



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2024 – 02:09 PM JST

PDB ID : 8IRE  
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)  
with a 200-nanosecond delay  
Authors : Li, H.; Suga, M.; Shen, J.R.  
Deposited on : 2023-03-17  
Resolution : 2.25 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](mailto: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

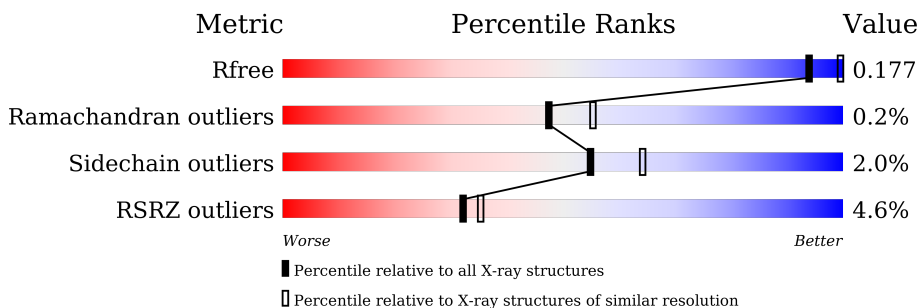
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



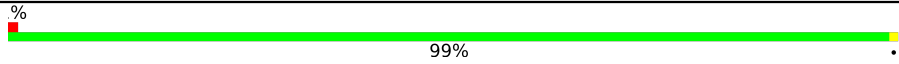
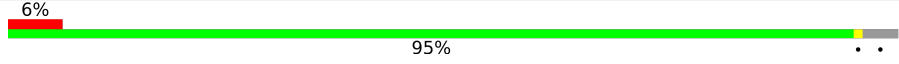
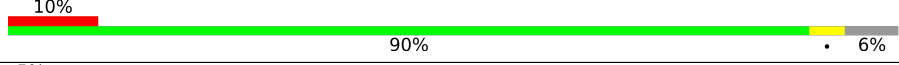

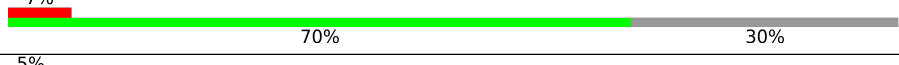
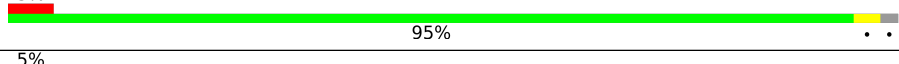
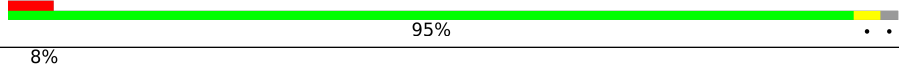
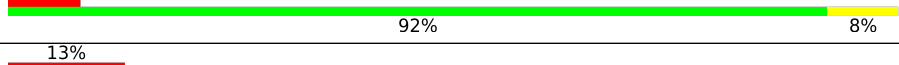
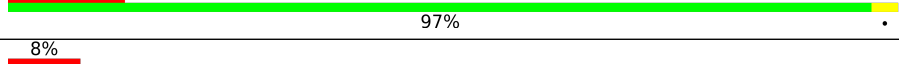
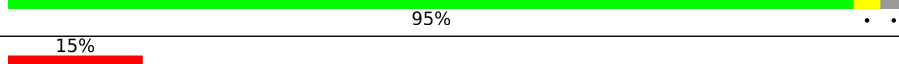
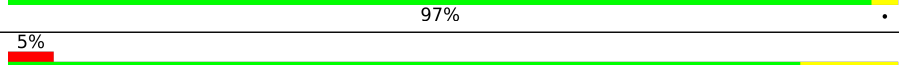
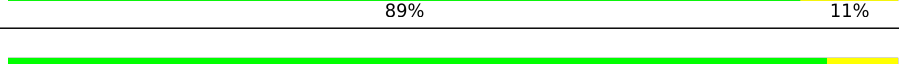
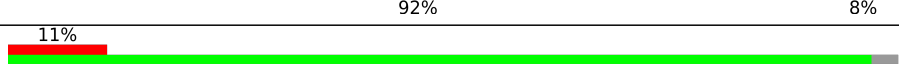
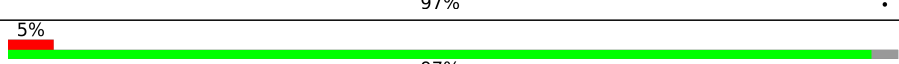
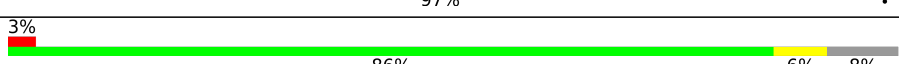
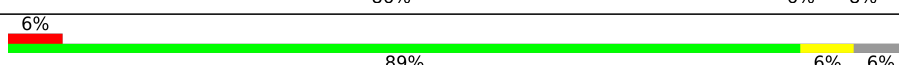
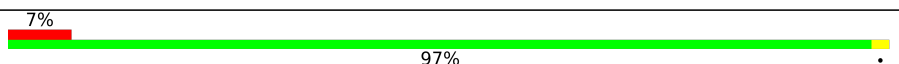
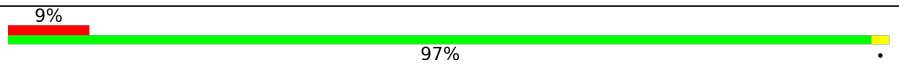
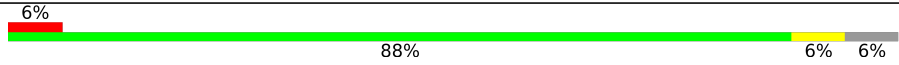
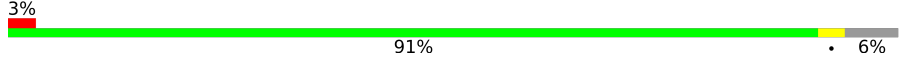
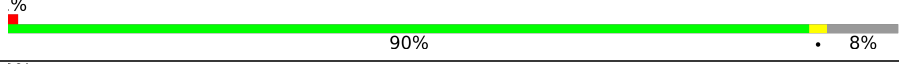
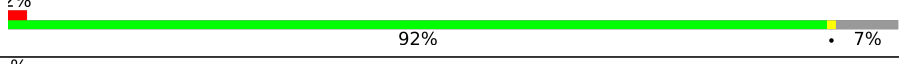
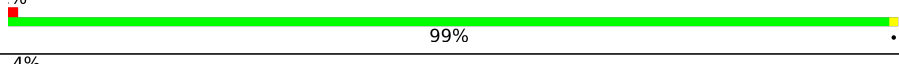
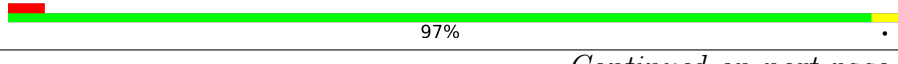

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	 97%
2	B	505	 99%
2	b	505	 98%
3	C	455	 98%
3	c	455	 98%
4	D	342	 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	d	342	 99%
5	E	84	 95%
5	e	84	 90%
6	F	44	 77%
6	f	44	 70%
7	H	65	 95%
7	h	65	 95%
8	I	38	 92%
8	i	38	 97%
9	J	39	 95%
9	j	39	 97%
10	K	37	 89%
10	k	37	 92%
11	L	37	 97%
11	l	37	 97%
12	M	36	 86%
12	m	36	 89%
13	O	244	 97%
13	o	244	 97%
14	T	32	 88%
14	t	32	 91%
15	U	104	 90%
15	u	104	 92%
16	V	137	 99%
16	v	137	 97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
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
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[A]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405[A]	X	-	-	-
23	CLA	D	405[B]	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	405[A]	X	-	-	-
23	CLA	a	405[B]	X	-	-	-
23	CLA	a	406[A]	X	-	-	-
23	CLA	a	406[B]	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	514	X	-	-	-
23	CLA	d	402[A]	X	-	-	-
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	D	701	-	X	-	-
27	GOL	a	701	-	-	-	X
30	UNL	b	626	-	-	-	X
30	UNL	c	525[A]	-	-	-	X
30	UNL	c	525[B]	-	-	-	X
32	LMT	E	102	-	-	-	X
32	LMT	a	420	-	-	-	X
32	LMT	e	102	-	-	-	X
34	HTG	b	623	-	-	-	X
37	LHG	e	101[A]	-	-	-	X
37	LHG	e	101[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 62600 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	4338	2836	717	760	25	0	222	0
1	a	334	4330	2830	716	759	25	0	221	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	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	4146	2721	692	720	13	0	20	0
2	b	504	4134	2718	687	716	13	0	19	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	4260	2788	713	741	18	0	97	0
3	c	455	4308	2821	719	750	18	0	100	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

- 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	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	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
			277	185	43	48	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	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	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	4	0
			800	508	133	159			
15	u	97	Total	C	N	O	0	4	0
			807	513	134	160			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	1	0
			289	194	46	49			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

- 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	34	Total	C	N	O	0	0	0
			273	186	47	40			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

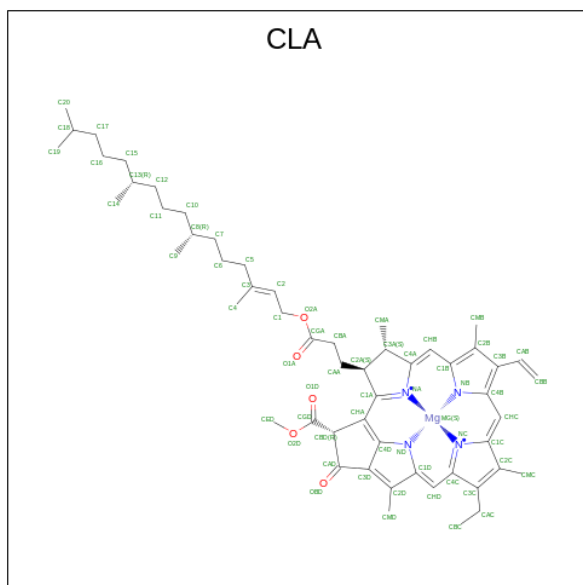
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

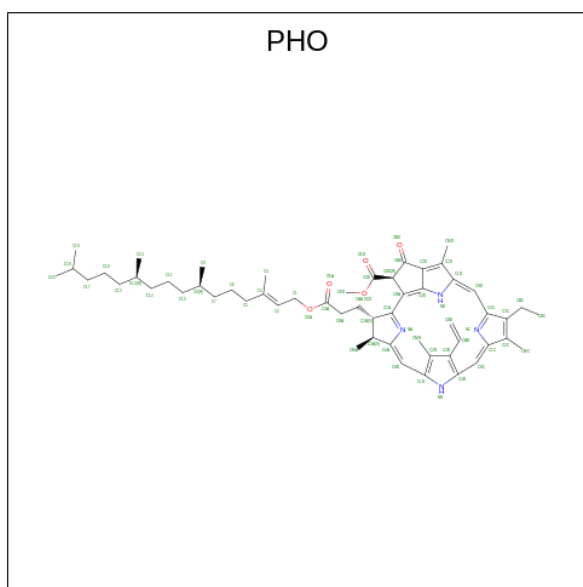
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

*Continued on next page...*

*Continued from previous page...*

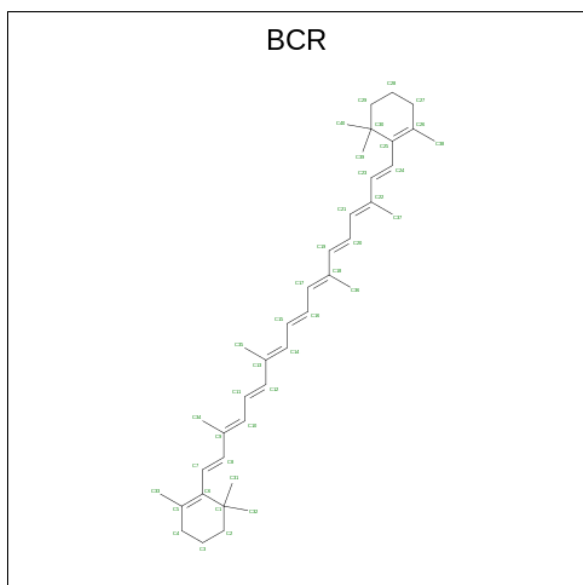
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

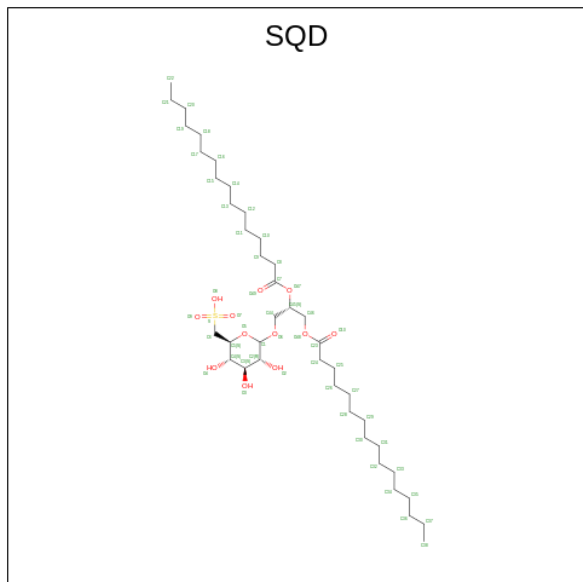
- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





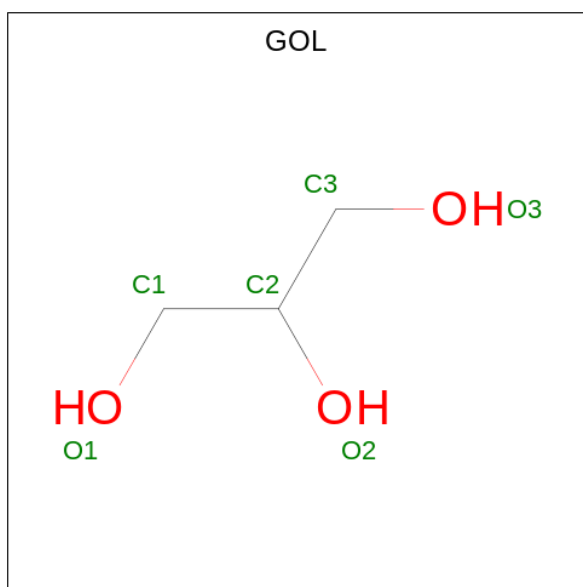
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	A	1	Total 108	C 82	O 24	S 2	0	1
26	A	1	Total 54	C 41	O 12	S 1	0	0
26	B	1	Total 54	C 41	O 12	S 1	0	0
26	F	1	Total 43	C 30	O 12	S 1	0	0
26	a	1	Total 108	C 82	O 24	S 2	0	1
26	a	1	Total 54	C 41	O 12	S 1	0	0
26	b	1	Total 54	C 41	O 12	S 1	0	0
26	f	1	Total 43	C 30	O 12	S 1	0	0

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



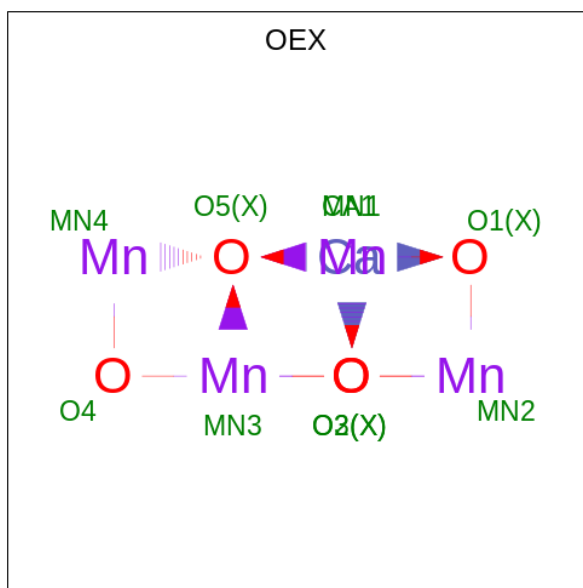
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 12 6 6	0	1
27	D	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O 12 6 6	0	1
27	a	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	1
			12	6	6		
27	c	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	1
			12	6	6		
27	o	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	1
			12	6	6		

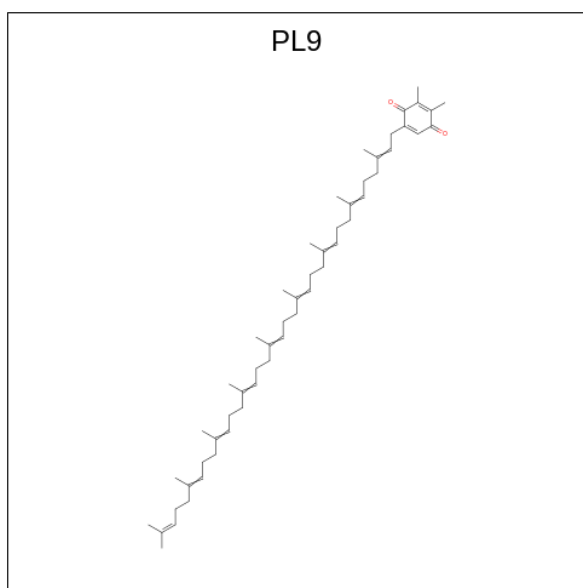
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
28	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	1
			110	106	4		
29	D	1	Total	C	O	0	1
			110	106	4		
29	a	1	Total	C	O	0	1
			110	106	4		
29	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

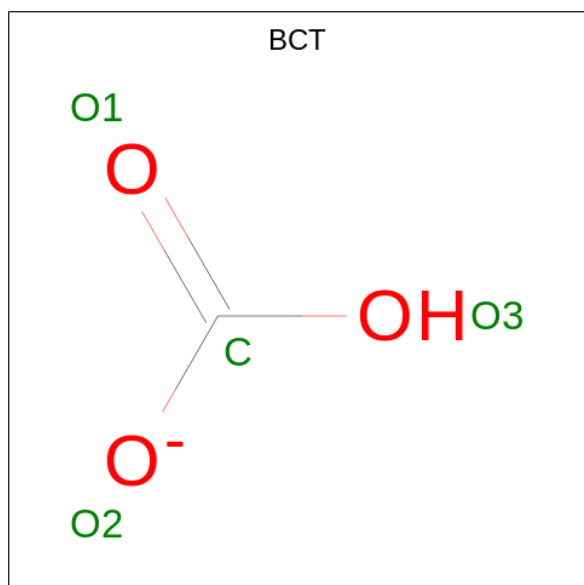
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	M	1	Total	C		0	0
			10	10			

*Continued on next page...*

Continued from previous page...

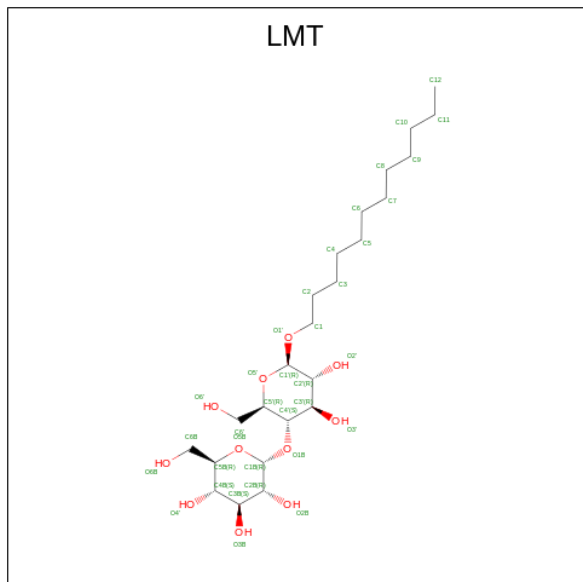
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			8	2	6		
31	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



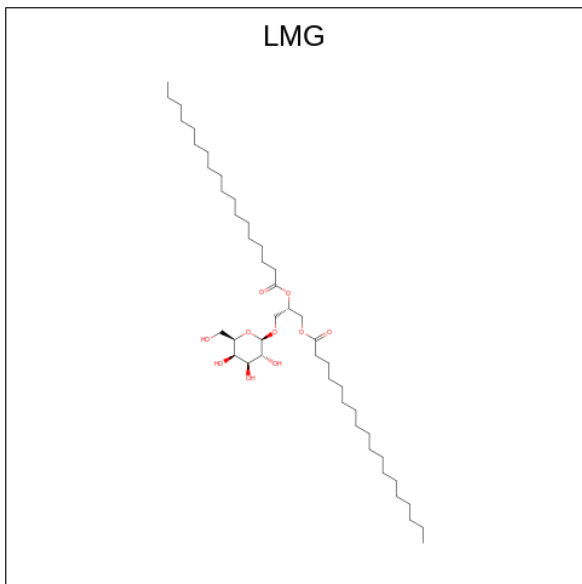
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 35 24 11	0	0
32	D	1	Total C O 35 24 11	0	0
32	E	1	Total C O 35 24 11	0	0
32	I	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 25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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	t	1	Total	C	O	0	0
			25	19	6		
32	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



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

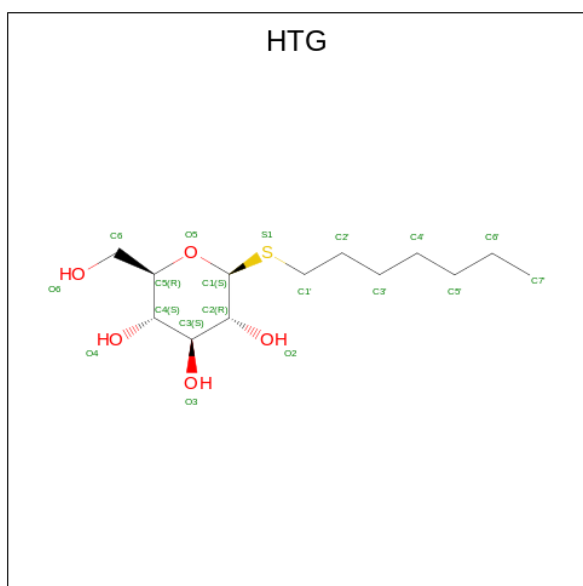
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	m	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



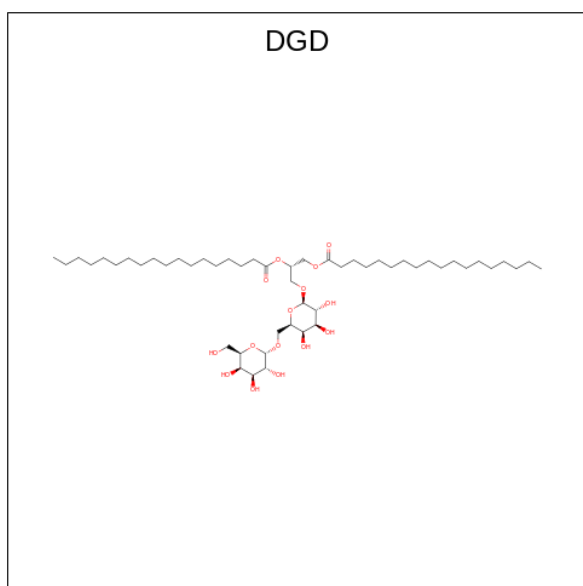
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16	10	5	1		
34	V	1	Total	C	O		0	0
			11	6	5			
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).

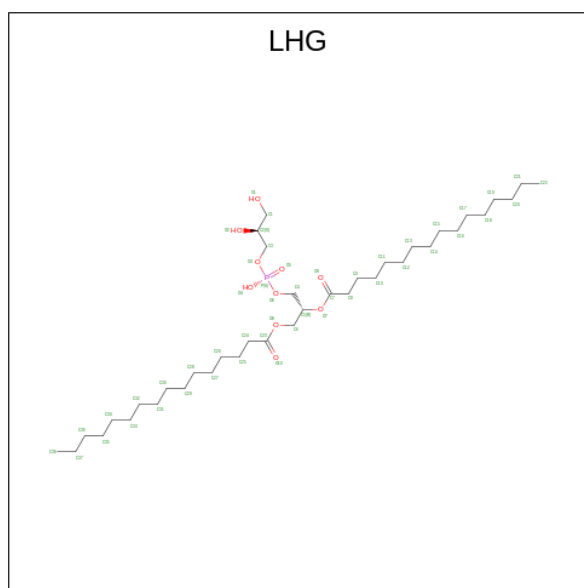


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	1
			124	94	30		
35	C	1	Total	C	O	0	1
			124	94	30		
35	C	1	Total	C	O	0	0
			62	47	15		
35	H	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	1
			124	94	30		
35	c	1	Total	C	O	0	1
			124	94	30		
35	c	1	Total	C	O	0	0
			62	47	15		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



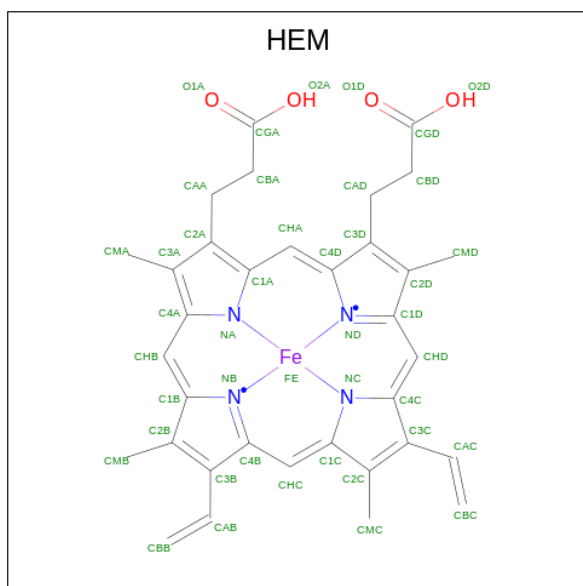
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 98 76 20 2	0	1
37	D	1	Total C O P 98 76 20 2	0	1
37	D	1	Total C O P 98 76 20 2	0	1
37	E	1	Total C O P 84 62 20 2	0	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	L	1	Total	C	O	P	0	1
			98	76	20	2		
37	d	1	Total	C	O	P	0	1
			98	76	20	2		
37	d	1	Total	C	O	P	0	1
			98	76	20	2		
37	d	1	Total	C	O	P	0	1
			98	76	20	2		
37	e	1	Total	C	O	P	0	1
			84	62	20	2		
37	l	1	Total	C	O	P	0	1
			98	76	20	2		

- 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	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

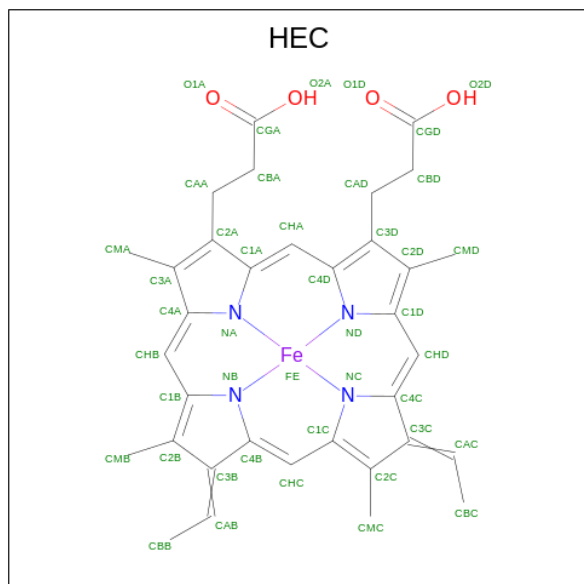
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 40 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	A	126	206	206	0	80
41	B	164	166	166	0	2
41	C	141	174	174	0	33
41	D	118	150	150	0	32
41	E	14	14	14	0	0
41	F	3	3	3	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	H	17	Total O 17 17	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	5	Total O 5 5	0	0
41	L	3	Total O 3 3	0	0
41	M	5	Total O 5 5	0	0
41	O	70	Total O 73 73	0	3
41	T	8	Total O 10 10	0	2
41	U	32	Total O 32 32	0	0
41	V	65	Total O 69 69	0	4
41	X	1	Total O 1 1	0	0
41	a	128	Total O 208 208	0	81
41	b	182	Total O 184 184	0	2
41	c	133	Total O 163 163	0	30
41	d	109	Total O 140 140	0	31
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0
41	h	15	Total O 15 15	0	0
41	i	3	Total O 3 3	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0

*Continued on next page...*

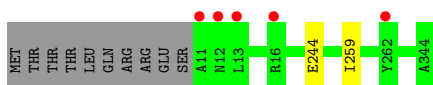
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
41	l	4	Total 4	O 4	0	0
41	m	14	Total 14	O 14	0	0
41	o	76	Total 81	O 81	0	5
41	t	6	Total 7	O 7	0	1
41	u	47	Total 48	O 48	0	1
41	v	41	Total 41	O 41	0	0
41	x	2	Total 2	O 2	0	0
41	y	1	Total 1	O 1	0	0
41	G	263	Total 286	O 286	0	24

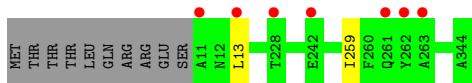
### 3 Residue-property plots [i](#)

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



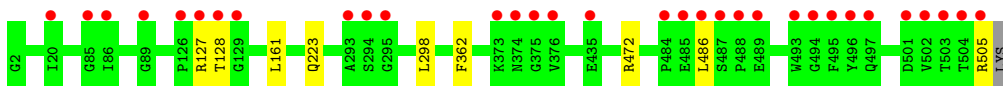
- Molecule 1: Photosystem II protein D1



- 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





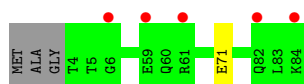
- Molecule 4: Photosystem II D2 protein



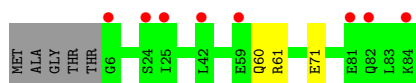
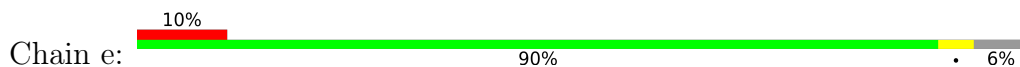
- Molecule 4: Photosystem II D2 protein



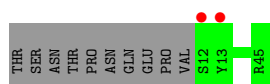
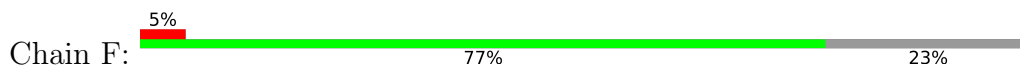
- Molecule 5: Cytochrome b559 subunit alpha



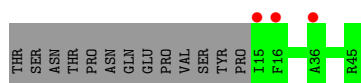
- Molecule 5: Cytochrome b559 subunit alpha



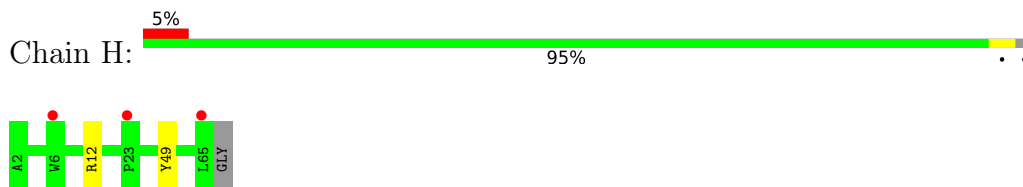
- Molecule 6: Cytochrome b559 subunit beta



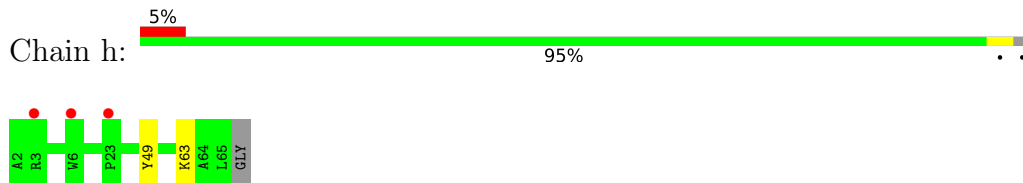
- Molecule 6: Cytochrome b559 subunit beta



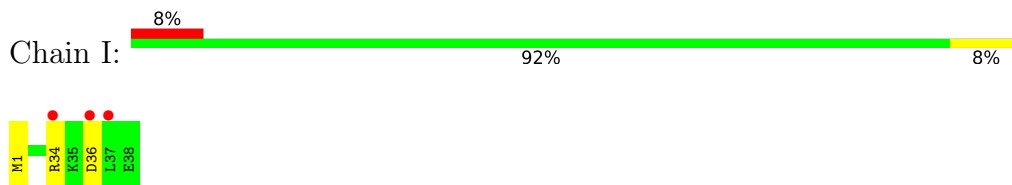
- Molecule 7: Photosystem II reaction center protein H



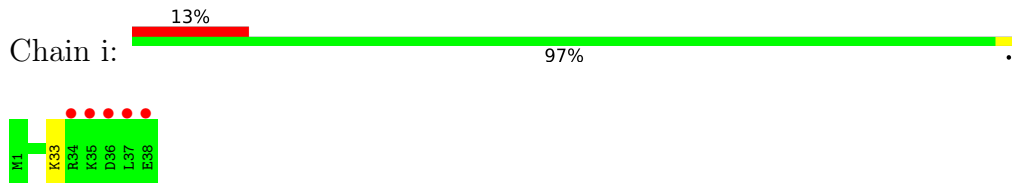
- Molecule 7: Photosystem II reaction center protein H



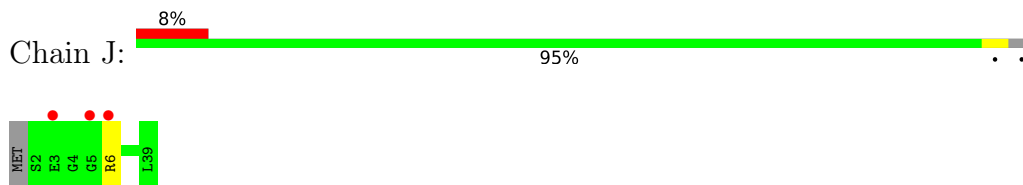
- Molecule 8: Photosystem II reaction center protein I



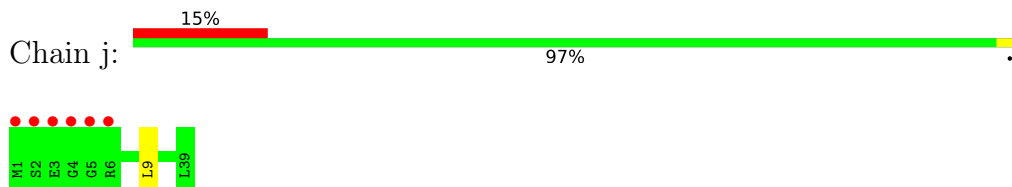
- Molecule 8: Photosystem II reaction center protein I



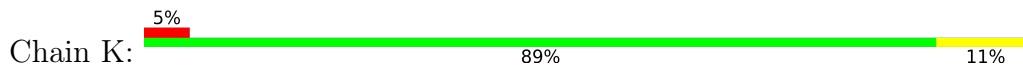
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

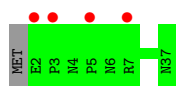




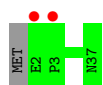
- Molecule 10: Photosystem II reaction center protein K



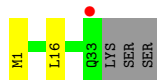
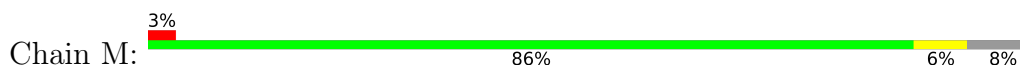
- Molecule 11: Photosystem II reaction center protein L



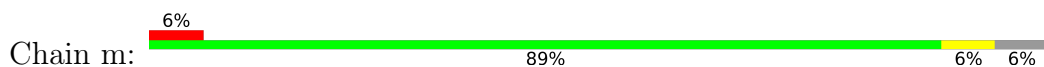
- Molecule 11: Photosystem II reaction center protein L



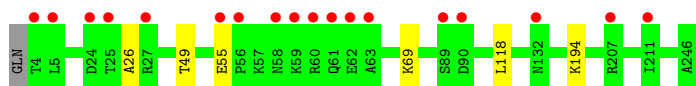
- Molecule 12: Photosystem II reaction center protein M



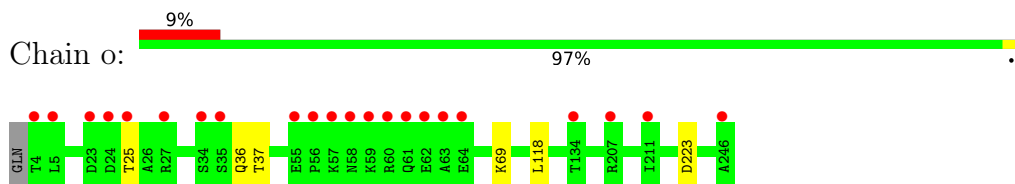
- Molecule 12: Photosystem II reaction center protein M



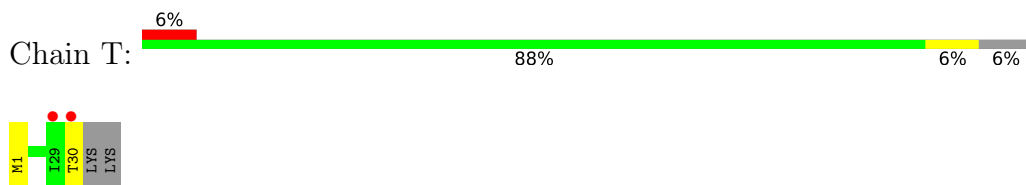
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



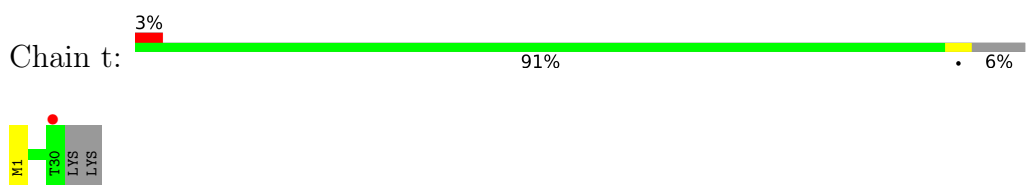
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



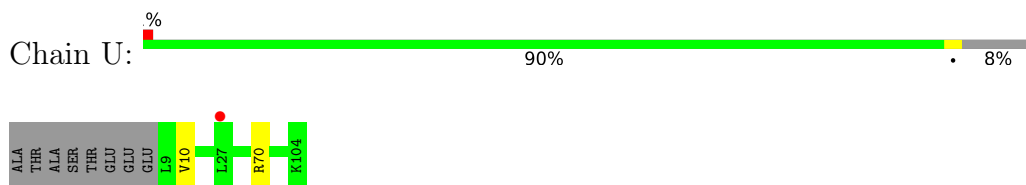
- Molecule 14: Photosystem II reaction center protein T



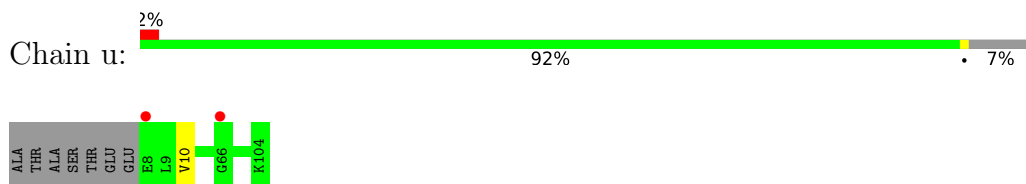
- Molecule 14: Photosystem II reaction center protein T



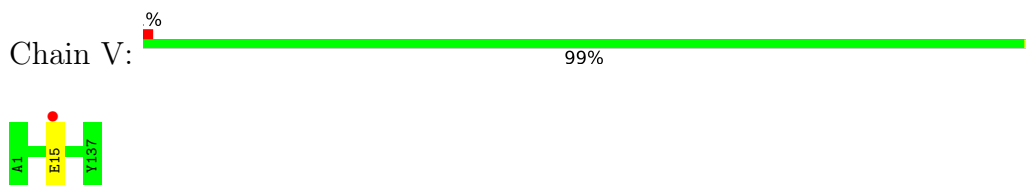
- Molecule 15: Photosystem II 12 kDa extrinsic protein



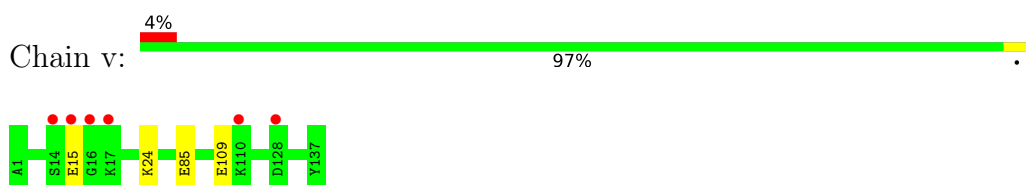
- Molecule 15: Photosystem II 12 kDa extrinsic protein



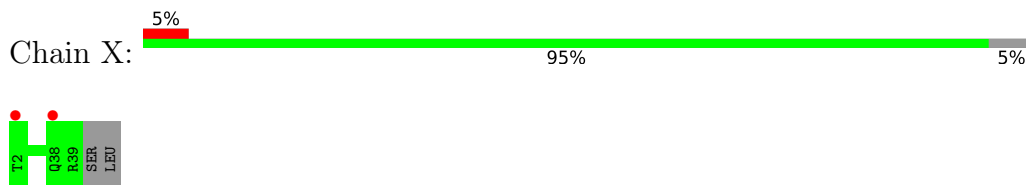
- Molecule 16: Cytochrome c-550



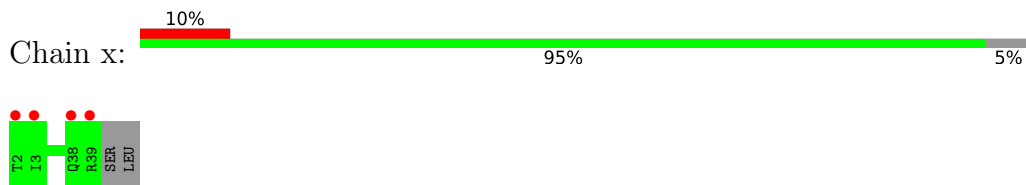
- Molecule 16: Cytochrome c-550



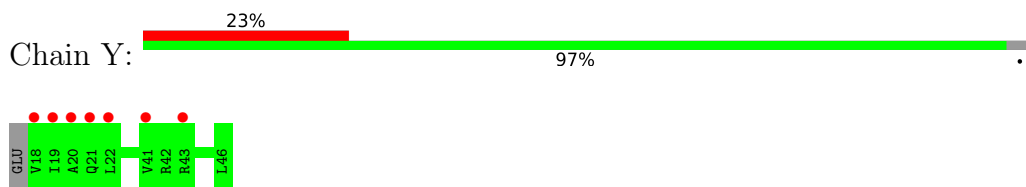
- Molecule 17: Photosystem II reaction center protein X



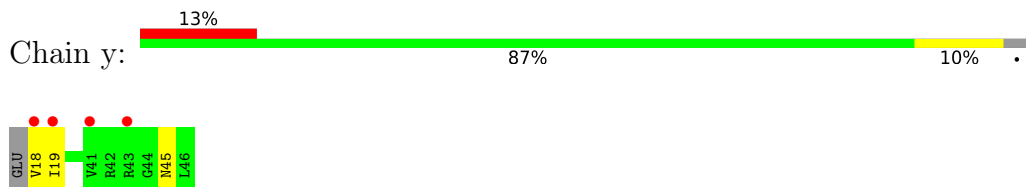
- Molecule 17: Photosystem II reaction center protein X



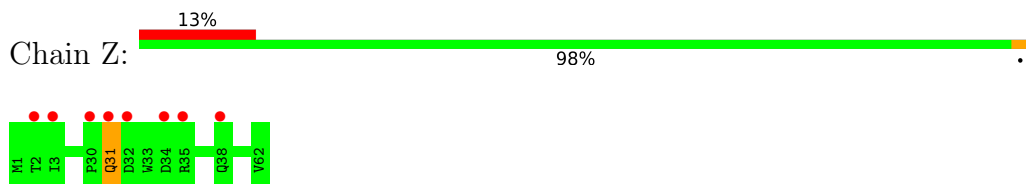
- Molecule 18: Photosystem II reaction center protein Ycf12



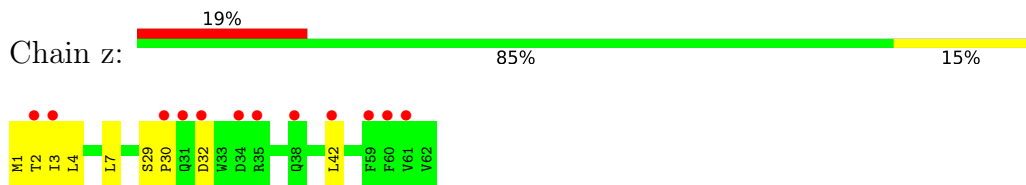
- Molecule 18: Photosystem II reaction center protein Ycf12



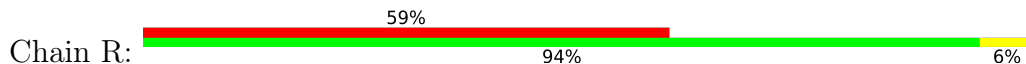
- Molecule 19: Photosystem II reaction center protein Z

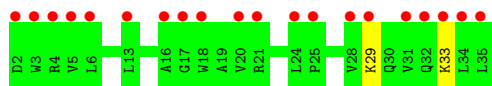


- Molecule 19: Photosystem II reaction center protein Z



- 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, $\alpha$ , $\beta$ , $\gamma$	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 100.0 (19.99-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.26Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.139 , 0.177 0.139 , 0.177	Depositor DCC
$R_{free}$ test set	19880 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtrriage
Anisotropy	0.483	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 86.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	62600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.44	0/4478	0.58	0/6098
1	a	0.42	0/4470	0.56	0/6087
2	B	0.45	0/4293	0.59	0/5851
2	b	0.44	0/4285	0.58	0/5841
3	C	0.41	0/4404	0.55	0/5997
3	c	0.40	0/4459	0.55	0/6071
4	D	0.48	0/3741	0.60	0/5095
4	d	0.45	0/3749	0.57	0/5106
5	E	0.41	0/681	0.58	0/928
5	e	0.39	0/690	0.54	0/939
6	F	0.41	0/284	0.54	0/387
6	f	0.37	0/269	0.52	0/365
7	H	0.40	0/519	0.62	0/708
7	h	0.38	0/530	0.59	0/722
8	I	0.39	0/311	0.55	0/419
8	i	0.41	0/311	0.57	0/419
9	J	0.38	0/278	0.54	0/376
9	j	0.38	0/283	0.56	0/383
10	K	0.38	0/303	0.51	0/416
10	k	0.40	0/303	0.51	0/416
11	L	0.41	0/318	0.57	0/433
11	l	0.48	0/318	0.54	0/433
12	M	0.47	0/261	0.50	0/357
12	m	0.41	0/279	0.53	0/380
13	O	0.42	0/1991	0.64	0/2698
13	o	0.41	0/1966	0.65	1/2665 (0.0%)
14	T	0.47	0/310	0.63	0/419
14	t	0.45	0/301	0.60	0/406
15	U	0.46	0/811	0.61	0/1095
15	u	0.45	0/818	0.63	0/1105
16	V	0.42	0/1142	0.58	0/1545



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.36	0/1139	0.55	0/1542
17	X	0.33	0/292	0.50	0/395
17	x	0.34	0/284	0.48	0/384
18	Y	0.32	0/216	0.54	0/289
18	y	0.31	0/216	0.51	0/289
19	Z	0.34	0/490	0.46	0/669
19	z	0.33	0/490	0.43	0/669
20	R	0.31	0/279	0.52	0/383
All	All	0.43	0/50562	0.57	1/68780 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	223	ASP	CB-CG-OD1	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	34	37
1	a	552/344 (160%)	544 (99%)	6 (1%)	2 (0%)	34	37
2	B	522/505 (103%)	514 (98%)	8 (2%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	546/455 (120%)	540 (99%)	5 (1%)	1 (0%)	47	55
3	c	553/455 (122%)	540 (98%)	12 (2%)	1 (0%)	47	55
4	D	453/342 (132%)	438 (97%)	15 (3%)	0	100	100
4	d	454/342 (133%)	443 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	9	5
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	34	37
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	98/104 (94%)	94 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	4
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6038 (98%)	122 (2%)	11 (0%)	47	55

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO

### 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	444/279 (159%)	442 (100%)	2 (0%)	88	92
1	a	443/279 (159%)	442 (100%)	1 (0%)	93	96
2	B	421/403 (104%)	416 (99%)	5 (1%)	71	80
2	b	420/403 (104%)	410 (98%)	10 (2%)	49	58
3	C	430/356 (121%)	424 (99%)	6 (1%)	67	76
3	c	436/356 (122%)	429 (98%)	7 (2%)	62	73
4	D	368/277 (133%)	366 (100%)	2 (0%)	88	92
4	d	369/277 (133%)	364 (99%)	5 (1%)	67	76
5	E	72/73 (99%)	71 (99%)	1 (1%)	67	76
5	e	72/73 (99%)	69 (96%)	3 (4%)	30	34
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/54 (100%)	52 (96%)	2 (4%)	34	40
7	h	55/54 (102%)	54 (98%)	1 (2%)	59	68
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	51
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	51
9	J	26/27 (96%)	25 (96%)	1 (4%)	33	39
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	39
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	28 (93%)	2 (7%)	16	15
12	m	32/32 (100%)	30 (94%)	2 (6%)	18	17
13	O	216/207 (104%)	211 (98%)	5 (2%)	50	59
13	o	213/207 (103%)	208 (98%)	5 (2%)	50	59
14	T	32/28 (114%)	30 (94%)	2 (6%)	18	17
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	50	59
15	u	87/89 (98%)	85 (98%)	2 (2%)	50	59
16	V	123/117 (105%)	122 (99%)	1 (1%)	81	88
16	v	123/117 (105%)	119 (97%)	4 (3%)	38	46
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	2
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	66
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	R	29/29 (100%)	27 (93%)	2 (7%)	15	14
All	All	5103/4403 (116%)	5008 (98%)	95 (2%)	55	66

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	230[A]	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	o	36	GLN
5	e	60	GLN
10	k	10	LYS
15	u	10[A]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	60	GLN
3	c	28	GLN
11	l	8	GLN
13	o	58	ASN
16	v	86	GLN

### 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	$\# Z  > 2$
12	FME	m	1	-	8,9,10	0.56	0	7,9,11	1.53	2 (28%)
8	FME	I	1	-	8,9,10	0.59	0	7,9,11	1.19	1 (14%)
12	FME	M	1	-	8,9,10	0.60	0	7,9,11	1.15	1 (14%)
14	FME	T	1	-	8,9,10	0.60	0	7,9,11	1.49	1 (14%)
14	FME	t	1	-	8,9,10	0.74	0	7,9,11	1.51	1 (14%)
8	FME	i	1	-	8,9,10	0.71	0	7,9,11	1.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	-2.59	118.84	122.82
14	T	1	FME	CG-CB-CA	2.48	119.83	112.95
14	t	1	FME	O-C-CA	-2.46	118.34	124.78
12	m	1	FME	O1-CN-N	-2.34	119.10	125.27
8	I	1	FME	O-C-CA	-2.16	119.11	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	601	-	65,73,73	2.06	17 (26%)	76,113,113	2.78	25 (32%)
23	CLA	B	616	-	65,73,73	2.07	16 (24%)	76,113,113	2.74	27 (35%)
23	CLA	c	510	-	65,73,73	2.06	16 (24%)	76,113,113	2.82	29 (38%)
25	BCR	A	409	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	9 (16%)
23	CLA	a	406[A]	-	65,73,73	2.02	15 (23%)	76,113,113	2.80	29 (38%)
32	LMT	M	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.05	2 (4%)
29	PL9	A	414[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
24	PHO	a	408[B]	-	51,69,69	1.83	8 (15%)	47,99,99	1.77	9 (19%)
27	GOL	c	742[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
35	DGD	c	517[B]	-	63,63,67	0.88	2 (3%)	77,77,81	1.06	6 (7%)
25	BCR	b	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.31	5 (8%)
32	LMT	M	101	-	36,36,36	1.12	4 (11%)	47,47,47	1.22	4 (8%)
32	LMT	t	101	-	25,25,36	0.91	2 (8%)	30,30,47	1.16	3 (10%)
37	LHG	d	711[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
23	CLA	a	406[B]	-	65,73,73	2.05	15 (23%)	76,113,113	2.79	30 (39%)
23	CLA	c	509	-	65,73,73	2.10	17 (26%)	76,113,113	2.73	27 (35%)
25	BCR	a	410	-	41,41,41	1.08	1 (2%)	56,56,56	1.37	9 (16%)
26	SQD	a	411[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
25	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.53	13 (23%)
27	GOL	c	742[B]	-	5,5,5	0.98	0	5,5,5	0.90	0
23	CLA	C	503	-	65,73,73	2.09	15 (23%)	76,113,113	2.68	27 (35%)
29	PL9	A	414[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.99	23 (33%)
28	OEX	a	415[A]	-	0,15,15	-	-	-	-	-
23	CLA	B	602	-	65,73,73	2.07	17 (26%)	76,113,113	2.88	34 (44%)
27	GOL	b	901	-	5,5,5	0.54	0	5,5,5	1.40	1 (20%)
32	LMT	I	101	-	36,36,36	1.04	2 (5%)	47,47,47	1.19	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	LHG	d	711[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
23	CLA	c	504	-	65,73,73	2.04	17 (26%)	76,113,113	2.78	25 (32%)
23	CLA	b	614	-	65,73,73	2.02	16 (24%)	76,113,113	2.89	27 (35%)
26	SQD	a	411[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.68	12 (19%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.60	15 (26%)
33	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.14	5 (8%)
28	OEX	a	415[B]	-	0,15,15	-	-	-	-	-
32	LMT	a	414	-	36,36,36	1.02	2 (5%)	47,47,47	1.17	5 (10%)
37	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	B	614	-	65,73,73	2.02	17 (26%)	76,113,113	3.01	30 (39%)
37	LHG	D	411[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
23	CLA	a	405[A]	-	65,73,73	2.01	16 (24%)	76,113,113	2.86	32 (42%)
23	CLA	C	505	-	65,73,73	1.98	15 (23%)	76,113,113	2.86	27 (35%)
27	GOL	b	624	-	5,5,5	1.12	1 (20%)	5,5,5	0.77	0
32	LMT	a	420	-	36,36,36	0.98	2 (5%)	47,47,47	1.04	2 (4%)
37	LHG	d	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
34	HTG	V	203	-	11,11,19	0.29	0	15,15,24	1.28	1 (6%)
32	LMT	D	404	-	36,36,36	1.18	4 (11%)	47,47,47	1.38	5 (10%)
37	LHG	D	411[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
26	SQD	A	410[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.72	11 (17%)
23	CLA	a	405[B]	-	65,73,73	2.10	17 (26%)	76,113,113	2.76	30 (39%)
23	CLA	c	511	-	65,73,73	1.99	14 (21%)	76,113,113	2.79	30 (39%)
34	HTG	b	625	-	19,19,19	1.06	2 (10%)	23,24,24	1.53	3 (13%)
27	GOL	A	411	-	5,5,5	1.09	0	5,5,5	0.78	0
23	CLA	c	503	-	65,73,73	2.00	13 (20%)	76,113,113	2.68	25 (32%)
34	HTG	D	414	-	16,16,19	0.98	1 (6%)	20,21,24	1.60	1 (5%)
25	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.32	8 (14%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
23	CLA	b	605	-	65,73,73	1.94	17 (26%)	76,113,113	2.96	27 (35%)
23	CLA	d	402[A]	-	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
23	CLA	C	510	-	65,73,73	2.11	17 (26%)	76,113,113	2.75	28 (36%)
25	BCR	K	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.50	13 (23%)
27	GOL	a	412	-	5,5,5	0.88	0	5,5,5	1.00	0
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.10	4 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	GOL	a	701	-	5,5,5	1.07	0	5,5,5	1.02	0
38	HEM	E	103	-	41,50,50	1.30	7 (17%)	45,82,82	2.10	12 (26%)
35	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.94	5 (6%)
23	CLA	B	606	-	65,73,73	1.93	15 (23%)	76,113,113	2.98	30 (39%)
23	CLA	b	608	-	65,73,73	2.01	16 (24%)	76,113,113	2.78	32 (42%)
35	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.01	4 (5%)
35	DGD	c	519	-	63,63,67	0.87	4 (6%)	77,77,81	1.06	4 (5%)
24	PHO	A	407[A]	-	51,69,69	1.77	8 (15%)	47,99,99	1.69	10 (21%)
33	LMG	C	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.61	8 (13%)
23	CLA	B	612	-	65,73,73	2.01	19 (29%)	76,113,113	2.73	28 (36%)
23	CLA	C	513	-	65,73,73	2.04	15 (23%)	76,113,113	2.76	32 (42%)
33	LMG	m	101	-	51,51,55	0.86	2 (3%)	59,59,63	1.32	7 (11%)
35	DGD	C	518[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
37	LHG	D	410[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	B	615	-	65,73,73	2.03	16 (24%)	76,113,113	2.85	27 (35%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.34	3 (5%)
34	HTG	B	622	-	19,19,19	1.08	2 (10%)	23,24,24	1.56	5 (21%)
26	SQD	b	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.70	12 (19%)
40	HEC	v	202	-	32,50,50	1.96	3 (9%)	24,82,82	2.07	6 (25%)
25	BCR	B	617	-	41,41,41	1.09	1 (2%)	56,56,56	1.27	8 (14%)
23	CLA	C	507	-	65,73,73	2.04	17 (26%)	76,113,113	2.78	29 (38%)
24	PHO	A	407[B]	-	51,69,69	1.80	7 (13%)	47,99,99	1.75	11 (23%)
32	LMT	A	359	-	36,36,36	0.91	0	47,47,47	1.10	1 (2%)
26	SQD	f	102	-	42,43,54	1.21	3 (7%)	51,54,65	1.48	12 (23%)
25	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.38	8 (14%)
27	GOL	v	401[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
33	LMG	d	412	-	51,51,55	0.89	2 (3%)	59,59,63	1.14	5 (8%)
34	HTG	B	623	-	19,19,19	0.76	1 (5%)	23,24,24	1.43	1 (4%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.30	4 (7%)
35	DGD	C	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	C	508	-	65,73,73	1.95	16 (24%)	76,113,113	2.70	28 (36%)
37	LHG	D	410[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.99	4 (7%)
37	LHG	l	101[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
27	GOL	o	601	-	5,5,5	1.15	1 (20%)	5,5,5	1.09	0
23	CLA	B	610	-	65,73,73	2.03	16 (24%)	76,113,113	2.80	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	607	-	65,73,73	2.01	17 (26%)	76,113,113	2.83	26 (34%)
33	LMG	D	415	-	51,51,55	0.81	2 (3%)	59,59,63	1.07	3 (5%)
34	HTG	C	522	-	19,19,19	0.84	1 (5%)	23,24,24	1.23	1 (4%)
27	GOL	v	401[B]	-	5,5,5	1.02	0	5,5,5	0.86	0
25	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	8 (14%)
23	CLA	B	605	-	65,73,73	1.99	16 (24%)	76,113,113	2.92	29 (38%)
37	LHG	l	101[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	2 (3%)
25	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	2.00	17 (30%)
23	CLA	c	512	-	65,73,73	2.09	17 (26%)	76,113,113	2.83	29 (38%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.13	5 (6%)
32	LMT	b	621	-	25,25,36	0.96	1 (4%)	30,30,47	1.21	3 (10%)
31	BCT	a	404[A]	-	2,3,3	0.59	0	2,3,3	1.49	0
23	CLA	c	506	-	65,73,73	1.99	16 (24%)	76,113,113	2.69	25 (32%)
35	DGD	C	517[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
24	PHO	a	353[A]	-	51,69,69	1.88	8 (15%)	47,99,99	1.99	12 (25%)
33	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.33	6 (10%)
23	CLA	b	606	-	65,73,73	2.01	16 (24%)	76,113,113	2.83	28 (36%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.29	4 (6%)
29	PL9	d	405[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
33	LMG	Z	101	-	37,37,55	1.02	2 (5%)	45,45,63	1.42	6 (13%)
27	GOL	d	701	-	5,5,5	1.26	1 (20%)	5,5,5	1.00	0
35	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	7 (9%)
23	CLA	b	613	-	65,73,73	1.97	17 (26%)	76,113,113	2.77	30 (39%)
25	BCR	t	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.63	11 (19%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.30	7 (11%)
23	CLA	b	612	-	65,73,73	2.04	15 (23%)	76,113,113	2.73	27 (35%)
24	PHO	a	353[B]	-	51,69,69	1.90	8 (15%)	47,99,99	1.94	11 (23%)
34	HTG	B	626	-	19,19,19	1.10	2 (10%)	23,24,24	1.34	3 (13%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	7 (12%)
32	LMT	E	102	-	36,36,36	1.03	1 (2%)	47,47,47	1.01	2 (4%)
29	PL9	d	405[B]	-	55,55,55	0.65	1 (1%)	68,69,69	1.65	17 (25%)
23	CLA	A	408	-	65,73,73	2.05	15 (23%)	76,113,113	2.93	30 (39%)
23	CLA	C	502	-	65,73,73	1.99	17 (26%)	76,113,113	2.83	28 (36%)
23	CLA	d	402[B]	-	65,73,73	2.03	16 (24%)	76,113,113	2.82	29 (38%)
23	CLA	C	509	-	65,73,73	2.06	16 (24%)	76,113,113	2.71	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	D	405[A]	-	65,73,73	2.04	16 (24%)	76,113,113	2.87	31 (40%)
23	CLA	C	514	-	65,73,73	2.07	16 (24%)	76,113,113	2.77	28 (36%)
27	GOL	d	801[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
23	CLA	B	603	-	65,73,73	2.05	17 (26%)	76,113,113	2.93	28 (36%)
23	CLA	B	611	-	65,73,73	2.76	17 (26%)	76,113,113	3.22	26 (34%)
27	GOL	D	701	-	5,5,5	1.52	2 (40%)	5,5,5	0.76	0
23	CLA	B	609	-	65,73,73	1.99	15 (23%)	76,113,113	2.70	28 (36%)
23	CLA	B	613	-	65,73,73	1.98	17 (26%)	76,113,113	2.78	29 (38%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.10	5 (10%)
28	OEX	A	413[A]	-	0,15,15	-	-	-	-	-
25	BCR	B	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.48	7 (12%)
29	PL9	D	408[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
34	HTG	b	622	-	19,19,19	1.13	2 (10%)	23,24,24	2.01	7 (30%)
23	CLA	D	405[B]	-	65,73,73	2.00	17 (26%)	76,113,113	2.86	28 (36%)
37	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
27	GOL	d	801[B]	-	5,5,5	0.89	0	5,5,5	0.98	0
23	CLA	b	602	-	65,73,73	2.05	16 (24%)	76,113,113	2.88	32 (42%)
23	CLA	C	512	-	65,73,73	2.07	17 (26%)	76,113,113	2.63	26 (34%)
23	CLA	A	405[A]	-	65,73,73	1.99	15 (23%)	76,113,113	2.79	30 (39%)
32	LMT	m	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.19	4 (8%)
28	OEX	A	413[B]	-	0,15,15	-	-	-	-	-
37	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
23	CLA	C	506	-	65,73,73	2.02	16 (24%)	76,113,113	2.76	27 (35%)
32	LMT	e	102	-	36,36,36	1.01	2 (5%)	47,47,47	1.02	1 (2%)
26	SQD	F	101	-	42,43,54	1.20	4 (9%)	51,54,65	2.18	14 (27%)
27	GOL	O	601	-	5,5,5	0.79	0	5,5,5	1.12	1 (20%)
34	HTG	d	411	-	16,16,19	0.92	1 (6%)	20,21,24	1.58	1 (5%)
37	LHG	d	407[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.06	4 (7%)
38	HEM	e	87	-	41,50,50	1.29	5 (12%)	45,82,82	1.87	11 (24%)
23	CLA	c	505	-	65,73,73	2.08	18 (27%)	76,113,113	2.74	26 (34%)
32	LMT	t	102	-	26,26,36	0.88	2 (7%)	31,31,47	1.33	3 (9%)
23	CLA	A	405[B]	-	65,73,73	2.03	16 (24%)	76,113,113	2.77	29 (38%)
27	GOL	C	523[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
27	GOL	c	743	-	5,5,5	1.04	0	5,5,5	0.97	0
37	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.10	3 (6%)
27	GOL	a	801	-	5,5,5	1.32	1 (20%)	5,5,5	1.09	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.36	7 (11%)
23	CLA	b	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.87	28 (36%)
23	CLA	b	610	-	65,73,73	2.02	16 (24%)	76,113,113	2.88	29 (38%)
26	SQD	B	620	-	53,54,54	1.08	4 (7%)	62,65,65	1.75	11 (17%)
23	CLA	c	502	-	65,73,73	2.00	17 (26%)	76,113,113	2.78	29 (38%)
31	BCT	A	348[A]	-	2,3,3	0.64	0	2,3,3	1.30	0
23	CLA	b	607	-	65,73,73	1.99	17 (26%)	76,113,113	2.67	28 (36%)
23	CLA	c	508	-	65,73,73	2.01	17 (26%)	76,113,113	2.83	27 (35%)
27	GOL	B	624	-	5,5,5	0.94	0	5,5,5	1.12	1 (20%)
25	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)
27	GOL	B	901	-	5,5,5	1.13	0	5,5,5	1.00	0
23	CLA	c	514	-	65,73,73	2.09	16 (24%)	76,113,113	2.78	27 (35%)
23	CLA	b	611	-	65,73,73	1.97	17 (26%)	76,113,113	2.80	25 (32%)
23	CLA	b	609	-	65,73,73	2.03	16 (24%)	76,113,113	2.79	27 (35%)
23	CLA	C	511	-	65,73,73	2.05	16 (24%)	76,113,113	2.83	32 (42%)
25	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.56	8 (14%)
27	GOL	O	501	-	5,5,5	0.91	0	5,5,5	0.91	0
31	BCT	a	404[B]	-	2,3,3	0.61	0	2,3,3	1.19	0
32	LMT	b	627	-	25,25,36	0.86	0	30,30,47	1.11	3 (10%)
23	CLA	c	507	-	65,73,73	2.08	17 (26%)	76,113,113	2.77	28 (36%)
23	CLA	A	404[A]	-	65,73,73	2.02	16 (24%)	76,113,113	2.85	30 (39%)
34	HTG	c	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.49	2 (8%)
31	BCT	A	348[B]	-	2,3,3	0.68	0	2,3,3	1.11	0
23	CLA	B	604	-	65,73,73	2.04	17 (26%)	76,113,113	2.61	29 (38%)
37	LHG	e	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
29	PL9	a	416[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
23	CLA	c	513	-	65,73,73	2.06	17 (26%)	76,113,113	2.72	28 (36%)
23	CLA	A	404[B]	-	65,73,73	2.12	17 (26%)	76,113,113	2.80	30 (39%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	7 (9%)
27	GOL	o	501	-	5,5,5	0.98	0	5,5,5	0.97	0
37	LHG	e	101[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.91	2 (4%)
23	CLA	b	603	-	65,73,73	1.99	15 (23%)	76,113,113	2.90	30 (39%)
23	CLA	b	601	-	65,73,73	2.15	17 (26%)	76,113,113	2.75	25 (32%)
29	PL9	a	416[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.95	20 (29%)
25	BCR	b	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.30	9 (16%)
26	SQD	a	413	-	53,54,54	1.08	4 (7%)	62,65,65	1.18	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	a	407[A]	-	65,73,73	1.98	16 (24%)	76,113,113	2.77	27 (35%)
25	BCR	D	407	-	41,41,41	1.12	1 (2%)	56,56,56	1.87	17 (30%)
23	CLA	a	409	-	65,73,73	1.94	14 (21%)	76,113,113	2.92	28 (36%)
33	LMG	a	419	-	51,51,55	0.91	2 (3%)	59,59,63	1.19	3 (5%)
23	CLA	B	608	-	65,73,73	1.93	15 (23%)	76,113,113	2.84	33 (43%)
37	LHG	D	409[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
23	CLA	b	615	-	65,73,73	2.03	17 (26%)	76,113,113	2.74	28 (36%)
27	GOL	V	401[A]	-	5,5,5	1.34	0	5,5,5	0.80	0
23	CLA	a	407[B]	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	29 (38%)
29	PL9	D	408[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.63	17 (25%)
37	LHG	D	409[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.20	5 (9%)
40	HEC	V	202	-	32,50,50	2.00	4 (12%)	24,82,82	2.02	7 (29%)
24	PHO	A	353[A]	-	51,69,69	1.92	8 (15%)	47,99,99	1.85	9 (19%)
34	HTG	b	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.97	3 (13%)
27	GOL	C	523[B]	-	5,5,5	1.07	0	5,5,5	0.84	0
27	GOL	V	401[B]	-	5,5,5	1.17	0	5,5,5	0.92	0
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.80	16 (28%)
23	CLA	A	406[A]	-	65,73,73	1.98	17 (26%)	76,113,113	2.76	30 (39%)
23	CLA	C	504	-	65,73,73	1.97	16 (24%)	76,113,113	2.78	27 (35%)
23	CLA	D	406	-	65,73,73	2.06	16 (24%)	76,113,113	2.71	29 (38%)
37	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
23	CLA	d	403	-	65,73,73	2.02	15 (23%)	76,113,113	2.86	29 (38%)
24	PHO	a	408[A]	-	51,69,69	1.83	8 (15%)	47,99,99	1.87	9 (19%)
24	PHO	A	353[B]	-	51,69,69	1.90	8 (15%)	47,99,99	1.88	10 (21%)
27	GOL	A	701	-	5,5,5	1.48	2 (40%)	5,5,5	0.89	0
23	CLA	b	604	-	65,73,73	2.02	16 (24%)	76,113,113	2.69	24 (31%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.47	9 (16%)
35	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
37	LHG	L	101[B]	-	48,48,48	0.93	3 (6%)	51,54,54	1.10	3 (5%)
23	CLA	A	406[B]	-	65,73,73	2.05	17 (26%)	76,113,113	2.78	28 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	601	-	1/1/15/20	13/37/115/115	-
23	CLA	B	616	-	1/1/15/20	7/37/115/115	-
23	CLA	c	510	-	1/1/15/20	14/37/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	a	406[A]	-	1/1/15/20	8/37/115/115	-
32	LMT	M	103	-	-	7/21/61/61	0/2/2/2
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
24	PHO	a	408[B]	-	-	5/37/103/103	0/5/6/6
27	GOL	c	742[A]	-	-	0/4/4/4	-
35	DGD	c	517[B]	-	-	20/51/91/95	0/2/2/2
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
32	LMT	t	101	-	-	9/17/37/61	0/1/1/2
37	LHG	d	711[A]	-	-	17/53/53/53	-
23	CLA	a	406[B]	-	1/1/15/20	3/37/115/115	-
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
25	BCR	a	410	-	-	3/29/63/63	0/2/2/2
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
27	GOL	c	742[B]	-	-	0/4/4/4	-
23	CLA	C	503	-	-	10/37/115/115	-
29	PL9	A	414[B]	-	-	12/53/73/73	0/1/1/1
23	CLA	B	602	-	1/1/15/20	7/37/115/115	-
27	GOL	b	901	-	-	0/4/4/4	-
32	LMT	I	101	-	-	15/21/61/61	0/2/2/2
37	LHG	d	711[B]	-	-	10/53/53/53	-
23	CLA	c	504	-	1/1/15/20	1/37/115/115	-
23	CLA	b	614	-	1/1/15/20	14/37/115/115	-
26	SQD	a	411[B]	-	-	8/49/69/69	0/1/1/1
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
32	LMT	a	414	-	-	12/21/61/61	0/2/2/2
37	LHG	d	408[A]	-	-	13/53/53/53	-
23	CLA	B	614	-	1/1/15/20	15/37/115/115	-
37	LHG	D	411[A]	-	-	14/53/53/53	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	405[A]	-	1/1/15/20	4/37/115/115	-
23	CLA	C	505	-	1/1/15/20	7/37/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
32	LMT	a	420	-	-	11/21/61/61	0/2/2/2
37	LHG	d	408[B]	-	-	16/53/53/53	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
32	LMT	D	404	-	-	12/21/61/61	0/2/2/2
37	LHG	D	411[B]	-	-	14/53/53/53	-
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
23	CLA	a	405[B]	-	1/1/15/20	4/37/115/115	-
23	CLA	c	511	-	1/1/15/20	11/37/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	c	503	-	1/1/15/20	5/37/115/115	-
34	HTG	D	414	-	-	3/7/27/30	0/1/1/1
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	7/37/115/115	-
23	CLA	d	402[A]	-	1/1/15/20	4/37/115/115	-
23	CLA	C	510	-	1/1/15/20	6/37/115/115	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
27	GOL	a	412	-	-	4/4/4/4	-
33	LMG	C	520	-	-	11/46/66/70	0/1/1/1
27	GOL	a	701	-	-	2/4/4/4	-
38	HEM	E	103	-	-	6/12/54/54	-
35	DGD	c	518[B]	-	-	16/51/91/95	0/2/2/2
23	CLA	B	606	-	1/1/15/20	8/37/115/115	-
23	CLA	b	608	-	-	6/37/115/115	-
35	DGD	C	519	-	-	19/51/91/95	0/2/2/2
35	DGD	c	519	-	-	10/51/91/95	0/2/2/2
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-
23	CLA	C	513	-	1/1/15/20	10/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	m	101	-	-	11/46/66/70	0/1/1/1
35	DGD	C	518[A]	-	-	13/51/91/95	0/2/2/2
37	LHG	D	410[A]	-	-	17/53/53/53	-
23	CLA	B	615	-	1/1/15/20	8/37/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
40	HEC	v	202	-	-	2/10/54/54	-
25	BCR	B	617	-	-	1/29/63/63	0/2/2/2
23	CLA	C	507	-	1/1/15/20	13/37/115/115	-
24	PHO	A	407[B]	-	-	3/37/103/103	0/5/6/6
32	LMT	A	359	-	-	8/21/61/61	0/2/2/2
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	GOL	v	401[A]	-	-	2/4/4/4	-
33	LMG	d	412	-	-	9/46/66/70	0/1/1/1
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
35	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	C	508	-	1/1/15/20	7/37/115/115	-
37	LHG	D	410[B]	-	-	16/53/53/53	-
37	LHG	l	101[A]	-	-	14/53/53/53	-
27	GOL	o	601	-	-	4/4/4/4	-
23	CLA	B	610	-	1/1/15/20	8/37/115/115	-
23	CLA	B	607	-	1/1/15/20	3/37/115/115	-
33	LMG	D	415	-	-	8/46/66/70	0/1/1/1
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
27	GOL	v	401[B]	-	-	2/4/4/4	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	605	-	1/1/15/20	6/37/115/115	-
37	LHG	l	101[B]	-	-	17/53/53/53	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
23	CLA	c	512	-	1/1/15/20	7/37/115/115	-
35	DGD	h	102	-	-	14/51/91/95	0/2/2/2
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
35	DGD	C	517[A]	-	-	14/51/91/95	0/2/2/2
24	PHO	a	353[A]	-	-	1/37/103/103	0/5/6/6
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1
23	CLA	b	606	-	1/1/15/20	12/37/115/115	-
33	LMG	B	621	-	-	16/46/66/70	0/1/1/1
29	PL9	d	405[A]	-	-	7/53/73/73	0/1/1/1
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
27	GOL	d	701	-	-	2/4/4/4	-
35	DGD	C	517[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	b	613	-	1/1/15/20	6/37/115/115	-
25	BCR	t	103	-	-	0/29/63/63	0/2/2/2
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
23	CLA	b	612	-	1/1/15/20	5/37/115/115	-
24	PHO	a	353[B]	-	-	2/37/103/103	0/5/6/6
34	HTG	B	626	-	-	4/10/30/30	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
29	PL9	d	405[B]	-	-	7/53/73/73	0/1/1/1
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
23	CLA	C	502	-	1/1/15/20	5/37/115/115	-
23	CLA	d	402[B]	-	1/1/15/20	5/37/115/115	-
23	CLA	C	509	-	1/1/15/20	6/37/115/115	-
23	CLA	D	405[A]	-	1/1/15/20	0/37/115/115	-
23	CLA	C	514	-	1/1/15/20	6/37/115/115	-
27	GOL	d	801[A]	-	-	1/4/4/4	-
23	CLA	B	603	-	1/1/15/20	5/37/115/115	-
23	CLA	B	611	-	1/1/15/20	2/37/115/115	-
27	GOL	D	701	-	-	4/4/4/4	-
23	CLA	B	609	-	1/1/15/20	1/37/115/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
29	PL9	D	408[A]	-	-	6/53/73/73	0/1/1/1
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	405[B]	-	1/1/15/20	3/37/115/115	-
37	LHG	d	407[A]	-	-	13/53/53/53	-
27	GOL	d	801[B]	-	-	2/4/4/4	-
23	CLA	b	602	-	1/1/15/20	3/37/115/115	-
23	CLA	C	512	-	1/1/15/20	4/37/115/115	-
23	CLA	A	405[A]	-	1/1/15/20	3/37/115/115	-
32	LMT	m	103	-	-	6/21/61/61	0/2/2/2
37	LHG	E	101[A]	-	-	22/46/46/53	-
23	CLA	C	506	-	1/1/15/20	7/37/115/115	-
32	LMT	e	102	-	-	14/21/61/61	0/2/2/2
26	SQD	F	101	-	-	15/38/58/69	0/1/1/1
27	GOL	O	601	-	-	2/4/4/4	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
37	LHG	d	407[B]	-	-	15/53/53/53	-
38	HEM	e	87	-	-	6/12/54/54	-
23	CLA	c	505	-	1/1/15/20	6/37/115/115	-
32	LMT	t	102	-	-	9/17/38/61	0/1/1/2
23	CLA	A	405[B]	-	1/1/15/20	6/37/115/115	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
27	GOL	c	743	-	-	4/4/4/4	-
37	LHG	E	101[B]	-	-	19/46/46/53	-
27	GOL	a	801	-	-	0/4/4/4	-
33	LMG	C	521	-	-	15/46/66/70	0/1/1/1
23	CLA	b	616	-	1/1/15/20	9/37/115/115	-
23	CLA	b	610	-	1/1/15/20	7/37/115/115	-
26	SQD	B	620	-	-	11/49/69/69	0/1/1/1
23	CLA	c	502	-	1/1/15/20	6/37/115/115	-
23	CLA	b	607	-	1/1/15/20	4/37/115/115	-
23	CLA	c	508	-	1/1/15/20	7/37/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	GOL	B	901	-	-	1/4/4/4	-
23	CLA	c	514	-	1/1/15/20	9/37/115/115	-
23	CLA	b	611	-	1/1/15/20	3/37/115/115	-
23	CLA	b	609	-	1/1/15/20	1/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	511	-	1/1/15/20	14/37/115/115	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
27	GOL	O	501	-	-	2/4/4/4	-
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	c	507	-	1/1/15/20	8/37/115/115	-
23	CLA	A	404[A]	-	1/1/15/20	3/37/115/115	-
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
23	CLA	B	604	-	1/1/15/20	2/37/115/115	-
37	LHG	e	101[A]	-	-	16/46/46/53	-
29	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	c	513	-	1/1/15/20	12/37/115/115	-
23	CLA	A	404[B]	-	1/1/15/20	6/37/115/115	-
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
27	GOL	o	501	-	-	2/4/4/4	-
37	LHG	e	101[B]	-	-	16/46/46/53	-
23	CLA	b	603	-	1/1/15/20	7/37/115/115	-
23	CLA	b	601	-	1/1/15/20	20/37/115/115	-
29	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	SQD	a	413	-	-	14/49/69/69	0/1/1/1
23	CLA	a	407[A]	-	-	6/37/115/115	-
25	BCR	D	407	-	-	4/29/63/63	0/2/2/2
23	CLA	a	409	-	1/1/15/20	10/37/115/115	-
33	LMG	a	419	-	-	11/46/66/70	0/1/1/1
23	CLA	B	608	-	-	3/37/115/115	-
37	LHG	D	409[A]	-	-	14/53/53/53	-
23	CLA	b	615	-	1/1/15/20	8/37/115/115	-
27	GOL	V	401[A]	-	-	2/4/4/4	-
23	CLA	a	407[B]	-	-	5/37/115/115	-
29	PL9	D	408[B]	-	-	10/53/73/73	0/1/1/1
37	LHG	D	409[B]	-	-	14/53/53/53	-
40	HEC	V	202	-	-	2/10/54/54	-
24	PHO	A	353[A]	-	-	1/37/103/103	0/5/6/6
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
27	GOL	C	523[B]	-	-	0/4/4/4	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	V	401[B]	-	-	2/4/4/4	-
25	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
23	CLA	A	406[A]	-	-	5/37/115/115	-
23	CLA	C	504	-	1/1/15/20	3/37/115/115	-
23	CLA	D	406	-	1/1/15/20	14/37/115/115	-
37	LHG	L	101[A]	-	-	20/53/53/53	-
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-
24	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
24	PHO	A	353[B]	-	-	1/37/103/103	0/5/6/6
27	GOL	A	701	-	-	2/4/4/4	-
23	CLA	b	604	-	1/1/15/20	11/37/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
35	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2
37	LHG	L	101[B]	-	-	20/53/53/53	-
23	CLA	A	406[B]	-	-	4/37/115/115	-

The worst 5 of 1560 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	10.98	1.55	1.40
23	B	611	CLA	CMB-C2B	7.94	1.68	1.51
23	B	603	CLA	C3B-C2B	6.96	1.50	1.40
23	B	616	CLA	C3B-C2B	6.82	1.49	1.40
23	C	503	CLA	C3B-C2B	6.79	1.49	1.40

The worst 5 of 3077 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1D-ND-C4D	-11.73	98.00	106.33
23	a	409	CLA	C1D-ND-C4D	-10.36	98.98	106.33
23	b	605	CLA	C1D-ND-C4D	-10.18	99.10	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-10.08	99.17	106.33
23	C	504	CLA	C1D-ND-C4D	-10.08	99.18	106.33

5 of 71 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
23	A	405[A]	CLA	ND
23	A	405[B]	CLA	ND
23	A	408	CLA	ND

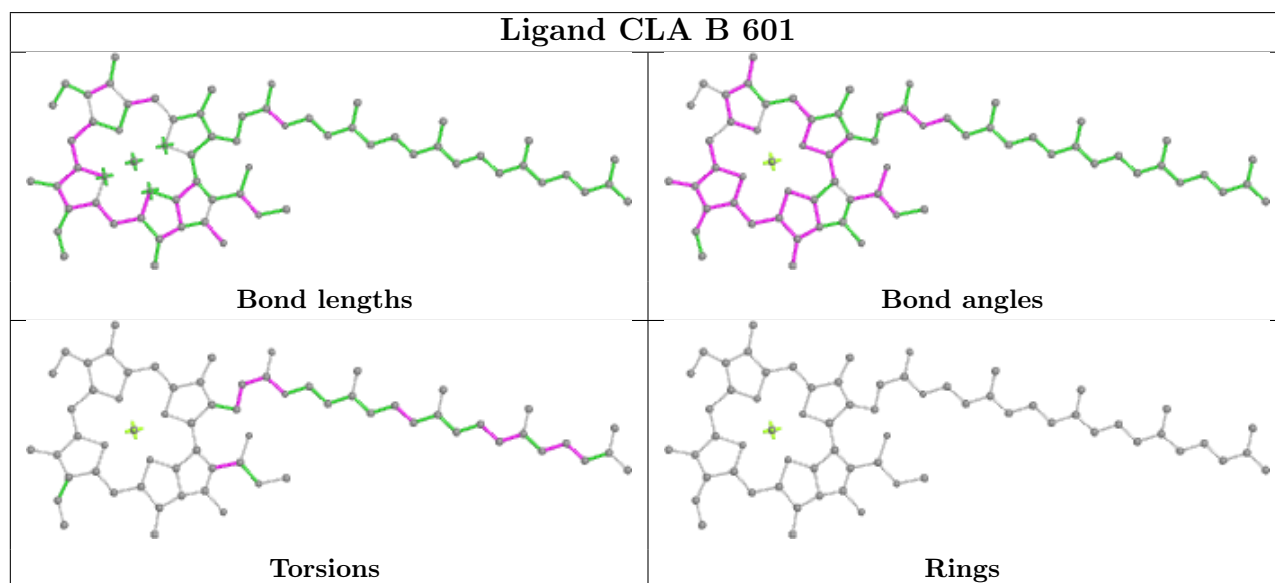
5 of 1655 torsion outliers are listed below:

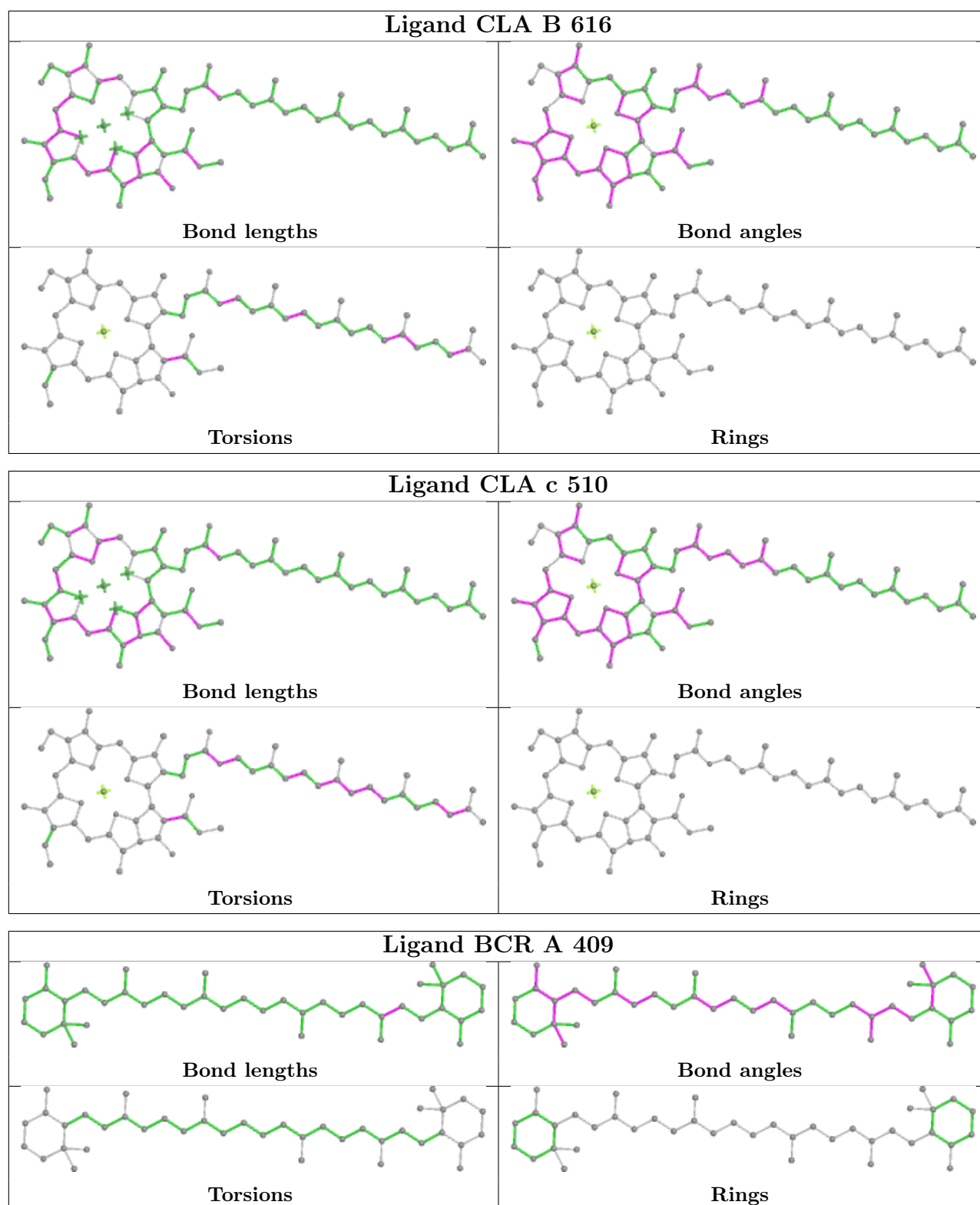
Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D

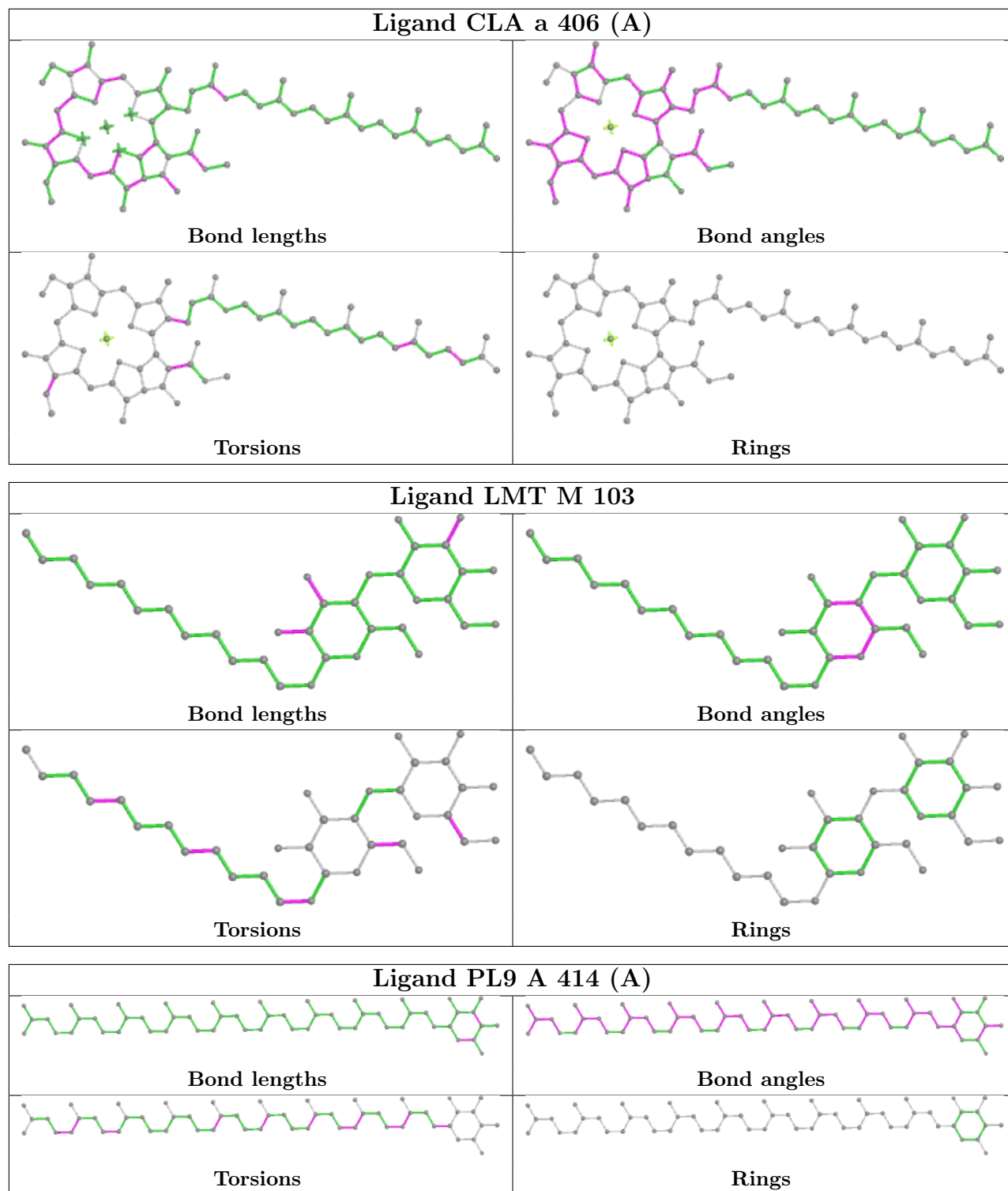
There are no ring outliers.

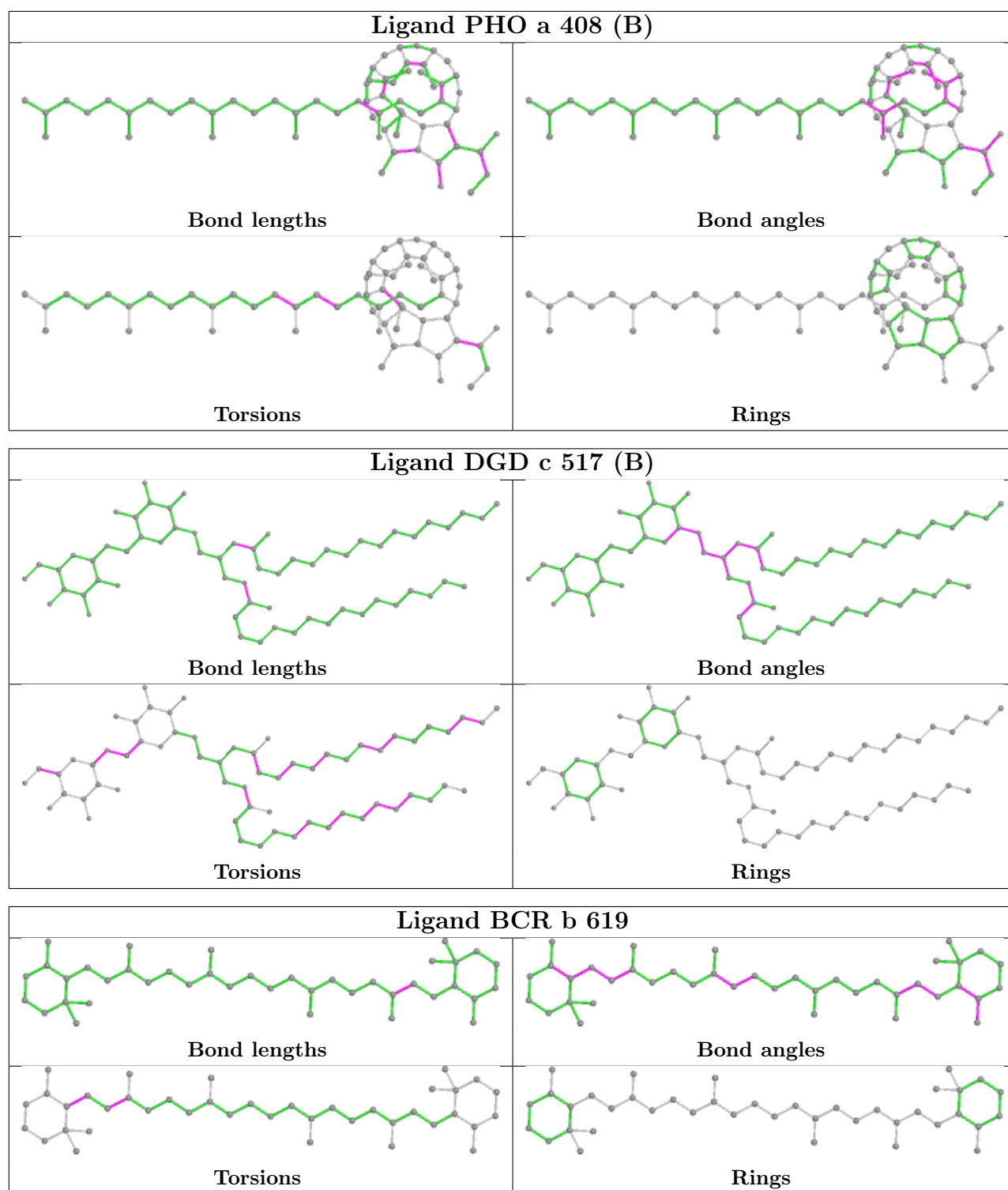
No monomer is involved in short contacts.

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

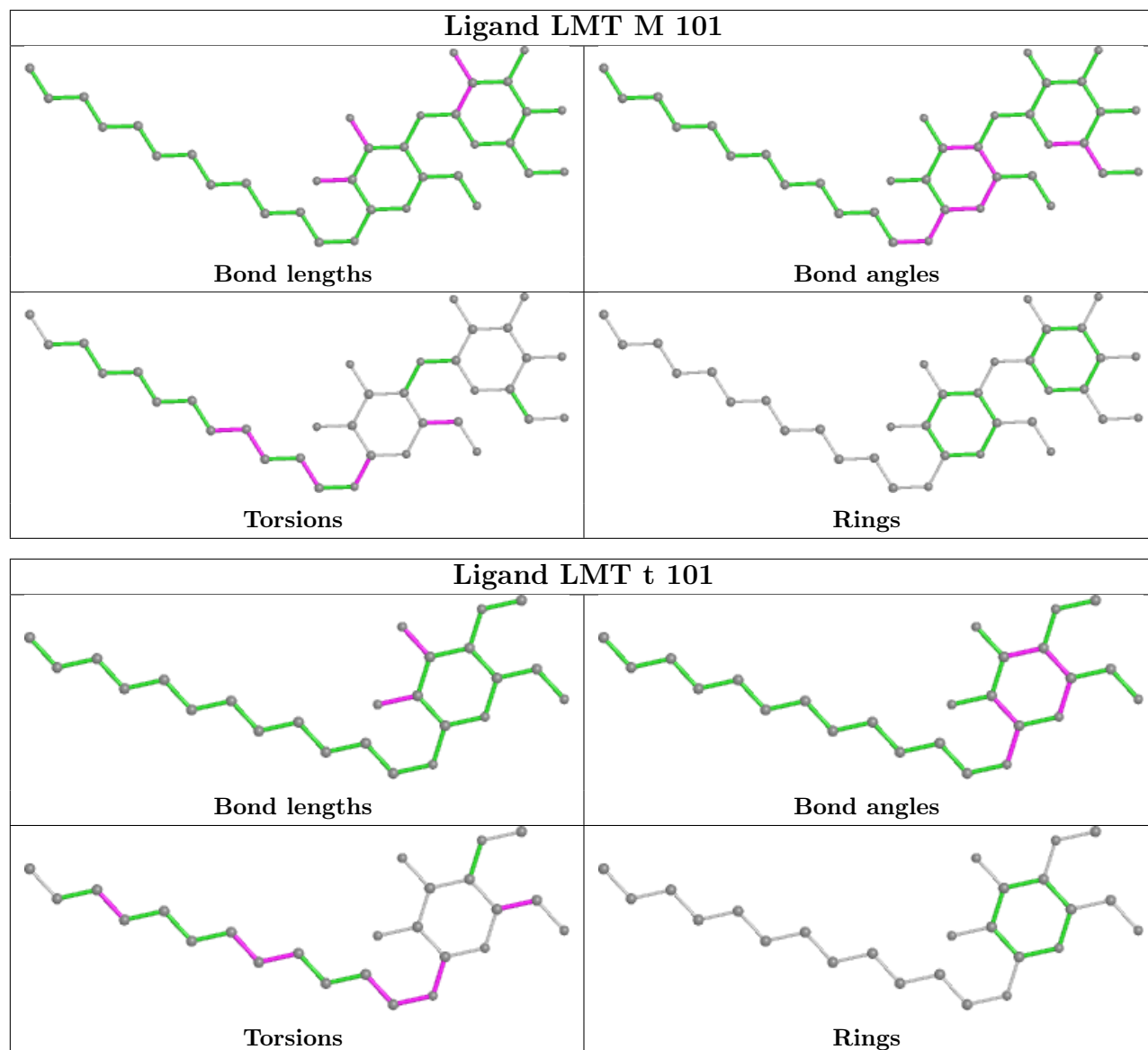


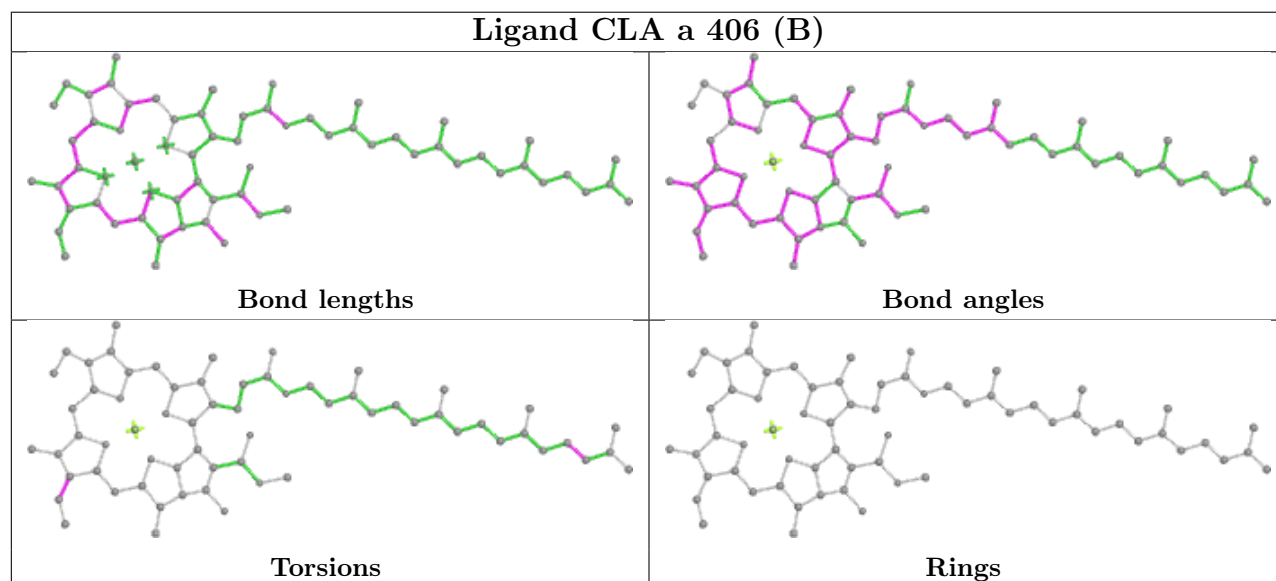
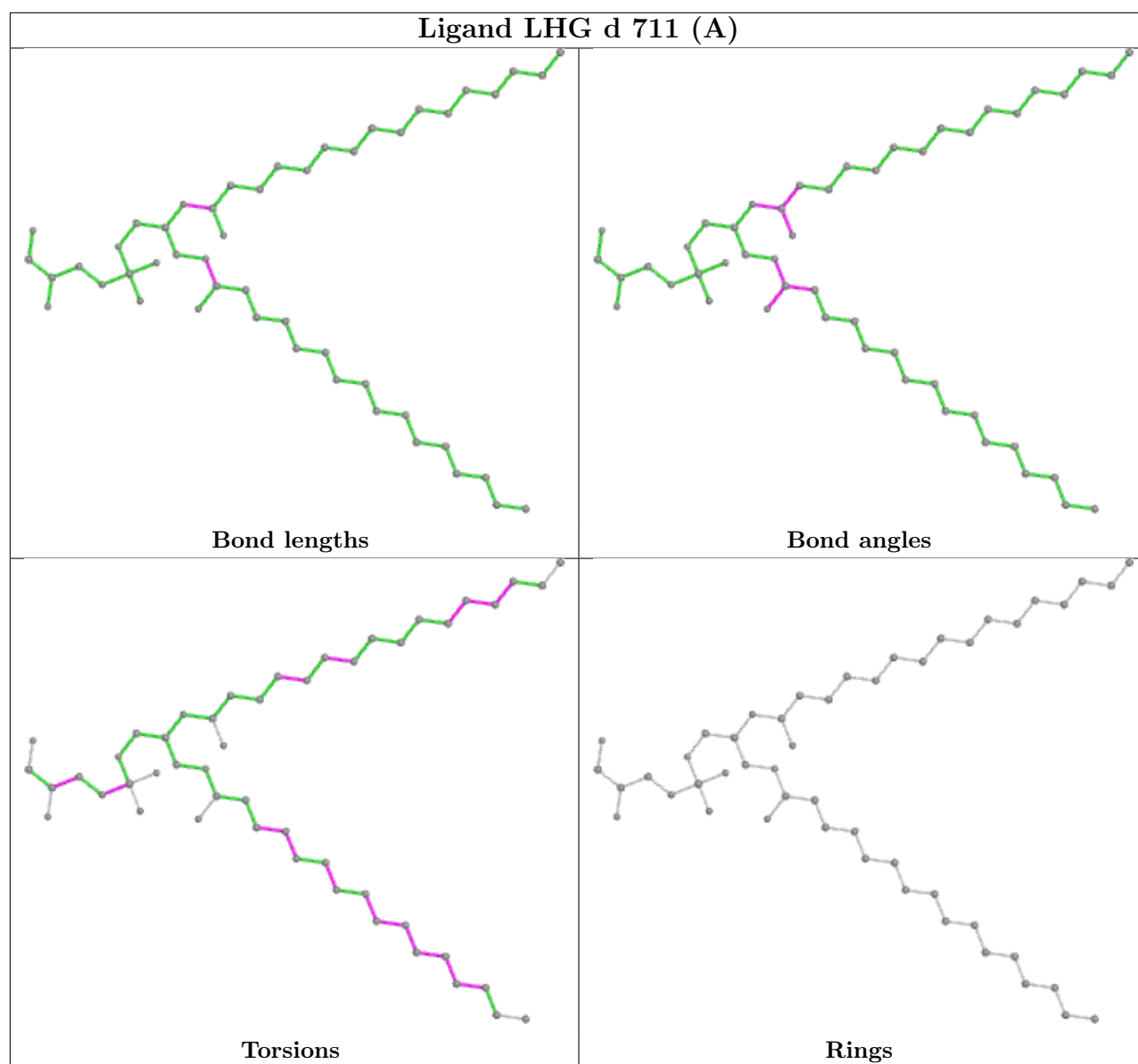


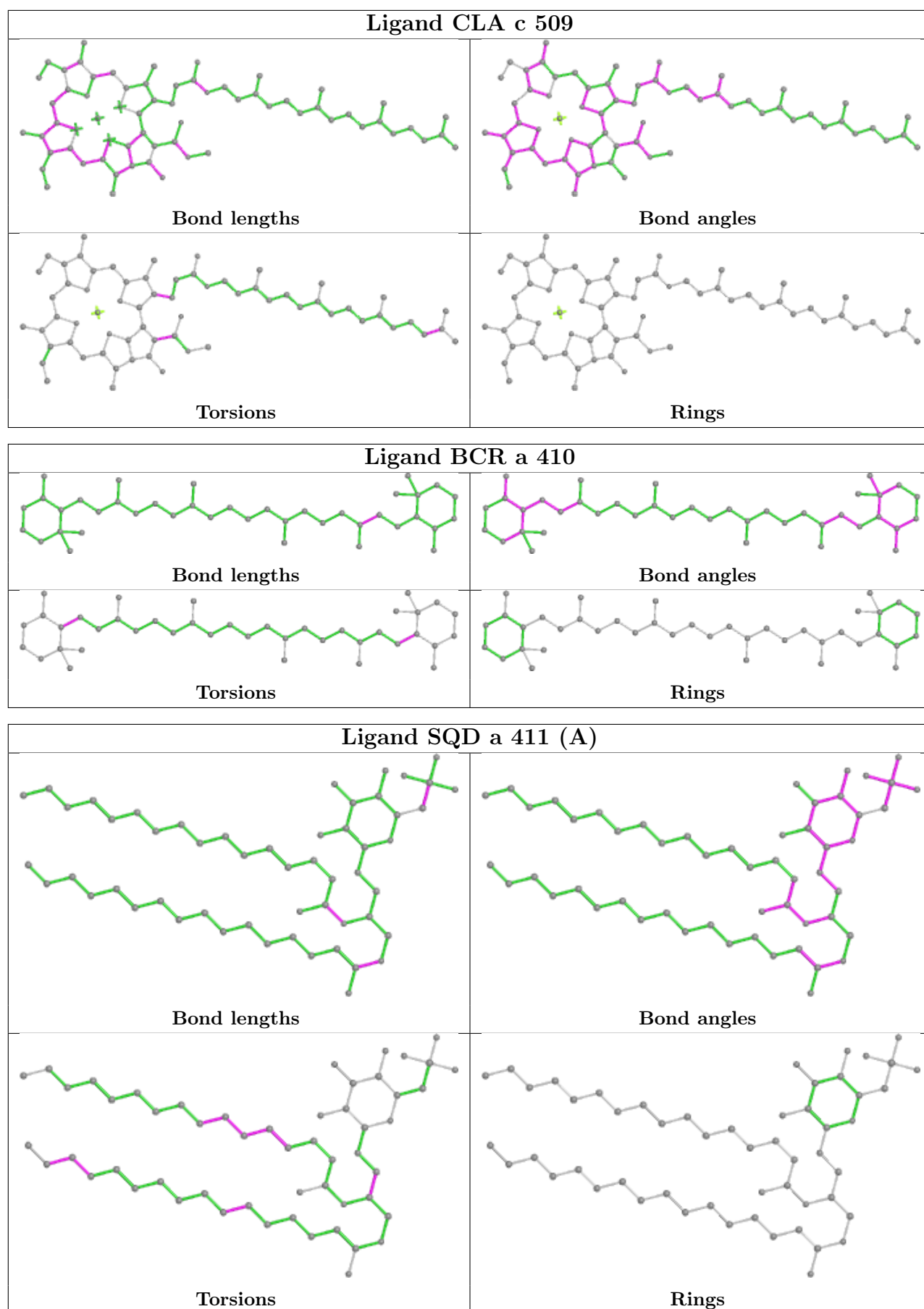


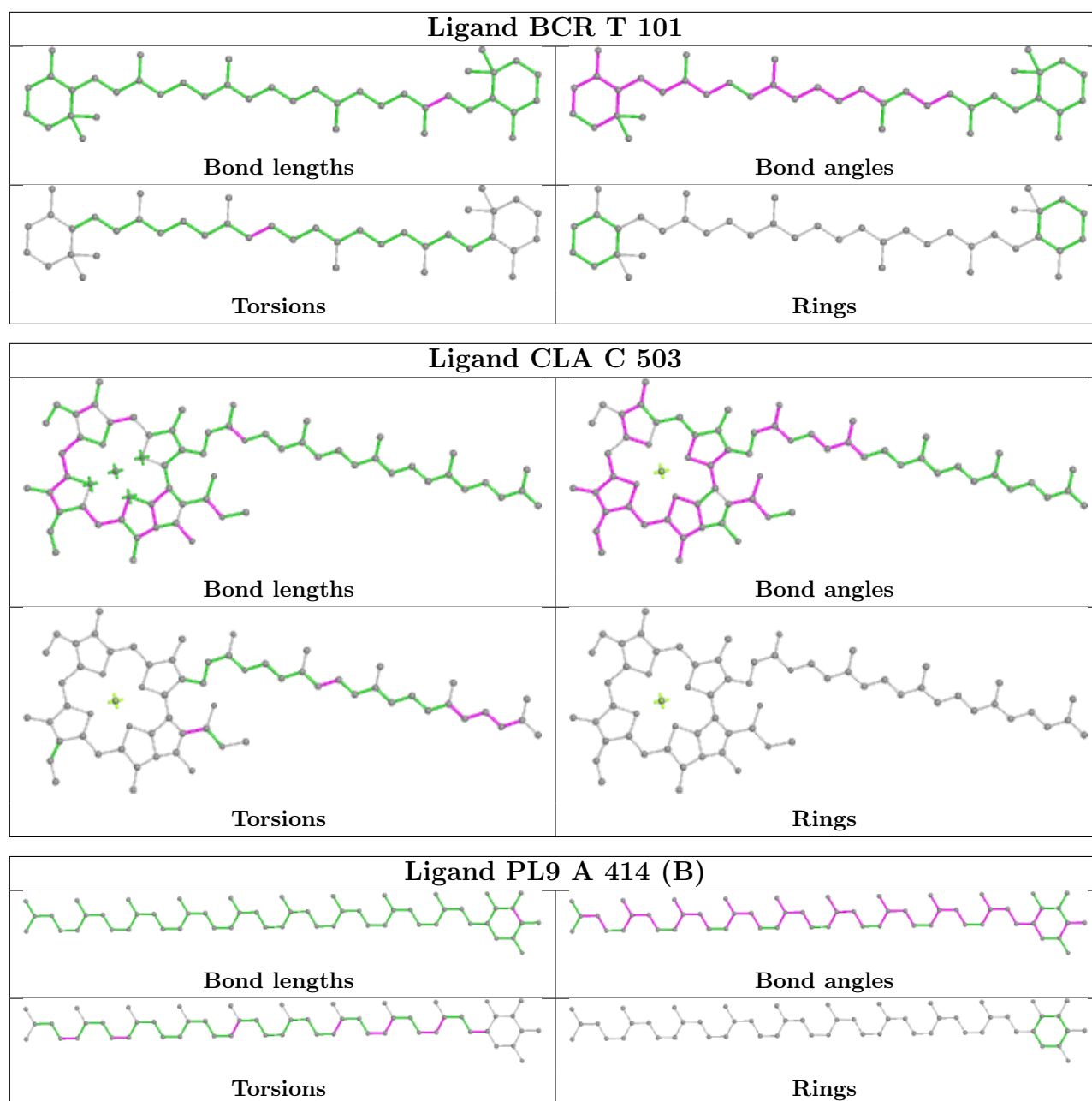


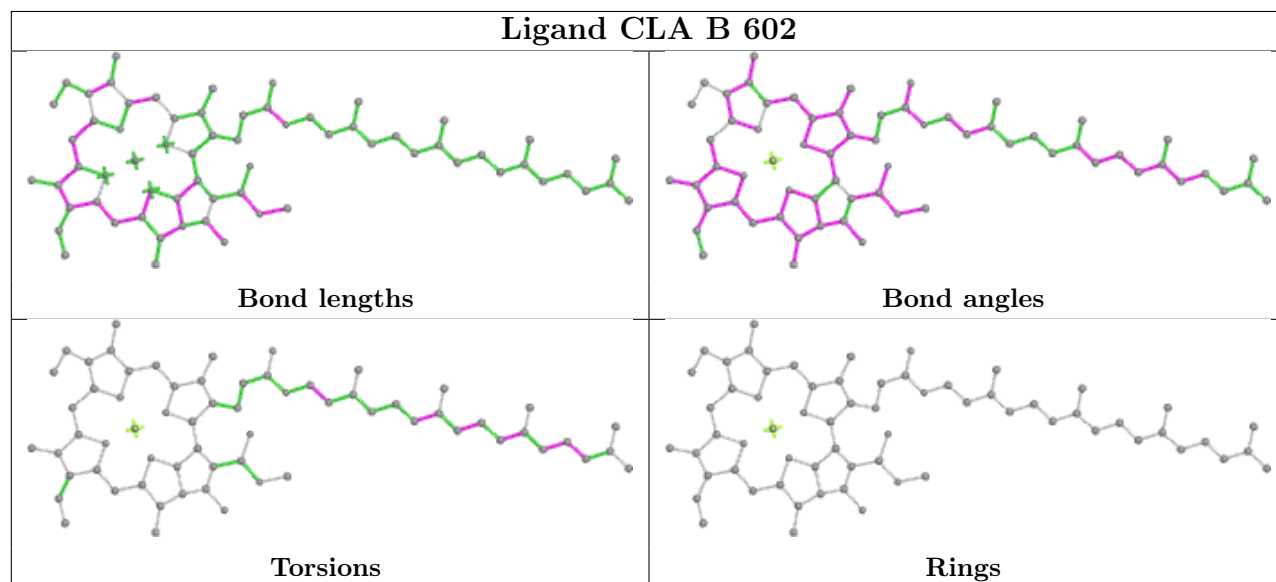
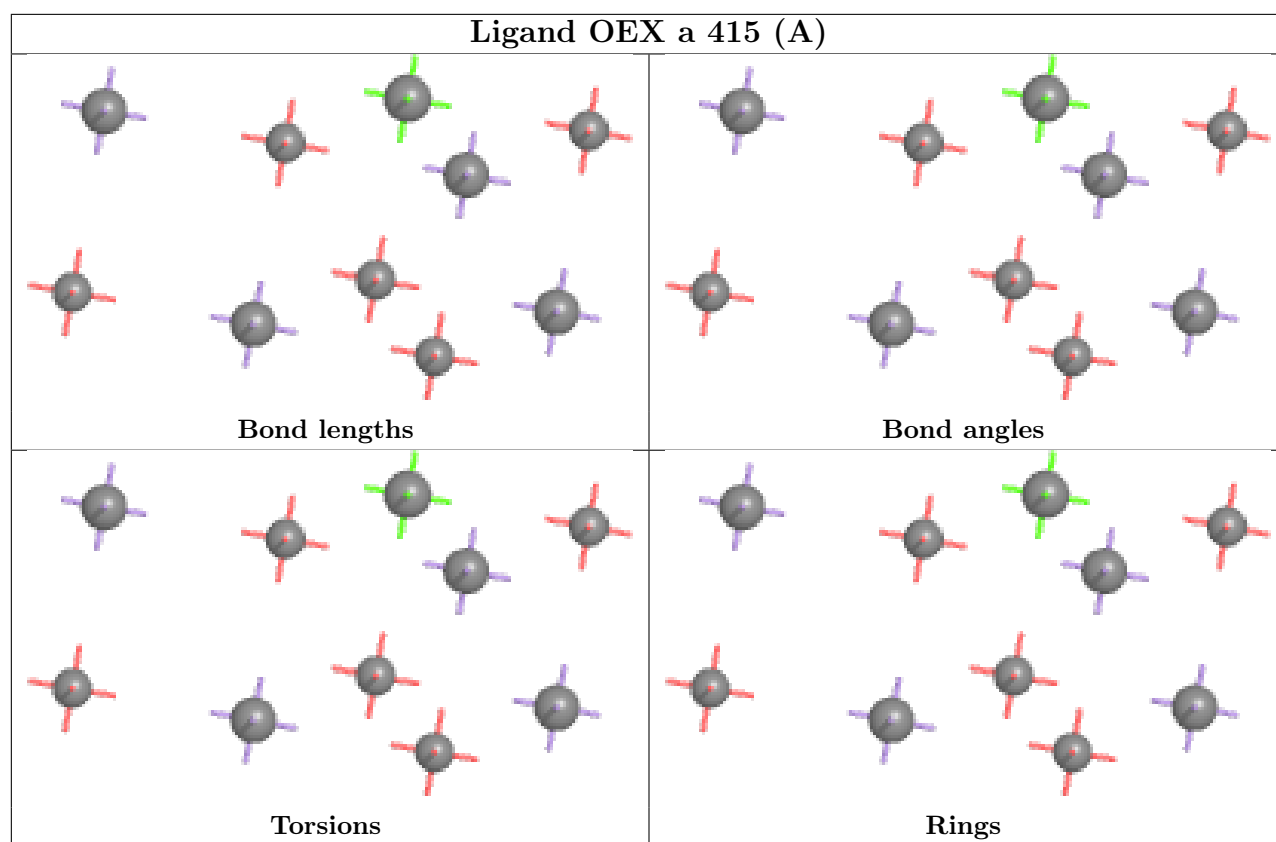


