



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:17 PM UTC

PDB ID : 5B5E / pdb_00005b5e
Title : Crystal structure analysis of Photosystem II complex
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on : 2016-05-02
Resolution : 1.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

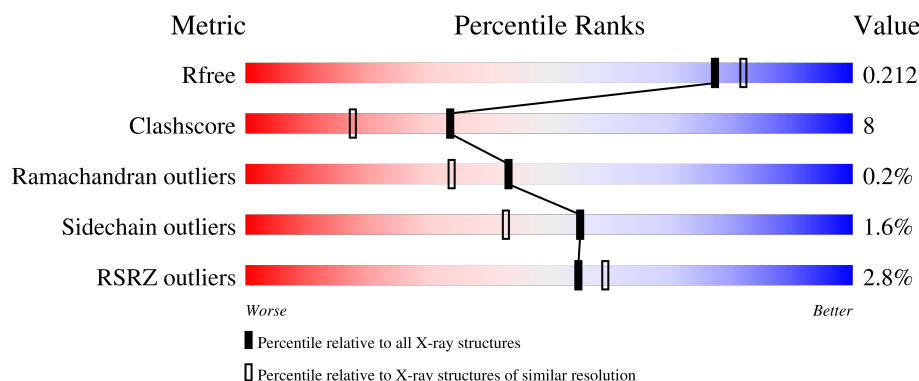
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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

Mol	Chain	Length	Quality of chain
1	A	344	87% 10% ..
1	a	344	2% 84% 13% .
2	B	505	3% 89% 11%
2	b	505	4% 88% 11% .
3	C	455	88% 11% .

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Mol	Chain	Length	Quality of chain
3	c	455	 88% 12%
4	D	342	 88% 11%
4	d	342	 89% 11%
5	E	83	 83% 14% 13%
5	e	83	 76% 14% 7% 5%
6	F	44	 73% 7% 20%
6	f	44	 64% 9% 27%
7	H	65	 82% 12%
7	h	65	 86% 11%
8	I	38	 89% 8%
8	i	38	 87% 13%
9	J	40	 78% 12% 10%
9	j	40	 85% 15%
10	K	37	 84% 16%
10	k	37	 76% 24%
11	L	37	 89% 11%
11	l	37	 89% 8%
12	M	36	 72% 19% 6%
12	m	36	 78% 17% 6%
13	O	244	 85% 13%
13	o	244	 88% 11%
14	T	32	 84% 6% 6%
14	t	32	 88% 6%
15	U	104	 82% 11% 7%
15	u	104	 83% 11% 7%

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	910	X	-	-	-
23	CLA	c	911	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	d	403	X	-	-	-
29	UNL	M	102	-	-	X	-
29	UNL	U	201	-	-	X	-
31	DMS	A	424	-	-	X	-
31	DMS	B	636	-	-	X	-
31	DMS	B	639	-	-	X	-
31	DMS	B	646	-	-	X	-
31	DMS	D	416	-	-	X	-
31	DMS	F	102	-	-	X	-
31	DMS	H	105	-	-	X	-
31	DMS	O	305	-	-	X	-
31	DMS	O	308	-	-	X	-
31	DMS	U	204	-	-	X	-
31	DMS	V	207	-	-	X	-
31	DMS	V	210	-	-	X	-
31	DMS	a	420	-	-	X	-
31	DMS	b	636	-	-	X	-
31	DMS	b	645	-	-	X	-
31	DMS	c	925	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	DMS	d	416	-	-	X	-
31	DMS	l	102	-	-	X	-
31	DMS	v	209	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 55401 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2622	1718	431	458	15			
1	a	334	Total	C	N	O	S	0	4	0
			2633	1727	431	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

- 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	4	0
			3992	2619	668	692	13			
2	b	501	Total	C	N	O	S	0	3	0
			3929	2582	653	681	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	4	0
			3511	2297	591	610	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

- 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	2	0
			2733	1813	446	462	12			
4	d	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			651	426	103	122			
5	e	79	Total	C	N	O	0	0	0
			637	419	101	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			280	190	46	43	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	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	2	0
			511	341	83	85	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	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
			285	195	45	44	1			
8	i	38	Total	C	N	O	S	0	0	0
			303	205	48	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			285	190	44	49	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			306	205	48	53			
11	l	36	Total	C	N	O	0	1	0
			297	200	47	50			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

- 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	2	0
			1861	1164	311	382	4			
13	o	243	Total	C	N	O	S	0	1	0
			1852	1159	310	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	31	Total	C	N	O	S	0	0	0
			261	183	37	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O		0	1	0
			776	493	129	154				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			210	137	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

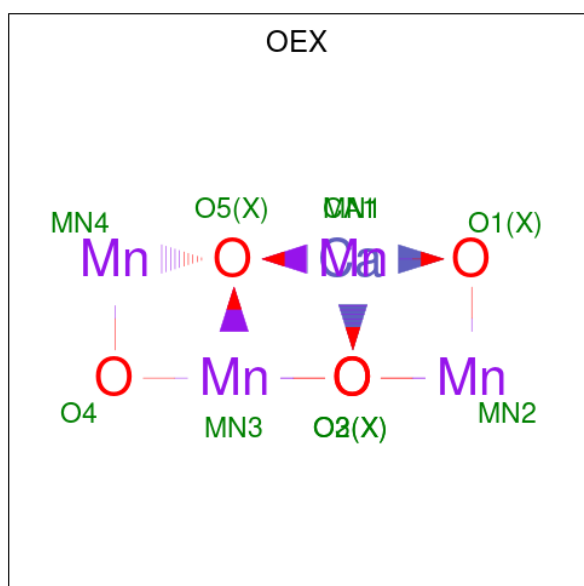
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O		0	0	0
			275	185	44	46				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			468	320	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			457	312	70	73	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		

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

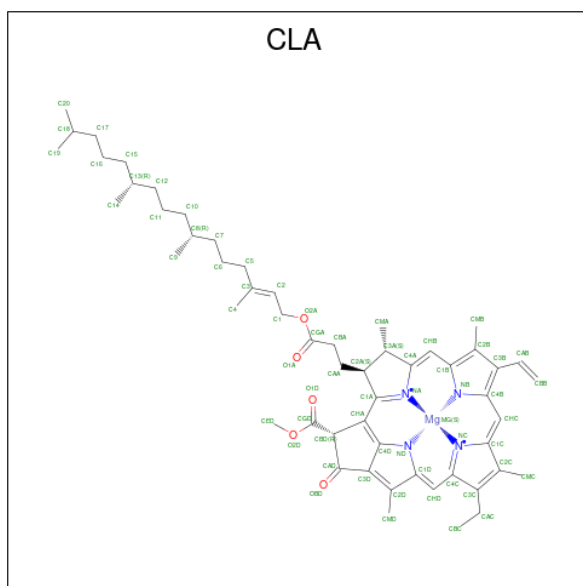
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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

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

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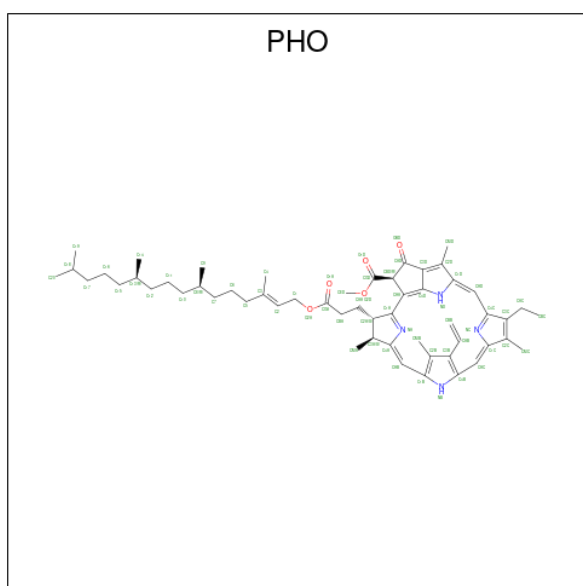
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23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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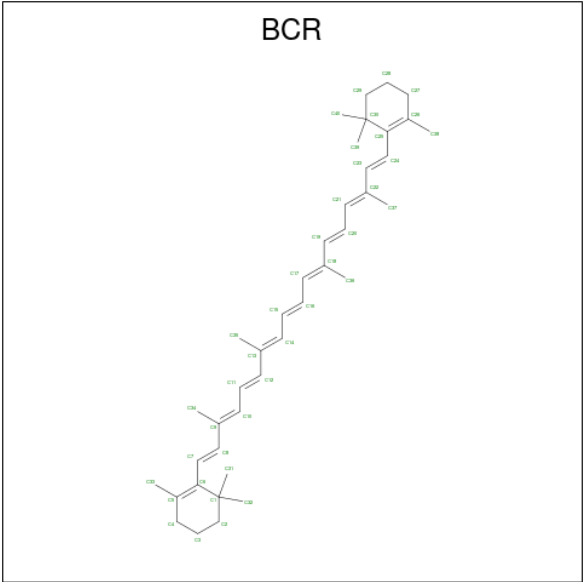
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



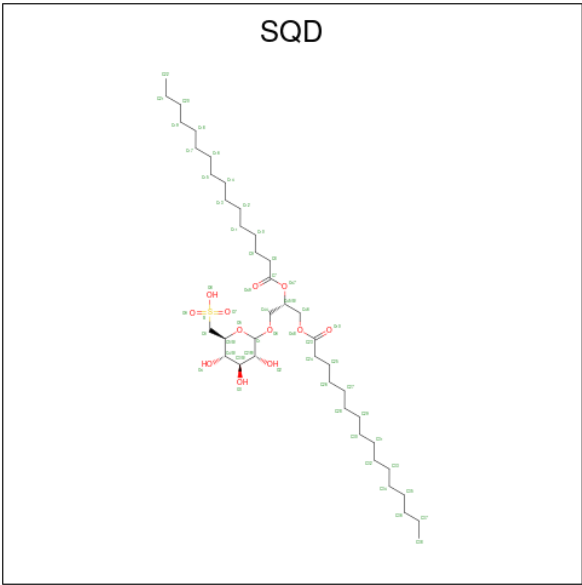
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total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

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

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



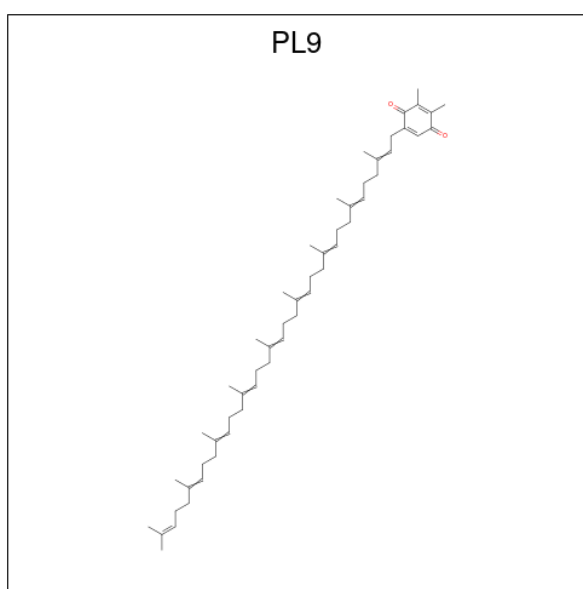
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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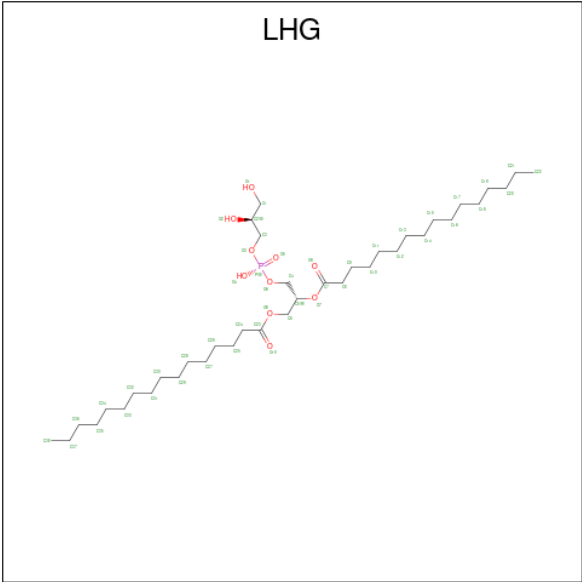
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	x	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 27 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: $C_{53}H_{80}O_2$).



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			46	35	10	1		
28	E	1	Total	C	O	P	0	0
			49	38	10	1		
28	K	1	Total	C	O	P	0	0
			44	35	8	1		
28	L	1	Total	C	O	P	0	0
			49	38	10	1		
28	a	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			44	33	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			46	35	10	1		
28	e	1	Total	C	O	P	0	0
			40	29	10	1		
28	l	1	Total	C	O	P	0	0
			49	38	10	1		

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

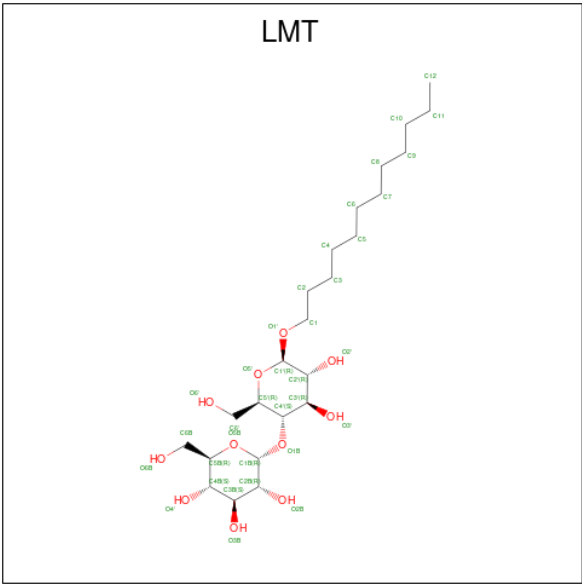
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	3	Total C 33 33	0	0
29	B	7	Total C 97 97	0	0
29	C	1	Total C 11 11	0	0
29	D	1	Total C 16 16	0	0
29	E	3	Total C 45 45	0	0
29	H	1	Total C 14 14	0	0
29	I	3	Total C 45 45	0	0
29	J	3	Total C 43 43	0	0
29	M	1	Total C 11 11	0	0
29	T	1	Total C 13 13	0	0
29	U	1	Total C 14 14	0	0
29	X	1	Total C 16 16	0	0
29	Z	2	Total C 23 23	0	0
29	a	2	Total C 16 16	0	0
29	b	7	Total C 102 102	0	0
29	c	1	Total C 10 10	0	0
29	d	2	Total C 27 27	0	0
29	e	1	Total C 16 16	0	0
29	i	4	Total C 64 64	0	0
29	j	1	Total C 16 16	0	0
29	k	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	m	1	Total	C	0	0
			11	11		
29	t	1	Total	C	0	0
			16	16		
29	u	2	Total	C	0	0
			27	27		
29	x	1	Total	C	0	0
			15	15		
29	z	1	Total	C	0	0
			13	13		

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



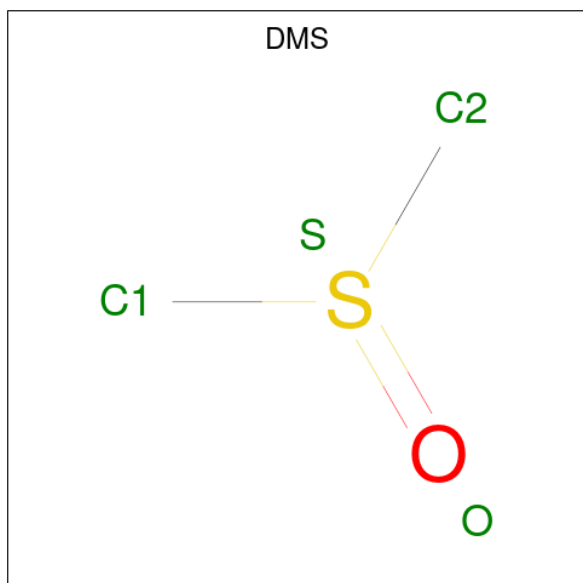
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			24	18	6		
30	B	1	Total	C	O	0	0
			24	18	6		
30	F	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	M	1	Total	C	O	0	0
			35	24	11		
30	T	1	Total	C	O	0	0
			24	18	6		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	e	1	Total	C	O	0	0
			25	19	6		
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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

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

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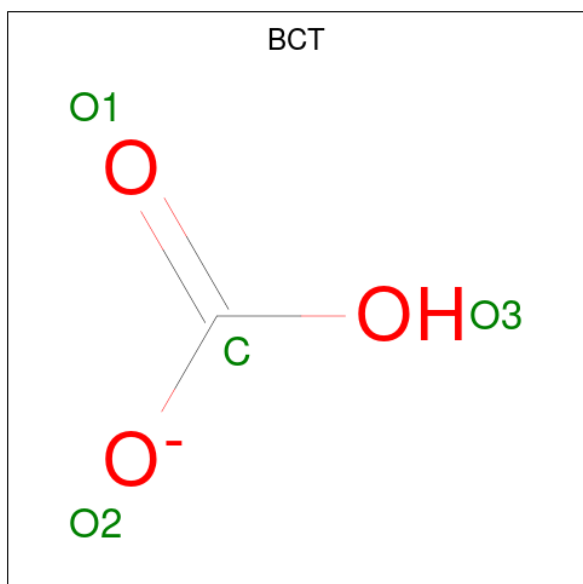
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	e	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	k	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

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

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

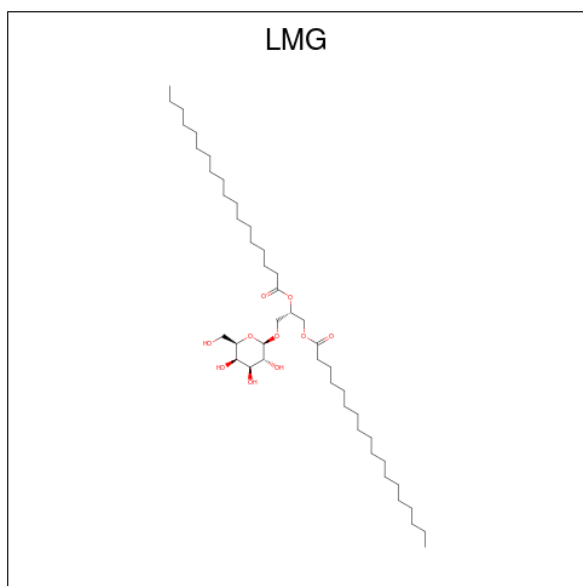
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		

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

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



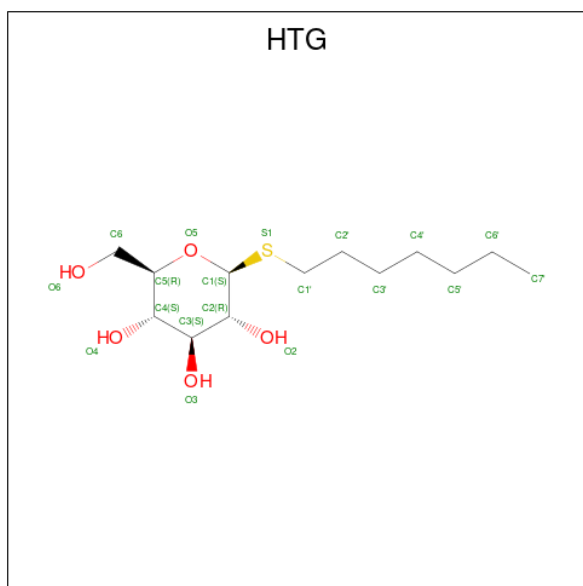
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		
34	a	1	Total	C	O	0	0
			51	41	10		

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



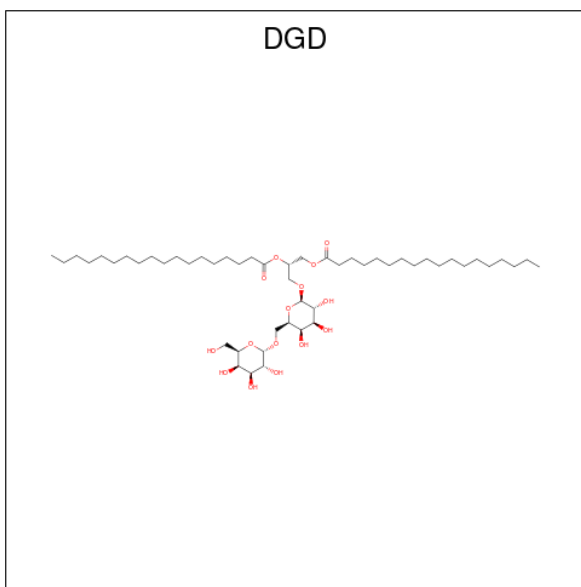
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		

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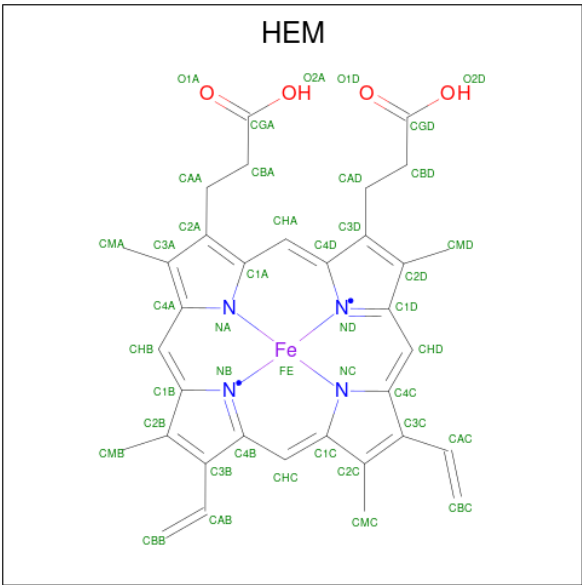
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			14	8	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			13	10	2	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	v	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



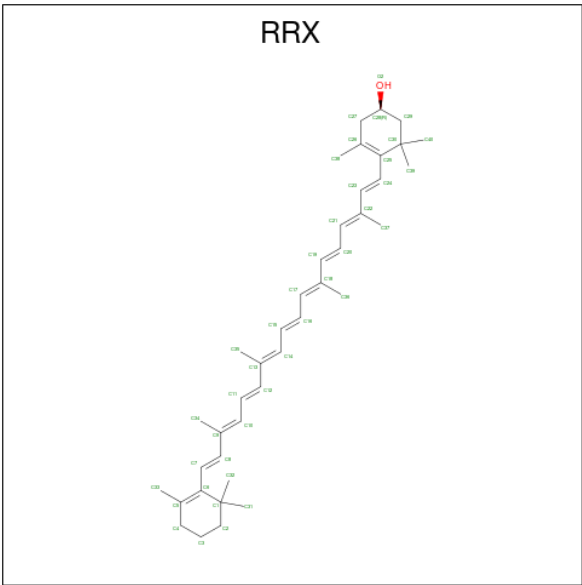
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			50	41	9		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
37	e	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).

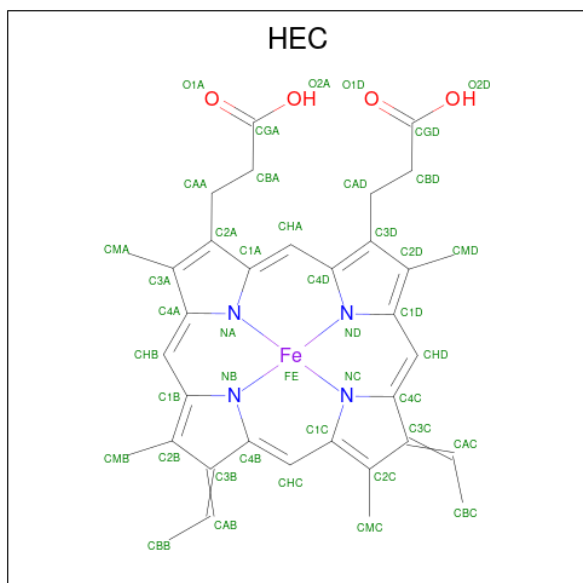


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	176	Total	O	0	11
			187	187		
41	B	420	Total	O	0	17
			437	437		
41	C	286	Total	O	0	8
			294	294		
41	D	159	Total	O	0	7
			166	166		
41	E	44	Total	O	0	3
			47	47		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	F	9	Total O 9 9	0	0
41	H	54	Total O 54 54	0	0
41	I	11	Total O 13 13	0	2
41	J	16	Total O 17 17	0	1
41	K	13	Total O 14 14	0	1
41	L	23	Total O 26 26	0	3
41	M	15	Total O 17 17	0	2
41	O	251	Total O 265 265	0	14
41	T	15	Total O 16 16	0	1
41	U	123	Total O 128 128	0	5
41	V	165	Total O 169 169	0	4
41	Y	8	Total O 8 8	0	0
41	X	14	Total O 14 14	0	0
41	Z	8	Total O 10 10	0	2
41	a	172	Total O 175 175	0	3
41	b	405	Total O 423 423	0	18
41	c	300	Total O 320 320	0	20
41	d	177	Total O 185 185	0	8
41	e	52	Total O 56 56	0	4
41	f	9	Total O 9 9	0	0
41	h	56	Total O 57 57	0	1

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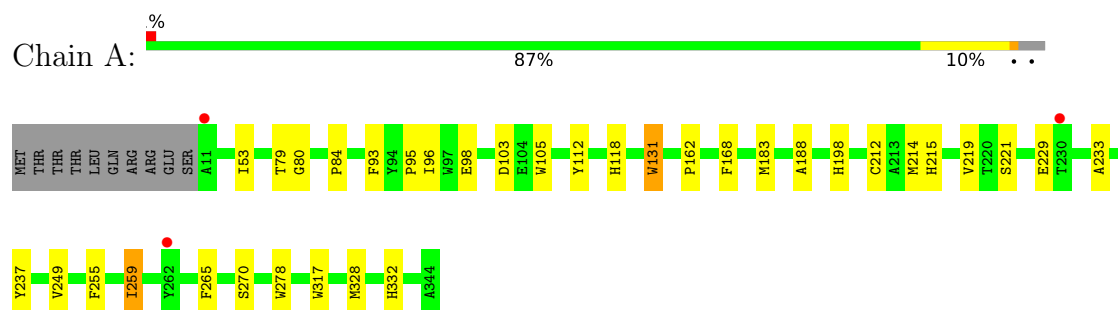
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	i	12	Total 13	O 13	0	1
41	j	13	Total 13	O 13	0	0
41	k	14	Total 14	O 14	0	0
41	l	16	Total 19	O 19	0	3
41	m	14	Total 15	O 15	0	1
41	o	223	Total 240	O 240	0	17
41	t	19	Total 21	O 21	0	2
41	u	146	Total 157	O 157	0	11
41	v	147	Total 154	O 154	0	7
41	y	16	Total 16	O 16	0	0
41	x	18	Total 19	O 19	0	1
41	z	5	Total 5	O 5	0	0

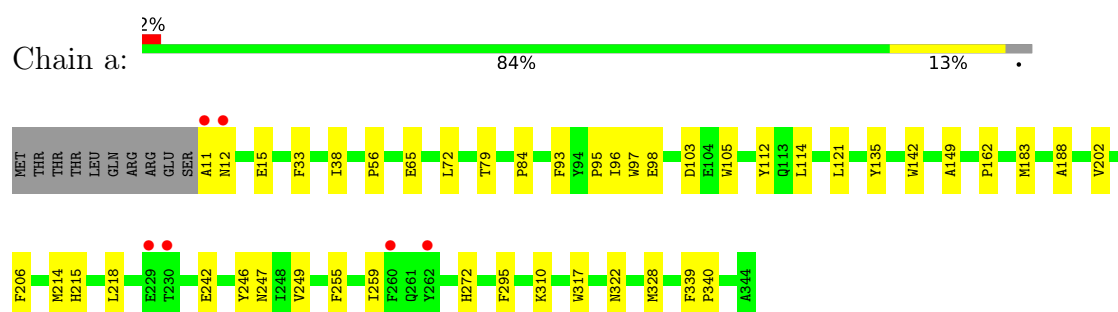
3 Residue-property plots [i](#)

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.

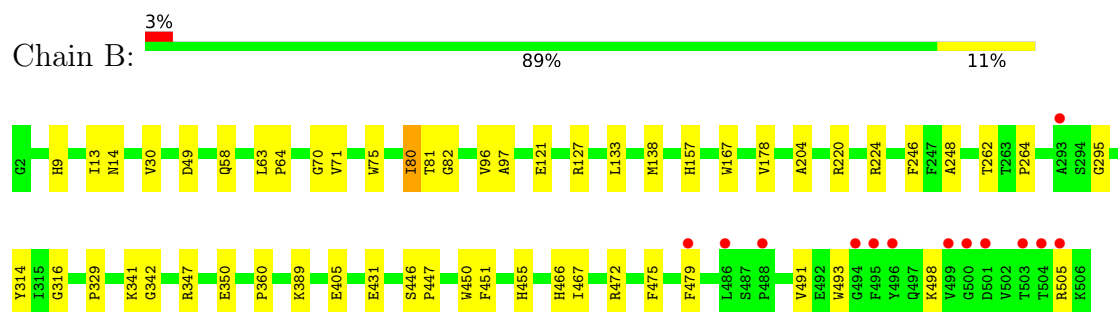
- Molecule 1: Photosystem II protein D1



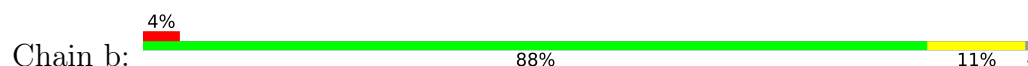
- Molecule 1: Photosystem II protein D1

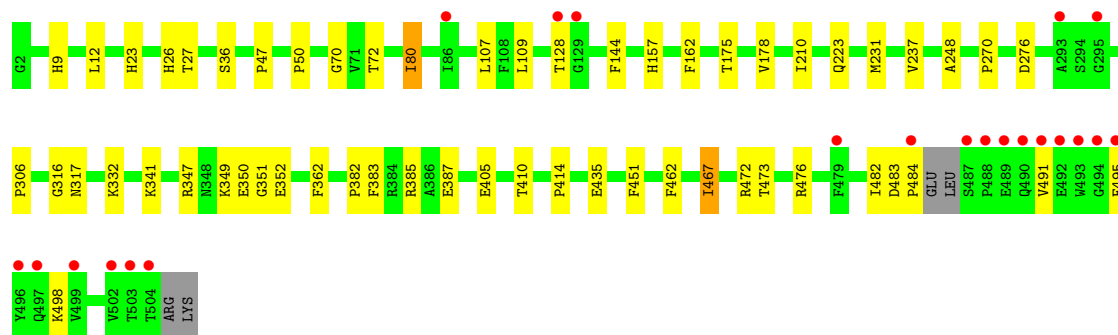


- Molecule 2: Photosystem II CP47 reaction center protein

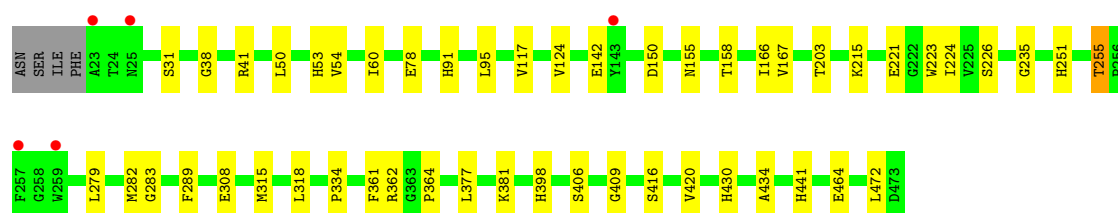
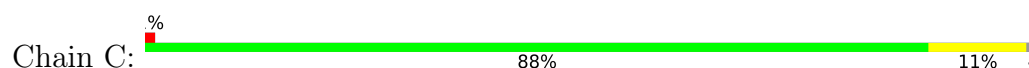


- Molecule 2: Photosystem II CP47 reaction center protein

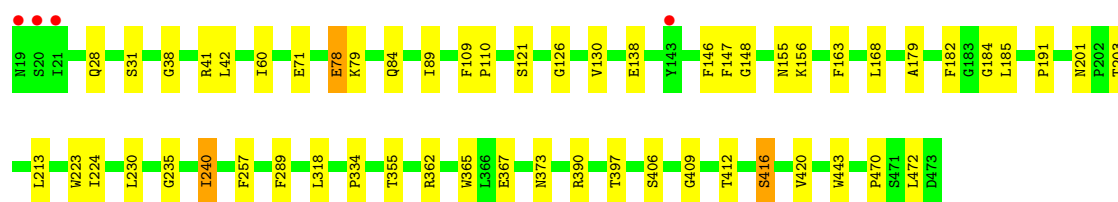
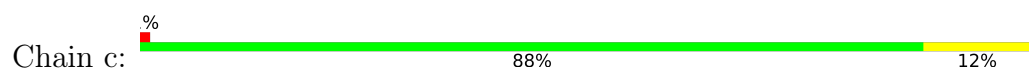




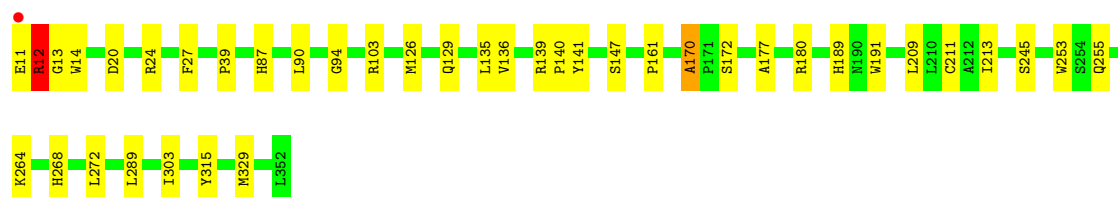
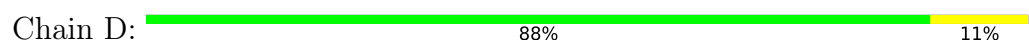
• Molecule 3: Photosystem II CP43 reaction center protein



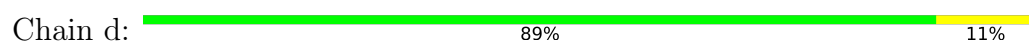
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein

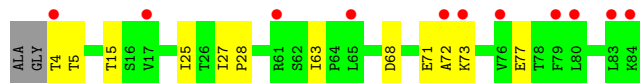
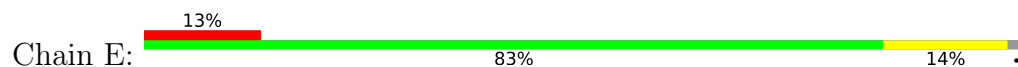


• Molecule 4: Photosystem II D2 protein

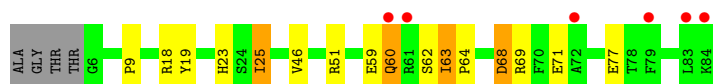
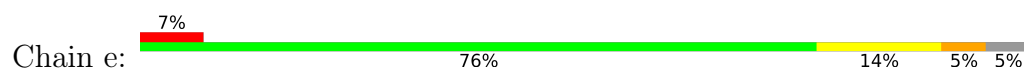




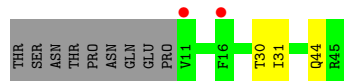
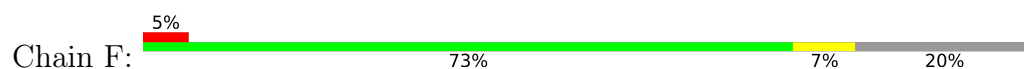
- Molecule 5: Cytochrome b559 subunit alpha



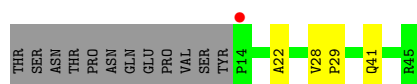
- Molecule 5: Cytochrome b559 subunit alpha



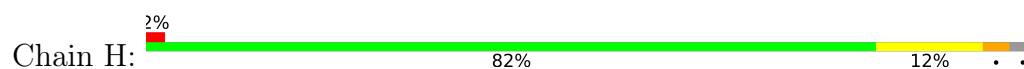
- Molecule 6: Cytochrome b559 subunit beta



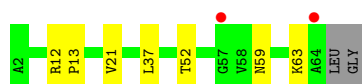
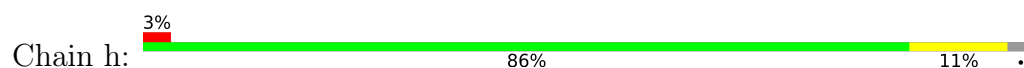
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

Chain I:  89% 8%



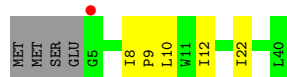
- Molecule 8: Photosystem II reaction center protein I

Chain i:  5% 87% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  2% 78% 12% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  5% 85% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  84% 16%

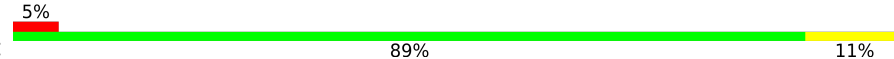


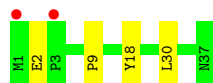
- Molecule 10: Photosystem II reaction center protein K

Chain k:  76% 24%

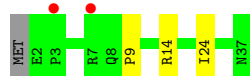
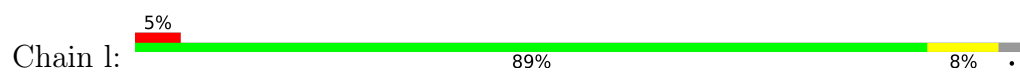


- Molecule 11: Photosystem II reaction center protein L

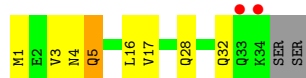
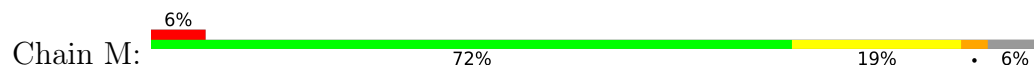
Chain L:  5% 89% 11%



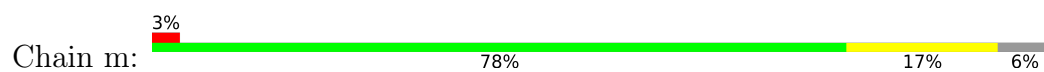
- Molecule 11: Photosystem II reaction center protein L



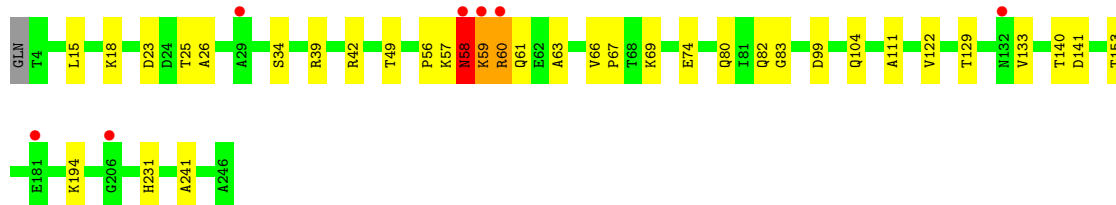
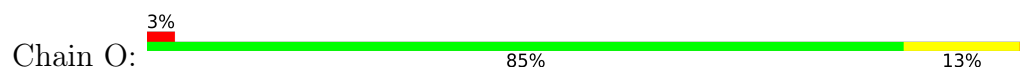
- Molecule 12: Photosystem II reaction center protein M



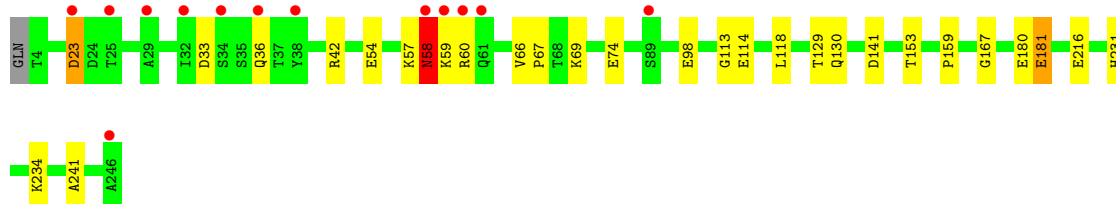
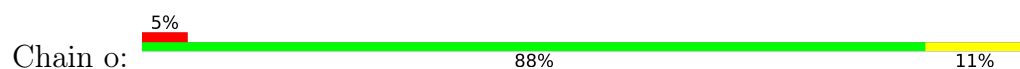
- Molecule 12: Photosystem II reaction center protein M



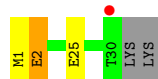
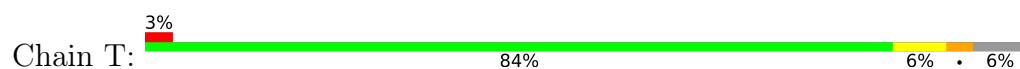
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



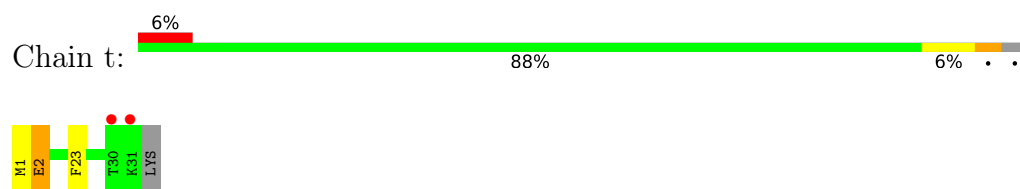
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



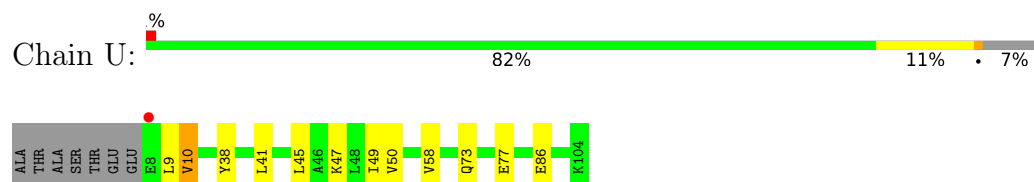
- Molecule 14: Photosystem II reaction center protein T



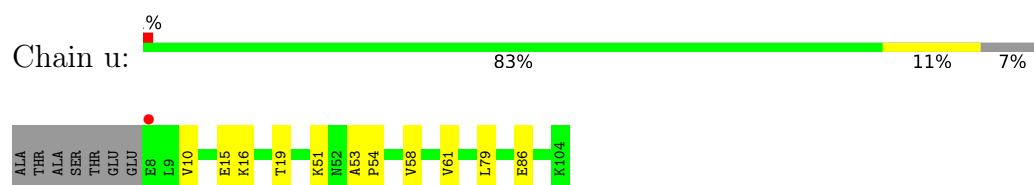
- Molecule 14: Photosystem II reaction center protein T



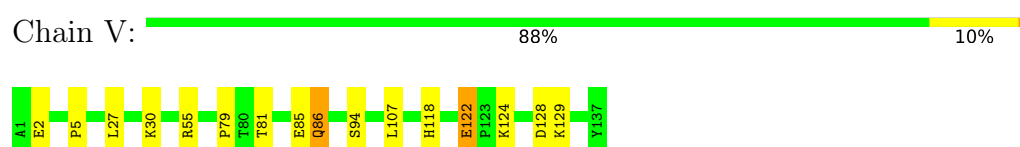
- Molecule 15: Photosystem II 12 kDa extrinsic protein



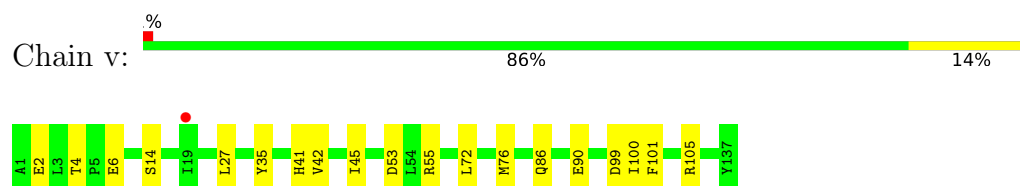
- Molecule 15: Photosystem II 12 kDa extrinsic protein



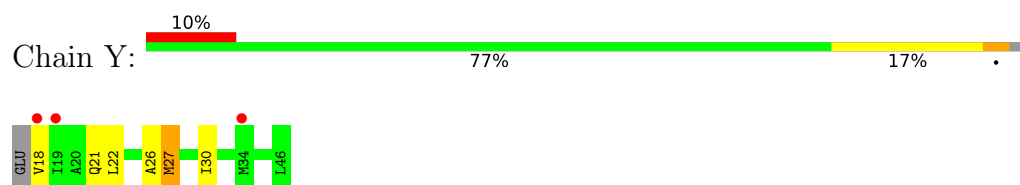
- Molecule 16: Cytochrome c-550



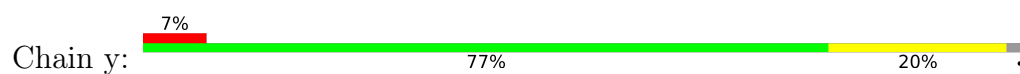
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12

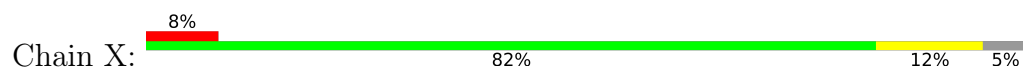


- Molecule 17: Photosystem II reaction center protein Ycf12

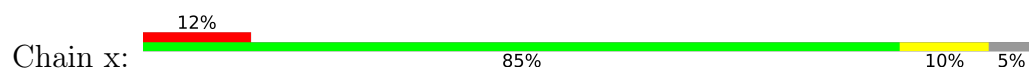




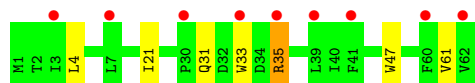
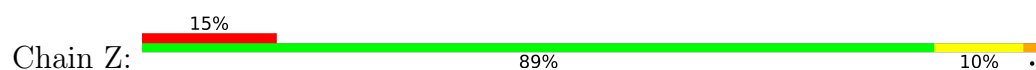
- Molecule 18: Photosystem II reaction center protein X



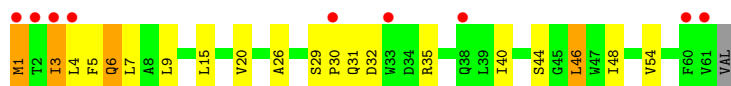
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.40Å 228.22Å 286.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.87 48.98 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.98-1.87) 99.8 (48.98-1.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.171 , 0.212 0.171 , 0.212	Depositor DCC
R_{free} test set	32518 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.2	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	55401	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: CA, DGD, FE2, LMT, HEM, MG, OEX, CL, LMG, HTG, UNL, PL9, DMS, PHO, FME, LHG, RRX, BCT, BCR, CLA, SQD, HEC

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	1.27	5/2710 (0.2%)	1.04	3/3696 (0.1%)
1	a	1.24	4/2730 (0.1%)	1.08	7/3723 (0.2%)
2	B	1.15	5/4144 (0.1%)	1.04	3/5647 (0.1%)
2	b	1.21	6/4076 (0.1%)	1.03	3/5558 (0.1%)
3	C	1.14	6/3633 (0.2%)	0.99	2/4945 (0.0%)
3	c	1.09	1/3638 (0.0%)	1.02	0/4953
4	D	1.25	5/2834 (0.2%)	1.05	5/3861 (0.1%)
4	d	1.24	6/2834 (0.2%)	1.00	0/3861
5	E	0.94	0/670	1.02	0/917
5	e	0.88	0/656	1.03	4/896 (0.4%)
6	F	0.96	0/289	0.92	0/394
6	f	0.97	0/262	0.99	0/356
7	H	0.97	0/530	0.98	0/722
7	h	1.03	0/522	0.95	1/711 (0.1%)
8	I	0.92	0/282	0.89	1/381 (0.3%)
8	i	0.91	0/300	0.92	0/406
9	J	0.91	0/257	0.98	0/349
9	j	0.95	0/291	0.99	2/393 (0.5%)
10	K	0.93	0/303	0.97	0/416
10	k	0.90	0/303	1.05	0/416
11	L	1.10	1/316 (0.3%)	1.00	0/430
11	l	1.12	0/307	1.00	0/418
12	M	1.06	0/270	1.08	2/369 (0.5%)
12	m	0.95	0/270	1.00	0/369
13	O	1.01	1/1898 (0.1%)	1.04	3/2577 (0.1%)
13	o	0.98	0/1886	1.05	4/2562 (0.2%)
14	T	0.97	0/255	1.02	2/346 (0.6%)
14	t	1.05	0/260	0.94	0/353
15	U	1.01	0/777	0.96	0/1055
15	u	1.02	0/790	0.97	0/1071
16	V	1.16	0/1096	1.05	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	1.03	0/1084	1.05	1/1475 (0.1%)
17	Y	0.80	0/211	1.06	0/282
17	y	0.71	0/208	1.08	1/278 (0.4%)
18	X	0.83	0/286	1.13	0/387
18	x	0.86	0/278	1.01	0/376
19	Z	0.76	0/479	1.00	0/656
19	z	0.71	0/468	0.97	0/640
All	All	1.12	40/42403 (0.1%)	1.02	45/57732 (0.1%)

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	TRP	N-CA	-7.33	1.41	1.46
4	D	87	HIS	ND1-CE1	7.15	1.39	1.32
4	D	87	HIS	CG-CD2	6.80	1.43	1.35
1	A	118	HIS	ND1-CE1	6.73	1.39	1.32
4	D	189	HIS	CG-CD2	6.50	1.43	1.35

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	142	TRP	N-CA-C	7.59	122.57	113.16
2	B	342	GLY	N-CA-C	-7.12	104.89	112.08
1	a	65	GLU	CA-C-N	-6.99	112.44	119.99
1	a	65	GLU	C-N-CA	-6.99	112.44	119.99
4	D	170	ALA	CA-C-N	-6.51	113.25	119.76

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	2622	0	2519	26	0
1	a	2633	0	2540	41	0
2	B	3992	0	3848	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3929	0	3774	69	0
3	C	3511	0	3440	37	0
3	c	3521	0	3439	50	0
4	D	2733	0	2647	33	0
4	d	2733	0	2647	38	0
5	E	651	0	626	9	0
5	e	637	0	617	12	0
6	F	280	0	284	2	0
6	f	255	0	263	3	0
7	H	511	0	535	12	0
7	h	506	0	531	4	0
8	I	285	0	305	0	0
8	i	303	0	313	6	0
9	J	251	0	257	3	0
9	j	285	0	293	3	0
10	K	293	0	305	4	0
10	k	293	0	305	6	0
11	L	306	0	320	4	0
11	l	297	0	311	3	0
12	M	264	0	283	6	0
12	m	264	0	283	7	0
13	O	1861	0	1825	30	0
13	o	1852	0	1812	20	0
14	T	256	0	256	1	0
14	t	261	0	258	2	0
15	U	766	0	758	11	0
15	u	776	0	775	9	0
16	V	1072	0	1086	19	0
16	v	1060	0	1053	20	0
17	Y	210	0	230	4	0
17	y	207	0	221	3	0
18	X	280	0	312	5	0
18	x	275	0	301	6	0
19	Z	468	0	492	11	0
19	z	457	0	471	10	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	195	0	216	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	1040	0	1152	25	0
23	C	845	0	936	24	0
23	D	195	0	216	5	0
23	a	195	0	216	8	0
23	b	1040	0	1152	34	0
23	c	845	0	936	27	0
23	d	195	0	216	9	0
24	A	64	0	74	1	0
24	D	64	0	74	2	0
24	a	128	0	148	4	0
25	A	40	0	56	3	0
25	B	120	0	168	8	0
25	C	120	0	168	7	0
25	D	40	0	56	5	0
25	T	40	0	56	6	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	11	0
25	c	80	0	112	6	0
25	d	40	0	56	2	0
25	j	40	0	56	4	0
25	k	40	0	56	1	0
25	t	40	0	56	7	0
26	A	108	0	155	11	0
26	B	54	0	78	4	0
26	D	45	0	57	2	0
26	L	54	0	78	4	0
26	a	108	0	156	5	0
26	x	41	0	49	2	0
27	A	55	0	80	12	0
27	D	55	0	80	0	0
27	a	55	0	80	14	0
27	d	55	0	80	0	0
28	A	49	0	74	1	0
28	D	144	0	213	7	0
28	E	49	0	74	3	0
28	K	44	0	67	0	0
28	L	49	0	74	1	0
28	a	49	0	74	1	0
28	d	188	0	274	6	0
28	e	40	0	53	5	0
28	l	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	33	0	0	1	0
29	B	97	0	0	1	0
29	C	11	0	0	0	0
29	D	16	0	0	0	0
29	E	45	0	0	0	0
29	H	14	0	0	0	0
29	I	45	0	0	0	0
29	J	43	0	0	1	0
29	M	11	0	0	3	0
29	T	13	0	0	0	0
29	U	14	0	0	3	0
29	X	16	0	0	0	0
29	Z	23	0	0	0	0
29	a	16	0	0	0	0
29	b	102	0	0	0	0
29	c	10	0	0	0	0
29	d	27	0	0	0	0
29	e	16	0	0	0	0
29	i	64	0	0	0	0
29	j	16	0	0	0	0
29	k	8	0	0	0	0
29	m	11	0	0	0	0
29	t	16	0	0	0	0
29	u	27	0	0	1	0
29	x	15	0	0	0	0
29	z	13	0	0	0	0
30	A	35	0	46	2	0
30	B	83	0	116	3	0
30	F	35	0	46	0	0
30	I	35	0	46	2	0
30	M	35	0	46	1	0
30	T	24	0	35	0	0
30	Z	35	0	46	6	0
30	a	70	0	92	8	0
30	b	25	0	35	4	0
30	e	25	0	35	1	0
30	m	70	0	92	3	0
30	z	32	0	33	1	0
31	A	24	0	36	8	0
31	B	48	0	72	25	0
31	C	28	0	42	6	0
31	D	12	0	18	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	F	4	0	6	5	0
31	H	8	0	12	7	0
31	O	36	0	54	16	0
31	U	12	0	18	5	0
31	V	36	0	54	16	0
31	a	16	0	24	12	0
31	b	60	0	90	34	0
31	c	48	0	72	17	0
31	d	20	0	30	7	0
31	e	4	0	6	1	0
31	h	16	0	24	3	0
31	i	8	0	12	3	0
31	k	4	0	6	0	0
31	l	4	0	6	5	0
31	o	12	0	18	4	0
31	u	16	0	24	5	0
31	v	32	0	48	14	0
32	A	4	0	0	0	0
32	a	4	0	0	1	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	4	0
34	D	51	0	72	5	0
34	J	51	0	72	3	0
34	a	51	0	72	8	0
34	c	102	0	144	4	0
34	d	51	0	72	5	0
34	j	51	0	72	0	0
34	m	51	0	72	3	0
35	B	95	0	130	4	0
35	C	57	0	78	1	0
35	D	19	0	26	3	0
35	O	19	0	26	2	0
35	V	14	0	13	0	0
35	b	76	0	104	5	0
35	c	51	0	70	2	0
35	d	19	0	26	0	0
35	v	19	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	C	186	0	246	2	0
36	D	50	0	69	4	0
36	H	62	0	82	0	0
36	c	186	0	246	3	0
36	d	50	0	69	6	0
36	h	62	0	82	0	0
37	E	43	0	30	1	0
37	e	43	0	30	1	0
38	H	41	0	56	0	0
38	x	41	0	56	4	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	187	0	0	7	0
41	B	437	0	0	10	0
41	C	294	0	0	6	0
41	D	166	0	0	4	0
41	E	47	0	0	0	0
41	F	9	0	0	0	0
41	H	54	0	0	1	0
41	I	13	0	0	0	0
41	J	17	0	0	3	0
41	K	14	0	0	0	0
41	L	26	0	0	1	0
41	M	17	0	0	1	0
41	O	265	0	0	12	0
41	T	16	0	0	0	0
41	U	128	0	0	2	0
41	V	169	0	0	7	0
41	X	14	0	0	0	0
41	Y	8	0	0	0	0
41	Z	10	0	0	2	0
41	a	175	0	0	5	0
41	b	423	0	0	15	0
41	c	320	0	0	2	0
41	d	185	0	0	0	0
41	e	56	0	0	1	0
41	f	9	0	0	0	0
41	h	57	0	0	1	0
41	i	13	0	0	0	0
41	j	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	k	14	0	0	1	0
41	l	19	0	0	2	0
41	m	15	0	0	2	0
41	o	240	0	0	7	0
41	t	21	0	0	0	0
41	u	157	0	0	7	0
41	v	154	0	0	5	0
41	x	19	0	0	0	0
41	y	16	0	0	0	0
41	z	5	0	0	0	0
All	All	55401	0	52590	803	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 8.

The worst 5 of 803 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)
31:O:311:DMS:H13	41:O:573:HOH:O	1.47	1.14
2:B:347[B]:ARG:NH2	41:B:1034[B]:HOH:O	1.80	1.13
1:A:214:MET:HG2	27:A:411:PL9:H102	1.20	1.12
2:b:347[A]:ARG:NH2	41:b:702[A]:HOH:O	1.81	1.10
1:a:97:TRP:HD1	31:a:420:DMS:H23	1.05	1.09

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	333/344 (97%)	325 (98%)	7 (2%)	1 (0%)	36	26
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	507/505 (100%)	497 (98%)	10 (2%)	0	100	100
2	b	500/505 (99%)	490 (98%)	10 (2%)	0	100	100
3	C	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	43	34
3	c	454/455 (100%)	441 (97%)	12 (3%)	1 (0%)	43	34
4	D	342/342 (100%)	333 (97%)	8 (2%)	1 (0%)	36	26
4	d	342/342 (100%)	333 (97%)	9 (3%)	0	100	100
5	E	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
5	e	77/83 (93%)	76 (99%)	1 (1%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	229 (94%)	11 (4%)	3 (1%)	10	2
13	o	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	1
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5210/5350 (97%)	5059 (97%)	140 (3%)	11 (0%)	43	34

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
19	Z	31	GLN
3	c	416	SER
19	z	31	GLN
3	C	416	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/279 (96%)	268 (100%)	1 (0%)	84	79
1	a	272/279 (98%)	271 (100%)	1 (0%)	84	79
2	B	403/403 (100%)	398 (99%)	5 (1%)	63	53
2	b	394/403 (98%)	390 (99%)	4 (1%)	68	60
3	C	355/356 (100%)	353 (99%)	2 (1%)	78	72
3	c	356/356 (100%)	351 (99%)	5 (1%)	59	48
4	D	278/277 (100%)	275 (99%)	3 (1%)	65	56
4	d	278/277 (100%)	277 (100%)	1 (0%)	84	79
5	E	70/72 (97%)	68 (97%)	2 (3%)	37	20
5	e	68/72 (94%)	64 (94%)	4 (6%)	18	5
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	53 (96%)	2 (4%)	31	14
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	31/34 (91%)	31 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	26	10
9	j	27/28 (96%)	27 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	3
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	16
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	33	16
12	m	30/33 (91%)	29 (97%)	1 (3%)	33	16
13	O	205/207 (99%)	202 (98%)	3 (2%)	57	46
13	o	203/207 (98%)	198 (98%)	5 (2%)	42	26
14	T	25/28 (89%)	24 (96%)	1 (4%)	28	11
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	11
15	U	82/89 (92%)	80 (98%)	2 (2%)	43	27
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	115 (98%)	3 (2%)	42	26
16	v	115/117 (98%)	114 (99%)	1 (1%)	70	63
17	Y	20/23 (87%)	19 (95%)	1 (5%)	22	7
17	y	19/23 (83%)	17 (90%)	2 (10%)	6	1
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	49/52 (94%)	46 (94%)	3 (6%)	17	4
19	z	46/52 (88%)	38 (83%)	8 (17%)	2	0
All	All	4255/4376 (97%)	4188 (98%)	67 (2%)	55	43

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	y	23	THR

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Mol	Chain	Res	Type
19	z	1	MET
19	z	29	SER
15	U	10	VAL
14	T	2	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
6	f	44	GLN
16	v	34	GLN
7	h	59	ASN
13	o	155	ASN
13	O	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.72	0	8,9,11	0.99	0
14	FME	t	1	14	8,9,10	0.56	0	8,9,11	1.57	2 (25%)
8	FME	i	1	8	8,9,10	0.63	0	8,9,11	1.45	3 (37%)
14	FME	T	1	14	8,9,10	0.57	0	8,9,11	1.84	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	2/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	-3.29	104.52	110.52
14	T	1	FME	O-C-CA	-2.53	118.27	124.77
14	t	1	FME	O-C-CA	-2.40	118.60	124.77
8	i	1	FME	O1-CN-N	-2.31	119.36	125.32
14	t	1	FME	C-CA-N	2.22	113.77	109.50

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
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	C-CA-CB-CG
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 366 ligands modelled in this entry, 13 are monoatomic and 53 are unknown - leaving 300 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
23	CLA	D	403	-	69,73,73	2.09	16 (23%)	82,113,113	2.41	30 (36%)
23	CLA	b	610	-	69,73,73	2.51	19 (27%)	82,113,113	2.01	27 (32%)
31	DMS	v	209	-	3,3,3	2.77	1 (33%)	3,3,3	0.74	0
23	CLA	b	604	-	69,73,73	2.29	20 (28%)	82,113,113	2.27	31 (37%)
23	CLA	C	504	-	69,73,73	2.42	25 (36%)	82,113,113	2.10	24 (29%)
23	CLA	b	613	-	69,73,73	2.07	18 (26%)	82,113,113	2.22	26 (31%)
25	BCR	A	409	-	41,41,41	1.08	4 (9%)	56,56,56	1.46	9 (16%)
23	CLA	B	602	41	69,73,73	2.37	17 (24%)	82,113,113	2.53	30 (36%)
31	DMS	U	202	-	3,3,3	2.75	1 (33%)	3,3,3	1.63	1 (33%)
31	DMS	c	934	-	3,3,3	2.76	1 (33%)	3,3,3	0.75	0
23	CLA	C	502	-	69,73,73	2.27	19 (27%)	82,113,113	2.15	24 (29%)
31	DMS	B	646	-	3,3,3	2.66	1 (33%)	3,3,3	0.72	0
37	HEM	e	105	6,5	50,50,50	2.07	12 (24%)	67,82,82	1.35	8 (11%)
36	DGD	c	919	-	63,63,67	0.95	3 (4%)	77,77,81	1.22	10 (12%)
23	CLA	b	605	-	69,73,73	2.07	19 (27%)	82,113,113	2.23	26 (31%)
31	DMS	b	635	-	3,3,3	2.78	1 (33%)	3,3,3	0.61	0
31	DMS	h	104	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
31	DMS	A	418	-	3,3,3	2.80	1 (33%)	3,3,3	0.67	0
23	CLA	C	506	-	69,73,73	2.28	21 (30%)	82,113,113	2.11	25 (30%)
23	CLA	B	614	-	69,73,73	1.79	15 (21%)	82,113,113	2.28	28 (34%)
31	DMS	C	533	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
31	DMS	U	203	-	3,3,3	2.77	1 (33%)	3,3,3	0.53	0
31	DMS	b	647	-	3,3,3	2.81	1 (33%)	3,3,3	0.73	0
23	CLA	d	404	-	69,73,73	1.95	21 (30%)	82,113,113	2.48	32 (39%)
31	DMS	C	524	-	3,3,3	2.45	1 (33%)	3,3,3	0.95	0
24	PHO	D	402	-	58,69,69	2.57	12 (20%)	55,99,99	3.03	16 (29%)
35	HTG	c	923	-	11,12,19	0.55	0	10,11,24	1.89	1 (10%)
30	LMT	Z	101	-	36,36,36	0.70	1 (2%)	47,47,47	0.92	2 (4%)
31	DMS	D	417	-	3,3,3	3.06	1 (33%)	3,3,3	0.79	0
31	DMS	V	206	-	3,3,3	2.72	1 (33%)	3,3,3	0.79	0
35	HTG	b	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.61	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	B	625	-	19,19,19	1.37	3 (15%)	23,24,24	2.01	8 (34%)
35	HTG	B	626	-	19,19,19	0.88	1 (5%)	23,24,24	1.41	1 (4%)
25	BCR	d	405	-	41,41,41	0.98	2 (4%)	56,56,56	1.96	19 (33%)
34	LMG	a	413	-	51,51,55	1.00	2 (3%)	59,59,63	1.11	4 (6%)
31	DMS	B	640	-	3,3,3	2.69	1 (33%)	3,3,3	0.79	0
36	DGD	C	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.13	8 (10%)
31	DMS	C	527	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
23	CLA	B	615	-	69,73,73	2.20	19 (27%)	82,113,113	2.58	31 (37%)
36	DGD	D	407	-	50,50,67	1.28	3 (6%)	58,58,81	1.75	8 (13%)
31	DMS	V	205	-	3,3,3	2.69	1 (33%)	3,3,3	0.98	0
23	CLA	c	906	-	69,73,73	2.20	23 (33%)	82,113,113	2.08	29 (35%)
23	CLA	b	612	-	69,73,73	2.09	15 (21%)	82,113,113	2.30	28 (34%)
31	DMS	h	101	-	3,3,3	2.75	1 (33%)	3,3,3	1.37	1 (33%)
23	CLA	B	609	-	69,73,73	2.04	20 (28%)	82,113,113	2.10	27 (32%)
31	DMS	k	103	-	3,3,3	2.72	1 (33%)	3,3,3	0.79	0
23	CLA	B	612	-	69,73,73	2.05	17 (24%)	82,113,113	2.22	27 (32%)
23	CLA	a	407	41	69,73,73	1.89	19 (27%)	82,113,113	2.24	25 (30%)
25	BCR	B	620	-	41,41,41	1.02	2 (4%)	56,56,56	1.60	12 (21%)
31	DMS	c	927	-	3,3,3	2.77	1 (33%)	3,3,3	1.30	1 (33%)
34	LMG	D	412	-	51,51,55	1.10	2 (3%)	59,59,63	1.34	8 (13%)
27	PL9	A	411	-	55,55,55	0.88	4 (7%)	68,69,69	1.68	15 (22%)
31	DMS	C	528	-	3,3,3	2.71	1 (33%)	3,3,3	0.73	0
25	BCR	C	530	-	41,41,41	0.83	0	56,56,56	1.57	9 (16%)
31	DMS	O	306	-	3,3,3	2.76	1 (33%)	3,3,3	0.56	0
31	DMS	u	203	-	3,3,3	2.64	1 (33%)	3,3,3	0.94	0
31	DMS	v	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.33	0
35	HTG	b	628	-	19,19,19	0.84	1 (5%)	23,24,24	1.34	1 (4%)
26	SQD	B	621	-	52,54,54	1.01	3 (5%)	62,65,65	1.53	7 (11%)
23	CLA	C	513	-	69,73,73	2.58	20 (28%)	82,113,113	2.15	25 (30%)
23	CLA	B	604	-	69,73,73	1.94	19 (27%)	82,113,113	2.48	32 (39%)
25	BCR	c	915	-	41,41,41	0.80	0	56,56,56	1.34	8 (14%)
26	SQD	A	410	-	52,54,54	0.95	2 (3%)	62,65,65	1.97	15 (24%)
40	HEC	v	203	16	46,50,50	2.09	9 (19%)	58,82,82	1.51	10 (17%)
31	DMS	b	643	-	3,3,3	2.74	1 (33%)	3,3,3	0.62	0
28	LHG	a	415	-	48,48,48	1.01	2 (4%)	51,54,54	1.08	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	610	-	69,73,73	2.19	18 (26%)	82,113,113	2.14	26 (31%)
25	BCR	b	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	6 (10%)
28	LHG	d	402	-	43,43,48	1.07	2 (4%)	46,49,54	0.98	3 (6%)
31	DMS	v	210	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
34	LMG	d	411	-	51,51,55	1.13	3 (5%)	59,59,63	1.33	6 (10%)
23	CLA	c	905	41	69,73,73	2.24	20 (28%)	82,113,113	2.62	29 (35%)
23	CLA	D	401	41	69,73,73	2.07	20 (28%)	82,113,113	2.03	20 (24%)
31	DMS	H	101	-	3,3,3	2.85	1 (33%)	3,3,3	0.59	0
31	DMS	V	201	-	3,3,3	2.63	1 (33%)	3,3,3	0.78	0
25	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.21	9 (16%)
23	CLA	c	904	-	69,73,73	2.70	20 (28%)	82,113,113	2.23	26 (31%)
31	DMS	b	636	-	3,3,3	2.81	1 (33%)	3,3,3	0.54	0
31	DMS	c	925	-	3,3,3	2.88	1 (33%)	3,3,3	0.86	0
35	HTG	B	624	-	19,19,19	1.43	3 (15%)	23,24,24	1.47	3 (13%)
30	LMT	A	416	-	36,36,36	0.84	1 (2%)	47,47,47	1.20	5 (10%)
31	DMS	C	529	-	3,3,3	2.61	1 (33%)	3,3,3	0.45	0
34	LMG	C	520	-	51,51,55	1.15	2 (3%)	59,59,63	1.36	9 (15%)
28	LHG	K	101	-	43,43,48	1.07	2 (4%)	46,48,54	1.11	4 (8%)
31	DMS	O	305	-	3,3,3	2.72	1 (33%)	3,3,3	0.90	0
31	DMS	O	303	-	3,3,3	2.75	1 (33%)	3,3,3	0.58	0
31	DMS	c	937	-	3,3,3	2.72	1 (33%)	3,3,3	0.63	0
31	DMS	l	102	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
31	DMS	v	208	-	3,3,3	2.79	1 (33%)	3,3,3	0.75	0
30	LMT	I	101	-	36,36,36	0.74	1 (2%)	47,47,47	1.44	5 (10%)
31	DMS	A	424	-	3,3,3	2.82	1 (33%)	3,3,3	1.10	0
31	DMS	B	637	-	3,3,3	2.32	1 (33%)	3,3,3	0.98	0
31	DMS	d	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.73	0
34	LMG	B	622	-	51,51,55	1.00	3 (5%)	59,59,63	1.31	9 (15%)
23	CLA	B	608	41	69,73,73	2.04	16 (23%)	82,113,113	2.19	30 (36%)
23	CLA	C	508	41	69,73,73	2.37	20 (28%)	82,113,113	2.37	30 (36%)
26	SQD	x	101	-	39,41,54	1.22	2 (5%)	49,52,65	1.40	9 (18%)
27	PL9	d	406	-	55,55,55	1.07	3 (5%)	68,69,69	1.58	11 (16%)
28	LHG	D	411	-	45,45,48	1.00	2 (4%)	48,51,54	1.05	4 (8%)
30	LMT	b	621	-	25,25,36	0.63	1 (4%)	30,30,47	1.32	4 (13%)
31	DMS	A	421	-	3,3,3	2.77	1 (33%)	3,3,3	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	B	648	-	3,3,3	2.55	1 (33%)	3,3,3	1.07	0
28	LHG	d	409	-	48,48,48	0.81	2 (4%)	51,54,54	1.29	8 (15%)
35	HTG	D	414	-	19,19,19	0.88	1 (5%)	23,24,24	1.15	1 (4%)
36	DGD	c	917	-	63,63,67	0.85	3 (4%)	77,77,81	1.22	8 (10%)
27	PL9	D	406	-	55,55,55	1.05	3 (5%)	68,69,69	1.43	11 (16%)
30	LMT	B	623	-	36,36,36	0.58	0	47,47,47	1.06	3 (6%)
31	DMS	o	303	-	3,3,3	2.74	1 (33%)	3,3,3	1.01	0
31	DMS	A	419	-	3,3,3	2.81	1 (33%)	3,3,3	0.73	0
25	BCR	C	515	-	41,41,41	0.86	0	56,56,56	1.53	11 (19%)
31	DMS	C	525	-	3,3,3	2.69	1 (33%)	3,3,3	0.92	0
28	LHG	D	409	-	48,48,48	0.86	1 (2%)	51,54,54	1.30	6 (11%)
31	DMS	b	640	-	3,3,3	2.76	1 (33%)	3,3,3	0.84	0
26	SQD	a	417	-	52,54,54	1.05	4 (7%)	62,65,65	1.34	4 (6%)
28	LHG	d	410	-	45,45,48	1.01	2 (4%)	48,51,54	1.04	3 (6%)
30	LMT	F	101	-	36,36,36	0.71	1 (2%)	47,47,47	1.20	5 (10%)
31	DMS	U	204	-	3,3,3	2.95	1 (33%)	3,3,3	0.82	0
31	DMS	b	638	-	3,3,3	3.00	1 (33%)	3,3,3	1.11	0
23	CLA	c	902	-	69,73,73	2.12	18 (26%)	82,113,113	2.63	27 (32%)
36	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.23	10 (12%)
31	DMS	V	209	-	3,3,3	2.58	1 (33%)	3,3,3	0.81	0
23	CLA	A	405	-	69,73,73	1.92	16 (23%)	82,113,113	2.20	30 (36%)
30	LMT	B	643	-	24,24,36	0.39	0	29,29,47	0.87	1 (3%)
31	DMS	V	211	-	3,3,3	3.04	1 (33%)	3,3,3	1.07	0
31	DMS	b	646	-	3,3,3	2.80	1 (33%)	3,3,3	0.71	0
23	CLA	c	910	-	69,73,73	2.46	19 (27%)	82,113,113	2.62	31 (37%)
28	LHG	D	410	-	48,48,48	0.83	2 (4%)	51,54,54	1.16	2 (3%)
25	BCR	c	916	-	41,41,41	0.82	1 (2%)	56,56,56	1.58	9 (16%)
23	CLA	C	509	-	69,73,73	2.25	18 (26%)	82,113,113	2.35	25 (30%)
23	CLA	c	909	-	69,73,73	2.26	19 (27%)	82,113,113	2.13	21 (25%)
36	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.19	9 (11%)
31	DMS	O	308	-	3,3,3	2.79	1 (33%)	3,3,3	0.71	0
31	DMS	A	423	-	3,3,3	1.95	1 (33%)	3,3,3	0.64	0
31	DMS	d	414	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
25	BCR	T	101	-	41,41,41	0.91	0	56,56,56	1.83	18 (32%)
24	PHO	a	408	-	58,69,69	2.26	13 (22%)	55,99,99	2.63	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	V	207	-	3,3,3	2.91	1 (33%)	3,3,3	1.28	0
28	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.26	3 (5%)
23	CLA	B	603	-	69,73,73	2.21	22 (31%)	82,113,113	2.17	30 (36%)
26	SQD	L	102	-	52,54,54	1.04	2 (3%)	62,65,65	1.64	12 (19%)
27	PL9	a	414	-	55,55,55	0.91	3 (5%)	68,69,69	1.67	19 (27%)
30	LMT	z	101	-	32,32,36	0.63	1 (3%)	42,42,47	1.21	5 (11%)
31	DMS	d	415	-	3,3,3	2.72	1 (33%)	3,3,3	0.90	0
36	DGD	d	407	-	50,50,67	1.11	2 (4%)	58,58,81	1.25	6 (10%)
23	CLA	c	903	-	69,73,73	2.04	17 (24%)	82,113,113	2.38	35 (42%)
31	DMS	v	205	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
28	LHG	E	101	-	48,48,48	1.06	2 (4%)	51,54,54	1.19	5 (9%)
23	CLA	c	907	-	69,73,73	2.51	20 (28%)	82,113,113	2.22	31 (37%)
31	DMS	D	415	-	3,3,3	2.81	1 (33%)	3,3,3	0.70	0
25	BCR	a	411	-	41,41,41	1.22	4 (9%)	56,56,56	1.36	5 (8%)
26	SQD	D	408	-	43,45,54	1.19	3 (6%)	53,56,65	2.20	13 (24%)
31	DMS	b	637	-	3,3,3	2.74	1 (33%)	3,3,3	1.04	0
31	DMS	b	639	-	3,3,3	2.83	1 (33%)	3,3,3	1.34	1 (33%)
23	CLA	b	614	-	69,73,73	1.96	17 (24%)	82,113,113	2.24	26 (31%)
31	DMS	v	207	-	3,3,3	2.78	1 (33%)	3,3,3	0.77	0
31	DMS	H	105	-	3,3,3	2.81	1 (33%)	3,3,3	0.67	0
35	HTG	C	521	-	19,19,19	0.88	2 (10%)	23,24,24	1.48	1 (4%)
31	DMS	e	104	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
34	LMG	c	920	-	51,51,55	0.96	2 (3%)	59,59,63	1.32	7 (11%)
34	LMG	c	930	-	51,51,55	1.07	3 (5%)	59,59,63	1.28	5 (8%)
23	CLA	a	406	-	69,73,73	1.88	17 (24%)	82,113,113	2.26	29 (35%)
31	DMS	a	421	-	3,3,3	2.74	1 (33%)	3,3,3	0.65	0
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.21	8 (10%)
35	HTG	b	622	-	19,19,19	1.26	3 (15%)	23,24,24	1.50	4 (17%)
36	DGD	C	518	-	63,63,67	0.96	4 (6%)	77,77,81	1.09	3 (3%)
23	CLA	C	510	-	69,73,73	2.26	17 (24%)	82,113,113	2.40	28 (34%)
23	CLA	b	615	-	69,73,73	2.10	18 (26%)	82,113,113	2.37	28 (34%)
25	BCR	t	101	-	41,41,41	1.04	0	56,56,56	1.54	14 (25%)
23	CLA	b	607	-	69,73,73	2.31	18 (26%)	82,113,113	2.24	29 (35%)
28	LHG	L	101	-	48,48,48	0.98	3 (6%)	51,54,54	1.15	3 (5%)
30	LMT	m	104	-	36,36,36	0.55	0	47,47,47	1.25	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	a	422	-	36,36,36	0.66	1 (2%)	47,47,47	0.96	3 (6%)
31	DMS	F	102	-	3,3,3	2.67	1 (33%)	3,3,3	0.26	0
31	DMS	i	105	-	3,3,3	2.75	1 (33%)	3,3,3	0.89	0
31	DMS	o	301	-	3,3,3	2.19	1 (33%)	3,3,3	0.40	0
34	LMG	J	101	39	51,51,55	0.93	2 (3%)	59,59,63	0.98	4 (6%)
31	DMS	v	201	-	3,3,3	2.48	1 (33%)	3,3,3	0.48	0
35	HTG	B	630	-	19,19,19	0.90	1 (5%)	23,24,24	1.19	2 (8%)
35	HTG	V	204	-	14,14,19	0.63	0	18,19,24	2.98	6 (33%)
23	CLA	C	507	-	69,73,73	2.14	21 (30%)	82,113,113	2.25	25 (30%)
23	CLA	b	609	-	69,73,73	2.22	18 (26%)	82,113,113	2.12	31 (37%)
32	BCT	a	424	21	3,3,3	1.65	1 (33%)	2,3,3	1.04	0
31	DMS	O	304	-	3,3,3	2.86	1 (33%)	3,3,3	0.89	0
30	LMT	e	103	-	25,25,36	0.72	1 (4%)	30,30,47	1.04	4 (13%)
34	LMG	C	531	-	51,51,55	1.03	2 (3%)	59,59,63	1.09	5 (8%)
35	HTG	B	631	-	19,19,19	1.02	1 (5%)	23,24,24	1.18	2 (8%)
23	CLA	B	617	-	69,73,73	2.00	20 (28%)	82,113,113	2.28	32 (39%)
23	CLA	c	913	-	69,73,73	2.45	20 (28%)	82,113,113	2.44	27 (32%)
31	DMS	d	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
31	DMS	B	647	-	3,3,3	2.79	1 (33%)	3,3,3	0.57	0
31	DMS	i	106	-	3,3,3	2.80	1 (33%)	3,3,3	0.68	0
25	BCR	Y	101	-	41,41,41	0.85	0	56,56,56	1.70	15 (26%)
31	DMS	b	634	-	3,3,3	2.51	1 (33%)	3,3,3	0.98	0
25	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.50	9 (16%)
31	DMS	O	307	-	3,3,3	2.81	1 (33%)	3,3,3	0.73	0
31	DMS	a	423	-	3,3,3	2.87	1 (33%)	3,3,3	0.85	0
31	DMS	b	633	-	3,3,3	1.87	1 (33%)	3,3,3	0.61	0
35	HTG	b	627	-	19,19,19	1.11	2 (10%)	23,24,24	1.37	2 (8%)
23	CLA	B	605	-	69,73,73	2.12	22 (31%)	82,113,113	2.06	27 (32%)
31	DMS	a	420	-	3,3,3	2.71	1 (33%)	3,3,3	0.38	0
31	DMS	b	644	-	3,3,3	2.85	1 (33%)	3,3,3	1.01	0
31	DMS	c	924	-	3,3,3	2.42	1 (33%)	3,3,3	0.42	0
28	LHG	A	412	-	48,48,48	1.06	2 (4%)	51,54,54	0.98	3 (5%)
30	LMT	B	644	-	24,24,36	0.34	0	29,29,47	1.26	4 (13%)
23	CLA	b	617	-	69,73,73	2.25	22 (31%)	82,113,113	2.08	28 (34%)
31	DMS	u	204	-	3,3,3	2.83	1 (33%)	3,3,3	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.16	4 (6%)
31	DMS	o	304	-	3,3,3	2.82	1 (33%)	3,3,3	0.83	0
31	DMS	v	206	-	3,3,3	2.66	1 (33%)	3,3,3	0.83	0
31	DMS	c	929	-	3,3,3	2.90	1 (33%)	3,3,3	0.71	0
23	CLA	c	908	41	69,73,73	2.16	17 (24%)	82,113,113	2.25	27 (32%)
25	BCR	C	516	-	41,41,41	1.01	0	56,56,56	1.38	8 (14%)
23	CLA	B	616	-	69,73,73	2.25	20 (28%)	82,113,113	2.30	27 (32%)
31	DMS	B	639	-	3,3,3	2.83	1 (33%)	3,3,3	0.91	0
20	OEX	A	401	41,3,1	0,15,15	-	-	-	-	-
28	LHG	e	101	-	39,39,48	1.16	2 (5%)	42,45,54	1.03	3 (7%)
31	DMS	O	311	-	3,3,3	2.71	1 (33%)	3,3,3	0.86	0
31	DMS	V	202	-	3,3,3	2.72	1 (33%)	3,3,3	0.83	0
31	DMS	a	401	-	3,3,3	2.77	1 (33%)	3,3,3	0.72	0
31	DMS	c	936	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
31	DMS	h	105	-	3,3,3	2.81	1 (33%)	3,3,3	0.70	0
35	HTG	C	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.83	3 (13%)
35	HTG	C	523	-	19,19,19	1.01	2 (10%)	23,24,24	1.52	1 (4%)
35	HTG	c	922	-	19,19,19	0.94	2 (10%)	23,24,24	1.58	4 (17%)
31	DMS	C	526	-	3,3,3	2.80	1 (33%)	3,3,3	0.60	0
31	DMS	B	642	-	3,3,3	2.99	1 (33%)	3,3,3	1.31	0
25	BCR	b	620	-	41,41,41	0.91	2 (4%)	56,56,56	1.25	5 (8%)
31	DMS	B	638	-	3,3,3	2.84	1 (33%)	3,3,3	1.04	0
31	DMS	b	641	-	3,3,3	2.71	1 (33%)	3,3,3	0.77	0
23	CLA	B	611	41	69,73,73	2.30	22 (31%)	82,113,113	2.32	28 (34%)
31	DMS	V	210	-	3,3,3	2.77	1 (33%)	3,3,3	0.54	0
23	CLA	d	403	-	69,73,73	1.90	17 (24%)	82,113,113	2.07	28 (34%)
31	DMS	d	418	-	3,3,3	2.81	1 (33%)	3,3,3	0.64	0
35	HTG	c	921	-	19,19,19	0.88	2 (10%)	23,24,24	1.33	2 (8%)
35	HTG	d	413	-	19,19,19	1.11	2 (10%)	23,24,24	1.90	4 (17%)
25	BCR	D	405	-	41,41,41	1.09	4 (9%)	56,56,56	2.03	13 (23%)
23	CLA	C	512	3	69,73,73	2.42	21 (30%)	82,113,113	2.40	27 (32%)
36	DGD	H	103	-	63,63,67	1.07	3 (4%)	77,77,81	1.33	8 (10%)
31	DMS	O	310	-	3,3,3	2.68	1 (33%)	3,3,3	0.73	0
23	CLA	b	608	41	69,73,73	2.14	22 (31%)	82,113,113	2.16	33 (40%)
23	CLA	b	602	41	69,73,73	2.79	20 (28%)	82,113,113	2.54	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	415	-	52,54,54	0.96	2 (3%)	62,65,65	1.87	11 (17%)
26	SQD	a	412	-	52,54,54	0.87	2 (3%)	62,65,65	2.09	12 (19%)
31	DMS	B	645	-	3,3,3	2.87	1 (33%)	3,3,3	0.72	0
31	DMS	O	309	-	3,3,3	2.94	1 (33%)	3,3,3	0.96	0
23	CLA	A	406	41	69,73,73	1.79	19 (27%)	82,113,113	2.51	29 (35%)
31	DMS	B	649	-	3,3,3	2.77	1 (33%)	3,3,3	0.56	0
24	PHO	A	407	-	58,69,69	2.18	12 (20%)	55,99,99	3.01	17 (30%)
23	CLA	c	911	-	69,73,73	2.20	18 (26%)	82,113,113	2.34	29 (35%)
31	DMS	c	932	-	3,3,3	2.71	1 (33%)	3,3,3	0.77	0
24	PHO	a	409	-	58,69,69	2.61	13 (22%)	55,99,99	3.27	17 (30%)
25	BCR	b	618	-	41,41,41	0.95	0	56,56,56	1.77	14 (25%)
37	HEM	E	105	6,5	50,50,50	2.12	9 (18%)	67,82,82	1.45	9 (13%)
40	HEC	V	203	16	46,50,50	2.04	10 (21%)	58,82,82	1.58	10 (17%)
23	CLA	D	404	-	69,73,73	2.04	20 (28%)	82,113,113	2.29	32 (39%)
23	CLA	C	503	-	69,73,73	2.26	19 (27%)	82,113,113	2.08	26 (31%)
38	RRX	H	102	-	42,42,42	0.90	2 (4%)	56,58,58	1.61	9 (16%)
31	DMS	h	103	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
23	CLA	C	514	-	69,73,73	2.57	22 (31%)	82,113,113	2.17	24 (29%)
30	LMT	T	103	-	24,24,36	0.50	0	29,29,47	1.32	4 (13%)
31	DMS	u	205	-	3,3,3	2.69	1 (33%)	3,3,3	1.08	0
23	CLA	d	401	41	69,73,73	1.97	14 (20%)	82,113,113	2.20	28 (34%)
23	CLA	B	606	-	69,73,73	2.05	19 (27%)	82,113,113	2.19	27 (32%)
30	LMT	m	103	-	36,36,36	0.61	1 (2%)	47,47,47	1.00	3 (6%)
34	LMG	j	101	39	51,51,55	0.99	4 (7%)	59,59,63	1.16	6 (10%)
31	DMS	c	933	-	3,3,3	2.73	1 (33%)	3,3,3	0.95	0
23	CLA	b	616	-	69,73,73	2.10	19 (27%)	82,113,113	2.13	31 (37%)
23	CLA	a	410	-	69,73,73	2.00	17 (24%)	82,113,113	2.20	30 (36%)
38	RRX	x	102	-	42,42,42	0.90	0	56,58,58	1.40	7 (12%)
23	CLA	c	912	3	69,73,73	2.48	21 (30%)	82,113,113	2.24	25 (30%)
31	DMS	B	641	-	3,3,3	2.89	1 (33%)	3,3,3	0.82	0
34	LMG	m	102	-	51,51,55	0.95	2 (3%)	59,59,63	1.34	7 (11%)
23	CLA	b	606	-	69,73,73	2.11	20 (28%)	82,113,113	2.29	27 (32%)
23	CLA	B	607	-	69,73,73	2.20	15 (21%)	82,113,113	2.40	26 (31%)
30	LMT	M	101	-	36,36,36	0.63	0	47,47,47	0.93	2 (4%)
23	CLA	b	603	-	69,73,73	2.07	22 (31%)	82,113,113	2.32	35 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	u	206	-	3,3,3	2.85	1 (33%)	3,3,3	0.65	0
23	CLA	C	511	-	69,73,73	2.30	17 (24%)	82,113,113	2.08	28 (34%)
31	DMS	D	416	-	3,3,3	2.55	1 (33%)	3,3,3	0.90	0
30	LMT	a	418	-	36,36,36	0.70	1 (2%)	47,47,47	1.31	6 (12%)
31	DMS	b	642	-	3,3,3	2.77	1 (33%)	3,3,3	0.59	0
31	DMS	c	928	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
25	BCR	j	104	-	41,41,41	0.82	0	56,56,56	1.51	13 (23%)
31	DMS	B	636	-	3,3,3	3.17	1 (33%)	3,3,3	0.78	0
23	CLA	b	611	41	69,73,73	2.15	22 (31%)	82,113,113	2.03	25 (30%)
31	DMS	c	935	-	3,3,3	2.74	1 (33%)	3,3,3	0.76	0
35	HTG	v	204	-	19,19,19	0.84	1 (5%)	23,24,24	2.49	8 (34%)
20	OEX	a	402	41,3,1	0,15,15	-	-	-	-	-
23	CLA	B	613	-	69,73,73	2.23	18 (26%)	82,113,113	2.18	27 (32%)
28	LHG	l	101	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	3 (5%)
35	HTG	O	302	-	19,19,19	1.38	2 (10%)	23,24,24	1.47	4 (17%)
31	DMS	c	926	-	3,3,3	2.68	1 (33%)	3,3,3	0.31	0
25	BCR	k	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.22	7 (12%)
31	DMS	b	645	-	3,3,3	2.75	1 (33%)	3,3,3	0.51	0
32	BCT	A	420	21	3,3,3	1.21	0	2,3,3	1.22	0
23	CLA	A	408	-	69,73,73	1.99	16 (23%)	82,113,113	2.65	33 (40%)
31	DMS	V	208	-	3,3,3	2.66	1 (33%)	3,3,3	0.42	0
31	DMS	A	422	-	3,3,3	2.74	1 (33%)	3,3,3	0.86	0
23	CLA	c	914	-	69,73,73	2.50	21 (30%)	82,113,113	2.20	27 (32%)
23	CLA	C	505	41	69,73,73	2.08	18 (26%)	82,113,113	2.38	30 (36%)

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
23	CLA	D	403	-	1/1/15/20	5/39/115/115	-
23	CLA	b	610	-	-	1/39/115/115	-
23	CLA	b	604	-	1/1/15/20	4/39/115/115	-
23	CLA	C	504	-	-	3/39/115/115	-
23	CLA	b	613	-	1/1/15/20	4/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	602	41	1/1/15/20	19/39/115/115	-
23	CLA	C	502	-	1/1/15/20	3/39/115/115	-
37	HEM	e	105	6,5	-	2/14/54/54	-
36	DGD	c	919	-	-	15/51/91/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	4/39/115/115	-
23	CLA	C	506	-	1/1/15/20	0/39/115/115	-
23	CLA	B	614	-	1/1/15/20	4/39/115/115	-
23	CLA	d	404	-	-	12/39/115/115	-
24	PHO	D	402	-	-	2/37/103/103	0/5/6/6
35	HTG	c	923	-	-	4/8/10/30	-
30	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
35	HTG	b	623	-	-	8/10/30/30	0/1/1/1
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
35	HTG	B	626	-	-	6/10/30/30	0/1/1/1
25	BCR	d	405	-	-	4/29/63/63	0/2/2/2
34	LMG	a	413	-	-	24/46/66/70	0/1/1/1
36	DGD	C	519	-	-	18/51/91/95	0/2/2/2
23	CLA	B	615	-	1/1/15/20	6/39/115/115	-
36	DGD	D	407	-	-	25/44/64/95	0/1/1/2
23	CLA	c	906	-	1/1/15/20	2/39/115/115	-
23	CLA	b	612	-	-	4/39/115/115	-
23	CLA	B	609	-	-	1/39/115/115	-
23	CLA	B	612	-	1/1/15/20	5/39/115/115	-
23	CLA	a	407	41	-	8/39/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
34	LMG	D	412	-	-	24/46/66/70	0/1/1/1
27	PL9	A	411	-	-	13/53/73/73	0/1/1/1
25	BCR	C	530	-	-	0/29/63/63	0/2/2/2
35	HTG	b	628	-	-	1/10/30/30	0/1/1/1
26	SQD	B	621	-	-	28/49/69/69	0/1/1/1
23	CLA	C	513	-	1/1/15/20	12/39/115/115	-
23	CLA	B	604	-	1/1/15/20	4/39/115/115	-
25	BCR	c	915	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410	-	-	20/49/69/69	0/1/1/1
40	HEC	v	203	16	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	a	415	-	-	20/53/53/53	-
23	CLA	B	610	-	-	3/39/115/115	-
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
28	LHG	d	402	-	-	24/48/48/53	-
34	LMG	d	411	-	-	25/46/66/70	0/1/1/1
23	CLA	c	905	41	-	8/39/115/115	-
23	CLA	D	401	41	-	2/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	904	-	-	3/39/115/115	-
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
30	LMT	A	416	-	-	7/21/61/61	0/2/2/2
34	LMG	C	520	-	-	20/46/66/70	0/1/1/1
28	LHG	K	101	-	-	24/45/45/53	-
30	LMT	I	101	-	-	8/21/61/61	0/2/2/2
34	LMG	B	622	-	-	15/46/66/70	0/1/1/1
23	CLA	B	608	41	1/1/15/20	2/39/115/115	-
23	CLA	C	508	41	1/1/15/20	11/39/115/115	-
26	SQD	x	101	-	-	19/36/56/69	0/1/1/1
27	PL9	d	406	-	-	4/53/73/73	0/1/1/1
28	LHG	D	411	-	-	14/50/50/53	-
30	LMT	b	621	-	-	12/17/37/61	0/1/1/2
35	HTG	D	414	-	-	4/10/30/30	0/1/1/1
36	DGD	c	917	-	-	13/51/91/95	0/2/2/2
28	LHG	d	409	-	-	9/53/53/53	-
27	PL9	D	406	-	-	3/53/73/73	0/1/1/1
30	LMT	B	623	-	-	15/21/61/61	0/2/2/2
25	BCR	C	515	-	-	3/29/63/63	0/2/2/2
28	LHG	D	409	-	-	9/53/53/53	-
26	SQD	a	417	-	-	15/49/69/69	0/1/1/1
28	LHG	d	410	-	-	10/50/50/53	-
30	LMT	F	101	-	-	10/21/61/61	0/2/2/2
36	DGD	h	102	-	-	18/51/91/95	0/2/2/2
23	CLA	c	902	-	1/1/15/20	4/39/115/115	-
23	CLA	A	405	-	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	B	643	-	-	6/15/35/61	0/1/1/2
23	CLA	c	910	-	1/1/15/20	8/39/115/115	-
28	LHG	D	410	-	-	9/53/53/53	-
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
23	CLA	C	509	-	1/1/15/20	4/39/115/115	-
23	CLA	c	909	-	-	2/39/115/115	-
36	DGD	c	918	-	-	15/51/91/95	0/2/2/2
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
24	PHO	a	408	-	-	4/37/103/103	0/5/6/6
28	LHG	d	408	-	-	14/53/53/53	-
23	CLA	B	603	-	1/1/15/20	0/39/115/115	-
26	SQD	L	102	-	-	27/49/69/69	0/1/1/1
27	PL9	a	414	-	-	10/53/73/73	0/1/1/1
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
36	DGD	d	407	-	-	22/44/64/95	0/1/1/2
23	CLA	c	903	-	-	6/39/115/115	-
28	LHG	E	101	-	-	28/53/53/53	-
23	CLA	c	907	-	1/1/15/20	9/39/115/115	-
25	BCR	a	411	-	-	0/29/63/63	0/2/2/2
26	SQD	D	408	-	-	19/40/60/69	0/1/1/1
23	CLA	b	614	-	1/1/15/20	3/39/115/115	-
35	HTG	C	521	-	-	3/10/30/30	0/1/1/1
34	LMG	c	920	-	-	20/46/66/70	0/1/1/1
34	LMG	c	930	-	-	7/46/66/70	0/1/1/1
23	CLA	a	406	-	1/1/15/20	5/39/115/115	-
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
35	HTG	b	622	-	-	4/10/30/30	0/1/1/1
36	DGD	C	518	-	-	14/51/91/95	0/2/2/2
23	CLA	C	510	-	1/1/15/20	10/39/115/115	-
23	CLA	b	615	-	1/1/15/20	10/39/115/115	-
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
23	CLA	b	607	-	1/1/15/20	9/39/115/115	-
28	LHG	L	101	-	-	17/53/53/53	-
30	LMT	m	104	-	-	2/21/61/61	0/2/2/2
30	LMT	a	422	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	J	101	39	-	15/46/66/70	0/1/1/1
40	HEC	V	203	16	-	6/14/54/54	-
35	HTG	B	630	-	-	4/10/30/30	0/1/1/1
35	HTG	V	204	-	-	0/5/25/30	0/1/1/1
23	CLA	C	507	-	1/1/15/20	14/39/115/115	-
23	CLA	b	609	-	-	1/39/115/115	-
30	LMT	e	103	-	-	6/17/37/61	0/1/1/2
34	LMG	C	531	-	-	18/46/66/70	0/1/1/1
35	HTG	B	631	-	-	3/10/30/30	0/1/1/1
23	CLA	B	617	-	1/1/15/20	8/39/115/115	-
23	CLA	c	913	-	1/1/15/20	6/39/115/115	-
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
23	CLA	B	605	-	1/1/15/20	6/39/115/115	-
28	LHG	A	412	-	-	28/53/53/53	-
30	LMT	B	644	-	-	8/15/35/61	0/1/1/2
23	CLA	b	617	-	1/1/15/20	18/39/115/115	-
34	LMG	C	501	-	-	24/46/66/70	0/1/1/1
23	CLA	c	908	41	1/1/15/20	10/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/15/20	5/39/115/115	-
28	LHG	e	101	-	-	18/44/44/53	-
35	HTG	C	522	-	-	5/10/30/30	0/1/1/1
35	HTG	C	523	-	-	4/10/30/30	0/1/1/1
35	HTG	c	922	-	-	3/10/30/30	0/1/1/1
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
23	CLA	B	611	41	1/1/15/20	4/39/115/115	-
35	HTG	c	921	-	-	5/10/30/30	0/1/1/1
23	CLA	d	403	-	1/1/15/20	3/39/115/115	-
35	HTG	d	413	-	-	7/10/30/30	0/1/1/1
25	BCR	D	405	-	-	4/29/63/63	0/2/2/2
23	CLA	C	512	3	-	0/39/115/115	-
36	DGD	H	103	-	-	11/51/91/95	0/2/2/2
23	CLA	b	608	41	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	602	41	1/1/15/20	17/39/115/115	-
26	SQD	A	415	-	-	24/49/69/69	0/1/1/1
26	SQD	a	412	-	-	23/49/69/69	0/1/1/1
23	CLA	A	406	41	-	7/39/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	c	911	-	1/1/15/20	1/39/115/115	-
24	PHO	a	409	-	-	4/37/103/103	0/5/6/6
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
23	CLA	D	404	-	1/1/15/20	11/39/115/115	-
23	CLA	C	503	-	-	5/39/115/115	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
23	CLA	C	514	-	-	9/39/115/115	-
30	LMT	T	103	-	-	7/15/35/61	0/1/1/2
23	CLA	d	401	41	-	3/39/115/115	-
23	CLA	B	606	-	1/1/15/20	6/39/115/115	-
30	LMT	m	103	-	-	10/21/61/61	0/2/2/2
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
23	CLA	b	616	-	1/1/15/20	8/39/115/115	-
23	CLA	a	410	-	-	8/39/115/115	-
38	RRX	x	102	-	-	0/29/65/65	0/2/2/2
23	CLA	c	912	3	-	1/39/115/115	-
34	LMG	m	102	-	-	18/46/66/70	0/1/1/1
23	CLA	b	606	-	1/1/15/20	4/39/115/115	-
23	CLA	B	607	-	1/1/15/20	6/39/115/115	-
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
23	CLA	b	603	-	1/1/15/20	2/39/115/115	-
37	HEM	E	105	6,5	-	6/14/54/54	-
23	CLA	C	511	-	1/1/15/20	1/39/115/115	-
30	LMT	a	418	-	-	12/21/61/61	0/2/2/2
25	BCR	j	104	-	-	2/29/63/63	0/2/2/2
23	CLA	b	611	41	1/1/15/20	4/39/115/115	-
35	HTG	v	204	-	-	7/10/30/30	0/1/1/1
23	CLA	B	613	-	1/1/15/20	2/39/115/115	-
28	LHG	l	101	-	-	13/53/53/53	-
35	HTG	O	302	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	k	102	-	-	2/29/63/63	0/2/2/2
23	CLA	A	408	-	-	17/39/115/115	-
23	CLA	c	914	-	-	9/39/115/115	-
23	CLA	C	505	41	1/1/15/20	8/39/115/115	-

The worst 5 of 1718 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	914	CLA	MG-NA	12.47	2.35	2.06
23	c	904	CLA	MG-NA	12.19	2.35	2.06
23	b	607	CLA	MG-NA	11.84	2.34	2.06
23	b	610	CLA	MG-NA	11.72	2.34	2.06
23	B	602	CLA	MG-NA	11.01	2.32	2.06

The worst 5 of 2770 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	905	CLA	C4A-NA-C1A	12.24	112.26	106.68
23	c	910	CLA	C4A-NA-C1A	12.18	112.23	106.68
23	C	512	CLA	C4A-NA-C1A	11.10	111.74	106.68
23	c	902	CLA	C4A-NA-C1A	10.91	111.66	106.68
24	A	407	PHO	C2D-C1D-ND	10.61	117.10	109.43

5 of 47 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND

5 of 1506 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	C4-C3-C5-C6
23	B	610	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

