



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 01:44 PM JST

PDB ID : 5B5E
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

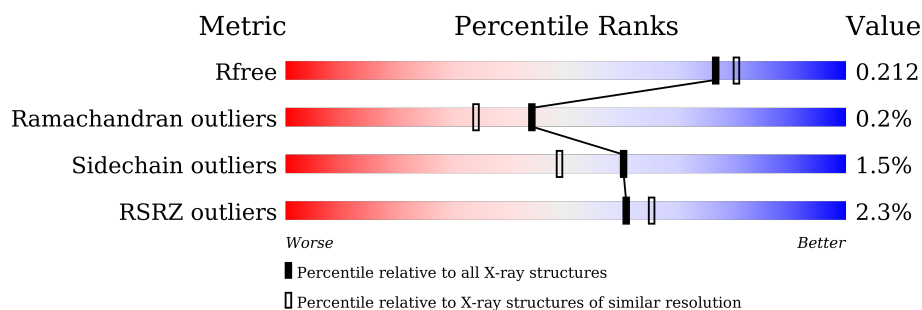
1 Overall quality at a glance

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}	164625	1090 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (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	95% . .
1	a	344	% 95% . .
2	B	505	2% 98% .
2	b	505	4% 96% . .
3	C	455	% 97% . .
3	c	455	% 97% .
4	D	342	97% .

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Mol	Chain	Length	Quality of chain
4	d	342	97% .
5	E	83	12% 94% . .
5	e	83	7% 89% 6% 5%
6	F	44	5% 75% 5% 20%
6	f	44	2% 70% . 27%
7	H	65	2% 92% 5% .
7	h	65	3% 92% 5% .
8	I	38	92% 8%
8	i	38	5% 97% .
9	J	40	2% 85% 5% 10%
9	j	40	5% 98% .
10	K	37	92% 8%
10	k	37	95% 5%
11	L	37	5% 100%
11	l	37	5% 97% .
12	M	36	3% 92% . 6%
12	m	36	3% 94% 6%
13	O	244	2% 96% .
13	o	244	4% 97% .
14	T	32	3% 88% 6% 6%
14	t	32	6% 91% 6% .
15	U	104	% 92% . 7%
15	u	104	% 93% 7%
16	V	137	97% .
16	v	137	99% .

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Mol	Chain	Length	Quality of chain
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	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	b	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-

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			

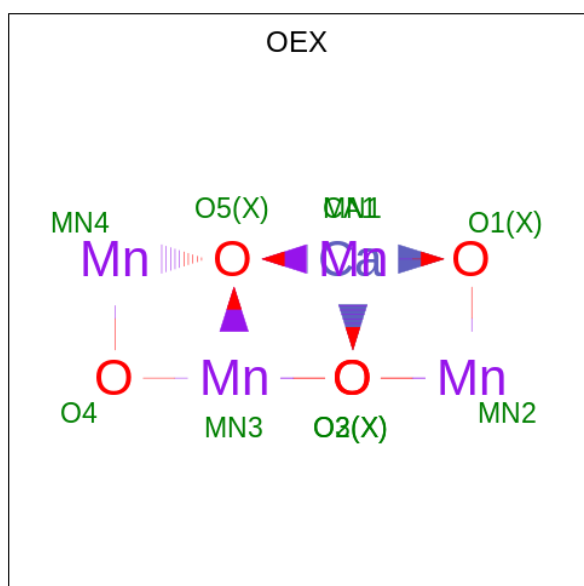
- Molecule 18 is a protein called Photosystem II reaction center protein X.

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 (three-letter code: OEX) (formula: CaMn_4O_5).



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

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

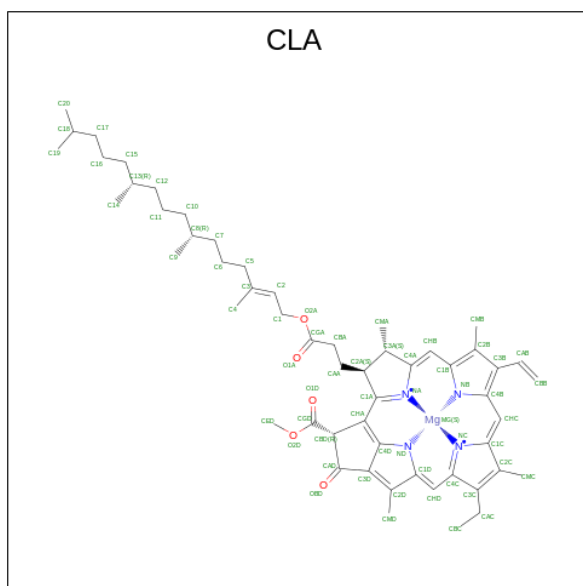
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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 (three-letter code: 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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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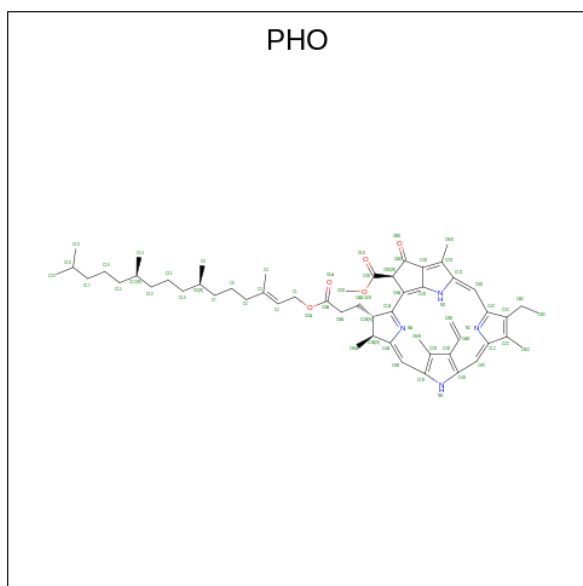
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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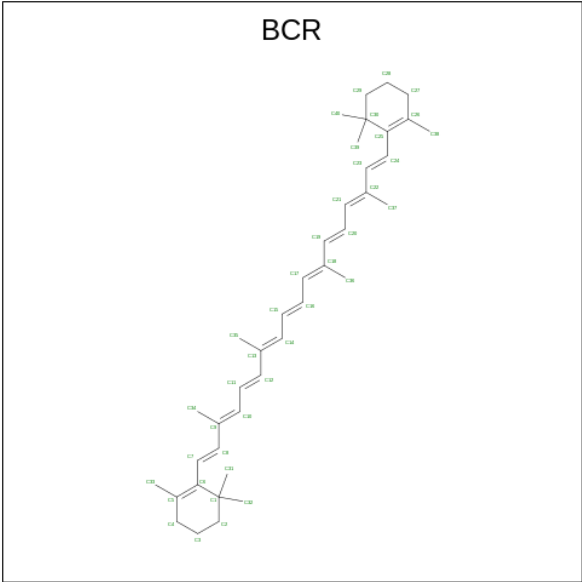
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: 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 (three-letter code: BCR) (formula: $C_{40}H_{56}$).



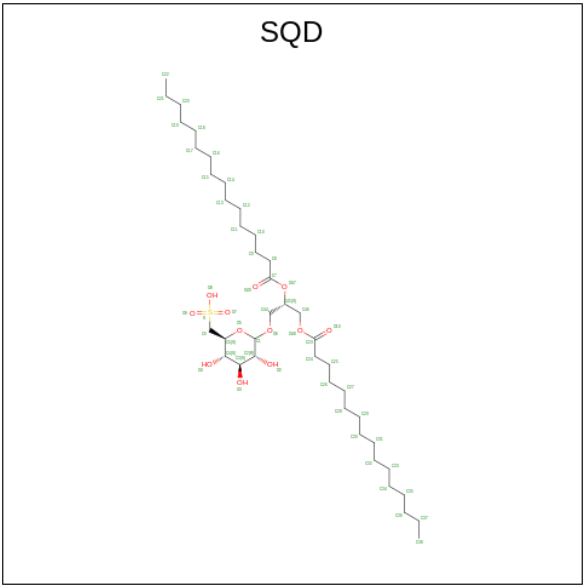
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total 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 (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



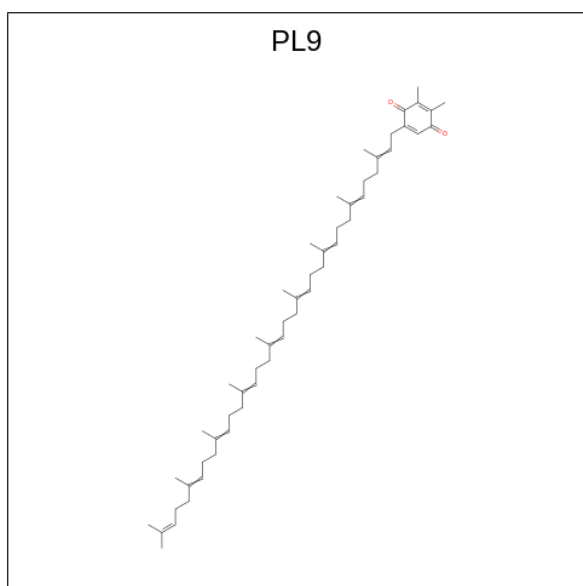
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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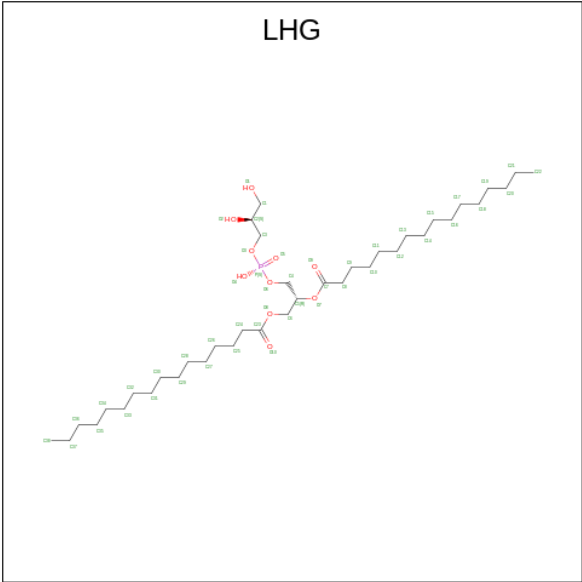
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	x	1	Total	C	O	S	0	0
			41	28	12	1		

- 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: UNL) (formula:).

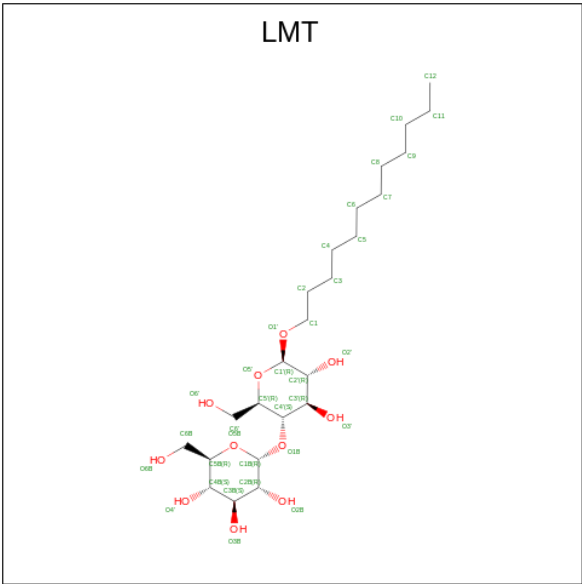
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	3	Total C 33 33	0	0
29	B	7	Total C 97 97	0	0
29	C	1	Total C 11 11	0	0
29	D	1	Total C 16 16	0	0
29	E	3	Total C 45 45	0	0
29	H	1	Total C 14 14	0	0
29	I	3	Total C 45 45	0	0
29	J	3	Total C 43 43	0	0
29	M	1	Total C 11 11	0	0
29	T	1	Total C 13 13	0	0
29	U	1	Total 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-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



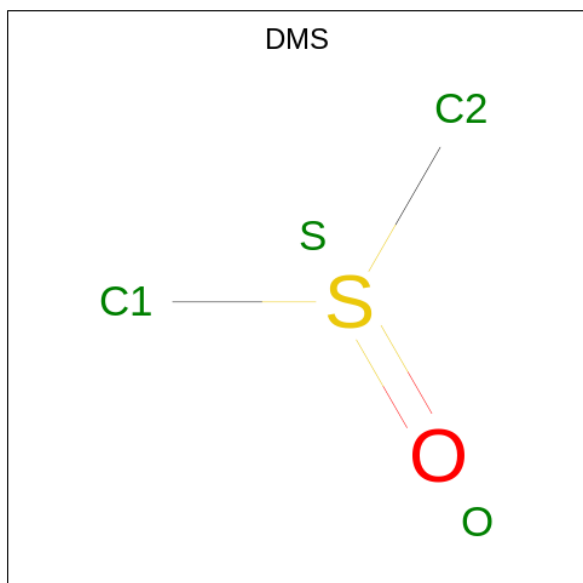
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			24	18	6		
30	B	1	Total	C	O	0	0
			24	18	6		
30	F	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		

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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 (three-letter code: 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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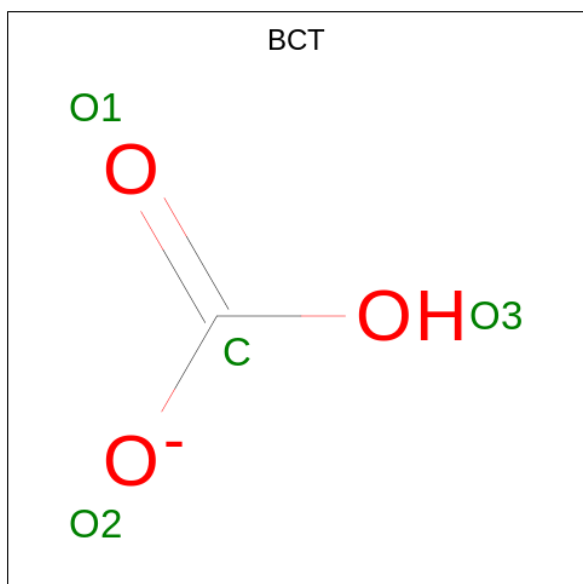
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	e	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 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 (three-letter code: 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 (three-letter code: CA) (formula: Ca).

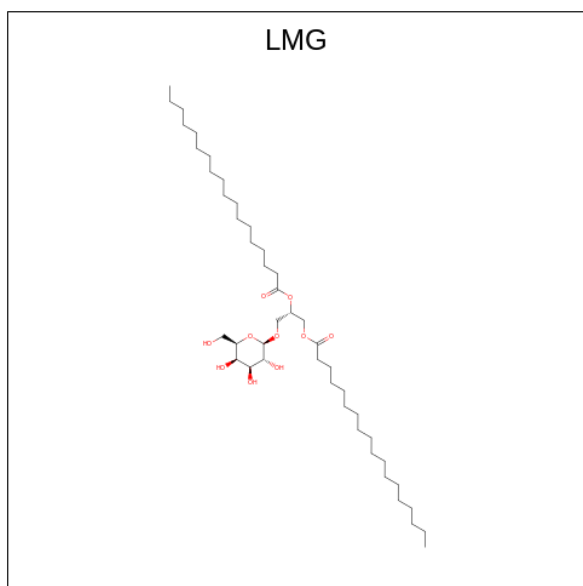
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		

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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 (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



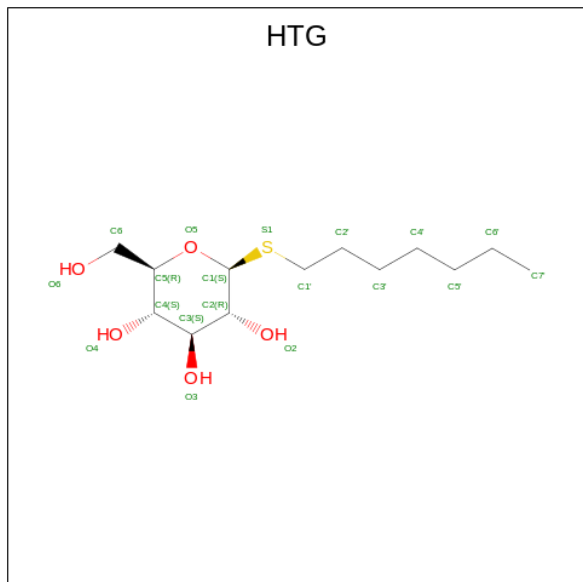
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		
34	a	1	Total	C	O	0	0
			51	41	10		

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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 (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



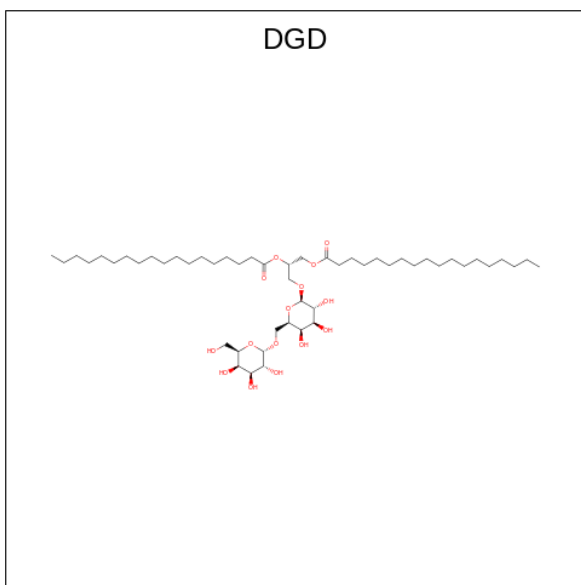
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		

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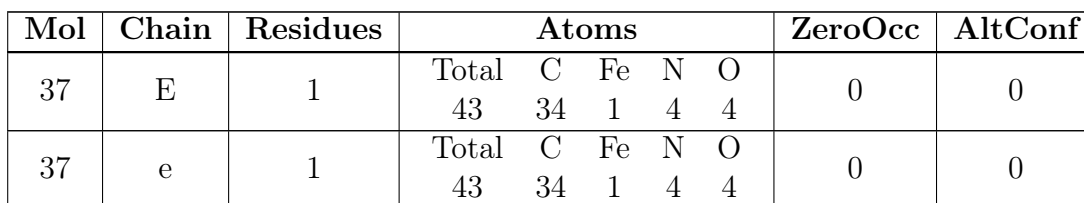
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			14	8	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	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) (three-letter code: 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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



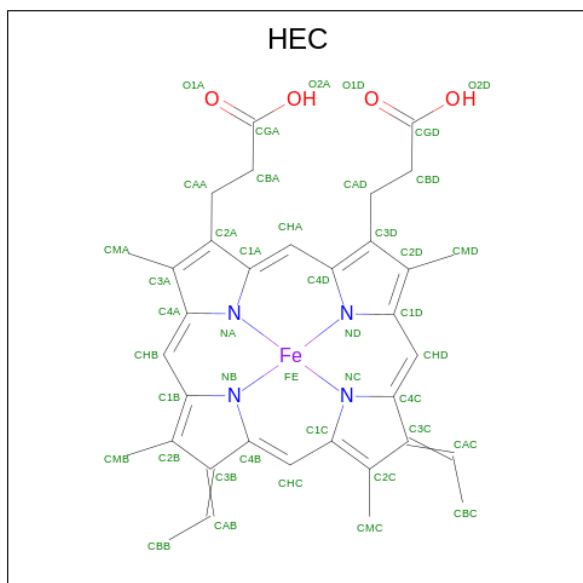
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

- Molecule 39 is MAGNESIUM ION (three-letter code: 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 (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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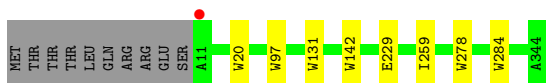
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	i	12	Total 13	O 13	0	1
41	j	13	Total 13	O 13	0	0
41	k	14	Total 14	O 14	0	0
41	l	16	Total 19	O 19	0	3
41	m	14	Total 15	O 15	0	1
41	o	223	Total 240	O 240	0	17
41	t	19	Total 21	O 21	0	2
41	u	146	Total 157	O 157	0	11
41	v	147	Total 154	O 154	0	7
41	y	16	Total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

Chain A:  95%



- Molecule 1: Photosystem II protein D1

Chain a:  95%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  98%



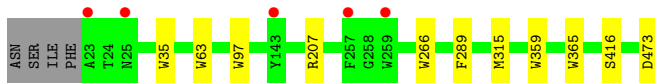
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  96%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  97%



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



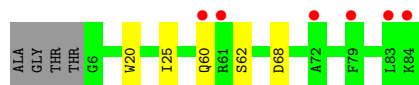
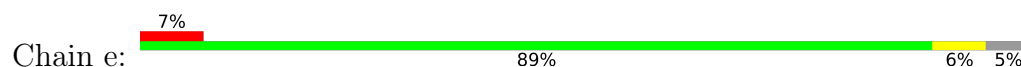
- Molecule 4: Photosystem II D2 protein



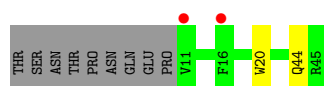
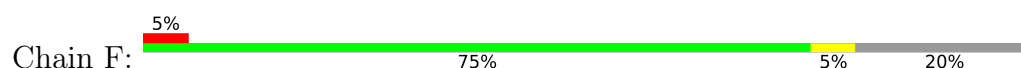
- Molecule 5: Cytochrome b559 subunit alpha



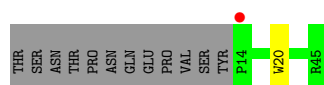
- Molecule 5: Cytochrome b559 subunit alpha



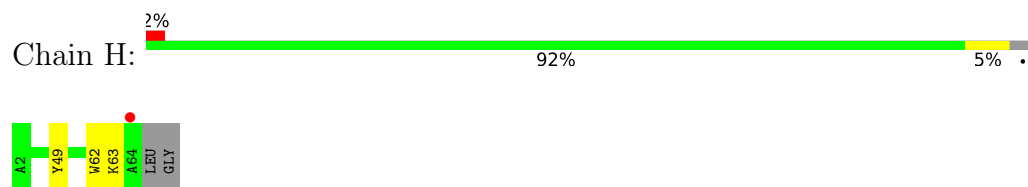
- Molecule 6: Cytochrome b559 subunit beta



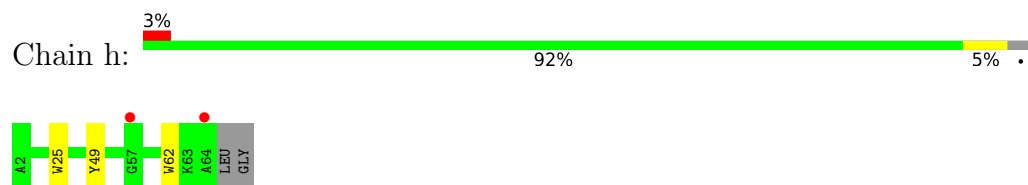
- Molecule 6: Cytochrome b559 subunit beta



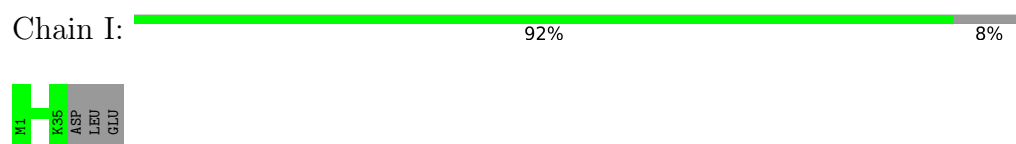
• Molecule 7: Photosystem II reaction center protein H



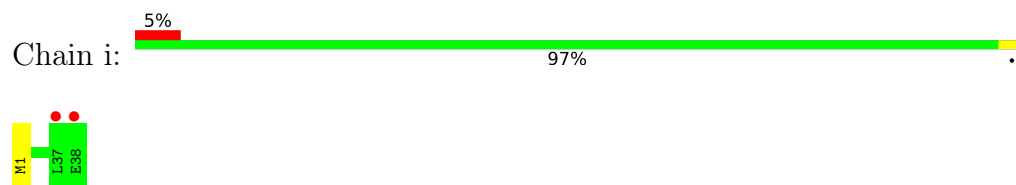
• Molecule 7: Photosystem II reaction center protein H



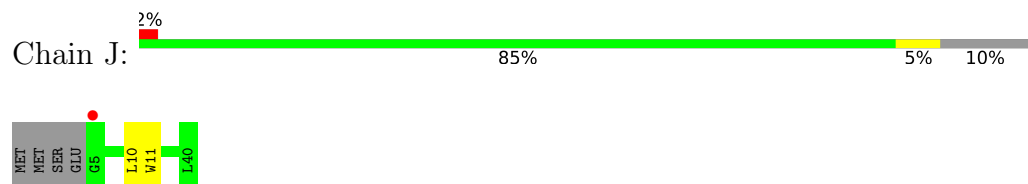
• Molecule 8: Photosystem II reaction center protein I



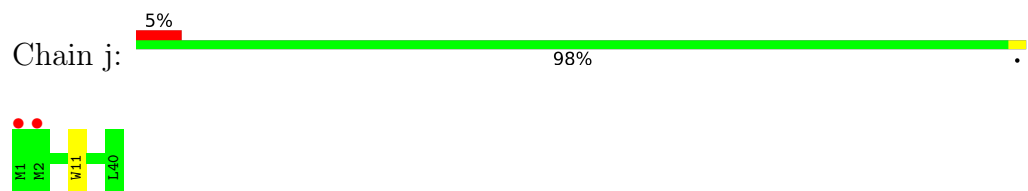
• Molecule 8: Photosystem II reaction center protein I



• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J



• Molecule 10: Photosystem II reaction center protein K





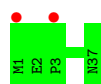
- Molecule 10: Photosystem II reaction center protein K

Chain k: 95% 5%



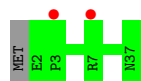
- Molecule 11: Photosystem II reaction center protein L

Chain L: 5% 100% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 5% 97% 5%



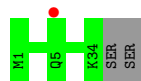
- Molecule 12: Photosystem II reaction center protein M

Chain M: 3% 92% 6% 6%



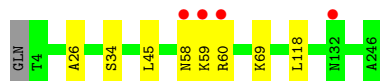
- Molecule 12: Photosystem II reaction center protein M

Chain m: 3% 94% 6%

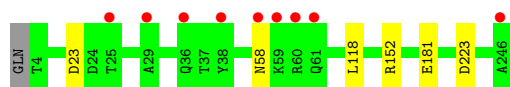


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

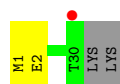
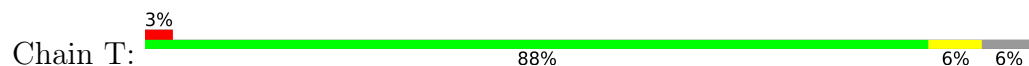
Chain O: 2% 96% 2%



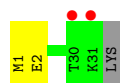
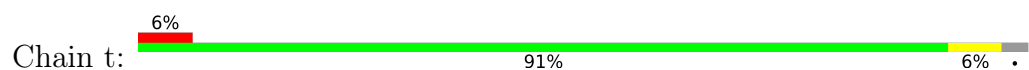
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



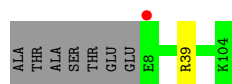
- Molecule 14: Photosystem II reaction center protein T



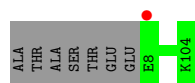
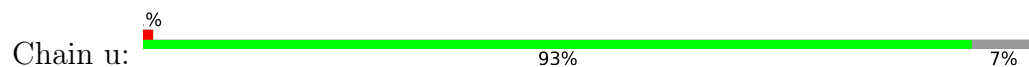
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



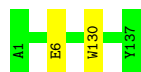
- Molecule 15: Photosystem II 12 kDa extrinsic protein



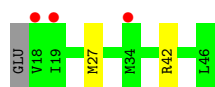
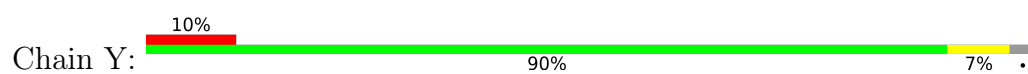
- Molecule 16: Cytochrome c-550



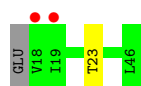
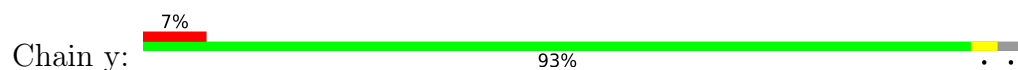
- Molecule 16: Cytochrome c-550



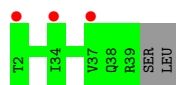
- Molecule 17: Photosystem II reaction center protein Ycf12



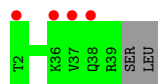
- Molecule 17: Photosystem II reaction center protein Ycf12



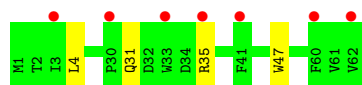
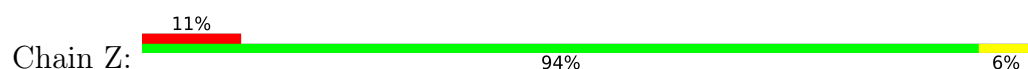
- Molecule 18: Photosystem II reaction center protein X



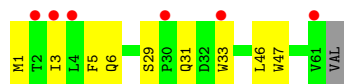
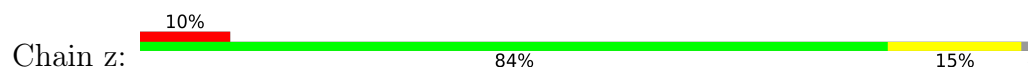
- Molecule 18: Photosystem II reaction center protein X



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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	5/2710 (0.2%)	0.81	1/3696 (0.0%)
1	a	0.99	4/2730 (0.1%)	0.81	1/3723 (0.0%)
2	B	0.94	4/4144 (0.1%)	0.82	4/5647 (0.1%)
2	b	0.98	9/4076 (0.2%)	0.83	3/5558 (0.1%)
3	C	0.91	6/3633 (0.2%)	0.78	1/4945 (0.0%)
3	c	0.91	9/3638 (0.2%)	0.78	1/4953 (0.0%)
4	D	1.01	4/2834 (0.1%)	0.83	2/3861 (0.1%)
4	d	1.02	8/2834 (0.3%)	0.82	1/3861 (0.0%)
5	E	0.74	1/670 (0.1%)	0.71	0/917
5	e	0.71	1/656 (0.2%)	0.73	0/896
6	F	0.83	1/289 (0.3%)	0.64	0/394
6	f	0.83	1/262 (0.4%)	0.65	0/356
7	H	0.85	1/530 (0.2%)	0.78	0/722
7	h	0.89	2/522 (0.4%)	0.79	0/711
8	I	0.66	0/282	0.67	0/381
8	i	0.68	0/300	0.67	0/406
9	J	0.80	1/257 (0.4%)	0.63	0/349
9	j	0.84	1/291 (0.3%)	0.69	0/393
10	K	0.73	1/303 (0.3%)	0.70	0/416
10	k	0.77	1/303 (0.3%)	0.71	0/416
11	L	0.94	0/316	0.80	0/430
11	l	0.98	0/307	0.80	0/418
12	M	0.78	0/270	0.75	0/369
12	m	0.72	0/270	0.74	0/369
13	O	0.78	0/1898	0.83	0/2577
13	o	0.74	0/1886	0.83	2/2562 (0.1%)
14	T	0.83	0/255	0.79	0/346
14	t	0.82	0/260	0.74	0/353
15	U	0.82	0/777	0.84	2/1055 (0.2%)
15	u	0.80	0/790	0.82	0/1071
16	V	0.88	0/1096	0.83	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.78	1/1084 (0.1%)	0.76	0/1475
17	Y	0.54	0/211	0.71	0/282
17	y	0.51	0/208	0.63	0/278
18	X	0.61	0/286	0.73	0/387
18	x	0.60	0/278	0.71	0/376
19	Z	0.67	1/479 (0.2%)	0.67	0/656
19	z	0.63	2/468 (0.4%)	0.61	0/640
All	All	0.90	64/42403 (0.2%)	0.80	19/57732 (0.0%)

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.28	1.50	1.41
1	a	131	TRP	CD2-CE2	6.83	1.49	1.41
3	c	35	TRP	CD2-CE2	6.66	1.49	1.41
2	b	56	TRP	CD2-CE2	6.63	1.49	1.41
10	k	39	TRP	CD2-CE2	6.56	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	152	ARG	NE-CZ-NH2	-7.84	116.38	120.30
4	d	297	ASP	CB-CG-OD1	7.14	124.73	118.30
2	B	357	ARG	NE-CZ-NH2	-6.52	117.04	120.30
15	U	39	ARG	NE-CZ-NH2	-6.50	117.05	120.30
4	D	100	ASP	CB-CG-OD1	6.18	123.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	325 (98%)	7 (2%)	1 (0%)	37	26
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	37	26
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%)	44	34
3	c	454/455 (100%)	441 (97%)	12 (3%)	1 (0%)	44	34
4	D	342/342 (100%)	333 (97%)	8 (2%)	1 (0%)	37	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%)	11	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	44	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%)	89	86
1	a	272/279 (98%)	271 (100%)	1 (0%)	89	86
2	B	403/403 (100%)	399 (99%)	4 (1%)	73	65
2	b	394/403 (98%)	389 (99%)	5 (1%)	65	55
3	C	355/356 (100%)	351 (99%)	4 (1%)	70	62
3	c	356/356 (100%)	351 (99%)	5 (1%)	62	52
4	D	278/277 (100%)	274 (99%)	4 (1%)	62	52
4	d	278/277 (100%)	276 (99%)	2 (1%)	81	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	70/72 (97%)	68 (97%)	2 (3%)	37	20
5	e	68/72 (94%)	64 (94%)	4 (6%)	16	4
6	F	28/38 (74%)	27 (96%)	1 (4%)	30	14
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	53 (96%)	2 (4%)	30	14
7	h	54/54 (100%)	53 (98%)	1 (2%)	52	38
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%)	25	9
9	j	27/28 (96%)	27 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	13	3
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	17
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	17
12	m	30/33 (91%)	30 (100%)	0	100	100
13	O	205/207 (99%)	200 (98%)	5 (2%)	44	28
13	o	203/207 (98%)	199 (98%)	4 (2%)	50	36
14	T	25/28 (89%)	24 (96%)	1 (4%)	27	10
14	t	25/28 (89%)	24 (96%)	1 (4%)	27	10
15	U	82/89 (92%)	82 (100%)	0	100	100
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%)	75	69
17	Y	20/23 (87%)	18 (90%)	2 (10%)	6	1
17	y	19/23 (83%)	18 (95%)	1 (5%)	19	6
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%)	47 (96%)	2 (4%)	26	10
19	z	46/52 (88%)	41 (89%)	5 (11%)	5	0
All	All	4255/4376 (97%)	4189 (98%)	66 (2%)	60	45

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	181	GLU
16	v	6	GLU
19	z	46	LEU
13	O	58	ASN
13	O	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	36	GLN
15	u	73	GLN
16	v	34	GLN
13	o	231	HIS
2	b	331	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	0.73	0	7,9,11	1.54	3 (42%)
14	FME	T	1	14	8,9,10	0.53	0	7,9,11	1.70	2 (28%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	1.70	3 (42%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CE-SD-CG	2.58	109.25	100.40
14	T	1	FME	O-C-CA	-2.49	118.27	124.78
14	t	1	FME	O-C-CA	-2.36	118.60	124.78
14	t	1	FME	CE-SD-CG	2.29	108.28	100.40
8	i	1	FME	O1-CN-N	-2.24	119.36	125.27

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	N-CA-CB-CG

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$
31	DMS	O	304	-	3,3,3	2.79	1 (33%)	3,3,3	0.87	0
31	DMS	b	641	-	3,3,3	2.64	1 (33%)	3,3,3	0.75	0
31	DMS	b	642	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
36	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.18	9 (11%)
31	DMS	C	533	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
31	DMS	U	203	-	3,3,3	2.71	1 (33%)	3,3,3	0.51	0
31	DMS	v	207	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
31	DMS	B	647	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
23	CLA	C	509	-	65,73,73	2.35	18 (27%)	76,113,113	2.43	23 (30%)
31	DMS	B	645	-	3,3,3	2.80	1 (33%)	3,3,3	0.70	0
35	HTG	B	630	-	19,19,19	0.98	2 (10%)	23,24,24	1.32	2 (8%)
23	CLA	b	602	41	65,73,73	2.57	18 (27%)	76,113,113	2.55	30 (39%)
31	DMS	V	207	-	3,3,3	2.84	1 (33%)	3,3,3	1.25	0
31	DMS	B	636	-	3,3,3	3.09	1 (33%)	3,3,3	0.77	0
31	DMS	i	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.88	0
23	CLA	c	913	-	65,73,73	2.40	17 (26%)	76,113,113	2.50	22 (28%)
34	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.15	4 (6%)
23	CLA	B	603	-	65,73,73	2.27	19 (29%)	76,113,113	2.21	27 (35%)
31	DMS	B	642	-	3,3,3	2.92	1 (33%)	3,3,3	1.28	0
30	LMT	m	103	-	36,36,36	0.61	1 (2%)	47,47,47	0.98	3 (6%)
20	OEX	A	401	41,1,3	0,15,15	-	-	-	-	-
23	CLA	c	906	-	65,73,73	2.14	21 (32%)	76,113,113	2.10	26 (34%)
31	DMS	O	309	-	3,3,3	2.88	1 (33%)	3,3,3	0.94	0
31	DMS	c	929	-	3,3,3	2.83	1 (33%)	3,3,3	0.69	0
26	SQD	A	415	-	53,54,54	1.03	3 (5%)	62,65,65	1.91	12 (19%)
28	LHG	d	402	-	43,43,48	1.06	2 (4%)	46,49,54	0.96	3 (6%)
30	LMT	F	101	-	36,36,36	0.71	1 (2%)	47,47,47	1.19	5 (10%)
25	BCR	b	618	-	41,41,41	0.95	0	56,56,56	1.75	13 (23%)
31	DMS	v	202	-	3,3,3	2.60	1 (33%)	3,3,3	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	h	105	-	3,3,3	2.74	1 (33%)	3,3,3	0.68	0
31	DMS	F	102	-	3,3,3	2.61	1 (33%)	3,3,3	0.25	0
23	CLA	b	616	-	65,73,73	2.14	15 (23%)	76,113,113	2.19	25 (32%)
23	CLA	B	616	-	65,73,73	2.26	20 (30%)	76,113,113	2.31	21 (27%)
31	DMS	c	927	-	3,3,3	2.71	1 (33%)	3,3,3	1.27	1 (33%)
35	HTG	c	921	-	19,19,19	0.95	2 (10%)	23,24,24	1.45	2 (8%)
23	CLA	C	502	-	65,73,73	2.11	14 (21%)	76,113,113	2.21	20 (26%)
31	DMS	A	423	-	3,3,3	1.91	1 (33%)	3,3,3	0.64	0
23	CLA	b	614	-	65,73,73	1.97	14 (21%)	76,113,113	2.28	21 (27%)
25	BCR	a	411	-	41,41,41	1.20	3 (7%)	56,56,56	1.35	5 (8%)
25	BCR	t	101	-	41,41,41	1.03	0	56,56,56	1.52	14 (25%)
23	CLA	B	612	-	65,73,73	2.01	14 (21%)	76,113,113	2.20	23 (30%)
31	DMS	A	424	-	3,3,3	2.76	1 (33%)	3,3,3	1.08	0
31	DMS	C	525	-	3,3,3	2.62	1 (33%)	3,3,3	0.90	0
31	DMS	O	310	-	3,3,3	2.61	1 (33%)	3,3,3	0.71	0
35	HTG	D	414	-	19,19,19	0.94	1 (5%)	23,24,24	1.31	1 (4%)
31	DMS	A	421	-	3,3,3	2.71	1 (33%)	3,3,3	0.80	0
35	HTG	B	631	-	19,19,19	1.11	1 (5%)	23,24,24	1.25	2 (8%)
31	DMS	H	101	-	3,3,3	2.78	1 (33%)	3,3,3	0.58	0
31	DMS	e	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
23	CLA	b	607	-	65,73,73	2.39	18 (27%)	76,113,113	2.25	25 (32%)
23	CLA	c	903	-	65,73,73	2.05	16 (24%)	76,113,113	2.34	30 (39%)
31	DMS	V	208	-	3,3,3	2.60	1 (33%)	3,3,3	0.41	0
32	BCT	a	424	21	2,3,3	0.66	0	2,3,3	1.00	0
25	BCR	d	405	-	41,41,41	0.99	1 (2%)	56,56,56	1.93	19 (33%)
31	DMS	c	925	-	3,3,3	2.81	1 (33%)	3,3,3	0.84	0
36	DGD	C	518	-	63,63,67	0.95	4 (6%)	77,77,81	1.09	4 (5%)
31	DMS	B	649	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
23	CLA	B	614	-	65,73,73	1.84	17 (26%)	76,113,113	2.37	22 (28%)
36	DGD	c	917	-	63,63,67	0.84	3 (4%)	77,77,81	1.24	8 (10%)
28	LHG	a	415	-	48,48,48	1.01	2 (4%)	51,54,54	1.07	4 (7%)
31	DMS	i	106	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
23	CLA	c	908	41	65,73,73	2.19	17 (26%)	76,113,113	2.29	22 (28%)
23	CLA	B	613	-	65,73,73	2.20	15 (23%)	76,113,113	2.22	23 (30%)
26	SQD	D	408	-	44,45,54	1.22	4 (9%)	53,56,65	2.21	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	B	643	-	24,24,36	0.39	0	29,29,47	0.88	1 (3%)
31	DMS	U	202	-	3,3,3	2.68	1 (33%)	3,3,3	1.60	1 (33%)
28	LHG	L	101	-	48,48,48	0.97	3 (6%)	51,54,54	1.13	3 (5%)
31	DMS	B	639	-	3,3,3	2.77	1 (33%)	3,3,3	0.89	0
31	DMS	c	924	-	3,3,3	2.36	1 (33%)	3,3,3	0.42	0
35	HTG	d	413	-	19,19,19	1.18	1 (5%)	23,24,24	2.11	5 (21%)
35	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.69	1 (4%)
40	HEC	v	203	16	32,50,50	2.14	10 (31%)	24,82,82	2.25	7 (29%)
23	CLA	a	406	-	65,73,73	1.89	15 (23%)	76,113,113	2.31	26 (34%)
23	CLA	b	604	-	65,73,73	2.24	17 (26%)	76,113,113	2.35	28 (36%)
31	DMS	B	641	-	3,3,3	2.82	1 (33%)	3,3,3	0.81	0
25	BCR	C	516	-	41,41,41	0.99	0	56,56,56	1.37	7 (12%)
31	DMS	U	204	-	3,3,3	2.88	1 (33%)	3,3,3	0.80	0
31	DMS	a	421	-	3,3,3	2.68	1 (33%)	3,3,3	0.63	0
31	DMS	u	205	-	3,3,3	2.62	1 (33%)	3,3,3	1.05	0
31	DMS	c	932	-	3,3,3	2.65	1 (33%)	3,3,3	0.75	0
23	CLA	c	909	-	65,73,73	2.26	19 (29%)	76,113,113	2.05	17 (22%)
31	DMS	b	633	-	3,3,3	1.83	1 (33%)	3,3,3	0.60	0
31	DMS	v	201	-	3,3,3	2.42	1 (33%)	3,3,3	0.47	0
31	DMS	d	415	-	3,3,3	2.65	1 (33%)	3,3,3	0.88	0
23	CLA	B	606	-	65,73,73	1.99	16 (24%)	76,113,113	2.23	24 (31%)
25	BCR	D	405	-	41,41,41	1.10	4 (9%)	56,56,56	1.99	14 (25%)
31	DMS	u	206	-	3,3,3	2.79	1 (33%)	3,3,3	0.63	0
35	HTG	B	624	-	19,19,19	1.52	3 (15%)	23,24,24	1.56	4 (17%)
35	HTG	B	625	-	19,19,19	1.41	3 (15%)	23,24,24	2.08	8 (34%)
30	LMT	a	422	-	36,36,36	0.65	1 (2%)	47,47,47	0.95	3 (6%)
31	DMS	c	928	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
23	CLA	b	603	-	65,73,73	2.04	20 (30%)	76,113,113	2.50	33 (43%)
31	DMS	V	206	-	3,3,3	2.65	1 (33%)	3,3,3	0.77	0
23	CLA	D	403	-	65,73,73	2.01	13 (20%)	76,113,113	2.48	28 (36%)
23	CLA	C	508	41	65,73,73	2.45	18 (27%)	76,113,113	2.35	24 (31%)
23	CLA	D	404	-	65,73,73	2.05	19 (29%)	76,113,113	2.27	29 (38%)
31	DMS	D	416	-	3,3,3	2.49	1 (33%)	3,3,3	0.88	0
34	LMG	D	412	-	51,51,55	1.10	2 (3%)	59,59,63	1.34	8 (13%)
26	SQD	A	410	-	53,54,54	0.99	3 (5%)	62,65,65	2.00	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	910	-	65,73,73	2.52	19 (29%)	76,113,113	2.56	25 (32%)
23	CLA	C	513	-	65,73,73	2.52	17 (26%)	76,113,113	2.14	24 (31%)
31	DMS	O	306	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
26	SQD	x	101	-	40,41,54	1.26	3 (7%)	49,52,65	1.46	9 (18%)
35	HTG	B	626	-	19,19,19	0.94	1 (5%)	23,24,24	1.59	1 (4%)
35	HTG	v	204	-	19,19,19	0.90	1 (5%)	23,24,24	2.78	8 (34%)
36	DGD	H	103	-	63,63,67	1.05	3 (4%)	77,77,81	1.32	7 (9%)
26	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.60	7 (11%)
23	CLA	D	401	41	65,73,73	1.99	18 (27%)	76,113,113	2.10	21 (27%)
31	DMS	b	646	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
31	DMS	V	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.81	0
31	DMS	a	423	-	3,3,3	2.80	1 (33%)	3,3,3	0.82	0
31	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
23	CLA	b	605	-	65,73,73	1.99	16 (24%)	76,113,113	2.30	25 (32%)
31	DMS	c	935	-	3,3,3	2.68	1 (33%)	3,3,3	0.74	0
23	CLA	C	511	-	65,73,73	2.23	17 (26%)	76,113,113	2.07	22 (28%)
30	LMT	M	101	-	36,36,36	0.64	0	47,47,47	0.92	2 (4%)
31	DMS	V	210	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
34	LMG	a	413	-	51,51,55	1.00	2 (3%)	59,59,63	1.10	4 (6%)
34	LMG	C	520	-	51,51,55	1.15	2 (3%)	59,59,63	1.35	9 (15%)
23	CLA	b	615	-	65,73,73	2.12	19 (29%)	76,113,113	2.36	25 (32%)
34	LMG	m	102	-	51,51,55	0.95	2 (3%)	59,59,63	1.33	6 (10%)
35	HTG	b	627	-	19,19,19	1.22	2 (10%)	23,24,24	1.49	2 (8%)
30	LMT	T	103	-	24,24,36	0.50	0	29,29,47	1.32	4 (13%)
28	LHG	D	409	-	48,48,48	0.85	1 (2%)	51,54,54	1.27	6 (11%)
31	DMS	A	422	-	3,3,3	2.68	1 (33%)	3,3,3	0.84	0
34	LMG	d	411	-	51,51,55	1.13	3 (5%)	59,59,63	1.32	6 (10%)
23	CLA	B	607	-	65,73,73	2.24	17 (26%)	76,113,113	2.23	21 (27%)
31	DMS	b	645	-	3,3,3	2.69	1 (33%)	3,3,3	0.49	0
31	DMS	v	208	-	3,3,3	2.73	1 (33%)	3,3,3	0.73	0
23	CLA	C	505	41	65,73,73	2.11	15 (23%)	76,113,113	2.36	22 (28%)
28	LHG	D	411	-	45,45,48	0.98	2 (4%)	48,51,54	1.03	4 (8%)
31	DMS	V	205	-	3,3,3	2.63	1 (33%)	3,3,3	0.95	0
20	OEX	a	402	41,1,3	0,15,15	-	-	-	-	-
31	DMS	b	636	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	510	-	65,73,73	2.24	13 (20%)	76,113,113	2.35	24 (31%)
31	DMS	b	643	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
38	RRX	x	102	-	42,42,42	0.90	0	57,58,58	1.38	7 (12%)
31	DMS	h	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
25	BCR	j	104	-	41,41,41	0.82	0	56,56,56	1.48	11 (19%)
31	DMS	C	526	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
31	DMS	C	529	-	3,3,3	2.55	1 (33%)	3,3,3	0.44	0
31	DMS	v	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
23	CLA	b	617	-	65,73,73	2.25	19 (29%)	76,113,113	2.15	26 (34%)
25	BCR	b	619	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	7 (12%)
31	DMS	V	201	-	3,3,3	2.57	1 (33%)	3,3,3	0.76	0
23	CLA	b	608	41	65,73,73	2.11	18 (27%)	76,113,113	2.13	27 (35%)
23	CLA	B	608	41	65,73,73	2.04	16 (24%)	76,113,113	2.24	26 (34%)
23	CLA	B	610	-	65,73,73	1.96	15 (23%)	76,113,113	2.19	23 (30%)
23	CLA	B	611	41	65,73,73	2.29	20 (30%)	76,113,113	2.32	23 (30%)
35	HTG	c	923	-	11,12,19	0.54	0	11,11,24	1.89	2 (18%)
24	PHO	A	407	-	51,69,69	1.36	7 (13%)	47,99,99	1.70	11 (23%)
31	DMS	b	647	-	3,3,3	2.75	1 (33%)	3,3,3	0.71	0
31	DMS	d	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
30	LMT	B	644	-	24,24,36	0.34	0	29,29,47	1.26	4 (13%)
31	DMS	C	524	-	3,3,3	2.39	1 (33%)	3,3,3	0.94	0
35	HTG	b	622	-	19,19,19	1.31	3 (15%)	23,24,24	1.51	4 (17%)
26	SQD	a	412	-	53,54,54	0.93	3 (5%)	62,65,65	2.14	13 (20%)
30	LMT	I	101	-	36,36,36	0.74	1 (2%)	47,47,47	1.40	5 (10%)
23	CLA	d	403	-	65,73,73	1.95	16 (24%)	76,113,113	2.10	21 (27%)
28	LHG	A	412	-	48,48,48	1.05	2 (4%)	51,54,54	0.96	3 (5%)
31	DMS	d	418	-	3,3,3	2.75	1 (33%)	3,3,3	0.62	0
23	CLA	b	613	-	65,73,73	1.97	15 (23%)	76,113,113	2.28	25 (32%)
27	PL9	d	406	-	55,55,55	1.05	4 (7%)	68,69,69	1.59	12 (17%)
34	LMG	j	101	39	51,51,55	0.98	4 (7%)	59,59,63	1.16	7 (11%)
25	BCR	C	530	-	41,41,41	0.84	0	56,56,56	1.56	8 (14%)
23	CLA	c	904	-	65,73,73	2.69	18 (27%)	76,113,113	2.29	22 (28%)
31	DMS	A	418	-	3,3,3	2.73	1 (33%)	3,3,3	0.65	0
23	CLA	C	507	-	65,73,73	2.15	18 (27%)	76,113,113	2.35	20 (26%)
31	DMS	V	209	-	3,3,3	2.52	1 (33%)	3,3,3	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	911	-	65,73,73	2.18	16 (24%)	76,113,113	2.39	27 (35%)
36	DGD	C	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.13	8 (10%)
31	DMS	d	419	-	3,3,3	2.69	1 (33%)	3,3,3	0.71	0
31	DMS	O	311	-	3,3,3	2.64	1 (33%)	3,3,3	0.85	0
25	BCR	Y	101	-	41,41,41	0.85	0	56,56,56	1.66	15 (26%)
27	PL9	a	414	-	55,55,55	0.94	3 (5%)	68,69,69	1.65	16 (23%)
28	LHG	d	409	-	48,48,48	0.79	2 (4%)	51,54,54	1.28	8 (15%)
37	HEM	e	105	6,5	41,50,50	2.04	10 (24%)	45,82,82	1.84	10 (22%)
31	DMS	c	933	-	3,3,3	2.67	1 (33%)	3,3,3	0.93	0
37	HEM	E	105	6,5	41,50,50	1.85	9 (21%)	45,82,82	1.89	13 (28%)
23	CLA	C	504	-	65,73,73	2.39	18 (27%)	76,113,113	2.02	23 (30%)
35	HTG	b	623	-	19,19,19	1.11	2 (10%)	23,24,24	1.79	4 (17%)
24	PHO	a	408	-	51,69,69	1.52	7 (13%)	47,99,99	1.30	7 (14%)
34	LMG	c	920	-	51,51,55	0.96	2 (3%)	59,59,63	1.31	7 (11%)
31	DMS	B	637	-	3,3,3	2.27	1 (33%)	3,3,3	0.96	0
27	PL9	A	411	-	55,55,55	0.90	4 (7%)	68,69,69	1.69	14 (20%)
25	BCR	C	515	-	41,41,41	0.83	0	56,56,56	1.50	10 (17%)
35	HTG	C	522	-	19,19,19	1.05	2 (10%)	23,24,24	1.95	4 (17%)
30	LMT	B	623	-	36,36,36	0.59	0	47,47,47	1.05	3 (6%)
23	CLA	b	612	-	65,73,73	2.13	14 (21%)	76,113,113	2.33	27 (35%)
35	HTG	O	302	-	19,19,19	1.45	3 (15%)	23,24,24	1.51	5 (21%)
31	DMS	u	204	-	3,3,3	2.76	1 (33%)	3,3,3	0.87	0
23	CLA	B	605	-	65,73,73	2.04	16 (24%)	76,113,113	2.08	22 (28%)
32	BCT	A	420	21	2,3,3	0.48	0	2,3,3	1.16	0
31	DMS	o	304	-	3,3,3	2.76	1 (33%)	3,3,3	0.81	0
25	BCR	A	409	-	41,41,41	1.06	4 (9%)	56,56,56	1.44	9 (16%)
31	DMS	c	936	-	3,3,3	2.73	1 (33%)	3,3,3	0.83	0
31	DMS	l	102	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
31	DMS	O	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
28	LHG	K	101	-	43,43,48	1.07	2 (4%)	47,48,54	1.14	5 (10%)
31	DMS	c	934	-	3,3,3	2.70	1 (33%)	3,3,3	0.73	0
23	CLA	b	610	-	65,73,73	2.39	15 (23%)	76,113,113	1.96	21 (27%)
27	PL9	D	406	-	55,55,55	1.02	3 (5%)	68,69,69	1.49	13 (19%)
38	RRX	H	102	-	42,42,42	0.89	1 (2%)	57,58,58	1.57	9 (15%)
31	DMS	b	640	-	3,3,3	2.70	1 (33%)	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	B	640	-	3,3,3	2.63	1 (33%)	3,3,3	0.77	0
36	DGD	c	919	-	63,63,67	0.94	3 (4%)	77,77,81	1.23	10 (12%)
34	LMG	B	622	-	51,51,55	0.99	3 (5%)	59,59,63	1.31	9 (15%)
31	DMS	B	638	-	3,3,3	2.78	1 (33%)	3,3,3	1.01	0
23	CLA	C	506	-	65,73,73	2.24	18 (27%)	76,113,113	2.13	22 (28%)
23	CLA	C	514	-	65,73,73	2.60	18 (27%)	76,113,113	2.10	20 (26%)
31	DMS	c	926	-	3,3,3	2.61	1 (33%)	3,3,3	0.30	0
31	DMS	O	305	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
31	DMS	O	308	-	3,3,3	2.72	1 (33%)	3,3,3	0.69	0
25	BCR	k	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.21	8 (14%)
31	DMS	a	420	-	3,3,3	2.65	1 (33%)	3,3,3	0.36	0
23	CLA	B	617	-	65,73,73	1.99	18 (27%)	76,113,113	2.24	28 (36%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.17	9 (16%)
30	LMT	Z	101	-	36,36,36	0.70	1 (2%)	47,47,47	0.90	2 (4%)
35	HTG	C	523	-	19,19,19	1.09	2 (10%)	23,24,24	1.74	1 (4%)
30	LMT	a	418	-	36,36,36	0.71	1 (2%)	47,47,47	1.30	6 (12%)
34	LMG	J	101	39	51,51,55	0.93	2 (3%)	59,59,63	0.97	4 (6%)
31	DMS	b	634	-	3,3,3	2.45	1 (33%)	3,3,3	0.96	0
31	DMS	B	648	-	3,3,3	2.49	1 (33%)	3,3,3	1.05	0
23	CLA	c	907	-	65,73,73	2.36	17 (26%)	76,113,113	2.25	24 (31%)
25	BCR	B	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.48	9 (16%)
31	DMS	b	639	-	3,3,3	2.77	1 (33%)	3,3,3	1.33	1 (33%)
23	CLA	b	611	41	65,73,73	2.10	19 (29%)	76,113,113	1.97	22 (28%)
23	CLA	B	604	-	65,73,73	1.87	16 (24%)	76,113,113	2.56	28 (36%)
24	PHO	D	402	-	51,69,69	1.77	7 (13%)	47,99,99	1.63	8 (17%)
23	CLA	d	401	41	65,73,73	2.02	11 (16%)	76,113,113	2.18	25 (32%)
23	CLA	A	406	41	65,73,73	1.70	14 (21%)	76,113,113	2.48	23 (30%)
25	BCR	c	916	-	41,41,41	0.81	0	56,56,56	1.56	10 (17%)
28	LHG	E	101	-	48,48,48	1.06	2 (4%)	51,54,54	1.17	5 (9%)
30	LMT	A	416	-	36,36,36	0.84	1 (2%)	47,47,47	1.19	6 (12%)
31	DMS	C	527	-	3,3,3	2.56	1 (33%)	3,3,3	0.63	0
31	DMS	b	635	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
36	DGD	d	407	-	50,50,67	1.11	2 (4%)	58,58,81	1.24	6 (10%)
23	CLA	c	912	3	65,73,73	2.53	17 (26%)	76,113,113	2.25	20 (26%)
23	CLA	d	404	-	65,73,73	1.91	17 (26%)	76,113,113	2.39	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	c	930	-	51,51,55	1.07	3 (5%)	59,59,63	1.26	5 (8%)
31	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	1.00	0
23	CLA	c	905	41	65,73,73	2.27	17 (26%)	76,113,113	2.68	26 (34%)
23	CLA	C	503	-	65,73,73	2.26	15 (23%)	76,113,113	2.09	20 (26%)
31	DMS	b	644	-	3,3,3	2.78	1 (33%)	3,3,3	0.99	0
30	LMT	e	103	-	25,25,36	0.71	1 (4%)	30,30,47	1.02	3 (10%)
23	CLA	B	602	41	65,73,73	2.43	17 (26%)	76,113,113	2.57	24 (31%)
31	DMS	v	206	-	3,3,3	2.60	1 (33%)	3,3,3	0.81	0
24	PHO	a	409	-	51,69,69	1.66	8 (15%)	47,99,99	2.03	10 (21%)
25	BCR	b	620	-	41,41,41	0.90	2 (4%)	56,56,56	1.24	5 (8%)
28	LHG	d	410	-	45,45,48	1.00	2 (4%)	48,51,54	1.02	3 (6%)
25	BCR	T	101	-	41,41,41	0.90	0	56,56,56	1.81	18 (32%)
28	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.24	3 (5%)
23	CLA	A	405	-	65,73,73	1.90	16 (24%)	76,113,113	2.26	28 (36%)
25	BCR	B	620	-	41,41,41	1.00	2 (4%)	56,56,56	1.57	13 (23%)
40	HEC	V	203	16	32,50,50	1.82	6 (18%)	24,82,82	1.70	5 (20%)
31	DMS	D	415	-	3,3,3	2.74	1 (33%)	3,3,3	0.69	0
31	DMS	D	417	-	3,3,3	2.99	1 (33%)	3,3,3	0.77	0
30	LMT	m	104	-	36,36,36	0.56	0	47,47,47	1.24	4 (8%)
31	DMS	H	105	-	3,3,3	2.74	1 (33%)	3,3,3	0.65	0
35	HTG	c	922	-	19,19,19	1.02	2 (10%)	23,24,24	1.74	3 (13%)
31	DMS	a	401	-	3,3,3	2.71	1 (33%)	3,3,3	0.70	0
25	BCR	c	915	-	41,41,41	0.79	0	56,56,56	1.33	8 (14%)
31	DMS	h	101	-	3,3,3	2.68	1 (33%)	3,3,3	1.34	1 (33%)
35	HTG	b	628	-	19,19,19	0.90	1 (5%)	23,24,24	1.51	1 (4%)
23	CLA	c	902	-	65,73,73	2.14	17 (26%)	76,113,113	2.70	22 (28%)
36	DGD	D	407	-	50,50,67	1.28	3 (6%)	58,58,81	1.74	8 (13%)
23	CLA	a	410	-	65,73,73	2.01	14 (21%)	76,113,113	2.32	28 (36%)
34	LMG	C	531	-	51,51,55	1.03	2 (3%)	59,59,63	1.08	4 (6%)
23	CLA	B	615	-	65,73,73	2.13	18 (27%)	76,113,113	2.58	27 (35%)
23	CLA	A	408	-	65,73,73	2.06	17 (26%)	76,113,113	2.71	27 (35%)
28	LHG	e	101	-	39,39,48	1.16	2 (5%)	42,45,54	1.02	3 (7%)
23	CLA	C	512	3	65,73,73	2.37	19 (29%)	76,113,113	2.36	22 (28%)
31	DMS	k	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.78	0
31	DMS	v	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	d	414	-	3,3,3	2.70	1 (33%)	3,3,3	0.77	0
31	DMS	o	301	-	3,3,3	2.14	1 (33%)	3,3,3	0.39	0
23	CLA	c	914	-	65,73,73	2.54	18 (27%)	76,113,113	2.30	23 (30%)
23	CLA	B	609	-	65,73,73	2.02	18 (27%)	76,113,113	2.16	25 (32%)
26	SQD	L	102	-	53,54,54	1.08	3 (5%)	62,65,65	1.68	12 (19%)
35	HTG	V	204	-	14,14,19	0.67	0	18,19,24	3.10	6 (33%)
36	DGD	h	102	-	63,63,67	0.93	3 (4%)	77,77,81	1.23	9 (11%)
30	LMT	b	621	-	25,25,36	0.63	1 (4%)	30,30,47	1.30	5 (16%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.22	8 (10%)
23	CLA	b	609	-	65,73,73	2.10	15 (23%)	76,113,113	2.11	26 (34%)
28	LHG	D	410	-	48,48,48	0.83	2 (4%)	51,54,54	1.13	2 (3%)
31	DMS	O	307	-	3,3,3	2.75	1 (33%)	3,3,3	0.72	0
31	DMS	V	211	-	3,3,3	2.97	1 (33%)	3,3,3	1.05	0
31	DMS	b	638	-	3,3,3	2.93	1 (33%)	3,3,3	1.08	0
31	DMS	C	528	-	3,3,3	2.64	1 (33%)	3,3,3	0.71	0
30	LMT	z	101	-	32,32,36	0.63	1 (3%)	42,42,47	1.19	5 (11%)
31	DMS	c	937	-	3,3,3	2.66	1 (33%)	3,3,3	0.62	0
31	DMS	b	637	-	3,3,3	2.68	1 (33%)	3,3,3	1.01	0
23	CLA	a	407	41	65,73,73	1.87	17 (26%)	76,113,113	2.25	23 (30%)
31	DMS	A	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.71	0
23	CLA	b	606	-	65,73,73	1.94	17 (26%)	76,113,113	2.41	25 (32%)
31	DMS	h	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.58	0
31	DMS	u	203	-	3,3,3	2.58	1 (33%)	3,3,3	0.92	0
28	LHG	l	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.03	3 (5%)
26	SQD	a	417	-	53,54,54	1.10	5 (9%)	62,65,65	1.35	4 (6%)
31	DMS	B	646	-	3,3,3	2.60	1 (33%)	3,3,3	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	c	918	-	-	16/51/91/95	0/2/2/2
23	CLA	C	509	-	1/1/15/20	6/37/115/115	-
35	HTG	B	630	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	602	41	1/1/15/20	18/37/115/115	-
23	CLA	c	913	-	1/1/15/20	7/37/115/115	-
34	LMG	C	501	-	-	24/46/66/70	0/1/1/1
23	CLA	B	603	-	1/1/15/20	4/37/115/115	-
30	LMT	m	103	-	-	10/21/61/61	0/2/2/2
23	CLA	c	906	-	1/1/15/20	4/37/115/115	-
26	SQD	A	415	-	-	24/49/69/69	0/1/1/1
28	LHG	d	402	-	-	24/48/48/53	-
30	LMT	F	101	-	-	11/21/61/61	0/2/2/2
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	8/37/115/115	-
23	CLA	B	616	-	1/1/15/20	5/37/115/115	-
35	HTG	c	921	-	-	5/10/30/30	0/1/1/1
23	CLA	C	502	-	1/1/15/20	3/37/115/115	-
23	CLA	b	614	-	1/1/15/20	3/37/115/115	-
25	BCR	a	411	-	-	1/29/63/63	0/2/2/2
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-
35	HTG	D	414	-	-	3/10/30/30	0/1/1/1
35	HTG	B	631	-	-	3/10/30/30	0/1/1/1
23	CLA	b	607	-	1/1/15/20	11/37/115/115	-
23	CLA	c	903	-	-	8/37/115/115	-
25	BCR	d	405	-	-	4/29/63/63	0/2/2/2
36	DGD	C	518	-	-	14/51/91/95	0/2/2/2
23	CLA	B	614	-	1/1/15/20	5/37/115/115	-
36	DGD	c	917	-	-	13/51/91/95	0/2/2/2
28	LHG	a	415	-	-	20/53/53/53	-
23	CLA	c	908	41	1/1/15/20	10/37/115/115	-
23	CLA	B	613	-	1/1/15/20	2/37/115/115	-
26	SQD	D	408	-	-	19/40/60/69	0/1/1/1
30	LMT	B	643	-	-	6/15/35/61	0/1/1/2
28	LHG	L	101	-	-	18/53/53/53	-
35	HTG	d	413	-	-	7/10/30/30	0/1/1/1
35	HTG	C	521	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	v	203	16	-	2/10/54/54	-
23	CLA	a	406	-	1/1/15/20	6/37/115/115	-
23	CLA	b	604	-	1/1/15/20	5/37/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	c	909	-	-	4/37/115/115	-
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
23	CLA	B	606	-	1/1/15/20	6/37/115/115	-
25	BCR	D	405	-	-	4/29/63/63	0/2/2/2
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
30	LMT	a	422	-	-	5/21/61/61	0/2/2/2
23	CLA	b	603	-	1/1/15/20	2/37/115/115	-
23	CLA	D	403	-	1/1/15/20	7/37/115/115	-
23	CLA	C	508	41	1/1/15/20	11/37/115/115	-
23	CLA	D	404	-	1/1/15/20	11/37/115/115	-
34	LMG	D	412	-	-	24/46/66/70	0/1/1/1
35	HTG	v	204	-	-	7/10/30/30	0/1/1/1
26	SQD	A	410	-	-	20/49/69/69	0/1/1/1
23	CLA	c	910	-	1/1/15/20	9/37/115/115	-
23	CLA	C	513	-	1/1/15/20	14/37/115/115	-
35	HTG	B	626	-	-	7/10/30/30	0/1/1/1
26	SQD	x	101	-	-	19/36/56/69	0/1/1/1
36	DGD	H	103	-	-	10/51/91/95	0/2/2/2
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
23	CLA	D	401	41	-	4/37/115/115	-
23	CLA	b	605	-	1/1/15/20	5/37/115/115	-
34	LMG	a	413	-	-	24/46/66/70	0/1/1/1
23	CLA	C	511	-	1/1/15/20	2/37/115/115	-
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
34	LMG	m	102	-	-	18/46/66/70	0/1/1/1
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
34	LMG	C	520	-	-	20/46/66/70	0/1/1/1
23	CLA	b	615	-	1/1/15/20	13/37/115/115	-
30	LMT	T	103	-	-	7/15/35/61	0/1/1/2
28	LHG	D	409	-	-	9/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	d	411	-	-	25/46/66/70	0/1/1/1
23	CLA	B	607	-	1/1/15/20	8/37/115/115	-
23	CLA	C	505	41	1/1/15/20	9/37/115/115	-
28	LHG	D	411	-	-	15/50/50/53	-
38	RRX	x	102	-	-	0/29/65/65	0/2/2/2
23	CLA	C	510	-	1/1/15/20	9/37/115/115	-
25	BCR	j	104	-	-	2/29/63/63	0/2/2/2
23	CLA	b	617	-	1/1/15/20	19/37/115/115	-
25	BCR	b	619	-	-	1/29/63/63	0/2/2/2
36	DGD	C	519	-	-	18/51/91/95	0/2/2/2
23	CLA	b	608	41	1/1/15/20	2/37/115/115	-
23	CLA	B	608	41	1/1/15/20	3/37/115/115	-
23	CLA	B	611	41	1/1/15/20	5/37/115/115	-
23	CLA	B	610	-	-	0/37/115/115	-
35	HTG	c	923	-	-	4/8/10/30	-
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
30	LMT	B	644	-	-	8/15/35/61	0/1/1/2
35	HTG	b	622	-	-	4/10/30/30	0/1/1/1
26	SQD	a	412	-	-	23/49/69/69	0/1/1/1
30	LMT	I	101	-	-	8/21/61/61	0/2/2/2
23	CLA	d	403	-	1/1/15/20	1/37/115/115	-
28	LHG	A	412	-	-	29/53/53/53	-
23	CLA	b	613	-	1/1/15/20	3/37/115/115	-
27	PL9	d	406	-	-	4/53/73/73	0/1/1/1
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
25	BCR	C	530	-	-	0/29/63/63	0/2/2/2
23	CLA	c	904	-	-	4/37/115/115	-
23	CLA	C	507	-	1/1/15/20	16/37/115/115	-
23	CLA	c	911	-	1/1/15/20	3/37/115/115	-
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
27	PL9	a	414	-	-	11/53/73/73	0/1/1/1
28	LHG	d	409	-	-	10/53/53/53	-
37	HEM	e	105	6,5	-	3/12/54/54	-
37	HEM	E	105	6,5	-	5/12/54/54	-
23	CLA	C	504	-	-	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	b	623	-	-	8/10/30/30	0/1/1/1
24	PHO	a	408	-	-	6/37/103/103	0/5/6/6
34	LMG	c	920	-	-	21/46/66/70	0/1/1/1
27	PL9	A	411	-	-	14/53/73/73	0/1/1/1
25	BCR	C	515	-	-	3/29/63/63	0/2/2/2
35	HTG	C	522	-	-	5/10/30/30	0/1/1/1
30	LMT	B	623	-	-	15/21/61/61	0/2/2/2
23	CLA	b	612	-	-	6/37/115/115	-
35	HTG	O	302	-	-	3/10/30/30	0/1/1/1
23	CLA	B	605	-	1/1/15/20	8/37/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
28	LHG	K	101	-	-	24/45/45/53	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
23	CLA	b	610	-	-	0/37/115/115	-
27	PL9	D	406	-	-	3/53/73/73	0/1/1/1
36	DGD	c	919	-	-	15/51/91/95	0/2/2/2
34	LMG	B	622	-	-	15/46/66/70	0/1/1/1
23	CLA	C	506	-	1/1/15/20	2/37/115/115	-
23	CLA	C	514	-	-	9/37/115/115	-
25	BCR	k	102	-	-	2/29/63/63	0/2/2/2
23	CLA	B	617	-	1/1/15/20	11/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
35	HTG	C	523	-	-	4/10/30/30	0/1/1/1
30	LMT	a	418	-	-	12/21/61/61	0/2/2/2
34	LMG	J	101	39	-	15/46/66/70	0/1/1/1
23	CLA	c	907	-	1/1/15/20	10/37/115/115	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
23	CLA	b	611	41	1/1/15/20	7/37/115/115	-
23	CLA	B	604	-	1/1/15/20	3/37/115/115	-
24	PHO	D	402	-	-	3/37/103/103	0/5/6/6
23	CLA	d	401	41	-	7/37/115/115	-
23	CLA	A	406	41	-	11/37/115/115	-
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
28	LHG	E	101	-	-	28/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	A	416	-	-	7/21/61/61	0/2/2/2
36	DGD	d	407	-	-	22/44/64/95	0/1/1/2
23	CLA	c	912	3	-	1/37/115/115	-
23	CLA	d	404	-	-	13/37/115/115	-
34	LMG	c	930	-	-	7/46/66/70	0/1/1/1
23	CLA	c	905	41	-	9/37/115/115	-
23	CLA	C	503	-	-	6/37/115/115	-
30	LMT	e	103	-	-	6/17/37/61	0/1/1/2
23	CLA	B	602	41	1/1/15/20	19/37/115/115	-
24	PHO	a	409	-	-	5/37/103/103	0/5/6/6
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
28	LHG	d	410	-	-	11/50/50/53	-
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
28	LHG	d	408	-	-	14/53/53/53	-
23	CLA	A	405	-	-	2/37/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
40	HEC	V	203	16	-	2/10/54/54	-
30	LMT	m	104	-	-	2/21/61/61	0/2/2/2
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
25	BCR	c	915	-	-	1/29/63/63	0/2/2/2
35	HTG	b	628	-	-	1/10/30/30	0/1/1/1
23	CLA	c	902	-	1/1/15/20	4/37/115/115	-
36	DGD	D	407	-	-	24/44/64/95	0/1/1/2
23	CLA	a	410	-	-	8/37/115/115	-
34	LMG	C	531	-	-	18/46/66/70	0/1/1/1
23	CLA	B	615	-	1/1/15/20	9/37/115/115	-
23	CLA	A	408	-	-	18/37/115/115	-
28	LHG	e	101	-	-	18/44/44/53	-
23	CLA	C	512	3	-	0/37/115/115	-
23	CLA	c	914	-	-	9/37/115/115	-
23	CLA	B	609	-	-	1/37/115/115	-
26	SQD	L	102	-	-	27/49/69/69	0/1/1/1
35	HTG	V	204	-	-	1/5/25/30	0/1/1/1
36	DGD	h	102	-	-	17/51/91/95	0/2/2/2
30	LMT	b	621	-	-	12/17/37/61	0/1/1/2
36	DGD	C	517	-	-	13/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	609	-	-	1/37/115/115	-
28	LHG	D	410	-	-	10/53/53/53	-
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
23	CLA	a	407	41	-	9/37/115/115	-
23	CLA	b	606	-	1/1/15/20	6/37/115/115	-
28	LHG	l	101	-	-	13/53/53/53	-
26	SQD	a	417	-	-	14/49/69/69	0/1/1/1

The worst 5 of 1542 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 2474 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	905	CLA	C4A-NA-C1A	12.36	112.26	106.71
23	c	910	CLA	C4A-NA-C1A	12.30	112.23	106.71
23	C	512	CLA	C4A-NA-C1A	11.20	111.74	106.71
23	c	902	CLA	C4A-NA-C1A	11.01	111.66	106.71
23	b	612	CLA	C4A-NA-C1A	10.40	111.38	106.71

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 1579 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6

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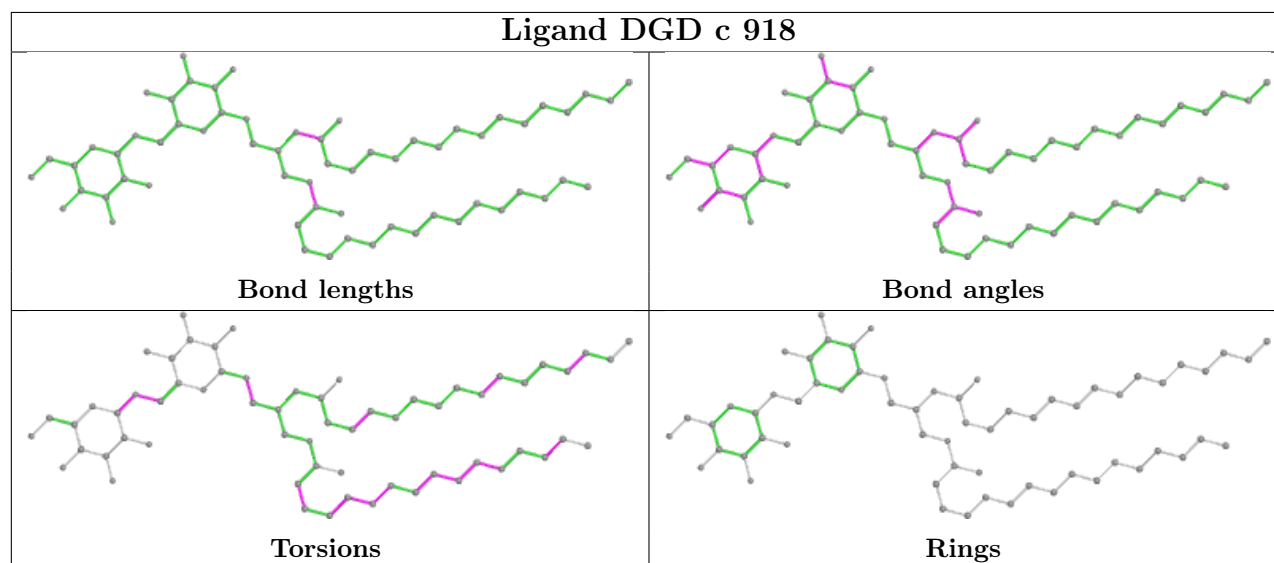
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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CAD-CBD-CGD-O1D

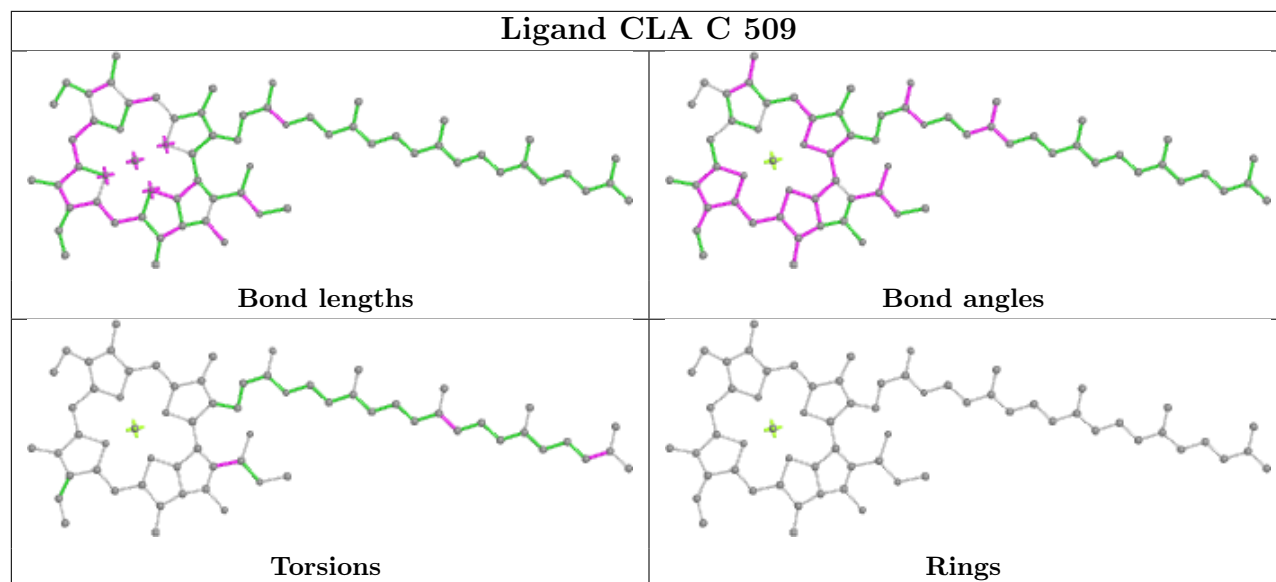
There are no ring outliers.

No monomer is involved in short contacts.

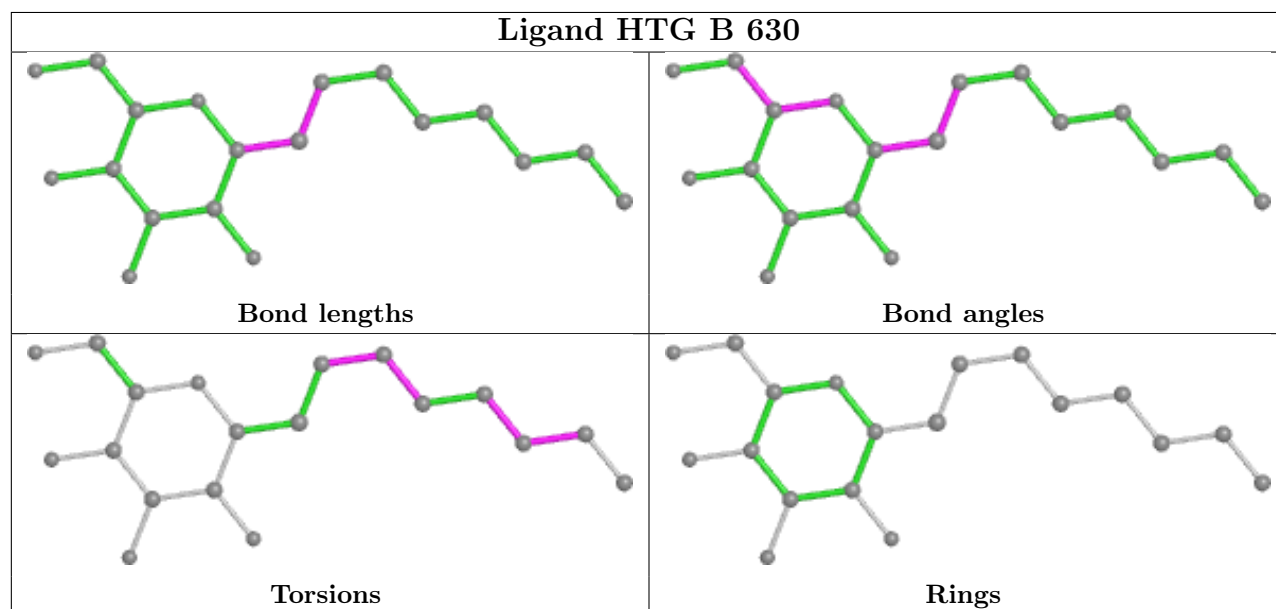
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



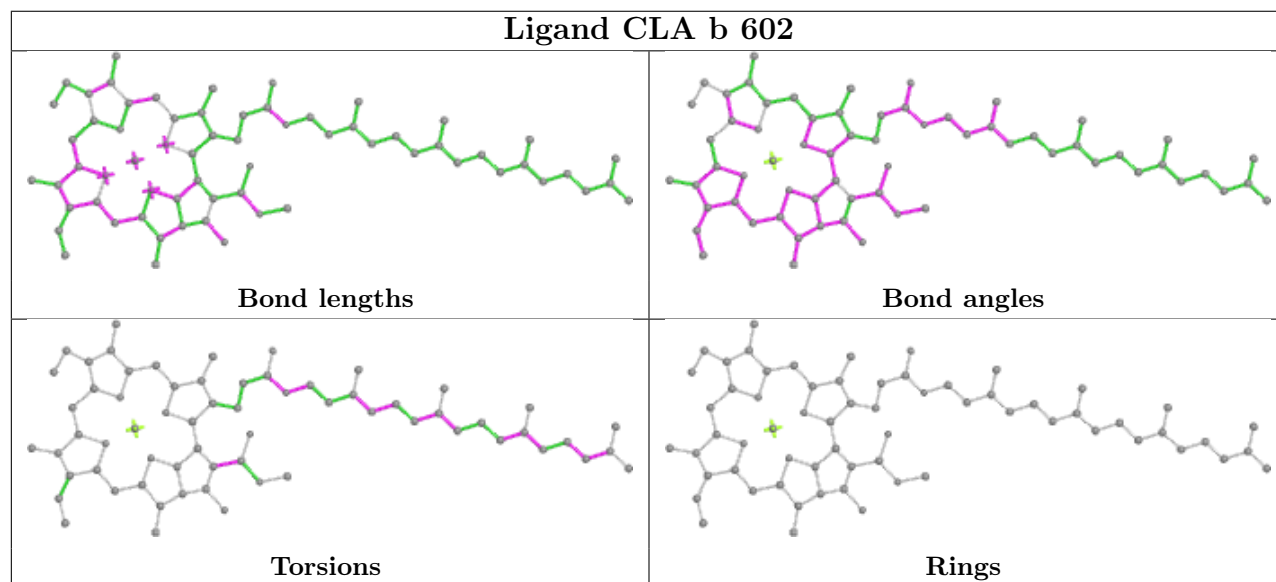
Ligand CLA C 509

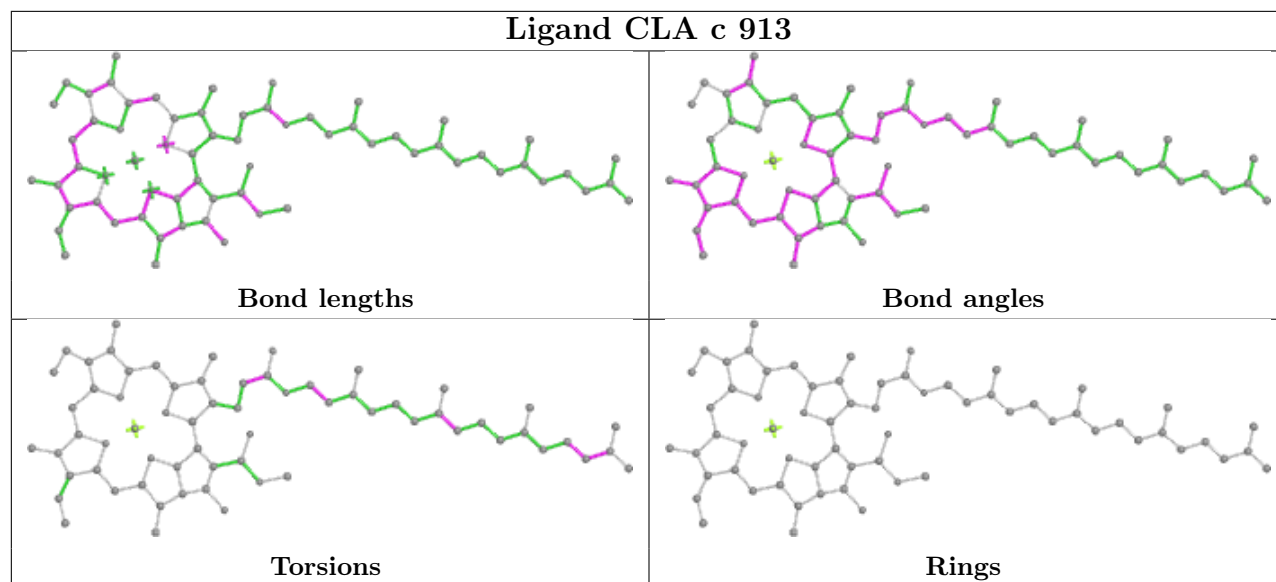
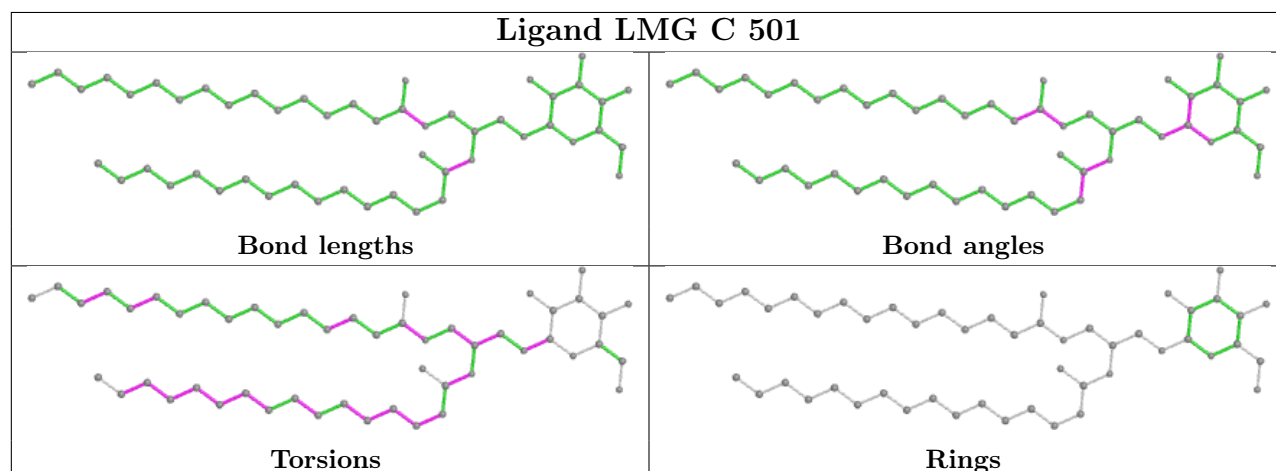
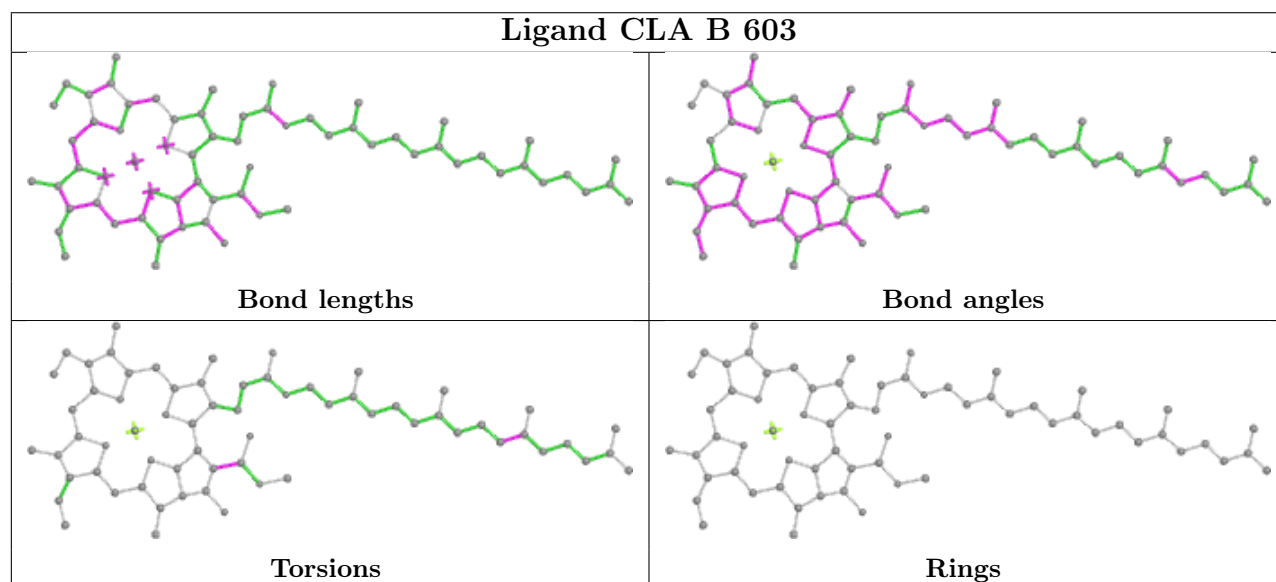


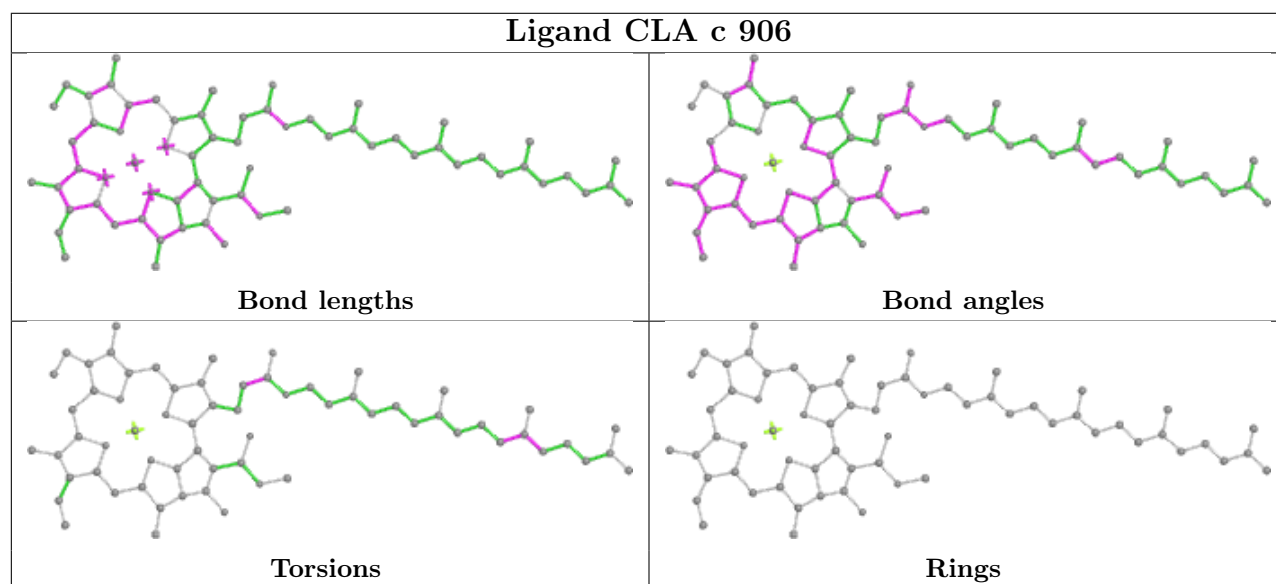
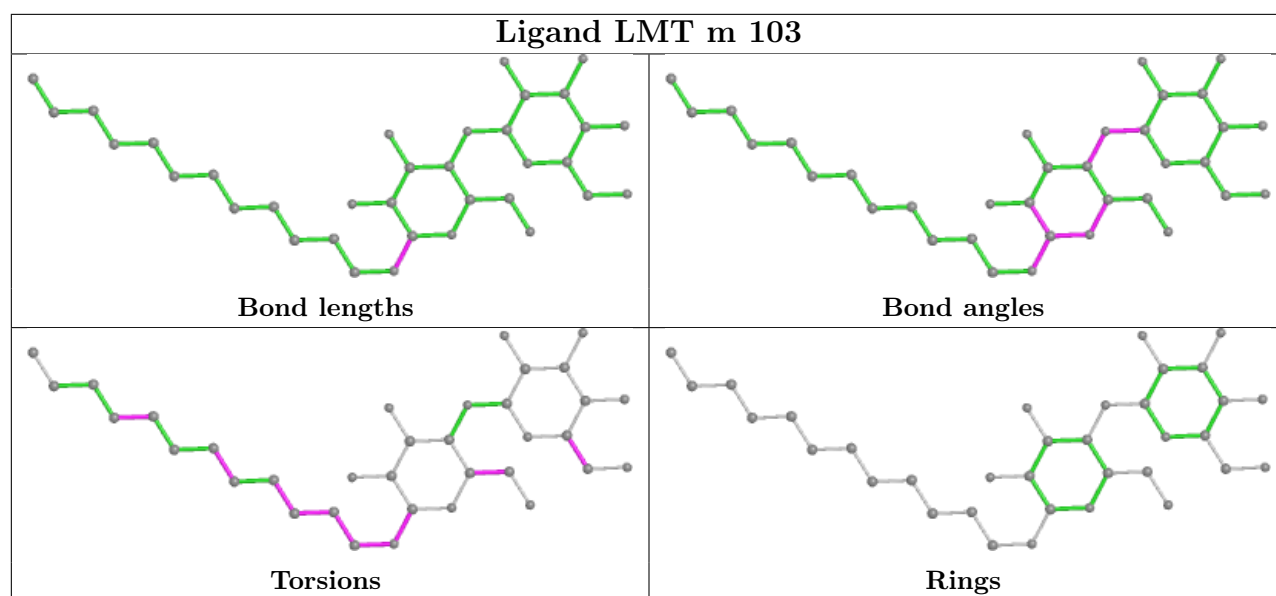
Ligand HTG B 630