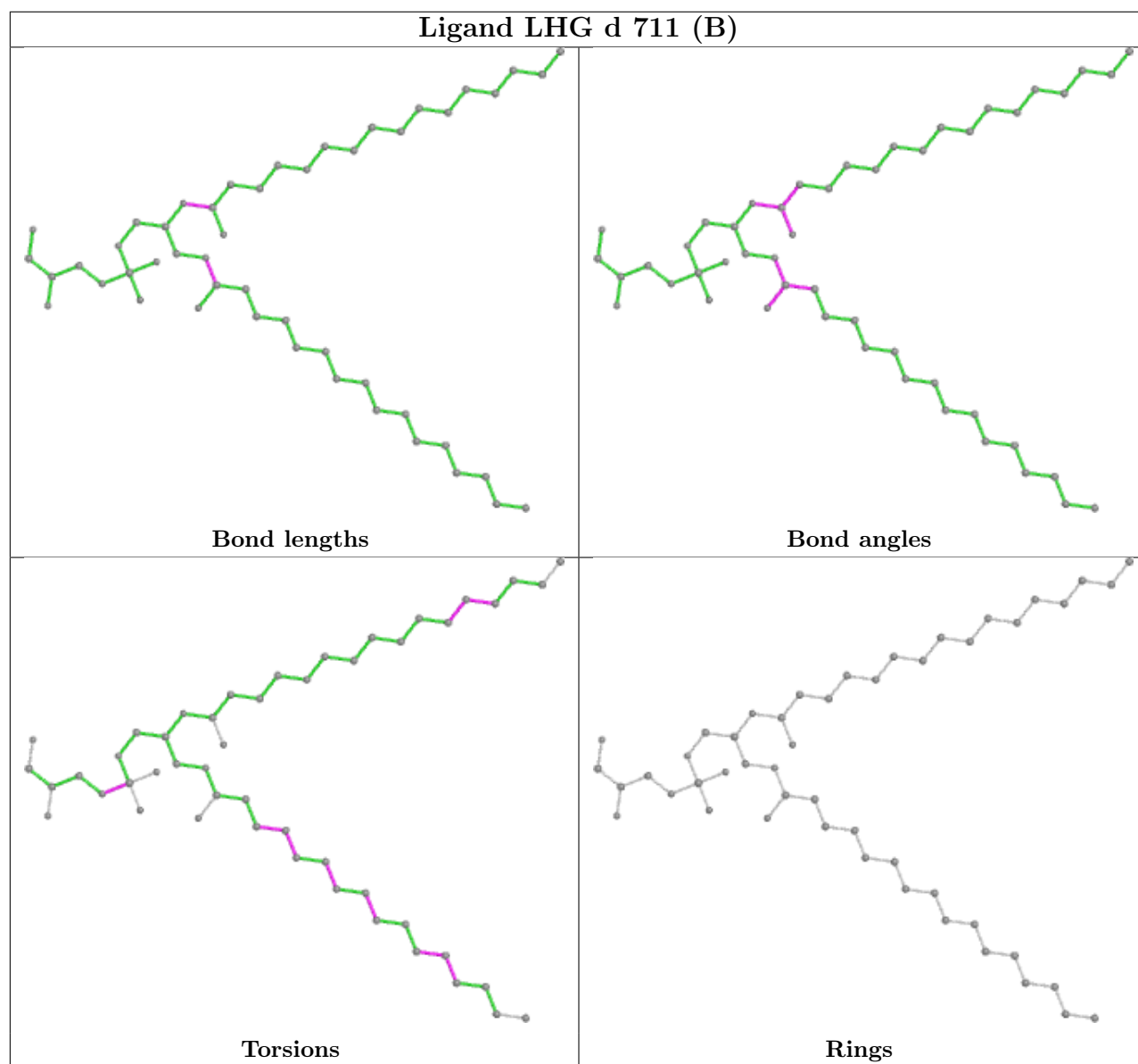
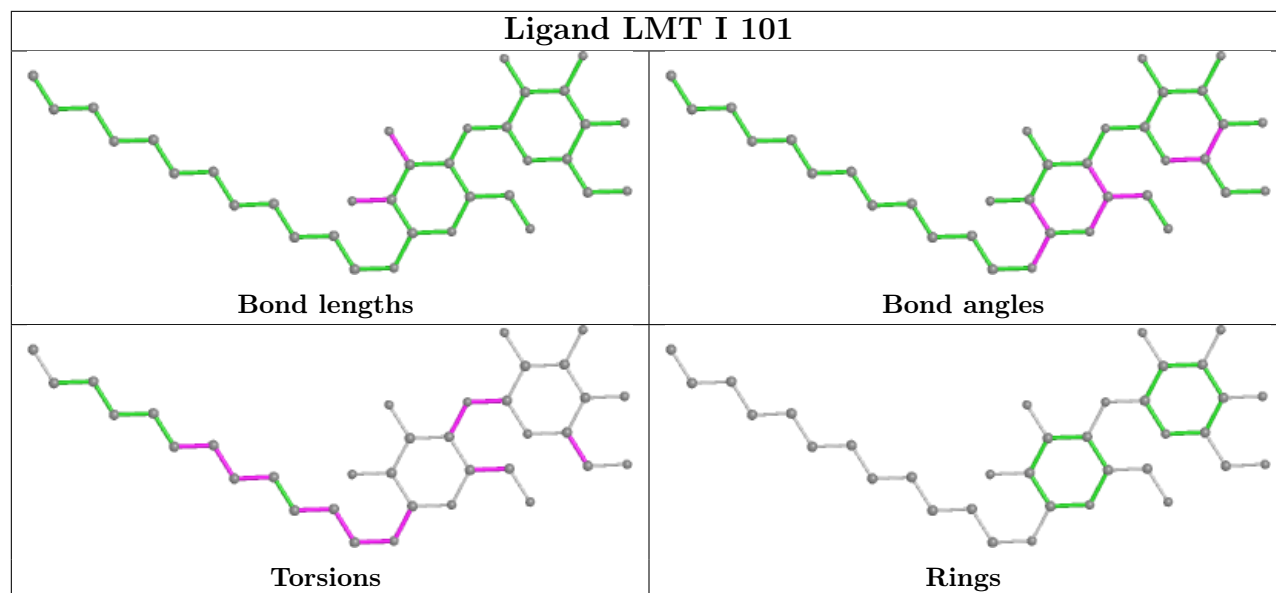


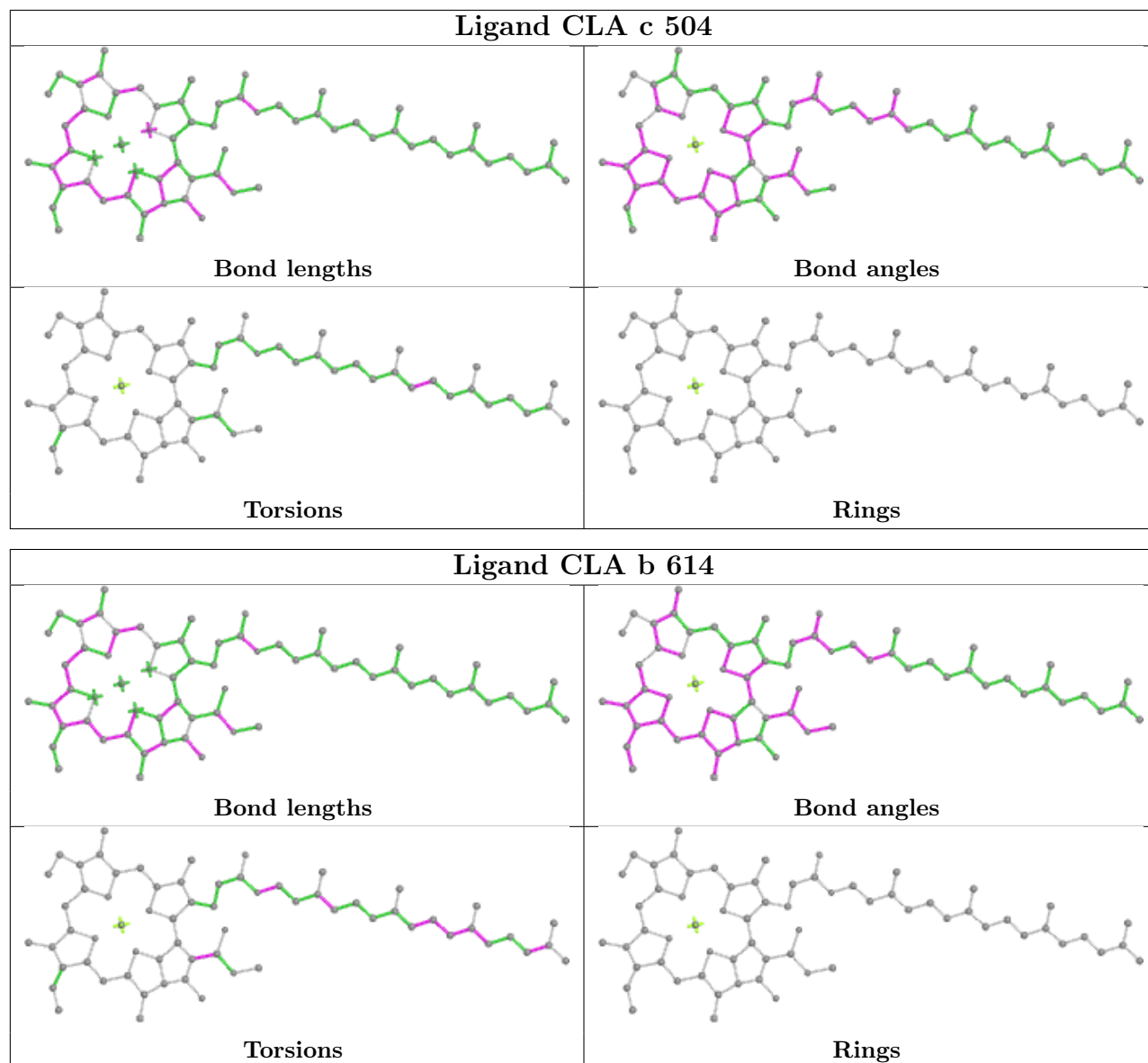


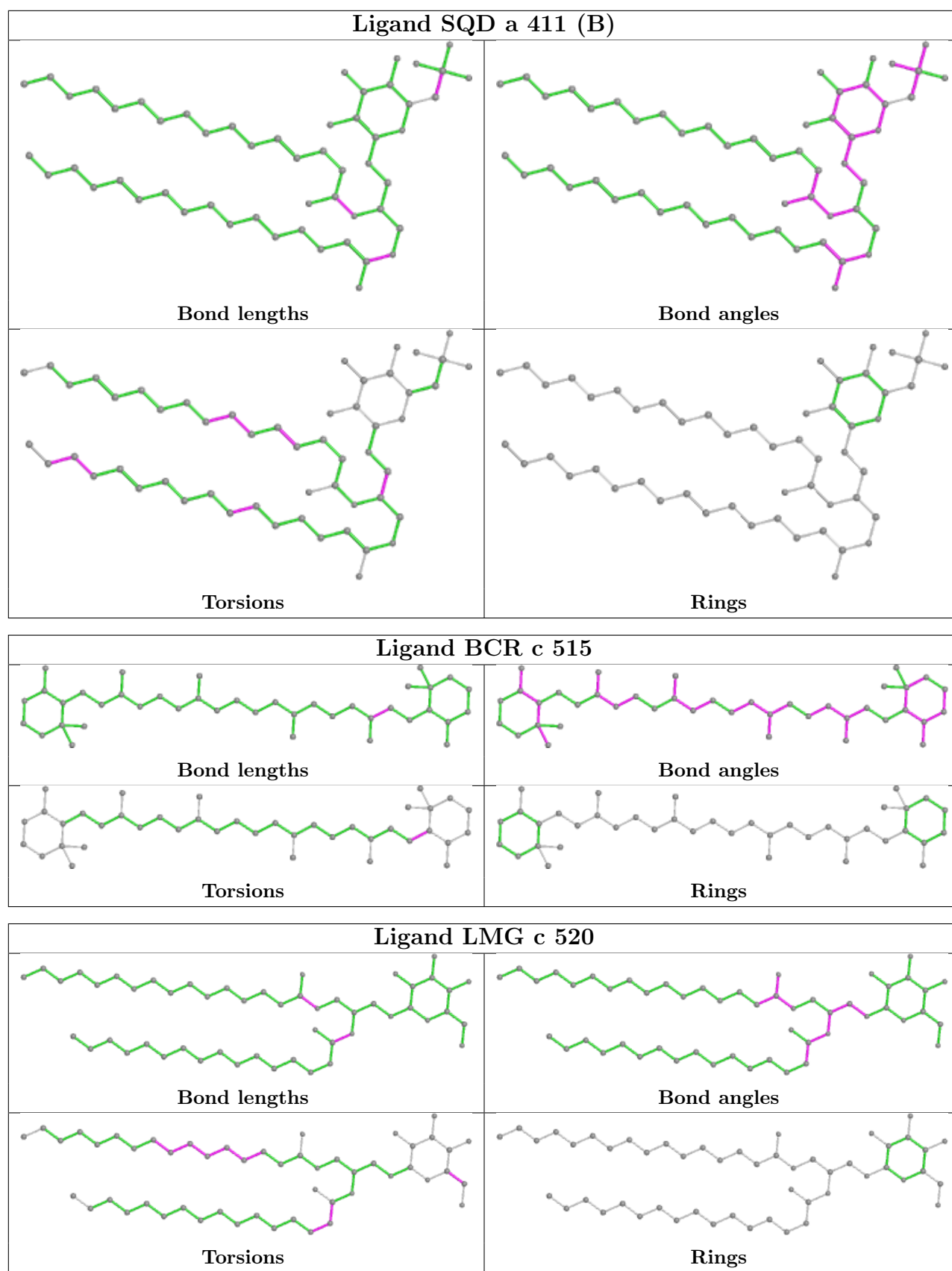




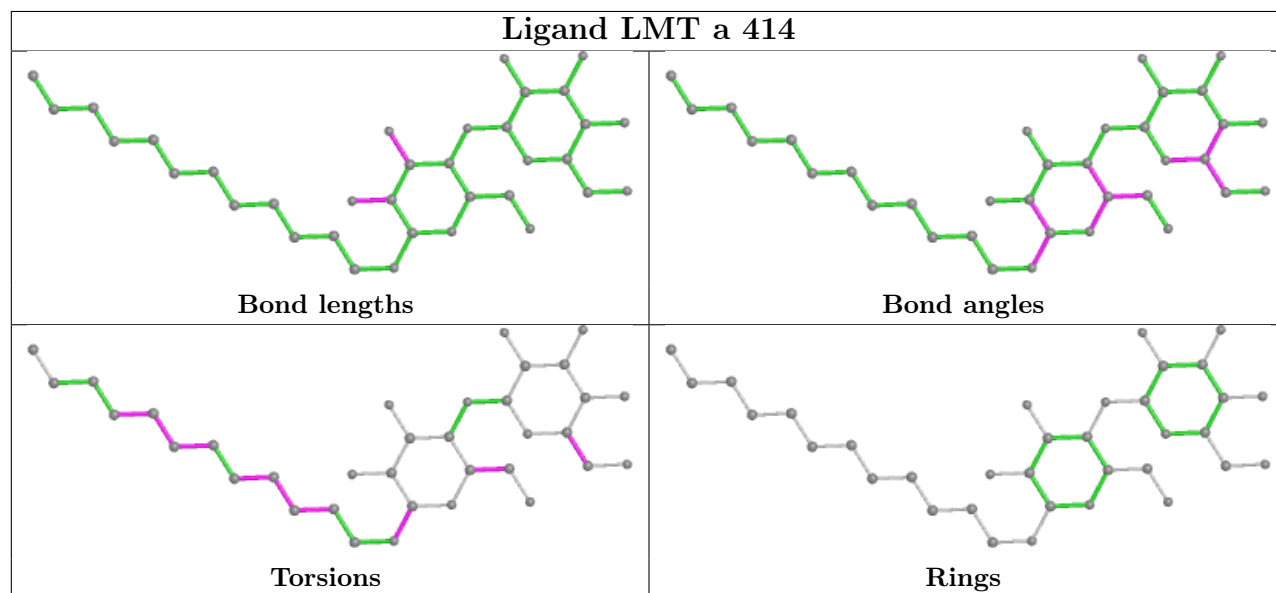
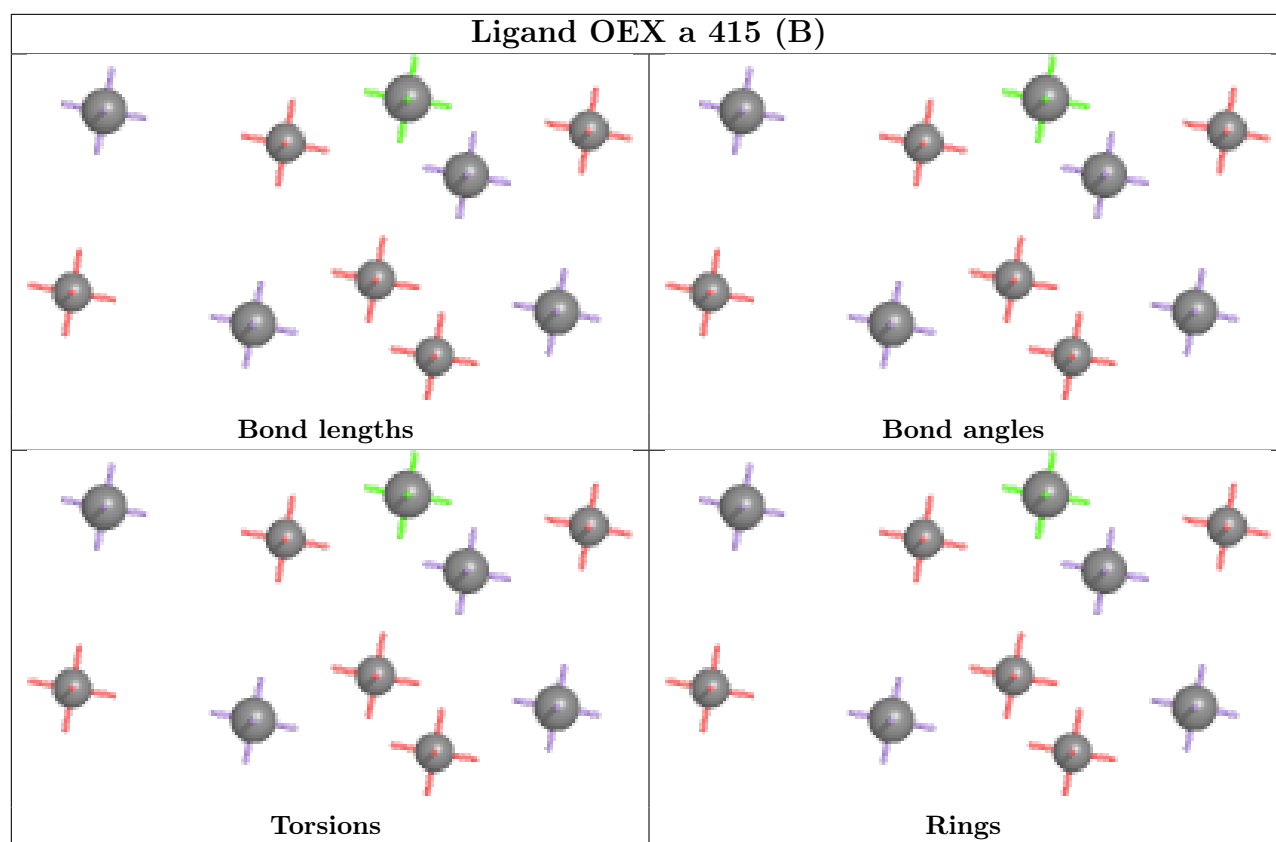


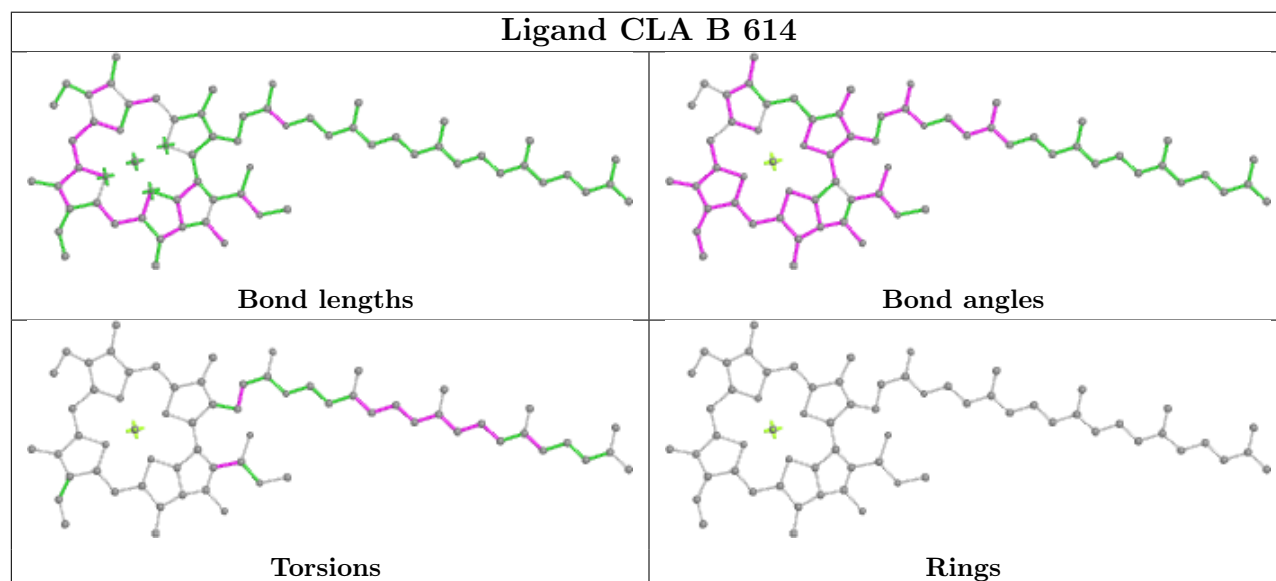
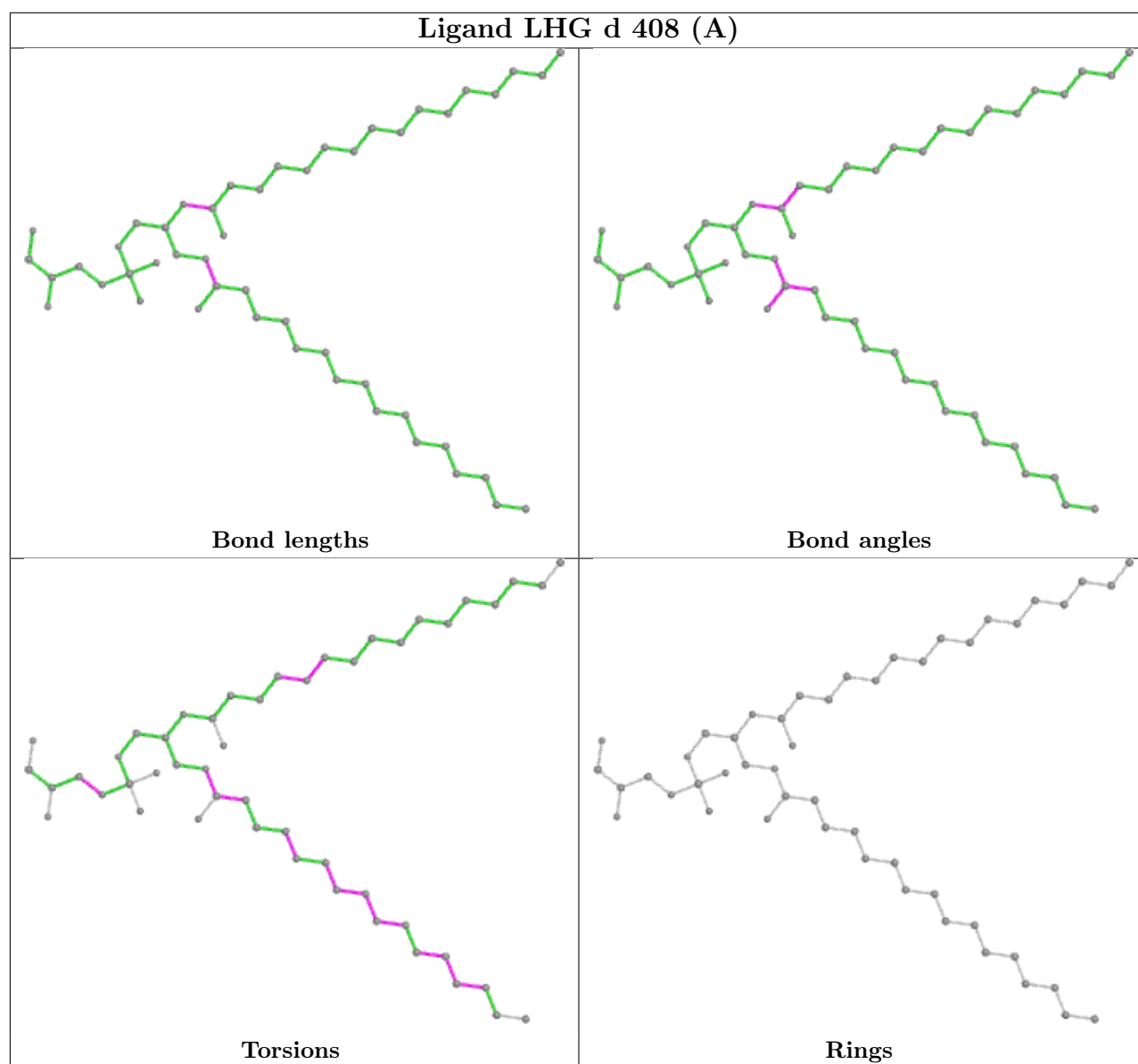


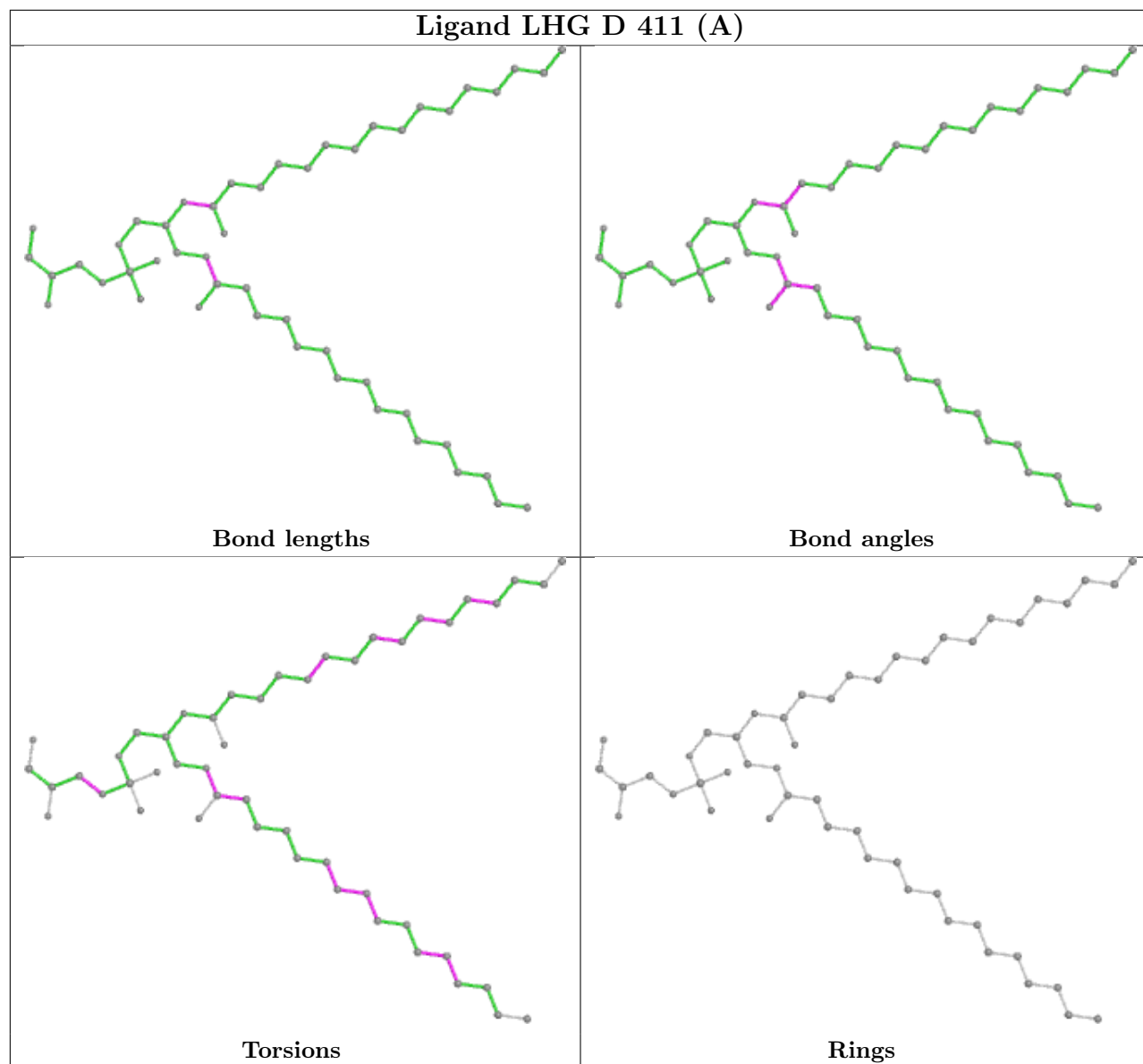


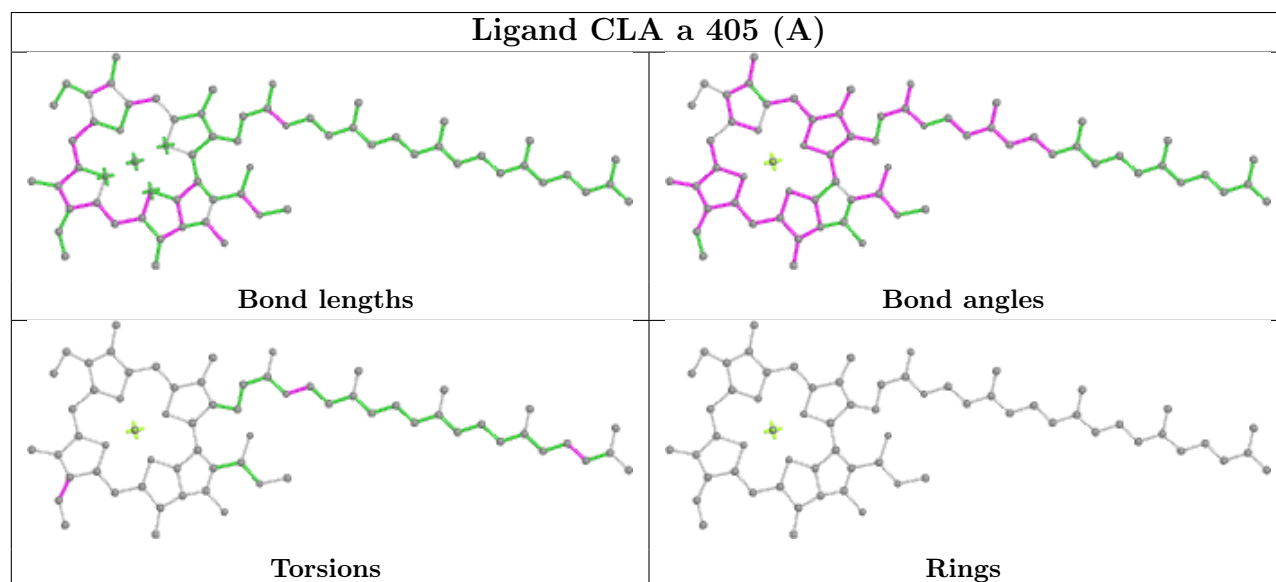
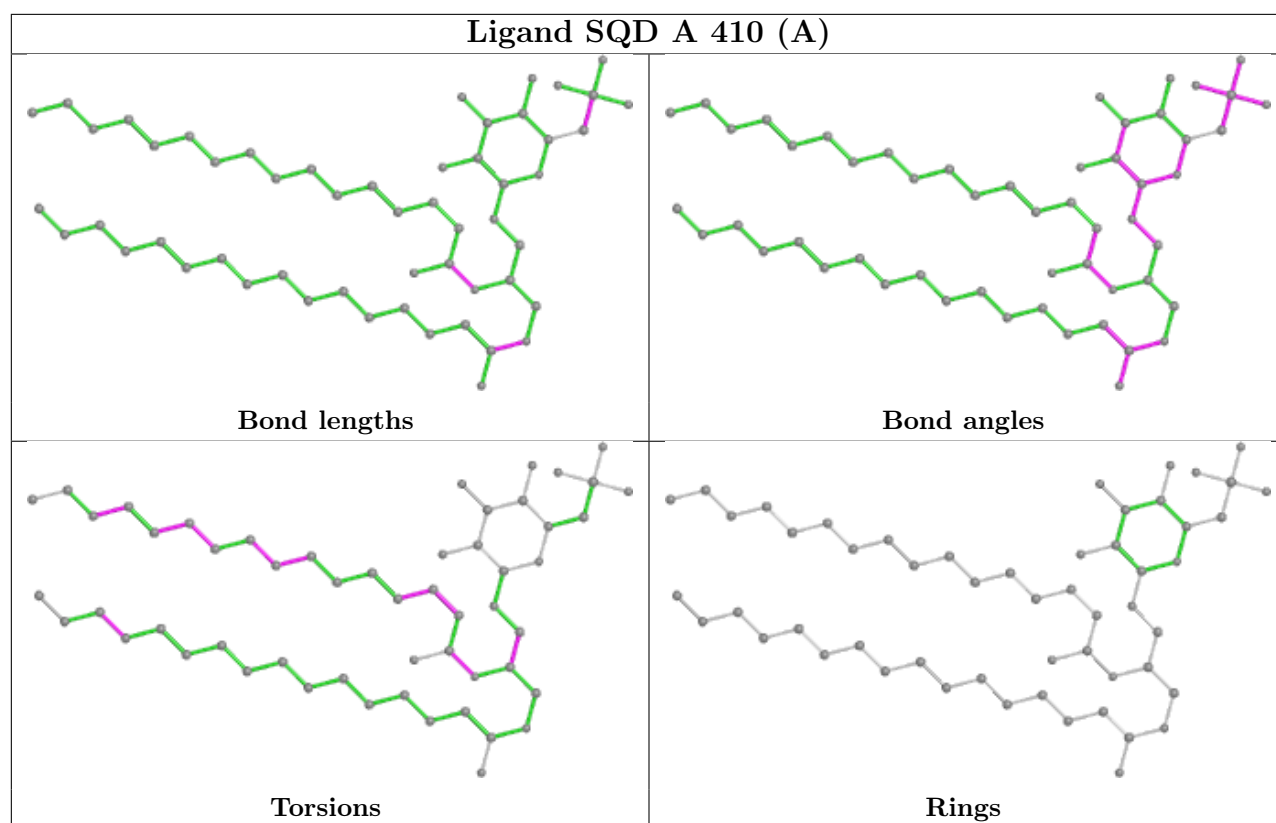


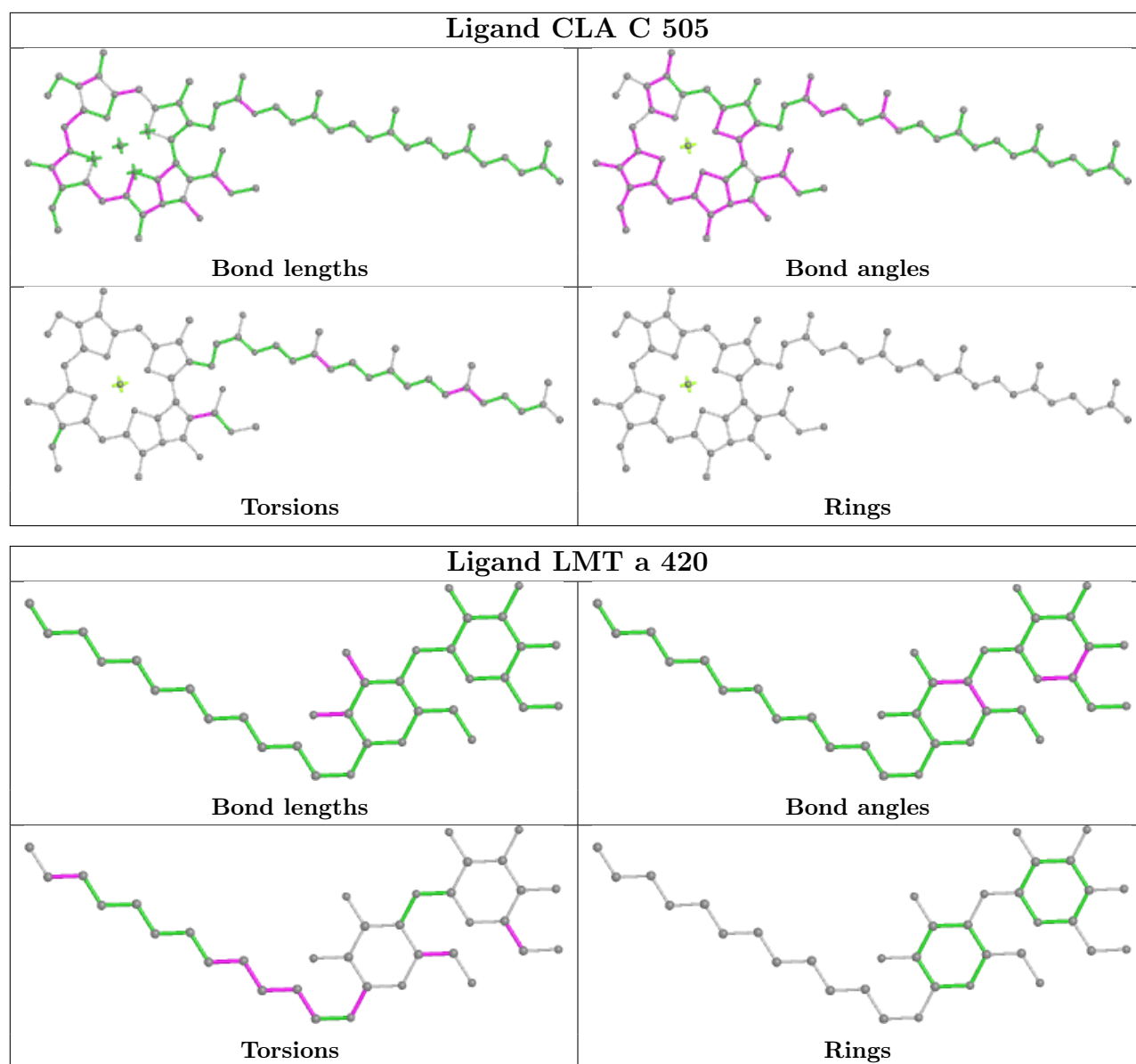


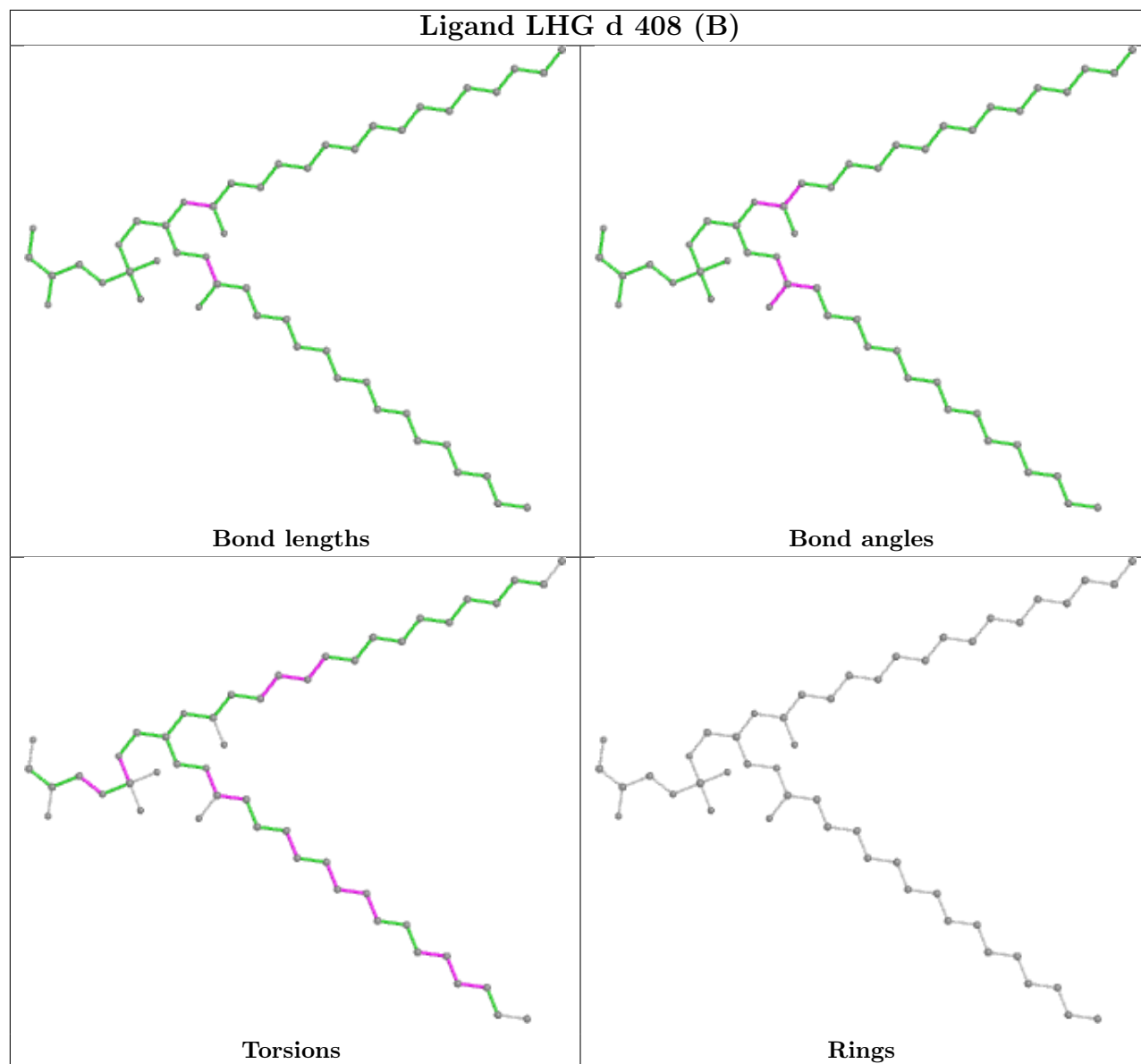


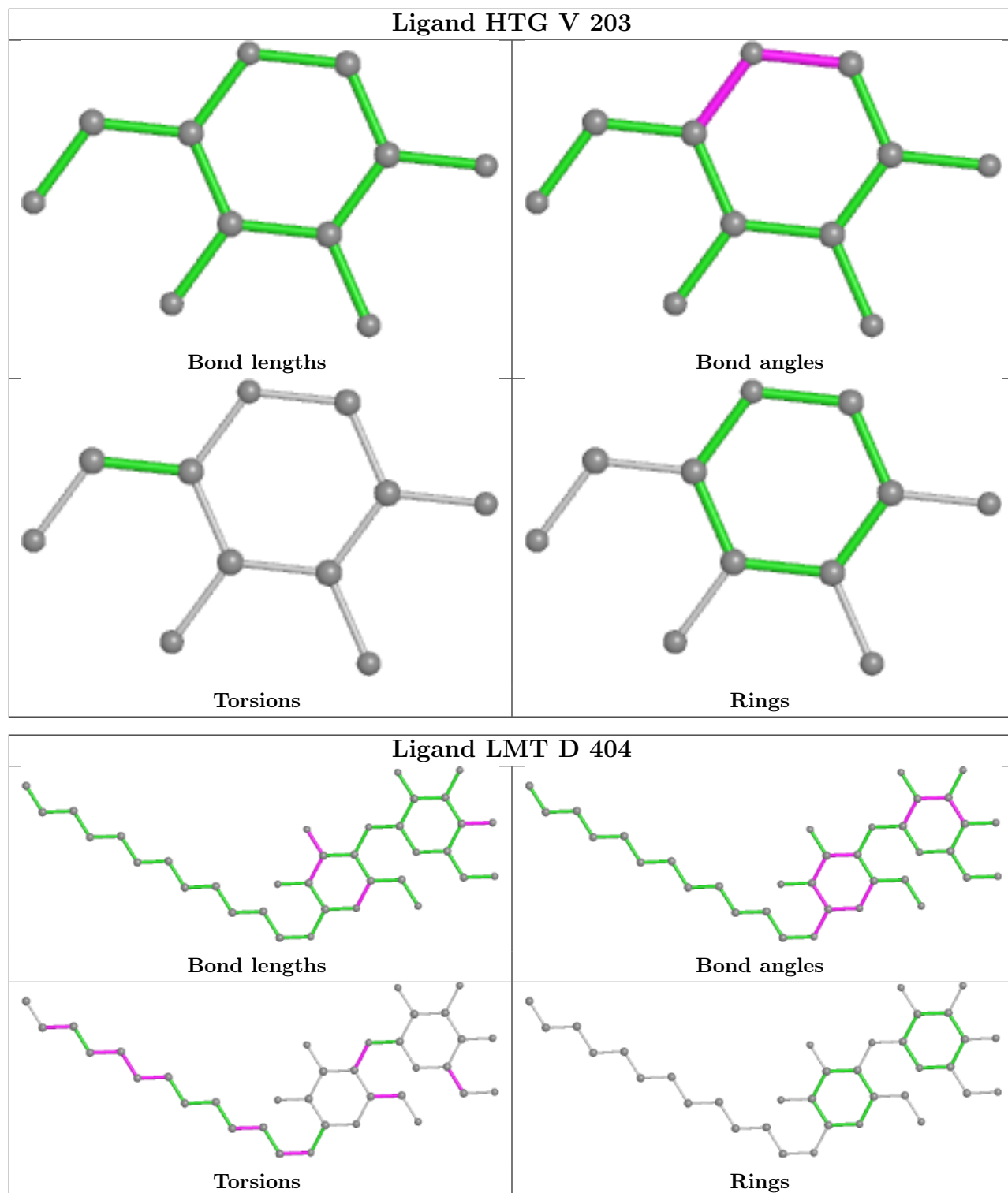


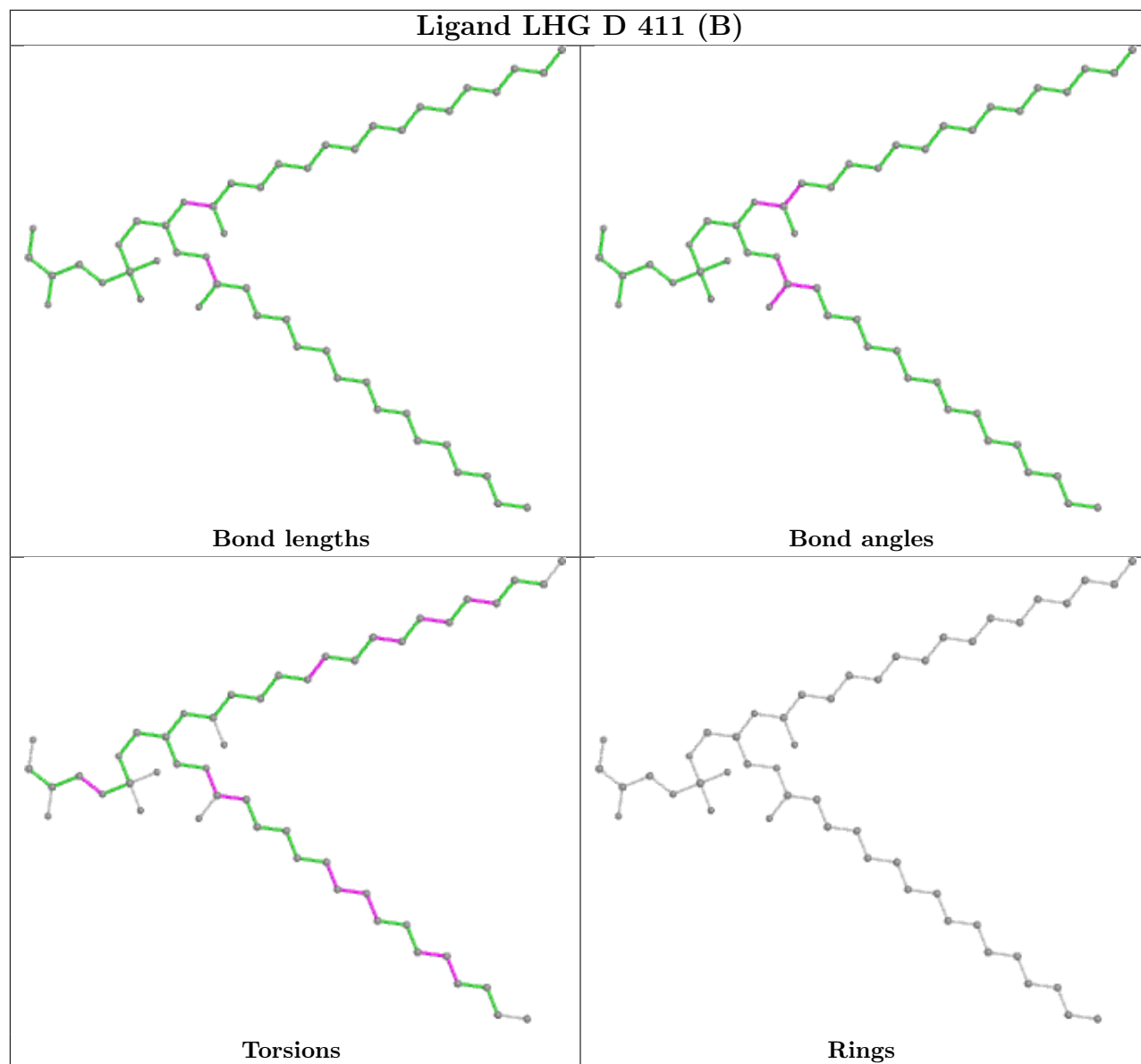




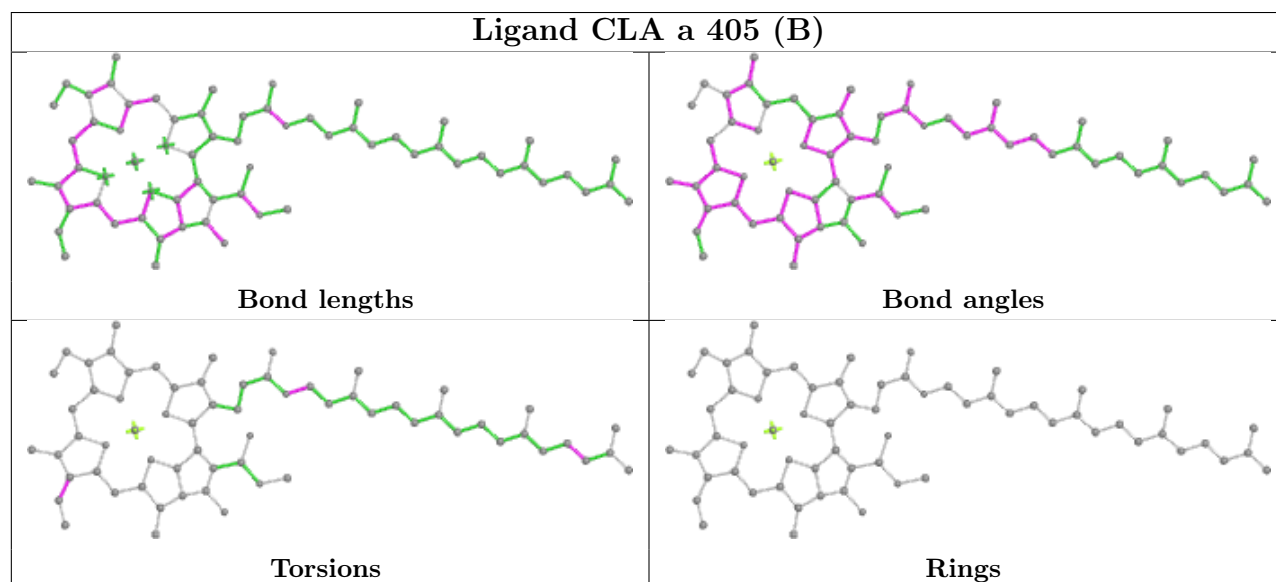
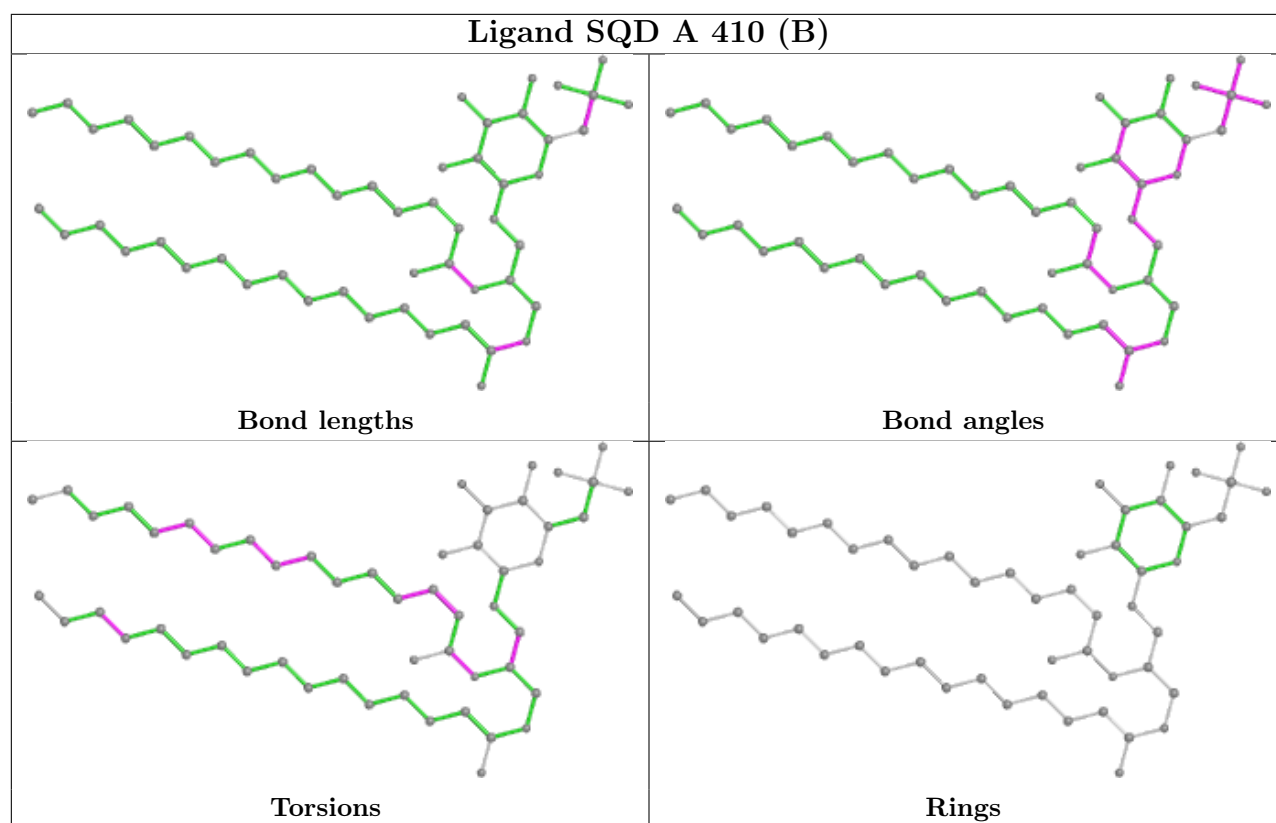


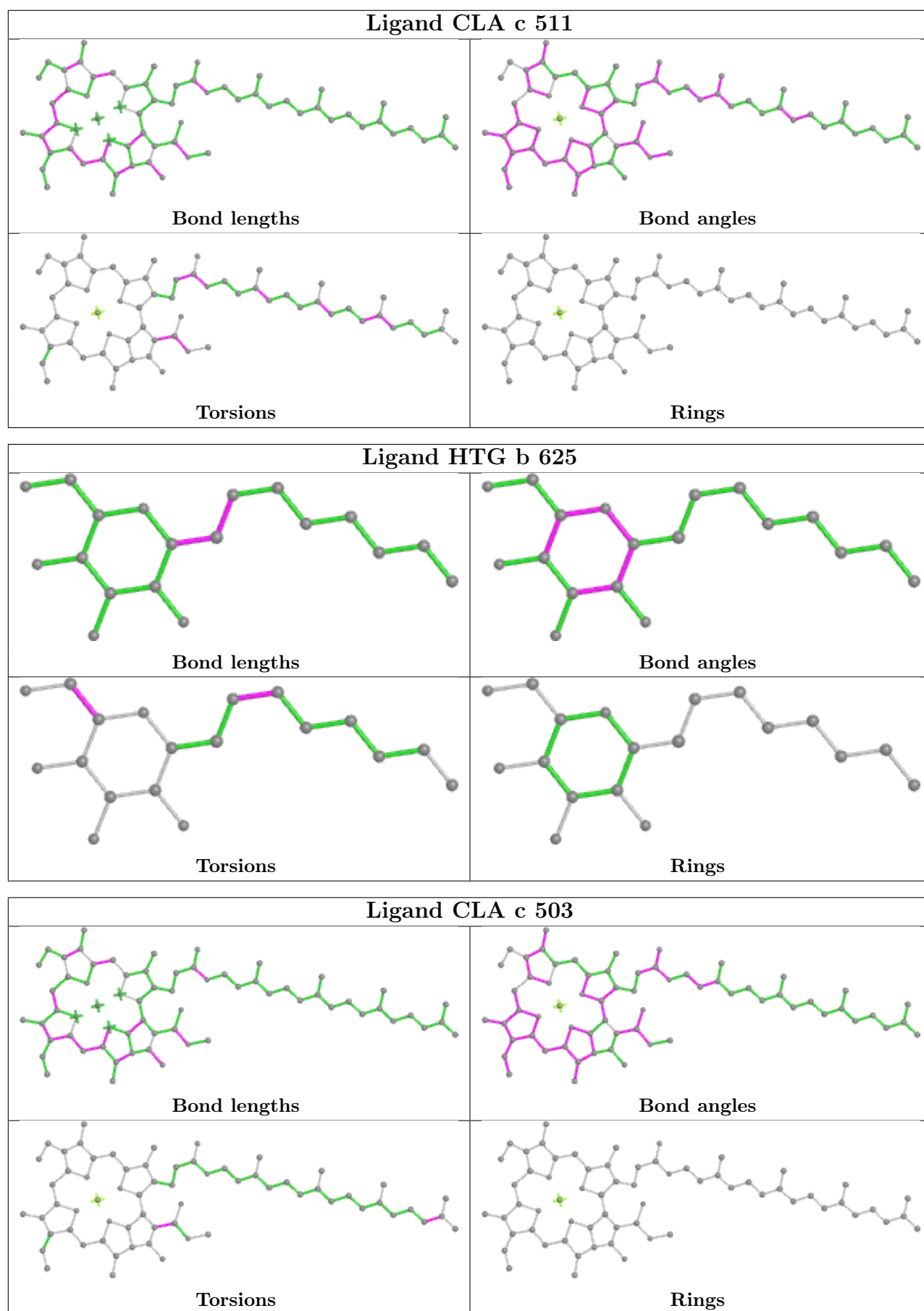


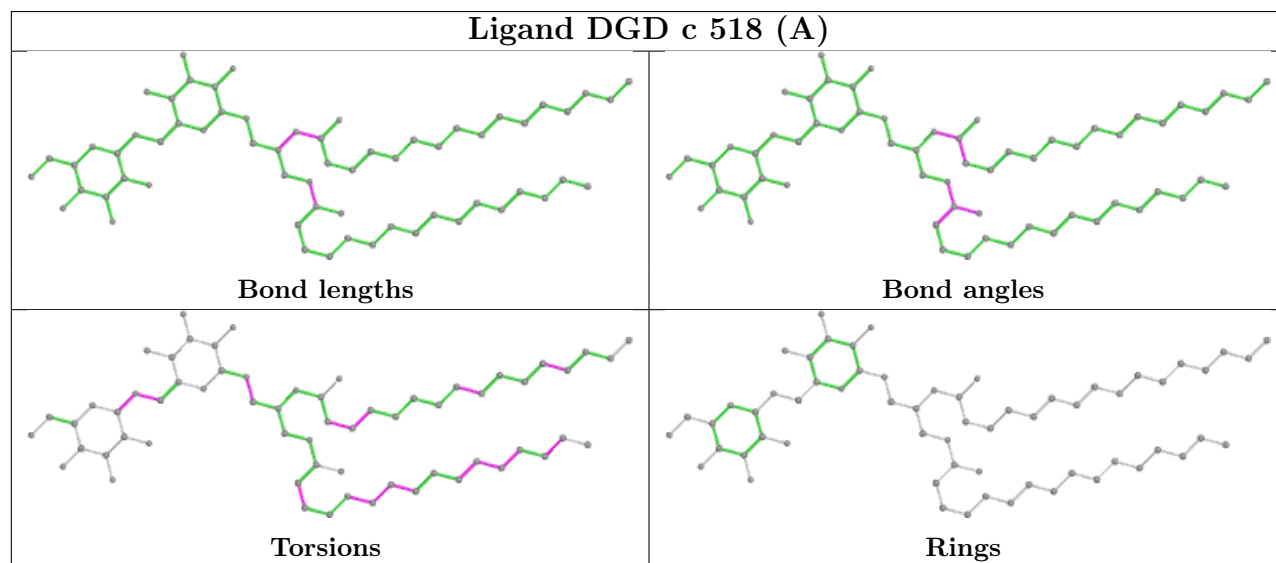
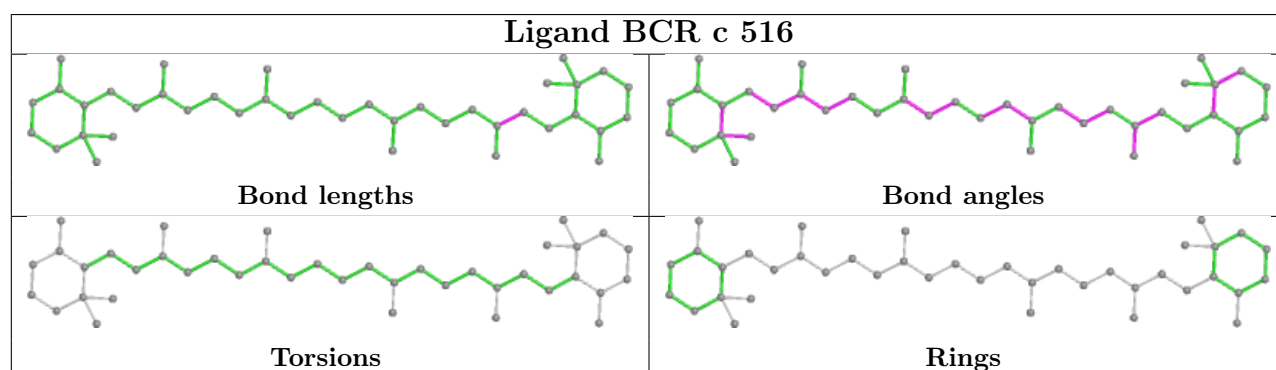
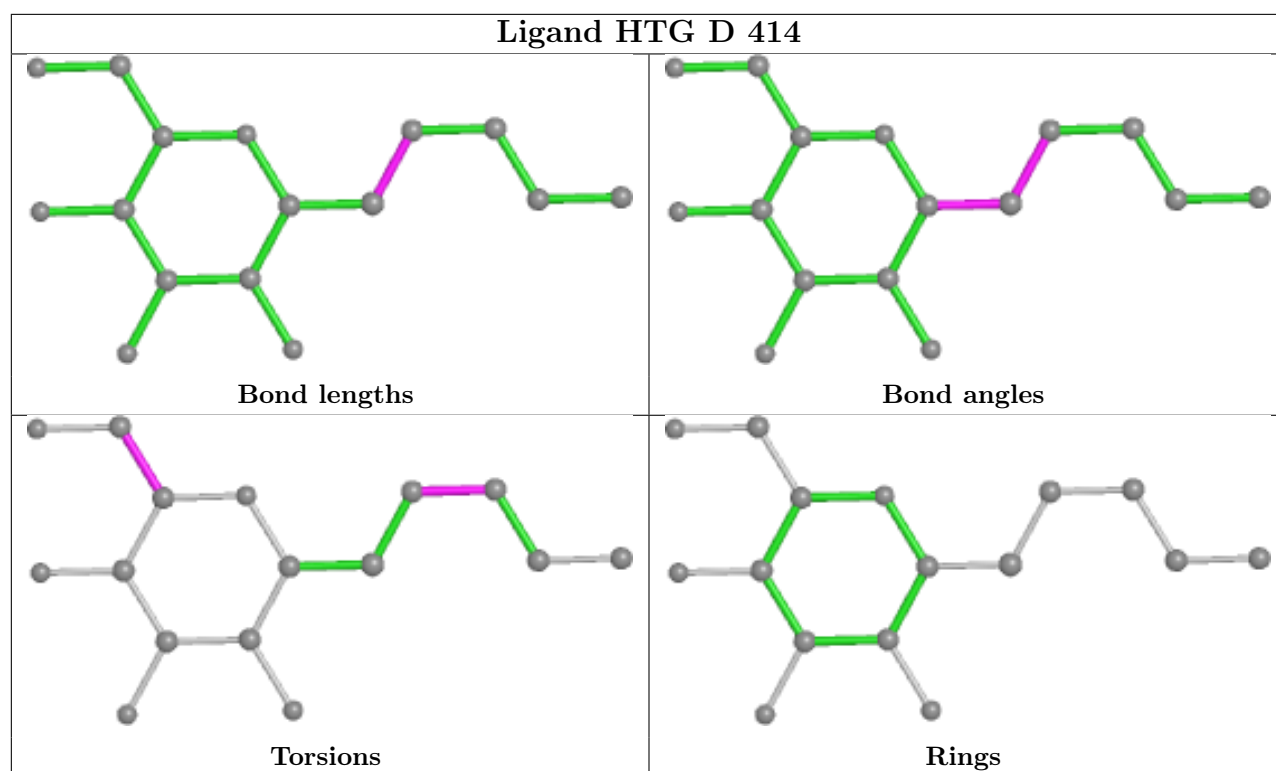


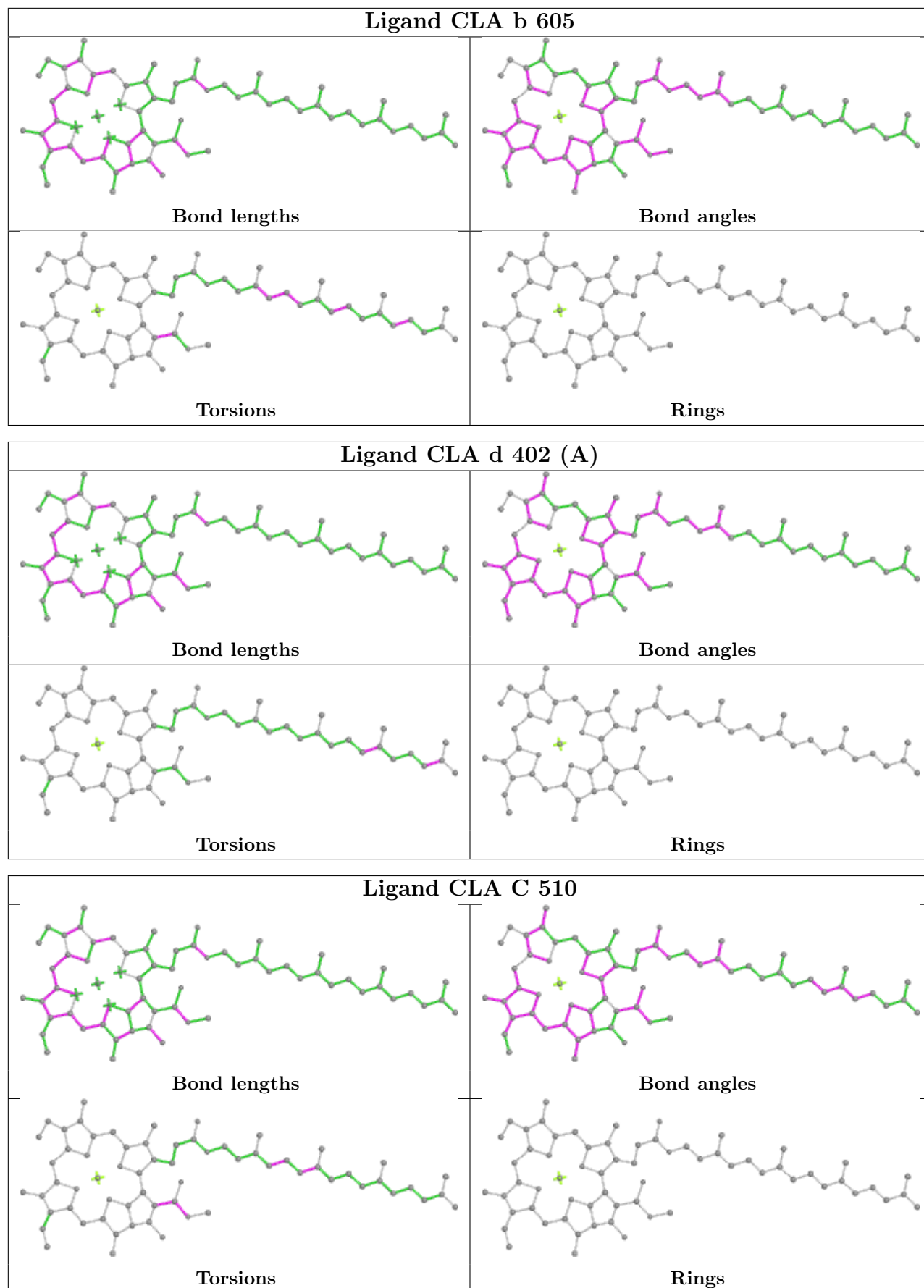


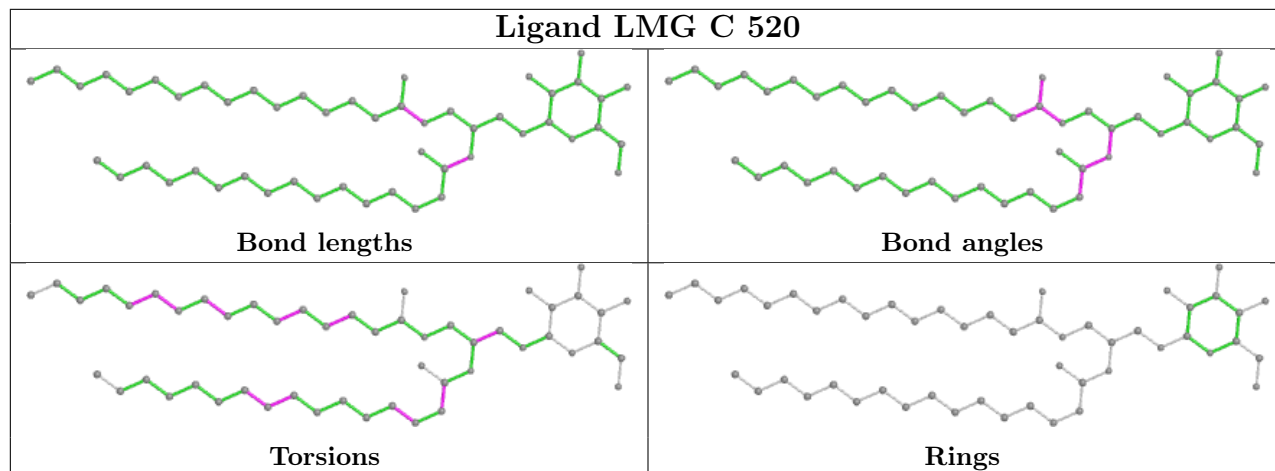
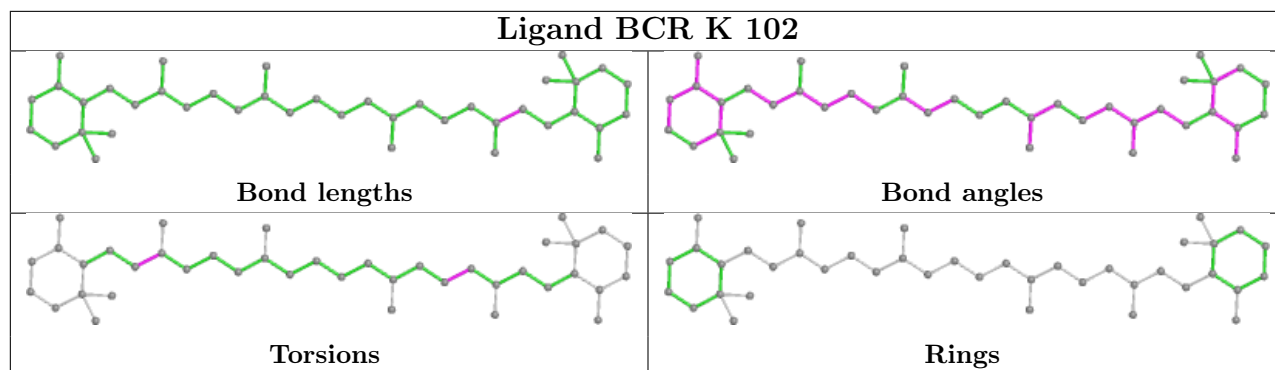


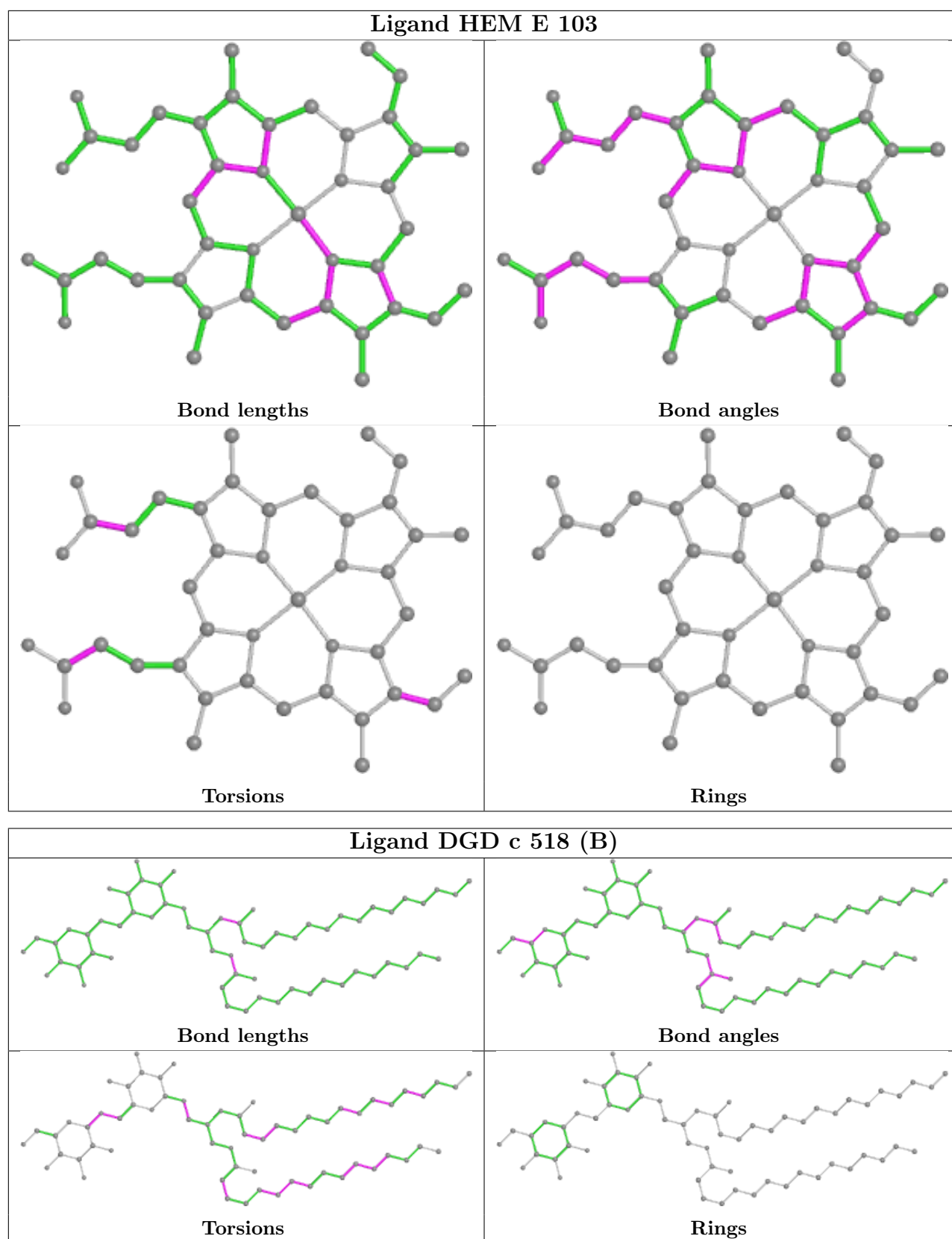


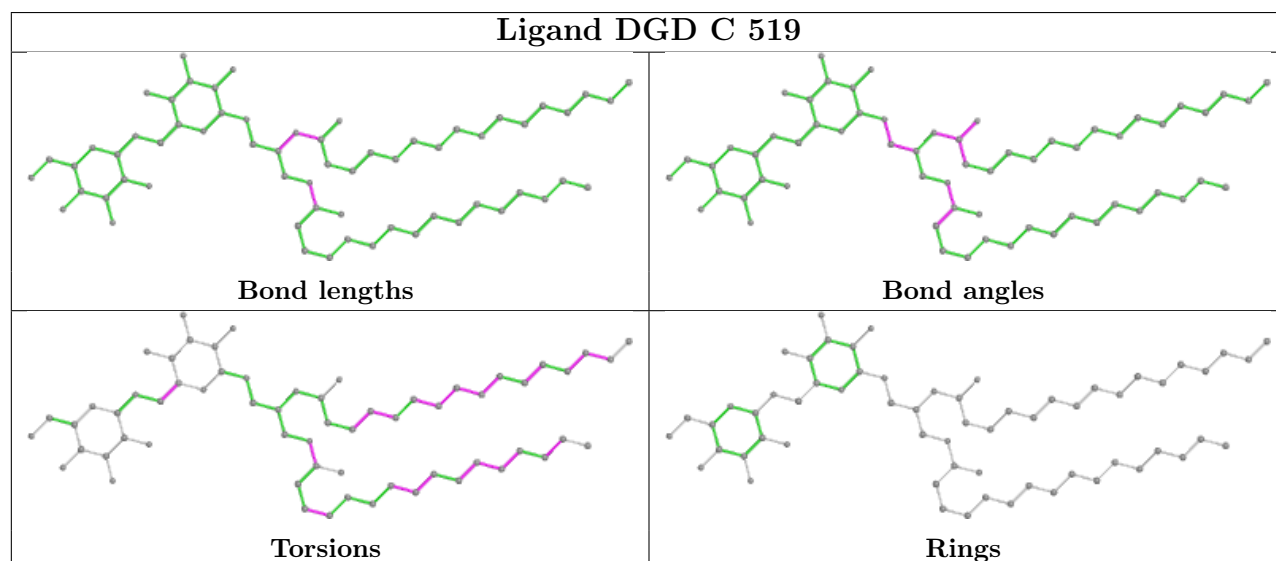
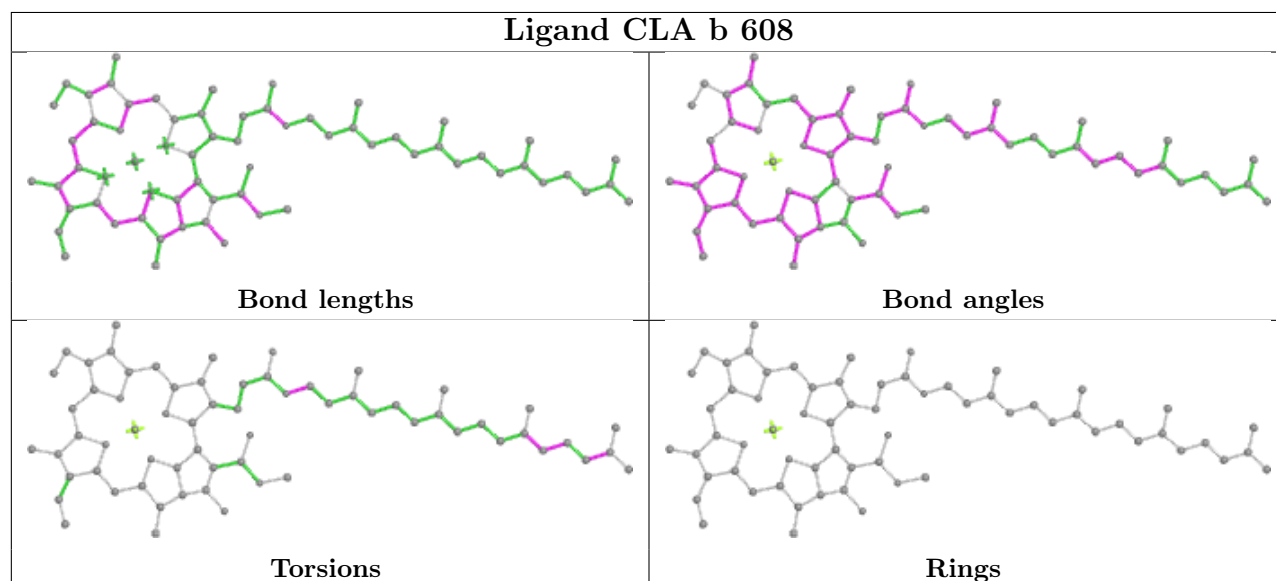
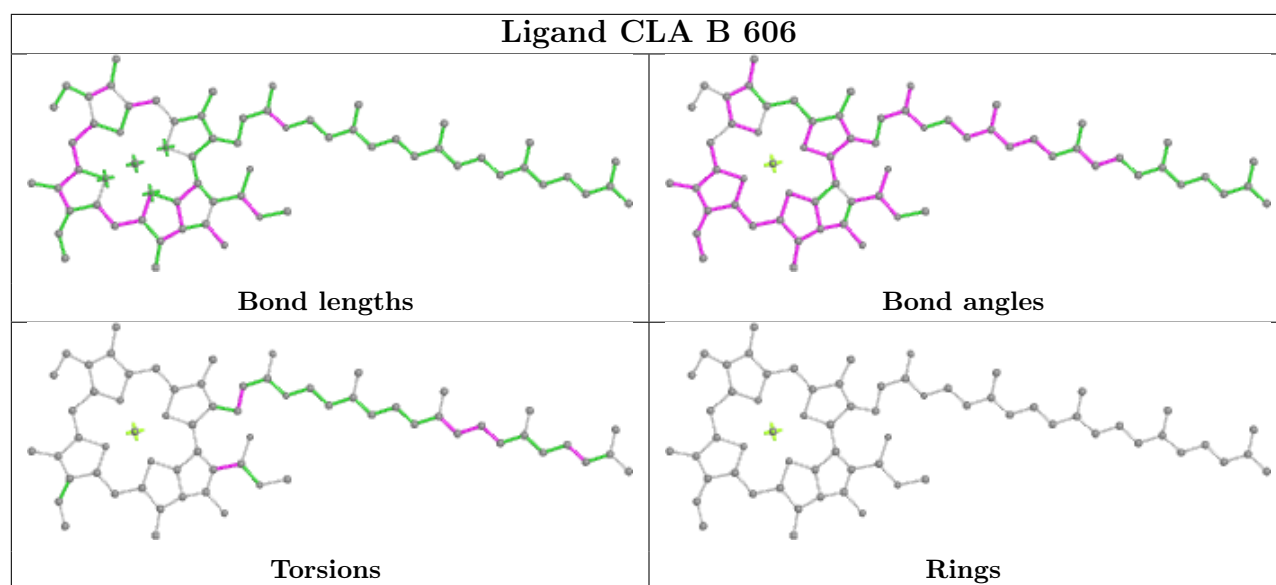


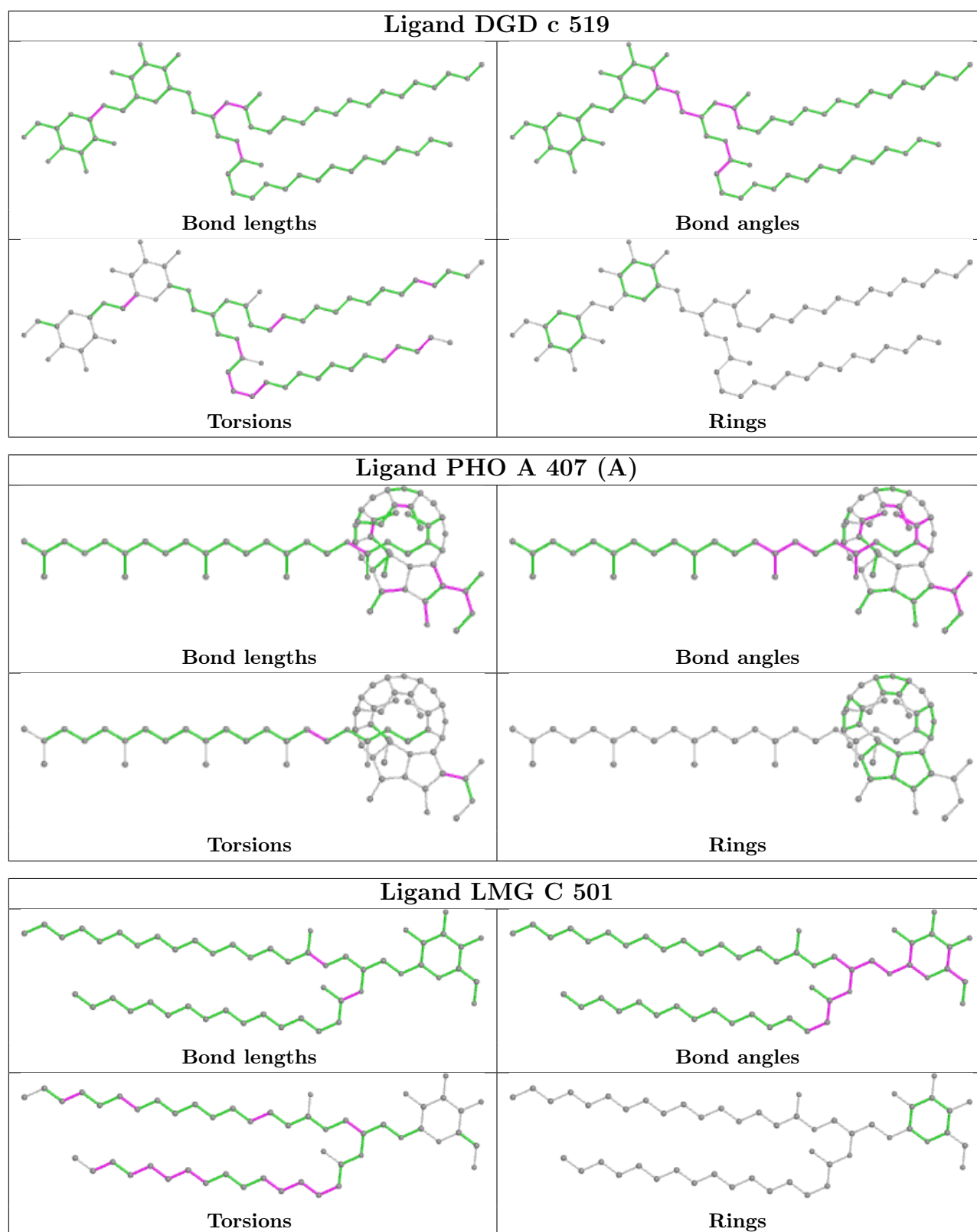




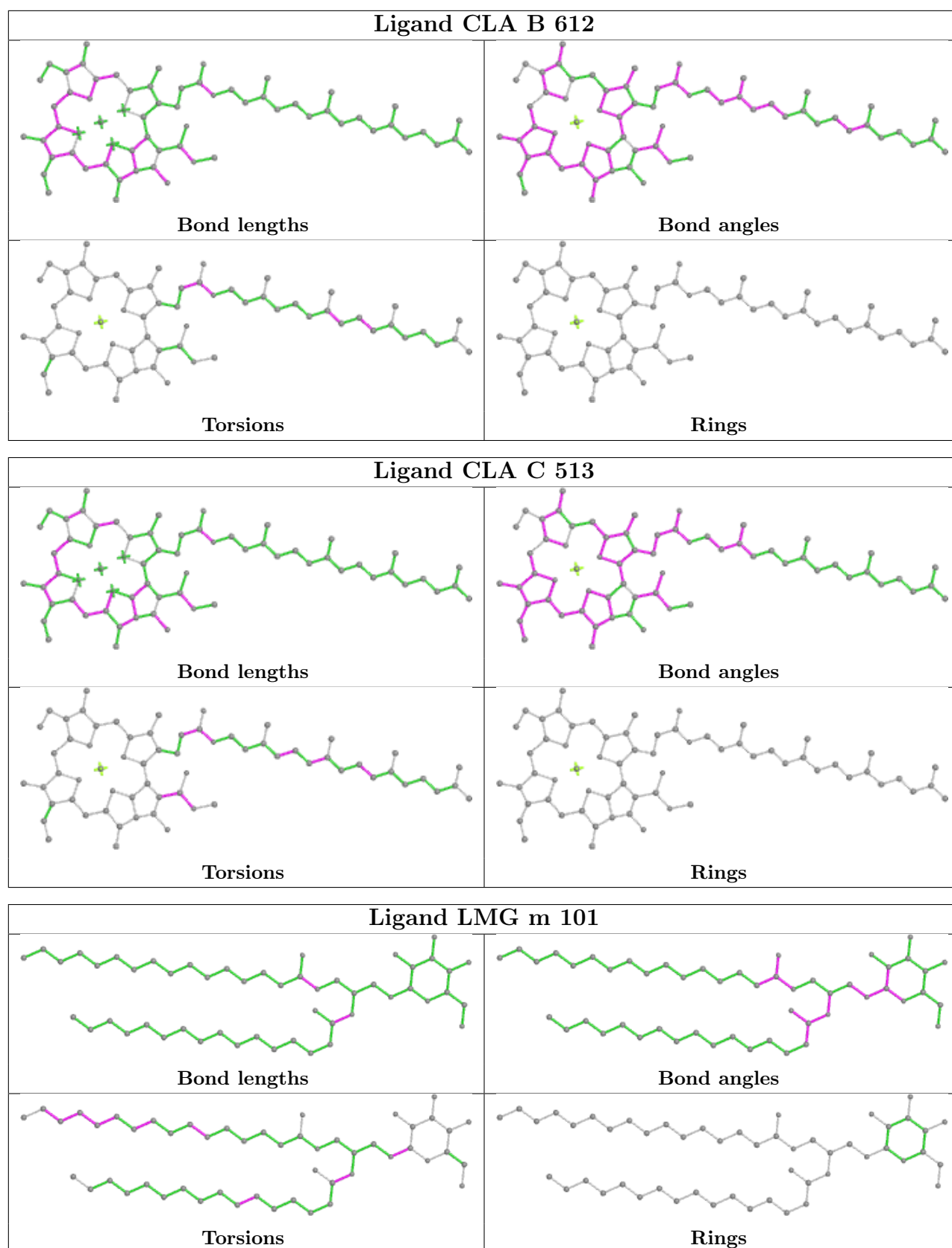


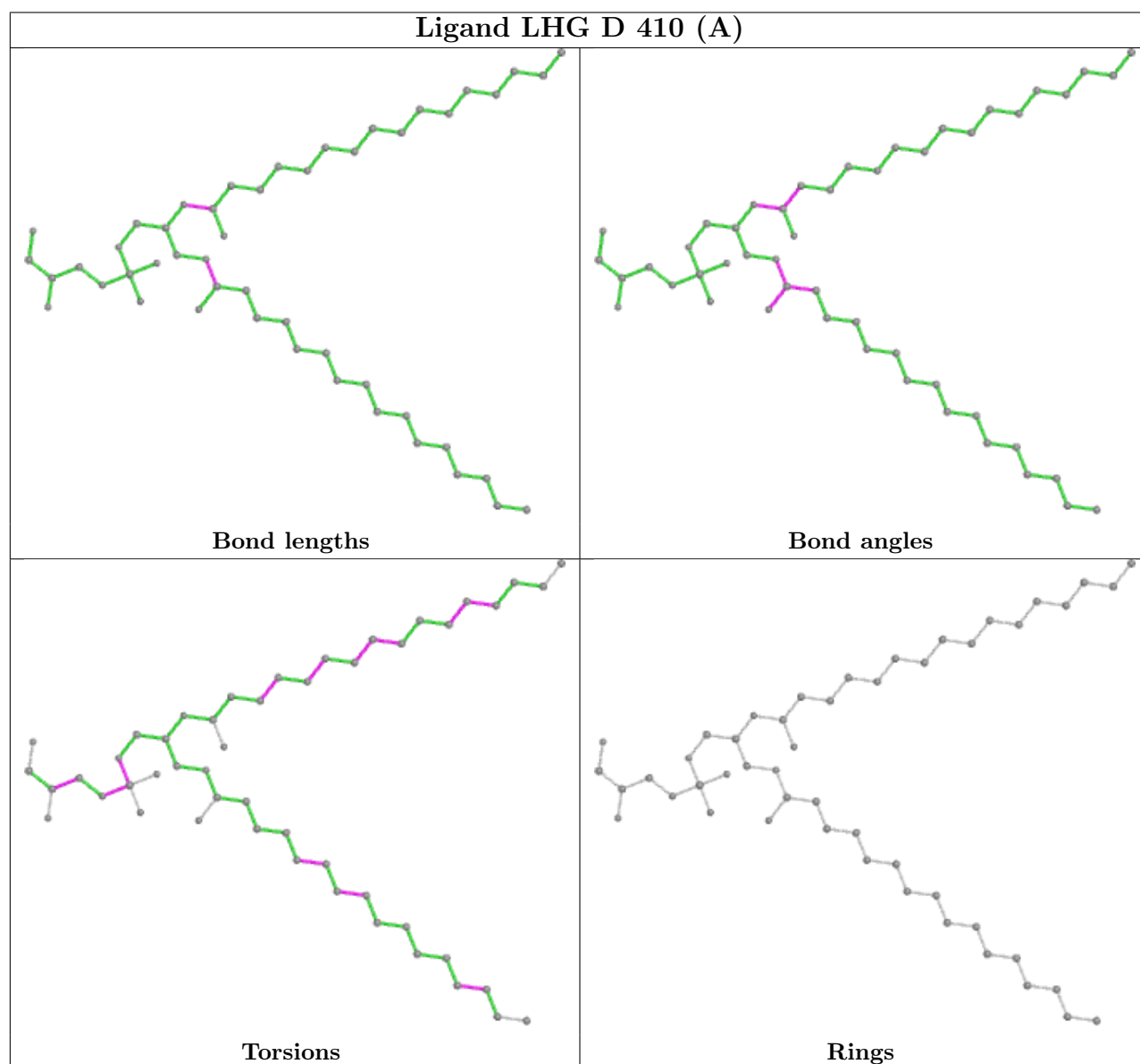
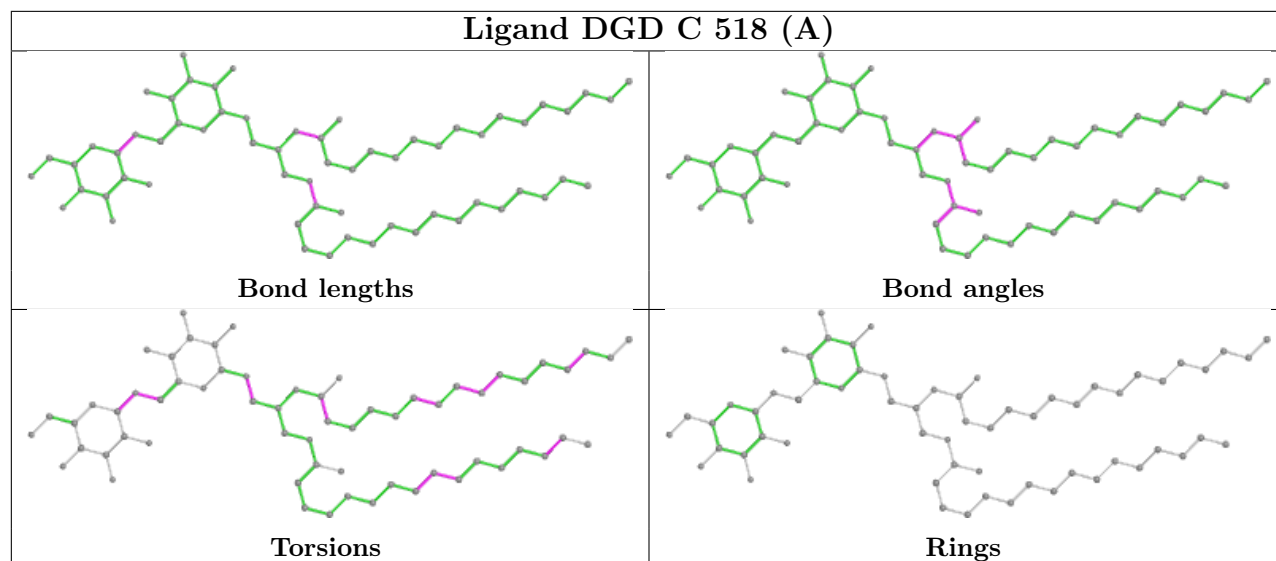


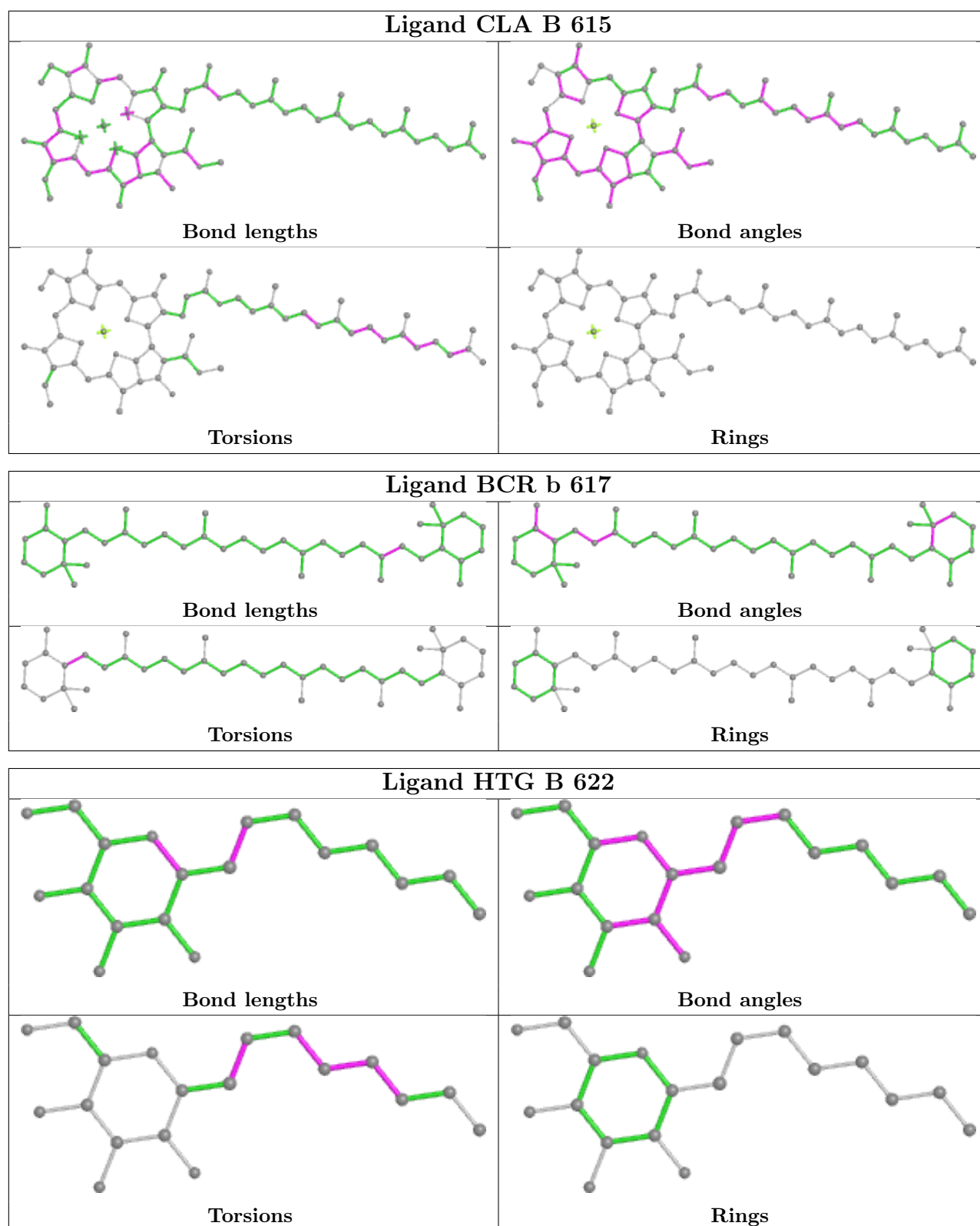


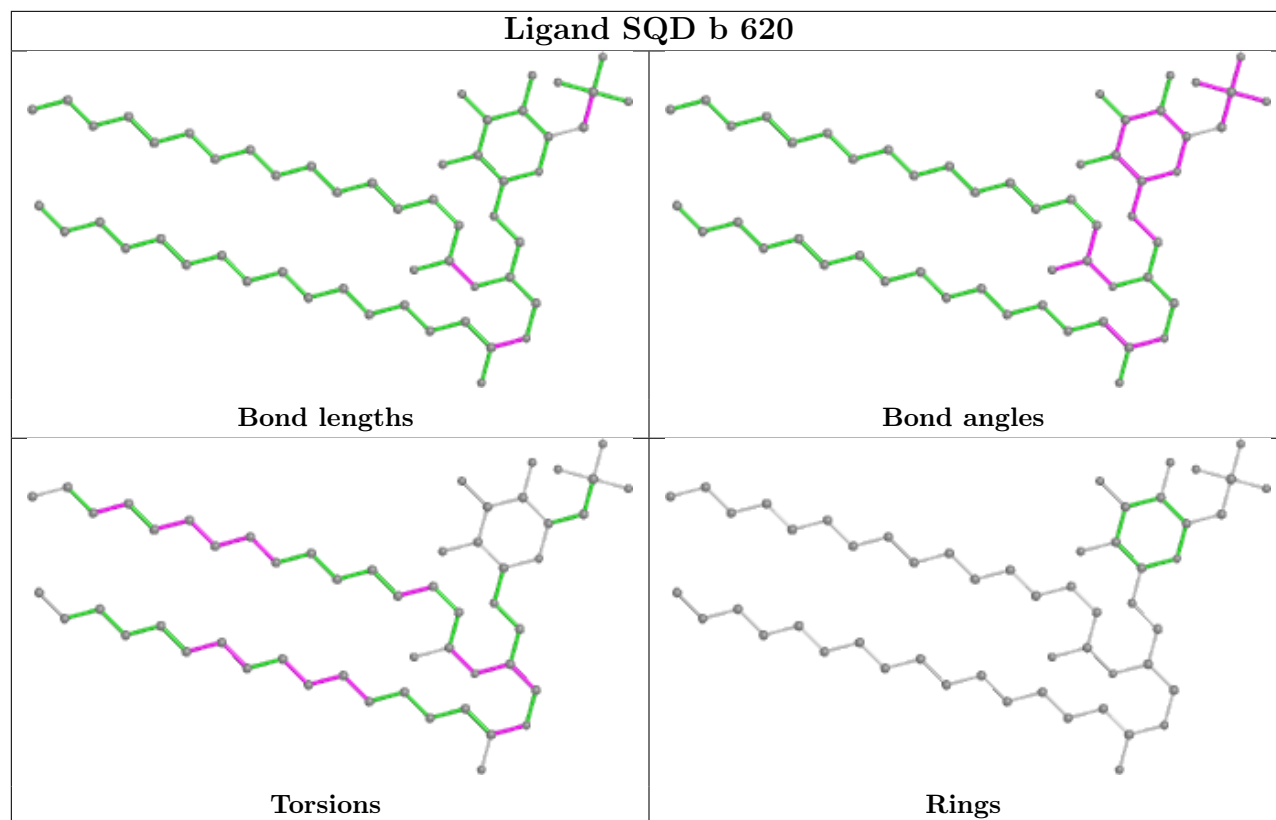


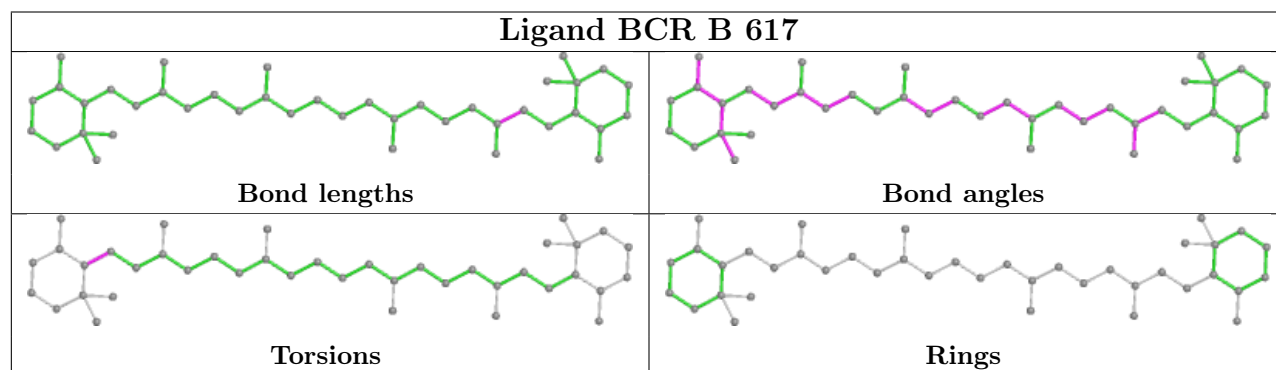
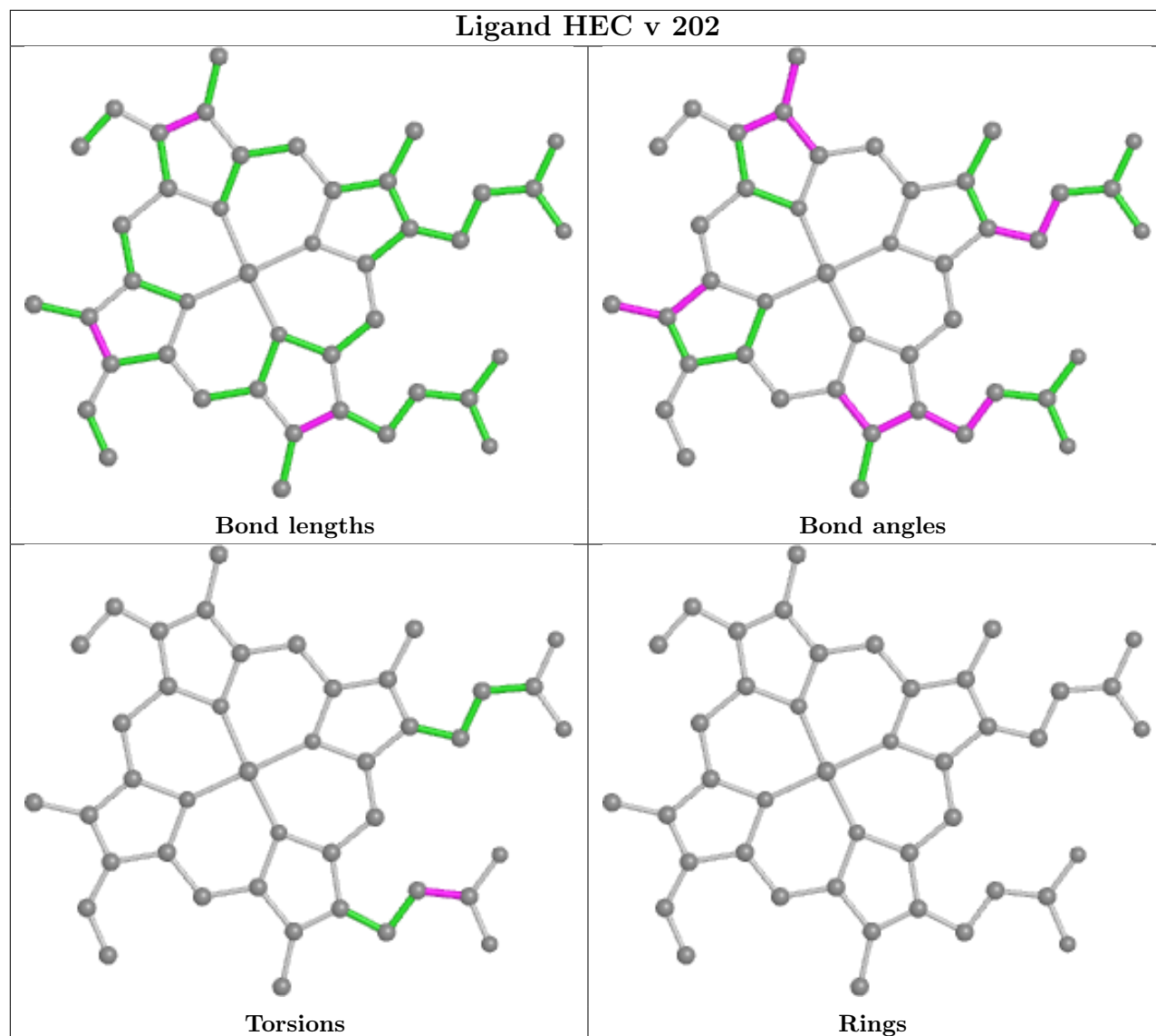


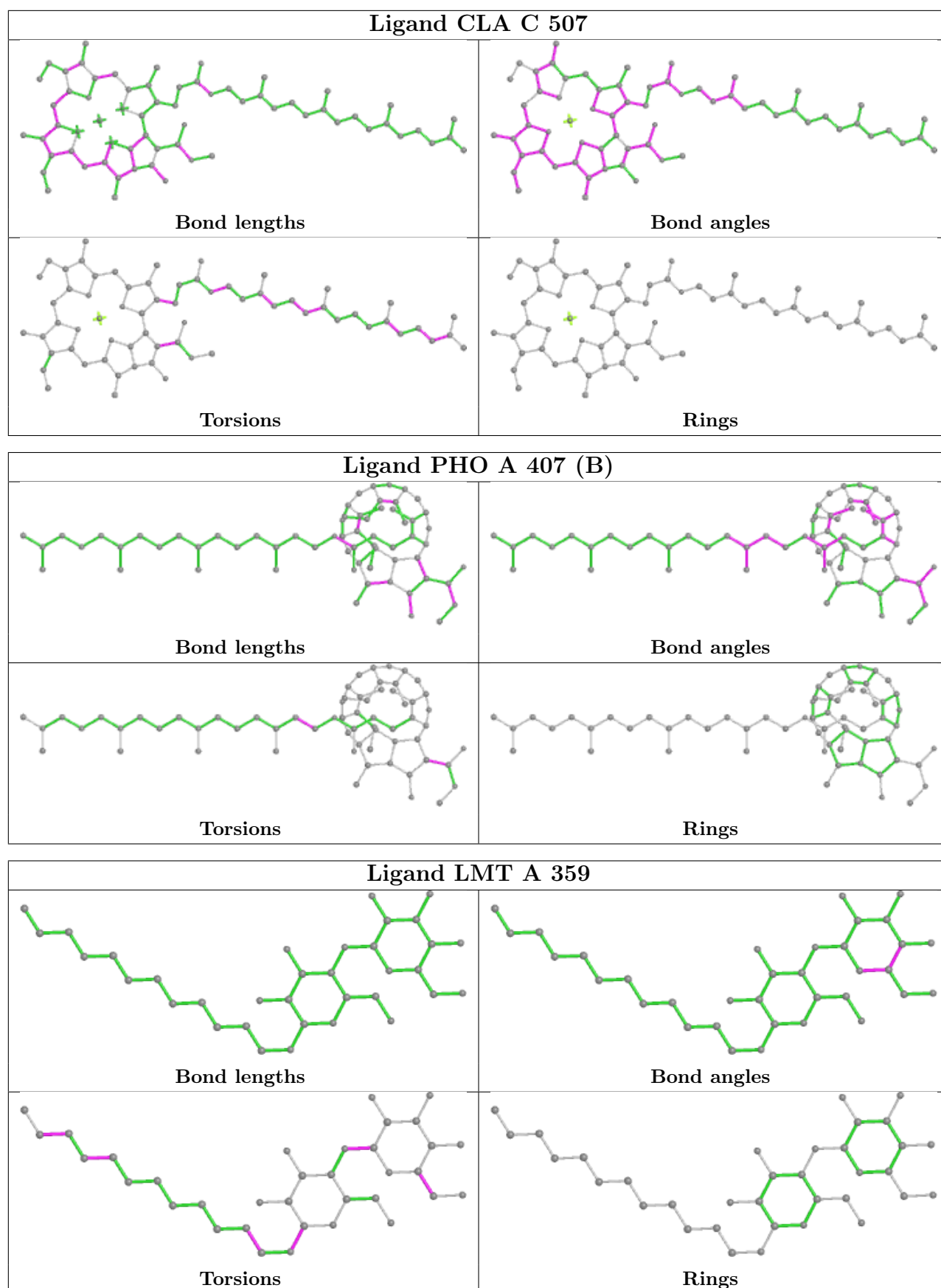


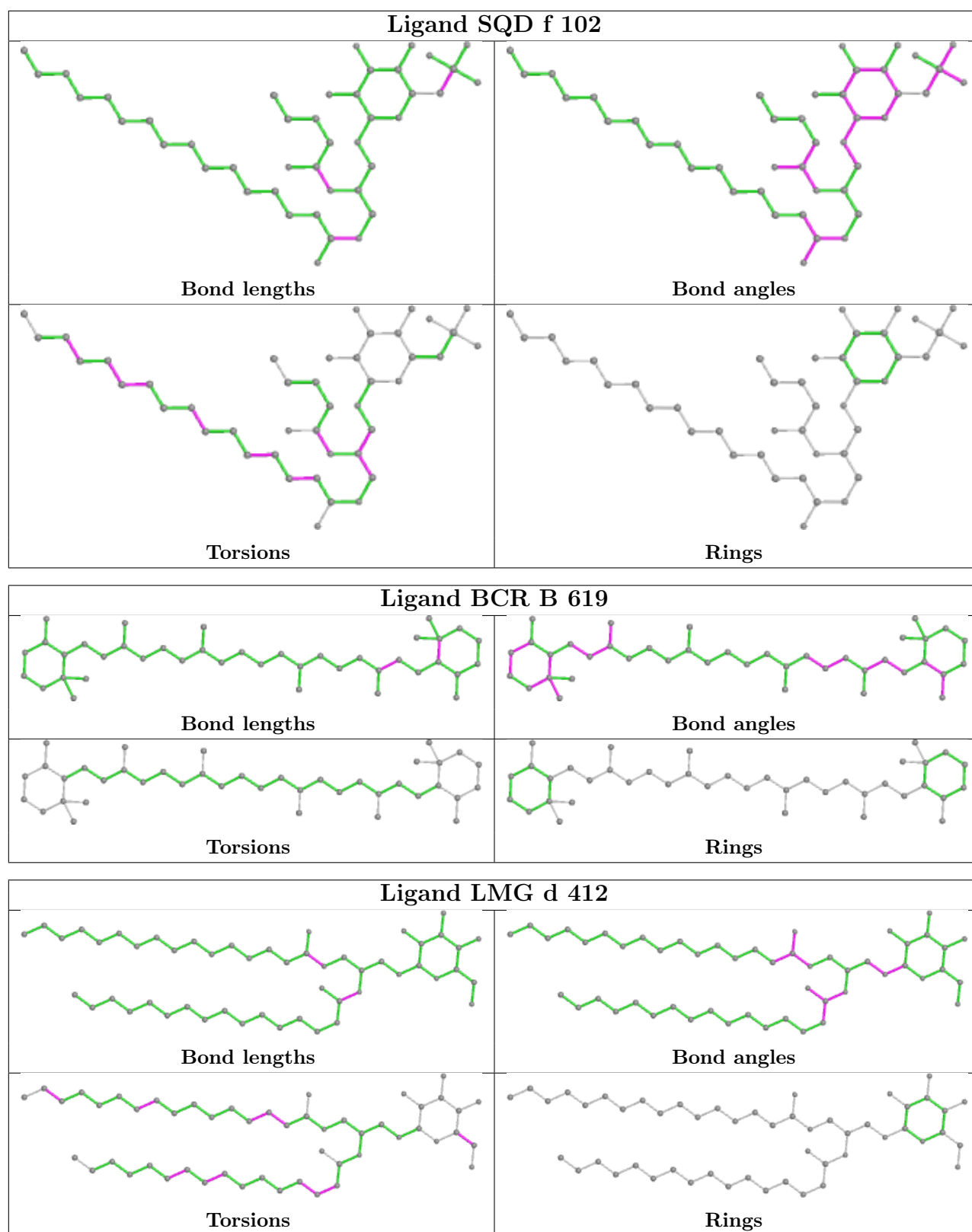


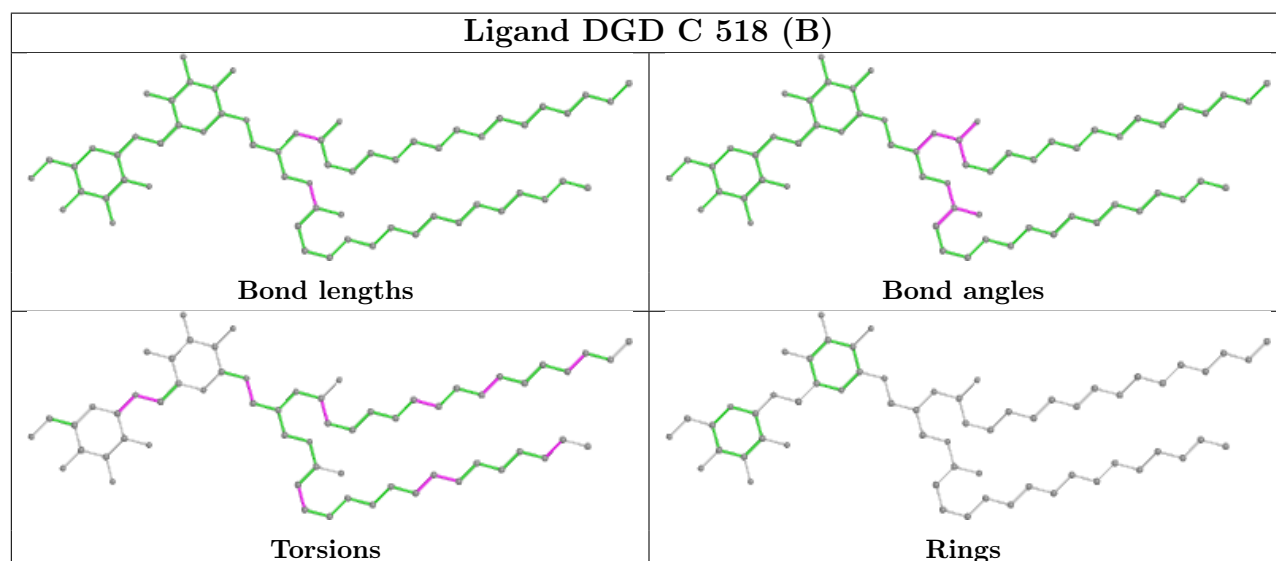
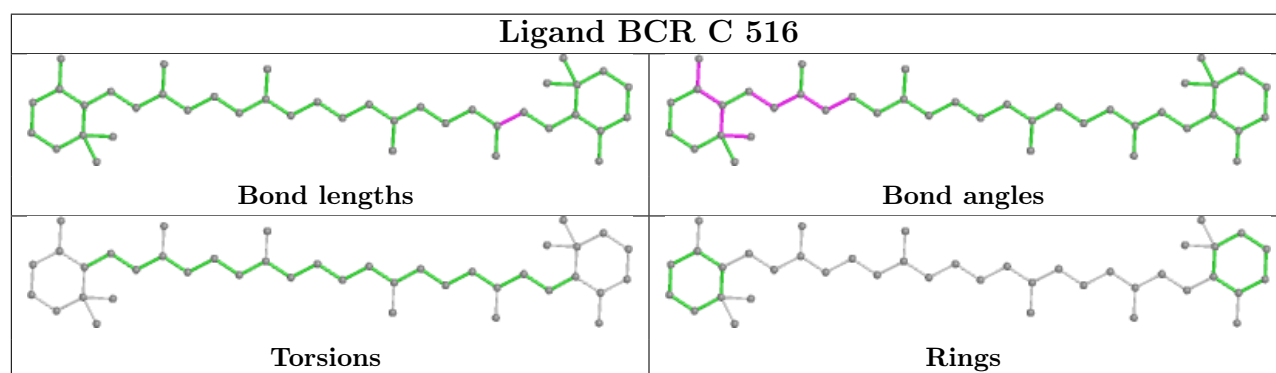
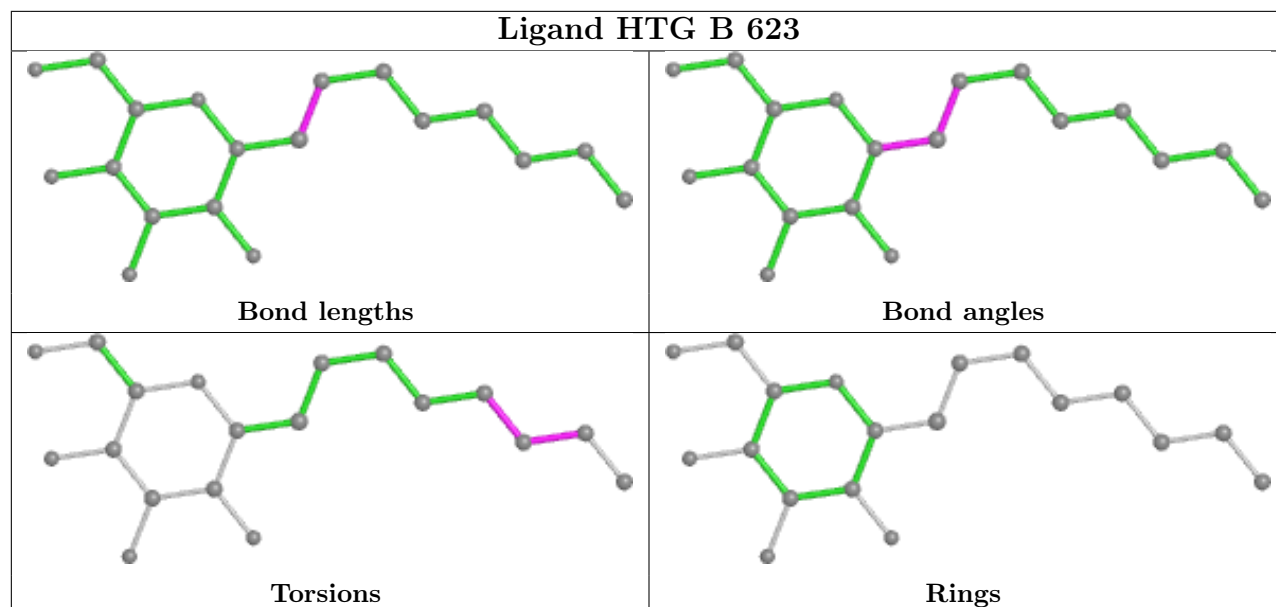




