



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 23, 2023 – 03:46 AM JST

PDB ID : 8GN0  
Title : Crystal structure of DCBQ-bound photosystem II complex  
Authors : Kamada, S.; Nakajima, Y.; Shen, J.-R.  
Deposited on : 2022-08-22  
Resolution : 2.15 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>.

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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

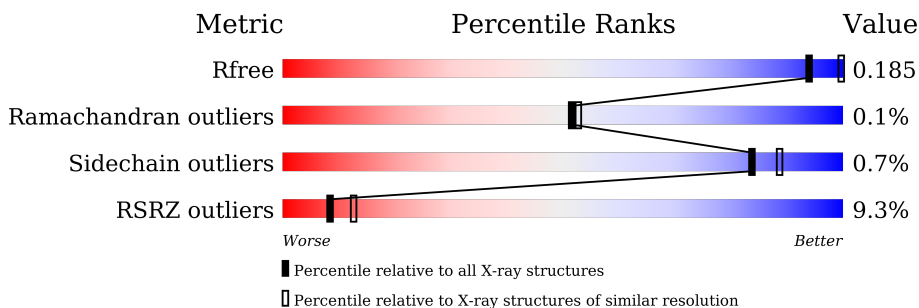
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	 3% 97%
1	a	344	 8% 96%
2	B	505	 10% 99%
2	b	505	 7% 95%
3	C	455	 6% 98%
3	c	455	 7% 99%
4	D	342	 2% 99%

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Mol	Chain	Length	Quality of chain
4	d	342	3% 99%
5	E	83	27% 94%
5	e	83	17% 95% 5%
6	F	44	11% 77% 23%
6	f	44	5% 73% 27%
7	H	63	8% 97%
7	h	63	27% 97%
8	I	38	16% 82% 16%
8	i	38	16% 82% 16%
9	J	40	5% 90% 10%
9	j	40	12% 98%
10	K	37	3% 100%
10	k	37	8% 100%
11	L	37	11% 100%
11	l	37	3% 97%
12	M	36	3% 92% 8%
12	m	36	6% 92% 6%
13	O	244	13% 99%
13	o	244	14% 99%
14	T	32	3% 91% 6%
14	t	32	6% 91% 6%
15	U	104	3% 93% 7%
15	u	104	% 92% 7%
16	V	137	2% 100%
16	v	137	16% 100%

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

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	405	X	-	-	-
23	CLA	A	410	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	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	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	513	X	-	-	-
23	CLA	D	2303	X	-	-	-
23	CLA	D	2304	X	-	-	-
23	CLA	a	2609	X	-	-	-
23	CLA	a	2613	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	b	621	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	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	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	c	516	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	408	X	-	-	-
23	CLA	d	409	X	-	-	-
28	LMT	f	101	-	-	-	X
29	GOL	v	204	-	-	-	X
30	UNL	B	629	-	-	-	X
30	UNL	T	101	-	-	-	X
30	UNL	a	2616	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	2702	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	JOX	a	2617	-	X	-	-
34	DMS	B	640	-	-	-	X
34	DMS	O	311	-	-	-	X
34	DMS	a	2620	-	-	-	X
34	DMS	c	541	-	-	-	X
34	DMS	c	547	-	-	-	X
34	DMS	o	309	-	-	-	X
36	HTG	B	625	-	-	-	X
36	HTG	C	522	-	-	-	X
36	HTG	c	524	-	-	-	X
36	HTG	d	407	-	-	-	X

## 2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 53814 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	2614	1715	428	456	15	0	3	0
1	a	334	2629	1722	432	460	15	0	4	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	505	4005	2628	667	697	13	0	7	0
2	b	483	3833	2520	637	663	13	0	9	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	3494	2286	585	610	13	0	2	0
3	c	455	3518	2303	589	613	13	0	0	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

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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	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	342	Total	C	N	O	S	0	3	0
			2738	1815	447	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	1	0
			643	422	101	120			
5	e	79	Total	C	N	O	0	1	0
			630	417	99	114			

- 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
			271	184	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	32	Total	C	N	O	S	0	0	0
			256	177	37	41	1			
8	i	32	Total	C	N	O	S	0	0	0
			259	178	37	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			274	184	40	48	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			297	208	43	46			
10	k	37	Total	C	N	O	0	0	0
			289	201	42	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	37	Total	C	N	O	S	0	1	0
			303	204	45	53	1			
11	l	36	Total	C	N	O		0	2	0
			305	206	47	52				

- 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	2	0
			267	180	38	48	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			270	182	39	48	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	244	Total	C	N	O	S	0	3	0
			1870	1171	314	380	5			
13	o	243	Total	C	N	O	S	0	4	0
			1874	1174	312	382	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			776	493	130	153			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1063	677	177	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			216	139	38	36	3			

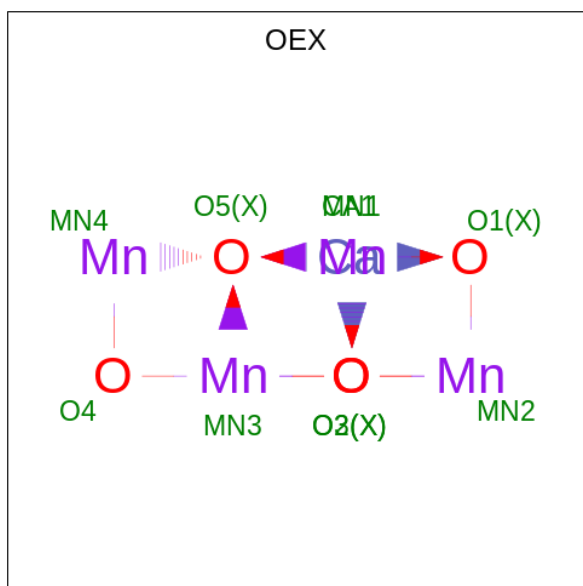
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	0	0
			275	185	44	46				
18	x	35	Total	C	N	O	S	0	1	0
			257	176	38	43				

- 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
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			456	312	70	72	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

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

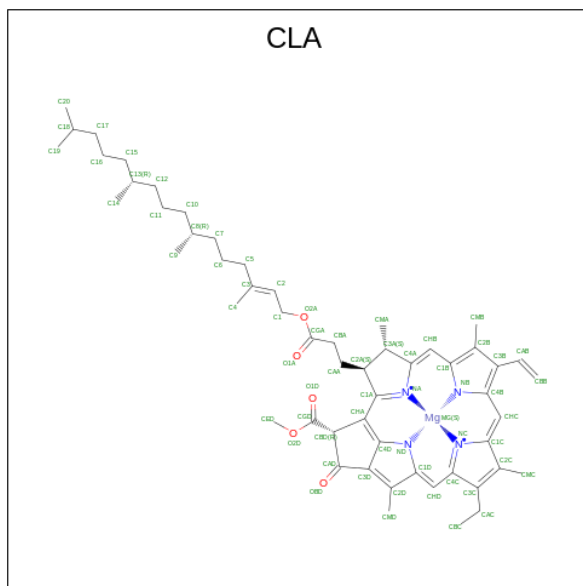
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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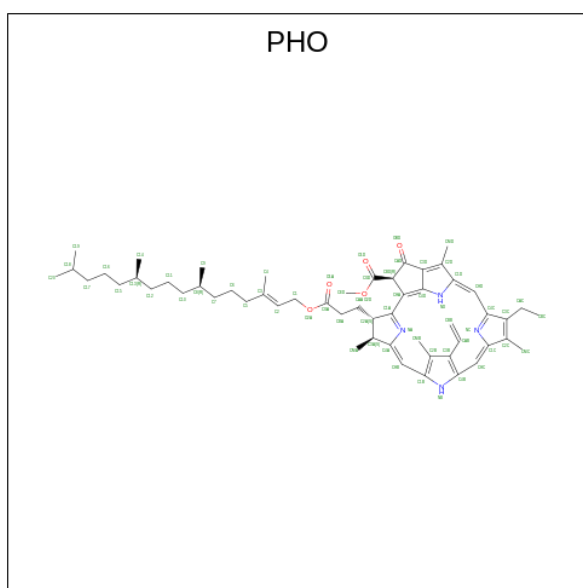
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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

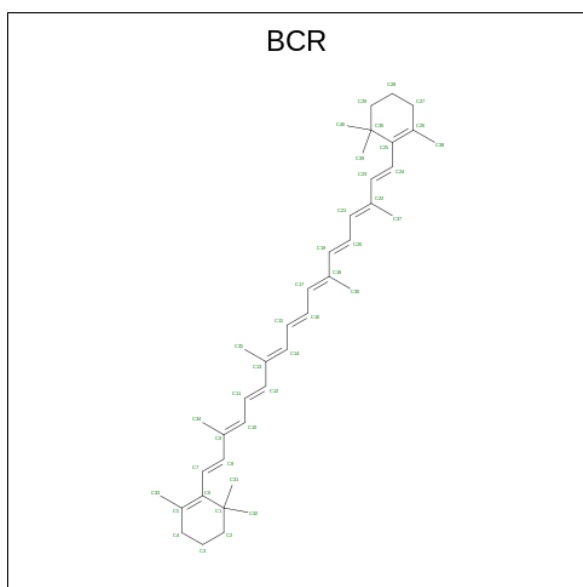
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

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





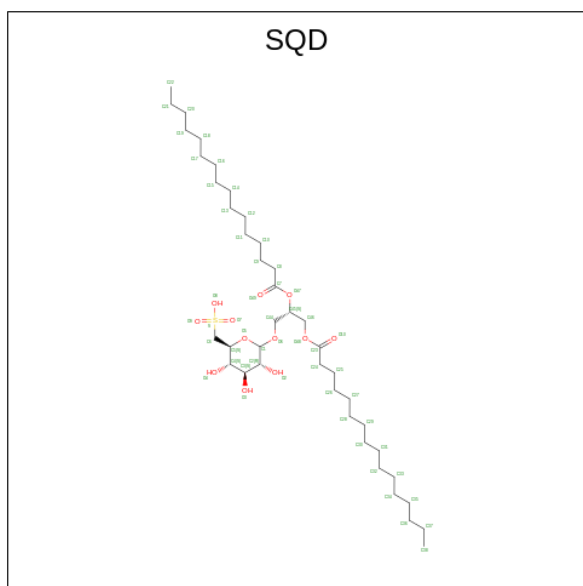
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	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	k	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	z	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:  $C_{41}H_{78}O_{12}S$ ).