219 monomers are involved in 526 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	403	CLA	2	0
23	b	610	CLA	1	0
31	v	209	DMS	7	0
23	b	604	CLA	2	0
23	C	504	CLA	4	0
23	b	613	CLA	1	0
25	A	409	BCR	3	0
23	B	602	CLA	2	0
31	U	202	DMS	1	0
31	c	934	DMS	1	0
23	C	502	CLA	1	0
31	B	646	DMS	4	0
37	e	105	HEM	1	0
23	b	605	CLA	1	0
31	h	104	DMS	1	0
23	C	506	CLA	1	0
23	B	614	CLA	4	0
31	b	647	DMS	3	0
23	d	404	CLA	5	0
24	D	402	PHO	2	0
30	Z	101	LMT	6	0
31	V	206	DMS	1	0
35	b	623	HTG	1	0
35	B	625	HTG	1	0
25	d	405	BCR	2	0
34	a	413	LMG	8	0
31	B	640	DMS	1	0
23	B	615	CLA	1	0
36	D	407	DGD	4	0
31	V	205	DMS	1	0
23	c	906	CLA	2	0
31	h	101	DMS	2	0
23	B	612	CLA	1	0
23	a	407	CLA	2	0
25	B	620	BCR	3	0
31	c	927	DMS	2	0
34	D	412	LMG	5	0
27	A	411	PL9	12	0
25	C	530	BCR	2	0
31	v	202	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	621	SQD	4	0
23	C	513	CLA	5	0
23	B	604	CLA	2	0
25	c	915	BCR	3	0
26	A	410	SQD	9	0
28	a	415	LHG	1	0
25	b	619	BCR	3	0
28	d	402	LHG	2	0
31	v	210	DMS	1	0
34	d	411	LMG	5	0
23	c	905	CLA	1	0
23	D	401	CLA	2	0
31	H	101	DMS	2	0
25	B	619	BCR	4	0
23	c	904	CLA	2	0
31	b	636	DMS	15	0
31	c	925	DMS	7	0
35	B	624	HTG	2	0
30	A	416	LMT	2	0
31	C	529	DMS	2	0
31	O	305	DMS	5	0
31	O	303	DMS	2	0
31	l	102	DMS	5	0
30	I	101	LMT	2	0
31	A	424	DMS	4	0
34	B	622	LMG	2	0
26	x	101	SQD	2	0
28	D	411	LHG	5	0
30	b	621	LMT	4	0
31	A	421	DMS	2	0
31	B	648	DMS	2	0
35	D	414	HTG	3	0
36	c	917	DGD	2	0
30	B	623	LMT	2	0
31	o	303	DMS	1	0
25	C	515	BCR	3	0
31	C	525	DMS	1	0
28	D	409	LHG	2	0
26	a	417	SQD	3	0
28	d	410	LHG	2	0
31	U	204	DMS	4	0
31	b	638	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	902	CLA	2	0
31	V	209	DMS	1	0
23	A	405	CLA	5	0
31	b	646	DMS	2	0
23	c	910	CLA	2	0
25	c	916	BCR	3	0
23	C	509	CLA	2	0
23	c	909	CLA	6	0
36	c	918	DGD	1	0
31	O	308	DMS	5	0
31	d	414	DMS	2	0
25	T	101	BCR	6	0
24	a	408	PHO	1	0
31	V	207	DMS	6	0
28	d	408	LHG	2	0
23	B	603	CLA	1	0
26	L	102	SQD	4	0
27	a	414	PL9	14	0
30	z	101	LMT	1	0
36	d	407	DGD	6	0
23	c	903	CLA	1	0
31	v	205	DMS	1	0
28	E	101	LHG	3	0
23	c	907	CLA	5	0
31	D	415	DMS	3	0
25	a	411	BCR	1	0
26	D	408	SQD	2	0
31	b	637	DMS	1	0
31	b	639	DMS	2	0
23	b	614	CLA	2	0
31	v	207	DMS	1	0
31	H	105	DMS	5	0
35	C	521	HTG	1	0
31	e	104	DMS	1	0
34	c	920	LMG	3	0
34	c	930	LMG	1	0
23	a	406	CLA	5	0
31	a	421	DMS	1	0
36	C	517	DGD	1	0
35	b	622	HTG	3	0
36	C	518	DGD	1	0
23	C	510	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	615	CLA	4	0
25	t	101	BCR	7	0
23	b	607	CLA	2	0
28	L	101	LHG	1	0
30	m	104	LMT	1	0
30	a	422	LMT	4	0
31	F	102	DMS	5	0
31	i	105	DMS	3	0
34	J	101	LMG	3	0
31	v	201	DMS	1	0
35	B	630	HTG	1	0
23	C	507	CLA	3	0
32	a	424	BCT	1	0
31	O	304	DMS	1	0
30	e	103	LMT	1	0
34	C	531	LMG	3	0
23	B	617	CLA	3	0
23	c	913	CLA	5	0
31	d	416	DMS	5	0
25	Y	101	BCR	1	0
25	B	618	BCR	1	0
31	a	423	DMS	2	0
31	b	633	DMS	1	0
35	b	627	HTG	1	0
23	B	605	CLA	1	0
31	a	420	DMS	9	0
31	b	644	DMS	1	0
28	A	412	LHG	1	0
30	B	644	LMT	1	0
23	b	617	CLA	9	0
34	C	501	LMG	1	0
31	o	304	DMS	3	0
31	v	206	DMS	2	0
31	c	929	DMS	2	0
23	c	908	CLA	3	0
25	C	516	BCR	2	0
23	B	616	CLA	3	0
31	B	639	DMS	8	0
28	e	101	LHG	5	0
31	O	311	DMS	3	0
31	V	202	DMS	1	0
31	c	936	DMS	1	0

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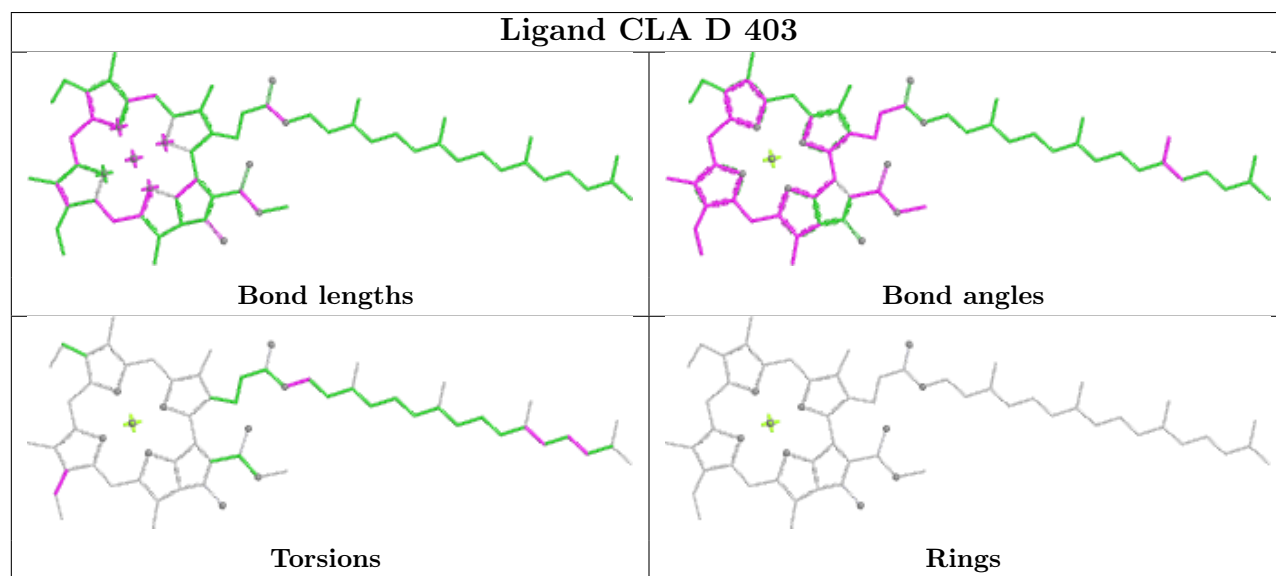
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35	c	922	HTG	1	0
31	C	526	DMS	3	0
25	b	620	BCR	8	0
31	B	638	DMS	3	0
31	b	641	DMS	2	0
23	B	611	CLA	4	0
31	V	210	DMS	6	0
23	d	403	CLA	1	0
35	c	921	HTG	1	0
25	D	405	BCR	5	0
23	C	512	CLA	2	0
23	b	608	CLA	1	0
23	b	602	CLA	6	0
26	A	415	SQD	2	0
26	a	412	SQD	2	0
31	B	645	DMS	1	0
23	A	406	CLA	1	0
24	A	407	PHO	1	0
31	c	932	DMS	2	0
24	a	409	PHO	3	0
37	E	105	HEM	1	0
23	D	404	CLA	1	0
23	C	503	CLA	2	0
23	C	514	CLA	3	0
31	u	205	DMS	2	0
23	d	401	CLA	3	0
23	B	606	CLA	6	0
30	m	103	LMT	2	0
31	c	933	DMS	2	0
23	b	616	CLA	3	0
23	a	410	CLA	1	0
38	x	102	RRX	4	0
23	c	912	CLA	3	0
31	B	641	DMS	1	0
34	m	102	LMG	3	0
23	b	606	CLA	1	0
30	M	101	LMT	1	0
23	b	603	CLA	2	0
31	u	206	DMS	3	0
23	C	511	CLA	1	0
31	D	416	DMS	6	0
30	a	418	LMT	4	0

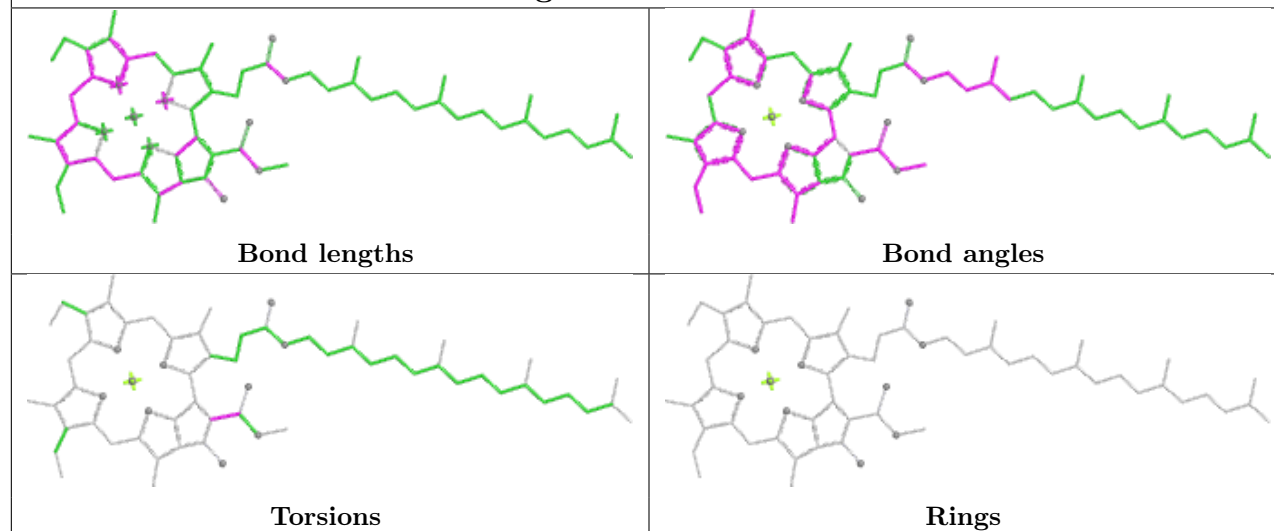
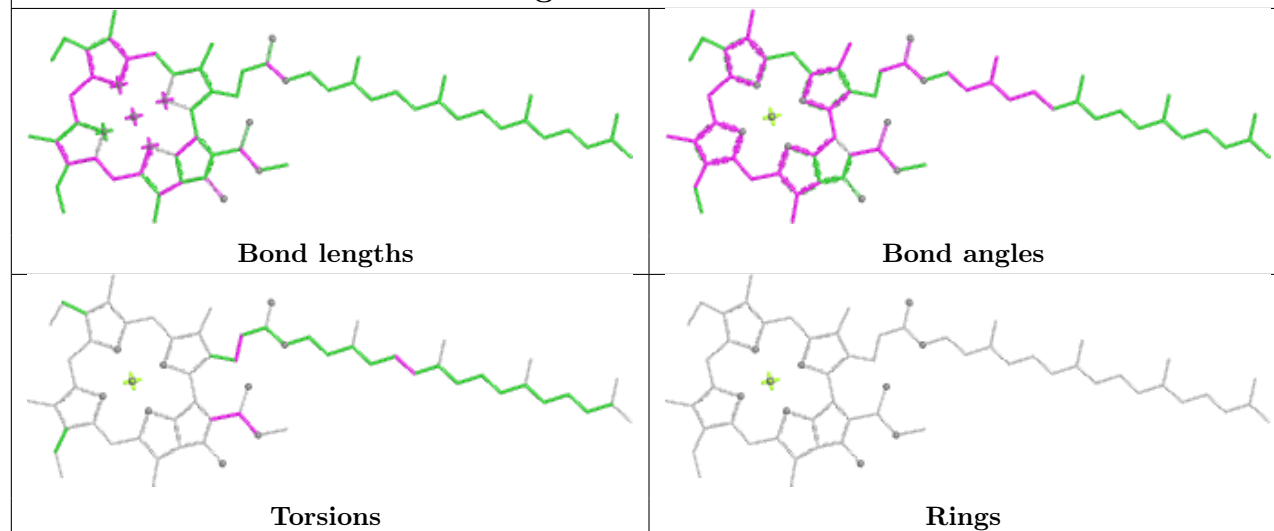
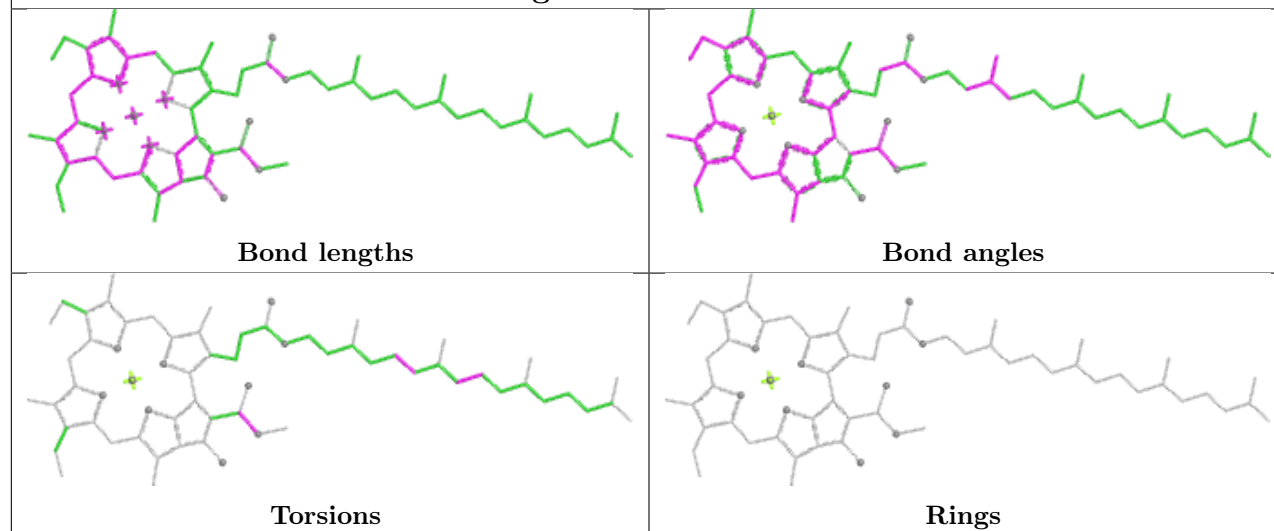
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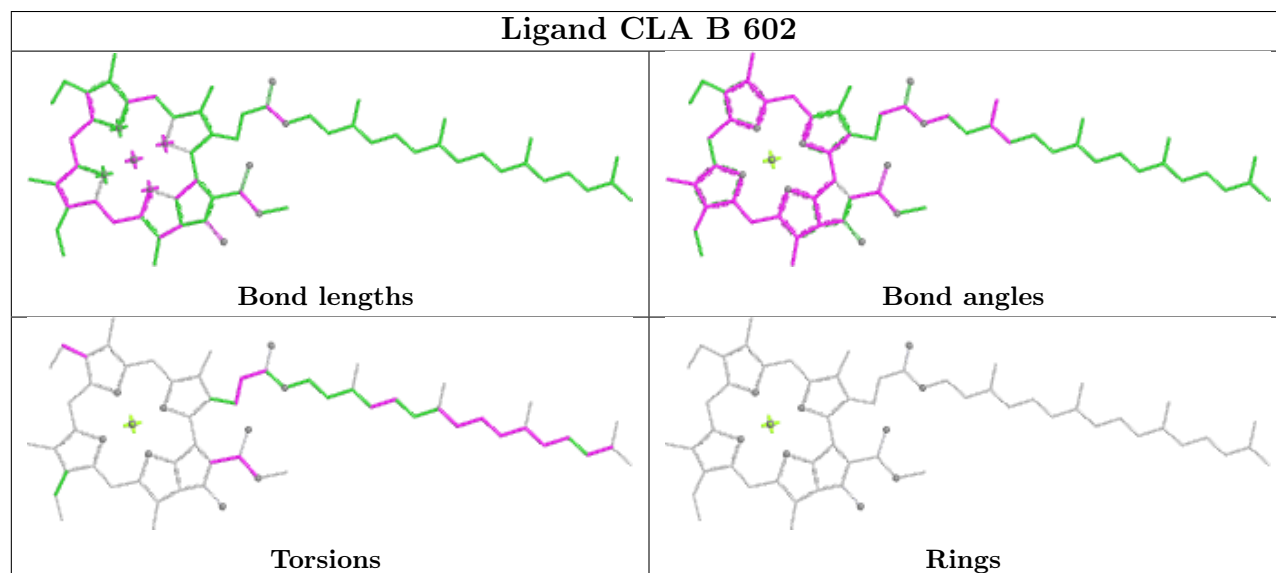
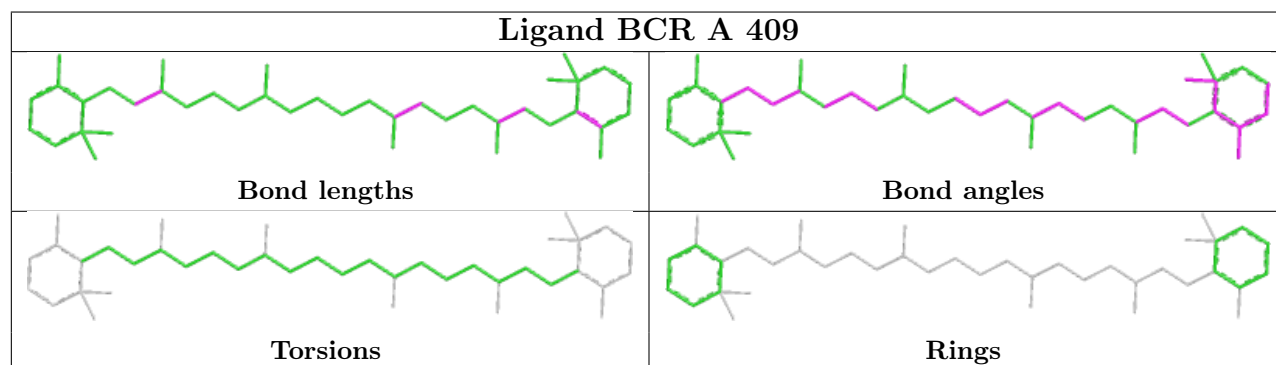
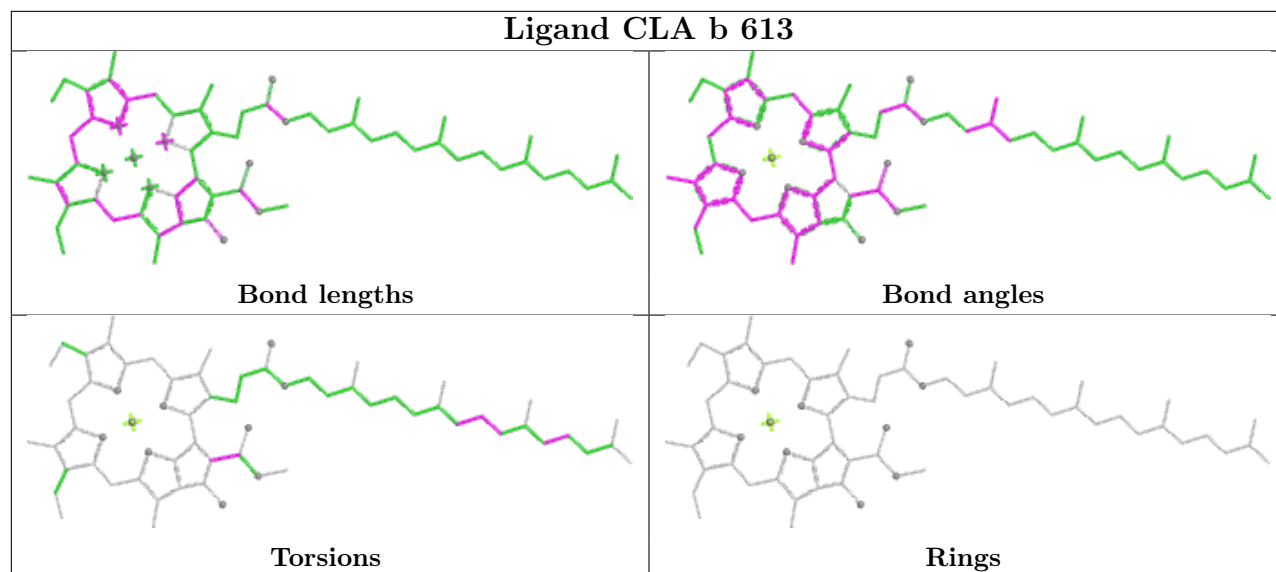
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	j	104	BCR	4	0
31	B	636	DMS	5	0
23	b	611	CLA	5	0
35	v	204	HTG	4	0
35	O	302	HTG	2	0
25	k	102	BCR	1	0
31	b	645	DMS	6	0
23	A	408	CLA	1	0
31	A	422	DMS	2	0
23	c	914	CLA	1	0
23	C	505	CLA	1	0

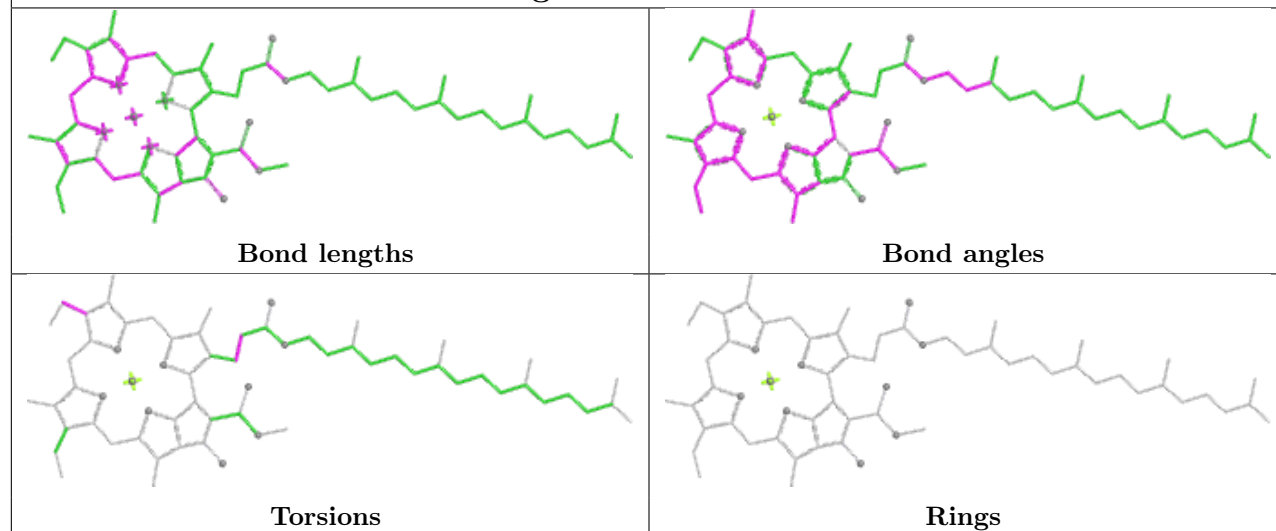
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



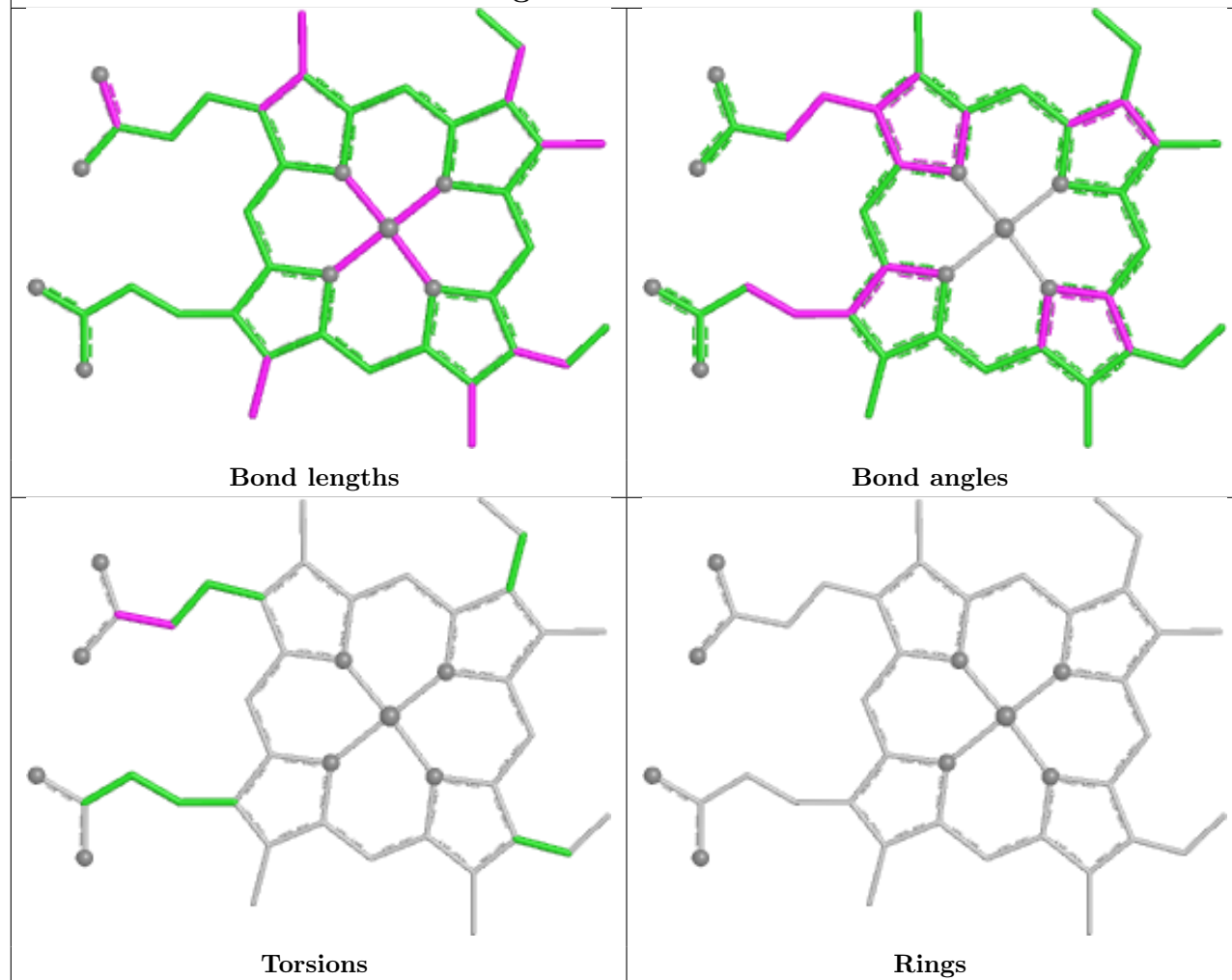
Ligand CLA b 610**Ligand CLA b 604****Ligand CLA C 504**

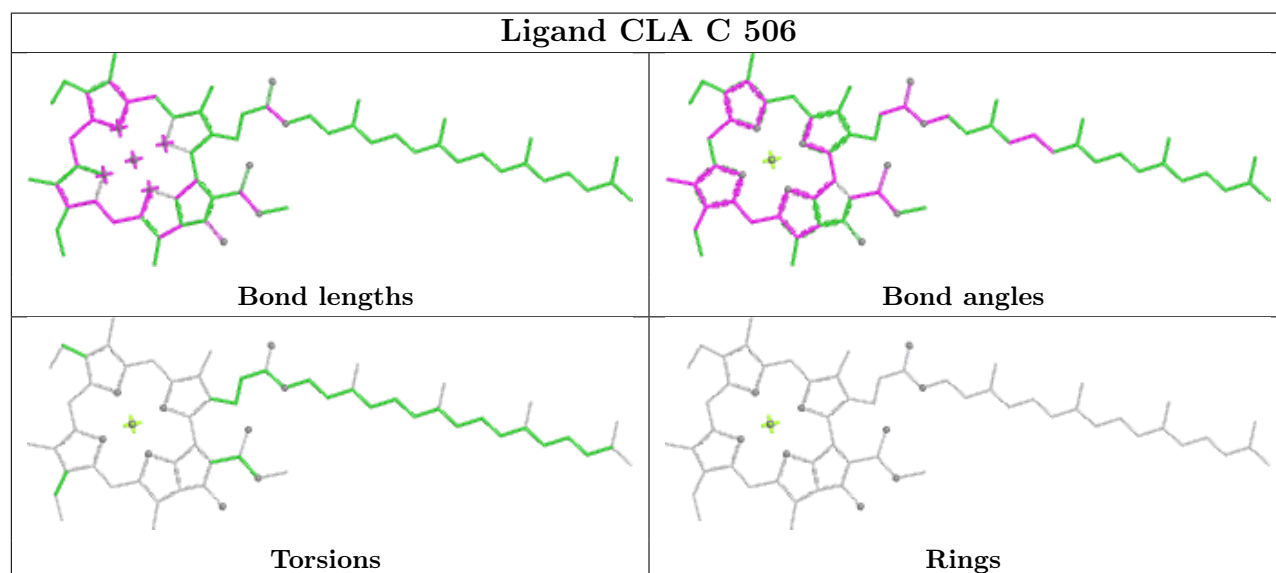
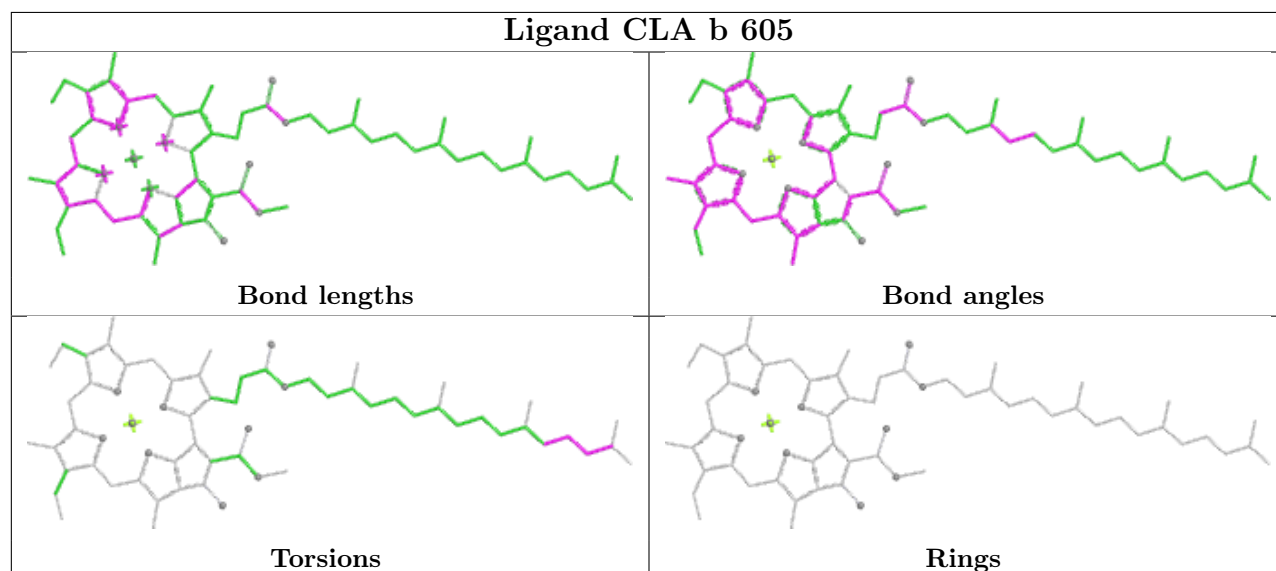
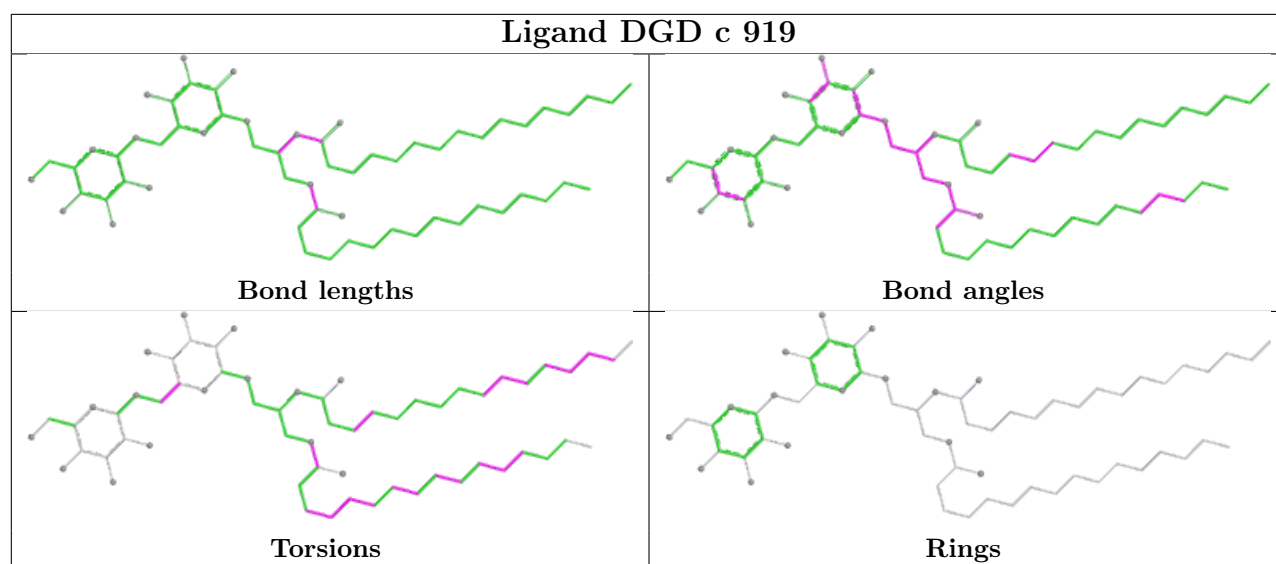


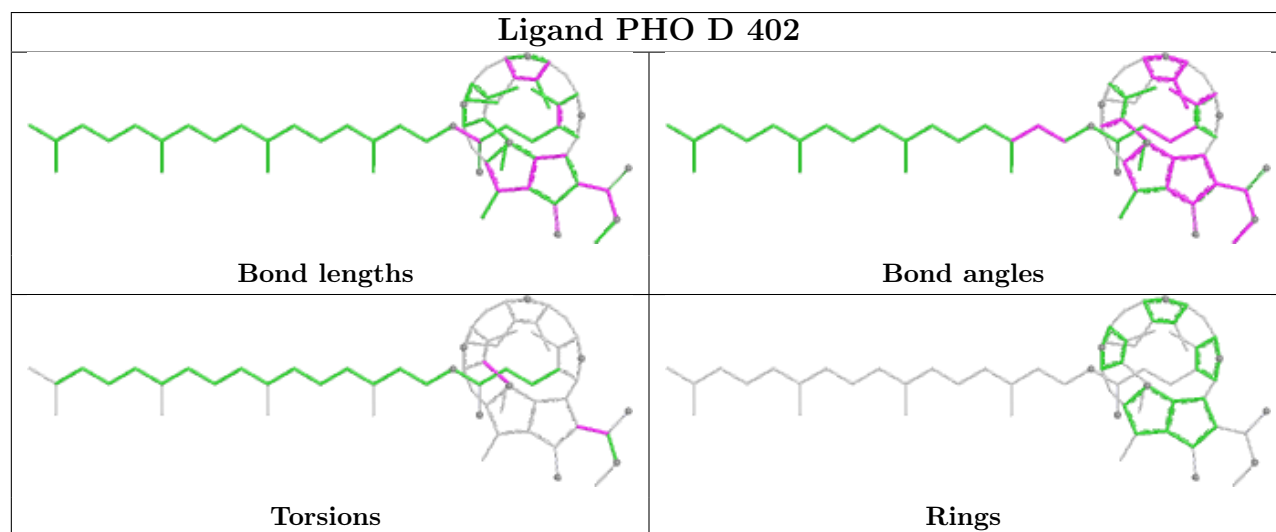
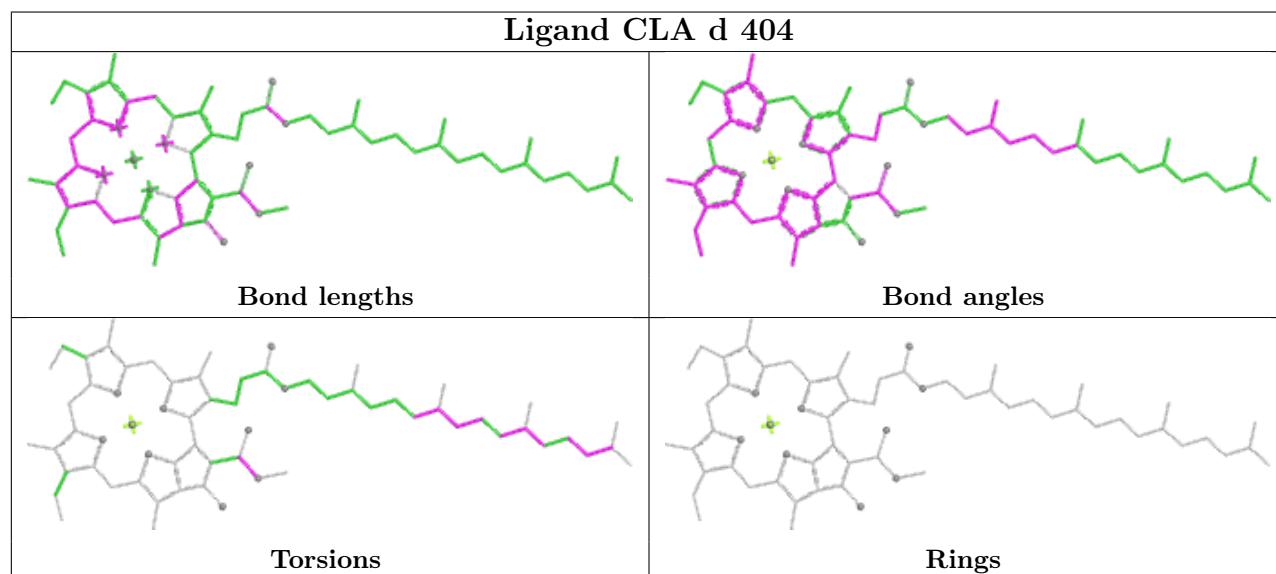
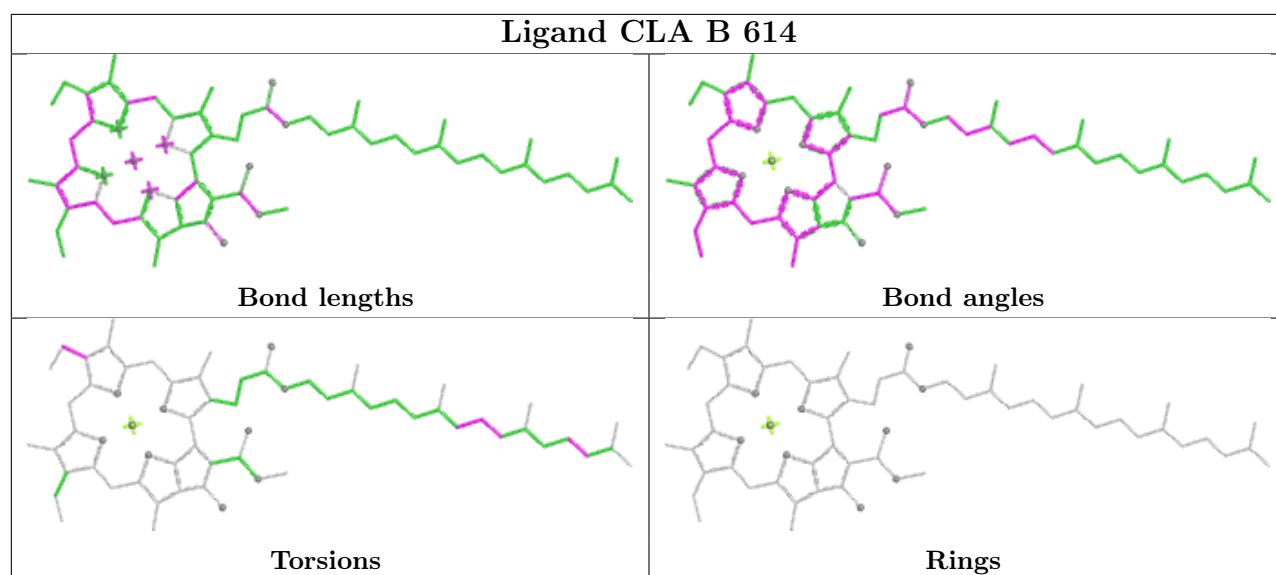
Ligand CLA C 502

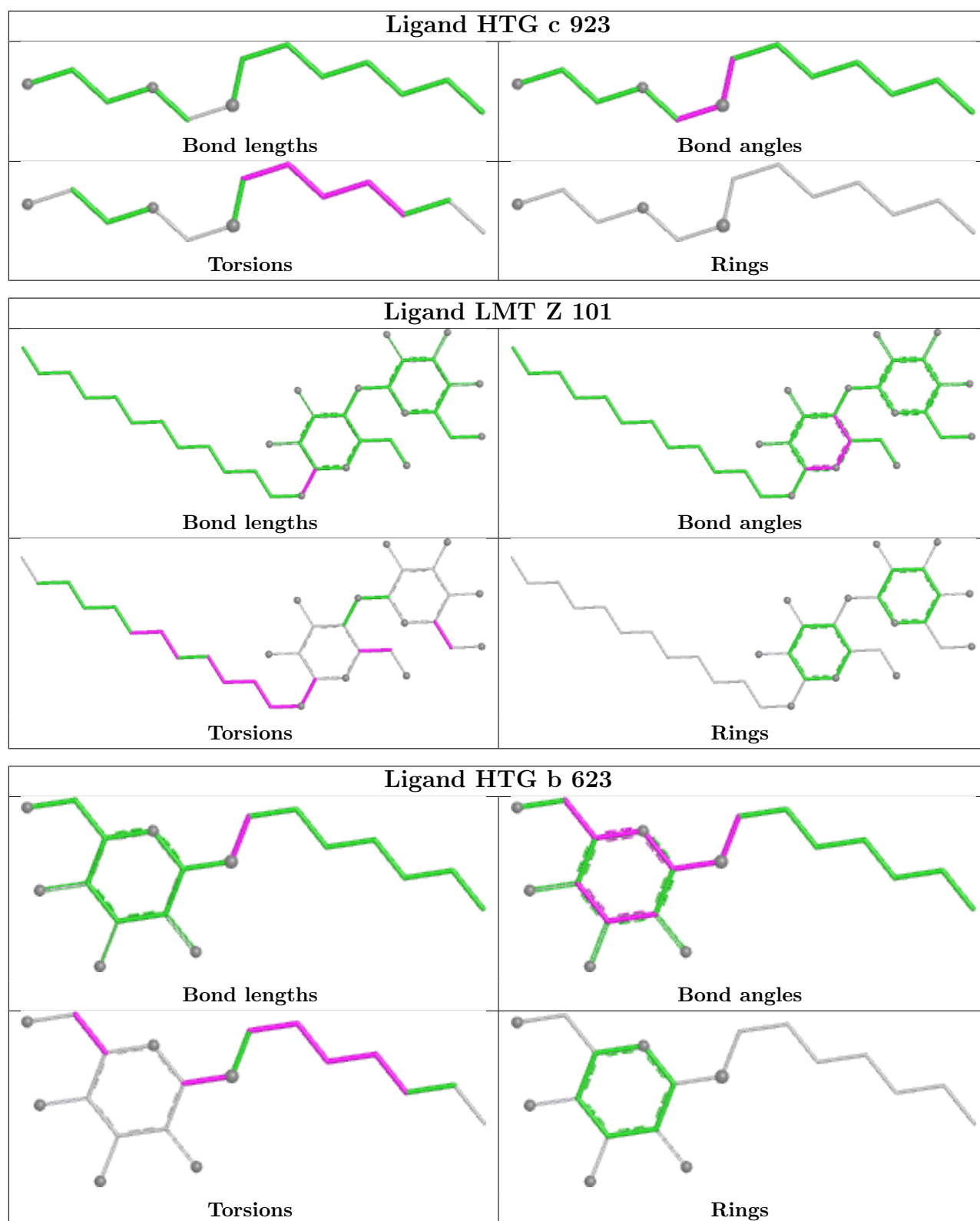


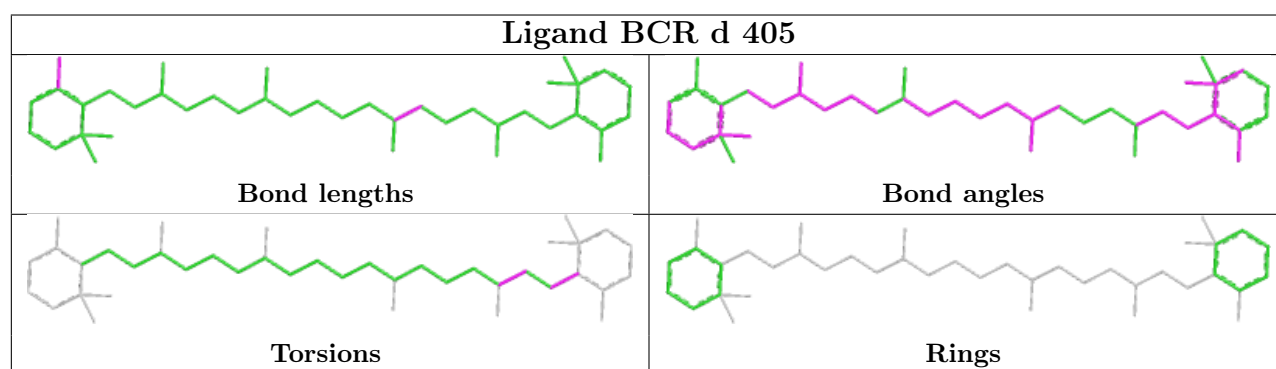
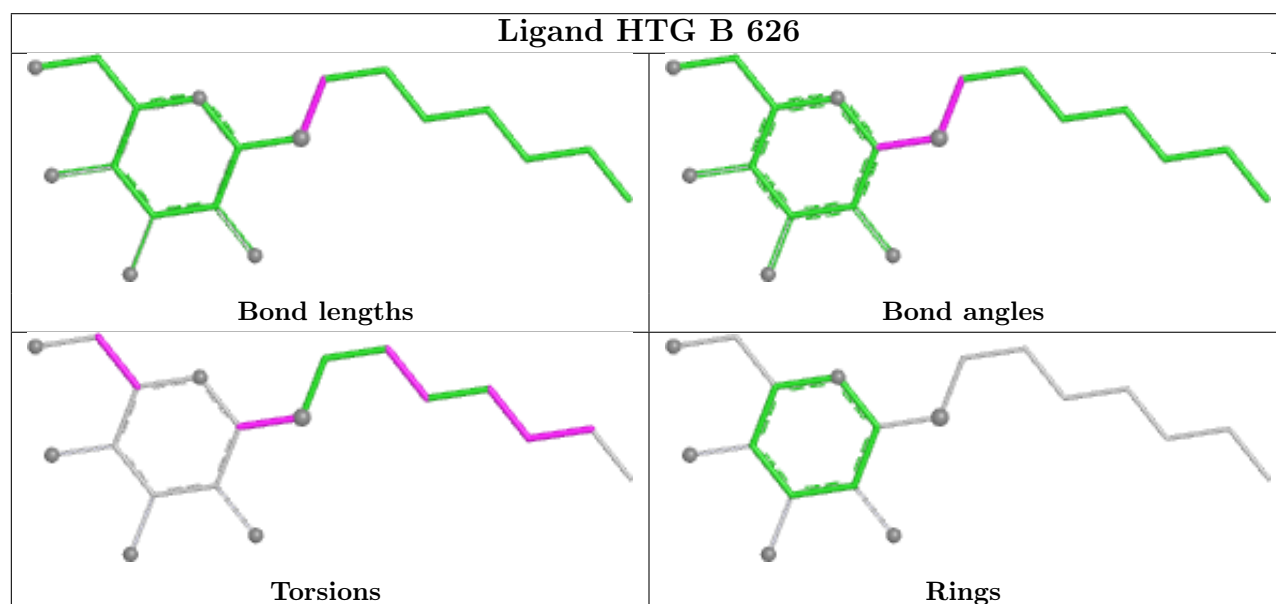
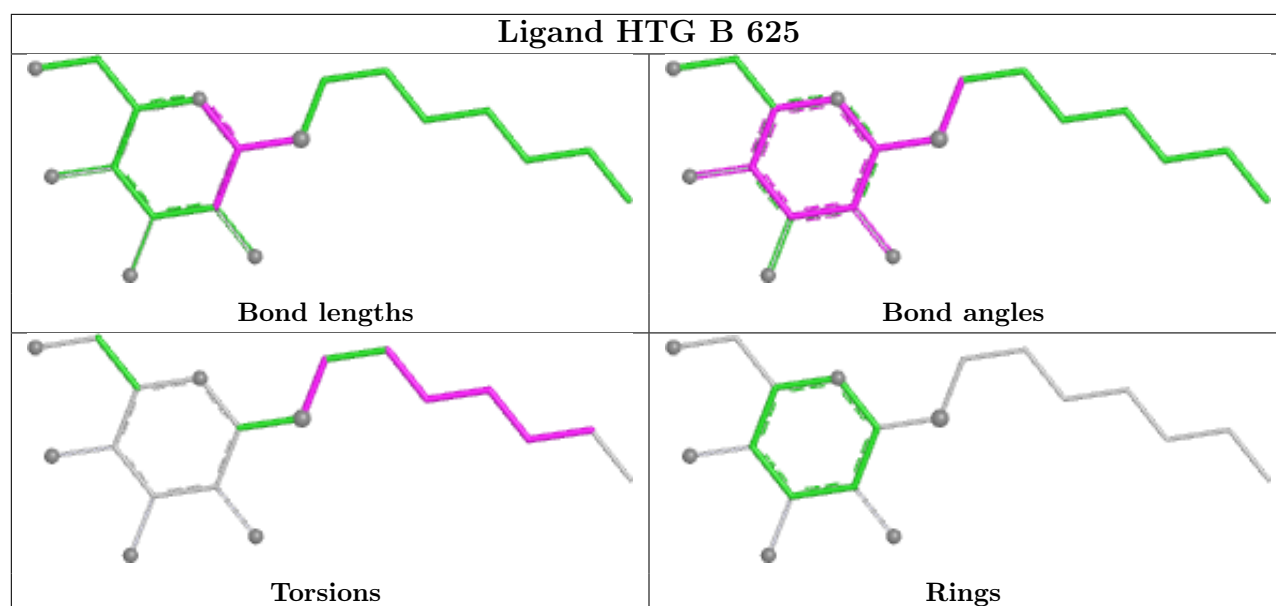
Ligand HEM e 105

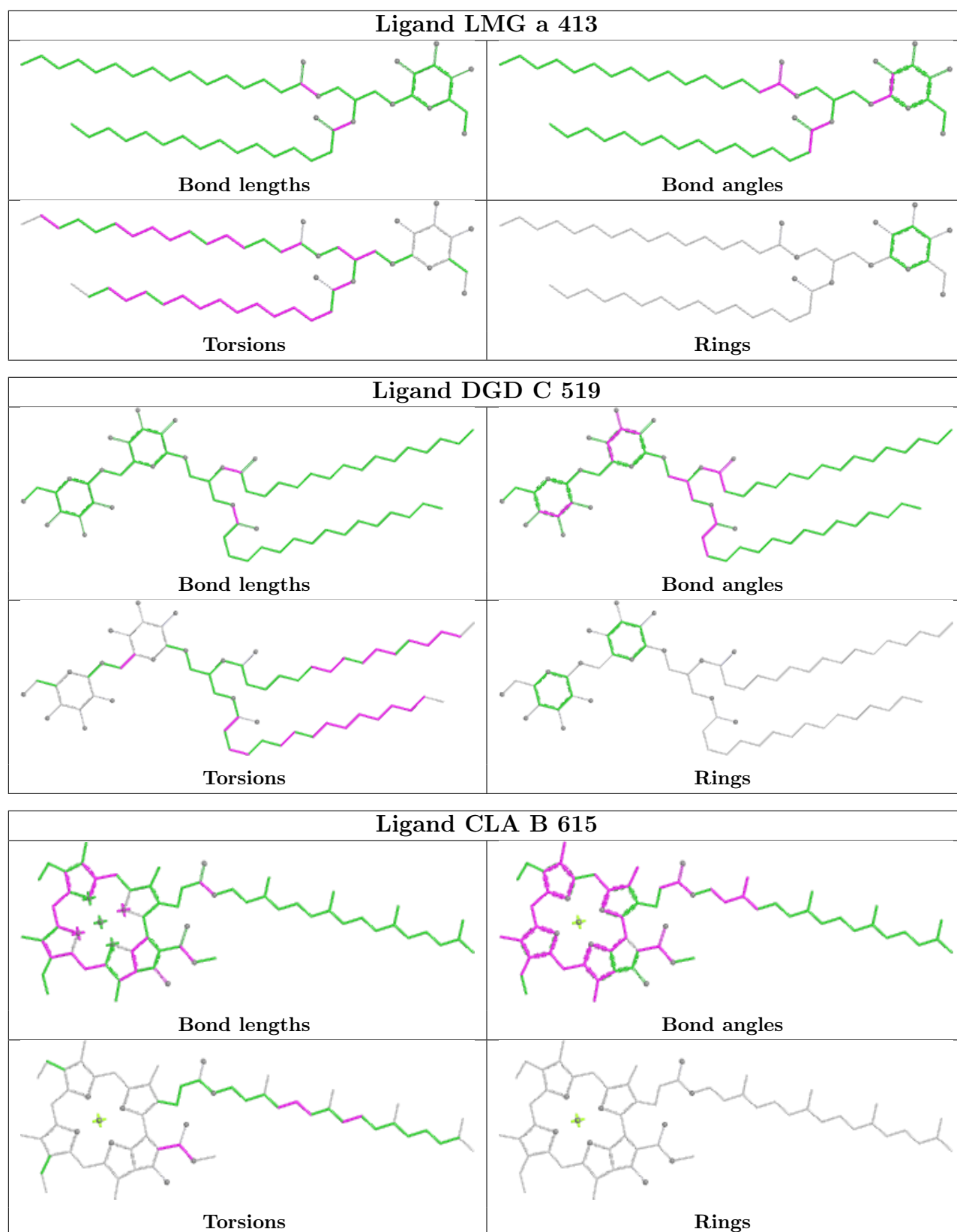


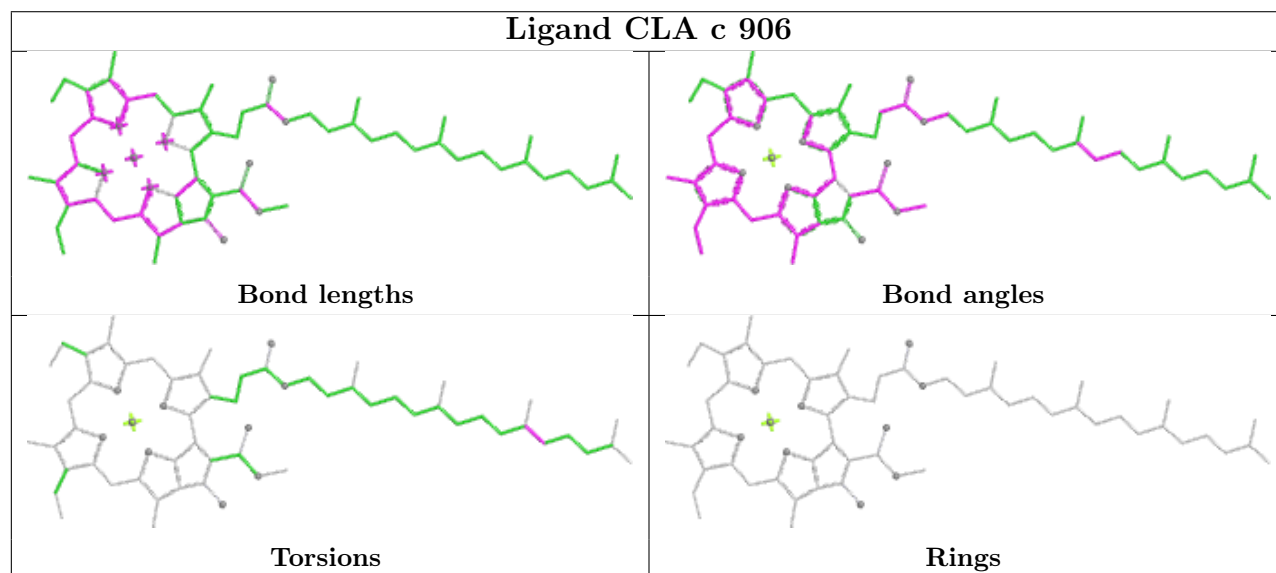
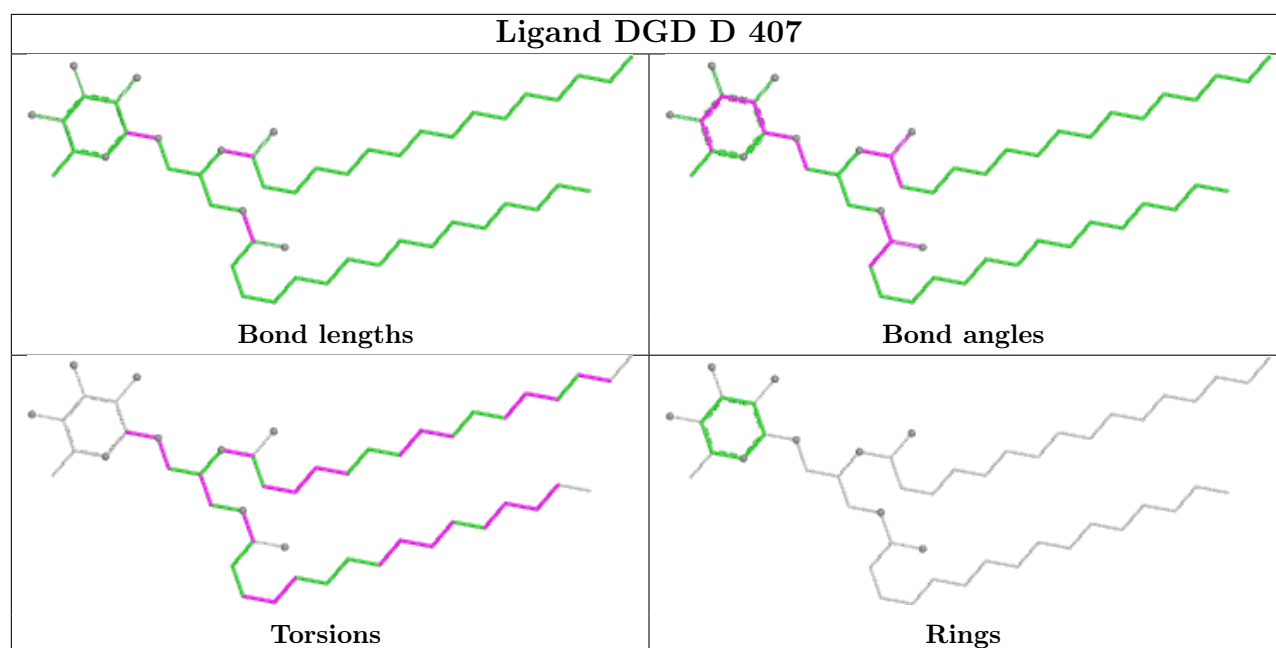


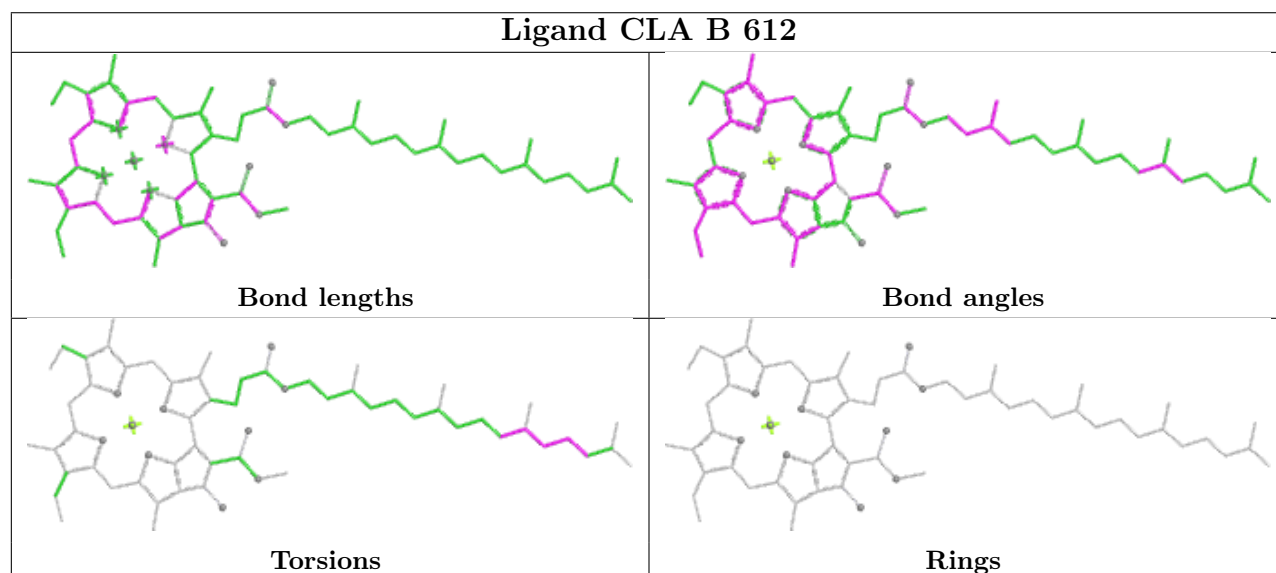
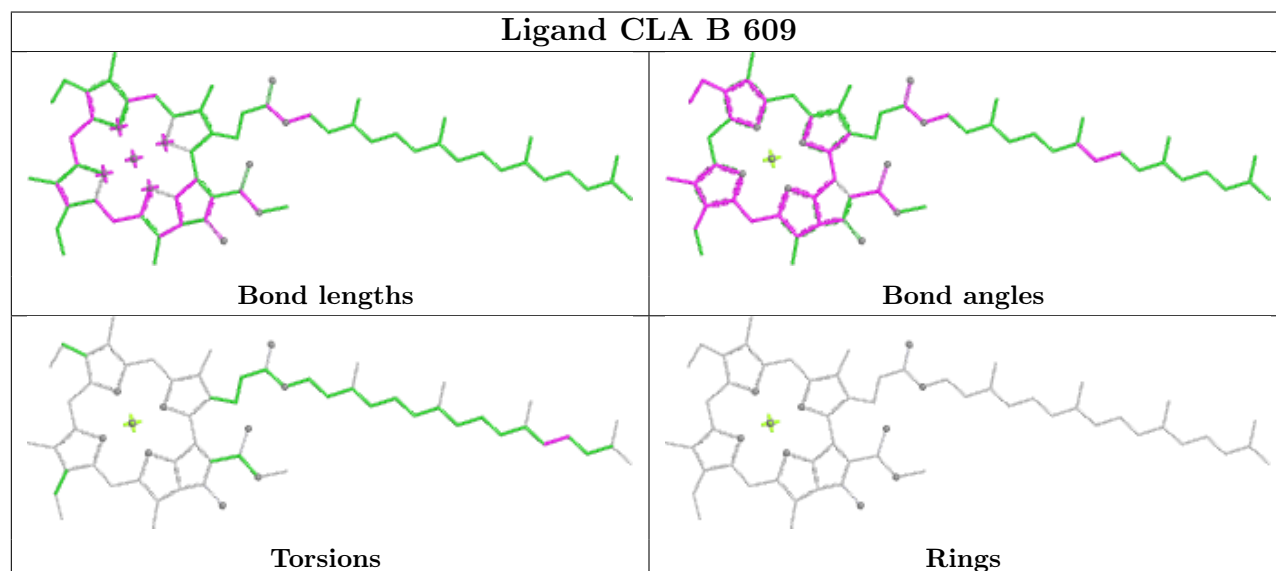
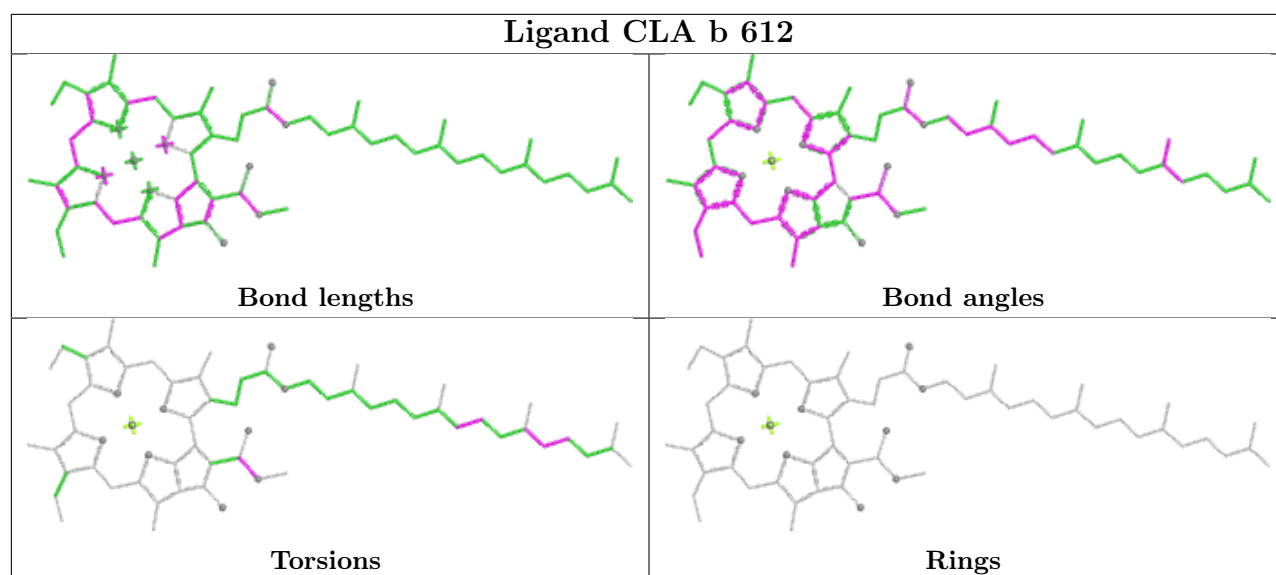


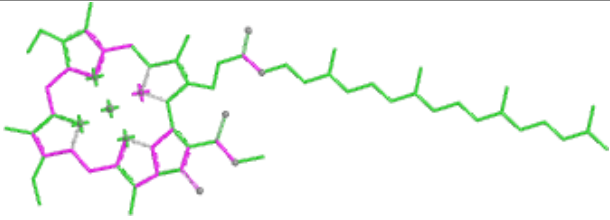
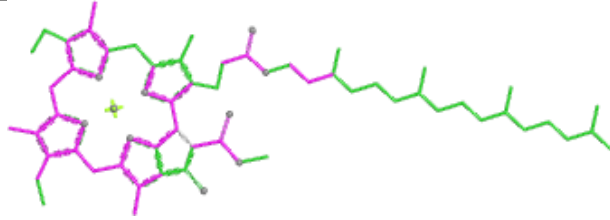
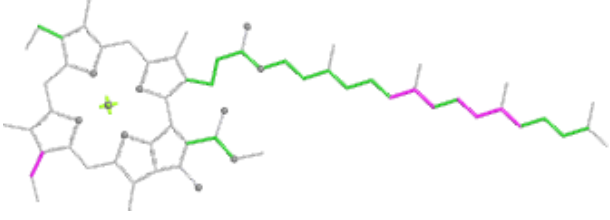
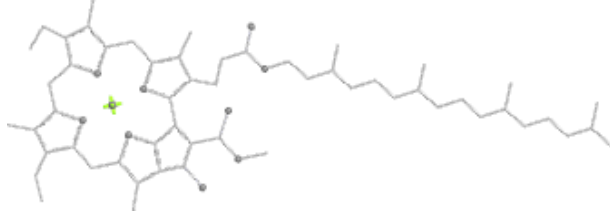
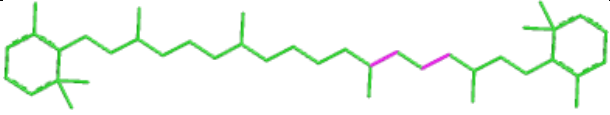
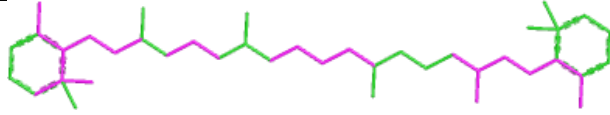
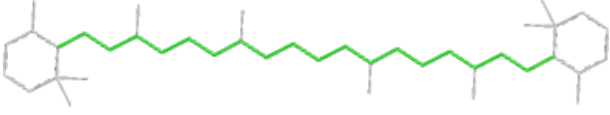
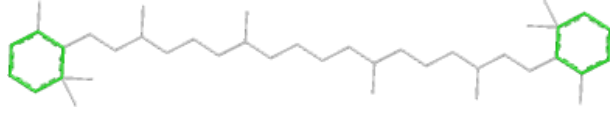
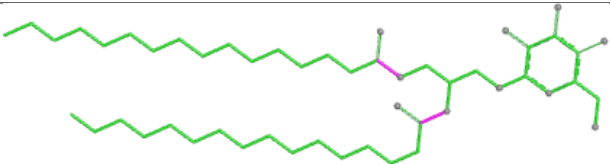
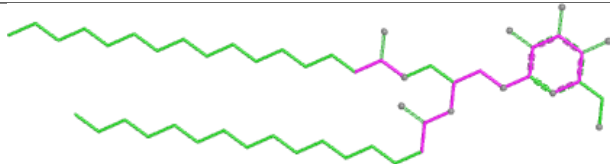
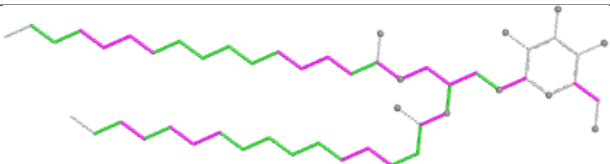
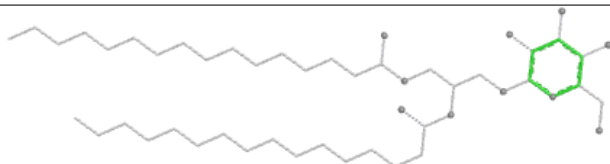
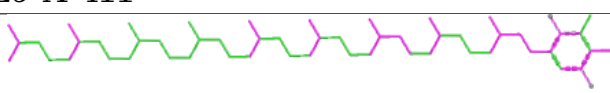
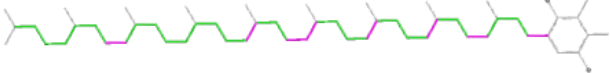
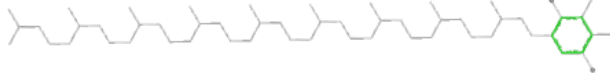


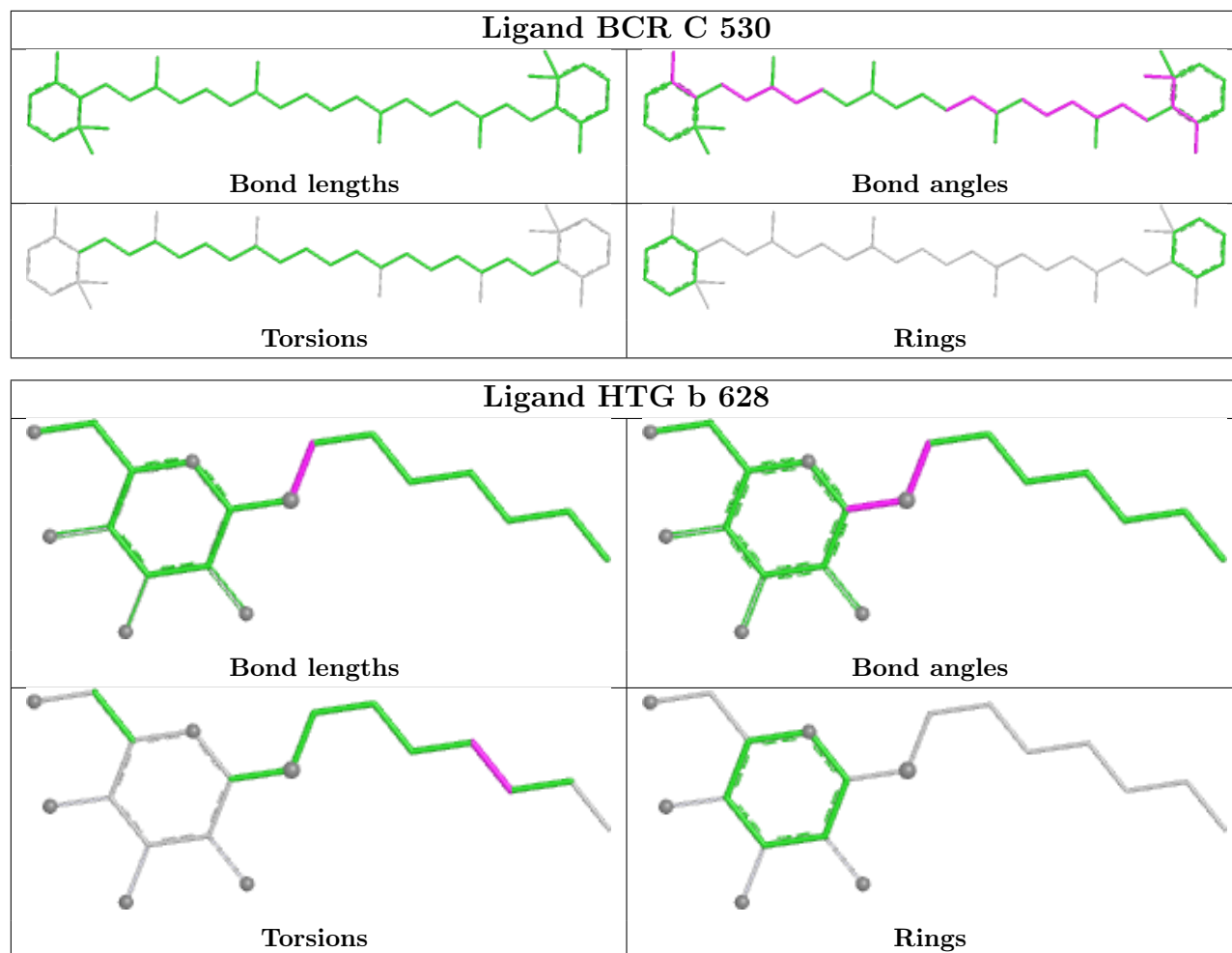


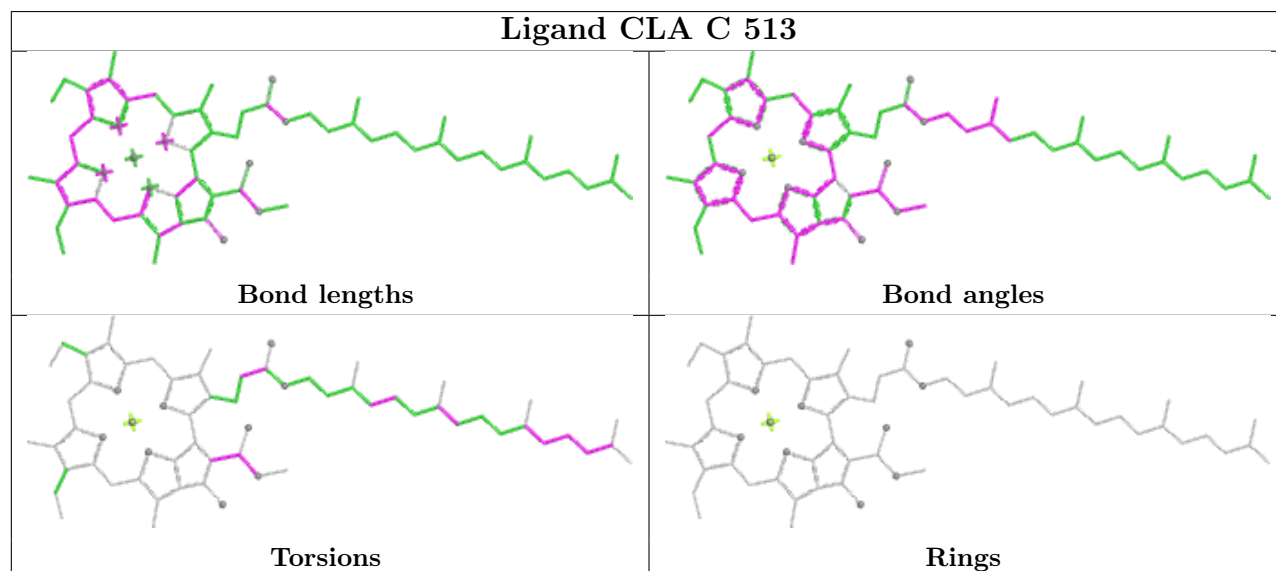
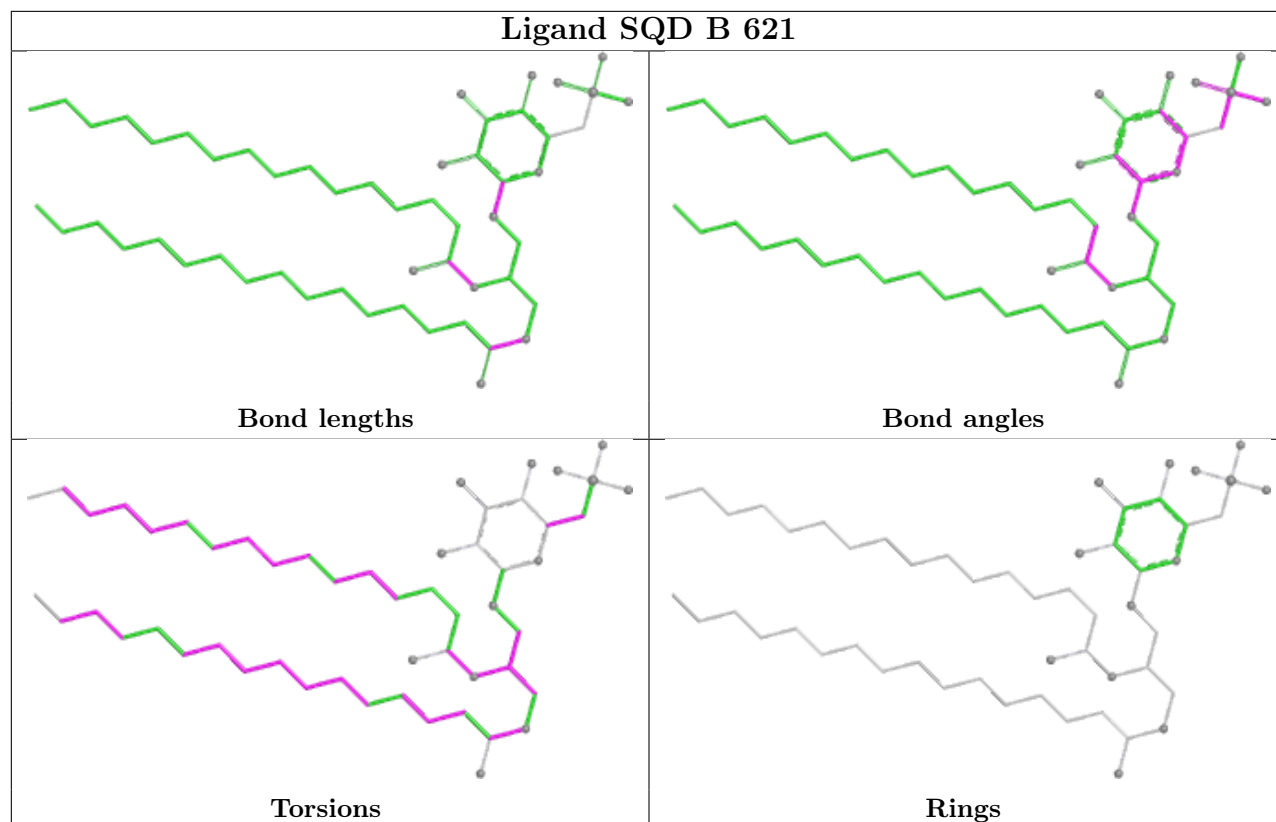


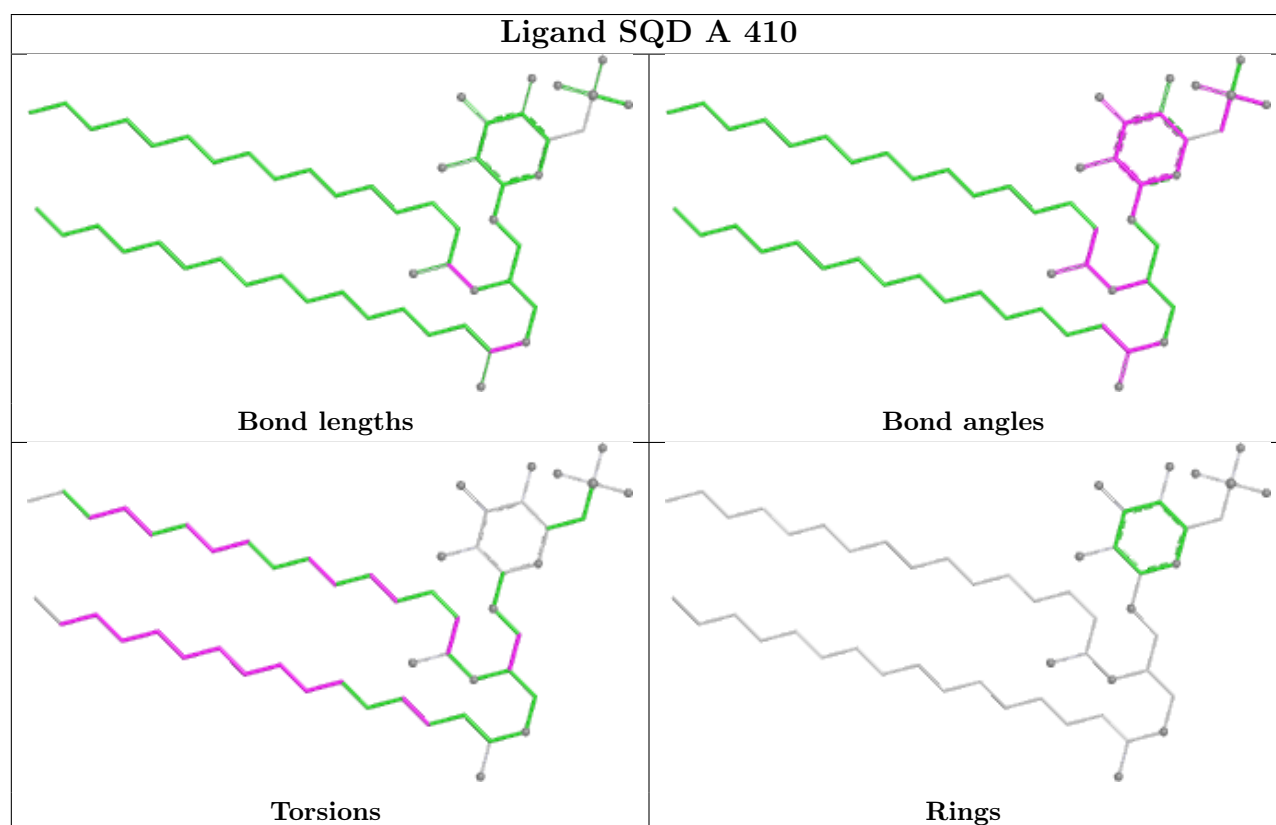
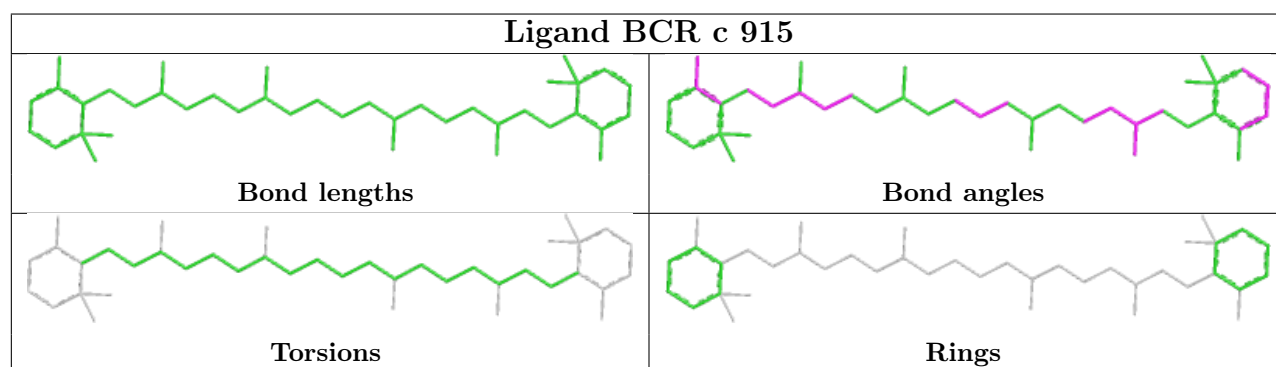
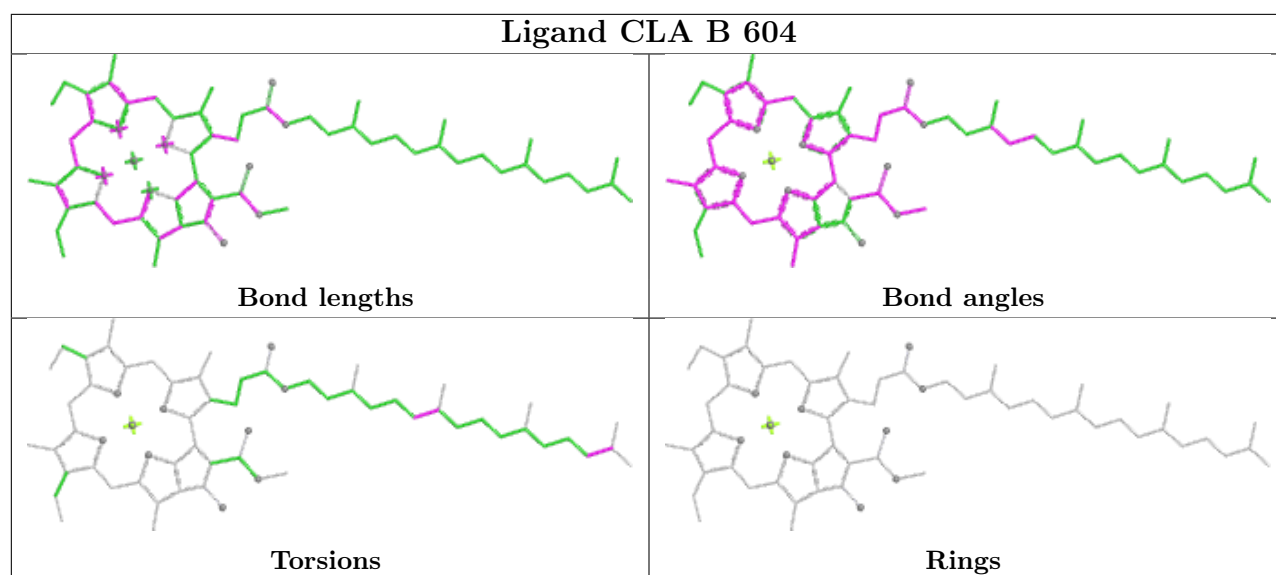




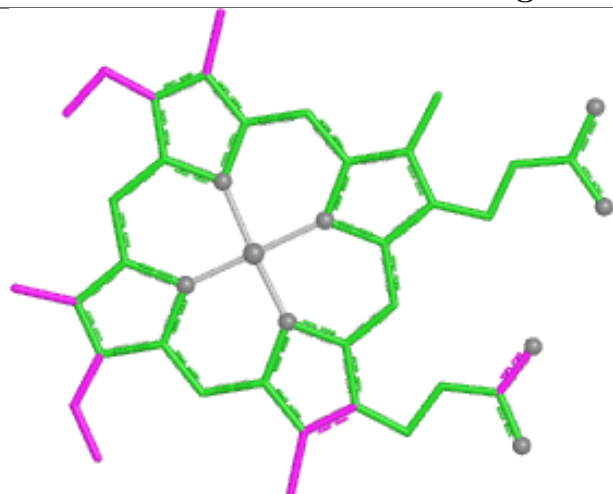
Ligand CLA a 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG D 412	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 411	
 Bond lengths	 Bond angles
 Torsions	 Rings



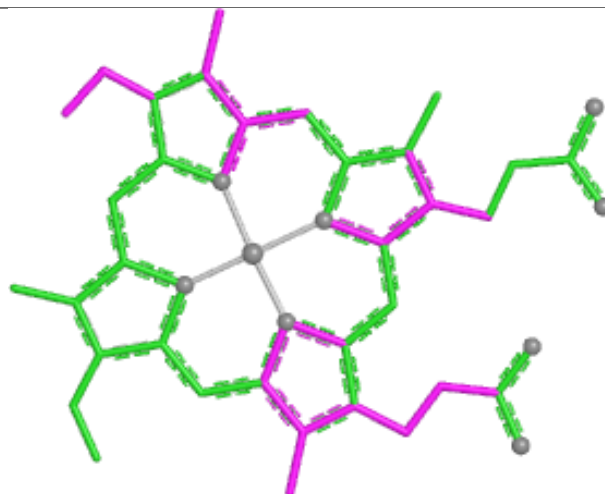




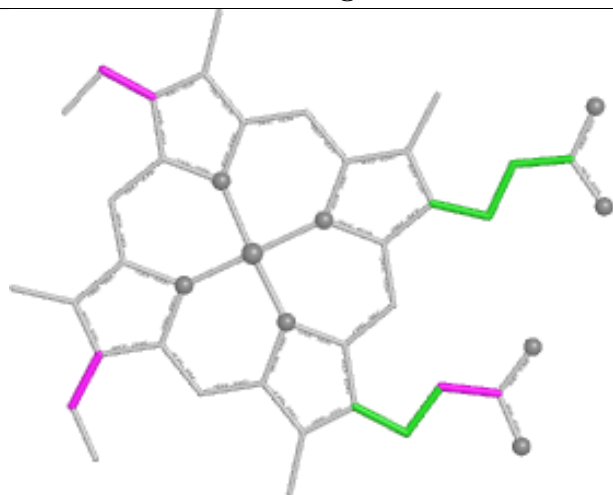
Ligand HEC v 203



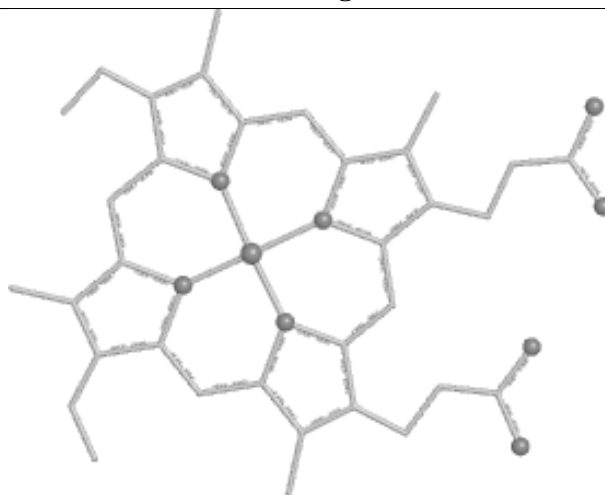
Bond lengths



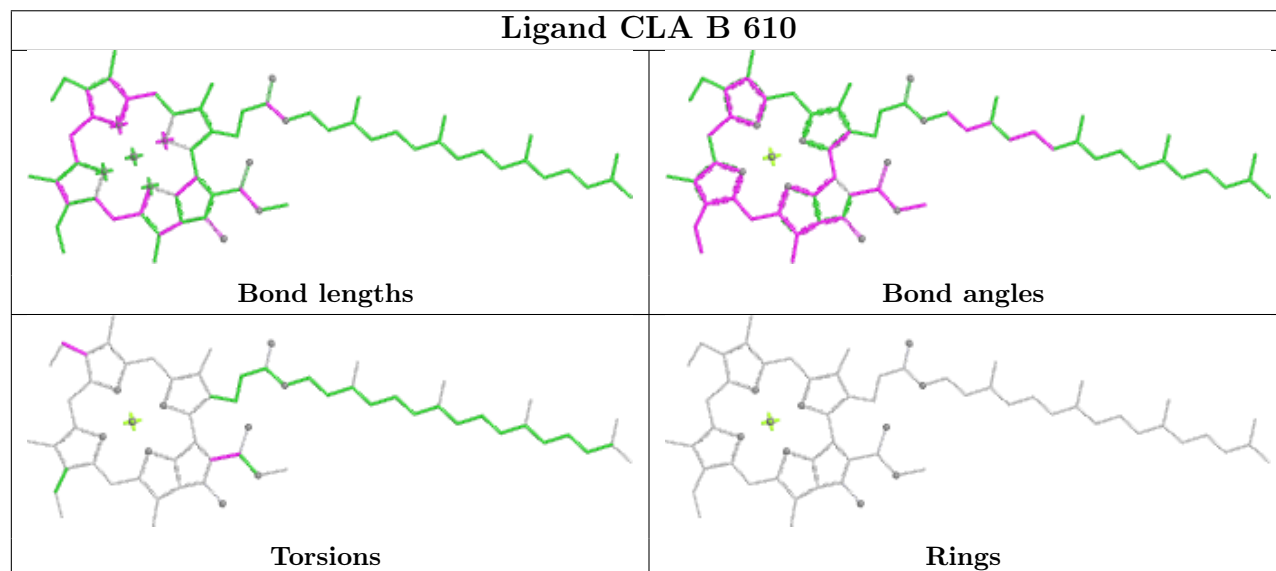
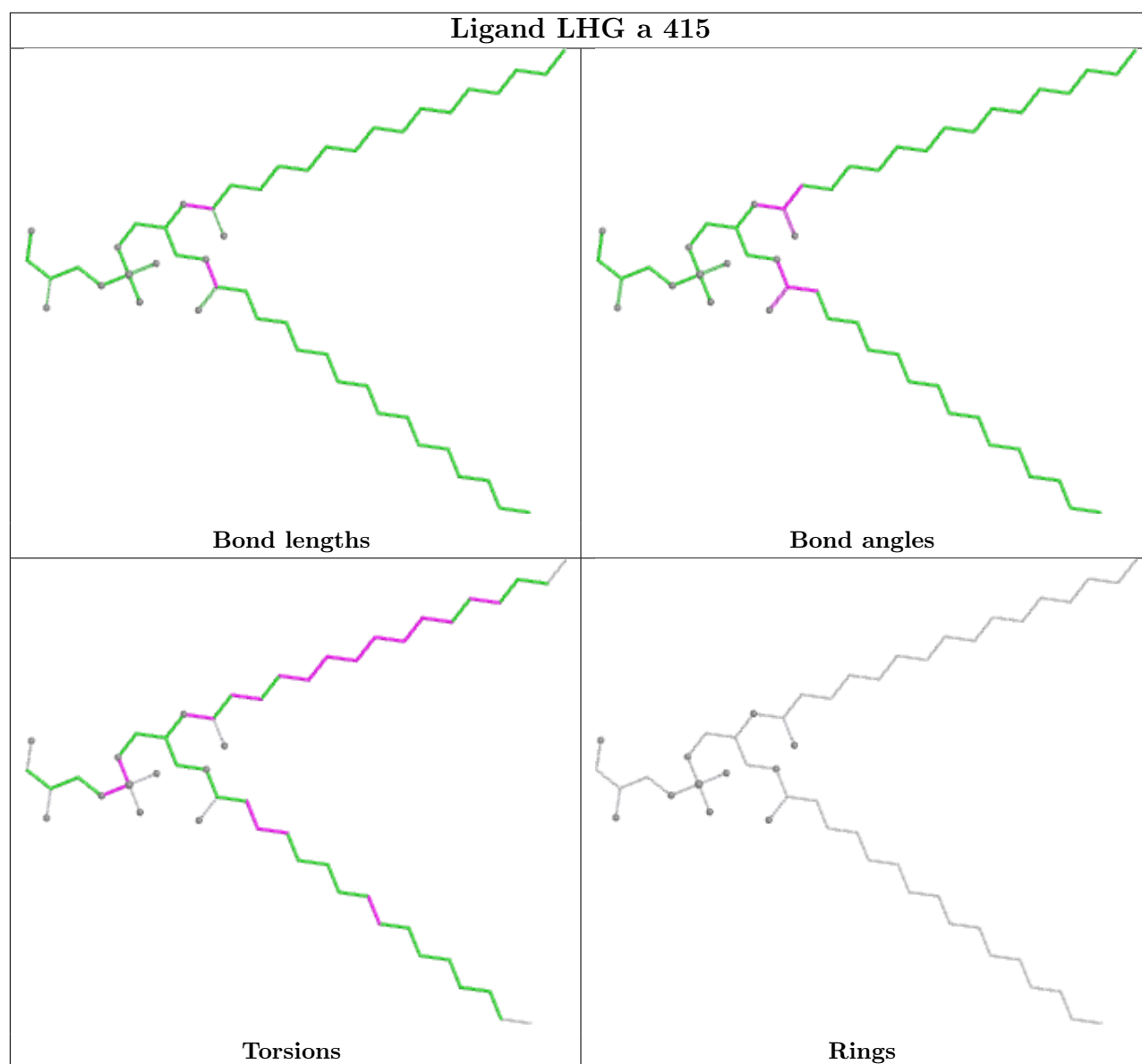
Bond angles

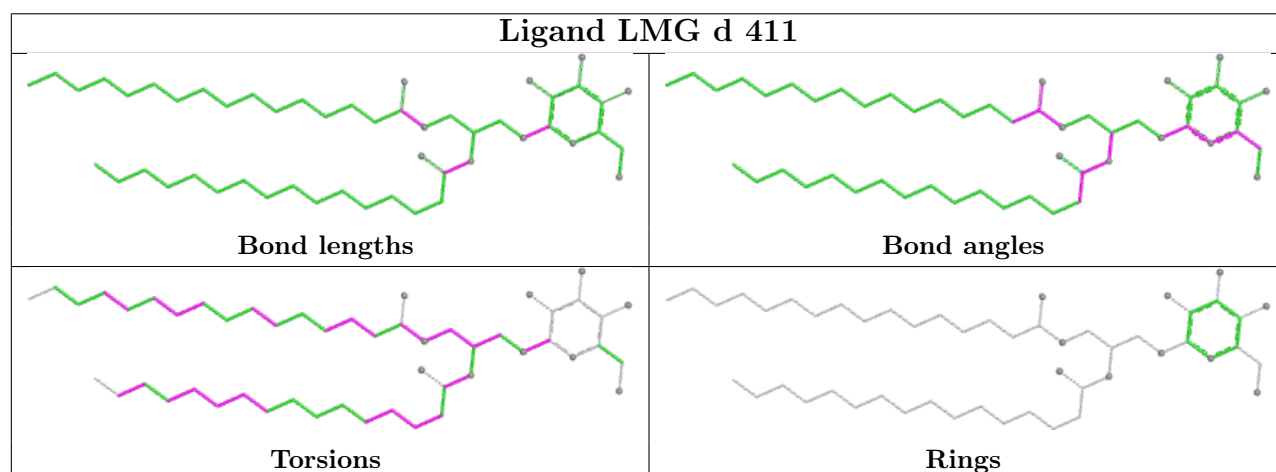
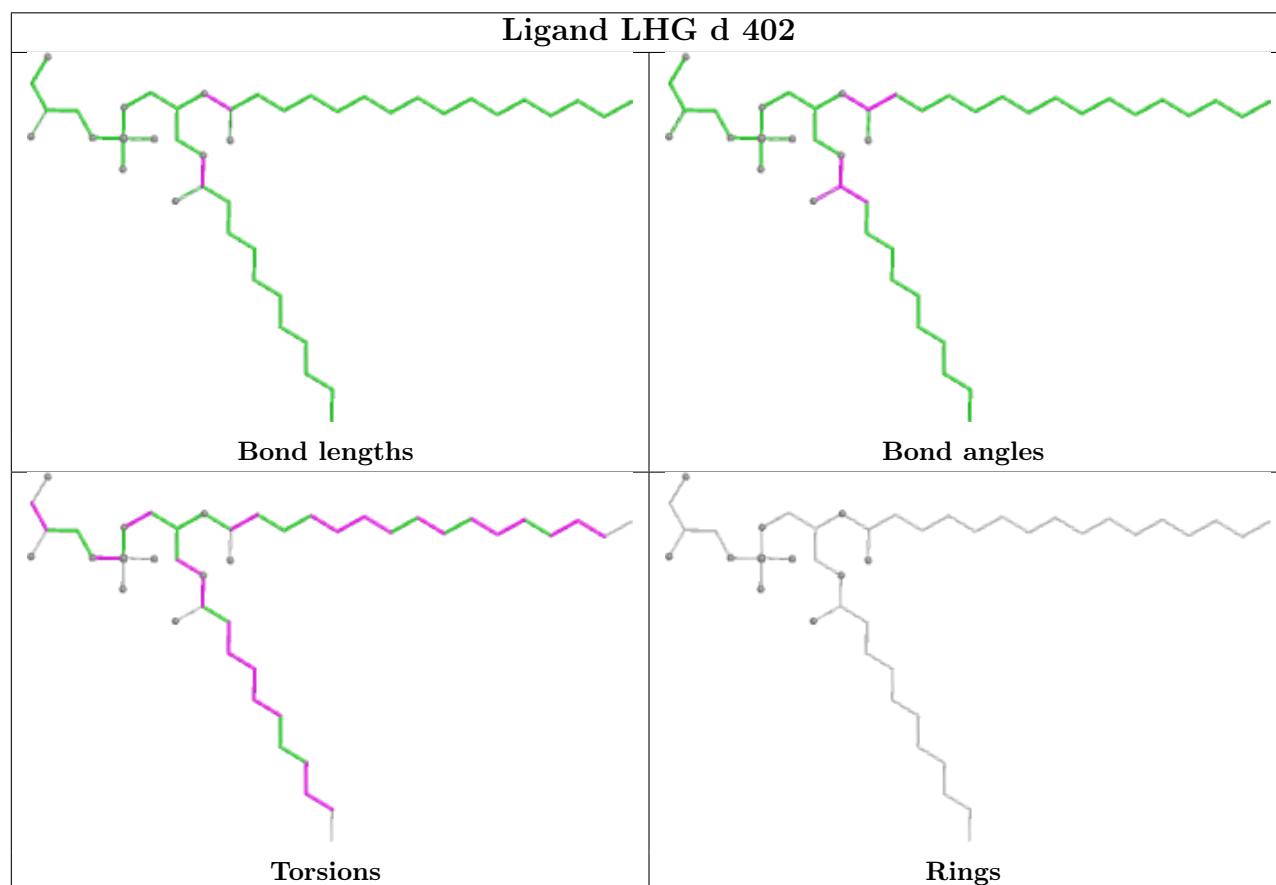
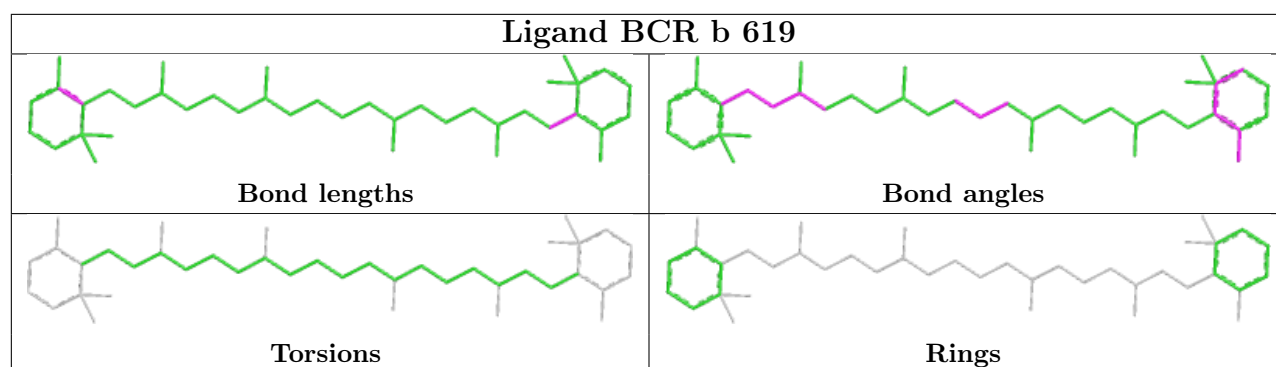


