



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2023 – 05:09 PM JST

PDB ID : 6JLM
Title : XFEL structure of cyanobacterial photosystem II (dark state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.35 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 : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

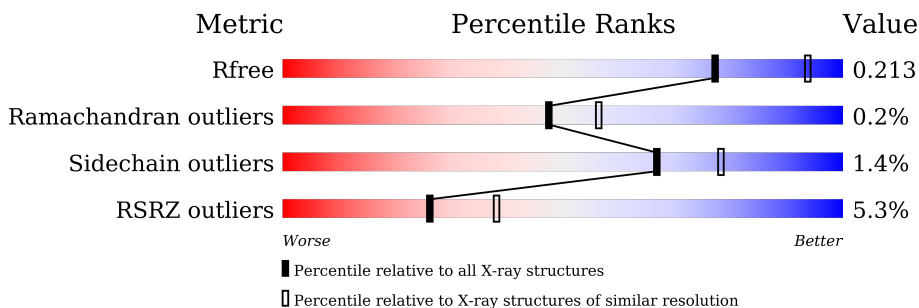
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	97%
1	a	344	96%
2	B	505	99%
2	b	505	99%
3	C	455	98%
3	c	455	98%
4	D	342	99%

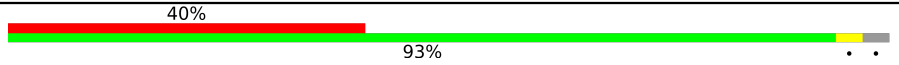
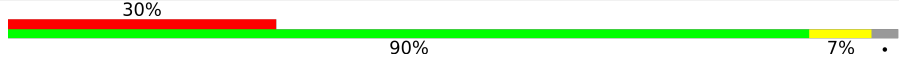
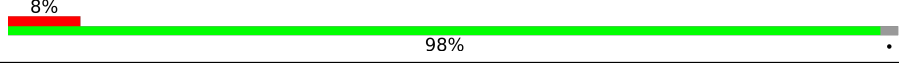
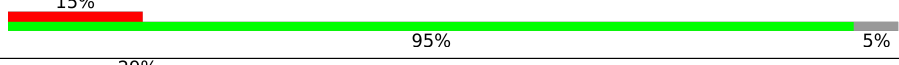
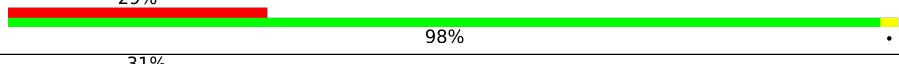
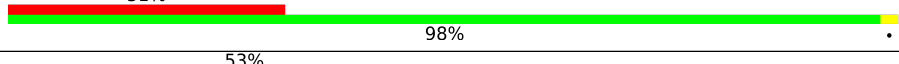
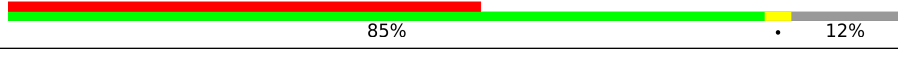
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Mol	Chain	Length	Quality of chain
4	d	342	99%
5	E	84	30% 96%
5	e	84	18% 96%
6	F	44	9% 77% 23%
6	f	44	5% 70% 27%
7	H	65	5% 97%
7	h	65	5% 98%
8	I	38	11% 92% 8%
8	i	38	11% 92% 8%
9	J	39	15% 97%
9	j	39	18% 97%
10	K	37	11% 97%
10	k	37	97%
11	L	37	97%
11	l	37	3% 100%
12	M	36	89% 6% 6%
12	m	36	94% 6%
13	O	244	5% 97%
13	o	244	2% 98%
14	T	32	3% 91% 6%
14	t	32	88% 6% 6%
15	U	104	89% 7%
15	u	104	93% 7%
16	V	137	99%
16	v	137	100%

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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	
20	R	34	

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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	912	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	d	406	X	-	-	-
28	GOL	V	204	-	-	-	X
29	LMT	F	101	-	-	-	X
37	DGD	e	101	-	-	-	X

2 Entry composition i

There are 40 unique types of molecules in this entry. The entry contains 54101 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
			Total	C	N	O	S			
1	A	334	2634	1728	432	459	15	0	3	0
1	a	334	2645	1737	432	461	15	0	6	0

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
			Total	C	N	O	S			
2	B	504	4021	2639	667	702	13	0	10	0
2	b	503	4022	2644	664	701	13	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3501	2291	584	613	13	0	4	0
3	c	455	3544	2323	589	619	13	0	6	0

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	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	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	S	0	2	0
			668	436	107	125				
5	e	81	Total	C	N	O	S	0	2	0
			670	439	107	124				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	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	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

- 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
			274	184	40	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	m	34	269	179	40	49	1	0	0	0

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
			Total	C	N	O	S			
13	O	243	1903	1191	315	392	5	0	8	0
13	o	243	1891	1183	315	388	5	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	264	185	36	41	2	0	1	0
14	t	30	264	185	36	41	2	0	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	97	774	491	129	154	0	0	0
15	u	97	774	491	129	154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1072	680	180	208	4	0	1	0
16	v	137	1064	675	177	208	4	0	0	0

- 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
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

- 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
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O		98	0	0
			239	163	41	35				

- 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	d	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

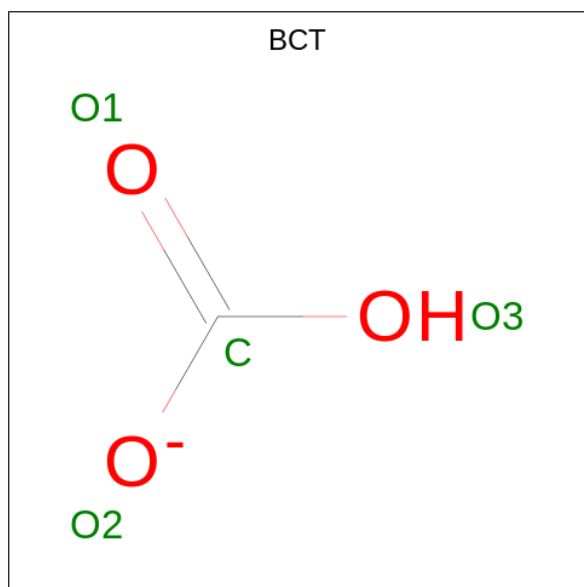
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

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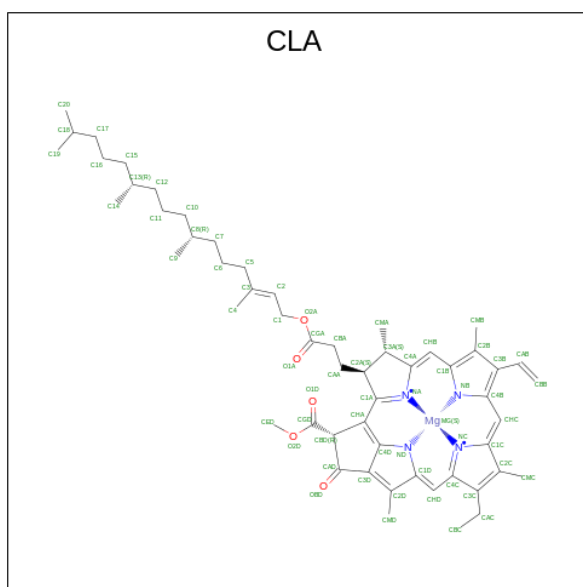
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 2 2	0	0
22	v	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 4 1 3	0	0
23	d	1	Total C O 4 1 3	0	0

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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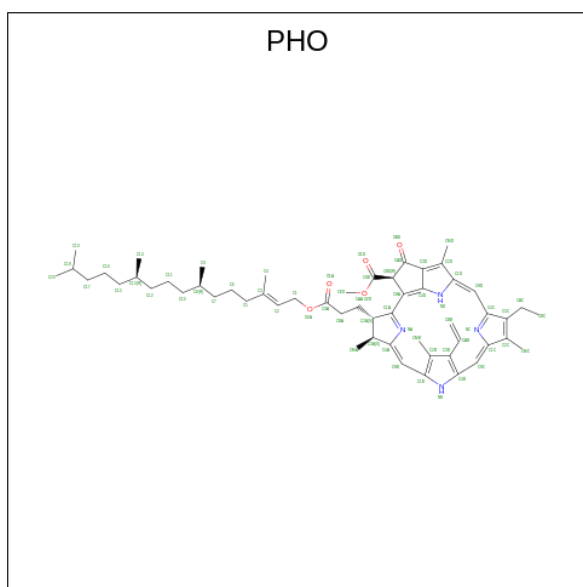
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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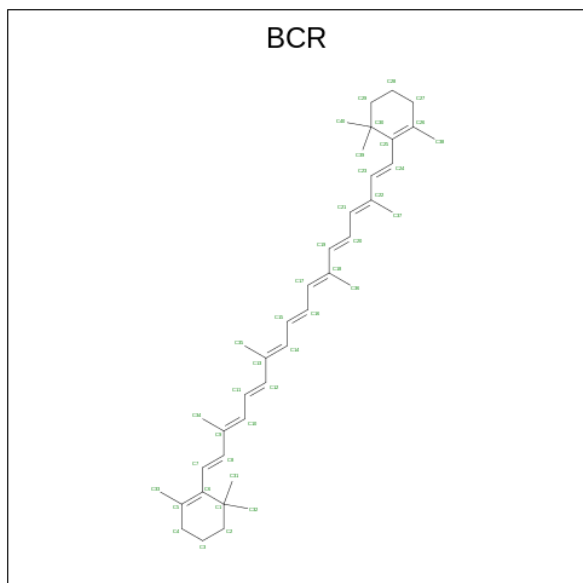
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



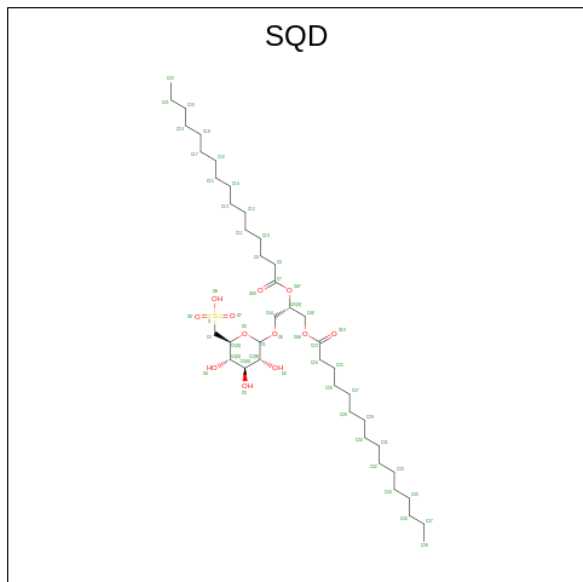
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
25	A	1	Total	64	55	4	5	0	0
25	D	1	Total	64	55	4	5	0	0
25	a	1	Total	64	55	4	5	0	0
25	d	1	Total	64	55	4	5	0	0

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
27	A	1	54	41	12	1	0	0
27	B	1	54	41	12	1	0	0
27	F	1	43	30	12	1	0	0
27	L	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	f	1	43	30	12	1	0	0

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



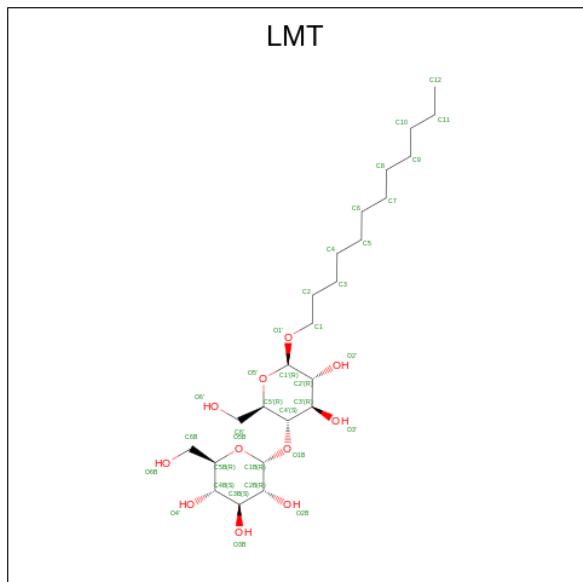
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	D	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0
28	T	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	l	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



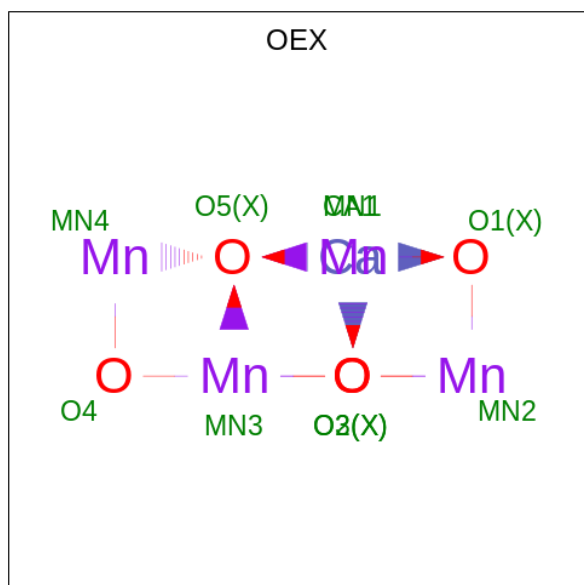
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	b	1	Total	C	O	0	0
			25	19	6		
29	e	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

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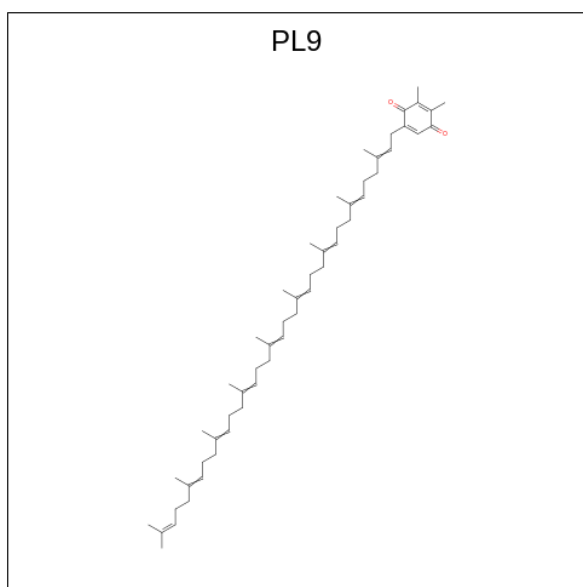
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		
29	t	1	Total	C	O	0	0
			25	19	6		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 31 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

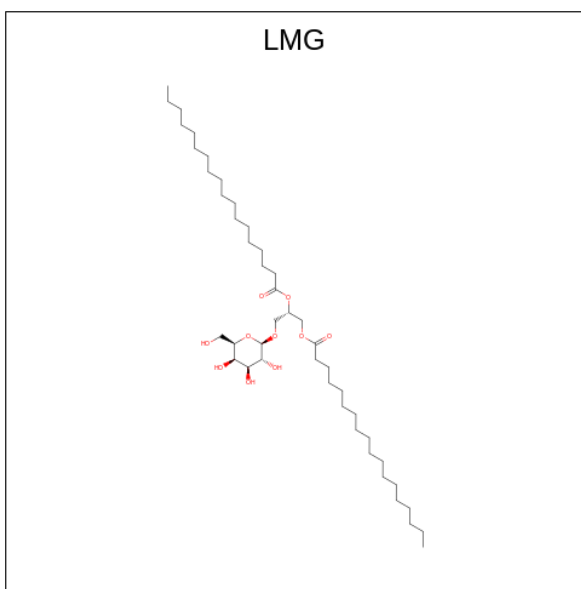
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	M	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	a	1	Total	C	O	0	0
			30	25	5		
32	b	1	Total	C	O	0	0
			33	28	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	d	2	Total	C	O	0	0
			53	47	6		
32	i	1	Total	C	O	0	0
			40	35	5		
32	j	1	Total	C		0	0
			10	10			
32	m	1	Total	C		0	0
			10	10			
32	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			51	41	10		
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		

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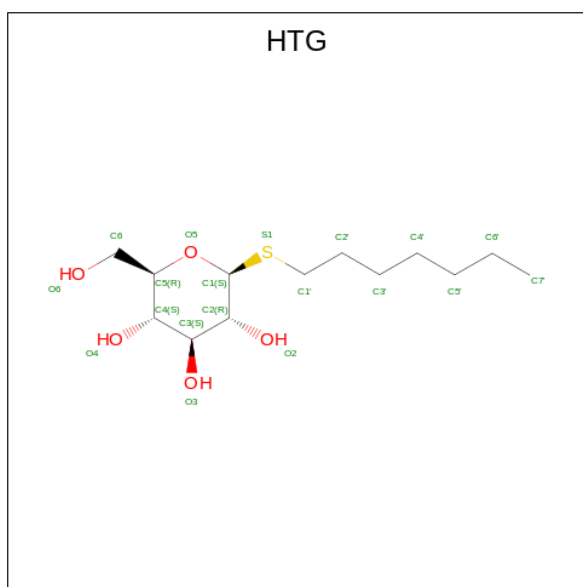
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	J	1	Total	C	O	0	0
			51	41	10		
33	Y	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	B	1	Total	Ca	0	0
			1	1		
34	C	1	Total	Ca	0	0
			1	1		
34	F	1	Total	Ca	0	0
			1	1		
34	O	1	Total	Ca	0	0
			1	1		
34	b	1	Total	Ca	0	0
			1	1		
34	c	2	Total	Ca	0	0
			2	2		
34	f	1	Total	Ca	0	0
			1	1		
34	o	1	Total	Ca	0	0
			1	1		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



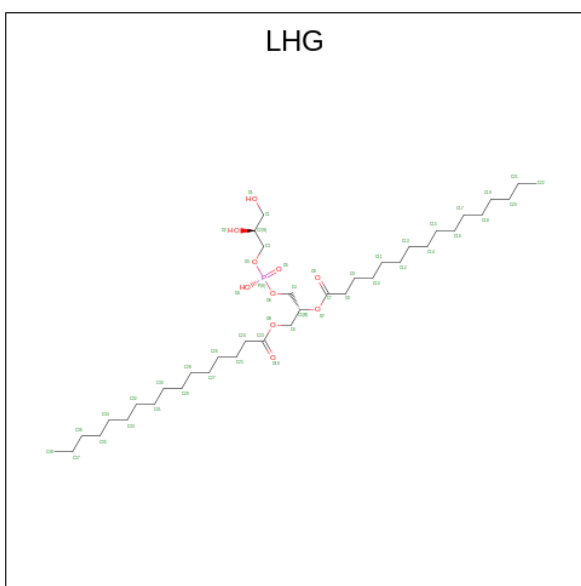
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	D	1	16	10	5	1	0	0
35	V	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	c	1	Total 19	C 13	O 5	S 1	0	0
35	c	1	Total 19	C 13	O 5	S 1	0	0
35	d	1	Total 16	C 10	O 5	S 1	0	0

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



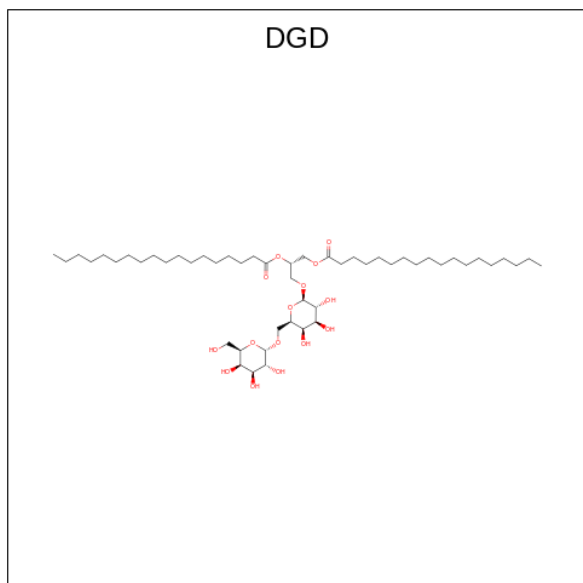
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
36	B	1	Total 49	C 38	O 10	P 1	0	0
36	D	1	Total 49	C 38	O 10	P 1	0	0
36	D	1	Total 49	C 38	O 10	P 1	0	0
36	E	1	Total 42	C 31	O 10	P 1	0	0
36	L	1	Total 49	C 38	O 10	P 1	0	0
36	a	1	Total 42	C 31	O 10	P 1	0	0
36	b	1	Total 49	C 38	O 10	P 1	0	0
36	d	1	Total 49	C 38	O 10	P 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
36	d	1	49	38	10	1	0	0
36	d	1	49	38	10	1	0	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



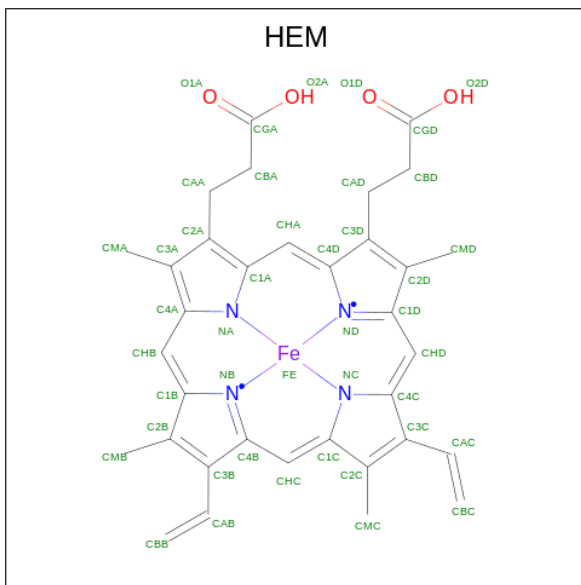
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
37	C	1	62	47	15	0	0
37	C	1	62	47	15	0	0
37	C	1	62	47	15	0	0
37	D	1	52	42	10	0	0
37	H	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	e	1	62	47	15	0	0

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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- 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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	164	Total O 167 167	0	3
40	B	295	Total O 299 299	0	4
40	C	232	Total O 234 234	0	2
40	D	140	Total O 144 144	0	4
40	E	30	Total O 31 31	0	1
40	F	10	Total O 10 10	0	0
40	H	48	Total O 48 48	0	0
40	I	6	Total O 6 6	0	0
40	J	12	Total O 12 12	0	0
40	K	7	Total O 7 7	0	0
40	L	14	Total O 15 15	0	1
40	M	13	Total O 13 13	0	0
40	O	179	Total O 181 181	0	2
40	T	16	Total O 17 17	0	1
40	U	80	Total O 80 80	0	0
40	V	114	Total O 116 116	0	2
40	Y	4	Total O 4 4	0	0
40	X	9	Total O 9 9	0	0
40	Z	1	Total O 1 1	0	0
40	a	158	Total O 159 159	0	1
40	b	262	Total O 265 265	0	3
40	c	207	Total O 210 210	0	3

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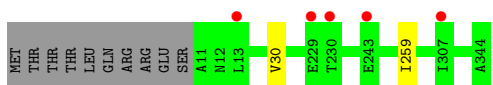
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	d	129	Total O 132 132	0	3
40	e	19	Total O 19 19	0	0
40	f	6	Total O 6 6	0	0
40	h	40	Total O 40 40	0	0
40	i	4	Total O 4 4	0	0
40	j	6	Total O 6 6	0	0
40	k	7	Total O 7 7	0	0
40	l	10	Total O 10 10	0	0
40	m	15	Total O 15 15	0	0
40	o	155	Total O 155 155	0	0
40	t	11	Total O 11 11	0	0
40	u	97	Total O 97 97	0	0
40	v	77	Total O 78 78	0	1
40	y	2	Total O 2 2	0	0
40	x	6	Total O 6 6	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1



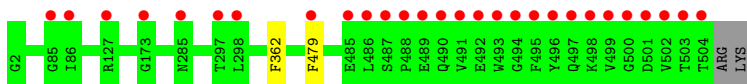
- Molecule 1: Photosystem II protein D1



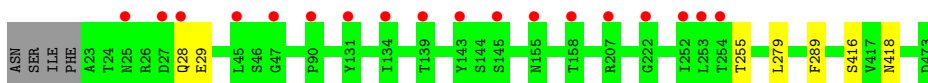
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



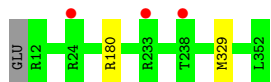
- Molecule 3: Photosystem II CP43 reaction center protein



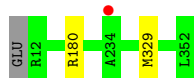
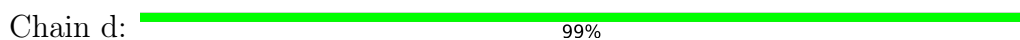
- Molecule 3: Photosystem II CP43 reaction center protein



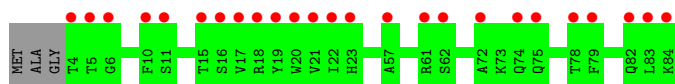
• Molecule 4: Photosystem II D2 protein



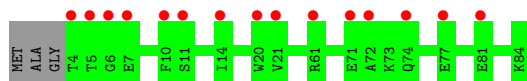
• Molecule 4: Photosystem II D2 protein



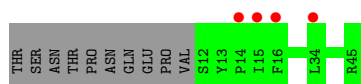
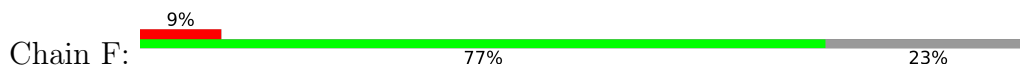
• Molecule 5: Cytochrome b559 subunit alpha



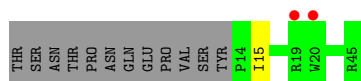
• Molecule 5: Cytochrome b559 subunit alpha



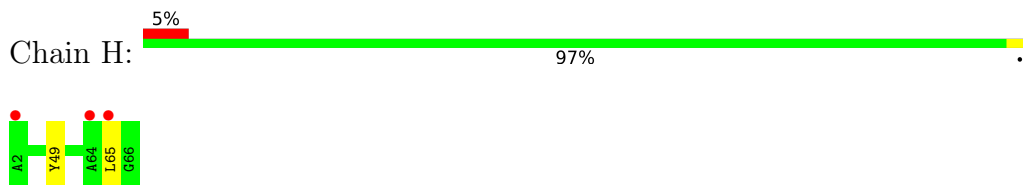
• Molecule 6: Cytochrome b559 subunit beta



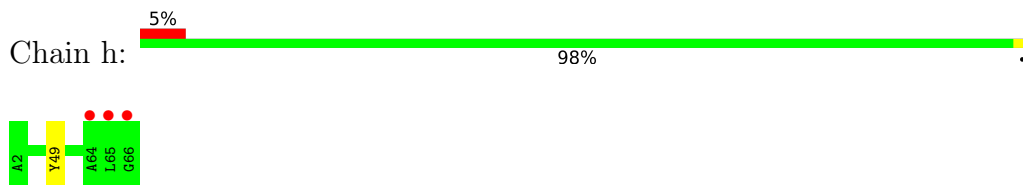
• Molecule 6: Cytochrome b559 subunit beta



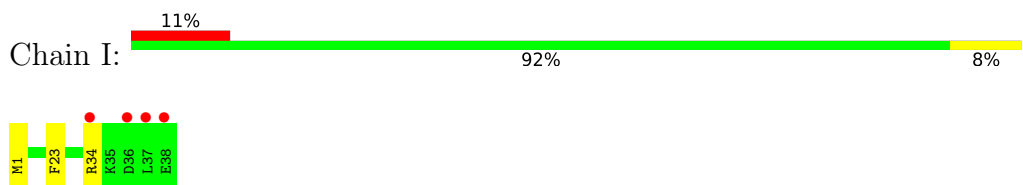
- Molecule 7: Photosystem II reaction center protein H



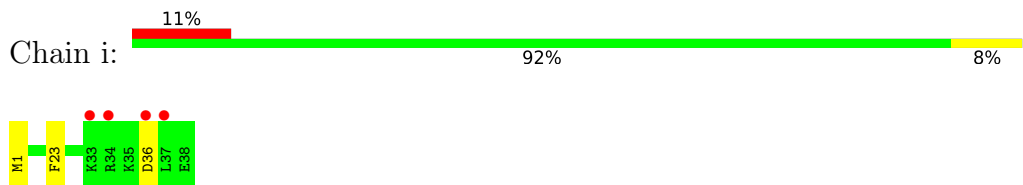
- Molecule 7: Photosystem II reaction center protein H



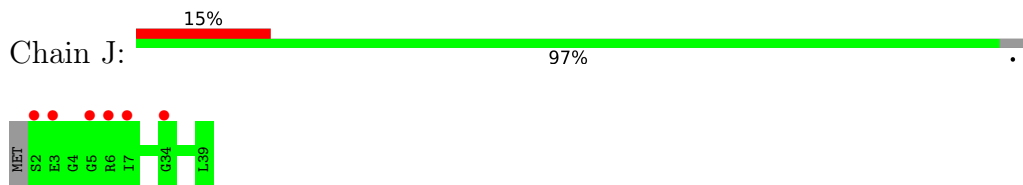
- Molecule 8: Photosystem II reaction center protein I



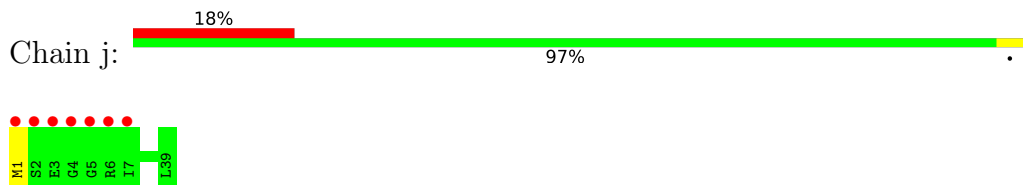
- Molecule 8: Photosystem II reaction center protein I



- 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: 97%



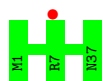
- Molecule 11: Photosystem II reaction center protein L

Chain L: 97%



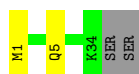
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 89% 6% 6%



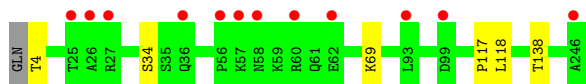
- Molecule 12: Photosystem II reaction center protein M

Chain m: 94% 6%



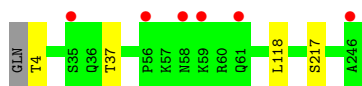
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 97%

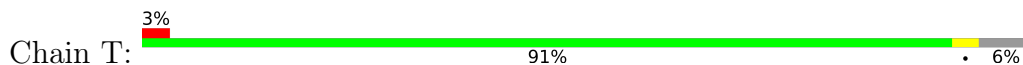


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

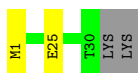
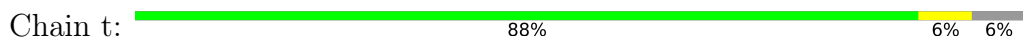
Chain o: 98%



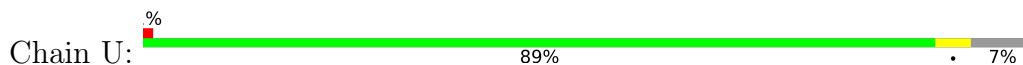
- Molecule 14: Photosystem II reaction center protein T



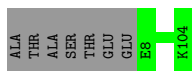
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



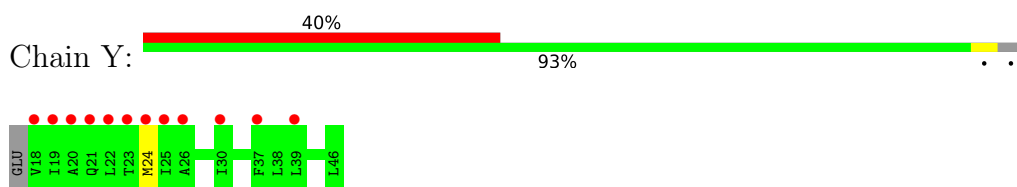
- Molecule 16: Cytochrome c-550



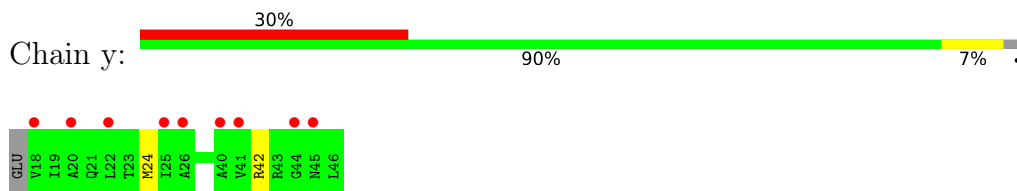
- Molecule 16: Cytochrome c-550



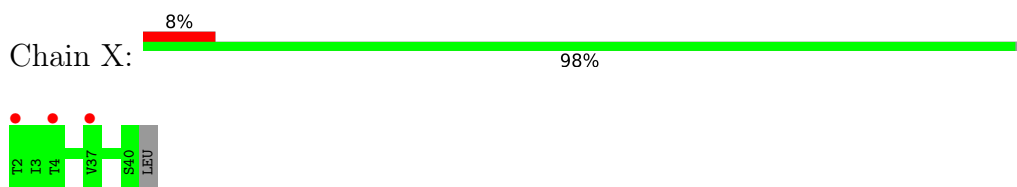
- Molecule 17: Photosystem II reaction center protein Ycf12



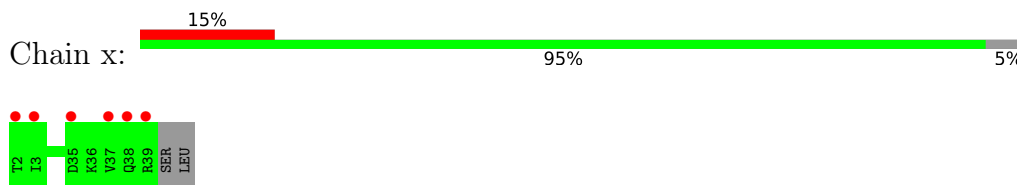
- Molecule 17: Photosystem II reaction center protein Ycf12



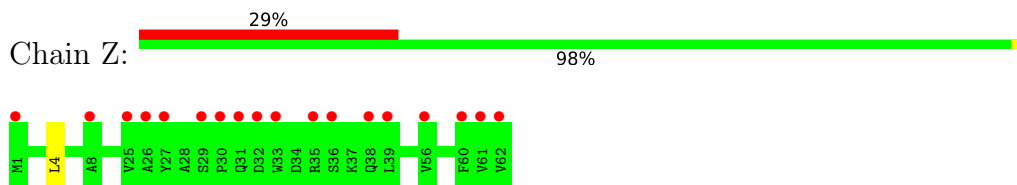
- Molecule 18: Photosystem II reaction center protein X



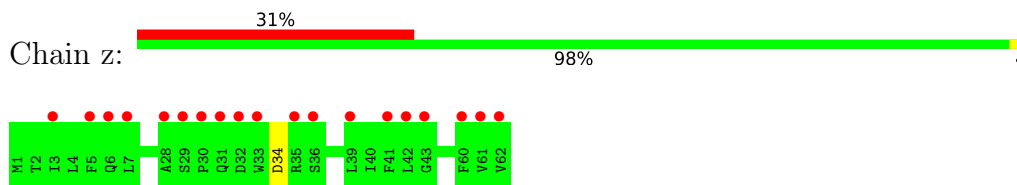
- Molecule 18: Photosystem II reaction center protein X



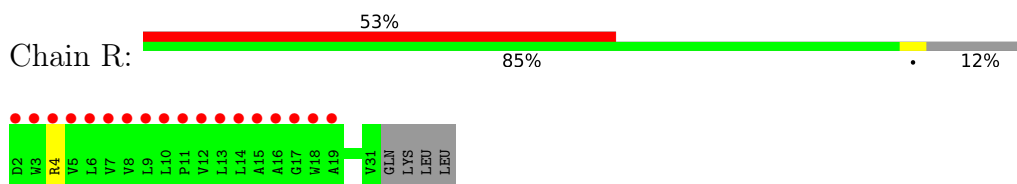
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.35 121.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.35) 99.9 (121.57-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.153 , 0.209 0.160 , 0.213	Depositor DCC
R_{free} test set	17809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtrriage
Anisotropy	0.577	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 83.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54101	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: PHO, GOL, HTG, LMG, CA, UNL, SQD, LHG, FE2, PL9, HEM, DGD, MG, CL, BCT, OEX, CLA, BCR, LMT, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/2728	0.56	0/3719
1	a	0.47	0/2748	0.57	0/3746
2	B	0.44	0/4191	0.54	0/5709
2	b	0.44	0/4198	0.54	0/5720
3	C	0.40	0/3626	0.52	0/4936
3	c	0.39	0/3676	0.52	0/5004
4	D	0.48	0/2818	0.56	0/3840
4	d	0.47	0/2818	0.56	0/3840
5	E	0.37	0/693	0.51	0/944
5	e	0.36	0/695	0.52	0/948
6	F	0.44	0/284	0.53	0/387
6	f	0.44	0/265	0.54	0/360
7	H	0.38	0/535	0.57	0/728
7	h	0.37	0/524	0.51	0/713
8	I	0.37	0/311	0.51	0/419
8	i	0.40	0/311	0.49	0/419
9	J	0.37	0/278	0.43	0/376
9	j	0.37	0/286	0.46	0/386
10	K	0.36	0/303	0.54	0/416
10	k	0.37	0/303	0.50	0/416
11	L	0.41	0/319	0.51	0/433
11	l	0.45	0/319	0.48	0/433
12	M	0.52	0/270	0.69	0/368
12	m	0.49	0/262	0.62	0/357
13	O	0.39	0/1958	0.56	0/2654
13	o	0.39	0/1937	0.57	0/2625
14	T	0.45	0/266	0.54	0/362
14	t	0.53	0/266	0.52	0/362
15	U	0.41	0/785	0.56	0/1064
15	u	0.41	0/785	0.56	0/1064
16	V	0.38	0/1096	0.52	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.37	0/1085	0.54	0/1473
17	Y	0.36	0/216	0.50	0/289
17	y	0.33	0/216	0.46	0/289
18	X	0.35	0/290	0.47	0/392
18	x	0.34	0/284	0.47	0/384
19	Z	0.32	0/490	0.48	0/669
19	z	0.29	0/490	0.50	0/669
20	R	0.24	0/245	0.39	0/338
All	All	0.42	0/43170	0.54	0/58738

There are no bond length outliers.

There are no bond angle outliers.

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	335/344 (97%)	328 (98%)	5 (2%)	2 (1%)	25	27
1	a	338/344 (98%)	331 (98%)	5 (2%)	2 (1%)	25	27
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	442 (98%)	9 (2%)	2 (0%)	34	38
3	c	459/455 (101%)	448 (98%)	9 (2%)	2 (0%)	34	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	2
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	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	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	242 (97%)	6 (2%)	1 (0%)	34	38
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	24 (89%)	3 (11%)	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%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5282/5384 (98%)	5151 (98%)	121 (2%)	10 (0%)	47	56

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	I	34	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	273 (99%)	2 (1%)	84	91
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	82
2	b	413/403 (102%)	411 (100%)	2 (0%)	88	94
3	C	356/356 (100%)	350 (98%)	6 (2%)	60	72
3	c	362/356 (102%)	352 (97%)	10 (3%)	43	53
4	D	277/277 (100%)	275 (99%)	2 (1%)	84	91
4	d	277/277 (100%)	275 (99%)	2 (1%)	84	91
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	74 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	41
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	43
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	52
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	22
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	42
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	46
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	46
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	53
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	30 (97%)	1 (3%)	39	47
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	61
13	o	211/207 (102%)	206 (98%)	5 (2%)	49	59
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	14
15	U	84/89 (94%)	81 (96%)	3 (4%)	35	43
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	89
16	v	117/117 (100%)	117 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	33
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	8
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	68
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	68
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	39
All	All	4387/4403 (100%)	4324 (99%)	63 (1%)	67	78

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Y	24	MET
13	o	118	LEU
3	c	19	ASN

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Mol	Chain	Res	Type
13	o	37	THR
14	t	25[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	315	ASN
16	v	86	GLN
2	b	331	ASN
19	z	58	ASN
13	o	147	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.44	1 (14%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.23	1 (14%)
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.16	1 (14%)
14	FME	t	1	14	8,9,10	0.80	0	7,9,11	2.51	5 (71%)
12	FME	m	1	12	8,9,10	0.67	0	7,9,11	1.08	0
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.26	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.15	116.44	122.82
14	t	1	FME	C-CA-N	3.05	115.23	109.73
14	T	1	FME	O-C-CA	-2.50	118.21	124.78
14	t	1	FME	O-C-CA	-2.47	118.31	124.78
14	t	1	FME	CE-SD-CG	-2.19	92.88	100.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 19 are monoatomic and 18 are unknown - leaving 214 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$
24	CLA	B	610	-	65,73,73	2.01	16 (24%)	76,113,113	2.66	26 (34%)
29	LMT	a	401	-	36,36,36	0.51	1 (2%)	47,47,47	1.15	3 (6%)
24	CLA	C	507	40	65,73,73	2.04	16 (24%)	76,113,113	2.73	27 (35%)
26	BCR	d	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.66	15 (26%)
24	CLA	B	604	-	65,73,73	2.08	16 (24%)	76,113,113	2.85	26 (34%)
24	CLA	b	613	-	65,73,73	2.09	16 (24%)	76,113,113	2.69	29 (38%)
24	CLA	B	617	-	65,73,73	2.04	15 (23%)	76,113,113	2.78	26 (34%)
24	CLA	A	405	-	65,73,73	2.08	16 (24%)	76,113,113	2.74	29 (38%)
24	CLA	C	511	3	65,73,73	2.10	16 (24%)	76,113,113	2.67	26 (34%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.49	0
35	HTG	b	628	-	19,19,19	1.21	2 (10%)	23,24,24	1.69	3 (13%)
24	CLA	B	615	-	65,73,73	2.10	16 (24%)	76,113,113	2.79	28 (36%)
24	CLA	b	609	-	65,73,73	2.08	18 (27%)	76,113,113	2.68	25 (32%)
33	LMG	a	411	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	5 (8%)
36	LHG	d	411	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
28	GOL	C	523	-	5,5,5	0.37	0	5,5,5	0.88	0
28	GOL	v	203	-	5,5,5	0.35	0	5,5,5	0.27	0
24	CLA	c	902	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	28 (36%)
24	CLA	C	502	-	65,73,73	2.07	16 (24%)	76,113,113	2.69	26 (34%)
36	LHG	D	410	-	48,48,48	0.97	2 (4%)	51,54,54	1.20	4 (7%)
24	CLA	c	908	40	65,73,73	2.03	16 (24%)	76,113,113	2.68	25 (32%)
27	SQD	F	103	-	42,43,54	1.17	3 (7%)	51,54,65	1.58	9 (17%)
36	LHG	B	635	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
36	LHG	d	410	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	4 (7%)
37	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.12	6 (7%)
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.41	9 (16%)
28	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.47	0
24	CLA	A	406	40	65,73,73	2.09	16 (24%)	76,113,113	2.88	30 (39%)
35	HTG	B	625	-	19,19,19	1.05	2 (10%)	23,24,24	1.64	2 (8%)
28	GOL	V	207	-	5,5,5	0.34	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.02	6 (7%)
35	HTG	c	921	-	19,19,19	1.00	2 (10%)	23,24,24	1.56	1 (4%)
33	LMG	A	419	-	51,51,55	0.96	2 (3%)	59,59,63	1.12	4 (6%)
24	CLA	b	616	-	65,73,73	1.99	16 (24%)	76,113,113	2.78	27 (35%)
24	CLA	c	912	3	65,73,73	2.03	16 (24%)	76,113,113	2.72	25 (32%)
24	CLA	c	904	-	65,73,73	2.05	15 (23%)	76,113,113	2.75	24 (31%)
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.49	0
28	GOL	a	413	-	5,5,5	0.41	0	5,5,5	0.26	0
27	SQD	A	414	-	53,54,54	1.03	3 (5%)	62,65,65	1.12	6 (9%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
24	CLA	B	602	40	65,73,73	2.07	17 (26%)	76,113,113	2.81	23 (30%)
24	CLA	C	510	-	65,73,73	2.11	16 (24%)	76,113,113	2.72	27 (35%)
29	LMT	t	101	-	25,25,36	0.50	0	30,30,47	0.77	1 (3%)
26	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.48	9 (16%)
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.64	11 (17%)
28	GOL	T	101	-	5,5,5	0.38	0	5,5,5	0.22	0
37	DGD	c	916	-	63,63,67	0.84	2 (3%)	77,77,81	1.07	7 (9%)
26	BCR	b	624	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
29	LMT	b	602	-	25,25,36	0.57	1 (4%)	30,30,47	1.12	2 (6%)
24	CLA	B	605	-	65,73,73	2.00	15 (23%)	76,113,113	2.76	27 (35%)
36	LHG	b	635	-	48,48,48	0.96	2 (4%)	51,54,54	1.12	3 (5%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.41	0
24	CLA	C	508	-	65,73,73	2.09	16 (24%)	76,113,113	2.74	26 (34%)
27	SQD	L	102	-	53,54,54	1.04	3 (5%)	62,65,65	1.55	11 (17%)
24	CLA	c	913	-	65,73,73	2.06	15 (23%)	76,113,113	2.86	28 (36%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.47	0
29	LMT	M	101	-	36,36,36	0.46	0	47,47,47	0.92	0
35	HTG	B	623	-	19,19,19	1.20	1 (5%)	23,24,24	1.28	1 (4%)
24	CLA	A	409	-	65,73,73	2.07	16 (24%)	76,113,113	2.61	29 (38%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.57	11 (17%)
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.61	0
28	GOL	c	928	-	5,5,5	0.41	0	5,5,5	0.25	0
24	CLA	c	906	-	65,73,73	1.99	16 (24%)	76,113,113	2.61	25 (32%)
28	GOL	D	402	-	5,5,5	0.43	0	5,5,5	0.35	0
24	CLA	b	612	40	65,73,73	2.00	15 (23%)	76,113,113	2.66	27 (35%)
24	CLA	B	616	-	65,73,73	2.04	16 (24%)	76,113,113	2.69	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HEM	V	202	16	41,50,50	1.36	5 (12%)	45,82,82	1.80	9 (20%)
24	CLA	c	903	-	65,73,73	2.08	16 (24%)	76,113,113	2.70	24 (31%)
30	OEX	A	416	3,40,1	0,15,15	-	-	-	-	-
24	CLA	b	619	-	65,73,73	2.07	16 (24%)	76,113,113	2.86	31 (40%)
35	HTG	B	624	-	19,19,19	0.82	1 (5%)	23,24,24	1.74	4 (17%)
26	BCR	C	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.52	9 (16%)
28	GOL	B	626	-	5,5,5	0.41	0	5,5,5	0.34	0
24	CLA	b	620	-	65,73,73	2.06	16 (24%)	76,113,113	2.73	29 (38%)
28	GOL	b	630	-	5,5,5	0.40	0	5,5,5	0.14	0
29	LMT	M	103	-	36,36,36	0.59	1 (2%)	47,47,47	1.08	4 (8%)
31	PL9	D	407	-	55,55,55	0.64	2 (3%)	68,69,69	1.89	22 (32%)
38	HEM	v	202	16	41,50,50	1.30	5 (12%)	45,82,82	1.74	9 (20%)
24	CLA	C	504	40	65,73,73	2.10	16 (24%)	76,113,113	2.80	27 (35%)
24	CLA	C	505	-	65,73,73	1.97	16 (24%)	76,113,113	2.63	26 (34%)
28	GOL	l	101	-	5,5,5	0.47	0	5,5,5	0.24	0
24	CLA	C	513	-	65,73,73	2.04	15 (23%)	76,113,113	2.74	27 (35%)
26	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.53	10 (17%)
35	HTG	d	414	-	16,16,19	1.14	2 (12%)	20,21,24	1.76	1 (5%)
24	CLA	B	611	40	65,73,73	2.05	17 (26%)	76,113,113	2.78	29 (38%)
26	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	9 (16%)
26	BCR	b	623	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)
28	GOL	V	201	34	5,5,5	0.34	0	5,5,5	0.26	0
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.47	12 (21%)
24	CLA	b	614	-	65,73,73	2.02	15 (23%)	76,113,113	2.82	26 (34%)
29	LMT	b	626	-	25,25,36	0.47	0	30,30,47	0.58	0
29	LMT	m	103	-	36,36,36	0.49	0	47,47,47	1.08	3 (6%)
35	HTG	B	633	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
29	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.86	1 (2%)
33	LMG	d	415	39	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
25	PHO	A	408	-	51,69,69	1.84	8 (15%)	47,99,99	1.73	8 (17%)
24	CLA	b	606	40	65,73,73	2.11	15 (23%)	76,113,113	2.75	24 (31%)
25	PHO	d	403	-	51,69,69	1.85	7 (13%)	47,99,99	1.96	12 (25%)
27	SQD	a	402	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	6 (9%)
28	GOL	A	412	-	5,5,5	0.39	0	5,5,5	0.29	0
24	CLA	b	611	-	65,73,73	2.04	16 (24%)	76,113,113	2.78	27 (35%)
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	a	412	-	5,5,5	0.39	0	5,5,5	0.53	0
24	CLA	c	911	-	65,73,73	2.09	16 (24%)	76,113,113	2.73	28 (36%)
24	CLA	b	610	-	65,73,73	2.01	16 (24%)	76,113,113	2.91	24 (31%)
35	HTG	B	632	-	19,19,19	0.96	2 (10%)	23,24,24	1.37	2 (8%)
24	CLA	C	506	-	65,73,73	2.07	16 (24%)	76,113,113	2.72	29 (38%)
24	CLA	C	501	-	65,73,73	2.08	16 (24%)	76,113,113	2.77	27 (35%)
35	HTG	b	603	-	19,19,19	1.00	2 (10%)	23,24,24	1.55	4 (17%)
27	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.45	6 (11%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	5 (6%)
26	BCR	A	410	-	41,41,41	1.11	1 (2%)	56,56,56	1.11	4 (7%)
24	CLA	D	405	-	65,73,73	2.01	17 (26%)	76,113,113	2.73	26 (34%)
35	HTG	c	922	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	3 (13%)
24	CLA	b	615	40	65,73,73	2.09	17 (26%)	76,113,113	2.70	30 (39%)
29	LMT	D	403	-	36,36,36	0.47	0	47,47,47	1.04	3 (6%)
31	PL9	A	417	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	23 (33%)
24	CLA	B	608	40	65,73,73	2.04	17 (26%)	76,113,113	2.74	27 (35%)
28	GOL	B	630	-	5,5,5	0.39	0	5,5,5	0.21	0
25	PHO	a	407	-	51,69,69	1.89	8 (15%)	47,99,99	1.81	11 (23%)
33	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.30	7 (11%)
35	HTG	C	521	-	19,19,19	1.02	2 (10%)	23,24,24	1.76	3 (13%)
24	CLA	B	612	-	65,73,73	1.98	16 (24%)	76,113,113	2.89	29 (38%)
24	CLA	b	608	-	65,73,73	2.02	17 (26%)	76,113,113	2.79	27 (35%)
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	4 (17%)
24	CLA	b	607	-	65,73,73	2.07	17 (26%)	76,113,113	2.88	30 (39%)
33	LMG	Y	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.00	4 (6%)
28	GOL	V	204	-	5,5,5	0.38	0	5,5,5	0.37	0
28	GOL	T	103	-	5,5,5	0.40	0	5,5,5	0.30	0
24	CLA	c	910	-	65,73,73	2.17	16 (24%)	76,113,113	2.76	27 (35%)
33	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.25	8 (13%)
26	BCR	b	622	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	9 (16%)
24	CLA	c	909	-	65,73,73	2.07	16 (24%)	76,113,113	2.78	27 (35%)
26	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	14 (25%)
28	GOL	V	206	-	5,5,5	0.43	0	5,5,5	0.32	0
36	LHG	d	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	6 (11%)
29	LMT	A	415	-	36,36,36	0.67	1 (2%)	47,47,47	1.43	5 (10%)
26	BCR	c	927	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	D	409	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	3 (5%)
26	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
28	GOL	A	413	-	5,5,5	0.38	0	5,5,5	0.22	0
29	LMT	a	417	-	36,36,36	0.42	0	47,47,47	0.79	1 (2%)
24	CLA	B	603	-	65,73,73	2.02	17 (26%)	76,113,113	2.86	29 (38%)
35	HTG	b	604	-	19,19,19	0.99	2 (10%)	23,24,24	1.11	1 (4%)
24	CLA	D	404	-	65,73,73	2.00	17 (26%)	76,113,113	2.90	31 (40%)
24	CLA	C	512	-	65,73,73	2.07	16 (24%)	76,113,113	2.73	27 (35%)
29	LMT	F	101	-	36,36,36	0.46	0	47,47,47	0.90	1 (2%)
33	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
24	CLA	B	613	-	65,73,73	2.02	15 (23%)	76,113,113	2.77	24 (31%)
24	CLA	a	406	40	65,73,73	2.04	15 (23%)	76,113,113	2.85	27 (35%)
24	CLA	c	914	-	65,73,73	2.05	16 (24%)	76,113,113	2.82	27 (35%)
24	CLA	B	614	-	65,73,73	2.12	15 (23%)	76,113,113	2.69	30 (39%)
36	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
28	GOL	B	629	-	5,5,5	0.35	0	5,5,5	0.31	0
28	GOL	c	923	-	5,5,5	0.37	0	5,5,5	0.22	0
24	CLA	c	905	40	65,73,73	2.06	16 (24%)	76,113,113	2.81	30 (39%)
37	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.04	5 (6%)
24	CLA	a	405	-	65,73,73	2.03	16 (24%)	76,113,113	2.80	30 (39%)
26	BCR	B	620	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	10 (17%)
24	CLA	B	609	-	65,73,73	2.09	16 (24%)	76,113,113	2.63	27 (35%)
24	CLA	B	606	-	65,73,73	2.03	15 (23%)	76,113,113	2.81	26 (34%)
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)
28	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.39	0
24	CLA	a	408	-	65,73,73	2.03	16 (24%)	76,113,113	2.84	29 (38%)
33	LMG	b	625	-	51,51,55	0.89	2 (3%)	59,59,63	1.11	5 (8%)
33	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	0.97	3 (5%)
28	GOL	b	632	-	5,5,5	0.38	0	5,5,5	0.33	0
33	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.39	6 (13%)
24	CLA	d	404	40	65,73,73	2.08	15 (23%)	76,113,113	2.77	29 (38%)
24	CLA	b	617	-	65,73,73	2.01	16 (24%)	76,113,113	2.74	29 (38%)
35	HTG	b	601	-	19,19,19	1.03	1 (5%)	23,24,24	1.28	1 (4%)
28	GOL	v	205	-	5,5,5	0.33	0	5,5,5	0.47	0
35	HTG	b	627	-	19,19,19	0.81	1 (5%)	23,24,24	1.54	3 (13%)
31	PL9	d	408	-	55,55,55	0.67	2 (3%)	68,69,69	1.69	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	406	-	65,73,73	2.08	16 (24%)	76,113,113	2.78	26 (34%)
31	PL9	a	415	-	55,55,55	0.64	2 (3%)	68,69,69	1.88	21 (30%)
38	HEM	f	101	5,6	41,50,50	1.28	6 (14%)	45,82,82	1.84	9 (20%)
28	GOL	B	631	-	5,5,5	0.33	0	5,5,5	0.43	0
24	CLA	C	503	-	65,73,73	2.08	16 (24%)	76,113,113	2.75	24 (31%)
24	CLA	b	621	-	65,73,73	2.06	15 (23%)	76,113,113	2.77	29 (38%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	13 (23%)
24	CLA	B	607	-	65,73,73	2.06	16 (24%)	76,113,113	2.88	28 (36%)
37	DGD	C	517	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	7 (9%)
37	DGD	c	917	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	6 (7%)
26	BCR	D	406	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	10 (17%)
35	HTG	V	203	-	19,19,19	1.02	2 (10%)	23,24,24	1.31	3 (13%)
24	CLA	C	509	-	65,73,73	2.14	16 (24%)	76,113,113	2.72	27 (35%)
24	CLA	b	618	-	65,73,73	2.06	15 (23%)	76,113,113	2.67	27 (35%)
26	BCR	a	409	-	41,41,41	1.05	1 (2%)	56,56,56	1.28	2 (3%)
24	CLA	d	405	-	65,73,73	1.98	17 (26%)	76,113,113	2.84	27 (35%)
24	CLA	c	907	-	65,73,73	2.03	17 (26%)	76,113,113	2.76	29 (38%)
36	LHG	L	101	-	48,48,48	0.95	3 (6%)	51,54,54	1.13	5 (9%)
36	LHG	a	418	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
26	BCR	c	915	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	10 (17%)
29	LMT	C	520	-	36,36,36	0.48	0	47,47,47	1.17	4 (8%)
26	BCR	T	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.85	17 (30%)
28	GOL	b	631	-	5,5,5	0.32	0	5,5,5	0.26	0
23	BCT	d	402	21	2,3,3	0.67	0	2,3,3	0.71	0
35	HTG	D	413	-	16,16,19	1.07	2 (12%)	20,21,24	1.52	1 (5%)
37	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	1.02	4 (5%)
30	OEX	a	416	3,40,1	0,15,15	-	-	-	-	-
24	CLA	A	407	40	65,73,73	2.04	16 (24%)	76,113,113	2.74	28 (36%)
38	HEM	F	102	5,6	41,50,50	1.31	5 (12%)	45,82,82	2.02	11 (24%)
25	PHO	D	401	-	51,69,69	1.86	7 (13%)	47,99,99	1.80	9 (19%)
26	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	8 (14%)
37	DGD	D	408	-	52,52,67	1.04	3 (5%)	60,60,81	1.17	5 (8%)
28	GOL	a	419	34	5,5,5	0.31	0	5,5,5	0.40	0
27	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.44	8 (12%)
33	LMG	c	919	-	51,51,55	0.88	2 (3%)	59,59,63	1.18	4 (6%)
28	GOL	C	524	-	5,5,5	0.41	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	v	204	-	5,5,5	0.36	0	5,5,5	0.34	0
23	BCT	A	404	21	2,3,3	0.65	0	2,3,3	1.14	0
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.57	0
26	BCR	Y	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.67	11 (19%)

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
24	CLA	B	610	-	1/1/15/20	3/37/115/115	-
29	LMT	a	401	-	-	7/21/61/61	0/2/2/2
24	CLA	C	507	40	1/1/15/20	3/37/115/115	-
26	BCR	d	407	-	-	4/29/63/63	0/2/2/2
24	CLA	B	604	-	1/1/15/20	4/37/115/115	-
24	CLA	b	613	-	-	1/37/115/115	-
24	CLA	B	617	-	1/1/15/20	8/37/115/115	-
24	CLA	A	405	-	1/1/15/20	4/37/115/115	-
24	CLA	C	511	3	1/1/15/20	4/37/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	B	615	-	1/1/15/20	18/37/115/115	-
24	CLA	b	609	-	1/1/15/20	3/37/115/115	-
33	LMG	a	411	-	-	14/46/66/70	0/1/1/1
36	LHG	d	411	-	-	12/53/53/53	-
28	GOL	C	523	-	-	2/4/4/4	-
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	c	902	-	1/1/15/20	5/37/115/115	-
24	CLA	C	502	-	1/1/15/20	8/37/115/115	-
36	LHG	D	410	-	-	18/53/53/53	-
24	CLA	c	908	40	1/1/15/20	4/37/115/115	-
27	SQD	F	103	-	-	15/38/58/69	0/1/1/1
36	LHG	B	635	-	-	13/53/53/53	-
36	LHG	d	410	-	-	9/53/53/53	-
37	DGD	C	516	-	-	16/51/91/95	0/2/2/2
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	628	-	-	2/4/4/4	-
24	CLA	A	406	40	1/1/15/20	4/37/115/115	-
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
28	GOL	V	207	-	-	4/4/4/4	-
37	DGD	H	102	-	-	9/51/91/95	0/2/2/2
35	HTG	c	921	-	-	4/10/30/30	0/1/1/1
33	LMG	A	419	-	-	21/46/66/70	0/1/1/1
24	CLA	b	616	-	1/1/15/20	3/37/115/115	-
24	CLA	c	912	3	1/1/15/20	6/37/115/115	-
24	CLA	c	904	-	1/1/15/20	6/37/115/115	-
28	GOL	b	629	-	-	0/4/4/4	-
28	GOL	a	413	-	-	2/4/4/4	-
27	SQD	A	414	-	-	13/49/69/69	0/1/1/1
33	LMG	z	101	-	-	11/34/54/70	0/1/1/1
24	CLA	B	602	40	1/1/15/20	14/37/115/115	-
24	CLA	C	510	-	1/1/15/20	8/37/115/115	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
28	GOL	T	101	-	-	0/4/4/4	-
37	DGD	c	916	-	-	12/51/91/95	0/2/2/2
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
29	LMT	b	602	-	-	7/17/37/61	0/1/1/2
24	CLA	B	605	-	1/1/15/20	4/37/115/115	-
36	LHG	b	635	-	-	20/53/53/53	-
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	C	508	-	1/1/15/20	5/37/115/115	-
27	SQD	L	102	-	-	22/49/69/69	0/1/1/1
24	CLA	c	913	-	1/1/15/20	12/37/115/115	-
28	GOL	B	636	-	-	2/4/4/4	-
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	A	409	-	1/1/15/20	10/37/115/115	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
28	GOL	c	924	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	c	928	-	-	2/4/4/4	-
24	CLA	c	906	-	1/1/15/20	8/37/115/115	-
28	GOL	D	402	-	-	4/4/4/4	-
24	CLA	b	612	40	1/1/15/20	1/37/115/115	-
24	CLA	B	616	-	1/1/15/20	11/37/115/115	-
38	HEM	V	202	16	-	4/12/54/54	-
24	CLA	c	903	-	-	5/37/115/115	-
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
24	CLA	b	619	-	1/1/15/20	20/37/115/115	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	b	620	-	1/1/15/20	7/37/115/115	-
28	GOL	b	630	-	-	0/4/4/4	-
29	LMT	M	103	-	-	11/21/61/61	0/2/2/2
31	PL9	D	407	-	-	9/53/73/73	0/1/1/1
38	HEM	v	202	16	-	4/12/54/54	-
24	CLA	C	504	40	1/1/15/20	7/37/115/115	-
24	CLA	C	505	-	1/1/15/20	6/37/115/115	-
28	GOL	l	101	-	-	0/4/4/4	-
24	CLA	C	513	-	1/1/15/20	8/37/115/115	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
24	CLA	B	611	40	1/1/15/20	4/37/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	BCR	b	623	-	-	1/29/63/63	0/2/2/2
28	GOL	V	201	34	-	2/4/4/4	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	CLA	b	614	-	1/1/15/20	3/37/115/115	-
29	LMT	b	626	-	-	5/17/37/61	0/1/1/2
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
29	LMT	e	102	-	-	9/21/61/61	0/2/2/2
33	LMG	d	415	39	-	10/46/66/70	0/1/1/1
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
24	CLA	b	606	40	1/1/15/20	16/37/115/115	-
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	a	402	-	-	10/49/69/69	0/1/1/1
28	GOL	A	412	-	-	0/4/4/4	-
24	CLA	b	611	-	1/1/15/20	14/37/115/115	-
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
28	GOL	a	412	-	-	4/4/4/4	-
24	CLA	c	911	-	1/1/15/20	7/37/115/115	-
24	CLA	b	610	-	1/1/15/20	4/37/115/115	-
35	HTG	B	632	-	-	0/10/30/30	0/1/1/1
24	CLA	C	506	-	1/1/15/20	6/37/115/115	-
24	CLA	C	501	-	1/1/15/20	7/37/115/115	-
35	HTG	b	603	-	-	1/10/30/30	0/1/1/1
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
26	BCR	A	410	-	-	4/29/63/63	0/2/2/2
24	CLA	D	405	-	1/1/15/20	4/37/115/115	-
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
24	CLA	b	615	40	1/1/15/20	5/37/115/115	-
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2
31	PL9	A	417	-	-	13/53/73/73	0/1/1/1
24	CLA	B	608	40	1/1/15/20	4/37/115/115	-
28	GOL	B	630	-	-	4/4/4/4	-
25	PHO	a	407	-	-	5/37/103/103	0/5/6/6
33	LMG	c	920	-	-	5/46/66/70	0/1/1/1
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
24	CLA	B	612	-	1/1/15/20	1/37/115/115	-
24	CLA	b	608	-	1/1/15/20	5/37/115/115	-
35	HTG	C	522	-	-	3/10/30/30	0/1/1/1
24	CLA	b	607	-	1/1/15/20	5/37/115/115	-
33	LMG	Y	101	-	-	10/46/66/70	0/1/1/1
28	GOL	V	204	-	-	2/4/4/4	-
28	GOL	T	103	-	-	2/4/4/4	-
24	CLA	c	910	-	1/1/15/20	15/37/115/115	-
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
24	CLA	c	909	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
28	GOL	V	206	-	-	2/4/4/4	-
36	LHG	d	409	-	-	18/53/53/53	-
29	LMT	A	415	-	-	5/21/61/61	0/2/2/2
26	BCR	c	927	-	-	0/29/63/63	0/2/2/2
36	LHG	D	409	-	-	11/53/53/53	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
28	GOL	A	413	-	-	2/4/4/4	-
29	LMT	a	417	-	-	4/21/61/61	0/2/2/2
24	CLA	B	603	-	1/1/15/20	3/37/115/115	-
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
24	CLA	D	404	-	1/1/15/20	0/37/115/115	-
24	CLA	C	512	-	1/1/15/20	9/37/115/115	-
29	LMT	F	101	-	-	6/21/61/61	0/2/2/2
33	LMG	B	622	-	-	8/46/66/70	0/1/1/1
24	CLA	B	613	-	1/1/15/20	5/37/115/115	-
24	CLA	a	406	40	-	11/37/115/115	-
24	CLA	c	914	-	-	5/37/115/115	-
24	CLA	B	614	-	1/1/15/20	8/37/115/115	-
36	LHG	E	101	-	-	19/46/46/53	-
28	GOL	B	629	-	-	3/4/4/4	-
28	GOL	c	923	-	-	0/4/4/4	-
24	CLA	c	905	40	1/1/15/20	4/37/115/115	-
37	DGD	c	918	-	-	13/51/91/95	0/2/2/2
24	CLA	a	405	-	1/1/15/20	4/37/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	B	609	-	-	1/37/115/115	-
24	CLA	B	606	-	1/1/15/20	6/37/115/115	-
37	DGD	e	101	-	-	26/51/91/95	0/2/2/2
28	GOL	O	302	-	-	0/4/4/4	-
24	CLA	a	408	-	1/1/15/20	10/37/115/115	-
33	LMG	b	625	-	-	8/46/66/70	0/1/1/1
33	LMG	J	101	39	-	11/46/66/70	0/1/1/1
28	GOL	b	632	-	-	2/4/4/4	-
33	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
24	CLA	d	404	40	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	617	-	1/1/15/20	4/37/115/115	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
28	GOL	v	205	-	-	2/4/4/4	-
35	HTG	b	627	-	-	2/10/30/30	0/1/1/1
31	PL9	d	408	-	-	3/53/73/73	0/1/1/1
24	CLA	d	406	-	1/1/15/20	6/37/115/115	-
31	PL9	a	415	-	-	15/53/73/73	0/1/1/1
38	HEM	f	101	5,6	-	8/12/54/54	-
28	GOL	B	631	-	-	1/4/4/4	-
24	CLA	C	503	-	1/1/15/20	2/37/115/115	-
24	CLA	b	621	-	1/1/15/20	9/37/115/115	-
26	BCR	t	102	-	-	5/29/63/63	0/2/2/2
24	CLA	B	607	-	1/1/15/20	5/37/115/115	-
37	DGD	C	517	-	-	19/51/91/95	0/2/2/2
37	DGD	c	917	-	-	18/51/91/95	0/2/2/2
26	BCR	D	406	-	-	8/29/63/63	0/2/2/2
35	HTG	V	203	-	-	5/10/30/30	0/1/1/1
24	CLA	C	509	-	1/1/15/20	14/37/115/115	-
24	CLA	b	618	-	1/1/15/20	3/37/115/115	-
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
24	CLA	d	405	-	1/1/15/20	5/37/115/115	-
24	CLA	c	907	-	1/1/15/20	13/37/115/115	-
36	LHG	L	101	-	-	16/53/53/53	-
36	LHG	a	418	-	-	15/46/46/53	-
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
29	LMT	C	520	-	-	6/21/61/61	0/2/2/2
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
28	GOL	b	631	-	-	4/4/4/4	-
35	HTG	D	413	-	-	0/7/27/30	0/1/1/1
37	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	A	407	40	-	6/37/115/115	-
38	HEM	F	102	5,6	-	4/12/54/54	-
25	PHO	D	401	-	-	4/37/103/103	0/5/6/6
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
37	DGD	D	408	-	-	18/47/67/95	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	a	419	34	-	3/4/4/4	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
33	LMG	c	919	-	-	12/46/66/70	0/1/1/1
28	GOL	C	524	-	-	2/4/4/4	-
28	GOL	v	204	-	-	2/4/4/4	-
28	GOL	V	205	-	-	0/4/4/4	-
26	BCR	Y	102	-	-	4/29/63/63	0/2/2/2

The worst 5 of 1326 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	910	CLA	C3B-C2B	6.68	1.49	1.40
24	A	406	CLA	C3B-C2B	6.68	1.49	1.40
24	c	912	CLA	C3B-C2B	6.65	1.49	1.40
24	C	509	CLA	C3B-C2B	6.59	1.49	1.40
24	C	504	CLA	C3B-C2B	6.45	1.49	1.40

The worst 5 of 2566 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	914	CLA	C1D-ND-C4D	-10.25	99.05	106.33
24	b	610	CLA	C1D-ND-C4D	-10.21	99.08	106.33
24	D	404	CLA	C1D-ND-C4D	-10.09	99.16	106.33
24	B	602	CLA	C1D-ND-C4D	-9.98	99.24	106.33
24	a	406	CLA	C1D-ND-C4D	-9.97	99.25	106.33

5 of 64 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	409	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND

5 of 1331 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D

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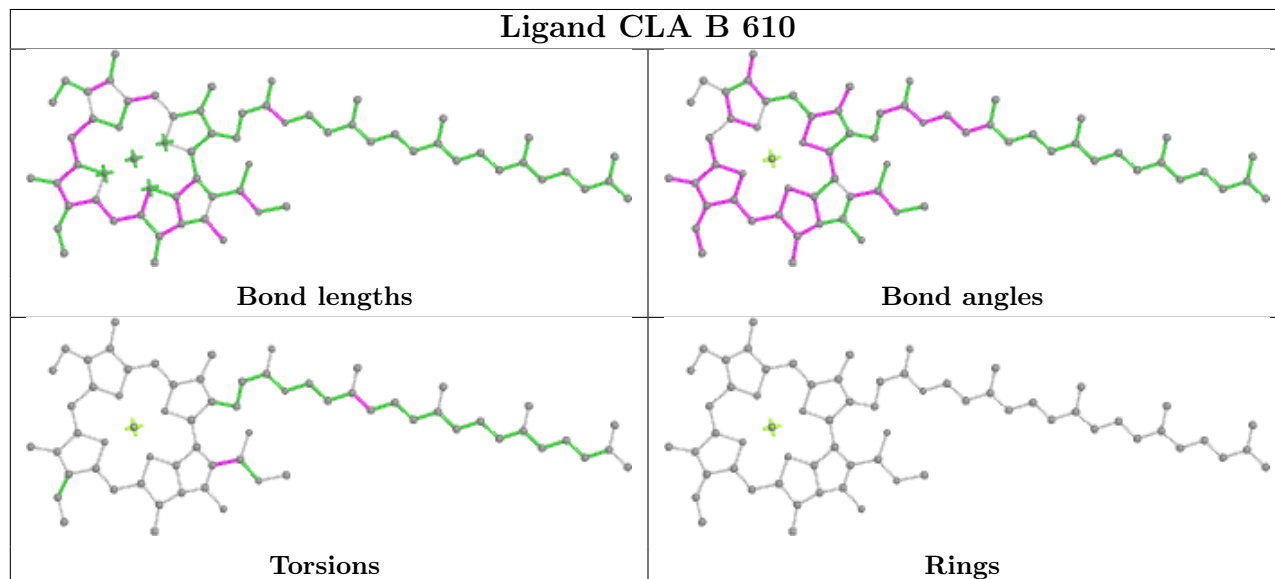
Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	C11-C10-C8-C9

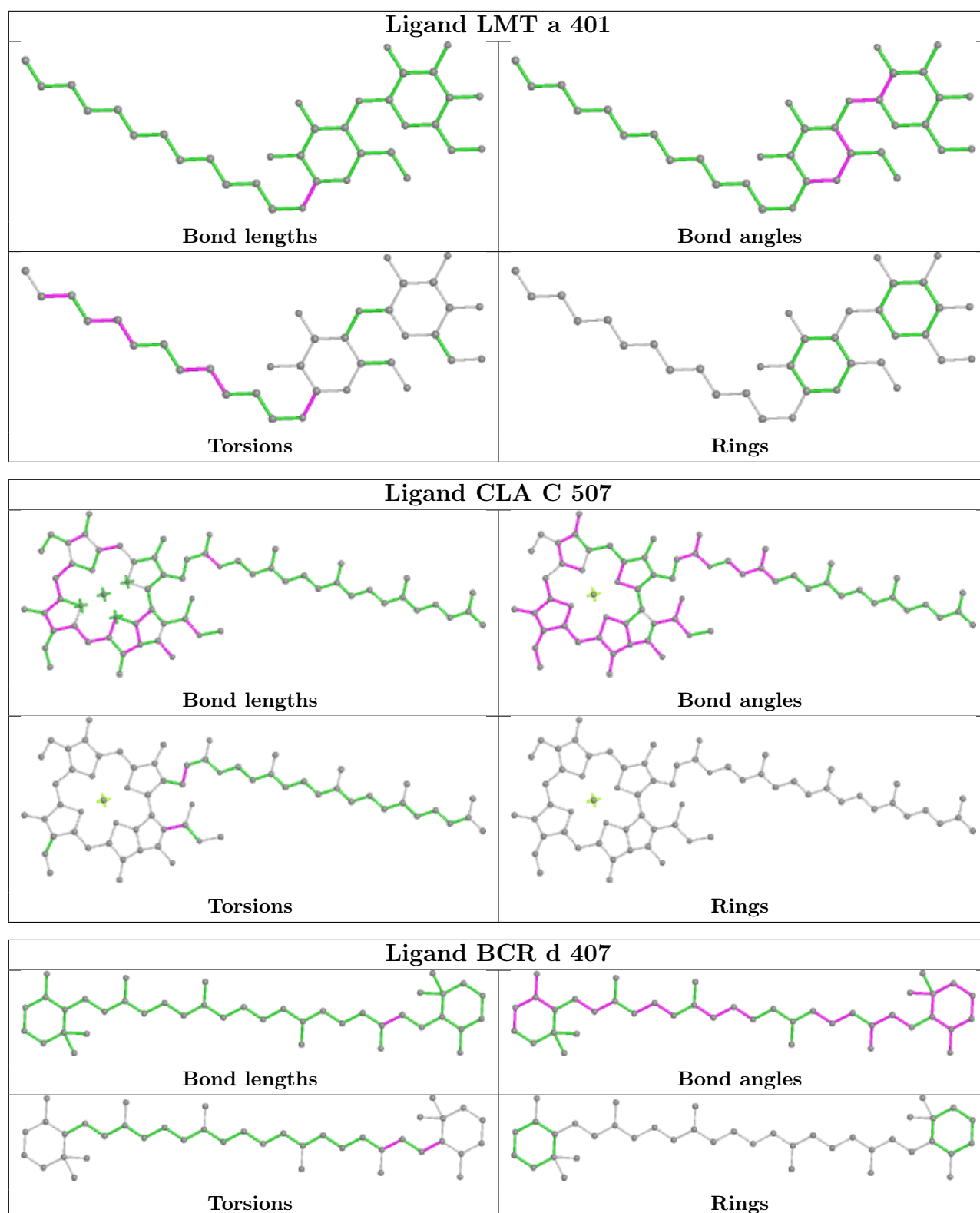
There are no ring outliers.

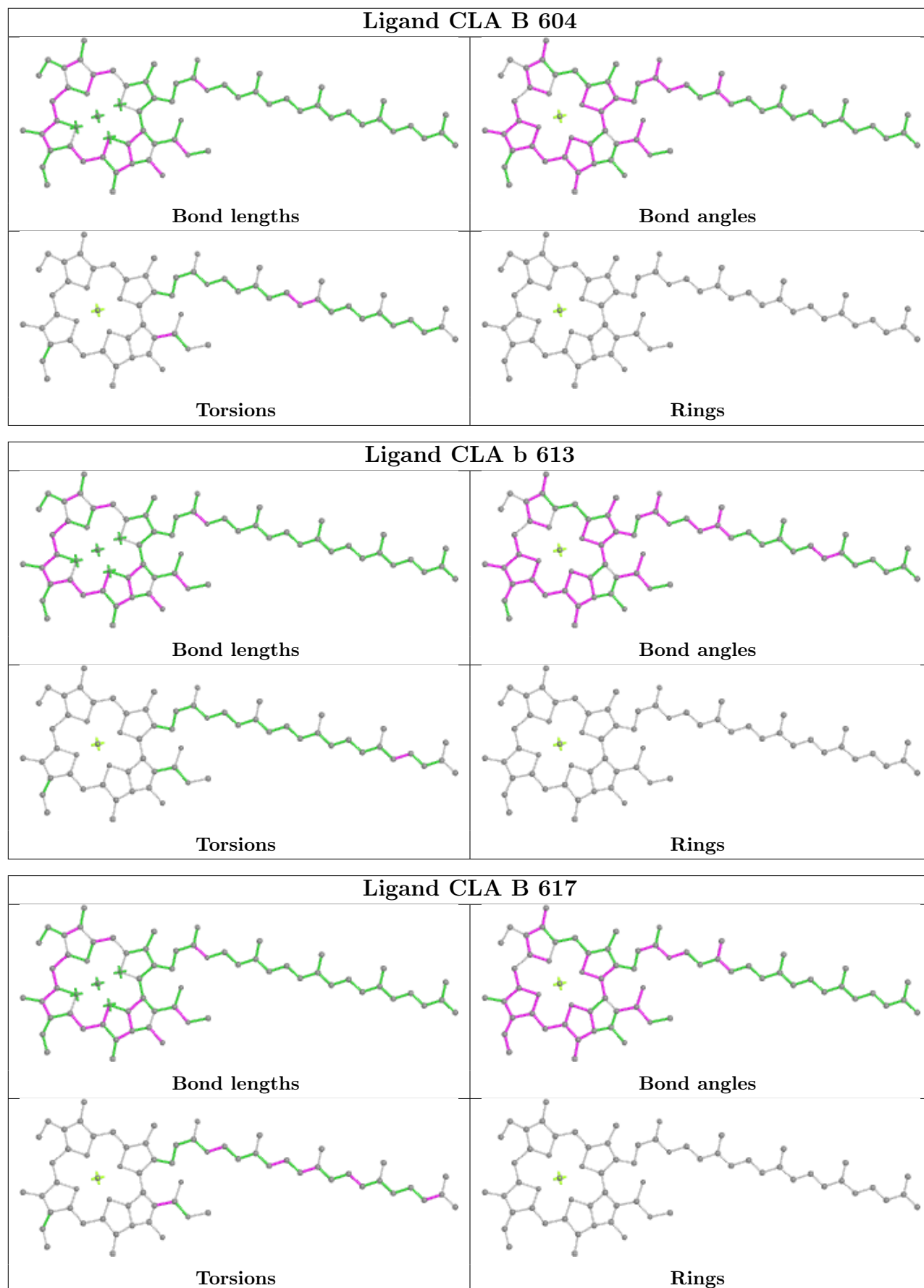
1 monomer is involved in 1 short contact:

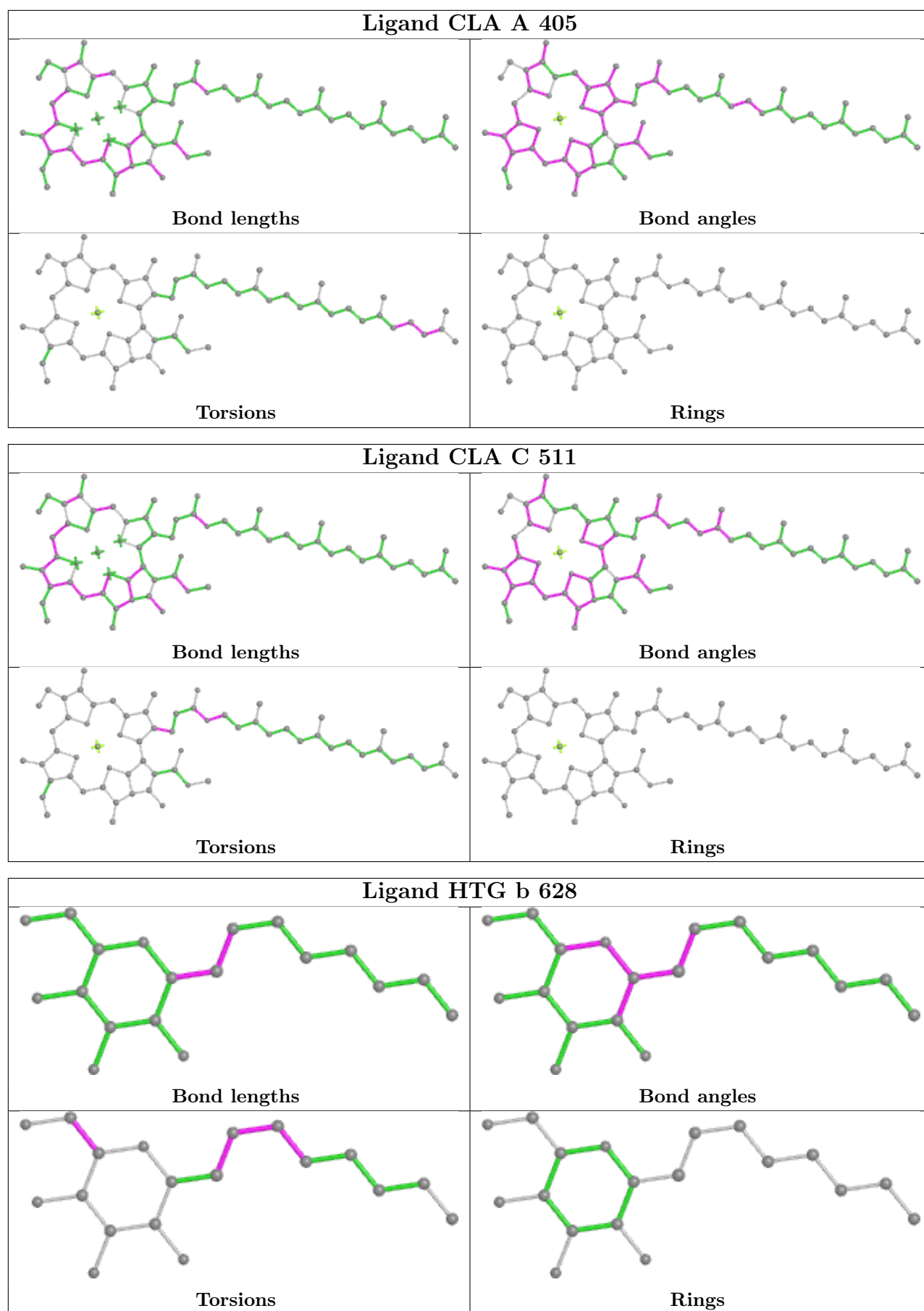
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	f	102	SQD	0	1

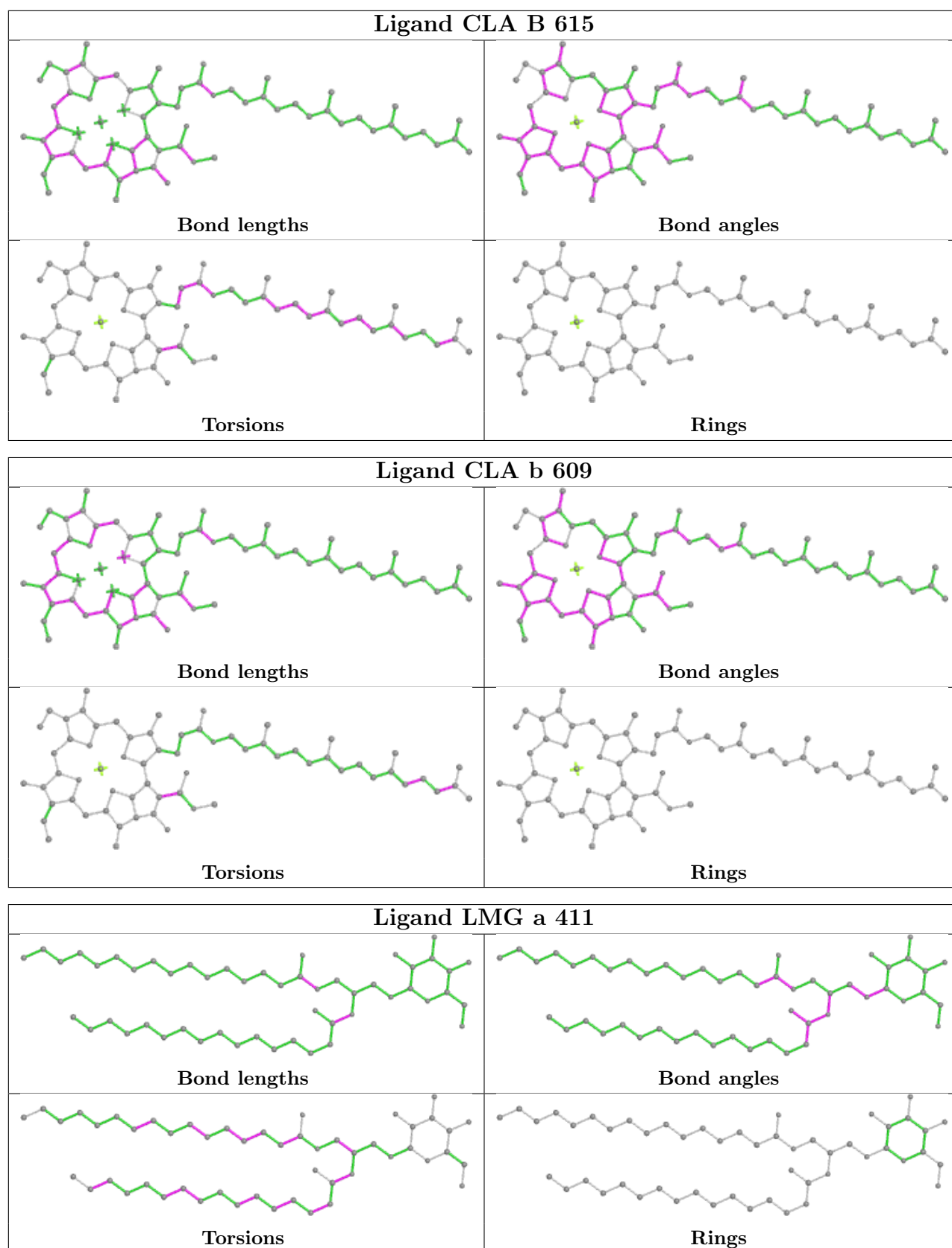
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

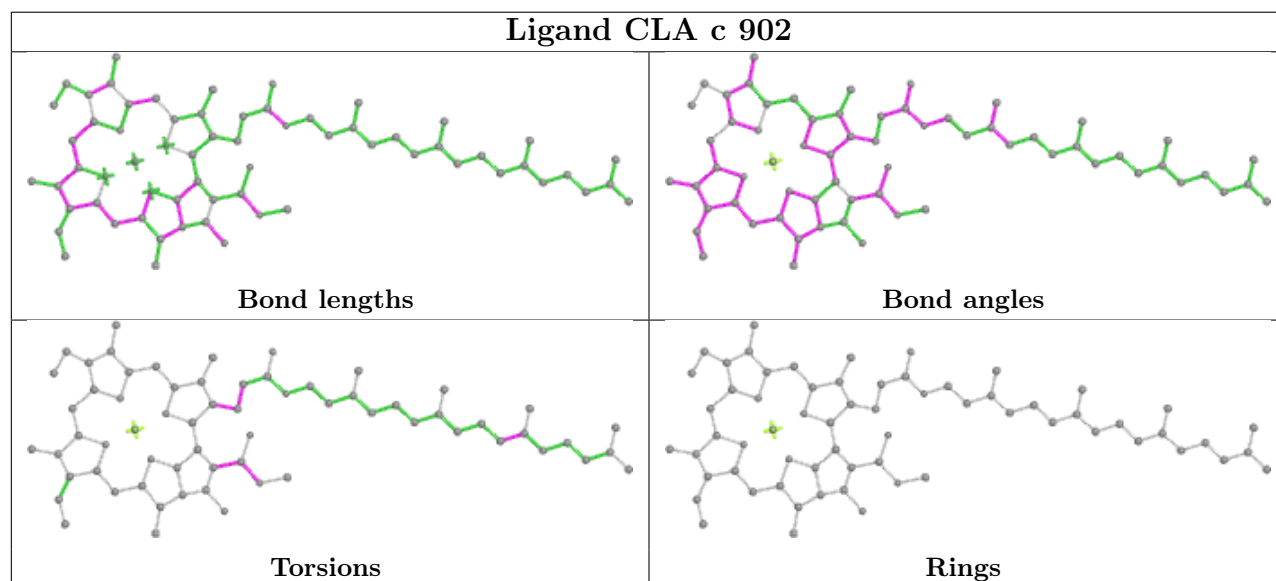
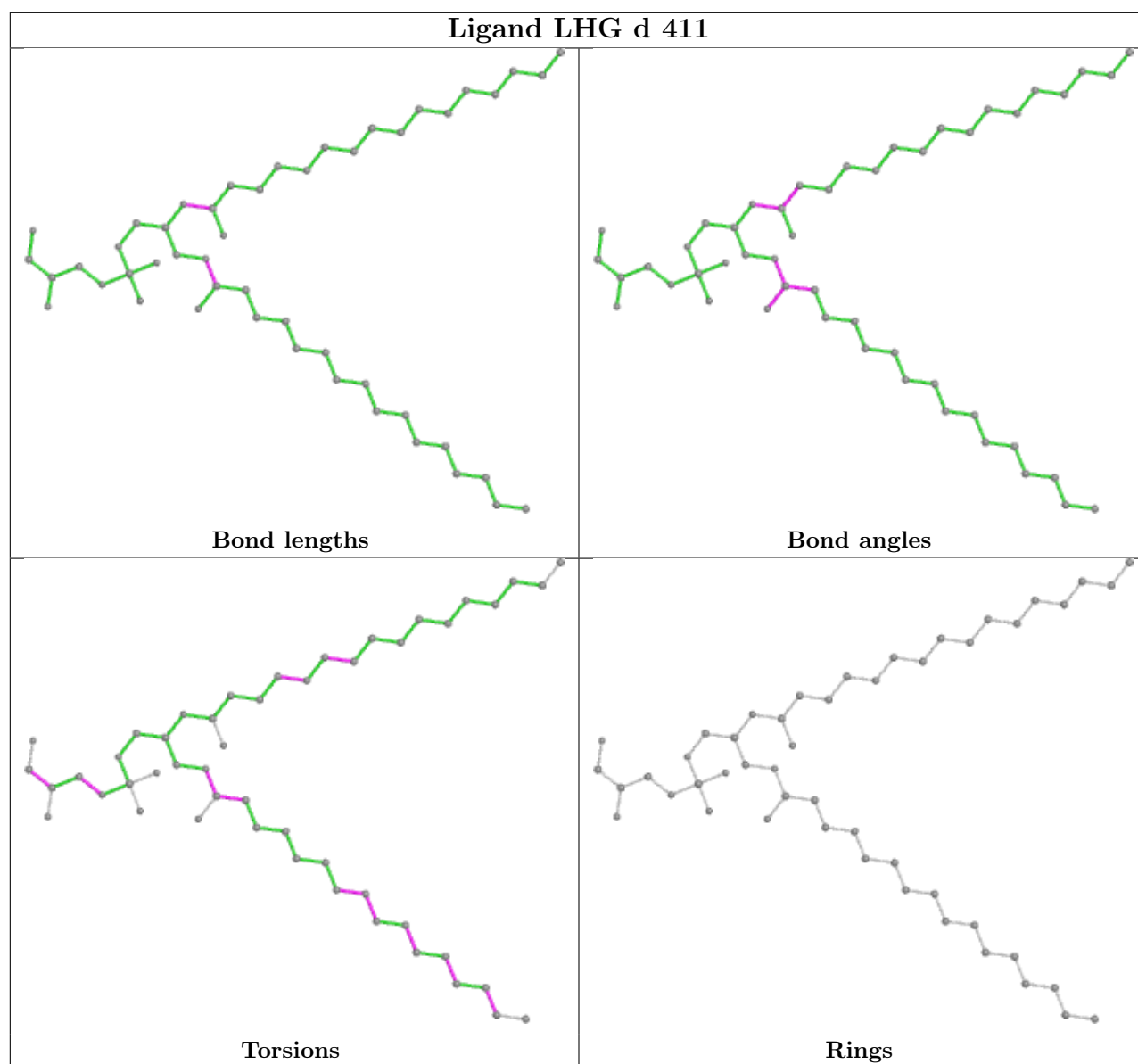