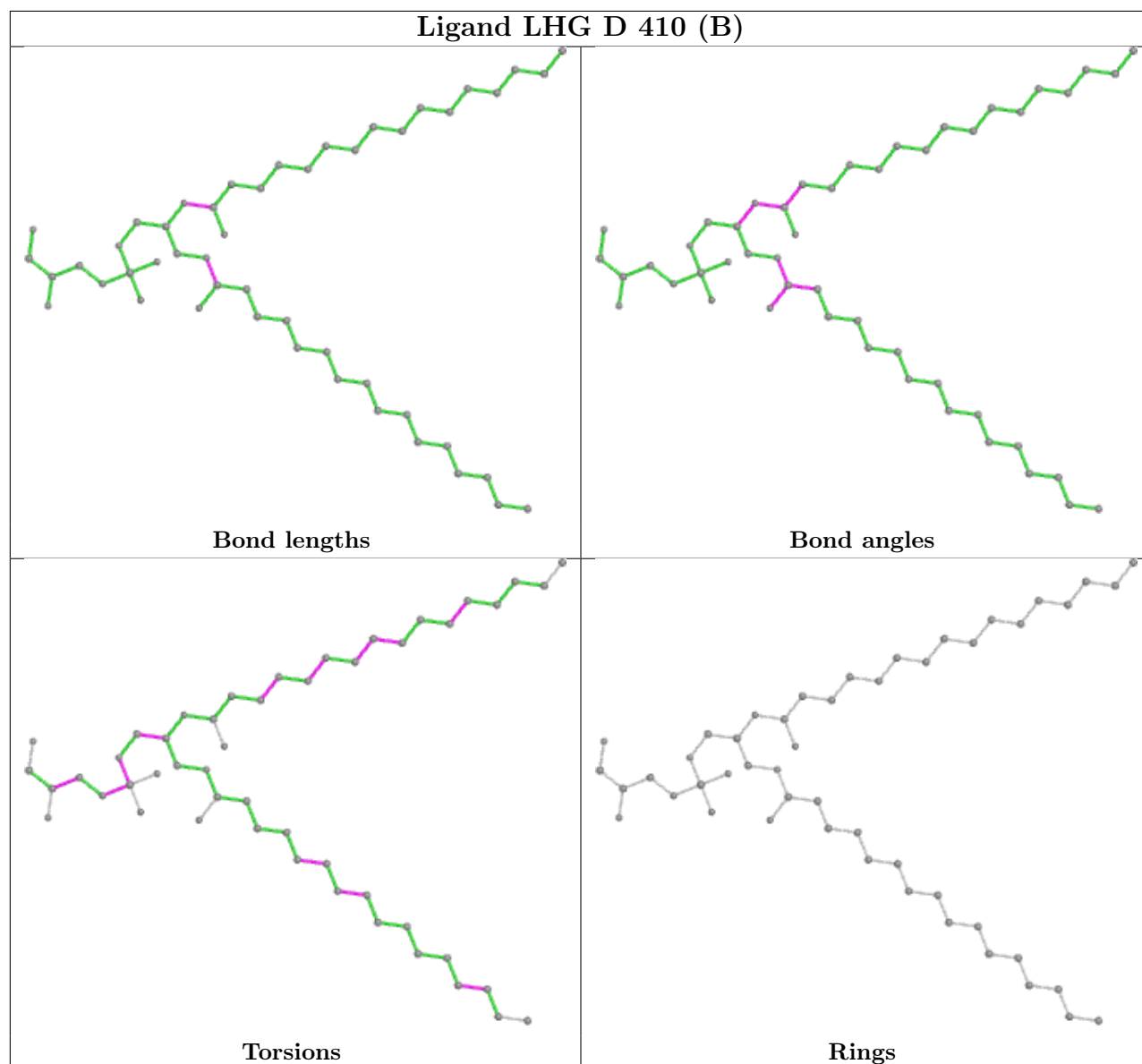
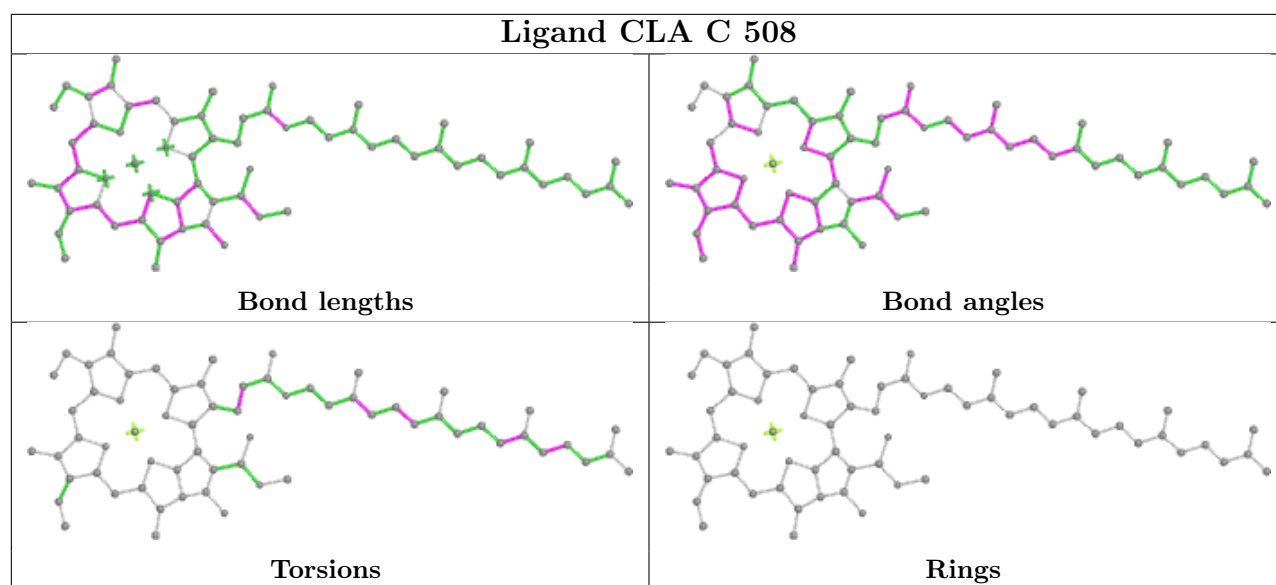


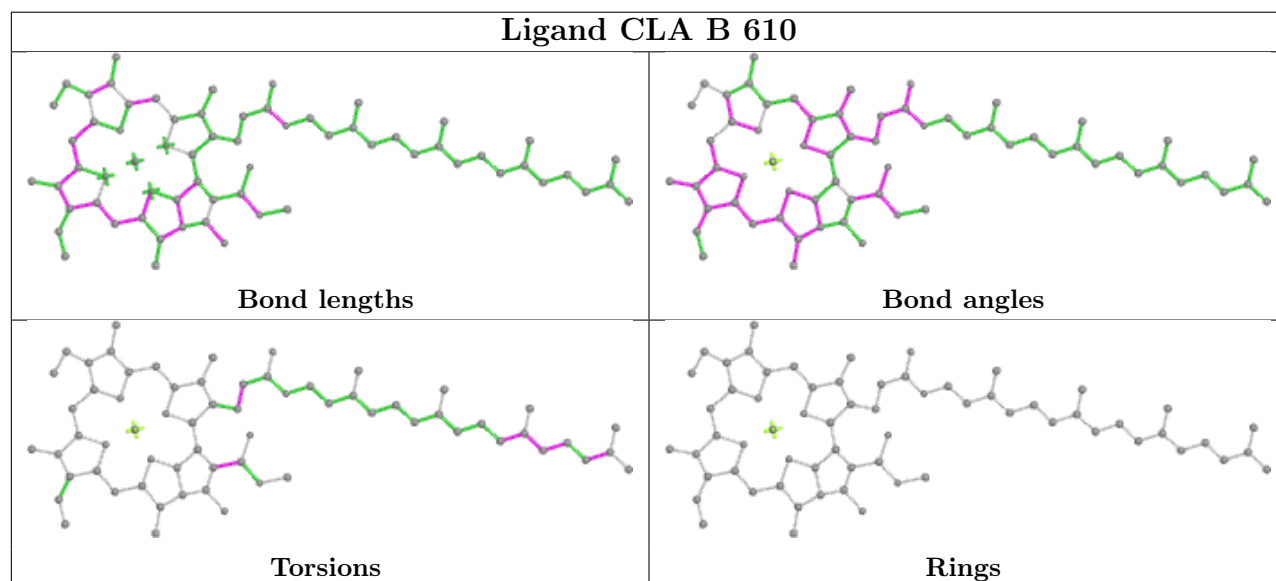
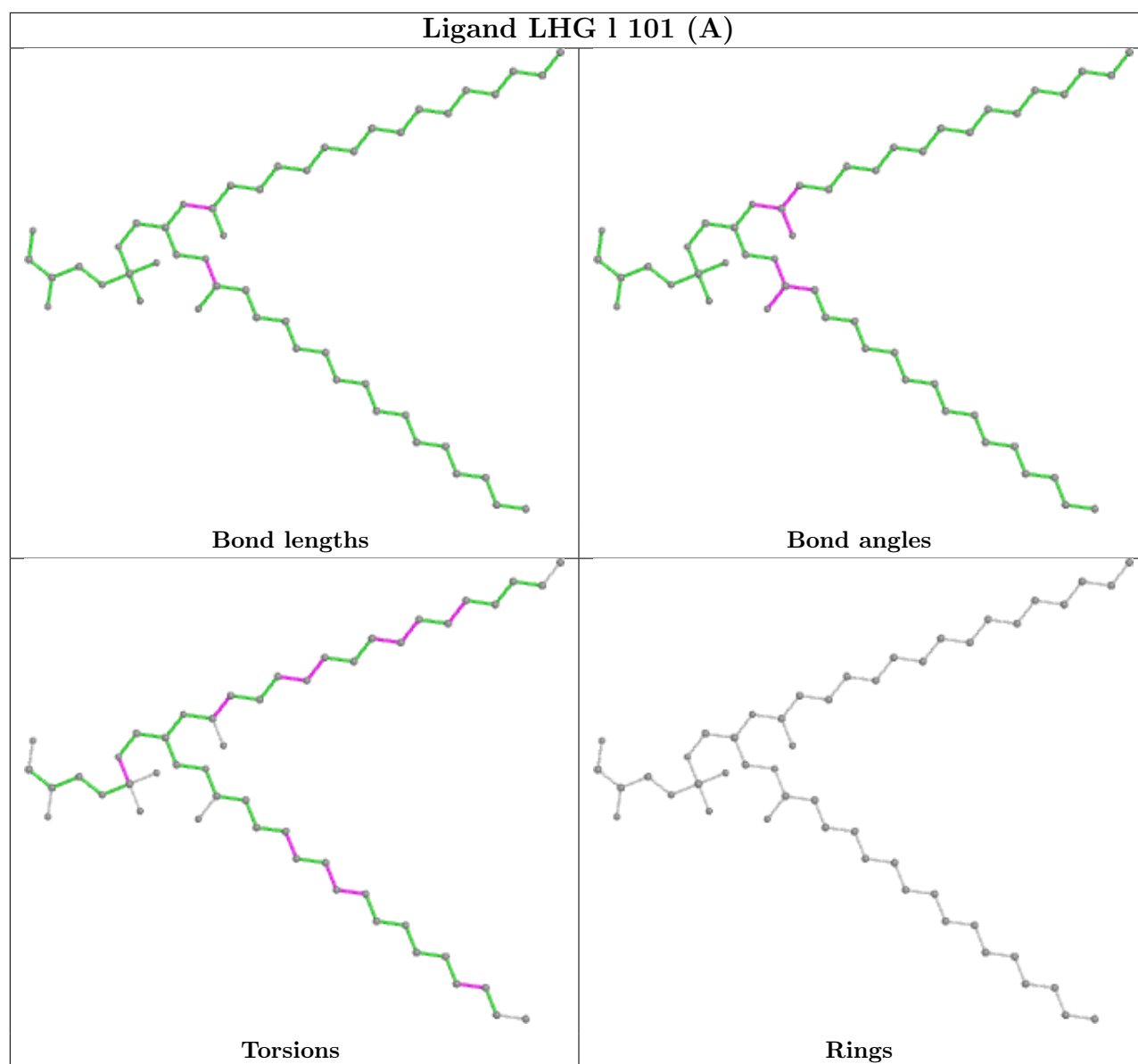


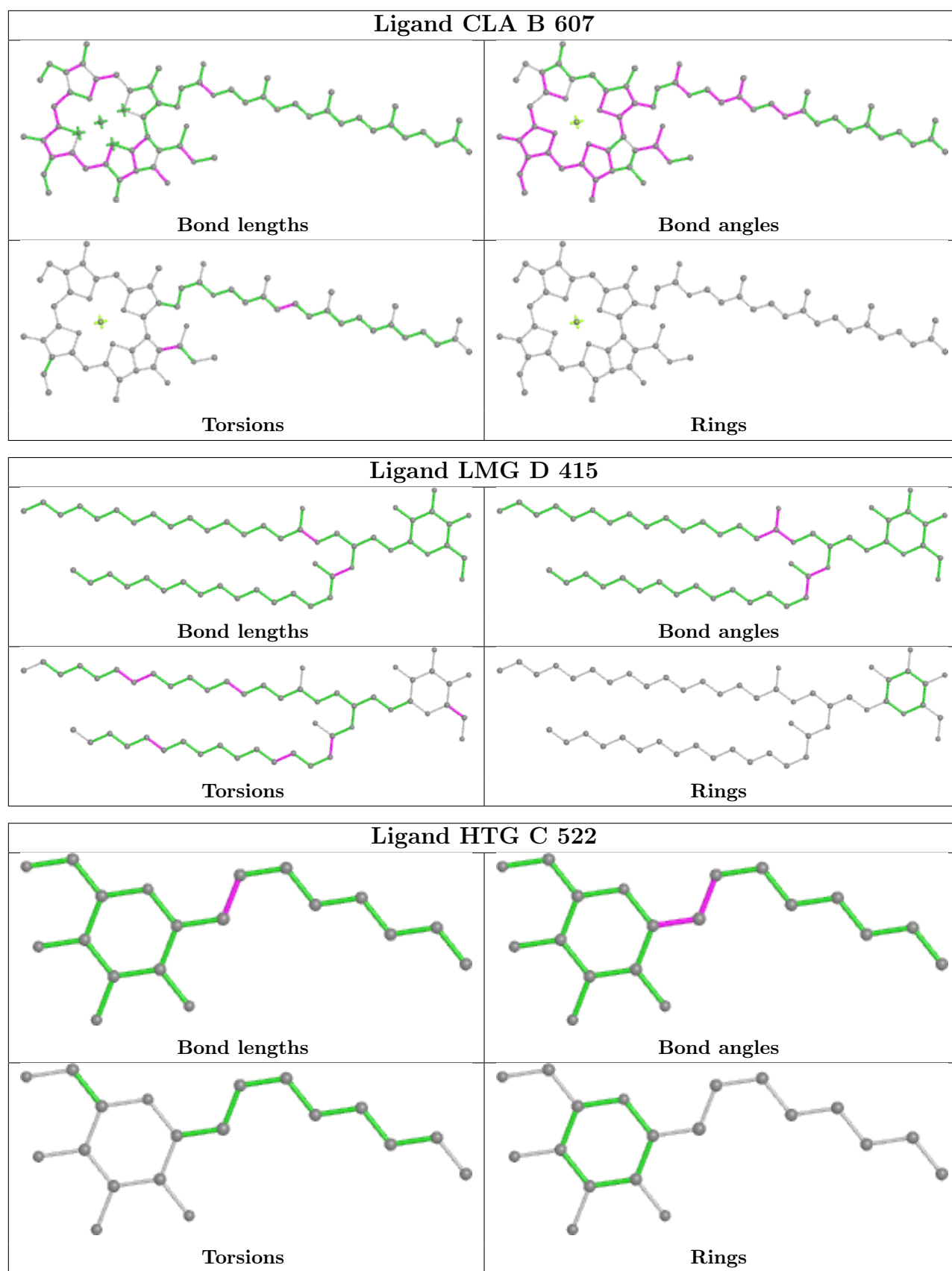


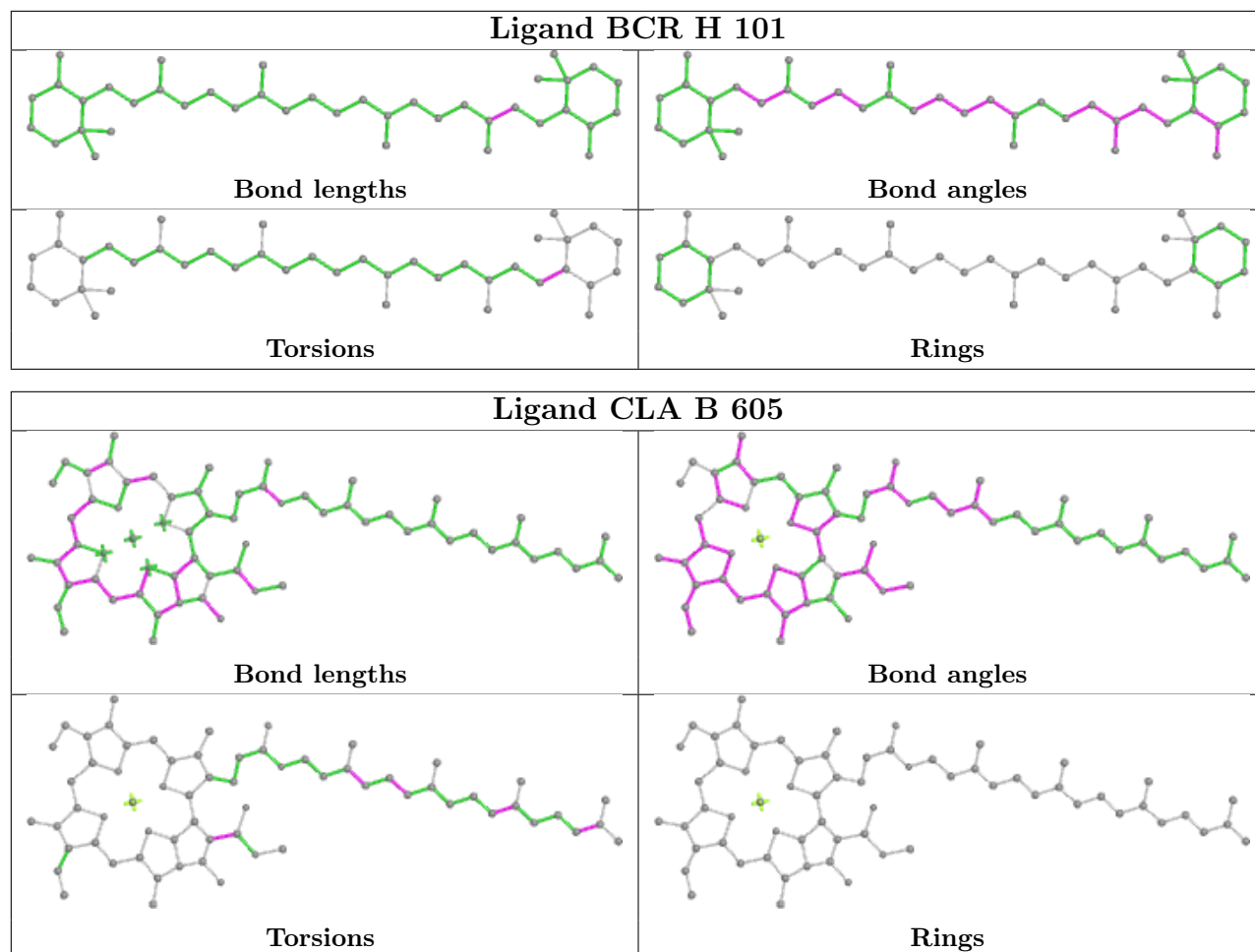


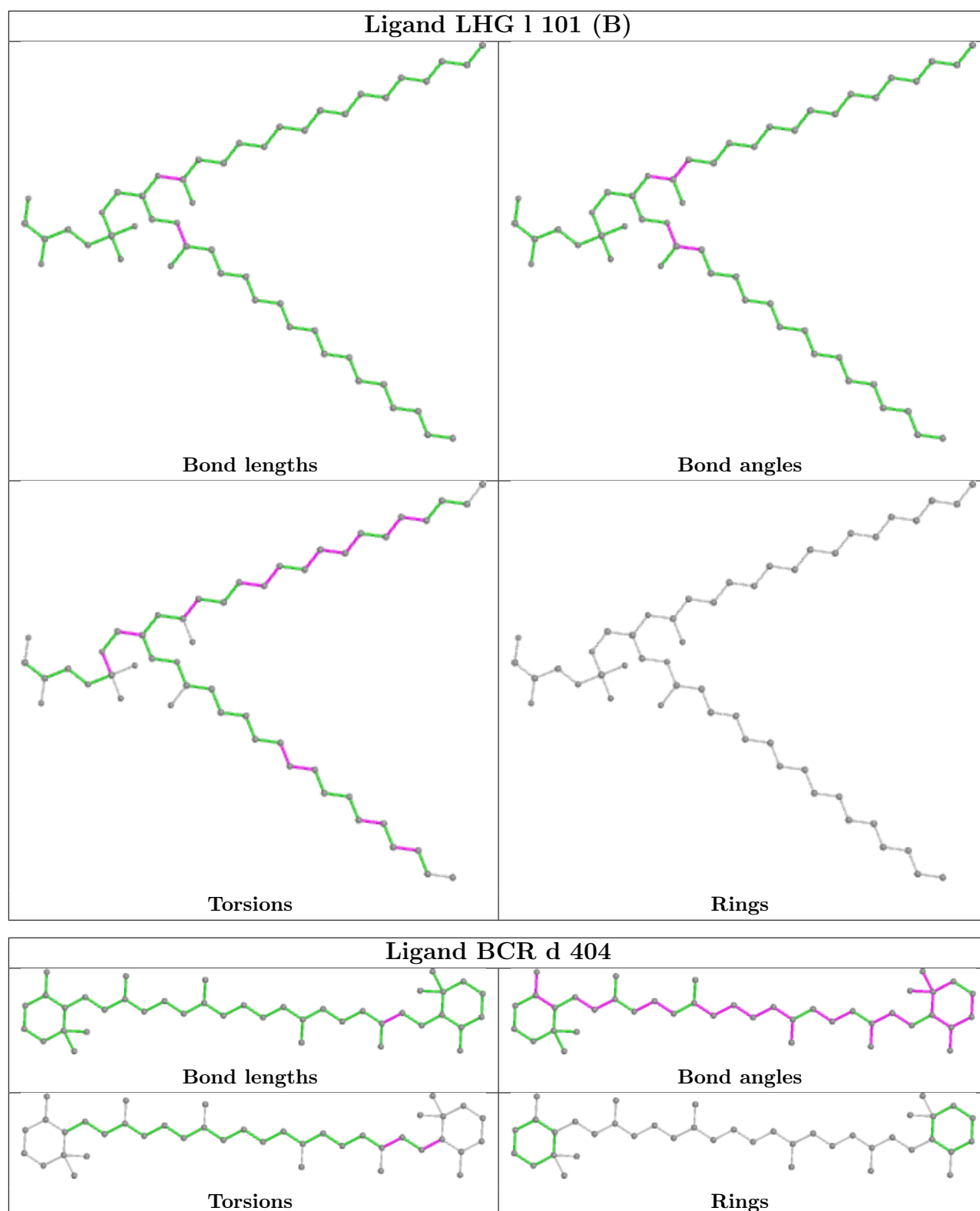


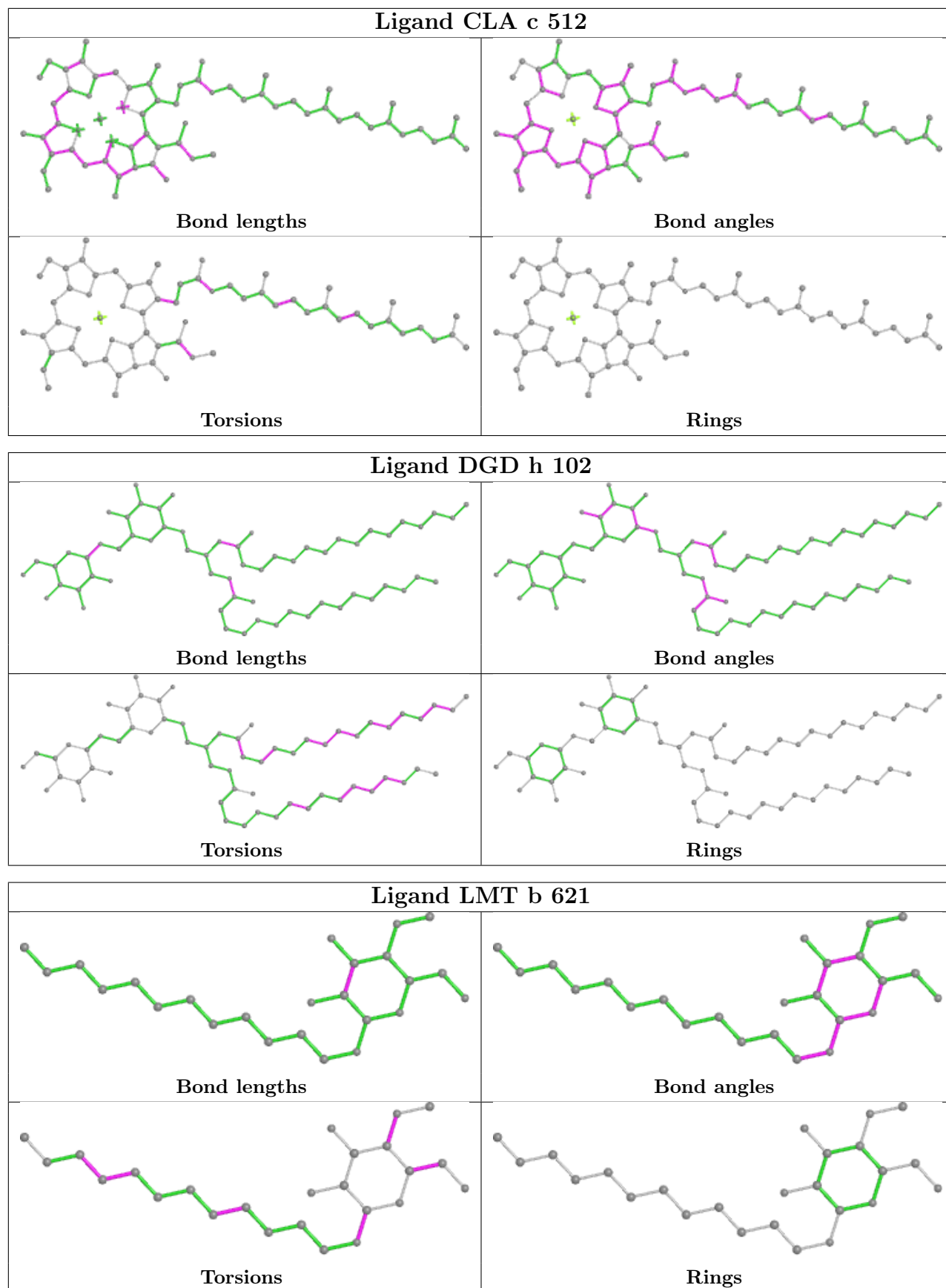


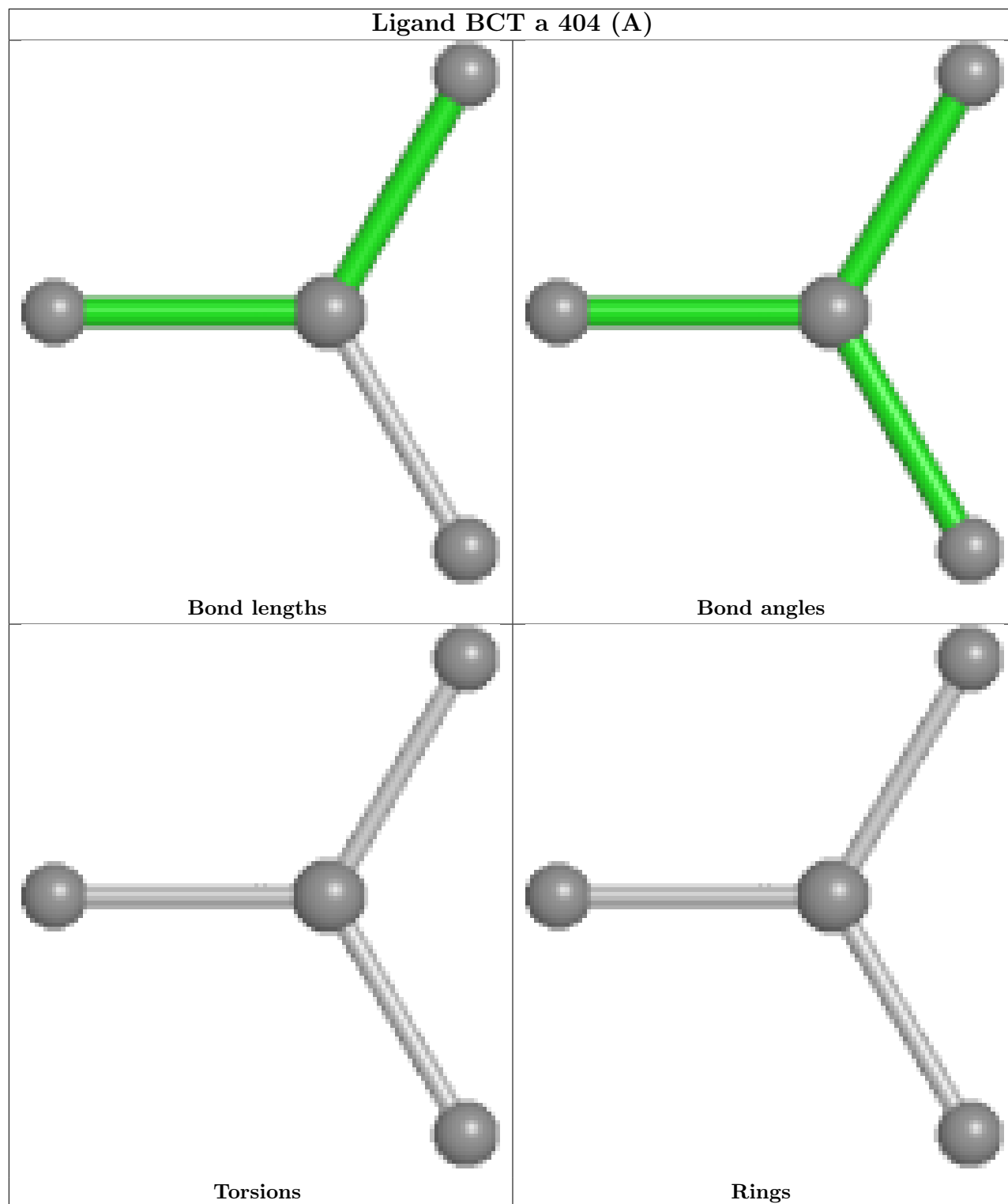


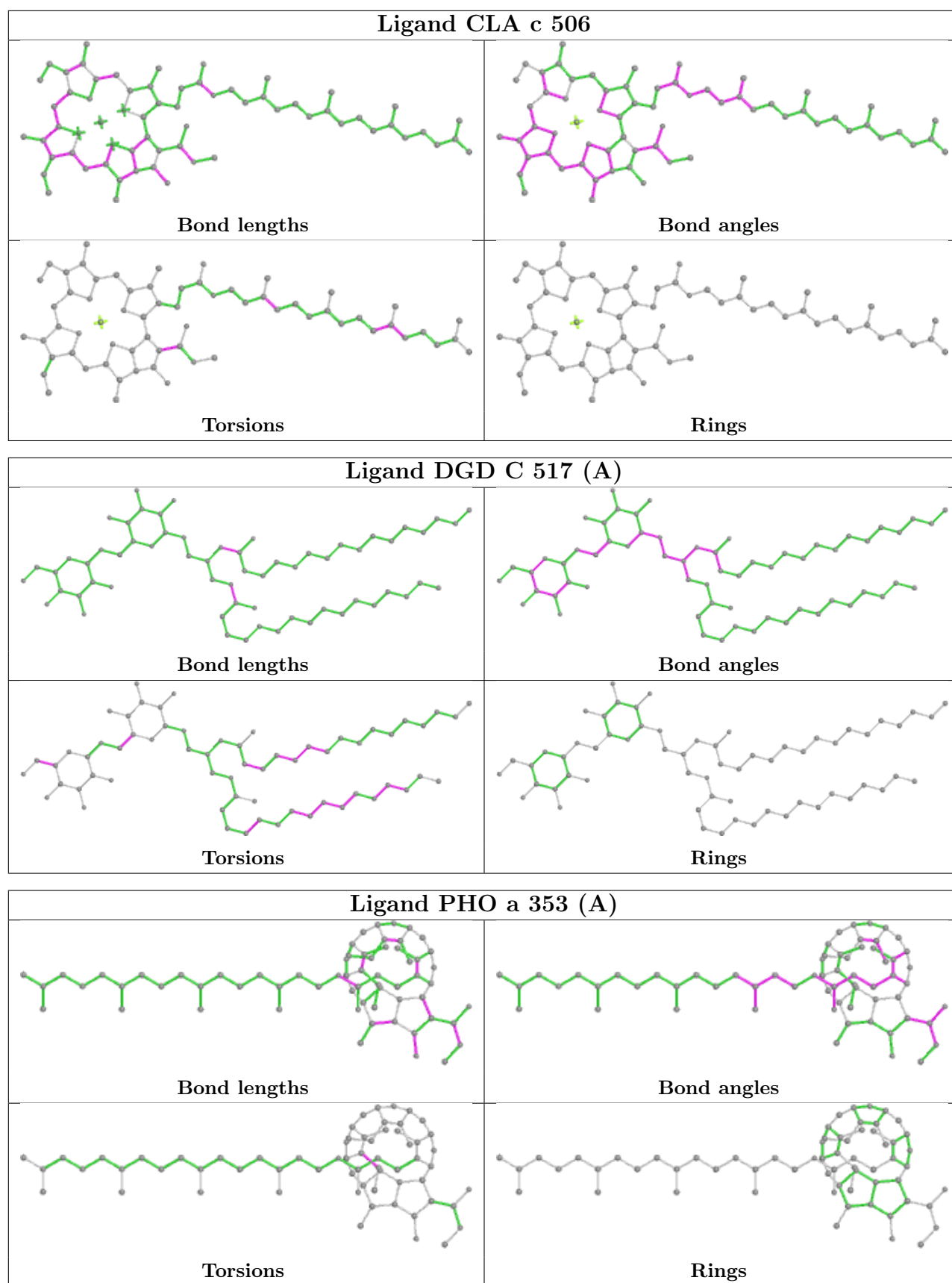




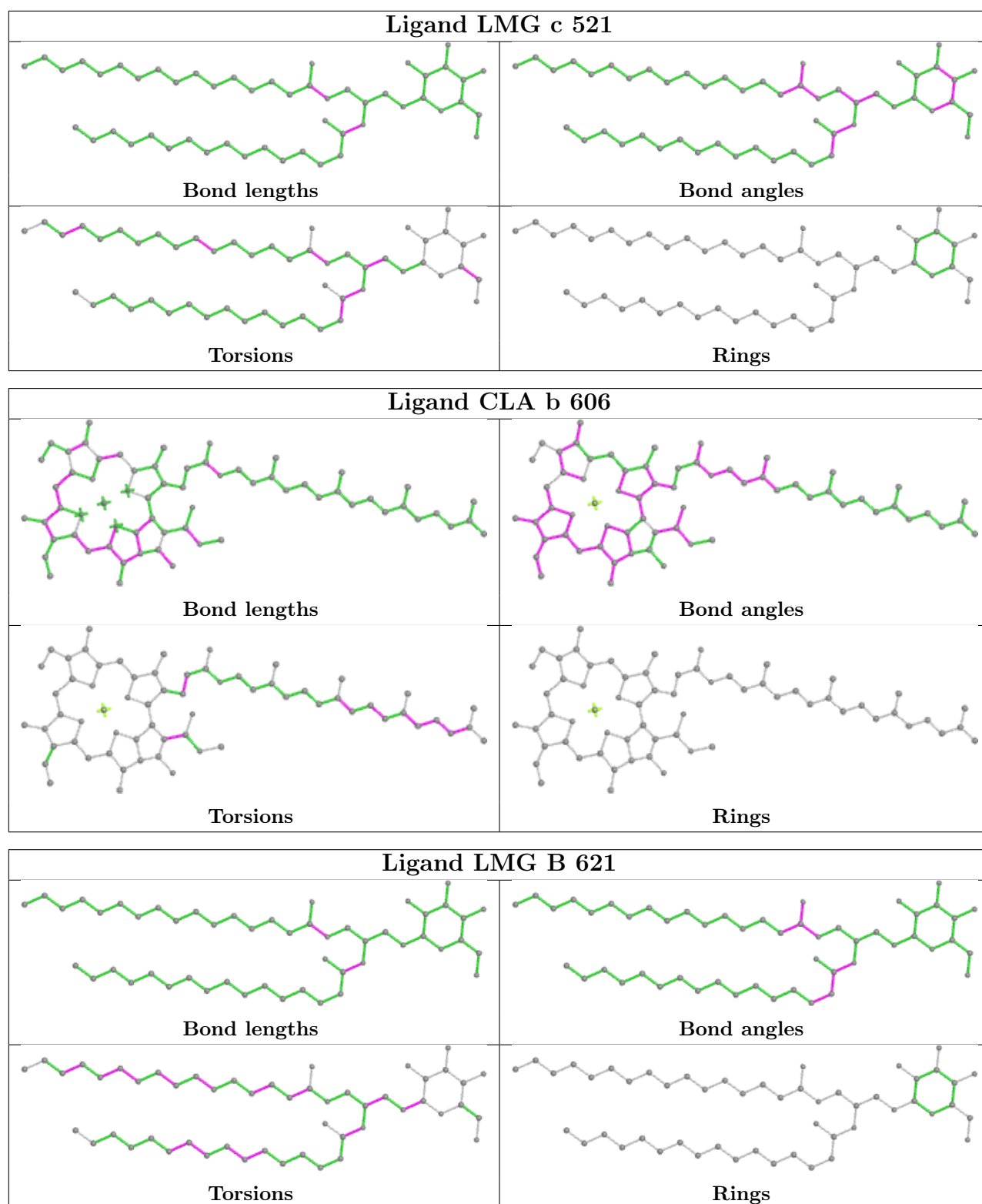


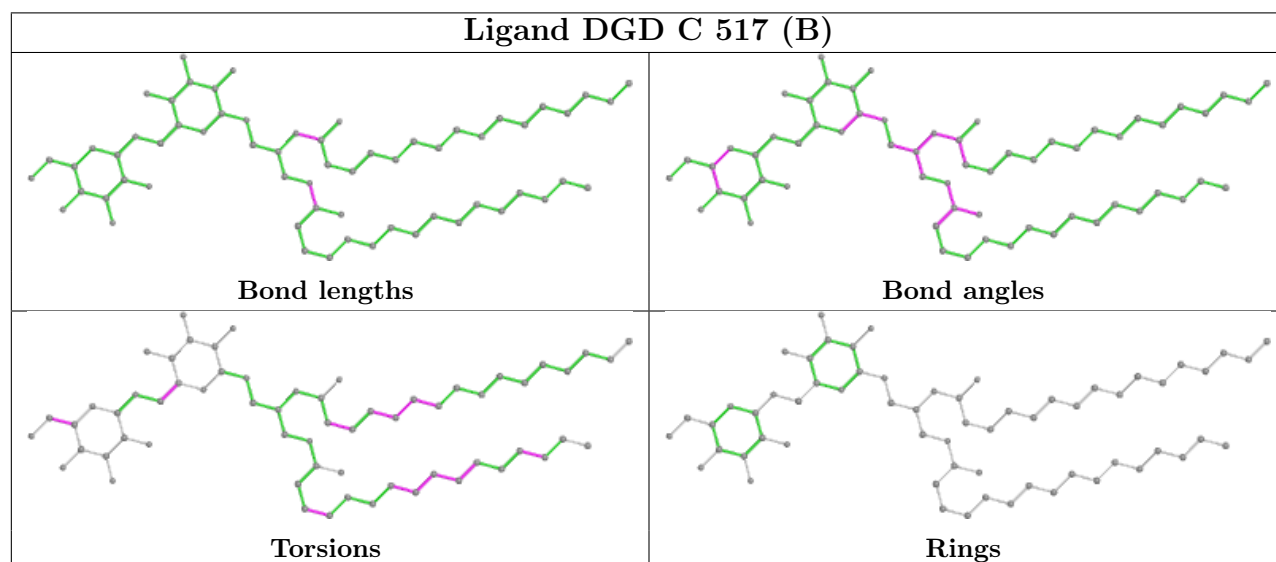
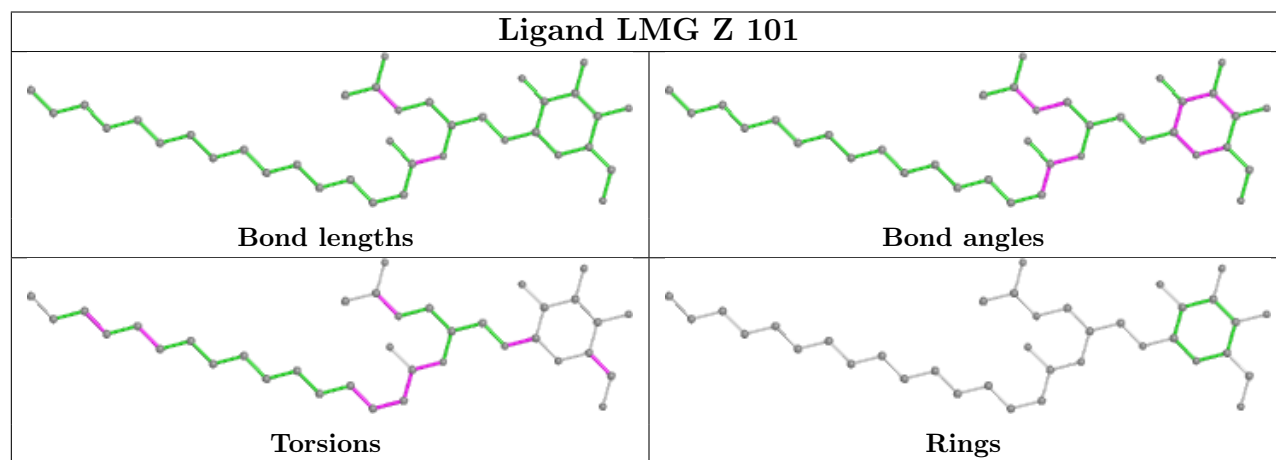
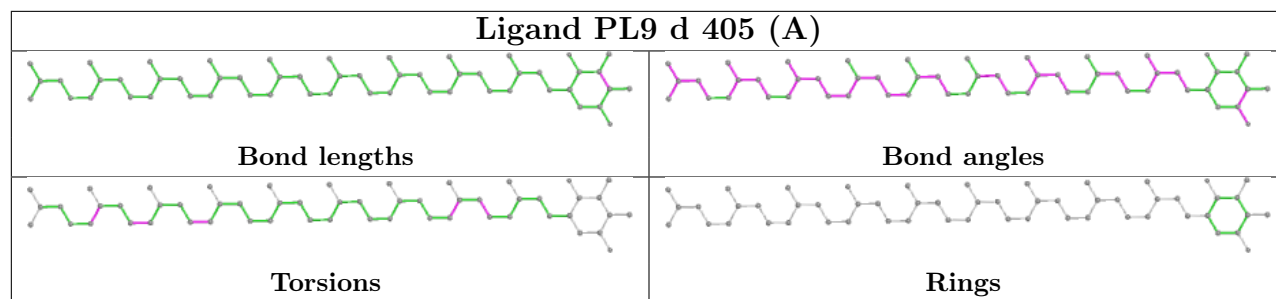


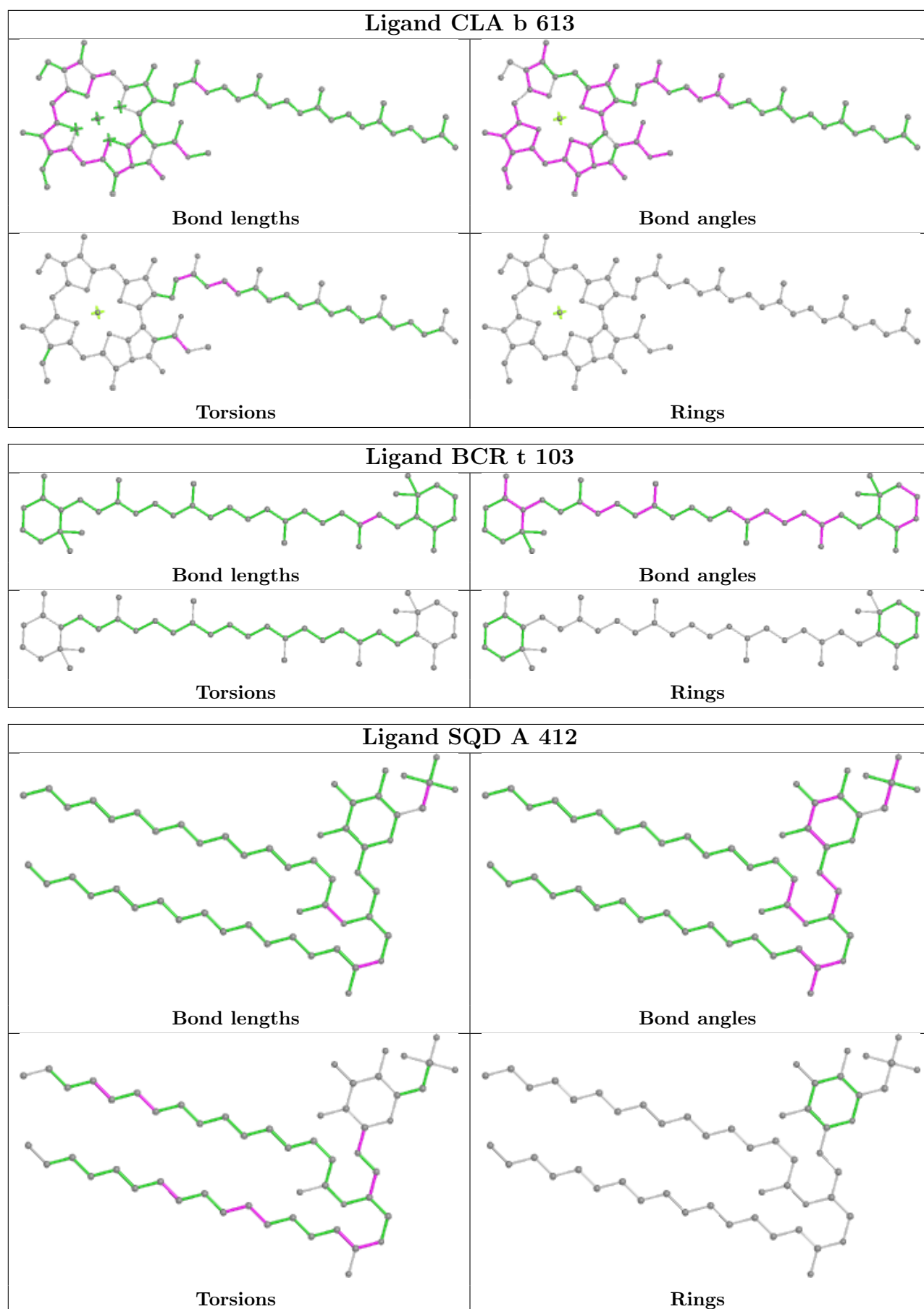


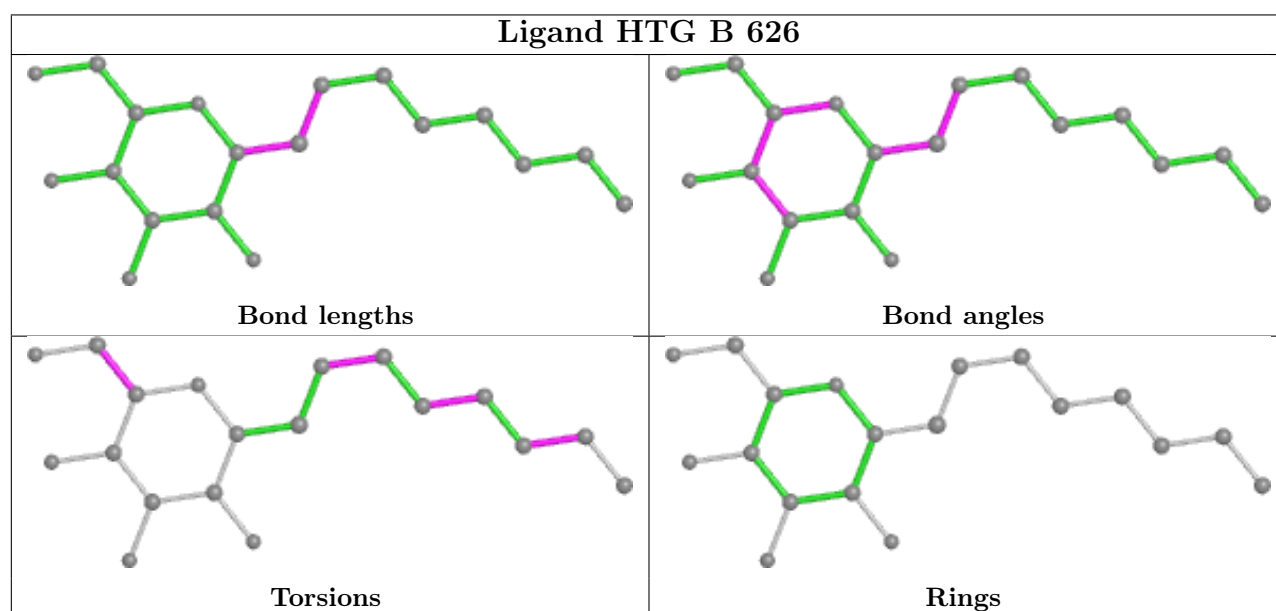
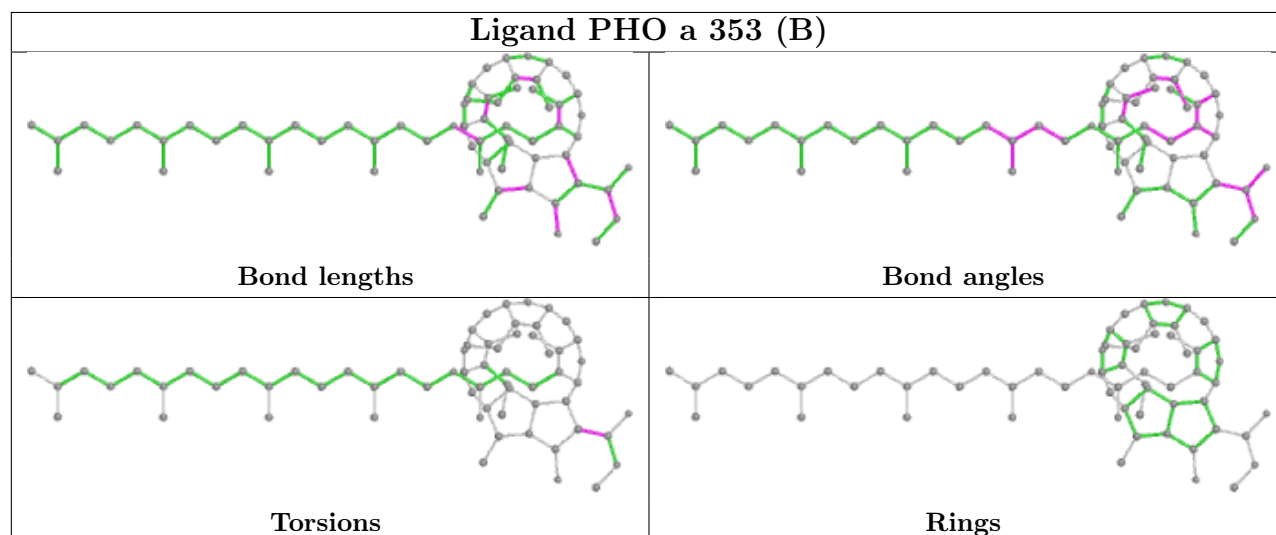
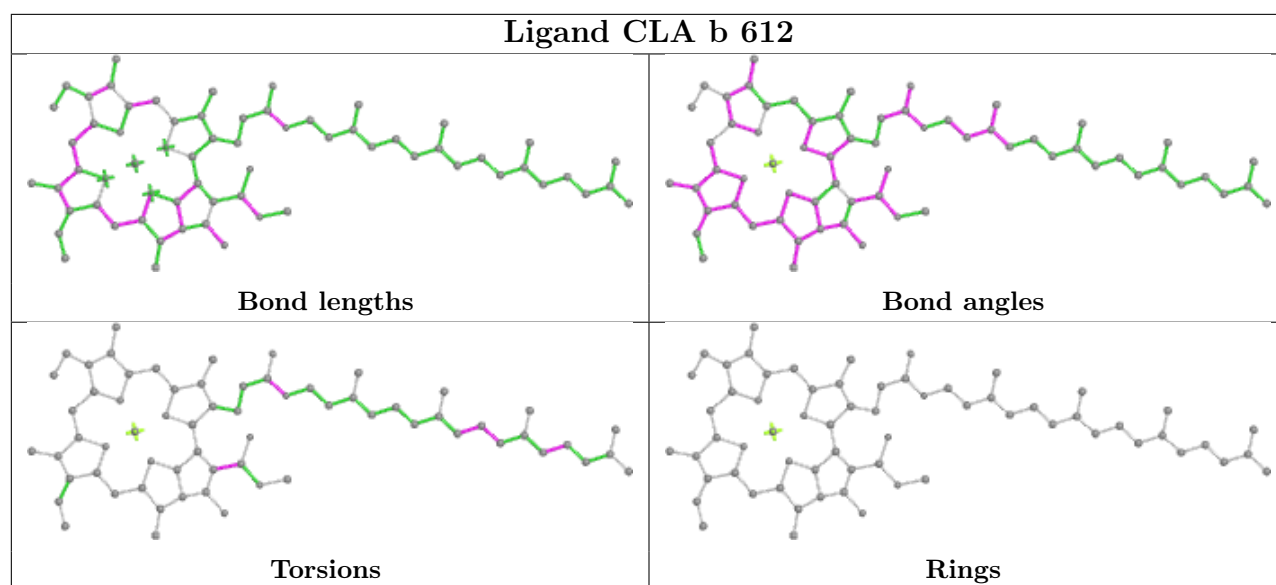


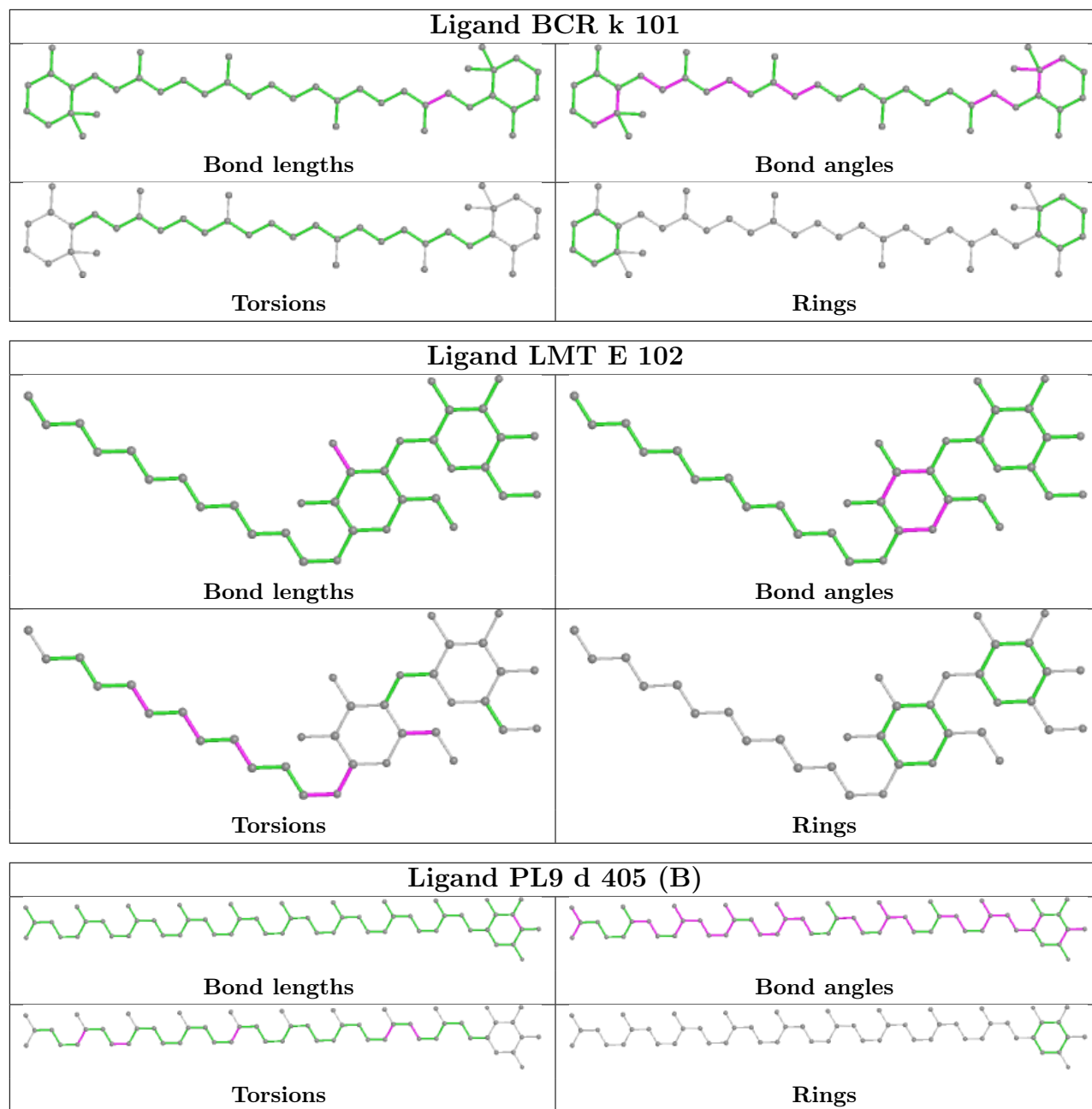


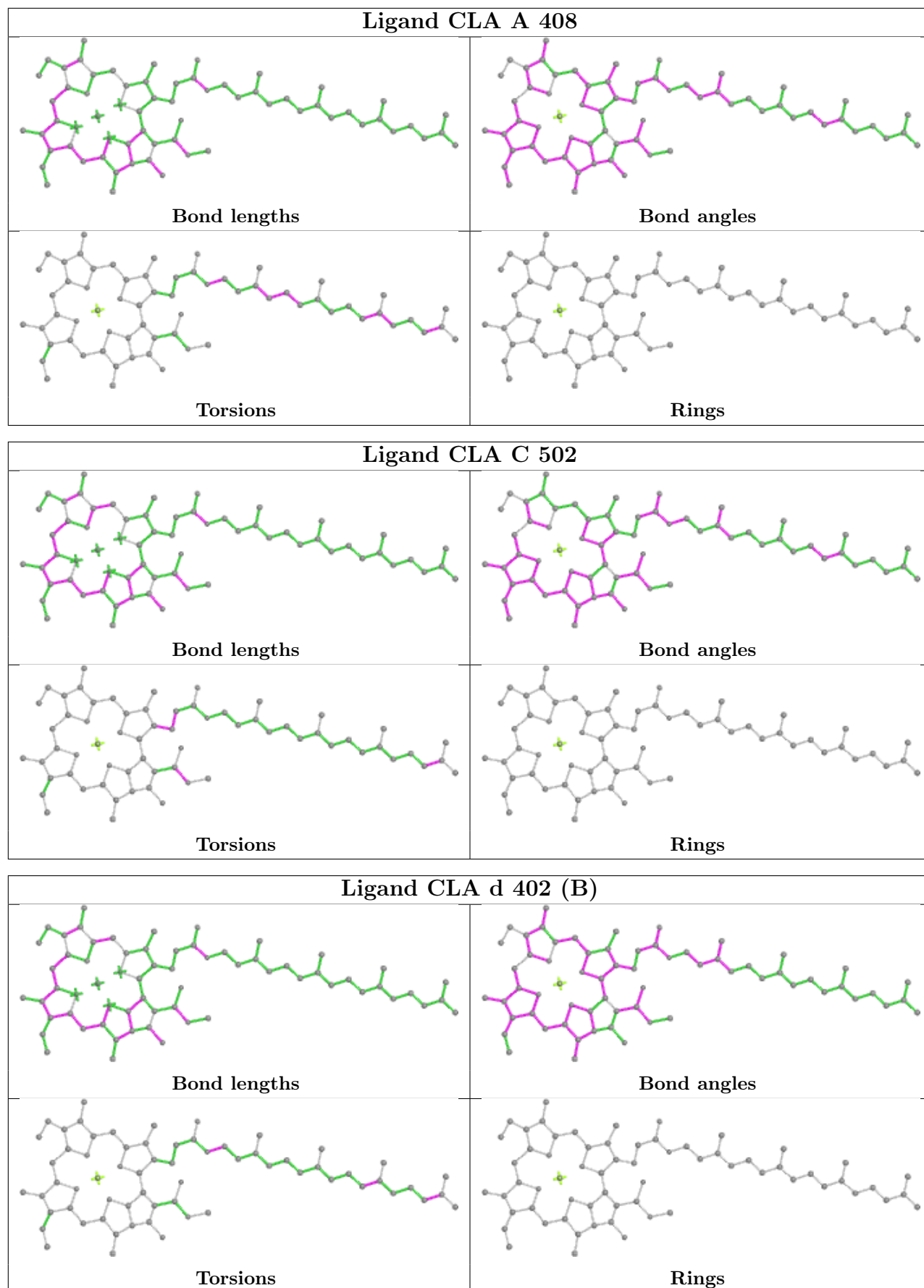


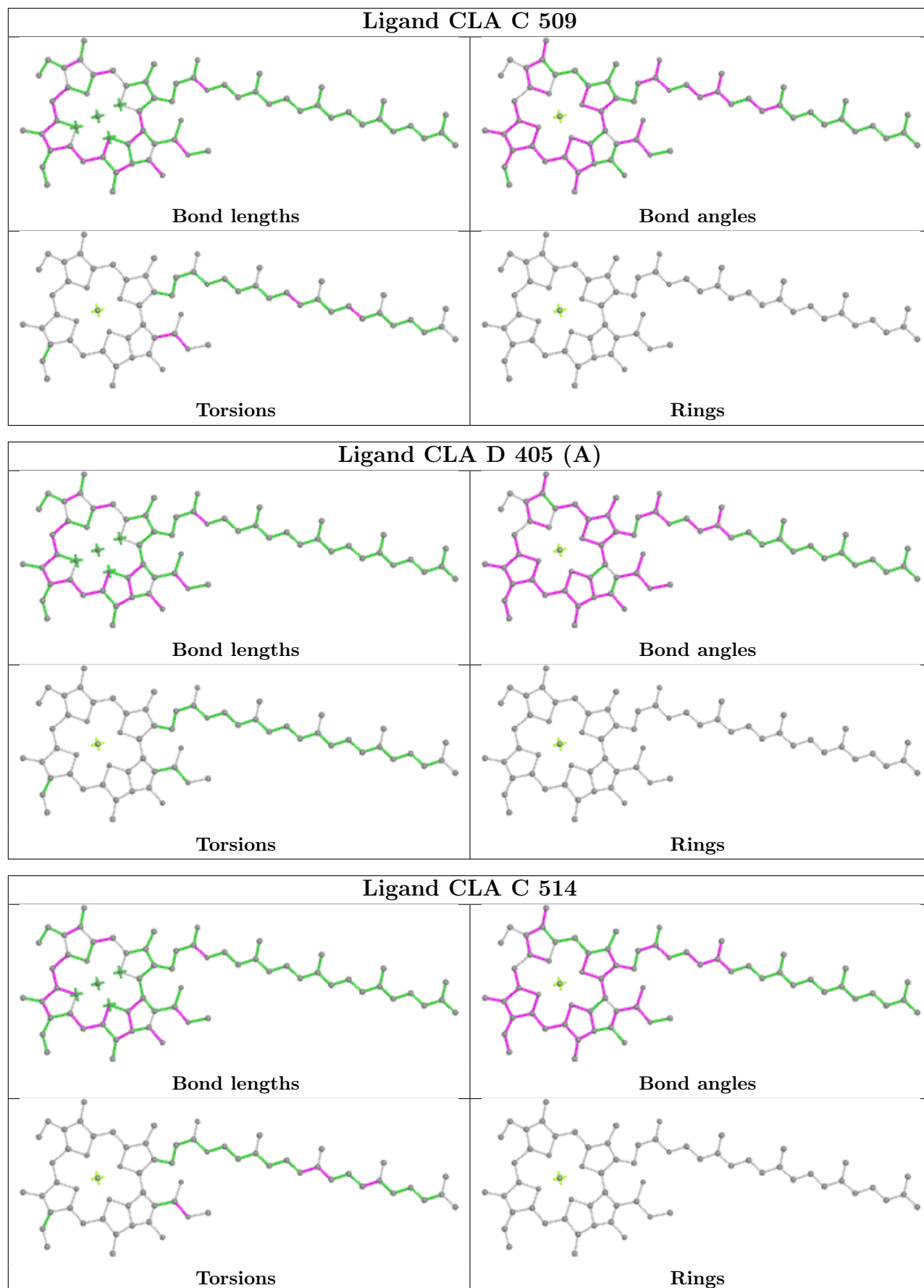


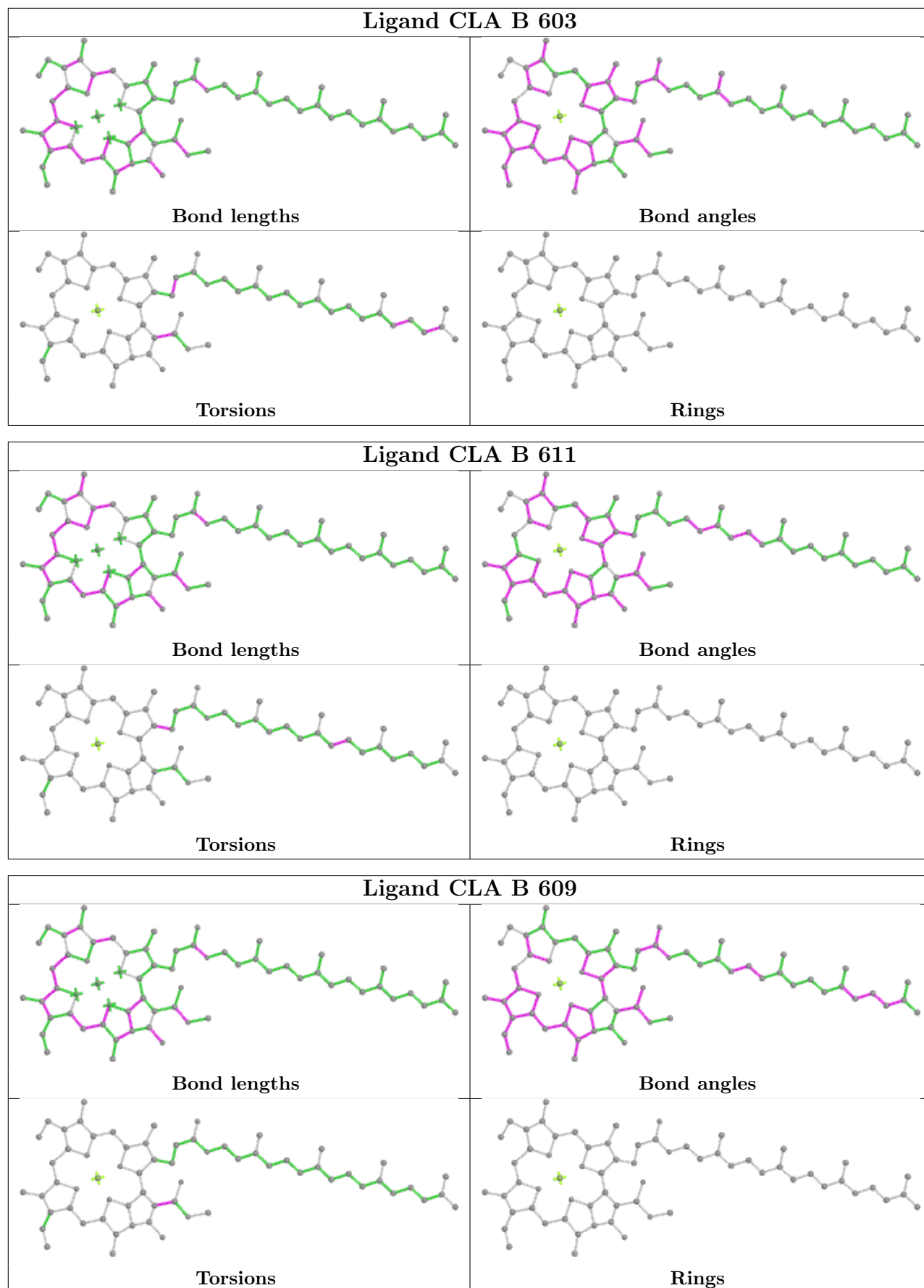




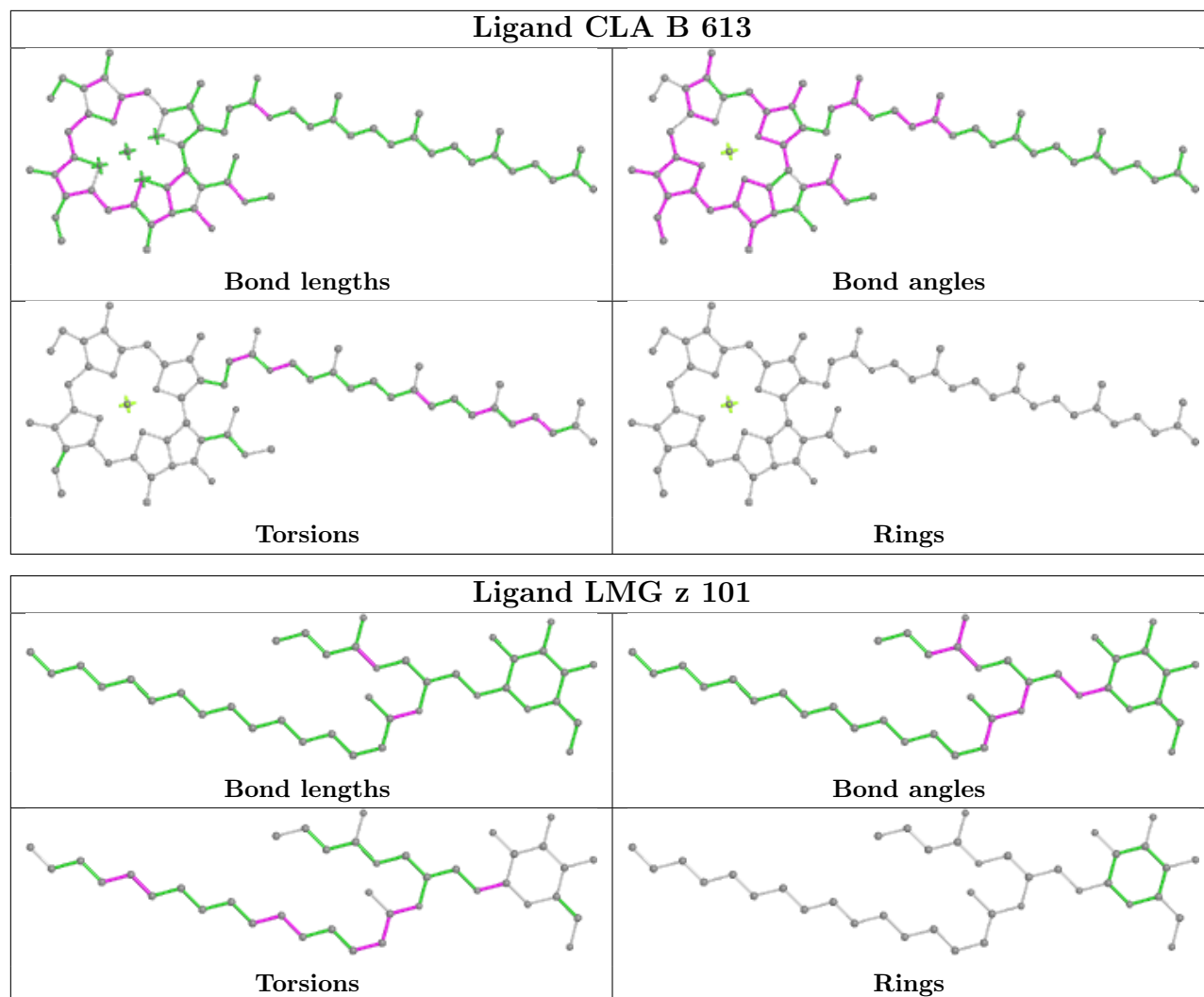


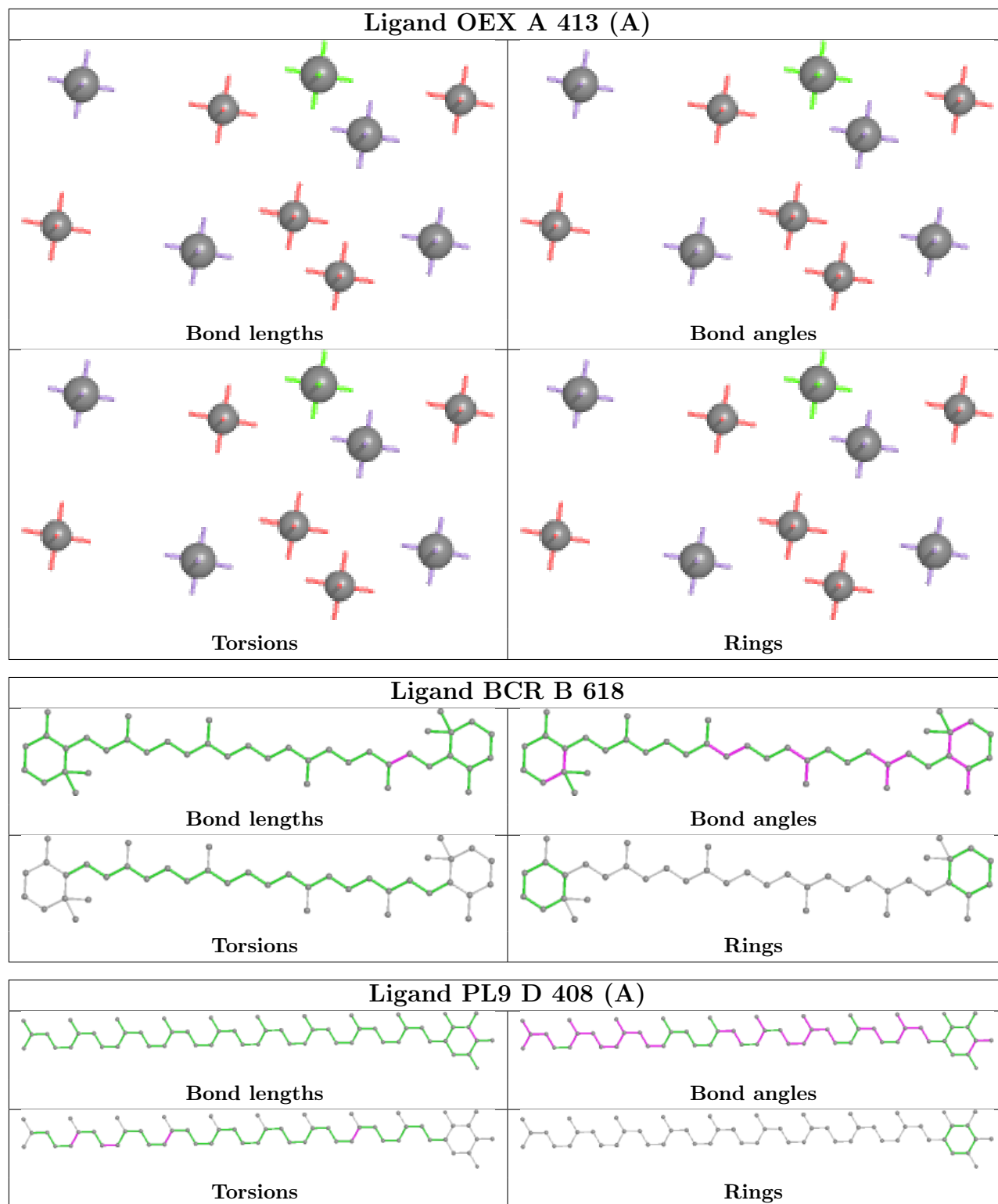


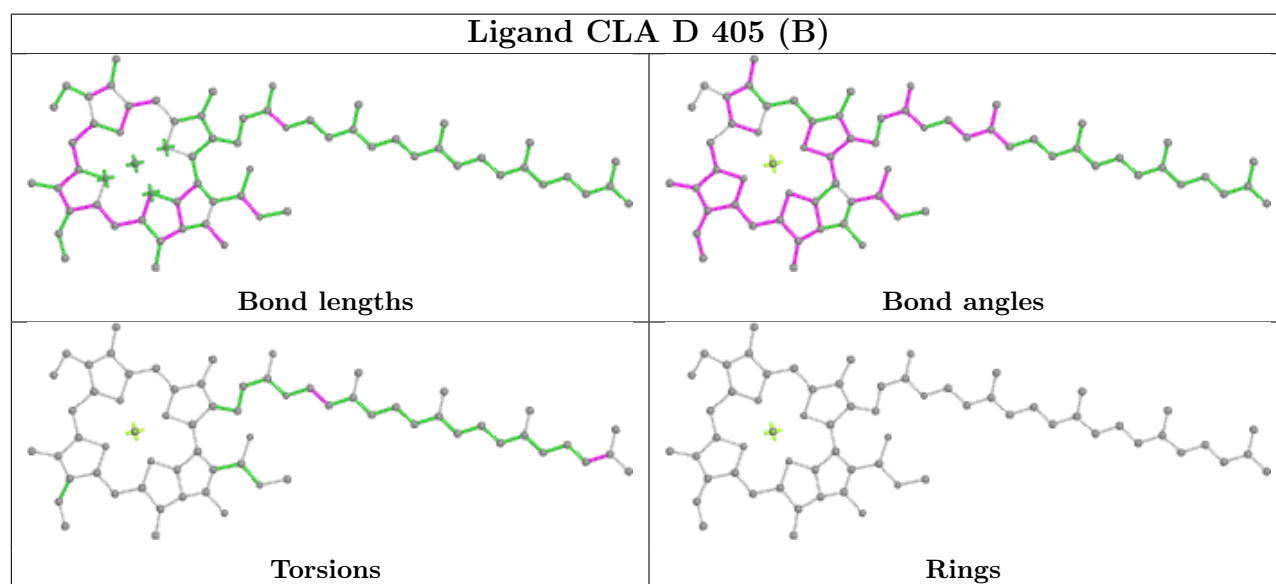
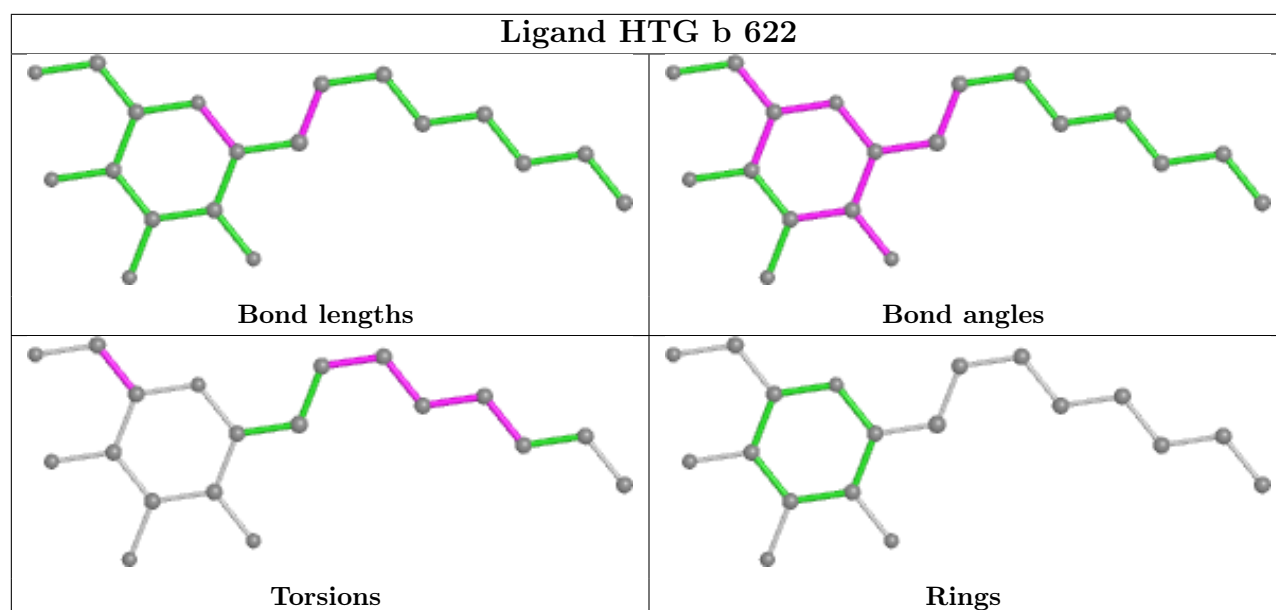


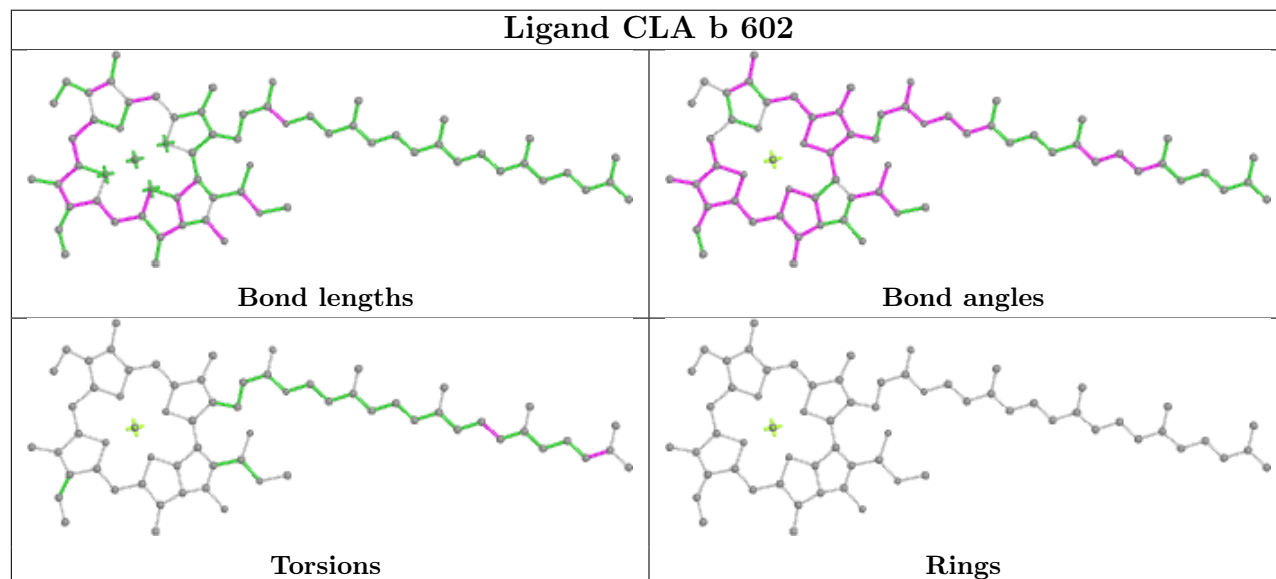
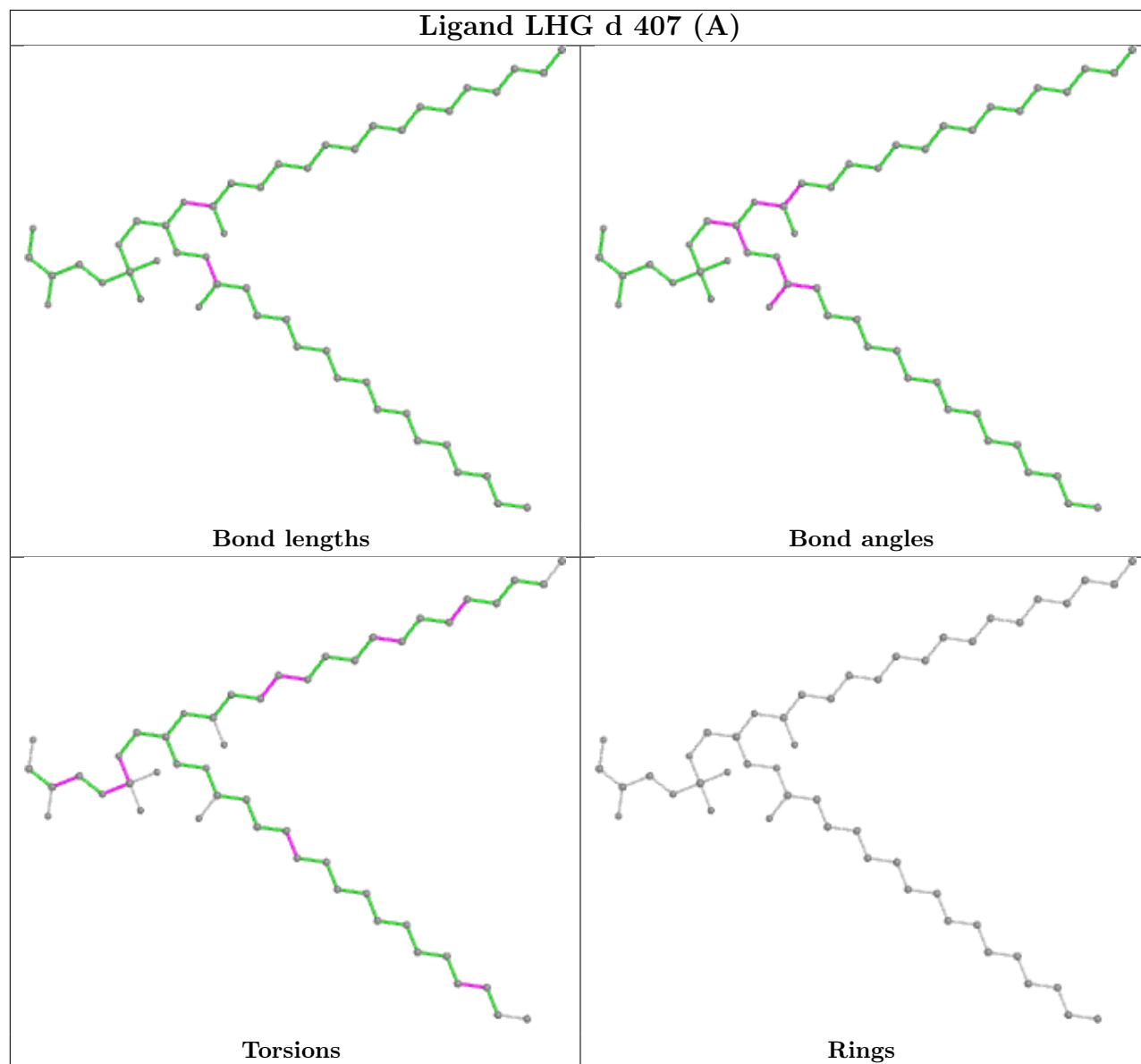


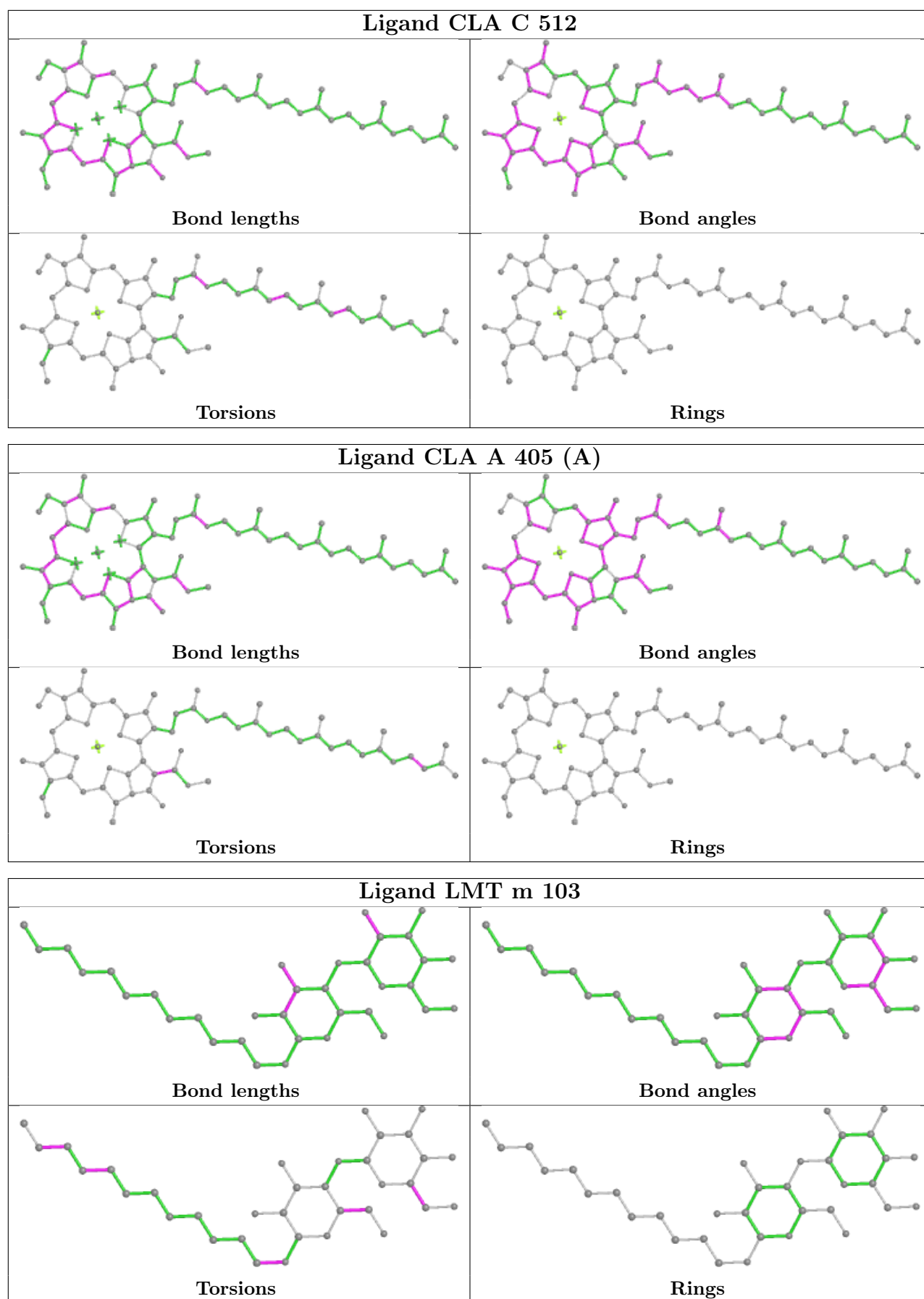


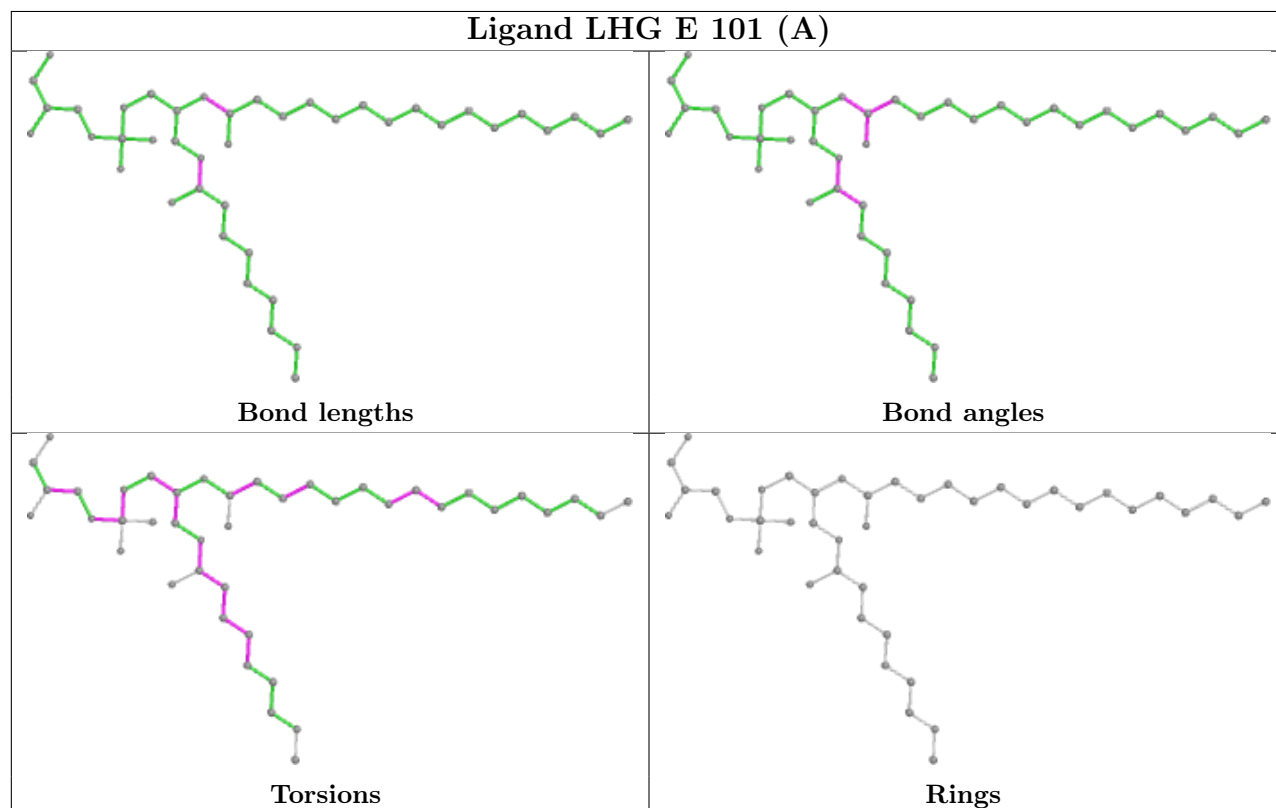
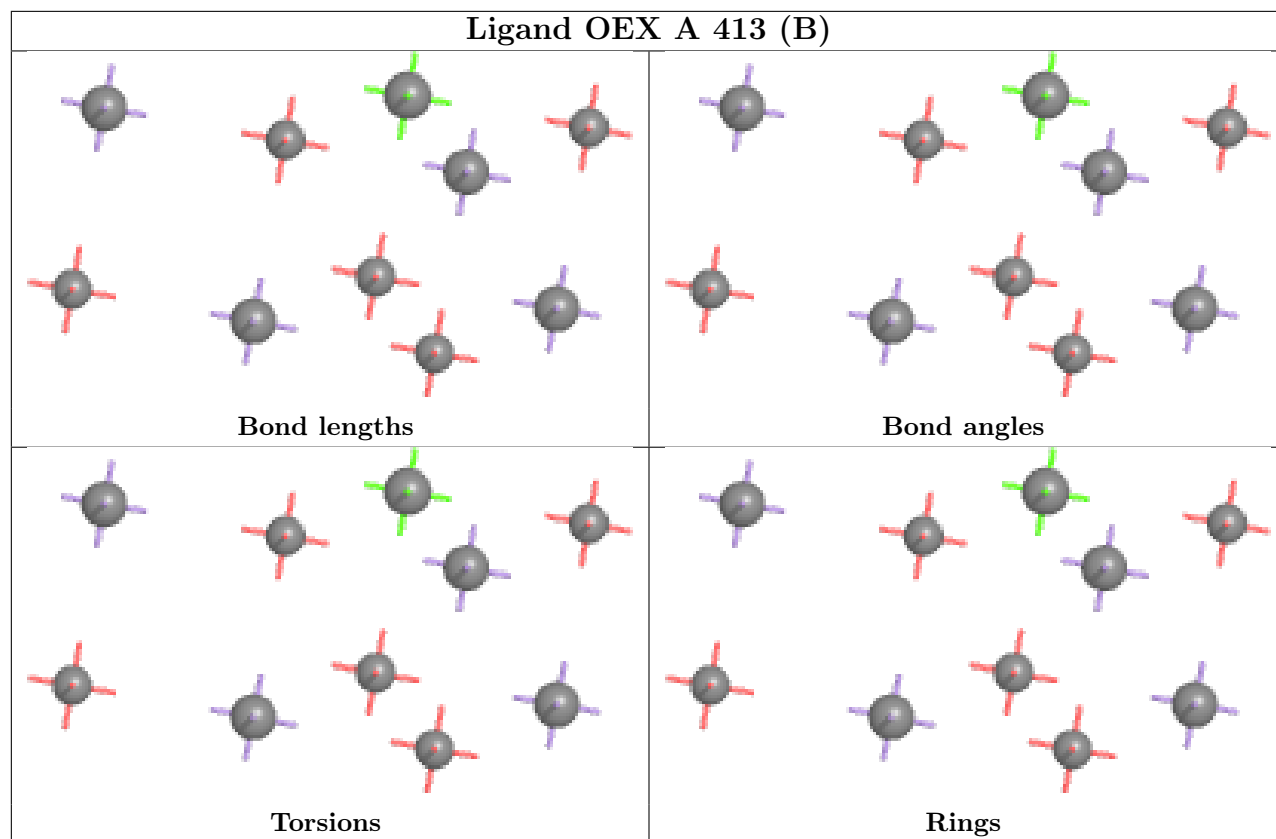


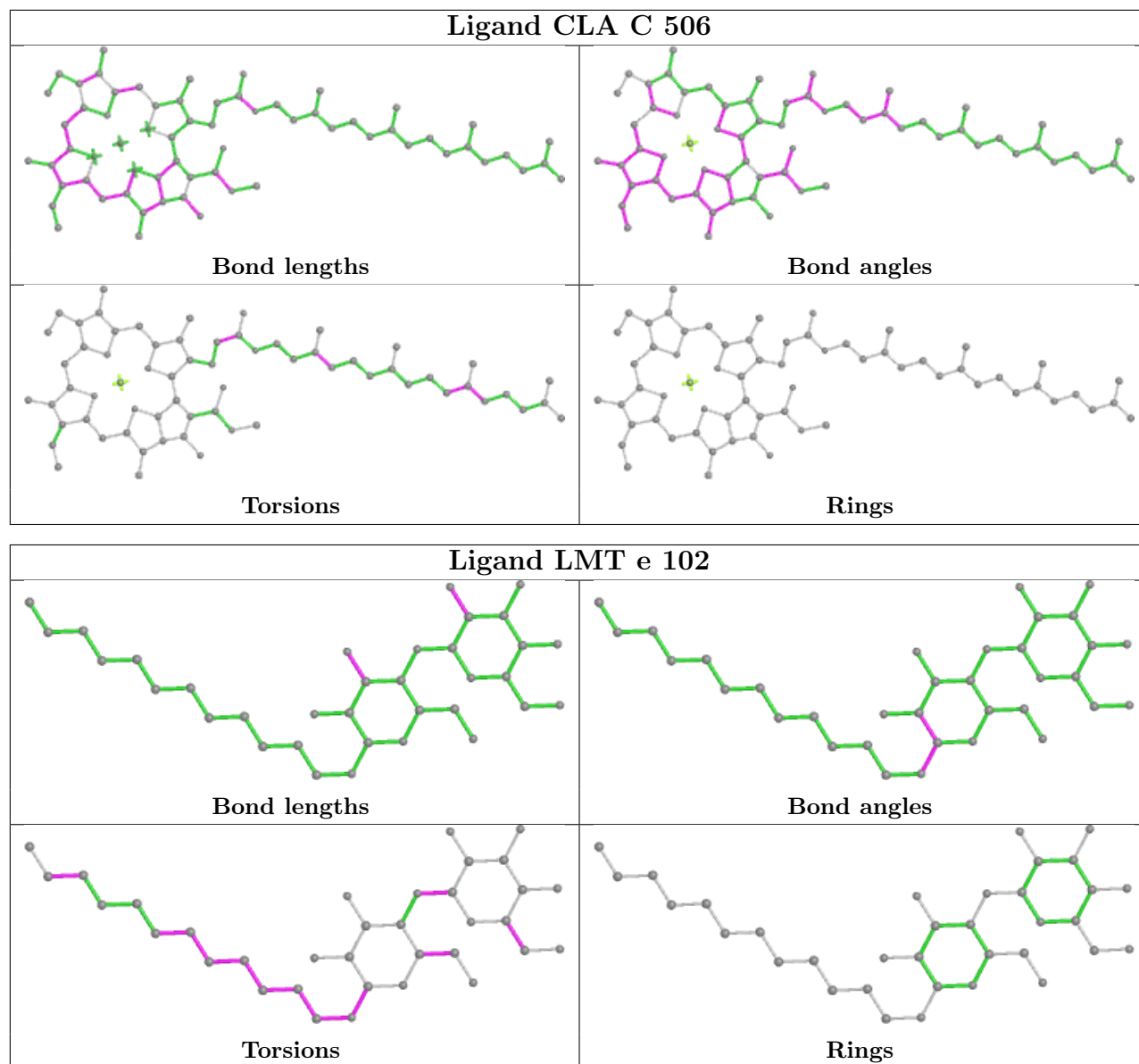


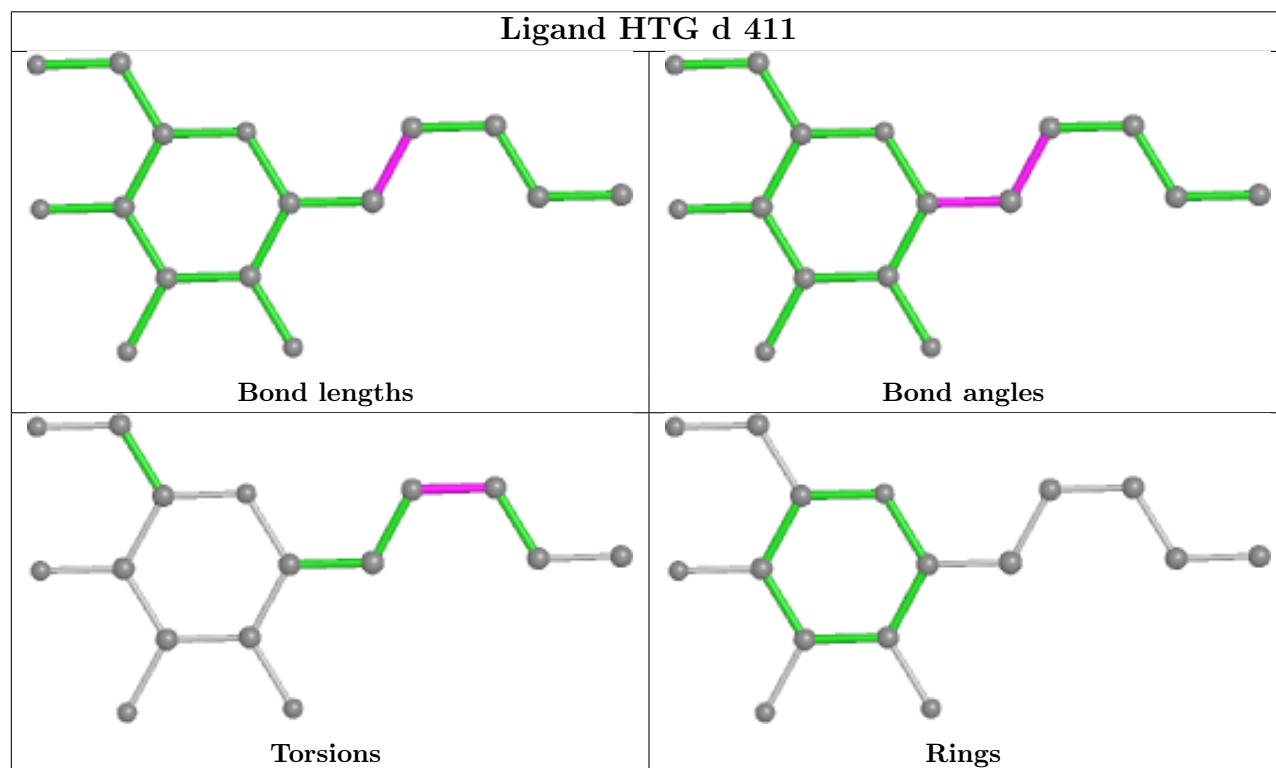
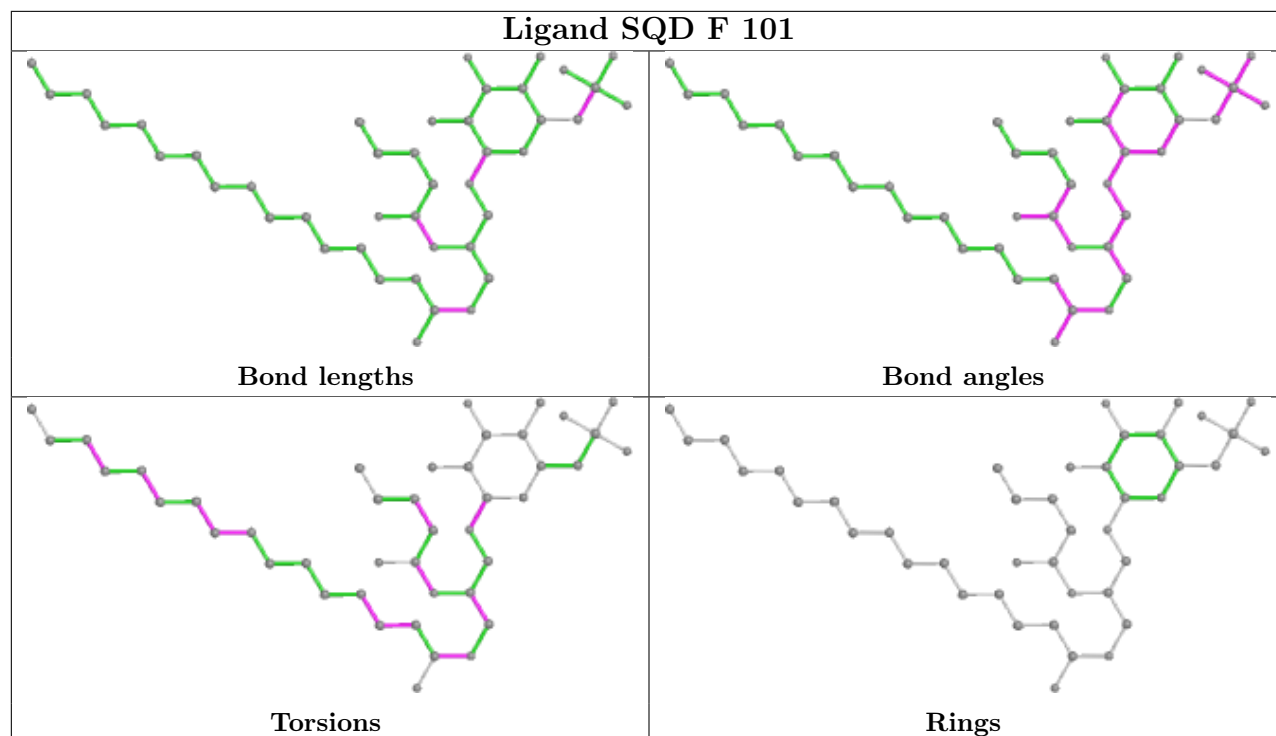




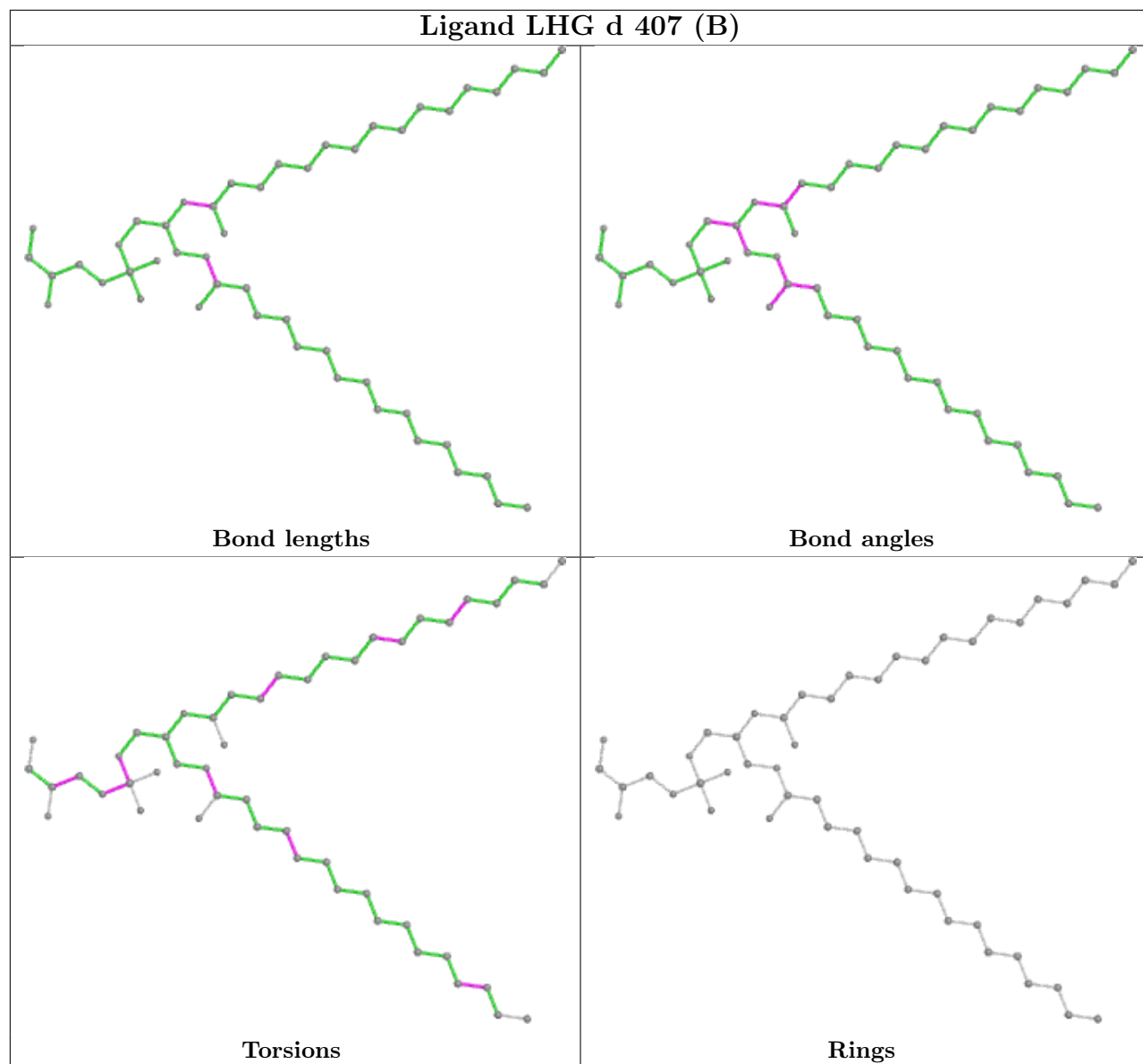


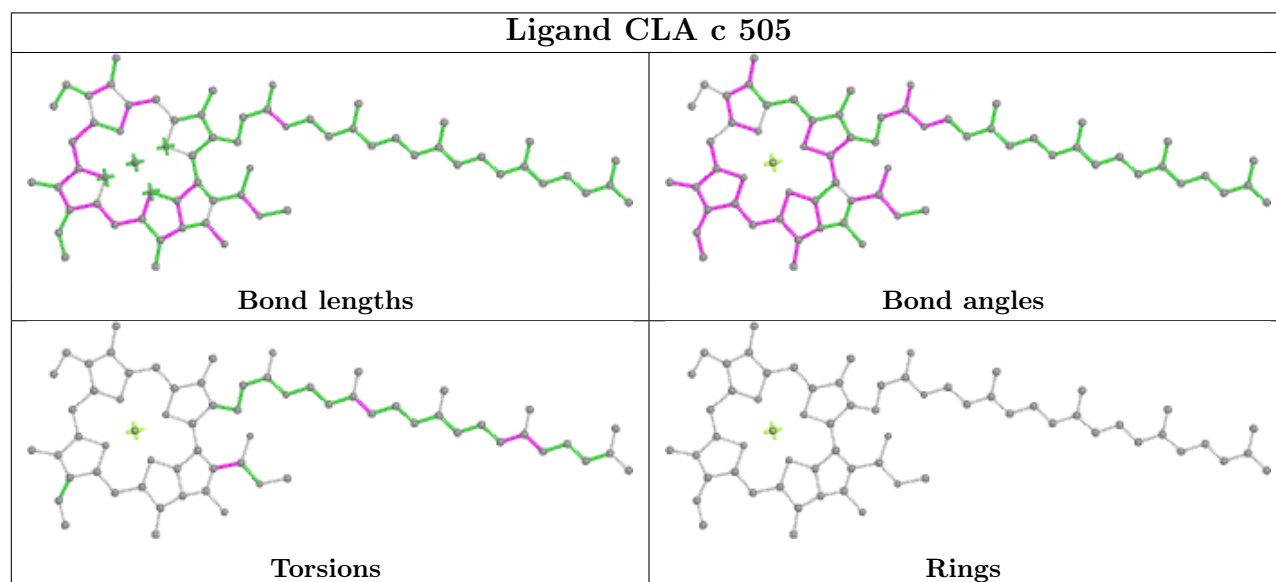
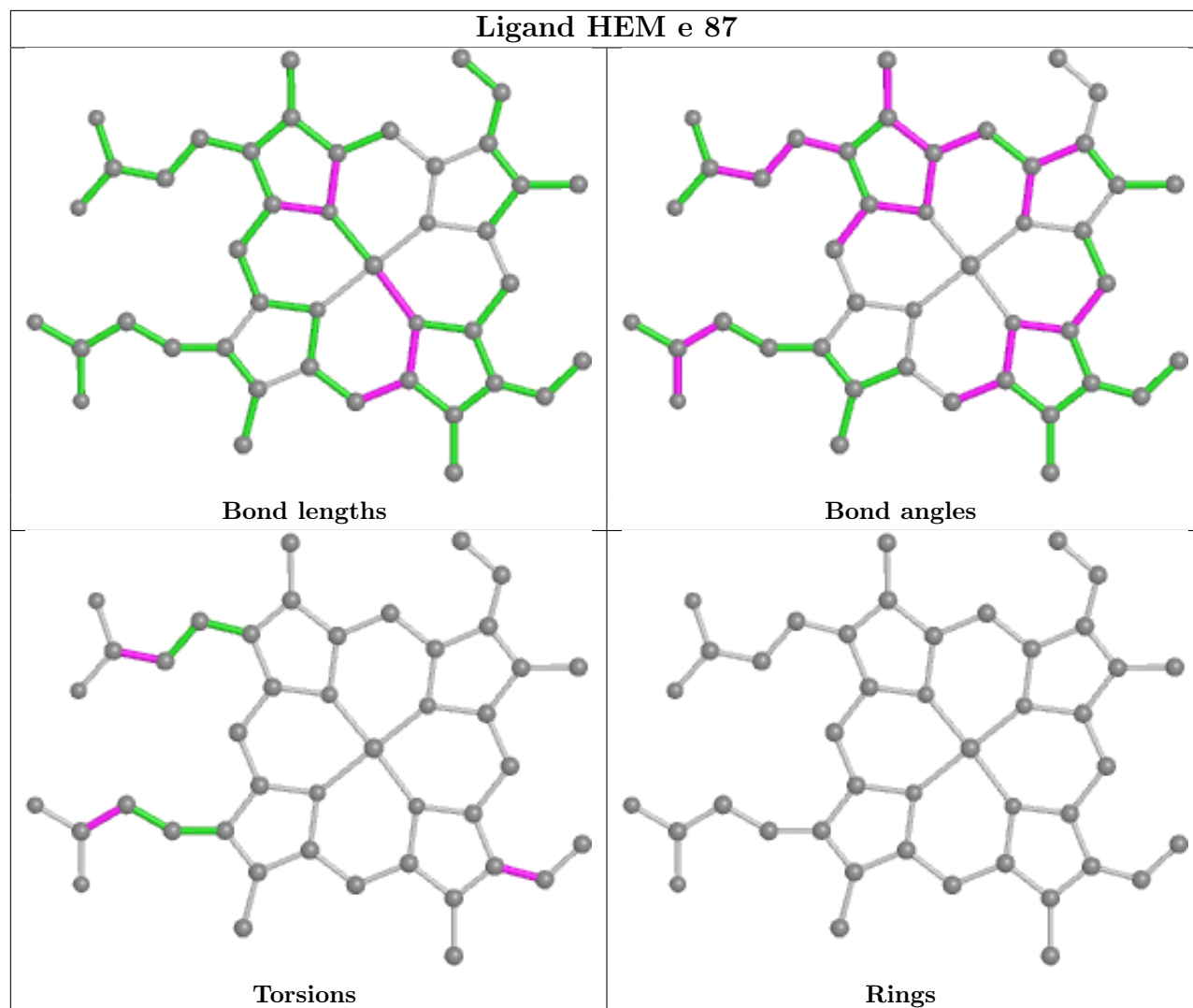