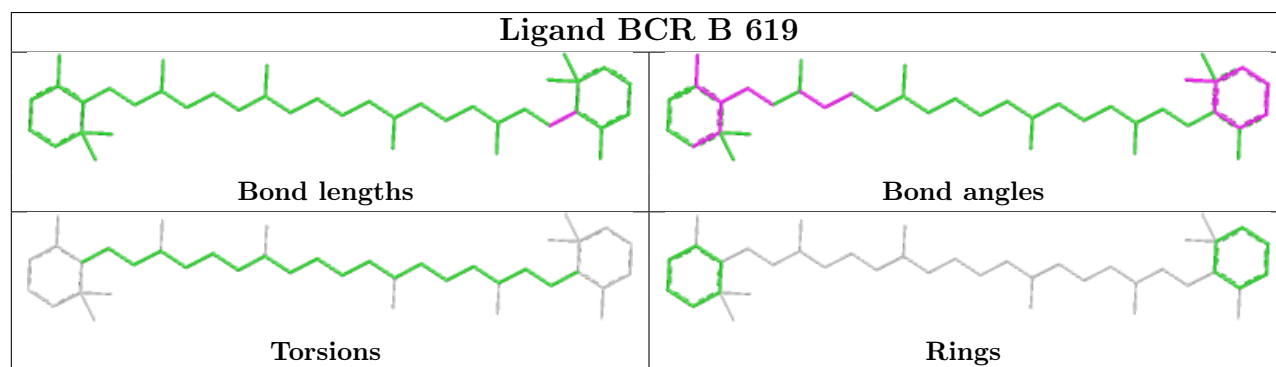
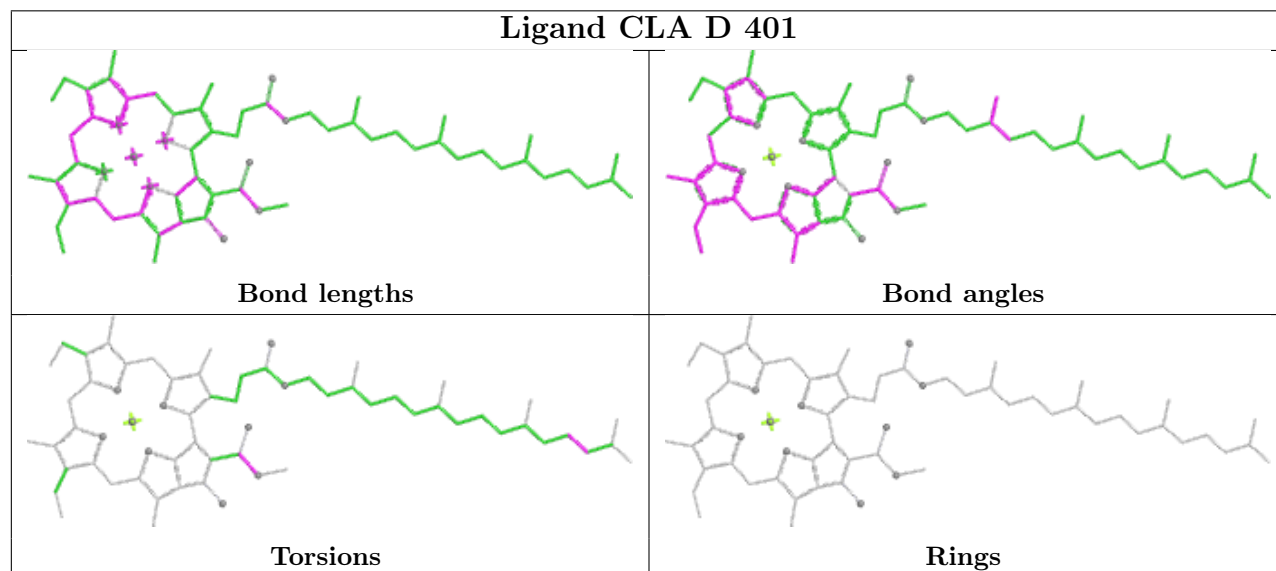
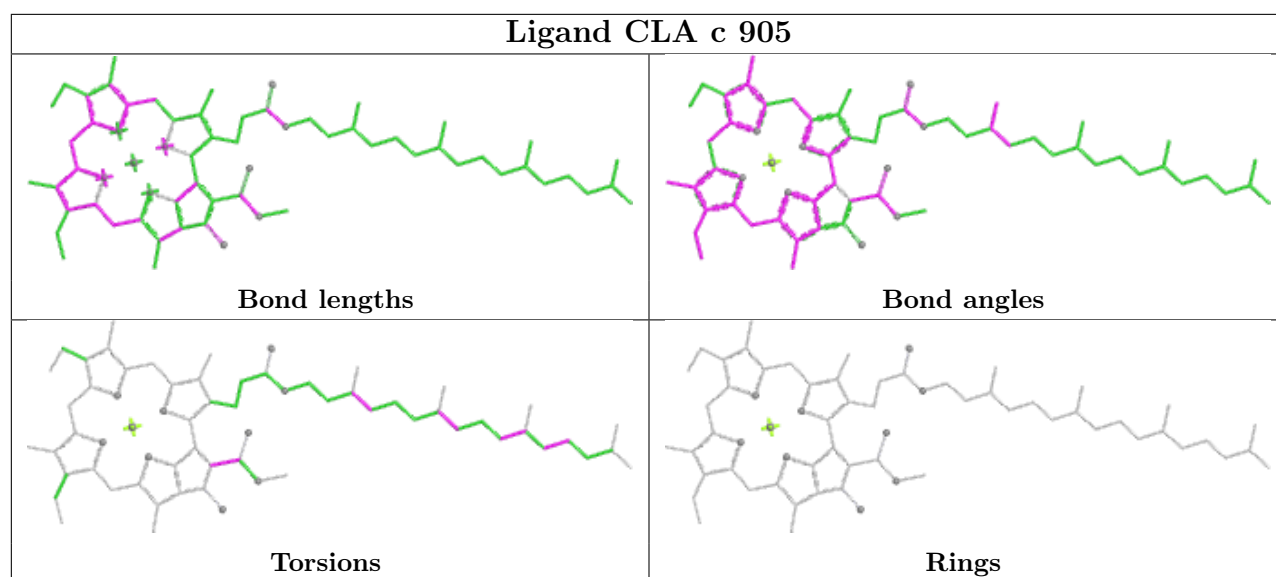
Torsions

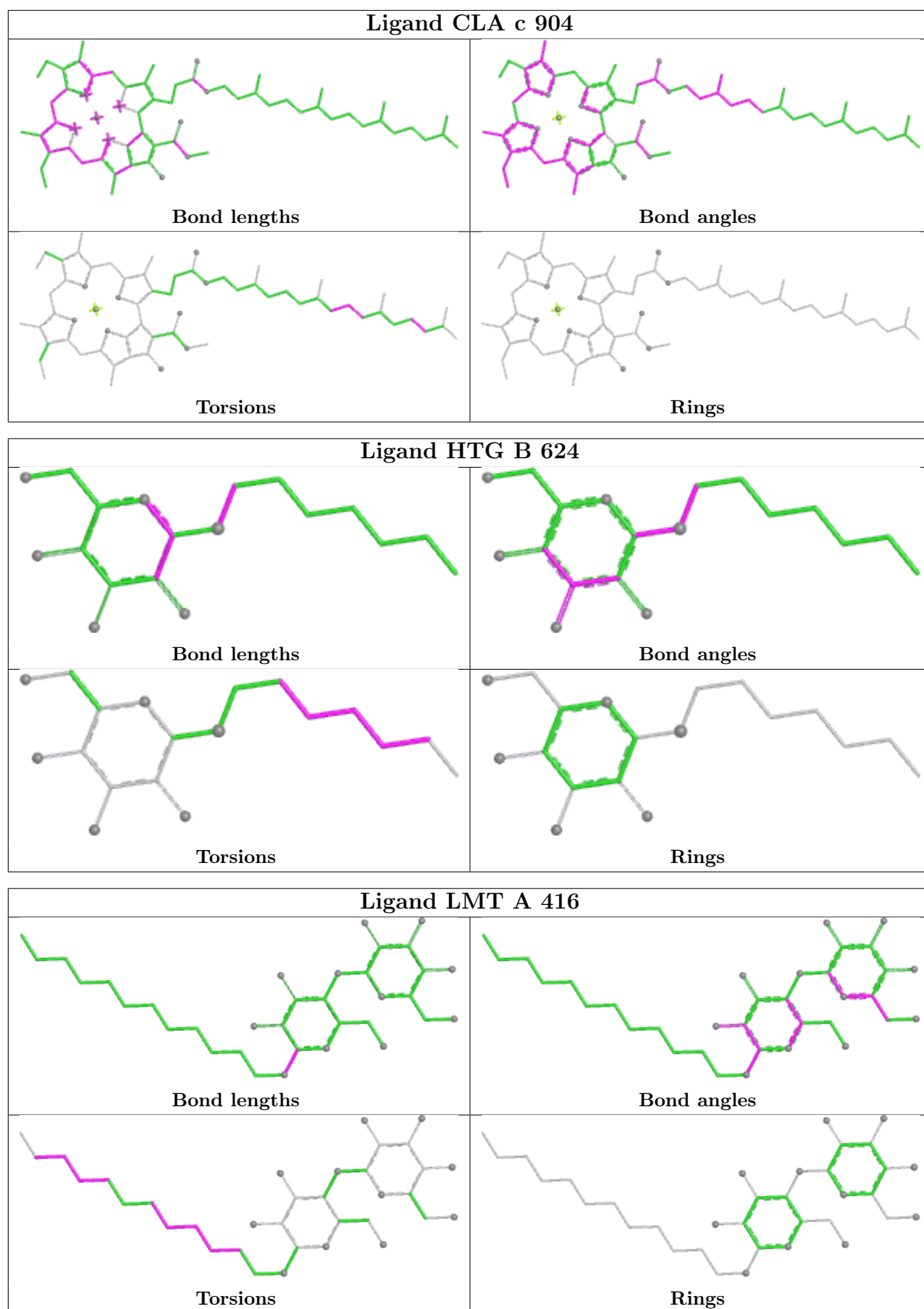


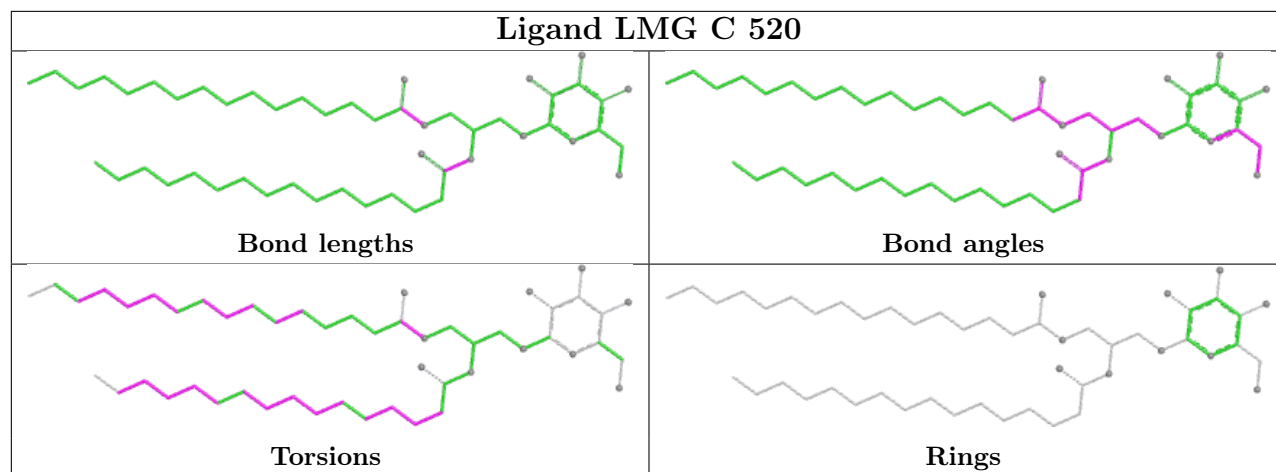
Rings

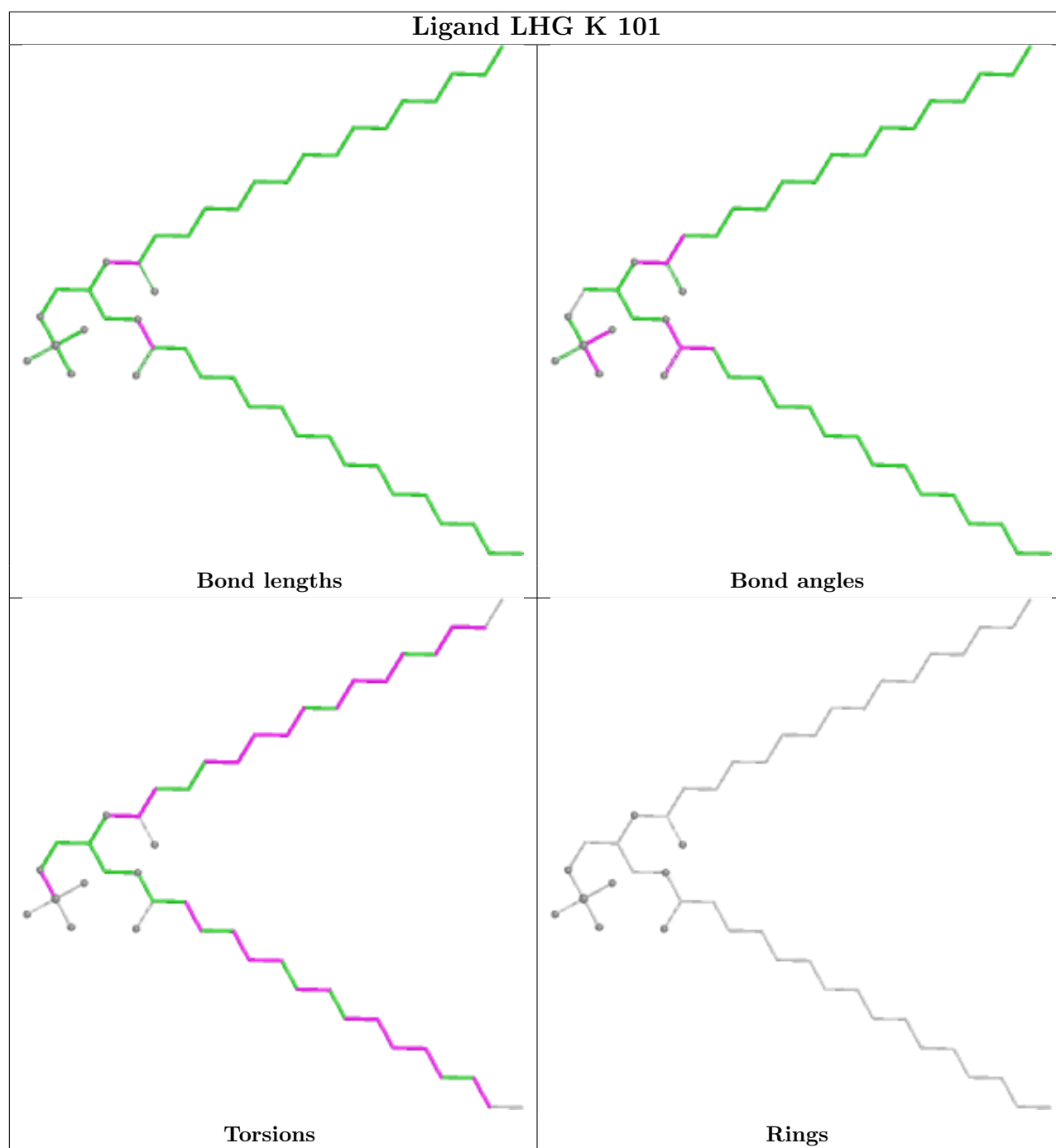


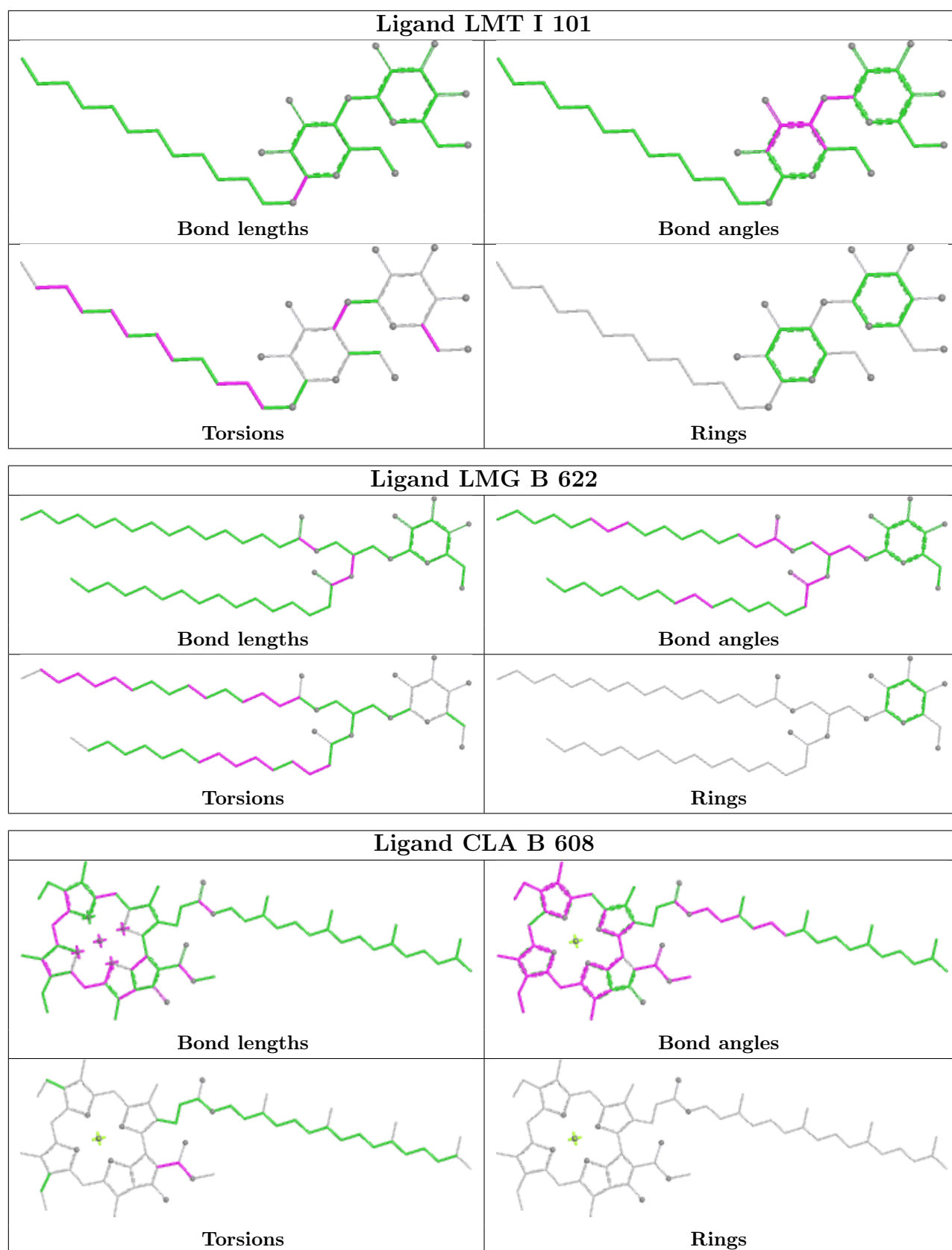


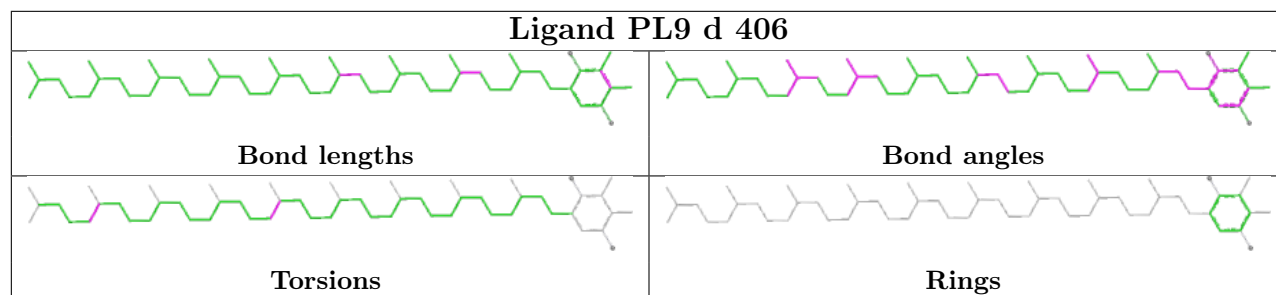
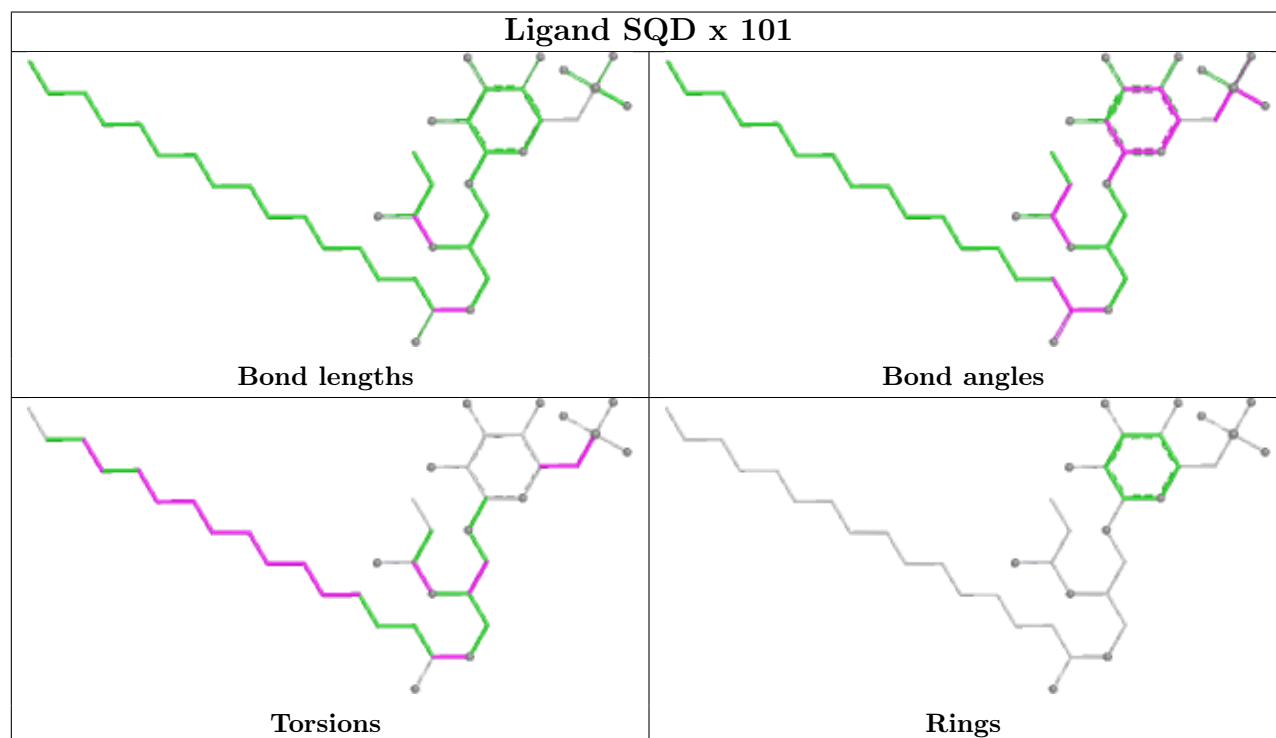
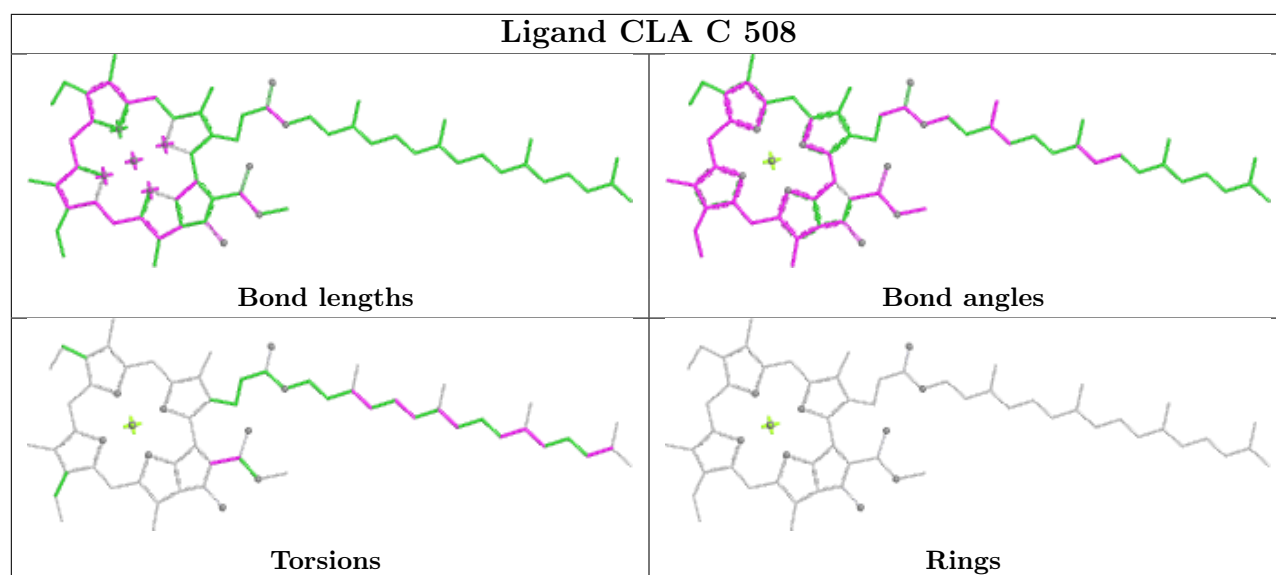


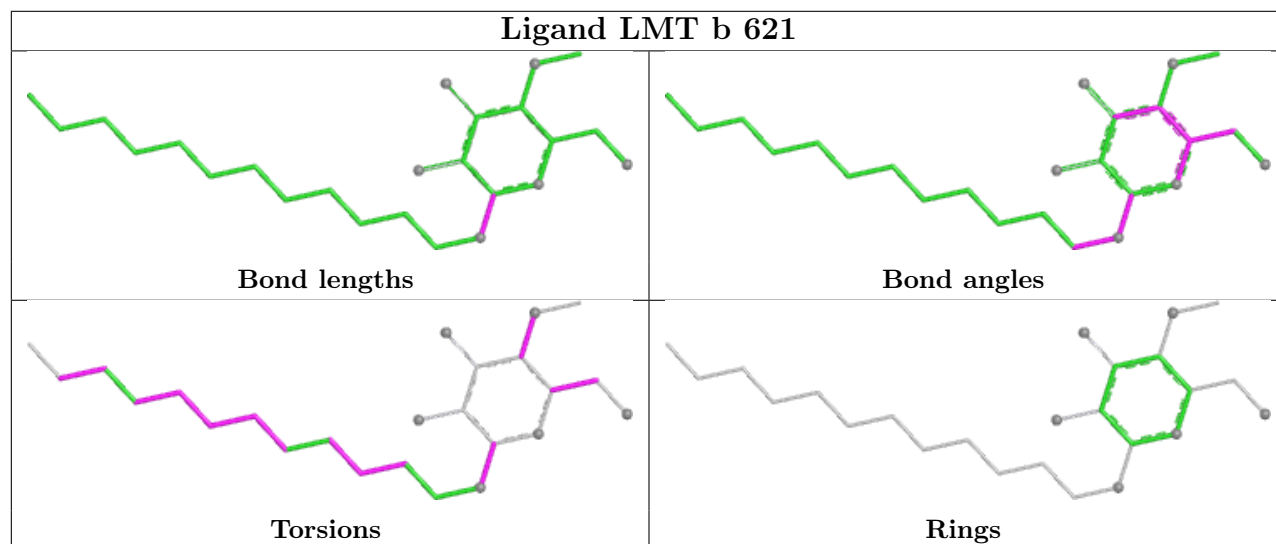
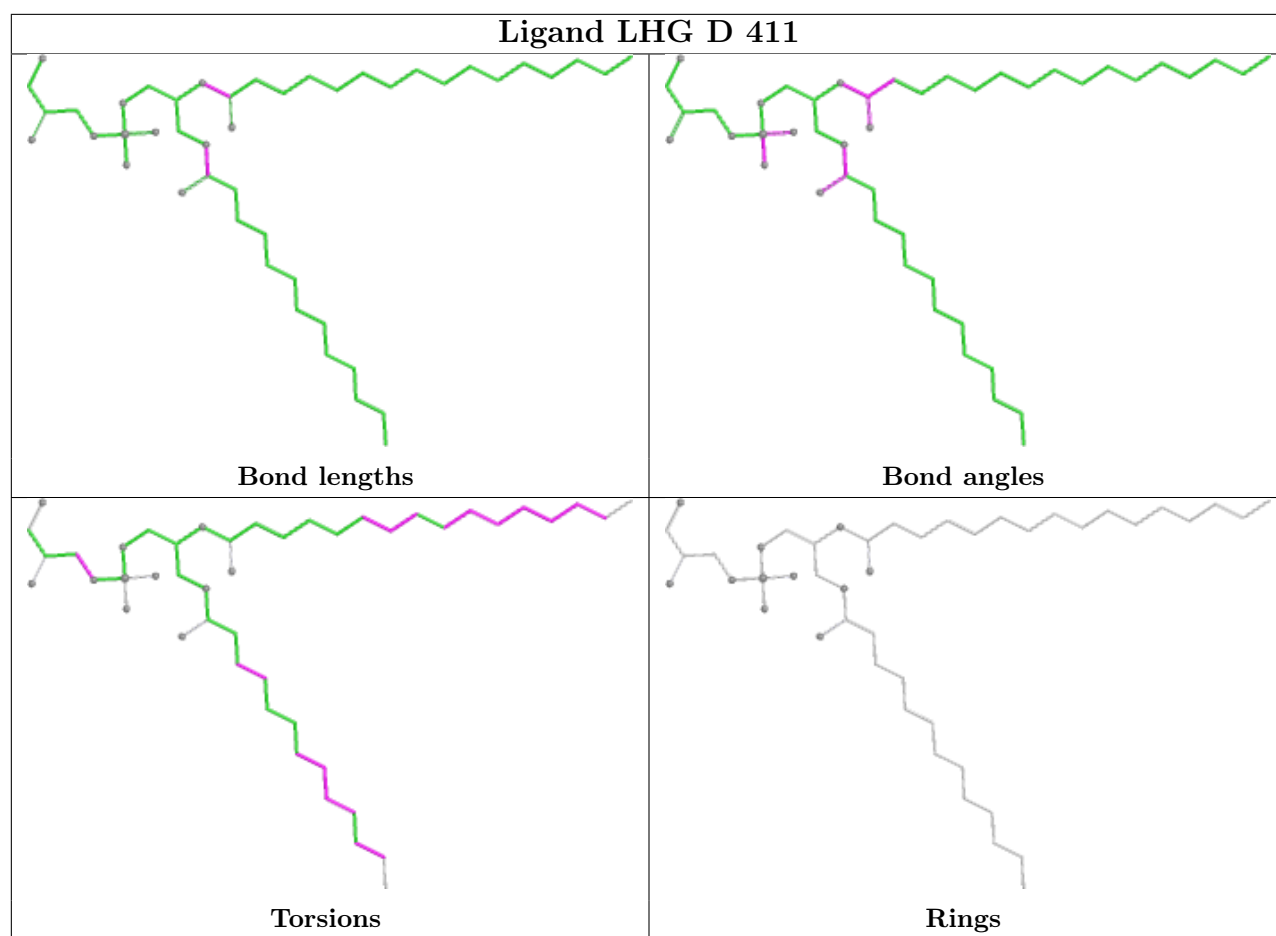


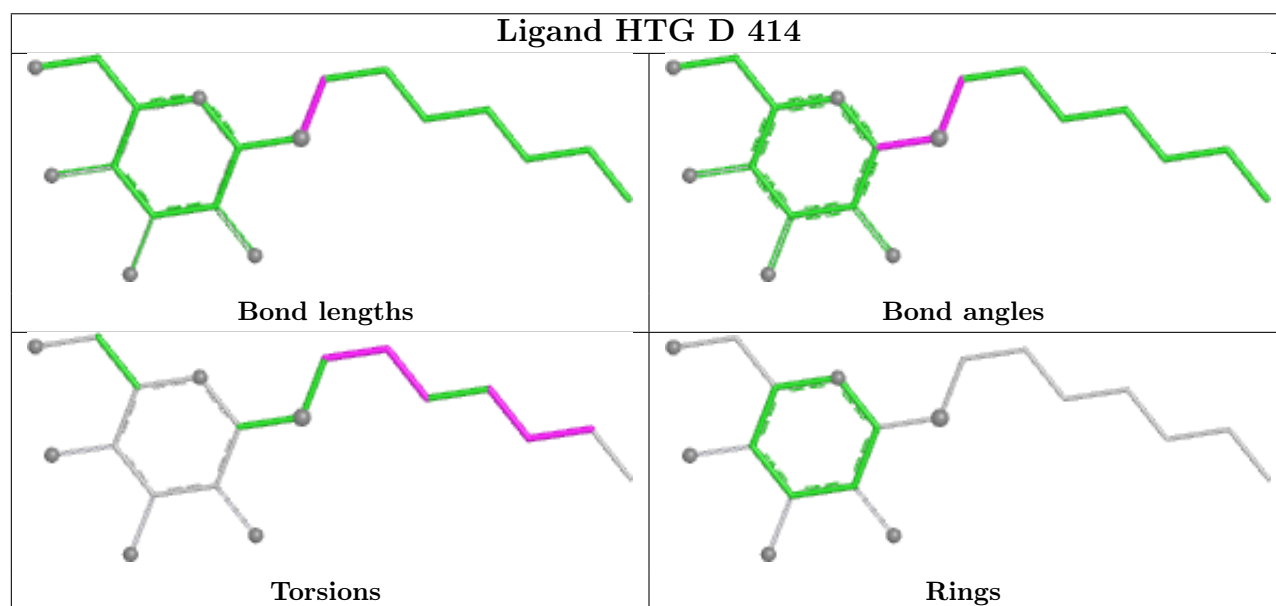
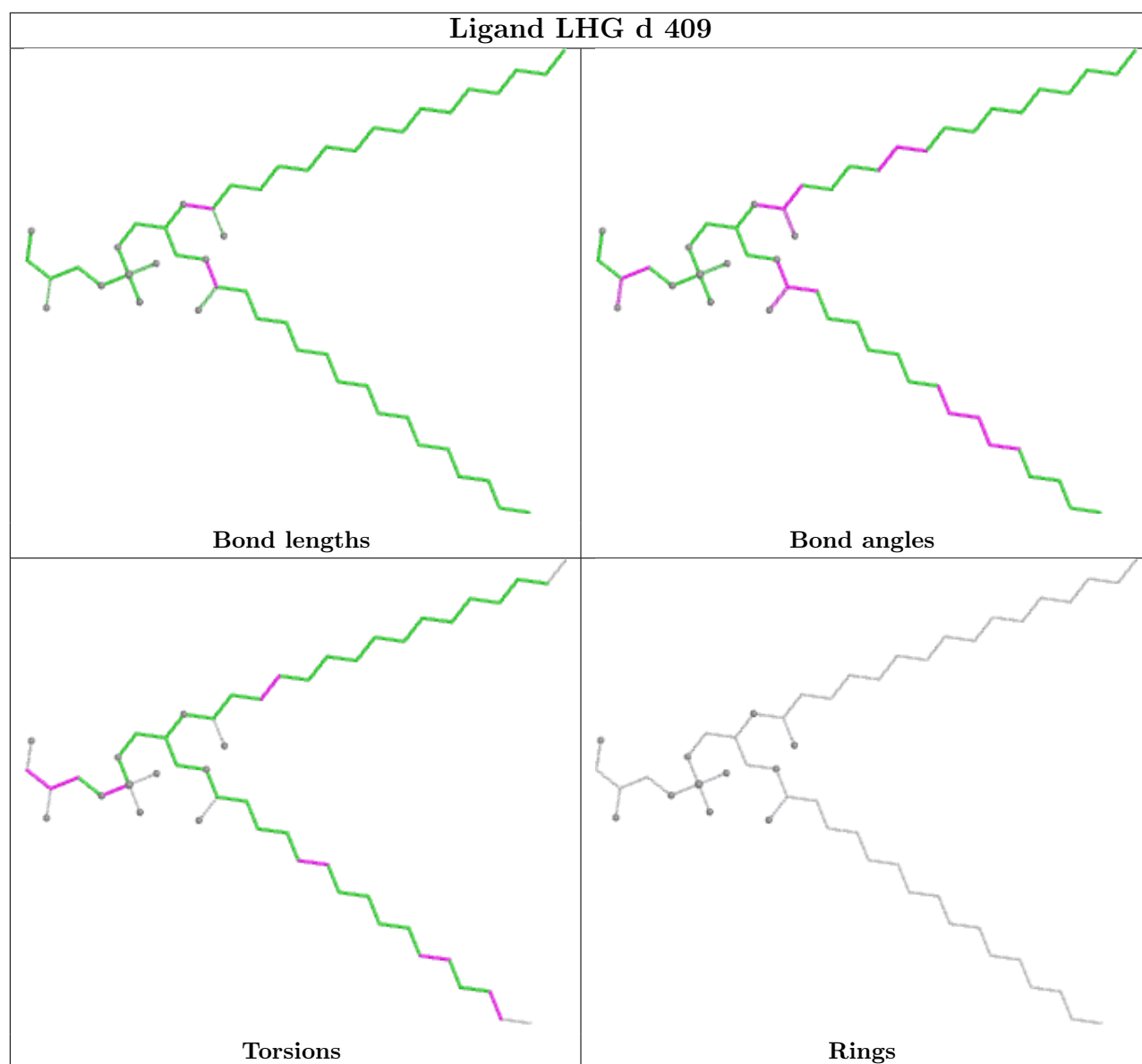


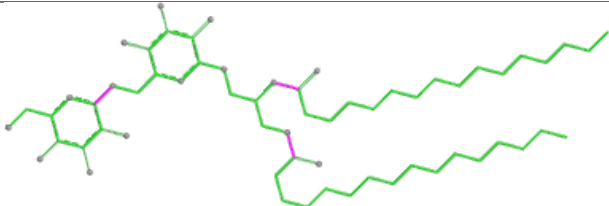
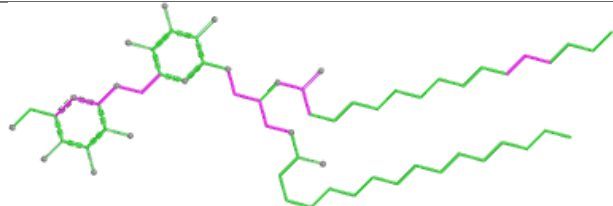
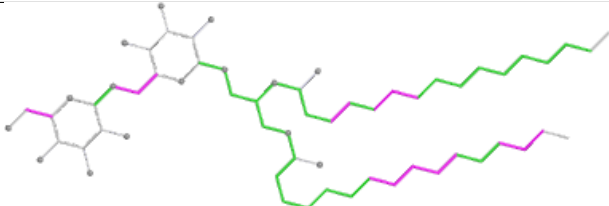
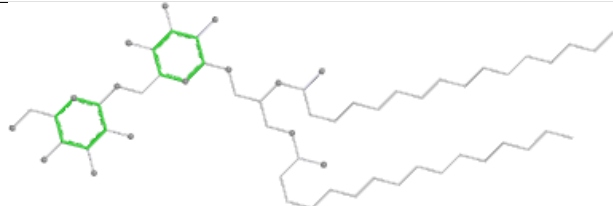


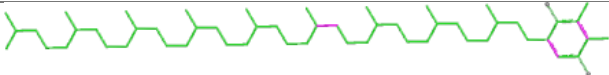
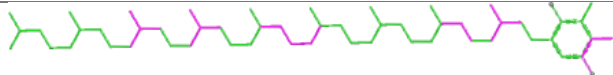
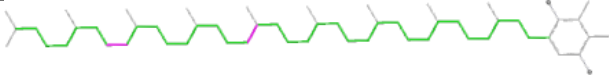
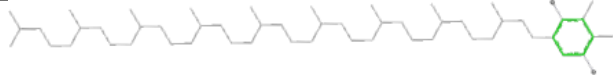


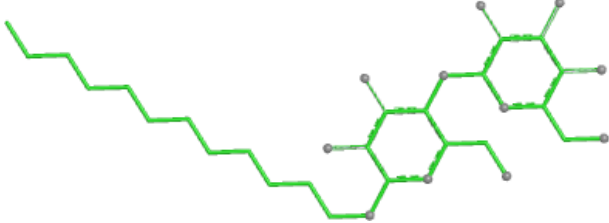
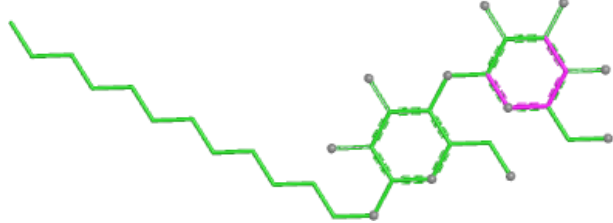
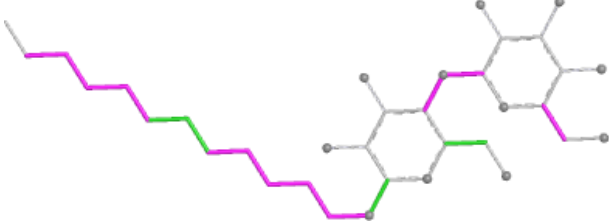
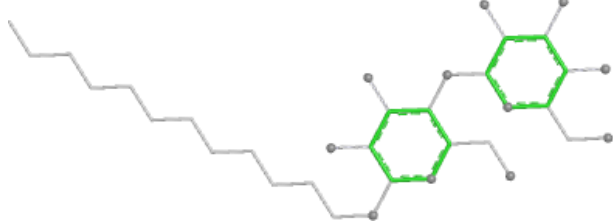


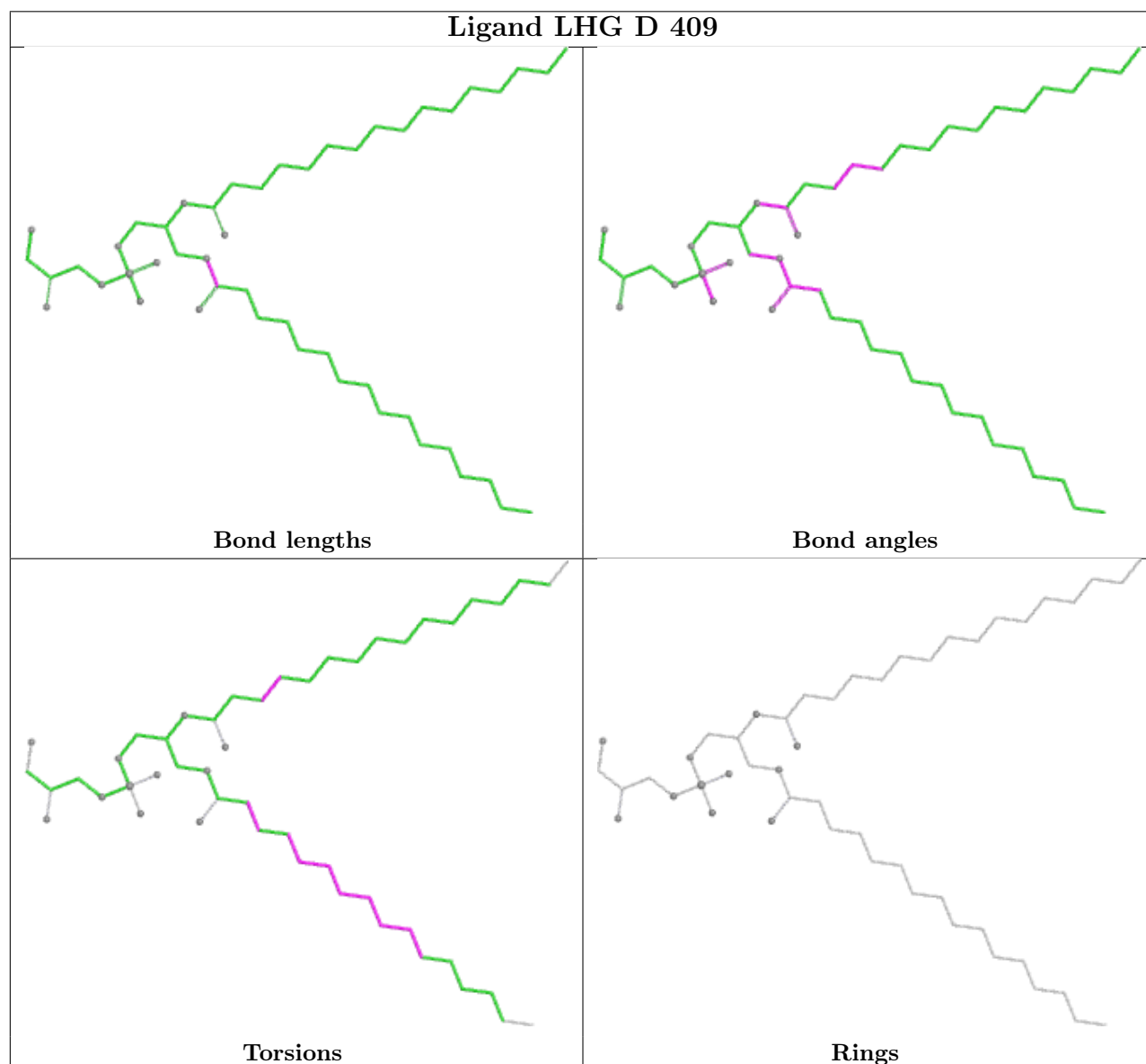
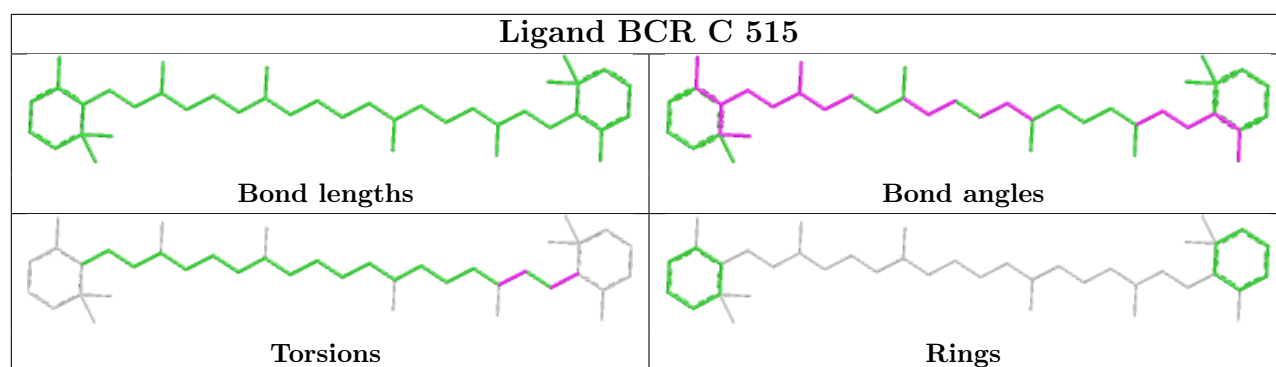


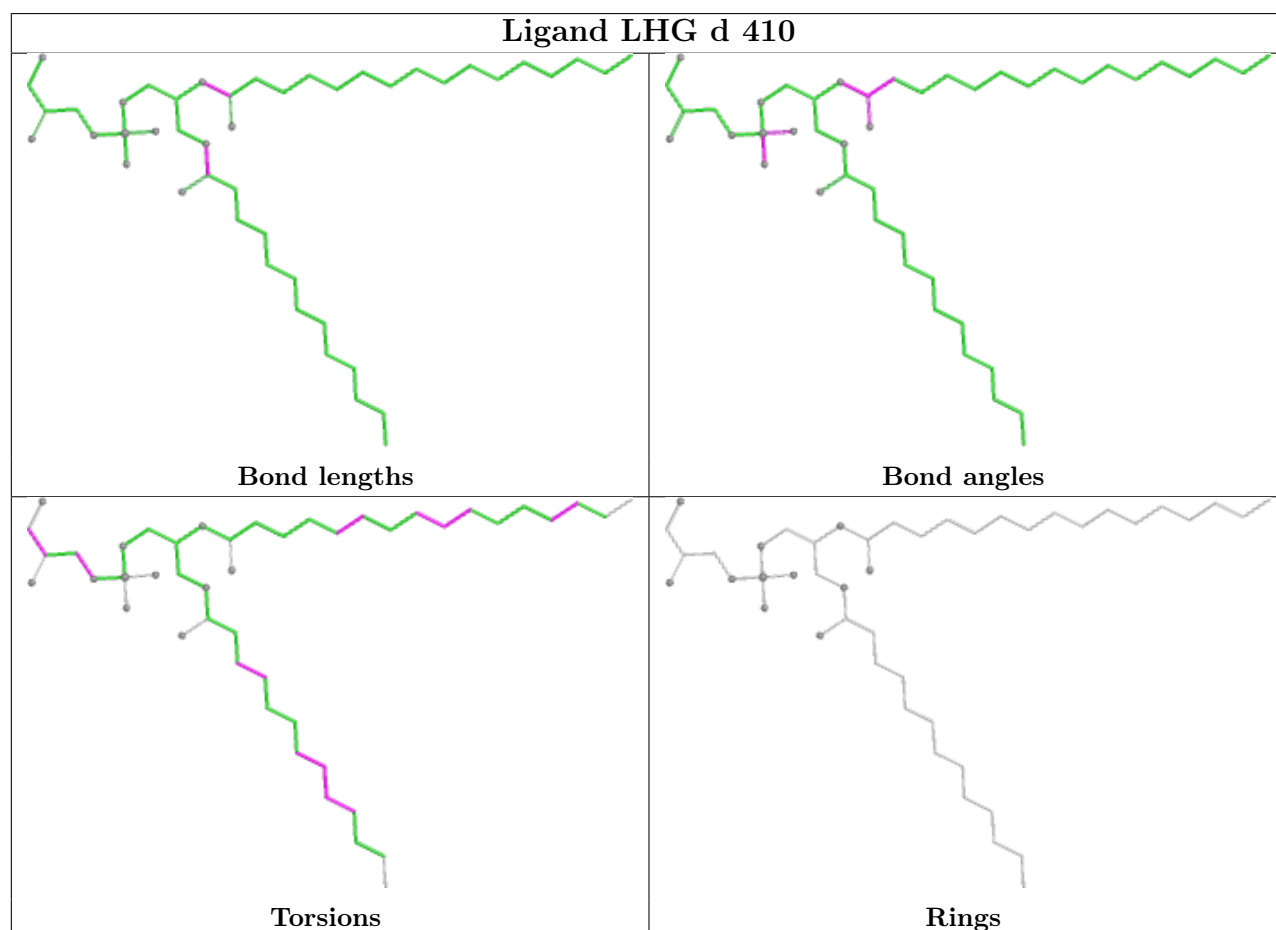
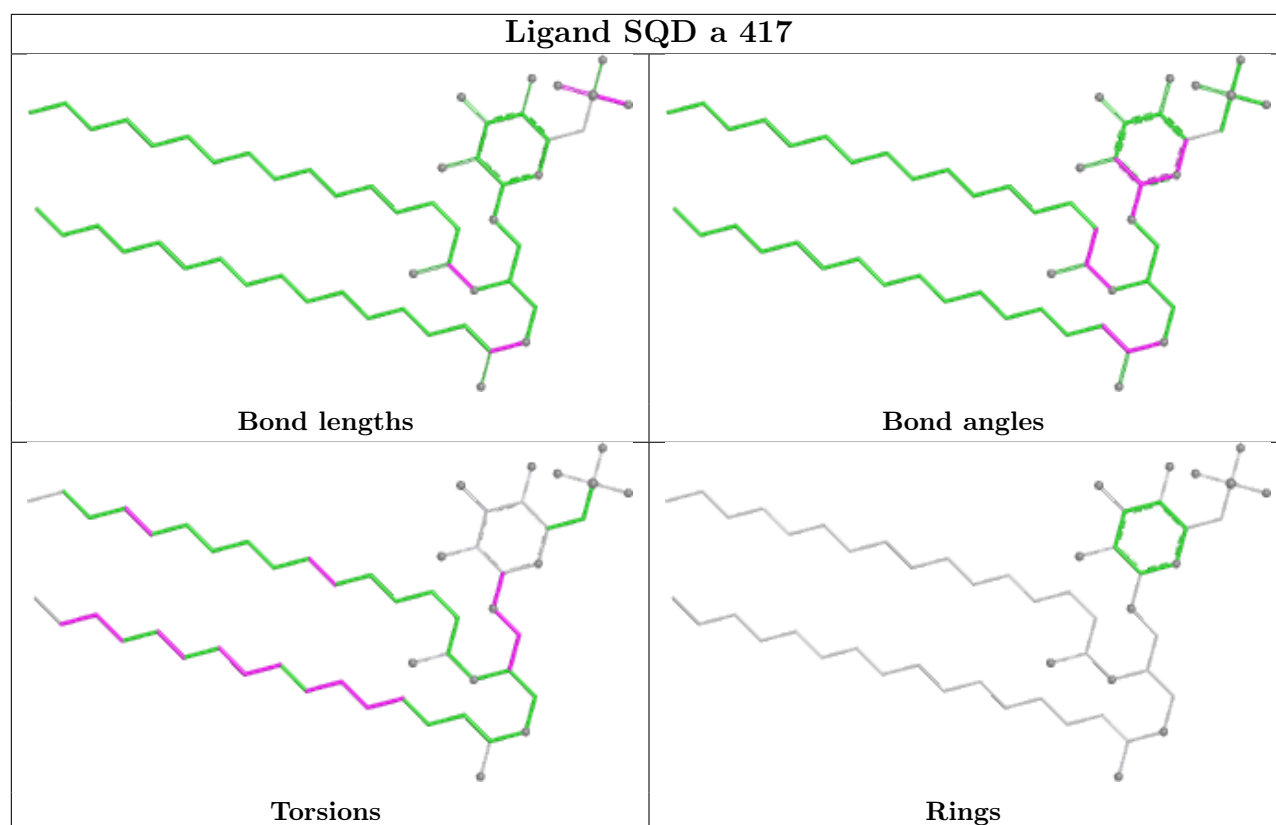


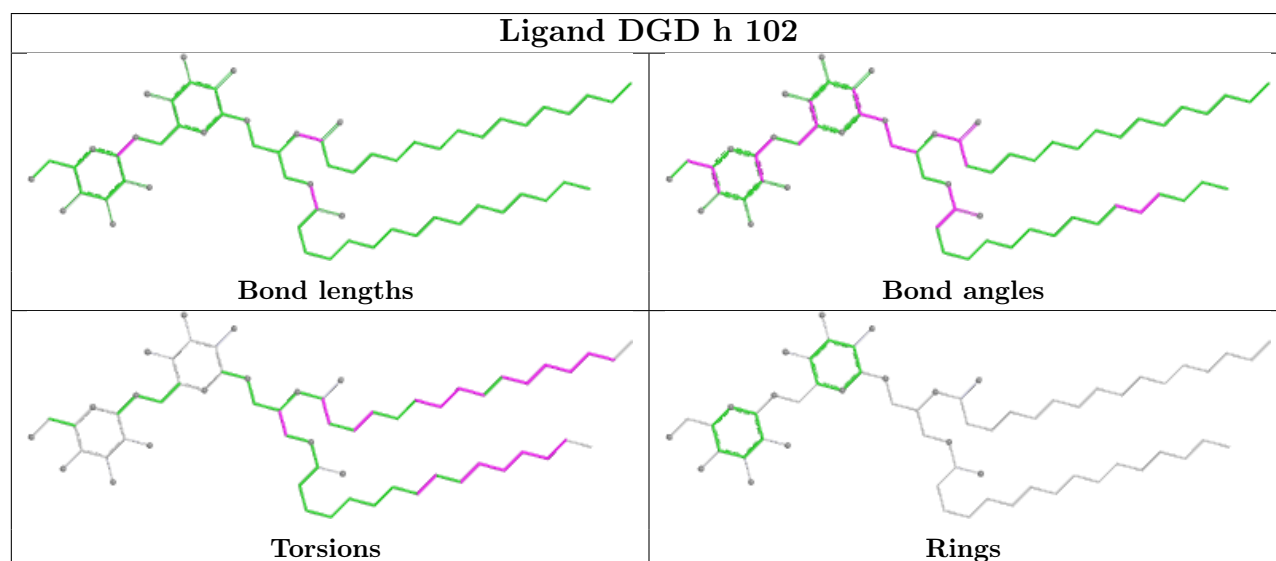
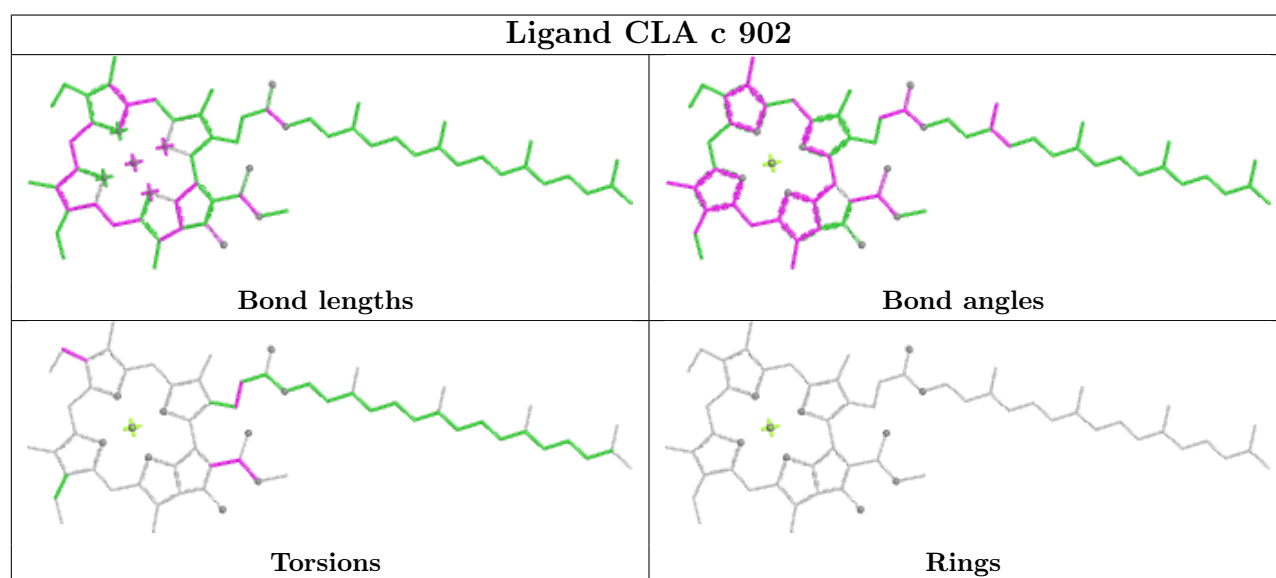
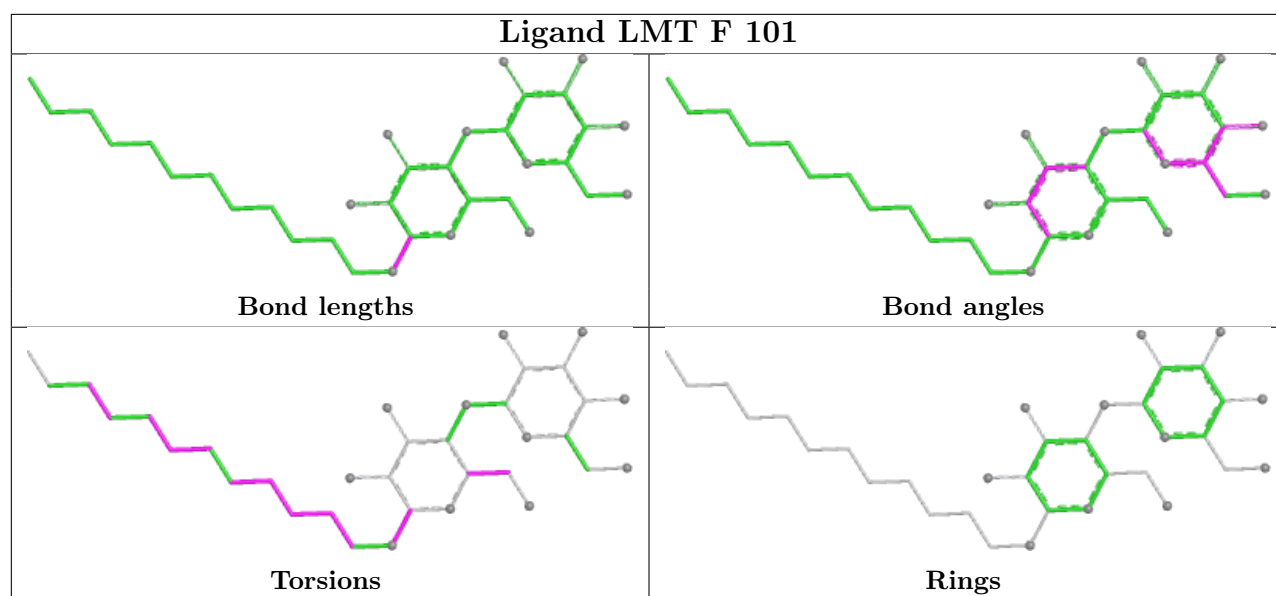
Ligand DGD c 917	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

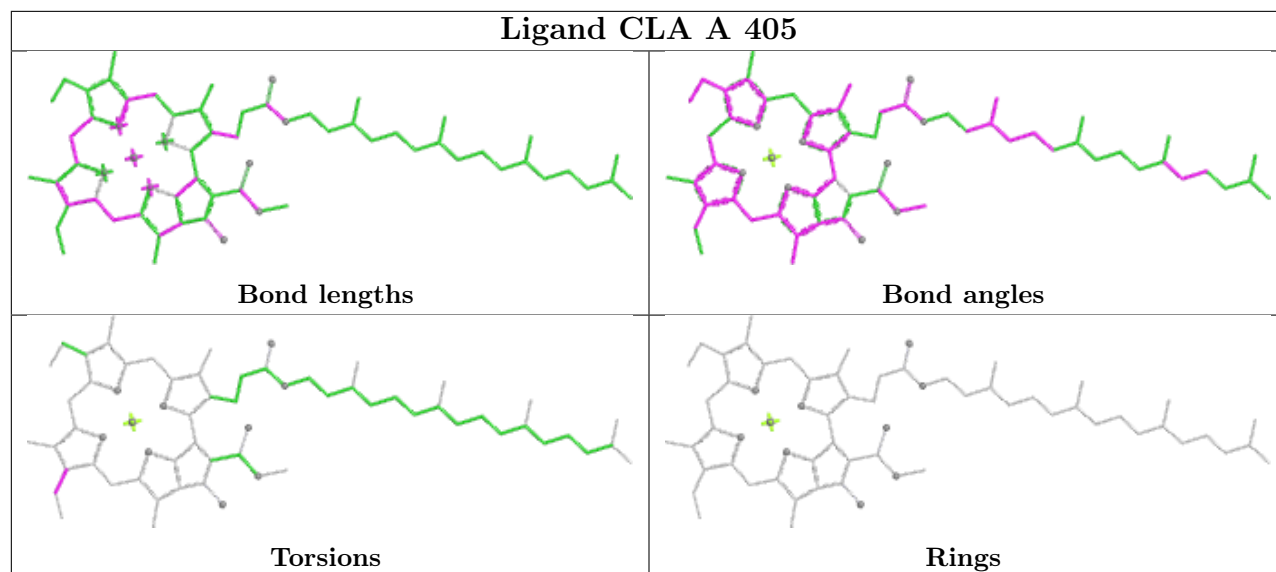
Ligand LMT B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings



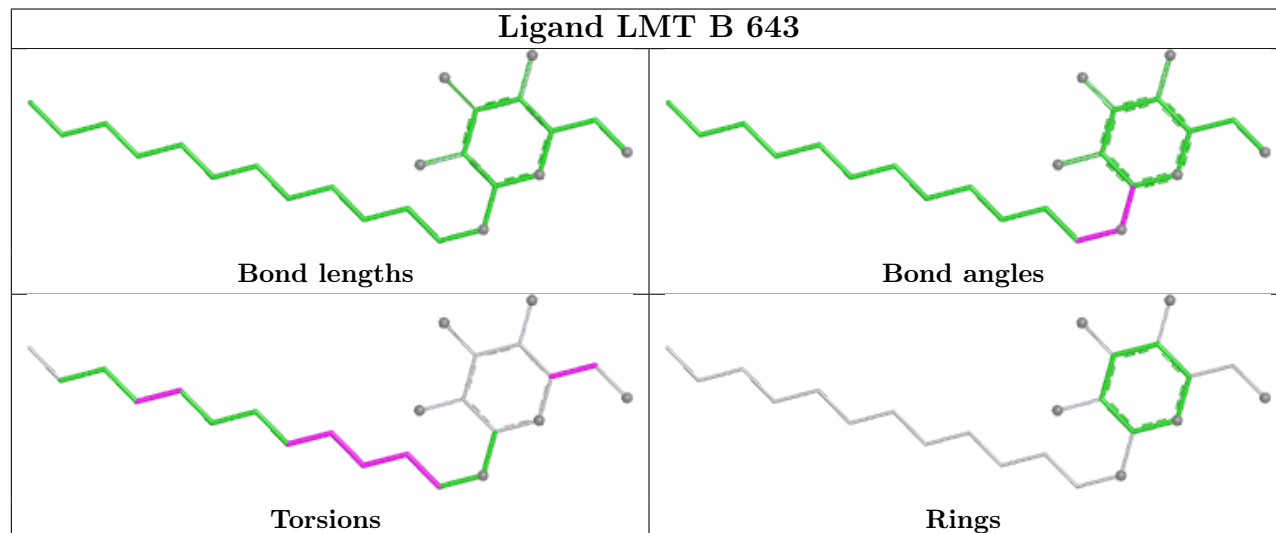




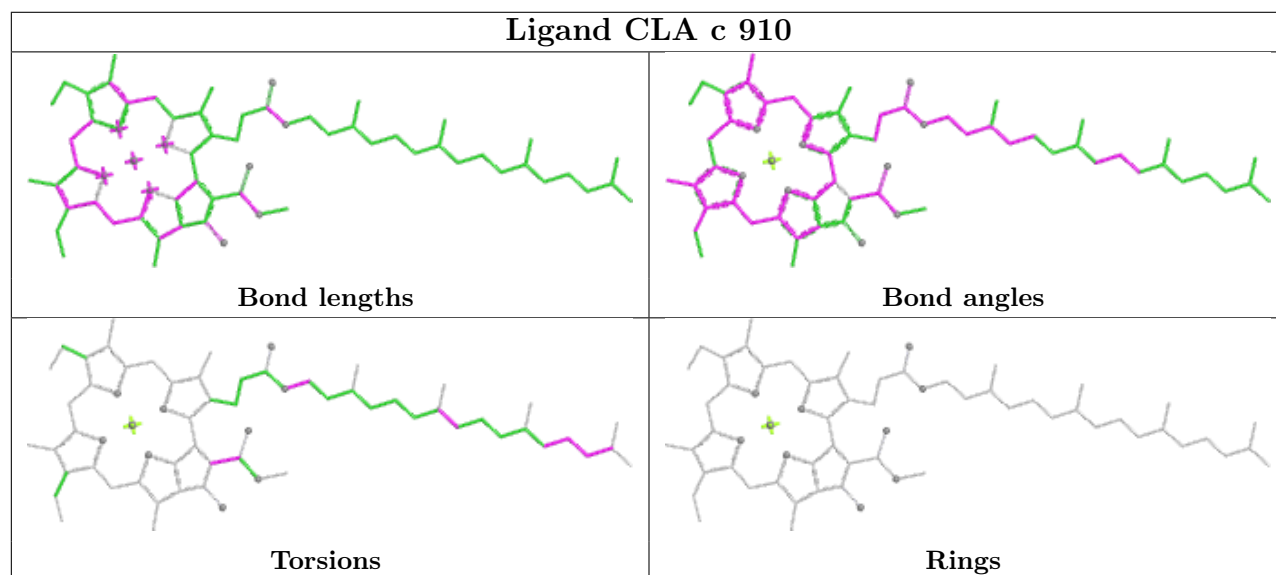
Ligand CLA A 405

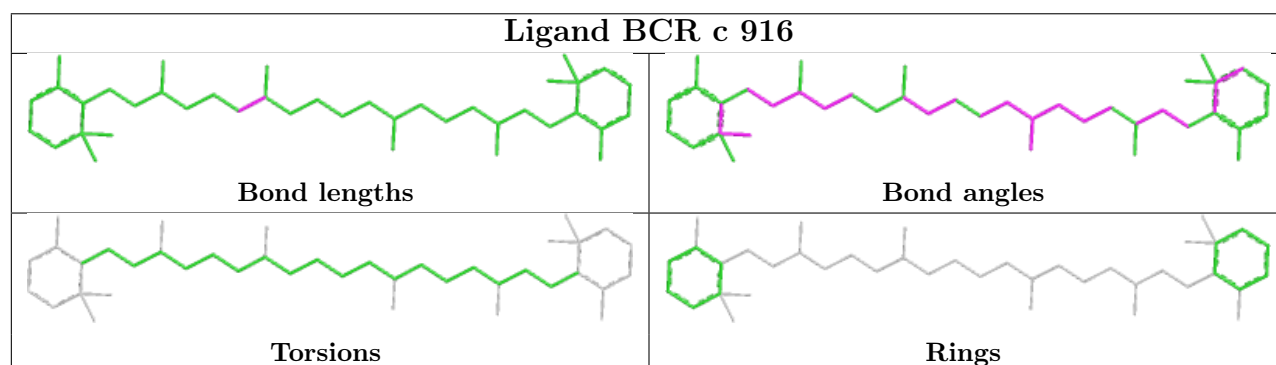
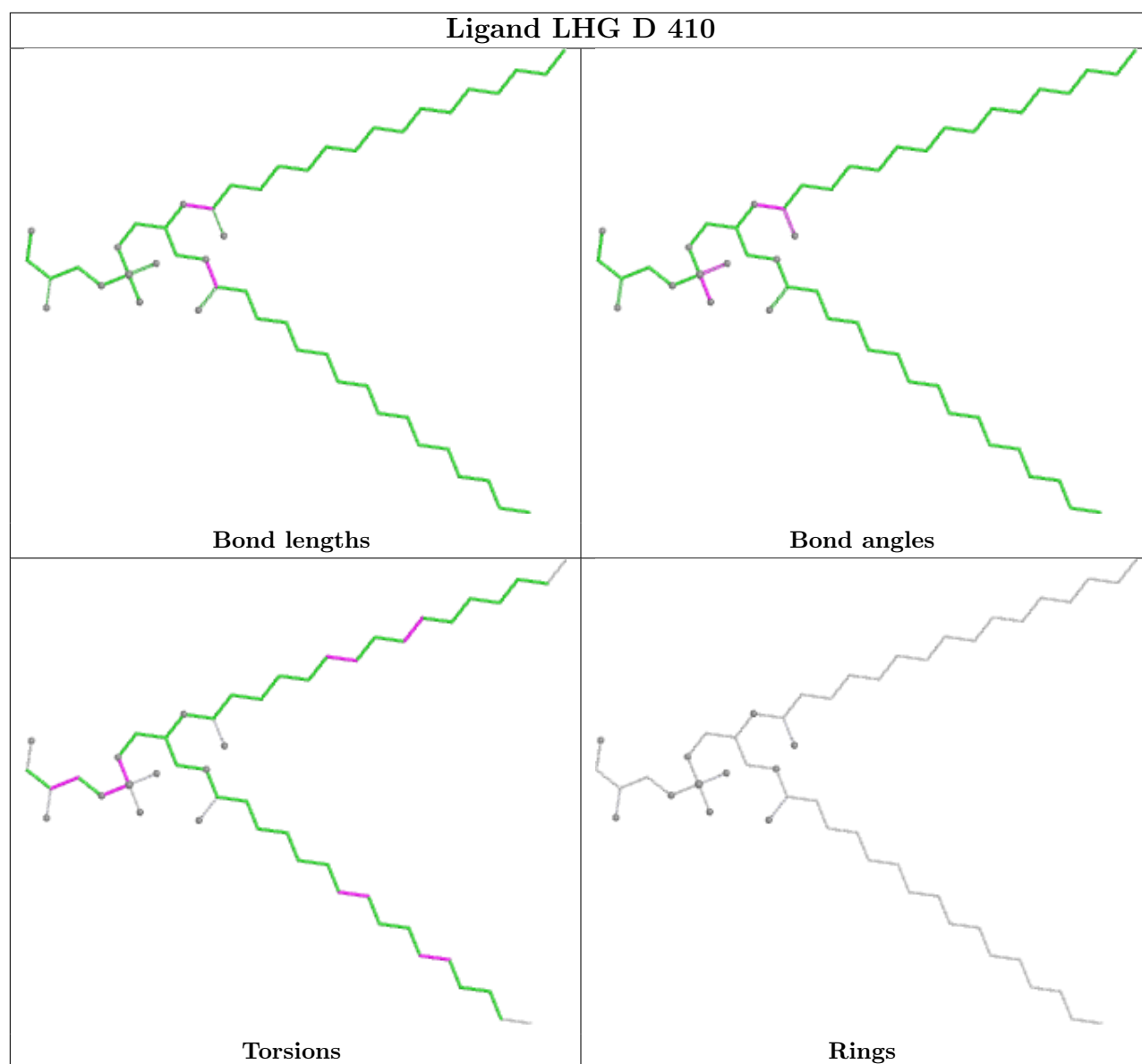


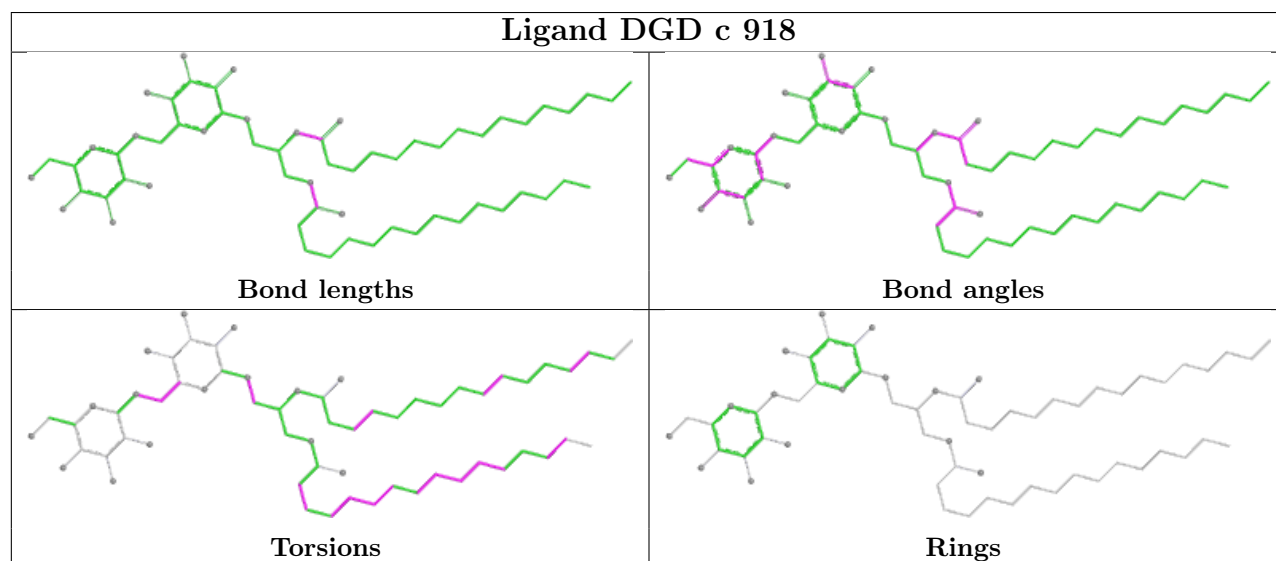
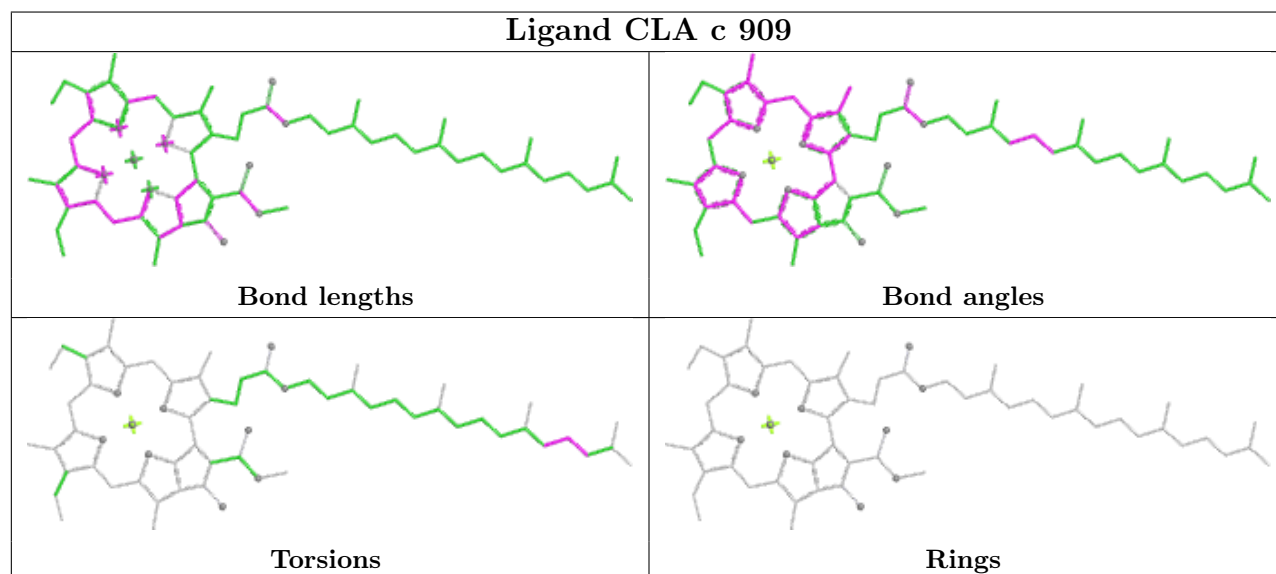
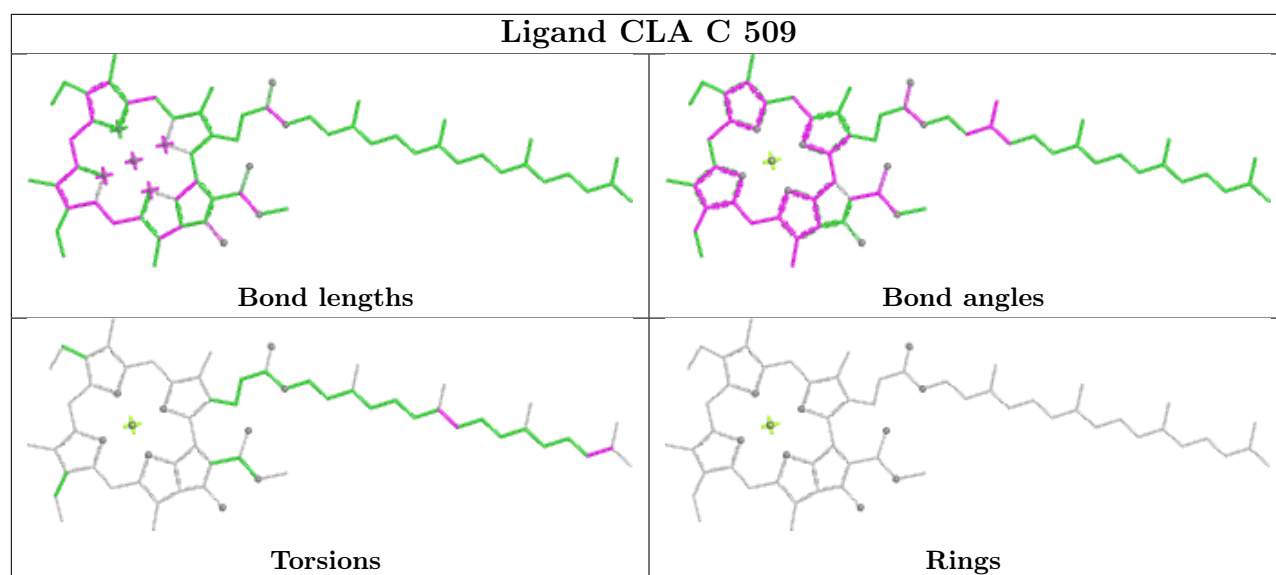
Ligand LMT B 643

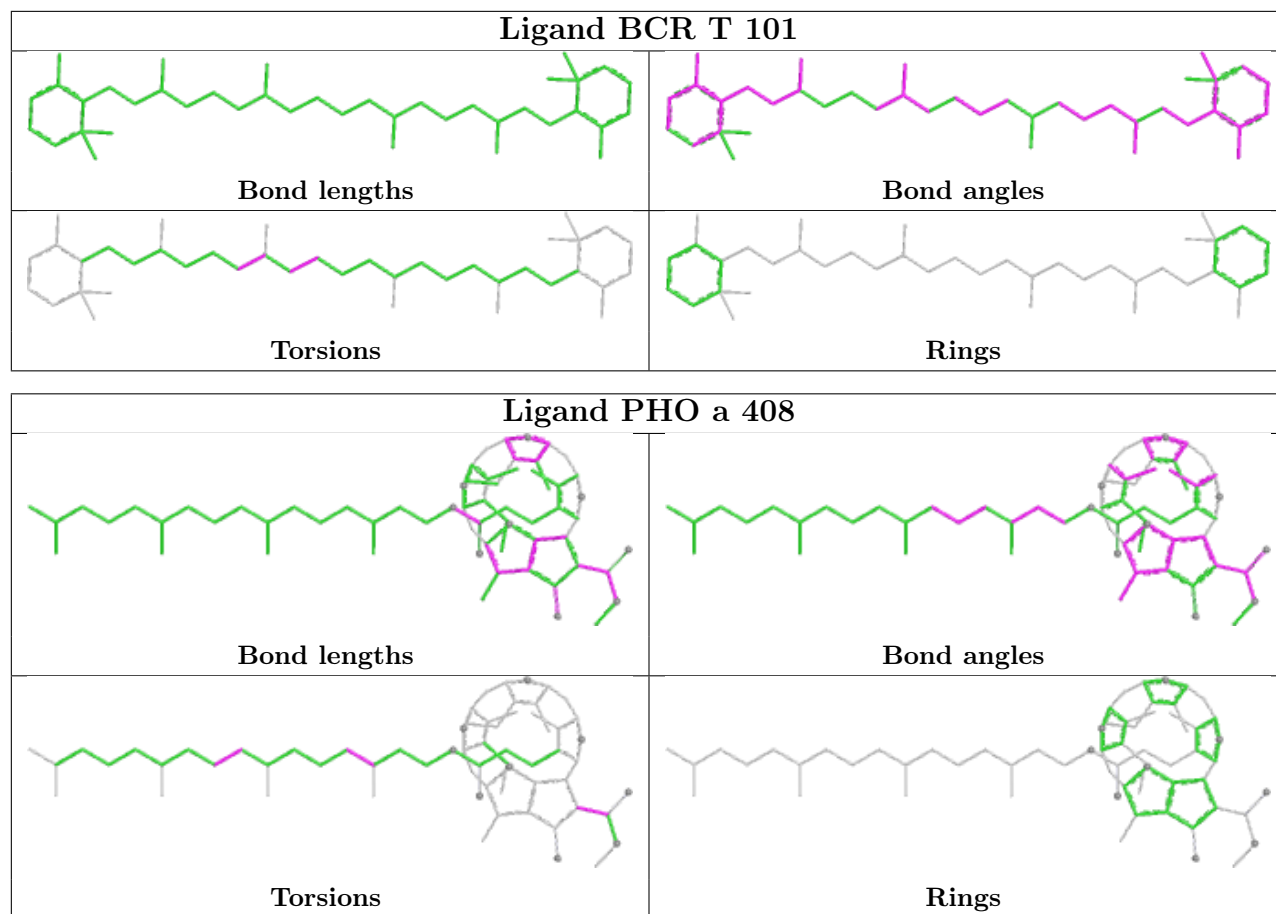


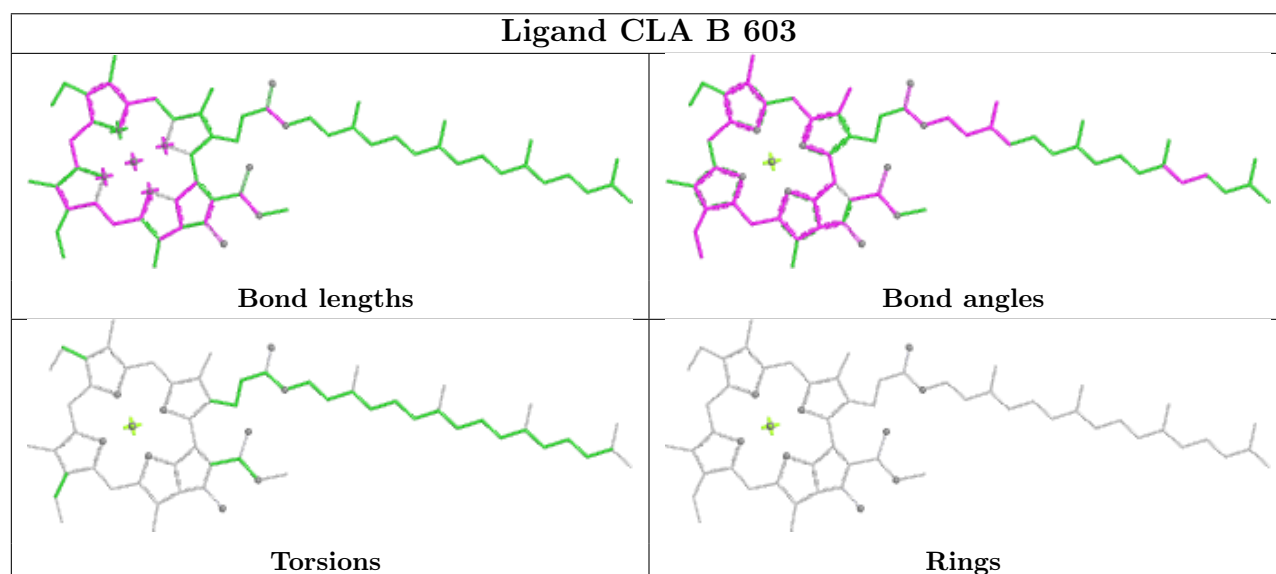
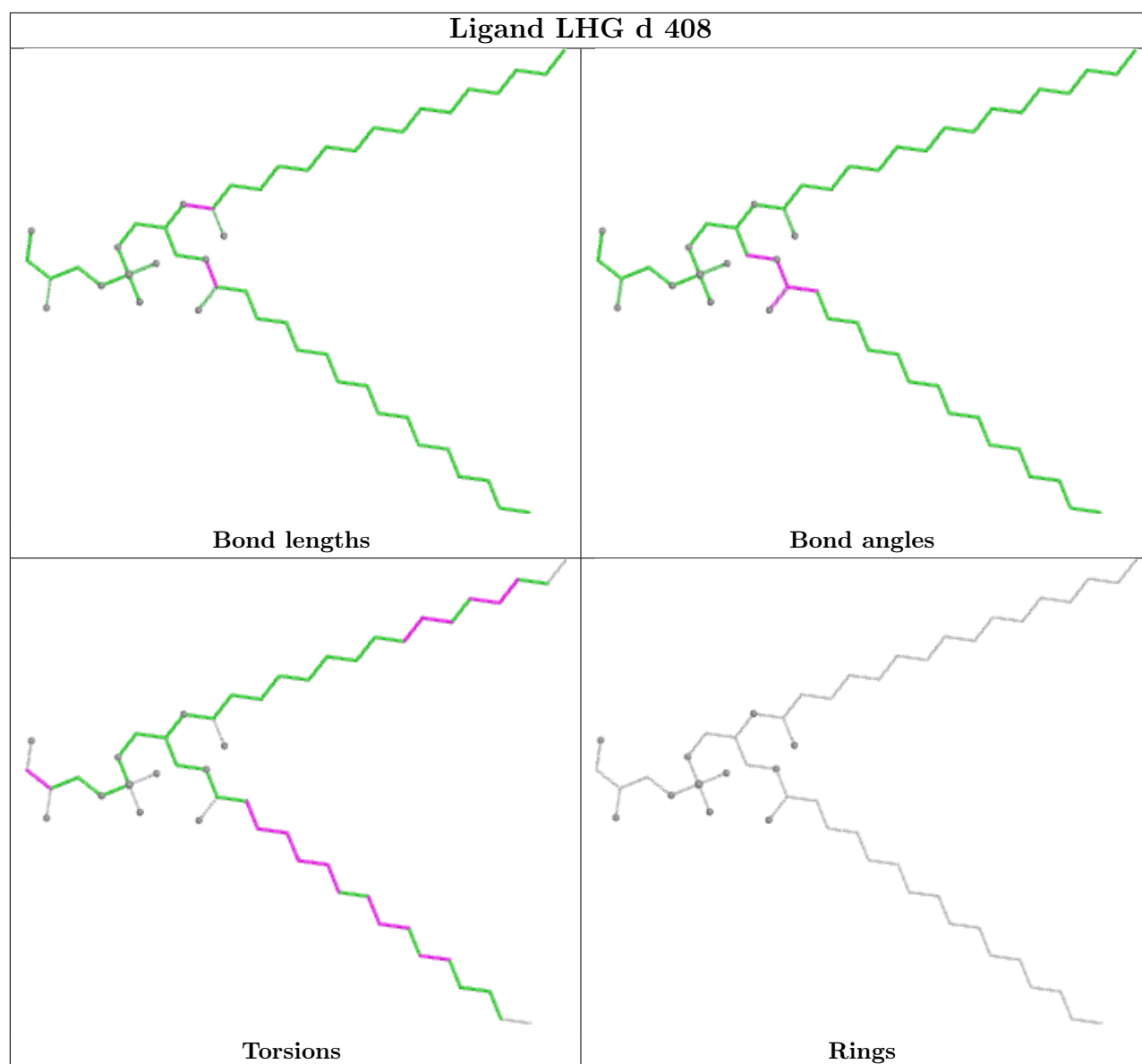
Ligand CLA c 910

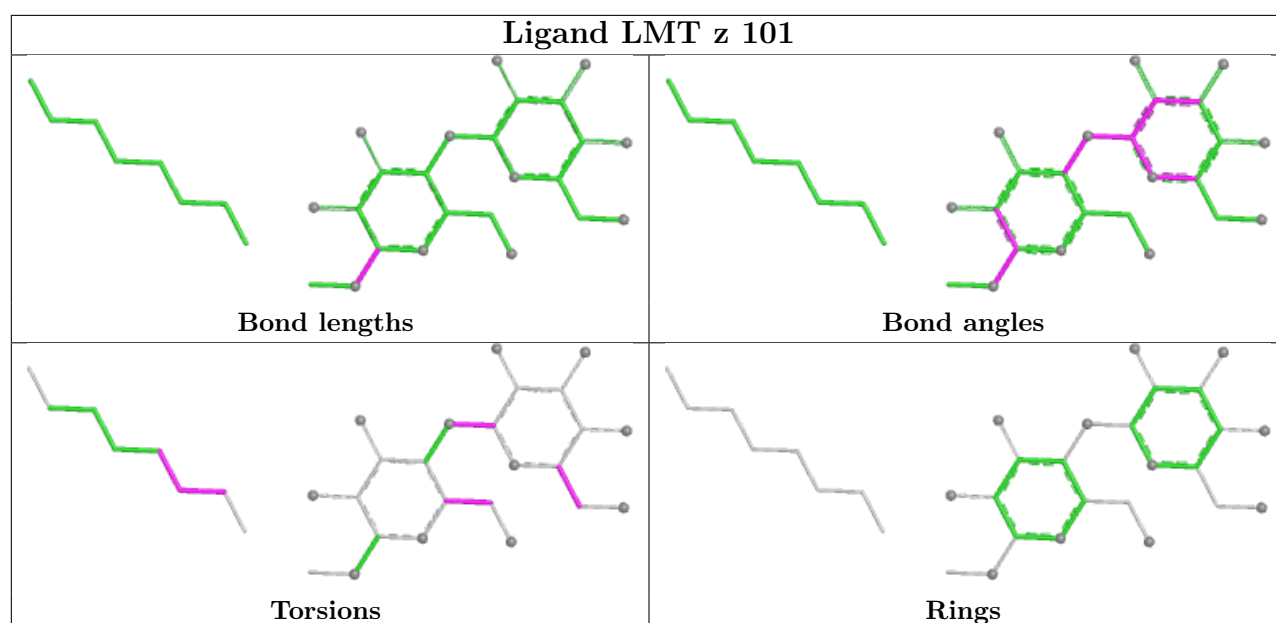
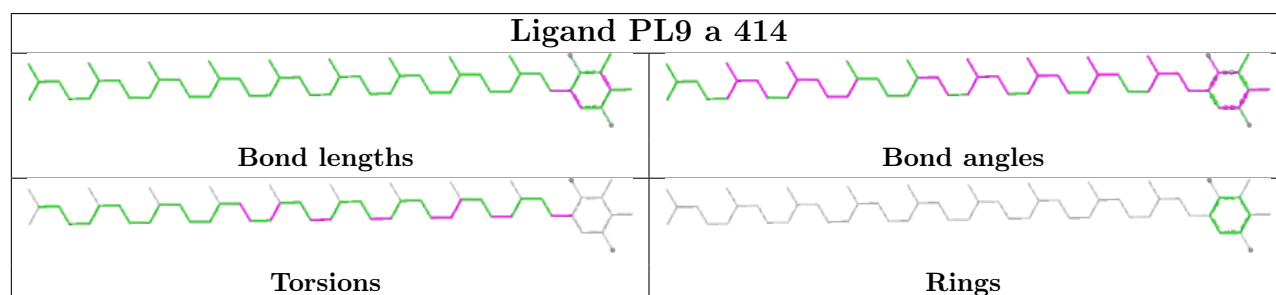
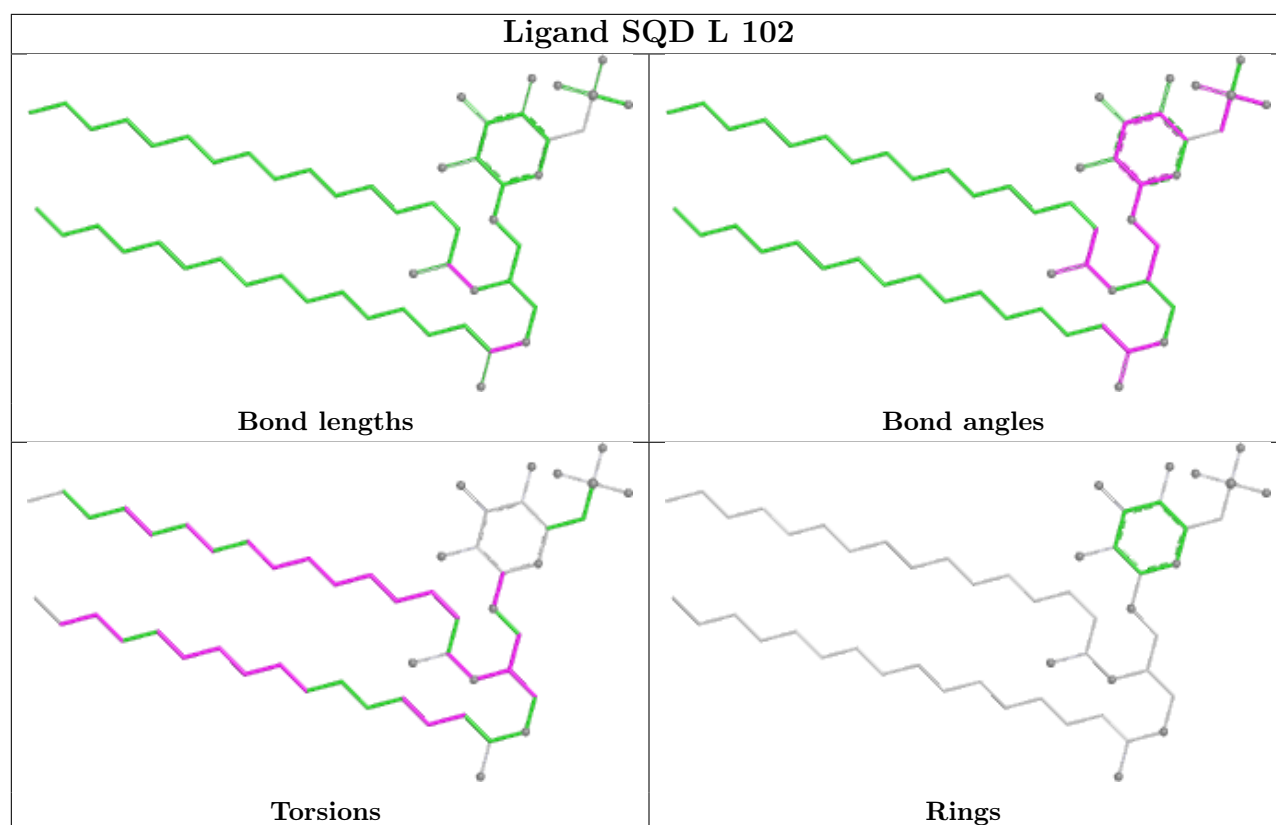