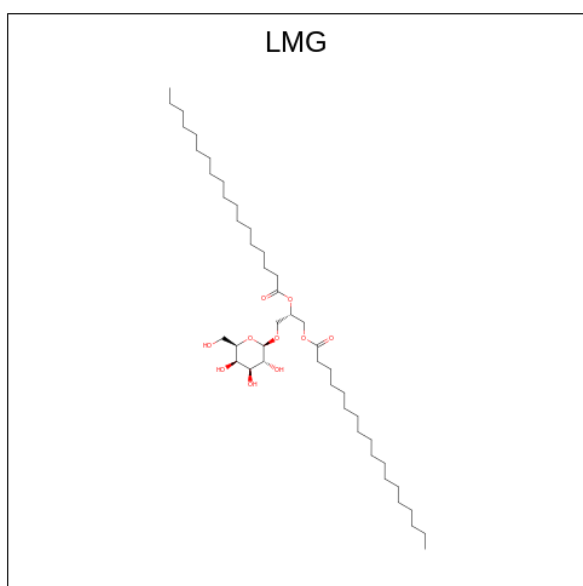
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 46 33 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	a	1	48	35	12	1	0	0
26	b	1	48	35	12	1	0	0
26	d	1	33	23	9	1	0	0
26	l	1	54	41	12	1	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



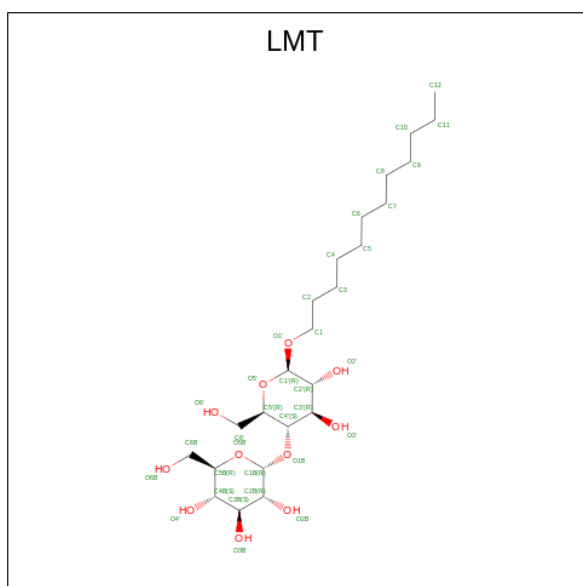
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	1	51	41	10	0	0
27	B	1	51	41	10	0	0
27	C	1	51	41	10	0	0
27	C	1	51	41	10	0	0
27	D	1	47	37	10	0	0
27	c	1	51	41	10	0	0
27	c	1	49	39	10	0	0

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

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



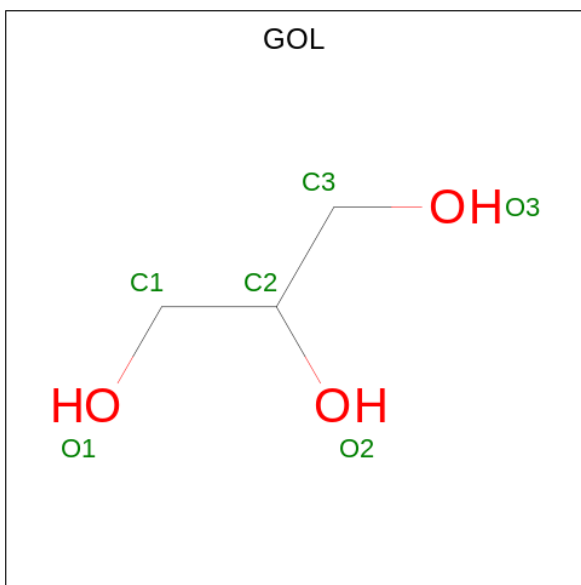
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			33	22	11		
28	A	1	Total	C	O	0	0
			24	18	6		
28	B	1	Total	C	O	0	0
			35	24	11		
28	B	1	Total	C	O	0	0
			35	24	11		
28	F	1	Total	C	O	0	0
			24	18	6		
28	J	1	Total	C	O	0	0
			24	18	6		
28	M	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			24	18	6		
28	Z	1	Total	C	O	0	0
			35	24	11		
28	d	1	Total	C	O	0	0
			35	24	11		
28	d	1	Total	C	O	0	0
			25	19	6		
28	f	1	Total	C	O	0	0
			24	18	6		
28	i	1	Total	C	O	0	0
			24	18	6		
28	j	1	Total	C	O	0	0
			34	23	11		
28	m	1	Total	C	O	0	0
			35	24	11		
28	m	1	Total	C	O	0	0
			35	24	11		
28	z	1	Total	C	O	0	0
			33	22	11		

- Molecule 29 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total 6	C 3	O 3	0	0
29	B	1	Total 6	C 3	O 3	0	0
29	B	1	Total 6	C 3	O 3	0	0
29	B	1	Total 6	C 3	O 3	0	0
29	C	1	Total 6	C 3	O 3	0	0
29	C	1	Total 6	C 3	O 3	0	0
29	D	1	Total 6	C 3	O 3	0	0
29	E	1	Total 6	C 3	O 3	0	0
29	J	1	Total 6	C 3	O 3	0	0
29	O	1	Total 6	C 3	O 3	0	0
29	O	1	Total 6	C 3	O 3	0	0
29	O	1	Total 6	C 3	O 3	0	0
29	O	1	Total 6	C 3	O 3	0	0
29	O	1	Total 6	C 3	O 3	0	0
29	U	1	Total 6	C 3	O 3	0	0
29	U	1	Total 6	C 3	O 3	0	0
29	V	1	Total 6	C 3	O 3	0	0
29	a	1	Total 6	C 3	O 3	0	0
29	a	1	Total 6	C 3	O 3	0	0
29	b	1	Total 6	C 3	O 3	0	0
29	b	1	Total 6	C 3	O 3	0	0
29	c	1	Total 6	C 3	O 3	0	0

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

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

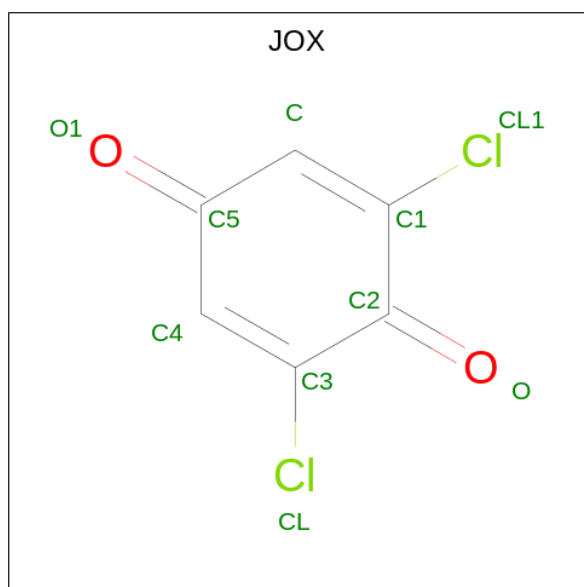
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	2	Total	C	O	0	0
			37	32	5		
30	B	3	Total	C	O	0	0
			65	58	7		
30	C	2	Total	C	O	0	0
			50	45	5		
30	D	3	Total	C	O	0	0
			48	44	4		
30	E	2	Total	C		0	0
			15	15			
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			5	5			
30	T	1	Total	C		0	0
			13	13			
30	Y	1	Total	C		0	0
			12	12			
30	a	2	Total	C	O	0	0
			42	37	5		
30	b	5	Total	C	O	0	0
			64	60	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	c	4	Total	C	O	0	0
			59	54	5		
30	d	2	Total	C	O	0	0
			55	48	7		
30	e	1	Total	C		0	0
			15	15			
30	i	1	Total	C	O	0	0
			19	15	4		
30	j	1	Total	C		0	0
			16	16			
30	k	1	Total	C		0	0
			16	16			
30	l	1	Total	C	O	0	0
			16	14	2		
30	m	1	Total	C	O	0	0
			15	13	2		
30	t	1	Total	C		0	0
			8	8			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is 2,6-bis(chloranyl)cyclohexa-2,5-diene-1,4-dione (three-letter code: JOX) (formula: C<sub>6</sub>H<sub>2</sub>Cl<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	Cl	O	0	0
			10	6	2	2		

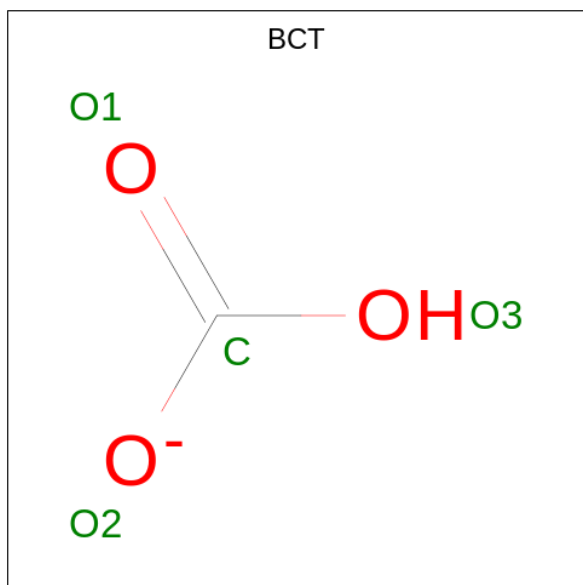
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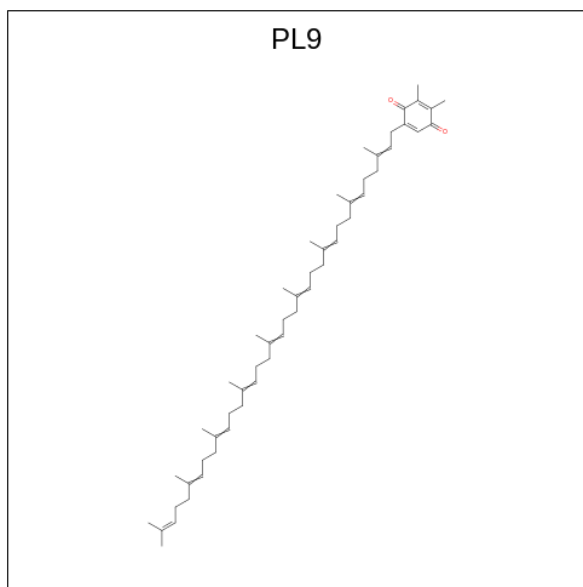
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	Cl	O	0	0
			10	6	2	2		
31	a	1	Total	C	Cl	O	0	0
			10	6	2	2		
31	a	1	Total	C	Cl	O	0	0
			10	6	2	2		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



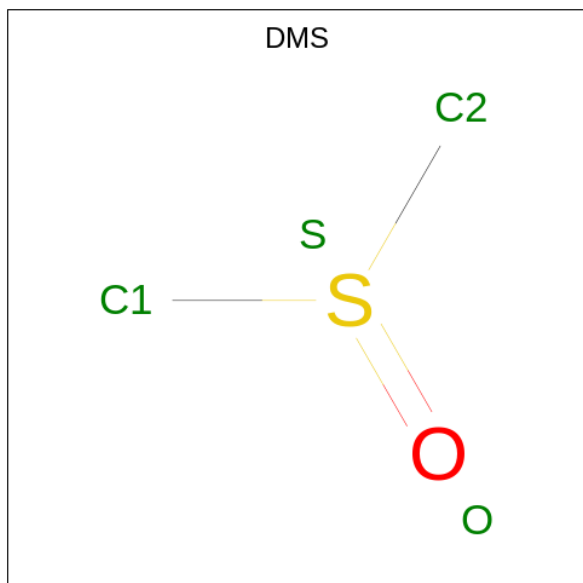
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C 39 39	0	0
33	D	1	Total C O 55 53 2	0	0
33	d	1	Total C O 55 53 2	0	0
33	x	1	Total C 39 39	0	0

- Molecule 34 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	l	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	o	1	Total	C	O	S	0	0
			4	2	1	1		
34	t	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	u	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		
34	v	1	Total	C	O	S	0	0
			4	2	1	1		

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

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

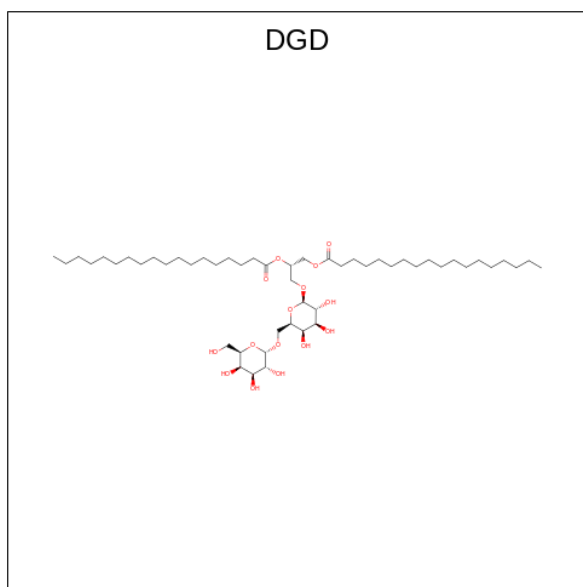
- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	i	1	Total	C	O	S	0	0
			19	13	5	1		
36	o	1	Total	C	O	S	0	0
			19	13	5	1		