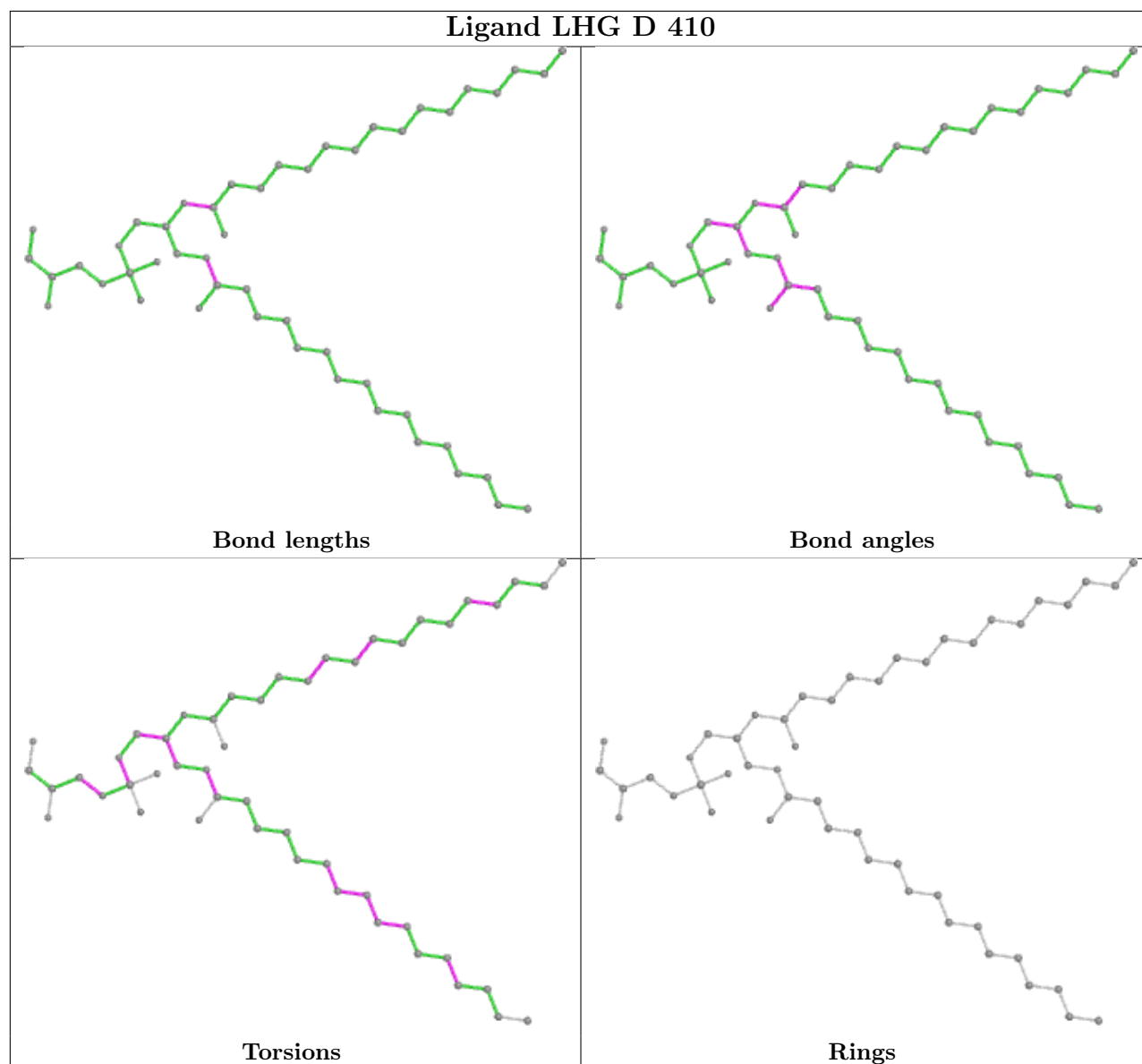
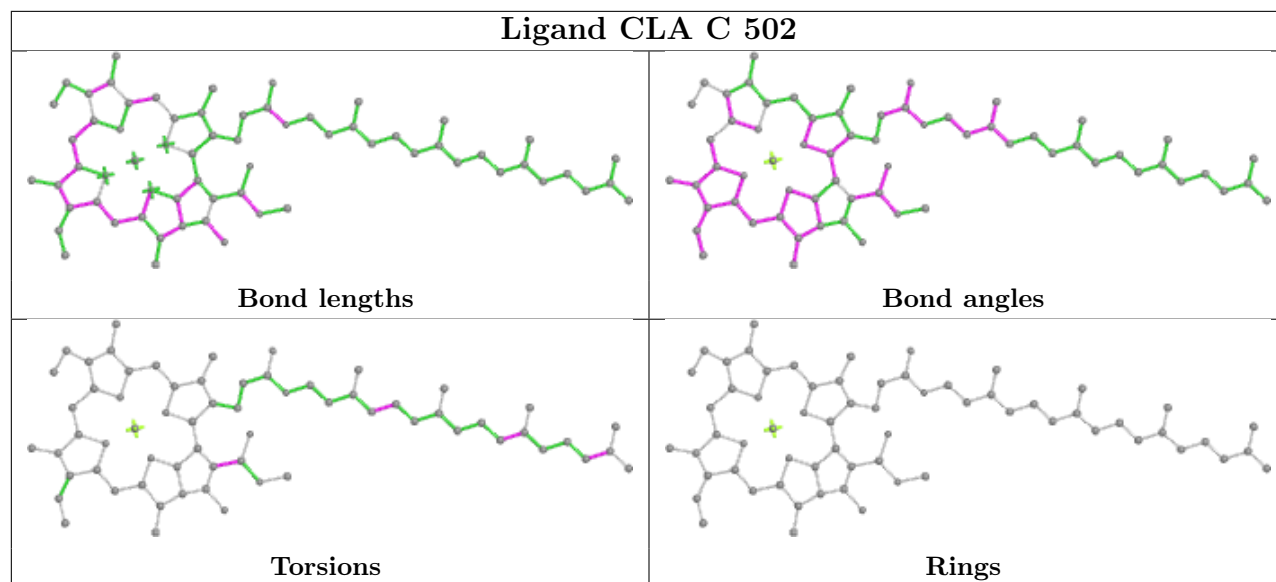


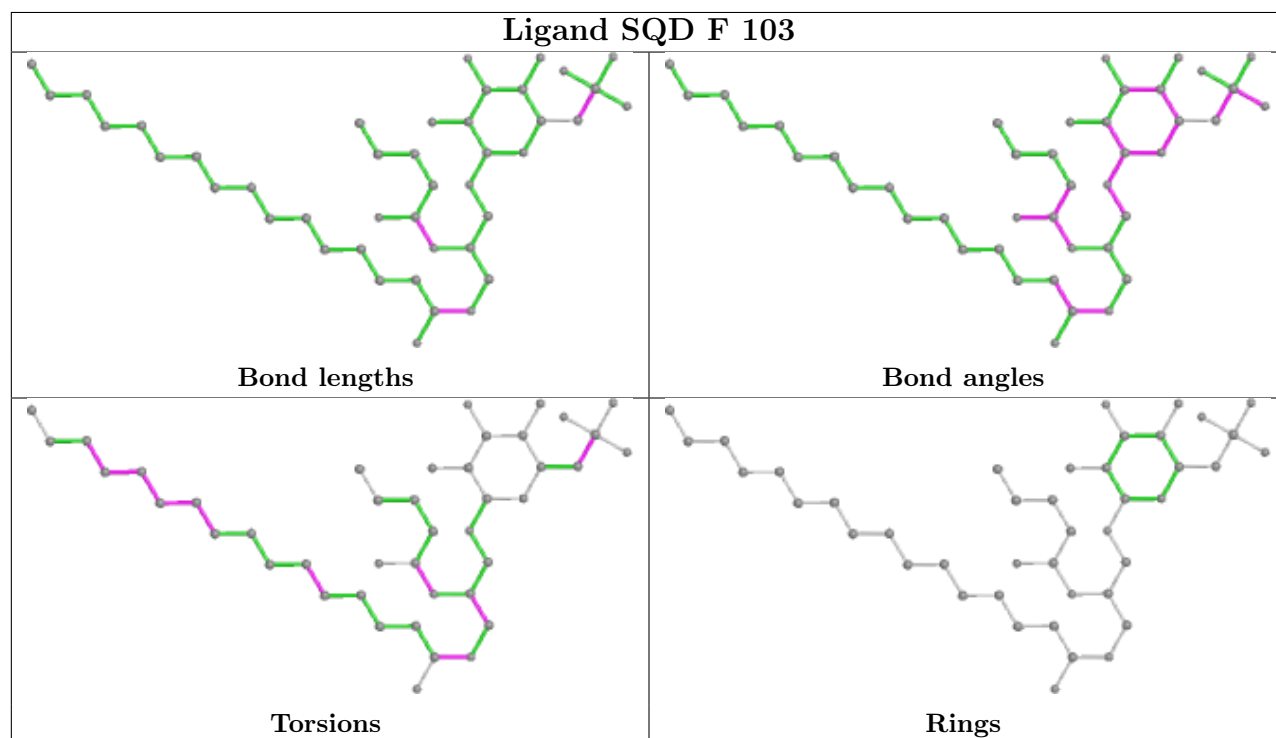
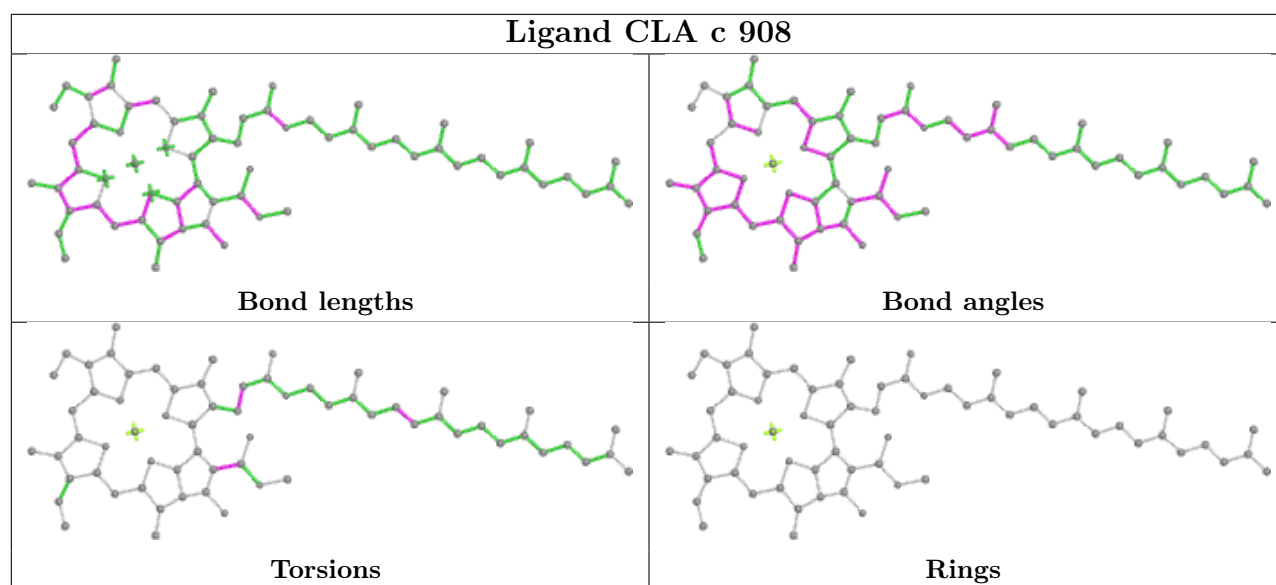


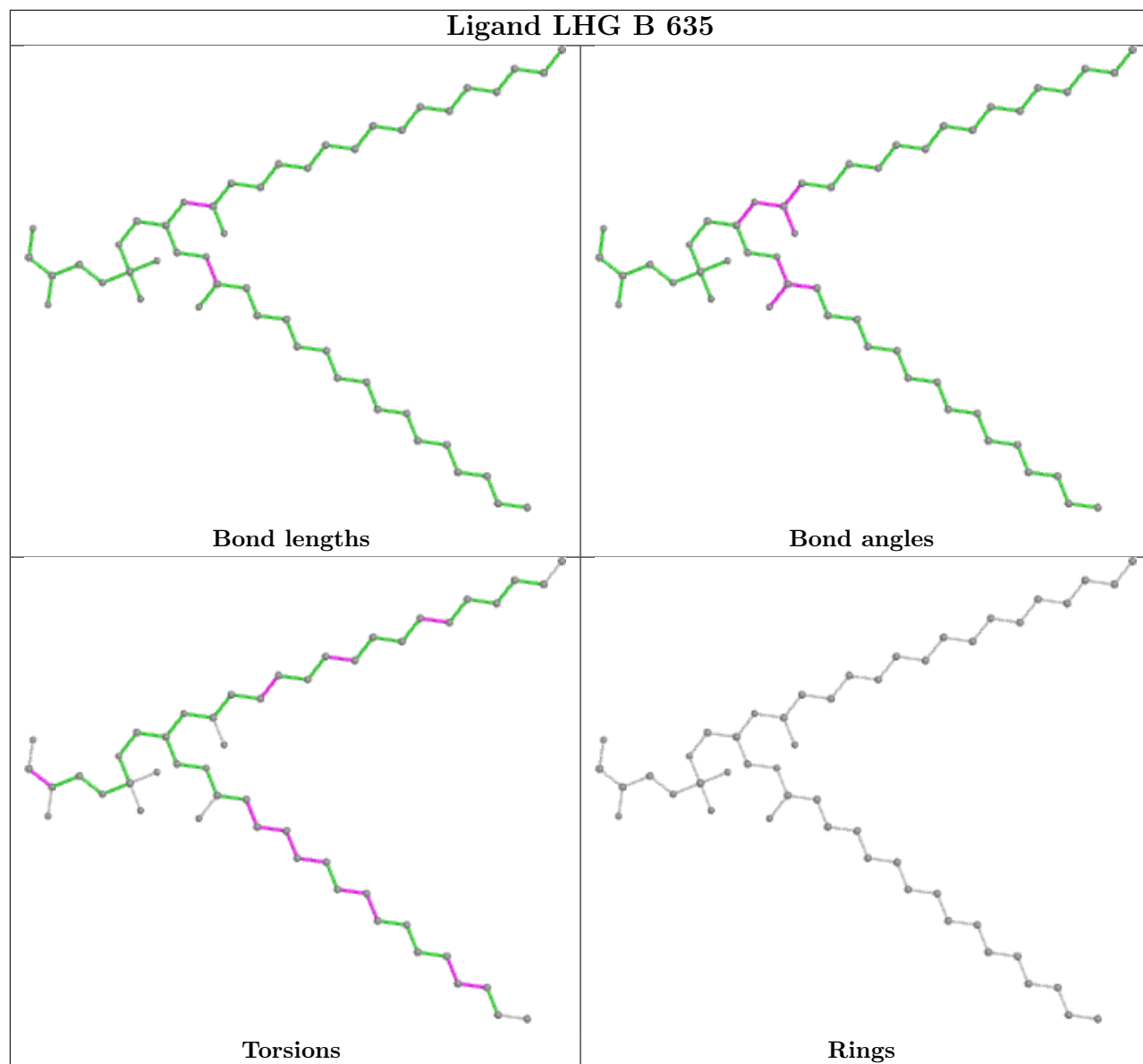


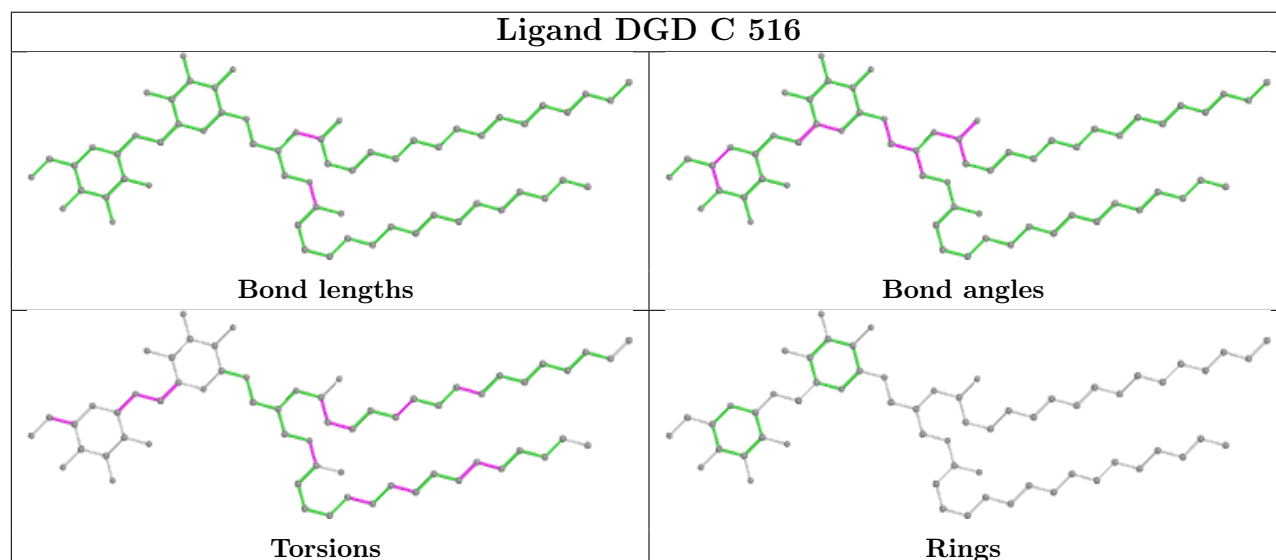
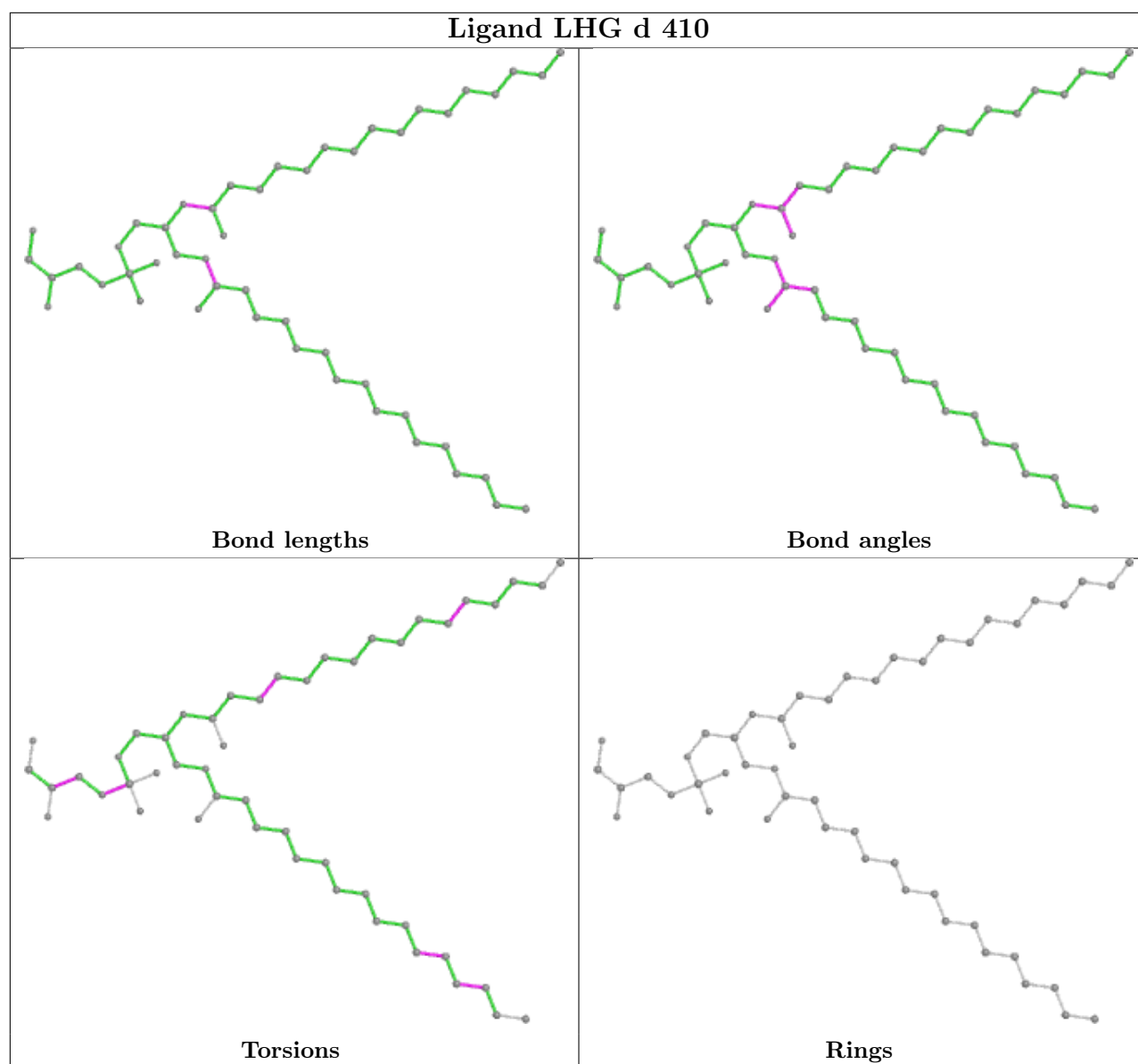


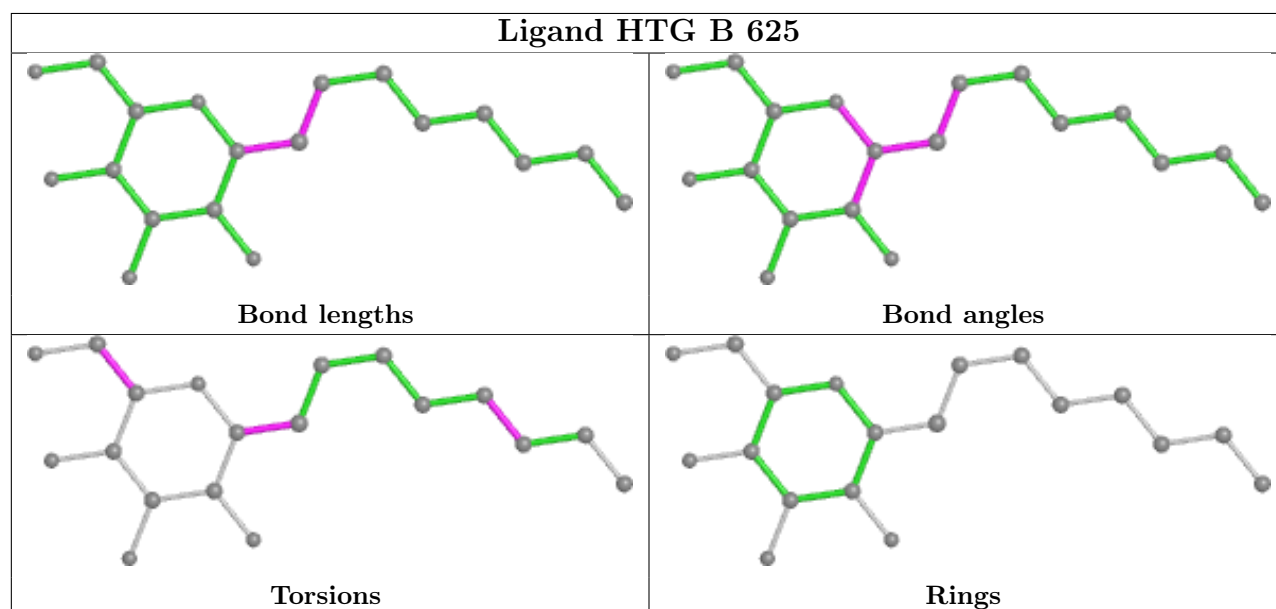
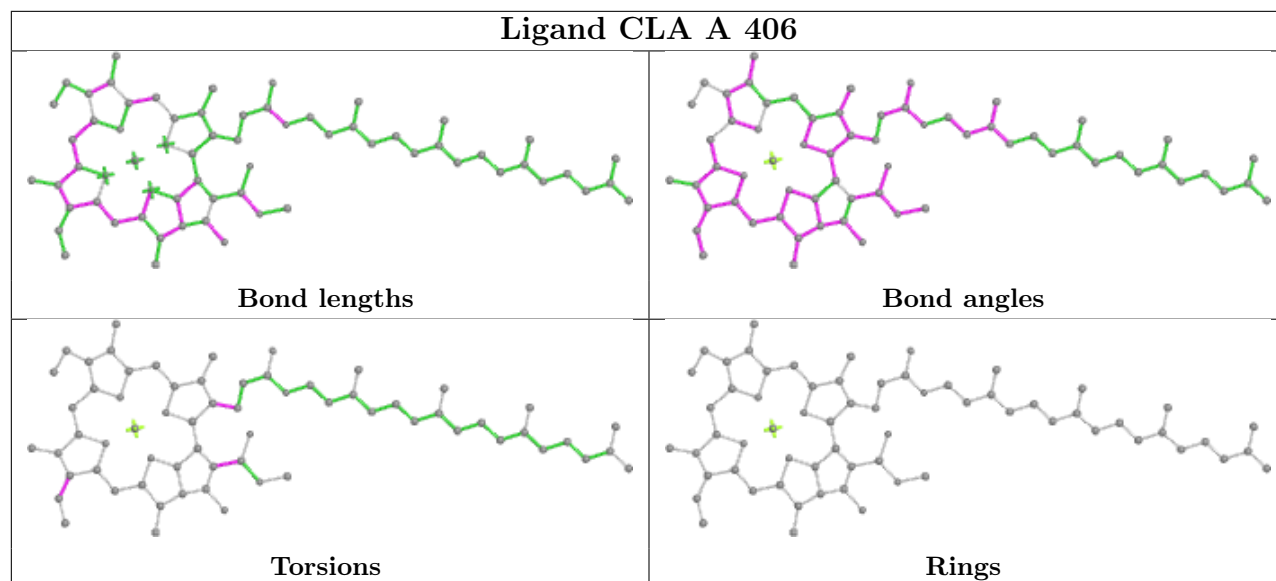
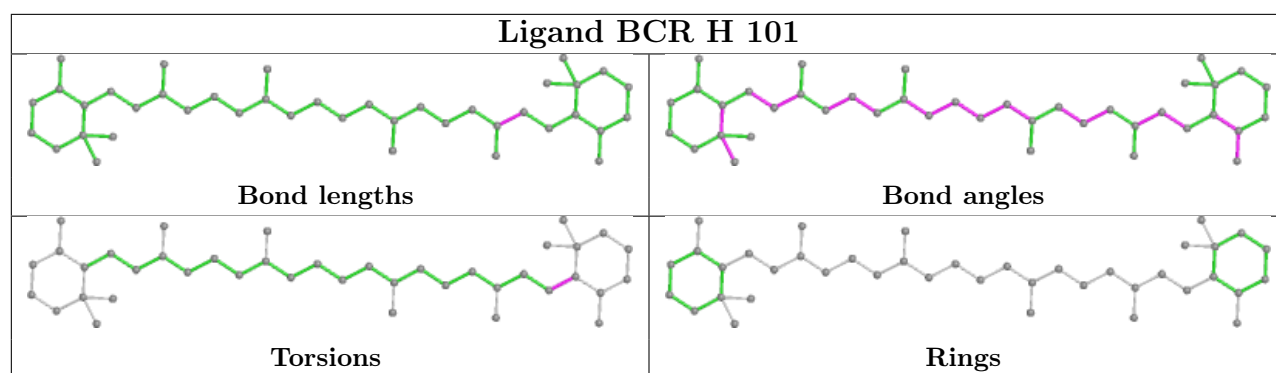


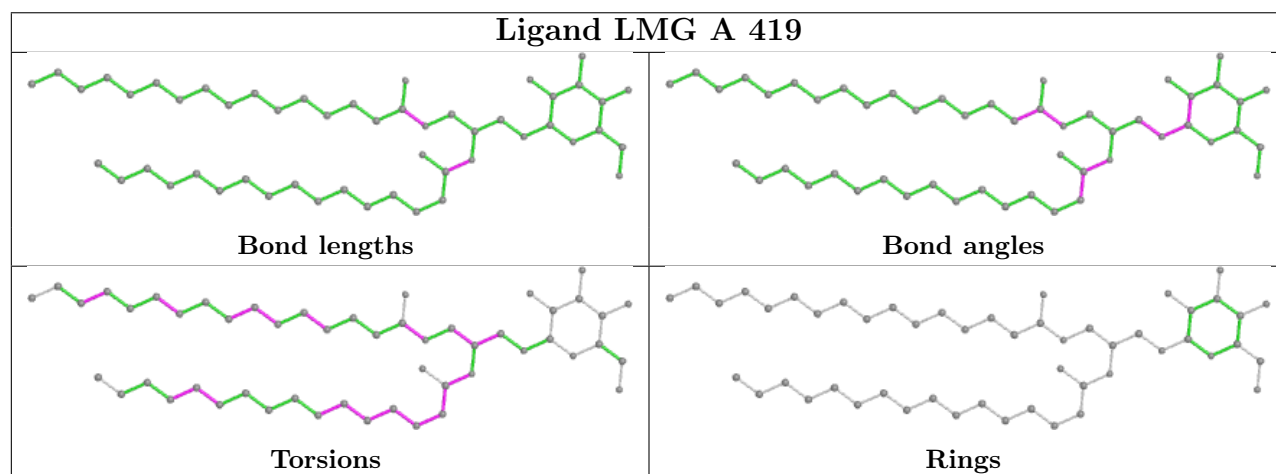
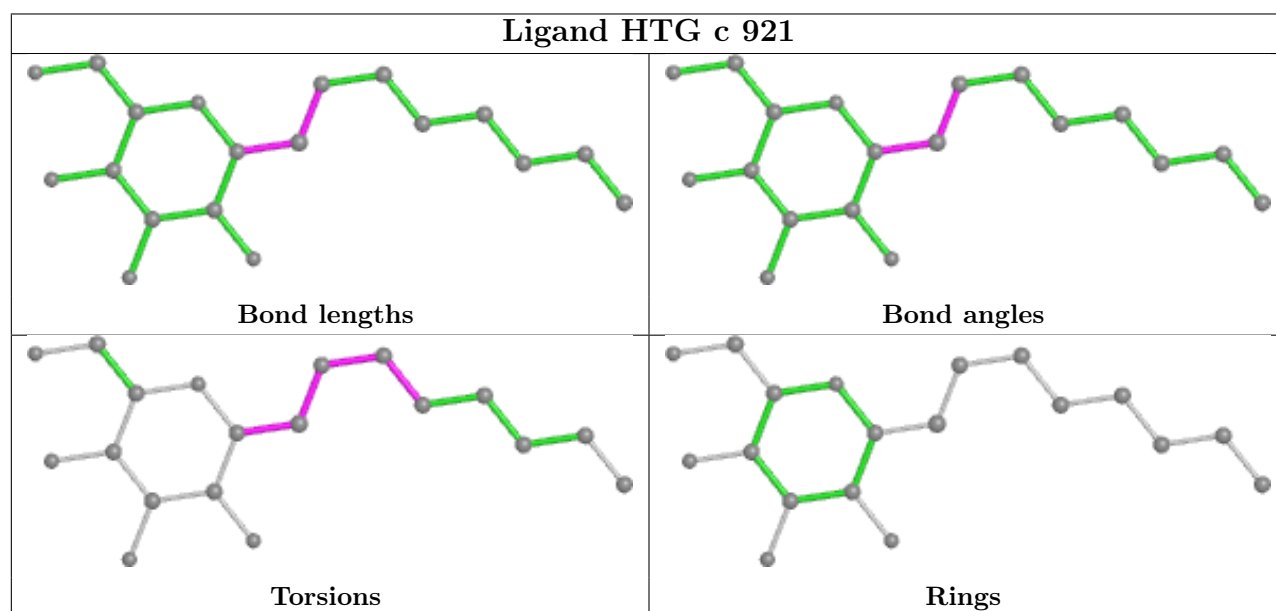
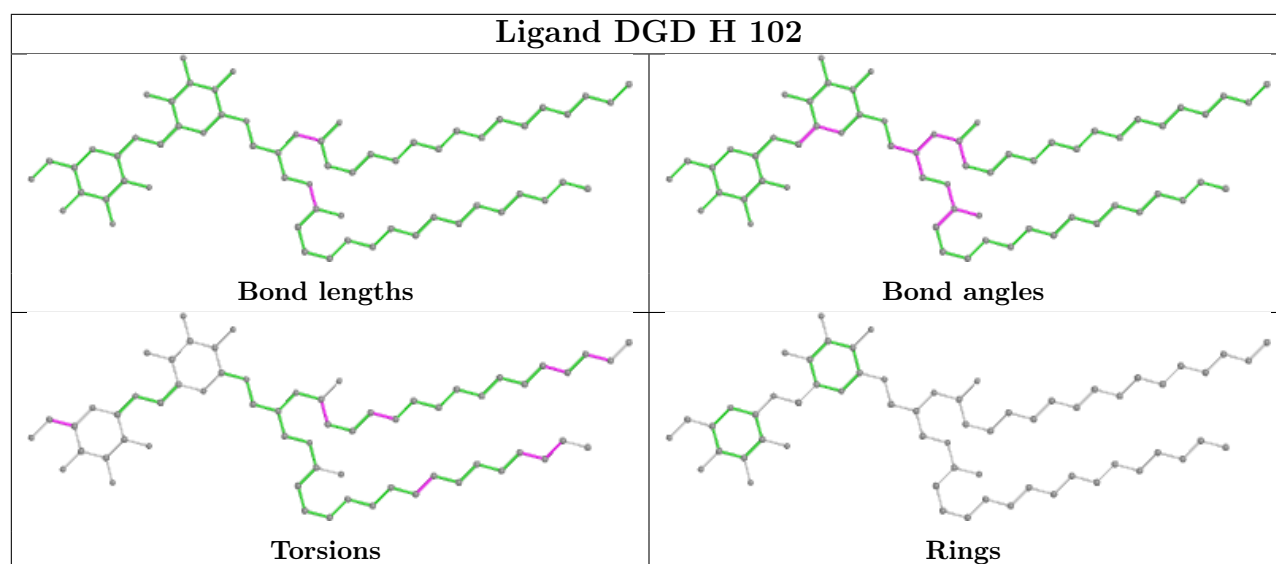


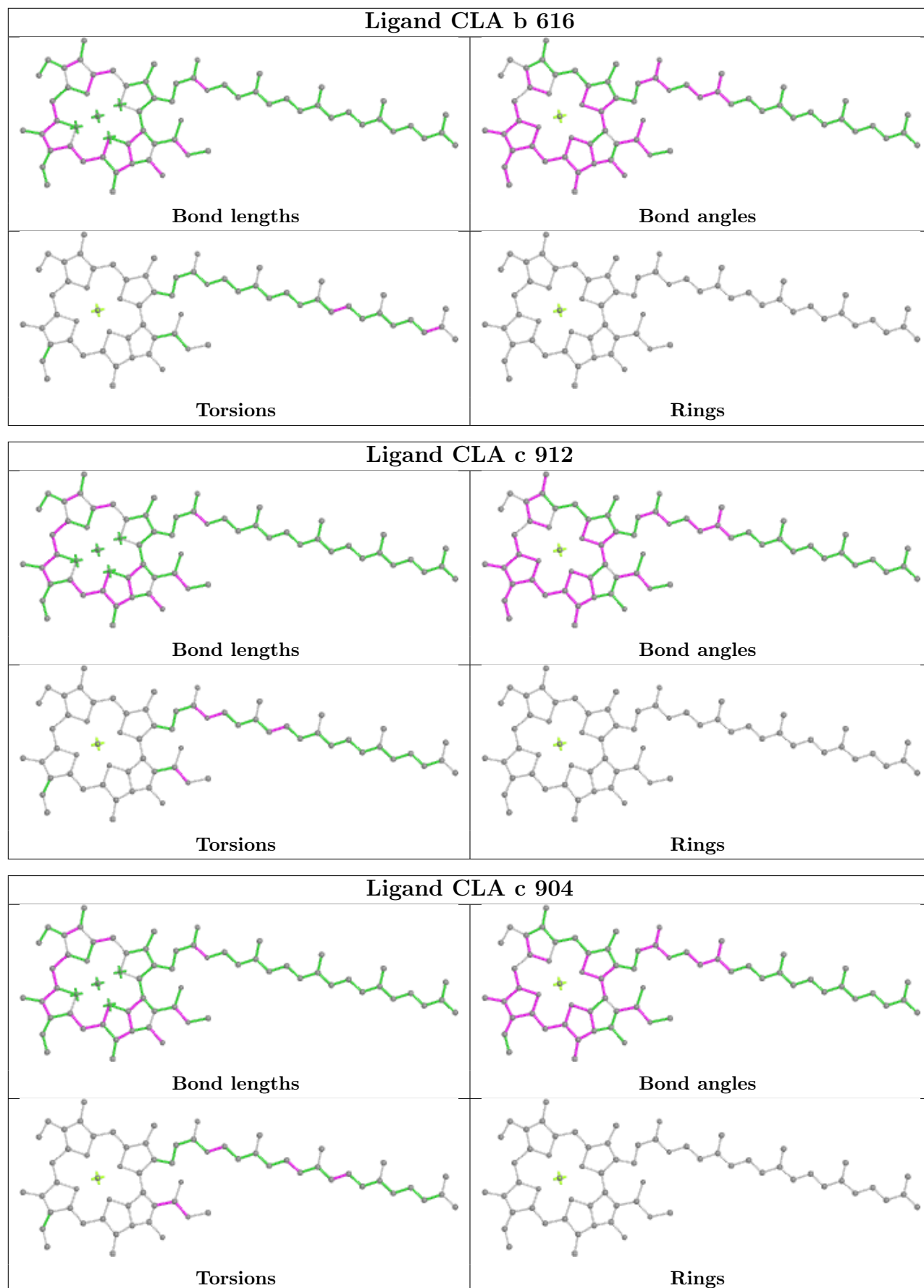


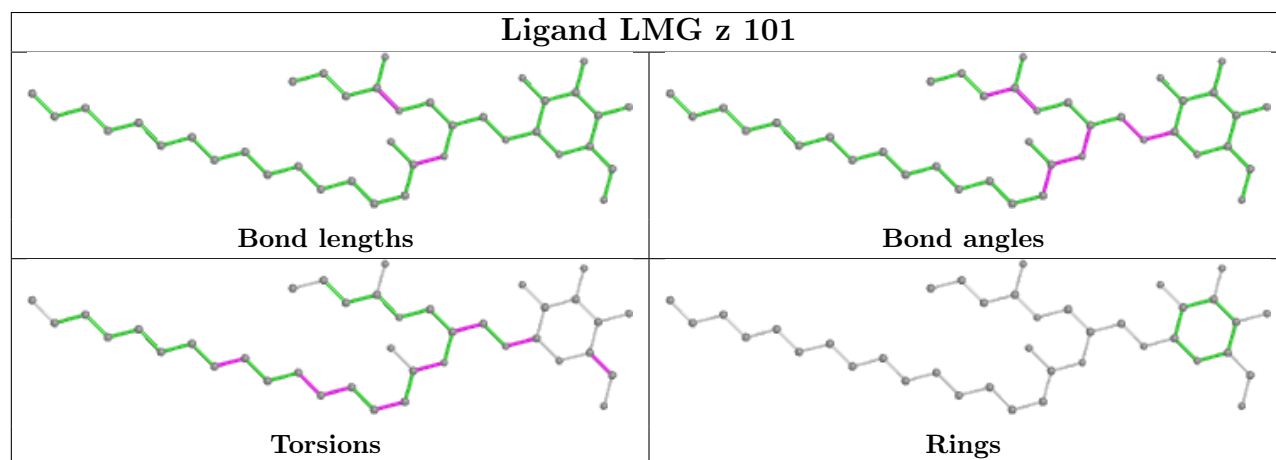
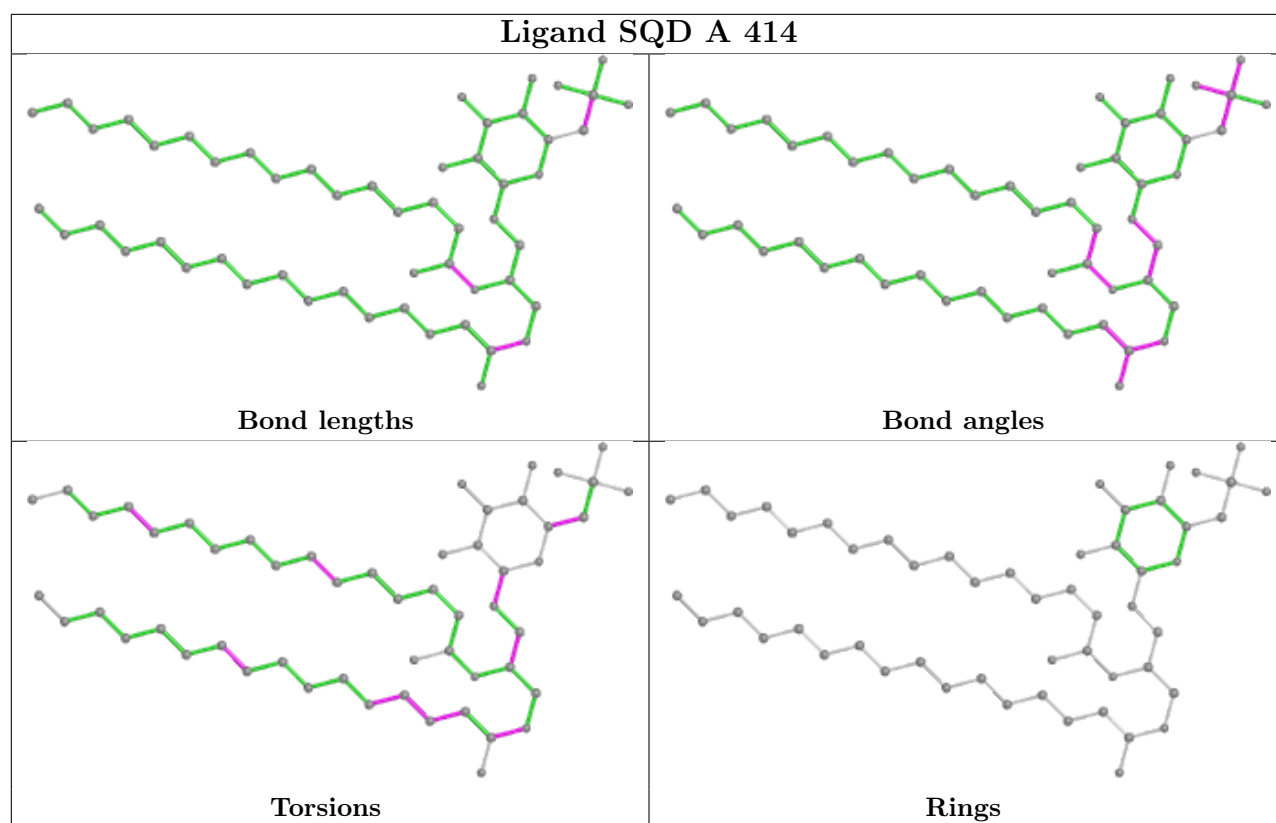


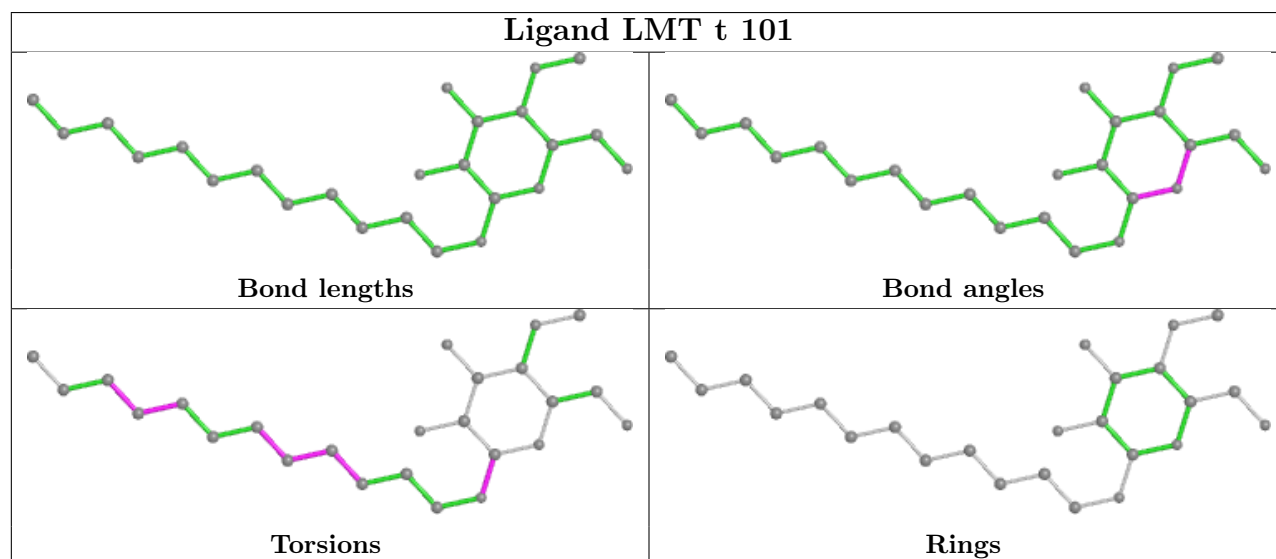
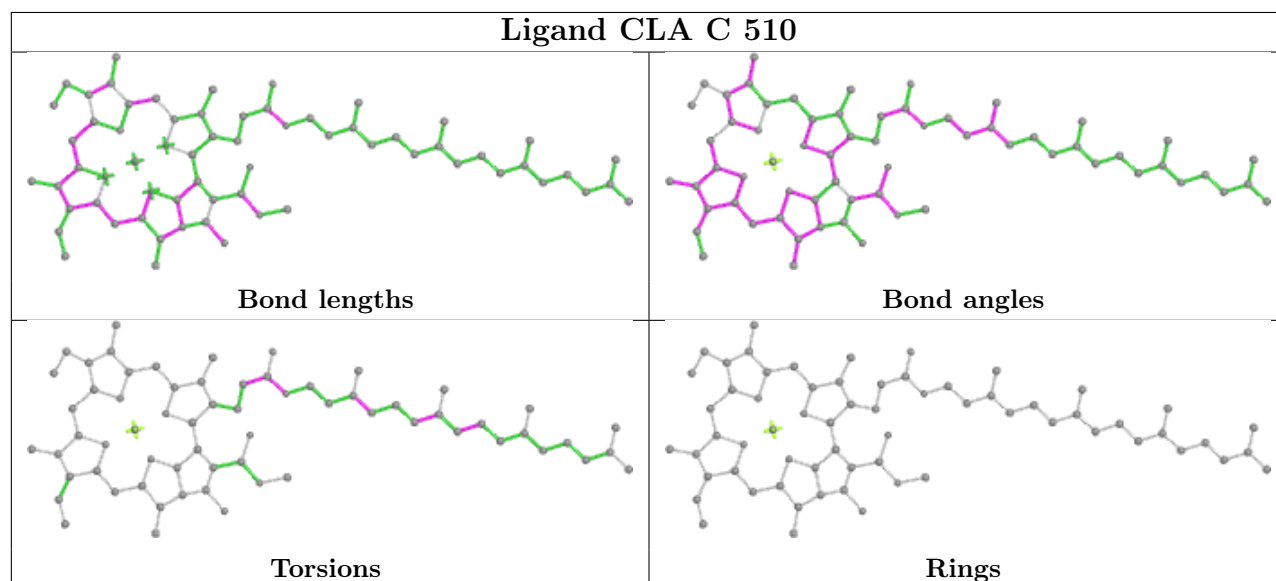
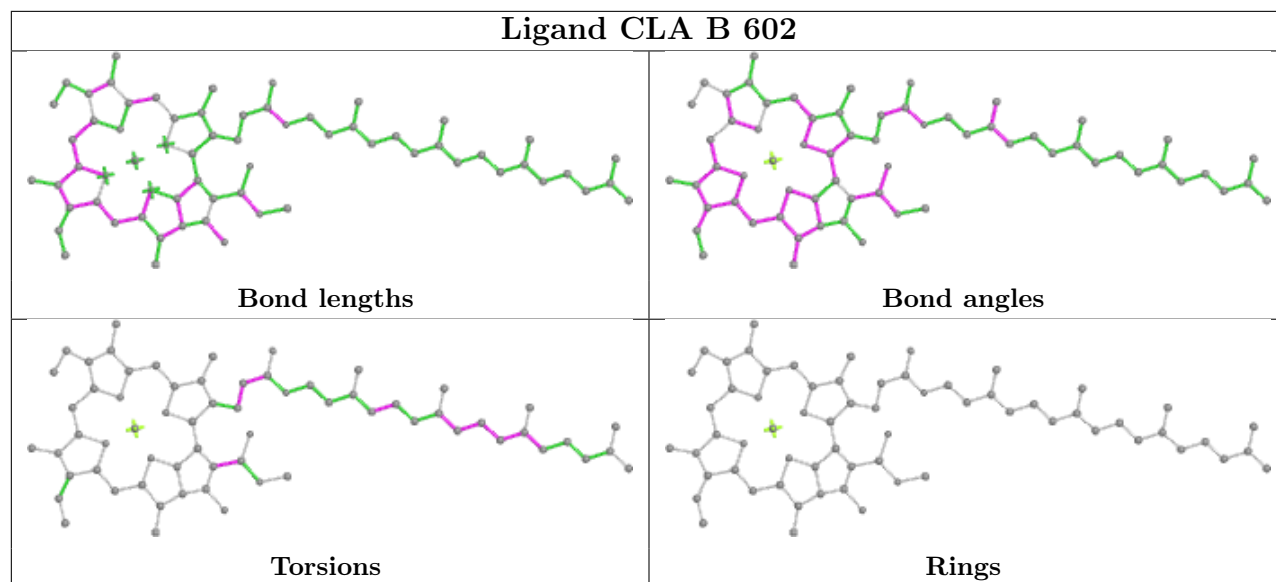


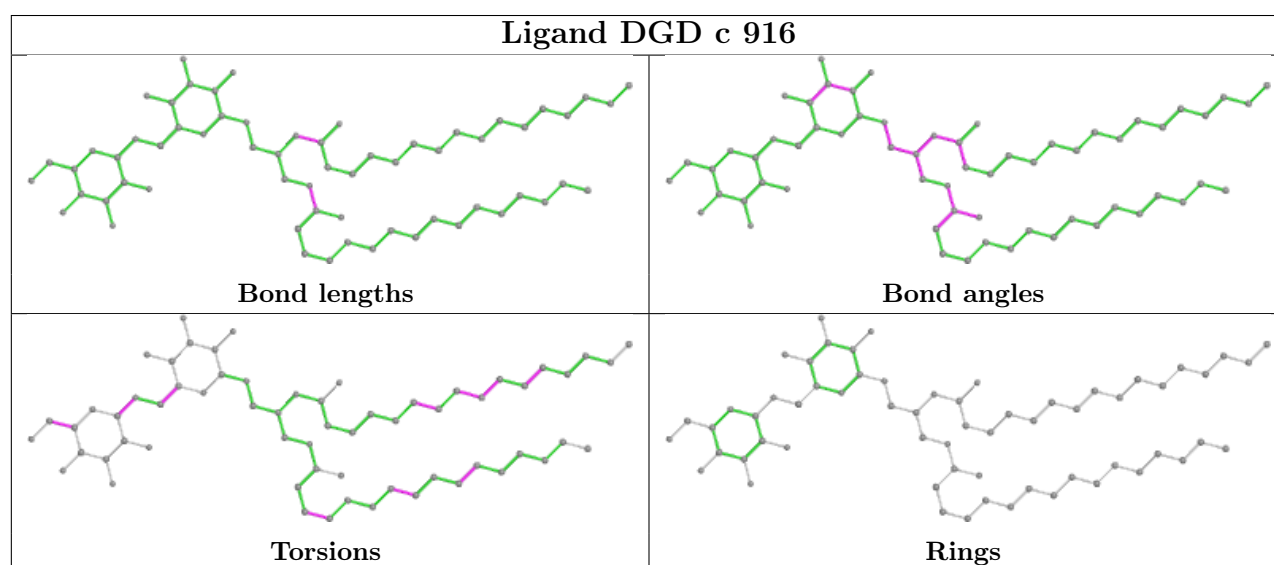
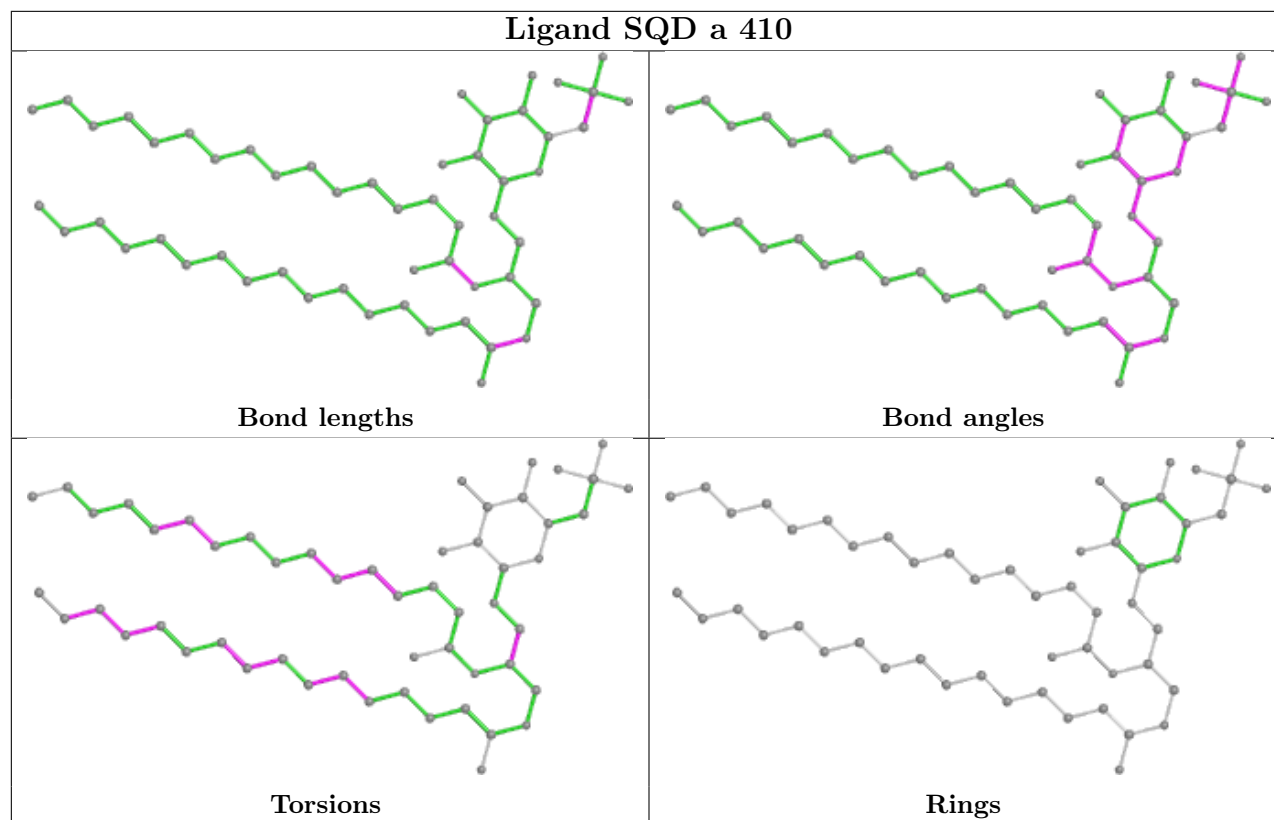
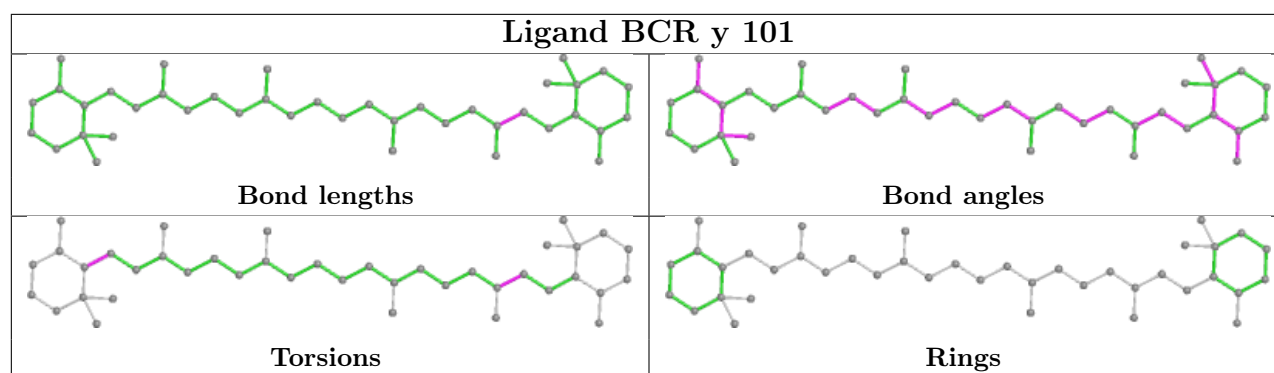


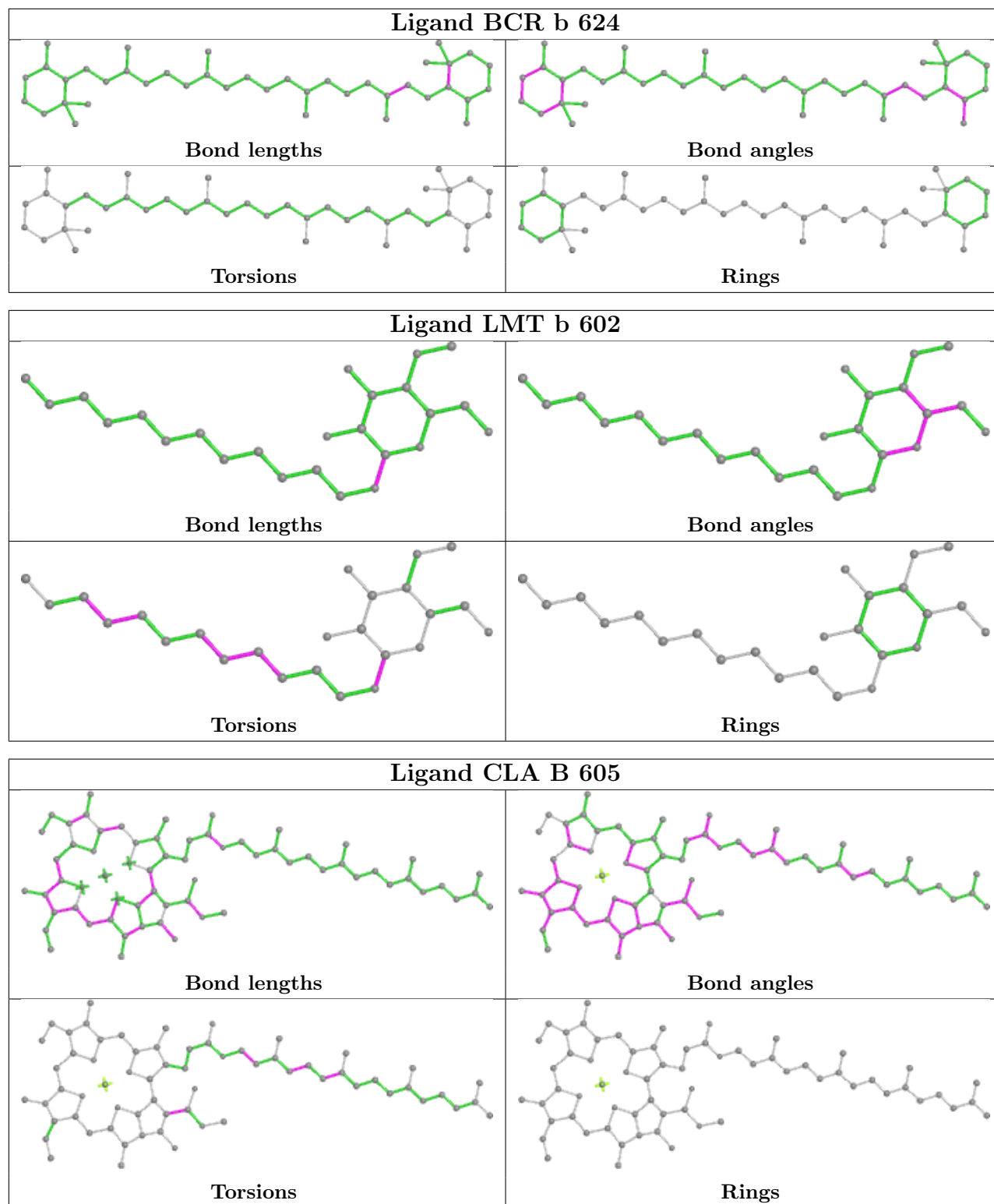


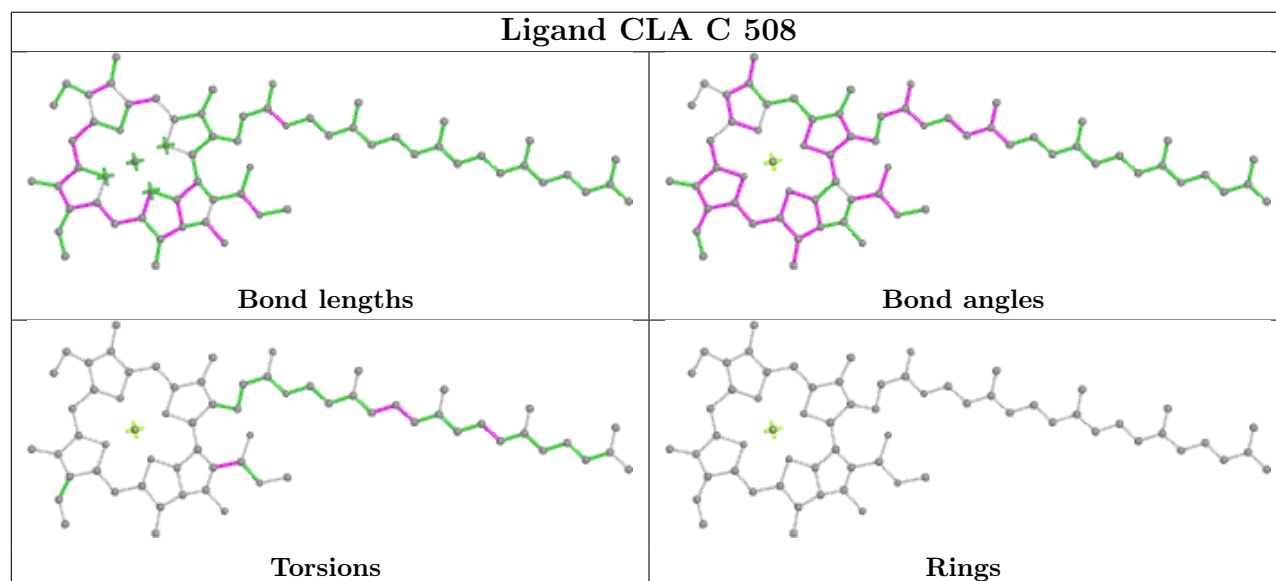
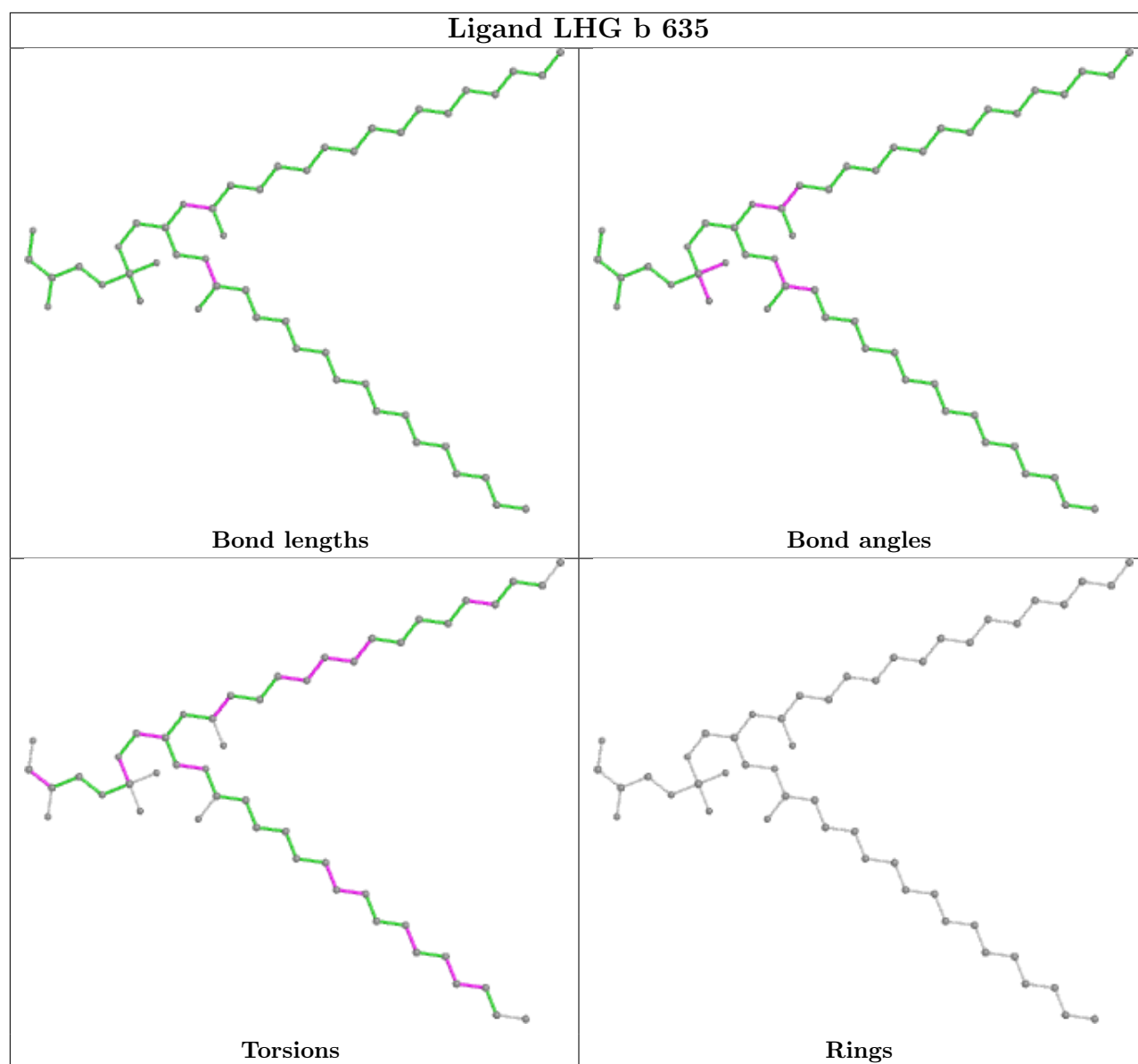


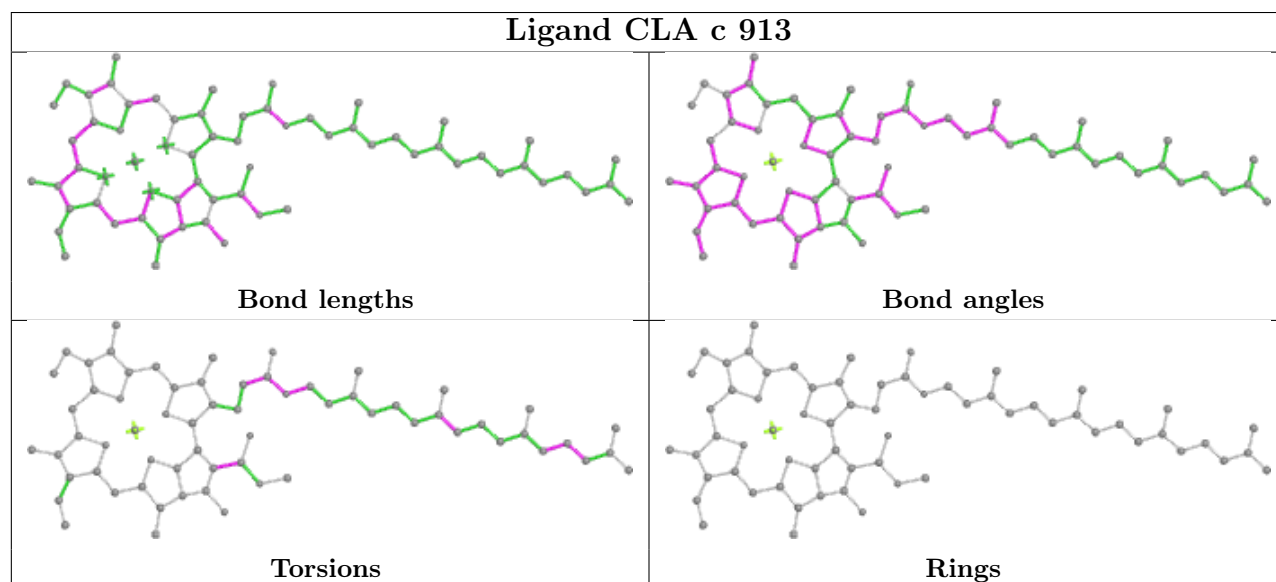
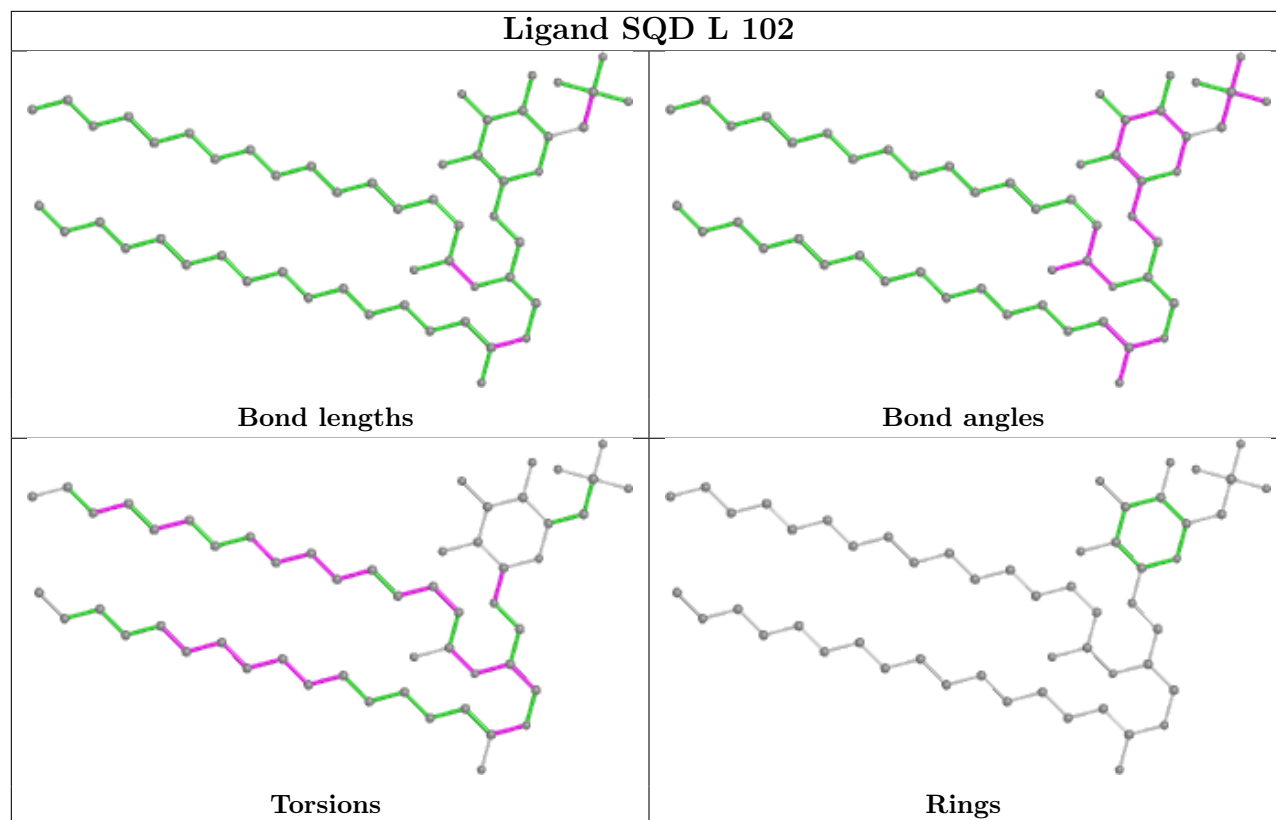


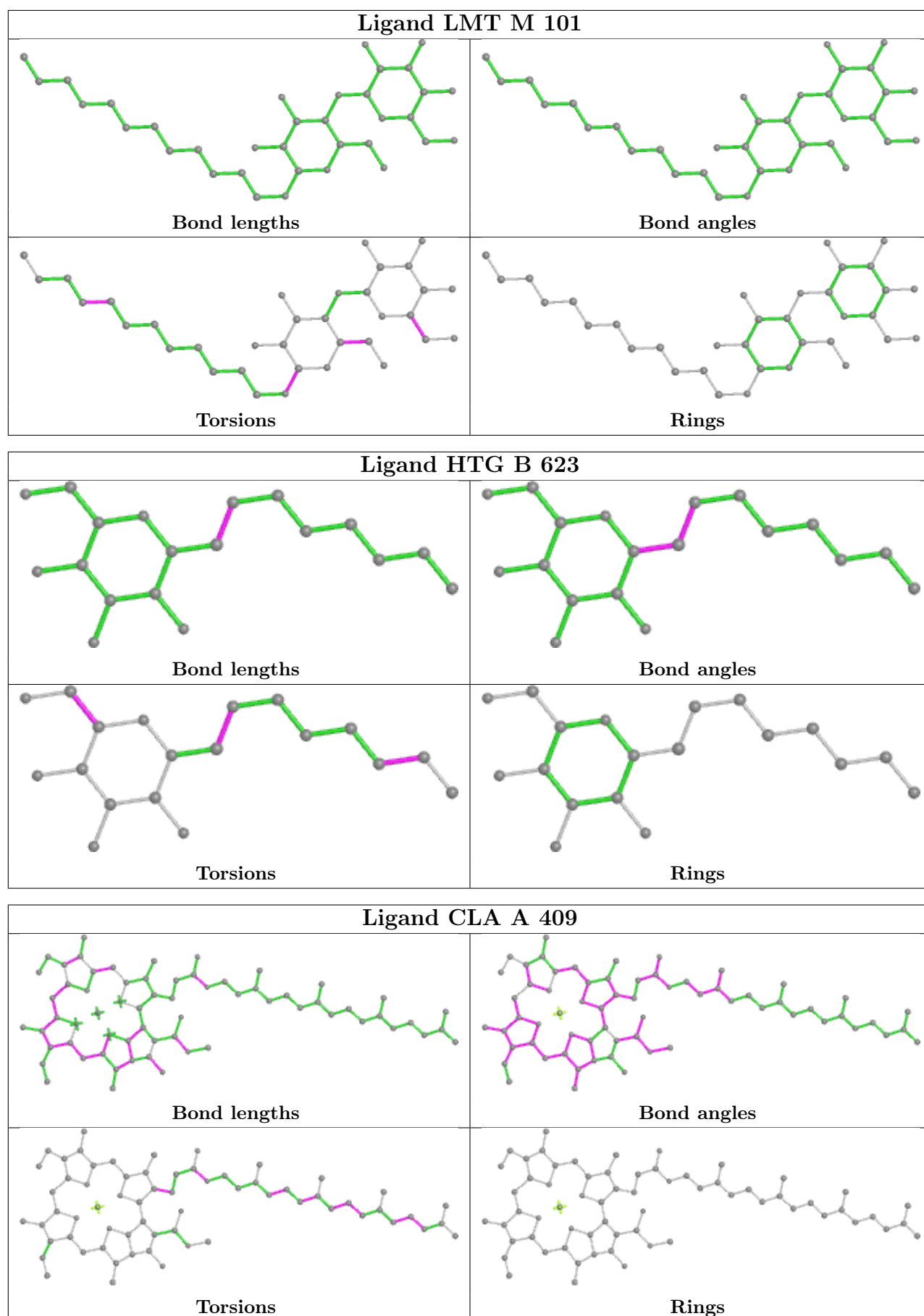


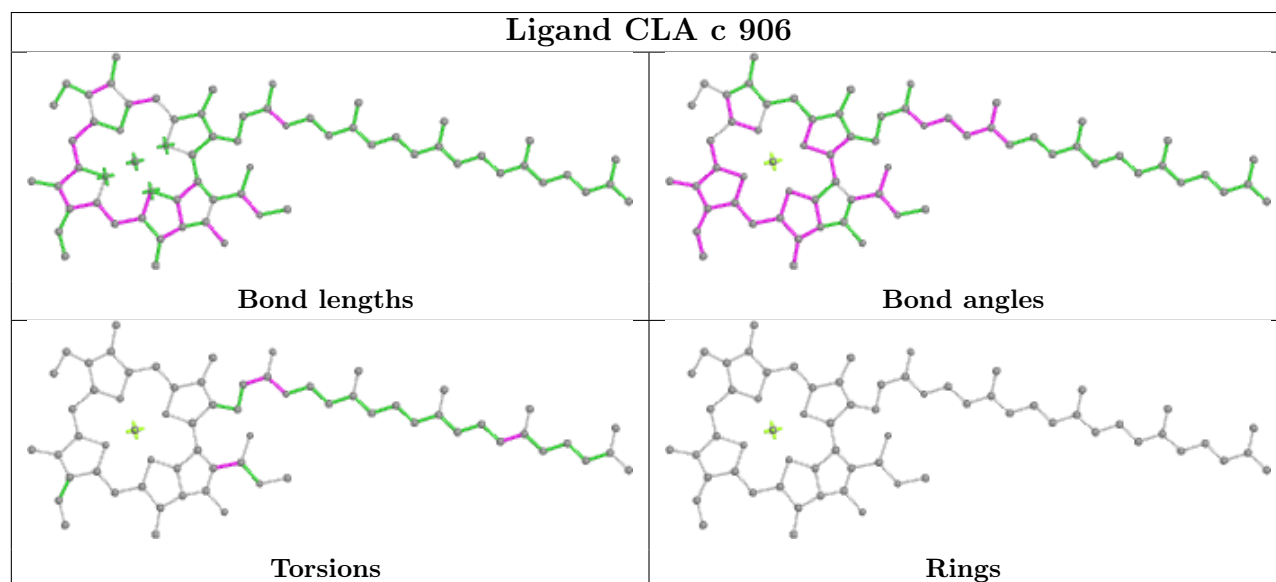
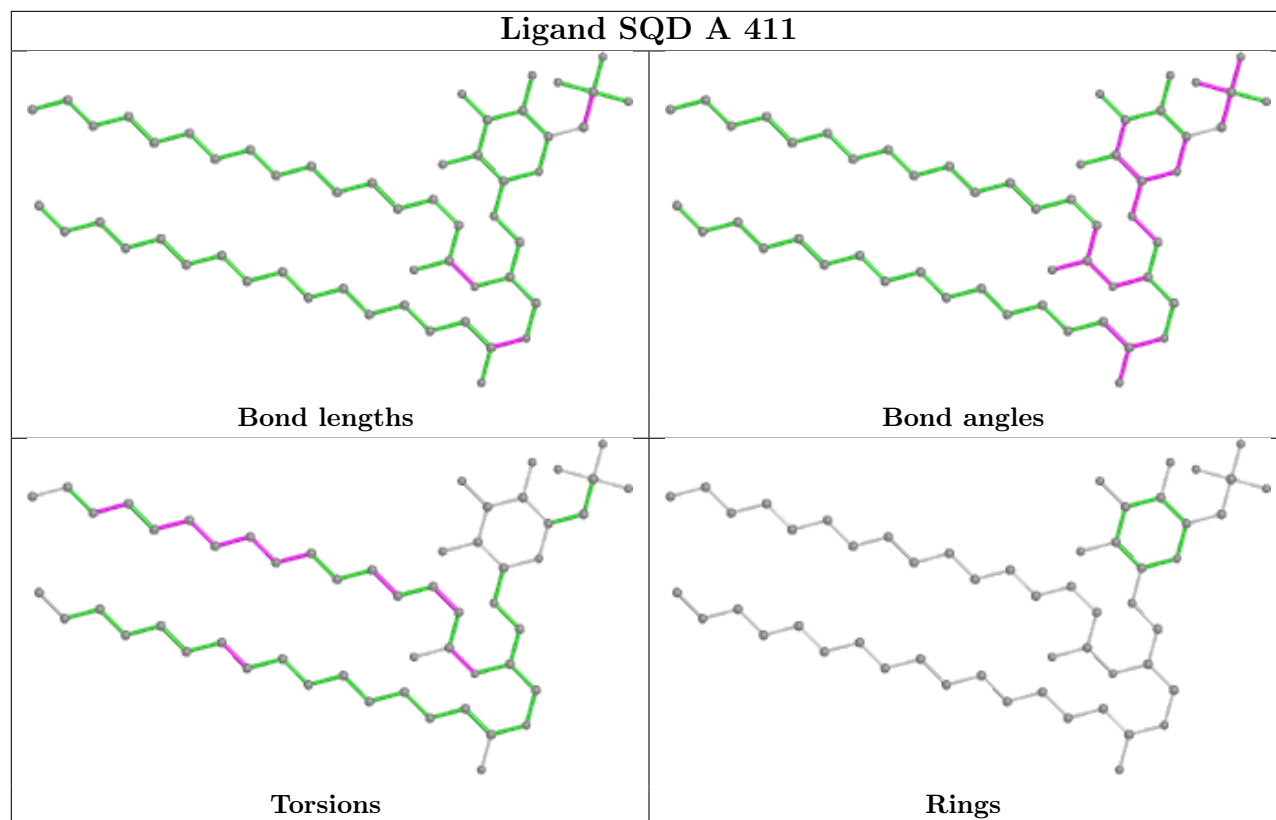


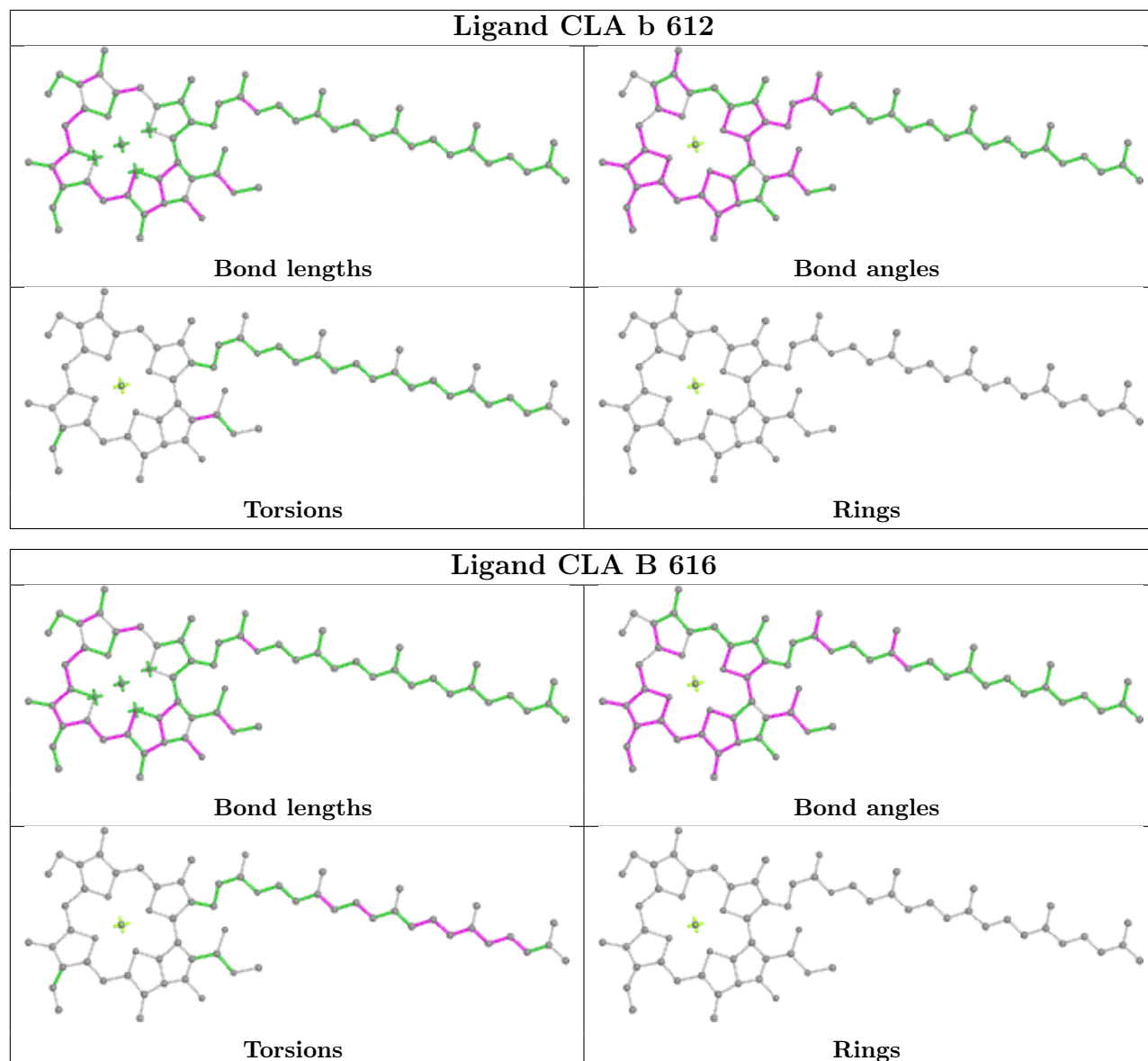


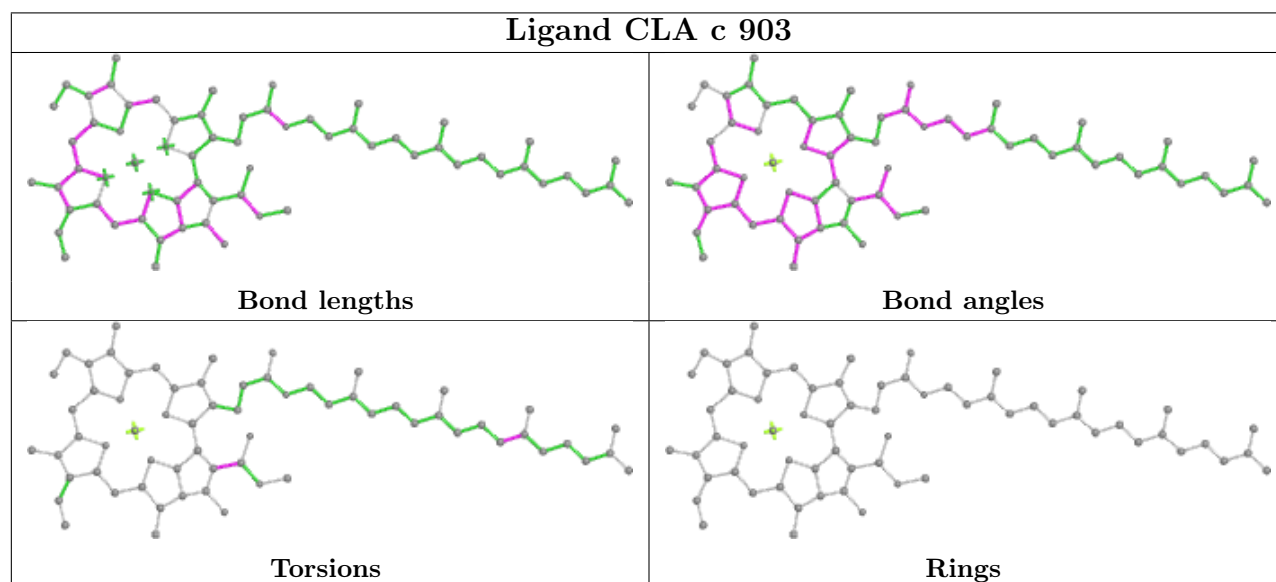
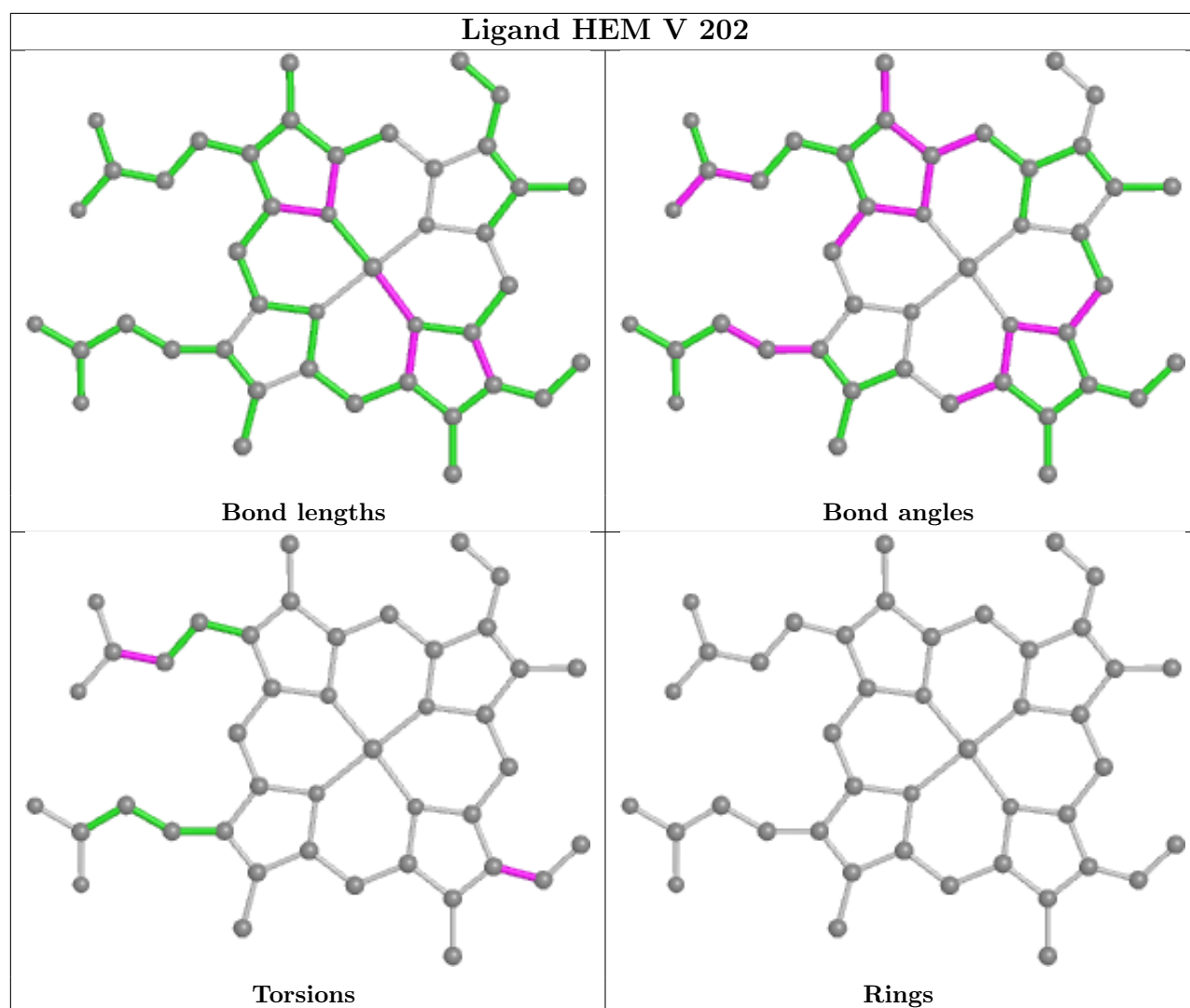