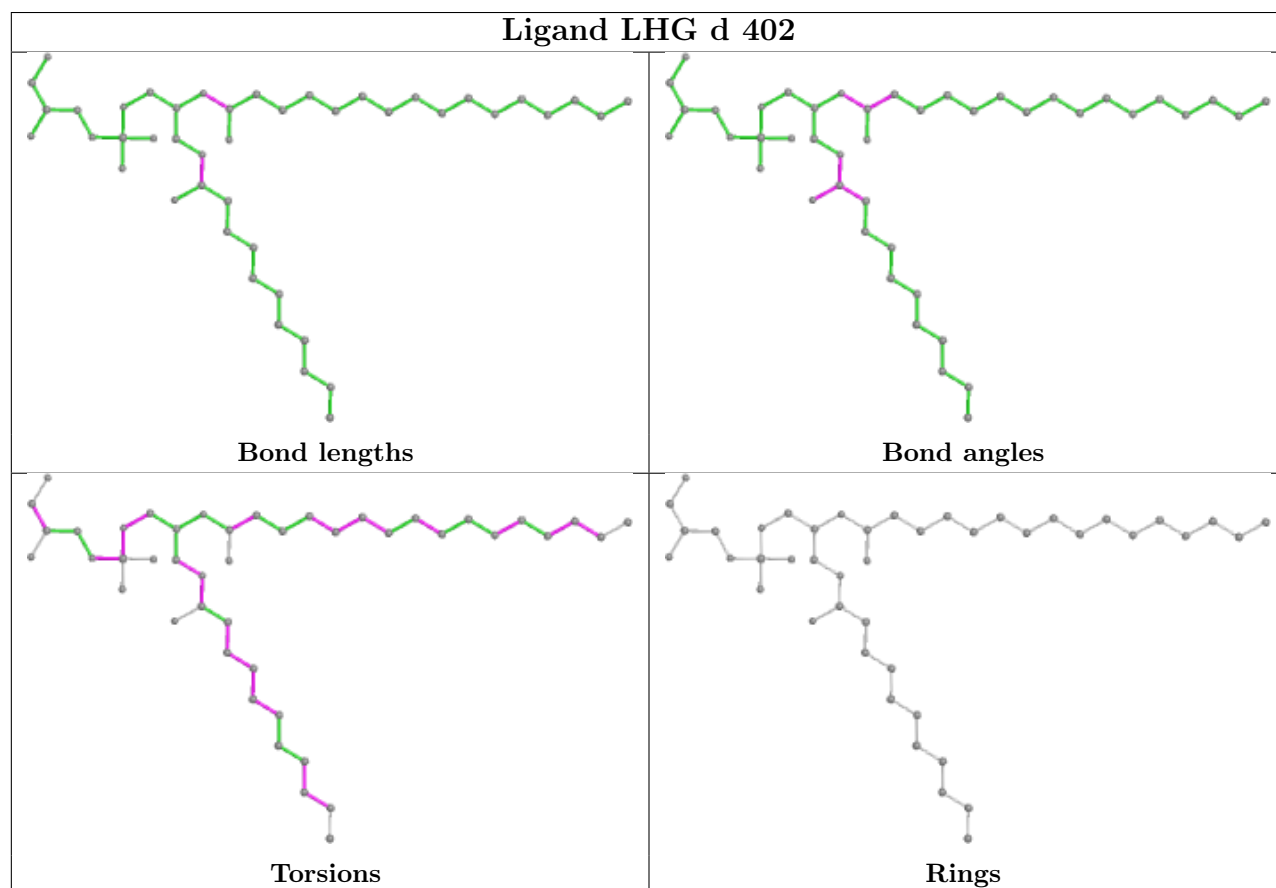
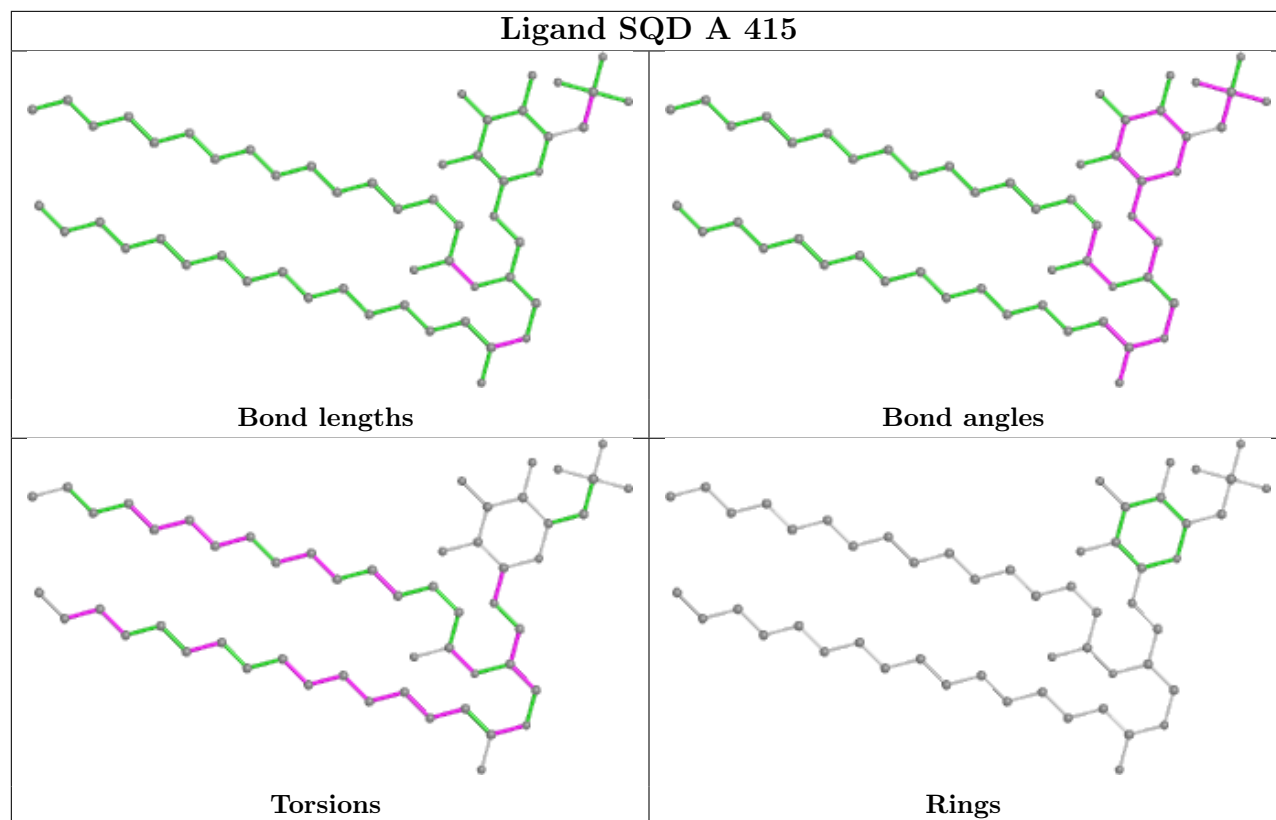


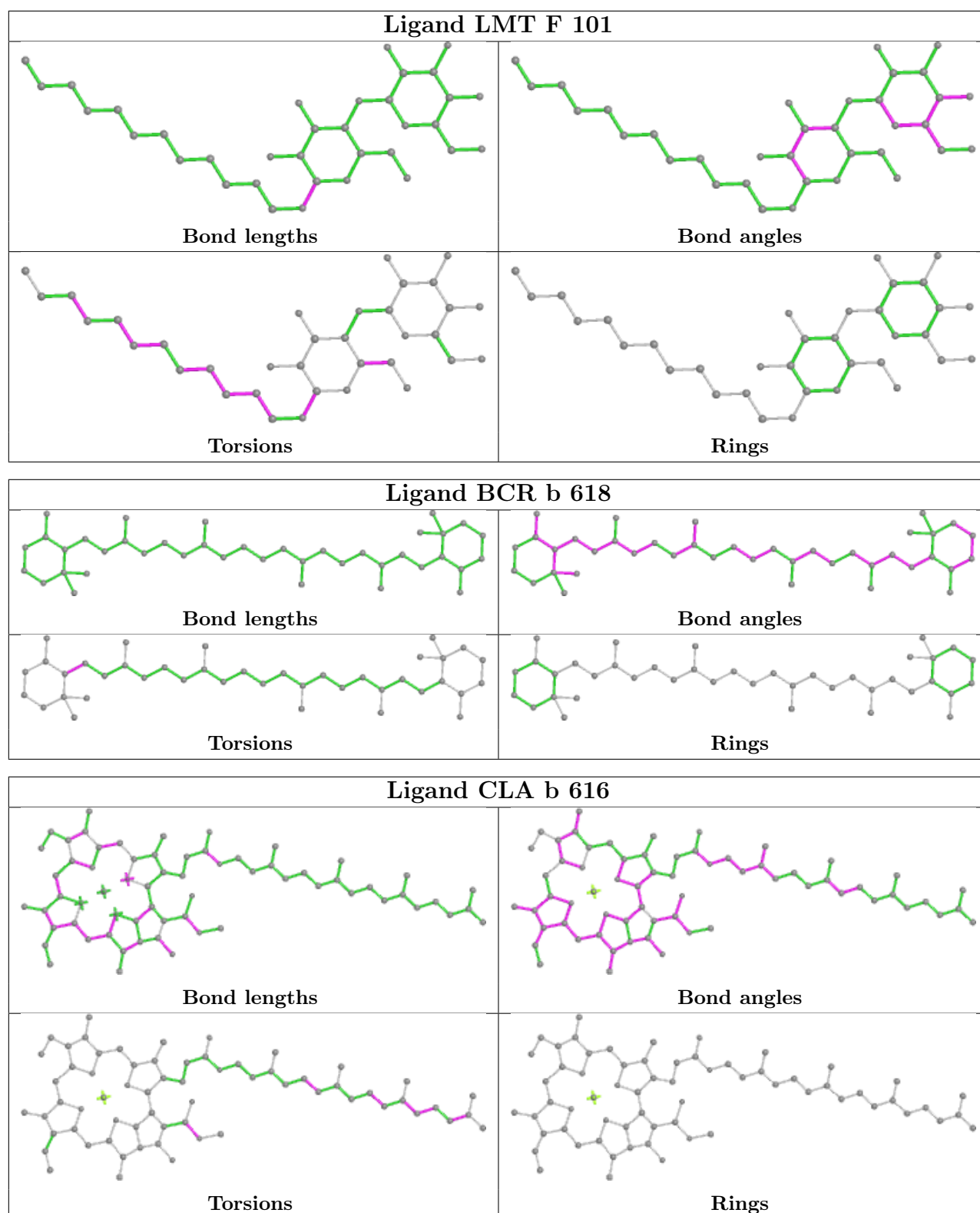
Ligand CLA b 602



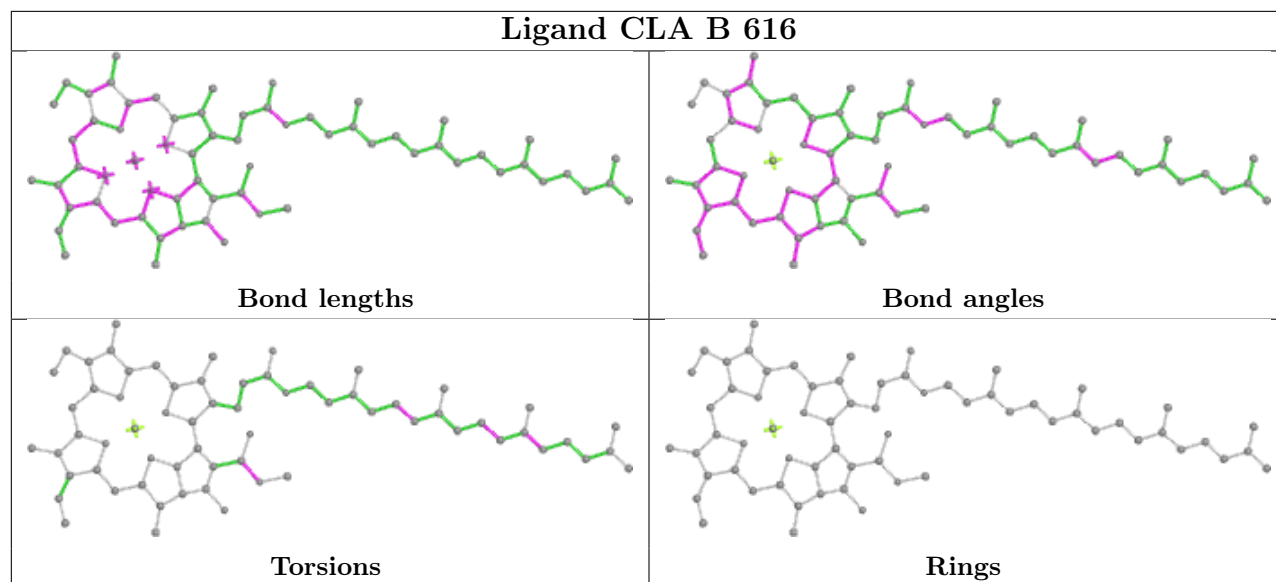
Ligand CLA c 913**Ligand LMG C 501****Ligand CLA B 603**



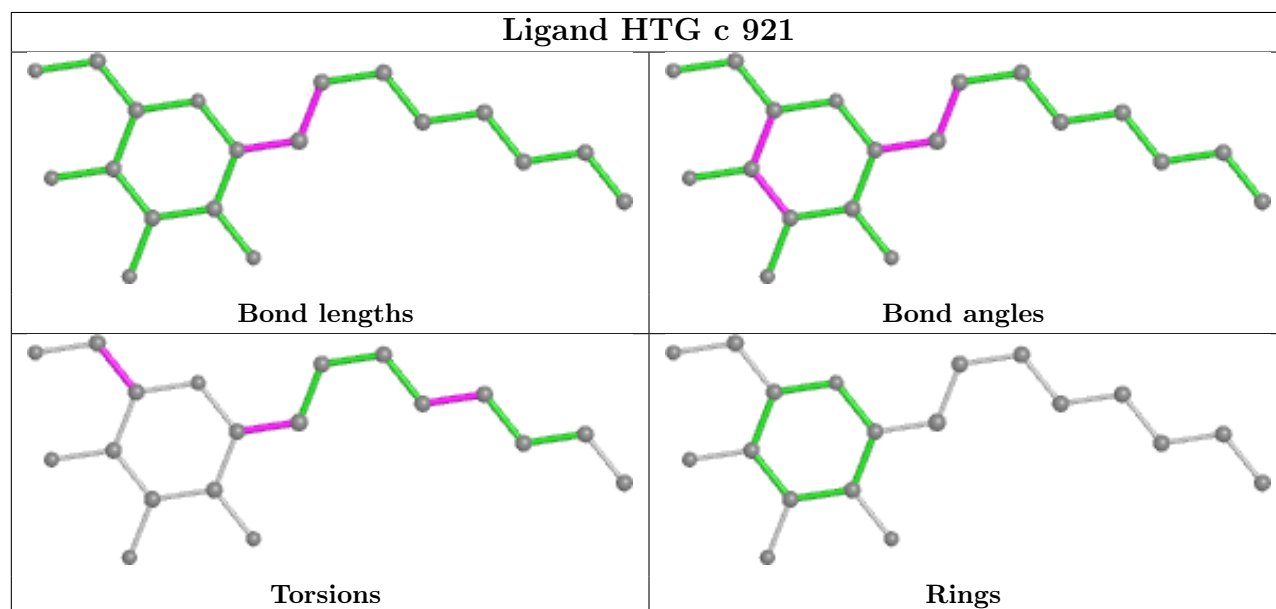




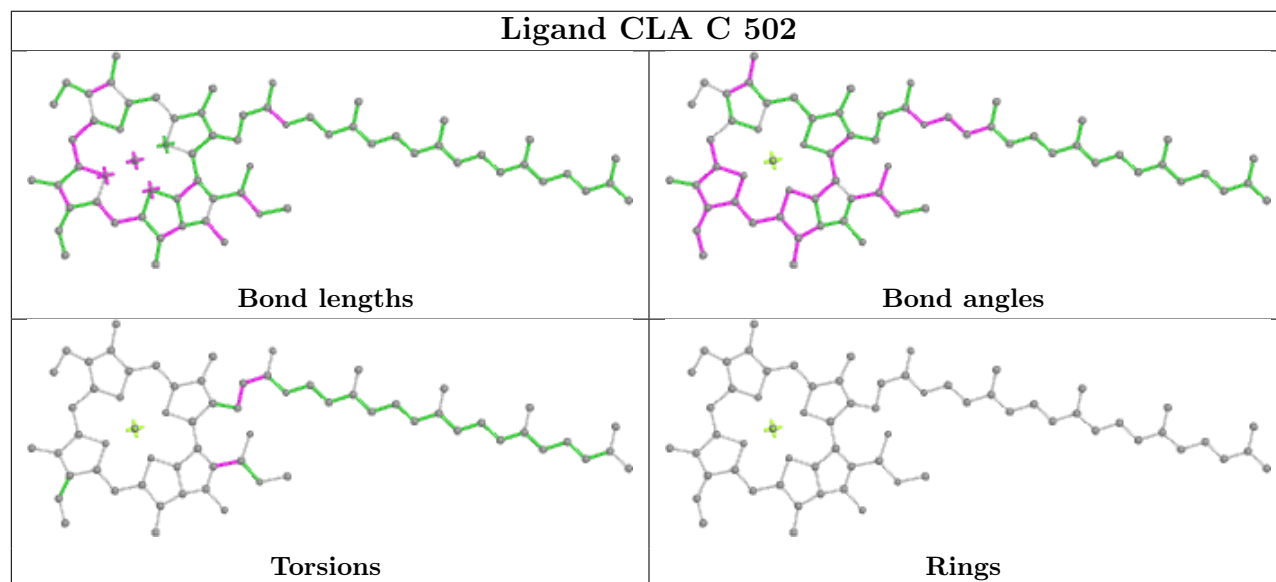
Ligand CLA B 616

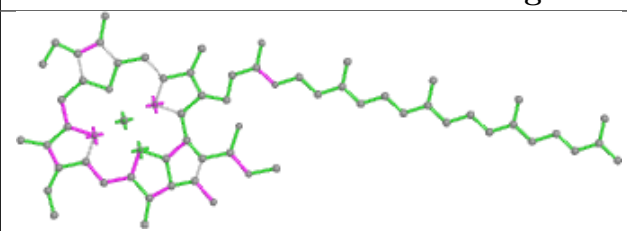
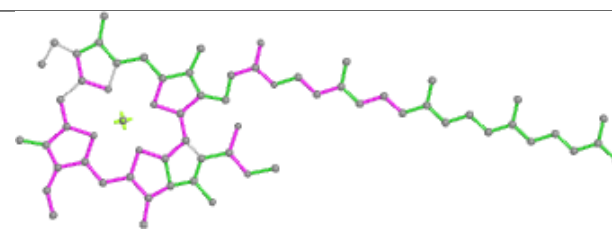
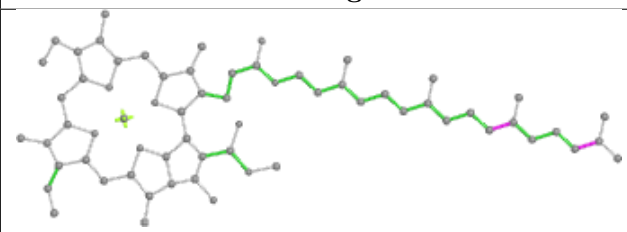
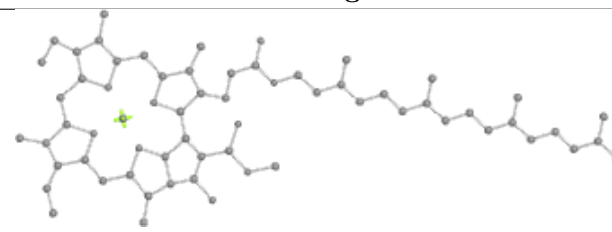


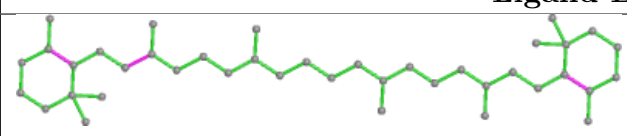
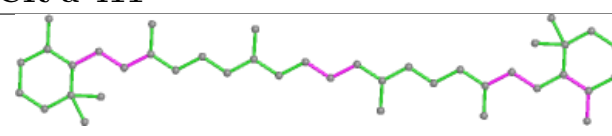
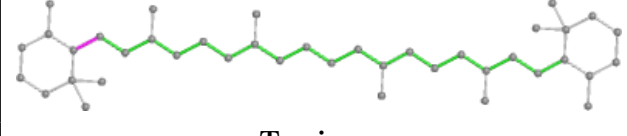
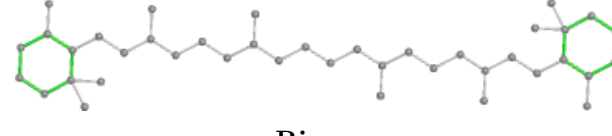
Ligand HTG c 921

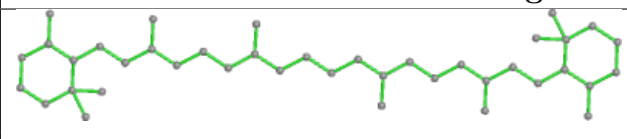
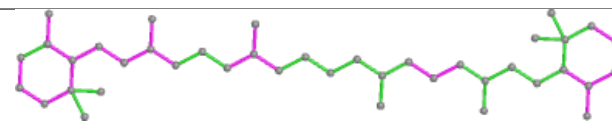
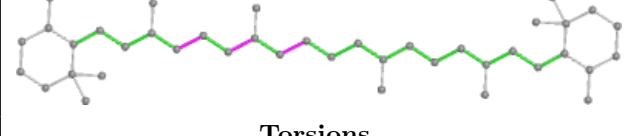



Ligand CLA C 502

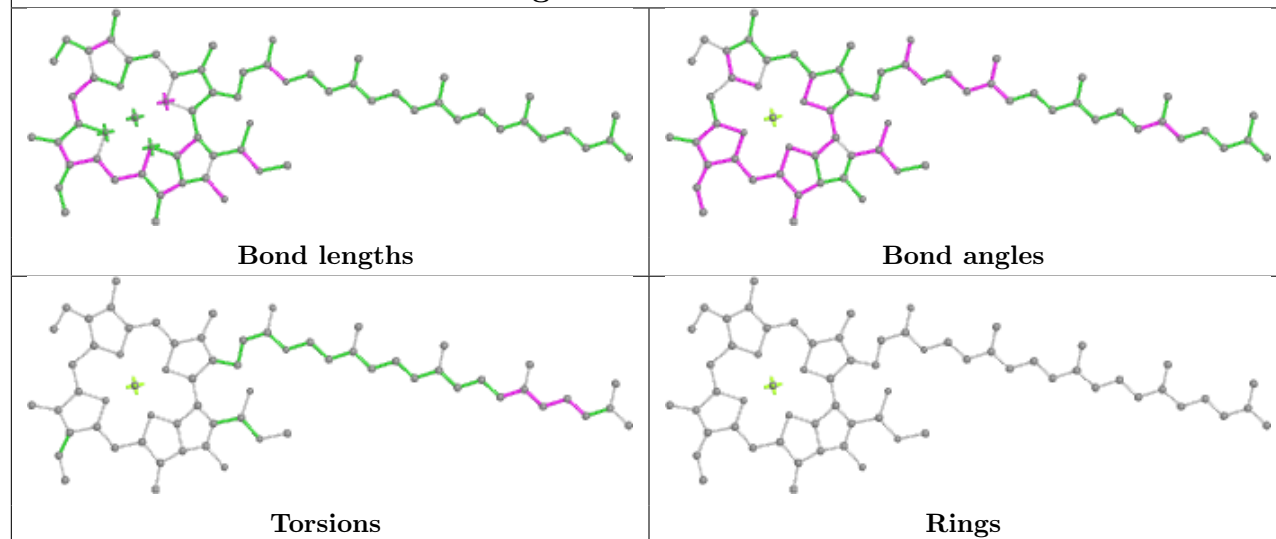


Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

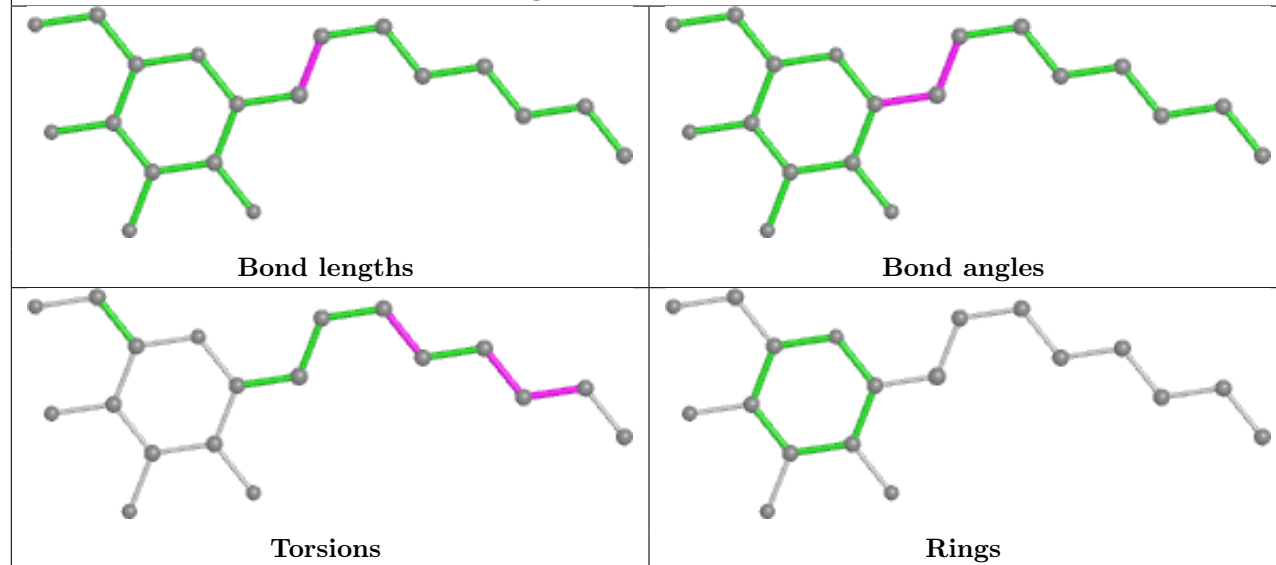
Ligand BCR a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

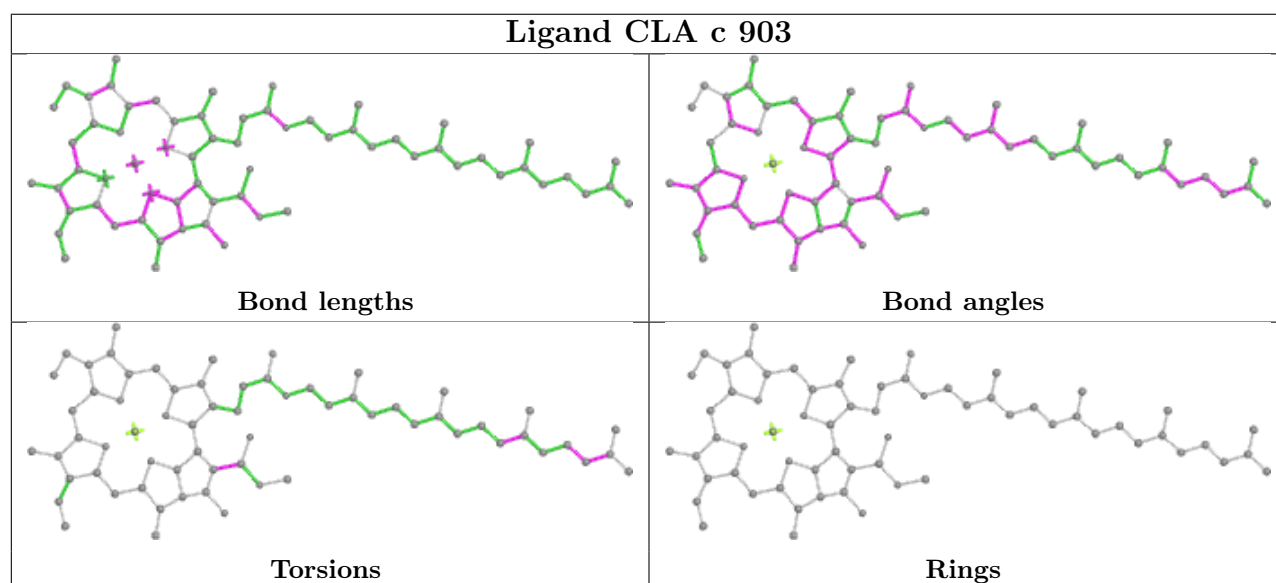
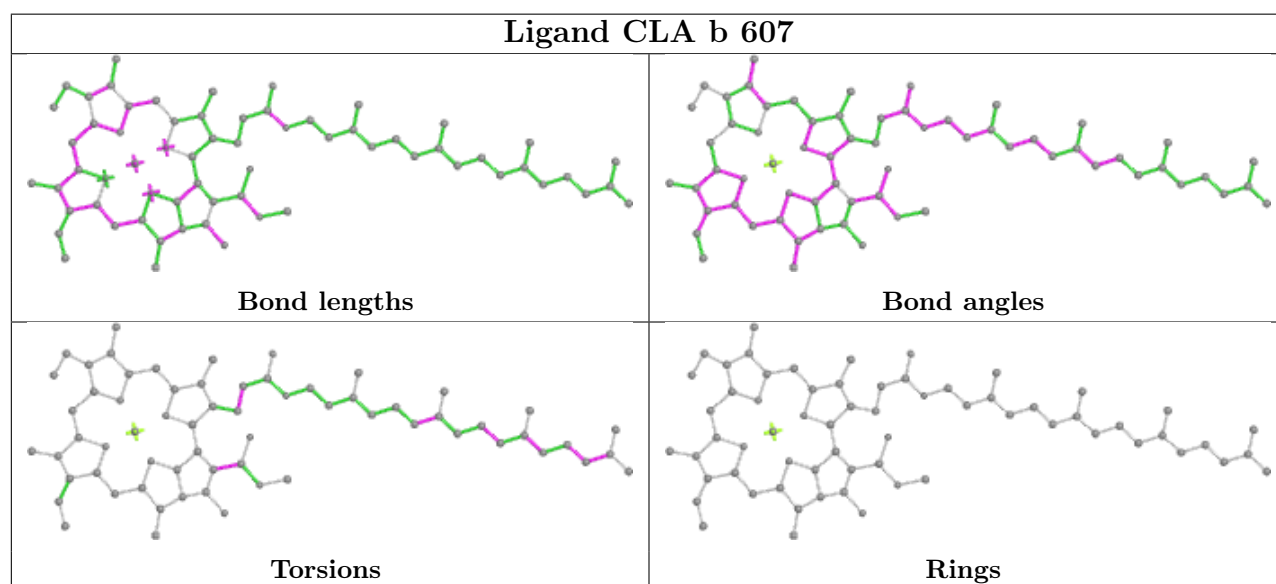
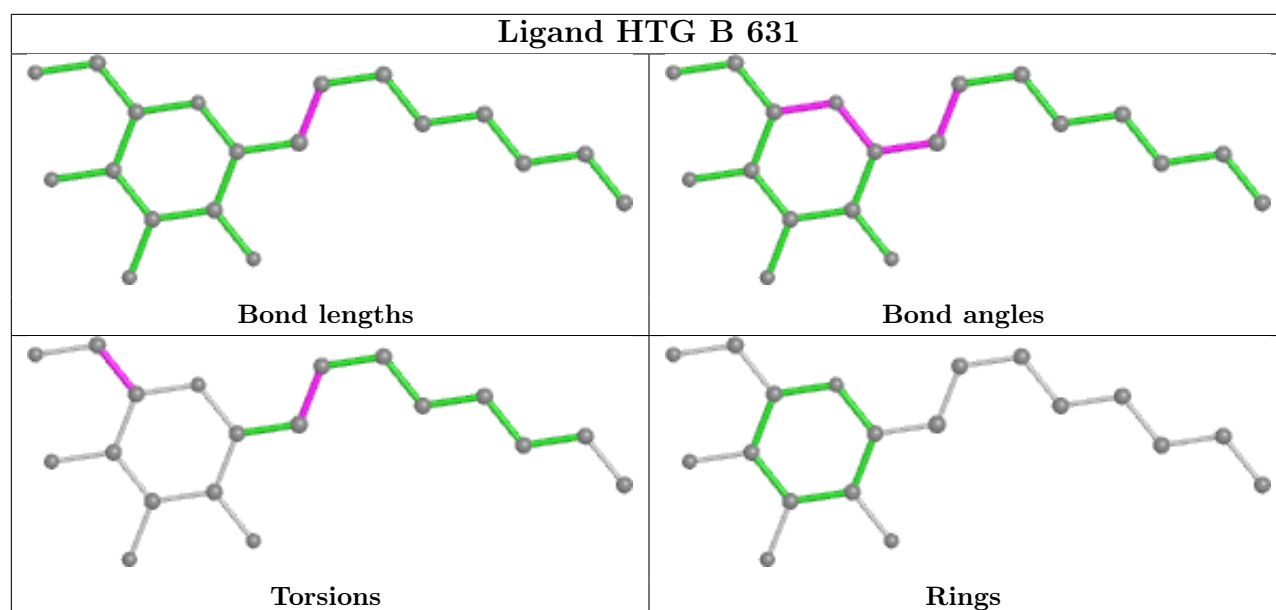
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

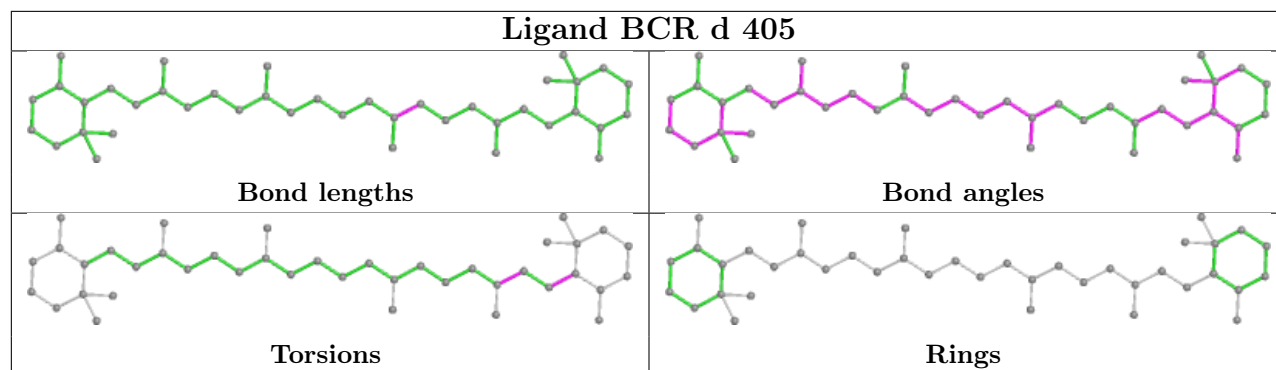
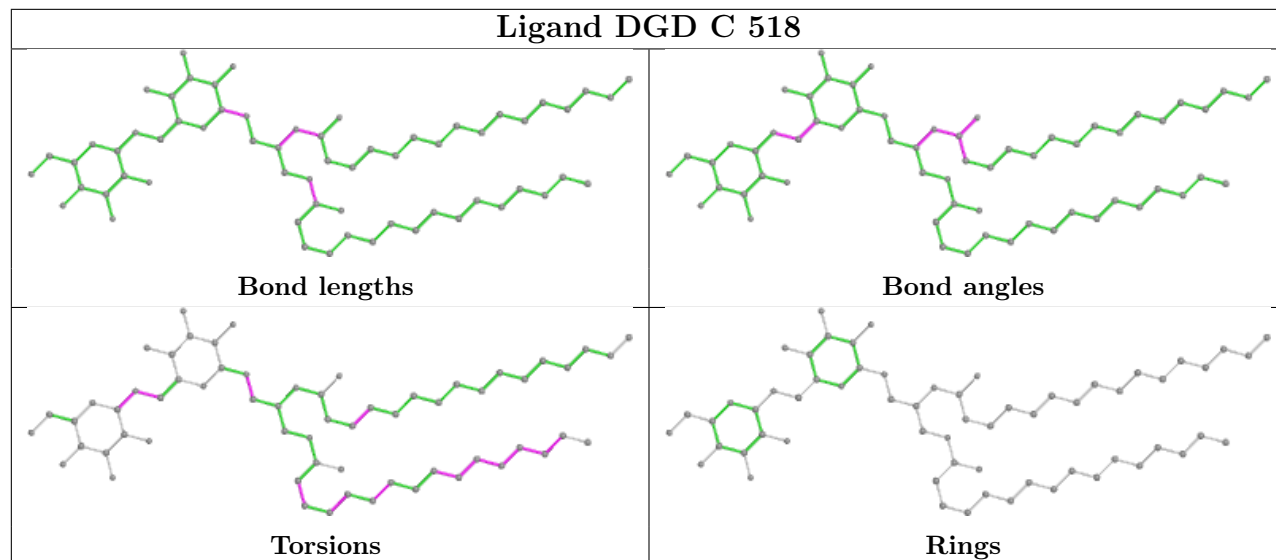
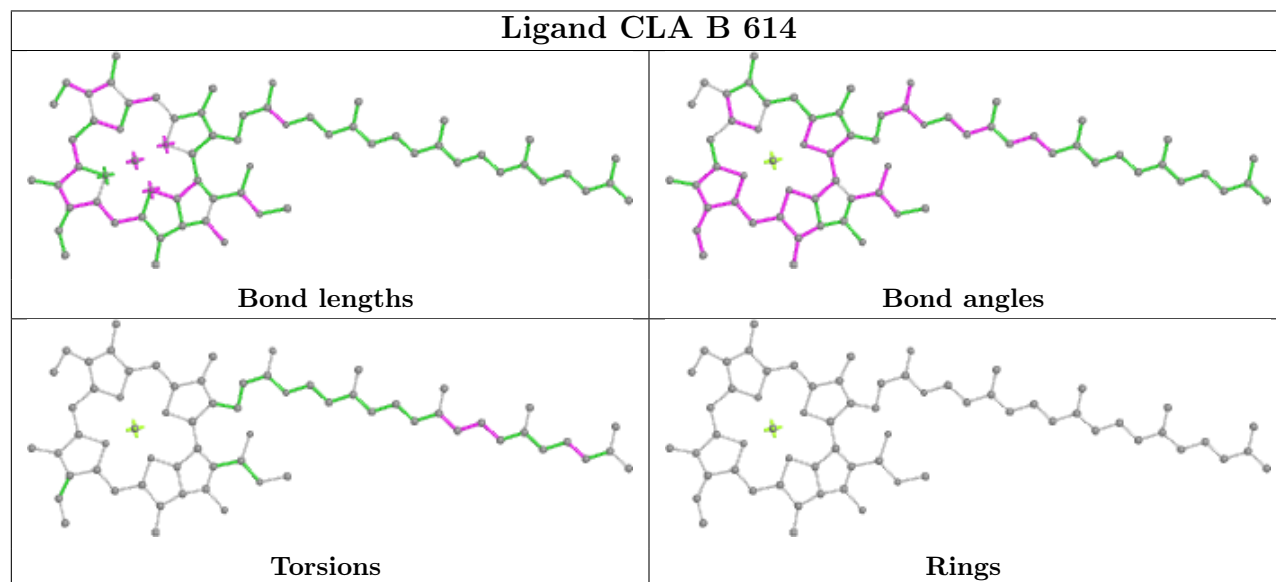
Ligand CLA B 612

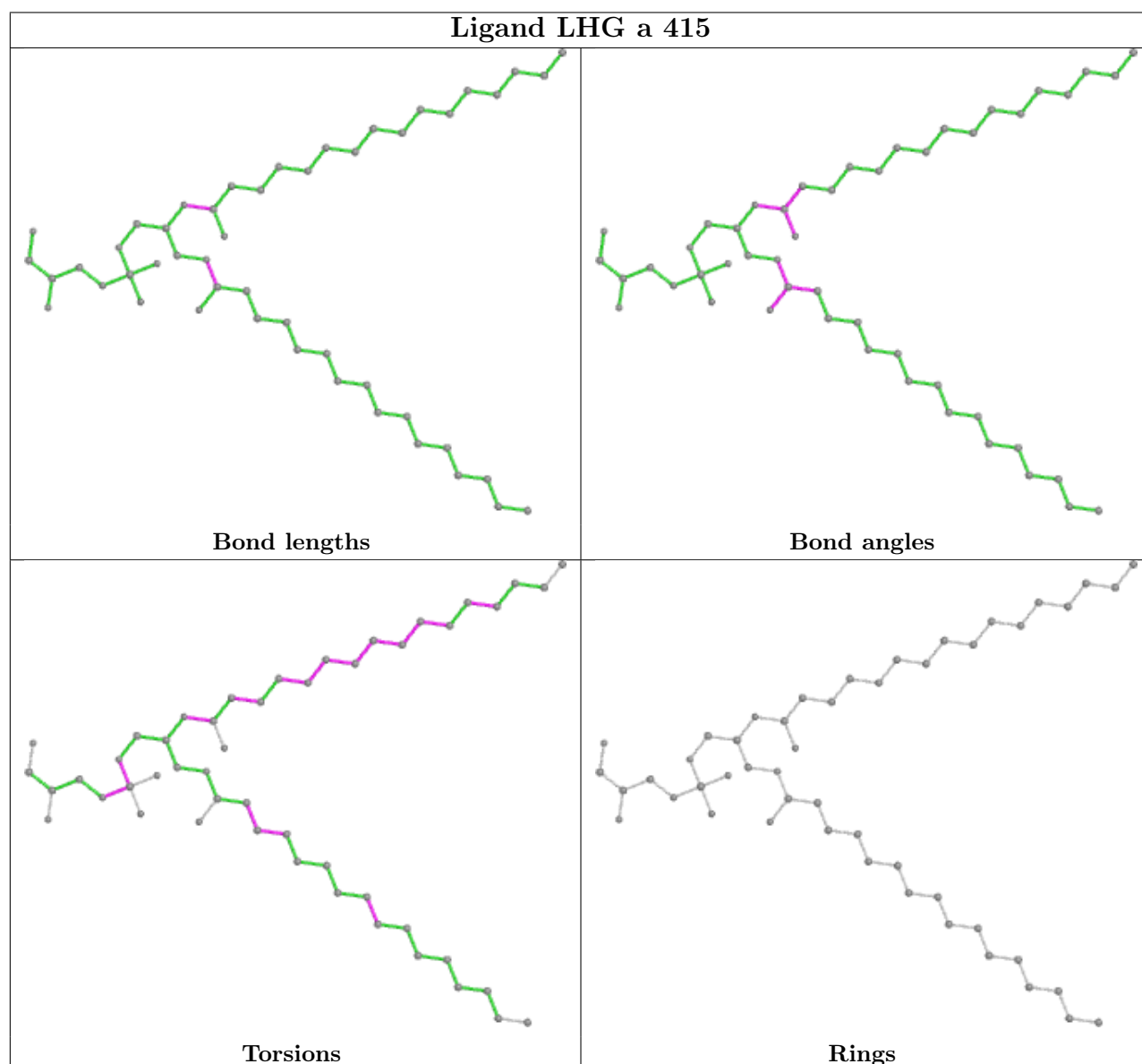
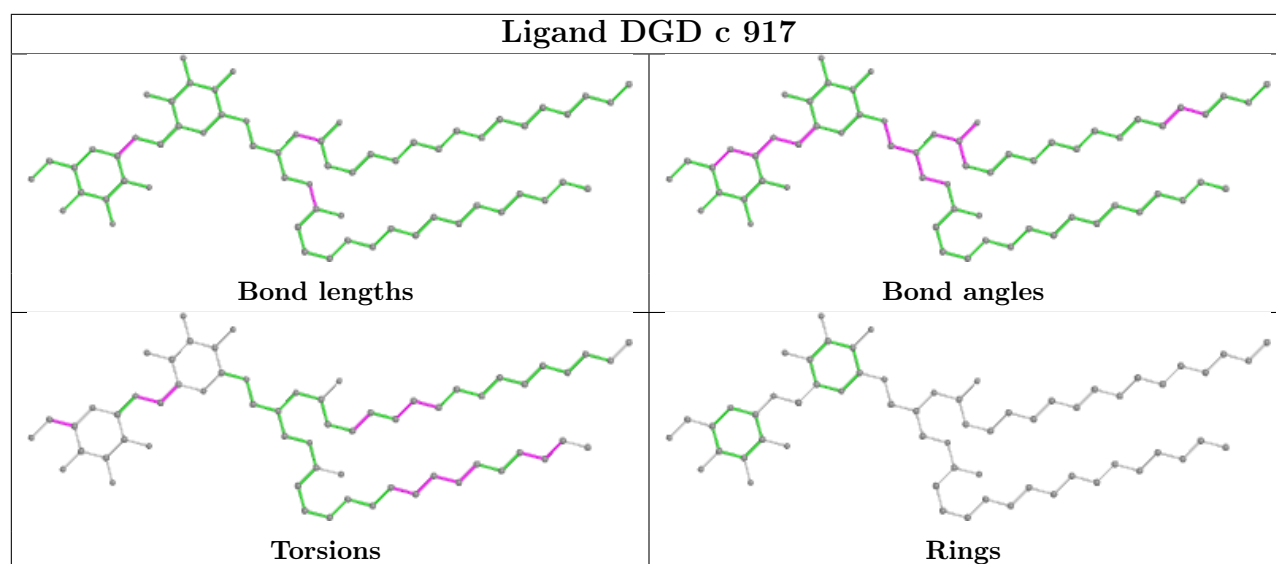


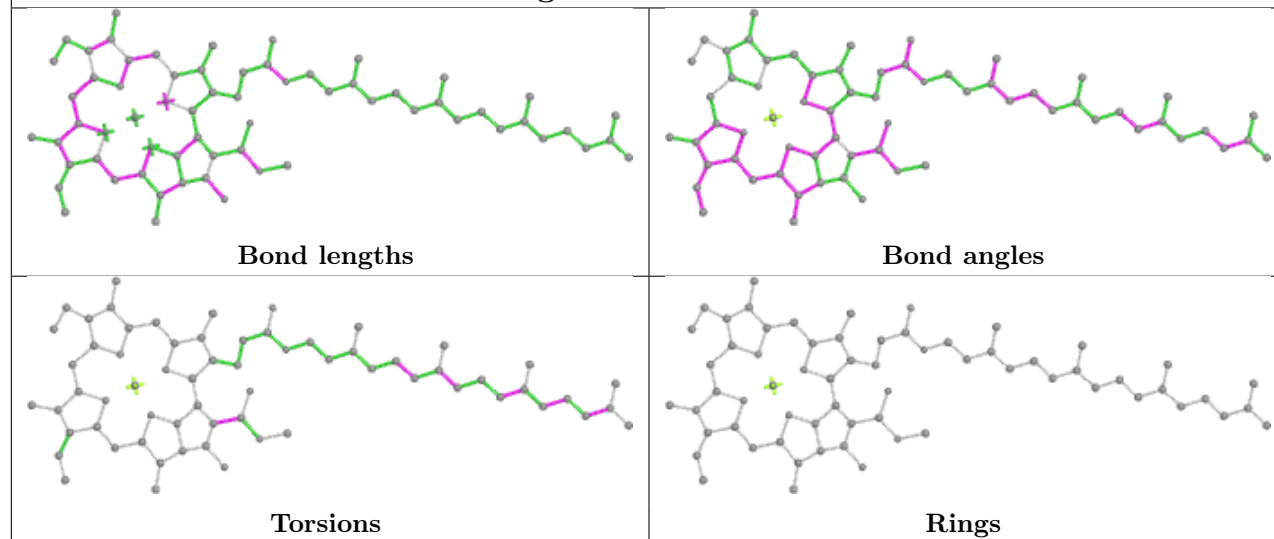
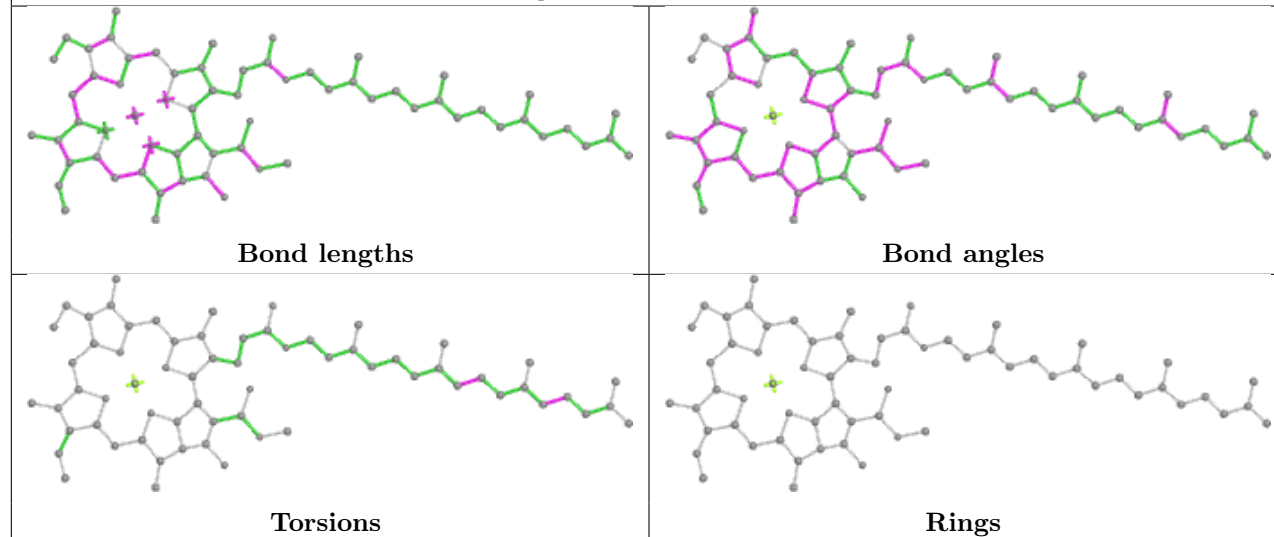
Ligand HTG D 414



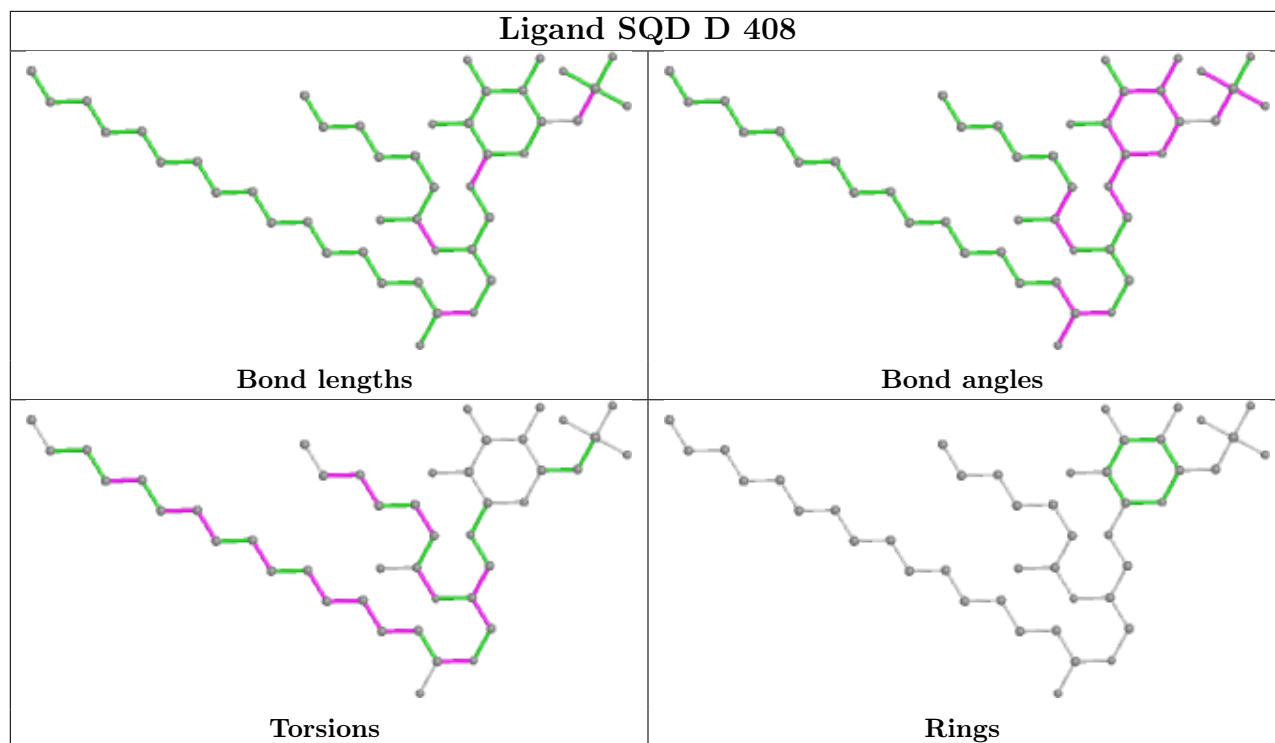


Ligand BCR d 405**Ligand DGD C 518****Ligand CLA B 614**

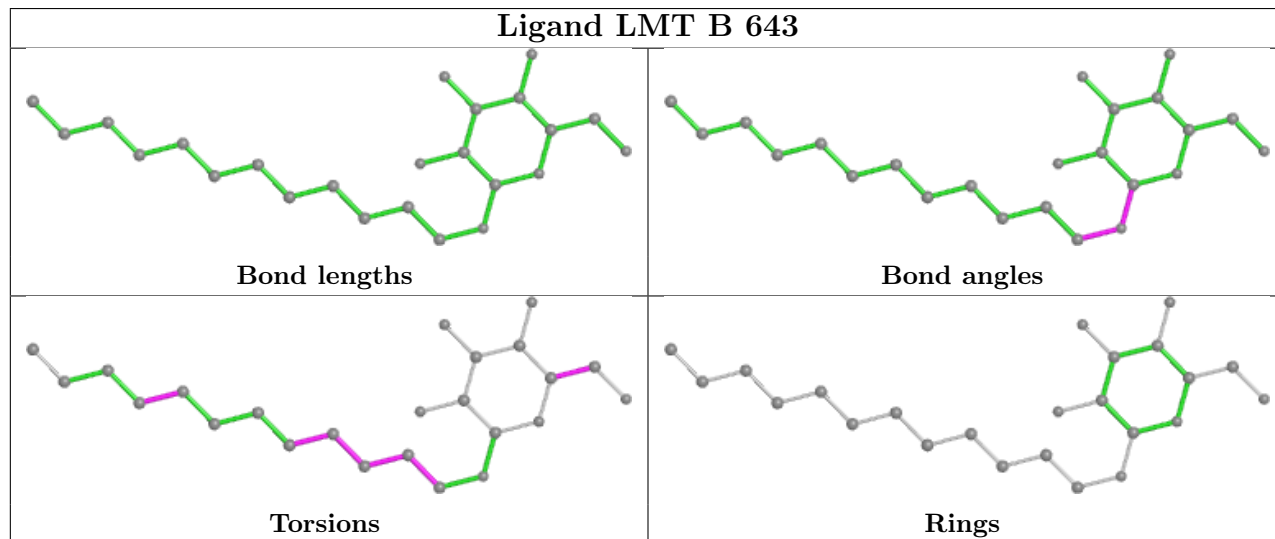


Ligand CLA c 908**Ligand CLA B 613**

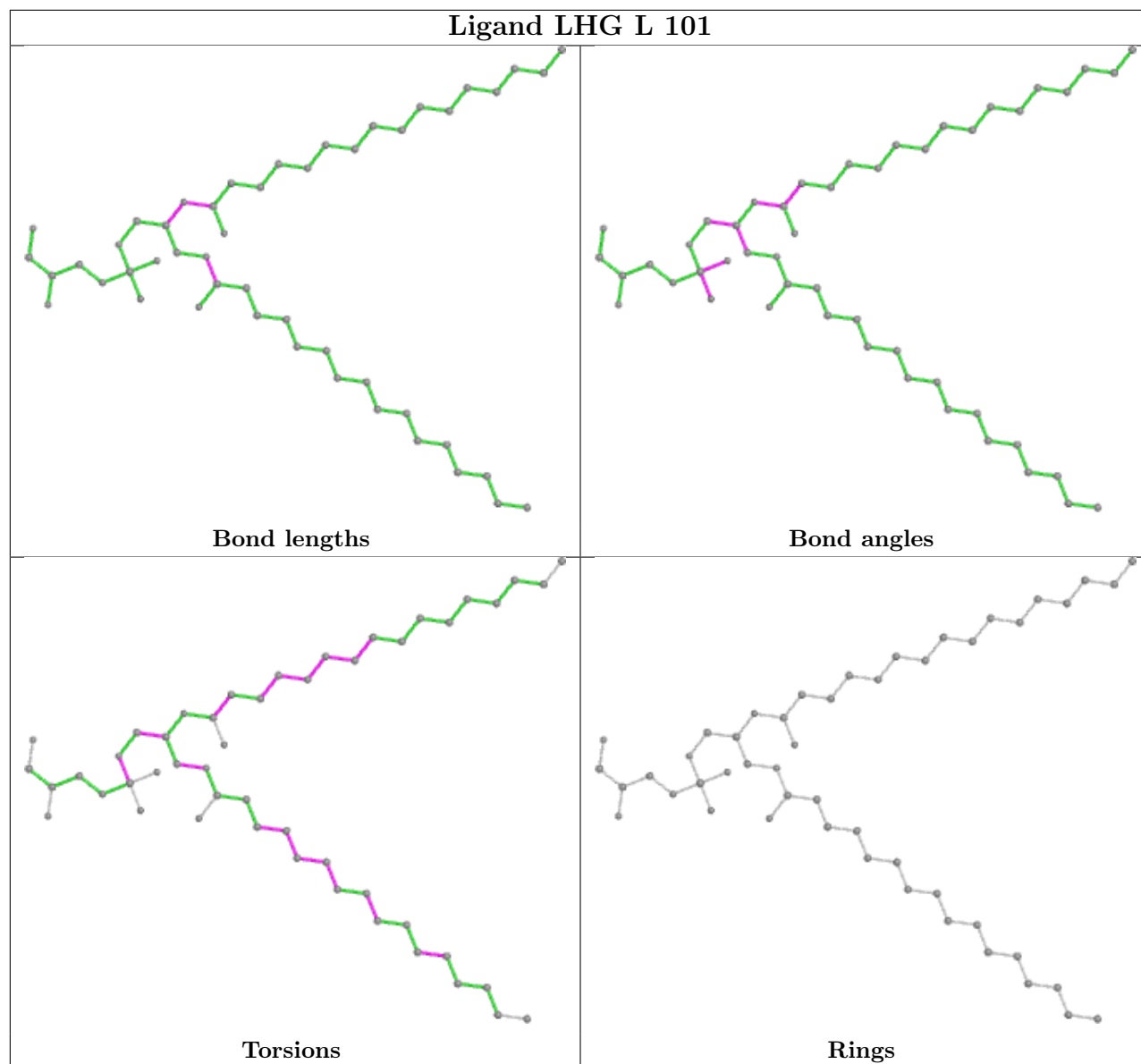
Ligand SQD D 408



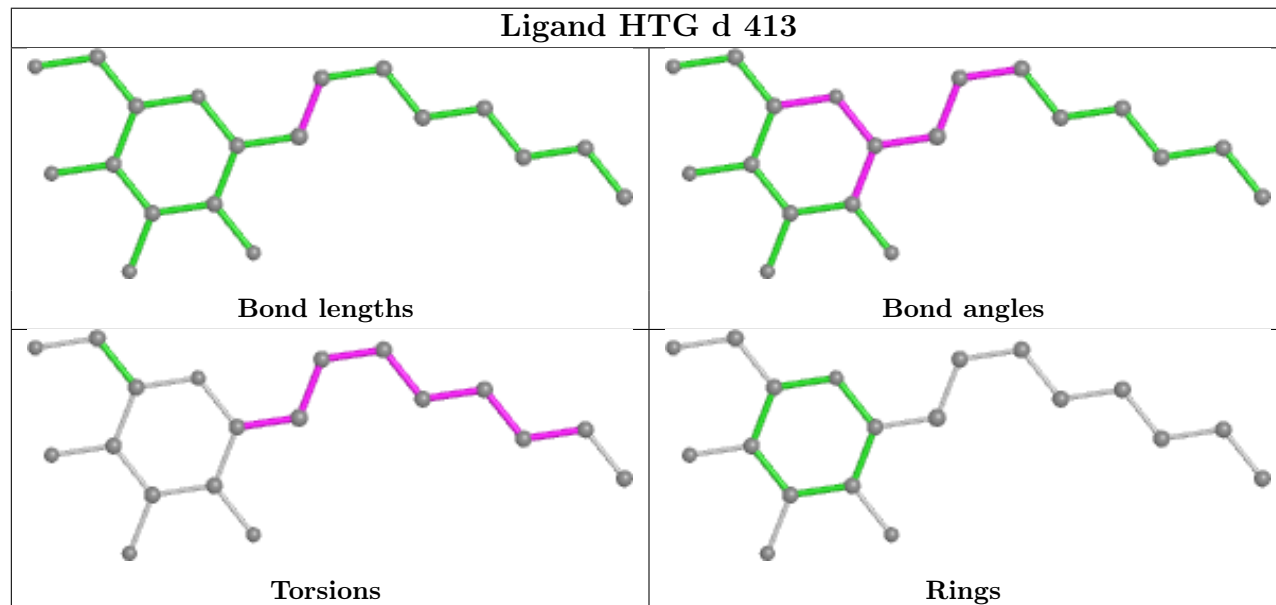
Ligand LMT B 643

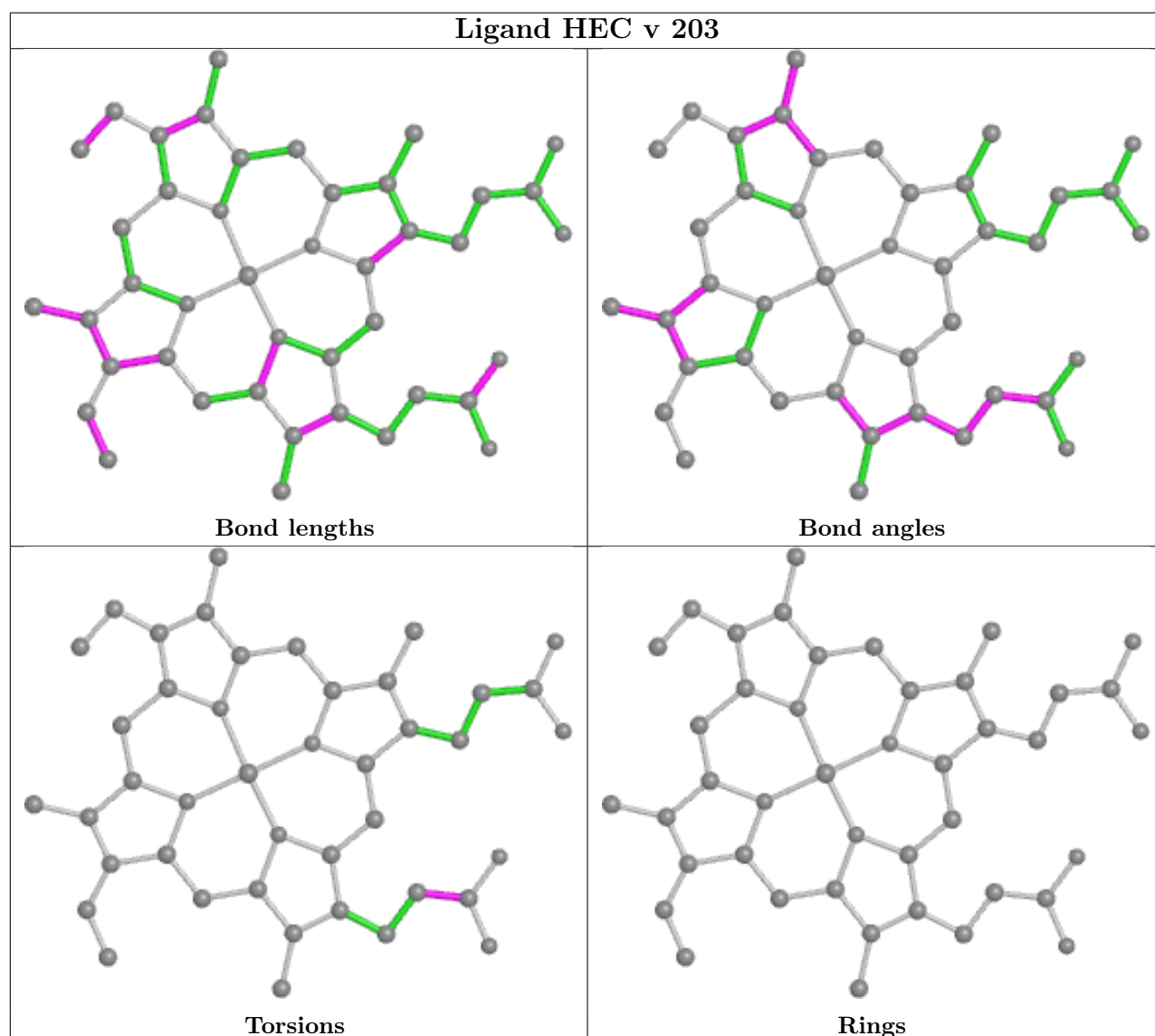
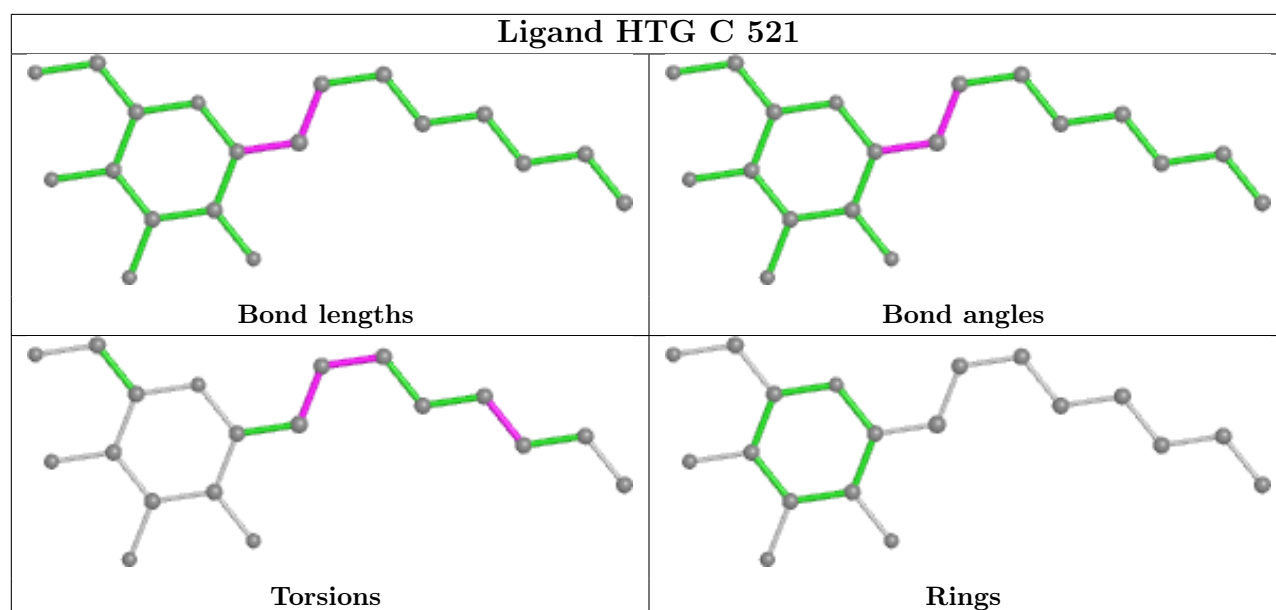


Ligand LHG L 101

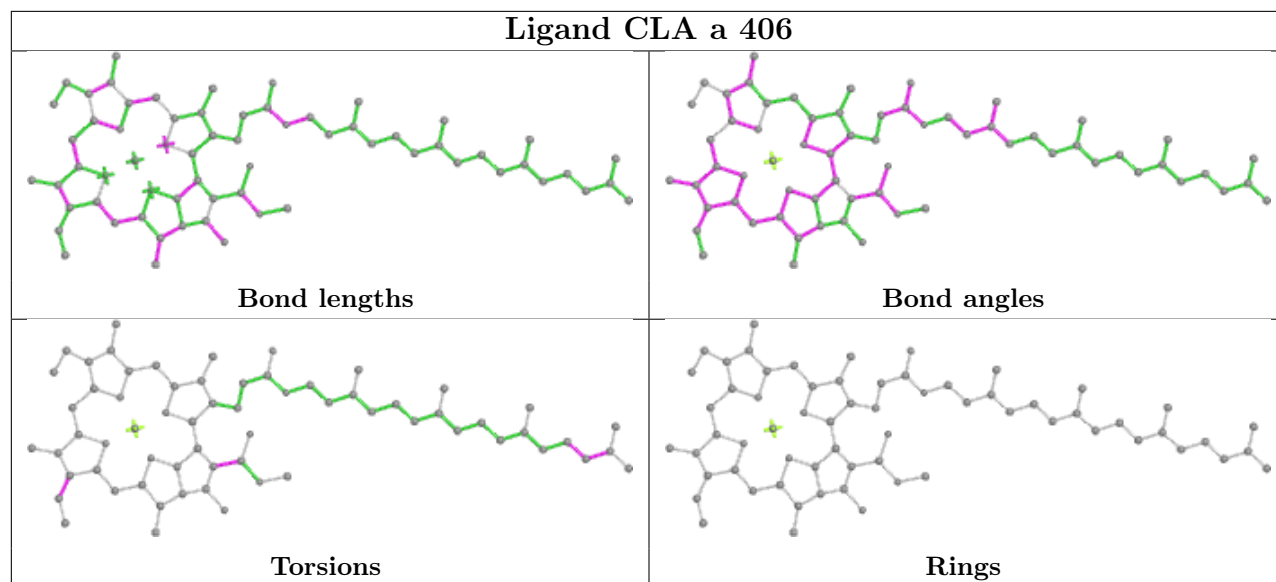


Ligand HTG d 413

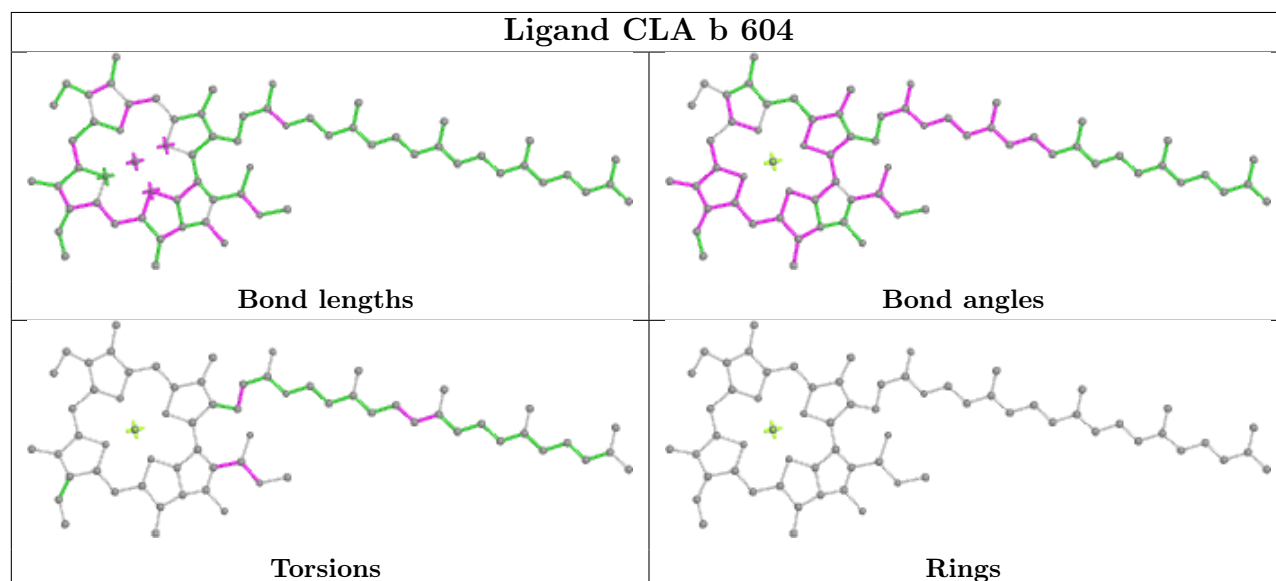




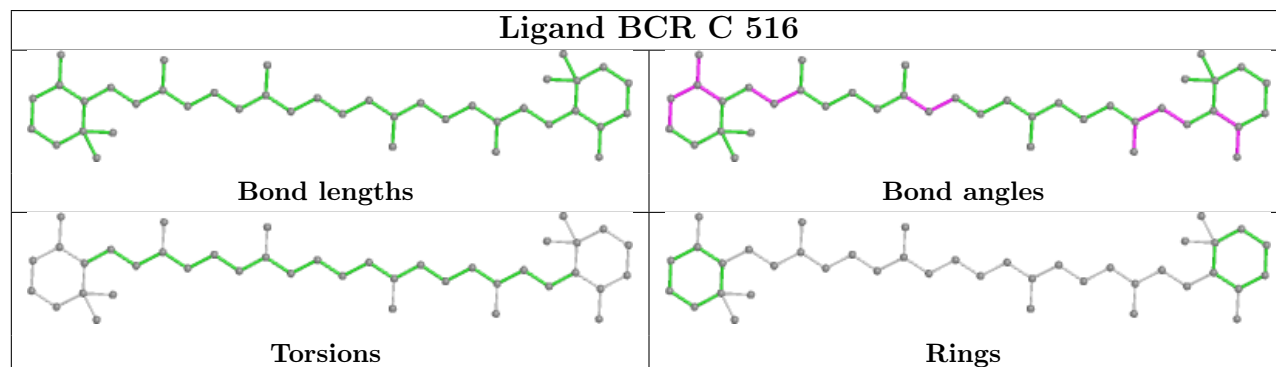
Ligand CLA a 406



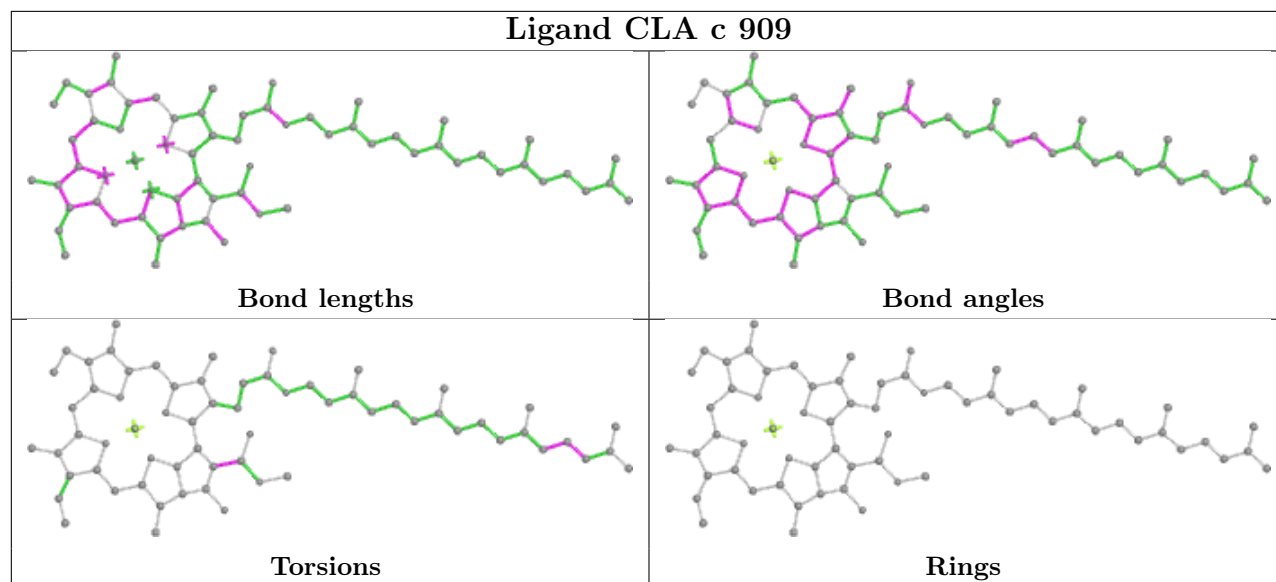
Ligand CLA b 604



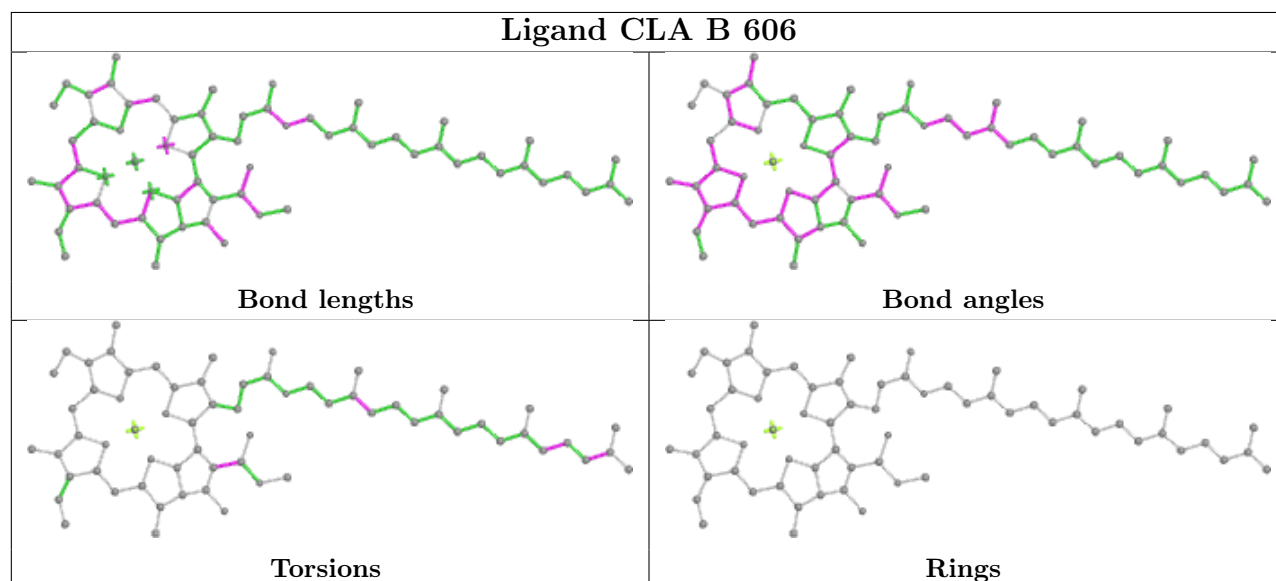
Ligand BCR C 516



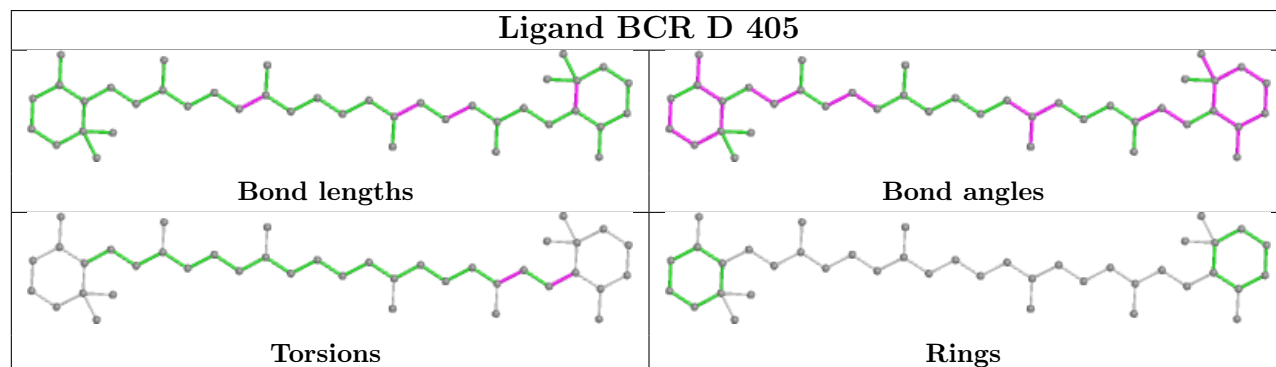
Ligand CLA c 909

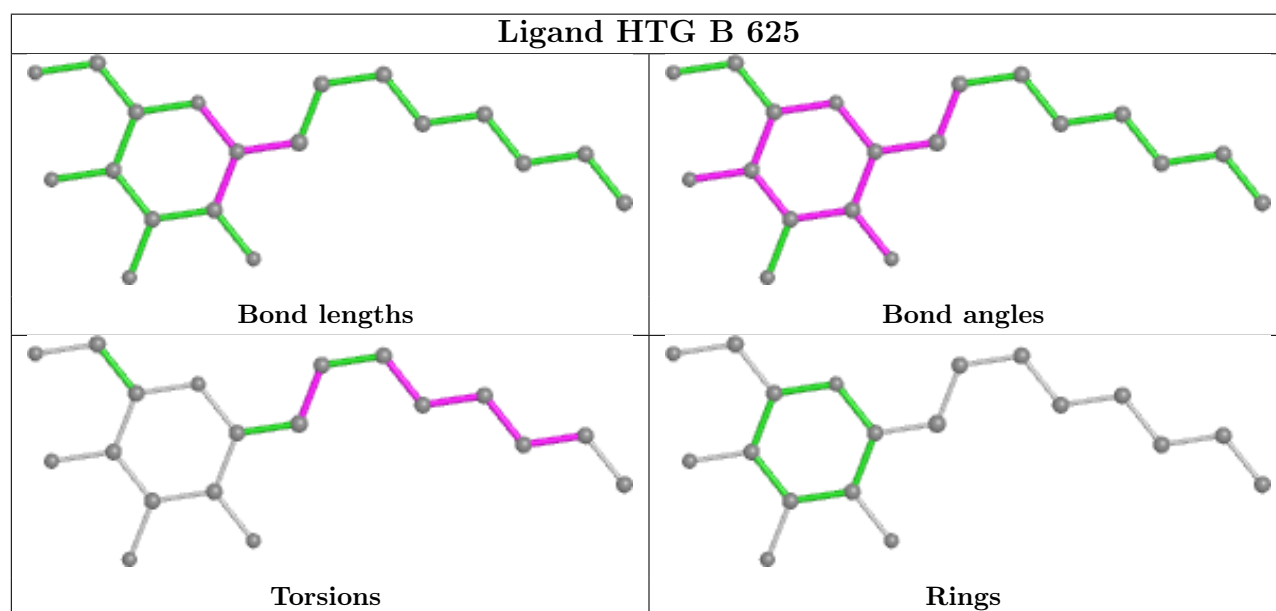
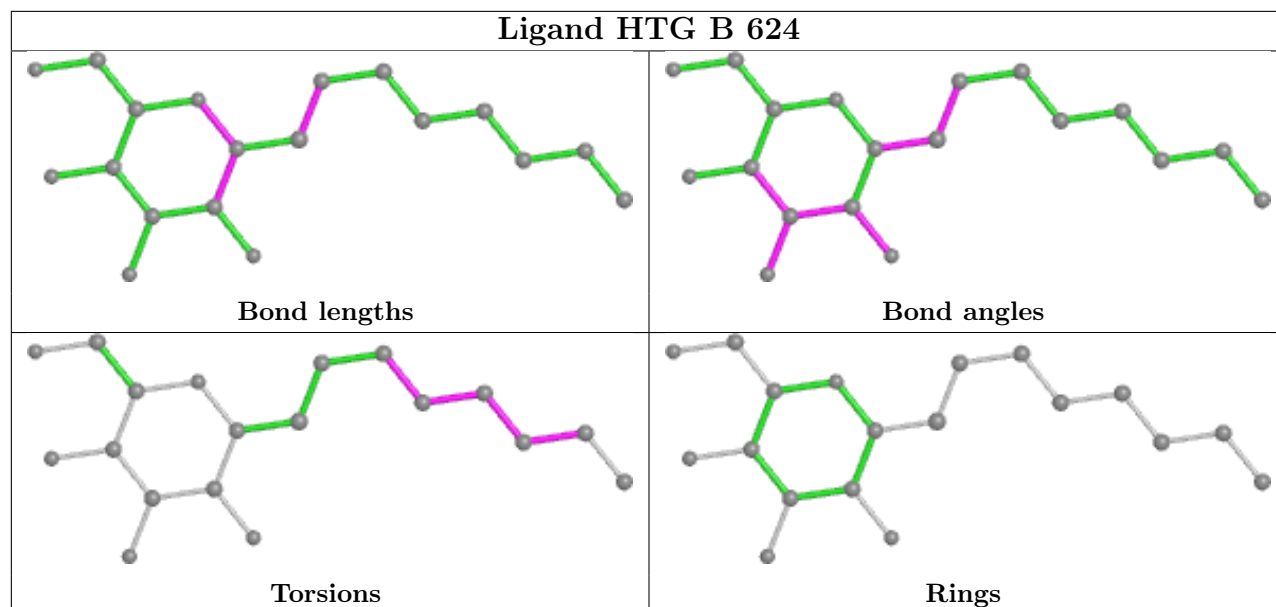


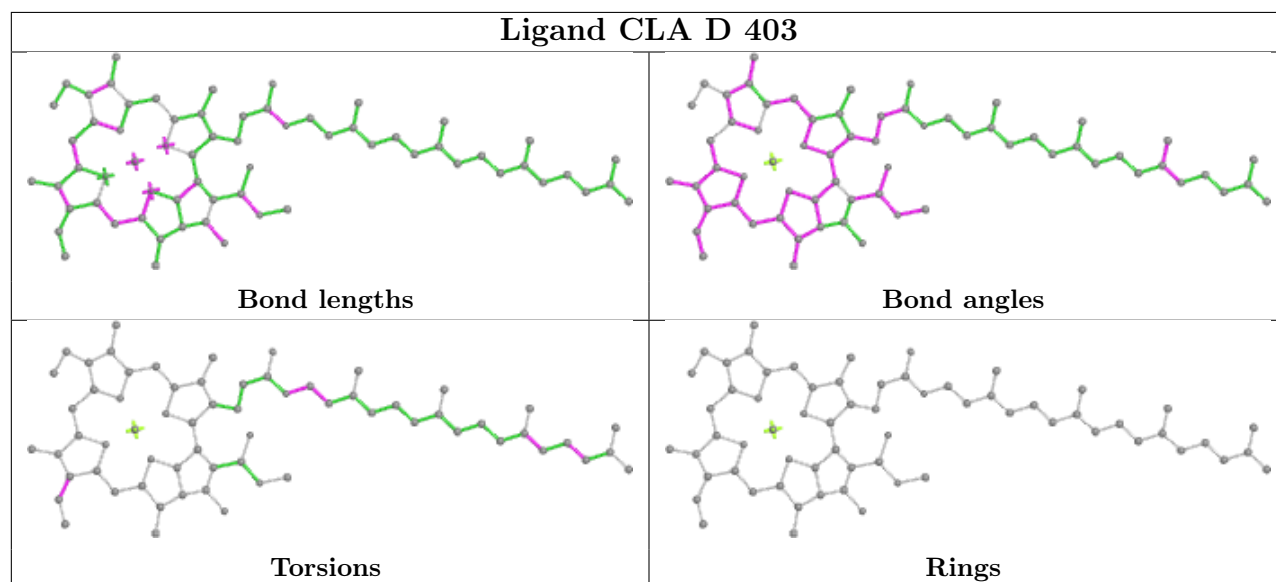
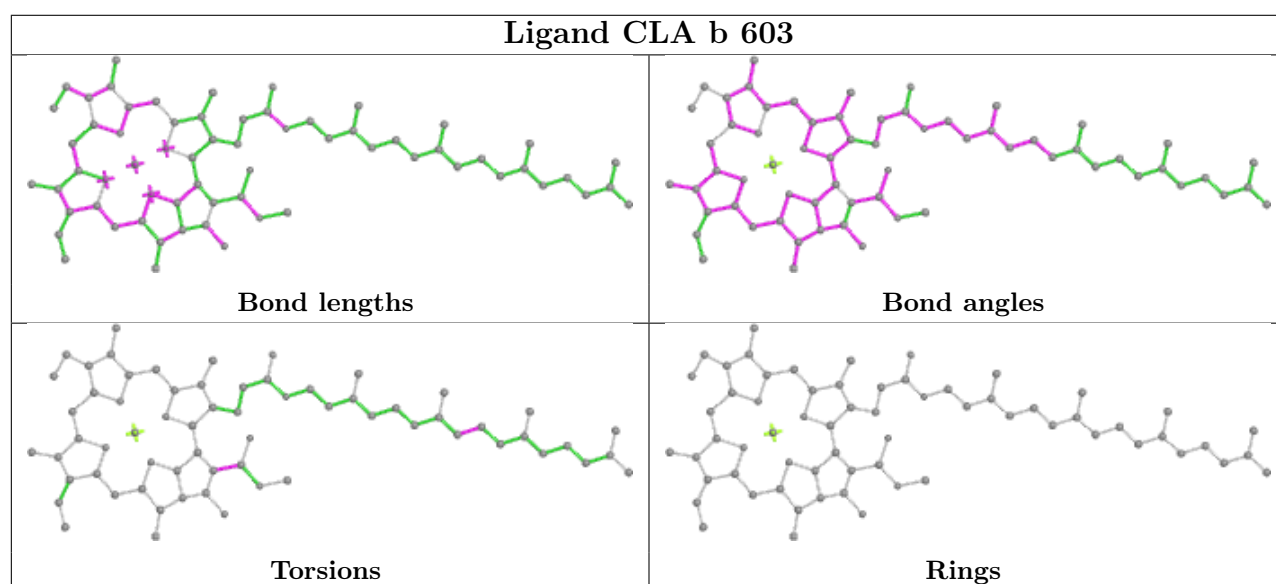
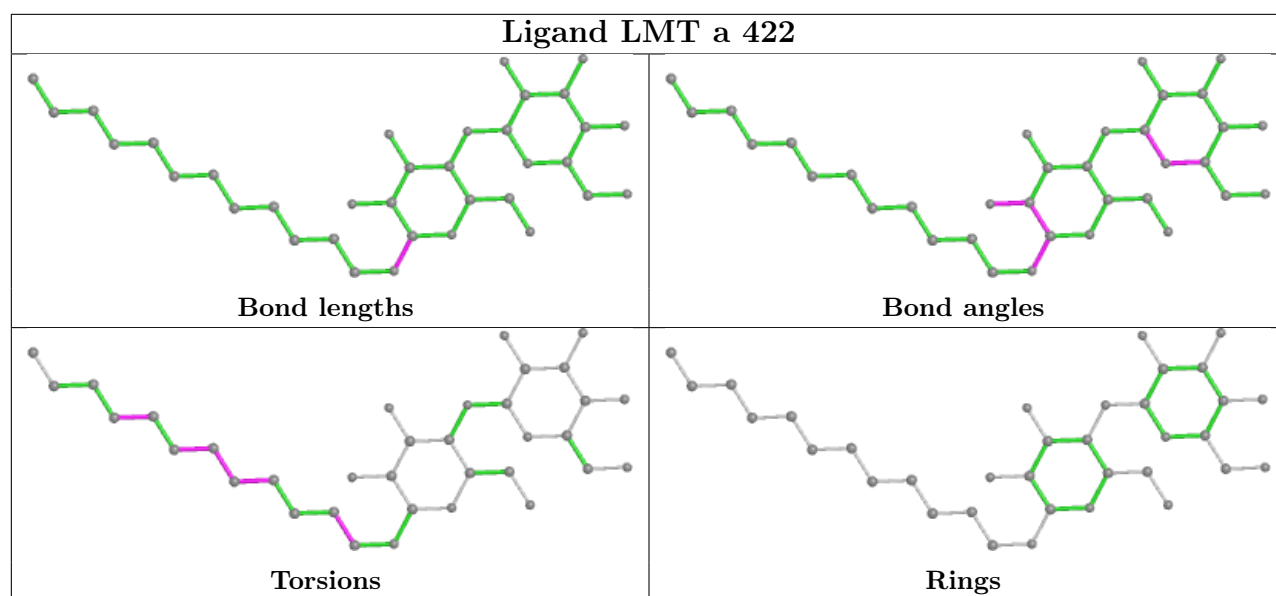
Ligand CLA B 606



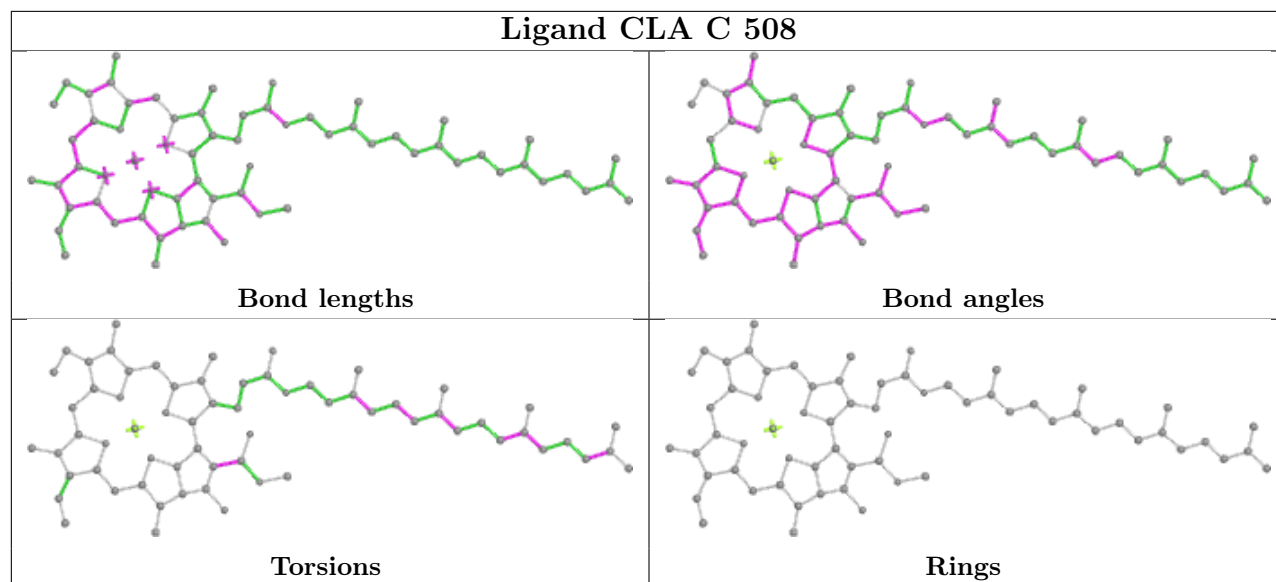
Ligand BCR D 405



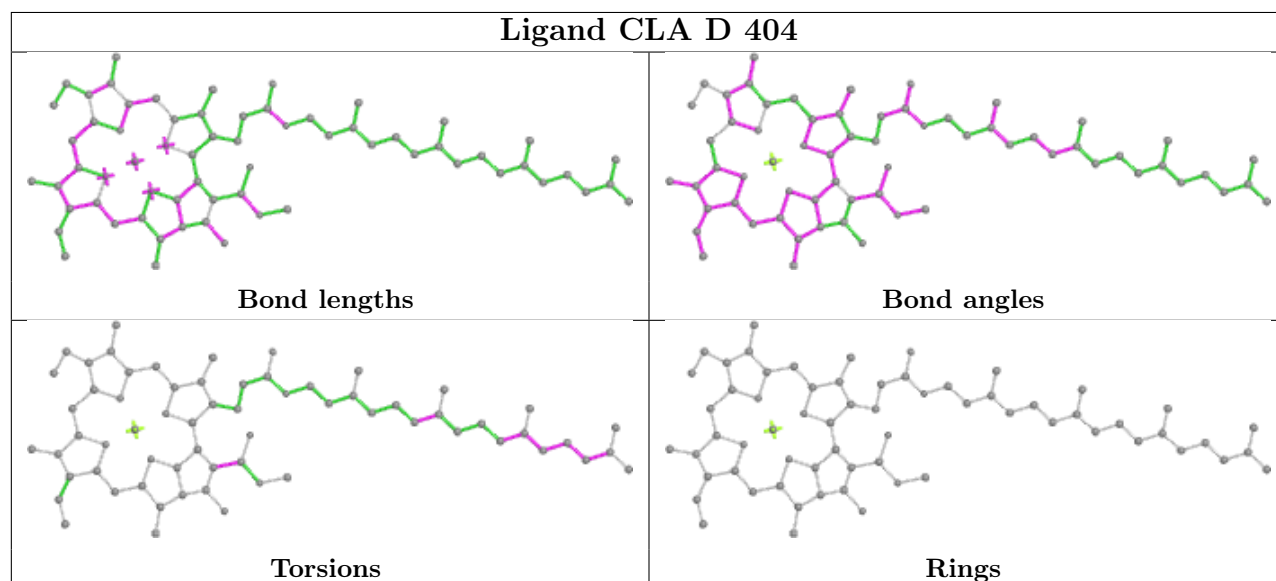




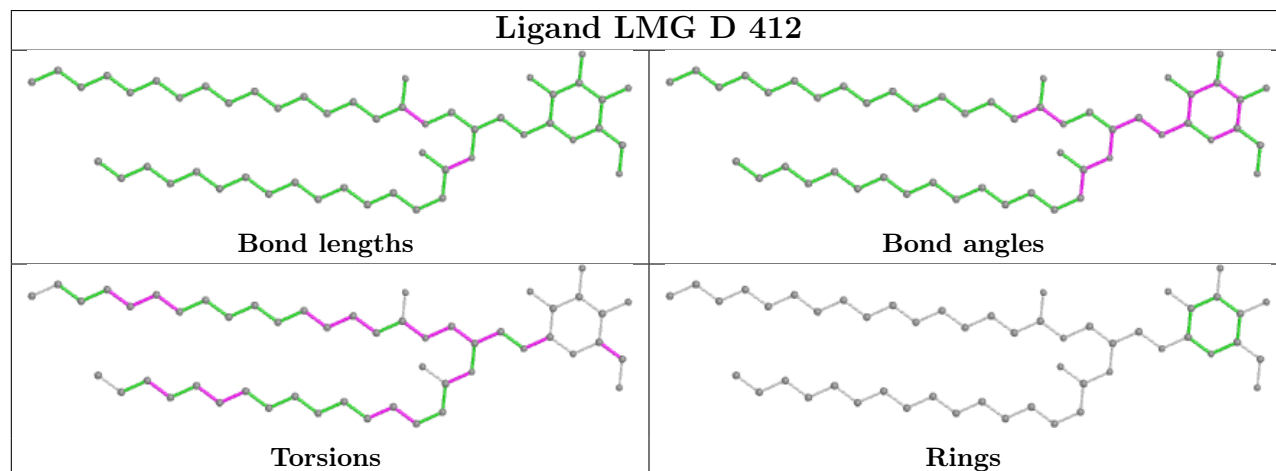
Ligand CLA C 508

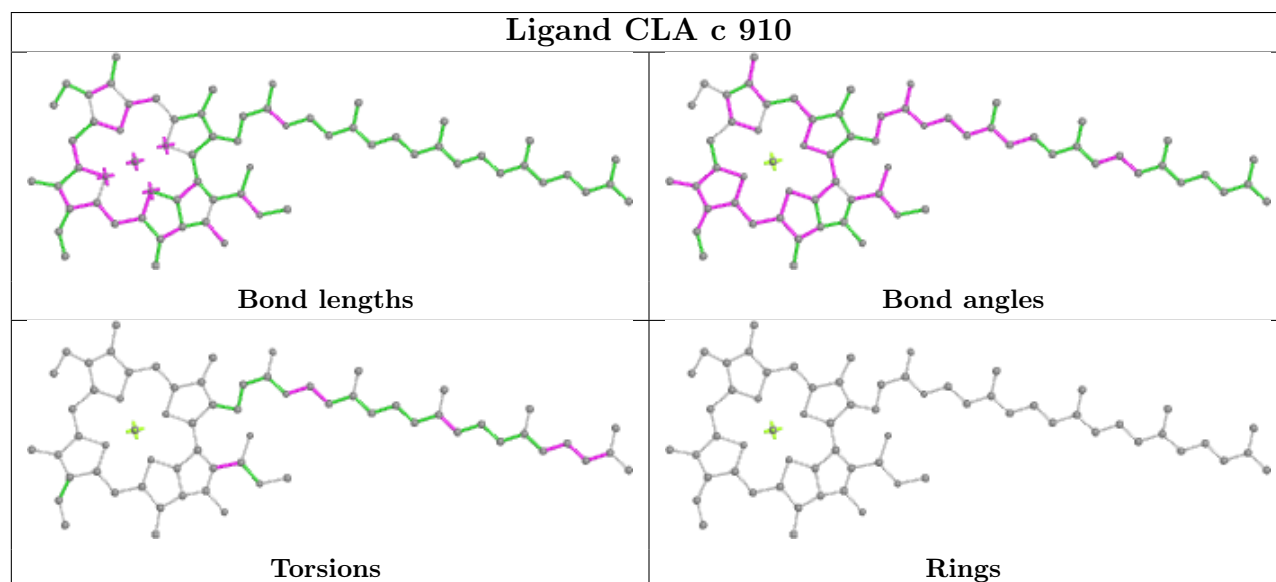
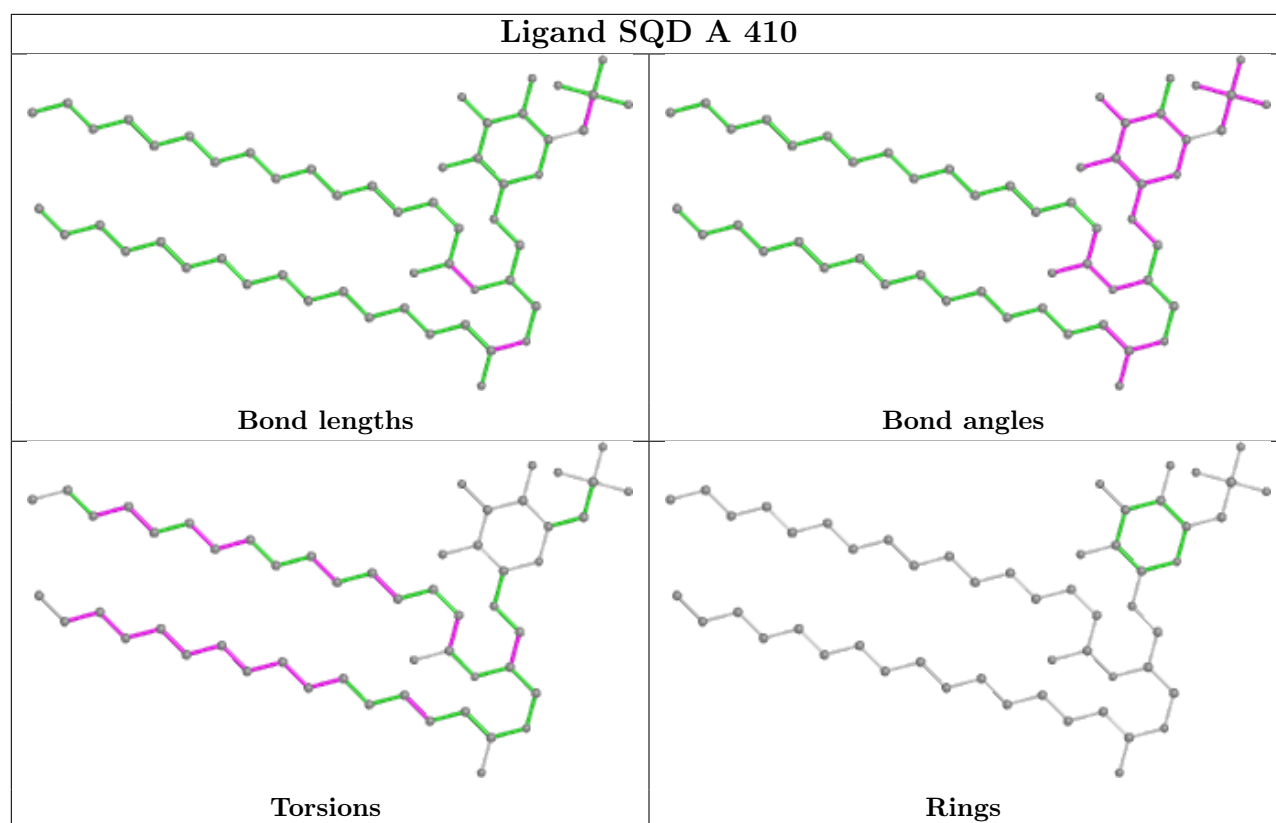


