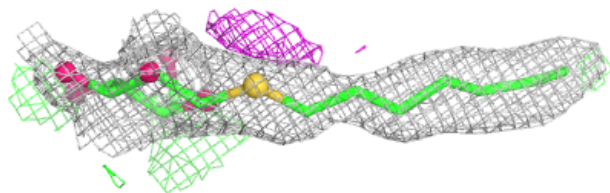
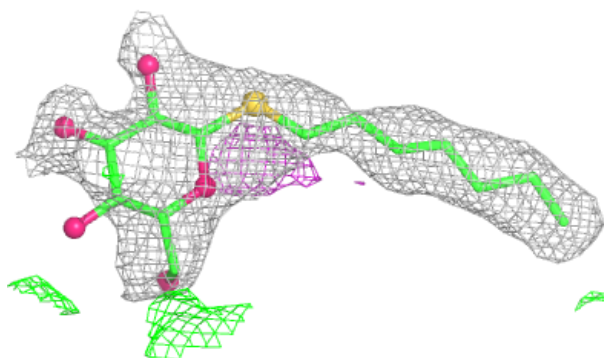


Electron density around HTG c 541:

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

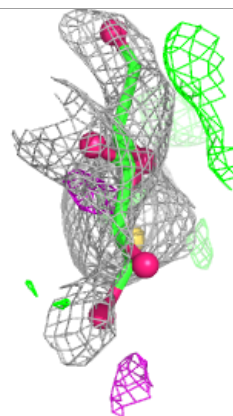
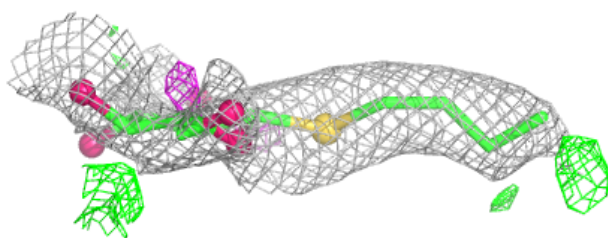
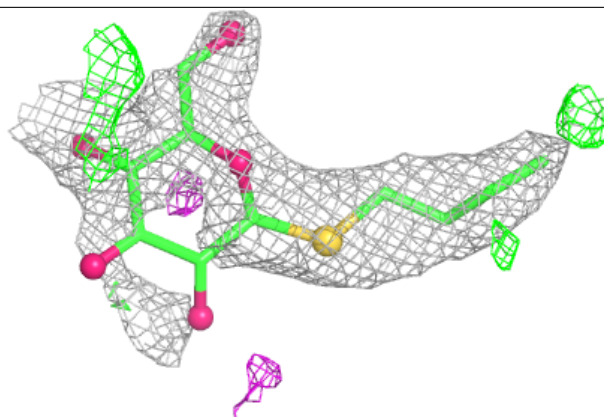
**Electron density around HTG B 629:**

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

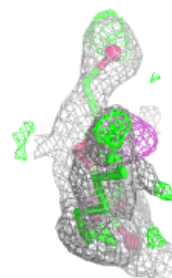
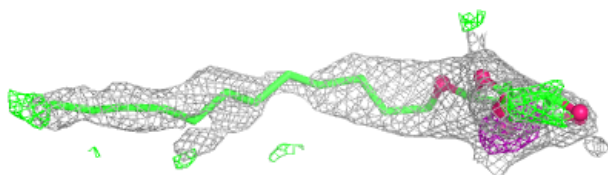
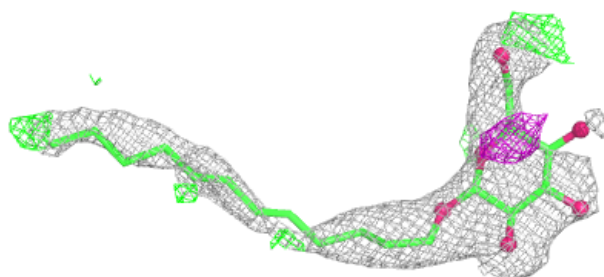


Electron density around HTG D 413:

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

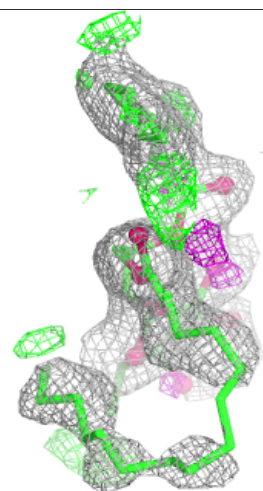
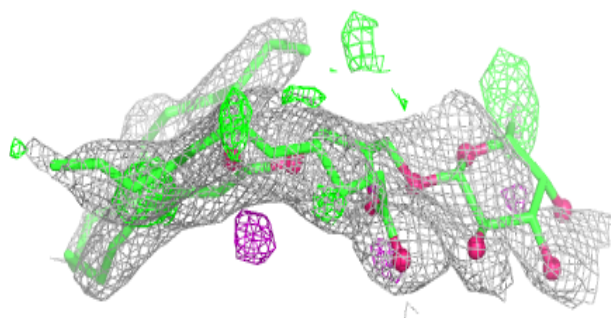
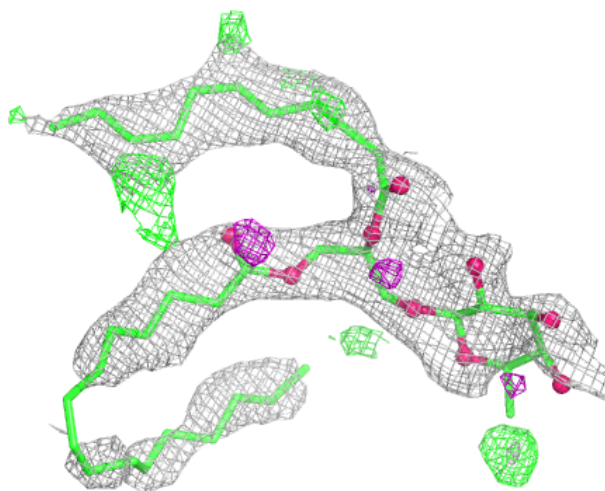
**Electron density around LMT F 102:**

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



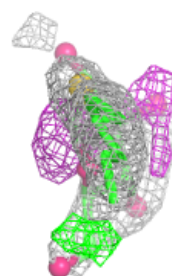
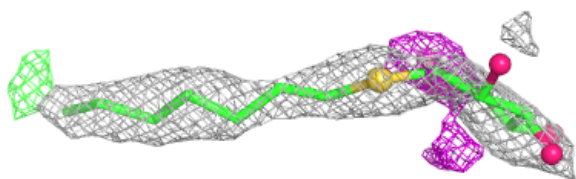
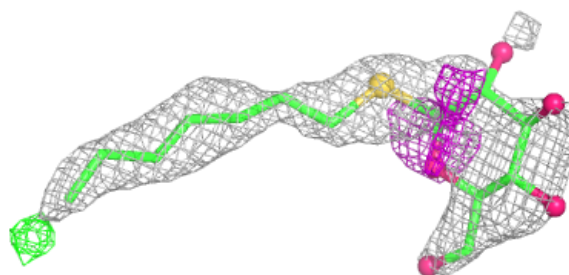
Electron density around DGD D 408:

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

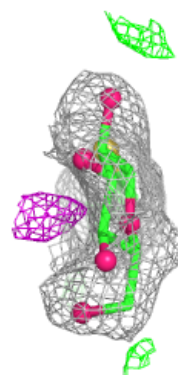
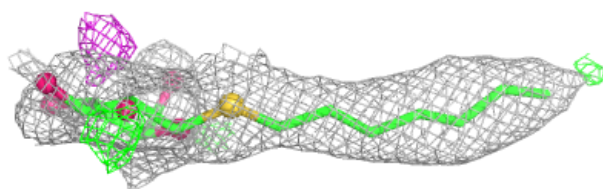
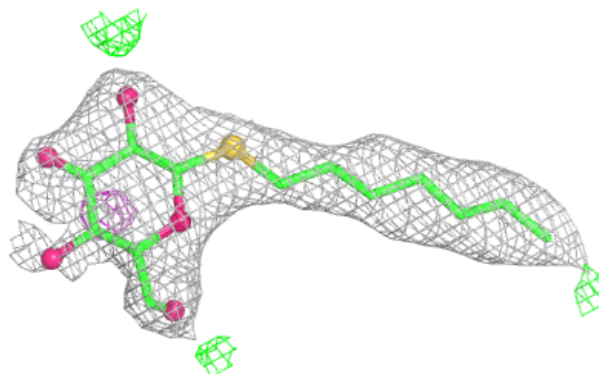


Electron density around HTG B 624:

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

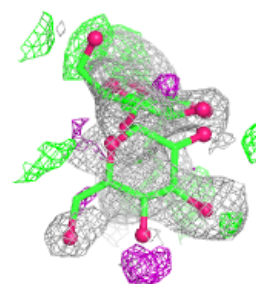
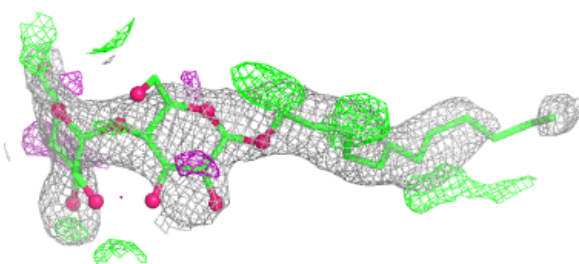
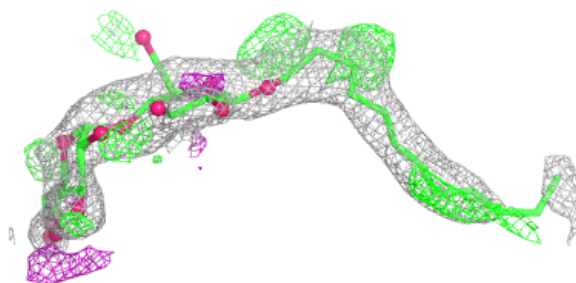
**Electron density around HTG b 602:**

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

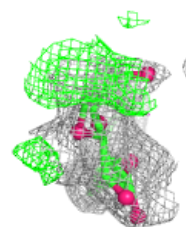
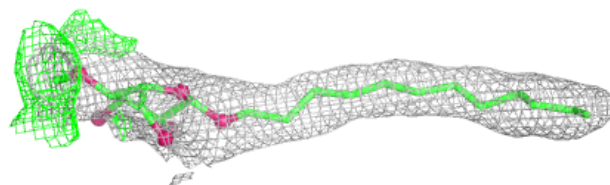
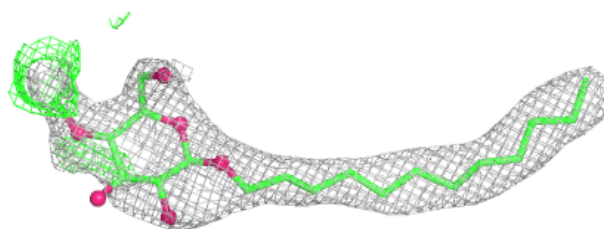


Electron density around LMT a 401:

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and green (positive)

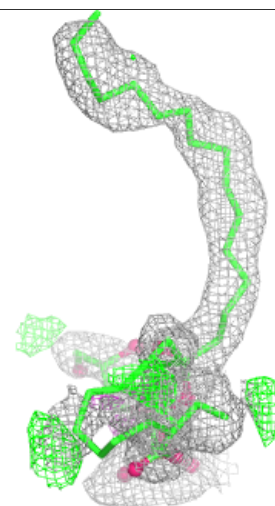
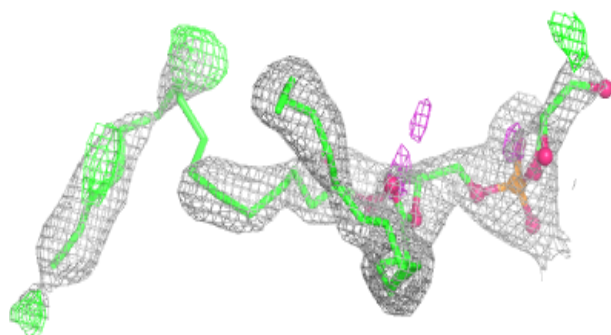
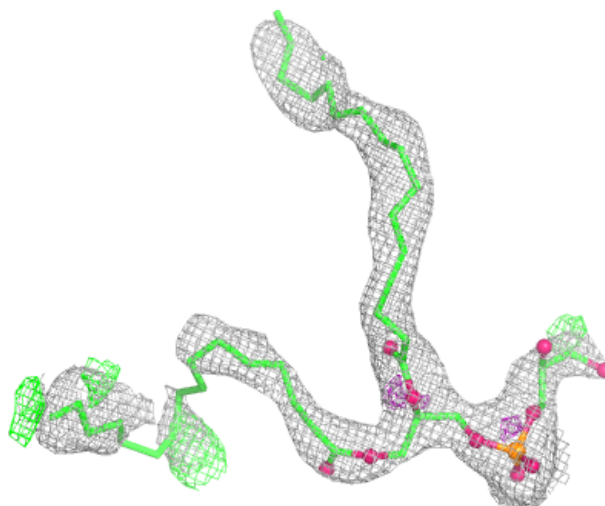
**Electron density around LMT b 626:**

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



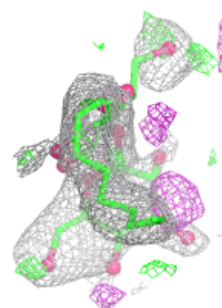
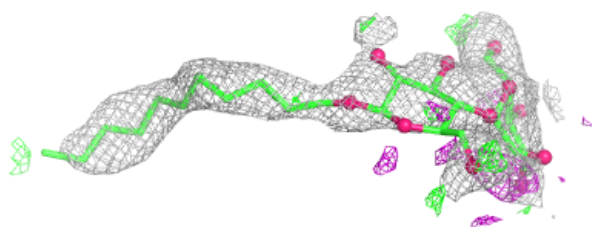
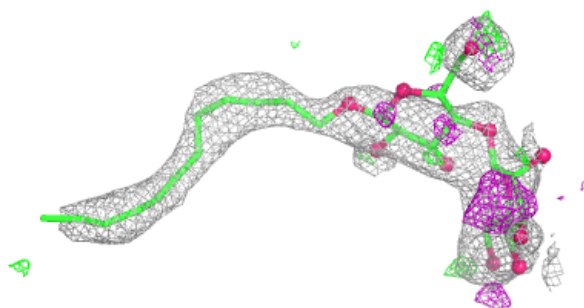
Electron density around LHG E 101:

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

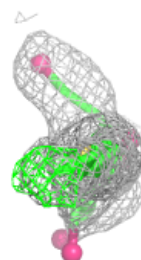
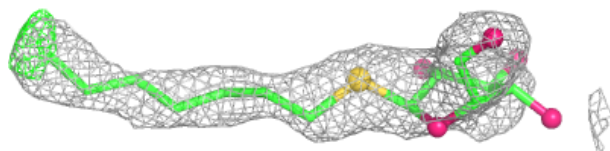
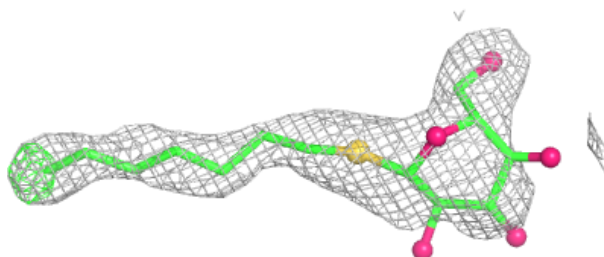


Electron density around LMT A 415:

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

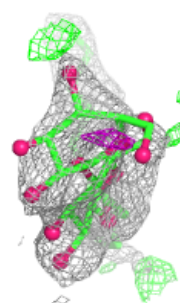
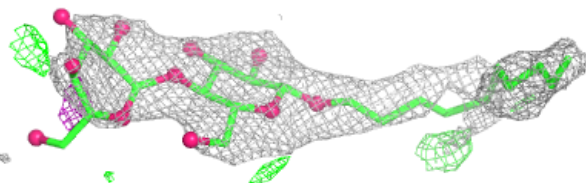
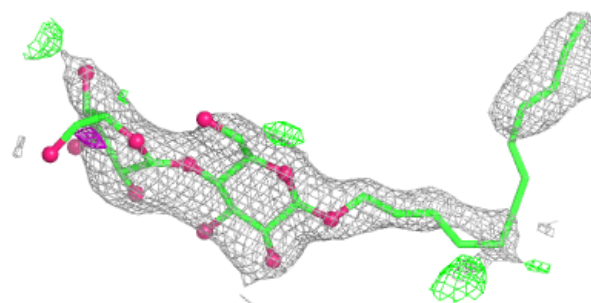
**Electron density around HTG C 522:**

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

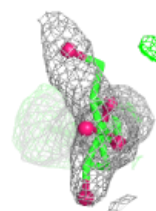
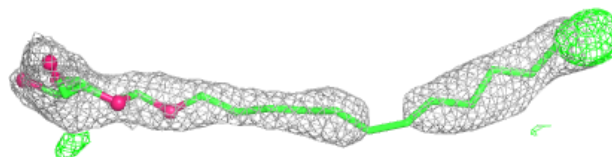
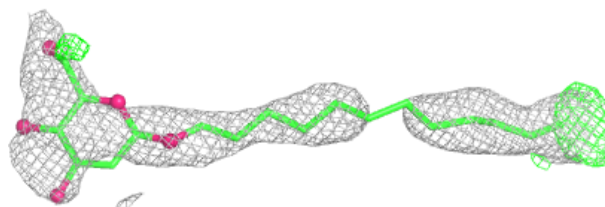


Electron density around LMT c 522:

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

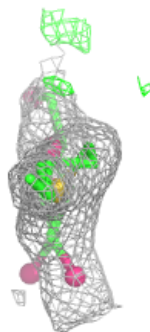
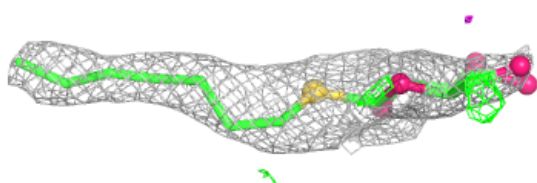
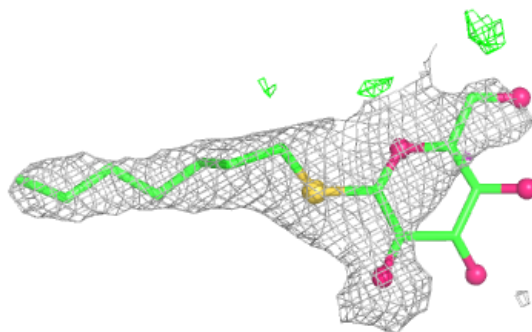
**Electron density around LMT j 102:**

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

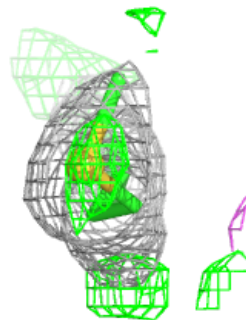
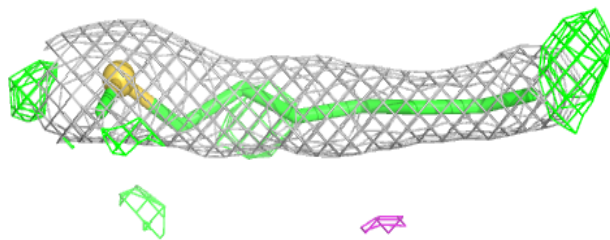
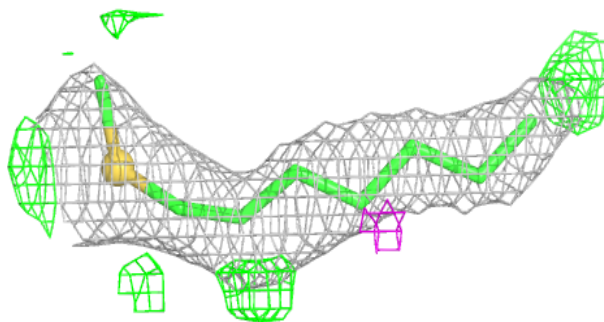


Electron density around HTG C 536:

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

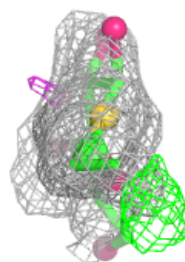
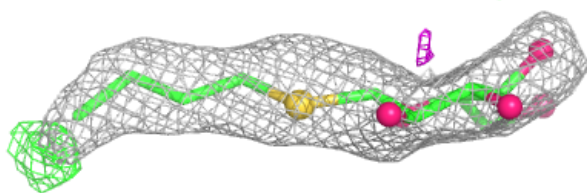
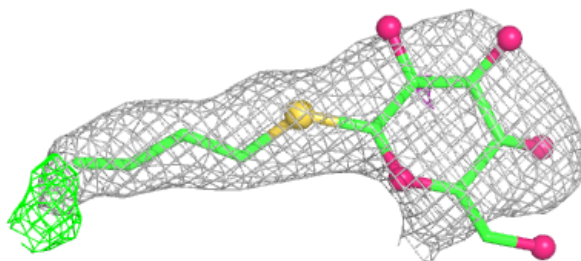
**Electron density around HTG c 524:**

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and green (positive)

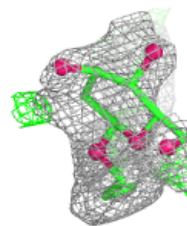
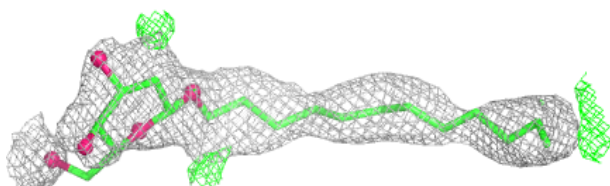
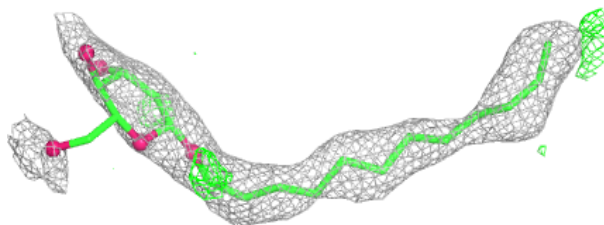


Electron density around HTG d 413:

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

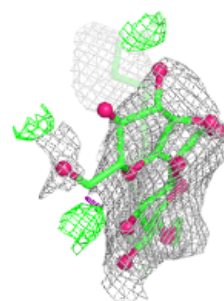
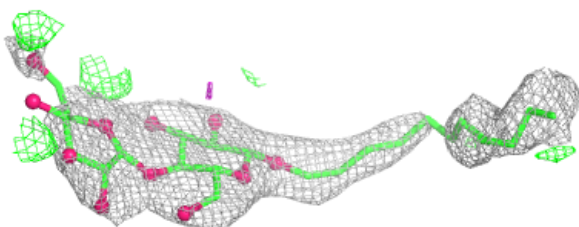
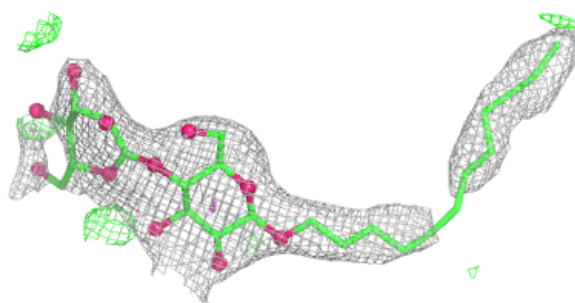
**Electron density around LMT m 103:**

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

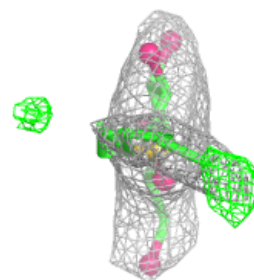
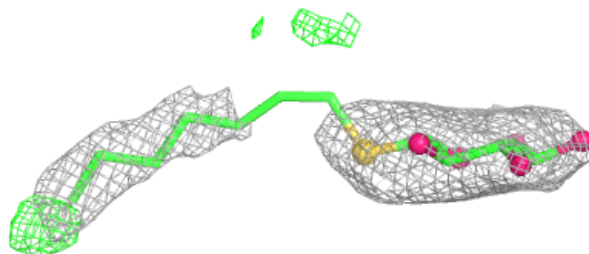
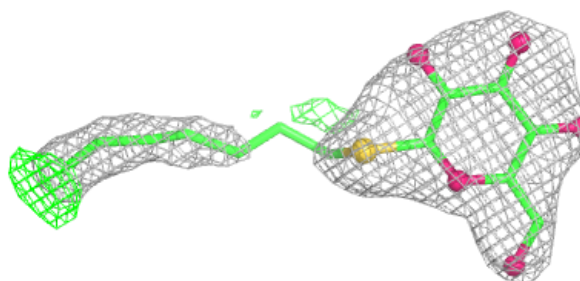


Electron density around LMT C 520:

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

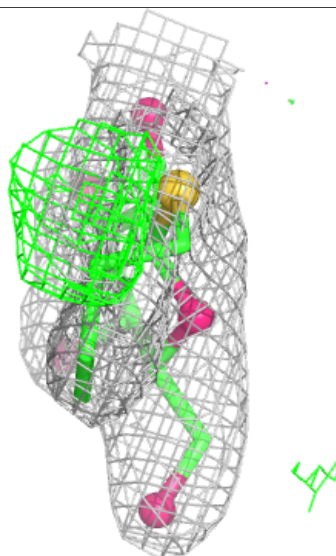
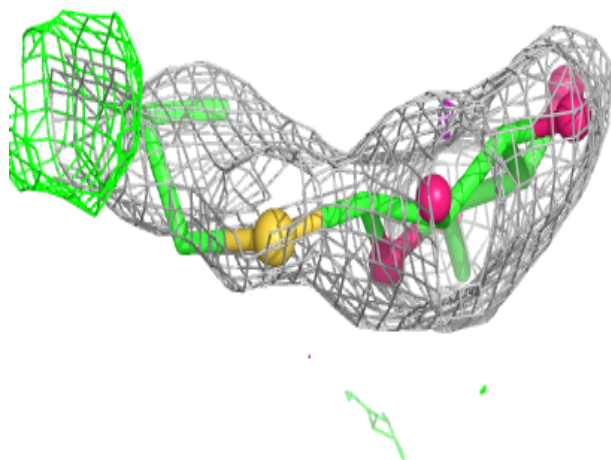
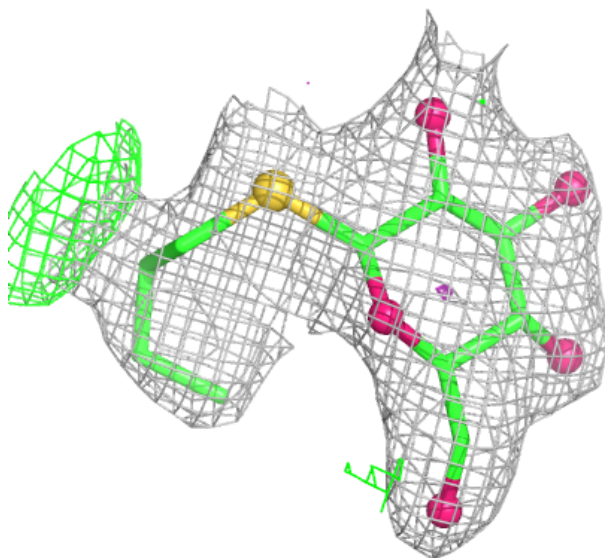
**Electron density around HTG c 523:**

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



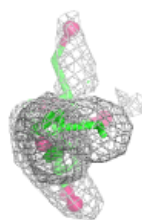
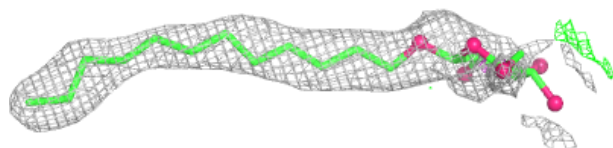
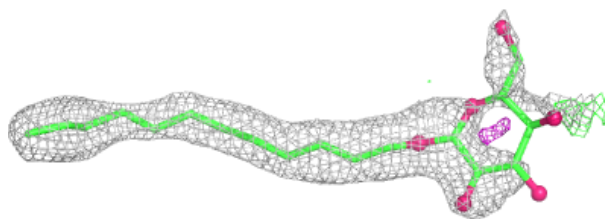
Electron density around HTG v 208:

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

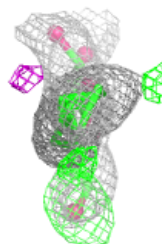
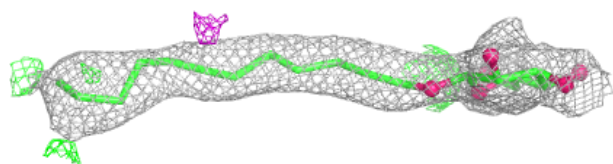
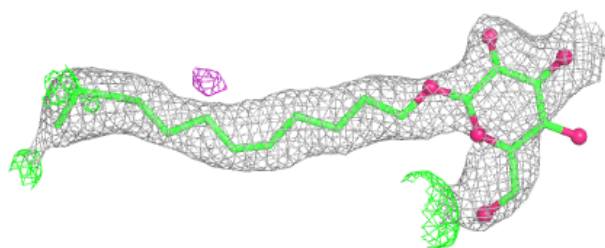


Electron density around LMT J 102:

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

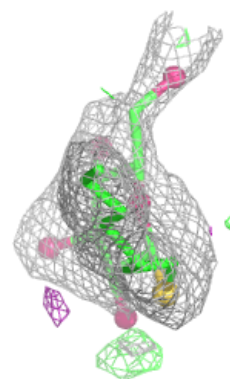
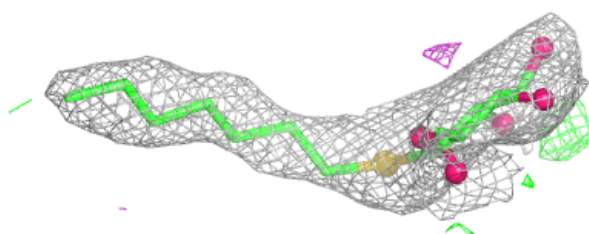
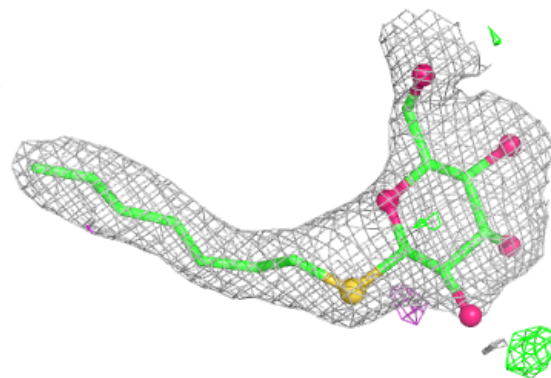
**Electron density around LMT I 101:**

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

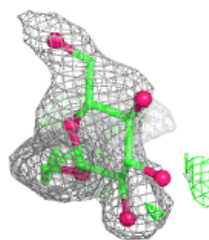
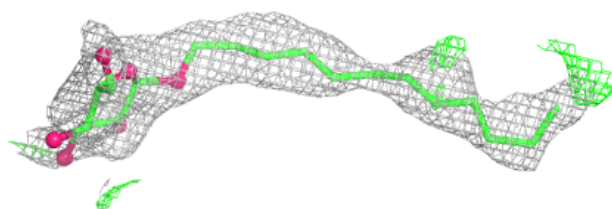
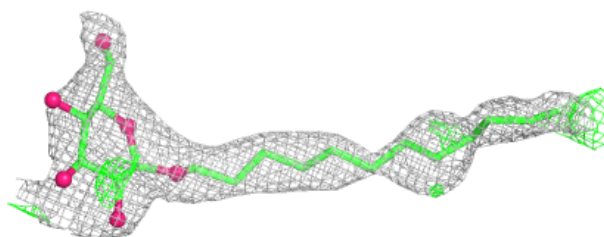


Electron density around HTG b 627:

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

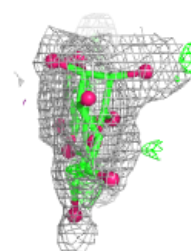
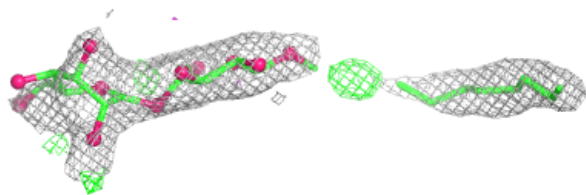
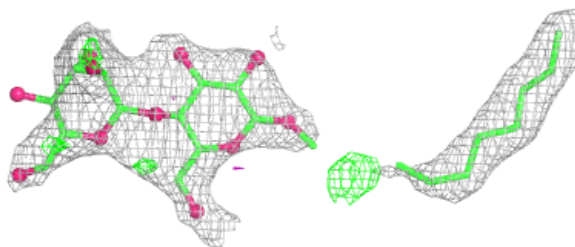
**Electron density around LMT t 102:**

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

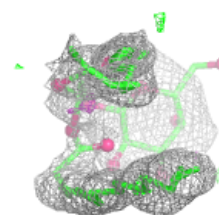
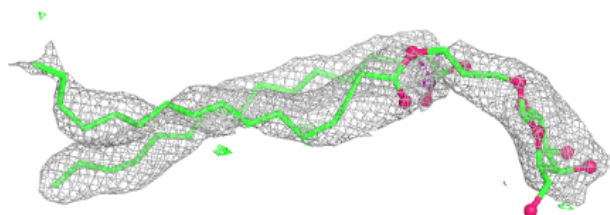
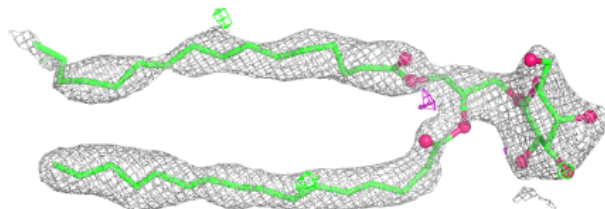


Electron density around LMT z 101:

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

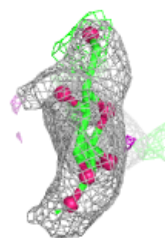
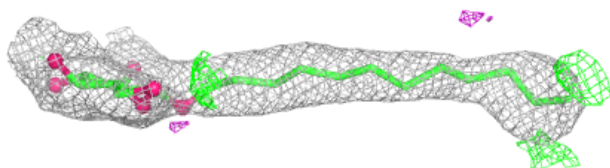
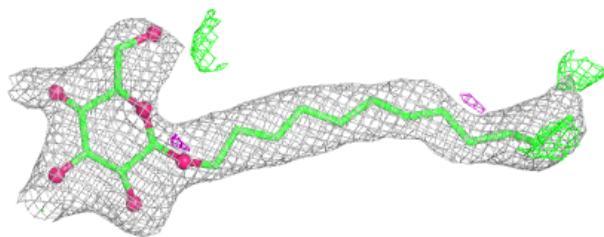
**Electron density around LMG c 521:**

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

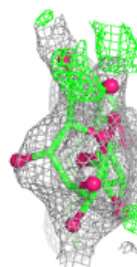
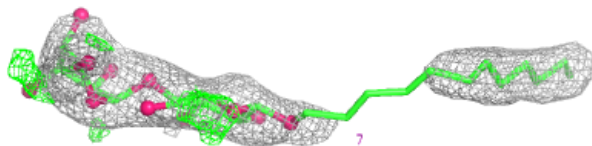
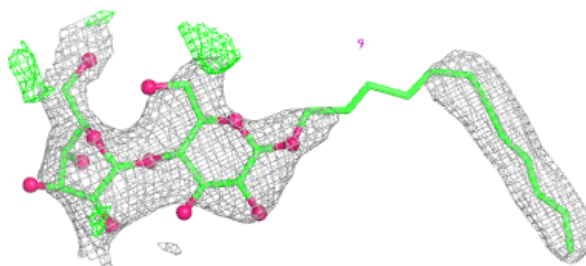


Electron density around LMT M 102:

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

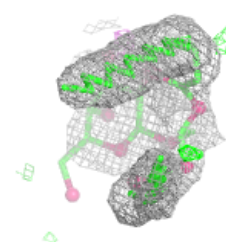
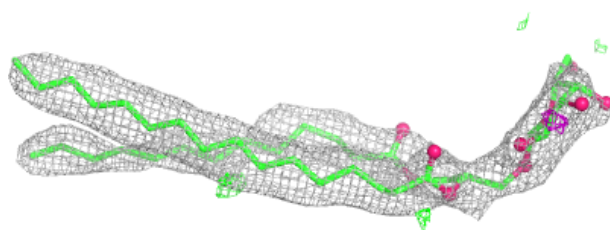
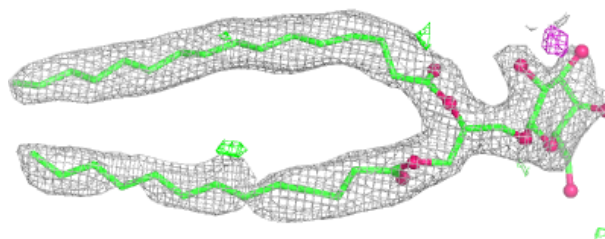
**Electron density around LMT Z 101:**

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

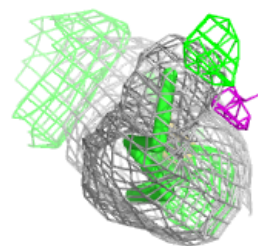
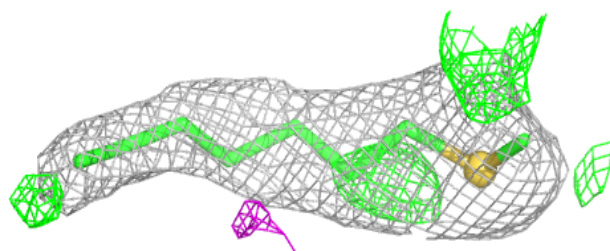
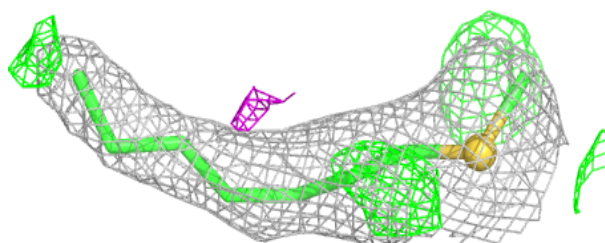


Electron density around LMG C 519:

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

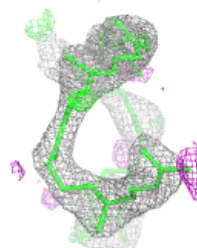
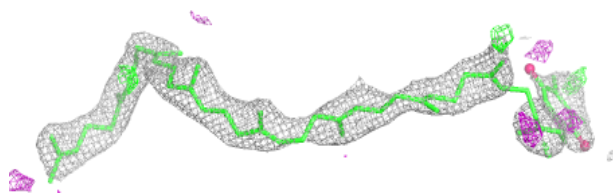
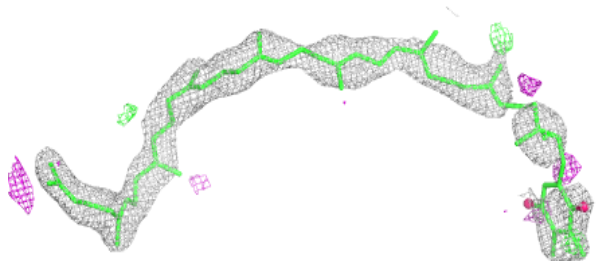
**Electron density around HTG C 535:**

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

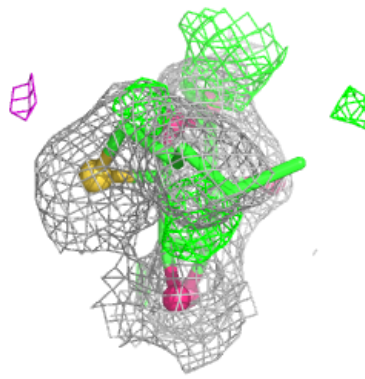
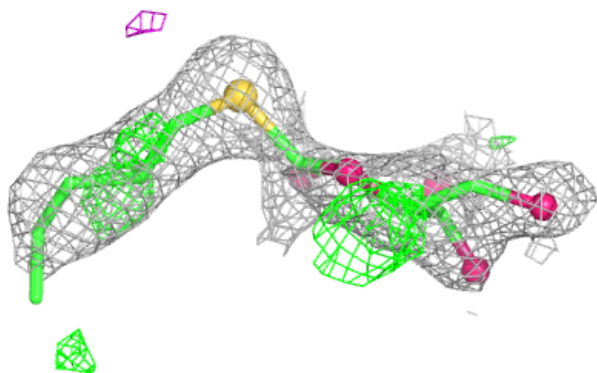
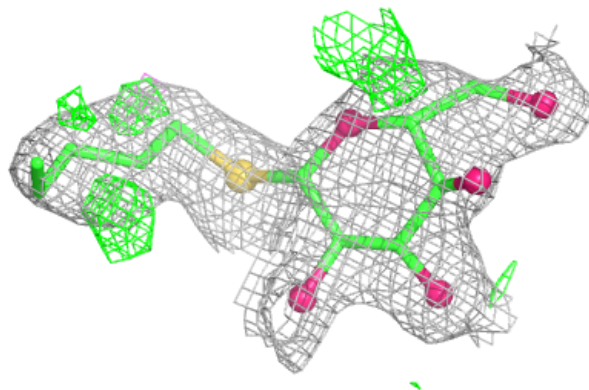


Electron density around PL9 A 410:

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

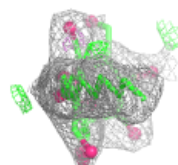
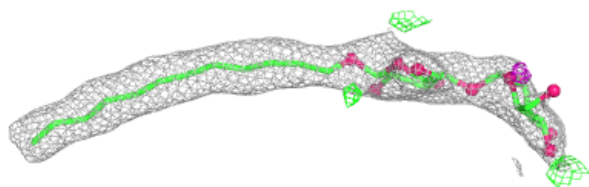
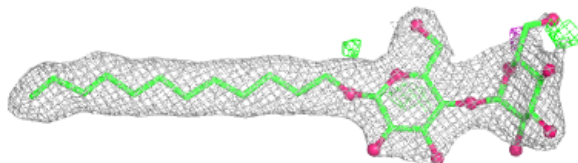
**Electron density around HTG b 640:**

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

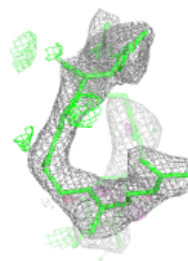
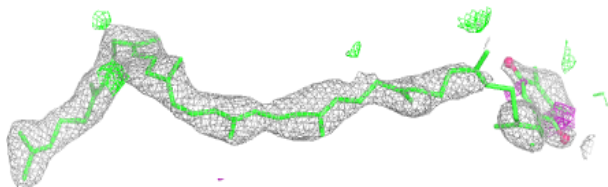
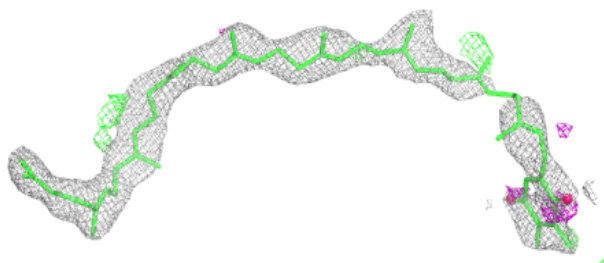


Electron density around LMT M 101:

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

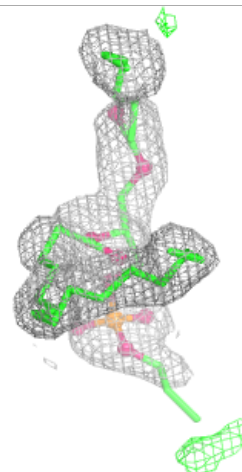
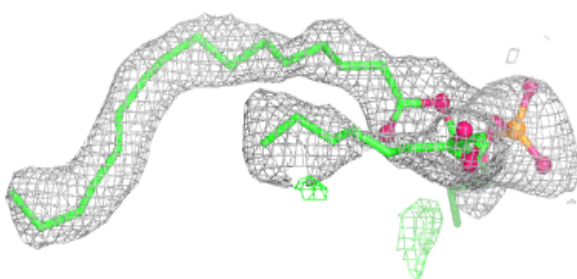
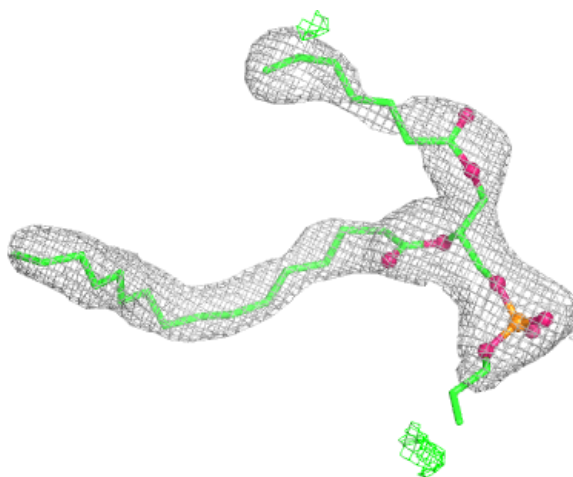
**Electron density around PL9 a 411:**

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



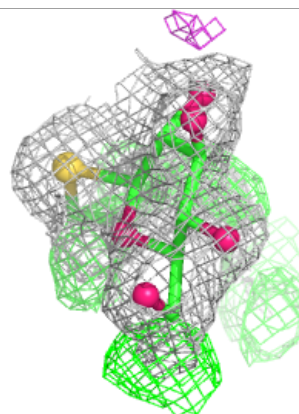
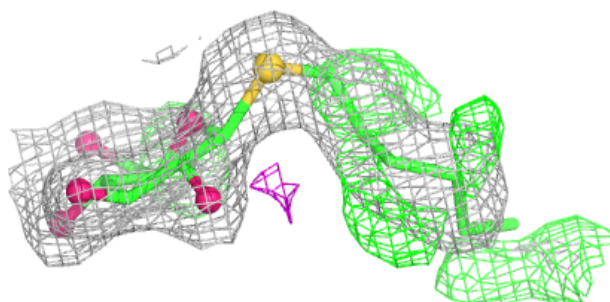
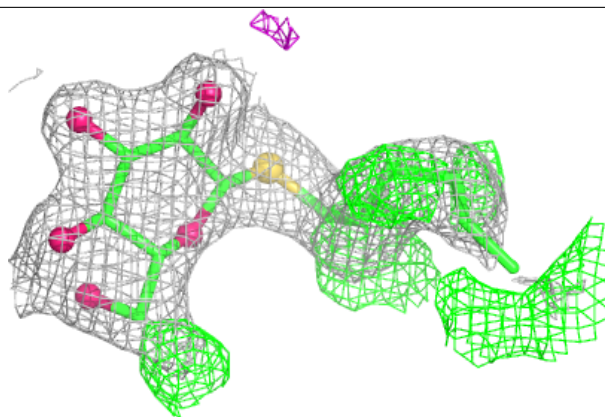
Electron density around LHG e 101:

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

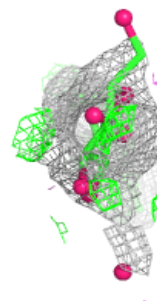
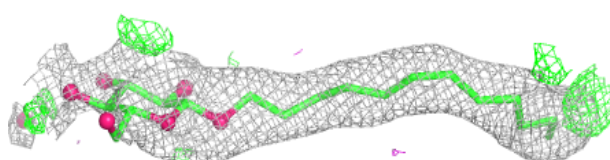
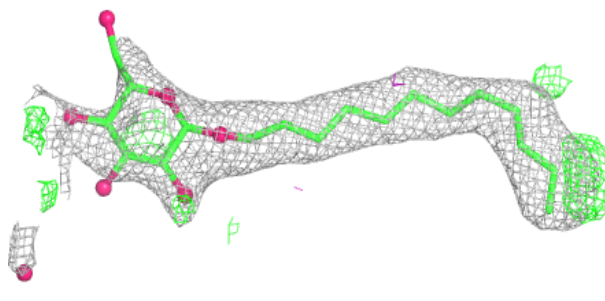


Electron density around HTG B 642:

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

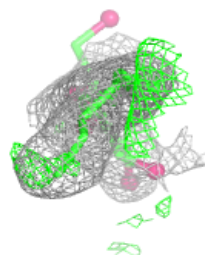
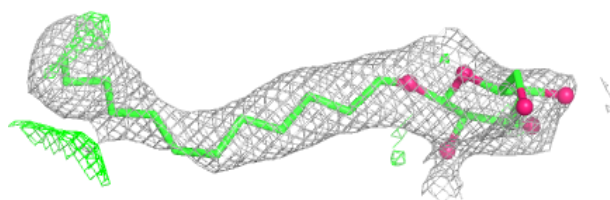
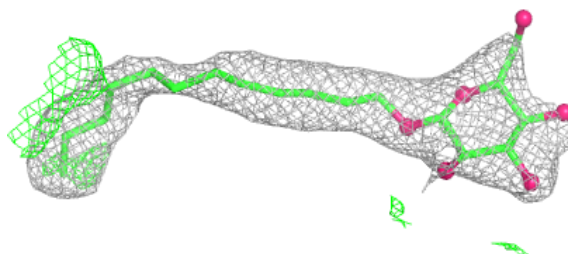
**Electron density around LMT m 102:**

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

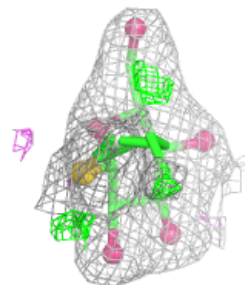
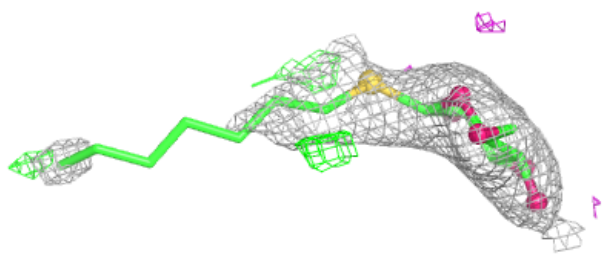
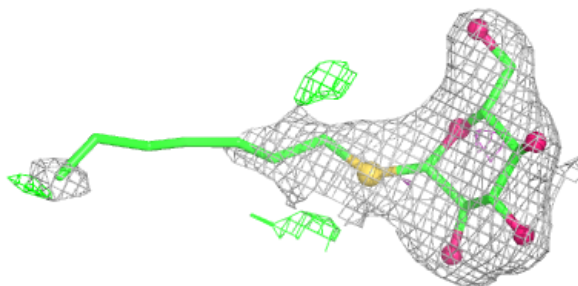


Electron density around LMT T 102:

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

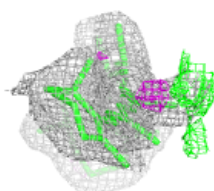
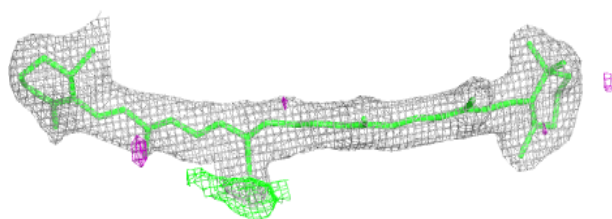
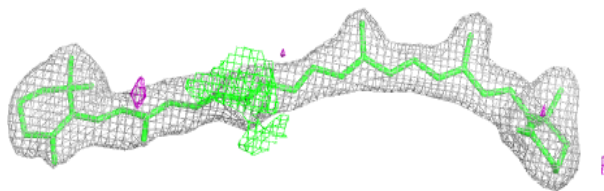
**Electron density around HTG V 202:**

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

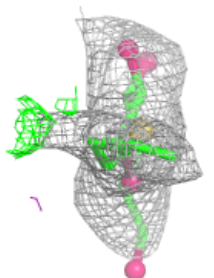
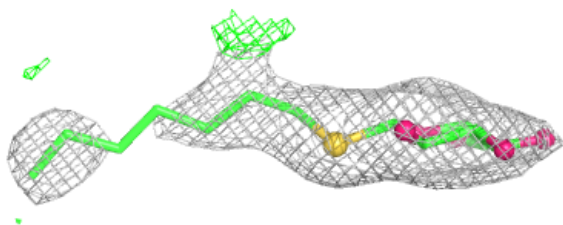
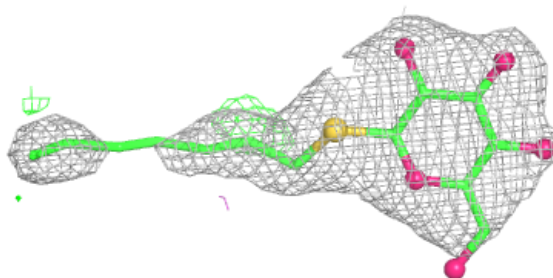


Electron density around BCR t 101:

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

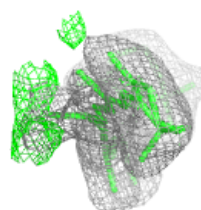
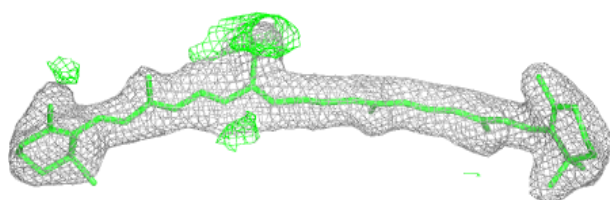
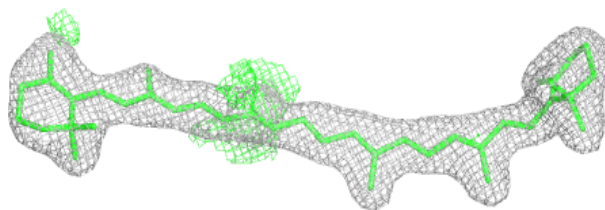
**Electron density around HTG C 521:**

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

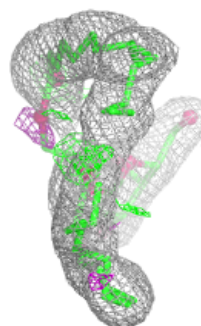
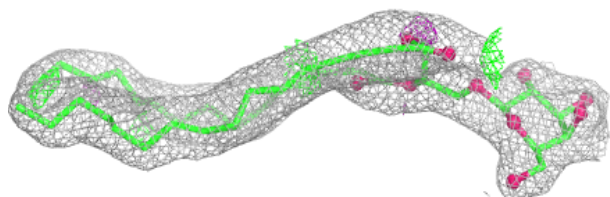
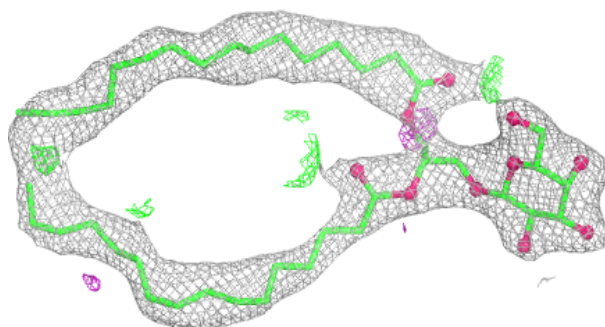


Electron density around BCR T 101:

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

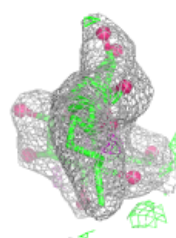
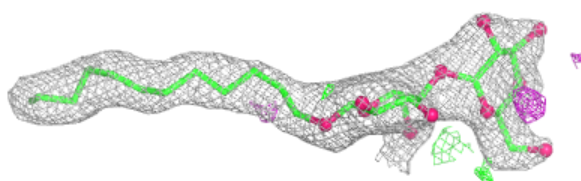
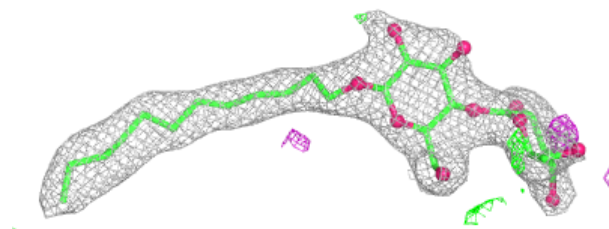
**Electron density around LMG a 412:**

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

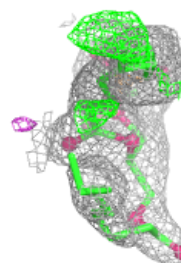
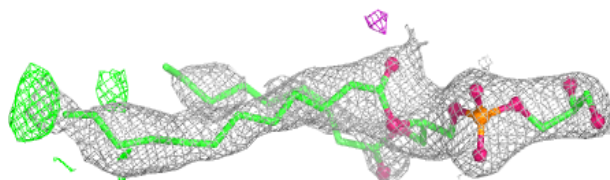
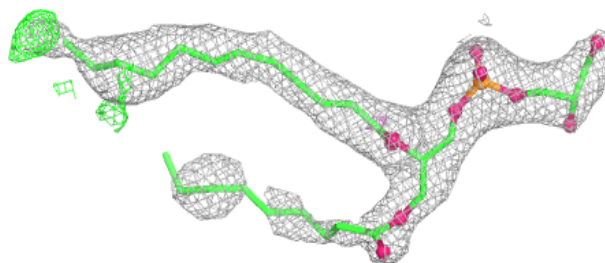


Electron density around LMT B 623:

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

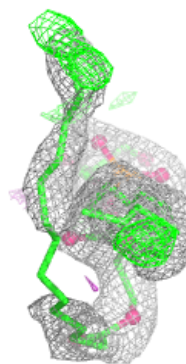
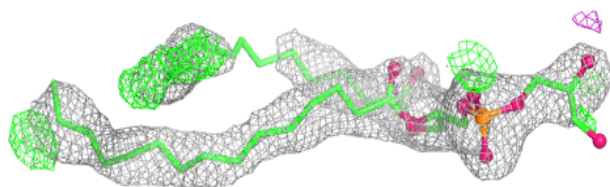
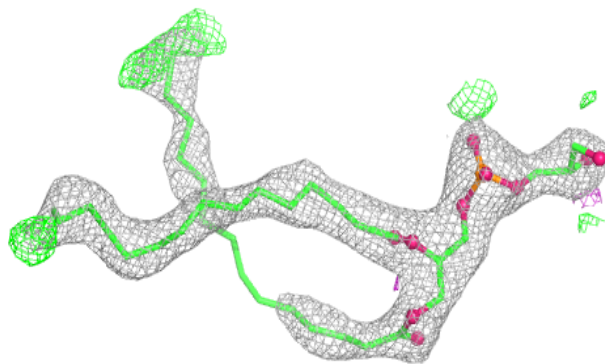
**Electron density around LHG F 103:**

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

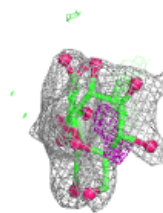
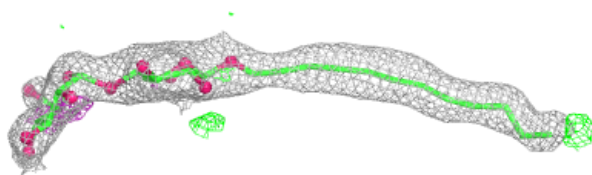
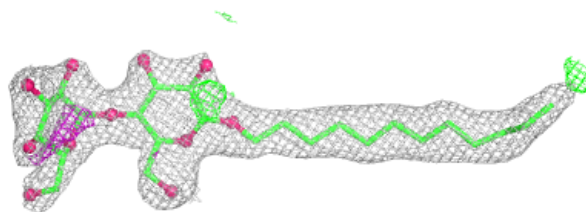


Electron density around LHG f 102:

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

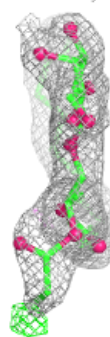
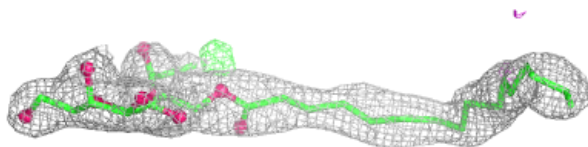
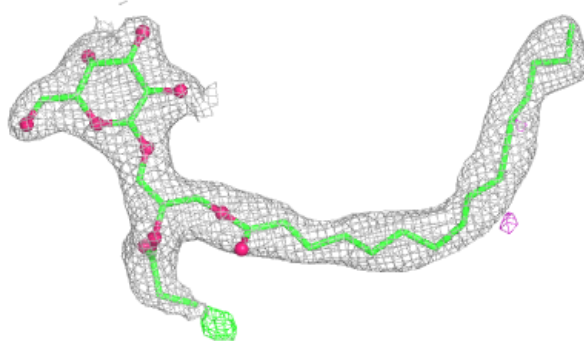
**Electron density around LMT m 101:**

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

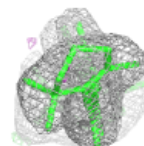
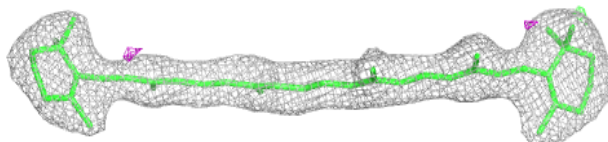
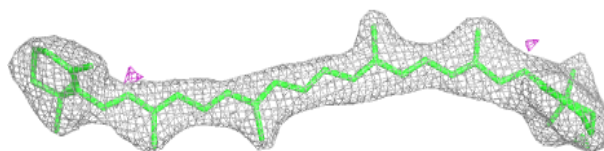


Electron density around LMG c 520:

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

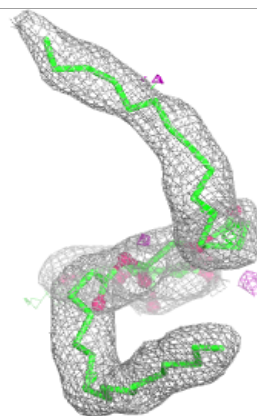
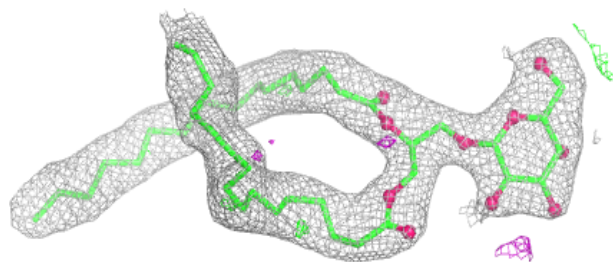
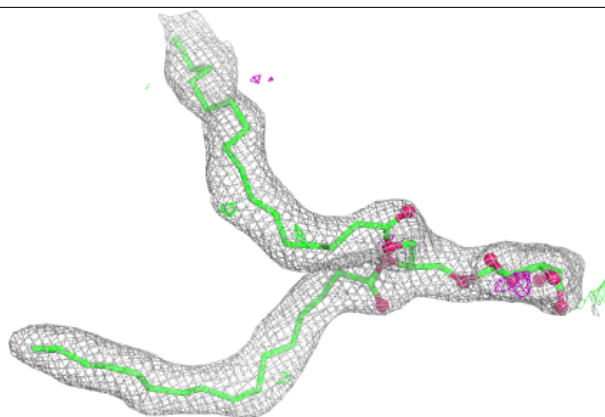
**Electron density around BCR c 515:**