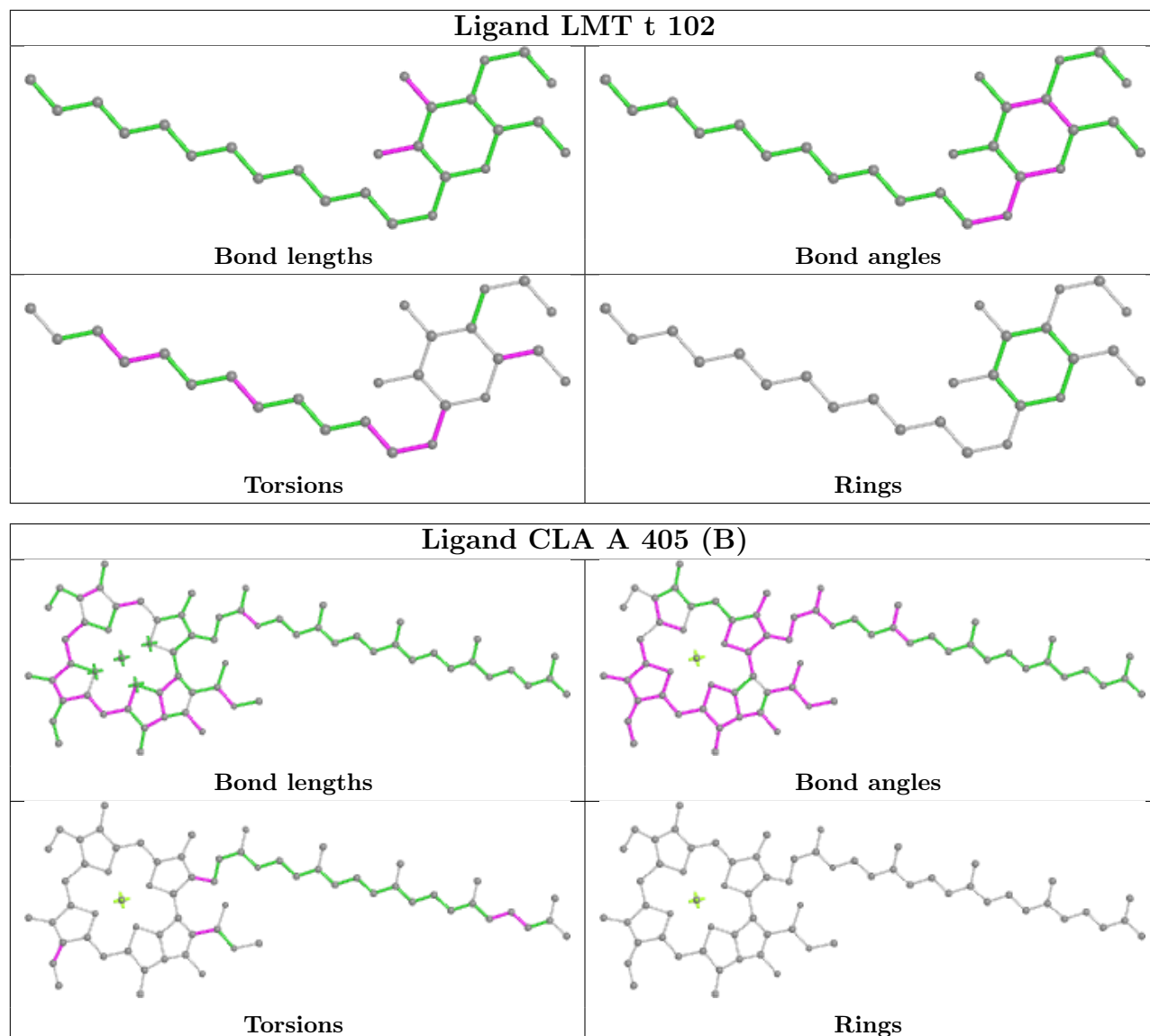


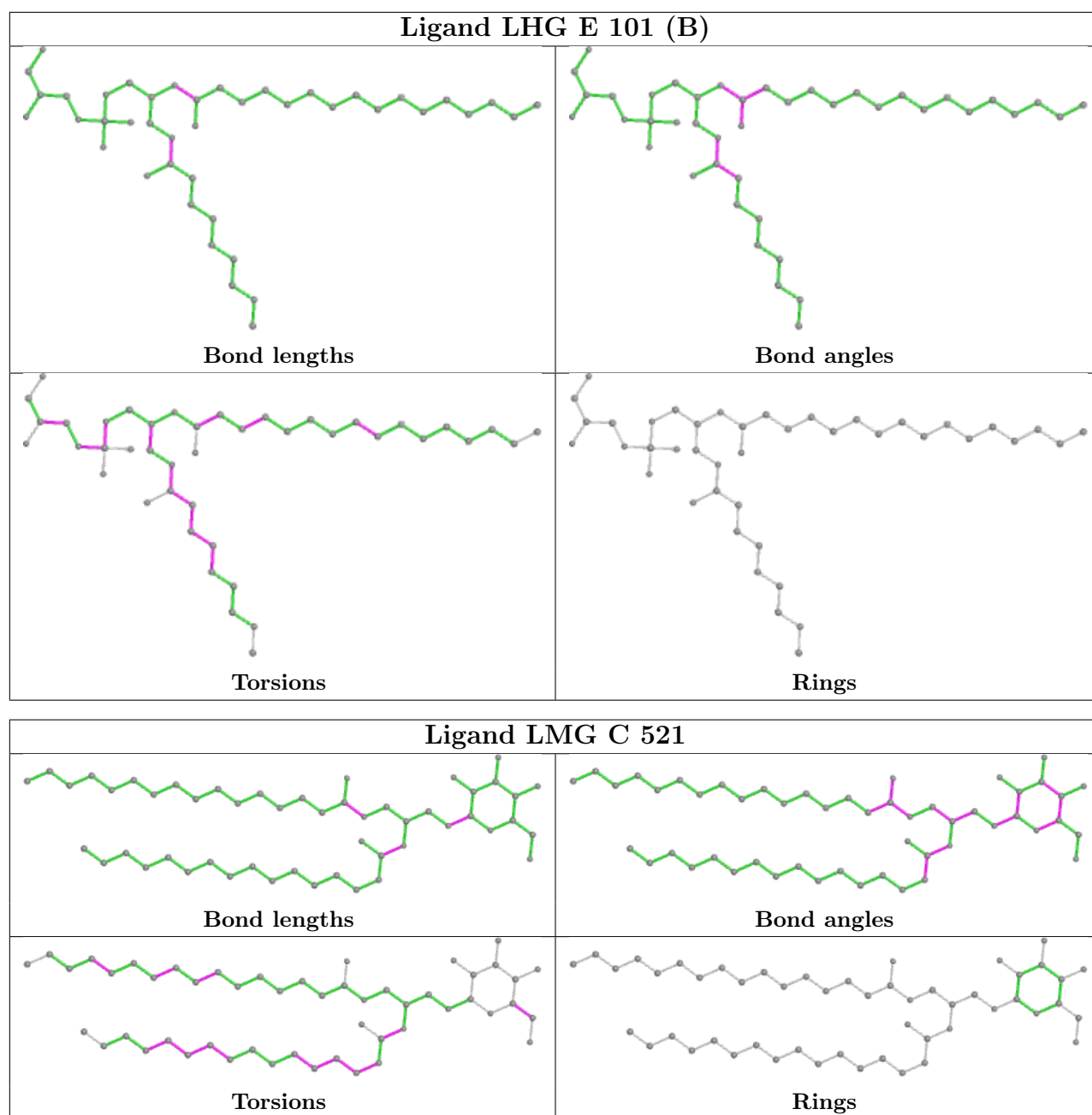


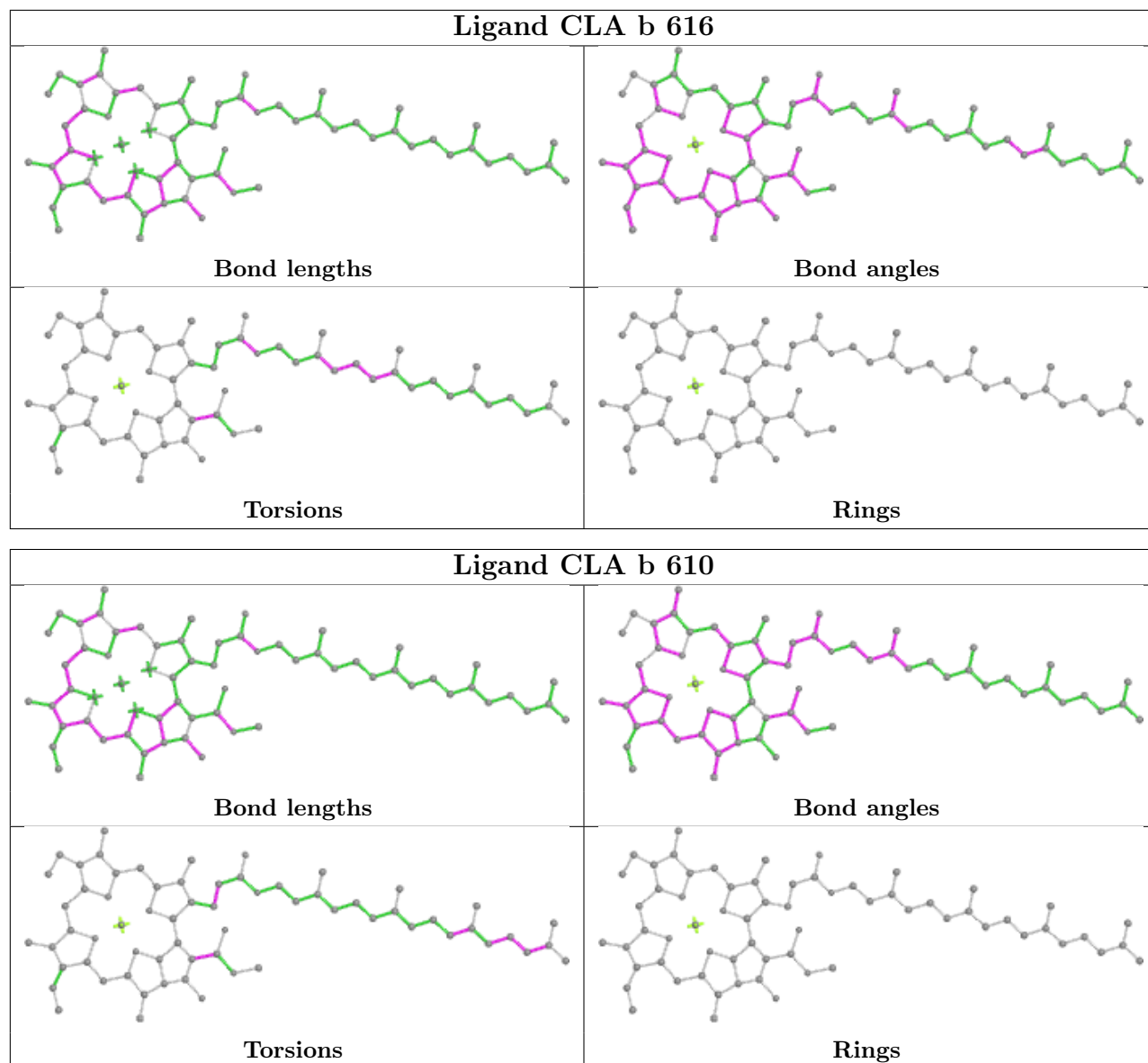


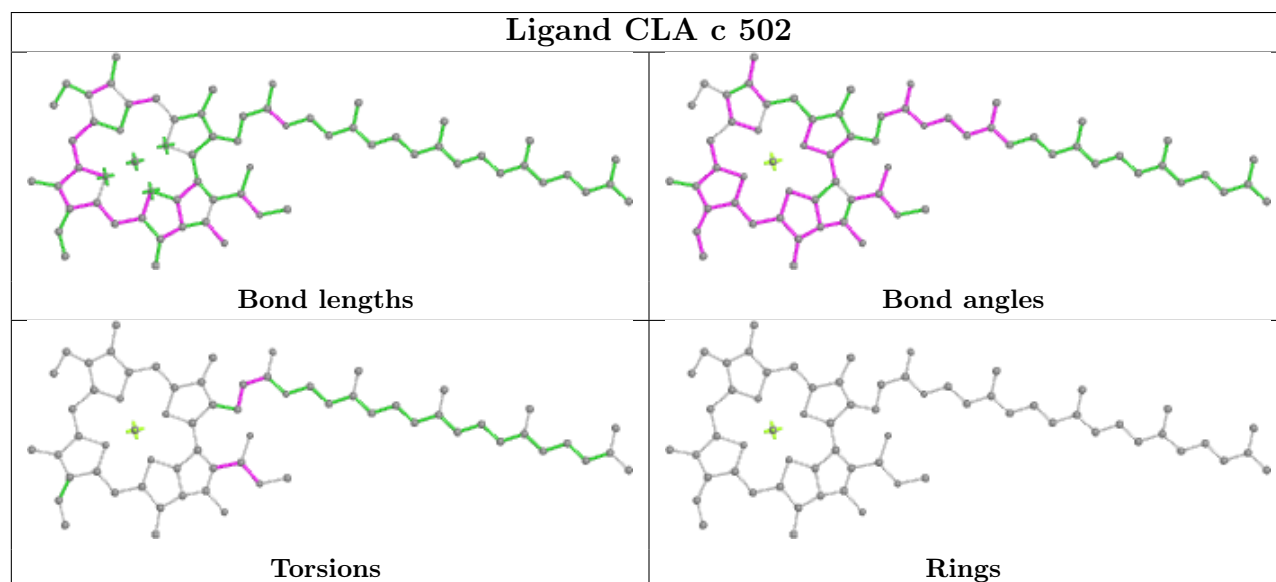
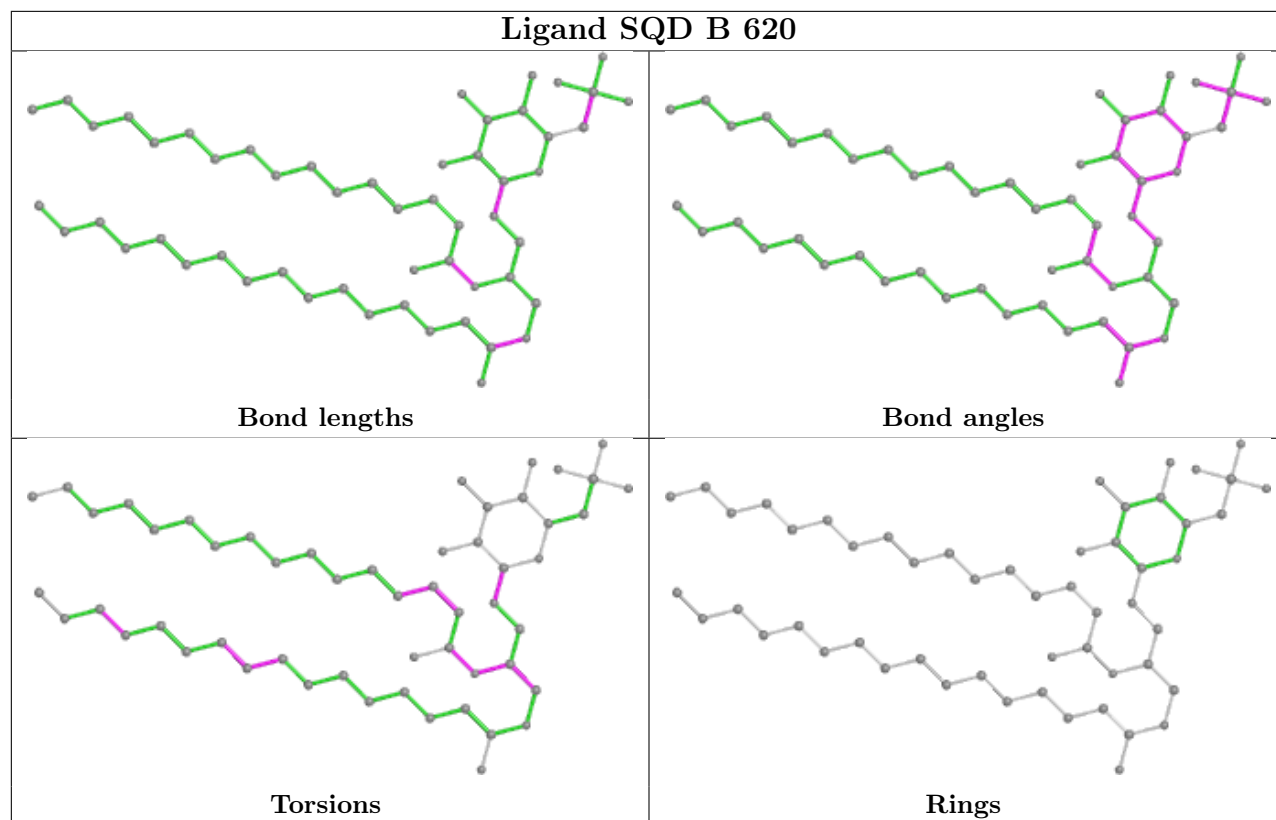


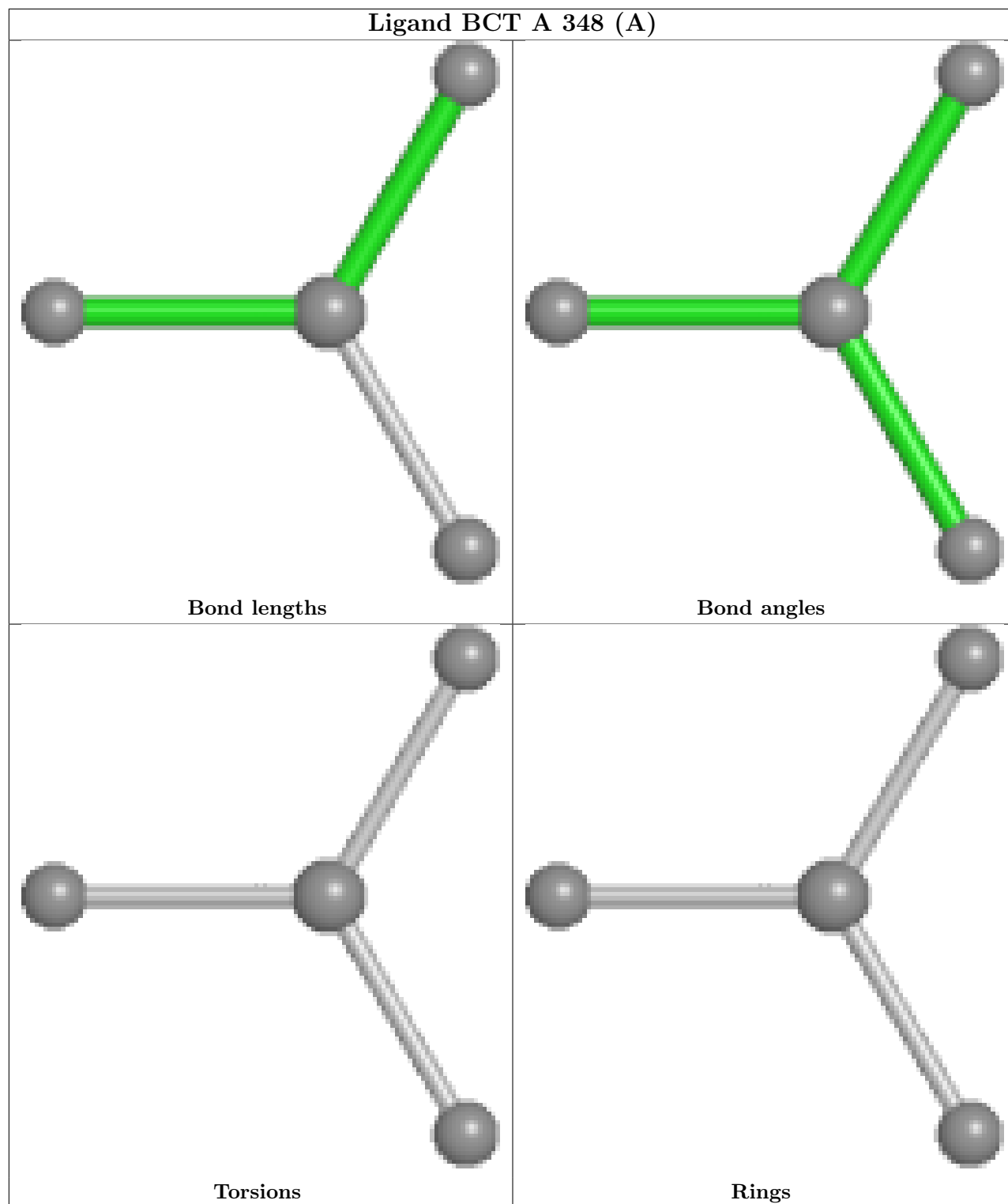


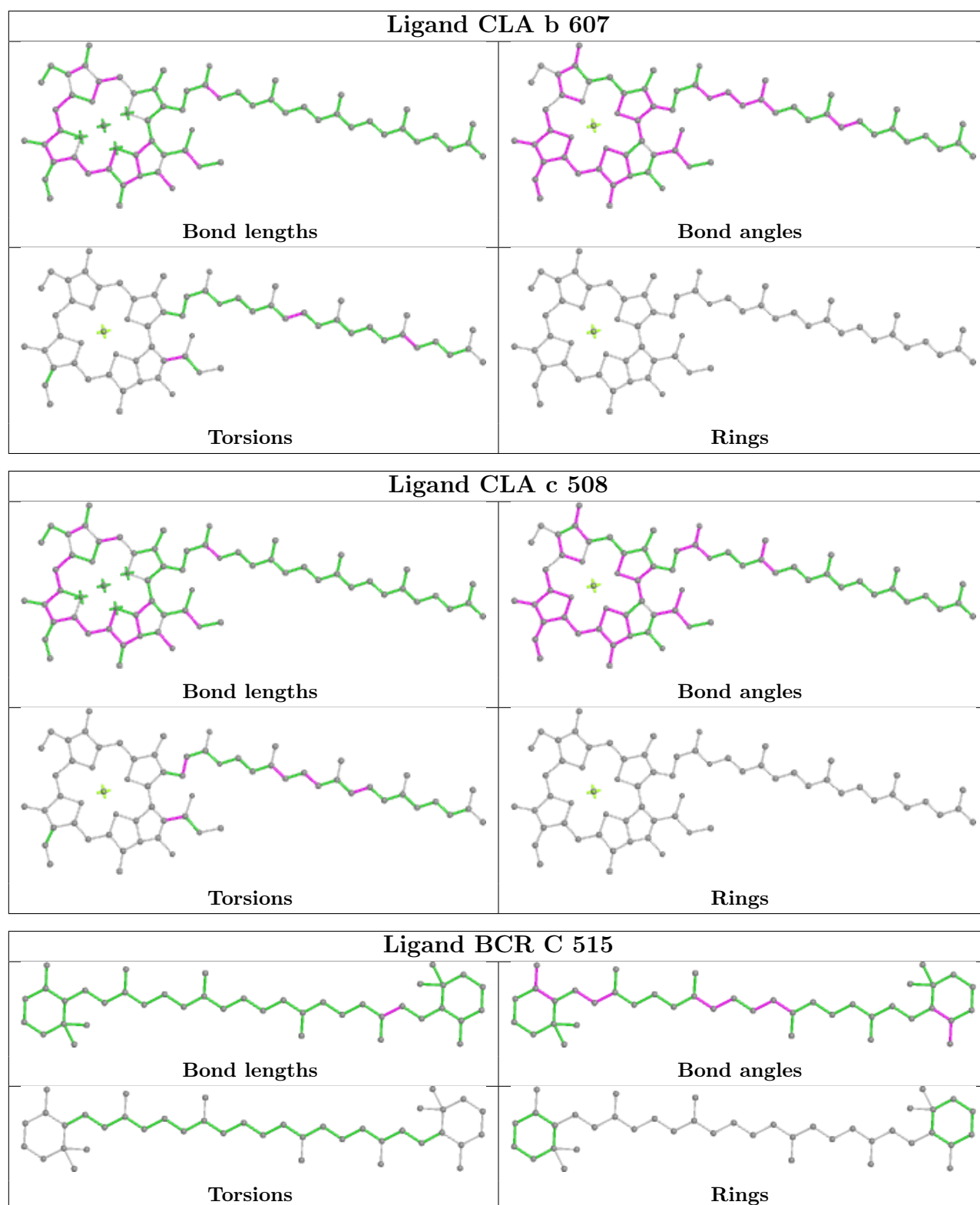




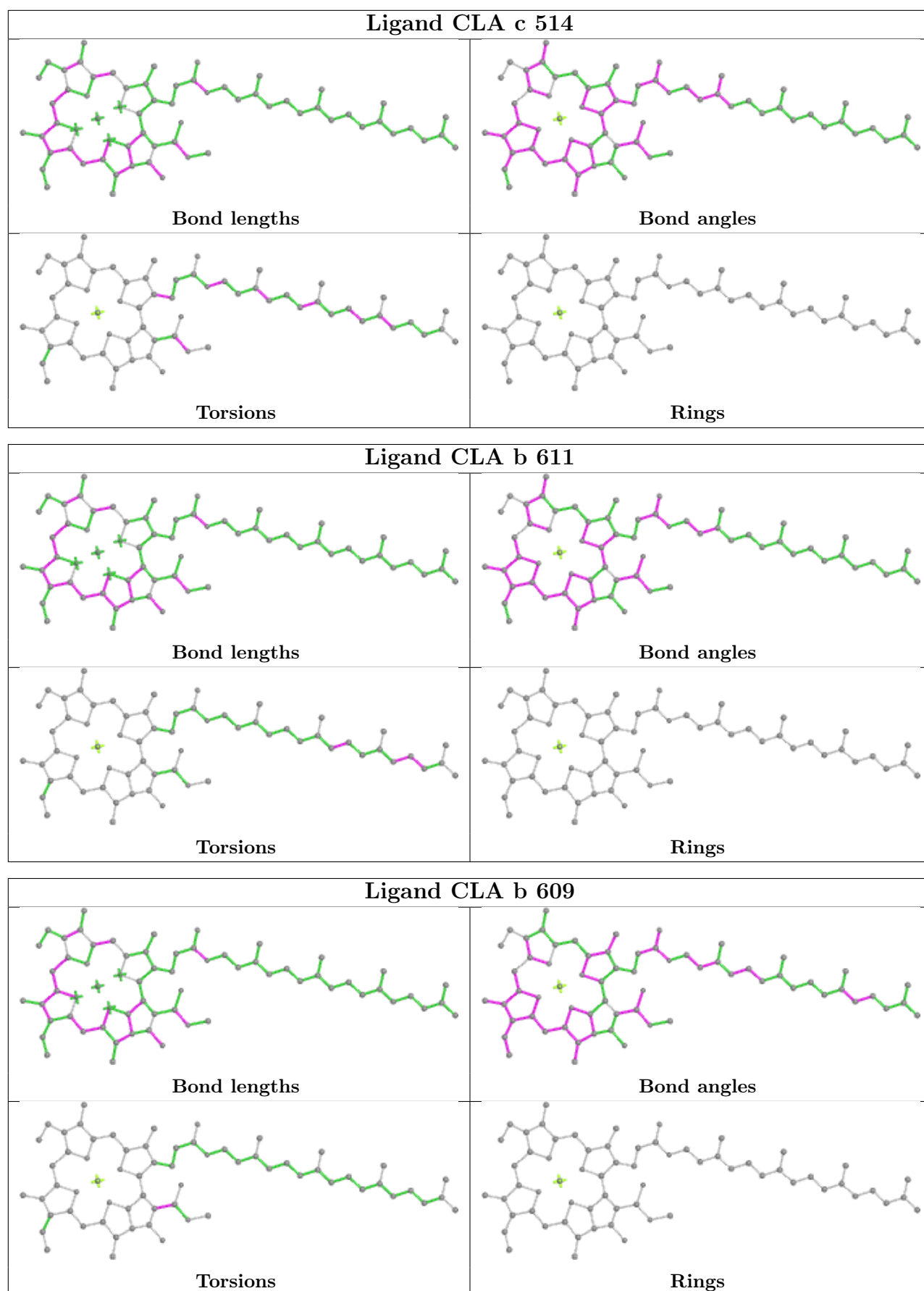


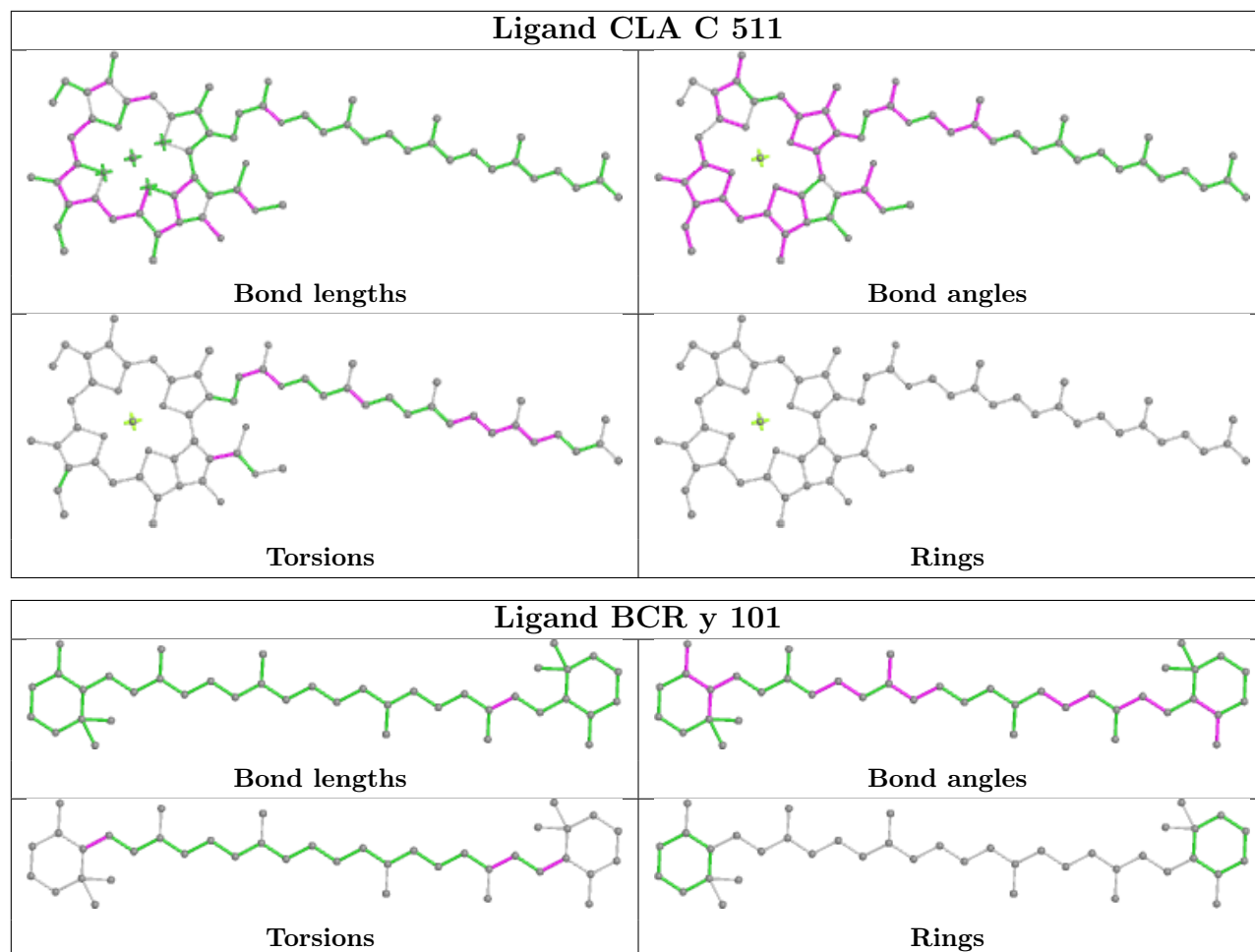


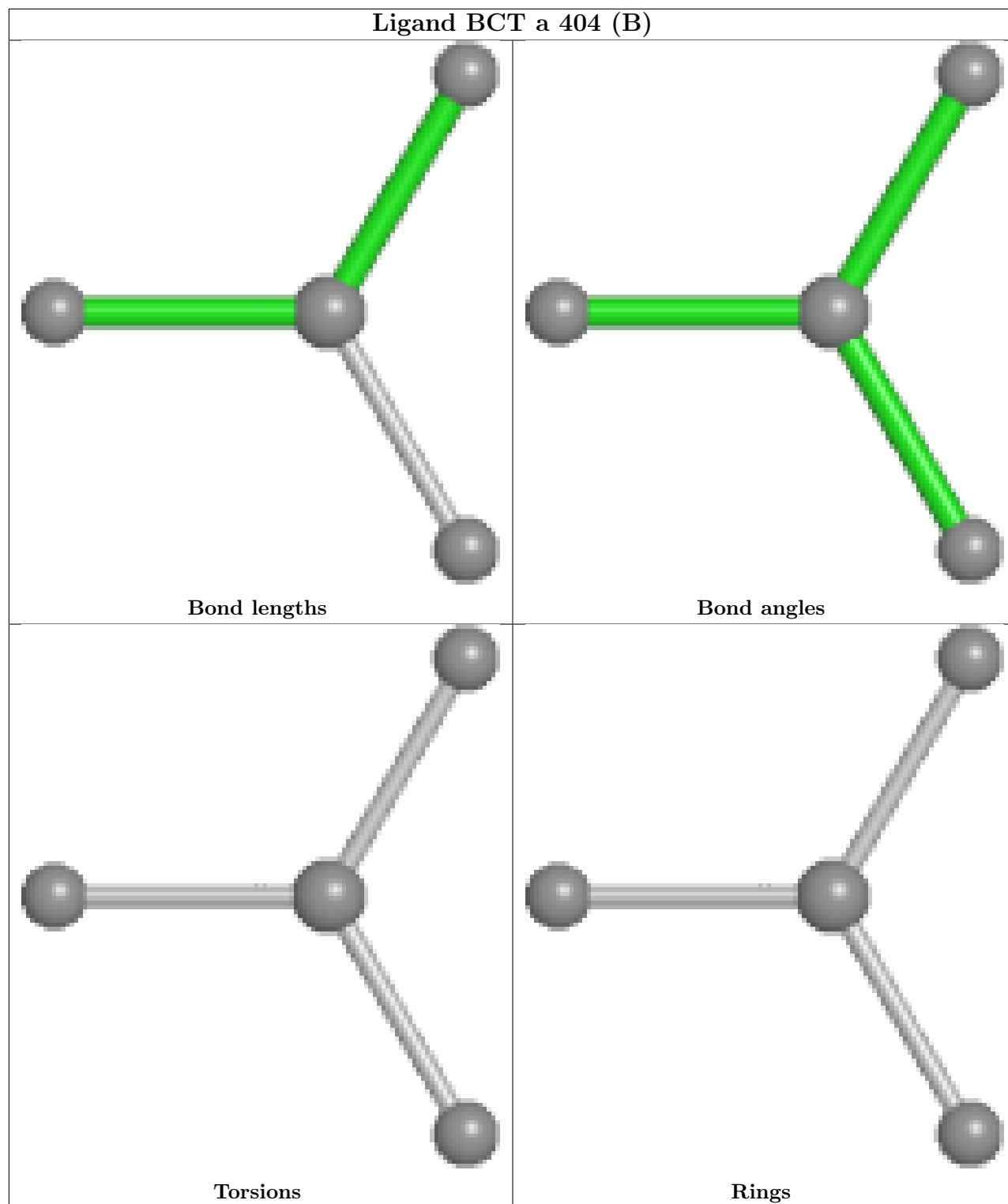


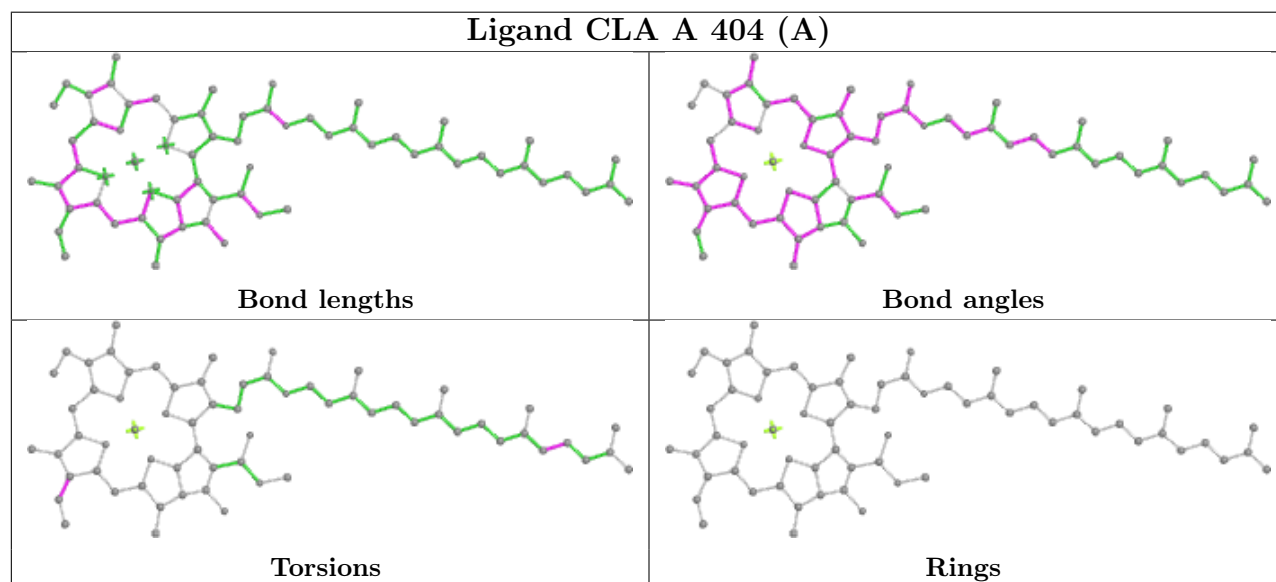
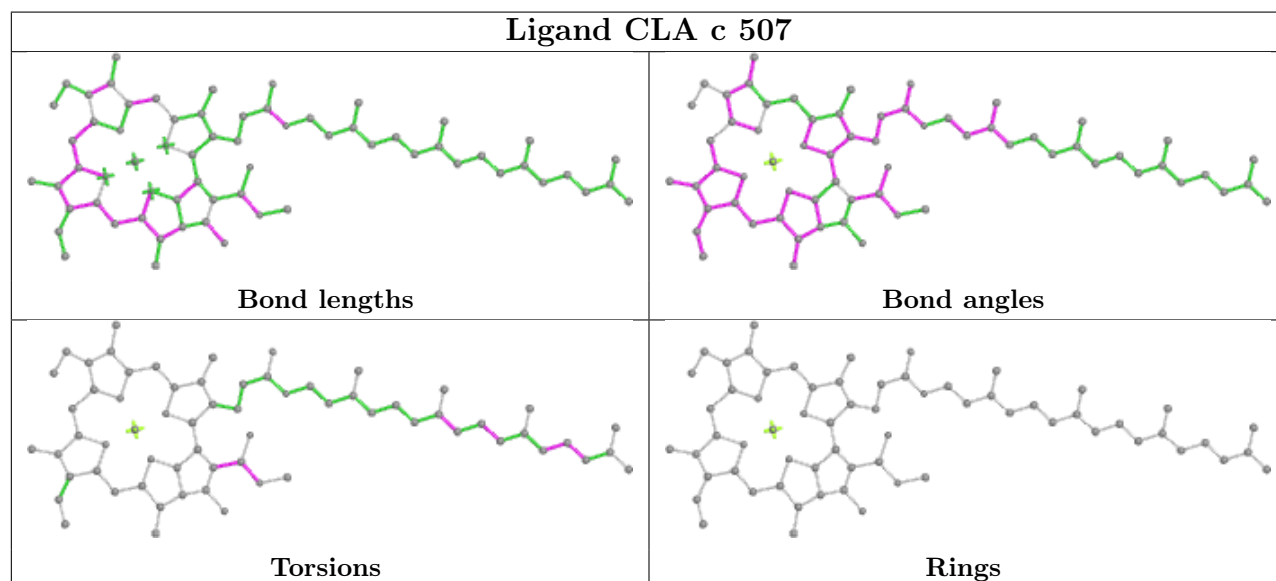
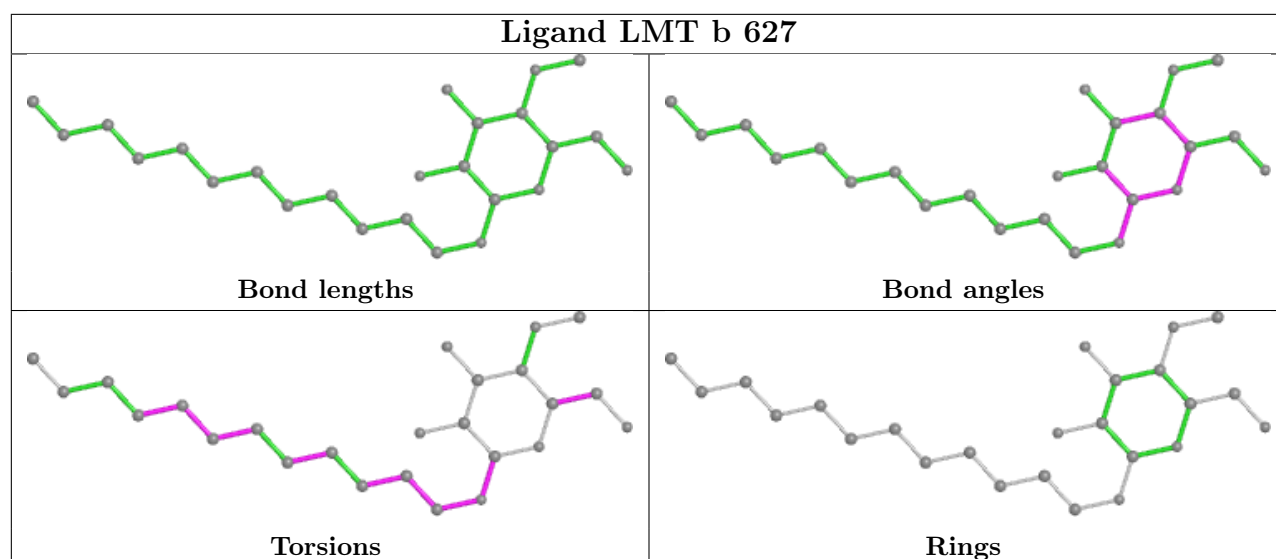


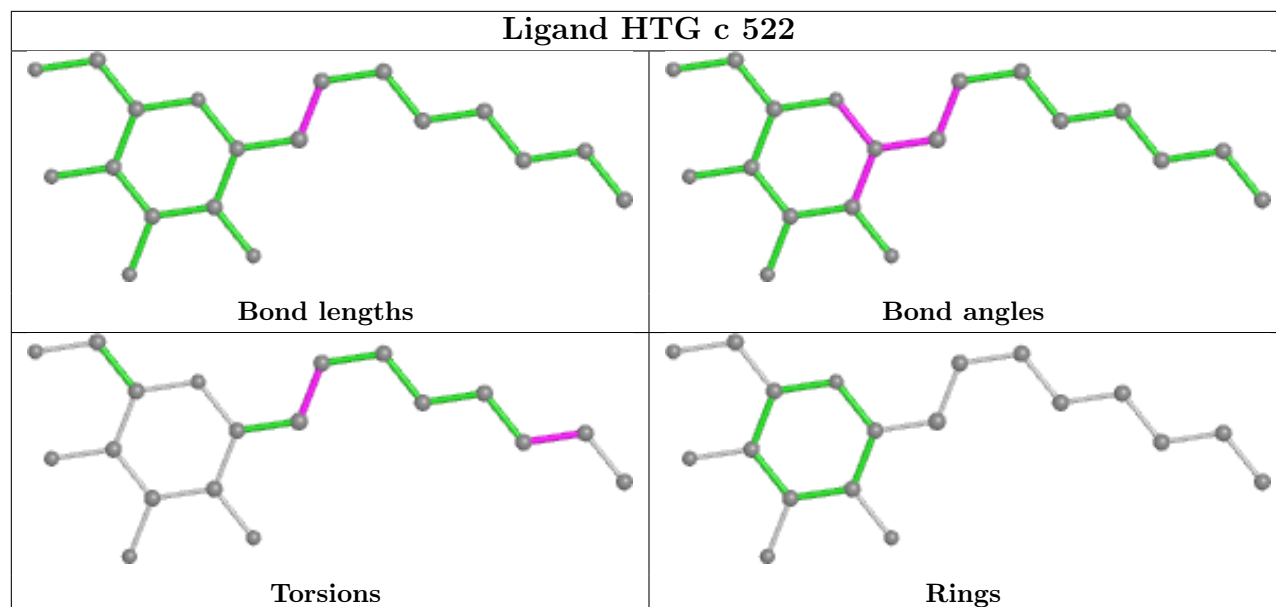


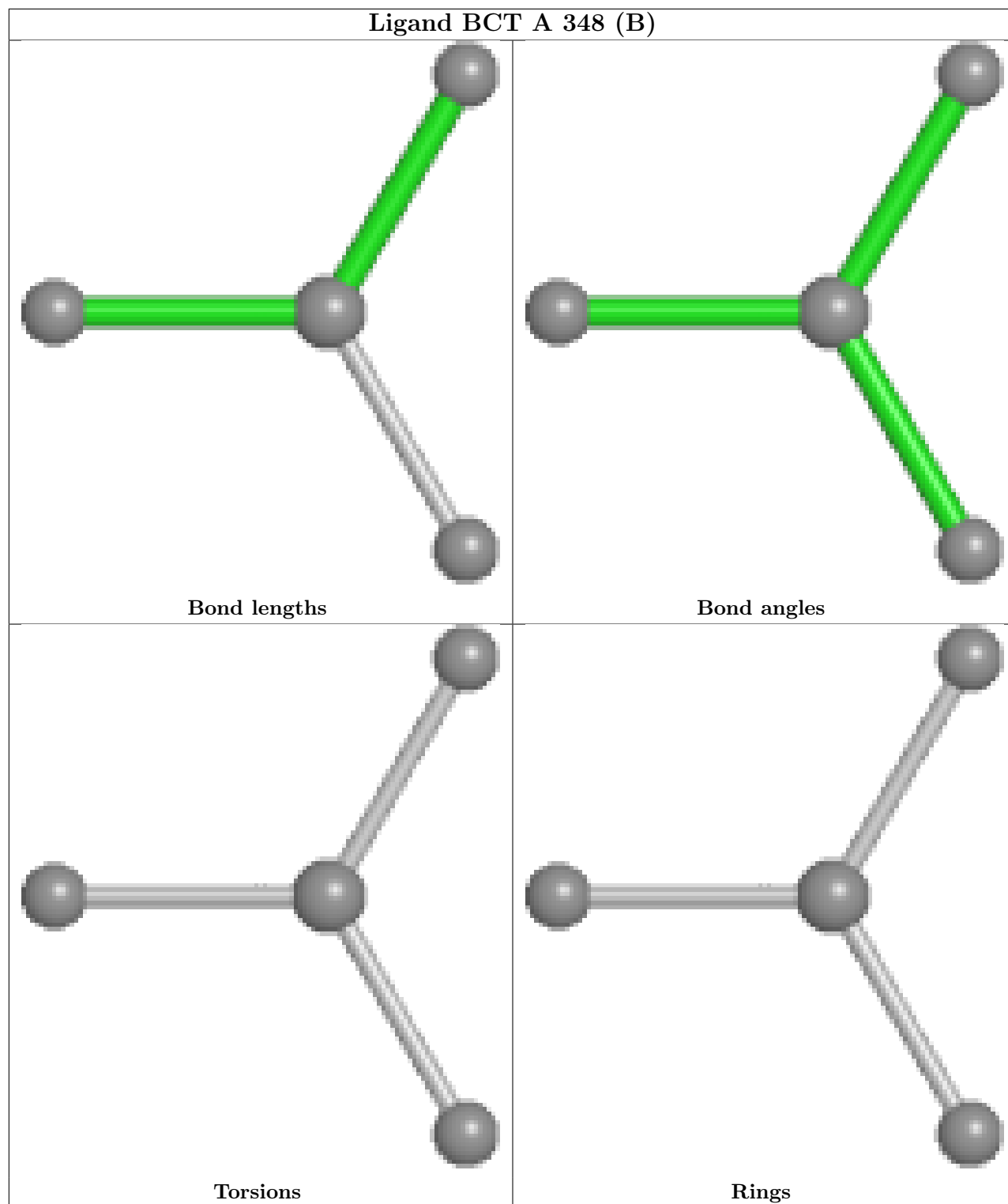


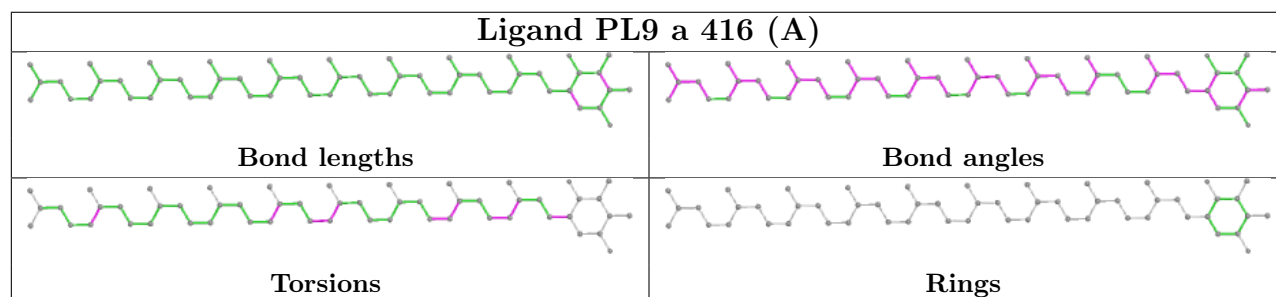
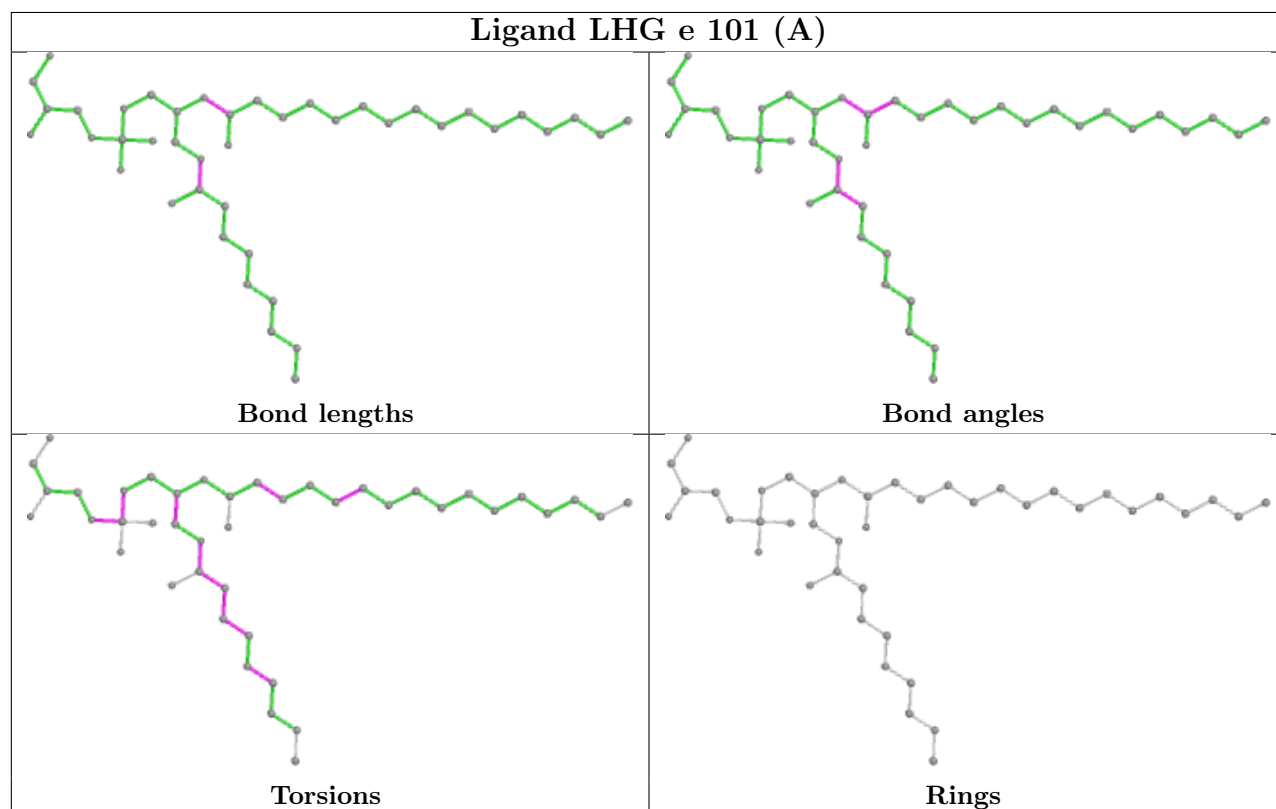
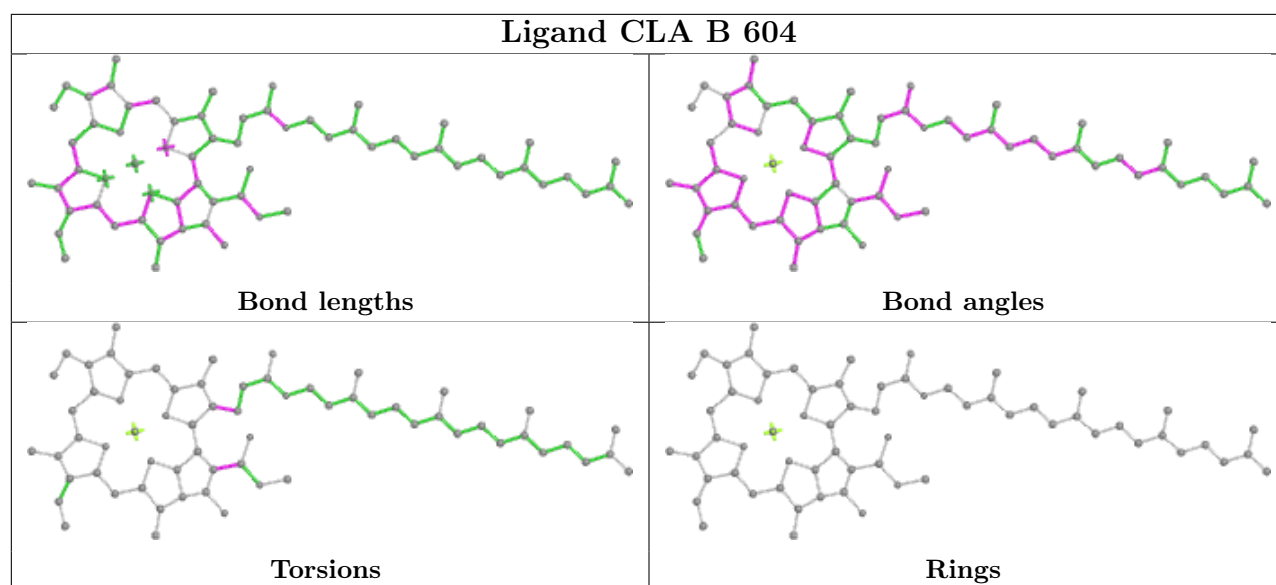


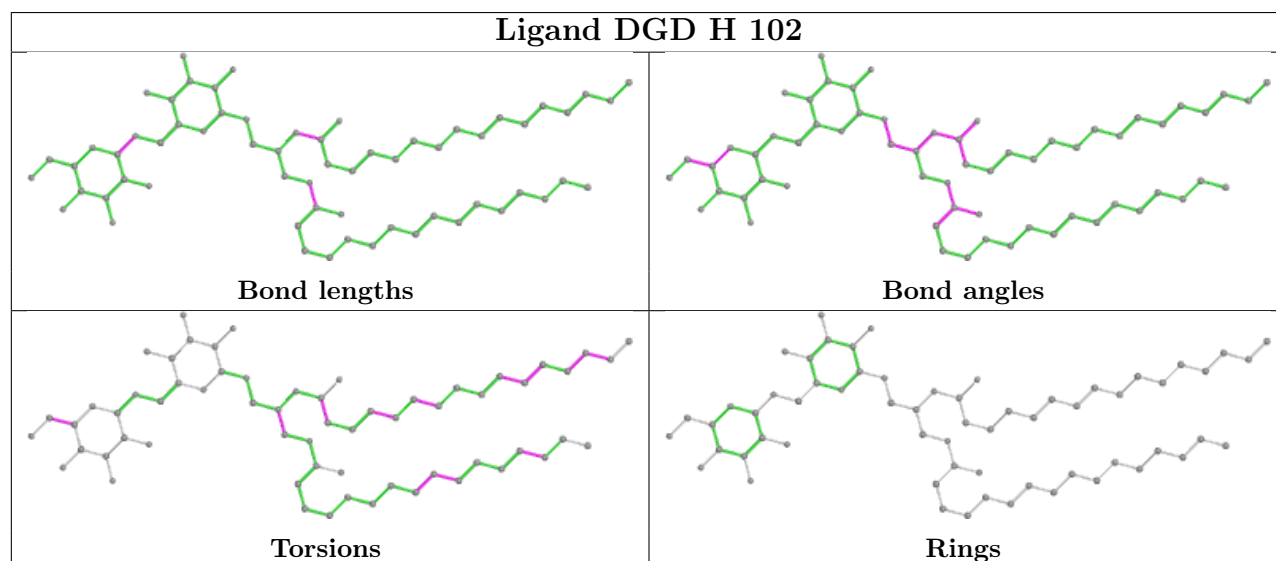
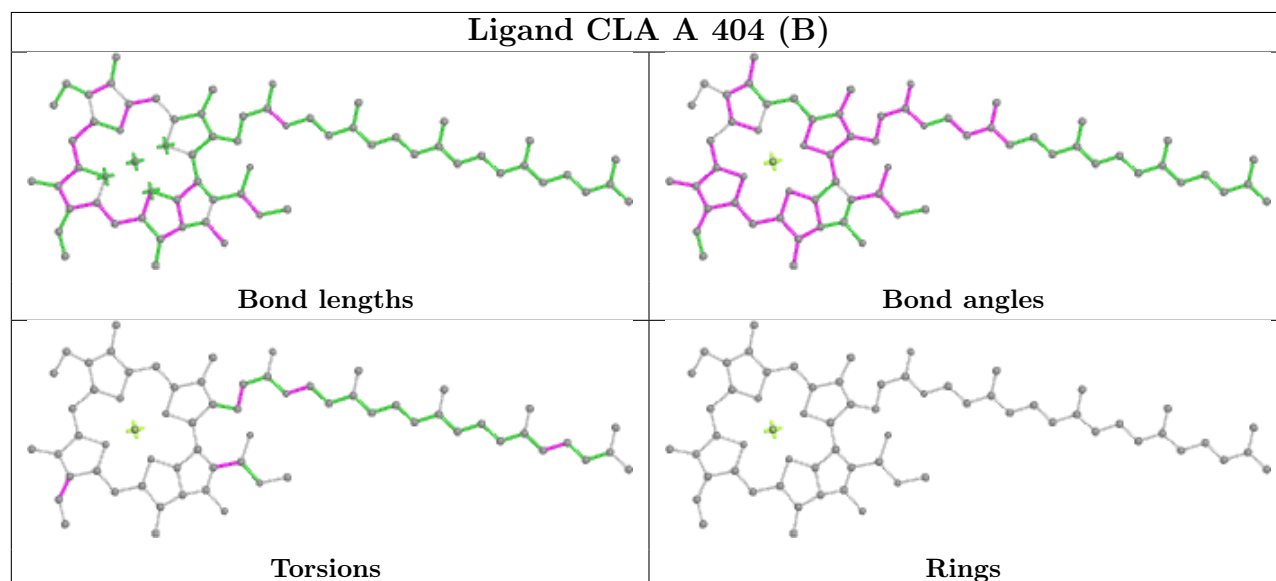
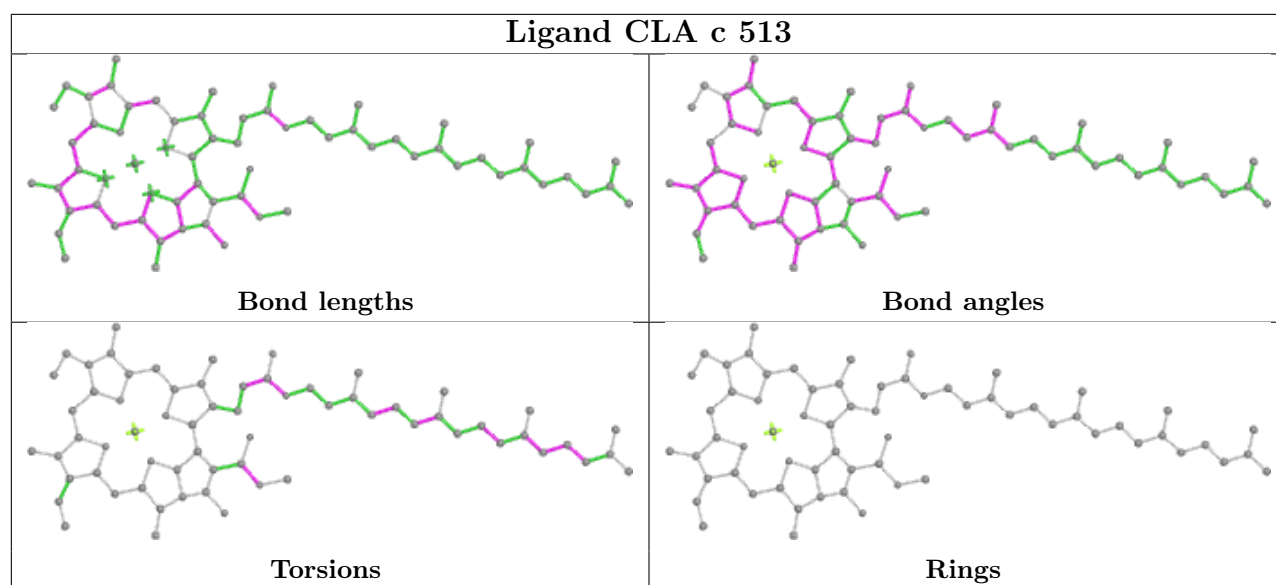




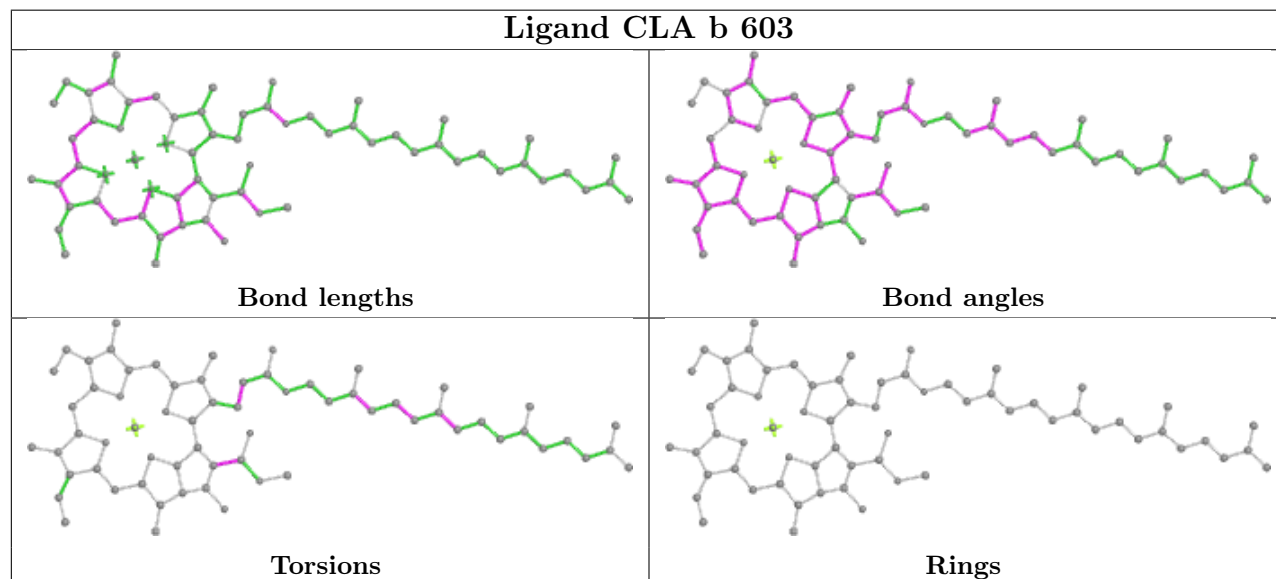
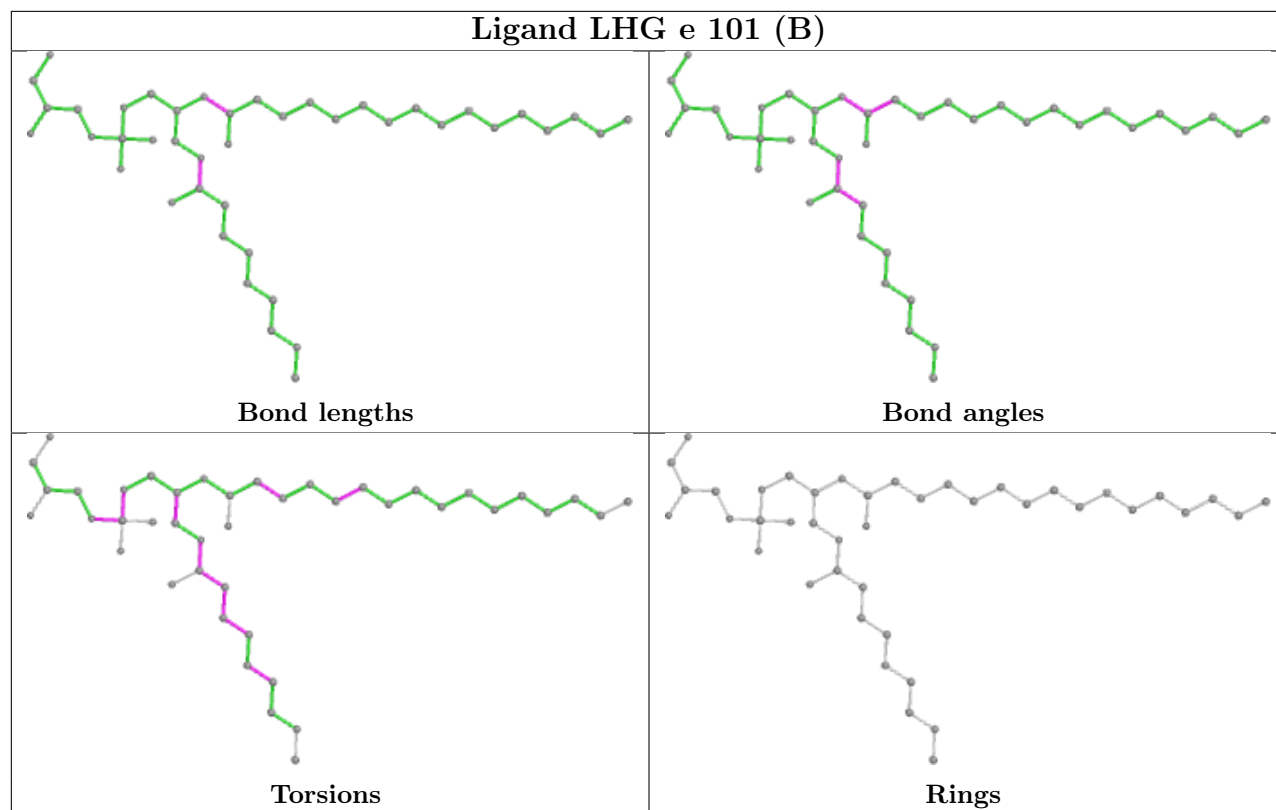


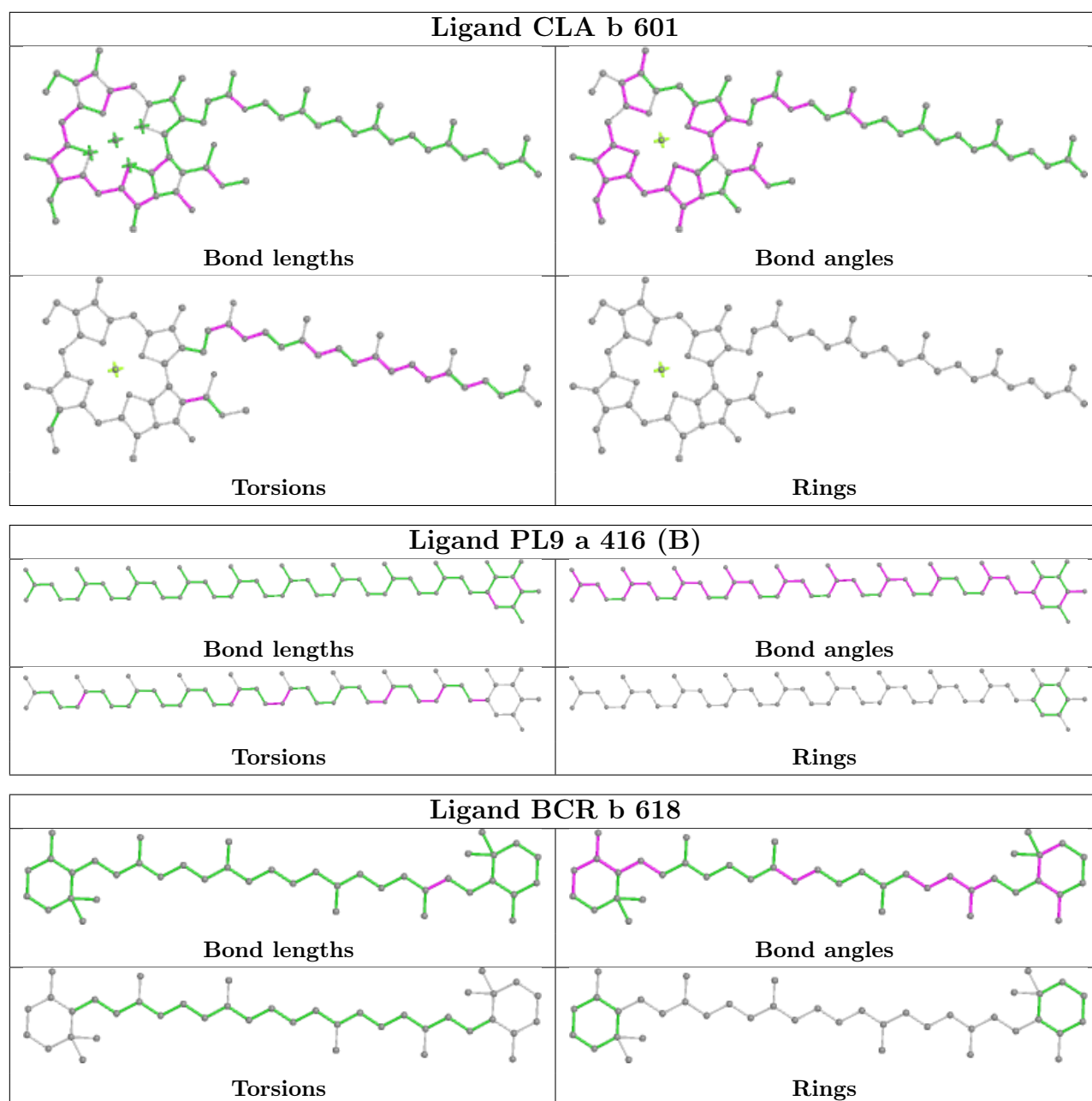


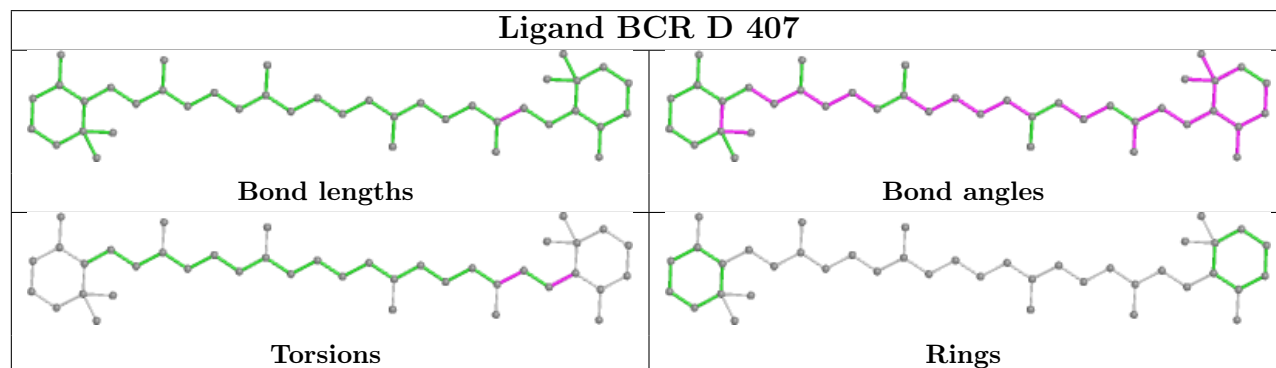
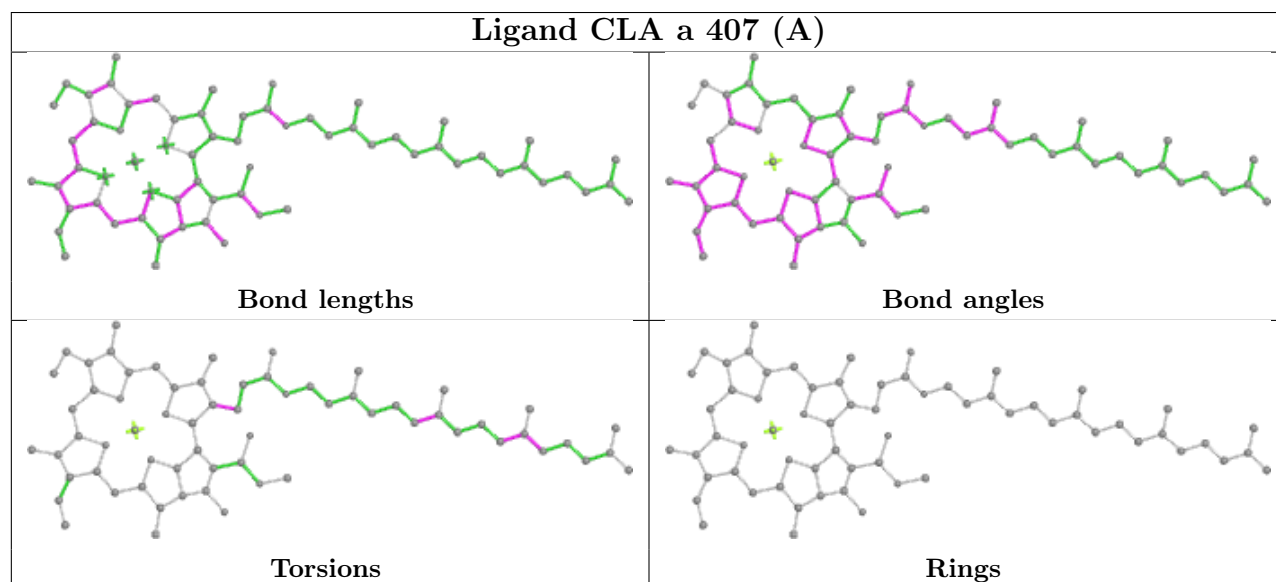
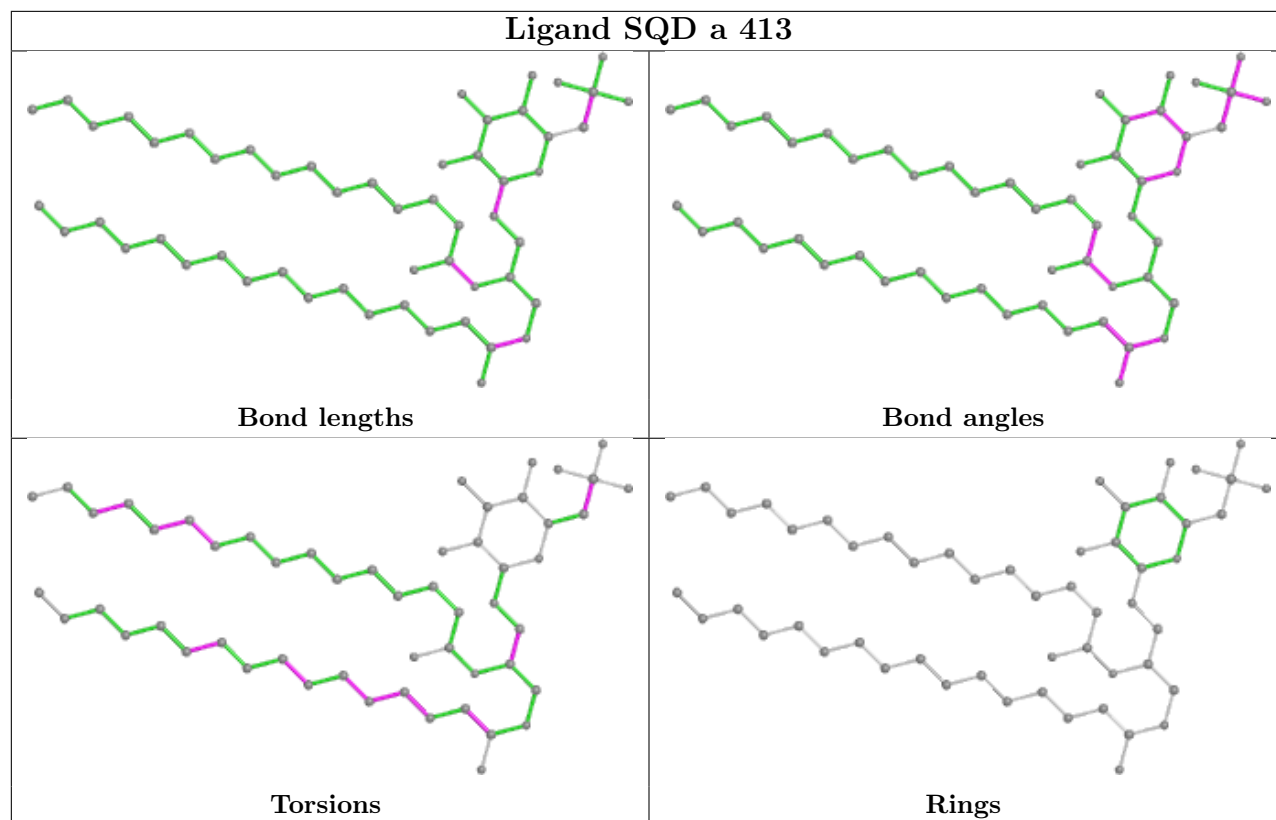


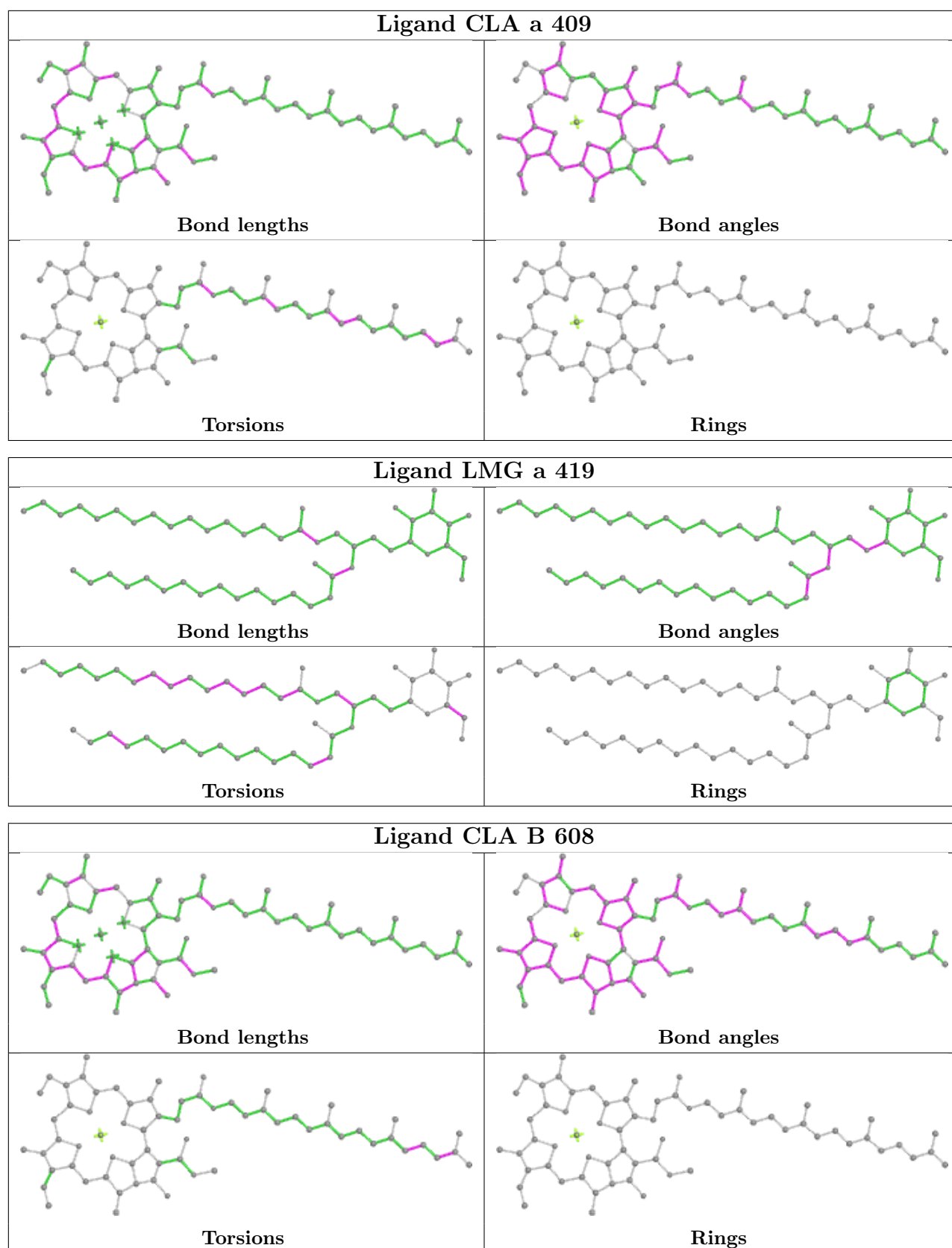


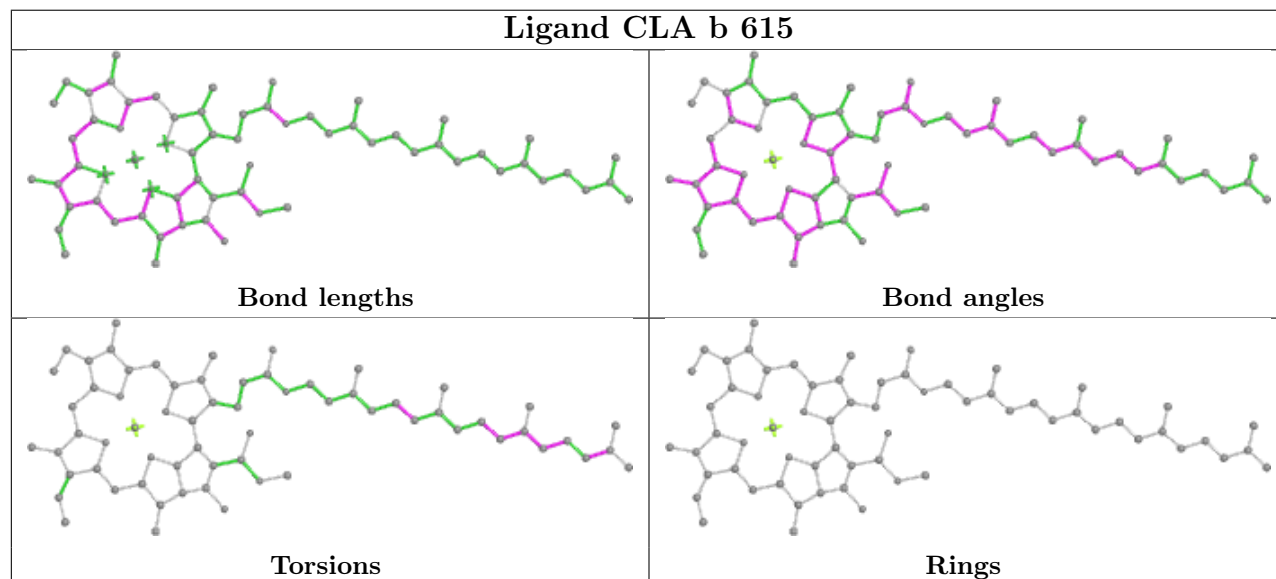
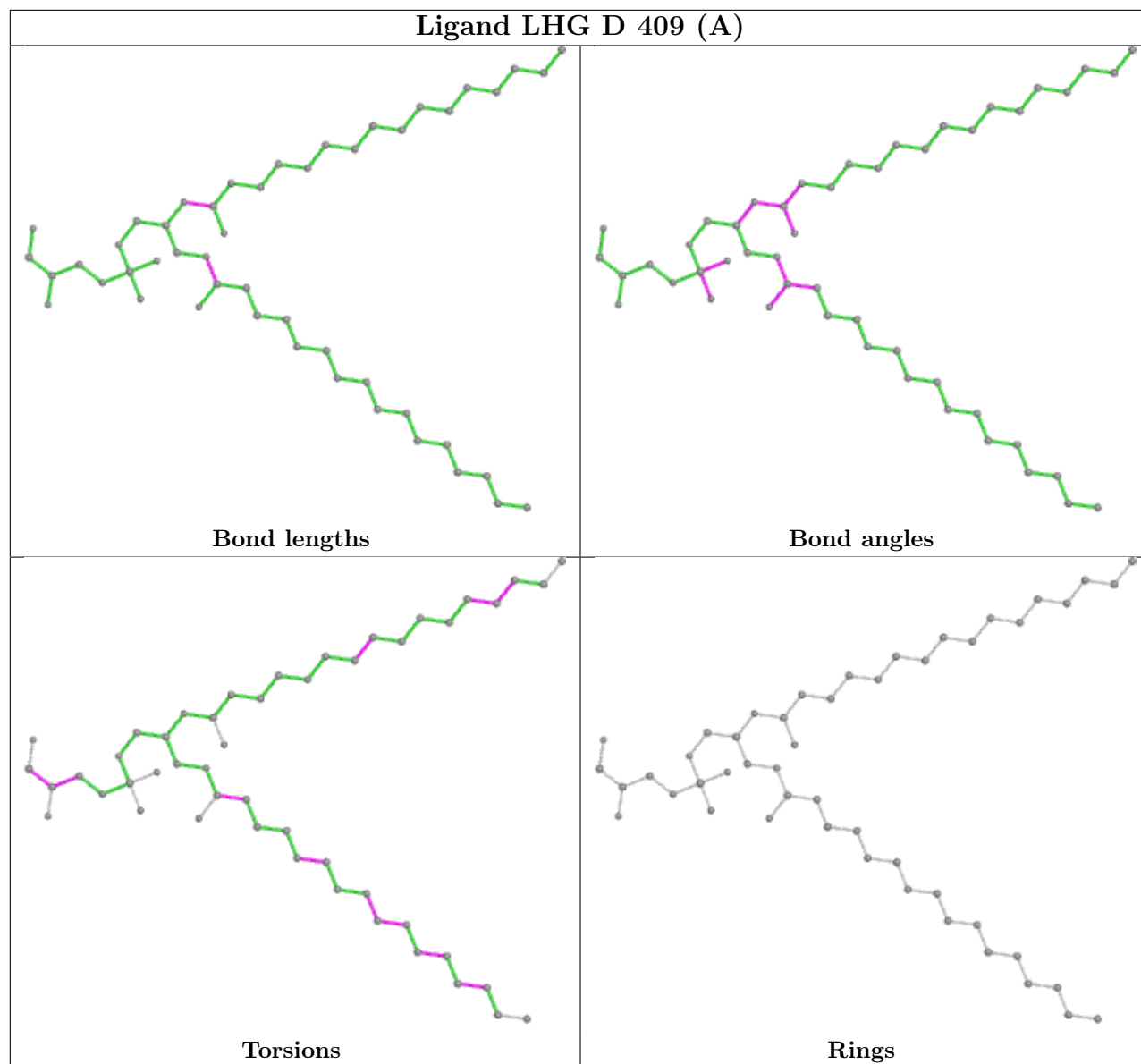


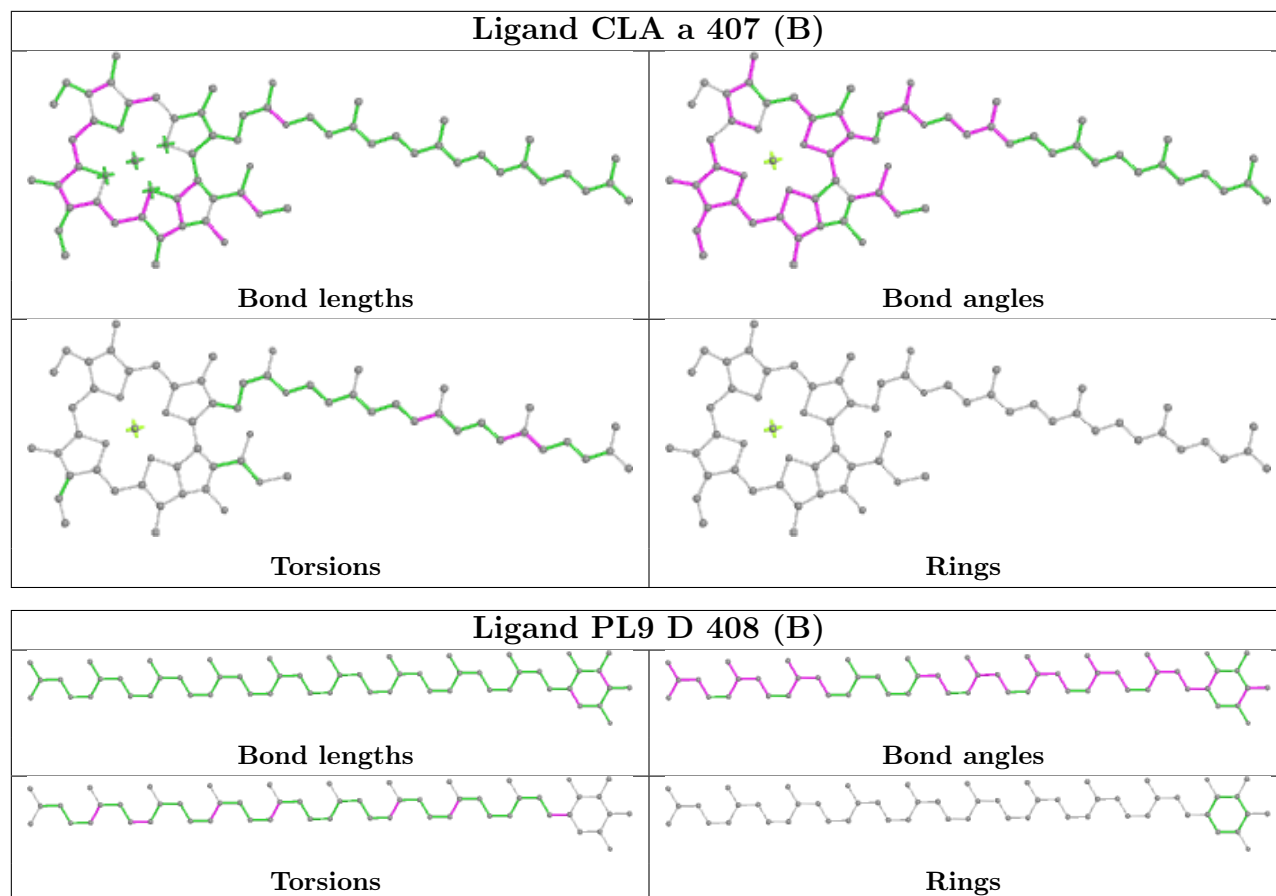


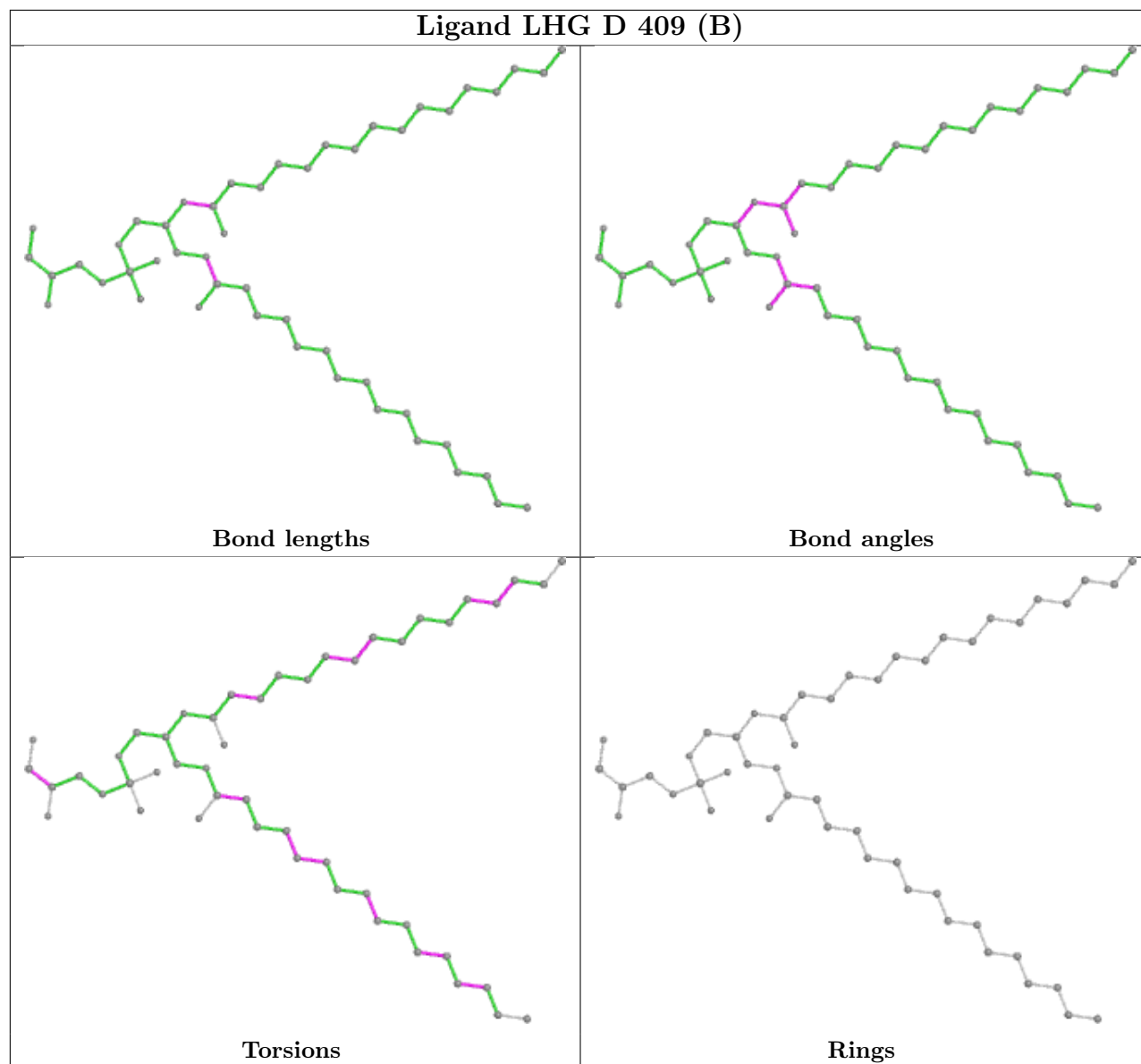


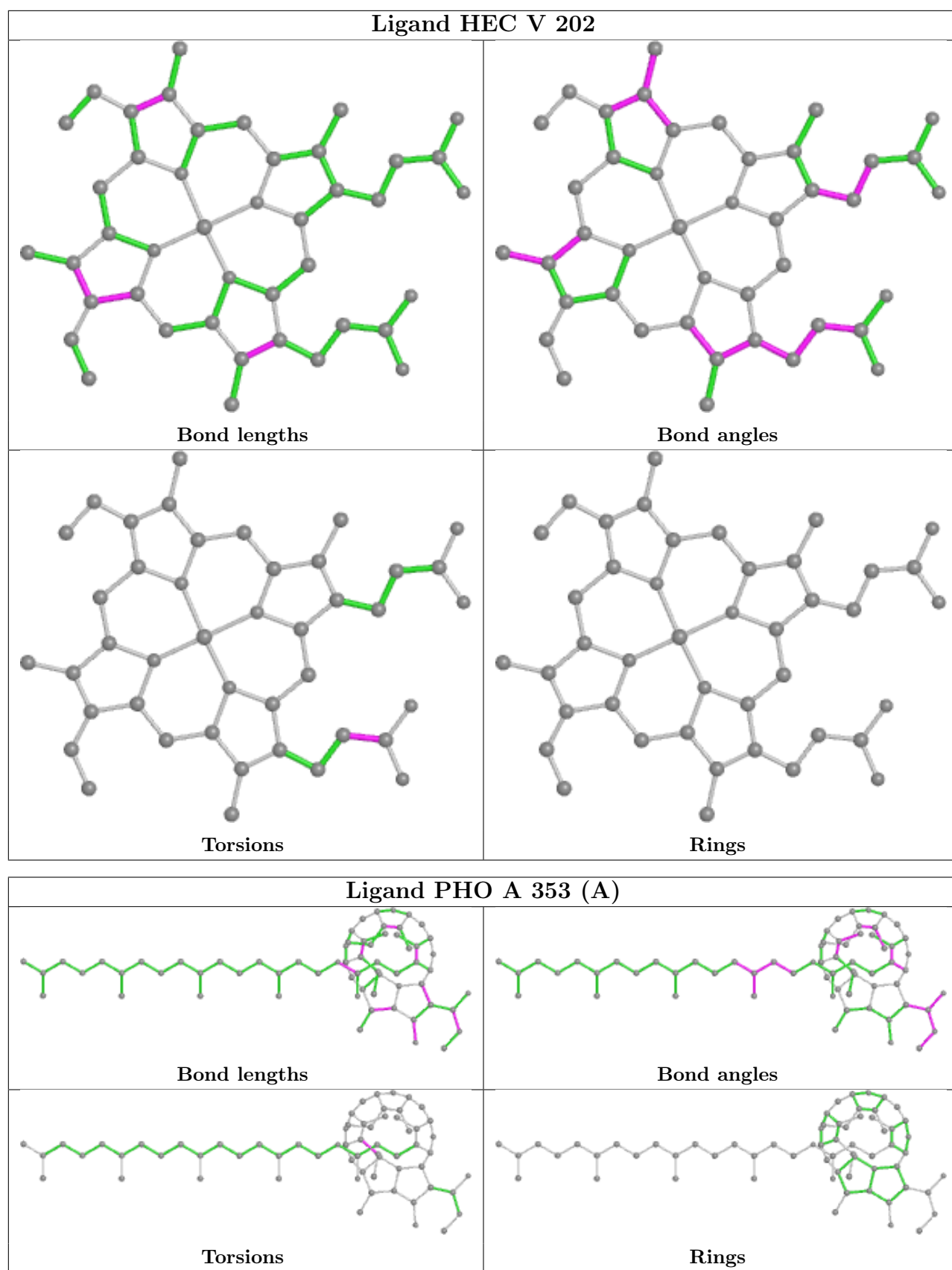




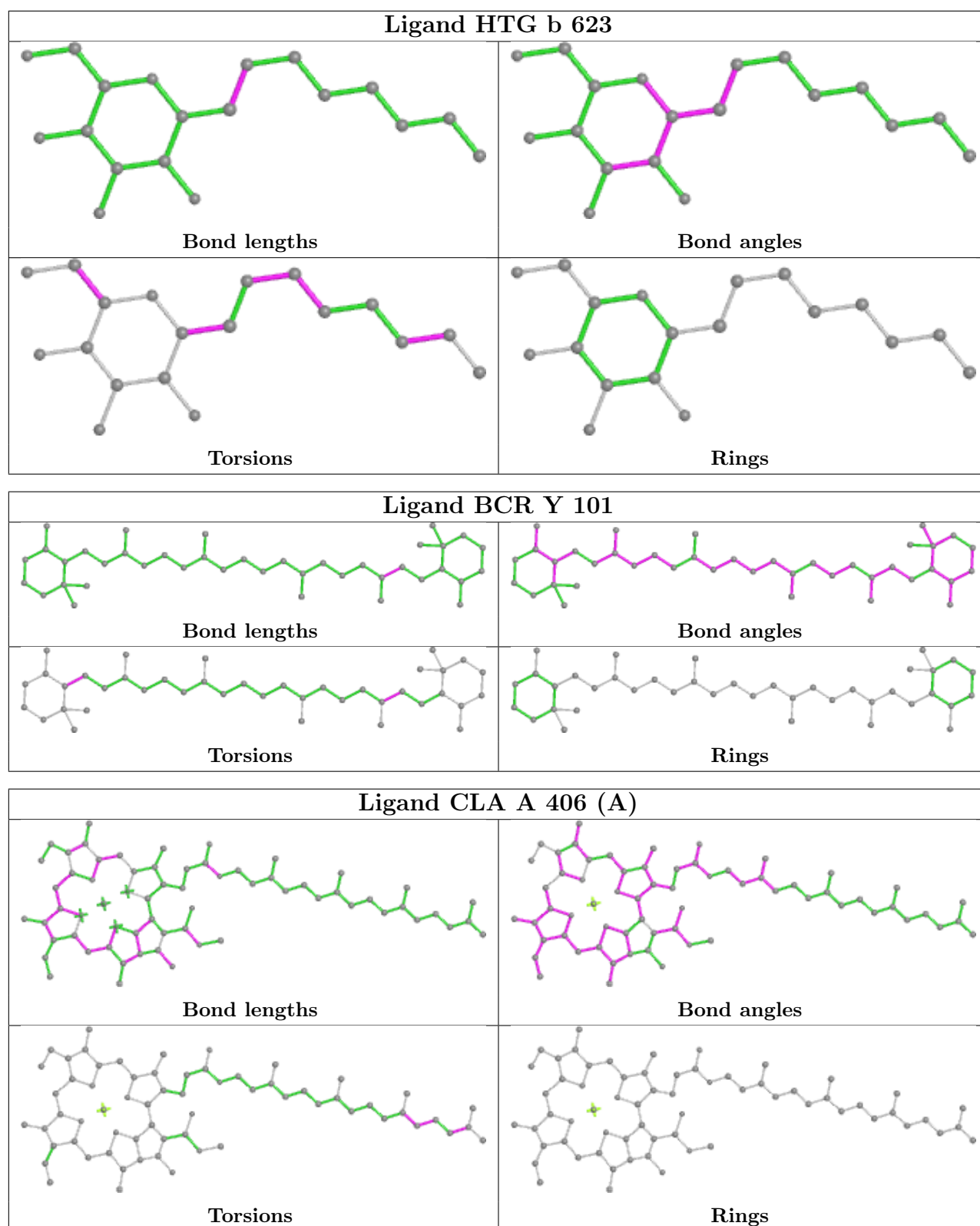


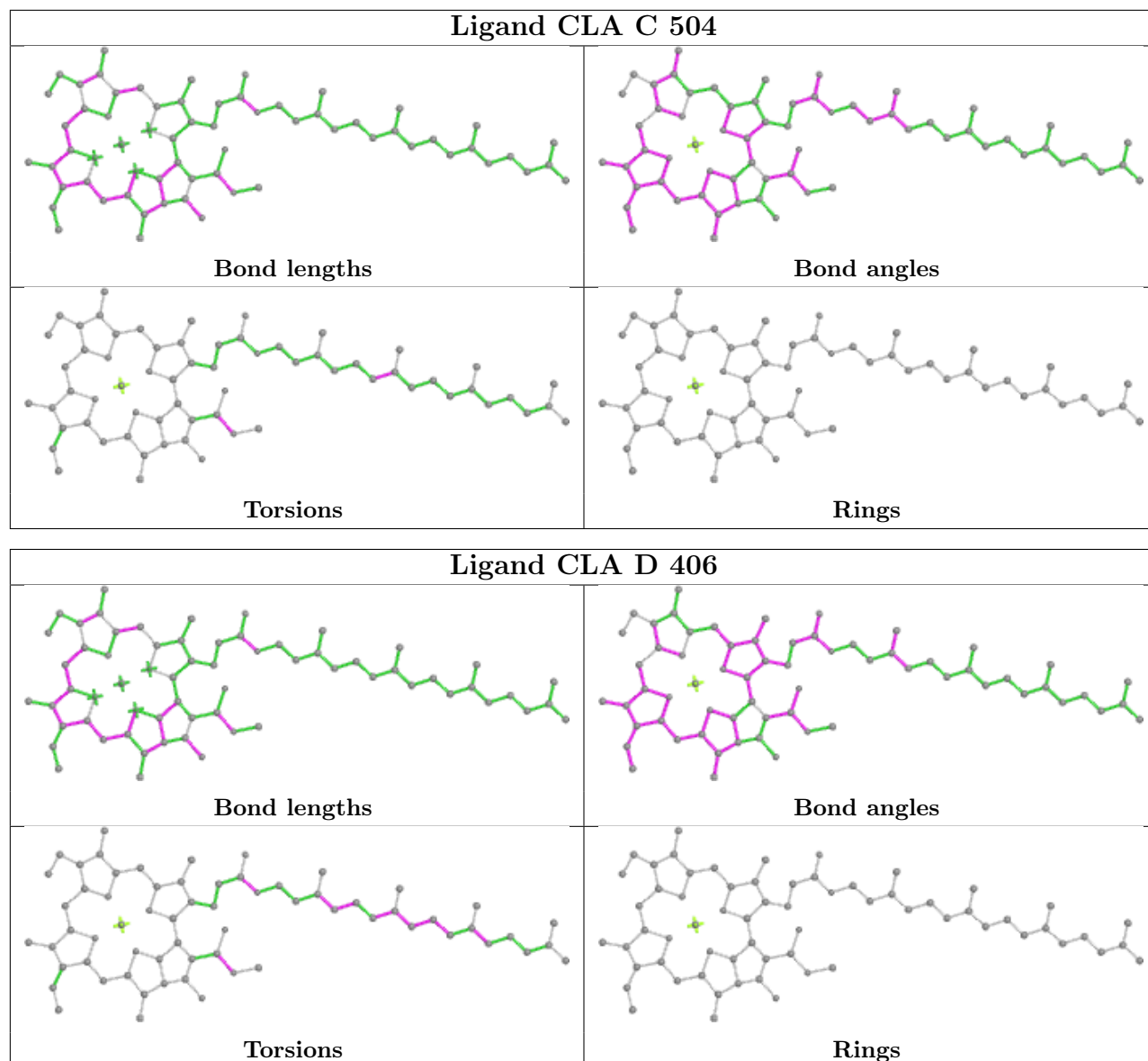


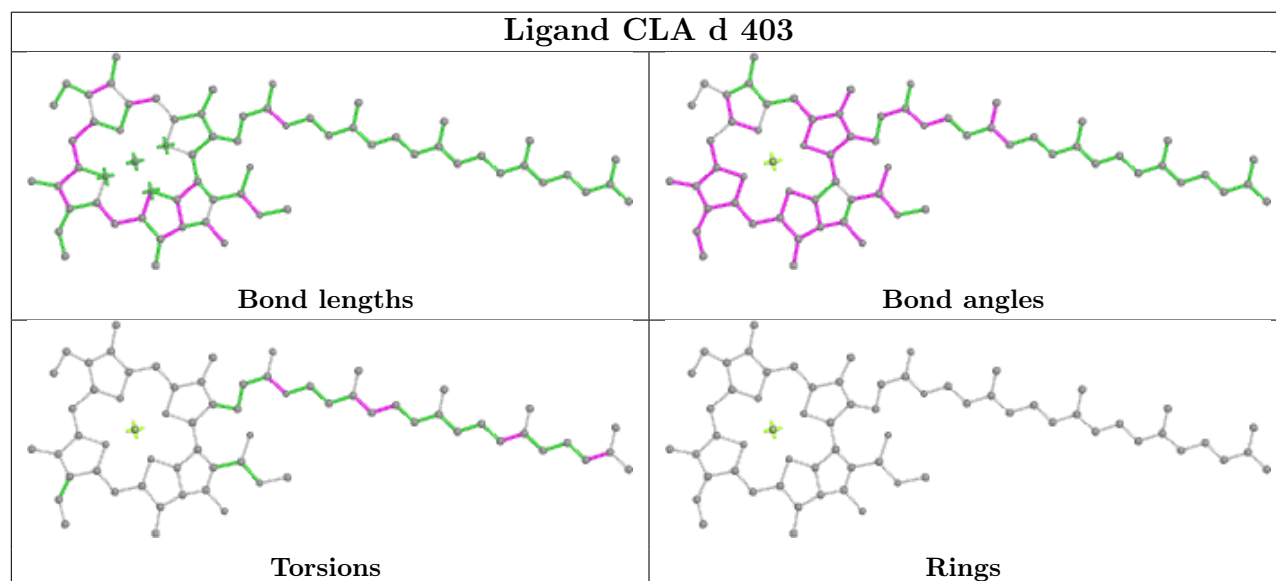
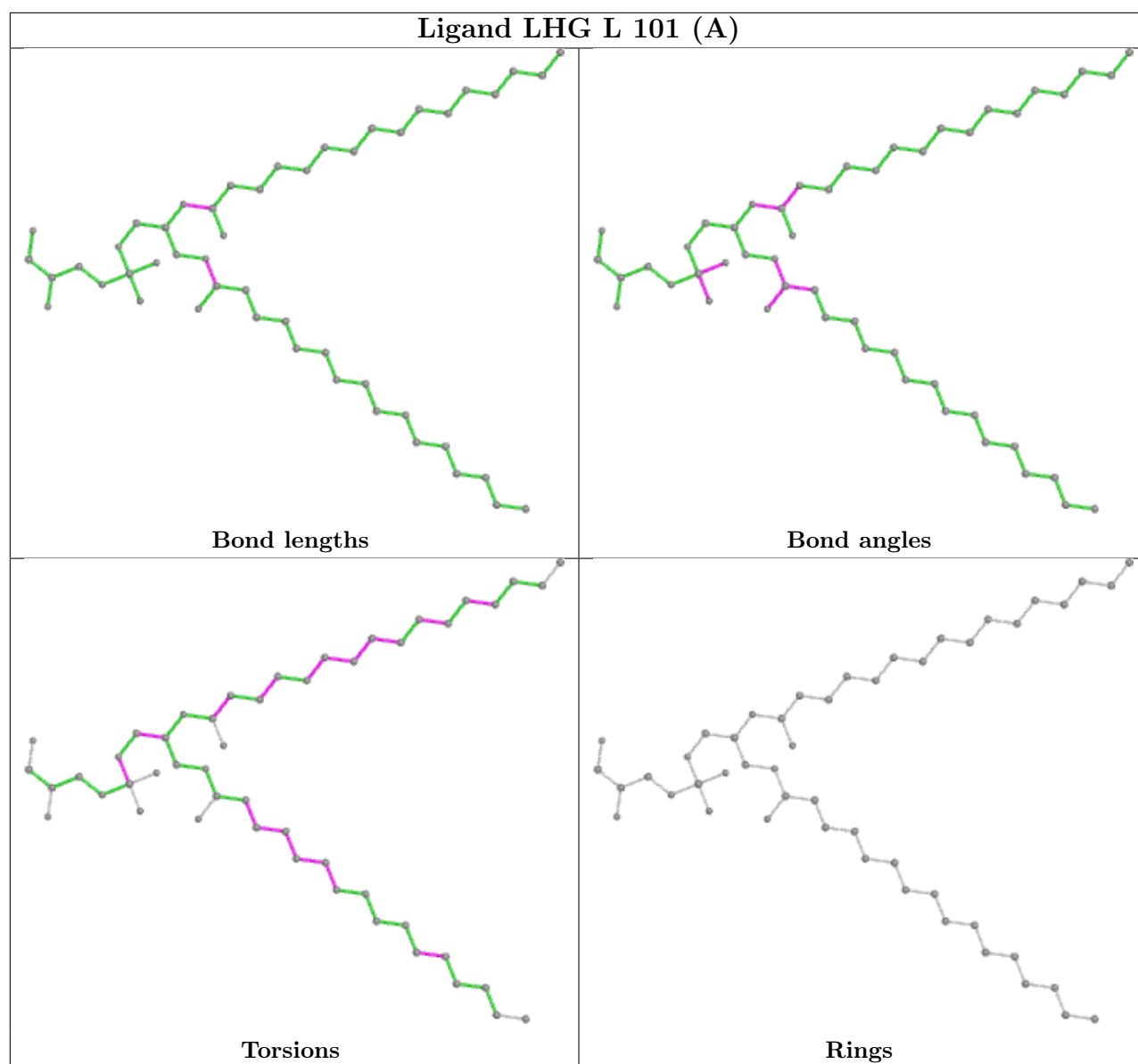


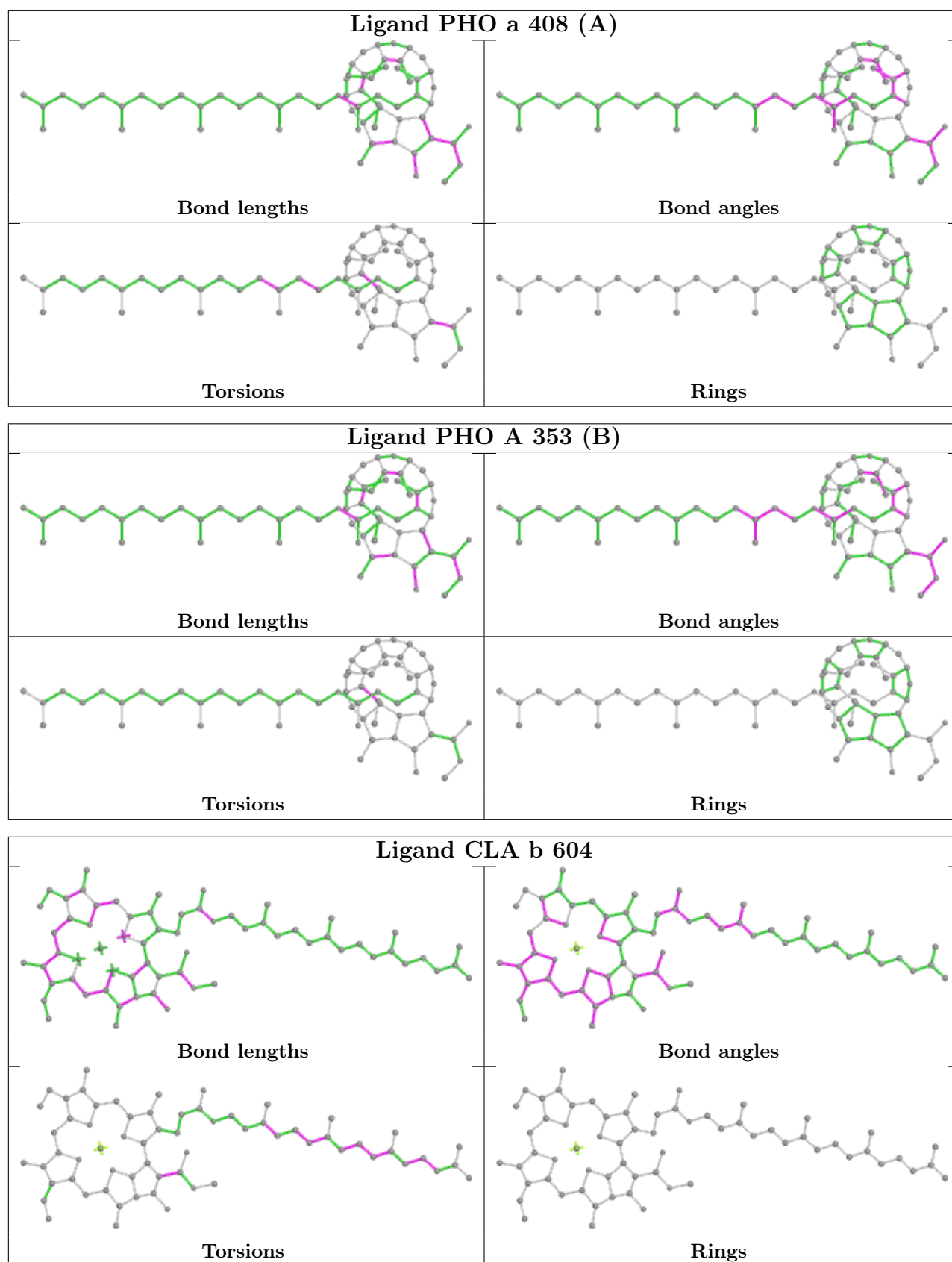


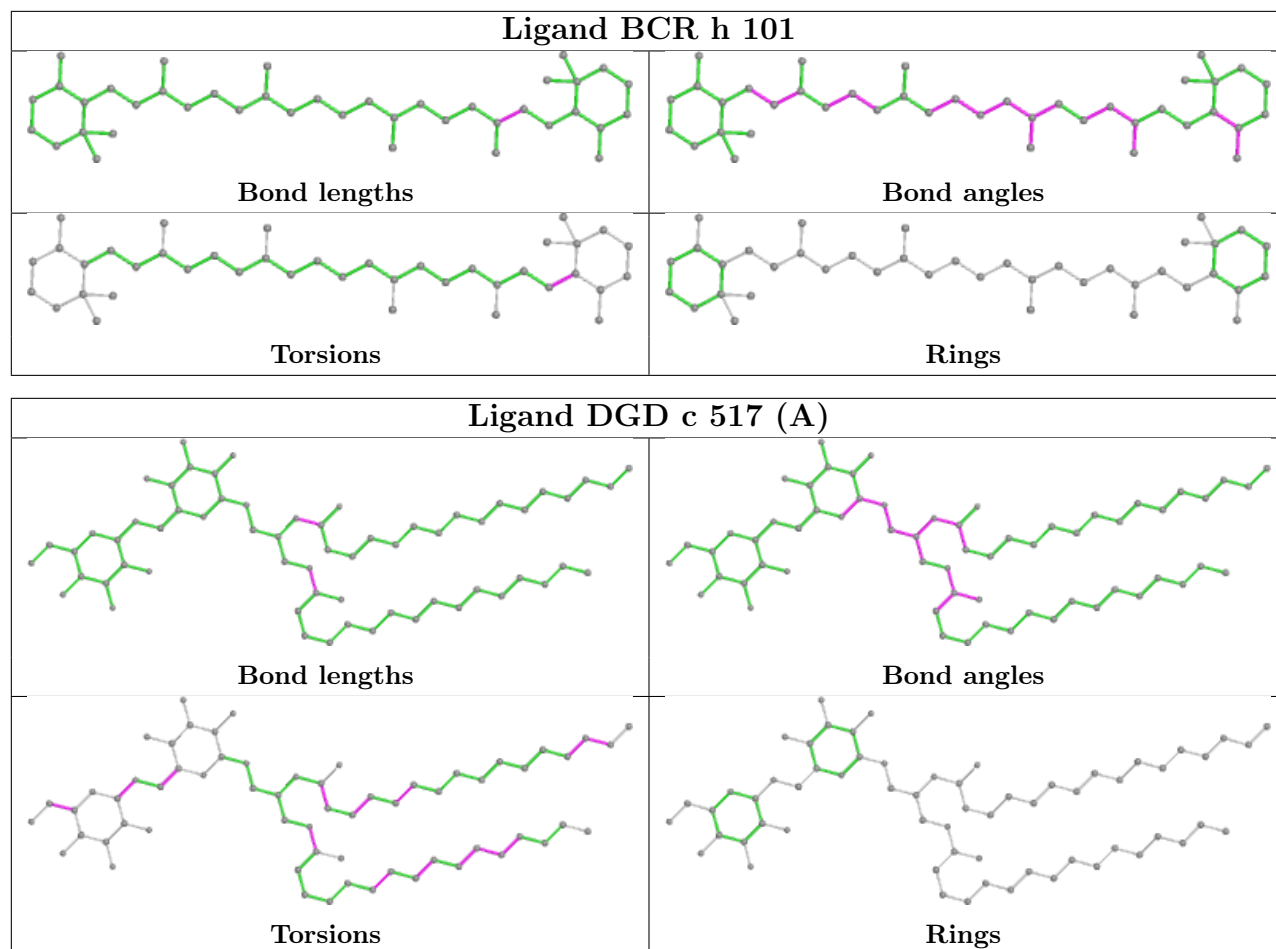


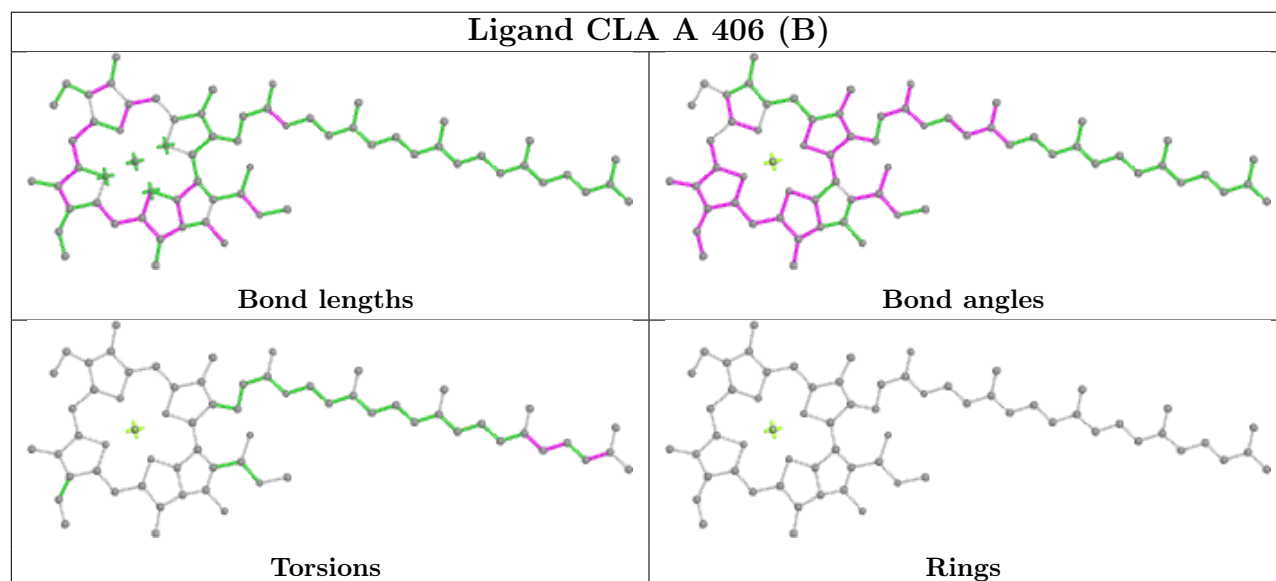
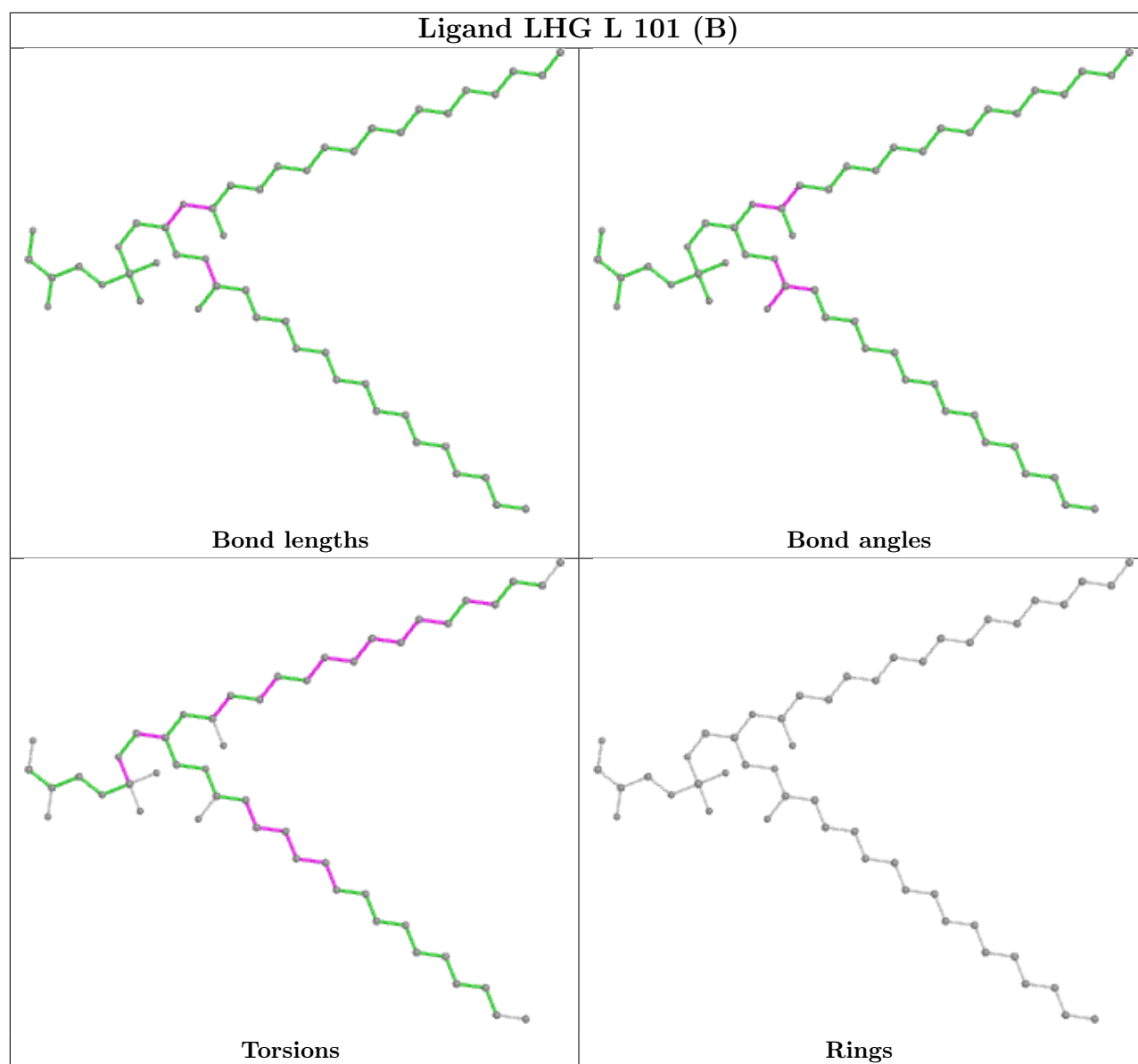