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



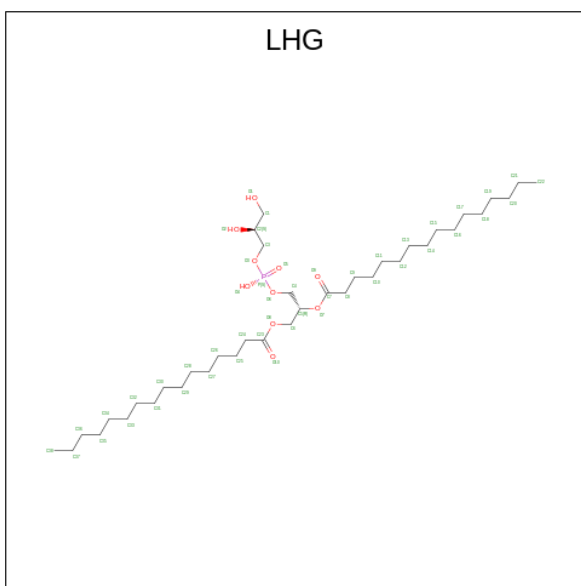
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			58	43	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			53	42	11		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	h	1	Total	C	O	0	0
			62	47	15		

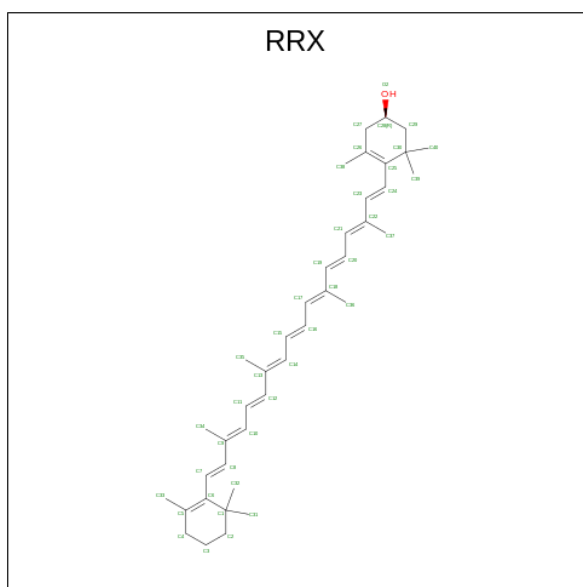
- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			39	28	10	1		
38	E	1	Total	C	O	P	0	0
			40	29	10	1		
38	L	1	Total	C	O	P	0	0
			49	38	10	1		

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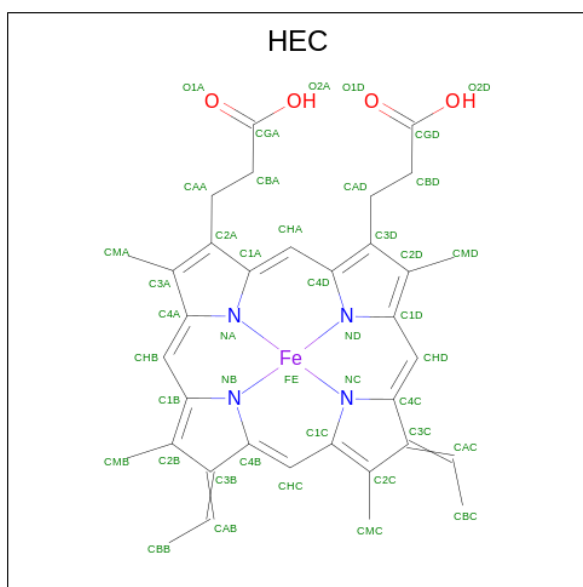


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	H	1	Total	C O	0	0
			41	40 1		
40	h	1	Total	C O	0	0
			41	40 1		

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	J	1	Total	Mg	0	0
			1	1		
41	K	1	Total	Mg	0	0
			1	1		
41	j	1	Total	Mg	0	0
			1	1		
41	k	1	Total	Mg	0	0
			1	1		

- Molecule 42 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	133	Total	O	0	0
			133	133		
43	B	302	Total	O	0	0
			302	302		
43	C	192	Total	O	0	0
			192	192		
43	D	146	Total	O	0	1
			147	147		
43	E	25	Total	O	0	0
			25	25		
43	F	9	Total	O	0	0
			9	9		
43	H	41	Total	O	0	0
			41	41		
43	I	8	Total	O	0	0
			8	8		
43	J	10	Total	O	0	0
			10	10		
43	K	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	L	15	Total O 15 15	0	0
43	M	12	Total O 12 12	0	0
43	O	144	Total O 145 145	0	1
43	T	12	Total O 12 12	0	0
43	U	79	Total O 79 79	0	0
43	V	113	Total O 113 113	0	0
43	Y	4	Total O 4 4	0	0
43	X	15	Total O 15 15	0	0
43	Z	8	Total O 8 8	0	0
43	a	122	Total O 122 122	0	0
43	b	250	Total O 251 251	0	1
43	c	211	Total O 211 211	0	0
43	d	146	Total O 147 147	0	1
43	e	19	Total O 19 19	0	0
43	f	7	Total O 7 7	0	0
43	h	27	Total O 27 27	0	0
43	i	8	Total O 8 8	0	0
43	j	10	Total O 10 10	0	0
43	k	5	Total O 5 5	0	0
43	l	20	Total O 20 20	0	0
43	m	11	Total O 11 11	0	0

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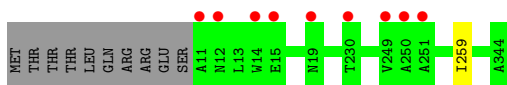
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
43	o	143	Total 144	O 144	0	1
43	t	10	Total 10	O 10	0	0
43	u	78	Total 78	O 78	0	0
43	v	93	Total 93	O 93	0	0
43	y	6	Total 6	O 6	0	0
43	x	4	Total 4	O 4	0	0
43	z	6	Total 6	O 6	0	0

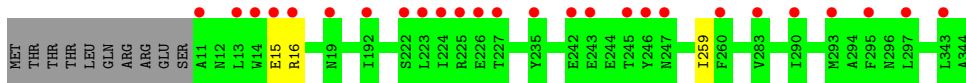
### 3 Residue-property plots

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.

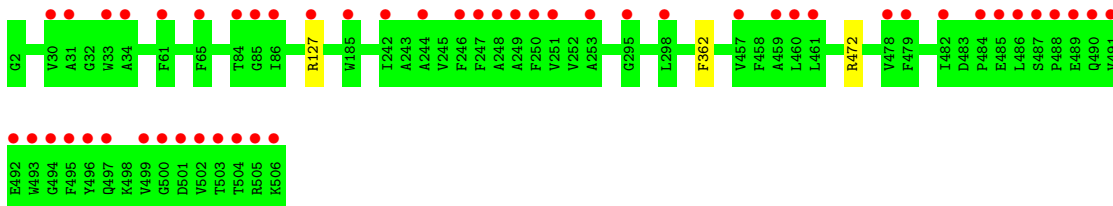
- Molecule 1: Photosystem II protein D1



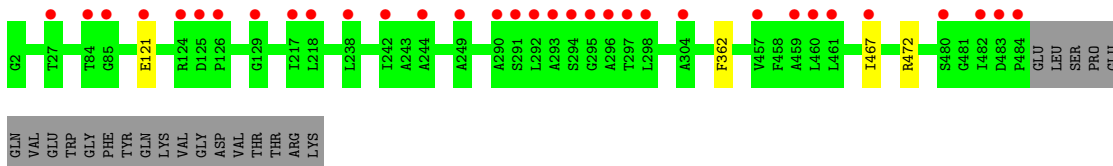
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

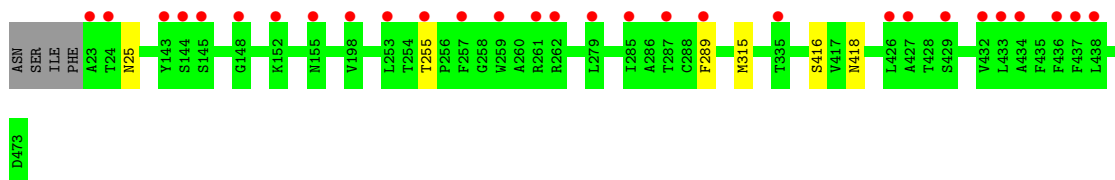


- Molecule 2: Photosystem II CP47 reaction center protein

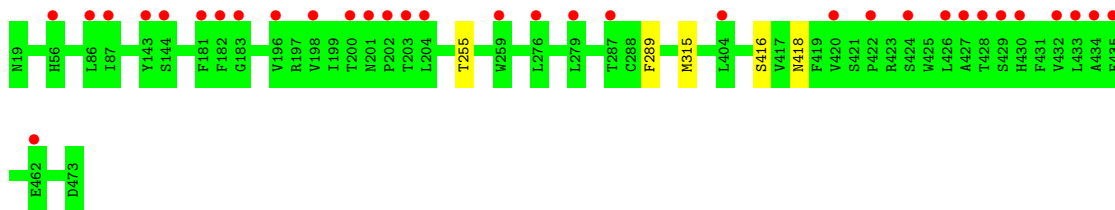


- Molecule 3: Photosystem II CP43 reaction center protein

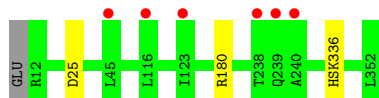




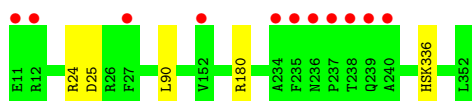
- Molecule 3: Photosystem II CP43 reaction center protein



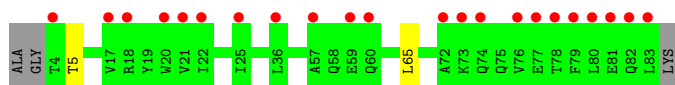
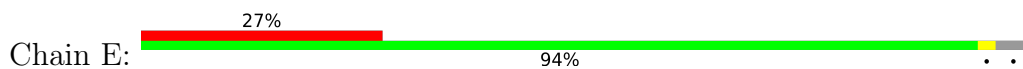
- Molecule 4: Photosystem II D2 protein



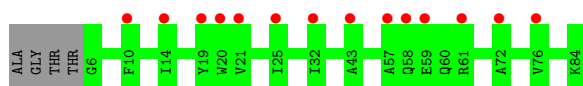
- Molecule 4: Photosystem II D2 protein



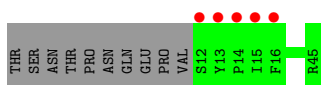
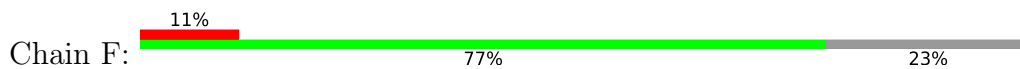
- Molecule 5: Cytochrome b559 subunit alpha



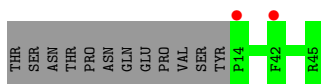
- Molecule 5: Cytochrome b559 subunit alpha



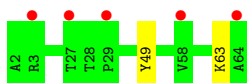
- Molecule 6: Cytochrome b559 subunit beta



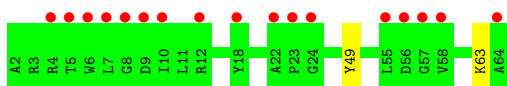
- Molecule 6: Cytochrome b559 subunit beta



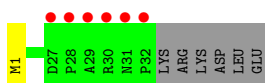
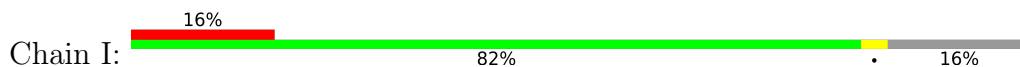
- Molecule 7: Photosystem II reaction center protein H