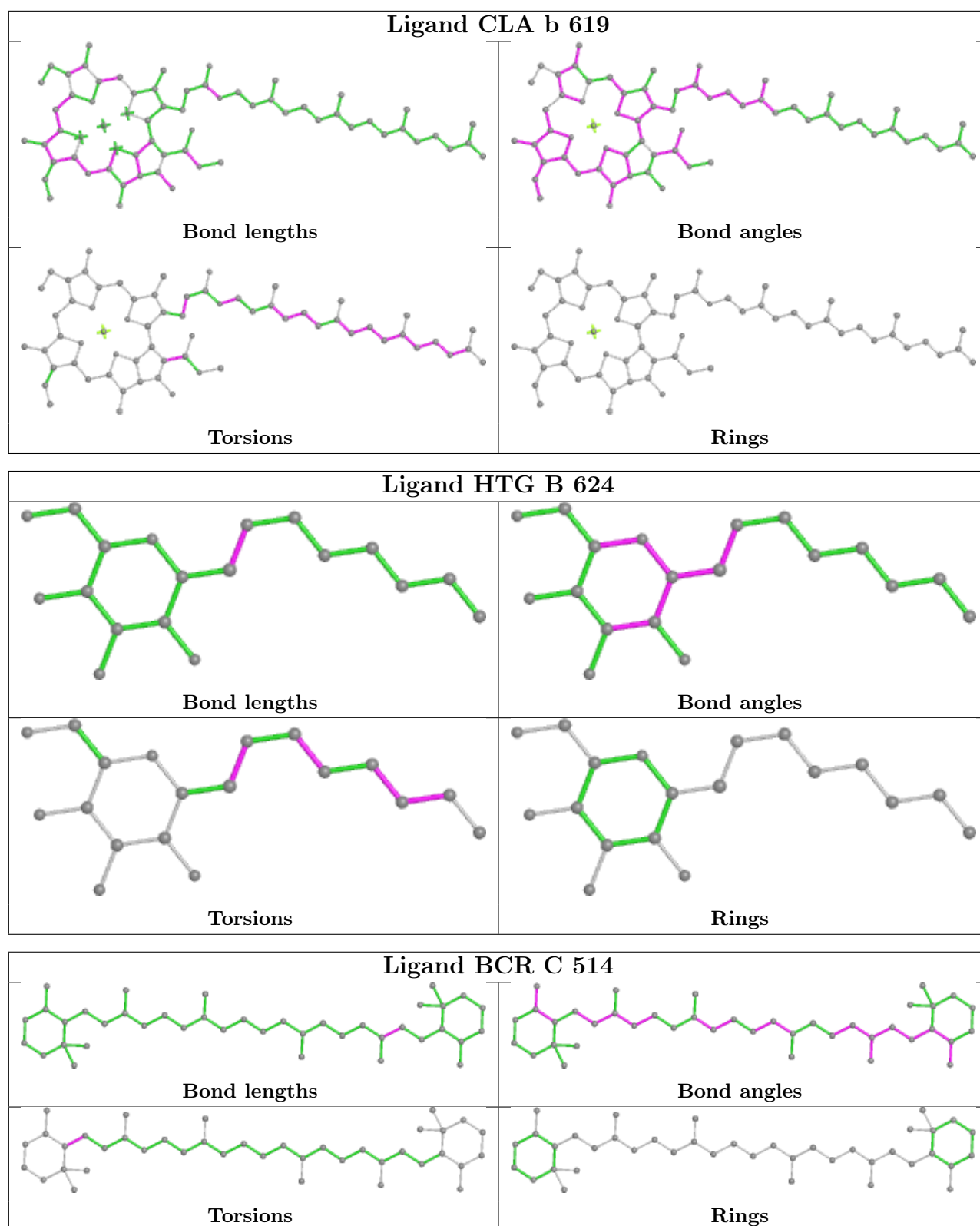


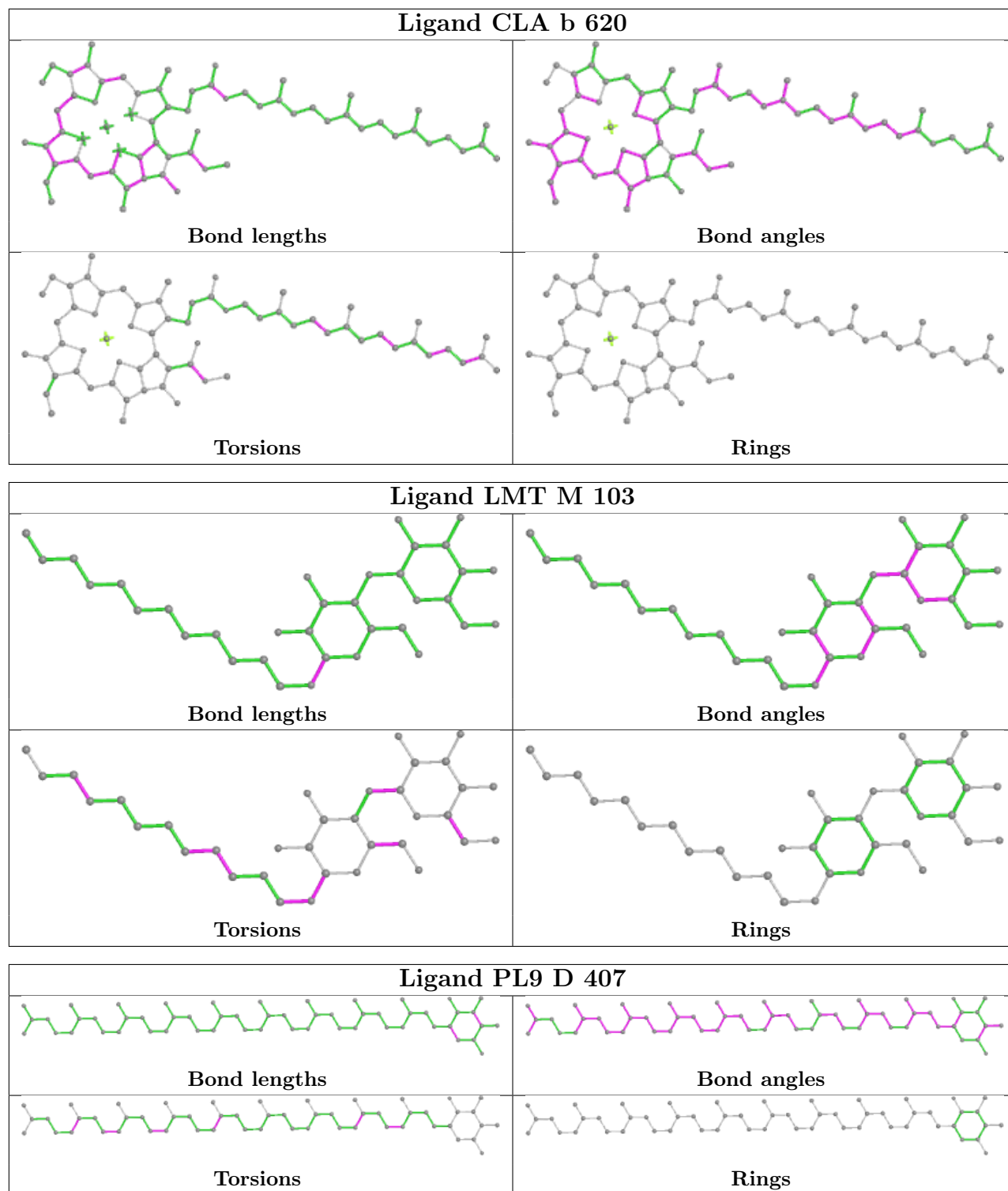


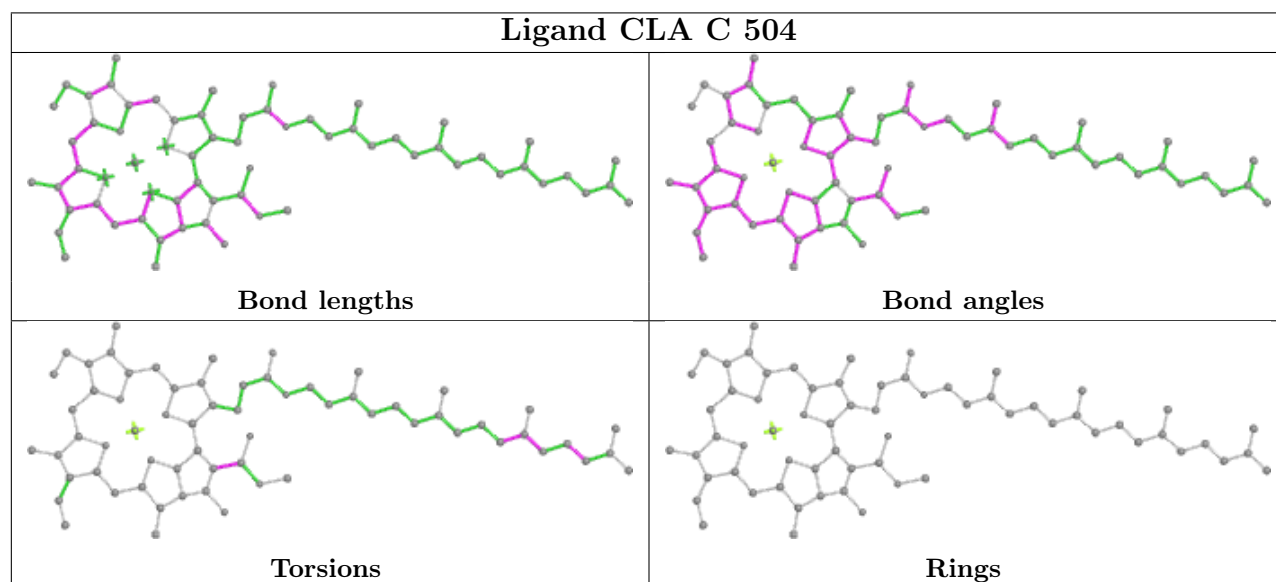
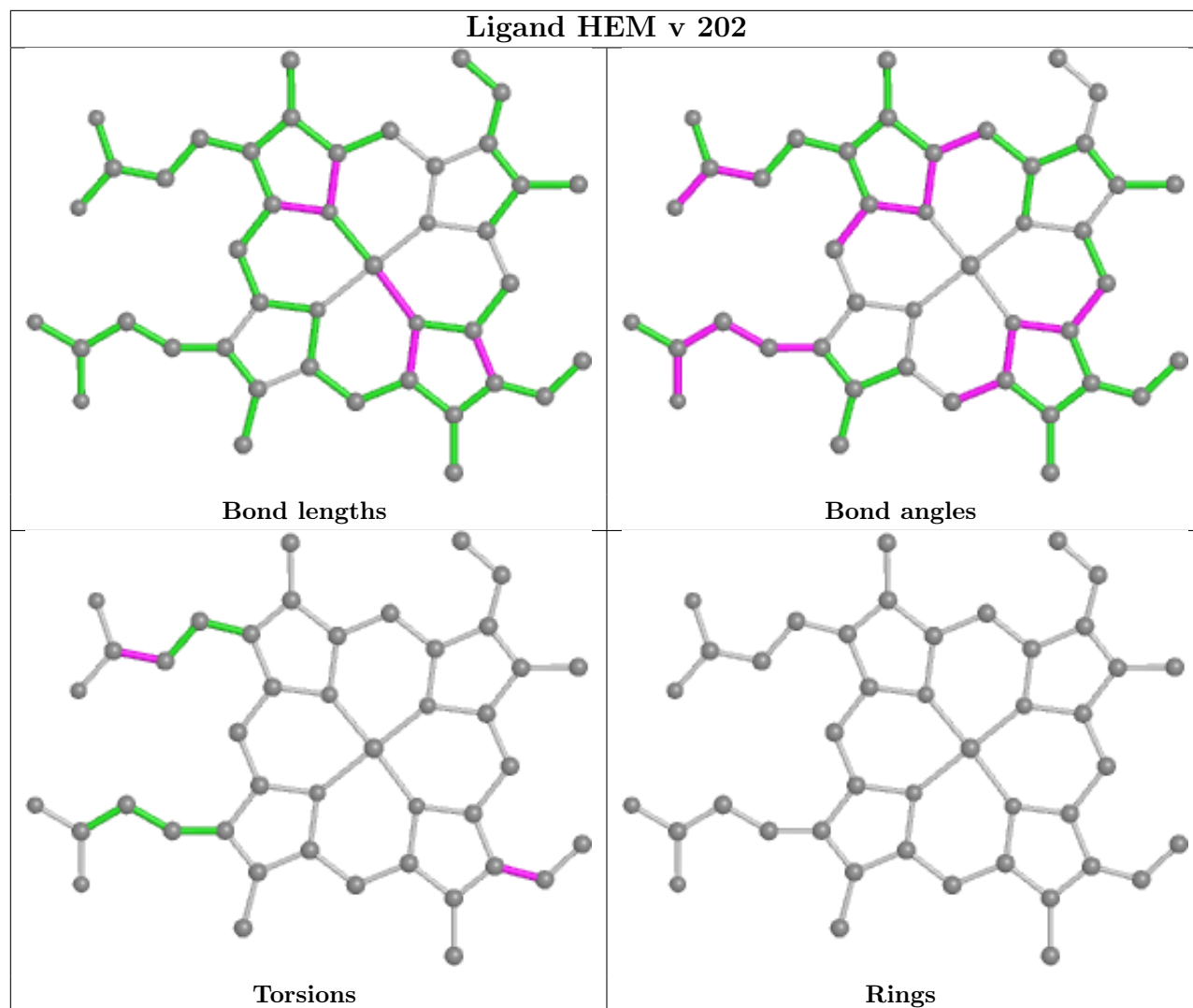


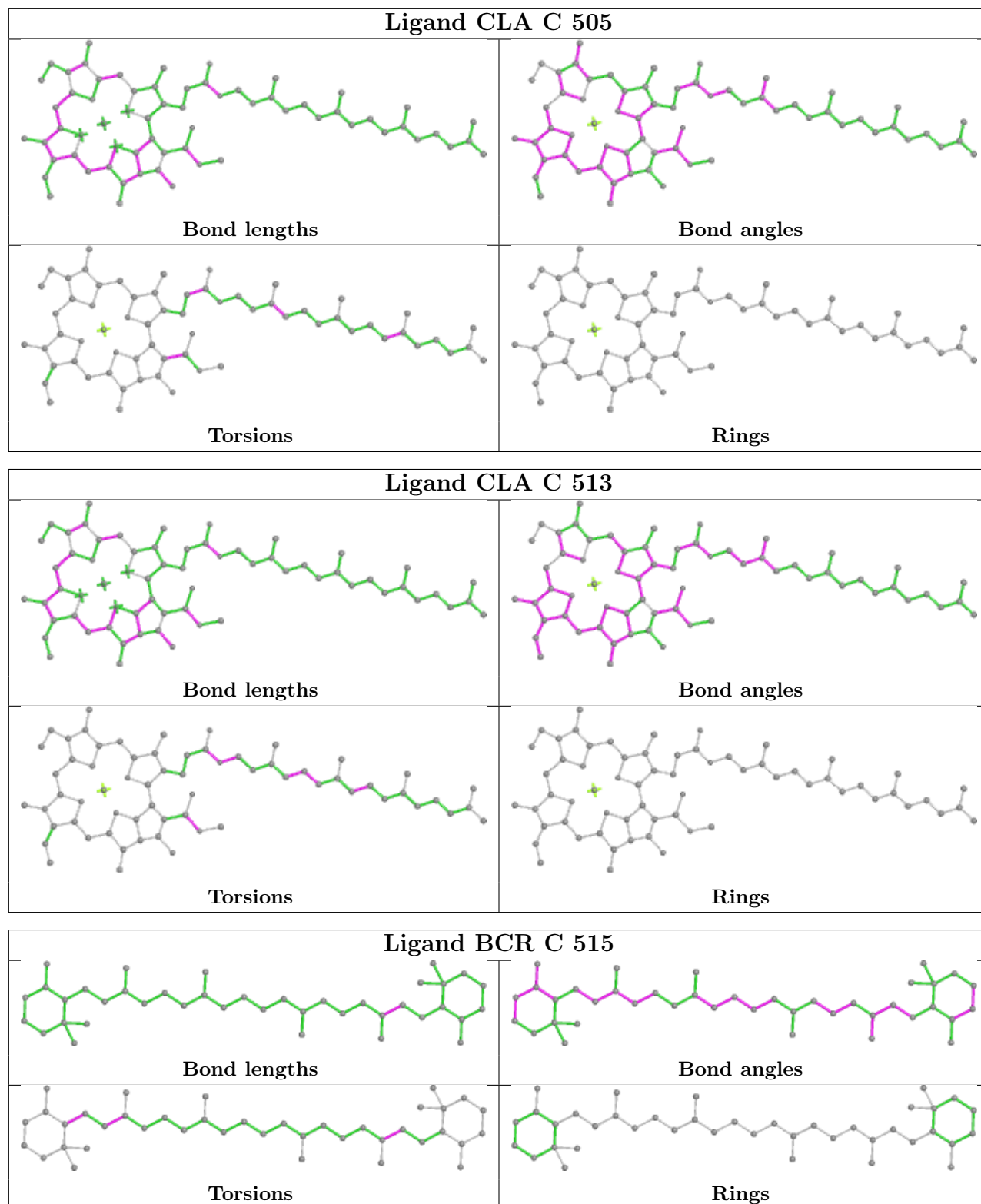


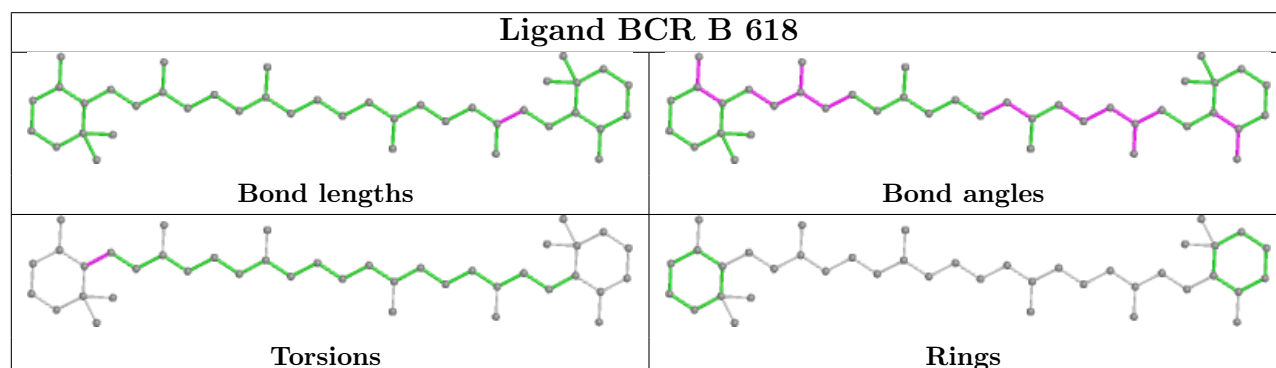
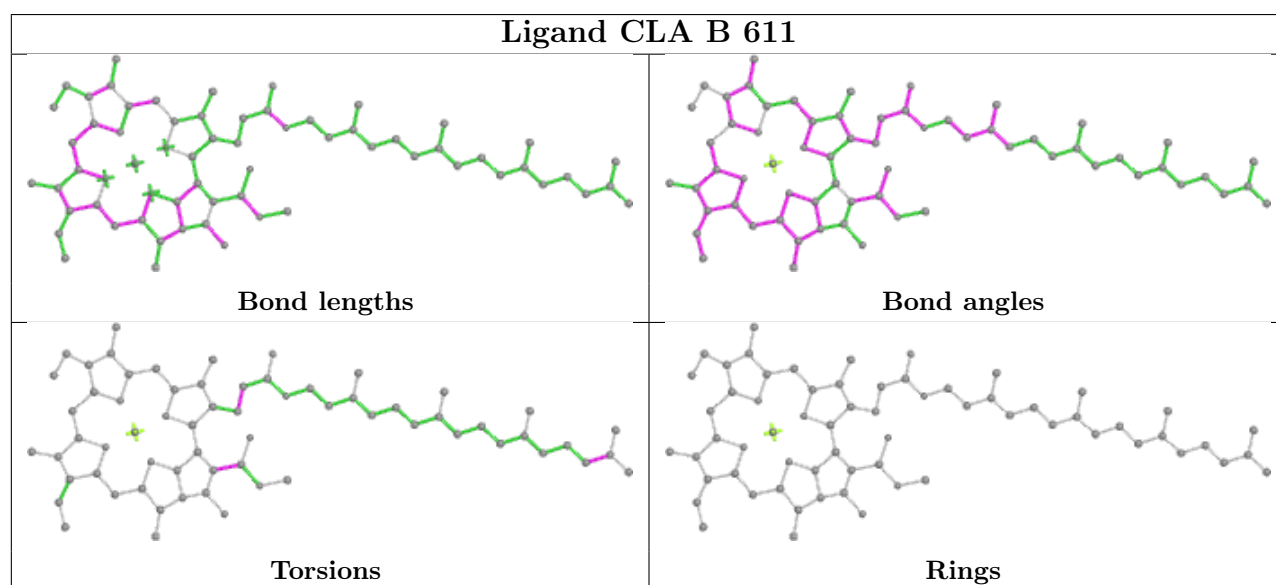
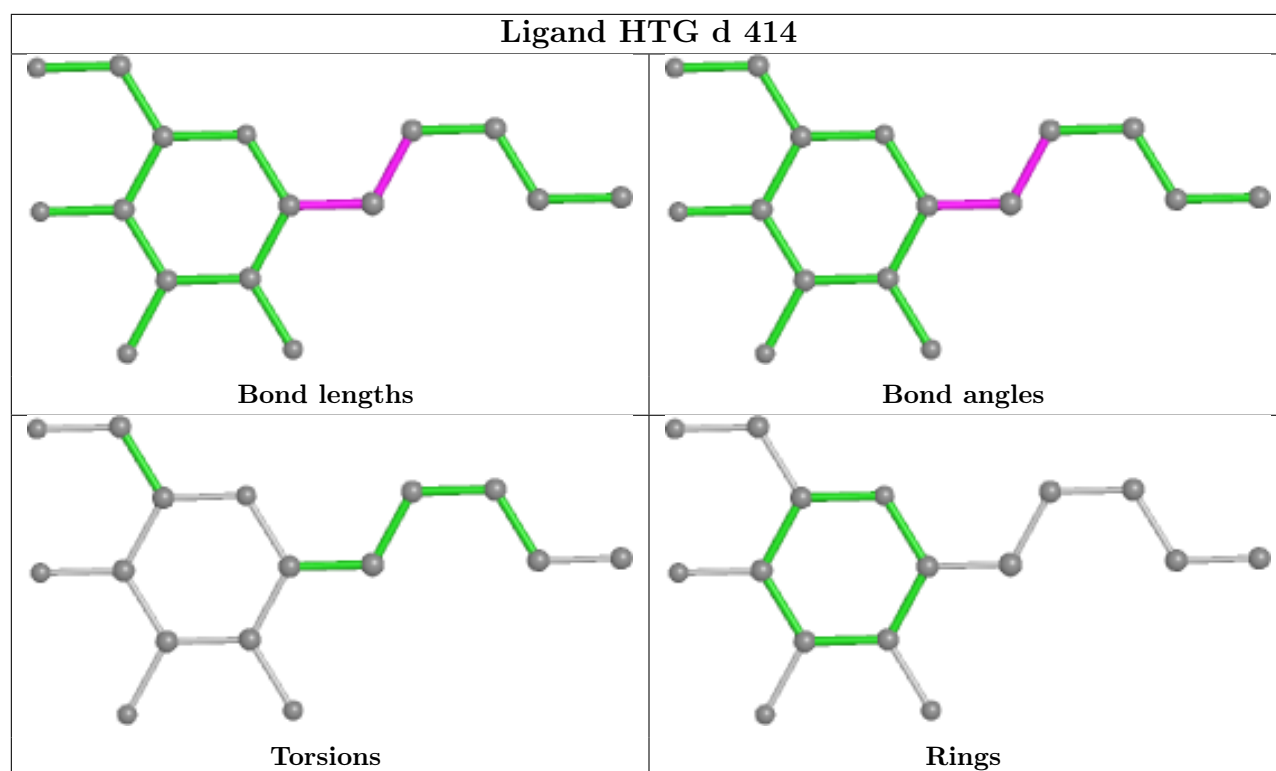


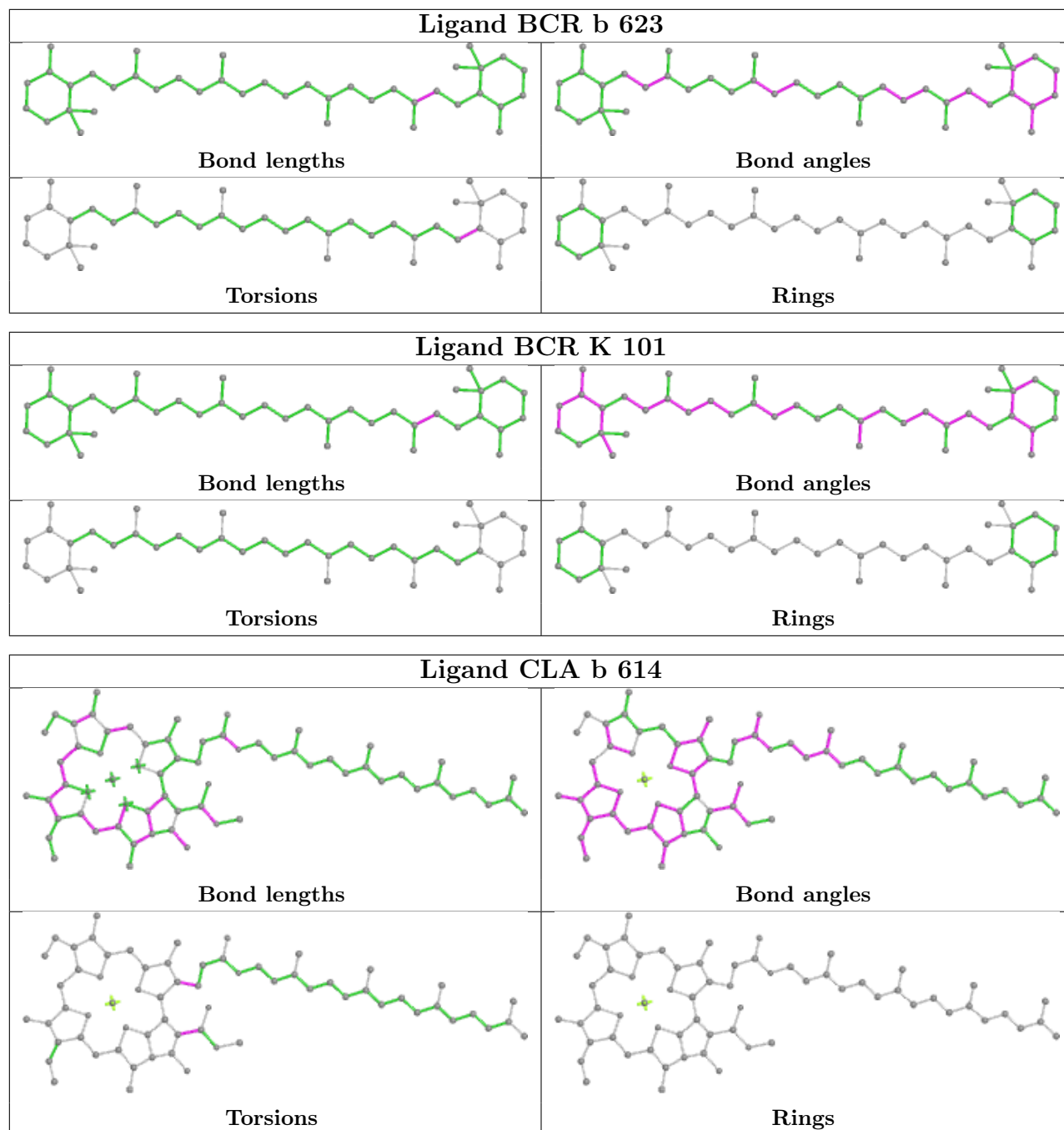


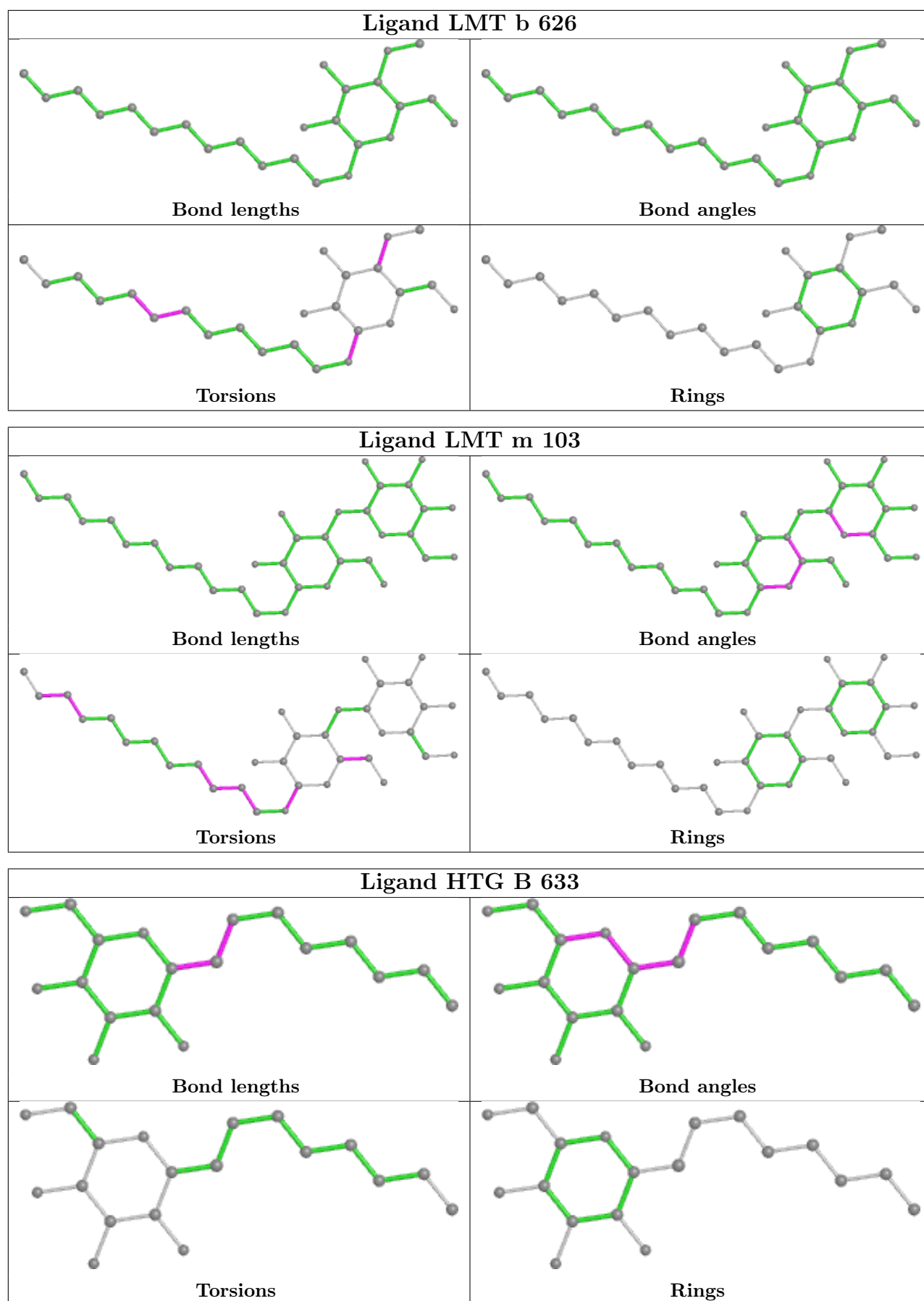


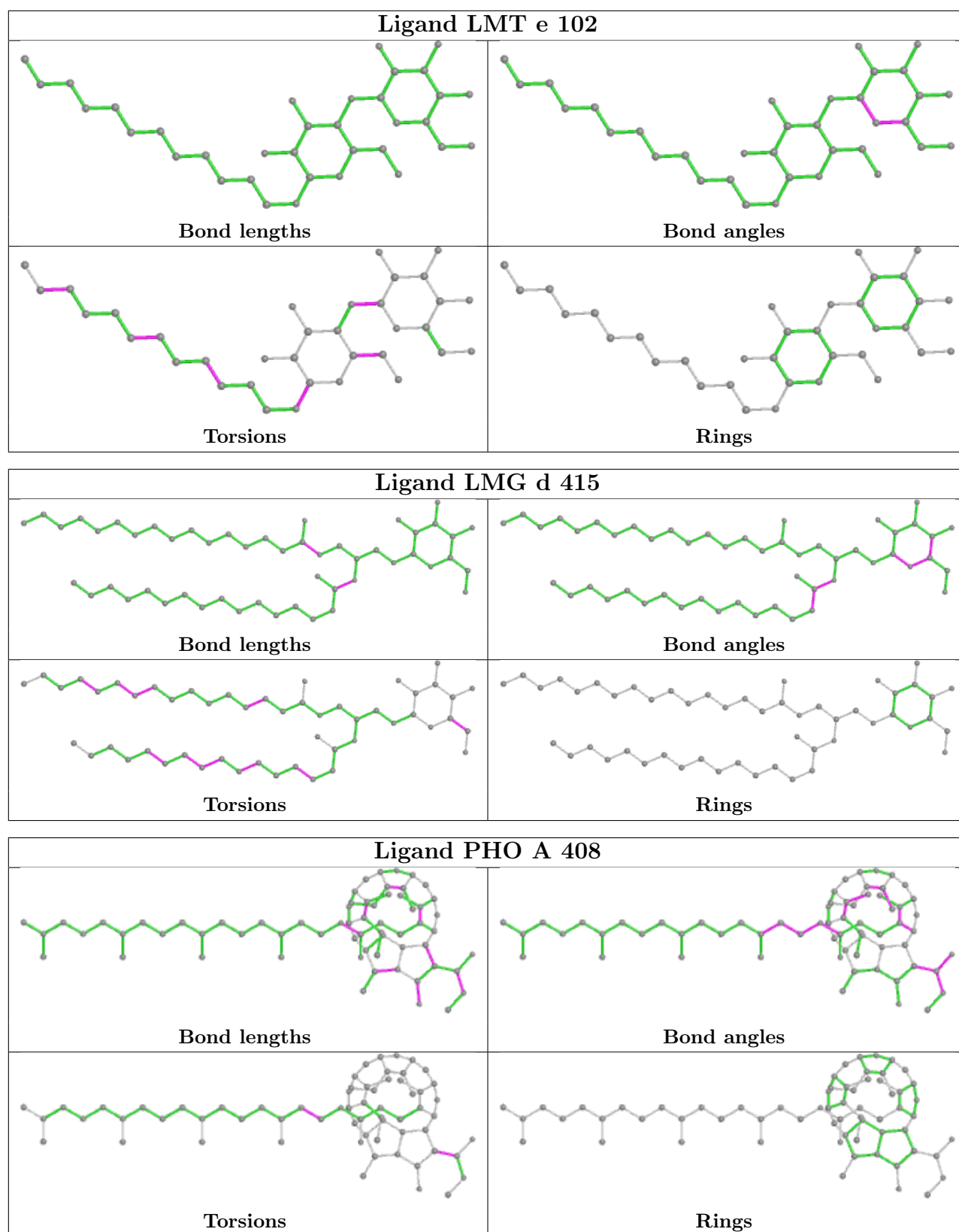


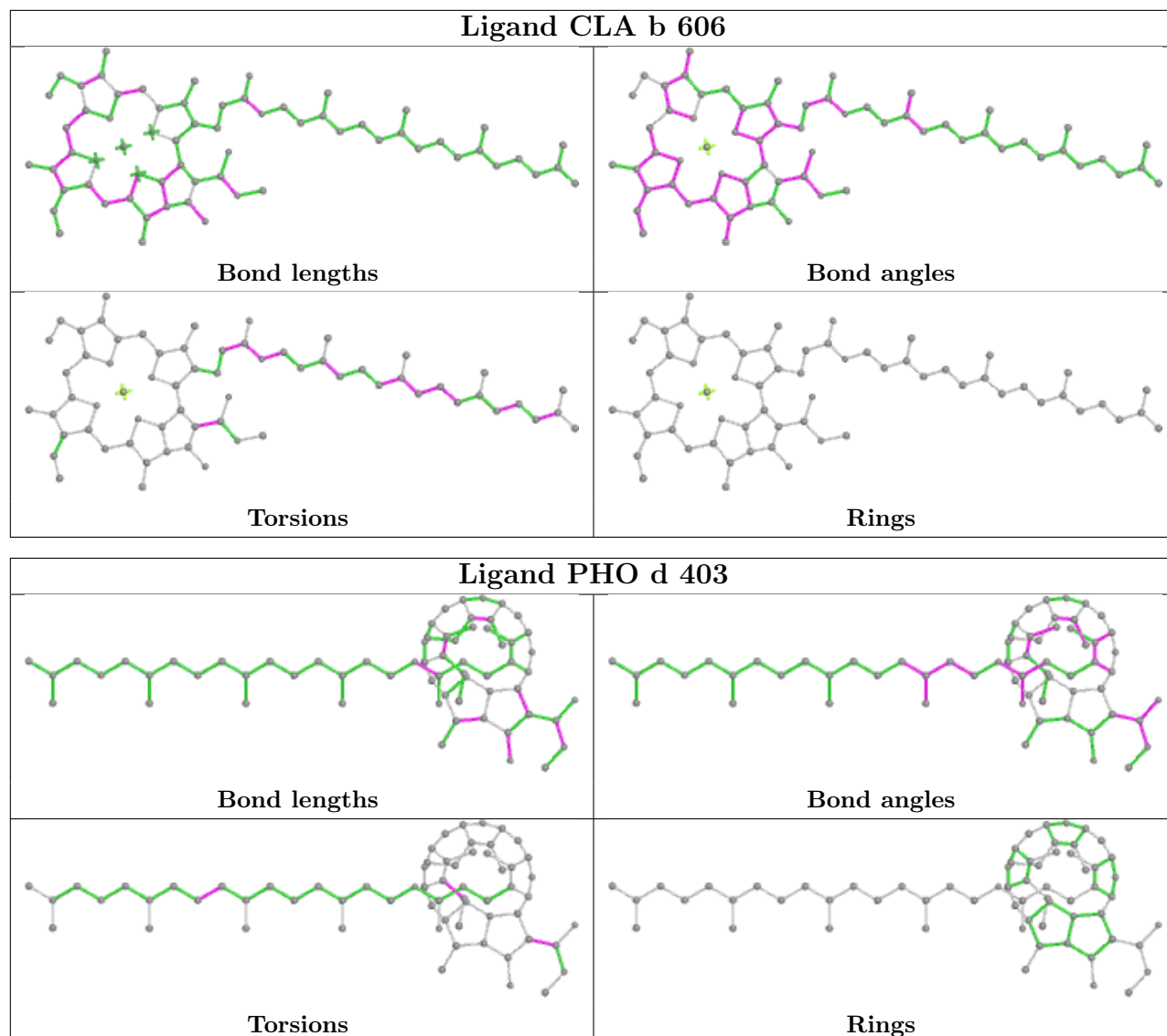


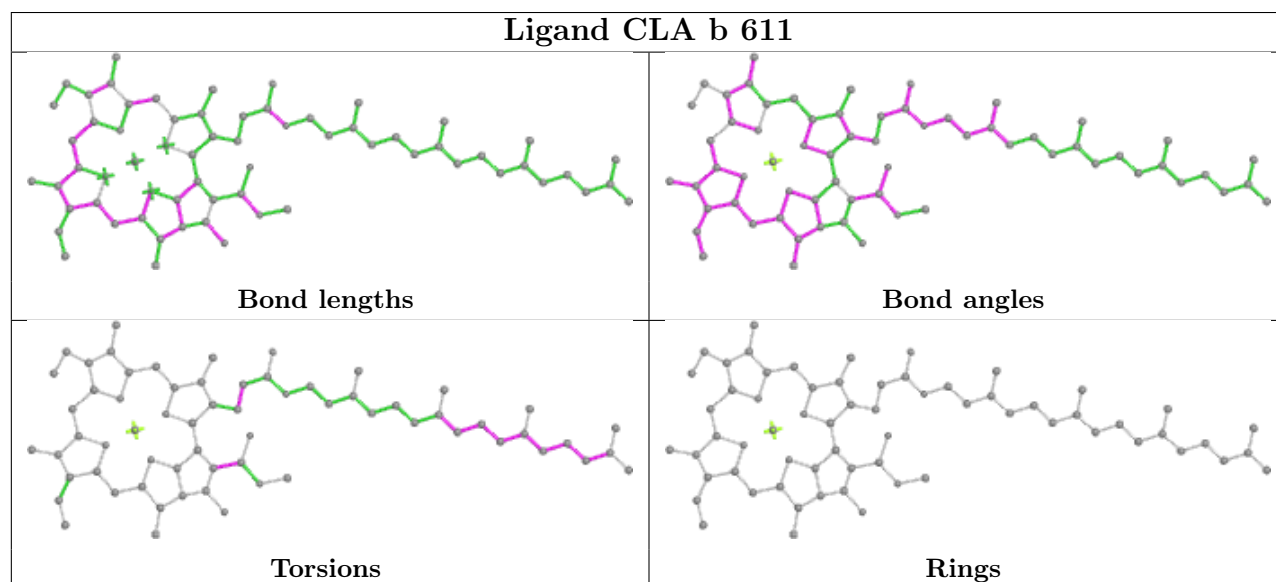
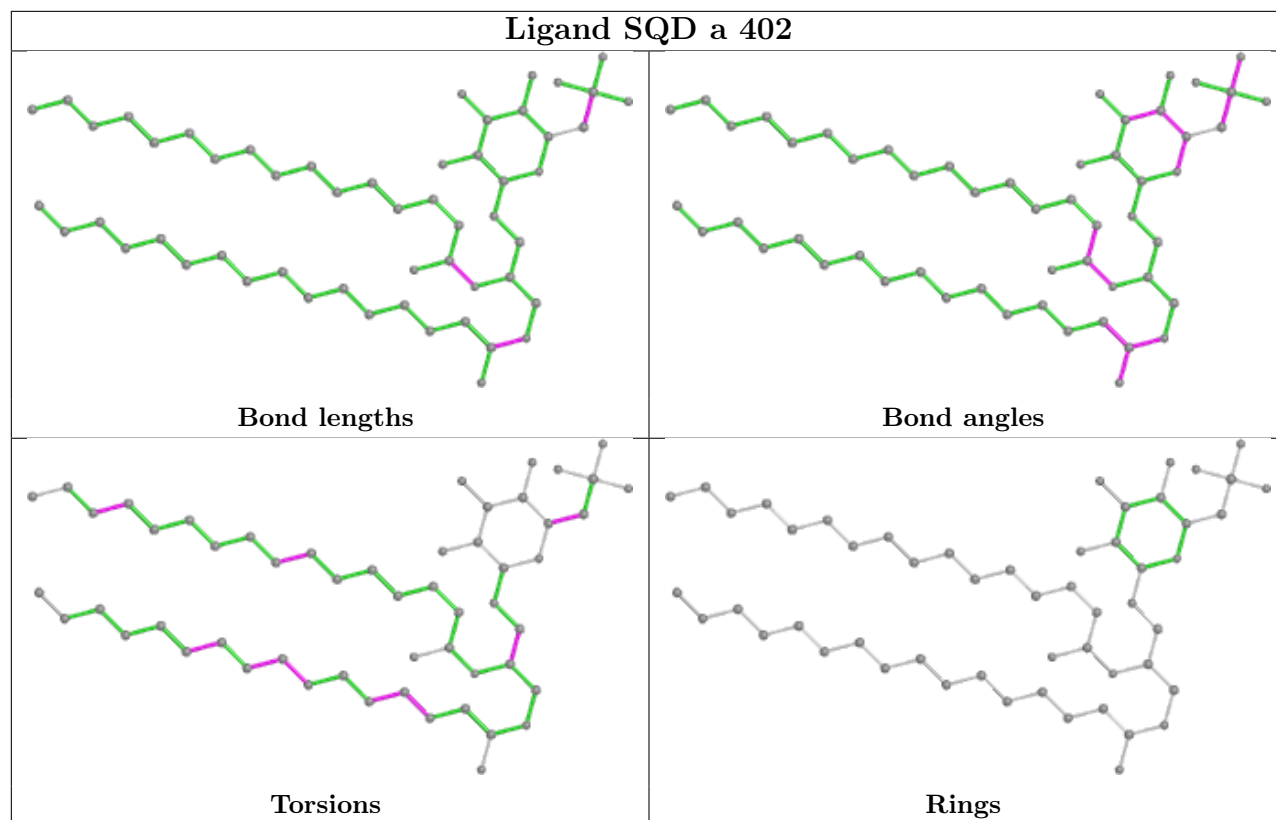


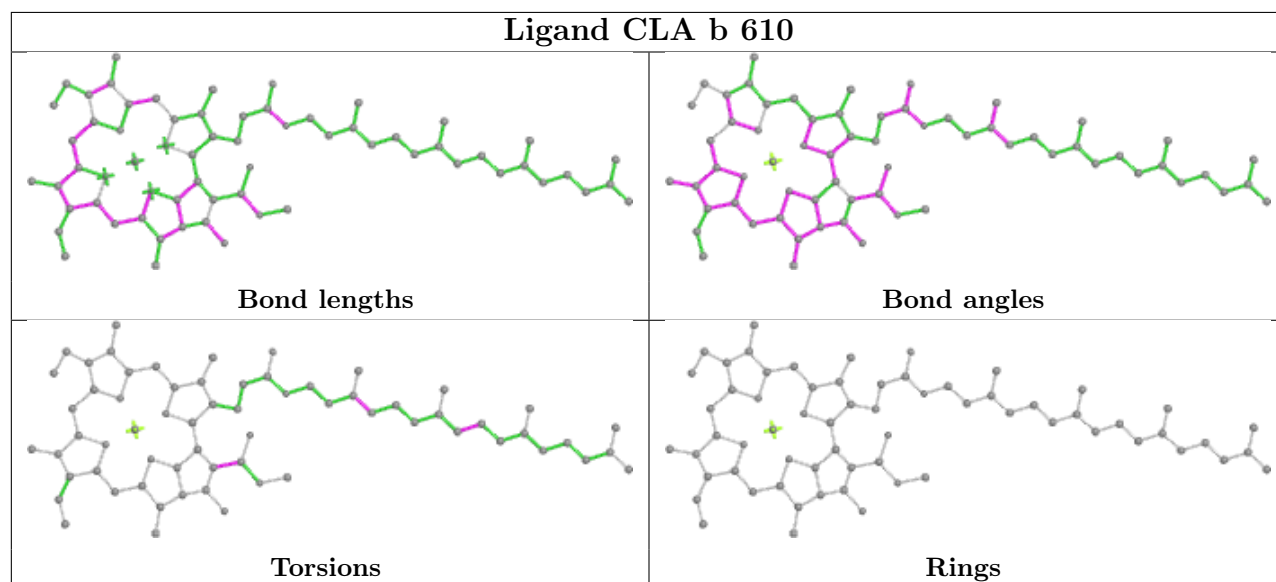
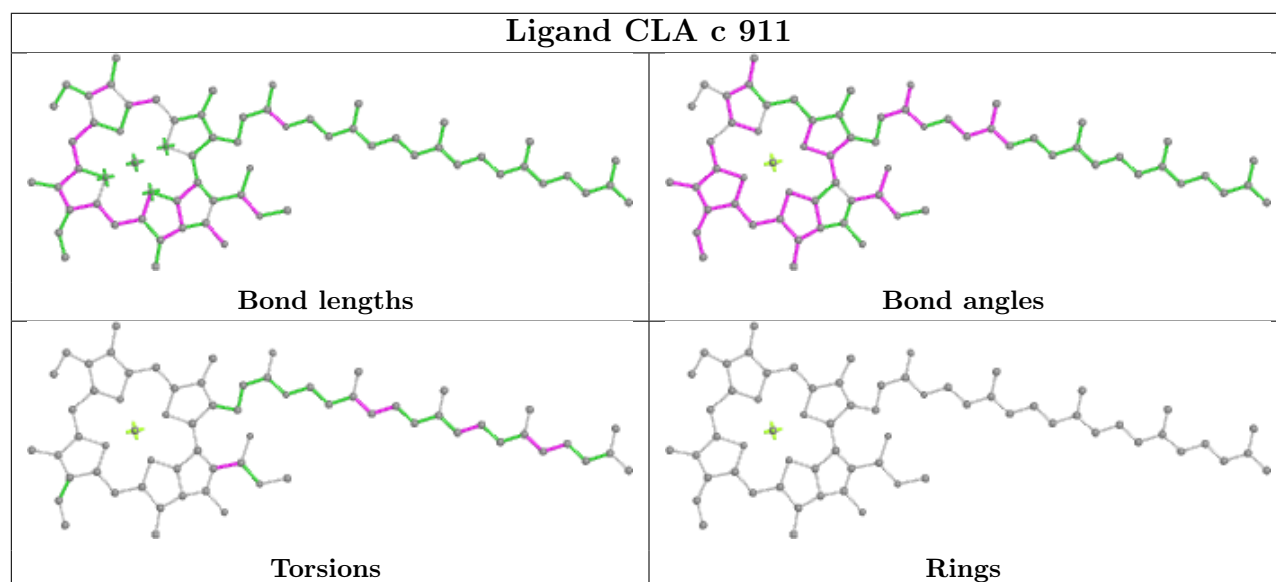
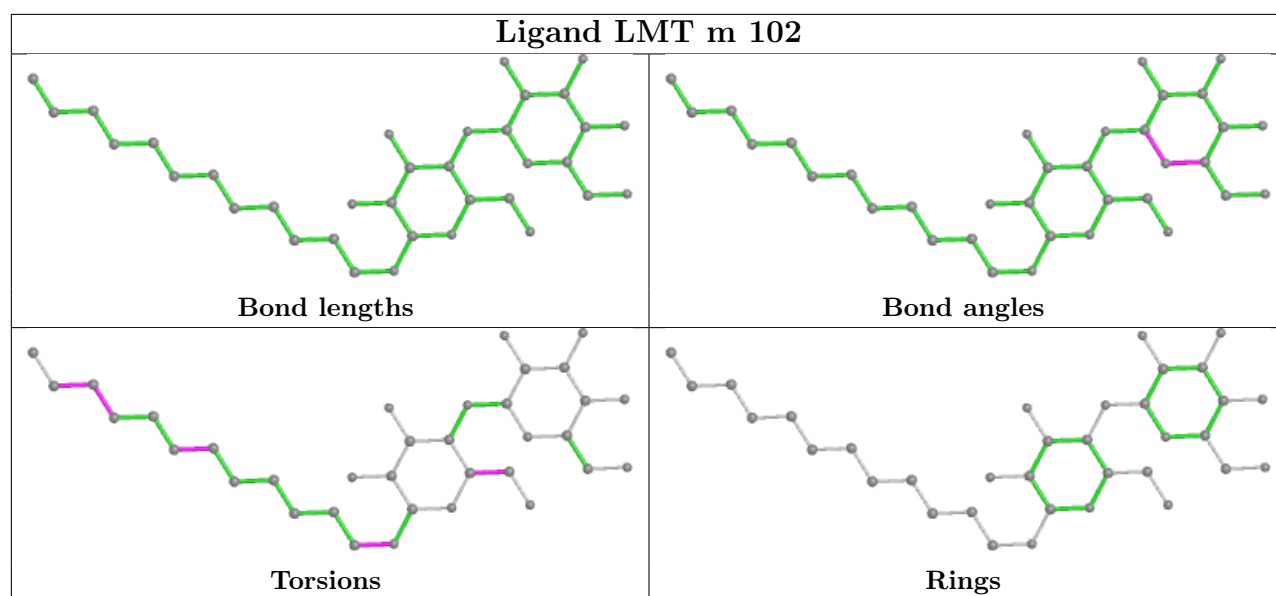


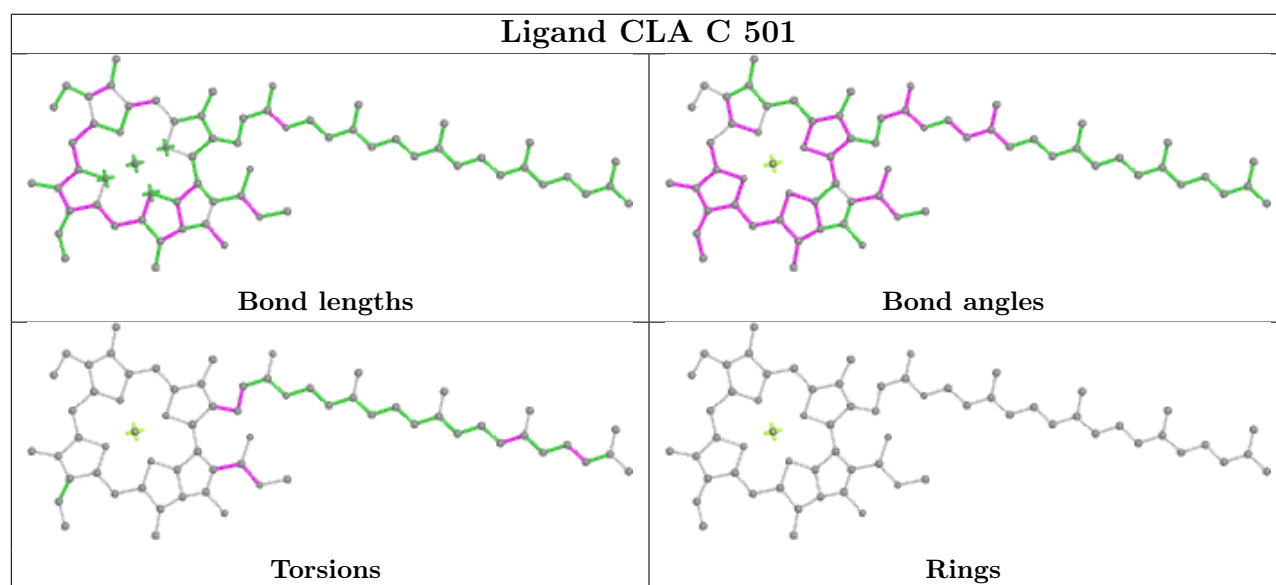
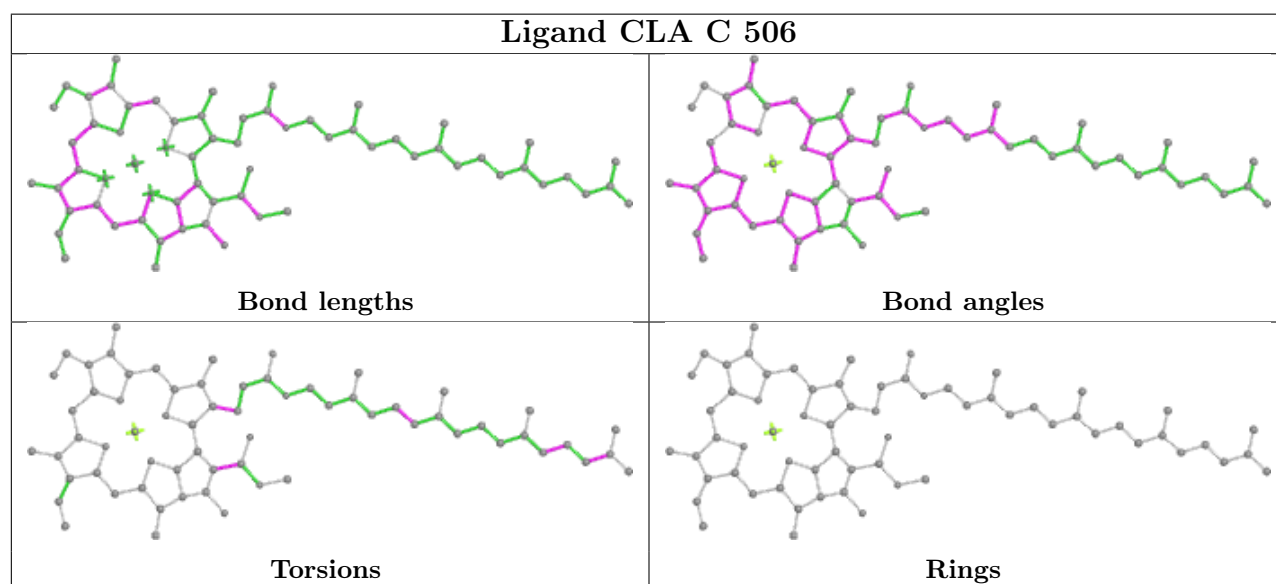
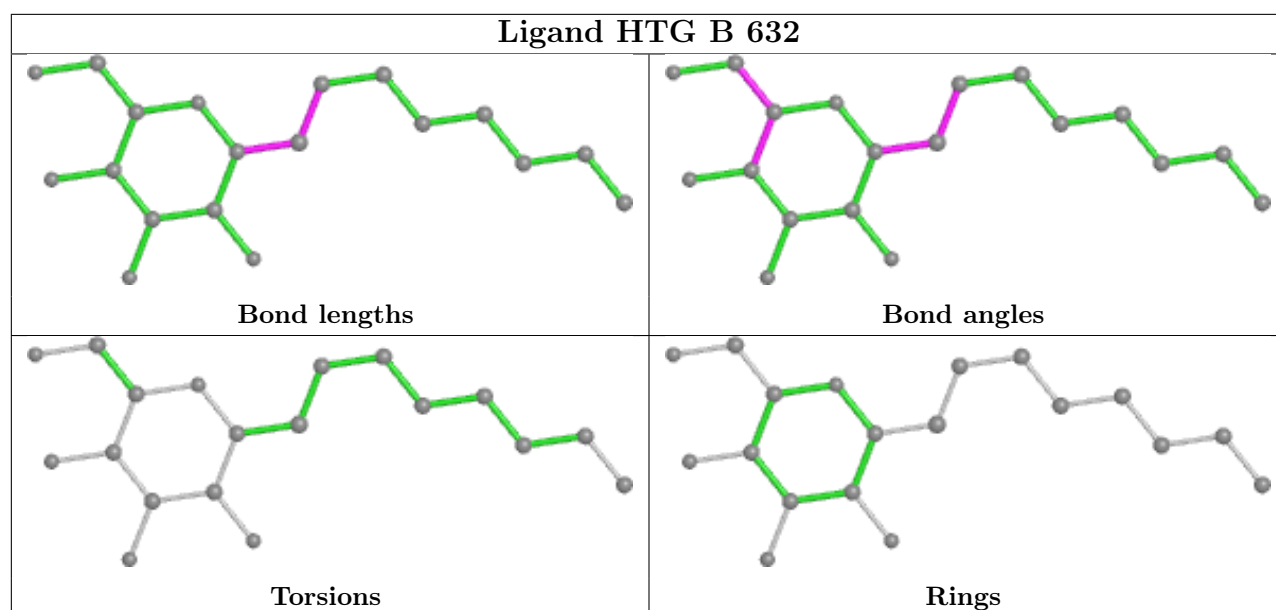


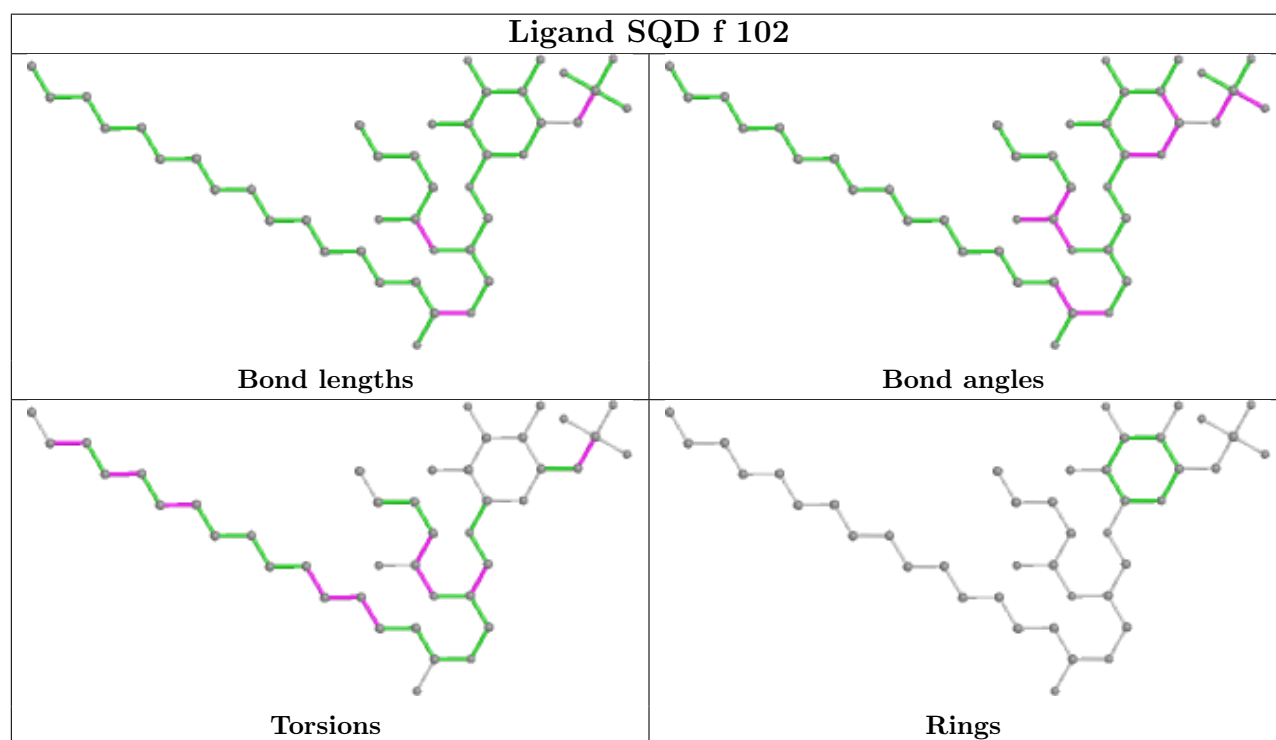
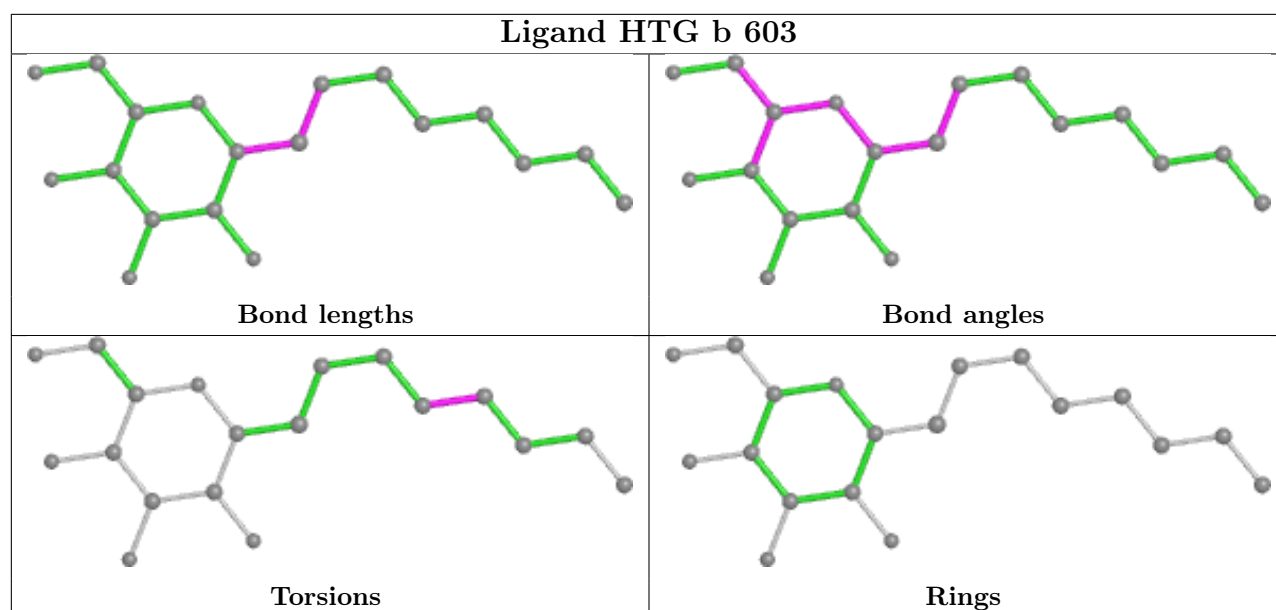


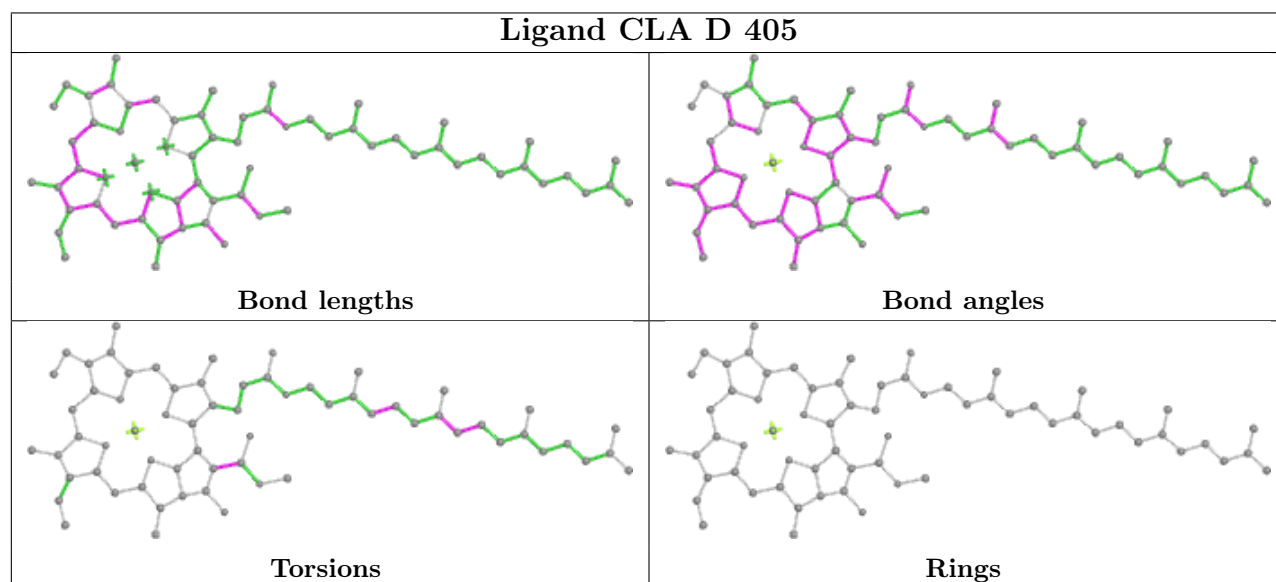
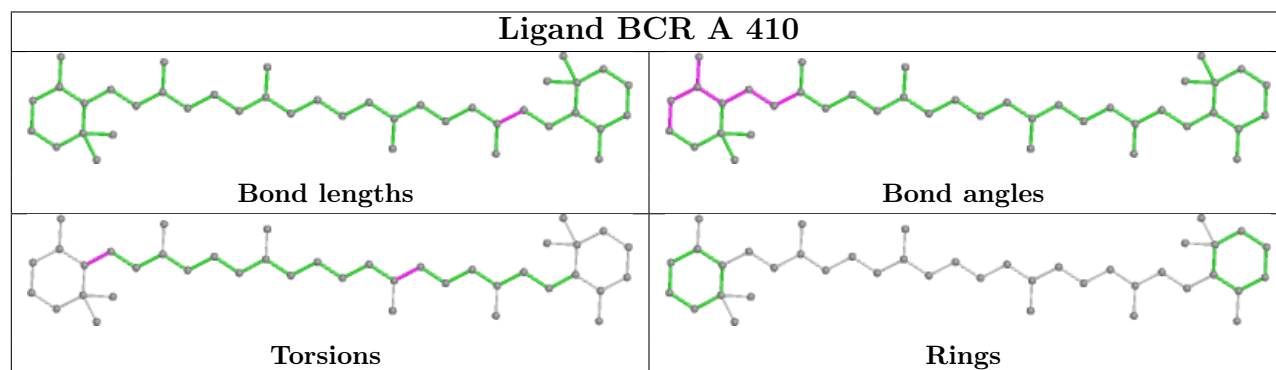
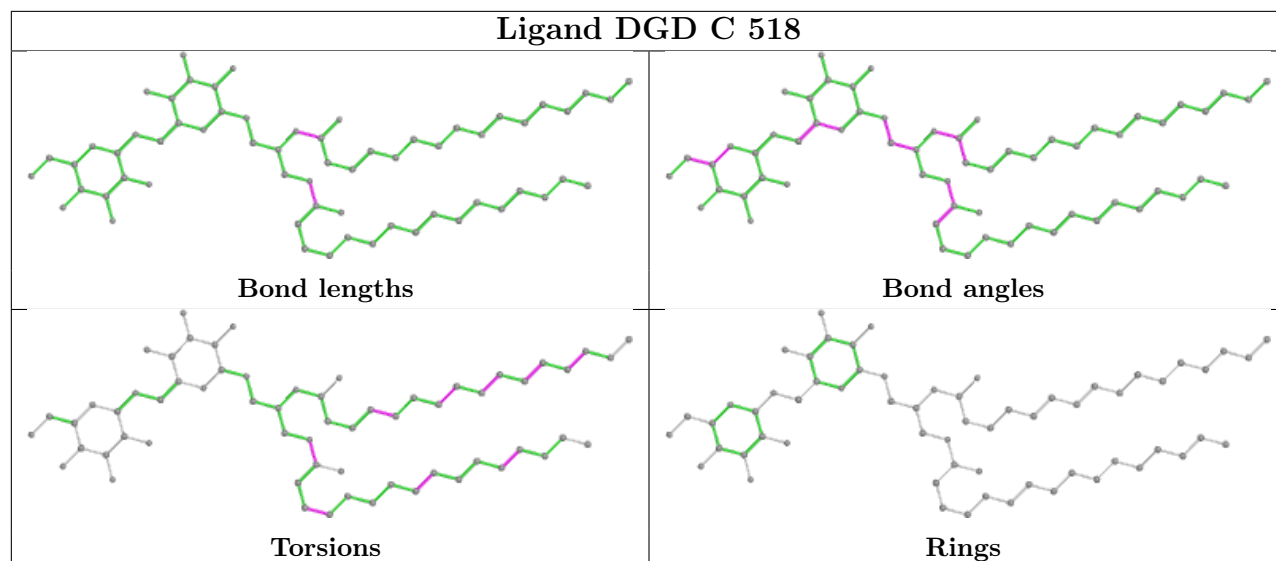


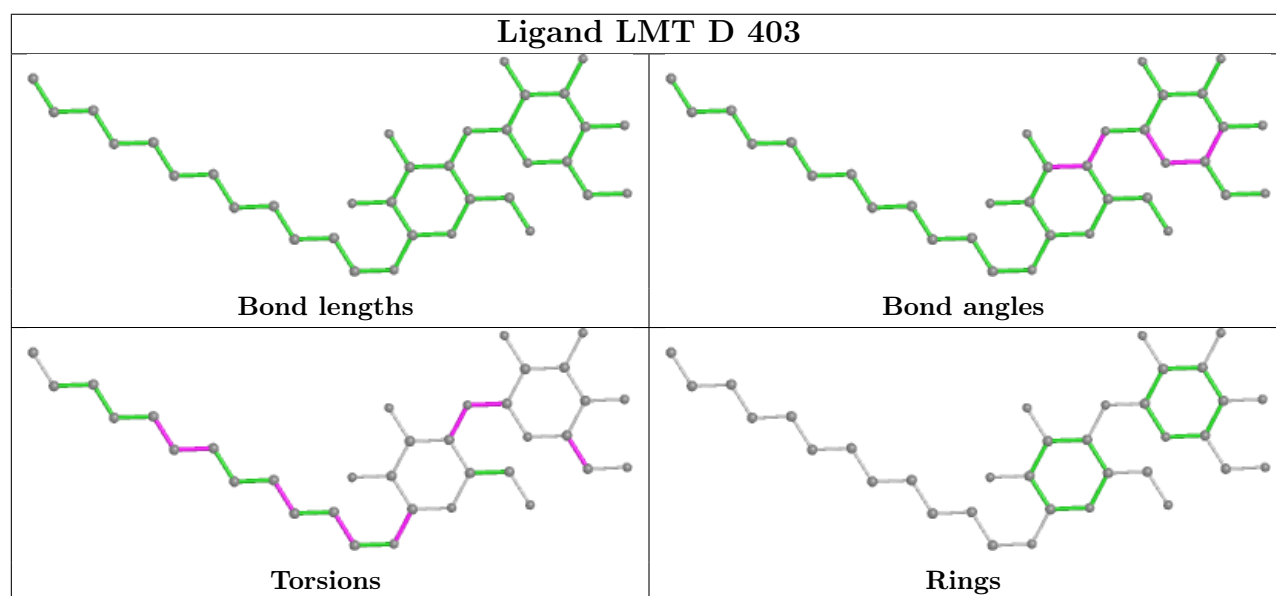
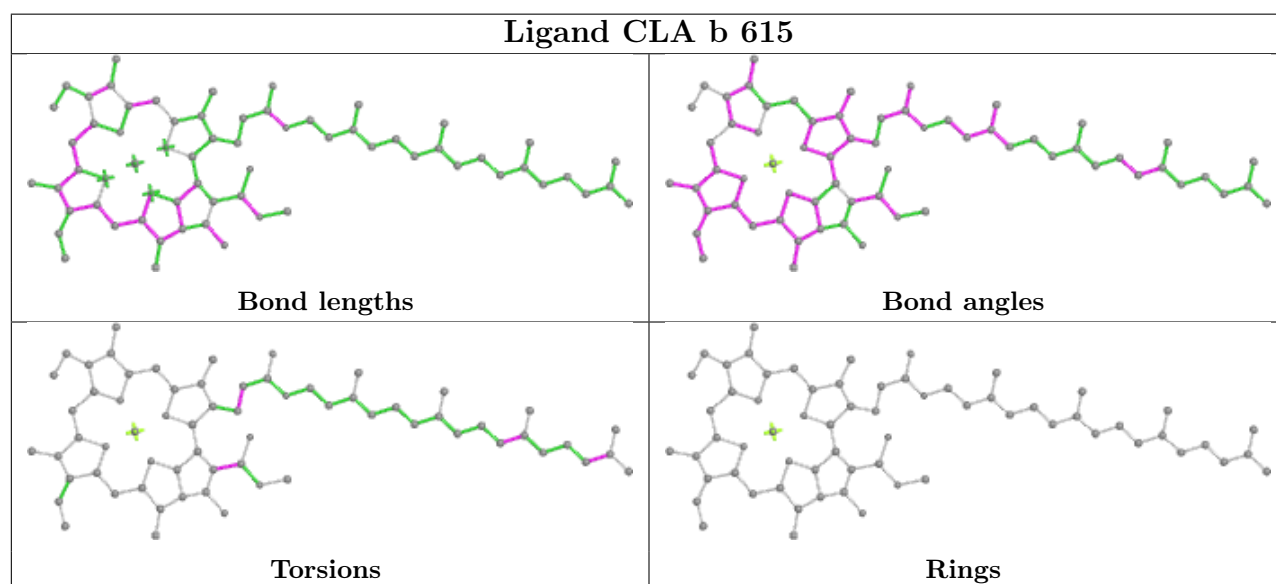
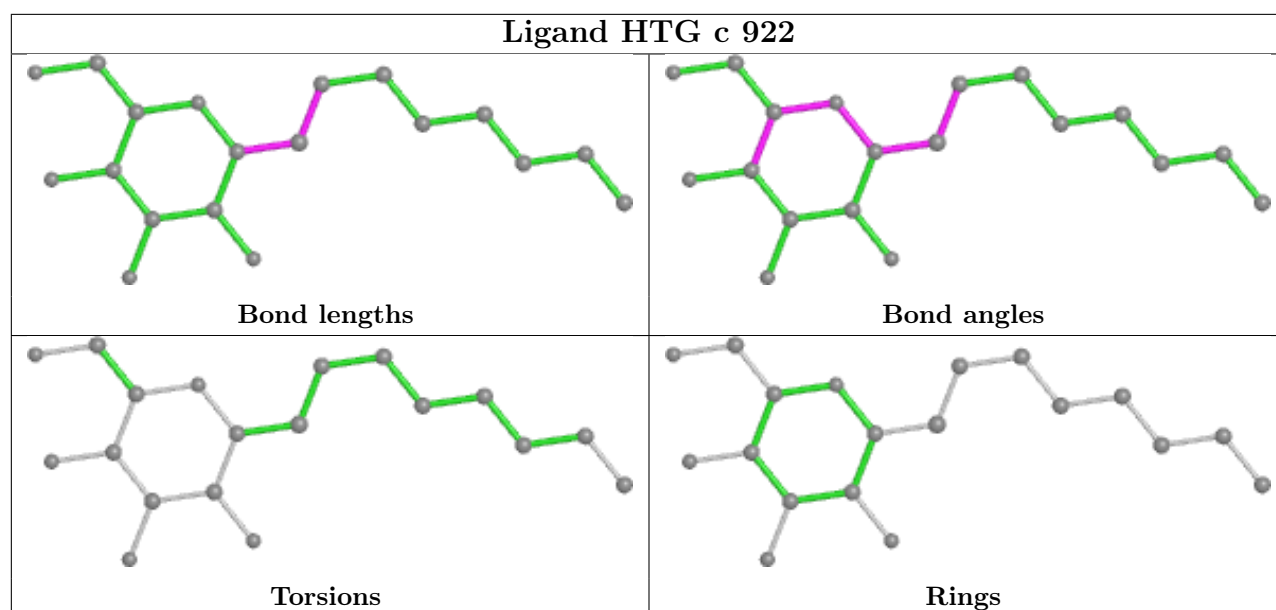


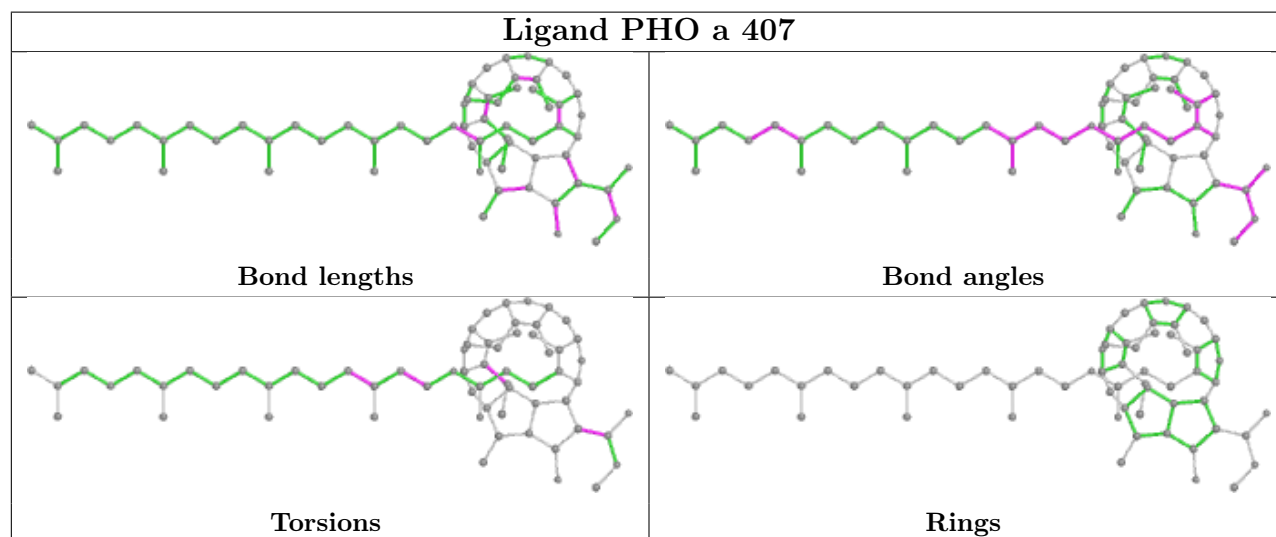
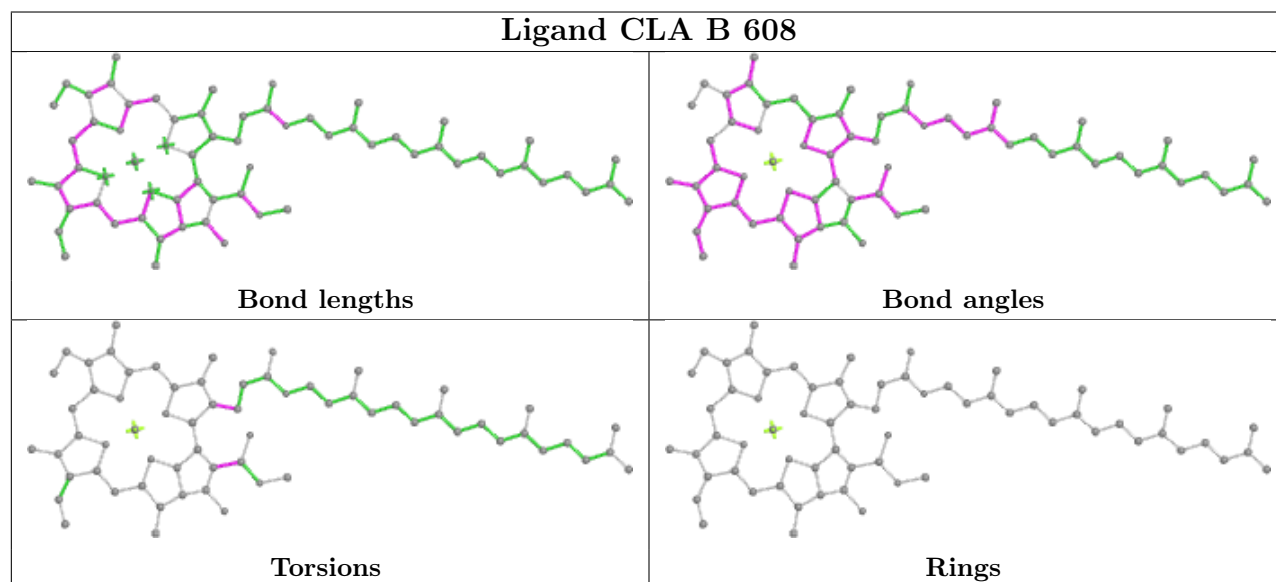
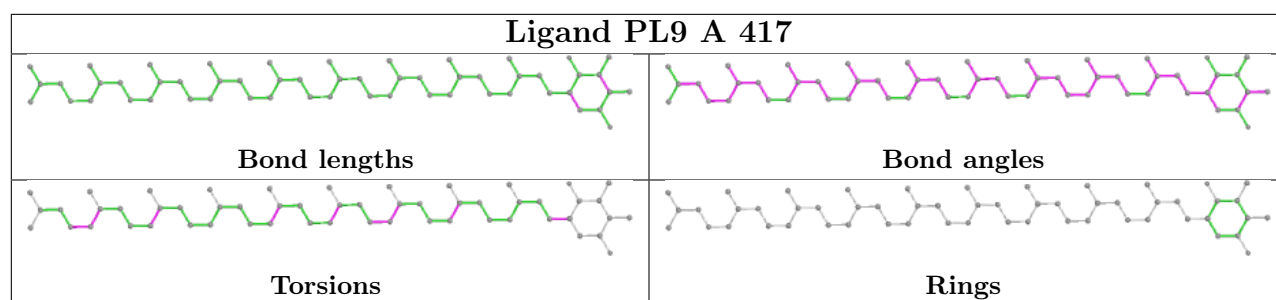


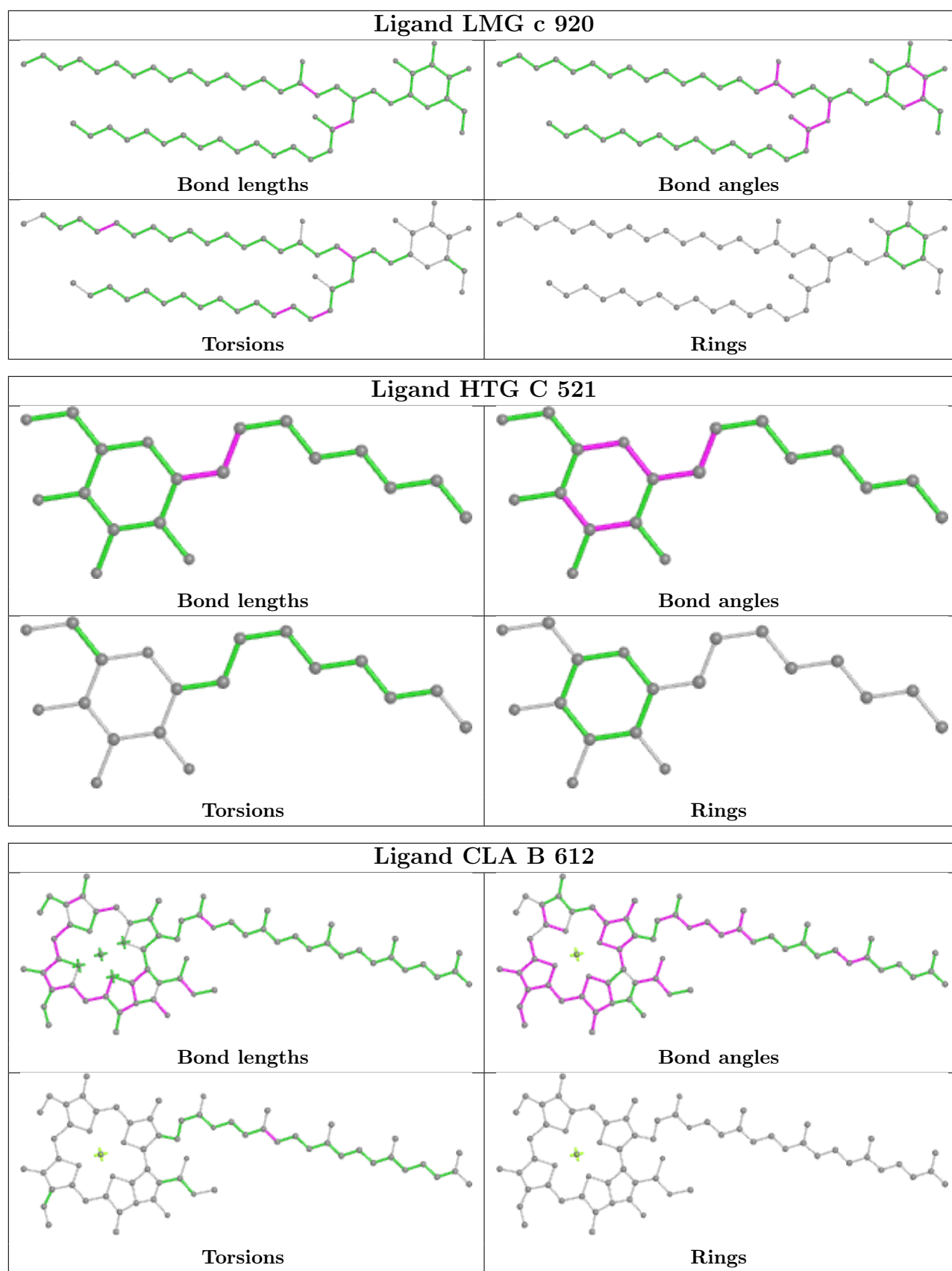


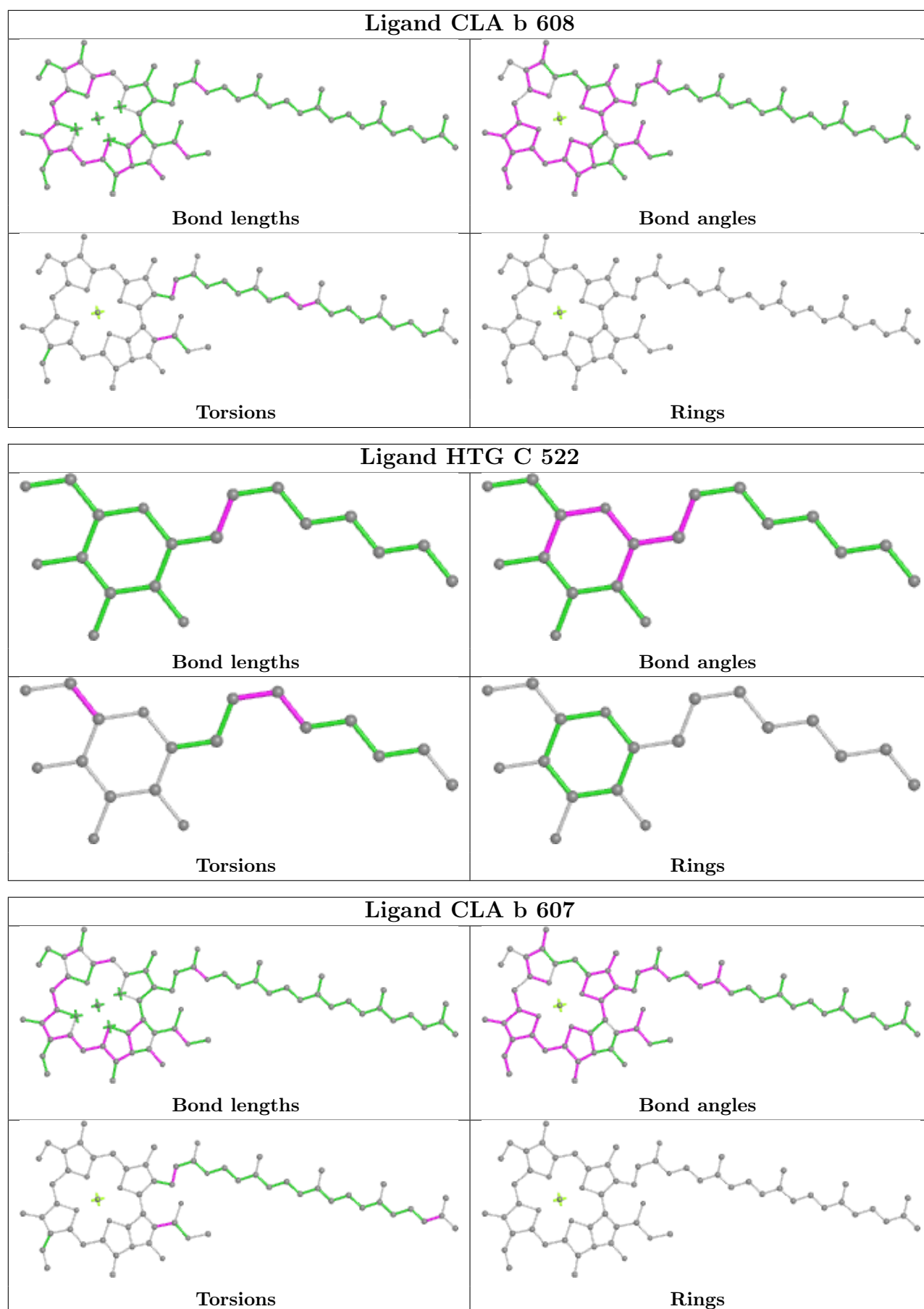


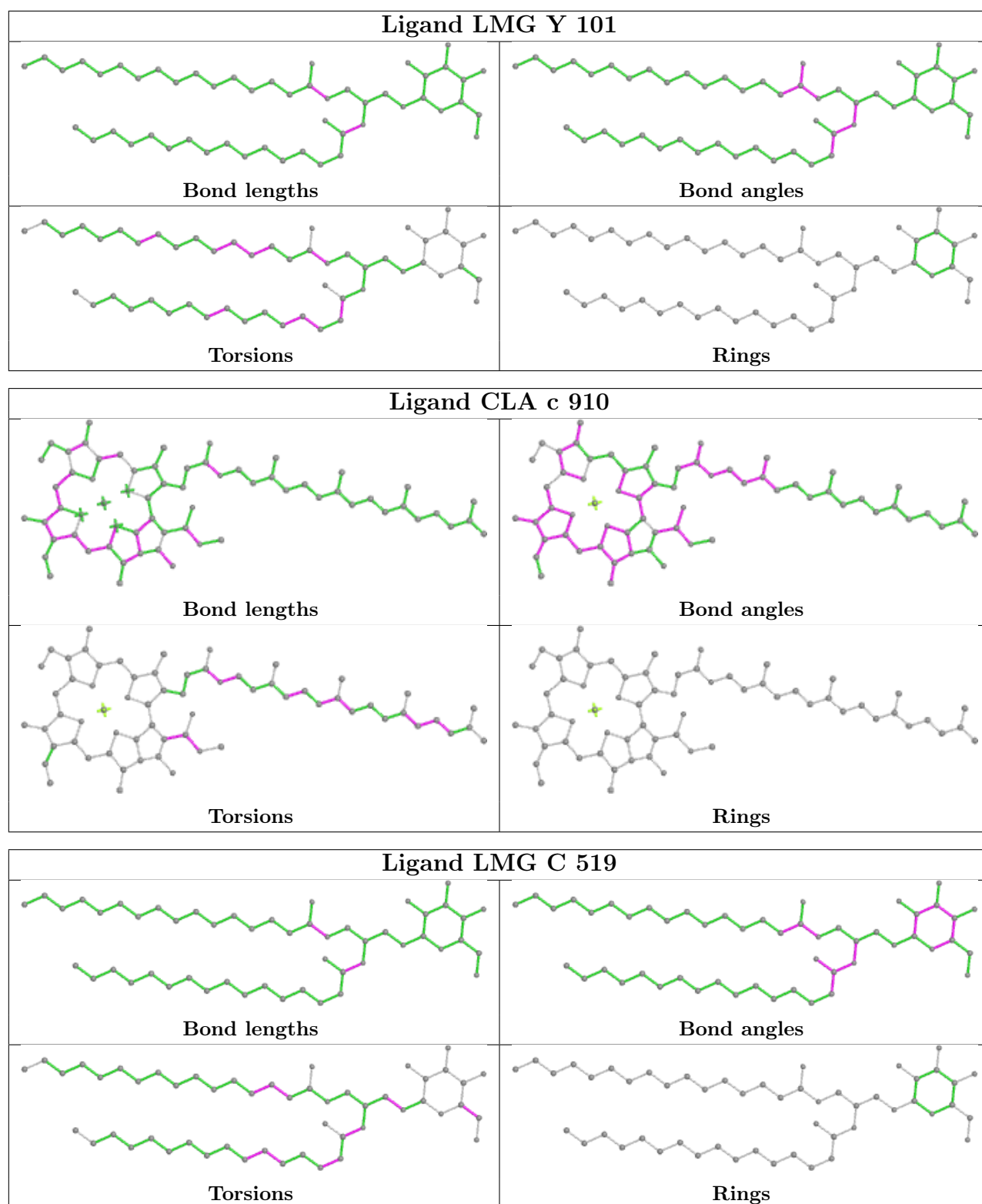


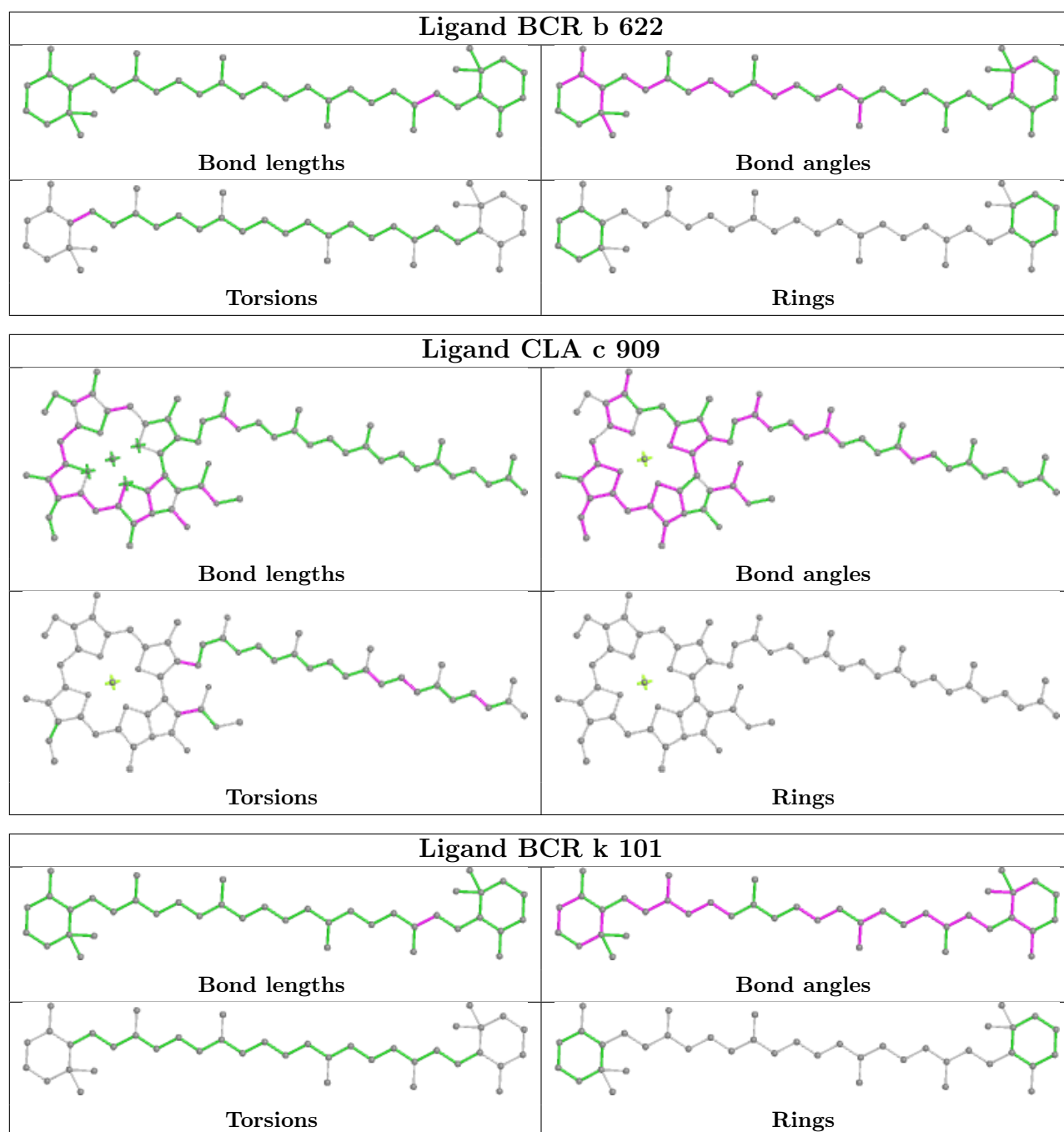


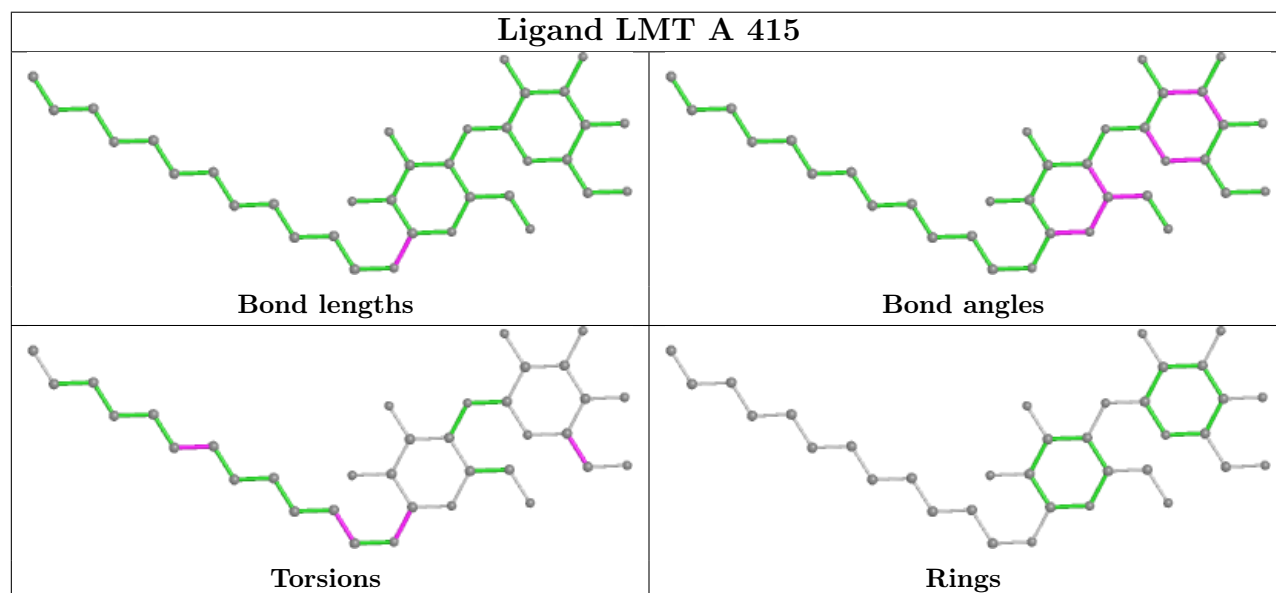
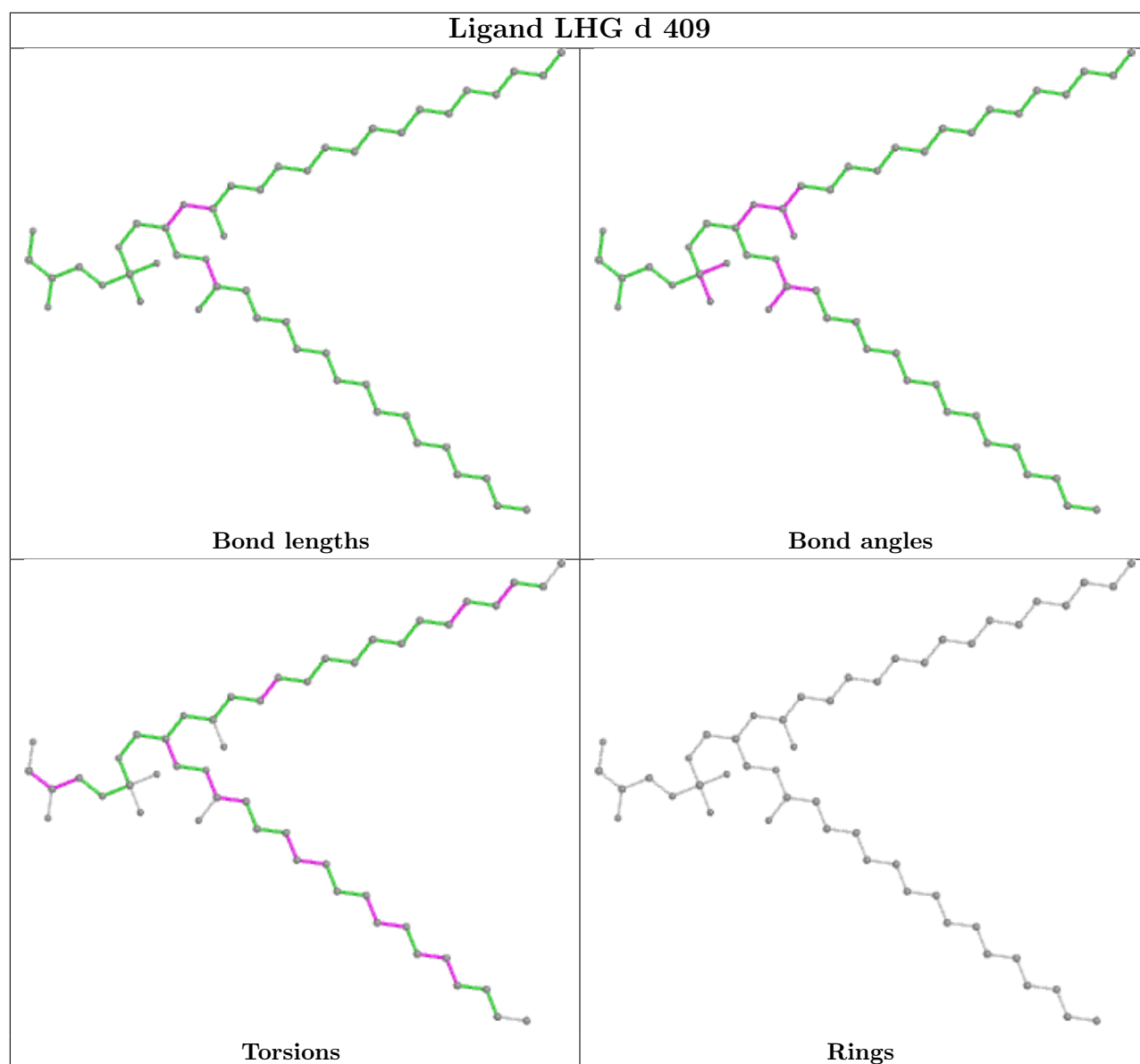