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.82	5 (1%) 73 75	38, 47, 68, 122	0
1	a	334/344 (97%)	-0.72	7 (2%) 63 66	39, 51, 82, 128	0
2	B	504/505 (99%)	-0.55	12 (2%) 59 62	38, 53, 85, 114	0
2	b	504/505 (99%)	-0.32	32 (6%) 20 22	42, 57, 101, 152	1 (0%)
3	C	451/455 (99%)	-0.58	8 (1%) 68 71	42, 60, 82, 133	0
3	c	455/455 (100%)	-0.47	12 (2%) 56 59	48, 66, 88, 127	2 (0%)
4	D	342/342 (100%)	-0.74	4 (1%) 79 81	37, 48, 67, 129	0
4	d	341/342 (99%)	-0.72	3 (0%) 84 85	41, 53, 79, 127	0
5	E	81/84 (96%)	-0.15	5 (6%) 20 22	52, 69, 97, 148	0
5	e	79/84 (94%)	0.23	8 (10%) 7 7	61, 77, 120, 141	0
6	F	34/44 (77%)	-0.51	2 (5%) 22 24	54, 61, 91, 116	0
6	f	31/44 (70%)	-0.26	3 (9%) 7 8	60, 68, 98, 137	0
7	H	64/65 (98%)	-0.32	3 (4%) 31 34	52, 63, 88, 112	0
7	h	64/65 (98%)	-0.29	3 (4%) 31 34	57, 73, 95, 105	0
8	I	37/38 (97%)	-0.16	3 (8%) 12 13	56, 65, 121, 145	0
8	i	37/38 (97%)	-0.05	5 (13%) 3 2	55, 64, 116, 133	0
9	J	38/39 (97%)	-0.18	3 (7%) 12 14	49, 67, 117, 155	0
9	j	39/39 (100%)	0.26	6 (15%) 2 2	57, 76, 132, 157	0
10	K	37/37 (100%)	-0.57	2 (5%) 25 28	56, 67, 86, 103	0
10	k	37/37 (100%)	-0.52	0 100 100	64, 75, 99, 111	0
11	L	36/37 (97%)	-0.38	4 (11%) 5 5	37, 44, 109, 130	0
11	l	36/37 (97%)	-0.46	2 (5%) 24 26	41, 47, 108, 119	0
12	M	32/36 (88%)	-0.75	1 (3%) 49 52	42, 47, 78, 123	0
12	m	33/36 (91%)	-0.48	2 (6%) 21 23	41, 48, 70, 137	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	-0.09	18 (7%) 14 15	41, 65, 118, 161	0
13	o	243/244 (99%)	-0.01	22 (9%) 9 10	42, 69, 122, 155	0
14	T	29/32 (90%)	-0.72	2 (6%) 16 18	42, 47, 79, 100	0
14	t	29/32 (90%)	-0.68	1 (3%) 45 47	43, 49, 78, 107	0
15	U	96/104 (92%)	-0.42	1 (1%) 82 84	46, 57, 88, 100	0
15	u	97/104 (93%)	-0.40	2 (2%) 63 66	51, 61, 80, 124	0
16	V	137/137 (100%)	-0.57	1 (0%) 87 88	45, 56, 83, 107	0
16	v	137/137 (100%)	-0.17	6 (4%) 34 37	52, 71, 101, 132	0
17	X	38/40 (95%)	-0.37	2 (5%) 26 29	62, 73, 93, 114	0
17	x	38/40 (95%)	0.05	4 (10%) 6 6	67, 80, 123, 152	0
18	Y	29/30 (96%)	0.92	7 (24%) 0 0	68, 83, 122, 124	0
18	y	29/30 (96%)	0.37	4 (13%) 2 2	74, 91, 113, 115	0
19	Z	62/62 (100%)	0.10	8 (12%) 3 3	67, 80, 132, 148	0
19	z	62/62 (100%)	0.49	12 (19%) 1 1	81, 95, 140, 165	0
20	R	34/34 (100%)	2.31	20 (58%) 0 0	87, 114, 135, 147	0
All	All	5283/5384 (98%)	-0.42	245 (4%) 32 35	37, 59, 102, 165	3 (0%)

The worst 5 of 245 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	8.9
5	E	84	LYS	8.7
13	O	60	ARG	7.9
3	c	20	SER	7.6
1	a	11	ALA	7.6

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	FME	i	1	10/11	0.92	0.16	59,70,80,86	0
14	FME	T	1	10/11	0.96	0.09	42,50,63,69	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.97	0.13	46,58,100,100	0
14	FME	t	1	10/11	0.97	0.08	42,47,56,74	0
12	FME	m	1	10/11	0.98	0.14	52,61,91,116	0
8	FME	I	1	10/11	0.98	0.07	61,69,83,84	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
30	UNL	b	626	33/-	0.40	0.40	67,95,148,162	0
30	UNL	I	102	40/-	0.47	0.33	75,100,151,158	0
30	UNL	B	627	33/-	0.47	0.35	53,105,143,149	0
32	LMT	M	103	35/35	0.50	0.30	64,121,173,173	0
32	LMT	b	621	25/35	0.53	0.30	80,106,154,170	0
30	UNL	i	101	40/-	0.57	0.32	74,103,146,164	0
33	LMG	C	521	51/55	0.57	0.32	59,112,155,180	0
32	LMT	M	101	35/35	0.63	0.26	58,103,129,138	0
27	GOL	a	701	6/6	0.63	0.45	76,98,100,110	0
32	LMT	E	102	35/35	0.64	0.52	91,128,168,171	0
32	LMT	a	414	35/35	0.64	0.34	63,118,143,159	0
30	UNL	x	101	18/-	0.65	0.26	70,76,127,129	0
32	LMT	t	101	25/35	0.67	0.24	58,84,141,151	0
30	UNL	j	101	10/-	0.67	0.23	75,87,105,106	0
33	LMG	Z	101	37/55	0.67	0.30	68,117,149,168	0
30	UNL	c	525[B]	32/-	0.68	0.41	86,103,117,128	32
33	LMG	c	521	51/55	0.68	0.29	77,128,157,190	0
30	UNL	c	525[A]	32/-	0.68	0.41	86,103,117,128	32
34	HTG	D	414	16/19	0.68	0.28	89,105,139,149	0
32	LMT	m	103	35/35	0.69	0.26	61,93,108,119	0
30	UNL	K	101[B]	34/-	0.70	0.38	77,99,112,119	34
30	UNL	K	101[A]	34/-	0.70	0.38	77,99,112,119	34
37	LHG	e	101[A]	42/49	0.70	0.40	87,125,143,156	42
37	LHG	e	101[B]	42/49	0.70	0.40	87,125,143,157	42

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
32	LMT	e	102	35/35	0.71	0.55	105,142,178,187	0
32	LMT	D	404	35/35	0.71	0.27	66,111,146,151	0
32	LMT	A	359	35/35	0.71	0.32	58,115,139,142	0
27	GOL	O	501	6/6	0.72	0.24	77,92,105,105	0
30	UNL	A	415	28/-	0.72	0.38	80,104,125,143	0
32	LMT	b	627	25/35	0.74	0.23	54,96,143,150	0
30	UNL	d	410	36/-	0.74	0.19	65,96,126,137	0
27	GOL	o	501	6/6	0.75	0.28	87,100,112,126	0
32	LMT	I	101	35/35	0.75	0.38	89,124,145,158	0
34	HTG	b	623	19/19	0.76	0.49	85,131,161,163	0
32	LMT	a	420	35/35	0.76	0.42	102,128,153,158	0
30	UNL	a	417	30/-	0.76	0.37	85,108,137,149	0
30	UNL	m	102	10/-	0.77	0.30	68,73,88,96	0
34	HTG	C	522	19/19	0.77	0.35	98,125,139,139	0
40	HEC	V	202	43/43	0.77	0.19	36,52,73,160	0
30	UNL	X	101	18/-	0.78	0.20	56,71,105,107	0
33	LMG	z	101	39/55	0.78	0.26	74,123,146,161	0
27	GOL	B	901	6/6	0.80	0.27	63,92,105,111	0
26	SQD	f	102	43/54	0.80	0.34	96,127,172,187	0
30	UNL	J	101	10/-	0.81	0.15	70,81,89,93	0
37	LHG	E	101[A]	42/49	0.81	0.26	71,98,113,121	42
37	LHG	E	101[B]	42/49	0.81	0.26	71,98,113,121	42
26	SQD	b	620	54/54	0.81	0.18	59,92,120,132	0
27	GOL	b	624	6/6	0.81	0.19	87,95,105,108	0
27	GOL	A	411	6/6	0.81	0.18	63,80,84,85	0
32	LMT	t	102	26/35	0.82	0.18	68,101,136,149	0
30	UNL	M	102	10/-	0.82	0.23	65,74,86,91	0
34	HTG	d	411	16/19	0.82	0.28	88,119,142,147	0
30	UNL	D	413	40/-	0.82	0.18	64,84,131,145	0
33	LMG	a	419	51/55	0.83	0.17	67,94,110,121	0
34	HTG	c	522	19/19	0.83	0.29	101,122,142,144	0
27	GOL	o	601	6/6	0.83	0.20	79,90,95,95	0
26	SQD	B	620	54/54	0.83	0.15	60,89,130,150	0
26	SQD	a	413	54/54	0.84	0.19	66,92,138,151	0
27	GOL	c	743	6/6	0.84	0.21	99,103,109,114	0
27	GOL	a	801	6/6	0.84	0.39	52,76,81,87	0
36	CA	f	103	1/1	0.85	0.09	124,124,124,124	0
27	GOL	d	801[B]	6/6	0.85	0.72	62,95,101,101	6
26	SQD	A	412	54/54	0.85	0.18	61,86,126,153	0
33	LMG	C	501	51/55	0.85	0.16	64,89,115,129	0
27	GOL	d	801[A]	6/6	0.85	0.72	63,95,101,101	6
34	HTG	B	623	19/19	0.85	0.23	64,98,120,127	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
27	GOL	O	601	6/6	0.86	0.25	74,91,94,104	0
29	PL9	A	414[A]	55/55	0.87	0.18	62,86,100,105	55
29	PL9	A	414[B]	55/55	0.87	0.18	62,86,100,105	55
23	CLA	b	601	65/65	0.87	0.16	64,87,123,160	0
33	LMG	d	412	51/55	0.87	0.19	53,73,117,144	0
27	GOL	v	401[A]	6/6	0.87	0.18	64,80,82,84	6
27	GOL	v	401[B]	6/6	0.87	0.18	64,80,82,84	6
23	CLA	b	616	65/65	0.88	0.16	48,63,124,134	0
27	GOL	d	701	6/6	0.88	0.25	49,68,78,91	0
29	PL9	a	416[A]	55/55	0.88	0.18	76,95,109,113	55
29	PL9	a	416[B]	55/55	0.88	0.18	76,95,109,113	55
34	HTG	b	622	19/19	0.88	0.15	59,85,118,122	0
25	BCR	C	515	40/40	0.88	0.14	53,77,89,90	0
25	BCR	h	101	40/40	0.88	0.16	59,73,94,96	0
27	GOL	V	401[B]	6/6	0.89	0.15	59,67,73,77	6
23	CLA	d	403	65/65	0.89	0.15	50,68,116,148	0
33	LMG	D	415	51/55	0.89	0.17	49,66,117,139	0
23	CLA	c	514	65/65	0.89	0.16	69,95,119,147	0
27	GOL	V	401[A]	6/6	0.89	0.15	59,67,73,76	6
36	CA	F	102	1/1	0.89	0.22	124,124,124,124	0
23	CLA	B	601	65/65	0.90	0.14	55,79,111,156	0
23	CLA	C	514	65/65	0.90	0.14	62,88,111,123	0
33	LMG	c	520	51/55	0.90	0.18	59,90,130,156	0
25	BCR	K	102	40/40	0.91	0.17	57,66,83,86	0
34	HTG	B	622	19/19	0.91	0.14	63,81,124,126	0
27	GOL	a	412	6/6	0.91	0.24	75,77,87,92	0
36	CA	o	301	1/1	0.91	0.06	116,116,116,116	0
25	BCR	d	404	40/40	0.91	0.12	48,65,105,108	0
23	CLA	c	513	65/65	0.91	0.17	59,82,121,133	0
33	LMG	B	621	51/55	0.91	0.13	47,68,91,111	0
27	GOL	A	701	6/6	0.91	0.32	49,73,80,83	0
33	LMG	C	520	51/55	0.91	0.16	54,84,115,125	0
35	DGD	c	518[A]	62/66	0.92	0.13	54,67,113,129	62
35	DGD	c	518[B]	62/66	0.92	0.13	54,67,113,129	62
23	CLA	B	606	65/65	0.92	0.14	41,55,101,128	0
30	UNL	d	409	17/-	0.92	0.13	64,79,116,123	0
23	CLA	B	616	65/65	0.92	0.17	41,58,131,139	0
23	CLA	C	507	65/65	0.92	0.14	54,70,121,141	0
30	UNL	D	412	17/-	0.92	0.14	58,77,99,114	0
23	CLA	C	513	65/65	0.92	0.15	59,78,111,125	0
26	SQD	F	101	43/54	0.92	0.17	69,103,128,137	0
25	BCR	Y	101	40/40	0.92	0.12	52,64,83,87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	606	65/65	0.93	0.13	44,61,120,133	0
35	DGD	C	518[A]	62/66	0.93	0.12	48,63,108,112	62
35	DGD	C	518[B]	62/66	0.93	0.12	48,63,108,112	62
35	DGD	C	519	62/66	0.93	0.11	42,58,93,111	0
25	BCR	c	515	40/40	0.93	0.11	69,84,96,97	0
33	LMG	m	101	51/55	0.93	0.11	47,73,96,109	0
35	DGD	c	519	62/66	0.93	0.12	49,64,99,125	0
35	DGD	h	102	62/66	0.93	0.12	51,66,81,95	0
25	BCR	k	101	40/40	0.94	0.15	60,73,90,92	0
25	BCR	D	407	40/40	0.94	0.10	43,58,100,103	0
34	HTG	V	203	11/19	0.94	0.44	80,115,125,142	0
23	CLA	c	507	65/65	0.94	0.12	51,68,125,135	0
27	GOL	D	701	6/6	0.94	0.17	45,60,70,92	0
34	HTG	b	625	19/19	0.94	0.10	62,76,93,109	0
23	CLA	a	409	65/65	0.94	0.17	44,57,138,156	0
23	CLA	B	609	65/65	0.94	0.16	50,59,72,83	0
23	CLA	C	509	65/65	0.94	0.10	47,56,116,149	0
23	CLA	D	406	65/65	0.94	0.13	46,59,123,146	0
34	HTG	B	626	19/19	0.94	0.10	67,81,97,106	0
35	DGD	H	102	62/66	0.94	0.11	42,61,79,101	0
23	CLA	a	407[B]	65/65	0.95	0.10	38,51,119,128	65
25	BCR	b	618	40/40	0.95	0.09	44,58,75,87	0
23	CLA	c	512	65/65	0.95	0.11	56,70,89,101	0
23	CLA	C	502	65/65	0.95	0.10	47,61,74,84	0
23	CLA	B	611	65/65	0.95	0.10	34,44,64,73	0
23	CLA	A	408	65/65	0.95	0.12	38,52,127,140	0
25	BCR	y	101	40/40	0.95	0.09	58,70,85,97	0
26	SQD	A	410[A]	54/54	0.95	0.13	57,78,112,116	54
26	SQD	A	410[B]	54/54	0.95	0.13	57,78,112,116	54
25	BCR	A	409	40/40	0.95	0.10	37,50,63,66	0
25	BCR	B	618	40/40	0.95	0.09	40,52,67,75	0
23	CLA	b	609	65/65	0.95	0.15	52,66,84,94	0
25	BCR	C	516	40/40	0.95	0.13	52,66,77,90	0
37	LHG	d	408[A]	49/49	0.95	0.14	50,62,109,125	49
37	LHG	d	408[B]	49/49	0.95	0.14	50,62,109,125	49
23	CLA	b	612	65/65	0.95	0.10	44,53,68,81	0
25	BCR	H	101	40/40	0.95	0.10	52,66,86,89	0
37	LHG	l	101[A]	49/49	0.95	0.13	48,58,72,93	49
37	LHG	l	101[B]	49/49	0.95	0.13	48,57,72,93	49
23	CLA	a	407[A]	65/65	0.95	0.10	38,51,119,128	65
23	CLA	c	502	65/65	0.96	0.11	56,67,80,86	0
23	CLA	c	504	65/65	0.96	0.09	48,70,86,92	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	GOL	b	901	6/6	0.96	0.21	78,79,83,88	0
23	CLA	c	505	65/65	0.96	0.09	50,63,108,146	0
23	CLA	c	506	65/65	0.96	0.10	50,64,92,101	0
26	SQD	a	411[A]	54/54	0.96	0.13	56,80,112,121	54
26	SQD	a	411[B]	54/54	0.96	0.13	56,80,112,121	54
35	DGD	c	517[A]	62/66	0.96	0.11	50,65,99,106	62
35	DGD	c	517[B]	62/66	0.96	0.11	50,65,99,106	62
23	CLA	C	505	65/65	0.96	0.09	40,55,102,129	0
23	CLA	c	508	65/65	0.96	0.10	56,69,85,90	0
25	BCR	a	410	40/40	0.96	0.08	44,54,61,69	0
23	CLA	c	509	65/65	0.96	0.11	46,63,125,155	0
36	CA	C	524	1/1	0.96	0.05	77,77,77,77	0
25	BCR	b	619	40/40	0.96	0.08	51,62,88,91	0
36	CA	O	301	1/1	0.96	0.06	105,105,105,105	0
27	GOL	B	624	6/6	0.96	0.21	65,73,81,84	0
23	CLA	b	602	65/65	0.96	0.14	50,60,82,92	0
37	LHG	D	409[A]	49/49	0.96	0.11	46,61,83,87	49
37	LHG	D	409[B]	49/49	0.96	0.11	46,61,83,87	49
37	LHG	D	411[A]	49/49	0.96	0.14	47,61,105,108	49
37	LHG	D	411[B]	49/49	0.96	0.14	47,60,105,108	49
27	GOL	C	523[A]	6/6	0.96	0.11	58,61,64,67	6
27	GOL	C	523[B]	6/6	0.96	0.11	57,62,65,66	6
37	LHG	d	407[A]	49/49	0.96	0.14	45,55,67,79	49
37	LHG	d	407[B]	49/49	0.96	0.14	45,56,68,79	49
25	BCR	c	516	40/40	0.96	0.12	57,67,80,96	0
23	CLA	C	510	65/65	0.96	0.10	45,58,82,88	0
37	LHG	d	711[A]	49/49	0.96	0.12	46,67,80,89	49
37	LHG	d	711[B]	49/49	0.96	0.12	45,67,80,89	49
23	CLA	C	511	65/65	0.96	0.09	48,57,79,89	0
23	CLA	C	512	65/65	0.96	0.13	51,62,81,87	0
25	BCR	t	103	40/40	0.96	0.08	43,58,77,81	0
23	CLA	b	615	65/65	0.96	0.11	52,62,83,88	0
38	HEM	e	87	43/43	0.96	0.13	63,85,118,137	0
39	MG	j	102	1/1	0.96	0.04	65,65,65,65	0
23	CLA	C	508	65/65	0.96	0.12	50,63,82,93	0
23	CLA	b	610	65/65	0.97	0.09	47,58,69,74	0
23	CLA	b	611	65/65	0.97	0.08	37,48,71,81	0
25	BCR	T	101	40/40	0.97	0.07	43,58,69,69	0
23	CLA	A	406[B]	65/65	0.97	0.09	38,47,110,122	65
23	CLA	b	613	65/65	0.97	0.08	39,50,88,105	0
35	DGD	C	517[A]	62/66	0.97	0.10	44,58,99,101	62
35	DGD	C	517[B]	62/66	0.97	0.10	44,58,99,101	62

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	b	617	40/40	0.97	0.08	45,52,61,70	0
23	CLA	b	614	65/65	0.97	0.08	40,51,102,120	0
23	CLA	B	610	65/65	0.97	0.11	39,54,66,83	0
27	GOL	c	742[A]	6/6	0.97	0.29	64,66,75,76	6
27	GOL	c	742[B]	6/6	0.97	0.29	65,66,75,76	6
23	CLA	A	404[A]	65/65	0.97	0.12	35,41,58,68	65
23	CLA	B	612	65/65	0.97	0.07	34,49,60,66	0
23	CLA	B	613	65/65	0.97	0.08	36,45,98,113	0
23	CLA	B	614	65/65	0.97	0.09	36,48,103,127	0
23	CLA	B	615	65/65	0.97	0.10	42,54,79,90	0
23	CLA	a	405[A]	65/65	0.97	0.12	33,44,60,74	65
23	CLA	a	405[B]	65/65	0.97	0.12	38,44,62,74	65
23	CLA	A	404[B]	65/65	0.97	0.12	35,42,60,68	65
23	CLA	c	510	65/65	0.97	0.10	46,61,90,95	0
23	CLA	c	511	65/65	0.97	0.10	47,63,79,93	0
29	PL9	D	408[A]	55/55	0.97	0.11	37,47,59,70	55
29	PL9	D	408[B]	55/55	0.97	0.11	37,47,59,71	55
23	CLA	B	602	65/65	0.97	0.11	46,58,75,94	0
23	CLA	C	504	65/65	0.97	0.09	48,61,73,79	0
29	PL9	d	405[A]	55/55	0.97	0.10	37,49,61,72	55
29	PL9	d	405[B]	55/55	0.97	0.10	36,49,61,72	55
23	CLA	B	603	65/65	0.97	0.10	40,53,74,81	0
23	CLA	d	402[A]	65/65	0.97	0.10	36,45,72,89	65
23	CLA	d	402[B]	65/65	0.97	0.10	36,45,72,89	65
23	CLA	C	506	65/65	0.97	0.09	45,61,88,104	0
24	PHO	a	353[A]	64/64	0.97	0.11	43,54,61,66	64
24	PHO	a	353[B]	64/64	0.97	0.11	43,54,61,66	64
23	CLA	b	604	65/65	0.97	0.11	41,52,96,119	0
25	BCR	B	617	40/40	0.97	0.09	40,49,62,66	0
23	CLA	b	605	65/65	0.97	0.10	38,50,77,79	0
25	BCR	B	619	40/40	0.97	0.08	48,58,88,99	0
23	CLA	A	406[A]	65/65	0.97	0.09	38,47,110,122	65
23	CLA	b	607	65/65	0.97	0.08	37,46,79,94	0
23	CLA	B	607	65/65	0.97	0.08	36,45,72,86	0
40	HEC	v	202	43/43	0.97	0.12	51,63,70,77	0
23	CLA	C	503	65/65	0.98	0.09	44,54,80,92	0
23	CLA	B	608	65/65	0.98	0.07	37,48,69,74	0
37	LHG	D	410[A]	49/49	0.98	0.13	43,54,67,76	49
37	LHG	D	410[B]	49/49	0.98	0.13	43,54,66,76	49
23	CLA	c	503	65/65	0.98	0.08	44,59,90,102	0
23	CLA	B	604	65/65	0.98	0.08	36,47,112,136	0
24	PHO	A	407[A]	64/64	0.98	0.08	35,45,50,56	64

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	PHO	A	407[B]	64/64	0.98	0.08	35,45,50,56	64
37	LHG	L	101[A]	49/49	0.98	0.11	45,55,66,88	49
37	LHG	L	101[B]	49/49	0.98	0.11	45,55,66,88	49
24	PHO	A	353[A]	64/64	0.98	0.09	38,48,54,62	64
24	PHO	A	353[B]	64/64	0.98	0.09	38,48,54,61	64
24	PHO	a	408[A]	64/64	0.98	0.07	38,47,55,57	64
24	PHO	a	408[B]	64/64	0.98	0.07	38,47,55,57	64
23	CLA	a	406[A]	65/65	0.98	0.07	36,43,59,68	65
23	CLA	b	608	65/65	0.98	0.07	42,54,78,91	0
23	CLA	a	406[B]	65/65	0.98	0.07	36,43,59,68	65
23	CLA	B	605	65/65	0.98	0.11	39,48,67,83	0
23	CLA	A	405[A]	65/65	0.98	0.09	32,42,54,71	65
23	CLA	A	405[B]	65/65	0.98	0.09	33,42,54,71	65
38	HEM	E	103	43/43	0.98	0.10	52,70,83,95	0
23	CLA	D	405[A]	65/65	0.98	0.11	32,43,68,76	65
36	CA	c	523	1/1	0.98	0.06	78,78,78,78	0
23	CLA	D	405[B]	65/65	0.98	0.11	32,43,68,76	65
23	CLA	b	603	65/65	0.98	0.08	43,56,81,93	0
31	BCT	a	404[B]	4/4	0.99	0.06	55,58,67,76	4
22	CL	A	403[A]	1/1	0.99	0.05	46,46,46,46	1
22	CL	A	403[B]	1/1	0.99	0.05	45,45,45,45	1
22	CL	a	402[A]	1/1	0.99	0.05	48,48,48,48	1
22	CL	a	402[B]	1/1	0.99	0.05	48,48,48,48	1
28	OEX	A	413[A]	10/10	0.99	0.04	37,45,50,50	10
36	CA	c	524	1/1	0.99	0.09	78,78,78,78	0
28	OEX	A	413[B]	10/10	0.99	0.04	37,45,49,50	10
28	OEX	a	415[A]	10/10	0.99	0.05	47,49,55,56	10
28	OEX	a	415[B]	10/10	0.99	0.05	47,49,55,56	10
21	FE2	a	401[A]	1/1	0.99	0.04	52,52,52,52	1
21	FE2	a	401[B]	1/1	0.99	0.04	52,52,52,52	1
22	CL	A	402[A]	1/1	0.99	0.02	41,41,41,41	1
22	CL	A	402[B]	1/1	0.99	0.02	41,41,41,41	1
39	MG	J	102	1/1	0.99	0.03	57,57,57,57	0
31	BCT	A	348[A]	4/4	0.99	0.10	51,52,58,68	4
31	BCT	A	348[B]	4/4	0.99	0.10	51,52,58,69	4
31	BCT	a	404[A]	4/4	0.99	0.06	55,58,67,76	4
22	CL	a	403[A]	1/1	1.00	0.02	53,53,53,53	1
22	CL	a	403[B]	1/1	1.00	0.02	53,53,53,53	1
21	FE2	A	401[A]	1/1	1.00	0.05	50,50,50,50	1
21	FE2	A	401[B]	1/1	1.00	0.05	50,50,50,50	1

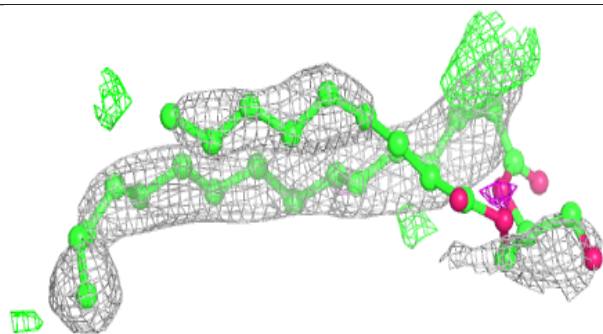
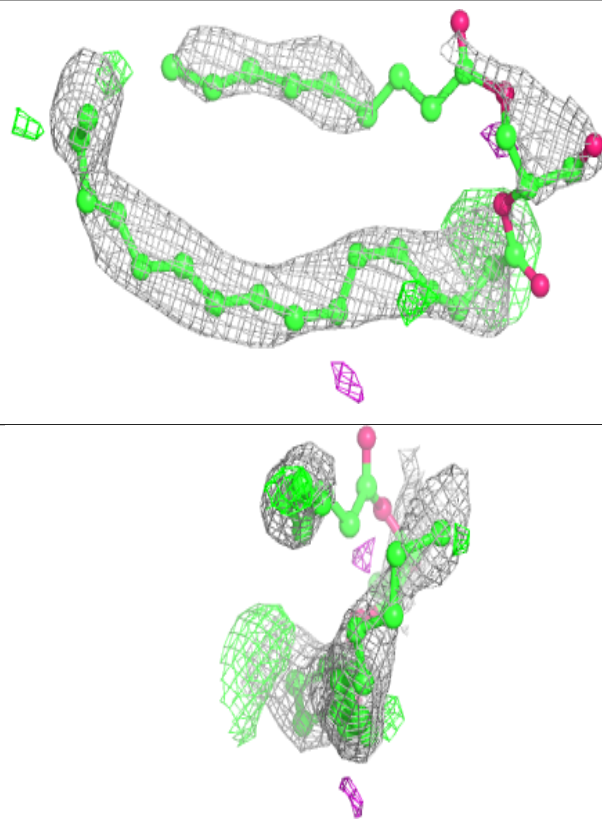
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

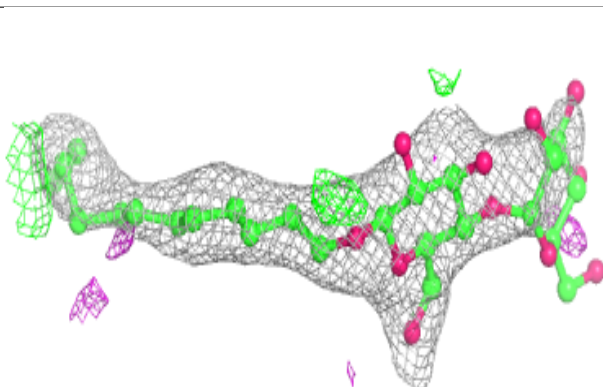
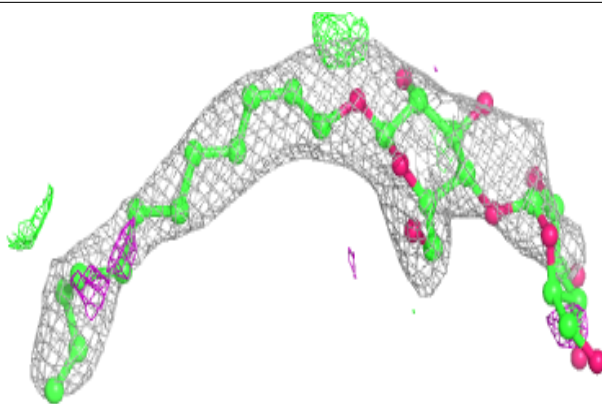
**Electron density around UNL b 626:**

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



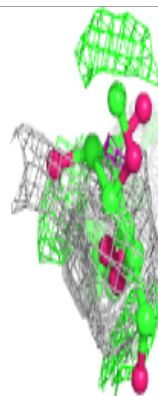
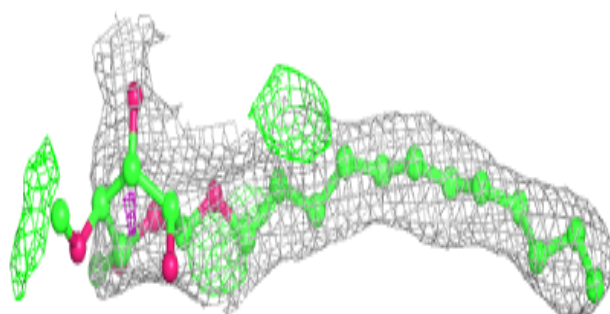
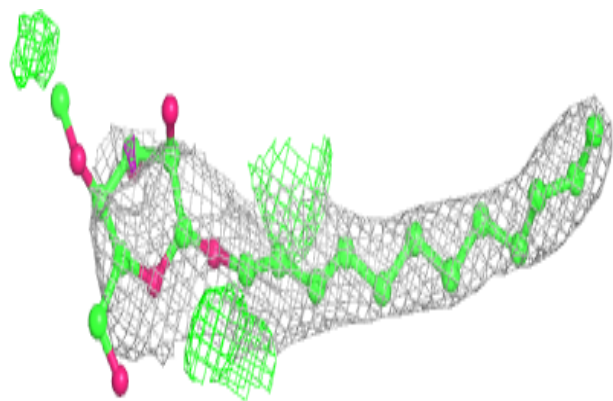
**Electron density around LMT M 103:**

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

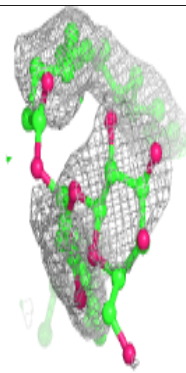
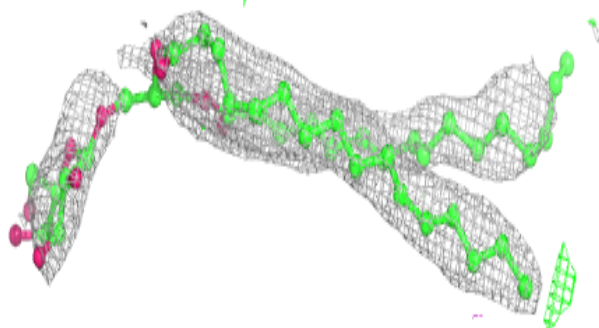
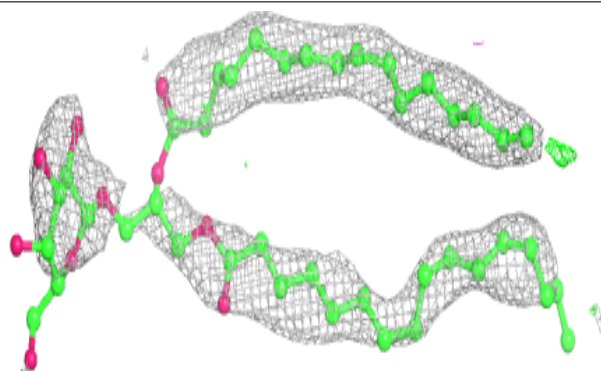


**Electron density around LMT b 621:**

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

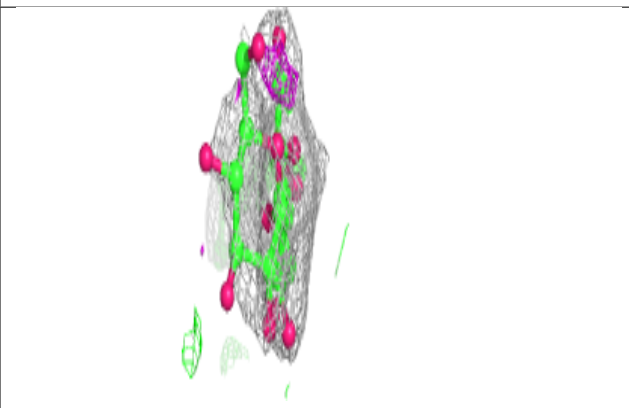
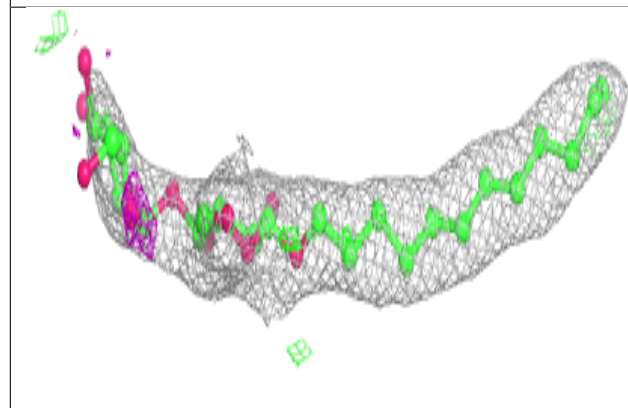
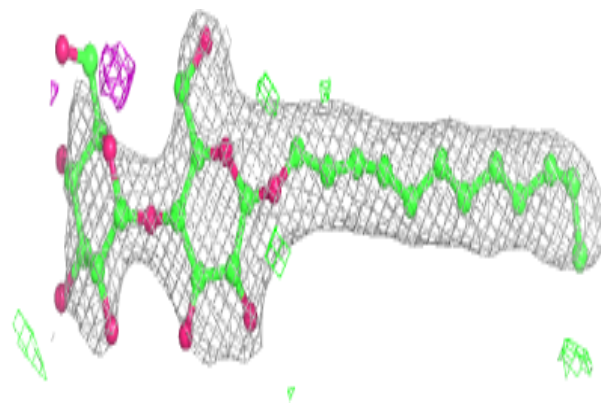
**Electron density around LMG C 521:**

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

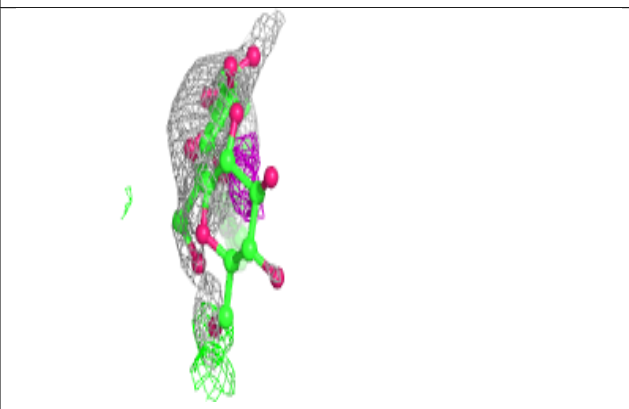
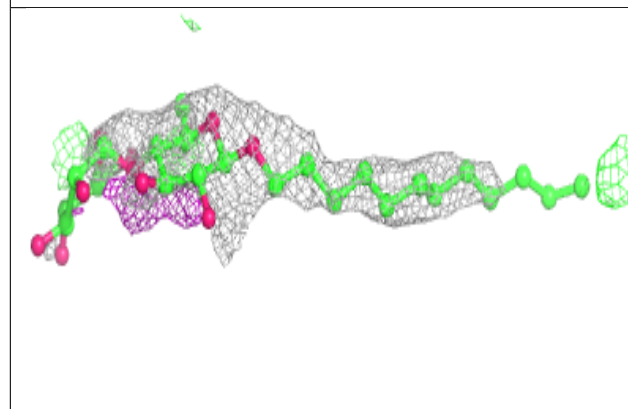
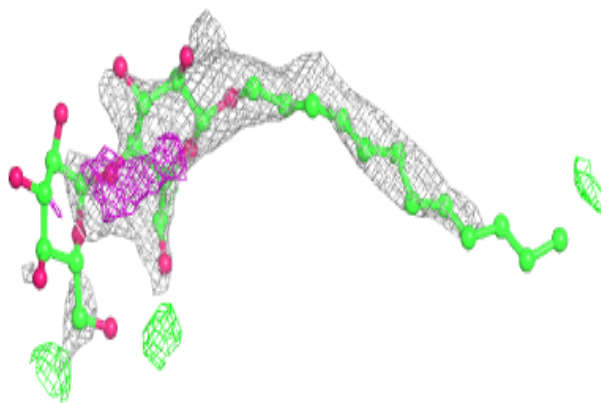


**Electron density around LMT M 101:**

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

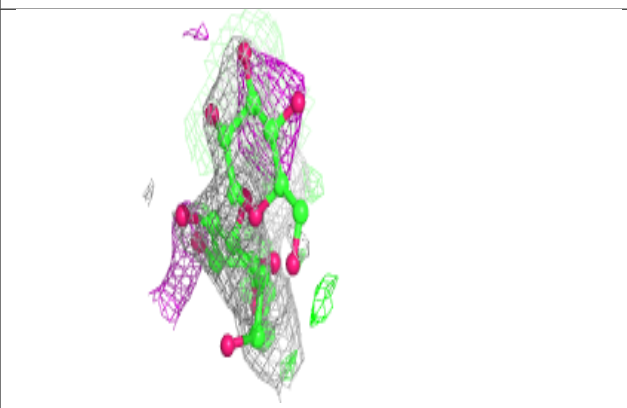
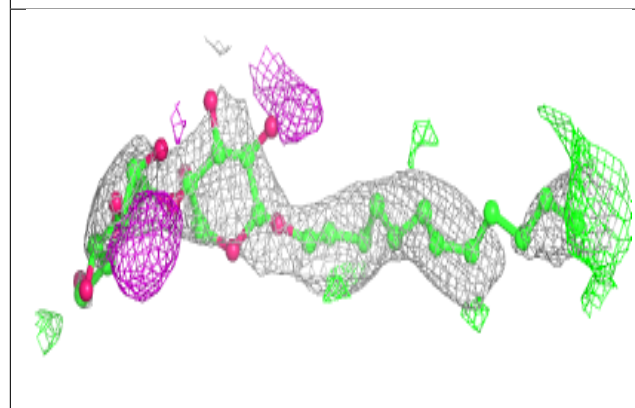
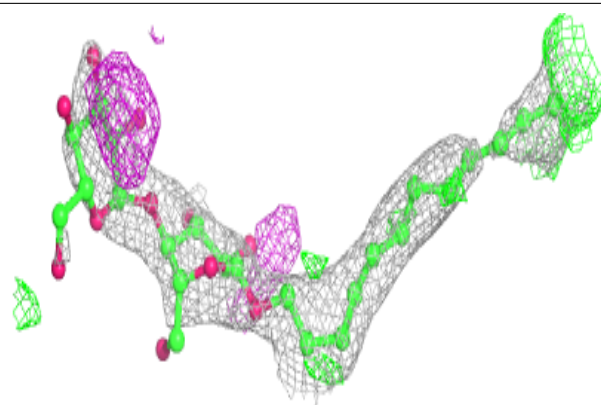
**Electron density around LMT E 102:**

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

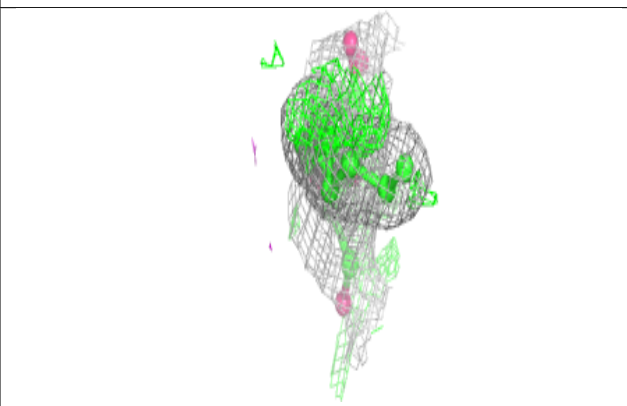
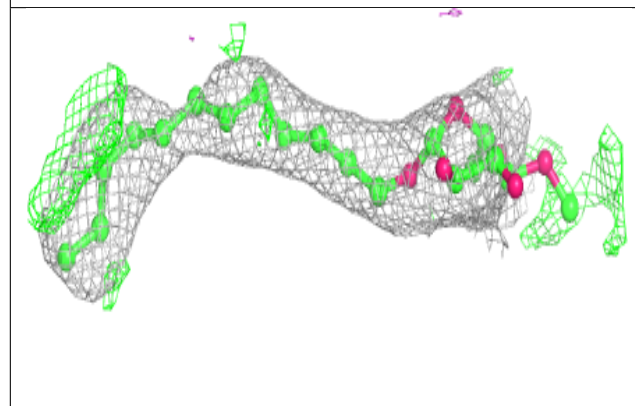
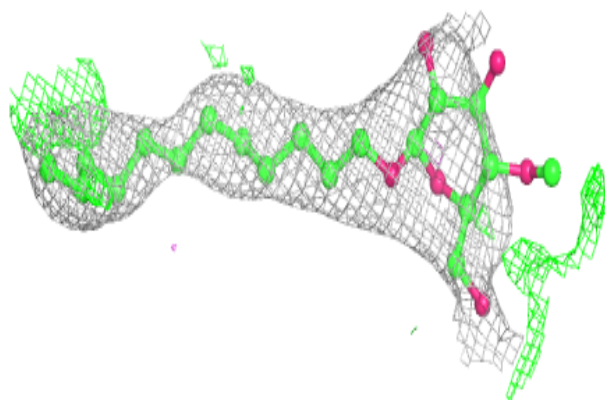


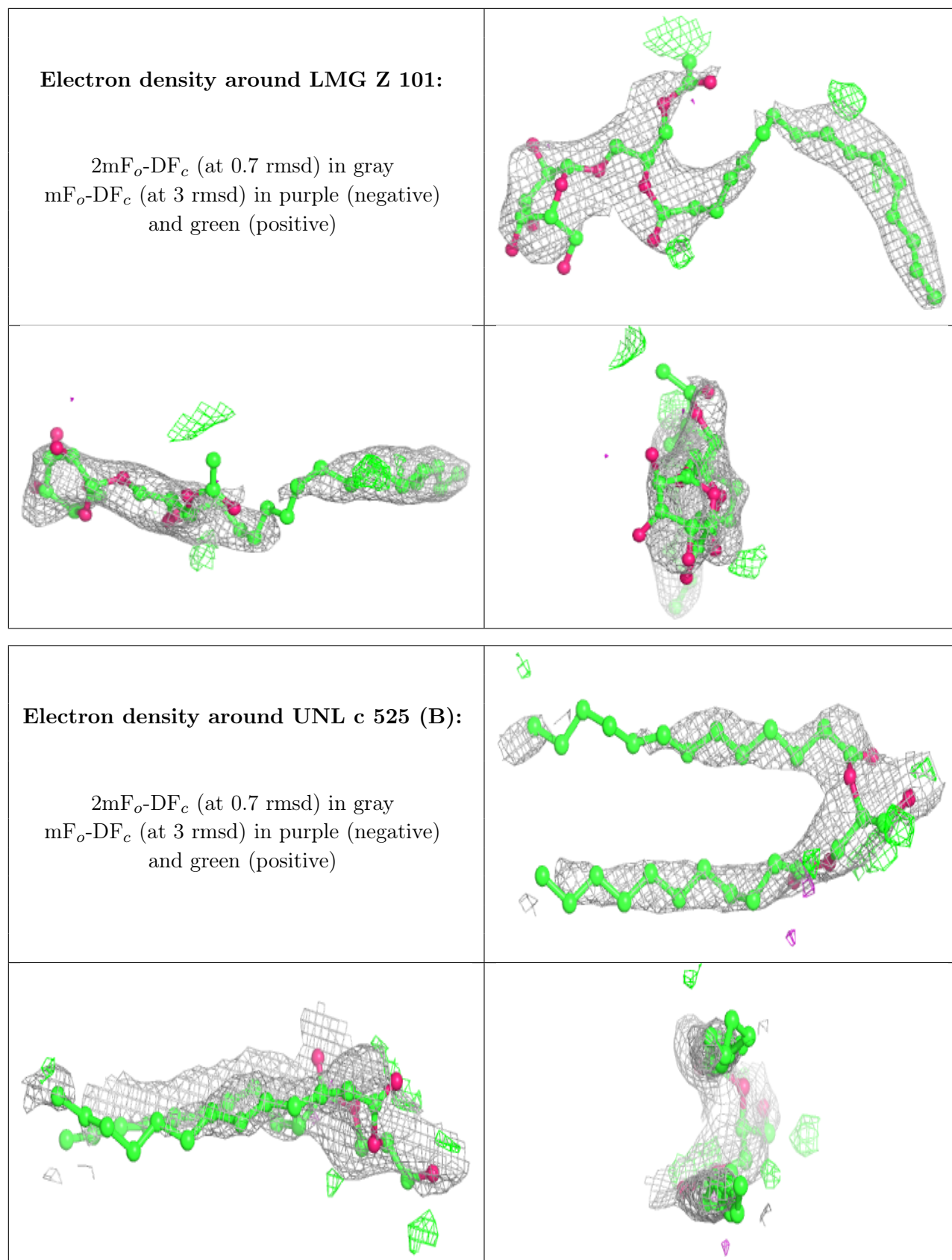
**Electron density around LMT a 414:**

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

**Electron density around LMT t 101:**

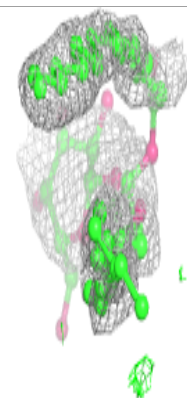
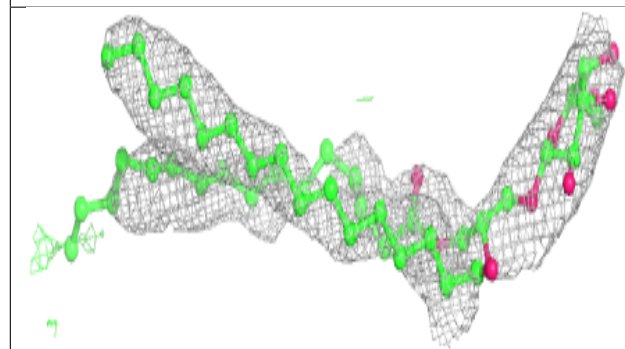
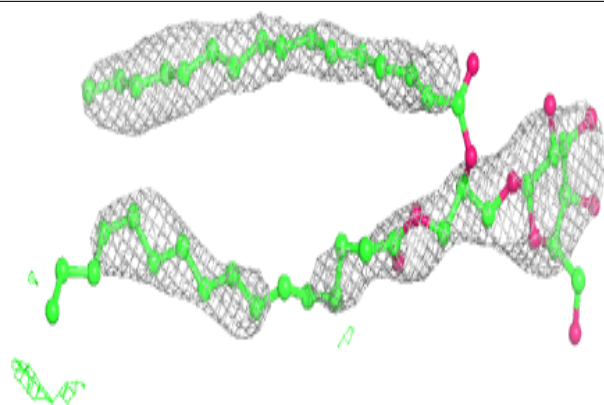
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



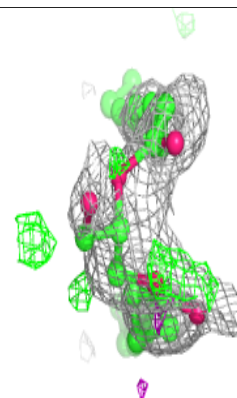
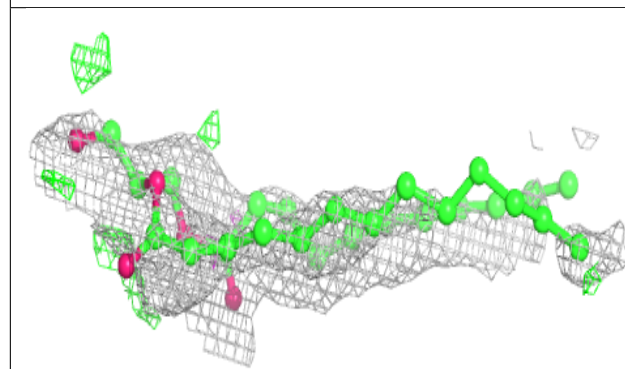
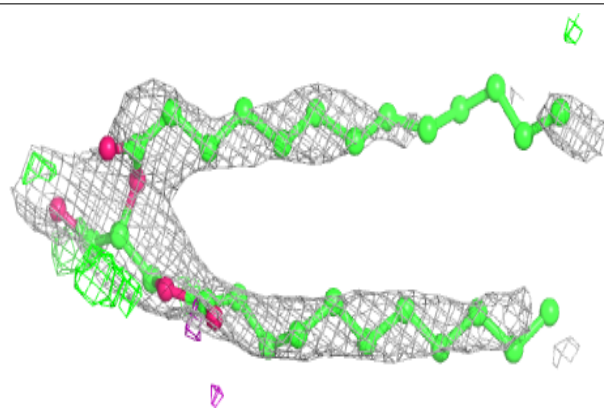


**Electron density around LMG c 521:**

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

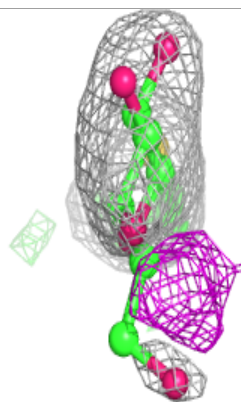
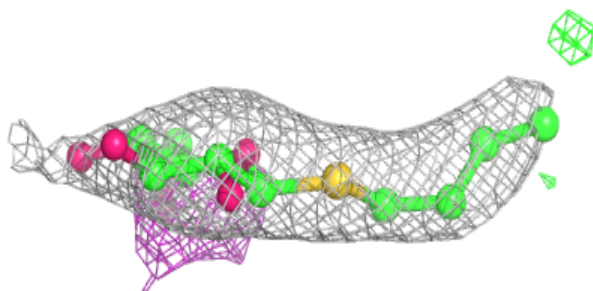
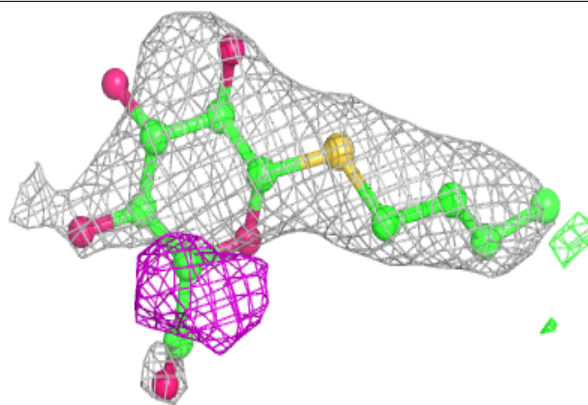
**Electron density around UNL c 525 (A):**

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

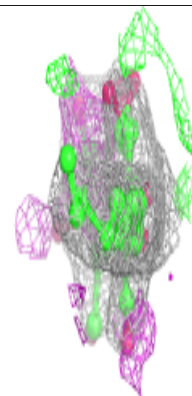
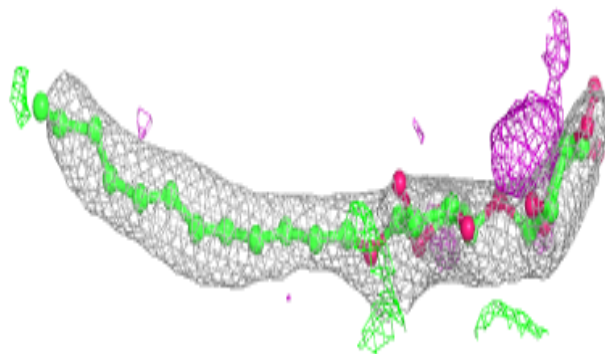
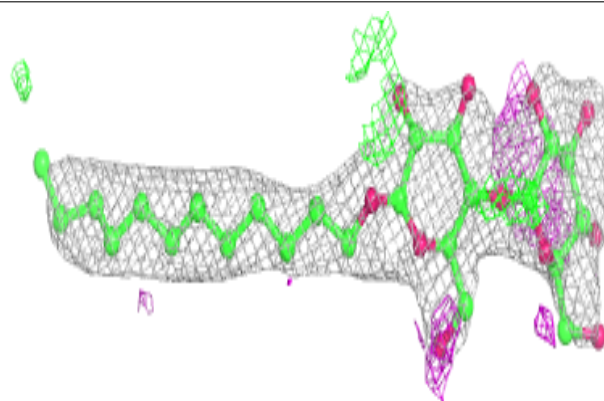


**Electron density around HTG D 414:**

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

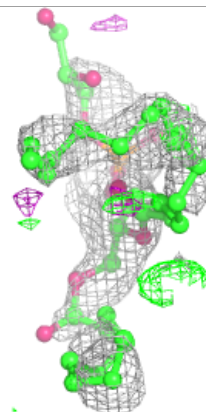
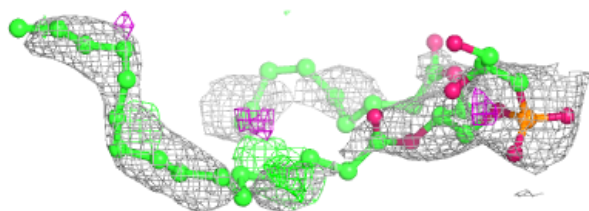
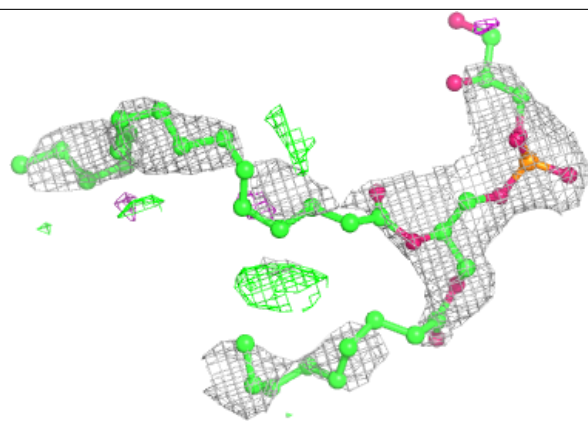
**Electron density around LMT m 103:**

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

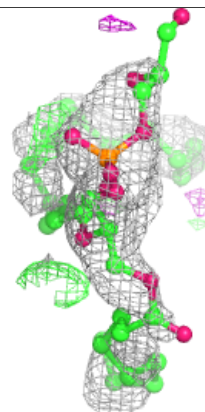
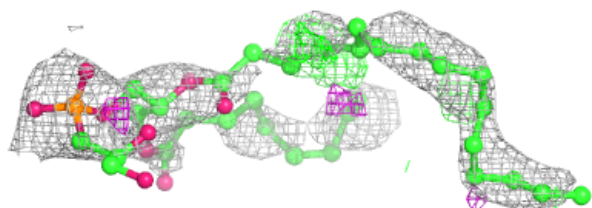
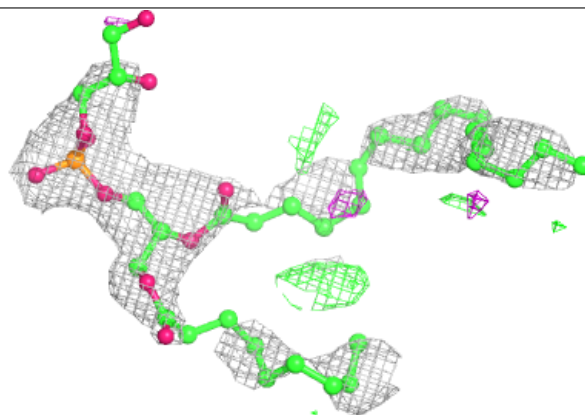


**Electron density around LHG e 101 (A):**

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

**Electron density around LHG e 101 (B):**

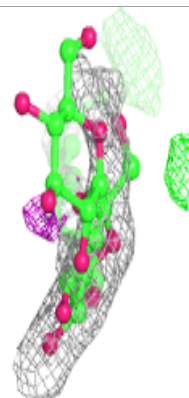
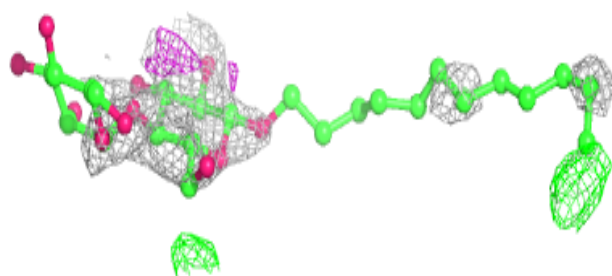
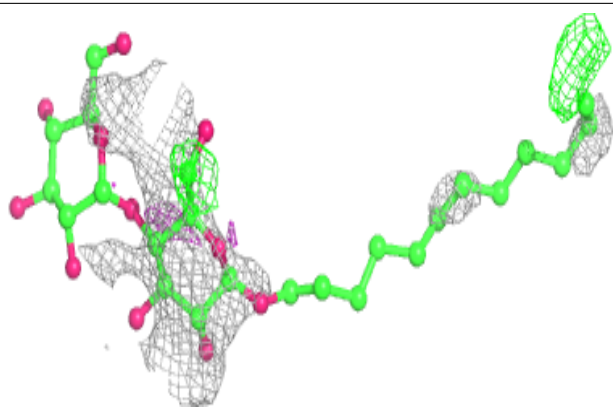
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



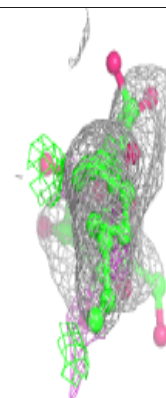
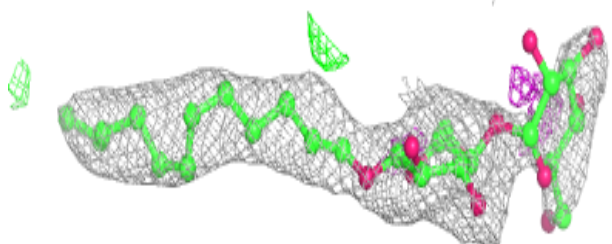
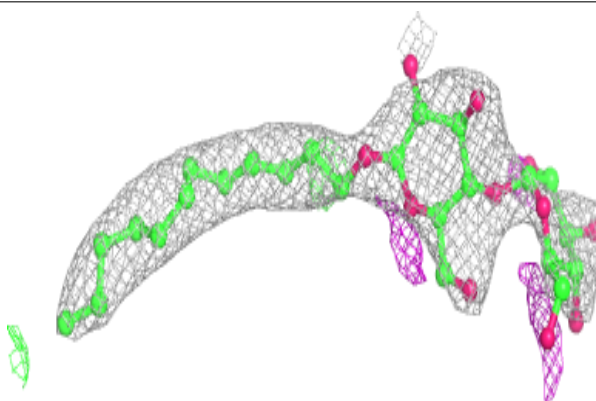


**Electron density around LMT e 102:**

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

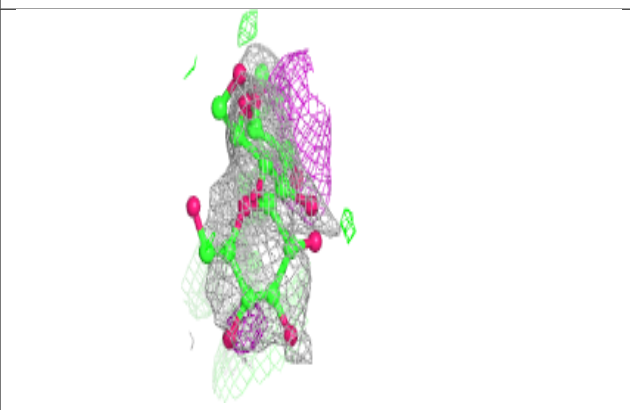
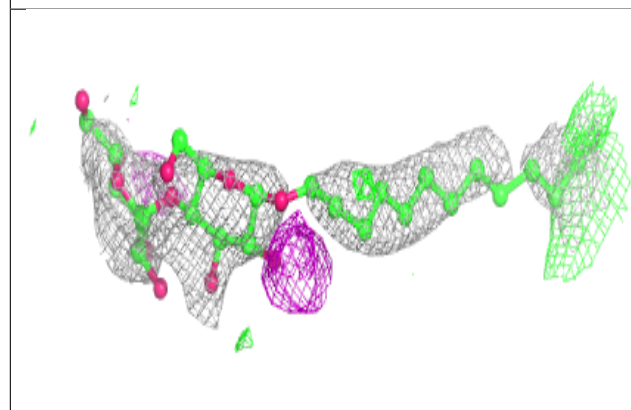
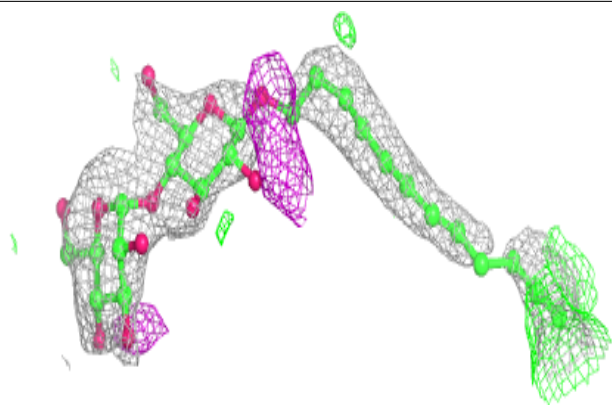
**Electron density around LMT D 404:**

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

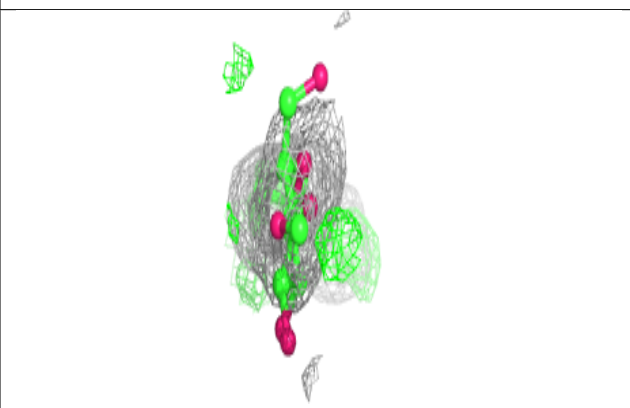
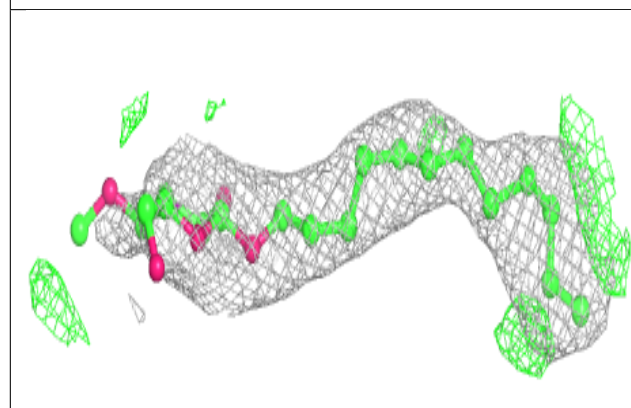
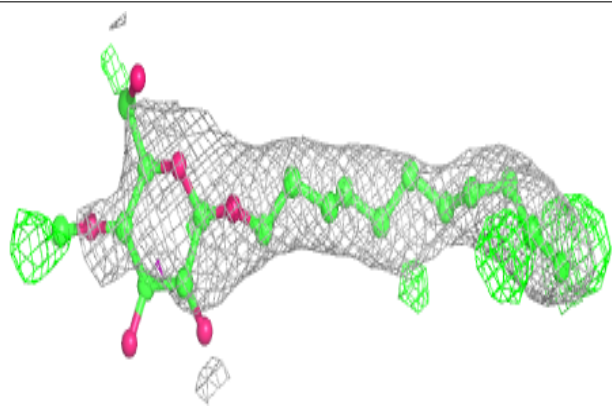


**Electron density around LMT A 359:**

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

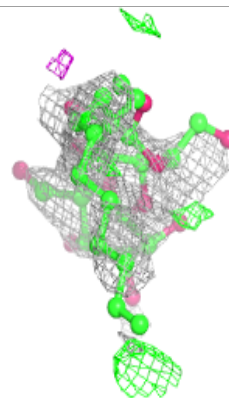
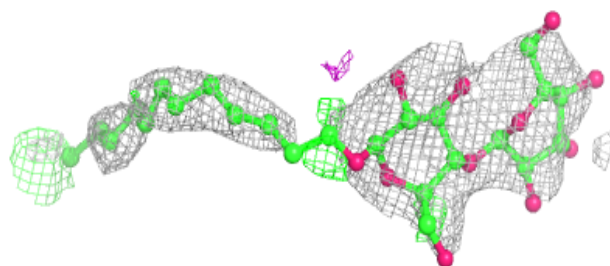
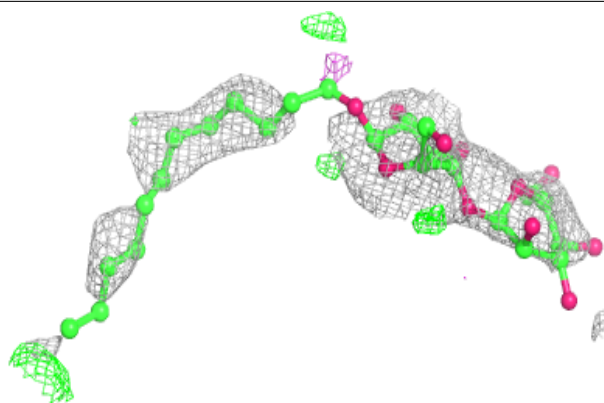
**Electron density around LMT b 627:**

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

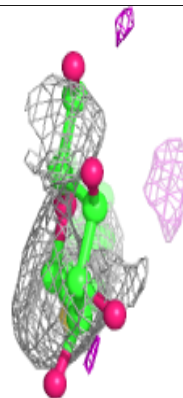
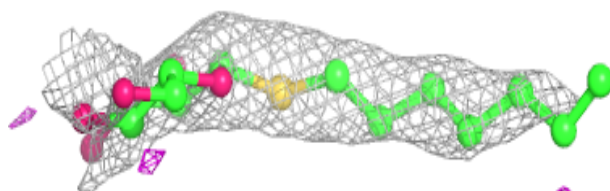
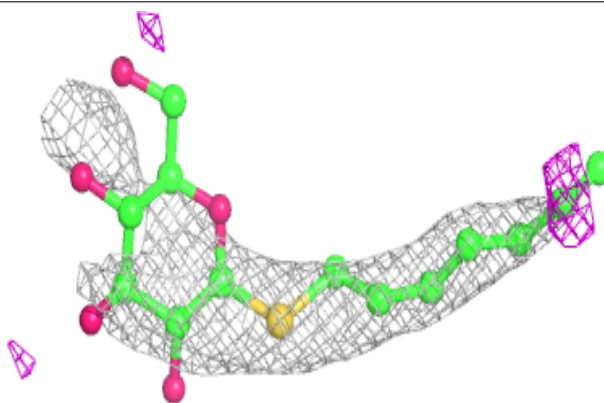


**Electron density around LMT I 101:**

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

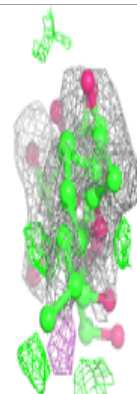
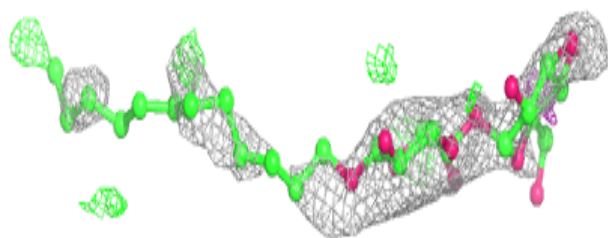
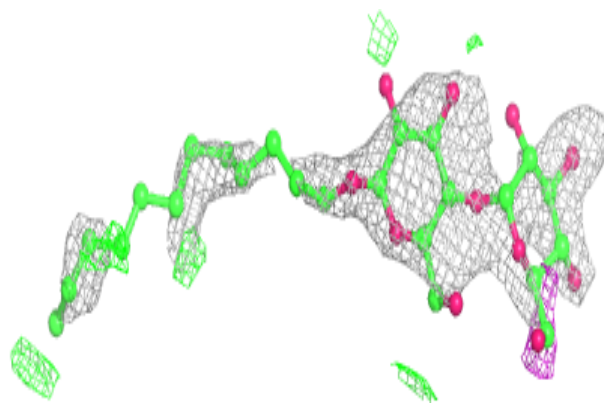
**Electron density around HTG b 623:**

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

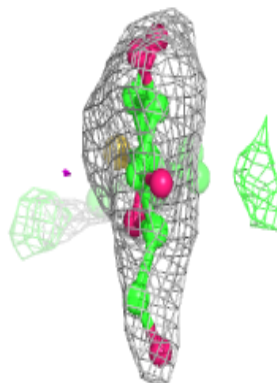
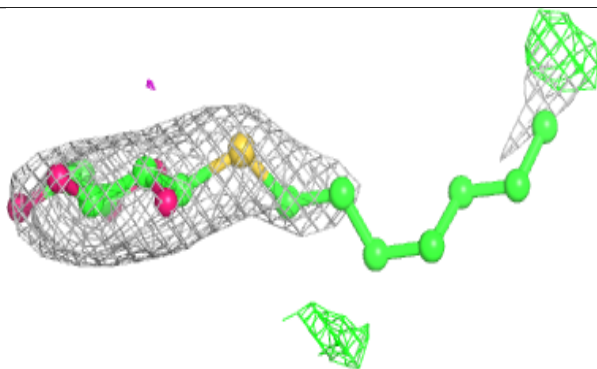
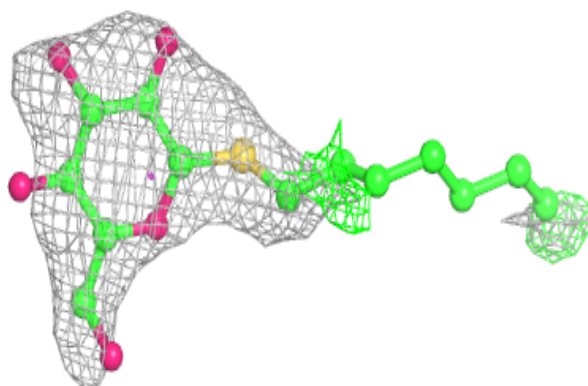


**Electron density around LMT a 420:**

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

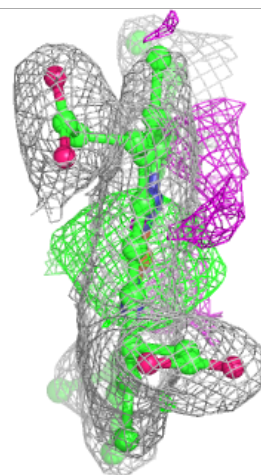
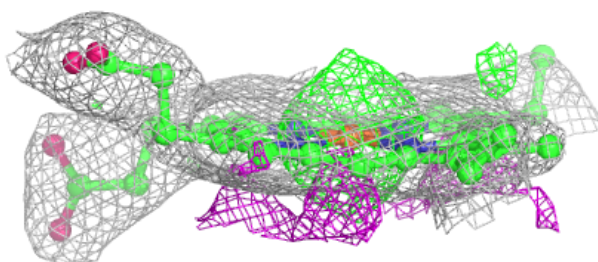
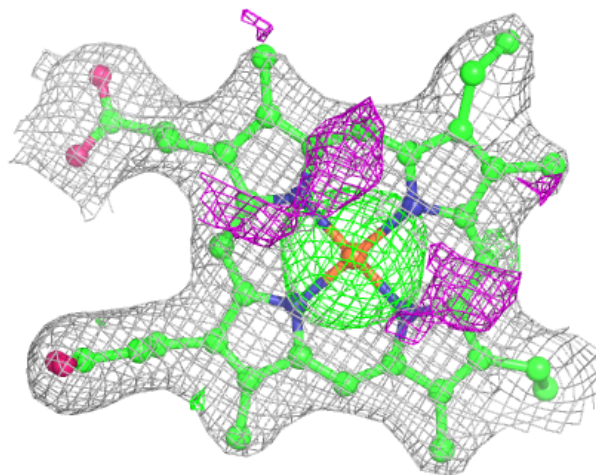
**Electron density around HTG C 522:**

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



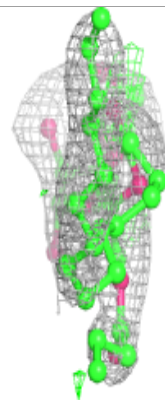
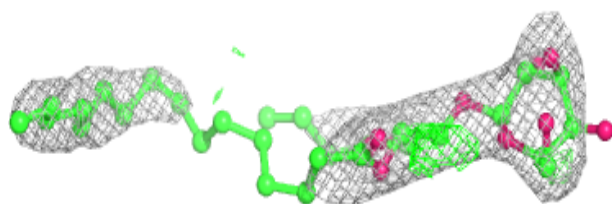
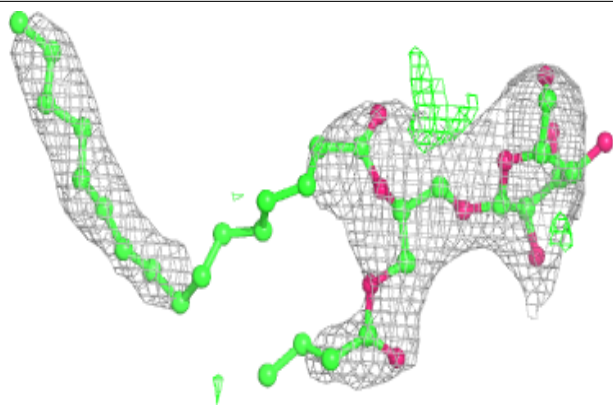
**Electron density around HEC V 202:**

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

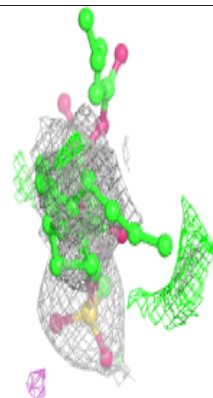
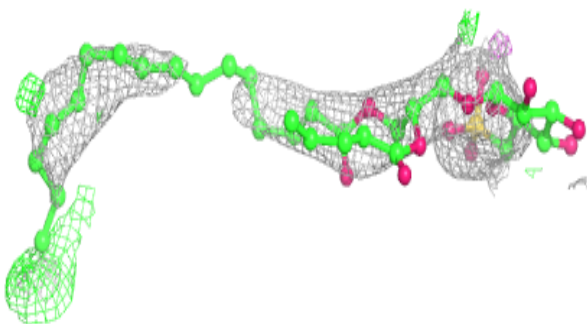
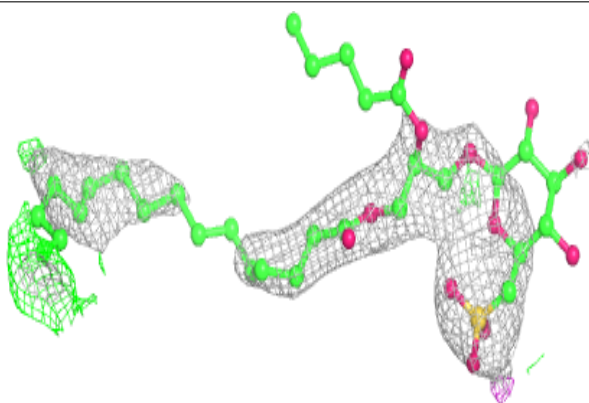


**Electron density around LMG z 101:**

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

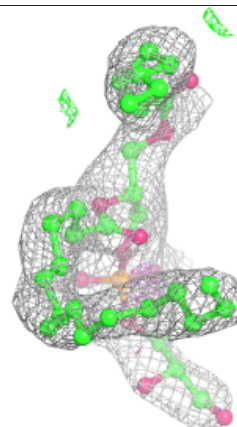
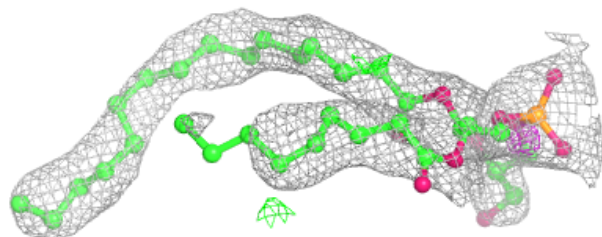
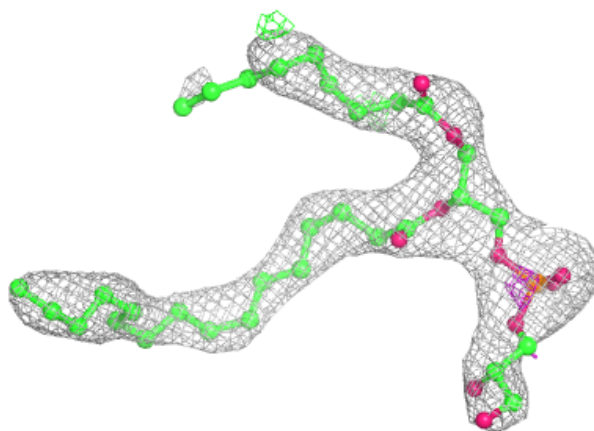
**Electron density around SQD f 102:**

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



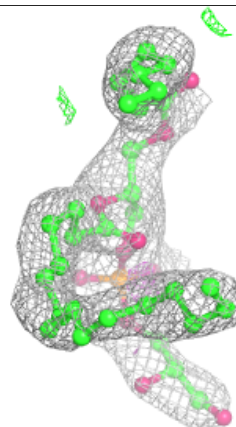
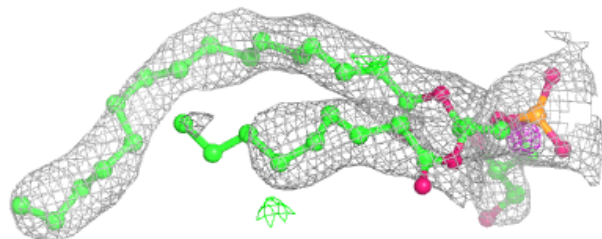
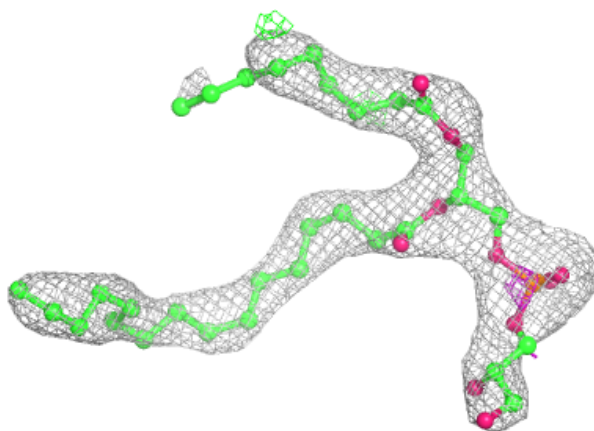
**Electron density around LHG E 101 (A):**

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

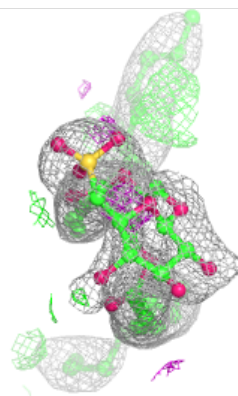
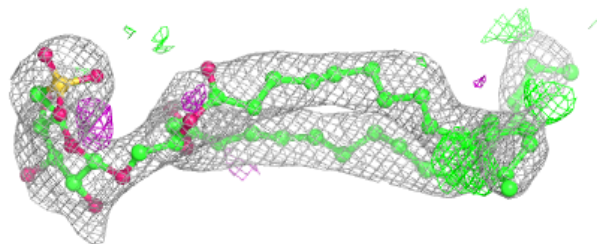
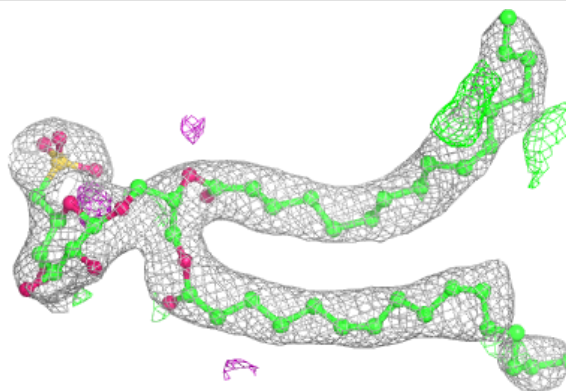


**Electron density around LHG E 101 (B):**

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

**Electron density around SQD b 620:**

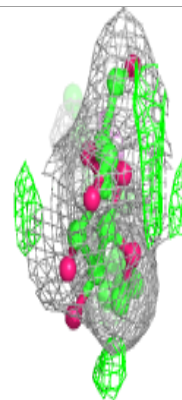
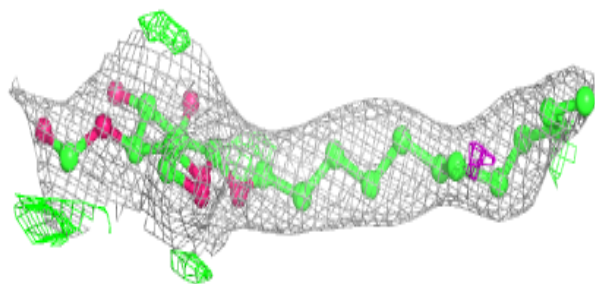
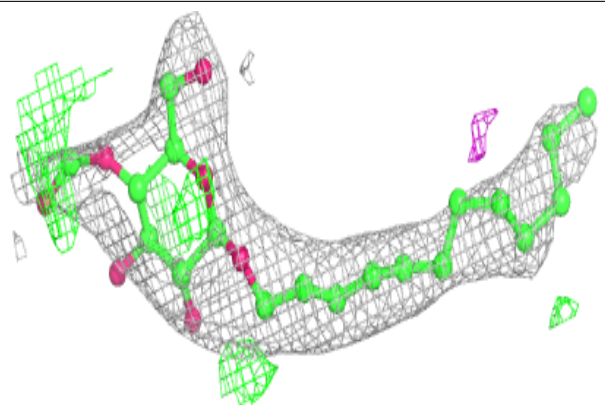
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



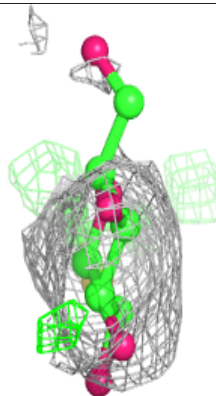
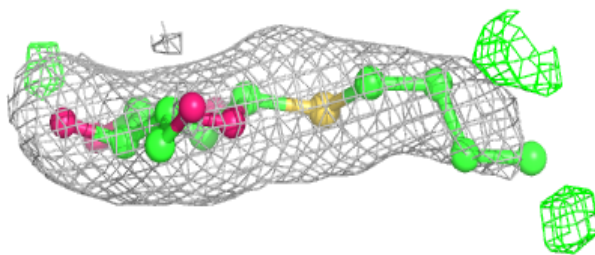
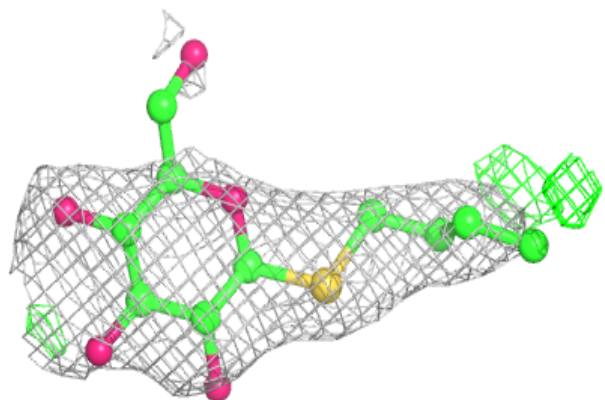


**Electron density around LMT t 102:**

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

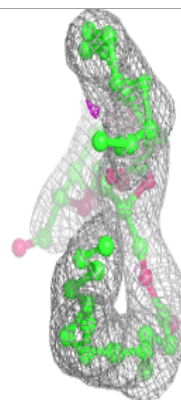
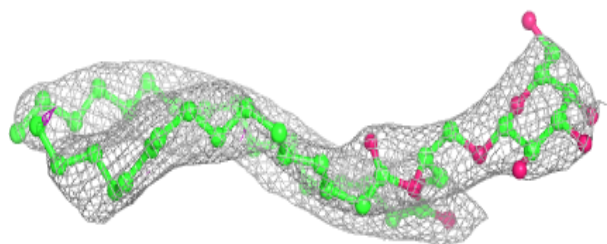
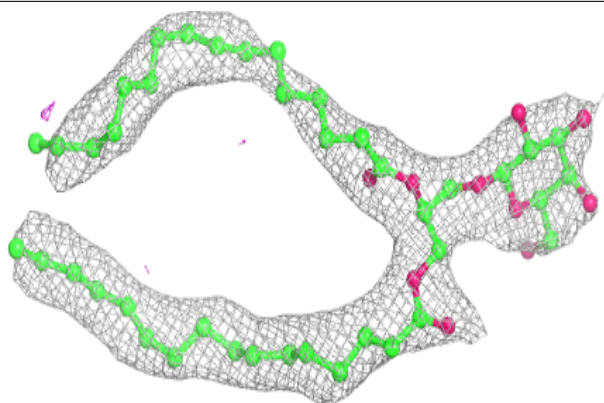
**Electron density around HTG d 411:**

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

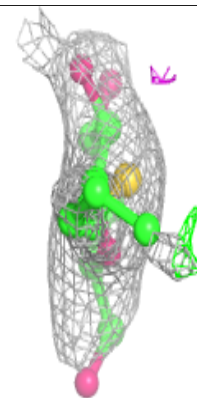
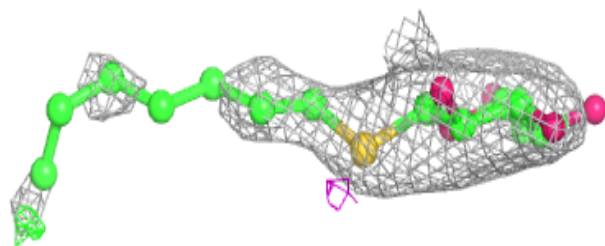
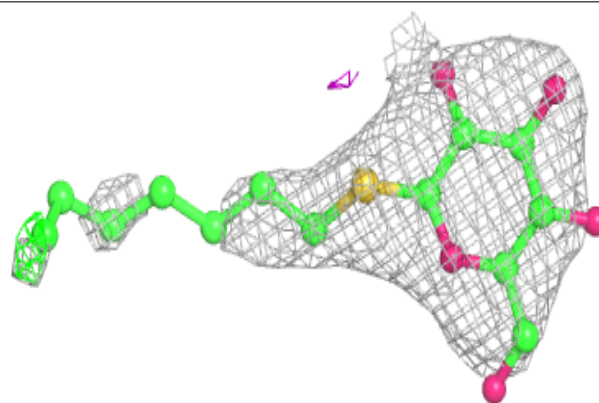


**Electron density around LMG a 419:**

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

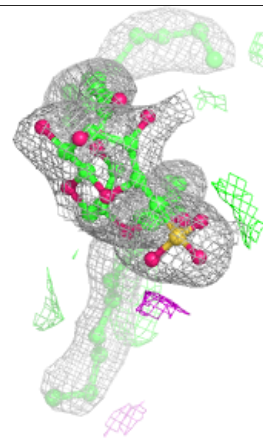
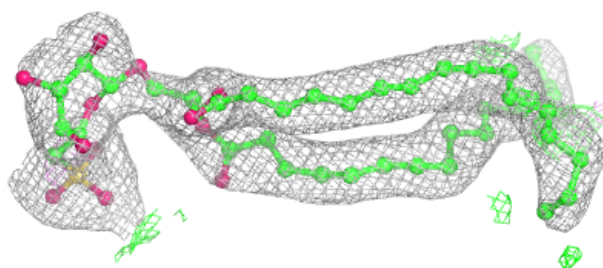
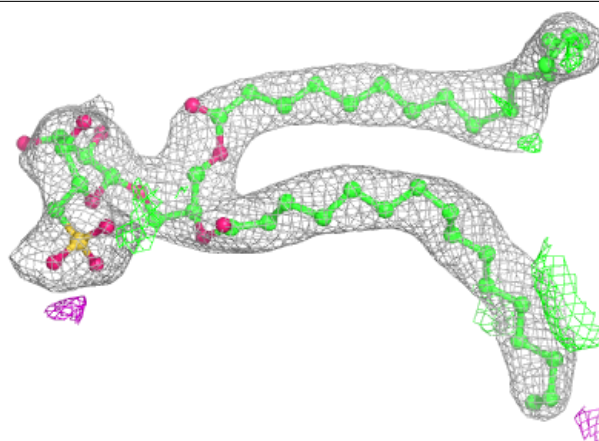
**Electron density around HTG c 522:**

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

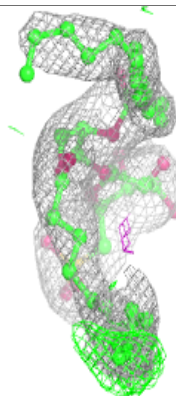
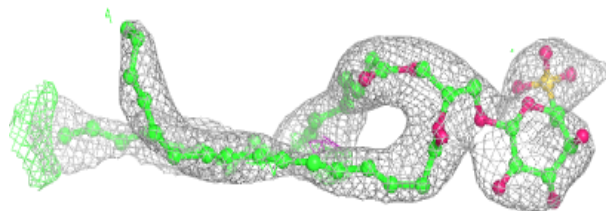
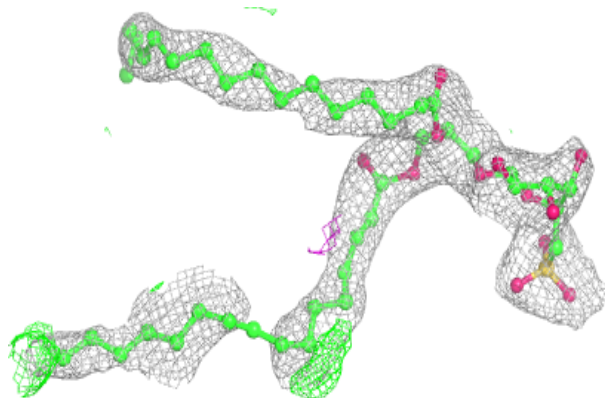


**Electron density around SQD B 620:**

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

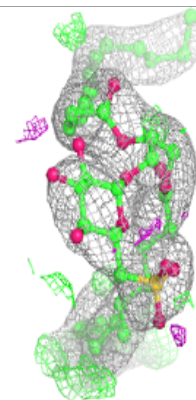
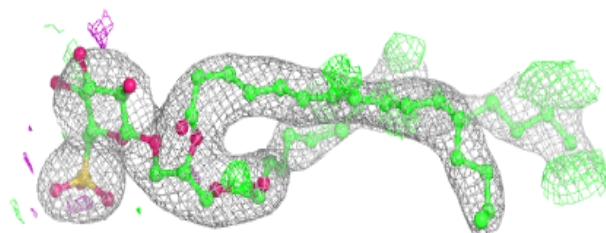
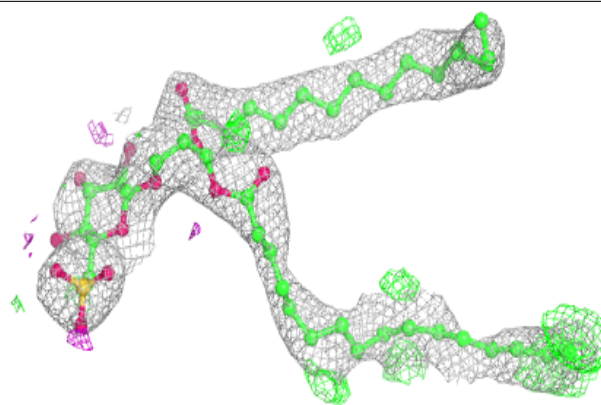
**Electron density around SQD a 413:**

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

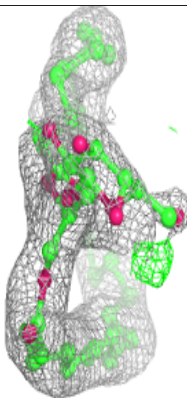
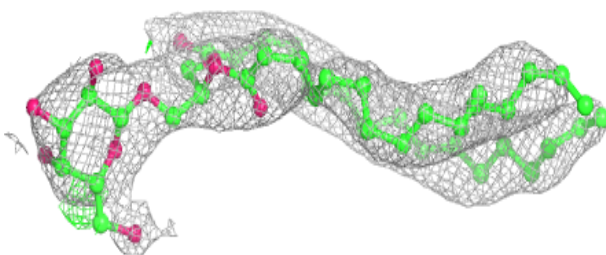
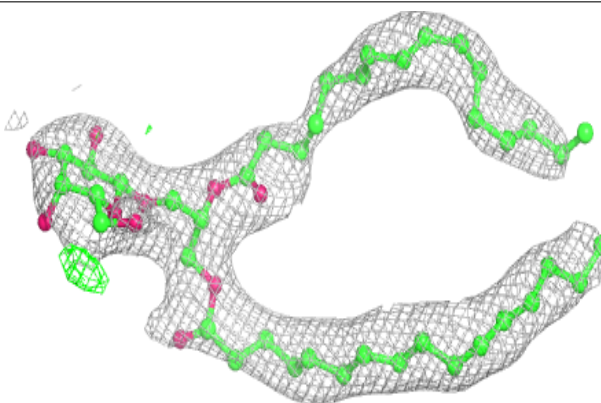


**Electron density around SQD A 412:**

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

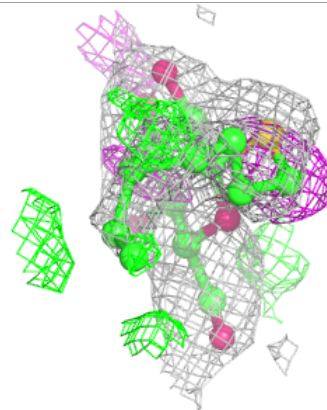
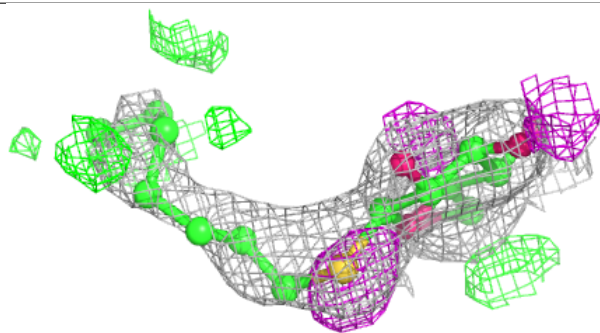
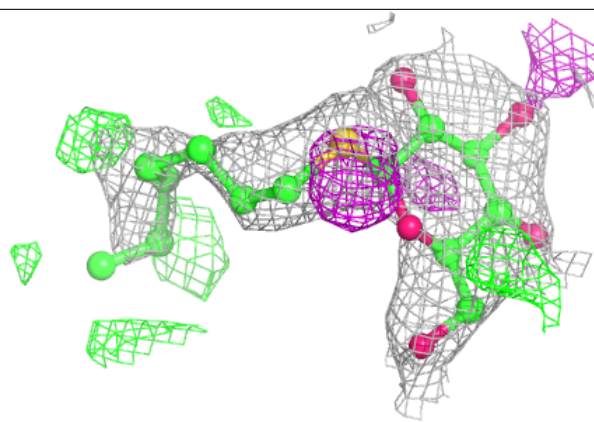
**Electron density around LMG C 501:**

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

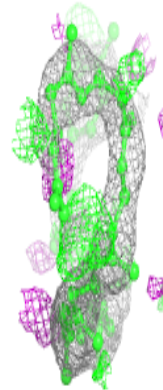
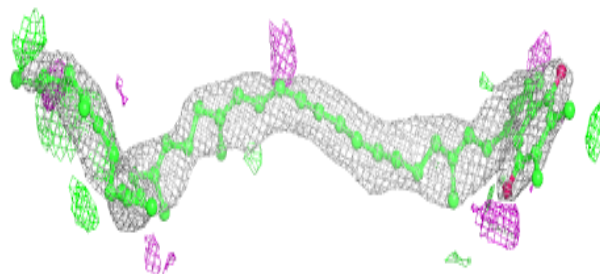
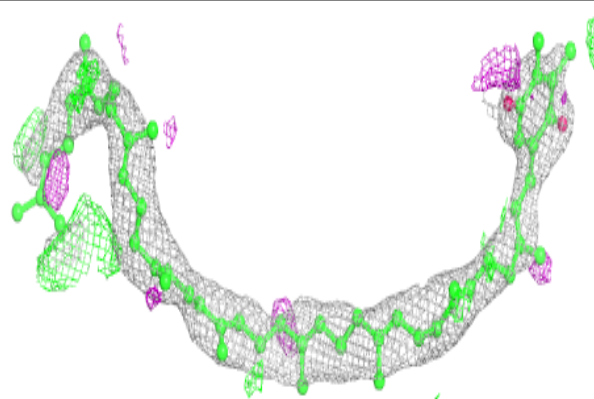


**Electron density around HTG B 623:**

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

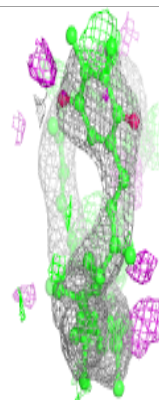
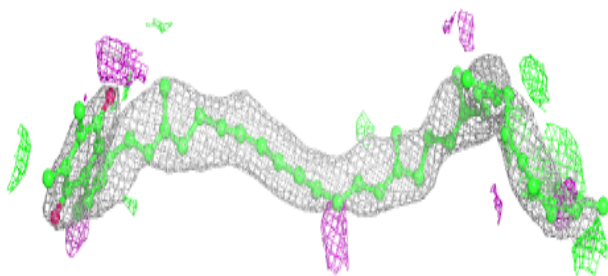
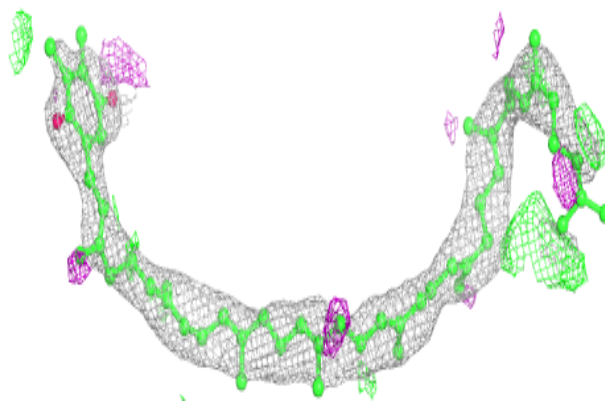
**Electron density around PL9 A 414 (A):**

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

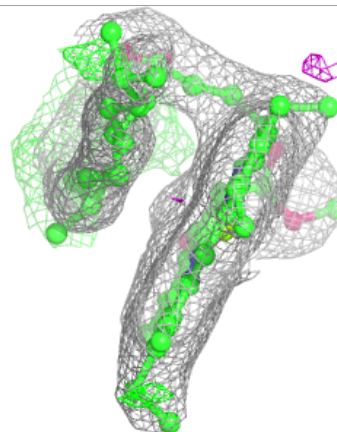
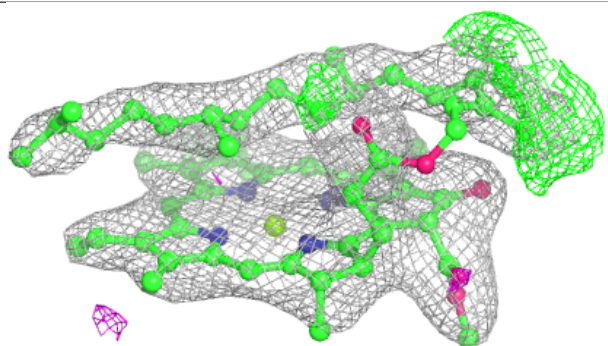
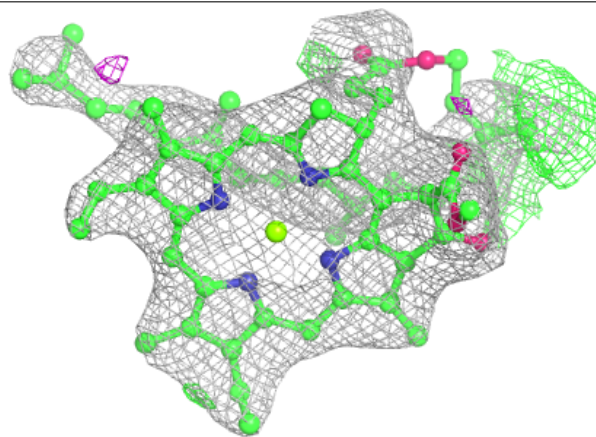


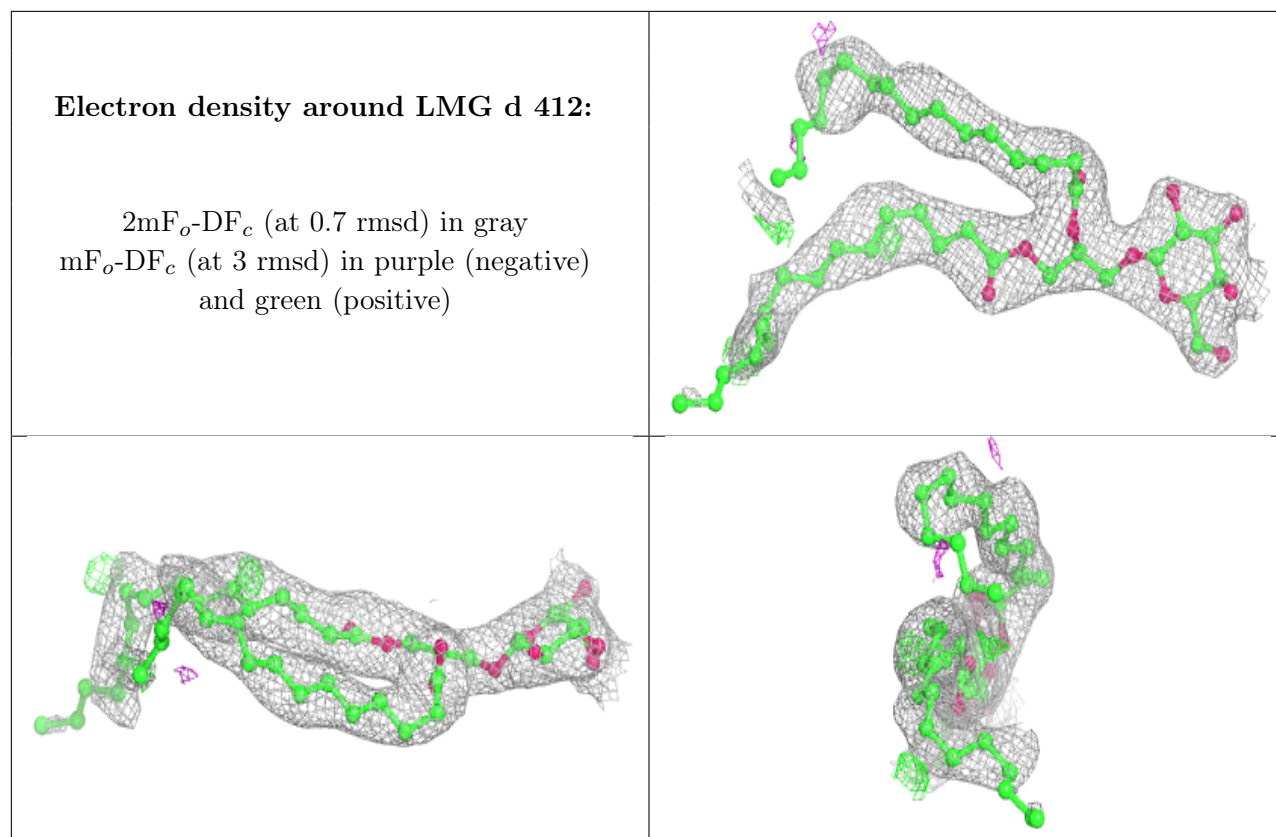
**Electron density around PL9 A 414 (B):**

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

**Electron density around CLA b 601:**

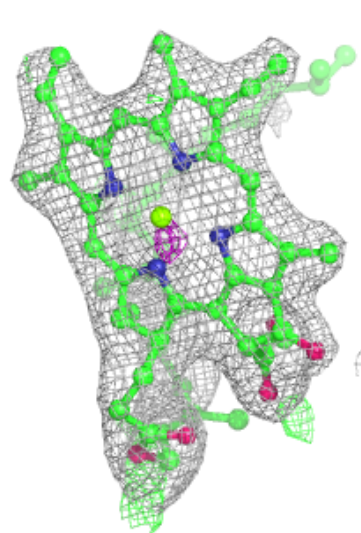
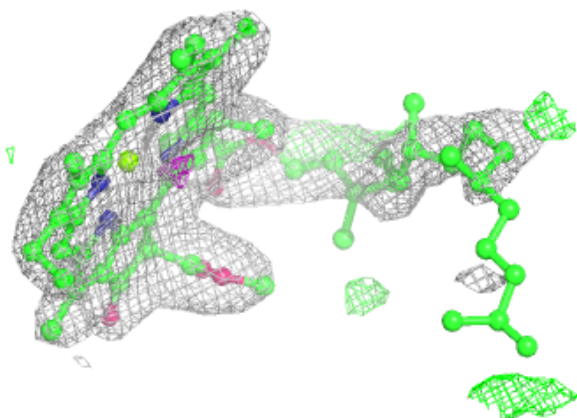
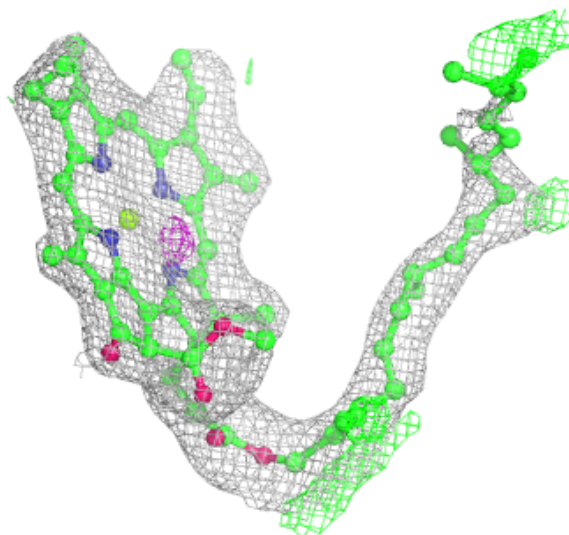
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA b 616:**

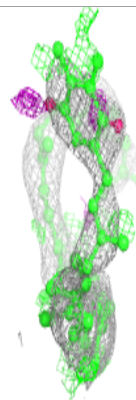
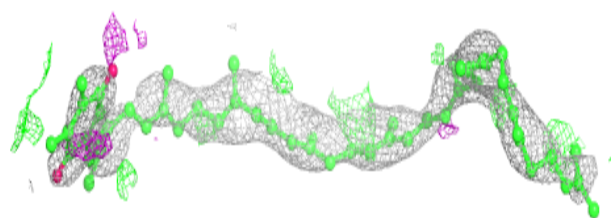
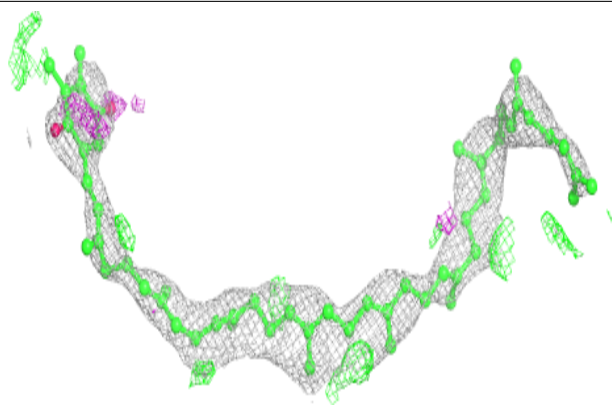
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



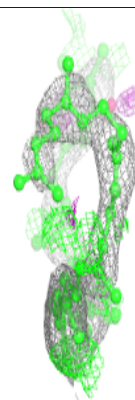
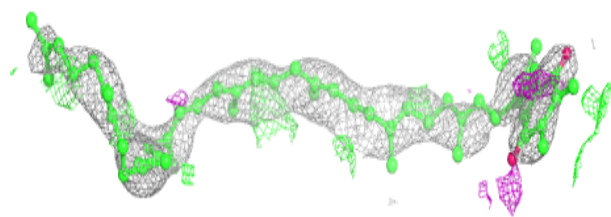
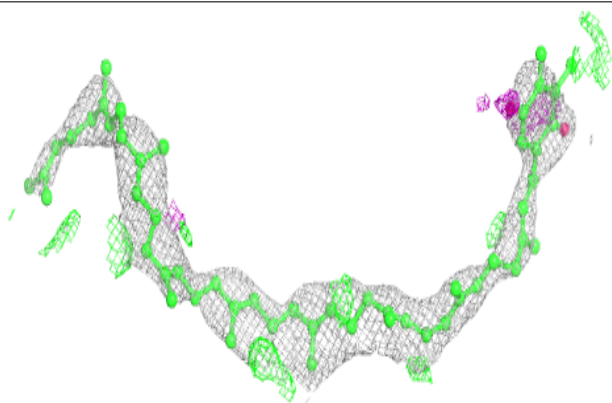


**Electron density around PL9 a 416 (A):**

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

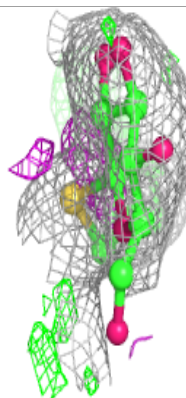
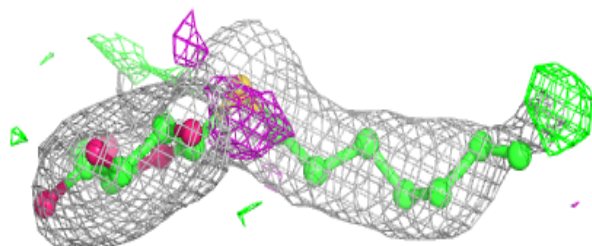
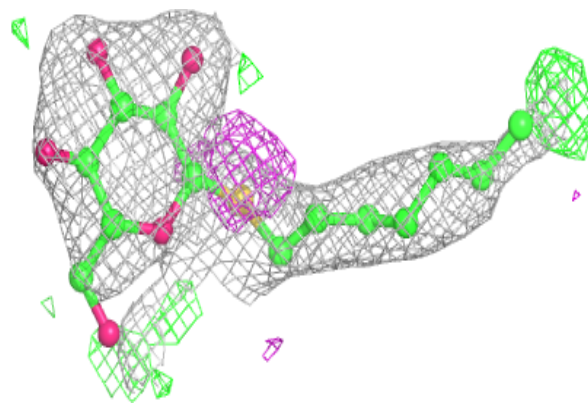
**Electron density around PL9 a 416 (B):**

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

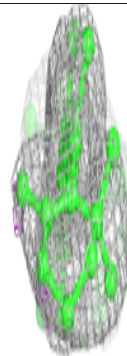
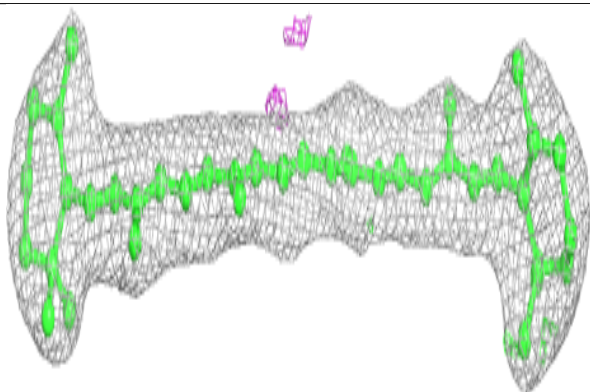
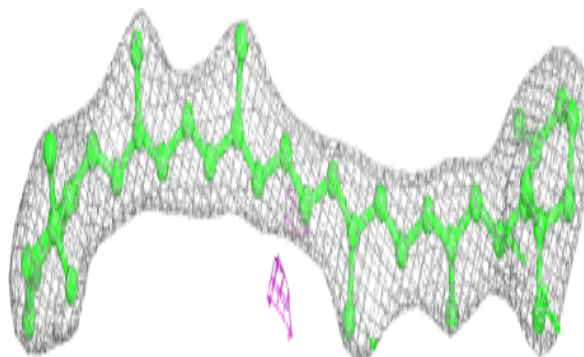


**Electron density around HTG b 622:**

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

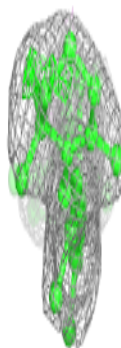
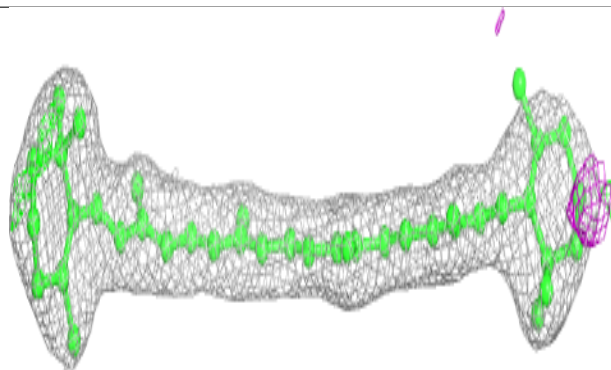
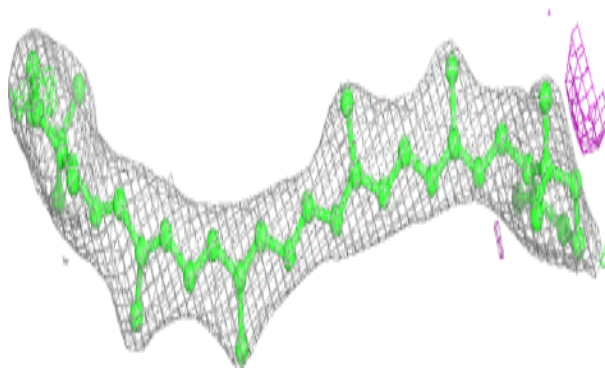
**Electron density around BCR C 515:**