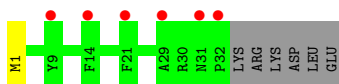
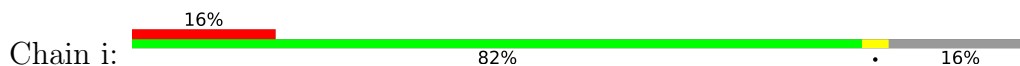
- Molecule 7: Photosystem II reaction center protein H



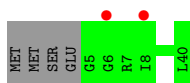
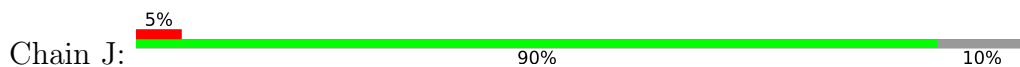
- Molecule 8: Photosystem II reaction center protein I



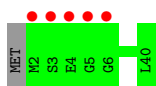
- Molecule 8: Photosystem II reaction center protein I



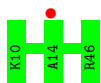
- Molecule 9: Photosystem II reaction center protein J



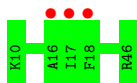
- Molecule 9: Photosystem II reaction center protein J



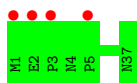
- Molecule 10: Photosystem II reaction center protein K



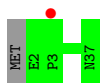
- Molecule 10: Photosystem II reaction center protein K



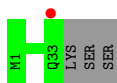
- Molecule 11: Photosystem II reaction center protein L



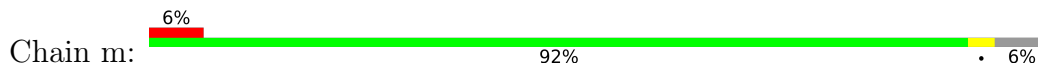
- Molecule 11: Photosystem II reaction center protein L

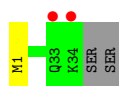


- Molecule 12: Photosystem II reaction center protein M

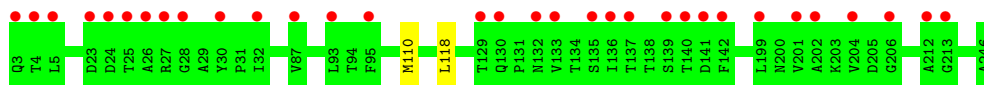


- Molecule 12: Photosystem II reaction center protein M

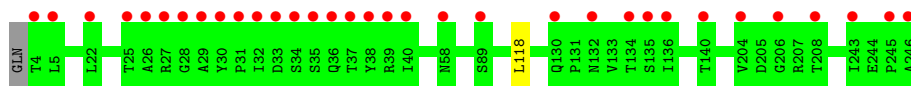




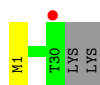
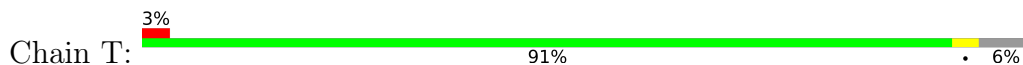
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



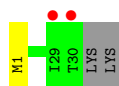
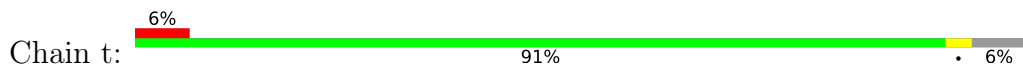
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



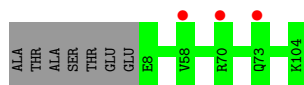
- Molecule 14: Photosystem II reaction center protein T



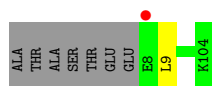
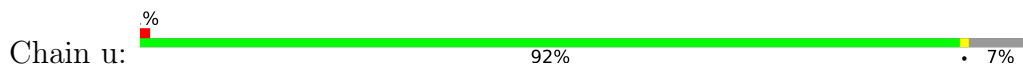
- Molecule 14: Photosystem II reaction center protein T



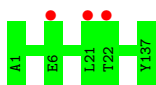
- Molecule 15: Photosystem II 12 kDa extrinsic protein



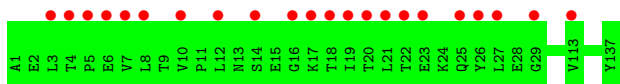
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



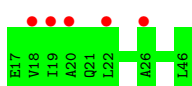
- Molecule 16: Cytochrome c-550



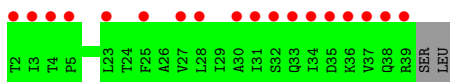
- Molecule 17: Photosystem II reaction center protein Ycf12



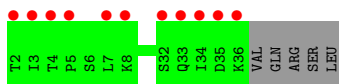
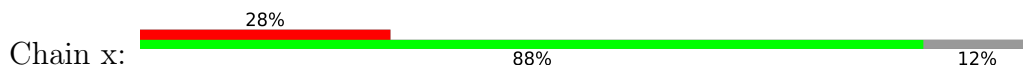
- Molecule 17: Photosystem II reaction center protein Ycf12



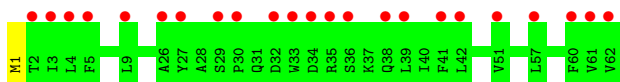
- Molecule 18: Photosystem II reaction center protein X



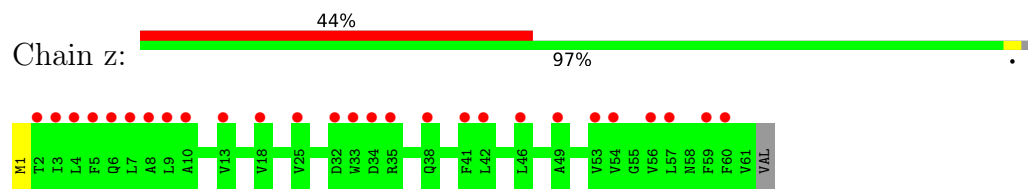
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



## ● Molecule 19: Photosystem II reaction center protein Z





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.22Å 228.21Å 287.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.15 49.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-2.15) 83.7 (49.00-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.06 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.151 , 0.185 0.151 , 0.185	Depositor DCC
$R_{free}$ test set	21442 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtrriage
Anisotropy	0.401	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 77.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	53814	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 1.64% 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: UNL, LMG, CL, MG, CA, HEM, FME, JOX, GOL, CLA, LMT, LHG, HEC, SQD, BCR, HSK, DMS, FE2, OEX, RRX, DGD, BCT, PL9, PHO, HTG

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	0.45	0/2708	0.53	0/3695
1	a	0.42	0/2725	0.55	0/3716
2	B	0.42	0/4163	0.53	0/5672
2	b	0.41	0/3994	0.54	0/5442
3	C	0.38	0/3613	0.49	0/4919
3	c	0.38	0/3632	0.50	0/4945
4	D	0.47	0/2804	0.54	0/3820
4	d	0.44	0/2819	0.53	0/3840
5	E	0.33	0/665	0.47	0/911
5	e	0.32	0/652	0.46	0/893
6	F	0.33	0/280	0.47	0/382
6	f	0.35	0/262	0.46	0/356
7	H	0.33	0/511	0.49	0/697
7	h	0.32	0/522	0.47	0/711
8	I	0.31	0/253	0.42	0/345
8	i	0.33	0/256	0.43	0/349
9	J	0.37	0/257	0.48	0/349
9	j	0.35	0/280	0.48	0/379
10	K	0.31	0/310	0.44	0/426
10	k	0.36	0/299	0.46	0/412
11	L	0.48	0/313	0.47	0/426
11	l	0.45	0/318	0.48	0/433
12	M	0.39	0/266	0.59	0/364
12	m	0.41	0/266	0.49	0/363
13	O	0.38	0/1910	0.58	0/2592
13	o	0.37	0/1917	0.58	0/2599
14	T	0.44	0/257	0.46	0/349
14	t	0.42	0/257	0.46	0/349
15	U	0.42	0/790	0.54	0/1071
15	u	0.40	0/785	0.57	0/1064
16	V	0.37	0/1087	0.53	0/1475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.33	0/1082	0.51	0/1472
17	Y	0.30	0/219	0.43	0/293
17	y	0.27	0/217	0.42	0/290
18	X	0.29	0/278	0.40	0/376
18	x	0.28	0/263	0.41	0/356
19	Z	0.29	0/472	0.42	0/646
19	z	0.30	0/457	0.41	0/626
All	All	0.40	0/42159	0.52	0/57403

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	41	37
1	a	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	41	37
2	B	510/505 (101%)	501 (98%)	9 (2%)	0	100	100
2	b	490/505 (97%)	484 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	441 (98%)	8 (2%)	2 (0%)	34	29
3	c	453/455 (100%)	444 (98%)	8 (2%)	1 (0%)	47	46
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	341/342 (100%)	335 (98%)	6 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	78/83 (94%)	78 (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	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	9	4
7	h	62/63 (98%)	59 (95%)	2 (3%)	1 (2%)	9	4
8	I	30/38 (79%)	29 (97%)	1 (3%)	0	100	100
8	i	30/38 (79%)	30 (100%)	0	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	245/244 (100%)	240 (98%)	5 (2%)	0	100	100
13	o	245/244 (100%)	240 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	28 (100%)	0	0	100	100
18	X	36/40 (90%)	36 (100%)	0	0	100	100
18	x	34/40 (85%)	34 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5191/5346 (97%)	5103 (98%)	81 (2%)	7 (0%)	51	53

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ASN
3	C	416	SER
3	c	416	SER
7	H	63	LYS
7	h	63	LYS

### 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	268/279 (96%)	268 (100%)	0	100	100
1	a	272/279 (98%)	270 (99%)	2 (1%)	84	89
2	B	406/403 (101%)	403 (99%)	3 (1%)	84	89
2	b	389/403 (96%)	385 (99%)	4 (1%)	76	81
3	C	354/356 (99%)	350 (99%)	4 (1%)	73	78
3	c	355/356 (100%)	351 (99%)	4 (1%)	73	78
4	D	275/276 (100%)	273 (99%)	2 (1%)	84	89
4	d	277/276 (100%)	273 (99%)	4 (1%)	67	72
5	E	69/72 (96%)	67 (97%)	2 (3%)	42	42
5	e	66/72 (92%)	66 (100%)	0	100	100
6	F	26/38 (68%)	26 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	53/53 (100%)	52 (98%)	1 (2%)	57	61
7	h	54/53 (102%)	53 (98%)	1 (2%)	57	61
8	I	27/34 (79%)	27 (100%)	0	100	100
8	i	28/34 (82%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	31/30 (103%)	31 (100%)	0	100	100
10	k	29/30 (97%)	29 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	206/207 (100%)	204 (99%)	2 (1%)	76	81
13	o	208/207 (100%)	207 (100%)	1 (0%)	88	92
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/89 (94%)	84 (100%)	0	100	100
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	76
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	115 (100%)	0	100	100
17	Y	21/23 (91%)	21 (100%)	0	100	100
17	y	20/23 (87%)	20 (100%)	0	100	100
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	28/33 (85%)	28 (100%)	0	100	100
19	Z	48/51 (94%)	48 (100%)	0	100	100
19	z	44/51 (86%)	44 (100%)	0	100	100
All	All	4239/4368 (97%)	4208 (99%)	31 (1%)	84	89

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	15	GLU
4	d	180	ARG
2	b	362	PHE
13	o	118	LEU
4	d	24	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	252	HIS
1	a	315	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	m	1	12	8,9,10	0.53	0	7,9,11	1.36	1 (14%)
4	HSK	D	336[B]	-	7,11,12	1.23	1 (14%)	3,14,16	1.51	1 (33%)
4	HSK	d	336[A]	-	7,10,12	1.07	1 (14%)	3,12,16	1.19	0
14	FME	t	1	14	8,9,10	0.69	0	7,9,11	1.76	4 (57%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.15	0
19	FME	Z	1	19	8,9,10	0.62	0	7,9,11	1.80	3 (42%)
14	FME	T	1	14	8,9,10	0.79	0	7,9,11	1.73	2 (28%)
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.72	3 (42%)
4	HSK	d	336[B]	-	7,11,12	1.32	1 (14%)	3,14,16	1.47	1 (33%)
4	HSK	D	336[A]	-	7,10,12	0.98	1 (14%)	3,12,16	1.19	0
19	FME	z	1	19	8,9,10	0.58	0	7,9,11	1.70	3 (42%)
8	FME	i	1	8	8,9,10	0.64	0	7,9,11	1.69	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	t	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
19	FME	Z	1	19	-	3/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
19	FME	z	1	19	-	5/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[B]	HSK	CE1-ND1	-2.94	1.33	1.36
4	D	336[B]	HSK	CE1-ND1	-2.77	1.33	1.36
4	d	336[A]	HSK	CE1-ND1	-2.18	1.34	1.36
4	D	336[A]	HSK	CE1-ND1	-2.05	1.34	1.36

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	1	FME	CE-SD-CG	2.89	110.32	100.40
12	m	1	FME	CE-SD-CG	2.80	110.00	100.40
14	T	1	FME	CE-SD-CG	2.73	109.79	100.40
19	Z	1	FME	CE-SD-CG	2.68	109.61	100.40
8	i	1	FME	CA-N-CN	-2.51	118.97	122.82

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
19	Z	1	FME	O-C-CA-CB
19	Z	1	FME	CA-CB-CG-SD
8	i	1	FME	O1-CN-N-CA
19	z	1	FME	O1-CN-N-CA

There are no ring outliers.