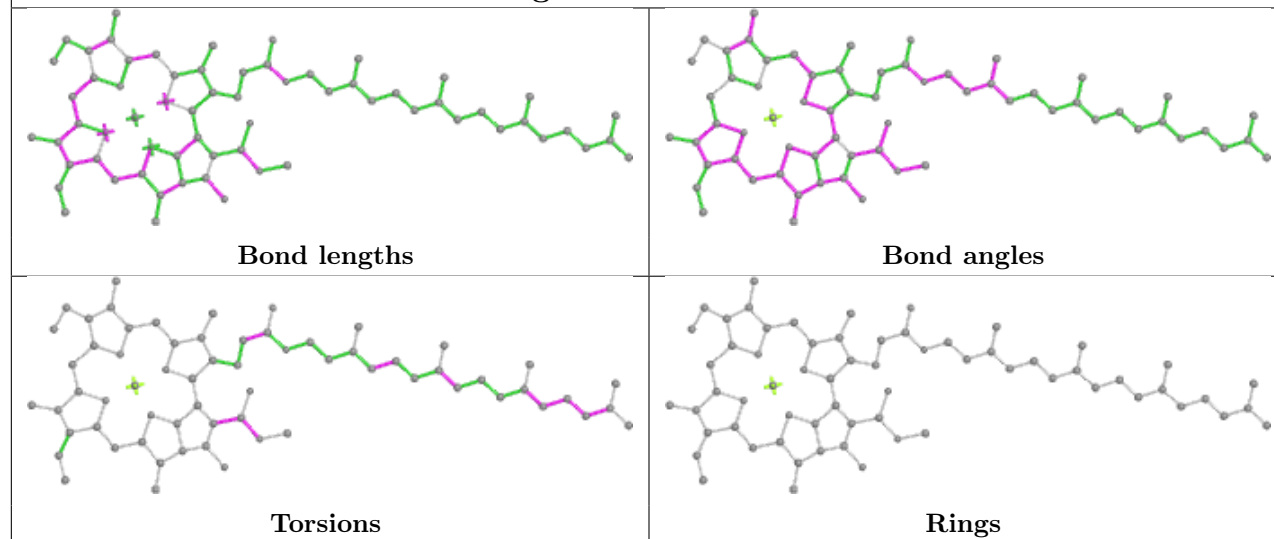
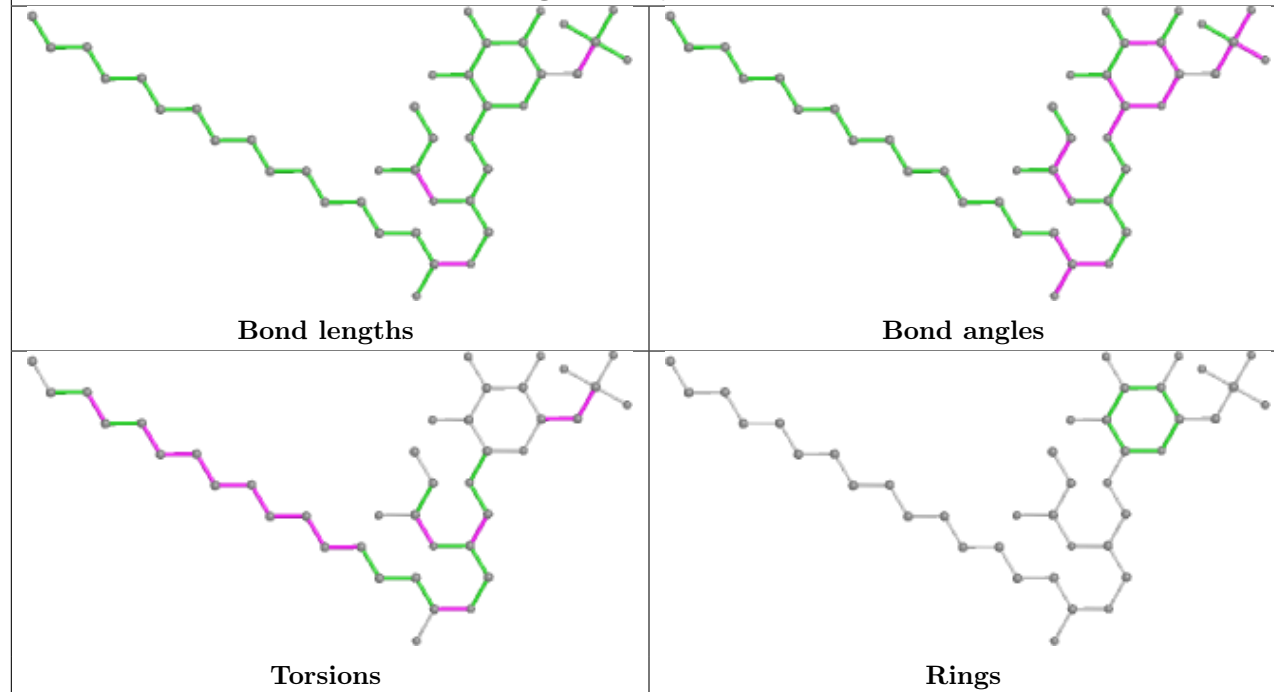
Ligand CLA D 404

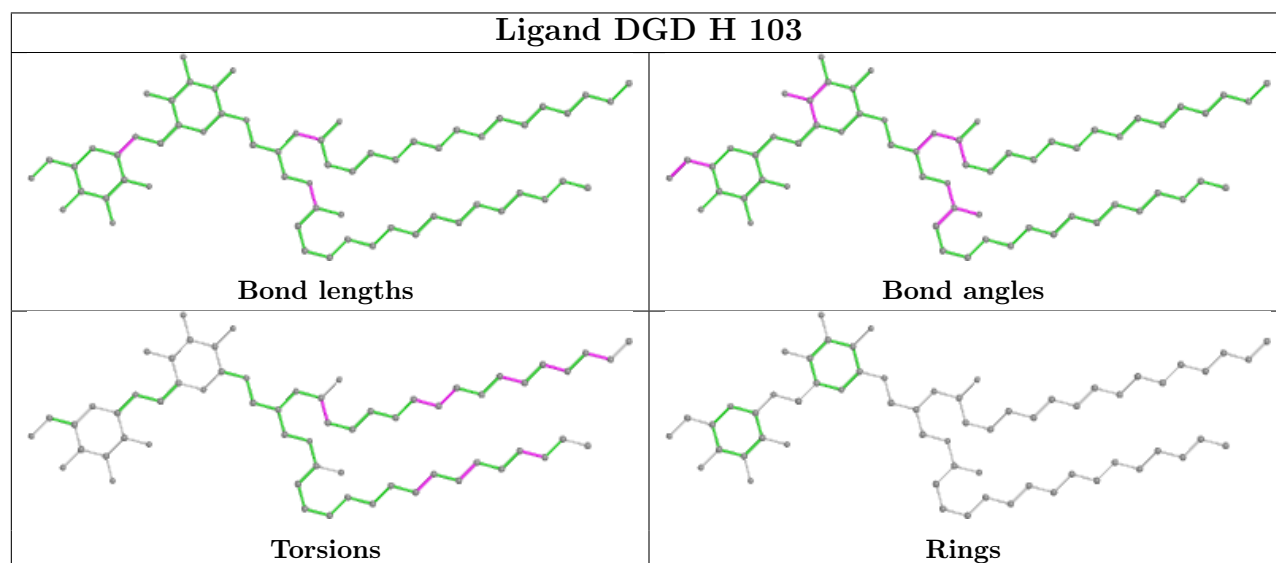
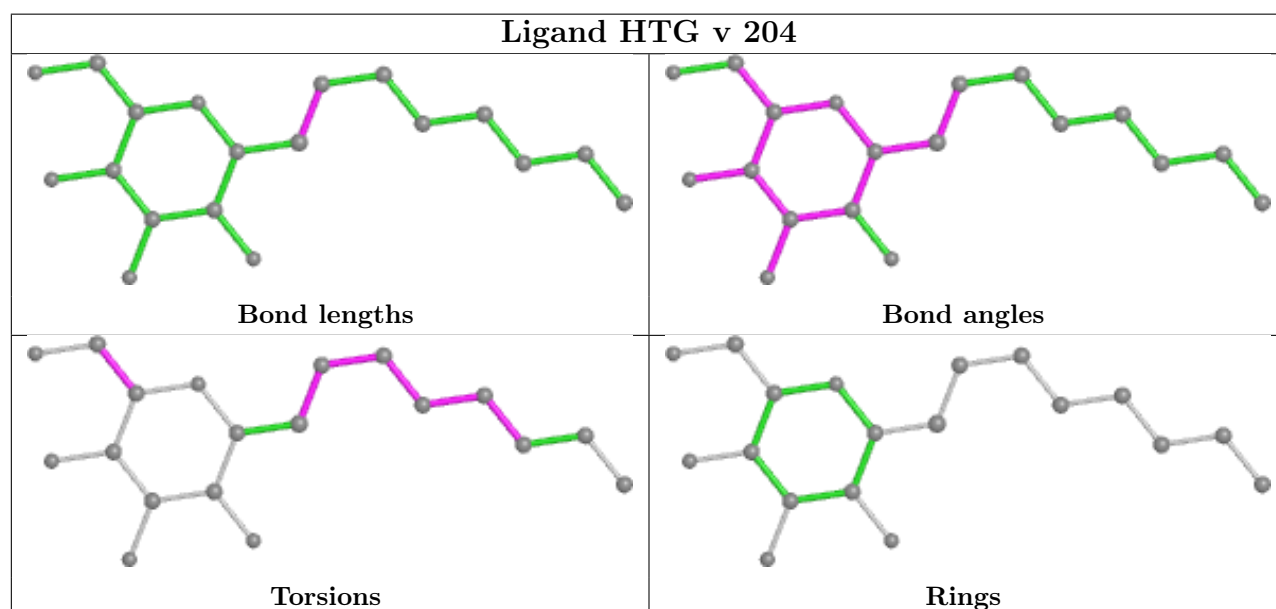
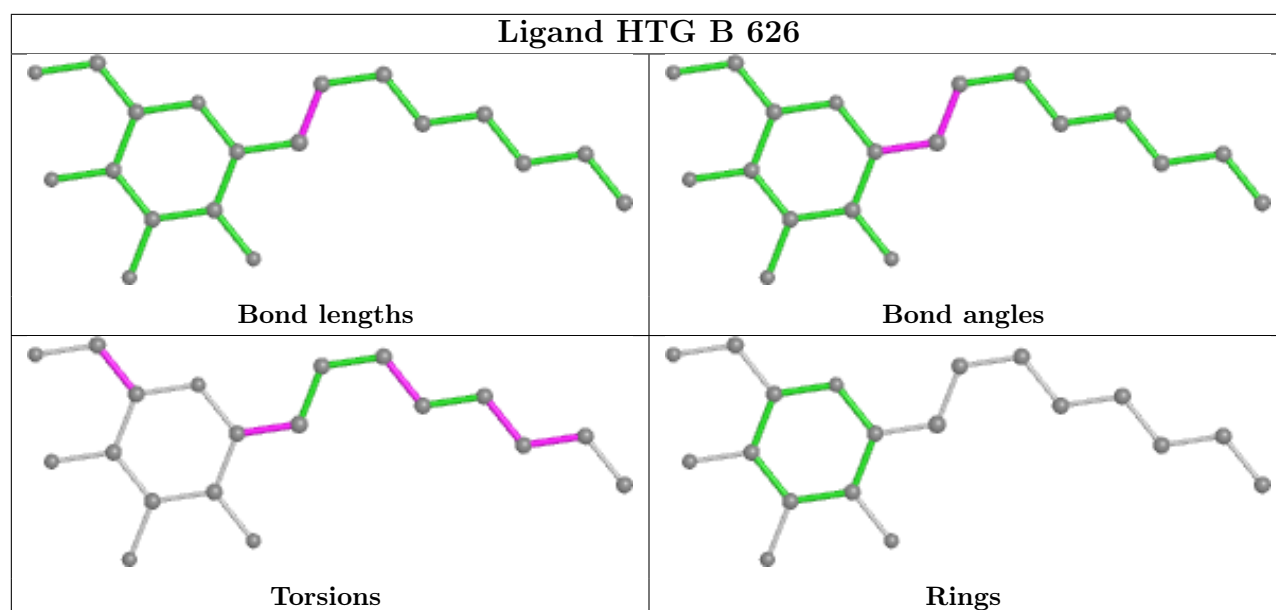


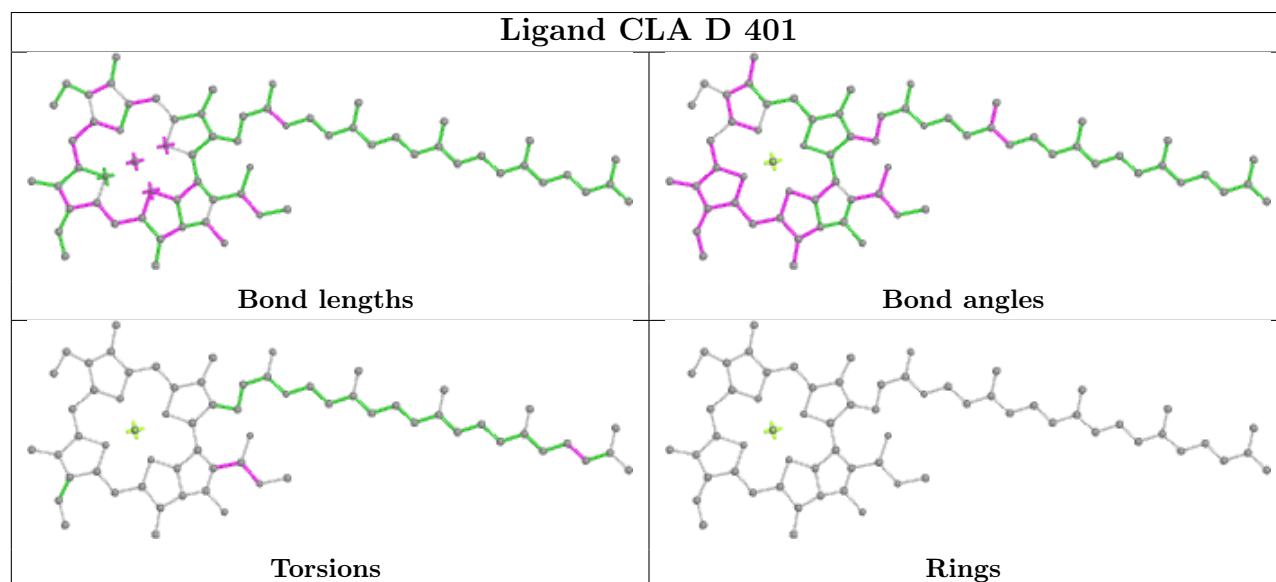
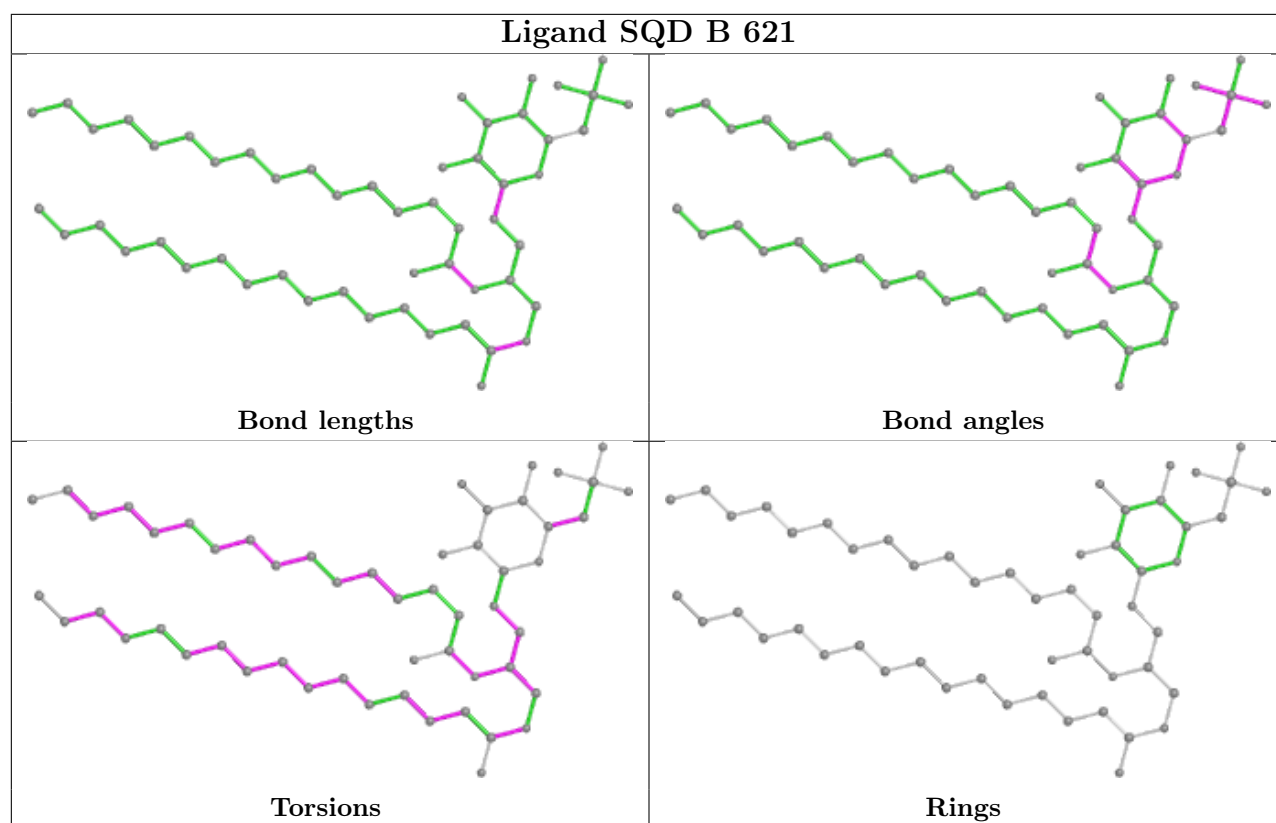
Ligand LMG D 412



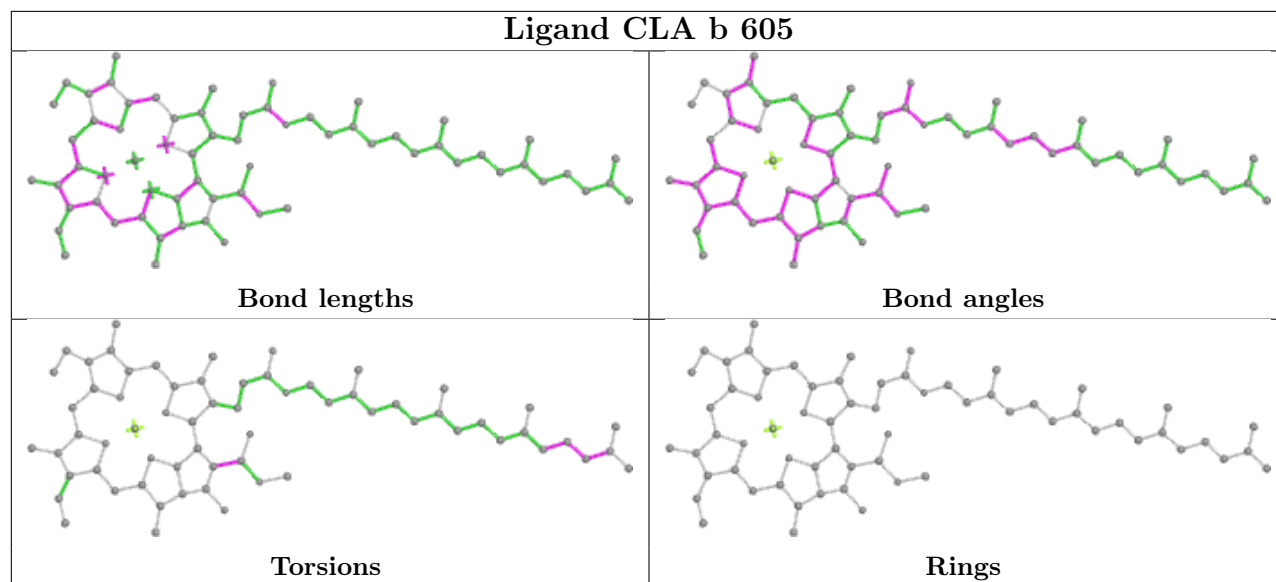


Ligand CLA C 513**Ligand SQD x 101**

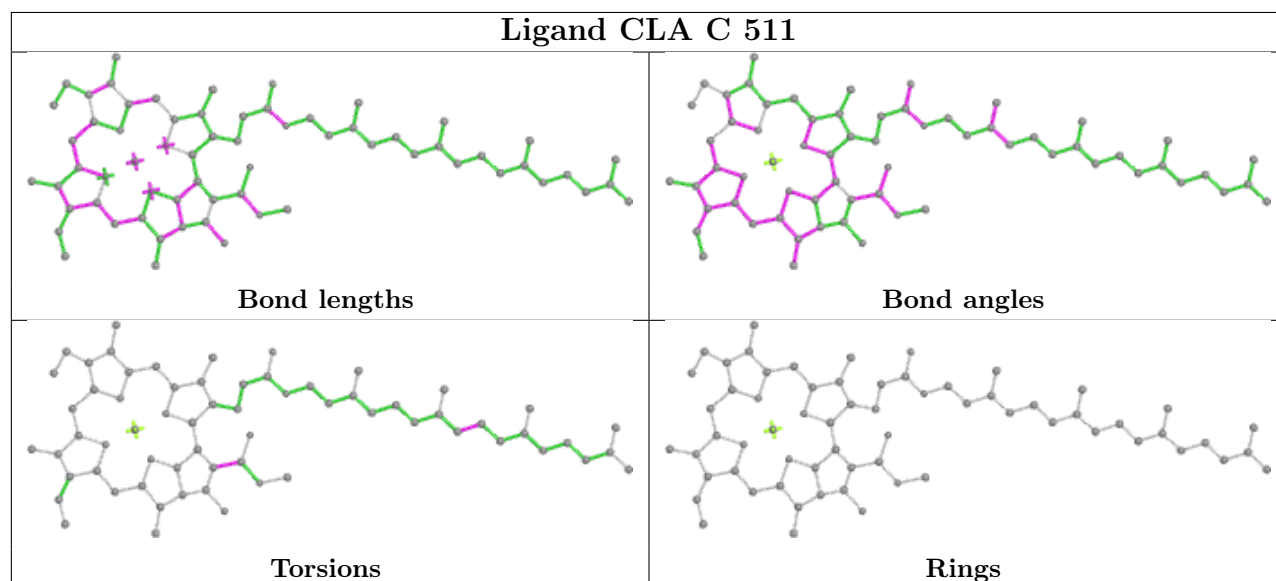




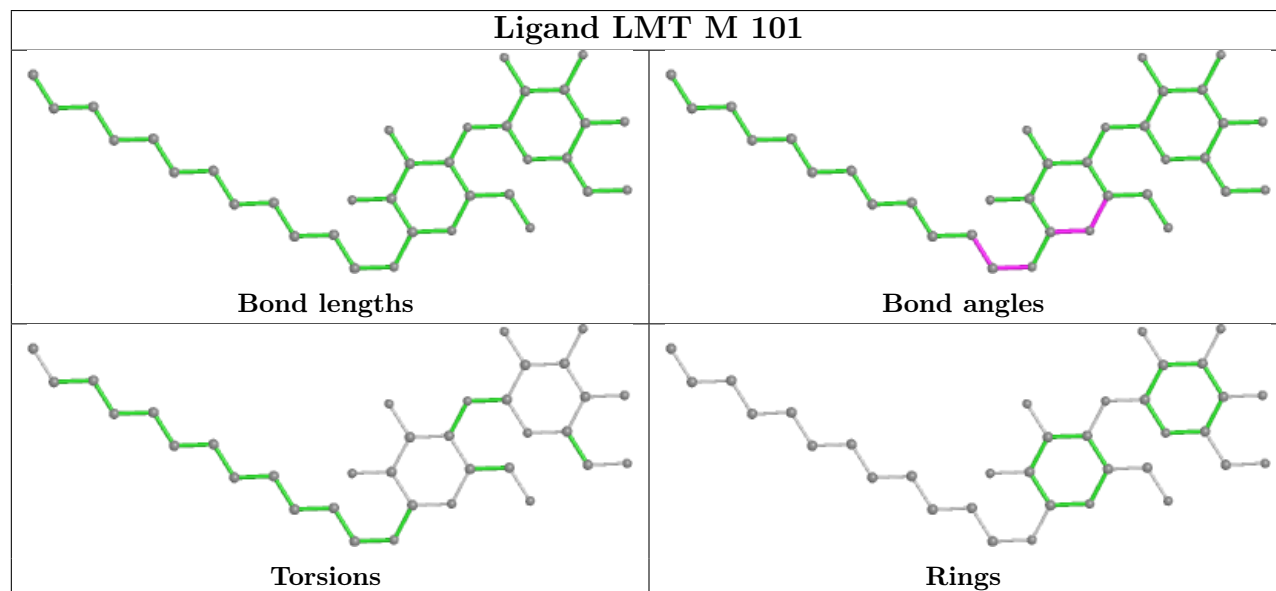
Ligand CLA b 605

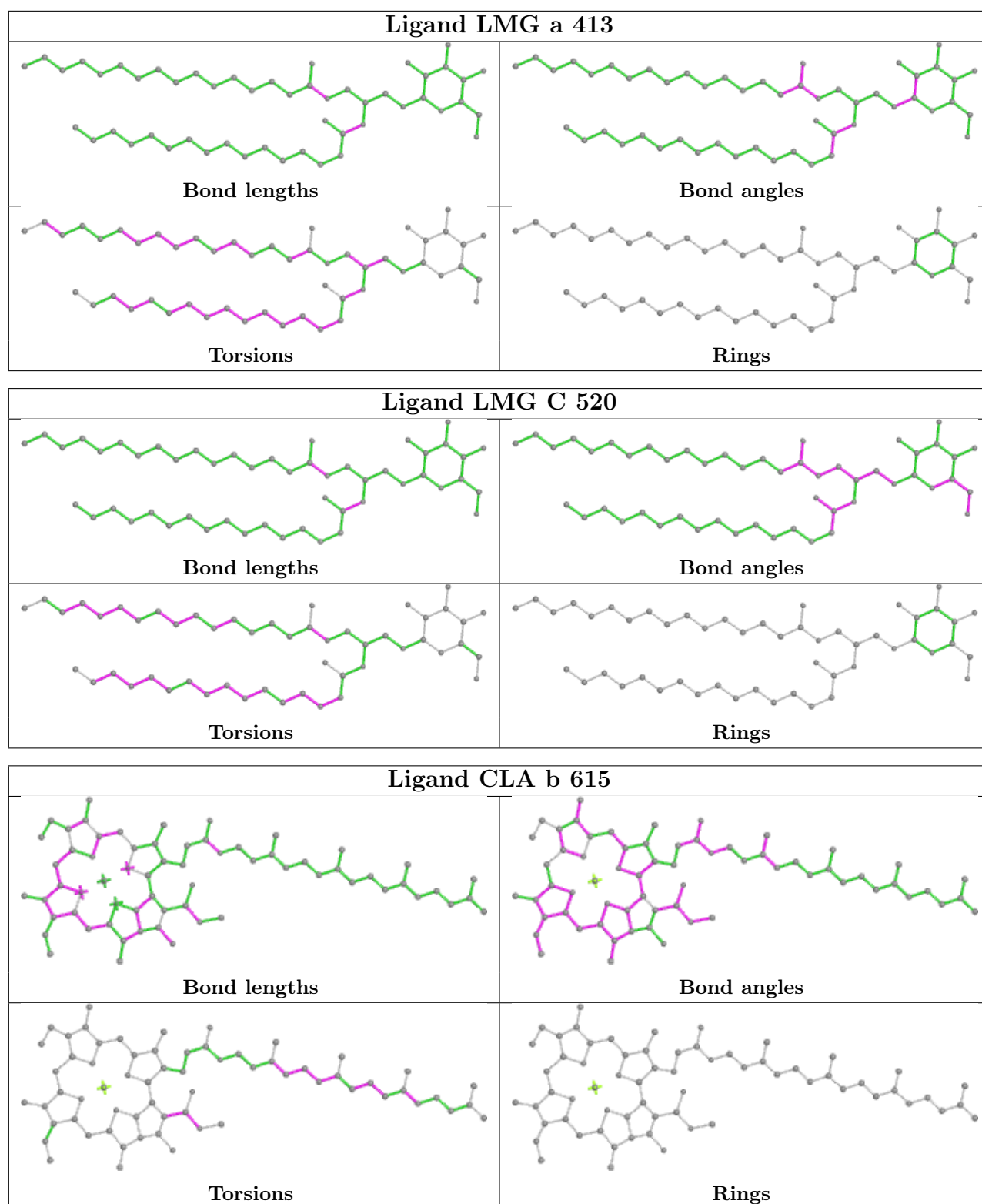


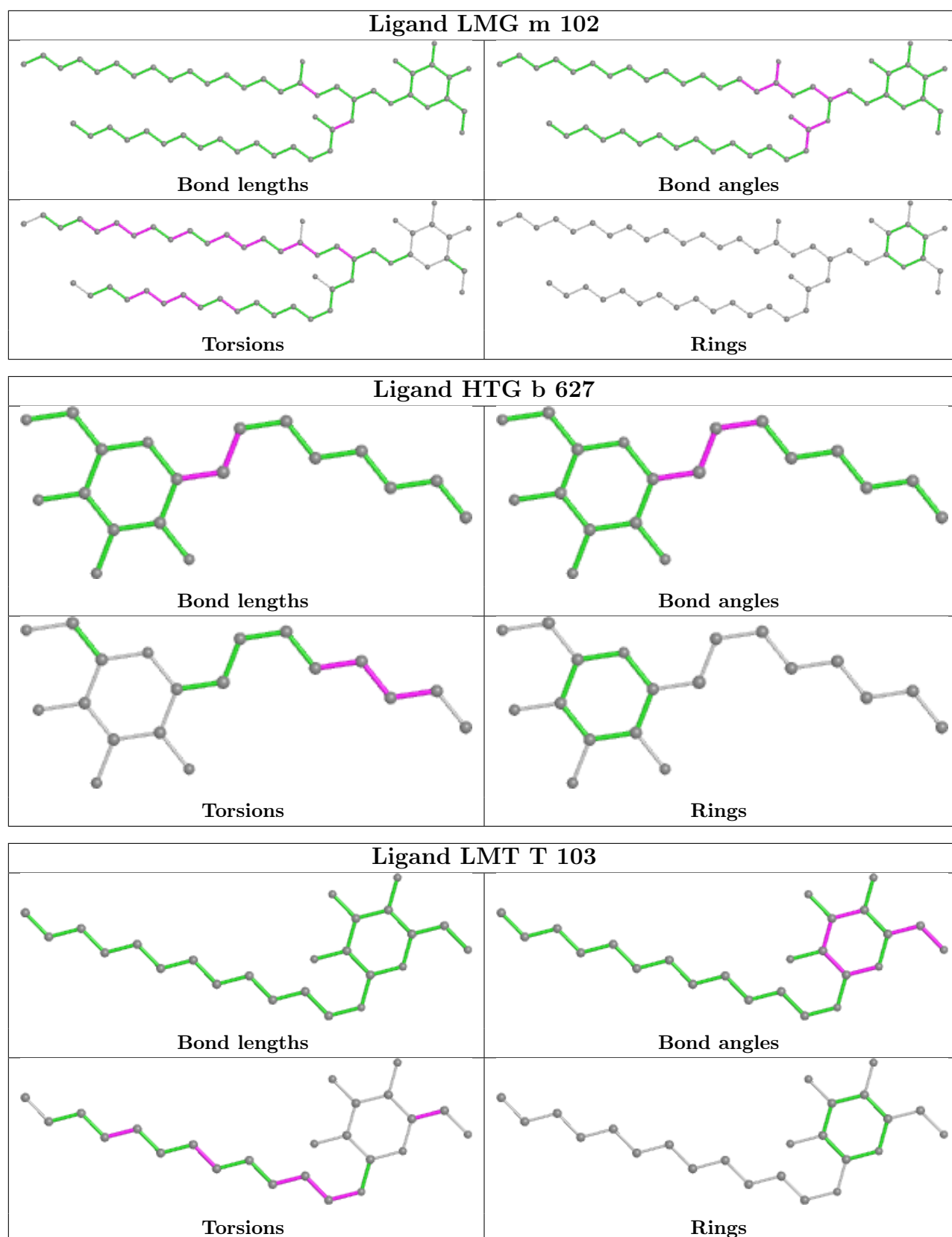
Ligand CLA C 511

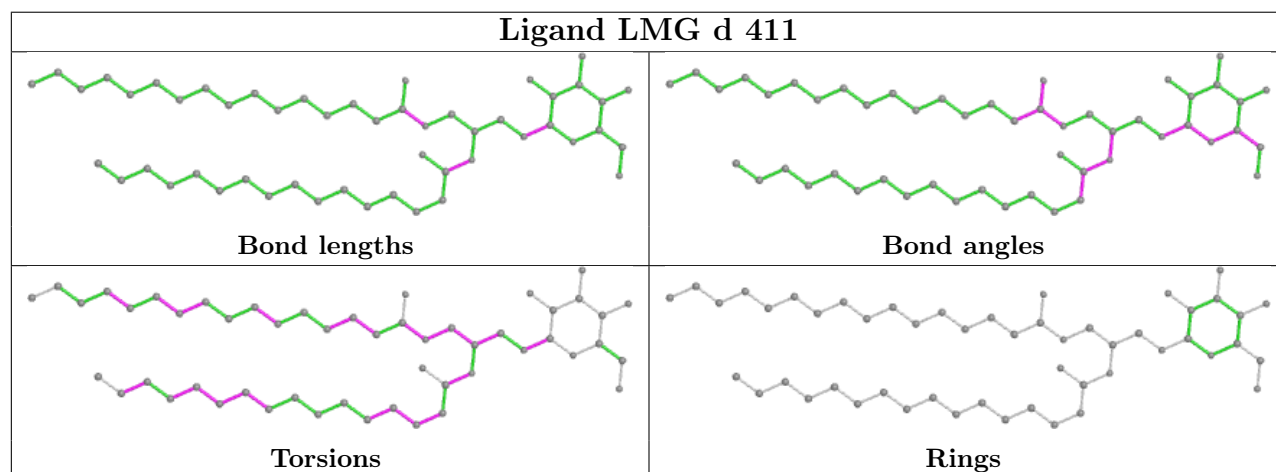
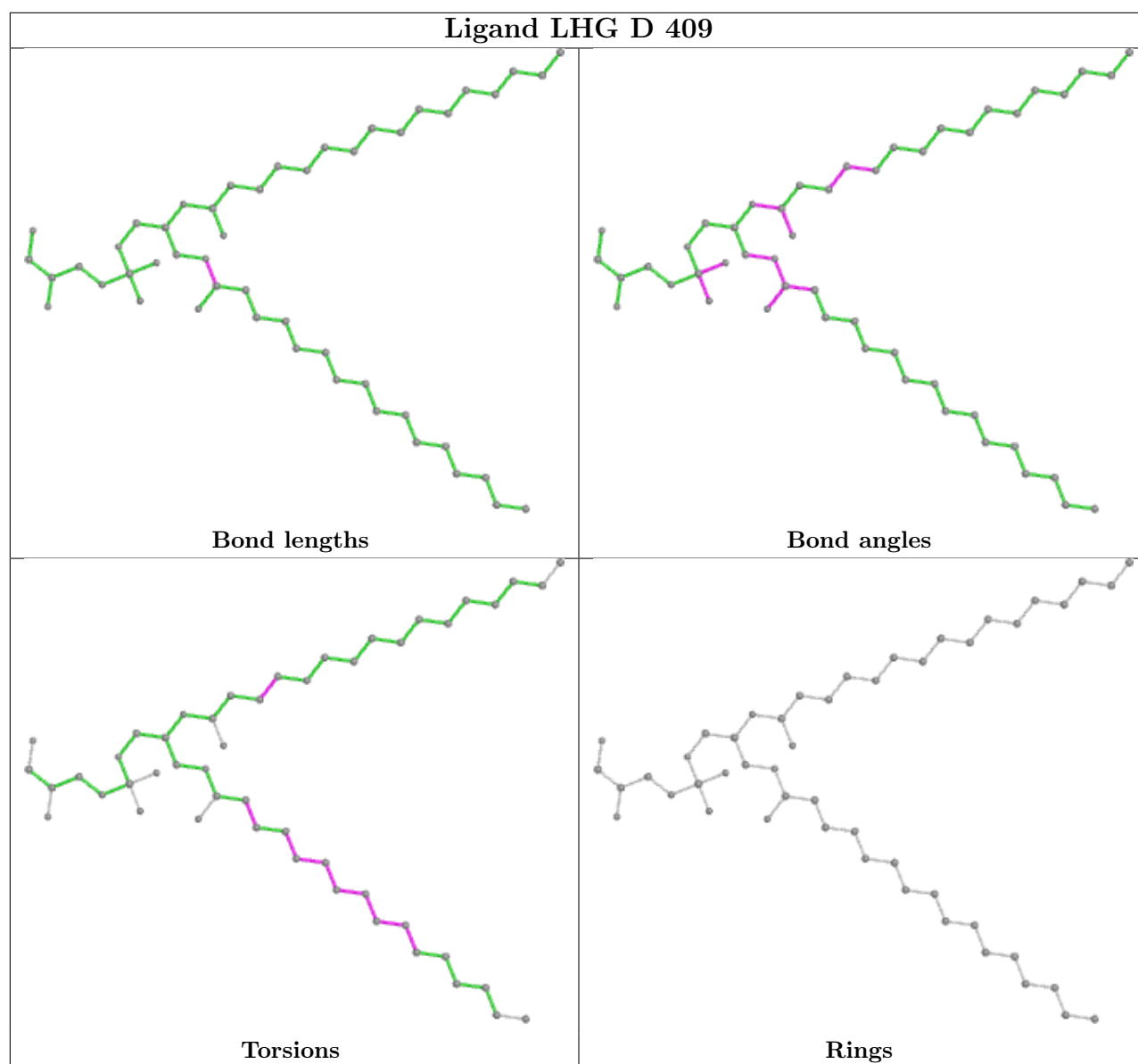


Ligand LMT M 101

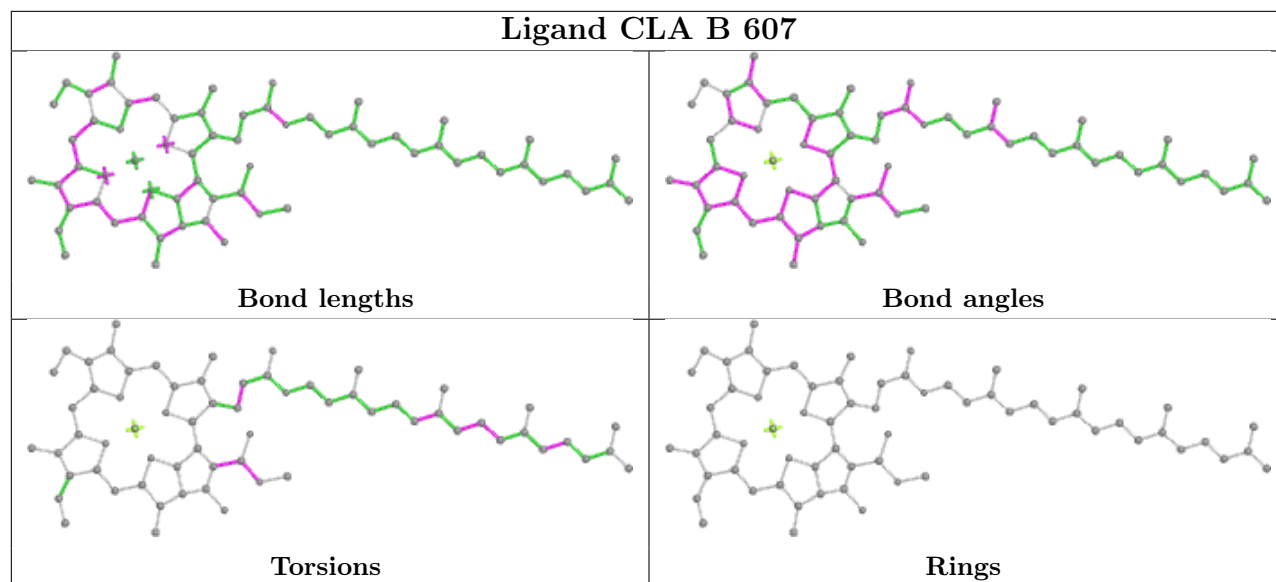




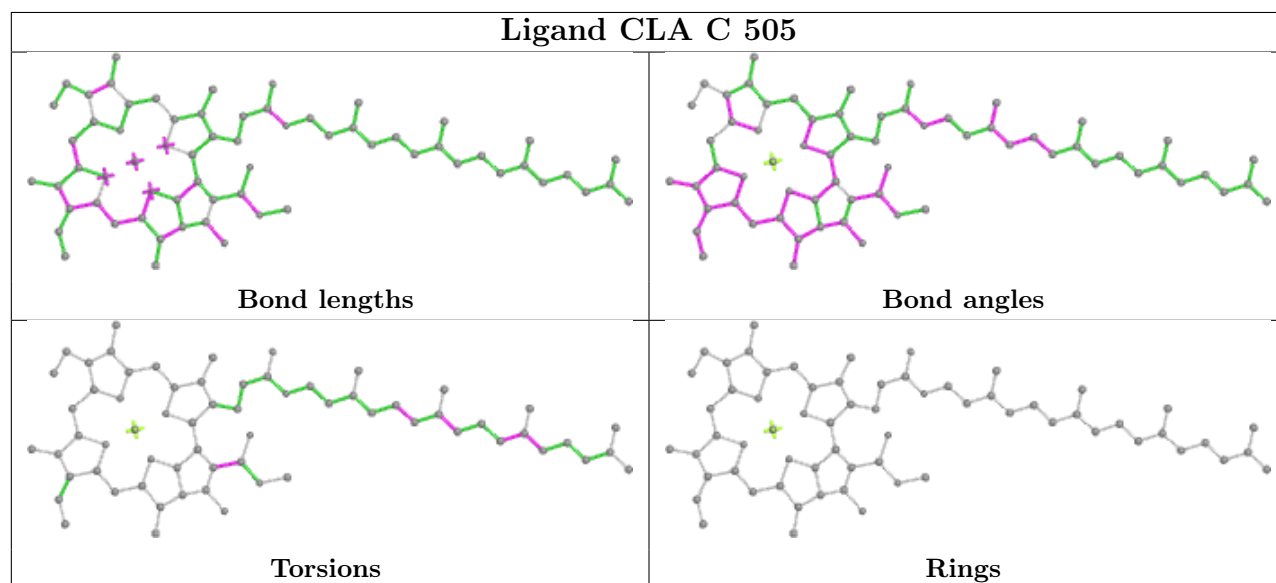


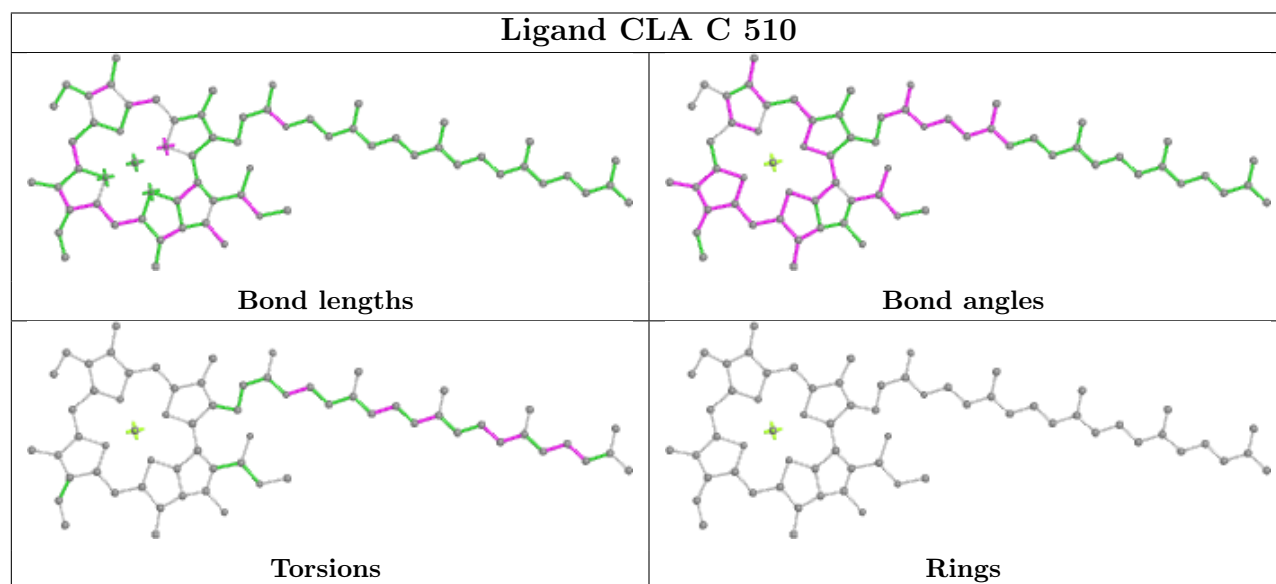
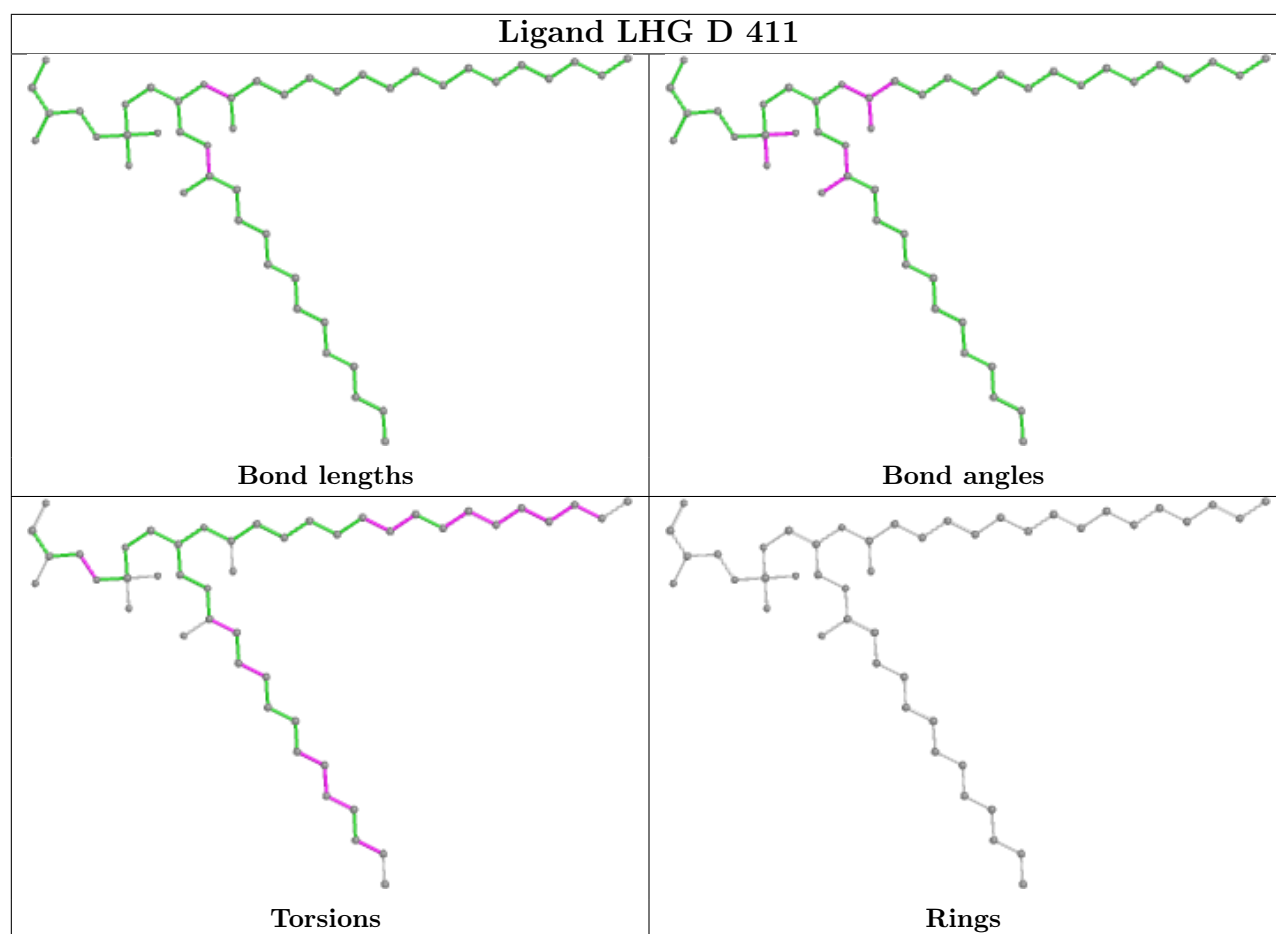


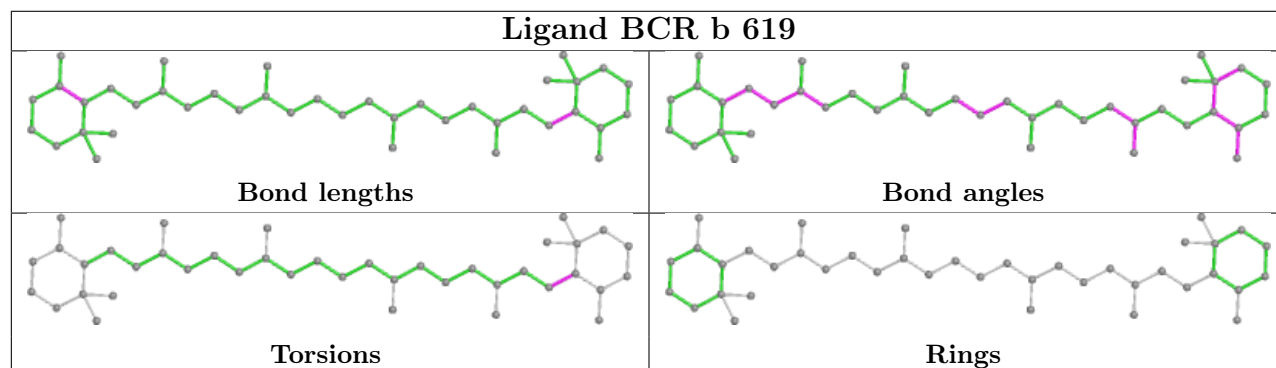
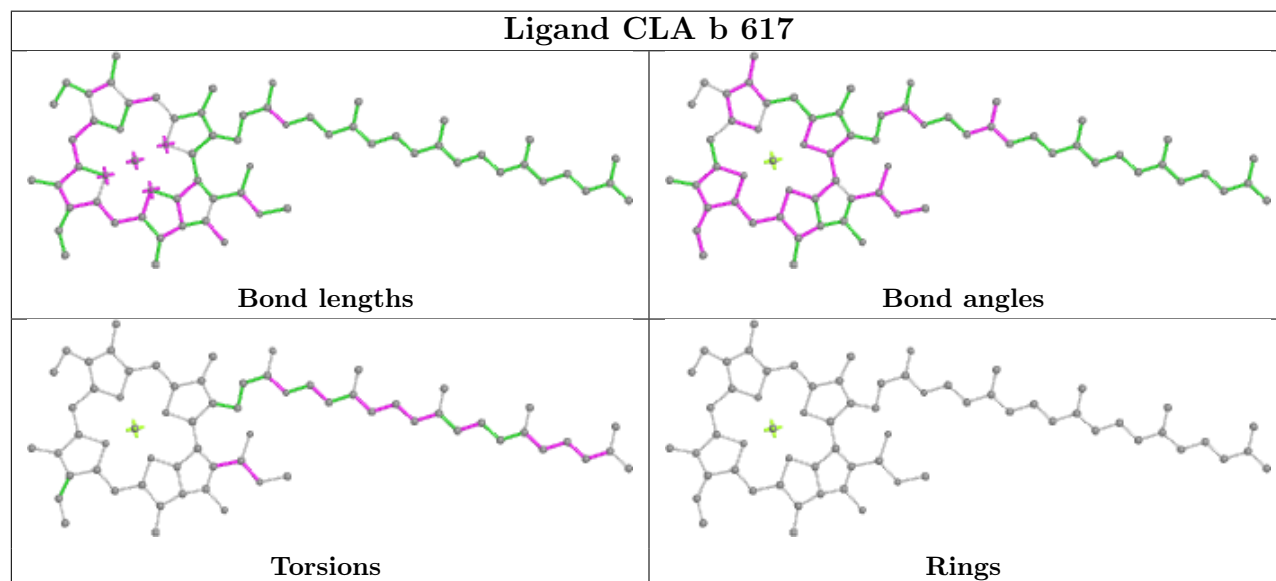
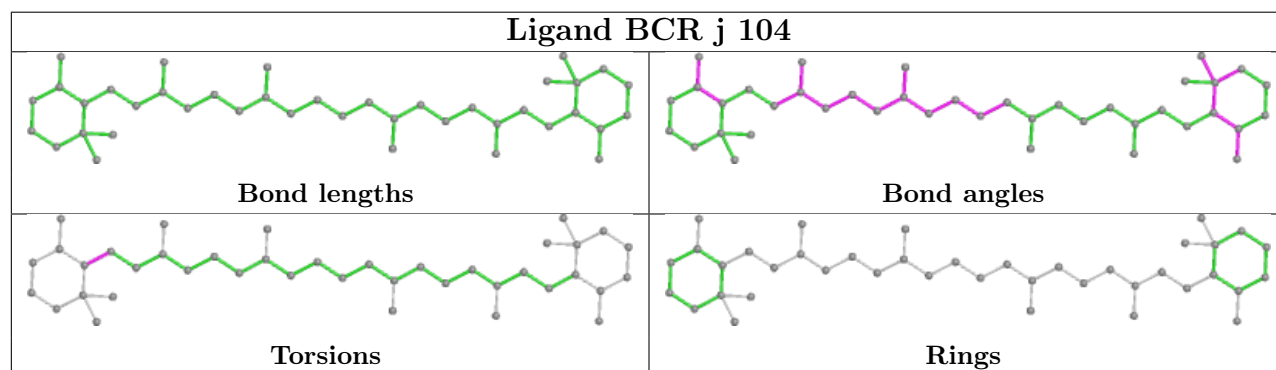
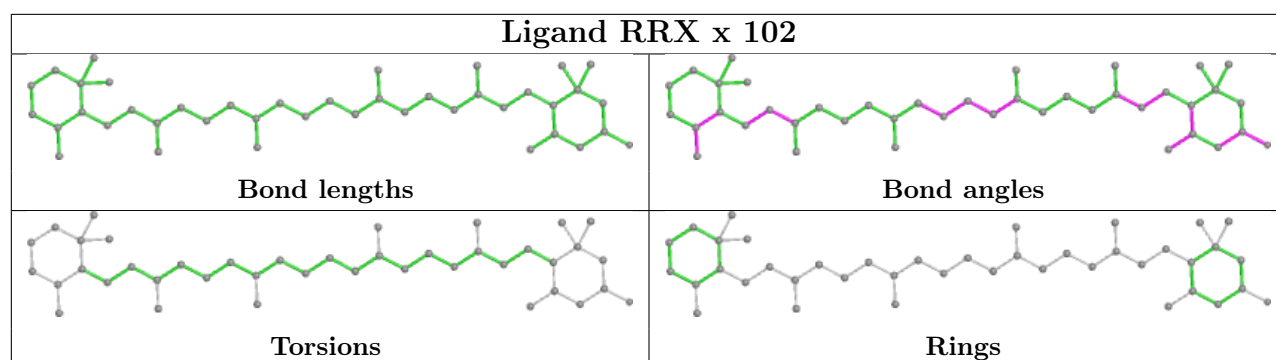
Ligand CLA B 607



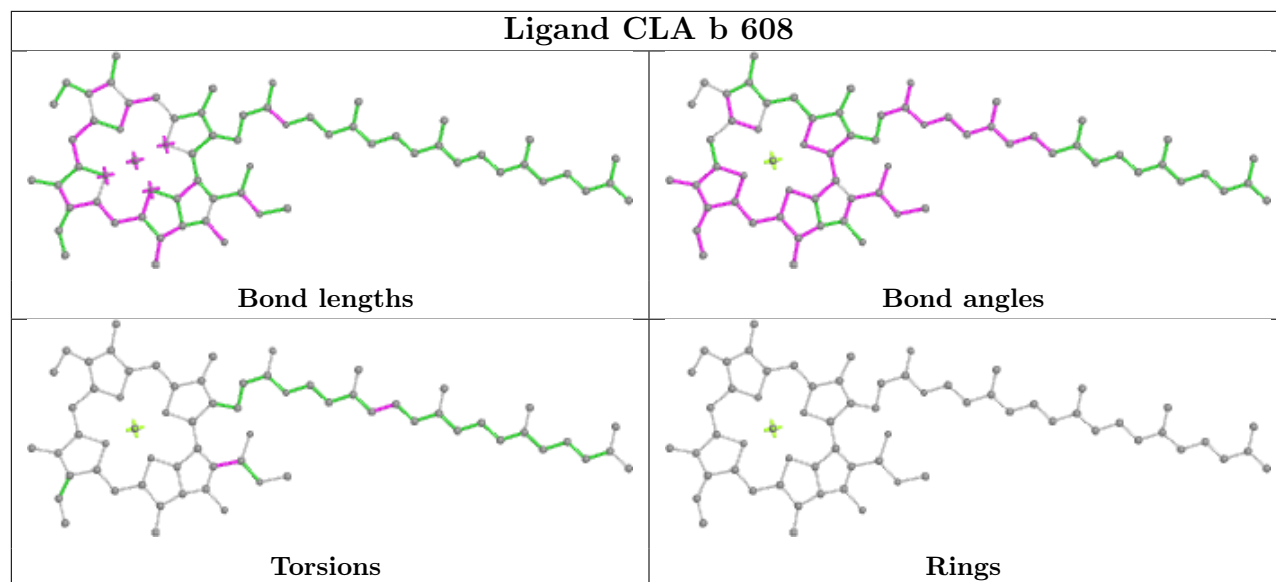
Ligand CLA C 505



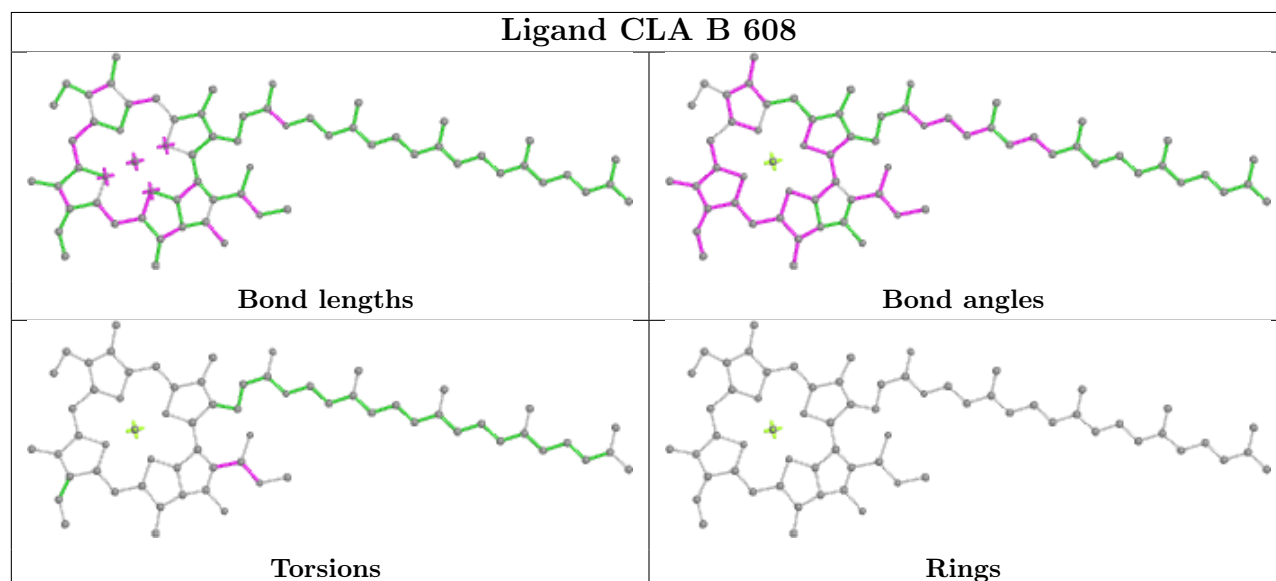




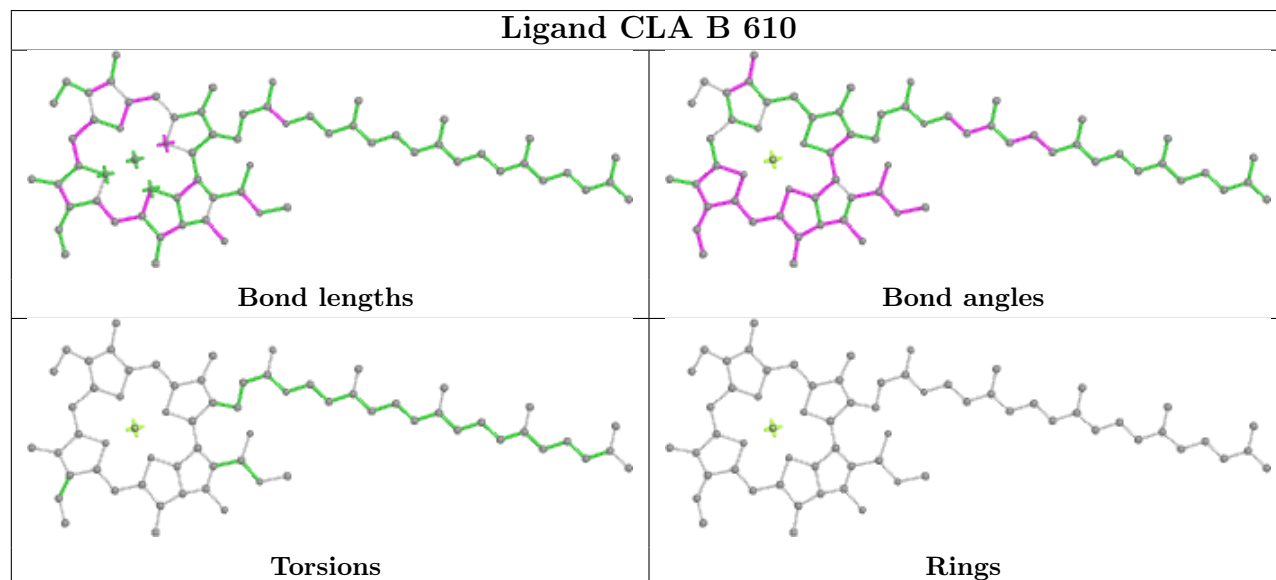
Ligand CLA b 608



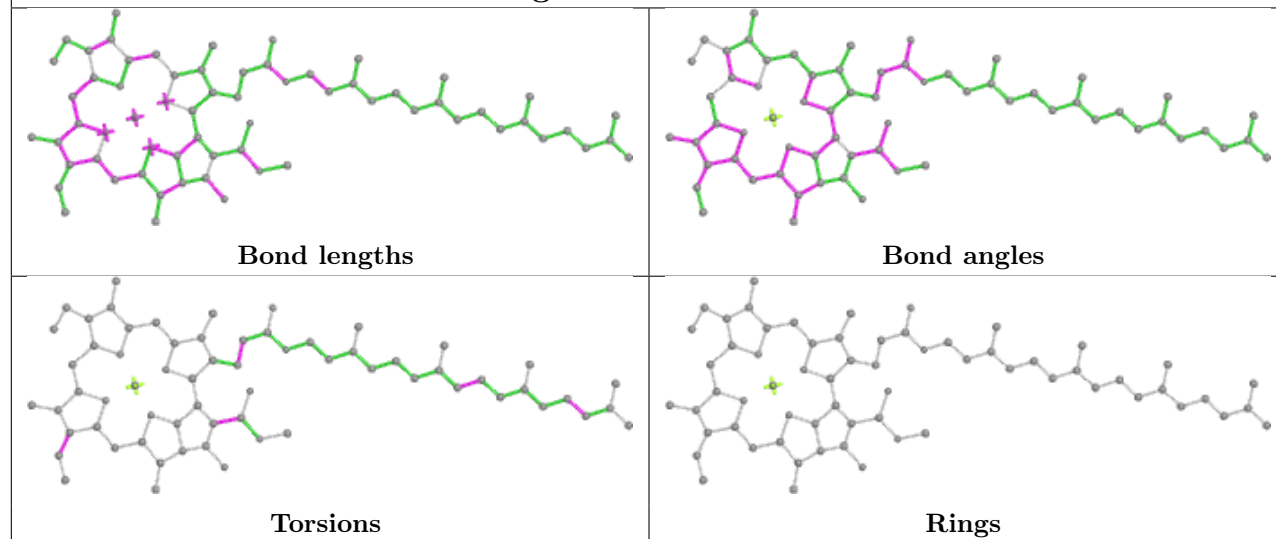
Ligand CLA B 608



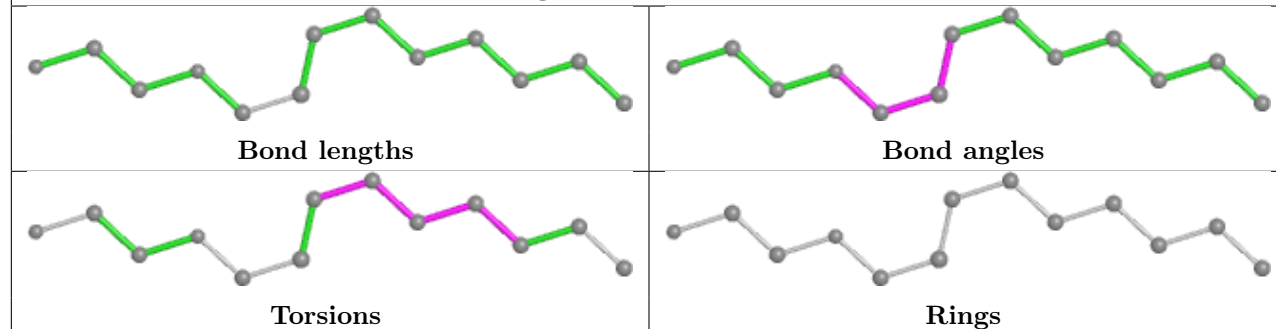
Ligand CLA B 610



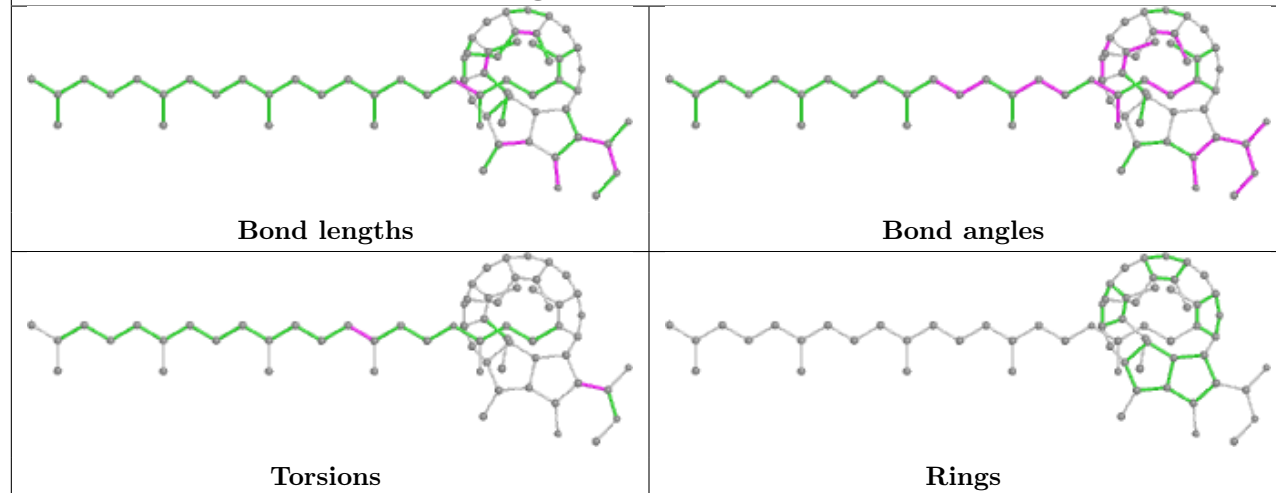
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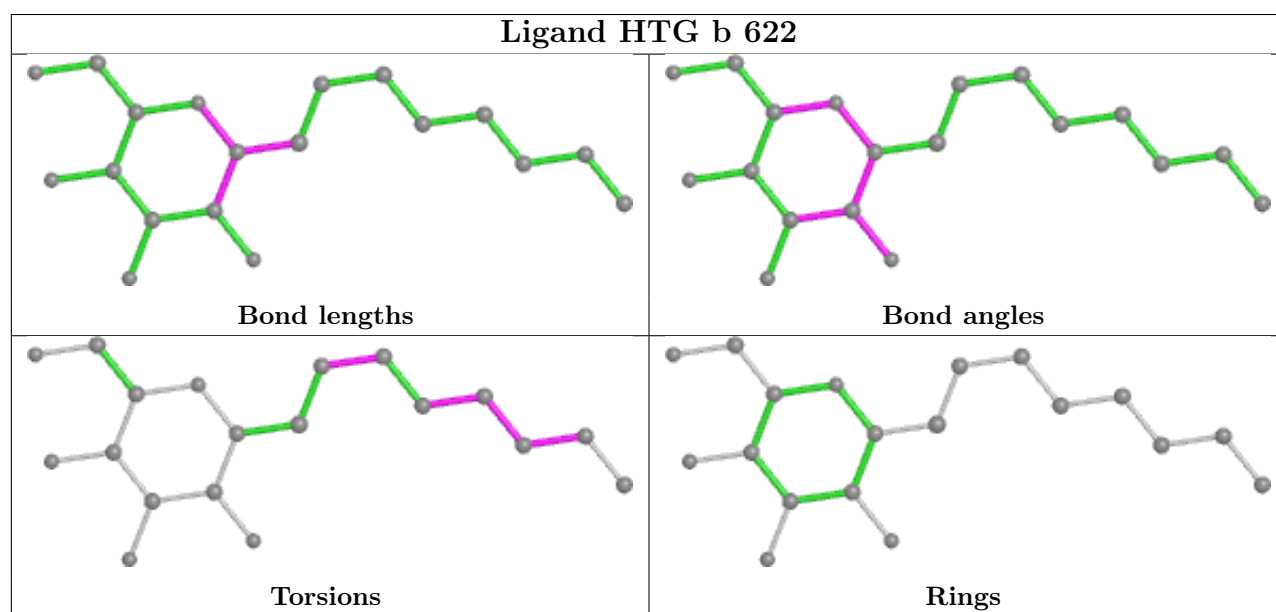
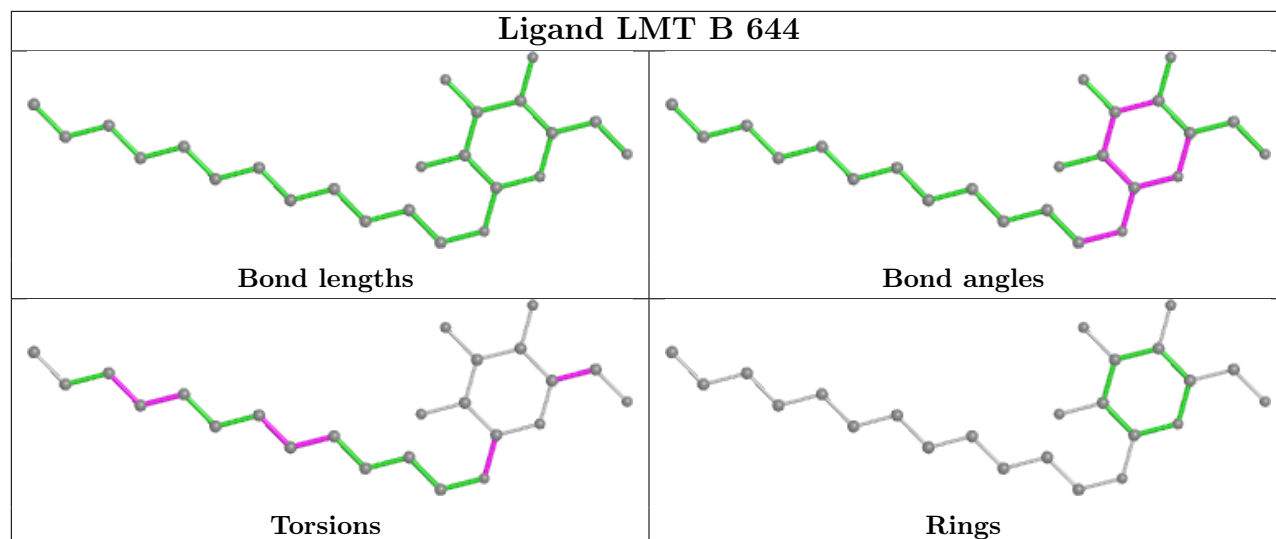


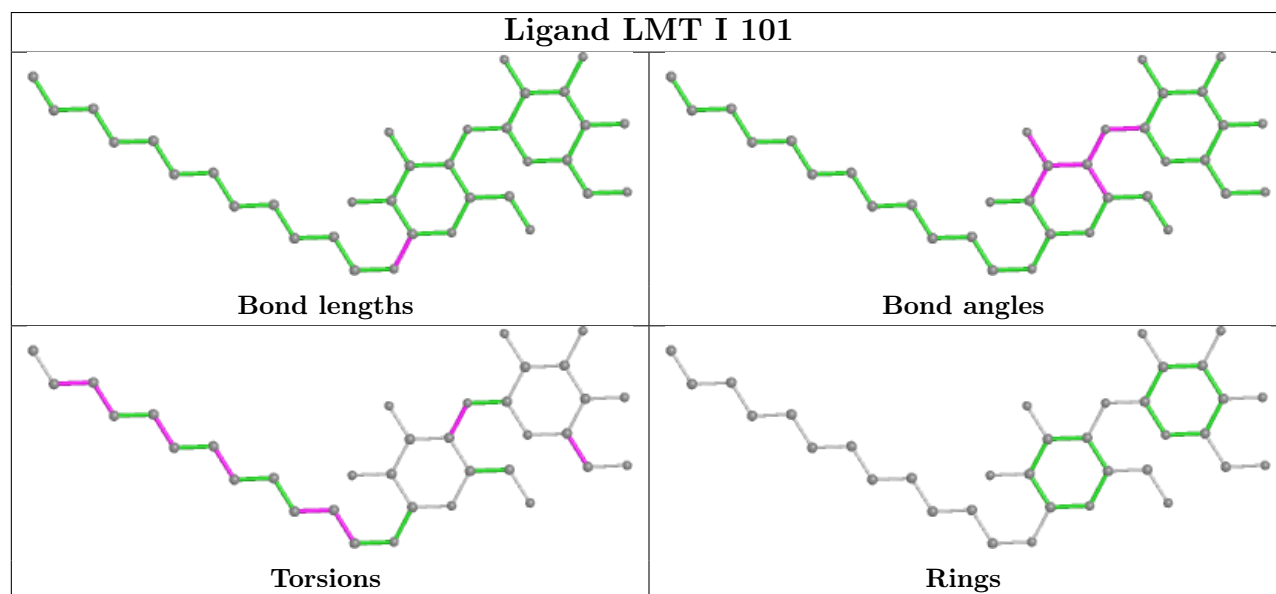
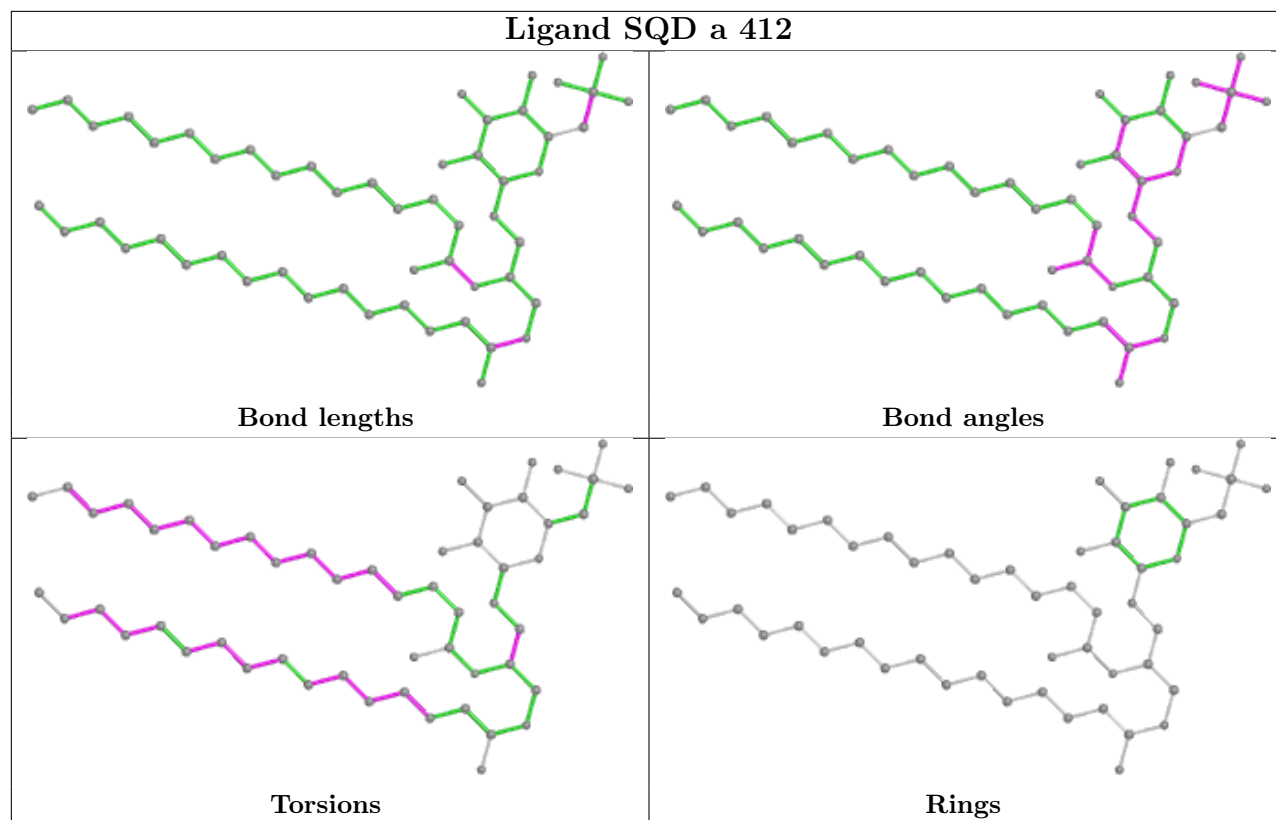
Ligand HTG c 923



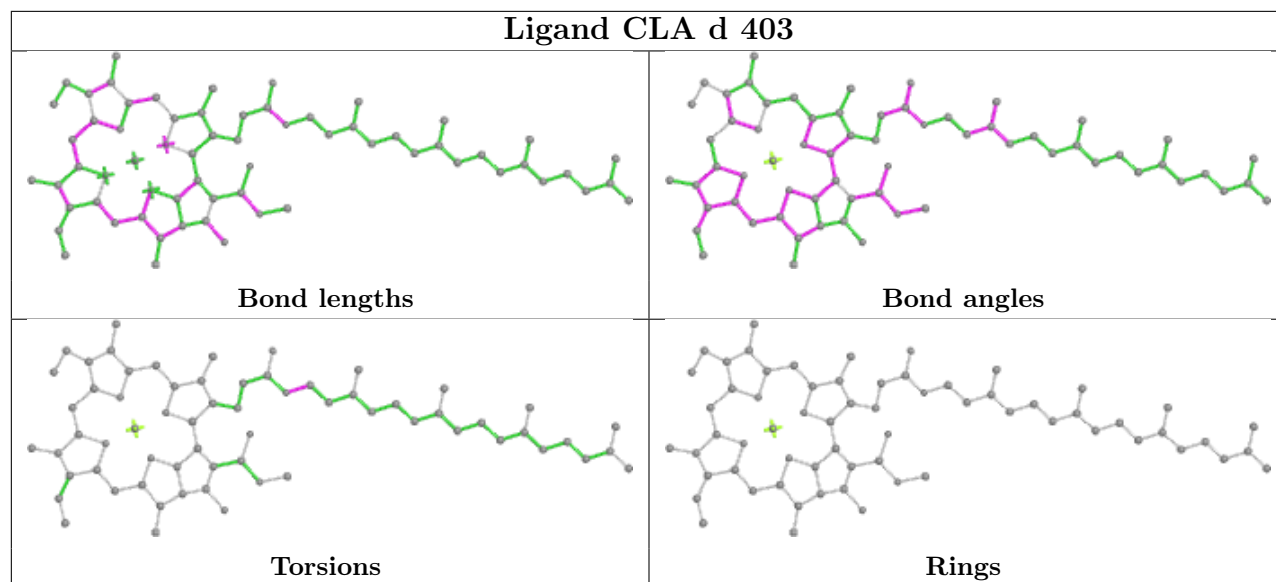
Ligand PHO A 407



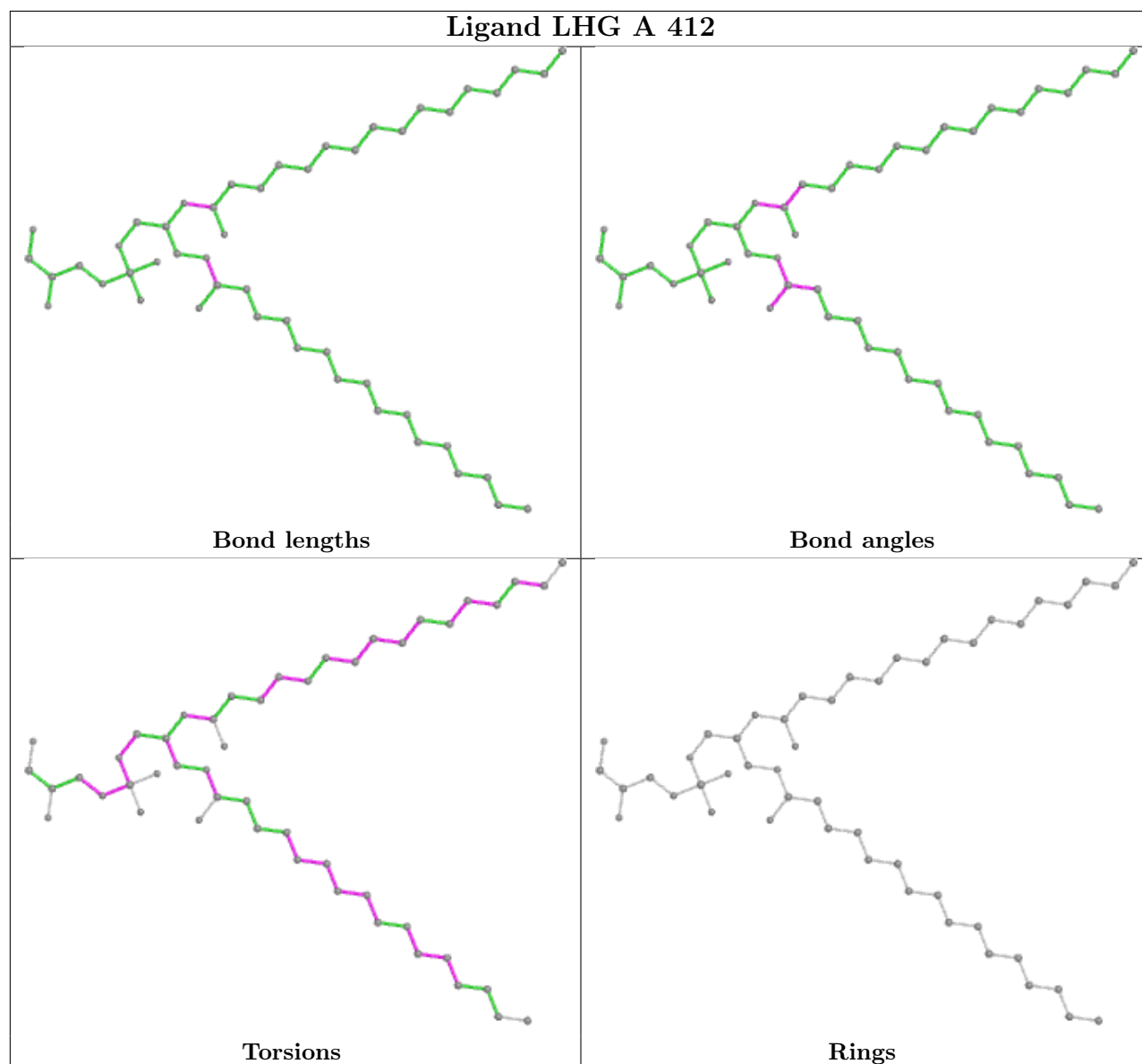


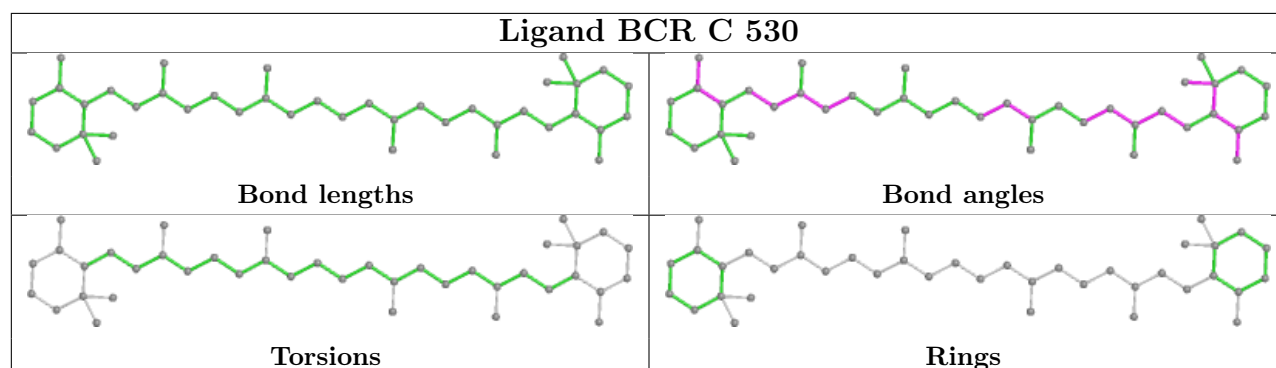
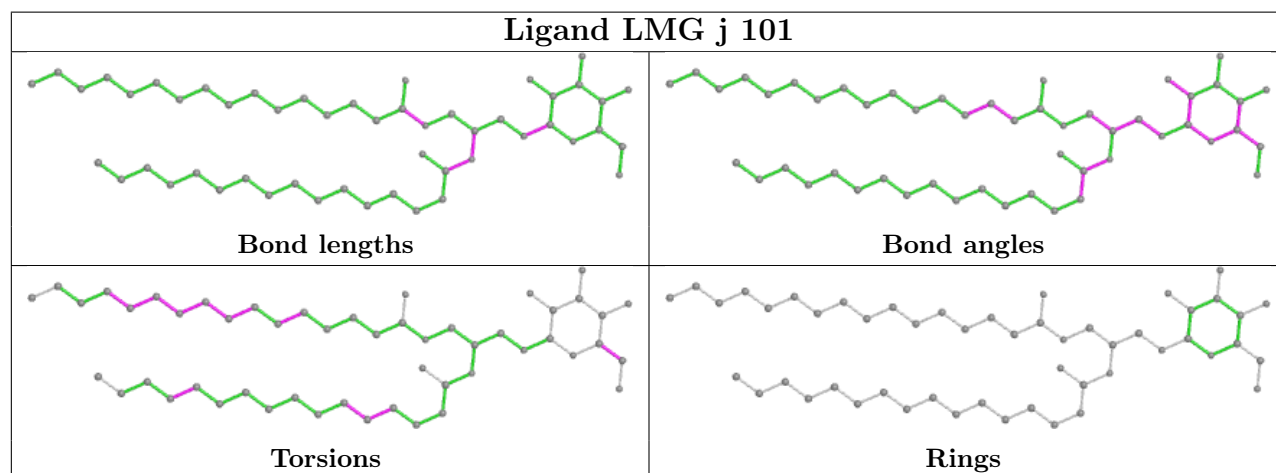
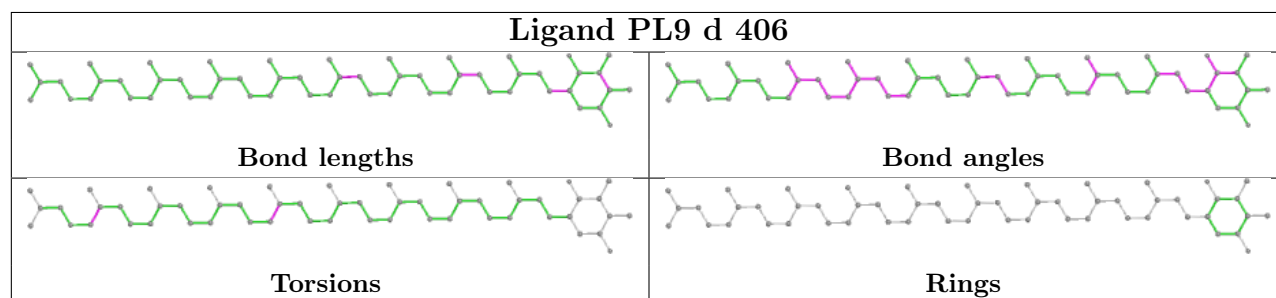
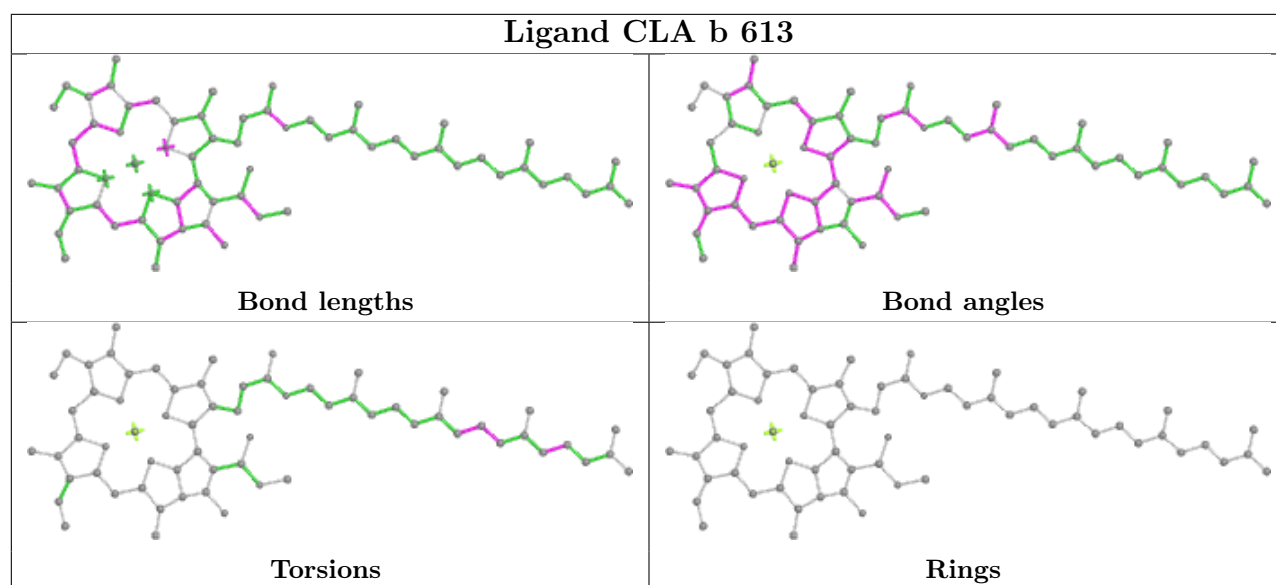