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

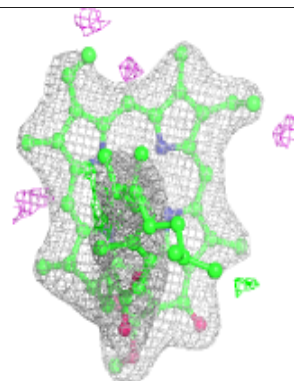
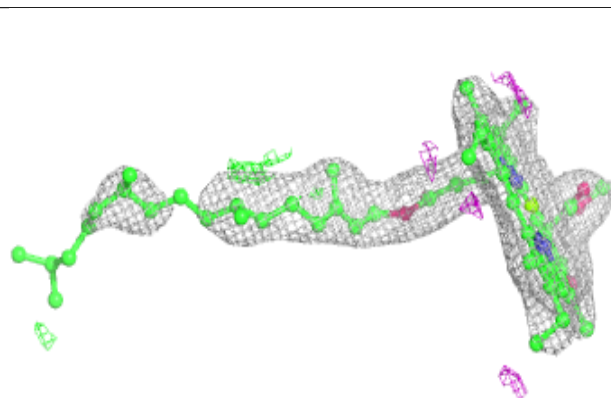
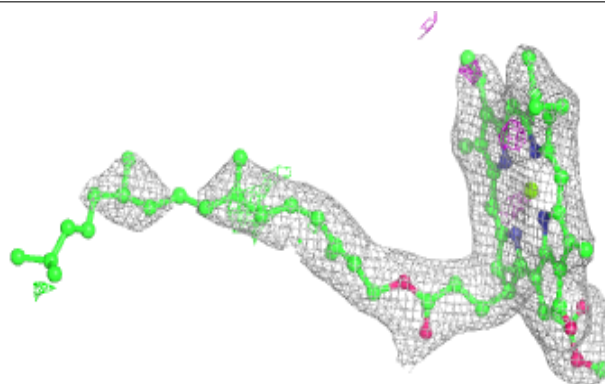


**Electron density around BCR h 101:**

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

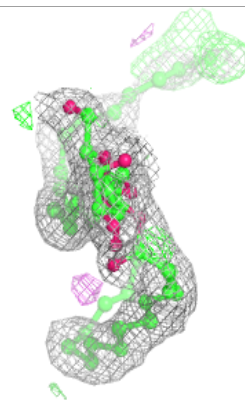
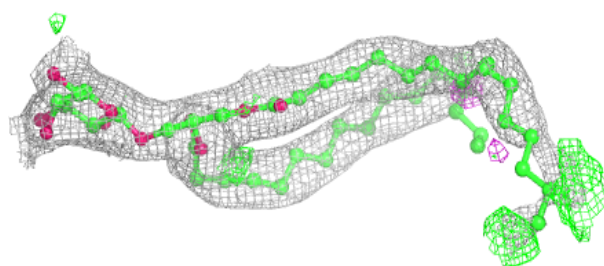
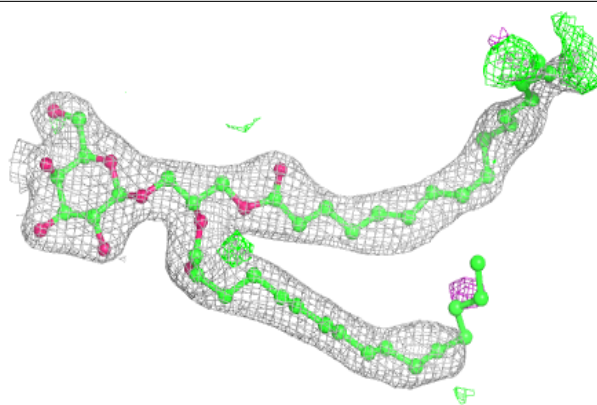
**Electron density around CLA d 403:**

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

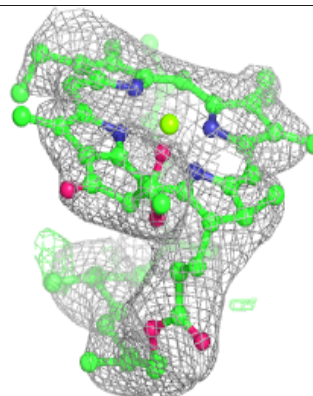
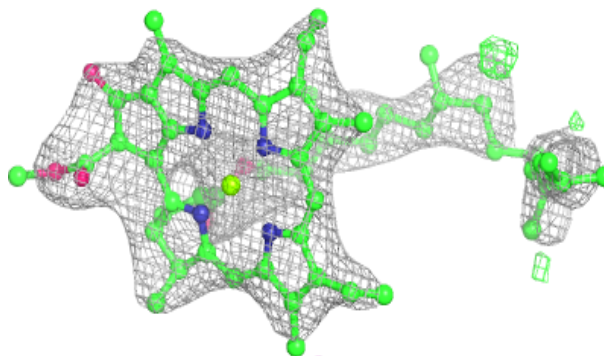
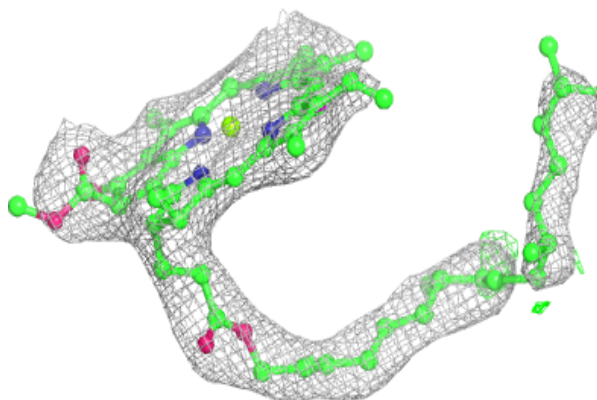


**Electron density around LMG D 415:**

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

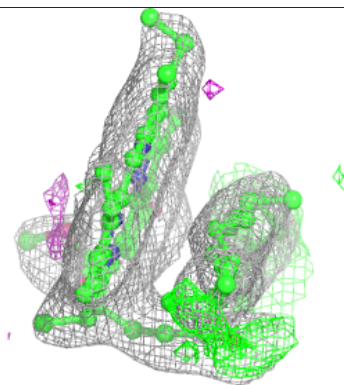
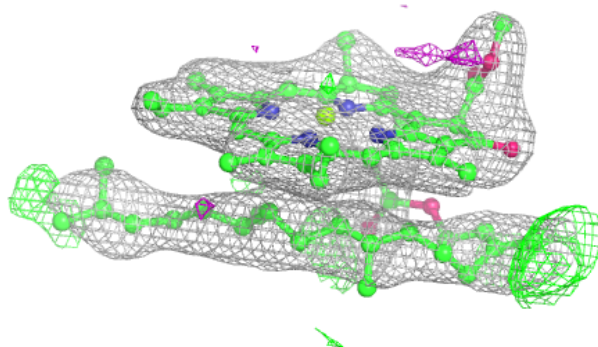
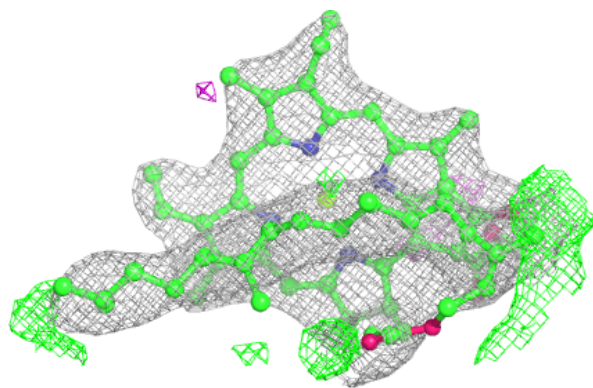
**Electron density around CLA c 514:**

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

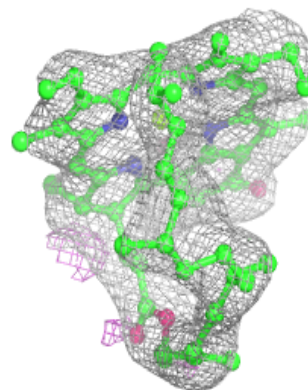
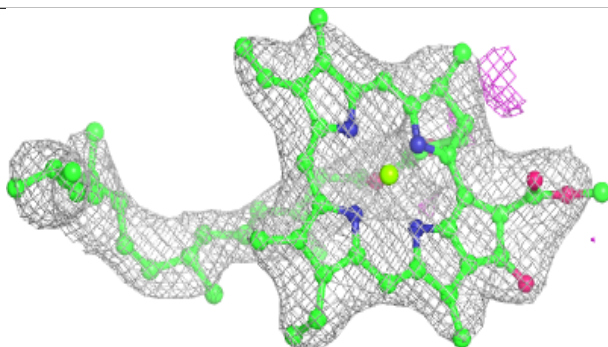
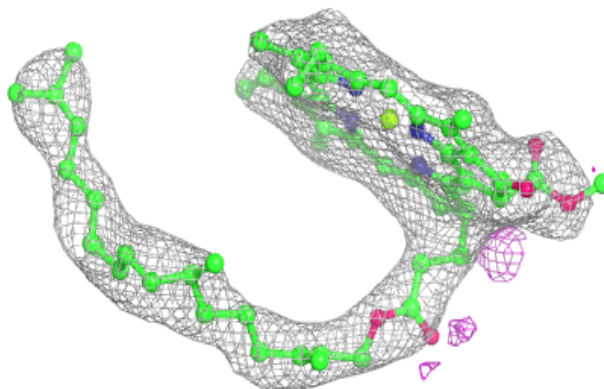


**Electron density around CLA B 601:**

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

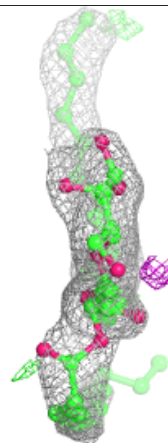
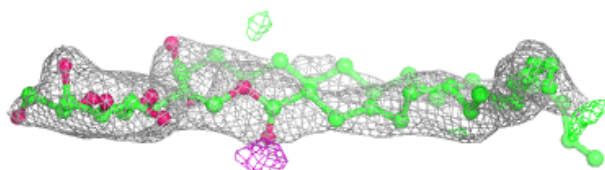
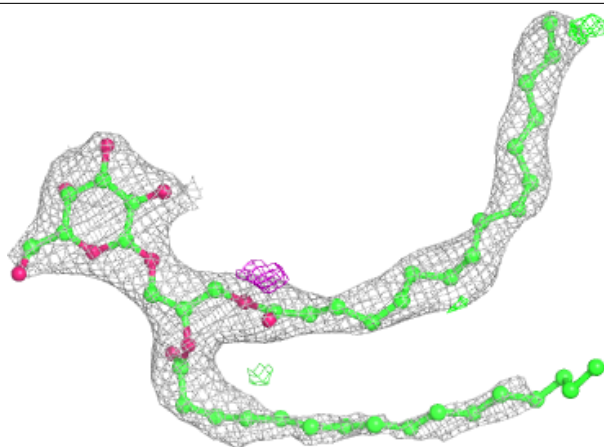
**Electron density around CLA C 514:**

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

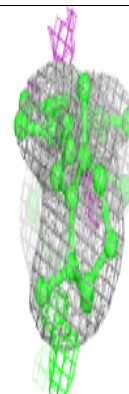
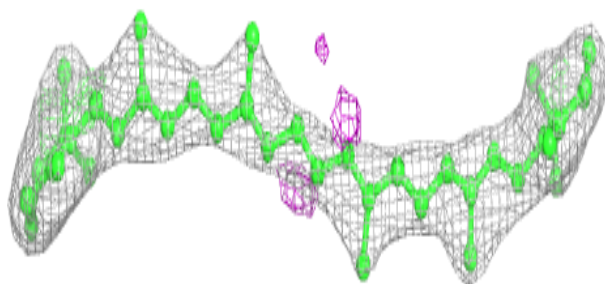
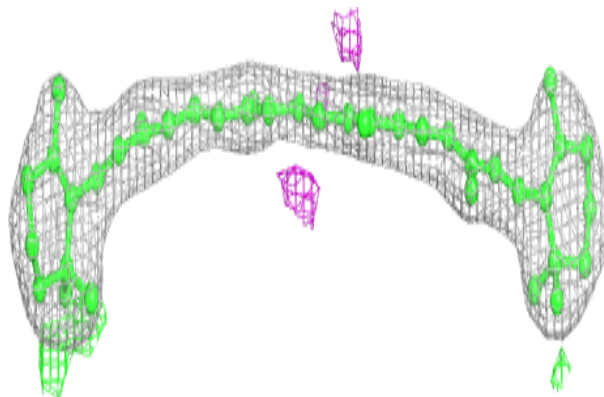


**Electron density around LMG c 520:**

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

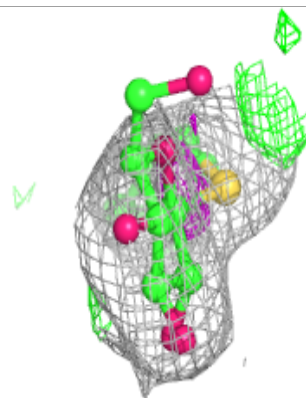
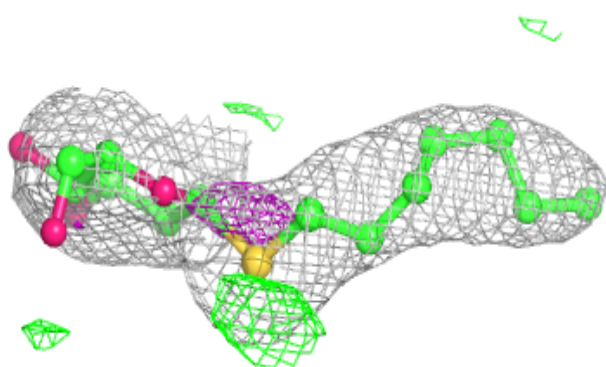
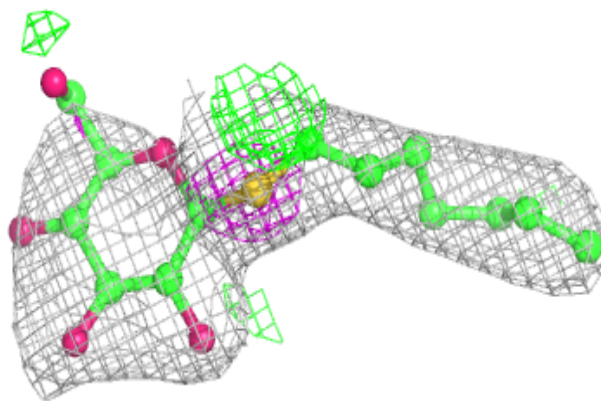
**Electron density around BCR K 102:**

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

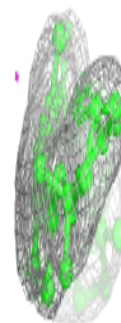
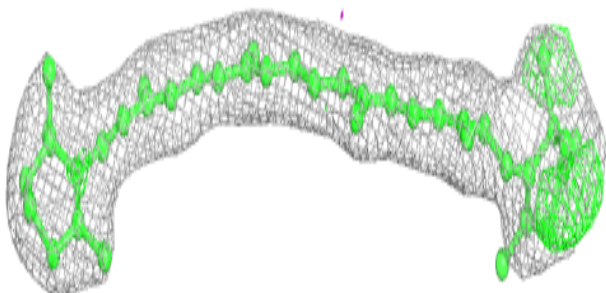
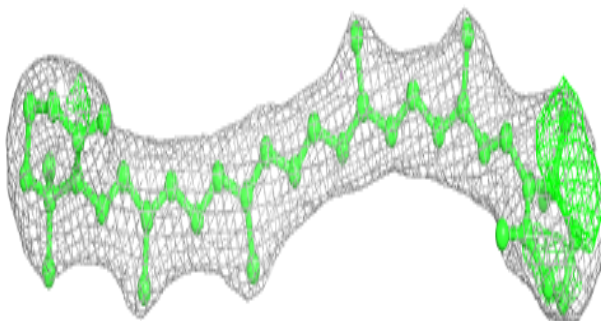


**Electron density around HTG B 622:**

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

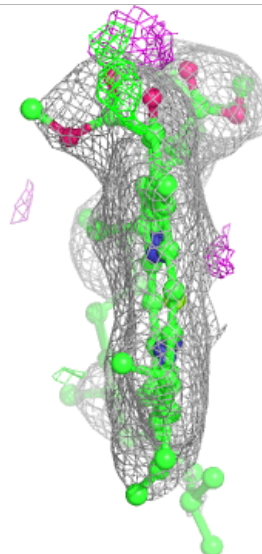
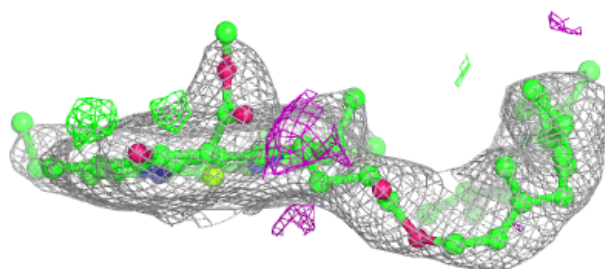
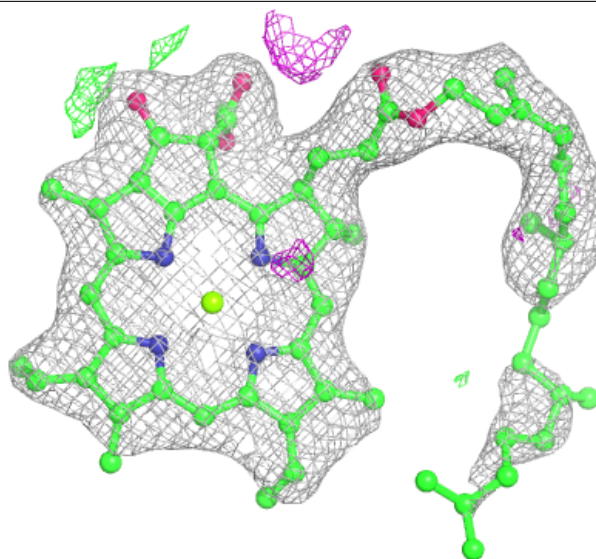
**Electron density around BCR d 404:**

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



**Electron density around CLA c 513:**

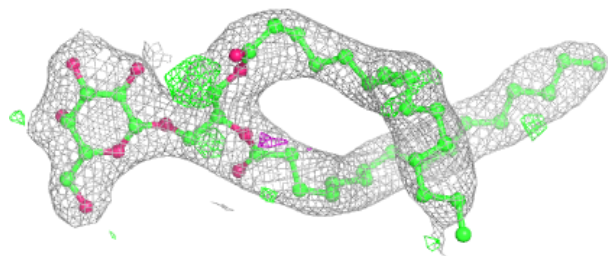
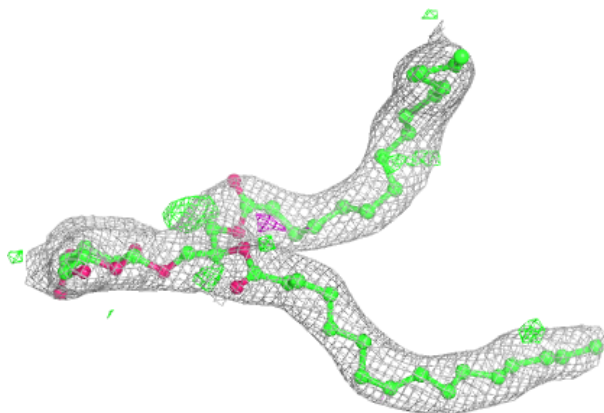
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





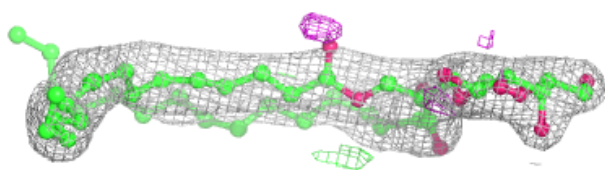
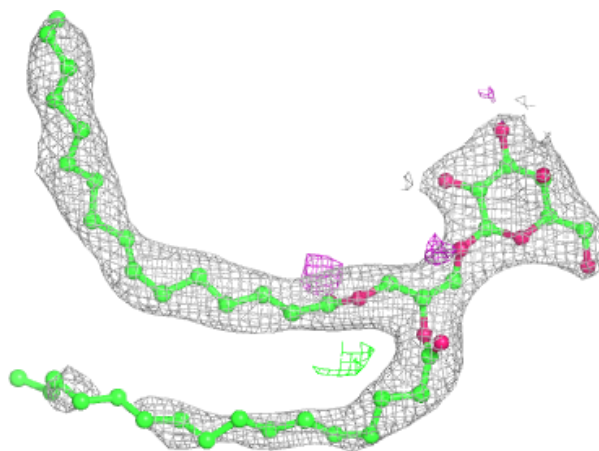
**Electron density around LMG B 621:**

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



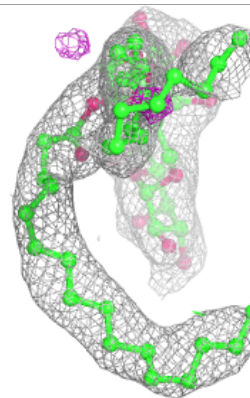
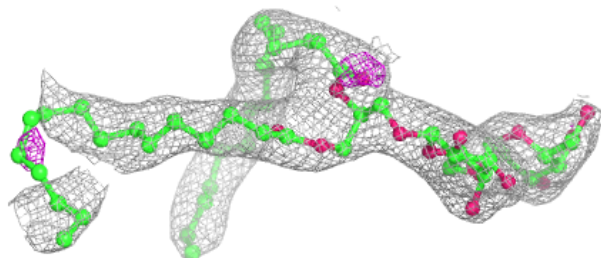
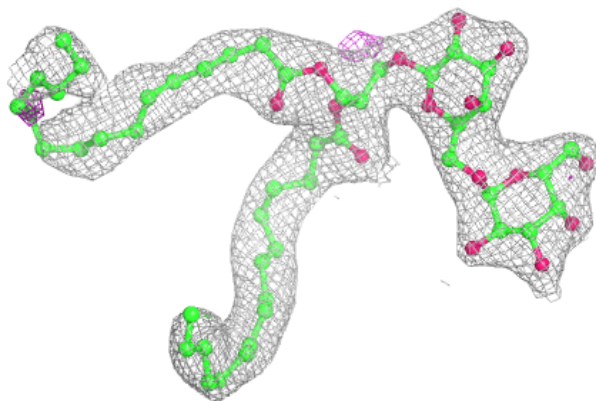
**Electron density around LMG C 520:**

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

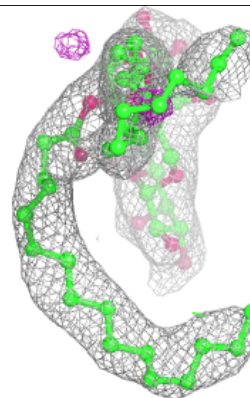
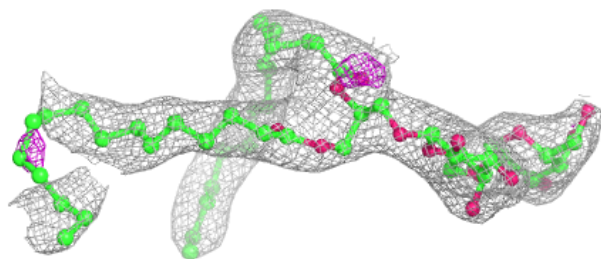
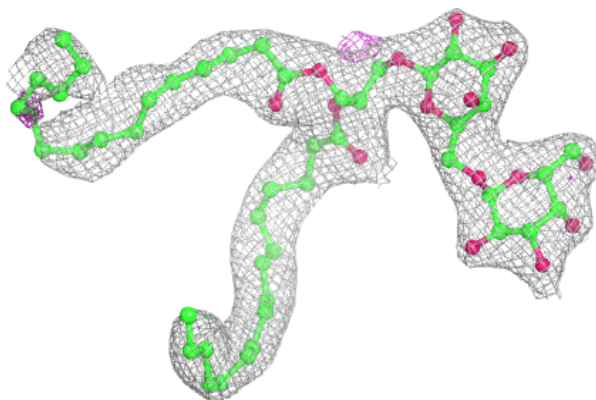


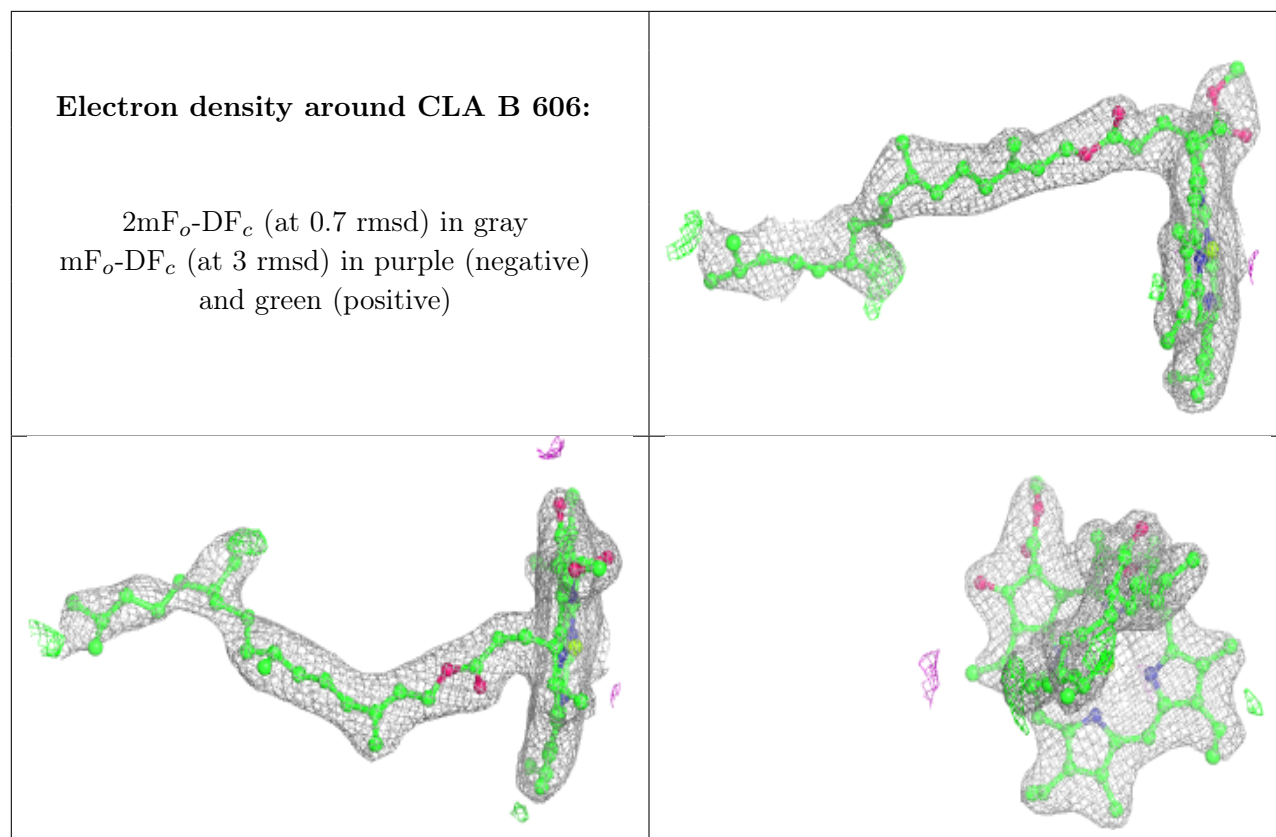
**Electron density around DGD c 518 (A):**

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

**Electron density around DGD c 518 (B):**

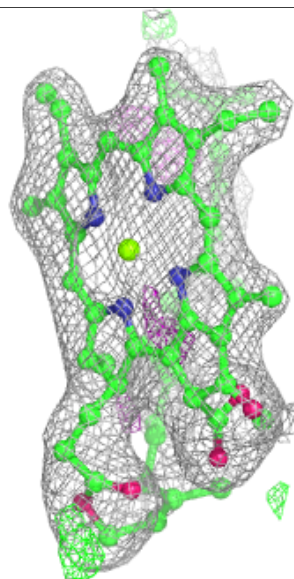
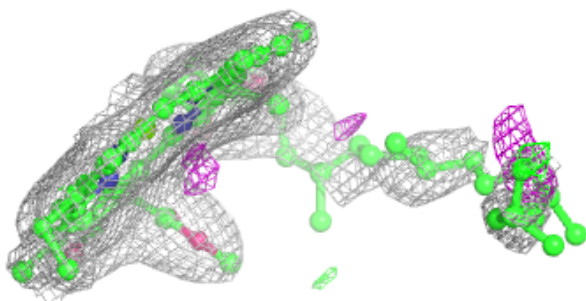
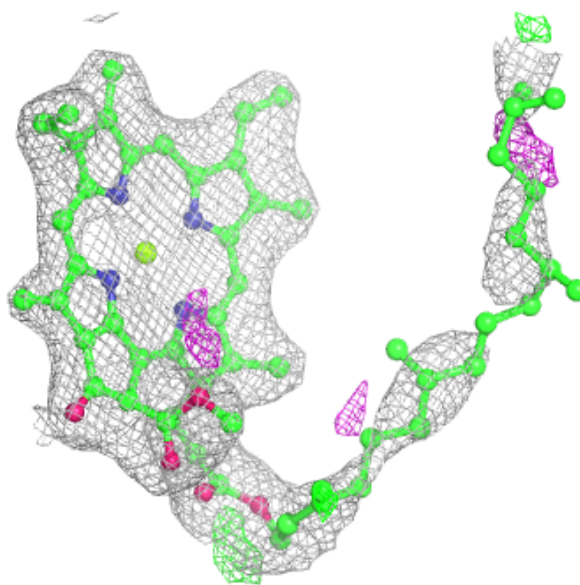
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





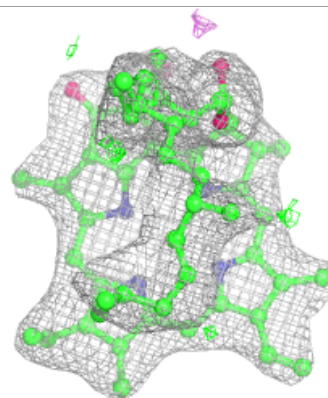
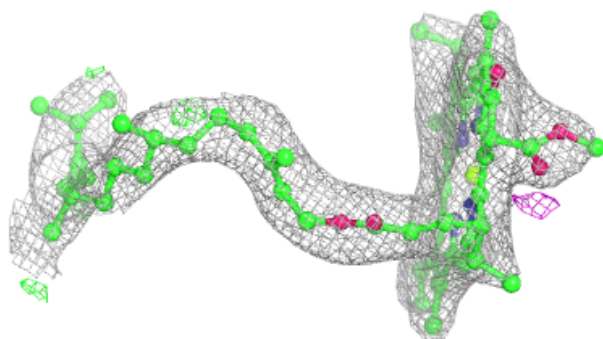
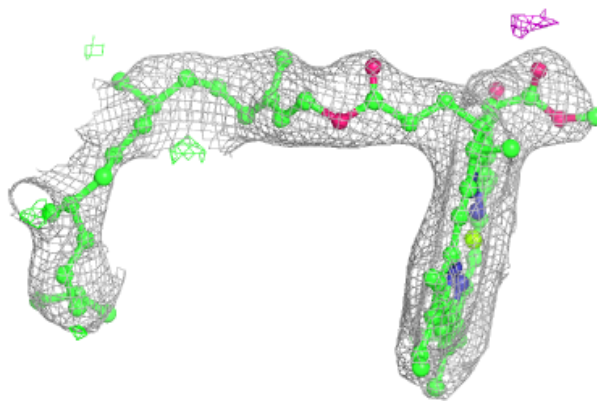
**Electron density around CLA B 616:**

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



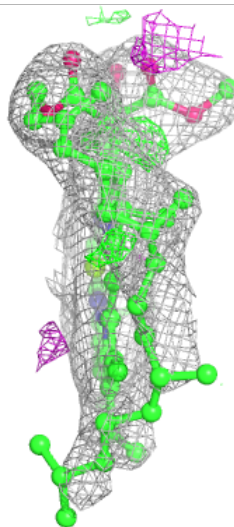
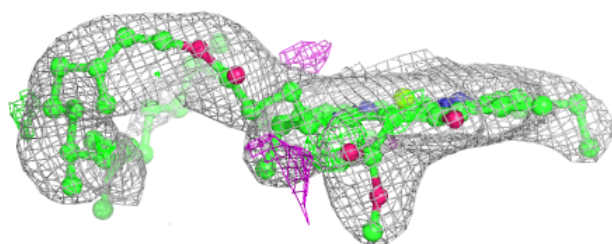
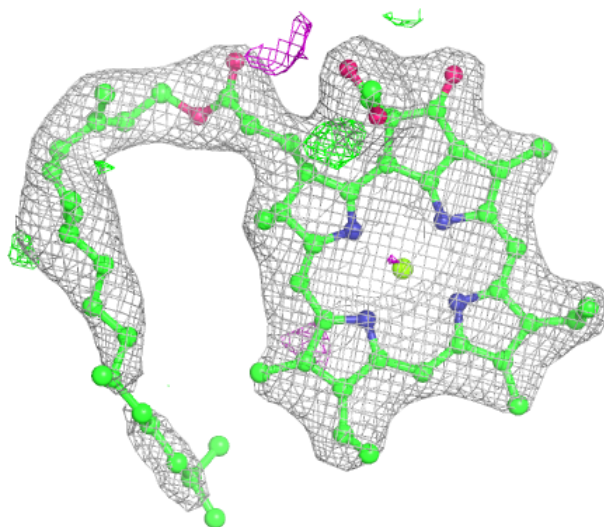
**Electron density around CLA C 507:**

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



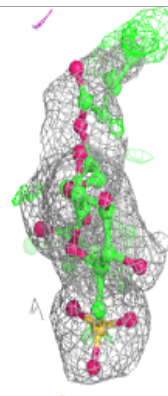
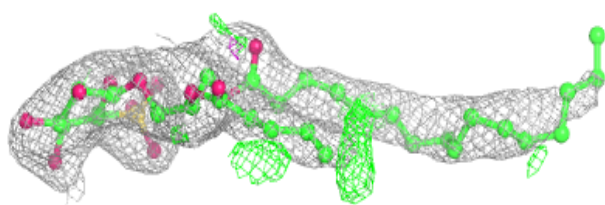
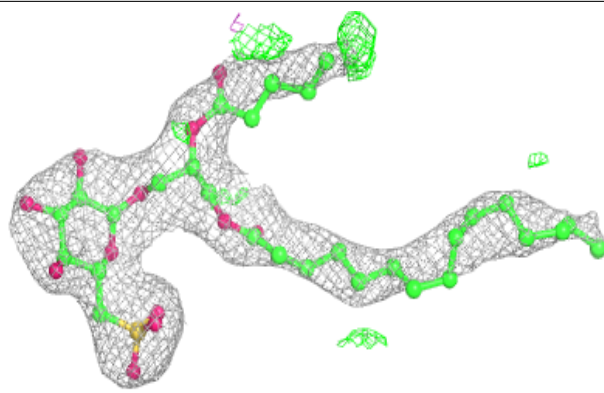
**Electron density around CLA C 513:**

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

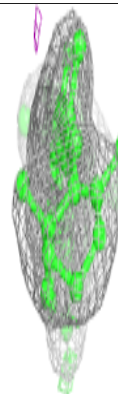
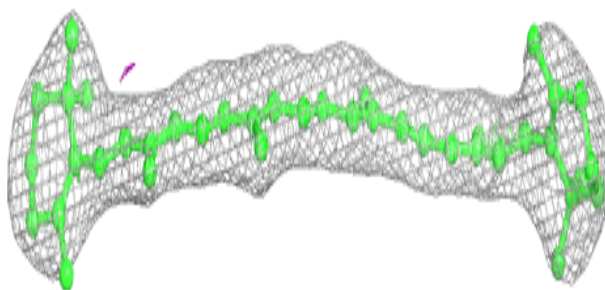
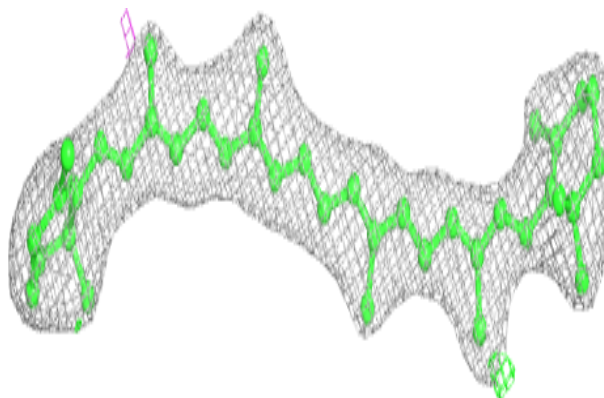


**Electron density around SQD F 101:**

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

**Electron density around BCR Y 101:**

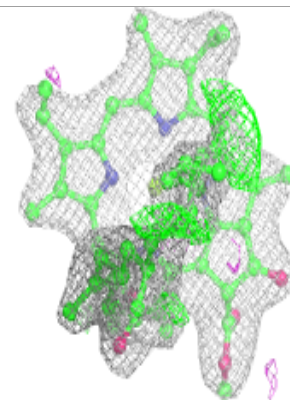
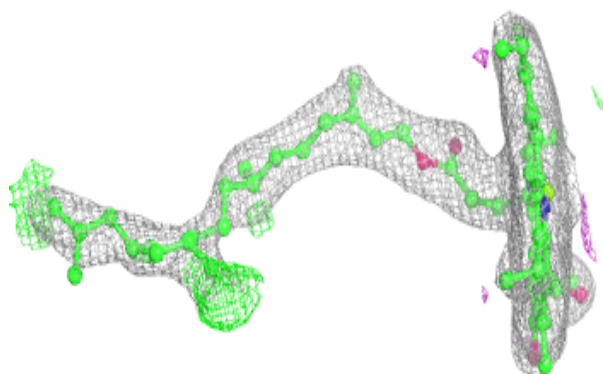
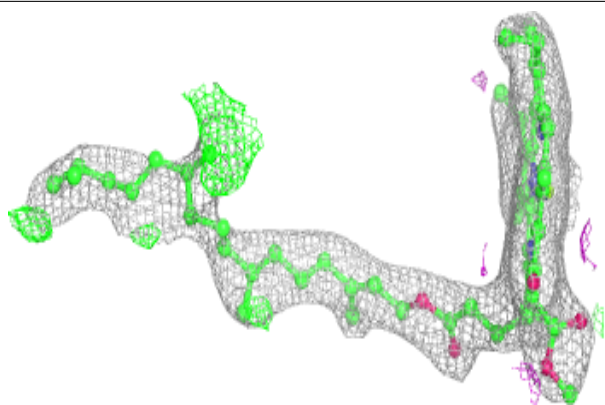
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



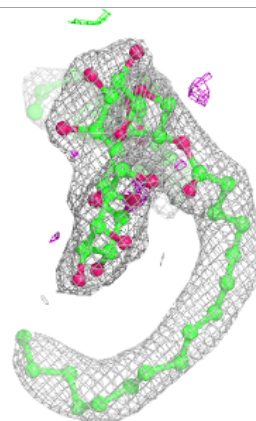
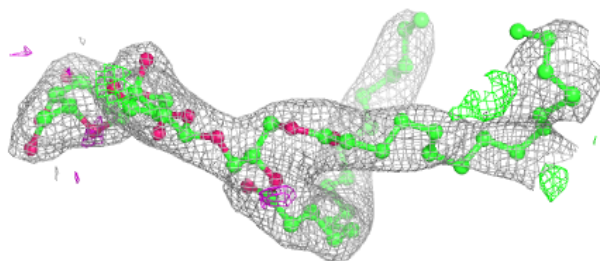
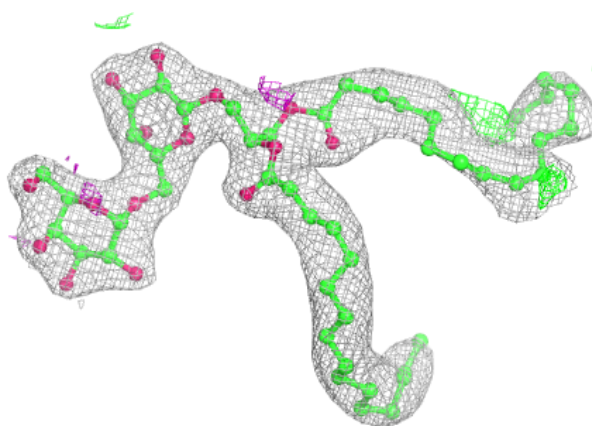


**Electron density around CLA b 606:**

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

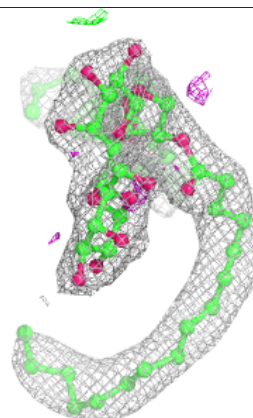
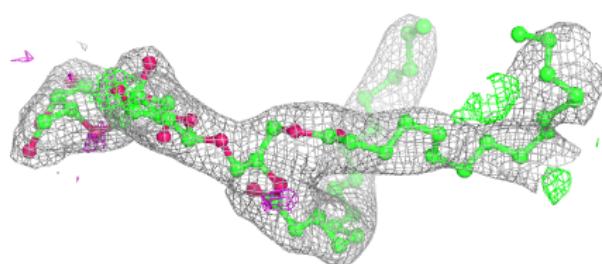
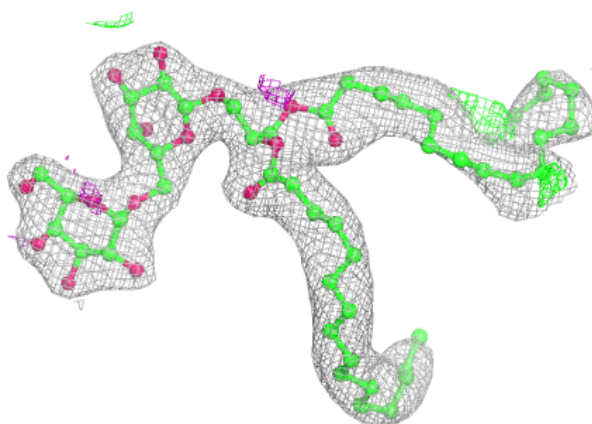
**Electron density around DGD C 518 (A):**

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

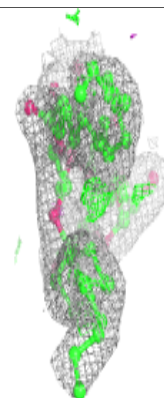
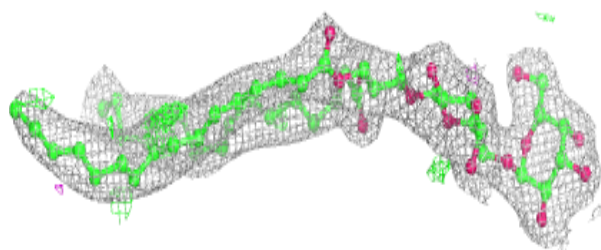
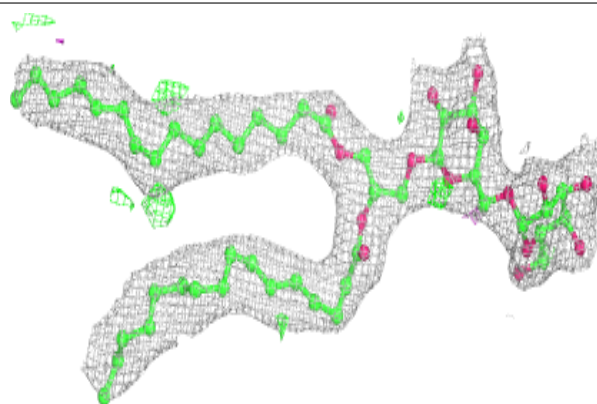


**Electron density around DGD C 518 (B):**

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

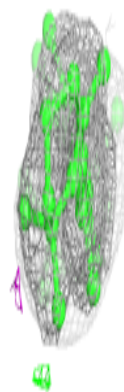
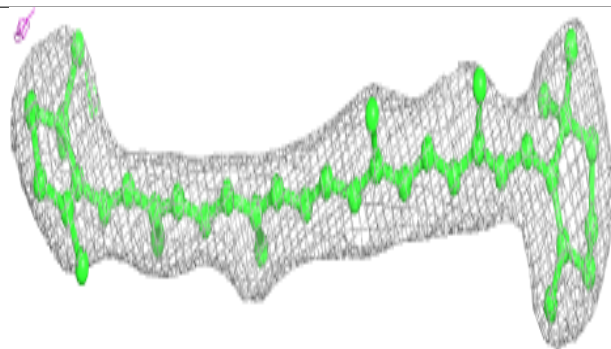
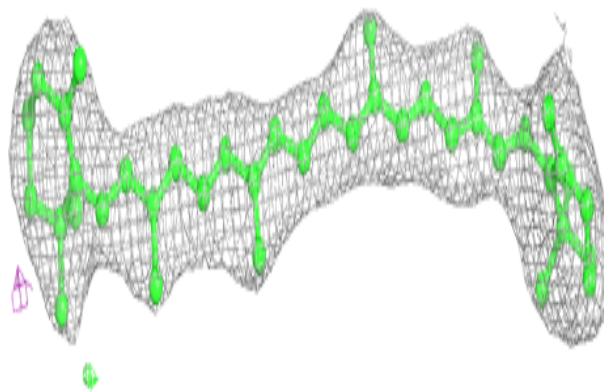
**Electron density around DGD C 519:**

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

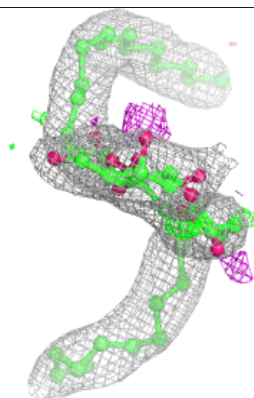
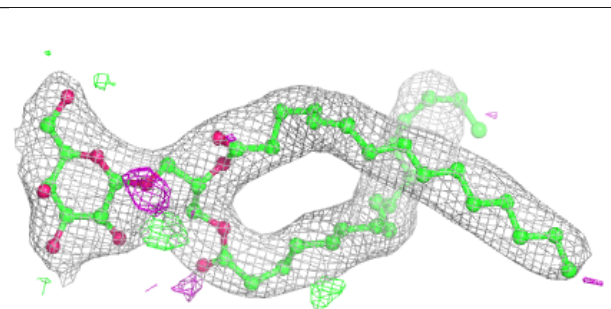
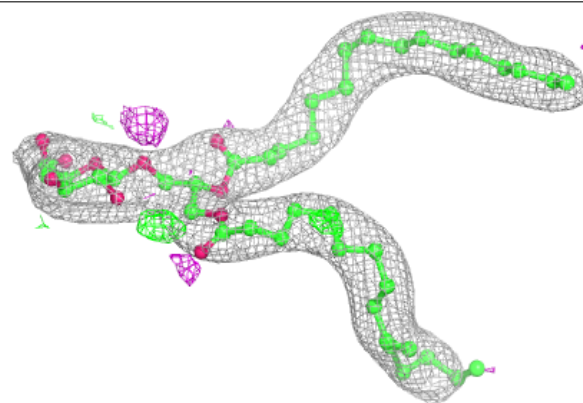


**Electron density around BCR c 515:**

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

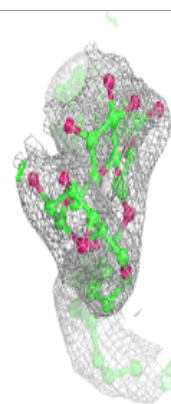
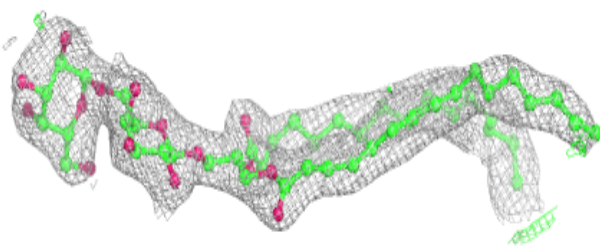
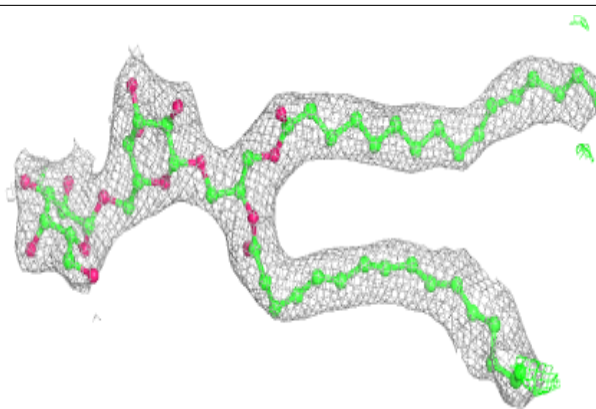
**Electron density around LMG m 101:**

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

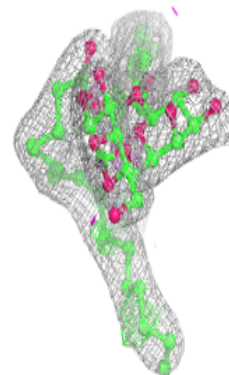
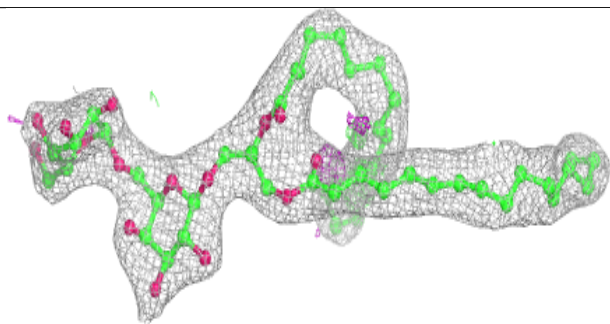
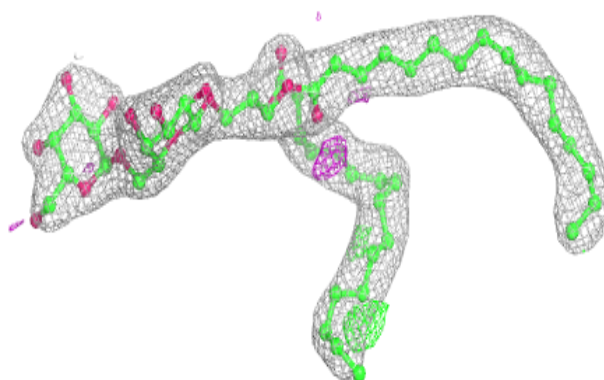


**Electron density around DGD c 519:**

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

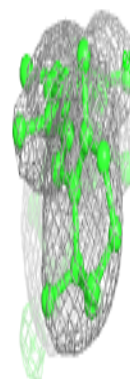
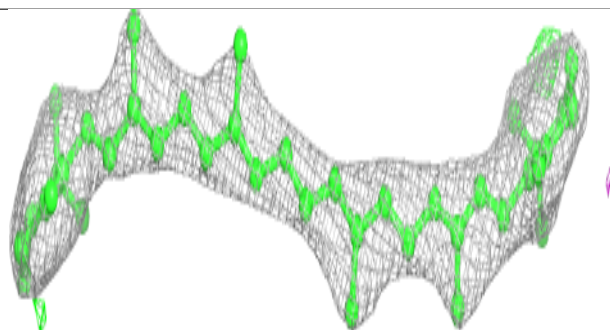
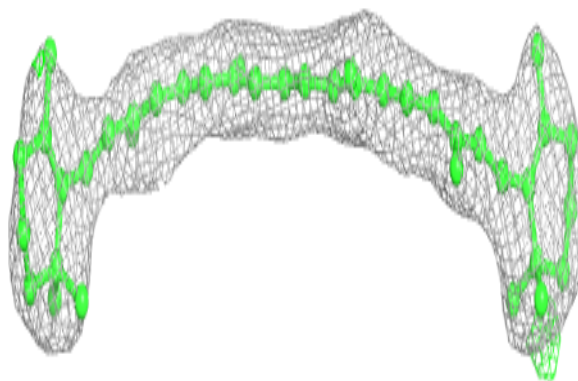
**Electron density around DGD h 102:**

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

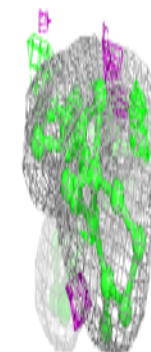
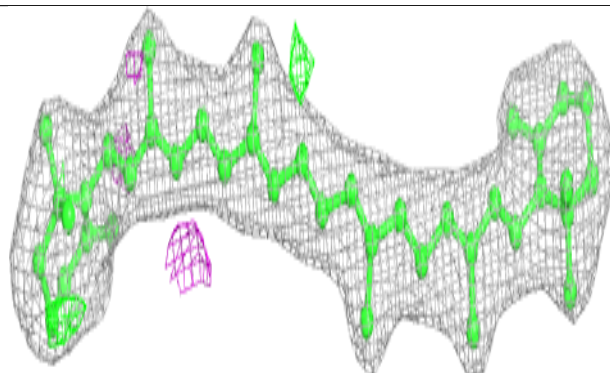
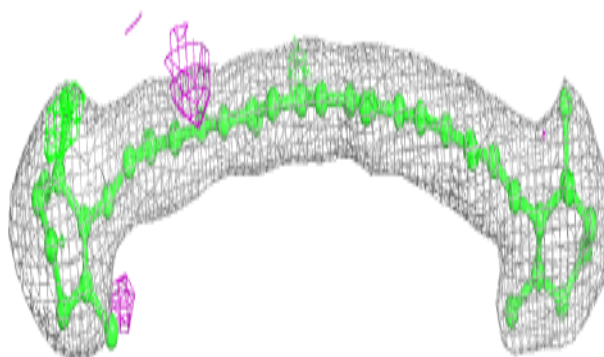


**Electron density around BCR k 101:**

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

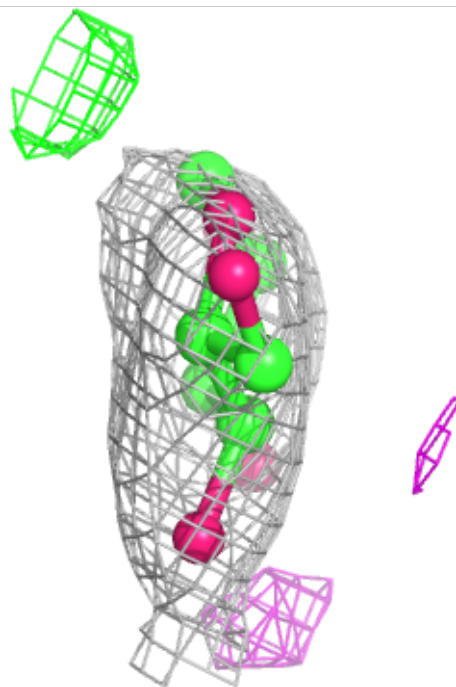
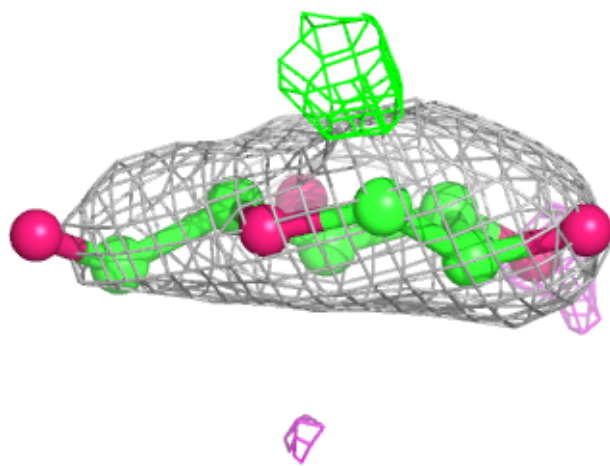
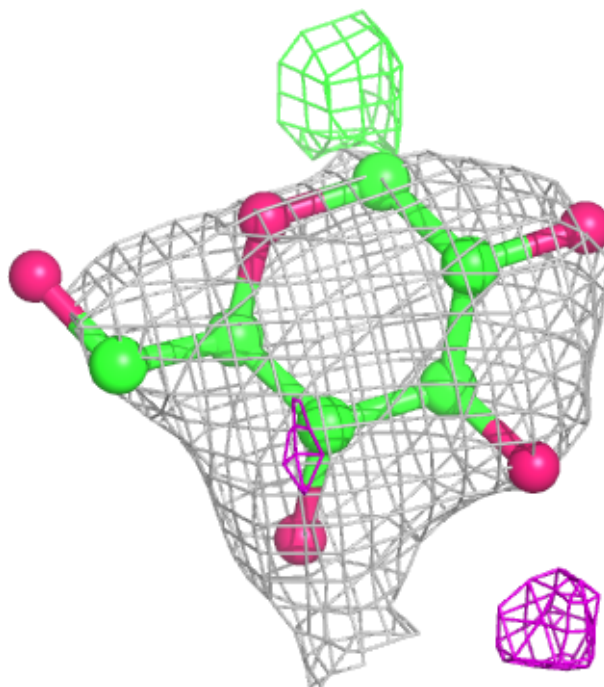
**Electron density around BCR D 407:**

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



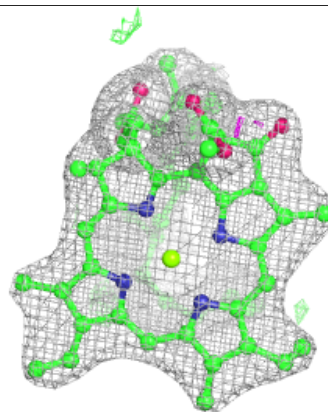
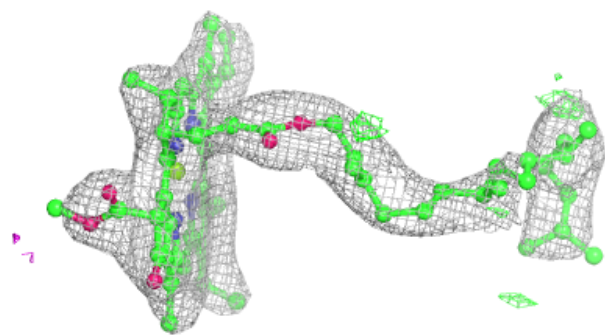
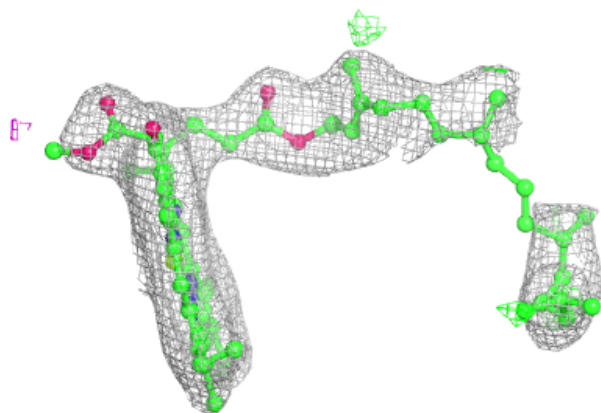
**Electron density around HTG V 203:**

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

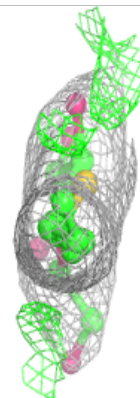
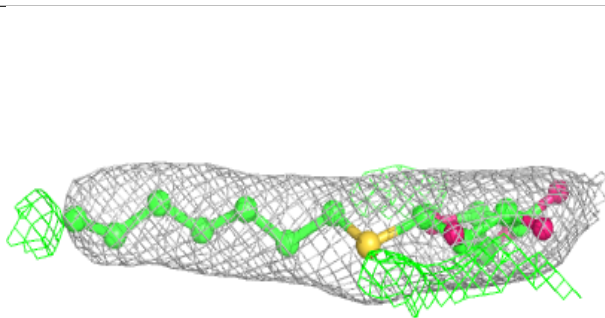
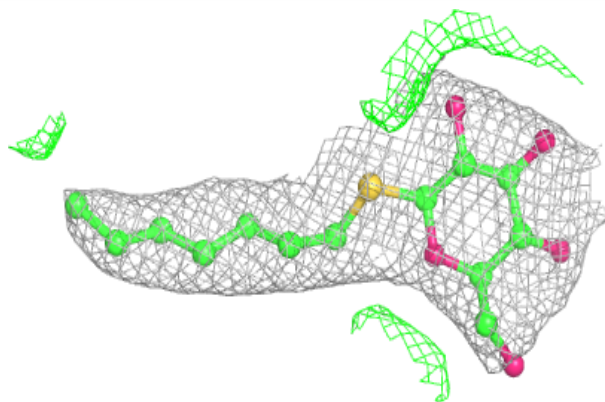


**Electron density around CLA c 507:**

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

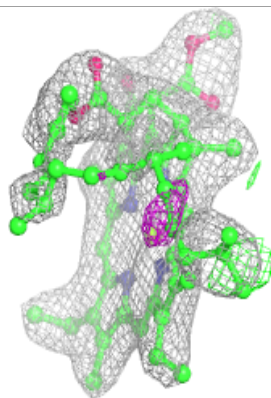
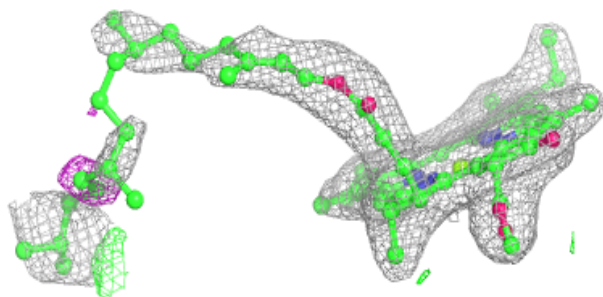
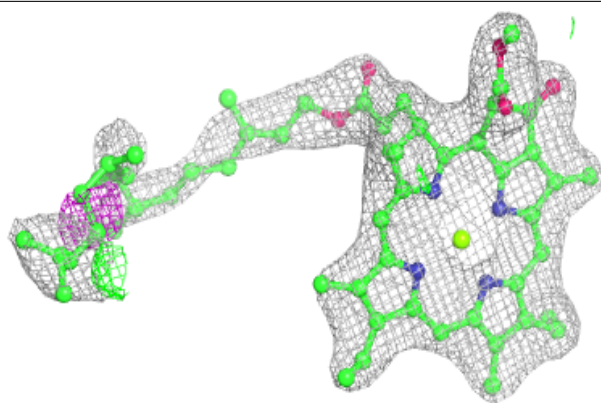
**Electron density around HTG b 625:**

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

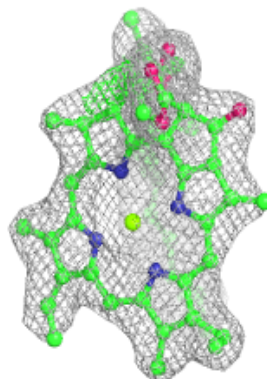
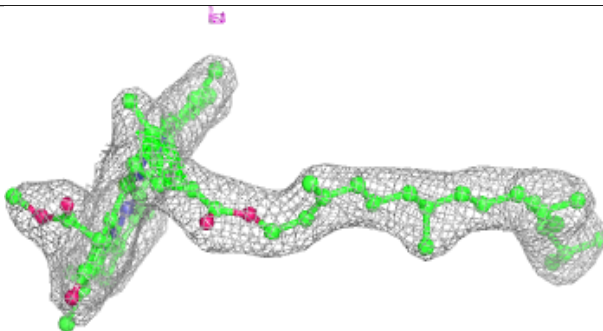
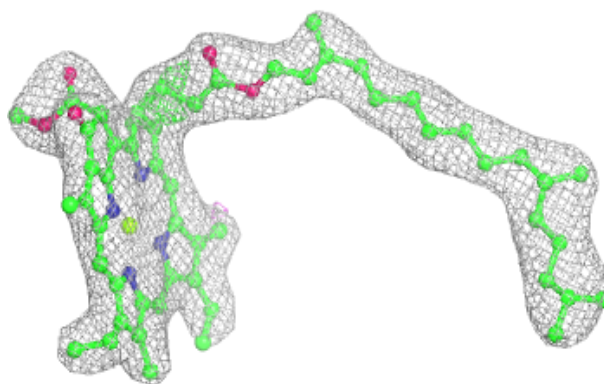


**Electron density around CLA a 409:**

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

**Electron density around CLA B 609:**

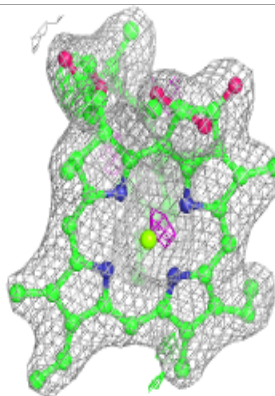
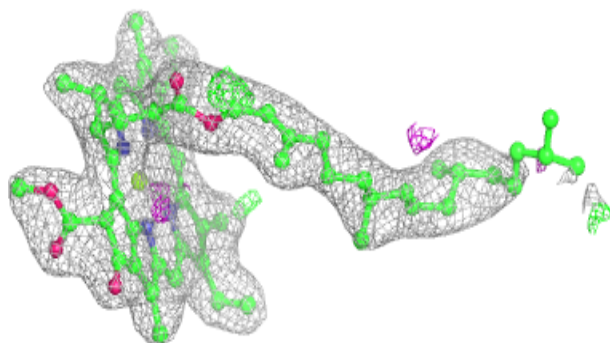
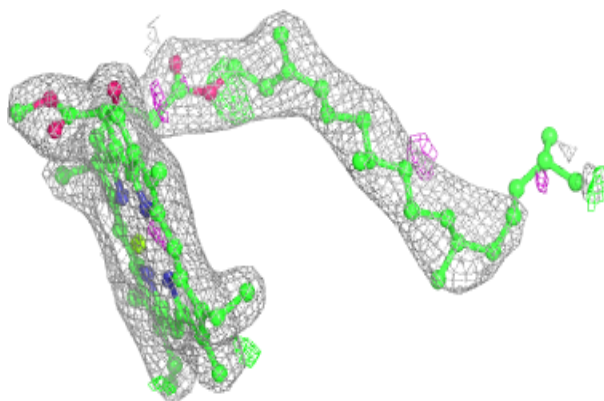
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



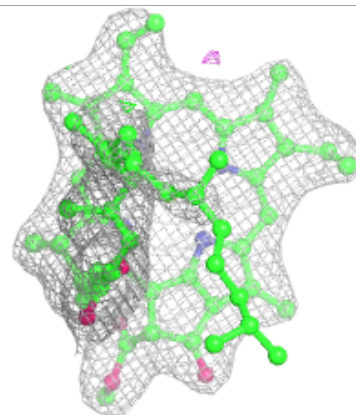
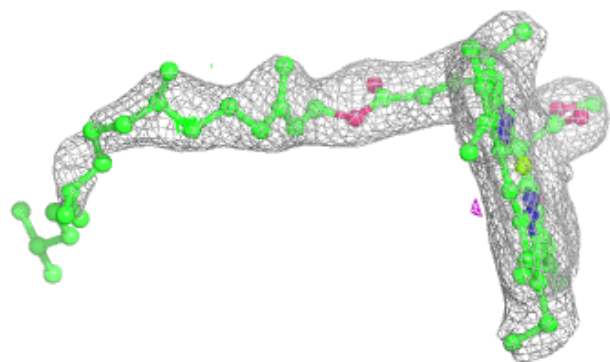
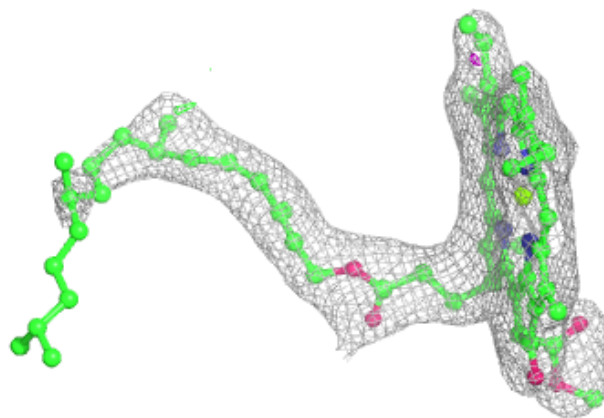


**Electron density around CLA C 509:**

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

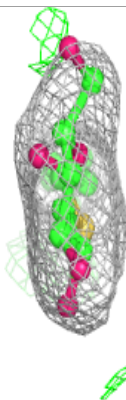
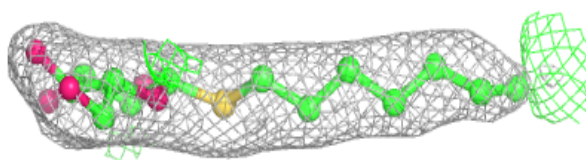
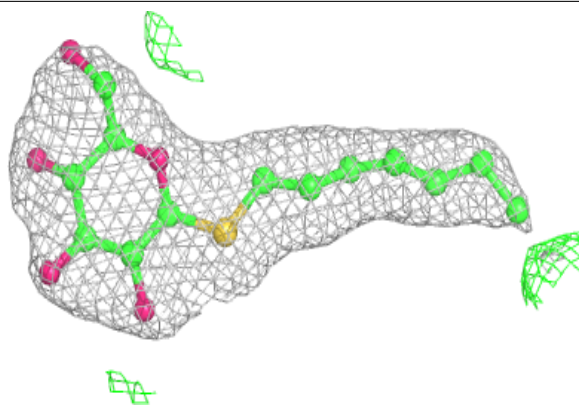
**Electron density around CLA D 406:**

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

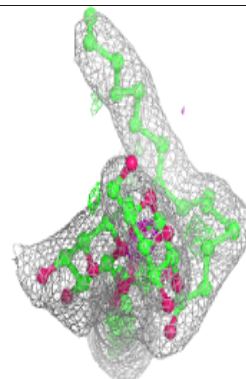
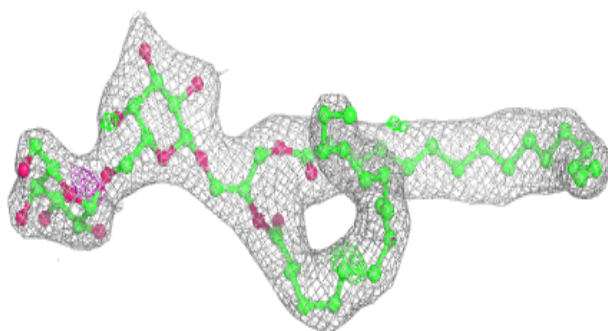
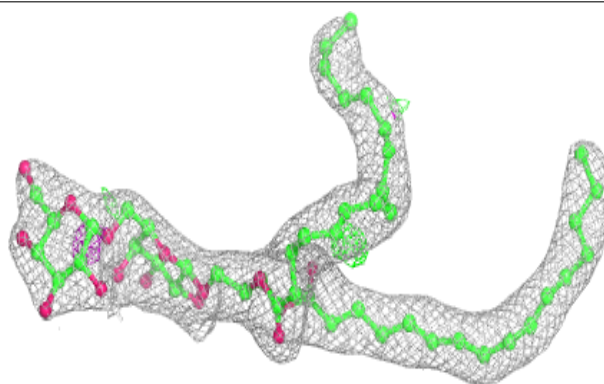


**Electron density around HTG B 626:**

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

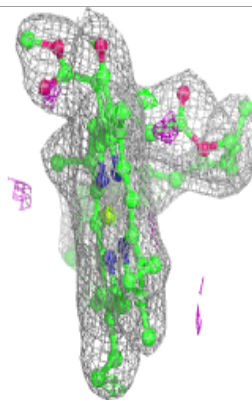
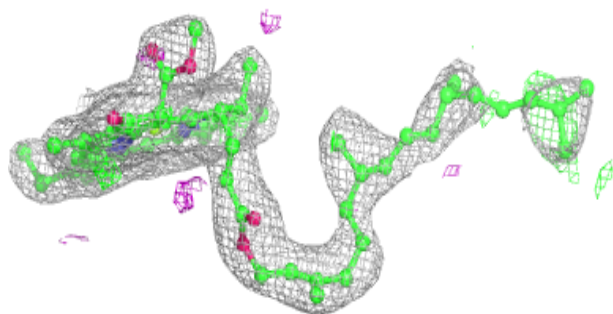
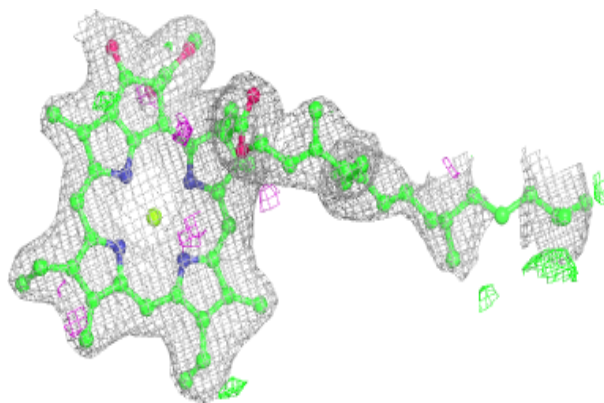
**Electron density around DGD H 102:**

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

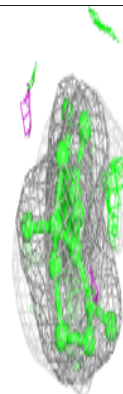
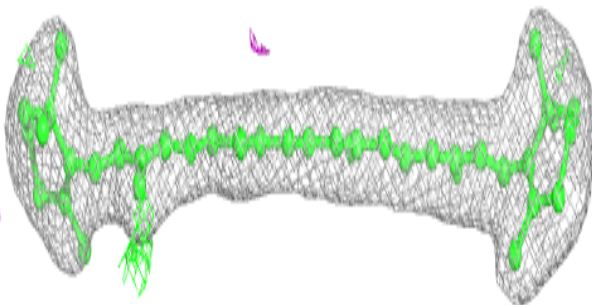
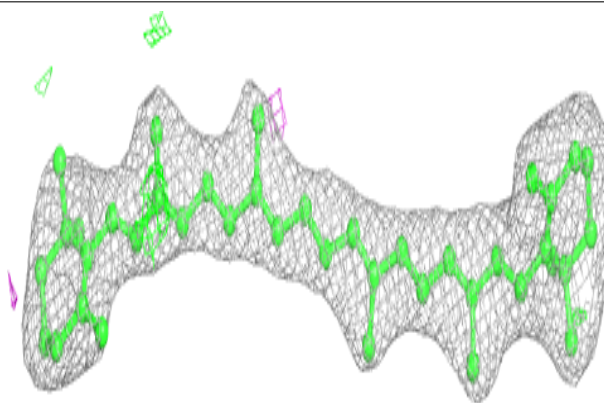


**Electron density around CLA a 407 (B):**

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

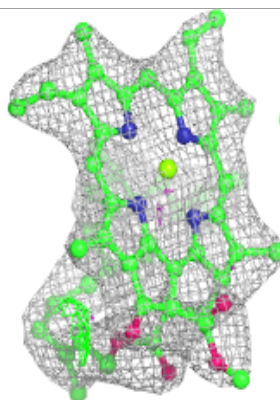
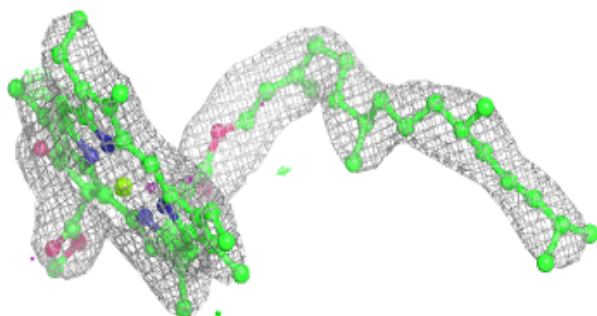
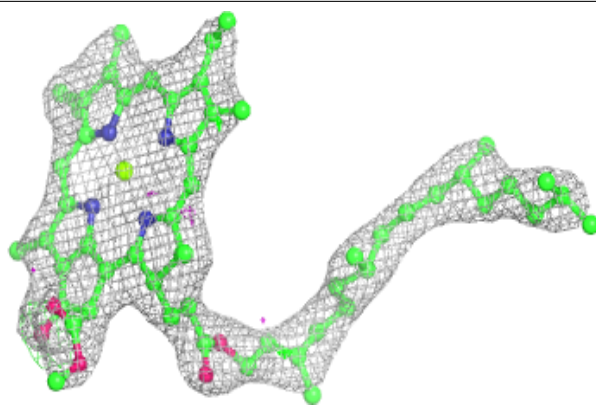
**Electron density around BCR b 618:**

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

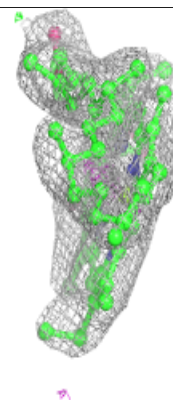
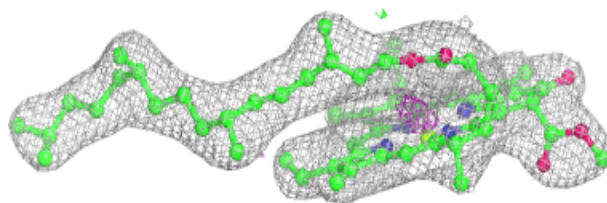
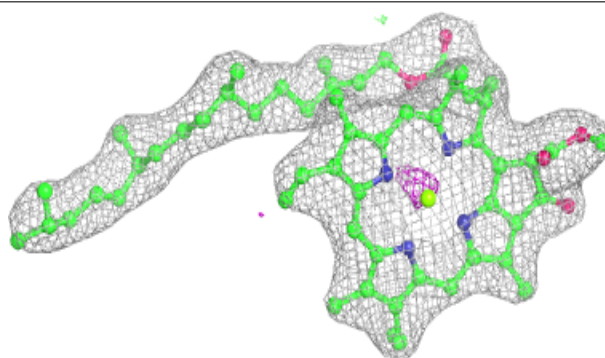


**Electron density around CLA c 512:**

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

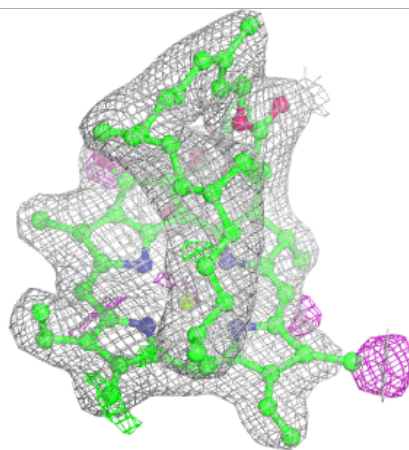
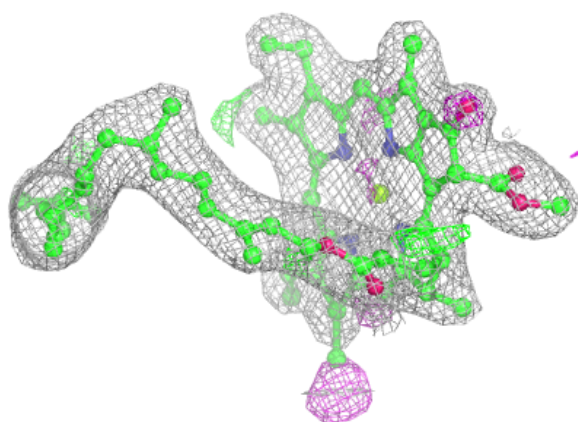
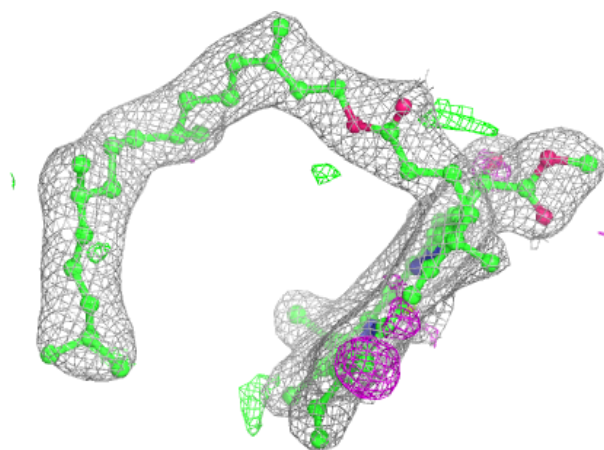
**Electron density around CLA C 502:**

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



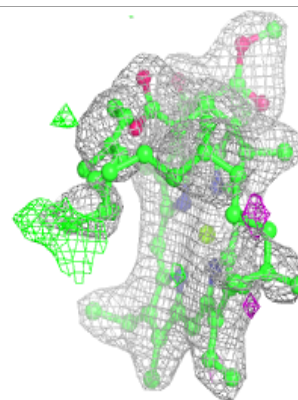
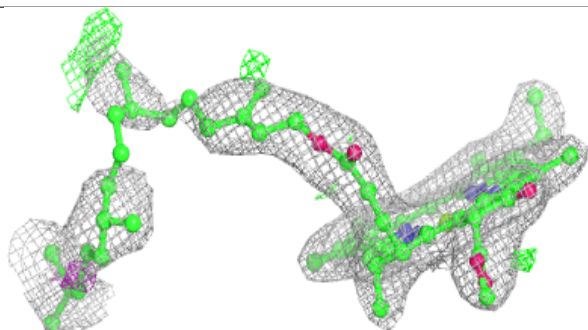
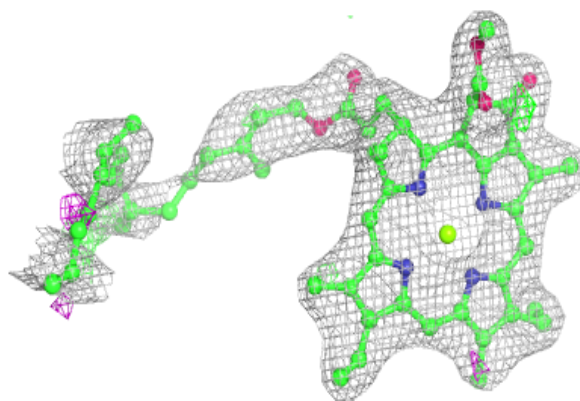
**Electron density around CLA B 611:**

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

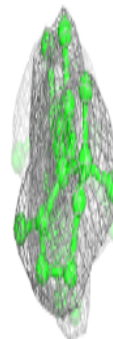
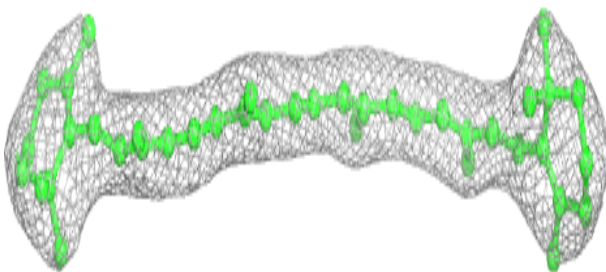
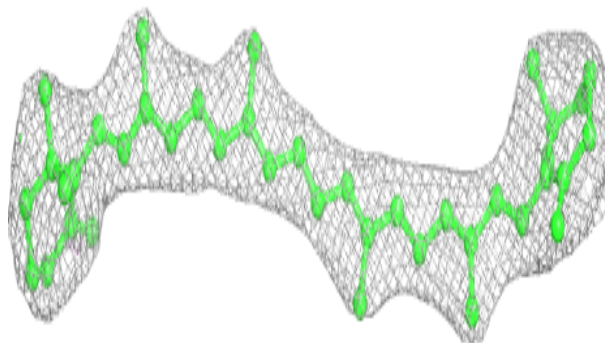


**Electron density around CLA A 408:**

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

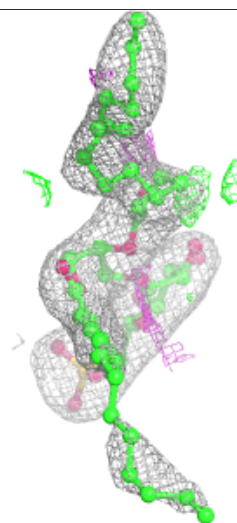
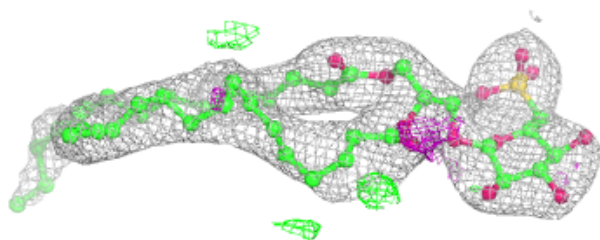
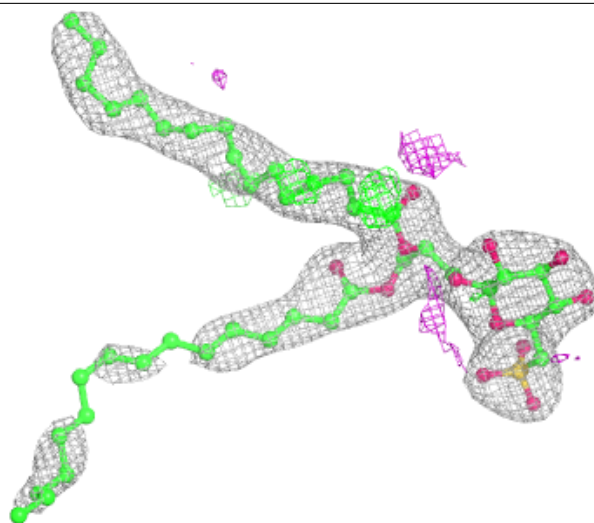
**Electron density around BCR y 101:**

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



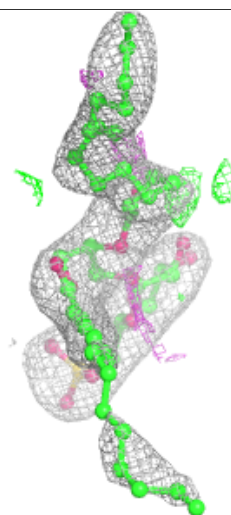
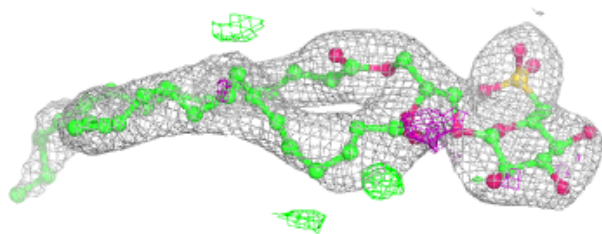
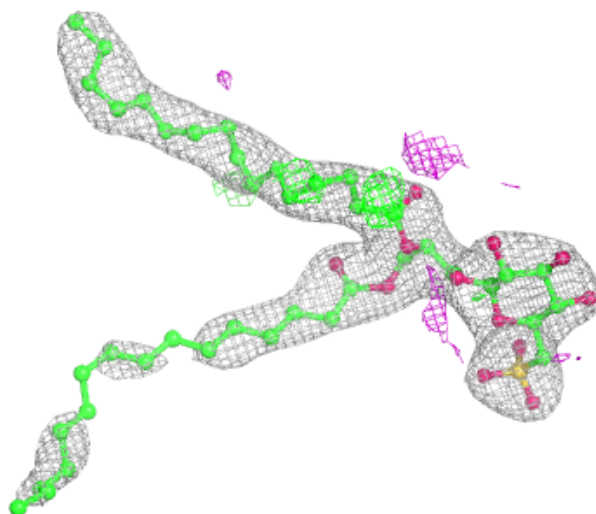
**Electron density around SQD A 410 (A):**

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

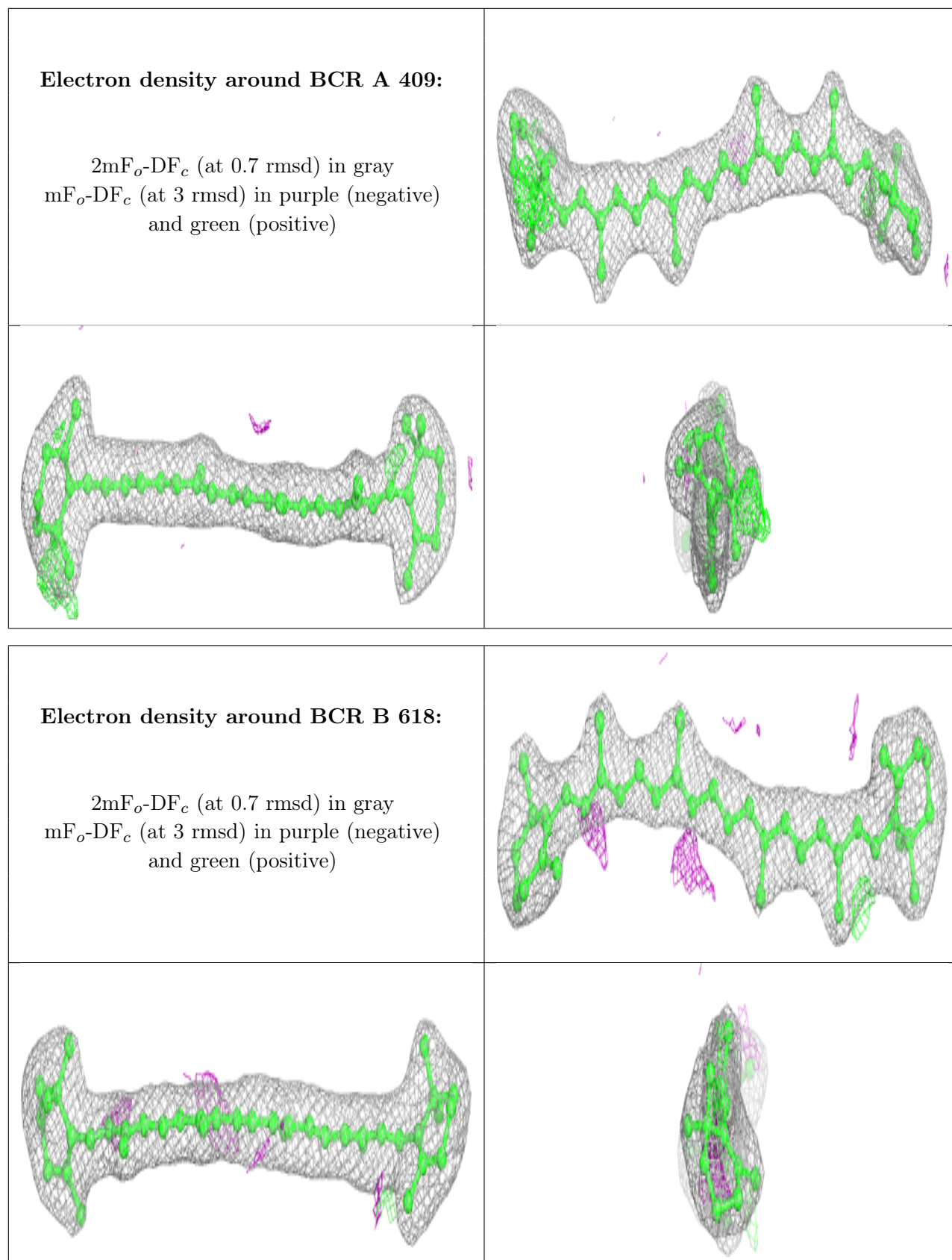


**Electron density around SQD A 410 (B):**

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

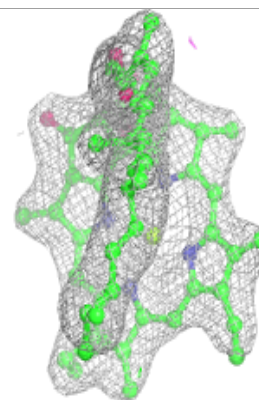
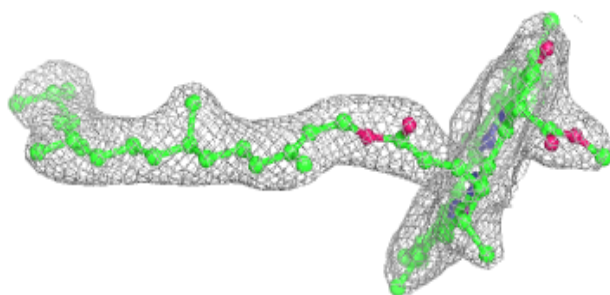
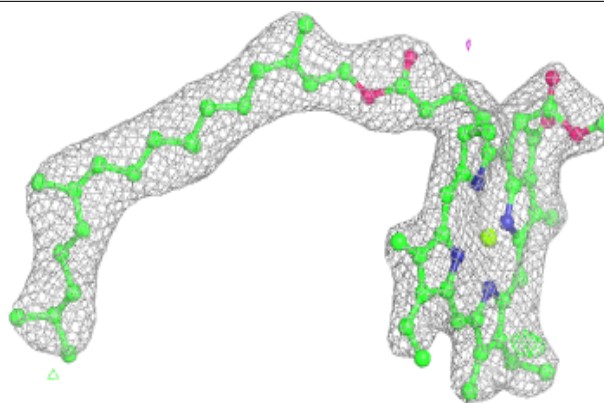




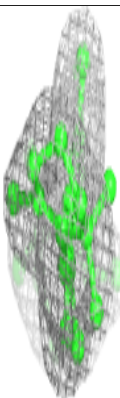
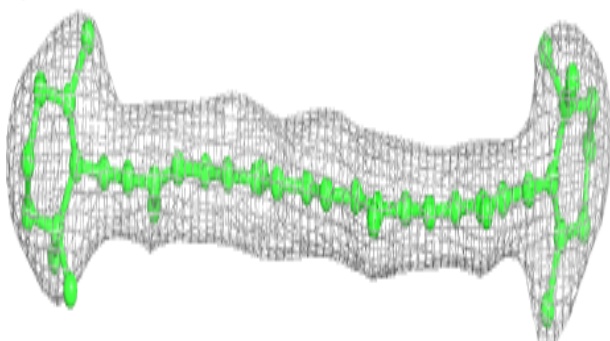
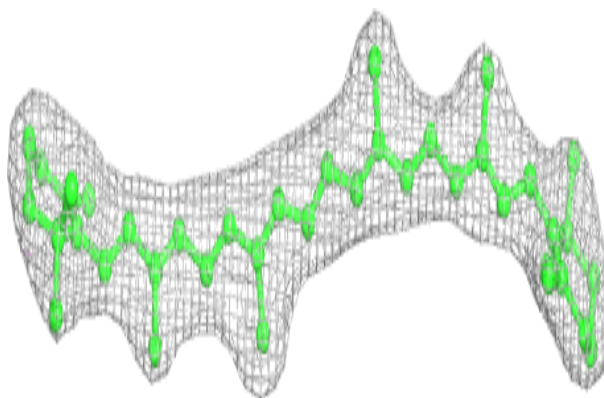


**Electron density around CLA b 609:**

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

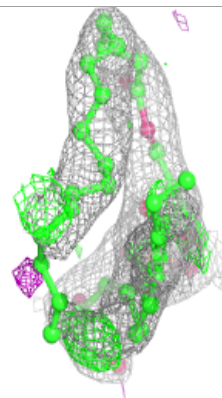
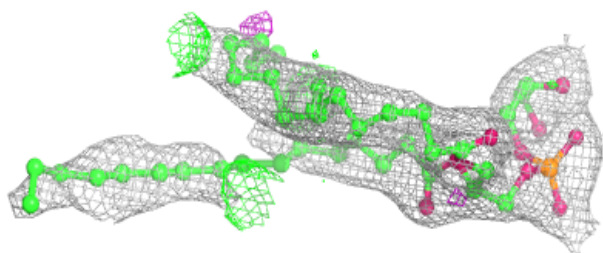
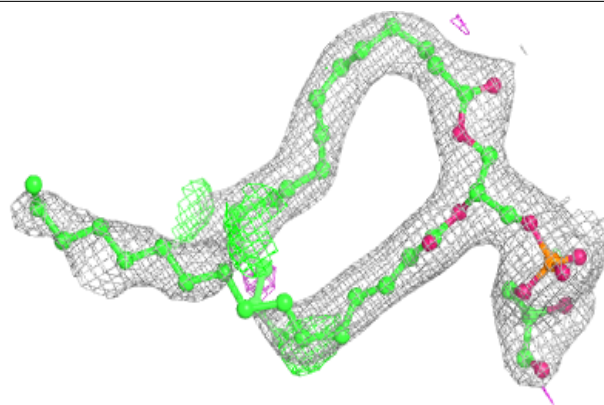
**Electron density around BCR C 516:**

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

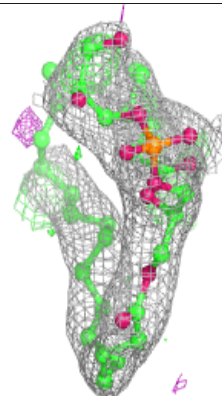
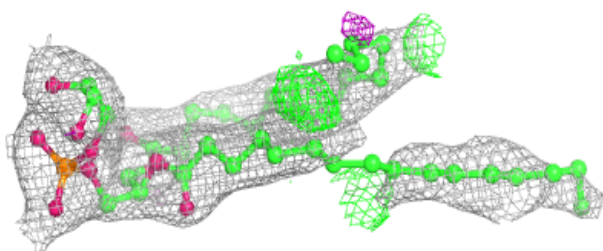
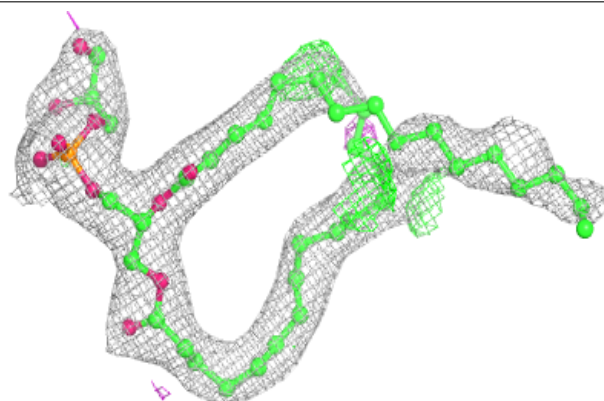


**Electron density around LHG d 408 (A):**

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

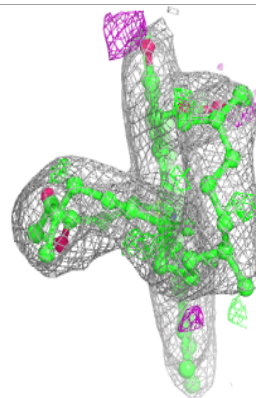
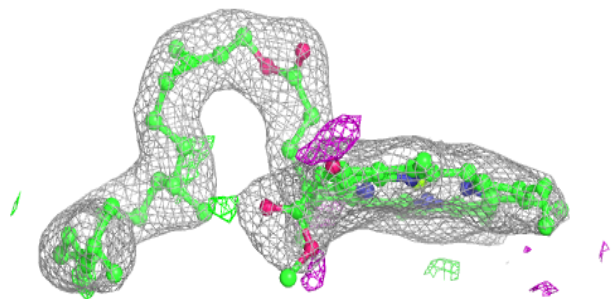
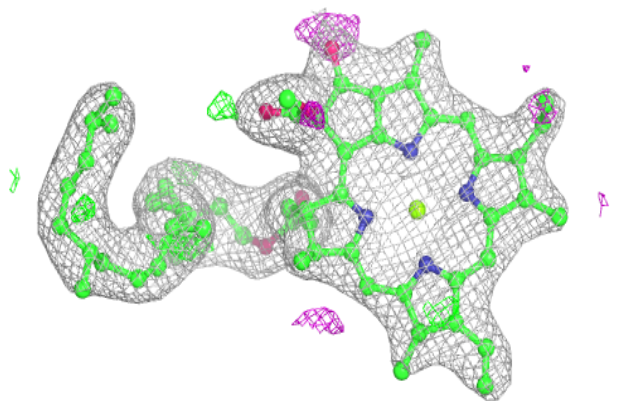
**Electron density around LHG d 408 (B):**

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

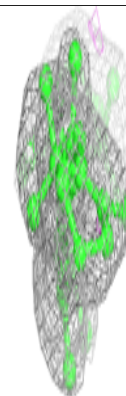
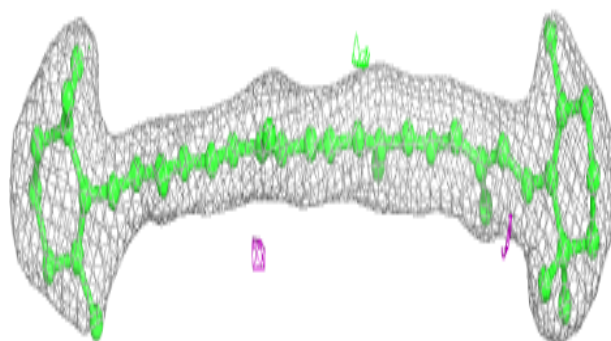
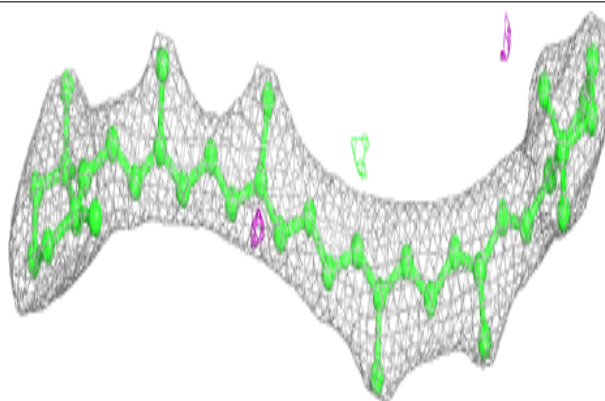


**Electron density around CLA b 612:**

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

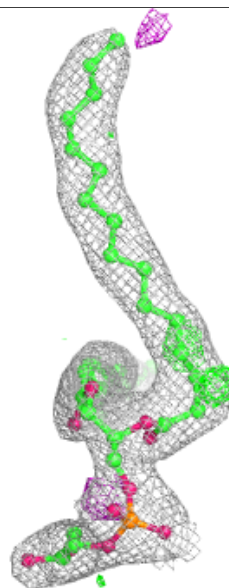
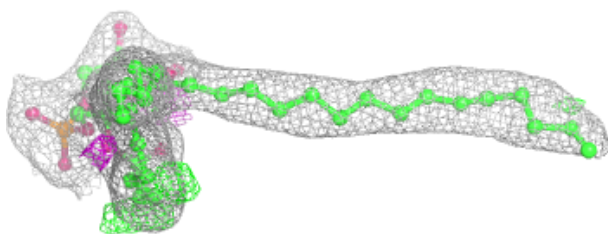
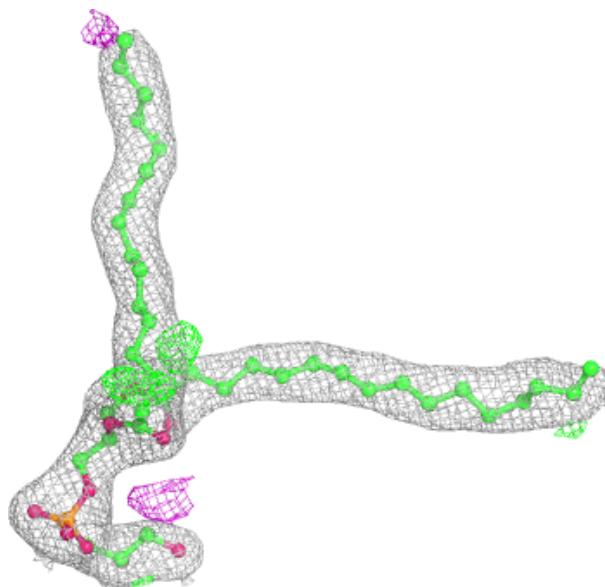
**Electron density around BCR H 101:**

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



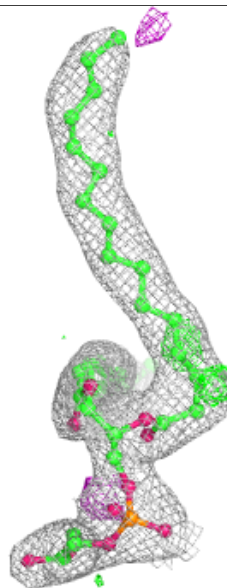
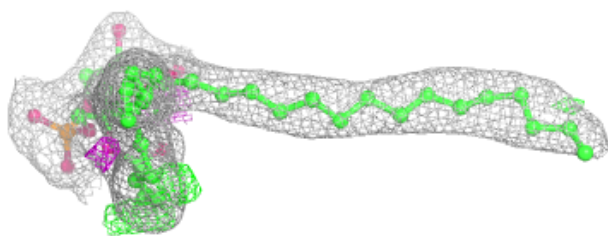
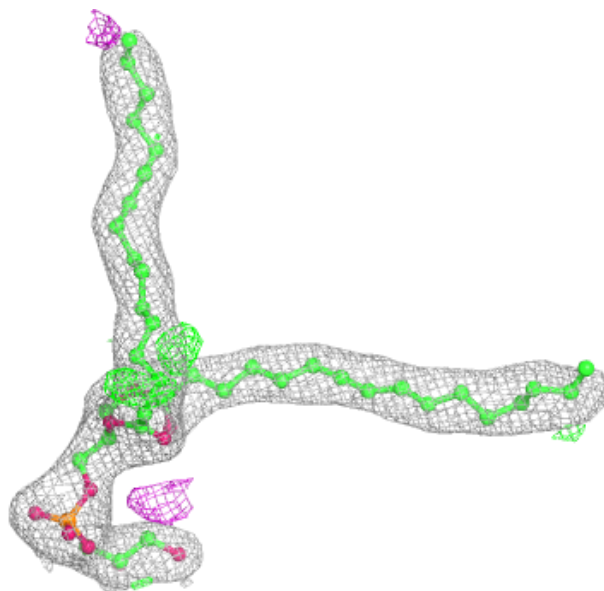
**Electron density around LHG 1 101 (A):**

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



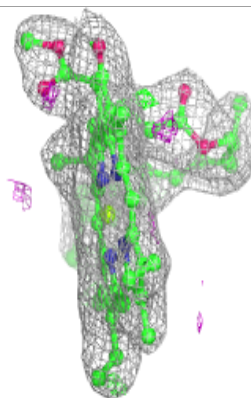
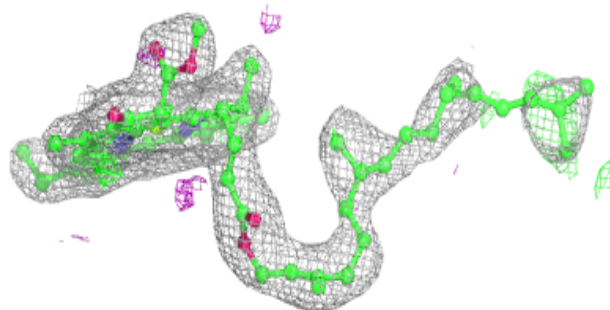
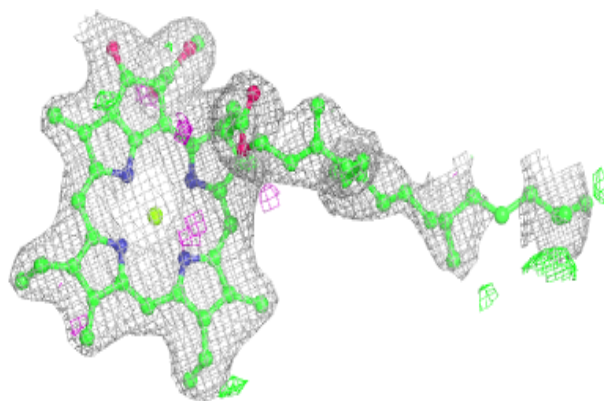
**Electron density around LHG 1 101 (B):**

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

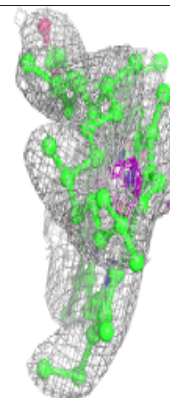
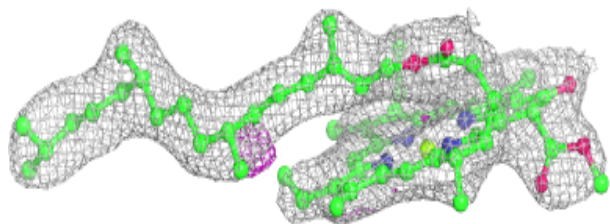
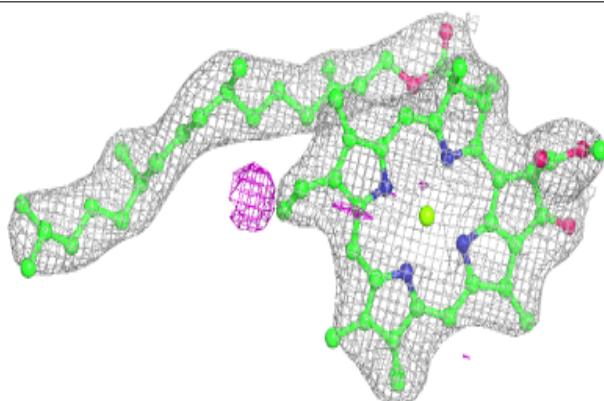


**Electron density around CLA a 407 (A):**

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

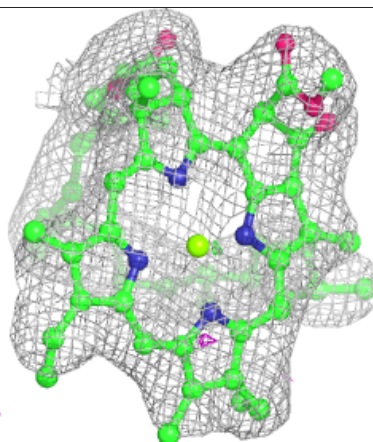
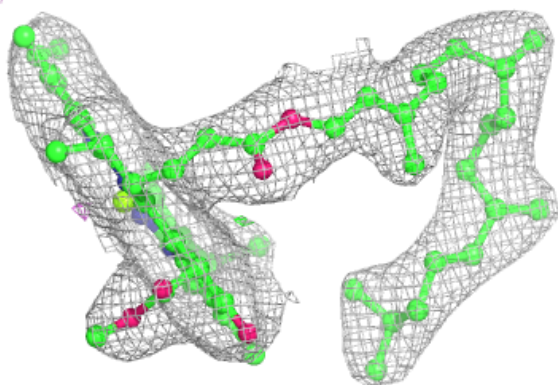
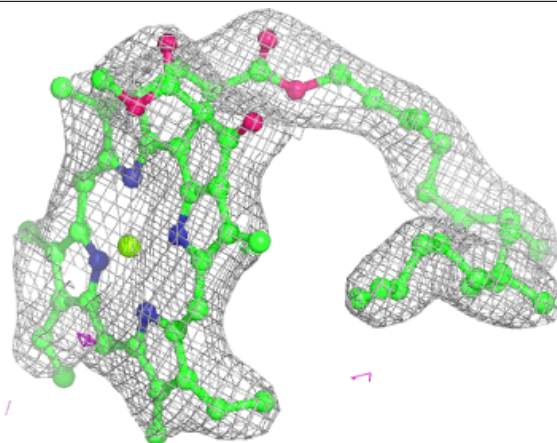
**Electron density around CLA c 502:**

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

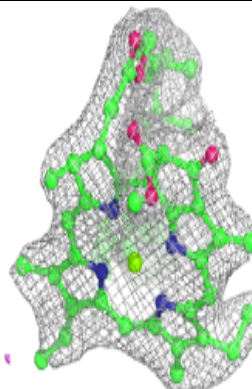
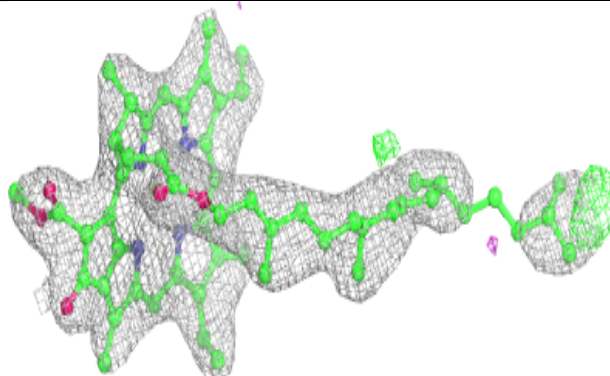
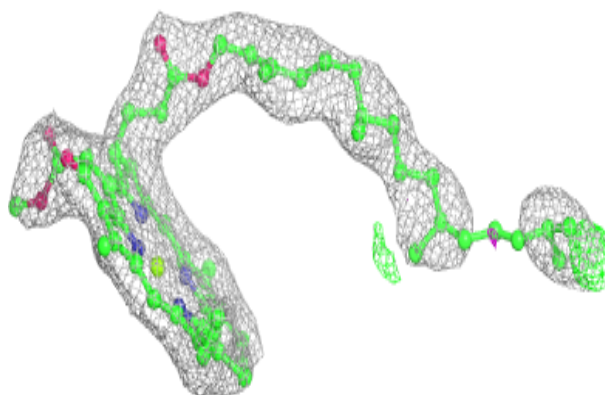


**Electron density around CLA c 504:**

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

**Electron density around CLA c 505:**

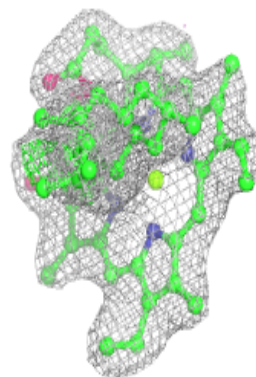
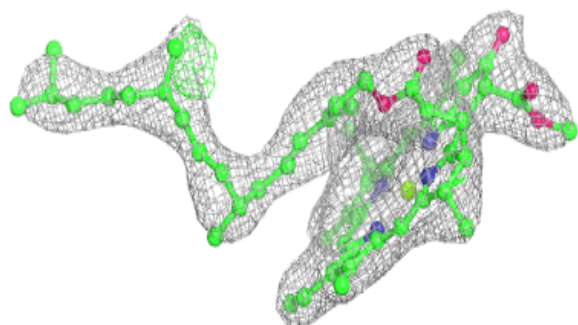
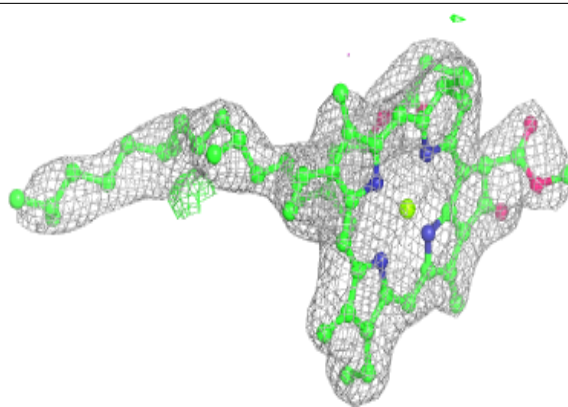
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





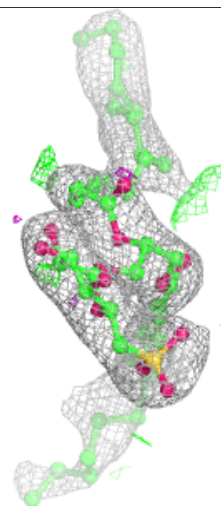
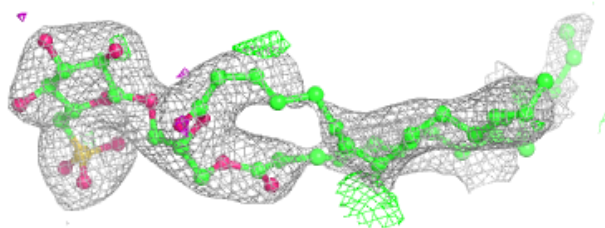
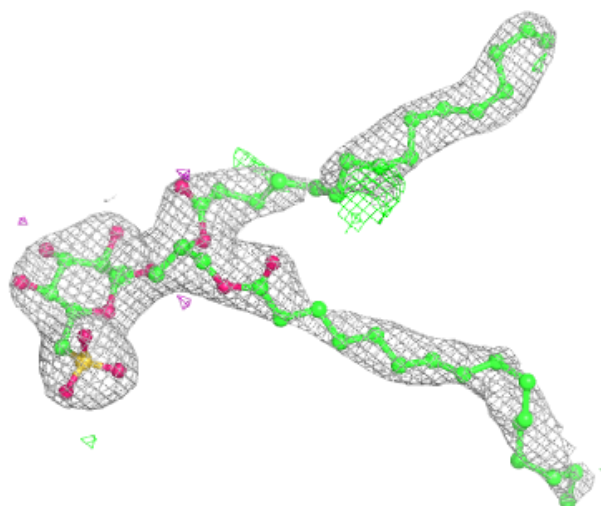
**Electron density around CLA c 506:**

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



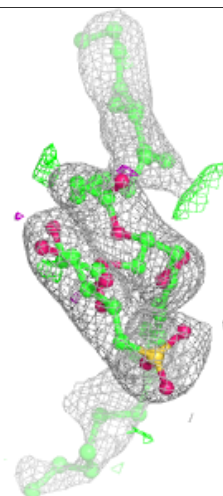
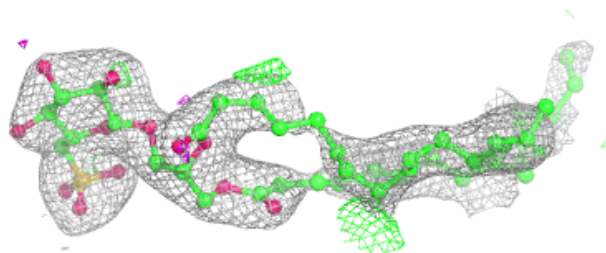
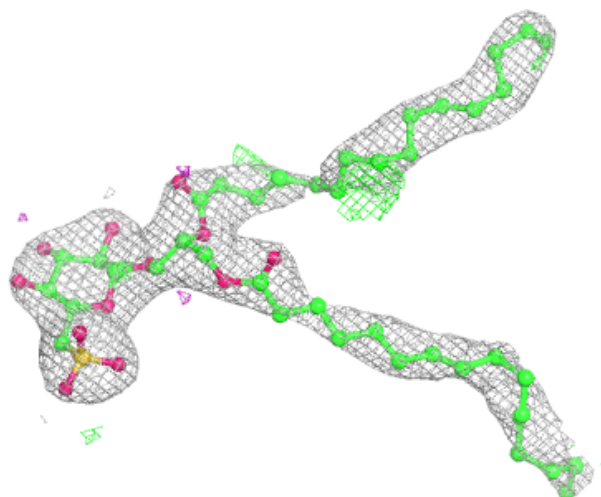
**Electron density around SQD a 411 (A):**

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



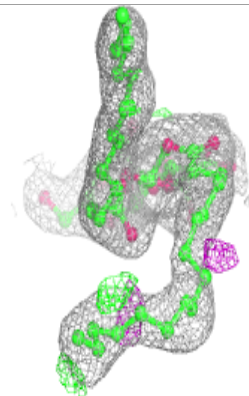
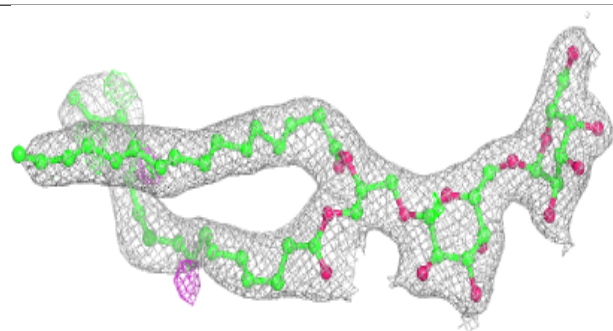
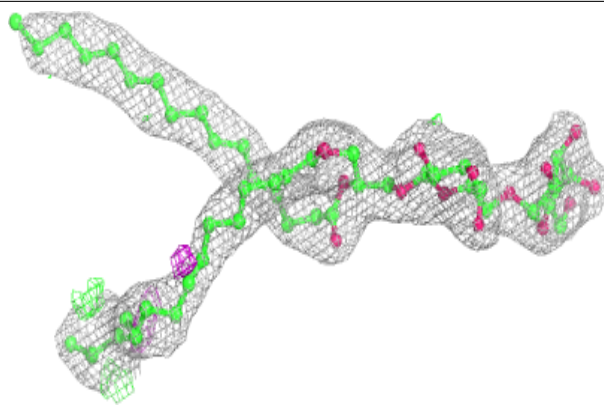
**Electron density around SQD a 411 (B):**