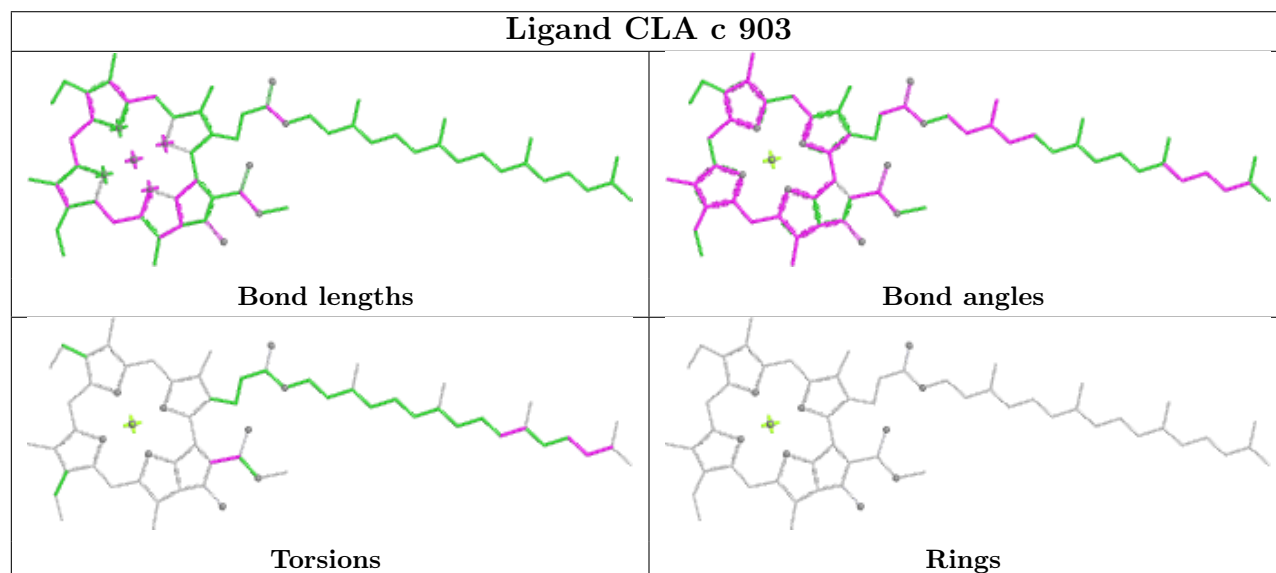
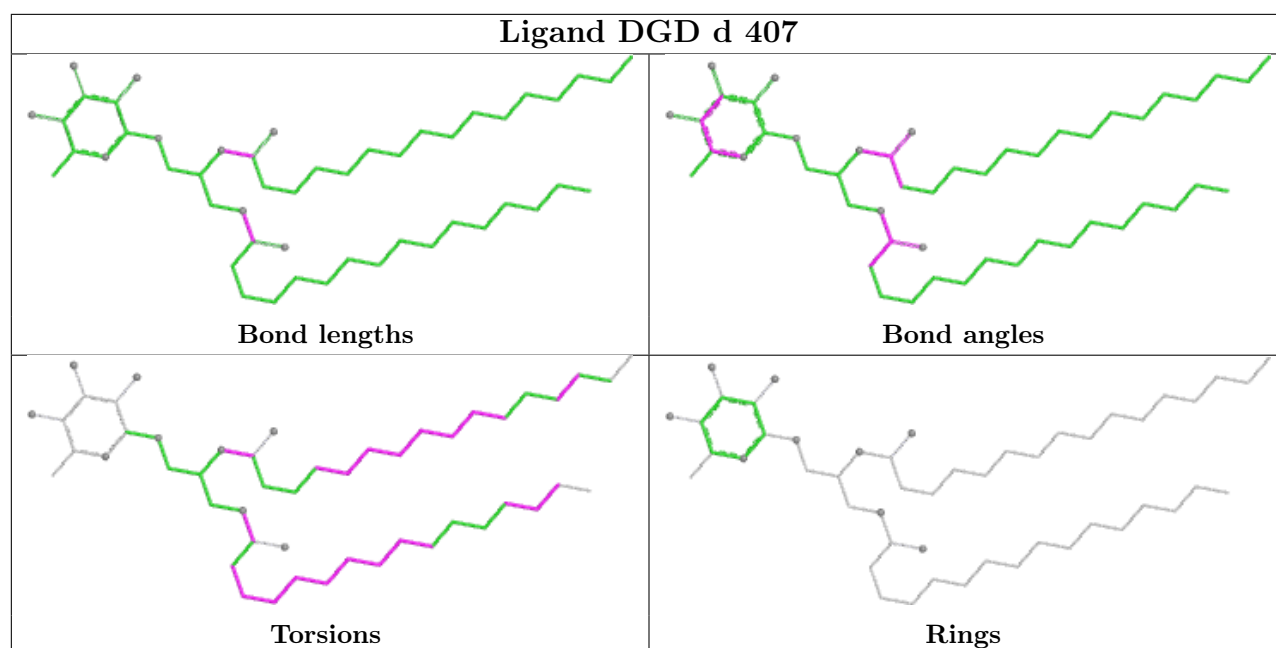


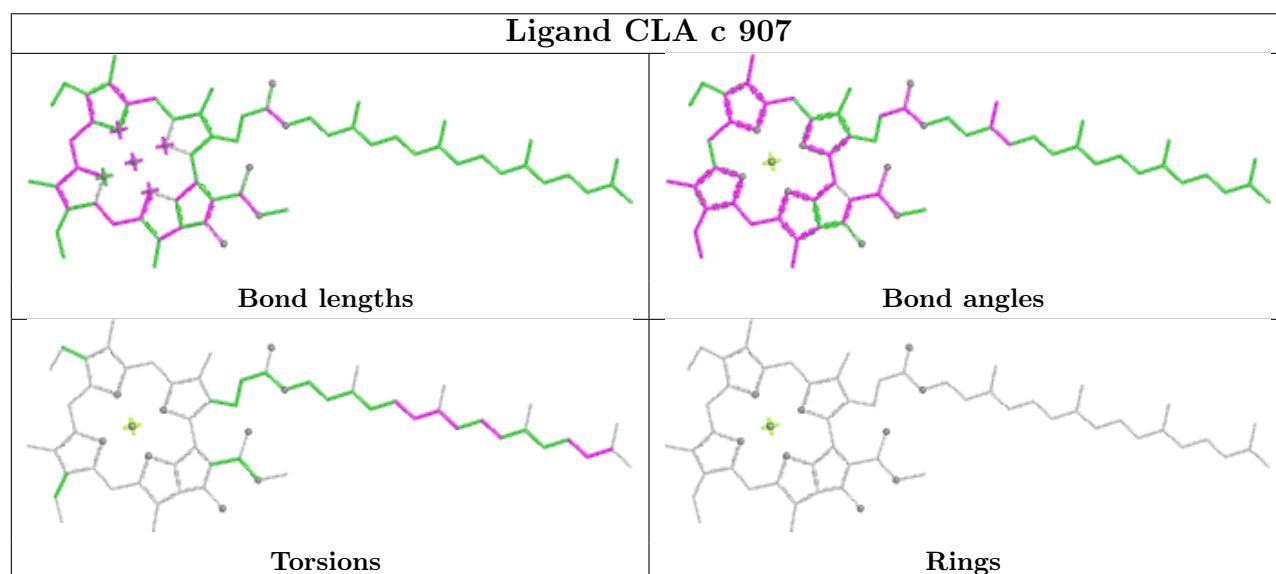
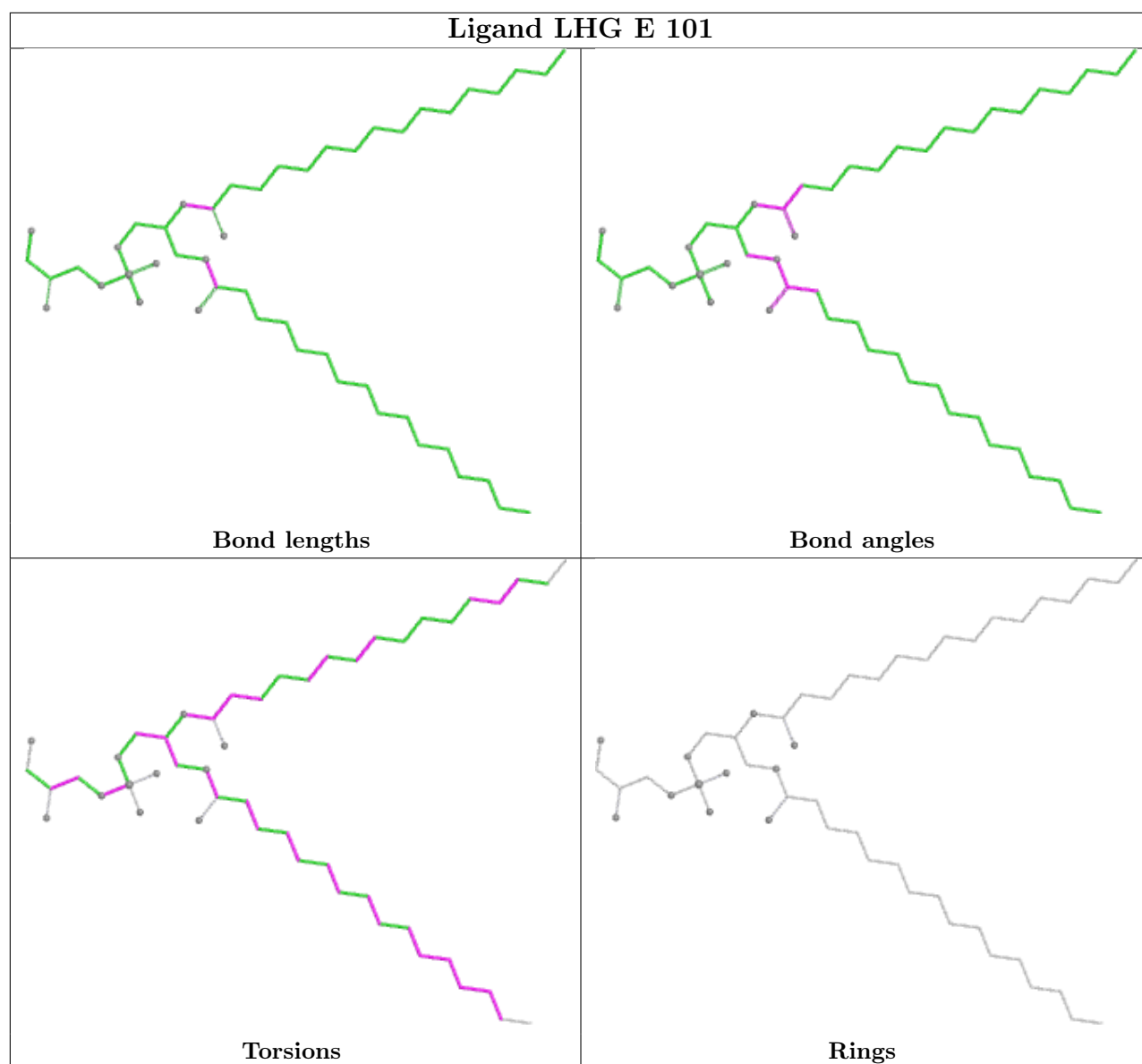


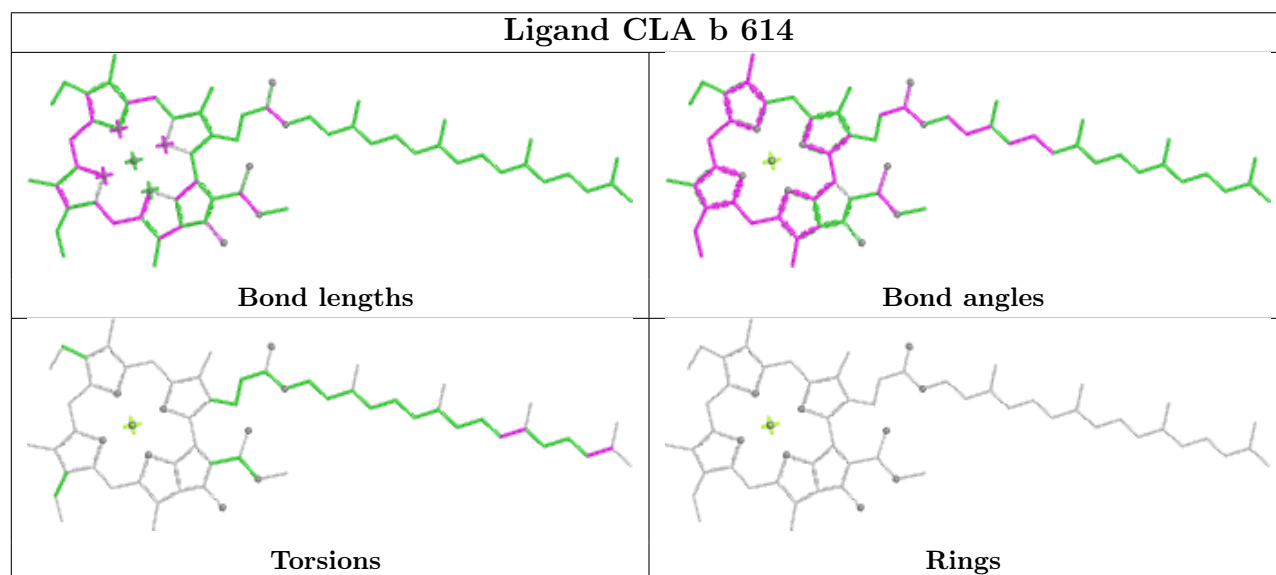
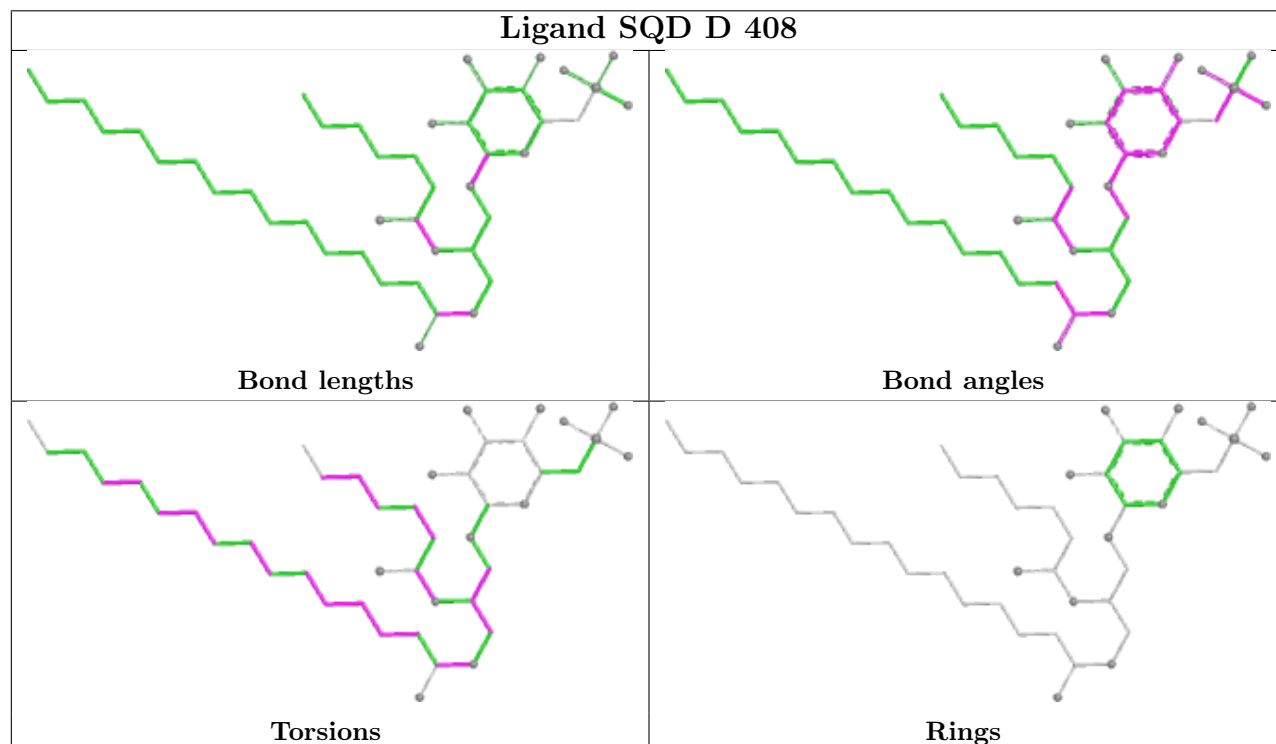
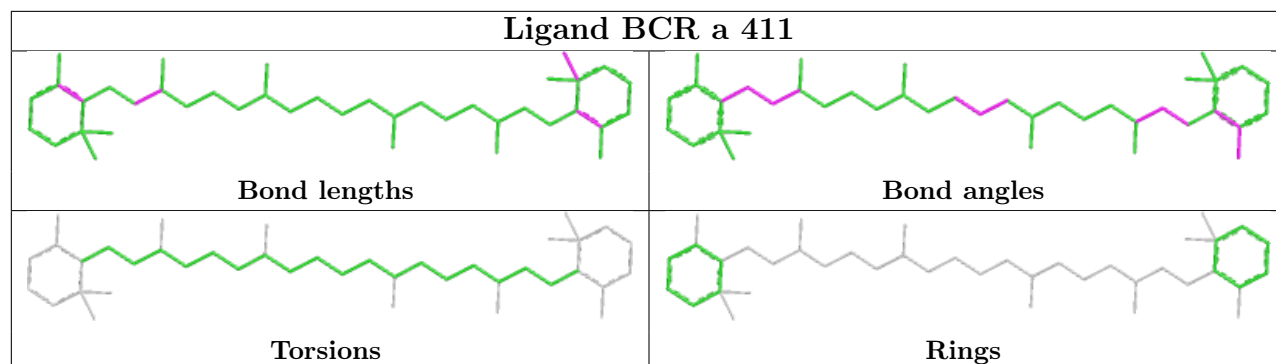


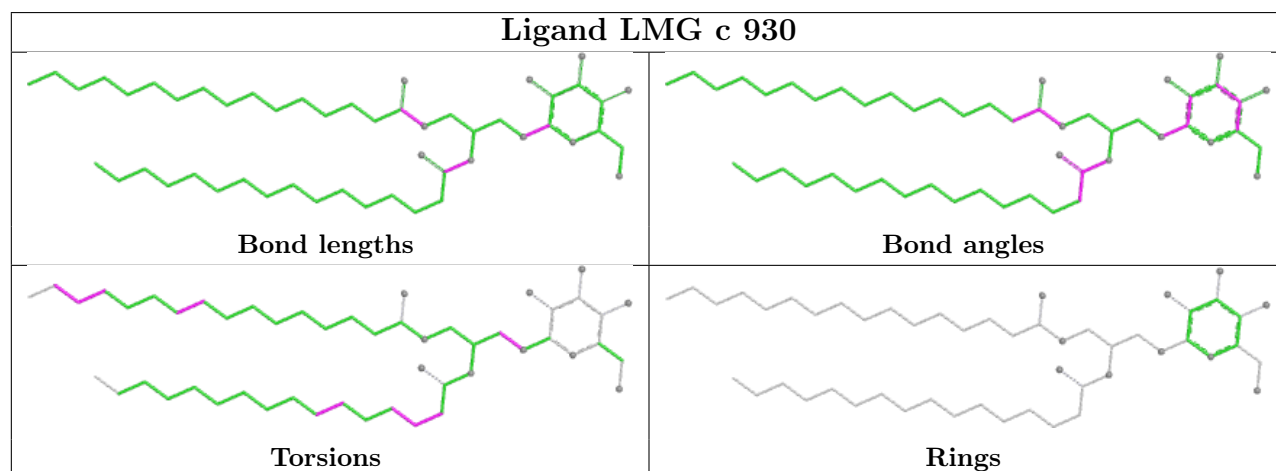
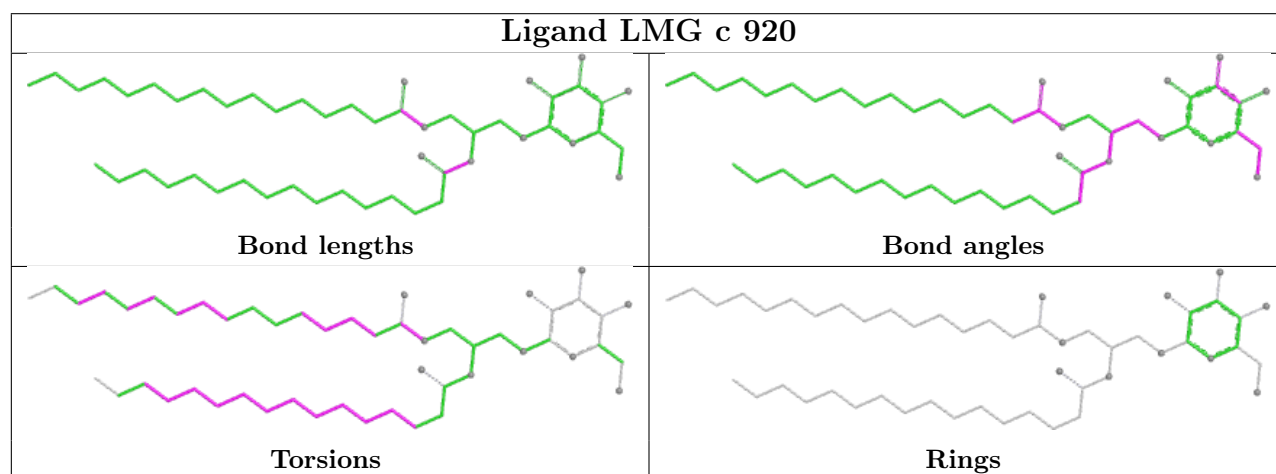
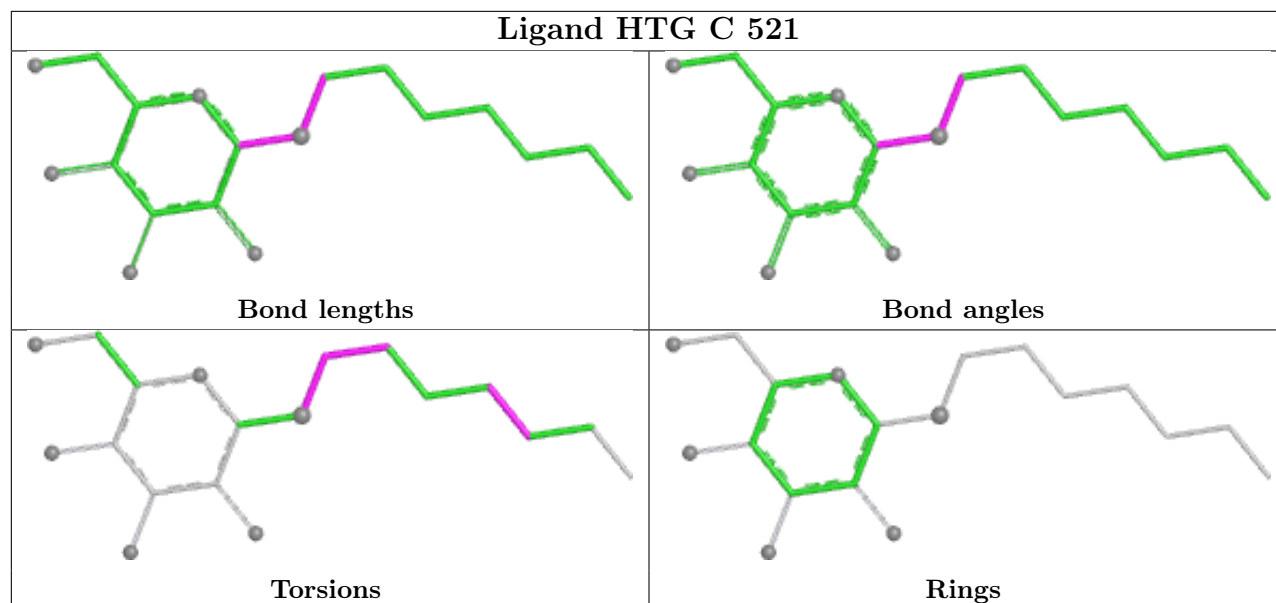


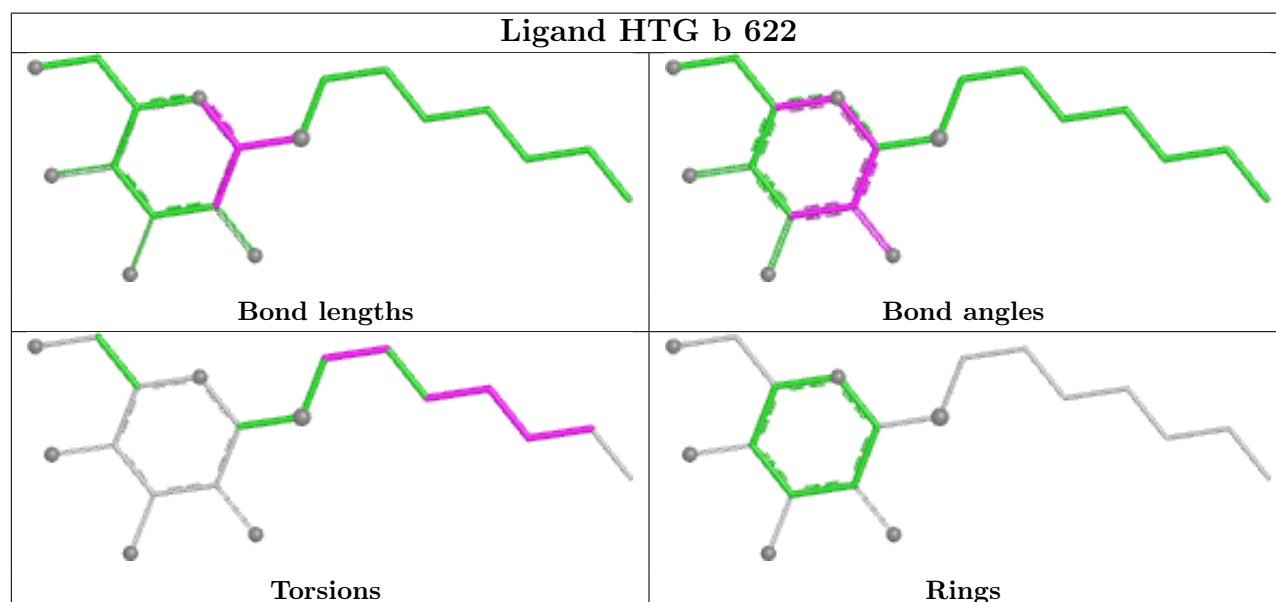
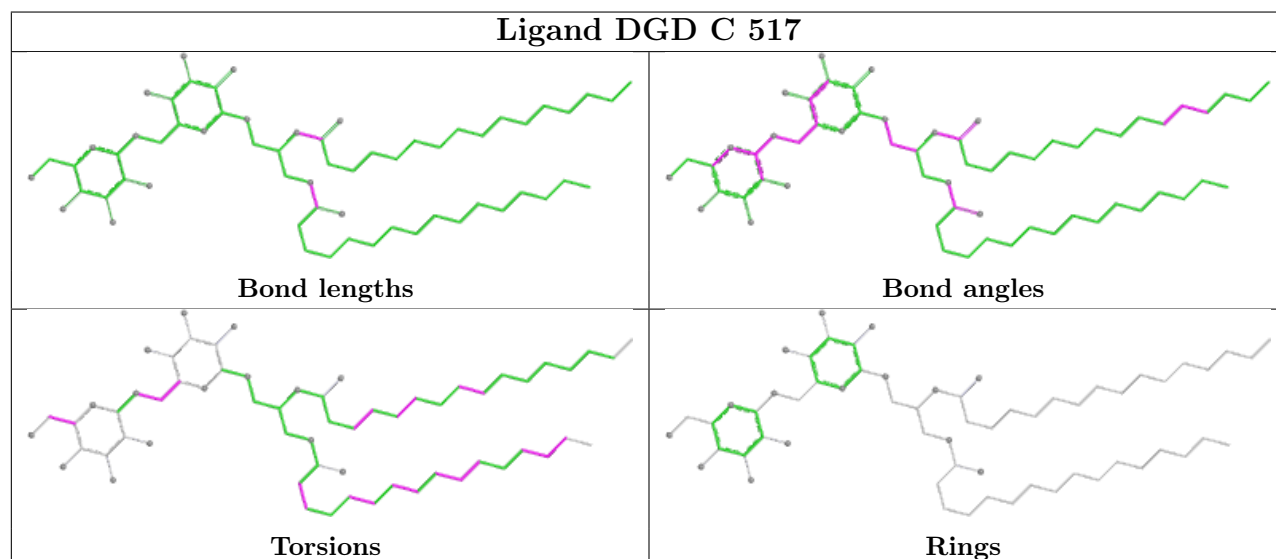
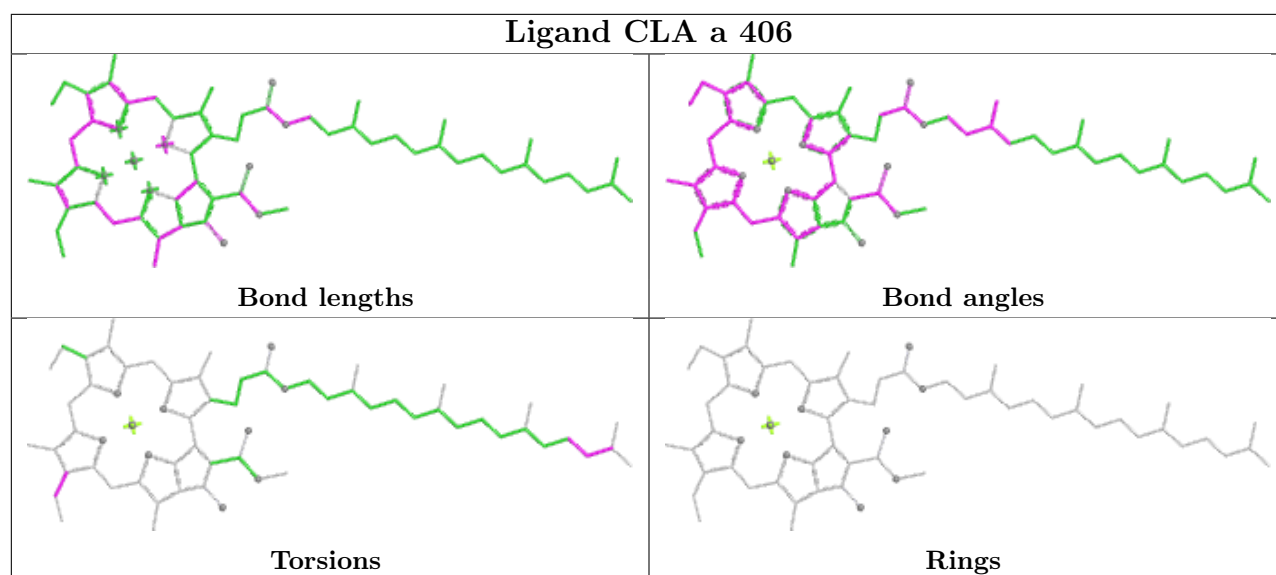


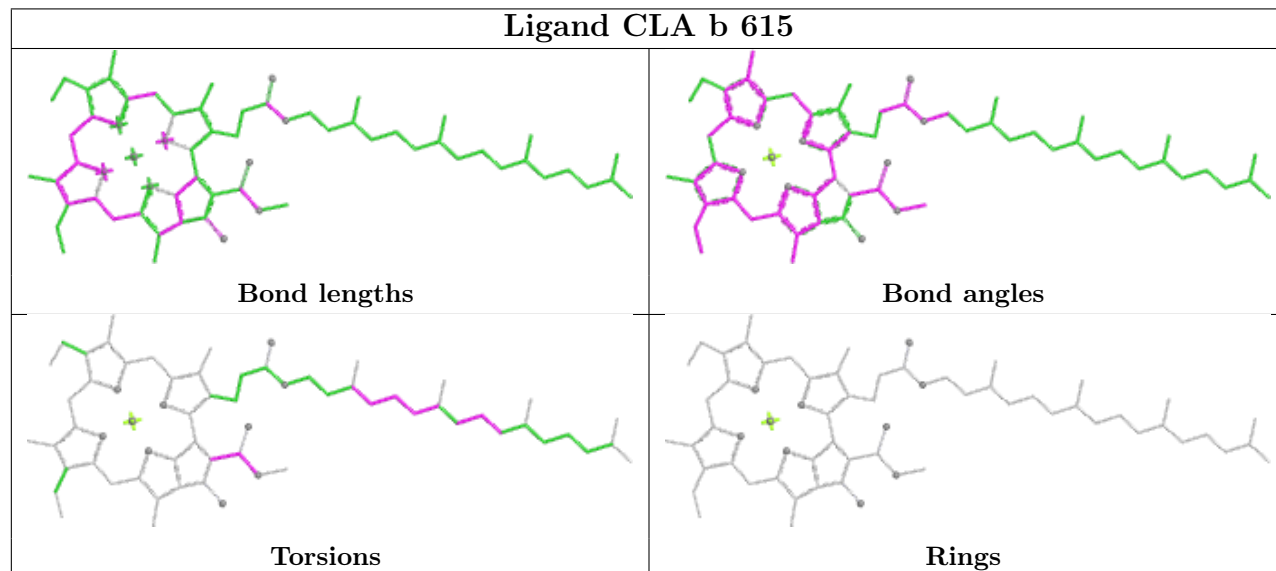
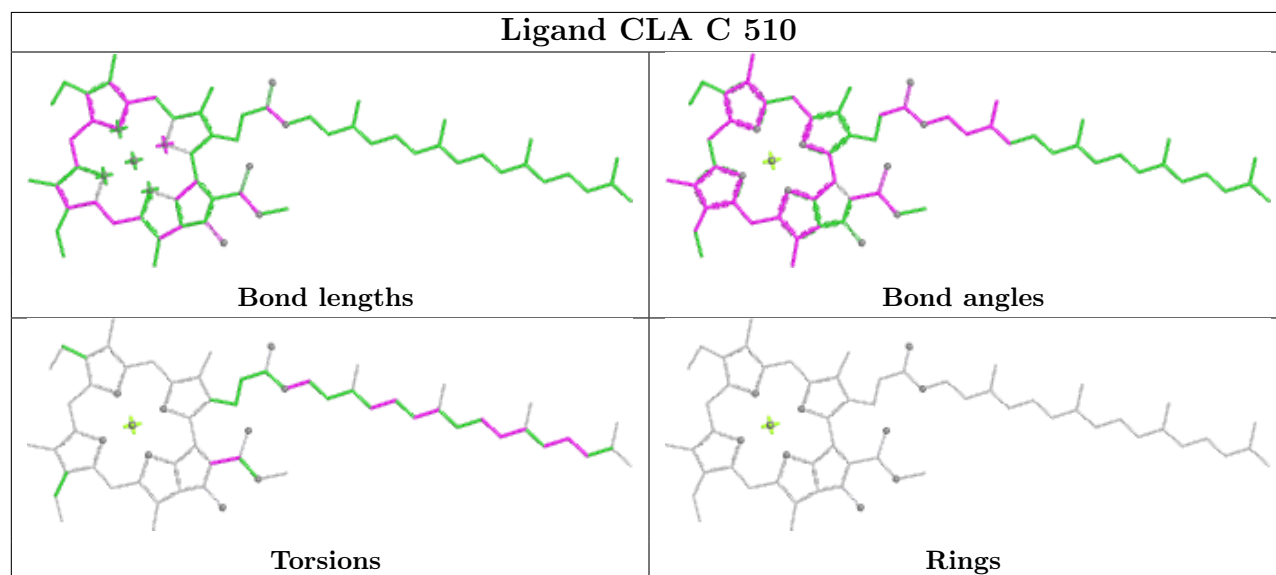
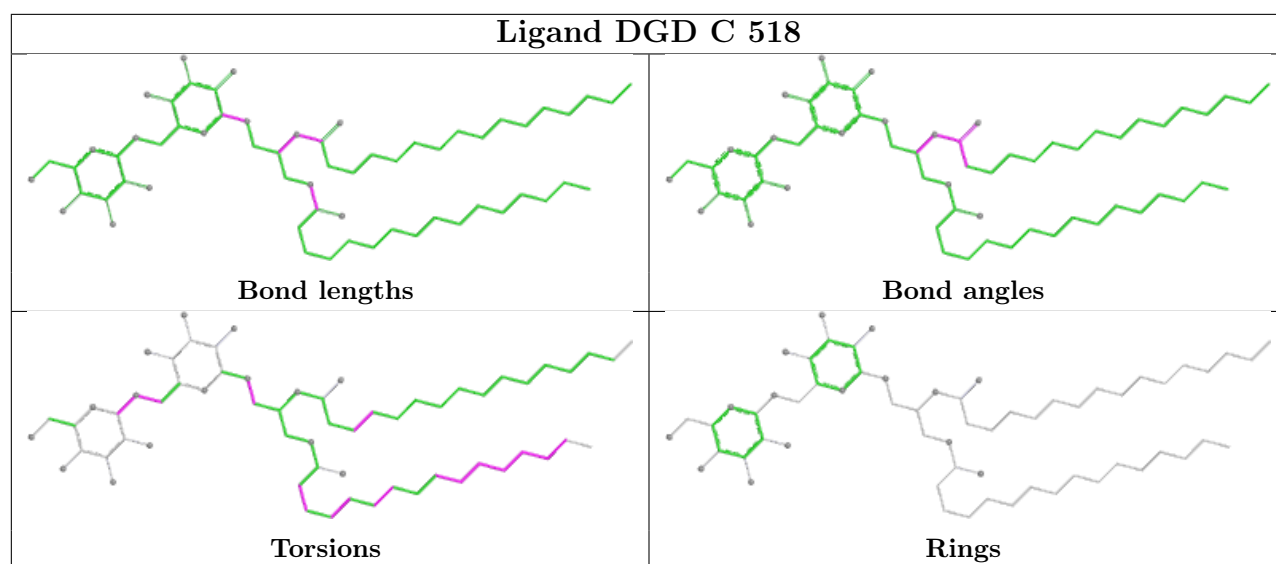


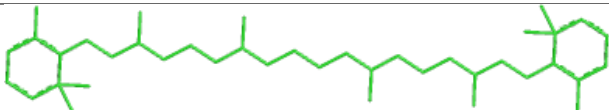
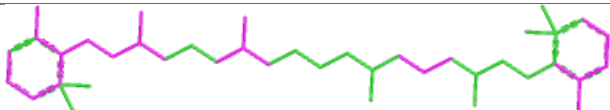
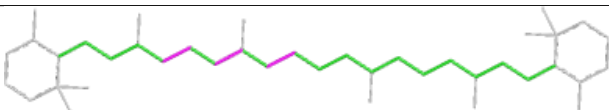
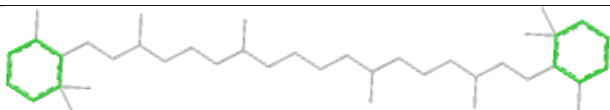


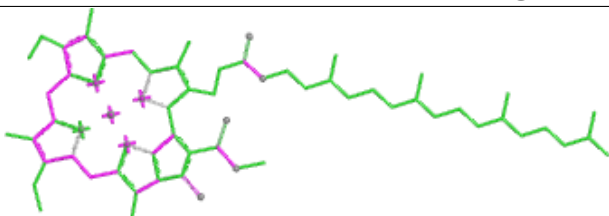
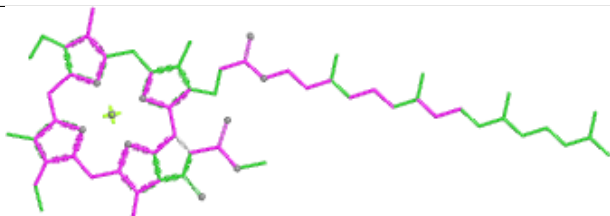
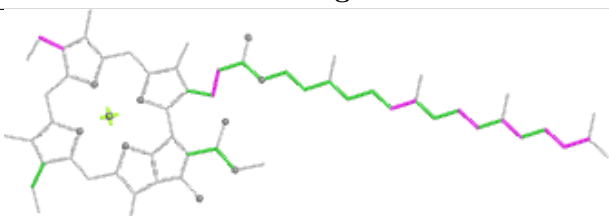
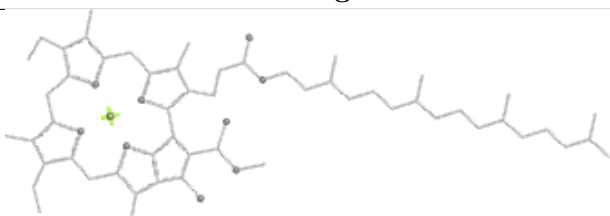


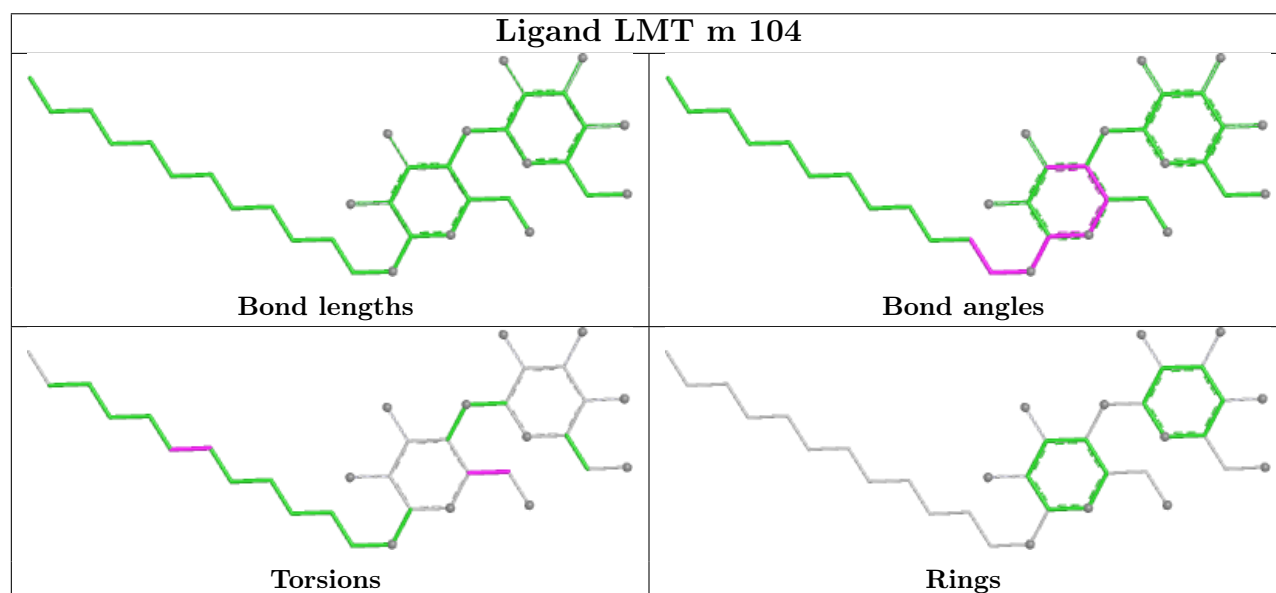
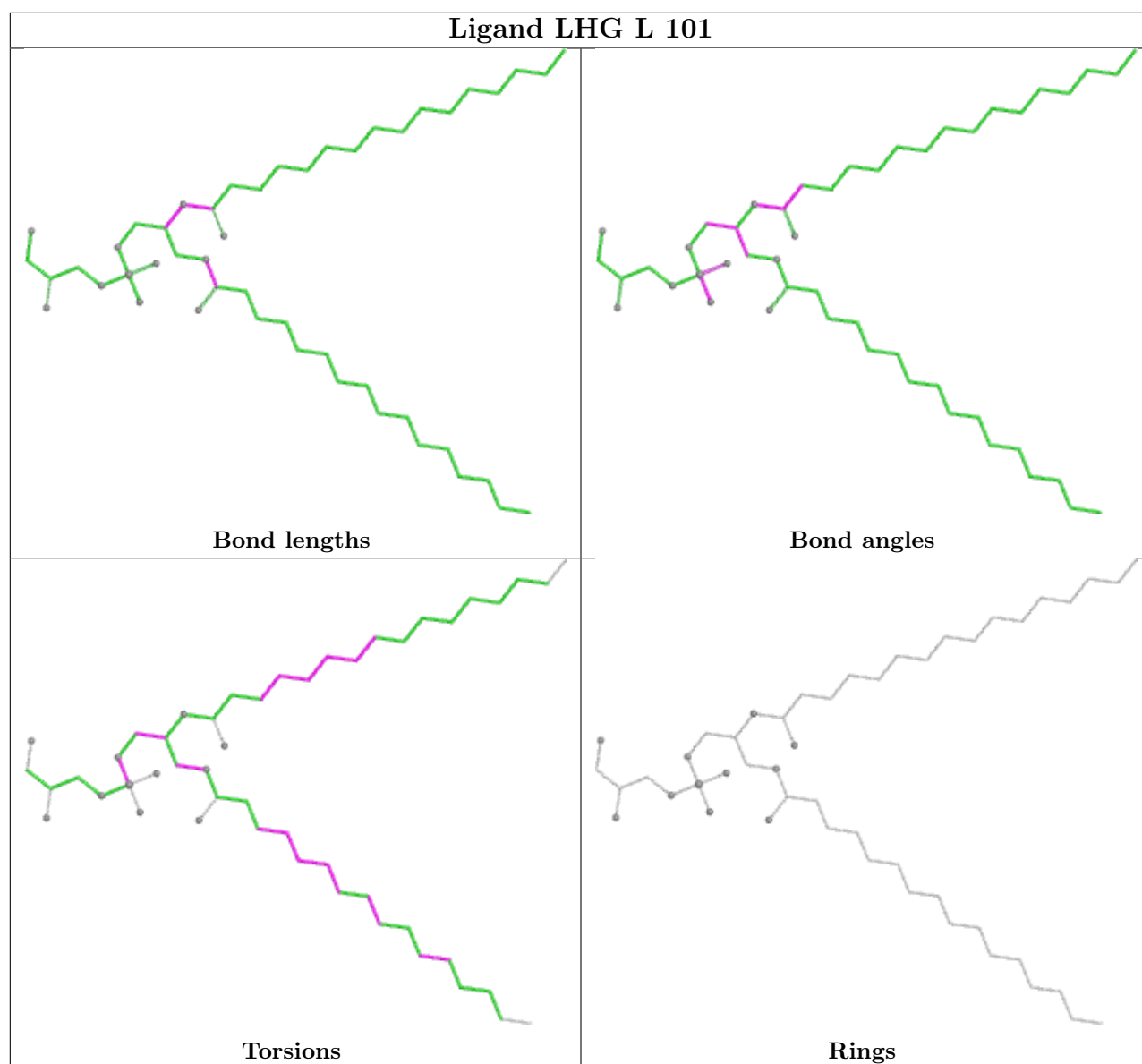


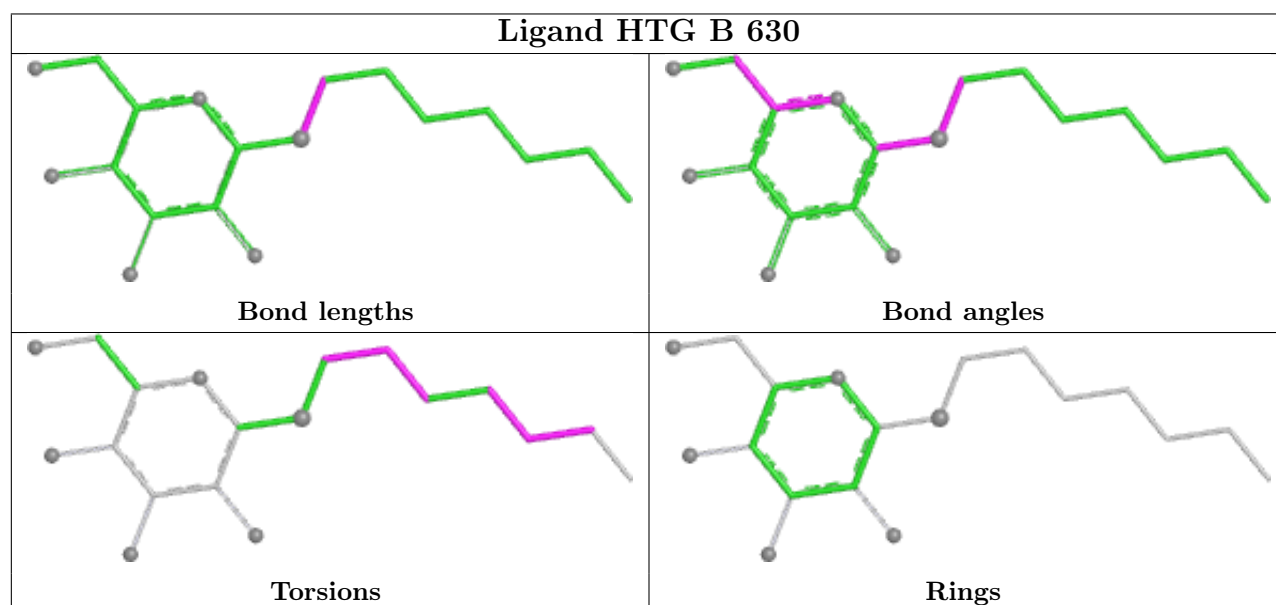
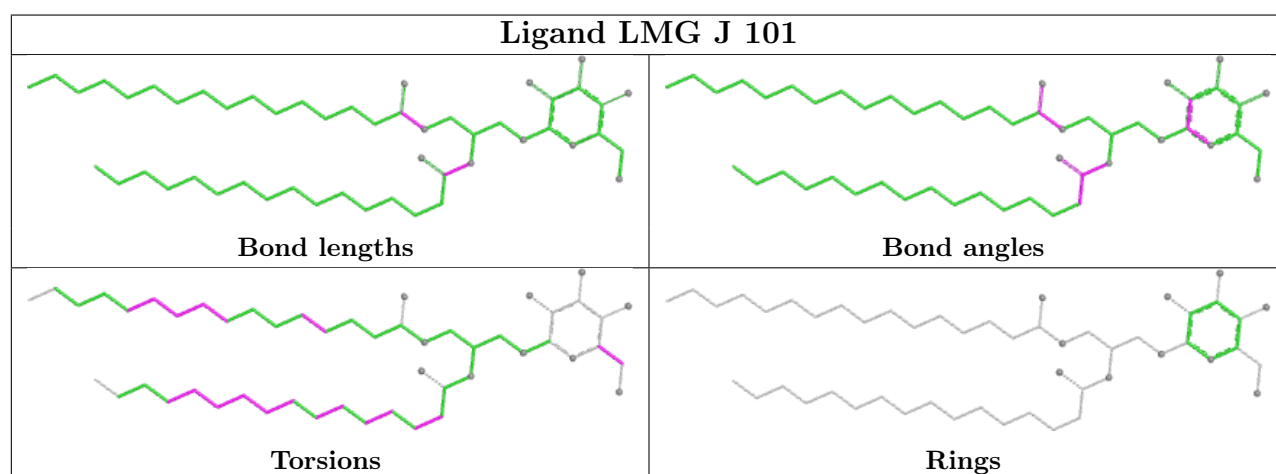
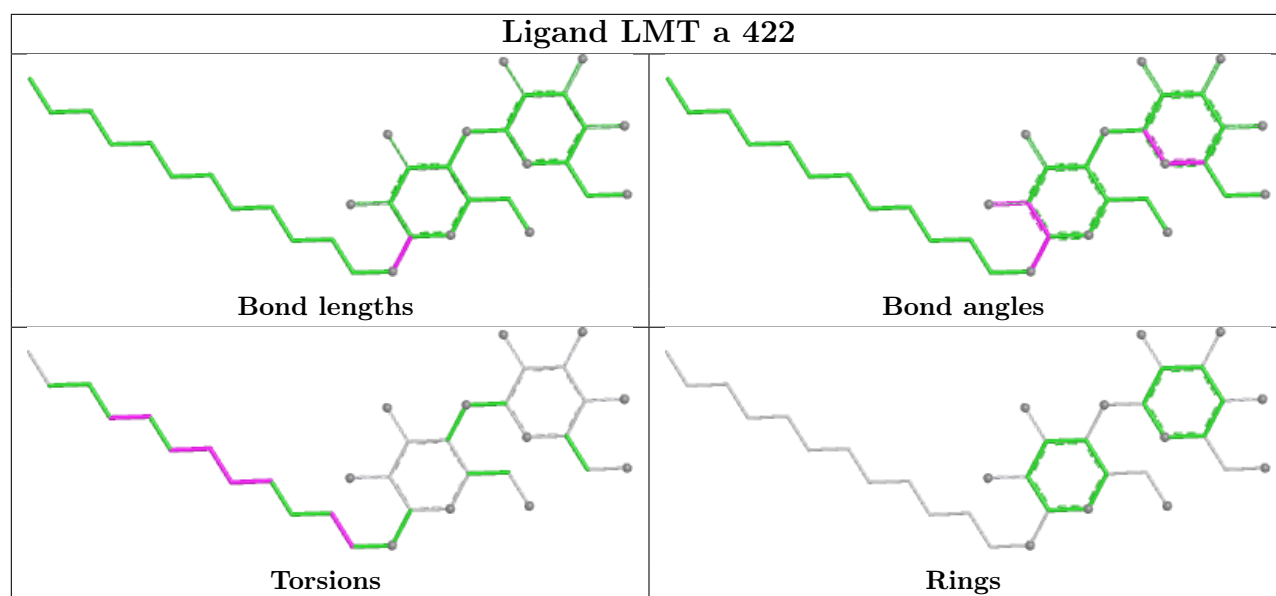


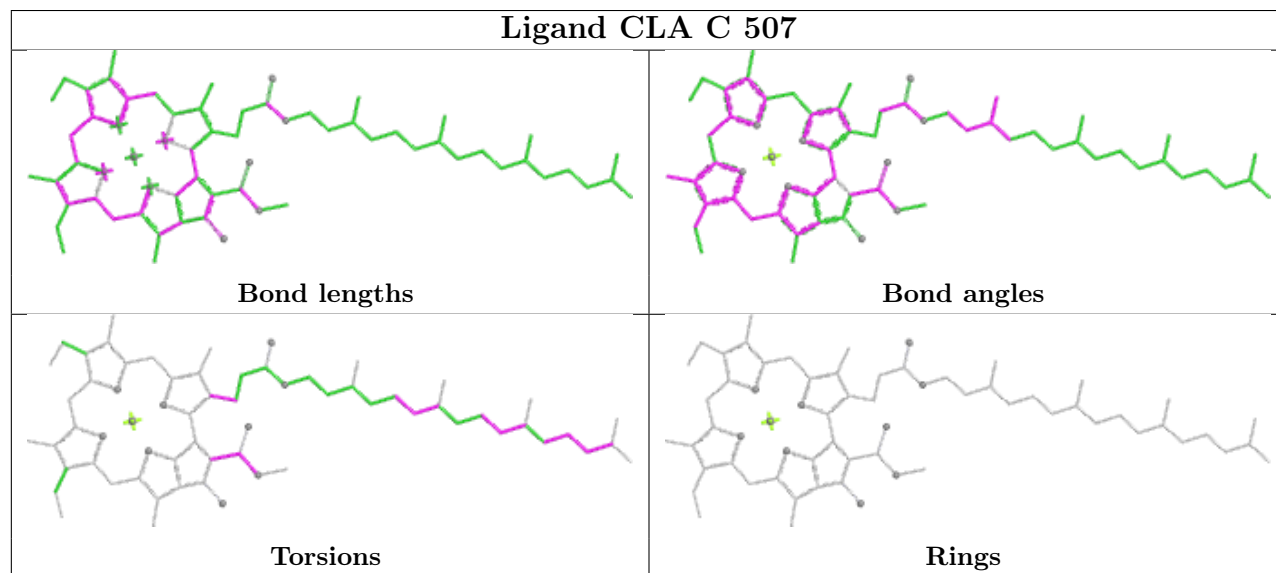
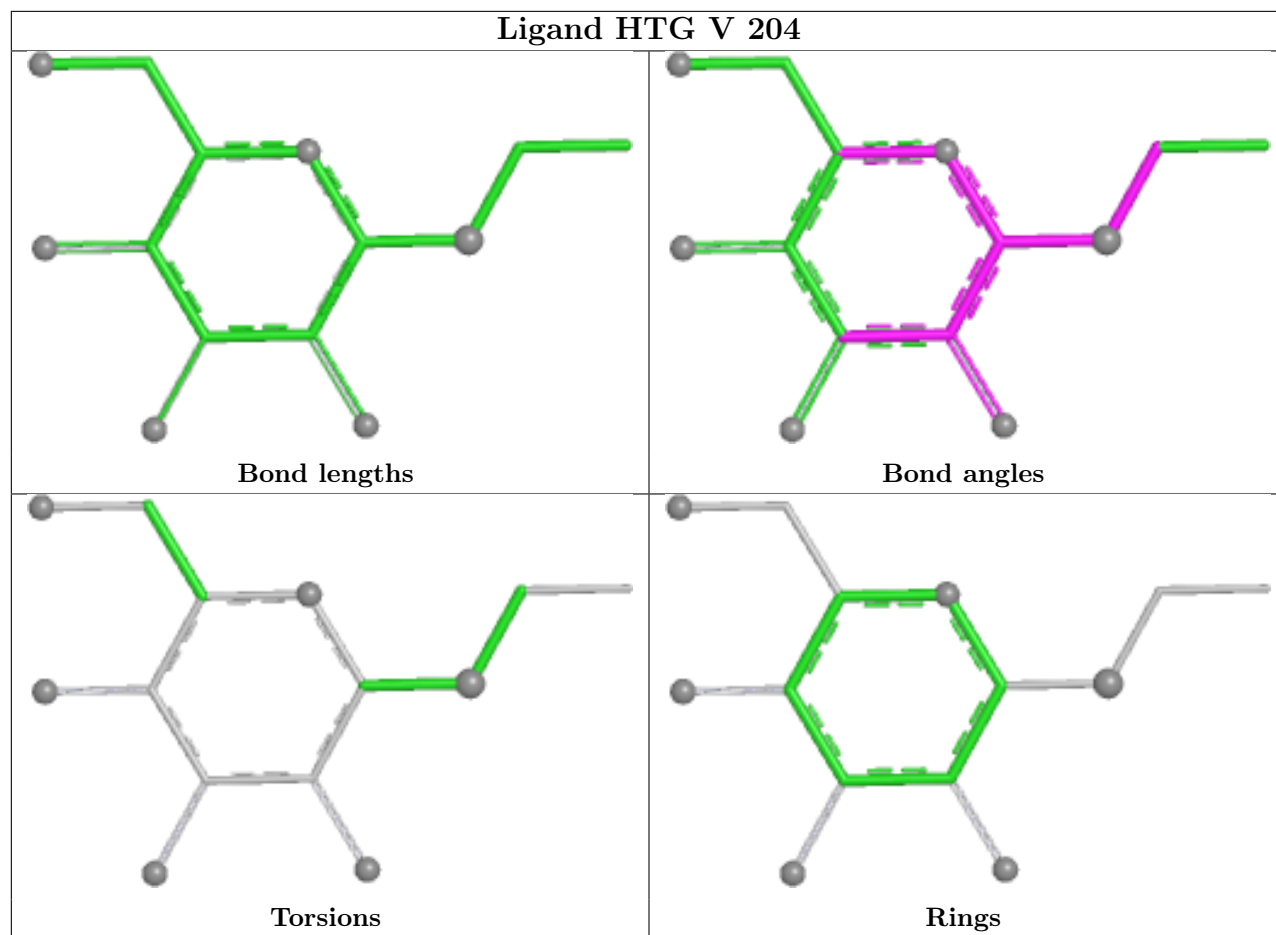


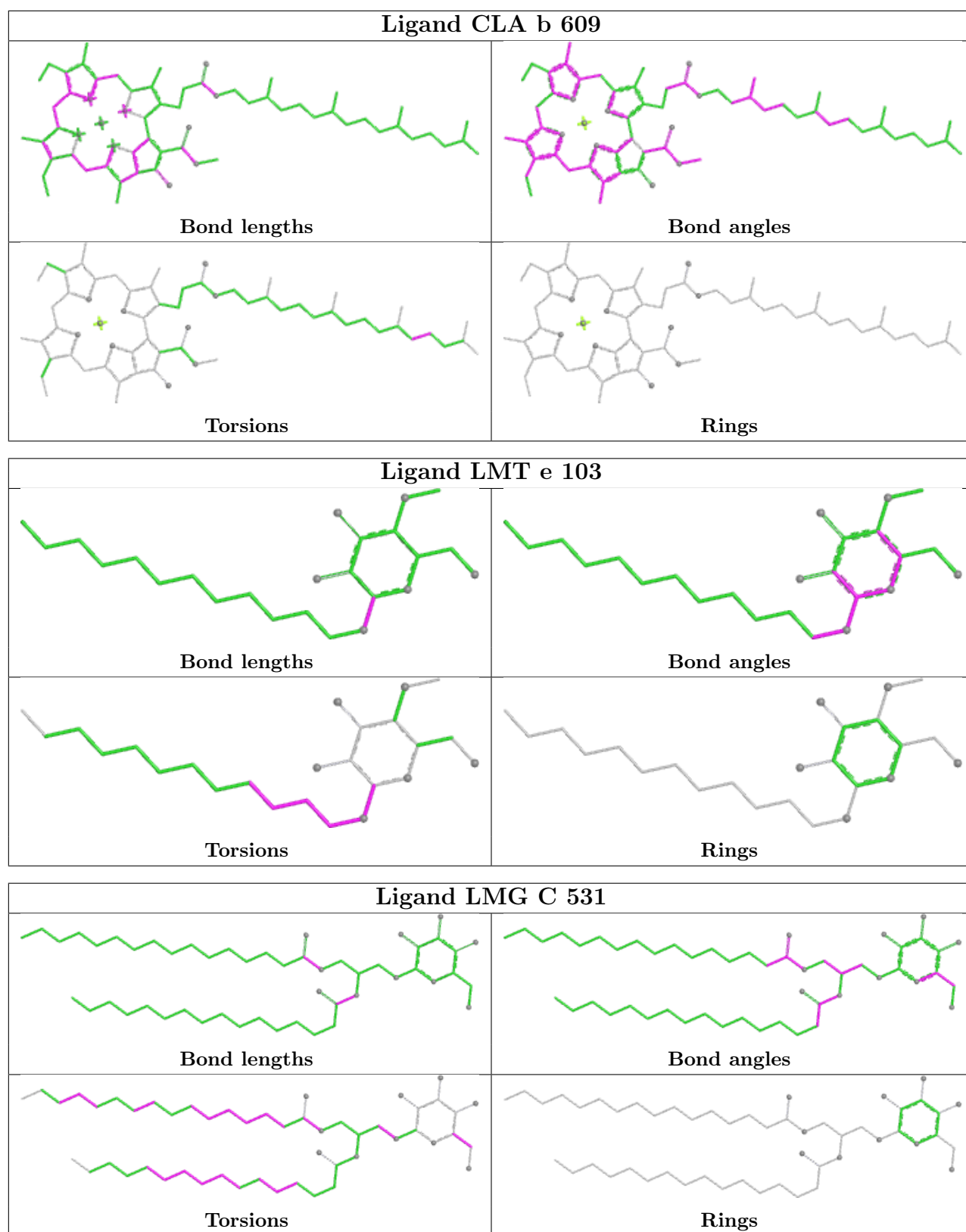
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

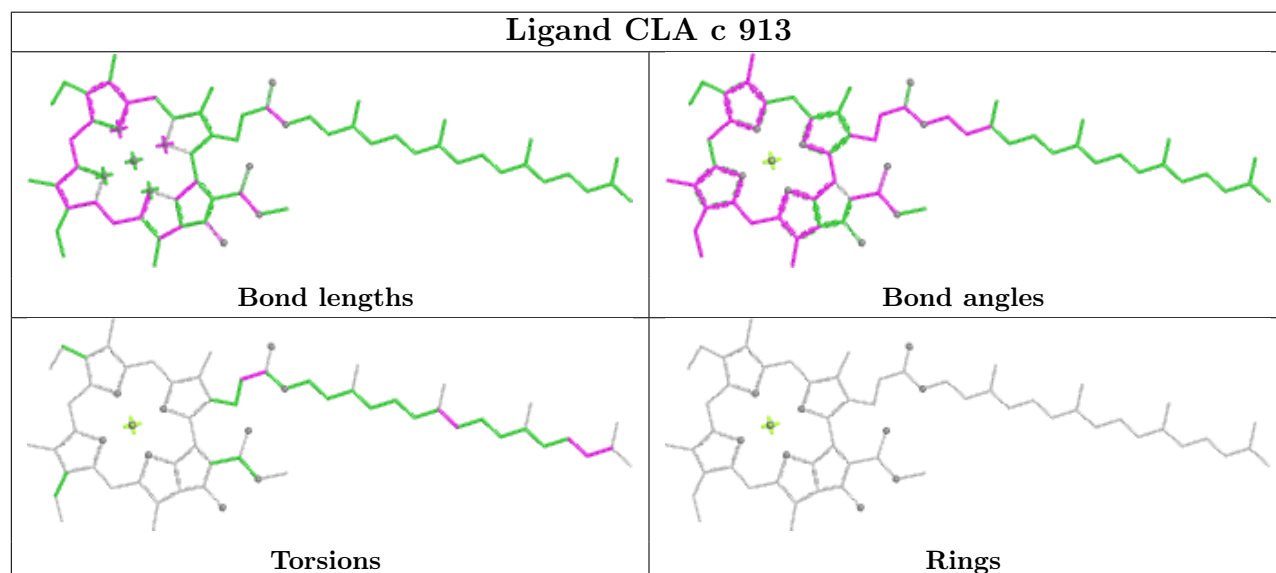
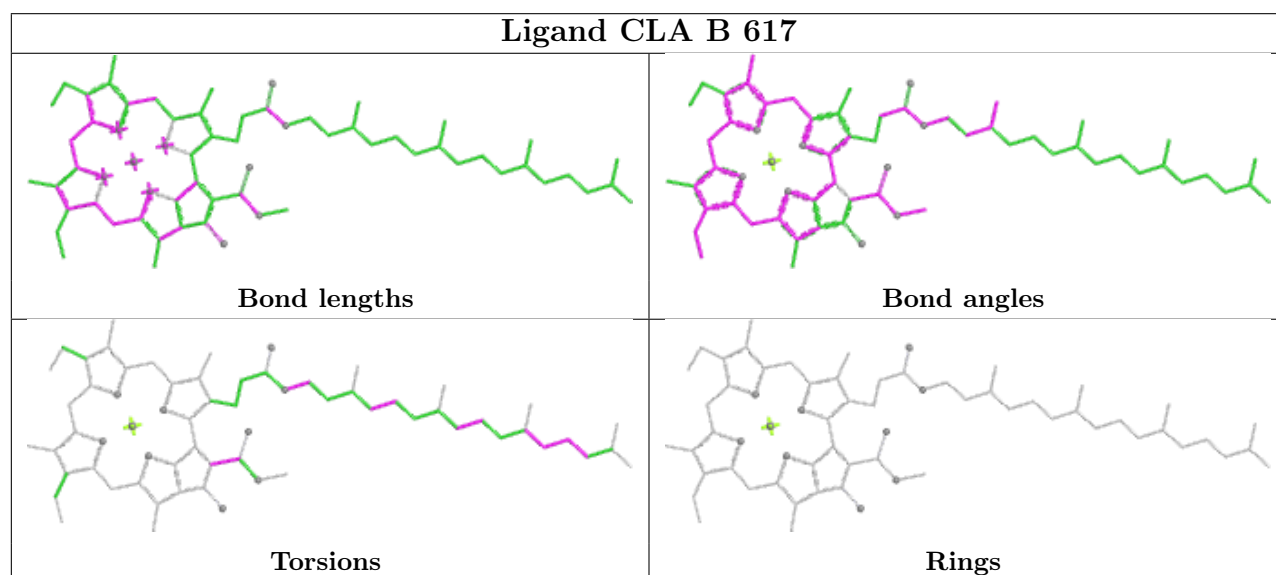
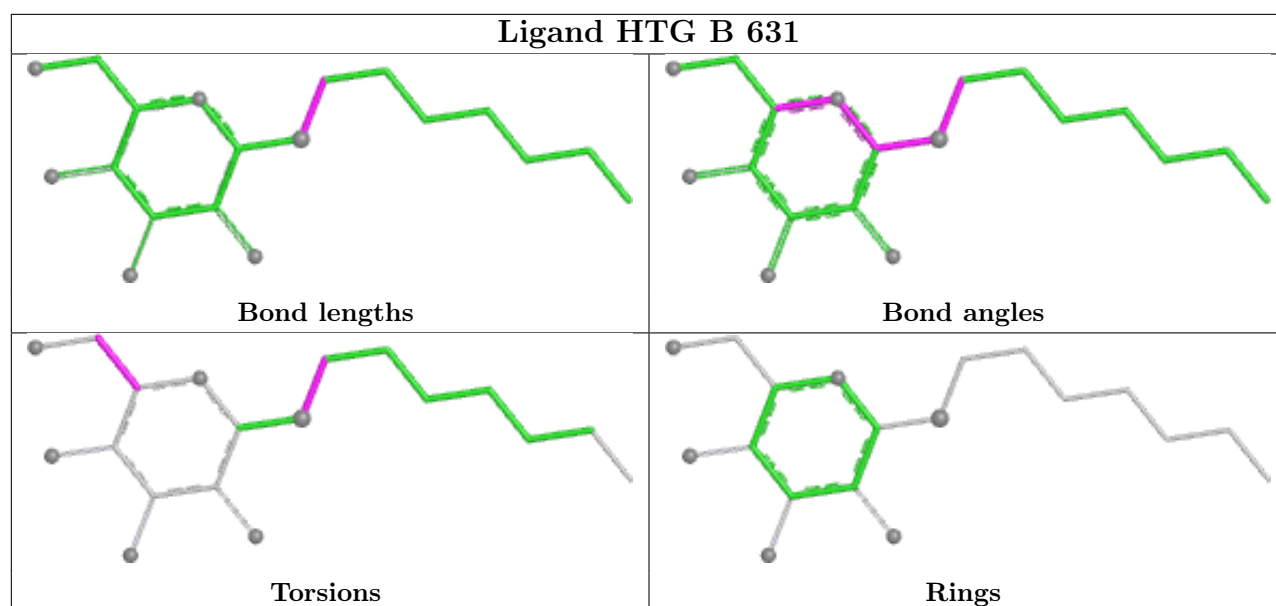
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

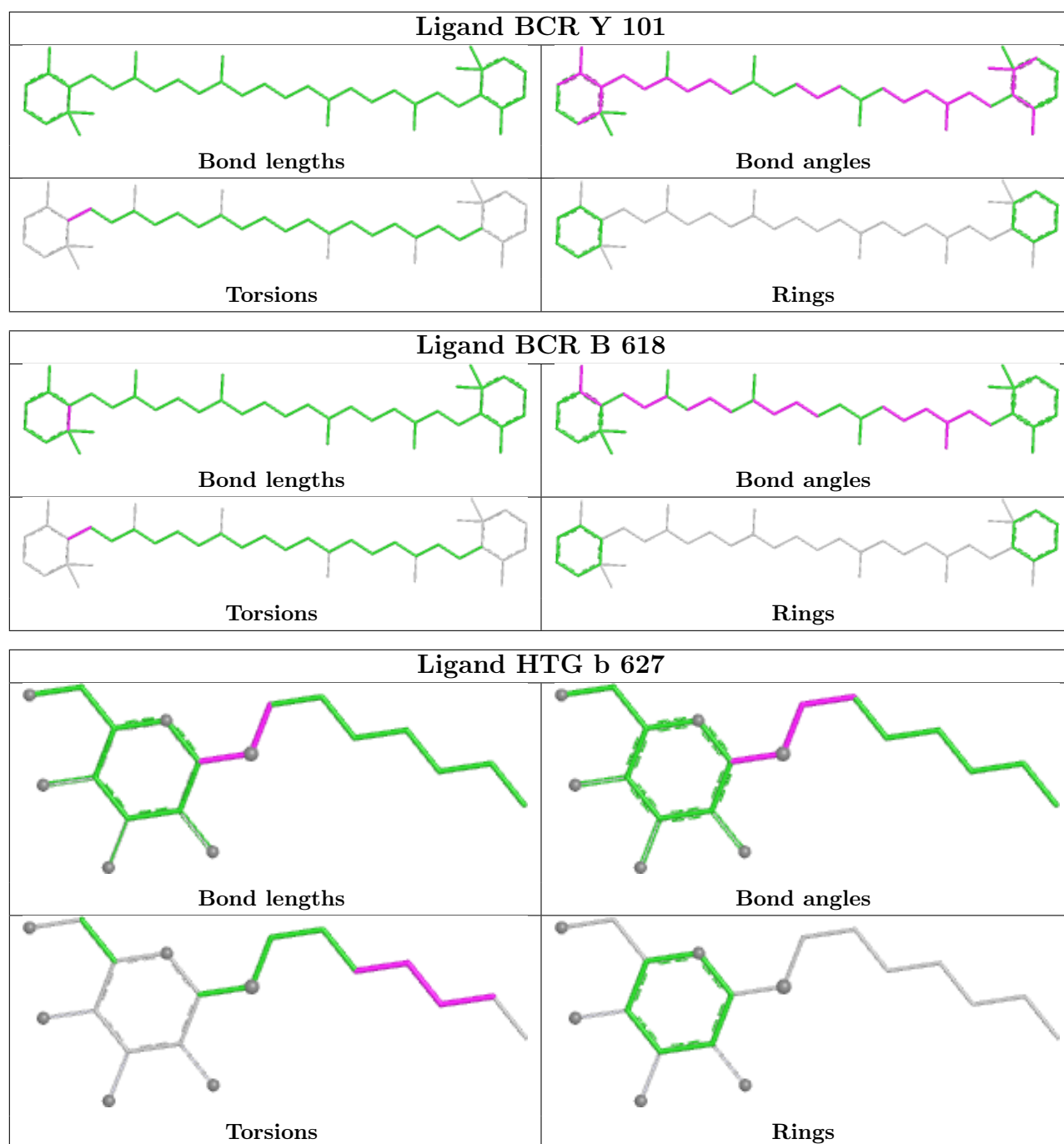


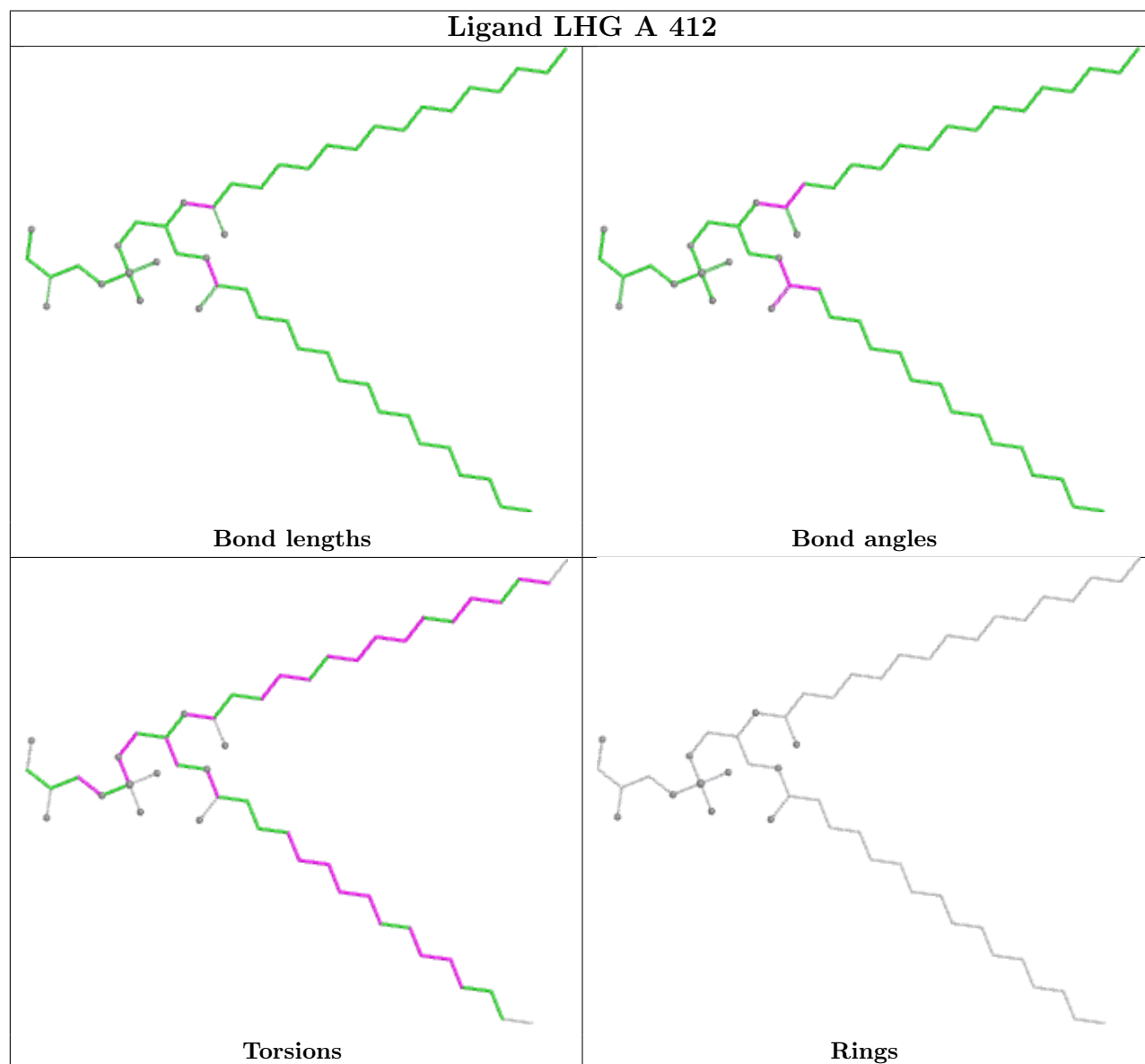
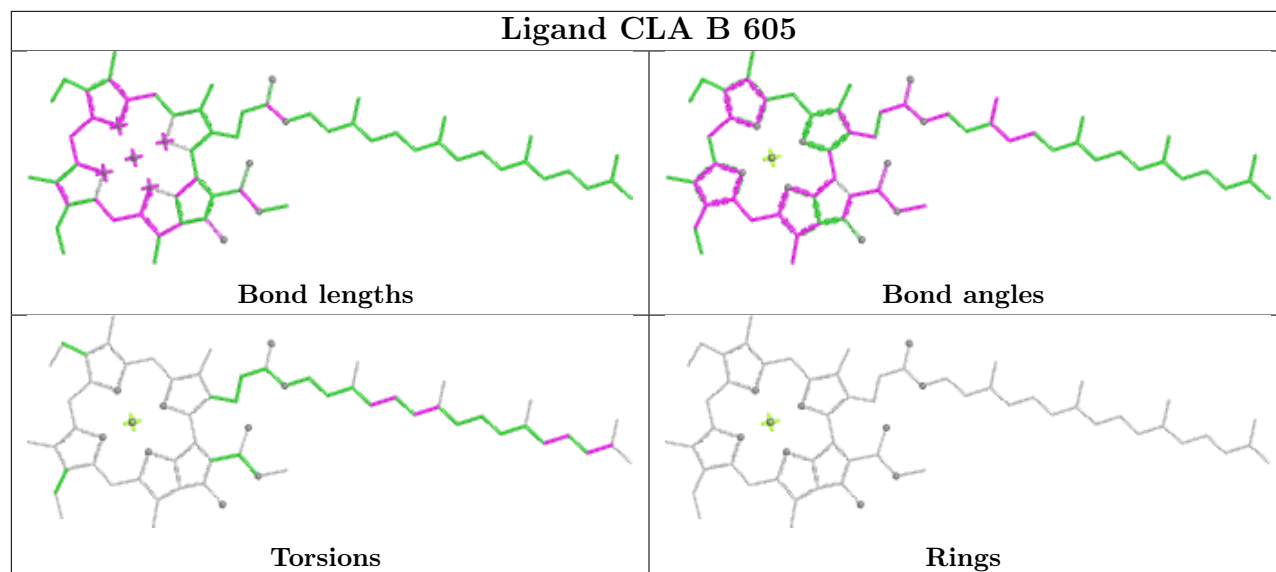


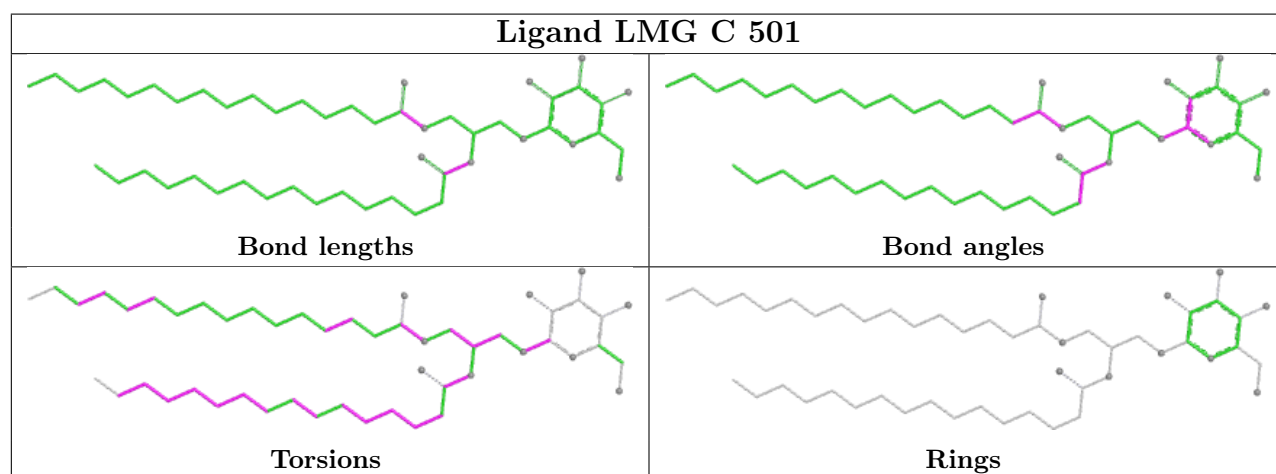
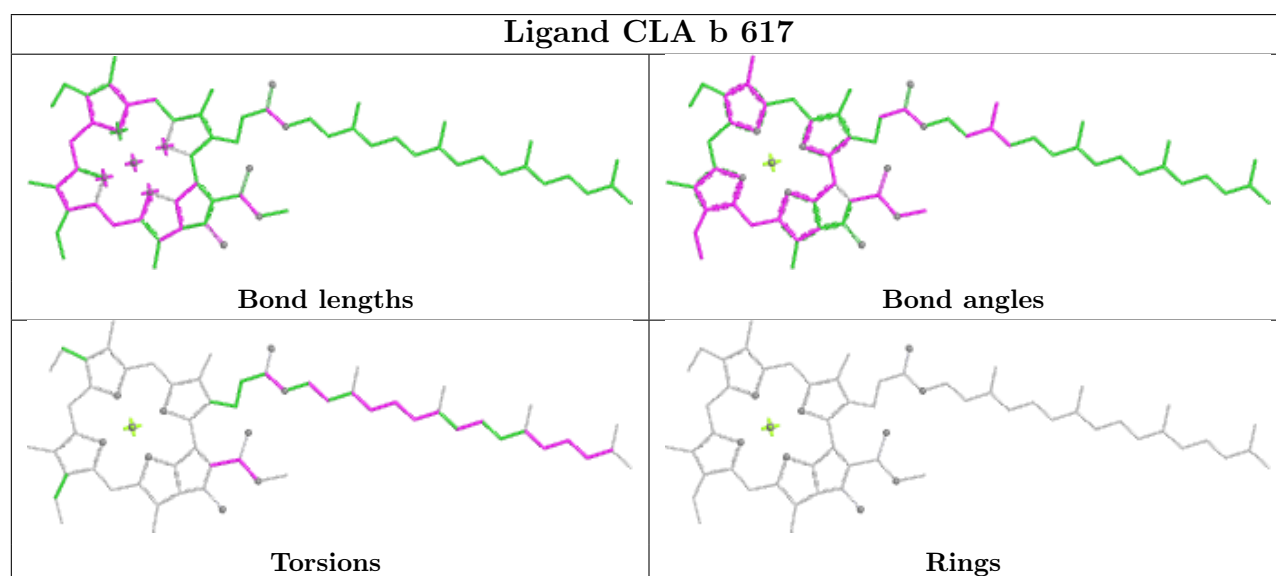
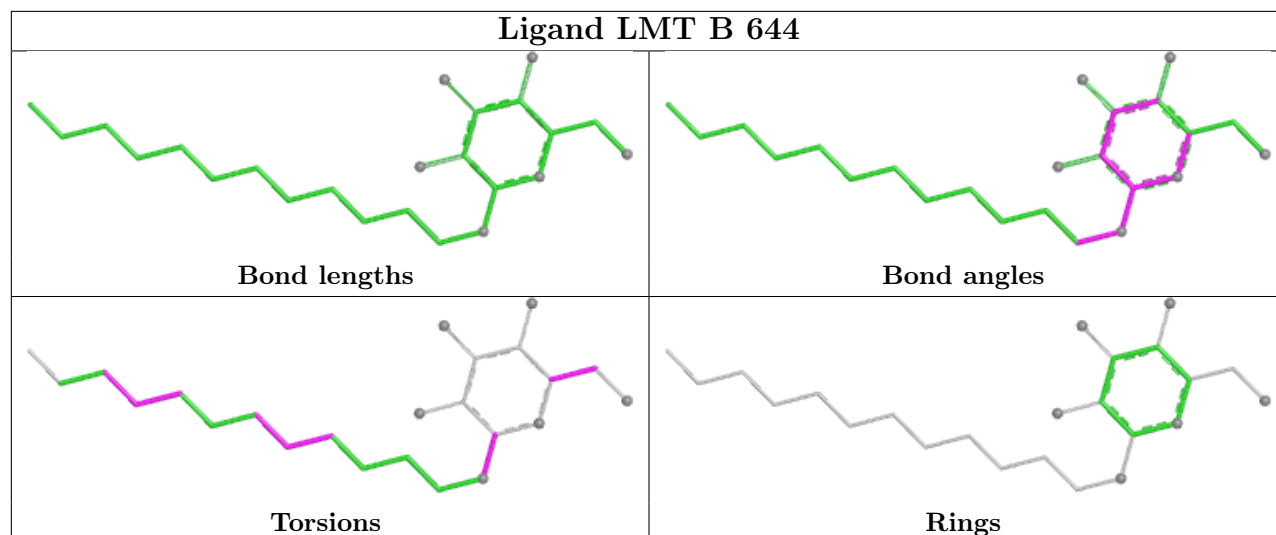


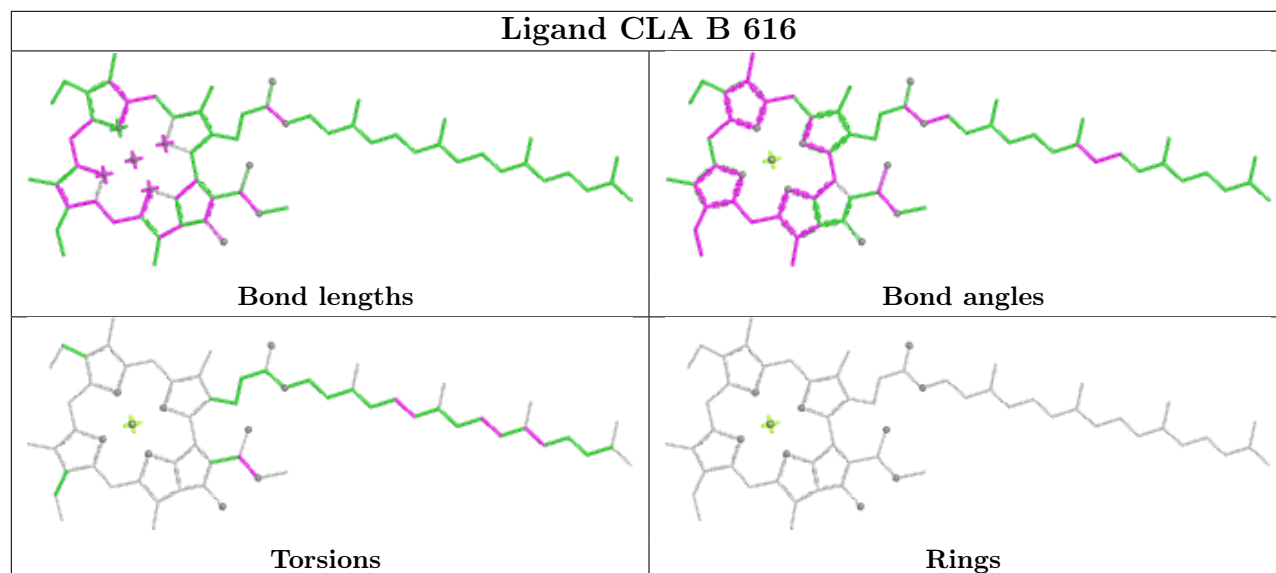
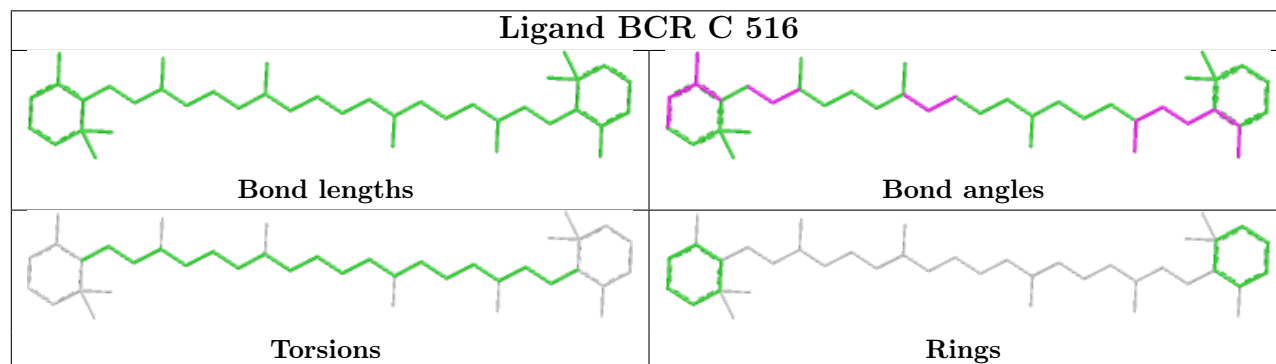
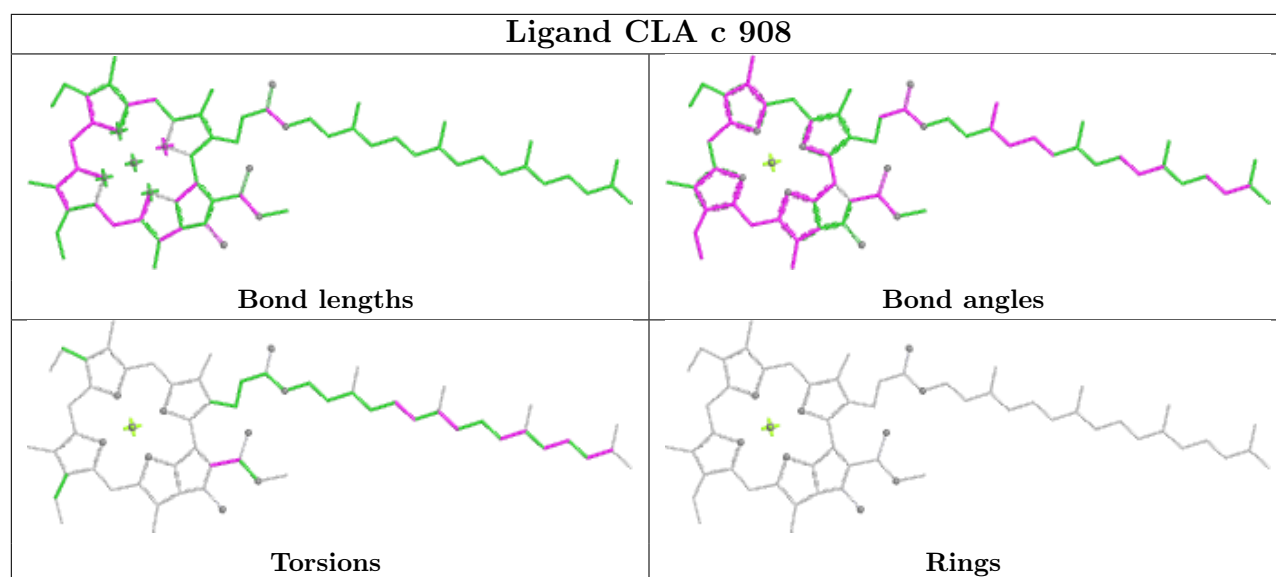




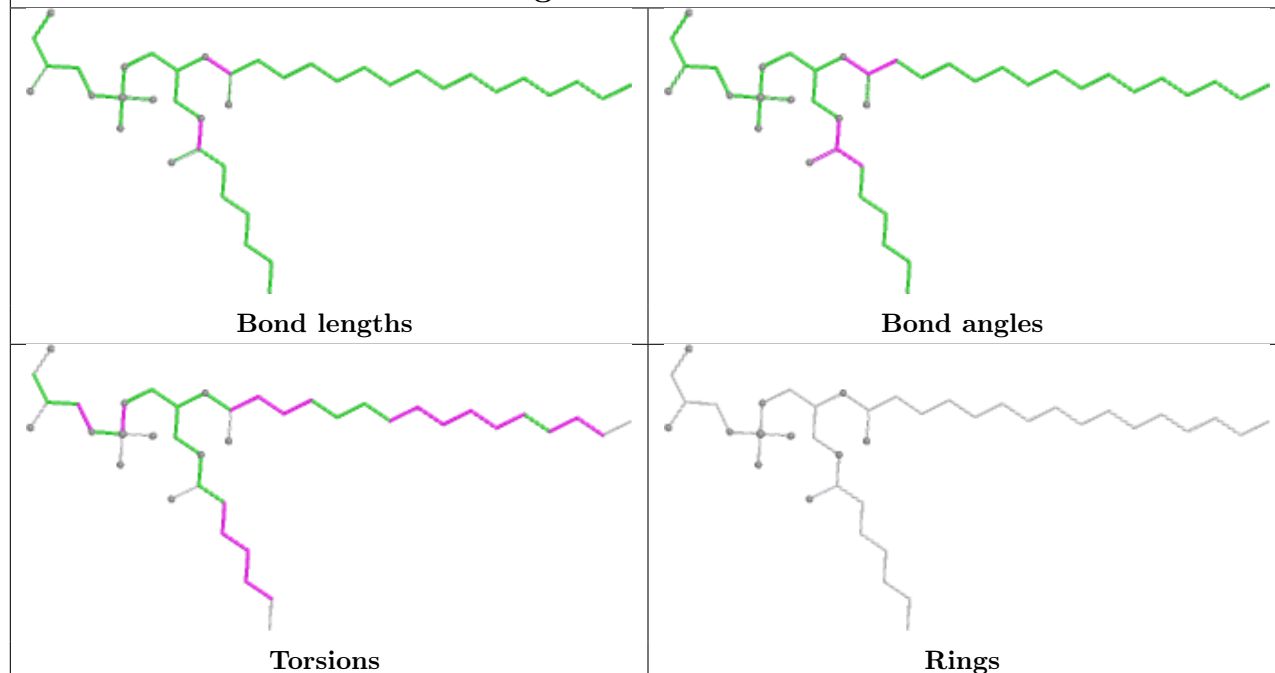




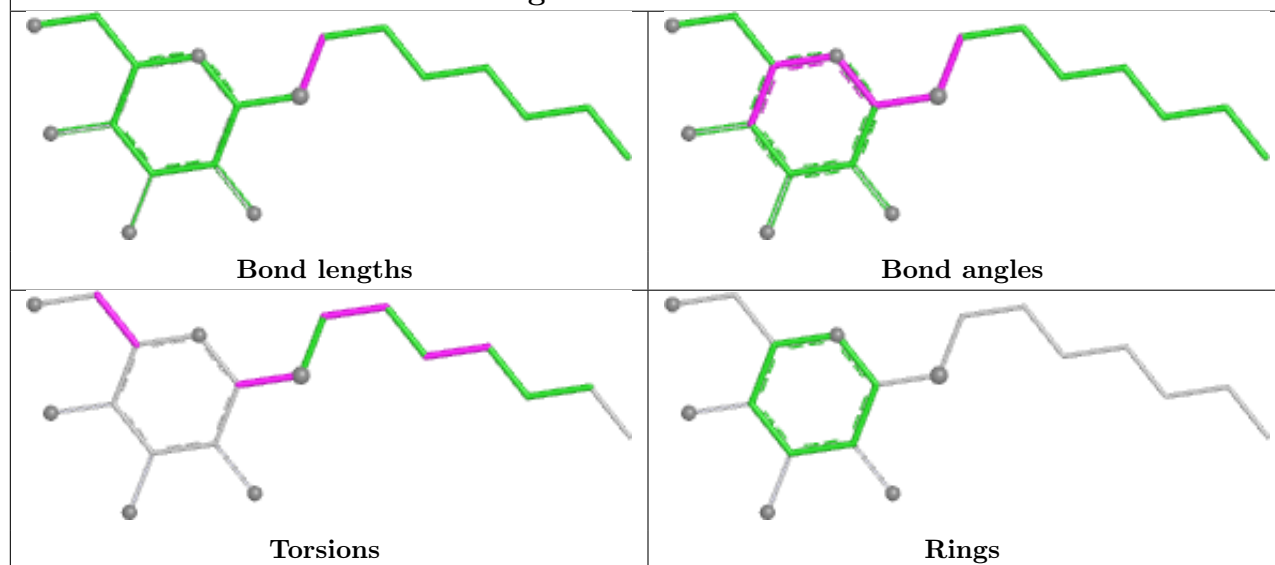


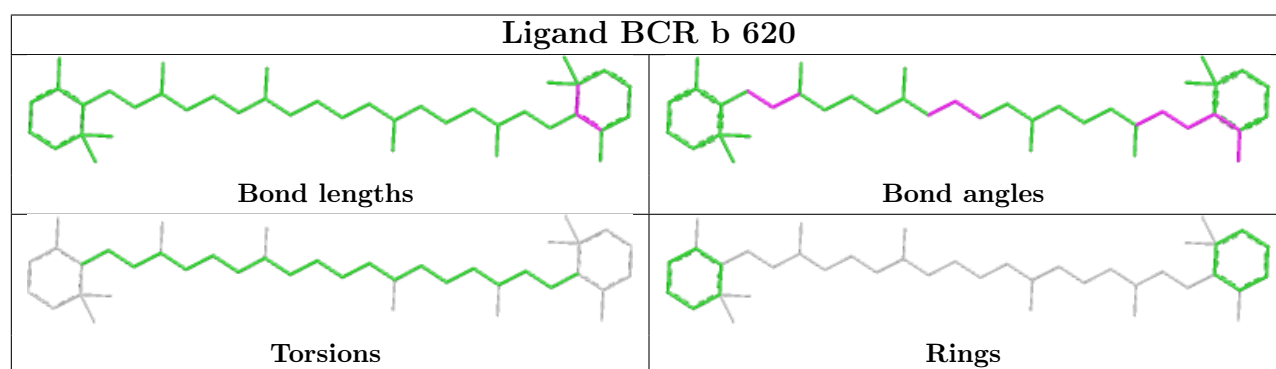
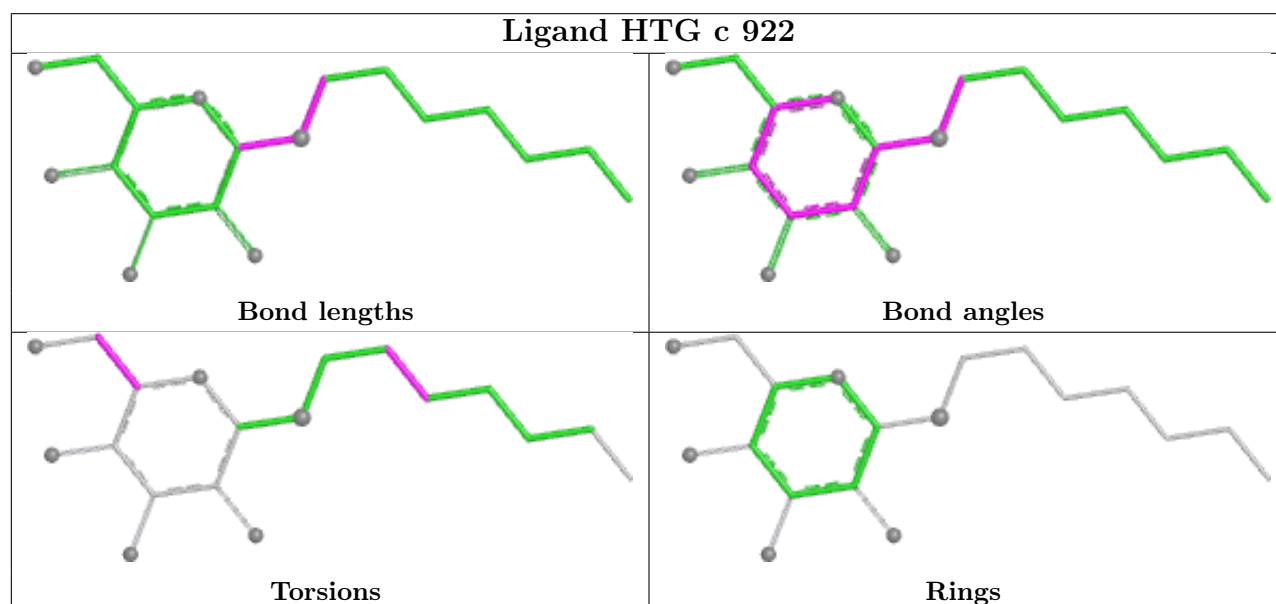
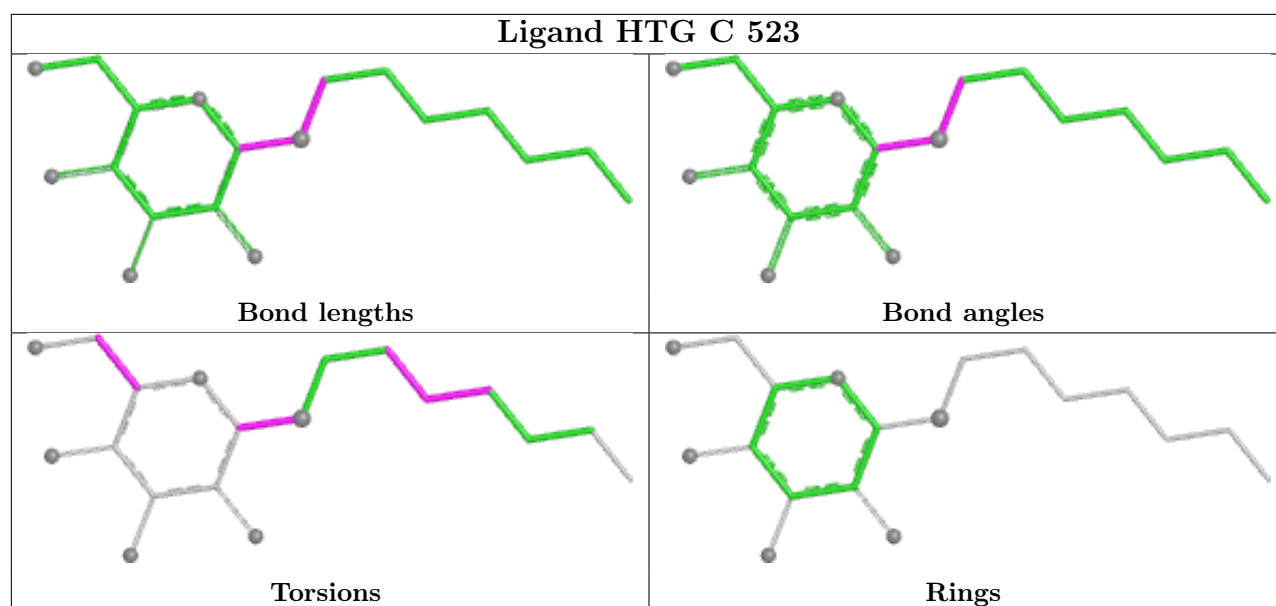