Ligand CLA d 403

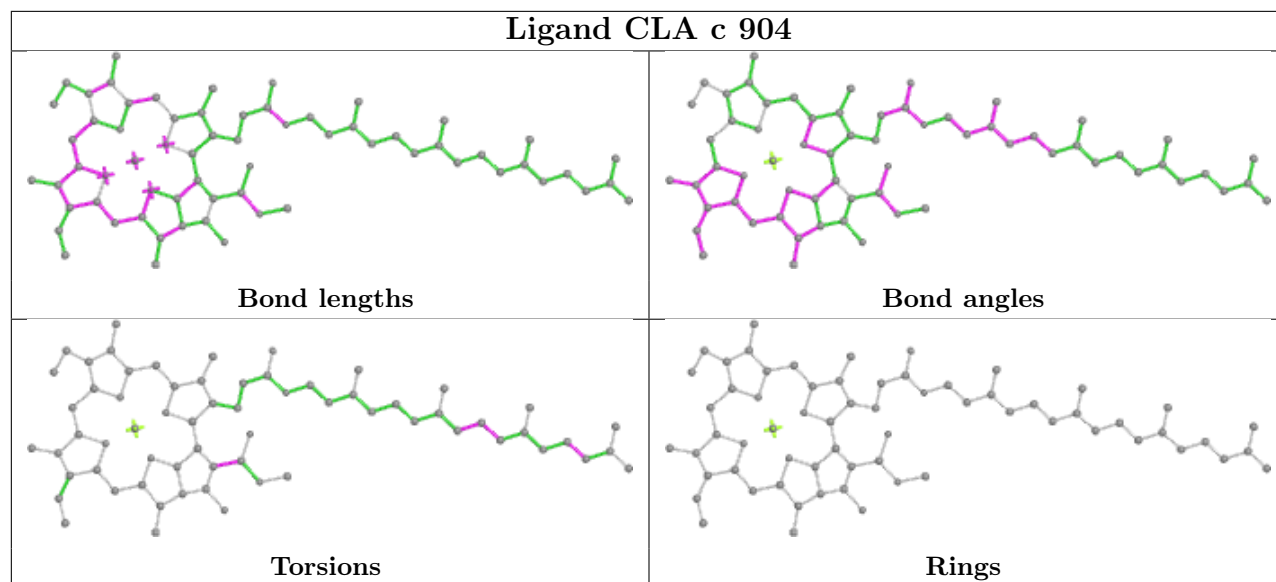


Ligand LHG A 412

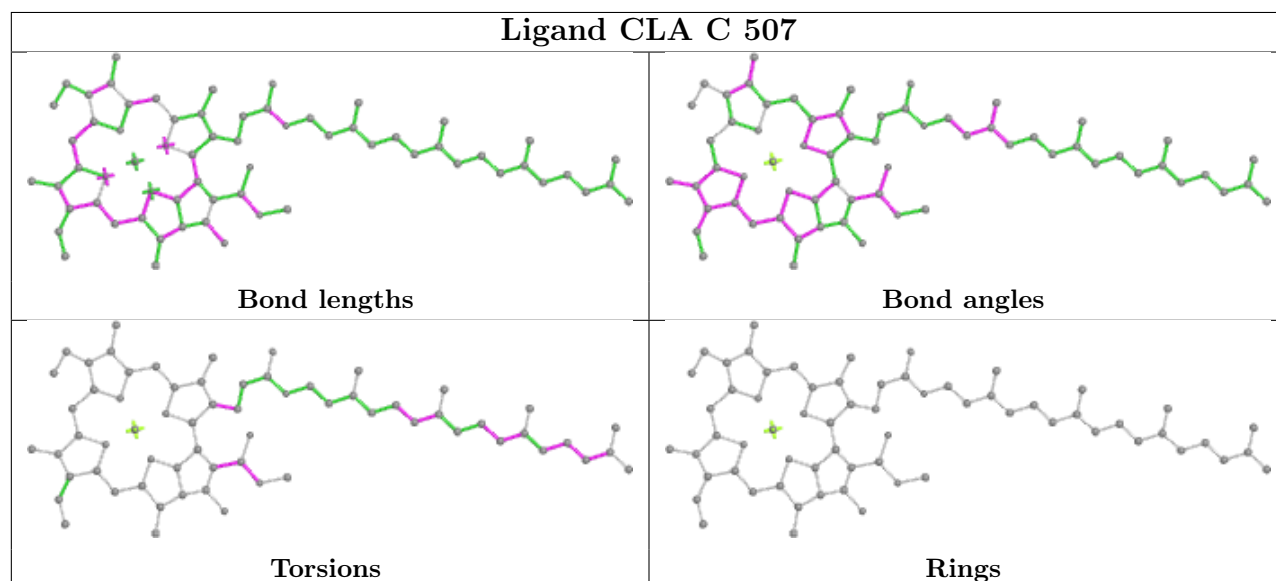




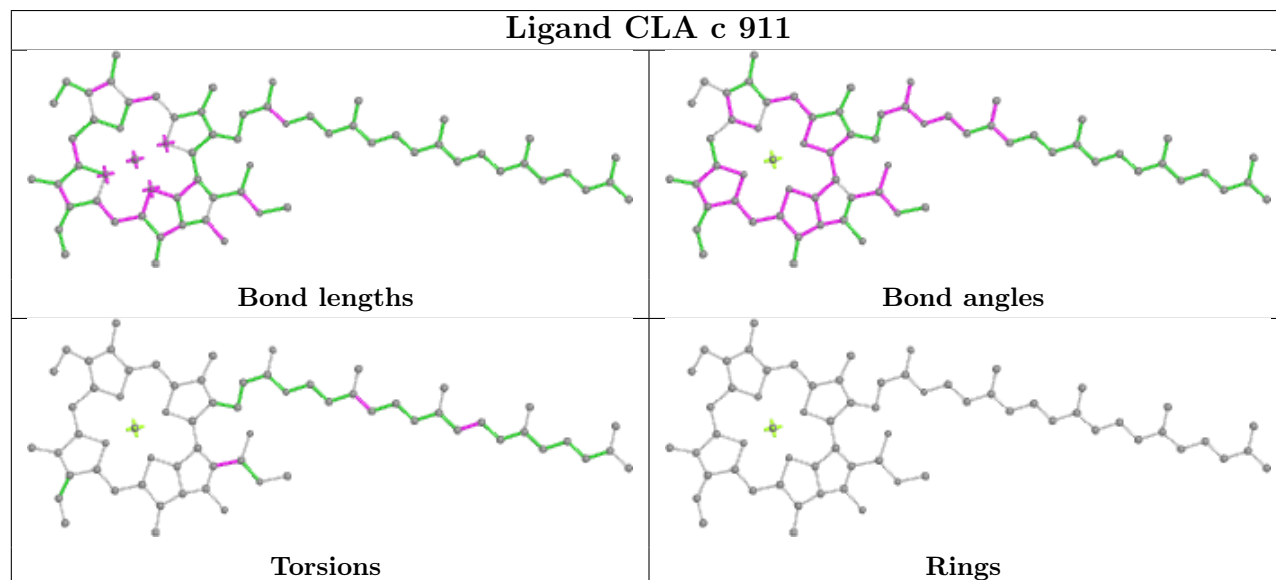
Ligand CLA c 904

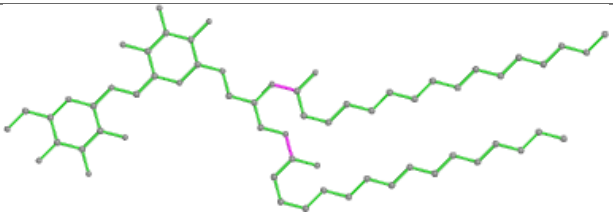
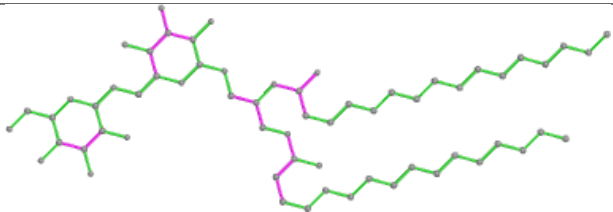
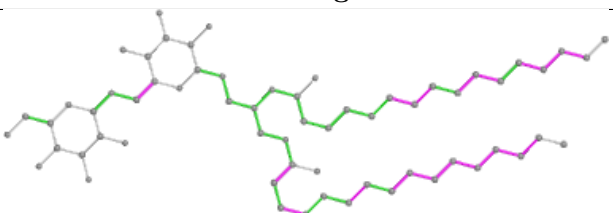
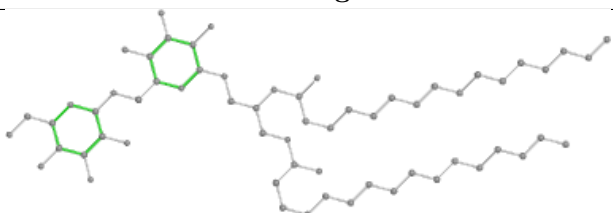


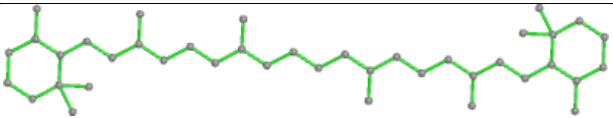
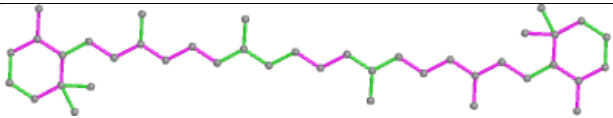
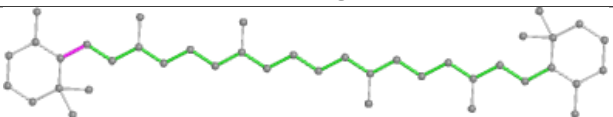
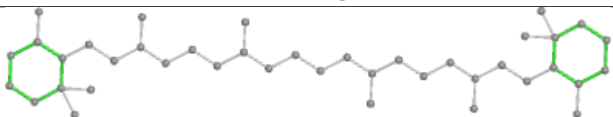
Ligand CLA C 507

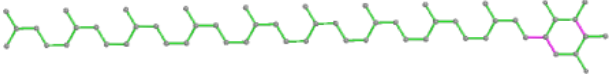
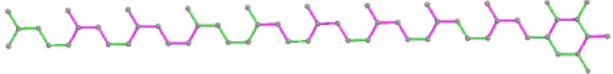
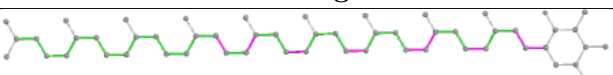
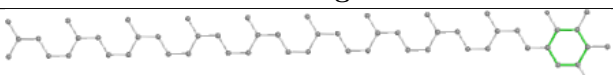


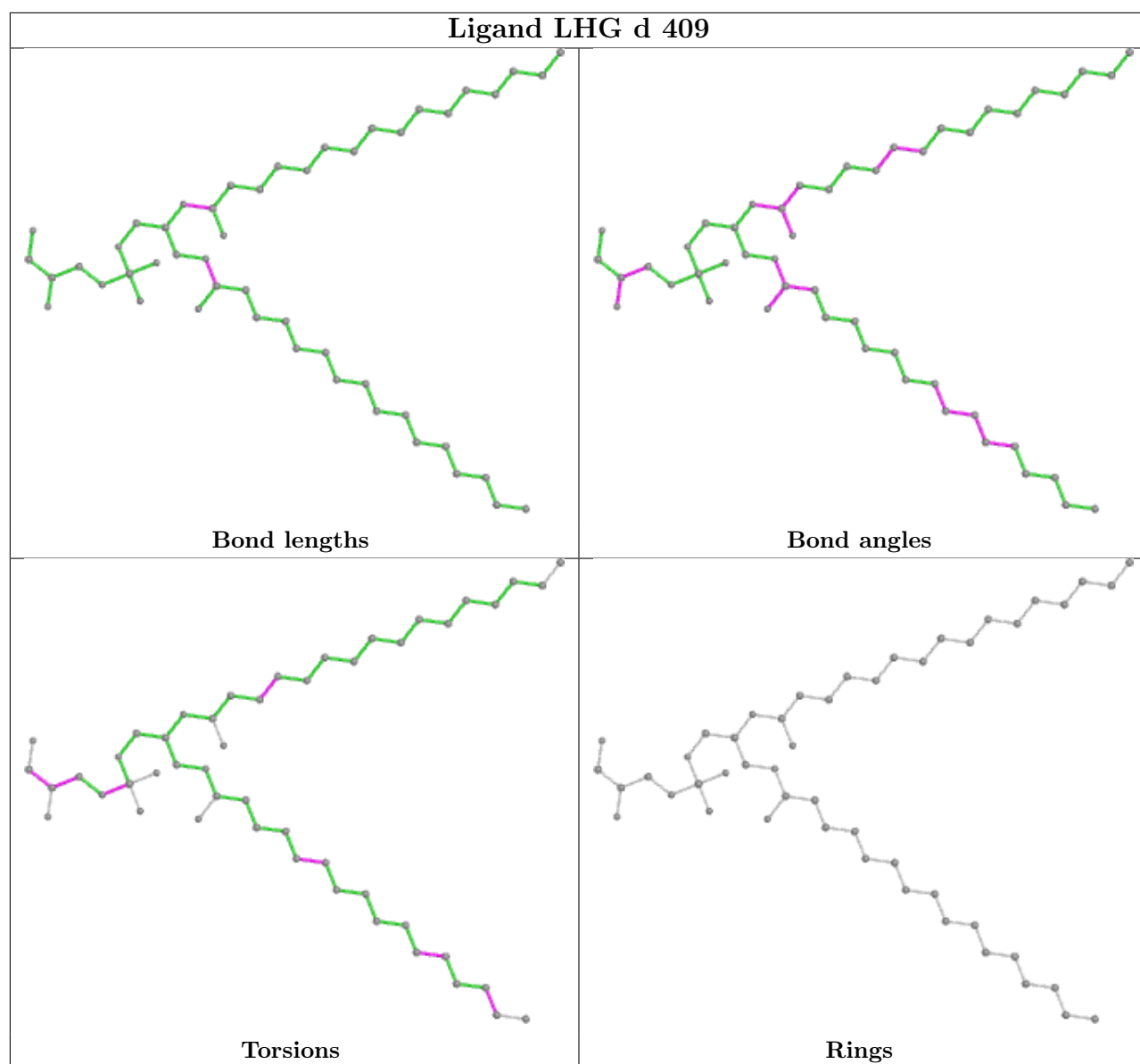
Ligand CLA c 911

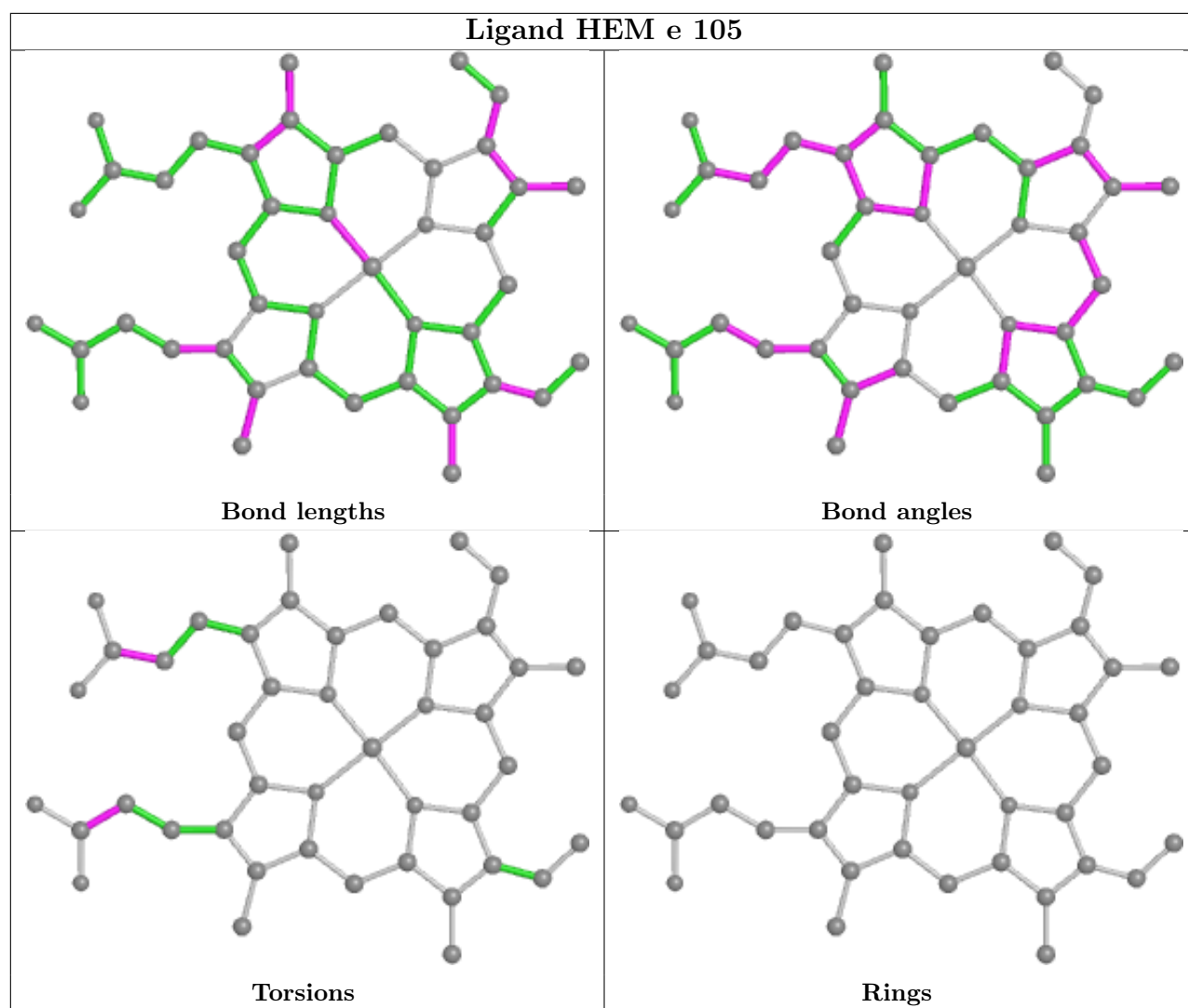


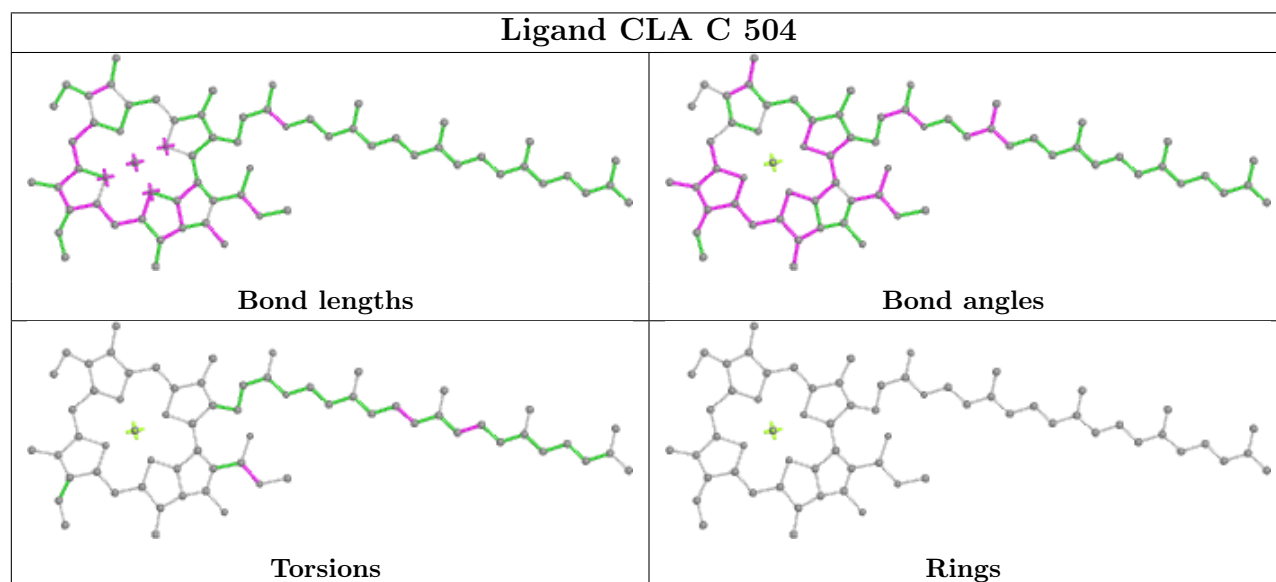
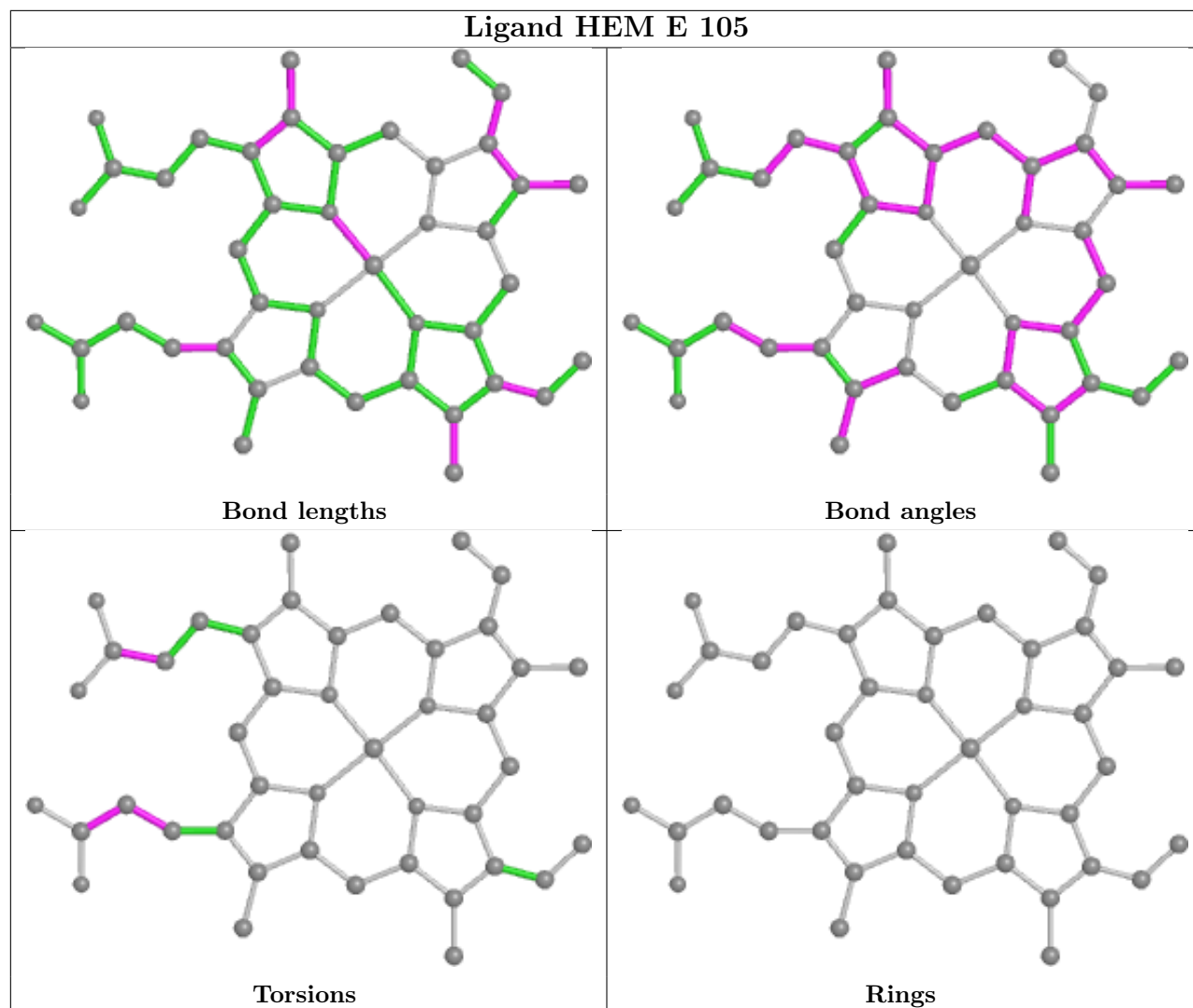
Ligand DGD C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

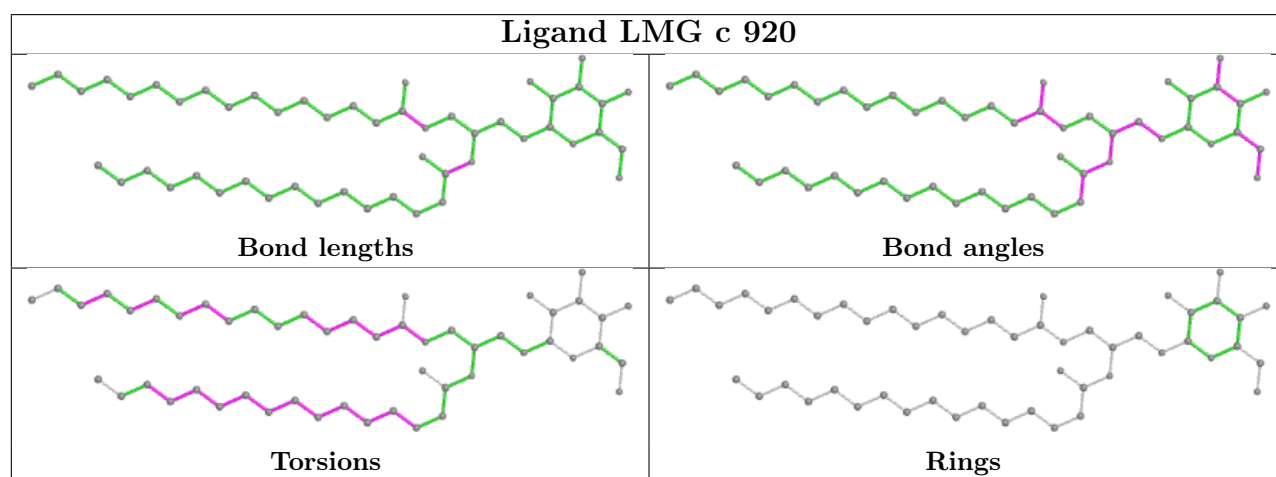
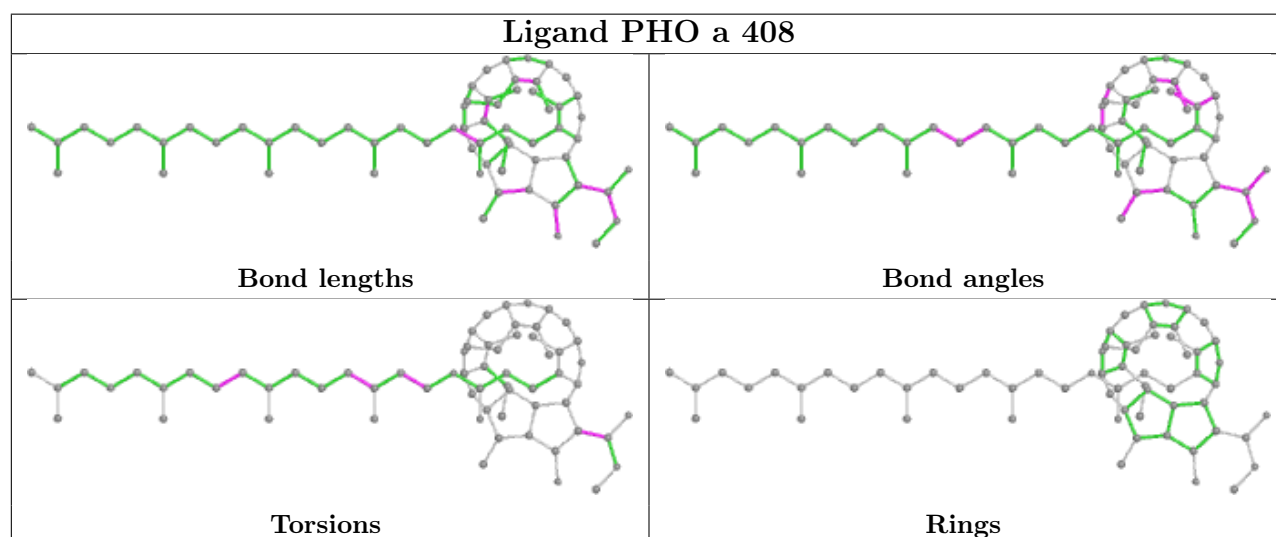
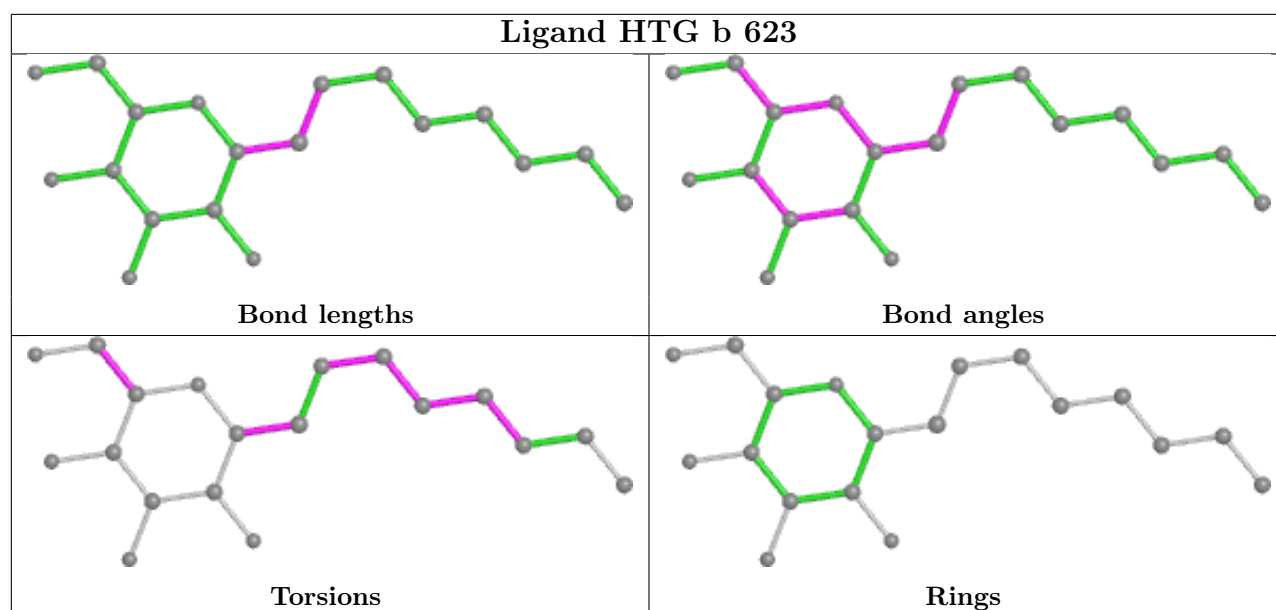
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

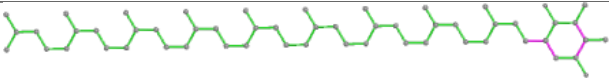
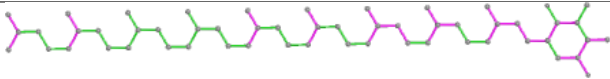
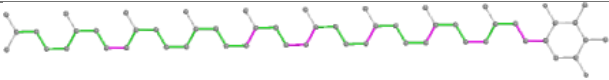
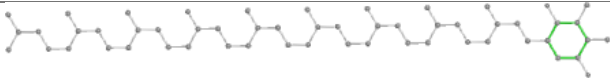
Ligand PL9 a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

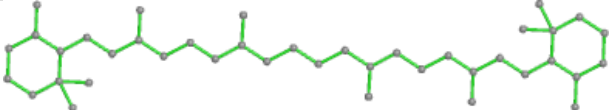
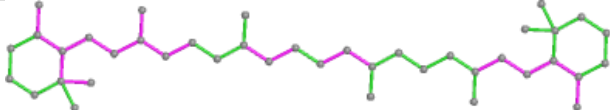
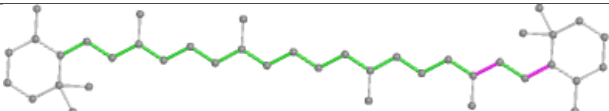
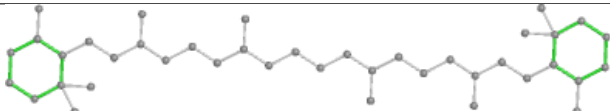


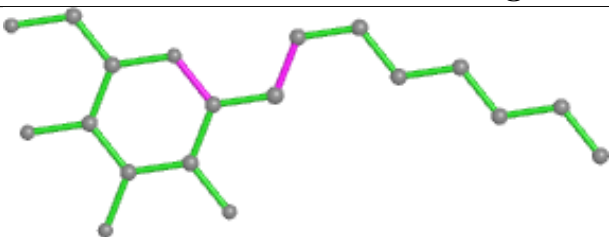
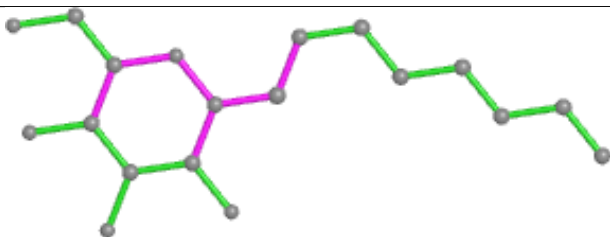
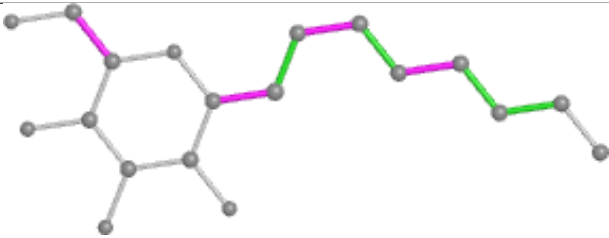
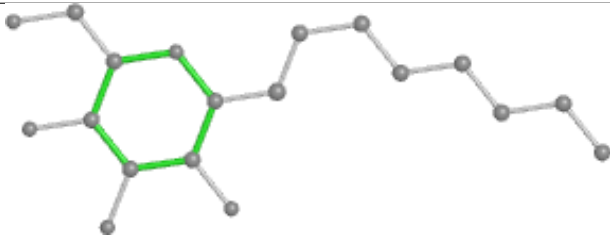


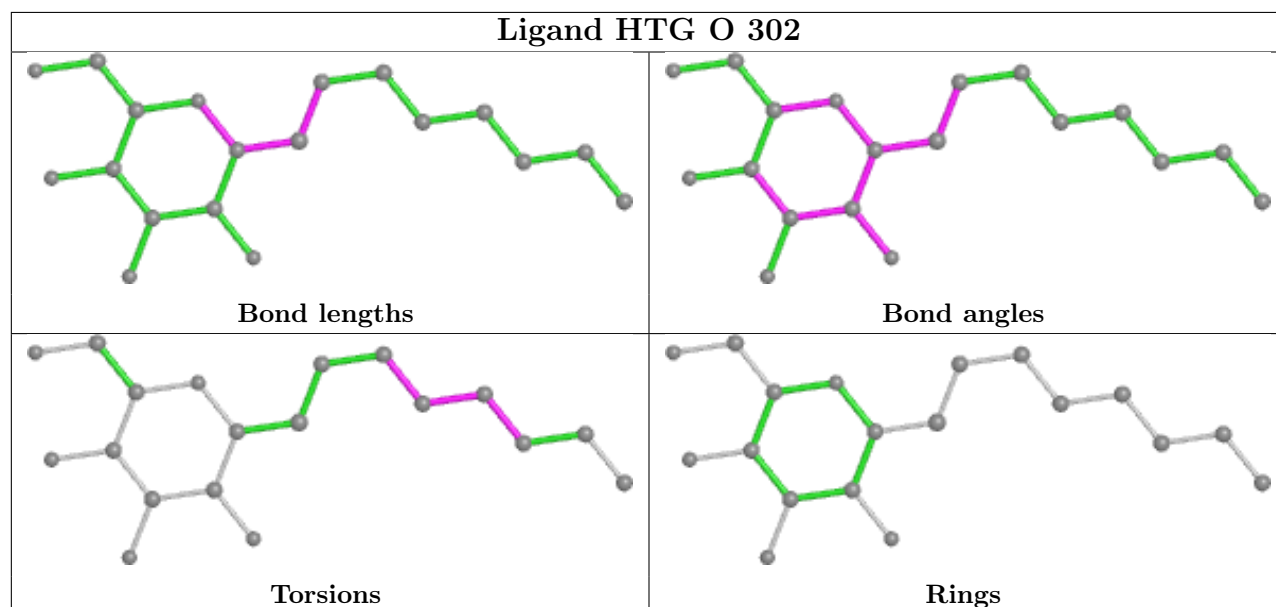
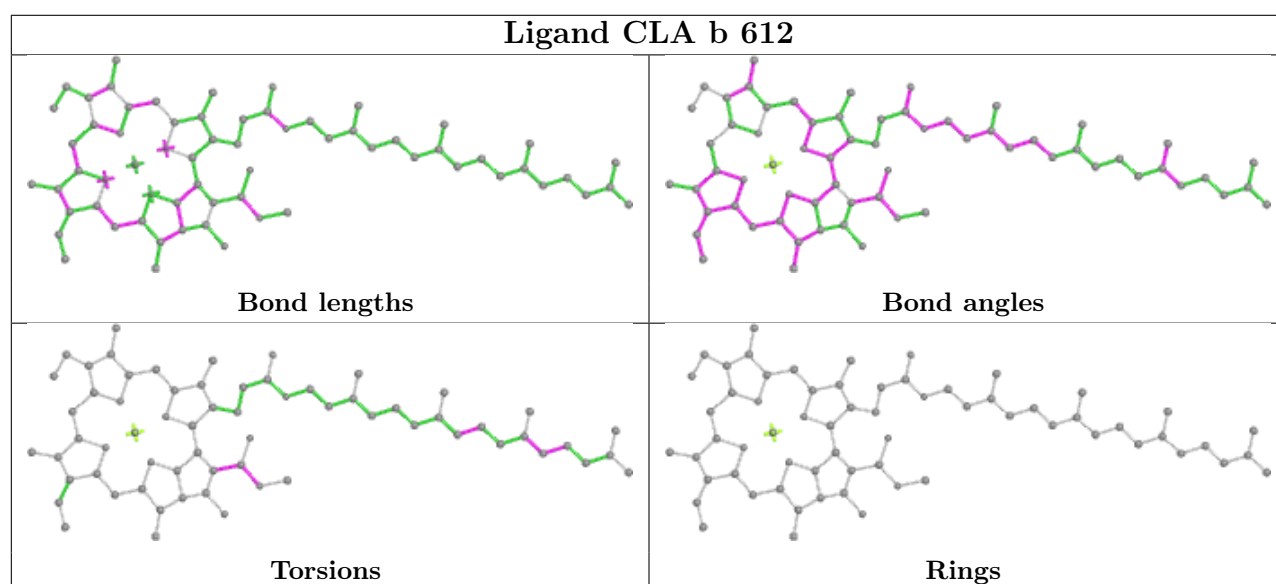
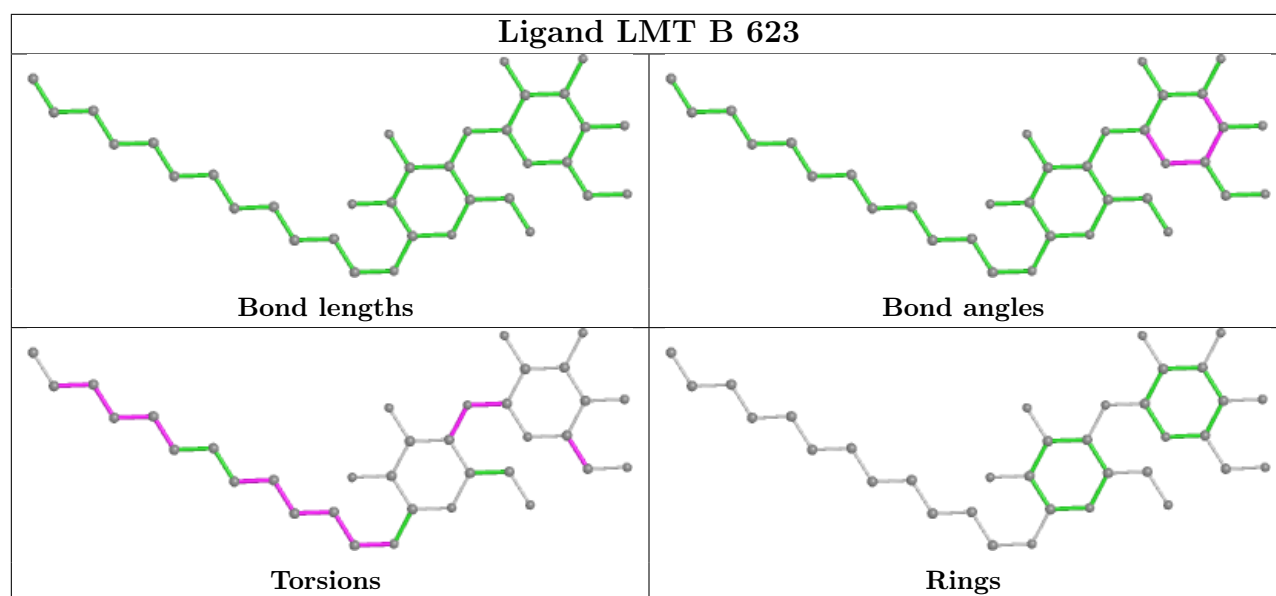


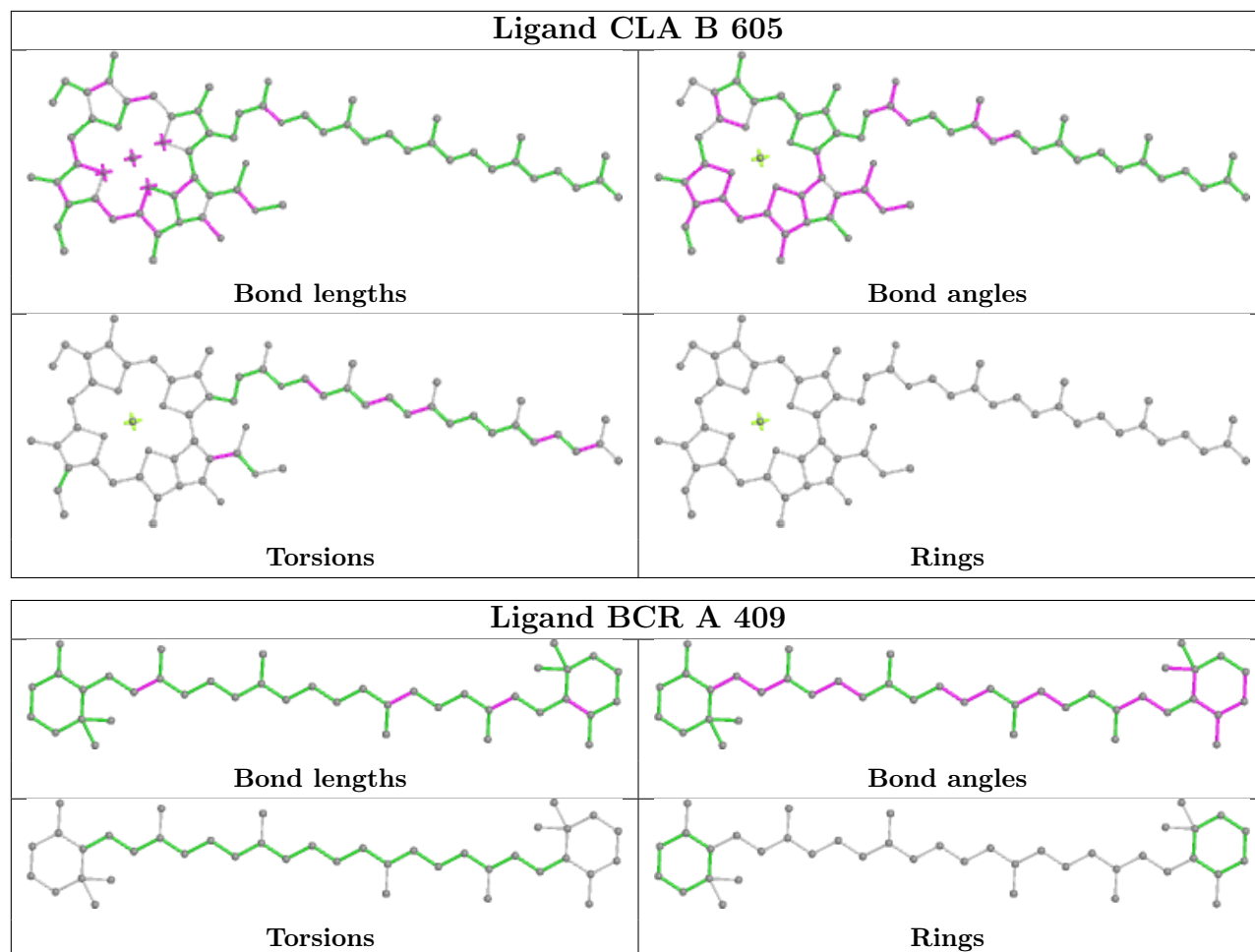


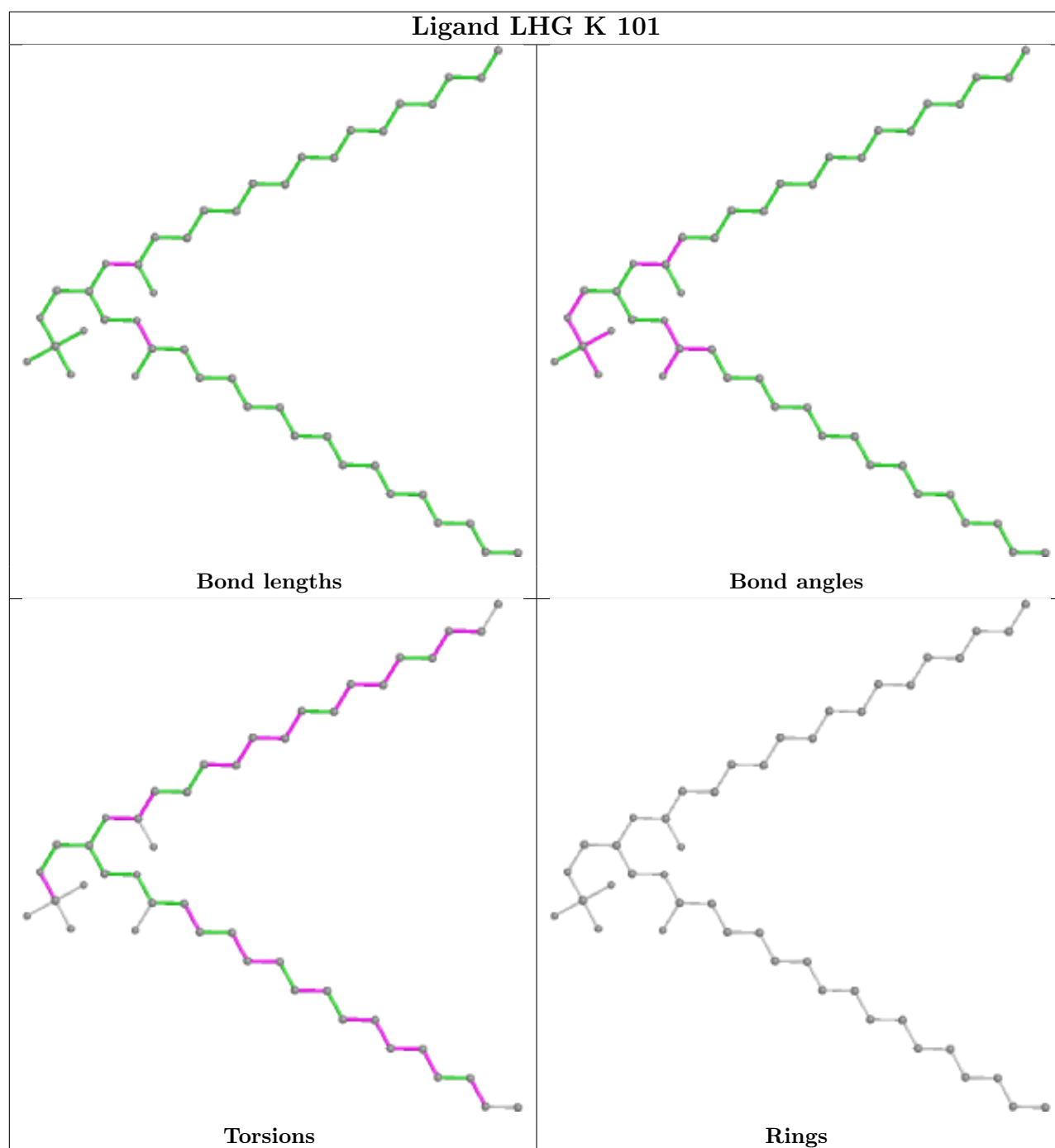
Ligand PL9 A 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

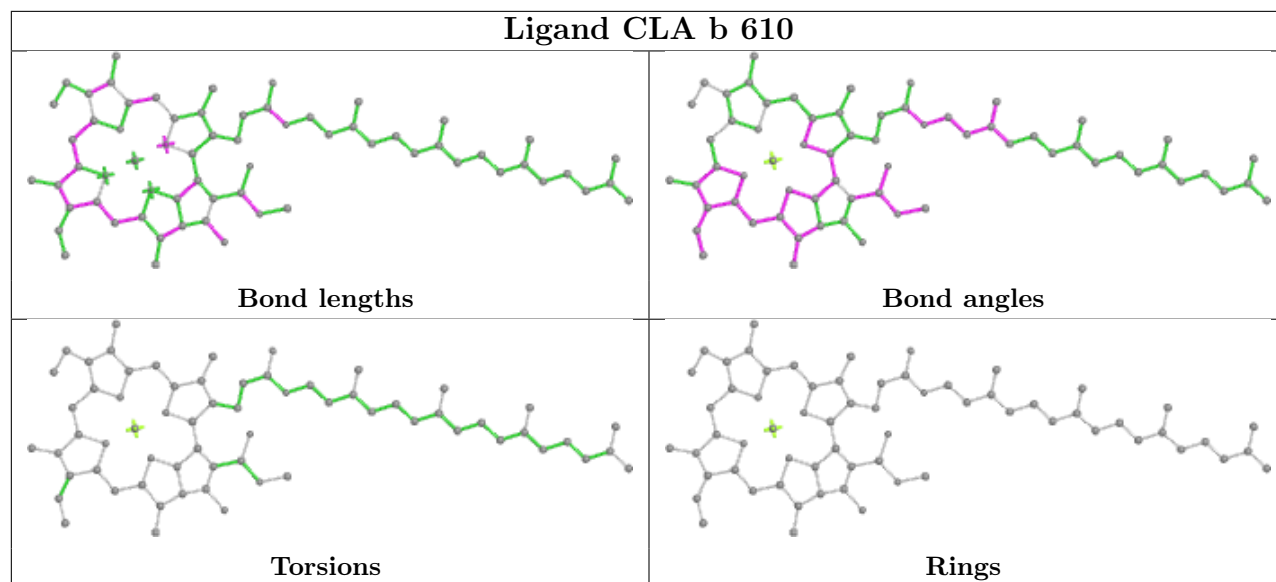
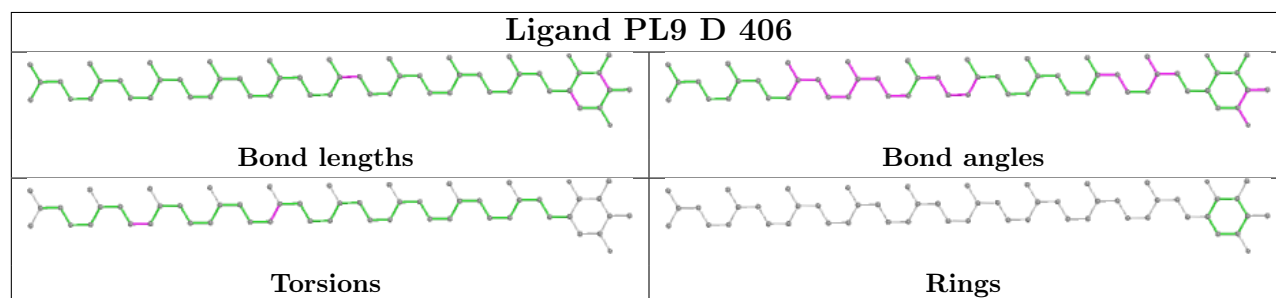
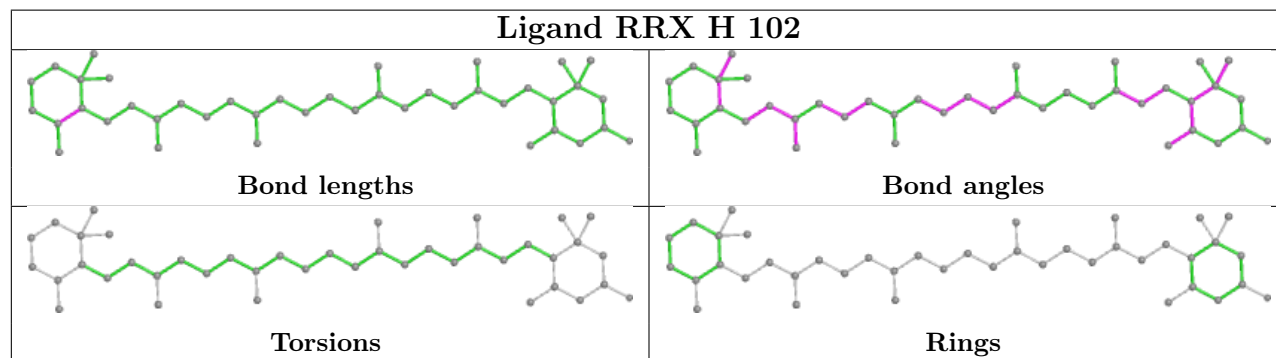
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG C 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

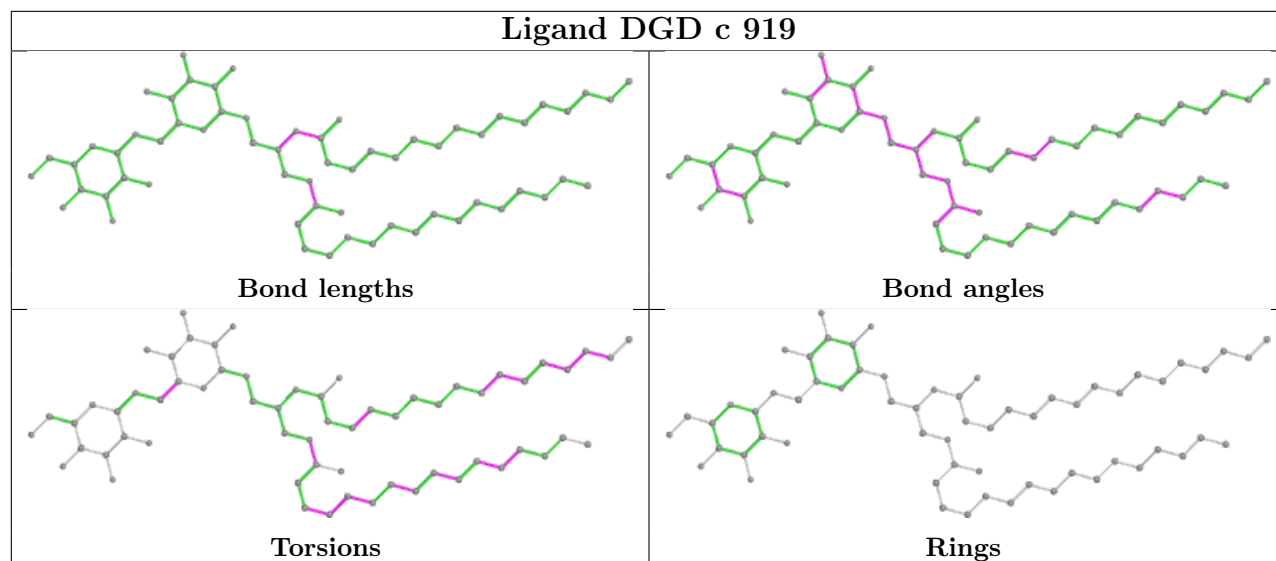




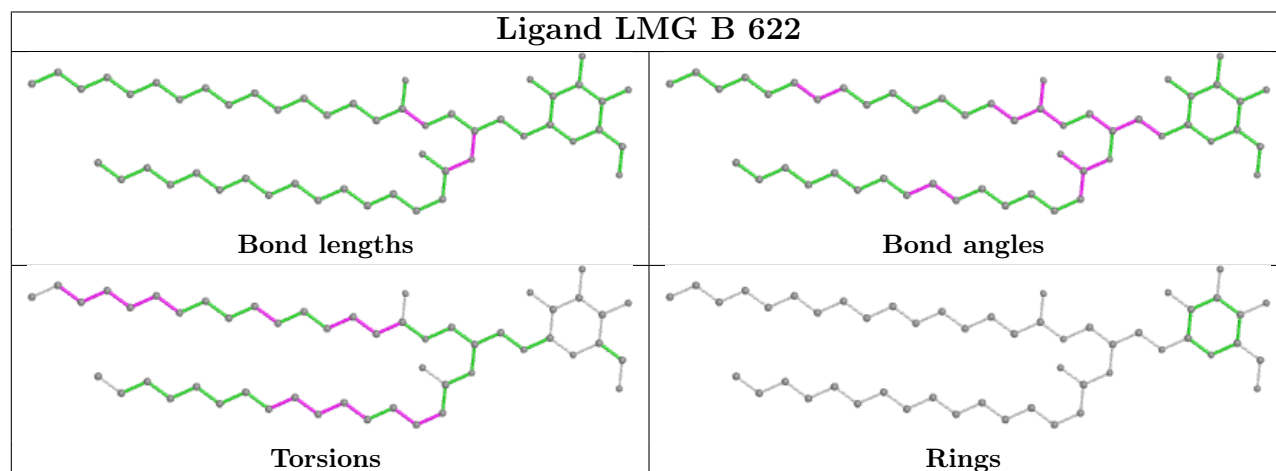


Ligand CLA b 610**Ligand PL9 D 406****Ligand RRX H 102**

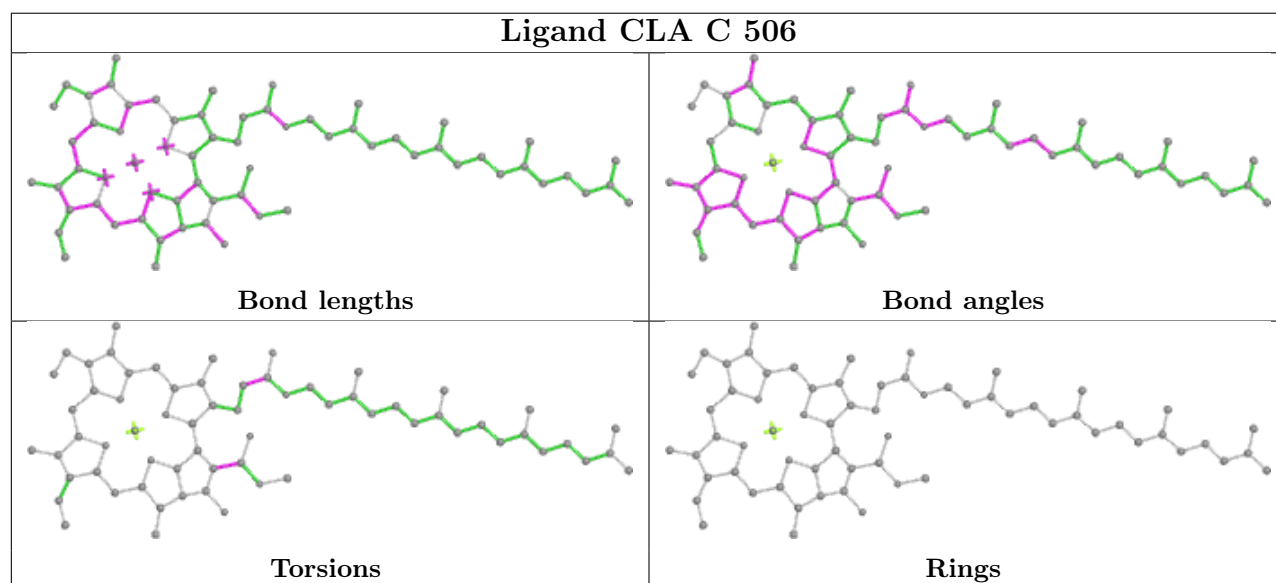
Ligand DGD c 919

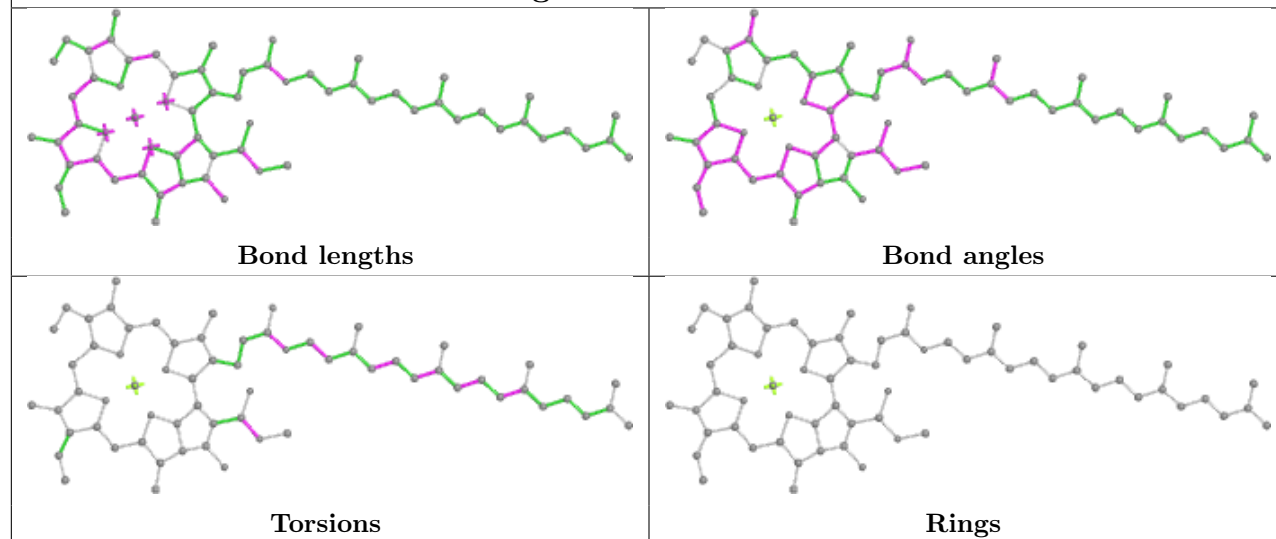
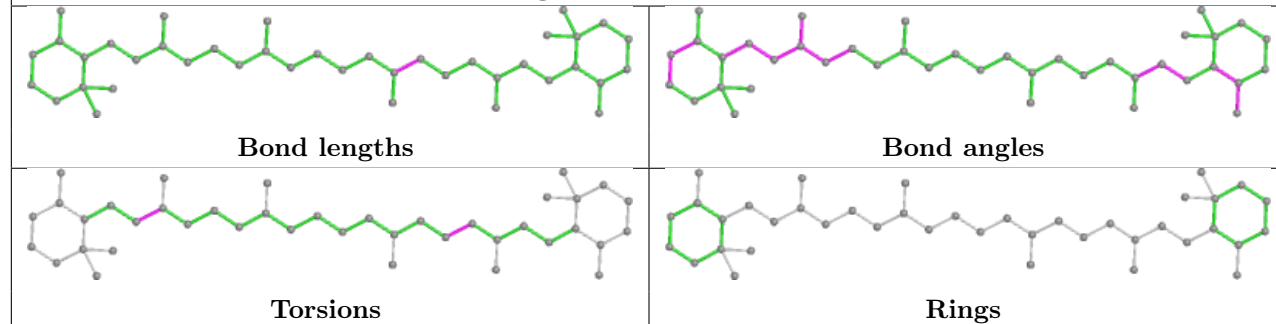
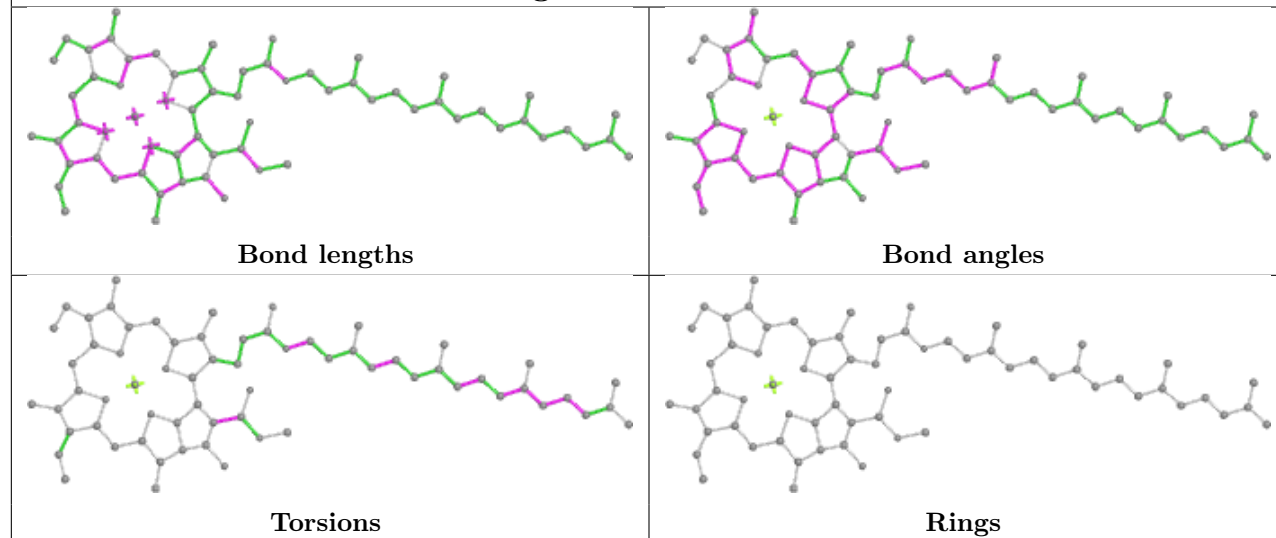


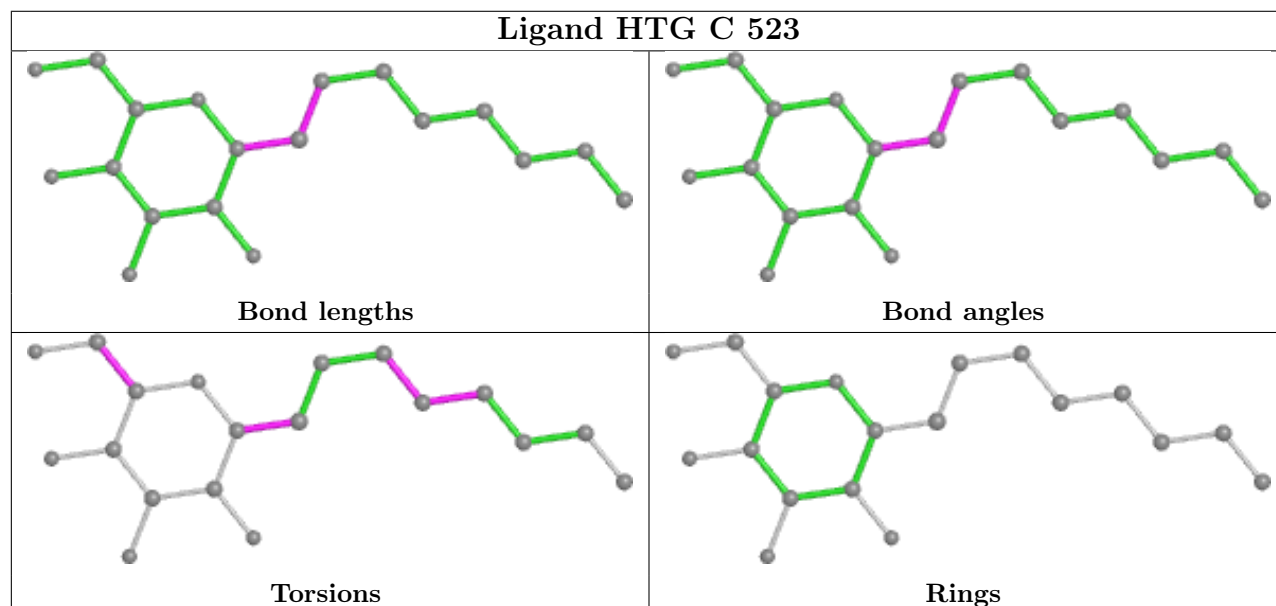
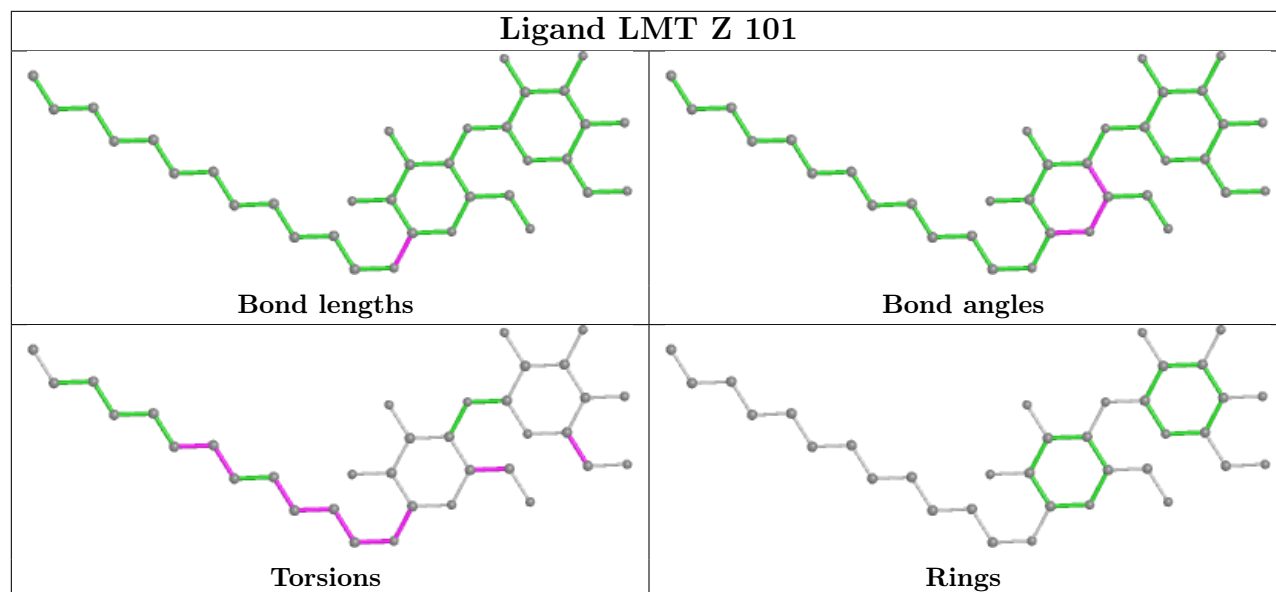
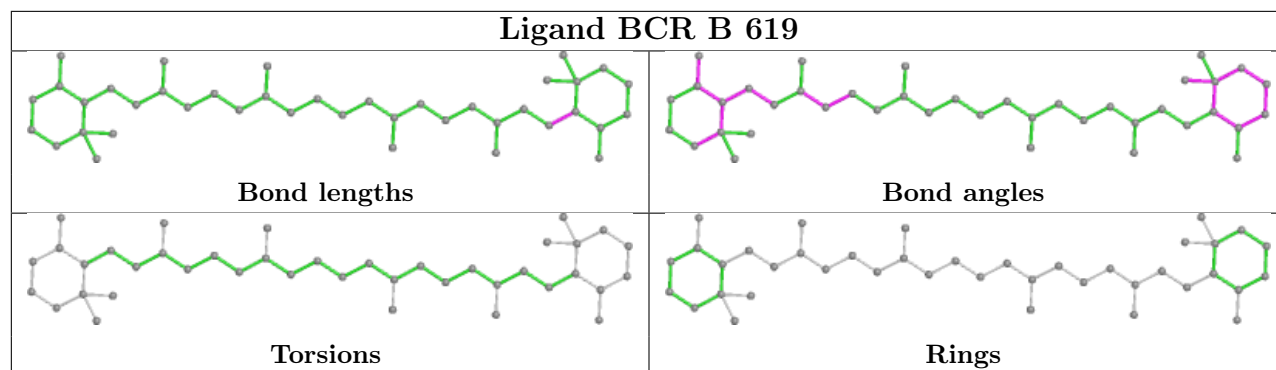
Ligand LMG B 622

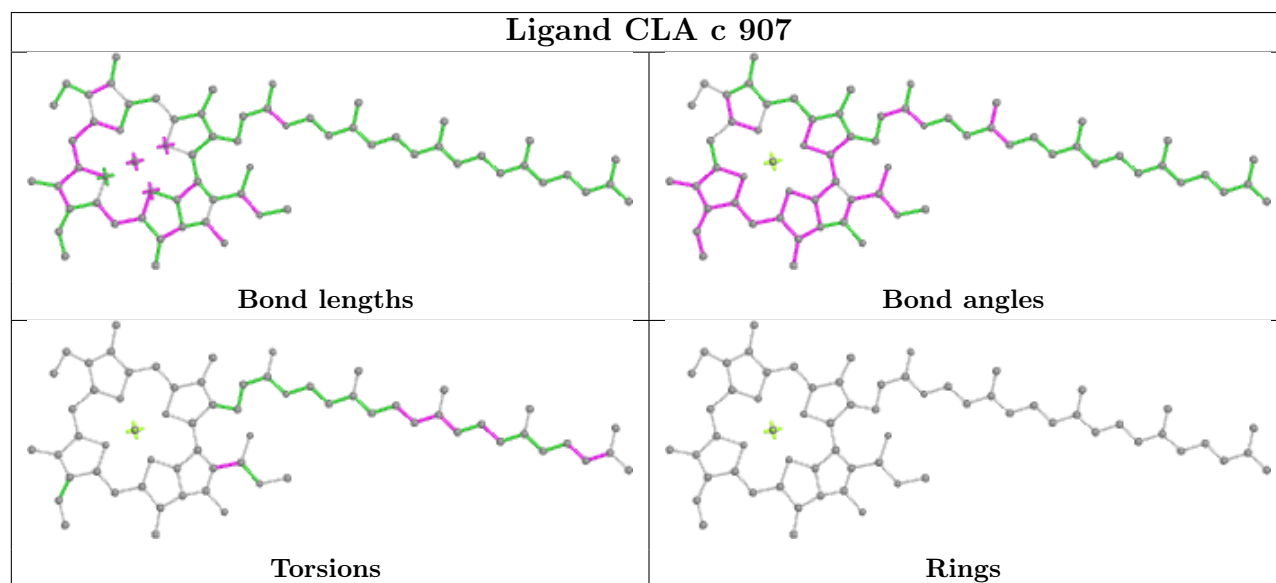
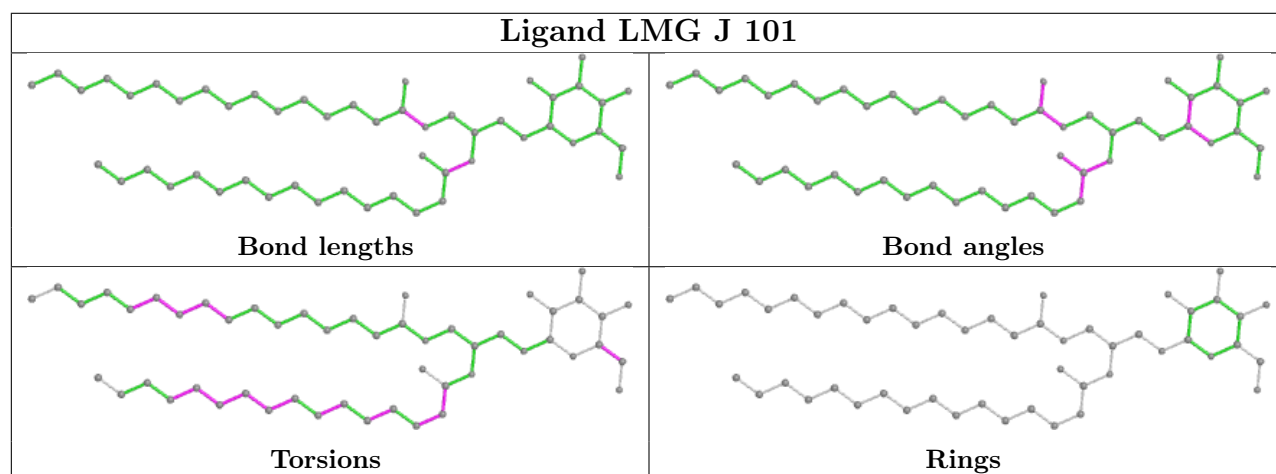
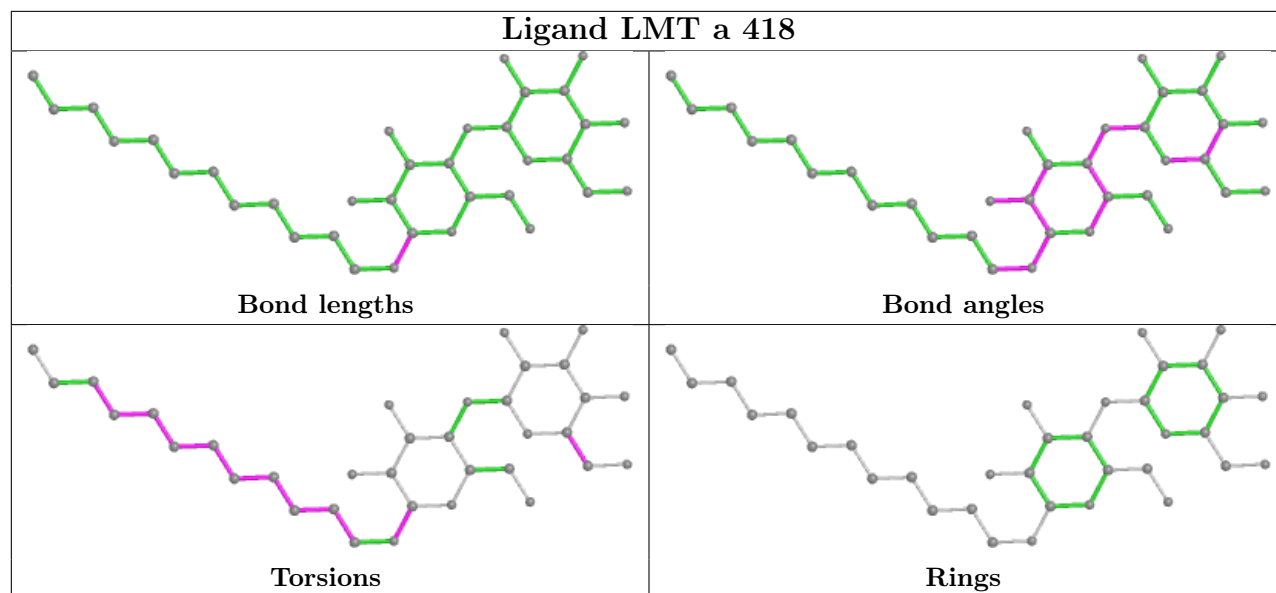


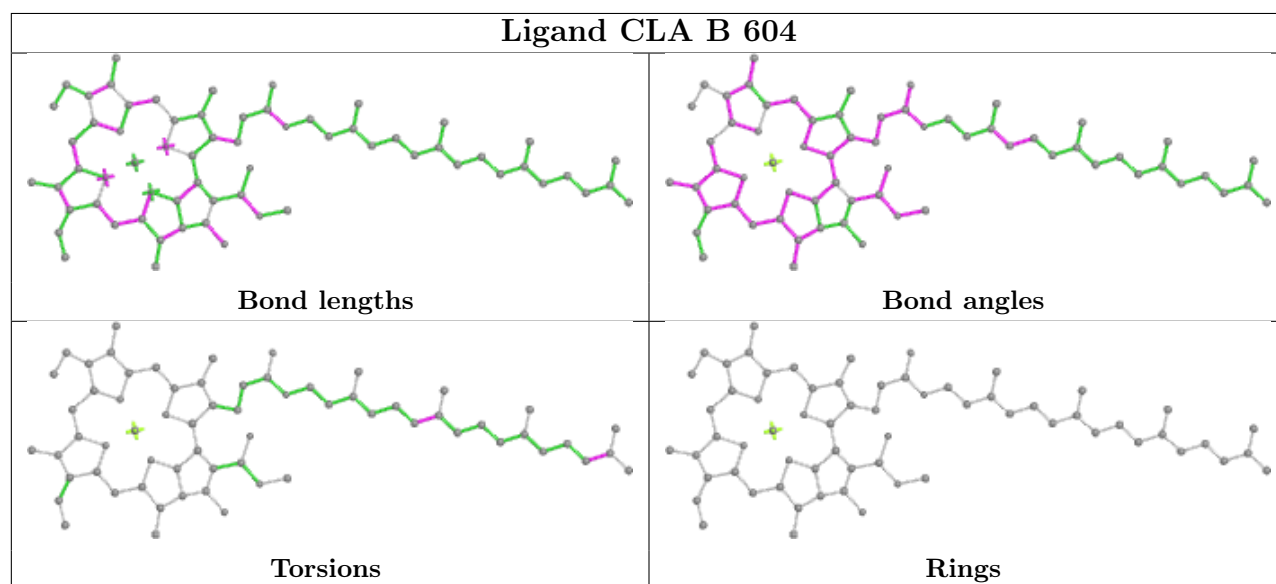
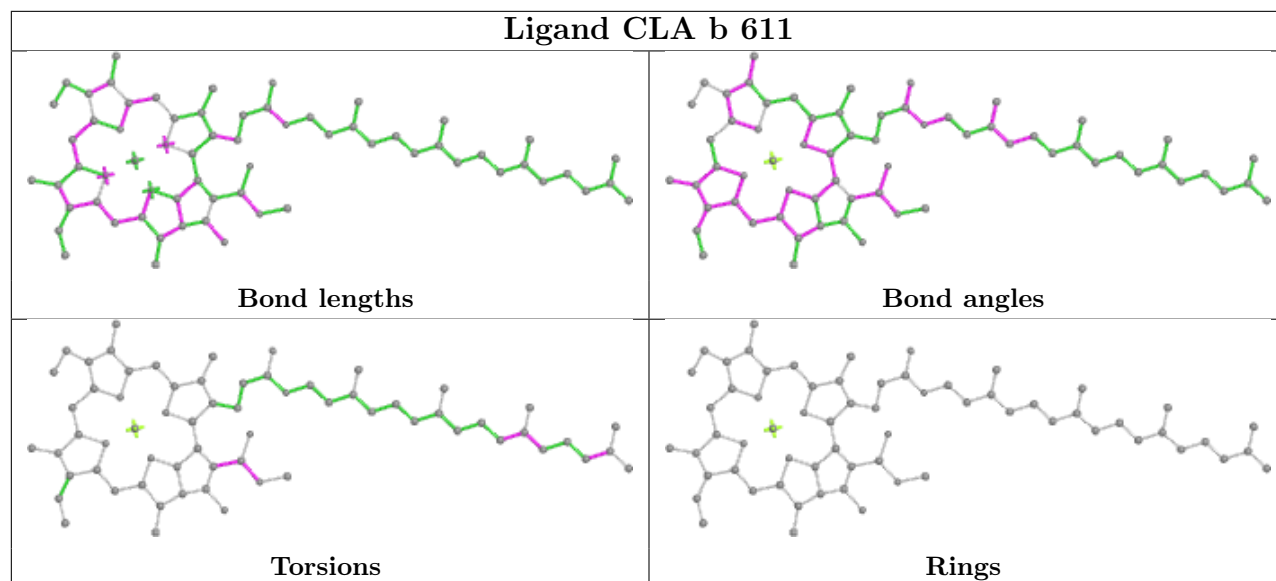
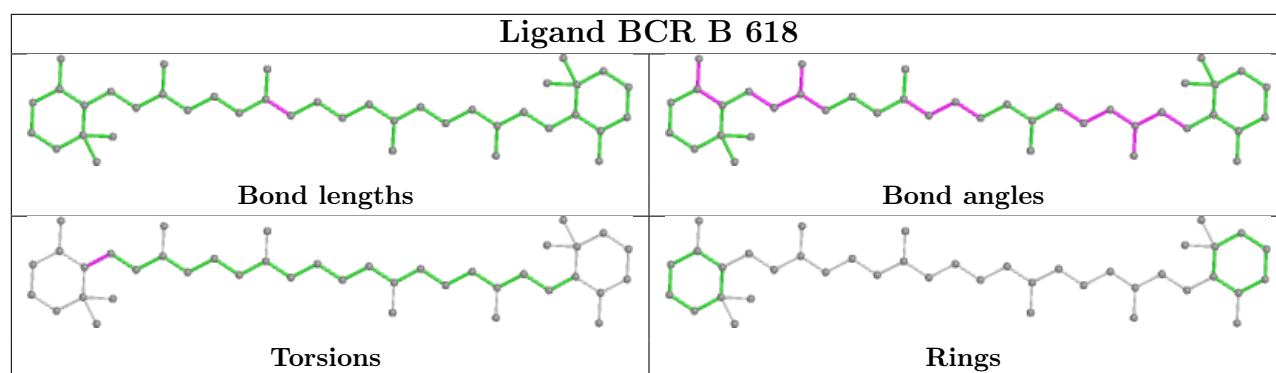
Ligand CLA C 506

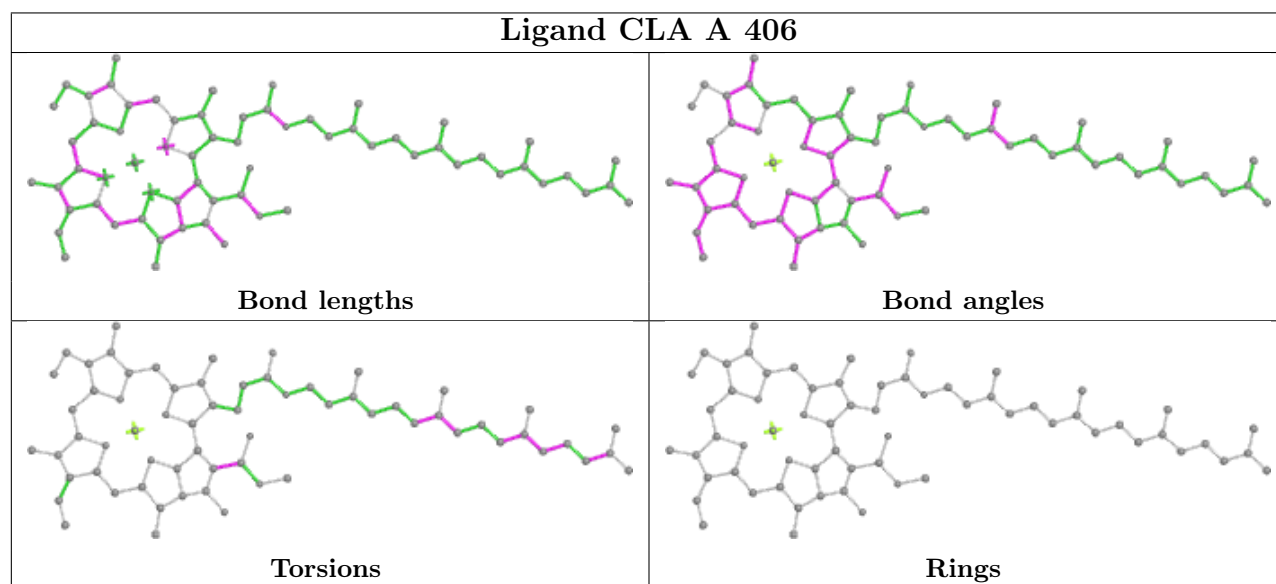
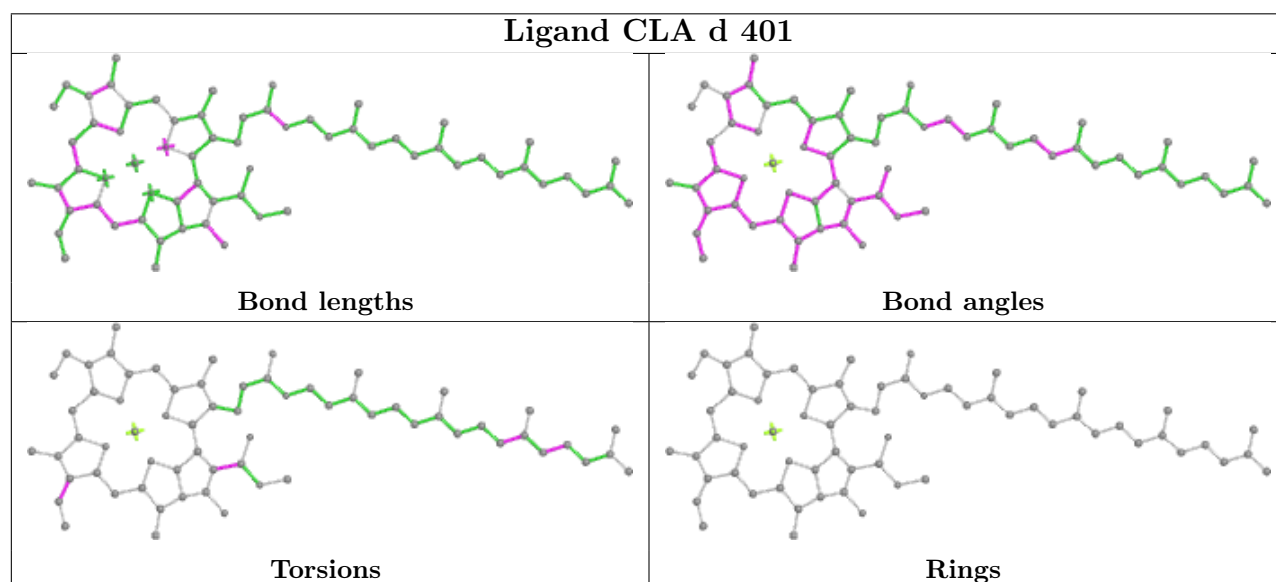
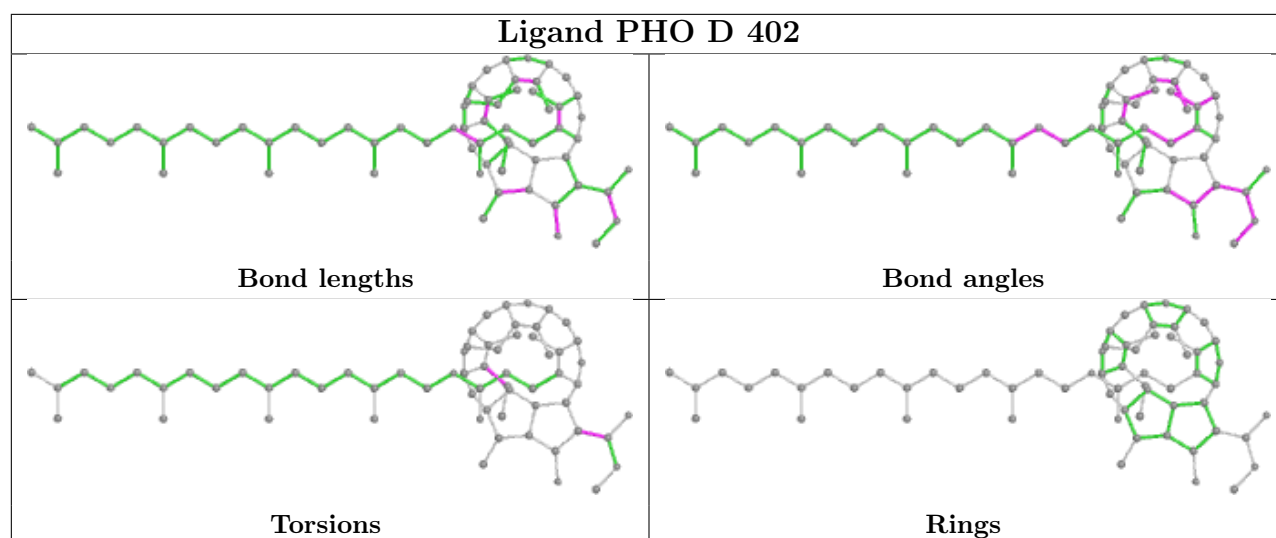


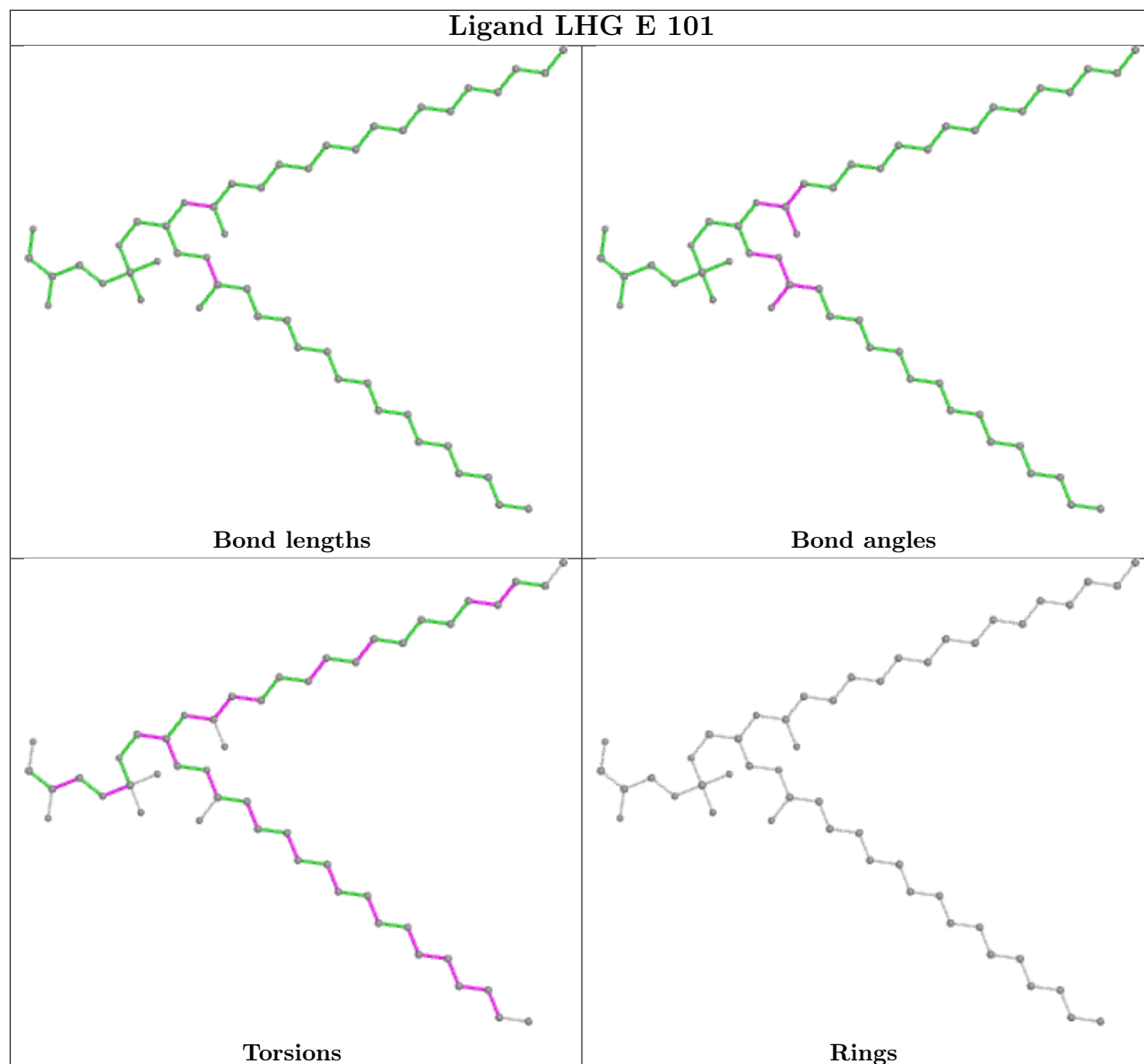
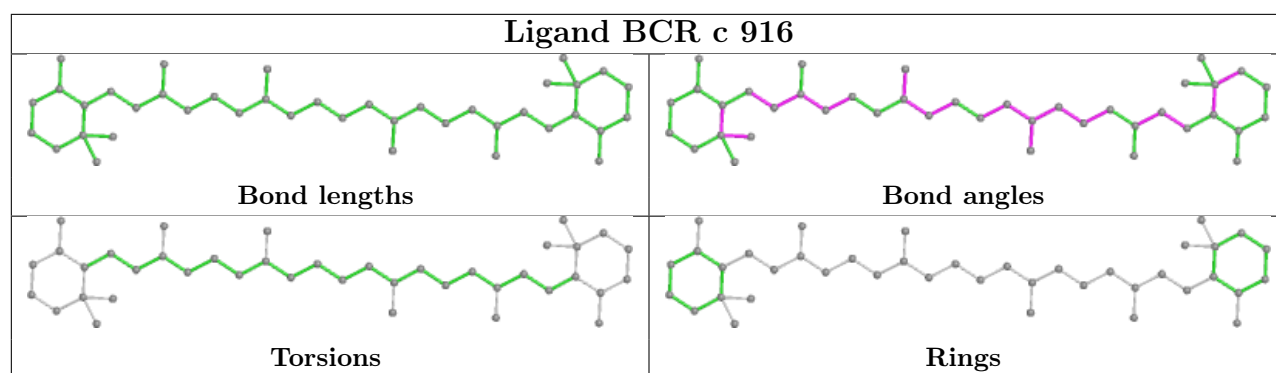
Ligand CLA C 514**Ligand BCR k 102****Ligand CLA B 617**