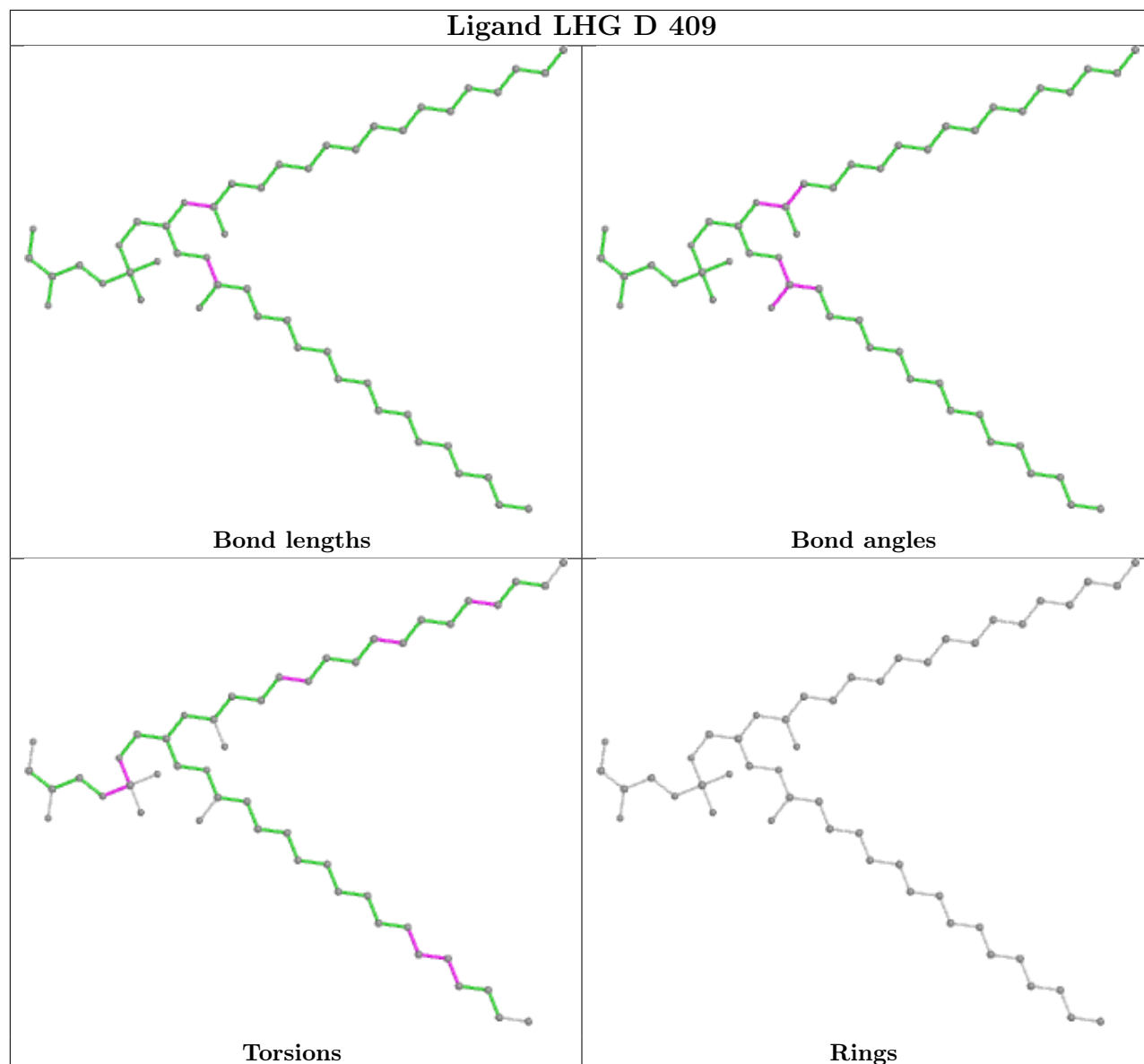
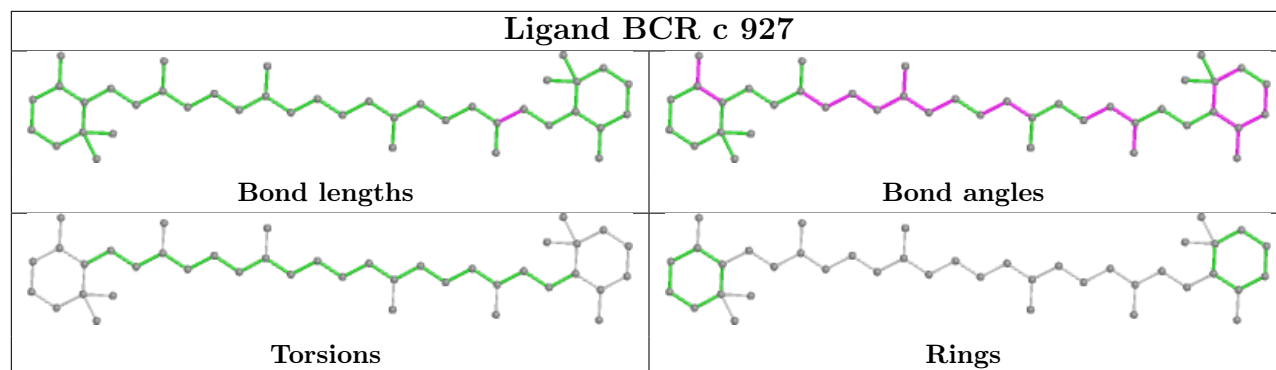


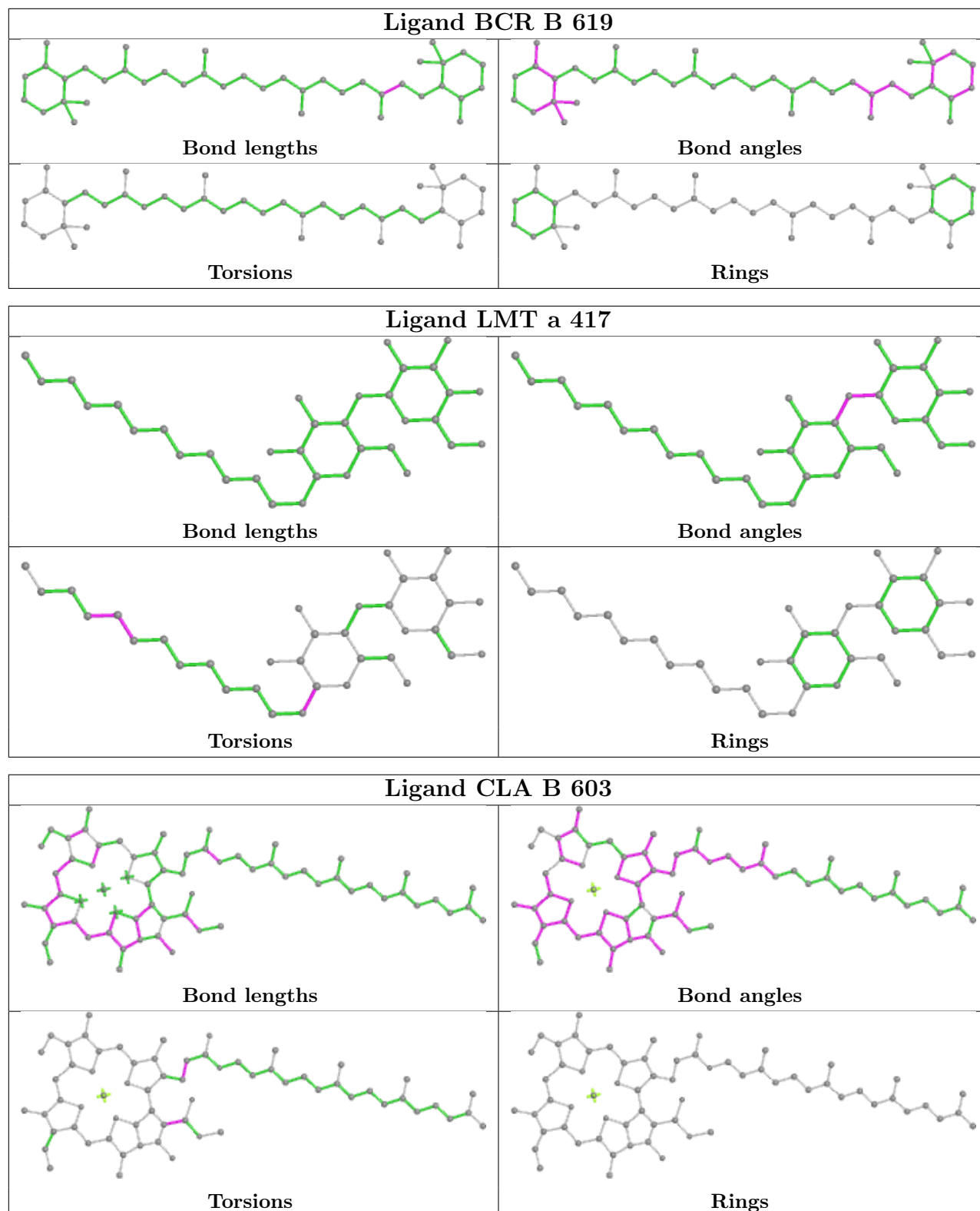


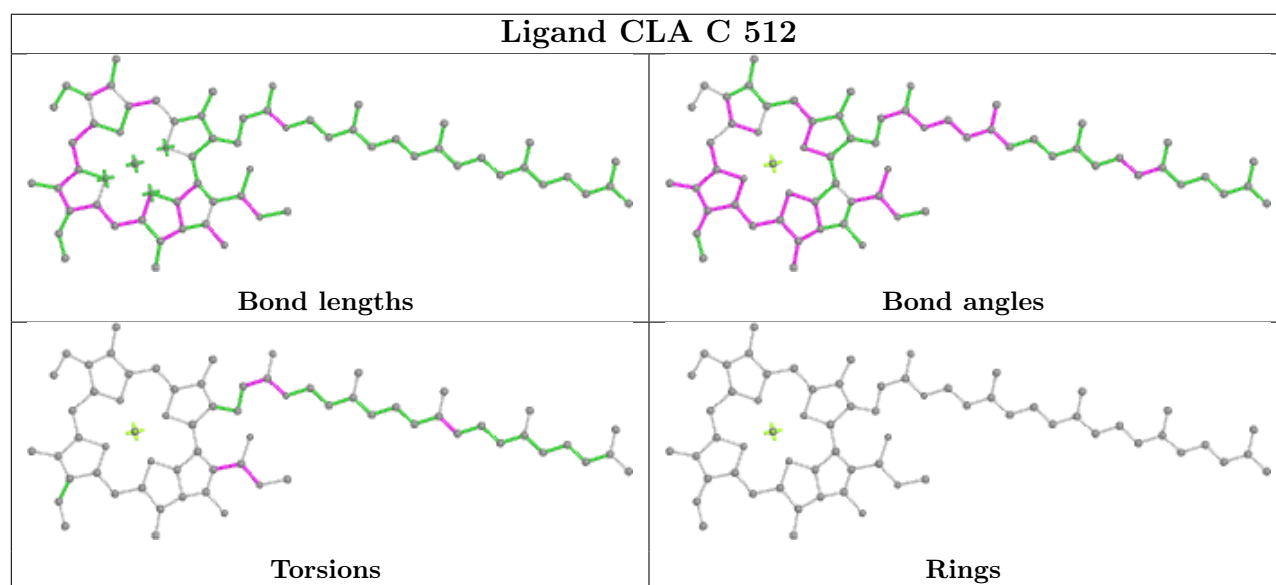
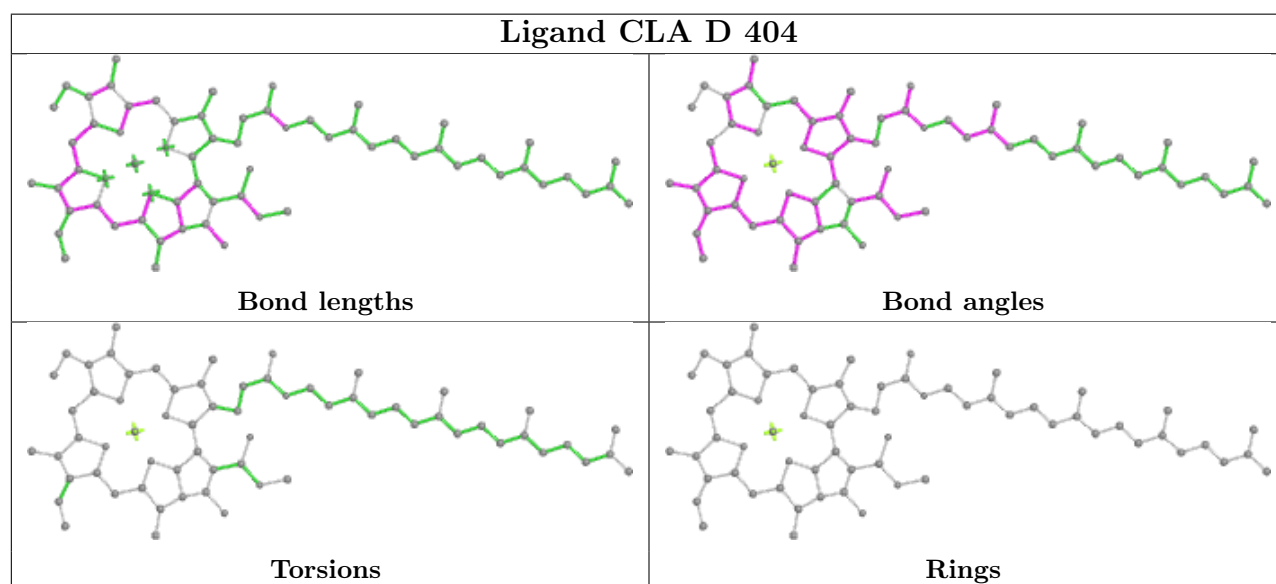
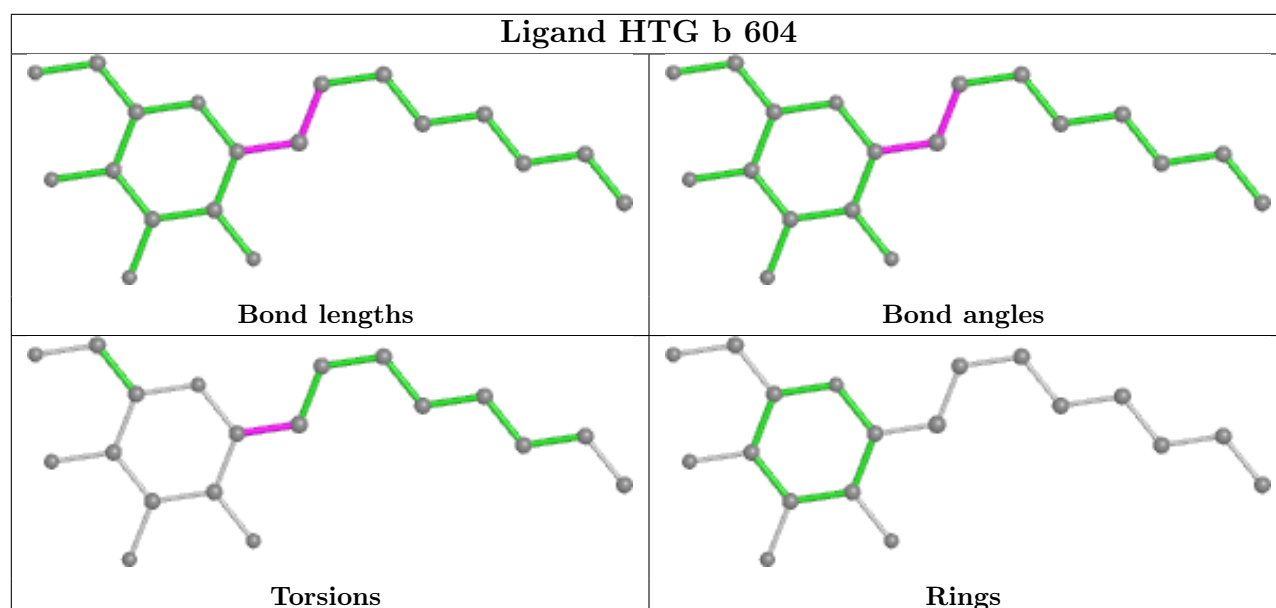


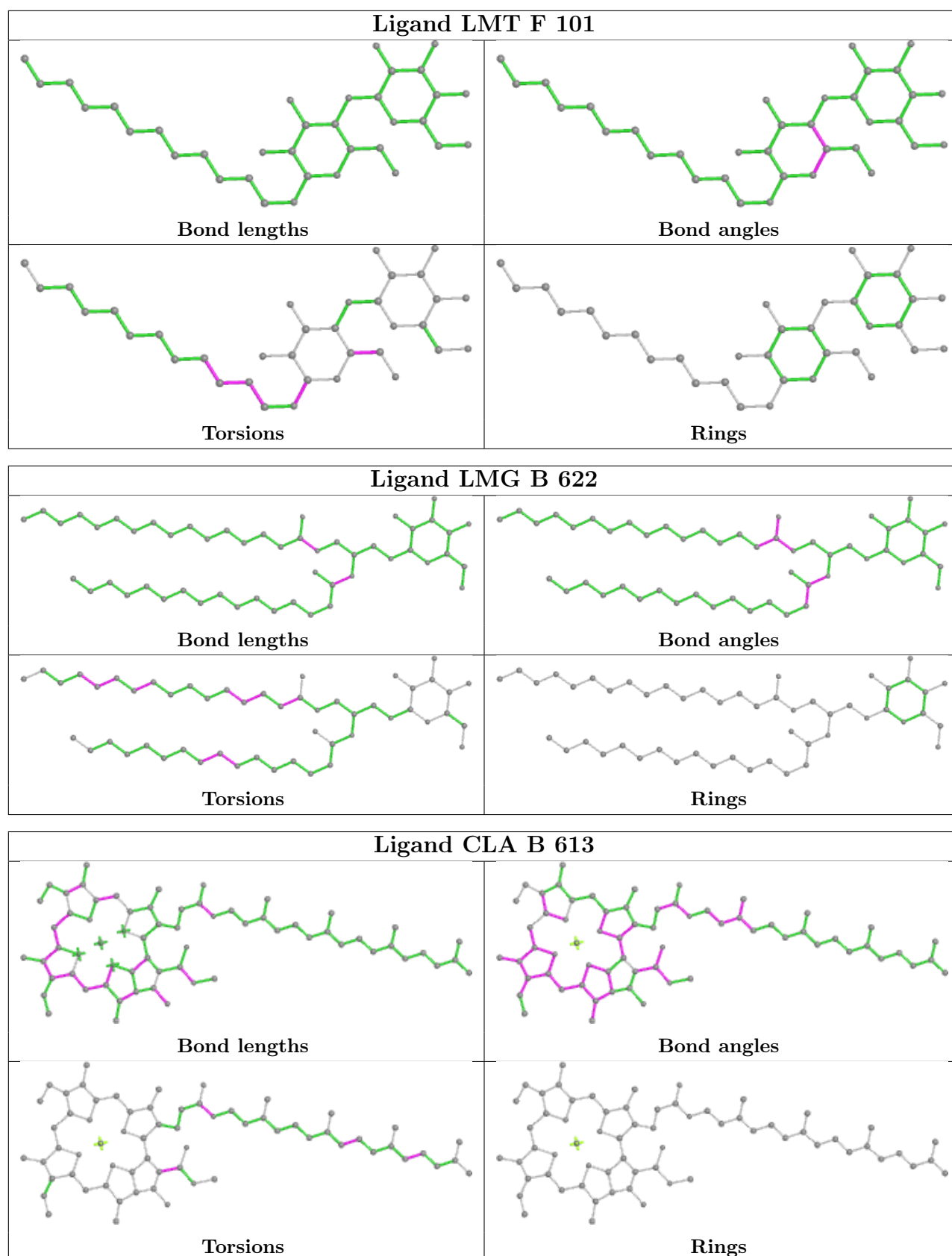


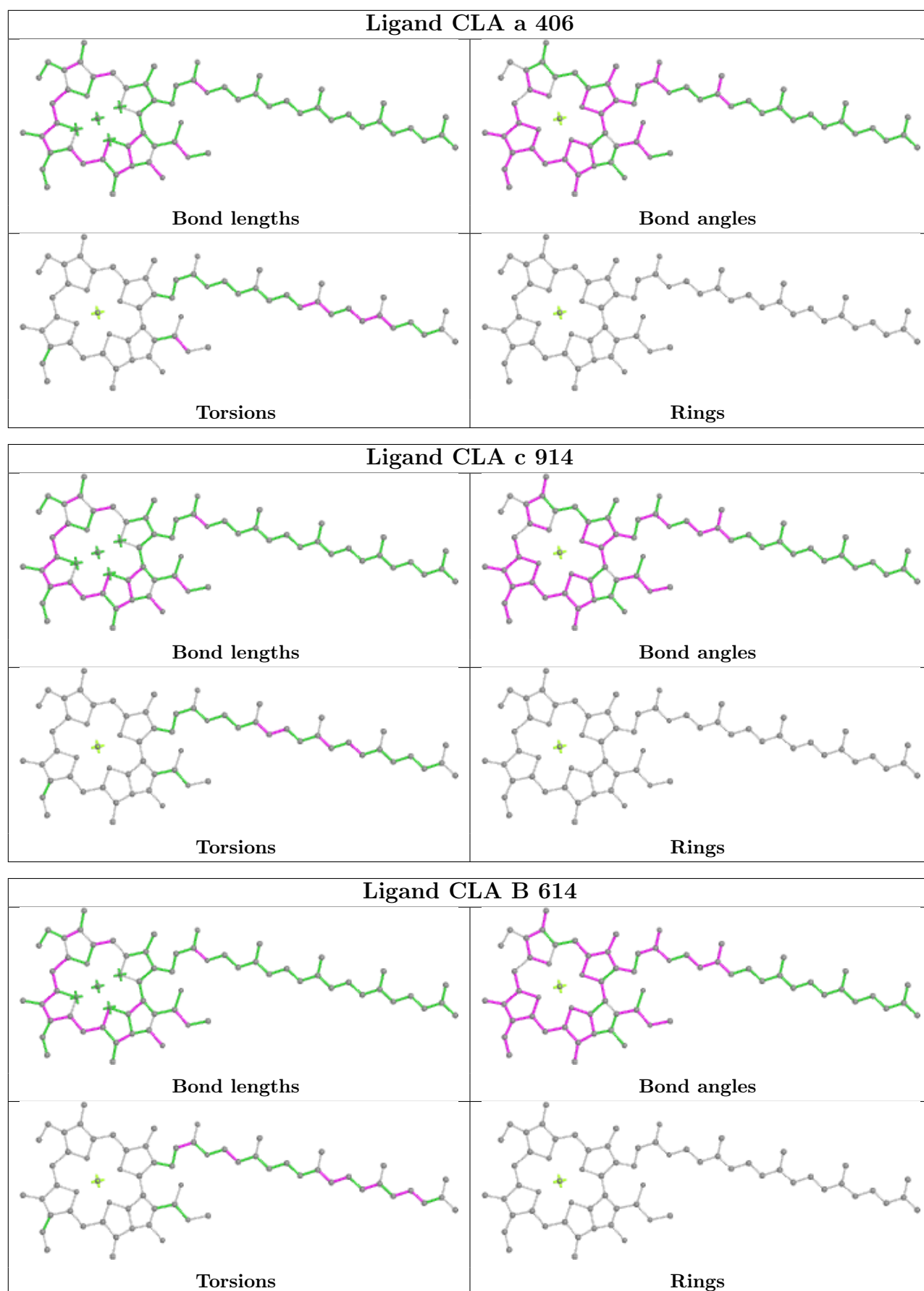


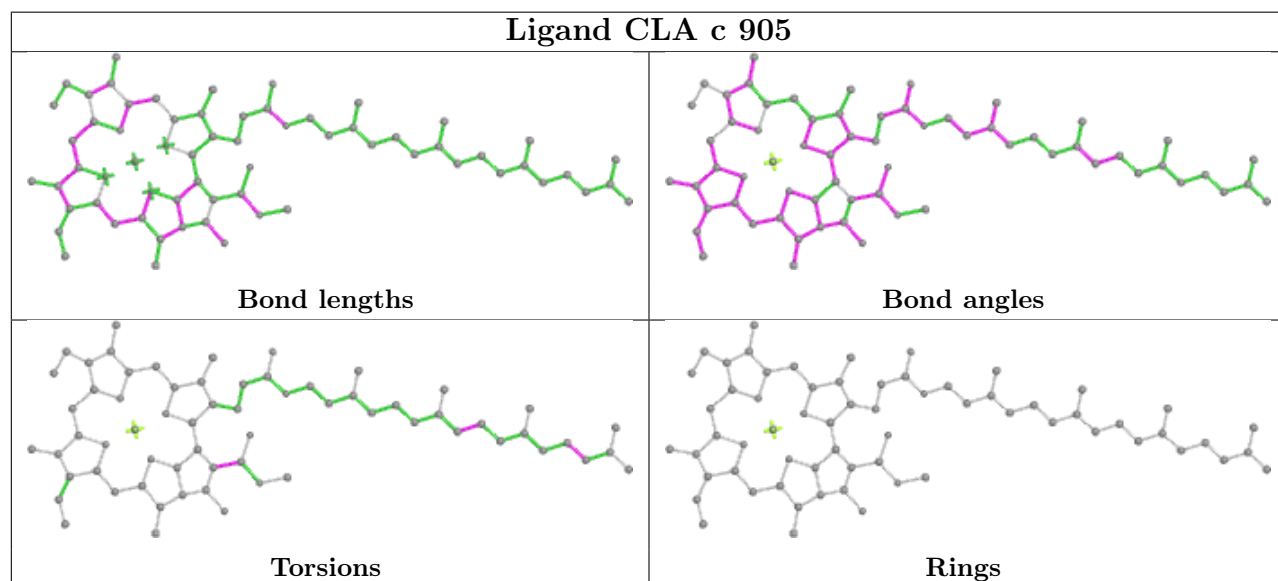
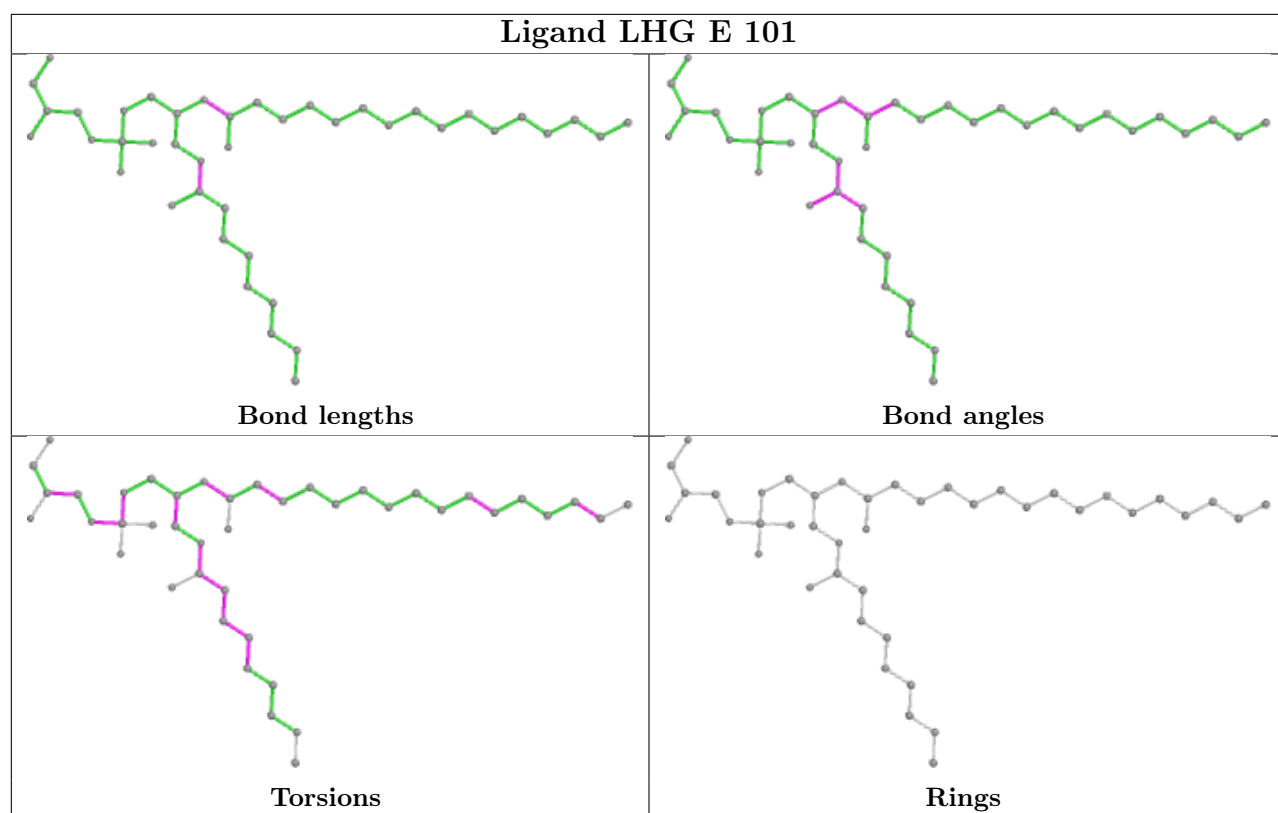


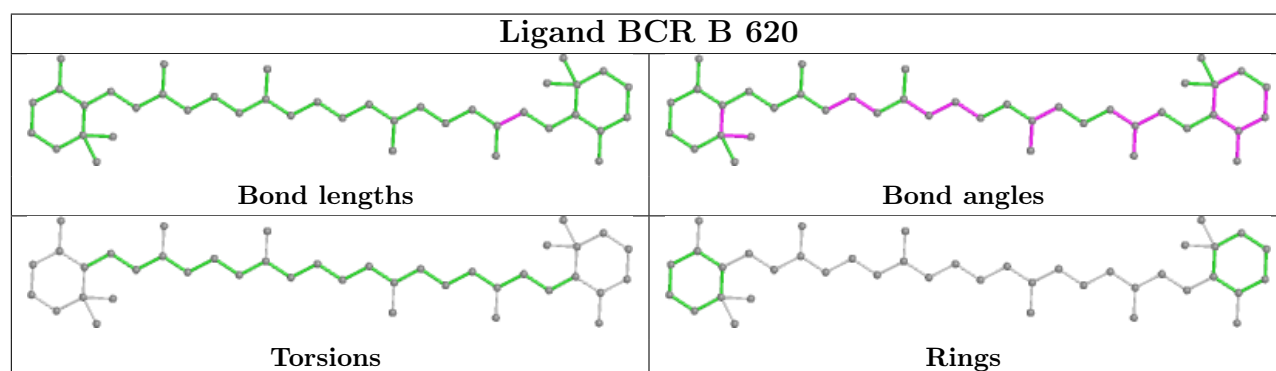
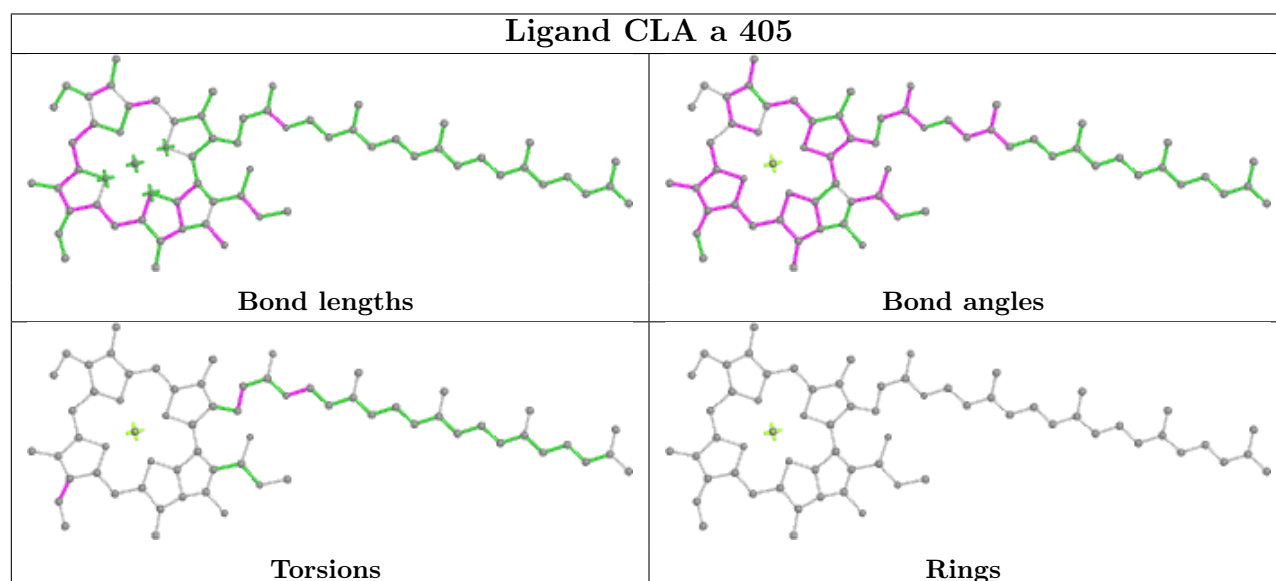
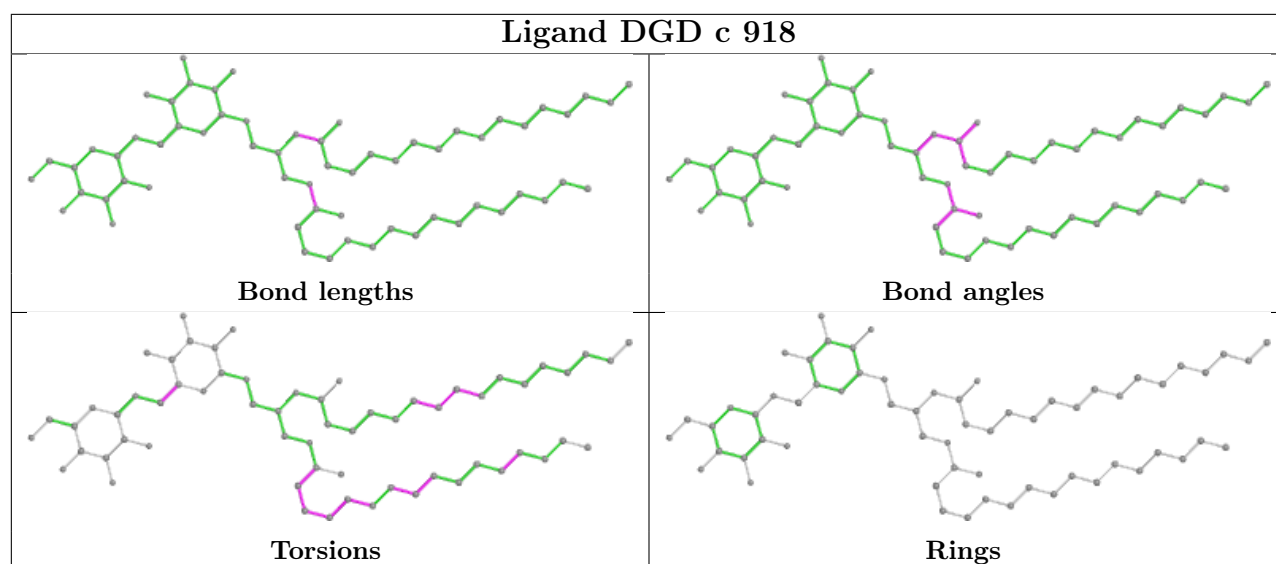


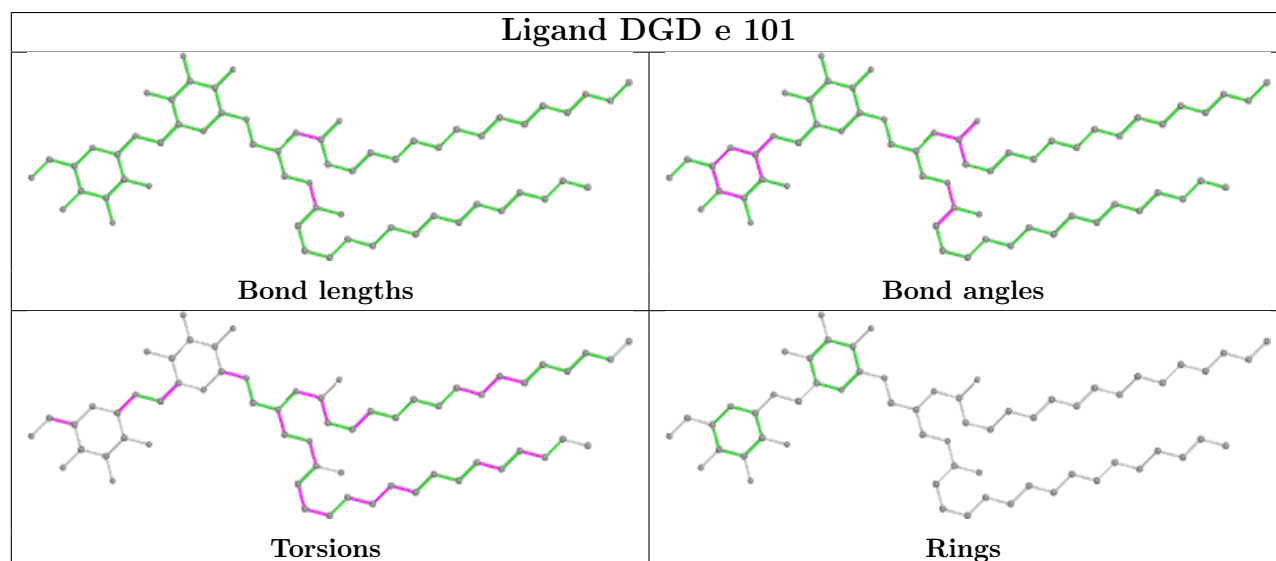
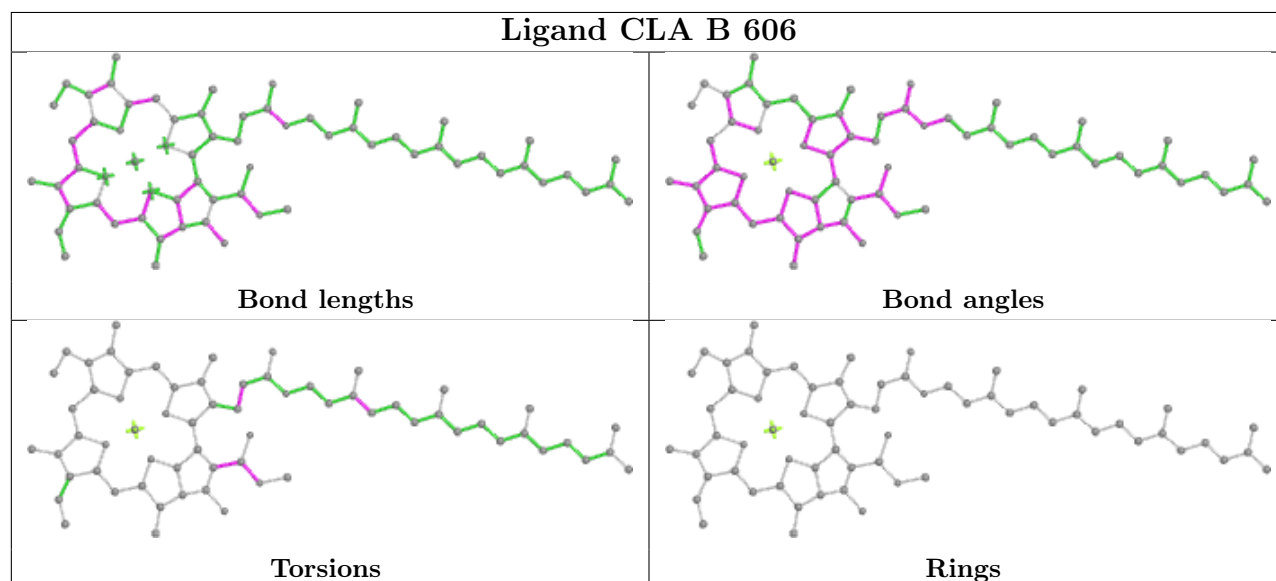
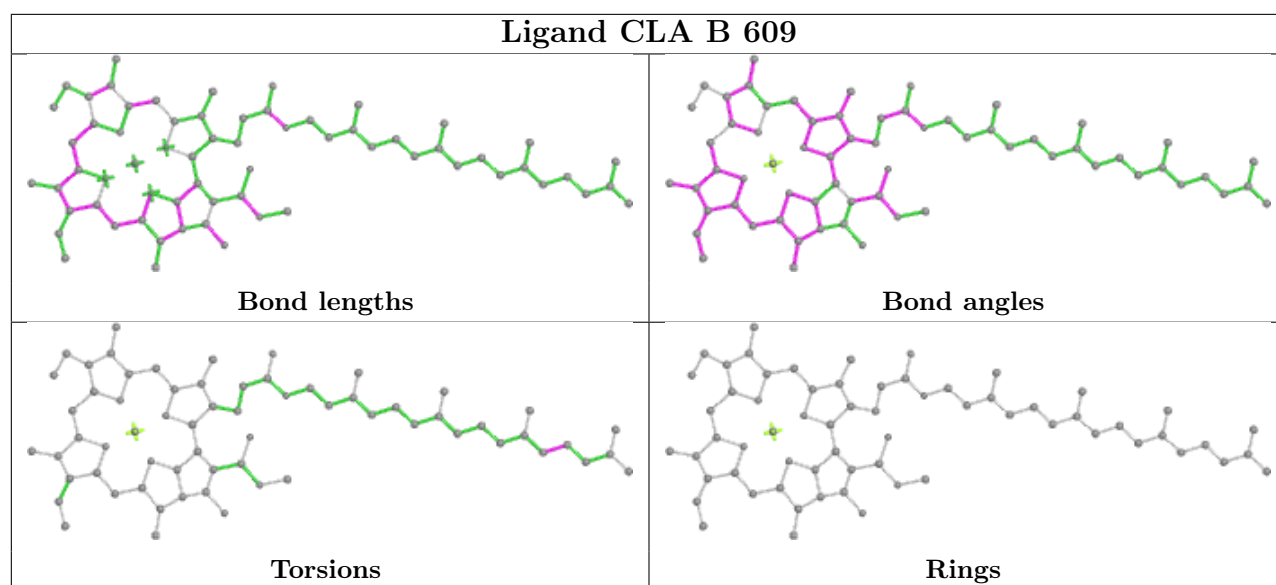


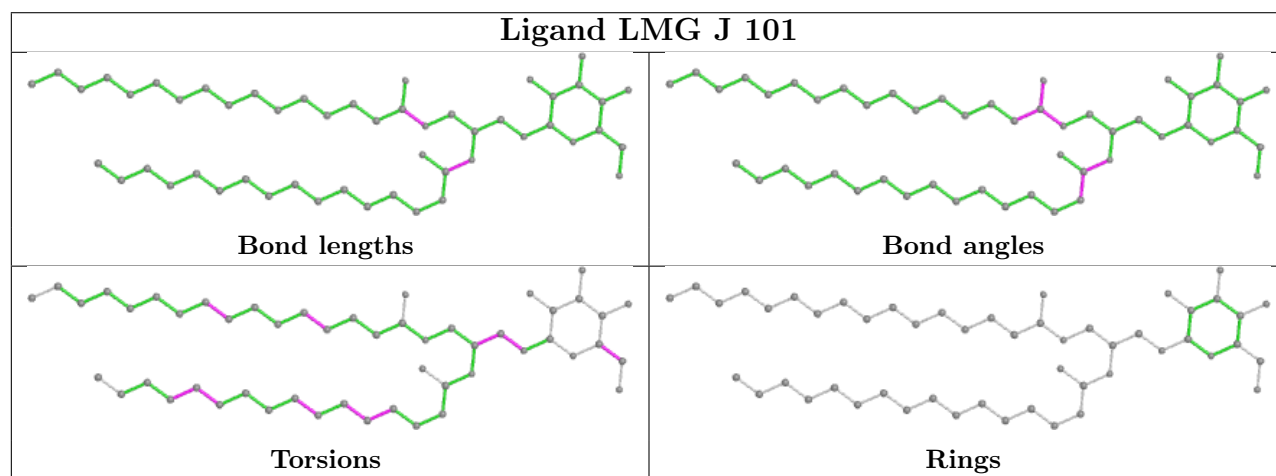
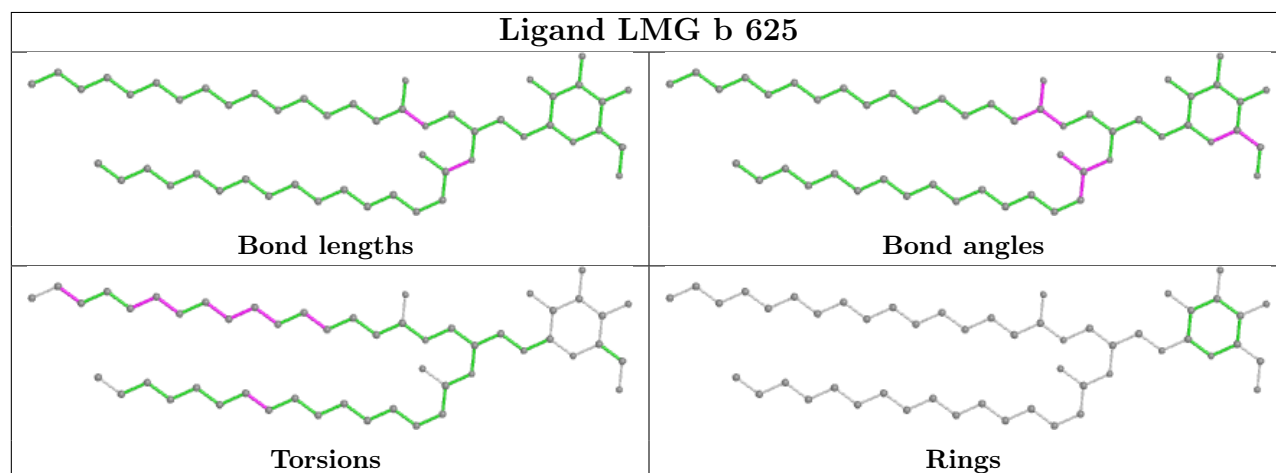
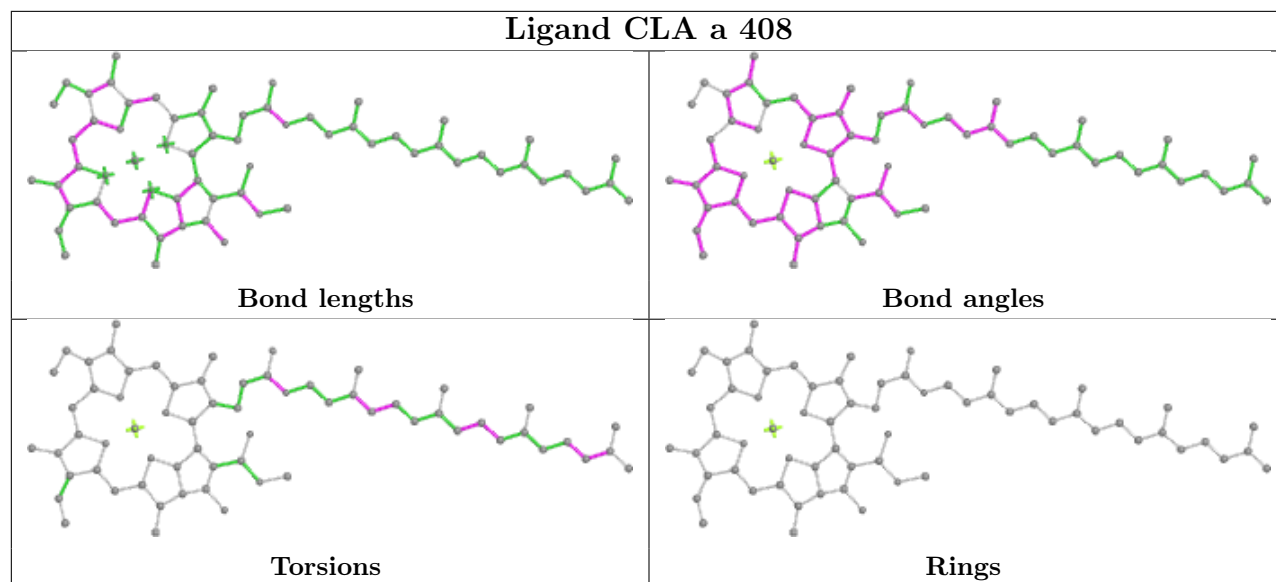


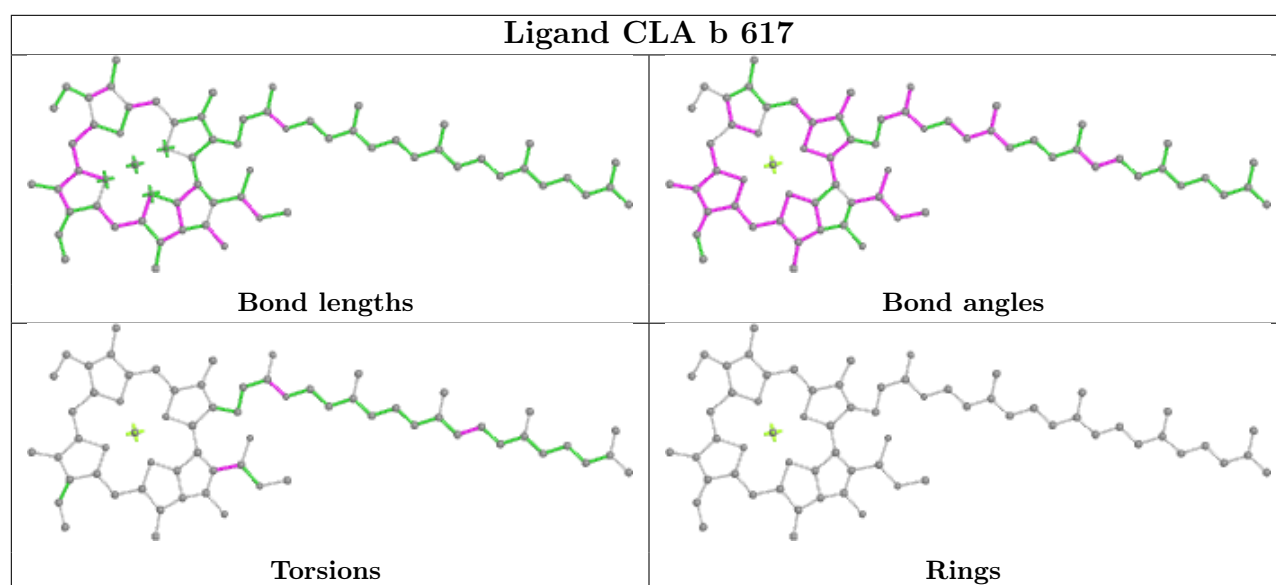
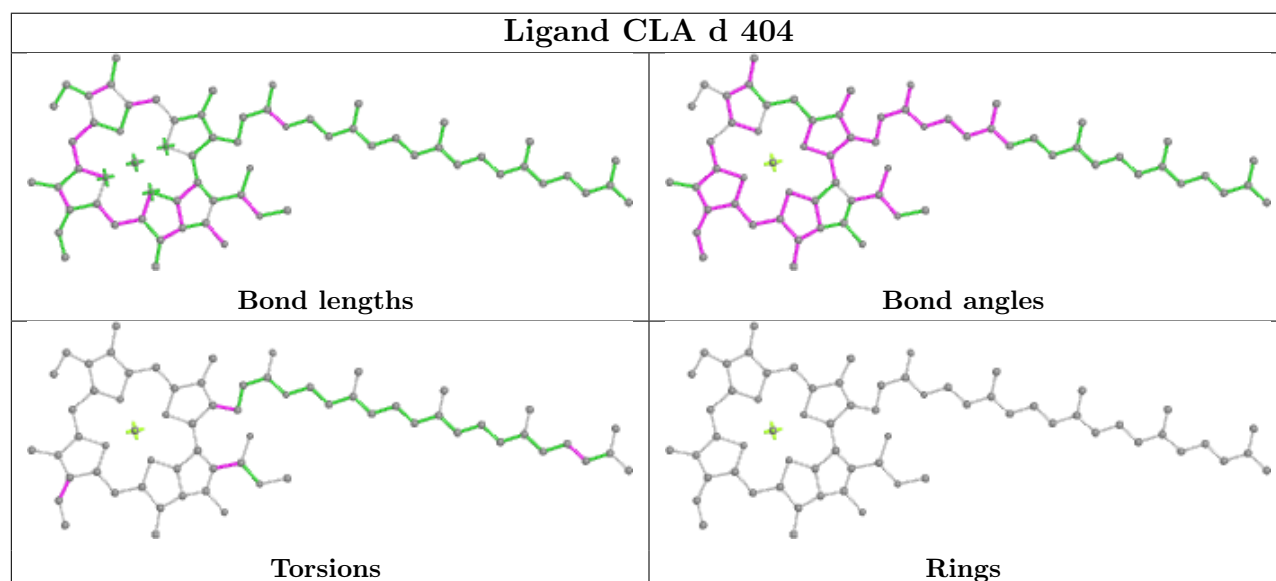
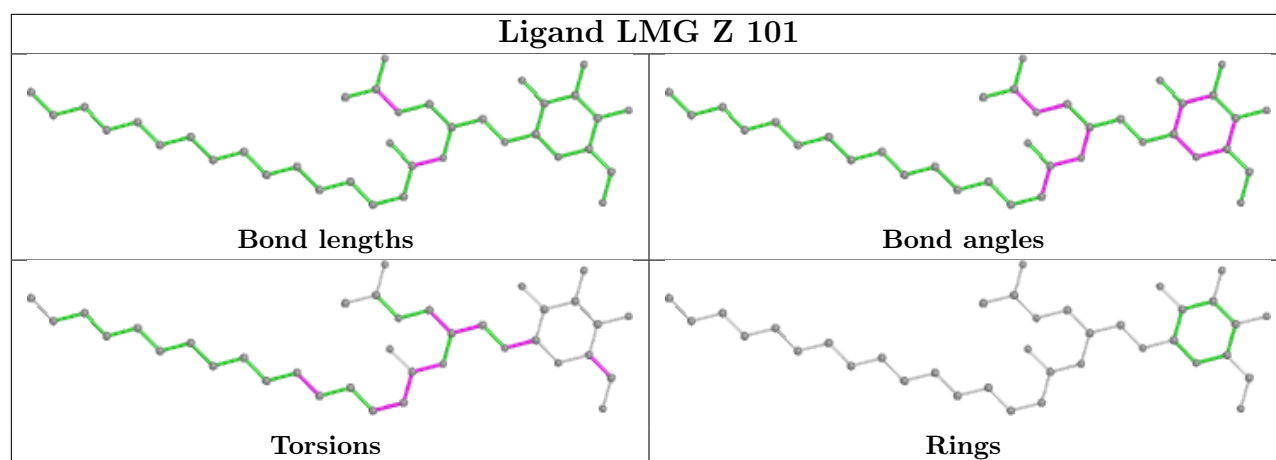


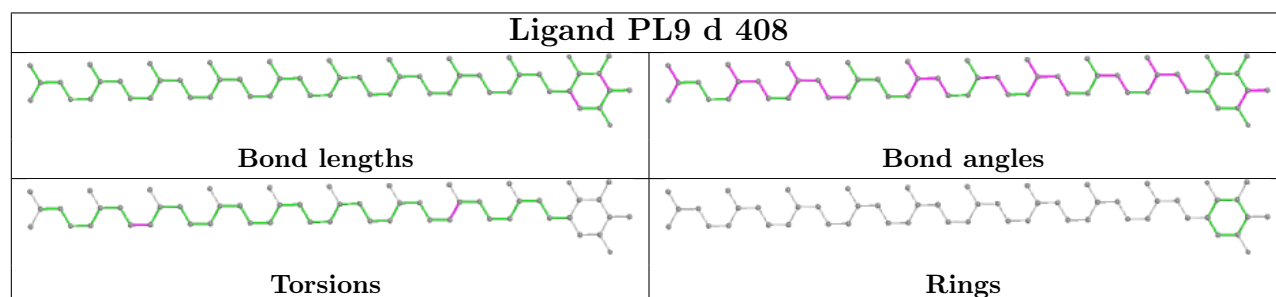
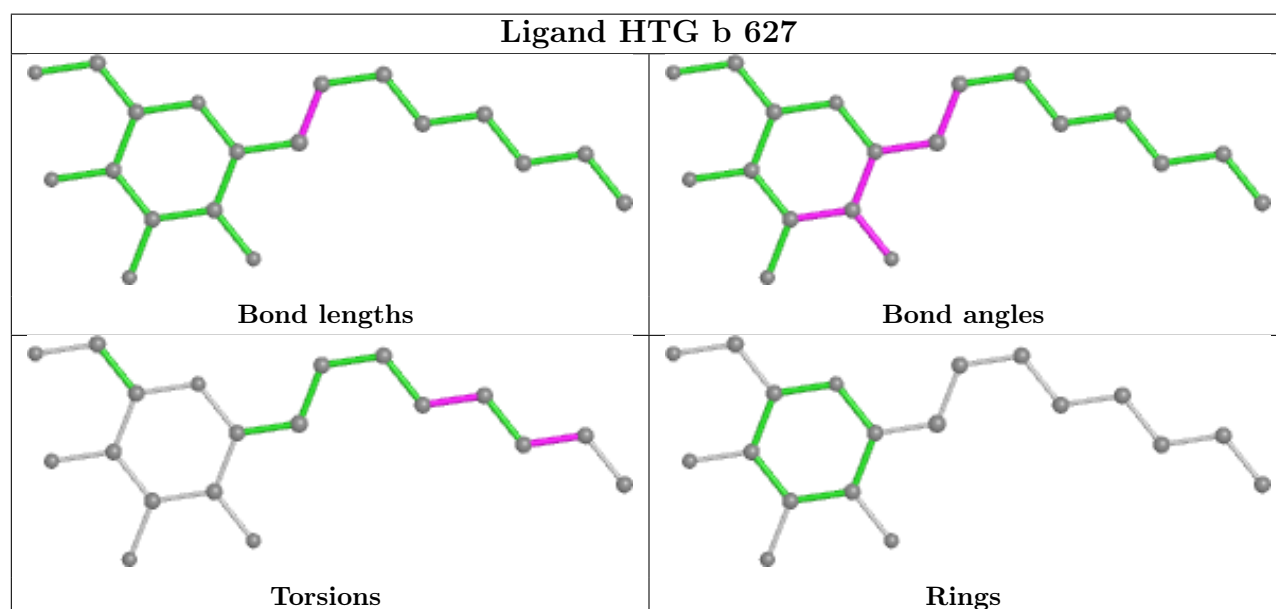
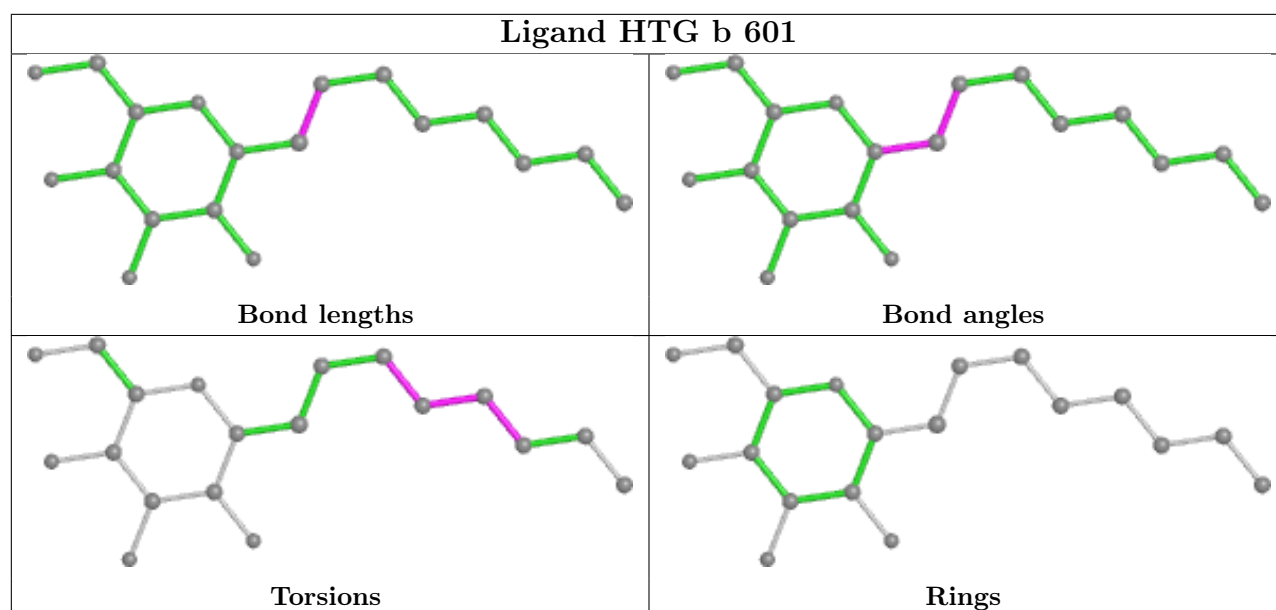


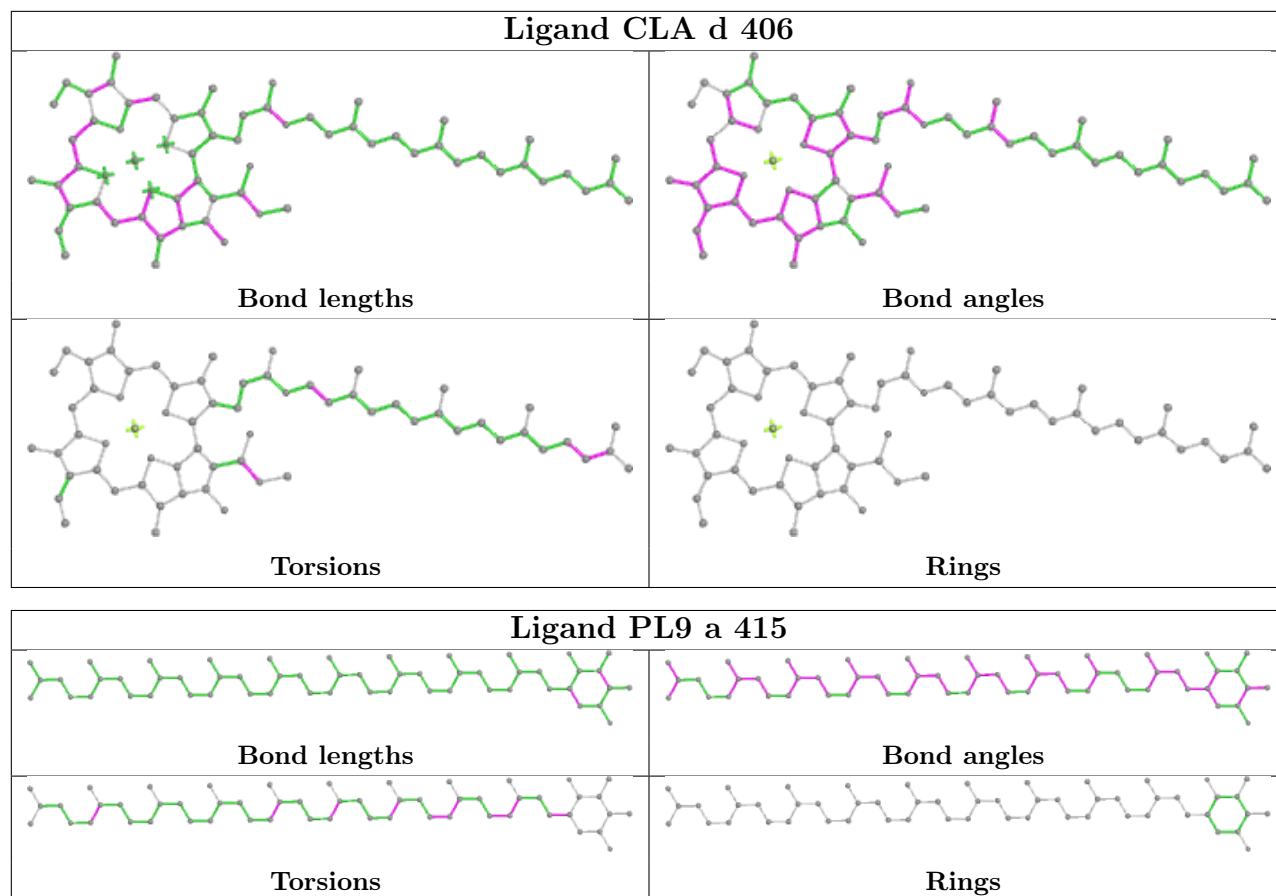


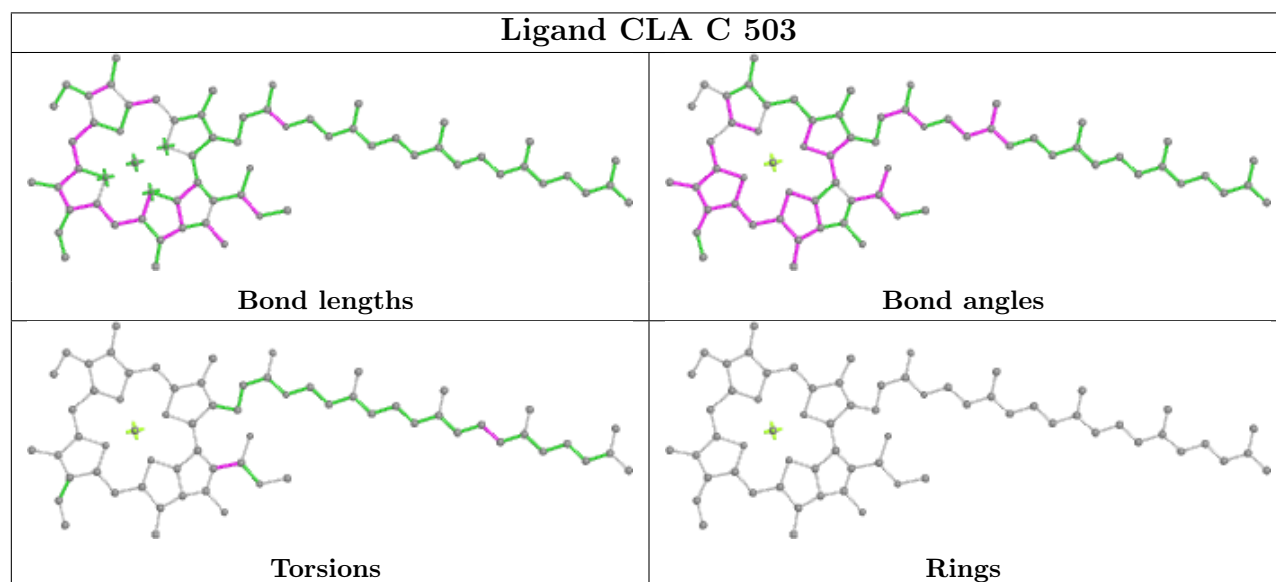
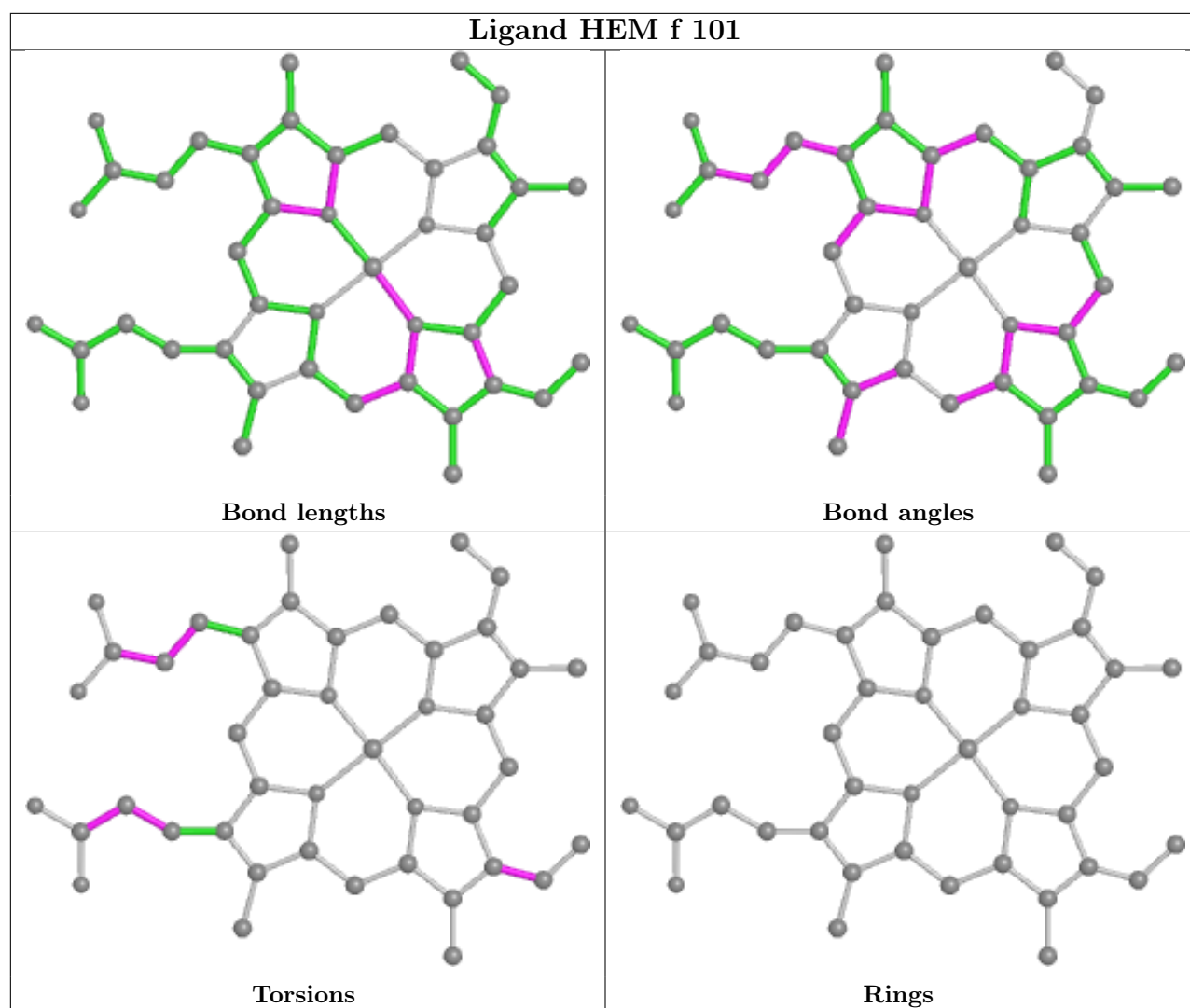


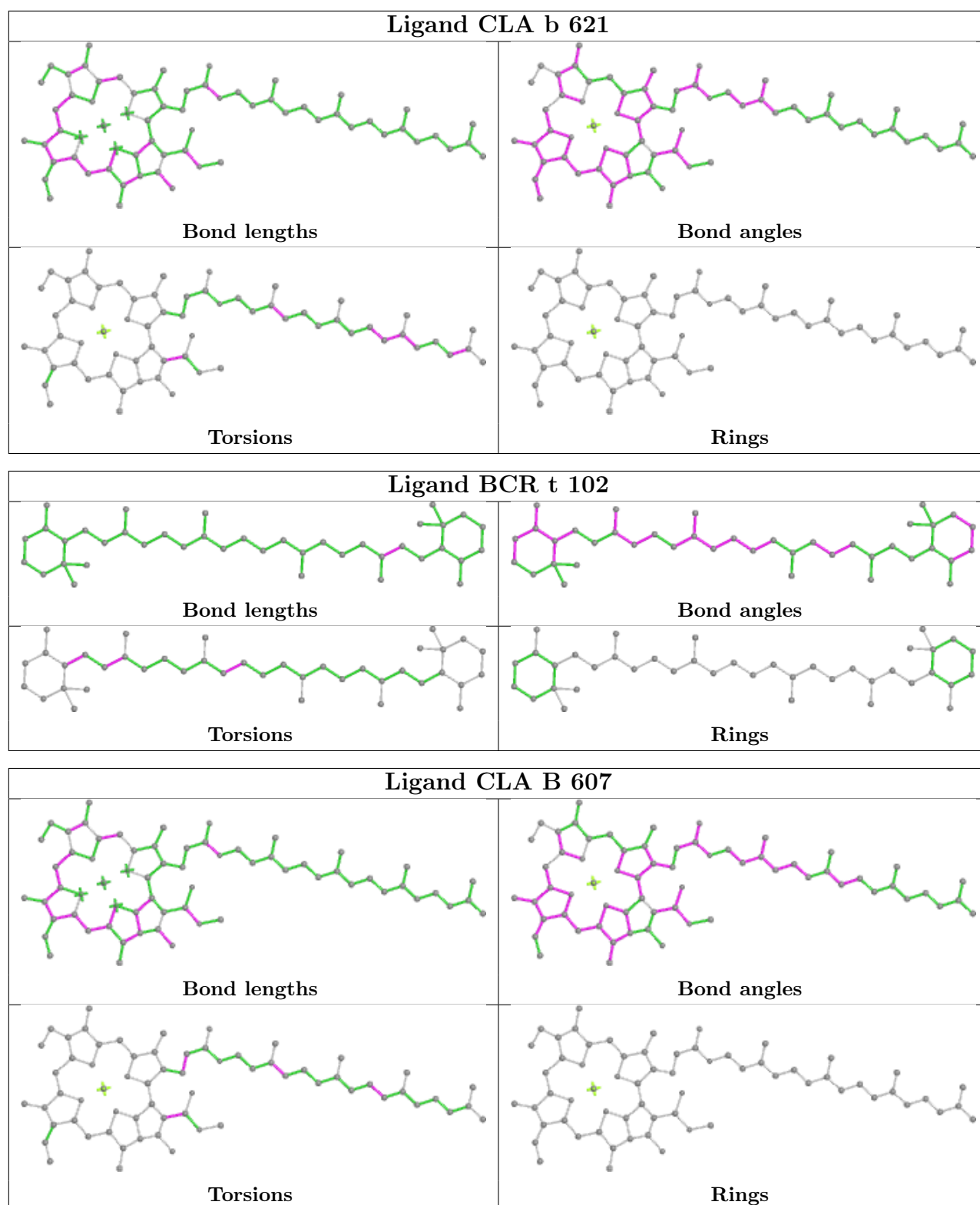


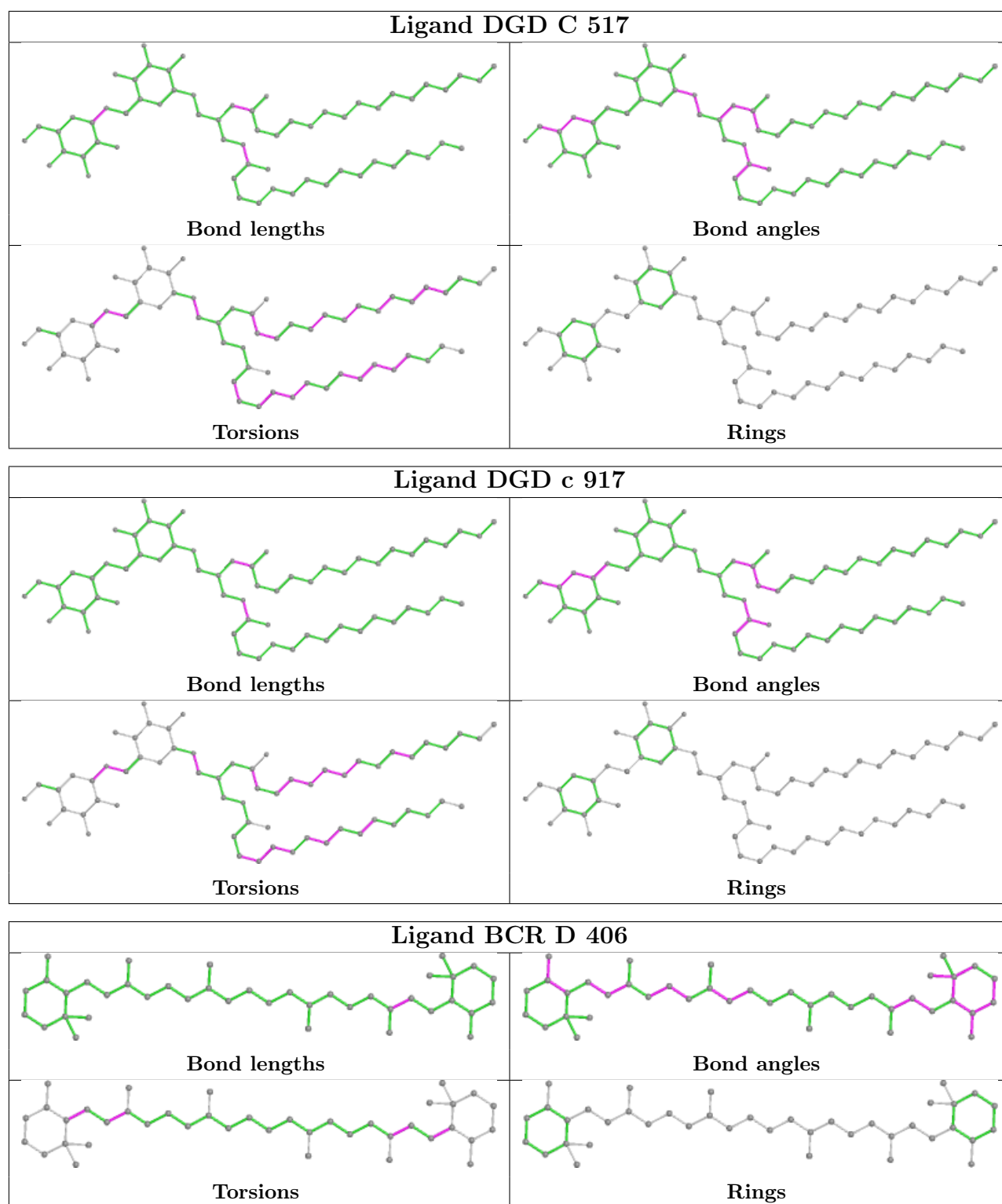


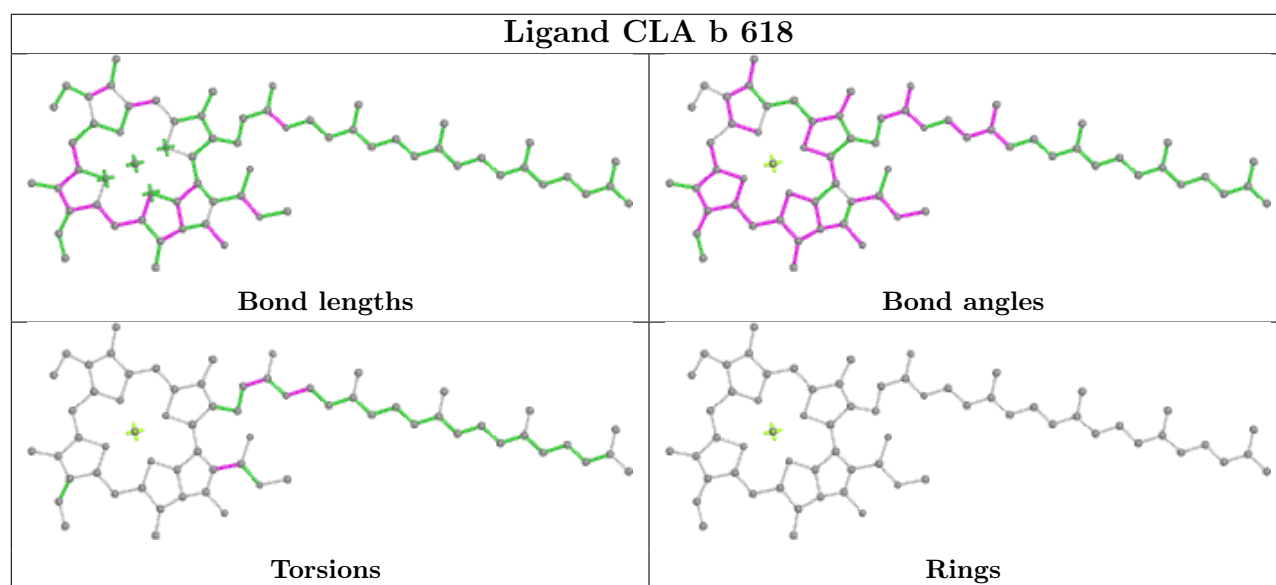
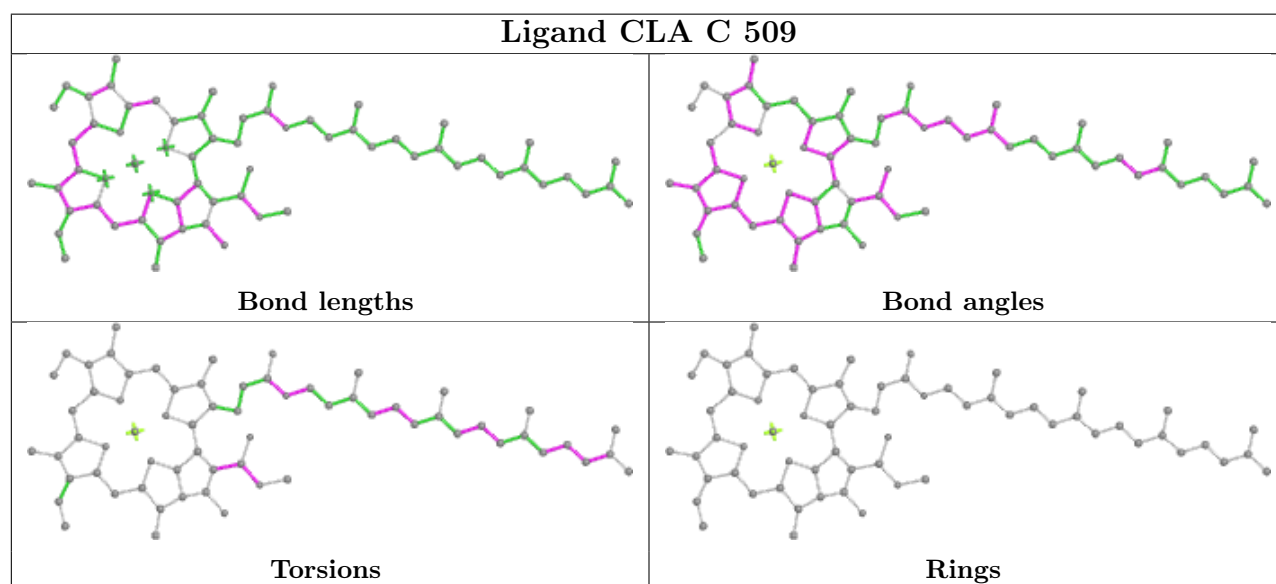
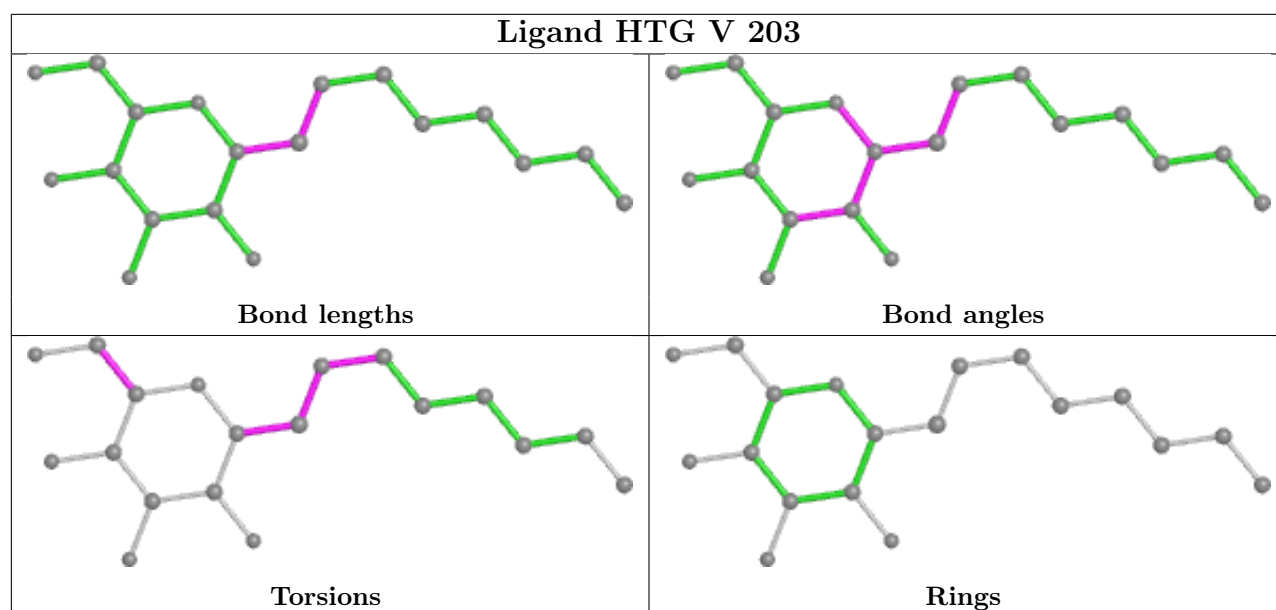


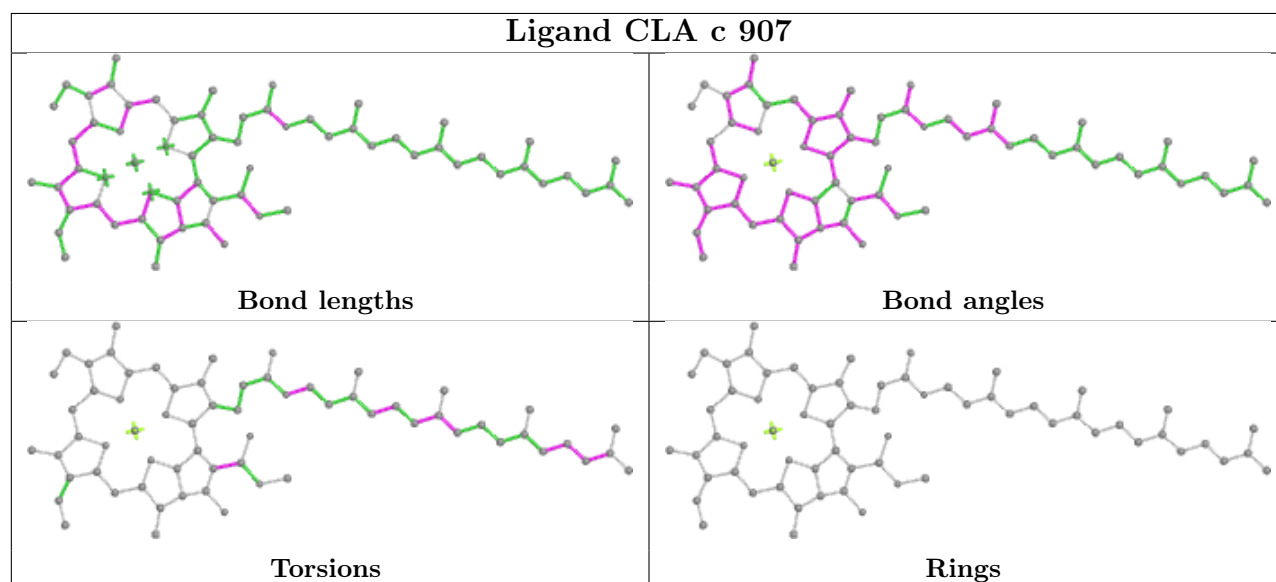
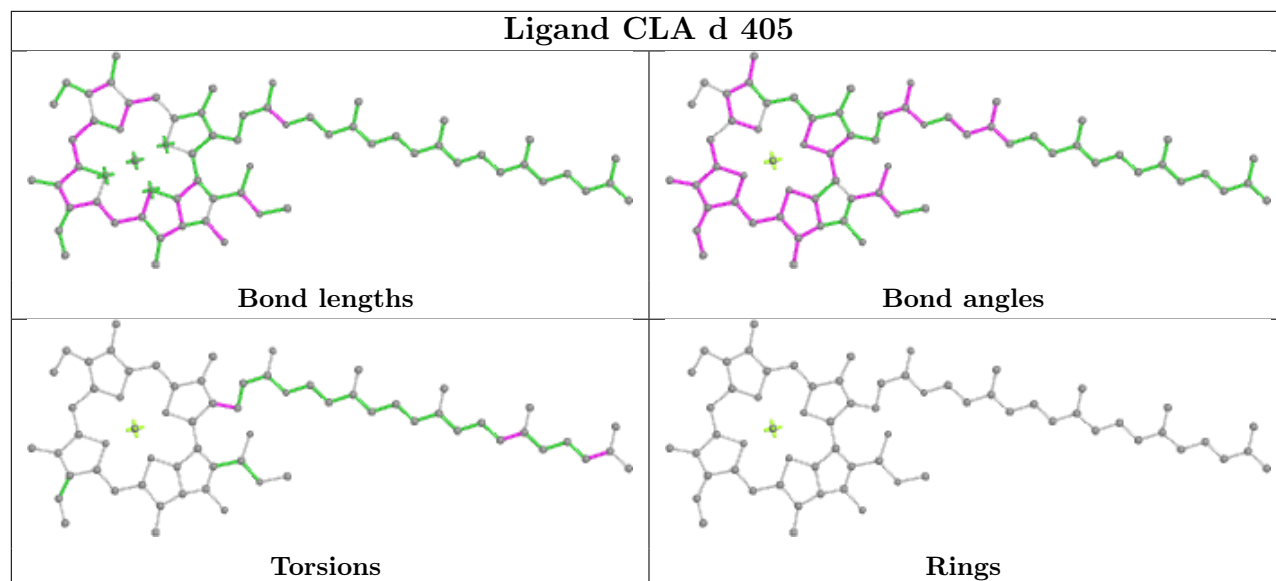
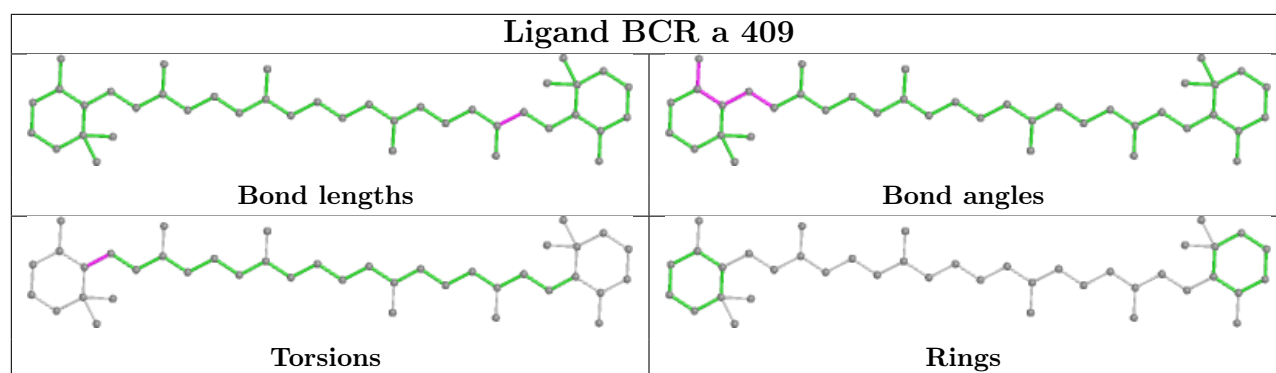