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

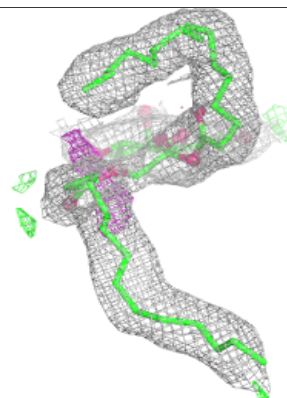
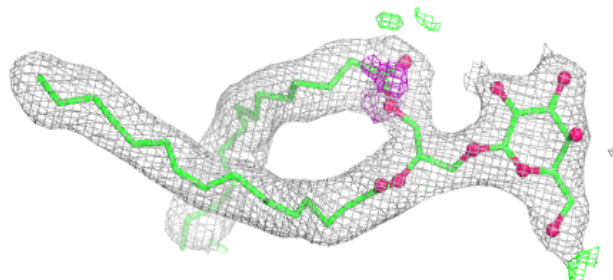
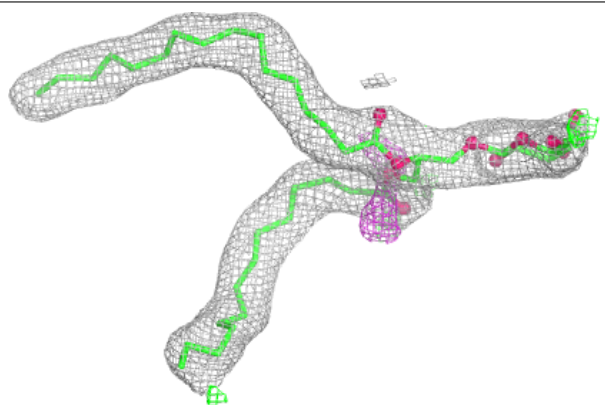


Electron density around LMG B 622:

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

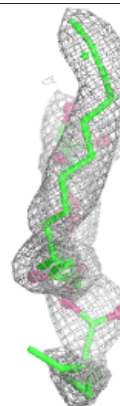
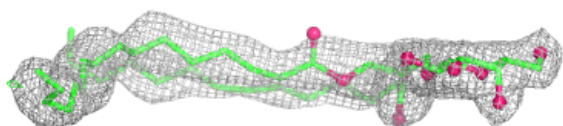
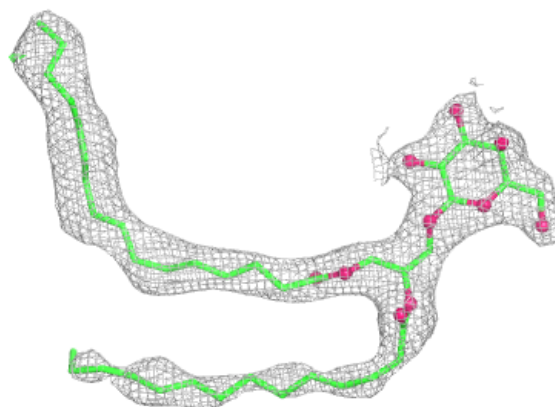
**Electron density around LMG b 625:**

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

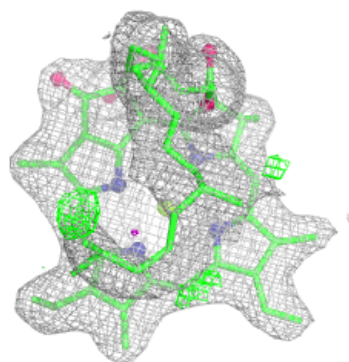
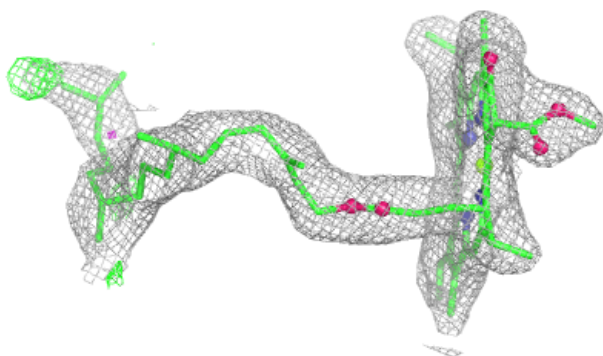
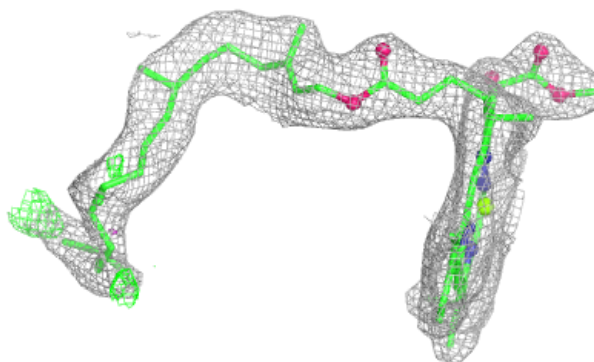


Electron density around LMG C 518:

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

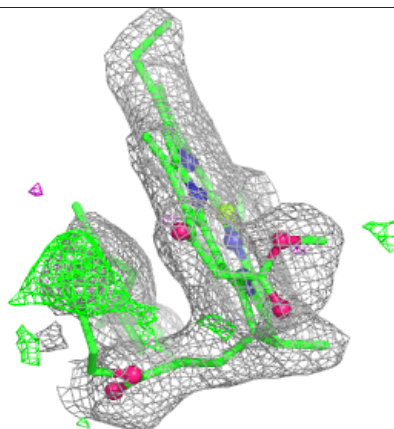
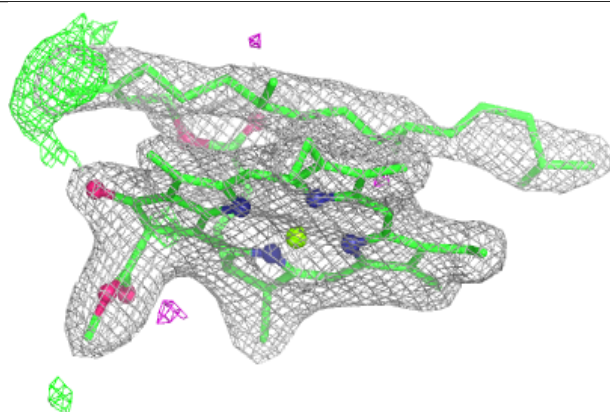
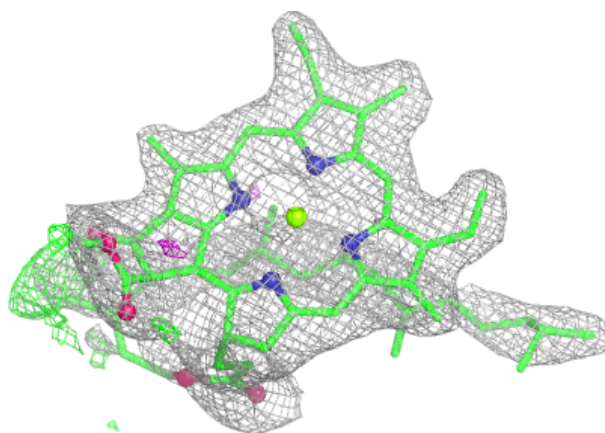
**Electron density around CLA C 506:**

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

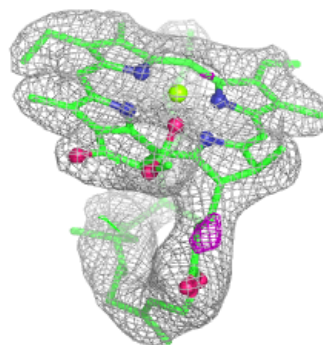
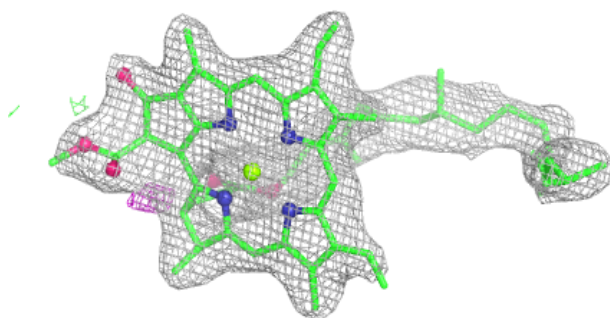
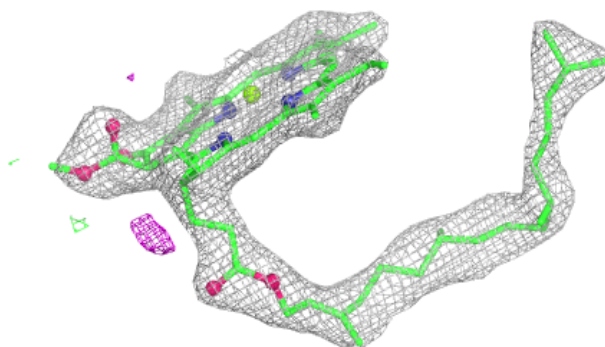


Electron density around CLA b 605:

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

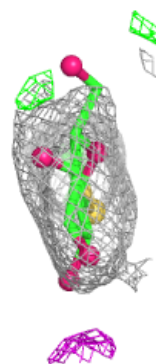
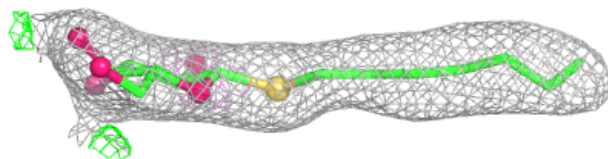
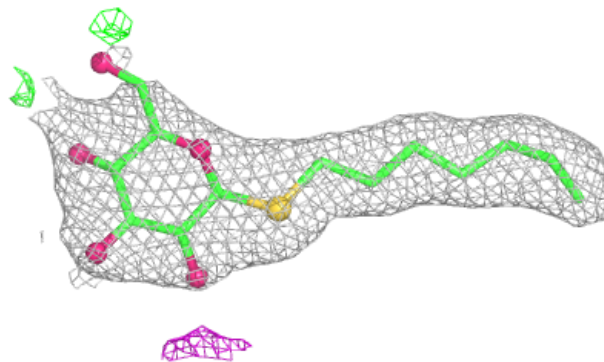
**Electron density around CLA c 514:**

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

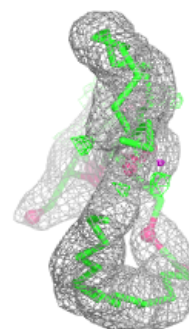
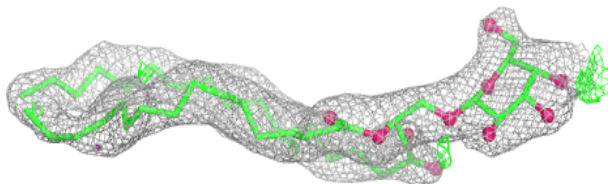
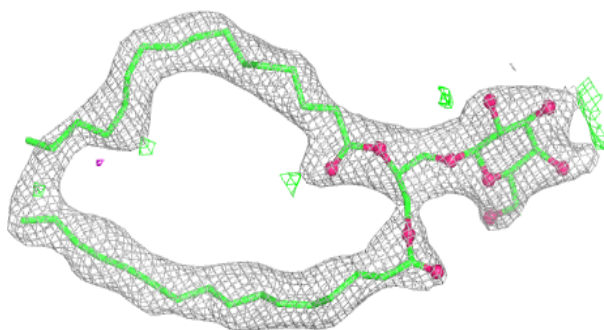


Electron density around HTG B 628:

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

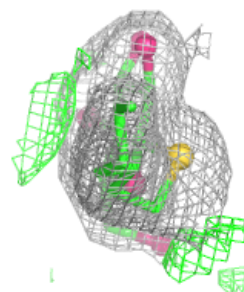
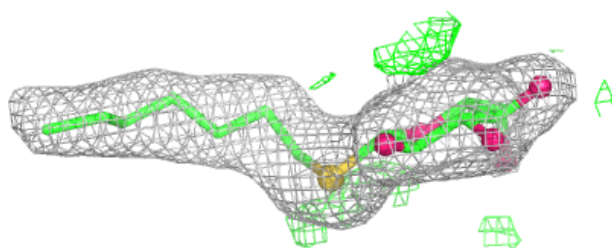
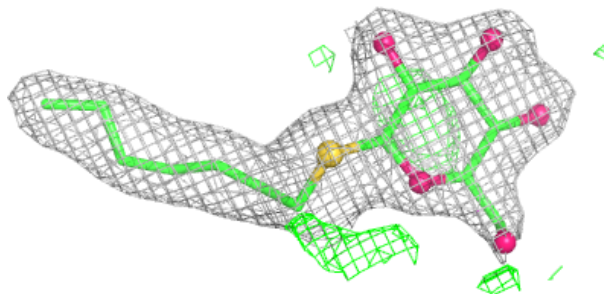
**Electron density around LMG A 411:**

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

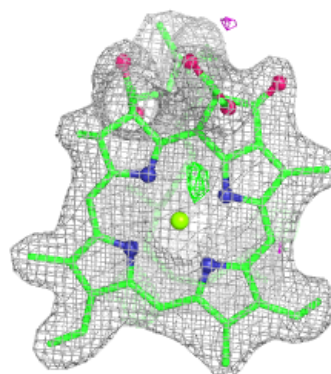
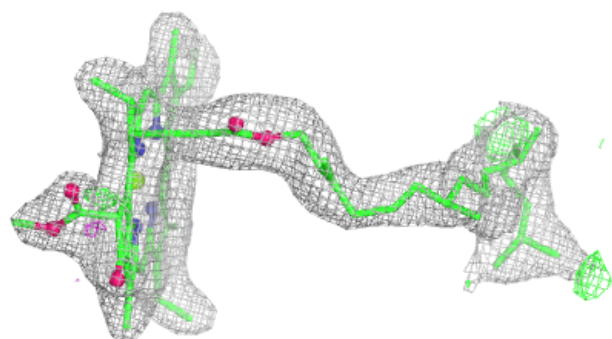
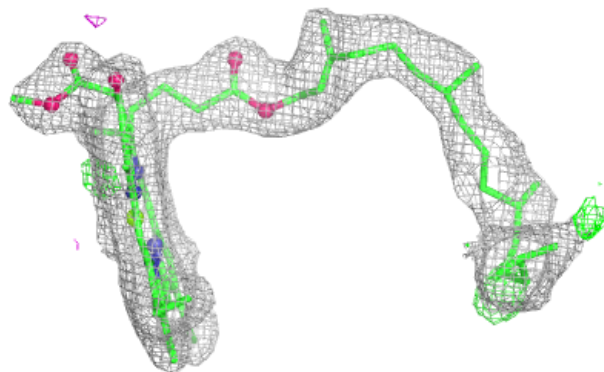


Electron density around HTG o 301:

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

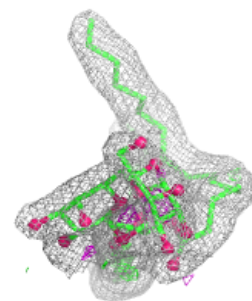
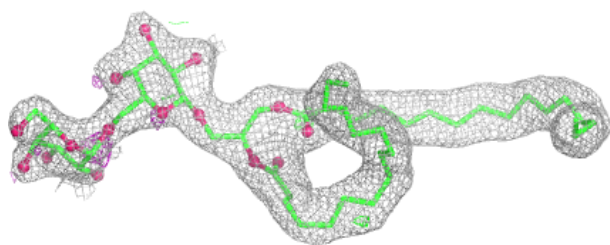
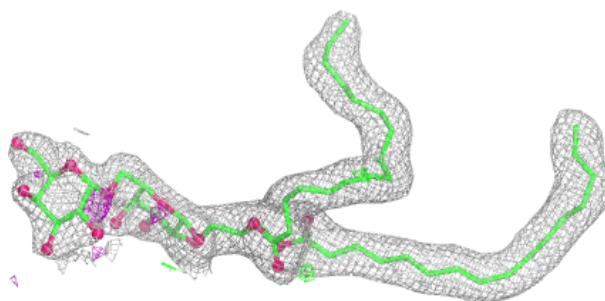
**Electron density around CLA c 507:**

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

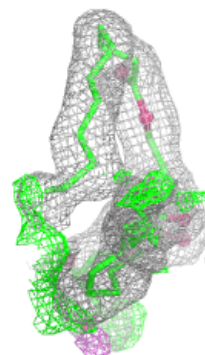
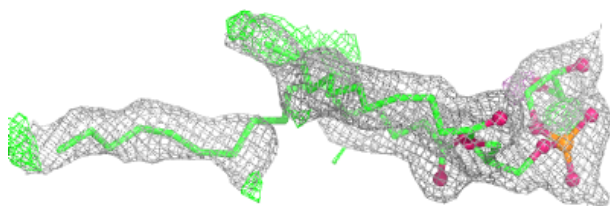
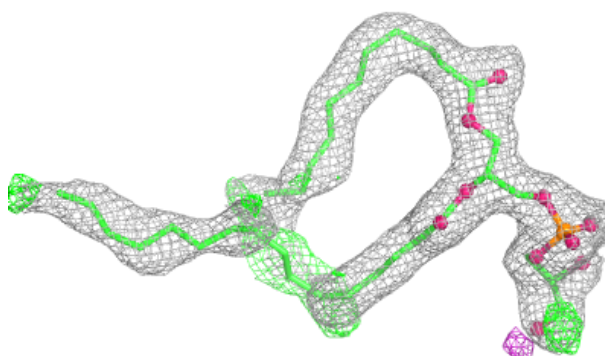


Electron density around DGD h 101:

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

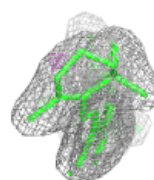
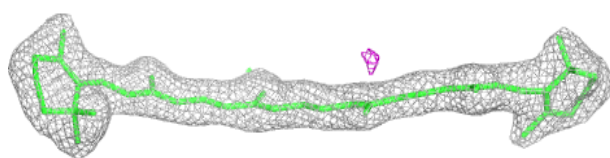
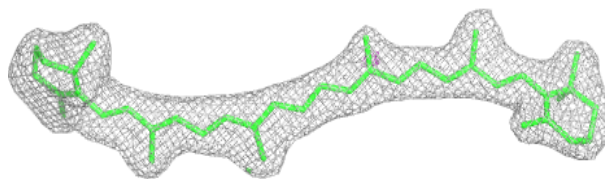
**Electron density around LHG D 411:**

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

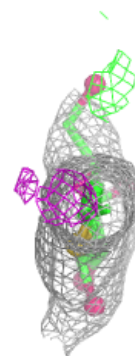
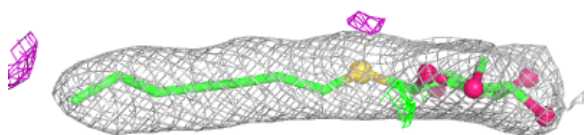
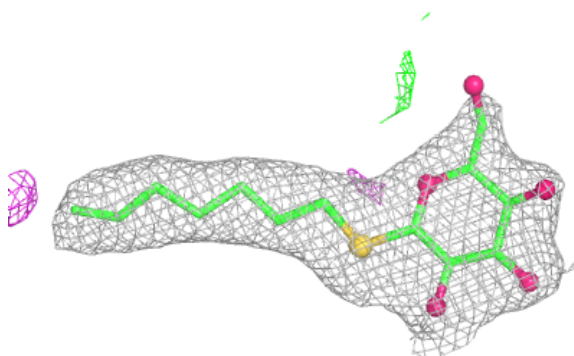


Electron density around BCR y 101:

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

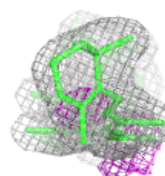
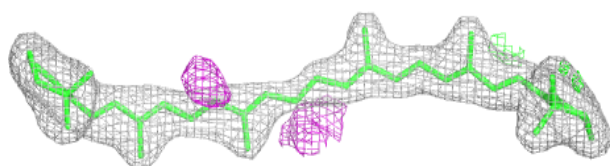
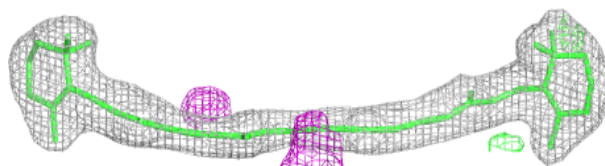
**Electron density around HTG b 601:**

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

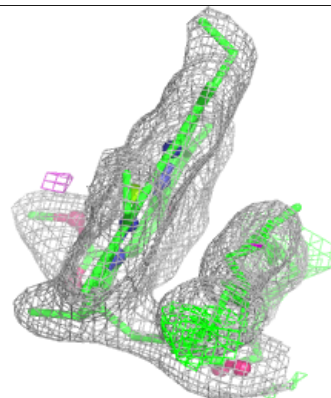
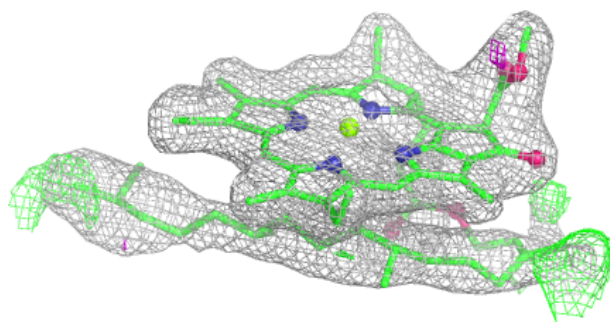
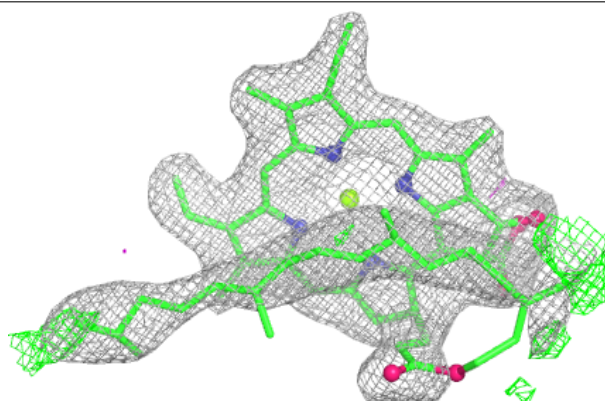


Electron density around BCR K 101:

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

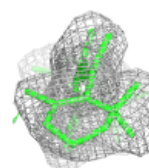
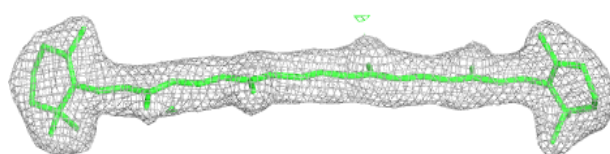
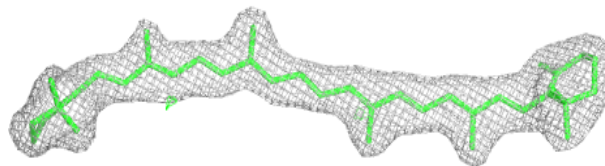
**Electron density around CLA B 602:**

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

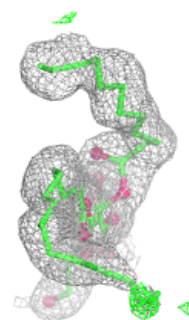
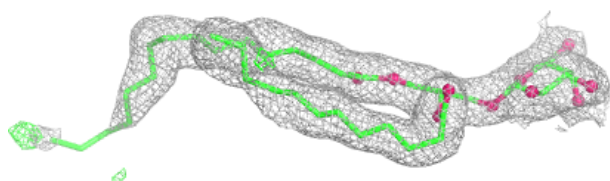
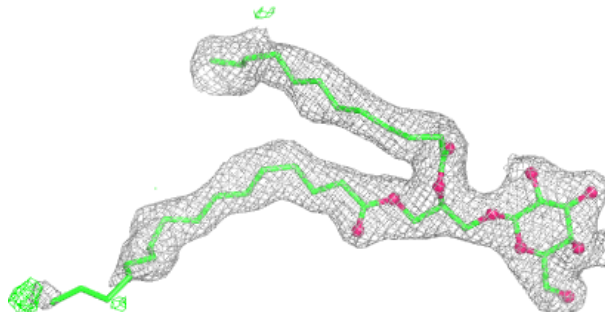


Electron density around BCR K 102:

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

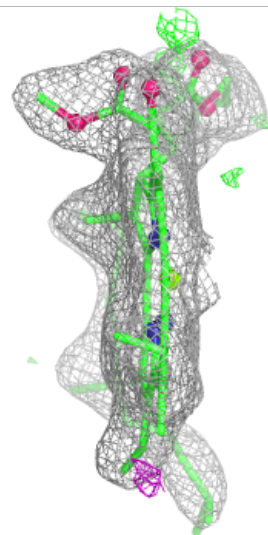
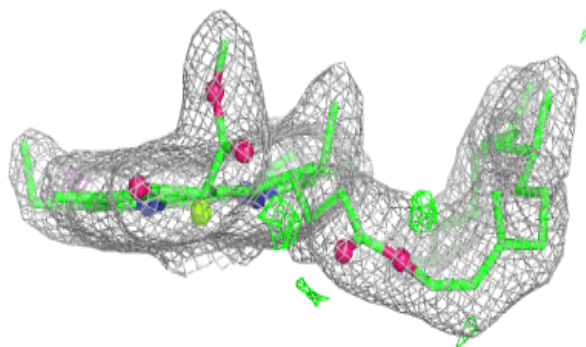
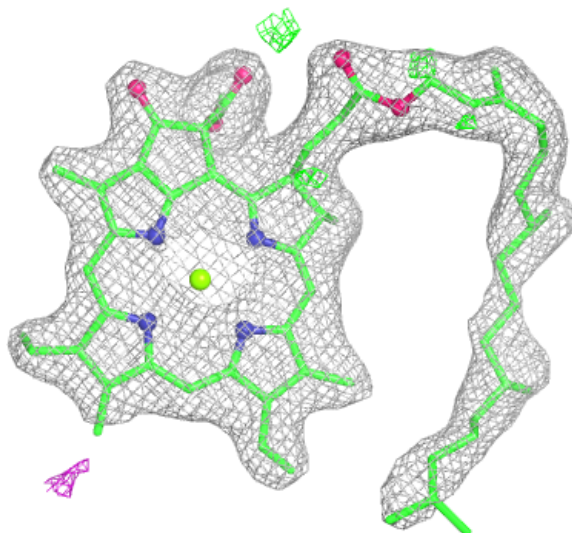
**Electron density around LMG d 412:**

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



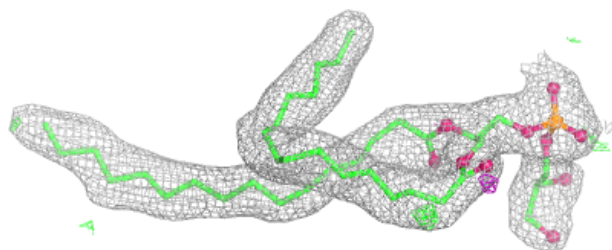
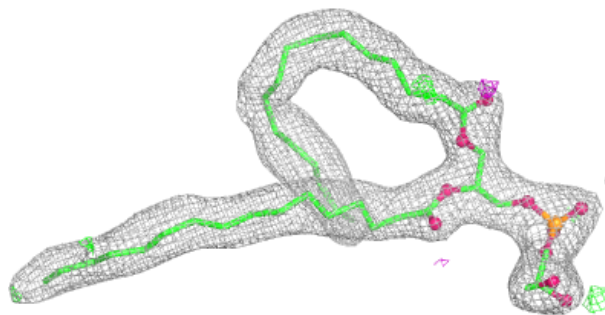
Electron density around CLA c 513:

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



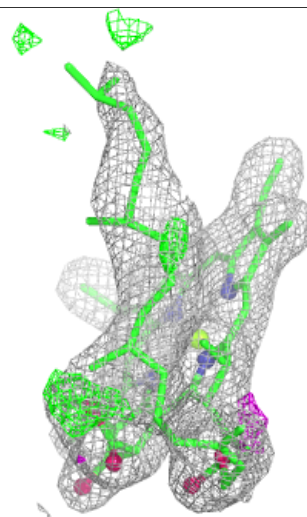
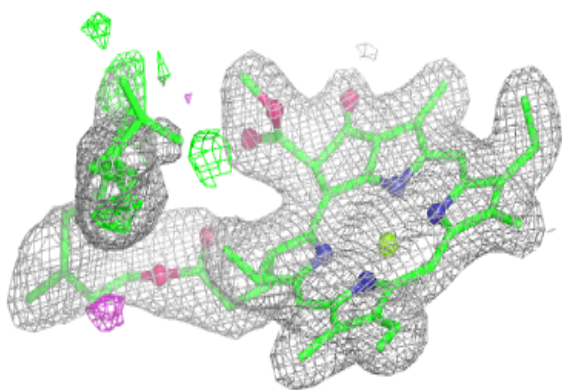
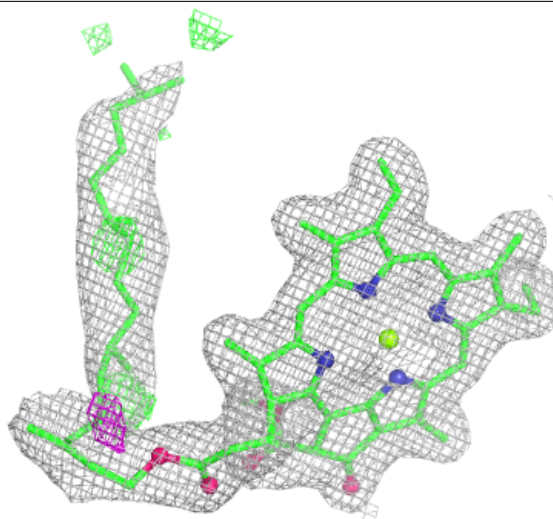
Electron density around LHG D 409:

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



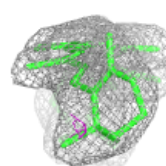
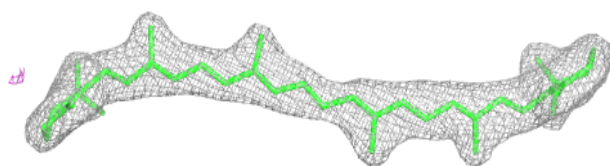
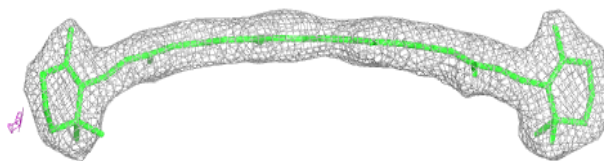
Electron density around CLA b 620:

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

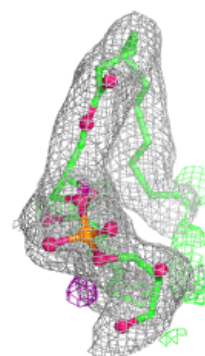
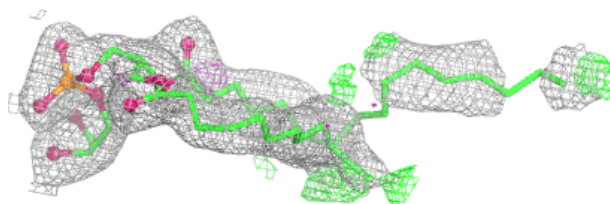
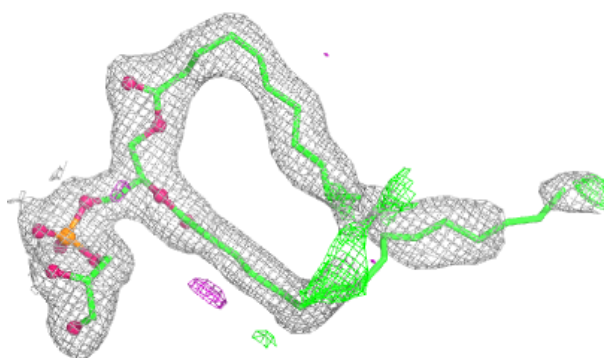


Electron density around BCR k 101:

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

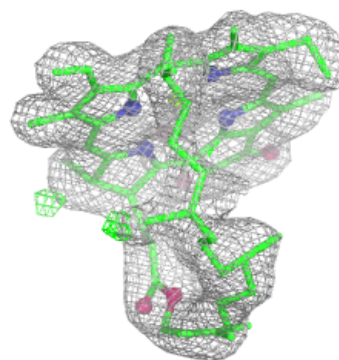
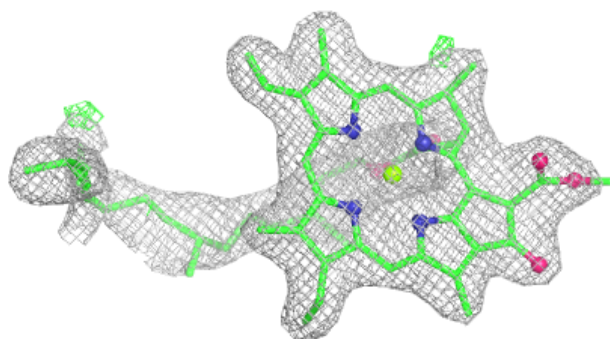
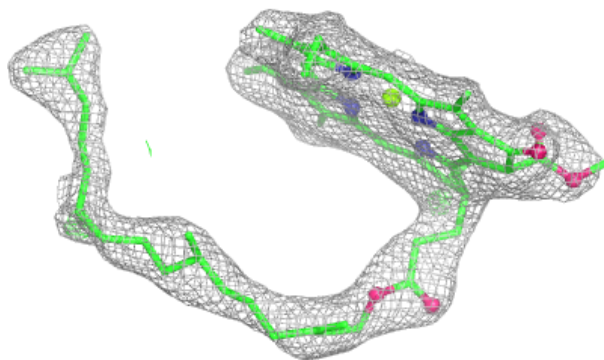
**Electron density around LHG d 411:**

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

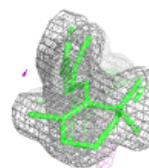
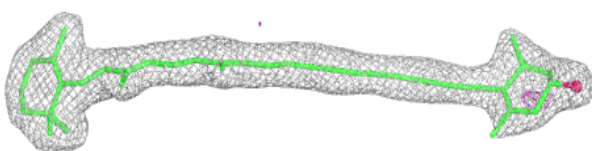
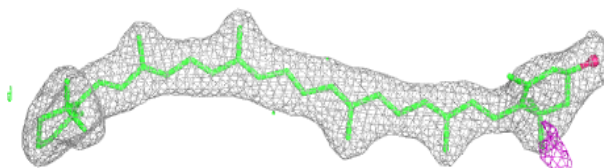


Electron density around CLA C 513:

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

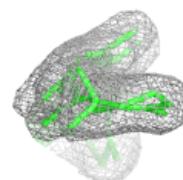
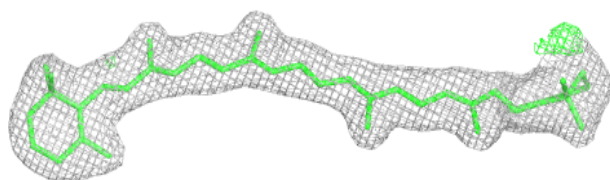
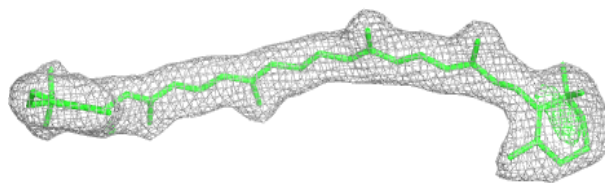
**Electron density around RRX H 102:**

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

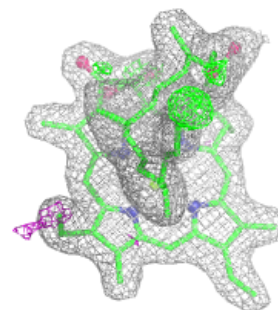
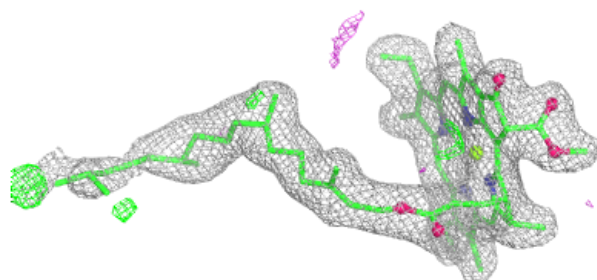
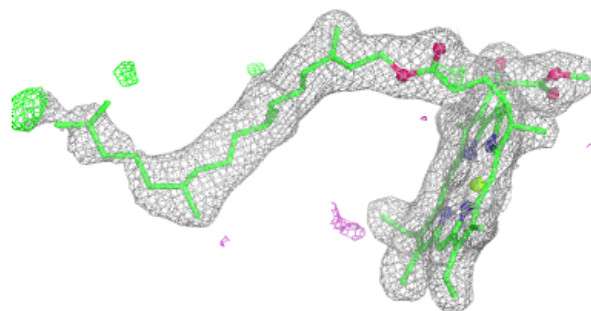


Electron density around BCR d 406:

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

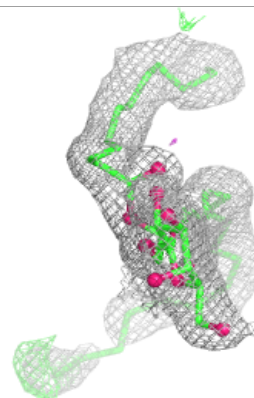
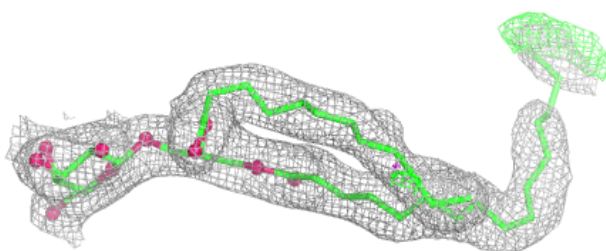
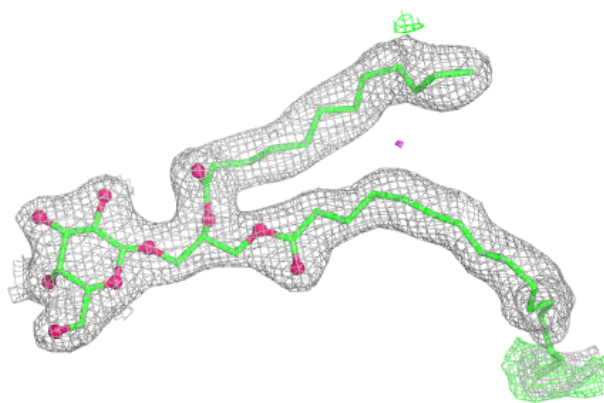
**Electron density around CLA c 509:**

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



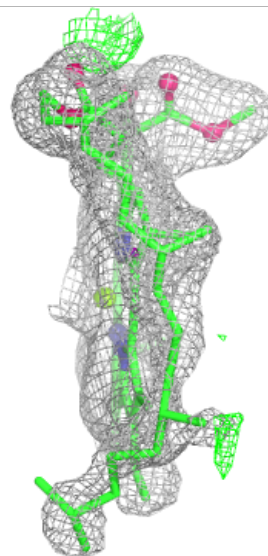
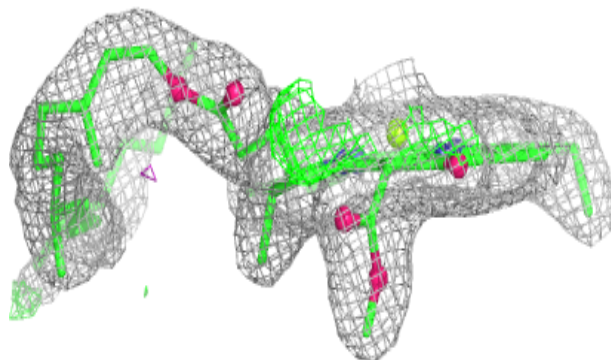
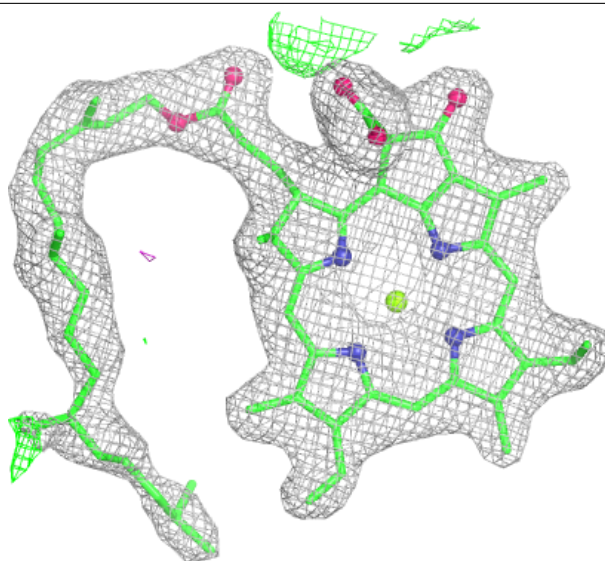
Electron density around LMG D 412:

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



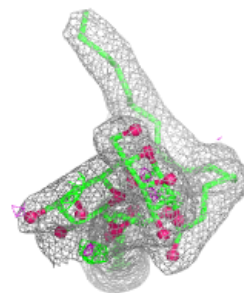
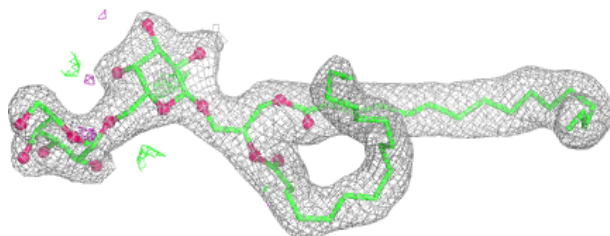
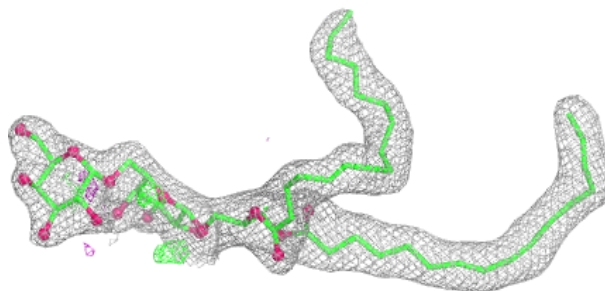
Electron density around CLA C 512:

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

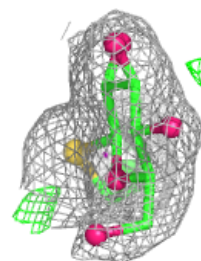
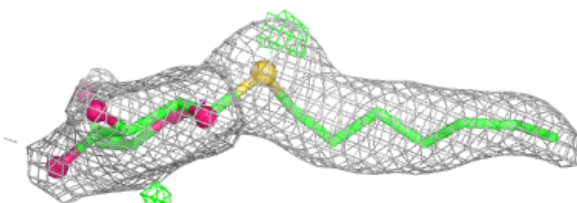
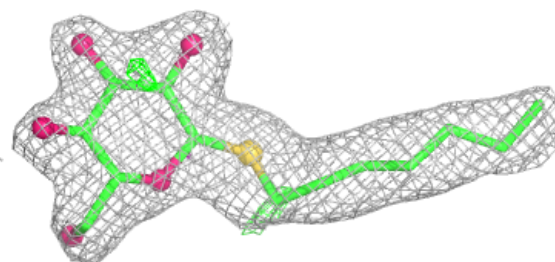


Electron density around DGD H 101:

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

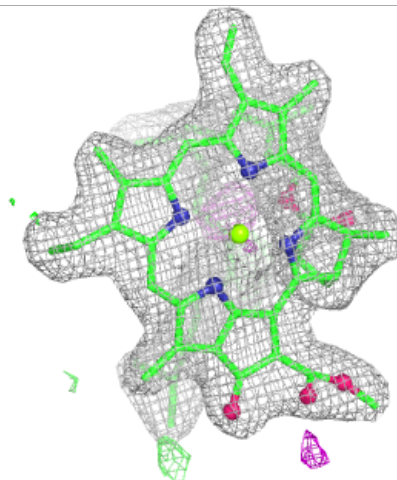
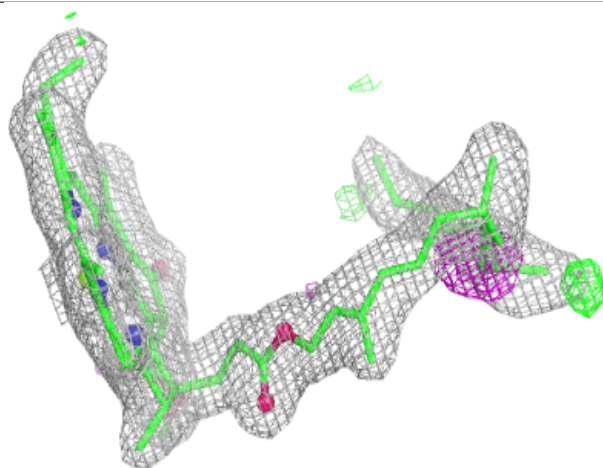
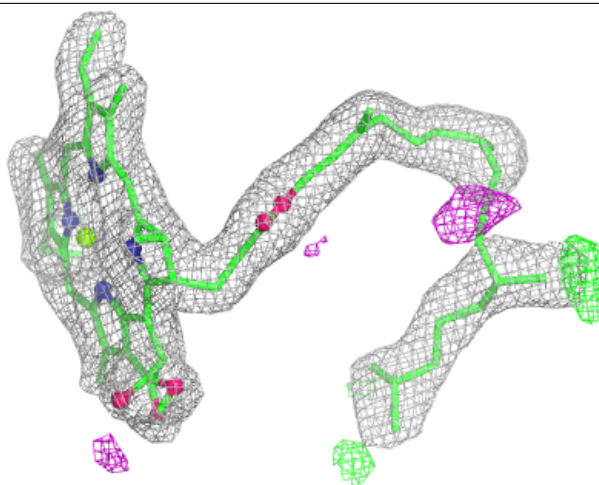
**Electron density around HTG O 302:**

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



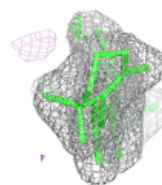
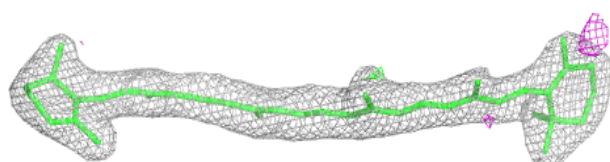
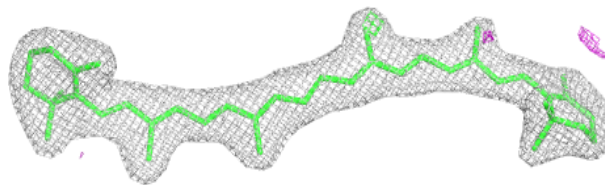
Electron density around CLA b 610:

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

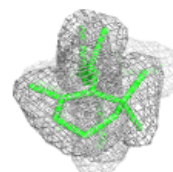
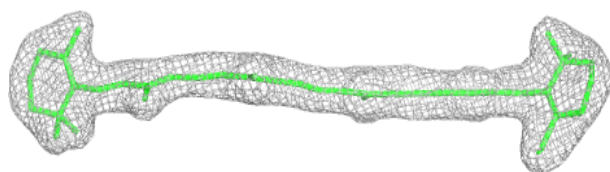
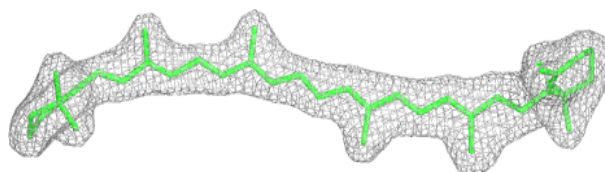


Electron density around BCR Y 101:

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

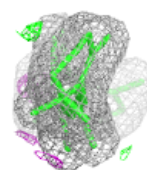
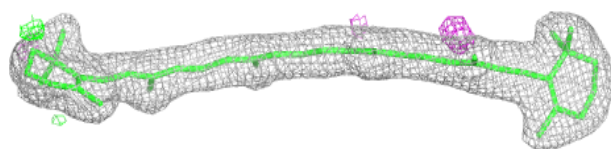
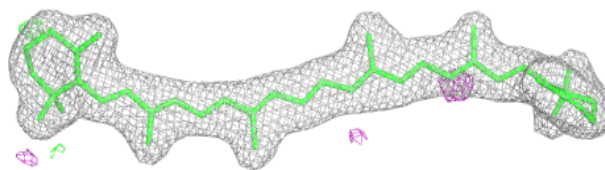
**Electron density around BCR a 410:**

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

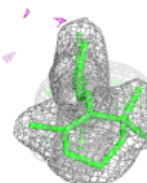
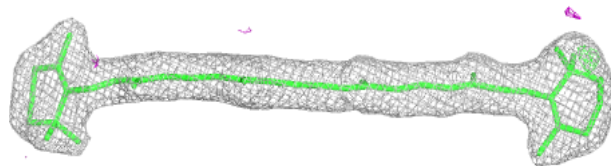
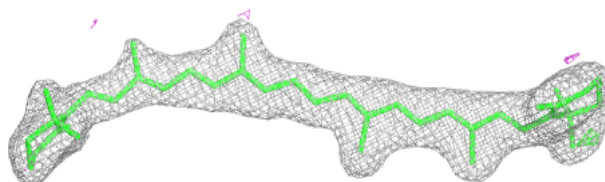


Electron density around BCR B 618:

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

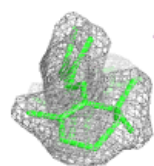
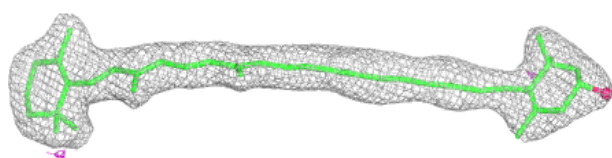
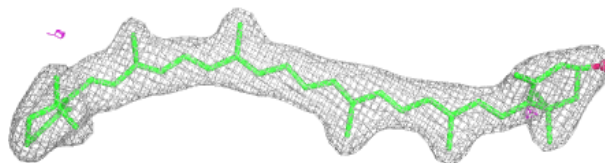
**Electron density around BCR c 516:**

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

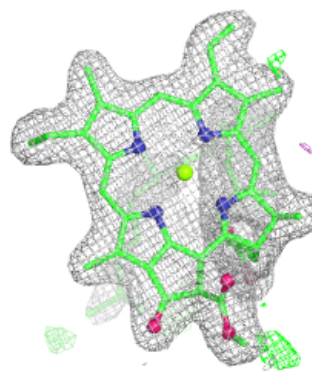
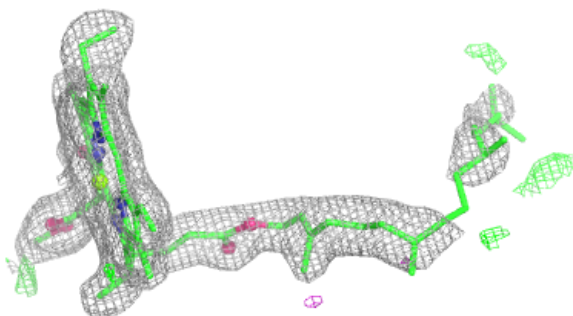
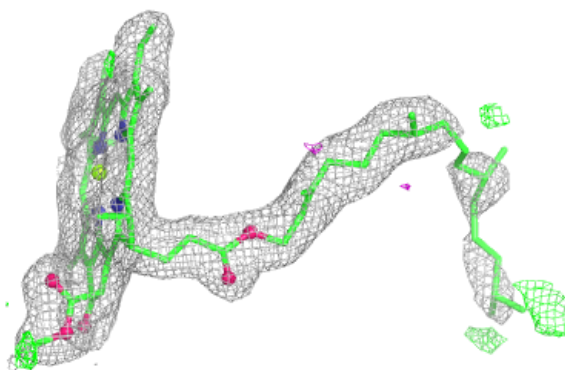


Electron density around RRX h 102:

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

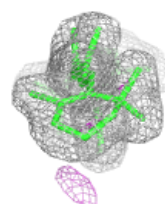
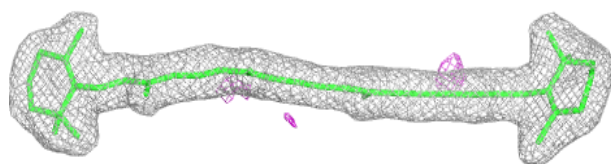
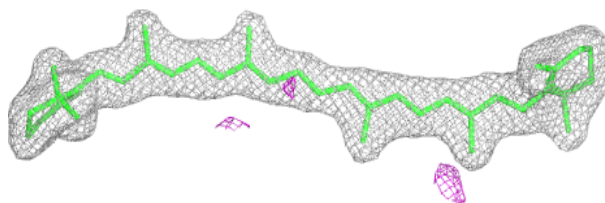
**Electron density around CLA d 405:**

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



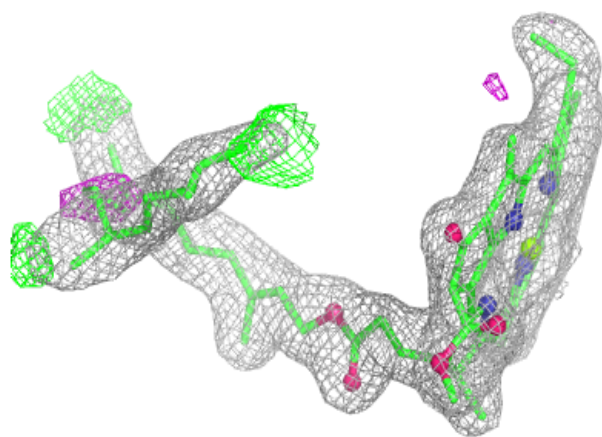
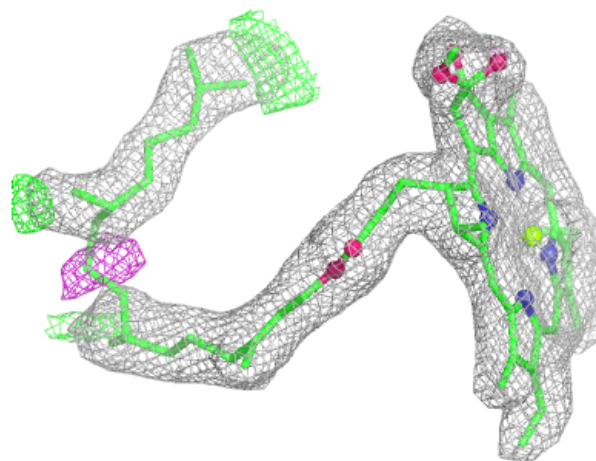
Electron density around BCR A 409:

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



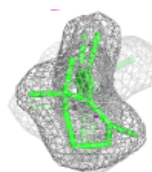
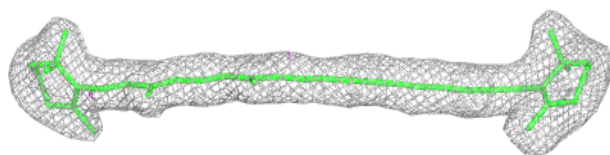
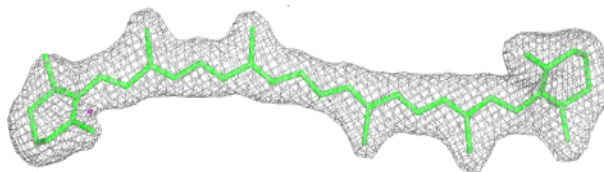
Electron density around CLA B 607:

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

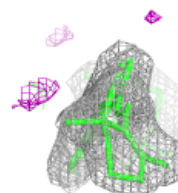
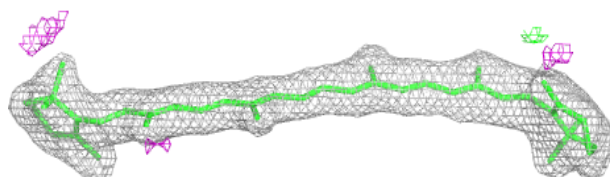
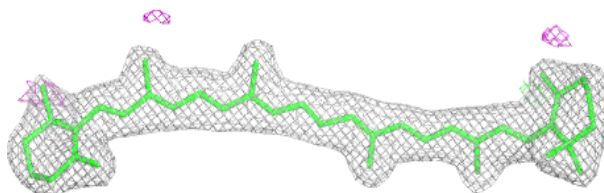


Electron density around BCR B 619:

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

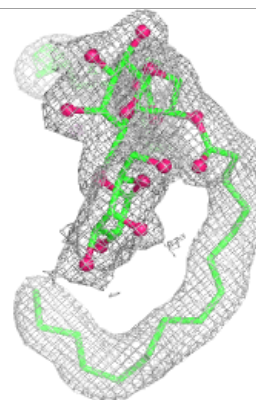
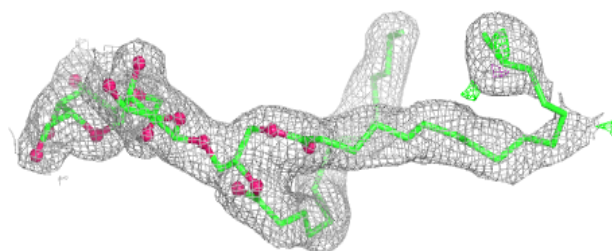
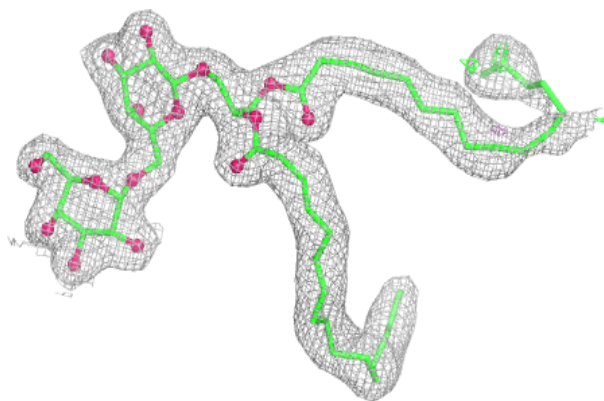
**Electron density around BCR B 620:**

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

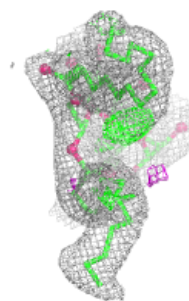
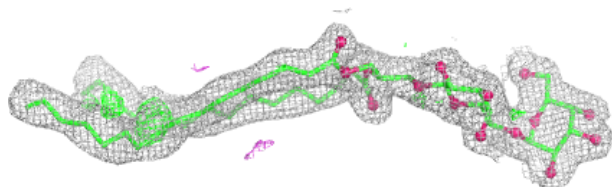
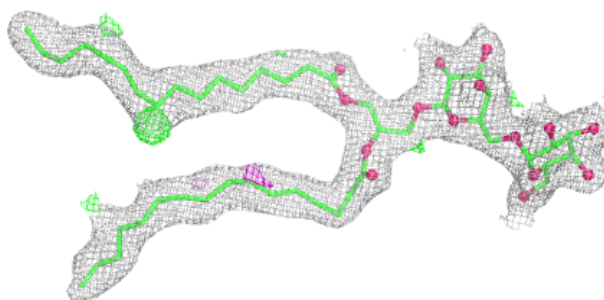


Electron density around DGD C 516:

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

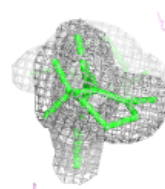
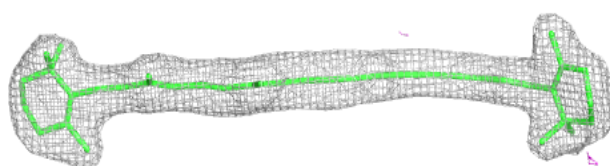
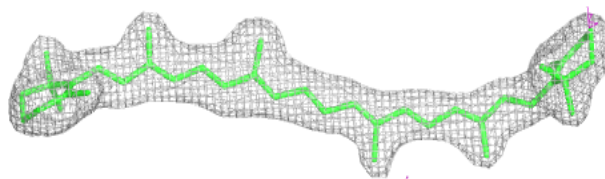
**Electron density around DGD C 517:**

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

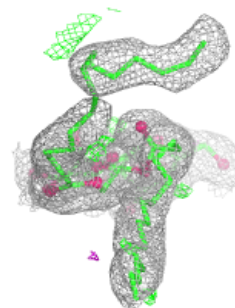
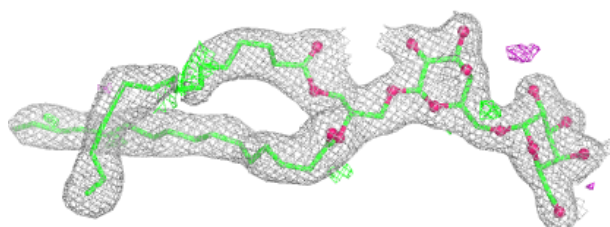
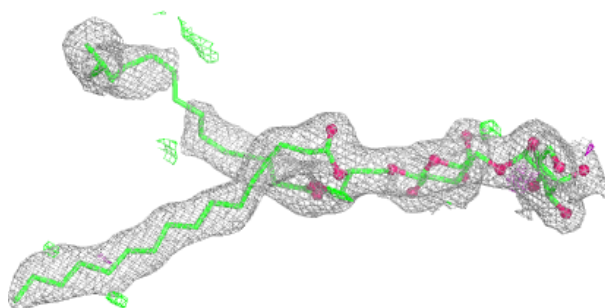


Electron density around BCR C 514:

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

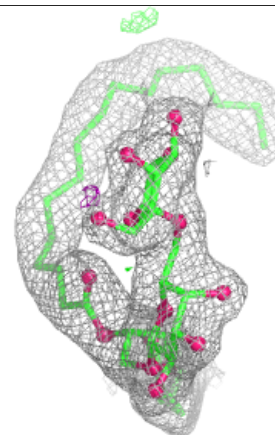
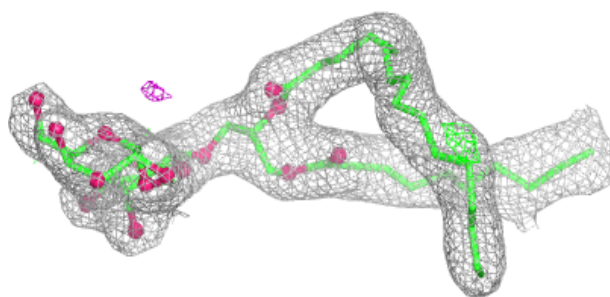
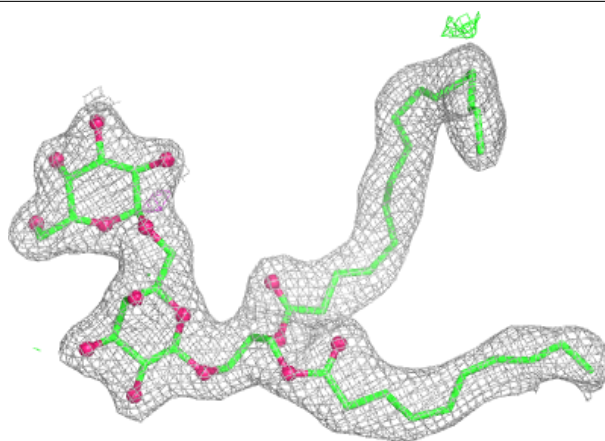
**Electron density around DGD c 517:**

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

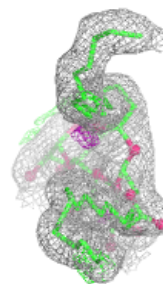
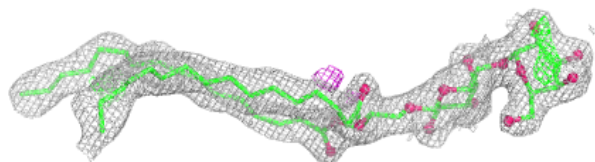
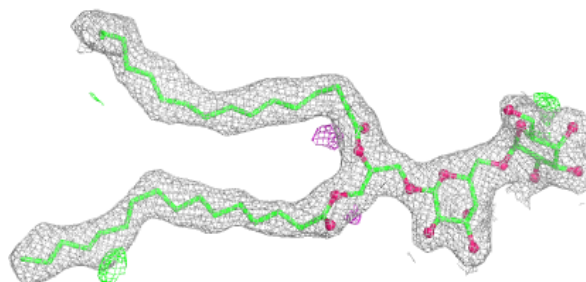


Electron density around DGD c 518:

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

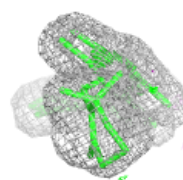
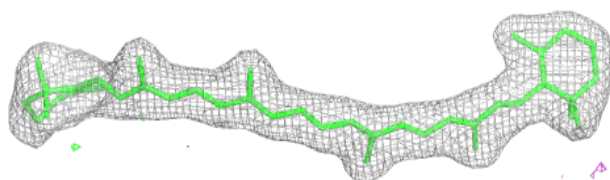
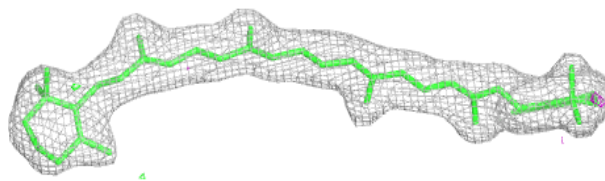
**Electron density around DGD c 519:**

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

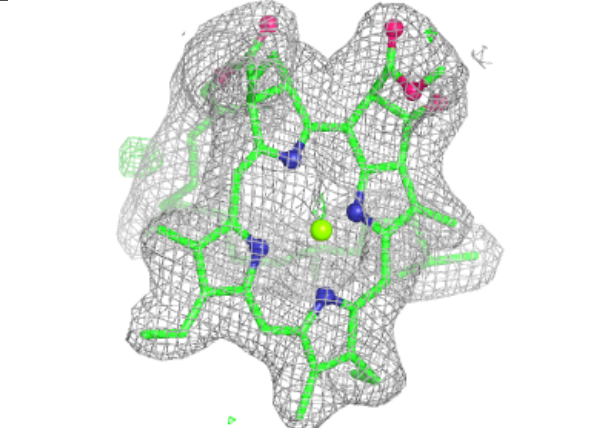
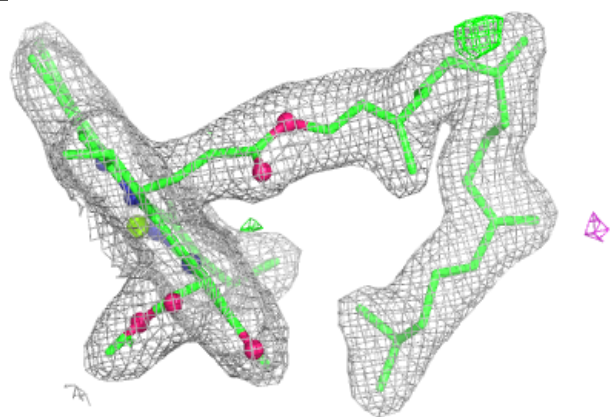
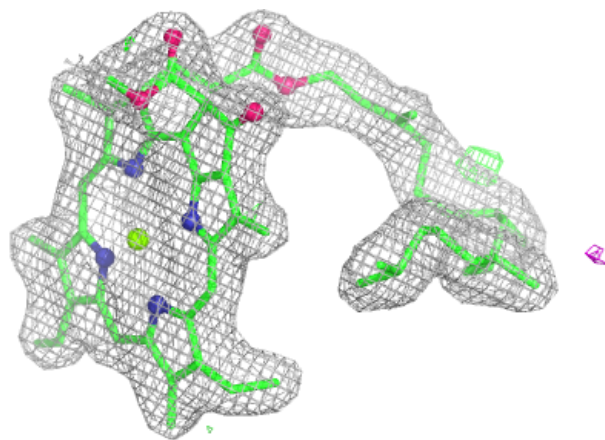


Electron density around BCR D 406:

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

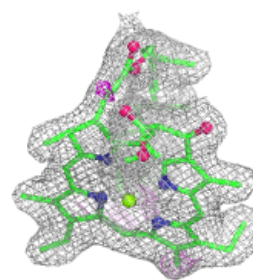
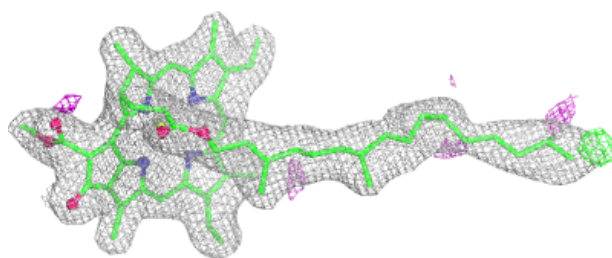
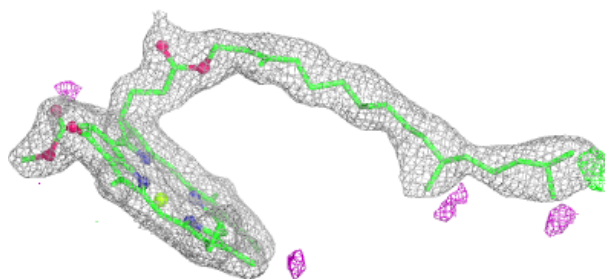
**Electron density around CLA c 504:**

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

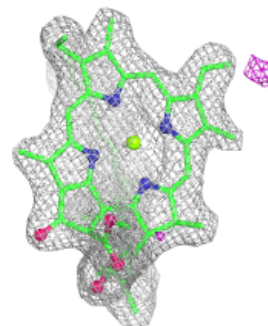
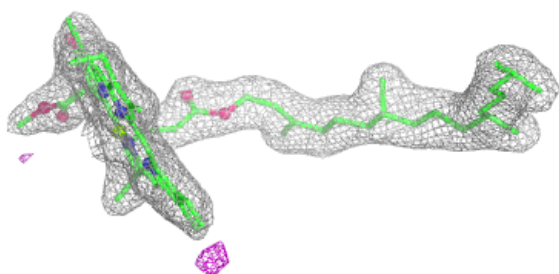
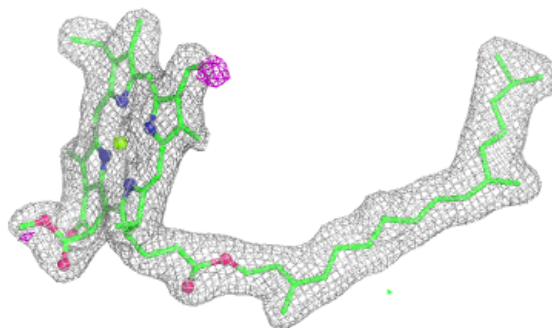


Electron density around CLA c 505:

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

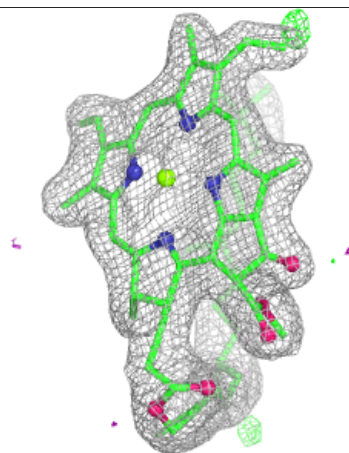
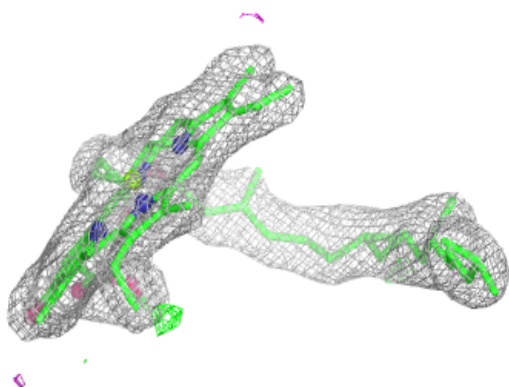
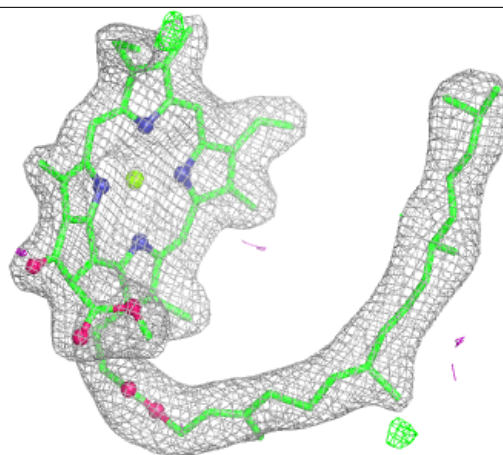
**Electron density around CLA B 610:**

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



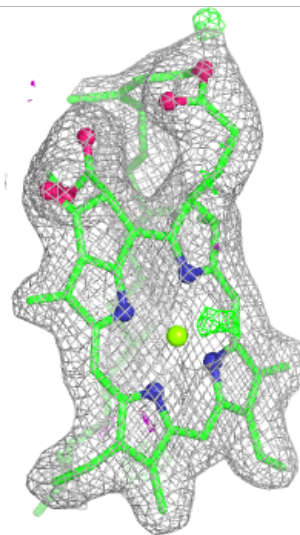
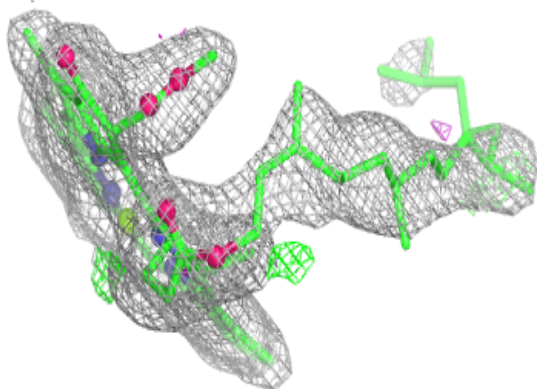
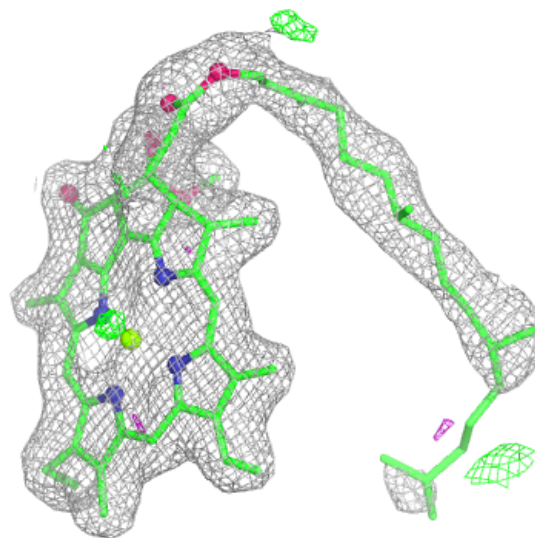
Electron density around CLA c 508:

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



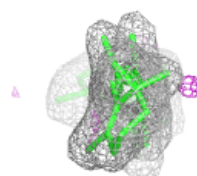
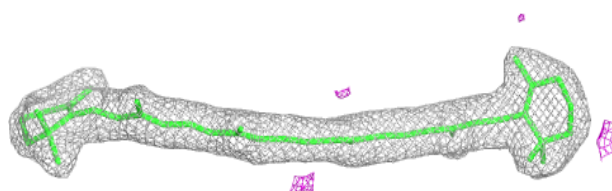
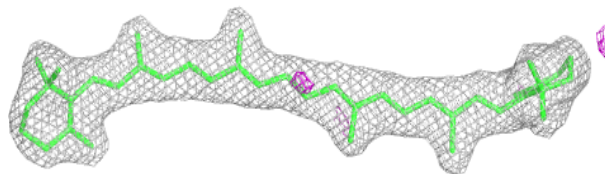
Electron density around CLA B 617:

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

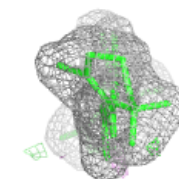
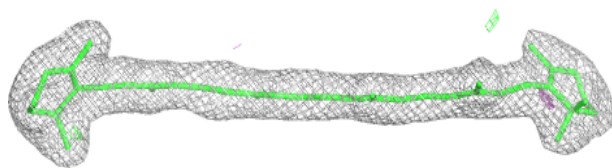
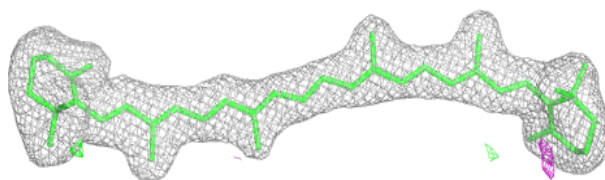


Electron density around BCR b 621:

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

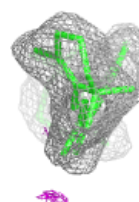
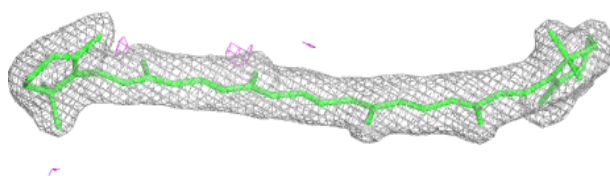
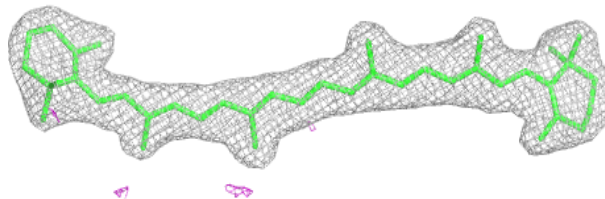
**Electron density around BCR b 622:**

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

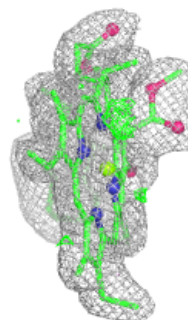
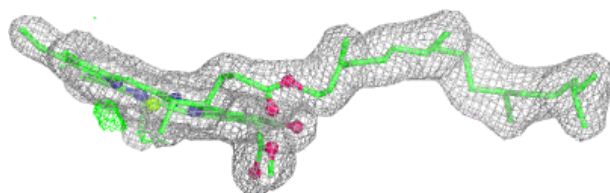
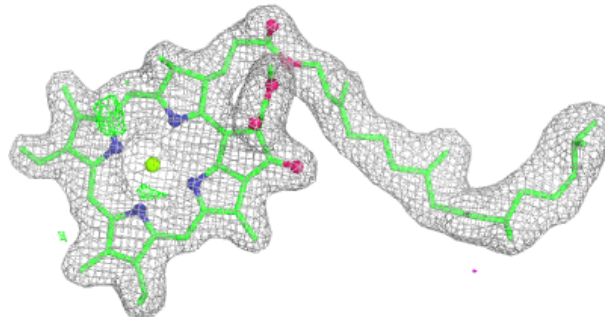


Electron density around BCR b 623:

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

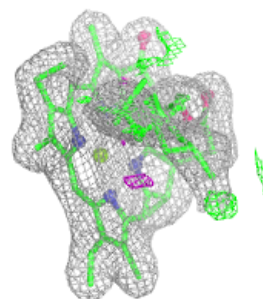
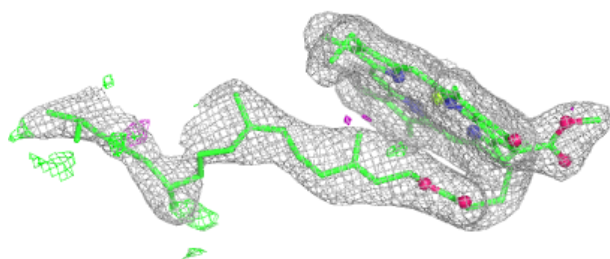
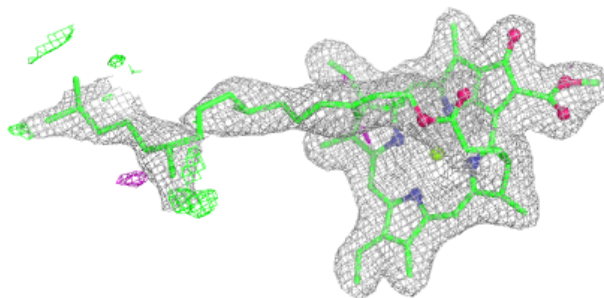
**Electron density around CLA B 603:**

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

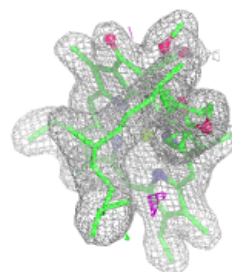
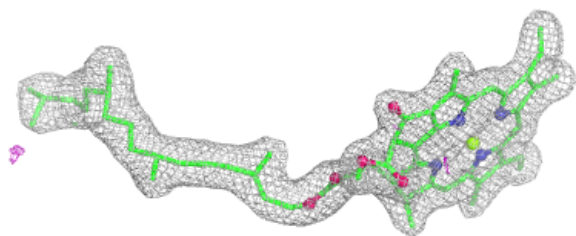
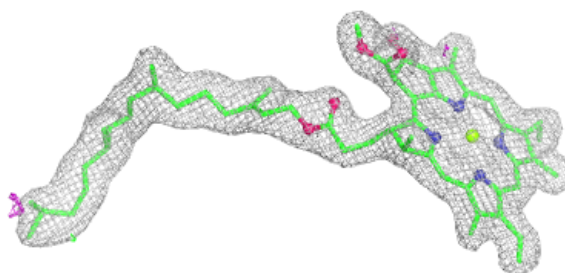


Electron density around CLA b 618:

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

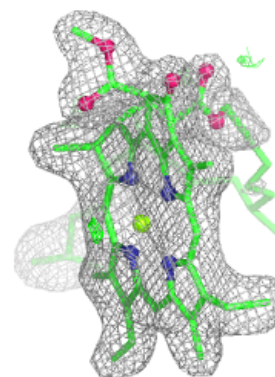
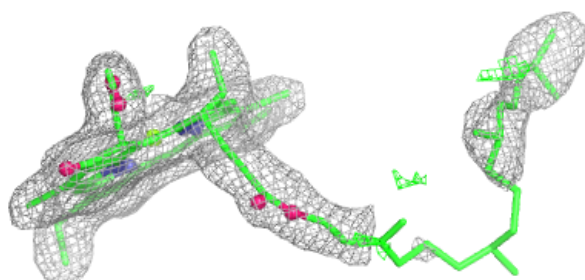
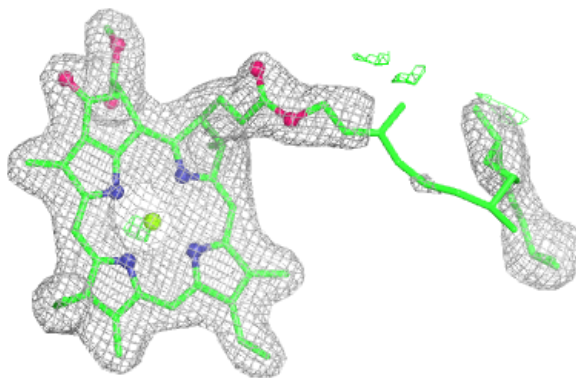
**Electron density around CLA a 406:**

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

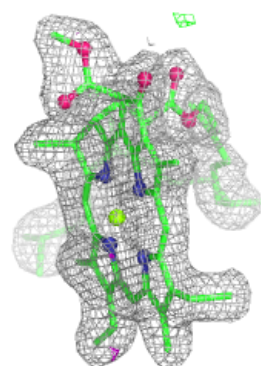
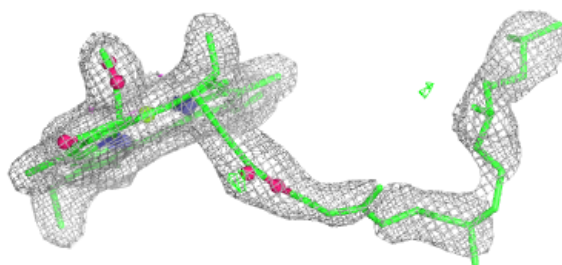
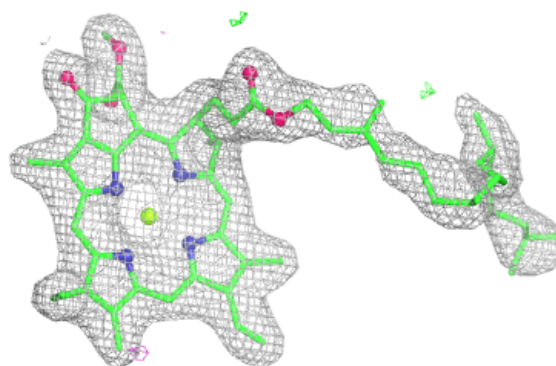


Electron density around CLA a 409:

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

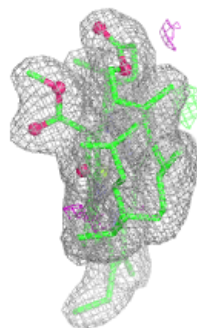
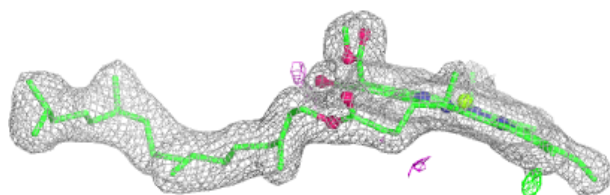
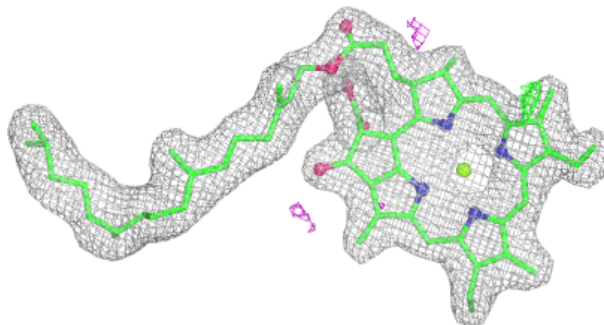
**Electron density around CLA A 408:**

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



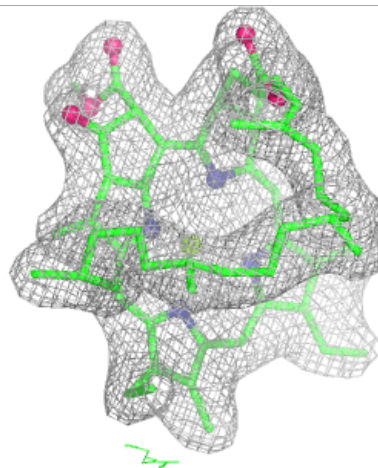
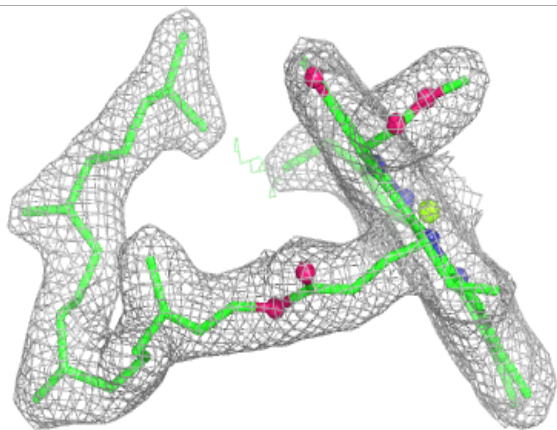
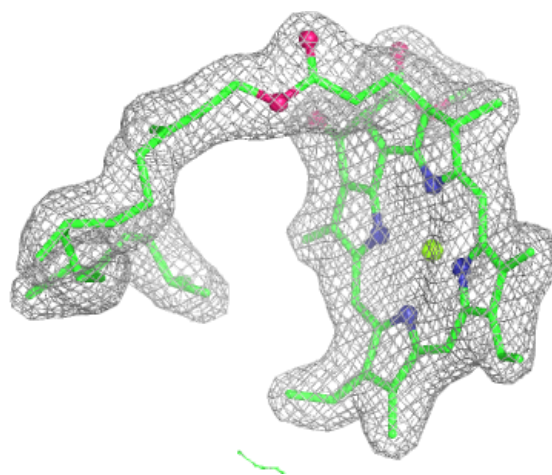
Electron density around CLA b 606:

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



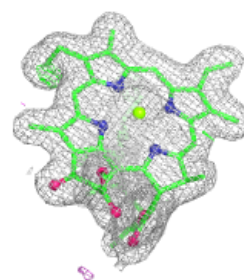
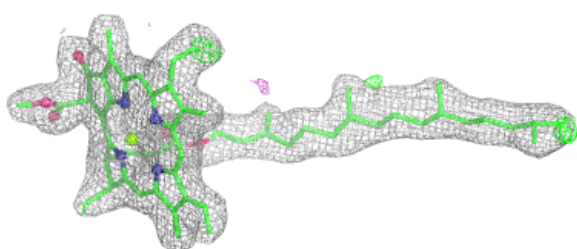
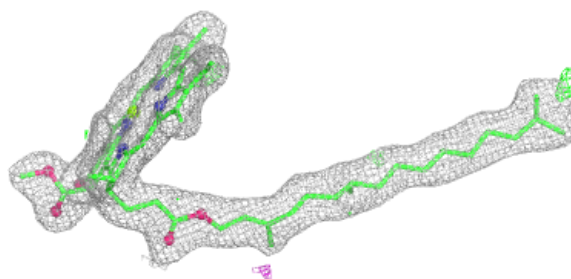
Electron density around CLA C 503:

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

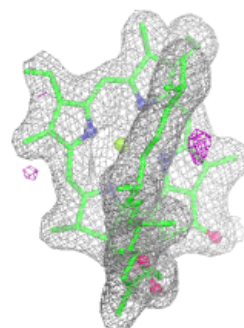
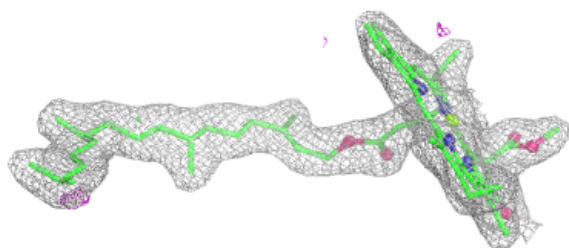
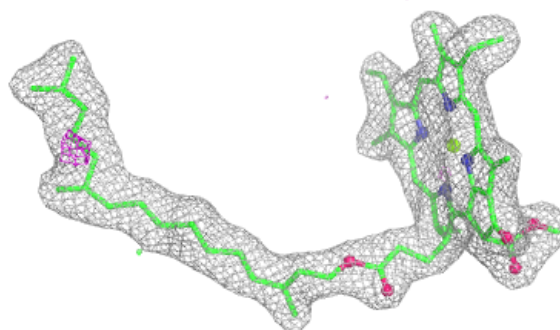


Electron density around CLA b 611:

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

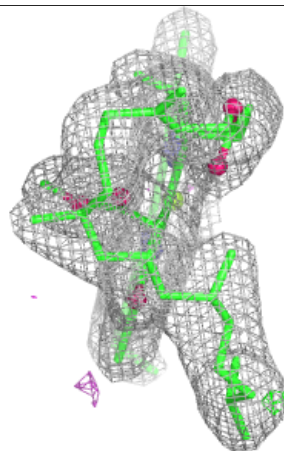
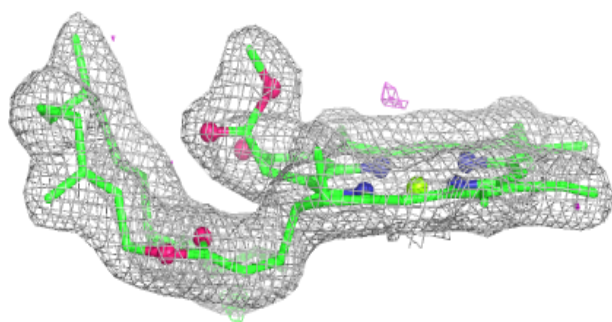
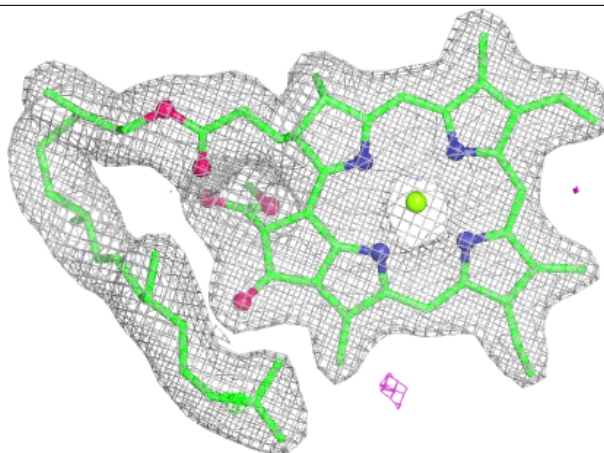
**Electron density around CLA b 613:**

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

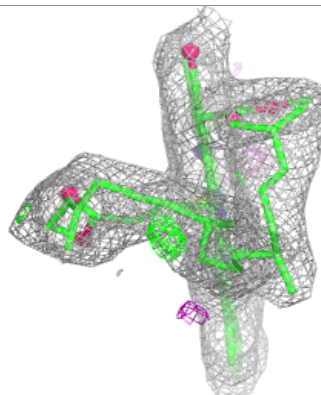
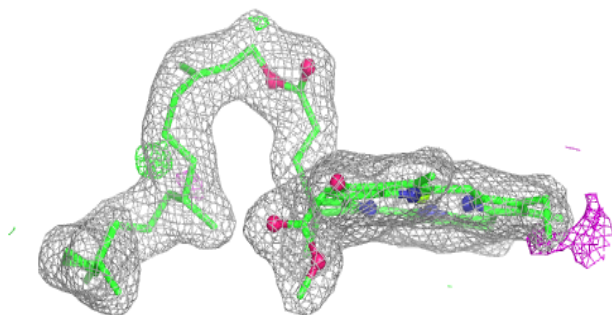
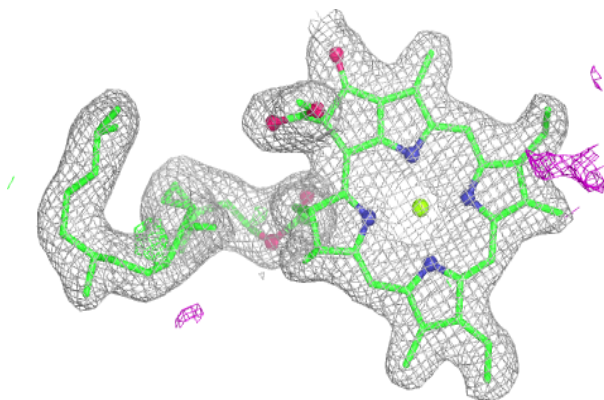


Electron density around CLA b 614:

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

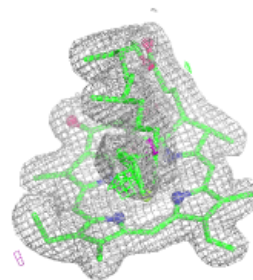
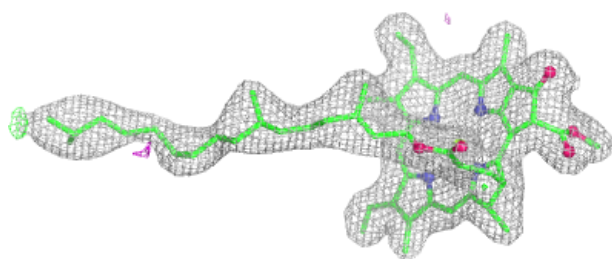
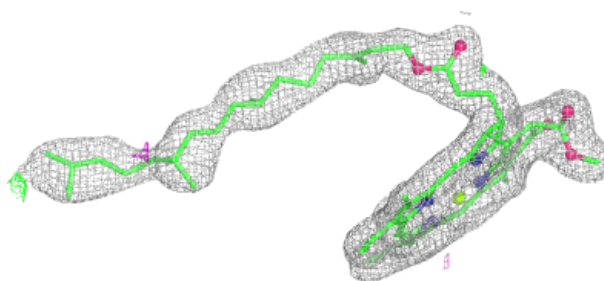
**Electron density around CLA b 616:**