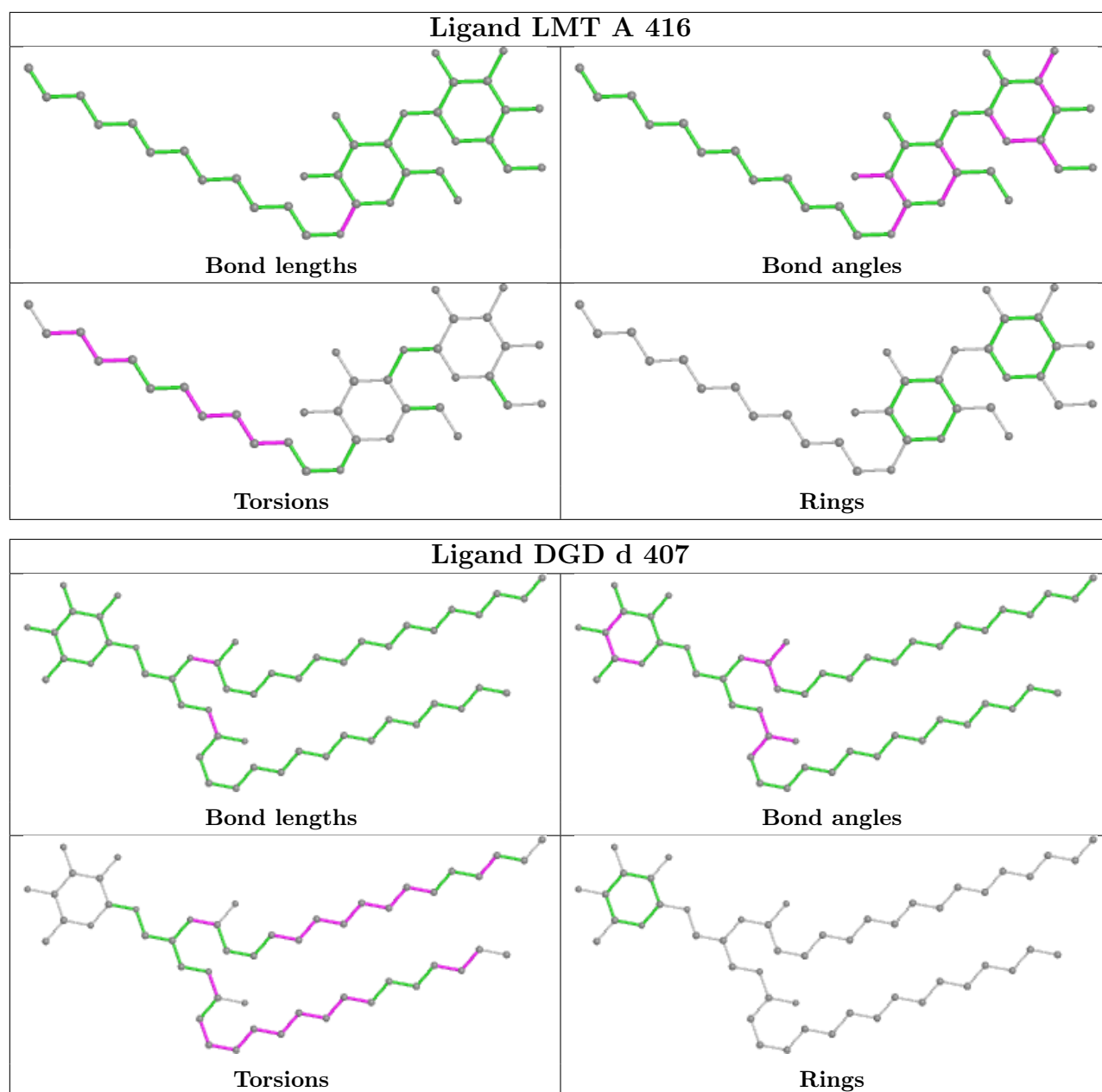




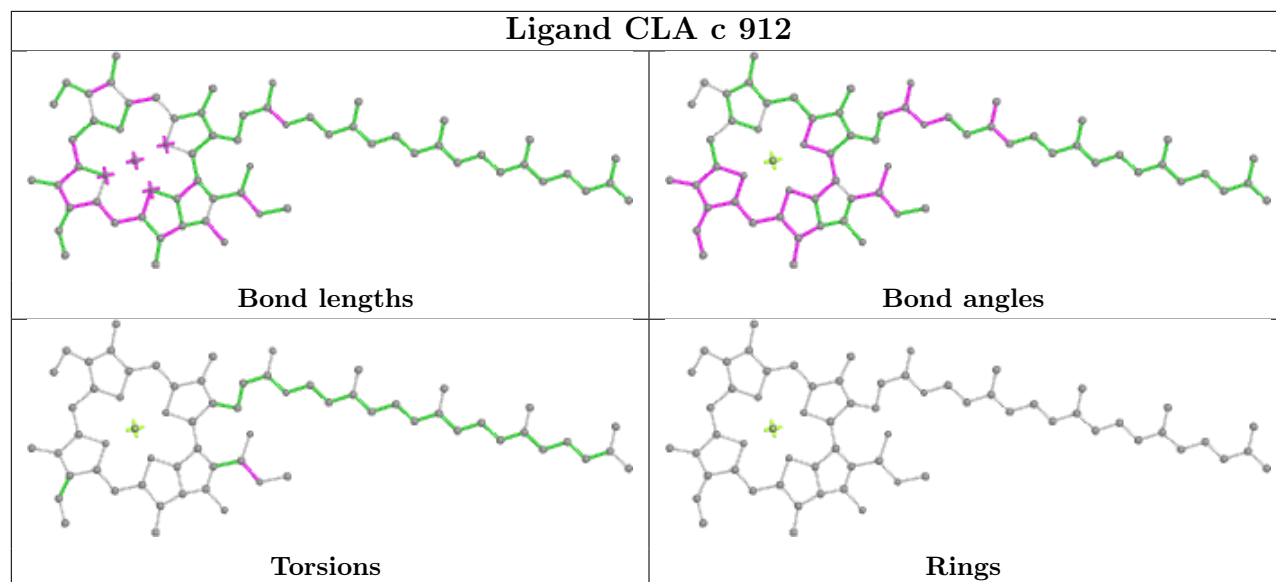




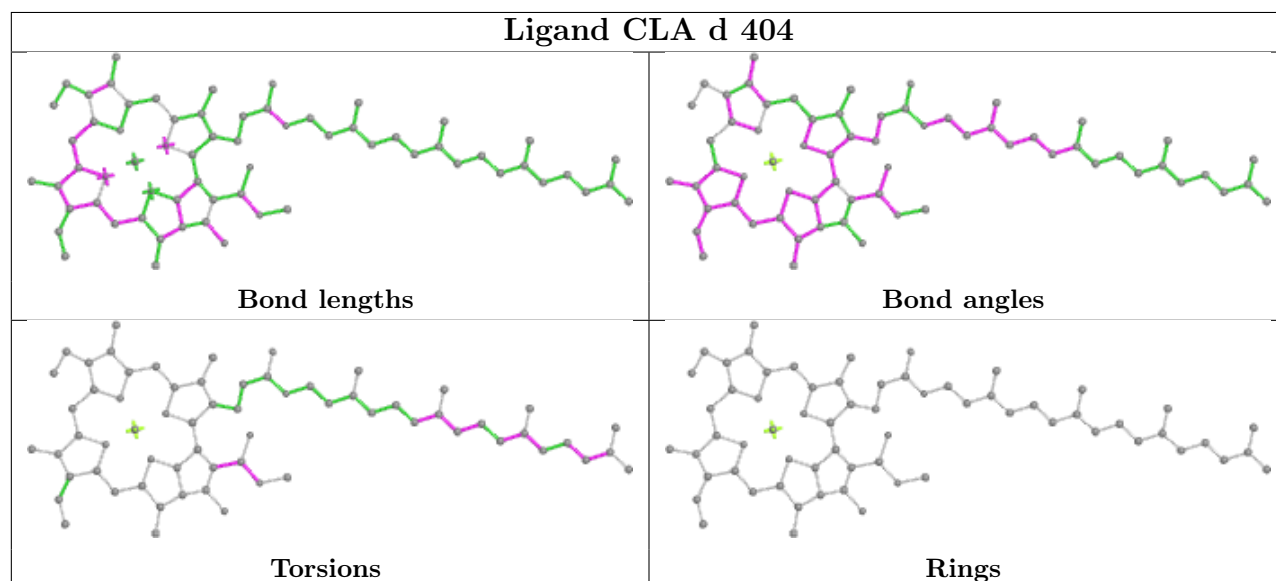




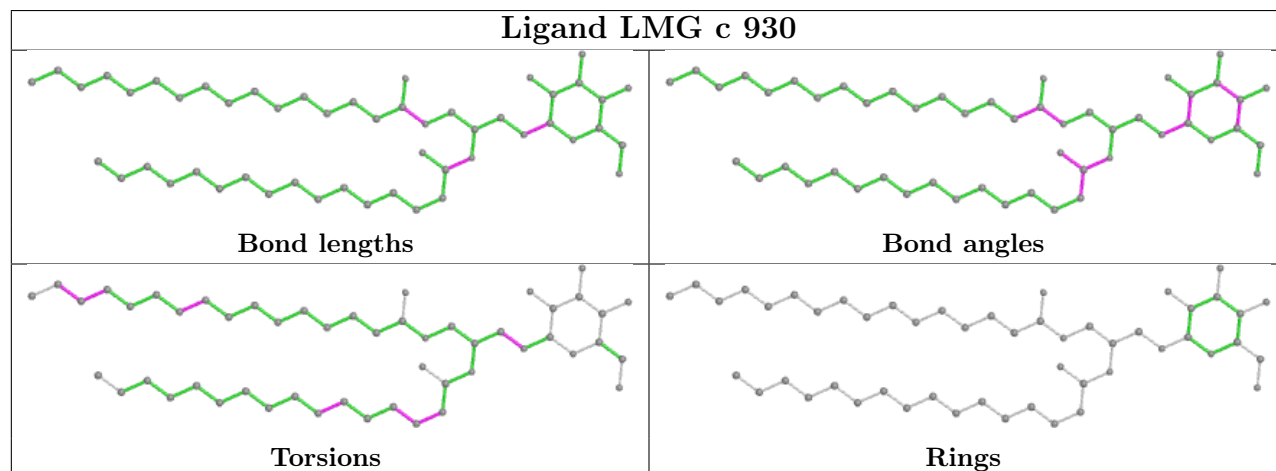
Ligand CLA c 912



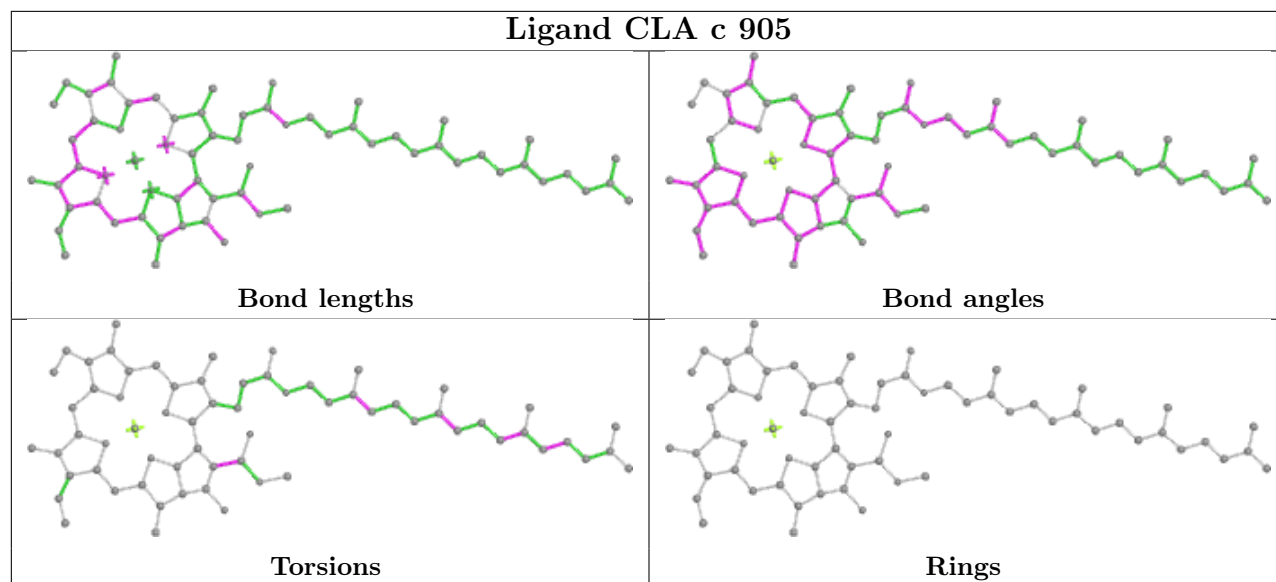
Ligand CLA d 404



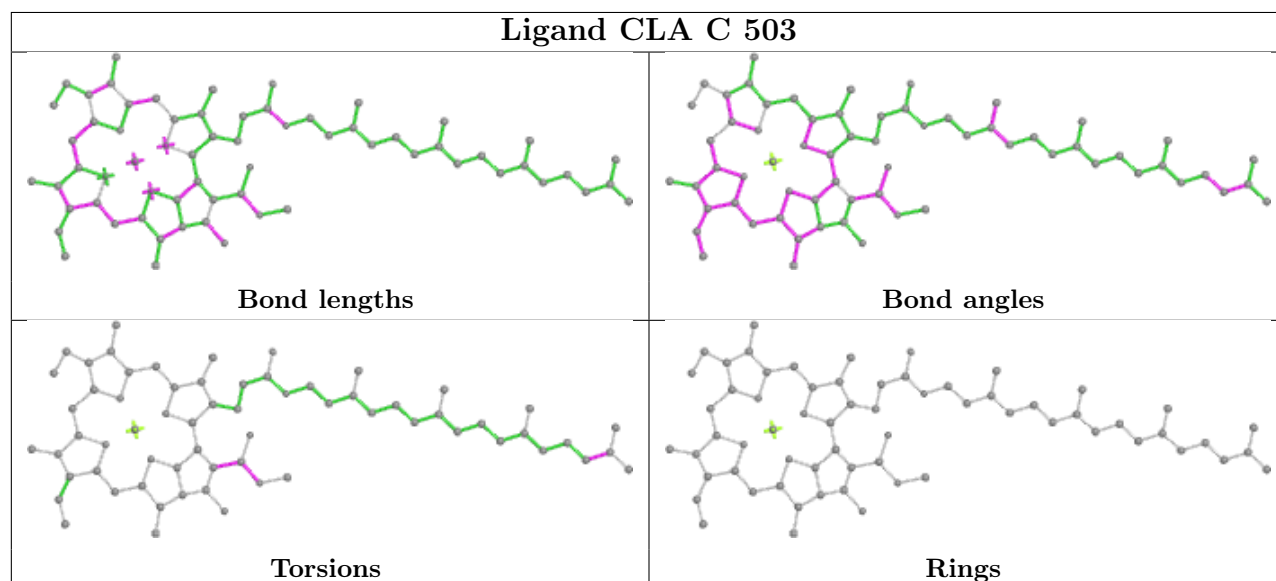
Ligand LMG c 930



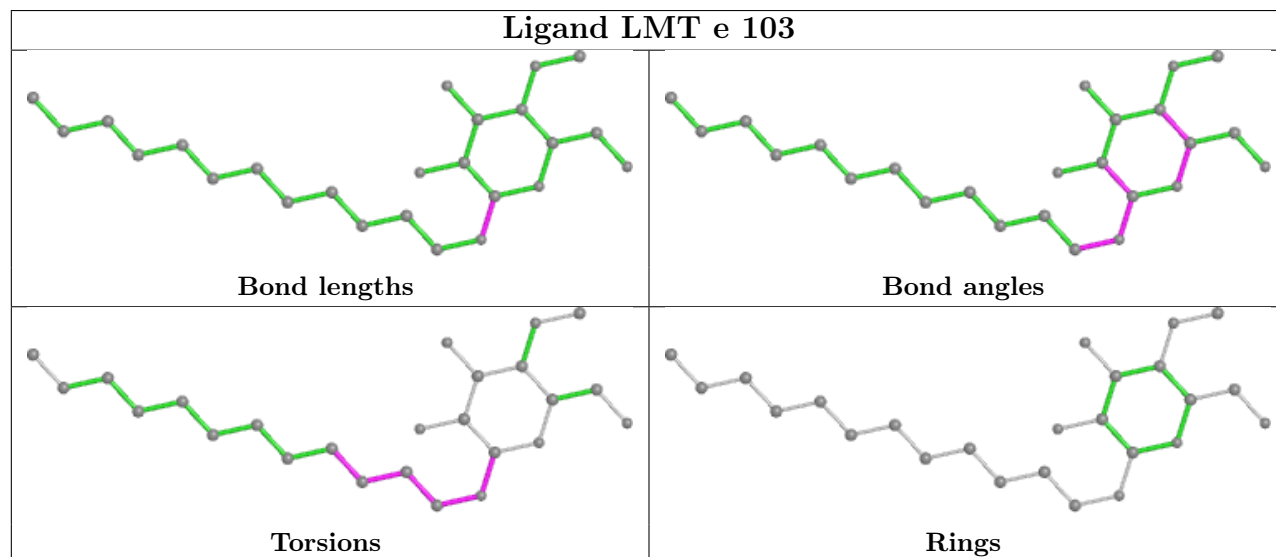
Ligand CLA c 905

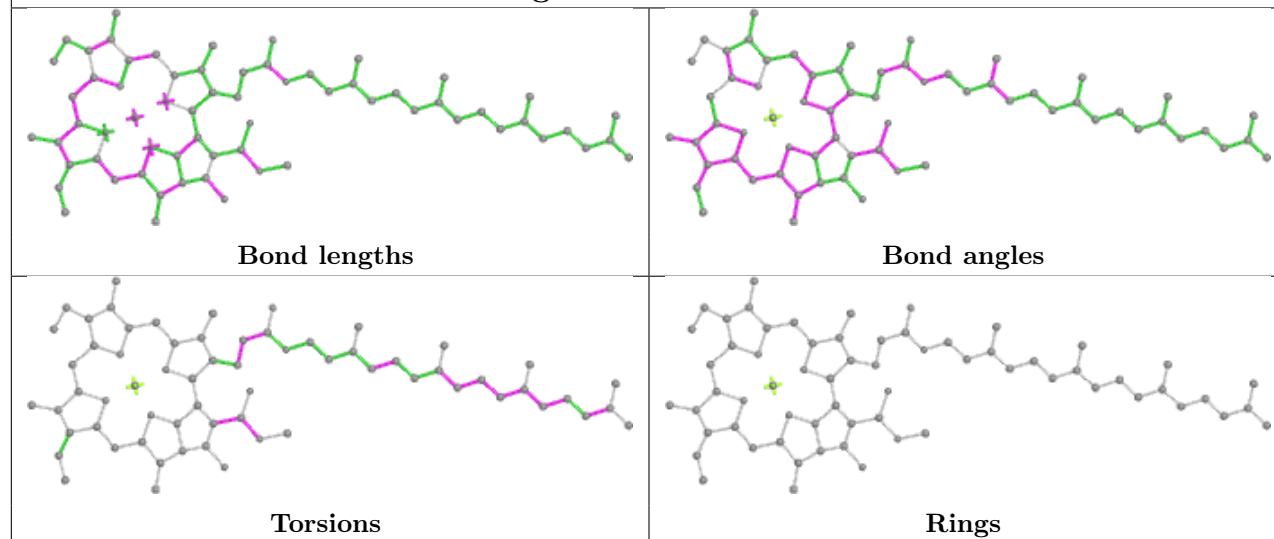
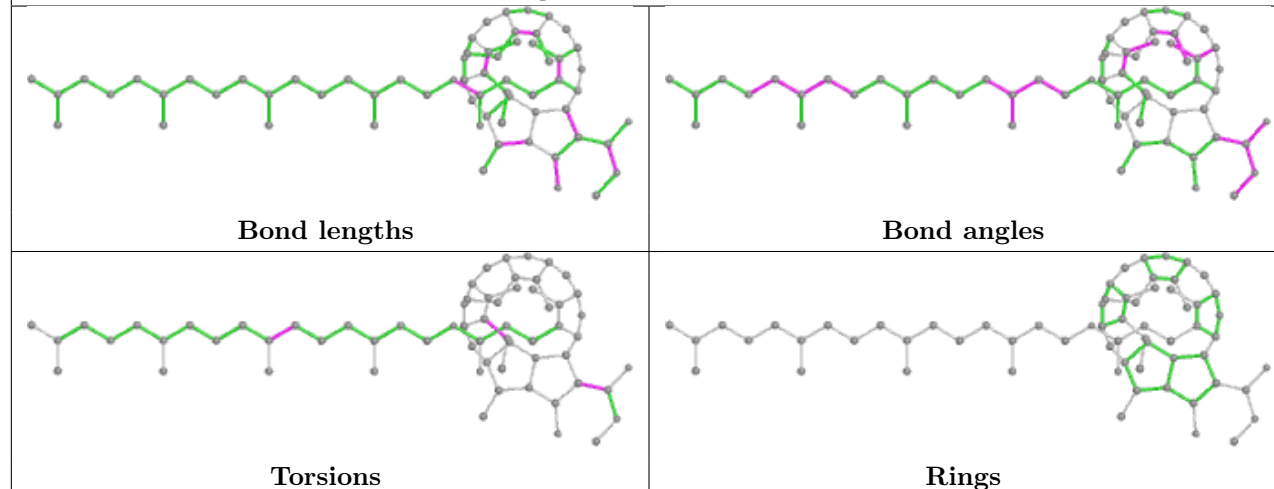
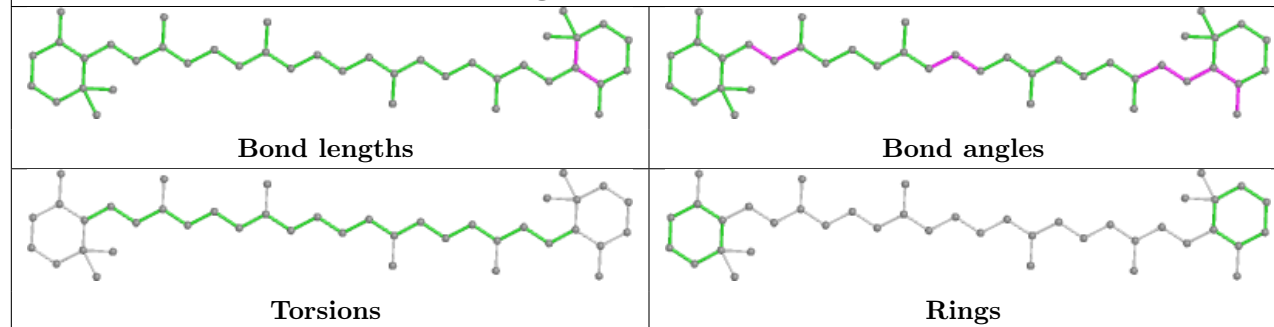


Ligand CLA C 503

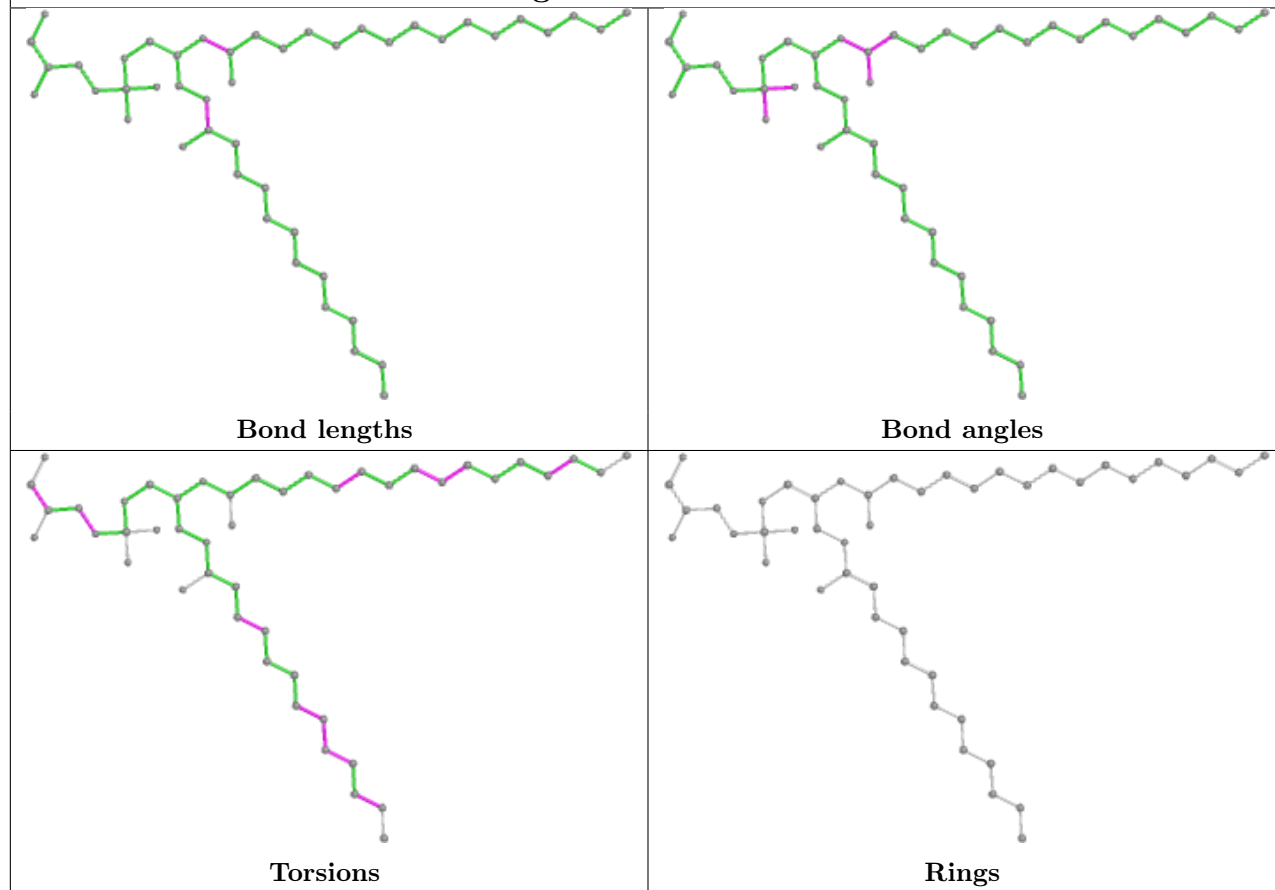


Ligand LMT e 103

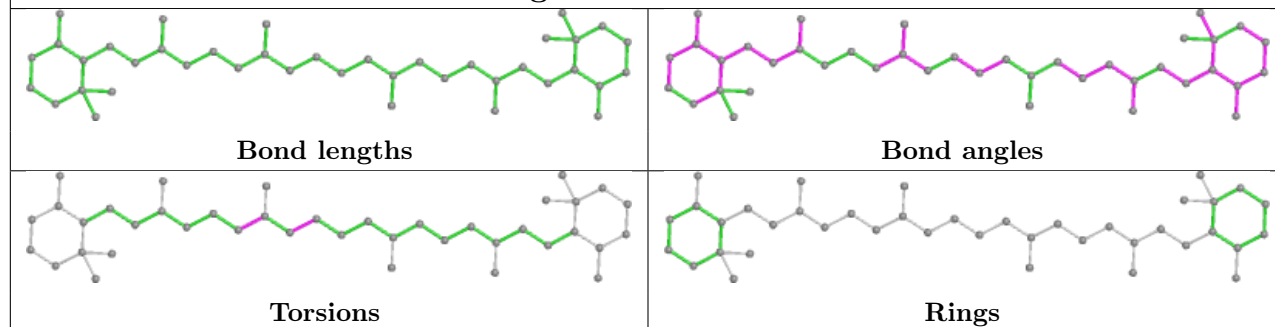


Ligand CLA B 602**Ligand PHO a 409****Ligand BCR b 620**

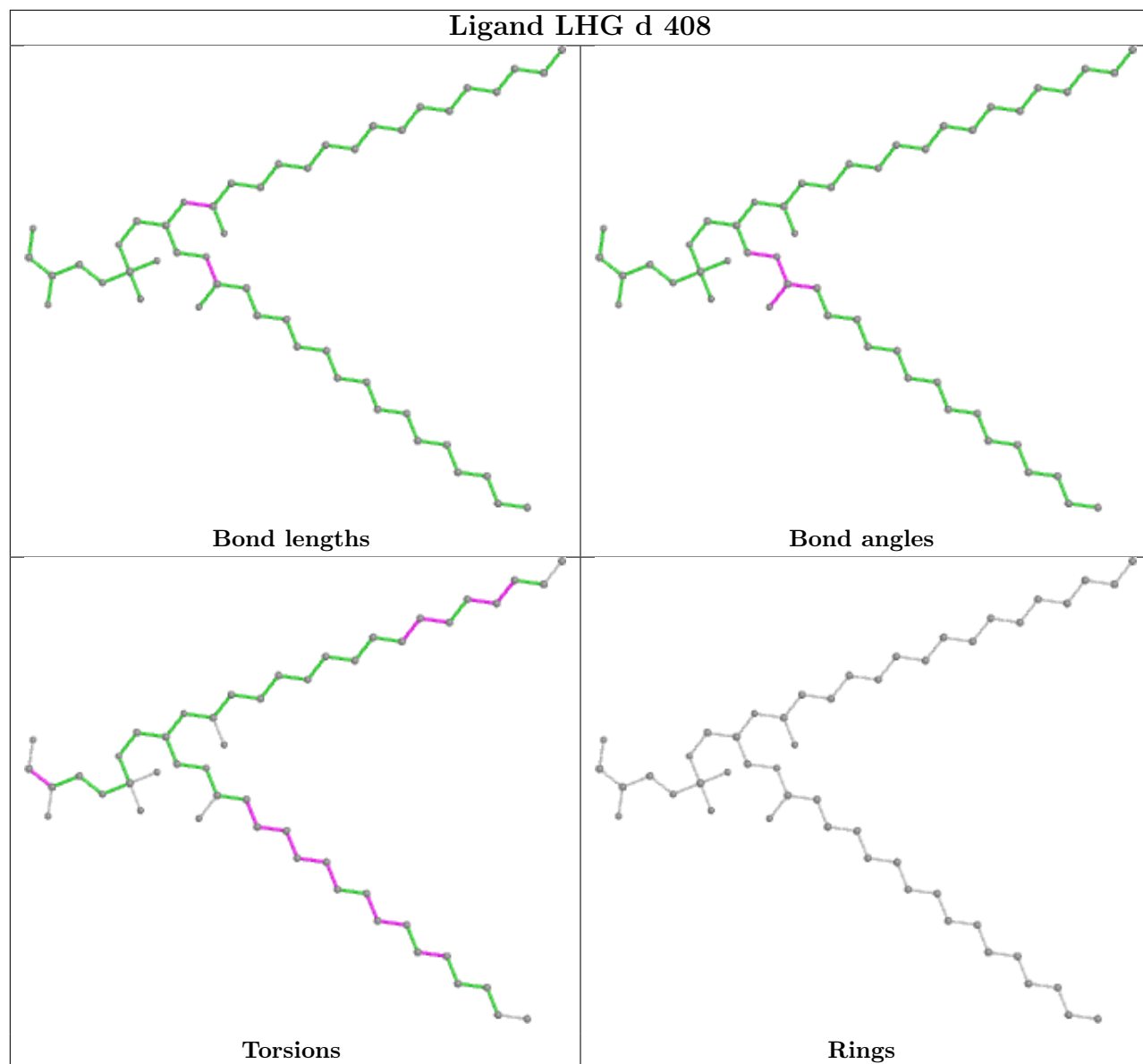
Ligand LHG d 410



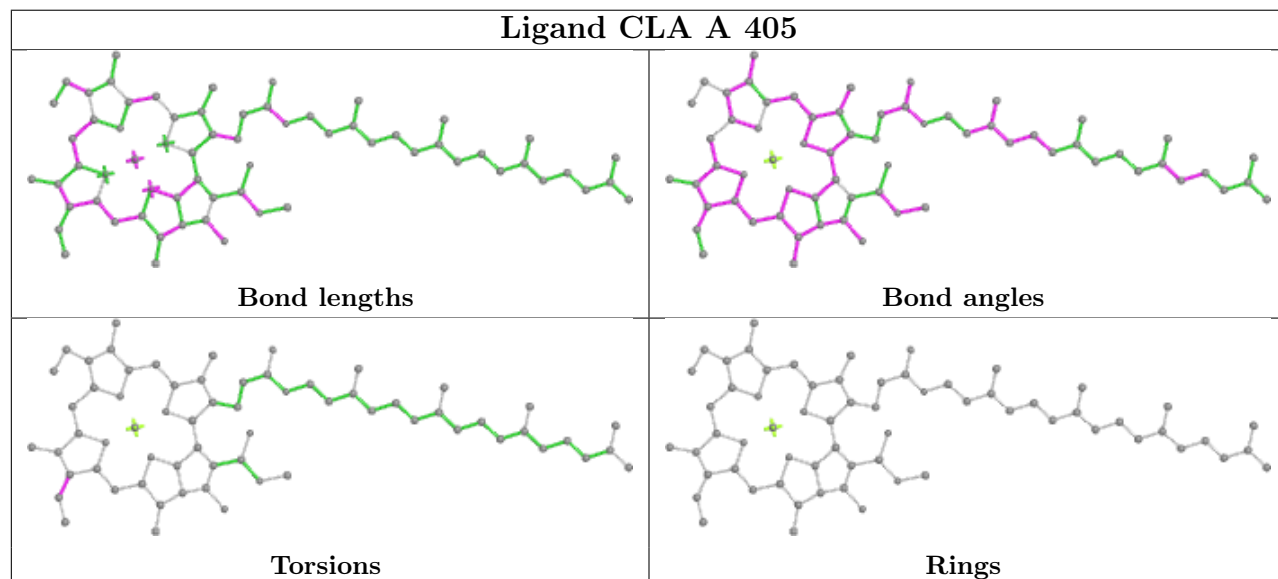
Ligand BCR T 101

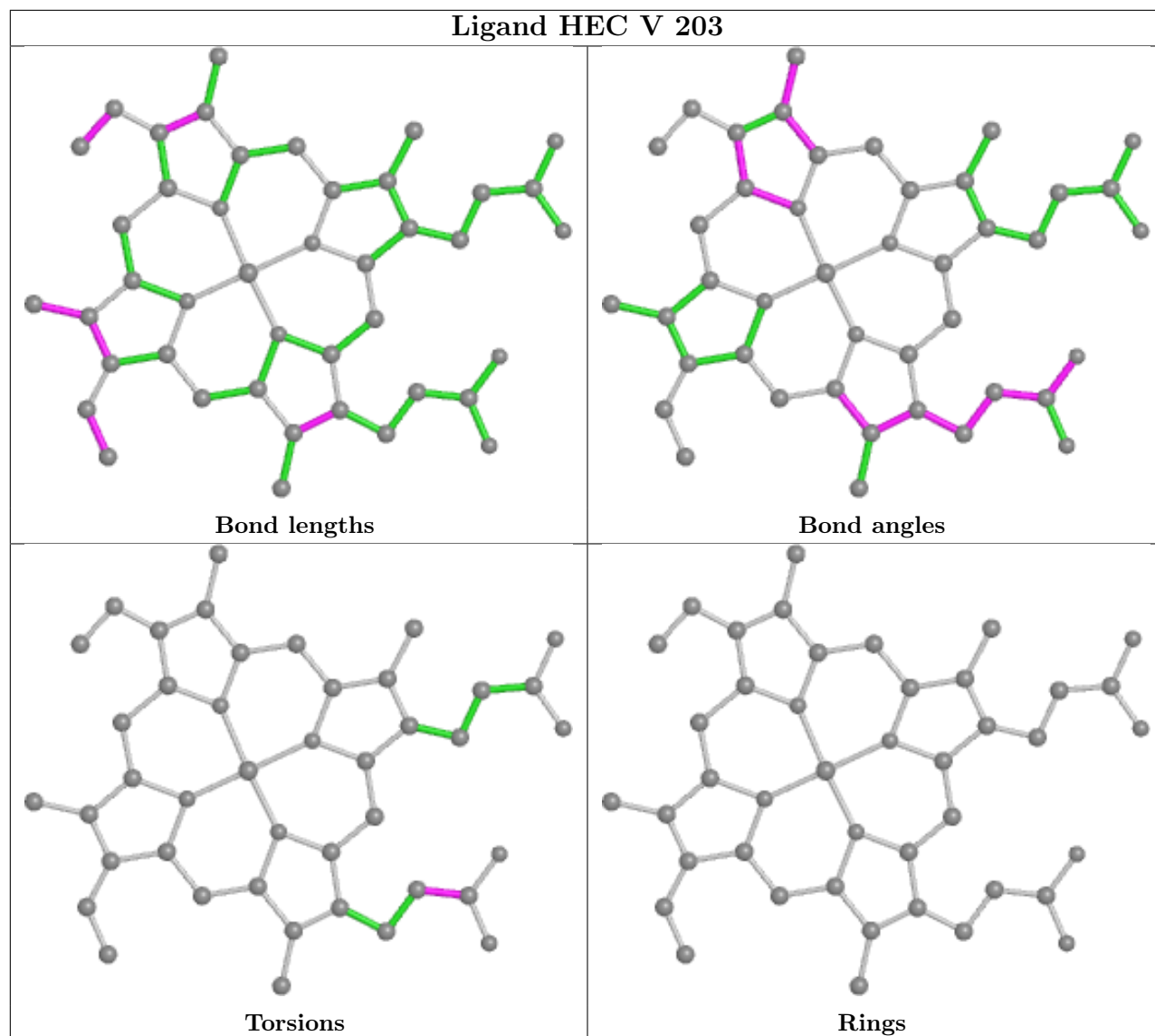
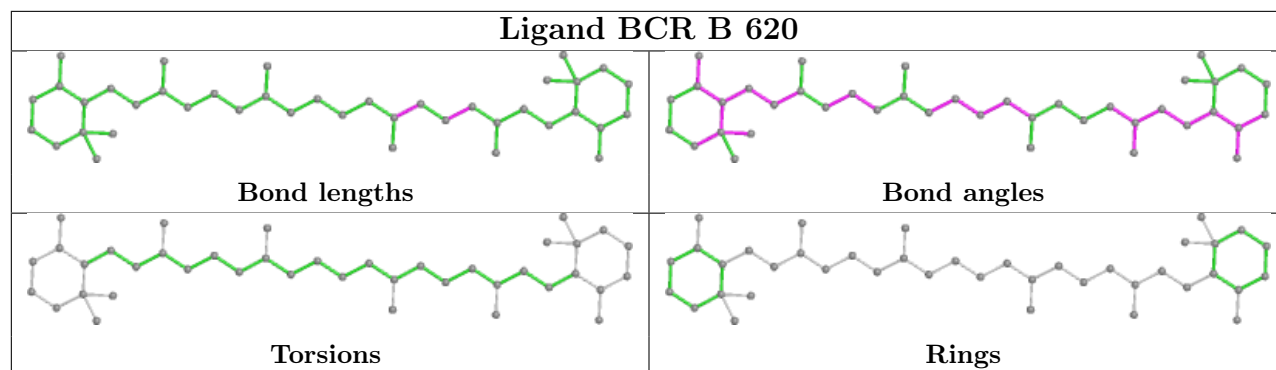


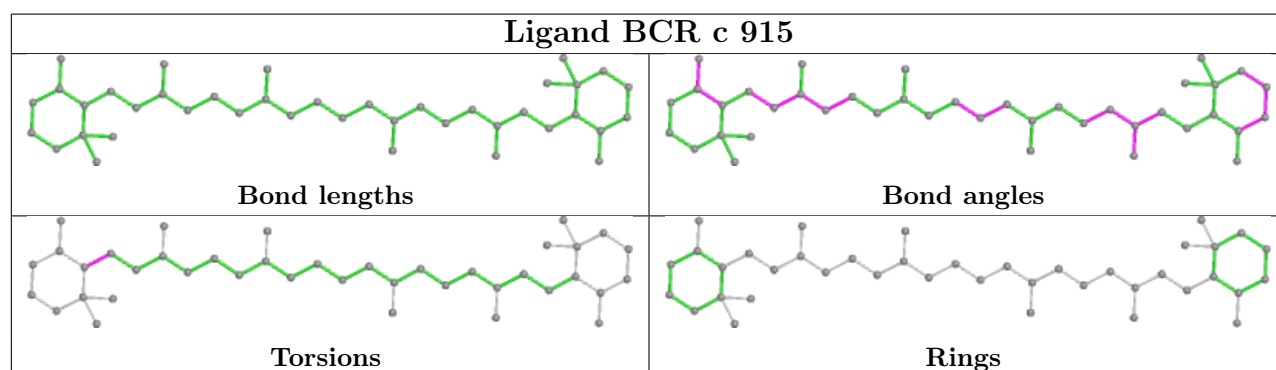
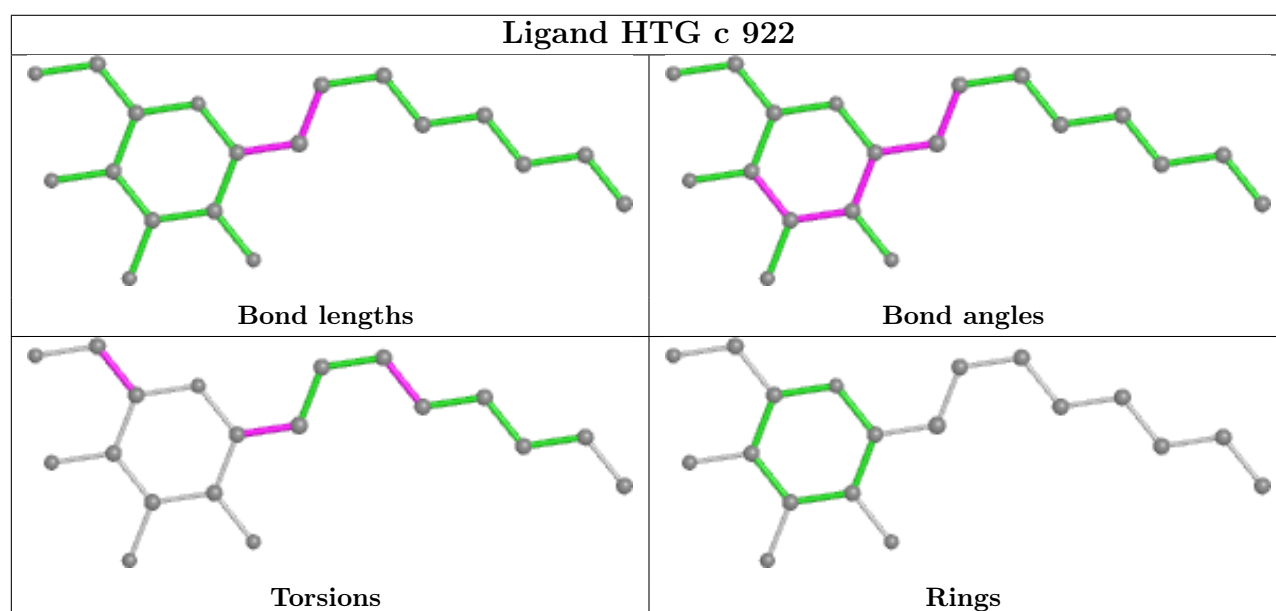
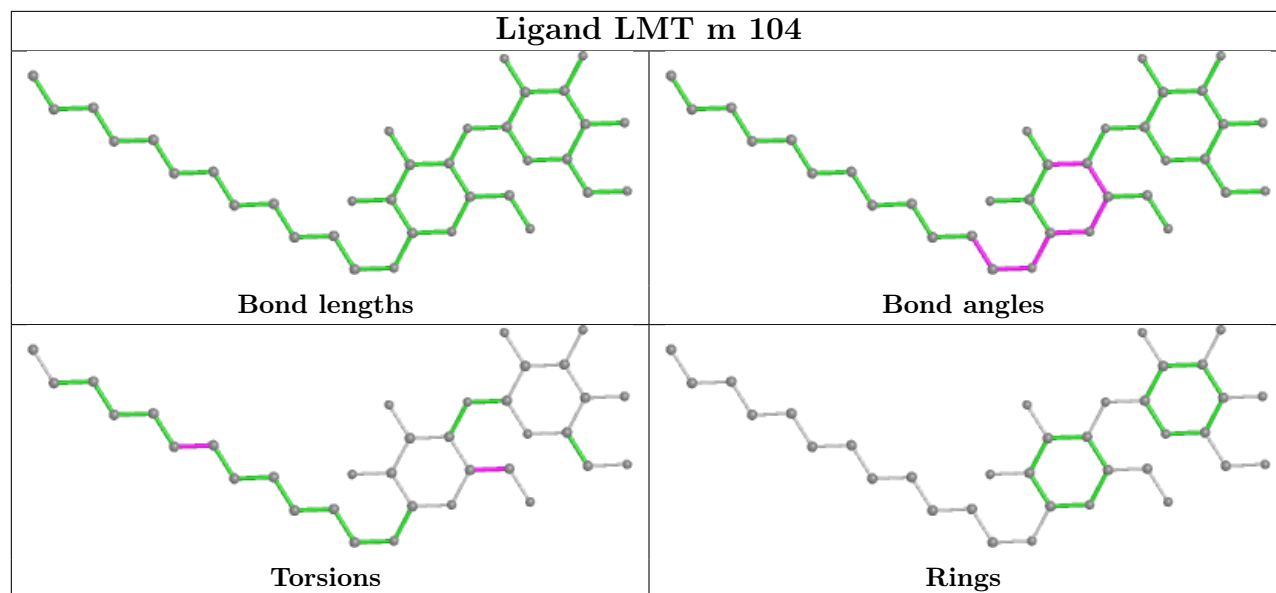
Ligand LHG d 408

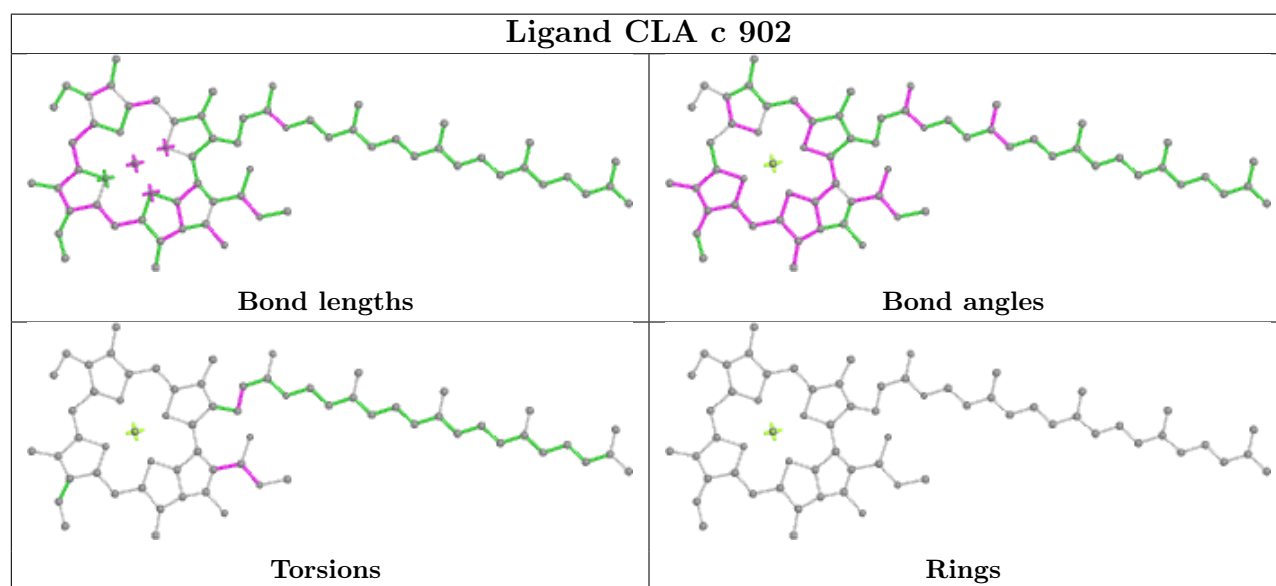
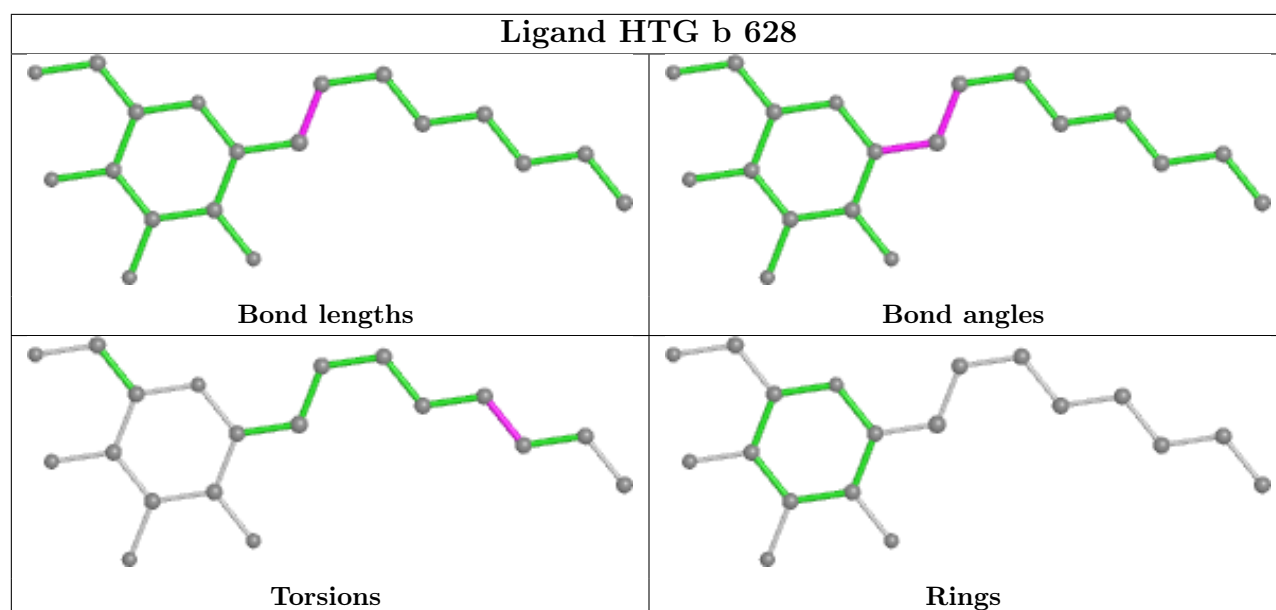


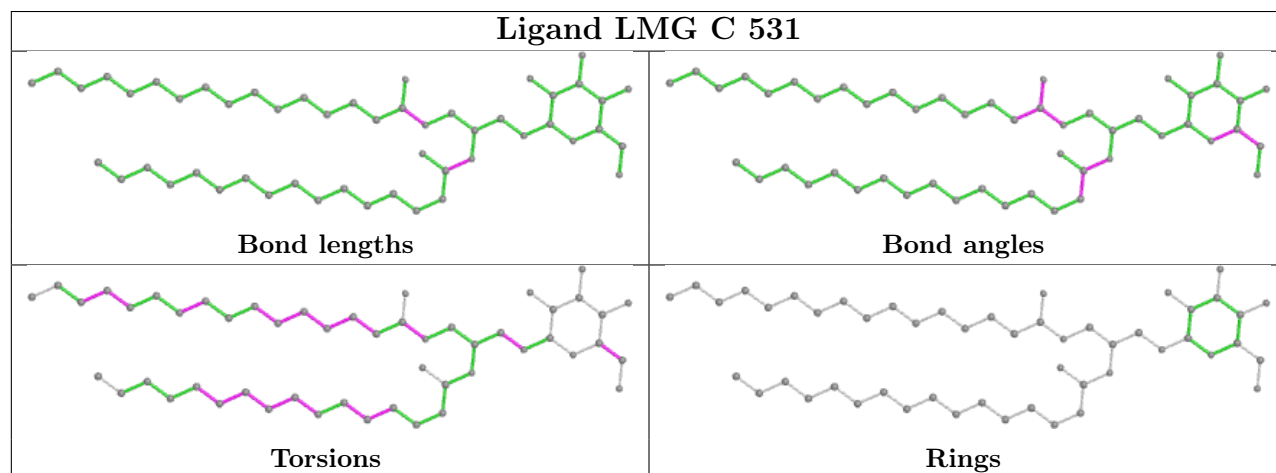
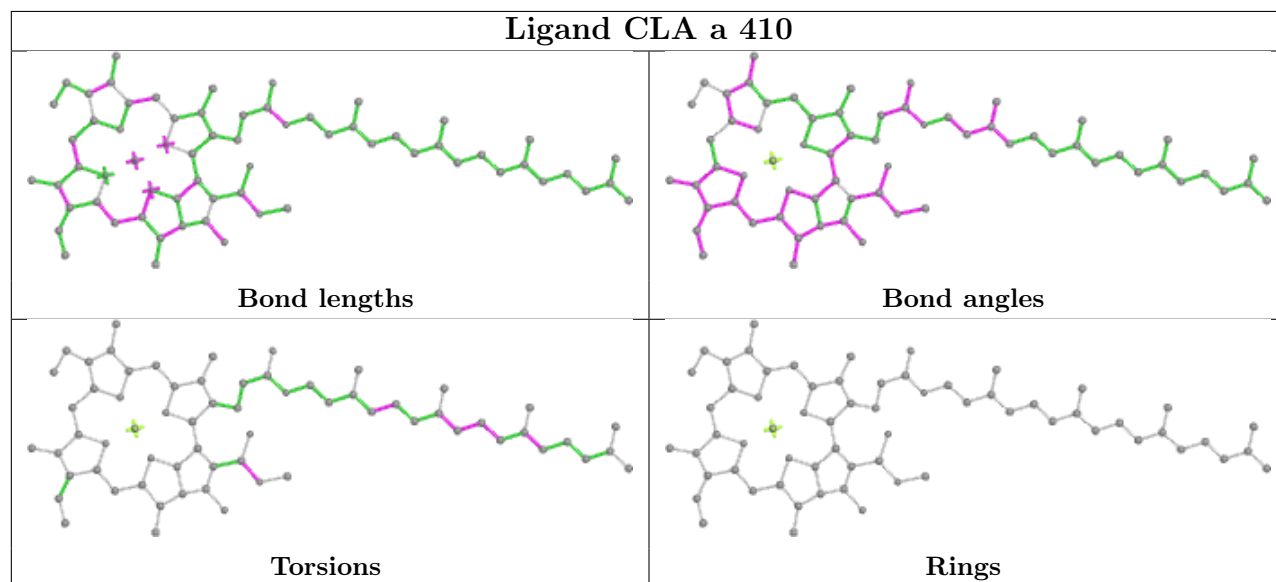
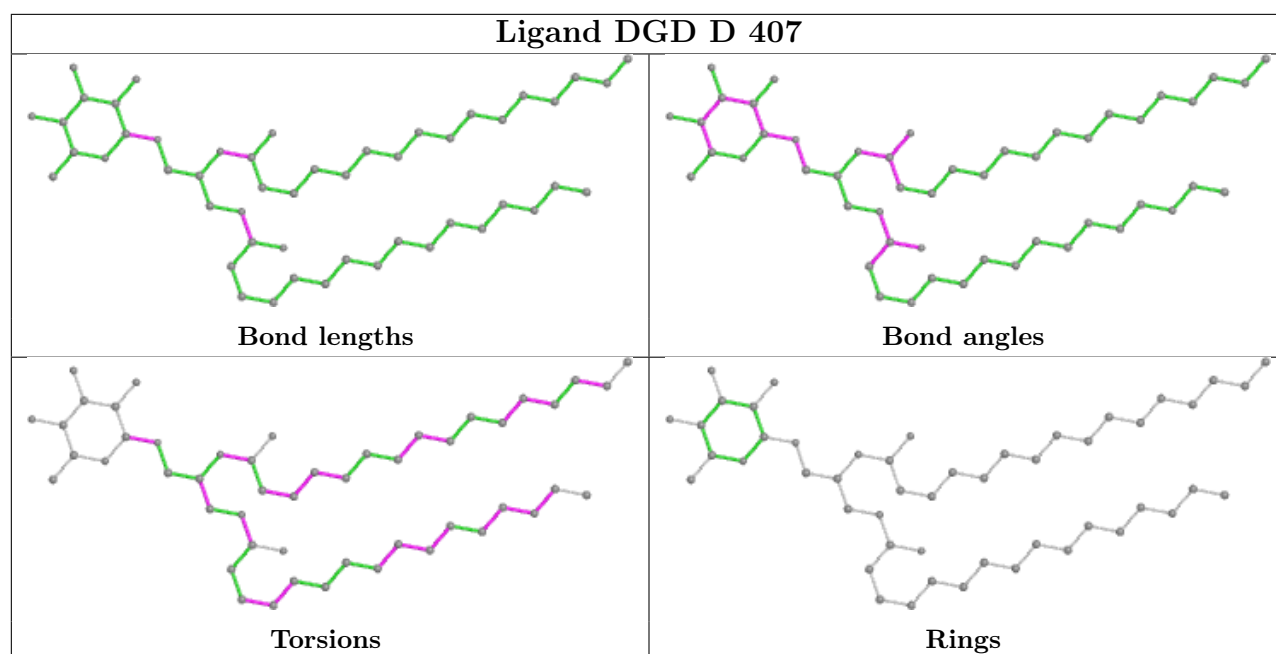
Ligand CLA A 405

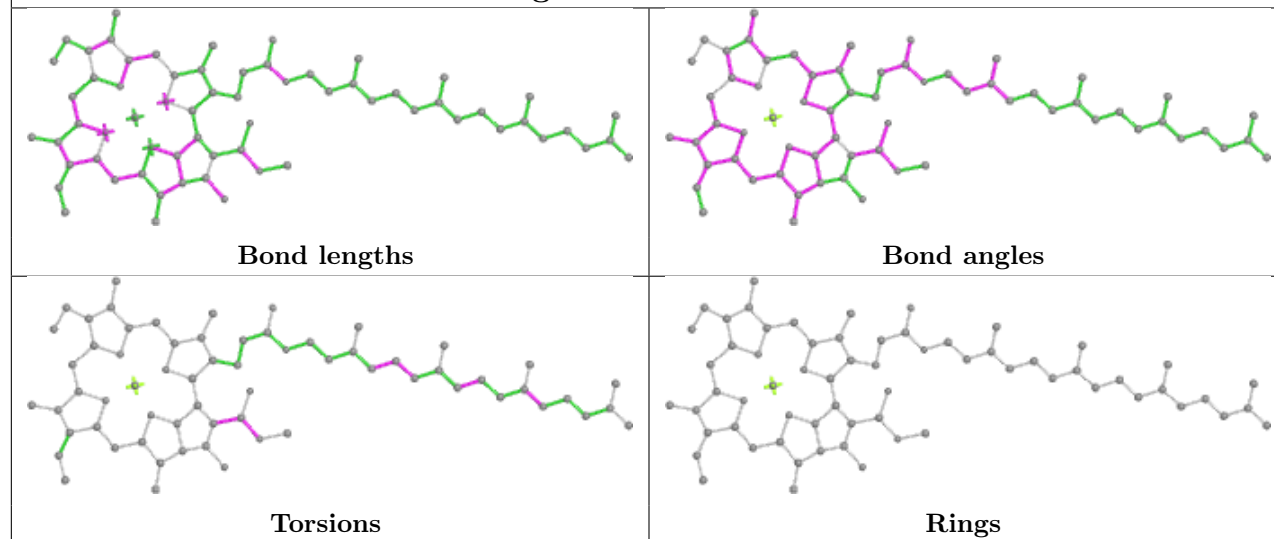
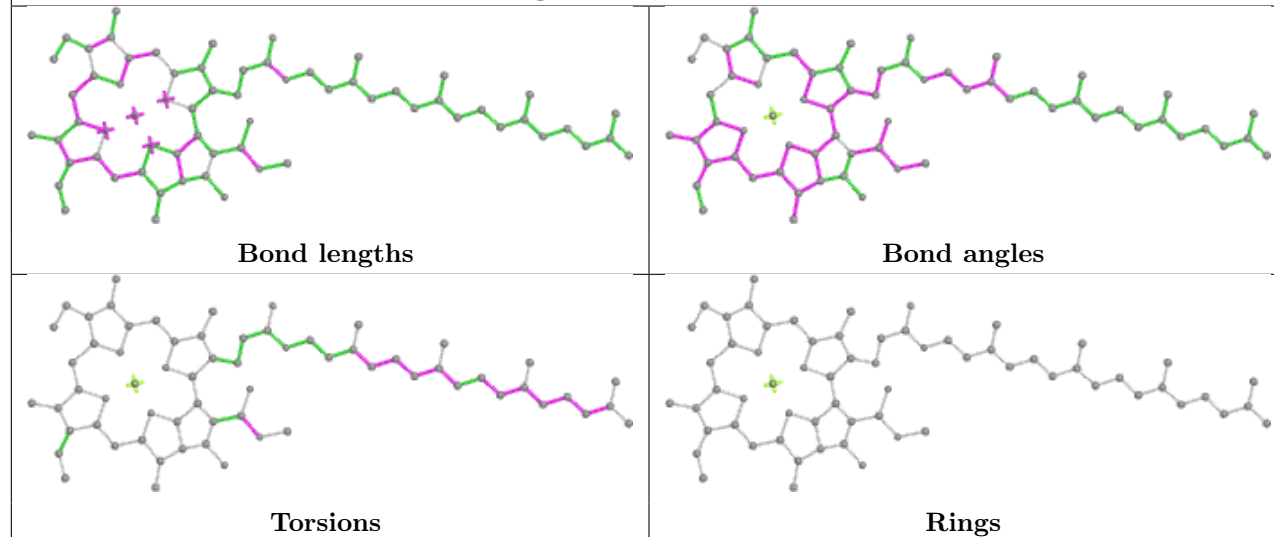




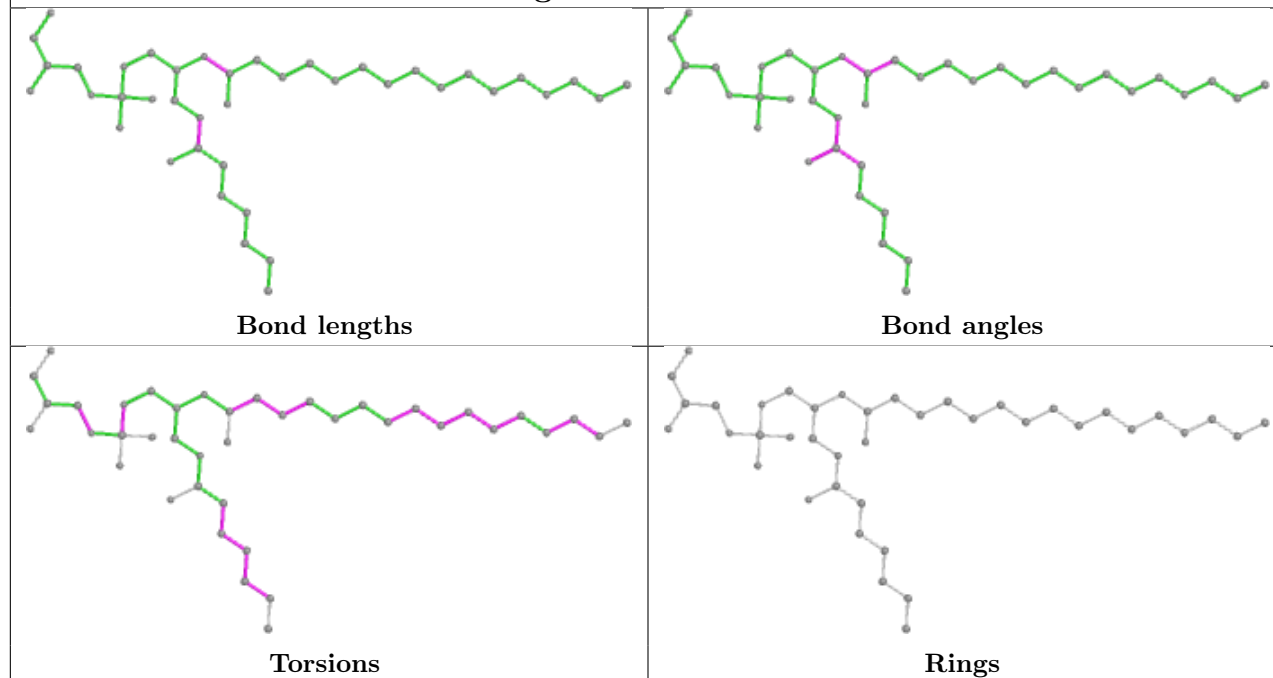




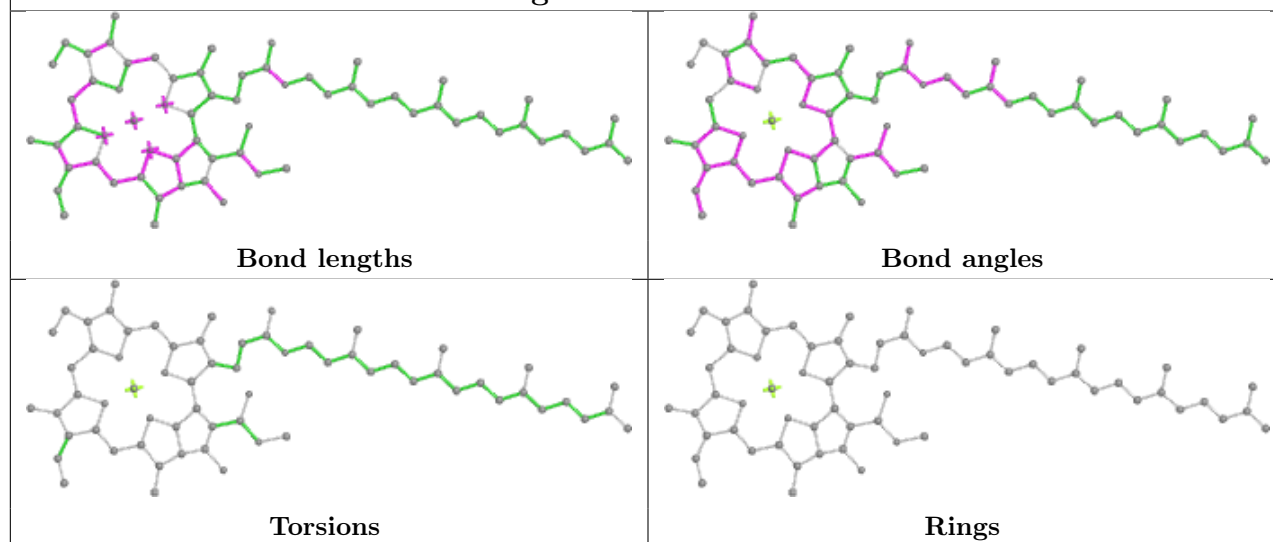


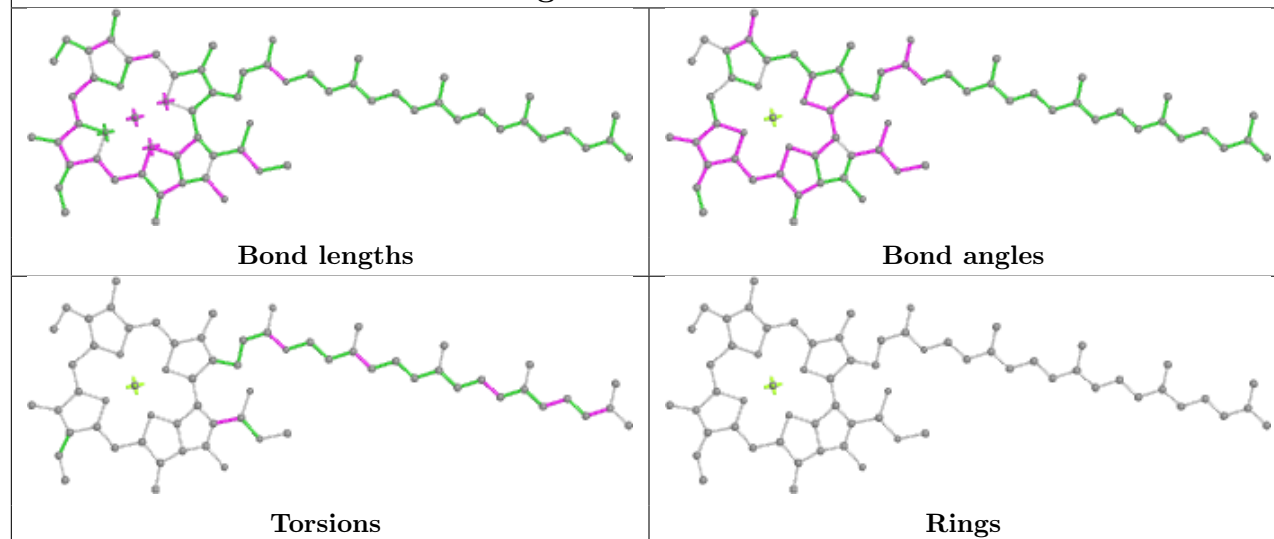
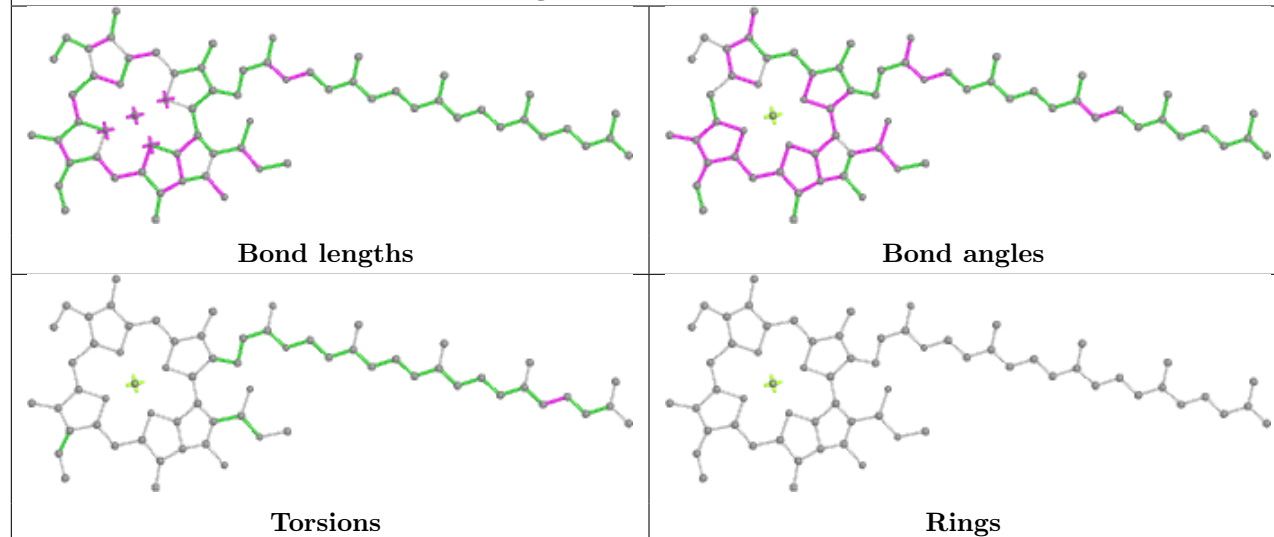
Ligand CLA B 615**Ligand CLA A 408**

Ligand LHG e 101

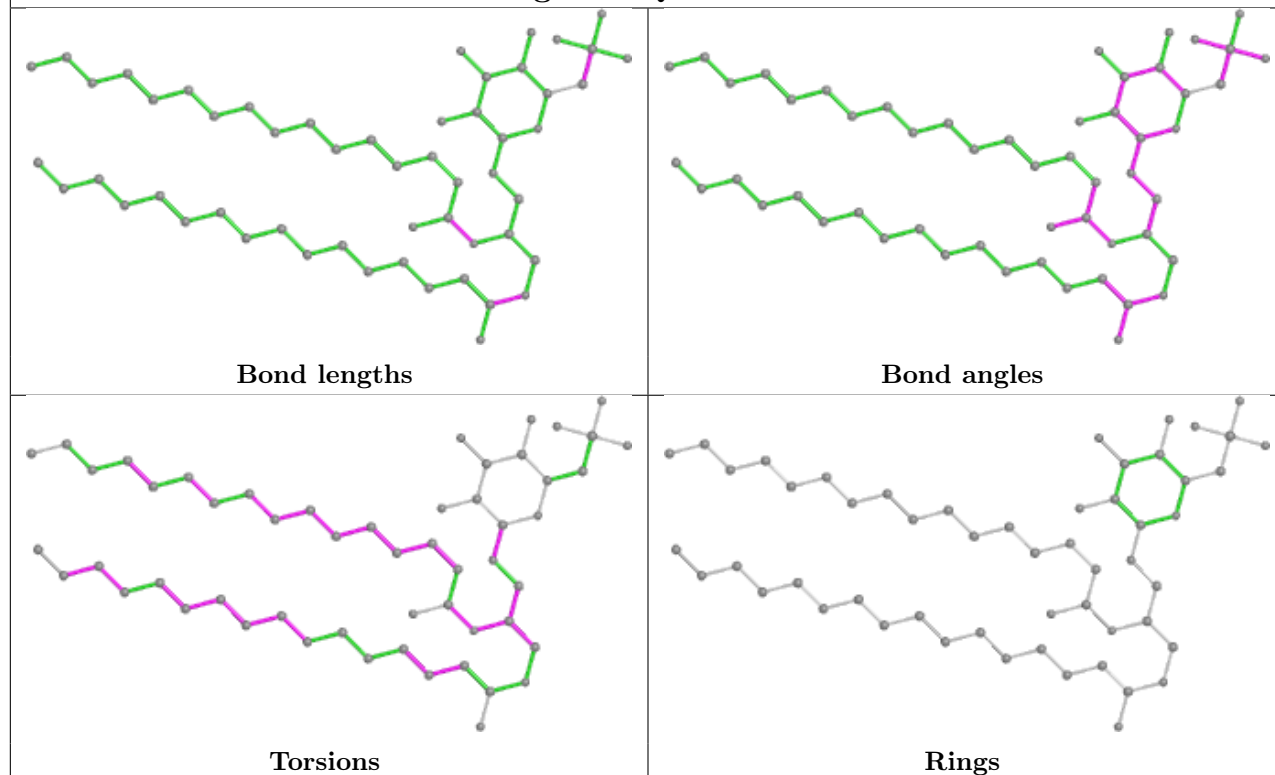


Ligand CLA C 512

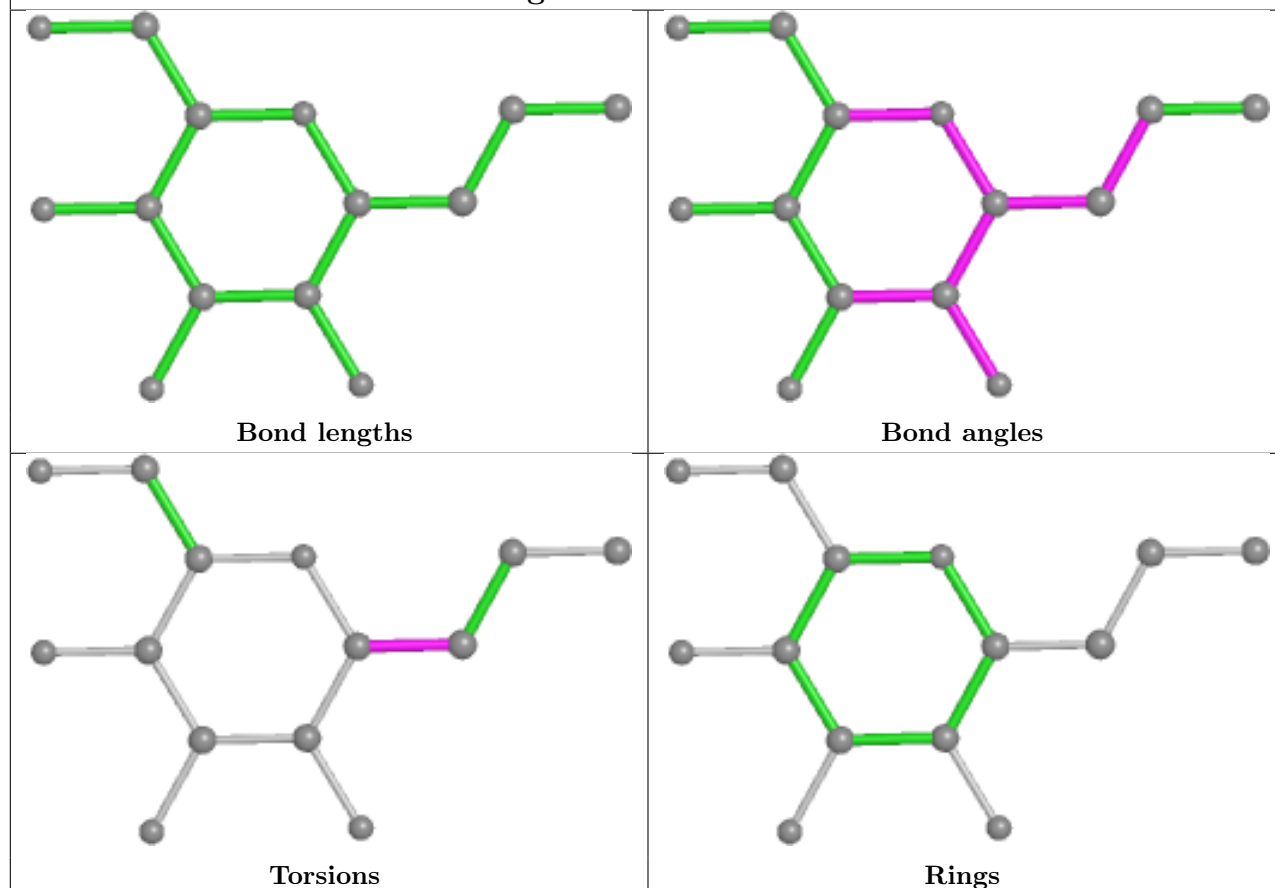


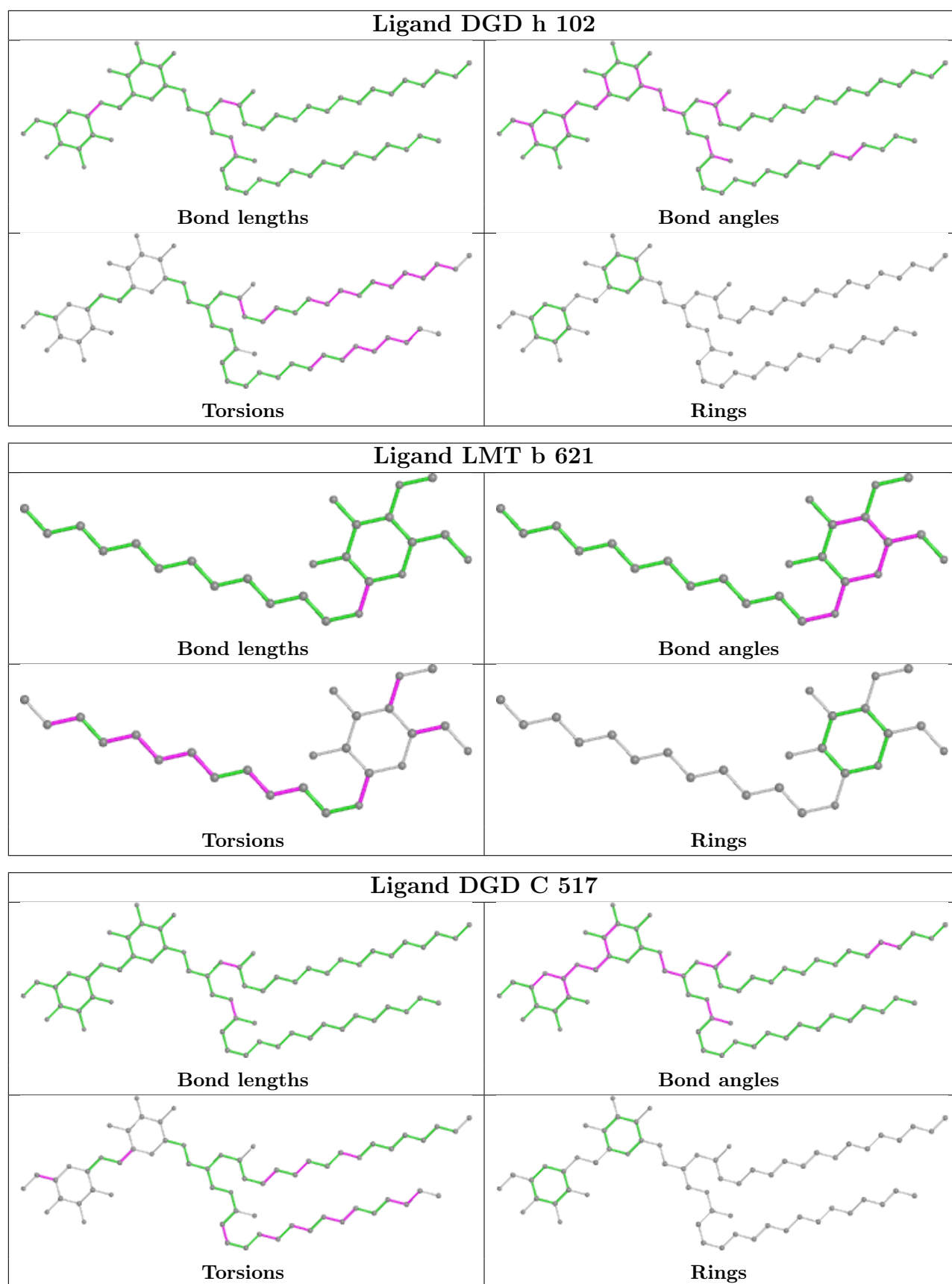
Ligand CLA c 914**Ligand CLA B 609**

Ligand SQD L 102

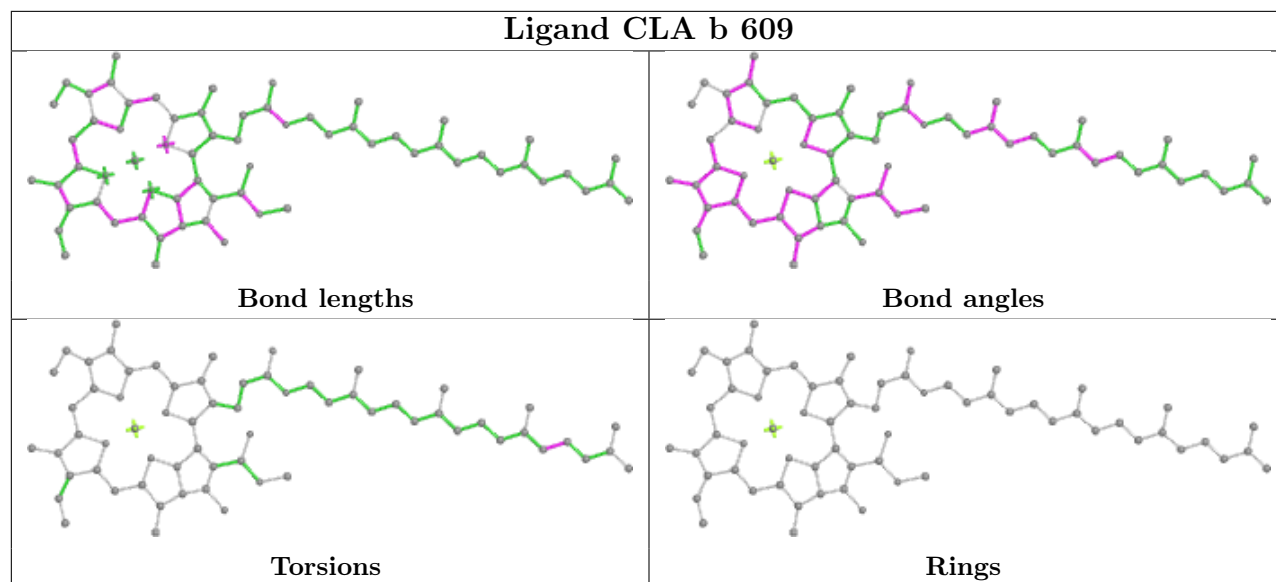


Ligand HTG V 204

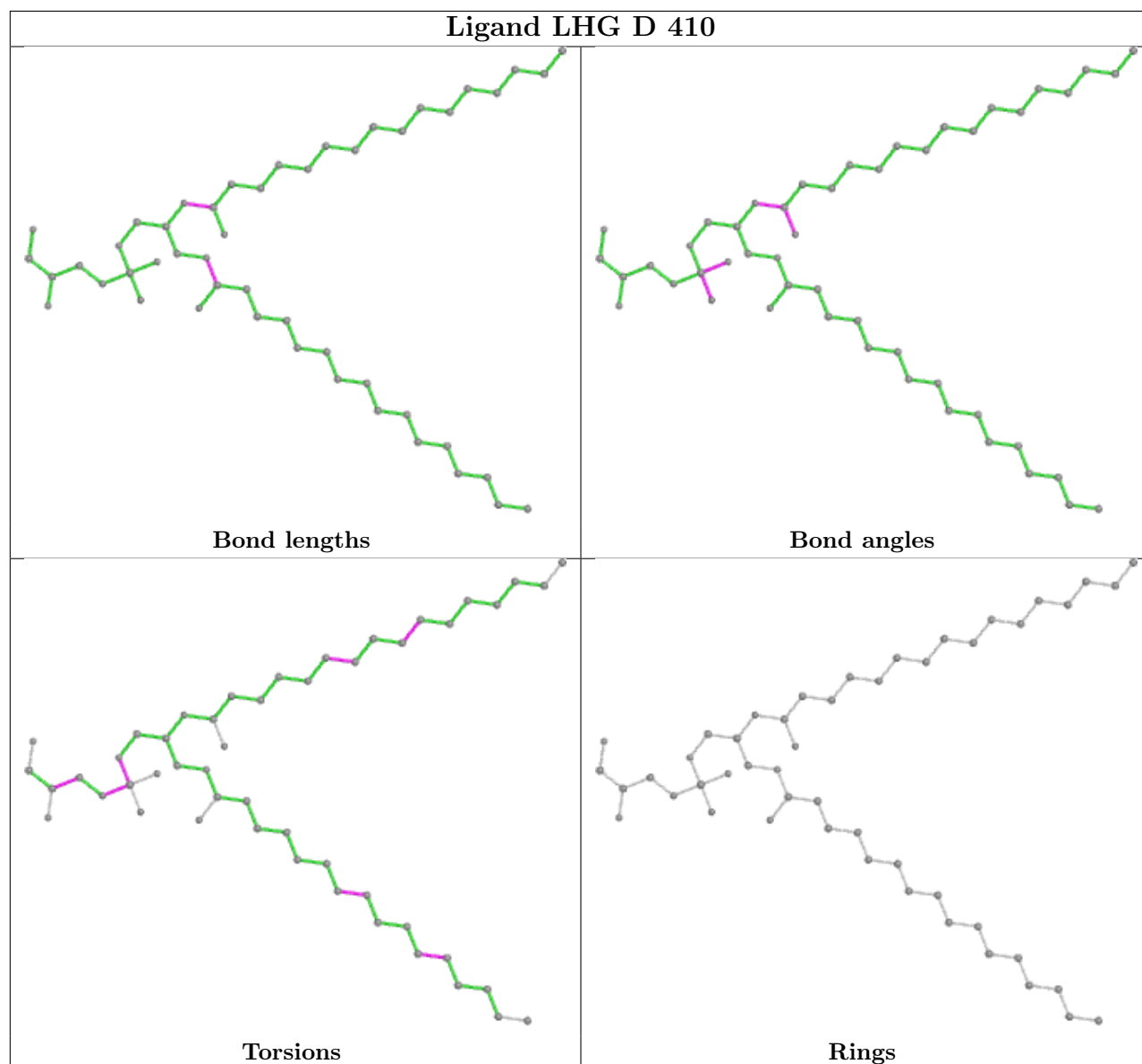


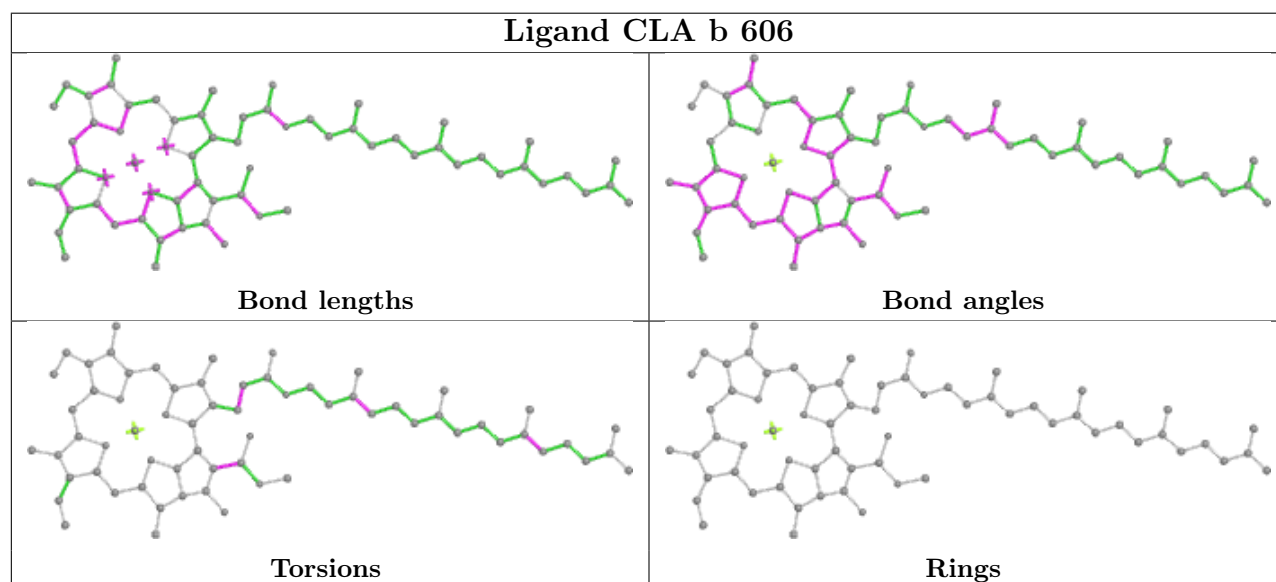
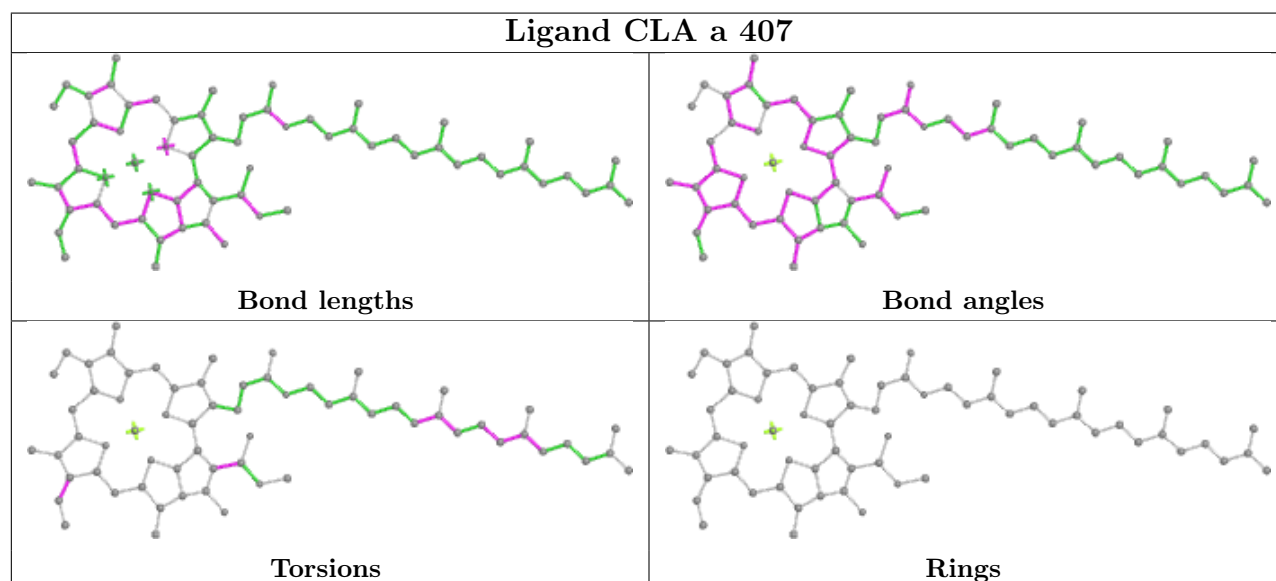
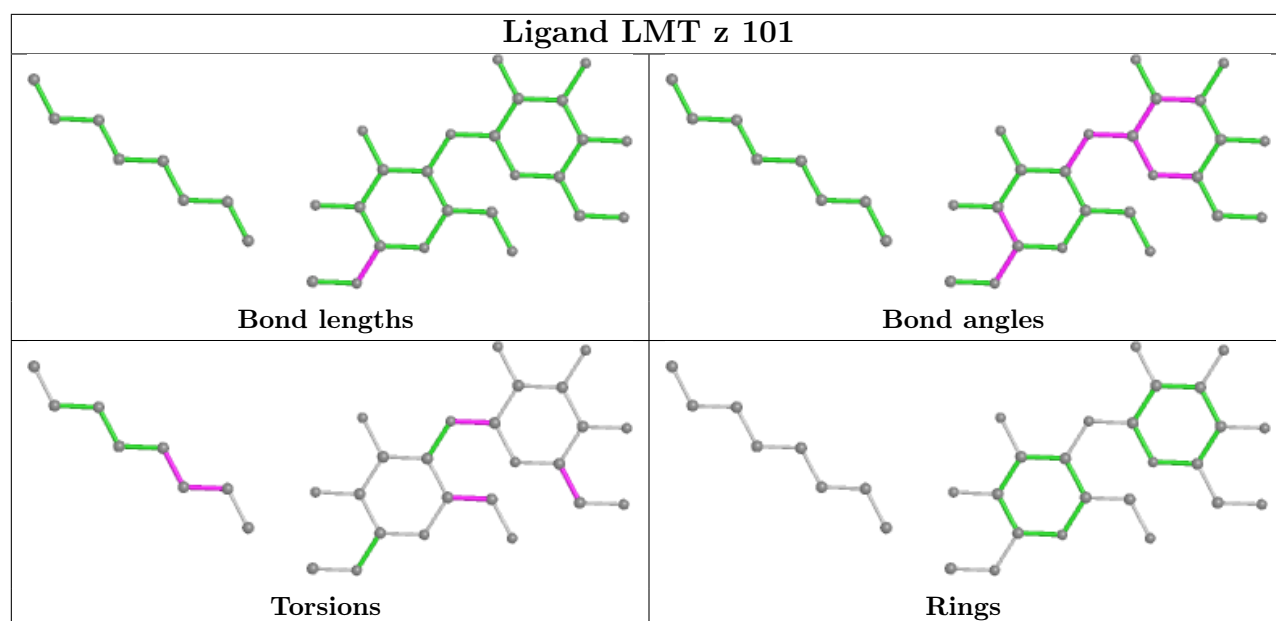