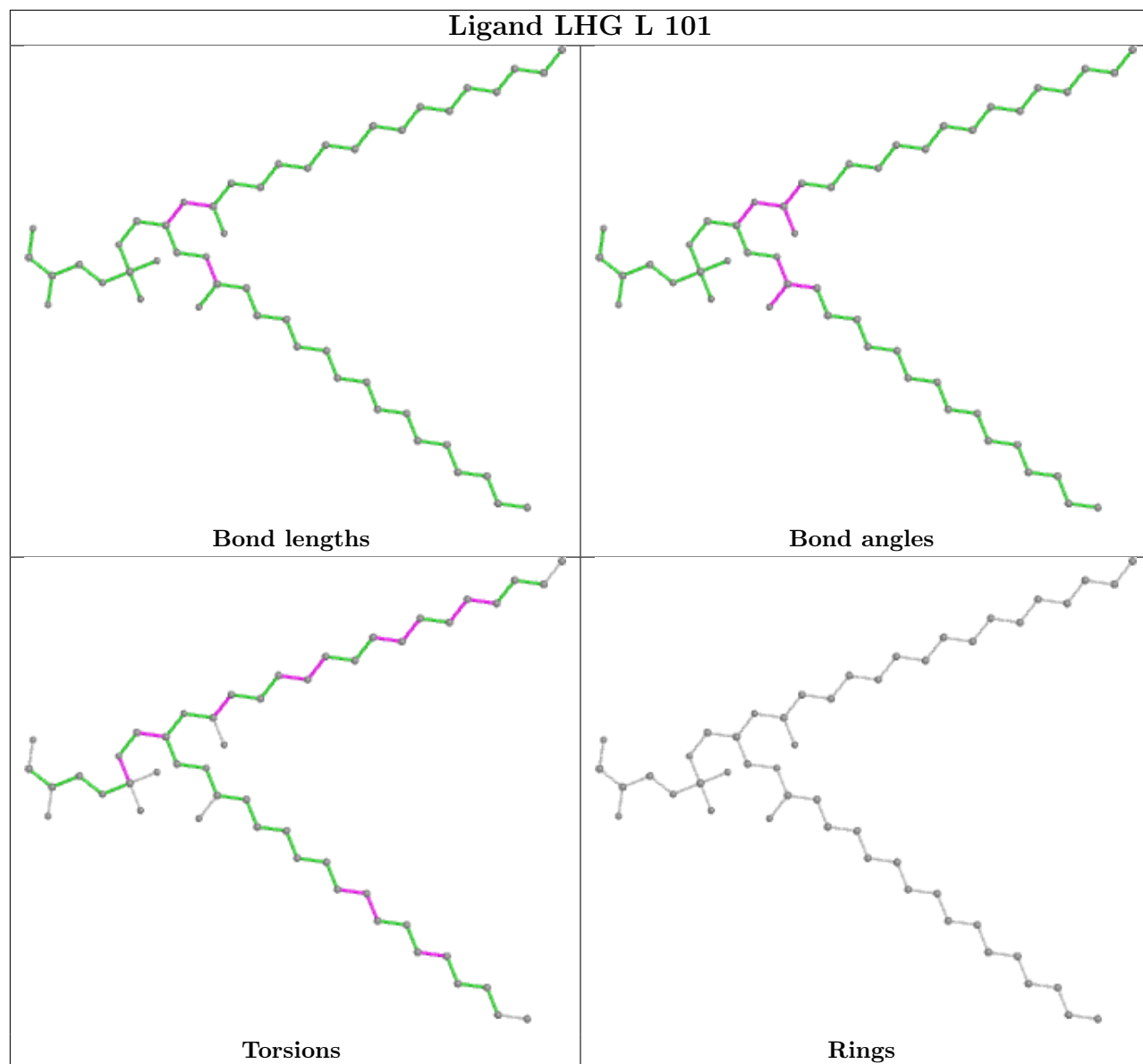


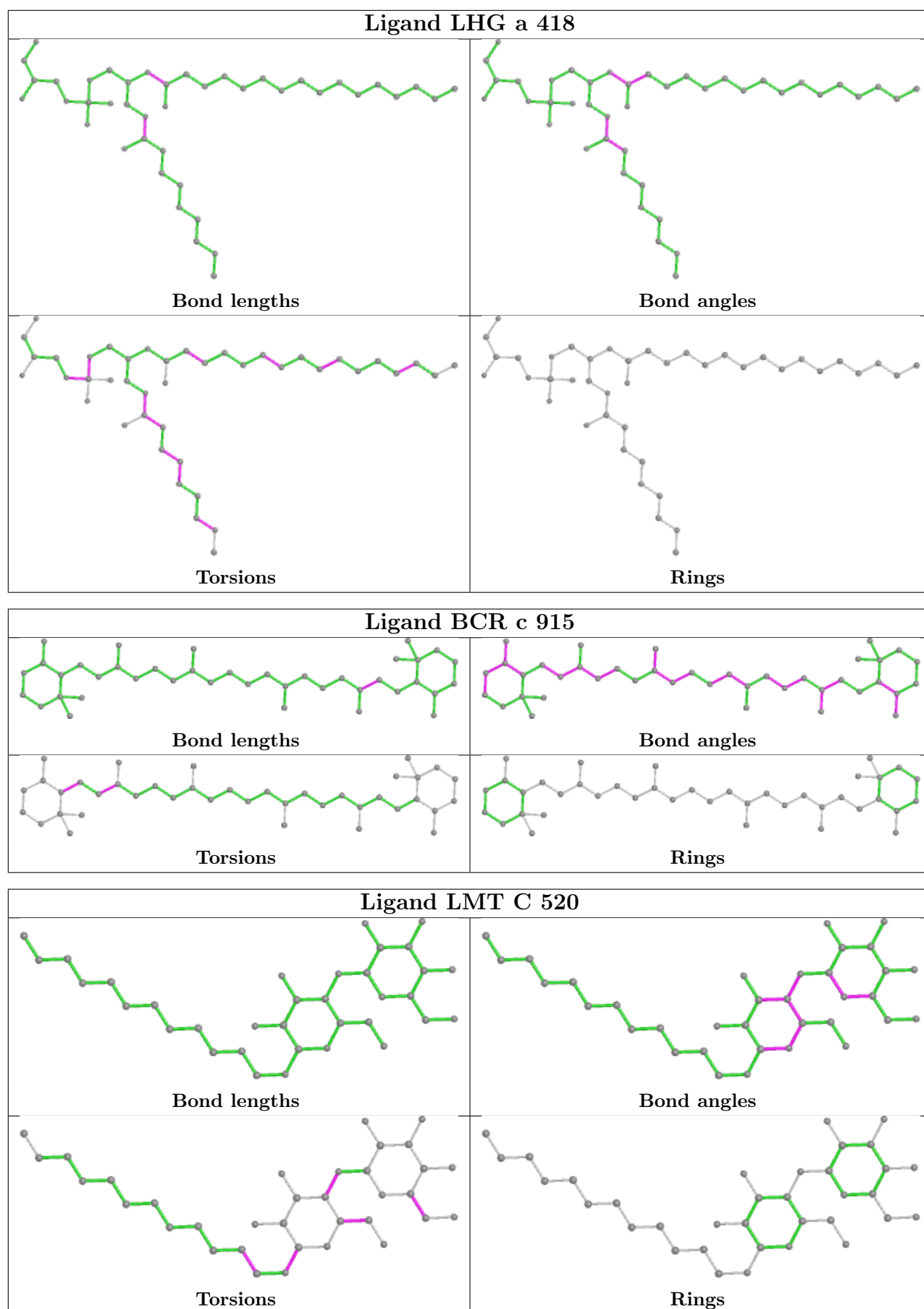


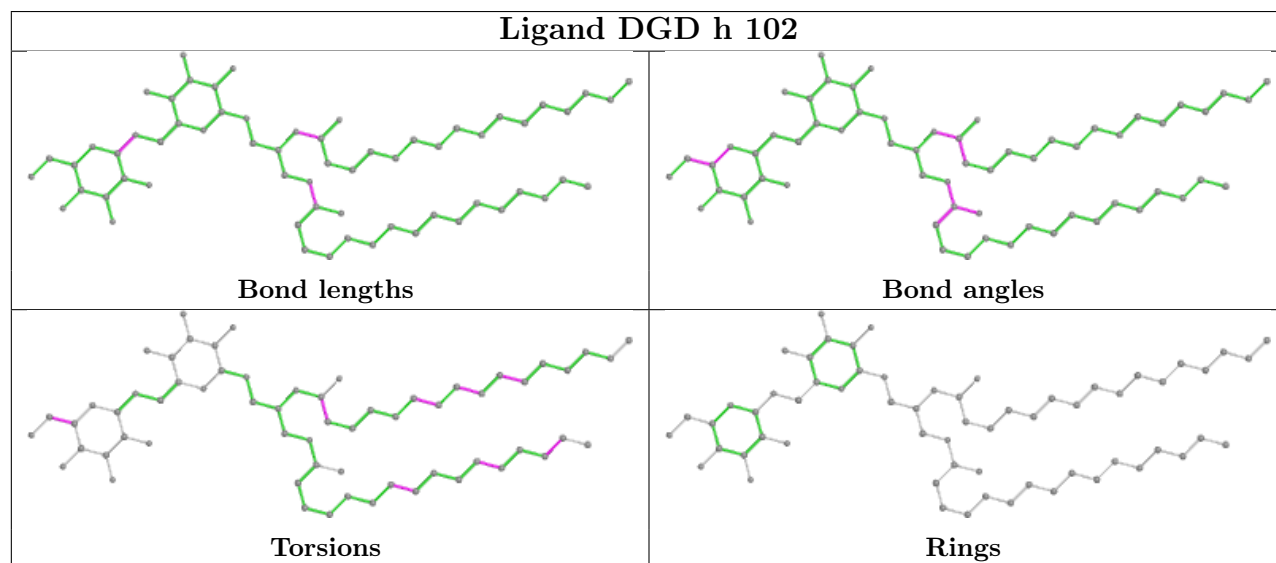
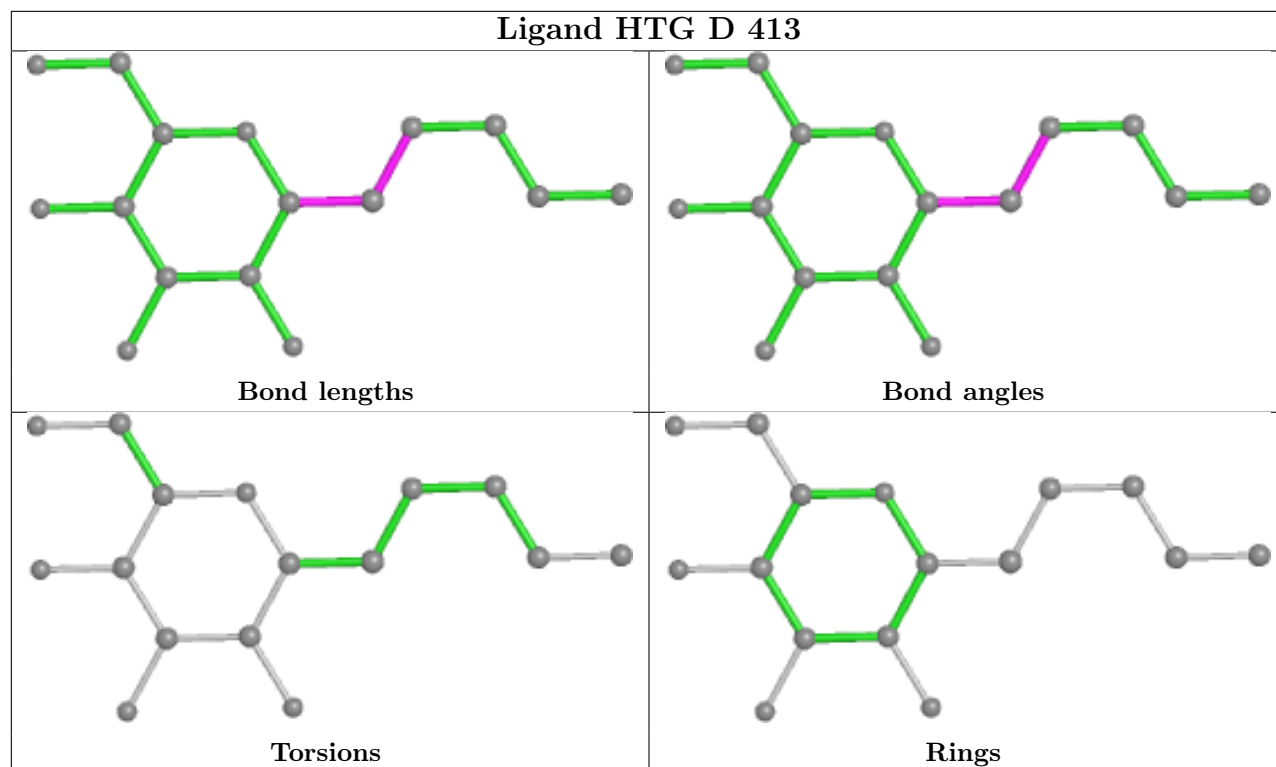
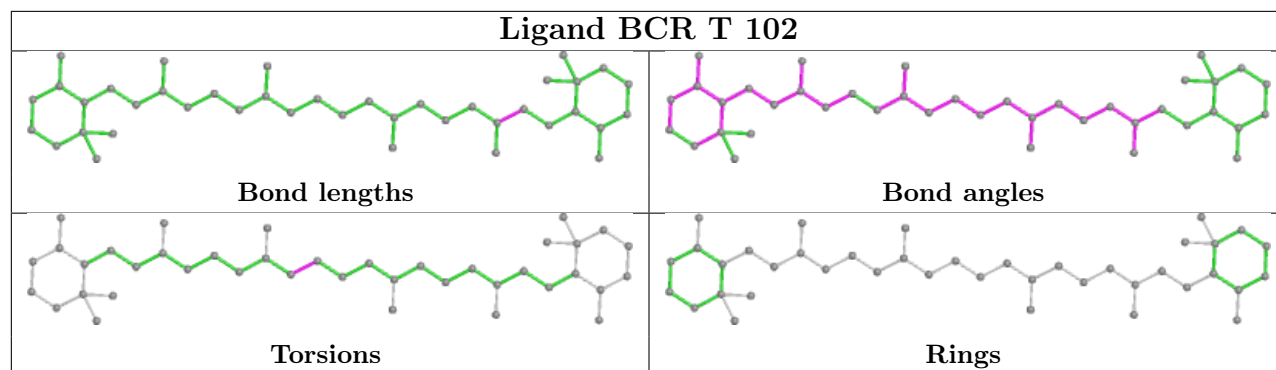


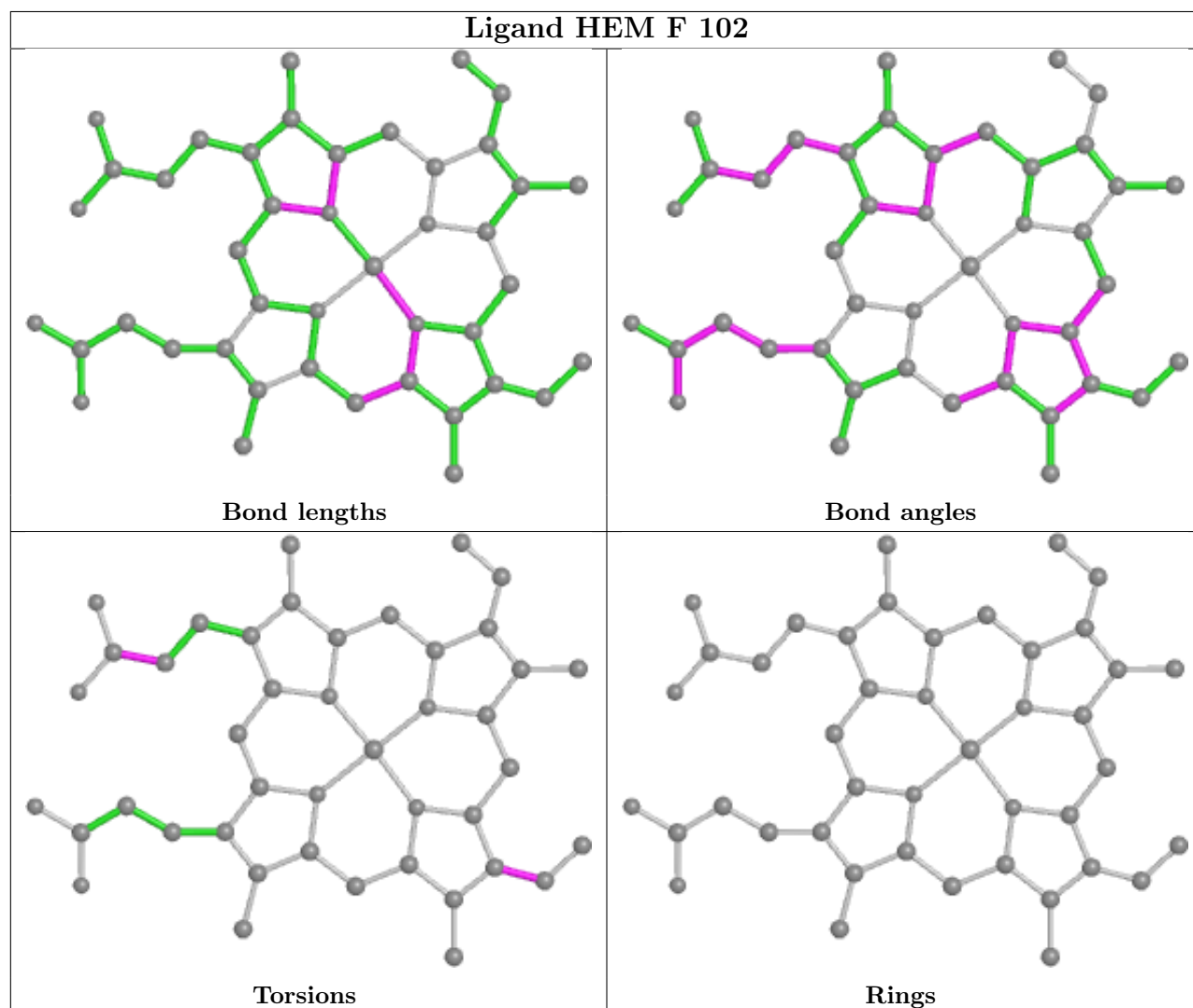
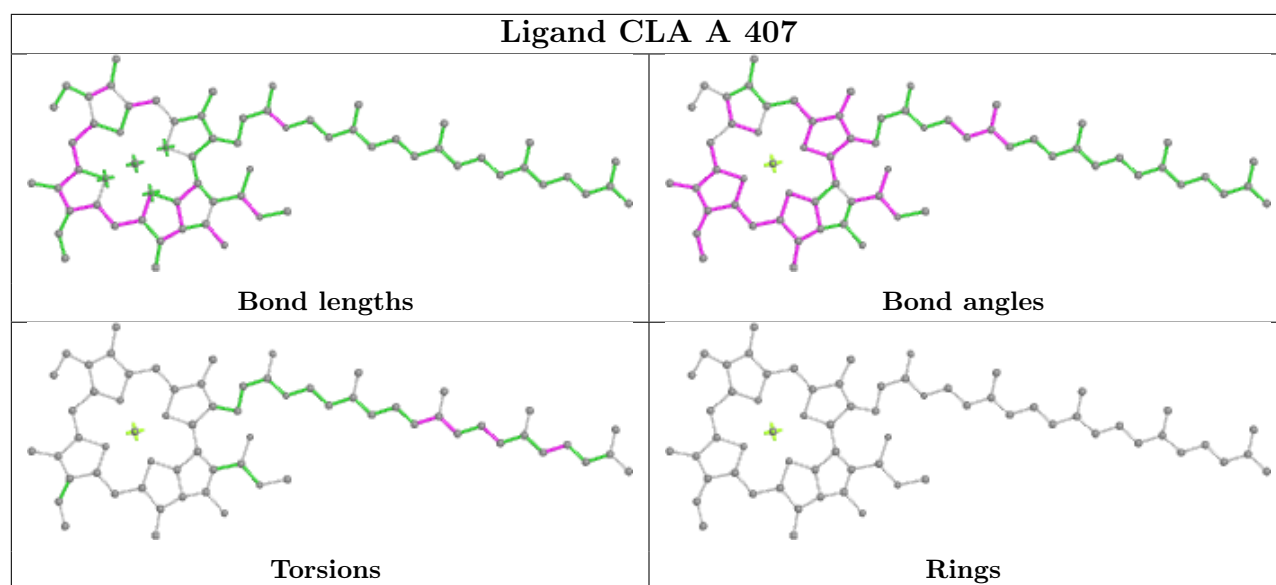


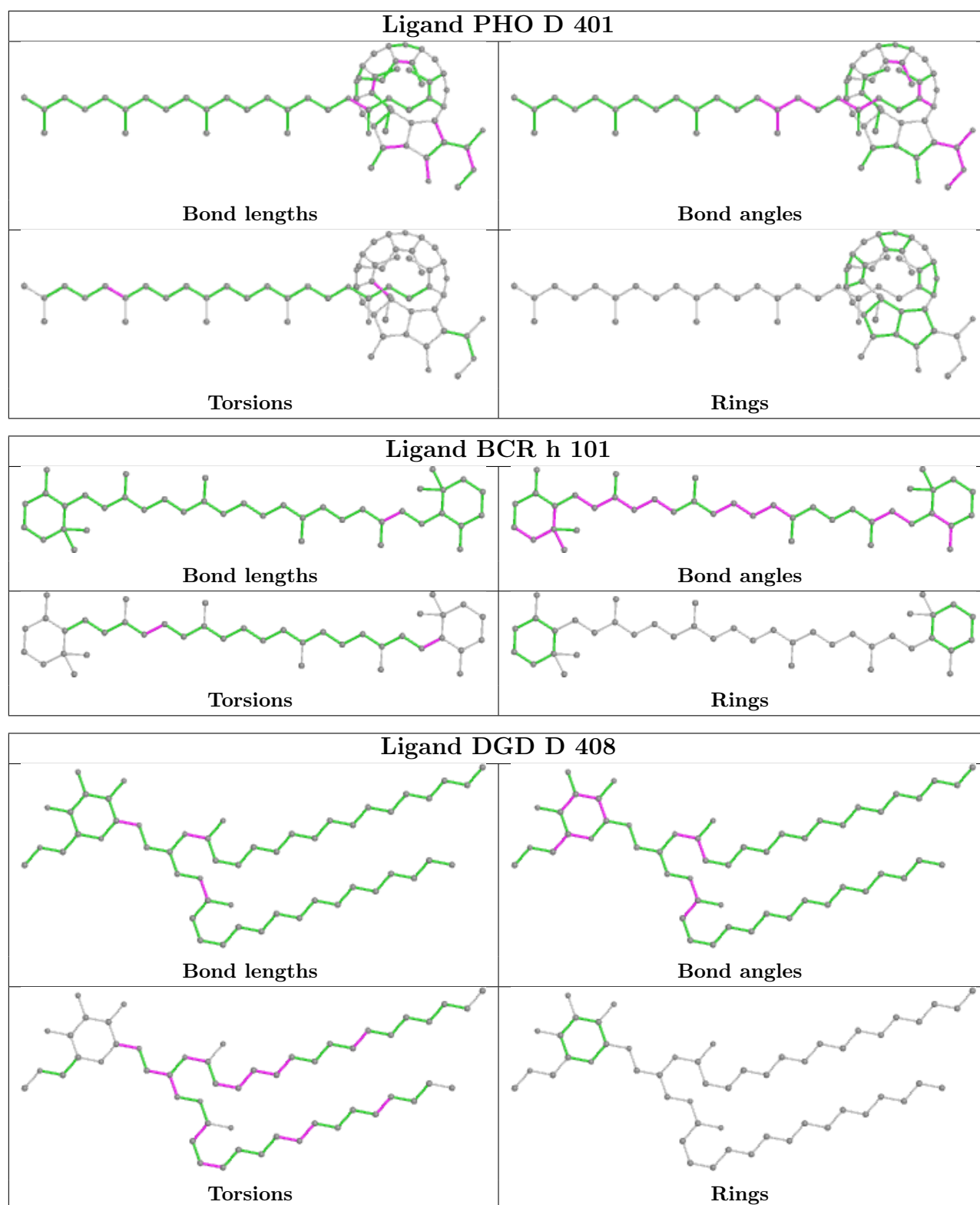


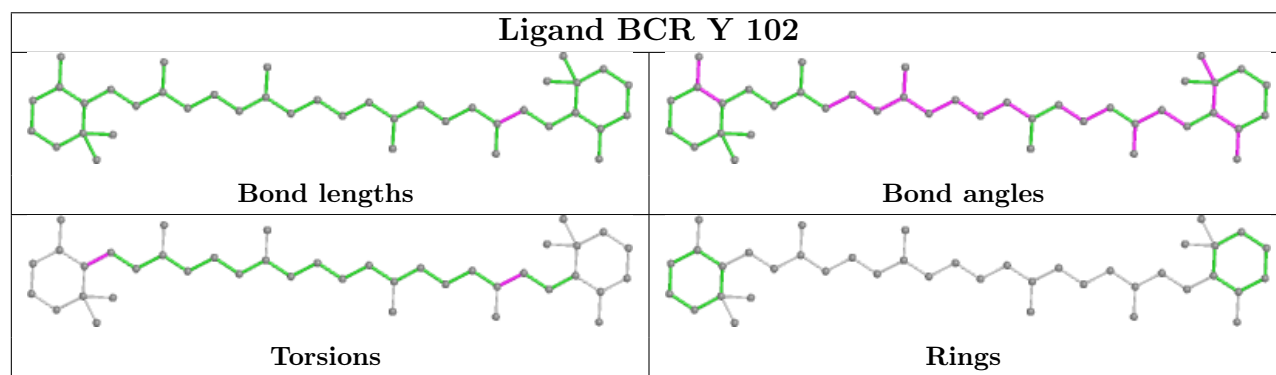
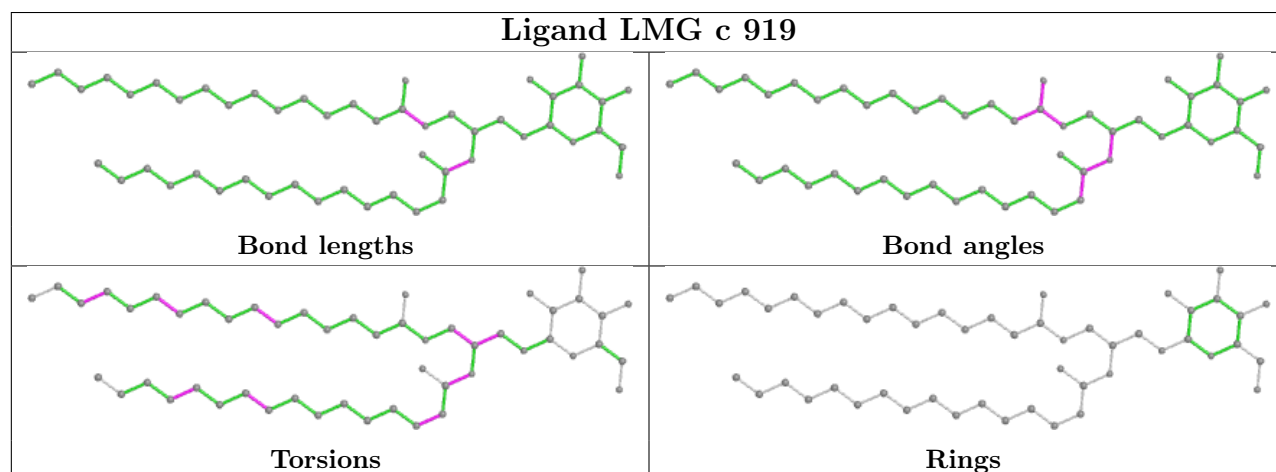
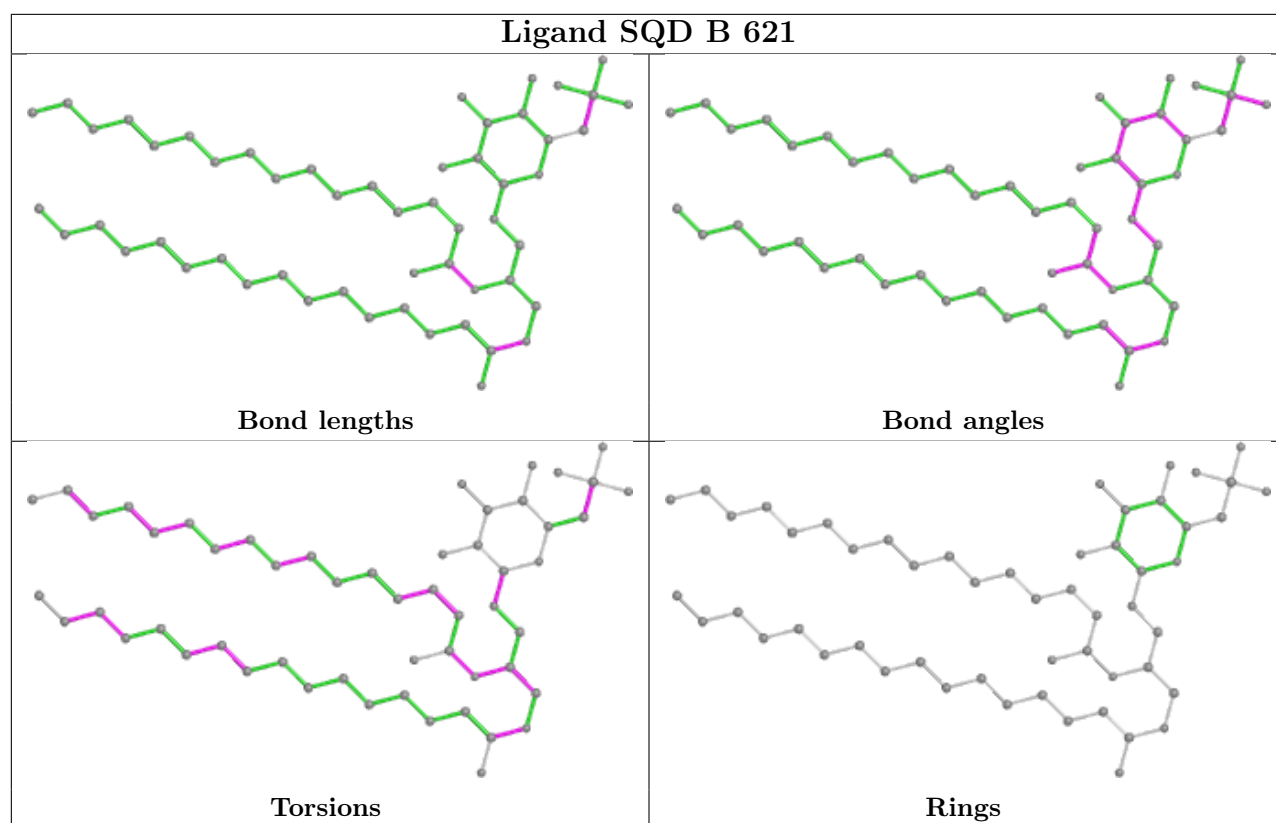












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.28	5 (1%) 73 81	33, 43, 75, 139	0
1	a	334/344 (97%)	0.48	15 (4%) 33 46	31, 44, 84, 146	0
2	B	504/505 (99%)	0.38	14 (2%) 53 64	34, 48, 86, 137	0
2	b	503/505 (99%)	0.50	28 (5%) 24 35	34, 48, 93, 193	0
3	C	451/455 (99%)	0.42	18 (3%) 38 51	37, 56, 82, 134	0
3	c	455/455 (100%)	0.27	8 (1%) 68 77	39, 58, 83, 118	0
4	D	341/342 (99%)	0.29	3 (0%) 84 90	32, 45, 70, 129	0
4	d	341/342 (99%)	0.35	1 (0%) 94 97	34, 45, 69, 115	0
5	E	81/84 (96%)	1.37	25 (30%) 0 0	50, 73, 116, 150	0
5	e	81/84 (96%)	0.84	15 (18%) 1 2	51, 71, 125, 201	0
6	F	34/44 (77%)	0.48	4 (11%) 4 7	51, 62, 103, 104	0
6	f	32/44 (72%)	0.31	2 (6%) 20 29	50, 62, 118, 148	0
7	H	65/65 (100%)	0.30	3 (4%) 32 45	47, 57, 83, 145	0
7	h	65/65 (100%)	0.36	3 (4%) 32 45	47, 60, 83, 167	0
8	I	37/38 (97%)	0.57	4 (10%) 5 9	45, 58, 123, 187	0
8	i	37/38 (97%)	0.64	4 (10%) 5 9	44, 57, 116, 159	0
9	J	38/39 (97%)	0.99	6 (15%) 2 3	52, 68, 151, 185	0
9	j	39/39 (100%)	0.75	7 (17%) 1 2	52, 68, 140, 190	0
10	K	37/37 (100%)	0.71	4 (10%) 5 9	60, 68, 88, 112	0
10	k	37/37 (100%)	0.42	0 100 100	59, 67, 88, 112	0
11	L	37/37 (100%)	0.40	0 100 100	34, 39, 101, 132	0
11	l	37/37 (100%)	0.51	1 (2%) 54 64	34, 40, 105, 130	0
12	M	33/36 (91%)	0.64	0 100 100	29, 41, 75, 126	0
12	m	33/36 (91%)	0.55	0 100 100	35, 42, 78, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.42	12 (4%) 29 42	36, 54, 102, 146	0
13	o	243/244 (99%)	0.31	6 (2%) 57 67	36, 56, 112, 179	0
14	T	29/32 (90%)	0.57	1 (3%) 45 57	35, 40, 70, 142	0
14	t	29/32 (90%)	0.45	0 100 100	35, 39, 68, 141	0
15	U	97/104 (93%)	0.20	1 (1%) 82 88	39, 51, 82, 128	0
15	u	97/104 (93%)	0.17	0 100 100	42, 52, 76, 126	0
16	V	137/137 (100%)	0.36	1 (0%) 87 92	41, 54, 88, 123	0
16	v	137/137 (100%)	0.21	1 (0%) 87 92	43, 58, 89, 121	0
17	Y	29/30 (96%)	3.31	12 (41%) 0 0	73, 85, 162, 203	0
17	y	29/30 (96%)	1.50	9 (31%) 0 0	75, 85, 164, 202	0
18	X	39/40 (97%)	0.57	3 (7%) 13 20	52, 67, 135, 143	0
18	x	38/40 (95%)	0.94	6 (15%) 2 3	55, 67, 130, 140	0
19	Z	62/62 (100%)	1.44	18 (29%) 0 0	75, 89, 144, 191	0
19	z	62/62 (100%)	1.64	19 (30%) 0 0	75, 90, 144, 188	0
20	R	18/34 (52%)	5.55	18 (100%) 0 0	102, 135, 170, 172	0
All	All	5275/5384 (97%)	0.48	277 (5%) 26 38	29, 52, 103, 203	0

The worst 5 of 277 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	14.8
17	Y	20	ALA	13.7
2	b	494	GLY	12.3
17	Y	19	ILE	11.9
20	R	6	LEU	10.3

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.14	30,49,67,82	0
14	FME	t	1	10/11	0.94	0.14	26,36,47,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.95	0.15	43,60,73,75	0
12	FME	m	1	10/11	0.95	0.16	31,50,100,103	0
12	FME	M	1	10/11	0.95	0.18	30,50,87,93	0
8	FME	I	1	10/11	0.96	0.12	28,49,62,64	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(Å ²)	Q<0.9
29	LMT	F	101	35/35	0.33	0.53	102,149,179,184	0
37	DGD	e	101	62/66	0.41	0.43	72,118,208,212	0
35	HTG	d	414	16/19	0.47	0.25	68,115,134,134	0
32	UNL	j	101	10/-	0.50	0.28	56,83,95,98	0
29	LMT	a	417	35/35	0.53	0.38	95,123,147,148	0
37	DGD	D	408	52/66	0.54	0.36	58,108,151,171	0
28	GOL	V	204	6/6	0.55	0.60	75,90,97,100	0
36	LHG	a	418	42/49	0.55	0.32	69,131,187,193	0
32	UNL	C	526	34/-	0.58	0.24	76,120,132,136	0
22	CL	v	201	1/1	0.58	0.10	124,124,124,124	0
29	LMT	a	401	35/35	0.59	0.32	52,87,118,142	0
29	LMT	b	626	25/35	0.59	0.39	71,102,168,175	0
32	UNL	J	102	10/-	0.60	0.24	50,85,104,107	0
29	LMT	m	103	35/35	0.60	0.31	42,109,140,144	0
29	LMT	e	102	35/35	0.60	0.31	83,129,164,170	0
29	LMT	C	520	35/35	0.62	0.36	88,135,162,175	0
33	LMG	Z	101	37/55	0.62	0.31	55,121,146,154	0
29	LMT	A	415	35/35	0.65	0.25	41,84,115,119	0
33	LMG	Y	101	51/55	0.67	0.25	60,93,118,127	0
27	SQD	f	102	43/54	0.67	0.29	97,116,175,182	0
29	LMT	M	103	35/35	0.68	0.28	47,99,150,158	0
35	HTG	B	633	19/19	0.68	0.24	53,103,141,160	0
32	UNL	a	414	30/-	0.68	0.26	64,85,117,134	0
32	UNL	c	925	32/-	0.69	0.25	66,101,138,147	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	0.69	0.29	73,114,134,192	0
36	LHG	E	101	42/49	0.70	0.26	59,115,138,140	0
32	UNL	A	418	28/-	0.70	0.26	59,88,108,111	0
29	LMT	b	602	25/35	0.71	0.28	41,91,134,149	0
35	HTG	b	604	19/19	0.71	0.19	51,112,150,150	0
29	LMT	D	403	35/35	0.72	0.27	58,132,172,179	0
35	HTG	D	413	16/19	0.72	0.27	76,142,160,166	0
32	UNL	b	634	33/-	0.72	0.26	47,86,155,158	0
28	GOL	O	302	6/6	0.73	0.17	68,79,84,89	0
33	LMG	z	101	39/55	0.73	0.28	65,124,153,161	0
35	HTG	B	625	19/19	0.73	0.23	75,132,140,190	0
29	LMT	M	101	35/35	0.74	0.23	45,93,118,133	0
37	DGD	C	517	62/66	0.74	0.23	48,65,94,116	0
35	HTG	C	522	19/19	0.75	0.31	81,112,138,140	0
32	UNL	B	634	33/-	0.75	0.29	54,73,126,134	0
29	LMT	t	101	25/35	0.76	0.31	43,92,140,150	0
29	LMT	m	102	35/35	0.76	0.26	42,90,122,128	0
27	SQD	L	102	54/54	0.76	0.23	48,79,126,149	0
33	LMG	C	519	51/55	0.77	0.25	53,121,145,151	0
35	HTG	b	628	19/19	0.77	0.22	72,130,158,159	0
31	PL9	A	417	55/55	0.77	0.25	61,98,125,131	0
33	LMG	c	920	51/55	0.78	0.24	50,111,142,145	0
32	UNL	M	102	10/-	0.78	0.31	50,55,74,86	0
33	LMG	b	625	51/55	0.78	0.23	40,54,73,98	0
35	HTG	c	921	19/19	0.79	0.18	93,101,107,111	0
27	SQD	a	402	54/54	0.79	0.22	45,75,125,133	0
28	GOL	l	101	6/6	0.79	0.39	48,92,98,103	0
34	CA	f	103	1/1	0.79	0.09	126,126,126,126	0
27	SQD	F	103	43/54	0.80	0.25	77,120,145,149	0
22	CL	U	201	1/1	0.80	0.08	117,117,117,117	0
24	CLA	C	513	65/65	0.80	0.28	53,84,113,119	0
33	LMG	B	622	51/55	0.80	0.22	38,53,78,91	0
27	SQD	B	621	54/54	0.80	0.25	53,88,137,156	0
32	UNL	d	413	36/-	0.81	0.25	60,85,140,142	0
34	CA	B	601	1/1	0.81	0.06	138,138,138,138	0
35	HTG	b	601	19/19	0.81	0.20	42,57,82,87	0
35	HTG	b	603	19/19	0.81	0.19	47,75,92,93	0
31	PL9	a	415	55/55	0.81	0.24	65,110,127,130	0
28	GOL	T	101	6/6	0.81	0.33	60,77,82,83	0
28	GOL	b	633	6/6	0.81	0.20	68,74,80,88	0
28	GOL	V	207	6/6	0.82	0.18	81,86,89,98	0
28	GOL	v	204	6/6	0.82	0.22	84,87,94,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	C	504	65/65	0.82	0.20	36,57,79,95	0
32	UNL	m	101	10/-	0.82	0.34	58,66,81,81	0
35	HTG	b	627	19/19	0.82	0.25	55,73,94,109	0
33	LMG	c	919	51/55	0.82	0.20	51,89,123,128	0
32	UNL	D	412	40/-	0.82	0.20	51,88,141,144	0
37	DGD	h	102	62/66	0.82	0.21	34,52,71,82	0
28	GOL	v	203	6/6	0.83	0.21	72,88,91,94	0
37	DGD	C	518	62/66	0.83	0.18	39,58,92,100	0
27	SQD	A	414	54/54	0.83	0.22	49,75,134,141	0
37	DGD	H	102	62/66	0.83	0.21	31,51,88,102	0
35	HTG	B	632	19/19	0.83	0.17	48,84,110,115	0
33	LMG	A	419	51/55	0.83	0.19	54,88,107,128	0
35	HTG	B	624	19/19	0.84	0.23	50,73,82,92	0
35	HTG	V	203	19/19	0.84	0.33	73,95,125,231	0
27	SQD	a	410	54/54	0.84	0.18	51,81,110,114	0
33	LMG	a	411	51/55	0.84	0.22	51,84,96,105	0
32	UNL	I	101	40/-	0.84	0.24	42,88,155,156	0
32	UNL	i	101	40/-	0.84	0.24	48,77,140,147	0
28	GOL	C	523	6/6	0.85	0.34	74,80,89,92	0
28	GOL	a	419	6/6	0.85	0.17	73,85,94,95	0
28	GOL	T	103	6/6	0.85	0.47	103,108,112,114	0
28	GOL	c	924	6/6	0.85	0.34	81,87,97,102	0
37	DGD	c	917	62/66	0.85	0.20	35,60,112,137	0
24	CLA	c	914	65/65	0.85	0.20	68,84,105,115	0
32	UNL	X	101	18/-	0.85	0.17	53,73,112,114	0
27	SQD	A	411	54/54	0.86	0.20	43,87,114,116	0
24	CLA	c	907	65/65	0.87	0.17	44,65,104,111	0
24	CLA	B	602	65/65	0.87	0.19	43,67,119,143	0
24	CLA	B	607	65/65	0.87	0.19	31,52,95,99	0
24	CLA	b	607	65/65	0.87	0.20	30,50,60,63	0
37	DGD	c	918	62/66	0.87	0.19	41,56,90,110	0
34	CA	F	104	1/1	0.87	0.06	107,107,107,107	0
24	CLA	b	612	65/65	0.87	0.20	27,38,48,58	0
33	LMG	d	415	51/55	0.88	0.20	38,61,112,126	0
24	CLA	c	904	65/65	0.88	0.17	41,60,73,84	0
33	LMG	J	101	51/55	0.88	0.20	44,65,120,137	0
24	CLA	b	614	65/65	0.88	0.18	39,51,61,72	0
24	CLA	c	908	65/65	0.88	0.17	45,63,74,84	0
32	UNL	x	101	18/-	0.89	0.22	51,71,116,116	0
28	GOL	V	201	6/6	0.89	0.23	88,99,104,109	0
24	CLA	c	906	65/65	0.89	0.17	36,51,70,76	0
24	CLA	B	614	65/65	0.89	0.19	29,41,64,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	GOL	a	413	6/6	0.89	0.20	73,83,95,97	0
24	CLA	b	606	65/65	0.89	0.20	39,67,123,145	0
28	GOL	b	632	6/6	0.89	0.24	77,78,102,105	0
36	LHG	B	635	49/49	0.89	0.26	30,52,68,77	0
24	CLA	C	511	65/65	0.89	0.16	48,67,85,109	0
35	HTG	B	623	19/19	0.90	0.18	38,56,78,93	0
24	CLA	C	501	65/65	0.90	0.15	39,57,85,91	0
24	CLA	C	512	65/65	0.90	0.15	49,76,99,106	0
24	CLA	B	610	65/65	0.90	0.18	36,52,65,82	0
36	LHG	D	410	49/49	0.90	0.23	47,67,121,138	0
24	CLA	c	909	65/65	0.90	0.15	38,54,125,137	0
35	HTG	C	521	19/19	0.90	0.19	70,99,121,123	0
24	CLA	c	910	65/65	0.90	0.16	43,58,77,81	0
24	CLA	c	912	65/65	0.90	0.16	43,63,83,99	0
24	CLA	C	506	65/65	0.90	0.15	41,70,114,128	0
28	GOL	B	630	6/6	0.90	0.21	51,59,70,81	0
37	DGD	c	916	62/66	0.90	0.18	38,56,100,114	0
24	CLA	d	404	65/65	0.90	0.18	29,39,48,56	0
28	GOL	c	928	6/6	0.90	0.14	75,83,90,98	0
26	BCR	C	514	40/40	0.90	0.17	50,72,86,87	0
24	CLA	c	905	65/65	0.90	0.16	31,57,74,85	0
24	CLA	b	611	65/65	0.91	0.17	37,51,97,108	0
24	CLA	C	503	65/65	0.91	0.18	36,59,72,85	0
36	LHG	b	635	49/49	0.91	0.22	30,48,61,64	0
36	LHG	d	411	49/49	0.91	0.20	37,53,112,120	0
28	GOL	A	412	6/6	0.91	0.18	49,55,57,69	0
24	CLA	A	405	65/65	0.91	0.17	24,37,51,66	0
28	GOL	B	636	6/6	0.91	0.18	49,56,64,65	0
24	CLA	b	619	65/65	0.91	0.18	25,43,86,108	0
28	GOL	D	402	6/6	0.91	0.31	52,57,83,90	0
24	CLA	b	620	65/65	0.91	0.17	36,50,64,69	0
24	CLA	c	911	65/65	0.91	0.15	43,55,69,81	0
24	CLA	B	616	65/65	0.91	0.17	37,50,65,77	0
24	CLA	B	605	65/65	0.91	0.17	28,41,72,78	0
26	BCR	k	101	40/40	0.92	0.14	51,64,75,80	0
24	CLA	D	405	65/65	0.92	0.15	39,55,106,121	0
24	CLA	a	405	65/65	0.92	0.19	24,38,53,67	0
24	CLA	C	508	65/65	0.92	0.15	35,61,138,148	0
24	CLA	C	509	65/65	0.92	0.15	53,65,82,93	0
34	CA	o	301	1/1	0.92	0.05	97,97,97,97	0
24	CLA	C	510	65/65	0.92	0.15	40,60,77,92	0
24	CLA	B	615	65/65	0.92	0.19	26,43,97,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	b	613	65/65	0.92	0.17	36,49,59,62	0
36	LHG	d	409	49/49	0.92	0.23	40,52,66,70	0
36	LHG	d	410	49/49	0.92	0.23	29,44,63,98	0
24	CLA	B	612	65/65	0.92	0.20	24,40,56,63	0
37	DGD	C	516	62/66	0.92	0.18	32,50,88,97	0
24	CLA	b	616	65/65	0.92	0.17	29,41,54,66	0
28	GOL	A	413	6/6	0.92	0.17	61,79,84,86	0
24	CLA	c	913	65/65	0.92	0.16	47,74,93,99	0
24	CLA	B	603	65/65	0.92	0.16	38,50,57,66	0
24	CLA	D	404	65/65	0.92	0.16	24,37,58,69	0
24	CLA	b	621	65/65	0.92	0.17	33,53,103,118	0
26	BCR	H	101	40/40	0.92	0.17	33,57,78,85	0
26	BCR	b	623	40/40	0.92	0.19	29,46,66,68	0
26	BCR	c	927	40/40	0.92	0.15	54,77,91,100	0
26	BCR	h	101	40/40	0.93	0.18	36,60,79,81	0
24	CLA	a	408	65/65	0.93	0.20	32,53,122,130	0
26	BCR	y	101	40/40	0.93	0.15	47,63,74,82	0
24	CLA	B	613	65/65	0.93	0.16	26,42,50,53	0
24	CLA	b	615	65/65	0.93	0.18	35,47,61,67	0
32	UNL	D	411	17/-	0.93	0.22	40,71,92,94	0
24	CLA	B	604	65/65	0.93	0.18	35,48,60,63	0
24	CLA	d	405	65/65	0.93	0.17	24,40,55,69	0
24	CLA	d	406	65/65	0.93	0.19	40,54,106,124	0
24	CLA	b	617	65/65	0.93	0.17	25,42,53,65	0
26	BCR	D	406	40/40	0.93	0.15	39,58,89,104	0
24	CLA	b	608	65/65	0.93	0.17	38,48,58,66	0
24	CLA	C	507	65/65	0.93	0.16	41,66,77,86	0
24	CLA	B	608	65/65	0.93	0.17	25,41,51,61	0
28	GOL	B	626	6/6	0.93	0.19	44,53,66,87	0
28	GOL	B	628	6/6	0.93	0.22	62,80,83,84	0
34	CA	b	605	1/1	0.93	0.06	124,124,124,124	0
26	BCR	d	407	40/40	0.93	0.19	39,54,85,88	0
28	GOL	b	630	6/6	0.94	0.17	50,82,94,95	0
24	CLA	c	903	65/65	0.94	0.15	39,52,76,80	0
32	UNL	d	412	17/-	0.94	0.25	47,62,95,102	0
36	LHG	D	409	49/49	0.94	0.22	31,46,67,79	0
28	GOL	B	627	6/6	0.94	0.25	54,64,88,102	0
24	CLA	A	406	65/65	0.94	0.16	23,36,45,55	0
36	LHG	L	101	49/49	0.94	0.22	36,47,56,62	0
24	CLA	B	617	65/65	0.94	0.20	34,54,130,139	0
24	CLA	A	407	65/65	0.94	0.15	28,43,106,119	0
31	PL9	D	407	55/55	0.94	0.21	29,42,52,60	0

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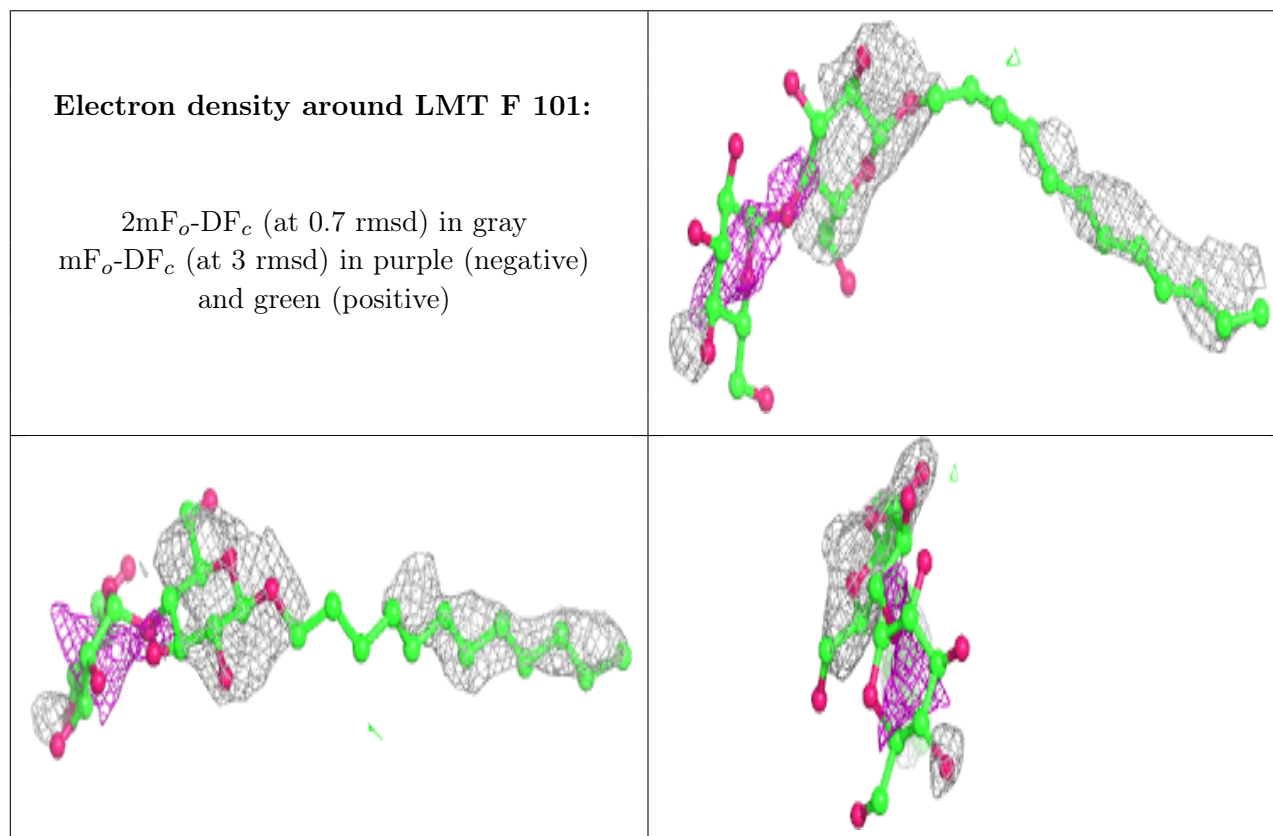
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	b	610	65/65	0.94	0.17	31,43,53,61	0
31	PL9	d	408	55/55	0.94	0.21	22,39,53,73	0
25	PHO	A	408	64/64	0.94	0.16	26,39,46,54	0
25	PHO	d	403	64/64	0.94	0.17	27,44,54,62	0
24	CLA	b	618	65/65	0.94	0.20	24,44,60,67	0
24	CLA	B	609	65/65	0.94	0.18	32,46,59,67	0
24	CLA	B	606	65/65	0.94	0.16	28,40,55,57	0
26	BCR	K	101	40/40	0.94	0.15	43,63,79,82	0
28	GOL	V	206	6/6	0.94	0.31	52,60,67,71	0
26	BCR	Y	102	40/40	0.94	0.14	51,71,90,107	0
24	CLA	C	505	65/65	0.94	0.15	41,54,71,89	0
24	CLA	c	902	65/65	0.94	0.16	44,60,72,81	0
24	CLA	b	609	65/65	0.95	0.17	27,42,74,77	0
26	BCR	c	915	40/40	0.95	0.18	32,56,67,75	0
26	BCR	A	410	40/40	0.95	0.18	32,42,54,54	0
24	CLA	C	502	65/65	0.95	0.14	42,56,69,85	0
26	BCR	C	515	40/40	0.95	0.18	38,55,68,78	0
24	CLA	B	611	65/65	0.95	0.20	31,50,62,66	0
24	CLA	A	409	65/65	0.95	0.16	33,50,116,132	0
28	GOL	v	205	6/6	0.95	0.21	48,59,69,78	0
28	GOL	V	205	6/6	0.95	0.17	45,51,58,72	0
24	CLA	a	406	65/65	0.95	0.19	31,44,118,125	0
26	BCR	T	102	40/40	0.95	0.17	29,46,64,65	0
34	CA	c	901	1/1	0.95	0.08	74,74,74,74	0
28	GOL	B	629	6/6	0.95	0.28	56,60,69,95	0
25	PHO	D	401	64/64	0.95	0.17	31,46,58,60	0
28	GOL	b	629	6/6	0.95	0.21	57,62,67,81	0
26	BCR	b	622	40/40	0.95	0.18	32,44,56,60	0
28	GOL	b	631	6/6	0.95	0.19	58,70,81,100	0
26	BCR	t	102	40/40	0.96	0.19	33,46,62,64	0
26	BCR	a	409	40/40	0.96	0.19	28,43,54,59	0
23	BCT	d	402	4/4	0.96	0.23	70,72,76,97	0
25	PHO	a	407	64/64	0.96	0.18	28,40,48,54	0
26	BCR	b	624	40/40	0.96	0.19	39,50,61,65	0
22	CL	A	403	1/1	0.96	0.09	38,38,38,38	0
34	CA	O	301	1/1	0.96	0.06	89,89,89,89	0
23	BCT	A	404	4/4	0.96	0.21	59,62,74,108	0
26	BCR	B	618	40/40	0.96	0.21	29,40,51,54	0
28	GOL	a	412	6/6	0.96	0.24	54,61,67,72	0
26	BCR	B	619	40/40	0.96	0.20	31,42,60,66	0
26	BCR	B	620	40/40	0.96	0.20	36,52,64,67	0
38	HEM	V	202	43/43	0.96	0.14	31,45,54,59	0

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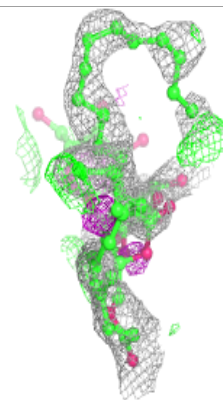
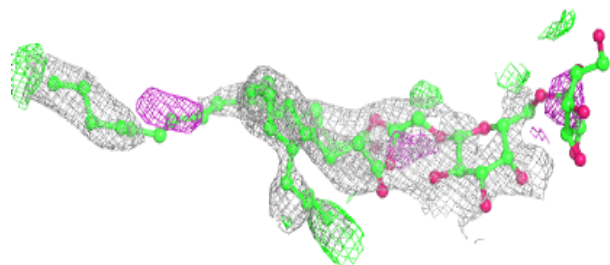
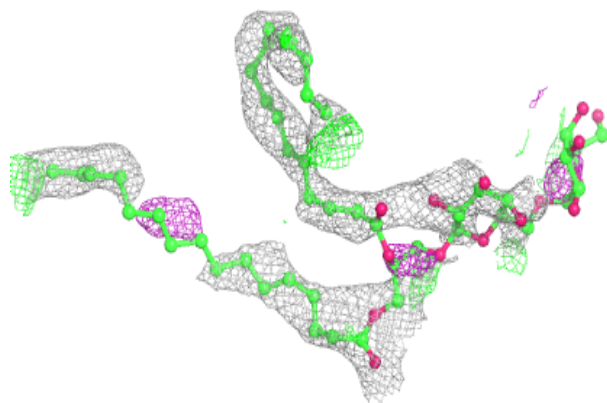
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	HEM	f	101	43/43	0.96	0.16	51,85,128,152	0
39	MG	j	102	1/1	0.96	0.13	61,61,61,61	0
34	CA	C	525	1/1	0.97	0.16	79,79,79,79	0
28	GOL	B	631	6/6	0.97	0.31	40,78,87,93	0
38	HEM	v	202	43/43	0.97	0.14	46,58,65,70	0
38	HEM	F	102	43/43	0.97	0.16	53,74,105,111	0
28	GOL	c	923	6/6	0.98	0.19	41,51,54,57	0
30	OEX	a	416	10/10	0.98	0.15	35,45,63,74	0
28	GOL	C	524	6/6	0.98	0.17	39,44,53,61	0
39	MG	J	103	1/1	0.98	0.12	54,54,54,54	0
34	CA	c	926	1/1	0.98	0.11	77,77,77,77	0
30	OEX	A	416	10/10	0.99	0.14	39,45,61,77	0
21	FE2	A	401	1/1	0.99	0.16	56,56,56,56	0
21	FE2	d	401	1/1	0.99	0.20	55,55,55,55	0
22	CL	a	403	1/1	0.99	0.17	37,37,37,37	0
22	CL	A	402	1/1	1.00	0.16	35,35,35,35	0
22	CL	a	404	1/1	1.00	0.14	42,42,42,42	0

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

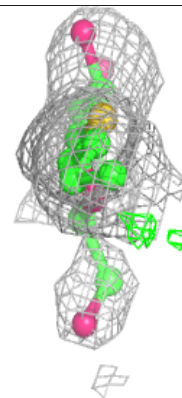
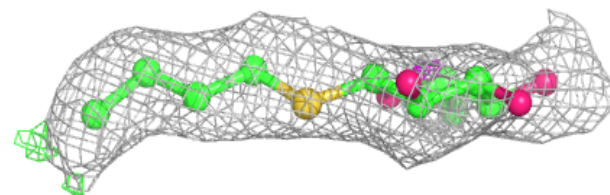
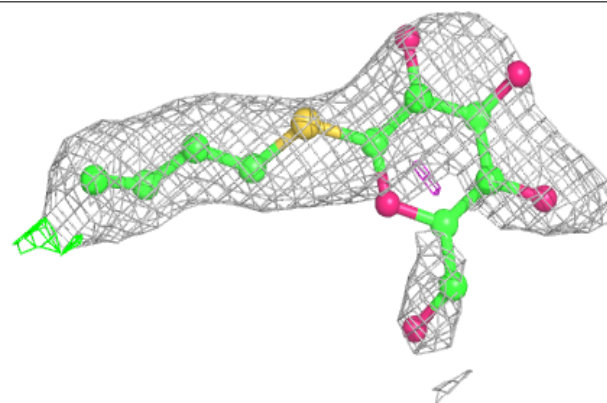


Electron density around DGD e 101:

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

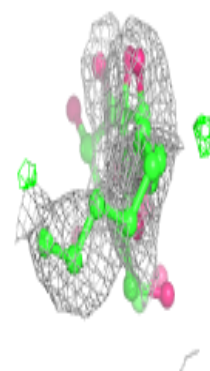
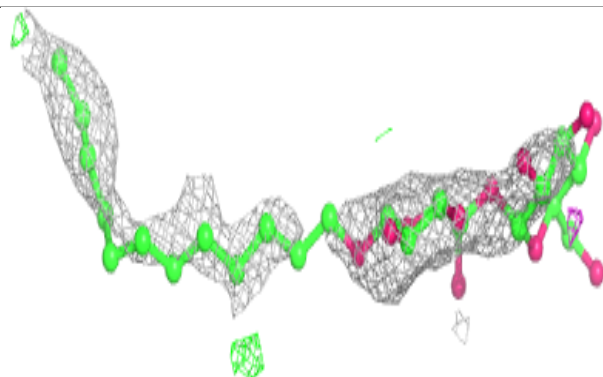
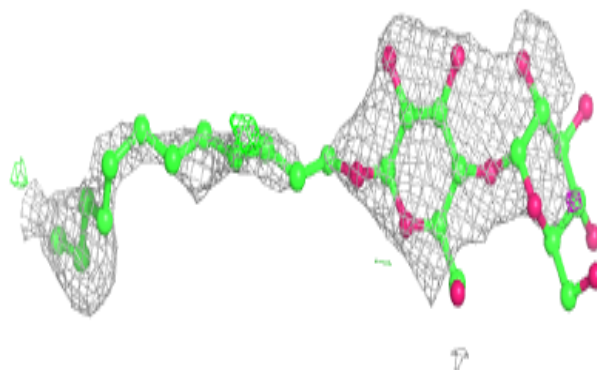
**Electron density around HTG d 414:**

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

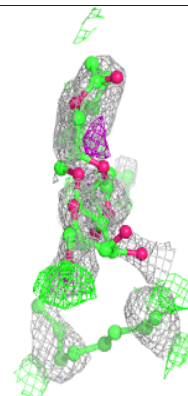
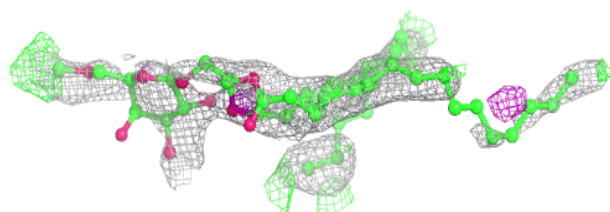
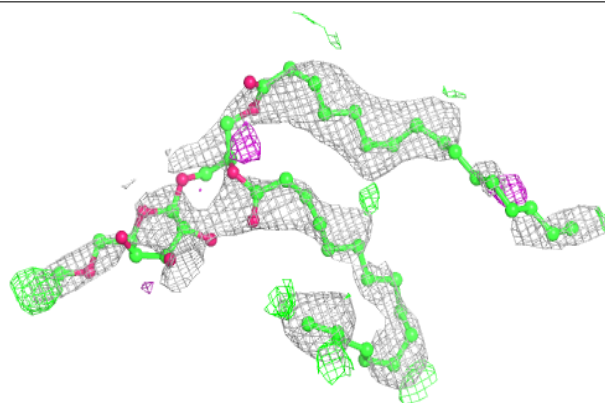


Electron density around LMT a 417:

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

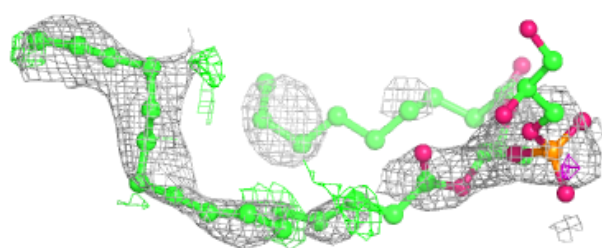
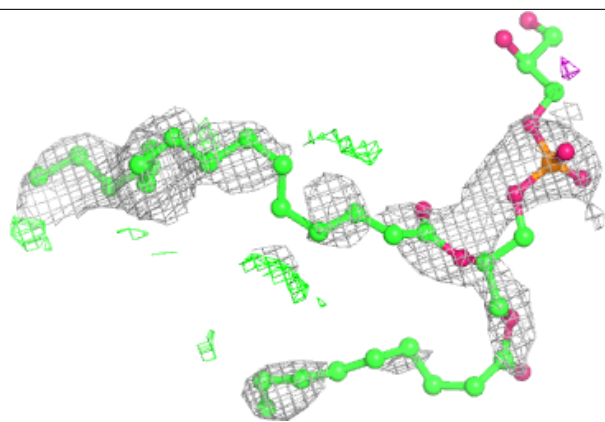
**Electron density around DGD D 408:**

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

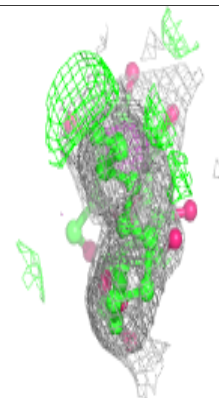
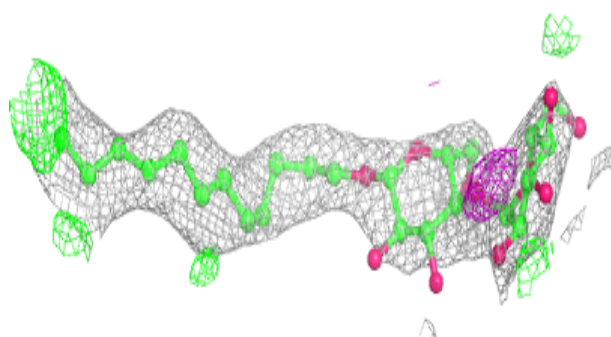
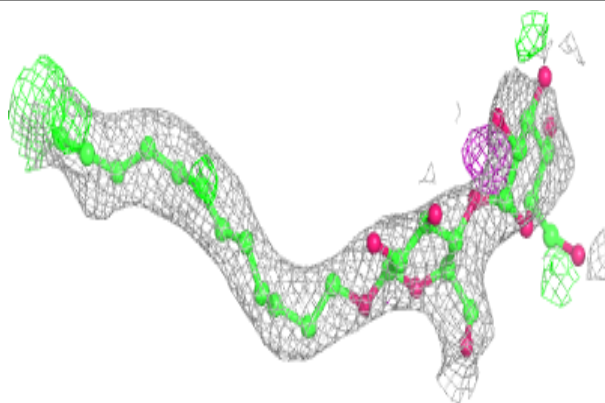


Electron density around LHG a 418:

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

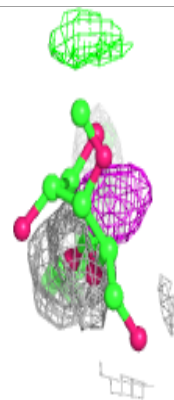
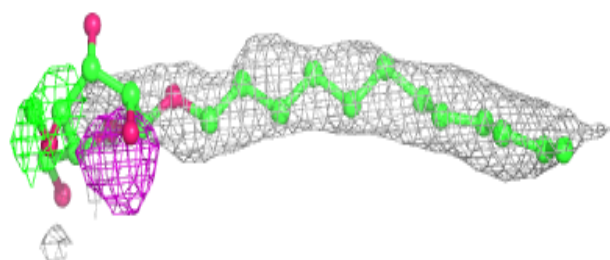
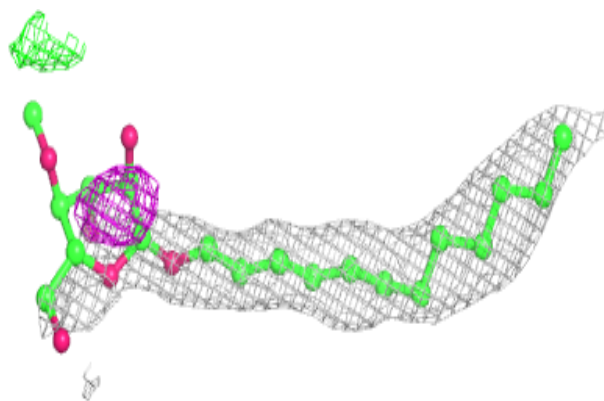
**Electron density around LMT a 401:**

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

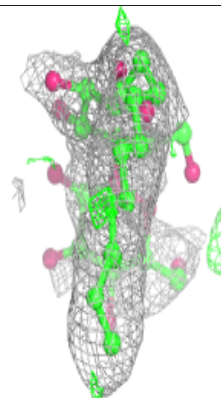
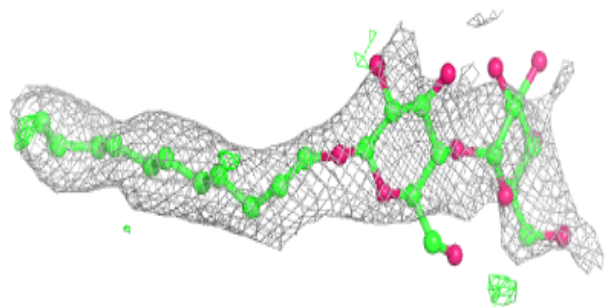
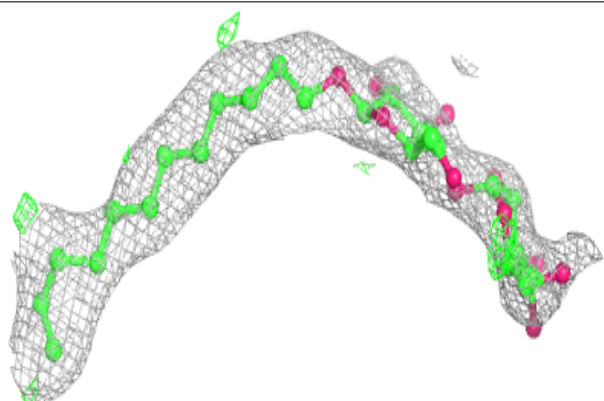


Electron density around LMT b 626:

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

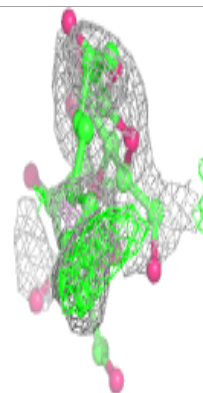
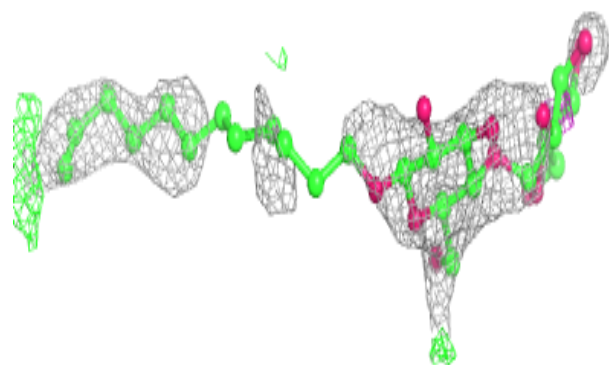
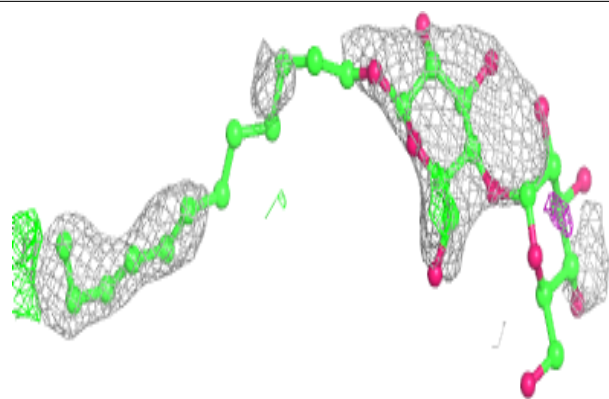
**Electron density around LMT m 103:**

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

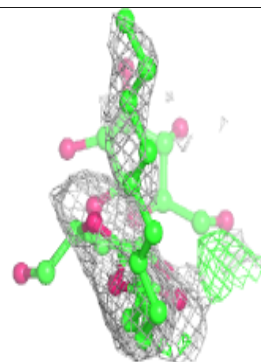
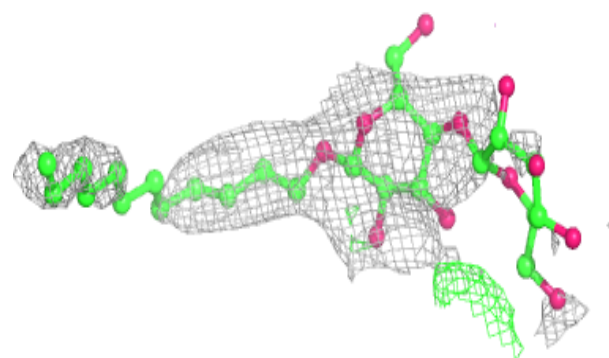
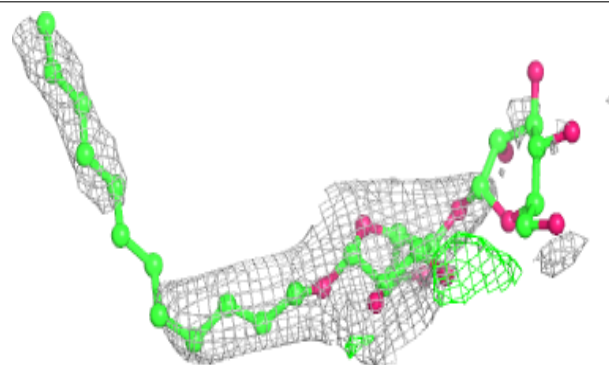


Electron density around LMT e 102:

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

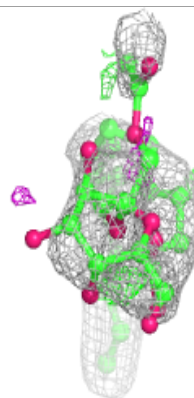
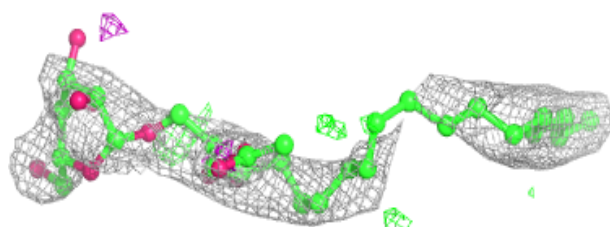
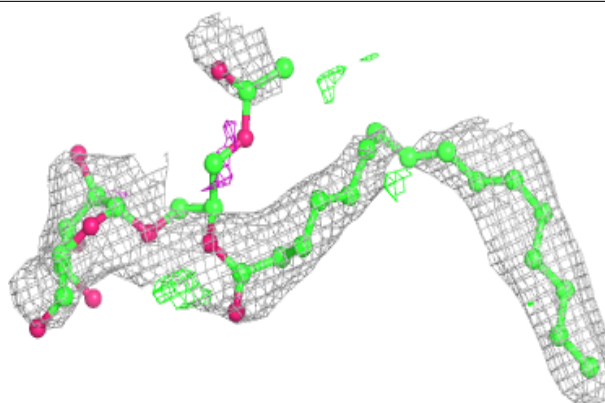
**Electron density around LMT C 520:**

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

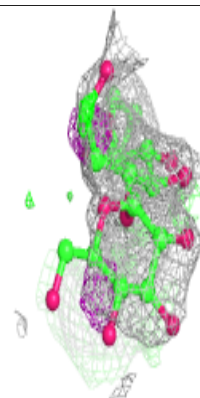
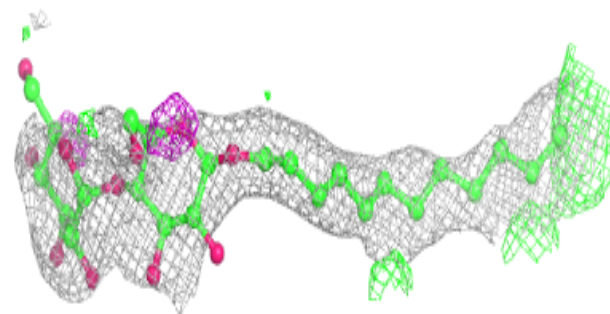
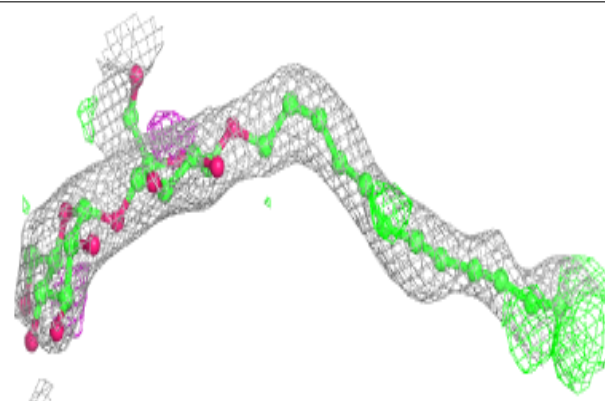


Electron density around LMG Z 101:

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

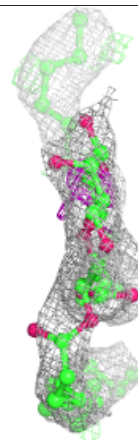
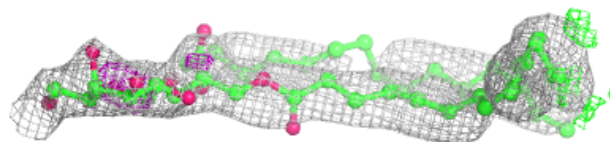
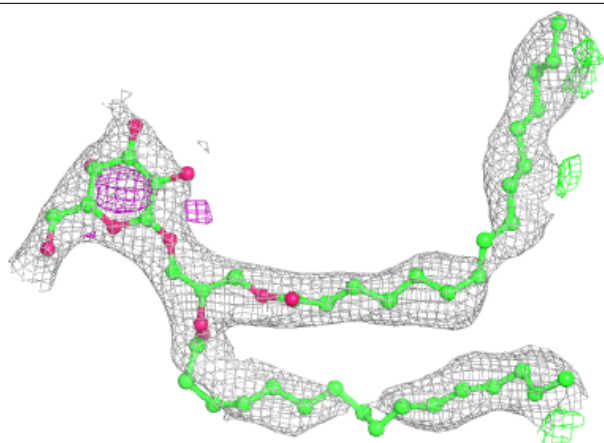
**Electron density around LMT A 415:**

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

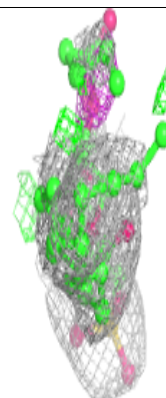
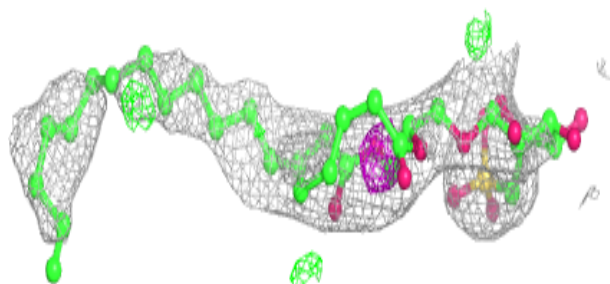
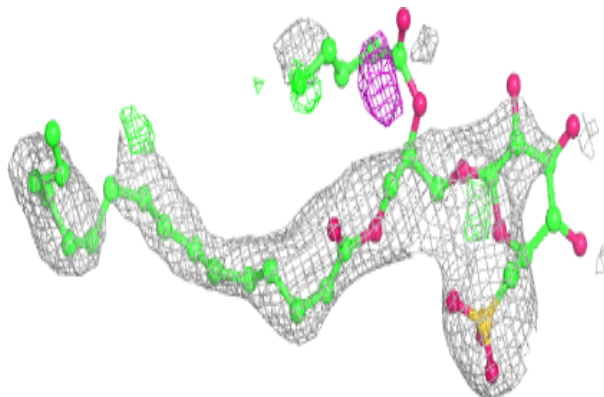


Electron density around LMG Y 101:

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

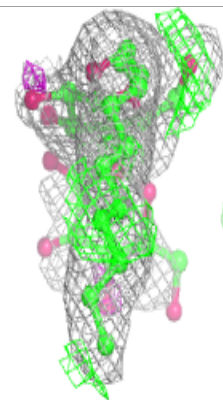
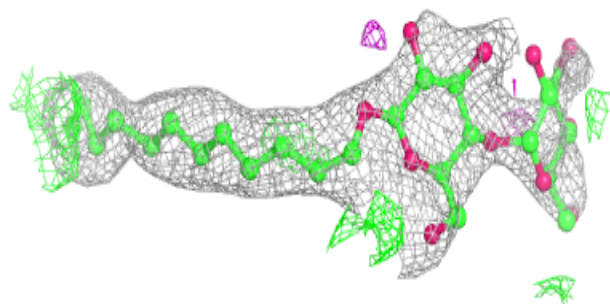
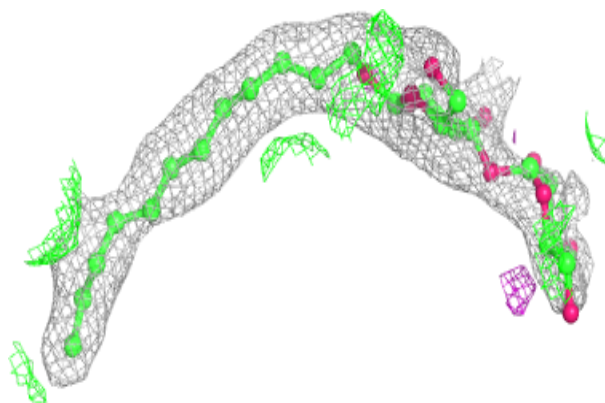
**Electron density around SQD f 102:**

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

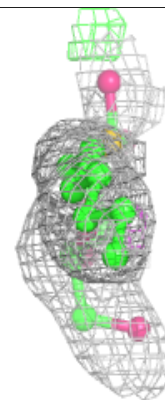
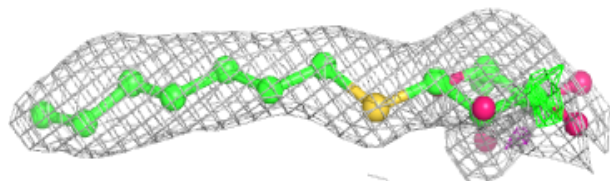
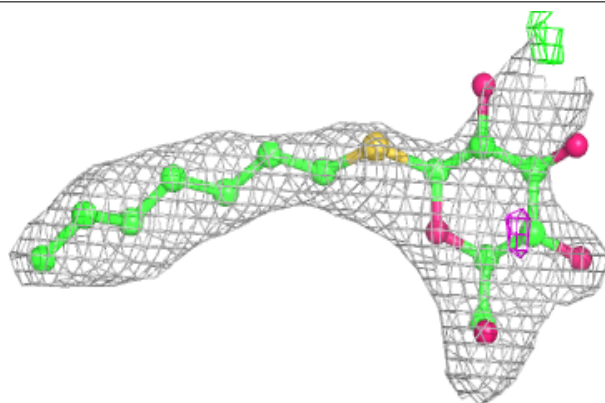


Electron density around LMT M 103:

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

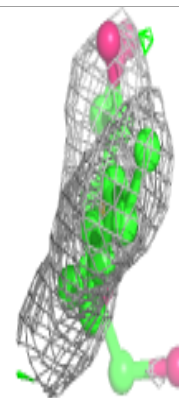
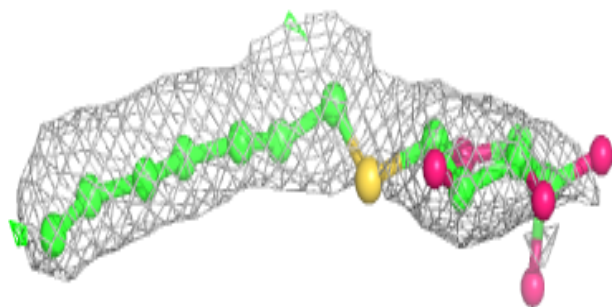
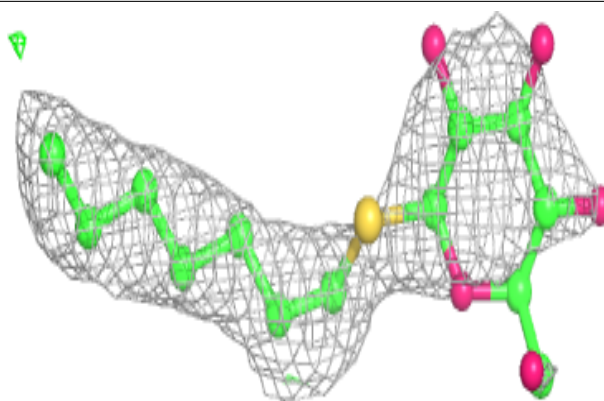
**Electron density around HTG B 633:**

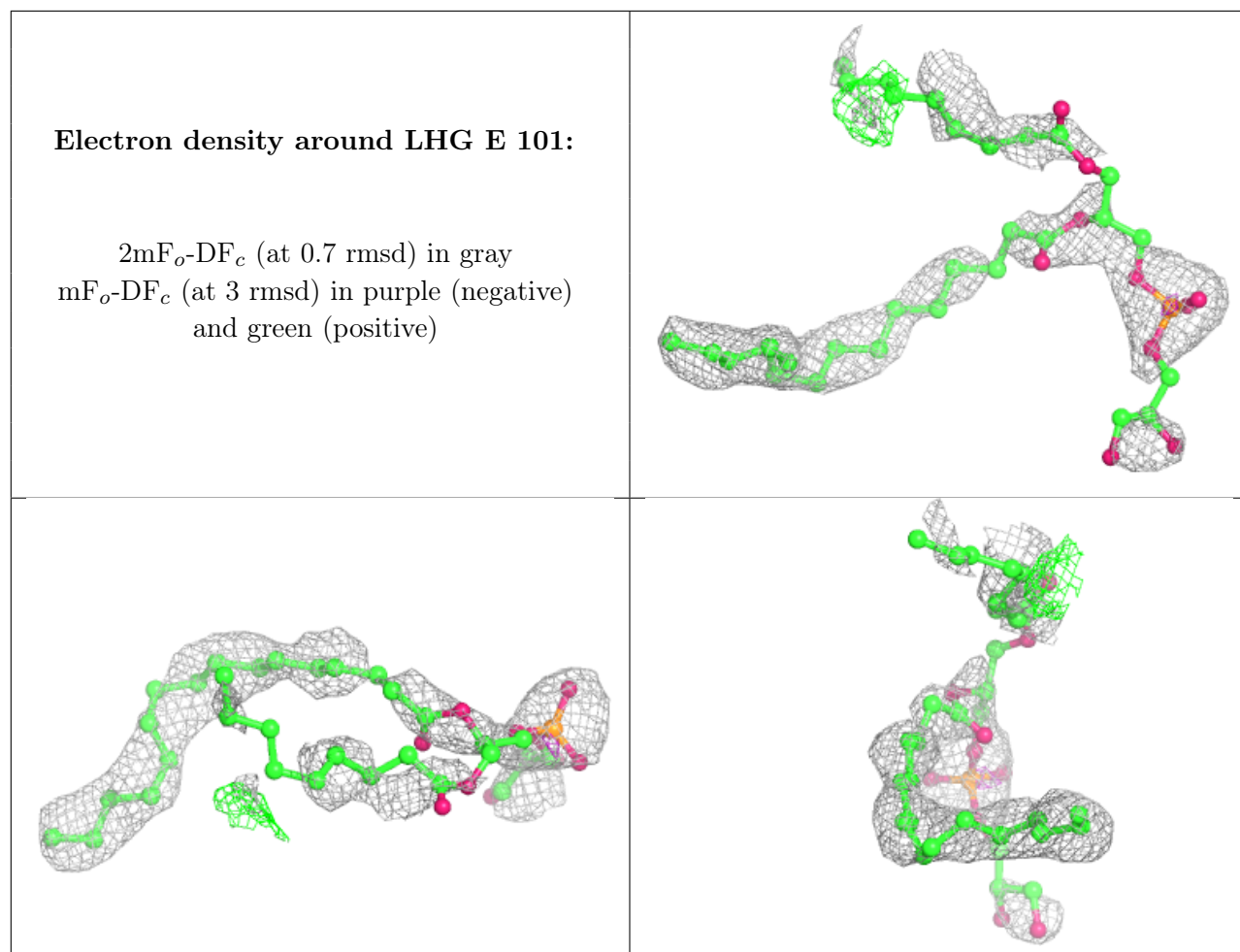
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HTG c 922:

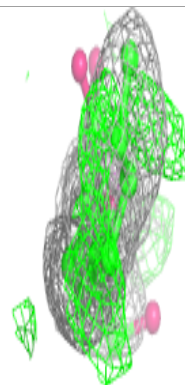
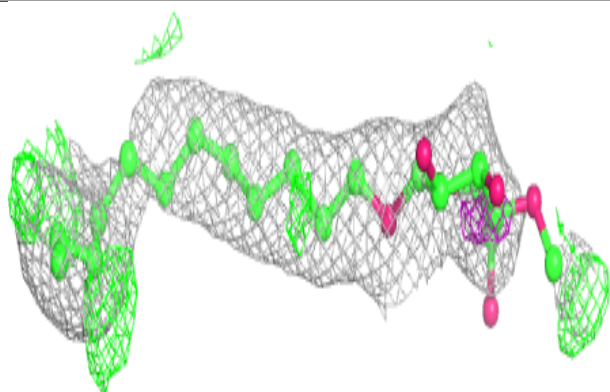
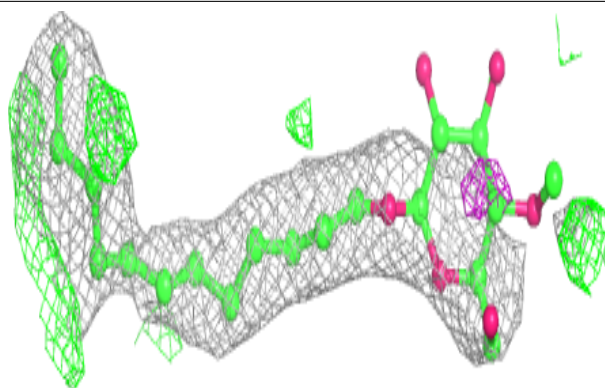
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



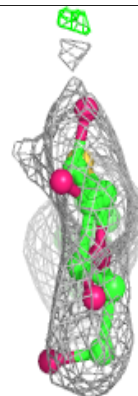
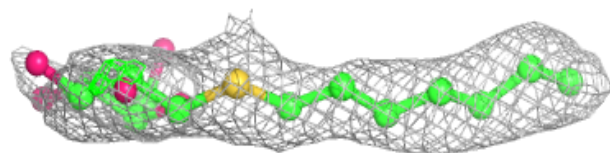
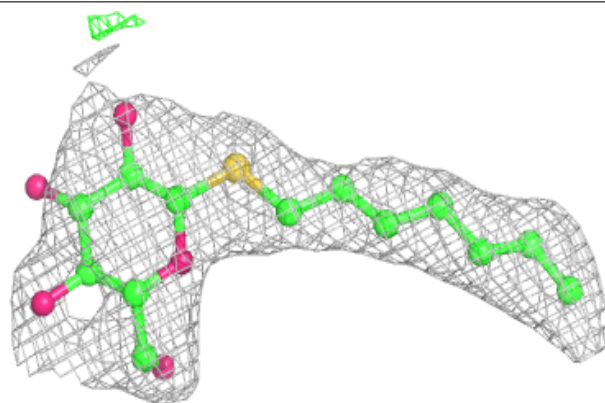


Electron density around LMT b 602:

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

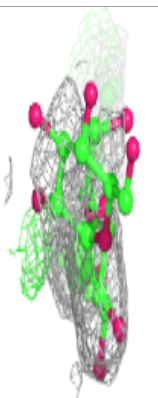
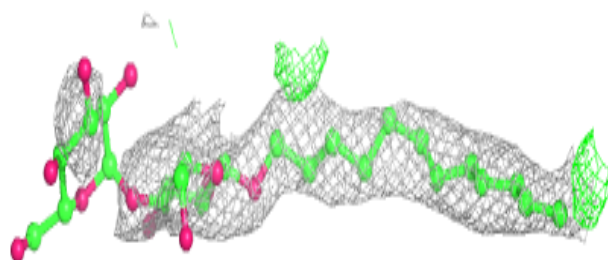
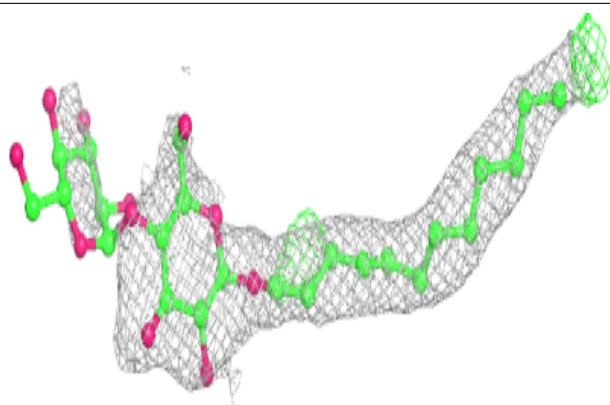
**Electron density around HTG b 604:**

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

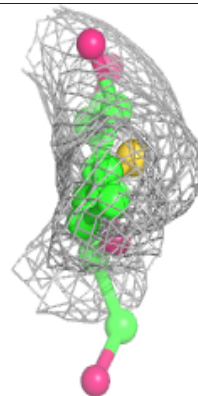
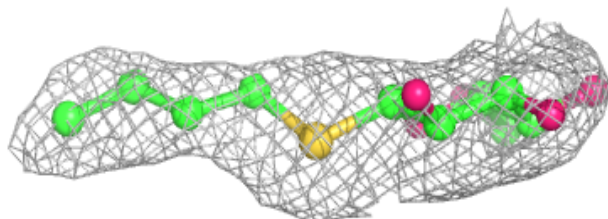
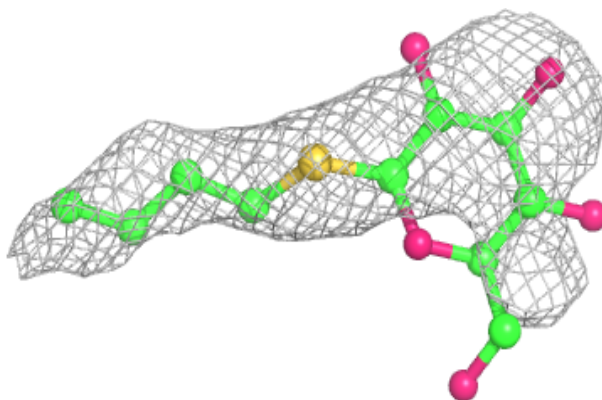


Electron density around LMT D 403:

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

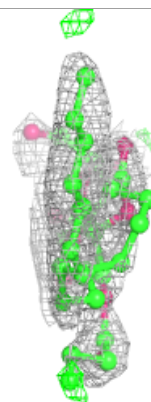
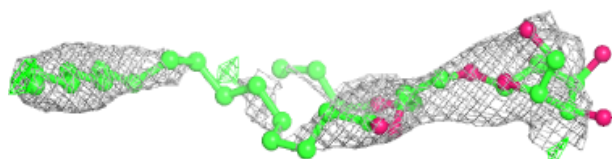
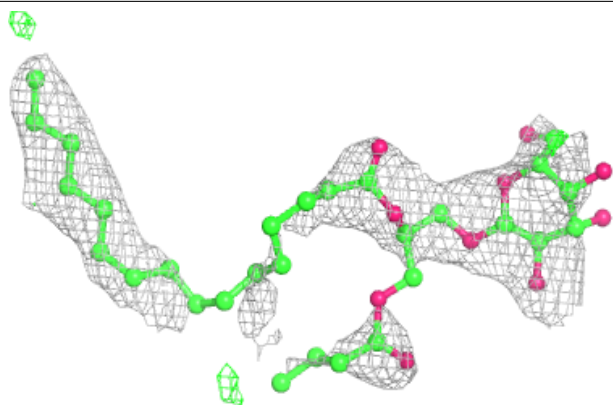
**Electron density around HTG D 413:**