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



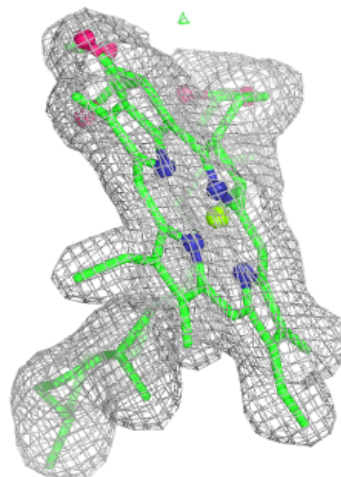
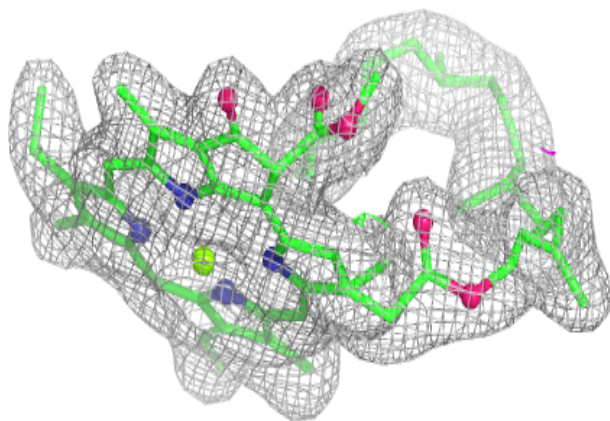
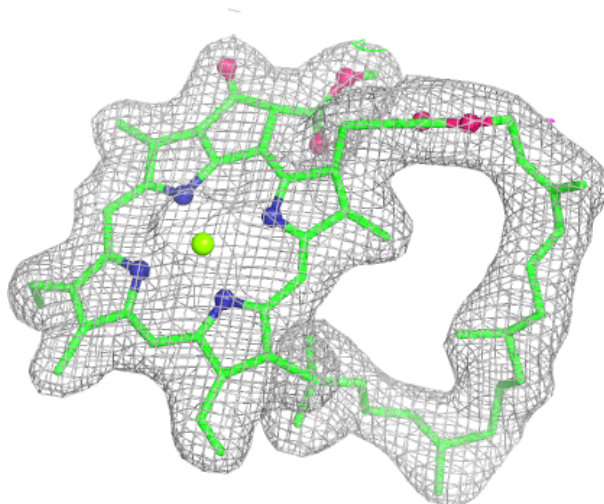
Electron density around CLA C 504:

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



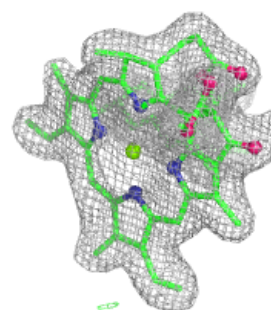
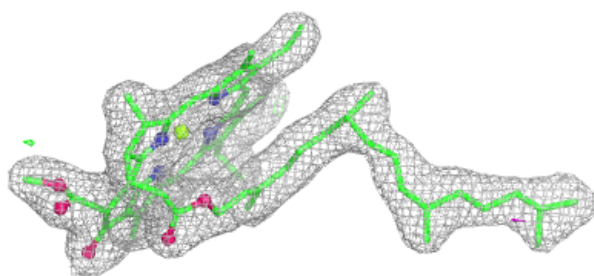
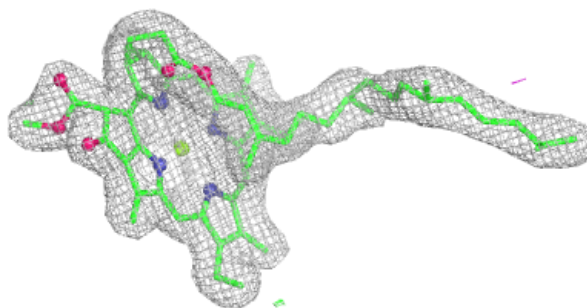
Electron density around CLA b 619:

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

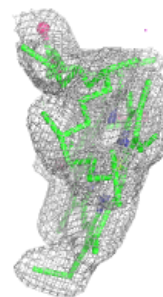
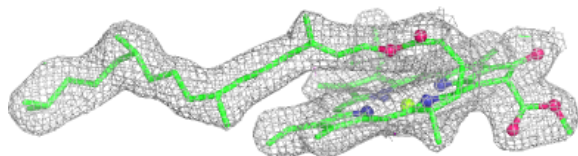
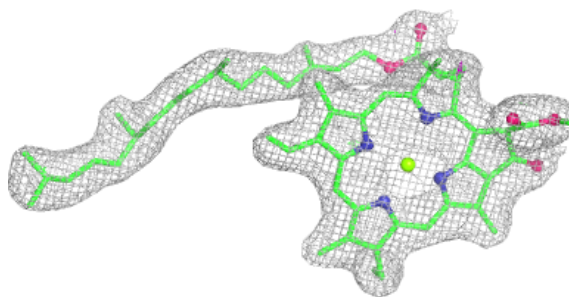


Electron density around CLA C 505:

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

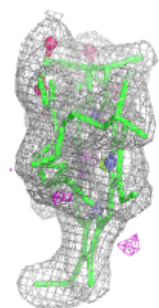
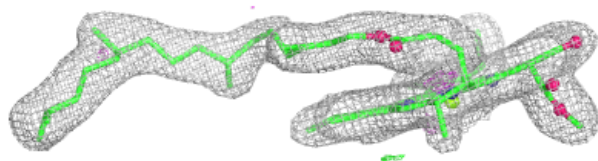
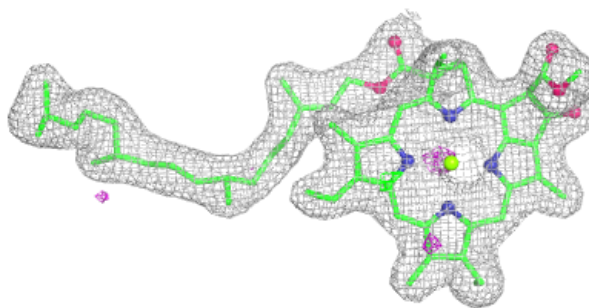
**Electron density around CLA c 502:**

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



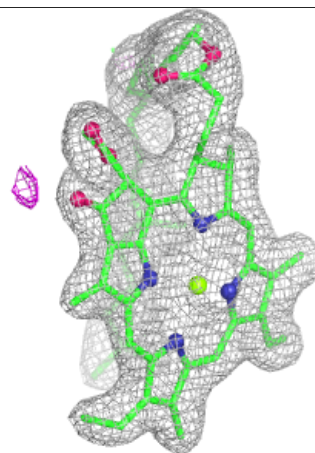
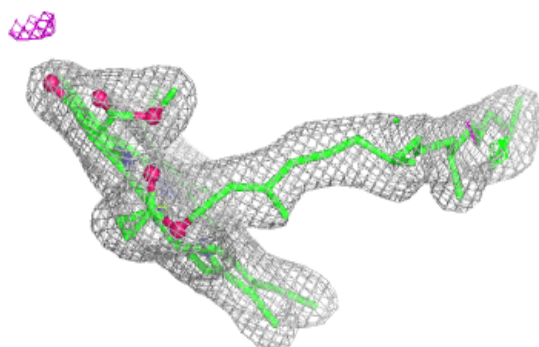
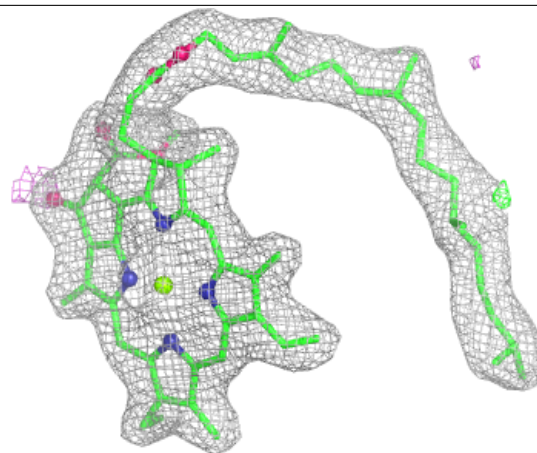
Electron density around CLA B 604:

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

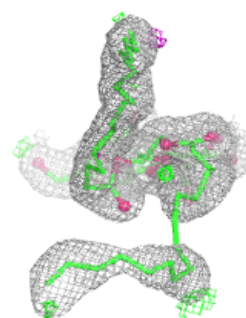
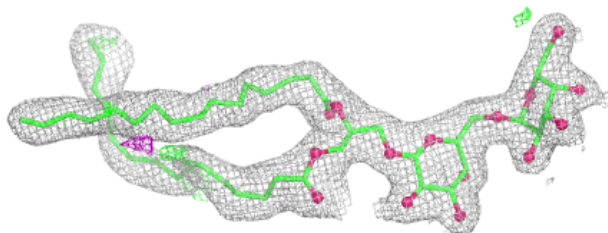
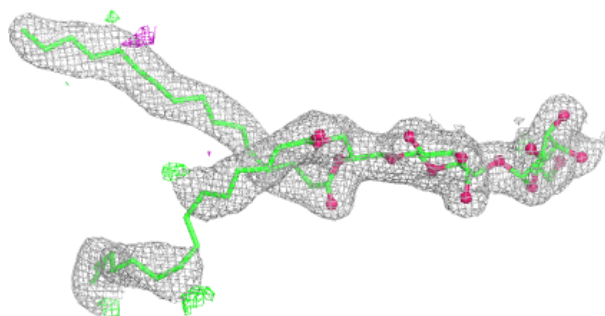


Electron density around CLA C 507:

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

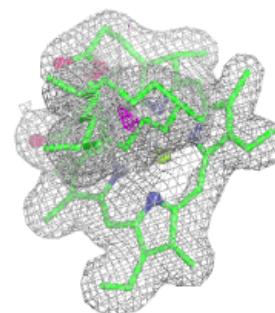
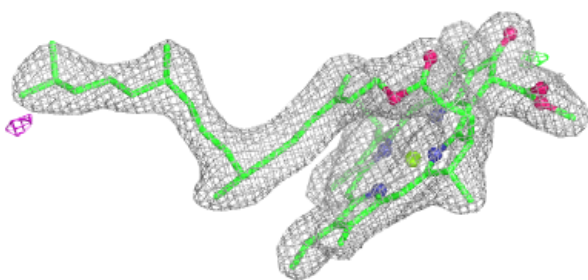
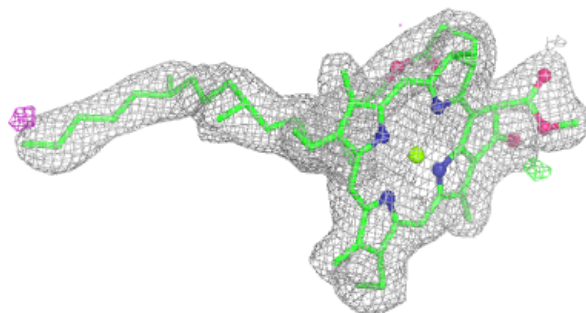
**Electron density around DGD C 515:**

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

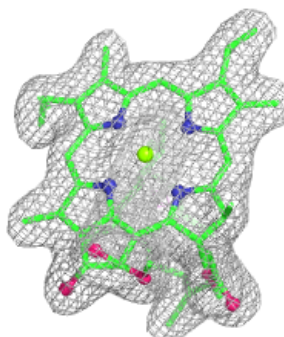
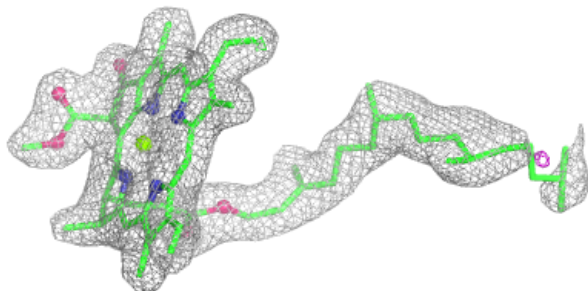
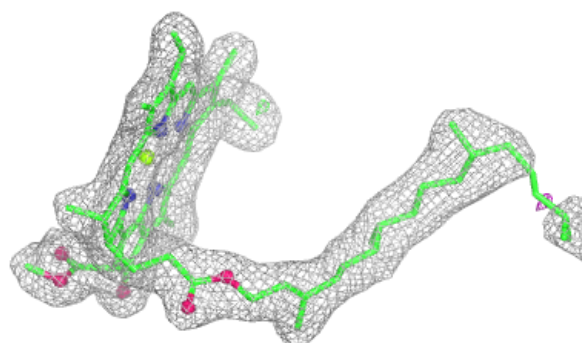


Electron density around CLA c 506:

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

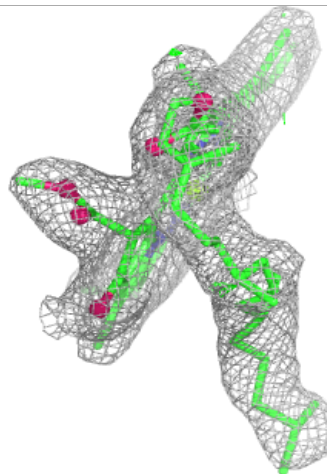
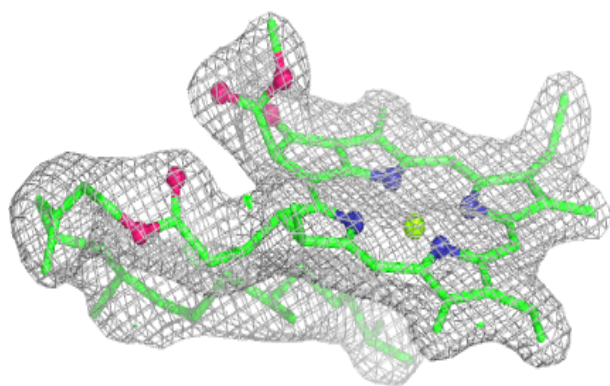
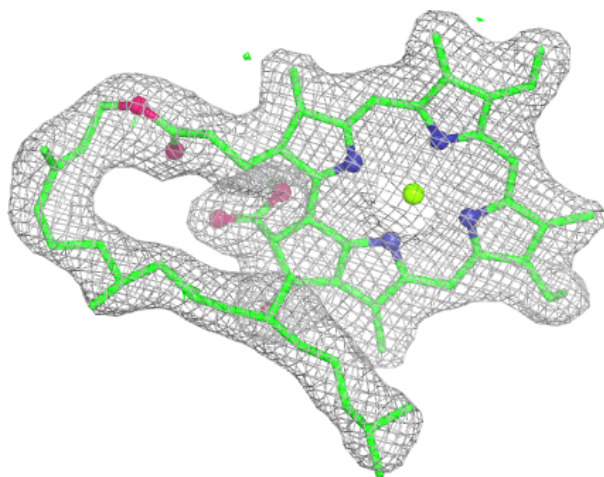
**Electron density around CLA C 508:**

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



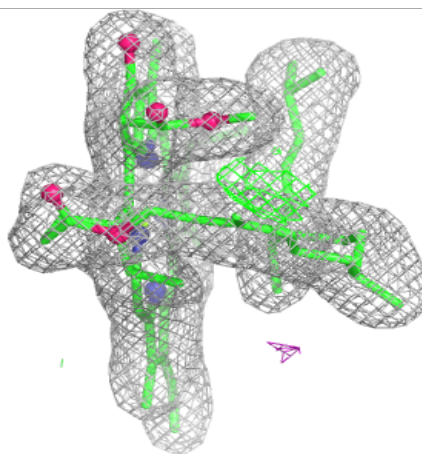
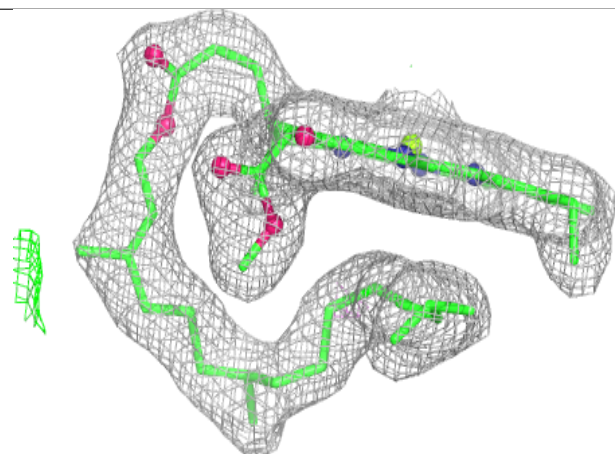
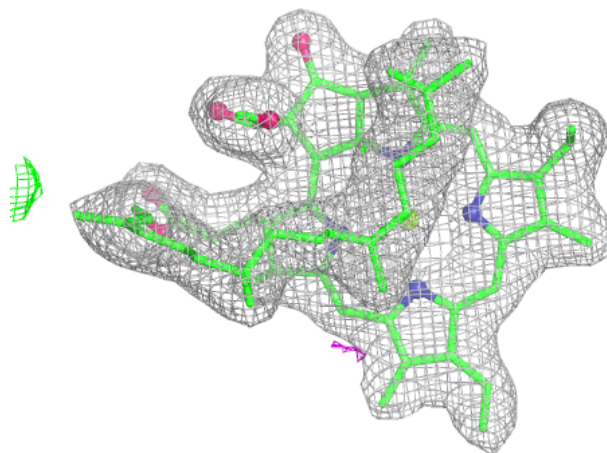
Electron density around CLA C 509:

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



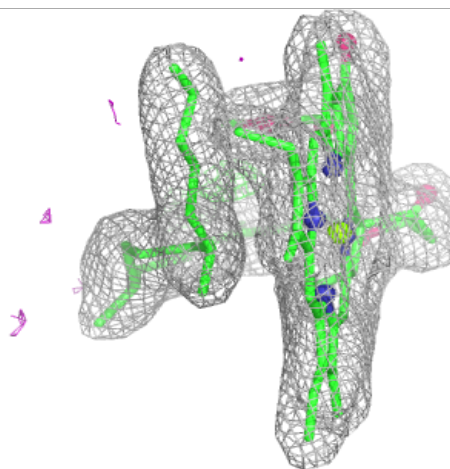
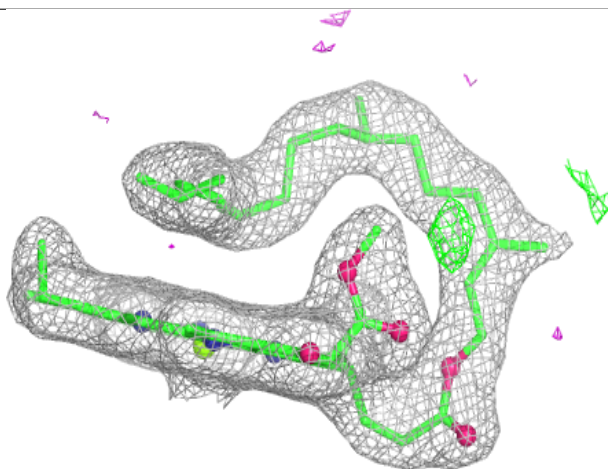
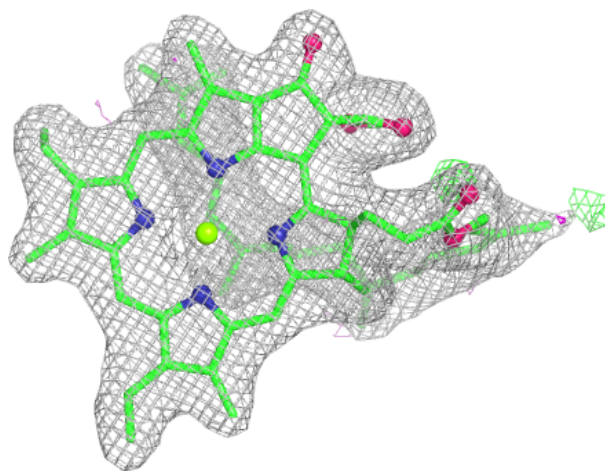
Electron density around CLA C 510:

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



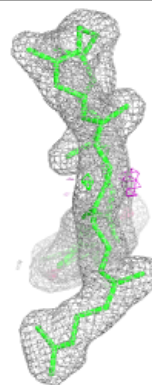
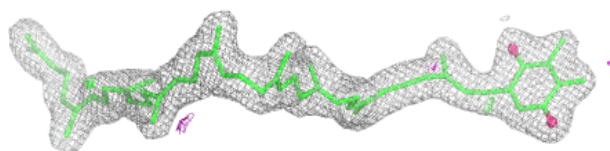
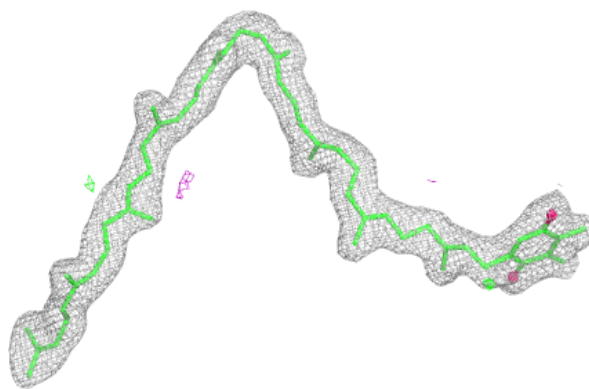
Electron density around CLA c 511:

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



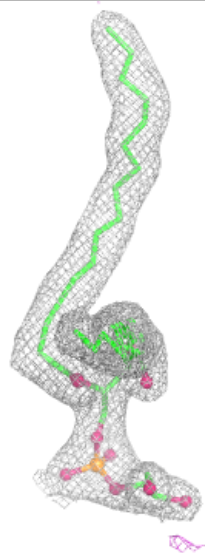
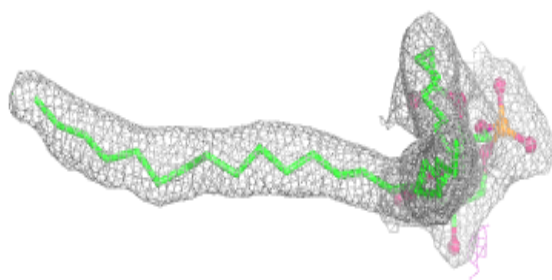
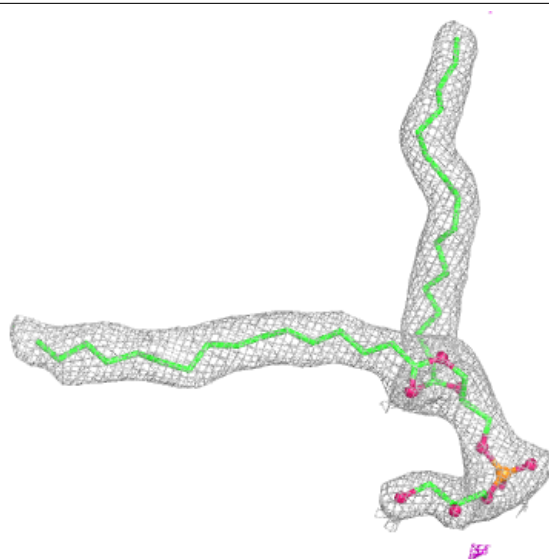
Electron density around PL9 D 407:

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



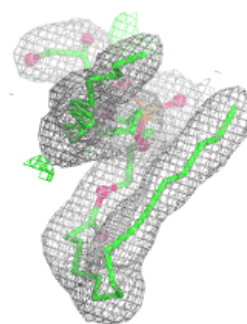
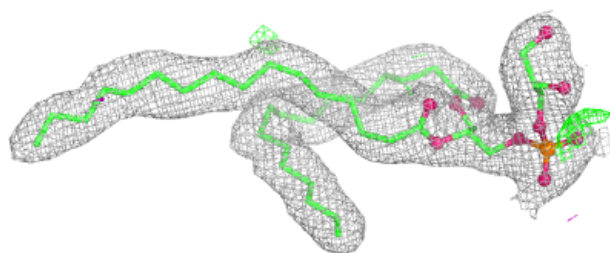
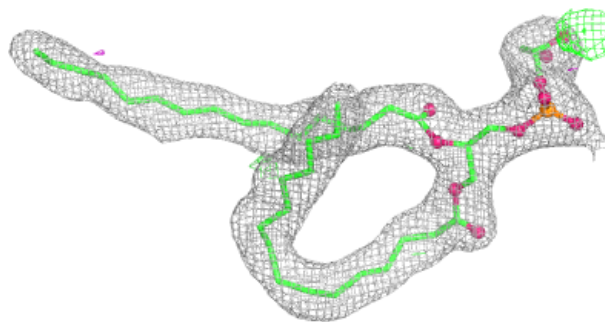
Electron density around LHG b 624:

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



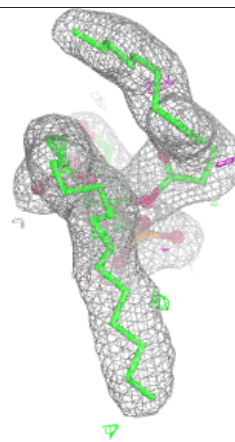
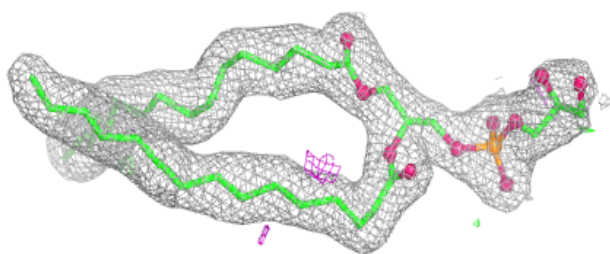
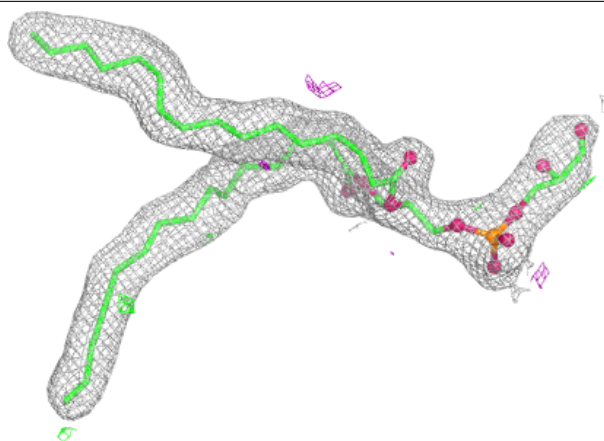
Electron density around LHG d 409:

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



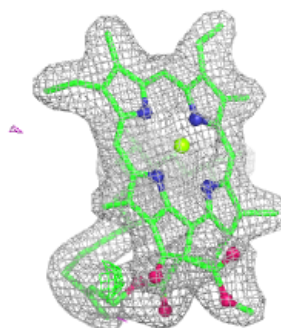
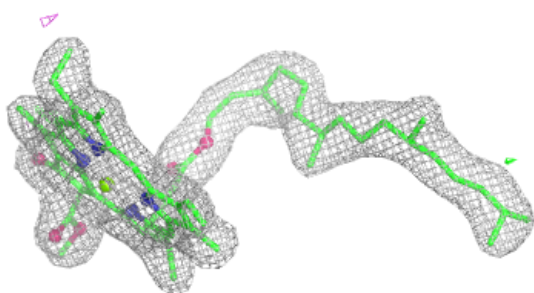
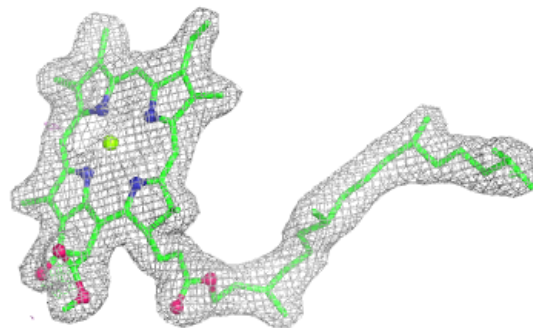
Electron density around LHG d 410:

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

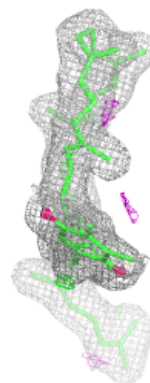
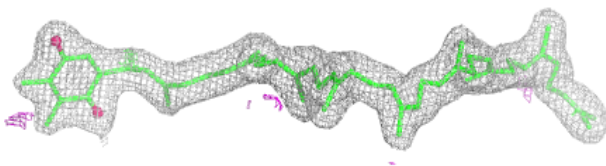
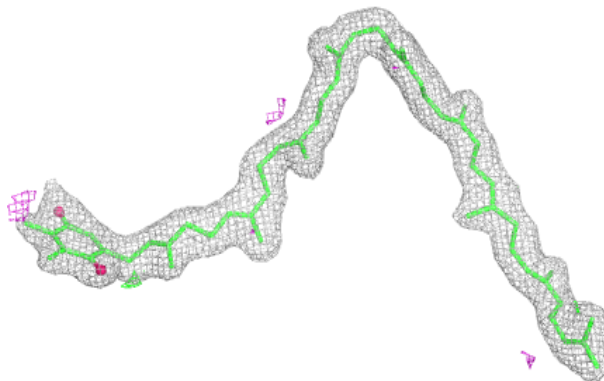


Electron density around CLA c 512:

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

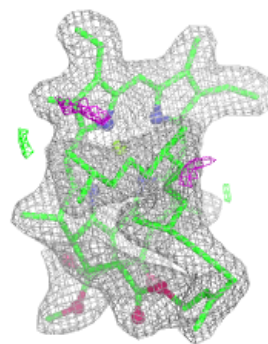
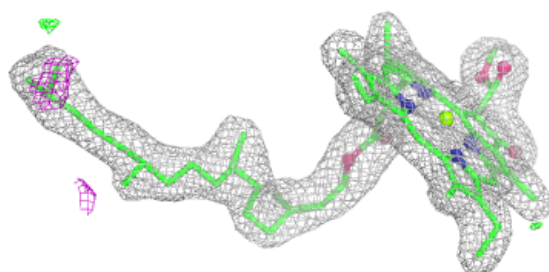
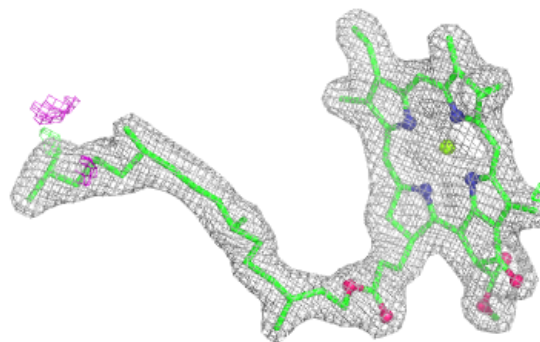
**Electron density around PL9 d 407:**

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

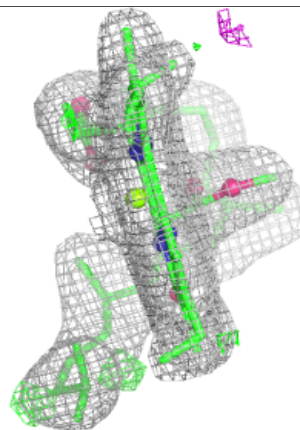
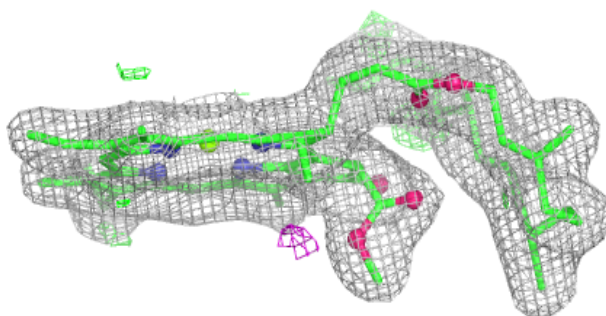
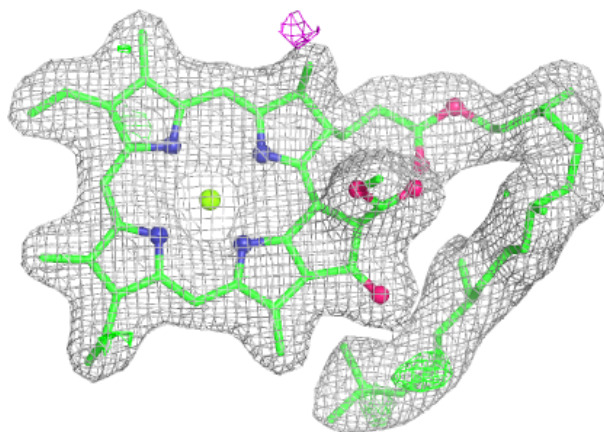