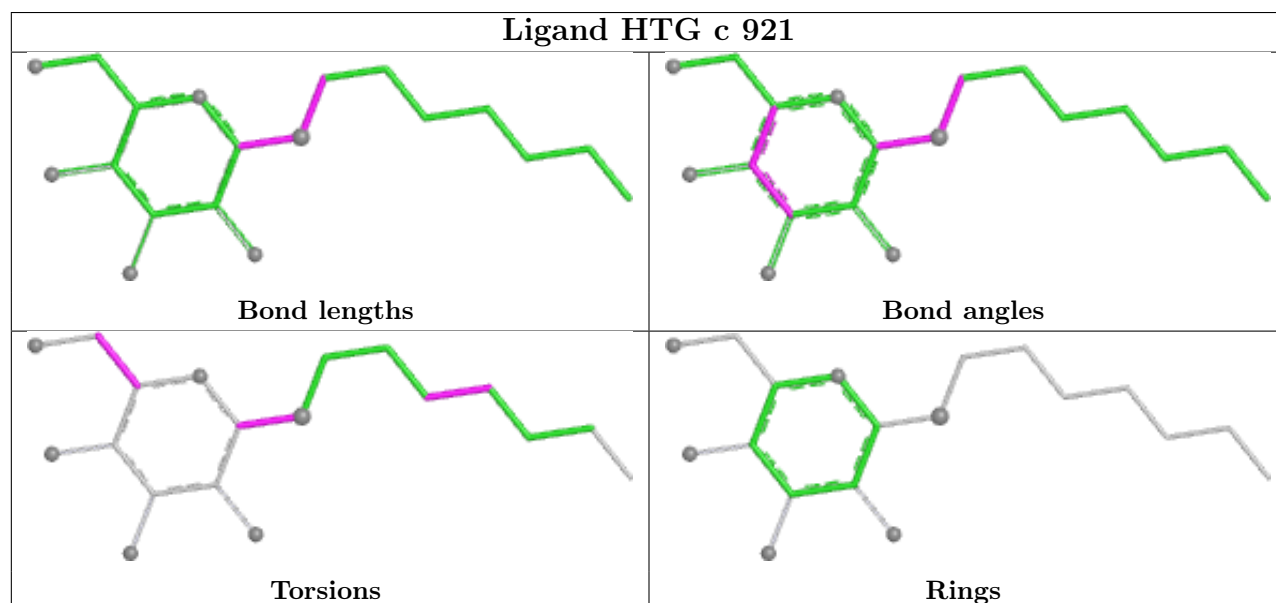
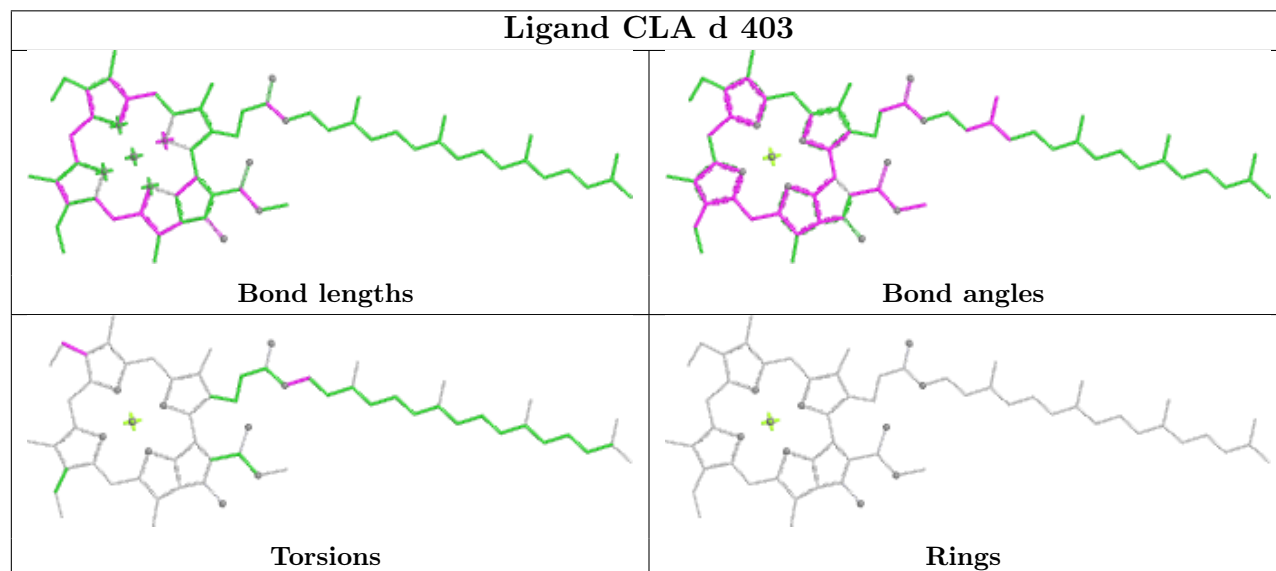
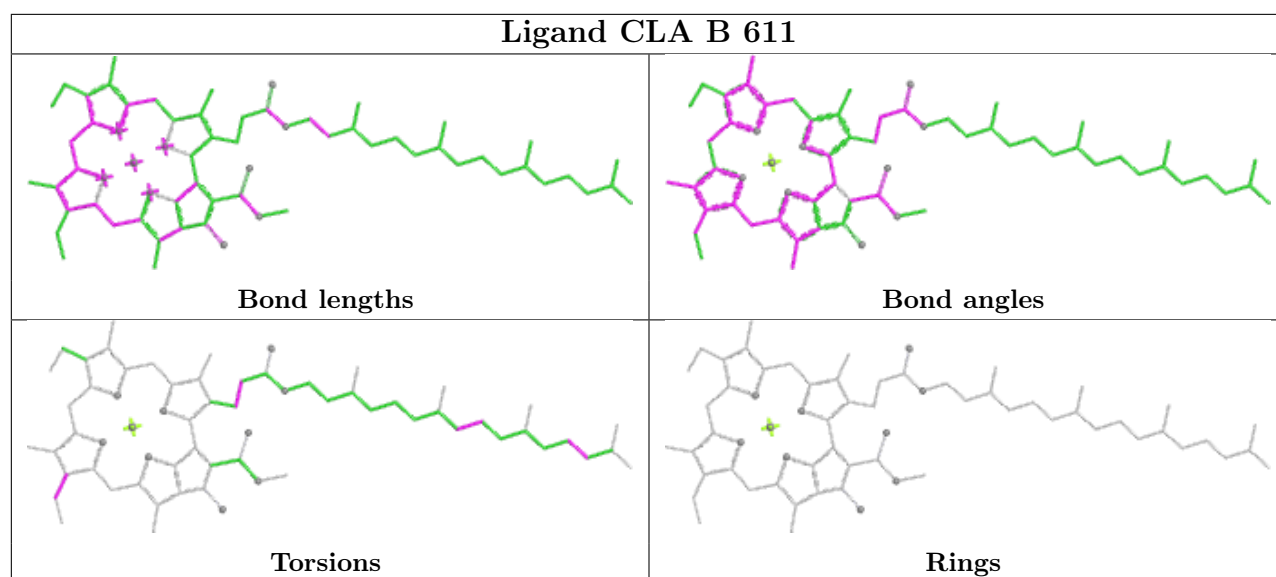
Ligand LHG e 101

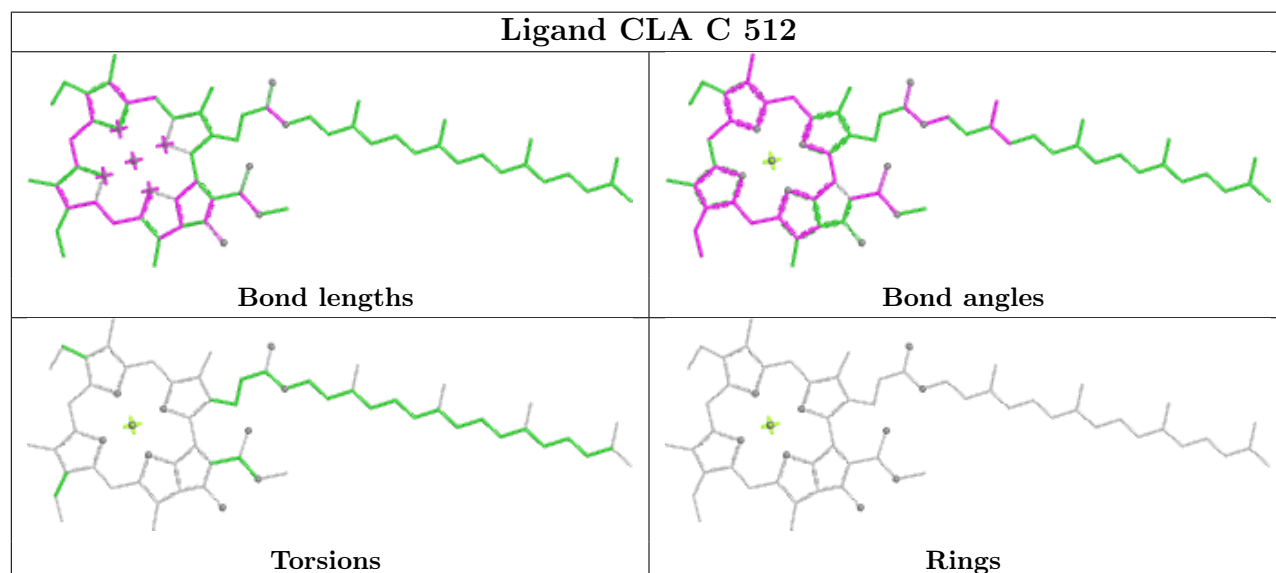
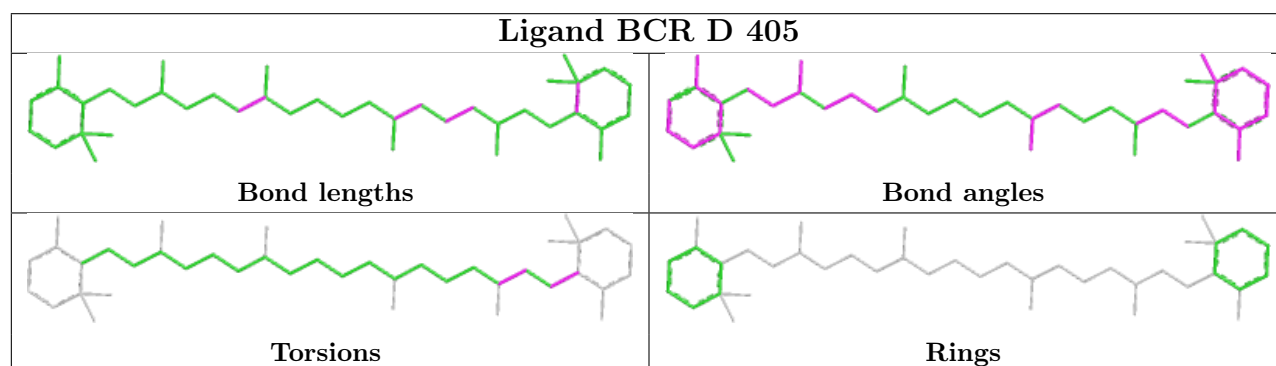
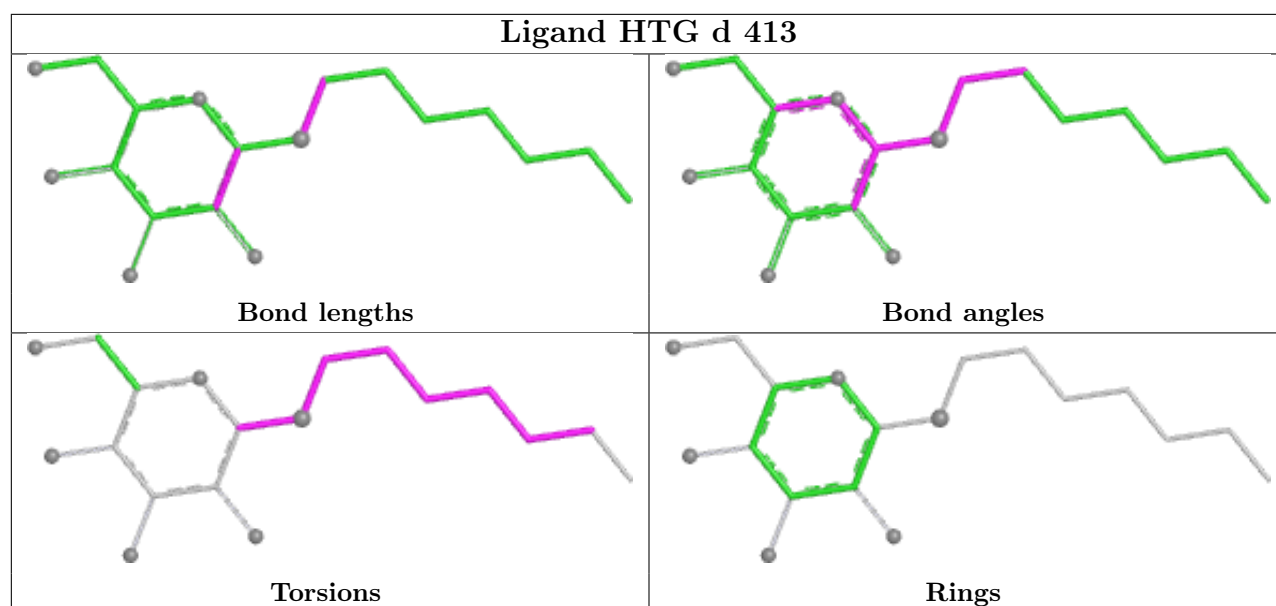


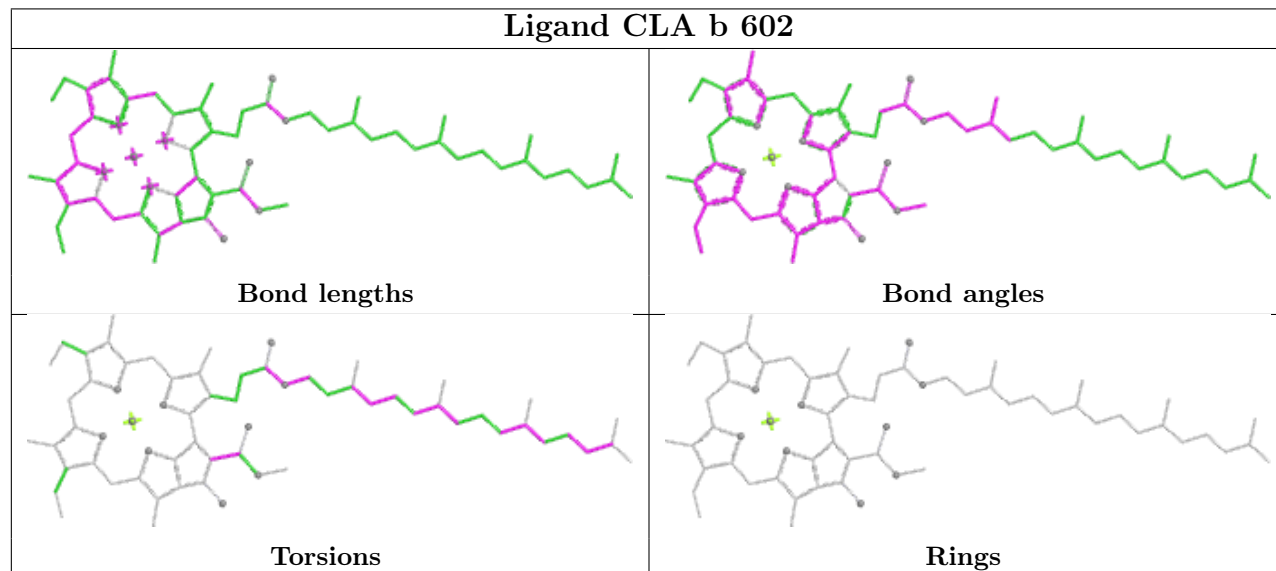
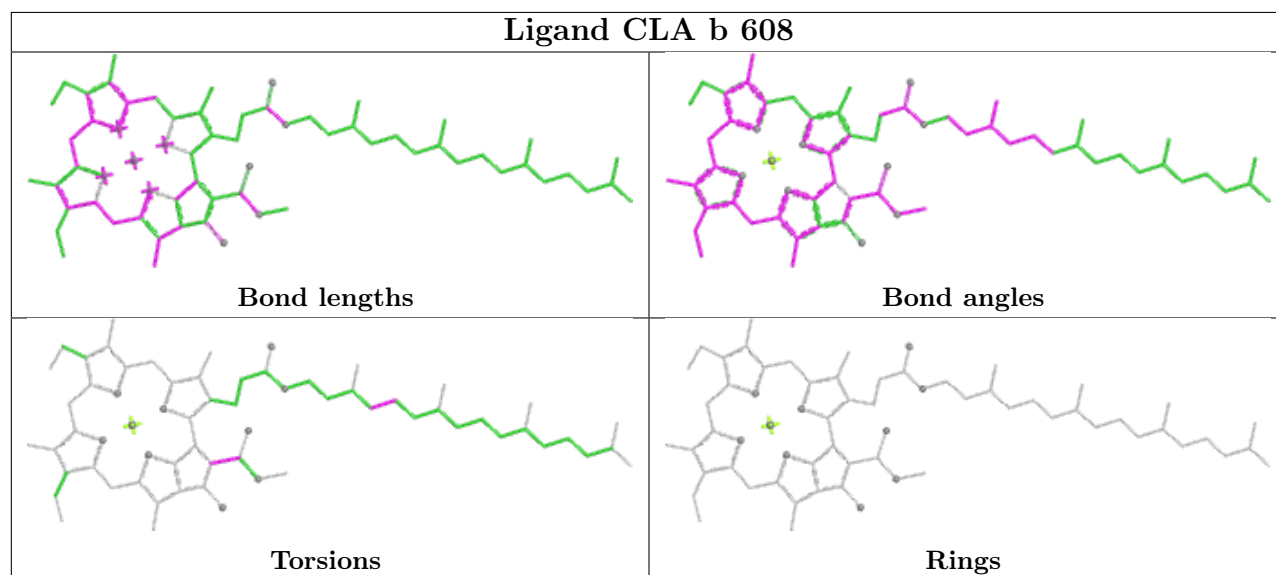
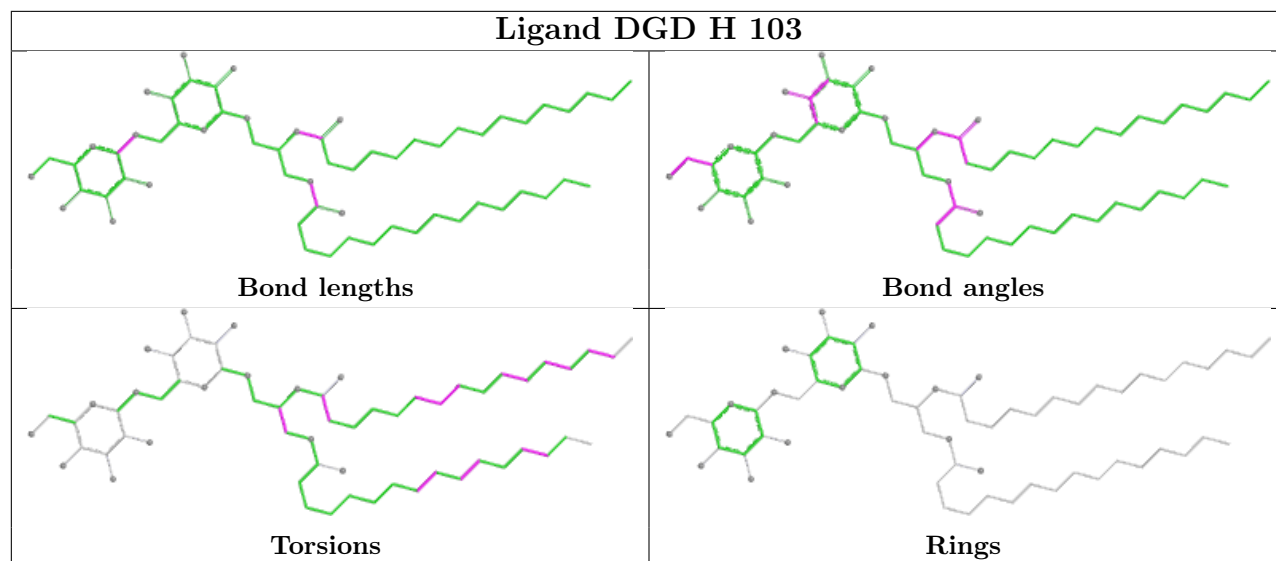
Ligand HTG C 522

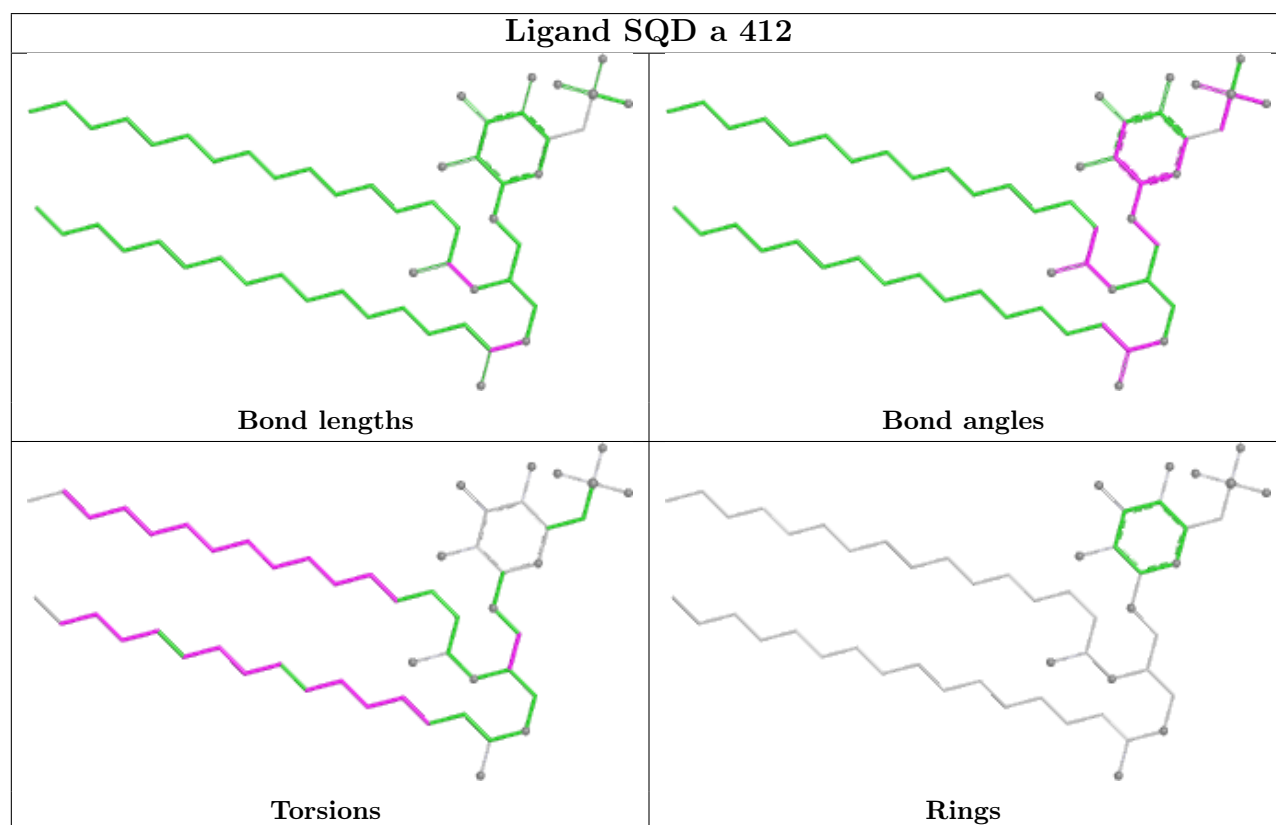
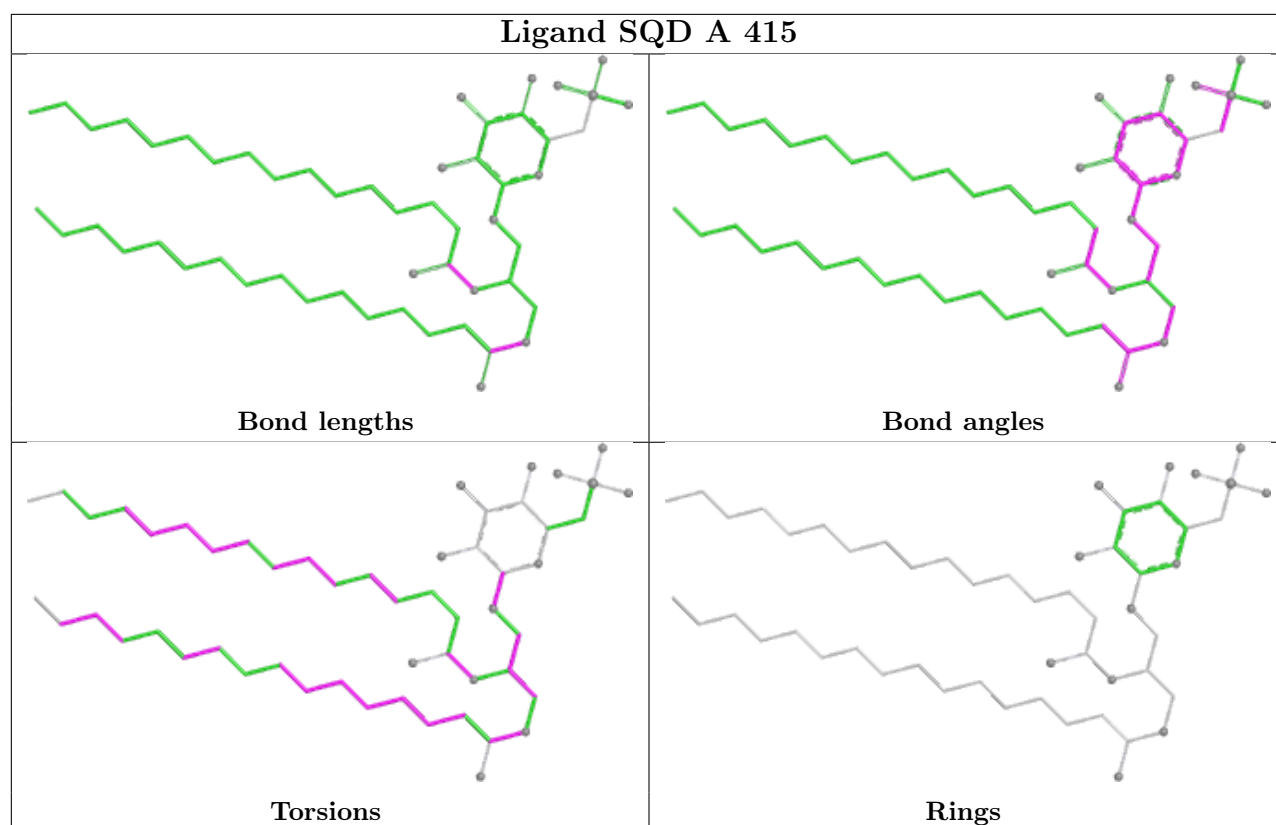


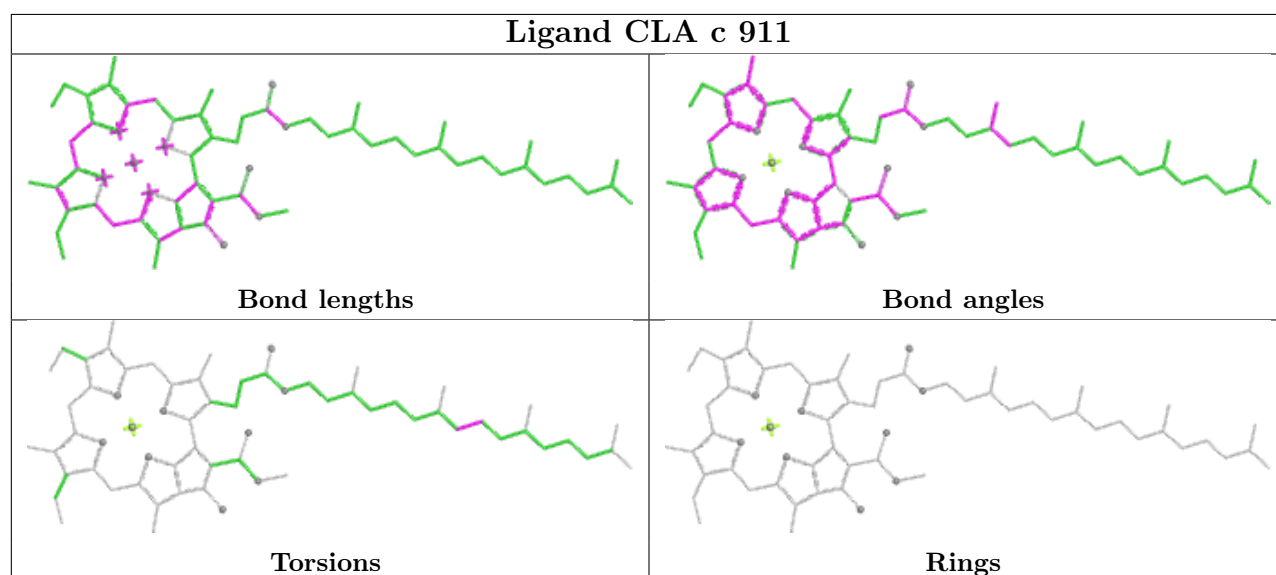
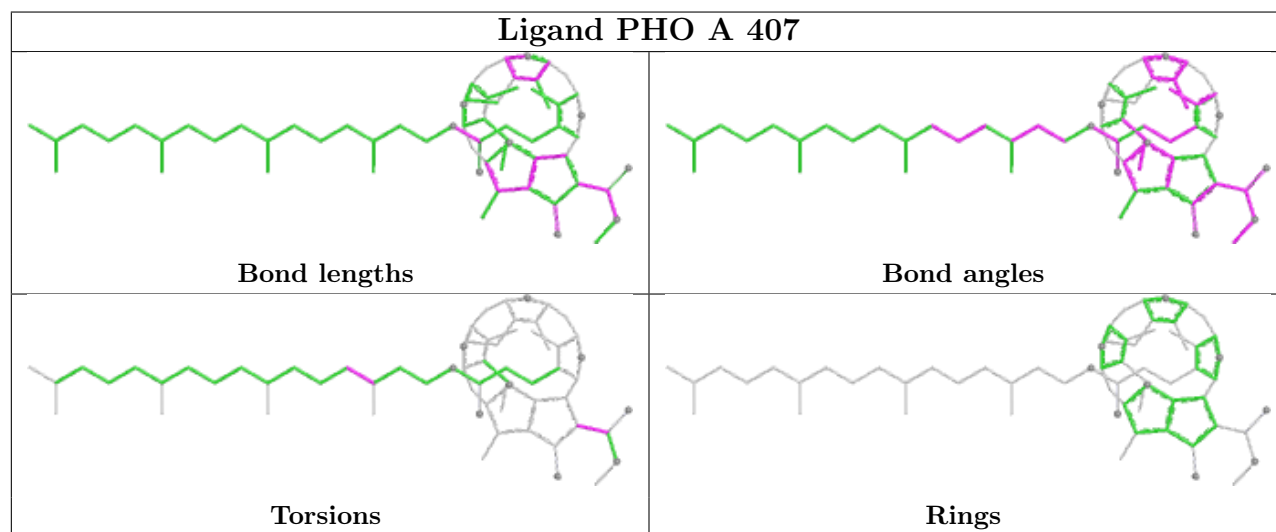
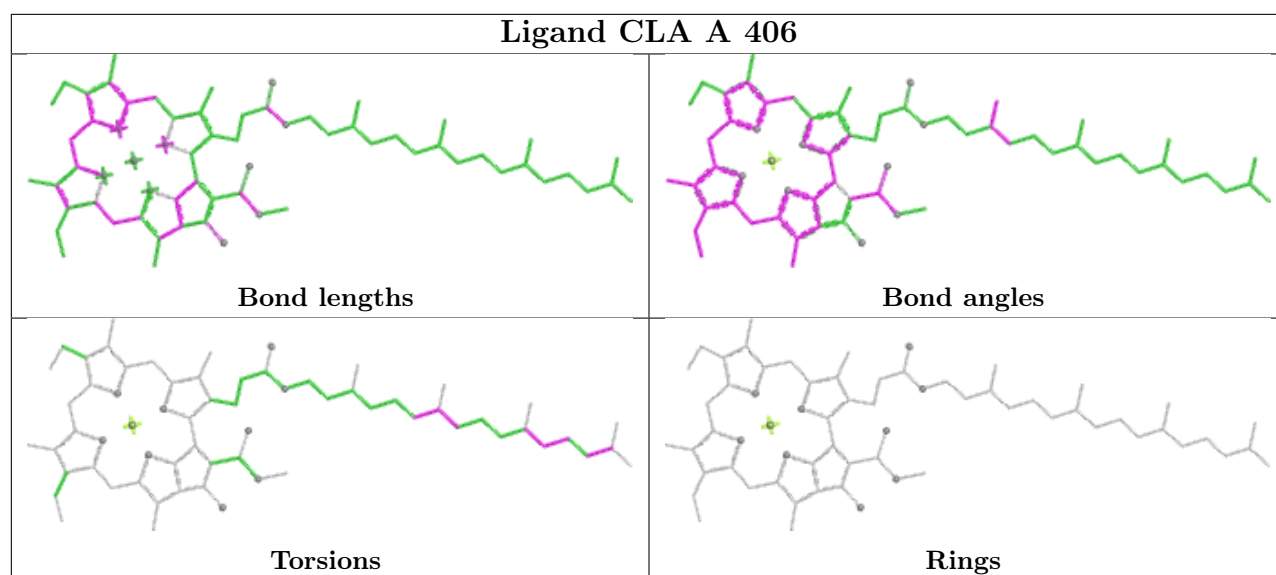


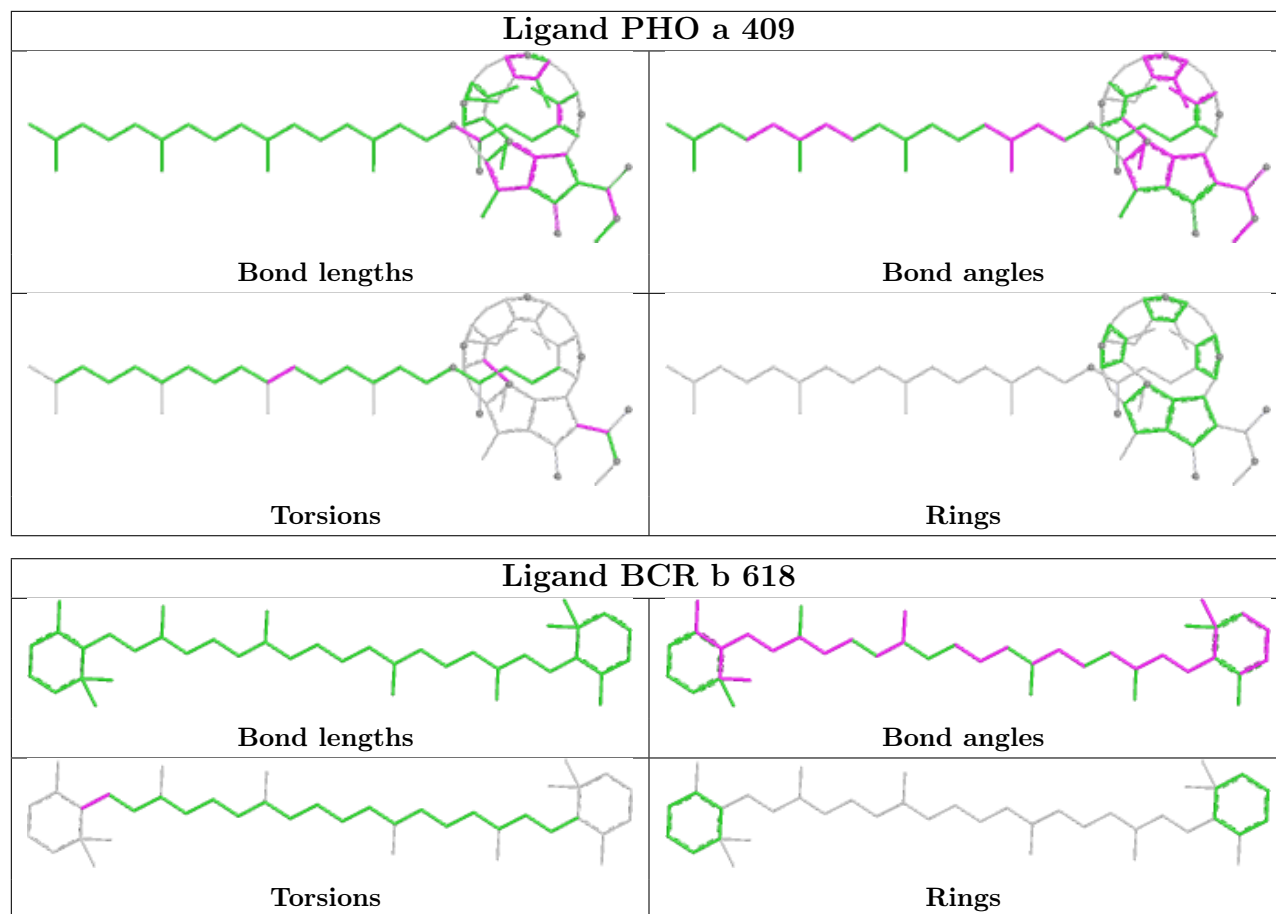




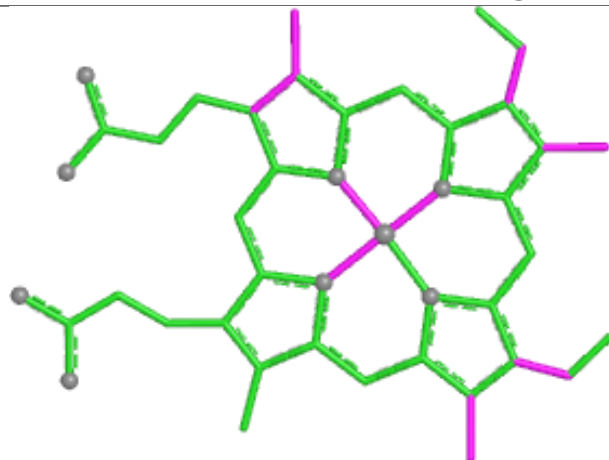




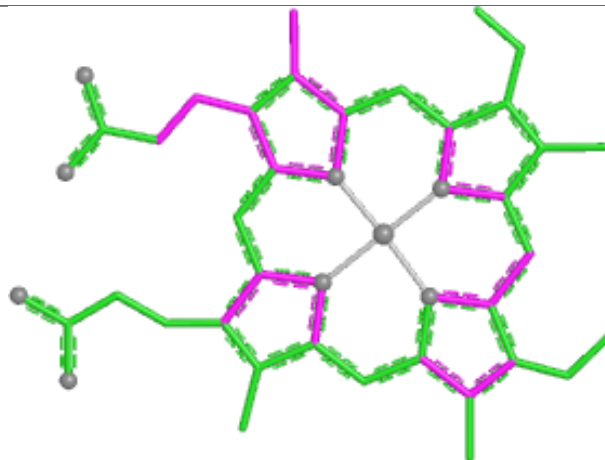




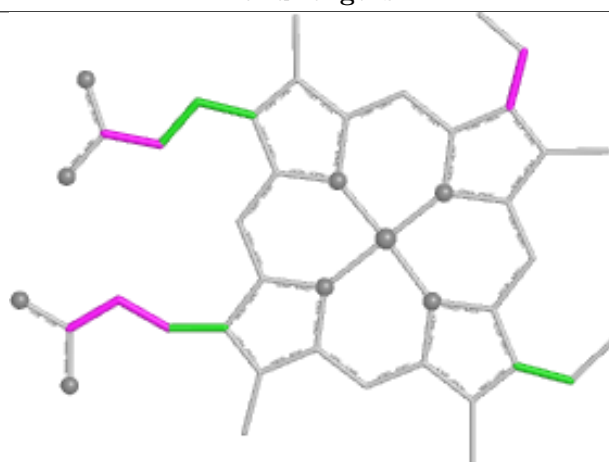
Ligand HEM E 105



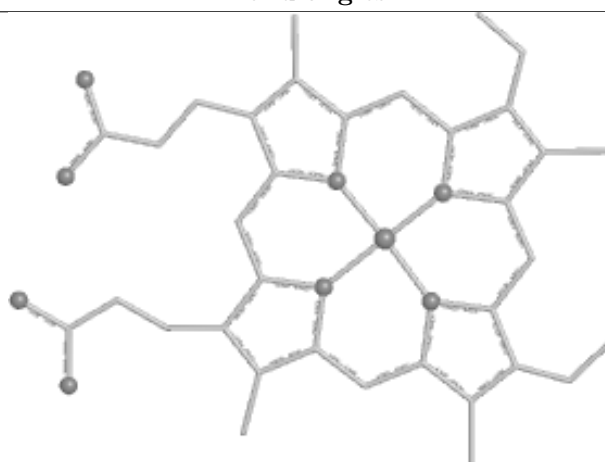
Bond lengths



Bond angles

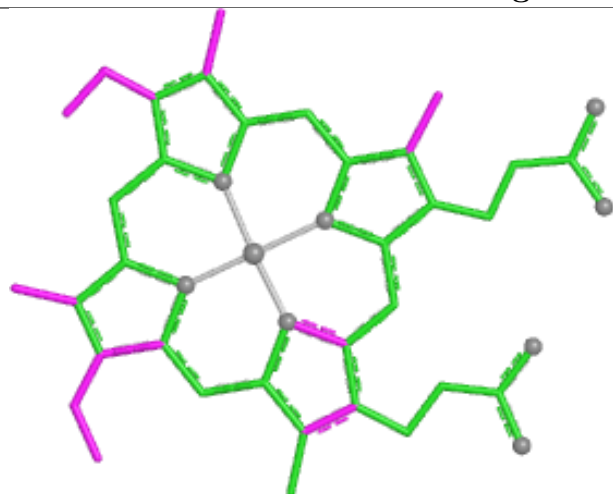


Torsions

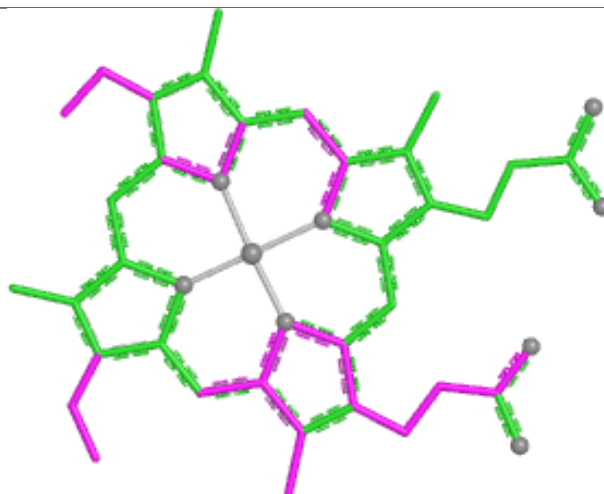


Rings

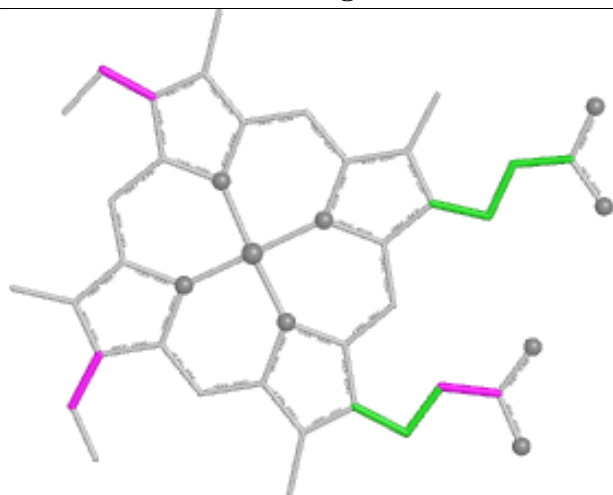
Ligand HEC V 203



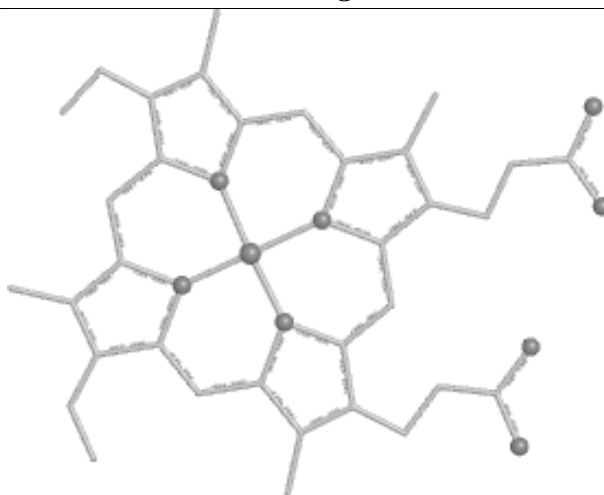
Bond lengths



Bond angles

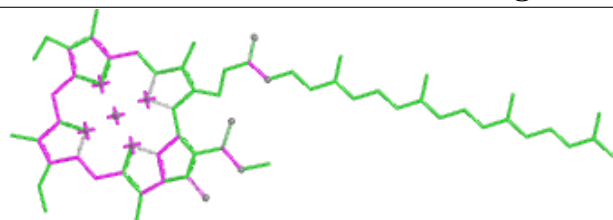


Torsions

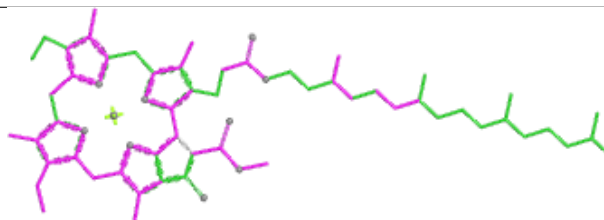


Rings

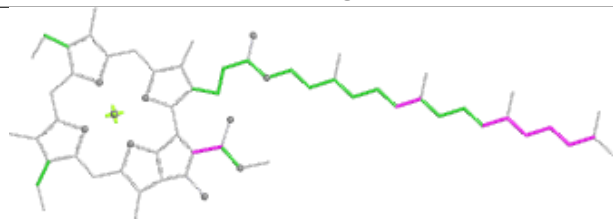
Ligand CLA D 404



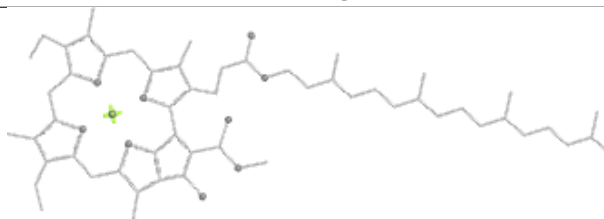
Bond lengths



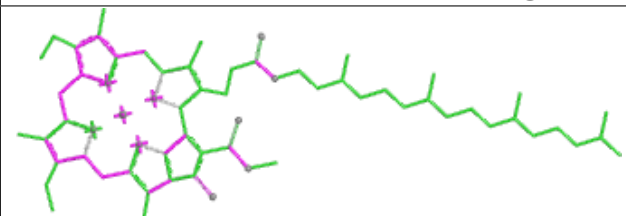
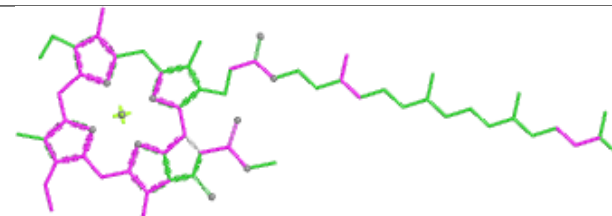
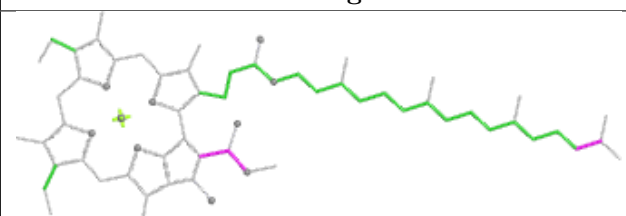
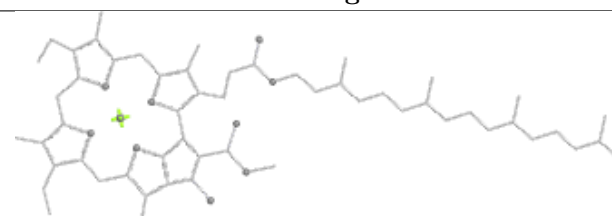
Bond angles

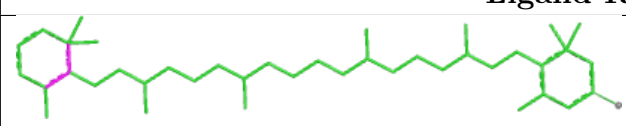
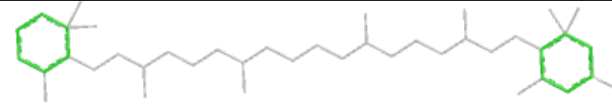


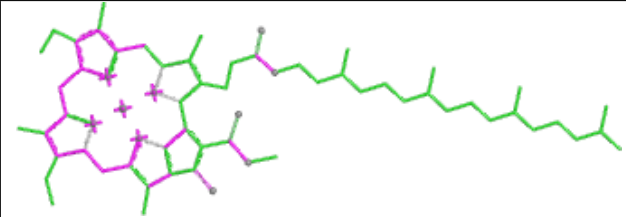
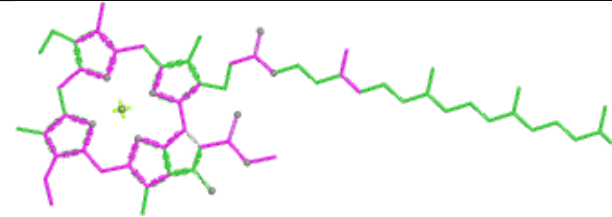
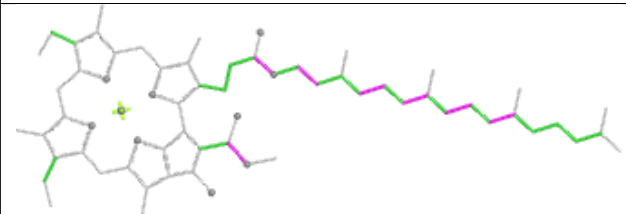
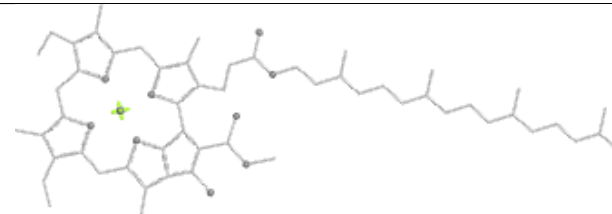
Torsions

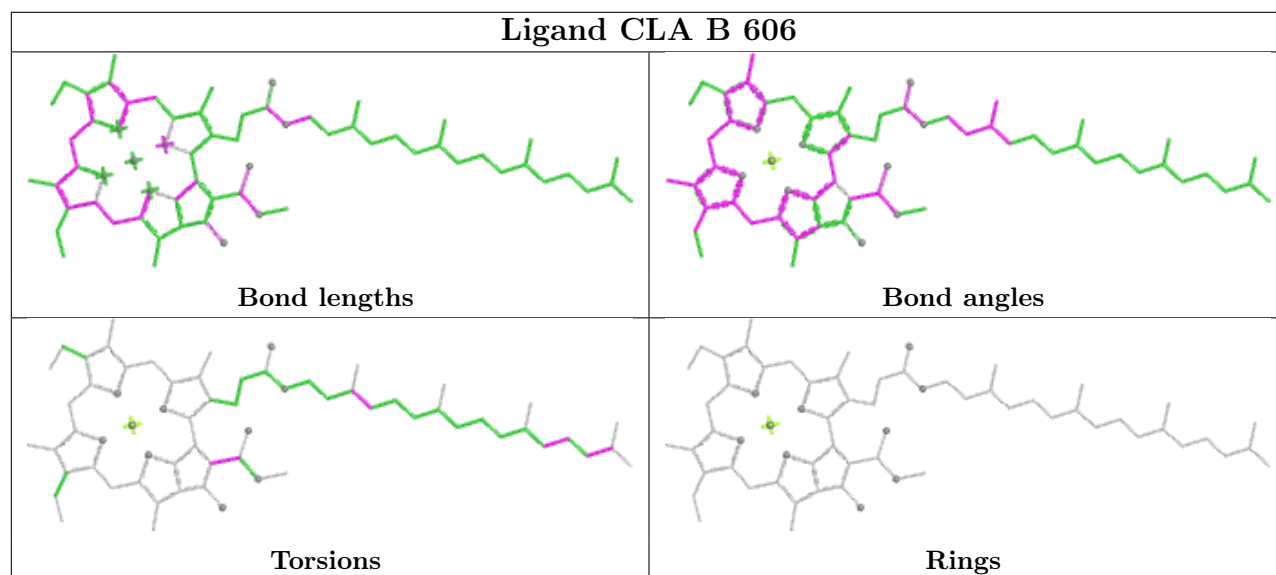
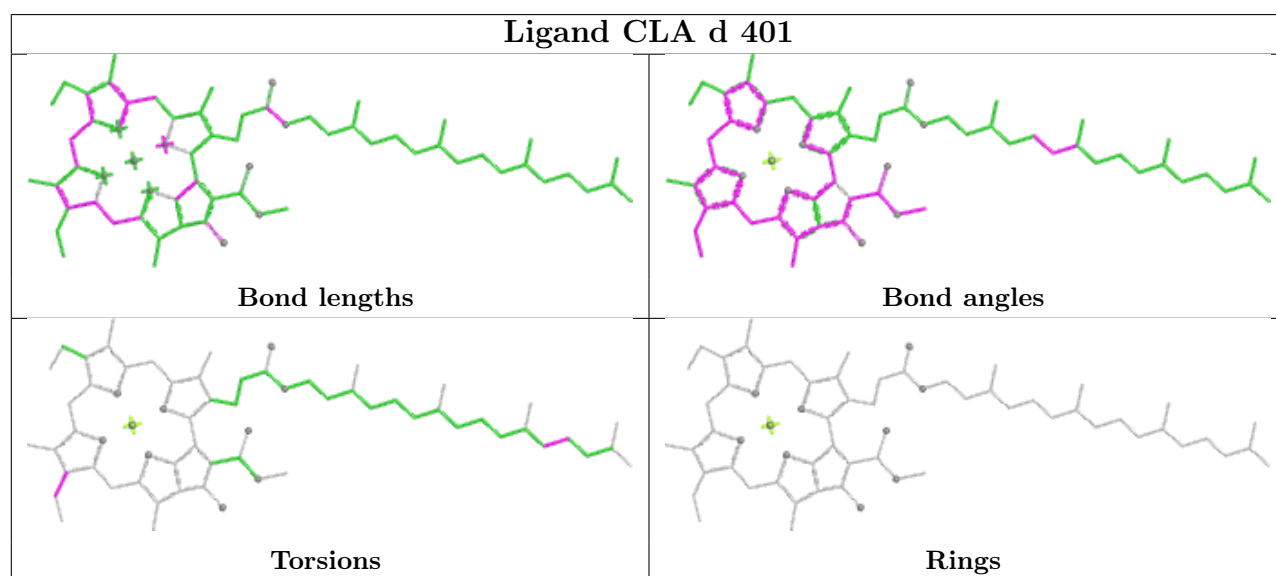
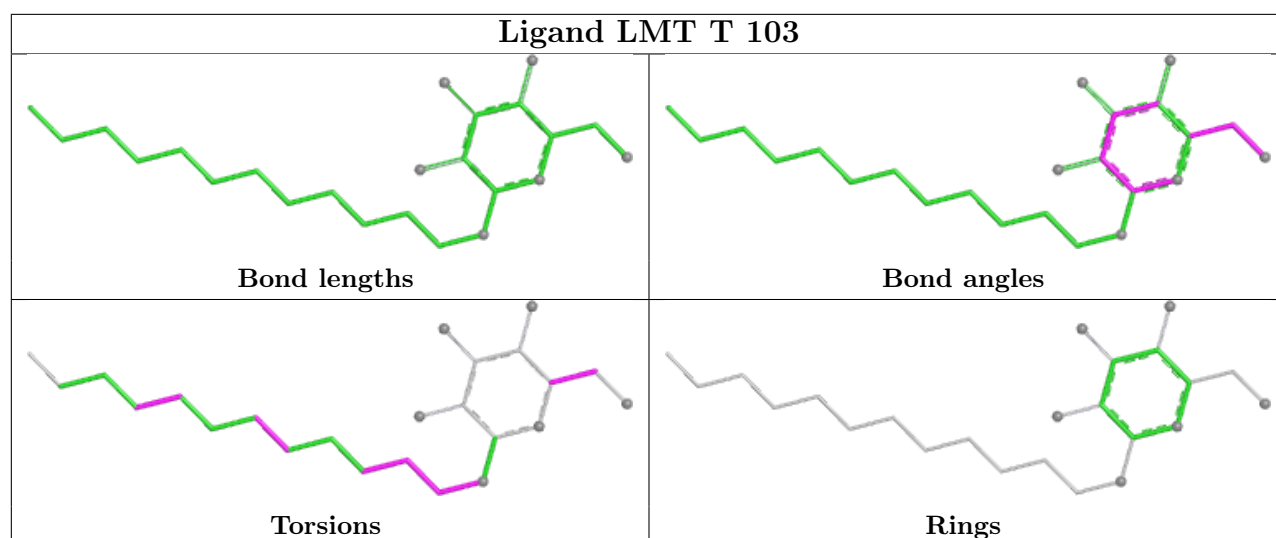


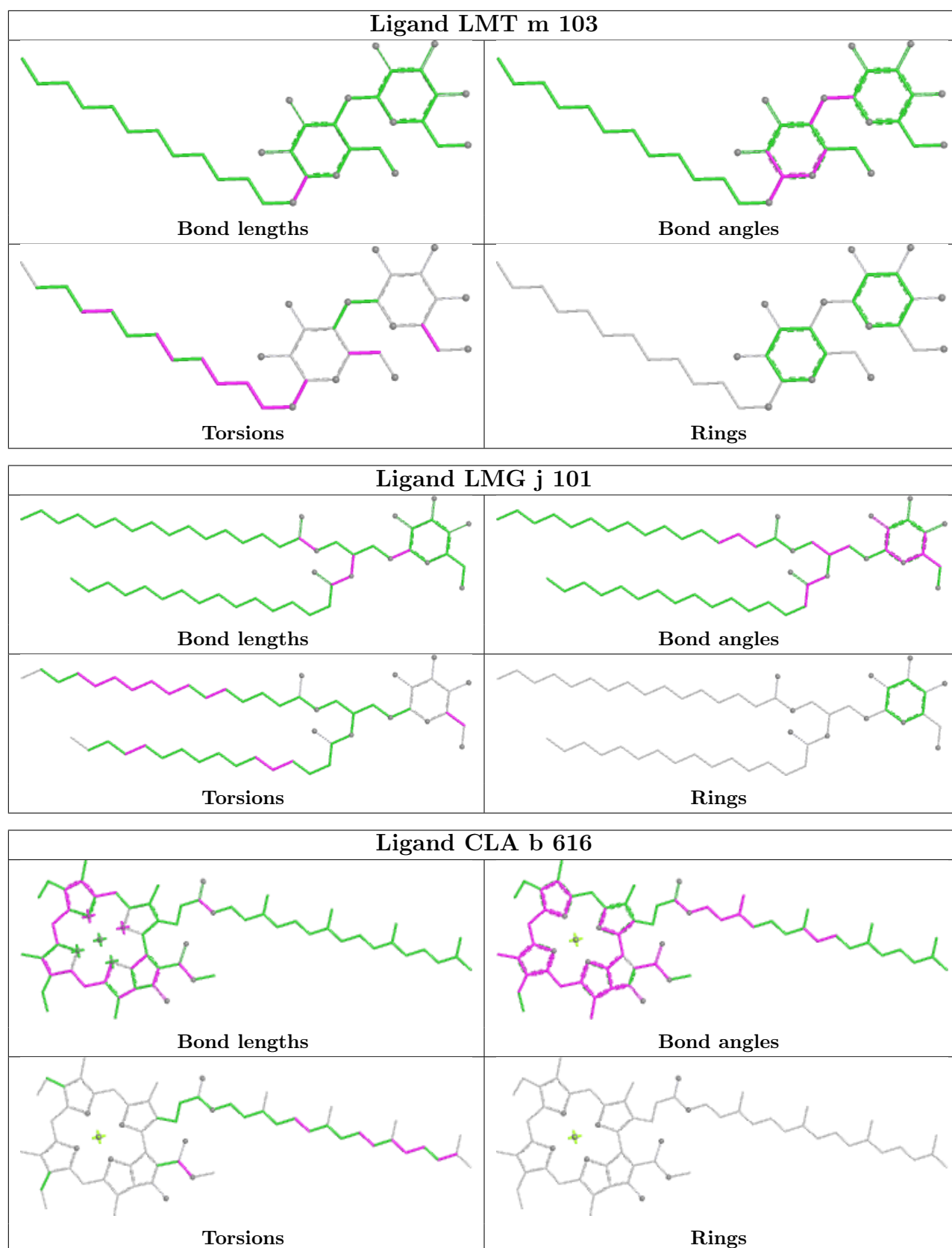
Rings

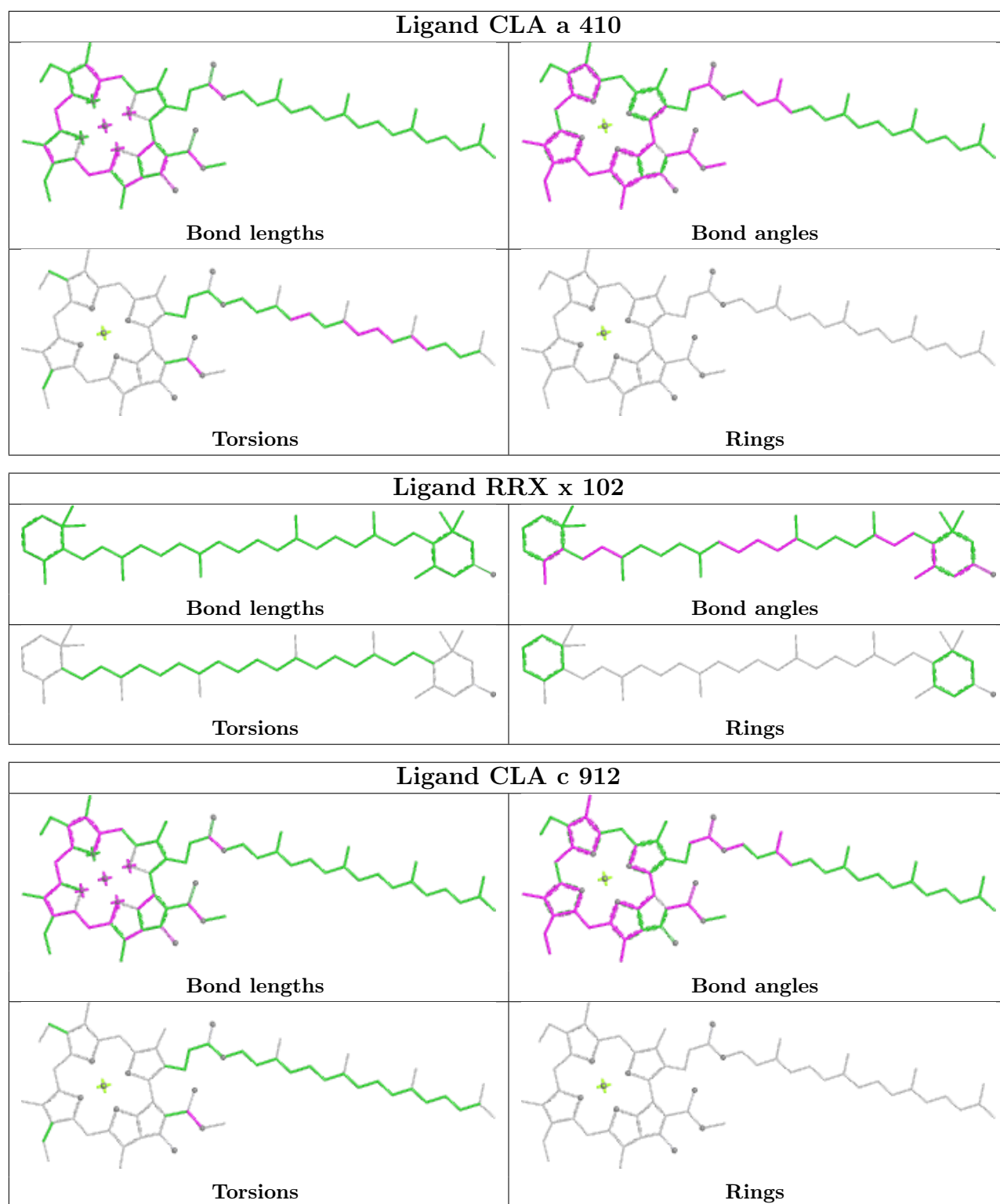
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

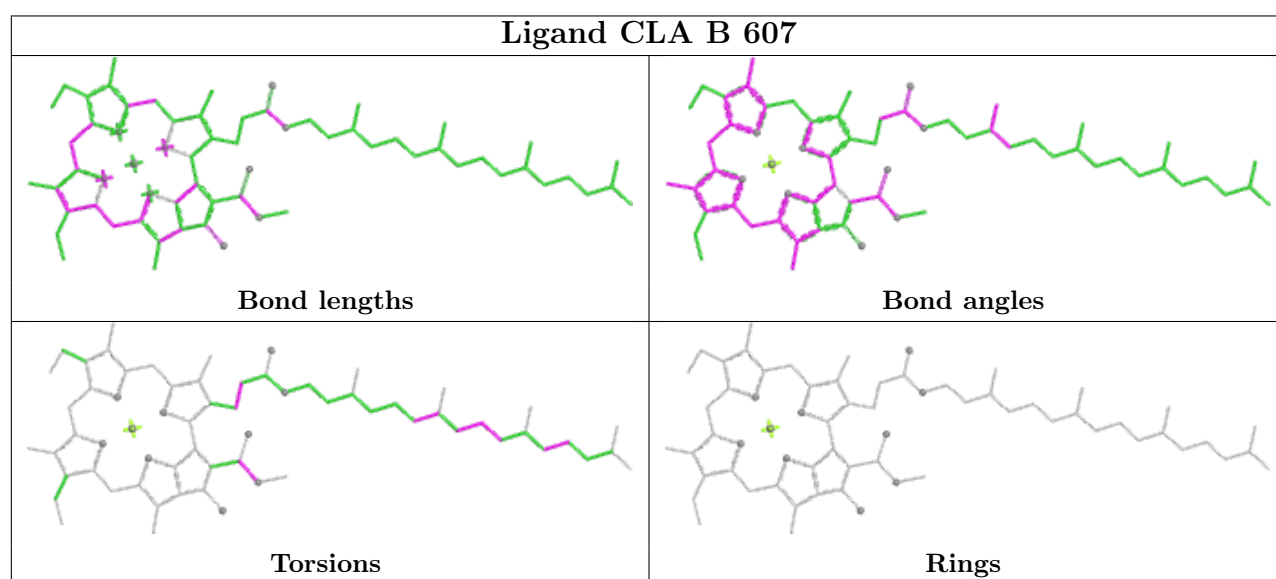
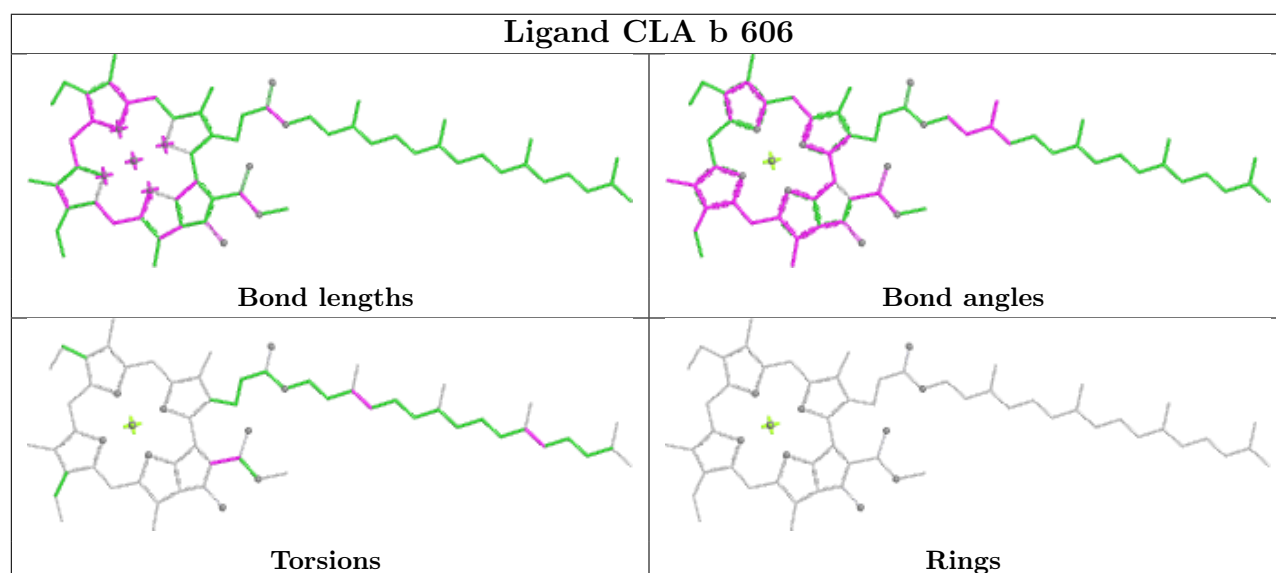
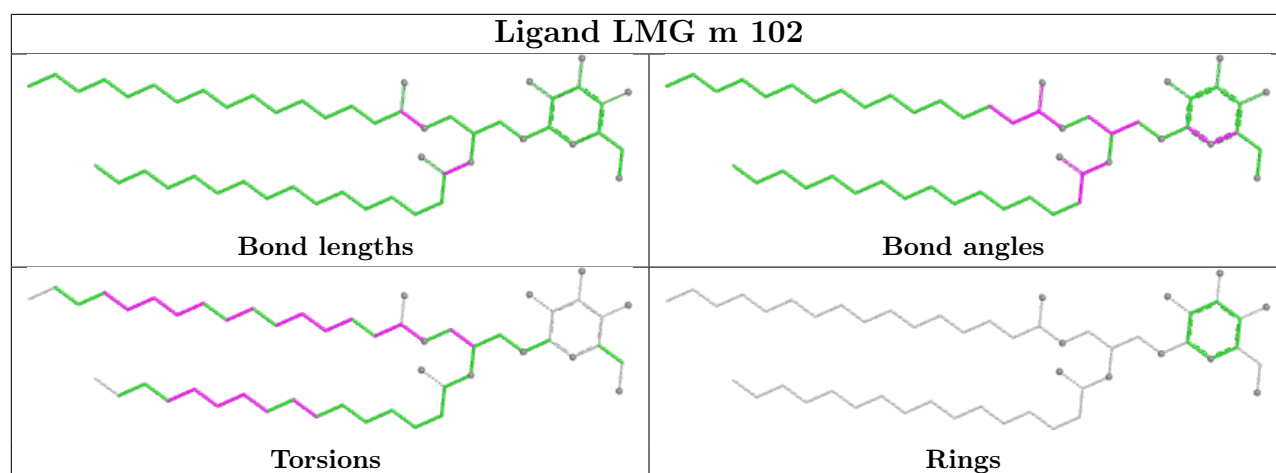
Ligand RRX H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

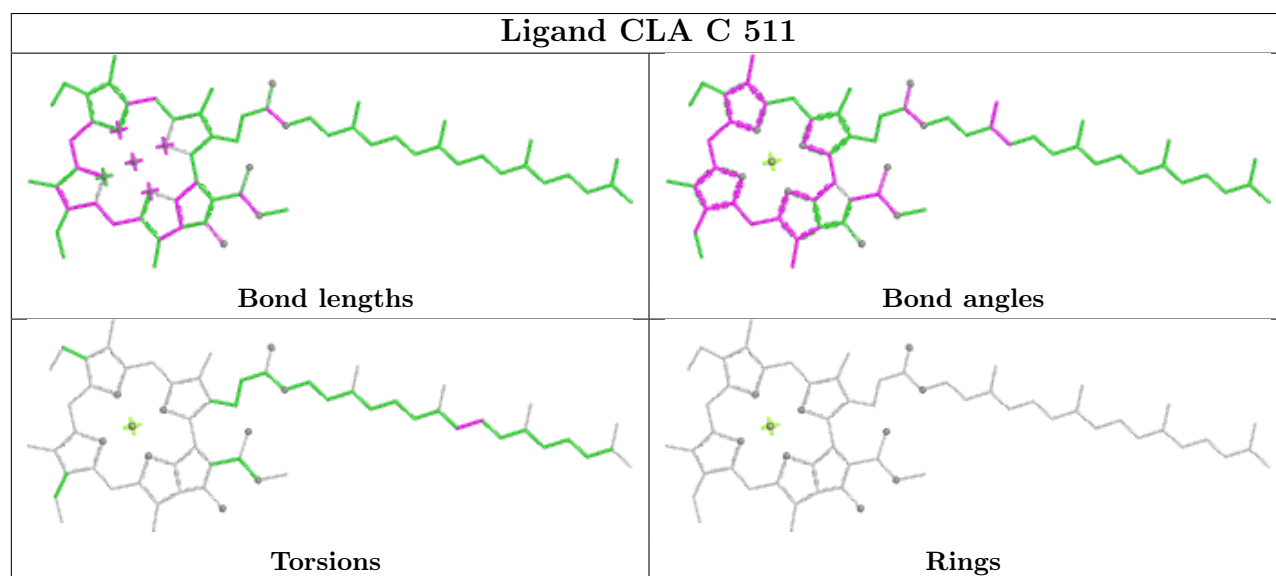
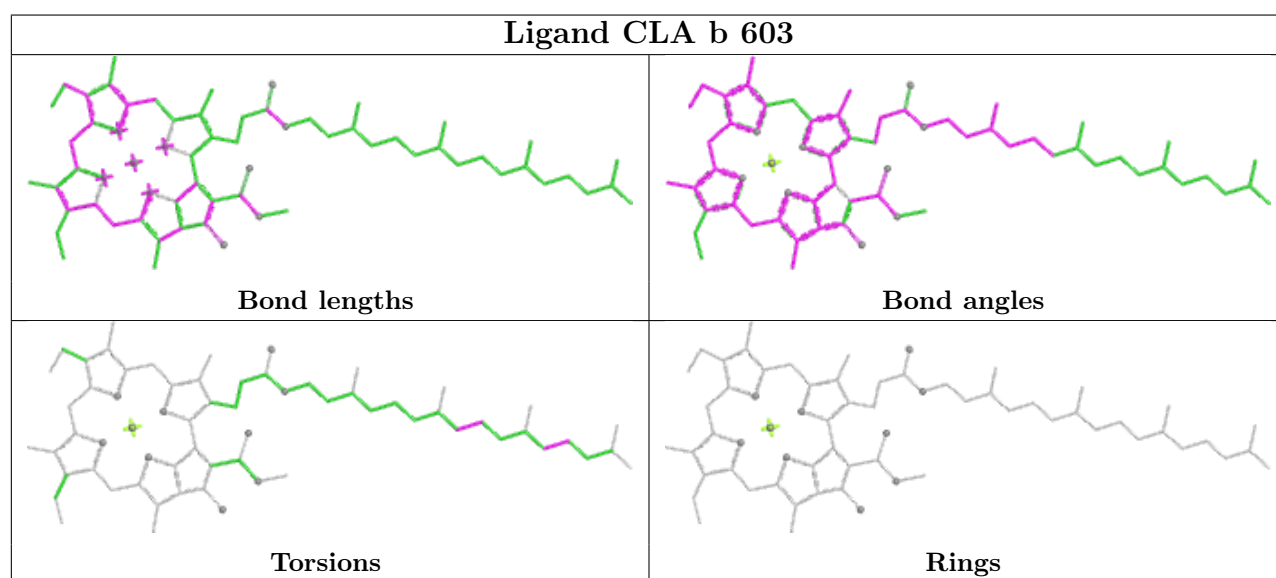
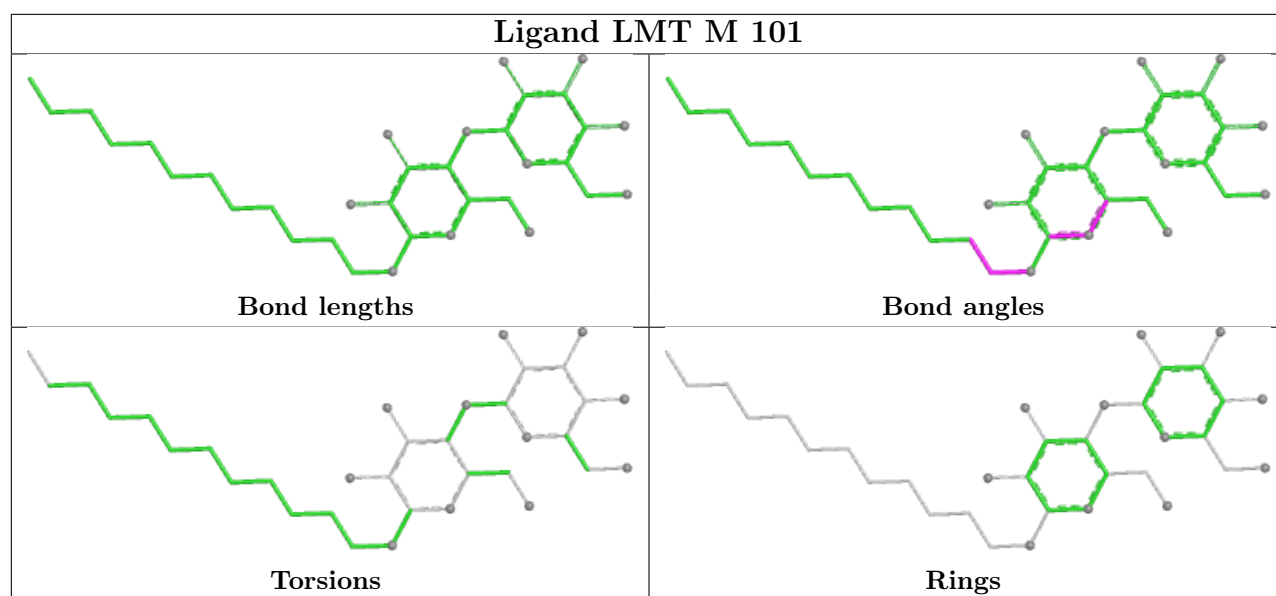
Ligand CLA C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

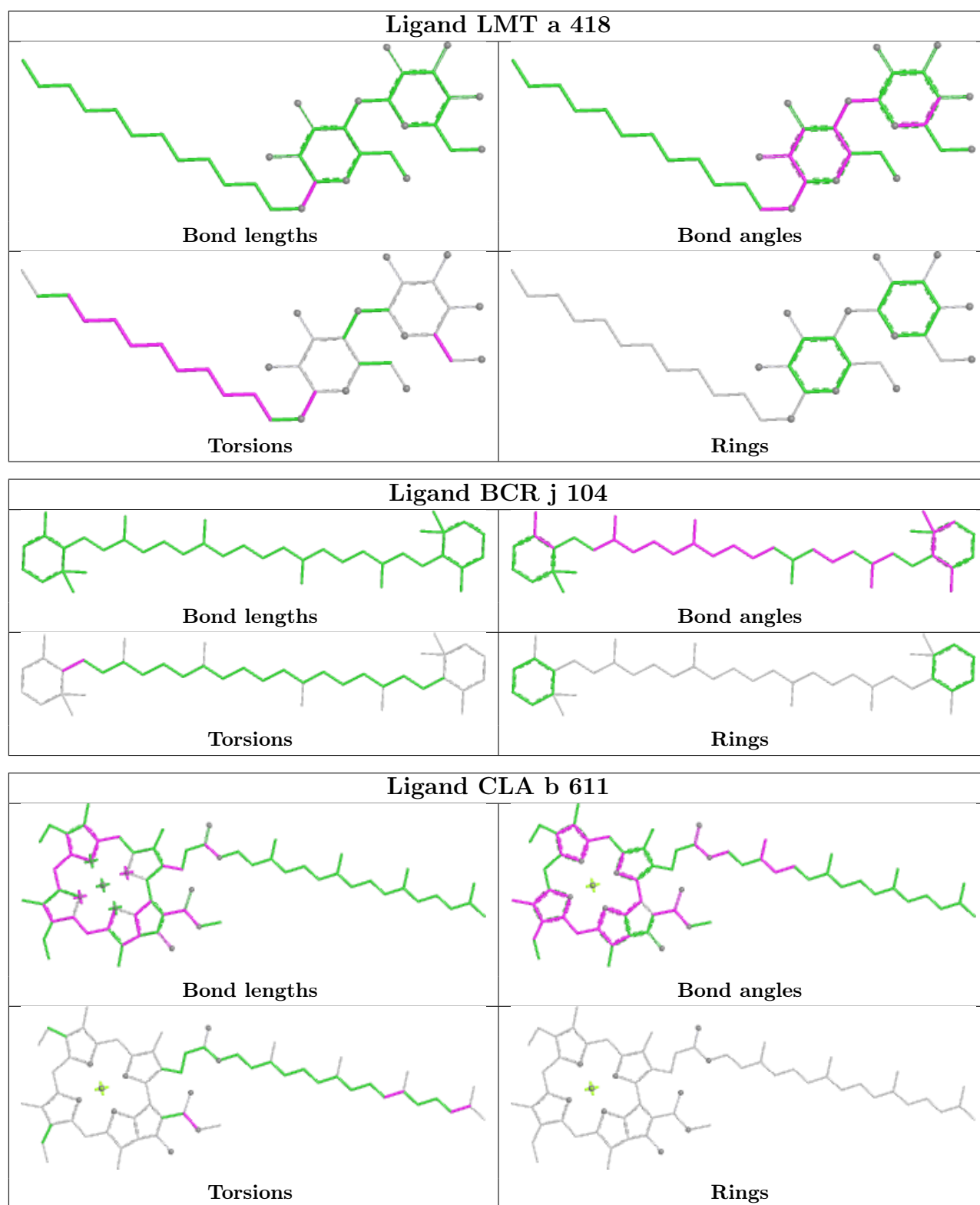


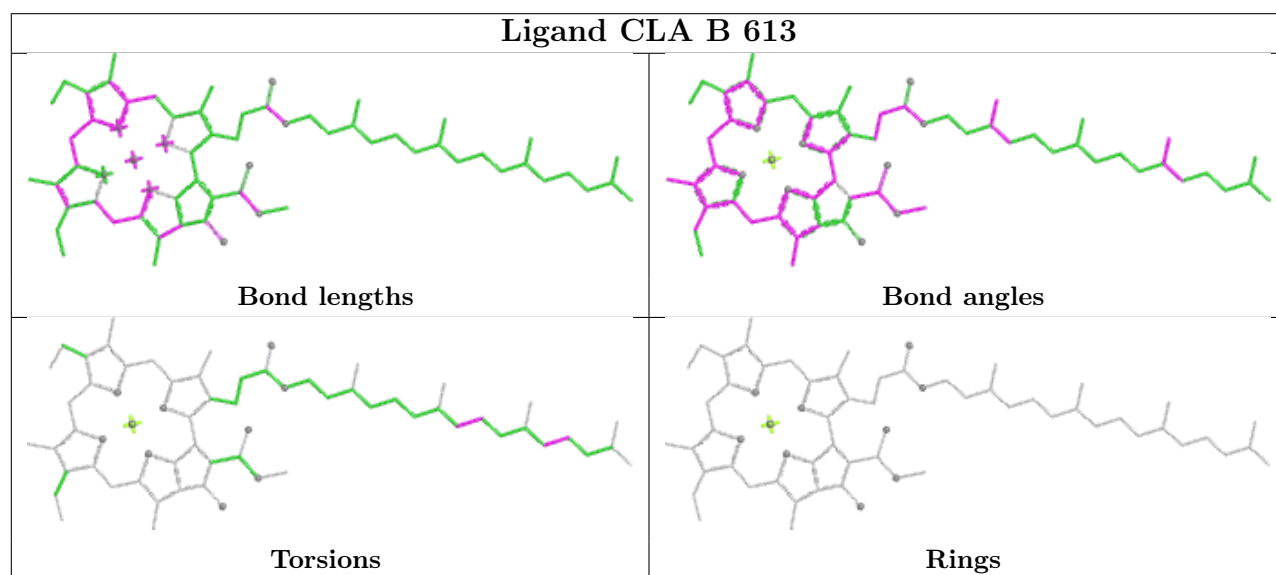
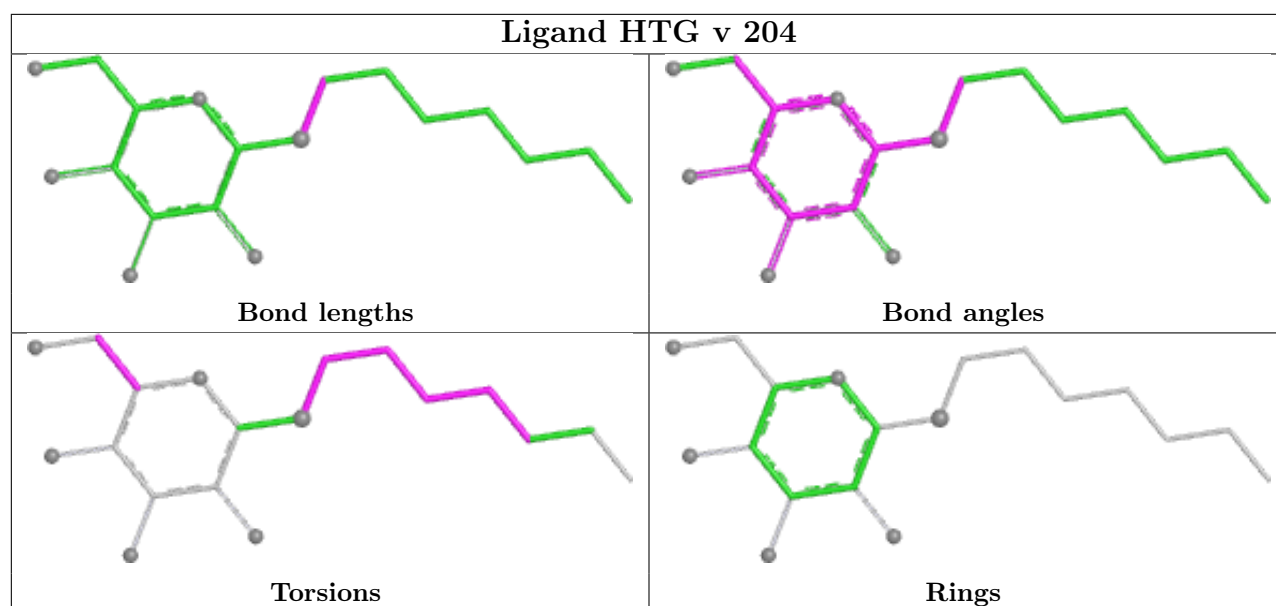


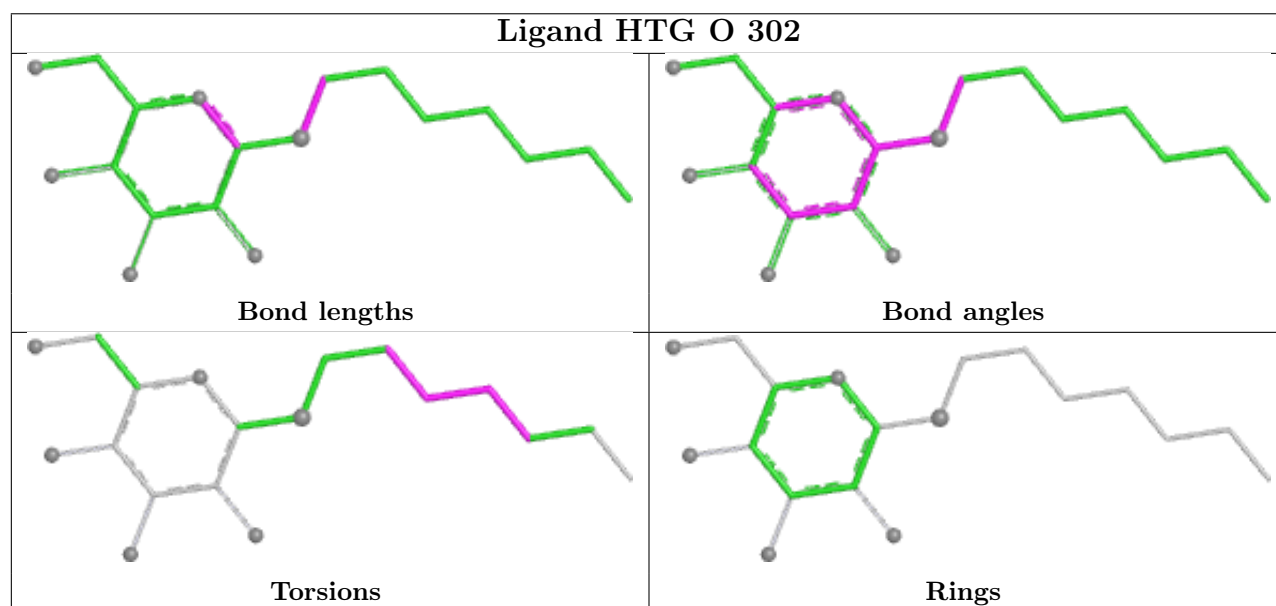
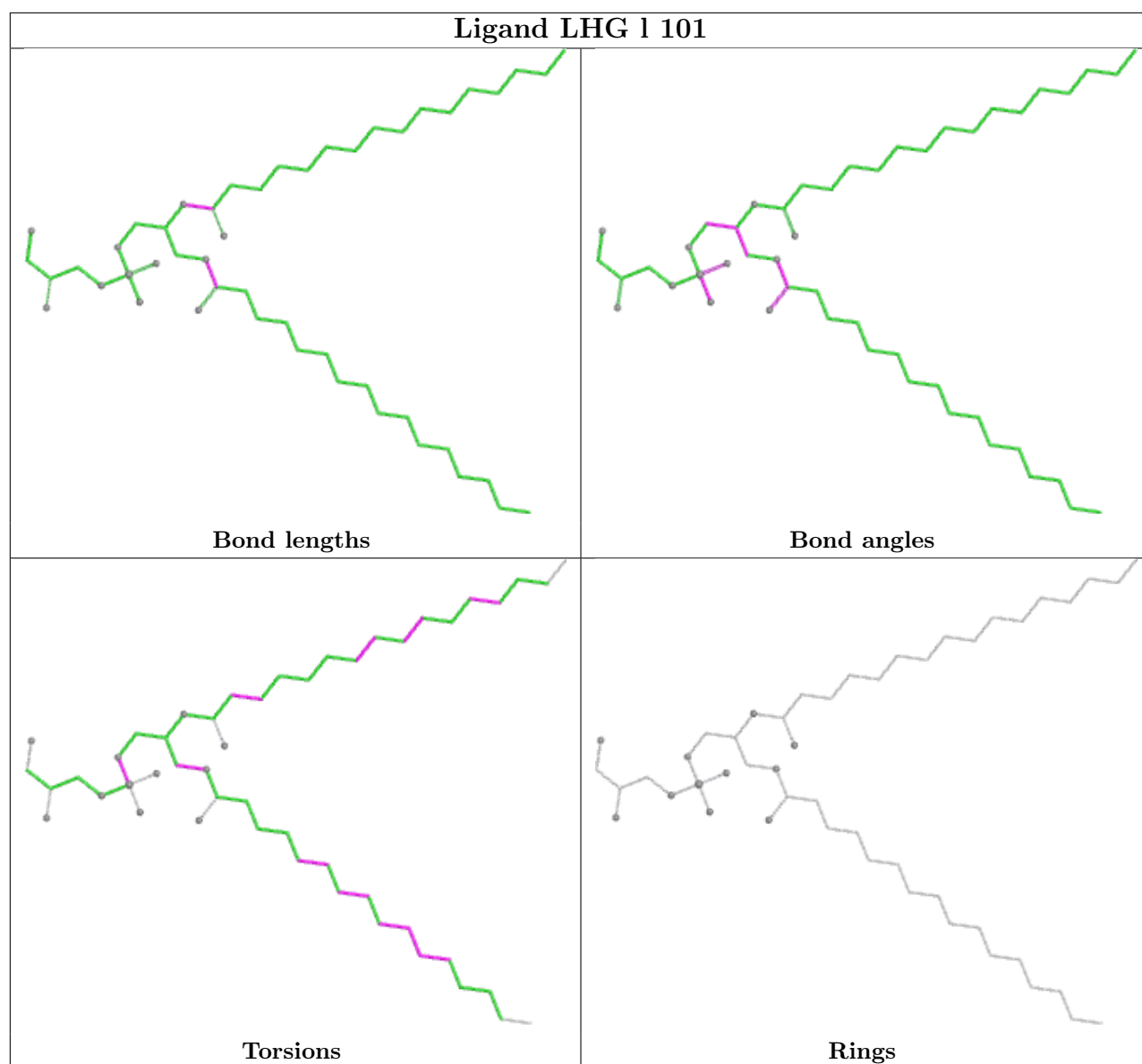


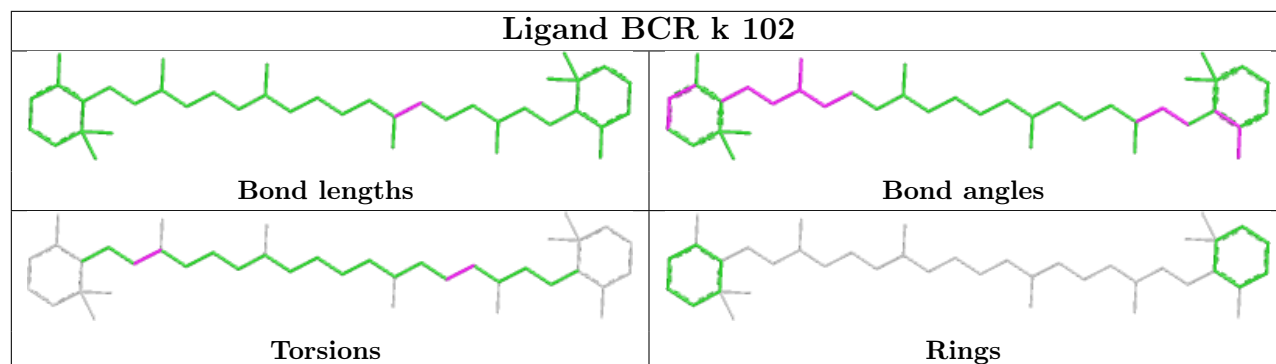
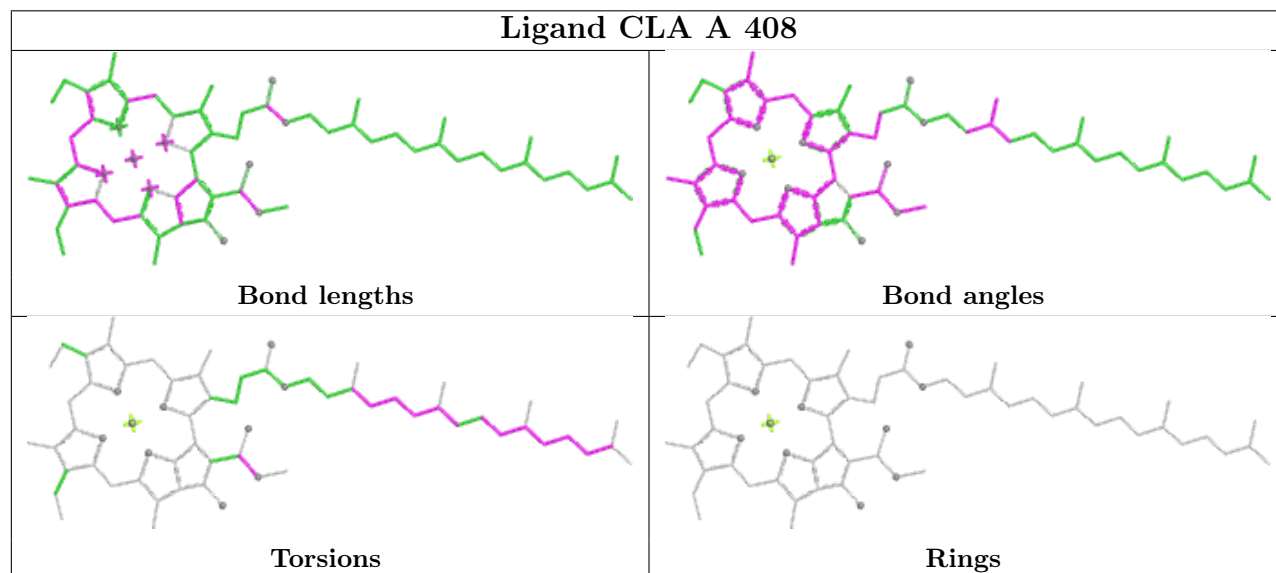
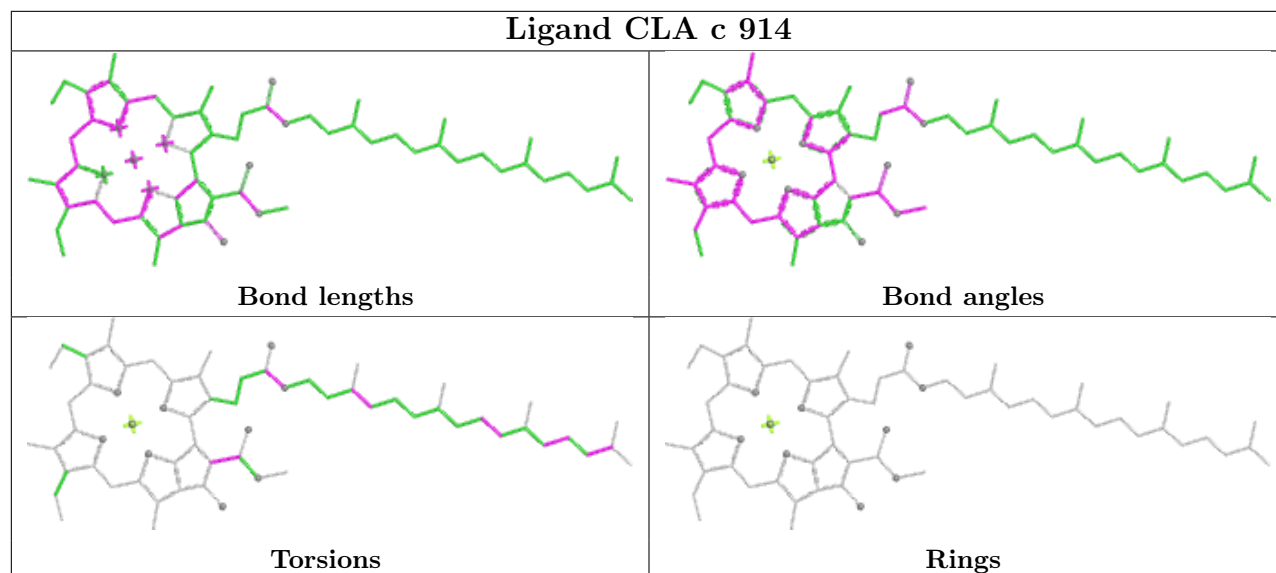