No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 407 ligands modelled in this entry, 15 are monoatomic and 37 are unknown - leaving 355 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
36	HTG	d	415	-	19,19,19	1.05	2 (10%)	23,24,24	1.52	1 (4%)
25	BCR	b	623	-	41,41,41	0.86	0	56,56,56	1.21	6 (10%)
23	CLA	C	511	-	65,73,73	2.60	20 (30%)	76,113,113	2.48	27 (35%)
36	HTG	b	626	-	19,19,19	1.14	2 (10%)	23,24,24	1.46	2 (8%)
34	DMS	u	502	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
36	HTG	c	526	-	19,19,19	1.00	2 (10%)	23,24,24	1.24	1 (4%)
23	CLA	B	608	43	65,73,73	2.44	18 (27%)	76,113,113	2.42	25 (32%)
34	DMS	C	536	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
23	CLA	C	509	-	65,73,73	2.49	18 (27%)	76,113,113	2.44	25 (32%)
26	SQD	a	2615	-	47,48,54	1.01	3 (6%)	56,59,65	1.79	12 (21%)
34	DMS	c	532	-	3,3,3	2.76	1 (33%)	3,3,3	0.80	0
26	SQD	D	2308	-	44,45,54	1.12	3 (6%)	53,56,65	1.31	8 (15%)
31	JOX	A	418	-	10,10,10	2.05	4 (40%)	14,14,14	3.36	10 (71%)
38	LHG	d	413	-	48,48,48	0.82	2 (4%)	51,54,54	0.99	3 (5%)
36	HTG	b	604	-	19,19,19	1.07	2 (10%)	23,24,24	1.66	4 (17%)
23	CLA	c	504	-	65,73,73	2.45	19 (29%)	76,113,113	2.63	22 (28%)
34	DMS	V	211	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
34	DMS	c	549	-	3,3,3	2.72	1 (33%)	3,3,3	0.62	0
34	DMS	O	308	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	b	633	-	3,3,3	2.50	1 (33%)	3,3,3	0.35	0
23	CLA	c	510	43	65,73,73	2.59	20 (30%)	76,113,113	2.53	29 (38%)
23	CLA	b	612	43	65,73,73	2.38	19 (29%)	76,113,113	2.44	26 (34%)
34	DMS	c	548	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
24	PHO	a	2611	-	51,69,69	1.81	7 (13%)	47,99,99	1.75	12 (25%)
28	LMT	F	102	-	24,24,36	0.47	0	29,29,47	0.73	0
34	DMS	V	205	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
34	DMS	A	426	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	V	206	-	3,3,3	2.71	1 (33%)	3,3,3	0.73	0
38	LHG	D	2309	-	48,48,48	0.90	2 (4%)	51,54,54	1.15	5 (9%)
34	DMS	o	310	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
27	LMG	d	414	41	51,51,55	0.90	2 (3%)	59,59,63	0.86	1 (1%)
23	CLA	C	506	-	65,73,73	2.75	21 (32%)	76,113,113	2.21	24 (31%)
23	CLA	C	508	43	65,73,73	2.63	20 (30%)	76,113,113	2.46	23 (30%)
23	CLA	a	2613	-	65,73,73	2.29	18 (27%)	76,113,113	2.49	27 (35%)
34	DMS	b	635	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
33	PL9	d	411	-	55,55,55	0.69	1 (1%)	68,69,69	1.60	15 (22%)
29	GOL	O	305	-	5,5,5	0.88	0	5,5,5	0.90	0
34	DMS	o	313	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
23	CLA	B	602	43	65,73,73	2.70	22 (33%)	76,113,113	2.25	24 (31%)
36	HTG	B	625	-	19,19,19	1.05	1 (5%)	23,24,24	2.09	4 (17%)
23	CLA	b	613	-	65,73,73	2.54	20 (30%)	76,113,113	2.47	29 (38%)
28	LMT	i	103	-	24,24,36	0.51	0	29,29,47	1.08	2 (6%)
29	GOL	c	529	-	5,5,5	0.91	0	5,5,5	0.98	0
34	DMS	b	642	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
38	LHG	D	2311	-	38,38,48	0.95	2 (5%)	41,44,54	1.11	3 (7%)
25	BCR	B	620	-	41,41,41	0.74	0	56,56,56	1.17	6 (10%)
23	CLA	b	608	-	65,73,73	2.55	21 (32%)	76,113,113	2.48	24 (31%)
27	LMG	c	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
20	OEX	A	401	3,43,1	0,15,15	-	-	-	-	-
25	BCR	b	622	-	41,41,41	0.78	0	56,56,56	1.39	9 (16%)
36	HTG	C	521	-	19,19,19	0.99	2 (10%)	23,24,24	1.04	1 (4%)
23	CLA	c	513	-	65,73,73	2.62	20 (30%)	76,113,113	2.32	27 (35%)
23	CLA	A	407	43	65,73,73	2.20	20 (30%)	76,113,113	2.50	28 (36%)
28	LMT	B	623	-	36,36,36	0.41	0	47,47,47	1.35	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	510	-	65,73,73	2.61	21 (32%)	76,113,113	2.45	25 (32%)
29	GOL	B	630	-	5,5,5	0.98	0	5,5,5	0.93	0
23	CLA	D	2303	-	65,73,73	2.17	18 (27%)	76,113,113	2.67	24 (31%)
34	DMS	c	542	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	O	317	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
36	HTG	d	407	-	19,19,19	1.15	2 (10%)	23,24,24	1.64	5 (21%)
34	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
34	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
36	HTG	b	602	-	19,19,19	1.04	1 (5%)	23,24,24	1.04	2 (8%)
28	LMT	d	401	-	36,36,36	0.47	0	47,47,47	0.81	1 (2%)
24	PHO	a	2612	-	51,69,69	1.82	8 (15%)	47,99,99	1.95	10 (21%)
34	DMS	d	422	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	D	2317	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
23	CLA	B	615	-	65,73,73	2.31	19 (29%)	76,113,113	2.58	27 (35%)
34	DMS	v	213	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
25	BCR	D	2305	-	41,41,41	0.82	1 (2%)	56,56,56	1.63	8 (14%)
34	DMS	B	637	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
23	CLA	b	620	-	65,73,73	2.52	19 (29%)	76,113,113	2.23	28 (36%)
23	CLA	B	614	-	65,73,73	2.41	18 (27%)	76,113,113	2.53	26 (34%)
29	GOL	O	304	-	5,5,5	0.86	0	5,5,5	0.99	0
34	DMS	O	315	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
34	DMS	a	2621	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
34	DMS	c	540	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
23	CLA	B	606	-	65,73,73	2.39	19 (29%)	76,113,113	2.44	23 (30%)
23	CLA	b	614	-	65,73,73	2.64	20 (30%)	76,113,113	2.29	25 (32%)
34	DMS	d	419	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
28	LMT	T	103	-	24,24,36	0.60	1 (4%)	29,29,47	0.94	2 (6%)
37	DGD	h	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.03	5 (6%)
36	HTG	B	627	-	19,19,19	1.02	2 (10%)	23,24,24	1.37	2 (8%)
32	BCT	a	2608	21	2,3,3	0.67	0	2,3,3	1.05	0
23	CLA	b	607	-	65,73,73	2.56	20 (30%)	76,113,113	2.42	25 (32%)
29	GOL	c	531	-	5,5,5	0.95	0	5,5,5	0.86	0
27	LMG	C	527	-	51,51,55	0.96	2 (3%)	59,59,63	1.27	5 (8%)
34	DMS	B	642	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
34	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	b	636	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
23	CLA	d	408	-	65,73,73	2.46	20 (30%)	76,113,113	2.53	24 (31%)
34	DMS	c	535	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
23	CLA	C	503	-	65,73,73	2.65	20 (30%)	76,113,113	2.46	25 (32%)
29	GOL	O	302	-	5,5,5	0.92	0	5,5,5	1.03	0
34	DMS	U	503	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
36	HTG	B	624[B]	-	19,19,19	0.96	1 (5%)	23,24,24	1.86	6 (26%)
39	HEM	F	101	6,5	41,50,50	1.94	6 (14%)	45,82,82	1.72	7 (15%)
23	CLA	c	515	-	65,73,73	2.63	20 (30%)	76,113,113	2.48	27 (35%)
23	CLA	b	621	-	65,73,73	2.63	19 (29%)	76,113,113	2.63	26 (34%)
34	DMS	u	504	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
31	JOX	a	2617	-	10,10,10	1.85	4 (40%)	14,14,14	4.93	14 (100%)
23	CLA	B	617	-	65,73,73	2.61	19 (29%)	76,113,113	2.46	27 (35%)
34	DMS	O	311	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
27	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.05	3 (5%)
23	CLA	B	609	-	65,73,73	2.47	20 (30%)	76,113,113	2.37	27 (35%)
25	BCR	T	102	-	41,41,41	0.69	0	56,56,56	1.85	14 (25%)
33	PL9	A	422	-	38,38,55	0.42	0	45,45,69	1.86	14 (31%)
34	DMS	V	209	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
34	DMS	c	538	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
34	DMS	O	306	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
42	HEC	v	201	16	32,50,50	2.35	6 (18%)	24,82,82	1.84	6 (25%)
25	BCR	B	619	-	41,41,41	0.81	0	56,56,56	1.20	5 (8%)
23	CLA	c	516	-	65,73,73	2.54	20 (30%)	76,113,113	2.35	24 (31%)
34	DMS	b	634	-	3,3,3	2.62	1 (33%)	3,3,3	0.35	0
38	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	5 (9%)
34	DMS	C	532	-	3,3,3	2.63	1 (33%)	3,3,3	0.72	0
39	HEM	e	103	6,5	41,50,50	1.93	6 (14%)	45,82,82	1.82	7 (15%)
36	HTG	c	524	-	19,19,19	1.05	2 (10%)	23,24,24	1.44	2 (8%)
28	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.81	0
34	DMS	d	418	-	3,3,3	2.65	1 (33%)	3,3,3	0.62	0
34	DMS	D	2318	-	3,3,3	2.57	1 (33%)	3,3,3	0.47	0
28	LMT	A	414	-	34,34,36	0.49	0	45,45,47	1.17	4 (8%)
23	CLA	b	611	-	65,73,73	2.69	18 (27%)	76,113,113	2.38	24 (31%)
23	CLA	c	514	3	65,73,73	2.49	19 (29%)	76,113,113	2.37	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	507	-	65,73,73	2.61	19 (29%)	76,113,113	2.61	27 (35%)
34	DMS	c	547	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
23	CLA	C	504	-	65,73,73	2.54	18 (27%)	76,113,113	2.37	24 (31%)
23	CLA	C	502	-	65,73,73	2.67	21 (32%)	76,113,113	2.26	21 (27%)
26	SQD	b	601	-	47,48,54	1.04	3 (6%)	56,59,65	1.46	9 (16%)
36	HTG	C	522	-	19,19,19	0.97	2 (10%)	23,24,24	2.32	4 (17%)
34	DMS	U	504	-	3,3,3	2.70	1 (33%)	3,3,3	0.64	0
34	DMS	B	638	-	3,3,3	2.54	1 (33%)	3,3,3	0.34	0
29	GOL	A	417	-	5,5,5	0.89	0	5,5,5	1.02	0
28	LMT	Z	101	-	36,36,36	0.45	0	47,47,47	0.91	2 (4%)
36	HTG	o	301	-	19,19,19	0.88	1 (5%)	23,24,24	1.15	2 (8%)
23	CLA	b	619	-	65,73,73	2.46	20 (30%)	76,113,113	2.58	30 (39%)
34	DMS	d	423	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
34	DMS	c	541	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
23	CLA	c	507	43	65,73,73	2.31	18 (27%)	76,113,113	2.62	22 (28%)
29	GOL	a	2602	-	5,5,5	0.85	0	5,5,5	1.03	0
28	LMT	m	2803	-	36,36,36	0.42	0	47,47,47	0.83	0
34	DMS	A	428	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
28	LMT	J	303	-	24,24,36	0.54	0	29,29,47	0.94	1 (3%)
29	GOL	C	526	-	5,5,5	1.12	1 (20%)	5,5,5	0.96	0
36	HTG	I	101	-	19,19,19	1.10	2 (10%)	23,24,24	1.81	4 (17%)
26	SQD	l	101	-	53,54,54	1.05	4 (7%)	62,65,65	1.69	10 (16%)
23	CLA	b	609	-	65,73,73	2.83	19 (29%)	76,113,113	2.39	23 (30%)
28	LMT	m	2804	-	36,36,36	0.45	0	47,47,47	1.13	6 (12%)
34	DMS	c	536	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
23	CLA	A	410	-	65,73,73	2.37	20 (30%)	76,113,113	2.53	26 (34%)
31	JOX	a	2619	1	10,10,10	1.91	6 (60%)	14,14,14	2.29	5 (35%)
23	CLA	B	603	-	65,73,73	2.57	19 (29%)	76,113,113	2.47	28 (36%)
34	DMS	B	646	-	3,3,3	2.69	1 (33%)	3,3,3	0.70	0
23	CLA	B	616	-	65,73,73	2.44	18 (27%)	76,113,113	2.58	28 (36%)
23	CLA	C	513	-	65,73,73	2.78	19 (29%)	76,113,113	2.40	25 (32%)
34	DMS	V	207	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
26	SQD	a	2603	-	53,54,54	1.03	3 (5%)	62,65,65	1.14	3 (4%)
29	GOL	E	104	-	5,5,5	1.00	0	5,5,5	0.88	0
34	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	C	525	-	19,19,19	1.10	2 (10%)	23,24,24	1.69	4 (17%)
34	DMS	v	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	D	2320	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