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

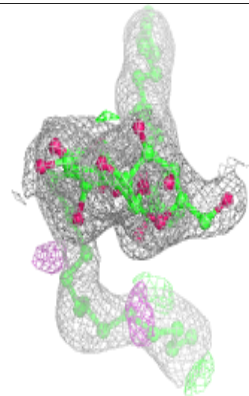
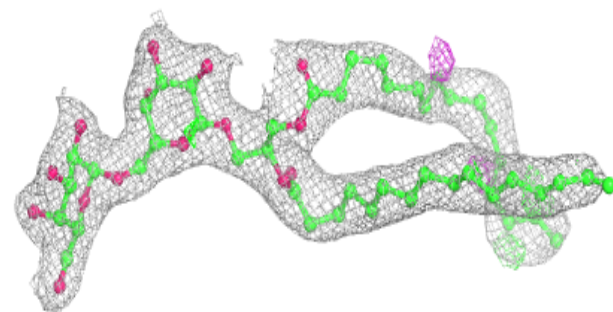
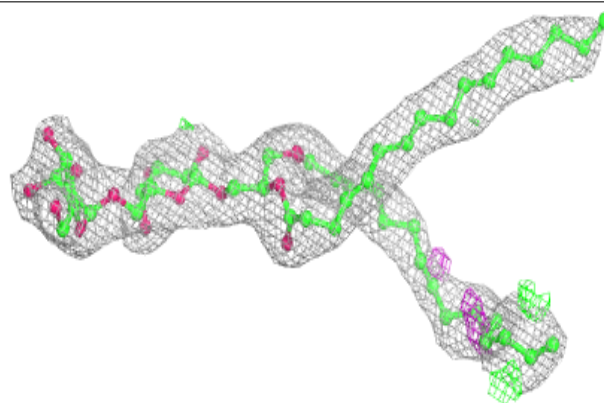


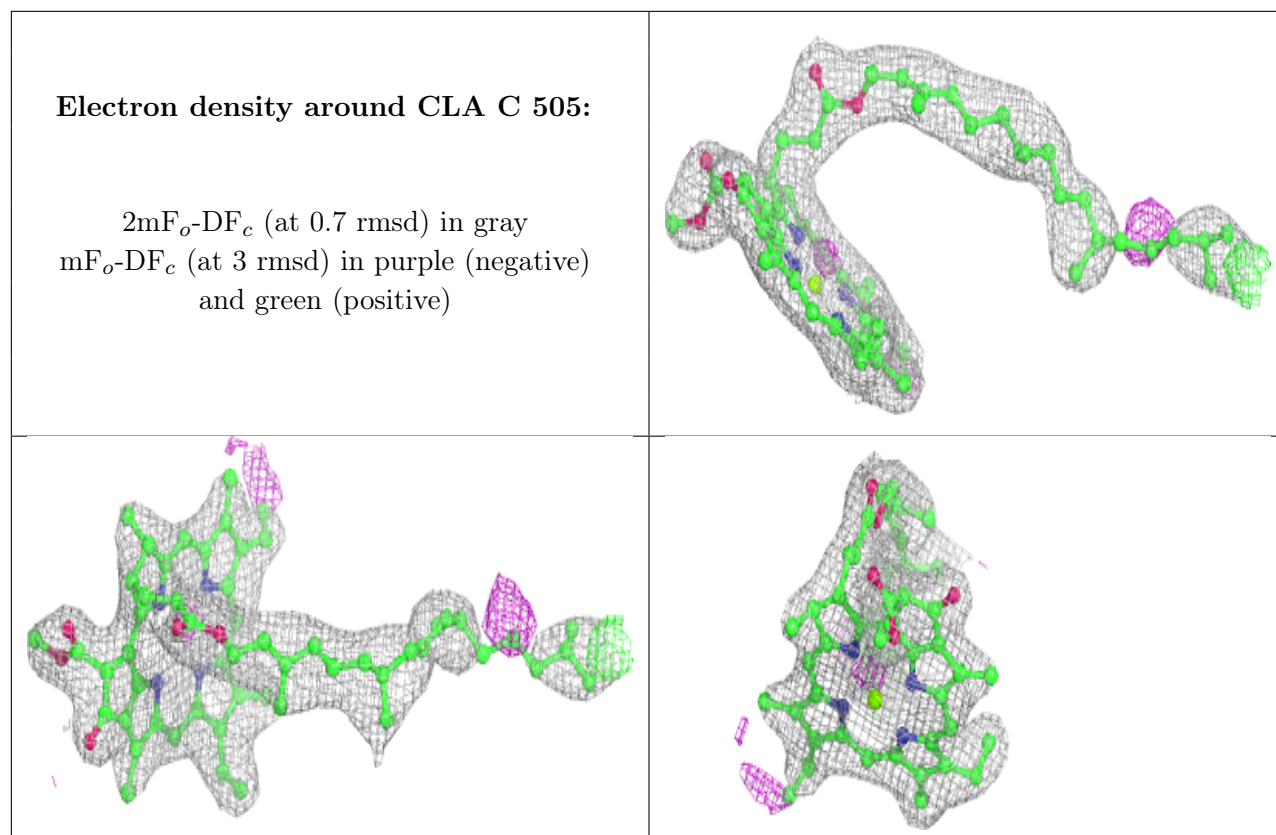
**Electron density around DGD c 517 (A):**

$2mF_o-DF_c$  (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 (B):**

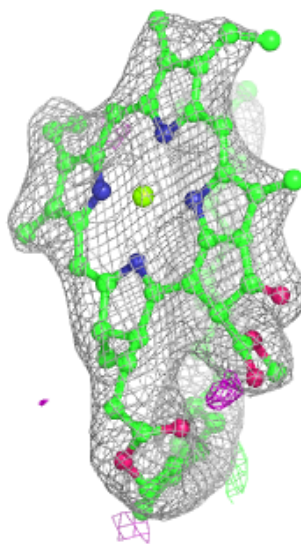
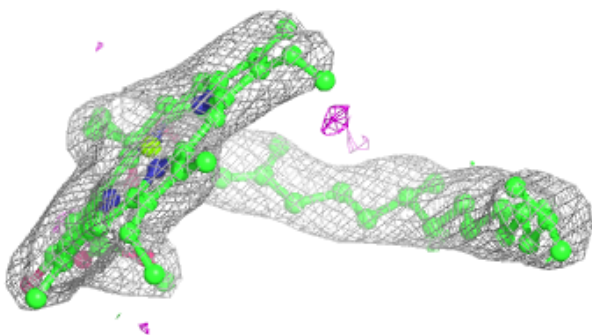
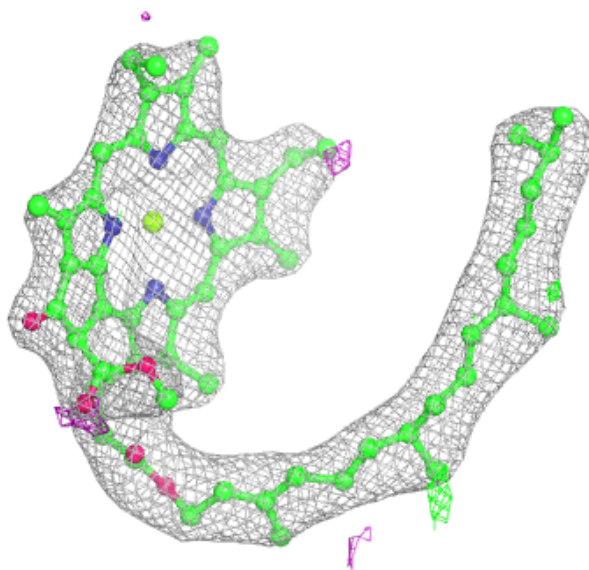
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





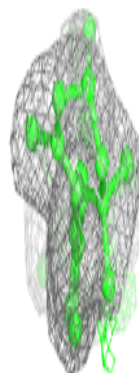
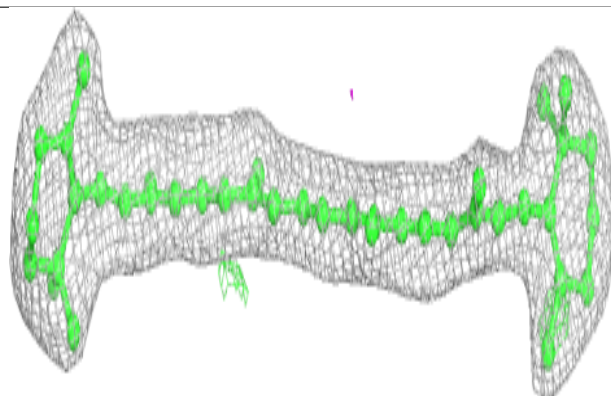
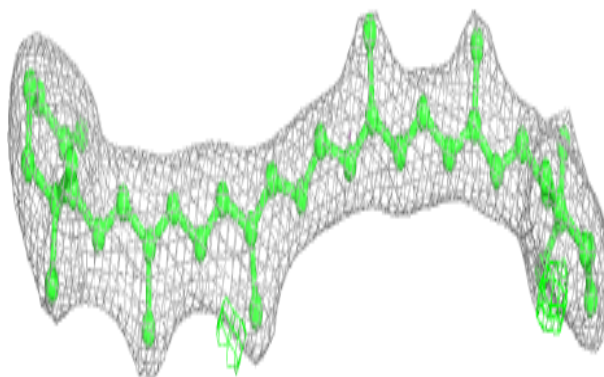
**Electron density around CLA c 508:**

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

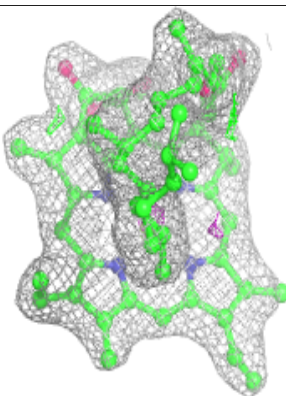
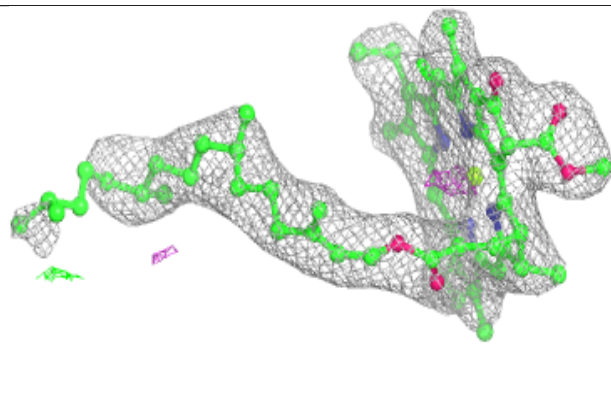
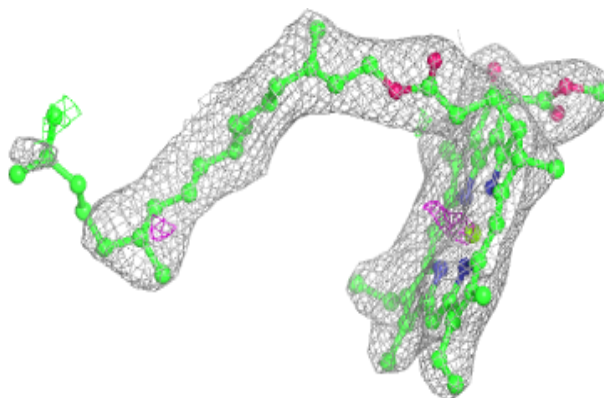


**Electron density around BCR a 410:**

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

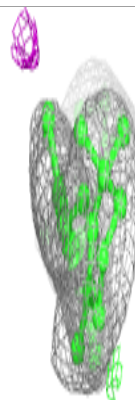
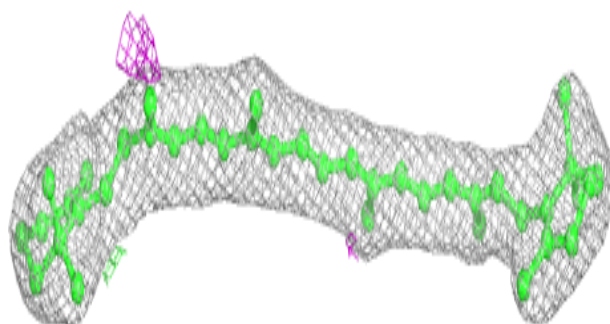
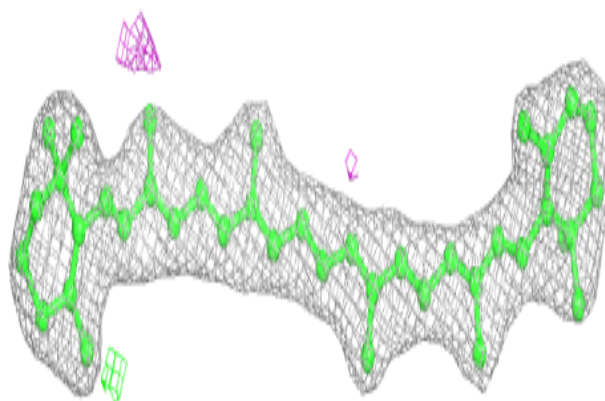
**Electron density around CLA c 509:**

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

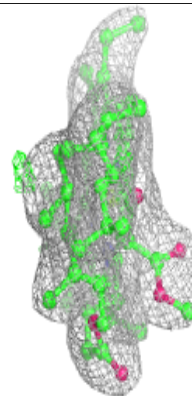
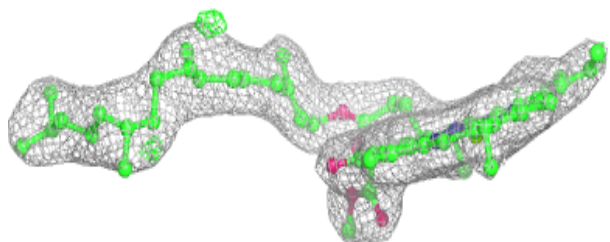
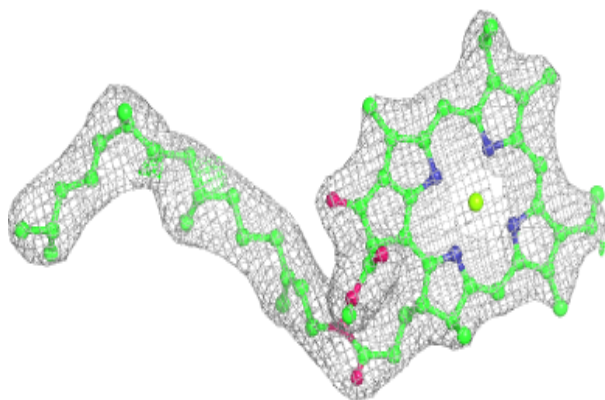


**Electron density around BCR b 619:**

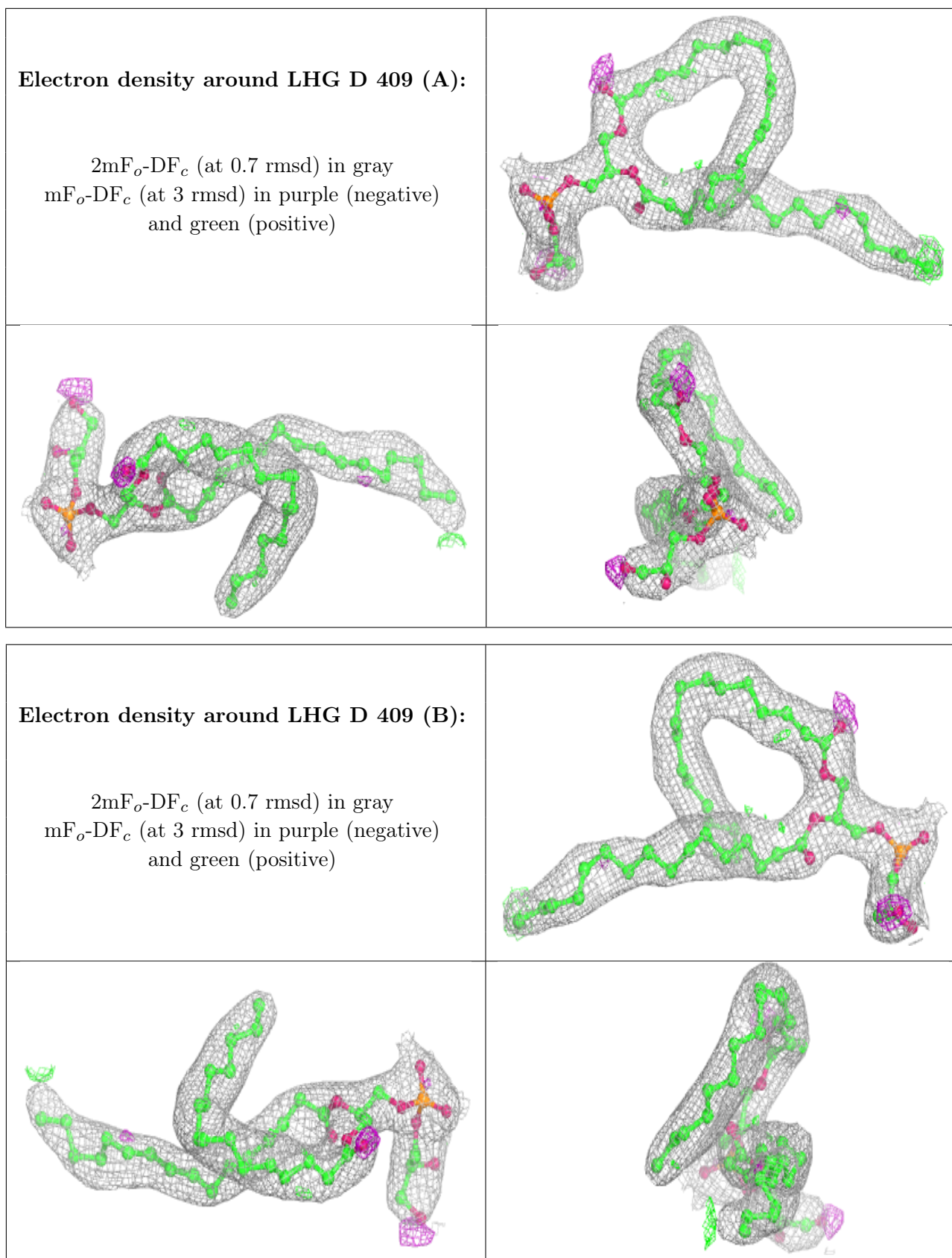
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

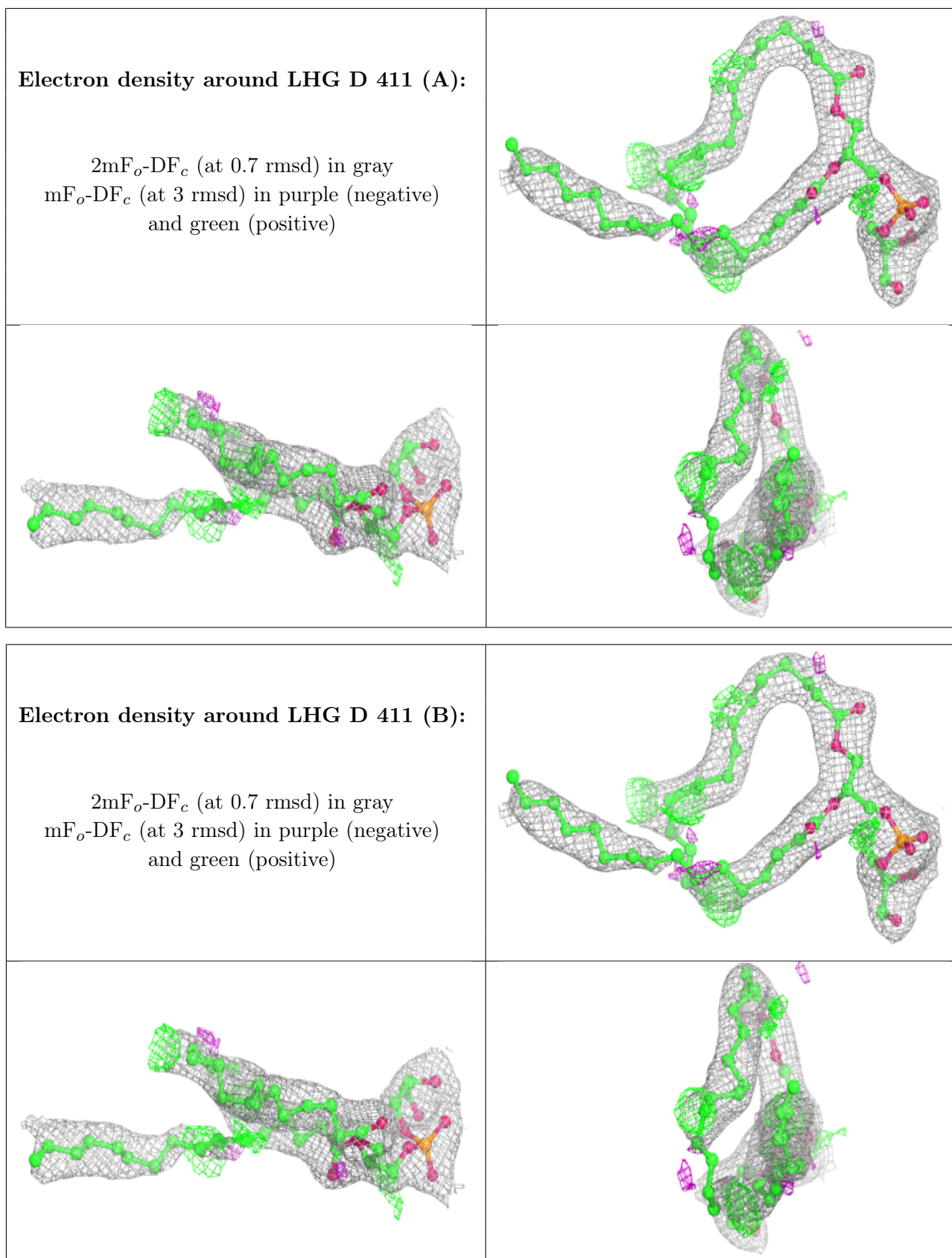
**Electron density around CLA b 602:**

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



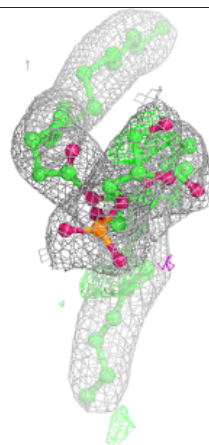
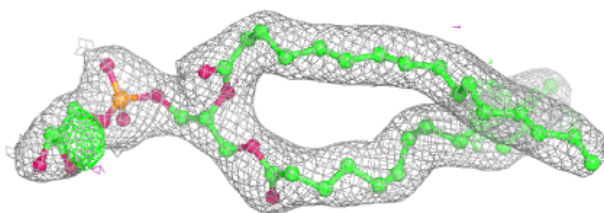
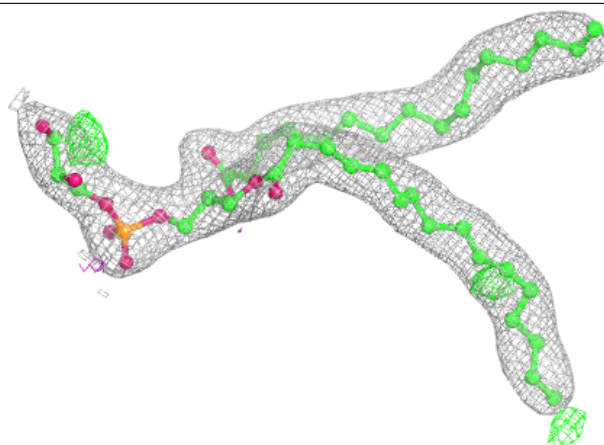






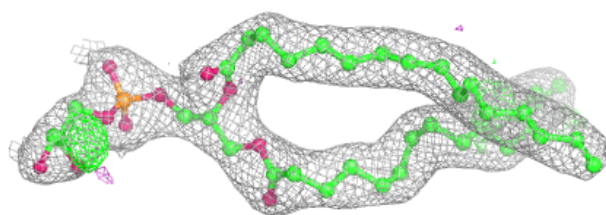
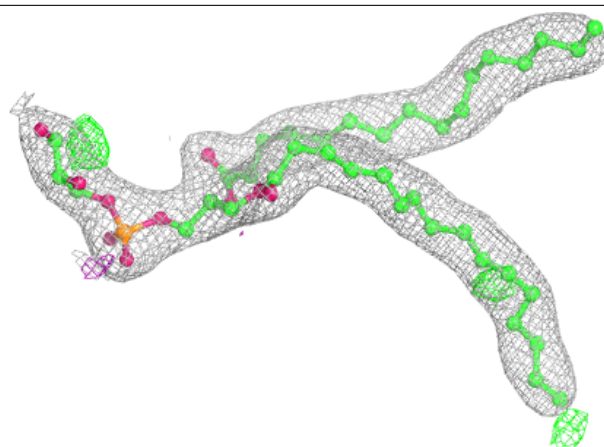
**Electron density around LHG d 407 (A):**

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

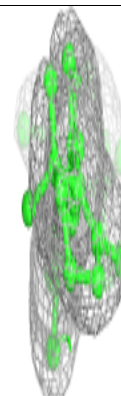
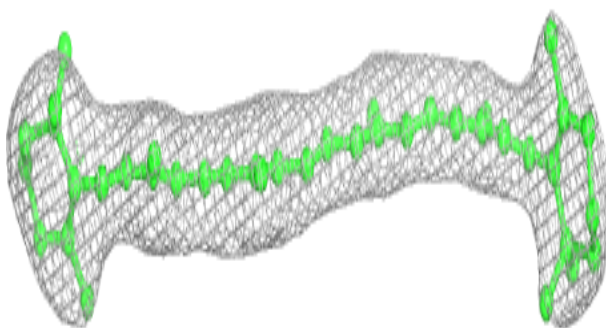
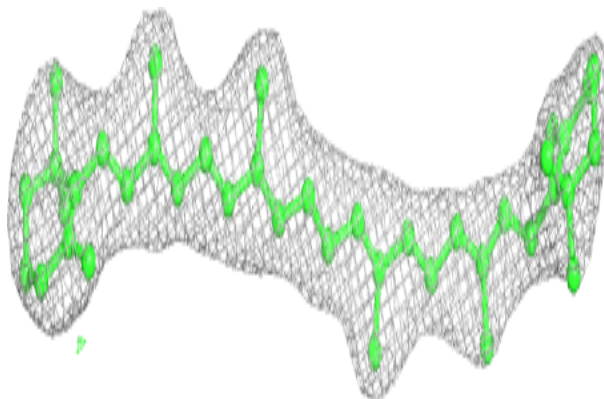


**Electron density around LHG d 407 (B):**

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

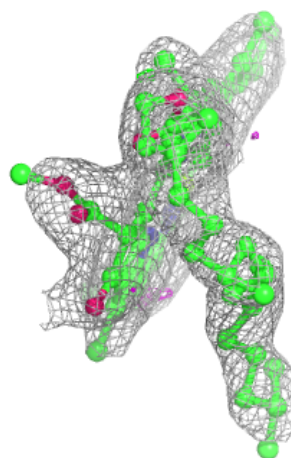
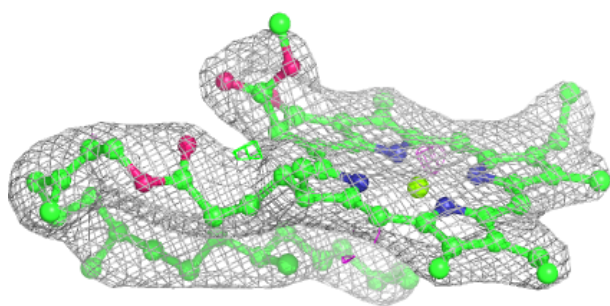
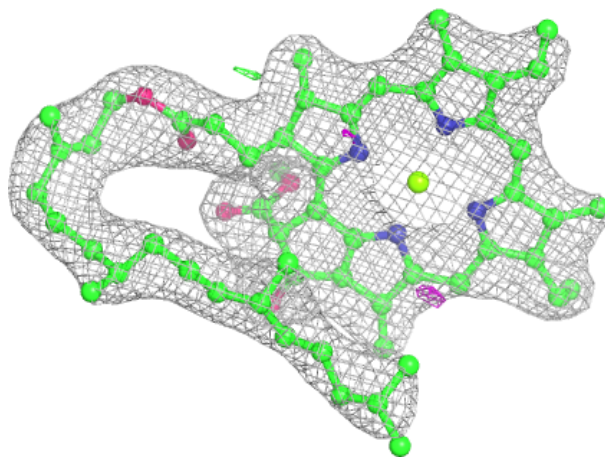
**Electron density around BCR c 516:**

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



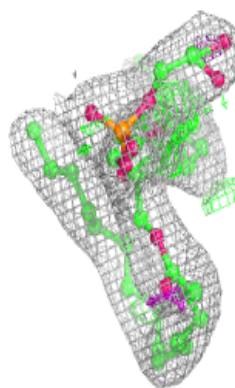
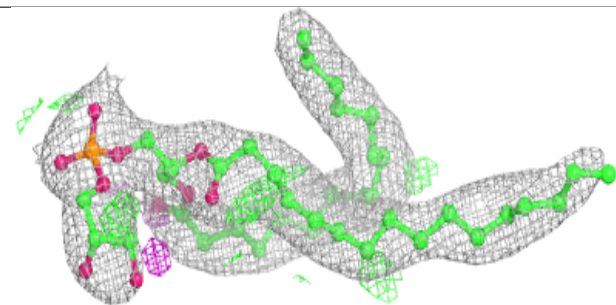
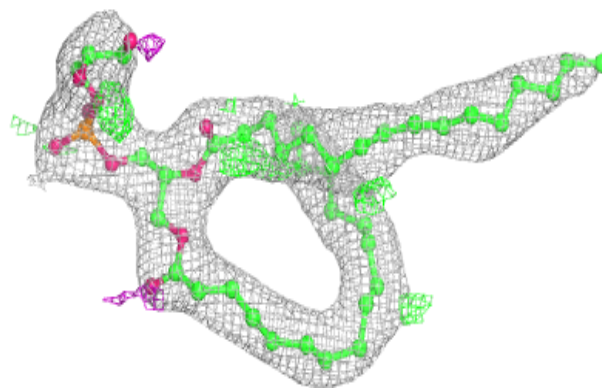
**Electron density around CLA C 510:**

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

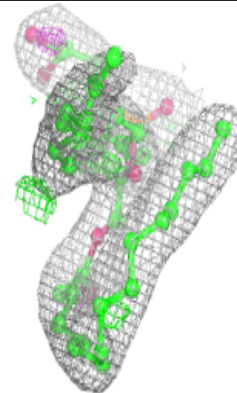
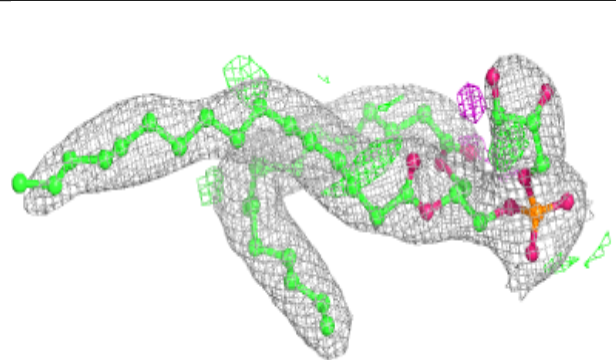
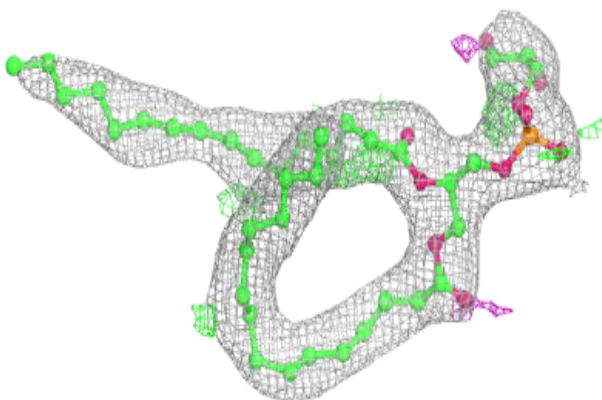


**Electron density around LHG d 711 (A):**

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

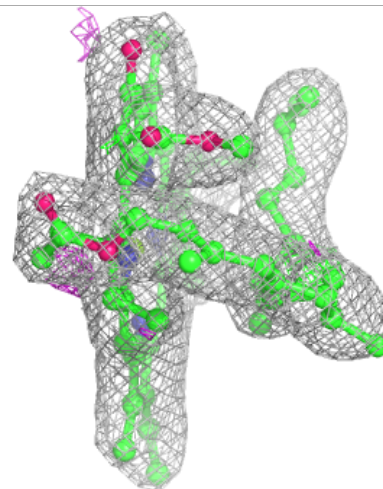
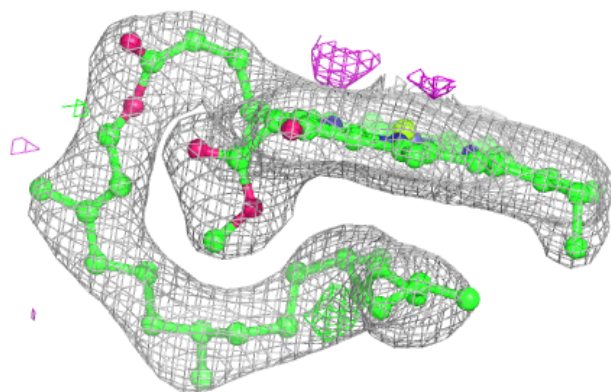
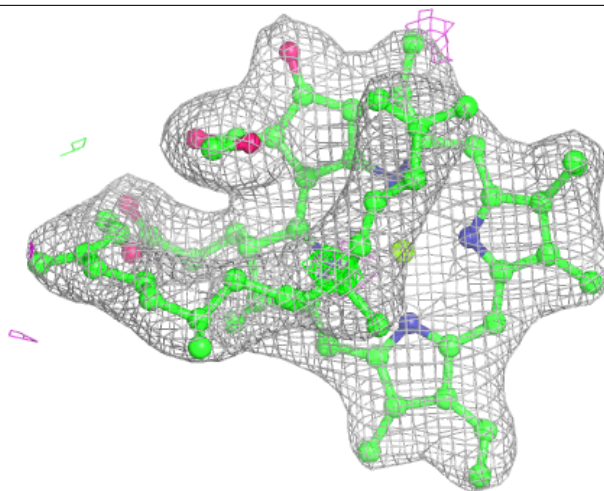
**Electron density around LHG d 711 (B):**

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



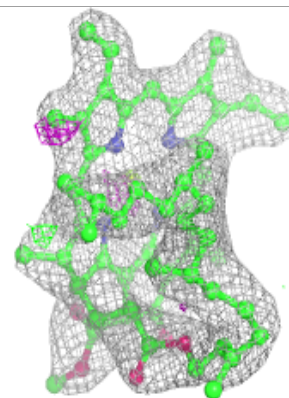
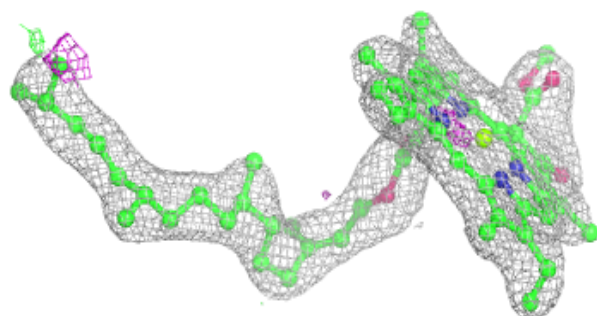
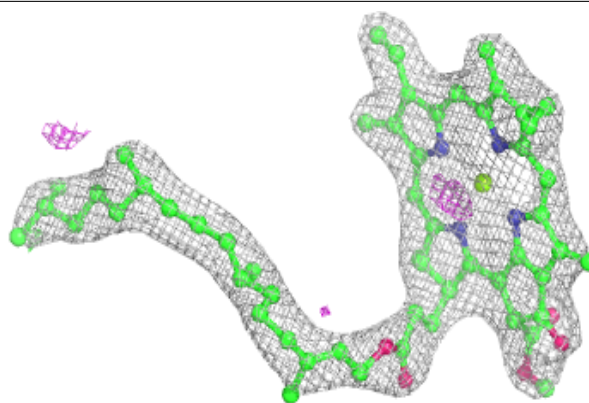
**Electron density around CLA C 511:**

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

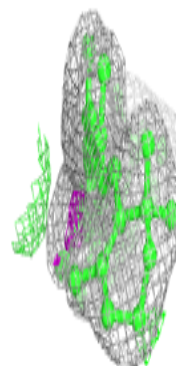
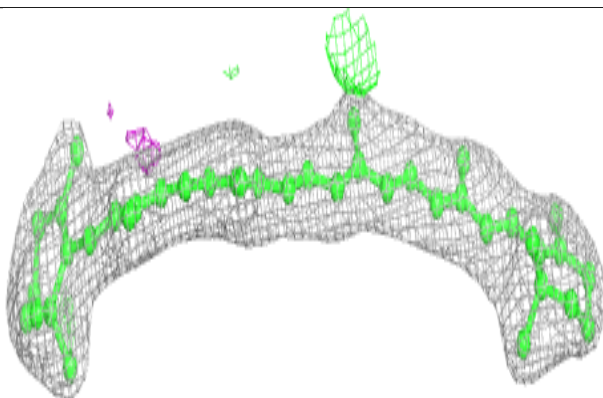
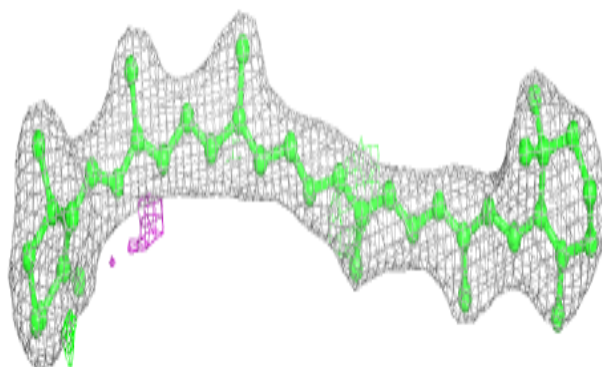


**Electron density around CLA C 512:**

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

**Electron density around BCR t 103:**

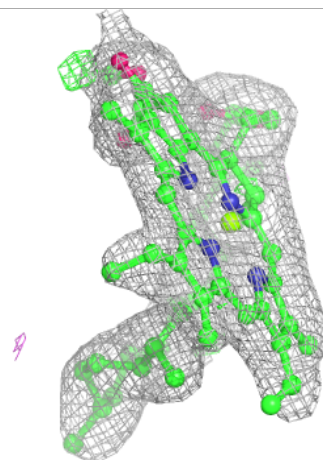
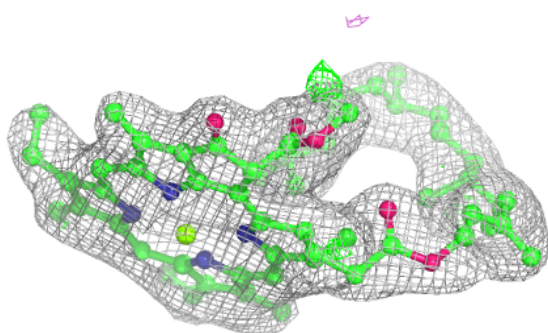
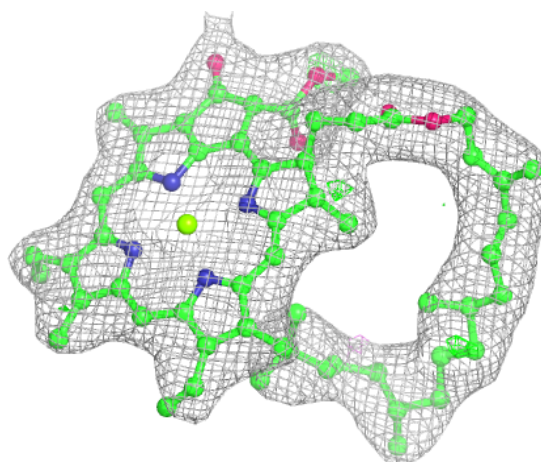
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





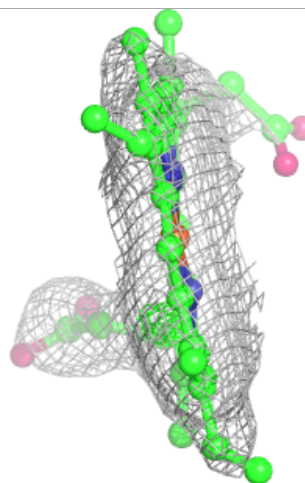
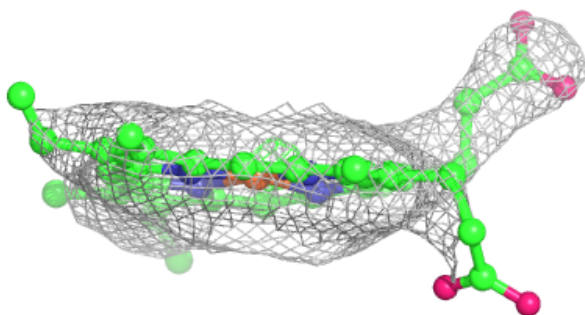
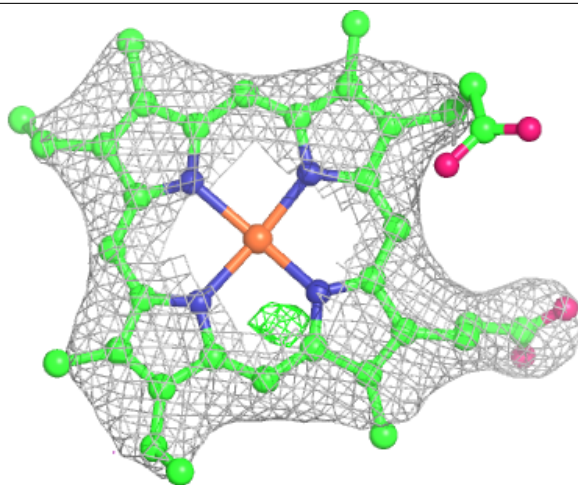
**Electron density around CLA b 615:**

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



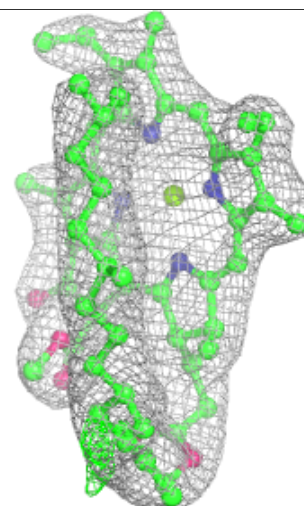
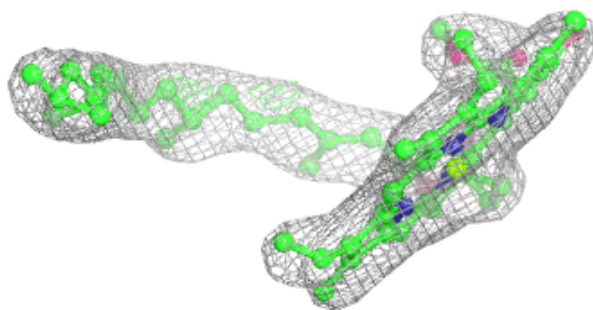
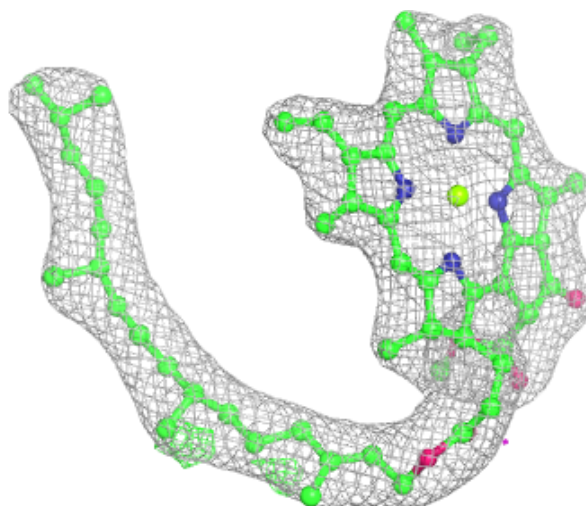
**Electron density around HEM e 87:**

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



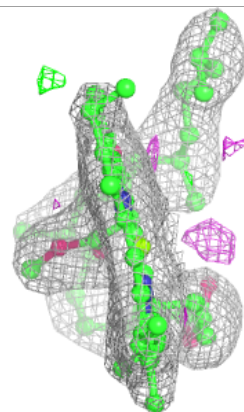
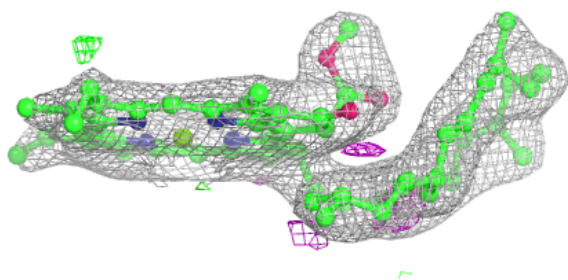
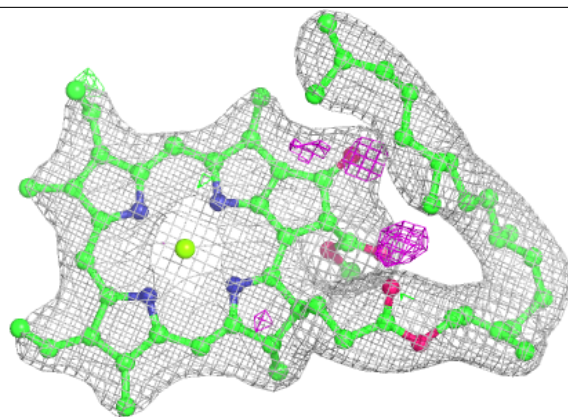
**Electron density around CLA C 508:**

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



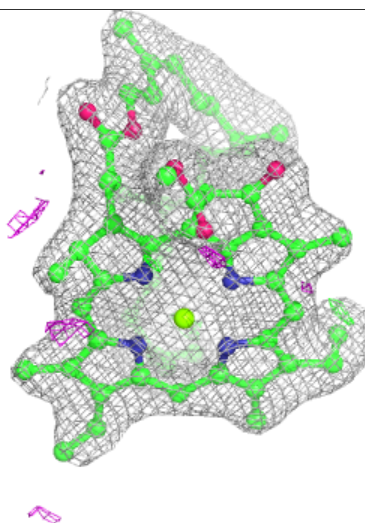
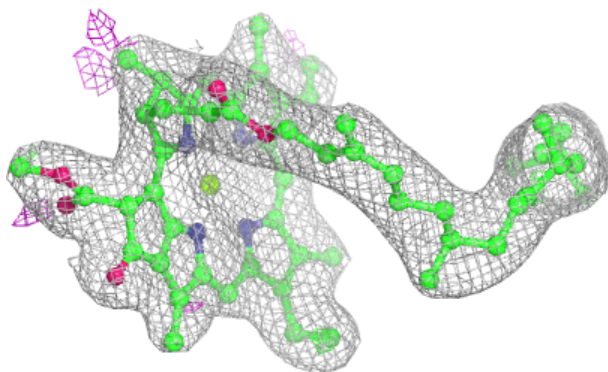
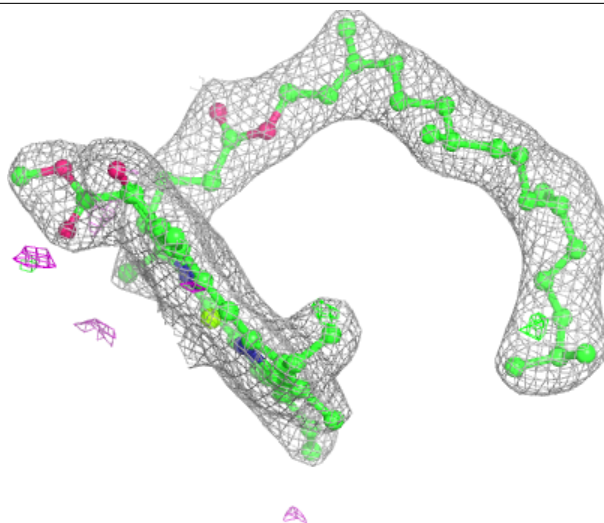
**Electron density around CLA b 610:**

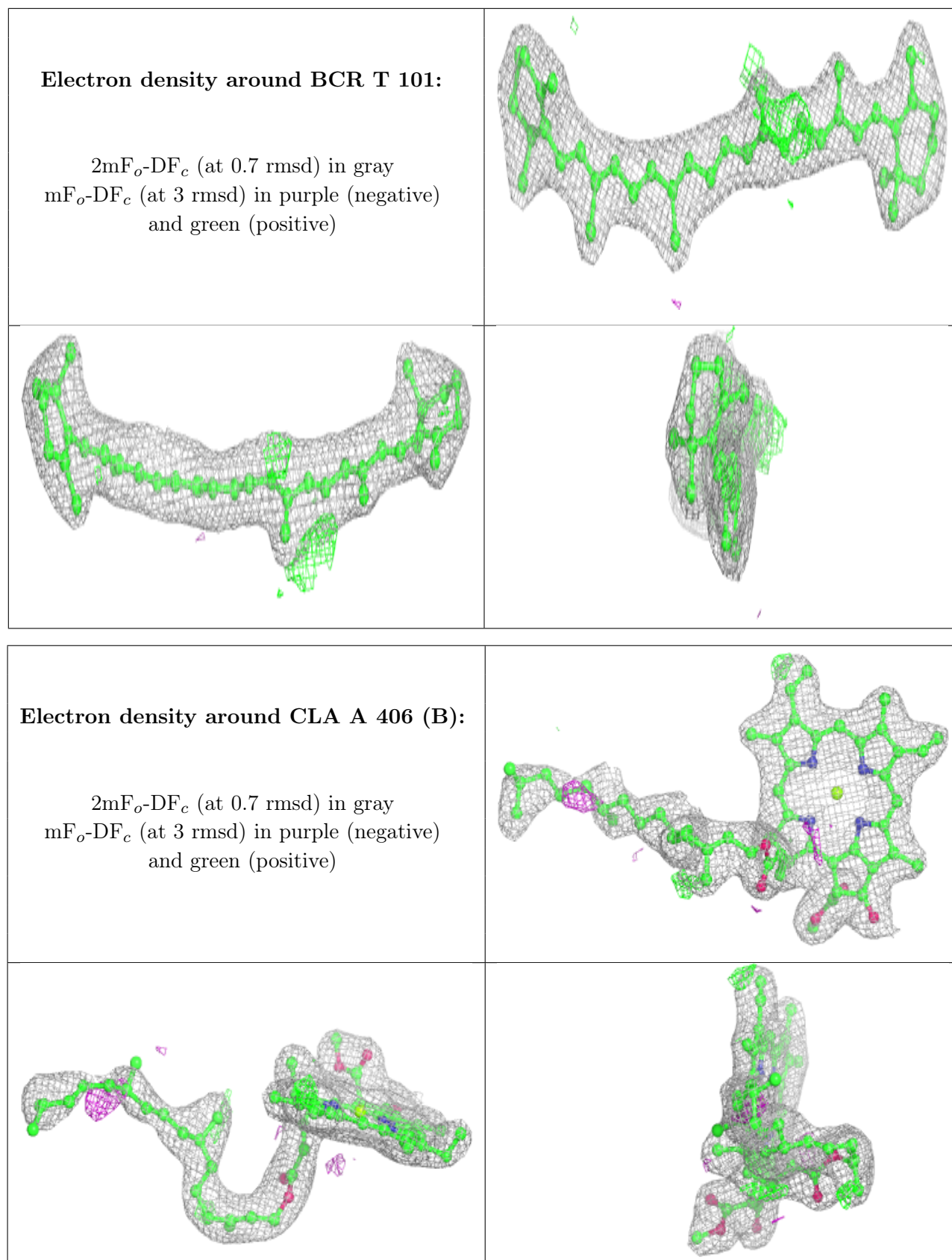
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA b 611:**

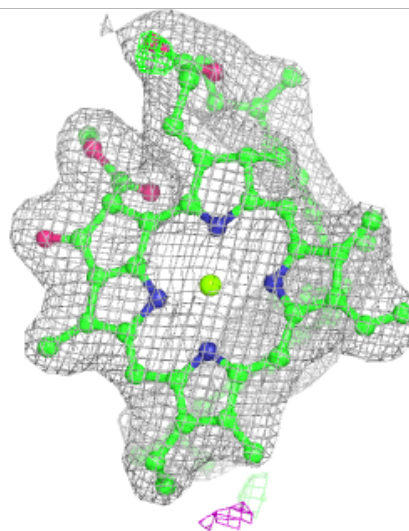
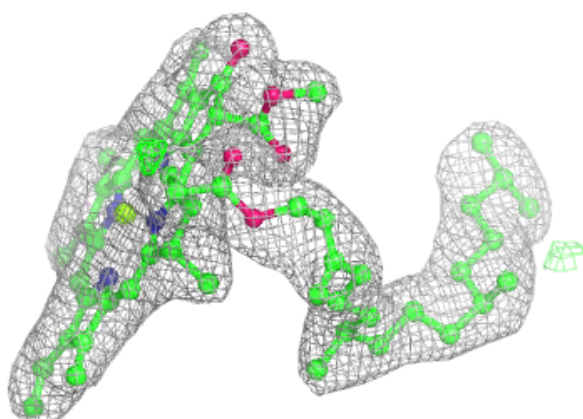
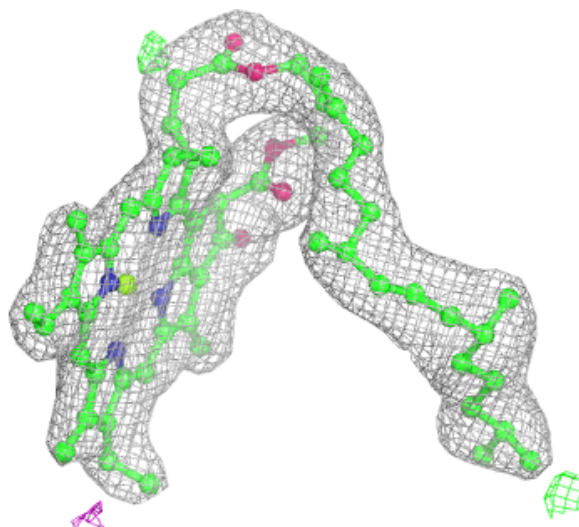
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





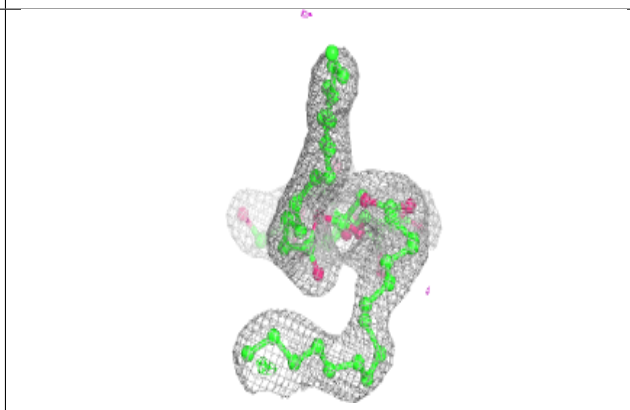
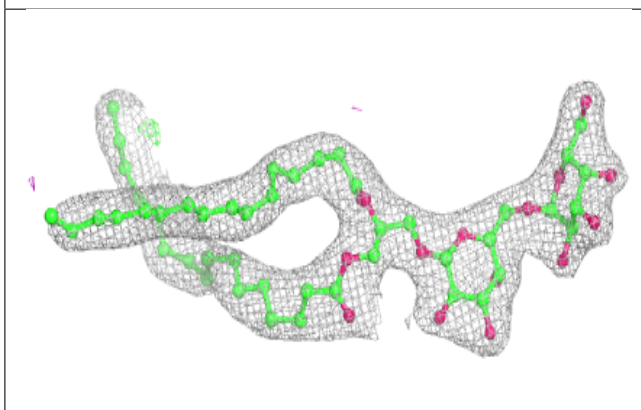
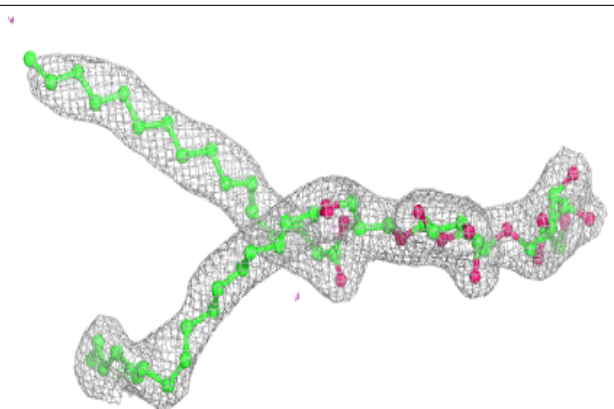
**Electron density around CLA b 613:**

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

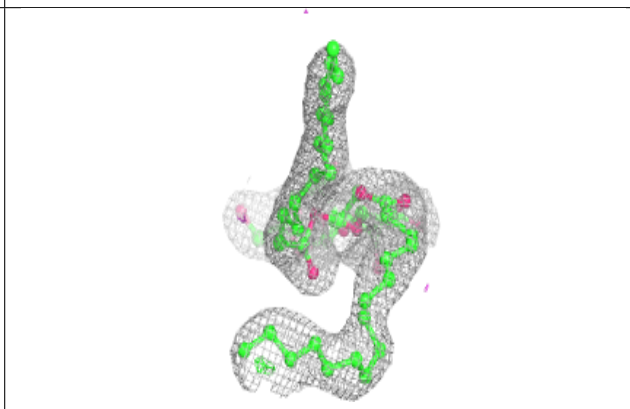
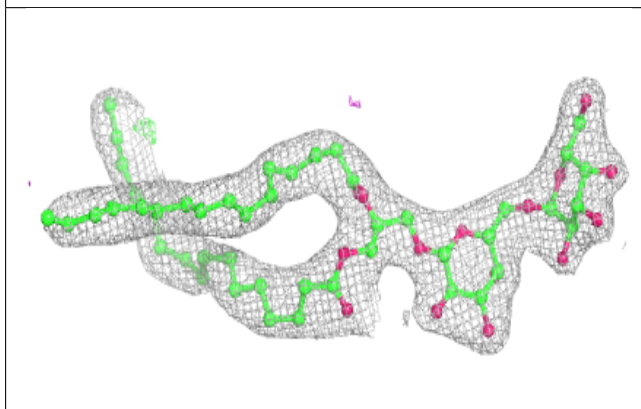
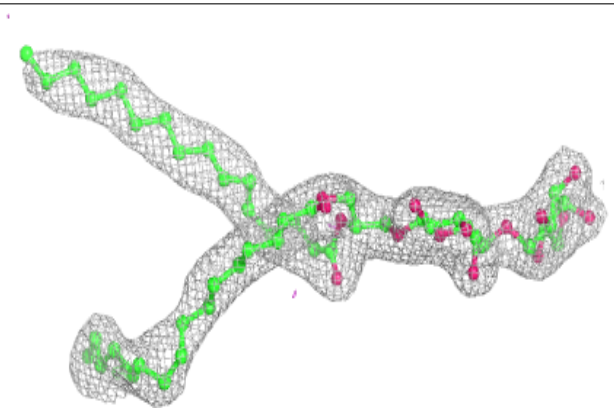


**Electron density around DGD C 517 (A):**

$2mF_o-DF_c$  (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 (B):**

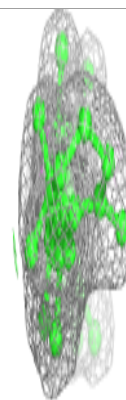
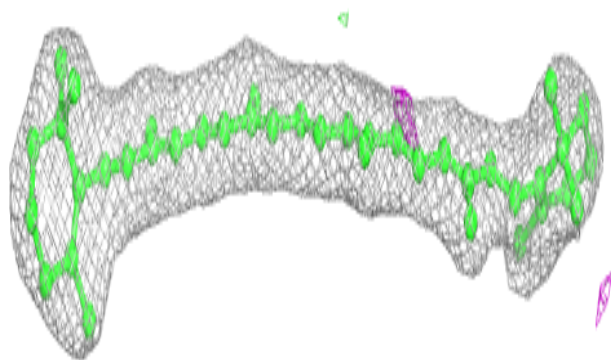
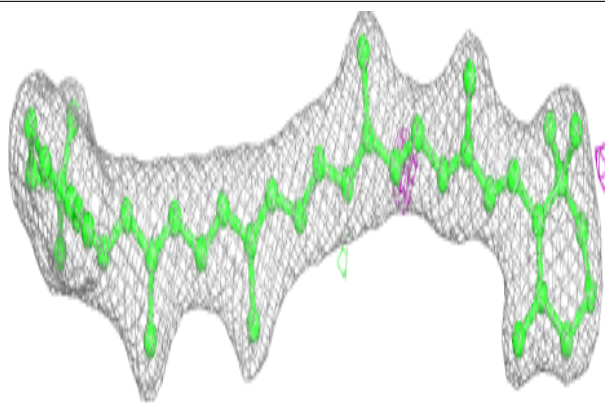
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



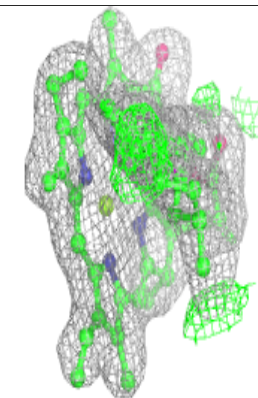
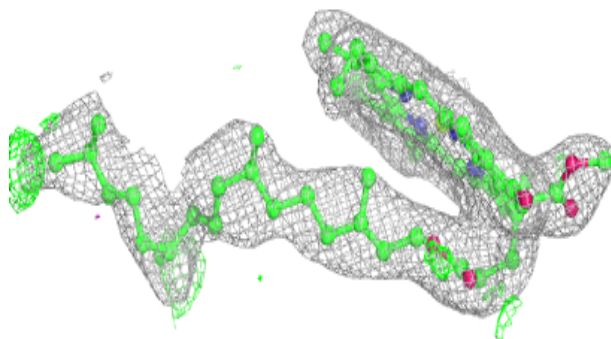
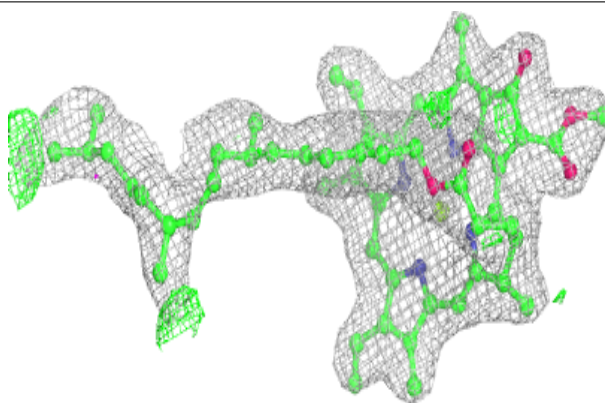


**Electron density around BCR b 617:**

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

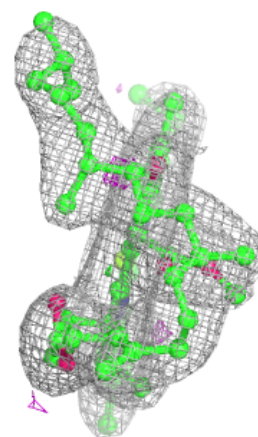
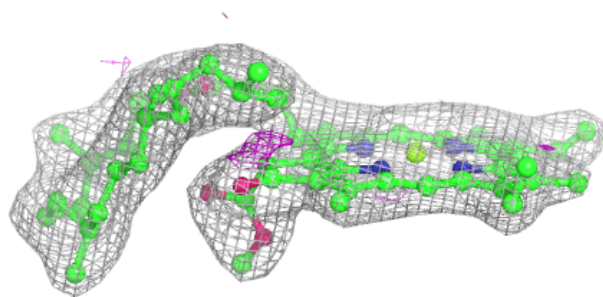
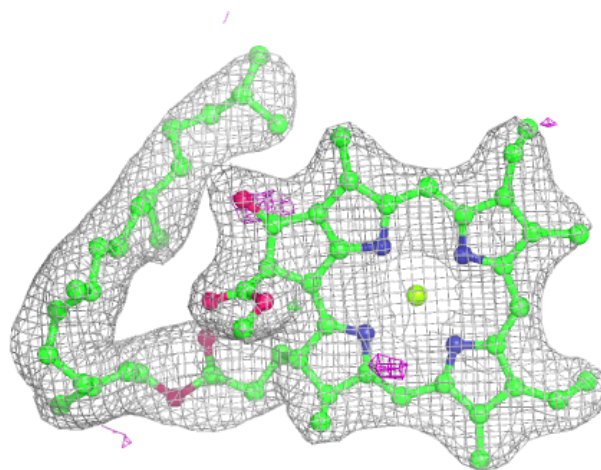
**Electron density around CLA b 614:**

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



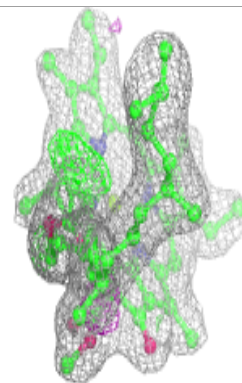
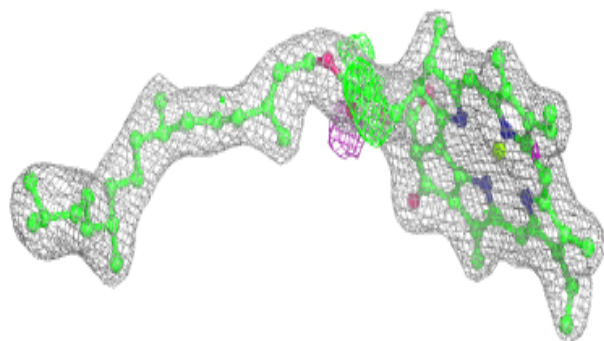
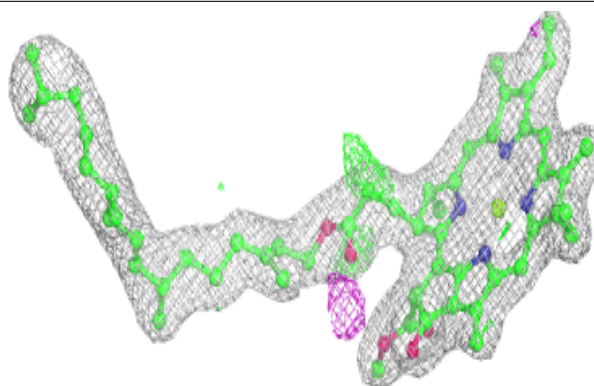
**Electron density around CLA B 610:**

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

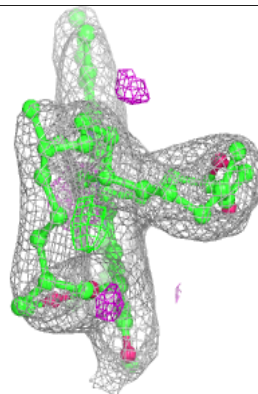
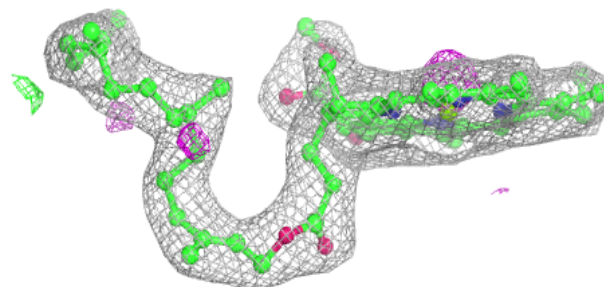
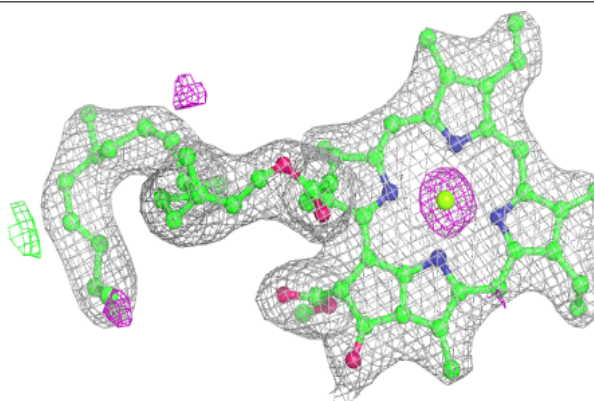


**Electron density around CLA A 404 (A):**

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

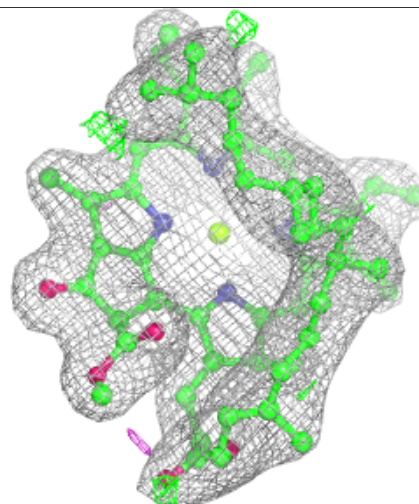
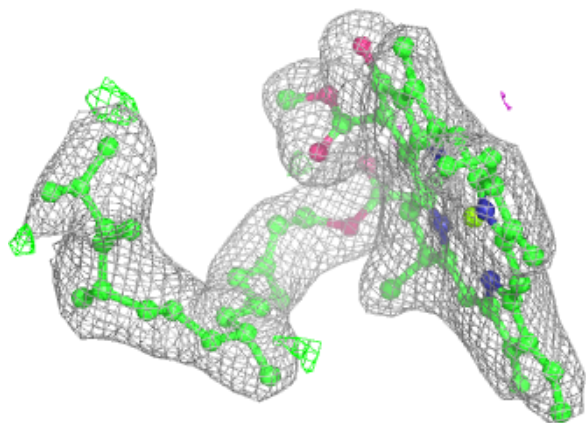
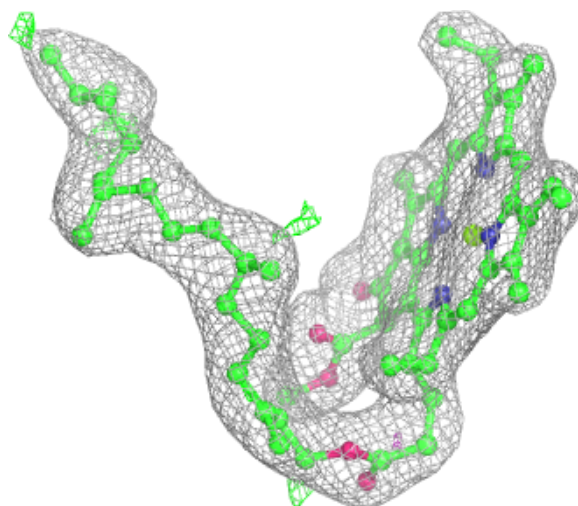
**Electron density around CLA B 612:**

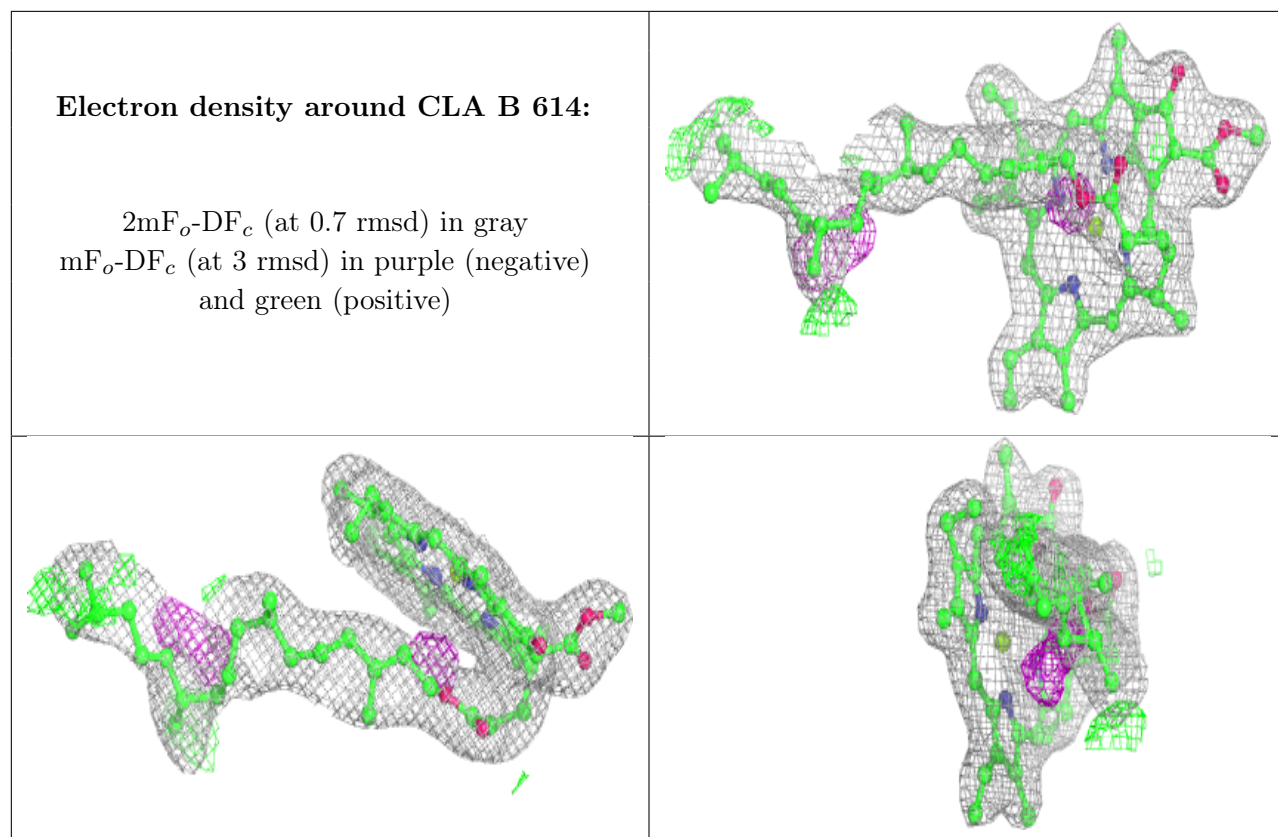
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 613:**

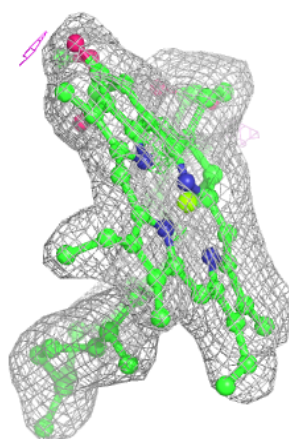
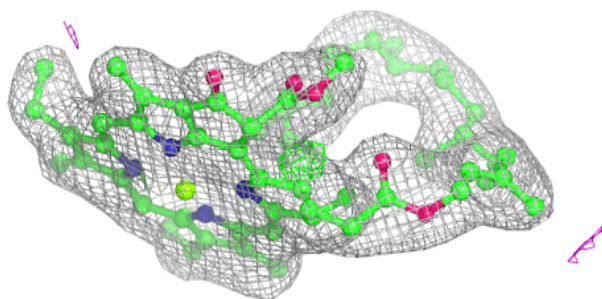
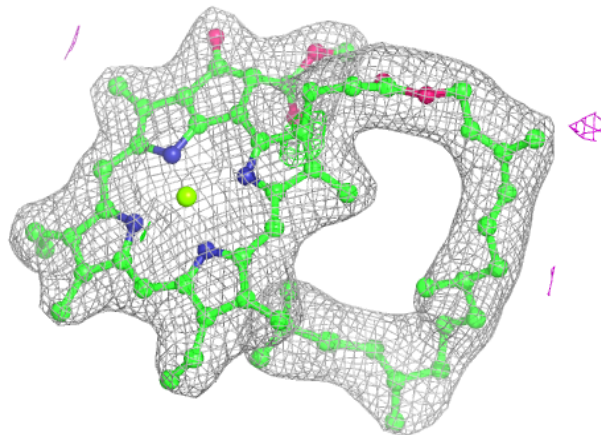
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





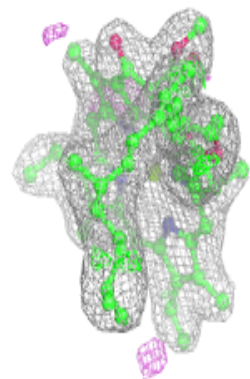
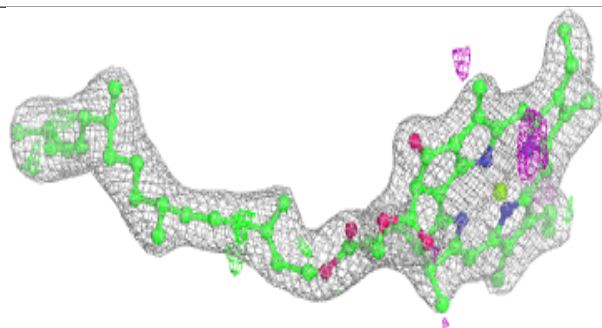
**Electron density around CLA B 615:**

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

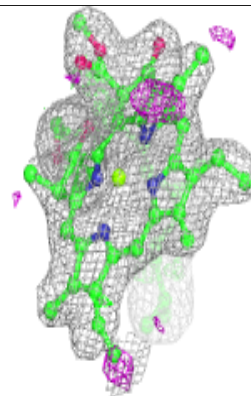
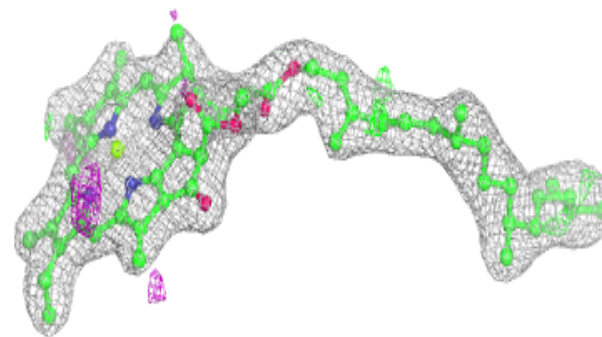
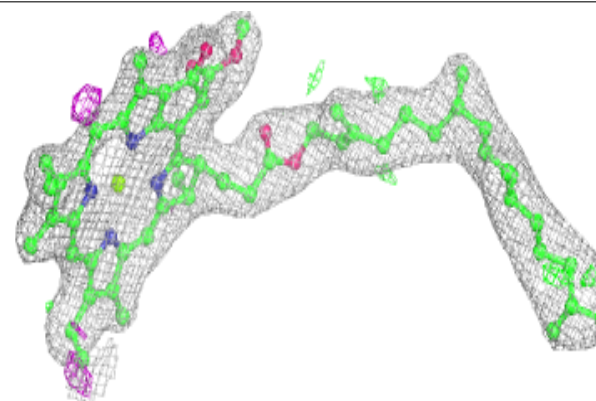


**Electron density around CLA a 405 (A):**

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

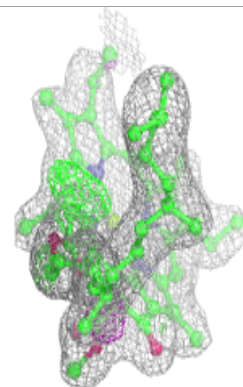
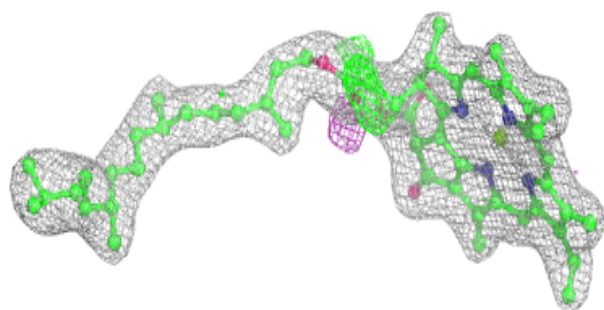
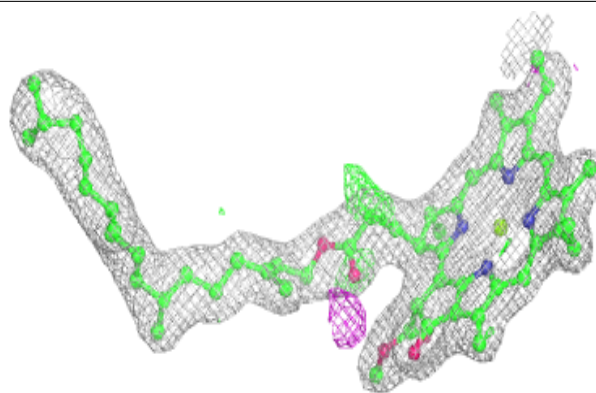
**Electron density around CLA a 405 (B):**

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

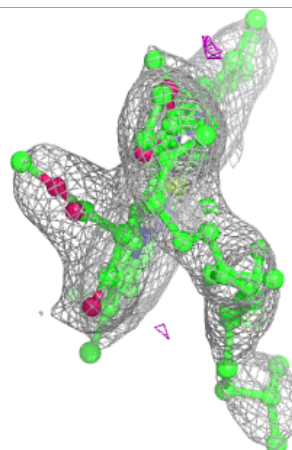
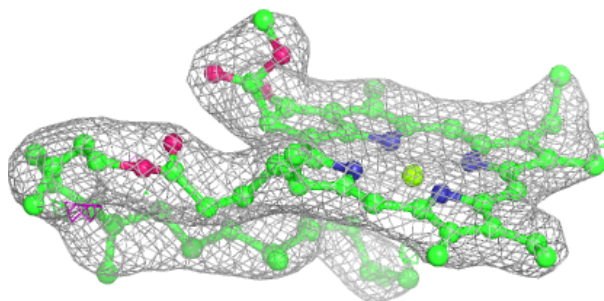
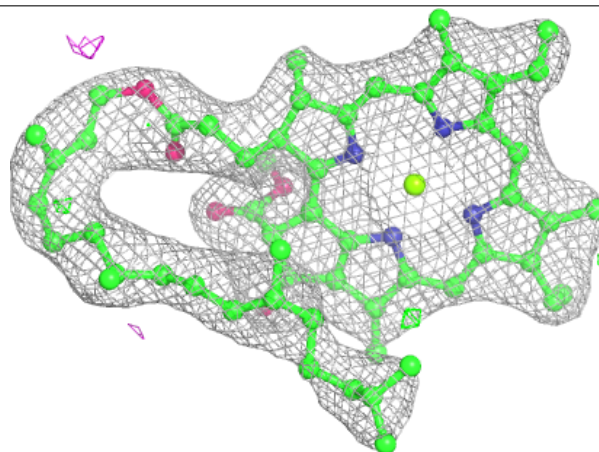


**Electron density around CLA A 404 (B):**

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

**Electron density around CLA c 510:**

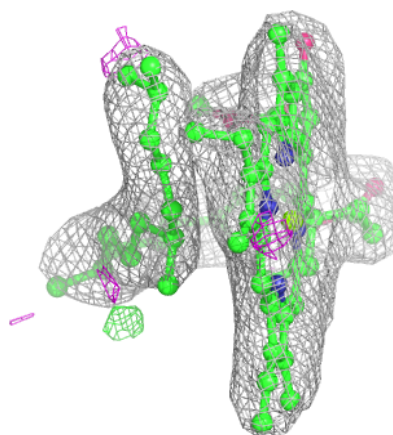
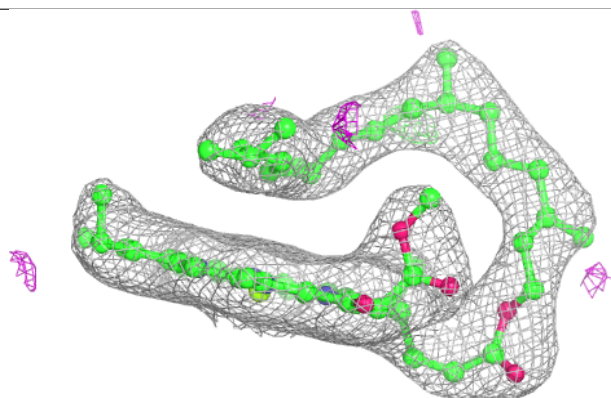
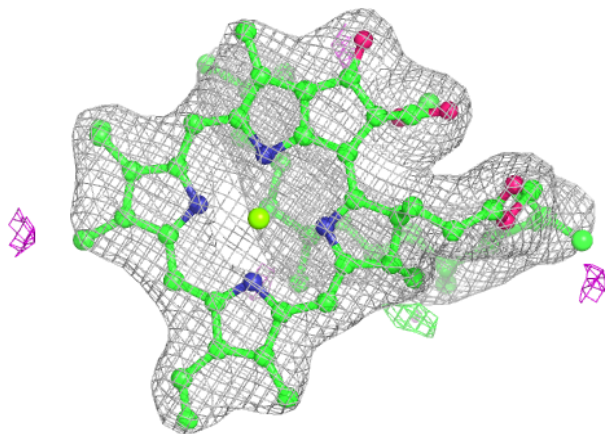
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





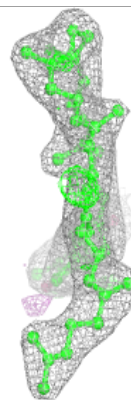
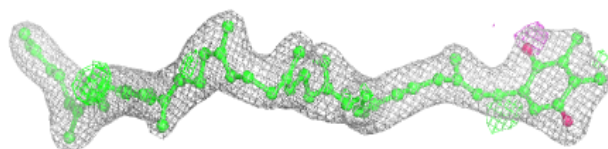
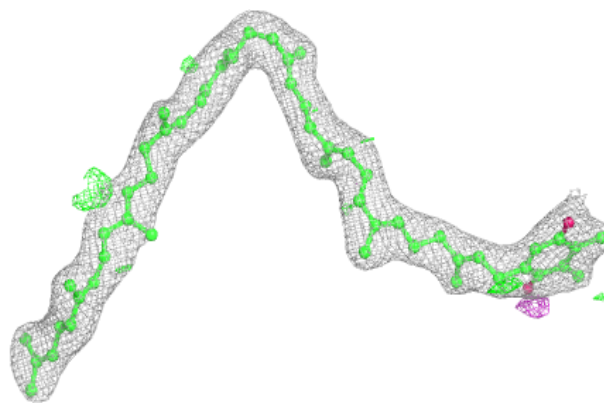
**Electron density around CLA c 511:**

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

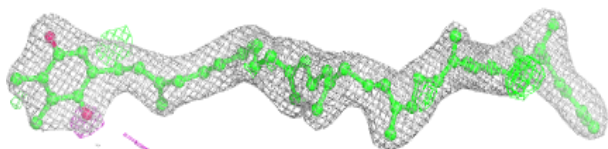
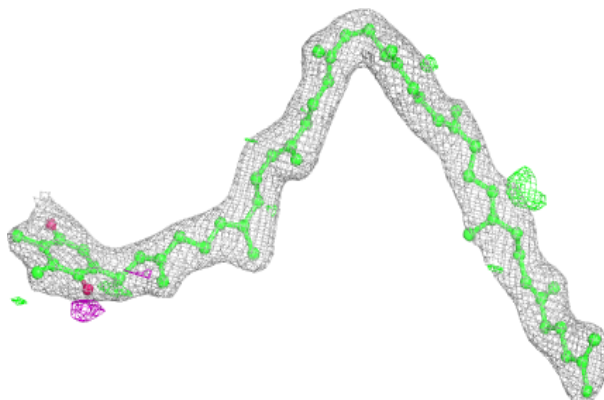


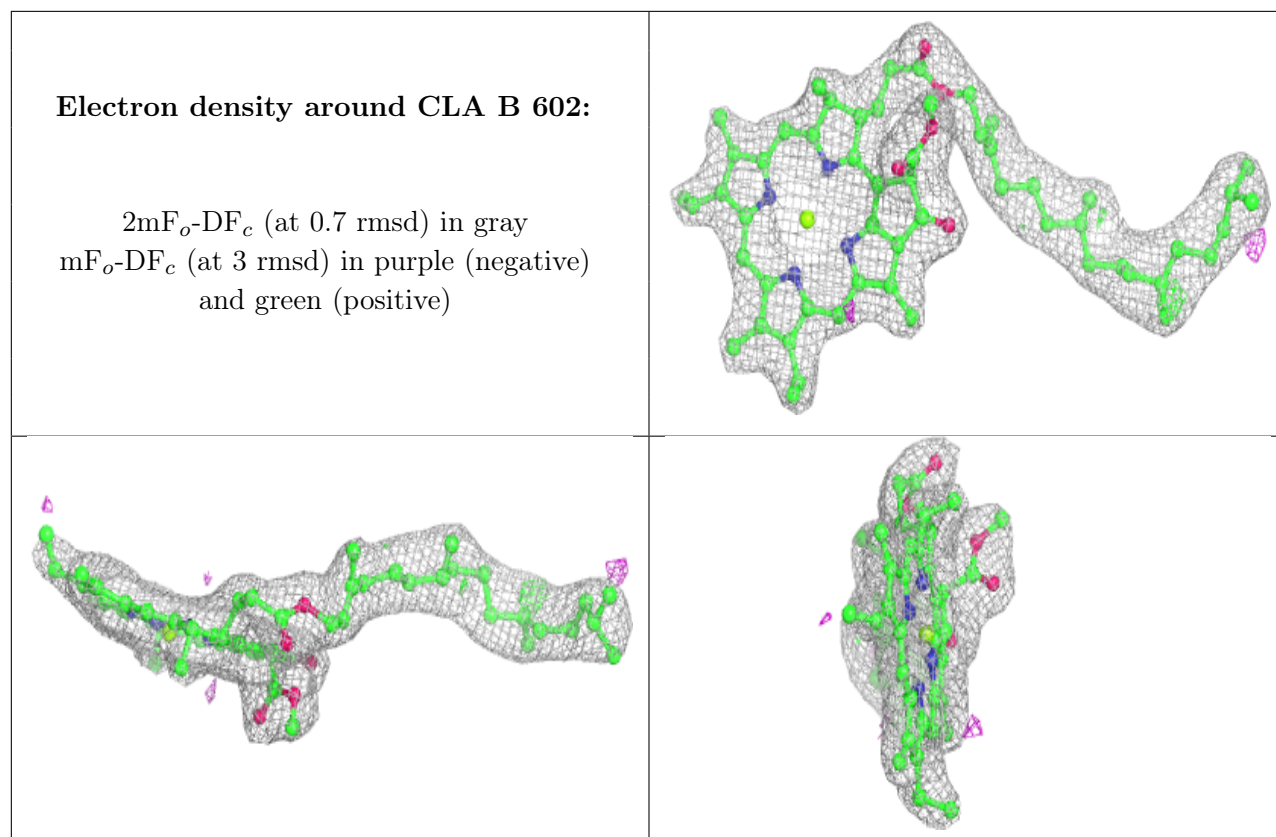
**Electron density around PL9 D 408 (A):**

$2mF_o-DF_c$  (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 (B):**

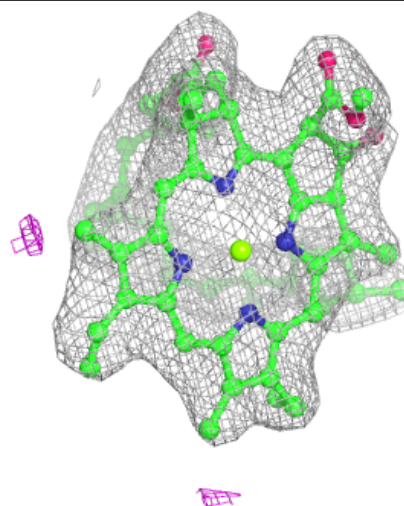
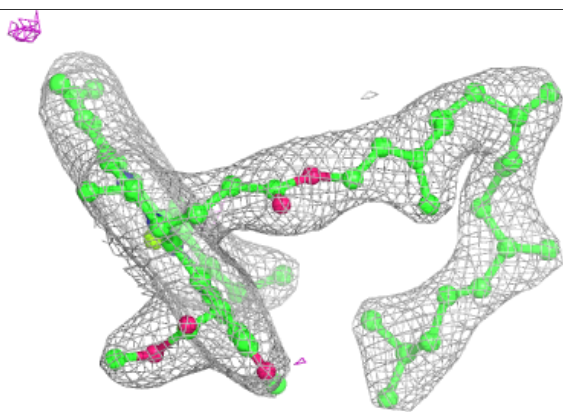
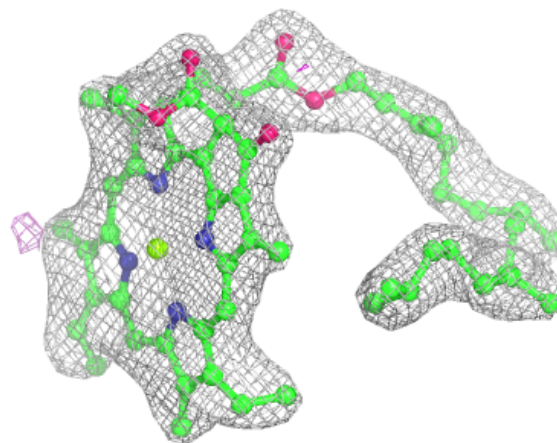
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





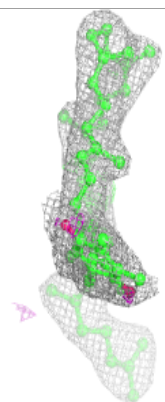
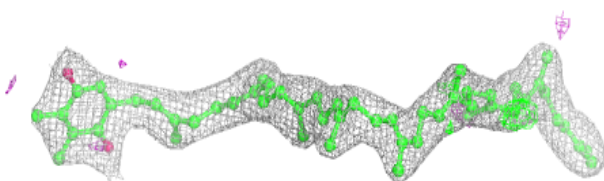
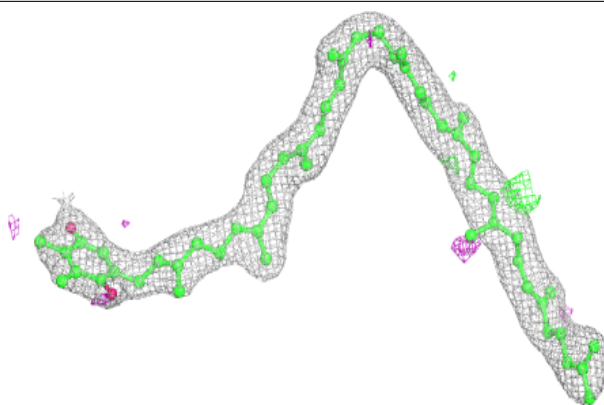
**Electron density around CLA C 504:**

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

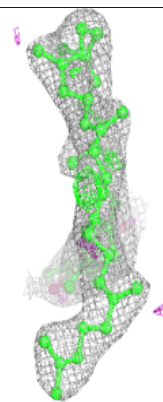
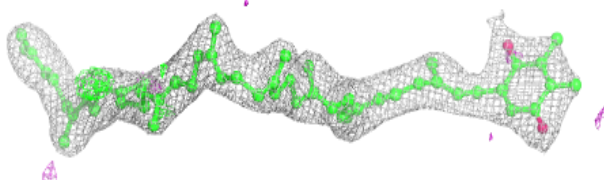
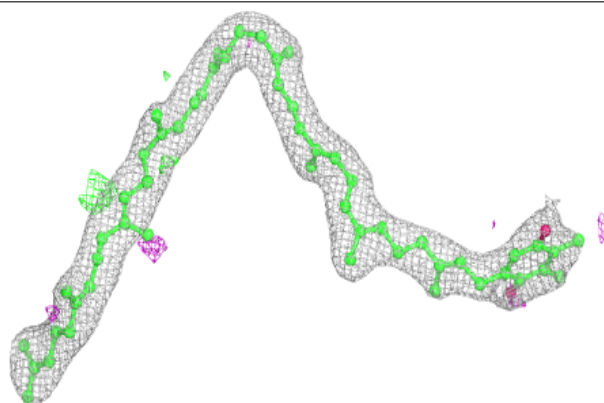


**Electron density around PL9 d 405 (A):**

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

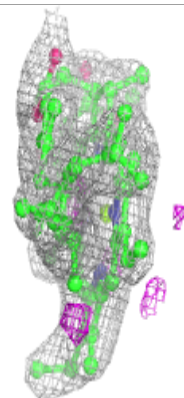
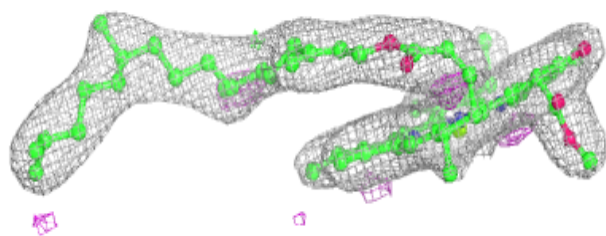
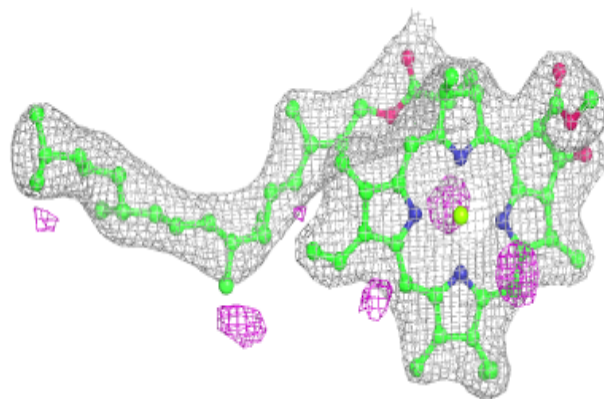
**Electron density around PL9 d 405 (B):**

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

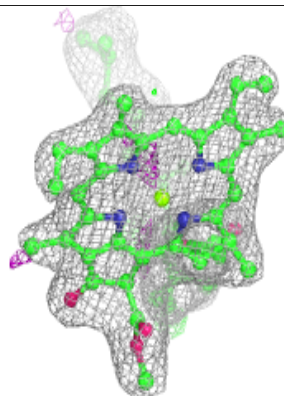
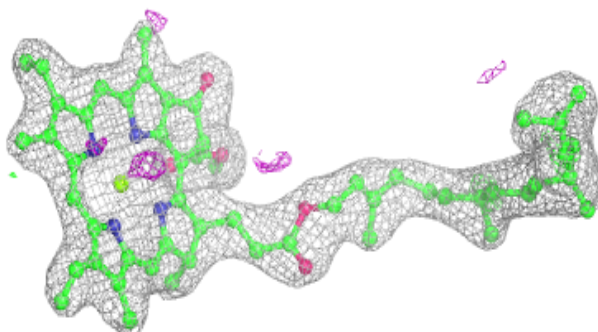
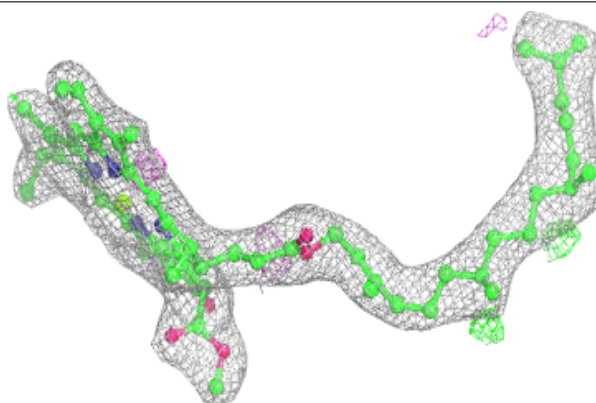


**Electron density around CLA B 603:**

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

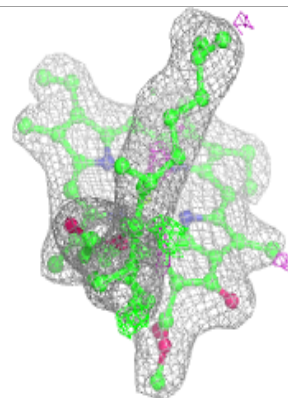
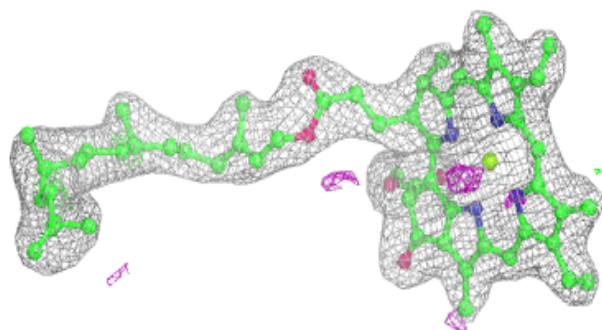
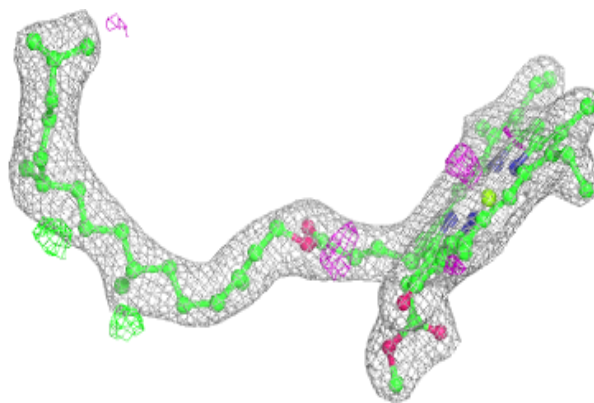
**Electron density around CLA d 402 (A):**

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

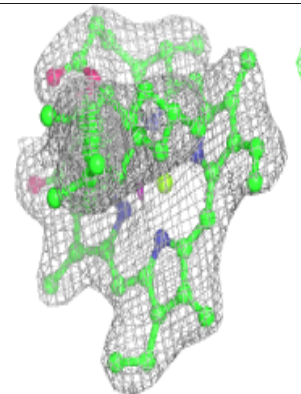
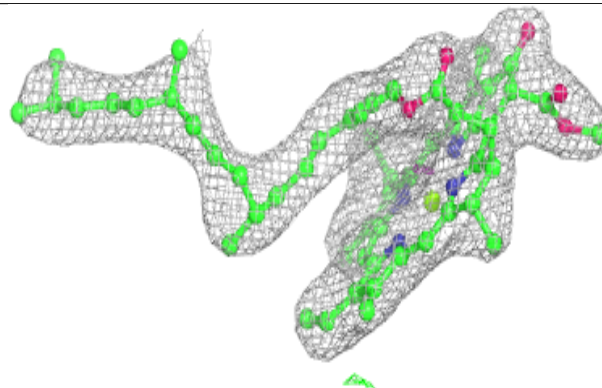
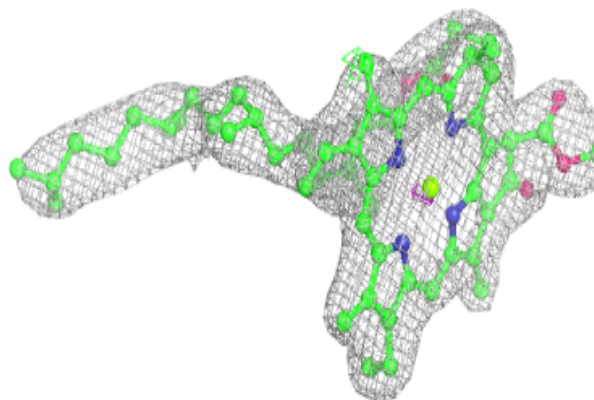


**Electron density around CLA d 402 (B):**

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

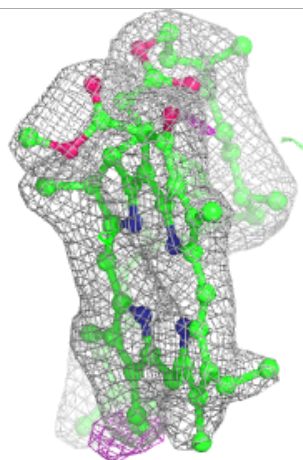
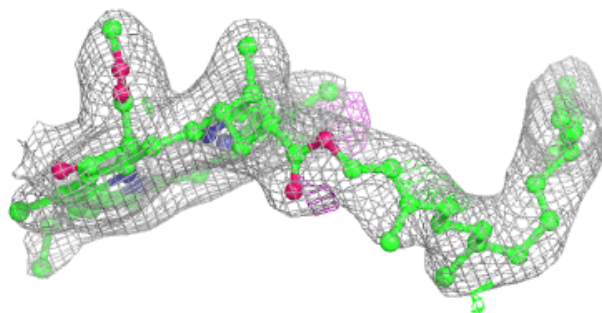
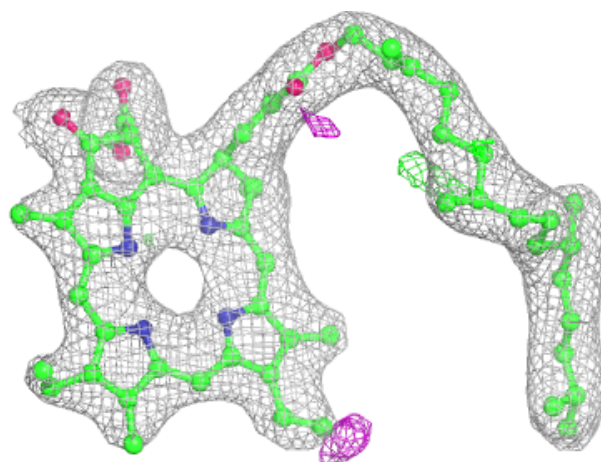
**Electron density around CLA C 506:**

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



**Electron density around PHO a 353 (A):**

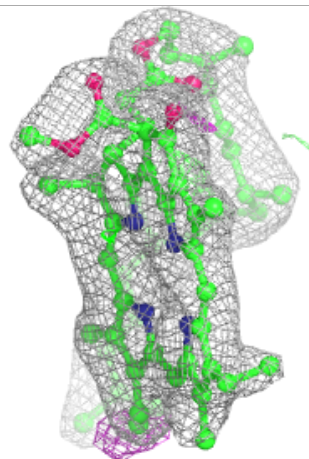
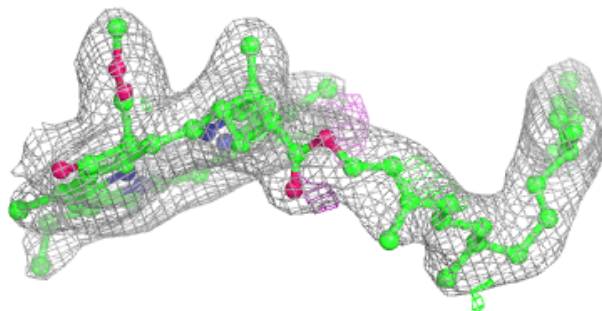
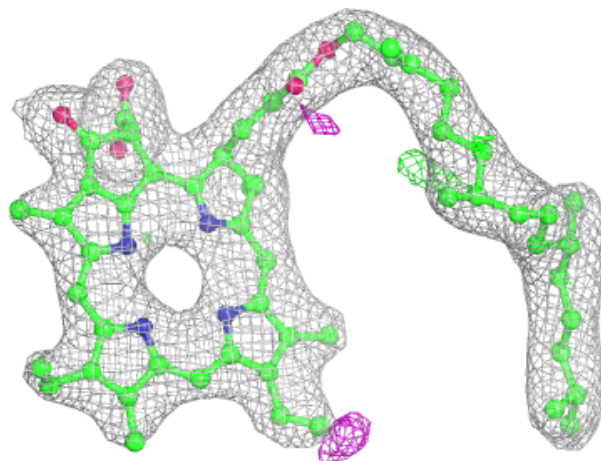
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





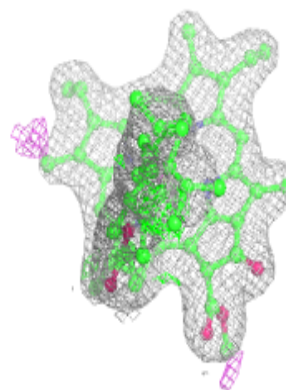
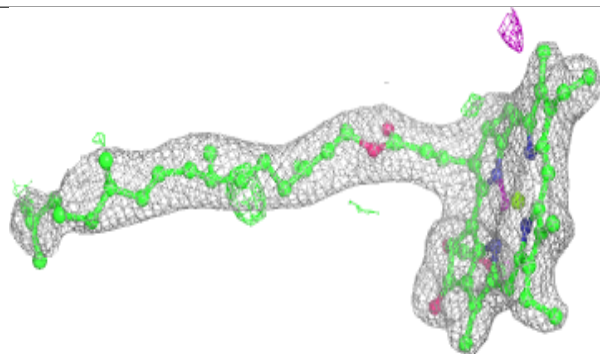
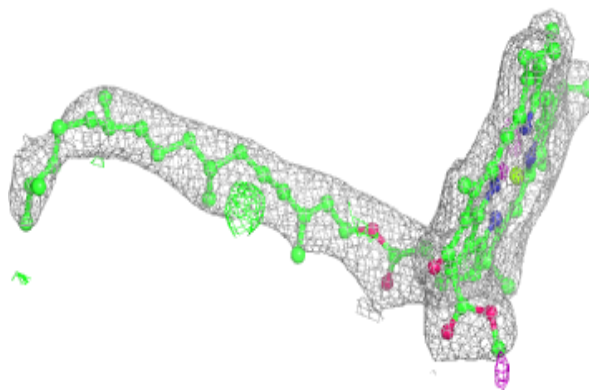
**Electron density around PHO a 353 (B):**

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

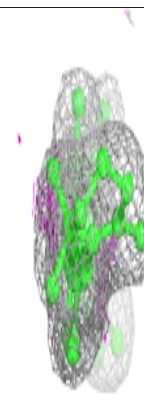
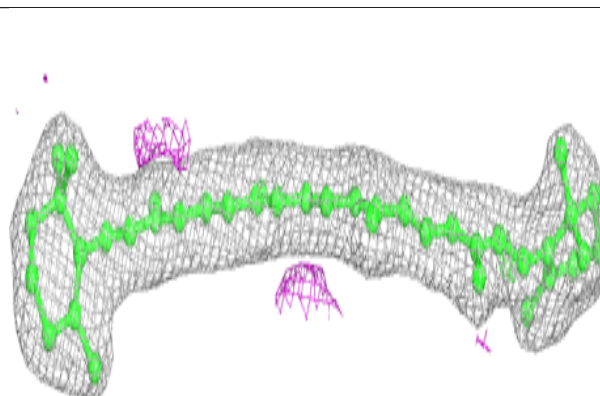
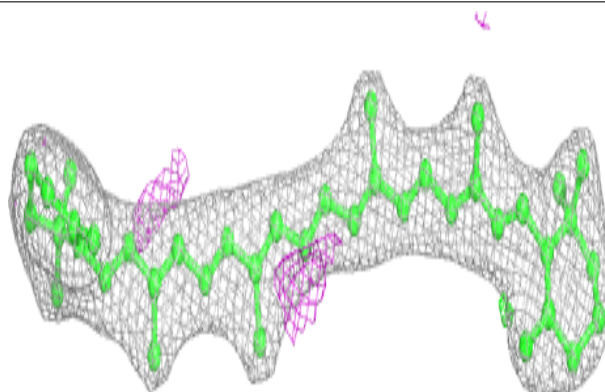


**Electron density around CLA b 604:**

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

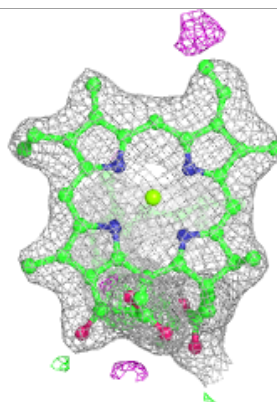
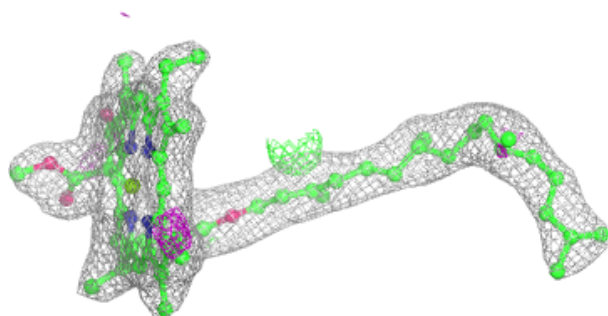
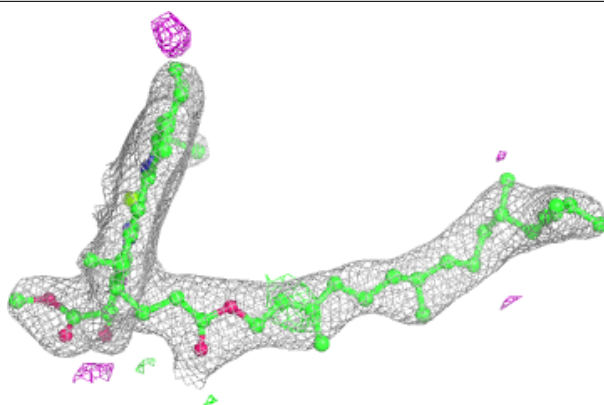
**Electron density around BCR B 617:**

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

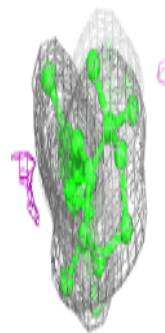
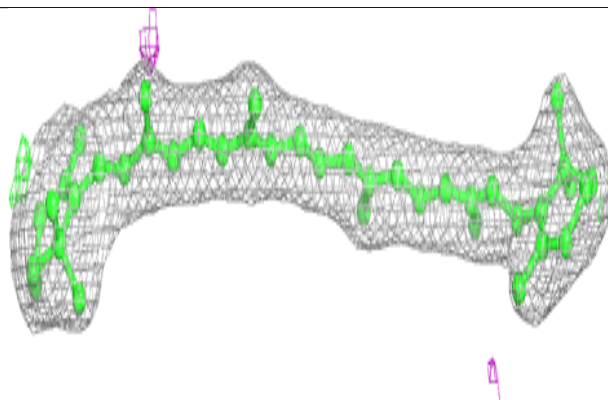
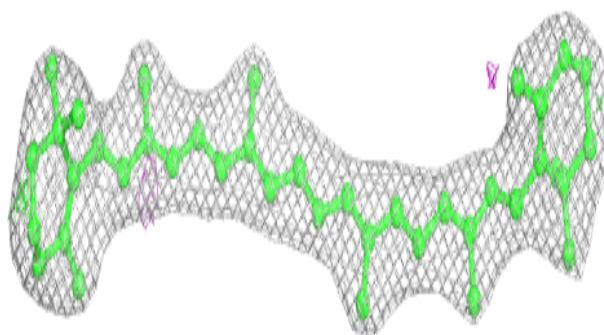


**Electron density around CLA b 605:**

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

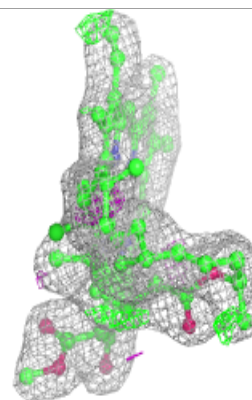
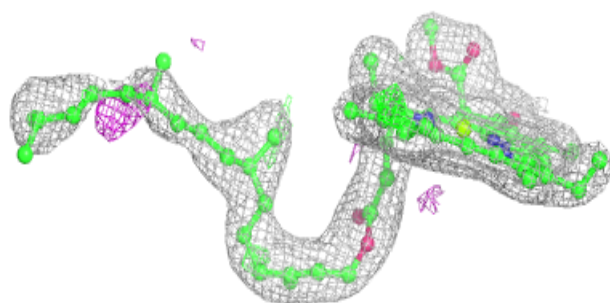
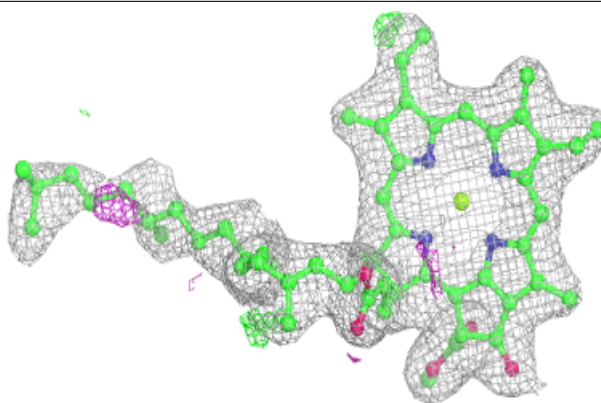
**Electron density around BCR B 619:**

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

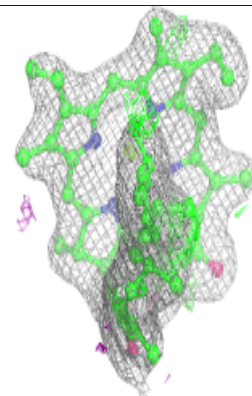
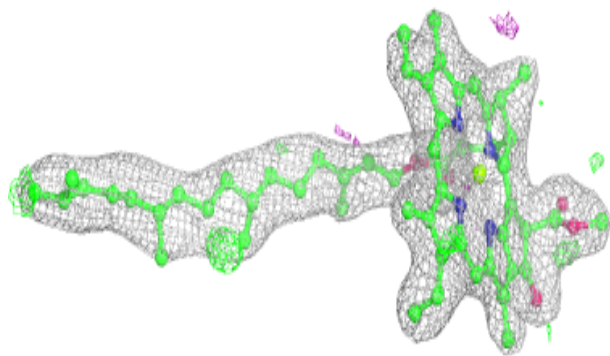
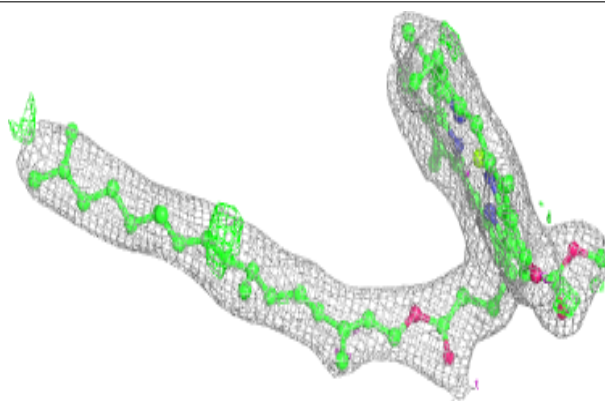


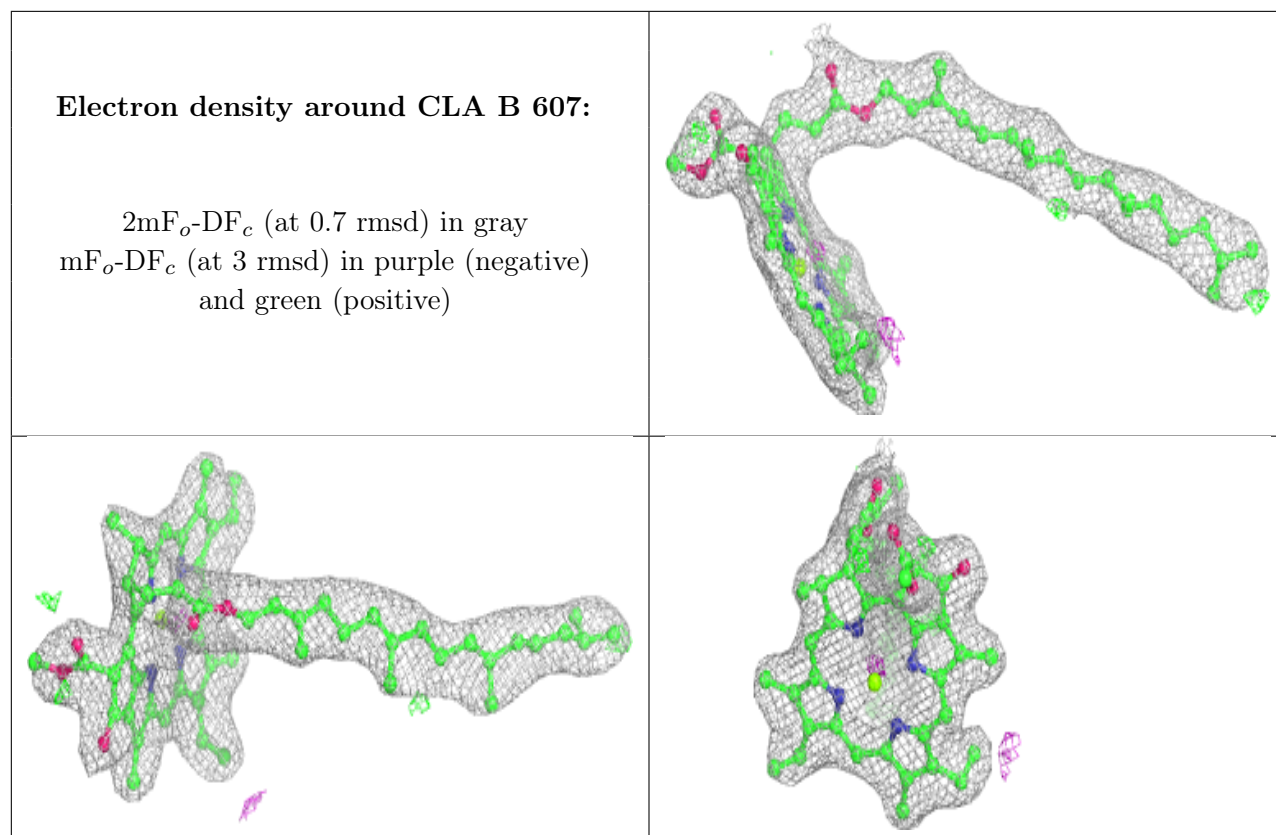
**Electron density around CLA A 406 (A):**