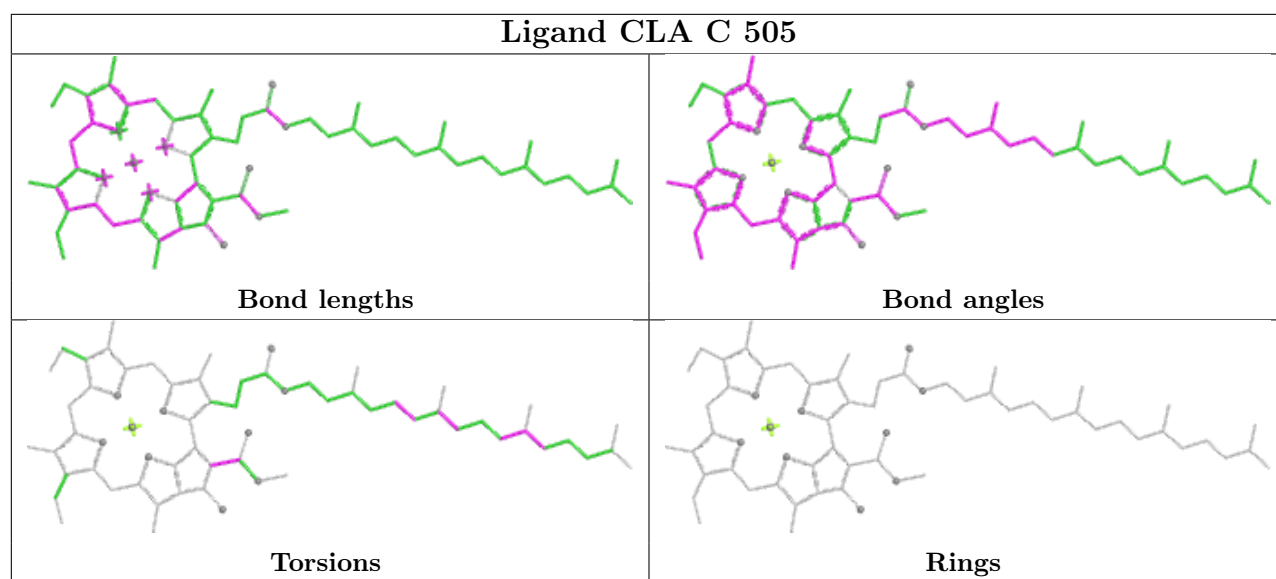








Ligand BCR k 102**Ligand CLA A 408****Ligand CLA c 914**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.44	3 (0%) 81 85	13, 21, 43, 67	1 (0%)
1	a	334/344 (97%)	-0.40	6 (1%) 67 73	13, 21, 44, 91	4 (1%)
2	B	505/505 (100%)	-0.19	13 (2%) 57 62	15, 25, 50, 81	4 (0%)
2	b	501/505 (99%)	-0.11	22 (4%) 39 42	15, 25, 53, 109	3 (0%)
3	C	451/455 (99%)	0.02	5 (1%) 78 82	16, 30, 46, 73	4 (0%)
3	c	455/455 (100%)	-0.02	4 (0%) 81 85	20, 31, 43, 68	1 (0%)
4	D	342/342 (100%)	-0.40	1 (0%) 90 93	12, 22, 41, 88	2 (0%)
4	d	342/342 (100%)	-0.49	1 (0%) 90 93	11, 22, 40, 73	2 (0%)
5	E	81/83 (97%)	0.87	11 (13%) 7 7	25, 45, 75, 97	0
5	e	79/83 (95%)	0.66	6 (7%) 20 22	28, 42, 67, 87	0
6	F	35/44 (79%)	0.35	2 (5%) 29 31	24, 35, 59, 96	0
6	f	32/44 (72%)	0.20	1 (3%) 51 56	26, 31, 70, 82	0
7	H	63/65 (96%)	0.30	1 (1%) 70 75	20, 33, 44, 77	2 (3%)
7	h	63/65 (96%)	0.44	2 (3%) 50 55	23, 34, 46, 72	1 (1%)
8	I	34/38 (89%)	0.31	0 100 100	27, 35, 58, 77	0
8	i	37/38 (97%)	0.37	2 (5%) 31 33	26, 32, 84, 89	0
9	J	36/40 (90%)	0.53	1 (2%) 55 59	24, 38, 65, 81	0
9	j	40/40 (100%)	0.42	2 (5%) 34 36	24, 36, 69, 76	0
10	K	37/37 (100%)	0.21	0 100 100	31, 37, 47, 56	0
10	k	37/37 (100%)	0.35	0 100 100	29, 37, 55, 66	0
11	L	37/37 (100%)	-0.34	2 (5%) 31 33	11, 20, 62, 80	1 (2%)
11	l	36/37 (97%)	-0.27	2 (5%) 30 32	12, 20, 68, 76	1 (2%)
12	M	34/36 (94%)	-0.26	2 (5%) 28 30	13, 23, 52, 75	1 (2%)
12	m	34/36 (94%)	-0.24	1 (2%) 53 58	15, 24, 53, 72	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.04	7 (2%) 53 58	16, 30, 55, 86	2 (0%)
13	o	243/244 (99%)	0.16	13 (5%) 32 34	16, 32, 65, 86	1 (0%)
14	T	29/32 (90%)	-0.21	1 (3%) 48 53	17, 21, 45, 81	0
14	t	30/32 (93%)	-0.13	2 (6%) 24 26	18, 22, 55, 85	0
15	U	97/104 (93%)	-0.07	1 (1%) 79 83	20, 28, 46, 59	0
15	u	97/104 (93%)	-0.14	1 (1%) 79 83	22, 27, 40, 63	1 (1%)
16	V	137/137 (100%)	-0.25	0 100 100	15, 26, 41, 59	1 (0%)
16	v	137/137 (100%)	0.15	1 (0%) 84 88	16, 33, 51, 71	1 (0%)
17	Y	29/30 (96%)	0.98	3 (10%) 12 14	38, 46, 69, 72	0
17	y	29/30 (96%)	0.78	2 (6%) 23 25	38, 47, 59, 69	0
18	X	38/40 (95%)	0.70	3 (7%) 18 20	21, 39, 58, 62	1 (2%)
18	x	38/40 (95%)	0.87	5 (13%) 7 8	30, 38, 83, 98	0
19	Z	62/62 (100%)	1.07	9 (14%) 6 6	36, 45, 83, 96	0
19	z	61/62 (98%)	1.36	9 (14%) 5 6	42, 52, 83, 103	0
All	All	5249/5350 (98%)	-0.05	147 (2%) 55 59	11, 27, 55, 109	35 (0%)

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	5.5
18	x	37	VAL	5.3
2	b	487	SER	5.0
7	h	64	ALA	4.9
8	i	38	GLU	4.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.97	0.07	27,32,36,36	0
14	FME	T	1	10/11	0.97	0.07	19,26,45,49	0
8	FME	i	1	10/11	0.97	0.06	28,29,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.97	0.07	18,24,45,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	V	211	4/4	0.52	0.29	61,61,68,79	0
31	DMS	i	106	4/4	0.53	0.21	120,121,124,138	0
31	DMS	b	644	4/4	0.56	0.29	73,76,78,96	0
31	DMS	k	103	4/4	0.58	0.29	90,92,93,104	0
29	UNL	b	630	16/-	0.60	0.21	74,86,106,110	0
31	DMS	c	936	4/4	0.60	0.24	80,80,81,90	0
35	HTG	c	923	13/19	0.65	0.21	59,72,86,87	0
31	DMS	b	646	4/4	0.66	0.22	84,87,89,96	0
29	UNL	H	104	14/-	0.67	0.25	64,69,74,76	0
29	UNL	i	104	16/-	0.68	0.20	69,76,78,79	0
29	UNL	b	631	16/-	0.68	0.17	61,73,81,82	0
36	DGD	D	407	50/66	0.68	0.19	54,71,97,97	0
29	UNL	I	104	16/-	0.69	0.20	69,76,89,92	0
29	UNL	B	629	14/-	0.69	0.22	62,72,81,82	0
36	DGD	d	407	50/66	0.69	0.22	58,74,97,98	0
29	UNL	B	634	16/-	0.70	0.20	73,80,95,97	0
35	HTG	D	414	19/19	0.70	0.19	76,92,111,112	0
30	LMT	F	101	35/35	0.70	0.19	64,88,93,96	0
29	UNL	J	104	16/-	0.70	0.24	62,82,99,99	0
31	DMS	b	642	4/4	0.70	0.21	90,90,97,101	0
29	UNL	B	633	16/-	0.71	0.17	61,80,87,88	0
35	HTG	v	204	19/19	0.71	0.20	62,70,81,91	0
31	DMS	o	304	4/4	0.71	0.22	63,68,70,84	0
31	DMS	U	204	4/4	0.71	0.20	53,62,62,80	0
30	LMT	e	103	25/35	0.72	0.18	60,77,93,95	0
31	DMS	O	304	4/4	0.72	0.28	69,71,78,87	0
29	UNL	u	202	16/-	0.73	0.19	41,54,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	HTG	c	922	19/19	0.73	0.15	53,84,96,100	0
29	UNL	c	931	10/-	0.73	0.25	55,60,62,64	0
35	HTG	d	413	19/19	0.73	0.17	62,86,104,106	0
29	UNL	J	105	11/-	0.73	0.21	61,67,75,78	0
31	DMS	c	935	4/4	0.73	0.20	71,72,75,83	0
31	DMS	u	206	4/4	0.73	0.22	70,71,76,93	0
31	DMS	O	307	4/4	0.74	0.22	64,69,69,84	0
31	DMS	U	203	4/4	0.74	0.22	70,74,80,89	0
31	DMS	A	419	4/4	0.74	0.27	75,76,91,97	0
28	LHG	e	101	40/49	0.74	0.17	55,93,121,126	0
28	LHG	K	101	44/49	0.75	0.16	63,93,124,137	0
29	UNL	b	632	16/-	0.75	0.18	58,83,101,101	0
35	HTG	b	628	19/19	0.75	0.17	52,96,109,112	0
35	HTG	c	921	19/19	0.75	0.16	68,82,88,91	0
29	UNL	Z	103	9/-	0.75	0.17	50,61,69,70	0
29	UNL	a	416	10/-	0.75	0.22	54,68,75,76	0
29	UNL	b	629	12/-	0.75	0.19	49,59,70,71	0
29	UNL	B	628	10/-	0.75	0.18	62,67,70,71	0
30	LMT	I	101	35/35	0.75	0.16	63,75,85,91	0
31	DMS	b	638	4/4	0.75	0.21	54,60,67,74	0
29	UNL	e	102	16/-	0.76	0.21	54,61,69,72	0
31	DMS	D	417	4/4	0.76	0.23	53,54,58,59	0
29	UNL	B	635	9/-	0.76	0.19	60,67,76,77	0
29	UNL	E	103	13/-	0.76	0.20	63,68,85,87	0
31	DMS	O	310	4/4	0.76	0.22	61,67,74,76	0
30	LMT	A	416	35/35	0.76	0.17	42,63,86,98	0
28	LHG	A	412	49/49	0.76	0.19	59,83,104,111	0
29	UNL	B	632	16/-	0.76	0.20	44,61,68,70	0
29	UNL	b	626	16/-	0.76	0.19	59,68,73,73	0
29	UNL	I	103	16/-	0.77	0.17	51,57,70,74	0
31	DMS	b	639	4/4	0.77	0.17	41,55,63,67	0
28	LHG	E	101	49/49	0.77	0.20	39,83,104,109	0
31	DMS	V	207	4/4	0.77	0.20	51,52,60,62	0
29	UNL	E	102	16/-	0.77	0.23	58,61,76,77	0
29	UNL	i	103	16/-	0.78	0.17	58,61,67,70	0
28	LHG	d	402	44/49	0.78	0.17	59,78,125,135	0
30	LMT	a	418	35/35	0.78	0.15	44,63,79,80	0
29	UNL	u	201	11/-	0.78	0.20	39,50,60,61	0
31	DMS	c	934	4/4	0.78	0.19	87,87,89,99	0
29	UNL	a	419	6/-	0.78	0.13	47,53,53,53	0
31	DMS	B	641	4/4	0.78	0.23	62,63,65,66	0
27	PL9	a	414	55/55	0.78	0.20	46,61,86,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	b	637	4/4	0.78	0.23	61,63,68,74	0
31	DMS	H	101	4/4	0.78	0.23	54,58,62,65	0
29	UNL	I	102	13/-	0.79	0.16	47,53,65,69	0
29	UNL	T	102	13/-	0.79	0.19	62,68,75,75	0
31	DMS	h	105	4/4	0.79	0.18	76,83,89,90	0
29	UNL	t	102	16/-	0.79	0.16	53,62,74,75	0
29	UNL	d	417	11/-	0.79	0.17	48,63,69,71	0
29	UNL	A	414	13/-	0.79	0.18	58,71,83,83	0
31	DMS	b	647	4/4	0.79	0.23	67,78,85,86	0
30	LMT	z	101	32/35	0.79	0.17	43,88,96,99	0
31	DMS	O	311	4/4	0.80	0.24	59,59,71,73	0
28	LHG	a	415	49/49	0.80	0.16	56,72,99,108	0
31	DMS	c	929	4/4	0.80	0.23	46,62,67,70	0
29	UNL	k	101	8/-	0.80	0.28	59,71,78,80	0
29	UNL	z	102	13/-	0.80	0.17	53,62,72,75	0
35	HTG	B	626	19/19	0.80	0.14	52,88,96,96	0
35	HTG	B	631	19/19	0.80	0.15	41,88,97,100	0
29	UNL	U	201	14/-	0.80	0.18	38,50,58,61	0
30	LMT	m	103	35/35	0.81	0.15	48,92,102,103	0
31	DMS	b	643	4/4	0.81	0.19	81,82,85,85	0
31	DMS	d	418	4/4	0.81	0.19	68,69,71,71	0
35	HTG	b	623	19/19	0.81	0.15	47,76,83,84	0
31	DMS	d	419	4/4	0.81	0.21	63,70,76,82	0
31	DMS	B	647	4/4	0.81	0.16	81,85,85,89	0
31	DMS	O	309	4/4	0.81	0.21	53,63,64,70	0
31	DMS	B	649	4/4	0.81	0.18	70,71,73,84	0
27	PL9	A	411	55/55	0.81	0.18	45,59,80,84	0
29	UNL	b	625	10/-	0.81	0.17	44,59,68,68	0
34	LMG	C	531	51/55	0.81	0.16	38,78,93,98	0
34	LMG	D	412	51/55	0.81	0.17	37,65,106,119	0
26	SQD	x	101	41/54	0.82	0.16	54,76,95,101	0
35	HTG	V	204	14/19	0.82	0.15	42,45,71,82	0
31	DMS	B	640	4/4	0.82	0.20	50,56,60,61	0
30	LMT	Z	101	35/35	0.82	0.16	41,88,100,102	0
31	DMS	B	645	4/4	0.82	0.21	50,61,64,69	0
26	SQD	D	408	45/54	0.82	0.16	45,67,86,93	0
29	UNL	Z	102	14/-	0.82	0.16	63,67,74,76	0
34	LMG	c	930	51/55	0.82	0.14	33,69,81,84	0
34	LMG	d	411	51/55	0.82	0.17	39,70,101,108	0
30	LMT	B	623	35/35	0.82	0.15	48,72,89,93	0
29	UNL	E	104	16/-	0.82	0.20	67,71,74,76	0
29	UNL	A	417	4/-	0.83	0.15	58,61,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	A	421	4/4	0.83	0.23	57,63,74,78	0
31	DMS	a	421	4/4	0.83	0.21	81,84,85,92	0
31	DMS	h	104	4/4	0.83	0.14	97,99,103,103	0
30	LMT	B	643	24/35	0.83	0.18	50,77,114,118	0
30	LMT	a	422	35/35	0.83	0.14	61,74,82,85	0
31	DMS	H	105	4/4	0.83	0.15	60,74,74,84	0
35	HTG	C	522	19/19	0.83	0.14	41,78,86,87	0
35	HTG	C	523	19/19	0.83	0.15	60,78,95,97	0
31	DMS	A	418	4/4	0.83	0.21	70,79,79,85	0
29	UNL	j	103	16/-	0.84	0.17	45,56,61,62	0
31	DMS	b	635	4/4	0.84	0.18	53,63,69,71	0
31	DMS	c	937	4/4	0.84	0.16	76,80,84,84	0
30	LMT	B	644	24/35	0.84	0.13	34,52,81,87	0
31	DMS	c	933	4/4	0.84	0.18	61,64,65,77	0
29	UNL	C	532	11/-	0.84	0.16	54,59,66,66	0
31	DMS	l	102	4/4	0.85	0.17	64,65,70,84	0
29	UNL	b	624	16/-	0.85	0.15	42,51,58,60	0
31	DMS	b	645	4/4	0.85	0.20	70,77,83,84	0
31	DMS	v	206	4/4	0.85	0.16	66,68,76,78	0
26	SQD	B	621	54/54	0.85	0.14	43,63,88,93	0
29	UNL	B	627	16/-	0.85	0.15	38,45,55,60	0
31	DMS	h	103	4/4	0.85	0.17	82,84,97,101	0
26	SQD	L	102	54/54	0.85	0.15	42,58,87,90	0
35	HTG	B	625	19/19	0.85	0.16	28,42,49,51	0
29	UNL	d	412	16/-	0.85	0.14	31,40,54,57	0
31	DMS	V	210	4/4	0.85	0.16	64,65,67,73	0
31	DMS	C	533	4/4	0.85	0.17	67,67,68,71	0
30	LMT	T	103	24/35	0.86	0.14	34,56,76,83	0
31	DMS	U	202	4/4	0.86	0.21	33,45,50,55	0
29	UNL	i	101	16/-	0.86	0.14	37,43,60,60	0
35	HTG	b	622	19/19	0.86	0.15	28,41,57,64	0
31	DMS	v	208	4/4	0.86	0.15	54,67,71,87	0
29	UNL	m	101	11/-	0.86	0.14	47,51,56,58	0
29	UNL	i	102	16/-	0.86	0.15	52,62,75,76	0
30	LMT	b	621	25/35	0.86	0.13	45,70,90,91	0
29	UNL	M	102	11/-	0.86	0.14	45,50,63,69	0
31	DMS	a	401	4/4	0.86	0.17	75,81,85,96	0
31	DMS	O	308	4/4	0.86	0.20	54,64,77,81	0
29	UNL	A	413	16/-	0.86	0.14	38,43,70,76	0
26	SQD	a	417	54/54	0.86	0.12	38,53,72,73	0
35	HTG	C	521	19/19	0.87	0.13	61,66,74,77	0
31	DMS	b	641	4/4	0.87	0.15	52,59,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	LMT	m	104	35/35	0.87	0.11	34,51,56,58	0
31	DMS	u	204	4/4	0.87	0.17	62,68,68,73	0
29	UNL	X	101	16/-	0.87	0.14	33,37,60,61	0
31	DMS	v	202	4/4	0.87	0.19	68,74,76,81	0
31	DMS	B	646	4/4	0.87	0.17	76,77,77,84	0
31	DMS	A	422	4/4	0.87	0.15	65,68,68,71	0
31	DMS	h	101	4/4	0.87	0.16	47,51,52,53	0
26	SQD	A	415	54/54	0.87	0.13	39,54,72,76	0
31	DMS	C	527	4/4	0.87	0.18	58,68,73,83	0
31	DMS	C	529	4/4	0.87	0.19	54,66,72,74	0
31	DMS	i	105	4/4	0.87	0.20	61,64,71,73	0
31	DMS	V	209	4/4	0.87	0.18	58,59,62,65	0
31	DMS	b	640	4/4	0.87	0.19	67,70,78,83	0
34	LMG	C	520	51/55	0.88	0.14	31,61,74,79	0
31	DMS	V	208	4/4	0.88	0.17	69,70,71,72	0
31	DMS	A	424	4/4	0.88	0.19	53,54,58,69	0
34	LMG	a	413	51/55	0.88	0.12	41,53,68,74	0
31	DMS	o	303	4/4	0.88	0.16	51,55,67,70	0
31	DMS	C	528	4/4	0.88	0.14	60,63,65,66	0
31	DMS	B	642	4/4	0.88	0.14	46,54,59,67	0
31	DMS	u	205	4/4	0.88	0.16	41,50,54,58	0
31	DMS	O	305	4/4	0.88	0.17	65,70,70,77	0
31	DMS	O	306	4/4	0.88	0.17	68,68,73,76	0
31	DMS	B	648	4/4	0.88	0.23	43,45,47,48	0
29	UNL	J	103	16/-	0.88	0.15	46,54,60,63	0
31	DMS	C	525	4/4	0.89	0.23	39,39,43,46	0
31	DMS	e	104	4/4	0.89	0.16	72,73,78,83	0
31	DMS	B	639	4/4	0.89	0.15	44,48,51,54	0
23	CLA	b	602	65/65	0.89	0.12	29,42,66,71	0
31	DMS	V	202	4/4	0.89	0.18	31,32,38,48	0
31	DMS	V	205	4/4	0.89	0.15	49,60,60,63	0
31	DMS	V	206	4/4	0.89	0.15	55,55,55,61	0
31	DMS	a	423	4/4	0.89	0.17	53,56,63,73	0
31	DMS	v	209	4/4	0.89	0.17	49,50,58,64	0
31	DMS	B	638	4/4	0.89	0.15	55,60,62,71	0
31	DMS	b	636	4/4	0.89	0.16	44,48,50,52	0
34	LMG	B	622	51/55	0.90	0.11	31,41,52,67	0
34	LMG	C	501	51/55	0.90	0.12	37,51,63,70	0
30	LMT	M	101	35/35	0.90	0.11	31,50,59,60	0
23	CLA	C	514	65/65	0.90	0.11	37,47,67,72	0
31	DMS	d	414	4/4	0.90	0.18	62,66,71,78	0
31	DMS	d	415	4/4	0.90	0.18	45,53,57,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	UNL	D	413	16/-	0.90	0.12	36,42,57,58	0
23	CLA	C	507	65/65	0.90	0.12	25,42,79,81	0
34	LMG	m	102	51/55	0.90	0.12	33,41,54,61	0
31	DMS	c	932	4/4	0.91	0.13	54,57,63,64	0
25	BCR	C	515	40/40	0.91	0.09	35,43,46,48	0
31	DMS	v	205	4/4	0.91	0.13	63,66,68,69	0
29	UNL	x	103	15/-	0.91	0.13	31,40,57,58	0
26	SQD	A	410	54/54	0.91	0.12	31,55,74,80	0
31	DMS	d	416	4/4	0.91	0.18	47,52,59,64	0
34	LMG	c	920	51/55	0.91	0.13	27,55,81,84	0
31	DMS	u	203	4/4	0.92	0.18	38,50,51,52	0
26	SQD	a	412	54/54	0.92	0.12	31,53,72,76	0
31	DMS	a	420	4/4	0.92	0.12	48,61,64,66	0
31	DMS	O	303	4/4	0.92	0.12	59,66,69,73	0
31	DMS	v	210	4/4	0.92	0.12	62,65,68,72	0
35	HTG	B	630	19/19	0.92	0.10	41,55,62,66	0
23	CLA	B	602	65/65	0.92	0.10	28,39,75,85	0
35	HTG	b	627	19/19	0.92	0.10	39,59,72,82	0
31	DMS	D	415	4/4	0.93	0.13	50,53,56,59	0
31	DMS	v	207	4/4	0.93	0.13	53,54,54,60	0
23	CLA	c	913	65/65	0.93	0.09	30,39,65,68	0
31	DMS	C	526	4/4	0.93	0.14	49,56,57,62	0
23	CLA	c	914	65/65	0.93	0.10	36,44,76,80	0
23	CLA	C	513	65/65	0.93	0.10	34,42,73,76	0
25	BCR	Y	101	40/40	0.93	0.08	29,33,40,41	0
35	HTG	O	302	19/19	0.93	0.10	36,39,48,49	0
35	HTG	B	624	19/19	0.93	0.11	35,39,46,47	0
25	BCR	d	405	40/40	0.93	0.09	21,27,50,54	0
38	RRX	H	102	41/41	0.93	0.09	25,29,38,44	0
28	LHG	D	409	49/49	0.94	0.09	27,34,41,47	0
31	DMS	v	201	4/4	0.94	0.13	46,48,51,51	0
25	BCR	j	104	40/40	0.94	0.07	27,32,39,43	0
25	BCR	t	101	40/40	0.94	0.07	19,26,38,40	0
23	CLA	C	512	65/65	0.94	0.08	26,34,39,40	0
23	CLA	C	508	65/65	0.94	0.09	28,35,49,55	0
23	CLA	b	617	65/65	0.94	0.10	20,30,81,89	0
25	BCR	C	516	40/40	0.94	0.08	28,34,40,43	0
25	BCR	C	530	40/40	0.94	0.07	27,32,36,37	0
32	BCT	A	420	4/4	0.94	0.08	31,32,35,40	0
25	BCR	D	405	40/40	0.94	0.09	22,28,54,57	0
31	DMS	c	925	4/4	0.94	0.18	35,37,42,49	0
31	DMS	c	926	4/4	0.94	0.17	66,68,69,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	c	927	4/4	0.94	0.20	30,37,37,44	0
25	BCR	T	101	40/40	0.94	0.07	22,29,40,41	0
34	LMG	J	101	51/55	0.94	0.11	25,31,85,93	0
23	CLA	c	904	65/65	0.94	0.08	25,32,37,40	0
31	DMS	b	634	4/4	0.94	0.12	42,45,48,48	0
25	BCR	c	915	40/40	0.94	0.09	36,44,48,50	0
36	DGD	C	518	62/66	0.94	0.10	24,33,70,80	0
25	BCR	c	916	40/40	0.94	0.08	25,32,38,38	0
36	DGD	H	103	62/66	0.94	0.09	23,32,38,39	0
23	CLA	c	907	65/65	0.94	0.10	23,36,73,76	0
36	DGD	h	102	62/66	0.94	0.09	24,31,41,47	0
31	DMS	F	102	4/4	0.94	0.12	48,48,50,64	0
38	RRX	x	102	41/41	0.94	0.08	23,29,46,52	0
23	CLA	C	502	65/65	0.95	0.07	25,31,41,51	0
23	CLA	C	503	65/65	0.95	0.07	23,27,37,42	0
25	BCR	B	619	40/40	0.95	0.07	20,25,41,45	0
25	BCR	B	620	40/40	0.95	0.07	21,29,41,42	0
23	CLA	C	504	65/65	0.95	0.07	24,31,36,41	0
23	CLA	C	506	65/65	0.95	0.08	25,31,40,44	0
23	CLA	b	603	65/65	0.95	0.07	21,24,33,41	0
23	CLA	b	607	65/65	0.95	0.08	22,27,54,63	0
32	BCT	a	424	4/4	0.95	0.07	32,35,37,41	0
23	CLA	b	615	65/65	0.95	0.09	19,24,71,76	0
23	CLA	B	607	65/65	0.95	0.08	20,26,53,60	0
27	PL9	D	406	55/55	0.95	0.06	17,22,28,30	0
25	BCR	a	411	40/40	0.95	0.06	20,23,27,28	0
25	BCR	b	619	40/40	0.95	0.07	20,27,41,43	0
23	CLA	B	610	65/65	0.95	0.07	21,28,32,34	0
28	LHG	D	411	46/49	0.95	0.10	25,30,82,85	0
31	DMS	c	928	4/4	0.95	0.10	57,59,61,61	0
31	DMS	B	637	4/4	0.95	0.12	35,38,40,42	0
23	CLA	c	906	65/65	0.95	0.07	25,29,44,47	0
34	LMG	j	101	51/55	0.95	0.10	22,33,80,85	0
23	CLA	C	509	65/65	0.95	0.08	24,29,76,85	0
23	CLA	c	908	65/65	0.95	0.08	23,28,46,54	0
25	BCR	k	102	40/40	0.95	0.07	27,32,38,40	0
28	LHG	d	408	49/49	0.95	0.09	25,33,43,44	0
23	CLA	b	604	65/65	0.96	0.06	19,23,29,32	0
23	CLA	B	617	65/65	0.96	0.10	20,27,93,106	0
23	CLA	b	610	65/65	0.96	0.07	22,27,31,39	0
23	CLA	b	611	65/65	0.96	0.07	19,24,32,37	0
23	CLA	B	603	65/65	0.96	0.06	20,26,33,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	616	65/65	0.96	0.07	21,26,42,44	0
23	CLA	C	510	65/65	0.96	0.09	25,31,52,55	0
23	CLA	c	902	65/65	0.96	0.07	24,27,38,46	0
23	CLA	C	511	65/65	0.96	0.06	24,30,35,40	0
25	BCR	b	618	40/40	0.96	0.06	20,25,32,33	0
28	LHG	L	101	49/49	0.96	0.08	22,31,42,48	0
23	CLA	c	905	65/65	0.96	0.07	21,27,51,54	0
25	BCR	b	620	40/40	0.96	0.07	25,29,40,44	0
23	CLA	B	604	65/65	0.96	0.07	18,21,30,36	0
31	DMS	V	201	4/4	0.96	0.11	41,46,47,47	0
28	LHG	d	409	49/49	0.96	0.07	18,24,44,47	0
28	LHG	d	410	46/49	0.96	0.10	24,27,73,84	0
23	CLA	B	611	65/65	0.96	0.07	20,24,33,39	0
28	LHG	l	101	49/49	0.96	0.08	20,28,48,52	0
23	CLA	C	505	65/65	0.96	0.07	25,28,58,60	0
23	CLA	c	909	65/65	0.96	0.08	22,26,79,92	0
23	CLA	c	910	65/65	0.96	0.07	23,27,49,60	0
33	CA	o	302	1/1	0.96	0.06	43,43,43,43	0
23	CLA	c	911	65/65	0.96	0.06	20,26,36,40	0
36	DGD	C	517	62/66	0.96	0.09	21,29,69,71	0
23	CLA	c	912	65/65	0.96	0.07	26,31,37,41	0
36	DGD	C	519	62/66	0.96	0.09	21,28,68,83	0
23	CLA	B	615	65/65	0.96	0.08	18,23,66,71	0
23	CLA	B	616	65/65	0.96	0.07	23,27,43,49	0
36	DGD	c	917	62/66	0.96	0.09	20,30,74,77	0
36	DGD	c	918	62/66	0.96	0.08	24,30,75,84	0
36	DGD	c	919	62/66	0.96	0.08	22,29,50,56	0
23	CLA	d	404	65/65	0.96	0.08	22,27,66,72	0
31	DMS	D	416	4/4	0.96	0.12	56,57,58,62	0
25	BCR	A	409	40/40	0.96	0.06	19,23,29,32	0
25	BCR	B	618	40/40	0.96	0.06	19,24,30,33	0
23	CLA	A	408	65/65	0.97	0.09	18,22,89,96	0
23	CLA	b	608	65/65	0.97	0.05	16,20,28,36	0
23	CLA	d	401	65/65	0.97	0.05	15,17,26,31	0
23	CLA	d	403	65/65	0.97	0.06	13,18,36,42	0
23	CLA	b	609	65/65	0.97	0.06	19,23,31,32	0
24	PHO	A	407	64/64	0.97	0.05	17,19,22,22	0
24	PHO	D	402	64/64	0.97	0.05	16,21,25,29	0
24	PHO	a	408	64/64	0.97	0.05	15,18,20,22	0
24	PHO	a	409	64/64	0.97	0.05	17,22,27,30	0
23	CLA	B	608	65/65	0.97	0.05	16,19,32,35	0
23	CLA	B	609	65/65	0.97	0.06	19,23,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DMS	B	636	4/4	0.97	0.09	18,20,22,28	0
23	CLA	b	612	65/65	0.97	0.06	18,21,36,42	0
27	PL9	d	406	55/55	0.97	0.05	16,21,27,34	0
23	CLA	b	613	65/65	0.97	0.06	18,24,29,34	0
23	CLA	b	614	65/65	0.97	0.06	17,21,47,54	0
28	LHG	D	410	49/49	0.97	0.07	20,27,42,46	0
23	CLA	A	406	65/65	0.97	0.07	18,20,90,96	0
23	CLA	B	605	65/65	0.97	0.07	18,21,52,53	0
23	CLA	B	612	65/65	0.97	0.06	17,20,36,52	0
23	CLA	D	403	65/65	0.97	0.05	13,17,33,41	0
33	CA	B	601	1/1	0.97	0.10	41,41,41,41	0
33	CA	O	301	1/1	0.97	0.06	42,42,42,42	0
23	CLA	c	903	65/65	0.97	0.06	20,24,37,43	0
23	CLA	D	404	65/65	0.97	0.08	23,27,67,73	0
23	CLA	a	406	65/65	0.97	0.05	14,17,25,37	0
23	CLA	a	407	65/65	0.97	0.08	17,20,95,102	0
23	CLA	a	410	65/65	0.97	0.10	17,22,91,94	0
23	CLA	B	613	65/65	0.97	0.06	18,23,28,31	0
23	CLA	B	614	65/65	0.97	0.05	18,20,44,51	0
23	CLA	B	606	65/65	0.97	0.06	18,22,32,34	0
31	DMS	b	633	4/4	0.97	0.08	21,23,24,25	0
37	HEM	E	105	43/43	0.97	0.08	36,42,46,47	0
37	HEM	e	105	43/43	0.97	0.08	35,39,51,63	0
23	CLA	b	605	65/65	0.97	0.07	17,22,53,55	0
23	CLA	b	606	65/65	0.97	0.06	18,22,29,33	0
33	CA	c	901	1/1	0.98	0.06	39,39,39,39	0
31	DMS	c	924	4/4	0.98	0.07	31,33,36,36	0
23	CLA	A	405	65/65	0.98	0.05	14,17,26,34	0
31	DMS	C	524	4/4	0.98	0.07	32,33,36,36	0
23	CLA	D	401	65/65	0.98	0.05	13,17,27,35	0
33	CA	b	601	1/1	0.98	0.07	41,41,41,41	0
40	HEC	v	203	43/43	0.98	0.07	22,27,29,32	0
31	DMS	A	423	4/4	0.99	0.05	23,27,27,28	0
21	FE2	a	403	1/1	0.99	0.02	25,25,25,25	0
22	CL	a	404	1/1	0.99	0.02	19,19,19,19	0
31	DMS	o	301	4/4	0.99	0.07	22,27,28,31	0
22	CL	a	405	1/1	0.99	0.02	21,21,21,21	0
39	MG	J	102	1/1	0.99	0.07	30,30,30,30	0
39	MG	j	102	1/1	0.99	0.07	28,28,28,28	0
40	HEC	V	203	43/43	0.99	0.05	19,22,26,29	0
21	FE2	A	402	1/1	0.99	0.03	28,28,28,28	0
20	OEX	A	401	10/10	1.00	0.03	19,21,23,24	0

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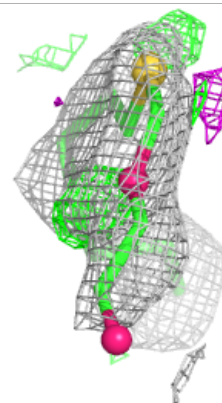
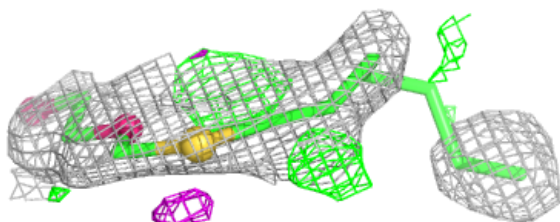
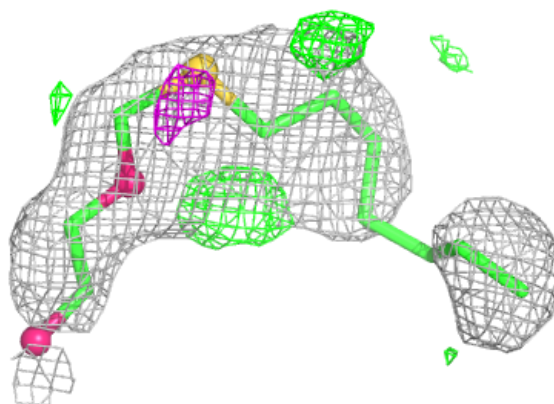
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	OEX	a	402	10/10	1.00	0.02	21,23,24,24	0
22	CL	A	403	1/1	1.00	0.02	19,19,19,19	0
22	CL	A	404	1/1	1.00	0.02	20,20,20,20	0

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

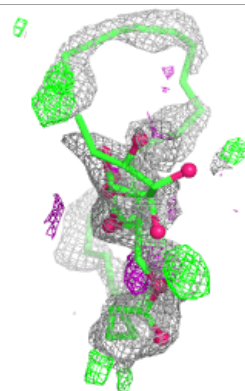
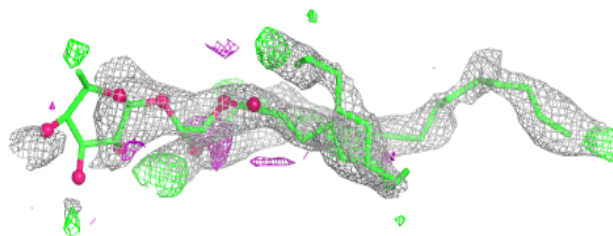
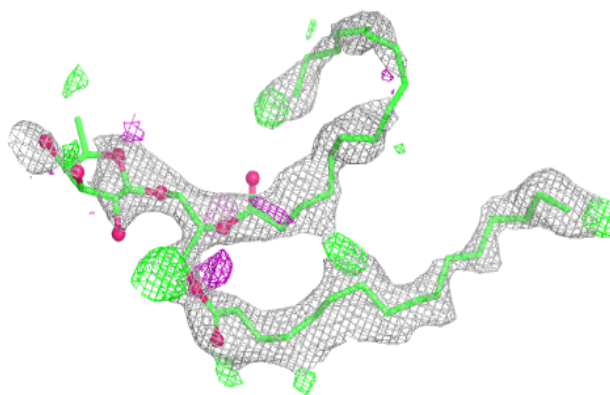
Electron density around HTG c 923:

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



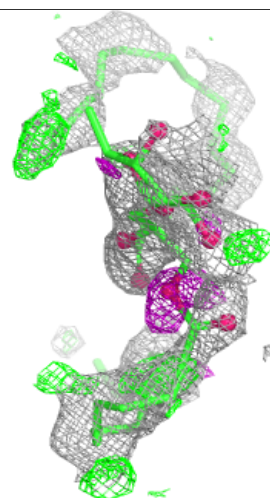
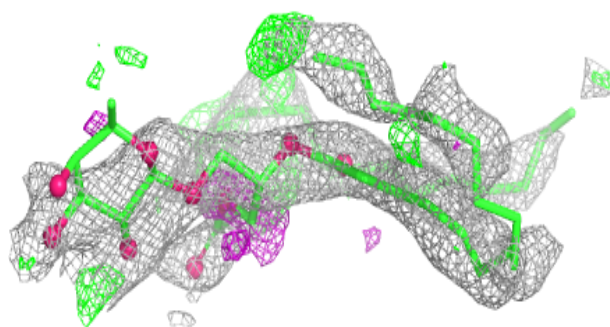
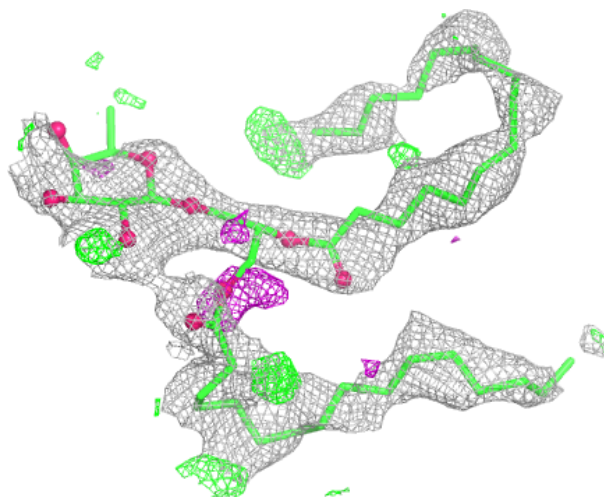
Electron density around DGD D 407:

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



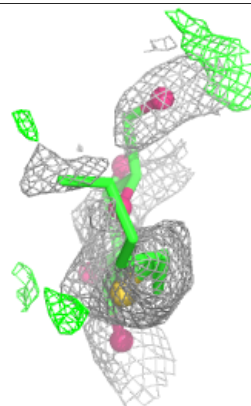
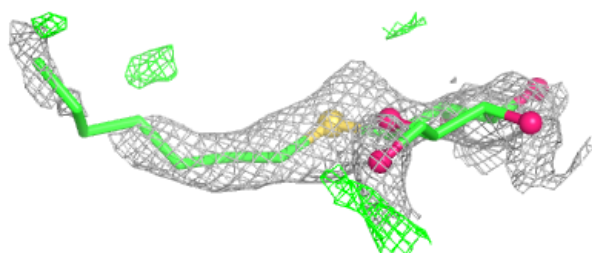
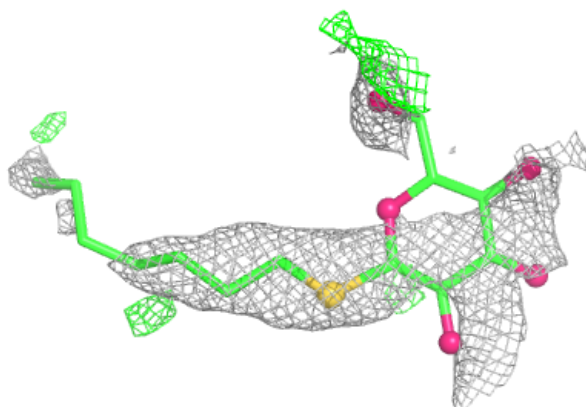
Electron density around DGD d 407:

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

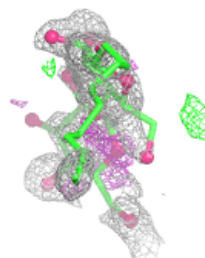
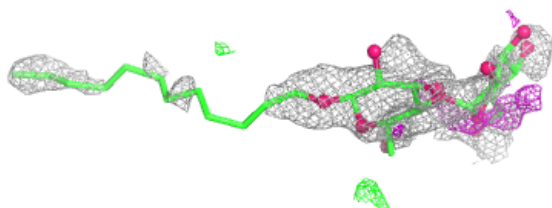
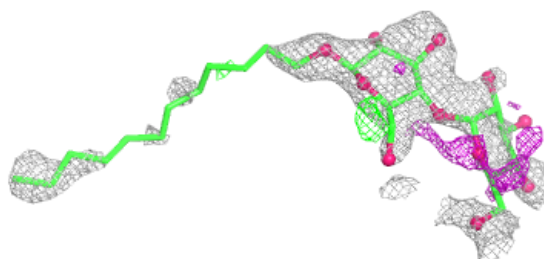


Electron density around HTG D 414:

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

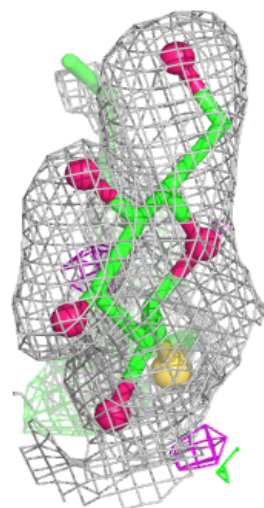
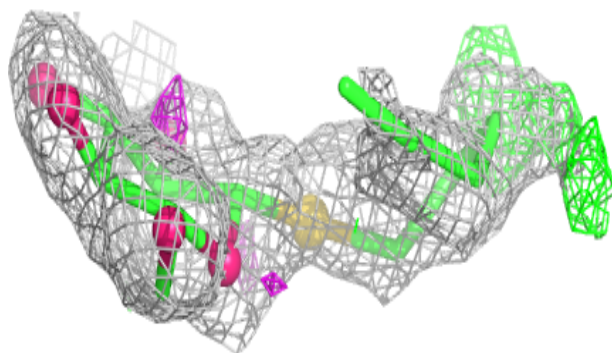
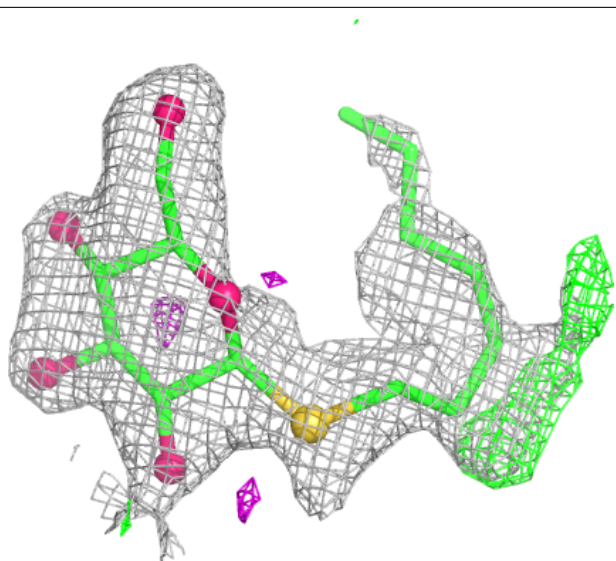
**Electron density around LMT F 101:**

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



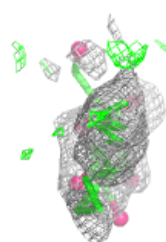
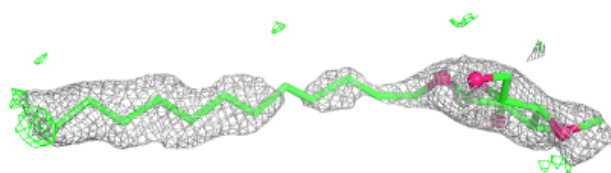
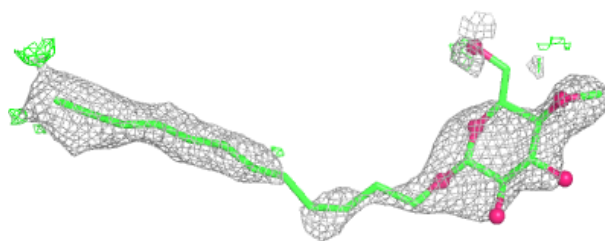
Electron density around HTG v 204:

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

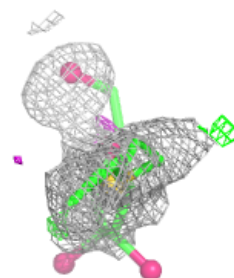
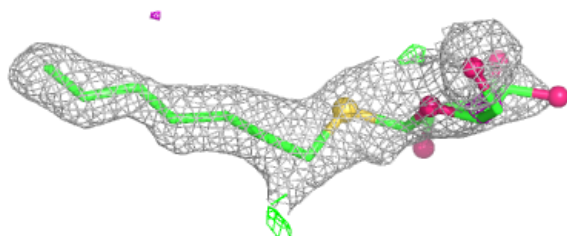
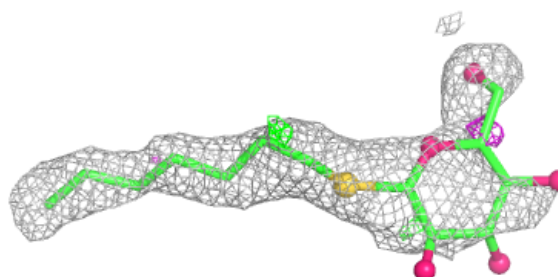


Electron density around LMT e 103:

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

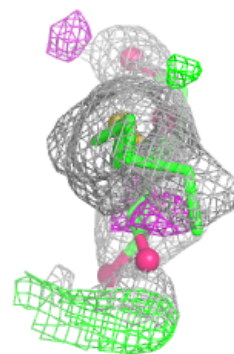
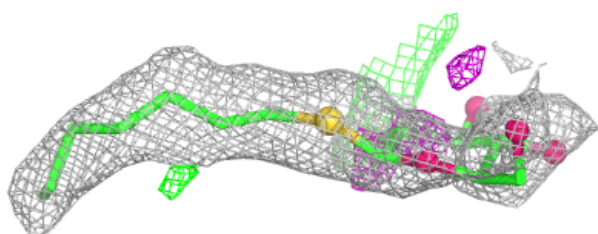
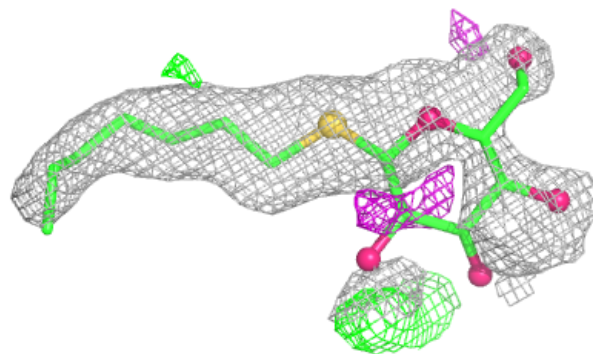
**Electron density around HTG c 922:**

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



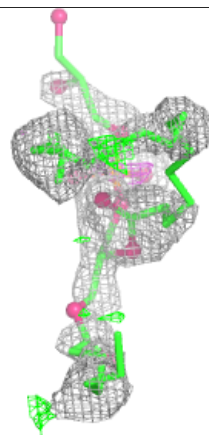
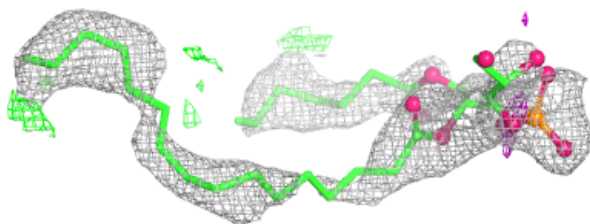
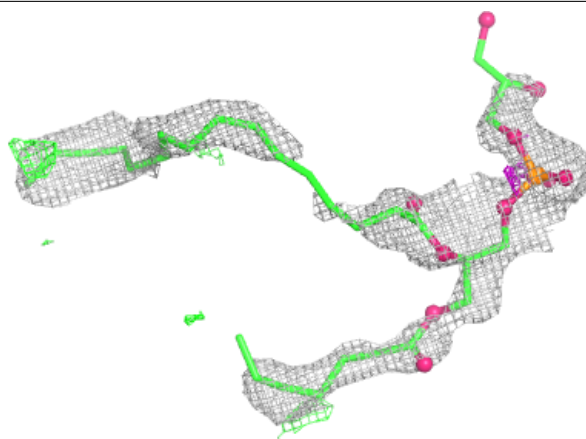
Electron density around HTG d 413:

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

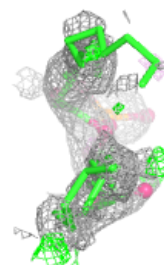
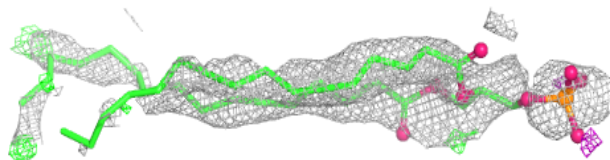
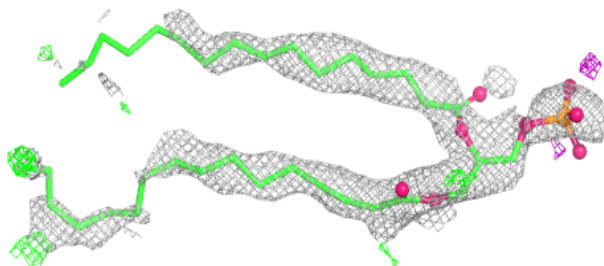


Electron density around LHG e 101:

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

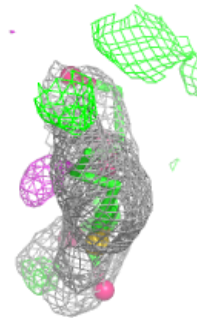
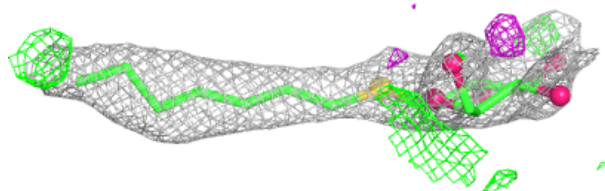
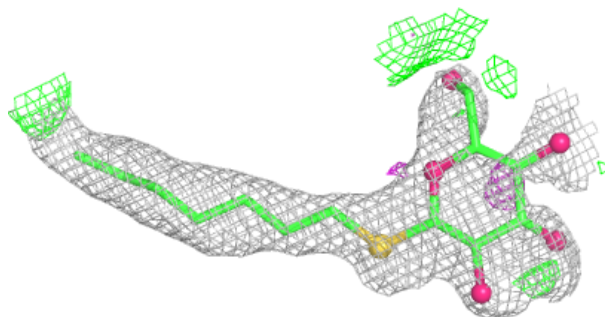
**Electron density around LHG K 101:**

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

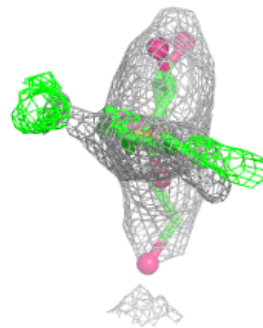
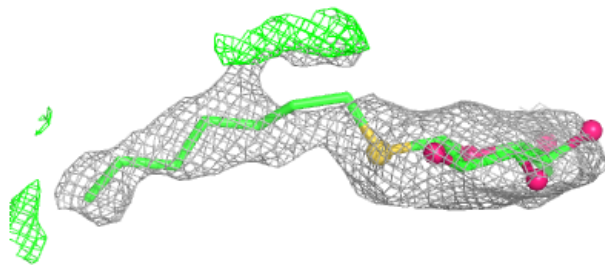
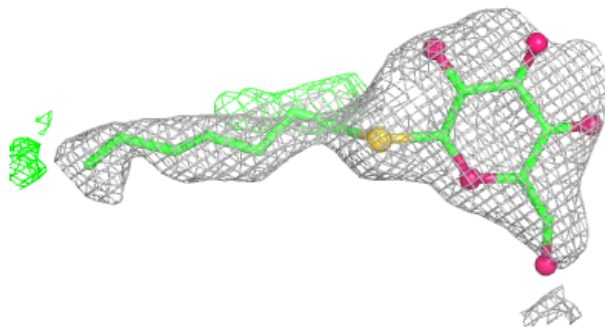


Electron density around HTG b 628:

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

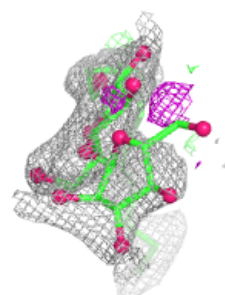
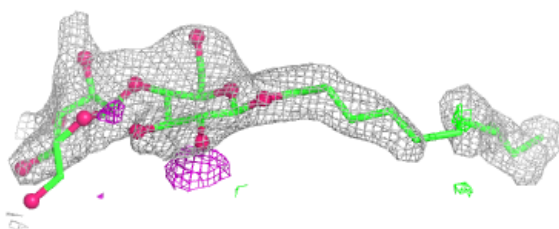
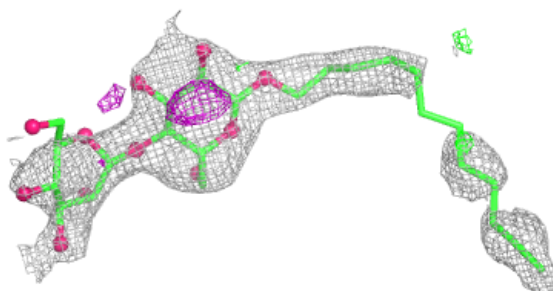
**Electron density around HTG c 921:**

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

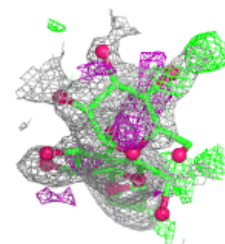
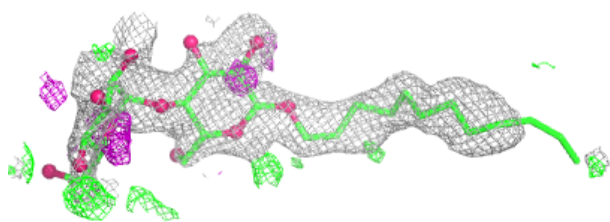
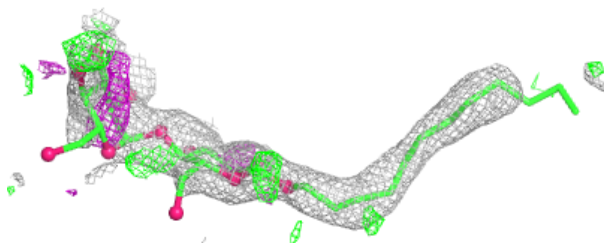


Electron density around LMT I 101:

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

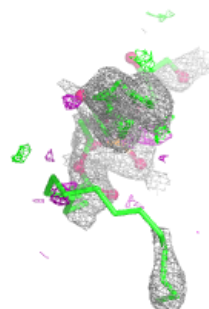
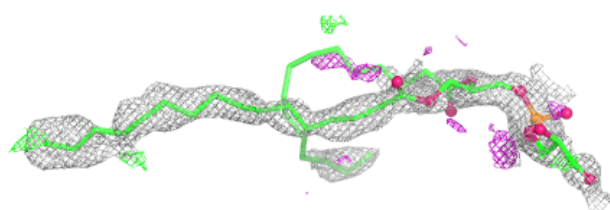
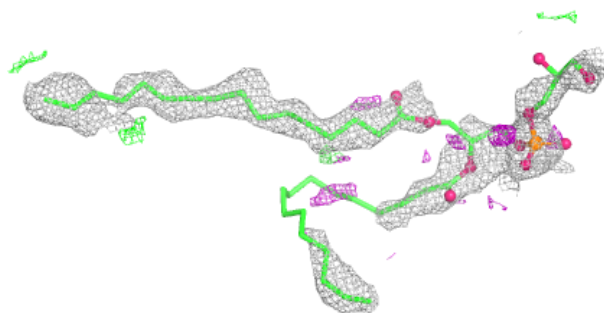
**Electron density around LMT A 416:**

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



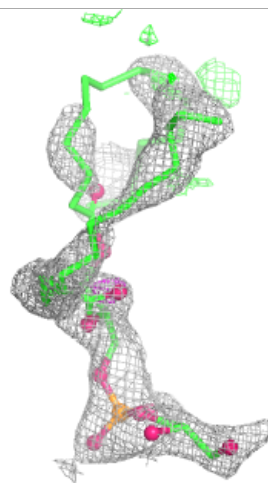
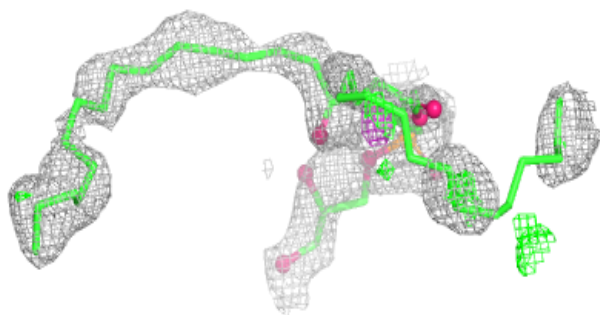
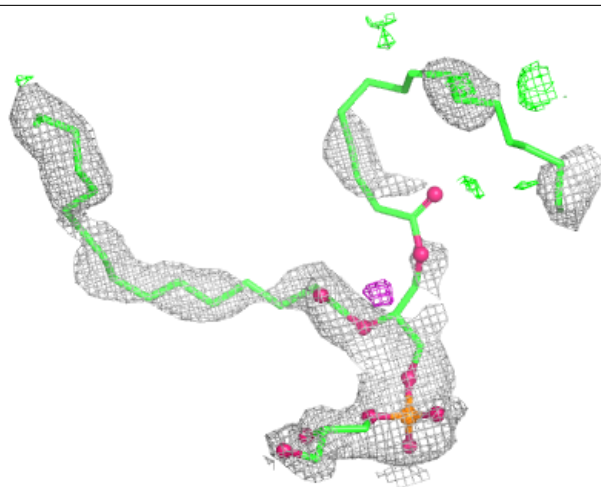
Electron density around LHG A 412:

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



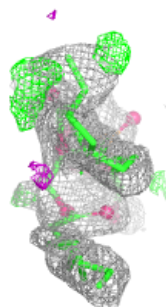
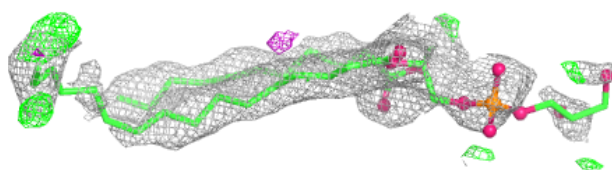
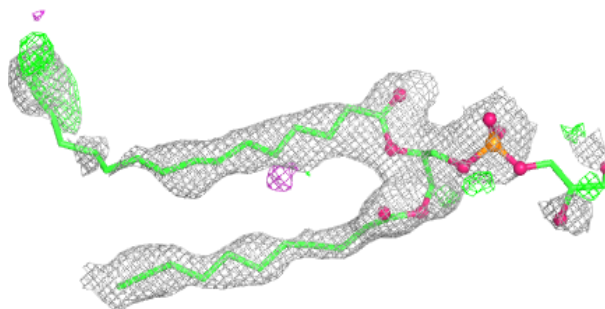
Electron density around LHG E 101:

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

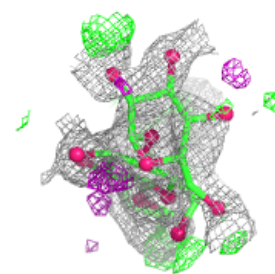
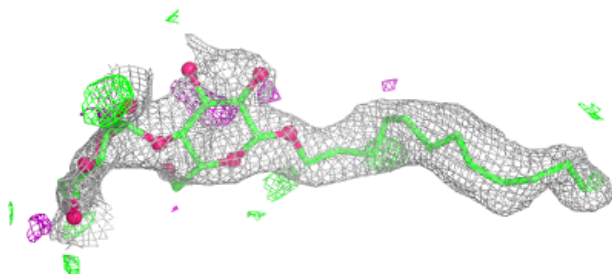
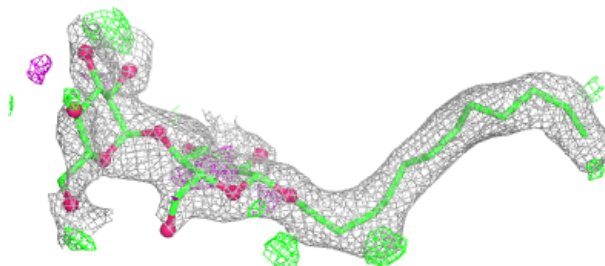


Electron density around LHG d 402:

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

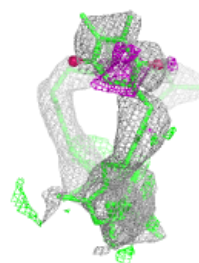
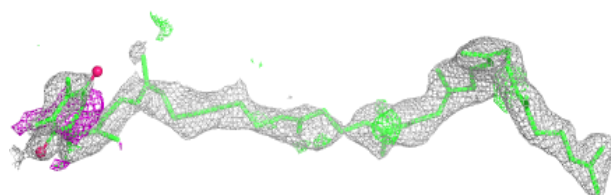
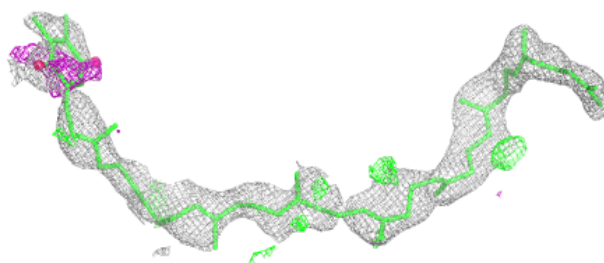
**Electron density around LMT a 418:**

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

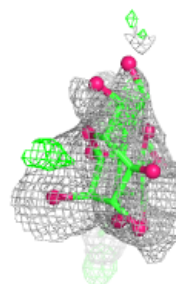
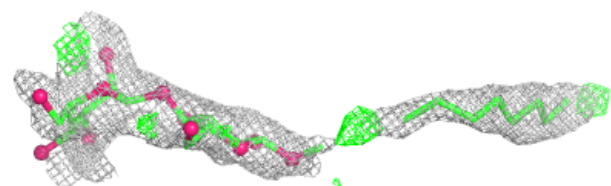
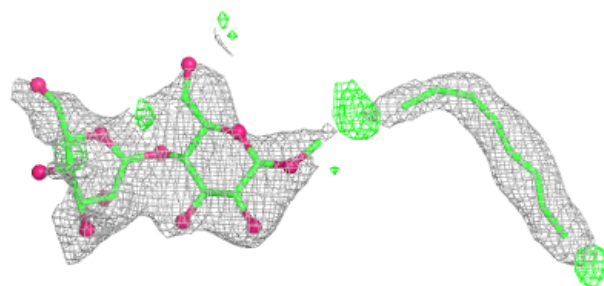


Electron density around PL9 a 414:

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

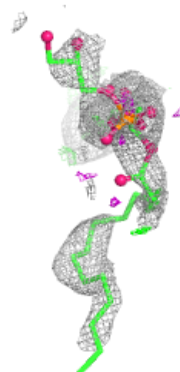
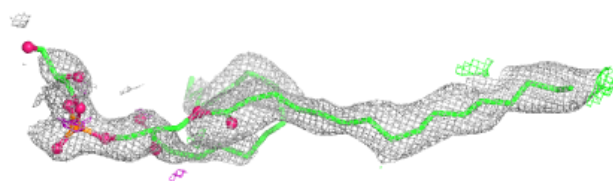
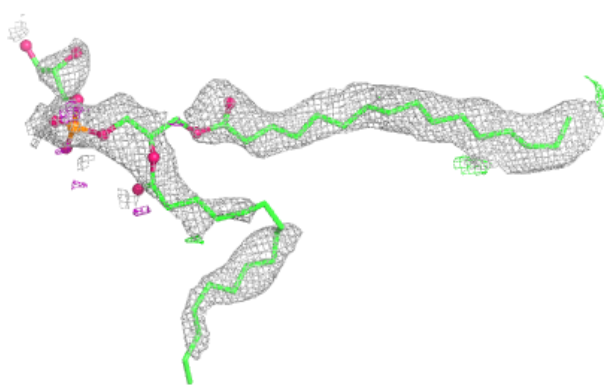
**Electron density around LMT z 101:**

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

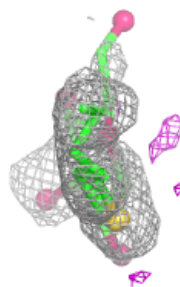
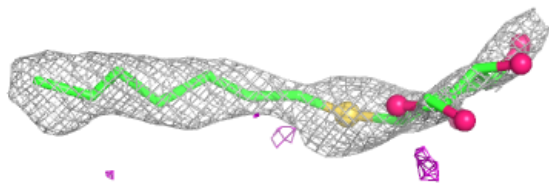
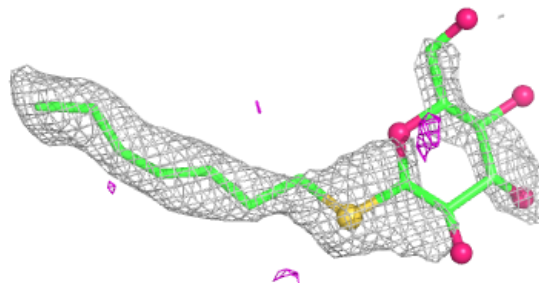


Electron density around LHG a 415:

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

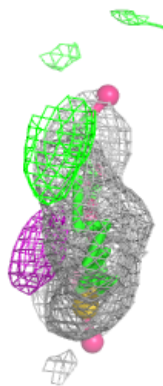
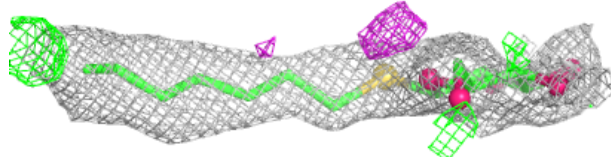
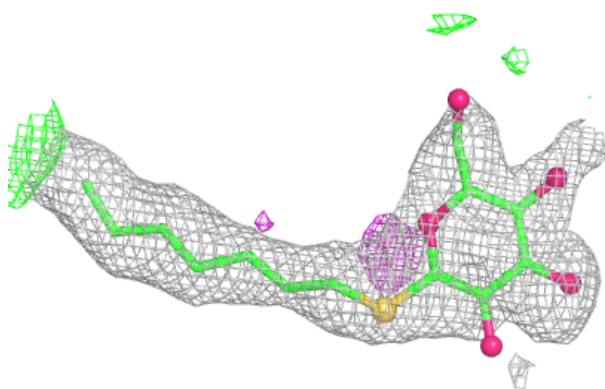
**Electron density around HTG B 626:**

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

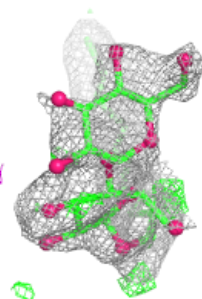
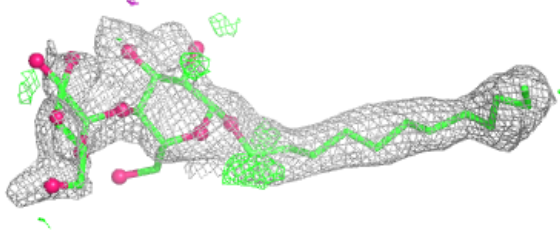
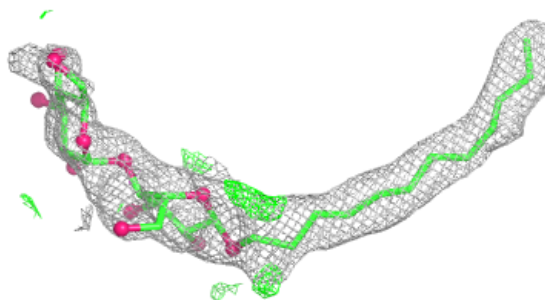


Electron density around HTG B 631:

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

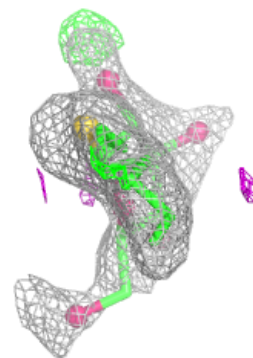
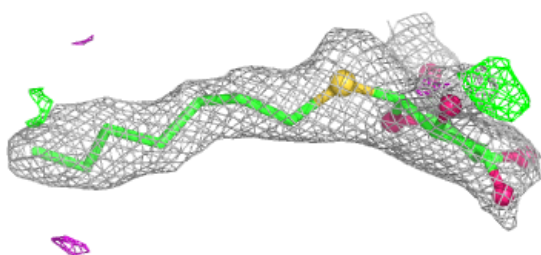
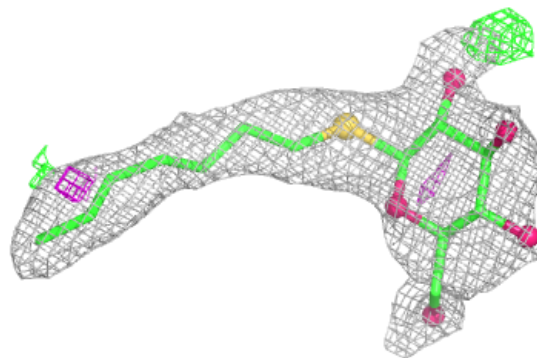
**Electron density around LMT m 103:**

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

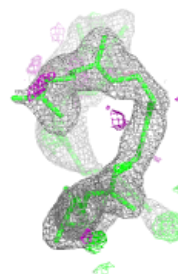
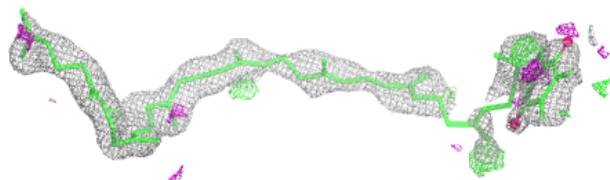
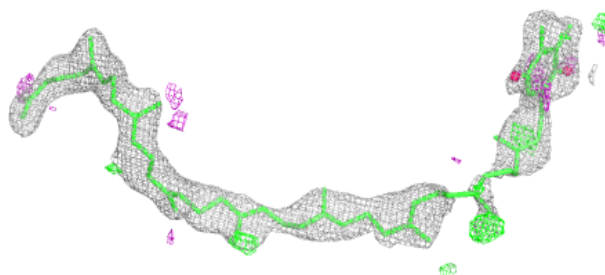


Electron density around HTG b 623:

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

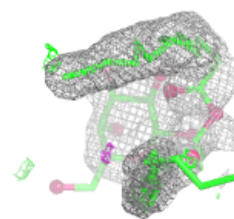
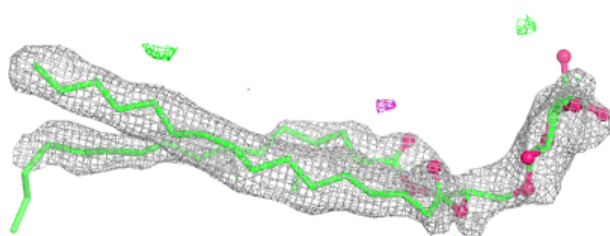
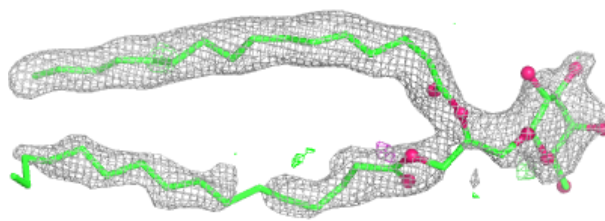
**Electron density around PL9 A 411:**

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

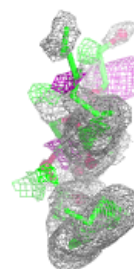
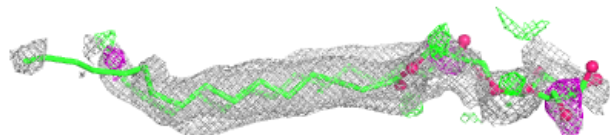
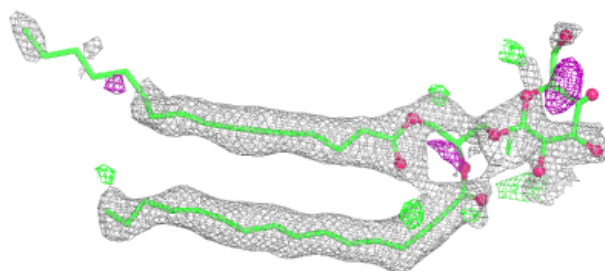


Electron density around LMG C 531:

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

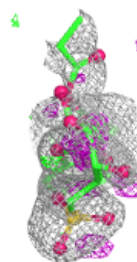
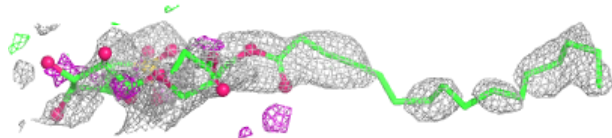
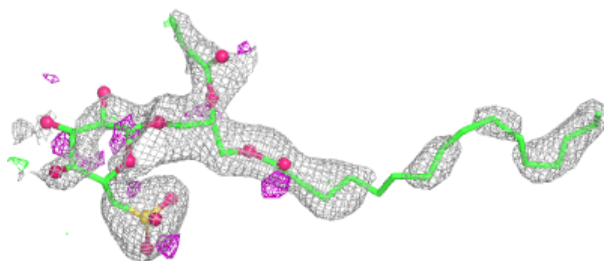
**Electron density around LMG D 412:**

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

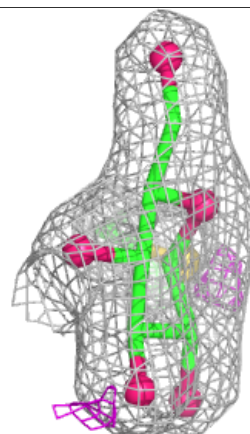
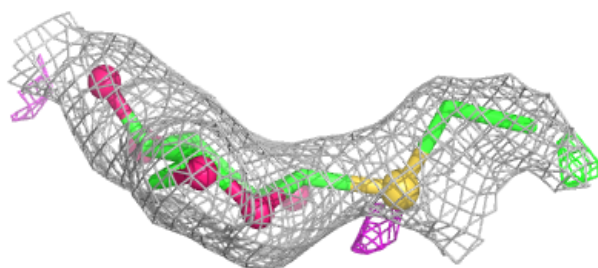
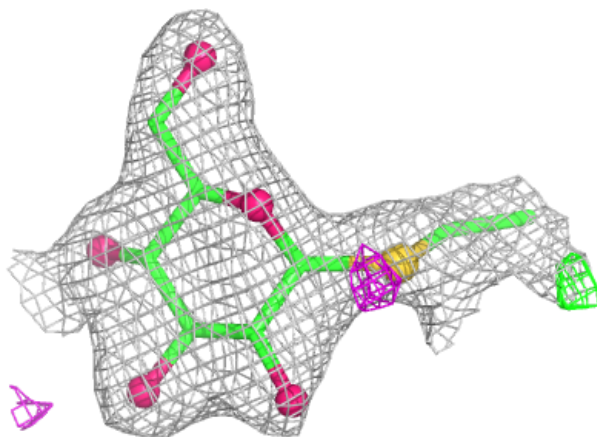


Electron density around SQD x 101:

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

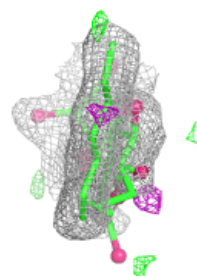
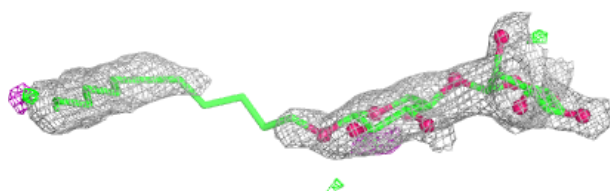
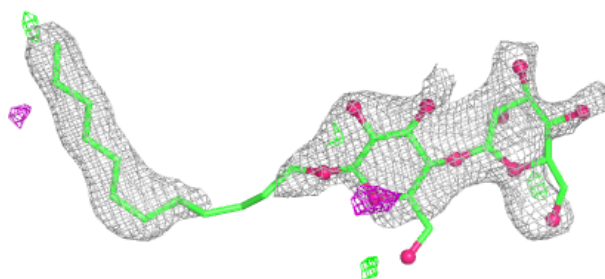
**Electron density around HTG V 204:**

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

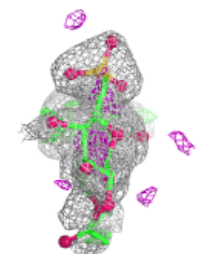
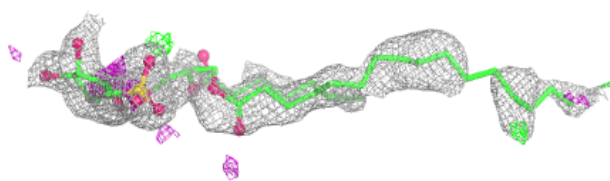
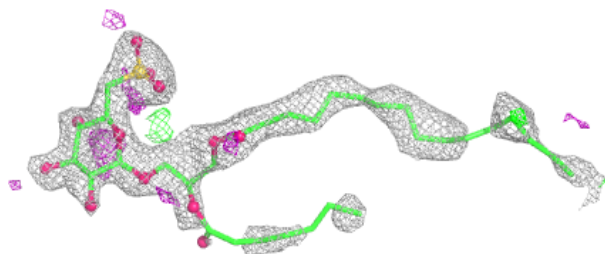


Electron density around LMT Z 101:

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

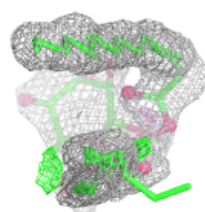
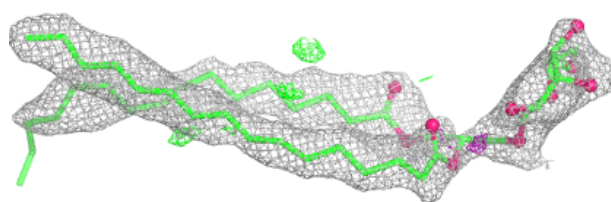
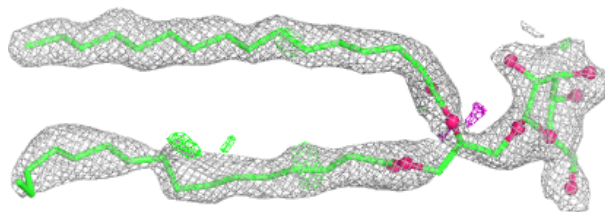
**Electron density around SQD D 408:**

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

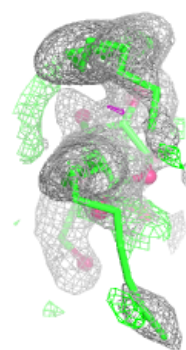
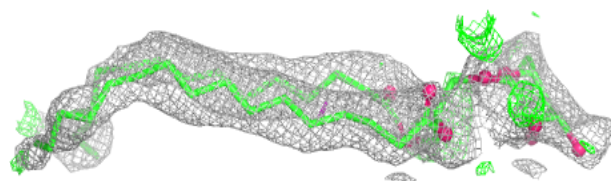
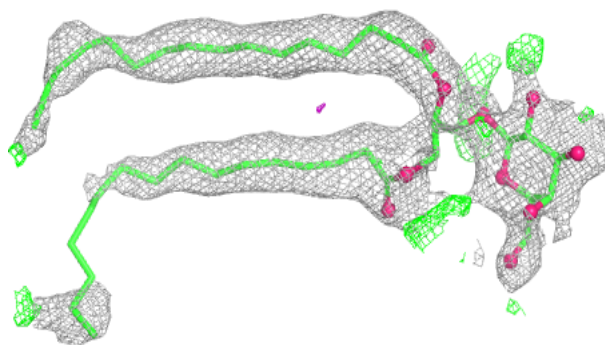


Electron density around LMG c 930:

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

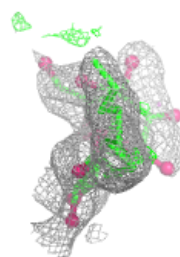
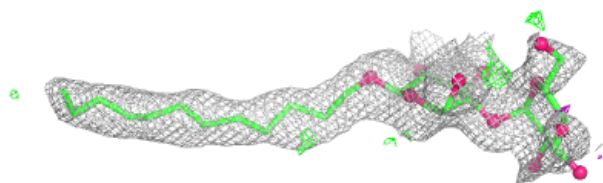
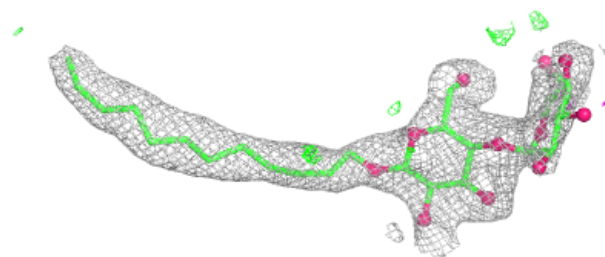
**Electron density around LMG d 411:**

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

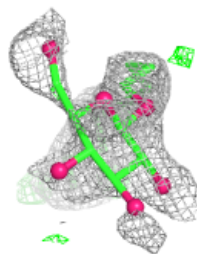
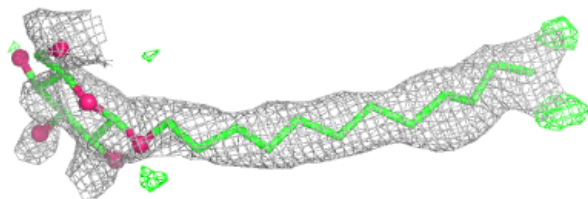
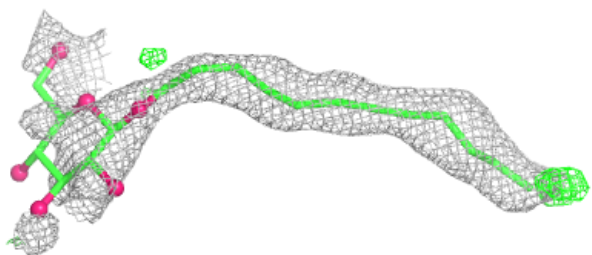


Electron density around LMT B 623:

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

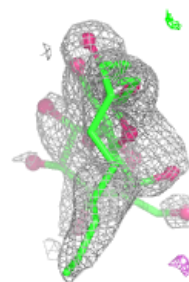
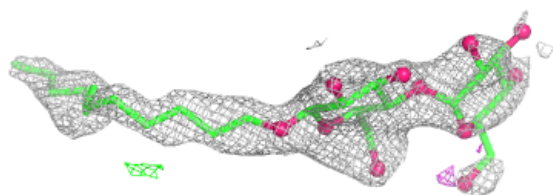
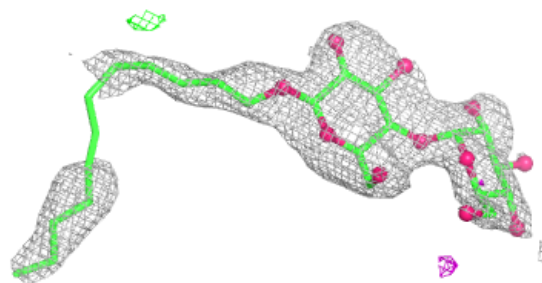
**Electron density around LMT B 643:**

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

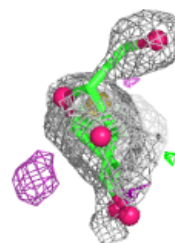
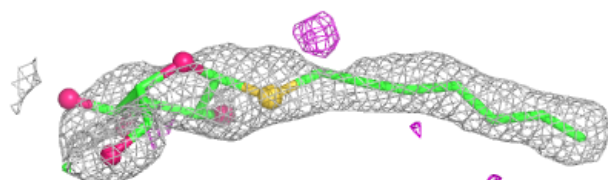


Electron density around LMT a 422:

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

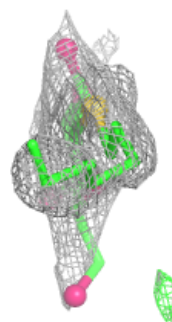
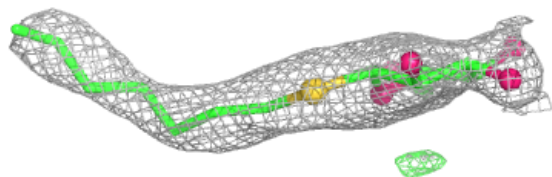
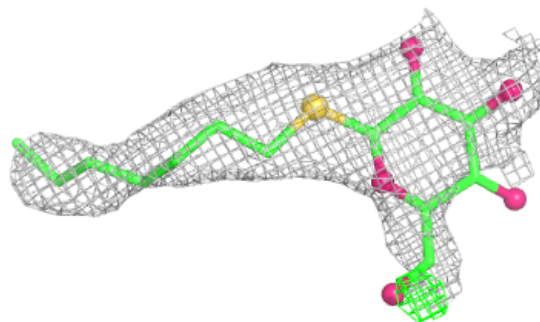
**Electron density around HTG C 522:**

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

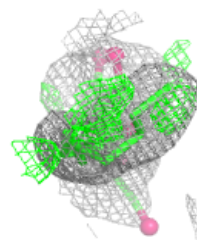
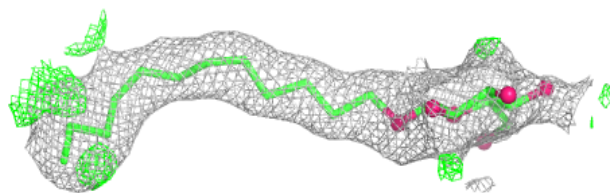
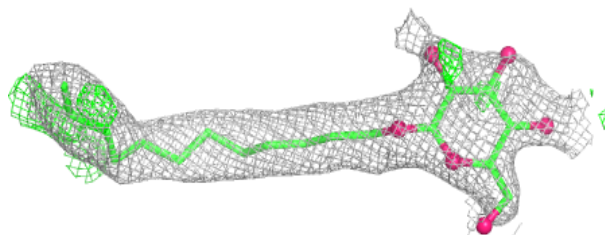


Electron density around HTG C 523:

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

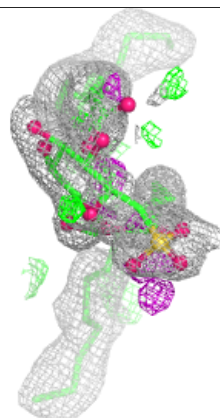
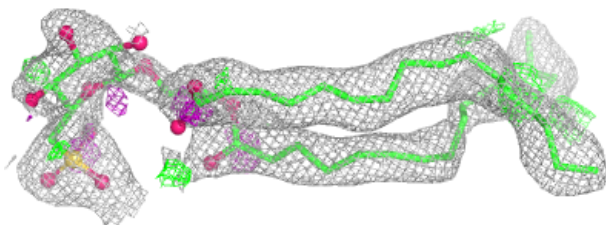
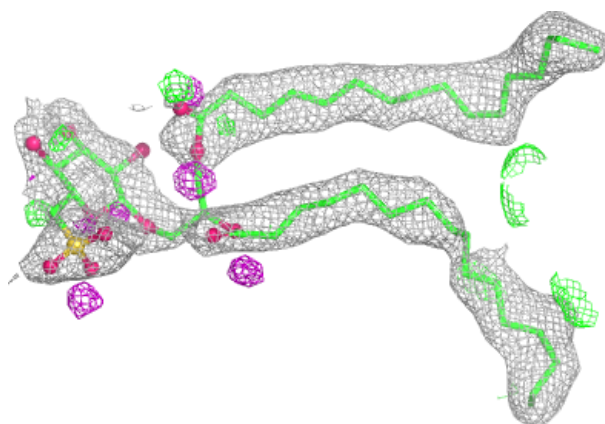
**Electron density around LMT B 644:**

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

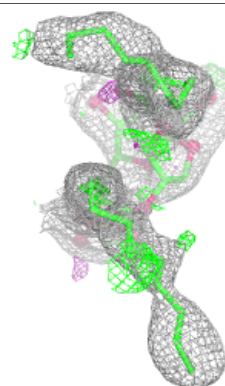
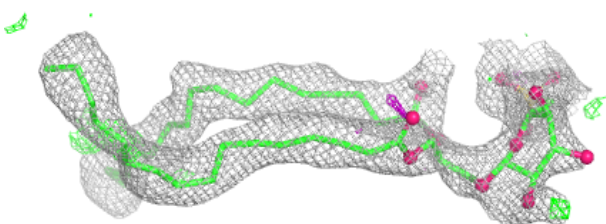
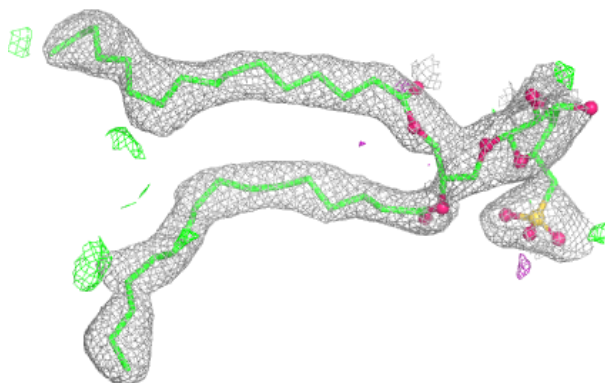


Electron density around SQD B 621:

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

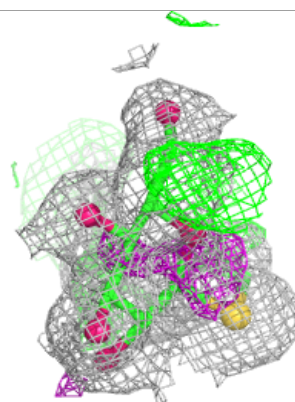
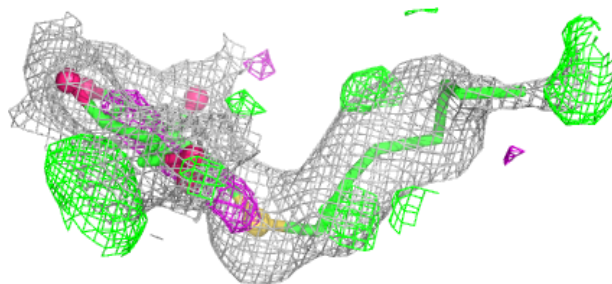
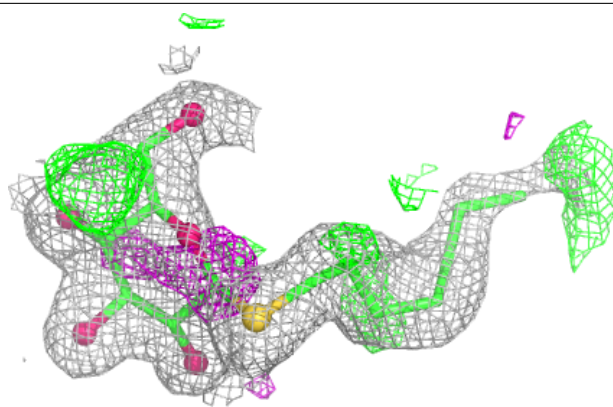
**Electron density around SQD L 102:**

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

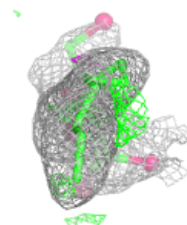
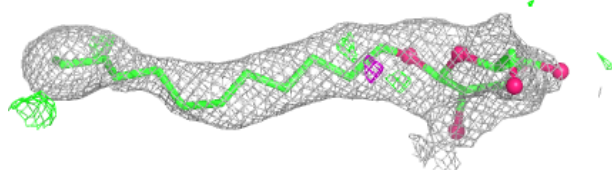
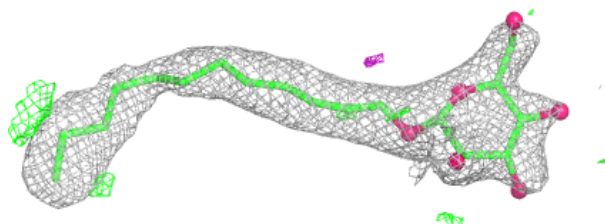


Electron density around HTG B 625:

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

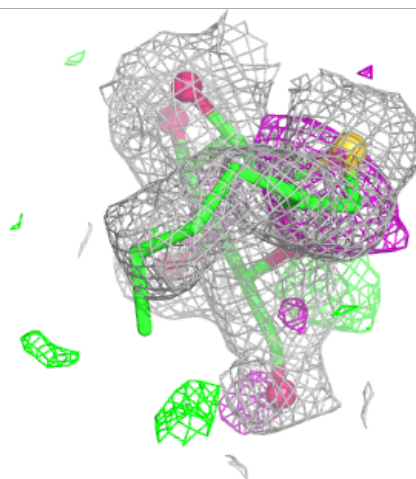
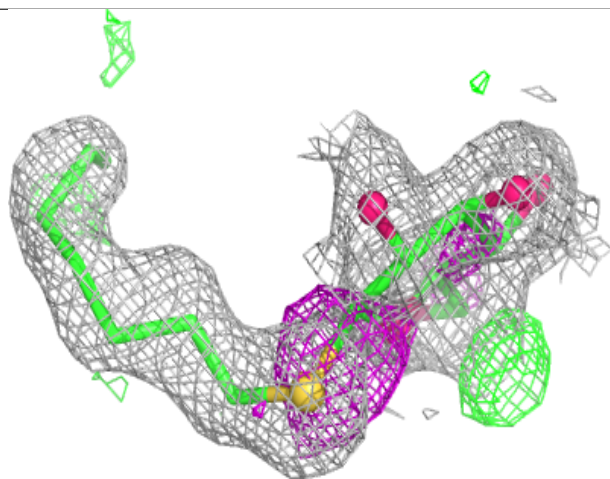
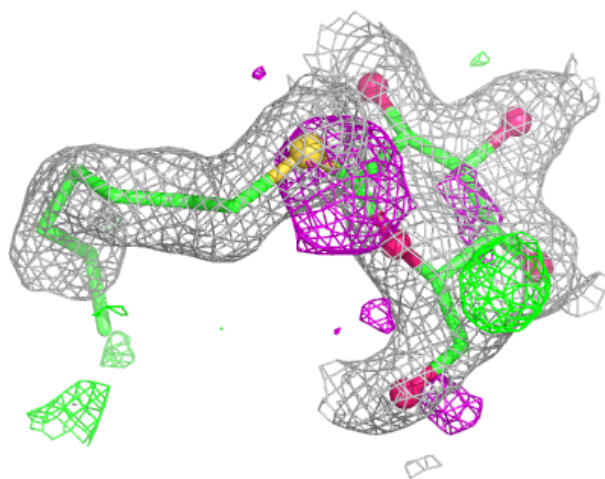
**Electron density around LMT T 103:**

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



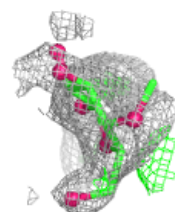
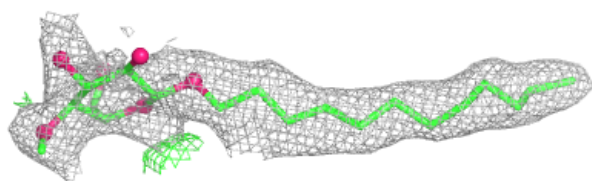
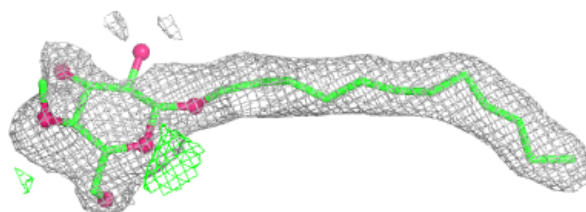
Electron density around HTG b 622:

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

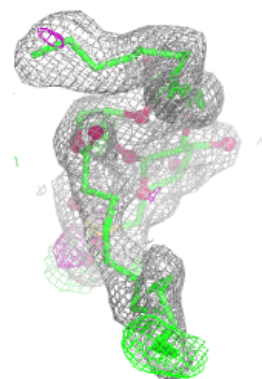
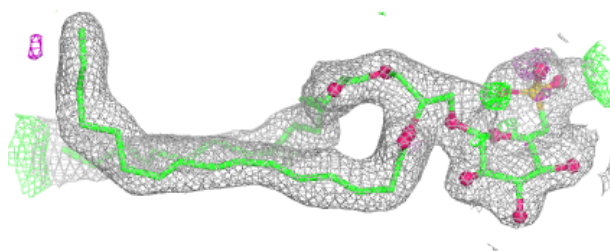
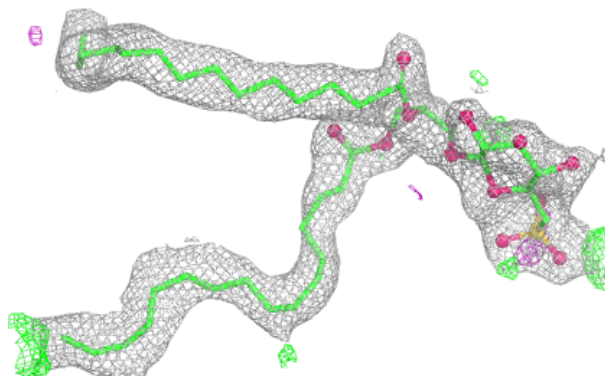


Electron density around LMT b 621:

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

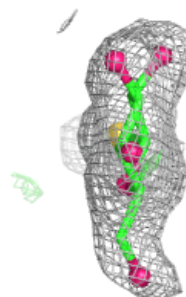
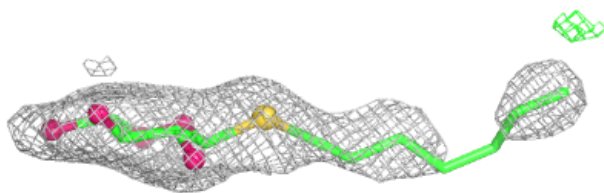
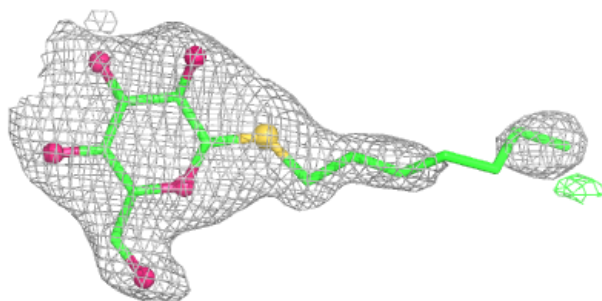
**Electron density around SQD a 417:**

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

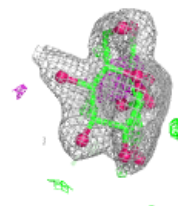
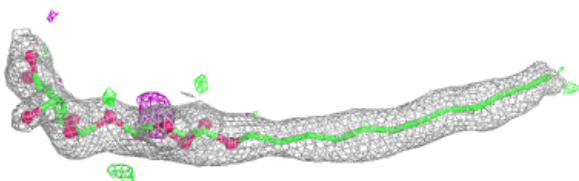
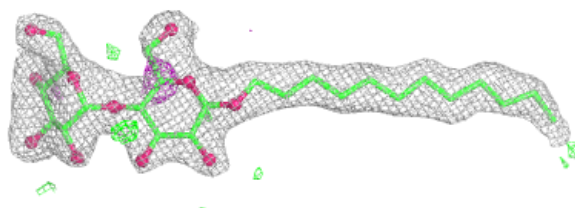


Electron density around HTG C 521:

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

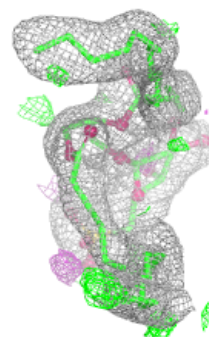
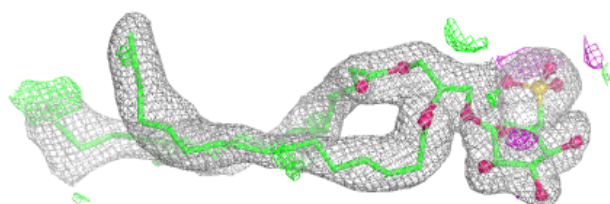
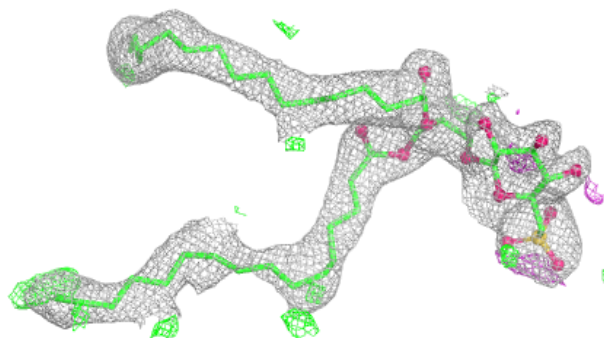
**Electron density around LMT m 104:**

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

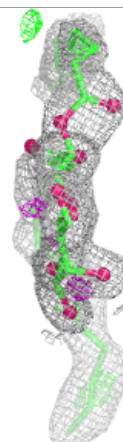
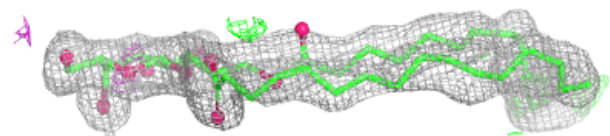
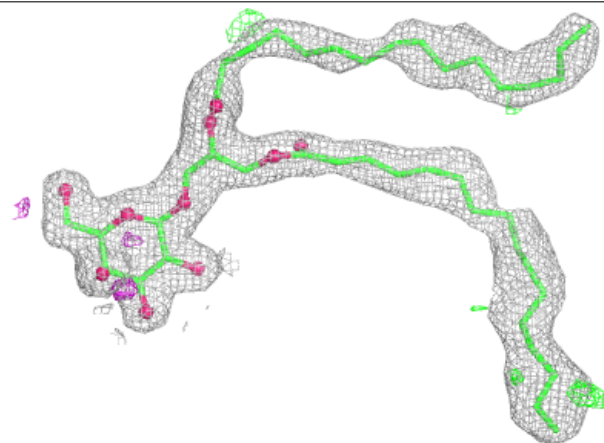


Electron density around SQD A 415:

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

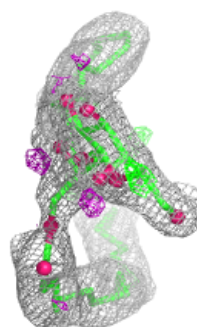
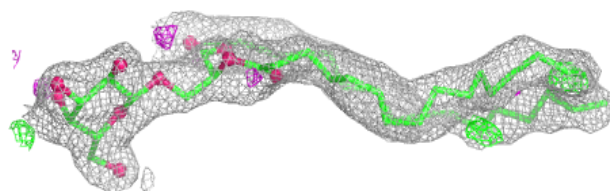
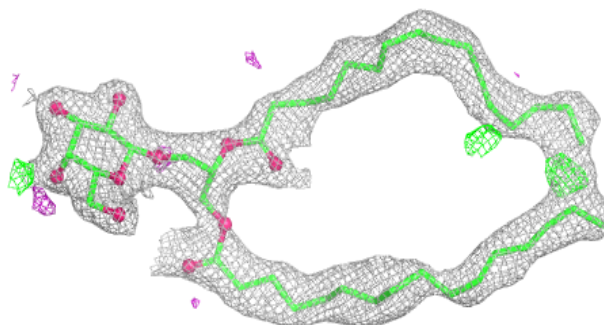
**Electron density around LMG C 520:**

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

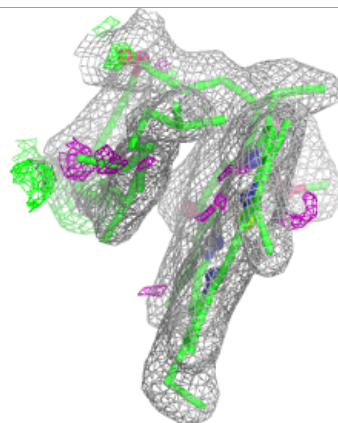
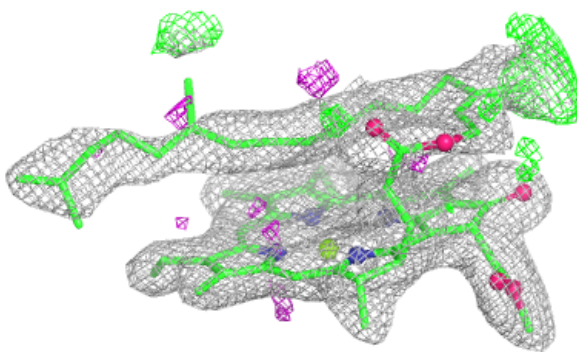
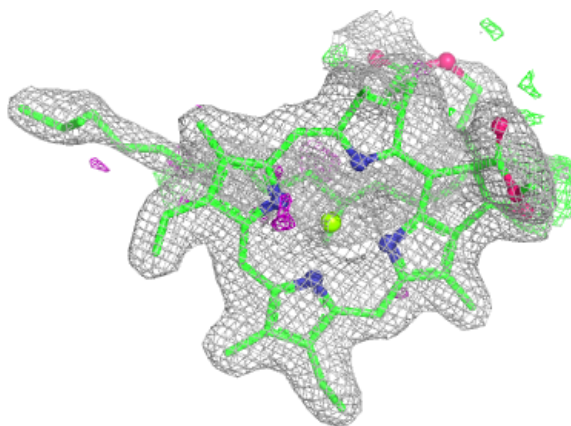


Electron density around LMG a 413:

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

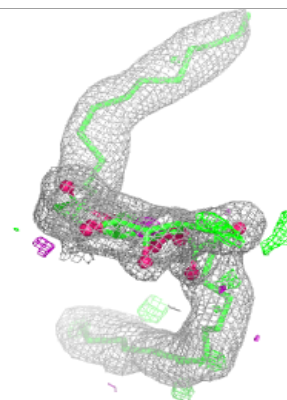
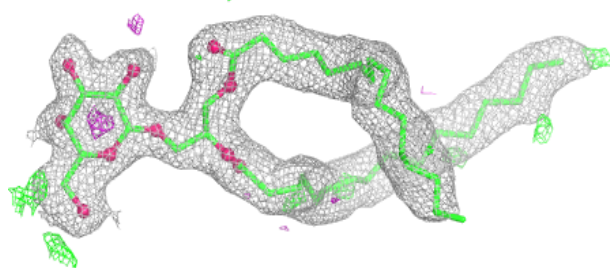
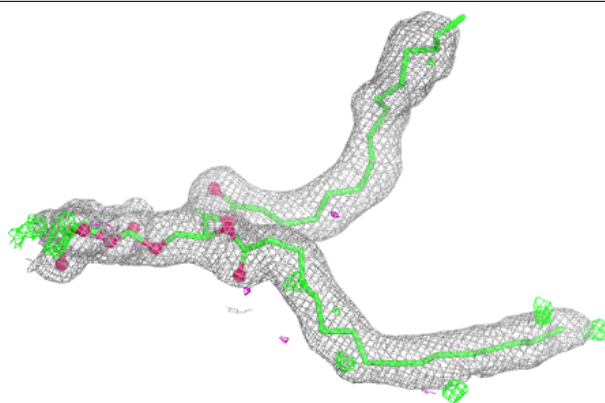
**Electron density around CLA b 602:**

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

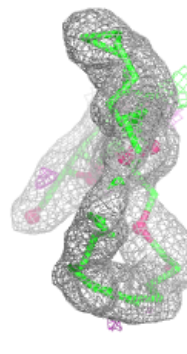
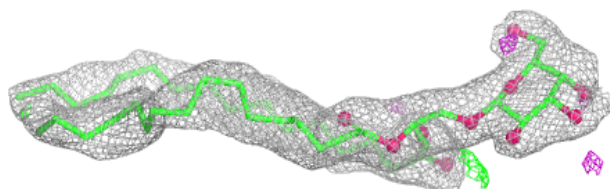
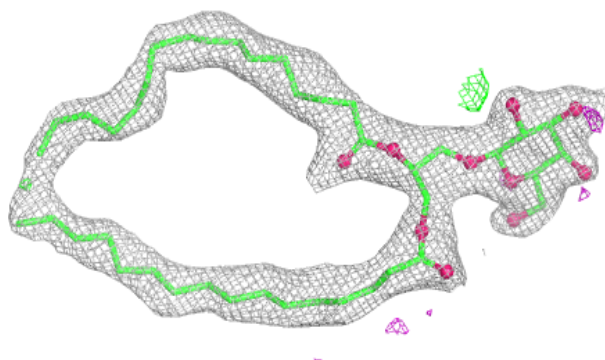


Electron density around LMG B 622:

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

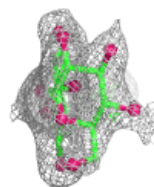
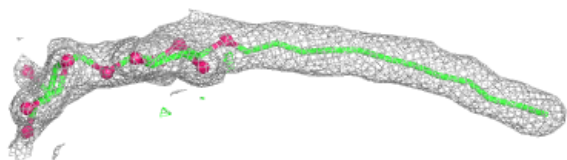
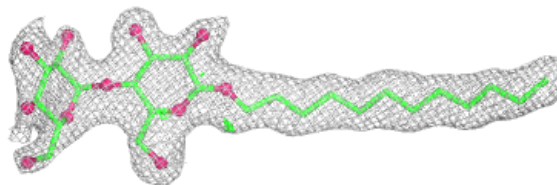
**Electron density around LMG C 501:**

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

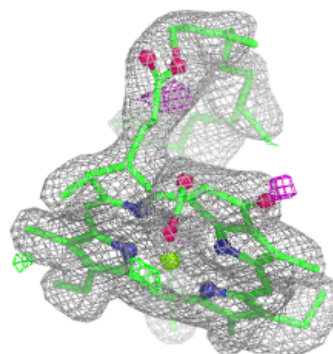
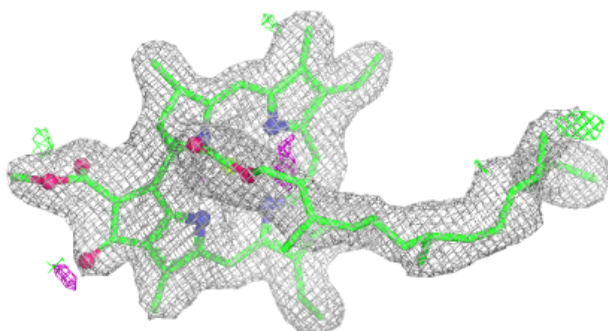
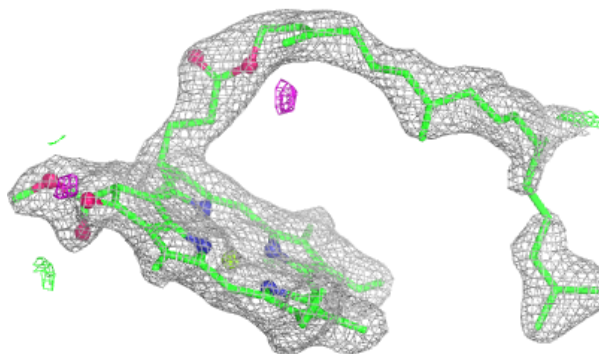


Electron density around LMT M 101:

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

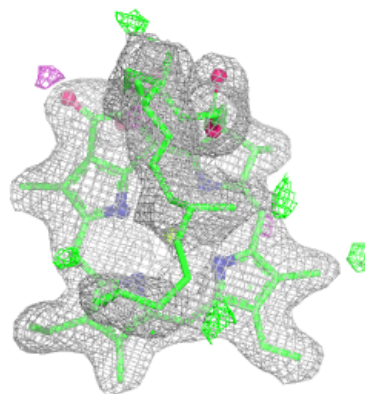
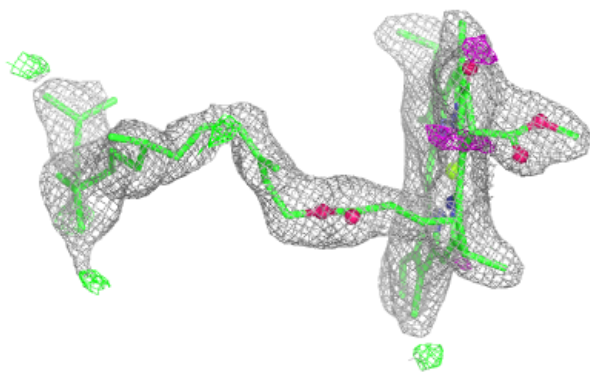
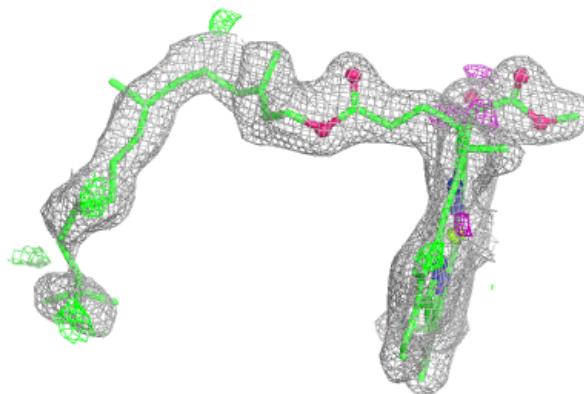
**Electron density around CLA C 514:**

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



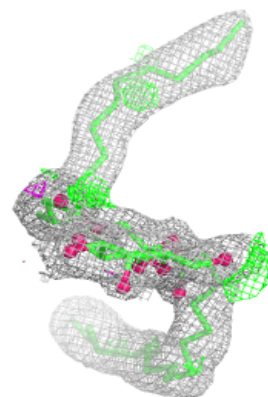
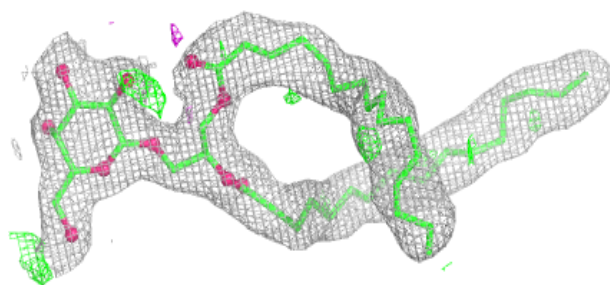
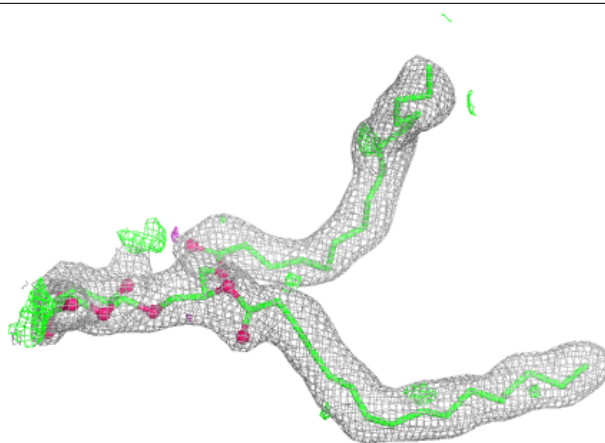
Electron density around CLA C 507:

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

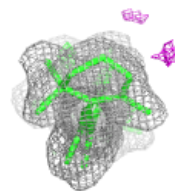
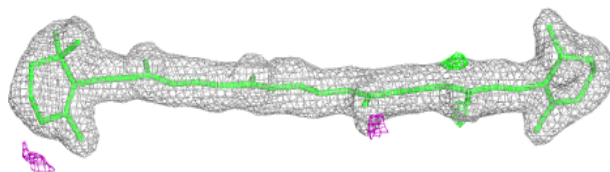
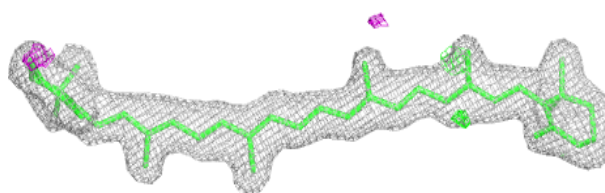


Electron density around LMG m 102:

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

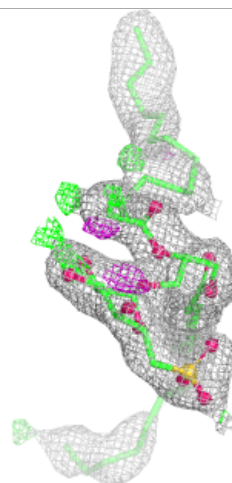
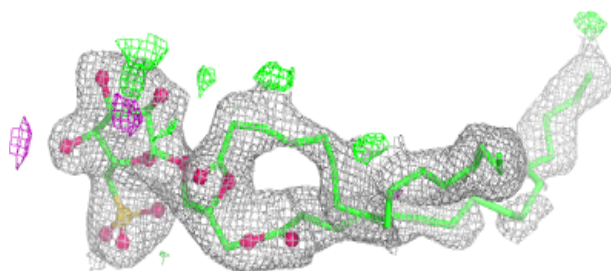
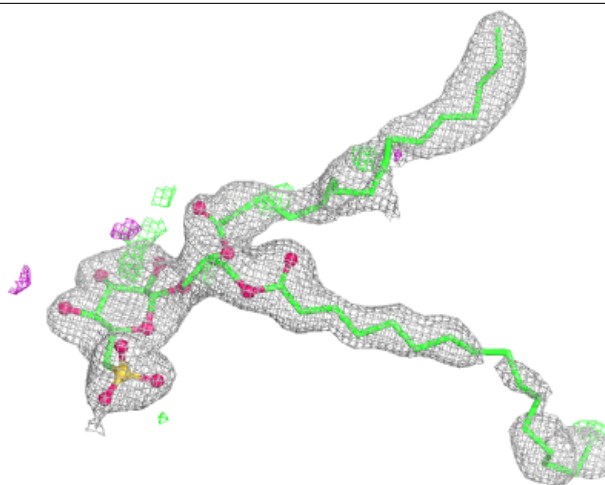
**Electron density around BCR C 515:**

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



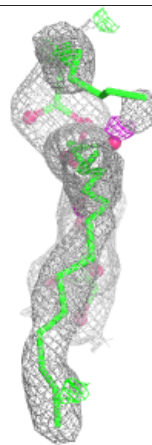
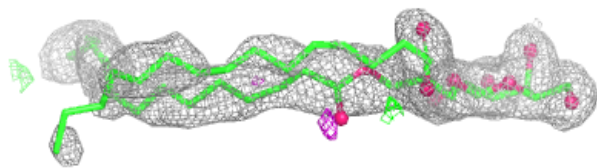
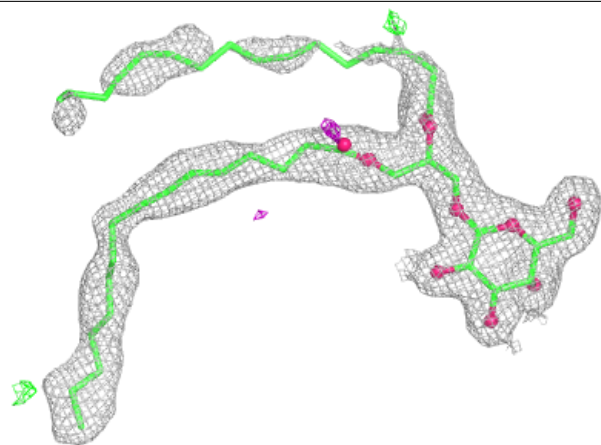
Electron density around SQD A 410:

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



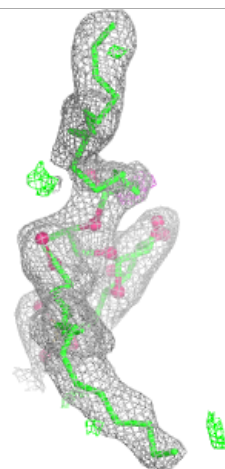
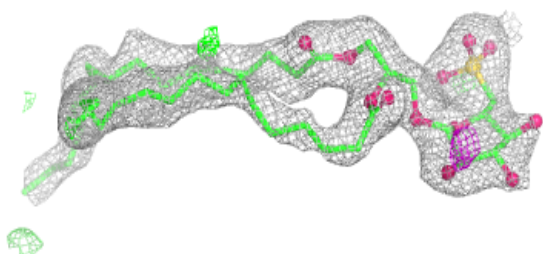
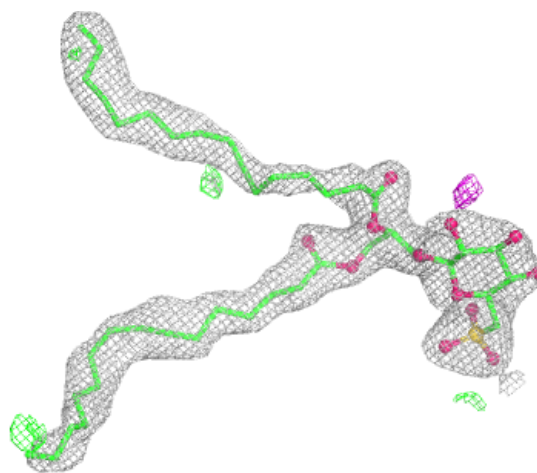
Electron density around LMG c 920:

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



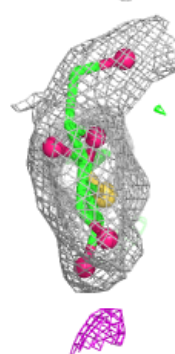
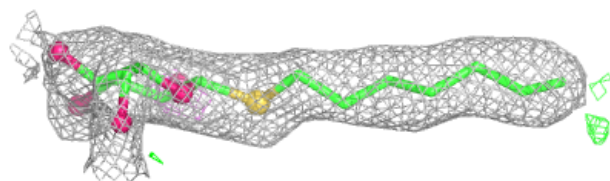
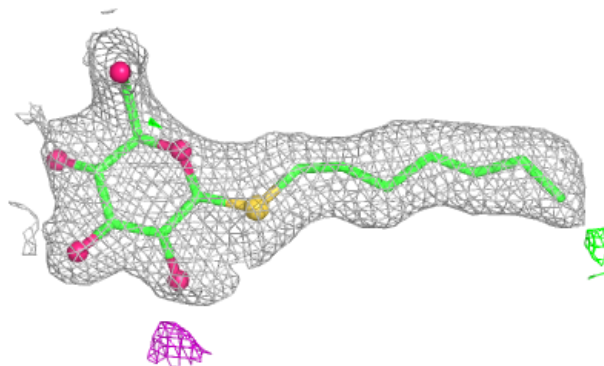
Electron density around SQD a 412:

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

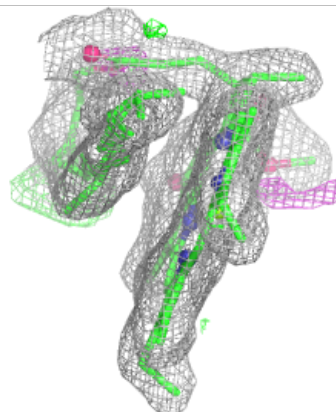
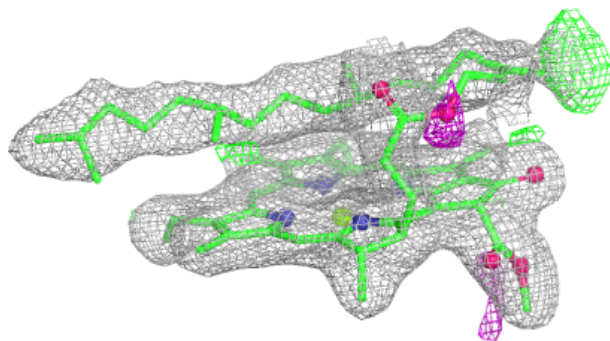
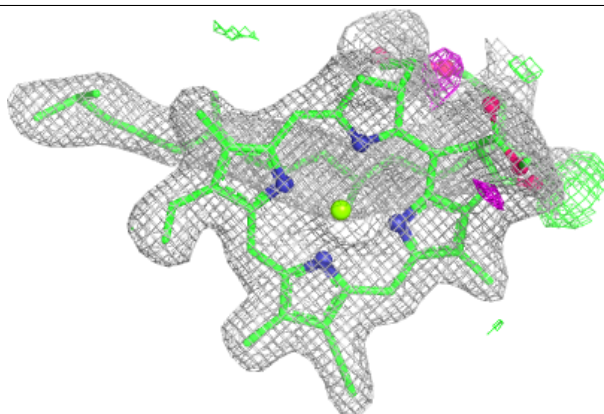


Electron density around HTG B 630:

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

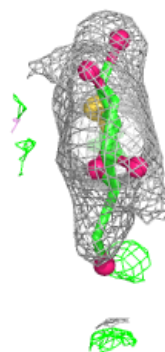
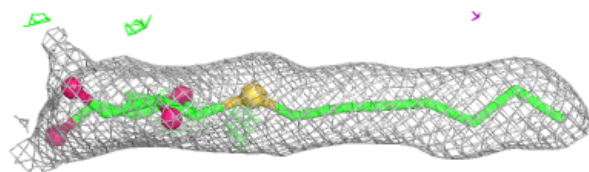
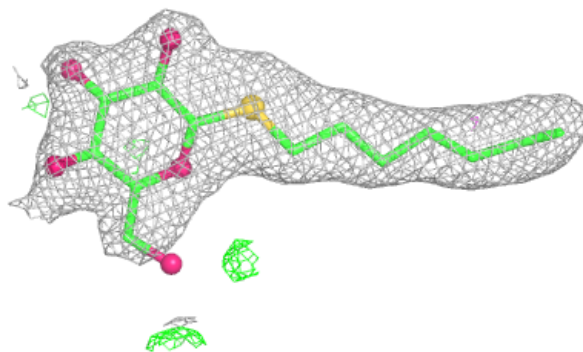
**Electron density around CLA B 602:**

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



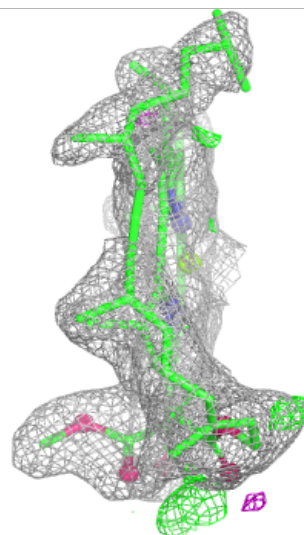
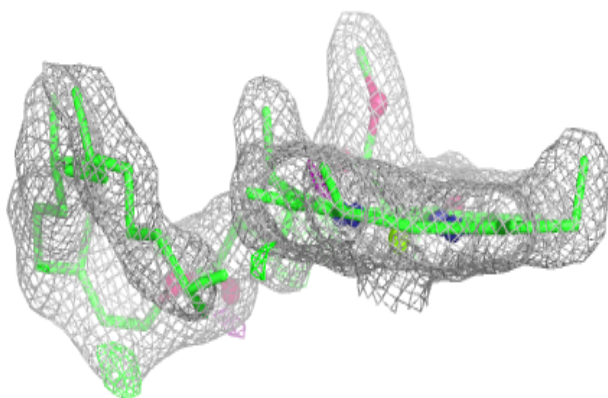
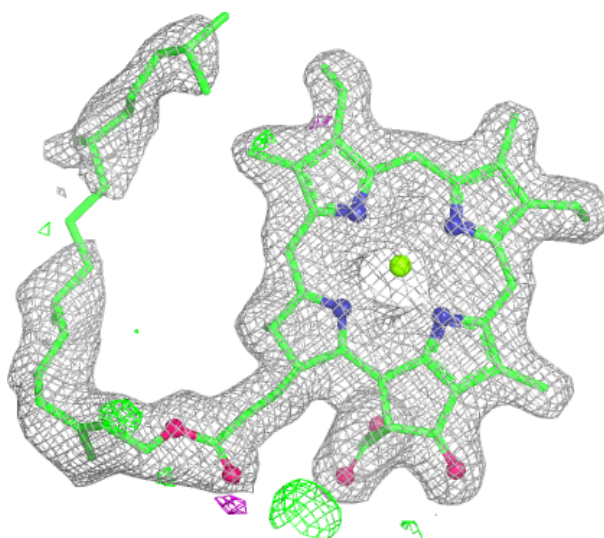
Electron density around HTG b 627:

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



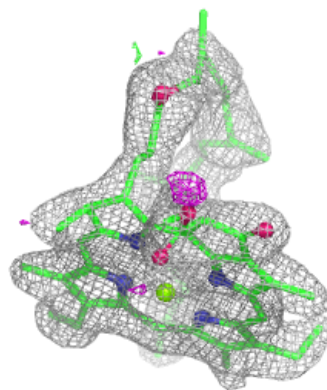
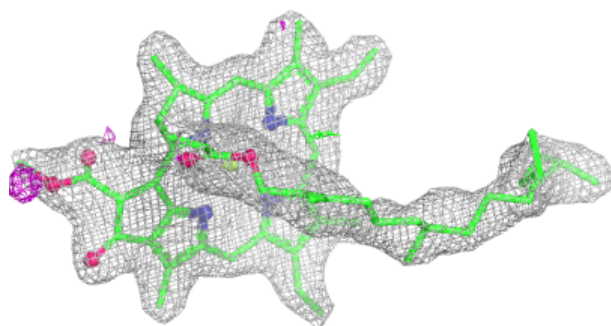
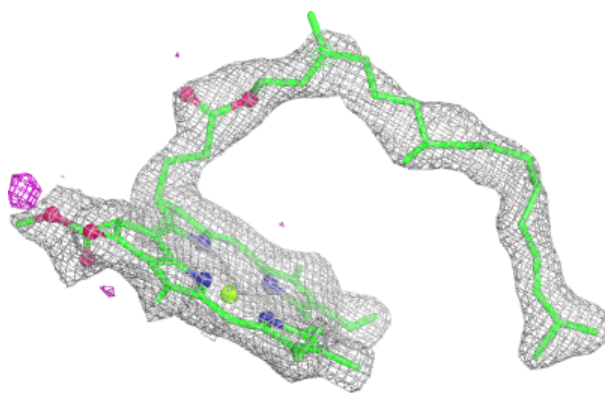
Electron density around CLA c 913:

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



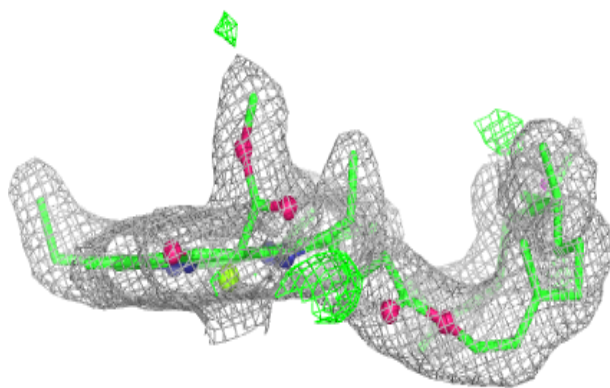
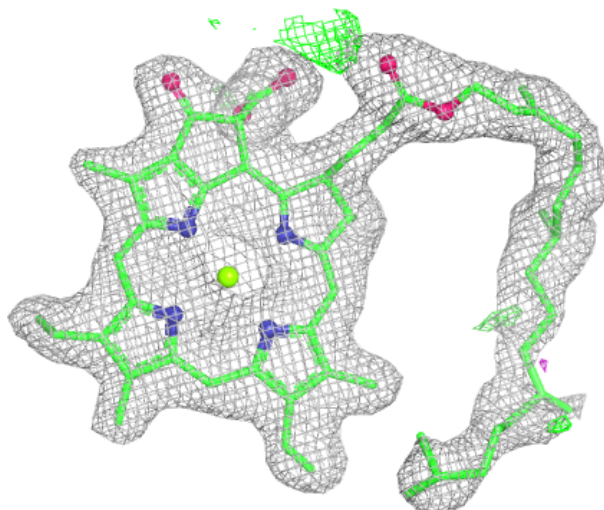
Electron density around CLA c 914:

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



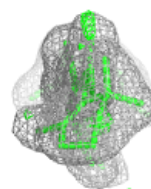
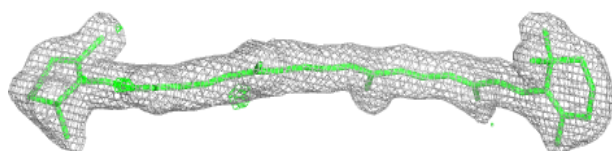
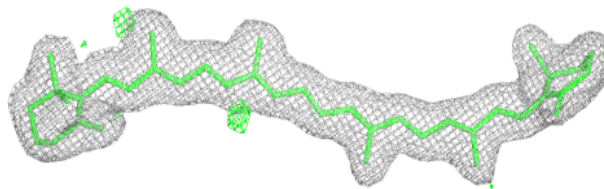
Electron density around CLA C 513:

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

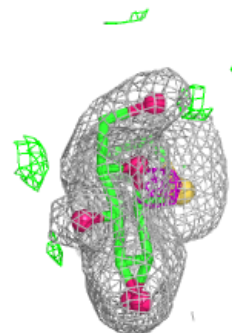
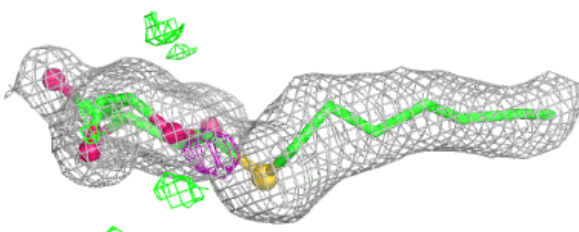
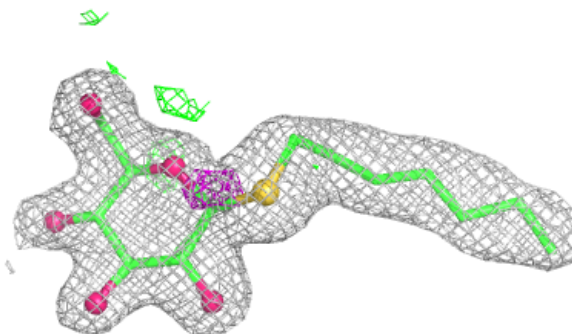


Electron density around BCR Y 101:

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

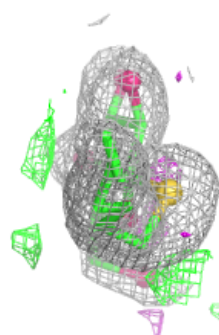
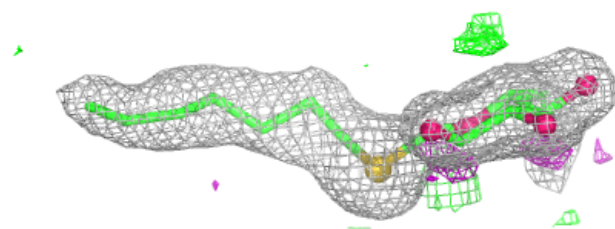
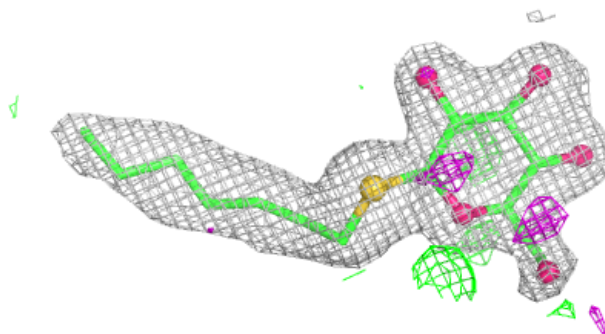
**Electron density around HTG O 302:**

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

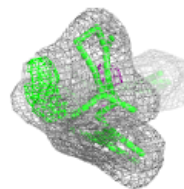
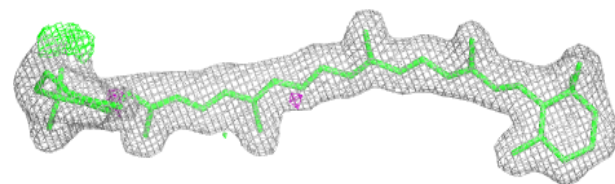
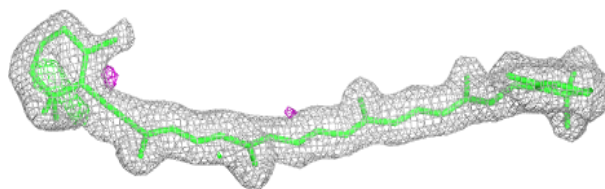


Electron density around HTG B 624:

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

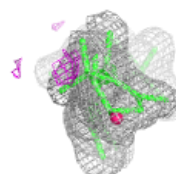
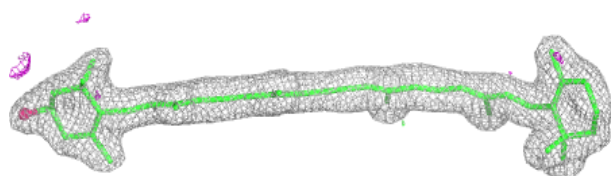
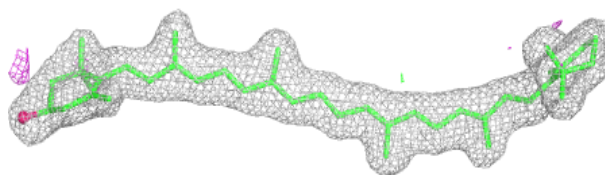
**Electron density around BCR d 405:**

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

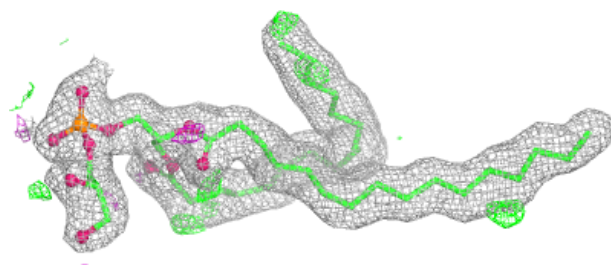
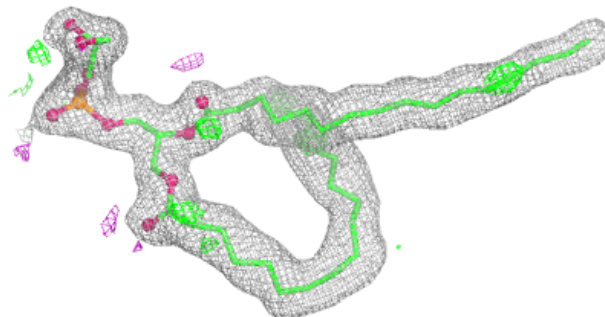


Electron density around RRX H 102:

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

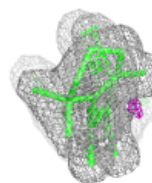
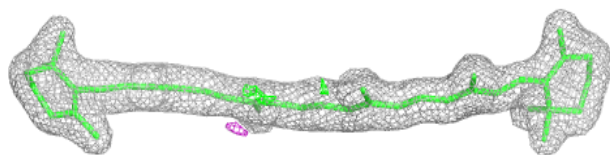
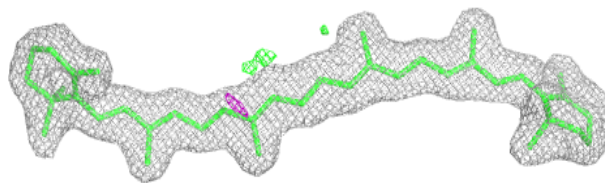
**Electron density around LHG D 409:**

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

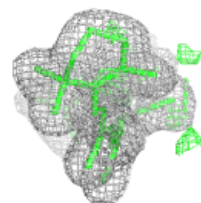
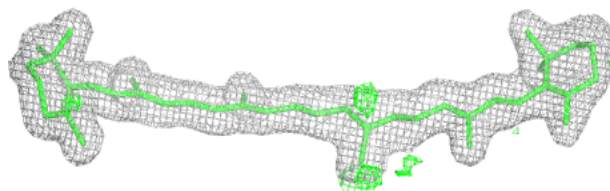
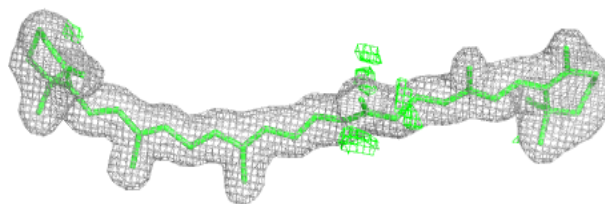


Electron density around BCR j 104:

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

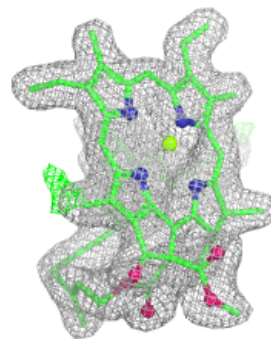
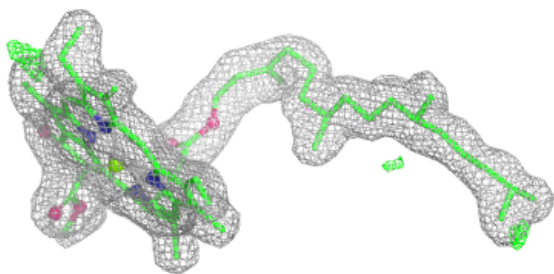
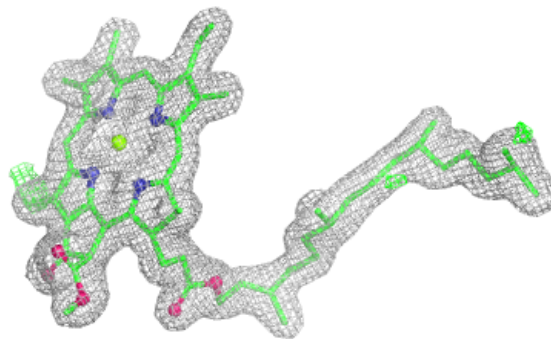
**Electron density around BCR t 101:**

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



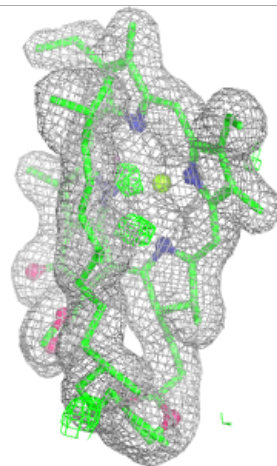
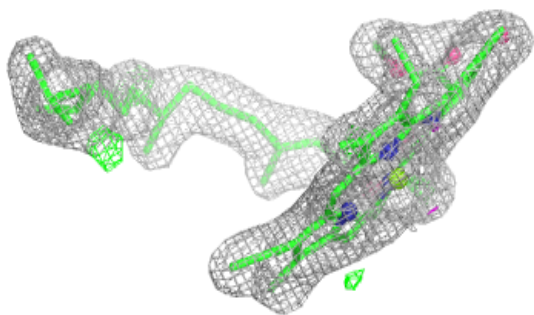
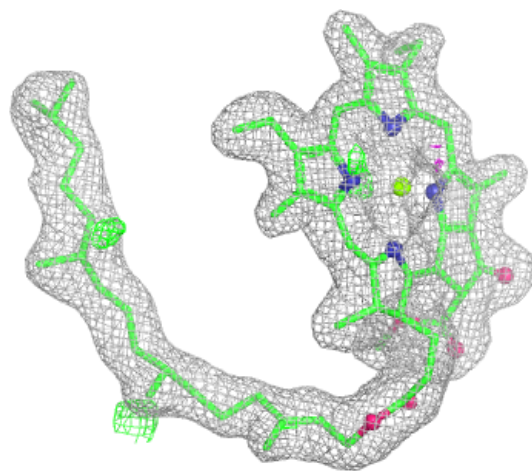
Electron density around CLA C 512:

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



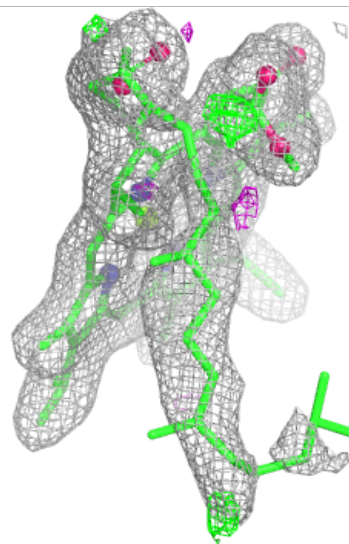
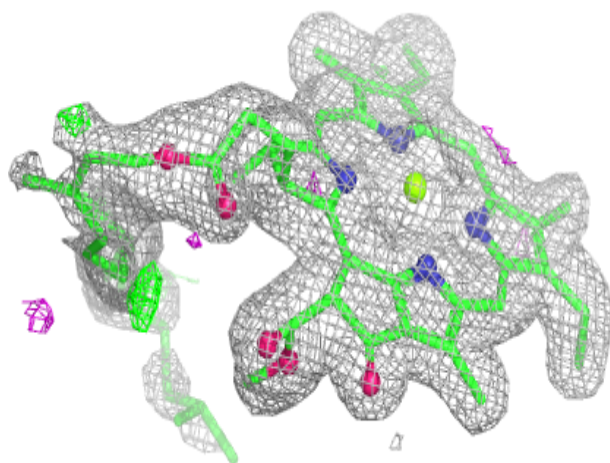
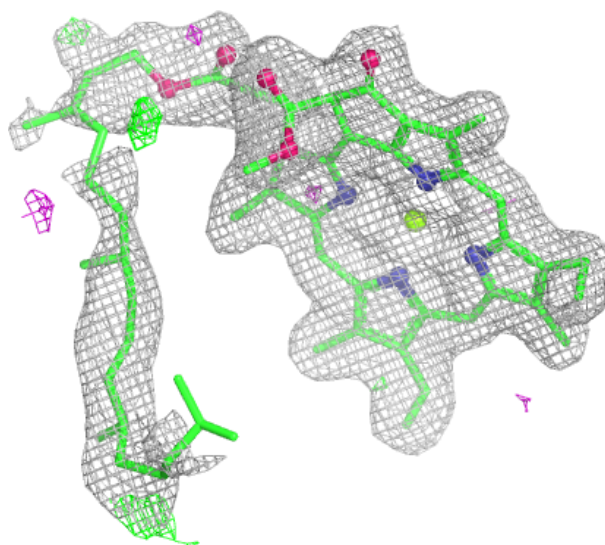
Electron density around CLA C 508:

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



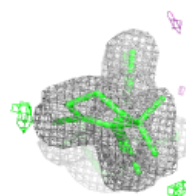
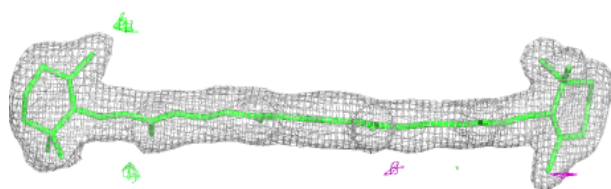
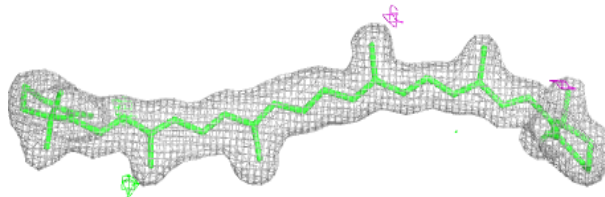
Electron density around CLA b 617:

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

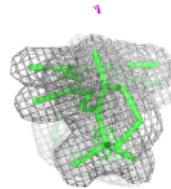
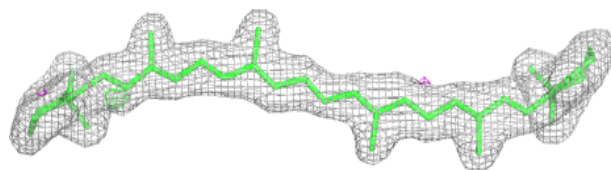
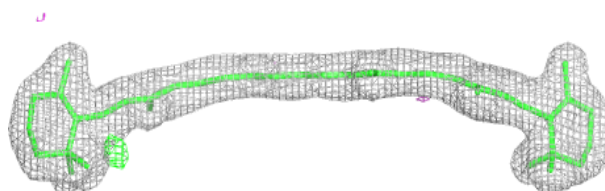


Electron density around BCR C 516:

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

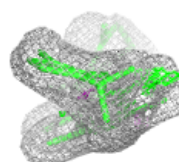
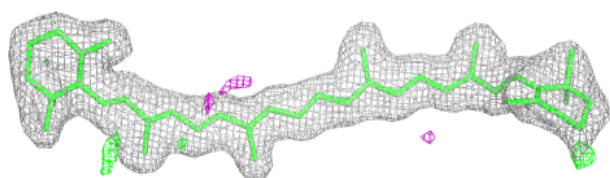
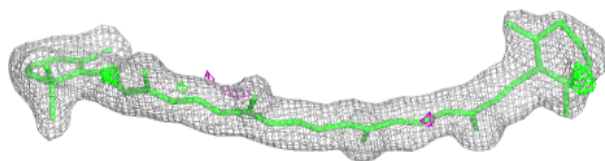
**Electron density around BCR C 530:**

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

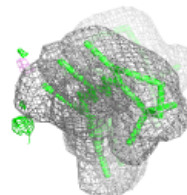
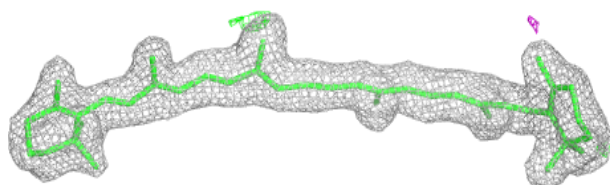
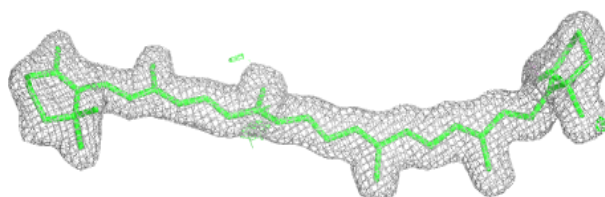


Electron density around BCR D 405:

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

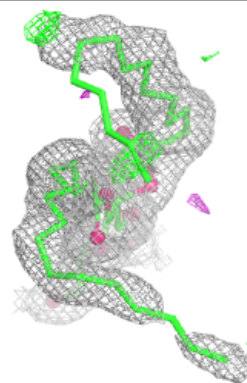
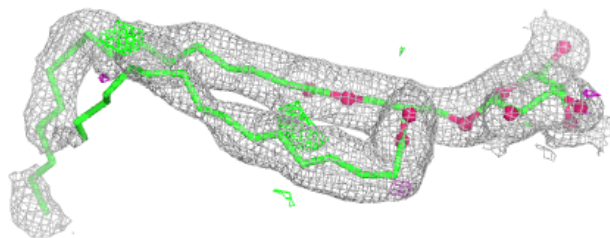
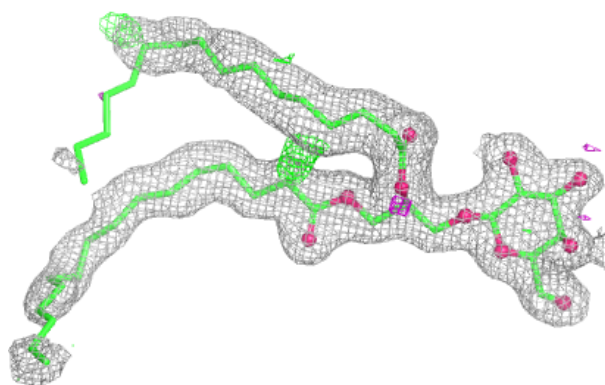
**Electron density around BCR T 101:**

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

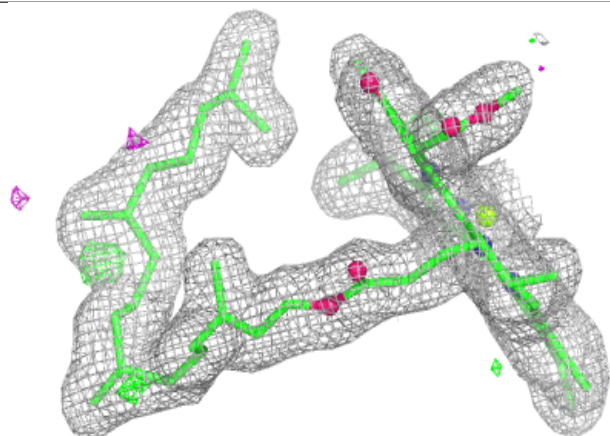
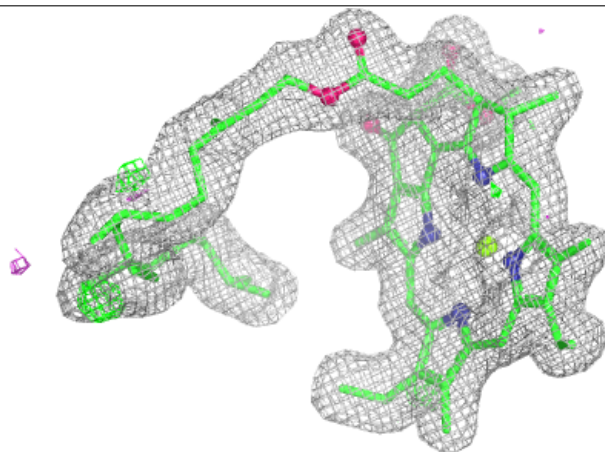


Electron density around LMG J 101:

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

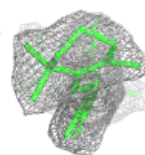
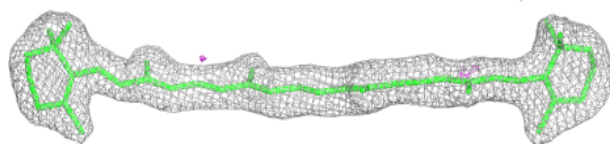
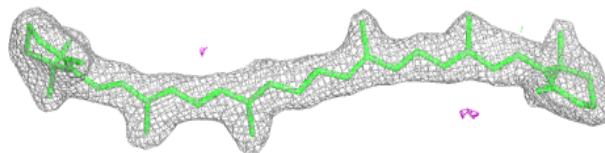
**Electron density around CLA c 904:**

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

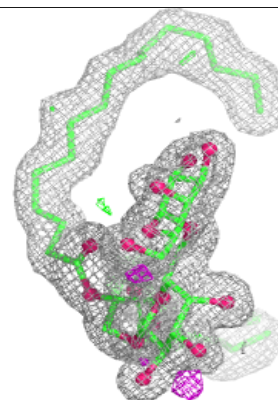
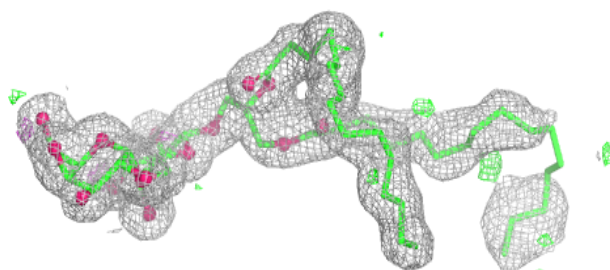
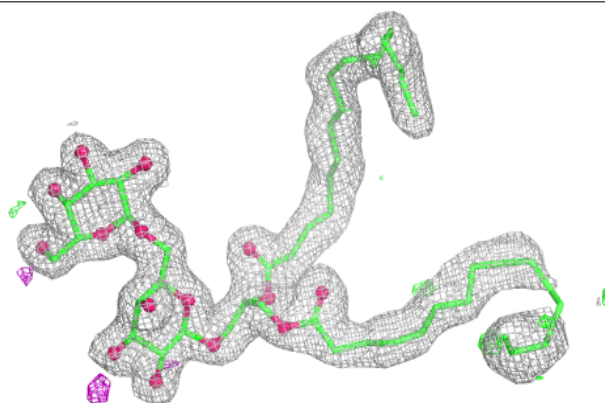


Electron density around BCR c 915:

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

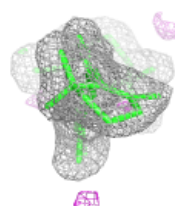
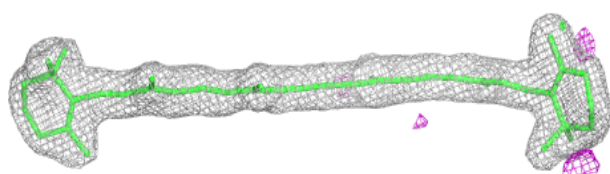
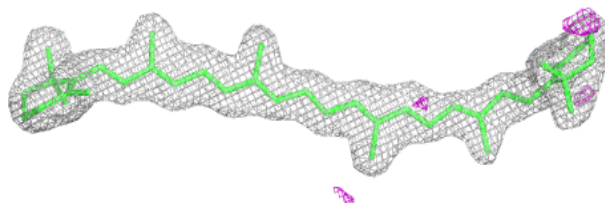
**Electron density around DGD C 518:**

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

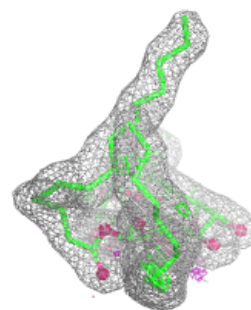
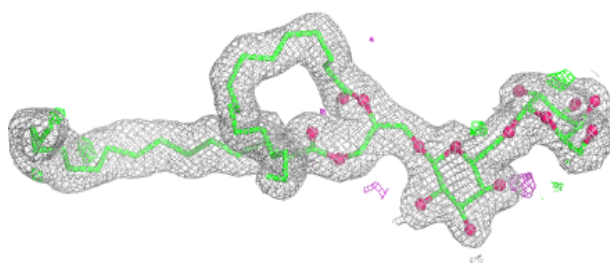
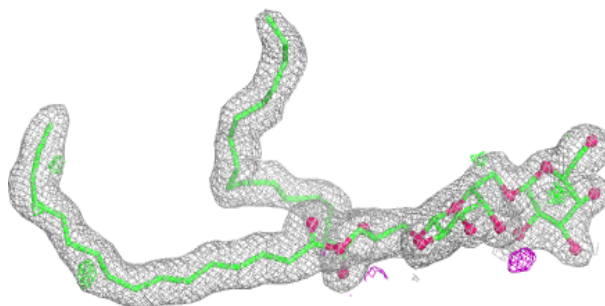


Electron density around BCR c 916:

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

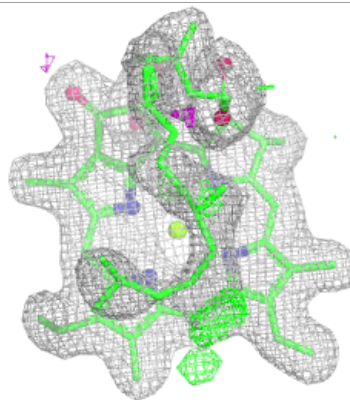
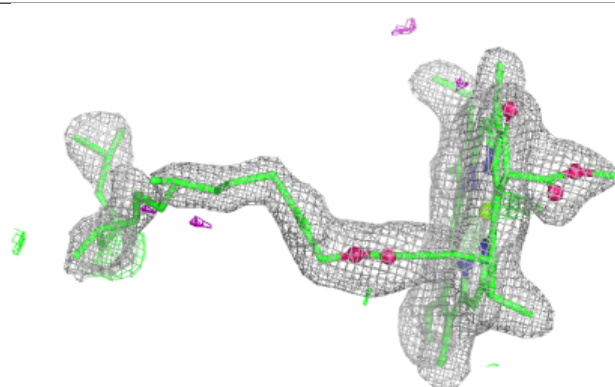
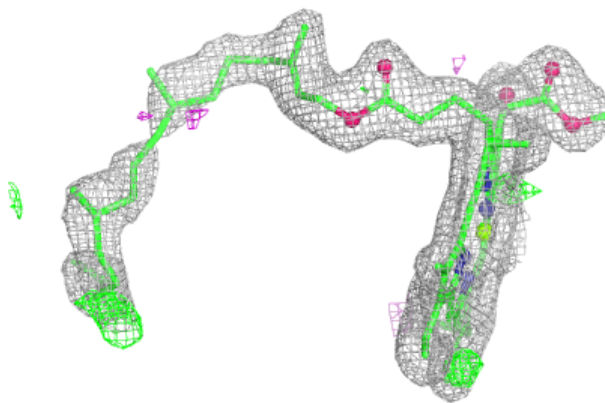
**Electron density around DGD H 103:**

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

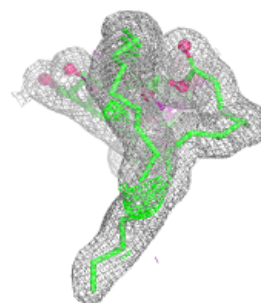
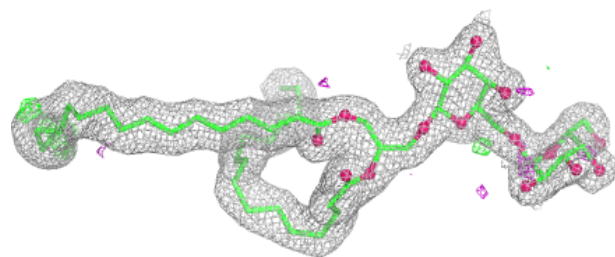
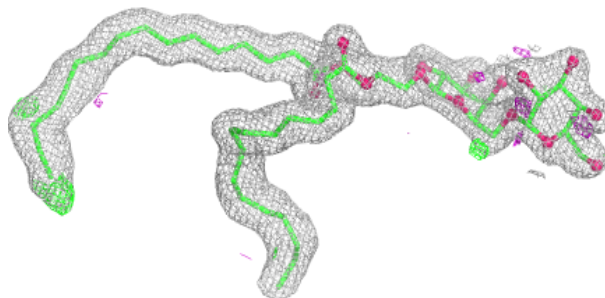


Electron density around CLA c 907:

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

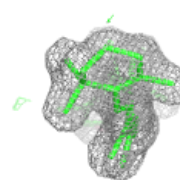
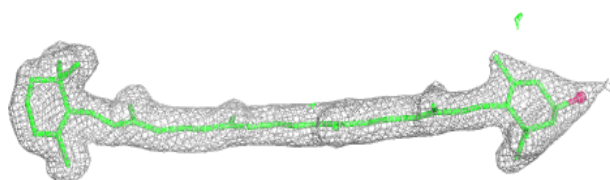
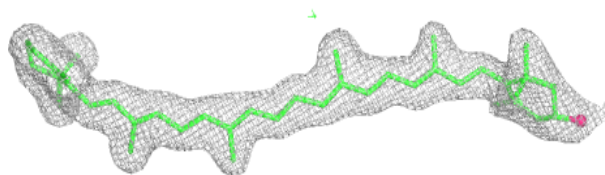
**Electron density around DGD h 102:**

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

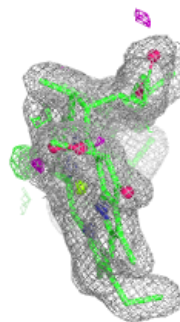
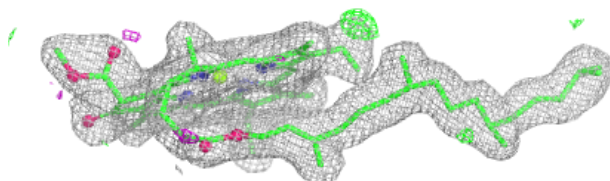
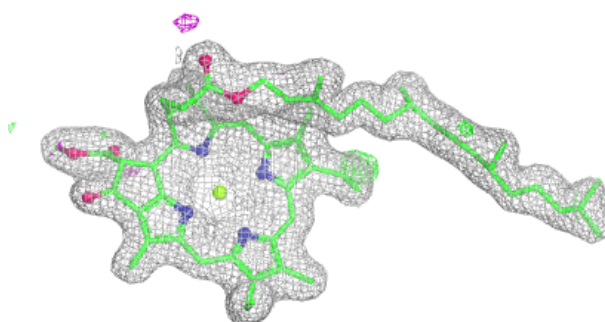


Electron density around RRX x 102:

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

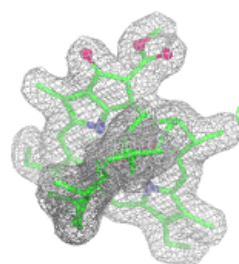
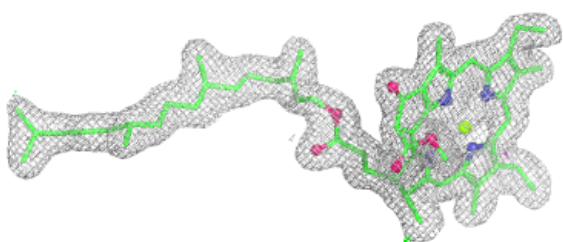
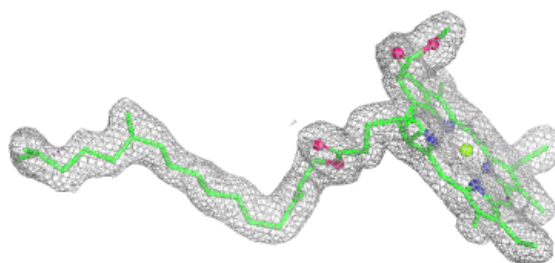
**Electron density around CLA C 502:**

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

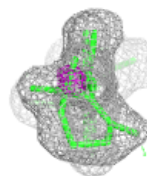
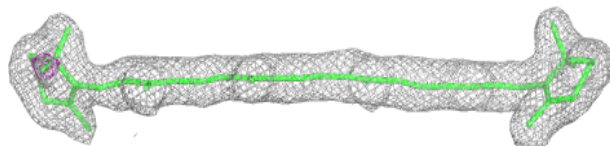
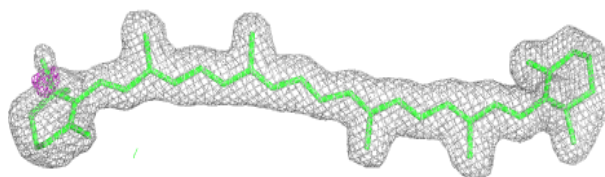


Electron density around CLA C 503:

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

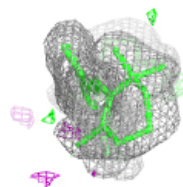
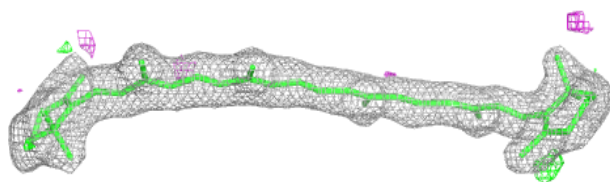
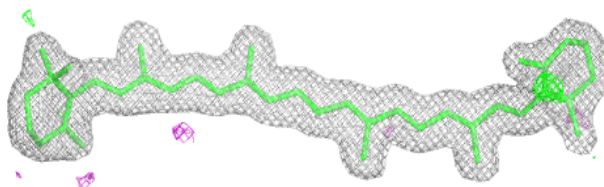
**Electron density around BCR B 619:**

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



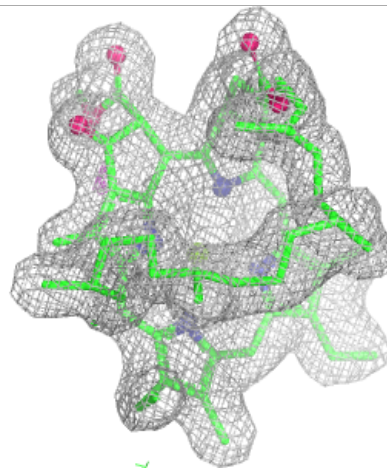
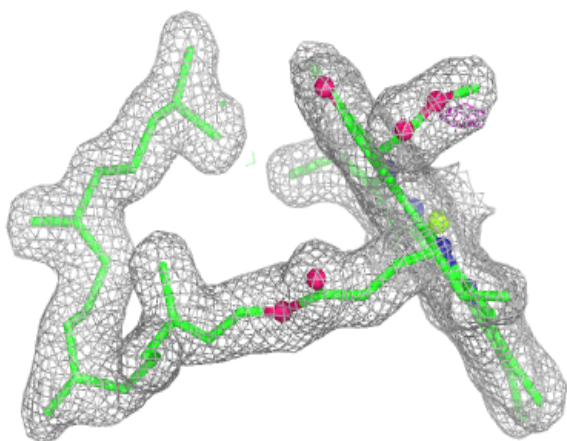
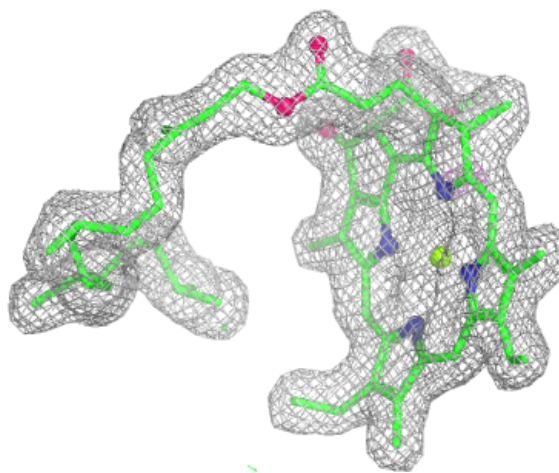
Electron density around BCR B 620:

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



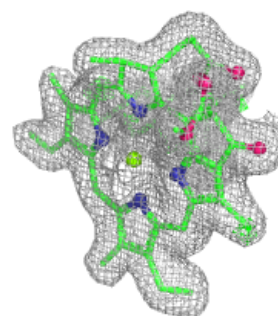
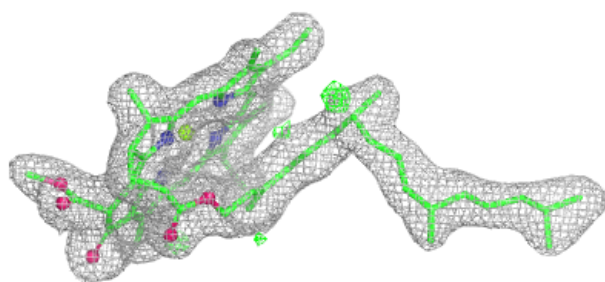
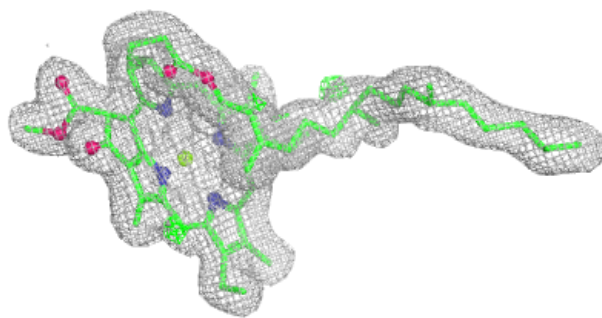
Electron density around CLA C 504:

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

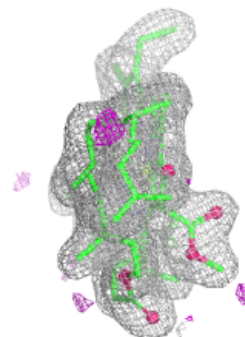
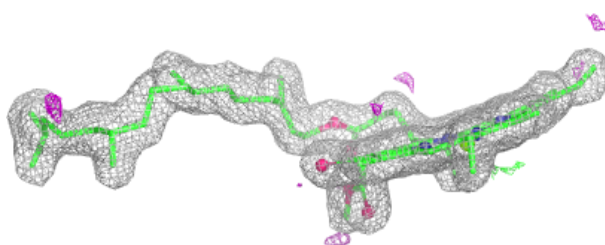
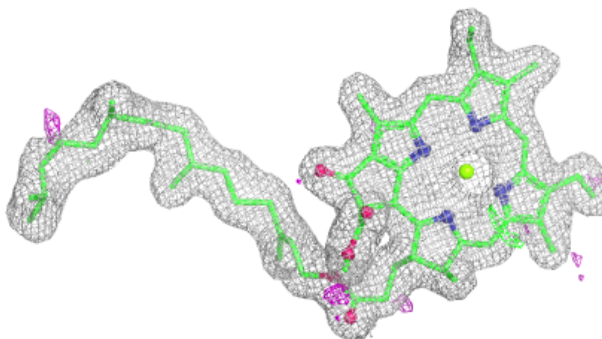


Electron density around CLA C 506:

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

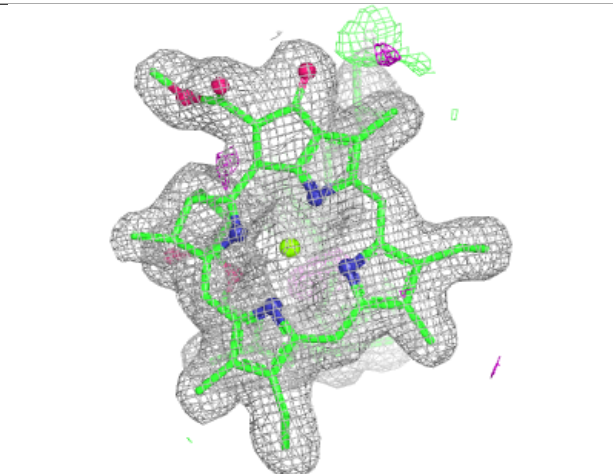
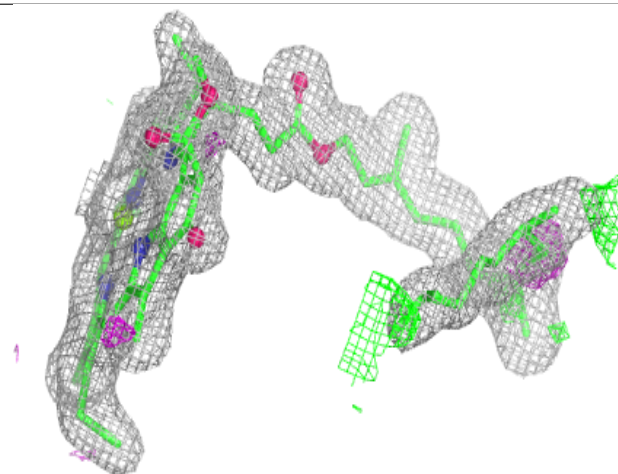
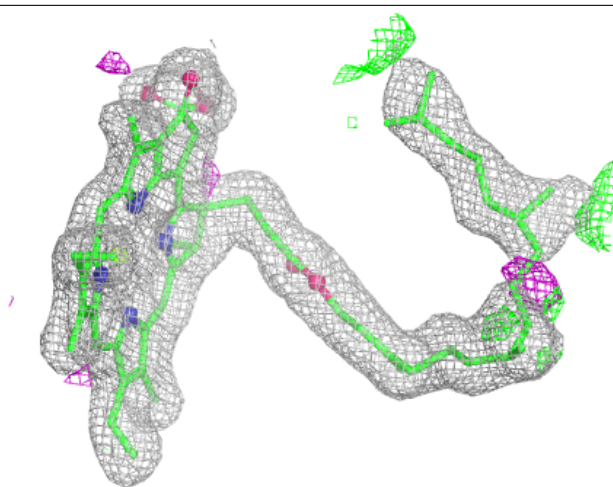
**Electron density around CLA b 603:**

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



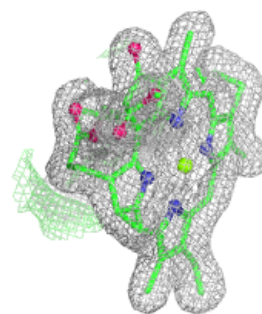
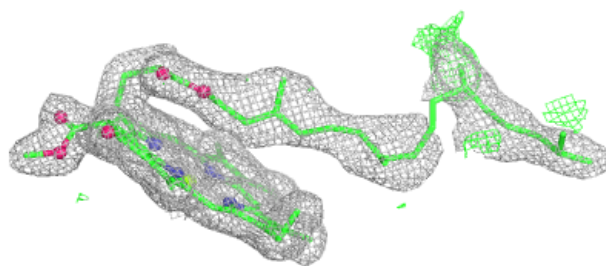
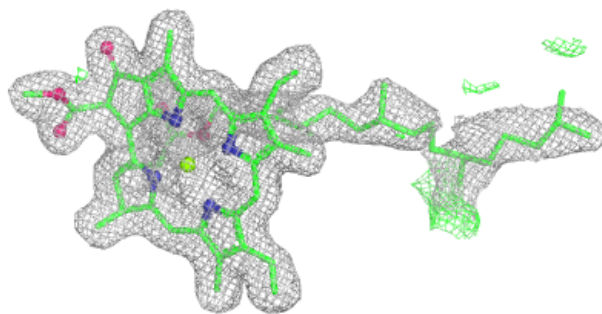
Electron density around CLA b 607:

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



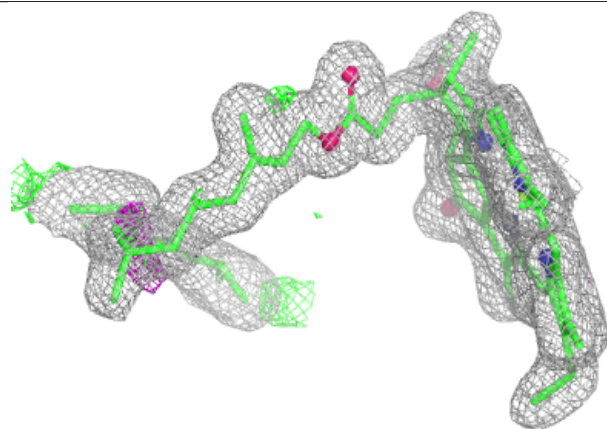
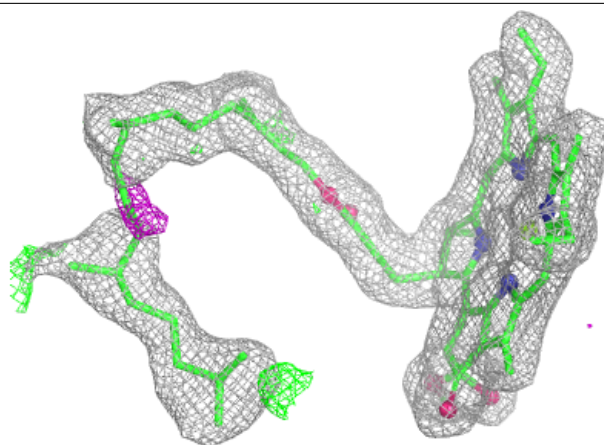
Electron density around CLA b 615:

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

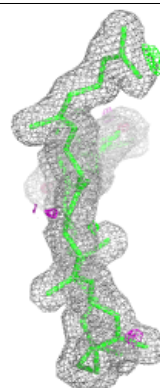
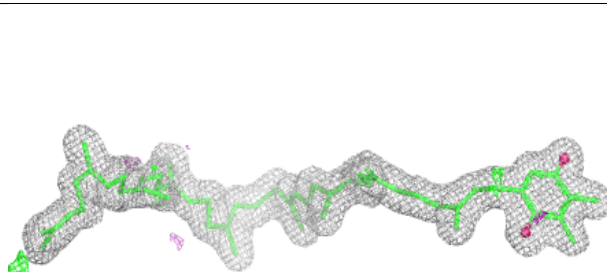
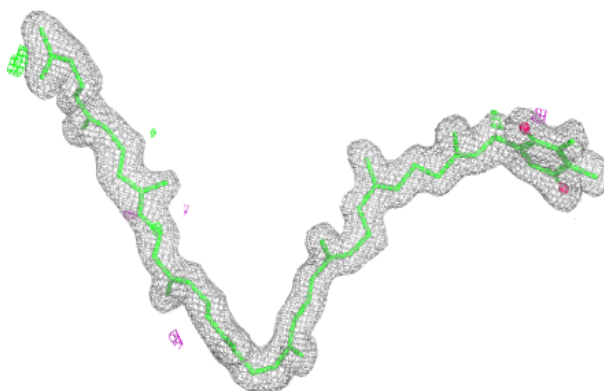


Electron density around CLA B 607:

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

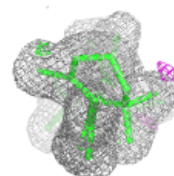
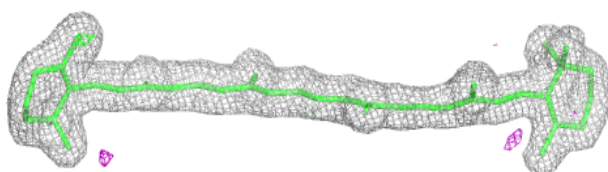
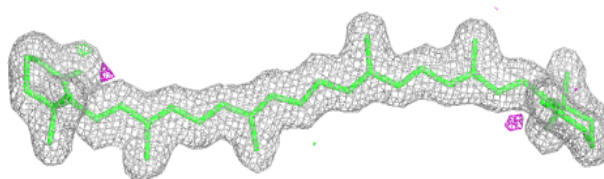
**Electron density around PL9 D 406:**

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

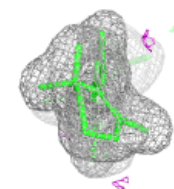
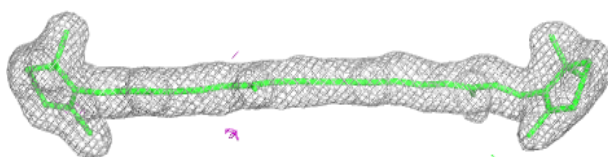
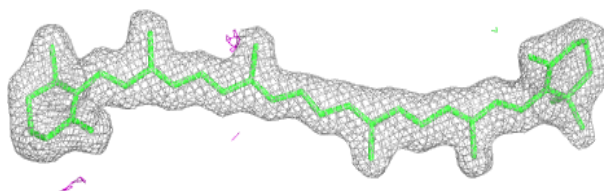


Electron density around BCR a 411:

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

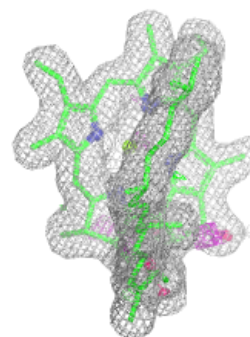
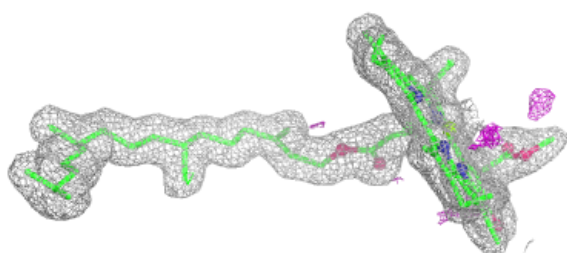
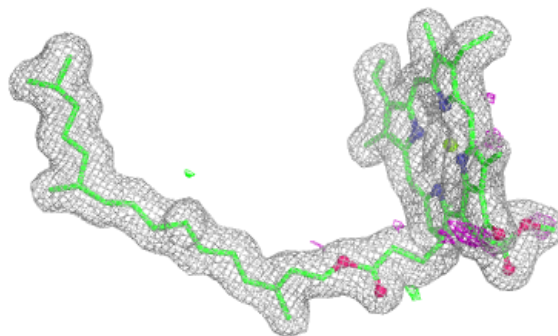
**Electron density around BCR b 619:**

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

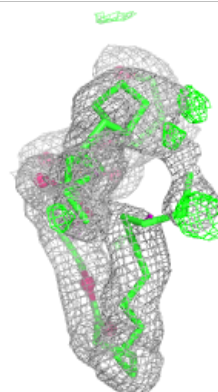
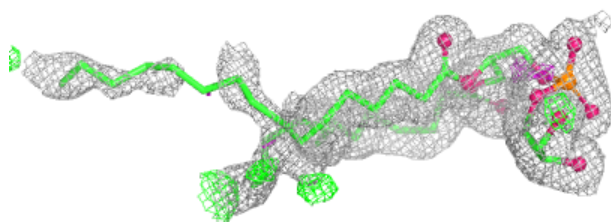
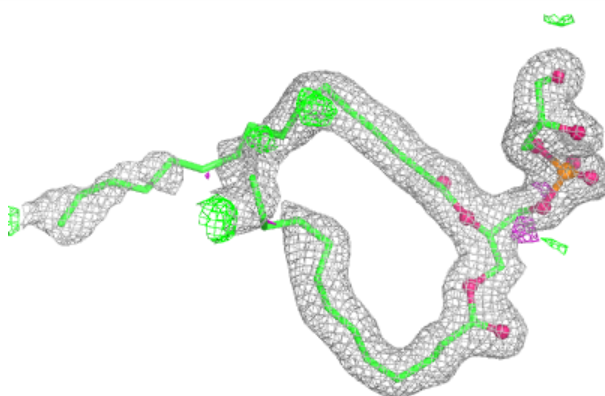


Electron density around CLA B 610:

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

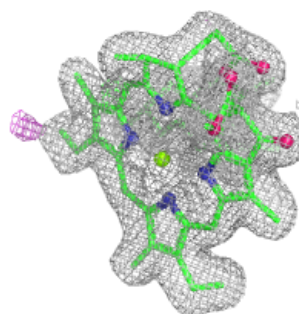
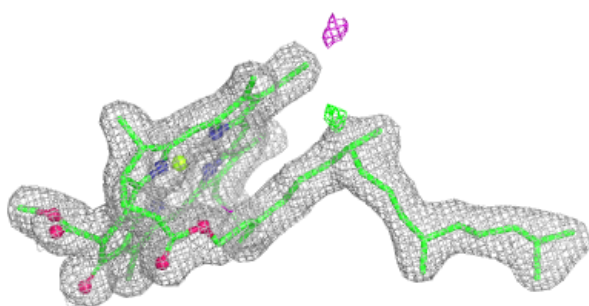
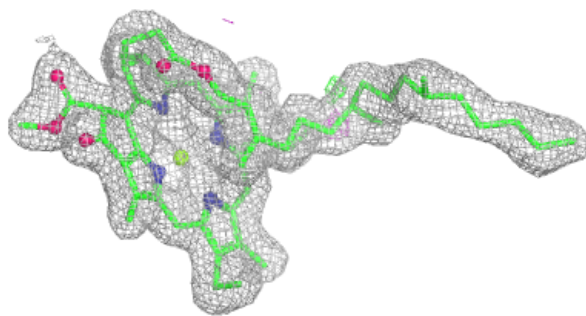
**Electron density around LHG D 411:**

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

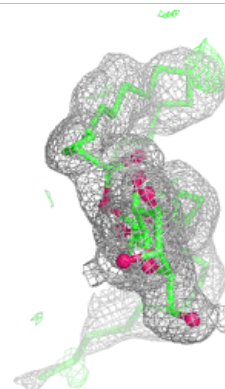
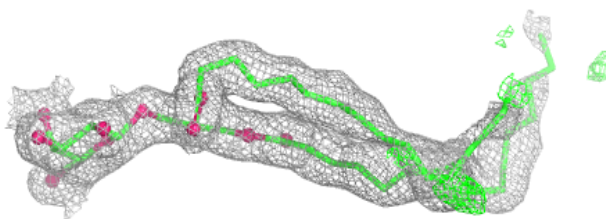
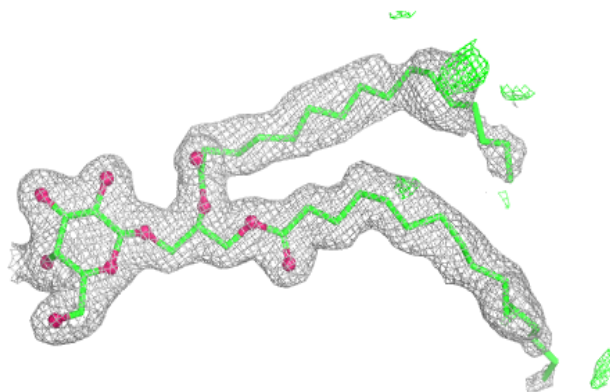


Electron density around CLA c 906:

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

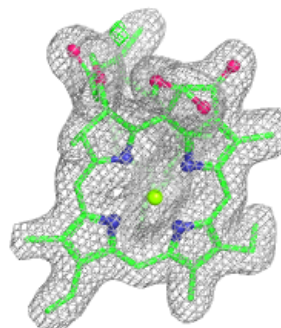
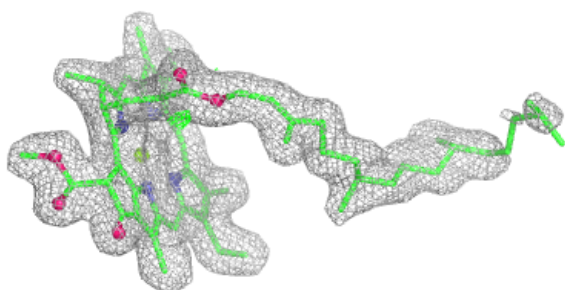
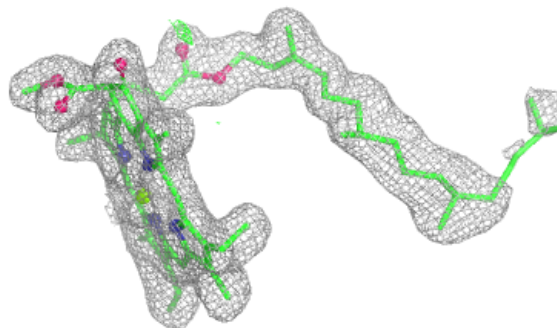
**Electron density around LMG j 101:**

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



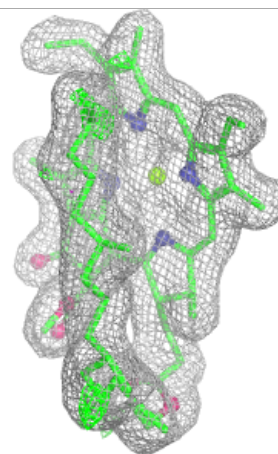
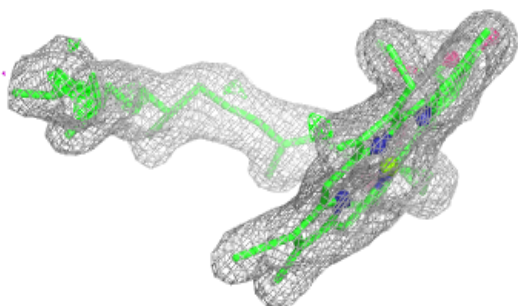
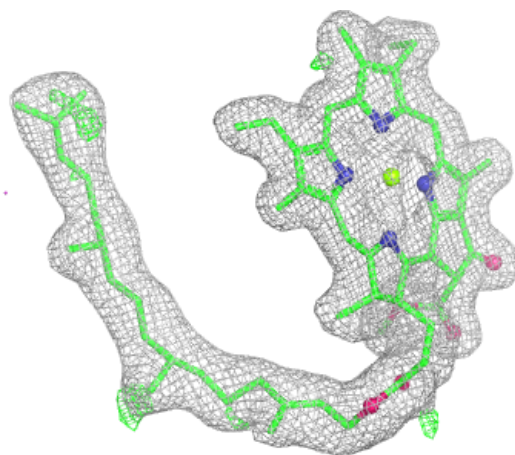
Electron density around CLA C 509:

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



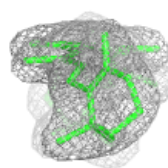
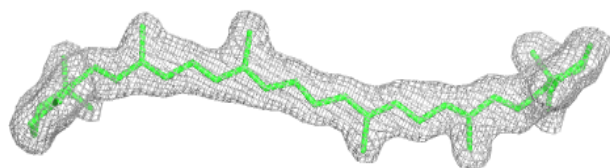
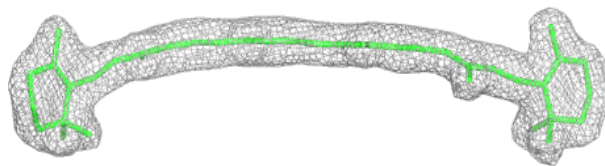
Electron density around CLA c 908:

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

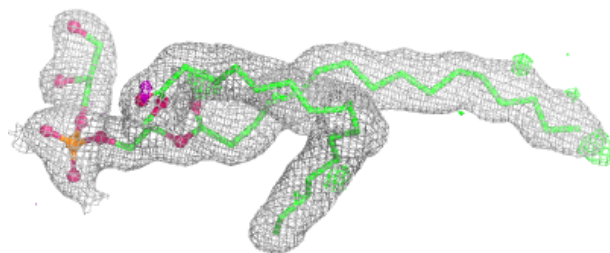
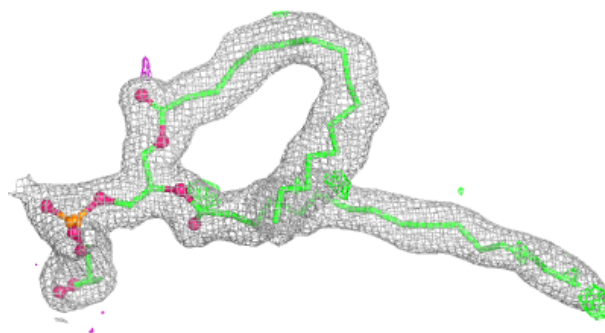


Electron density around BCR k 102:

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

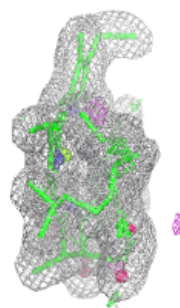
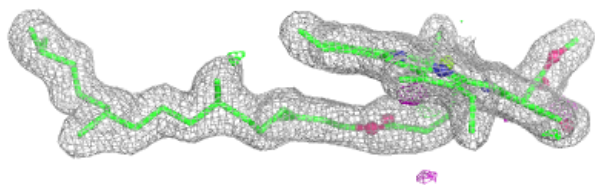
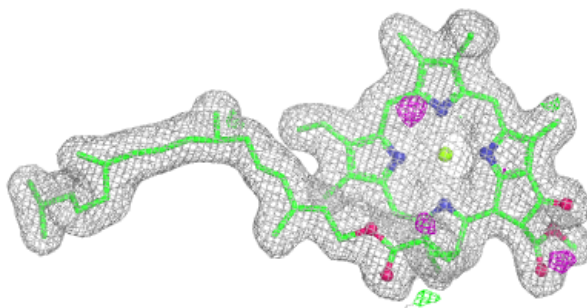
**Electron density around LHG d 408:**

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



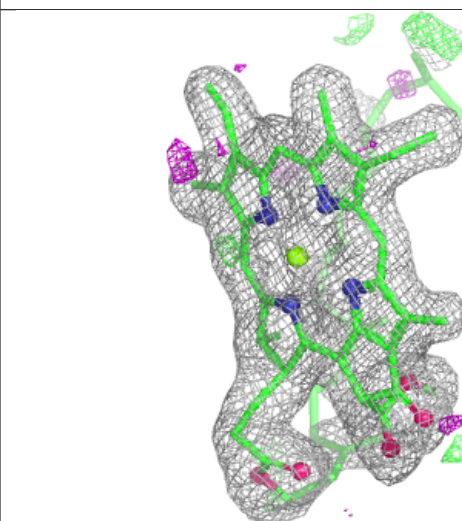
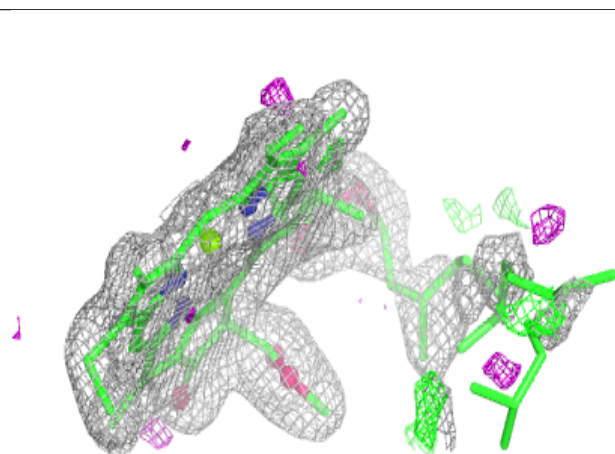
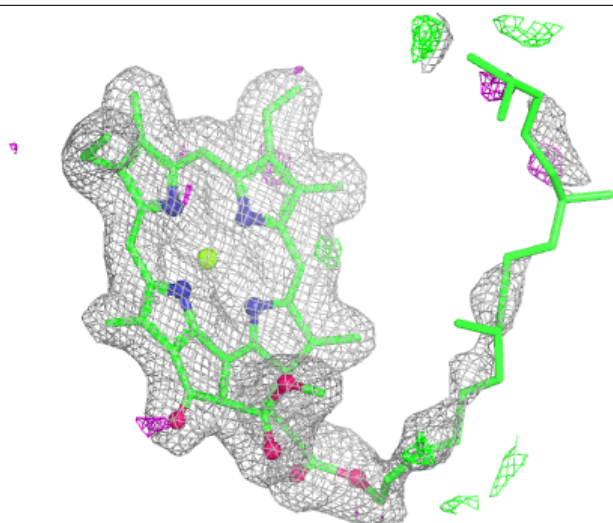
Electron density around CLA b 604:

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



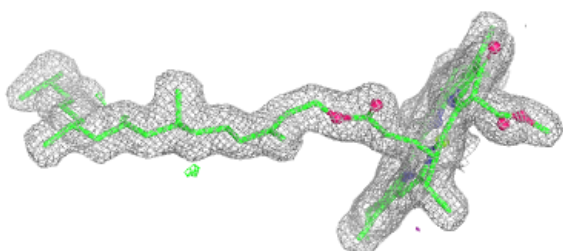
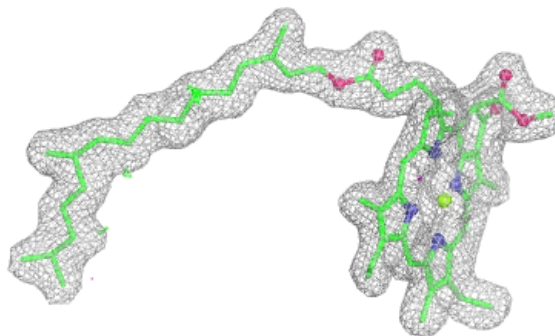
Electron density around CLA B 617:

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

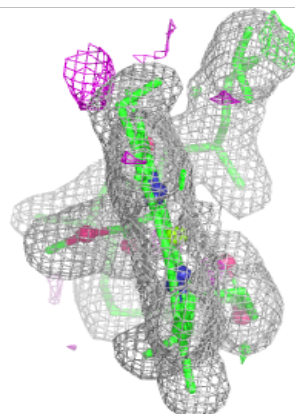
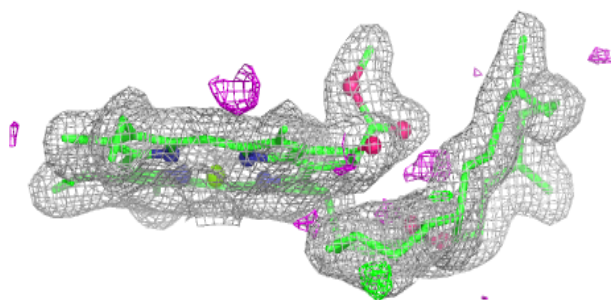
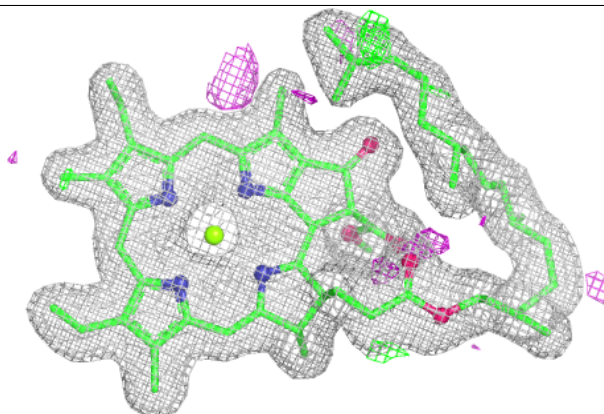


Electron density around CLA b 610:

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

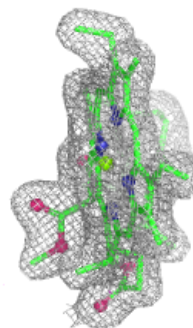
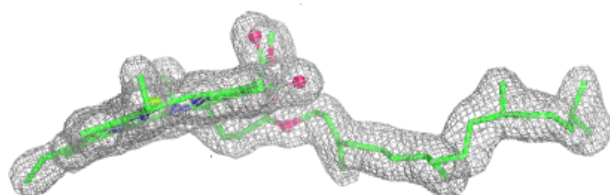
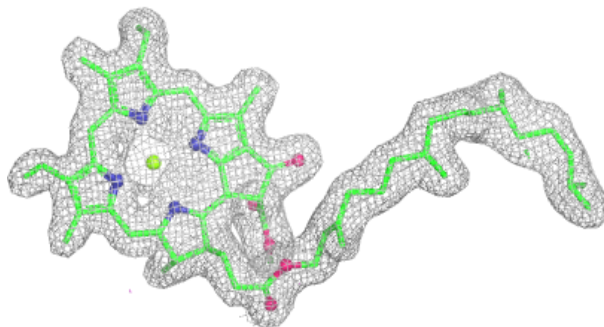
**Electron density around CLA b 611:**

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



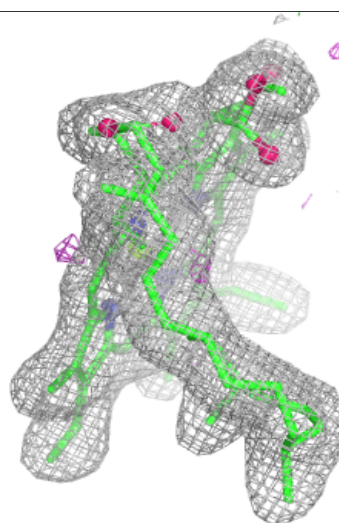
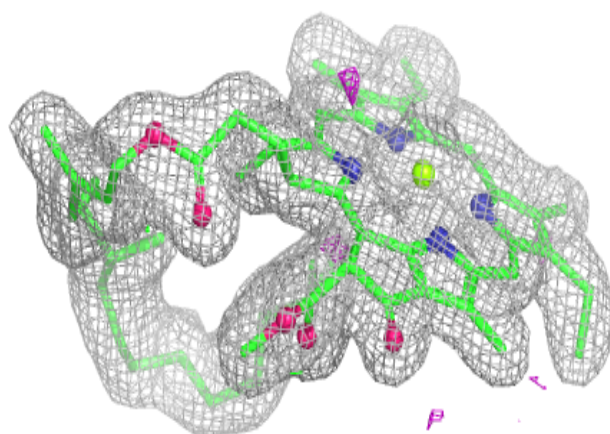
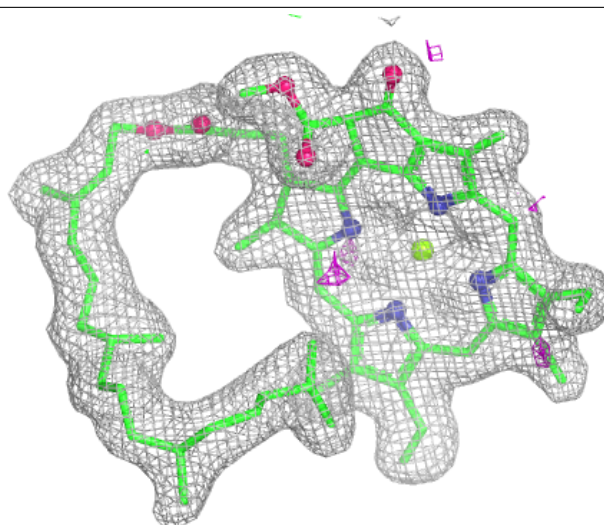
Electron density around CLA B 603:

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



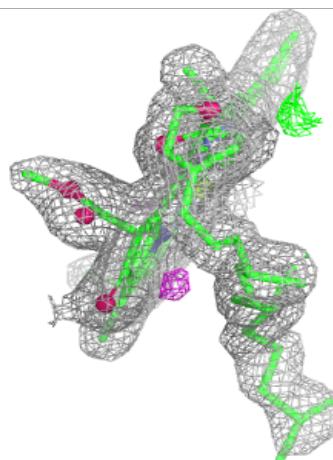
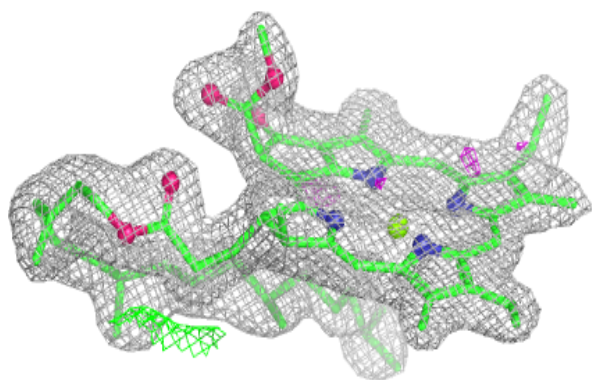
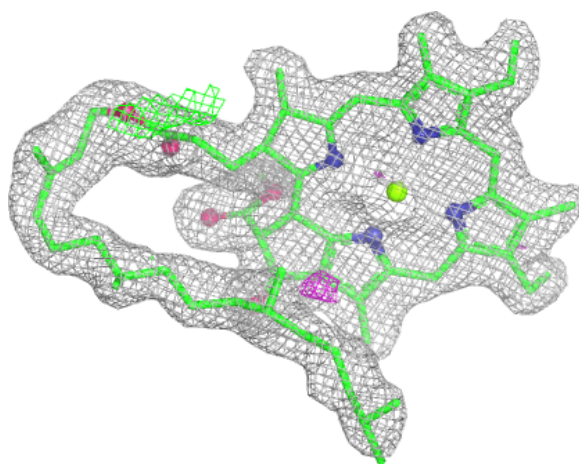
Electron density around CLA b 616:

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



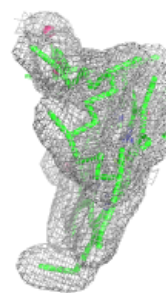
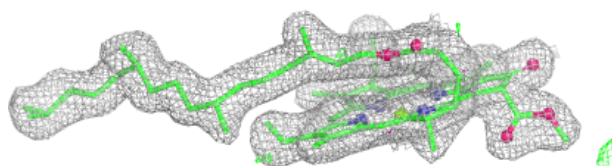
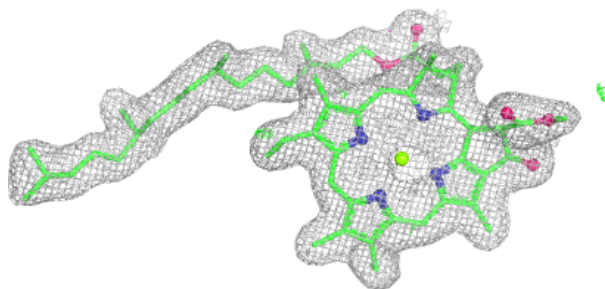
Electron density around CLA C 510:

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



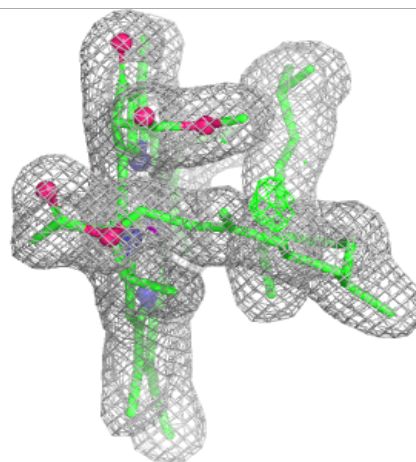
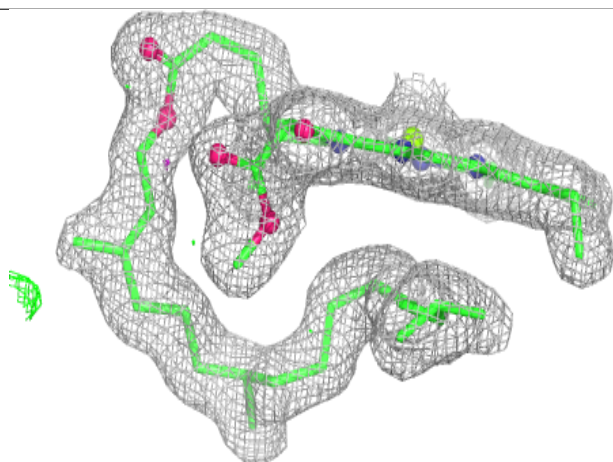
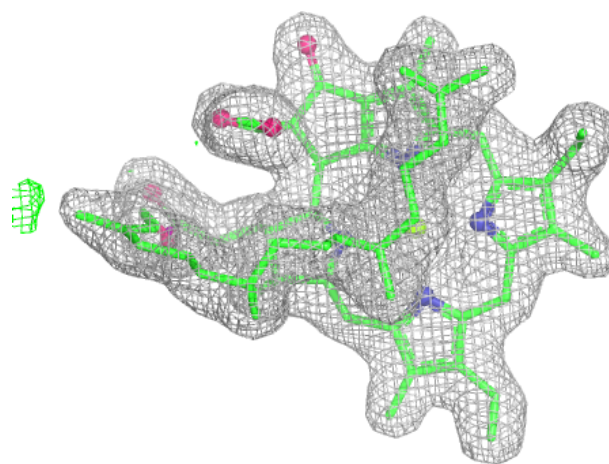
Electron density around CLA c 902:

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



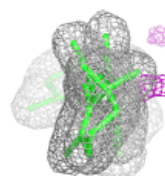
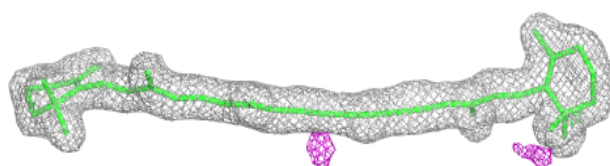
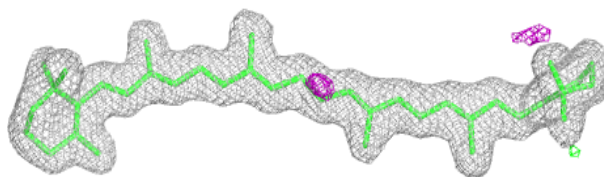
Electron density around CLA C 511:

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



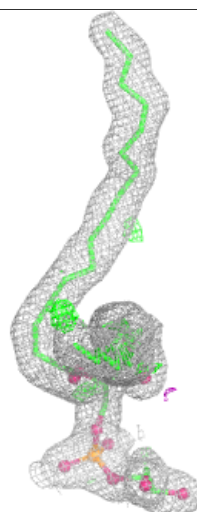
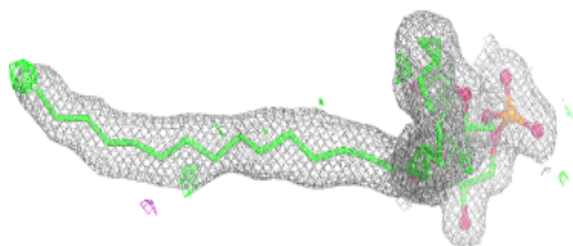
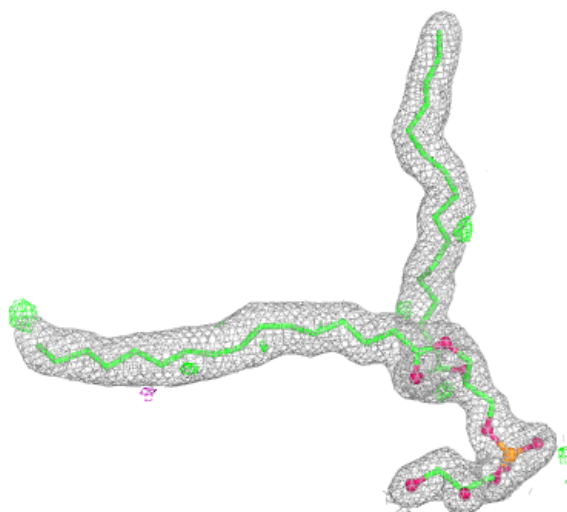
Electron density around BCR b 618:

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



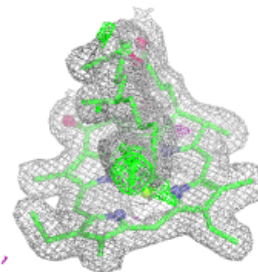
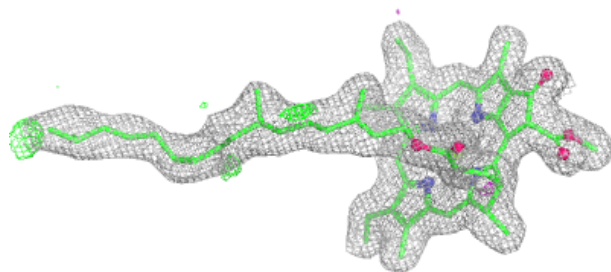
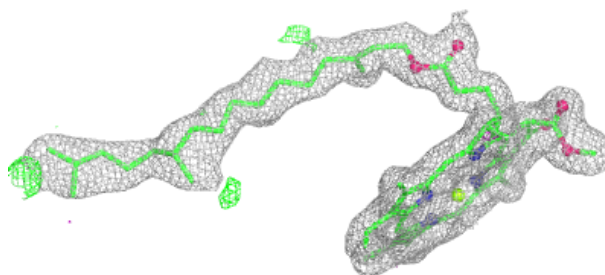
Electron density around LHG L 101:

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

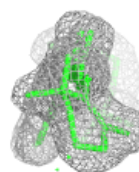
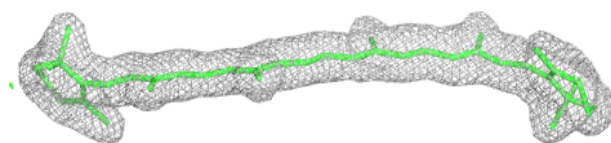
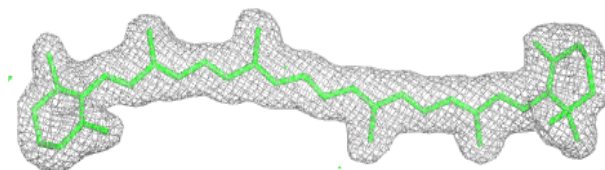


Electron density around CLA c 905:

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

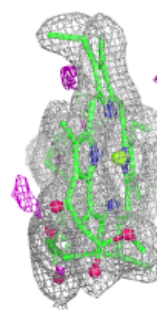
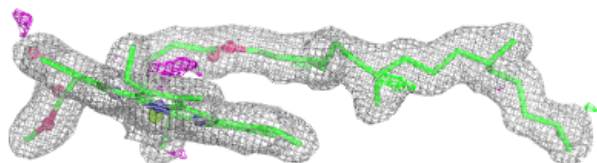
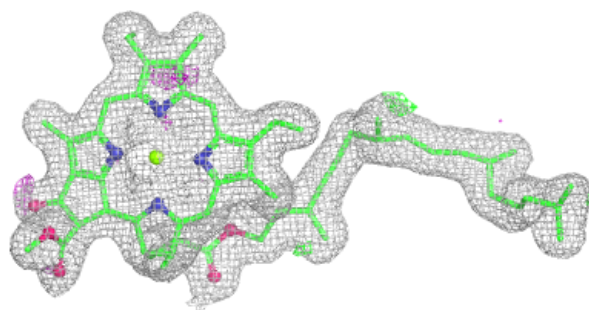
**Electron density around BCR b 620:**

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

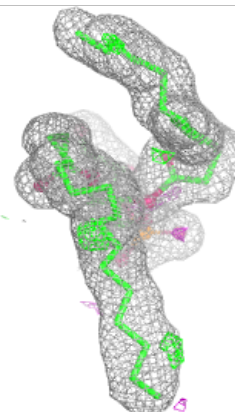
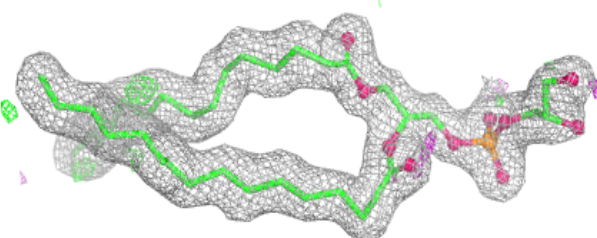
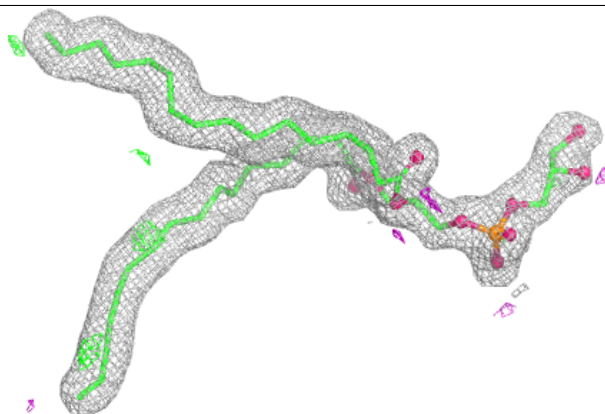


Electron density around CLA B 604:

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

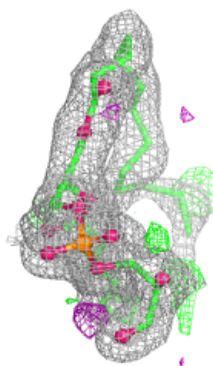
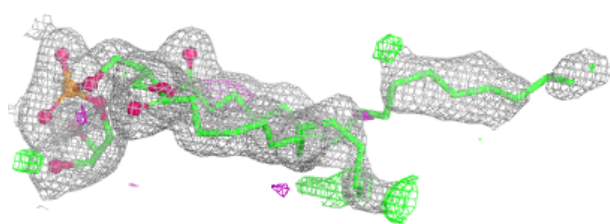
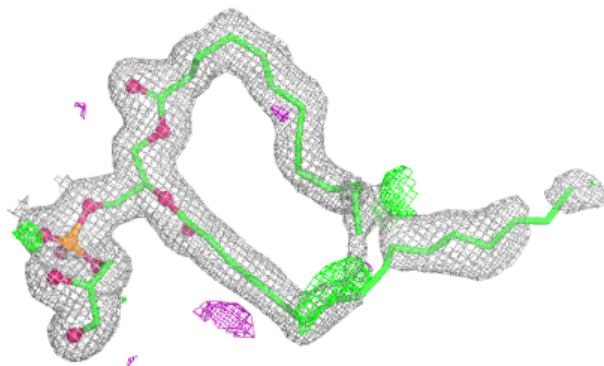
**Electron density around LHG d 409:**

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

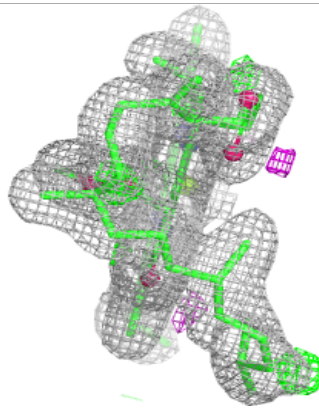
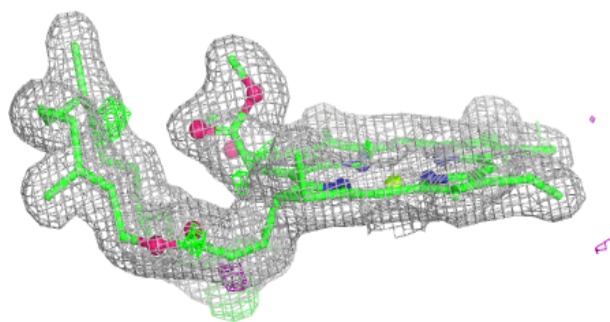
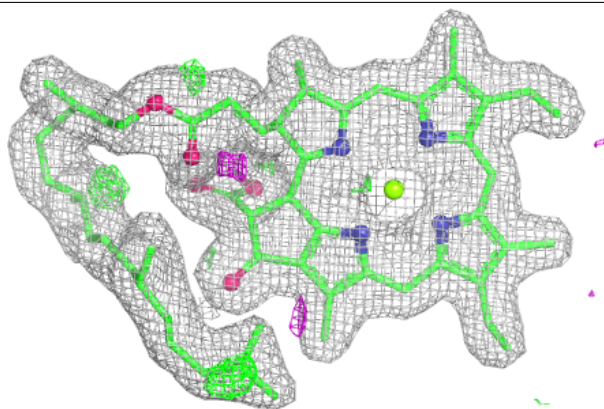


Electron density around LHG d 410:

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

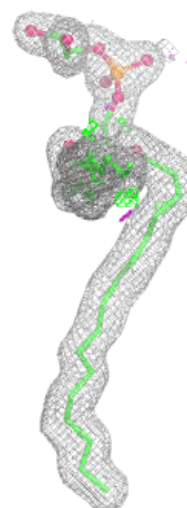
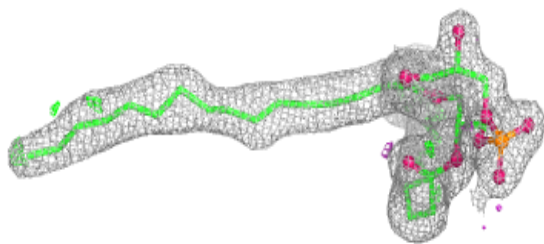
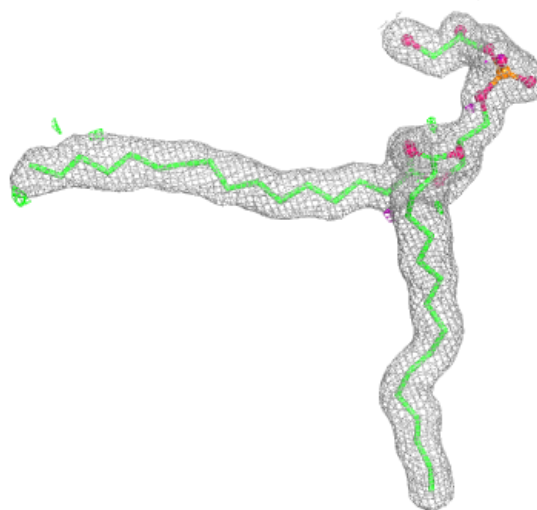
**Electron density around CLA B 611:**

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



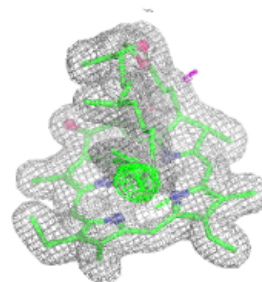
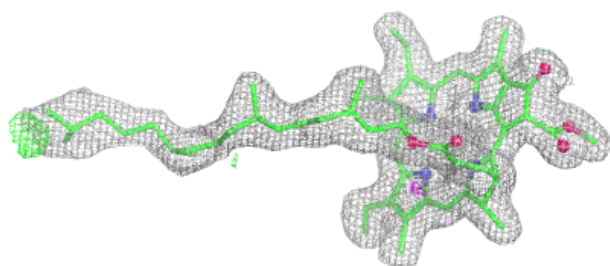
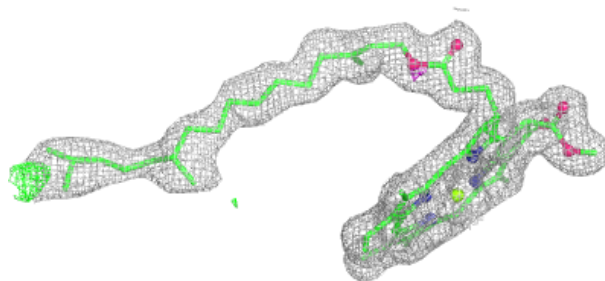
Electron density around LHG 1 101:

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

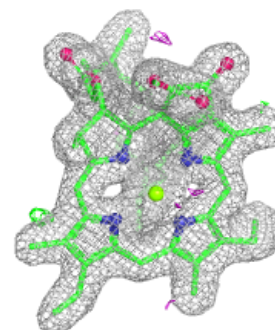
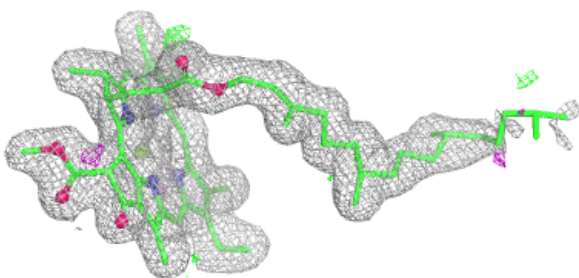
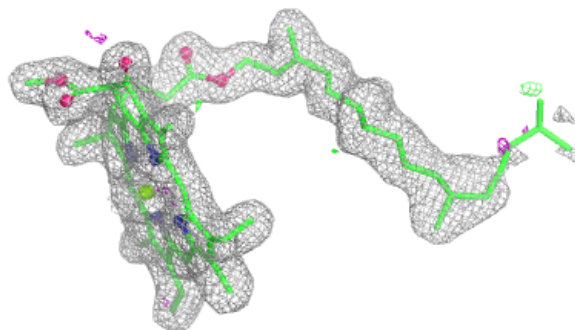


Electron density around CLA C 505:

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

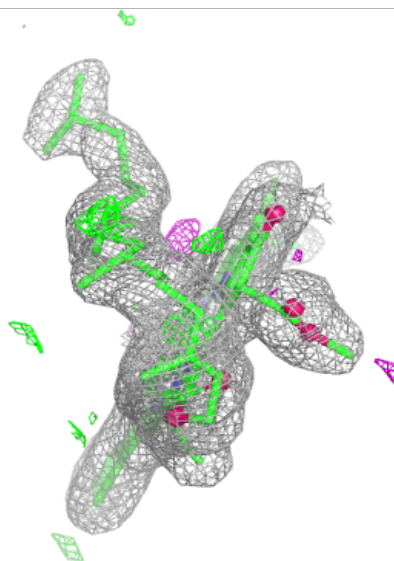
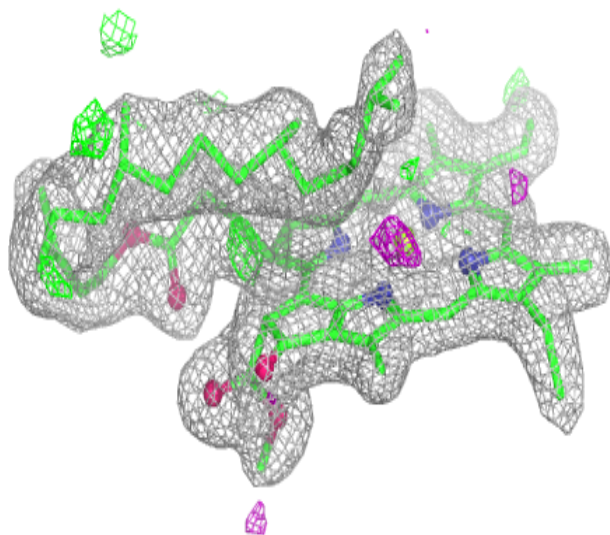
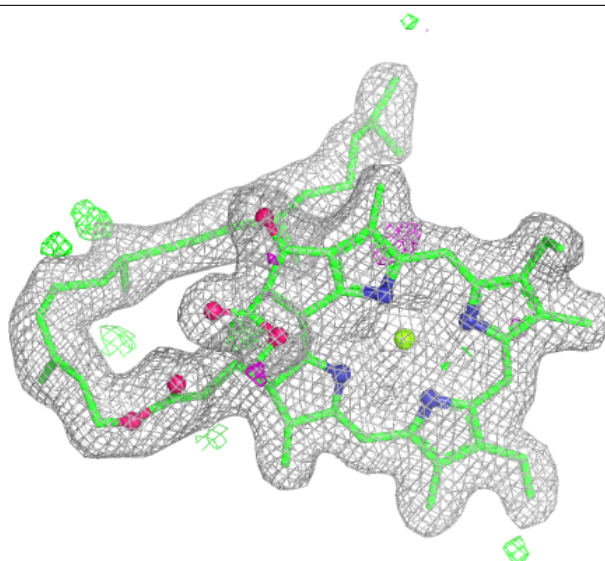
**Electron density around CLA c 909:**

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



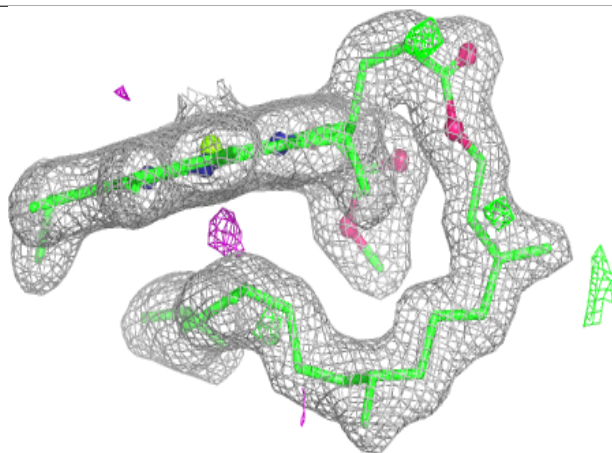
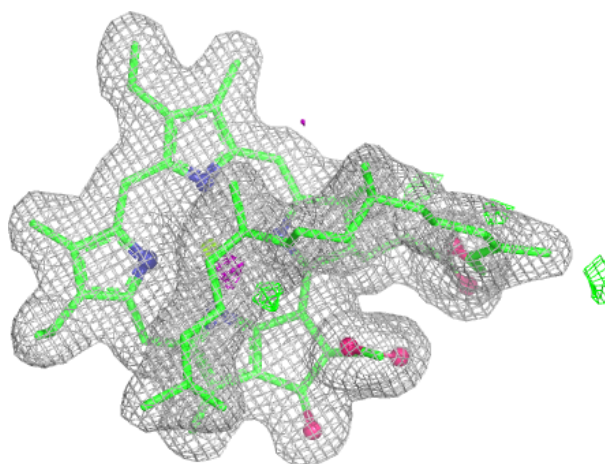
Electron density around CLA c 910:

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



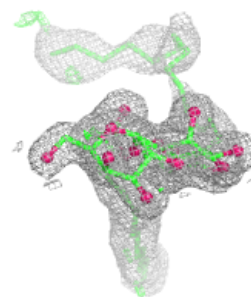
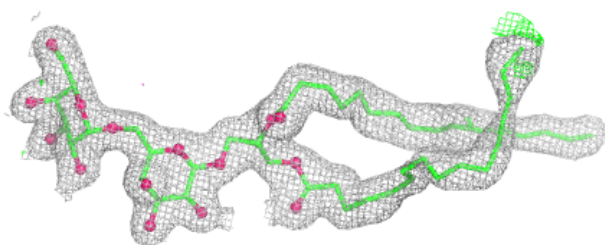
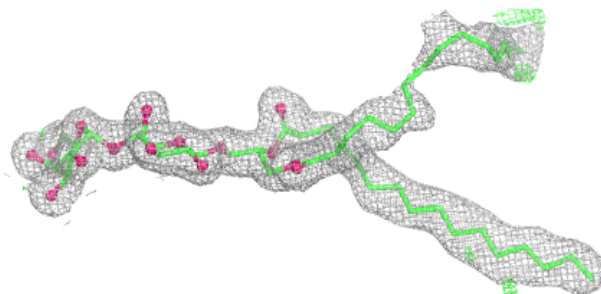
Electron density around CLA c 911:

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

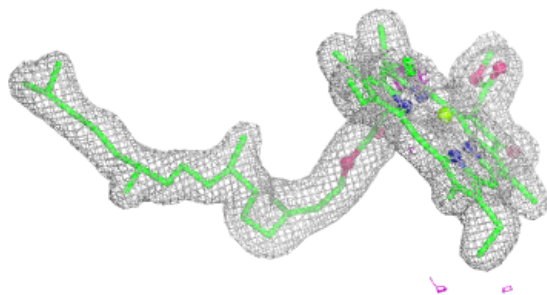
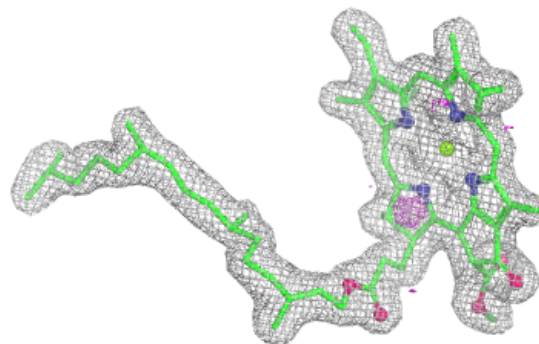


Electron density around DGD C 517:

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

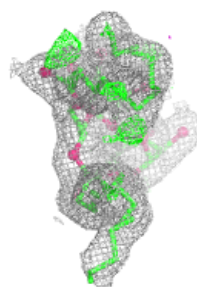
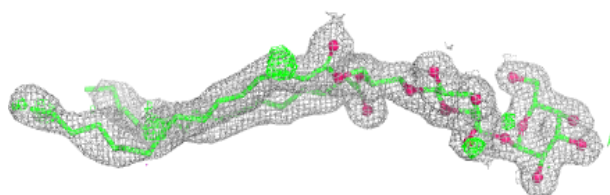
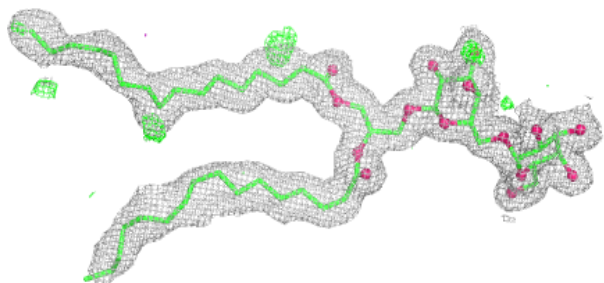
**Electron density around CLA c 912:**

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

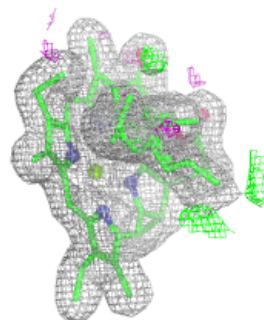
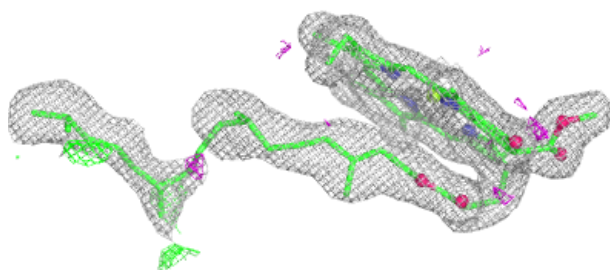
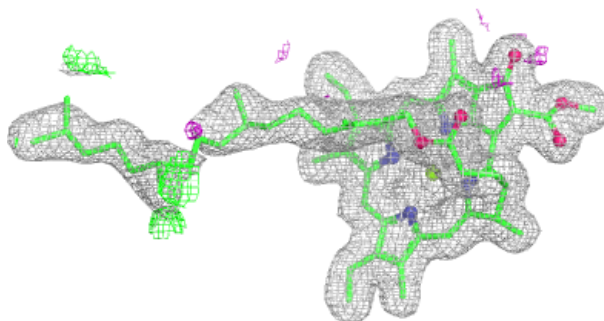


Electron density around DGD C 519:

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

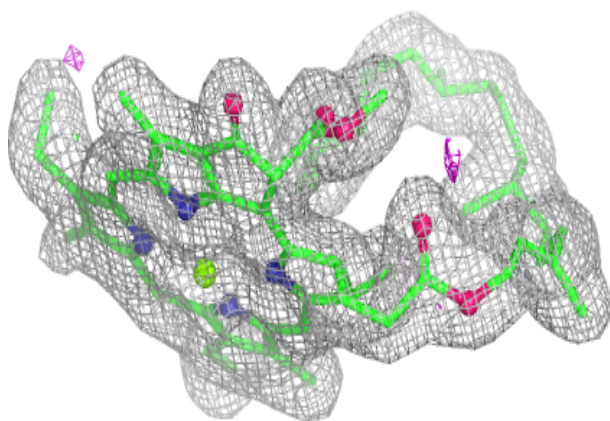
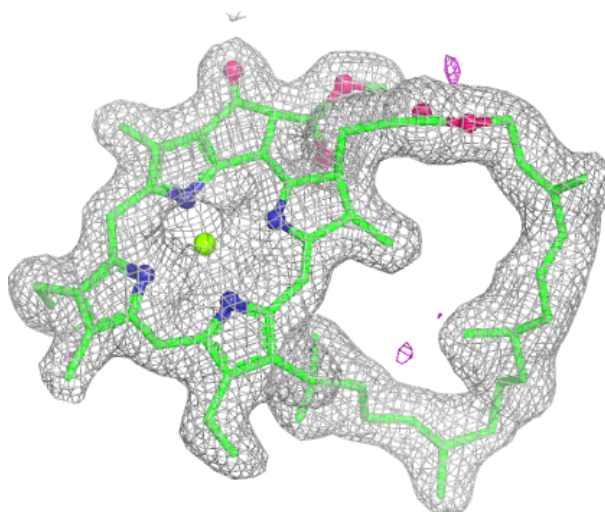
**Electron density around CLA B 615:**

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



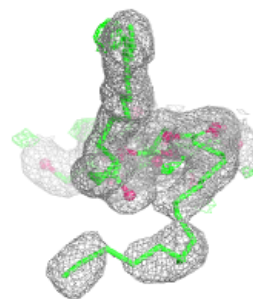
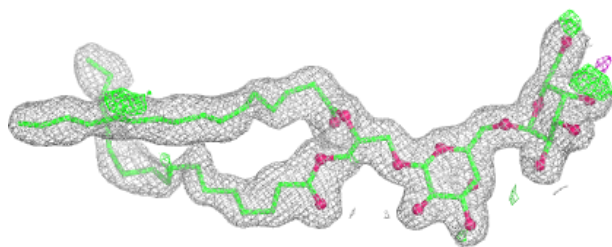
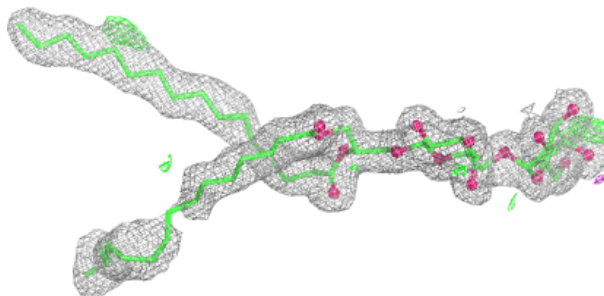
Electron density around CLA B 616:

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

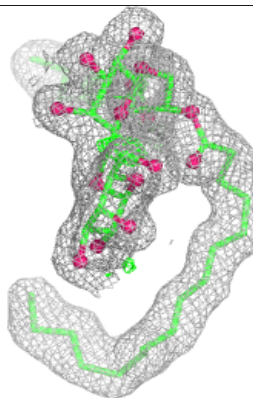
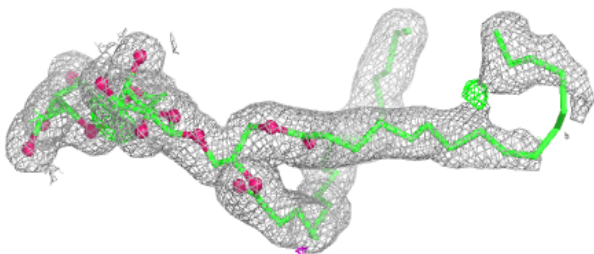
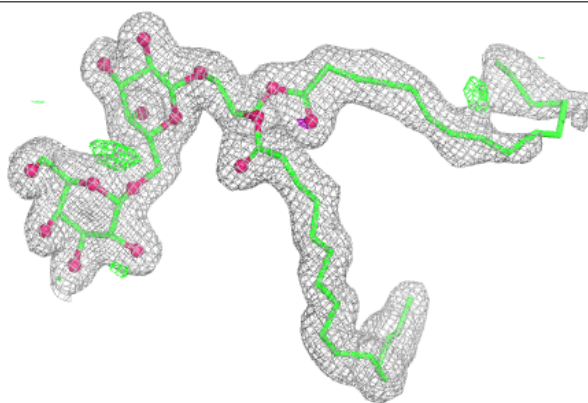


Electron density around DGD c 917:

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

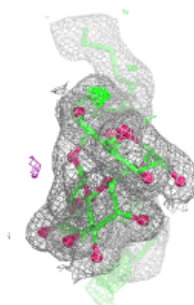
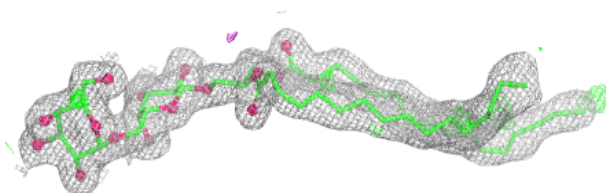
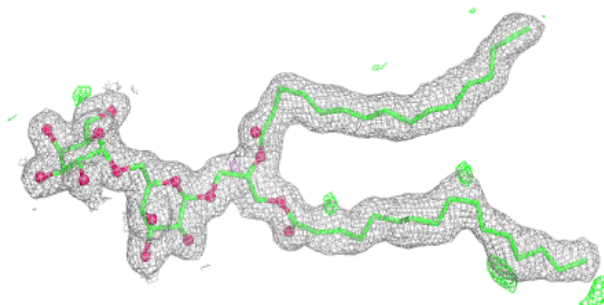
**Electron density around DGD c 918:**

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

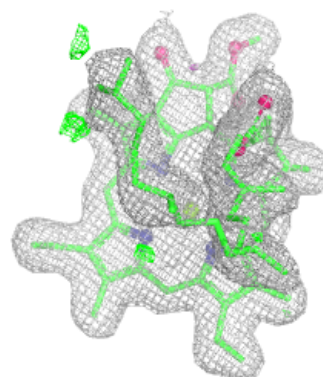
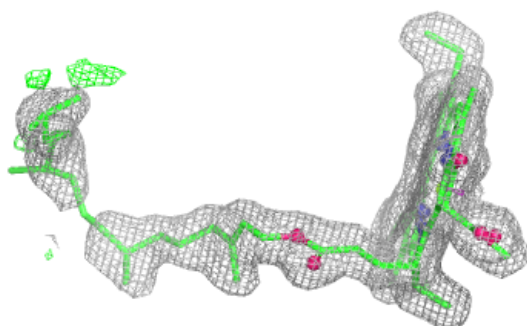
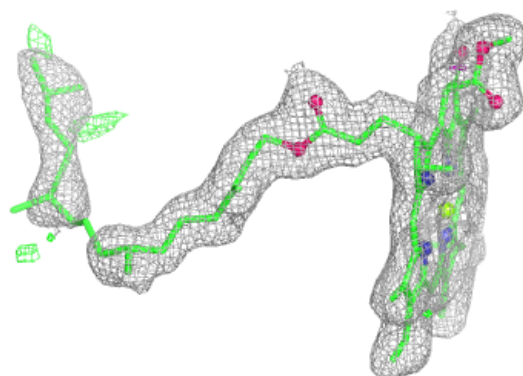


Electron density around DGD c 919:

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

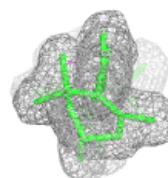
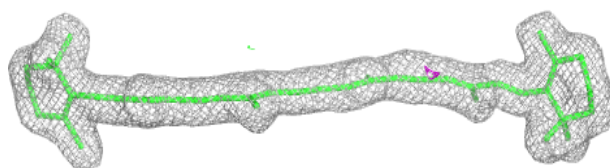
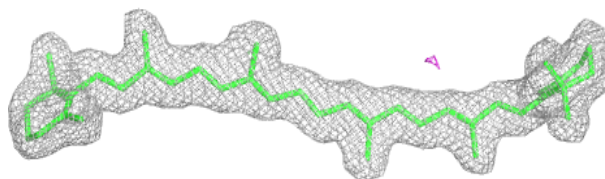
**Electron density around CLA d 404:**

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

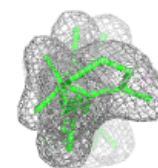
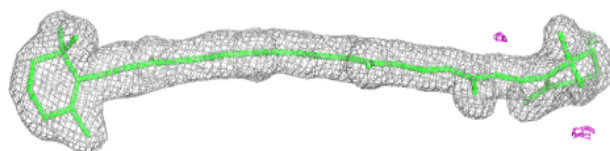
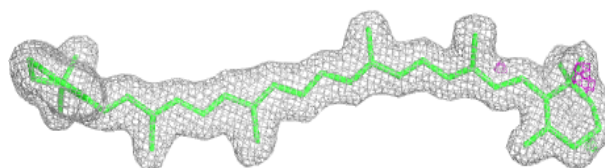


Electron density around BCR A 409:

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

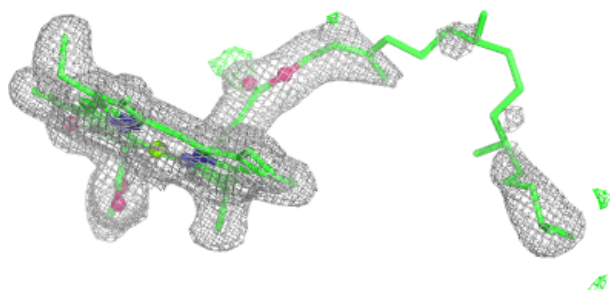
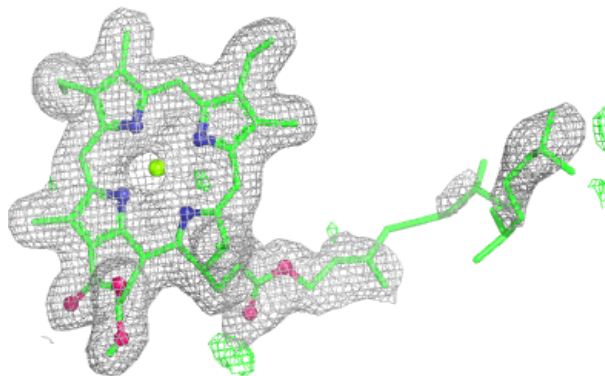
**Electron density around BCR B 618:**

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

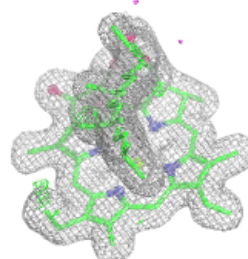
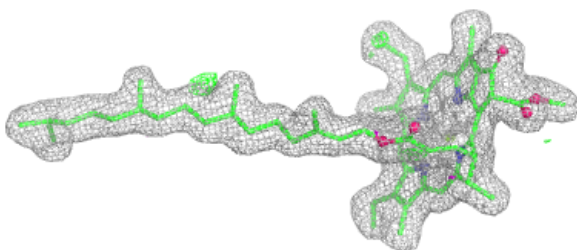
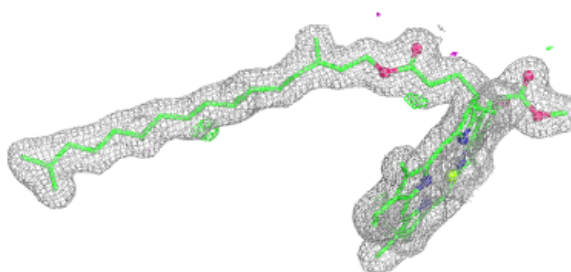


Electron density around CLA A 408:

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

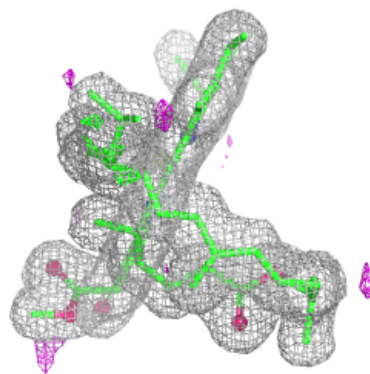
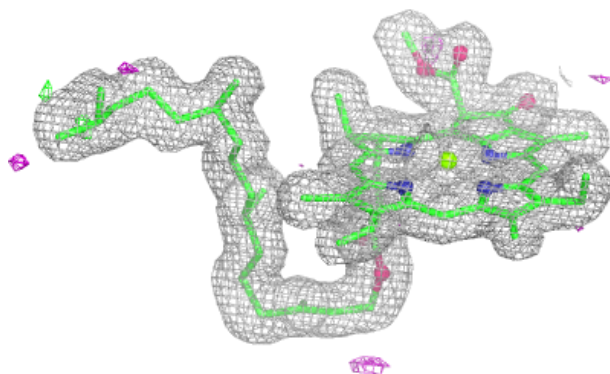
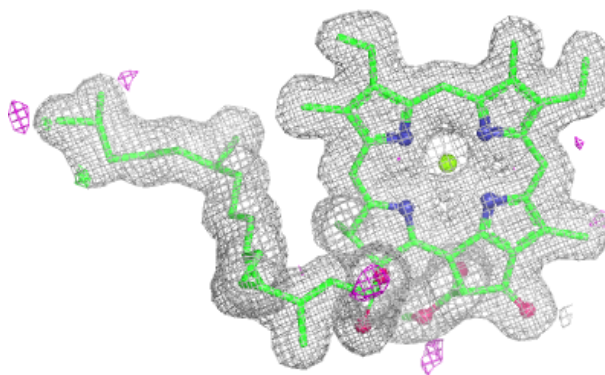
**Electron density around CLA b 608:**

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

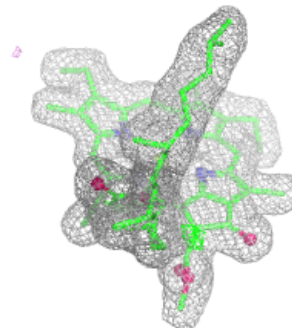
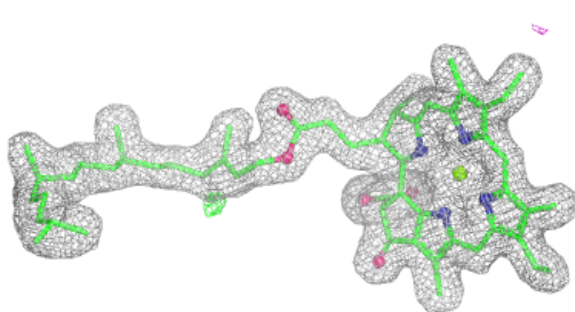
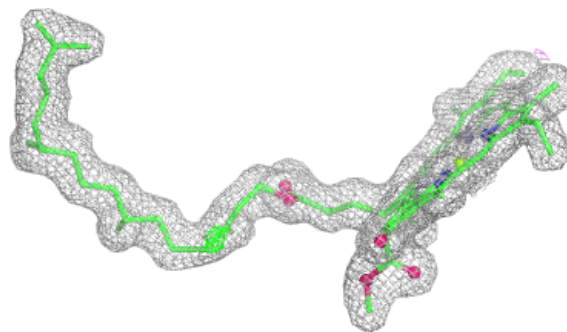


Electron density around CLA d 401:

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

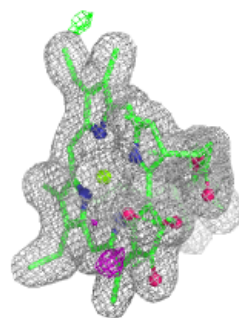
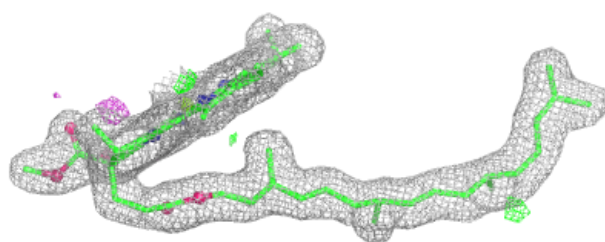
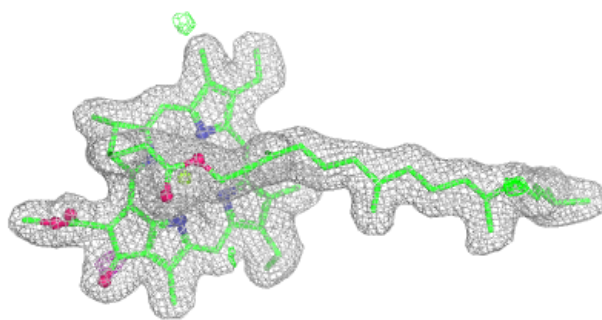
**Electron density around CLA d 403:**

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



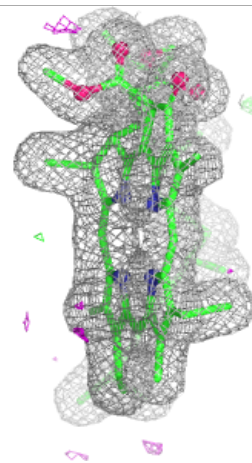
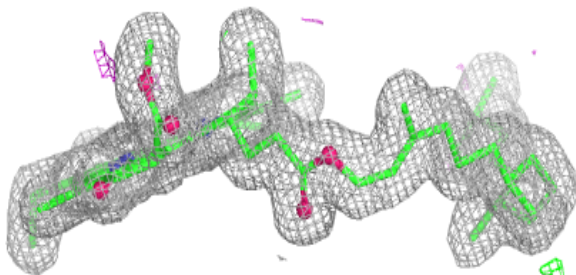
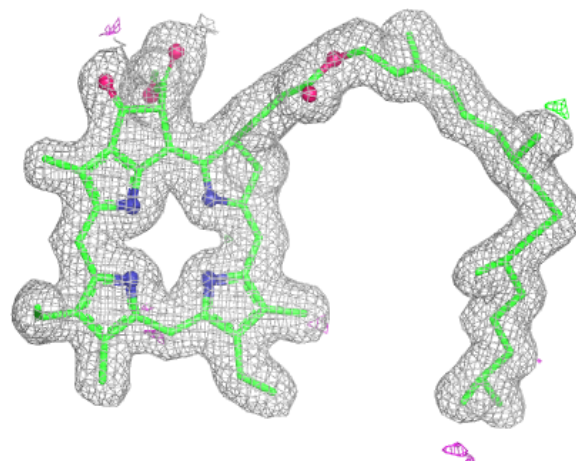
Electron density around CLA b 609:

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



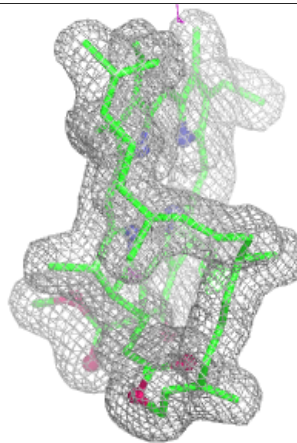
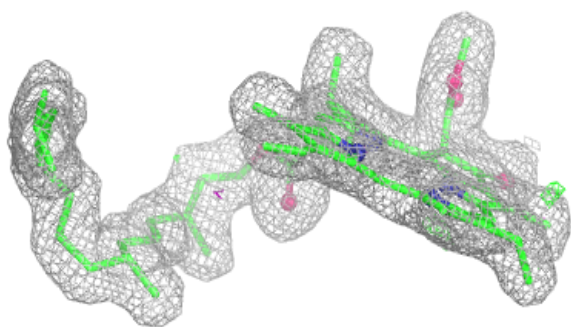
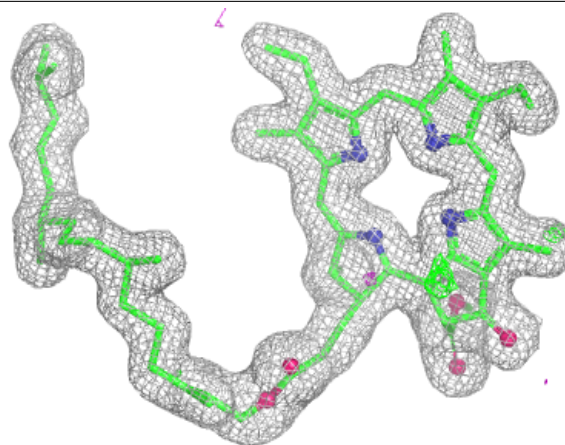
Electron density around PHO A 407:

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



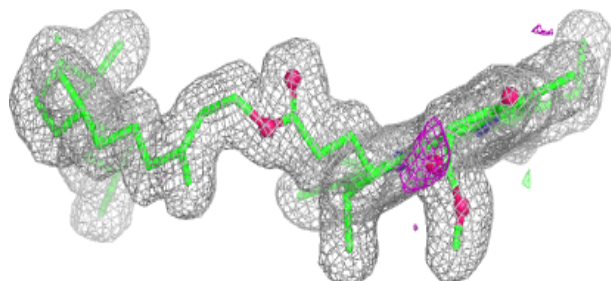
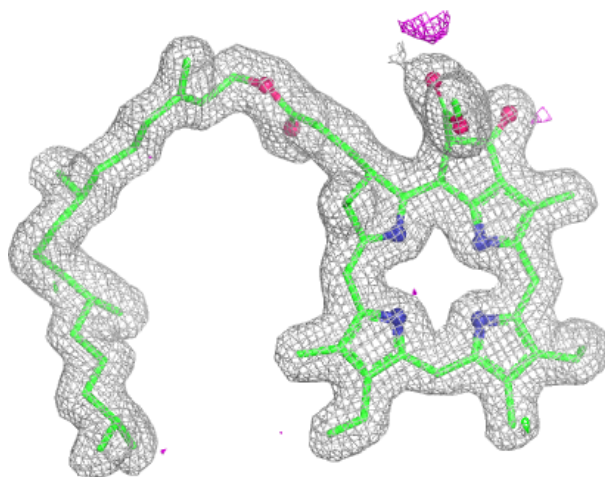
Electron density around PHO D 402:

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



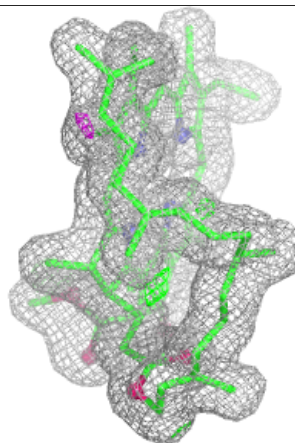
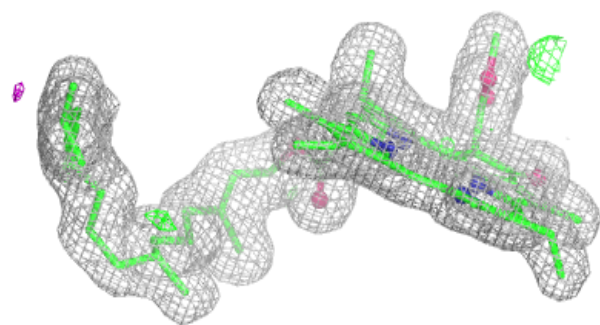
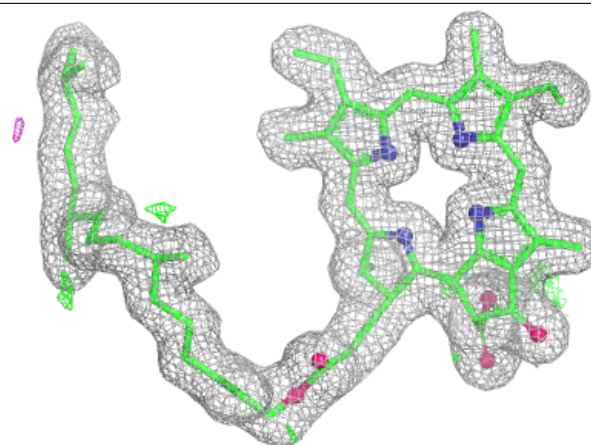
Electron density around PHO a 408:

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



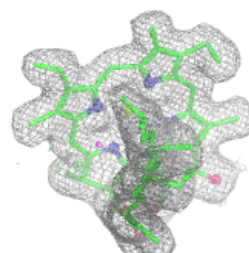
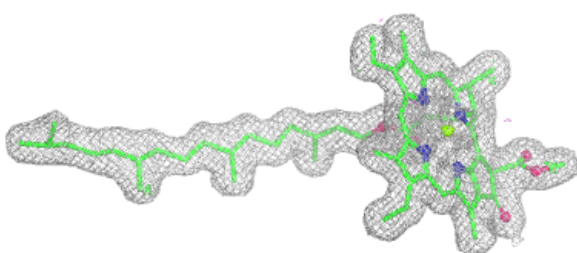
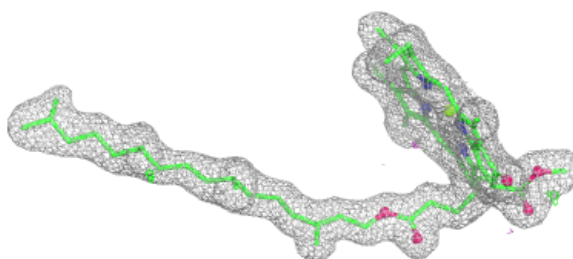
Electron density around PHO a 409:

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

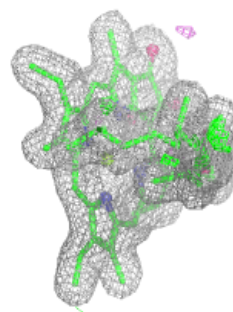
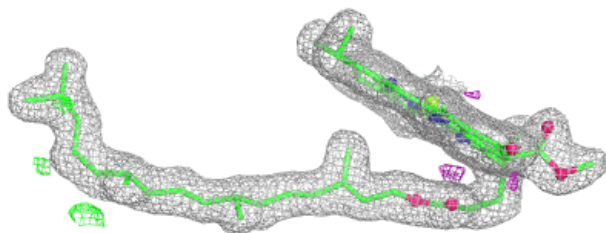
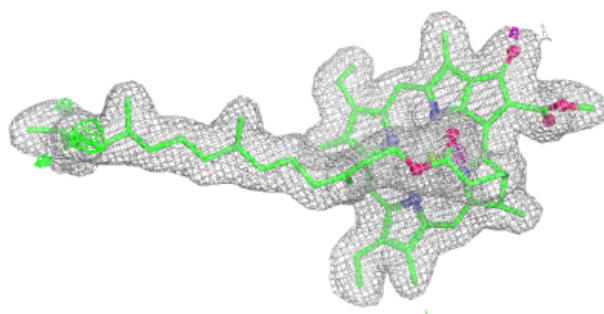


Electron density around CLA B 608:

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

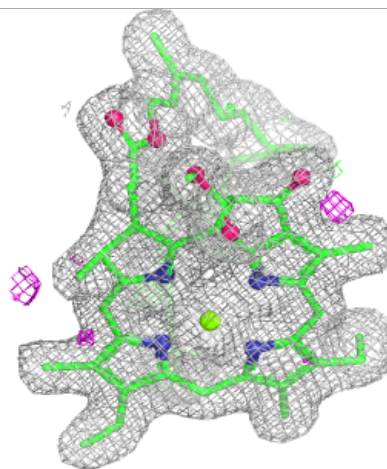
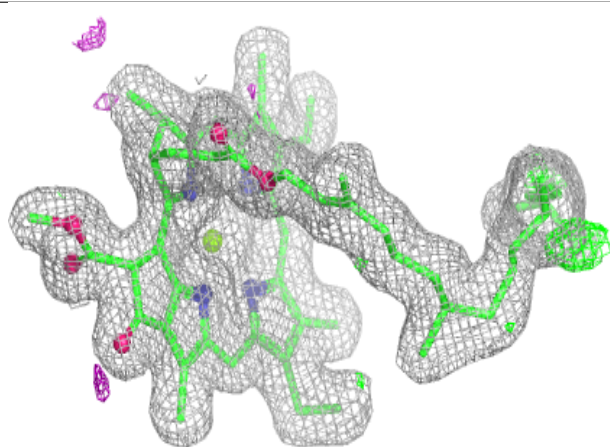
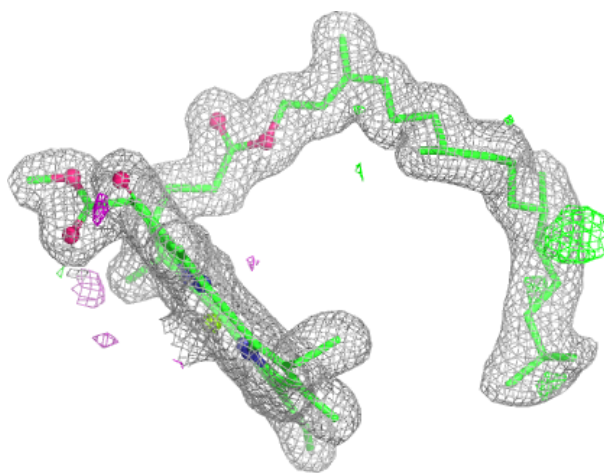
**Electron density around CLA B 609:**

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



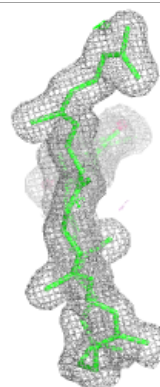
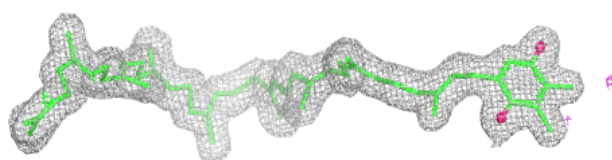
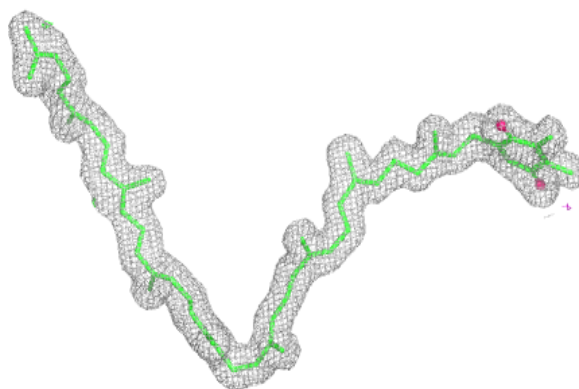
Electron density around CLA b 612:

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

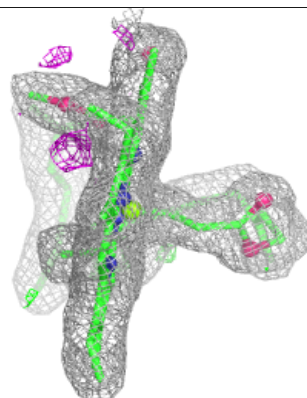
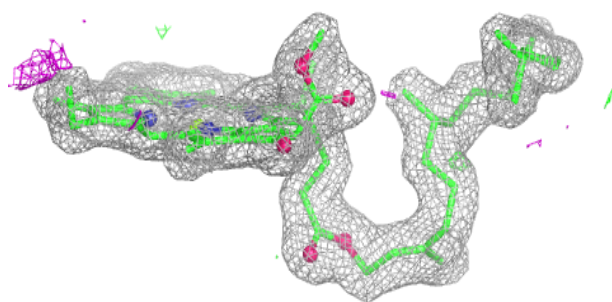
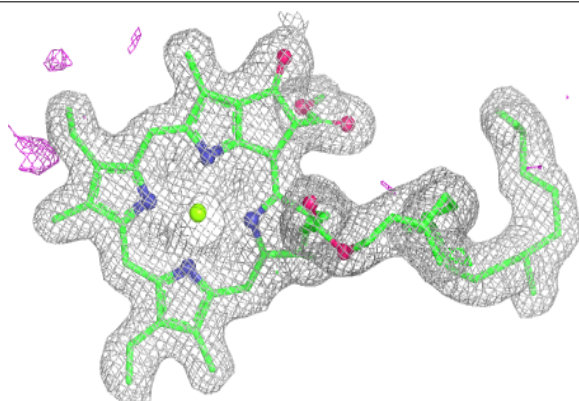


Electron density around PL9 d 406:

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

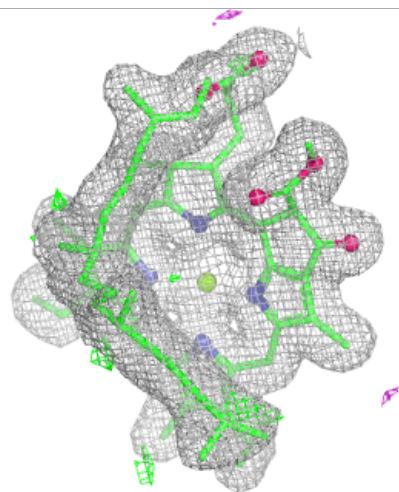
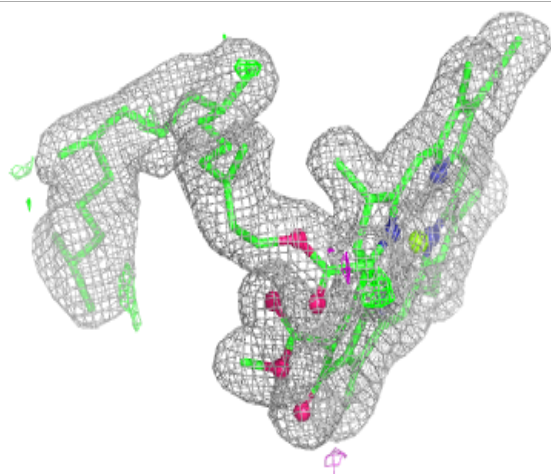
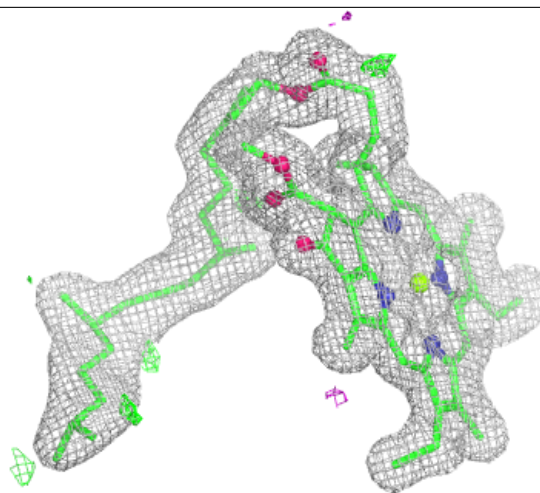
**Electron density around CLA b 613:**

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



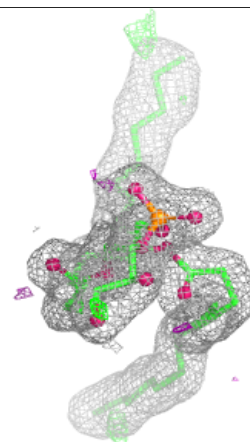
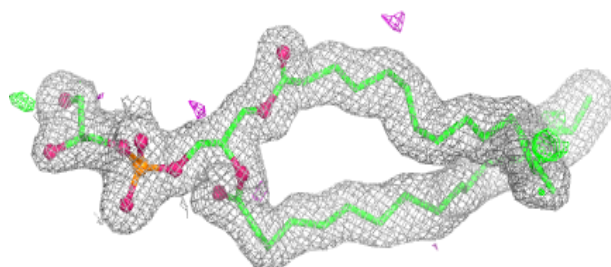
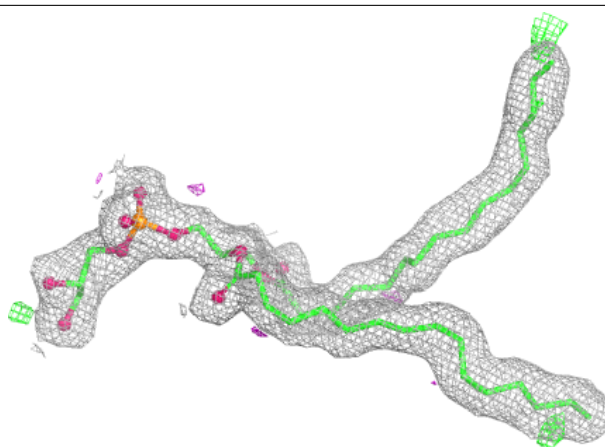
Electron density around CLA b 614:

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



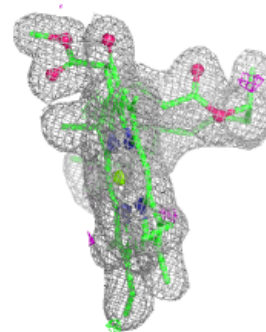
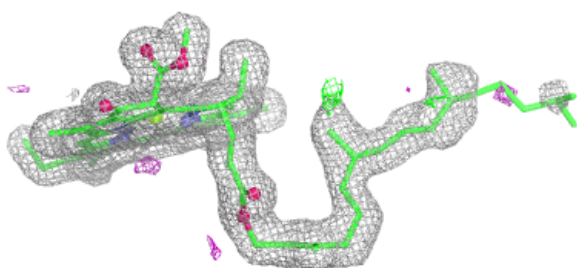
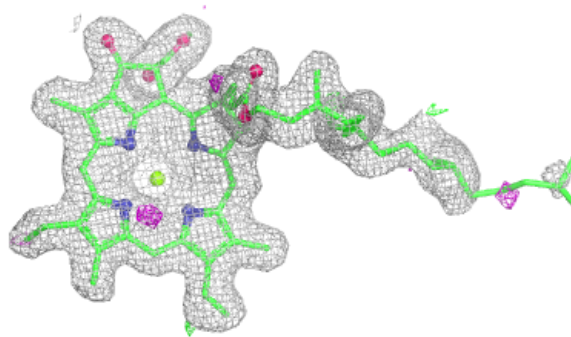
Electron density around LHG D 410:

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

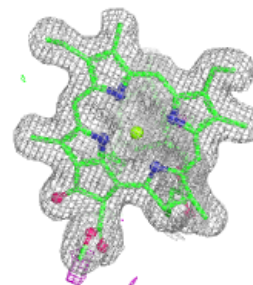
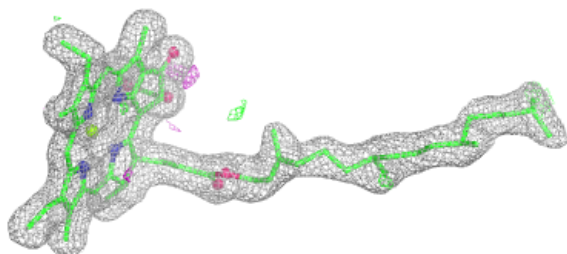
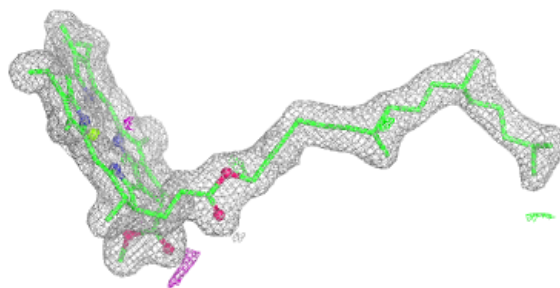


Electron density around CLA A 406:

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

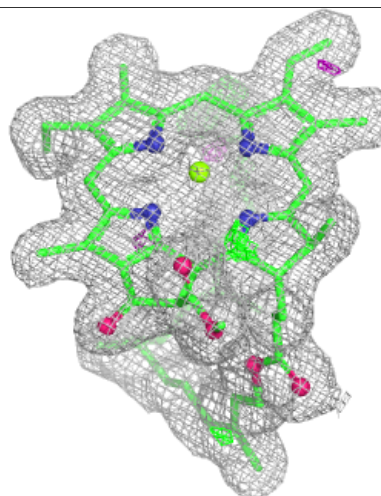
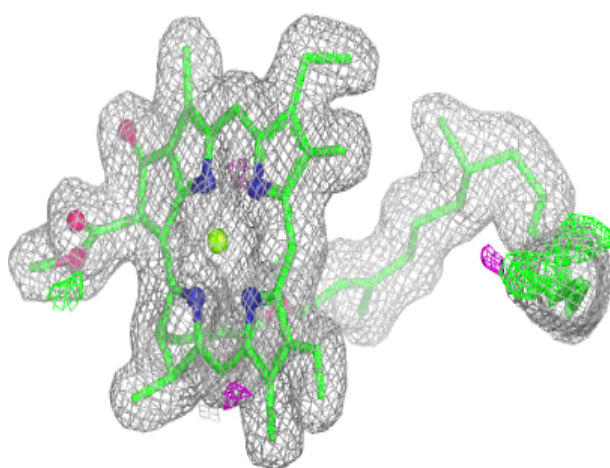
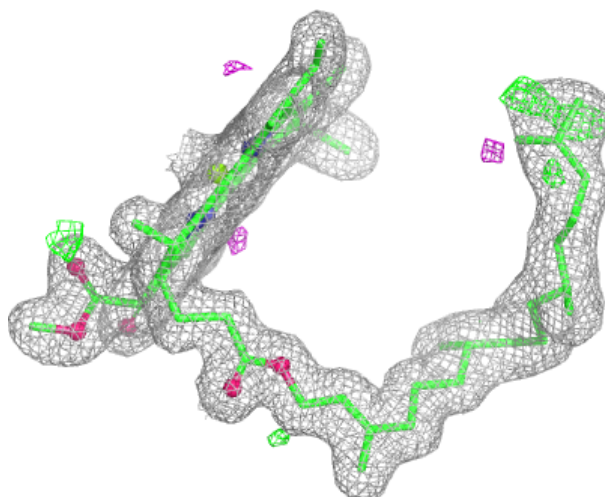
**Electron density around CLA B 605:**

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



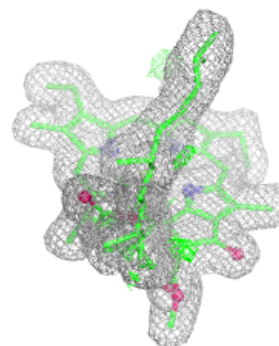
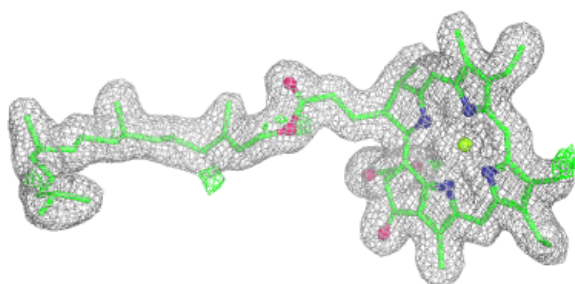
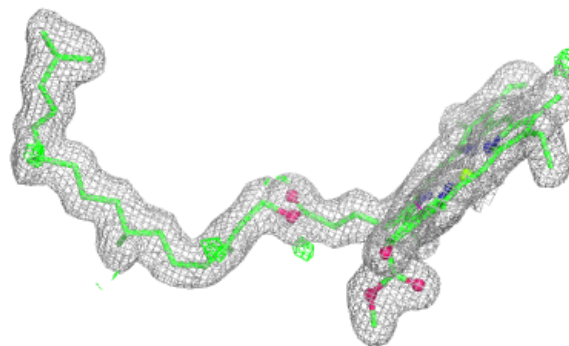
Electron density around CLA B 612:

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

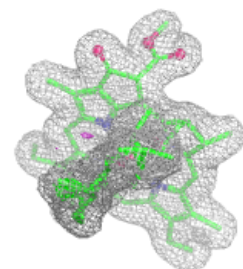
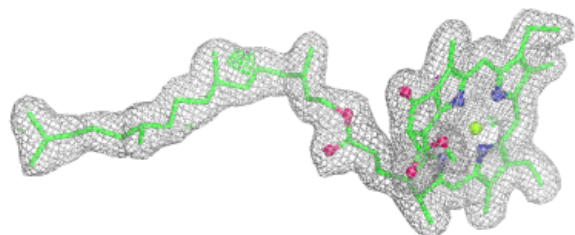
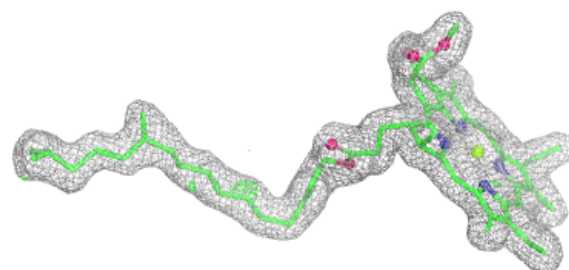


Electron density around CLA D 403:

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

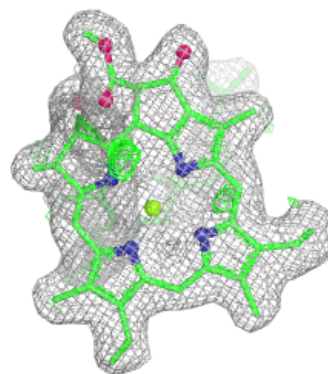
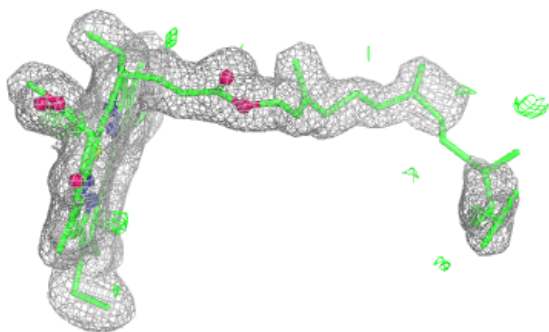
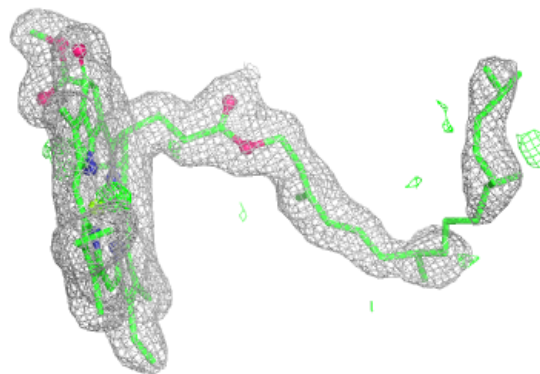
**Electron density around CLA c 903:**

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

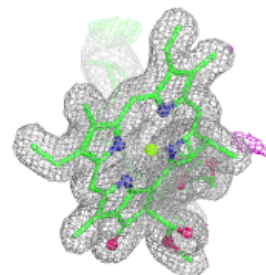
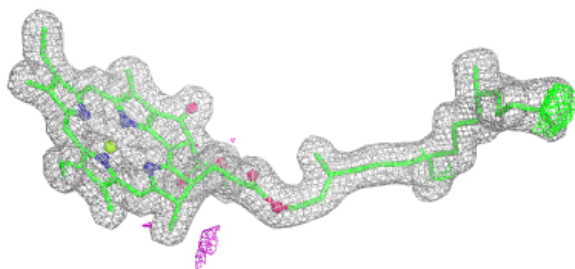
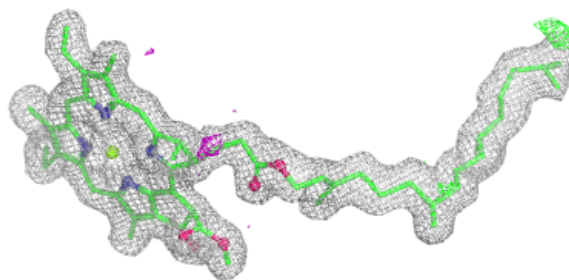


Electron density around CLA D 404:

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

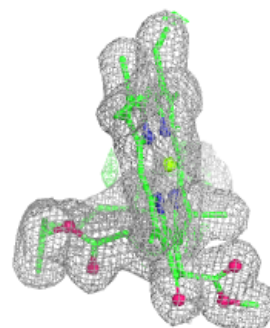
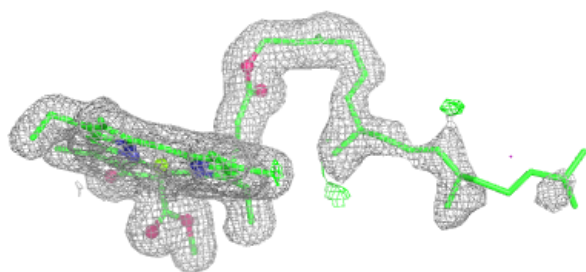
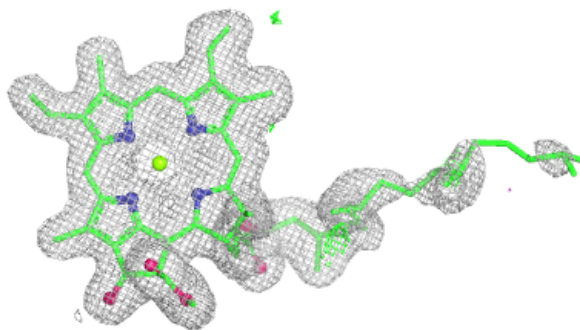
**Electron density around CLA a 406:**

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

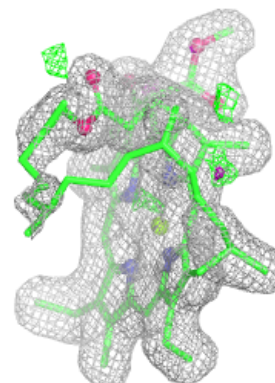
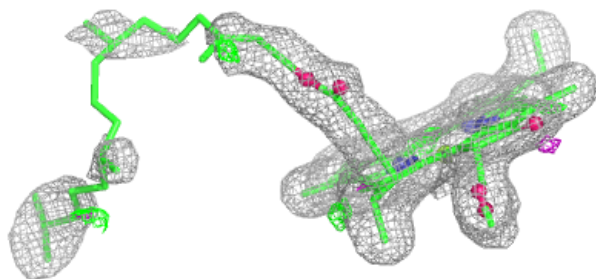
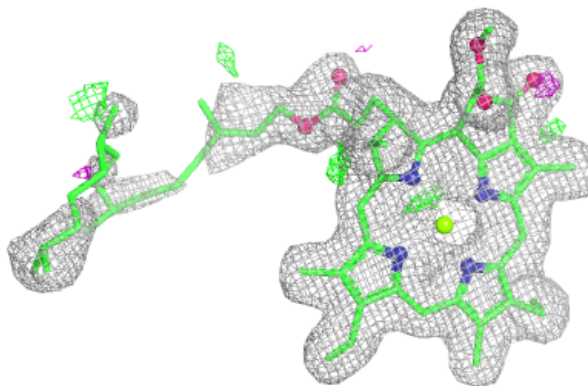


Electron density around CLA a 407:

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

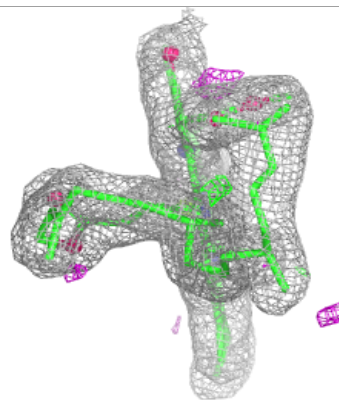
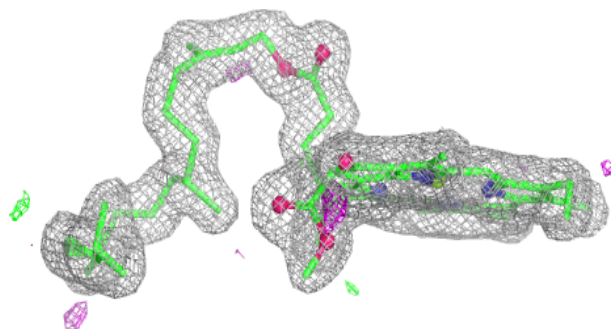
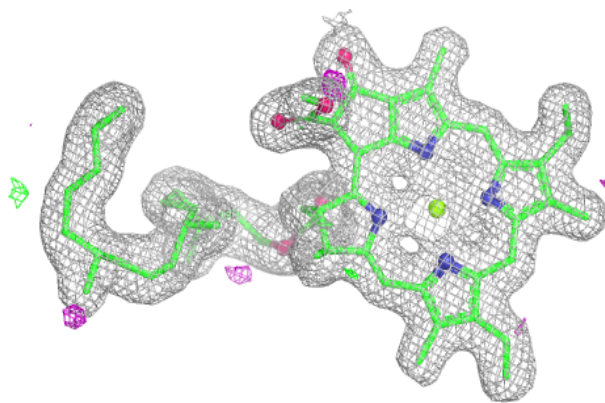
**Electron density around CLA a 410:**

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



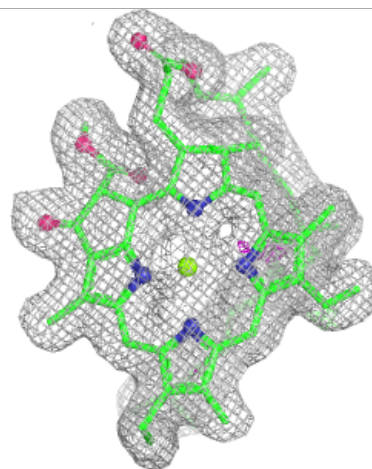
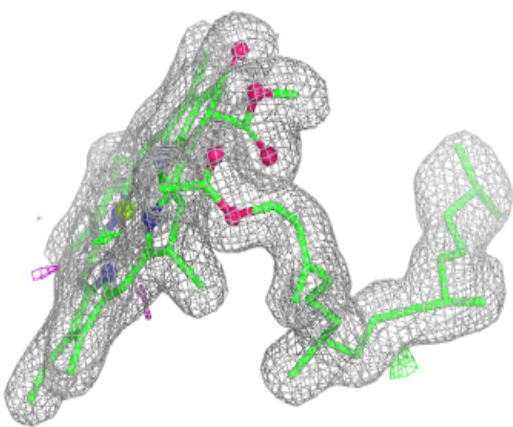
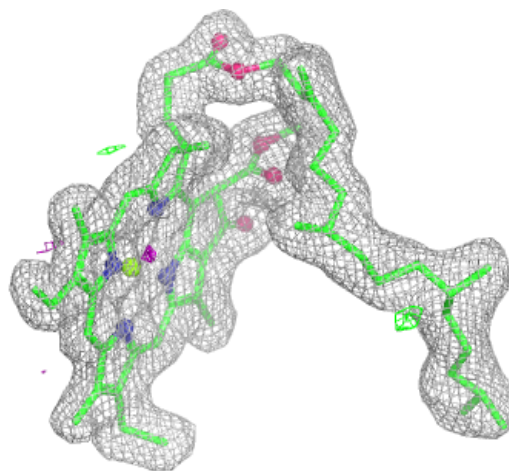
Electron density around CLA B 613:

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



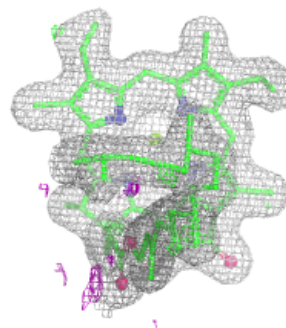
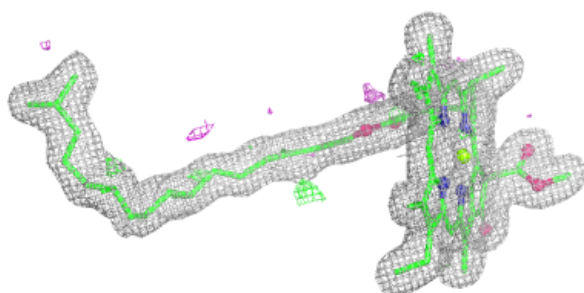
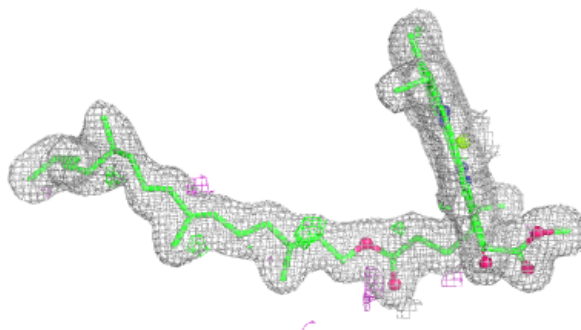
Electron density around CLA B 614:

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



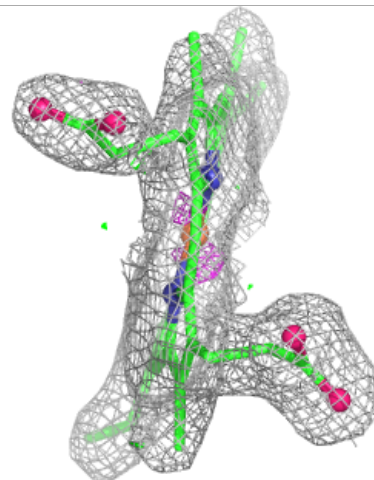
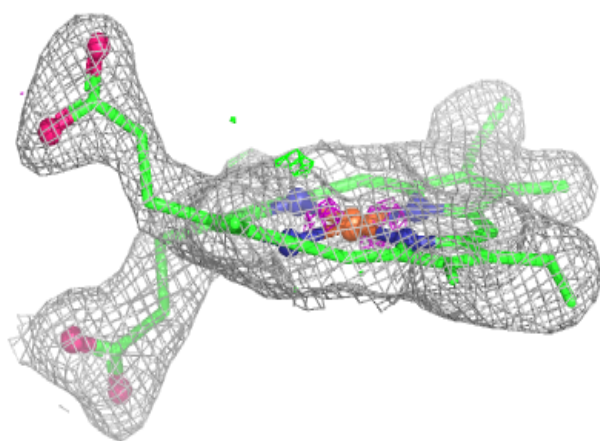
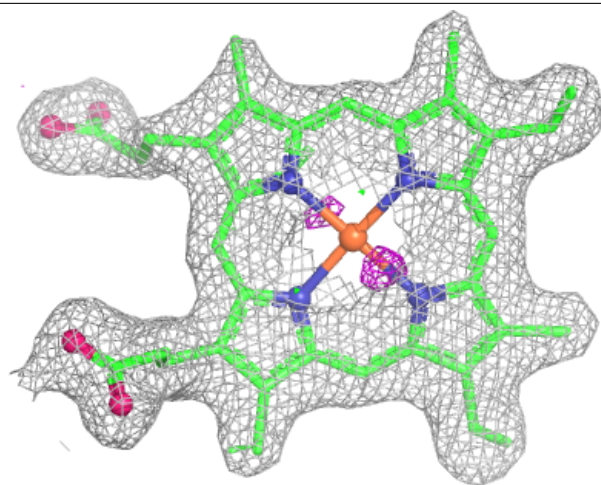
Electron density around CLA B 606:

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



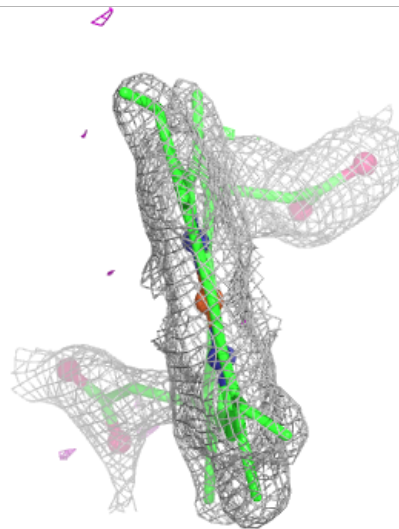
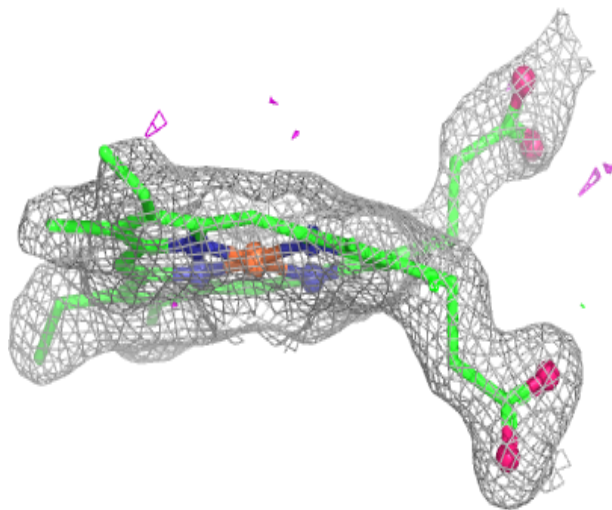
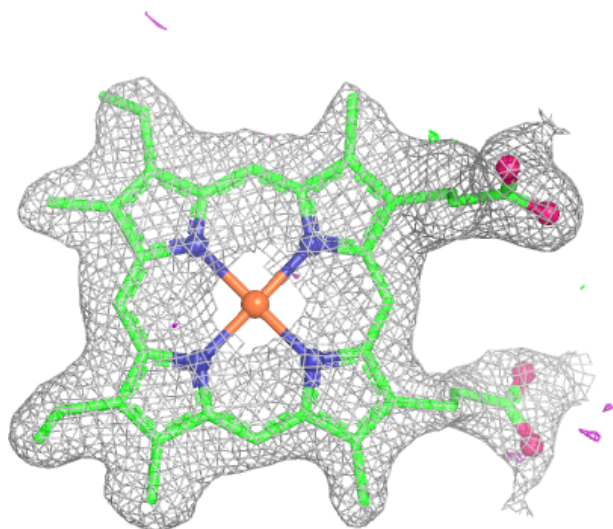
Electron density around HEM E 105:

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



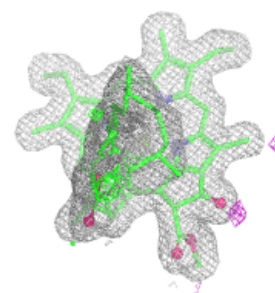
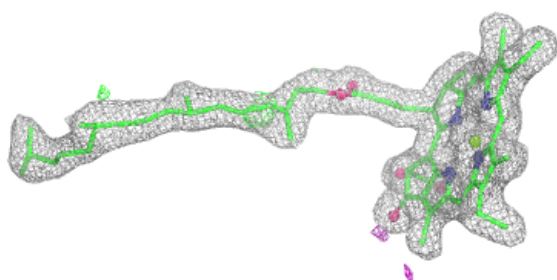
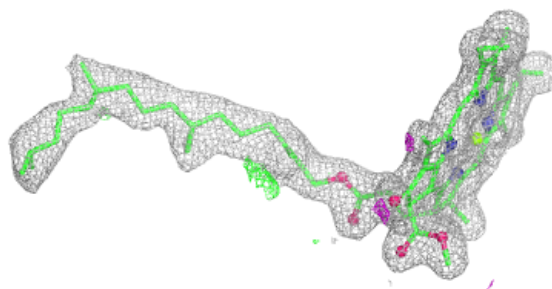
Electron density around HEM e 105:

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

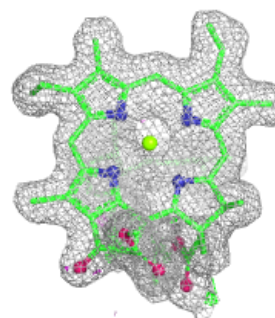
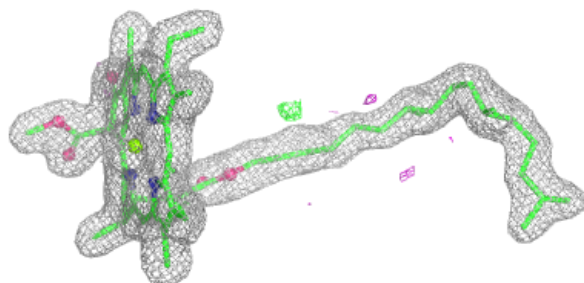
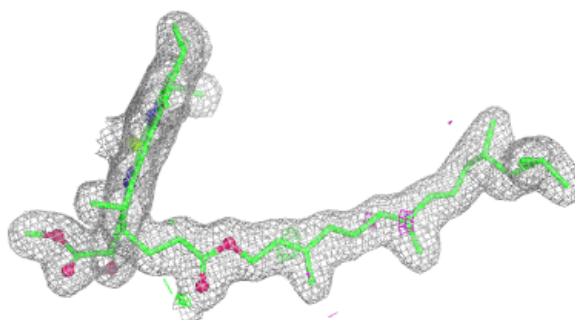


Electron density around CLA b 605:

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

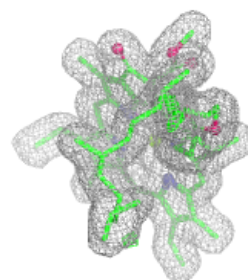
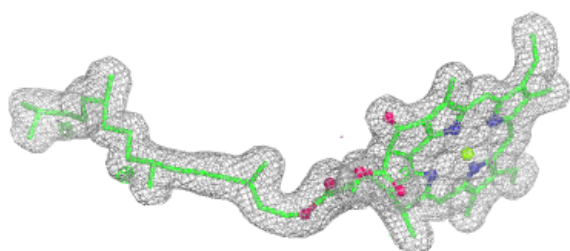
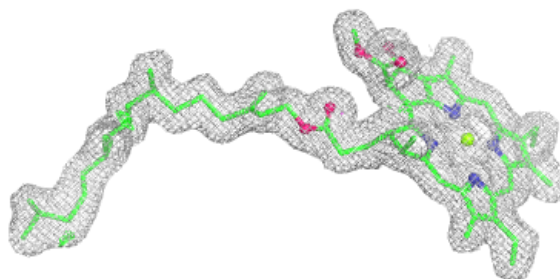
**Electron density around CLA b 606:**

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

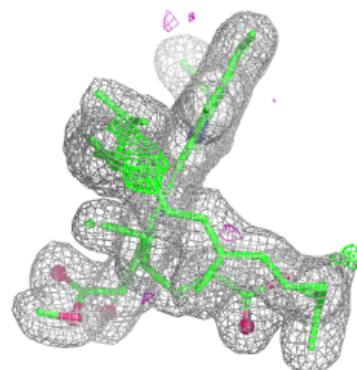
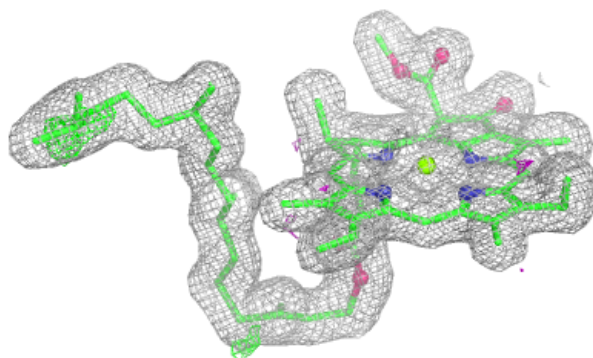
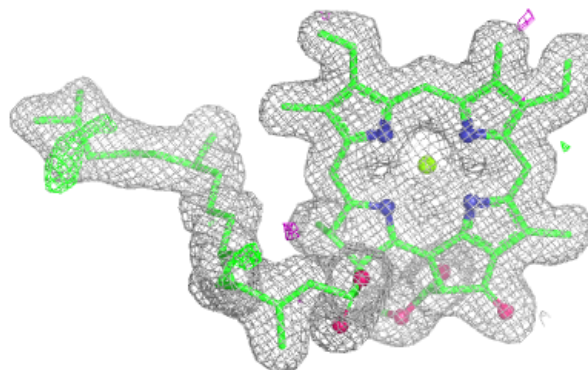


Electron density around CLA A 405:

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

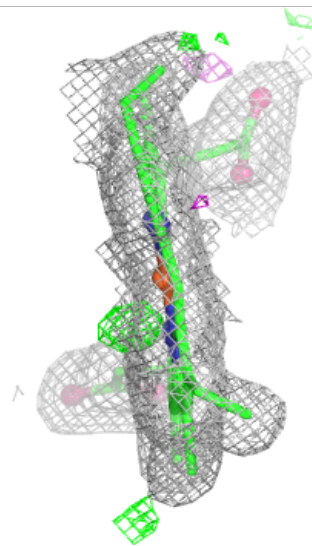
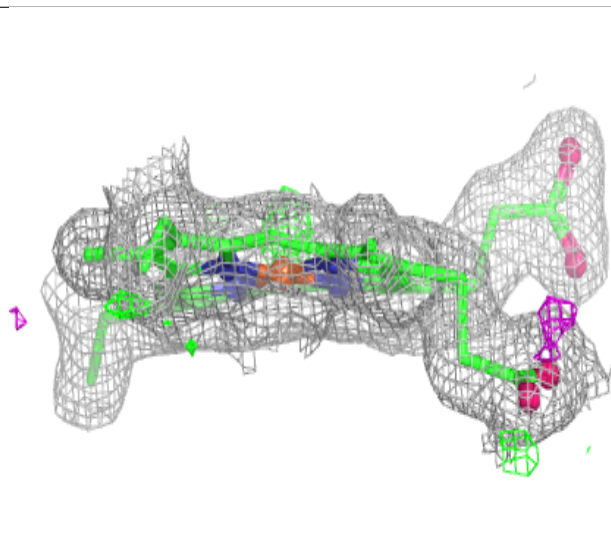
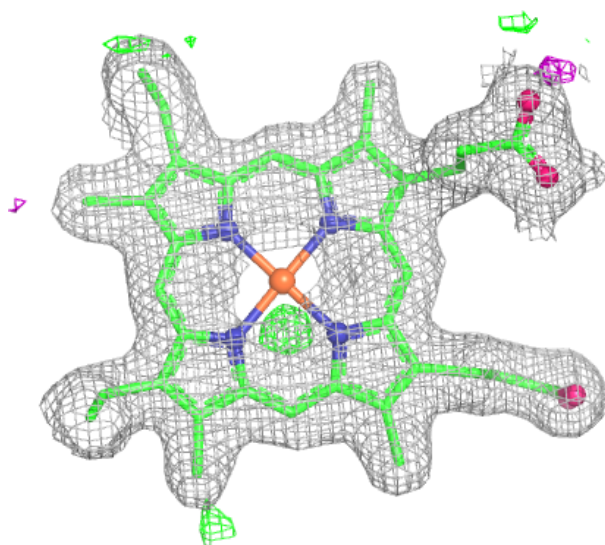
**Electron density around CLA D 401:**

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



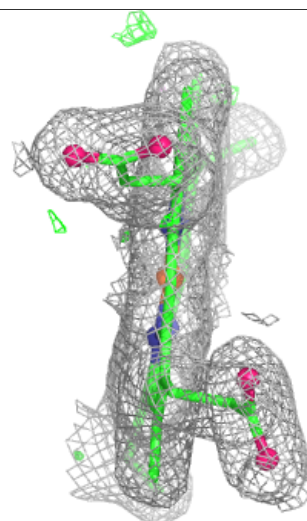
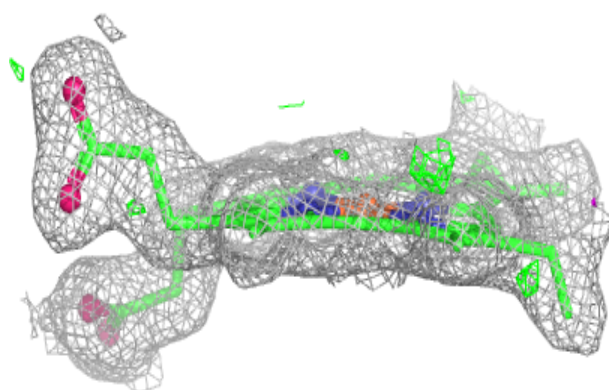
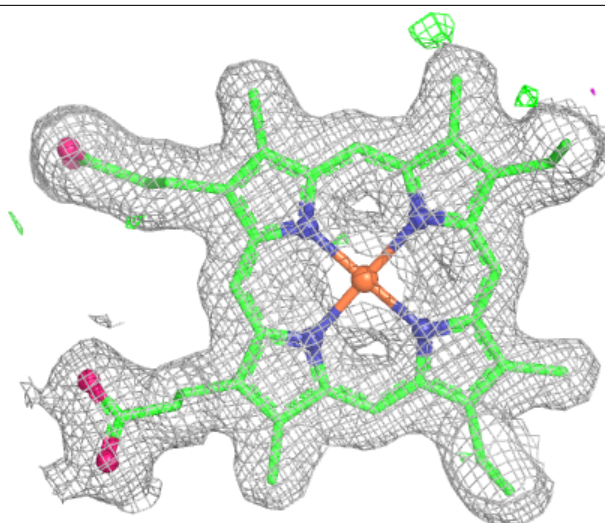
Electron density around HEC v 203:

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



Electron density around HEC V 203:

$2mF_o-DF_c$ (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.