Electron density around CLA C 511:

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

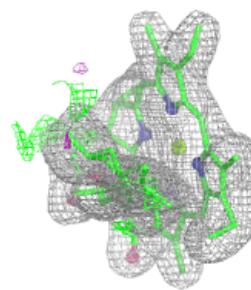
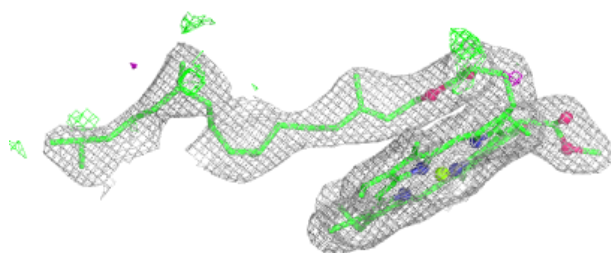
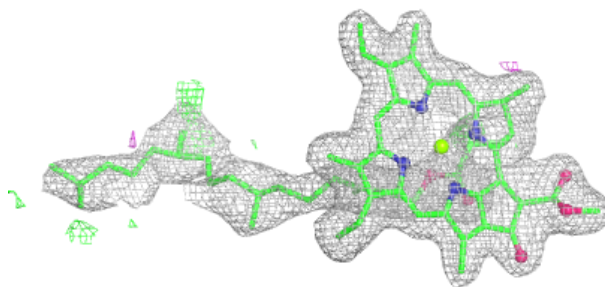
**Electron density around CLA B 611:**

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



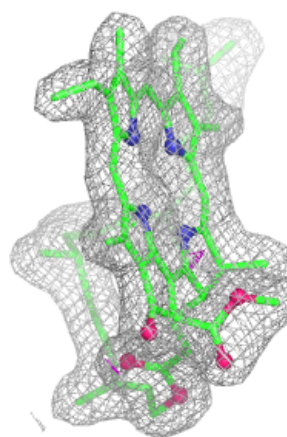
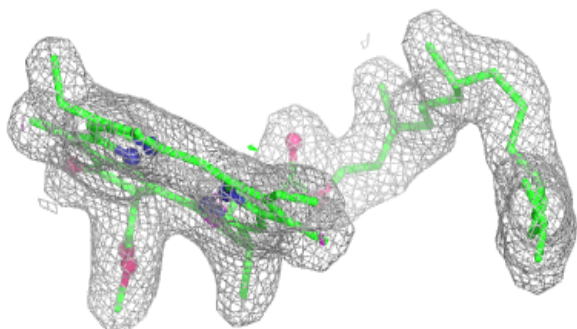
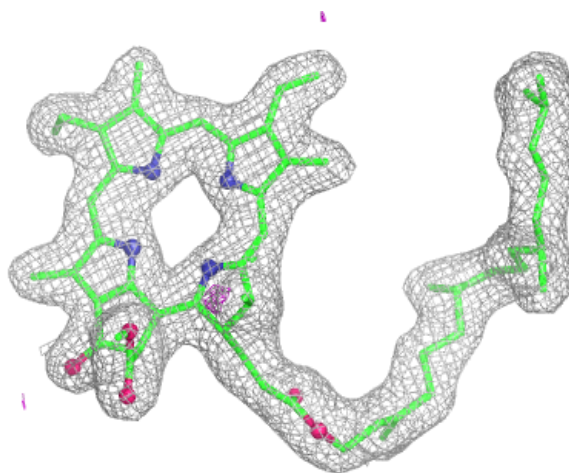
Electron density around CLA B 615:

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



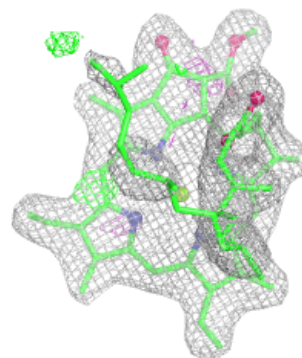
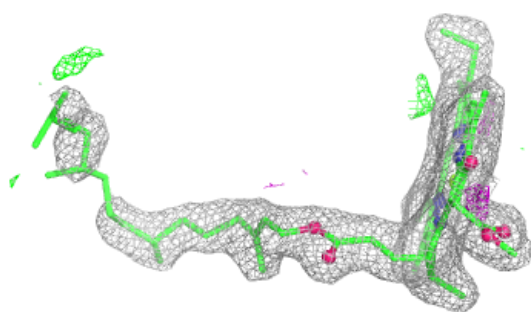
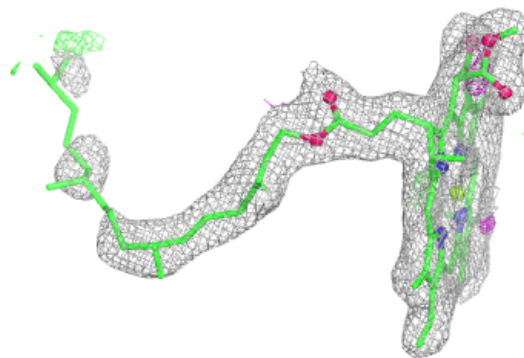
Electron density around PHO D 404:

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

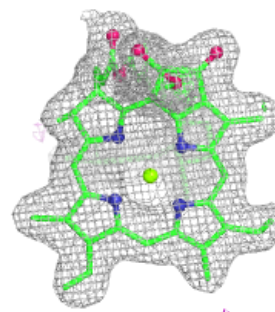
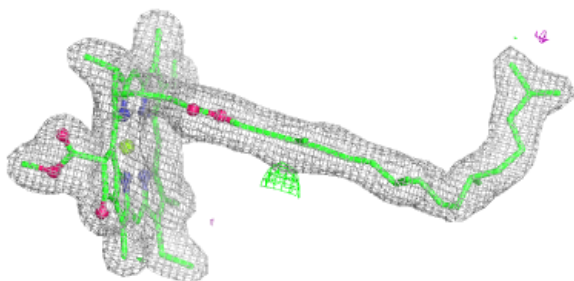
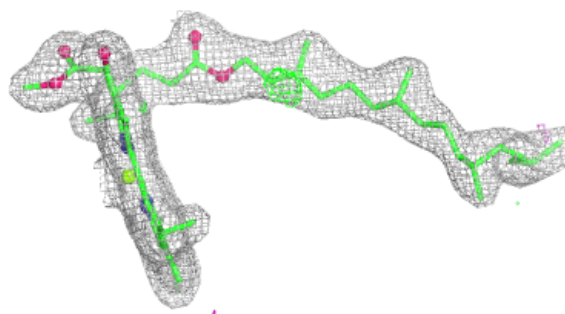


Electron density around CLA D 405:

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

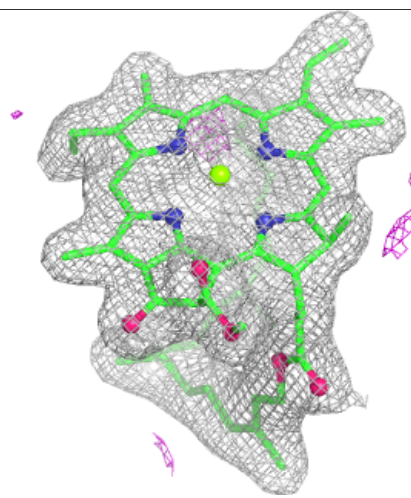
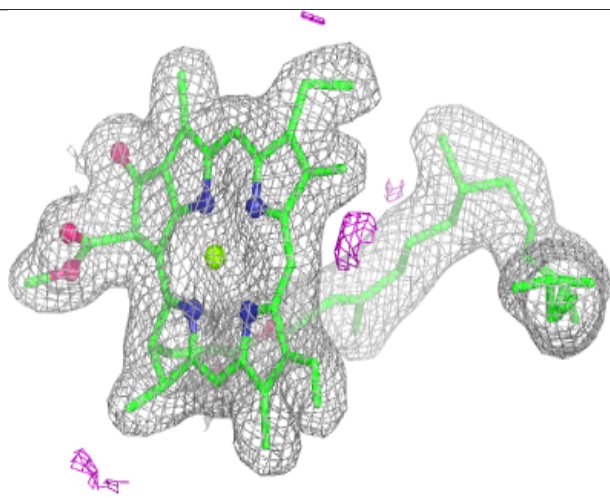
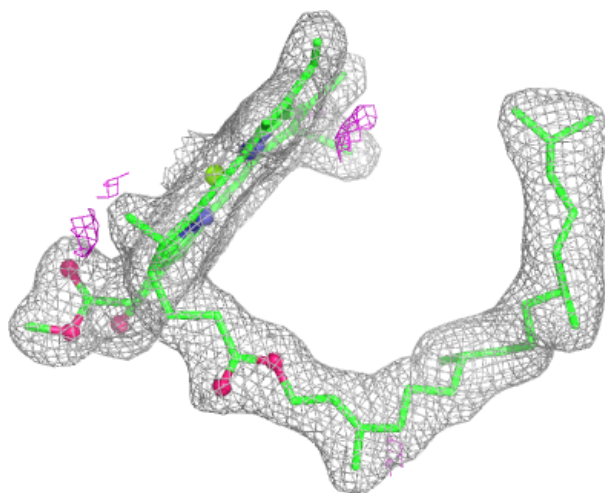
**Electron density around CLA B 606:**

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



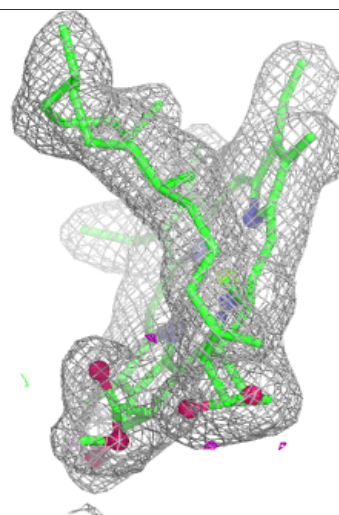
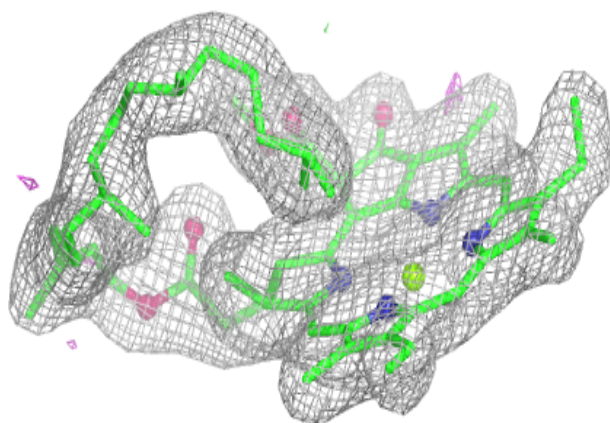
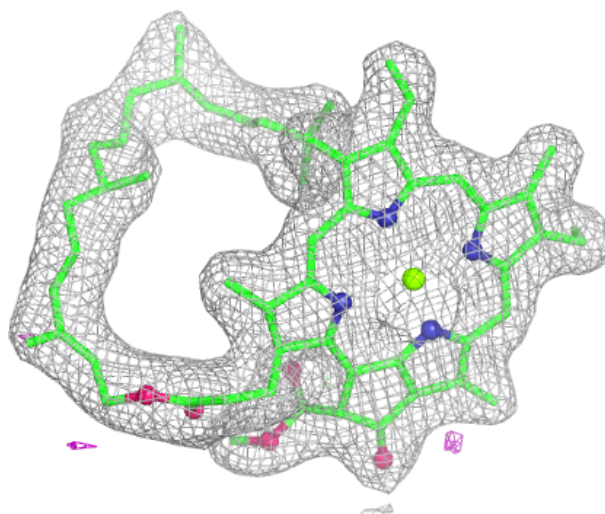
Electron density around CLA b 615:

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



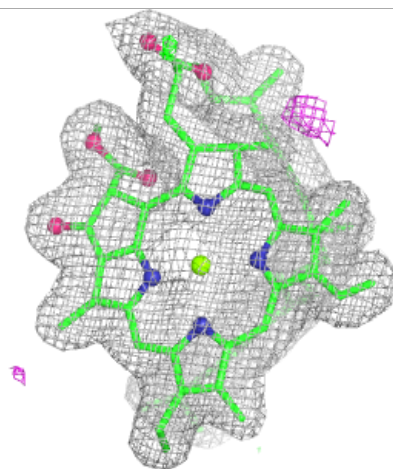
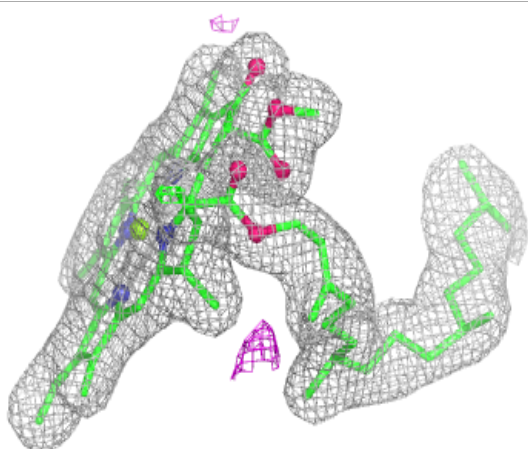
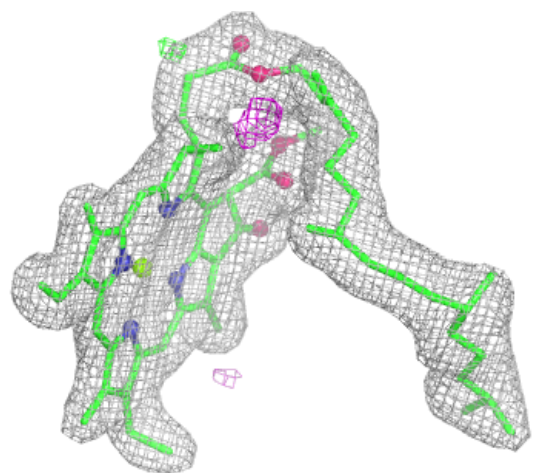
Electron density around CLA B 616:

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



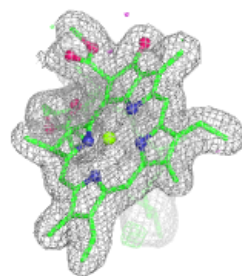
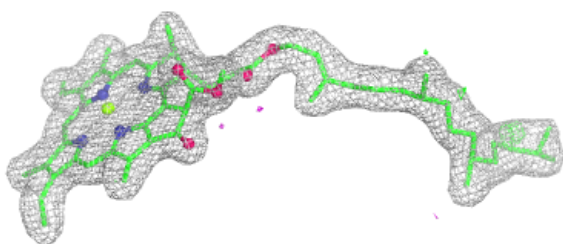
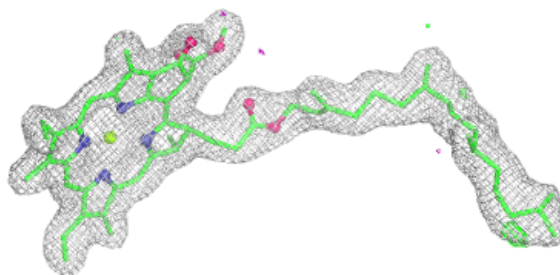
Electron density around CLA b 617:

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



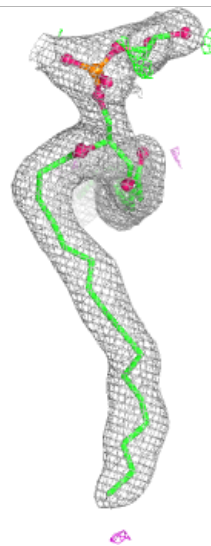
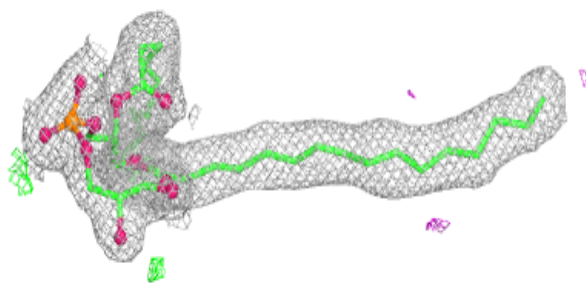
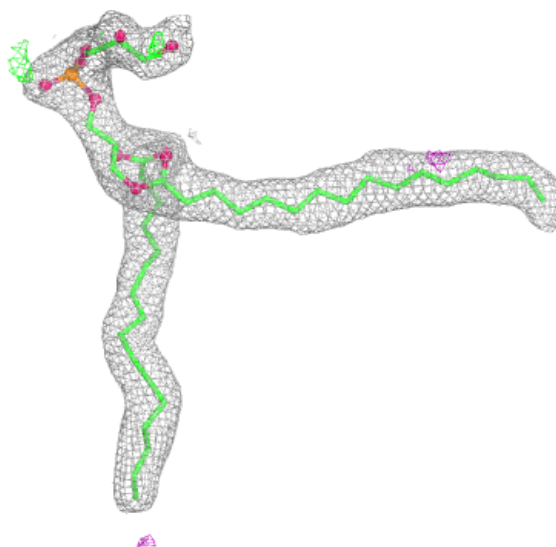
Electron density around CLA A 404:

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



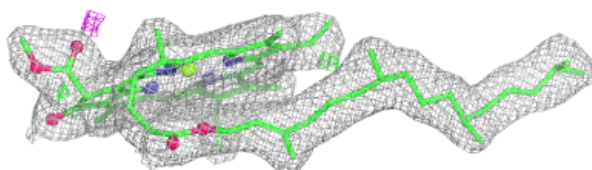
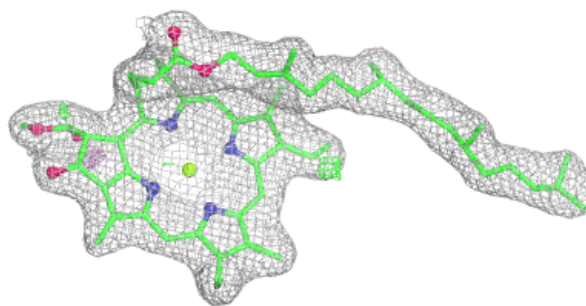
Electron density around LHG B 621:

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

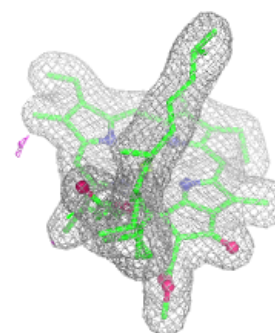
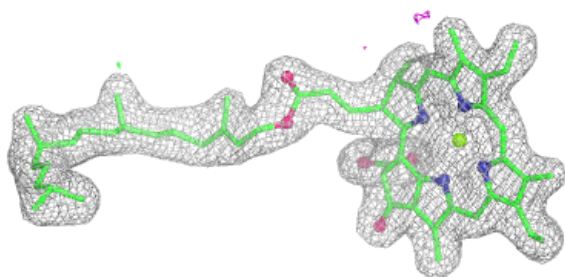
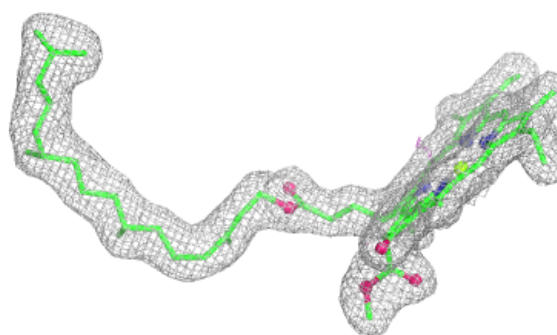


Electron density around CLA C 501:

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

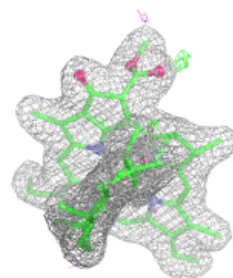
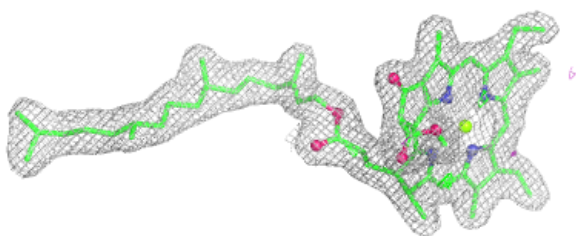
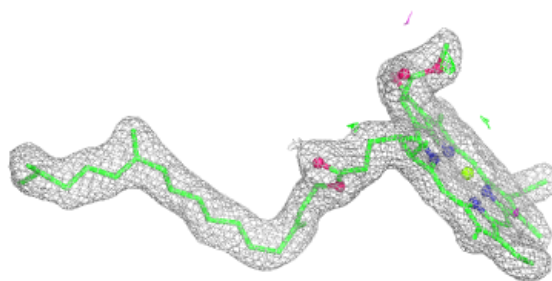
**Electron density around CLA D 403:**

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

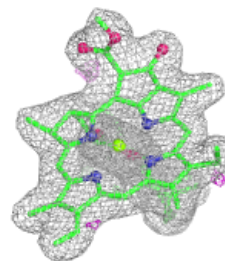
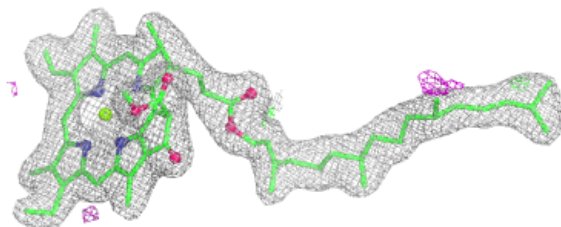
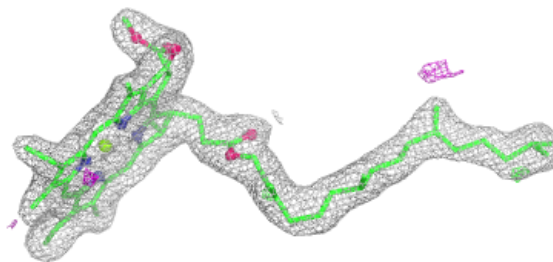


Electron density around CLA C 502:

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

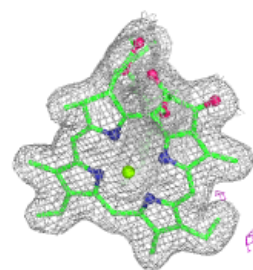
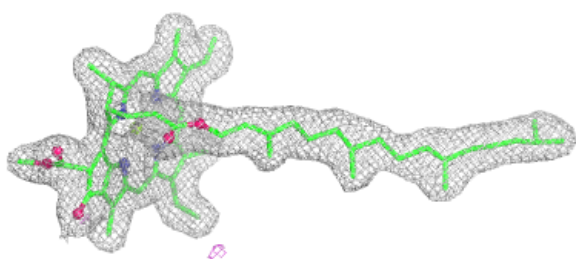
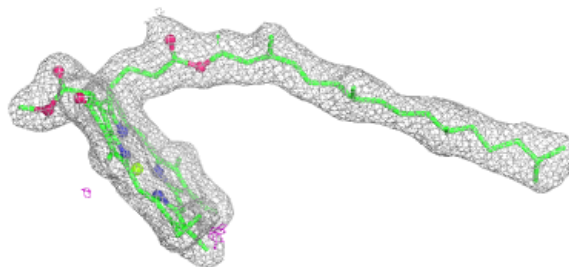
**Electron density around CLA c 503:**

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

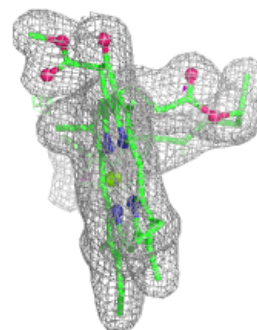
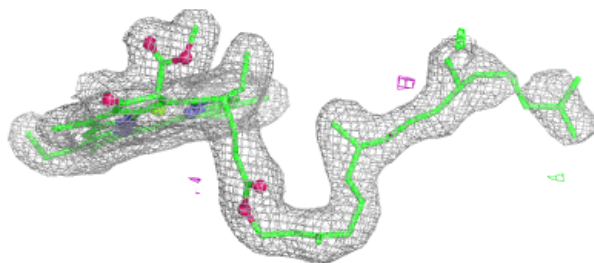
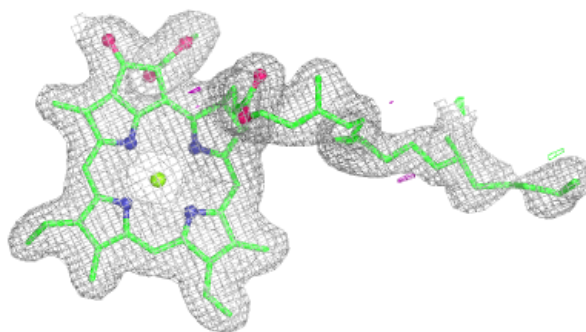


Electron density around CLA B 608:

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

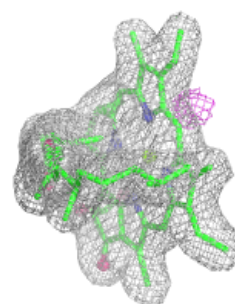
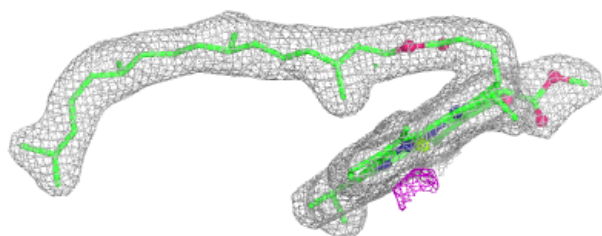
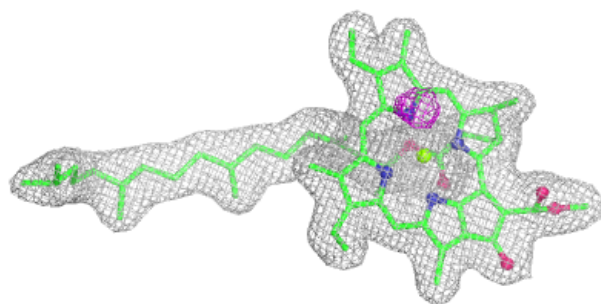
**Electron density around CLA a 407:**

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

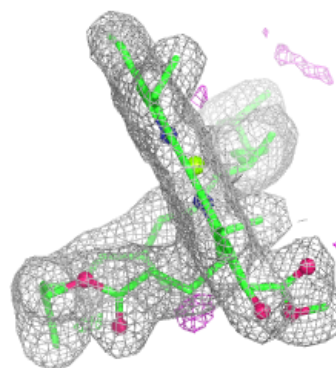
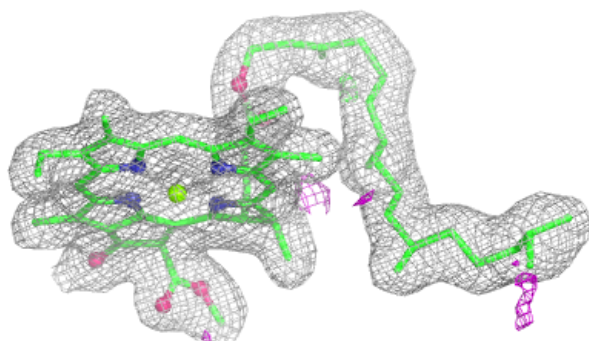
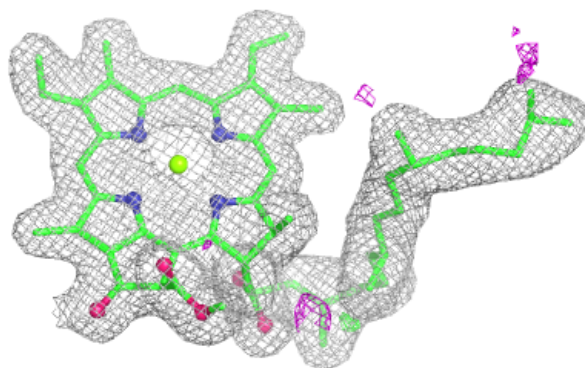


Electron density around CLA B 609:

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

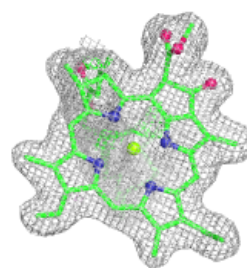
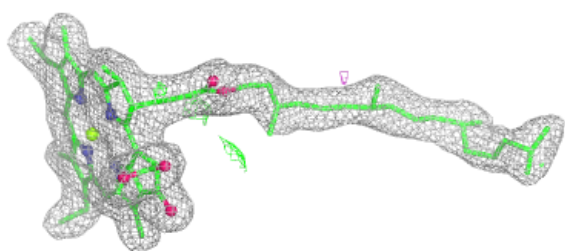
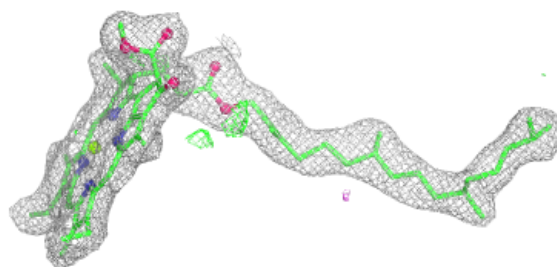
**Electron density around CLA A 405:**

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

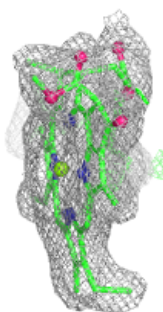
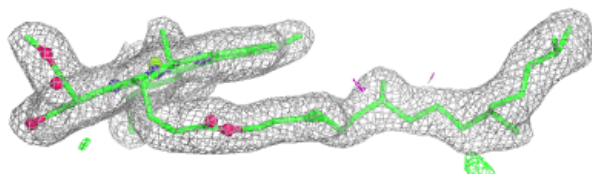
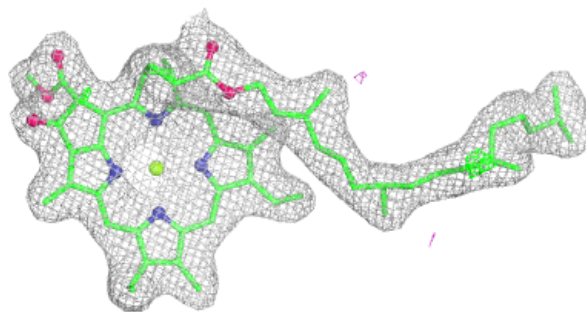


Electron density around CLA B 605:

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

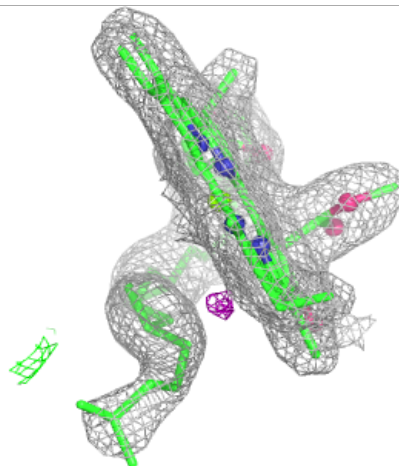
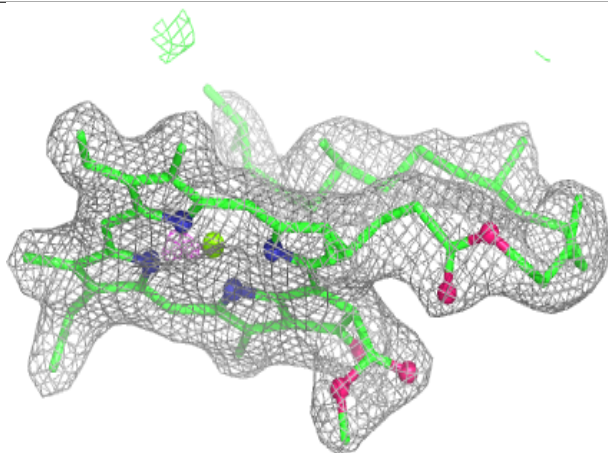
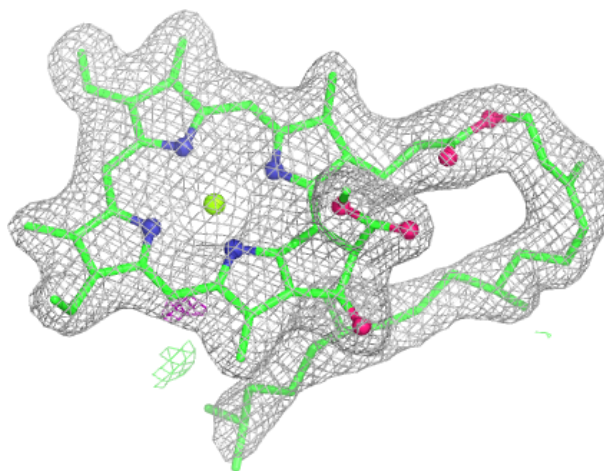
**Electron density around CLA b 607:**