$2mF_o-DF_c$  (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:**

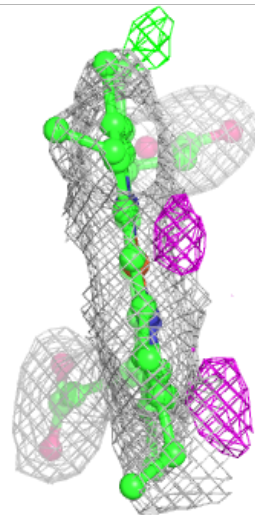
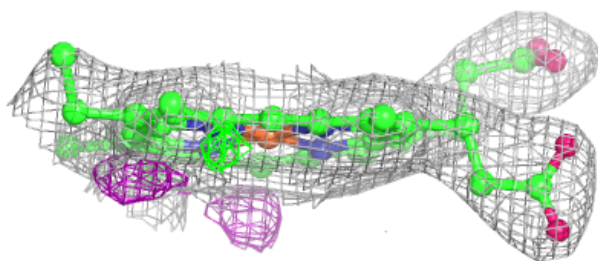
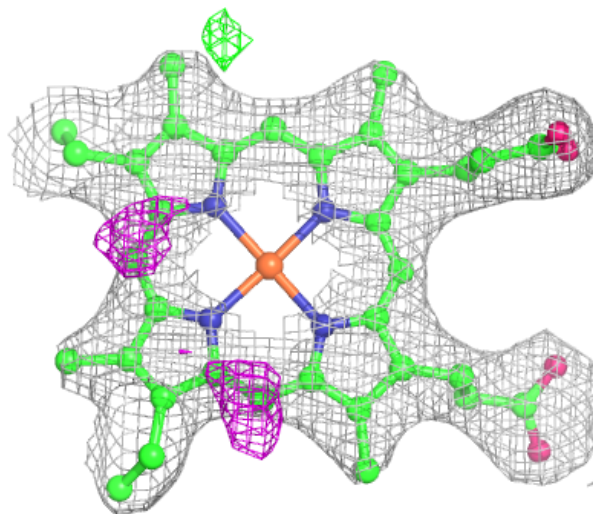
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





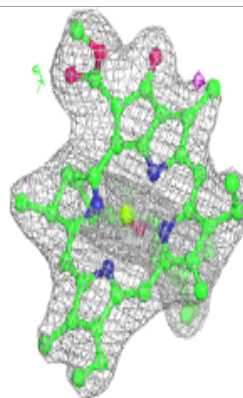
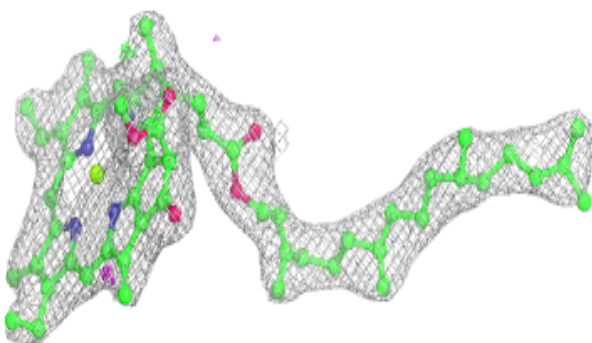
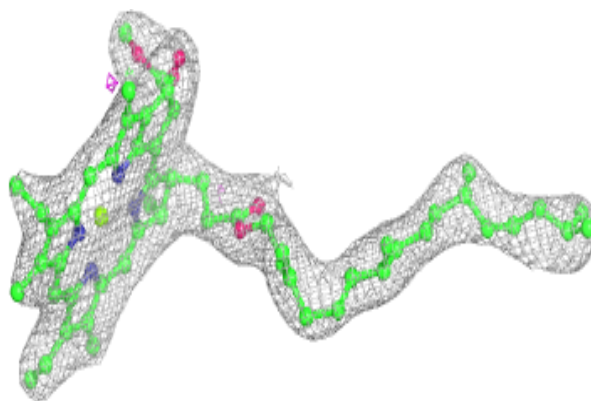
**Electron density around HEC v 202:**

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

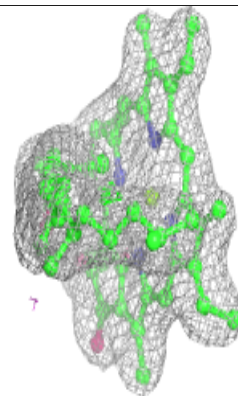
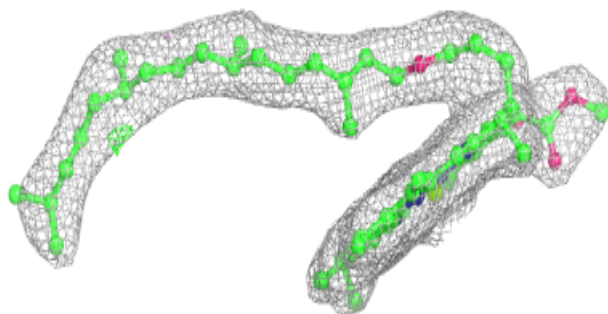
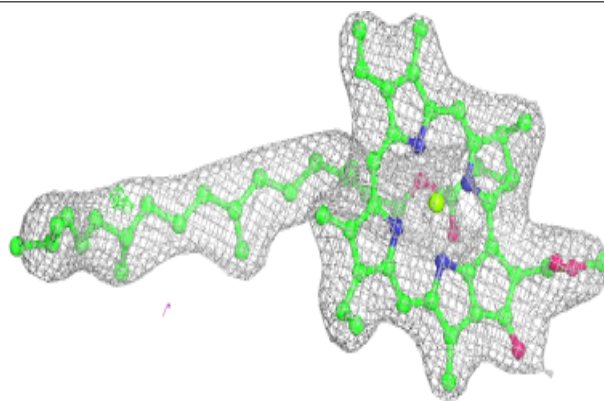


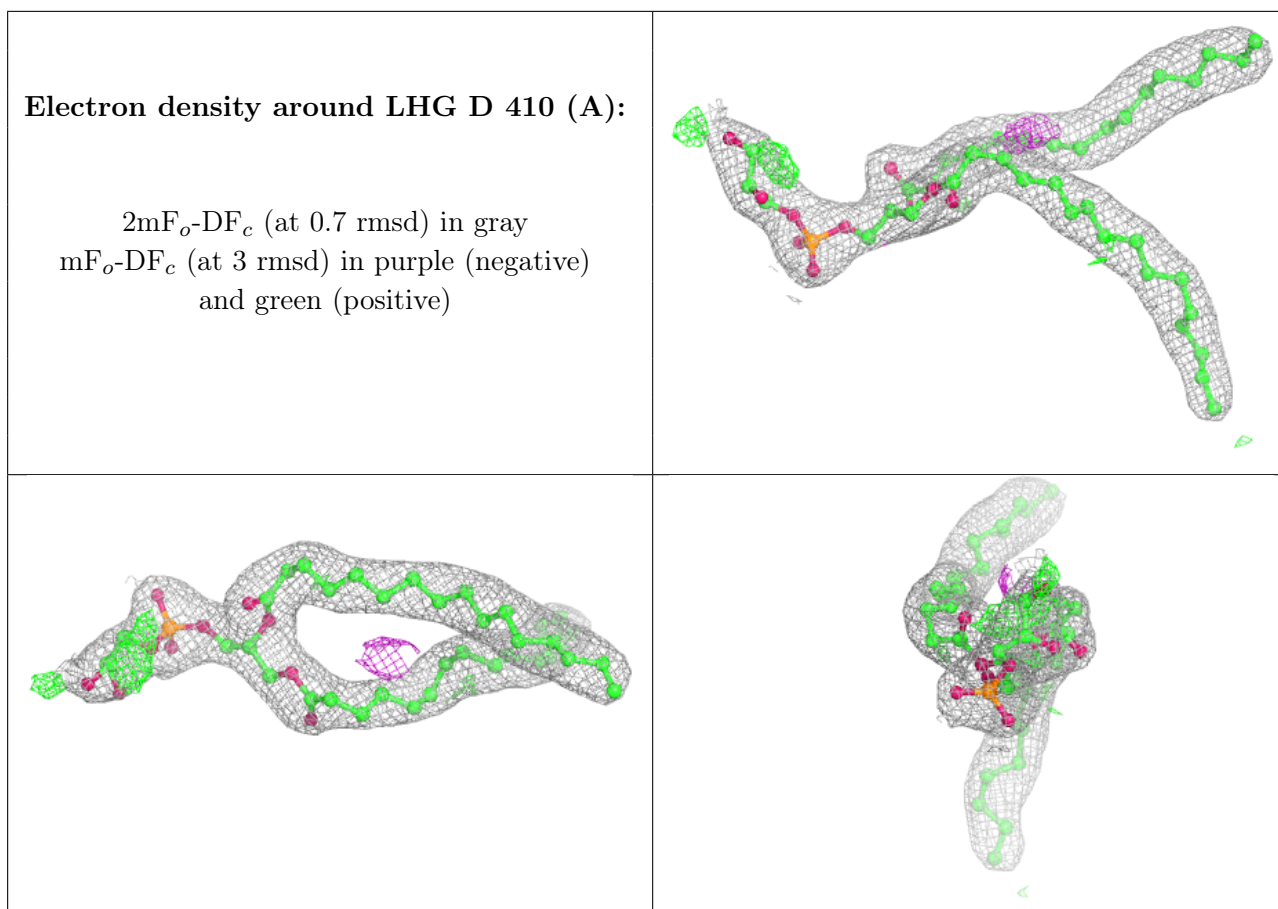
**Electron density around CLA C 503:**

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

**Electron density around CLA B 608:**

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

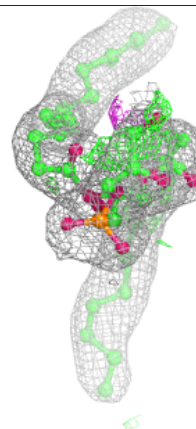
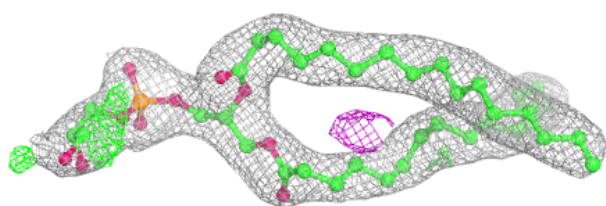
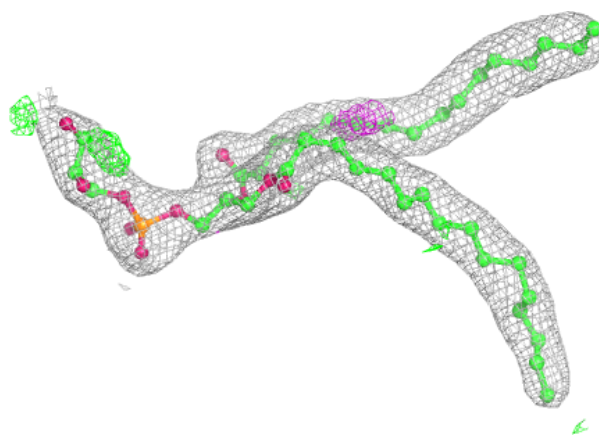




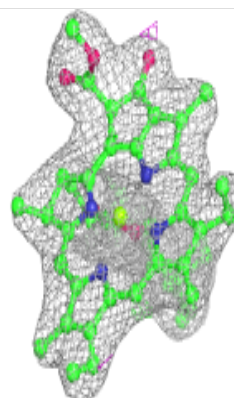
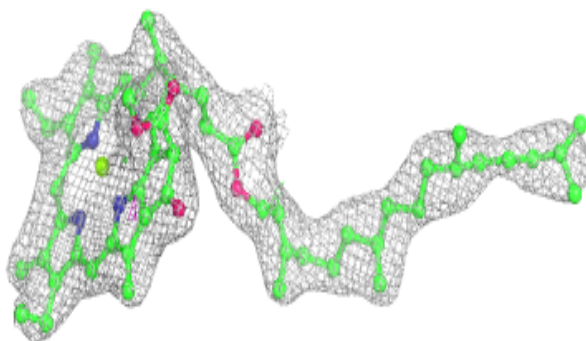
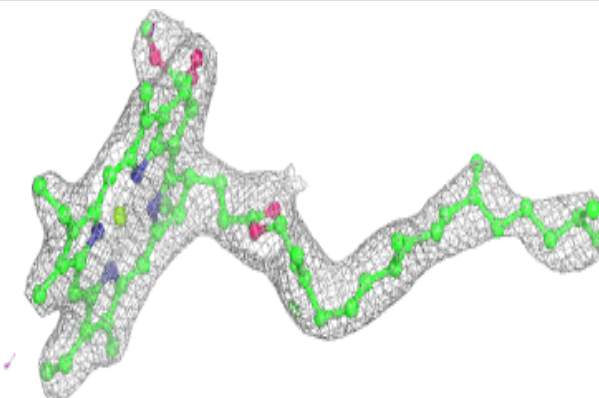


**Electron density around LHG D 410 (B):**

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

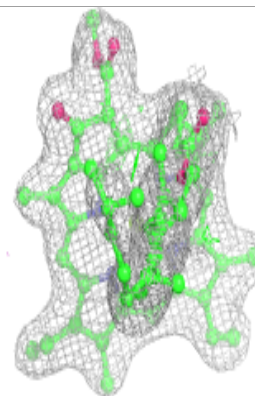
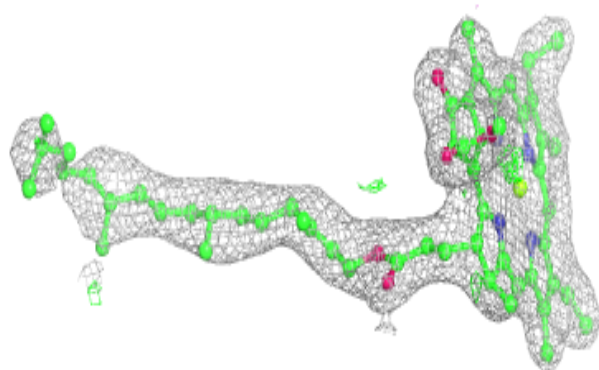
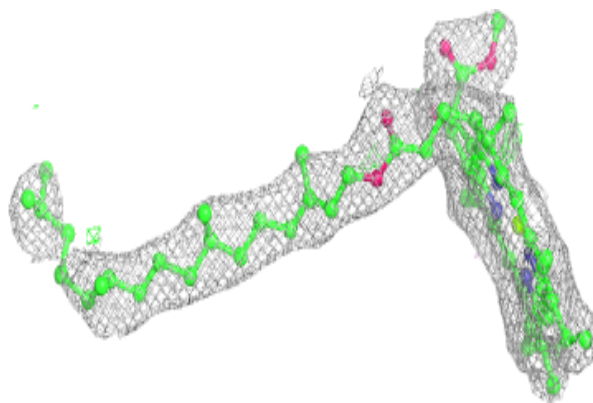
**Electron density around CLA c 503:**

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

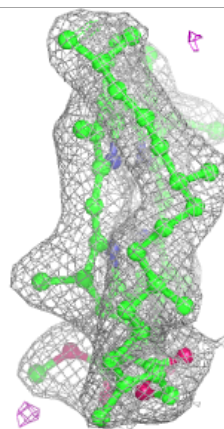
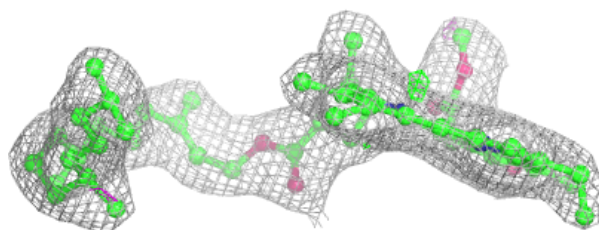
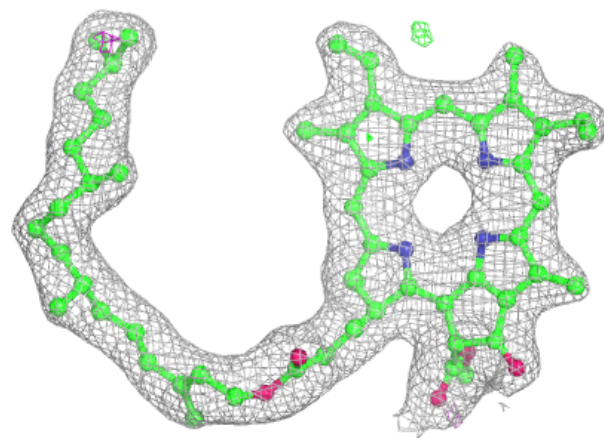


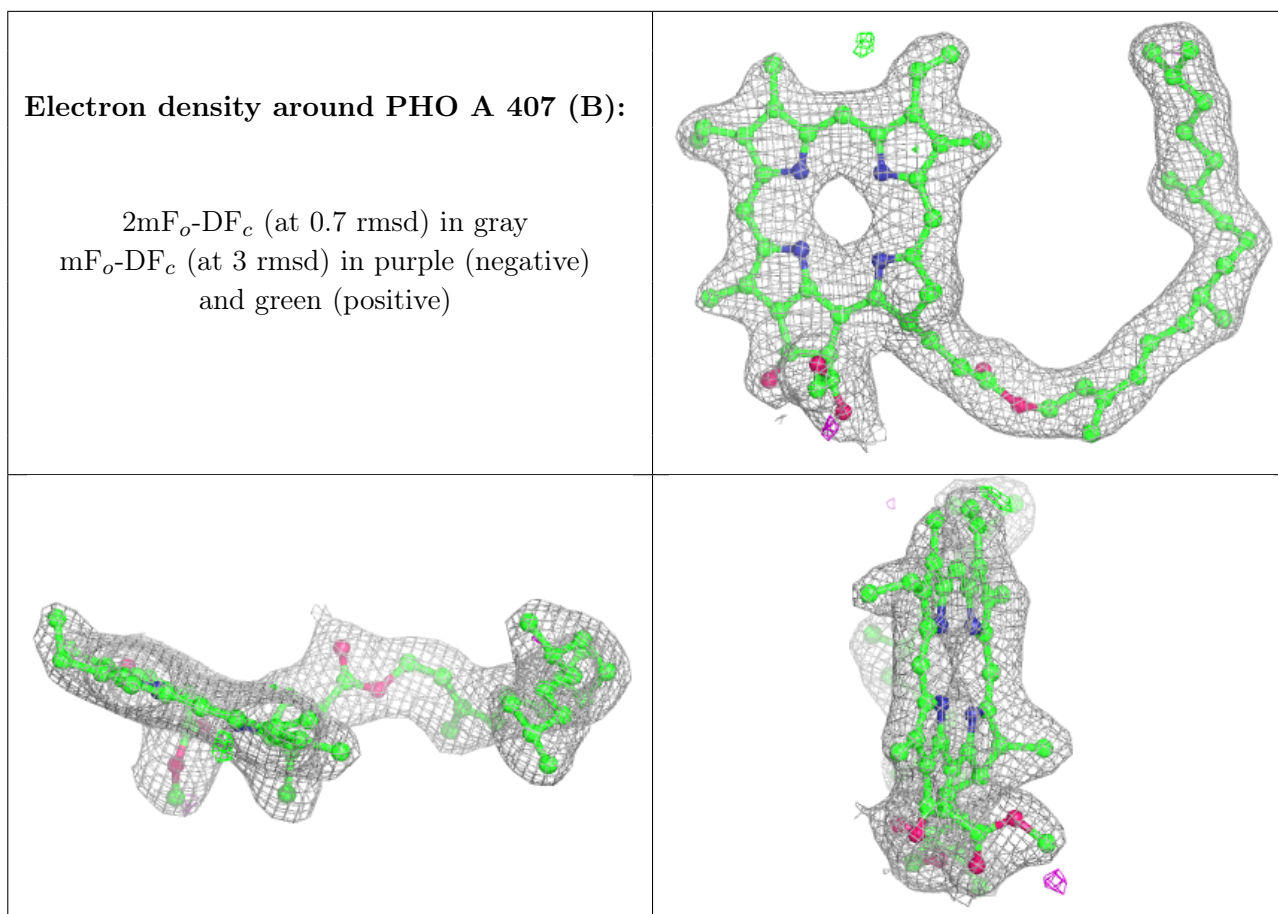
**Electron density around CLA B 604:**

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

**Electron density around PHO A 407 (A):**

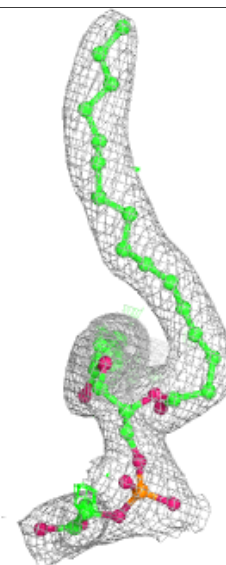
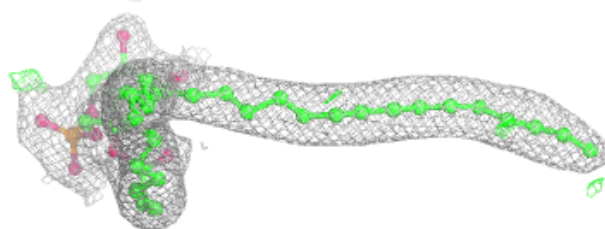
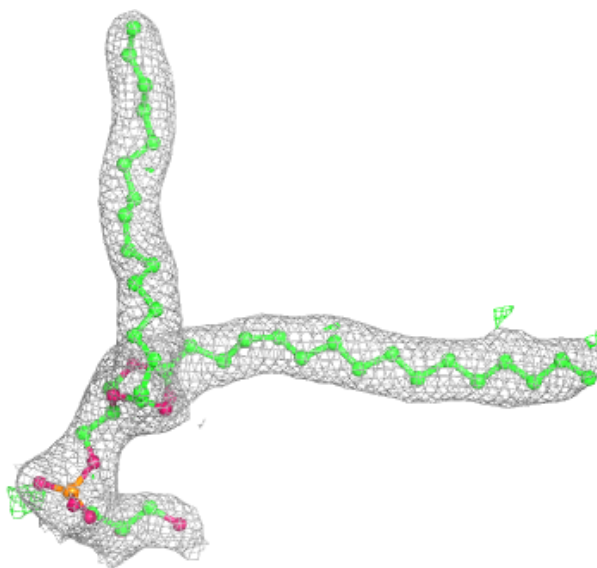
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





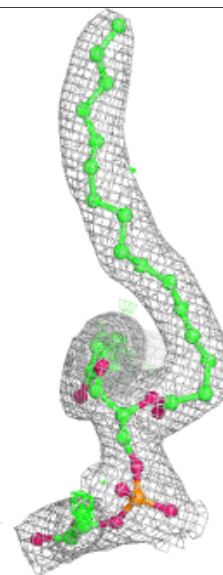
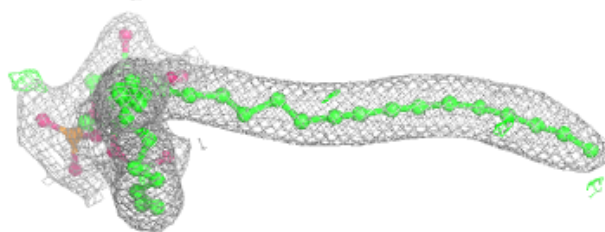
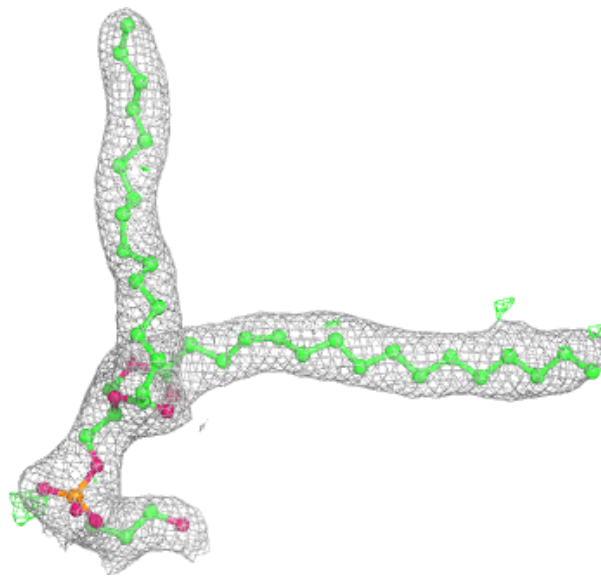
**Electron density around LHG L 101 (A):**

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



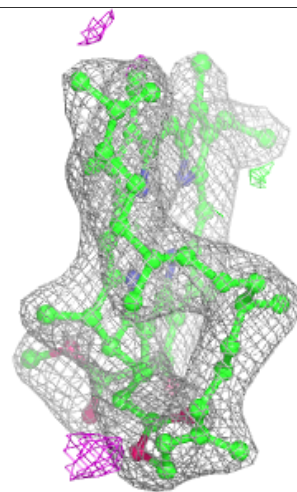
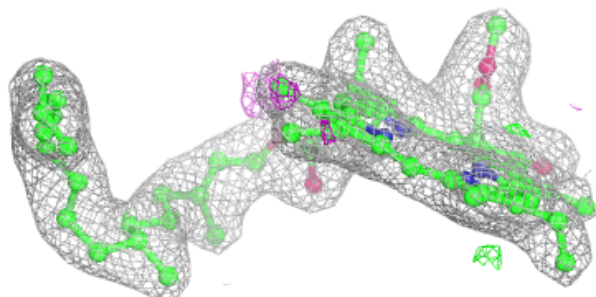
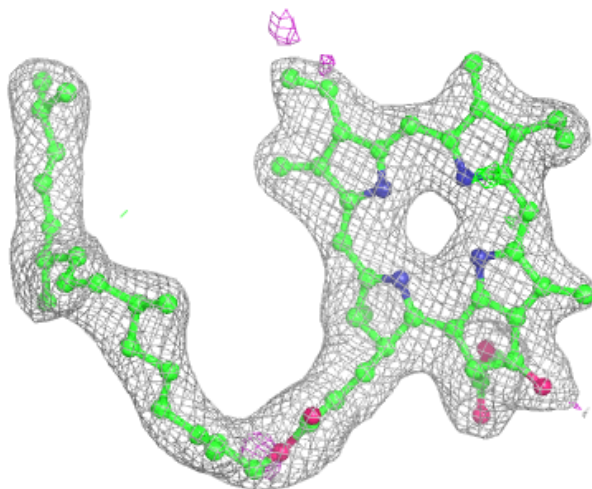
**Electron density around LHG L 101 (B):**

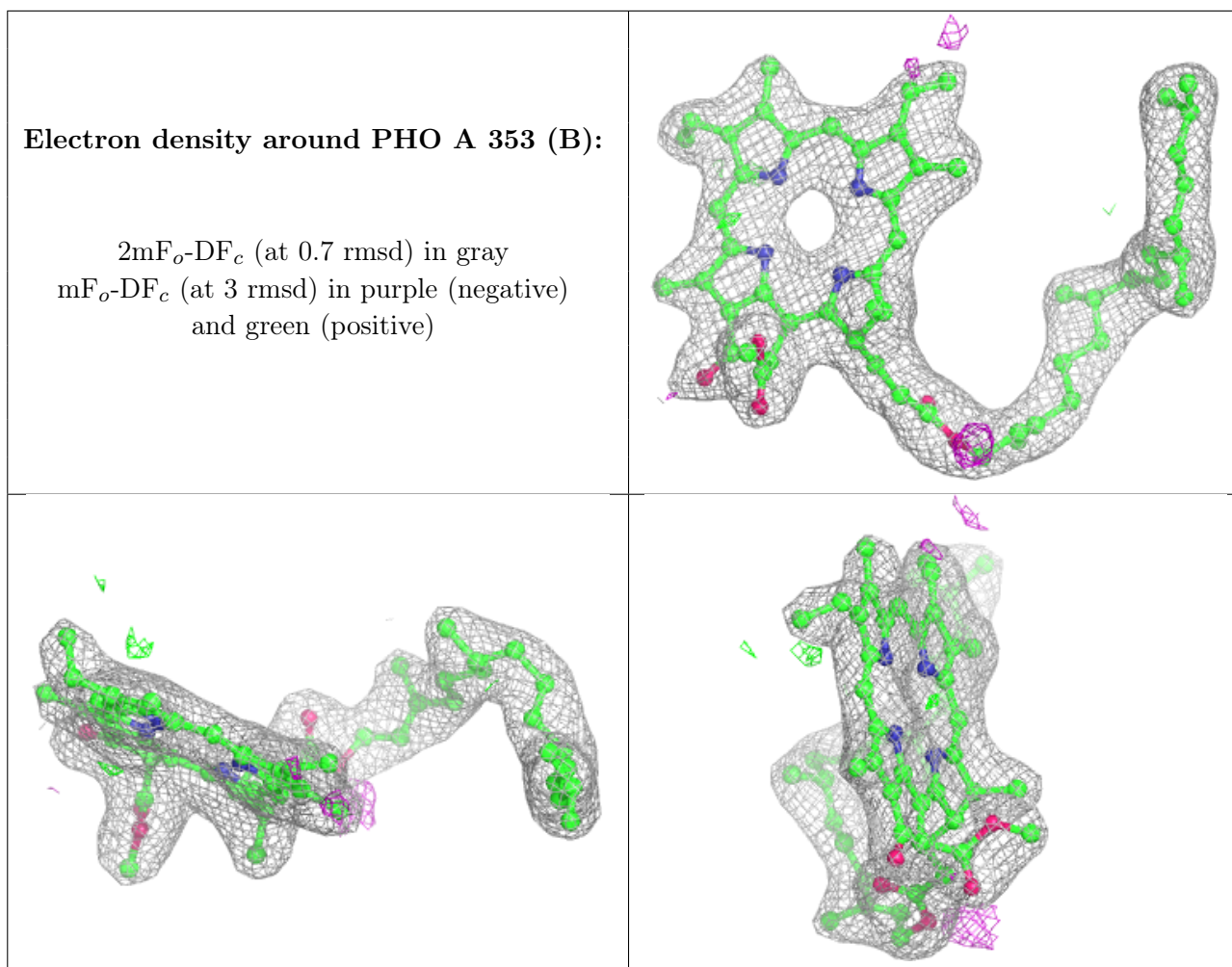
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO A 353 (A):**

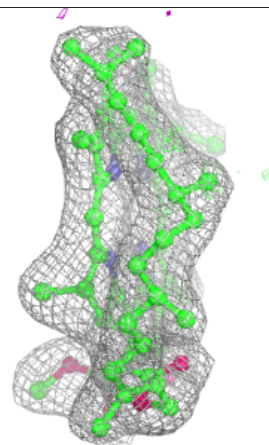
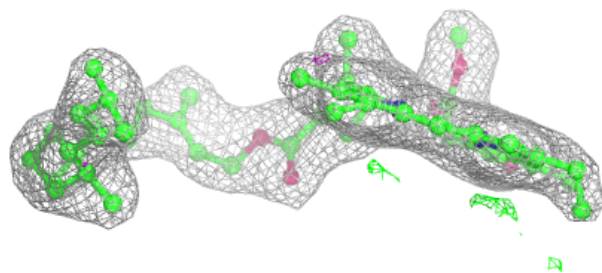
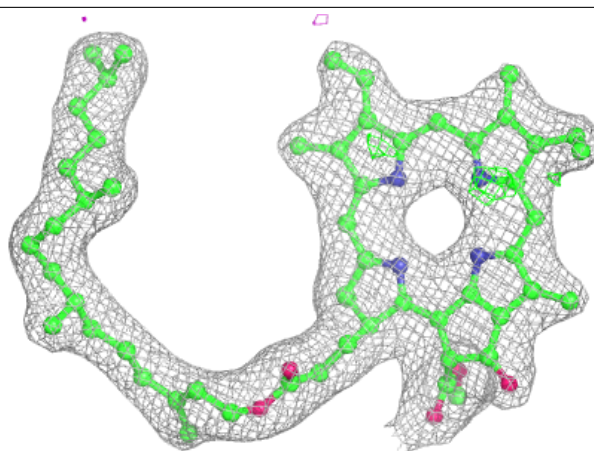
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PHO a 408 (A):**

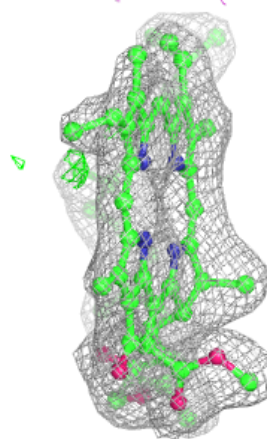
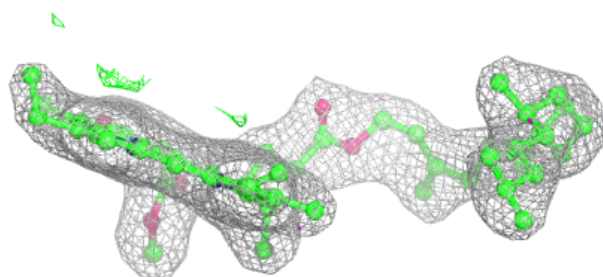
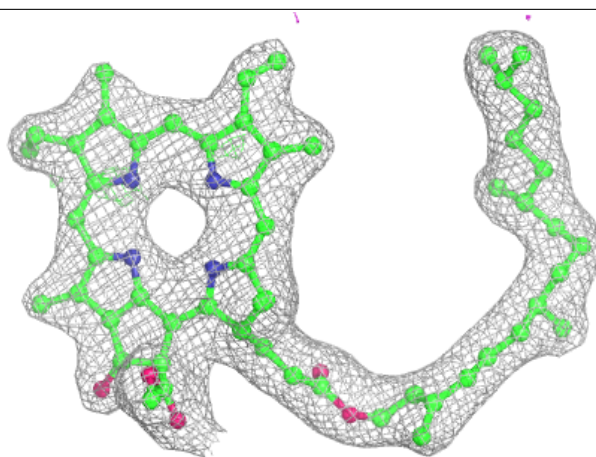
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





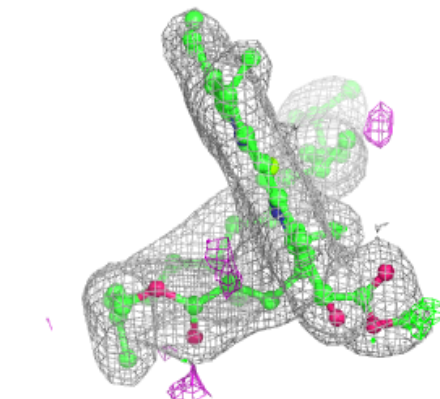
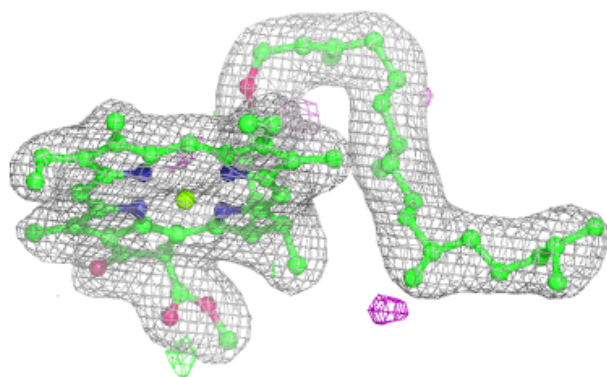
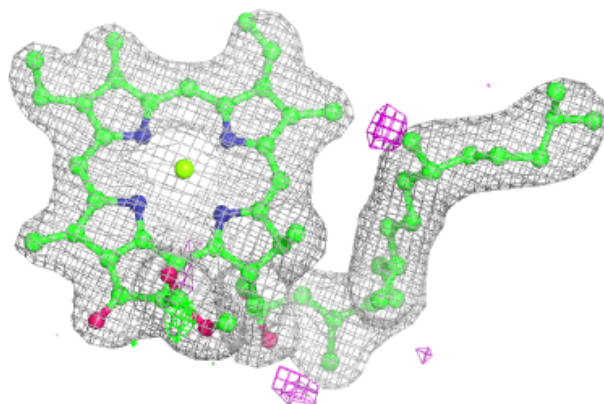
**Electron density around PHO a 408 (B):**

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

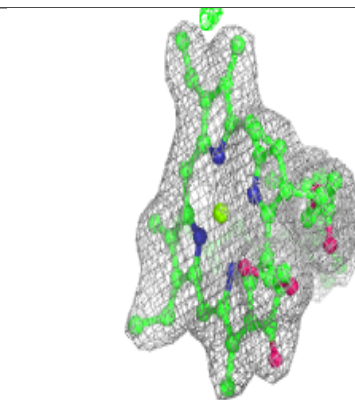
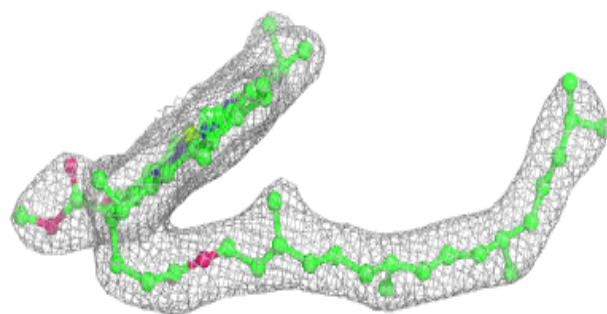
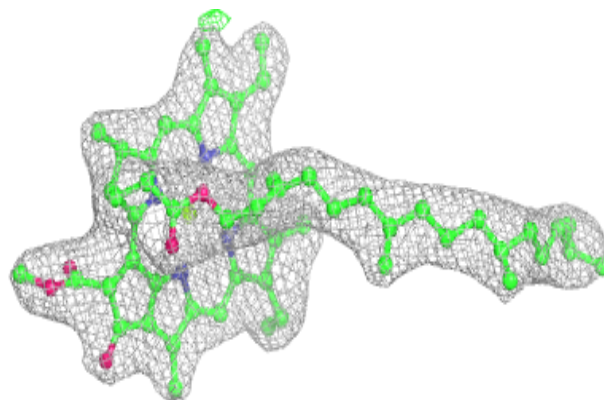


**Electron density around CLA a 406 (A):**

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

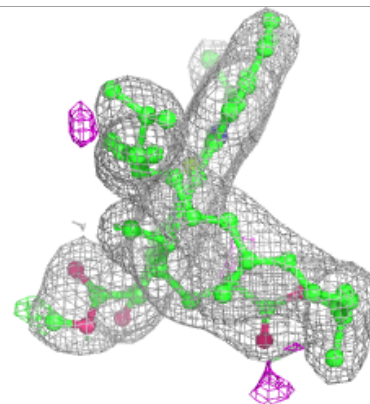
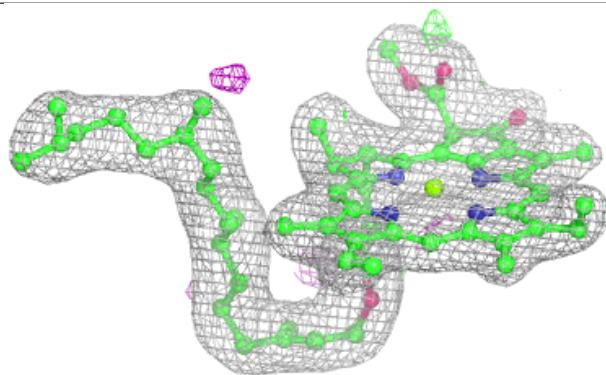
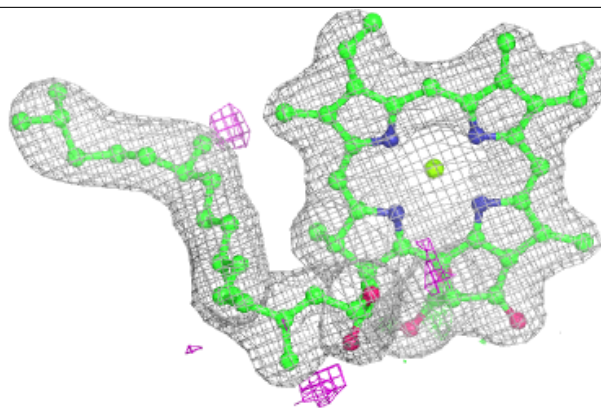
**Electron density around CLA b 608:**

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

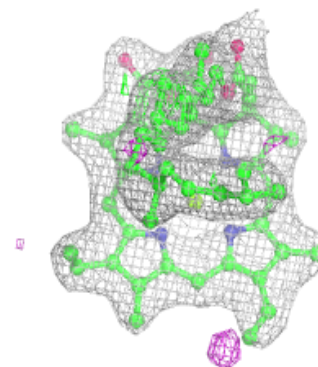
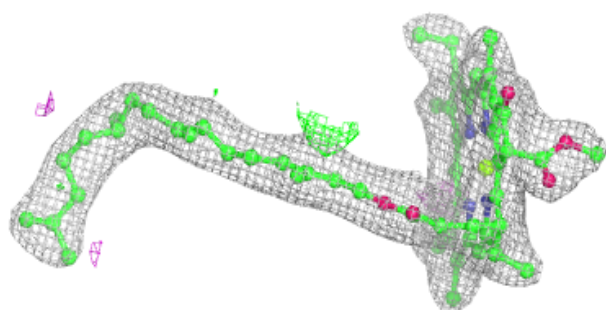
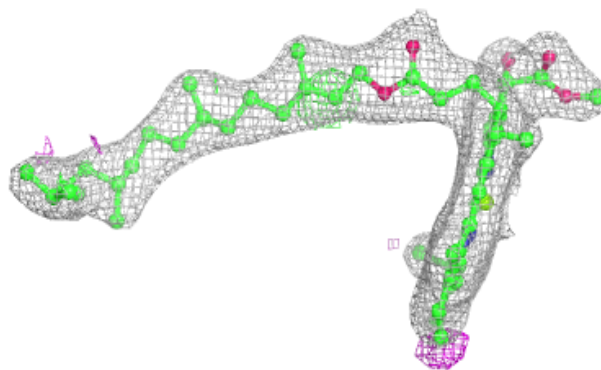


**Electron density around CLA a 406 (B):**

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

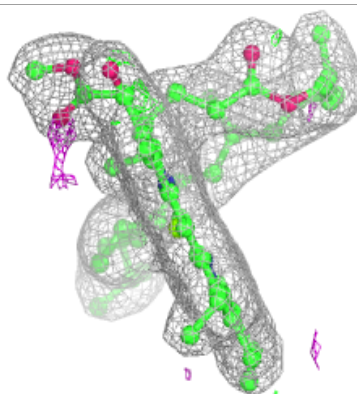
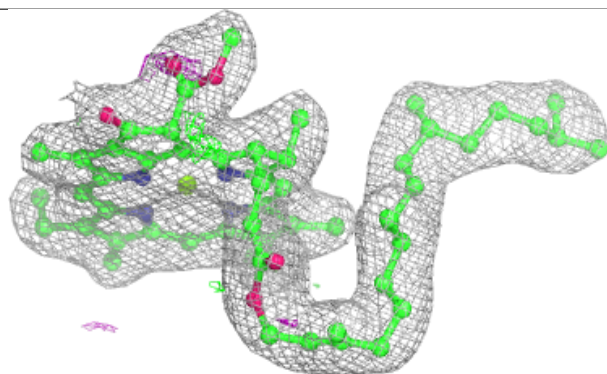
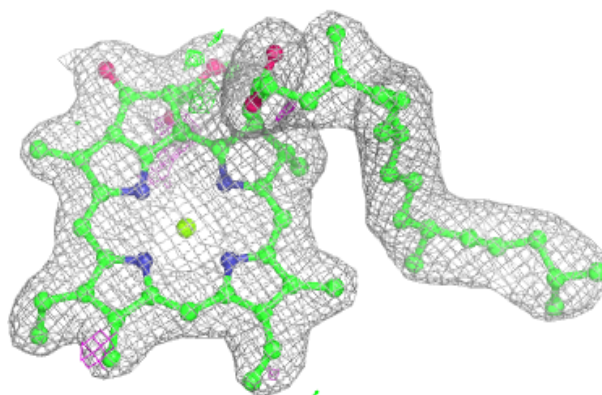
**Electron density around CLA B 605:**

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

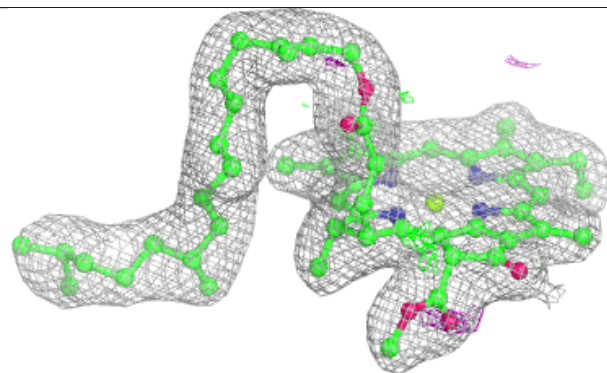
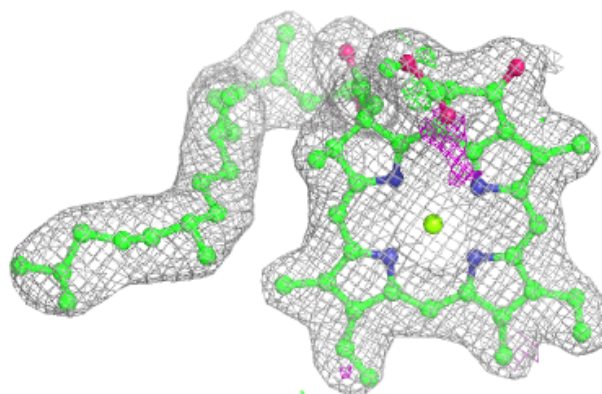


**Electron density around CLA A 405 (A):**

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

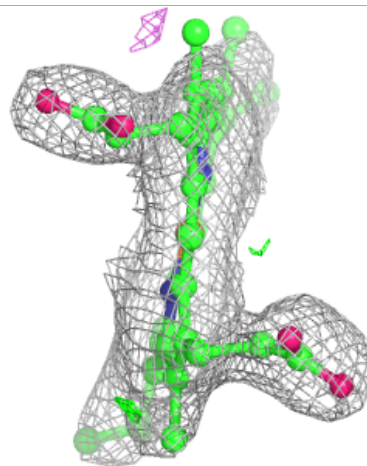
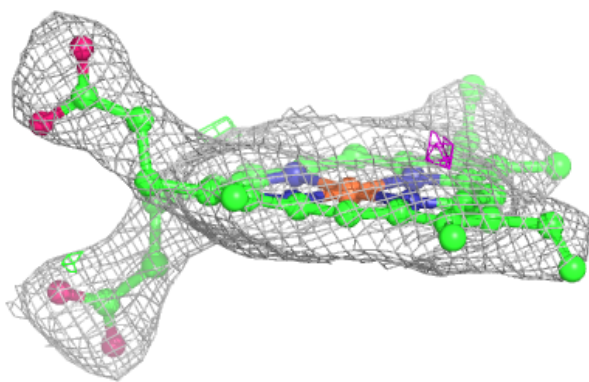
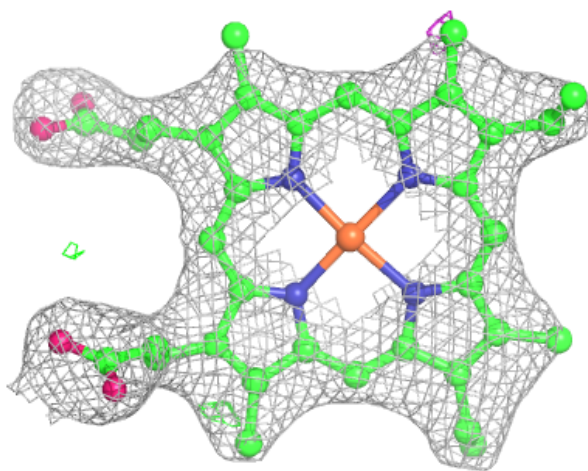
**Electron density around CLA A 405 (B):**

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



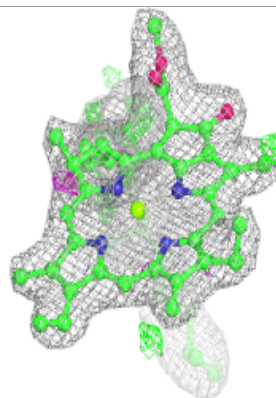
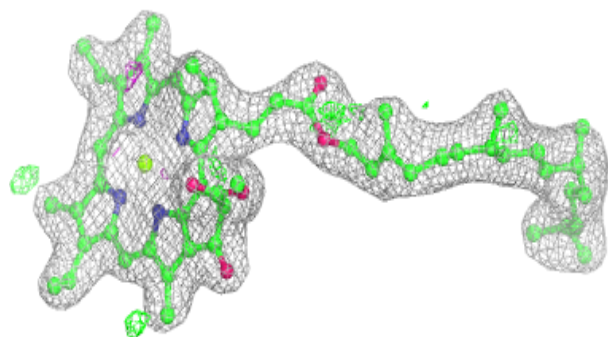
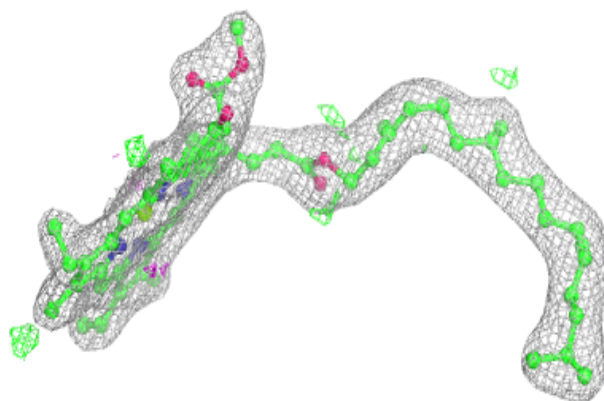
**Electron density around HEM E 103:**

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

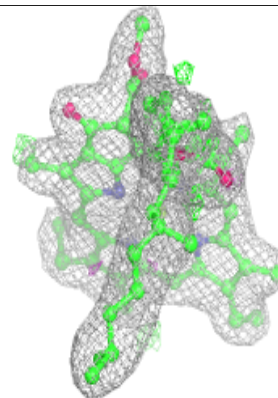
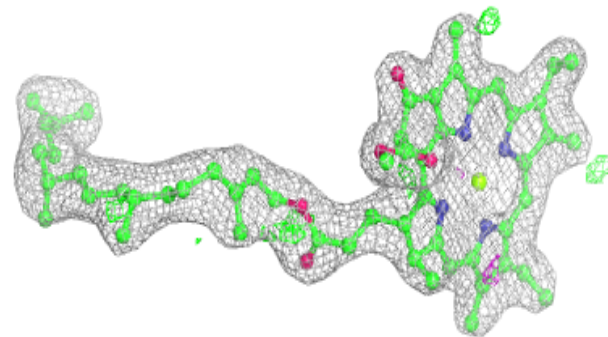
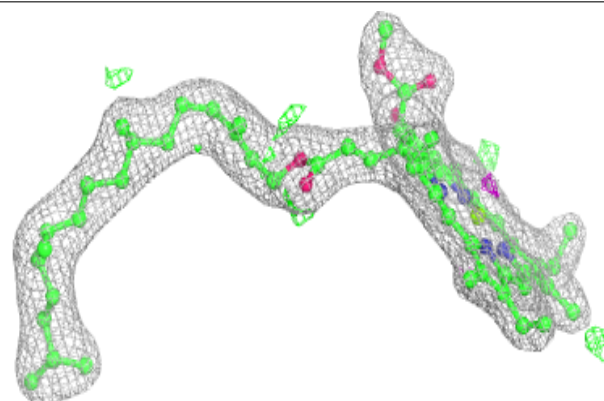


**Electron density around CLA D 405 (A):**

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

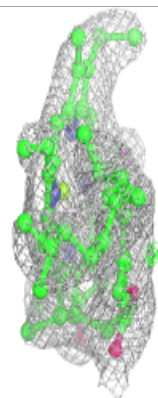
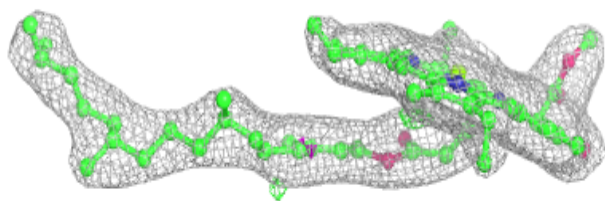
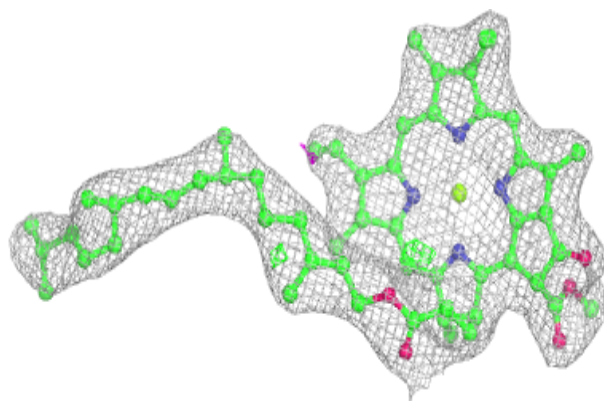
**Electron density around CLA D 405 (B):**

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



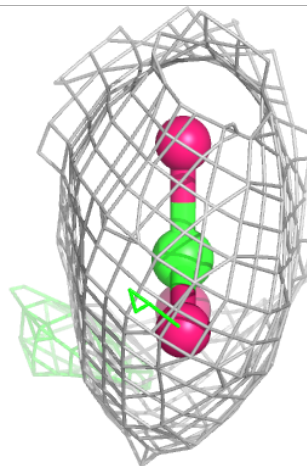
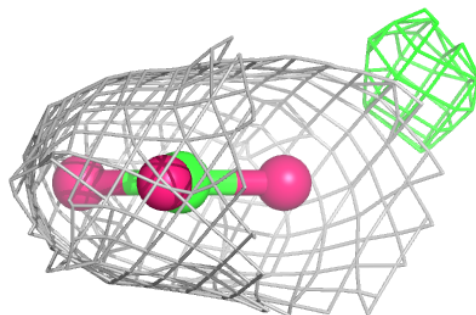
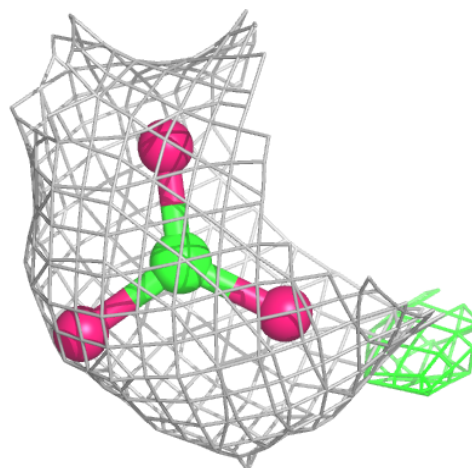
**Electron density around CLA b 603:**

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

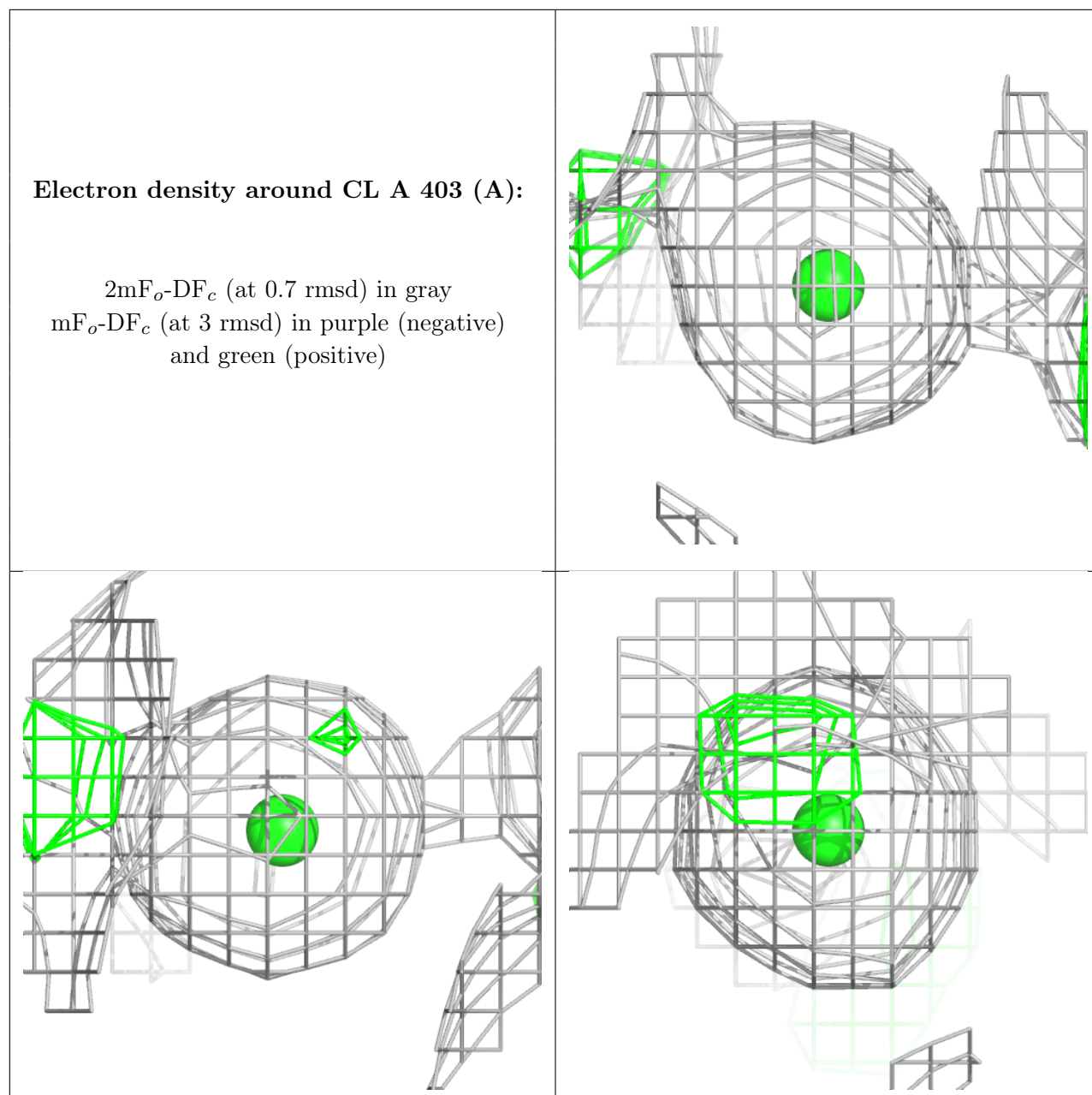


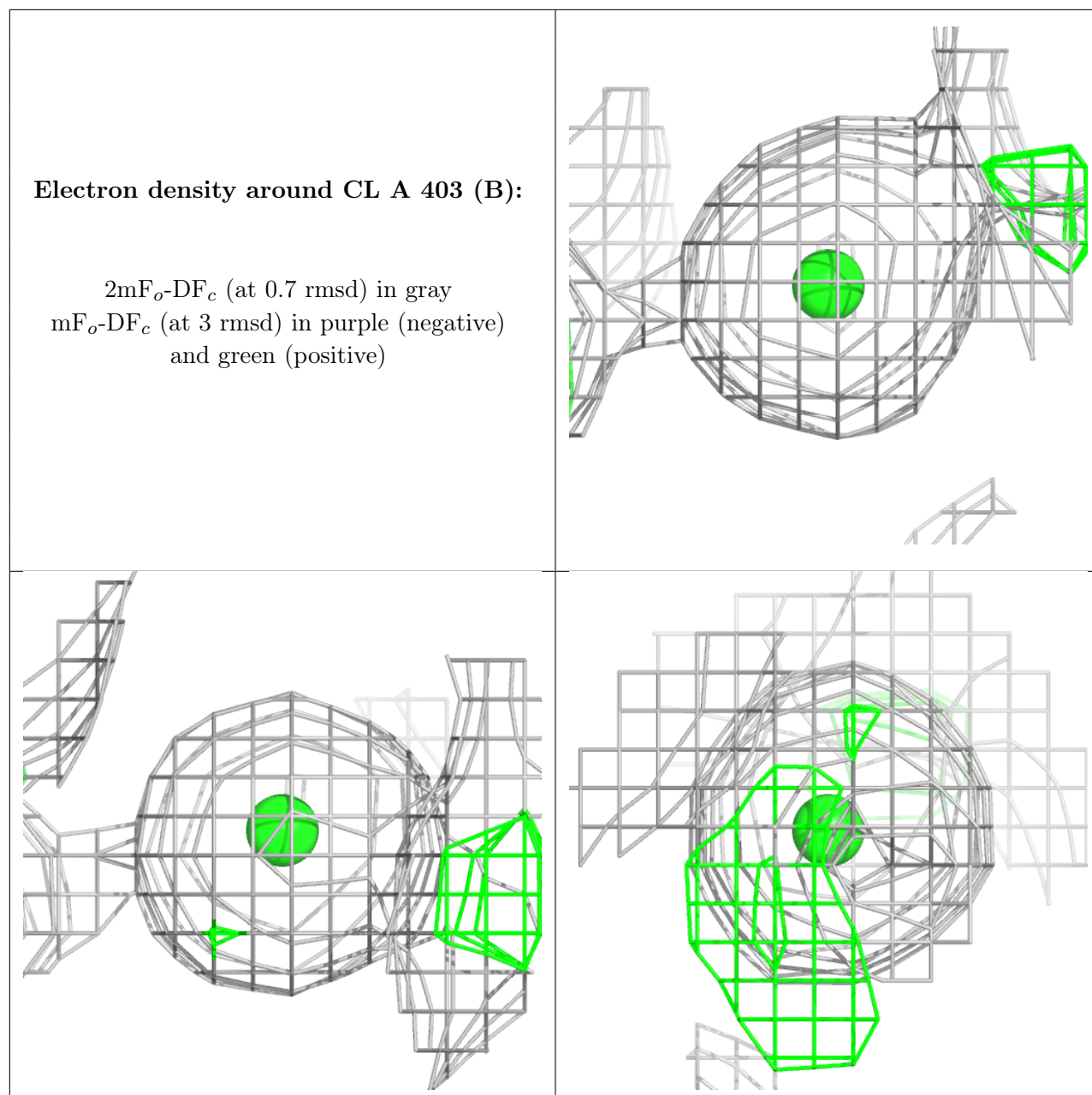
**Electron density around BCT a 404 (B):**

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



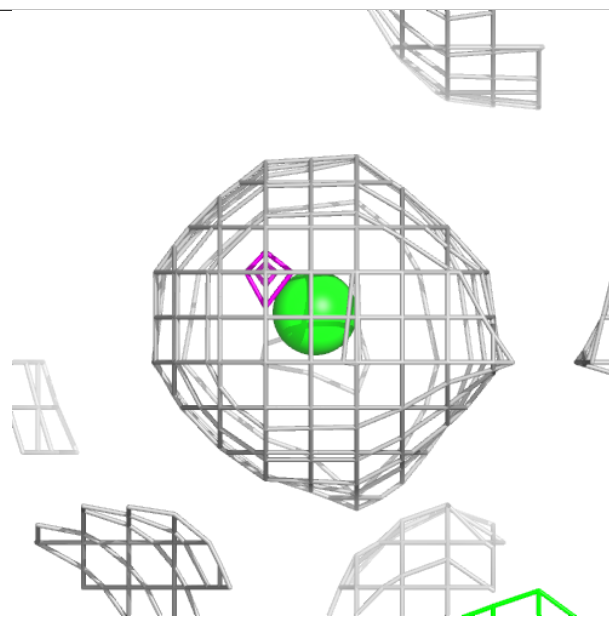
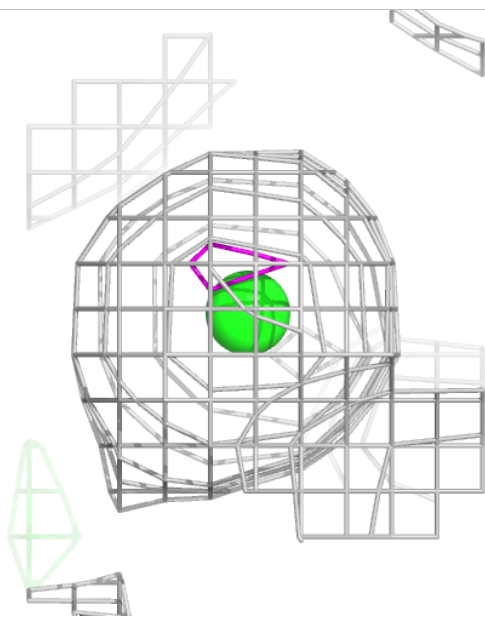
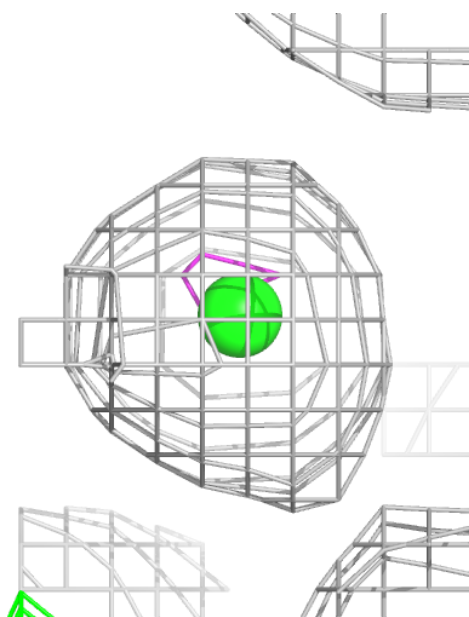






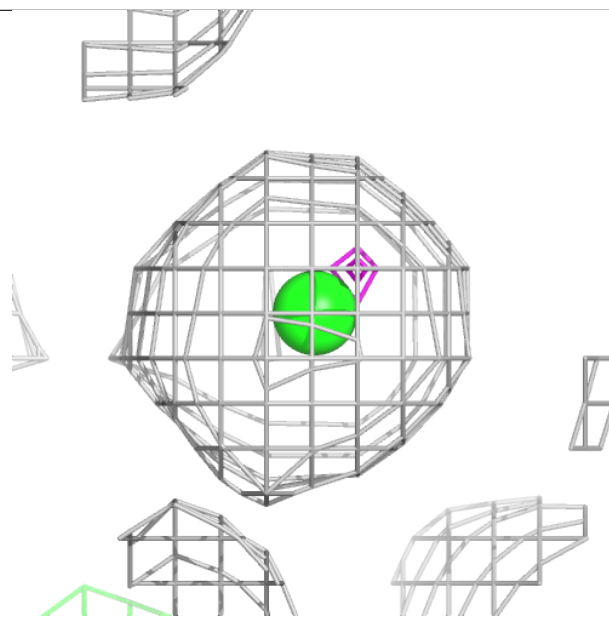
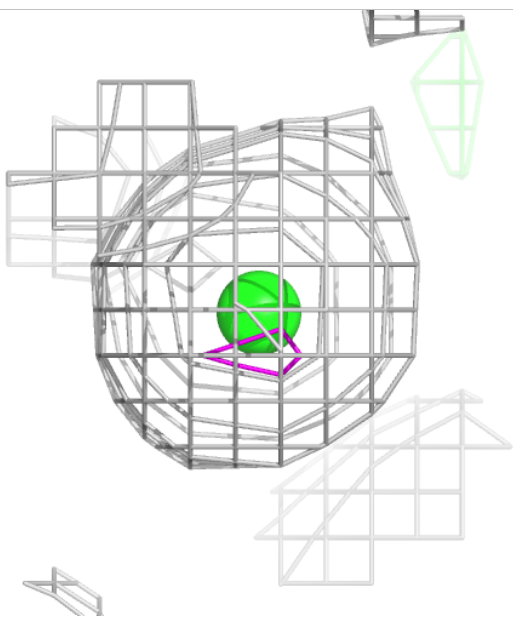
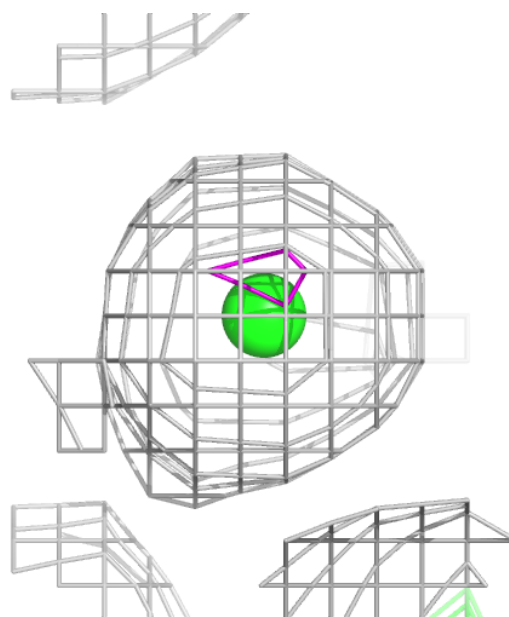
**Electron density around CL a 402 (A):**

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



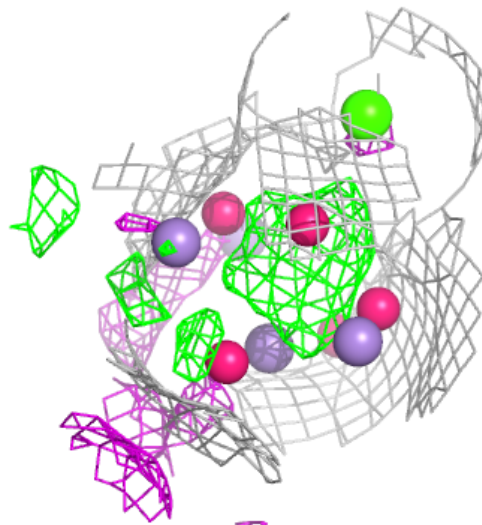
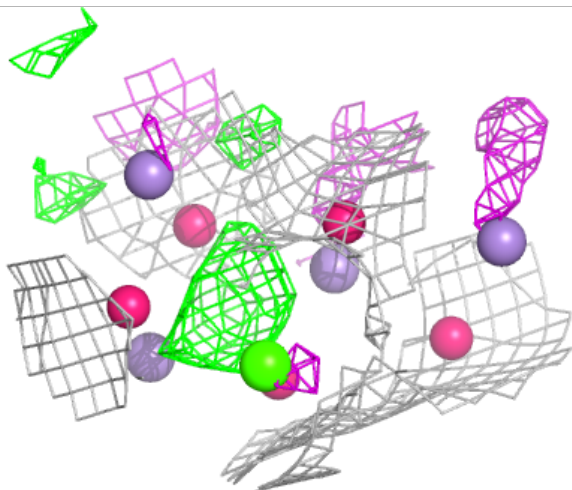
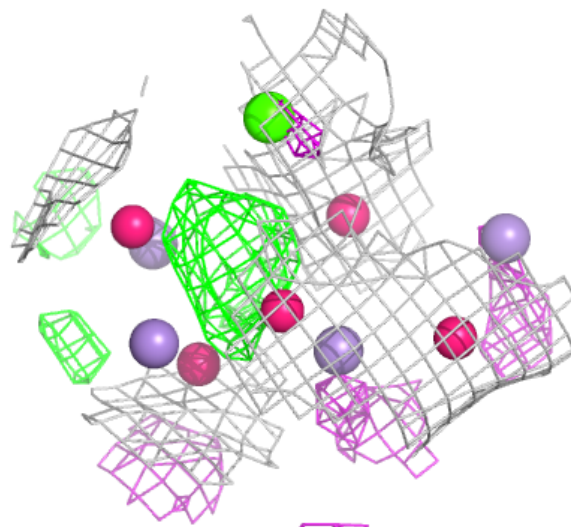
**Electron density around CL a 402 (B):**

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



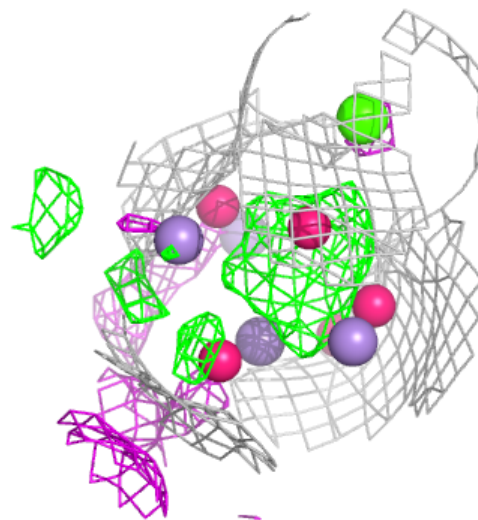
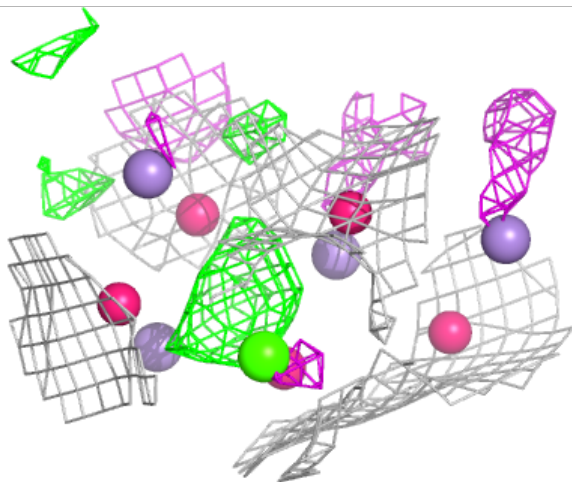
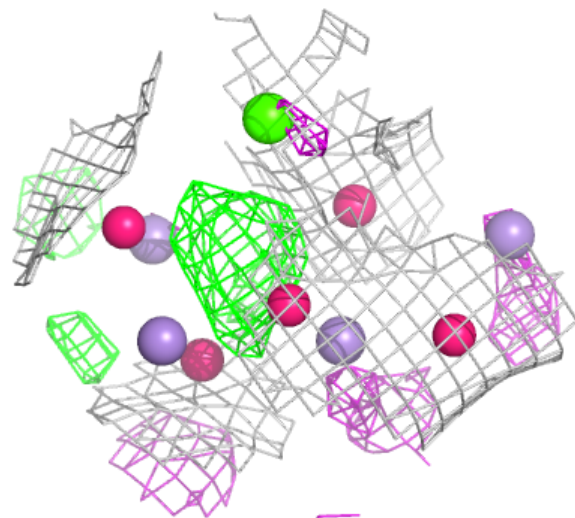
**Electron density around OEX A 413 (A):**

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



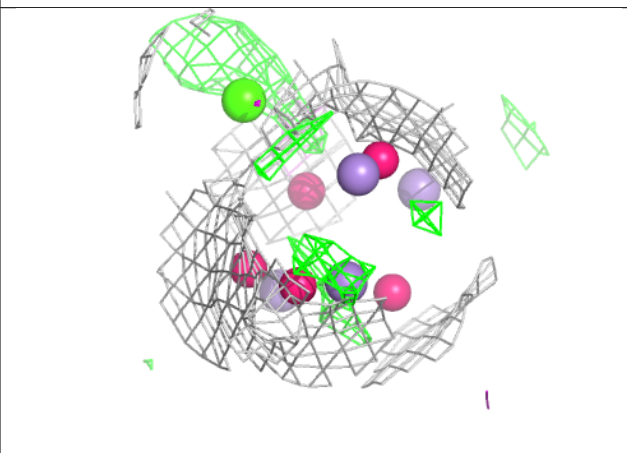
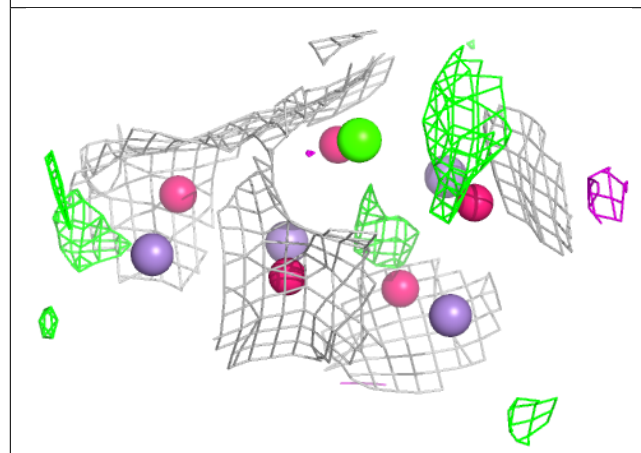
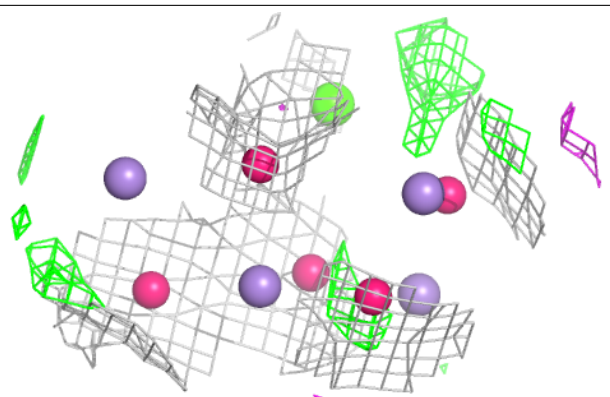
**Electron density around OEX A 413 (B):**

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



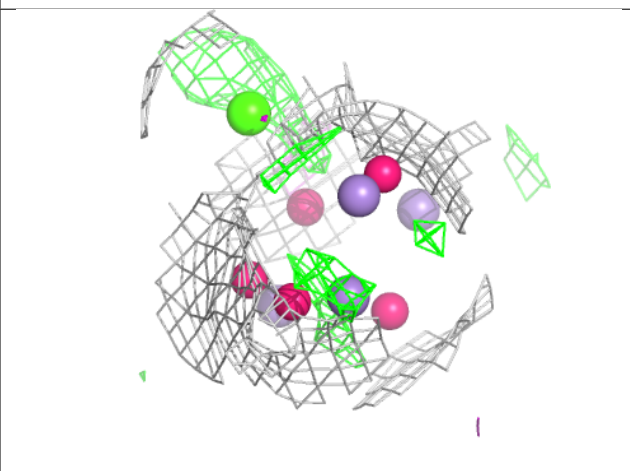
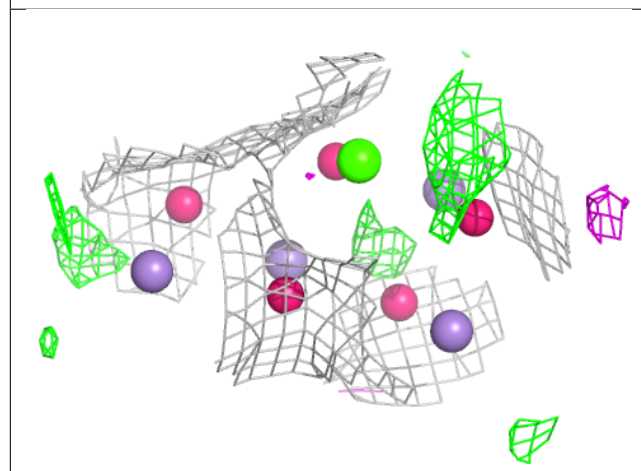
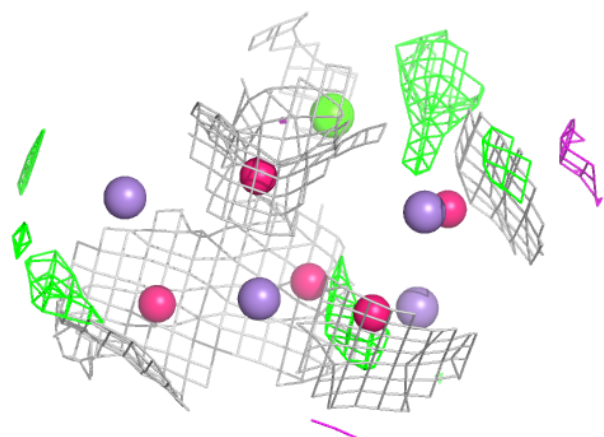
**Electron density around OEX a 415 (A):**

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



**Electron density around OEX a 415 (B):**

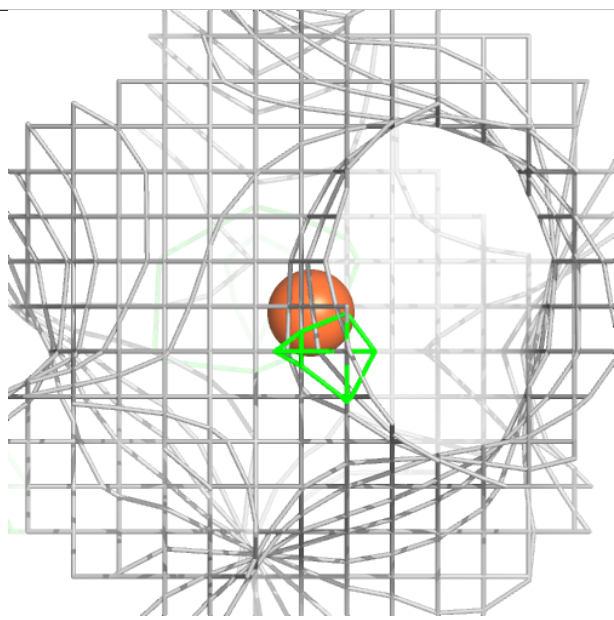
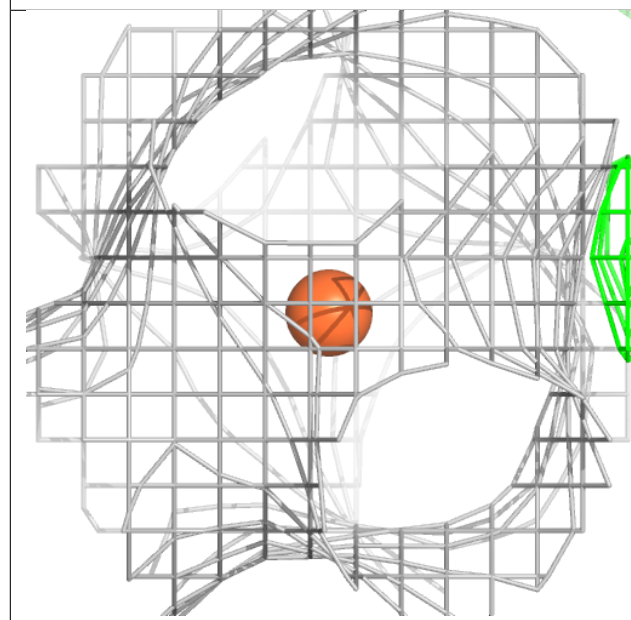
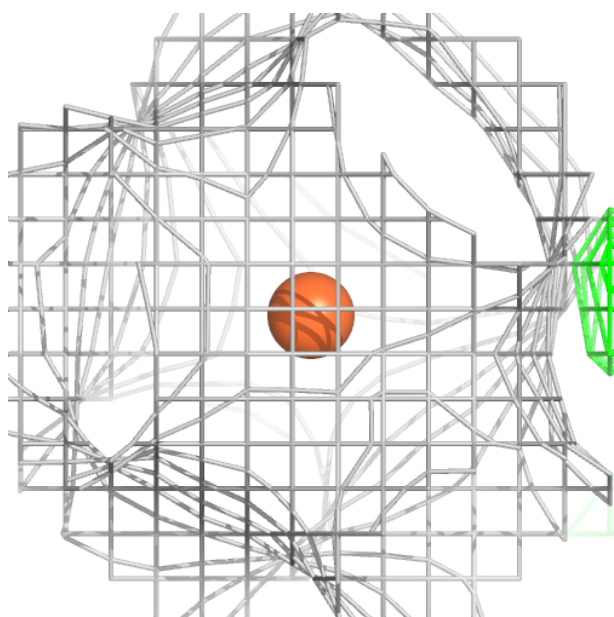
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





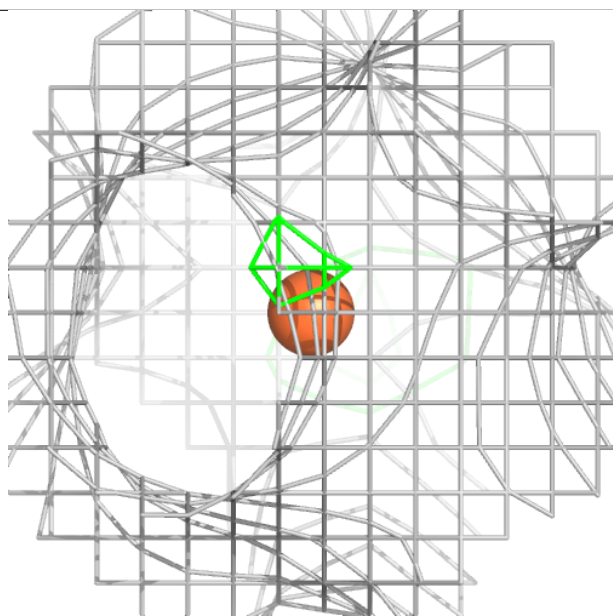
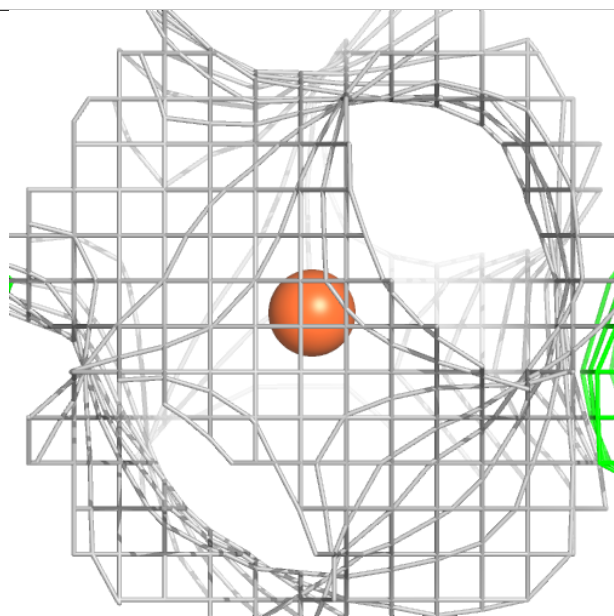
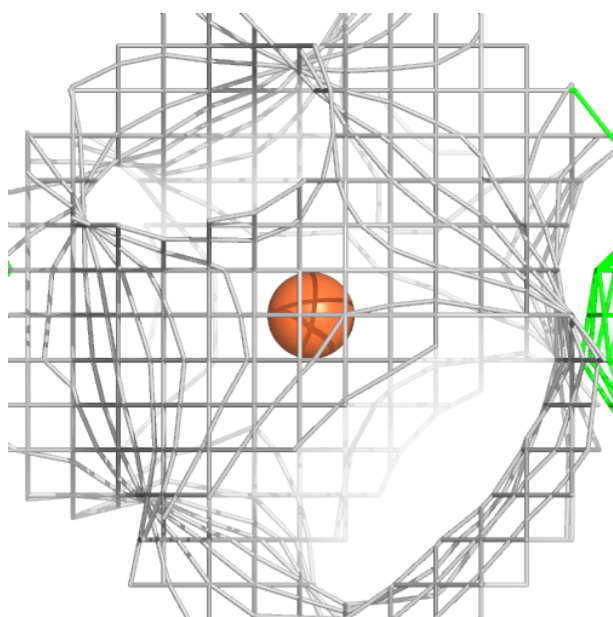
**Electron density around FE2 a 401 (A):**

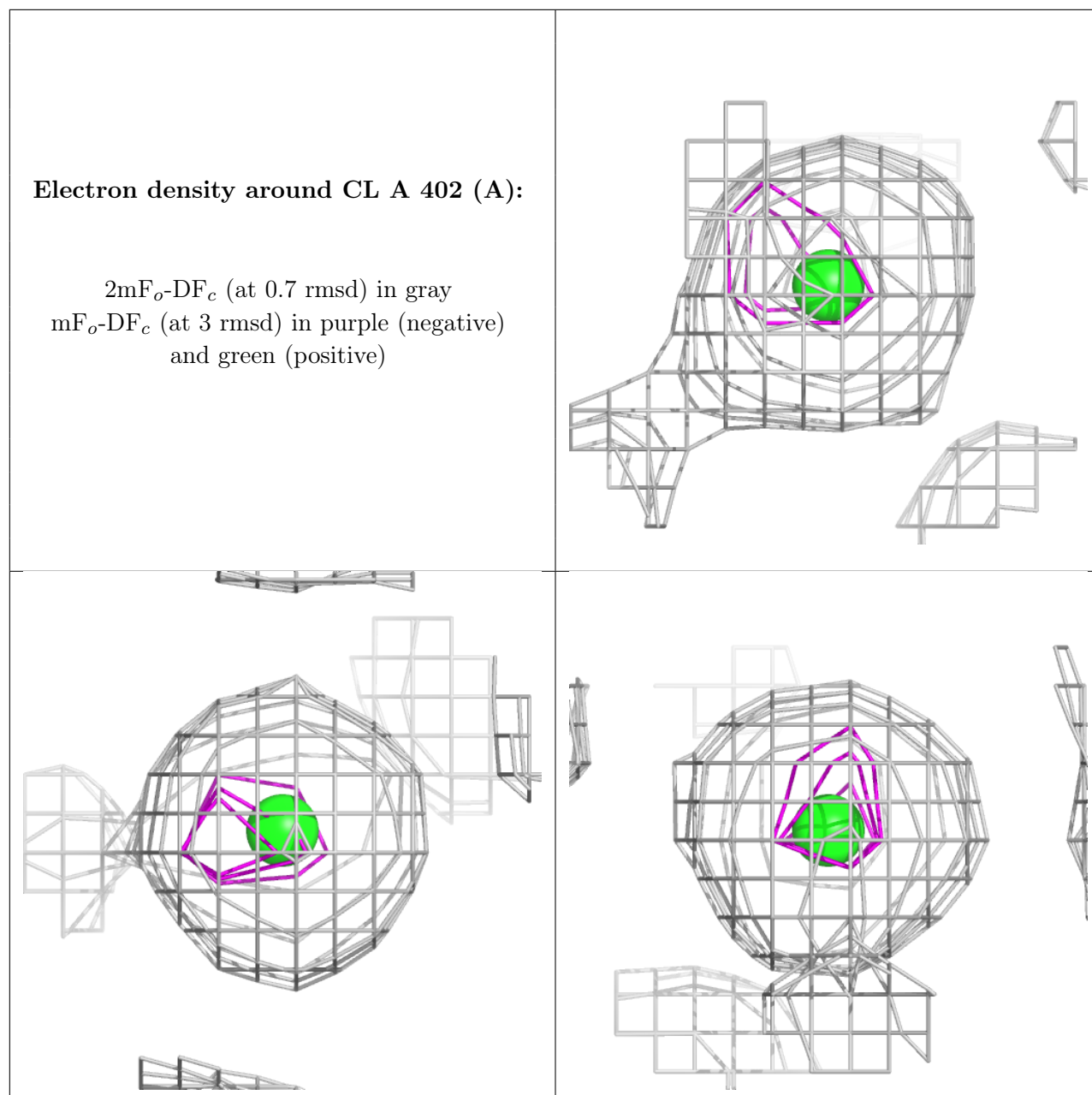
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

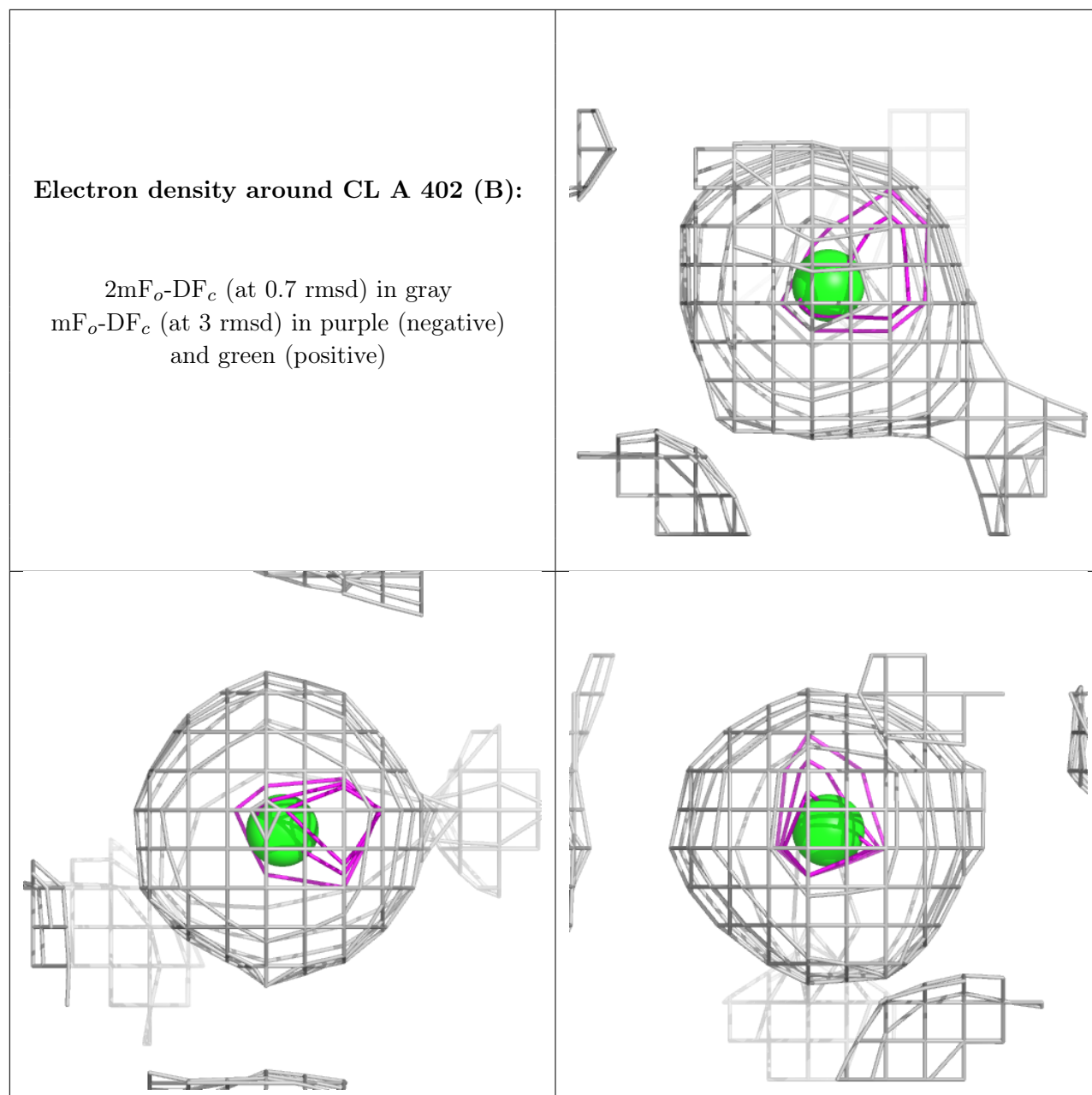


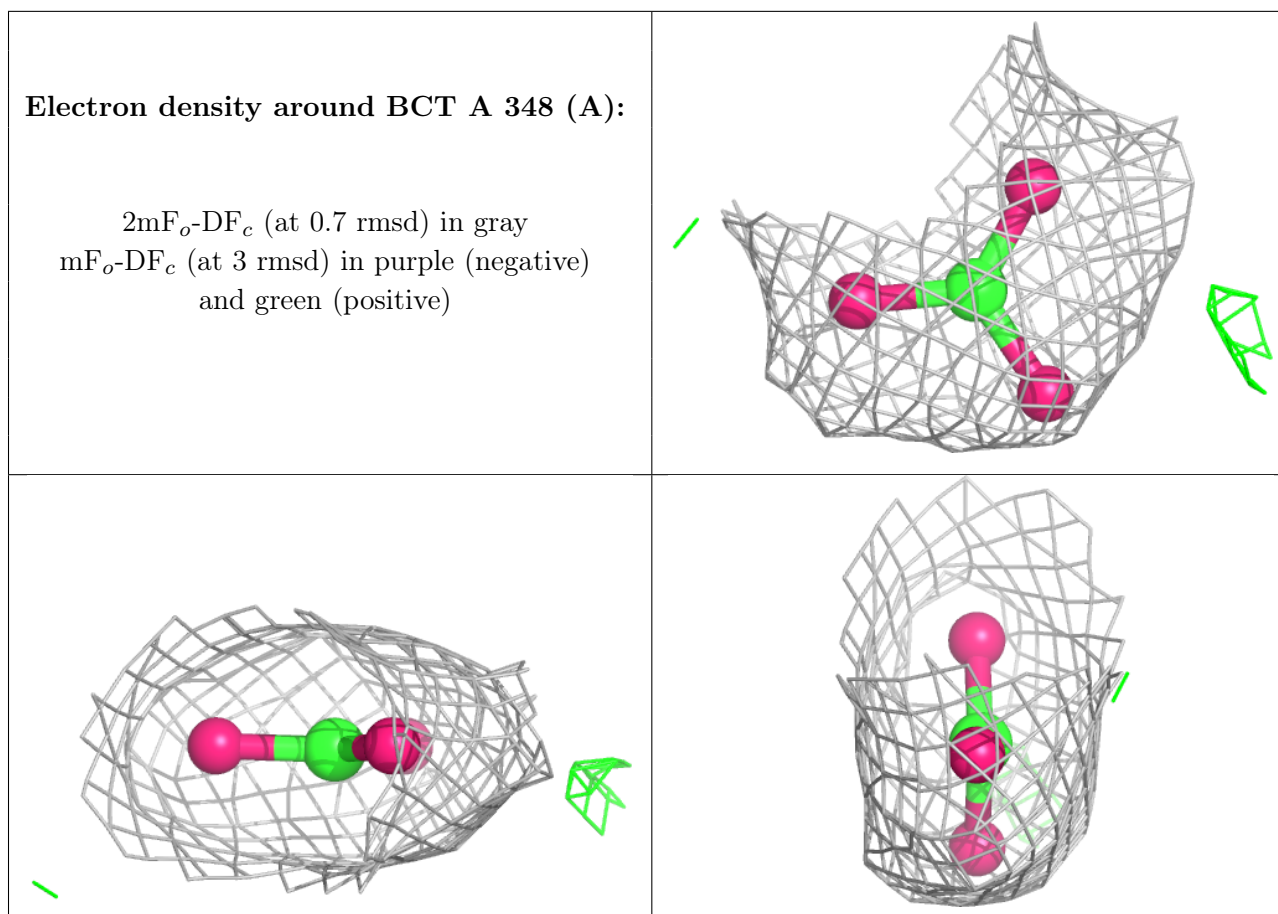
**Electron density around FE2 a 401 (B):**

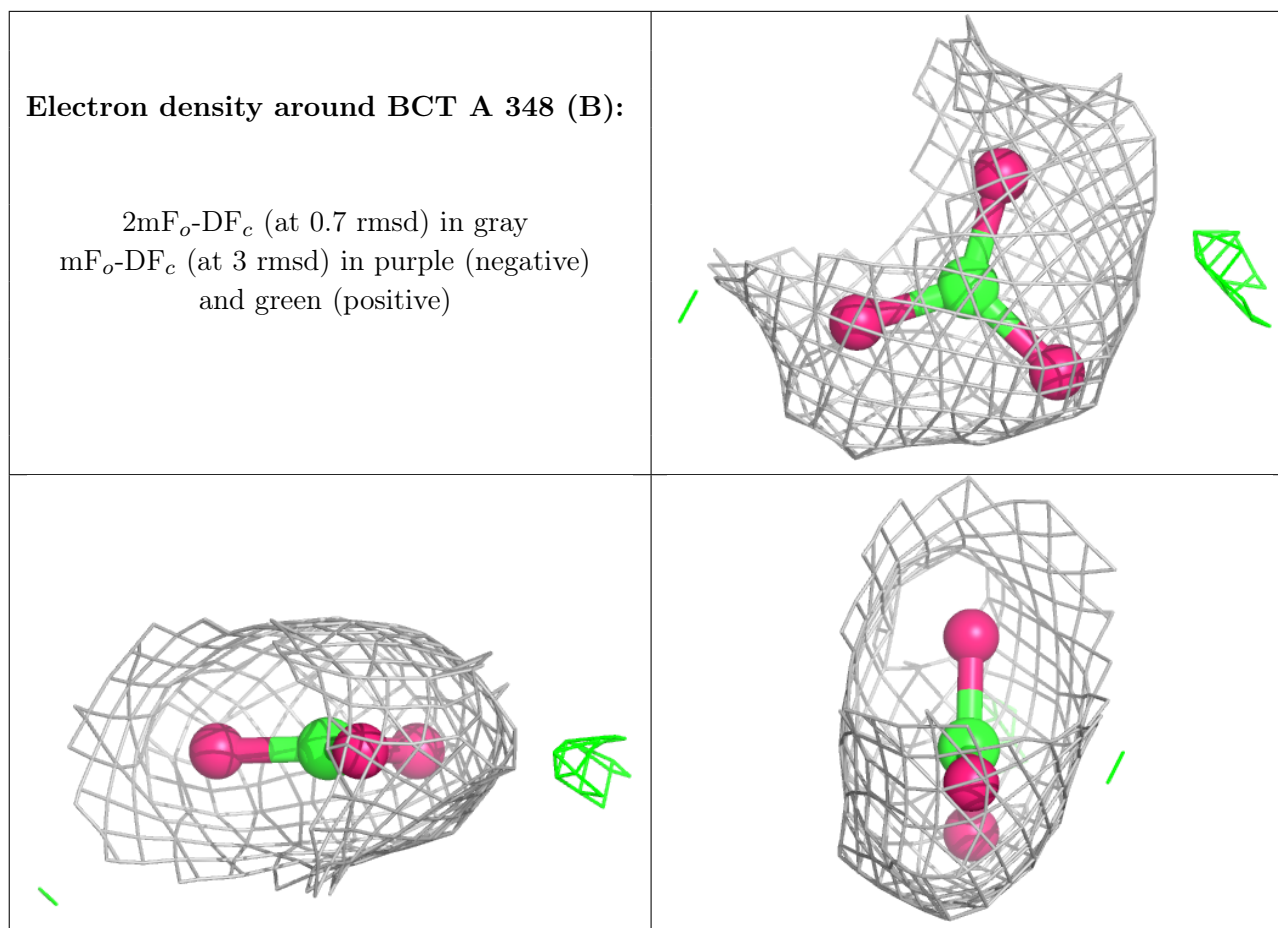
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





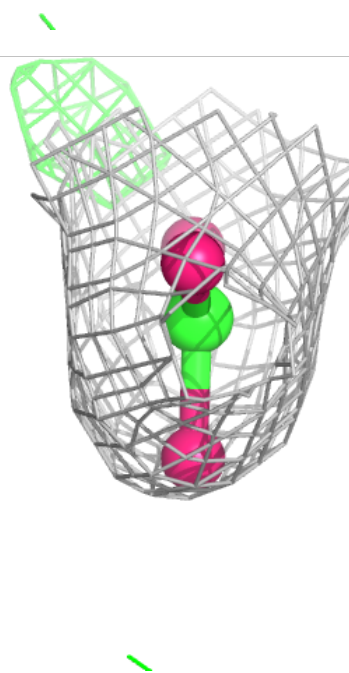
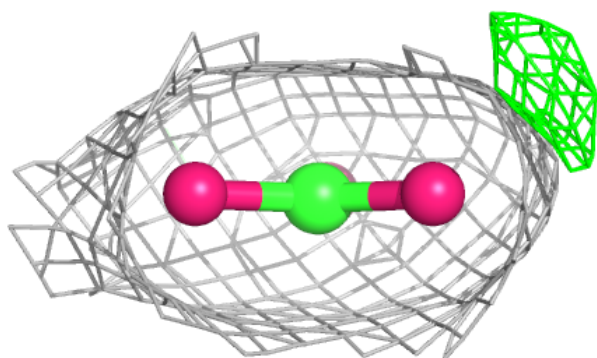
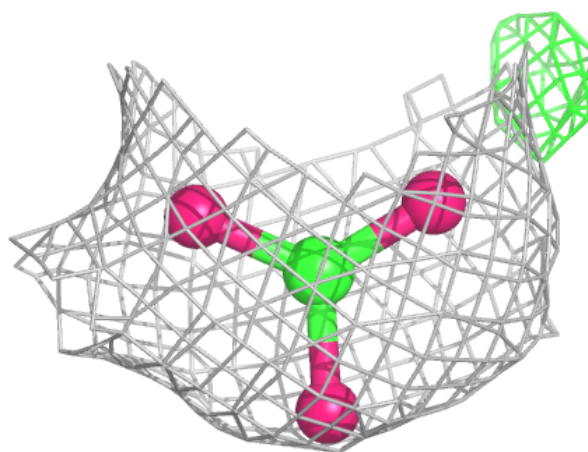






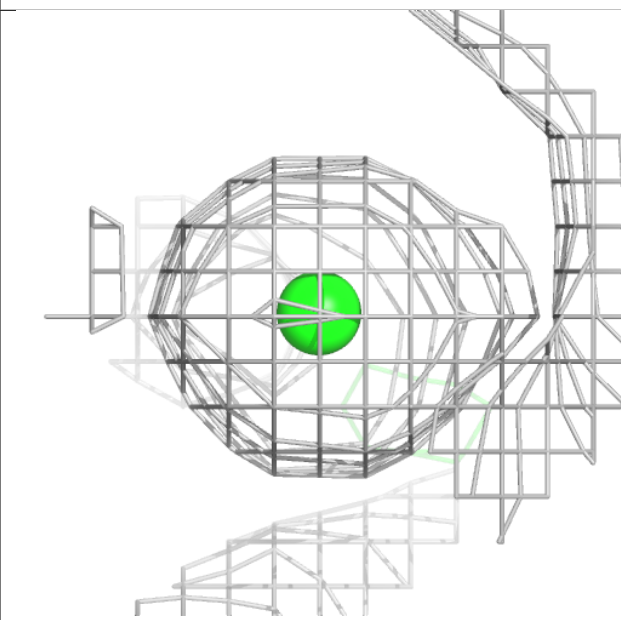
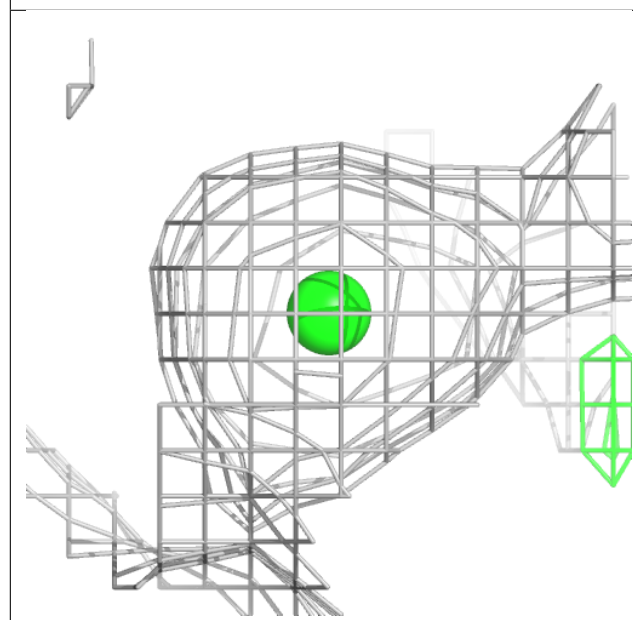
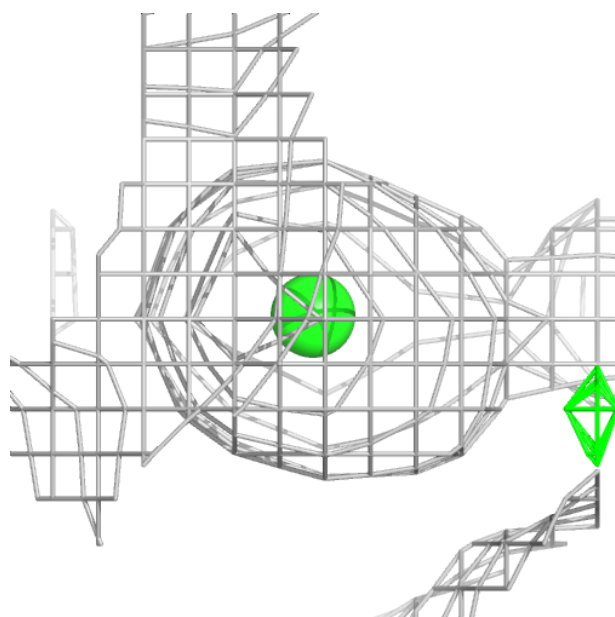
**Electron density around BCT a 404 (A):**

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



**Electron density around CL a 403 (A):**

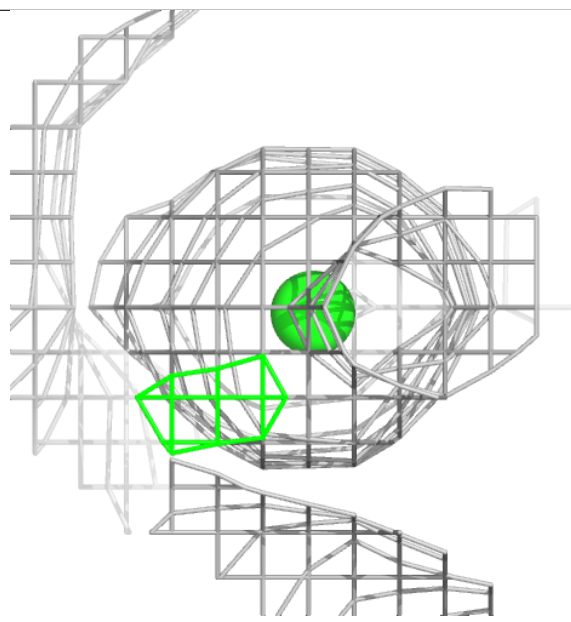
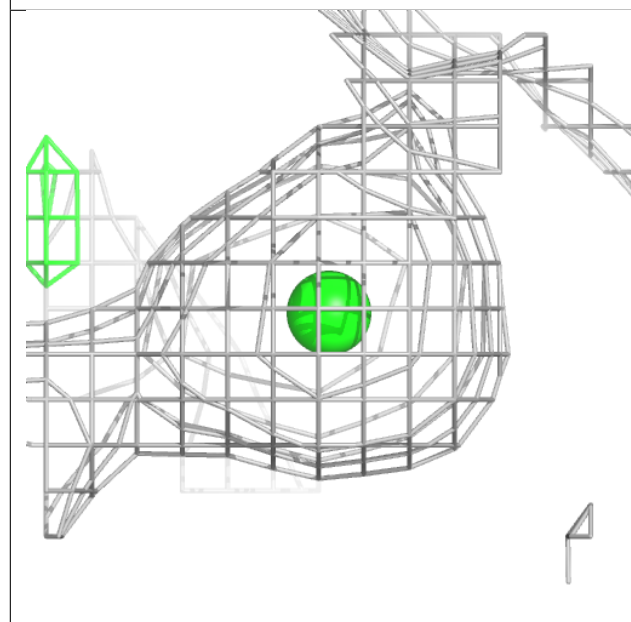
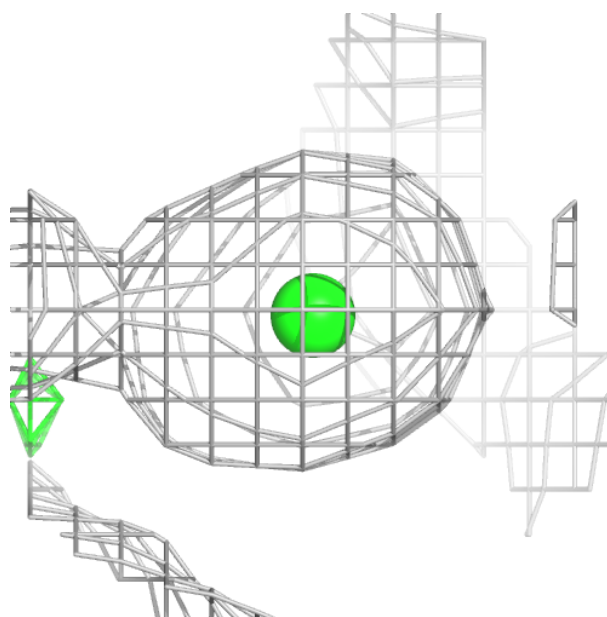
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





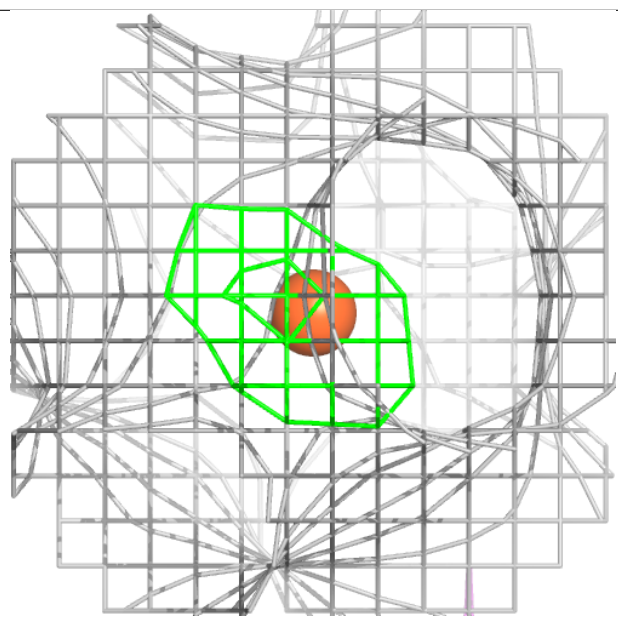
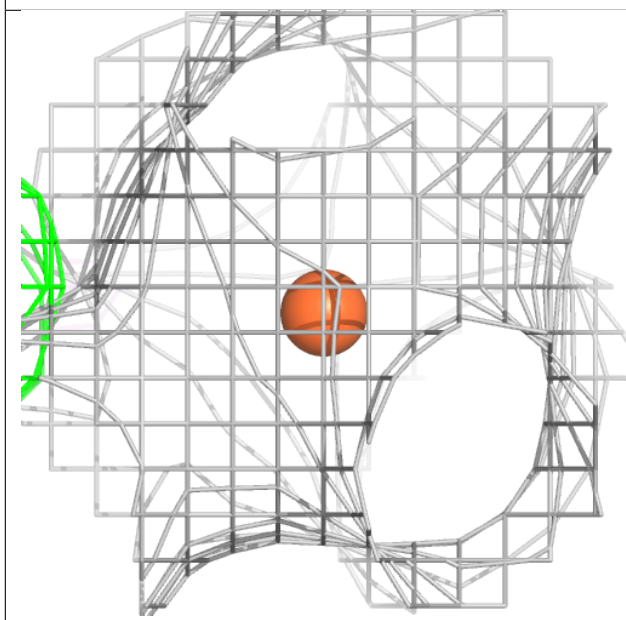
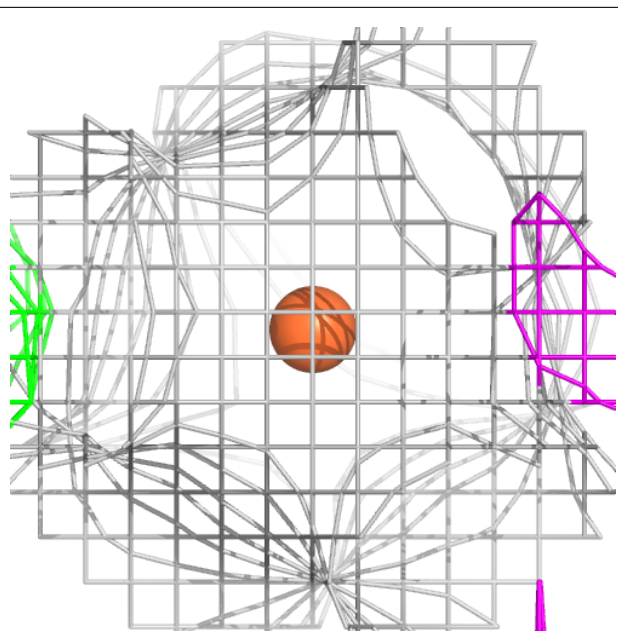
**Electron density around CL a 403 (B):**

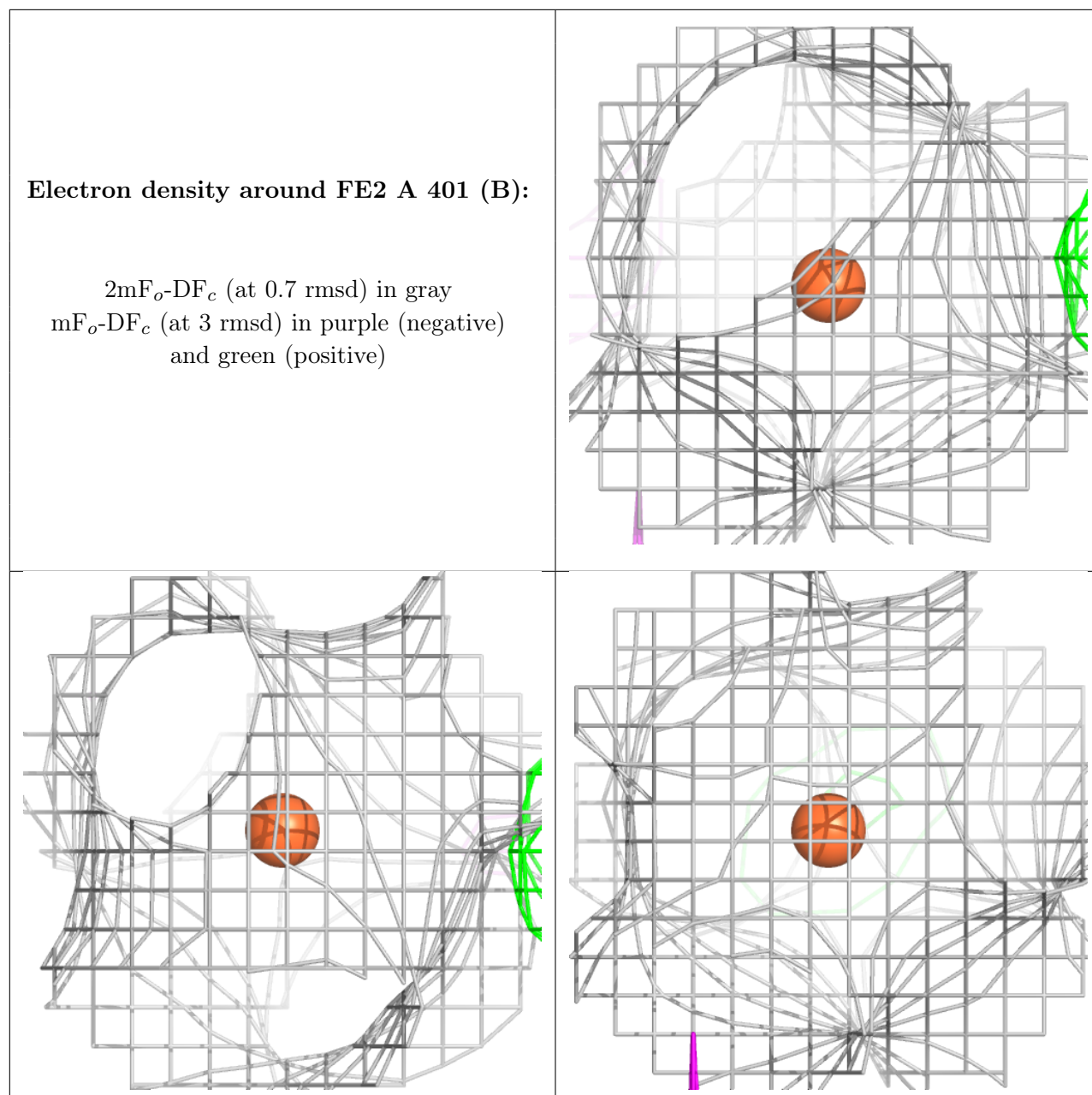
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE2 A 401 (A):**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.