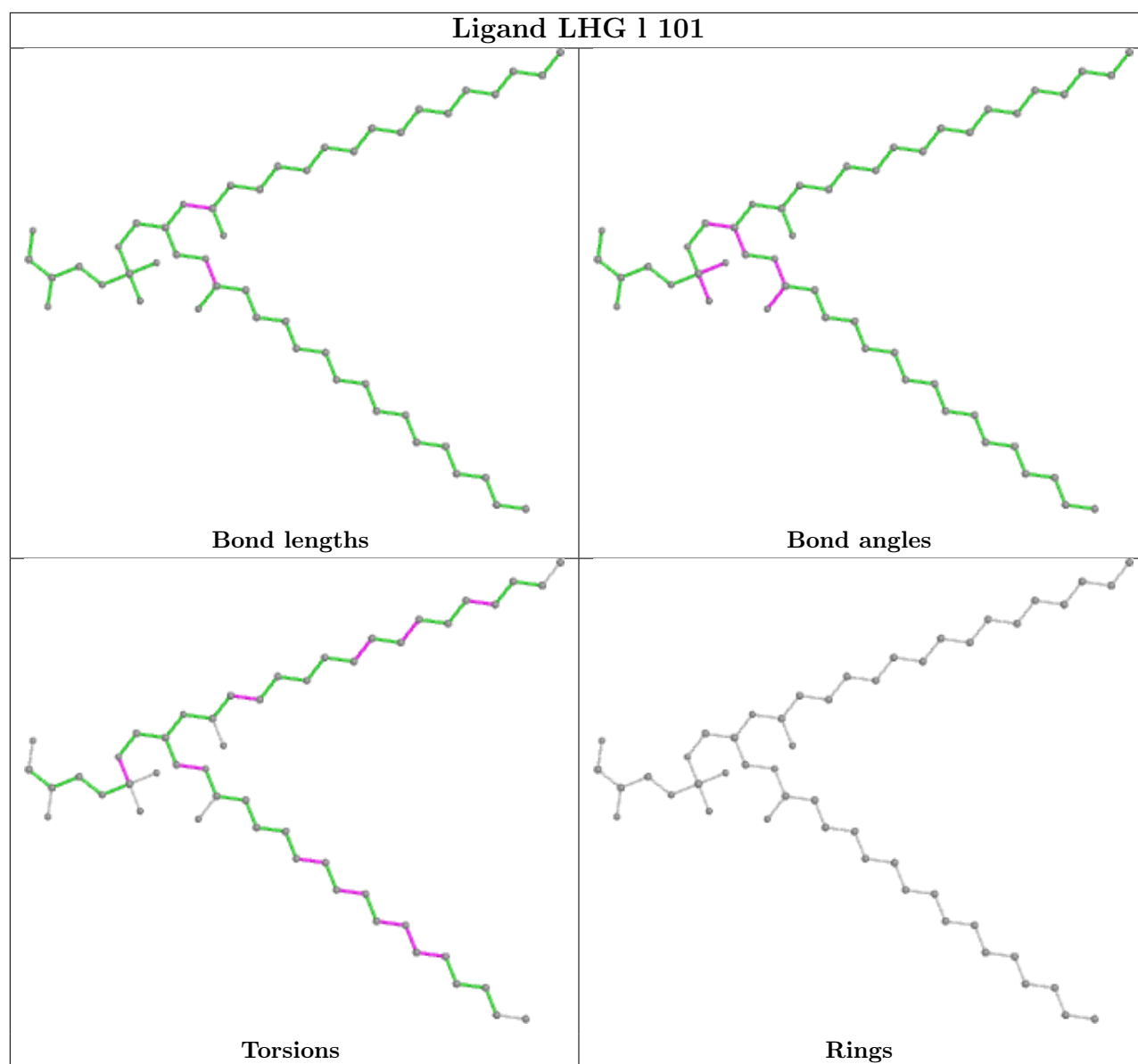
Ligand CLA b 609

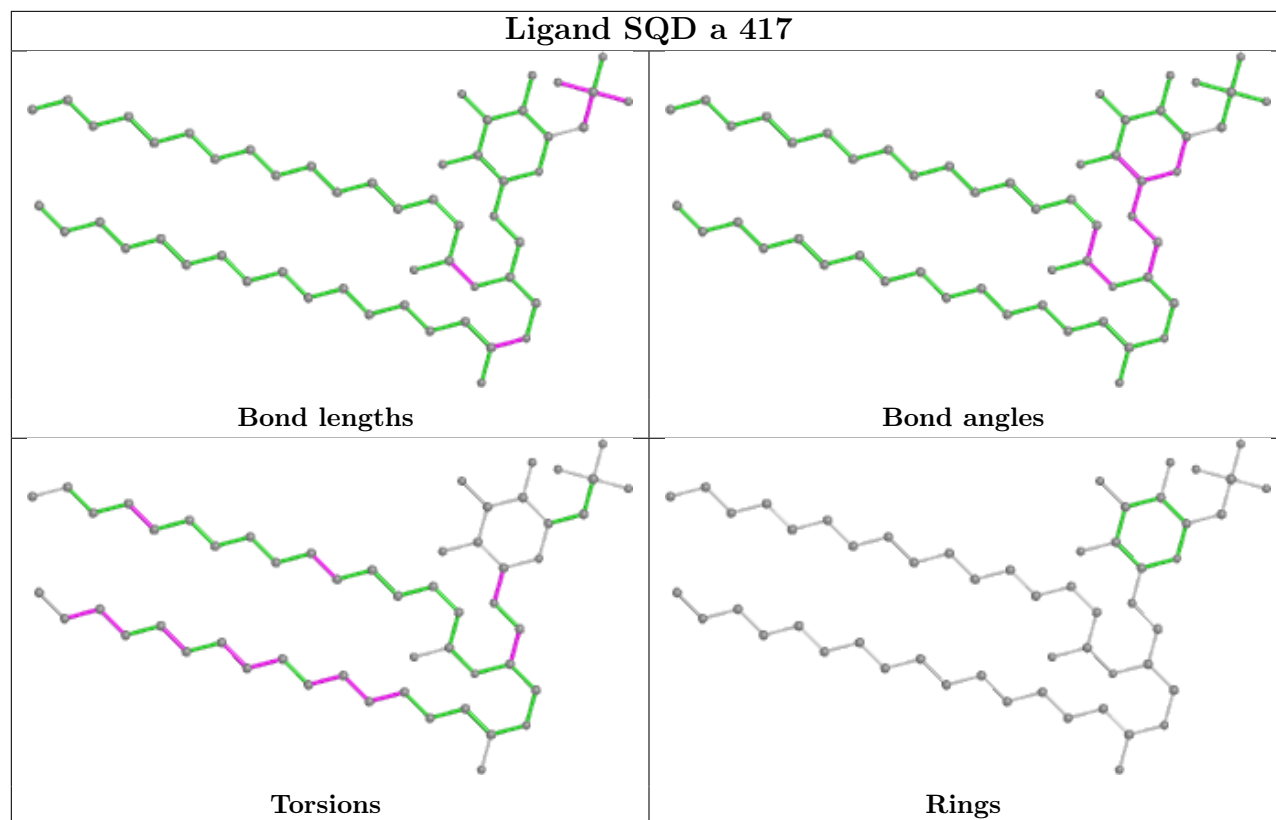


Ligand LHG D 410









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%)	-0.53	1 (0%) 90 93	13, 21, 43, 67	1 (0%)
1	a	334/344 (97%)	-0.49	5 (1%) 71 77	13, 21, 44, 91	4 (1%)
2	B	505/505 (100%)	-0.29	11 (2%) 62 67	15, 25, 50, 81	4 (0%)
2	b	501/505 (99%)	-0.21	19 (3%) 44 47	15, 25, 53, 109	3 (0%)
3	C	451/455 (99%)	-0.08	5 (1%) 77 82	16, 30, 46, 73	4 (0%)
3	c	455/455 (100%)	-0.12	4 (0%) 81 85	20, 31, 43, 68	1 (0%)
4	D	342/342 (100%)	-0.49	1 (0%) 90 93	12, 22, 41, 88	2 (0%)
4	d	342/342 (100%)	-0.58	0 100 100	11, 22, 40, 73	2 (0%)
5	E	81/83 (97%)	0.75	10 (12%) 9 10	25, 45, 75, 97	0
5	e	79/83 (95%)	0.54	6 (7%) 21 23	28, 42, 67, 87	0
6	F	35/44 (79%)	0.25	2 (5%) 30 31	24, 35, 59, 96	0
6	f	32/44 (72%)	0.09	1 (3%) 51 55	26, 31, 70, 82	0
7	H	63/65 (96%)	0.19	1 (1%) 70 75	20, 33, 44, 77	2 (3%)
7	h	63/65 (96%)	0.33	2 (3%) 50 53	23, 34, 46, 72	1 (1%)
8	I	34/38 (89%)	0.21	0 100 100	27, 35, 58, 77	0
8	i	37/38 (97%)	0.27	2 (5%) 32 33	26, 32, 84, 89	0
9	J	36/40 (90%)	0.42	1 (2%) 55 59	24, 38, 65, 81	0
9	j	40/40 (100%)	0.31	2 (5%) 35 36	24, 36, 69, 76	0
10	K	37/37 (100%)	0.10	0 100 100	31, 37, 47, 56	0
10	k	37/37 (100%)	0.24	0 100 100	29, 37, 55, 66	0
11	L	37/37 (100%)	-0.43	2 (5%) 32 33	11, 20, 62, 80	1 (2%)
11	l	36/37 (97%)	-0.36	2 (5%) 31 32	12, 20, 68, 76	1 (2%)
12	M	34/36 (94%)	-0.35	1 (2%) 54 57	13, 23, 52, 75	1 (2%)
12	m	34/36 (94%)	-0.33	1 (2%) 54 57	15, 24, 53, 72	1 (2%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.06	4 (1%) 70 75	16, 30, 55, 86	2 (0%)
13	o	243/244 (99%)	0.05	9 (3%) 45 48	16, 32, 65, 86	1 (0%)
14	T	29/32 (90%)	-0.30	1 (3%) 48 51	17, 21, 45, 81	0
14	t	30/32 (93%)	-0.22	2 (6%) 25 27	18, 22, 55, 85	0
15	U	97/104 (93%)	-0.17	1 (1%) 79 83	20, 28, 46, 59	0
15	u	97/104 (93%)	-0.24	1 (1%) 79 83	22, 27, 40, 63	1 (1%)
16	V	137/137 (100%)	-0.35	0 100 100	15, 26, 41, 59	1 (0%)
16	v	137/137 (100%)	0.05	0 100 100	16, 33, 51, 71	1 (0%)
17	Y	29/30 (96%)	0.86	3 (10%) 13 15	38, 46, 69, 72	0
17	y	29/30 (96%)	0.66	2 (6%) 24 26	38, 47, 59, 69	0
18	X	38/40 (95%)	0.59	3 (7%) 20 22	21, 39, 58, 62	1 (2%)
18	x	38/40 (95%)	0.75	4 (10%) 13 14	30, 38, 83, 98	0
19	Z	62/62 (100%)	0.95	7 (11%) 11 12	36, 45, 83, 96	0
19	z	61/62 (98%)	1.23	6 (9%) 14 17	42, 52, 83, 103	0
All	All	5249/5350 (98%)	-0.15	122 (2%) 61 65	11, 27, 55, 109	35 (0%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	5.3
18	x	37	VAL	5.0
2	b	487	SER	4.8
8	i	38	GLU	4.7
7	h	64	ALA	4.7

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(\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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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	0.25	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	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
35	HTG	D	414	19/19	0.70	0.19	76,92,111,112	0
29	UNL	B	634	16/-	0.70	0.20	73,80,95,97	0
30	LMT	F	101	35/35	0.70	0.19	64,88,93,96	0
31	DMS	U	204	4/4	0.70	0.20	53,62,62,80	0
35	HTG	v	204	19/19	0.71	0.20	62,70,81,91	0
29	UNL	B	633	16/-	0.71	0.17	61,80,87,88	0
31	DMS	o	304	4/4	0.71	0.22	63,68,70,84	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(\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	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
31	DMS	c	934	4/4	0.78	0.19	87,87,89,99	0
27	PL9	a	414	55/55	0.78	0.20	46,61,86,88	0
31	DMS	H	101	4/4	0.78	0.23	54,58,62,65	0
31	DMS	b	637	4/4	0.78	0.23	61,63,68,74	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	UNL	u	201	11/-	0.78	0.20	39,50,60,61	0
31	DMS	b	647	4/4	0.79	0.23	67,78,85,86	0
29	UNL	t	102	16/-	0.79	0.16	53,62,74,75	0
30	LMT	a	418	35/35	0.79	0.15	44,63,79,80	0
29	UNL	d	417	11/-	0.79	0.17	48,63,69,71	0
31	DMS	h	105	4/4	0.79	0.18	76,83,89,90	0
30	LMT	z	101	32/35	0.79	0.17	43,88,96,99	0
29	UNL	A	414	13/-	0.79	0.18	58,71,83,83	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	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	0.21	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(\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(\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(\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(\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	510	65/65	0.95	0.09	25,31,52,55	0
23	CLA	C	502	65/65	0.95	0.07	25,31,41,51	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	503	65/65	0.95	0.07	23,27,37,42	0
23	CLA	C	504	65/65	0.95	0.07	24,31,36,41	0
23	CLA	C	506	65/65	0.95	0.07	25,31,40,44	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(\AA^2)	Q<0.9
23	CLA	b	616	65/65	0.96	0.07	21,26,42,44	0
23	CLA	B	604	65/65	0.96	0.07	18,21,30,36	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	611	65/65	0.96	0.07	20,24,33,39	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	C	505	65/65	0.96	0.07	25,28,58,60	0
28	LHG	l	101	49/49	0.96	0.08	20,28,48,52	0
23	CLA	B	615	65/65	0.96	0.08	18,23,66,71	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	616	65/65	0.96	0.07	23,27,43,49	0
23	CLA	b	603	65/65	0.96	0.07	21,24,33,41	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(\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	0.08	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	0.07	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	0.08	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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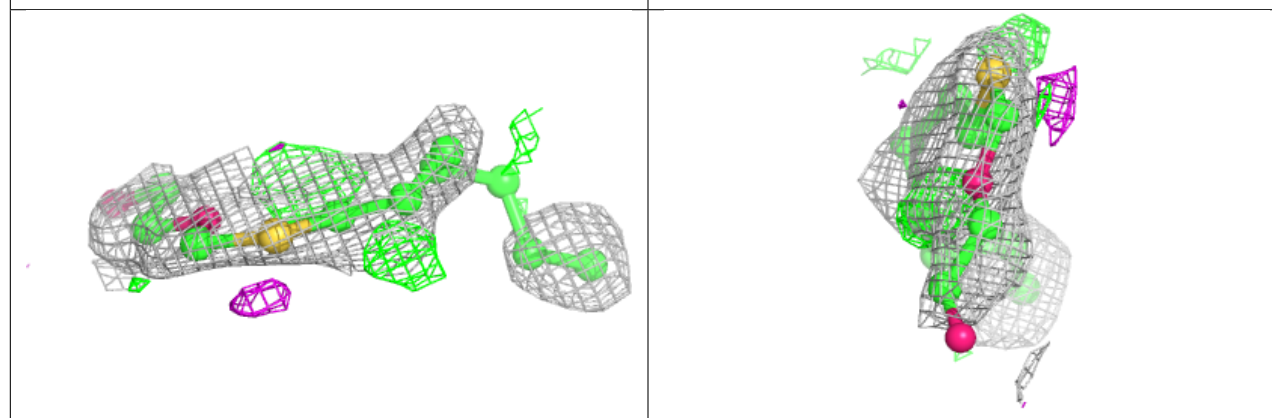
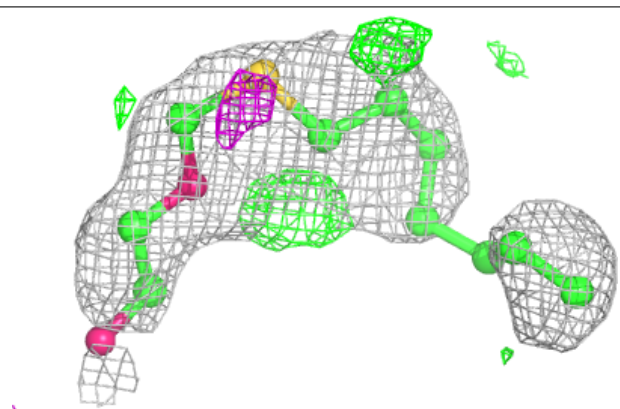
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	OEX	a	402	10/10	1.00	0.02	21,23,24,24	0
22	CL	A	403	1/1	1.00	0.02	19,19,19,19	0
22	CL	A	404	1/1	1.00	0.02	20,20,20,20	0

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.

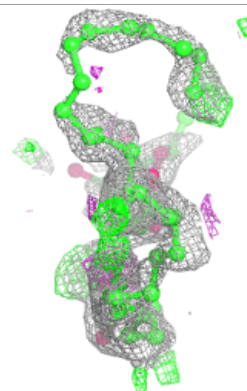
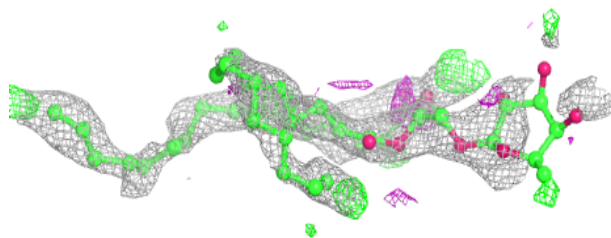
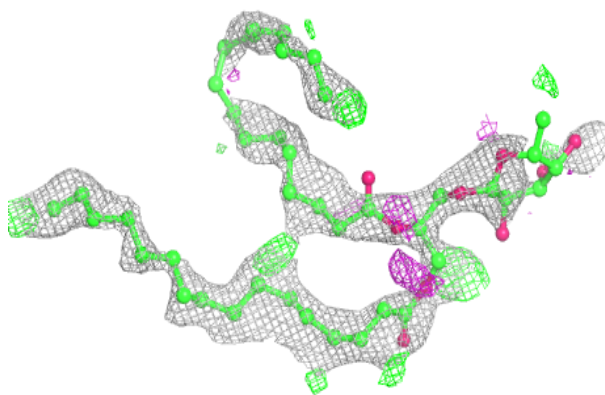
Electron density around HTG c 923:

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



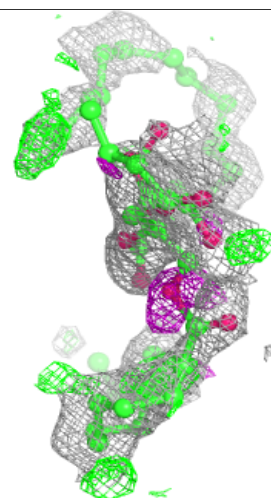
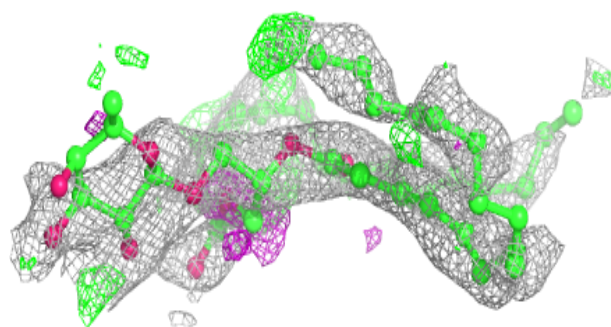
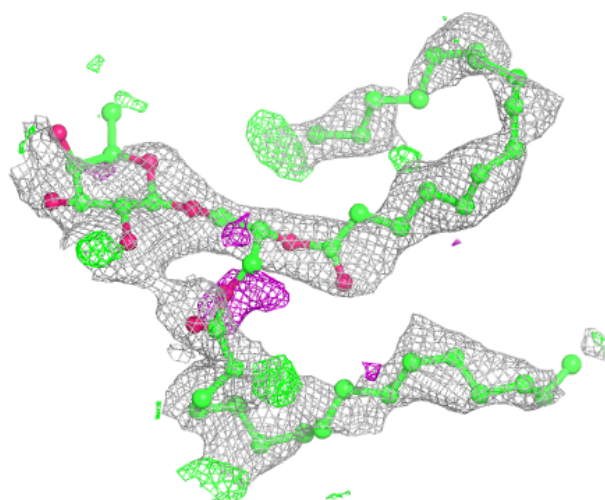
Electron density around DGD D 407:

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



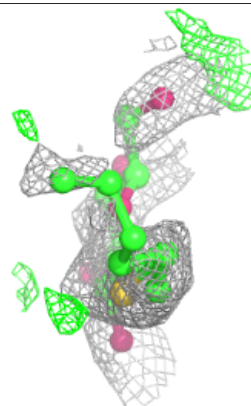
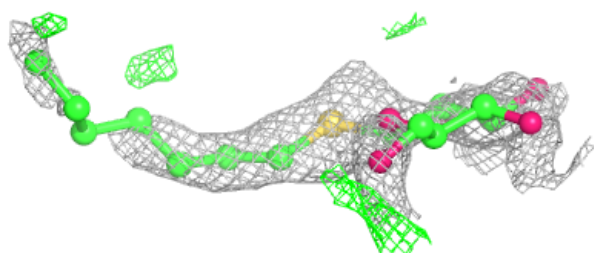
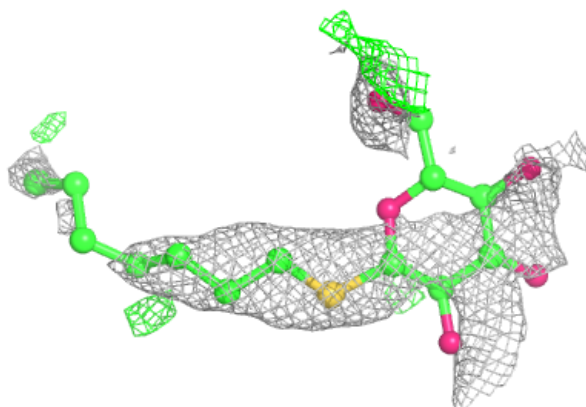
Electron density around DGD d 407:

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

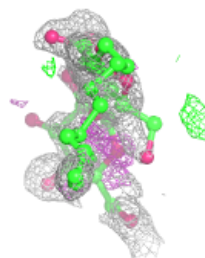
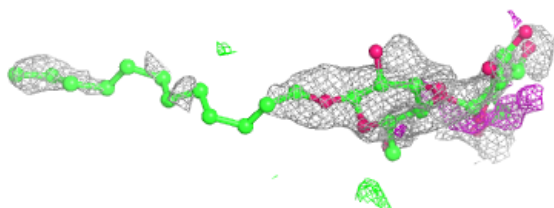
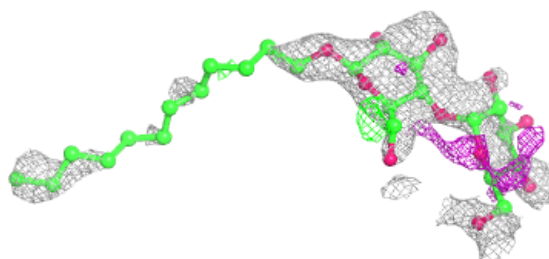


Electron density around HTG D 414:

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

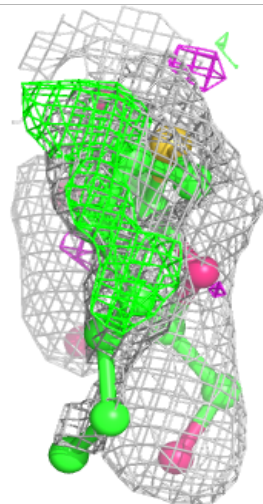
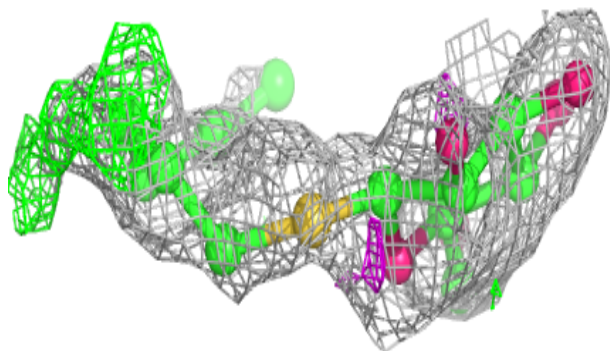
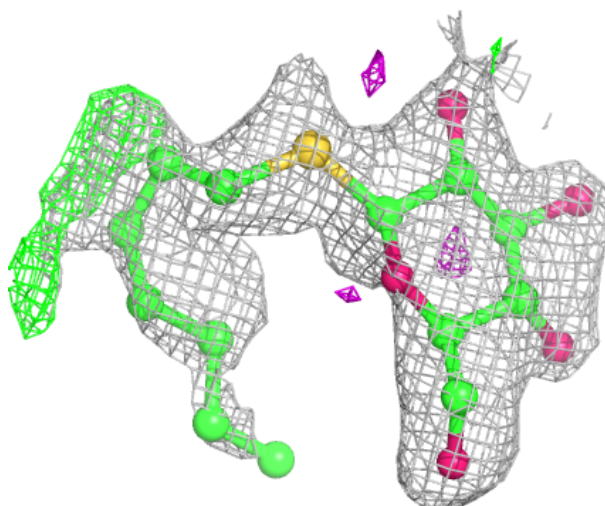
**Electron density around LMT F 101:**

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



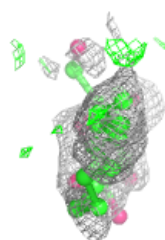
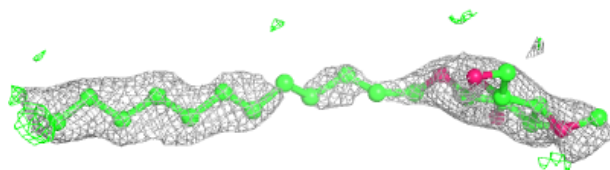
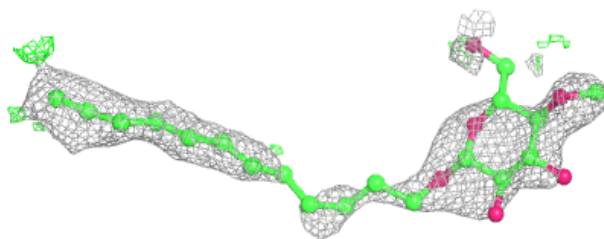
Electron density around HTG v 204:

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

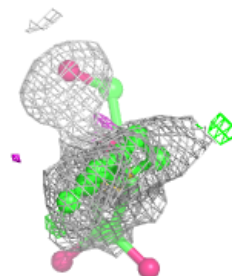
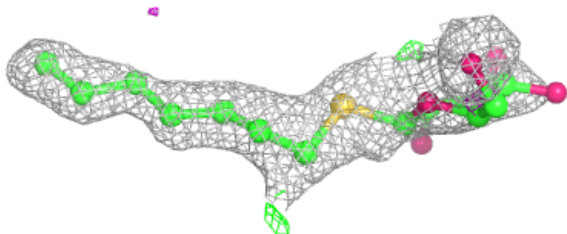
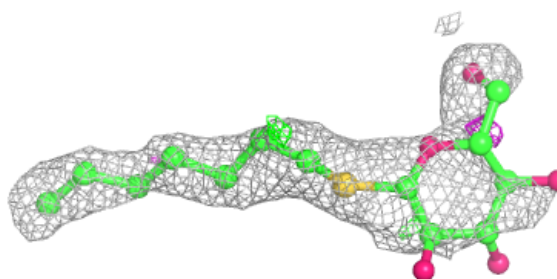


Electron density around LMT e 103:

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

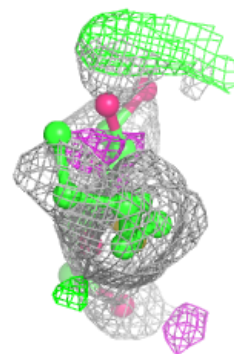
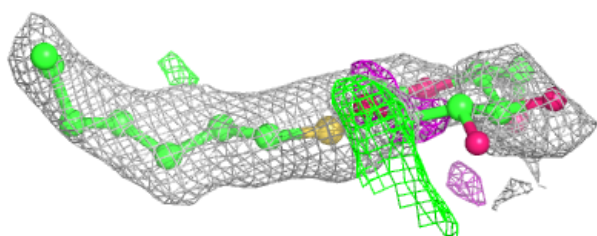
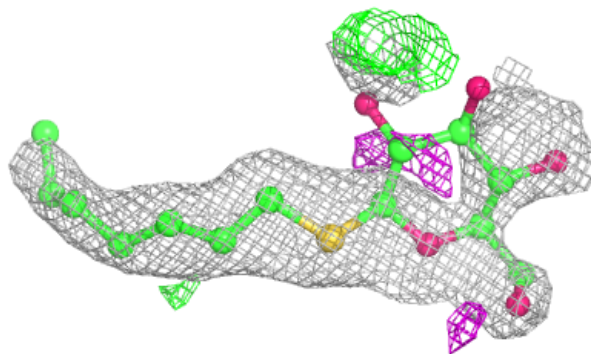
**Electron density around HTG c 922:**

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



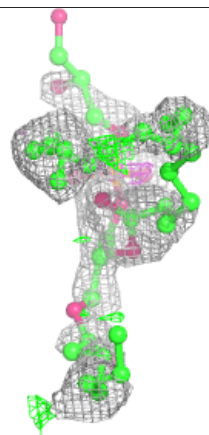
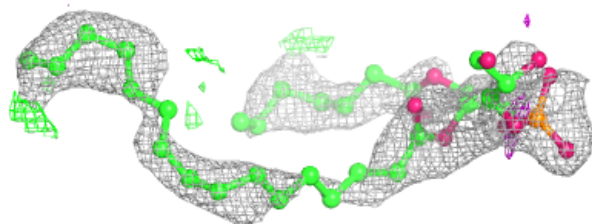
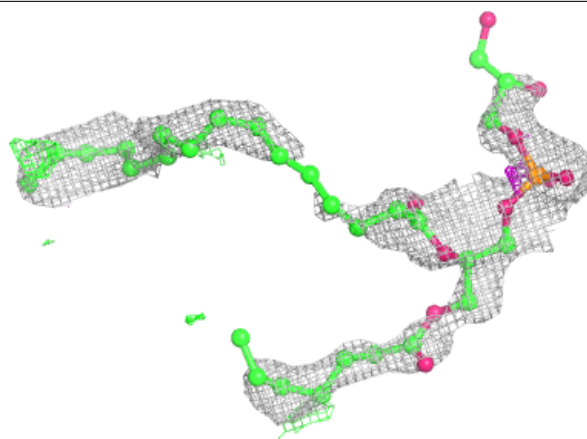
Electron density around HTG d 413:

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

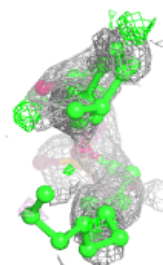
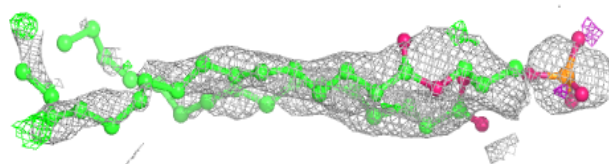
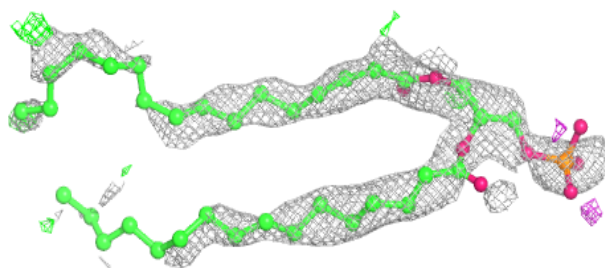


Electron density around LHG e 101:

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

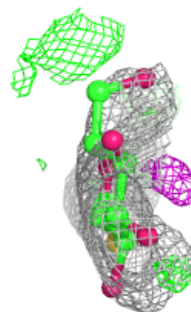
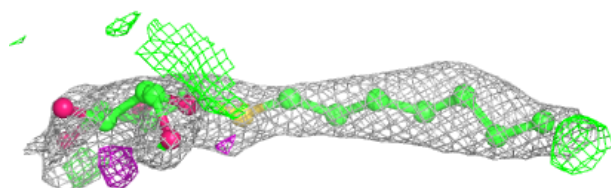
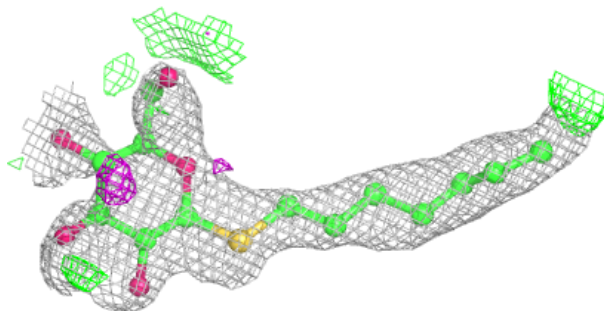
**Electron density around LHG K 101:**

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

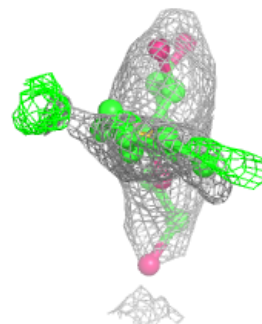
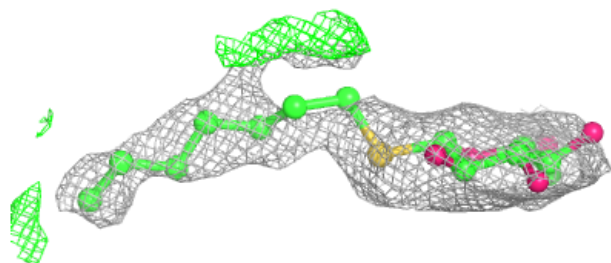
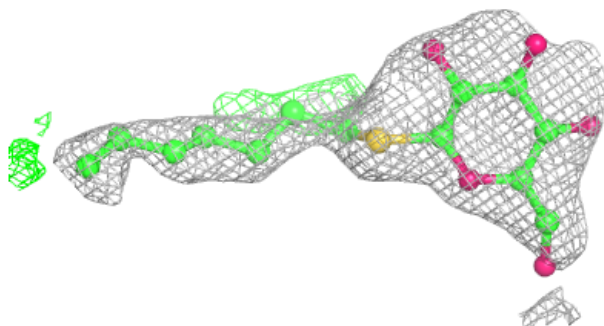


Electron density around HTG b 628:

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

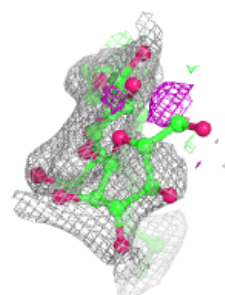
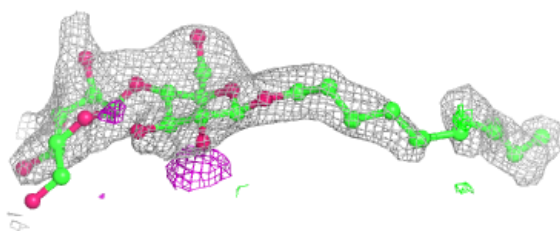
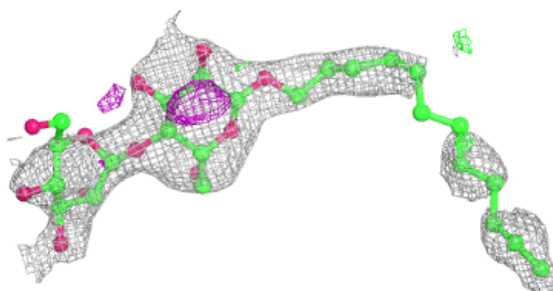
**Electron density around HTG c 921:**

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

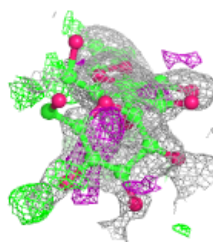
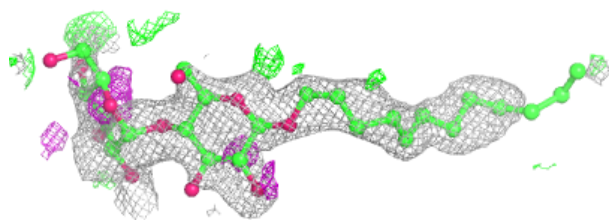
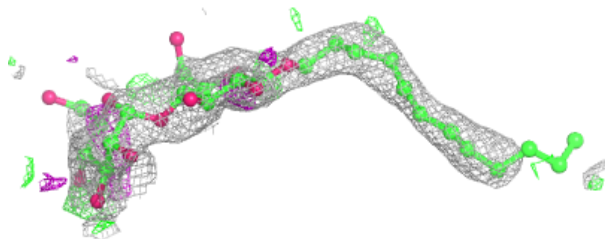


Electron density around LMT I 101:

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

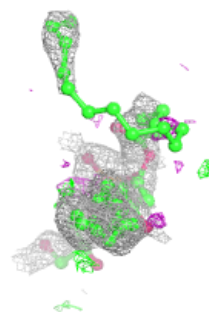
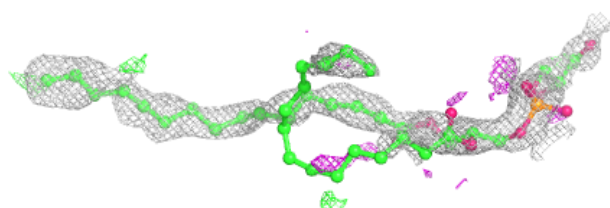
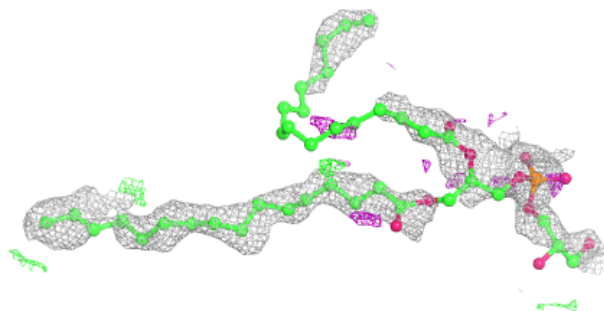
**Electron density around LMT A 416:**

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



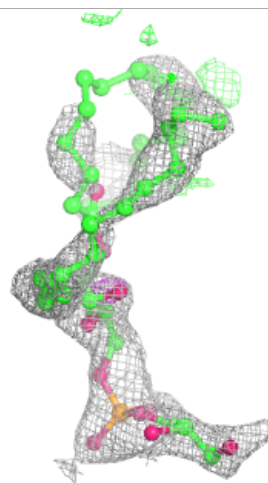
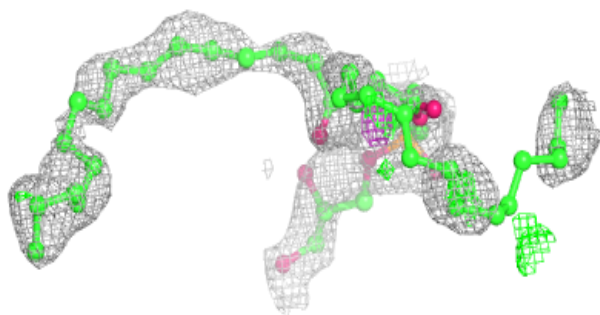
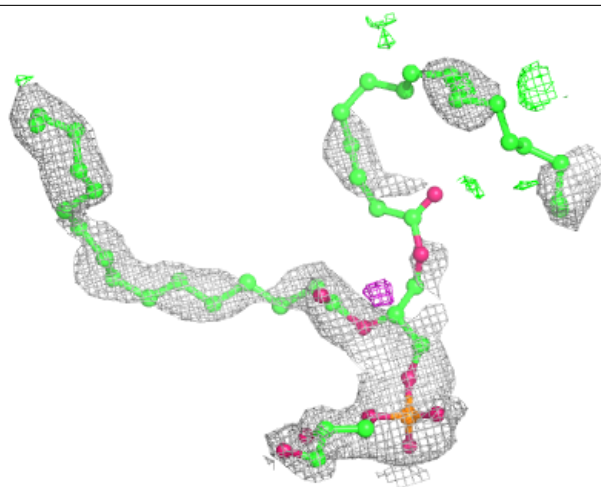
Electron density around LHG A 412:

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



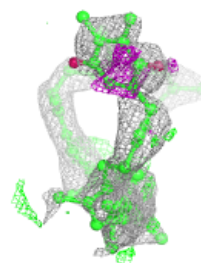
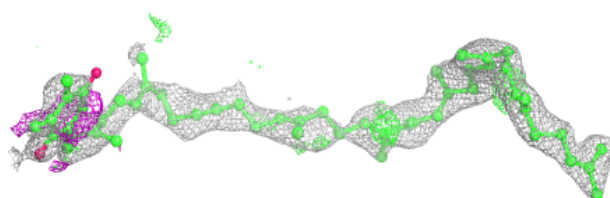
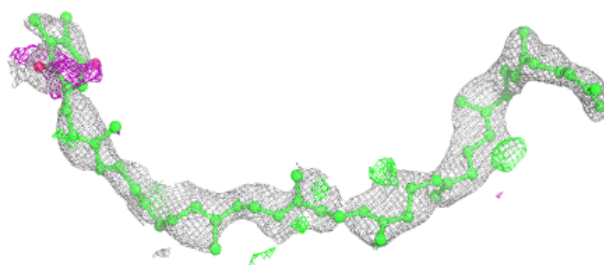
Electron density around LHG E 101:

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

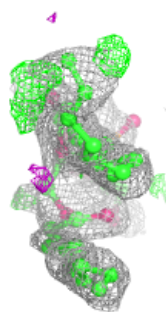
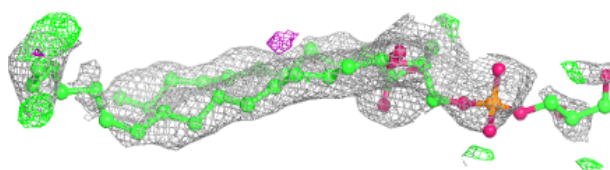
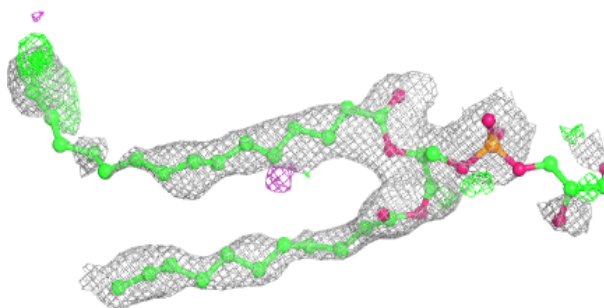


Electron density around PL9 a 414:

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

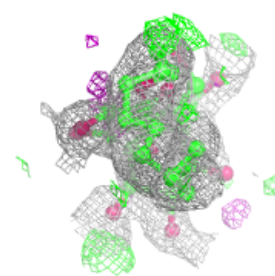
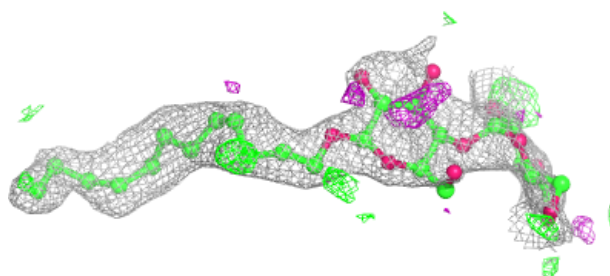
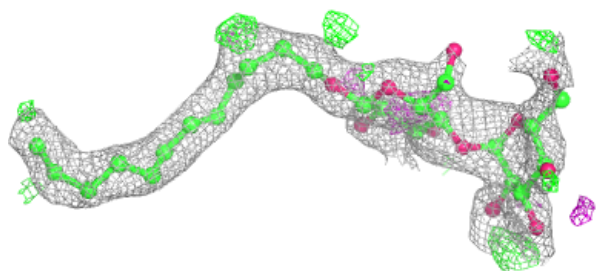
**Electron density around LHG d 402:**

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

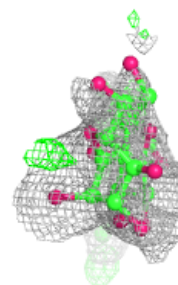
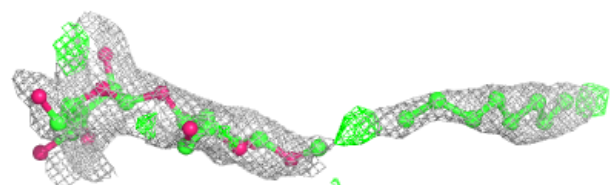
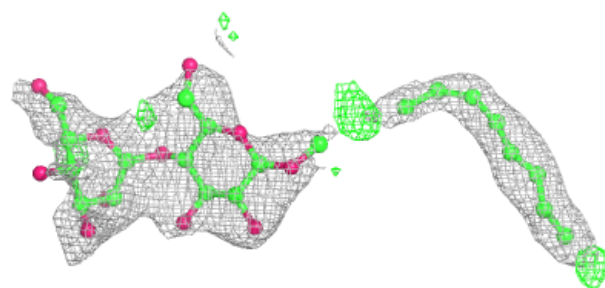


Electron density around LMT a 418:

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

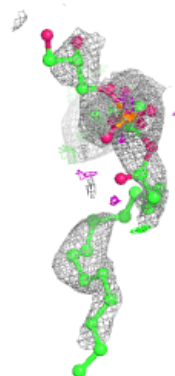
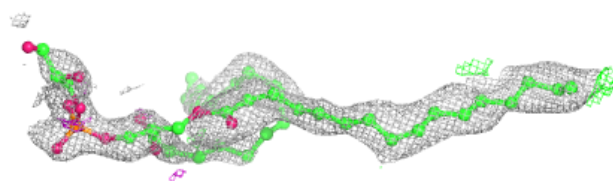
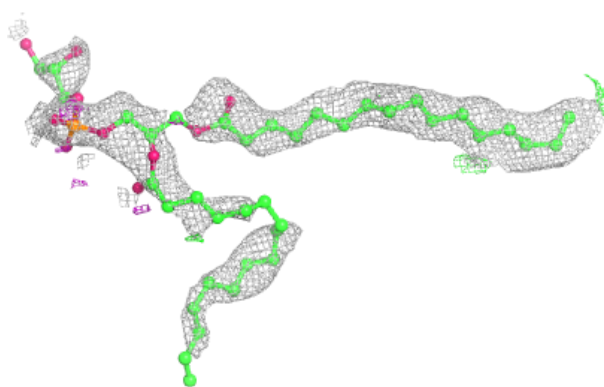
**Electron density around LMT z 101:**

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

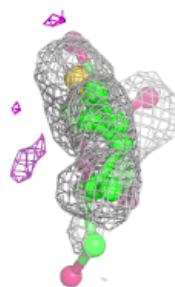
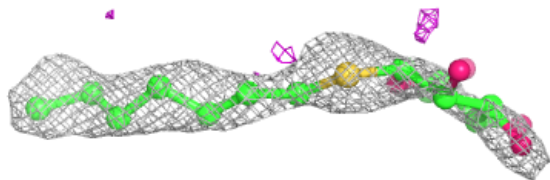
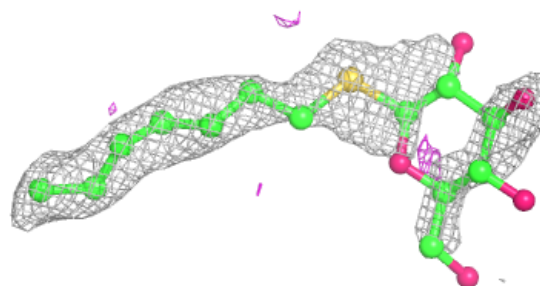


Electron density around LHG a 415:

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

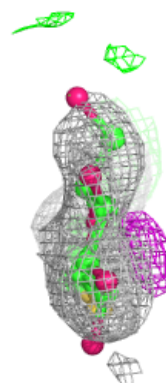
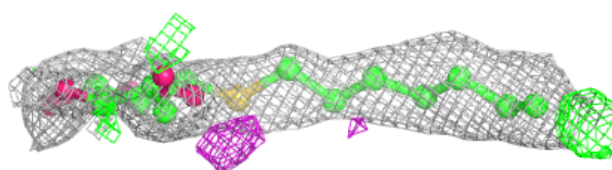
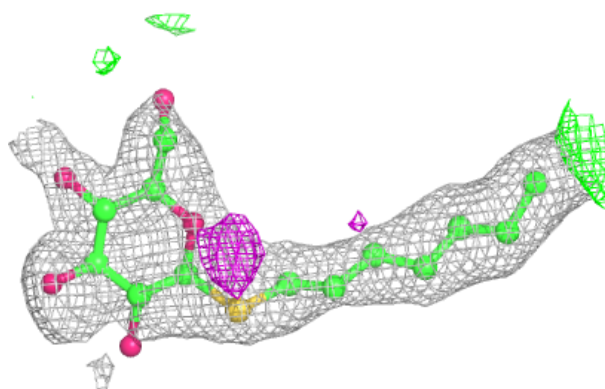
**Electron density around HTG B 626:**

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

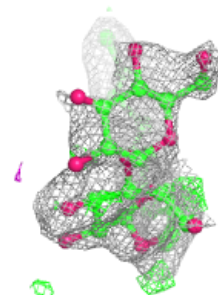
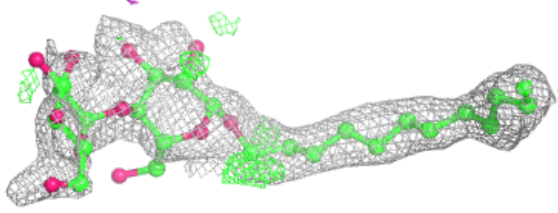
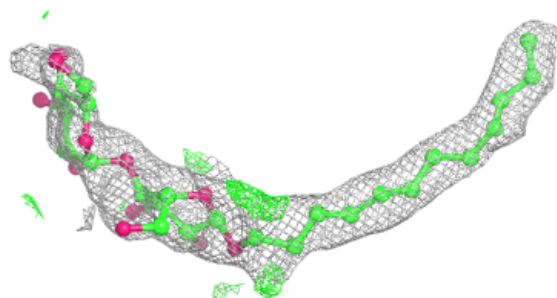


Electron density around HTG B 631:

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

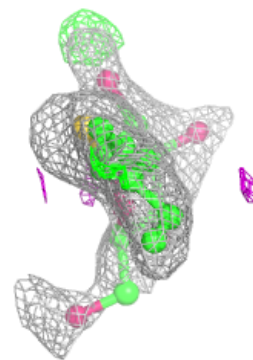
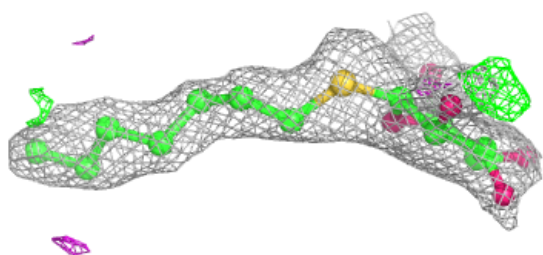
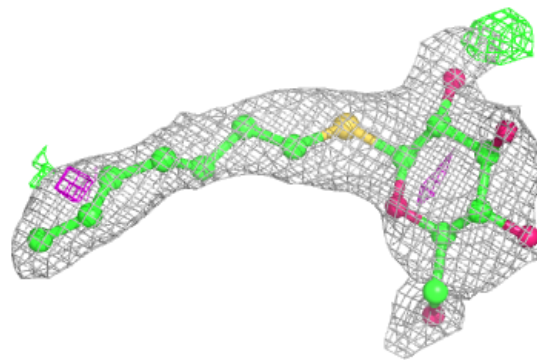
**Electron density around LMT m 103:**

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

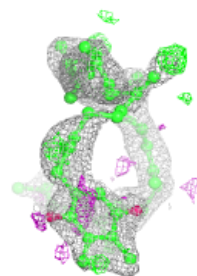
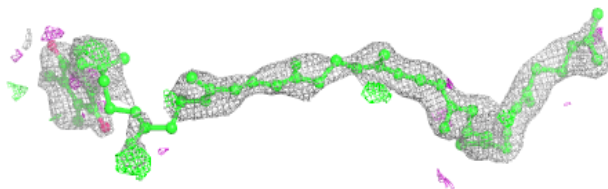
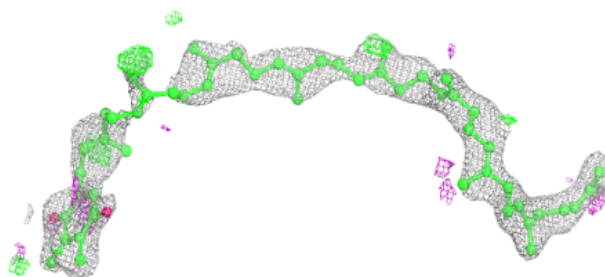


Electron density around HTG b 623:

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

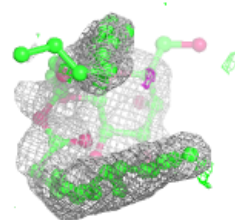
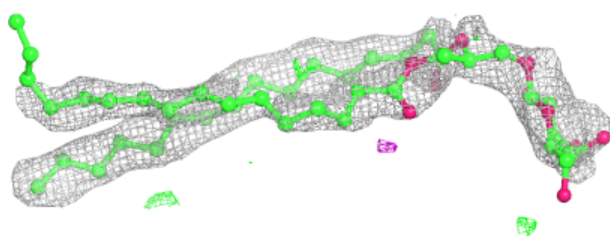
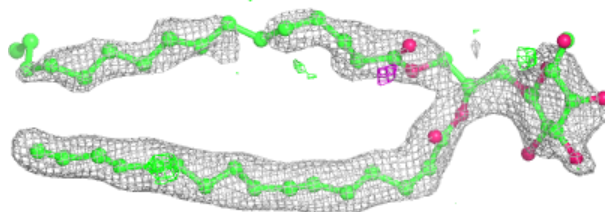
**Electron density around PL9 A 411:**

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

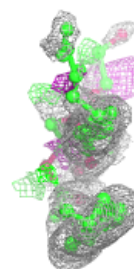
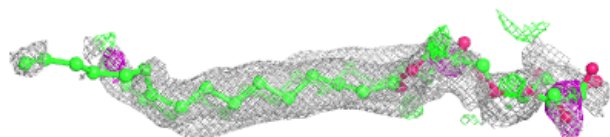
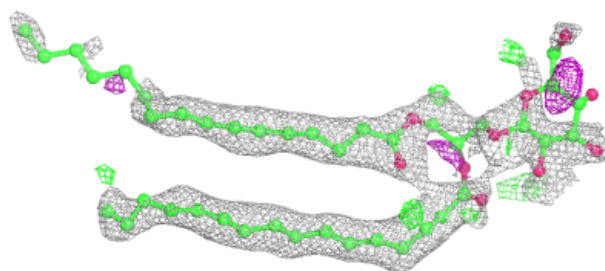


Electron density around LMG C 531:

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

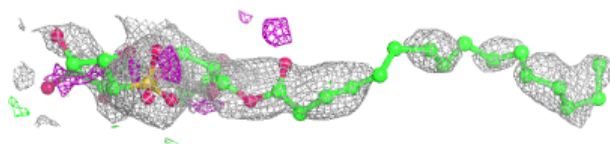
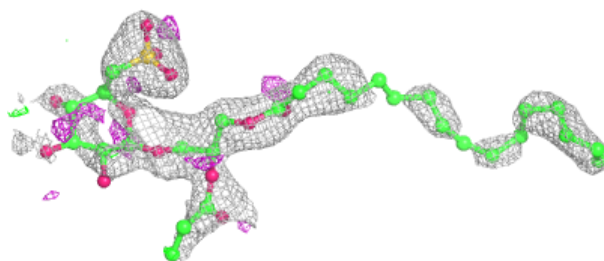
**Electron density around LMG D 412:**

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

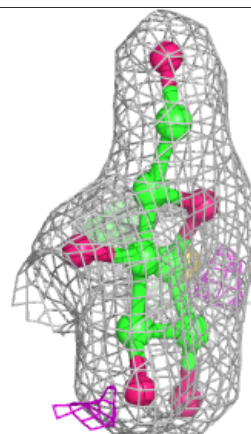
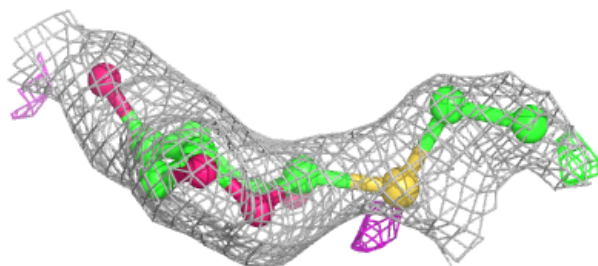
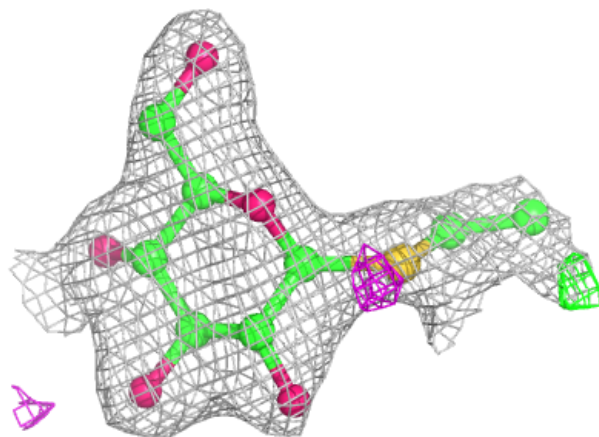


Electron density around SQD x 101:

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

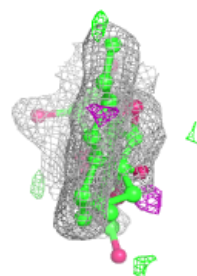
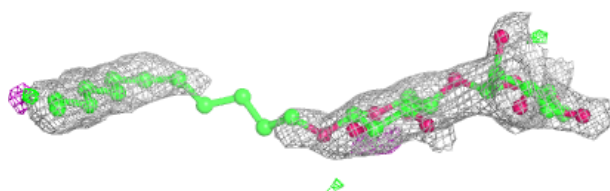
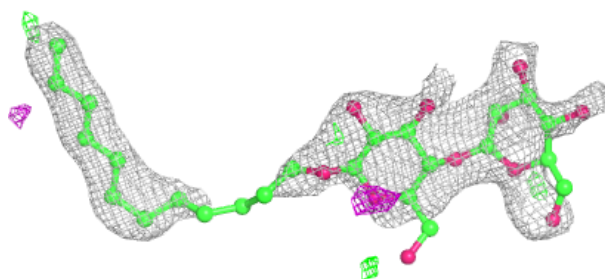
**Electron density around HTG V 204:**

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

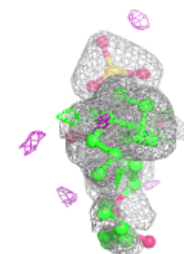
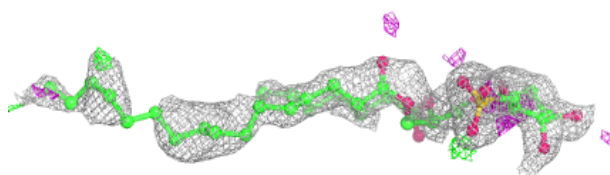
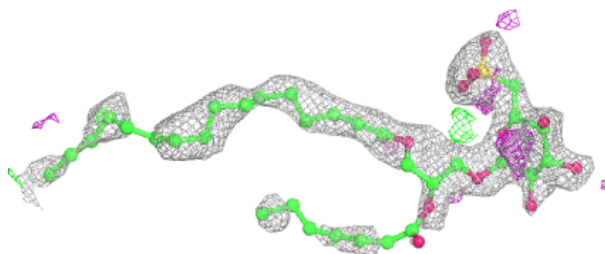


Electron density around LMT Z 101:

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

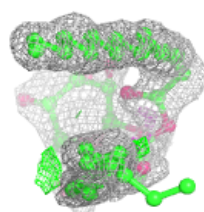
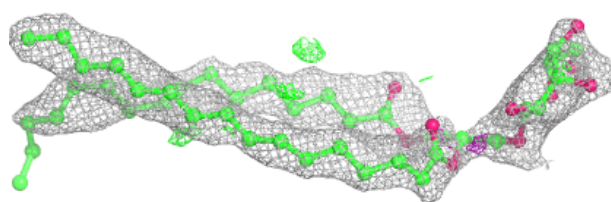
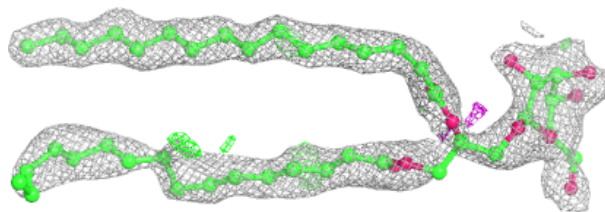
**Electron density around SQD D 408:**

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

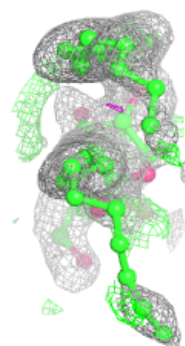
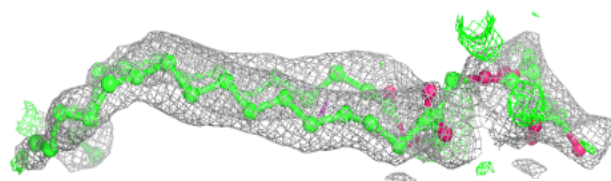
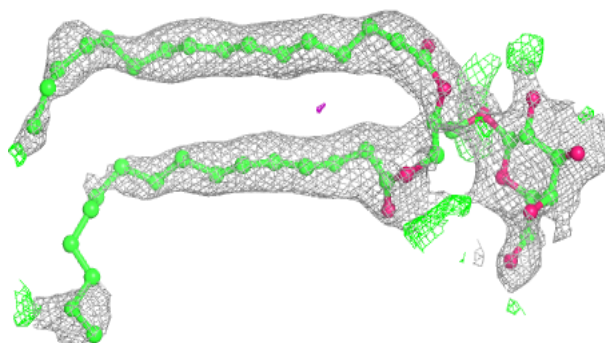


Electron density around LMG c 930:

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

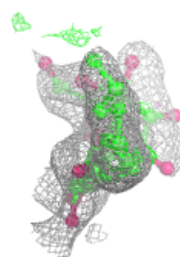
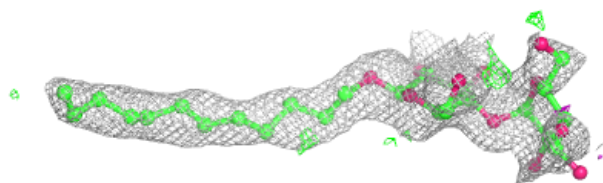
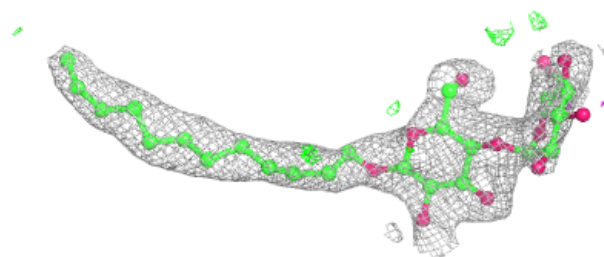
**Electron density around LMG d 411:**

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

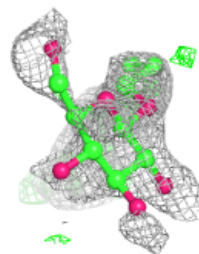
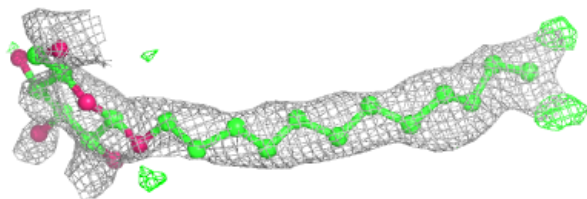
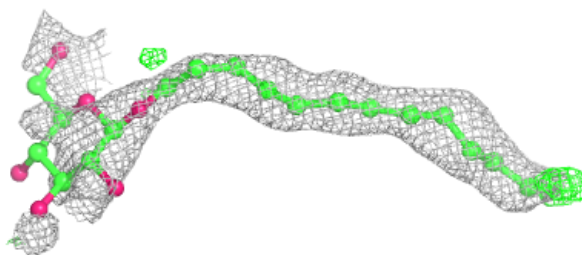


Electron density around LMT B 623:

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

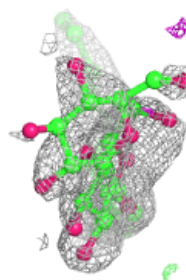
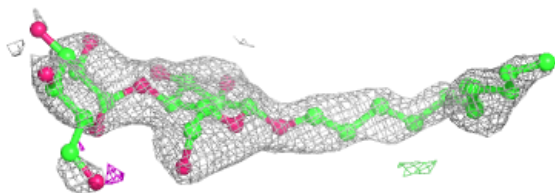
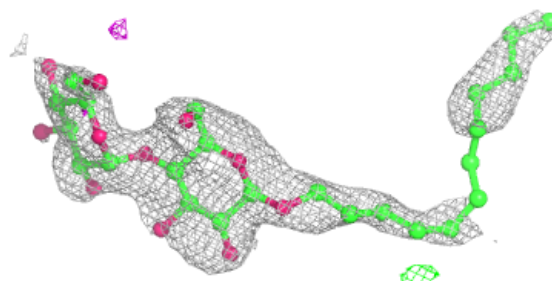
**Electron density around LMT B 643:**

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

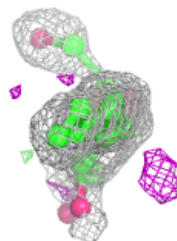
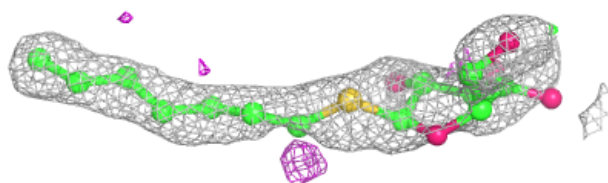
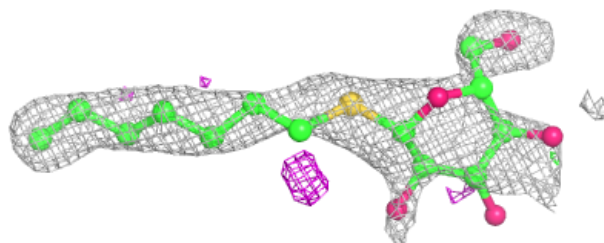


Electron density around LMT a 422:

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

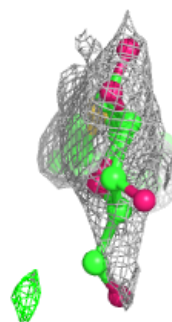
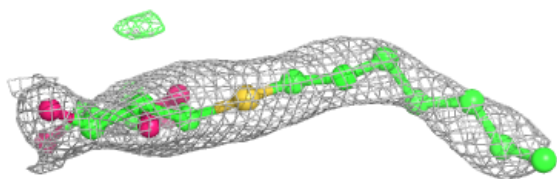
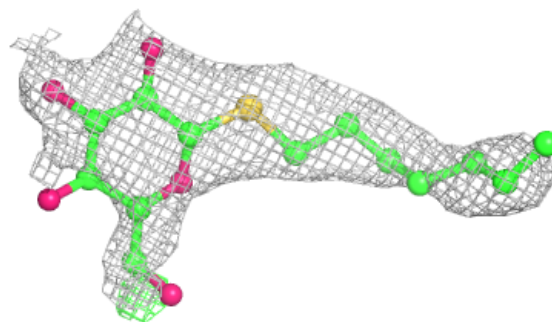
**Electron density around HTG C 522:**

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

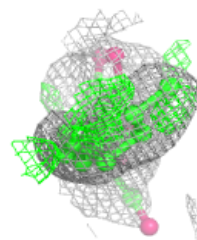
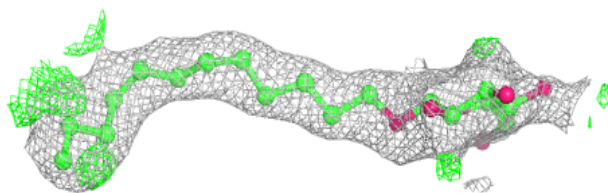
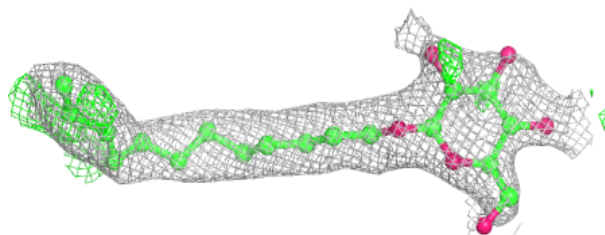


Electron density around HTG C 523:

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

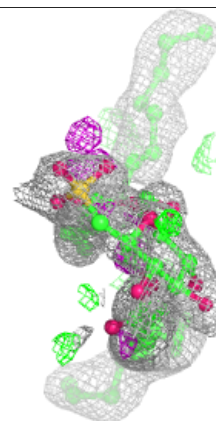
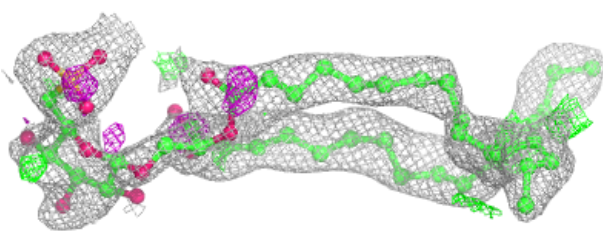
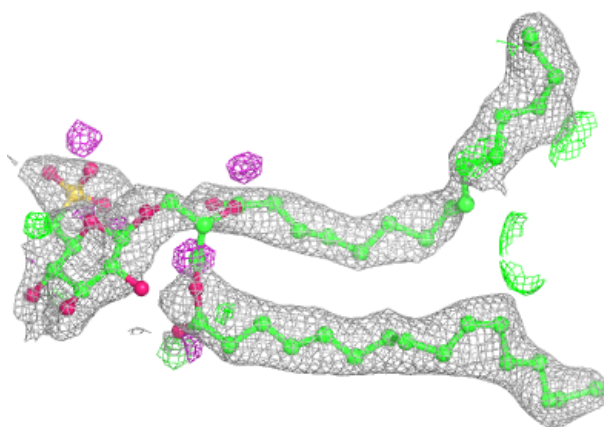
**Electron density around LMT B 644:**

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

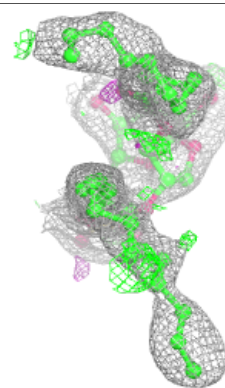
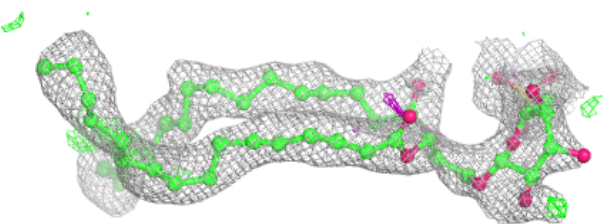
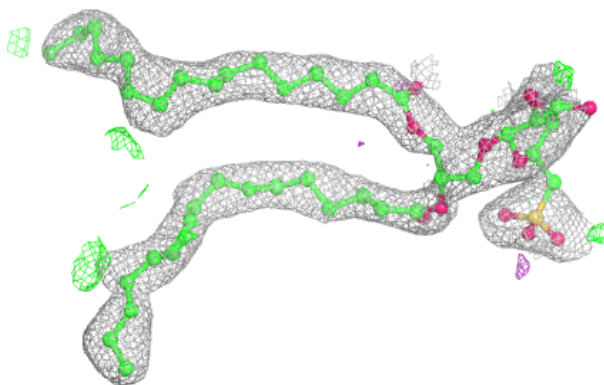


Electron density around SQD B 621:

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

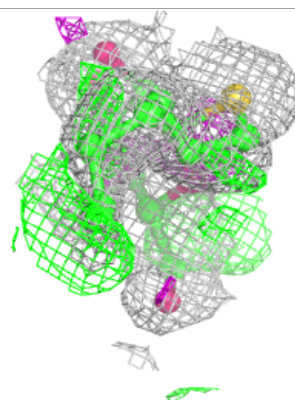
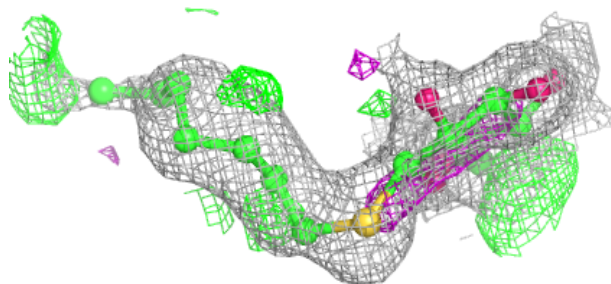
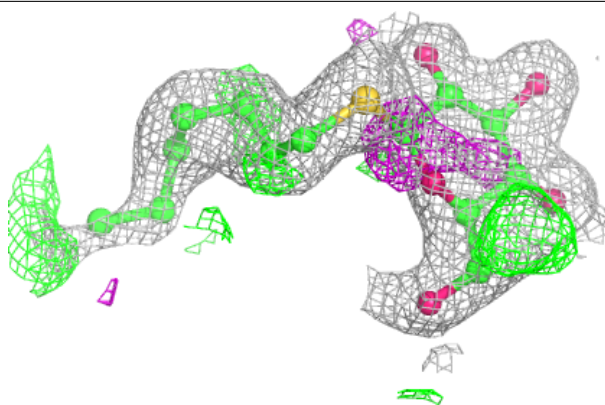
**Electron density around SQD L 102:**

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

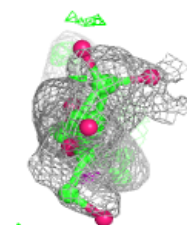
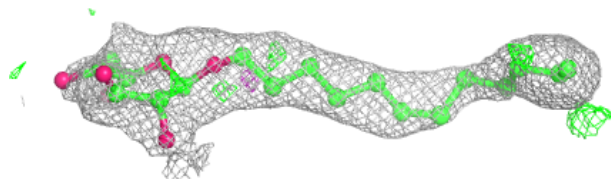
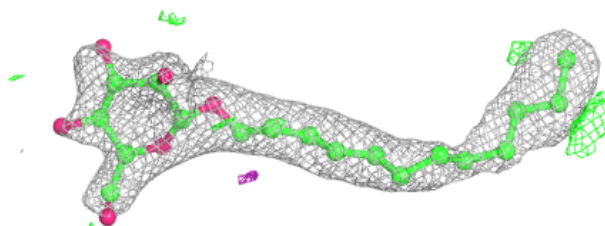


Electron density around HTG B 625:

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

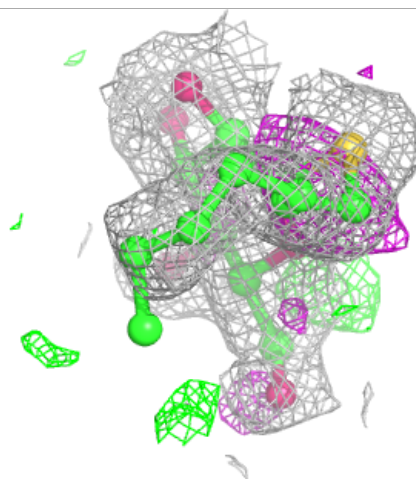
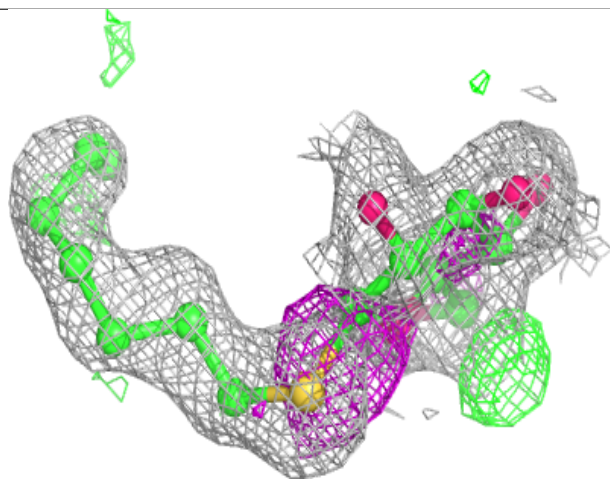
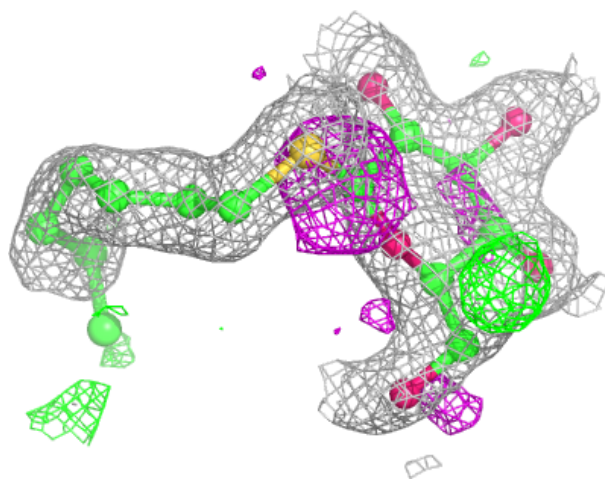
**Electron density around LMT T 103:**

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



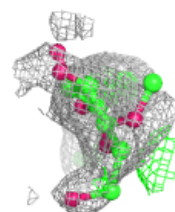
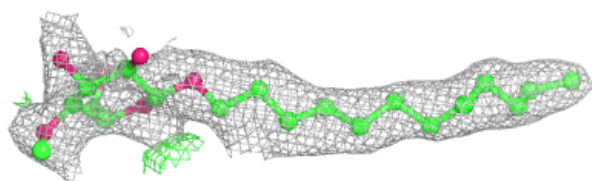
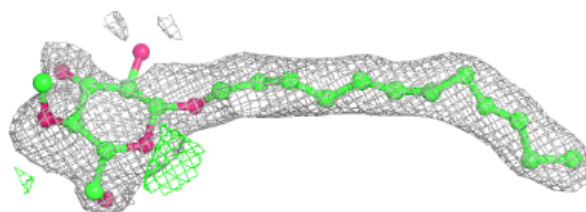
Electron density around HTG b 622:

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

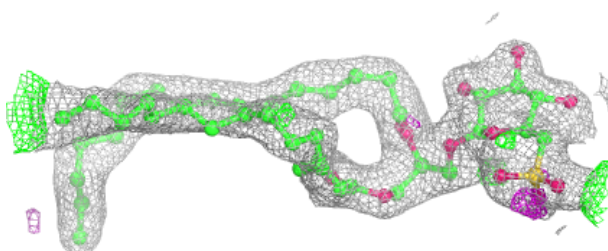
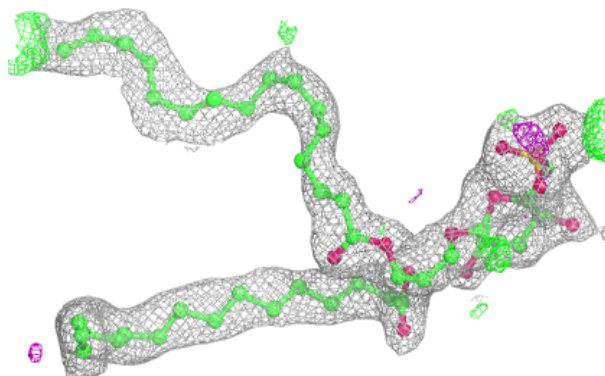


Electron density around LMT b 621:

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

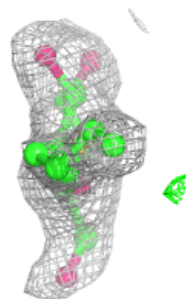
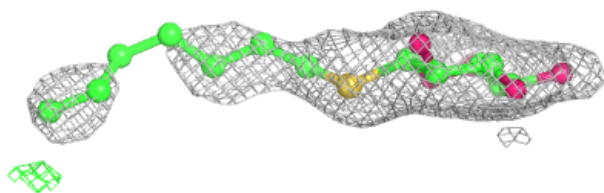
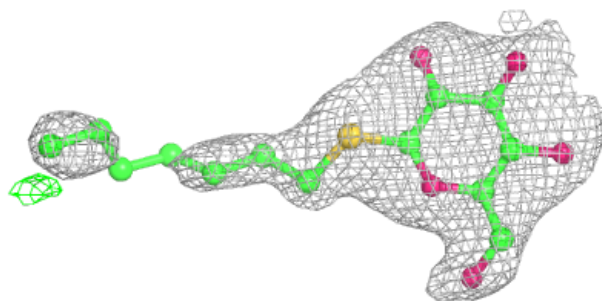
**Electron density around SQD a 417:**

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

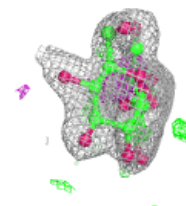
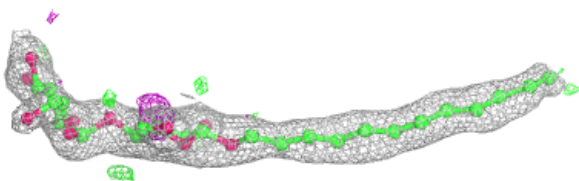
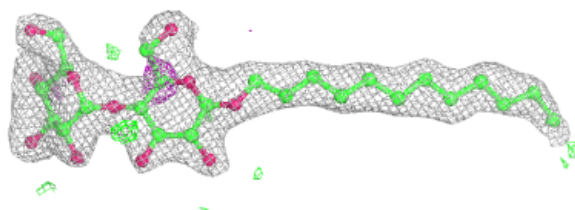


Electron density around HTG C 521:

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

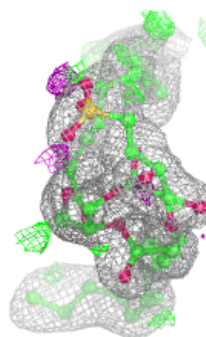
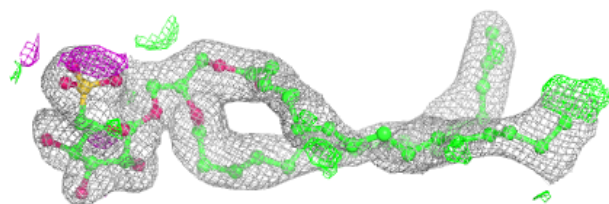
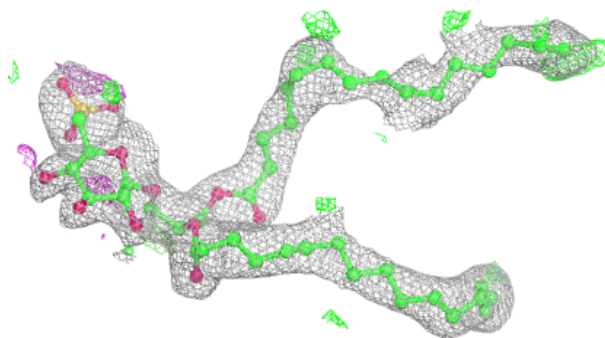
**Electron density around LMT m 104:**

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

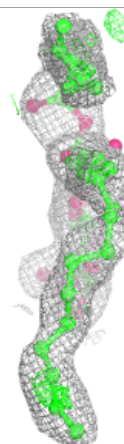
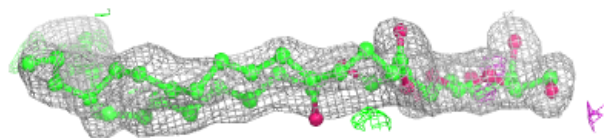
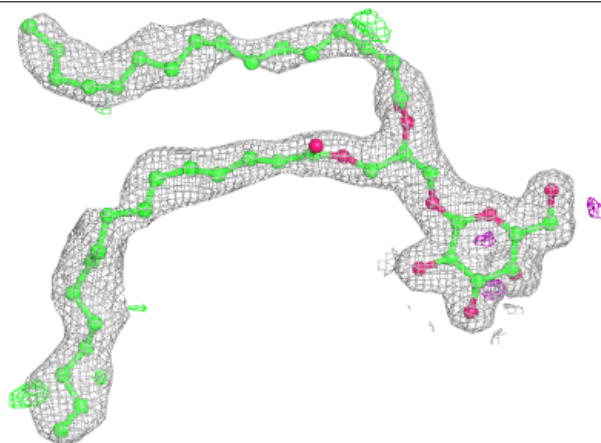


Electron density around SQD A 415:

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

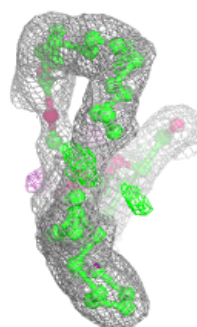
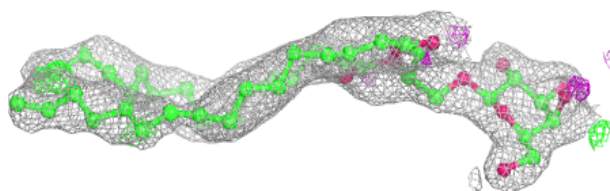
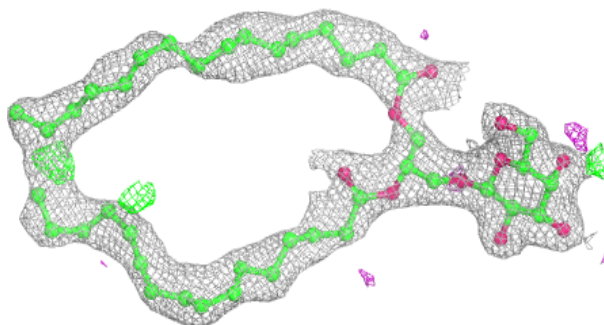
**Electron density around LMG C 520:**

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

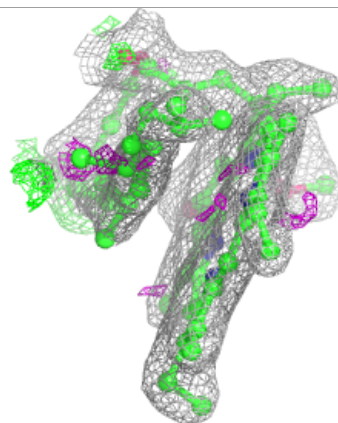
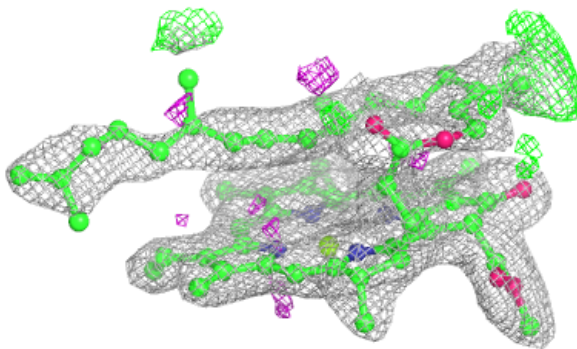
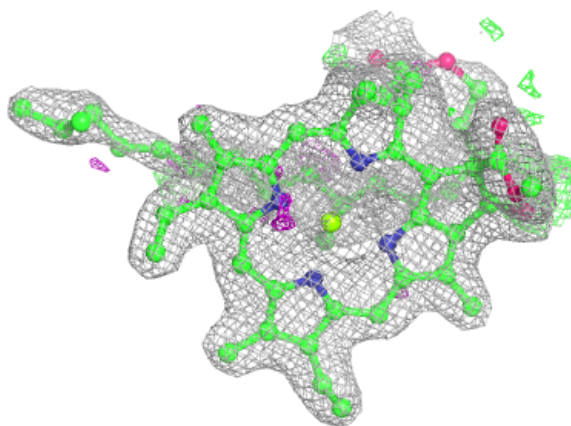


Electron density around LMG a 413:

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

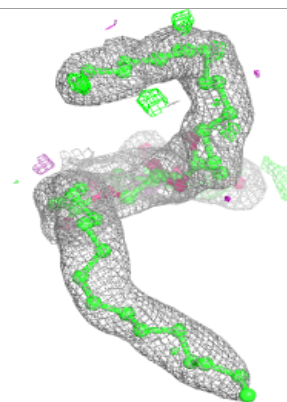
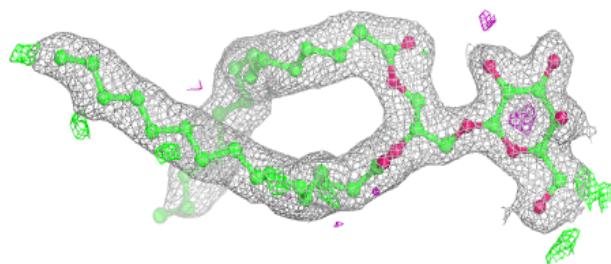
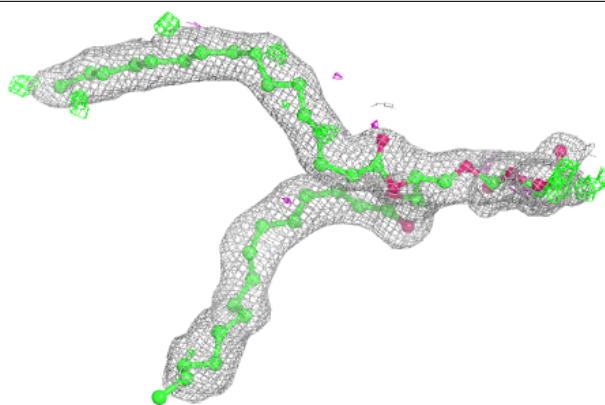
**Electron density around CLA b 602:**

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

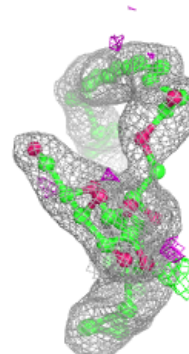
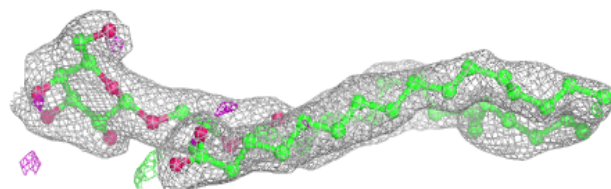
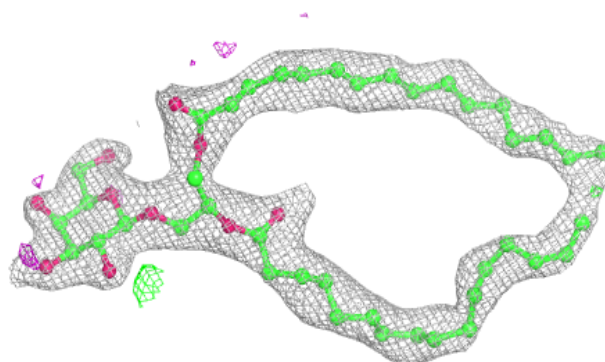


Electron density around LMG B 622:

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

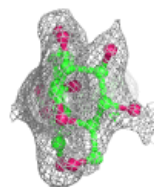
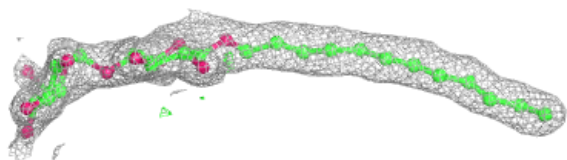
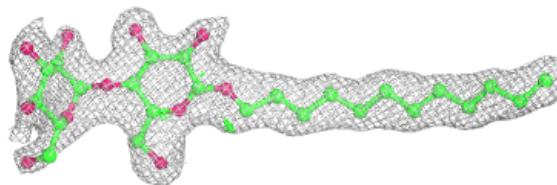
**Electron density around LMG C 501:**

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

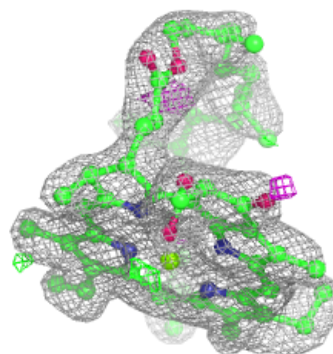
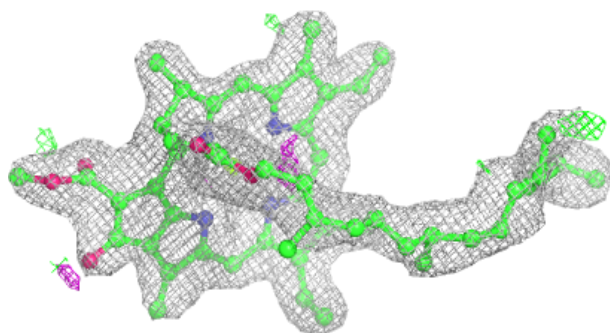
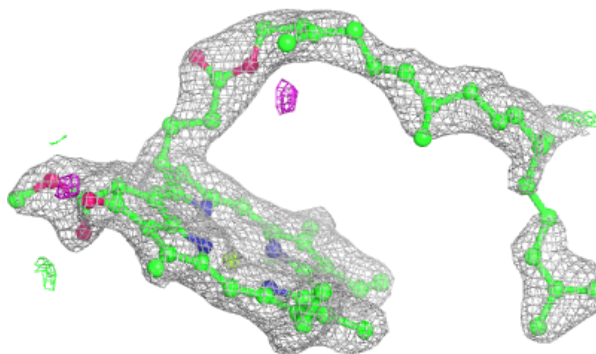


Electron density around LMT M 101:

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

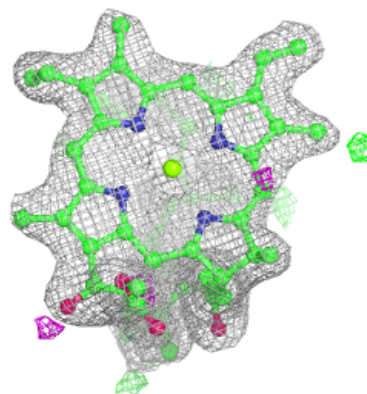
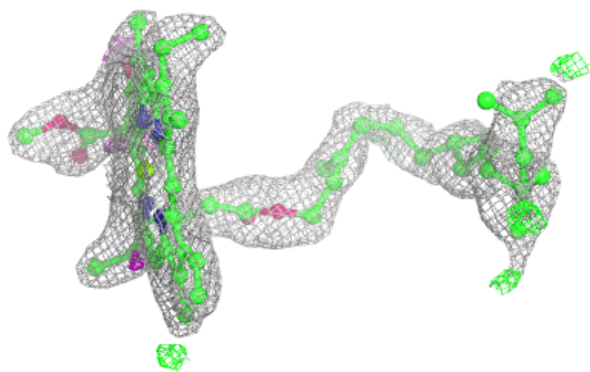
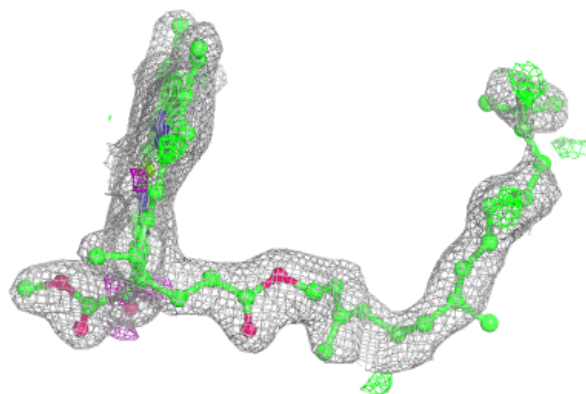
**Electron density around CLA C 514:**

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



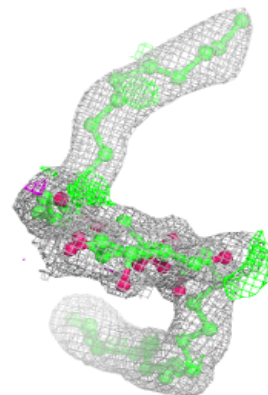
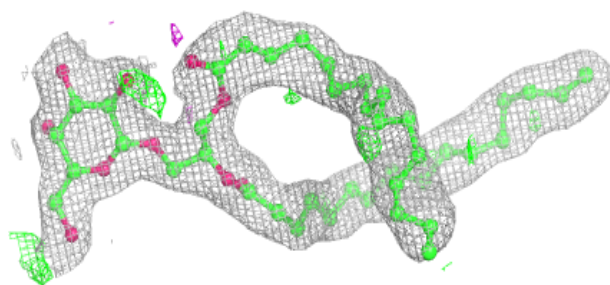
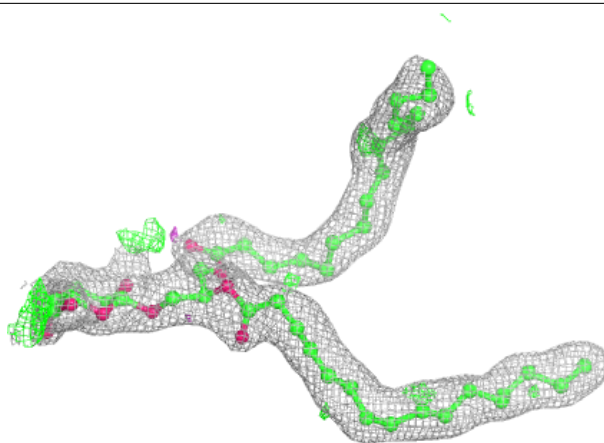
Electron density around CLA C 507:

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

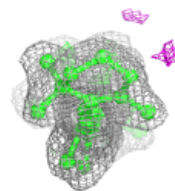
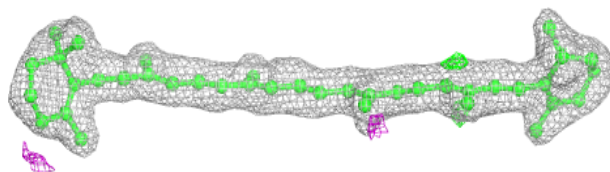
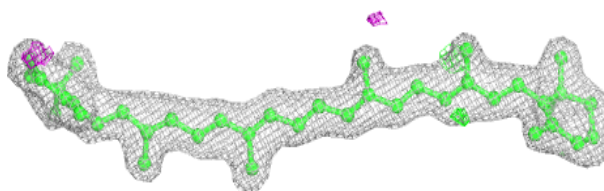


Electron density around LMG m 102:

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

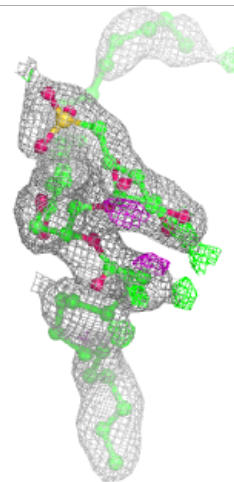
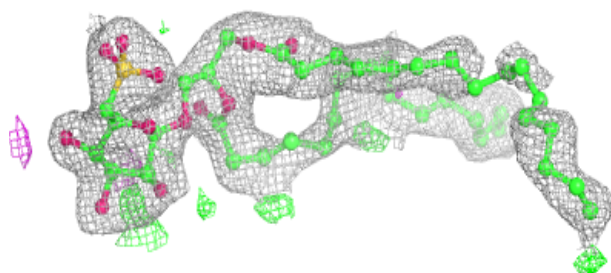
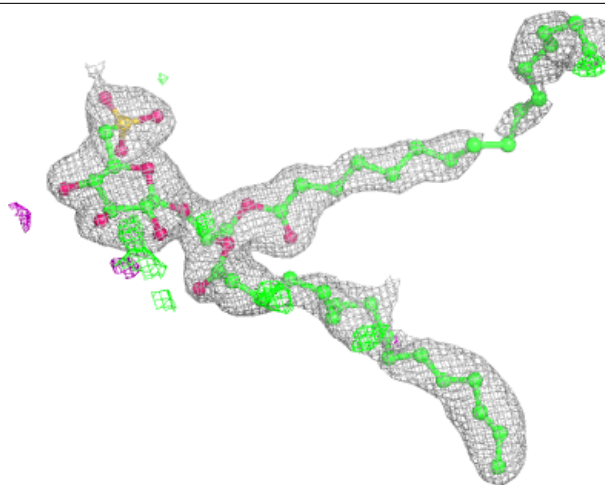
**Electron density around BCR C 515:**

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



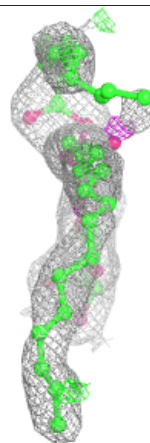
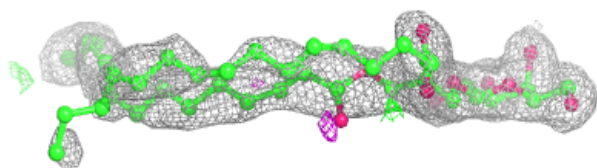
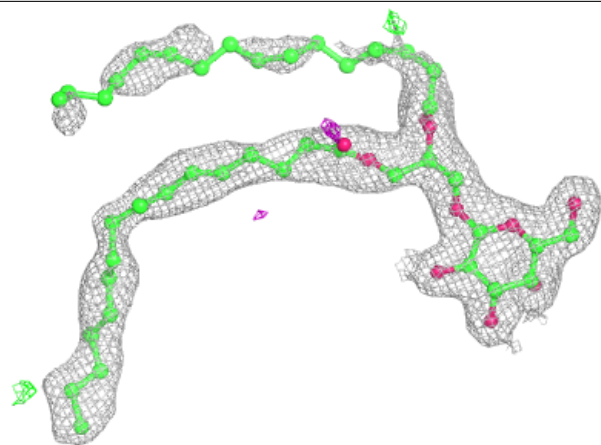
Electron density around SQD A 410:

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



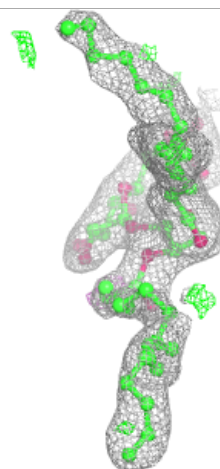
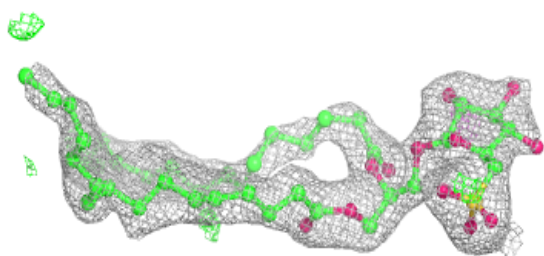
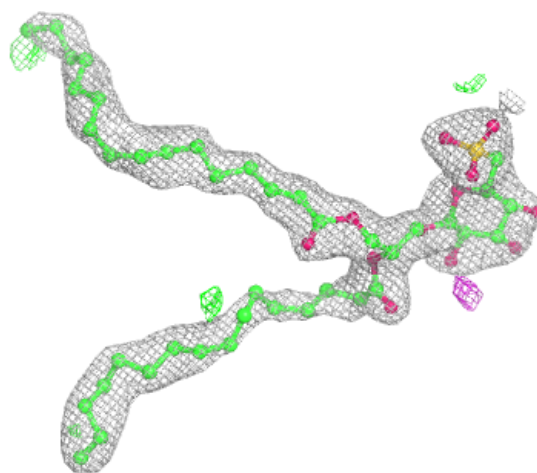
Electron density around LMG c 920:

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



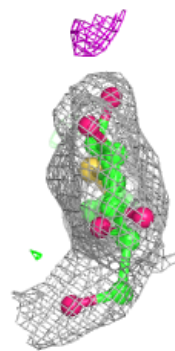
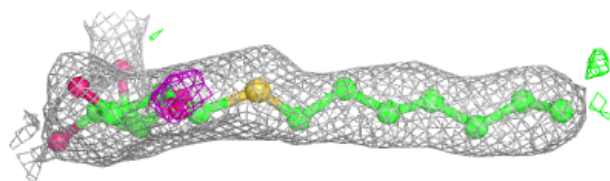
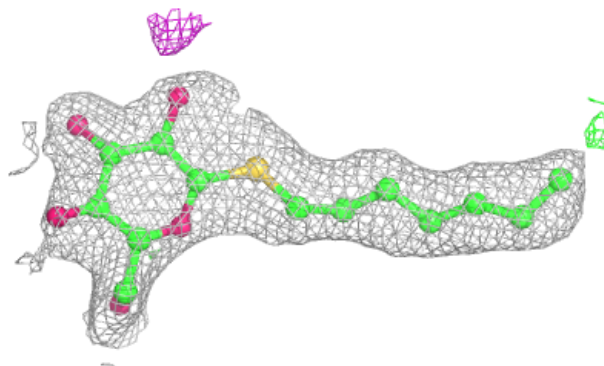
Electron density around SQD a 412:

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

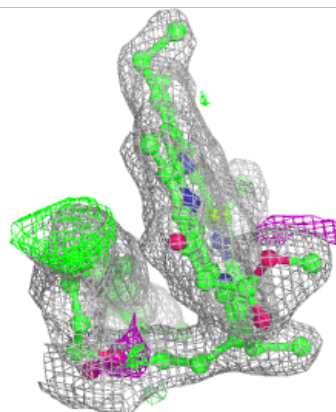
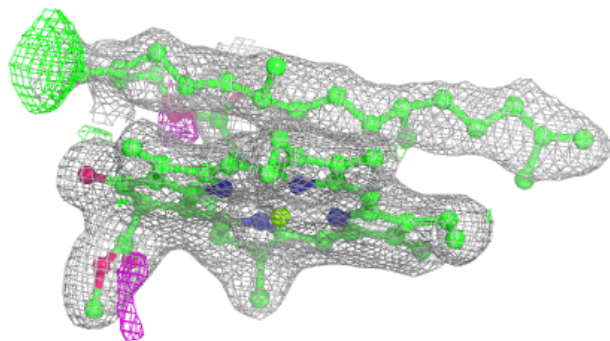
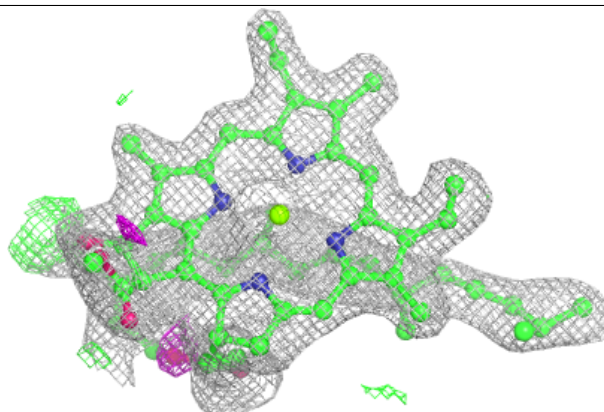


Electron density around HTG B 630:

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

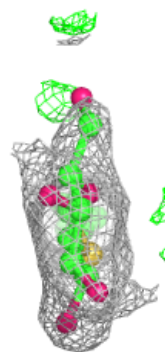
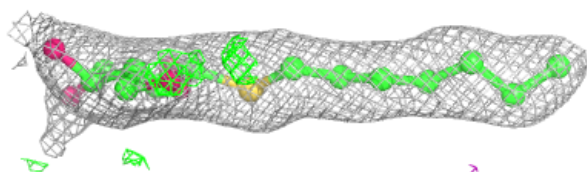
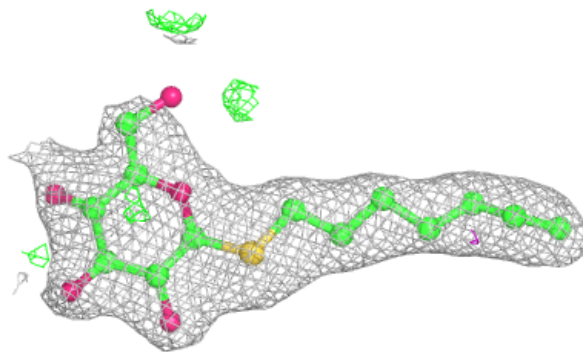
**Electron density around CLA B 602:**

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



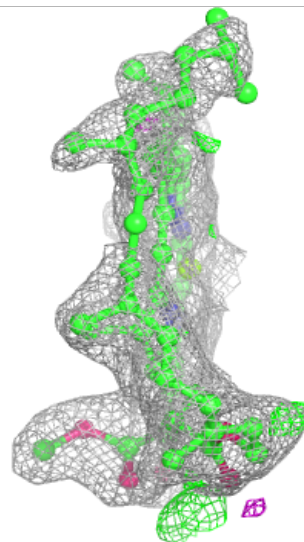
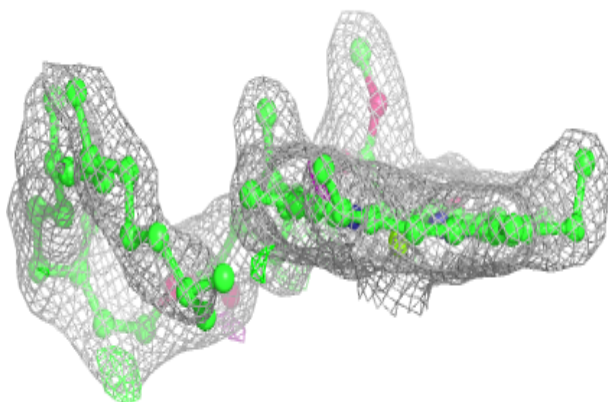
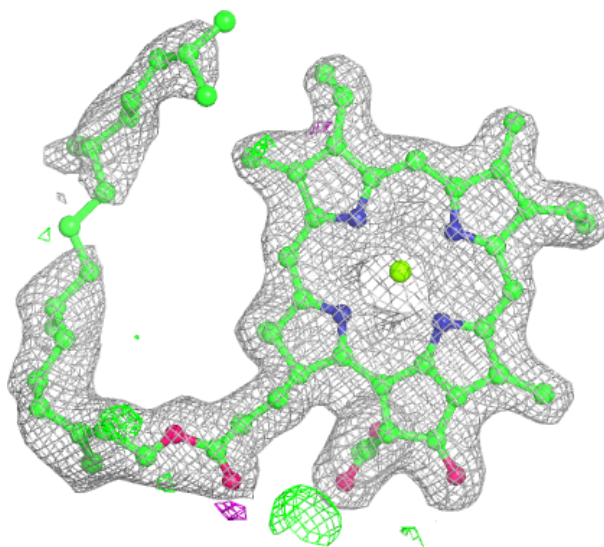
Electron density around HTG b 627:

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



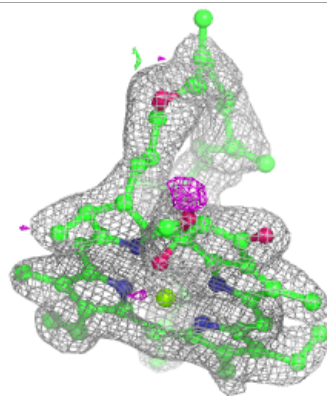
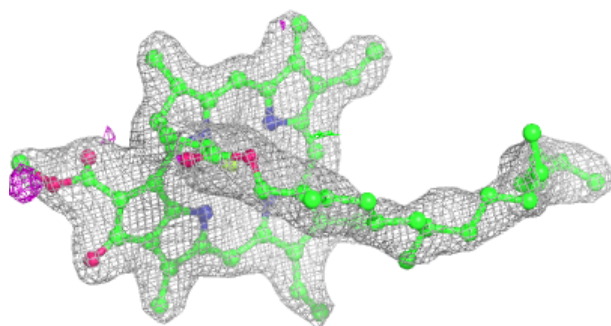
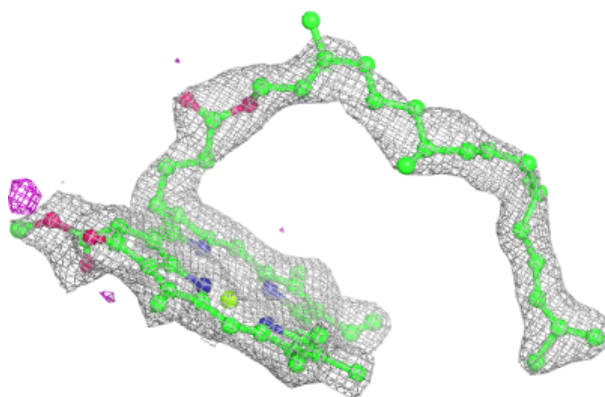
Electron density around CLA c 913:

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



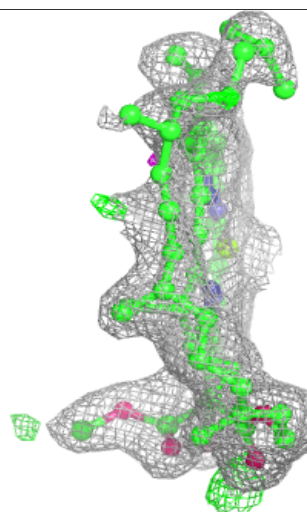
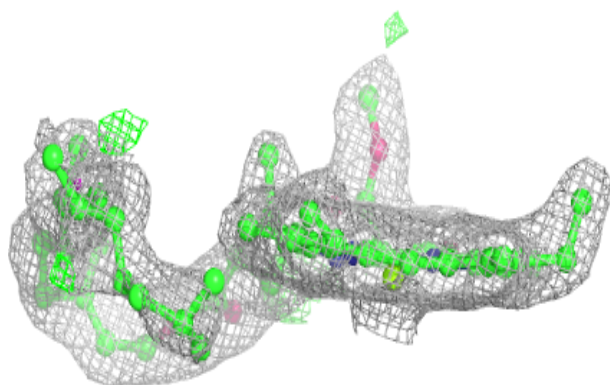
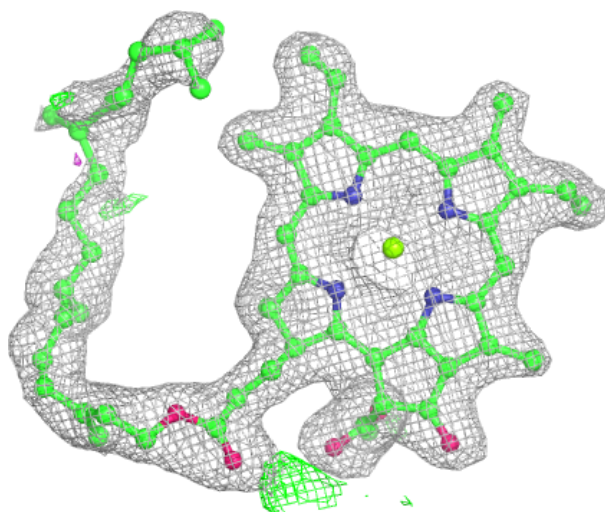
Electron density around CLA c 914:

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



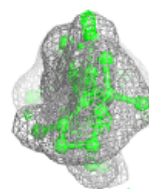
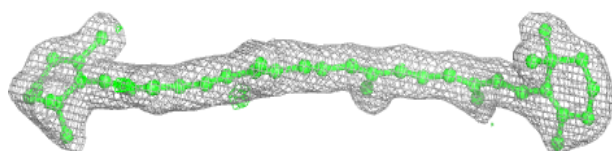
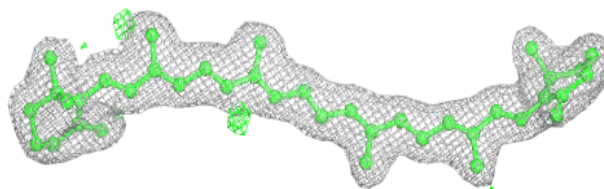
Electron density around CLA C 513:

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

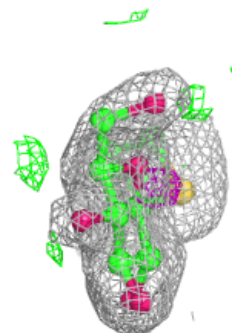
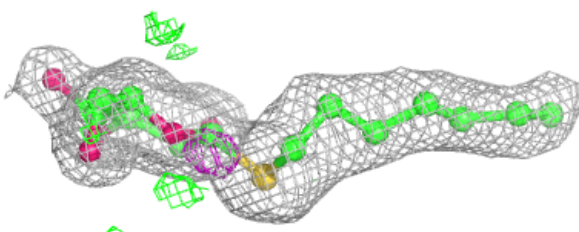
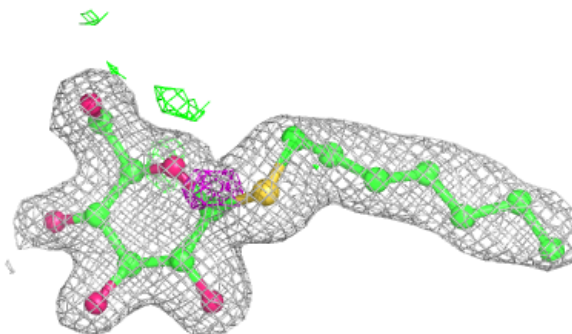


Electron density around BCR Y 101:

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

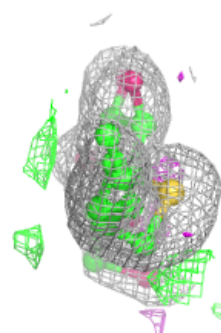
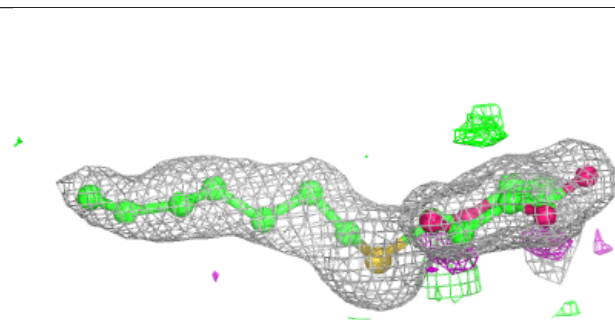
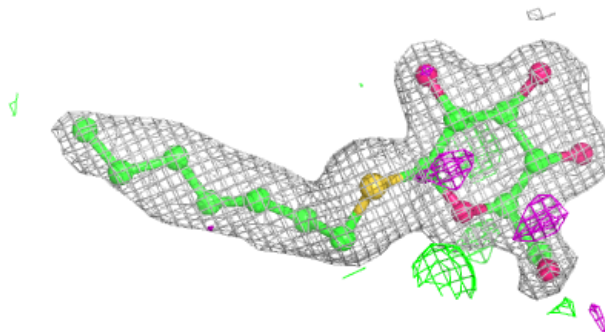
**Electron density around HTG O 302:**

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

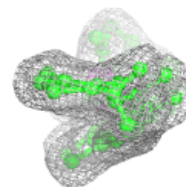
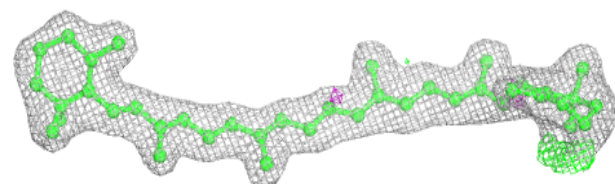
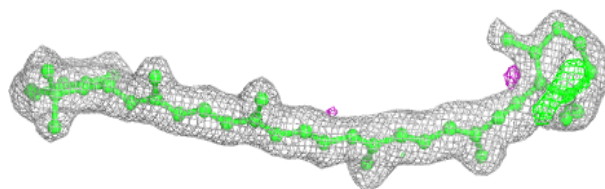


Electron density around HTG B 624:

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

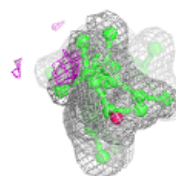
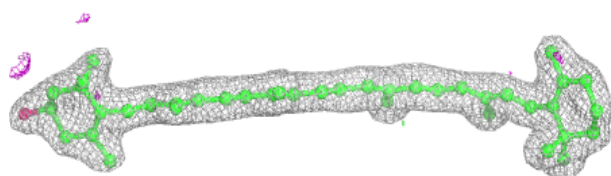
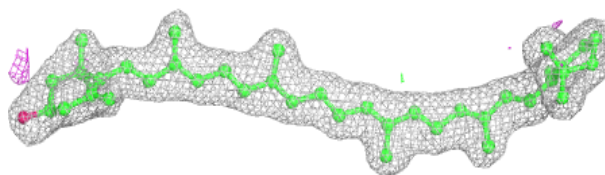
**Electron density around BCR d 405:**

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

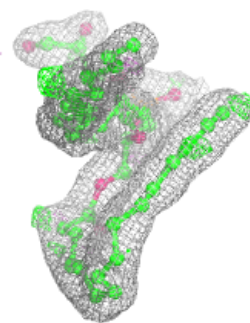
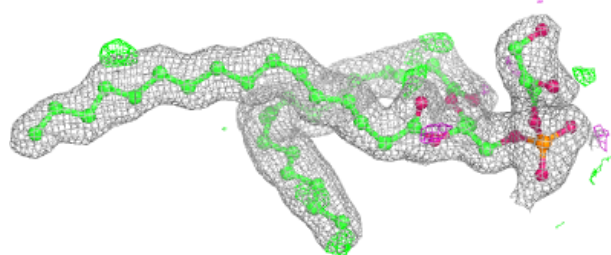
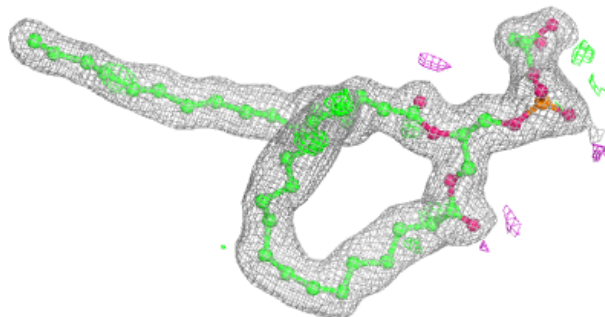


Electron density around RRX H 102:

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

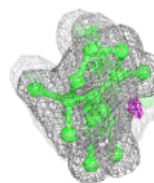
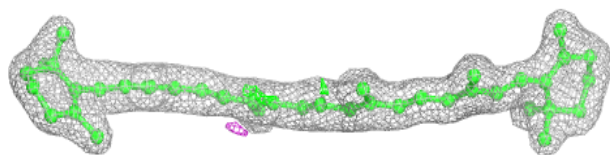
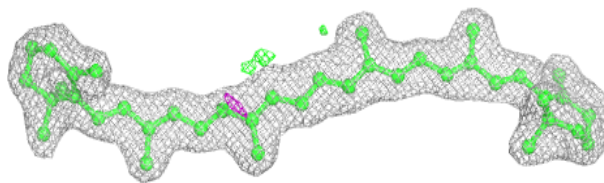
**Electron density around LHG D 409:**

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

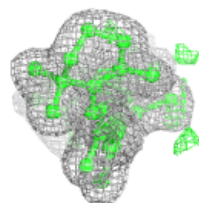
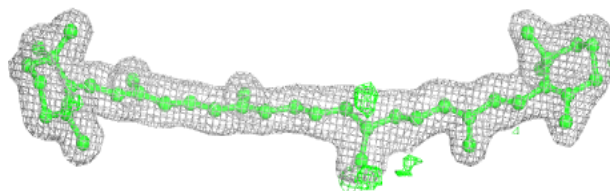
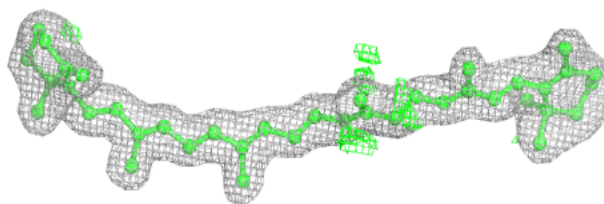


Electron density around BCR j 104:

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

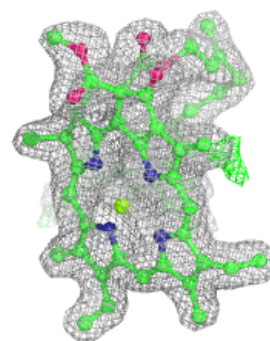
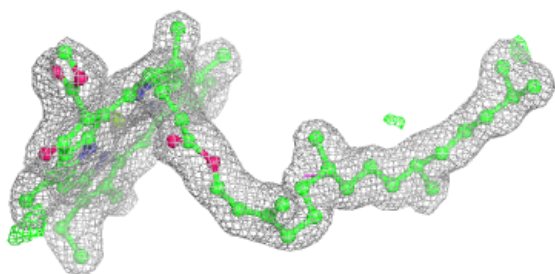
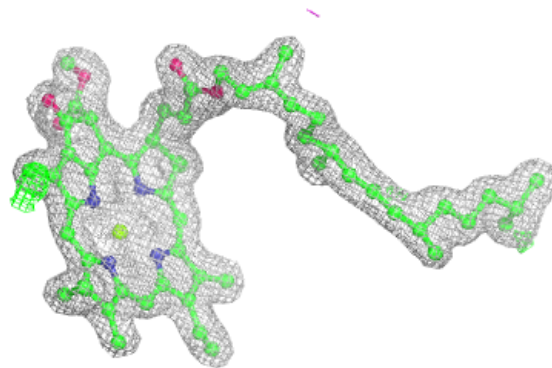
**Electron density around BCR t 101:**

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



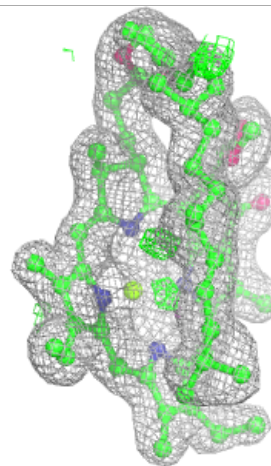
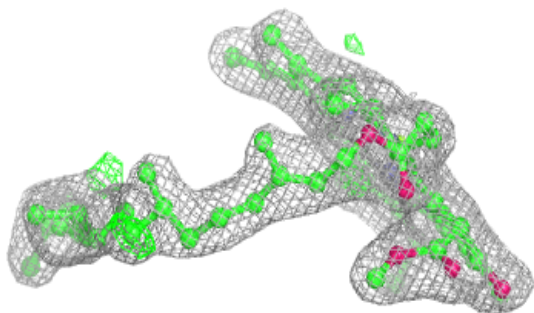
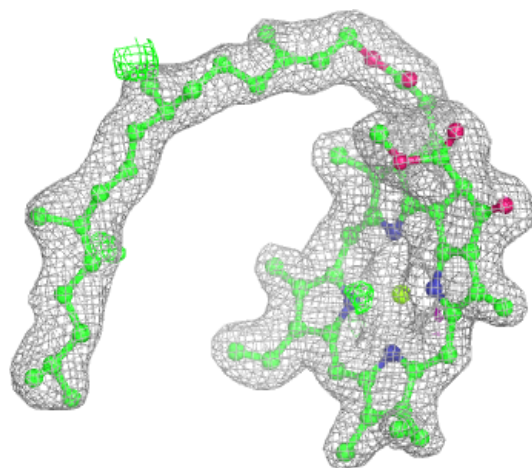
Electron density around CLA C 512:

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



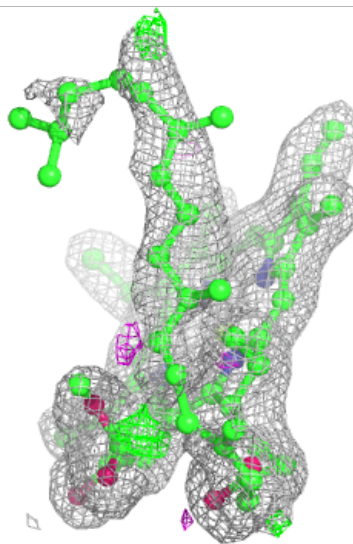
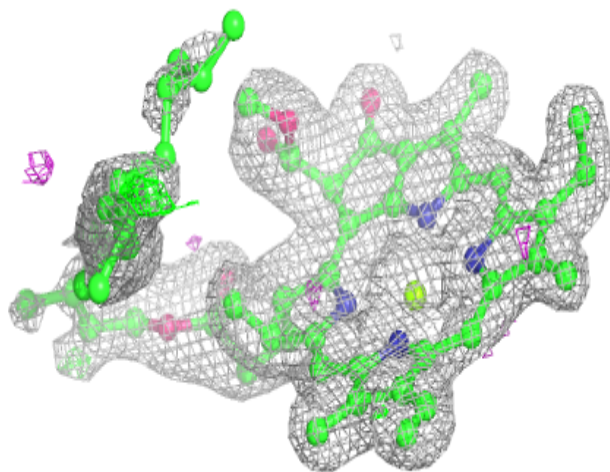
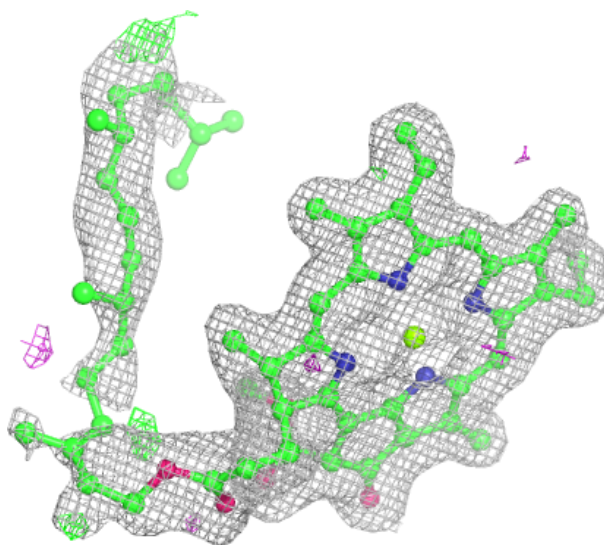
Electron density around CLA C 508:

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



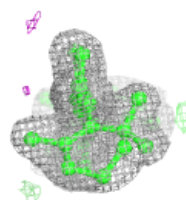
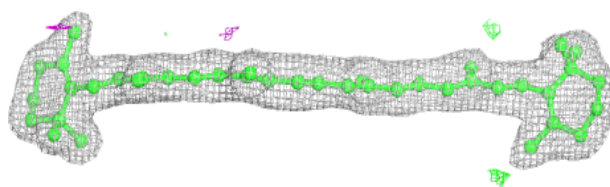
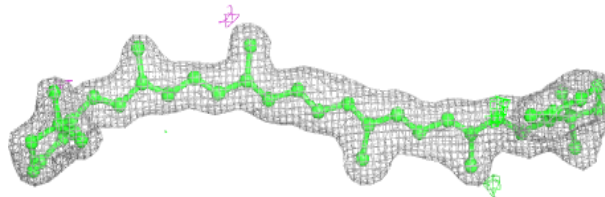
Electron density around CLA b 617:

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

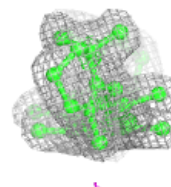
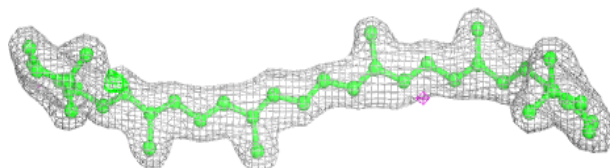
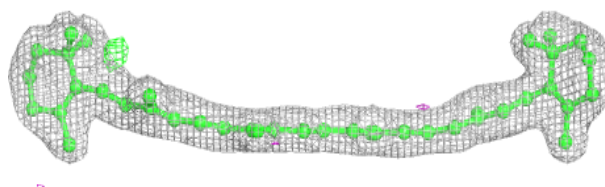


Electron density around BCR C 516:

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

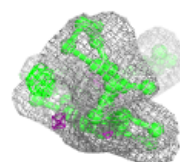
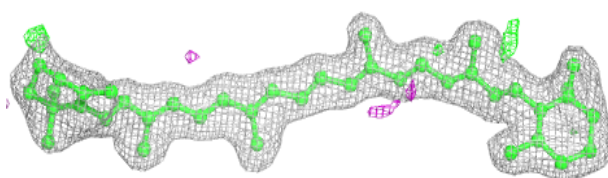
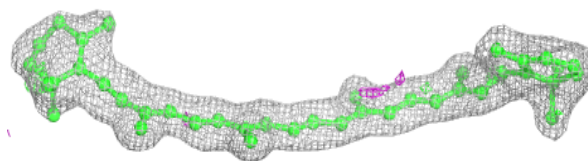
**Electron density around BCR C 530:**

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

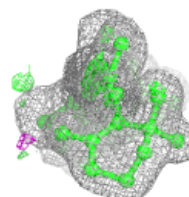
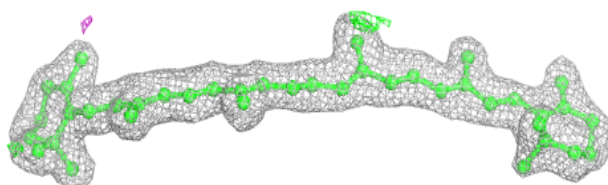
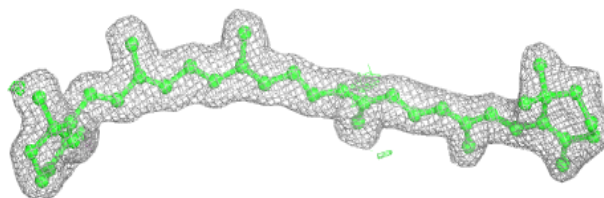


Electron density around BCR D 405:

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

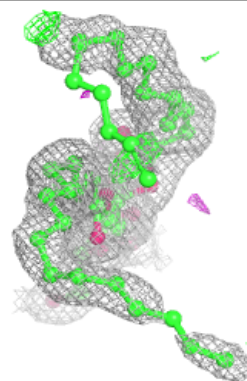
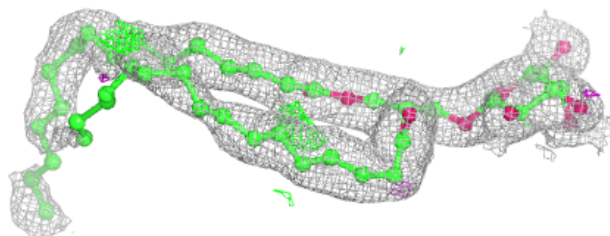
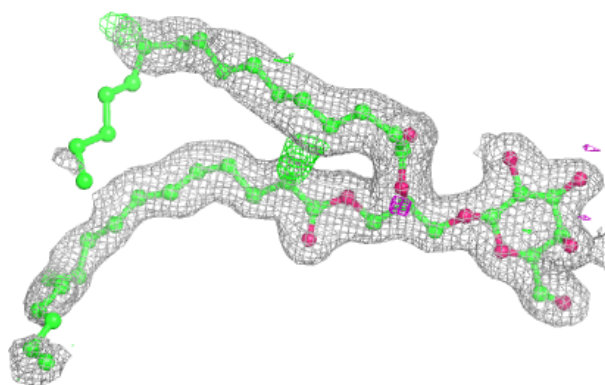
**Electron density around BCR T 101:**

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

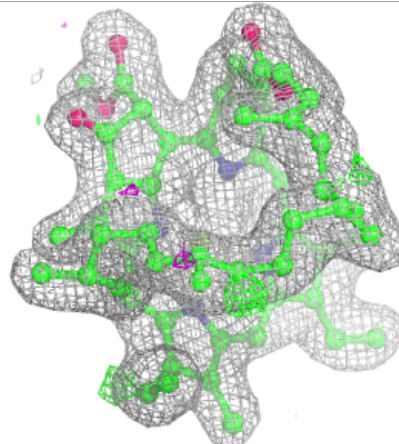
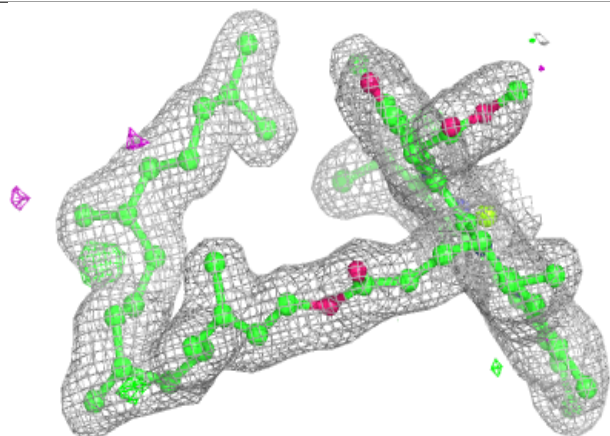
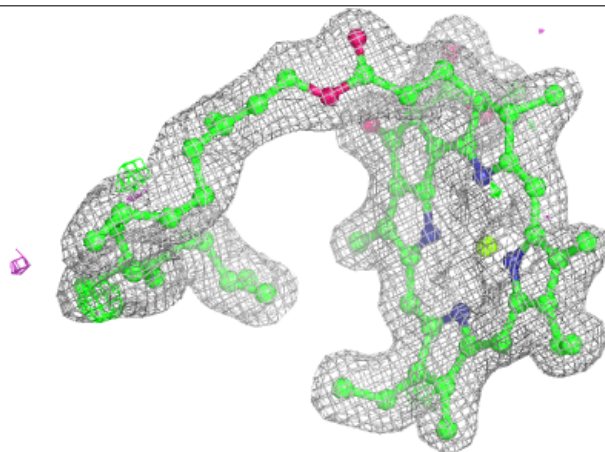


Electron density around LMG J 101:

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

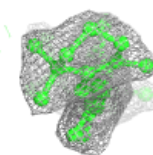
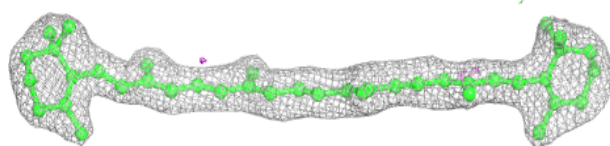
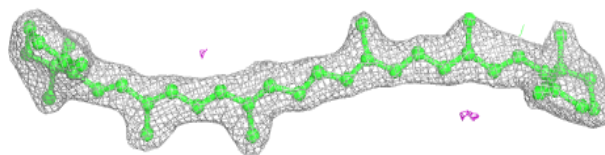
**Electron density around CLA c 904:**

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

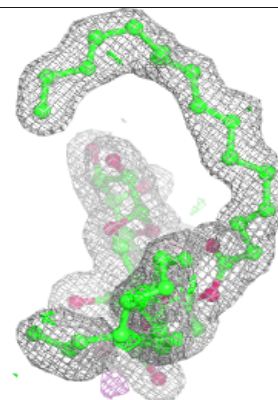
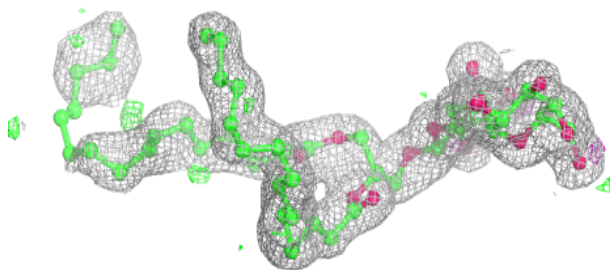
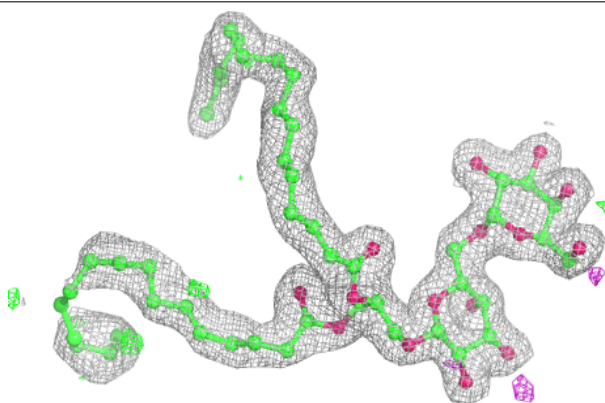


Electron density around BCR c 915:

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

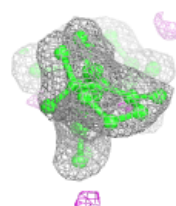
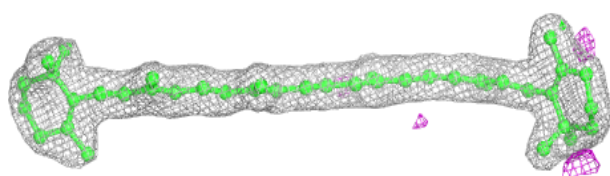
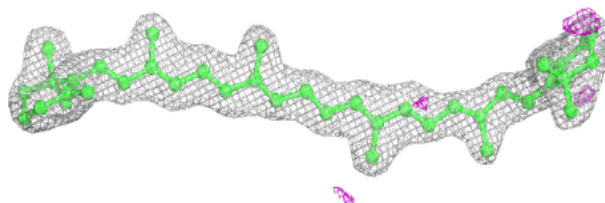
**Electron density around DGD C 518:**

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

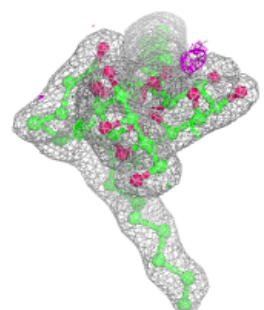
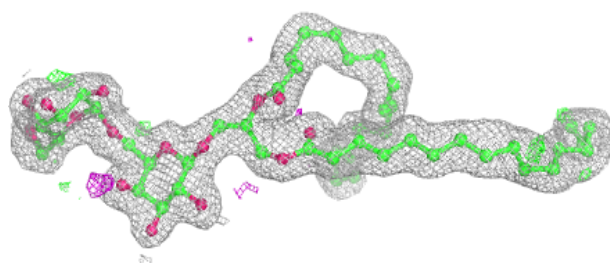
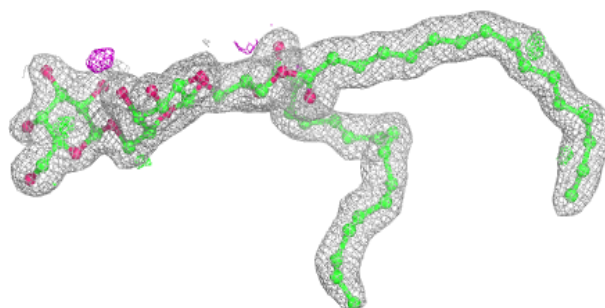


Electron density around BCR c 916:

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

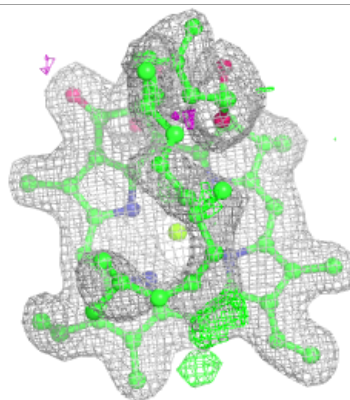
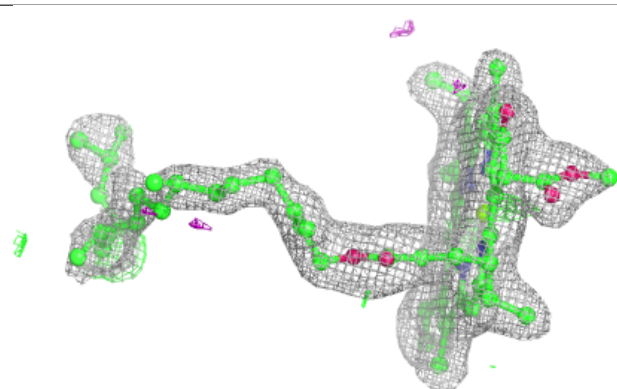
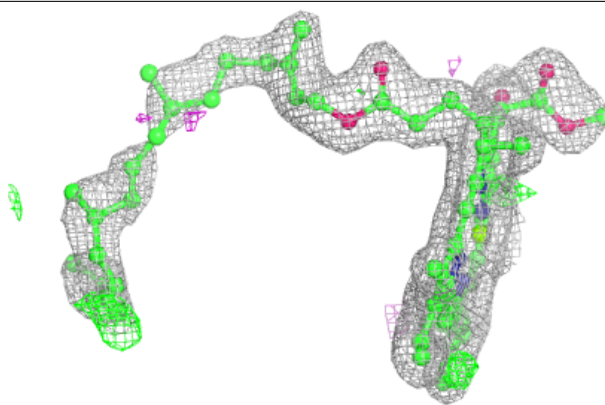
**Electron density around DGD H 103:**

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

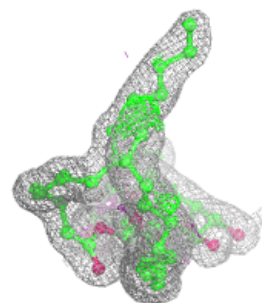
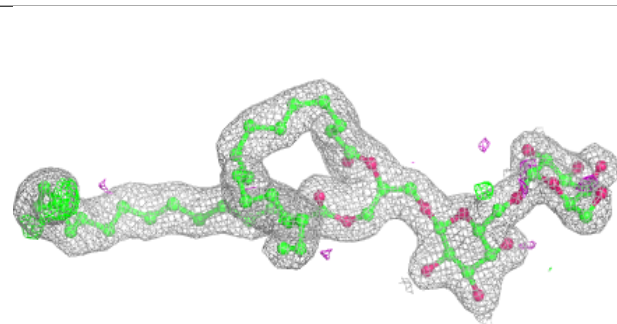
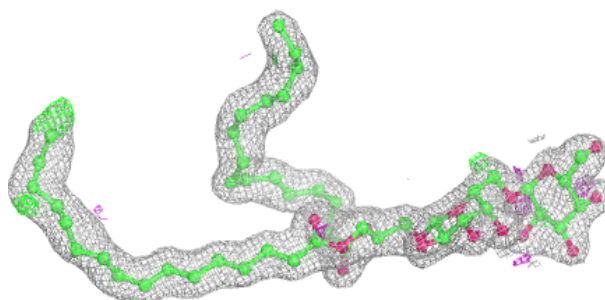


Electron density around CLA c 907:

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

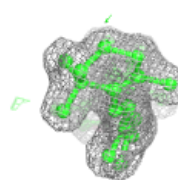
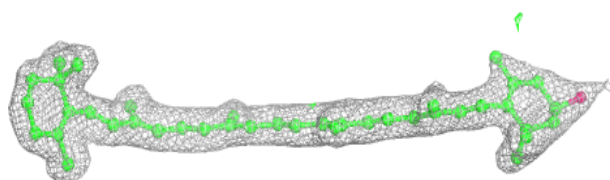
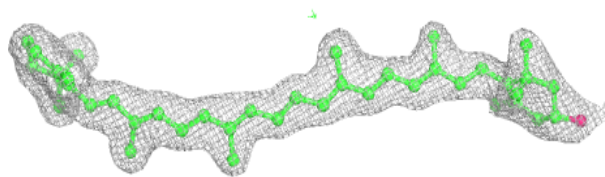
**Electron density around DGD h 102:**

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



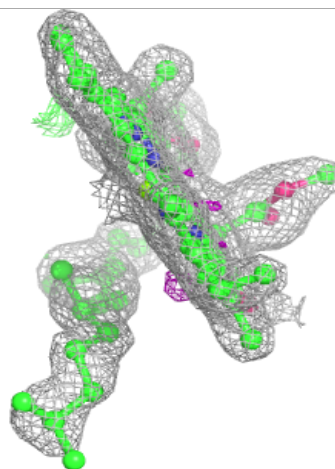
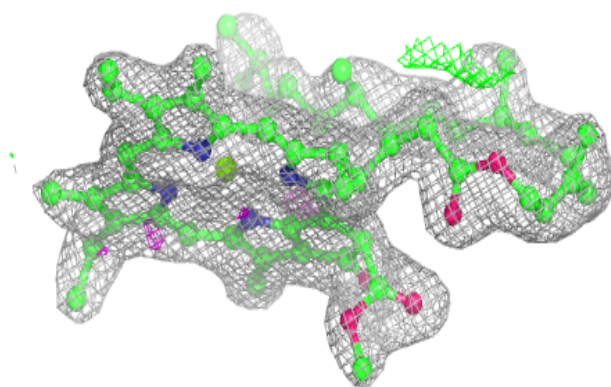
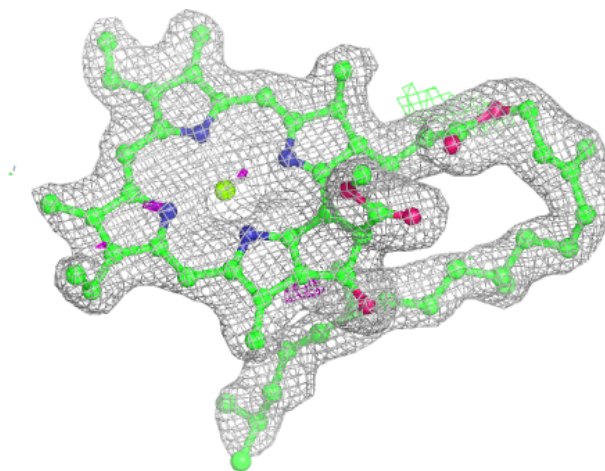
Electron density around RRX x 102:

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



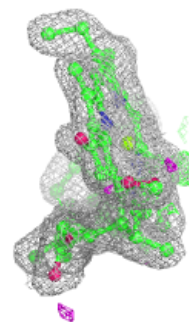
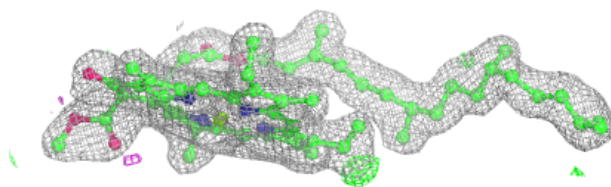
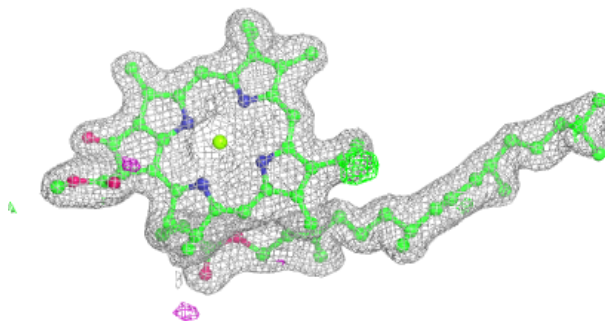
Electron density around CLA C 510:

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

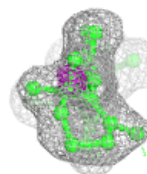
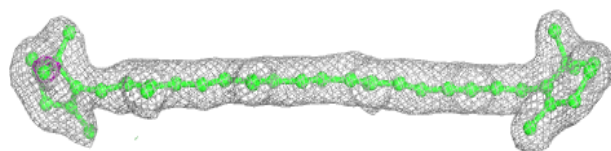
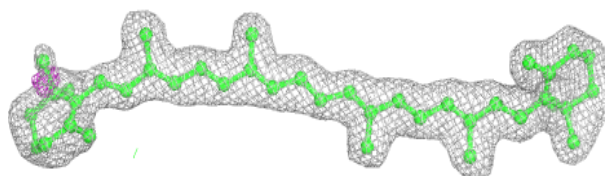


Electron density around CLA C 502:

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

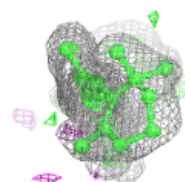
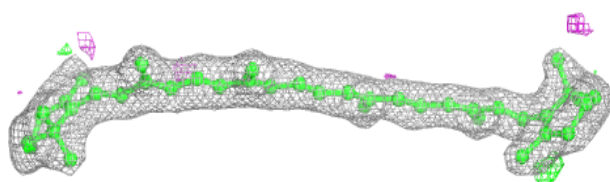
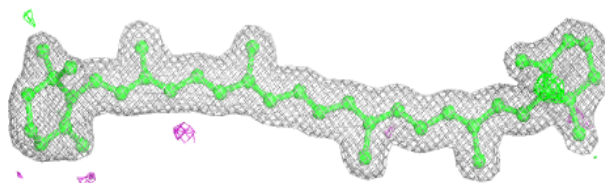
**Electron density around BCR B 619:**

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

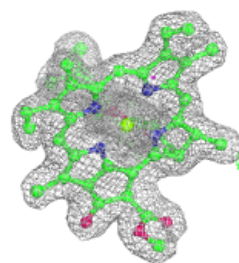
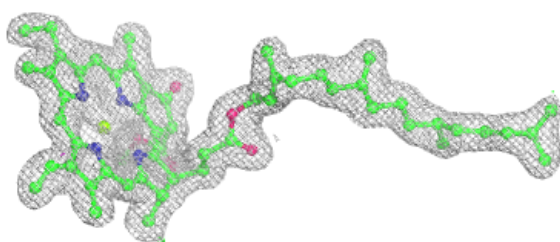
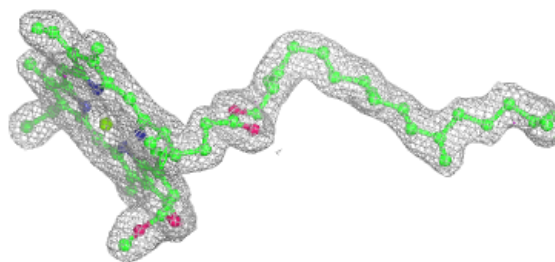


Electron density around BCR B 620:

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

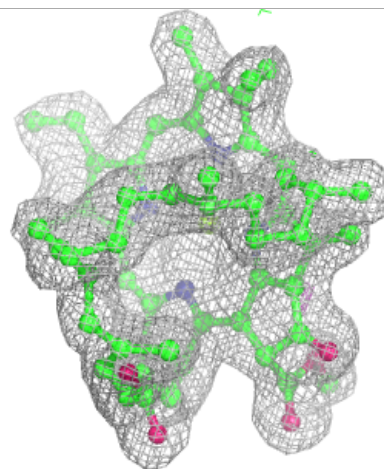
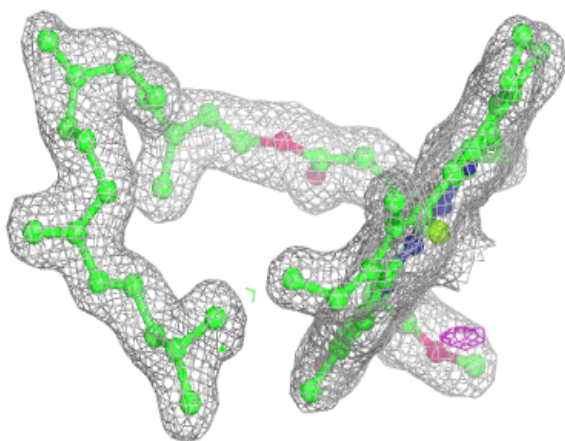
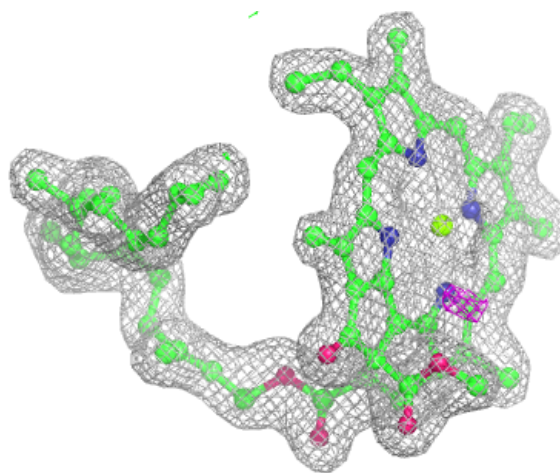
**Electron density around CLA C 503:**

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



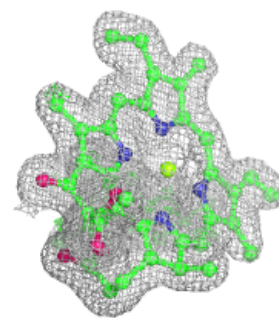
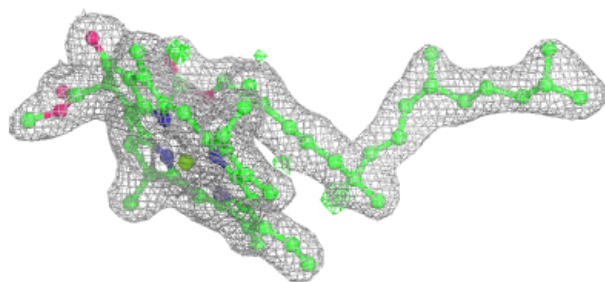
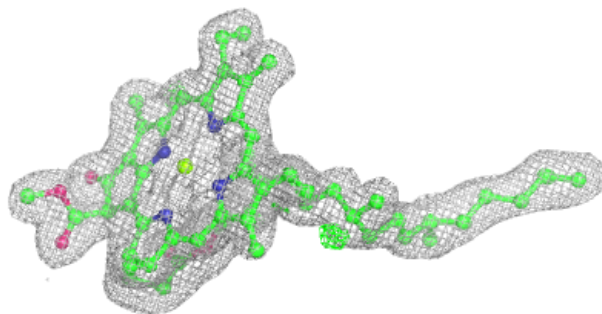
Electron density around CLA C 504:

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



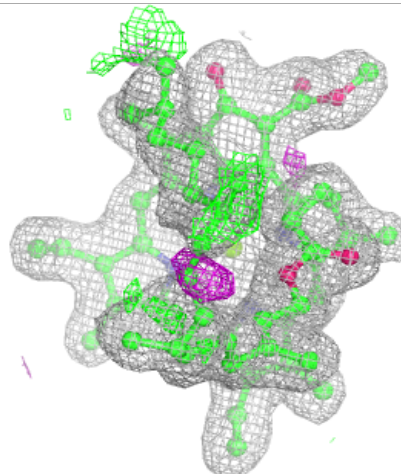
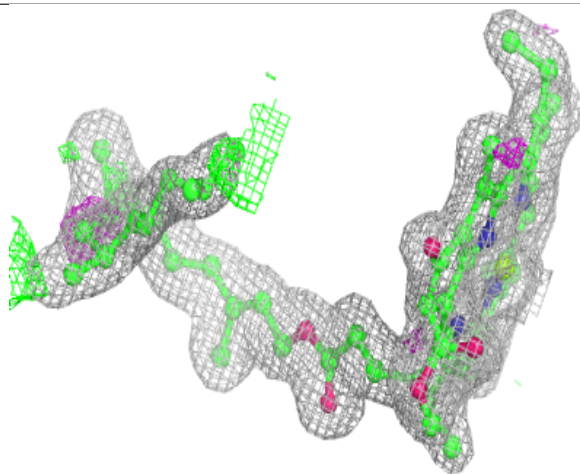
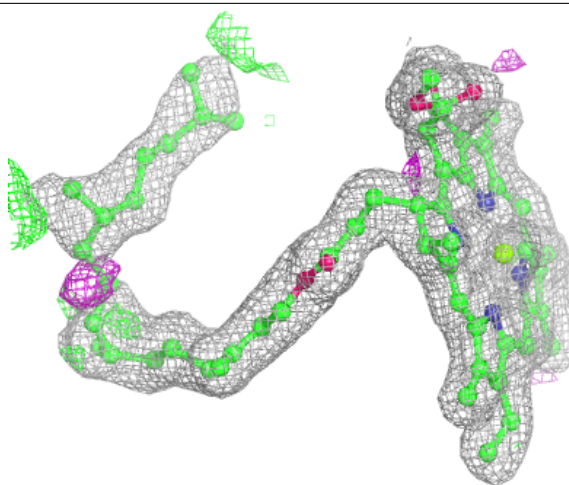
Electron density around CLA C 506:

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



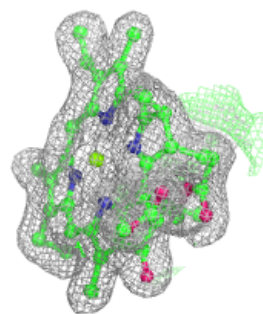
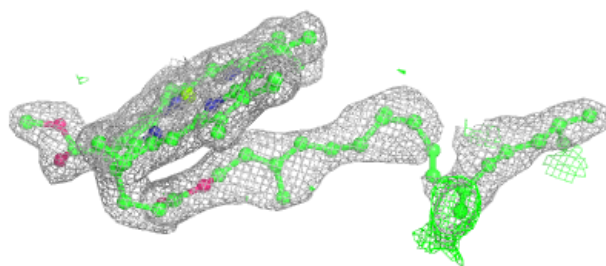
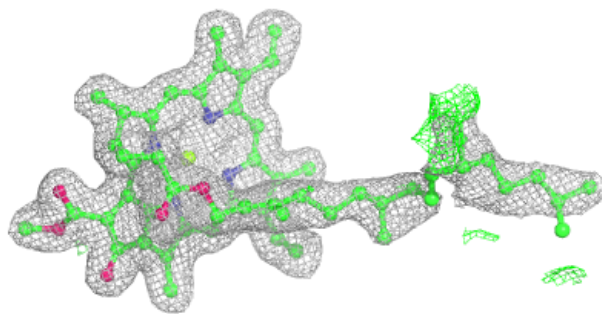
Electron density around CLA b 607:

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



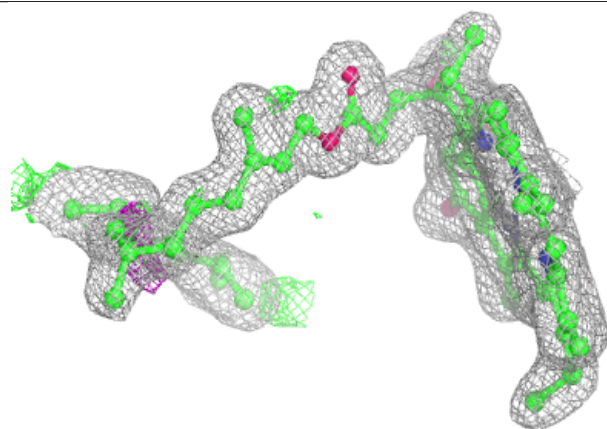
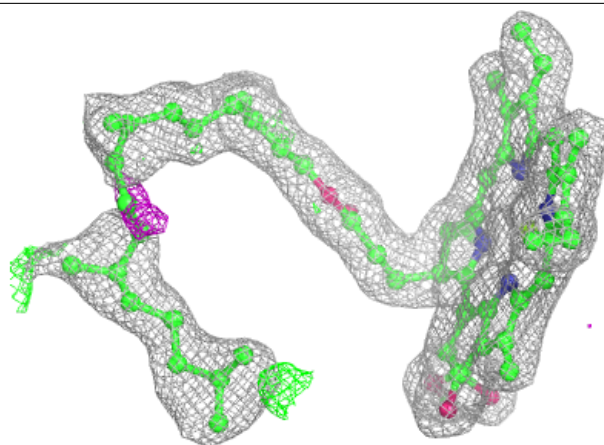
Electron density around CLA b 615:

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

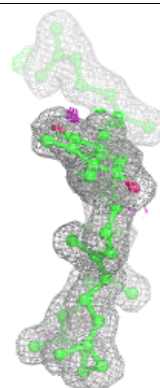
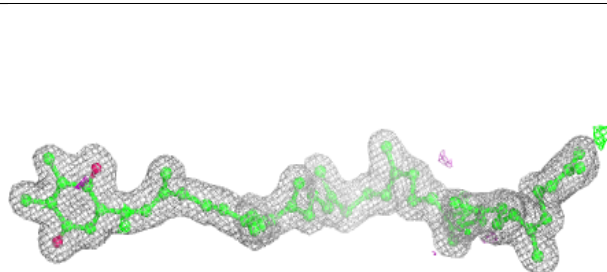
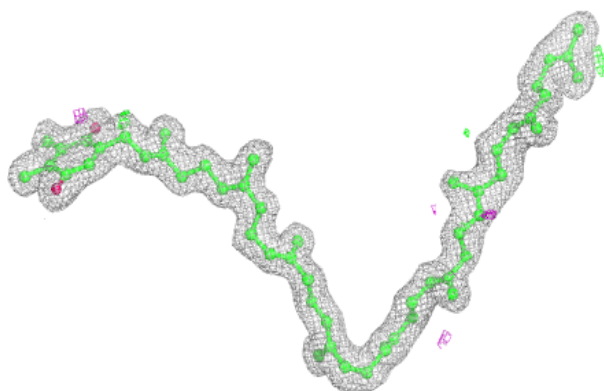


Electron density around CLA B 607:

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

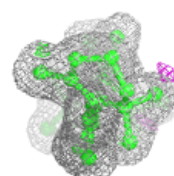
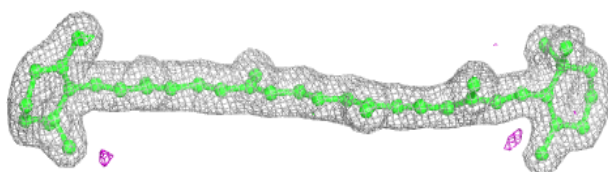
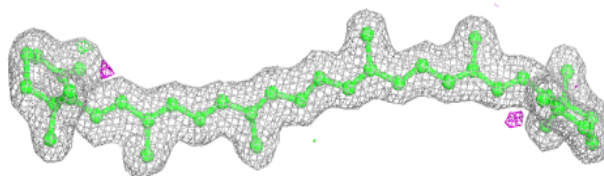
**Electron density around PL9 D 406:**

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

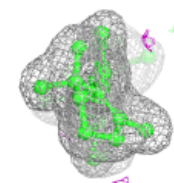
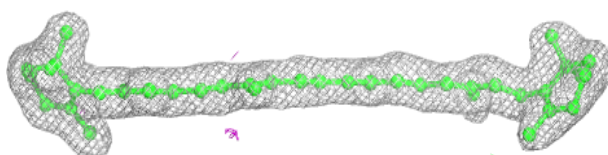
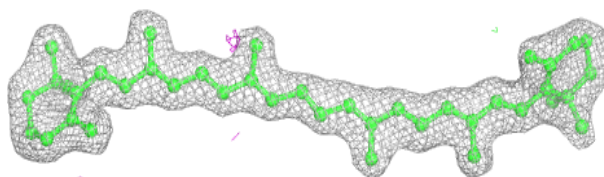


Electron density around BCR a 411:

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

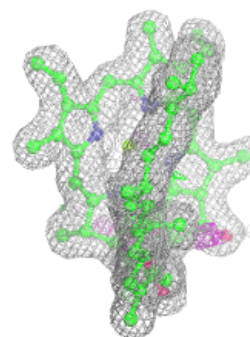
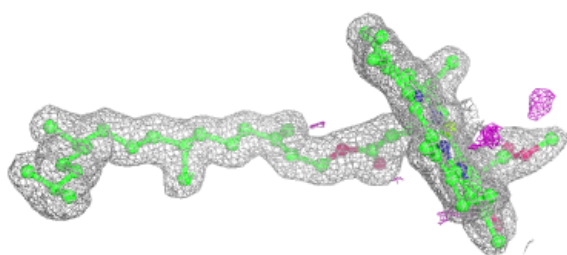
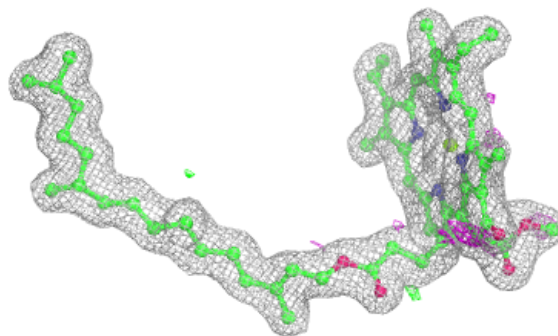
**Electron density around BCR b 619:**

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

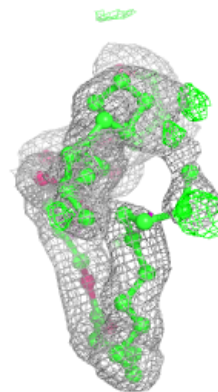
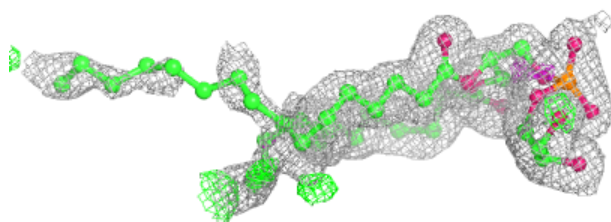
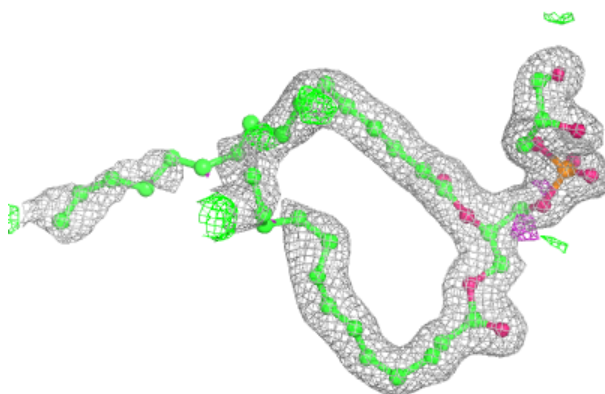


Electron density around CLA B 610:

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

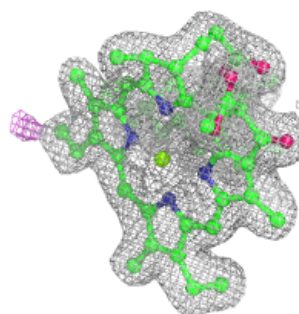
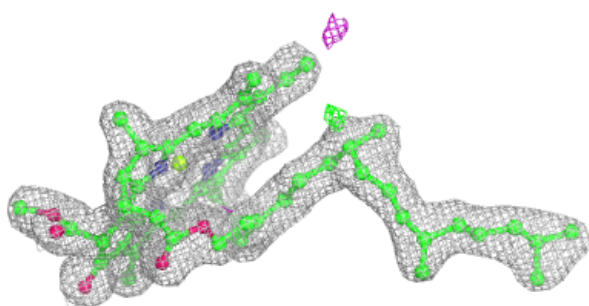
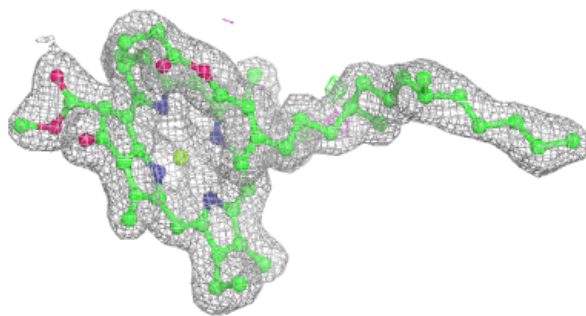
**Electron density around LHG D 411:**

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

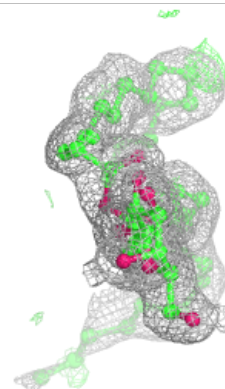
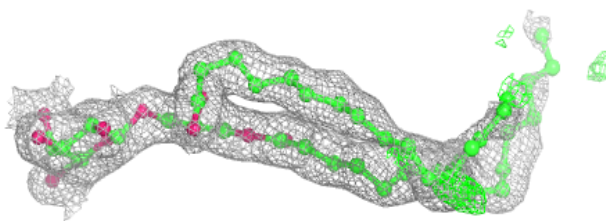
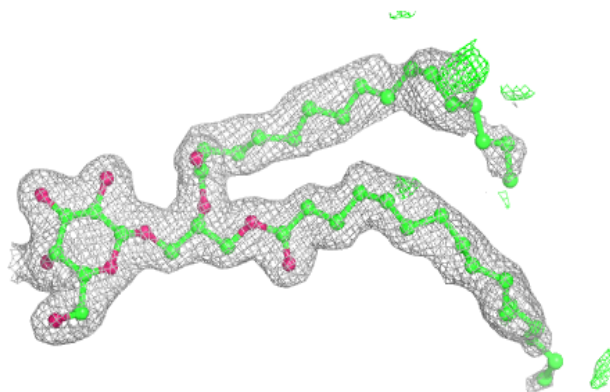


Electron density around CLA c 906:

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

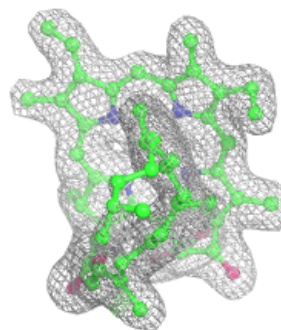
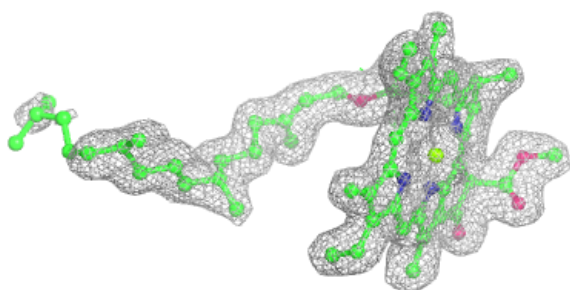
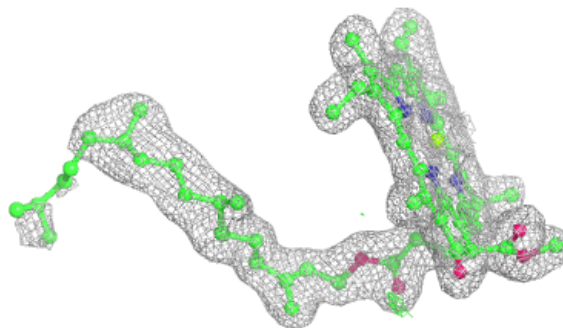
**Electron density around LMG j 101:**

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



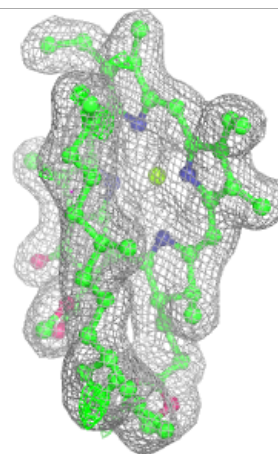
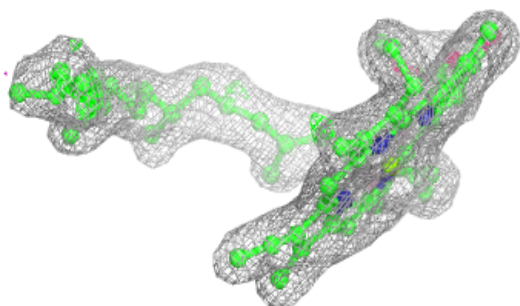
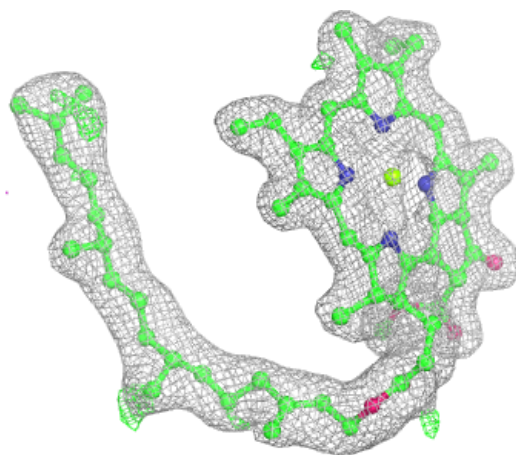
Electron density around CLA C 509:

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



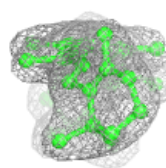
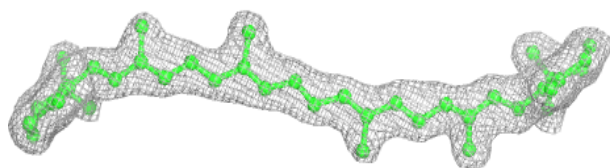
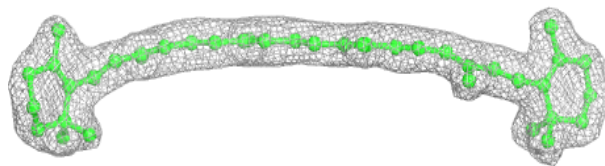
Electron density around CLA c 908:

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

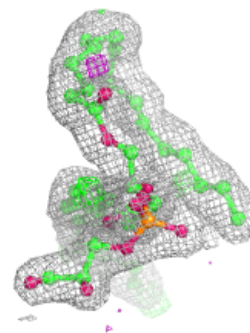
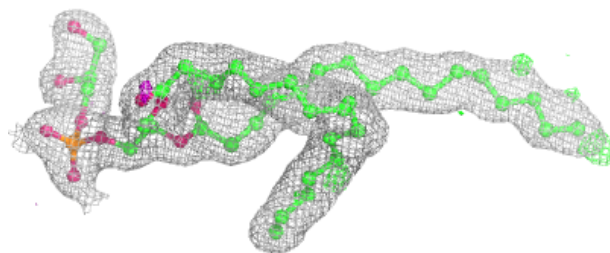
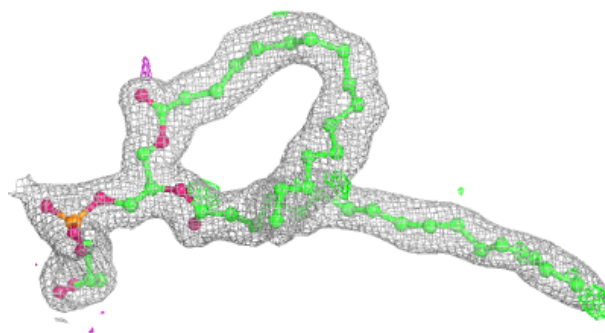


Electron density around BCR k 102:

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

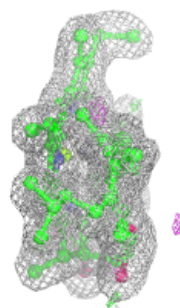
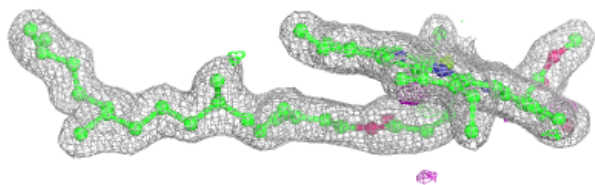
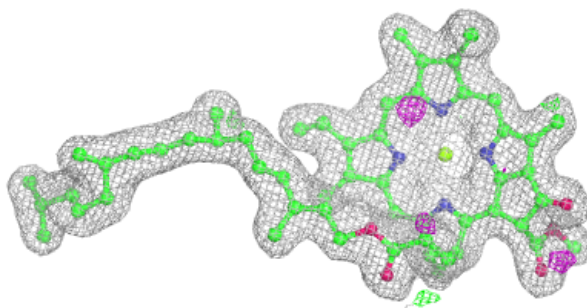
**Electron density around LHG d 408:**

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



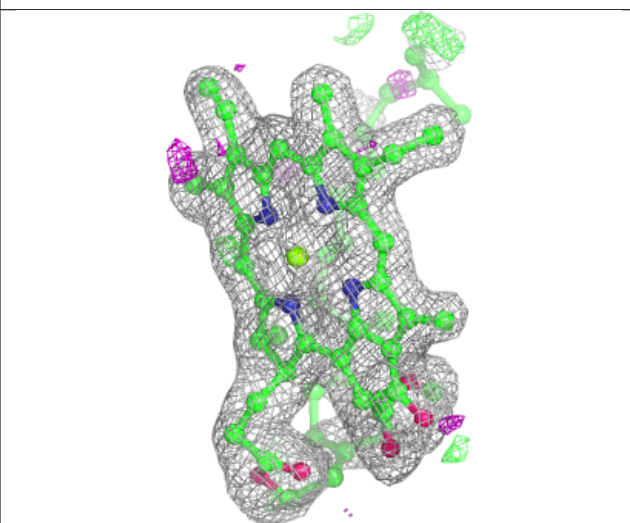
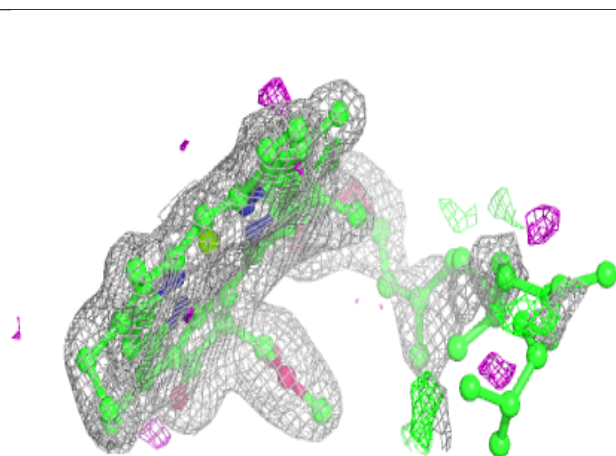
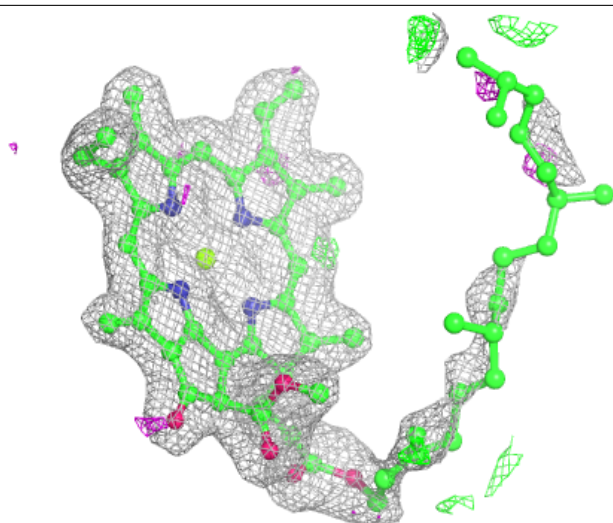
Electron density around CLA b 604:

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



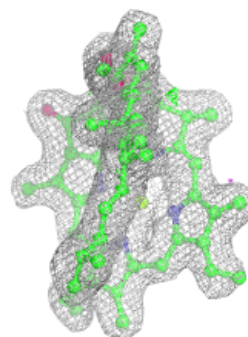
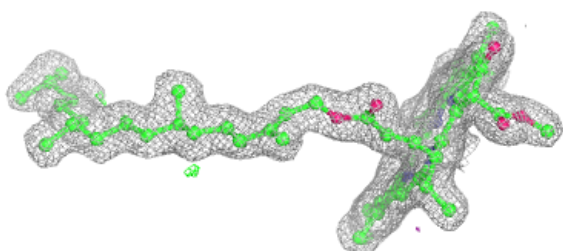
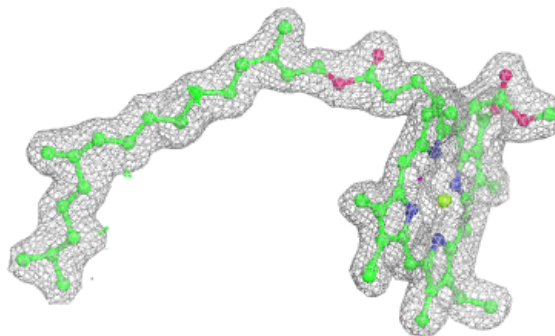
Electron density around CLA B 617:

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

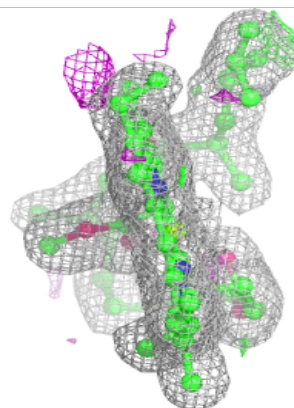
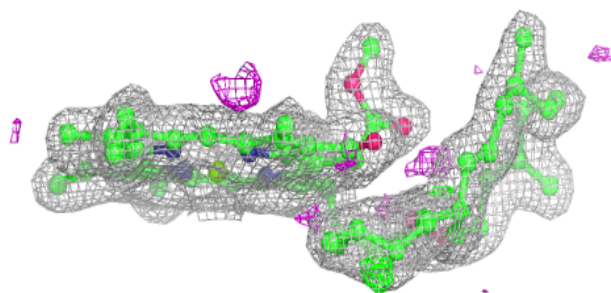
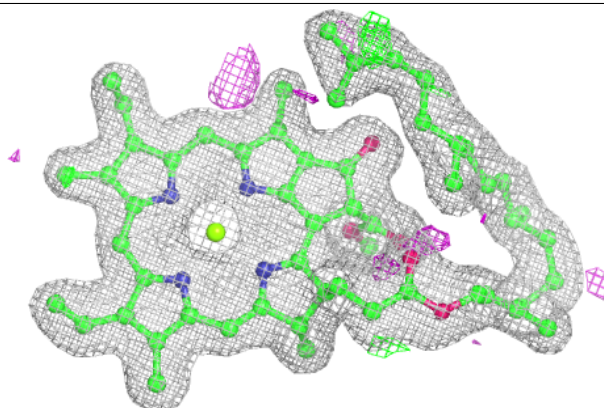


Electron density around CLA b 610:

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

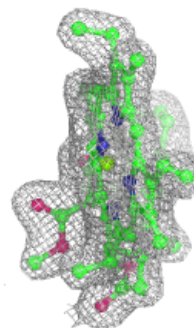
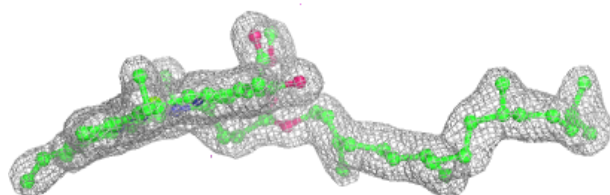
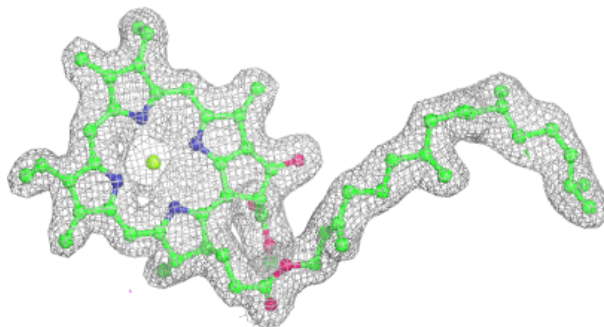
**Electron density around CLA b 611:**

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



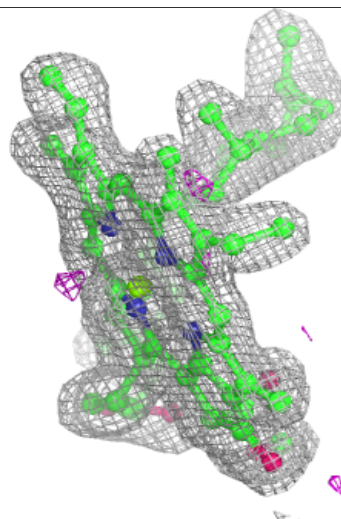
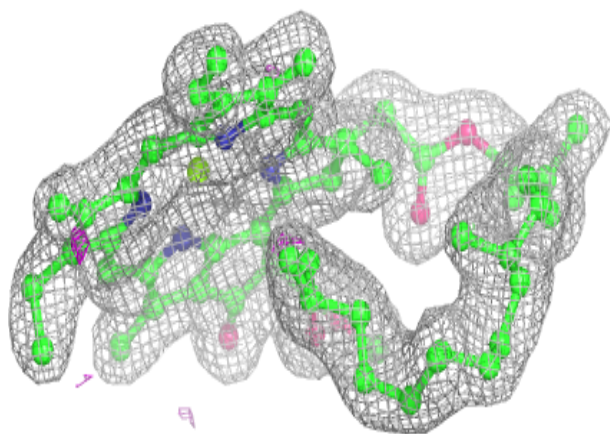
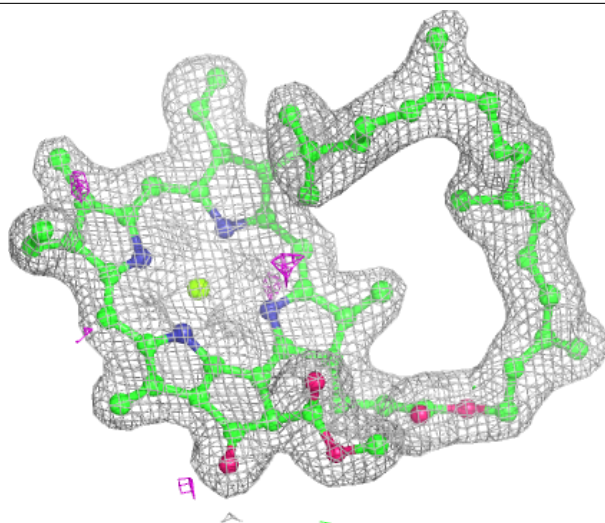
Electron density around CLA B 603:

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



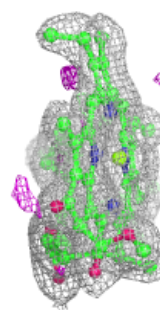
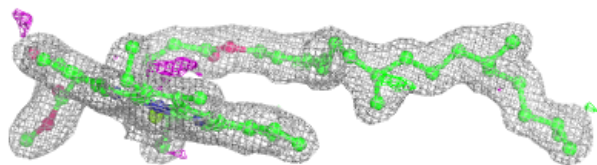
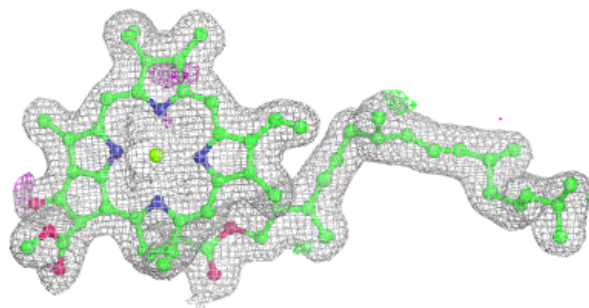
Electron density around CLA b 616:

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

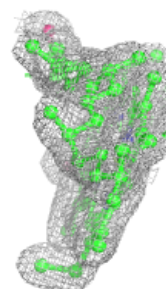
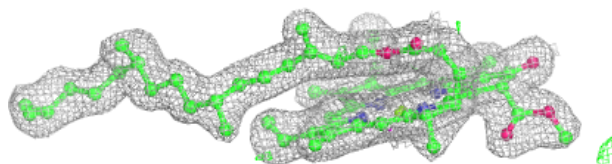
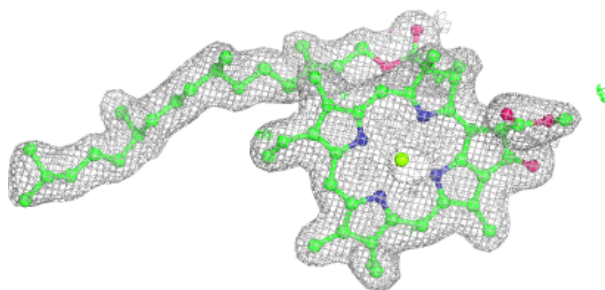


Electron density around CLA B 604:

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

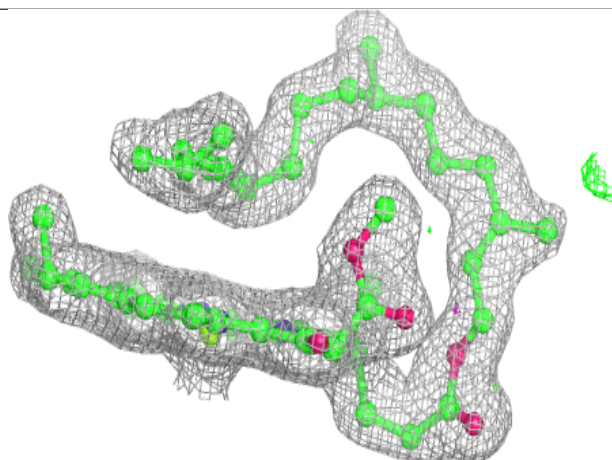
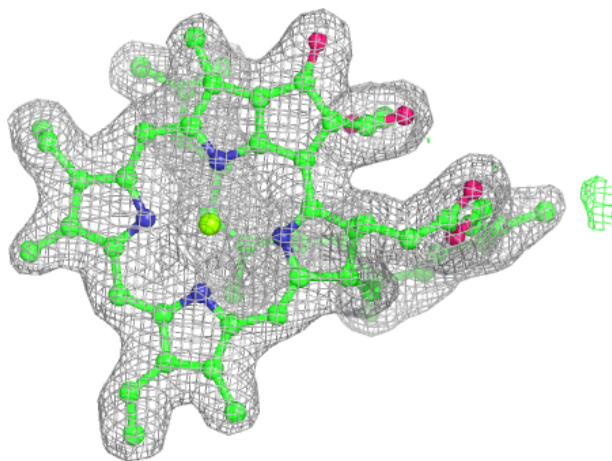
**Electron density around CLA c 902:**

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



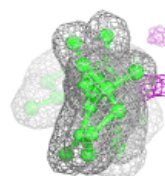
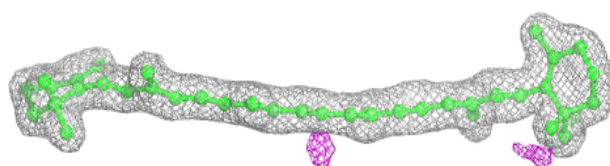
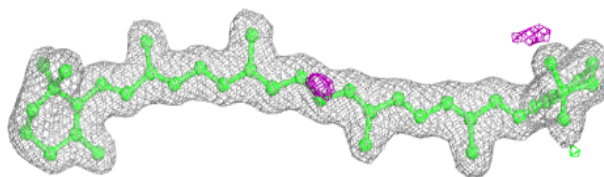
Electron density around CLA C 511:

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



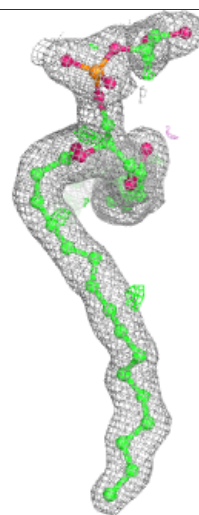
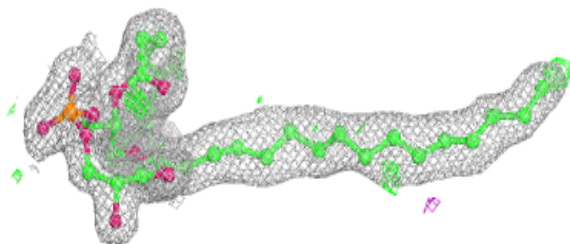
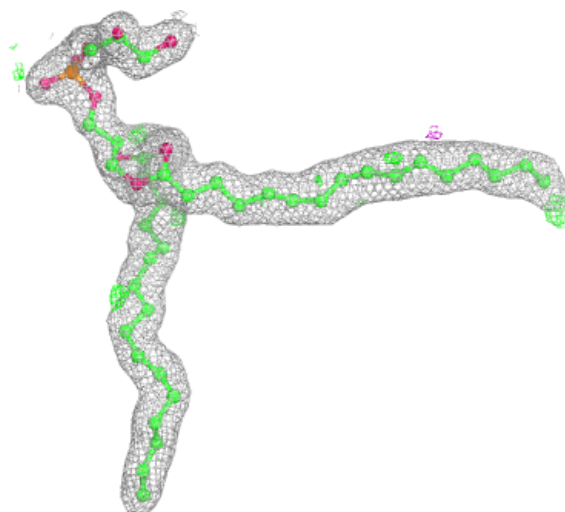
Electron density around BCR b 618:

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



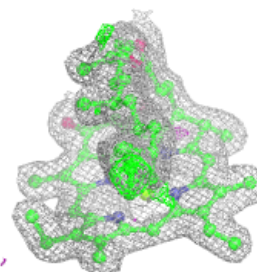
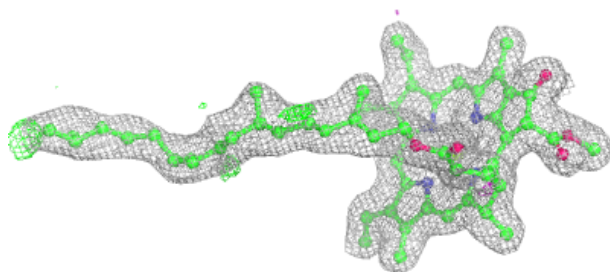
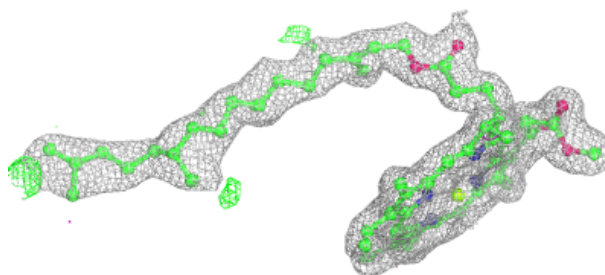
Electron density around LHG L 101:

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

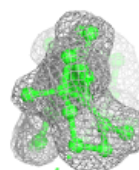
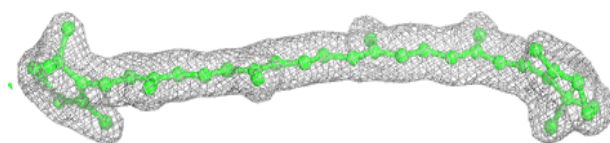
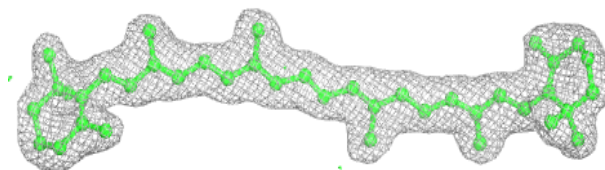


Electron density around CLA c 905:

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

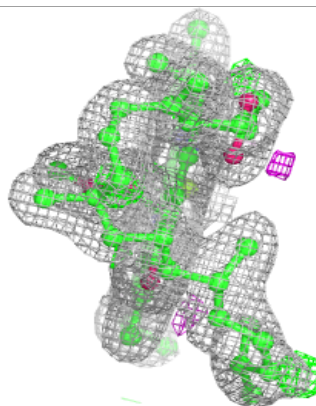
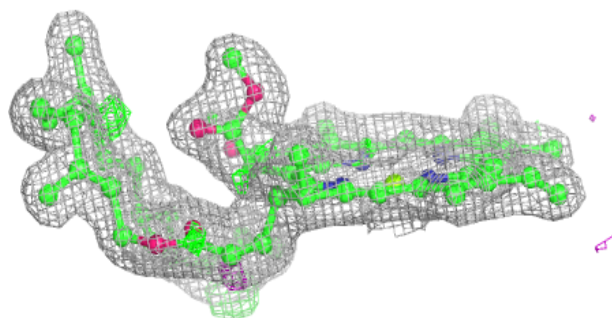
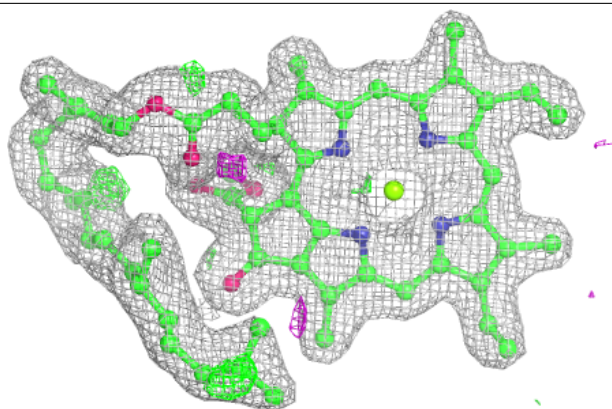
**Electron density around BCR b 620:**

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

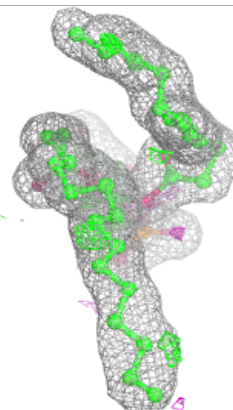
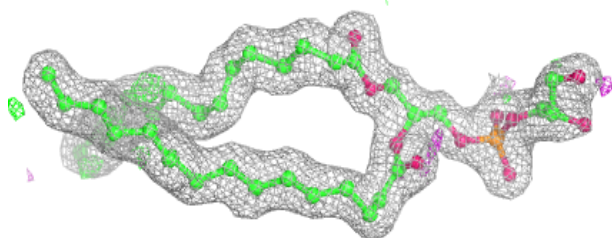
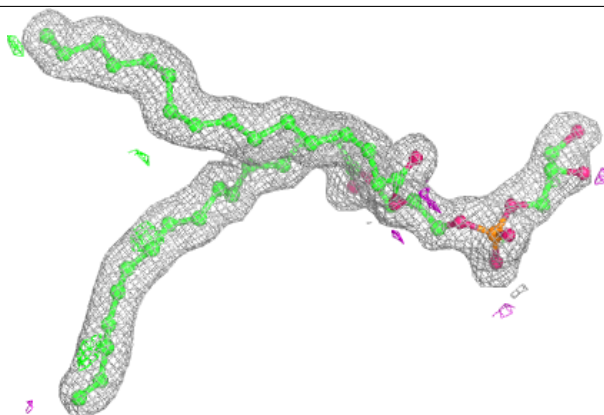


Electron density around CLA B 611:

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

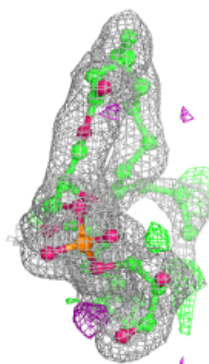
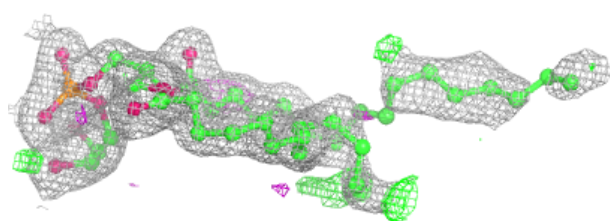
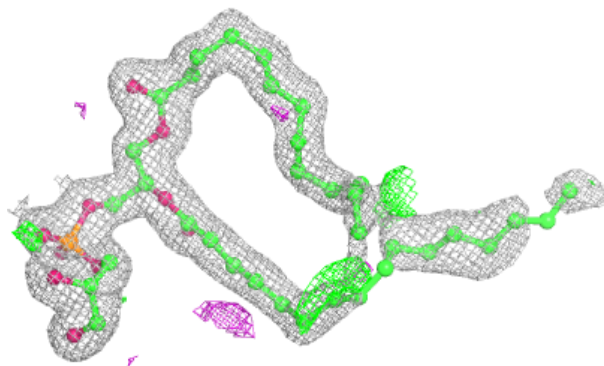
**Electron density around LHG d 409:**

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

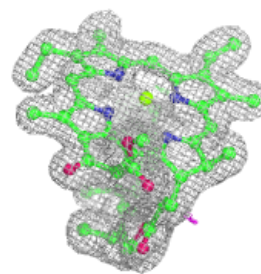
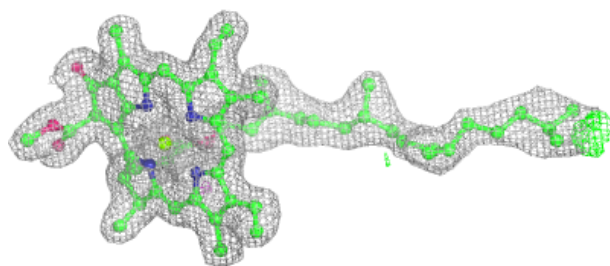
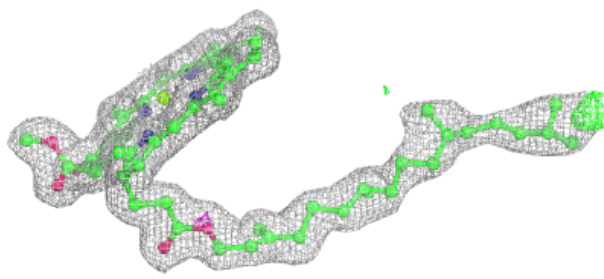


Electron density around LHG d 410:

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

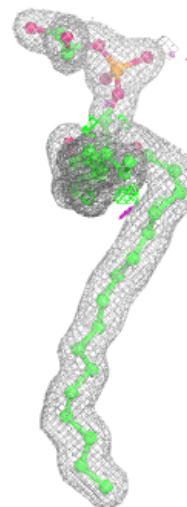
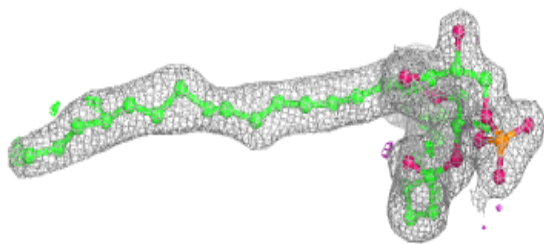
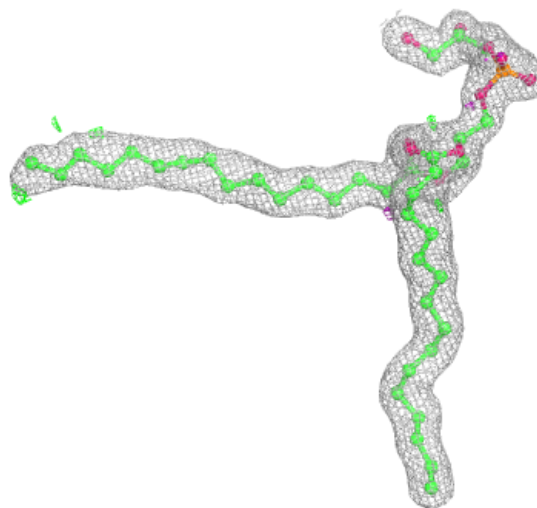
**Electron density around CLA C 505:**

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



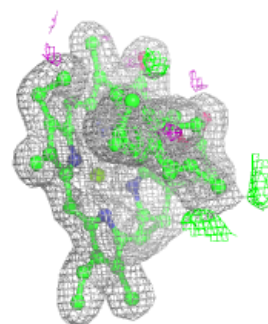
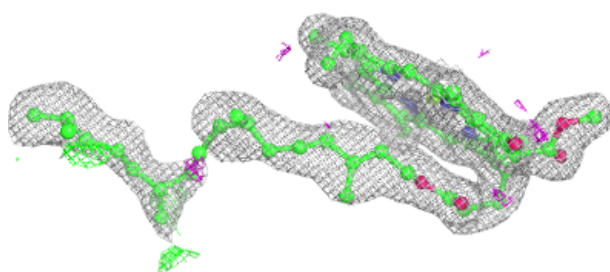
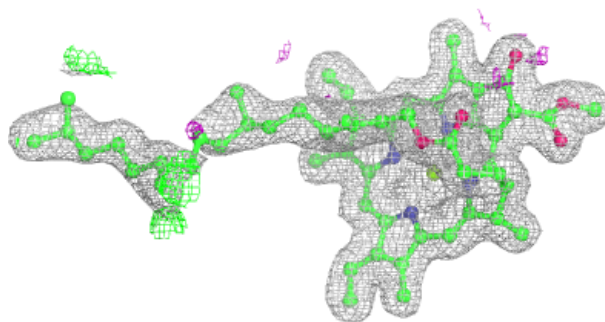
Electron density around LHG 1 101:

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

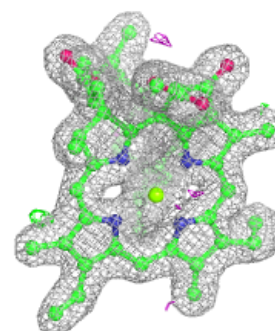
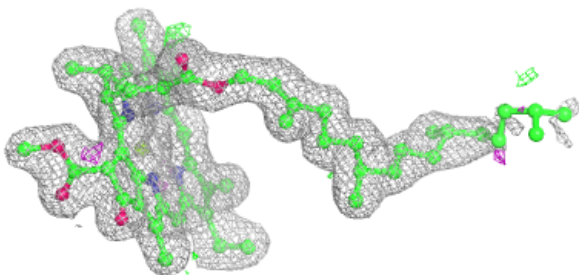
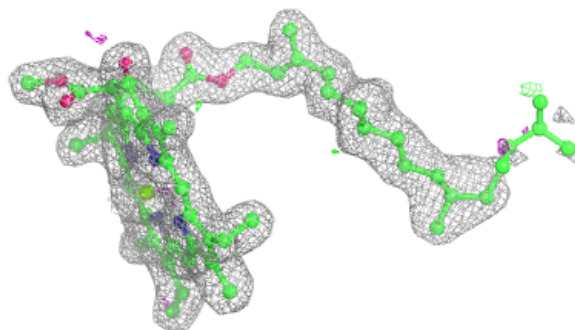


Electron density around CLA B 615:

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

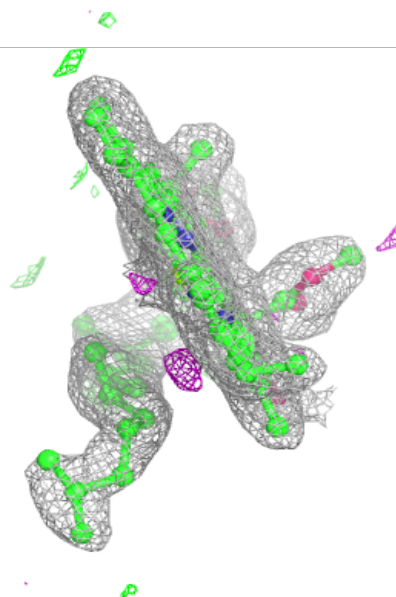
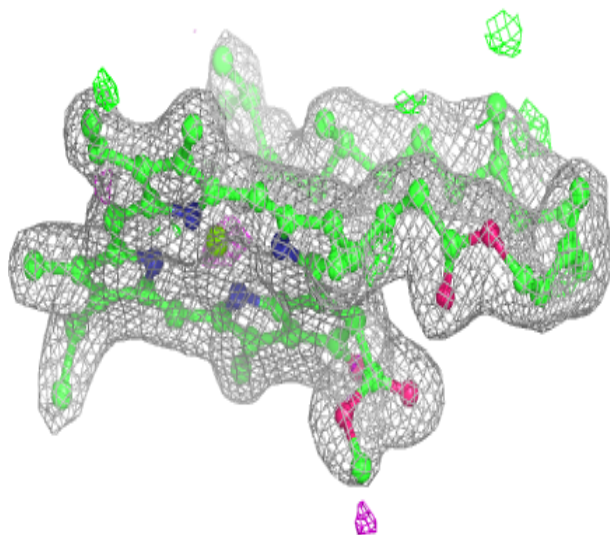
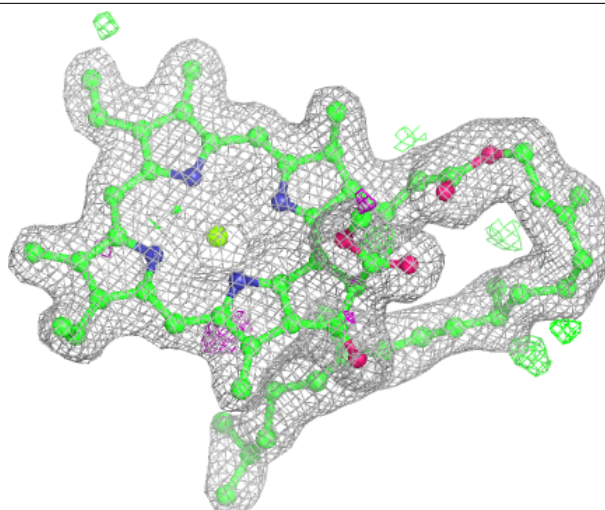
**Electron density around CLA c 909:**

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



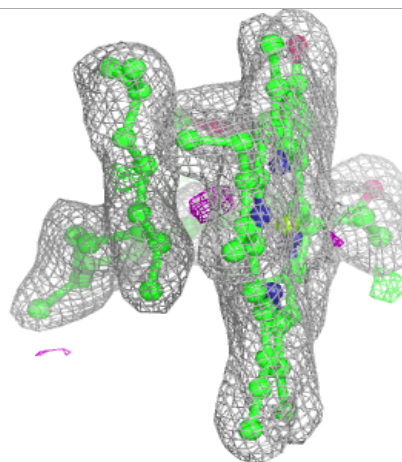
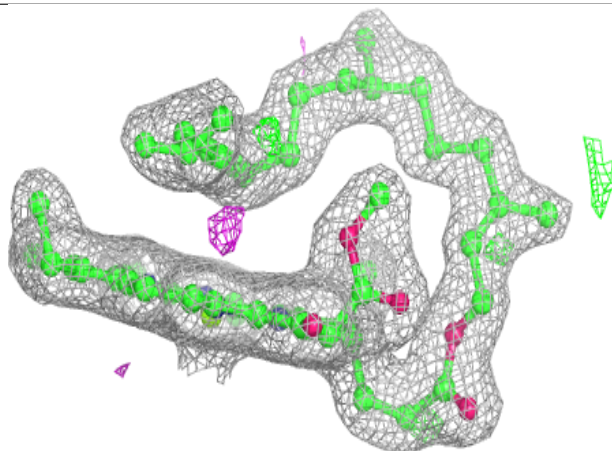
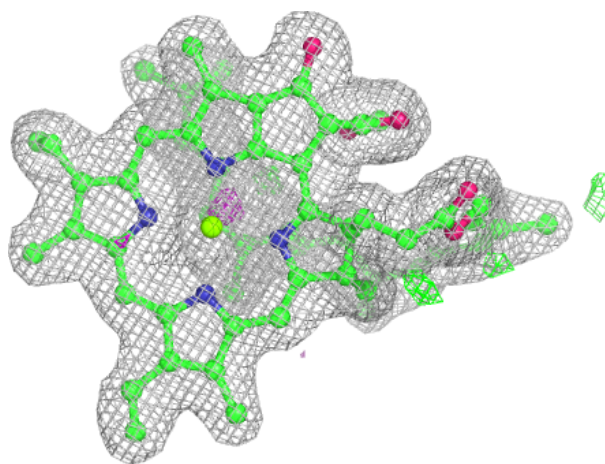
Electron density around CLA c 910:

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



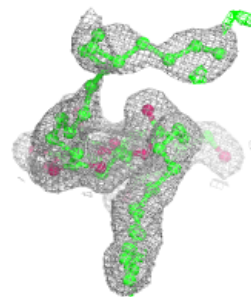
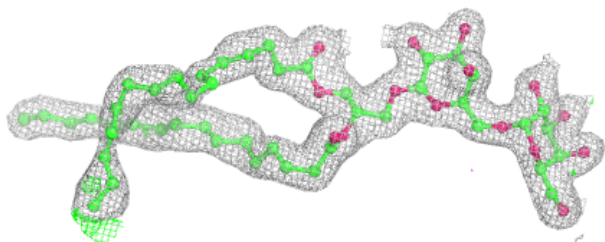
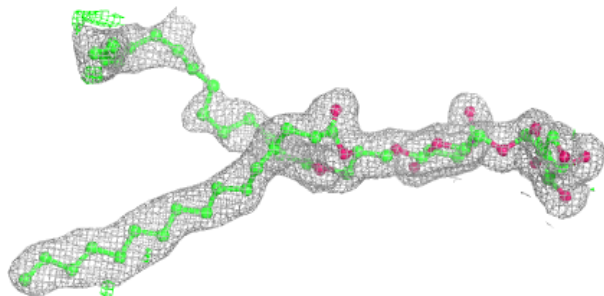
Electron density around CLA c 911:

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

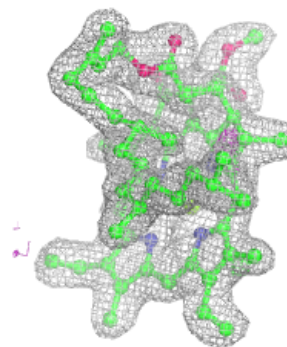
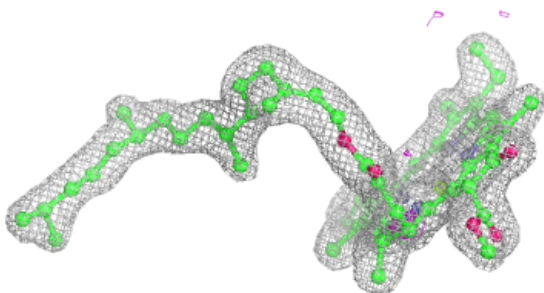
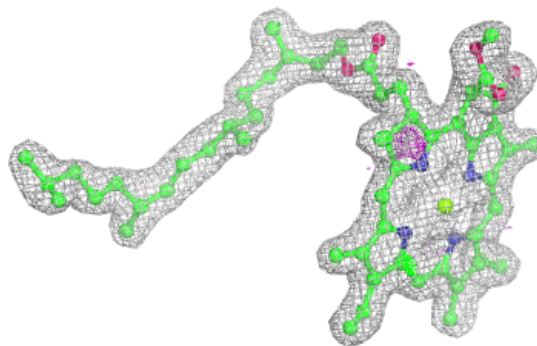


Electron density around DGD C 517:

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

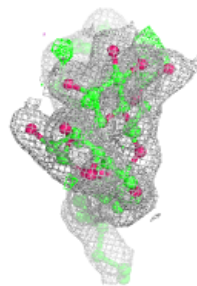
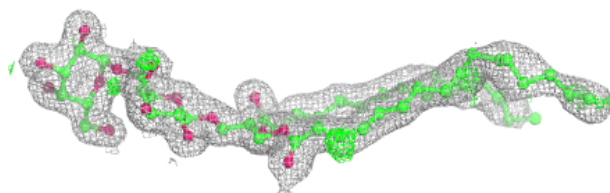
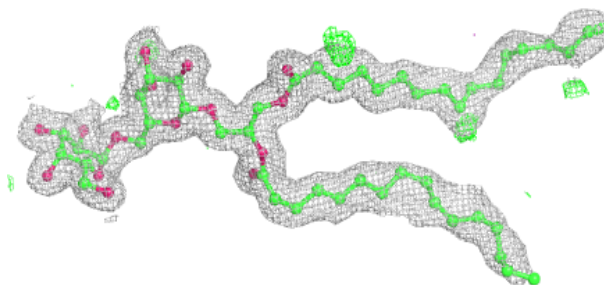
**Electron density around CLA c 912:**

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



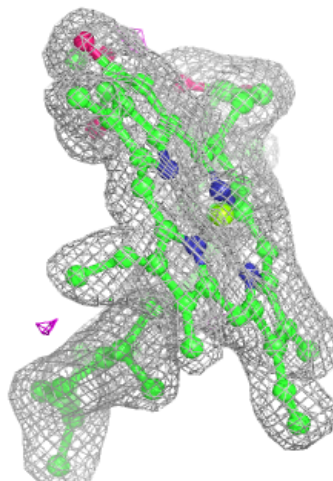
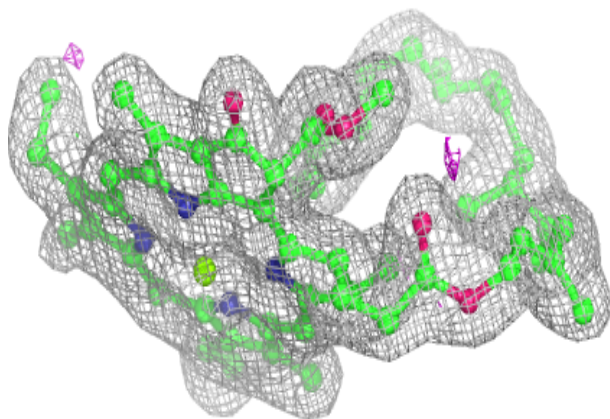
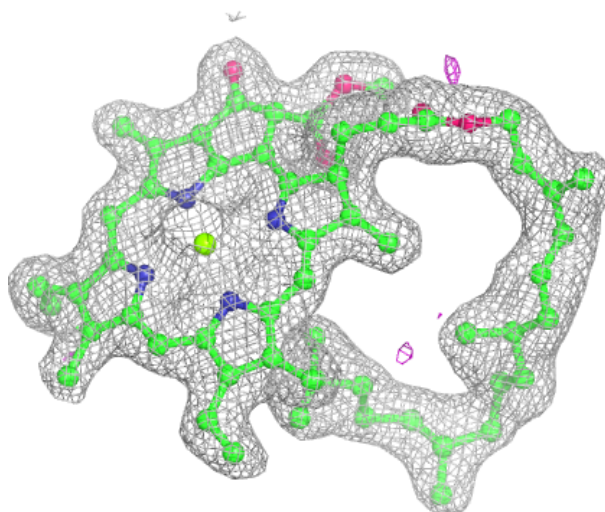
Electron density around DGD C 519:

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



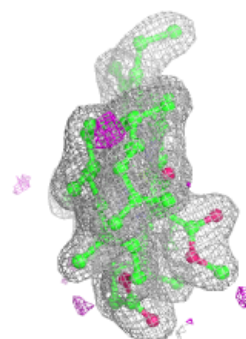
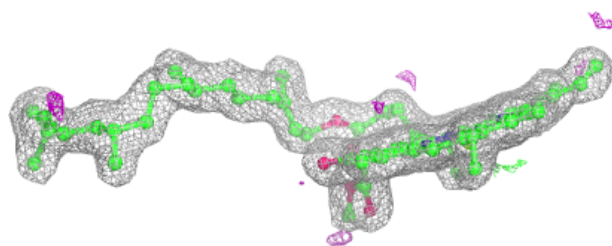
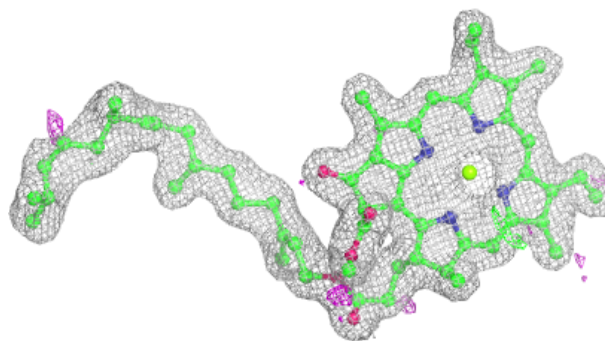
Electron density around CLA B 616:

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

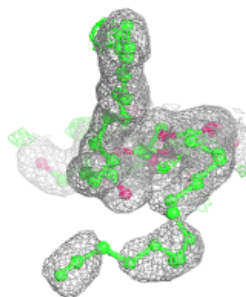
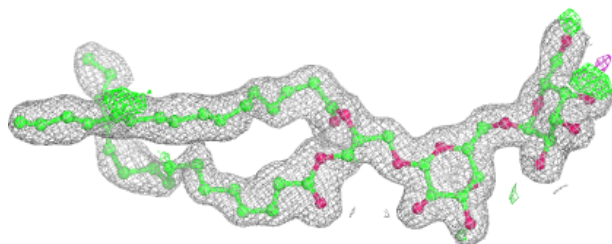
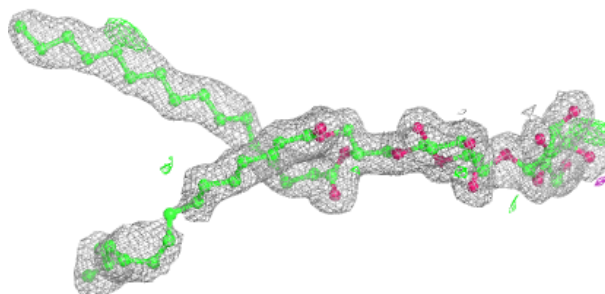


Electron density around CLA b 603:

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

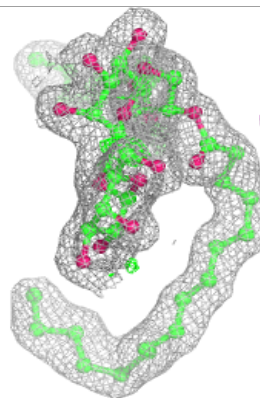
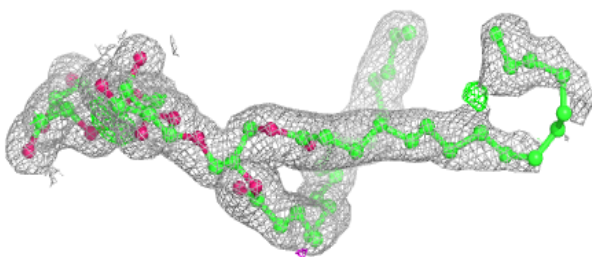
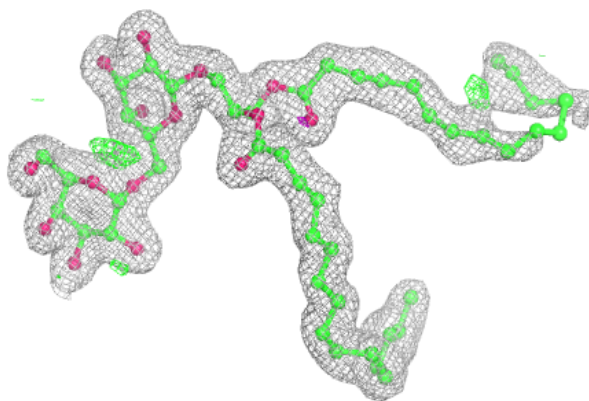
**Electron density around DGD c 917:**

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

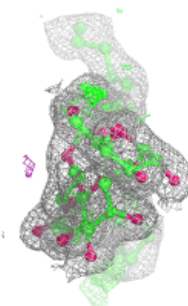
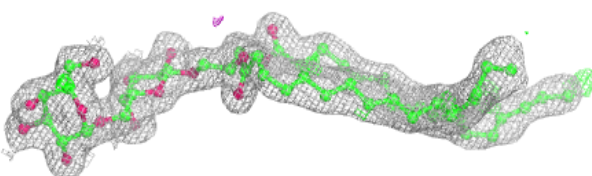
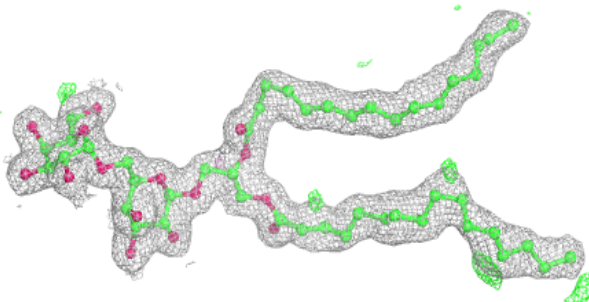


Electron density around DGD c 918:

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

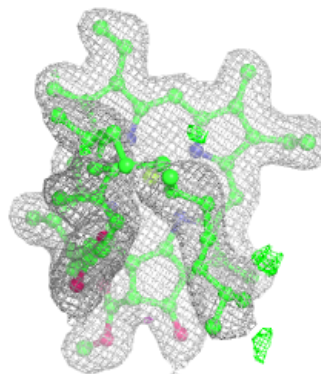
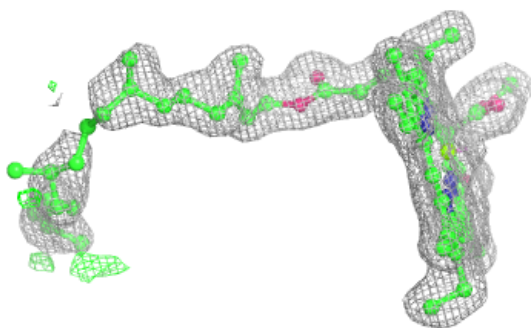
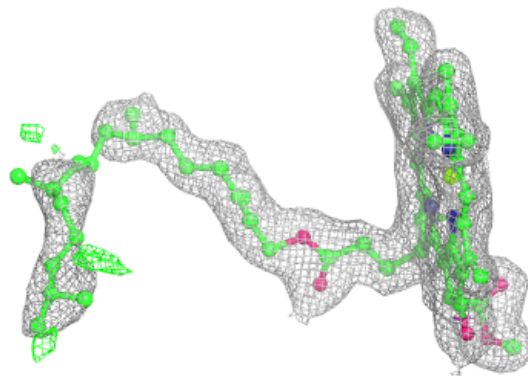
**Electron density around DGD c 919:**

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

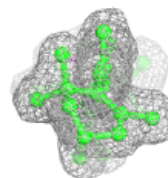
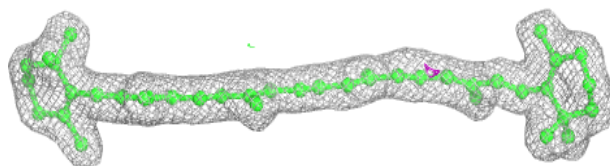
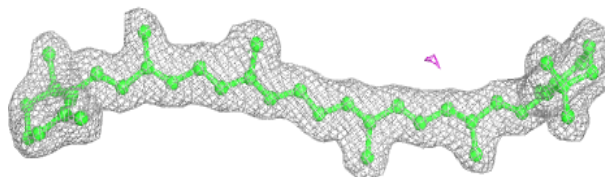


Electron density around CLA d 404:

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

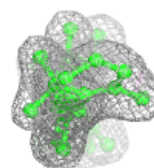
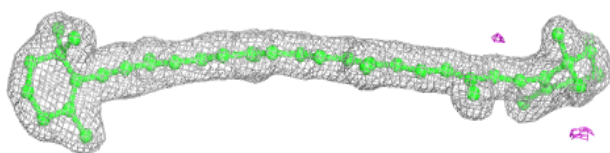
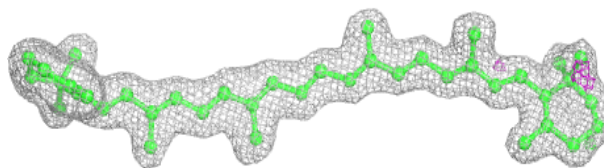
**Electron density around BCR A 409:**

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

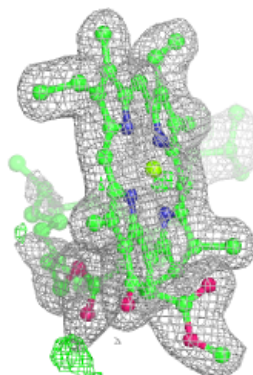
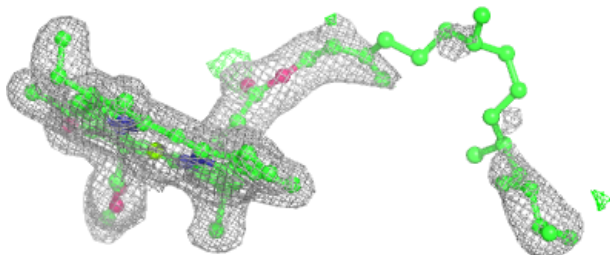
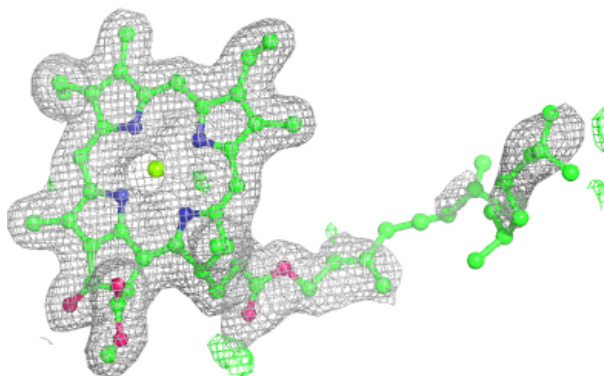


Electron density around BCR B 618:

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

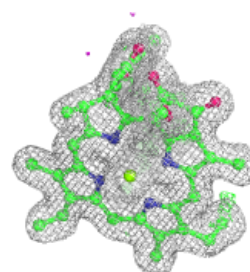
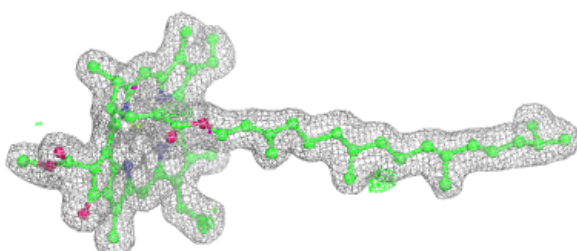
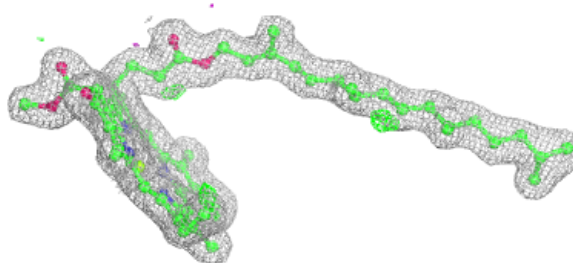
**Electron density around CLA A 408:**

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

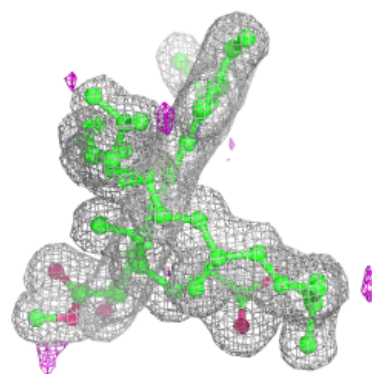
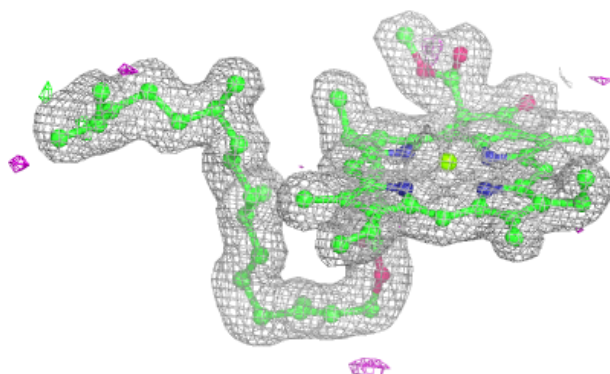
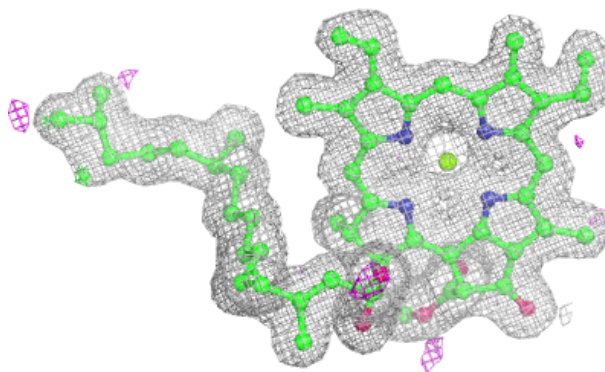


Electron density around CLA b 608:

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

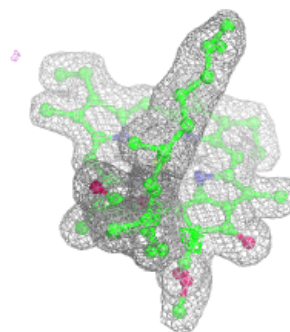
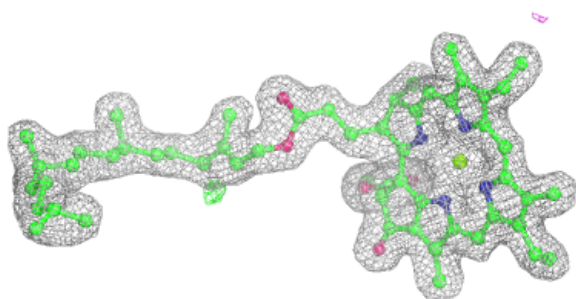
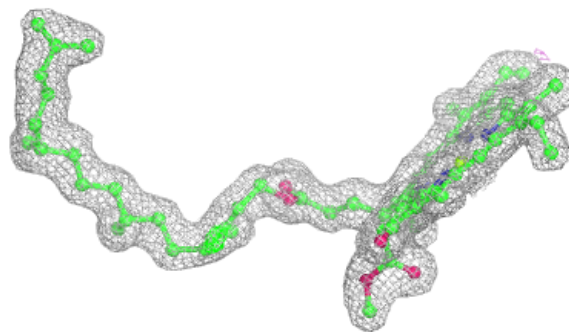
**Electron density around CLA d 401:**

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

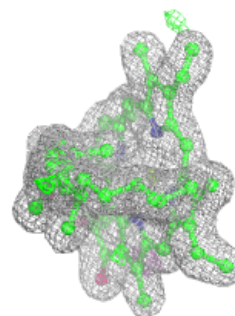
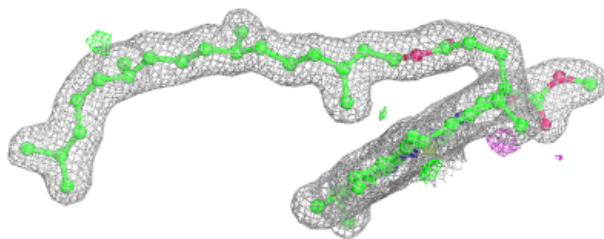
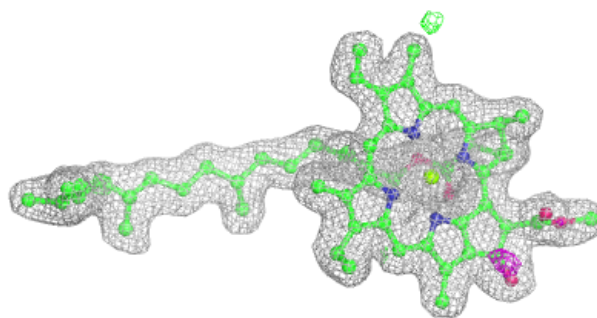


Electron density around CLA d 403:

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

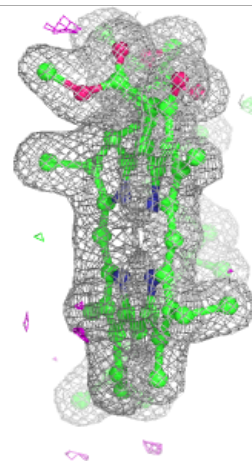
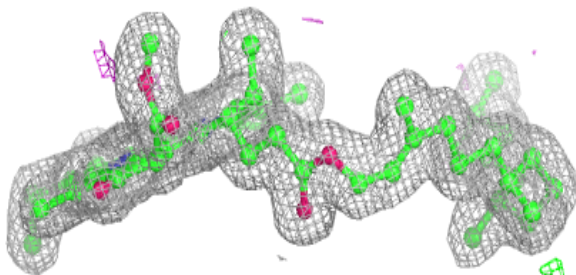
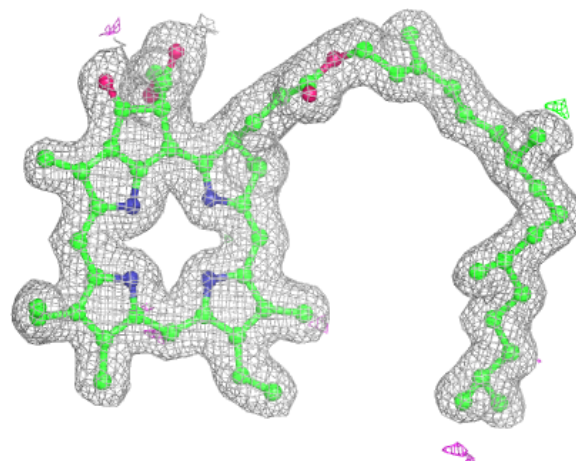
**Electron density around CLA b 609:**

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



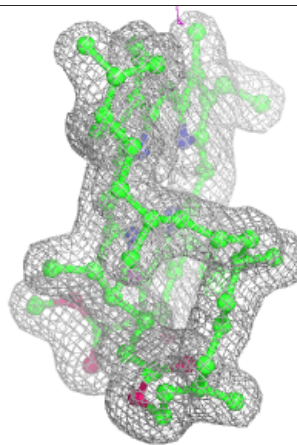
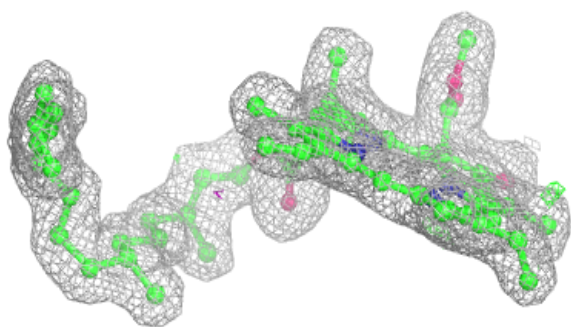
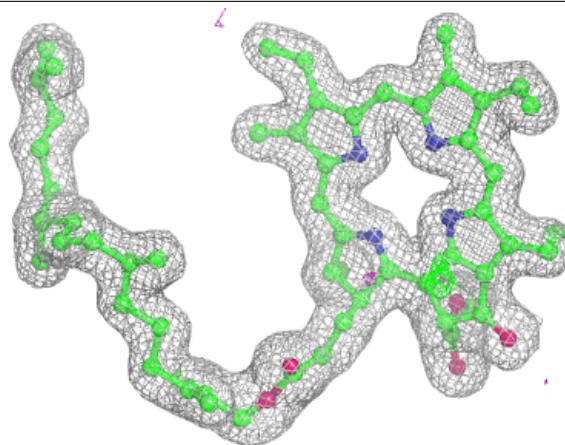
Electron density around PHO A 407:

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



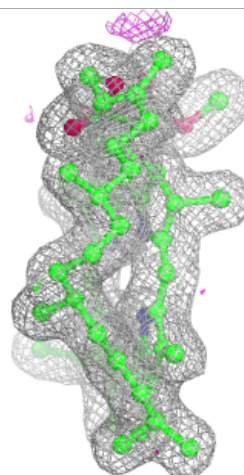
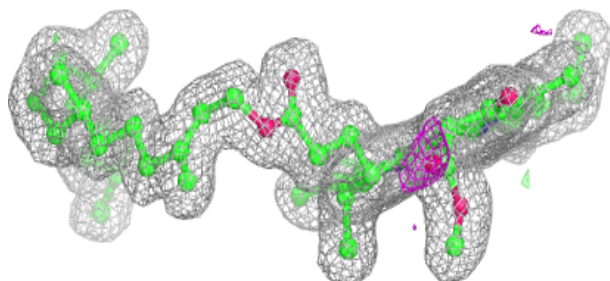
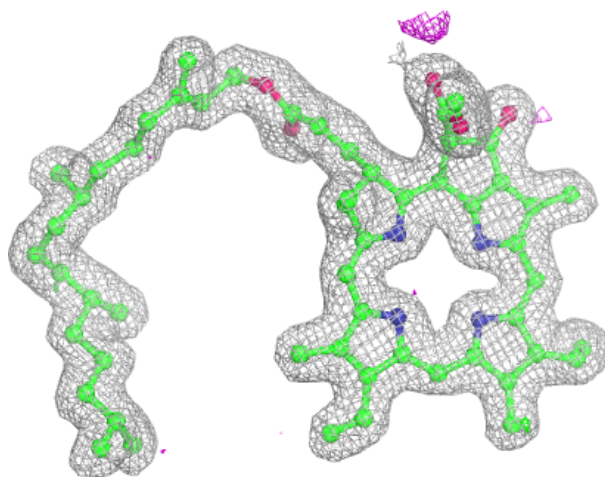
Electron density around PHO D 402:

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



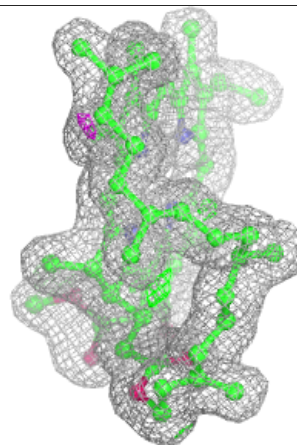
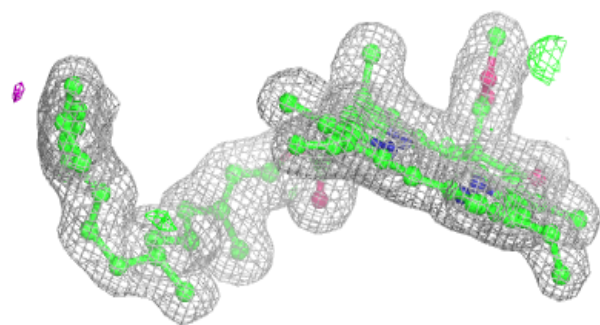
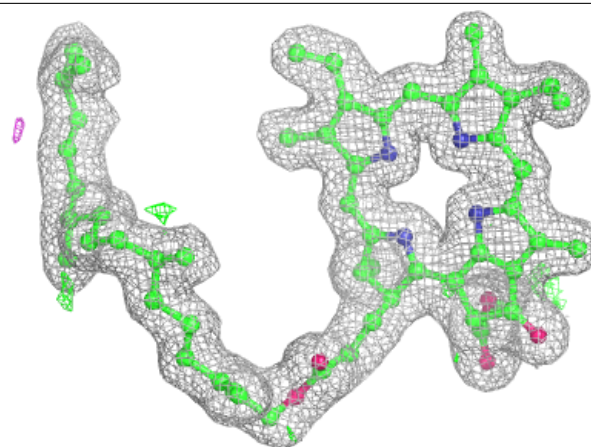
Electron density around PHO a 408:

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



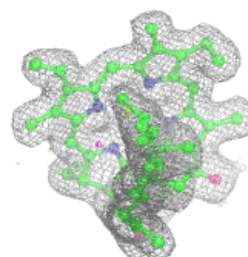
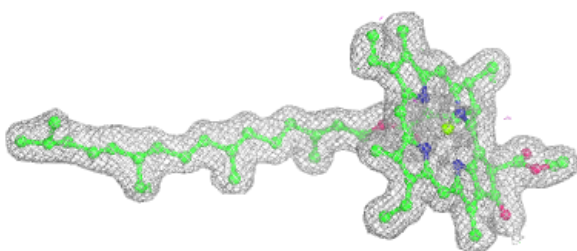
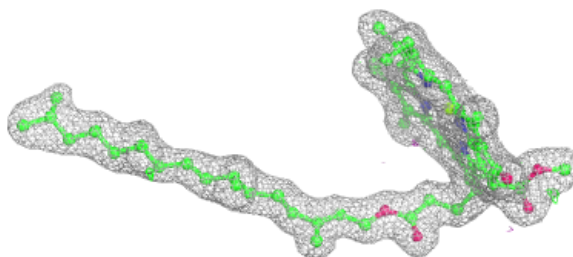
Electron density around PHO a 409:

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

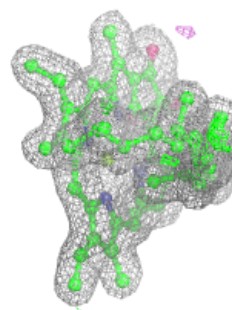
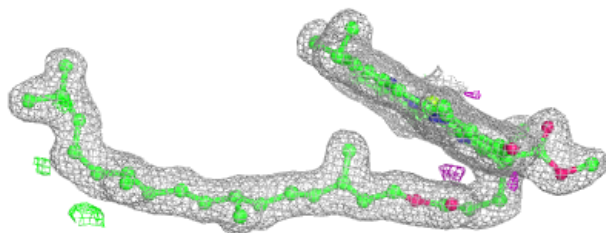
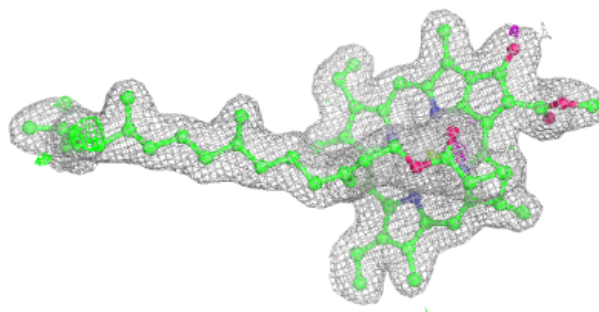


Electron density around CLA B 608:

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

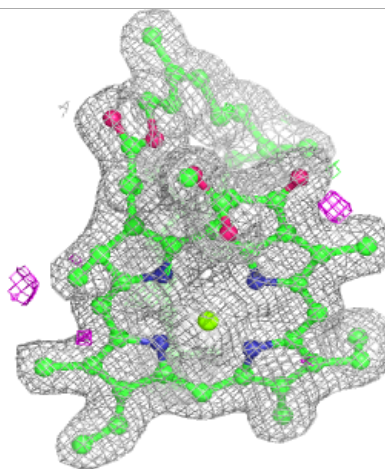
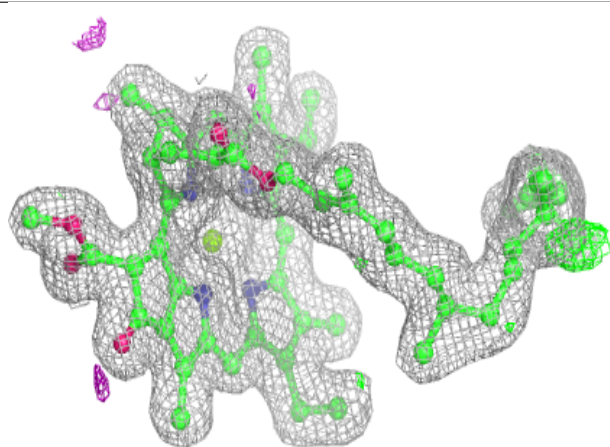
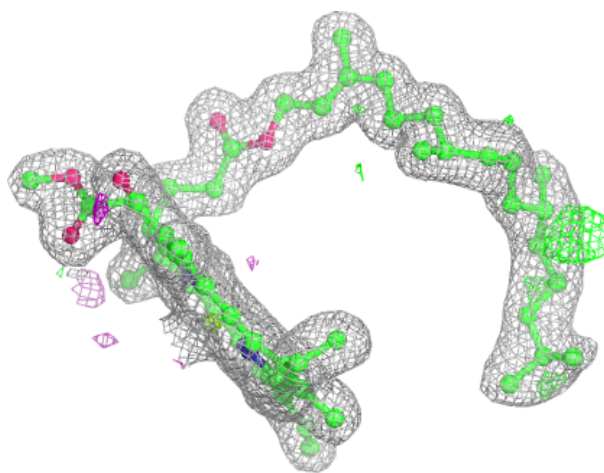
**Electron density around CLA B 609:**

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



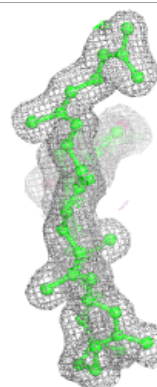
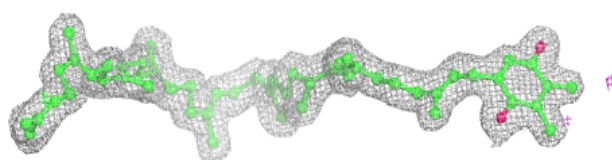
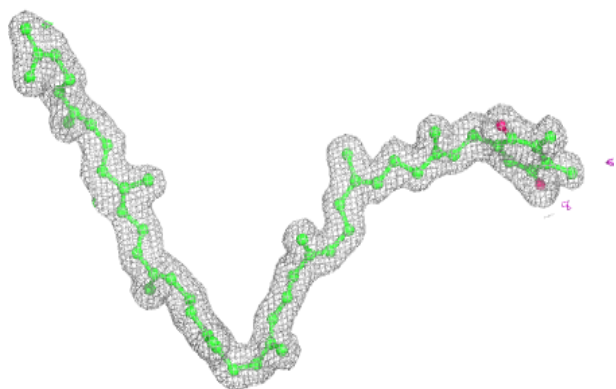
Electron density around CLA b 612:

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

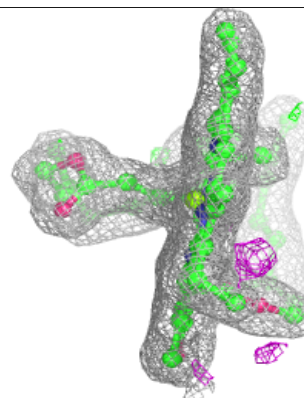
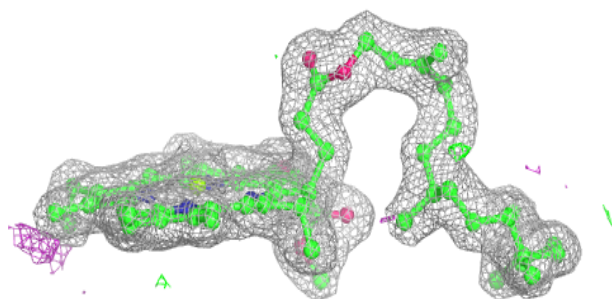
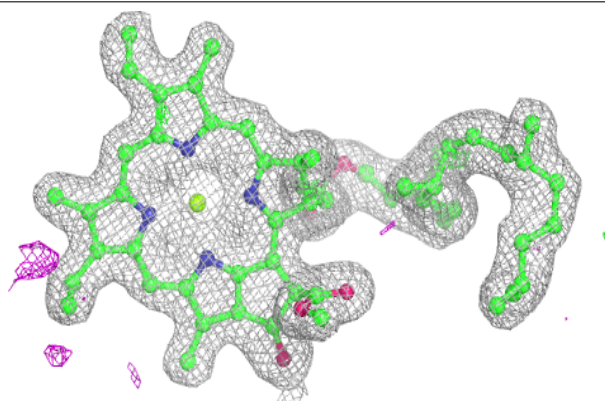


Electron density around PL9 d 406:

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

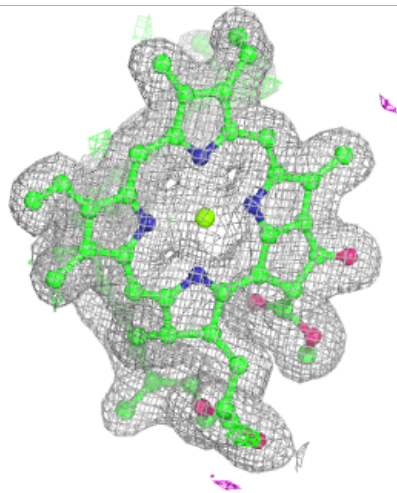
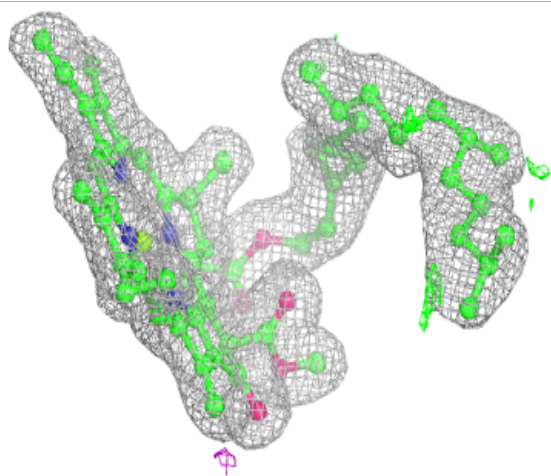
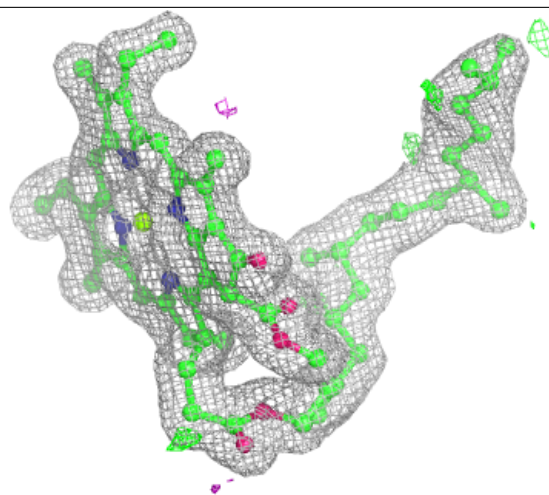
**Electron density around CLA b 613:**

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



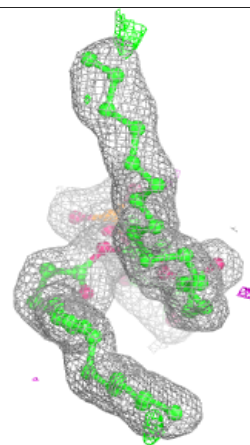
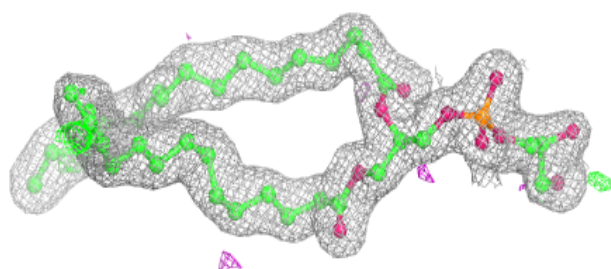
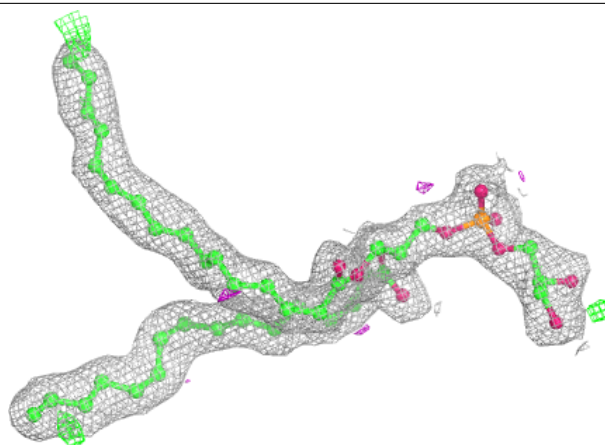
Electron density around CLA b 614:

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



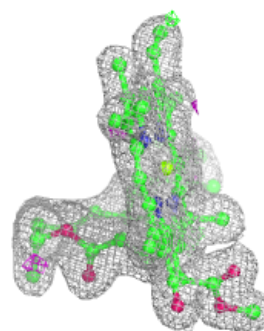
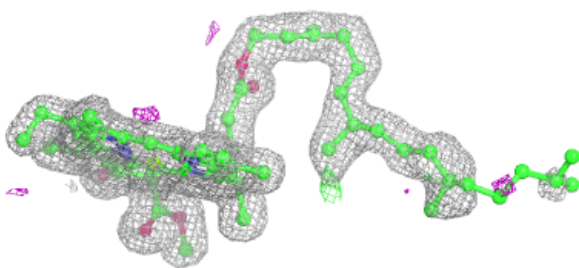
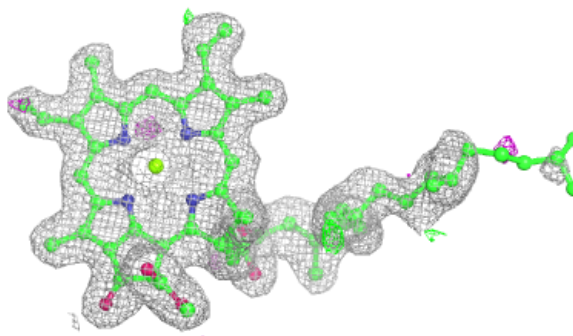
Electron density around LHG D 410:

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

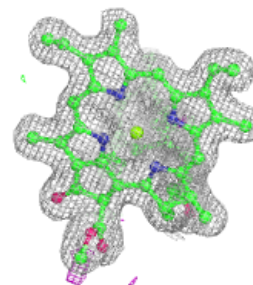
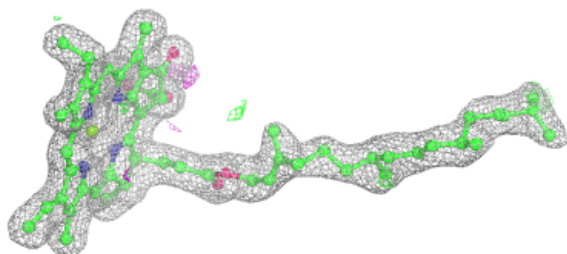
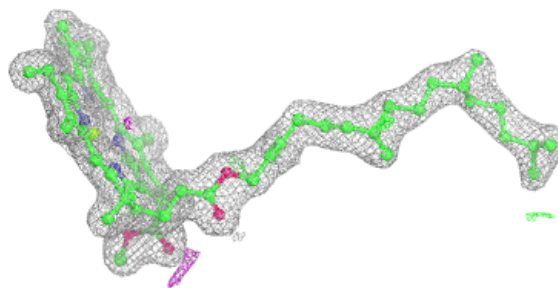


Electron density around CLA A 406:

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

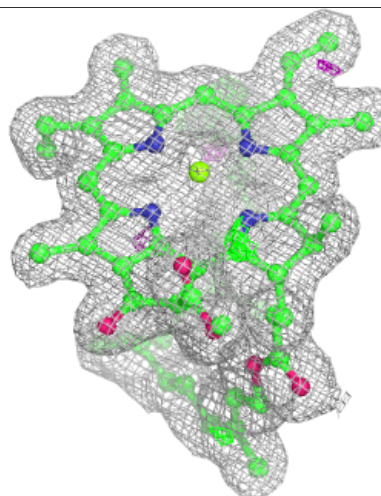
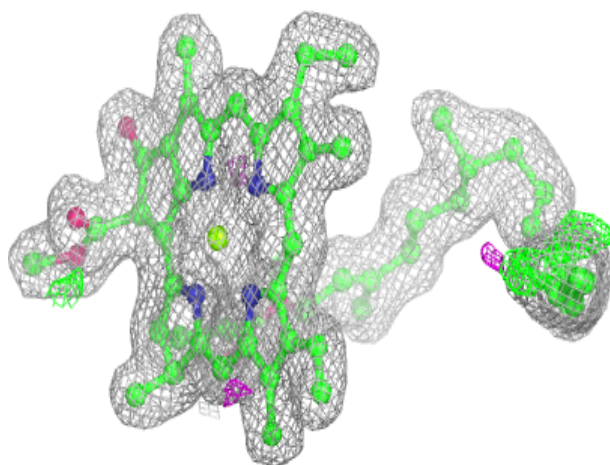
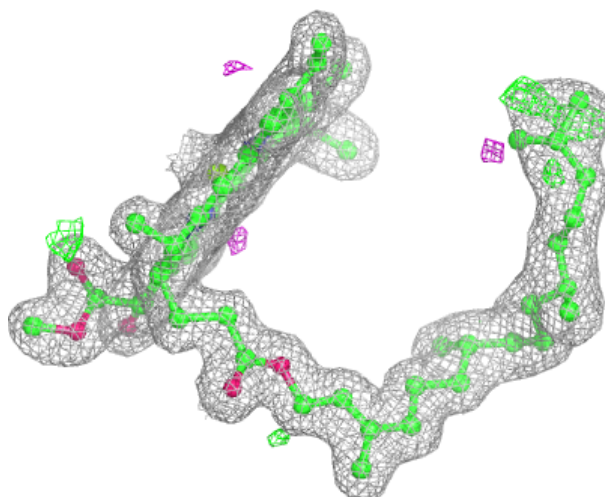
**Electron density around CLA B 605:**

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



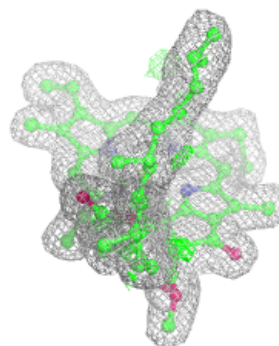
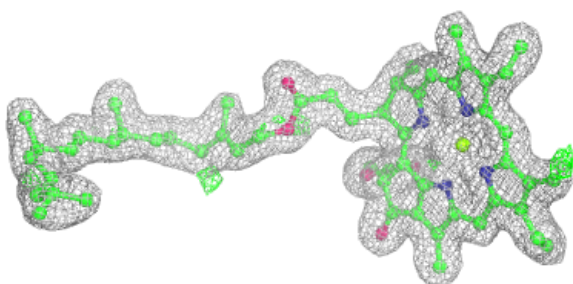
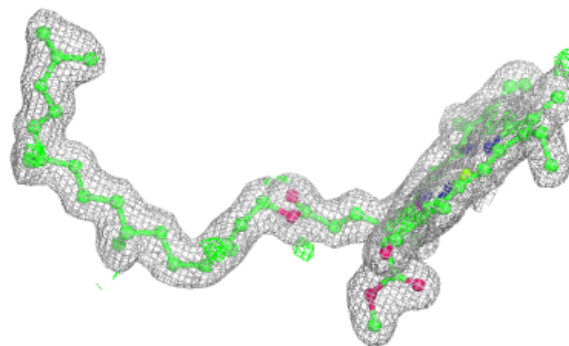
Electron density around CLA B 612:

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

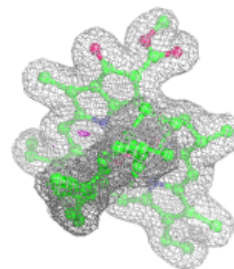
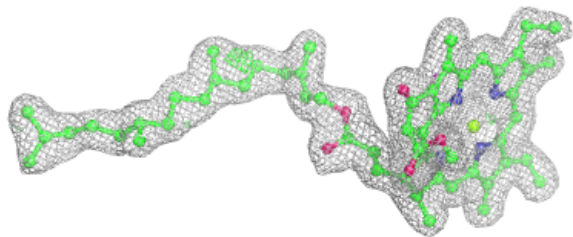
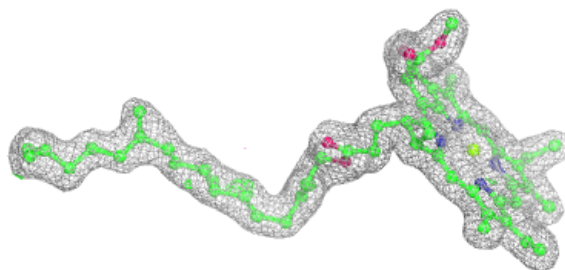


Electron density around CLA D 403:

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

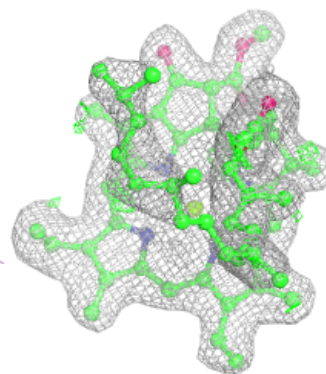
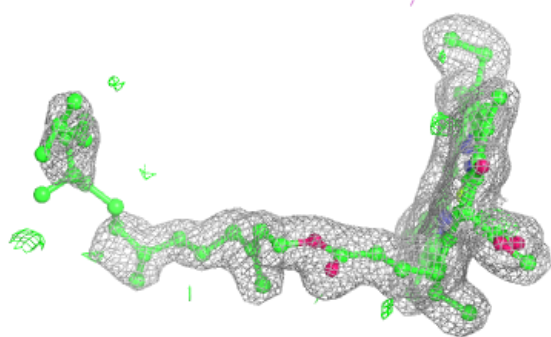
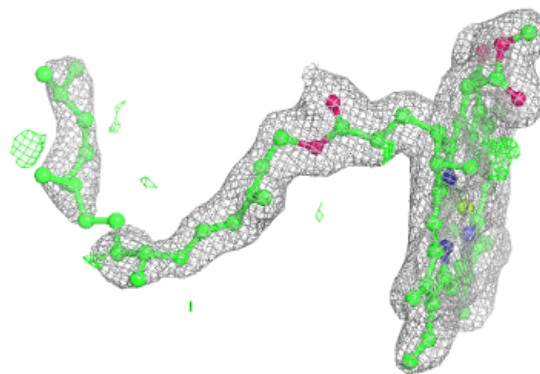
**Electron density around CLA c 903:**

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

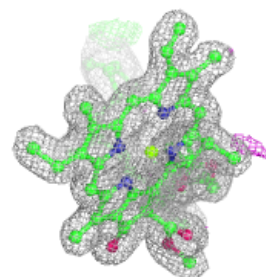
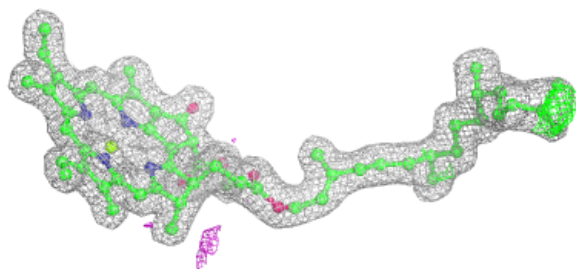
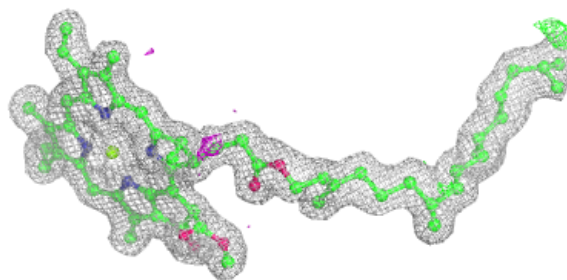


Electron density around CLA D 404:

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

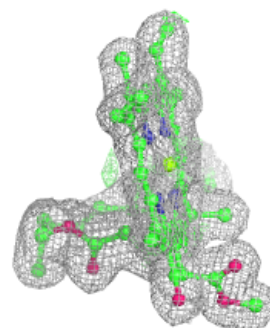
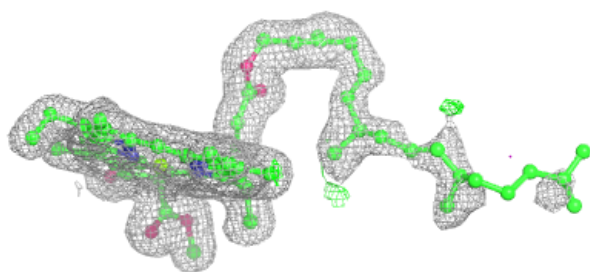
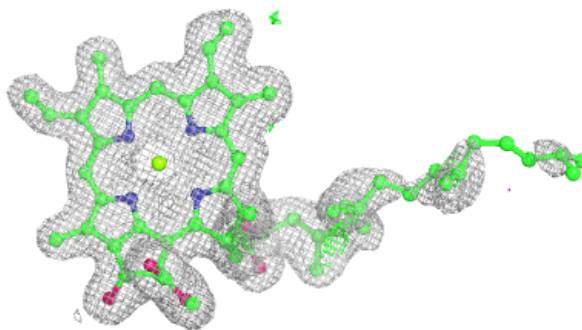
**Electron density around CLA a 406:**

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

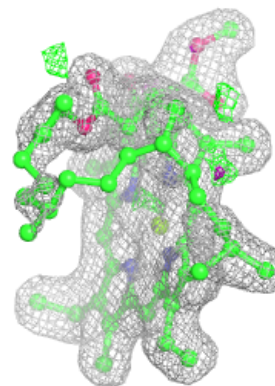
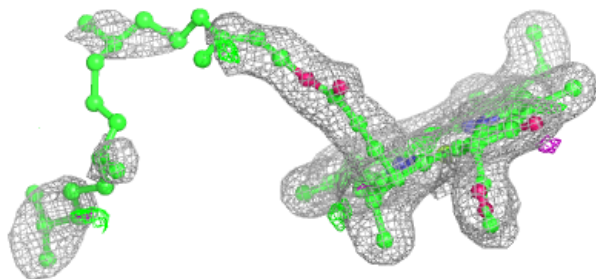
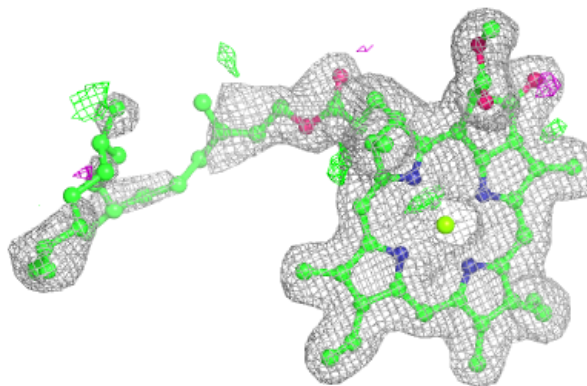


Electron density around CLA a 407:

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

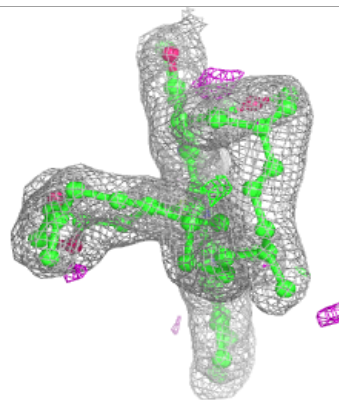
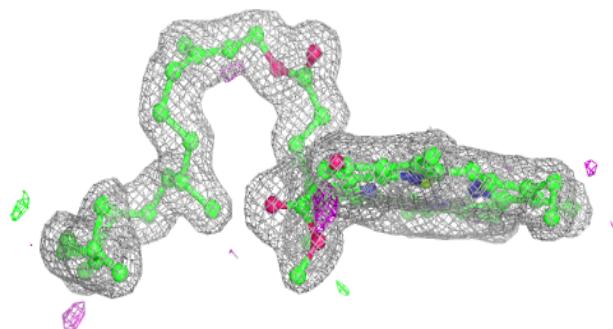
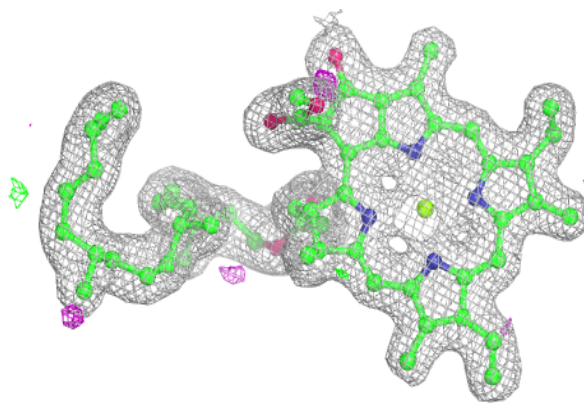
**Electron density around CLA a 410:**

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



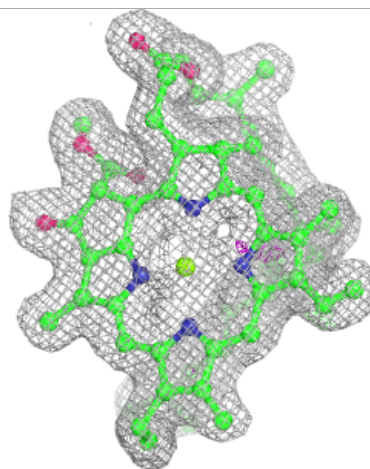
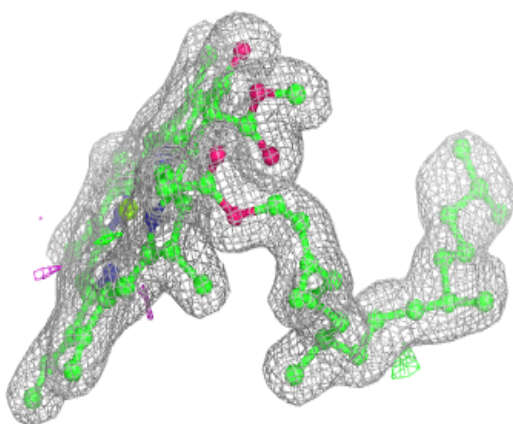
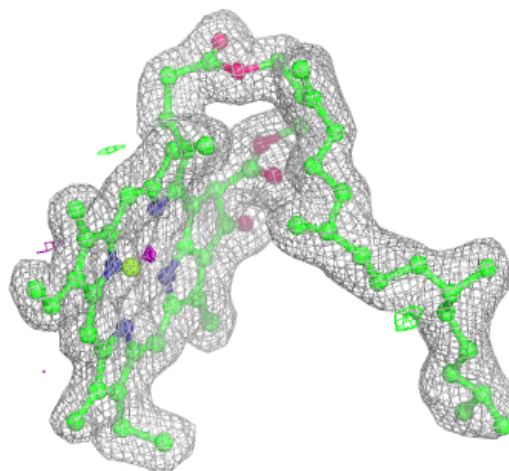
Electron density around CLA B 613:

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



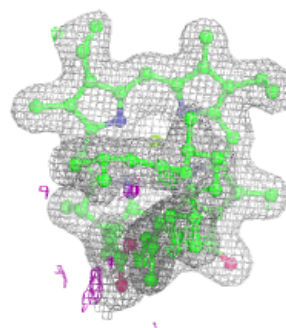
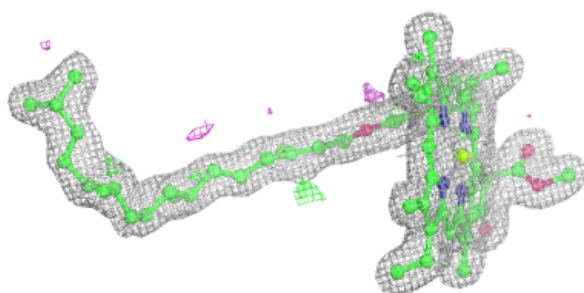
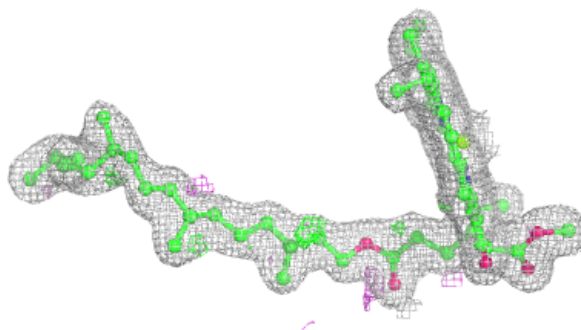
Electron density around CLA B 614:

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



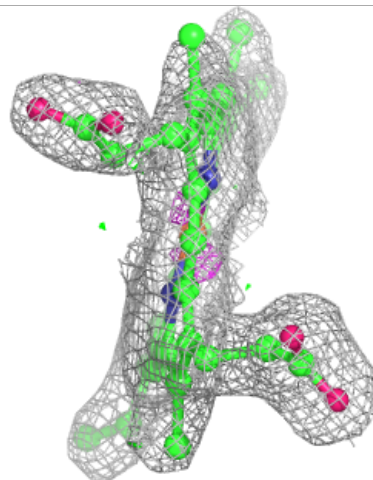
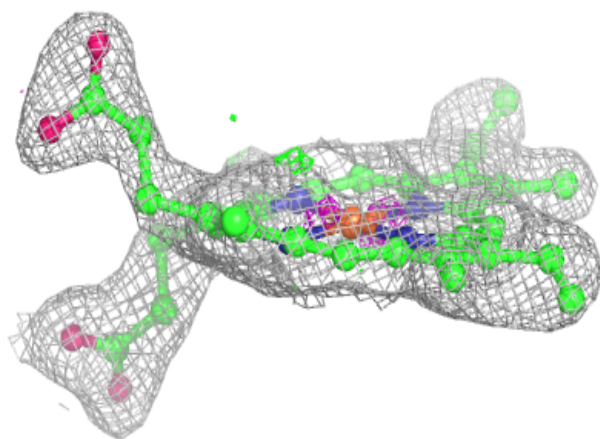
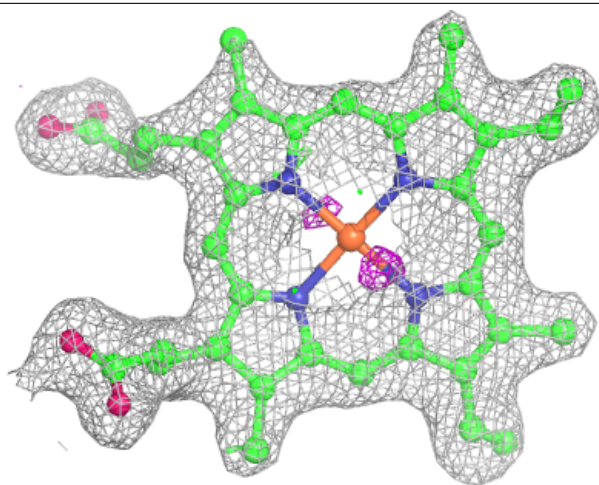
Electron density around CLA B 606:

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



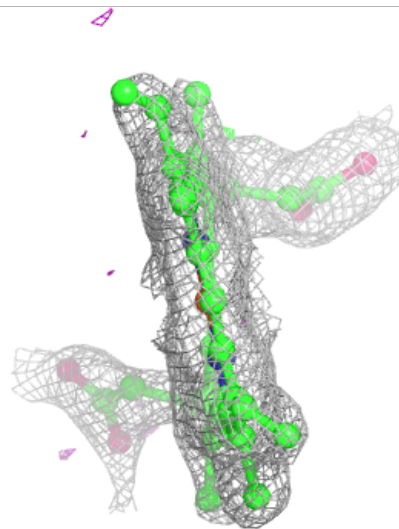
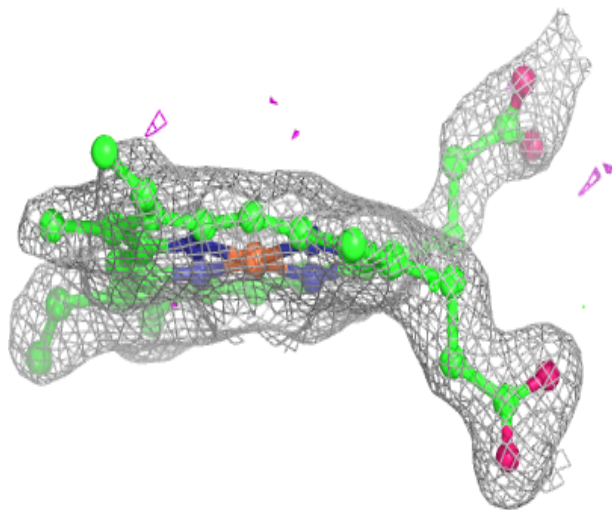
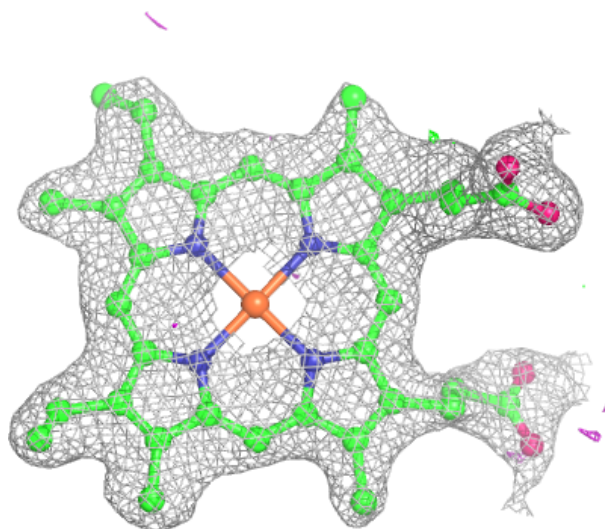
Electron density around HEM E 105:

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



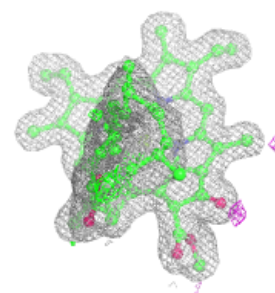
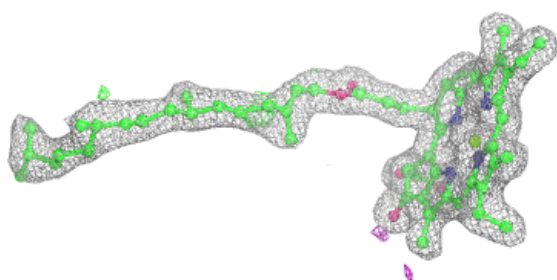
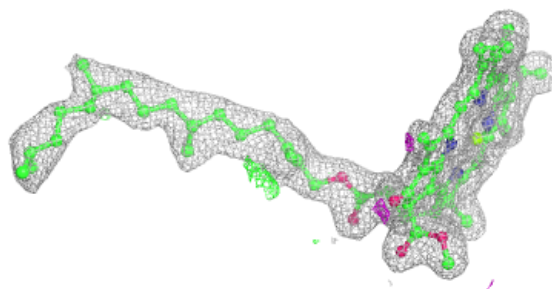
Electron density around HEM e 105:

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

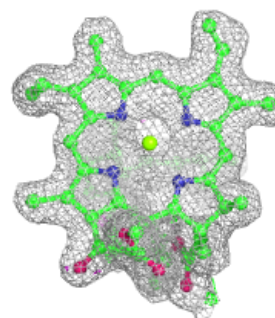
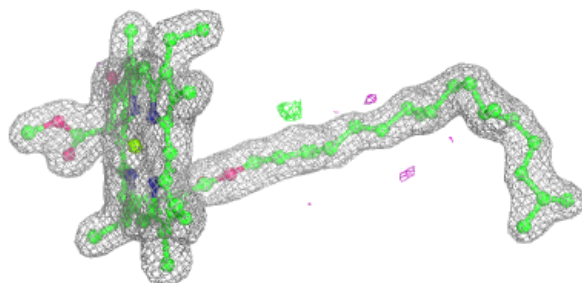
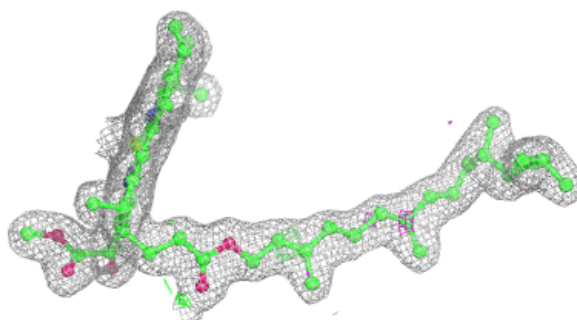


Electron density around CLA b 605:

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

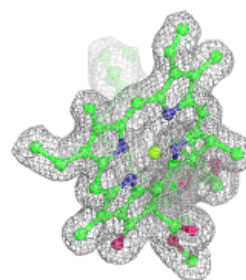
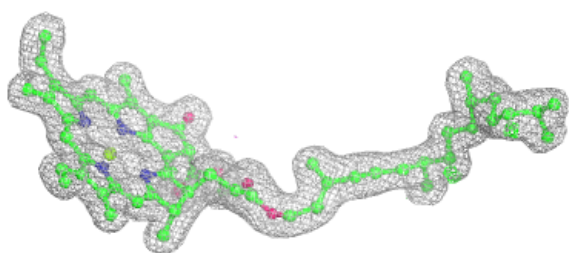
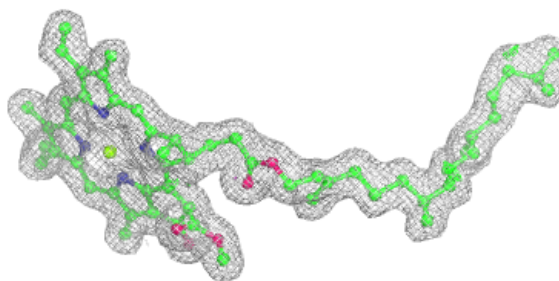
**Electron density around CLA b 606:**

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

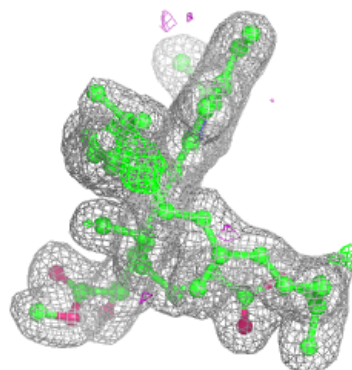
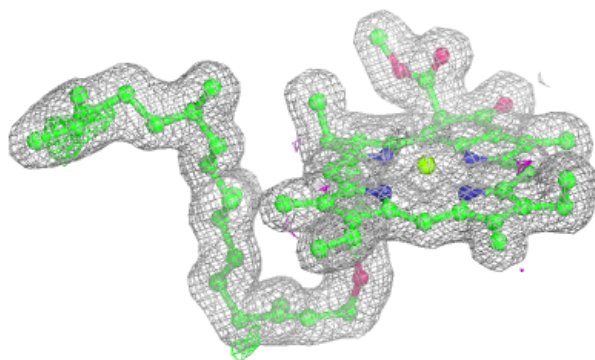
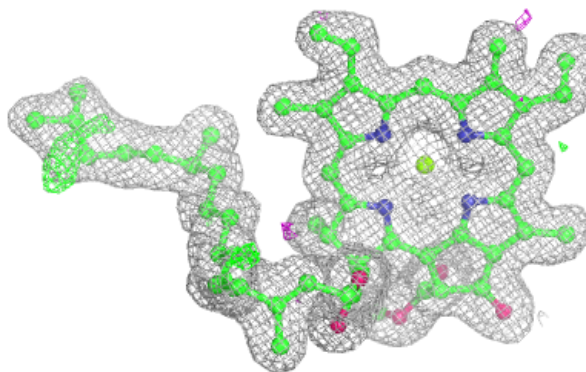


Electron density around CLA A 405:

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

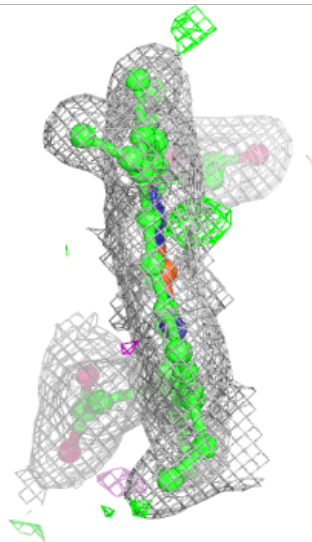
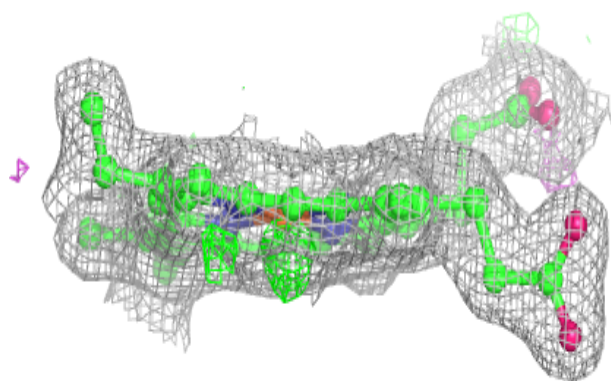
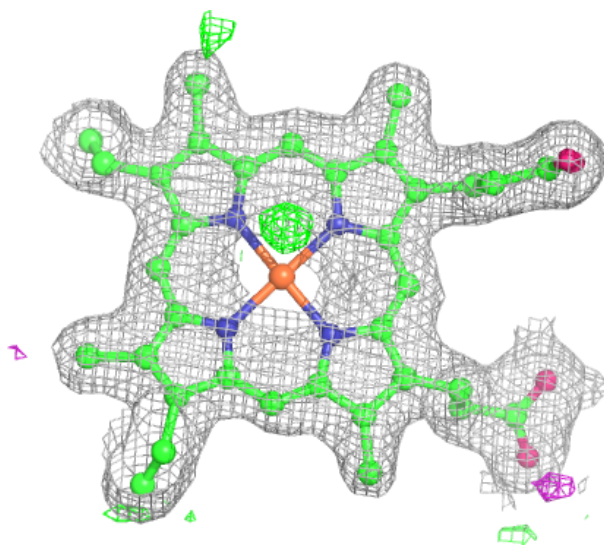
**Electron density around CLA D 401:**

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



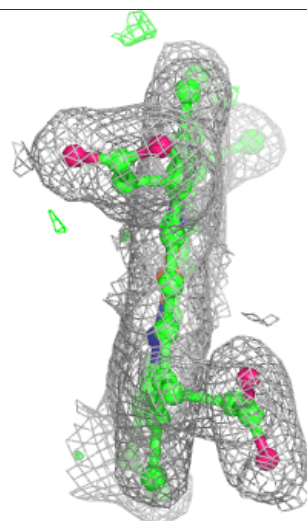
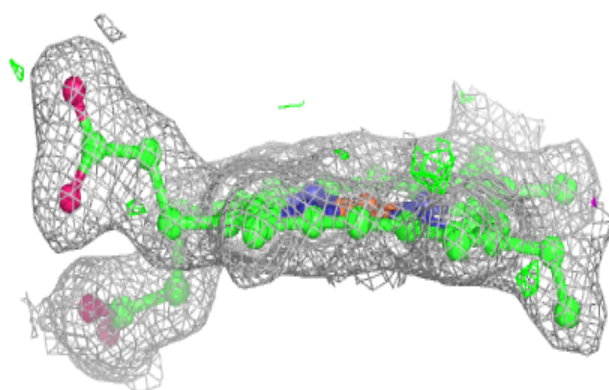
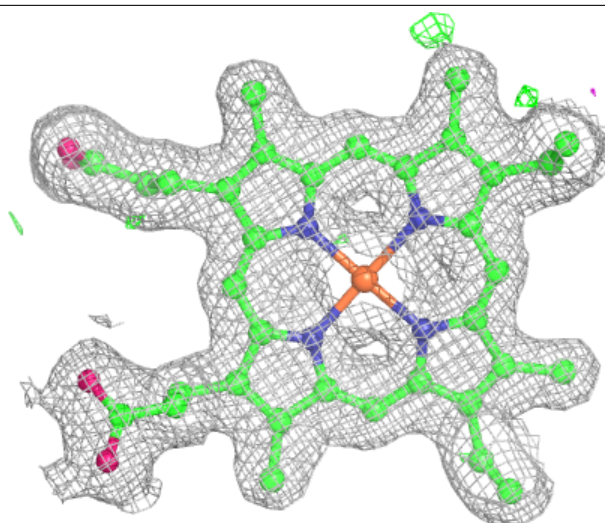
Electron density around HEC v 203:

$2mF_o-DF_c$ (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.