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



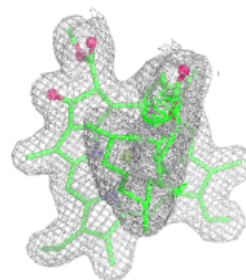
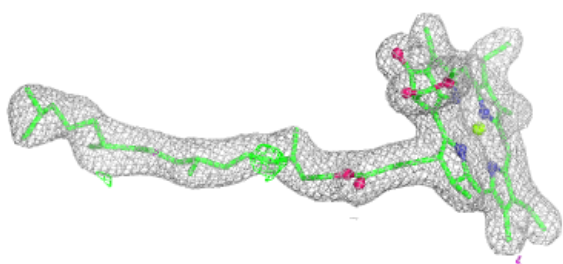
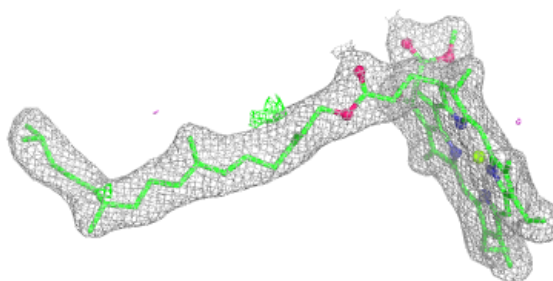
Electron density around CLA c 510:

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

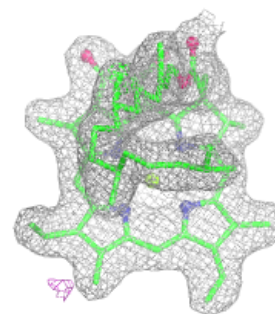
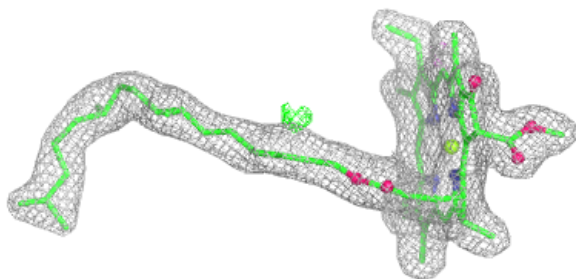
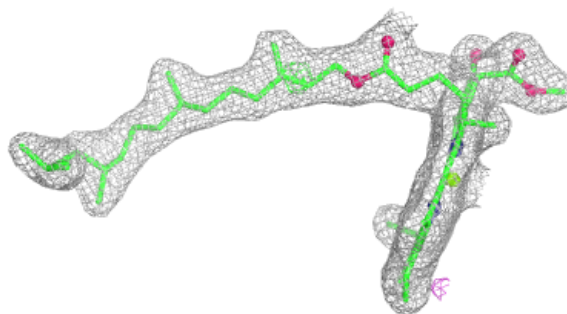


Electron density around CLA b 608:

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

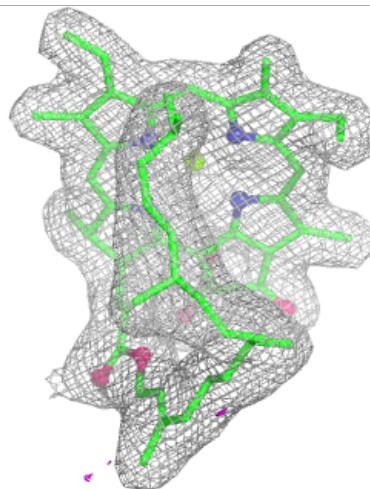
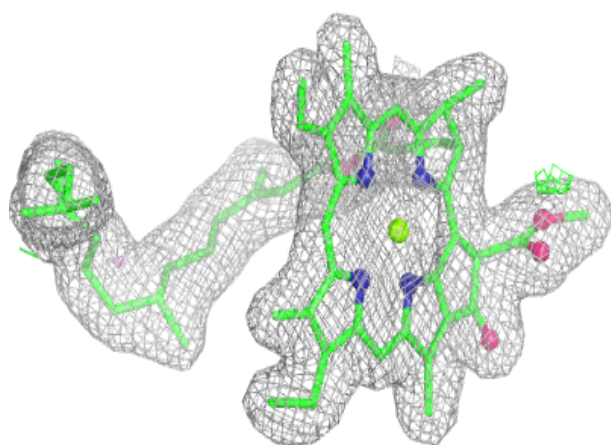
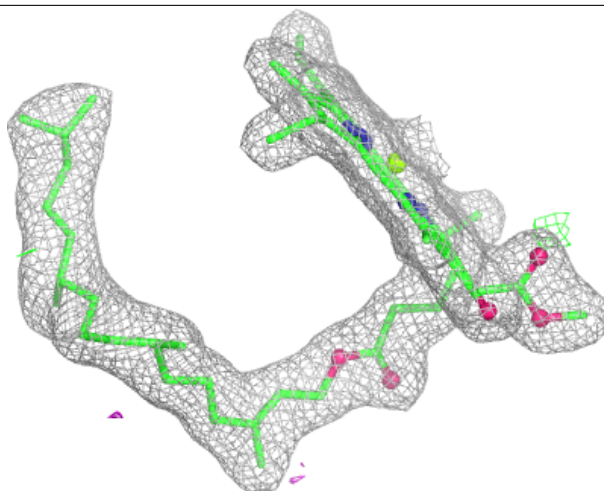
**Electron density around CLA b 609:**

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



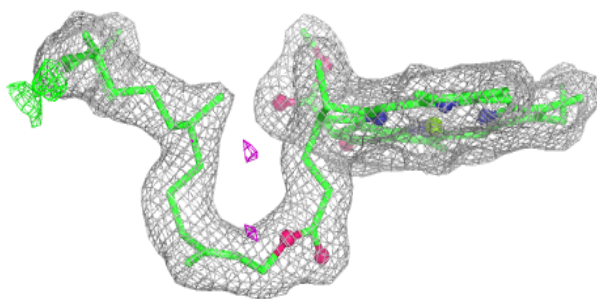
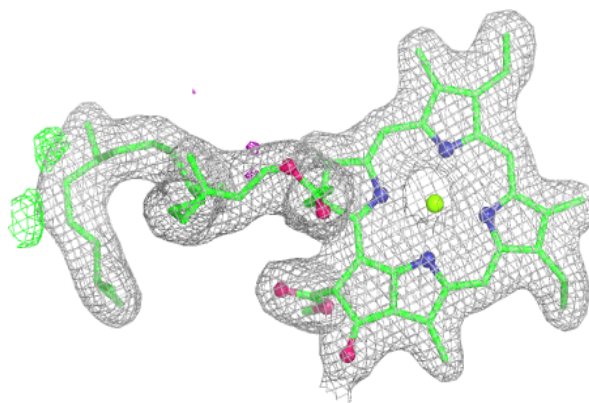
Electron density around CLA B 612:

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

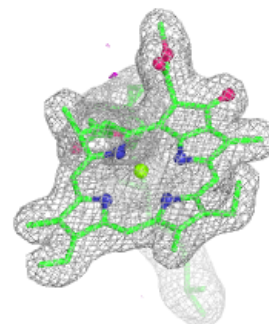
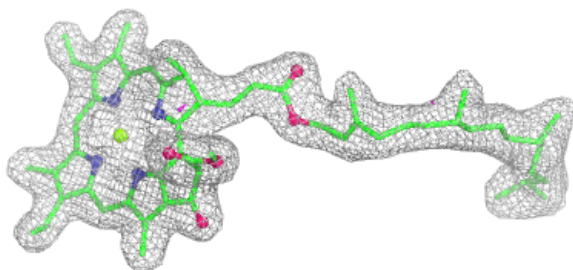
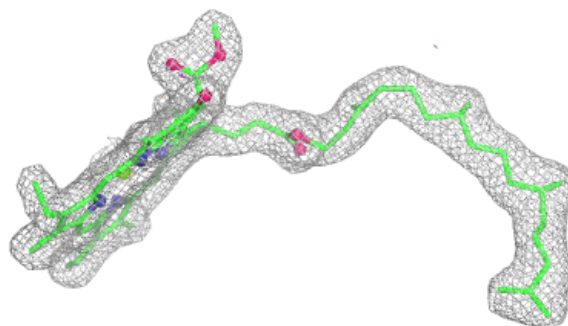


Electron density around CLA B 613:

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

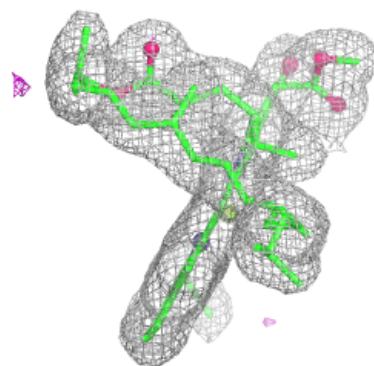
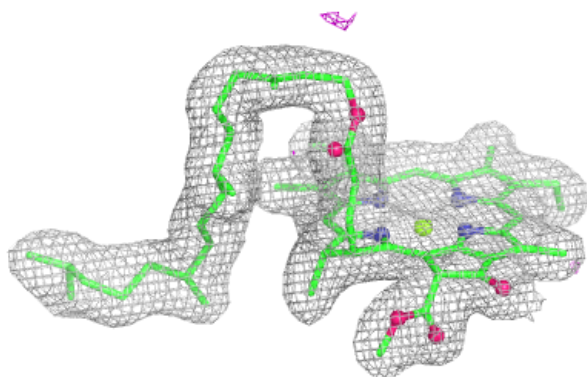
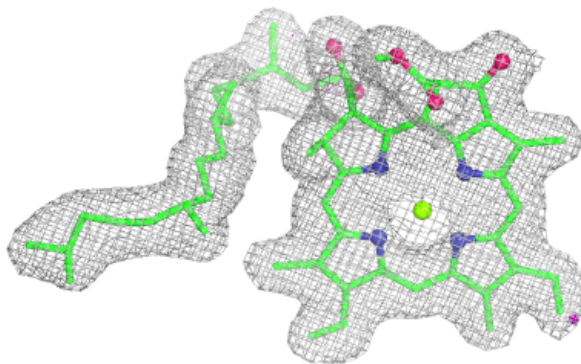
**Electron density around CLA d 402:**

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

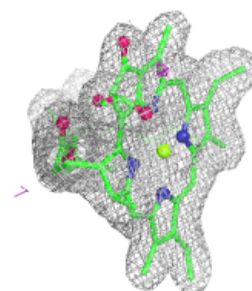
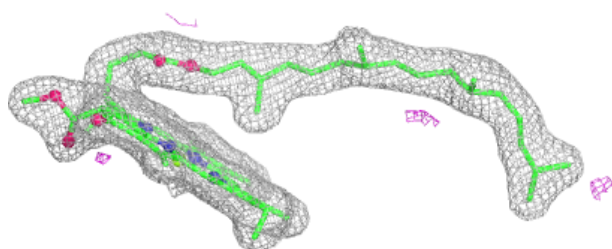
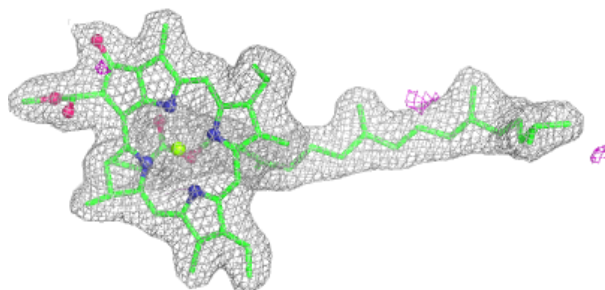


Electron density around CLA d 403:

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

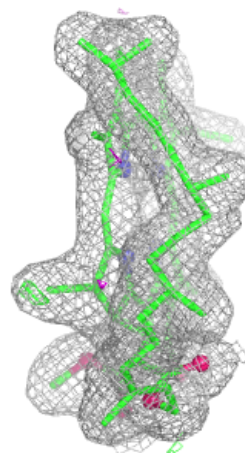
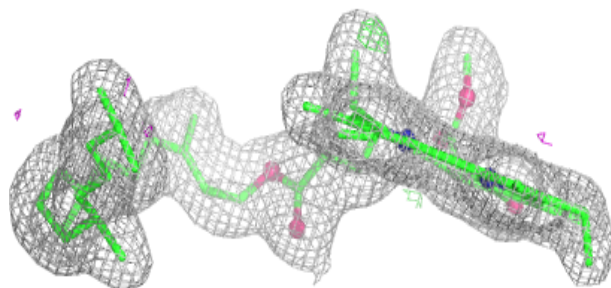
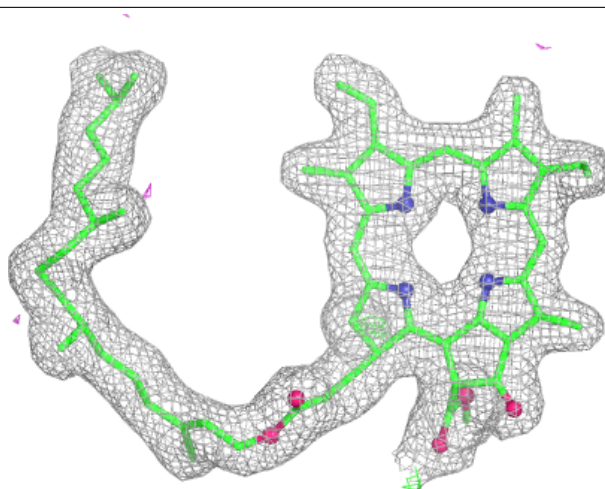
**Electron density around CLA b 612:**

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



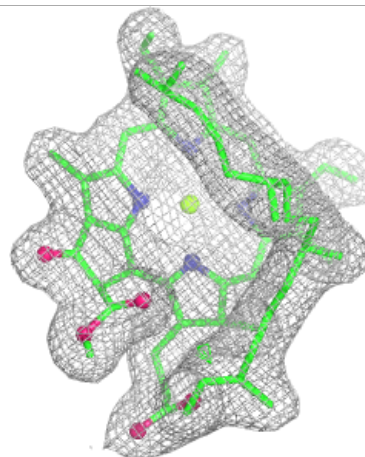
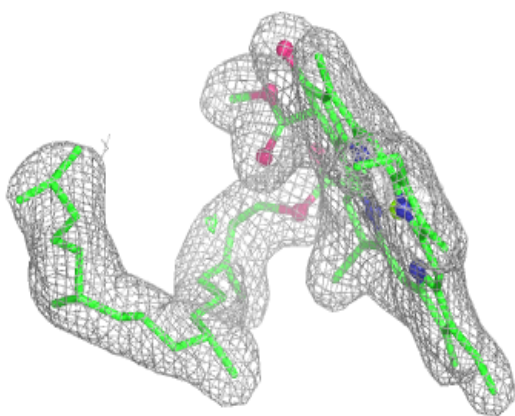
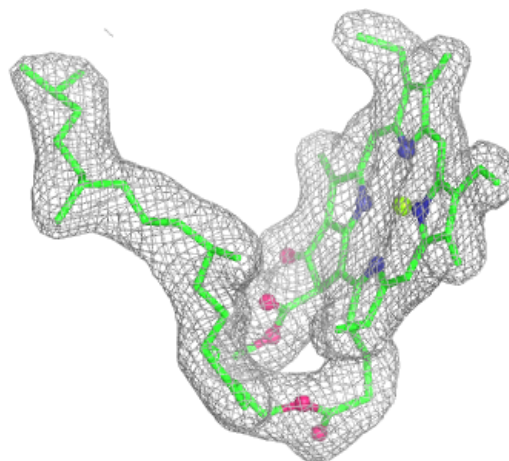
Electron density around PHO A 407:

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



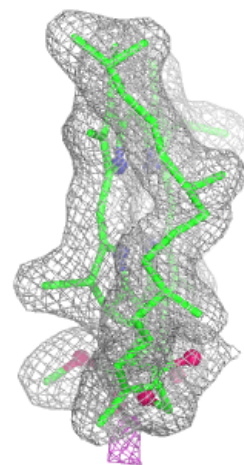
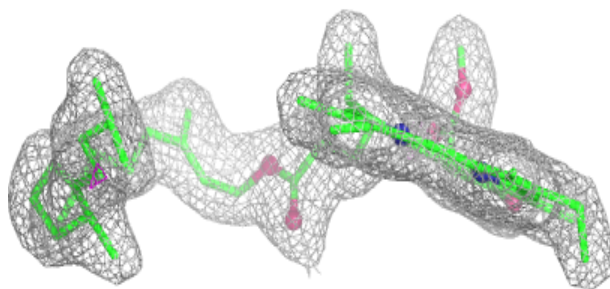
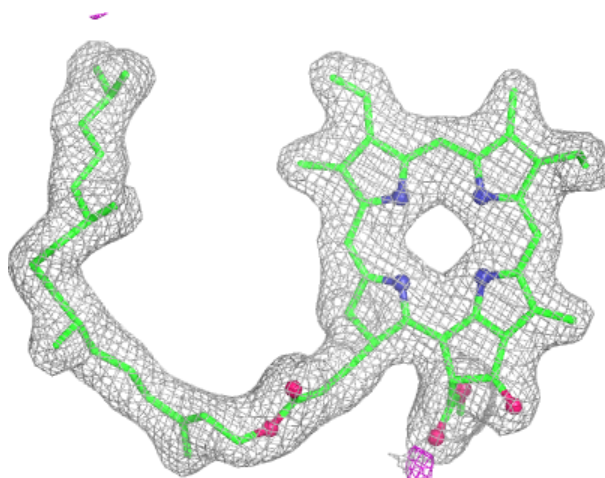
Electron density around CLA B 614:

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



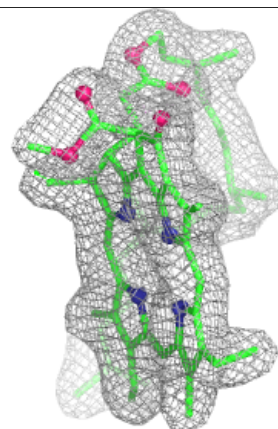
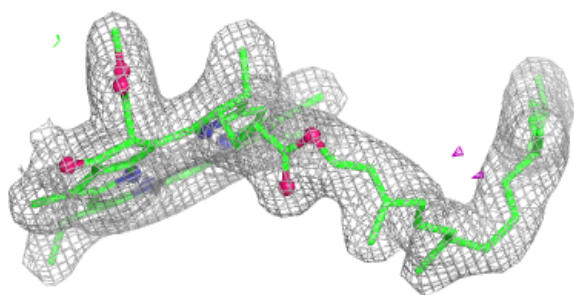
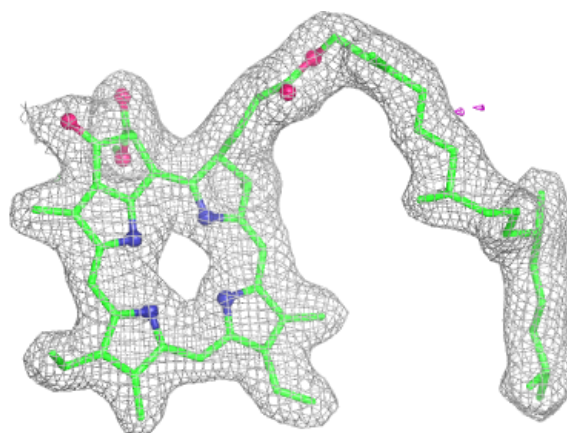
Electron density around PHO a 408:

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



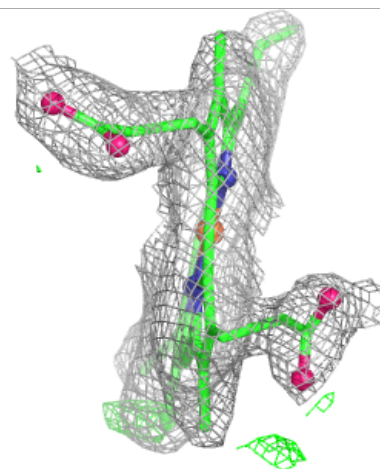
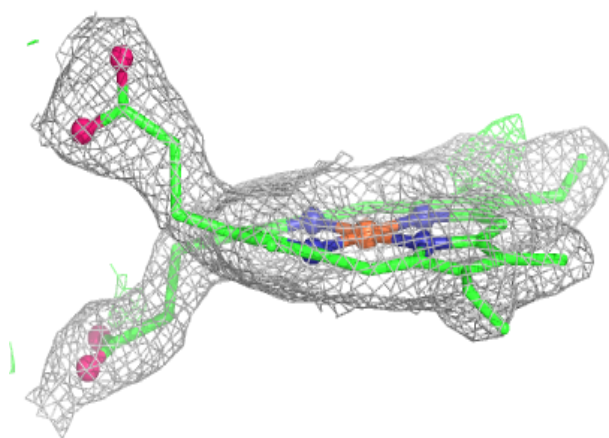
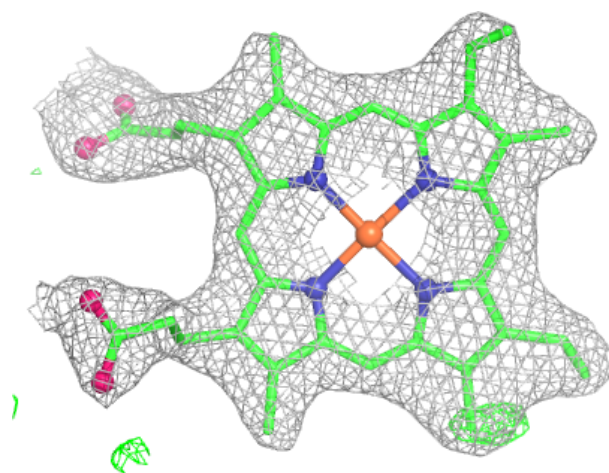
Electron density around PHO d 404:

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



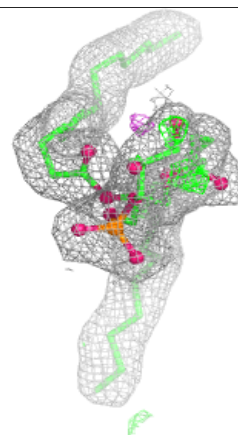
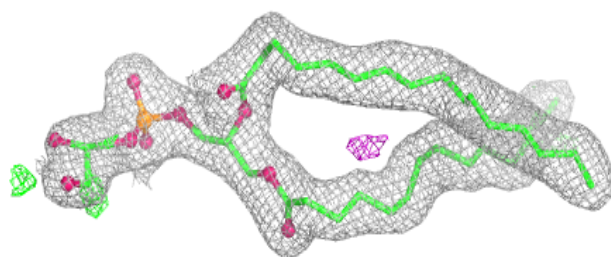
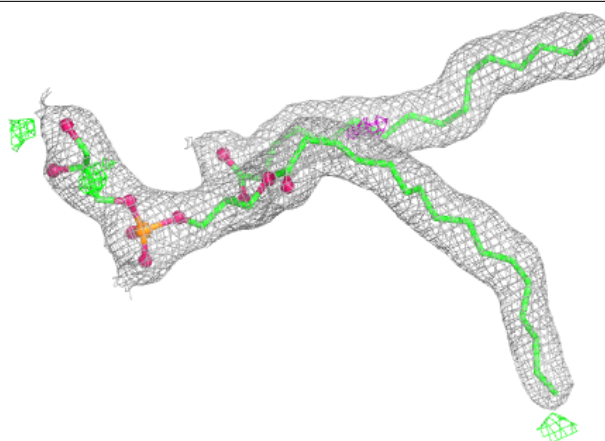
Electron density around HEM f 101:

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



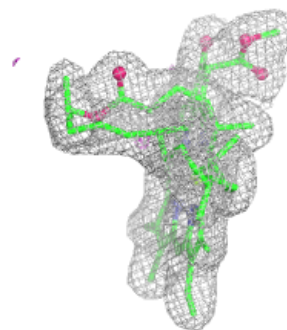
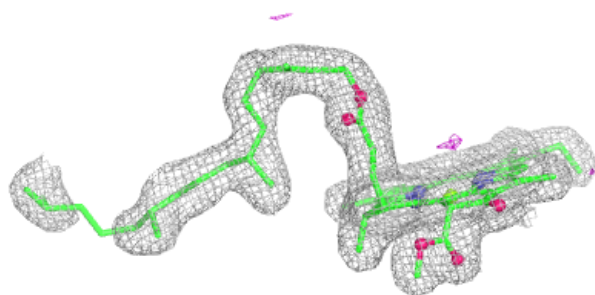
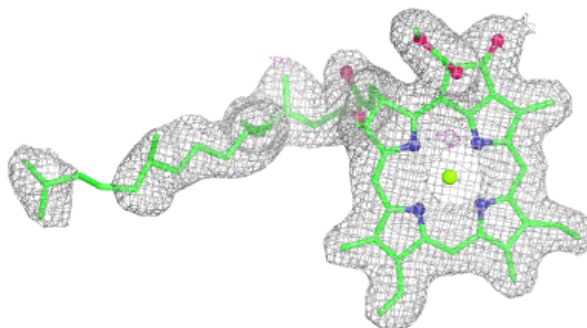
Electron density around LHG D 410:

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



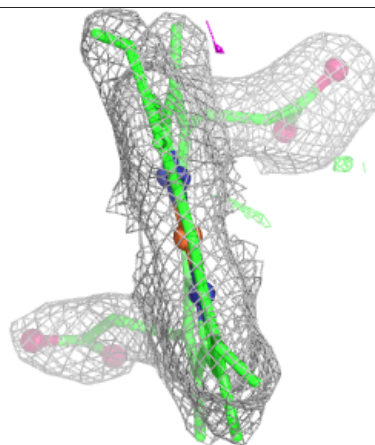
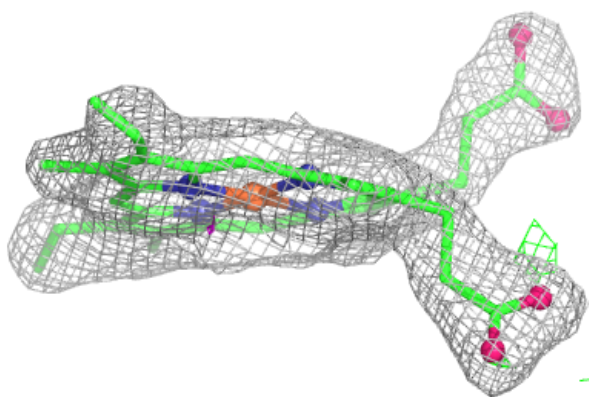
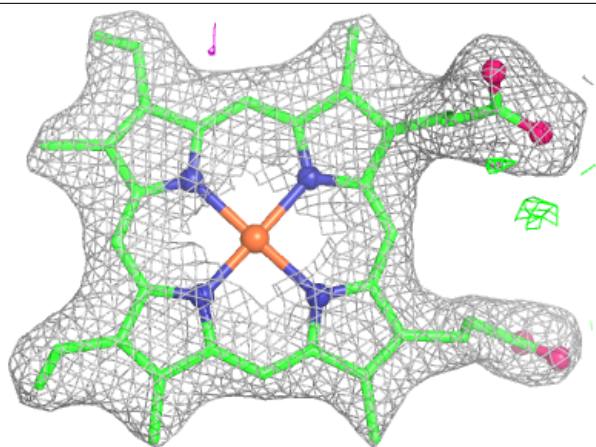
Electron density around CLA A 406:

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



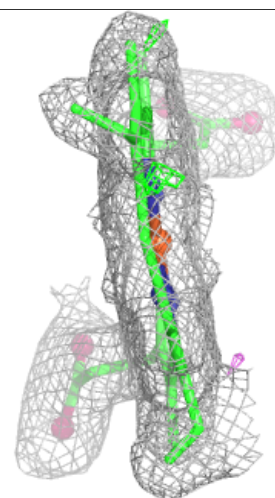
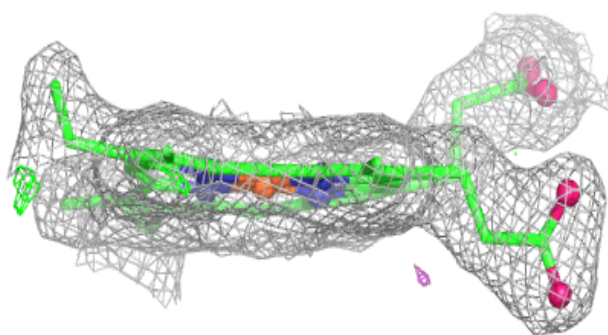
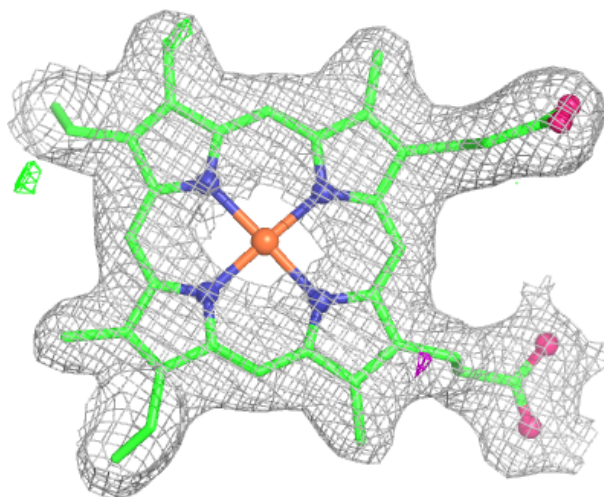
Electron density around HEM F 101:

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



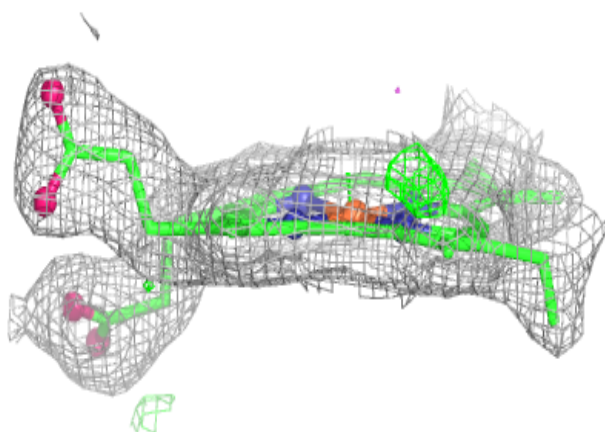
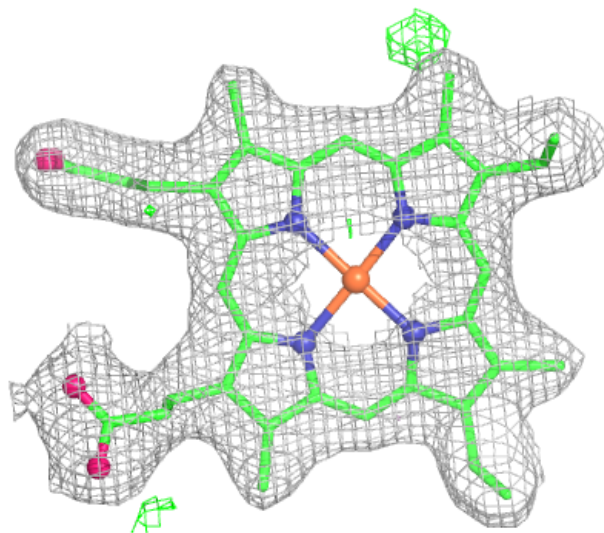
Electron density around HEC V 201:

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



Electron density around HEC v 202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.