34	DMS	B	647	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
34	DMS	d	421	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
34	DMS	O	319	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
34	DMS	O	312	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
23	CLA	B	607	-	65,73,73	2.54	19 (29%)	76,113,113	2.36	24 (31%)
36	HTG	b	603	-	19,19,19	0.95	2 (10%)	23,24,24	2.00	4 (17%)
25	BCR	B	633	-	41,41,41	0.69	0	56,56,56	1.72	12 (21%)
25	BCR	K	101	-	41,41,41	0.68	0	56,56,56	1.33	9 (16%)
40	RRX	H	102	-	42,42,42	0.69	0	57,58,58	1.47	9 (15%)
26	SQD	d	417	-	31,32,54	1.97	4 (12%)	34,36,65	1.57	4 (11%)
36	HTG	B	624[A]	-	19,19,19	0.90	1 (5%)	23,24,24	1.25	4 (17%)
34	DMS	a	2624	-	3,3,3	2.74	1 (33%)	3,3,3	0.70	0
25	BCR	d	410	-	41,41,41	0.80	0	56,56,56	1.65	5 (8%)
23	CLA	c	512	-	65,73,73	2.61	20 (30%)	76,113,113	2.45	23 (30%)
34	DMS	v	207	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
28	LMT	B	634	-	36,36,36	0.53	1 (2%)	47,47,47	0.85	0
34	DMS	v	210	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
34	DMS	O	314	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	c	537	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
34	DMS	o	316	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
24	PHO	A	409	-	51,69,69	1.92	8 (15%)	47,99,99	1.95	9 (19%)
20	OEX	a	2604	3,43,1	0,15,15	-	-	-	-	-
34	DMS	T	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
40	RRX	h	101	-	42,42,42	0.69	0	57,58,58	1.41	8 (14%)
36	HTG	b	625	-	19,19,19	0.89	1 (5%)	23,24,24	1.54	4 (17%)
34	DMS	D	2319	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
34	DMS	O	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
27	LMG	c	522	-	51,51,55	0.98	2 (3%)	59,59,63	1.34	6 (10%)
34	DMS	v	211	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
32	BCT	A	421	21	2,3,3	0.65	0	2,3,3	1.06	0
37	DGD	D	2307	-	53,53,67	0.96	2 (3%)	60,61,81	1.20	5 (8%)
29	GOL	V	203	-	5,5,5	0.90	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	v	214	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
23	CLA	b	606	43	65,73,73	2.72	22 (33%)	76,113,113	2.22	25 (32%)
36	HTG	H	101	-	17,17,19	1.23	2 (11%)	19,21,24	1.61	4 (21%)
34	DMS	c	533	-	3,3,3	2.61	1 (33%)	3,3,3	0.39	0
29	GOL	A	415	-	5,5,5	0.82	0	5,5,5	1.08	0
23	CLA	c	505	-	65,73,73	2.48	20 (30%)	76,113,113	2.34	22 (28%)
34	DMS	o	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
36	HTG	V	204	-	19,19,19	0.96	1 (5%)	23,24,24	1.84	4 (17%)
34	DMS	T	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
23	CLA	B	605	-	65,73,73	2.51	19 (29%)	76,113,113	2.42	25 (32%)
26	SQD	D	2302	-	53,54,54	1.05	4 (7%)	62,65,65	1.42	9 (14%)
34	DMS	A	427	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
34	DMS	V	210	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
34	DMS	o	307	-	3,3,3	2.63	1 (33%)	3,3,3	0.50	0
23	CLA	b	615	43	65,73,73	2.51	20 (30%)	76,113,113	2.42	27 (35%)
34	DMS	b	637	-	3,3,3	2.74	1 (33%)	3,3,3	0.67	0
28	LMT	z	102	-	33,33,36	0.54	0	43,43,47	1.06	4 (9%)
25	BCR	C	516	-	41,41,41	0.74	0	56,56,56	1.53	7 (12%)
38	LHG	e	101	-	39,39,48	1.08	2 (5%)	42,45,54	1.07	3 (7%)
28	LMT	j	2701	41	34,34,36	0.56	1 (2%)	44,44,47	1.05	3 (6%)
38	LHG	d	412	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
29	GOL	o	303	-	5,5,5	0.97	0	5,5,5	0.94	0
36	HTG	B	626	-	19,19,19	1.01	2 (10%)	23,24,24	1.49	1 (4%)
34	DMS	B	641	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	V	202	-	3,3,3	2.65	1 (33%)	3,3,3	0.57	0
34	DMS	o	308	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
24	PHO	A	408	-	51,69,69	1.85	7 (13%)	47,99,99	1.56	9 (19%)
29	GOL	B	648	-	5,5,5	0.89	0	5,5,5	0.94	0
29	GOL	d	416	-	5,5,5	0.89	0	5,5,5	0.99	0
23	CLA	c	506	-	65,73,73	2.58	20 (30%)	76,113,113	2.36	24 (31%)
29	GOL	a	2618	-	5,5,5	0.87	0	5,5,5	1.04	0
34	DMS	B	635	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
34	DMS	b	641	-	3,3,3	2.68	1 (33%)	3,3,3	0.40	0
29	GOL	b	644	-	5,5,5	0.69	0	5,5,5	1.21	1 (20%)
34	DMS	O	313	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
23	CLA	B	613	-	65,73,73	2.39	20 (30%)	76,113,113	2.53	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	A	413	-	51,51,55	0.93	2 (3%)	59,59,63	1.24	6 (10%)
34	DMS	c	543	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
23	CLA	c	511	-	65,73,73	2.74	20 (30%)	76,113,113	2.37	22 (28%)
38	LHG	l	103	-	48,48,48	0.87	2 (4%)	51,54,54	1.02	3 (5%)
34	DMS	t	102	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
29	GOL	J	301	-	5,5,5	0.96	0	5,5,5	0.89	0
23	CLA	D	2304	-	65,73,73	2.24	17 (26%)	76,113,113	2.53	26 (34%)
23	CLA	c	509	-	65,73,73	2.68	21 (32%)	76,113,113	2.44	28 (36%)
34	DMS	v	208	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	DMS	b	643	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
34	DMS	b	638	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
29	GOL	C	524	-	5,5,5	0.83	0	5,5,5	0.97	0
23	CLA	b	617	-	65,73,73	2.40	19 (29%)	76,113,113	2.57	25 (32%)
34	DMS	o	312	-	3,3,3	2.64	1 (33%)	3,3,3	0.49	0
37	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	6 (7%)
34	DMS	B	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0
25	BCR	z	101	-	41,41,41	0.74	0	56,56,56	1.52	12 (21%)
25	BCR	a	2614	-	41,41,41	0.80	0	56,56,56	1.31	6 (10%)
34	DMS	o	304	-	3,3,3	2.54	1 (33%)	3,3,3	0.32	0
23	CLA	d	402	43	65,73,73	2.41	18 (27%)	76,113,113	2.55	25 (32%)
23	CLA	b	610	-	65,73,73	2.40	19 (29%)	76,113,113	2.68	25 (32%)
25	BCR	C	515	-	41,41,41	0.76	0	56,56,56	1.49	8 (14%)
23	CLA	A	405	-	65,73,73	2.39	20 (30%)	76,113,113	2.51	28 (36%)
34	DMS	A	425	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
29	GOL	v	203	-	5,5,5	0.93	0	5,5,5	1.14	1 (20%)
34	DMS	A	424	-	3,3,3	2.61	1 (33%)	3,3,3	0.62	0
37	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	4 (5%)
37	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	0.86	5 (6%)
23	CLA	a	2610	43	65,73,73	2.36	18 (27%)	76,113,113	2.59	27 (35%)
23	CLA	c	508	-	65,73,73	2.60	21 (32%)	76,113,113	2.43	20 (26%)
28	LMT	d	404	-	25,25,36	0.52	0	30,30,47	0.90	2 (6%)
29	GOL	U	501	-	5,5,5	1.02	0	5,5,5	0.93	0
34	DMS	V	213	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
27	LMG	D	2312	41	47,47,55	0.90	2 (4%)	55,55,63	0.88	3 (5%)
25	BCR	Y	302	-	41,41,41	0.81	0	56,56,56	1.76	11 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LMT	A	420	-	24,24,36	0.42	0	29,29,47	0.96	0
42	HEC	V	201	16	32,50,50	2.18	6 (18%)	24,82,82	1.82	5 (20%)
34	DMS	A	429	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
34	DMS	d	420	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
36	HTG	i	102	-	19,19,19	1.13	2 (10%)	23,24,24	1.92	3 (13%)
29	GOL	u	501	-	5,5,5	1.25	0	5,5,5	0.83	0
23	CLA	B	612	-	65,73,73	2.58	17 (26%)	76,113,113	2.56	29 (38%)
25	BCR	k	302	-	41,41,41	0.69	0	56,56,56	1.47	12 (21%)
23	CLA	C	512	3	65,73,73	2.59	18 (27%)	76,113,113	2.37	25 (32%)
29	GOL	B	632	-	5,5,5	0.95	0	5,5,5	0.91	0
31	JOX	A	419	-	10,10,10	1.98	4 (40%)	14,14,14	4.85	11 (78%)
34	DMS	a	2620	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
34	DMS	v	209	-	3,3,3	2.67	1 (33%)	3,3,3	0.64	0
29	GOL	v	202	-	5,5,5	1.01	0	5,5,5	0.89	0
34	DMS	l	104	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
34	DMS	o	314	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
34	DMS	B	636	-	3,3,3	2.57	1 (33%)	3,3,3	0.58	0
34	DMS	u	503	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
34	DMS	C	537	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
29	GOL	b	631	-	5,5,5	1.07	0	5,5,5	0.60	0
28	LMT	f	101	-	24,24,36	0.46	0	29,29,47	0.76	0
34	DMS	B	639	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
34	DMS	c	544	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
29	GOL	U	502	-	5,5,5	1.29	1 (20%)	5,5,5	0.80	0
28	LMT	M	101	-	36,36,36	0.47	0	47,47,47	1.27	7 (14%)
34	DMS	O	316	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
34	DMS	b	640	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
33	PL9	x	1301	-	38,38,55	0.44	0	45,45,69	1.72	11 (24%)
36	HTG	c	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.49	2 (8%)
27	LMG	m	2802	-	51,51,55	0.95	2 (3%)	59,59,63	1.06	2 (3%)
26	SQD	A	412	-	45,46,54	1.05	3 (6%)	54,57,65	1.55	11 (20%)
29	GOL	c	530	-	5,5,5	0.92	0	5,5,5	0.80	0
25	BCR	A	411	-	41,41,41	0.75	0	56,56,56	1.39	8 (14%)
38	LHG	d	403	-	42,42,48	0.98	2 (4%)	45,48,54	0.91	3 (6%)
23	CLA	d	409	-	65,73,73	2.58	20 (30%)	76,113,113	2.42	25 (32%)
37	DGD	H	103	-	63,63,67	0.90	2 (3%)	77,77,81	1.09	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	616	-	65,73,73	2.36	20 (30%)	76,113,113	2.47	29 (38%)
34	DMS	C	535	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
23	CLA	C	514	-	65,73,73	2.49	20 (30%)	76,113,113	2.35	22 (28%)
26	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.45	9 (14%)
34	DMS	O	310	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
34	DMS	U	505	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
23	CLA	B	611	43	65,73,73	2.33	21 (32%)	76,113,113	2.53	28 (36%)
23	CLA	A	406	43	65,73,73	2.35	18 (27%)	76,113,113	2.73	29 (38%)
34	DMS	B	644	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
37	DGD	C	519	-	59,59,67	0.92	2 (3%)	73,73,81	1.28	6 (8%)
34	DMS	c	546	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
34	DMS	H	104	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
25	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.28	5 (8%)
25	BCR	y	101	-	41,41,41	0.76	0	56,56,56	1.56	12 (21%)
34	DMS	C	534	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
34	DMS	V	208	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
34	DMS	O	318	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
34	DMS	o	306	-	3,3,3	2.69	1 (33%)	3,3,3	0.64	0
34	DMS	o	305	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
34	DMS	C	529	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0
37	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
34	DMS	o	315	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
34	DMS	v	206	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
34	DMS	C	530	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
34	DMS	X	101	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