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

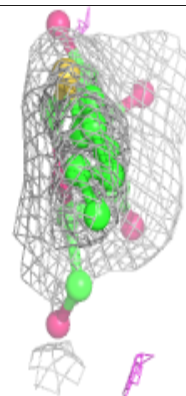
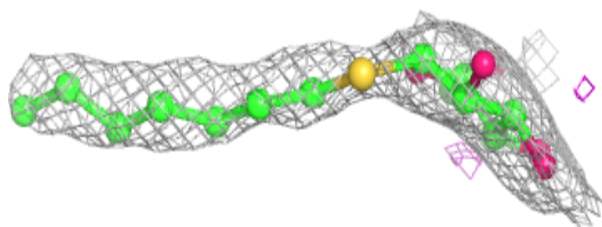
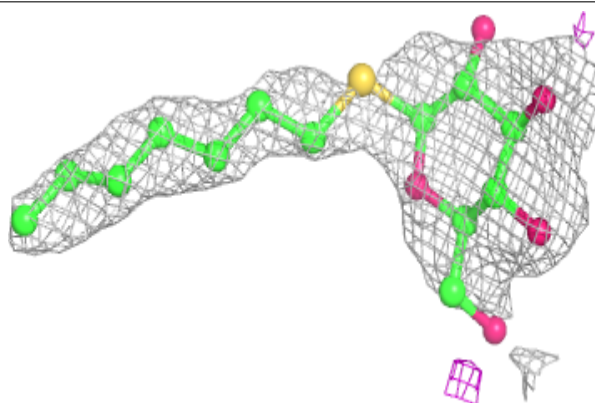


Electron density around LMG z 101:

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

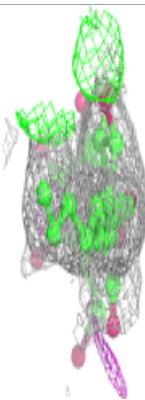
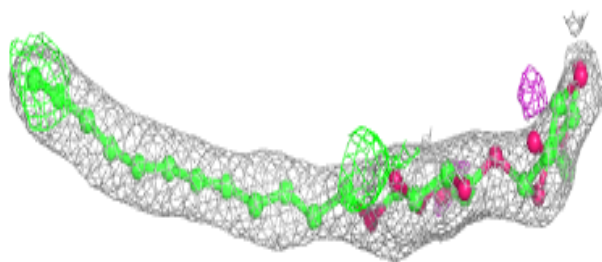
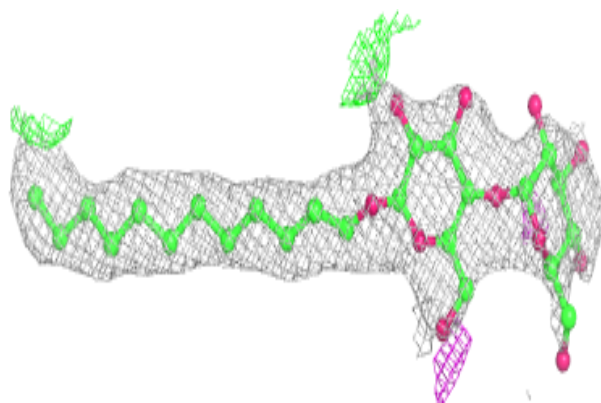
**Electron density around HTG B 625:**

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

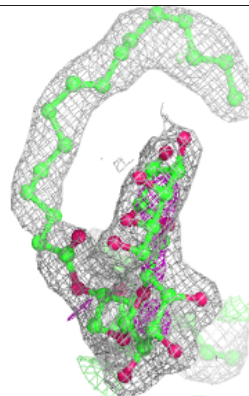
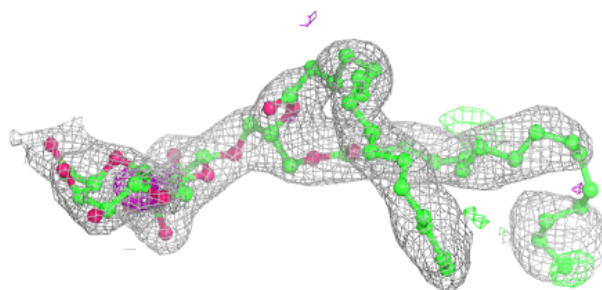
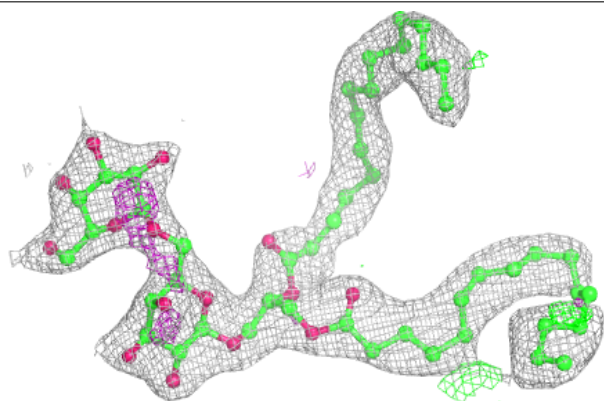


Electron density around LMT M 101:

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

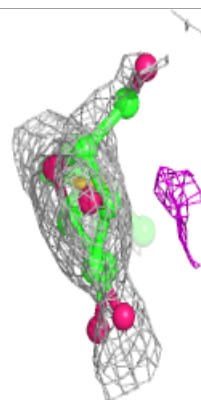
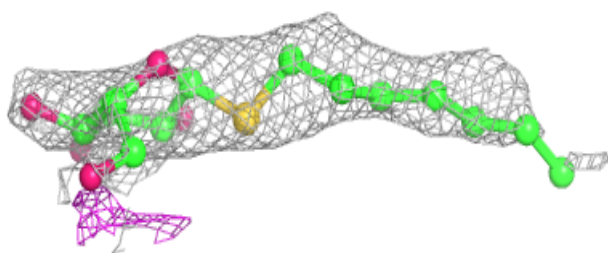
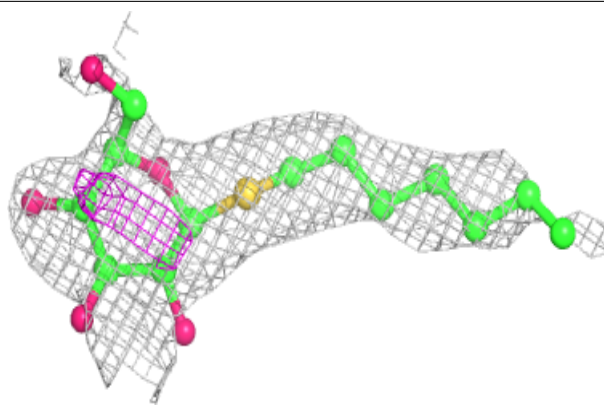
**Electron density around DGD C 517:**

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

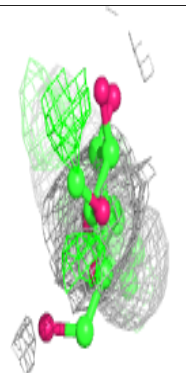
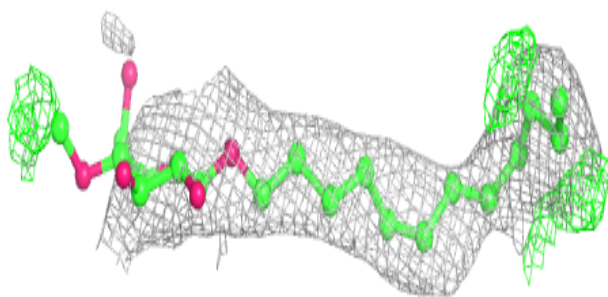
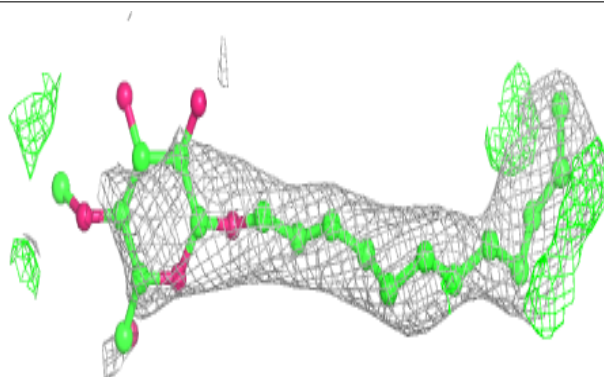


Electron density around HTG C 522:

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

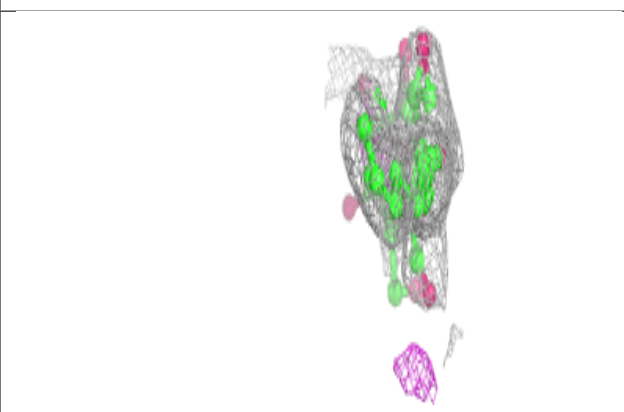
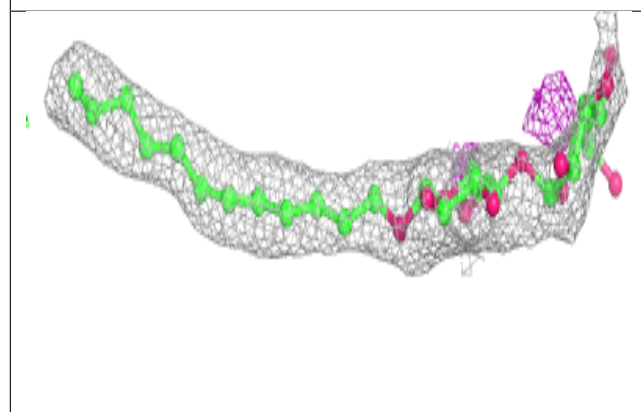
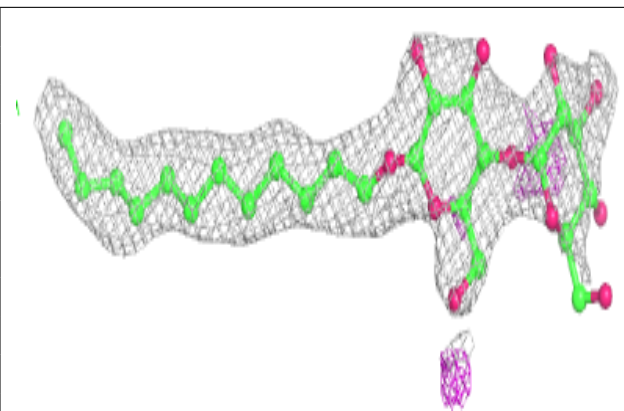
**Electron density around LMT t 101:**

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

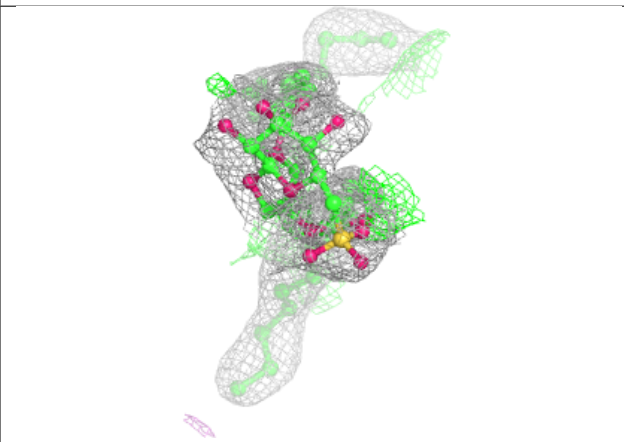
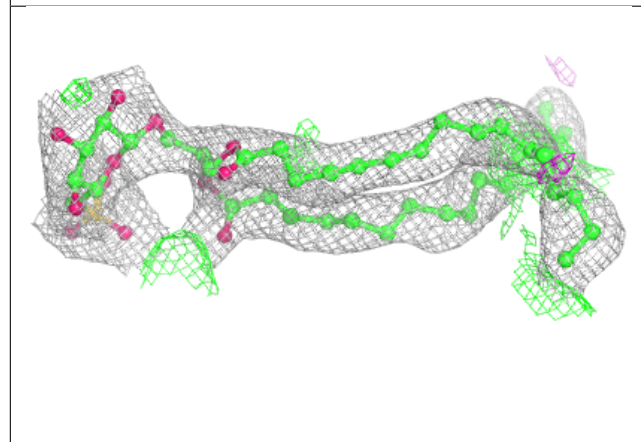
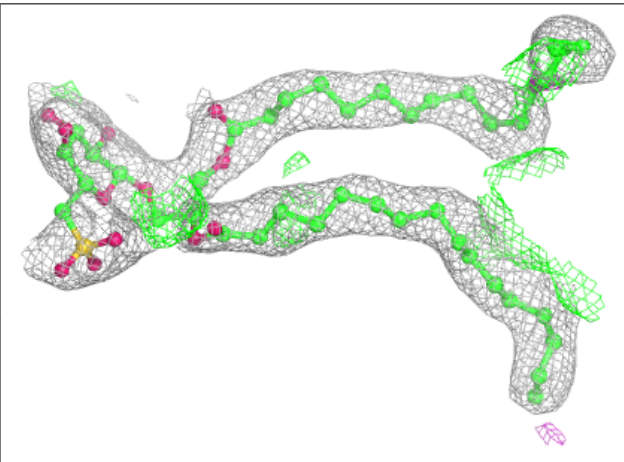


Electron density around LMT m 102:

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

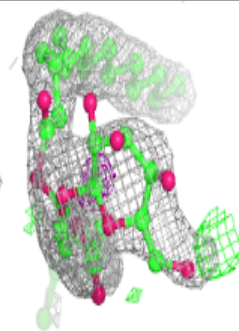
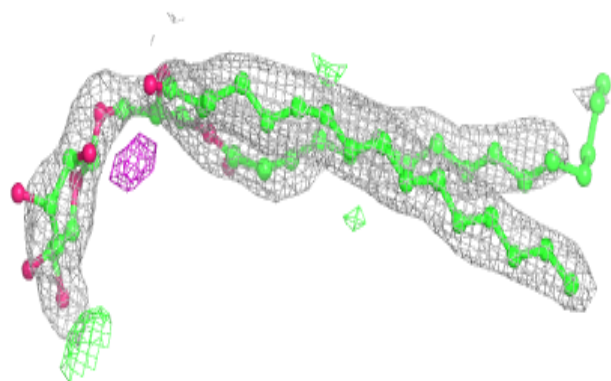
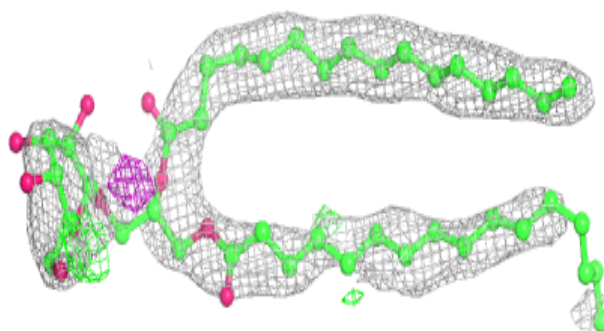
**Electron density around SQD L 102:**

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

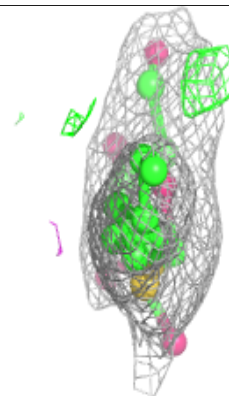
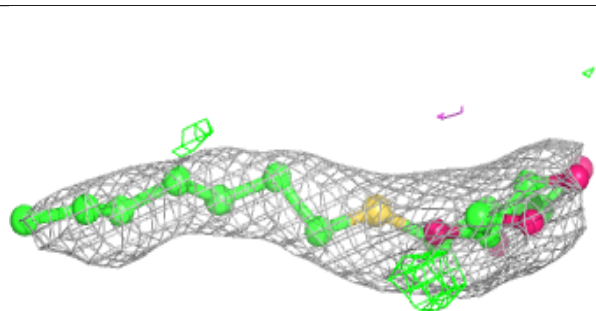
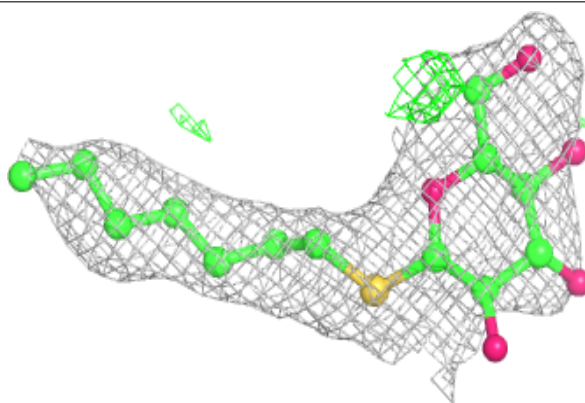


Electron density around LMG C 519:

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

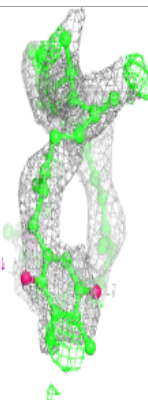
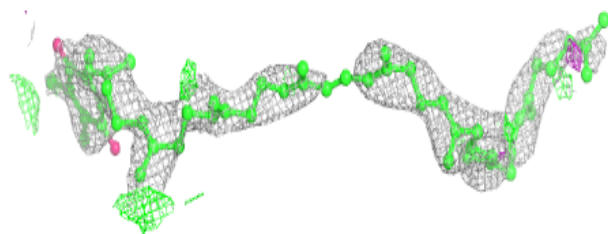
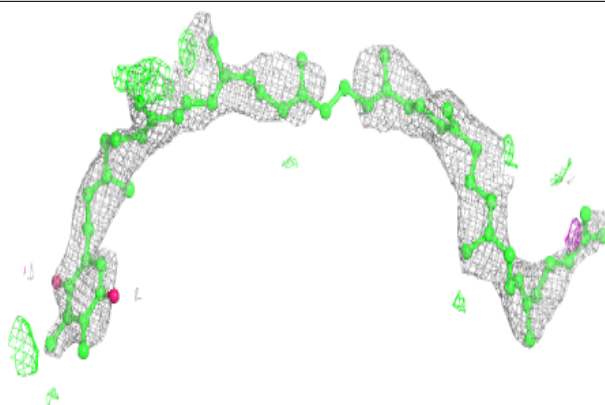
**Electron density around HTG b 628:**

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

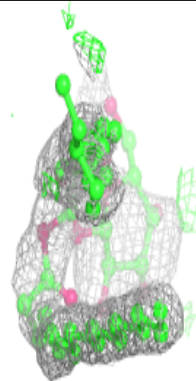
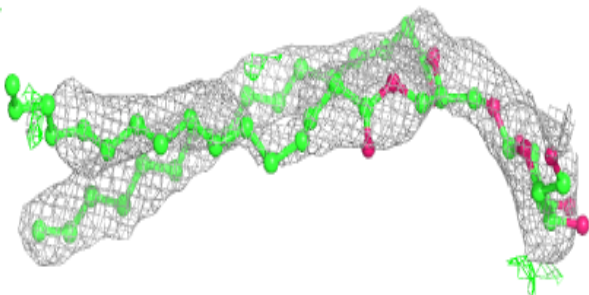
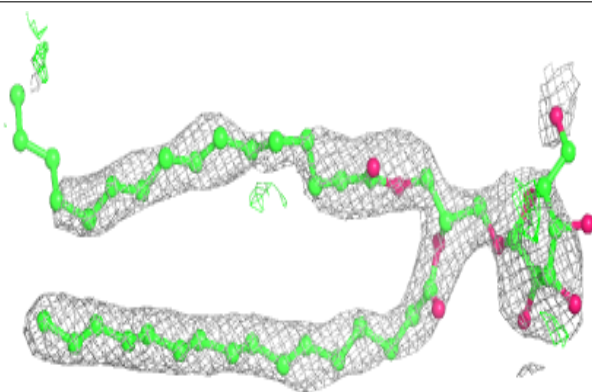


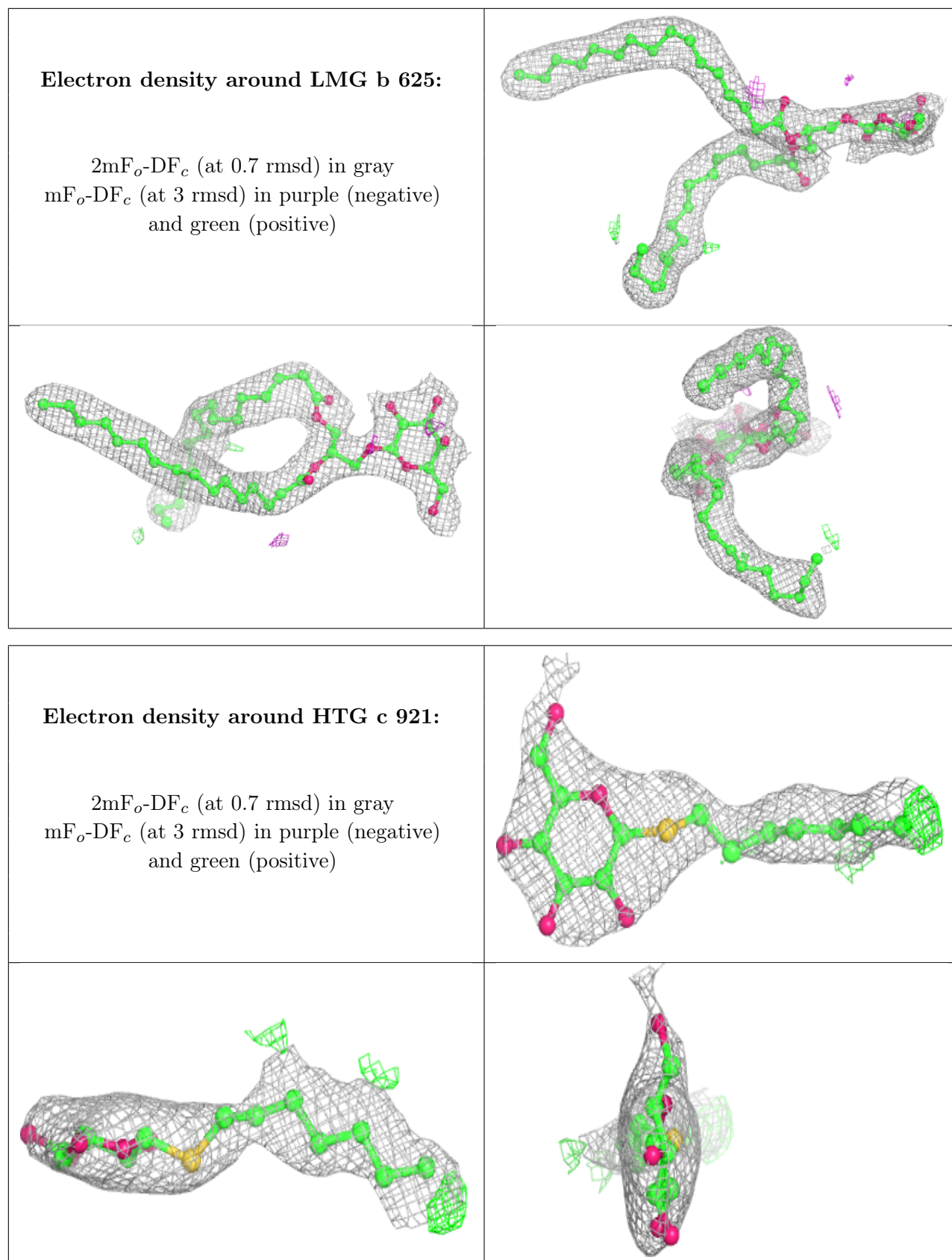
Electron density around PL9 A 417:

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

**Electron density around LMG c 920:**

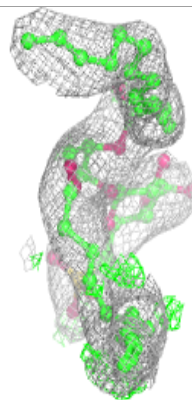
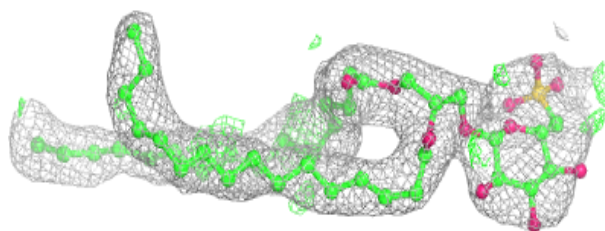
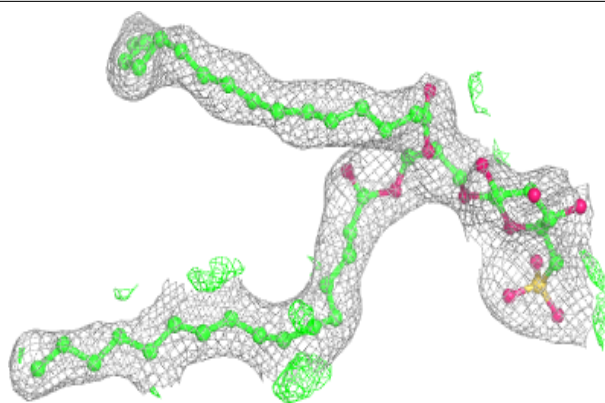
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



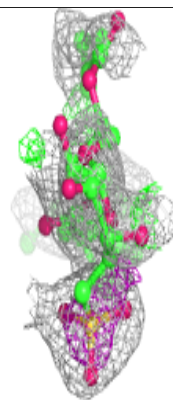
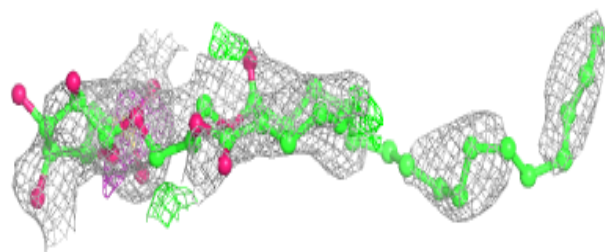
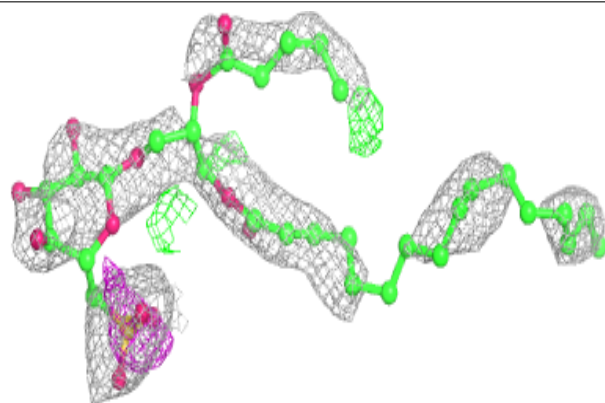


Electron density around SQD a 402:

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

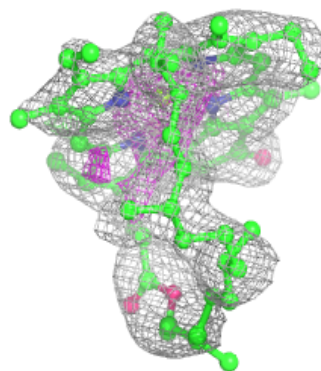
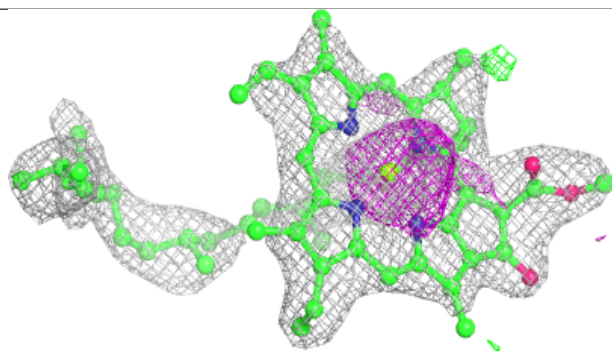
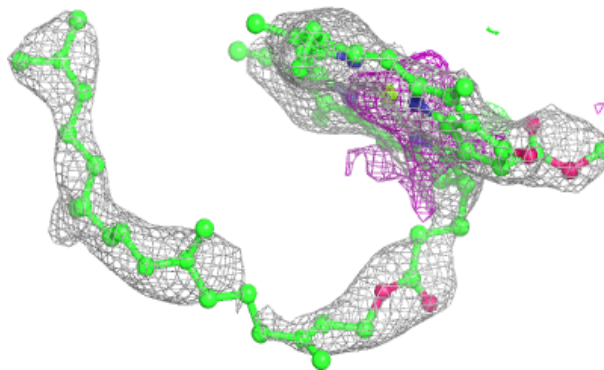
**Electron density around SQD F 103:**

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

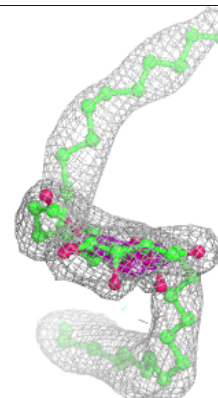
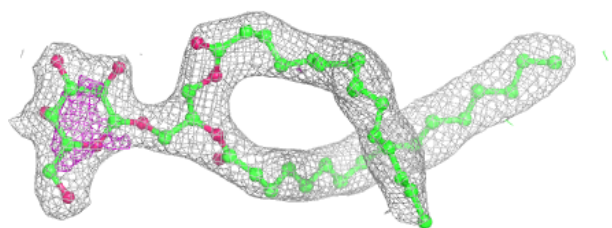
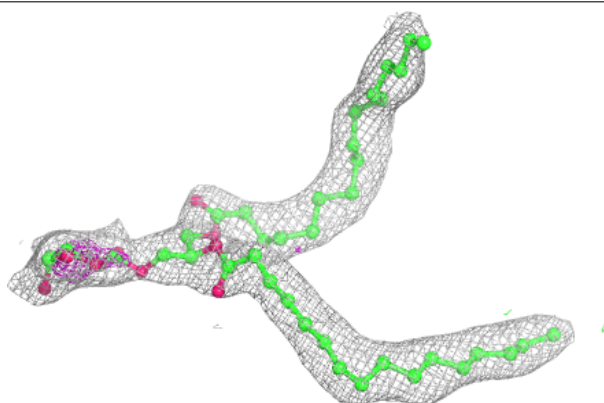


Electron density around CLA C 513:

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

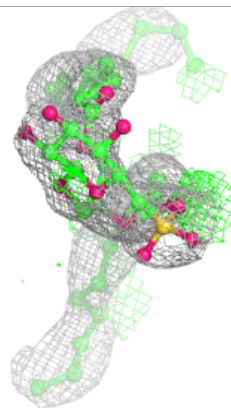
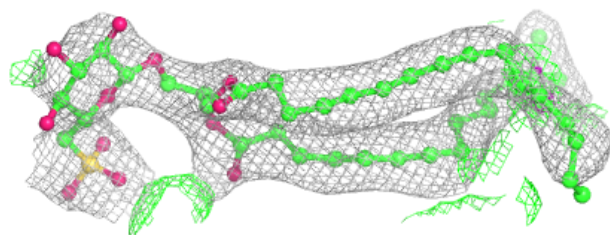
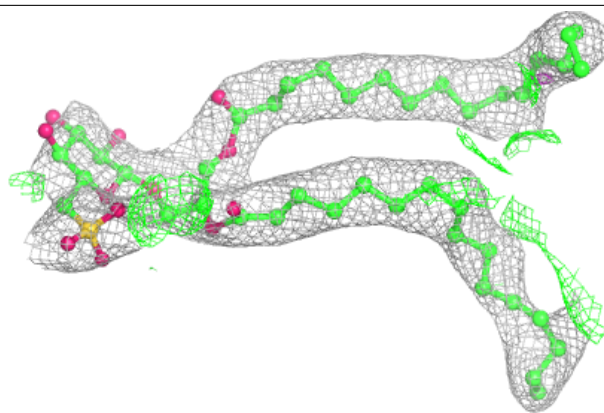
**Electron density around LMG B 622:**

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

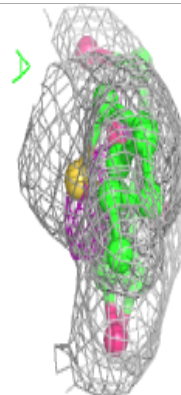
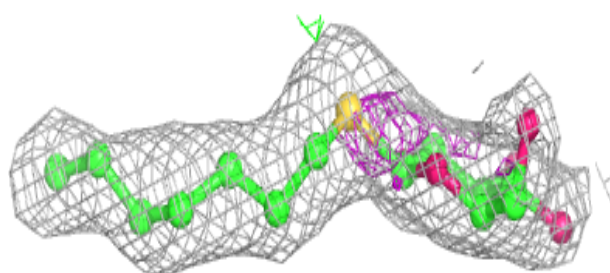
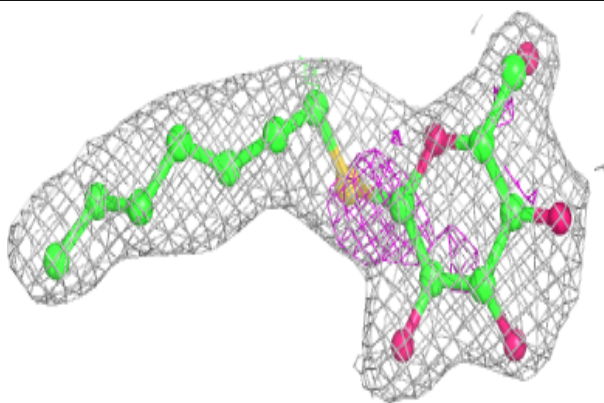


Electron density around SQD B 621:

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

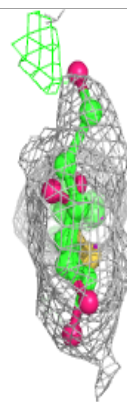
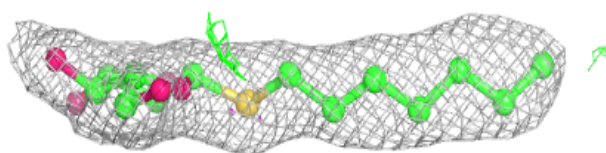
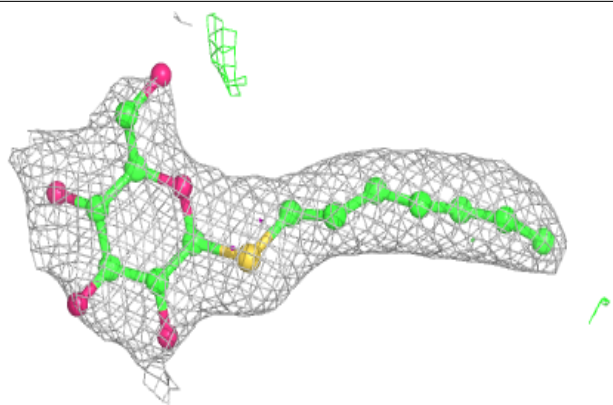
**Electron density around HTG b 601:**

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

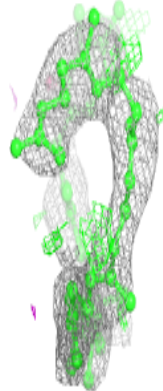
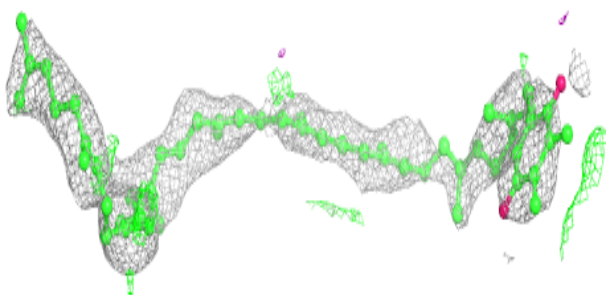
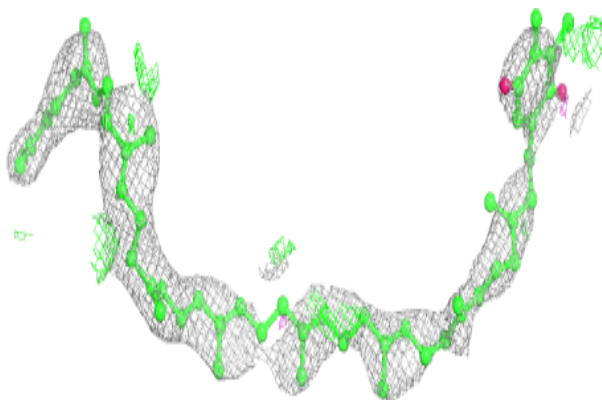


Electron density around HTG b 603:

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

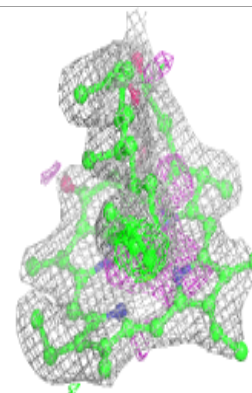
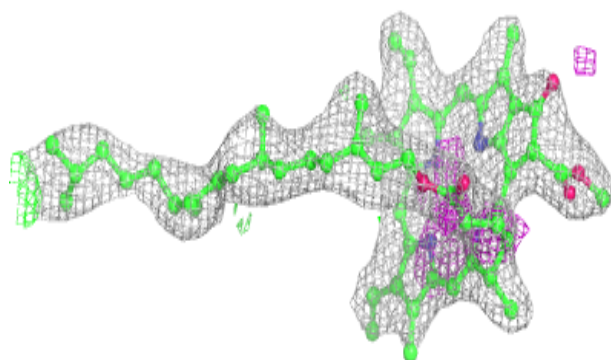
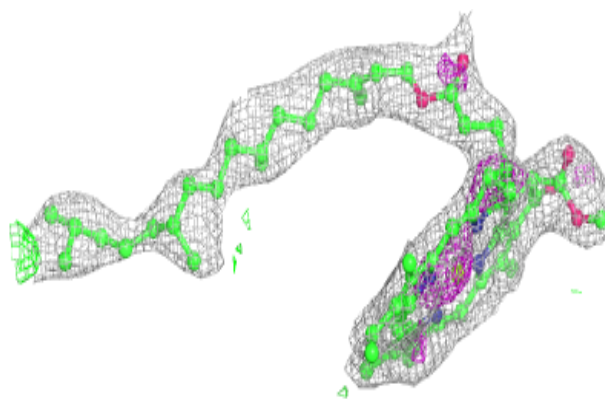
**Electron density around PL9 a 415:**

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

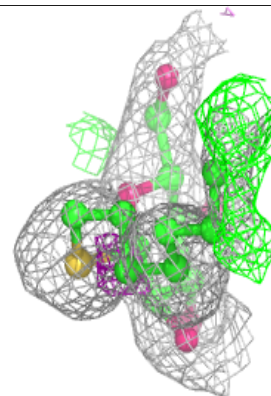
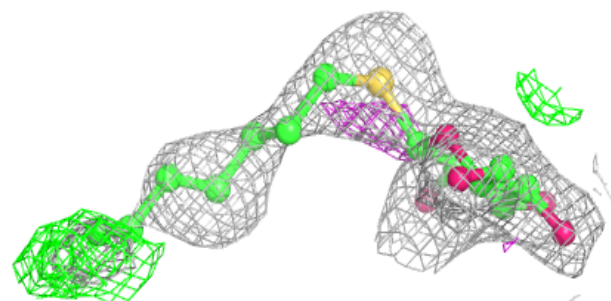
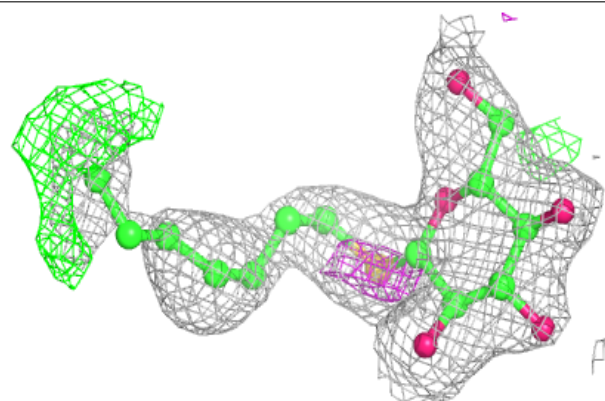


Electron density around CLA C 504:

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

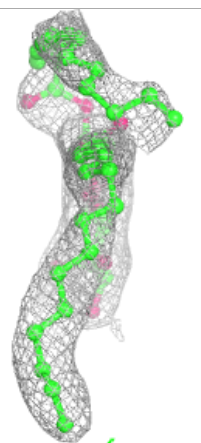
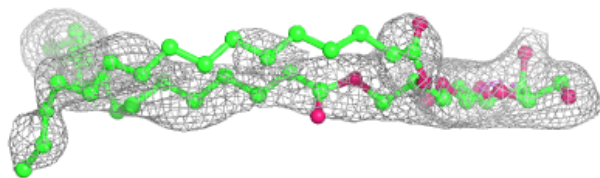
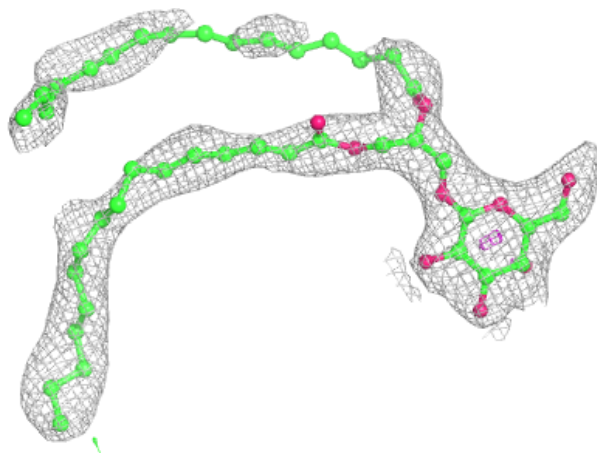
**Electron density around HTG b 627:**

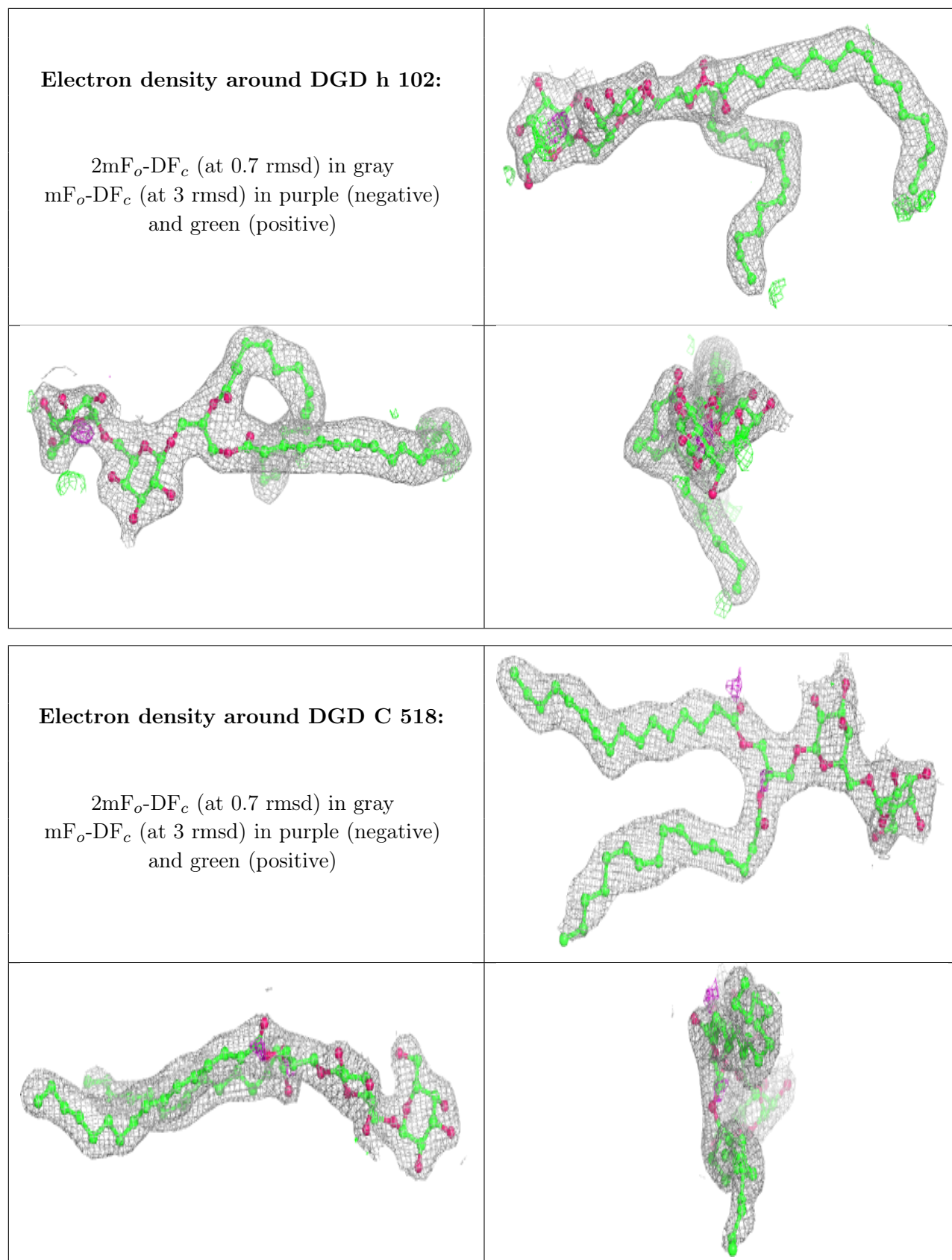
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMG c 919:

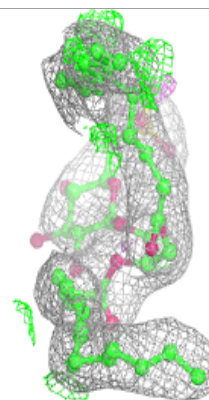
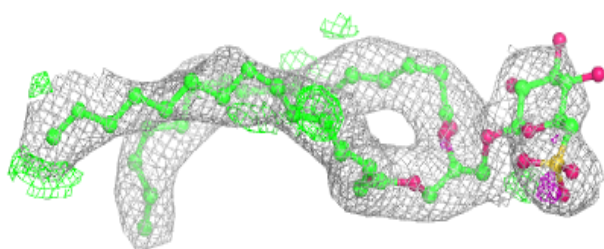
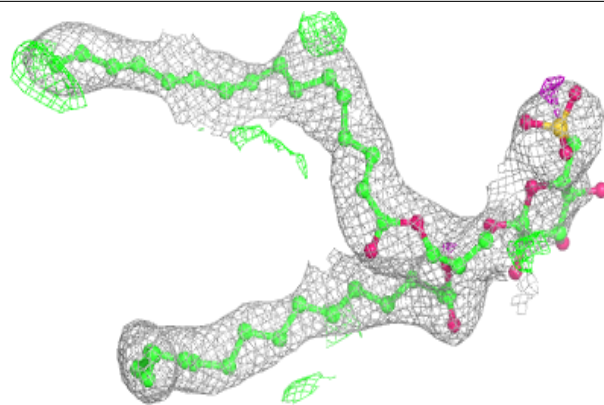
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



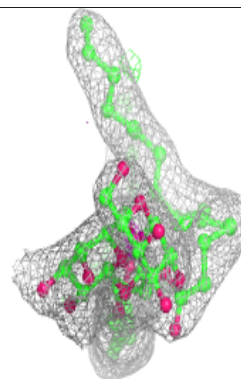
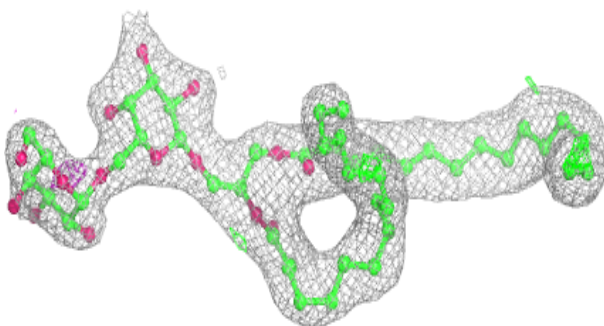
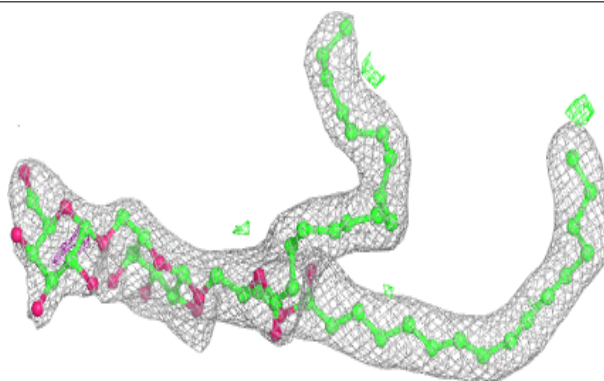


Electron density around SQD A 414:

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

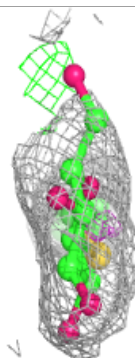
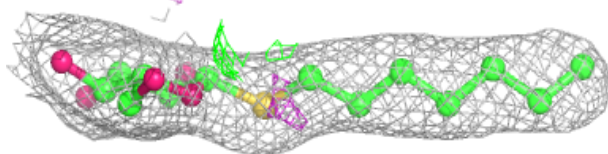
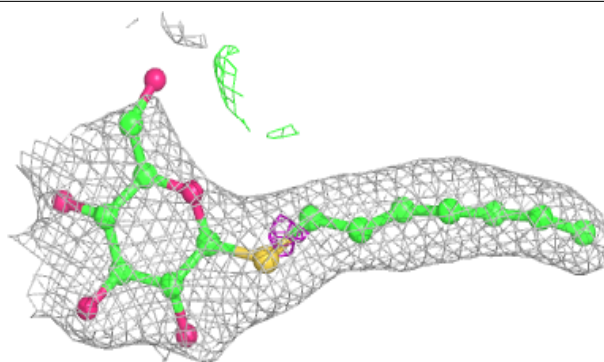
**Electron density around DGD H 102:**

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

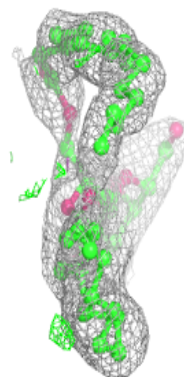
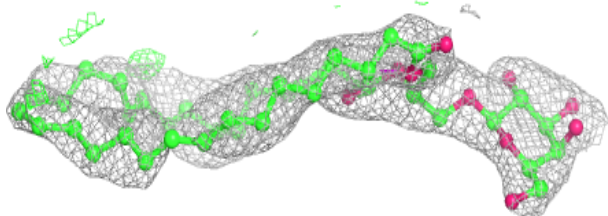
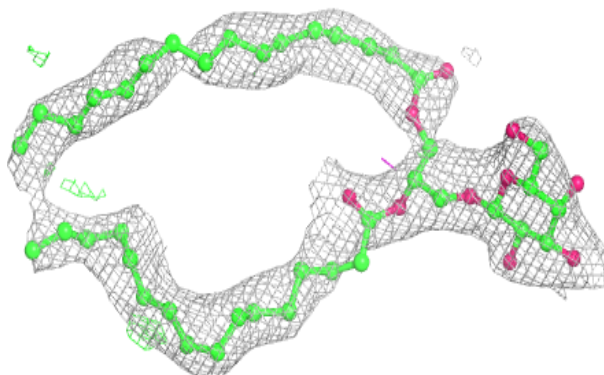


Electron density around HTG B 632:

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

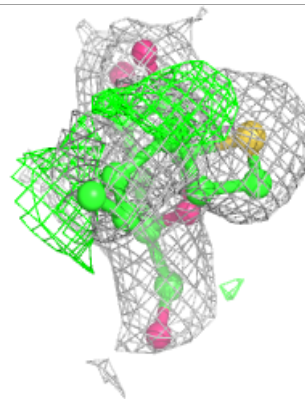
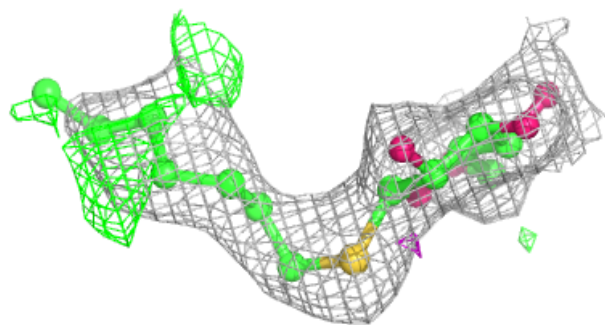
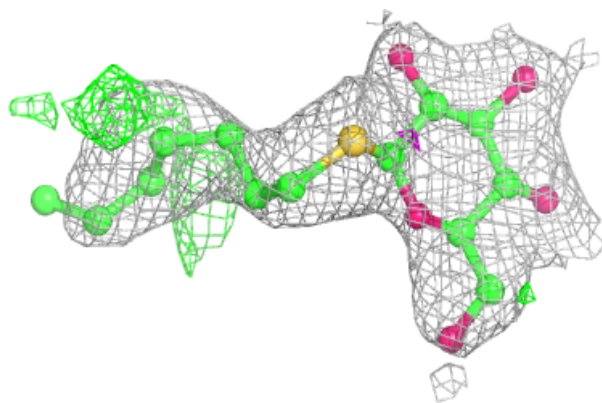
**Electron density around LMG A 419:**

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

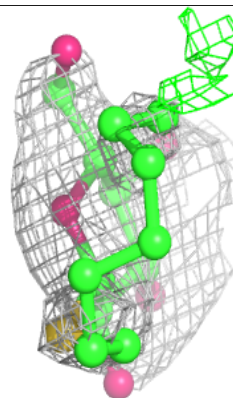
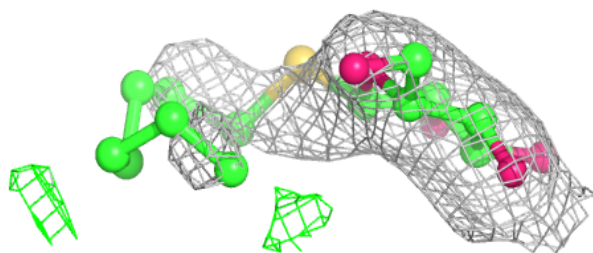
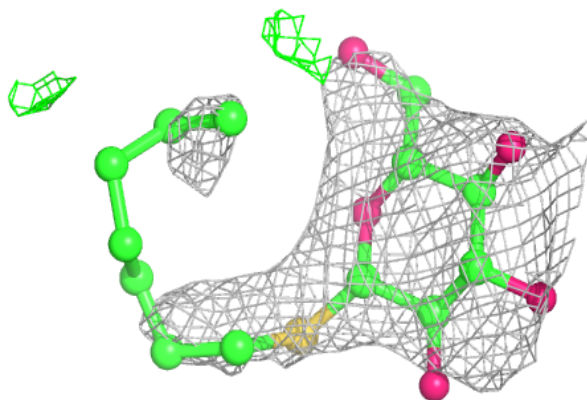


Electron density around HTG B 624:

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

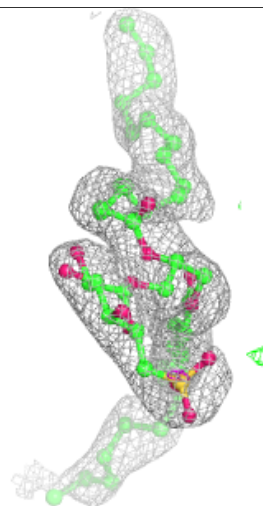
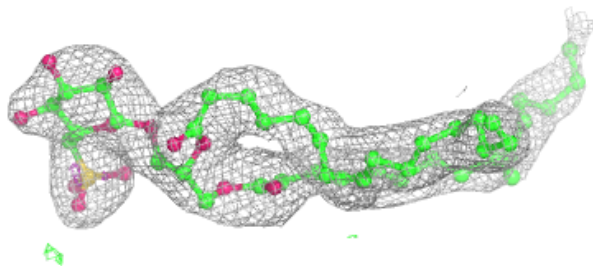
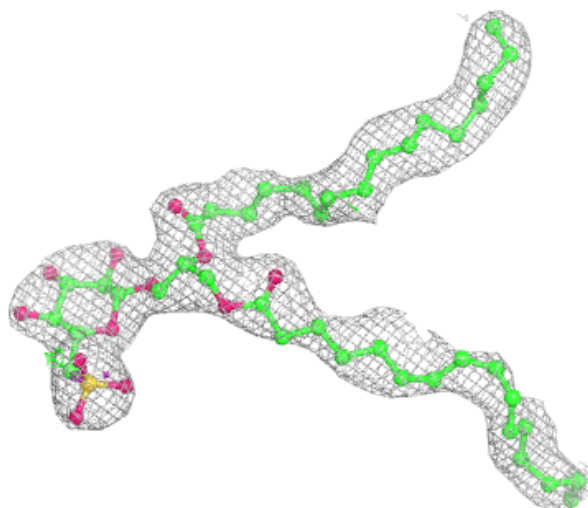
**Electron density around HTG V 203:**

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



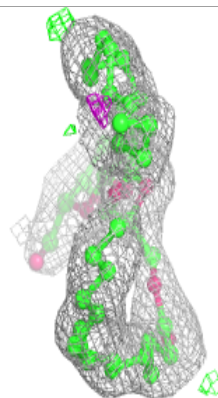
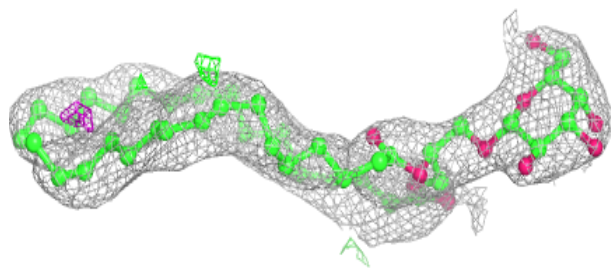
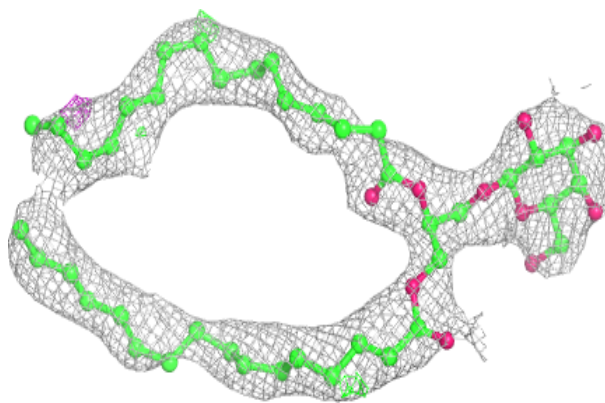
Electron density around SQD a 410:

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

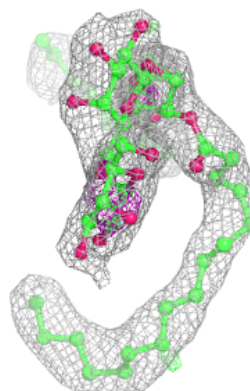
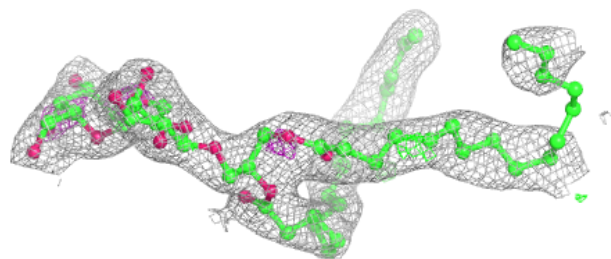
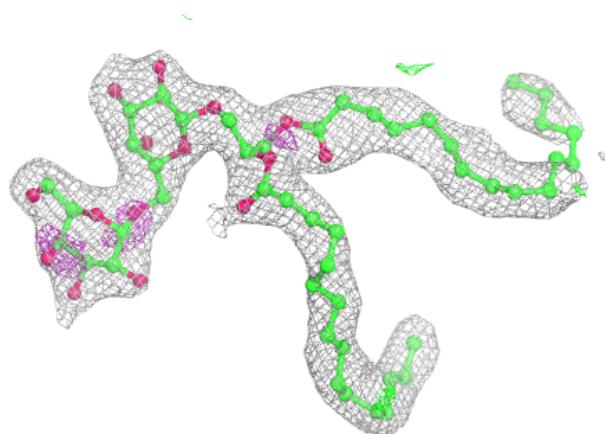


Electron density around LMG a 411:

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

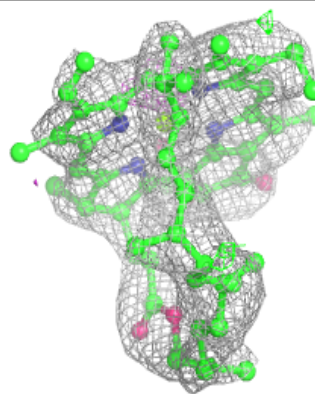
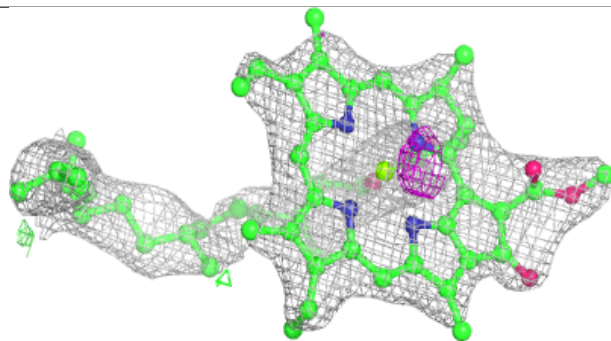
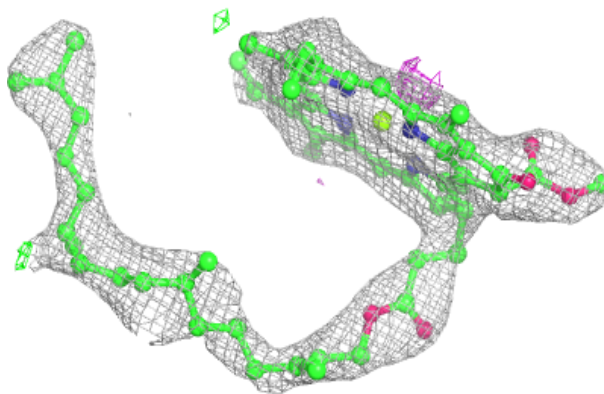
**Electron density around DGD c 917:**

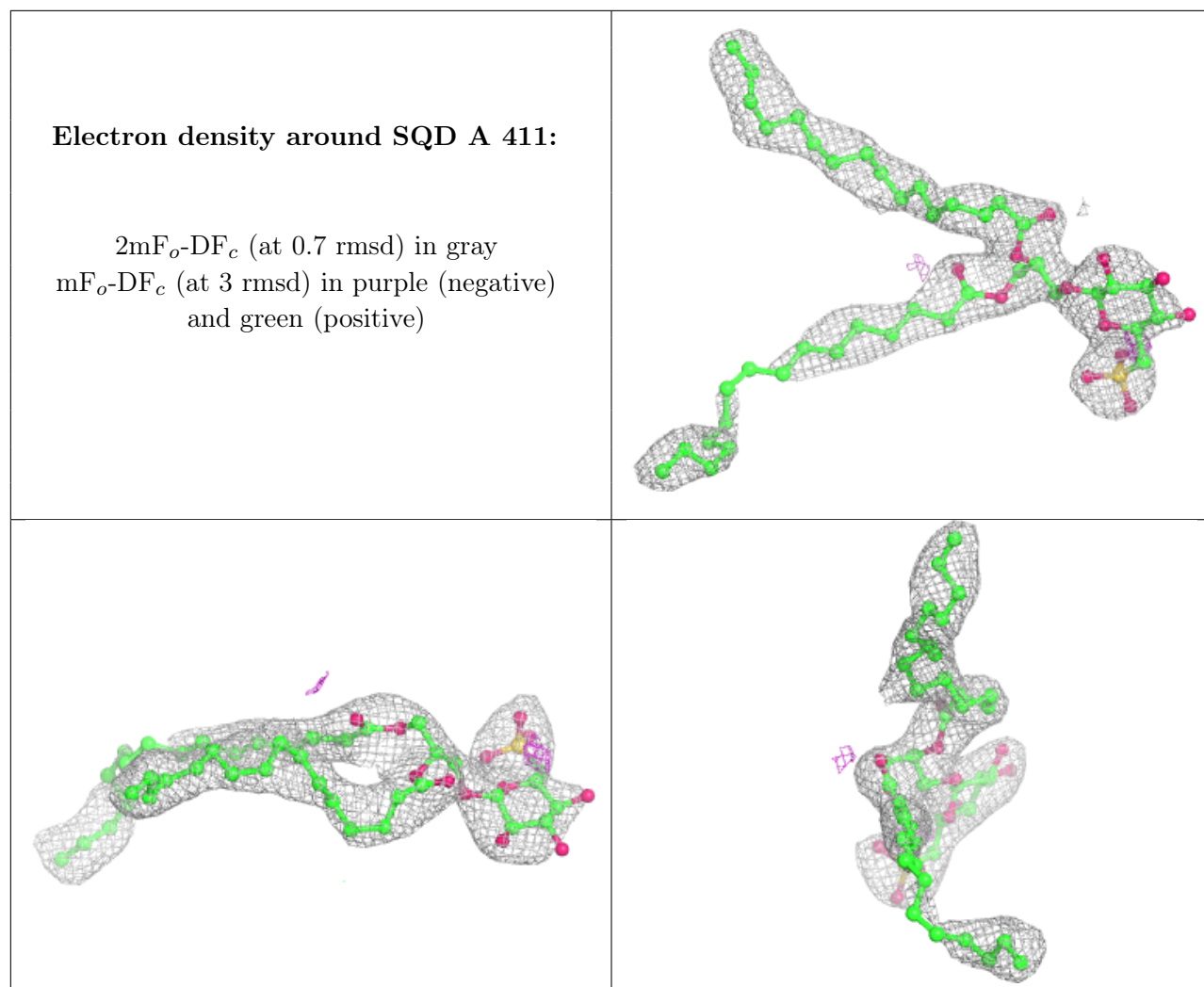
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 914:

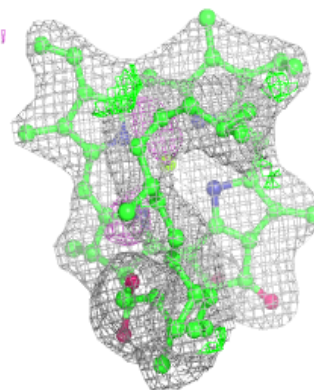
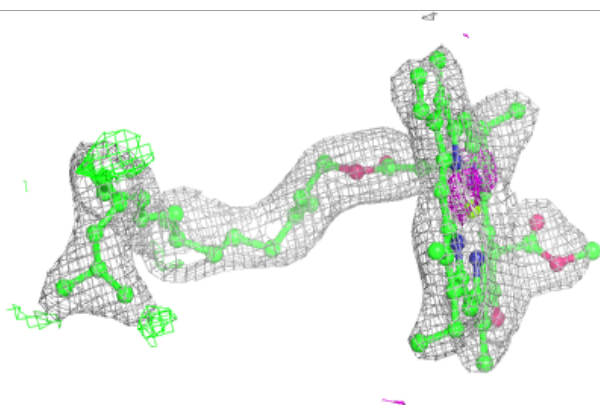
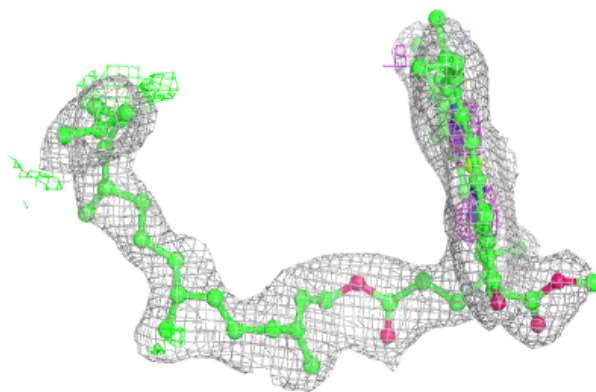
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



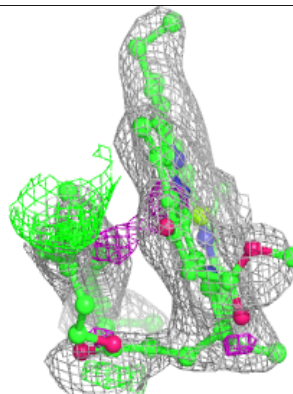
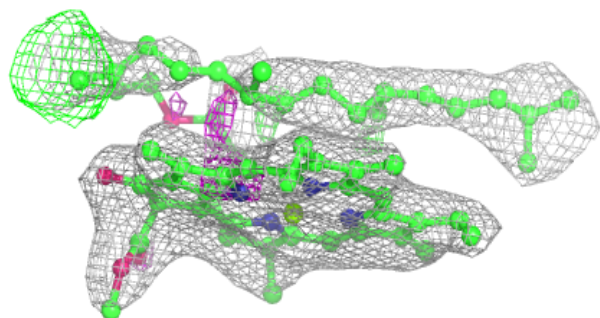
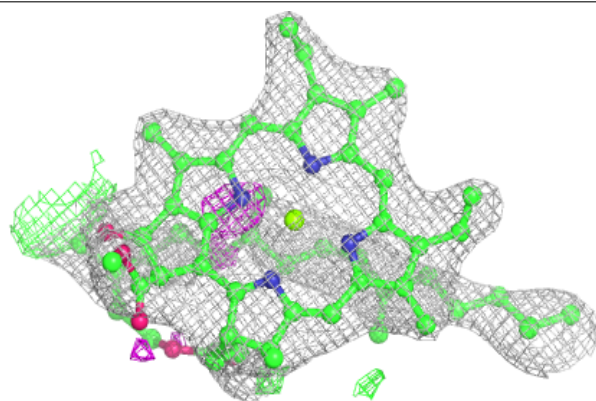


Electron density around CLA c 907:

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

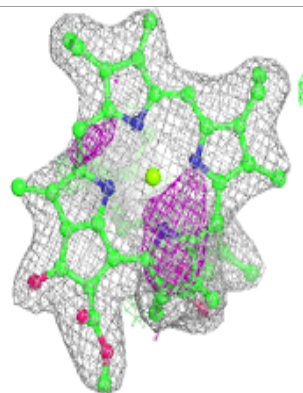
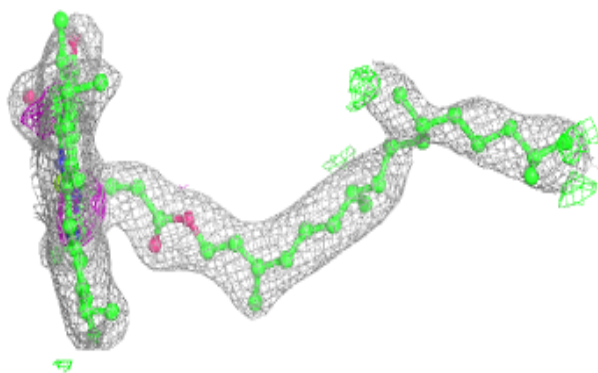
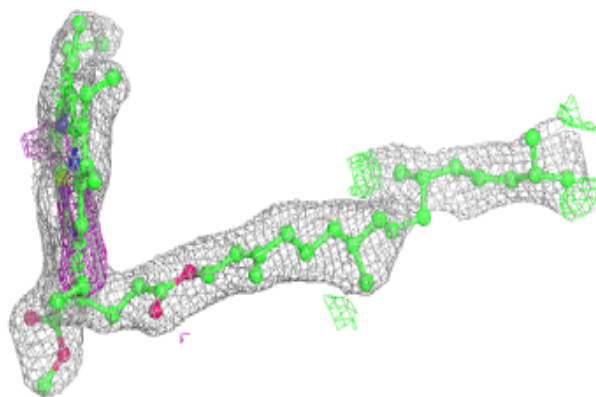
**Electron density around CLA B 602:**

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

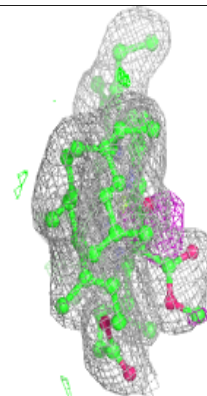
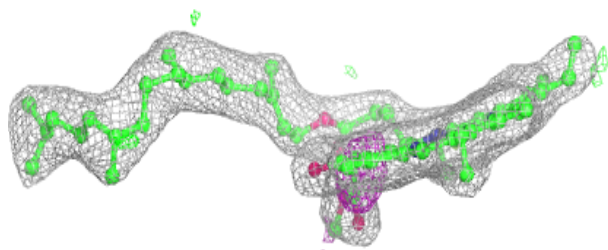
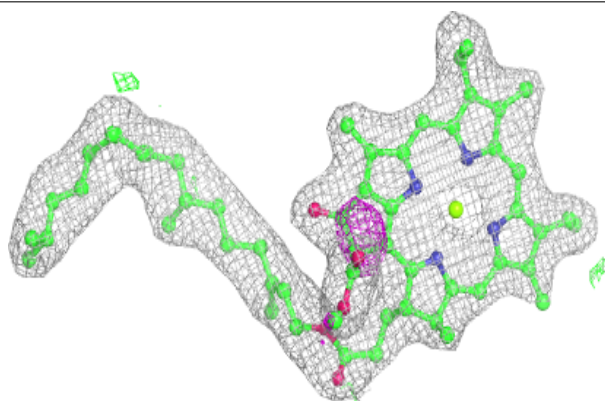


Electron density around CLA B 607:

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

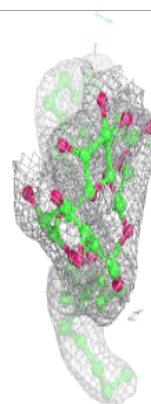
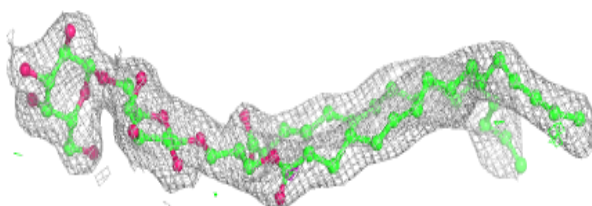
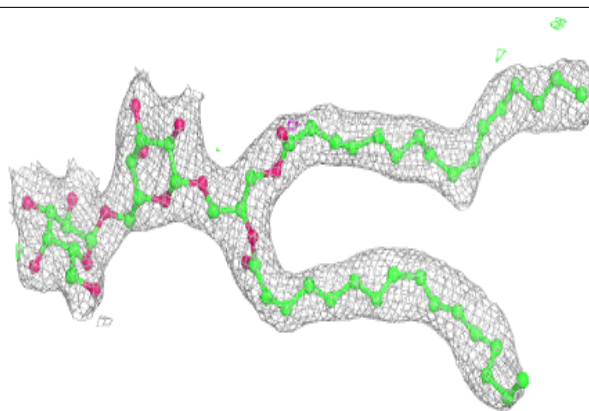
**Electron density around CLA b 607:**

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

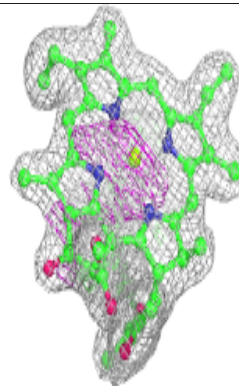
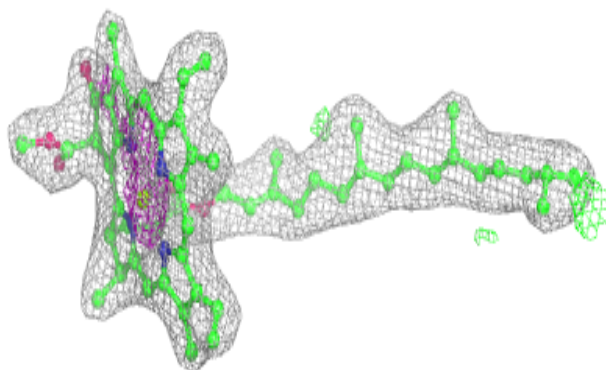
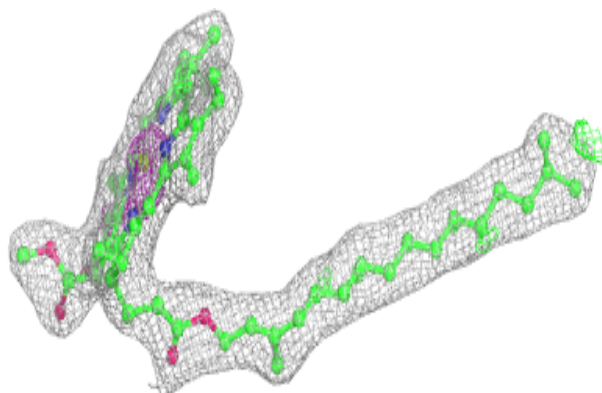


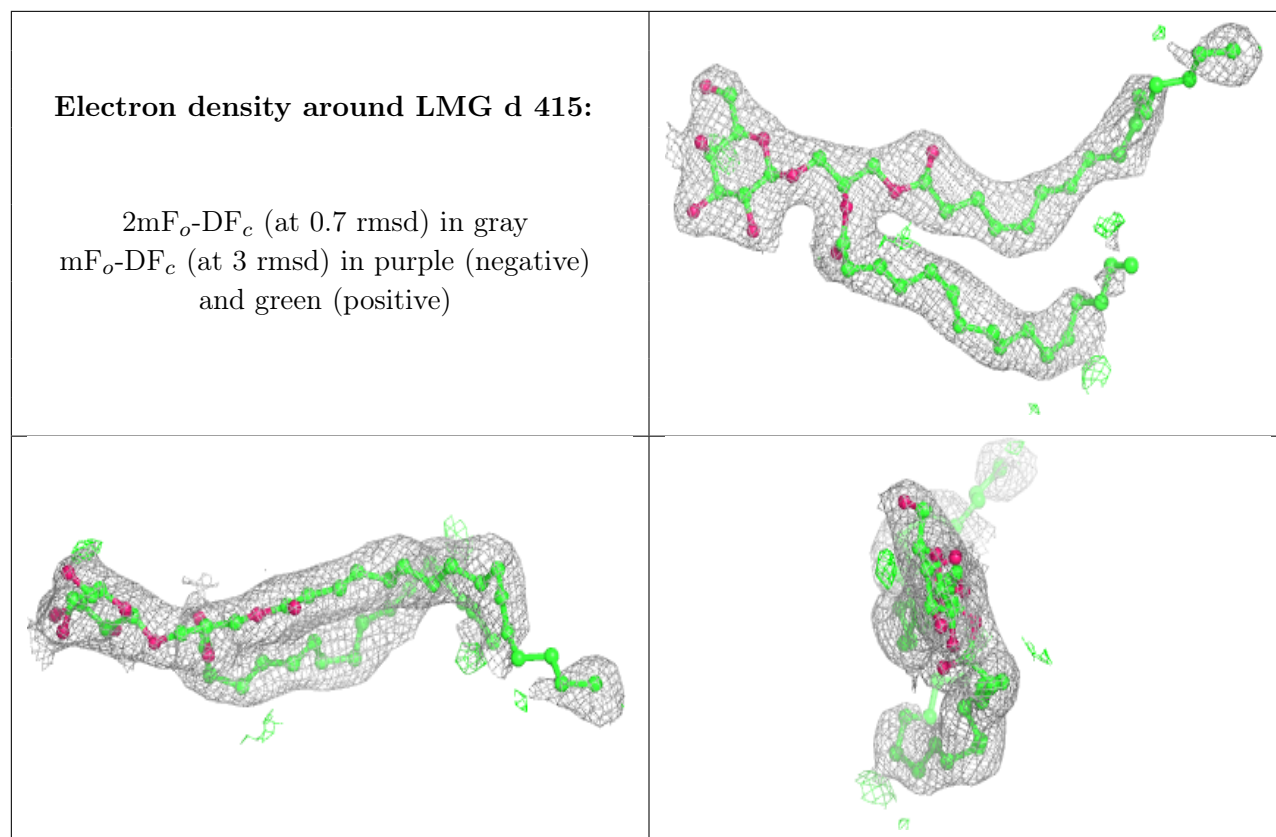
Electron density around DGD c 918:

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

**Electron density around CLA b 612:**

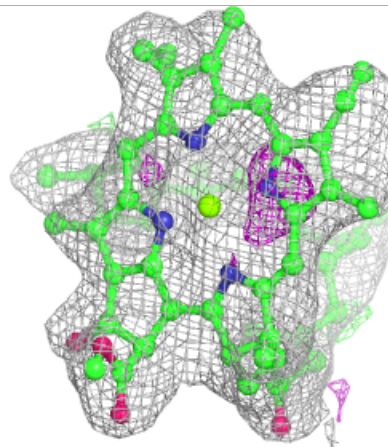
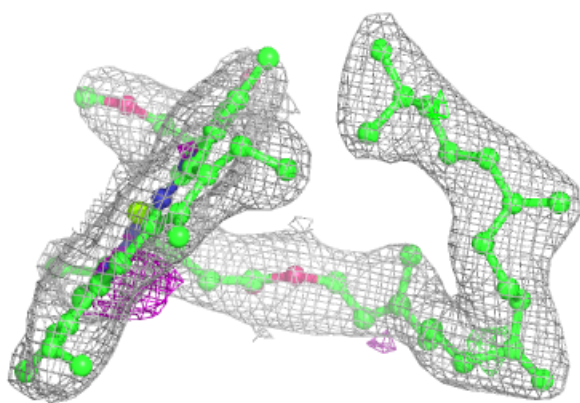
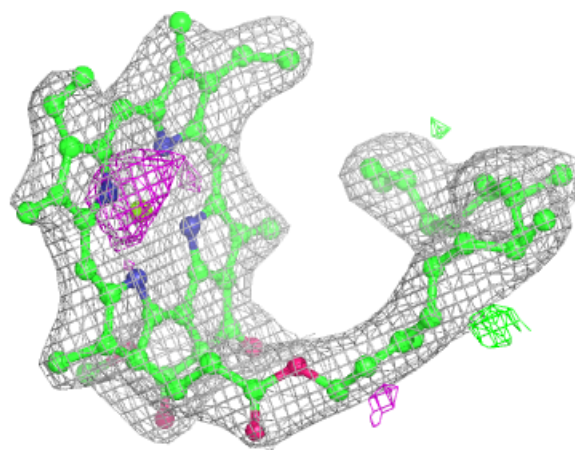
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

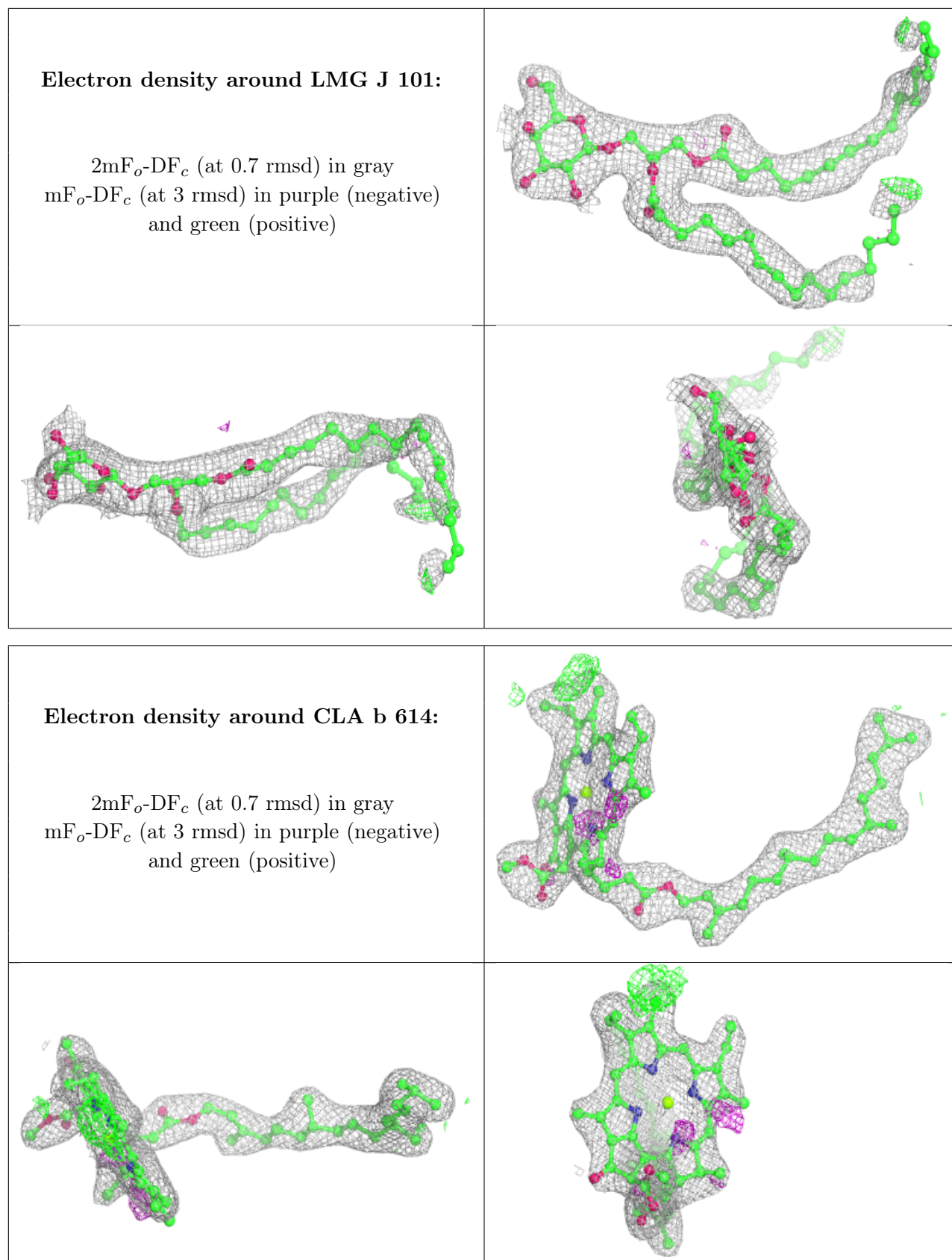




Electron density around CLA c 904:

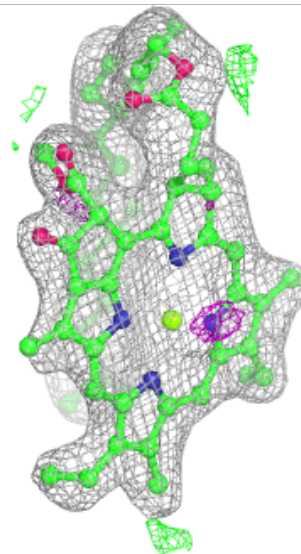
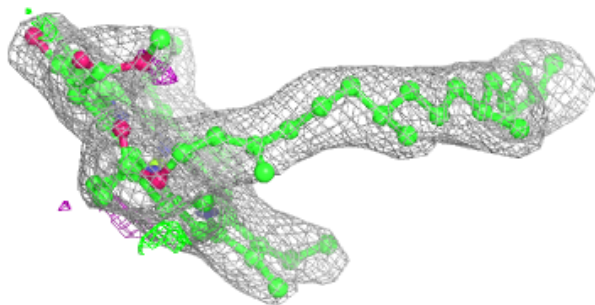
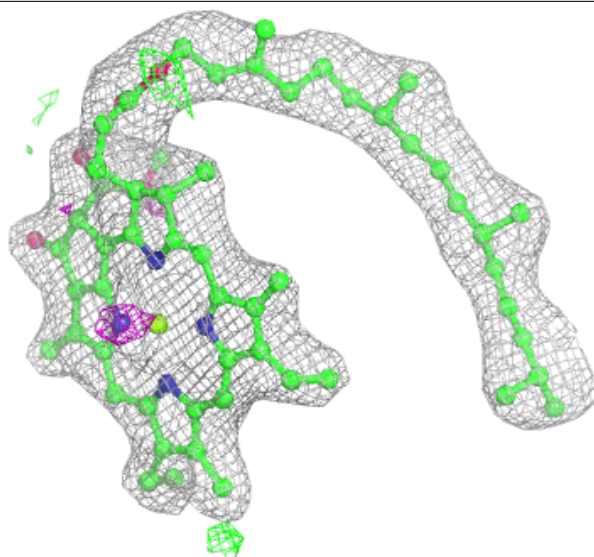
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





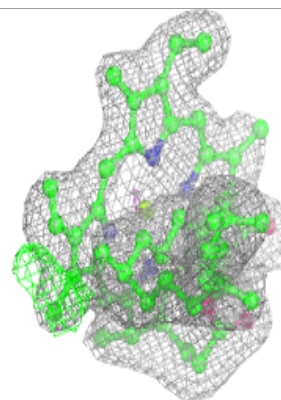
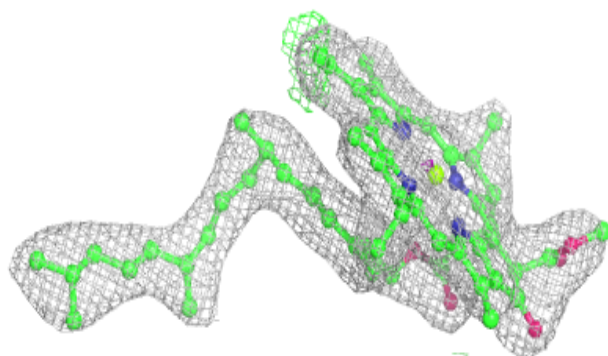
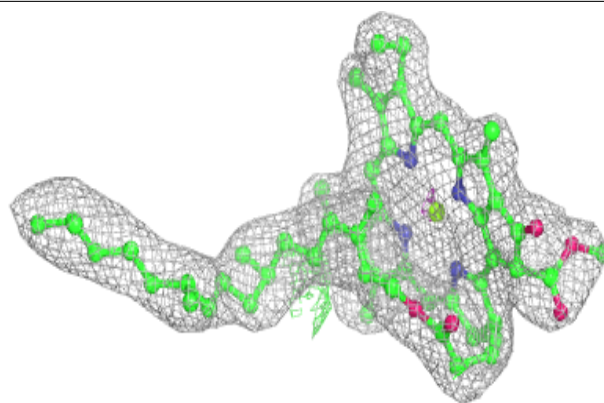
Electron density around CLA c 908:

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



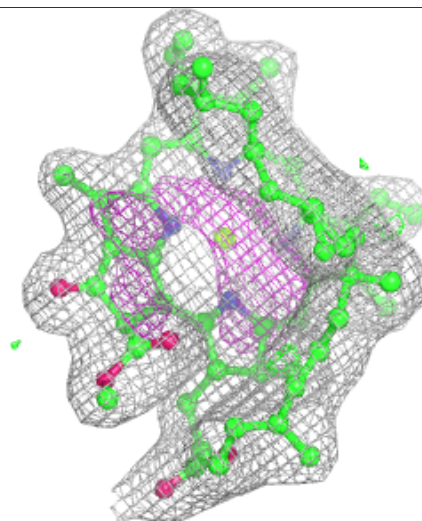
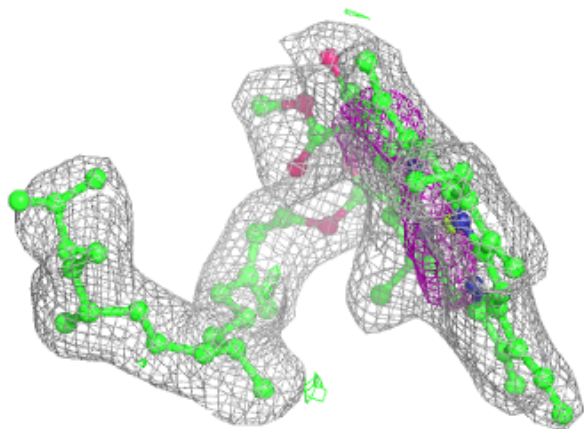
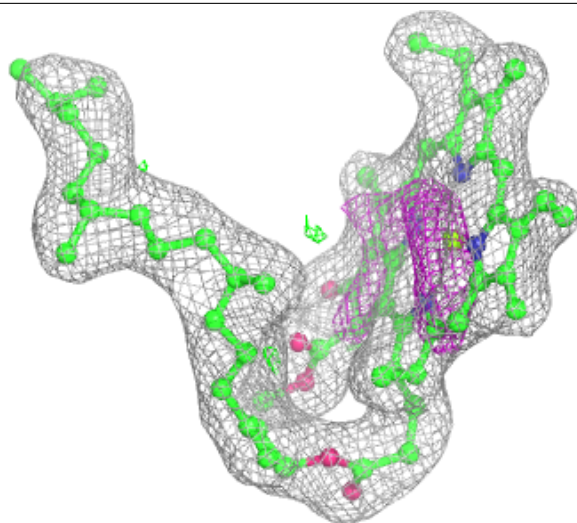
Electron density around CLA c 906:

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



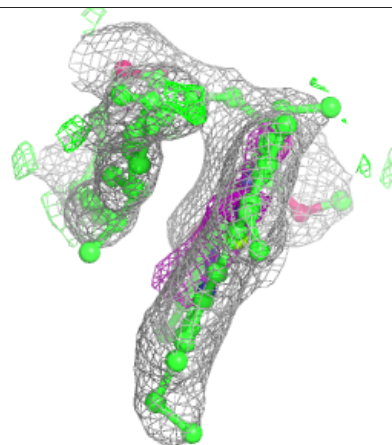
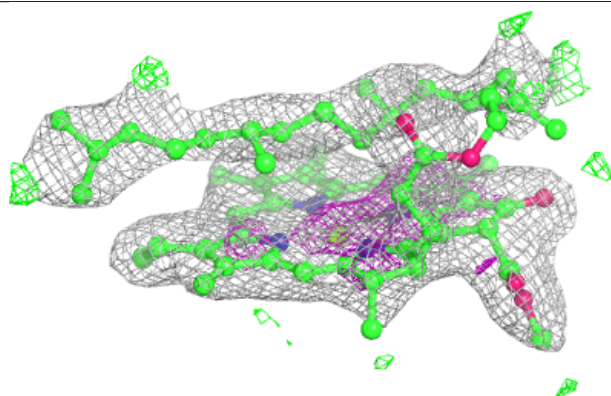
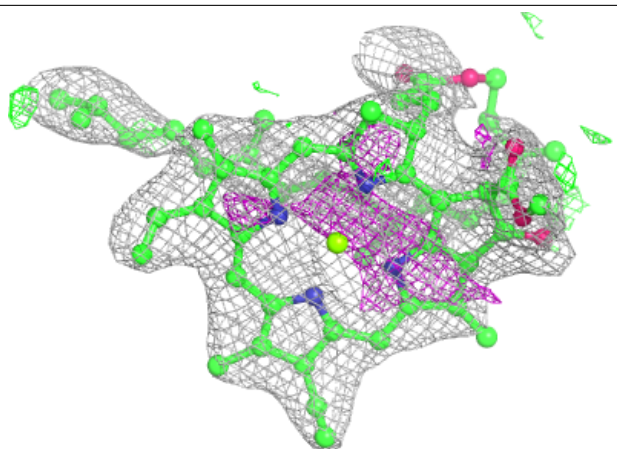
Electron density around CLA B 614:

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

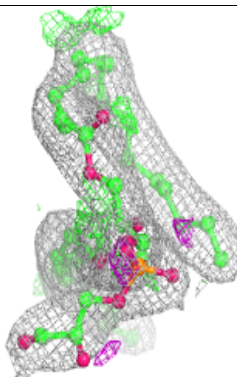
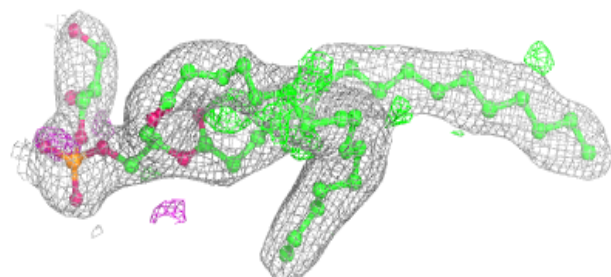
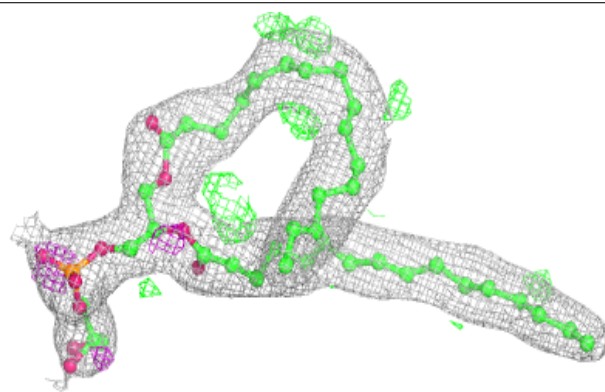


Electron density around CLA b 606:

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

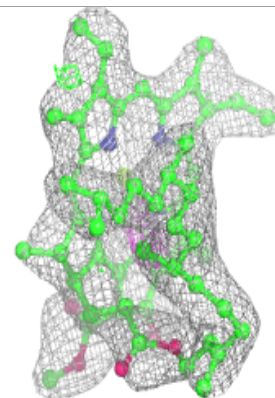
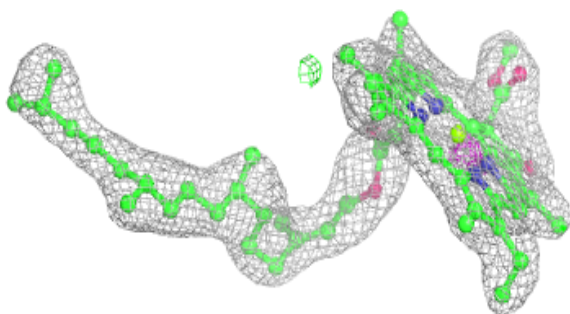
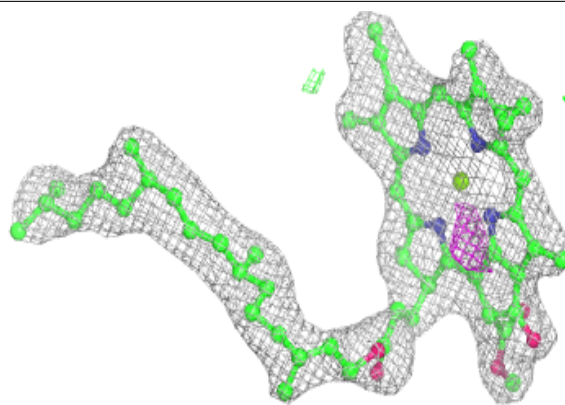
**Electron density around LHG B 635:**

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

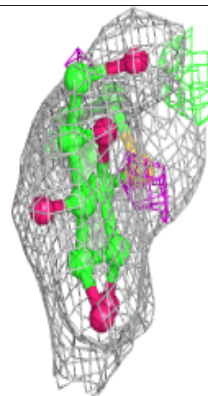
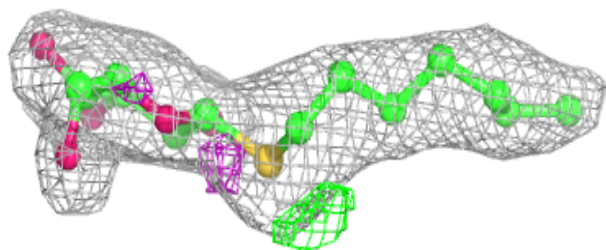
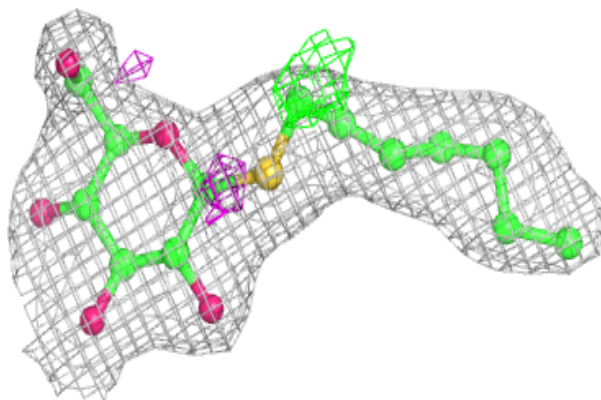


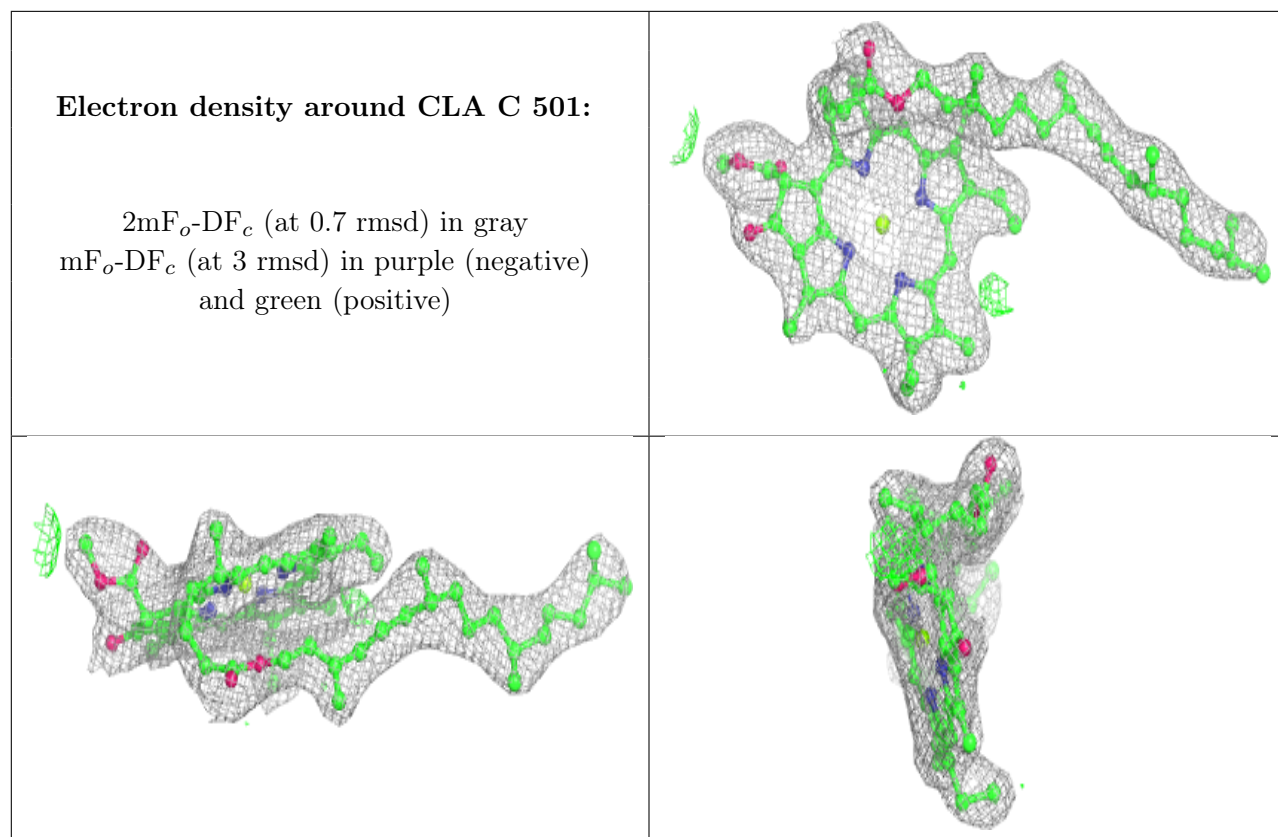
Electron density around CLA C 511:

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

**Electron density around HTG B 623:**

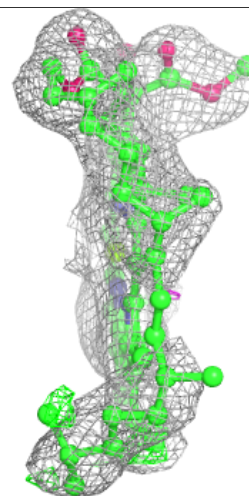
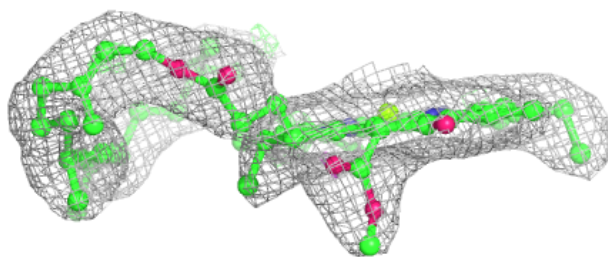
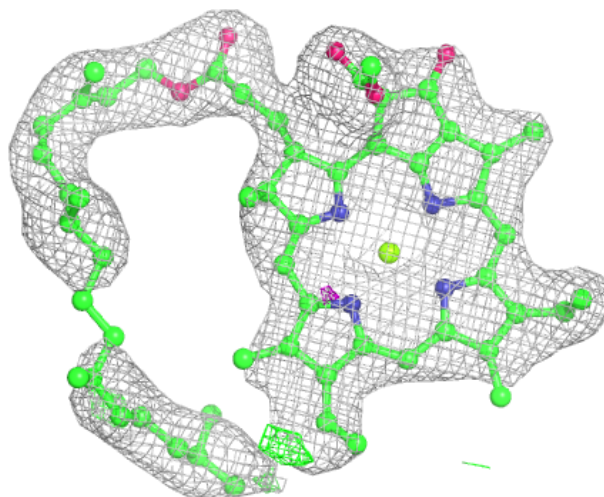
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





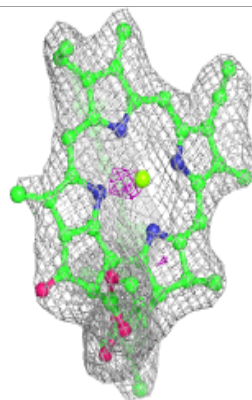
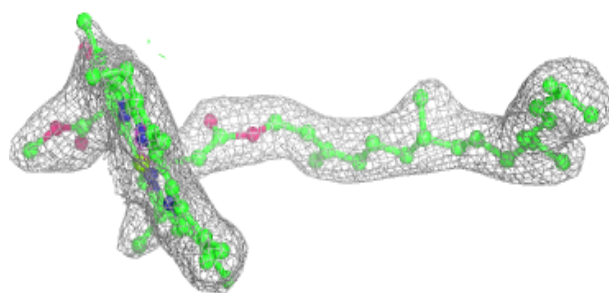
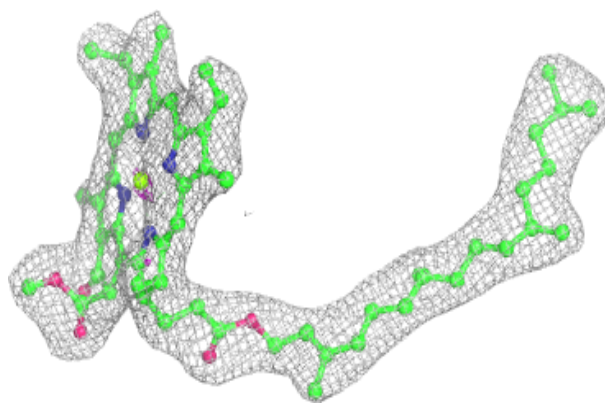
Electron density around CLA C 512:

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

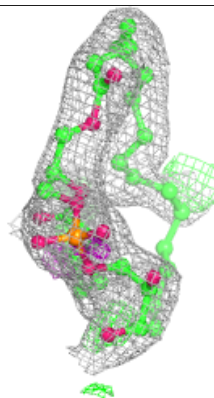
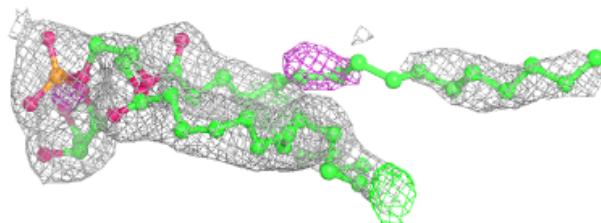
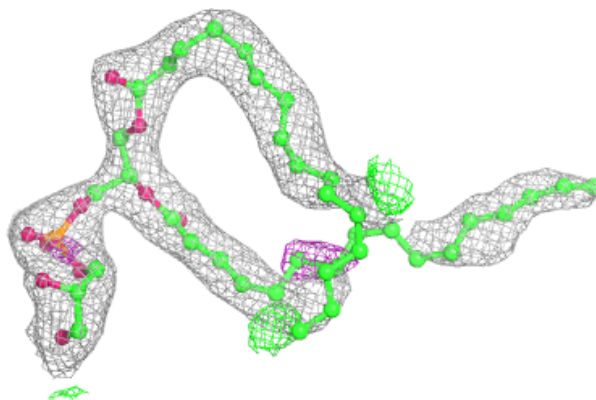


Electron density around CLA B 610:

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

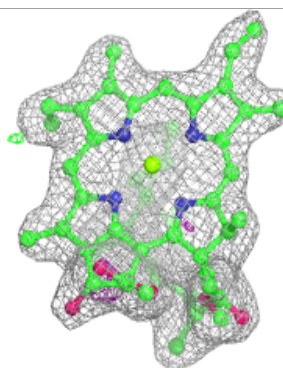
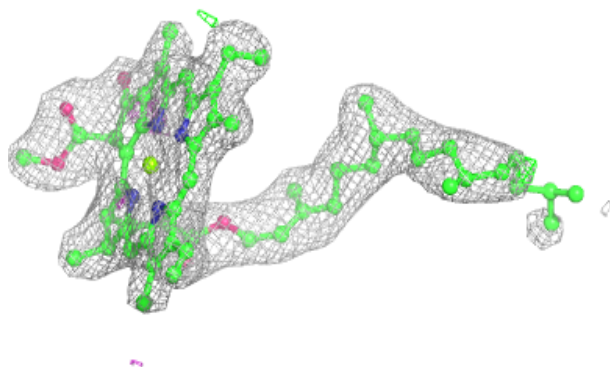
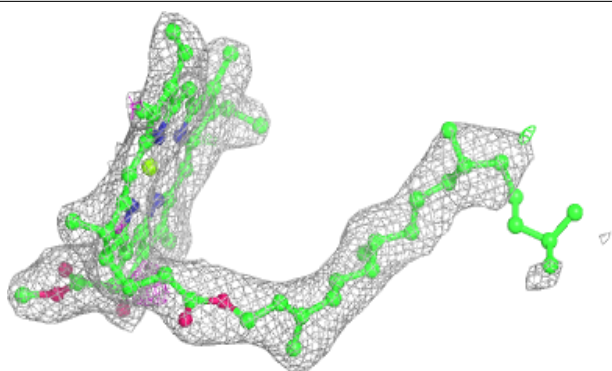
**Electron density around LHG D 410:**

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

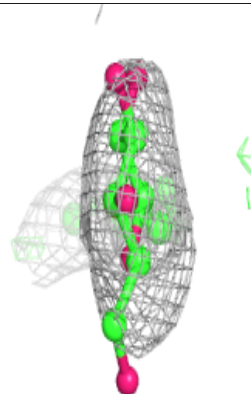
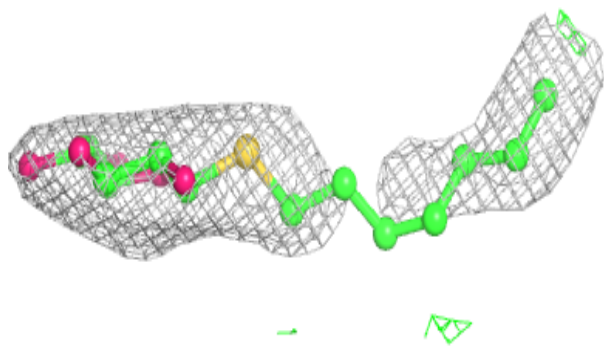
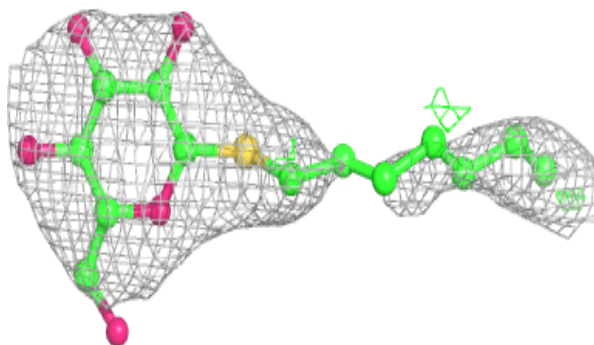


Electron density around CLA c 909:

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

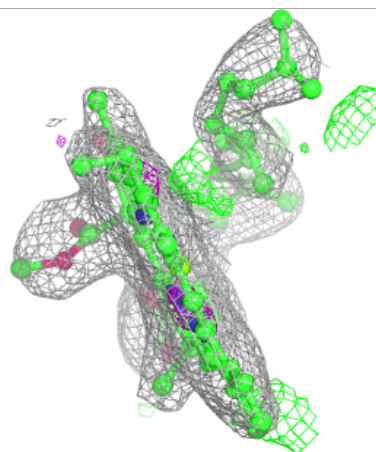
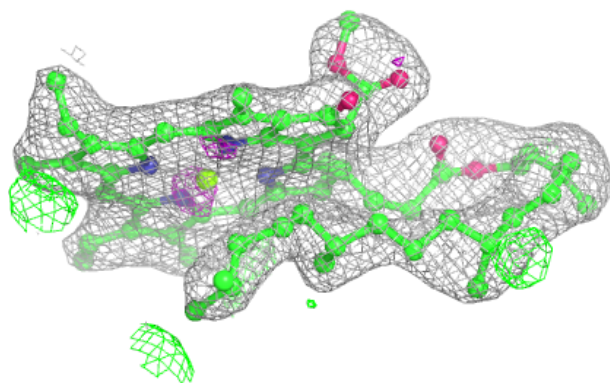
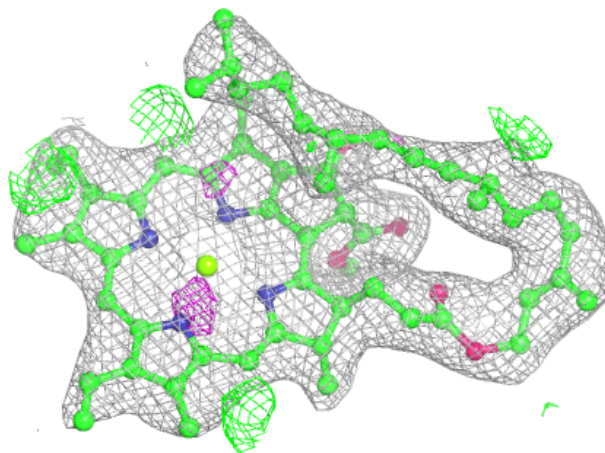
**Electron density around HTG C 521:**

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



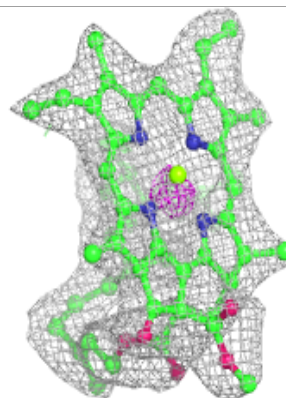
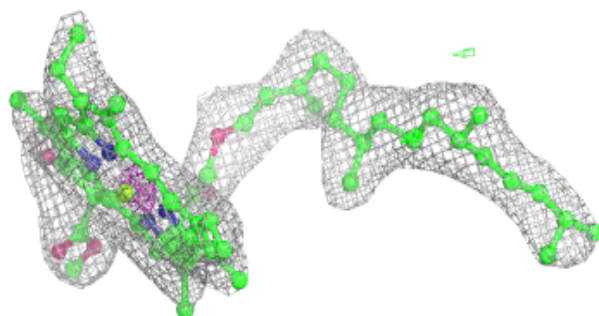
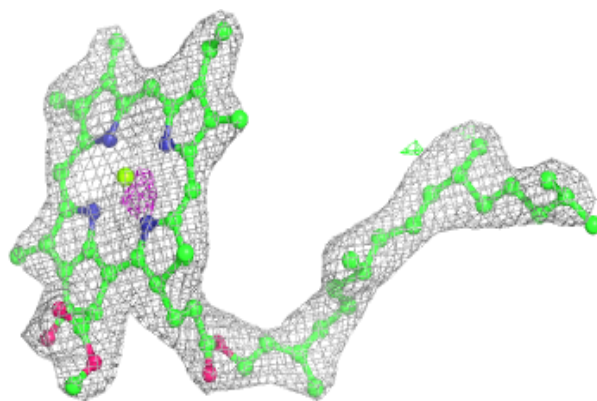
Electron density around CLA c 910:

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

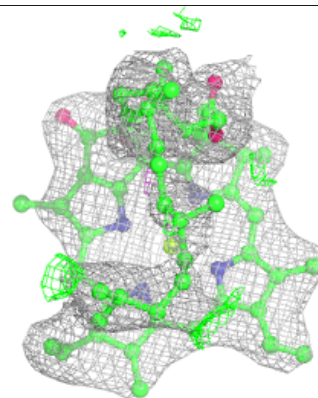
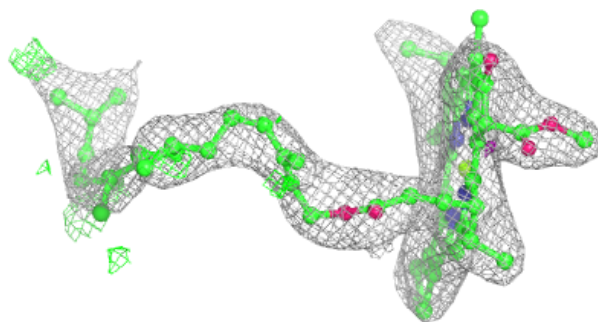
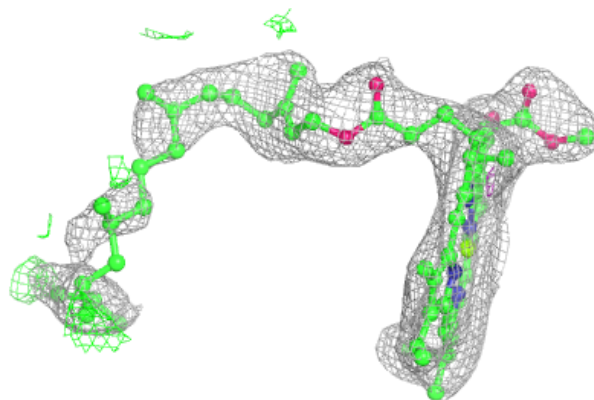


Electron density around CLA c 912:

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

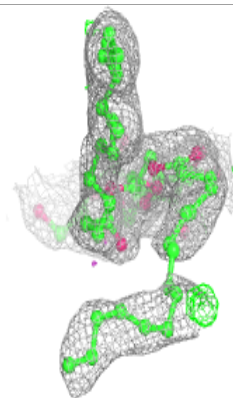
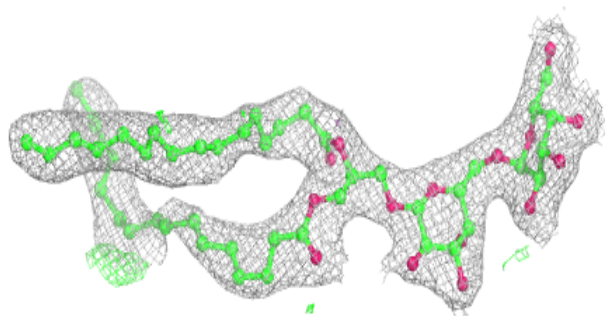
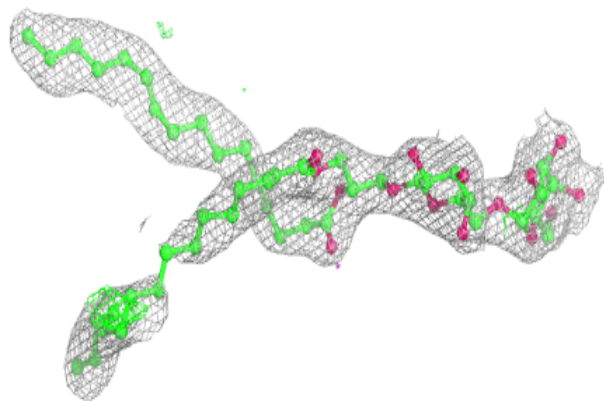
**Electron density around CLA C 506:**

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

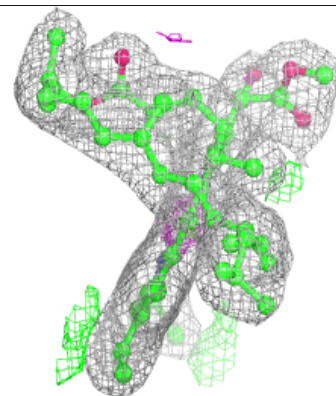
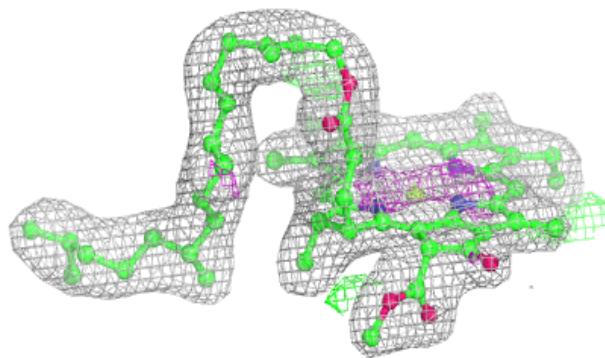
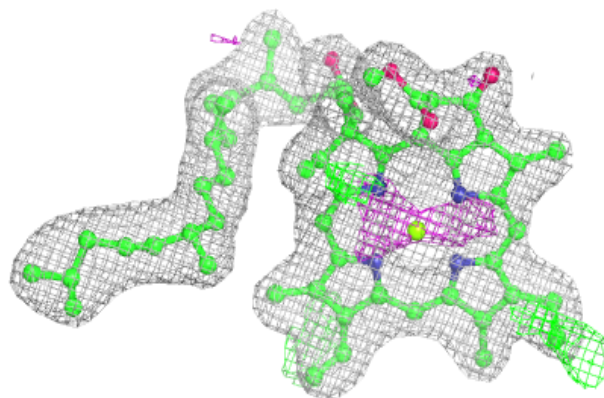


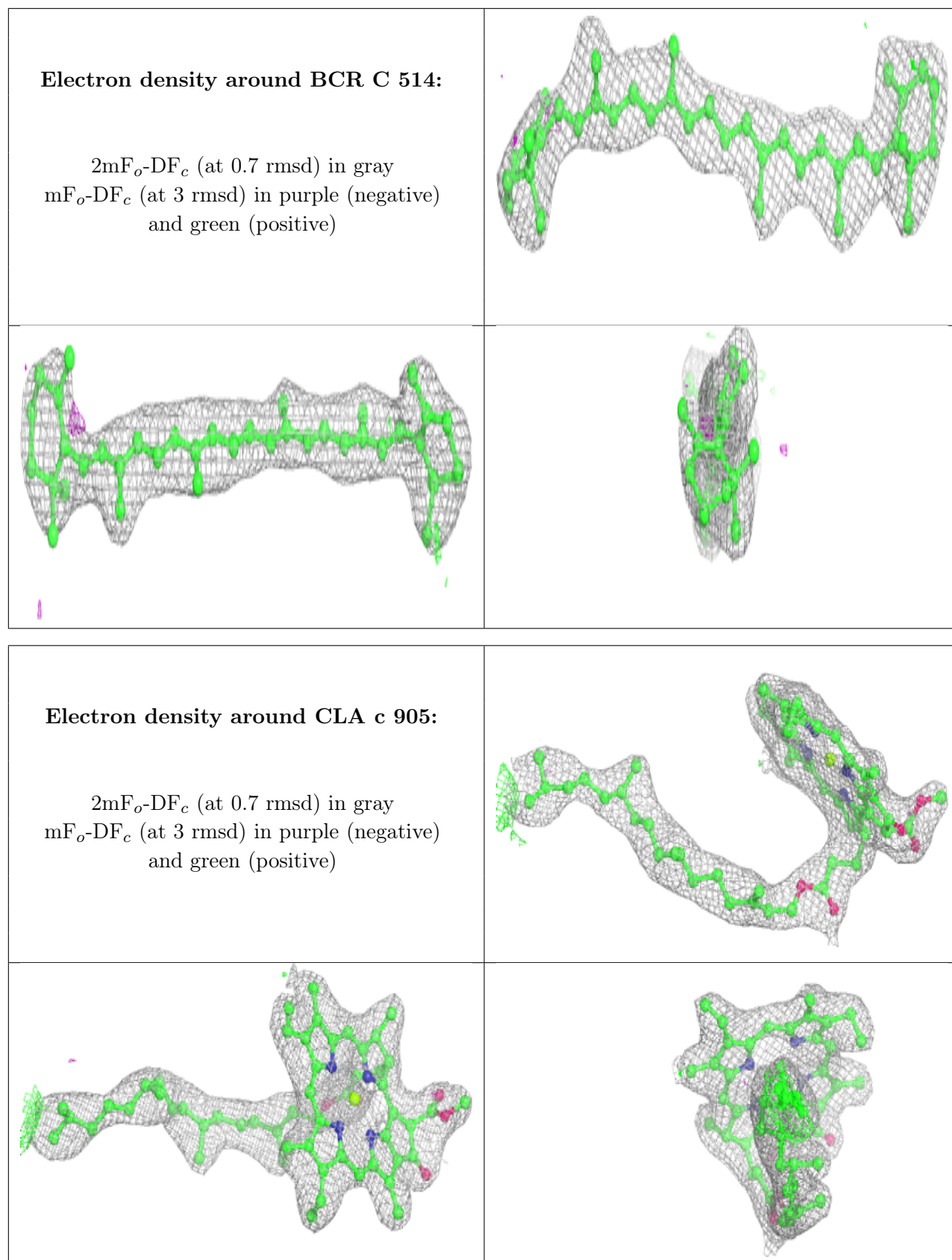
Electron density around DGD c 916:

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

**Electron density around CLA d 404:**

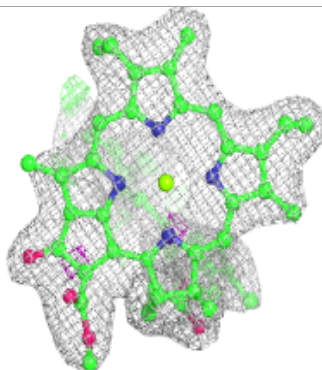
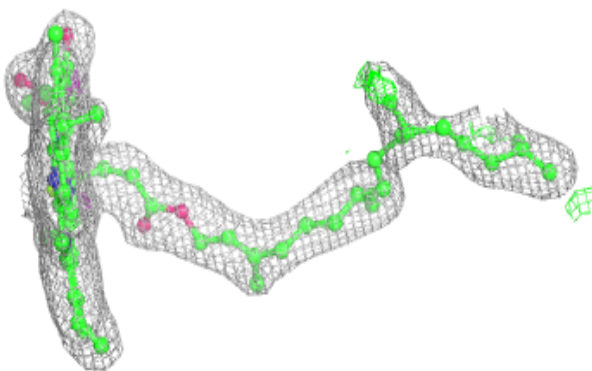
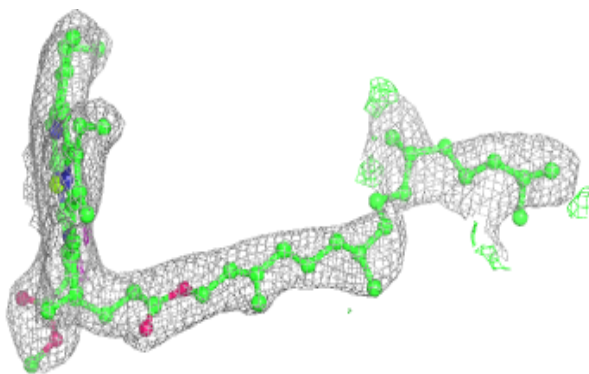
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





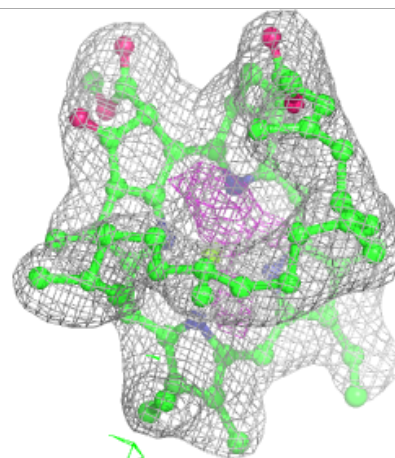
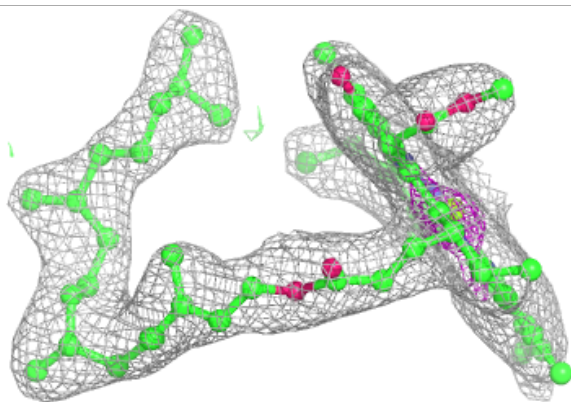
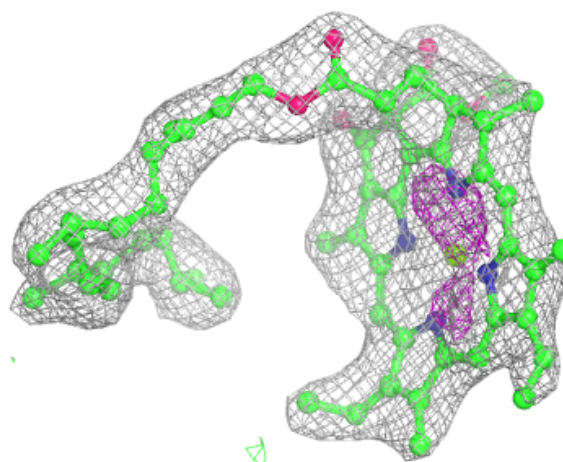
Electron density around CLA b 611:

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



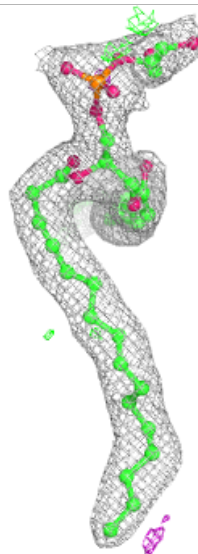
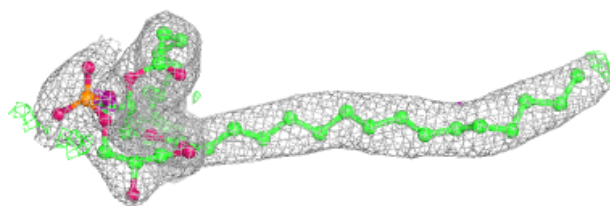
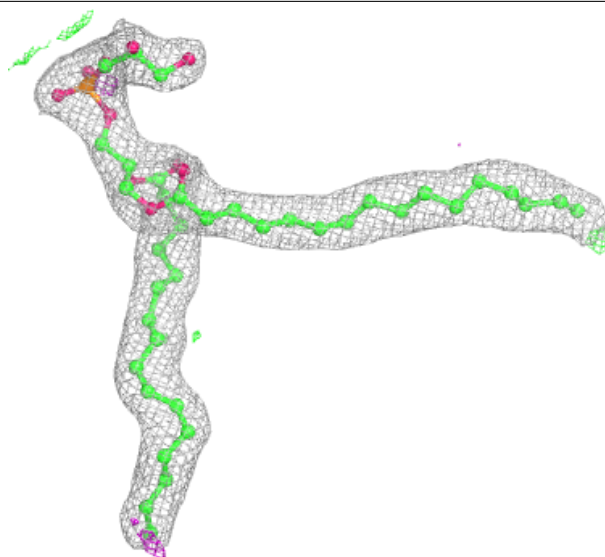
Electron density around CLA C 503:

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



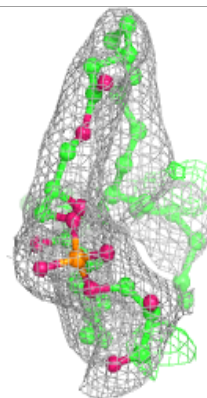
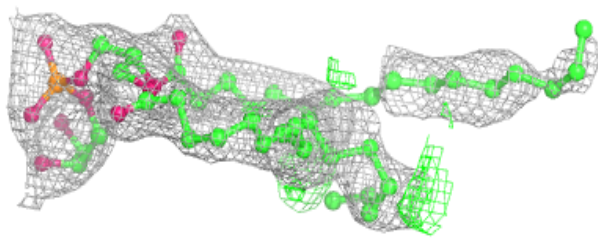
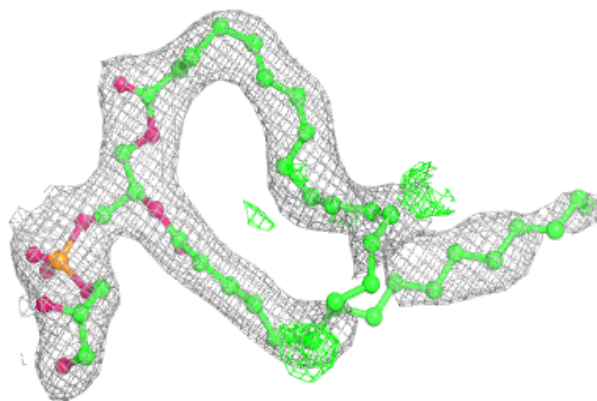
Electron density around LHG b 635:

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

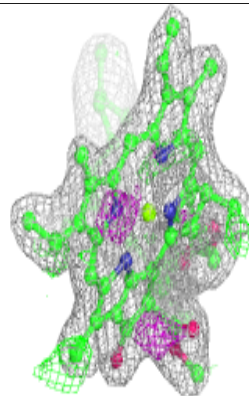
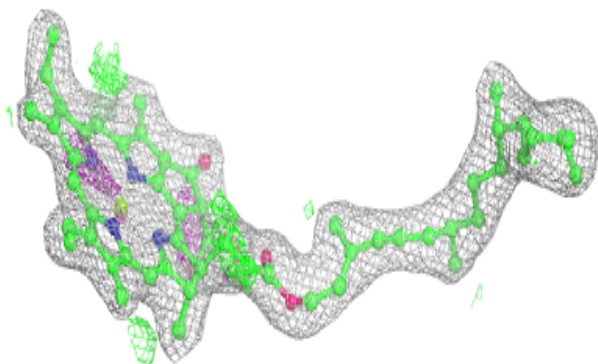
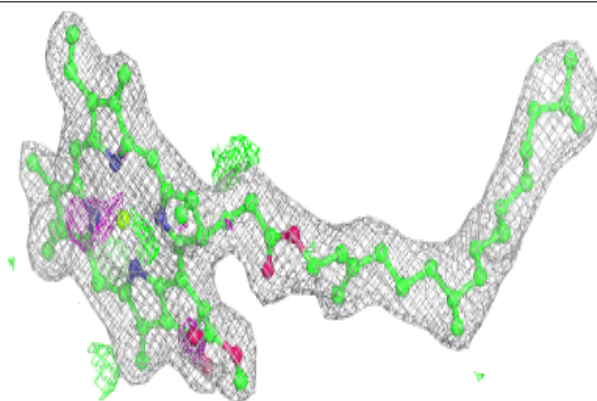


Electron density around LHG d 411:

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

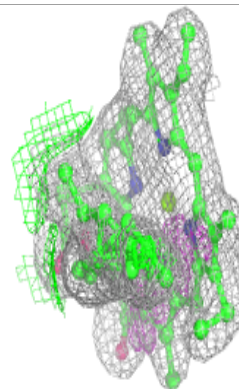
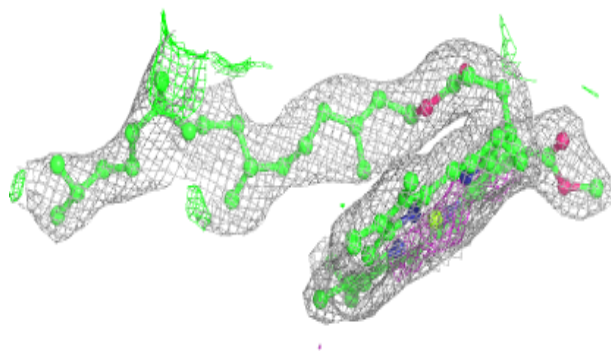
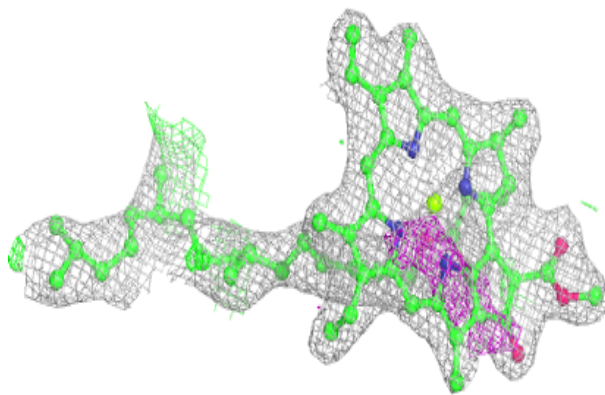
**Electron density around CLA A 405:**

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

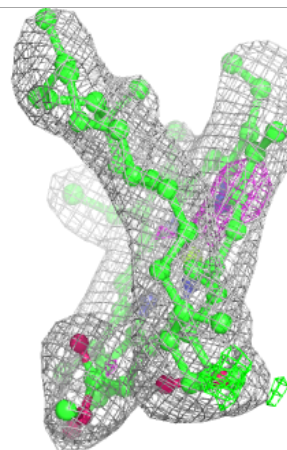
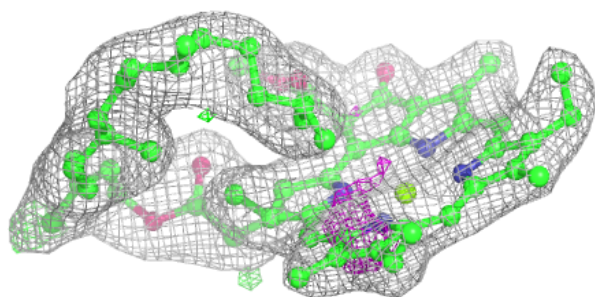
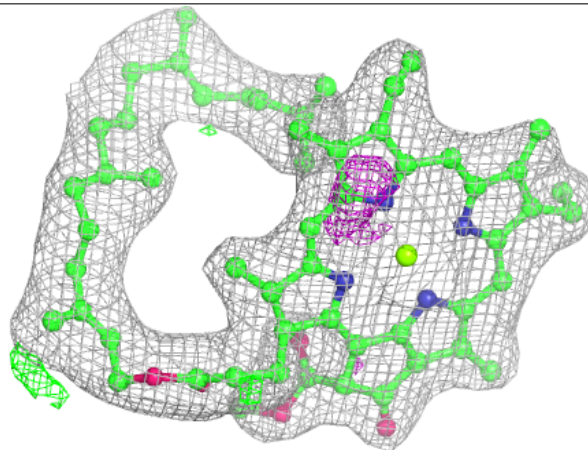


Electron density around CLA b 619:

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

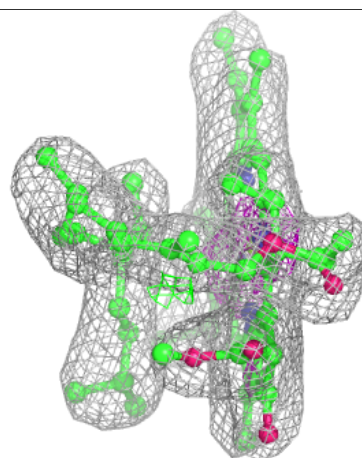
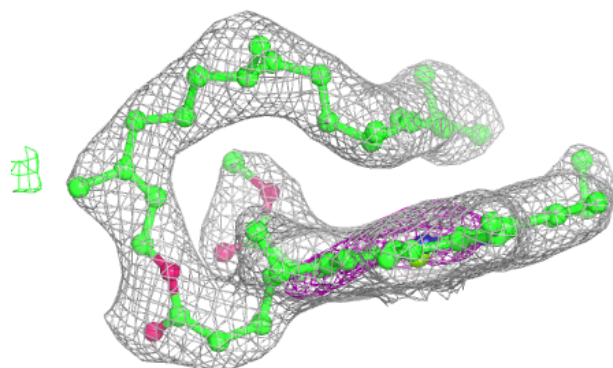
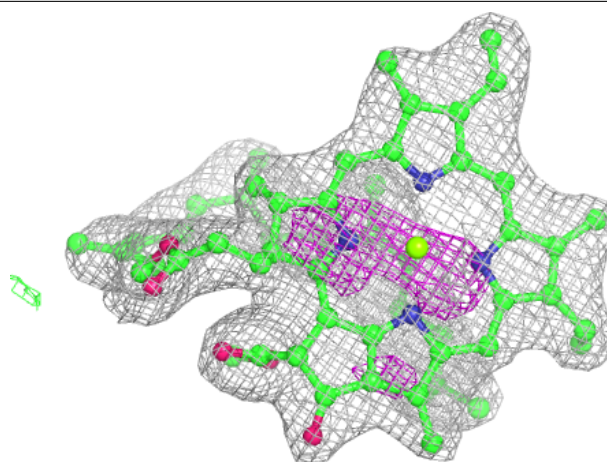
**Electron density around CLA b 620:**

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



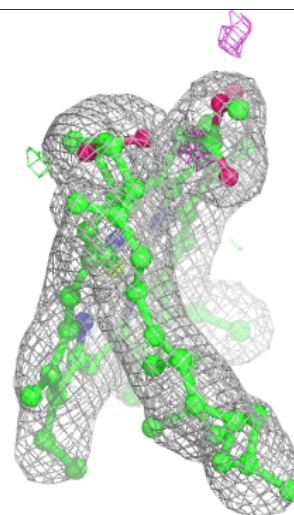
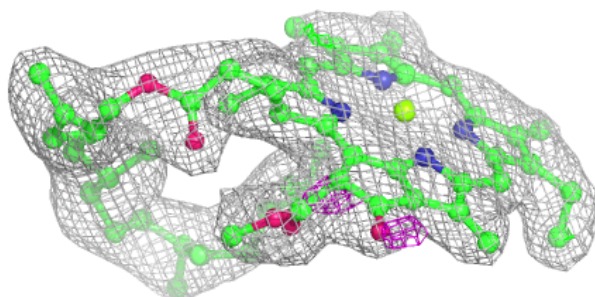
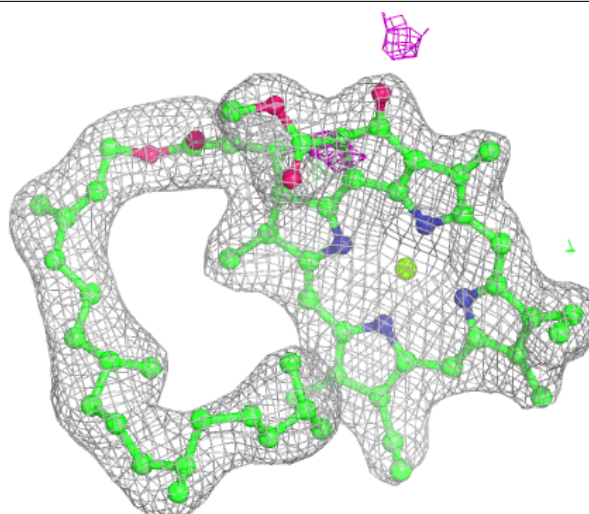
Electron density around CLA c 911:

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



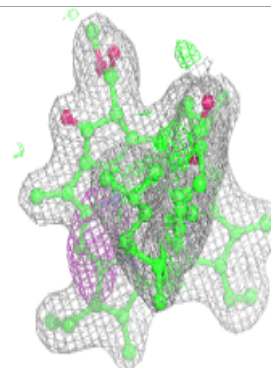
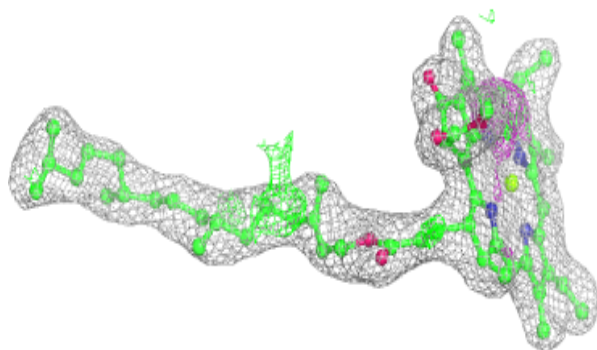
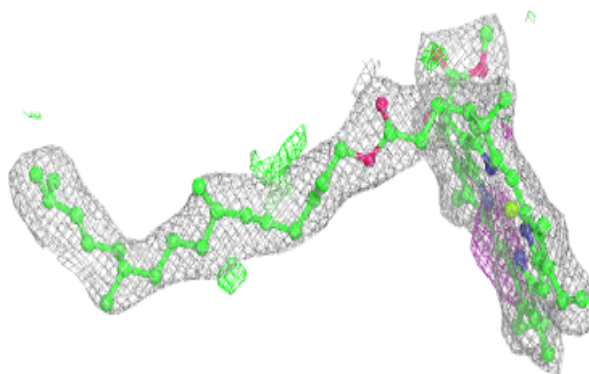
Electron density around CLA B 616:

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

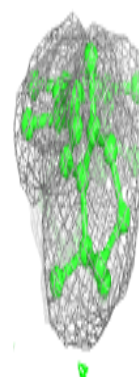
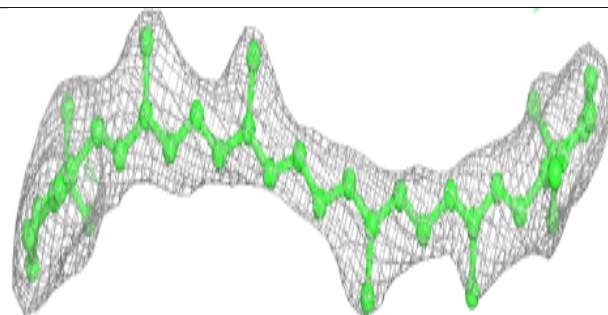
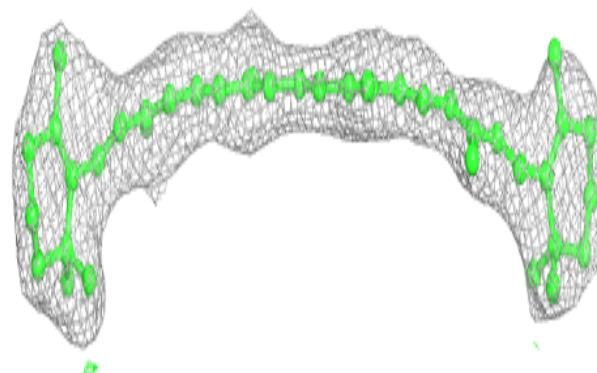


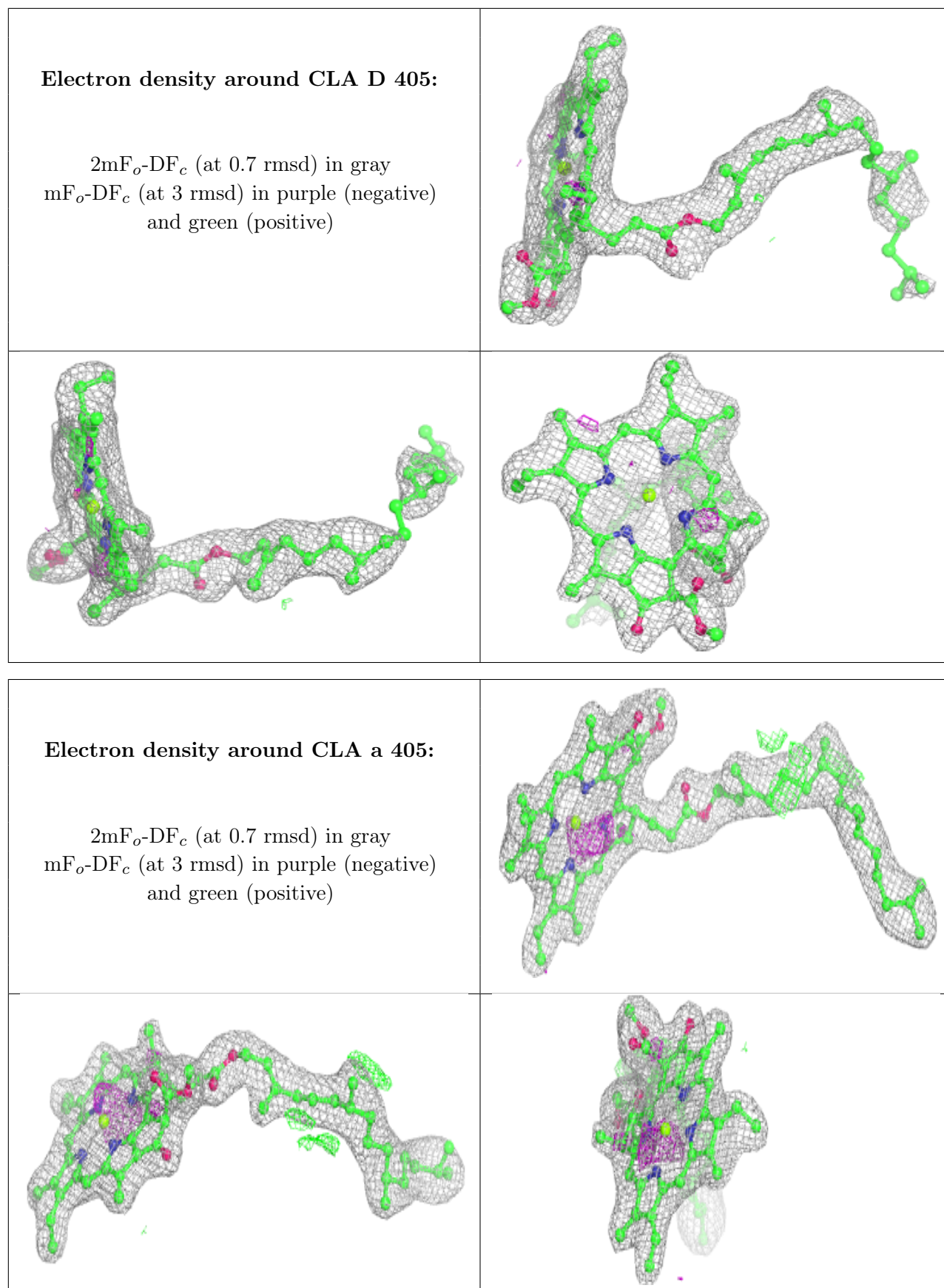
Electron density around CLA B 605:

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

**Electron density around BCR k 101:**

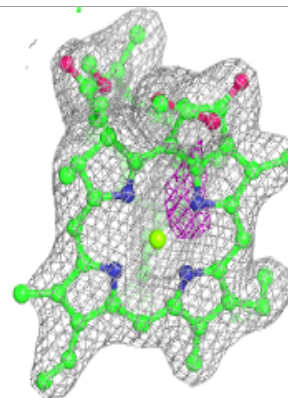
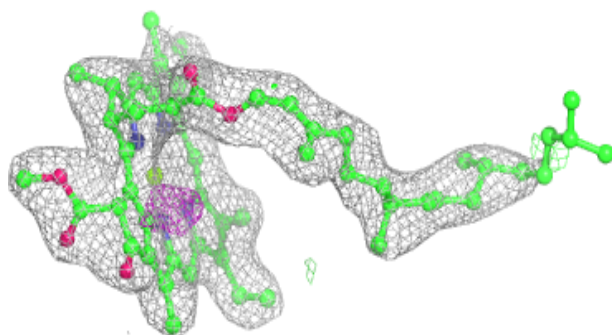
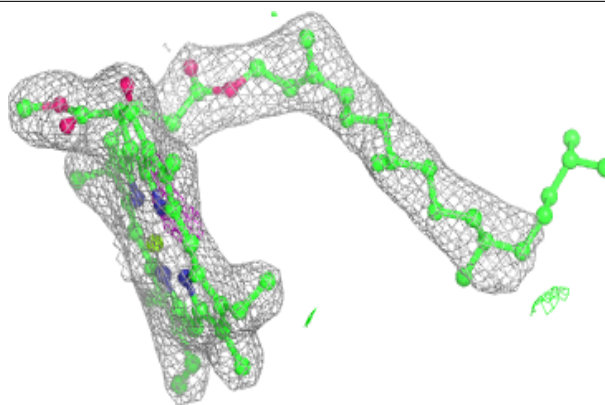
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



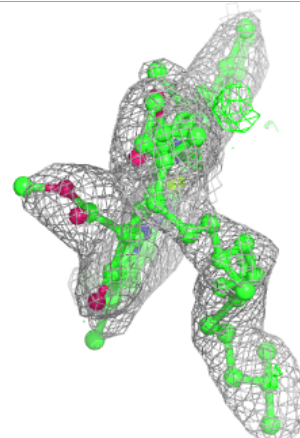
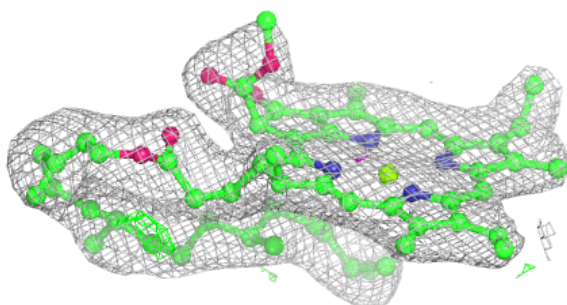
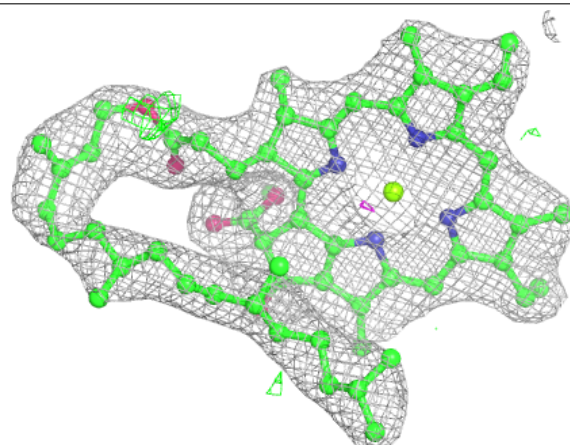


Electron density around CLA C 508:

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

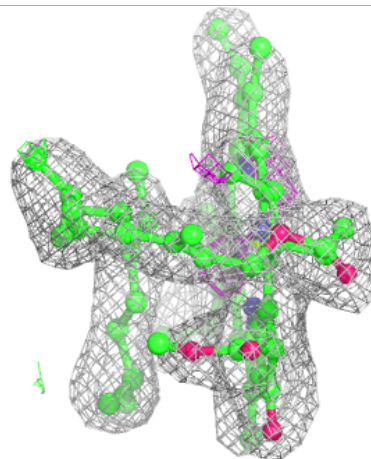
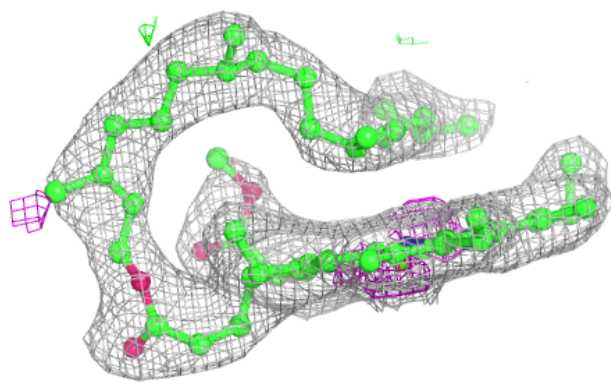
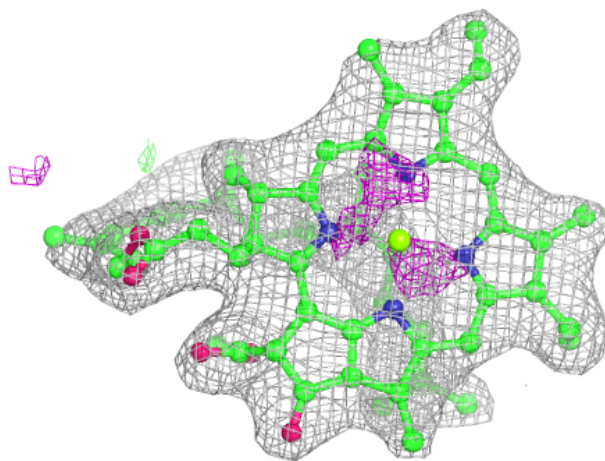
**Electron density around CLA C 509:**

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



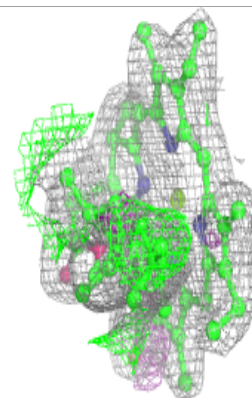
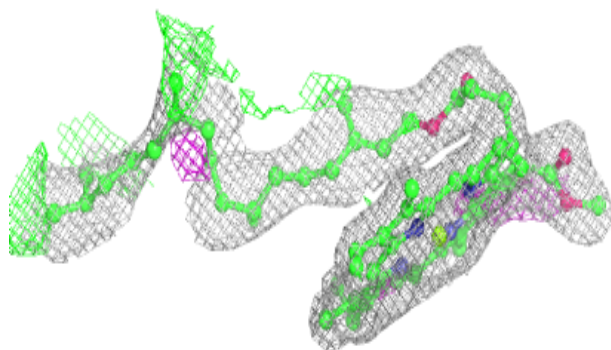
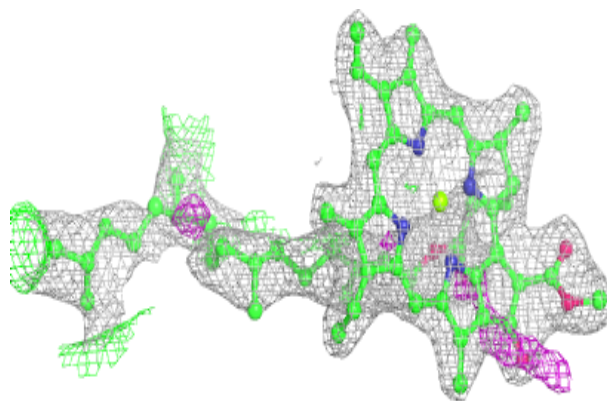
Electron density around CLA C 510:

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

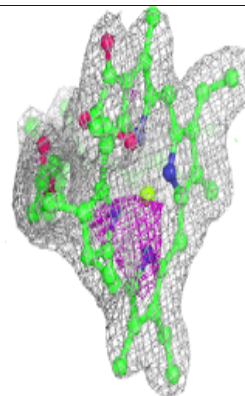
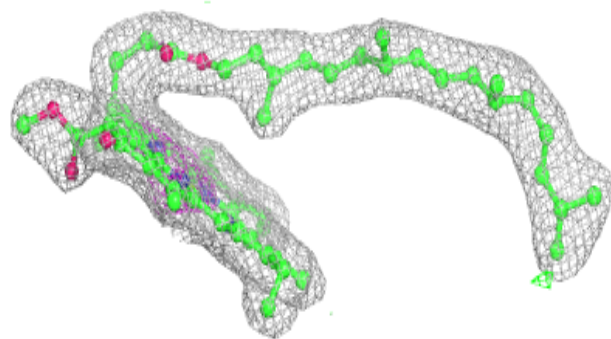
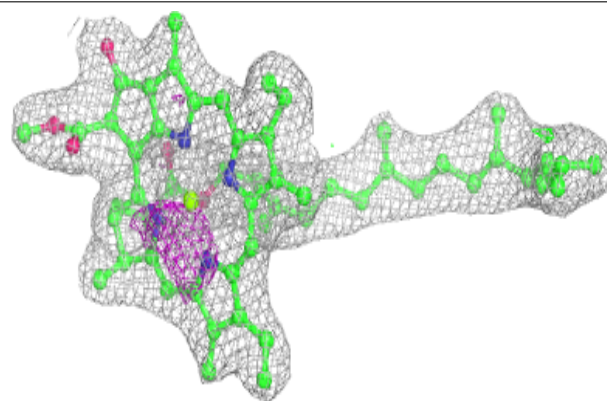


Electron density around CLA B 615:

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

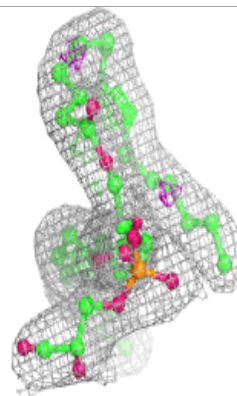
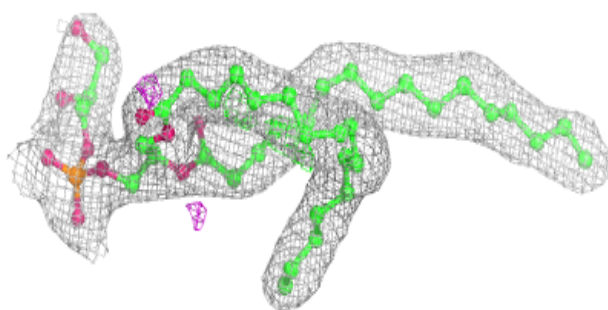
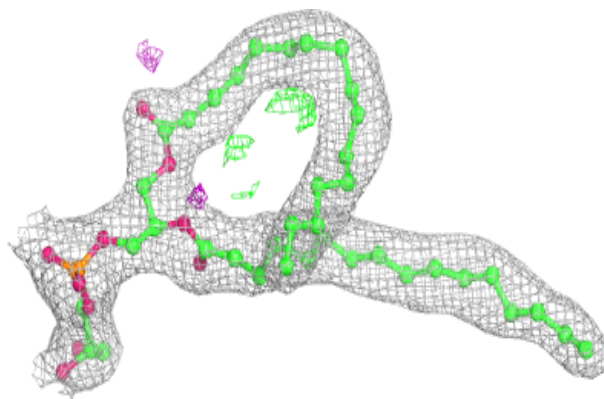
**Electron density around CLA b 613:**

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



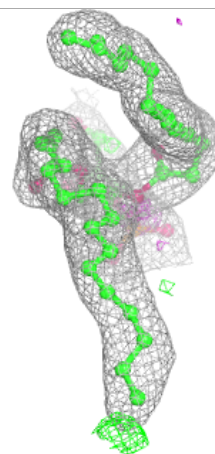
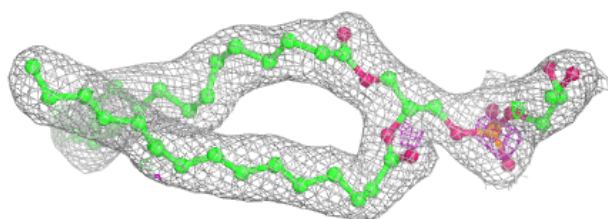
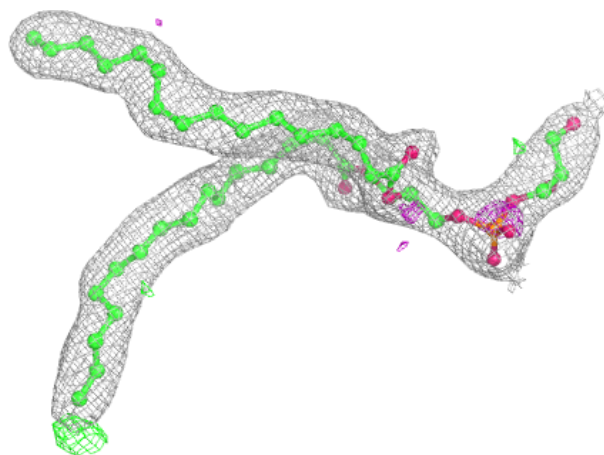
Electron density around LHG d 409:

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



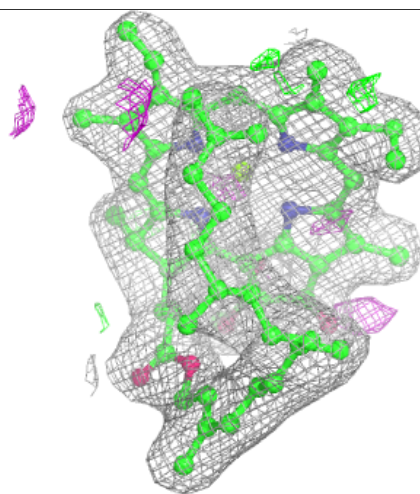
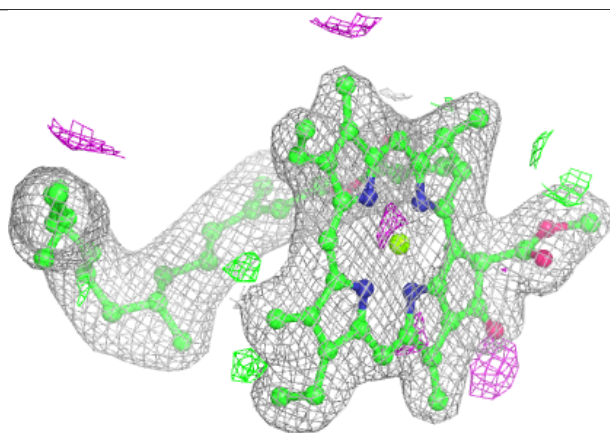
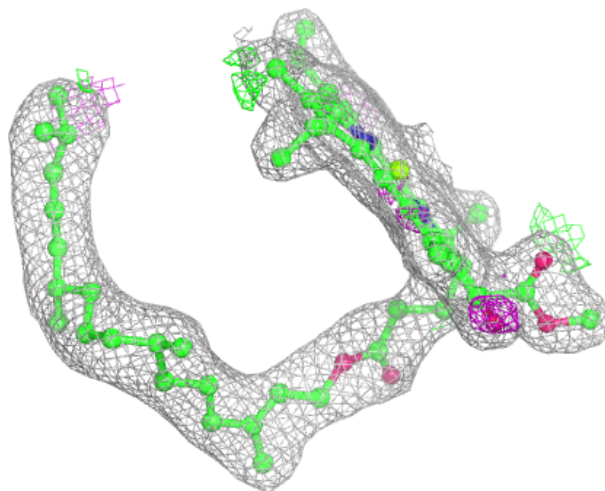
Electron density around LHG d 410:

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



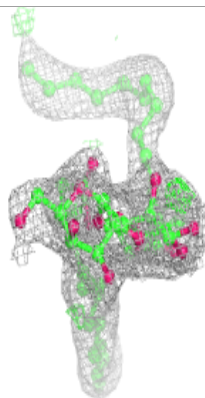
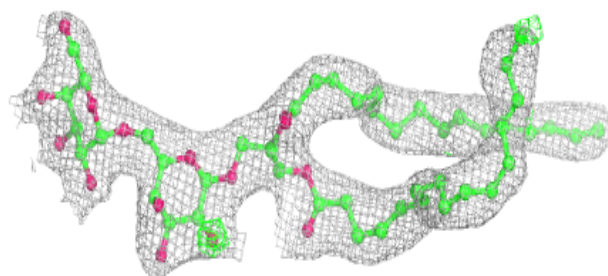
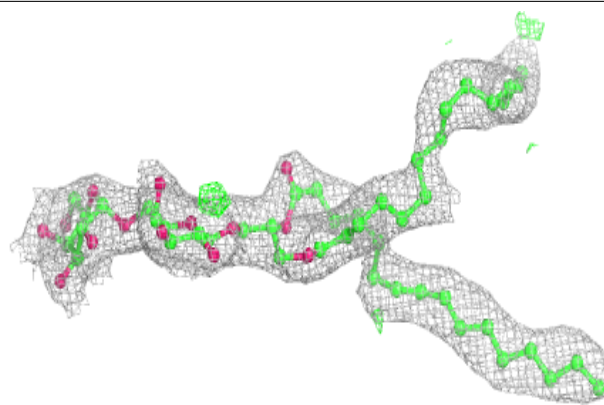
Electron density around CLA B 612:

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

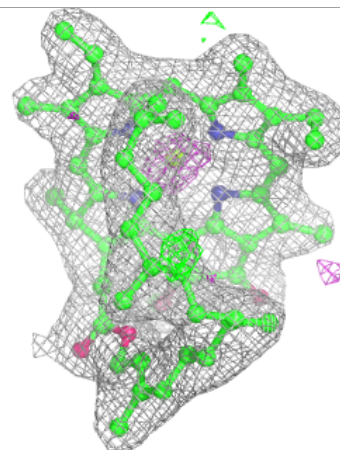
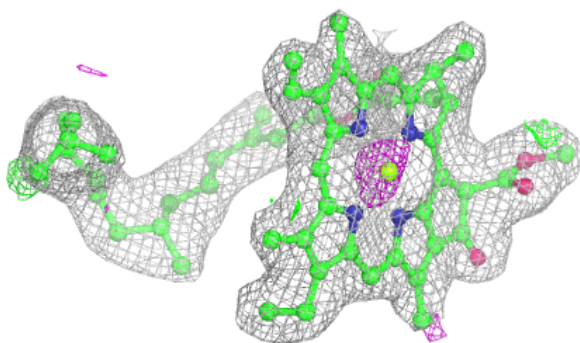
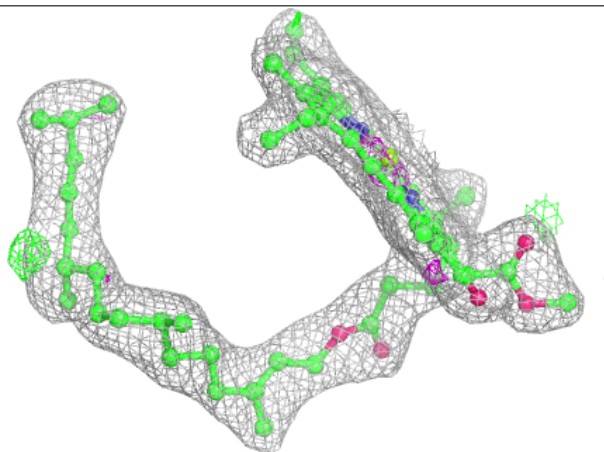


Electron density around DGD C 516:

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

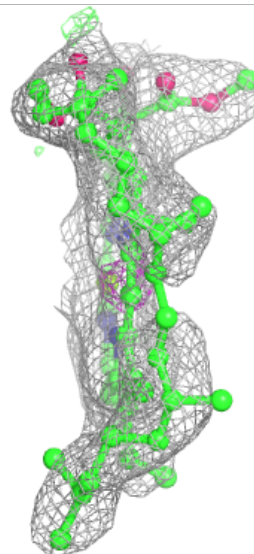
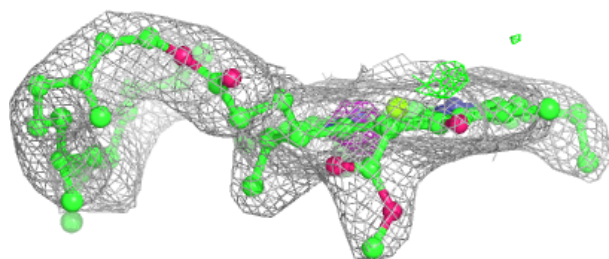
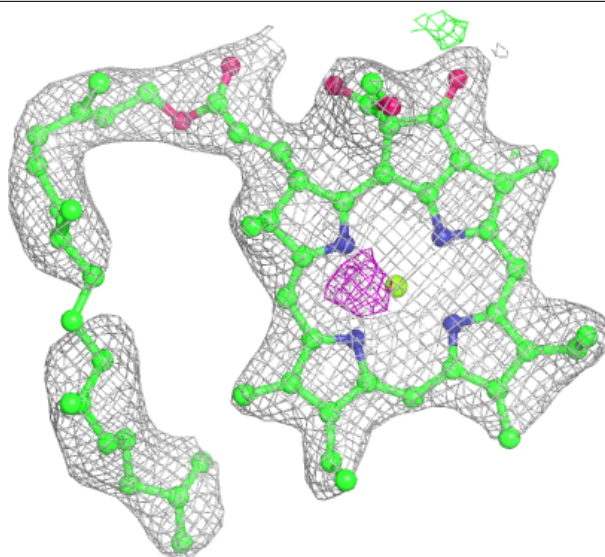
**Electron density around CLA b 616:**

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



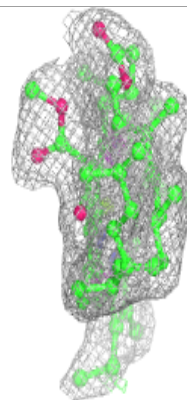
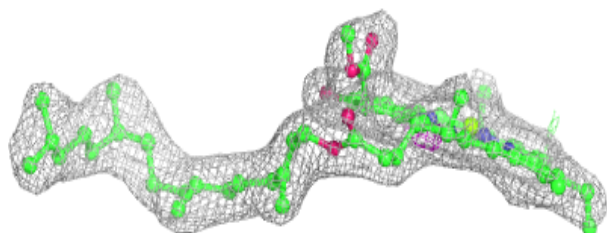
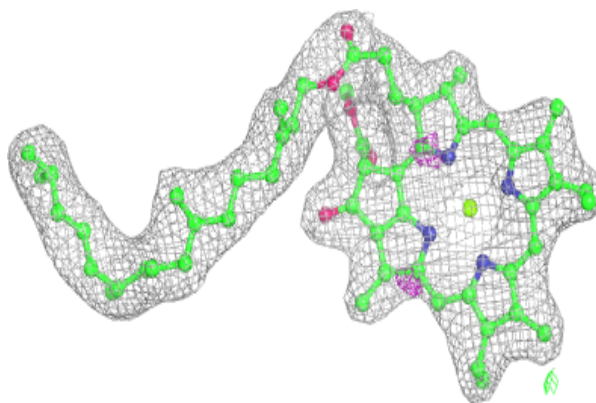
Electron density around CLA c 913:

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

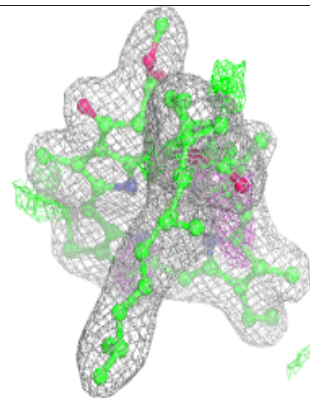
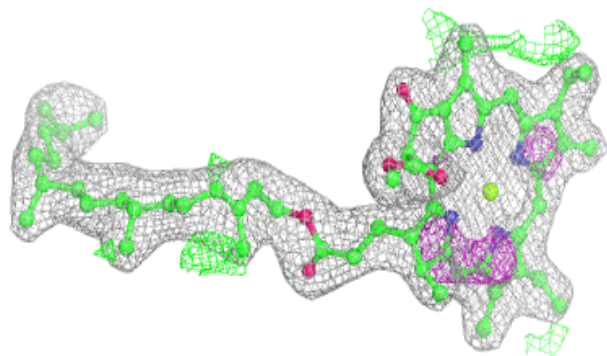
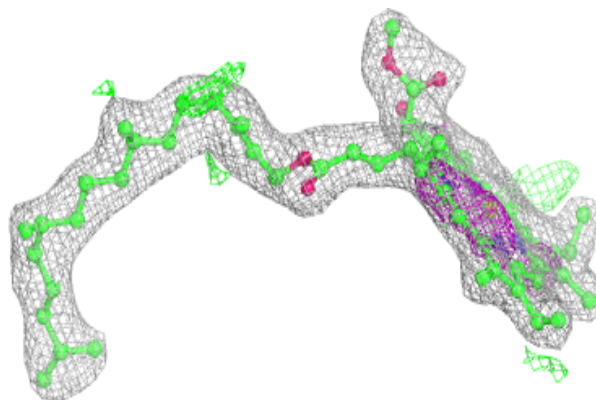


Electron density around CLA B 603:

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

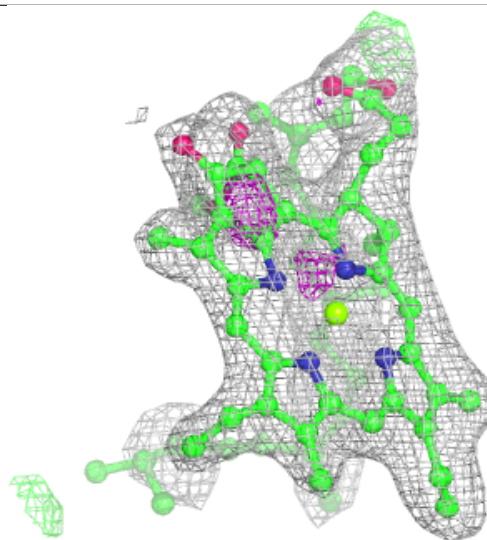
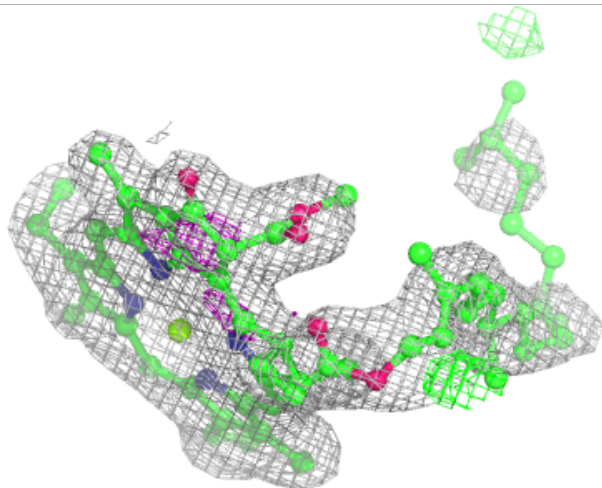
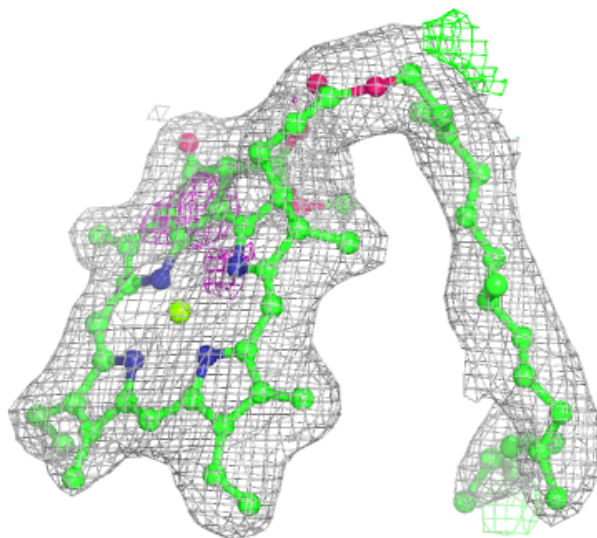
**Electron density around CLA D 404:**

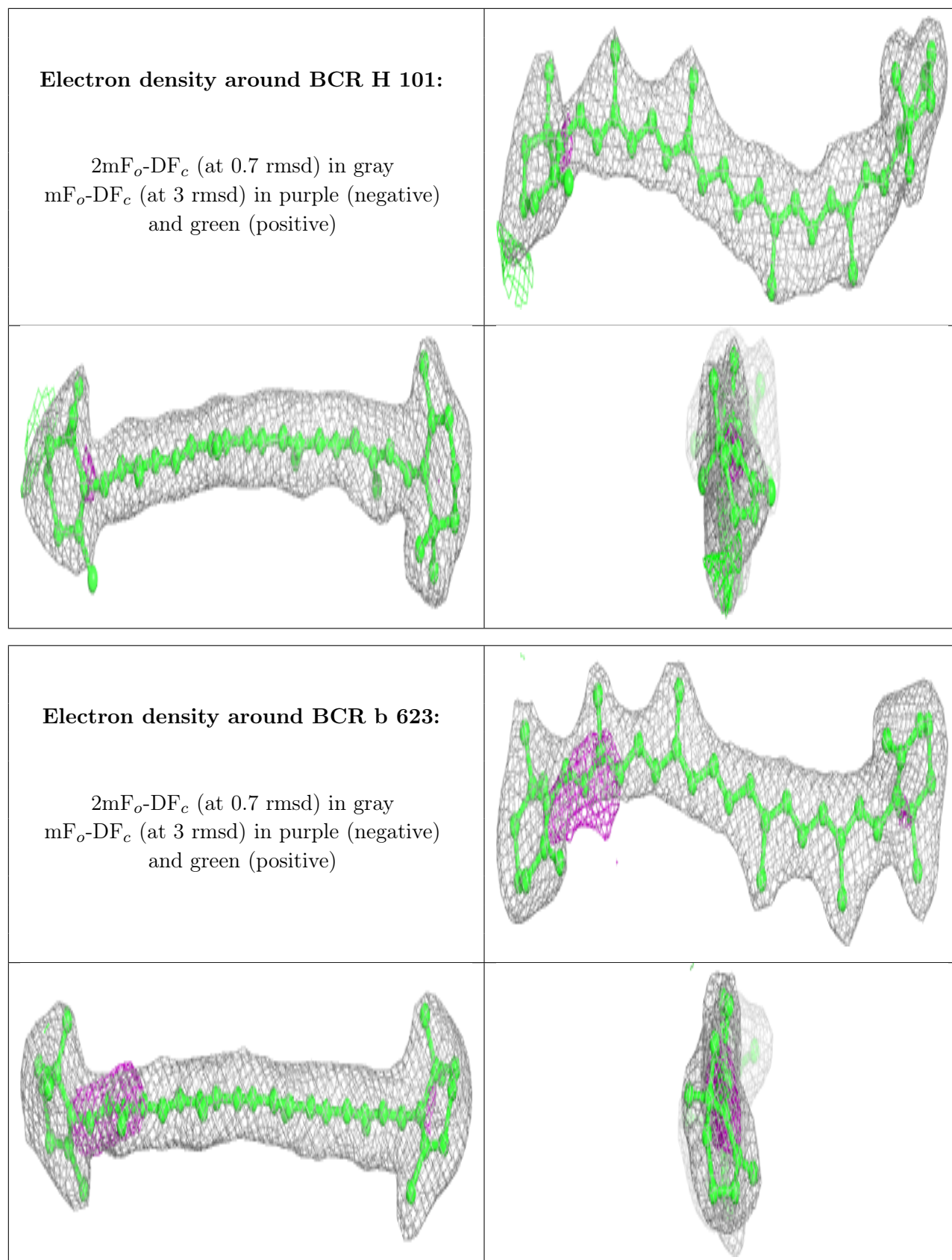
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 621:

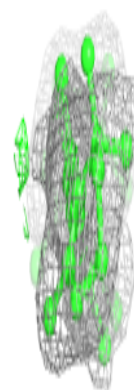
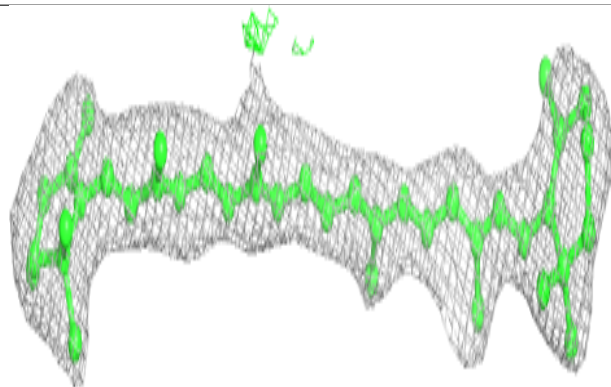
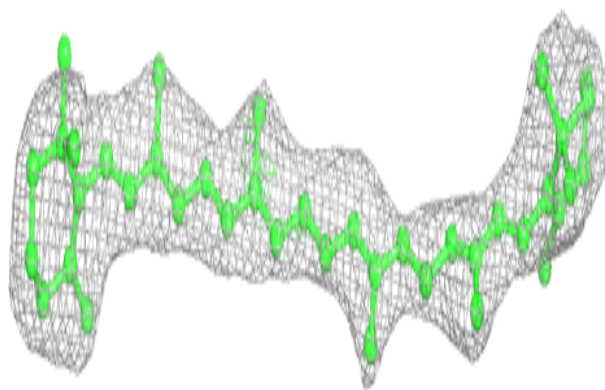
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



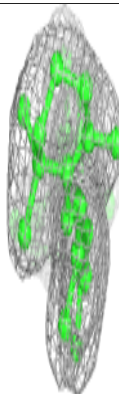
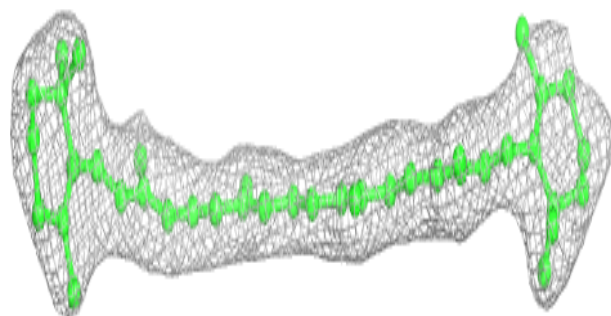
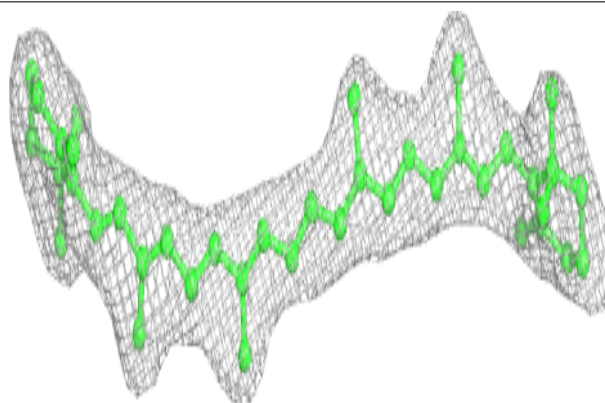


Electron density around BCR c 927:

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

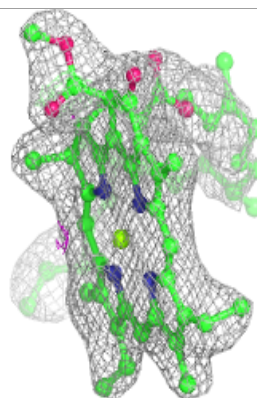
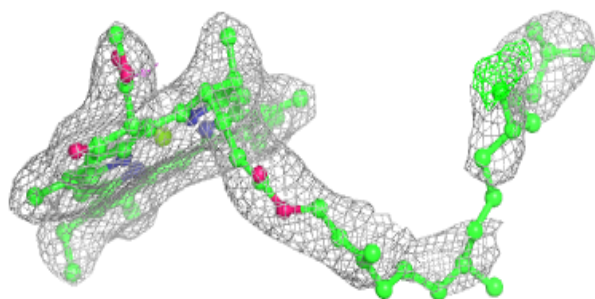
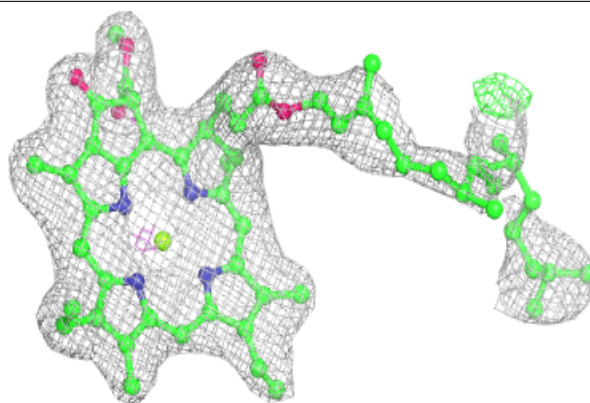
**Electron density around BCR h 101:**

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

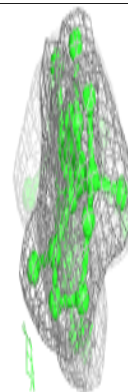
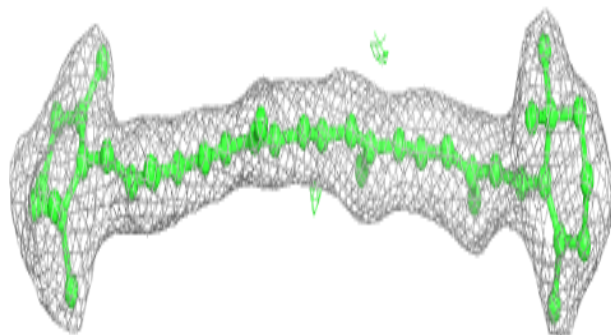
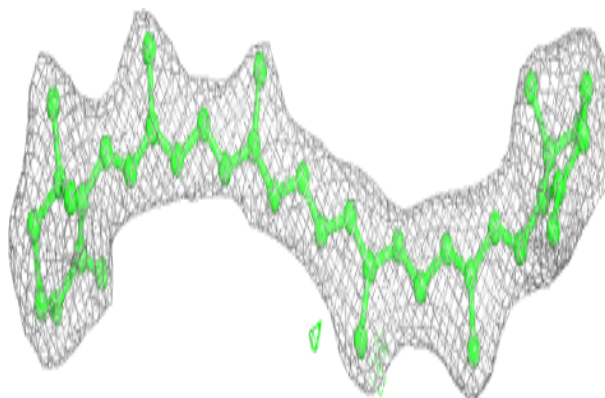


Electron density around CLA a 408:

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

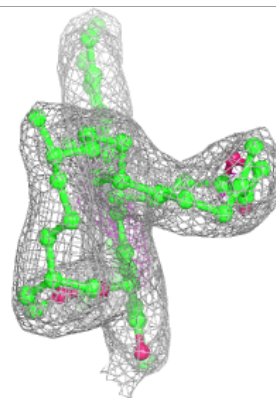
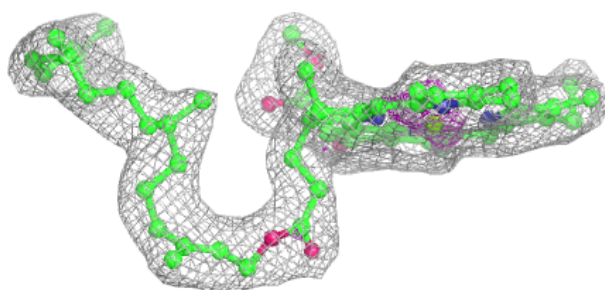
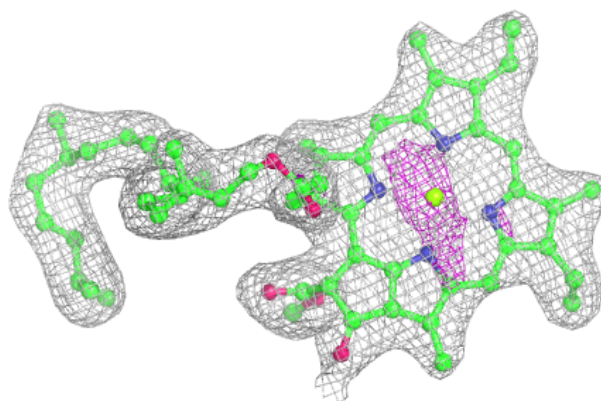
**Electron density around BCR y 101:**

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

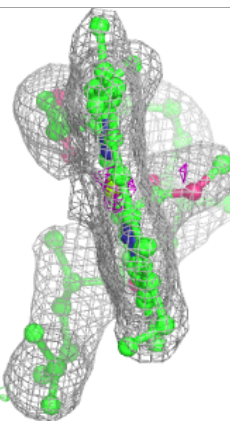
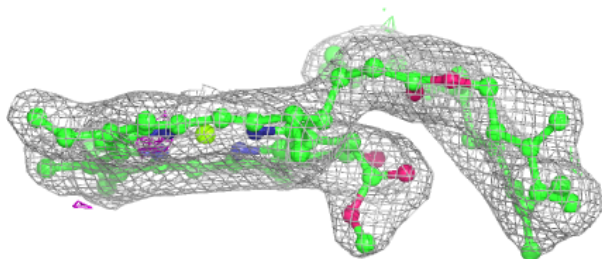
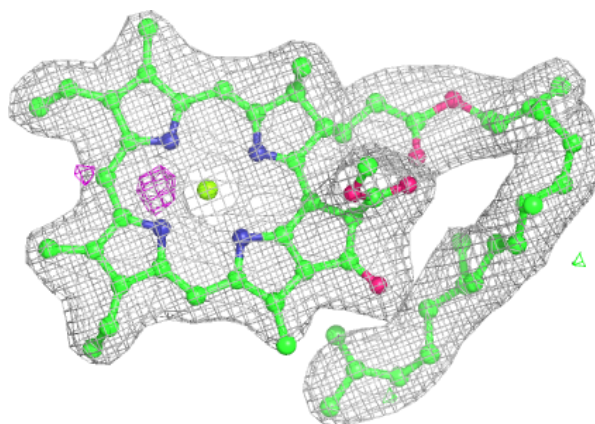


Electron density around CLA B 613:

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

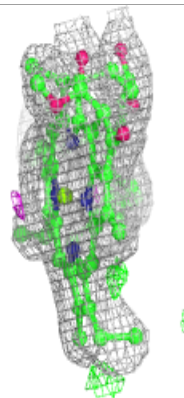
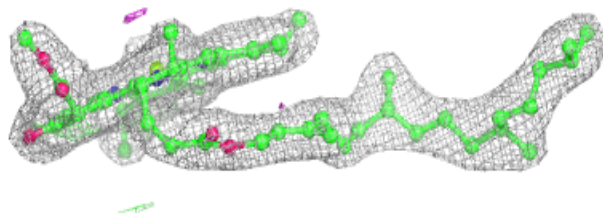
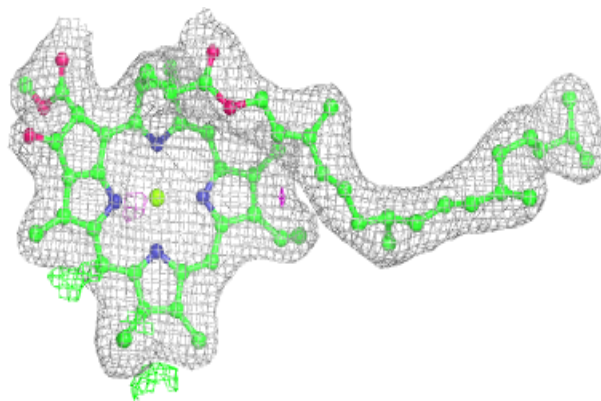
**Electron density around CLA b 615:**

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

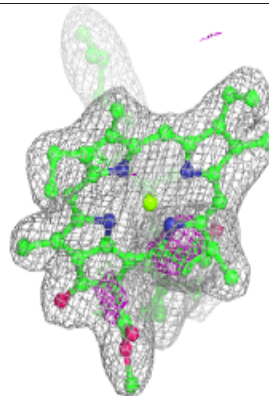
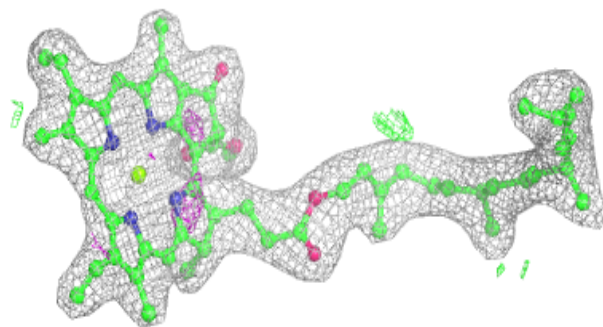
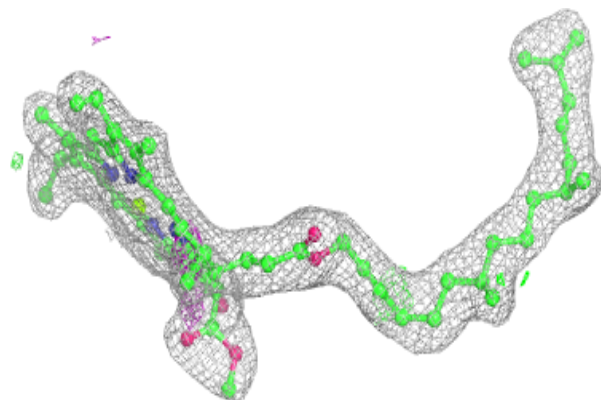


Electron density around CLA B 604:

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

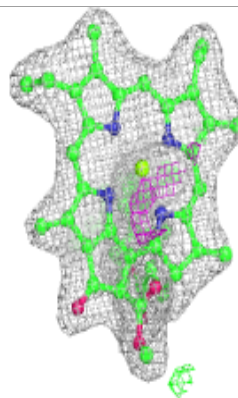
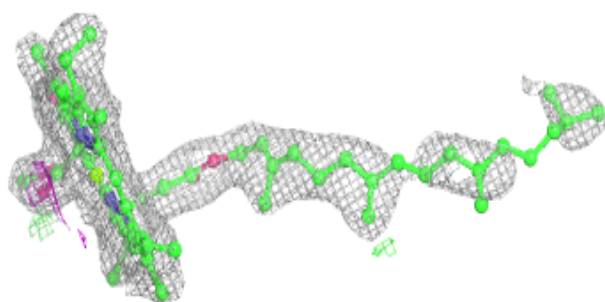
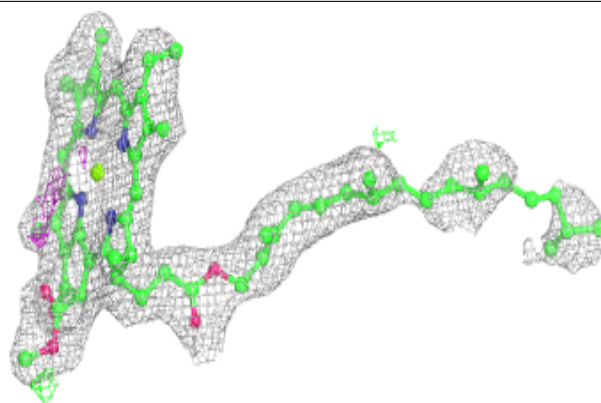
**Electron density around CLA d 405:**

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

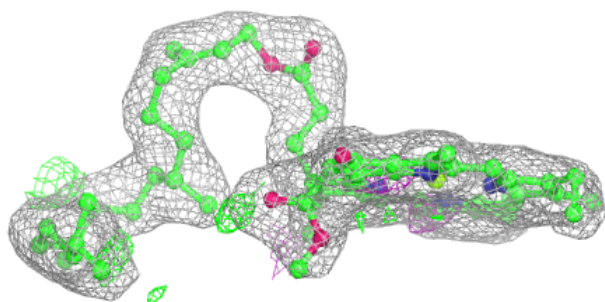
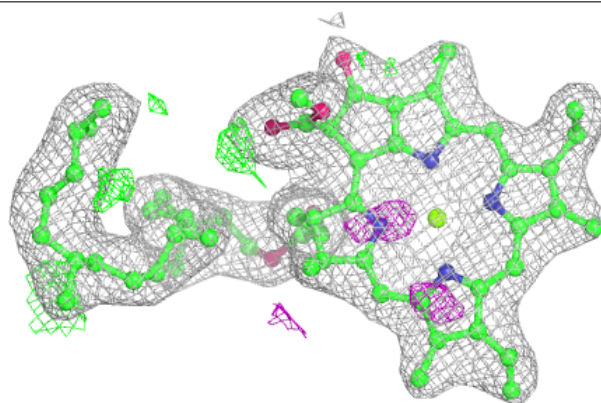


Electron density around CLA d 406:

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

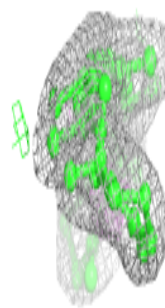
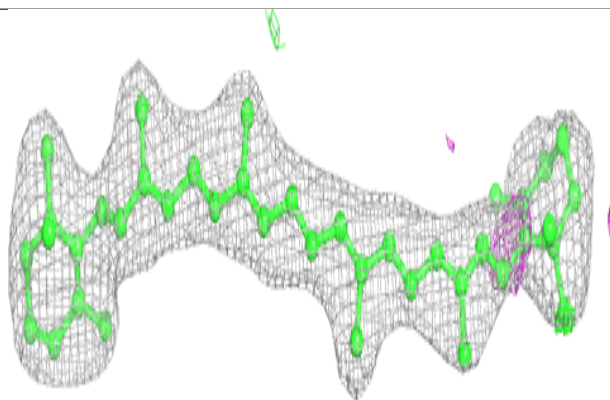
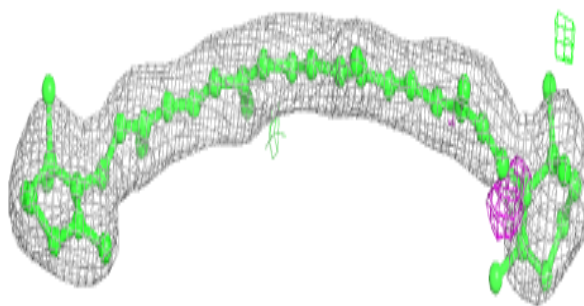
**Electron density around CLA b 617:**

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

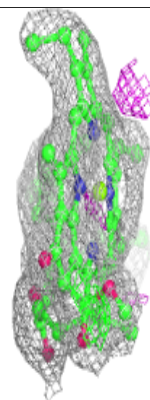
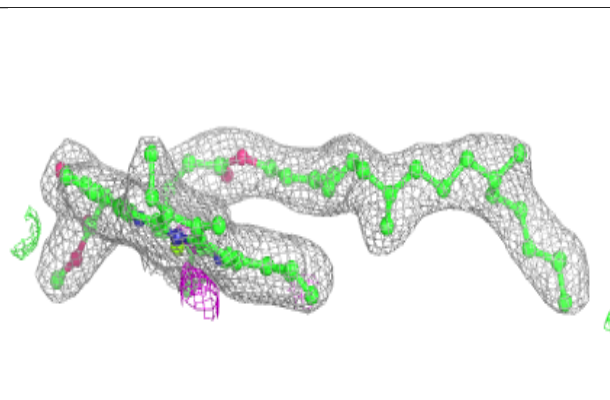
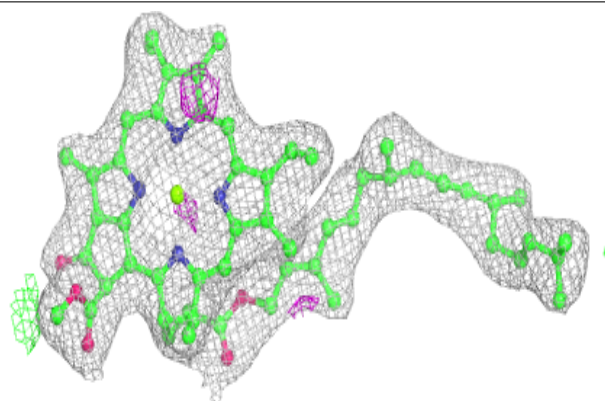


Electron density around BCR D 406:

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

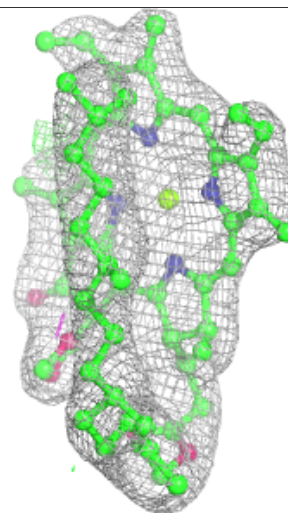
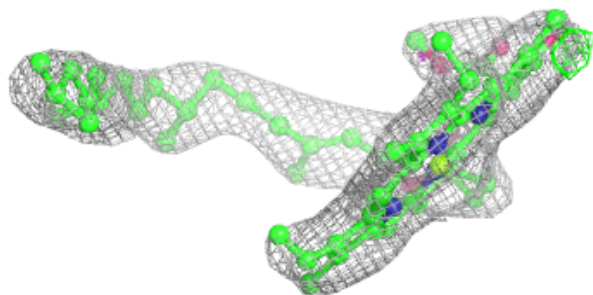
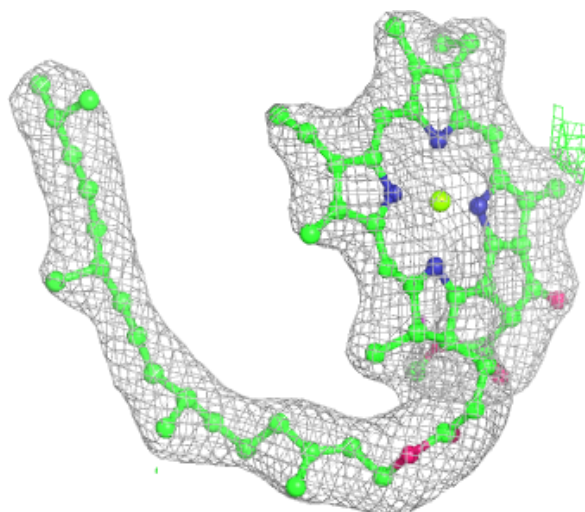
**Electron density around CLA b 608:**

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



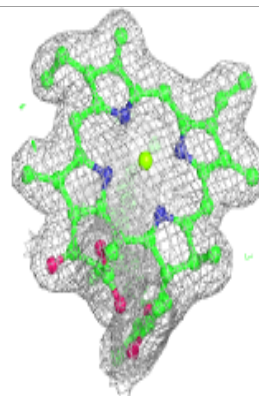
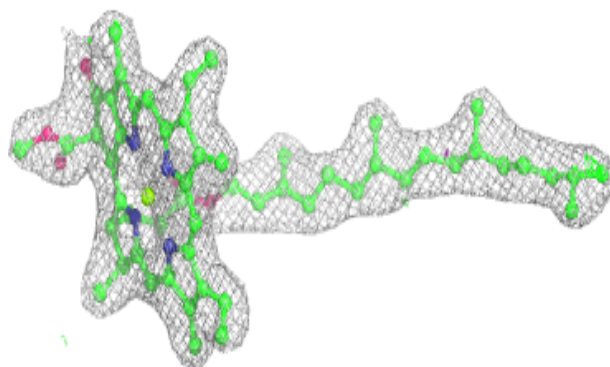
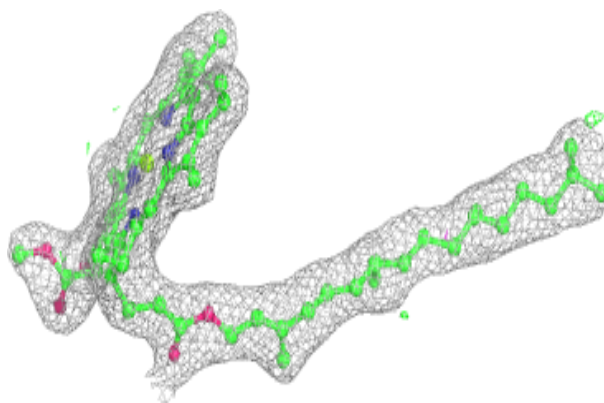
Electron density around CLA C 507:

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

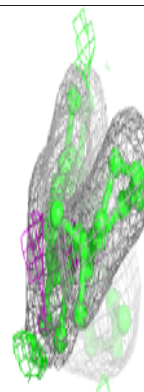
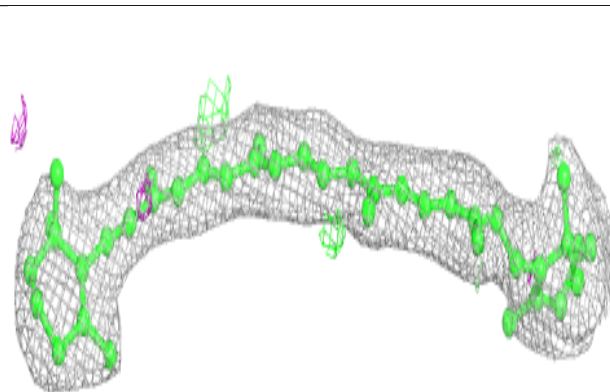
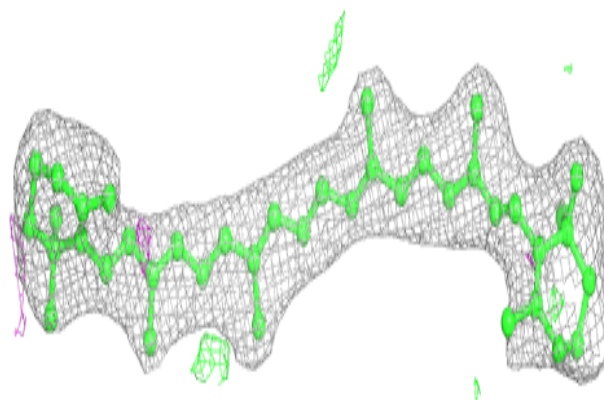


Electron density around CLA B 608:

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

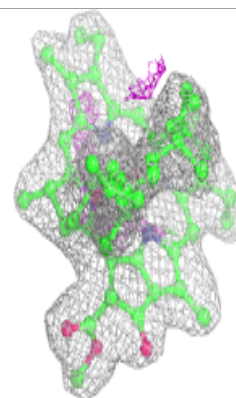
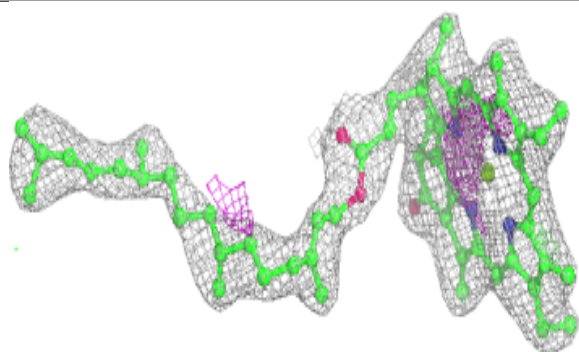
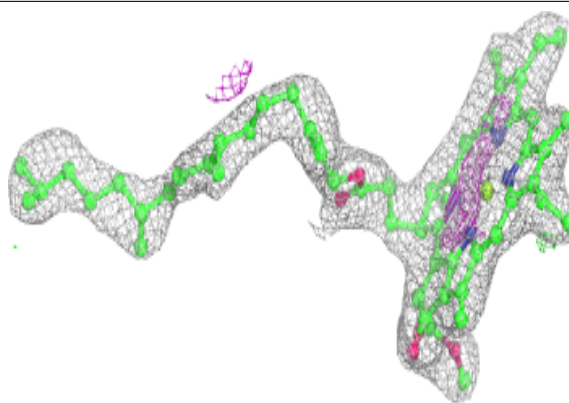
**Electron density around BCR d 407:**

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

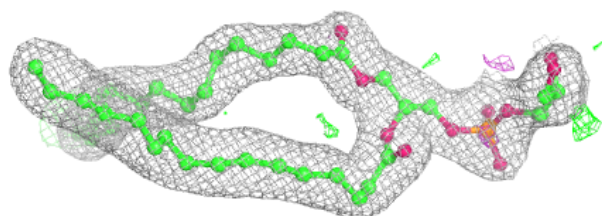
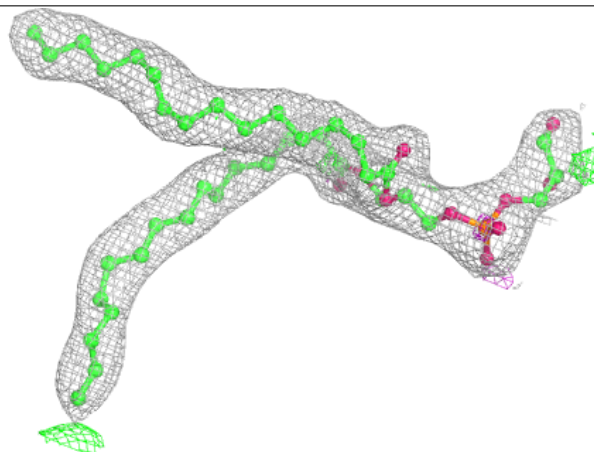


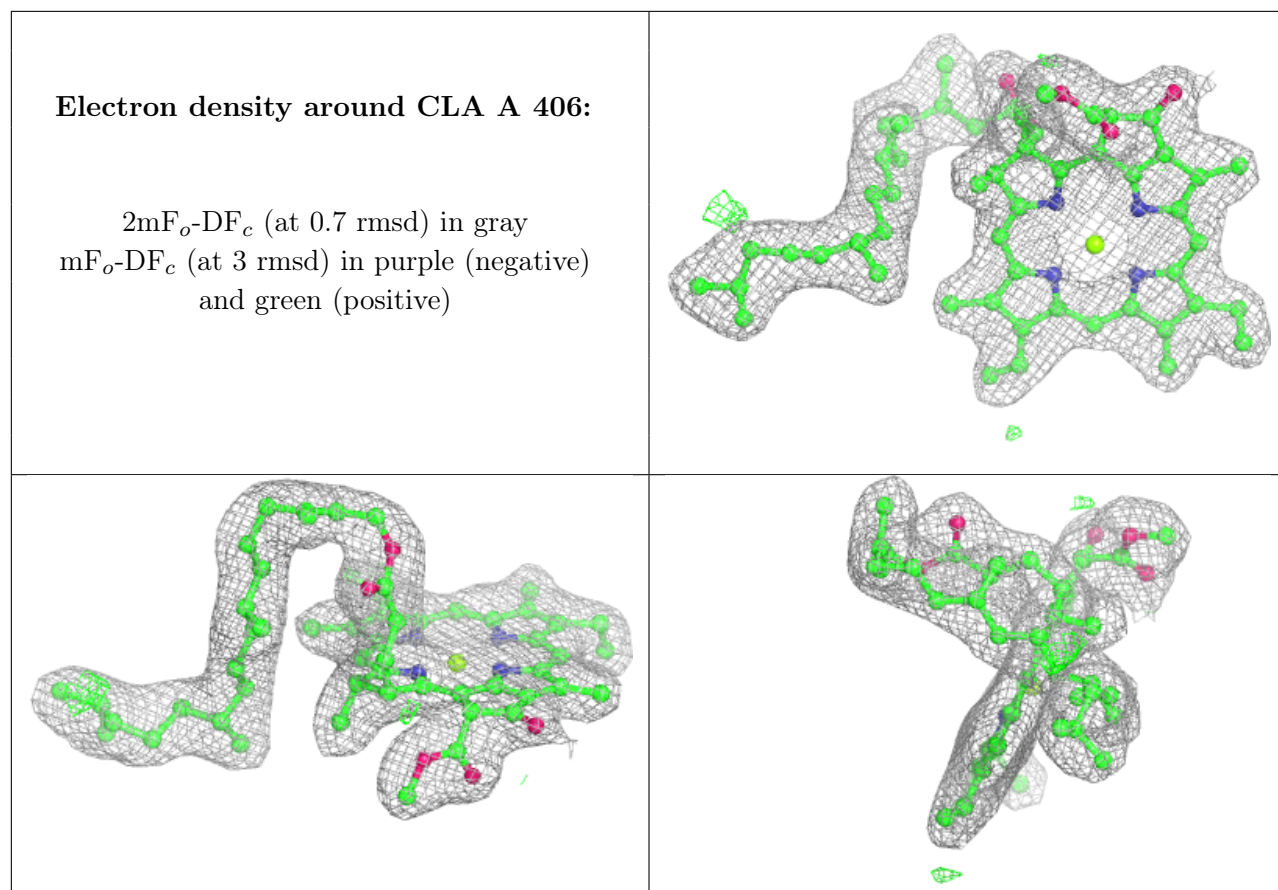
Electron density around CLA c 903:

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

**Electron density around LHG D 409:**

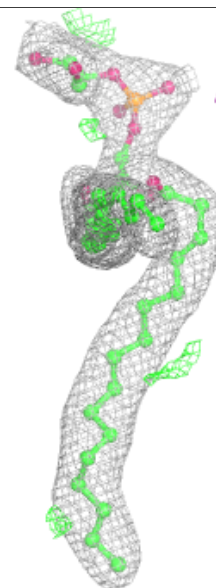
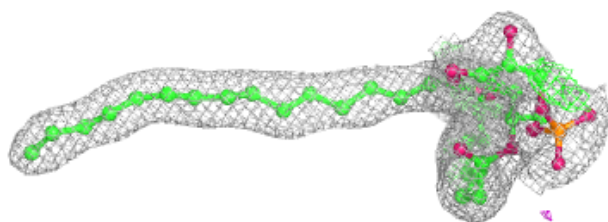
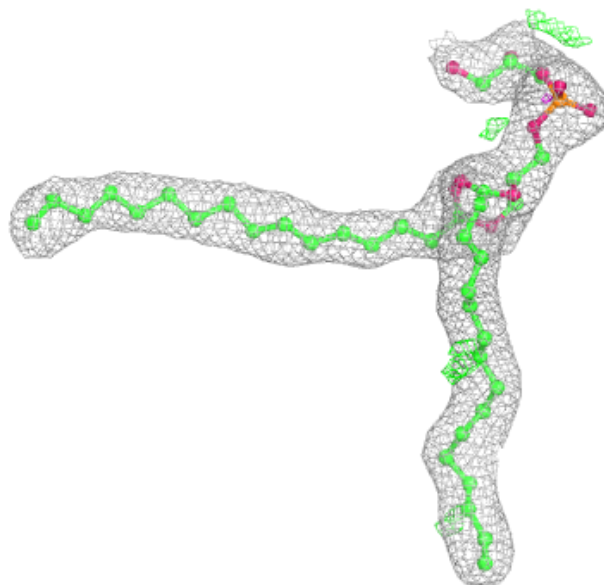
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





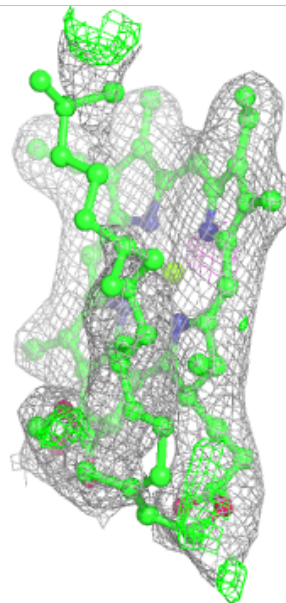
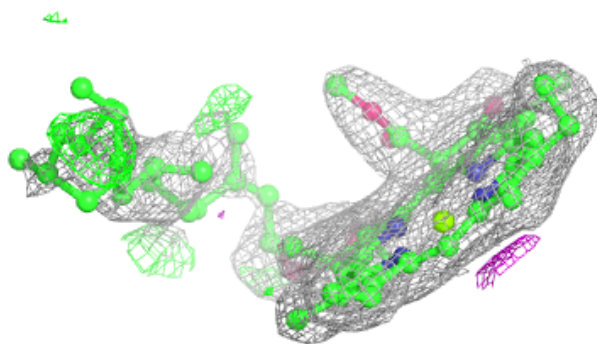
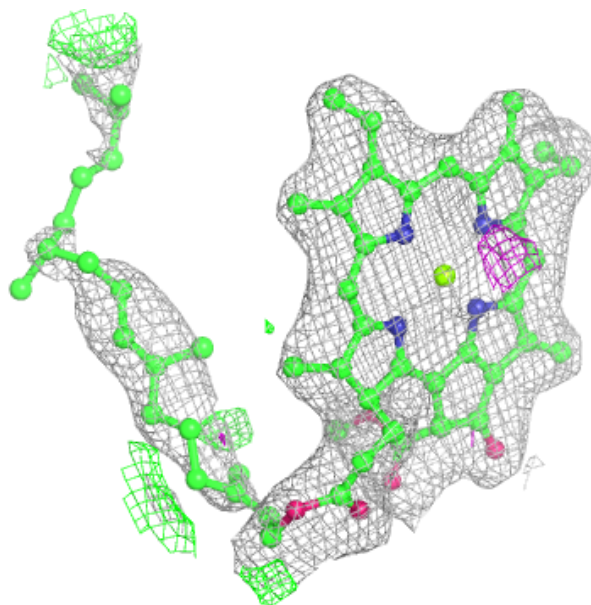
Electron density around LHG L 101:

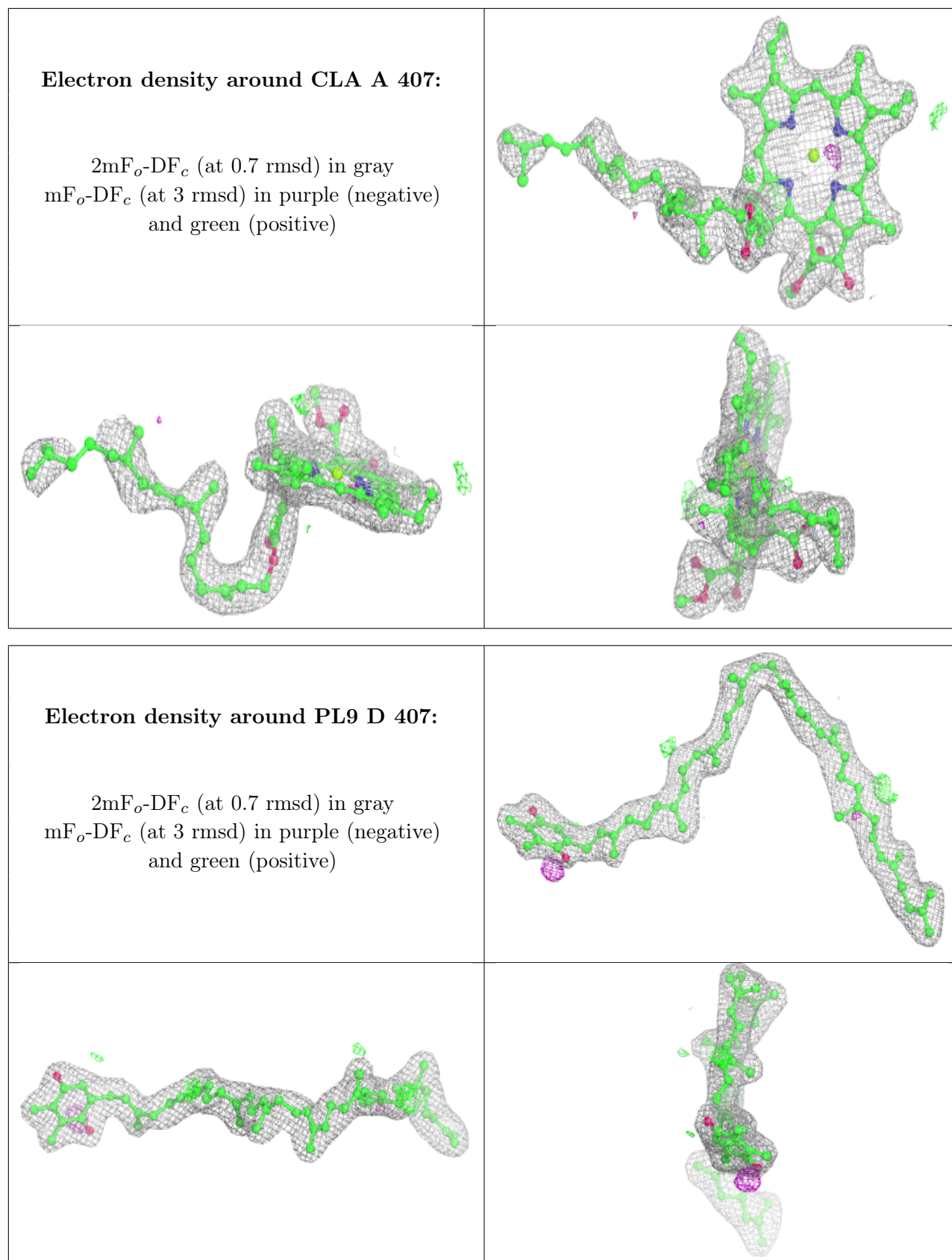
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 617:

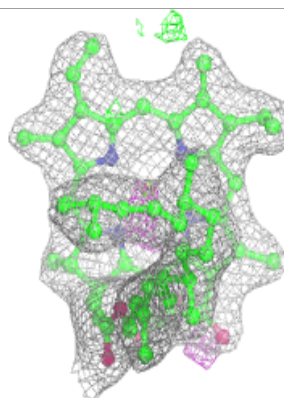
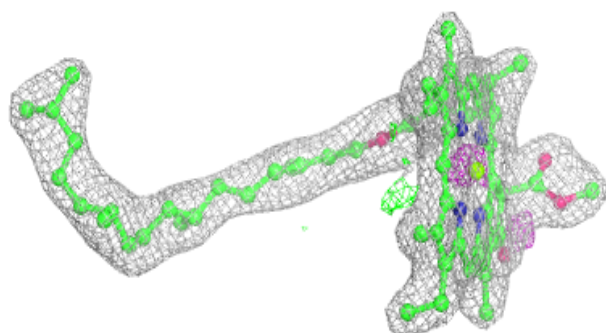
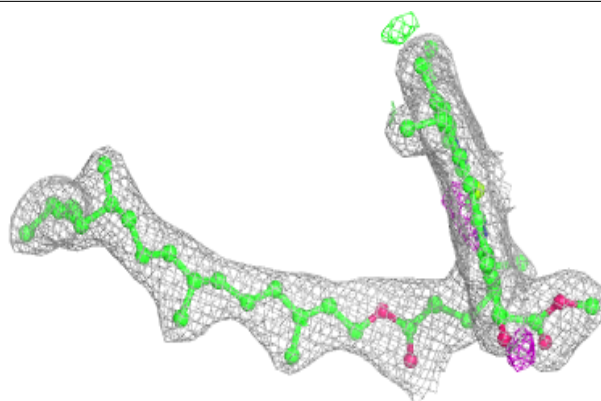
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



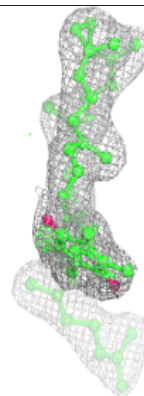
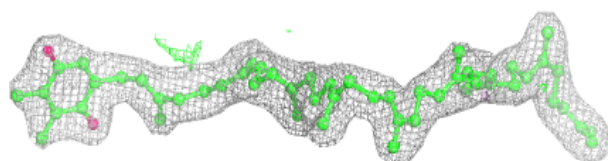
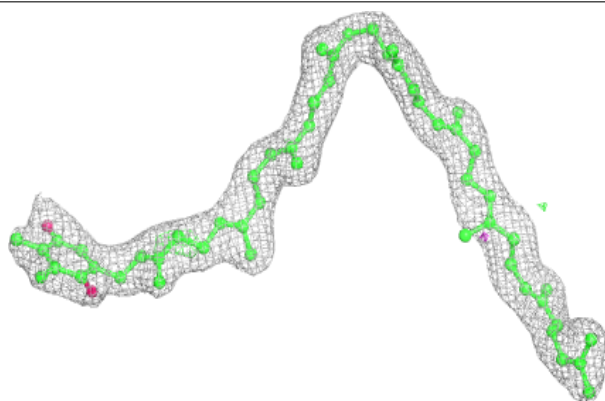


Electron density around CLA b 610:

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

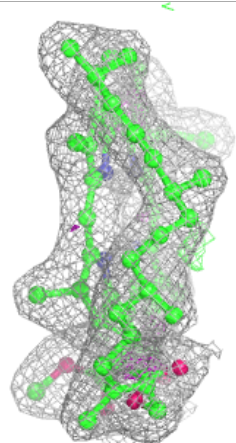
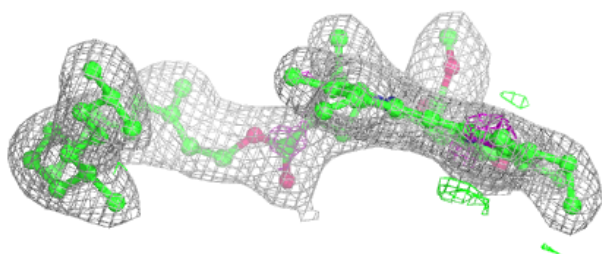
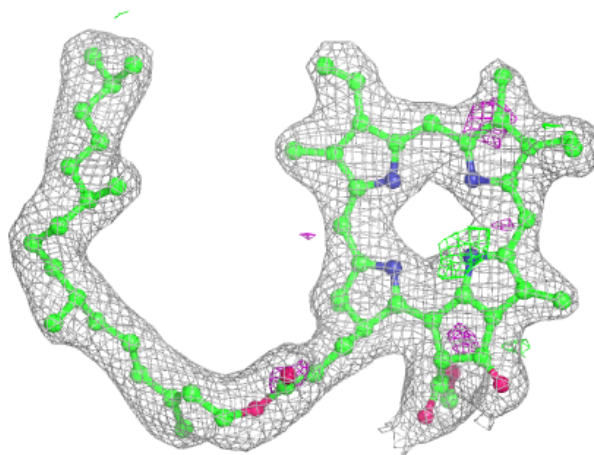
**Electron density around PL9 d 408:**

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



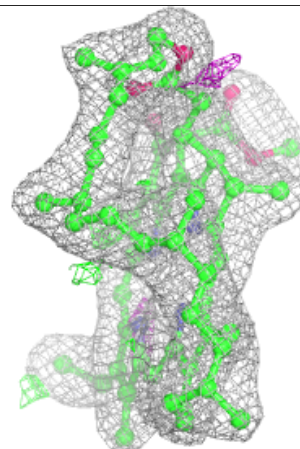
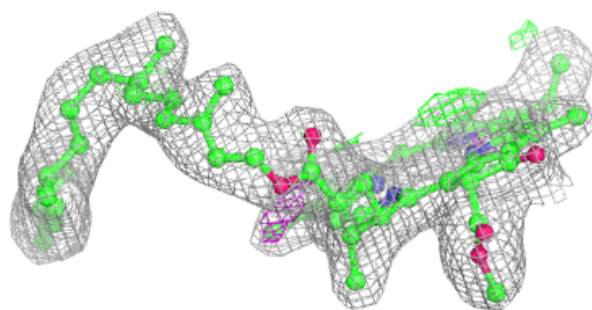
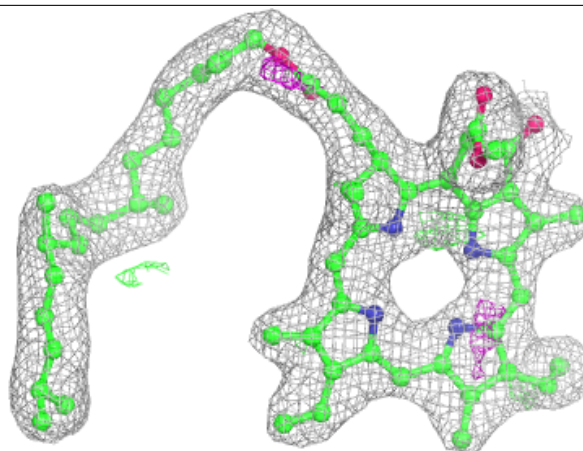
Electron density around PHO A 408:

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



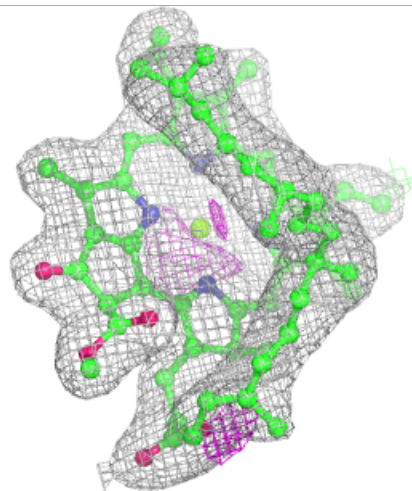
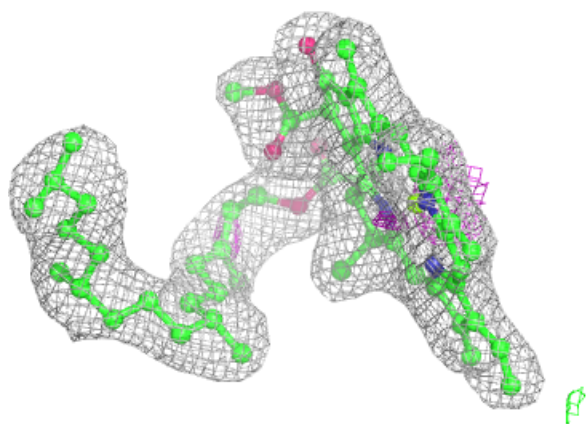
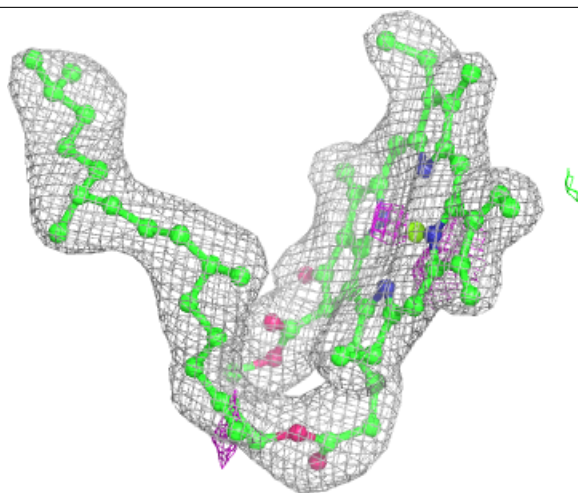
Electron density around PHO d 403:

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



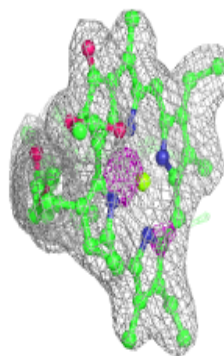
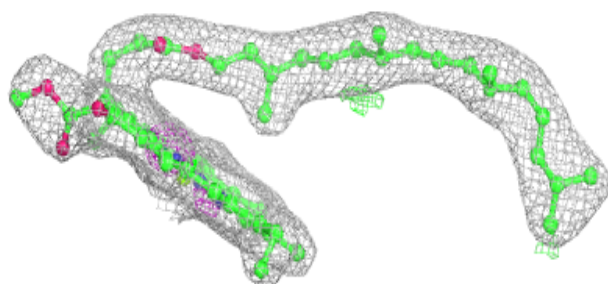
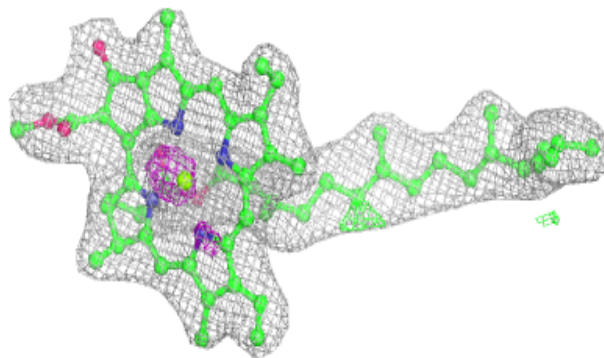
Electron density around CLA b 618:

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

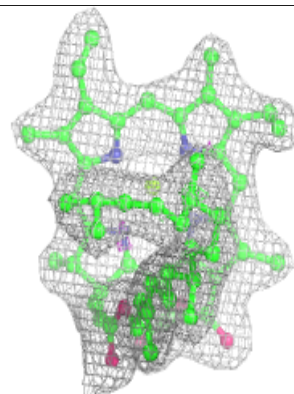
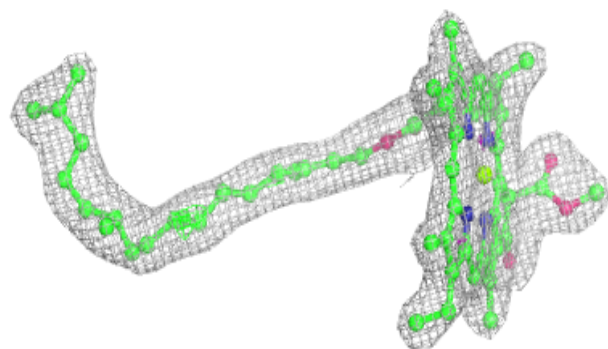
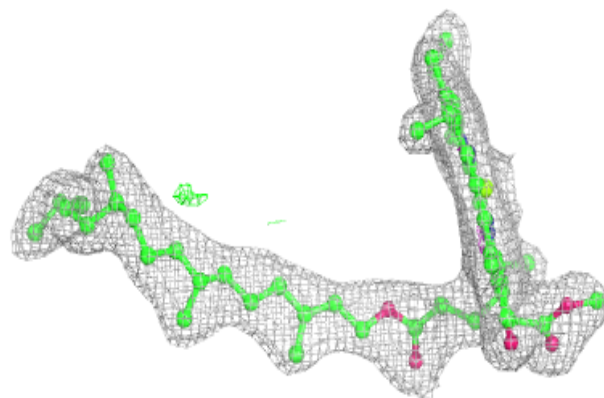


Electron density around CLA B 609:

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

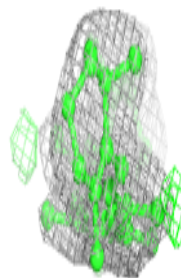
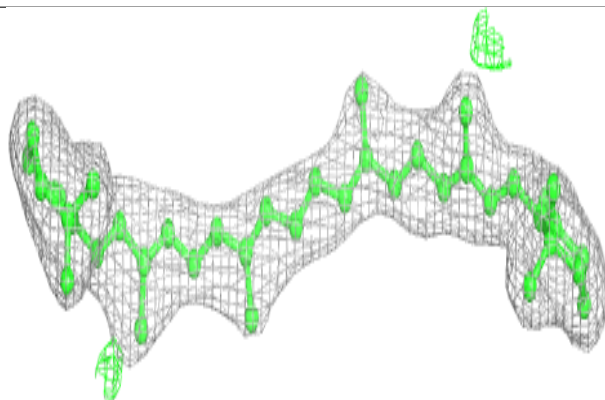
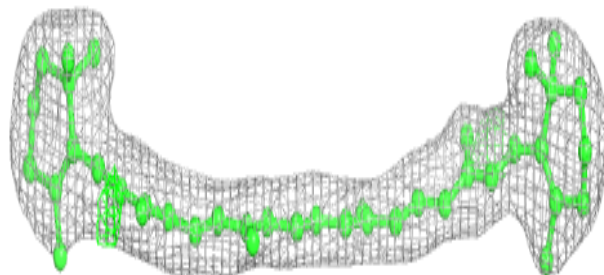
**Electron density around CLA B 606:**

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

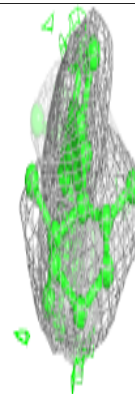
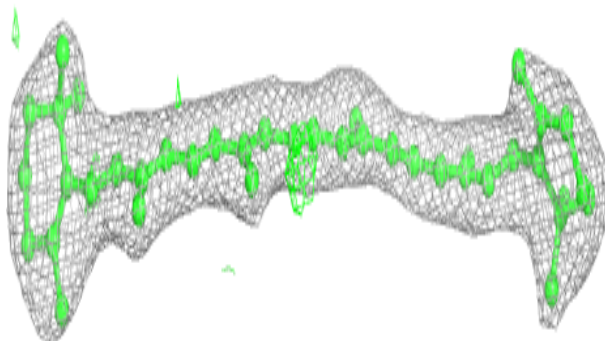
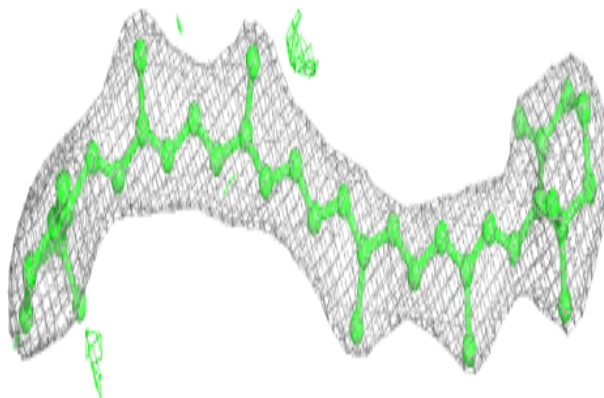


Electron density around BCR K 101:

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

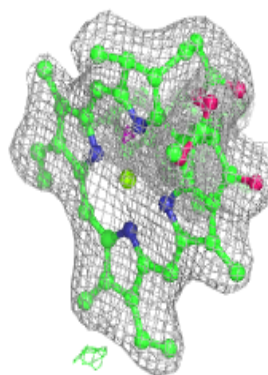
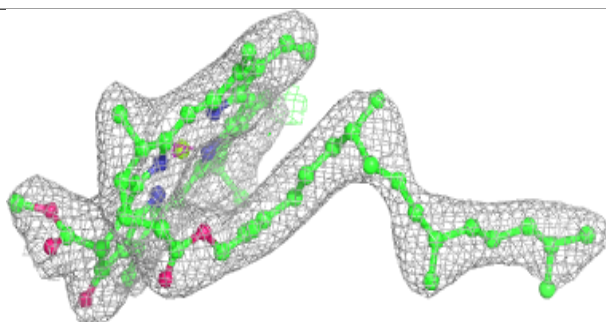
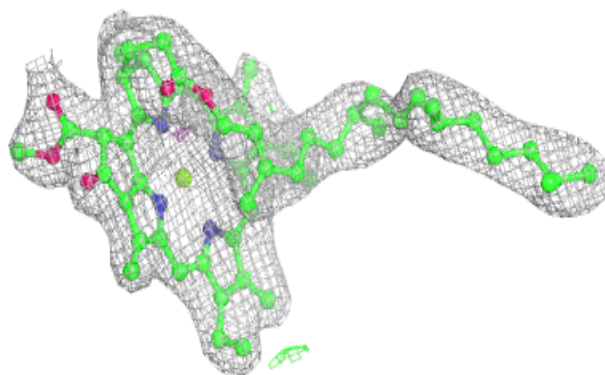
**Electron density around BCR Y 102:**

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

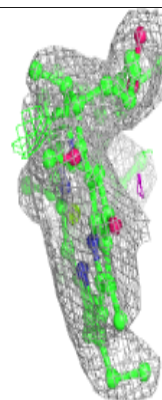
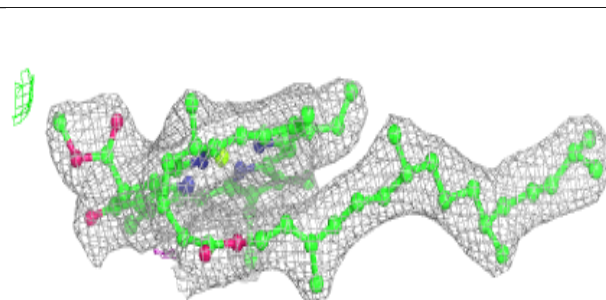
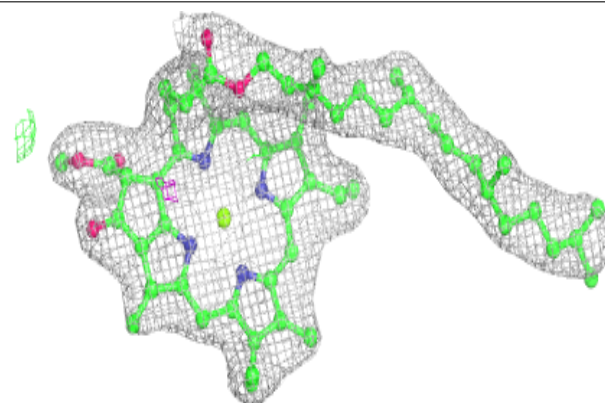


Electron density around CLA C 505:

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

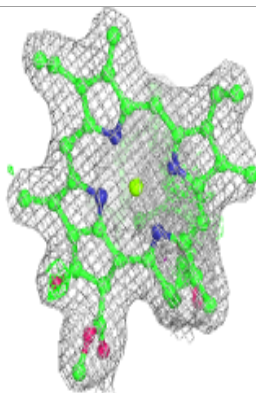
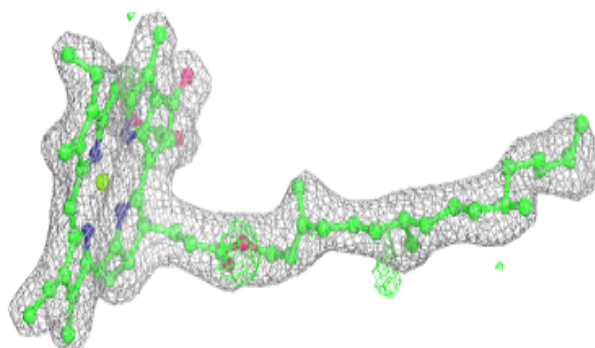
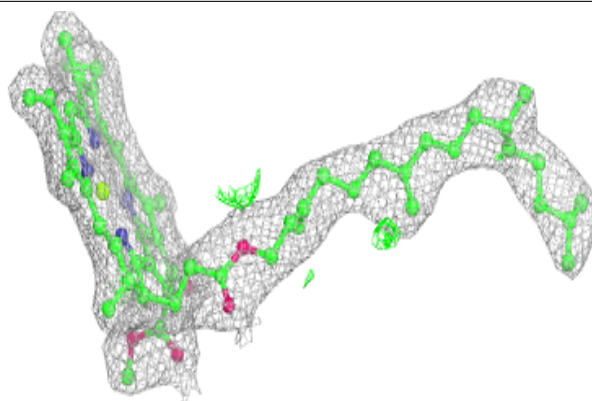
**Electron density around CLA c 902:**

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

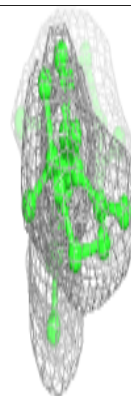
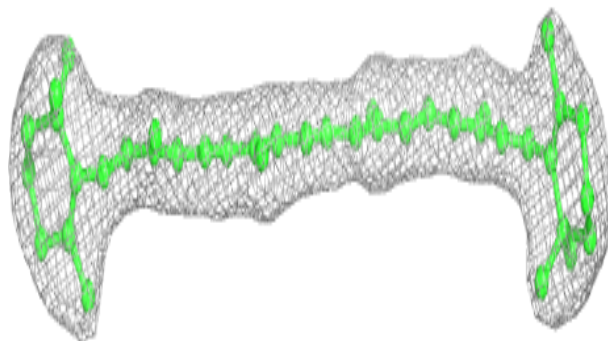
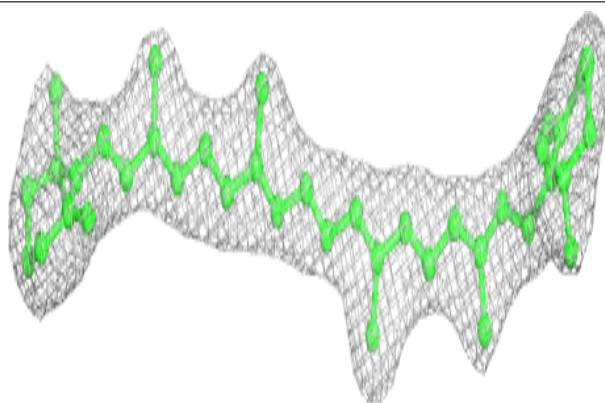


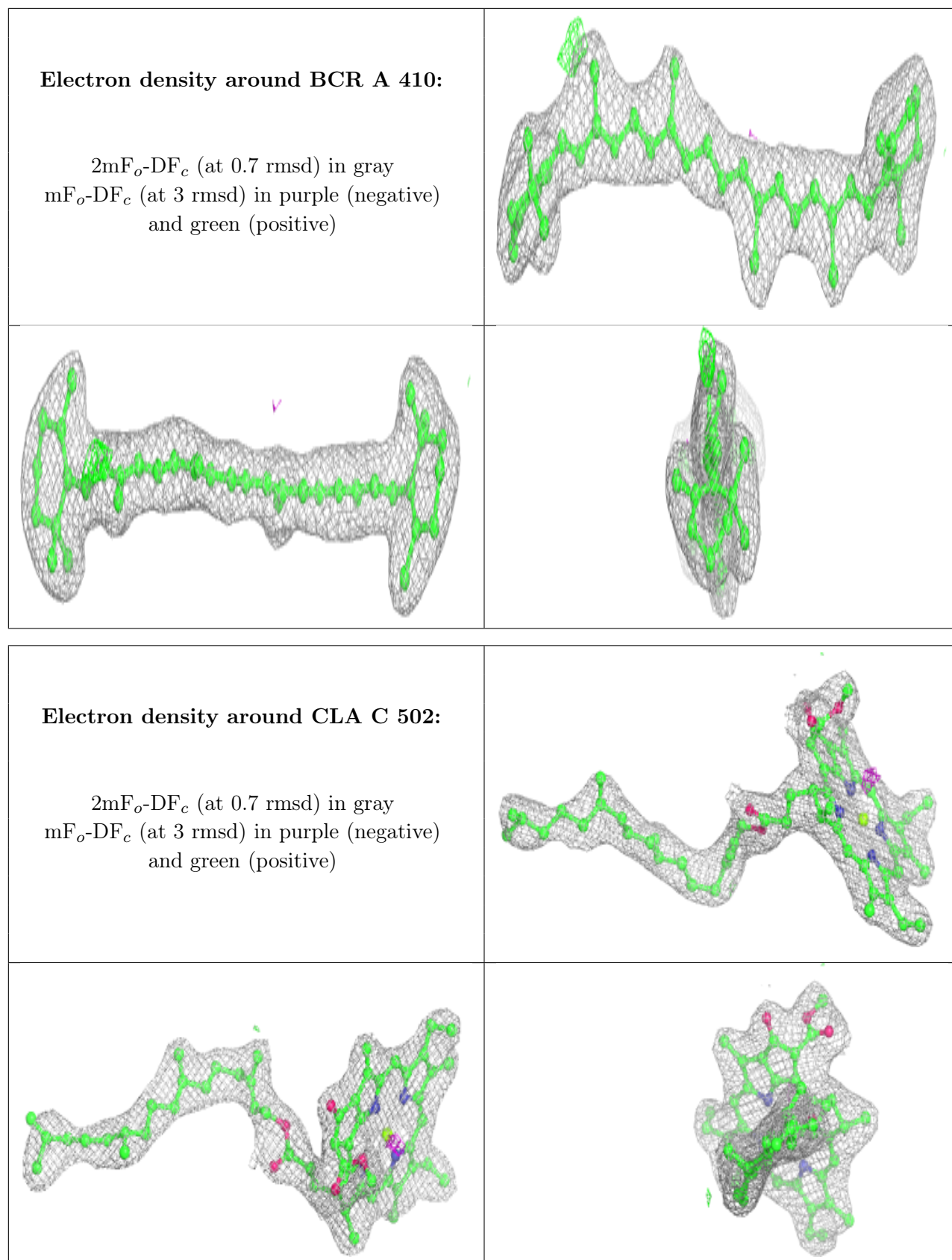
Electron density around CLA b 609:

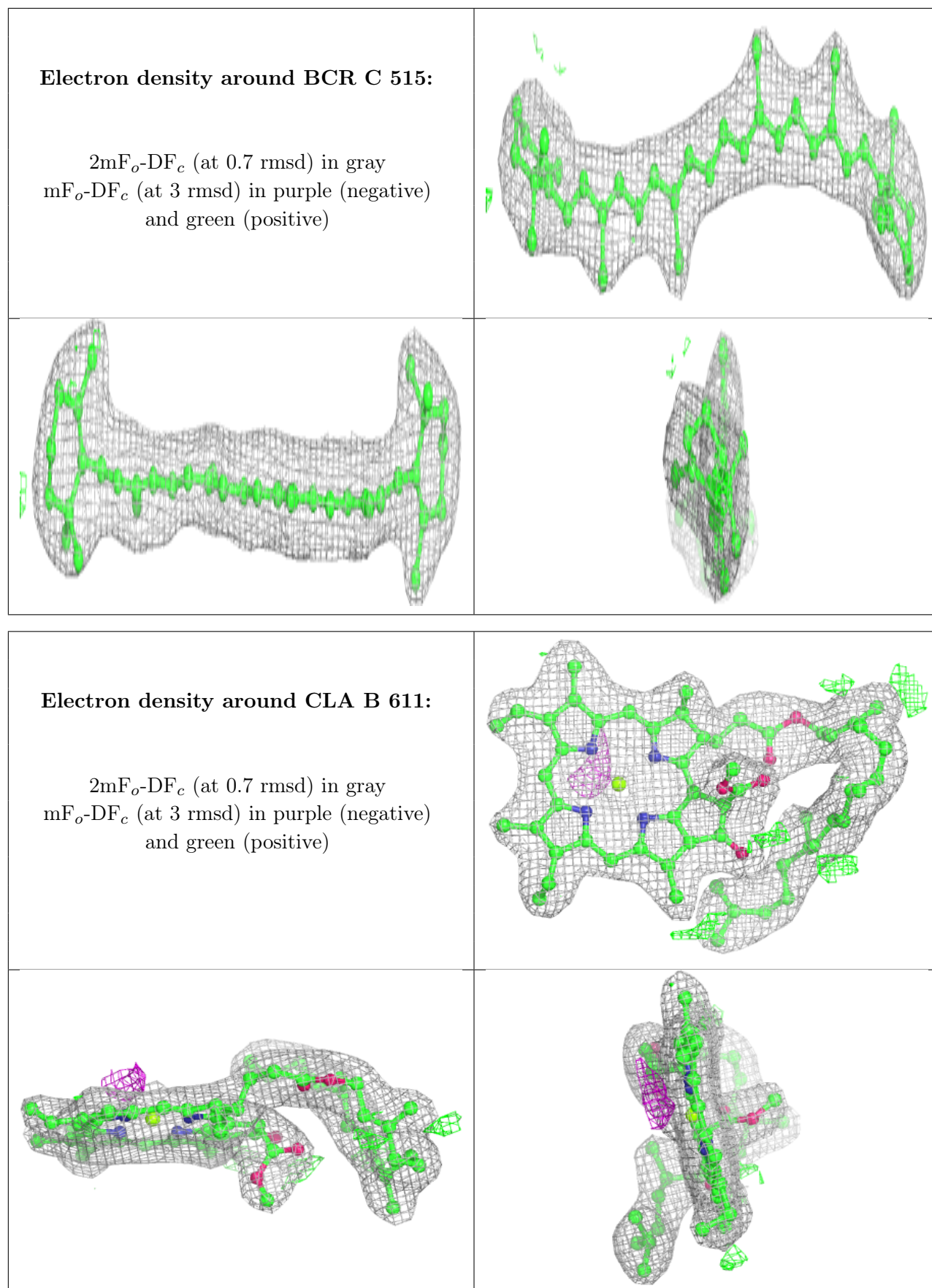
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

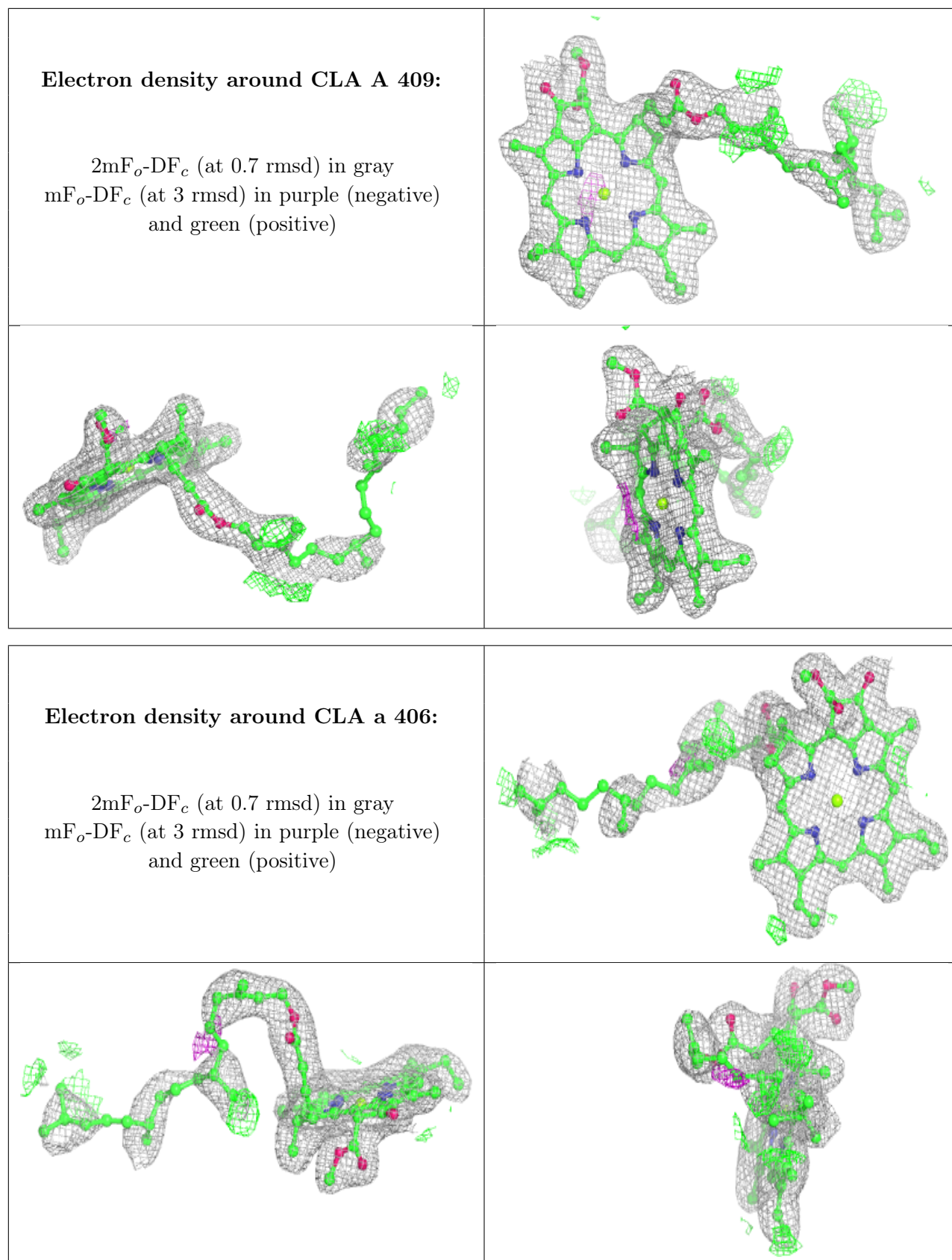
**Electron density around BCR c 915:**

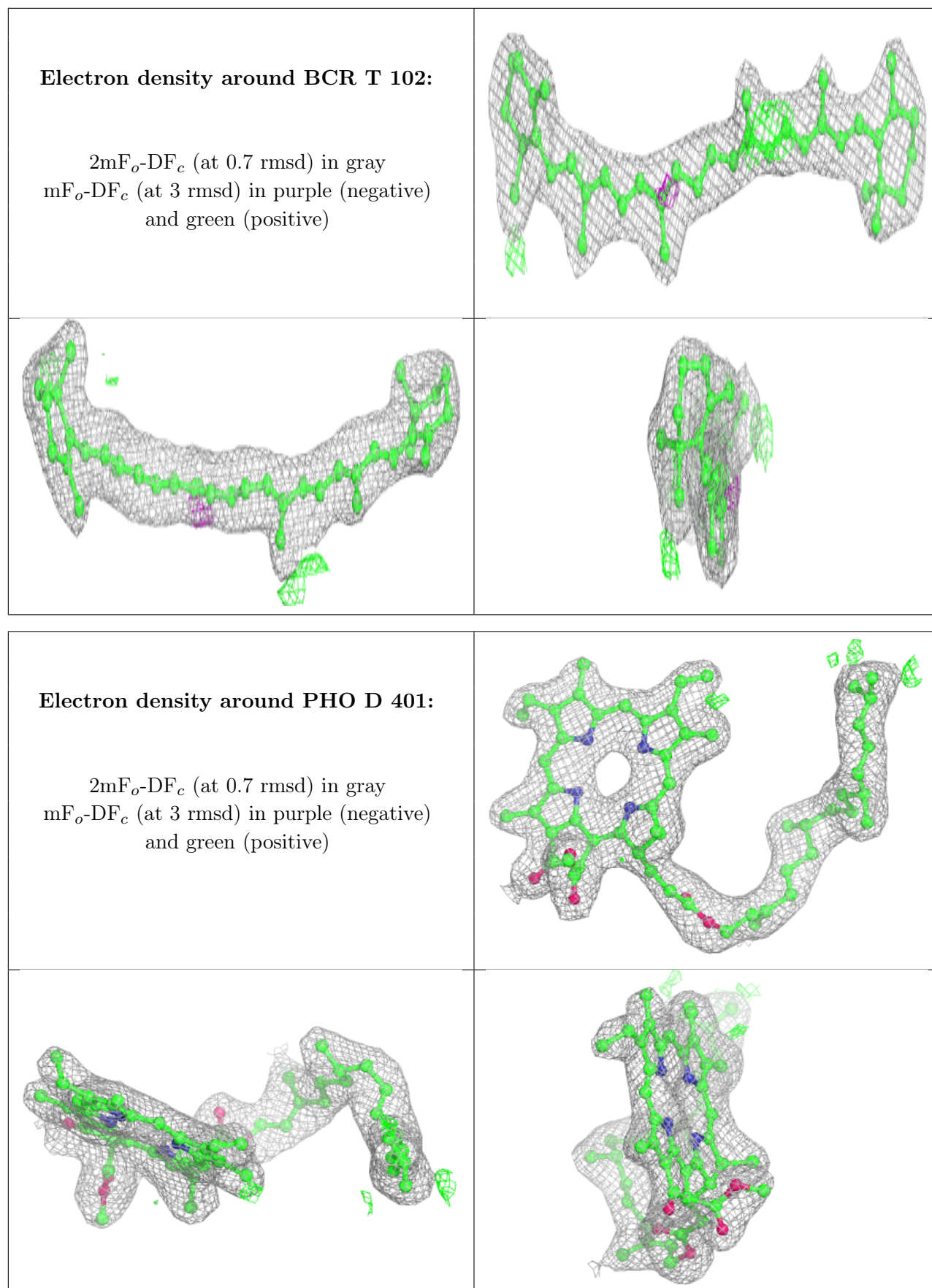
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





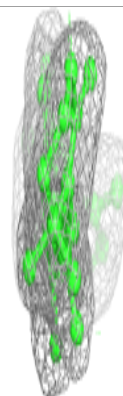
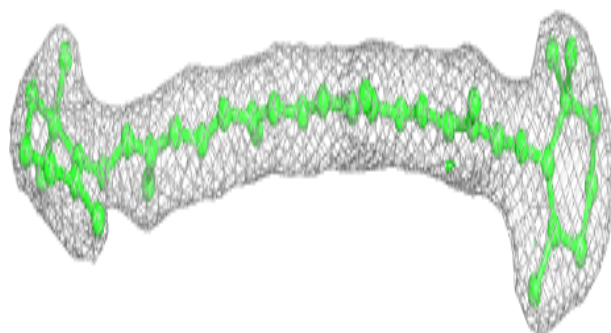
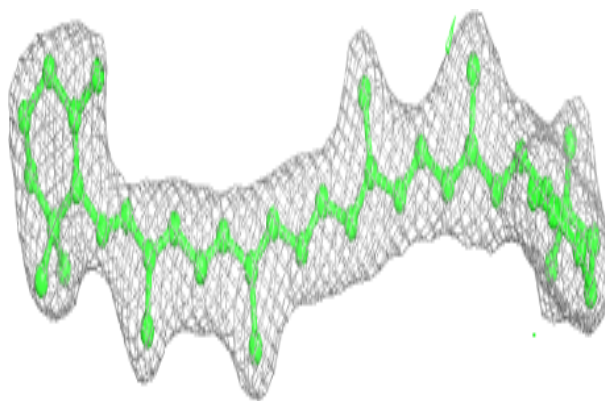




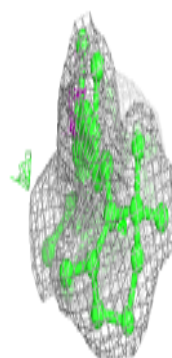
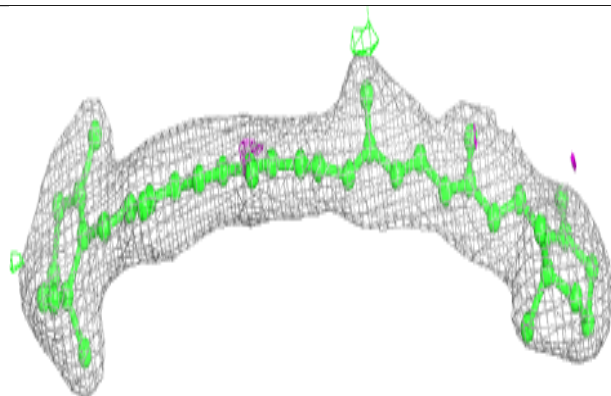
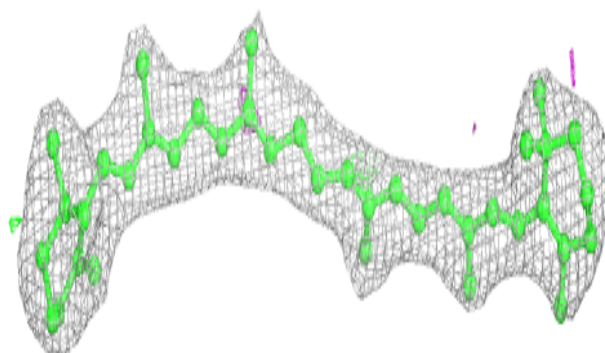


Electron density around BCR b 622:

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

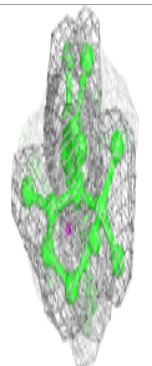
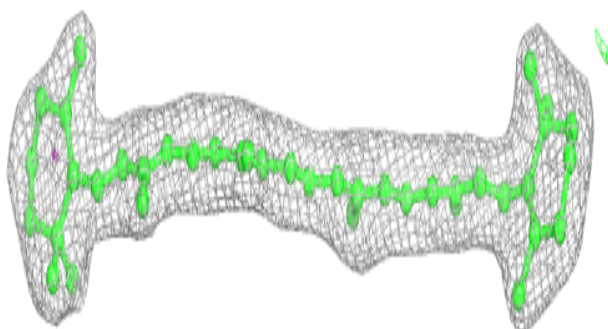
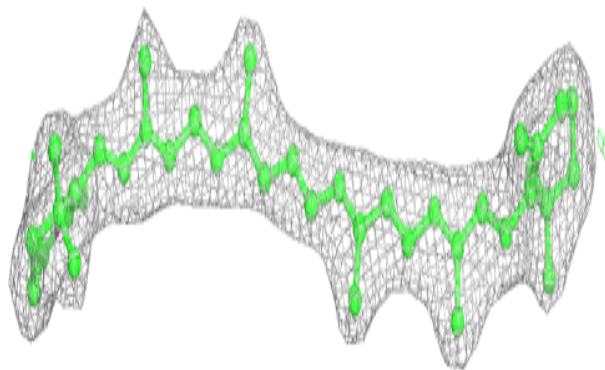
**Electron density around BCR t 102:**

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



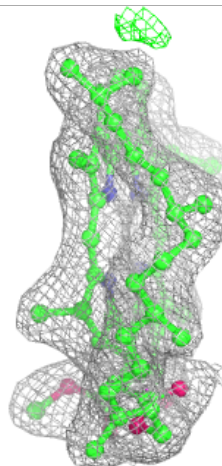
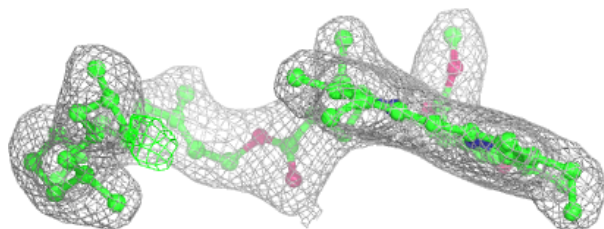
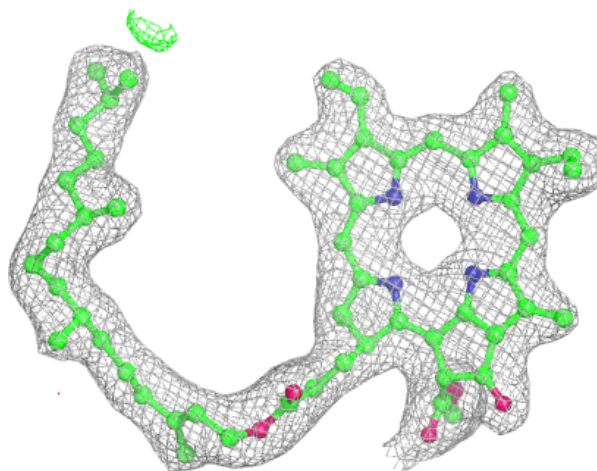
Electron density around BCR a 409:

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



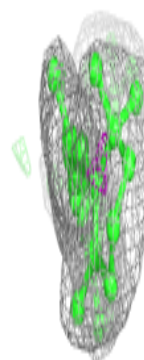
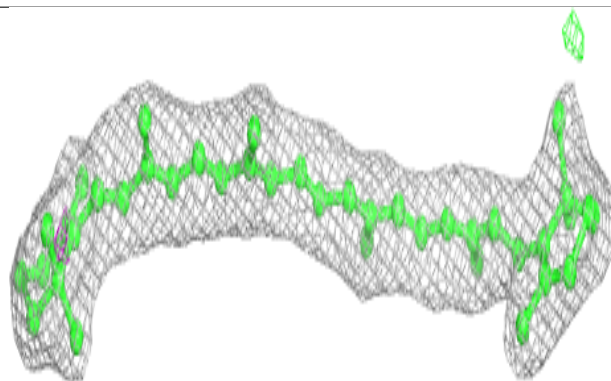
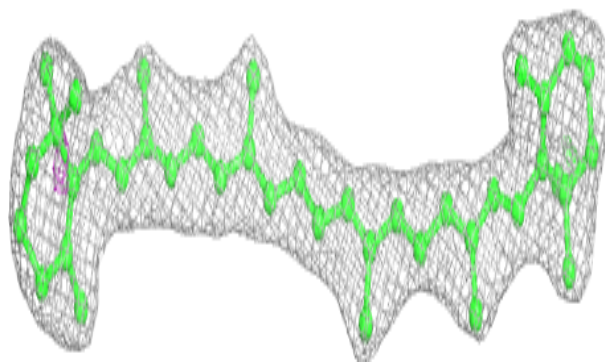
Electron density around PHO a 407:

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

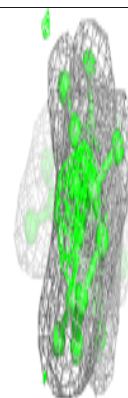
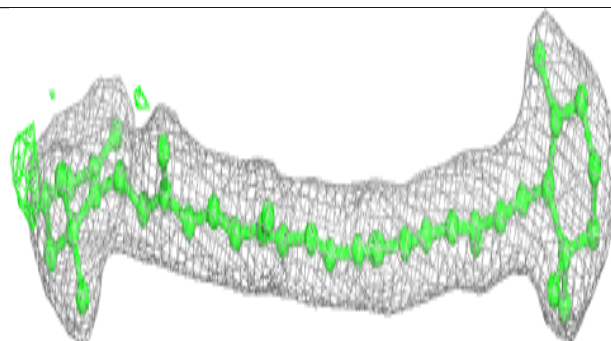
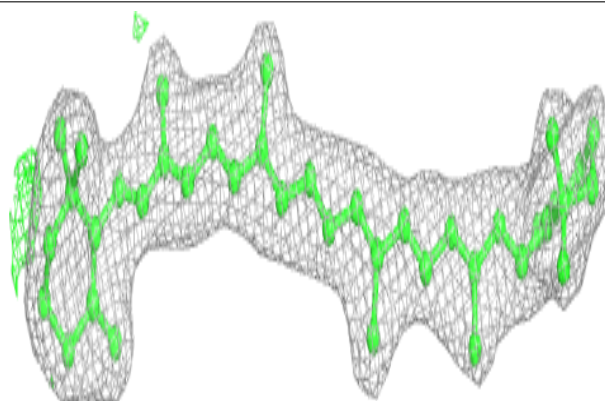


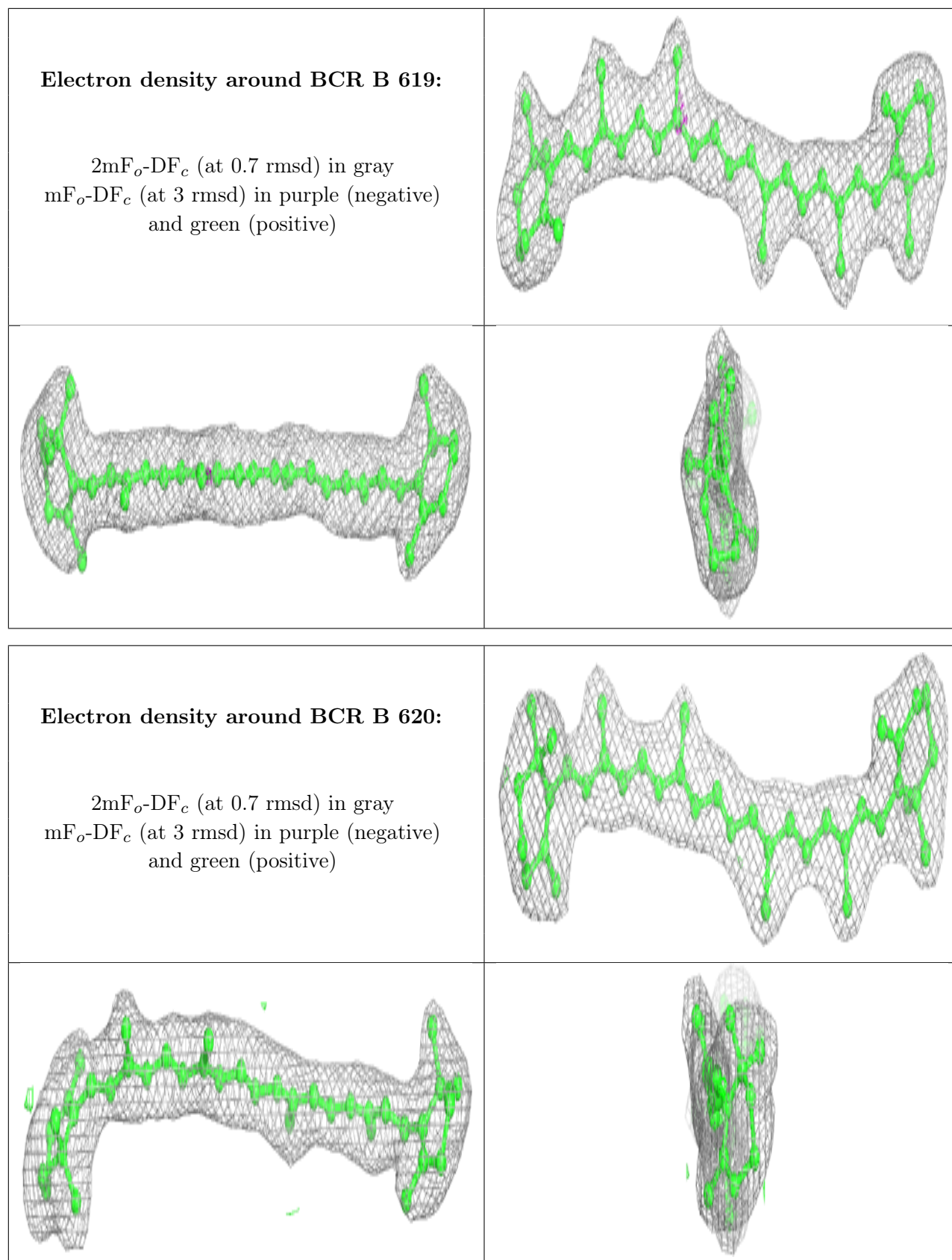
Electron density around BCR b 624:

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

**Electron density around BCR B 618:**

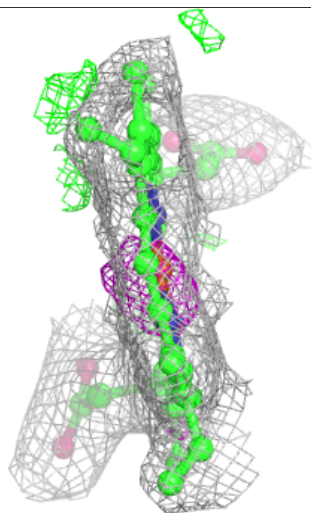
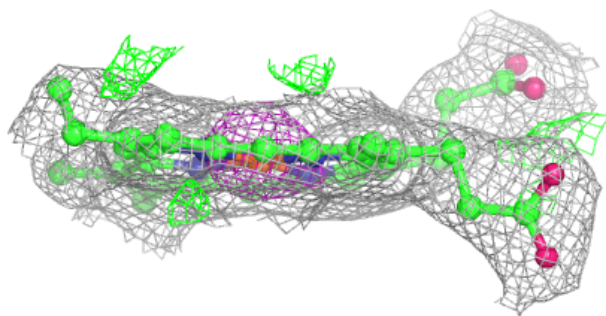
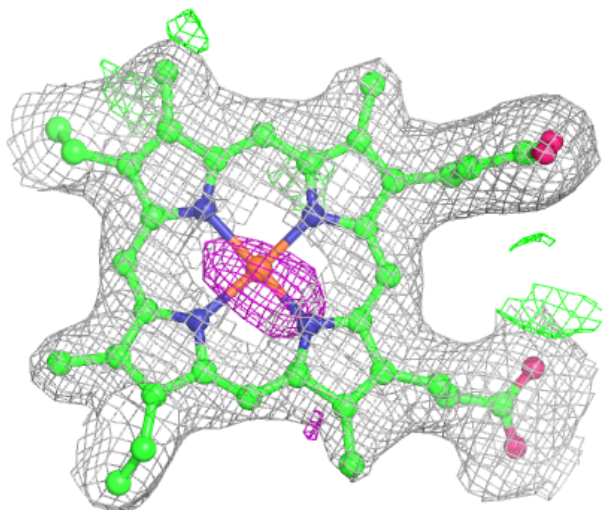
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





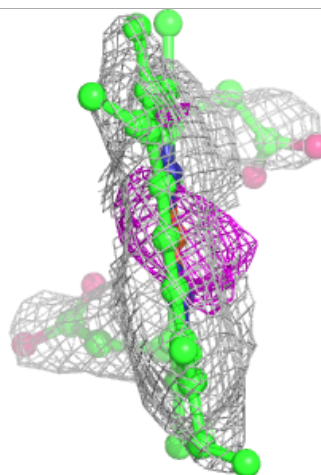
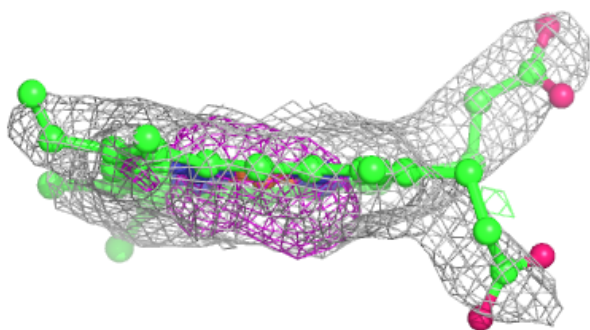
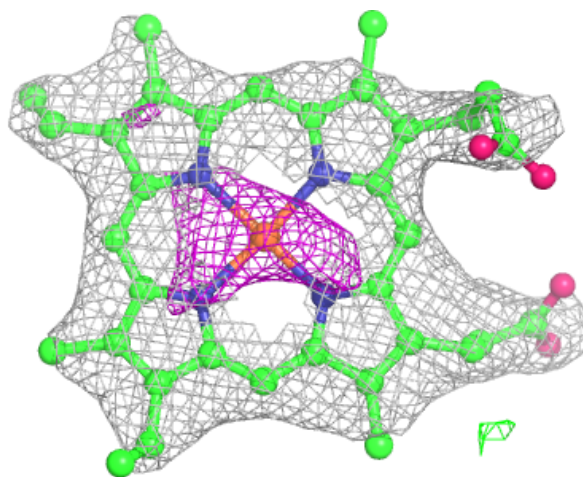
Electron density around HEM V 202:

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



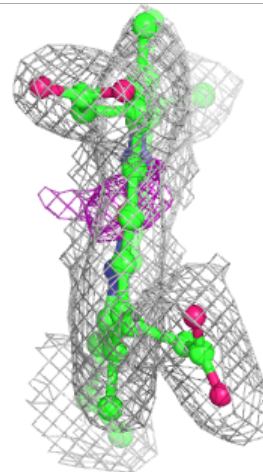
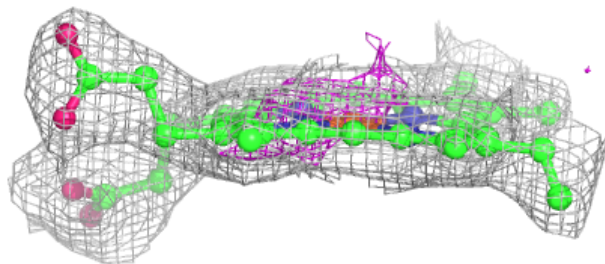
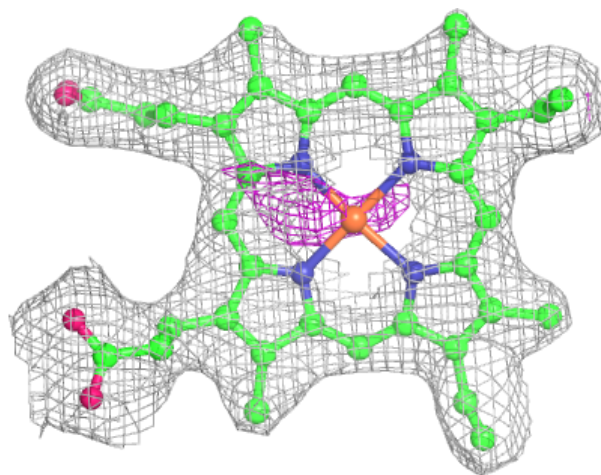
Electron density around HEM f 101:

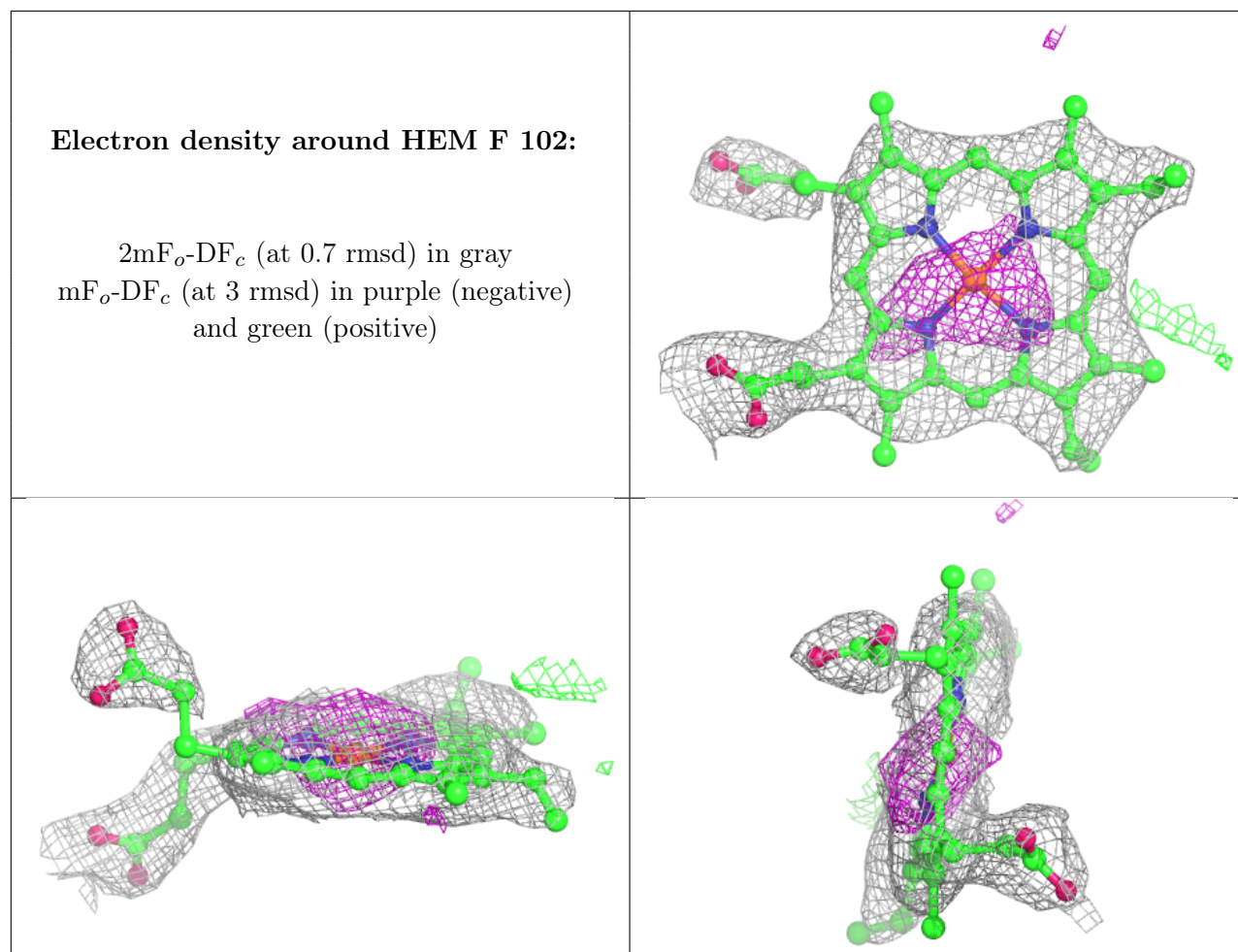
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM v 202:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.