23	CLA	a	2609	-	65,73,73	2.53	19 (29%)	76,113,113	2.48	25 (32%)
34	DMS	c	534	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
34	DMS	O	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
25	BCR	b	624	-	41,41,41	0.72	0	56,56,56	1.59	12 (21%)
34	DMS	b	639	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
29	GOL	D	2301	-	5,5,5	1.00	0	5,5,5	0.79	0
23	CLA	b	618	-	65,73,73	2.49	20 (30%)	76,113,113	2.39	23 (30%)
23	CLA	C	505	43	65,73,73	2.39	20 (30%)	76,113,113	2.45	24 (31%)
29	GOL	O	303	-	5,5,5	0.93	0	5,5,5	0.94	0
34	DMS	c	539	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DMS	C	531	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
34	DMS	V	212	-	3,3,3	2.68	1 (33%)	3,3,3	0.63	0
34	DMS	o	311	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
27	LMG	c	521	-	49,49,55	0.91	2 (4%)	57,57,63	1.13	5 (8%)
34	DMS	A	430	-	3,3,3	2.72	1 (33%)	3,3,3	0.60	0
38	LHG	D	2310	-	48,48,48	0.87	2 (4%)	51,54,54	0.95	3 (5%)
23	CLA	B	604	-	65,73,73	2.57	20 (30%)	76,113,113	2.50	25 (32%)
23	CLA	B	610	-	65,73,73	2.69	20 (30%)	76,113,113	2.41	22 (28%)
33	PL9	D	2306	-	55,55,55	0.69	1 (1%)	68,69,69	1.60	18 (26%)
27	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
34	DMS	c	545	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
34	DMS	B	643	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
34	DMS	a	2622	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
38	LHG	E	101	-	39,39,48	1.06	2 (5%)	42,45,54	1.12	3 (7%)
37	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	6 (7%)
34	DMS	a	2623	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
29	GOL	v	204	-	5,5,5	0.88	0	5,5,5	0.96	0
34	DMS	D	2316	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
25	BCR	c	517	-	41,41,41	0.75	0	56,56,56	1.57	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	d	415	-	-	2/10/30/30	0/1/1/1
25	BCR	b	623	-	-	1/29/63/63	0/2/2/2
27	LMG	B	622	-	-	16/46/66/70	0/1/1/1
23	CLA	C	511	-	1/1/15/20	6/37/115/115	-
36	HTG	b	626	-	-	6/10/30/30	0/1/1/1
36	HTG	c	526	-	-	2/10/30/30	0/1/1/1
23	CLA	B	608	43	1/1/15/20	3/37/115/115	-
23	CLA	B	609	-	-	1/37/115/115	-
42	HEC	V	201	16	-	2/10/54/54	-
23	CLA	C	509	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	2615	-	-	8/43/63/69	0/1/1/1
25	BCR	T	102	-	-	3/29/63/63	0/2/2/2
36	HTG	i	102	-	-	6/10/30/30	0/1/1/1
29	GOL	u	501	-	-	1/4/4/4	-
33	PL9	A	422	-	-	10/42/42/73	-
26	SQD	D	2308	-	-	16/40/60/69	0/1/1/1
23	CLA	B	612	-	1/1/15/20	3/37/115/115	-
25	BCR	k	302	-	-	0/29/63/63	0/2/2/2
31	JOX	A	418	-	-	-	0/1/1/1
42	HEC	v	201	16	-	2/10/54/54	-
38	LHG	d	413	-	-	10/53/53/53	-
24	PHO	A	409	-	-	4/37/103/103	0/5/6/6
23	CLA	C	512	3	1/1/15/20	2/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	GOL	B	632	-	-	3/4/4/4	-
36	HTG	b	604	-	-	1/10/30/30	0/1/1/1
31	JOX	A	419	-	-	-	0/1/1/1
23	CLA	c	516	-	1/1/15/20	10/37/115/115	-
23	CLA	c	504	-	1/1/15/20	2/37/115/115	-
40	RRX	h	101	-	-	2/29/65/65	0/2/2/2
29	GOL	v	202	-	-	2/4/4/4	-
38	LHG	L	101	-	-	15/53/53/53	-
39	HEM	e	103	6,5	-	4/12/54/54	-
36	HTG	b	625	-	-	2/10/30/30	0/1/1/1
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
29	GOL	b	631	-	-	0/4/4/4	-
27	LMG	c	522	-	-	5/46/66/70	0/1/1/1
28	LMT	M	102	-	-	4/21/61/61	0/2/2/2
28	LMT	A	414	-	-	8/19/59/61	0/2/2/2
23	CLA	c	510	43	1/1/15/20	10/37/115/115	-
28	LMT	f	101	-	-	4/15/35/61	0/1/1/2
37	DGD	D	2307	-	-	23/47/68/95	0/1/1/2
23	CLA	b	611	-	1/1/15/20	9/37/115/115	-
23	CLA	c	514	3	1/1/15/20	1/37/115/115	-
23	CLA	C	507	-	1/1/15/20	14/37/115/115	-
29	GOL	V	203	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	612	43	1/1/15/20	1/37/115/115	-
24	PHO	a	2611	-	-	3/37/103/103	0/5/6/6
23	CLA	C	504	-	-	3/37/115/115	-
23	CLA	C	502	-	1/1/15/20	4/37/115/115	-
26	SQD	b	601	-	-	16/43/63/69	0/1/1/1
28	LMT	F	102	-	-	5/15/35/61	0/1/1/2
28	LMT	M	101	-	-	6/21/61/61	0/2/2/2
29	GOL	U	502	-	-	2/4/4/4	-
36	HTG	C	522	-	-	2/10/30/30	0/1/1/1
29	GOL	A	417	-	-	3/4/4/4	-
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
23	CLA	b	606	43	1/1/15/20	8/37/115/115	-
36	HTG	o	301	-	-	6/10/30/30	0/1/1/1
36	HTG	H	101	-	-	2/8/25/30	0/1/1/1
33	PL9	x	1301	-	-	12/42/42/73	-
38	LHG	D	2309	-	-	13/53/53/53	-
36	HTG	c	523	-	-	2/10/30/30	0/1/1/1
23	CLA	b	619	-	1/1/15/20	8/37/115/115	-
29	GOL	A	415	-	-	2/4/4/4	-
23	CLA	c	505	-	1/1/15/20	4/37/115/115	-
27	LMG	d	414	41	-	11/46/66/70	0/1/1/1
23	CLA	C	506	-	1/1/15/20	8/37/115/115	-
27	LMG	m	2802	-	-	10/46/66/70	0/1/1/1
26	SQD	A	412	-	-	8/41/61/69	0/1/1/1
29	GOL	c	530	-	-	4/4/4/4	-
36	HTG	V	204	-	-	5/10/30/30	0/1/1/1
23	CLA	C	508	43	1/1/15/20	9/37/115/115	-
23	CLA	c	507	43	1/1/15/20	6/37/115/115	-
23	CLA	B	605	-	1/1/15/20	6/37/115/115	-
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
23	CLA	a	2613	-	1/1/15/20	7/37/115/115	-
26	SQD	D	2302	-	-	14/49/69/69	0/1/1/1
38	LHG	d	403	-	-	7/47/47/53	-
23	CLA	d	409	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	H	103	-	-	12/51/91/95	0/2/2/2
33	PL9	d	411	-	-	4/53/73/73	0/1/1/1
29	GOL	O	305	-	-	2/4/4/4	-
23	CLA	b	616	-	1/1/15/20	4/37/115/115	-
29	GOL	a	2602	-	-	4/4/4/4	-
23	CLA	B	602	43	1/1/15/20	10/37/115/115	-
36	HTG	B	625	-	-	1/10/30/30	0/1/1/1
23	CLA	C	514	-	-	6/37/115/115	-
23	CLA	b	613	-	-	1/37/115/115	-
23	CLA	b	615	43	1/1/15/20	6/37/115/115	-
26	SQD	B	621	-	-	22/49/69/69	0/1/1/1
28	LMT	m	2803	-	-	3/21/61/61	0/2/2/2
28	LMT	J	303	-	-	5/15/35/61	0/1/1/2
29	GOL	C	526	-	-	2/4/4/4	-
36	HTG	I	101	-	-	6/10/30/30	0/1/1/1
23	CLA	B	611	43	1/1/15/20	5/37/115/115	-
28	LMT	i	103	-	-	8/15/35/61	0/1/1/2
28	LMT	z	102	-	-	12/16/56/61	0/2/2/2
29	GOL	c	529	-	-	0/4/4/4	-
23	CLA	A	406	43	-	4/37/115/115	-
26	SQD	l	101	-	-	23/49/69/69	0/1/1/1
38	LHG	D	2311	-	-	9/43/43/53	-
37	DGD	C	519	-	-	14/47/87/95	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	3/29/63/63	0/2/2/2
38	LHG	e	101	-	-	14/44/44/53	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
23	CLA	b	608	-	1/1/15/20	3/37/115/115	-
23	CLA	b	609	-	1/1/15/20	2/37/115/115	-
27	LMG	c	501	-	-	12/46/66/70	0/1/1/1
25	BCR	b	622	-	-	2/29/63/63	0/2/2/2
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
28	LMT	j	2701	41	-	3/17/57/61	0/2/2/2
36	HTG	C	521	-	-	2/10/30/30	0/1/1/1
23	CLA	c	513	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMT	m	2804	-	-	10/21/61/61	0/2/2/2
38	LHG	d	412	-	-	13/53/53/53	-
29	GOL	o	303	-	-	0/4/4/4	-
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
23	CLA	A	407	43	-	6/37/115/115	-
28	LMT	B	623	-	-	12/21/61/61	0/2/2/2
23	CLA	A	410	-	1/1/15/20	10/37/115/115	-
23	CLA	C	510	-	1/1/15/20	6/37/115/115	-
29	GOL	B	630	-	-	0/4/4/4	-
24	PHO	A	408	-	-	4/37/103/103	0/5/6/6
29	GOL	B	648	-	-	0/4/4/4	-
29	GOL	d	416	-	-	2/4/4/4	-
23	CLA	c	506	-	-	3/37/115/115	-
23	CLA	D	2303	-	1/1/15/20	1/37/115/115	-
31	JOX	a	2619	1	-	-	0/1/1/1
29	GOL	a	2618	-	-	1/4/4/4	-
37	DGD	C	517	-	-	18/51/91/95	0/2/2/2
23	CLA	B	603	-	1/1/15/20	3/37/115/115	-
36	HTG	d	407	-	-	7/10/30/30	0/1/1/1
23	CLA	B	616	-	1/1/15/20	7/37/115/115	-
29	GOL	b	644	-	-	2/4/4/4	-
23	CLA	a	2609	-	1/1/15/20	4/37/115/115	-
28	LMT	d	401	-	-	8/21/61/61	0/2/2/2
23	CLA	C	513	-	1/1/15/20	7/37/115/115	-
24	PHO	a	2612	-	-	1/37/103/103	0/5/6/6
26	SQD	a	2603	-	-	16/49/69/69	0/1/1/1
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
23	CLA	B	613	-	1/1/15/20	5/37/115/115	-
23	CLA	B	615	-	1/1/15/20	12/37/115/115	-
27	LMG	A	413	-	-	20/46/66/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	5/37/115/115	-
38	LHG	l	103	-	-	13/53/53/53	-
29	GOL	J	301	-	-	4/4/4/4	-
23	CLA	D	2304	-	1/1/15/20	6/37/115/115	-
23	CLA	c	509	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	624	-	-	4/29/63/63	0/2/2/2
29	GOL	E	104	-	-	0/4/4/4	-
25	BCR	D	2305	-	-	8/29/63/63	0/2/2/2
23	CLA	b	620	-	1/1/15/20	3/37/115/115	-
23	CLA	B	614	-	1/1/15/20	8/37/115/115	-
29	GOL	D	2301	-	-	2/4/4/4	-
29	GOL	O	304	-	-	2/4/4/4	-
23	CLA	b	618	-	1/1/15/20	6/37/115/115	-
23	CLA	C	505	43	1/1/15/20	6/37/115/115	-
29	GOL	C	524	-	-	2/4/4/4	-
36	HTG	C	525	-	-	0/10/30/30	0/1/1/1
23	CLA	b	617	-	1/1/15/20	2/37/115/115	-
37	DGD	C	518	-	-	17/51/91/95	0/2/2/2
29	GOL	O	303	-	-	0/4/4/4	-
23	CLA	B	606	-	1/1/15/20	7/37/115/115	-
25	BCR	z	101	-	-	0/29/63/63	0/2/2/2
25	BCR	Y	302	-	-	5/29/63/63	0/2/2/2
25	BCR	a	2614	-	-	3/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/15/20	5/37/115/115	-
28	LMT	T	103	-	-	9/15/35/61	0/1/1/2
27	LMG	c	521	-	-	14/44/64/70	0/1/1/1
37	DGD	h	102	-	-	12/51/91/95	0/2/2/2
23	CLA	d	402	43	1/1/15/20	5/37/115/115	-
36	HTG	B	627	-	-	3/10/30/30	0/1/1/1
38	LHG	D	2310	-	-	8/53/53/53	-
23	CLA	B	604	-	1/1/15/20	5/37/115/115	-
23	CLA	B	610	-	1/1/15/20	3/37/115/115	-
23	CLA	B	607	-	1/1/15/20	4/37/115/115	-
23	CLA	b	610	-	1/1/15/20	3/37/115/115	-
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
23	CLA	b	607	-	1/1/15/20	3/37/115/115	-
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
33	PL9	D	2306	-	-	3/53/73/73	0/1/1/1
23	CLA	A	405	-	1/1/15/20	2/37/115/115	-
27	LMG	C	520	-	-	13/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	GOL	c	531	-	-	2/4/4/4	-
27	LMG	C	527	-	-	14/46/66/70	0/1/1/1
25	BCR	B	633	-	-	3/29/63/63	0/2/2/2
29	GOL	v	203	-	-	1/4/4/4	-
37	DGD	c	518	-	-	17/51/91/95	0/2/2/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
37	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	a	2610	43	-	11/37/115/115	-
40	RRX	H	102	-	-	1/29/65/65	0/2/2/2
23	CLA	d	408	-	1/1/15/20	1/37/115/115	-
26	SQD	d	417	-	-	13/33/33/69	-
36	HTG	B	624[A]	-	-	2/10/30/30	0/1/1/1
23	CLA	C	503	-	1/1/15/20	4/37/115/115	-
23	CLA	c	508	-	1/1/15/20	9/37/115/115	-
25	BCR	d	410	-	-	8/29/63/63	0/2/2/2
28	LMT	d	404	-	-	5/17/37/61	0/1/1/2
29	GOL	O	302	-	-	2/4/4/4	-
29	GOL	U	501	-	-	0/4/4/4	-
36	HTG	B	624[B]	-	-	4/10/30/30	0/1/1/1
38	LHG	E	101	-	-	13/44/44/53	-
37	DGD	c	519	-	-	18/51/91/95	0/2/2/2
23	CLA	c	512	-	1/1/15/20	5/37/115/115	-
23	CLA	c	515	-	1/1/15/20	6/37/115/115	-
23	CLA	b	621	-	1/1/15/20	12/37/115/115	-
29	GOL	v	204	-	-	1/4/4/4	-
27	LMG	D	2312	41	-	6/42/62/70	0/1/1/1
39	HEM	F	101	6,5	-	4/12/54/54	-
28	LMT	B	634	-	-	8/21/61/61	0/2/2/2
25	BCR	c	517	-	-	3/29/63/63	0/2/2/2
31	JOX	a	2617	-	-	-	0/1/1/1
23	CLA	B	617	-	1/1/15/20	9/37/115/115	-
28	LMT	A	420	-	-	6/15/35/61	0/1/1/2

The worst 5 of 1705 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	MG-NA	10.59	2.31	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	MG-NA	10.28	2.30	2.06
23	c	506	CLA	MG-NA	10.17	2.30	2.06
23	c	511	CLA	MG-ND	-9.74	1.86	2.05
23	b	609	CLA	MG-ND	-9.39	1.87	2.05

The worst 5 of 2435 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C1D-ND-C4D	-10.80	98.66	106.33
23	b	617	CLA	C1D-ND-C4D	-10.14	99.13	106.33
23	B	613	CLA	C1D-ND-C4D	-10.14	99.14	106.33
23	a	2610	CLA	C1D-ND-C4D	-10.08	99.17	106.33
23	a	2609	CLA	C1D-ND-C4D	-9.95	99.27	106.33

5 of 62 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	405	CLA	ND
23	A	410	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND

5 of 1254 torsion outliers are listed below:

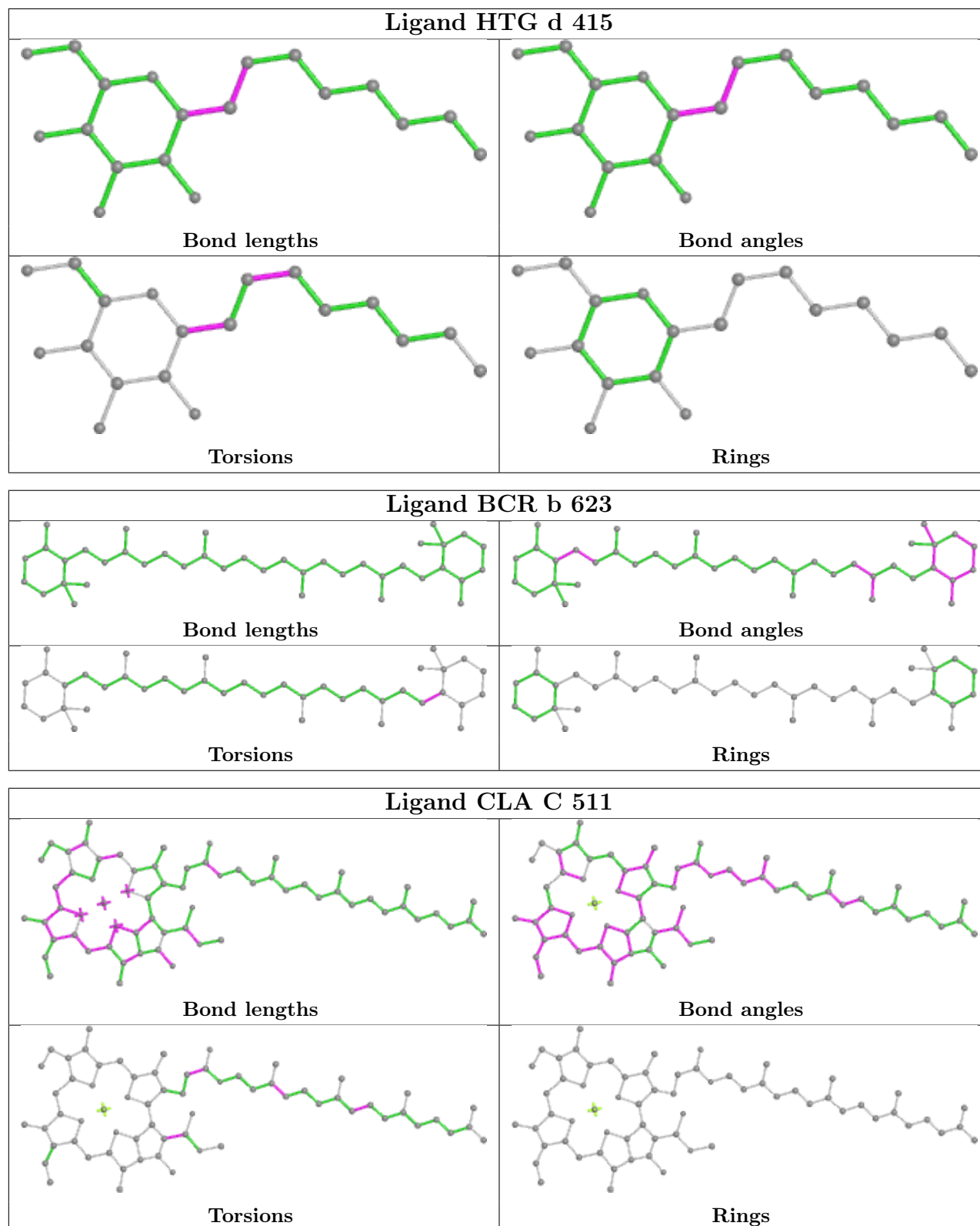
Mol	Chain	Res	Type	Atoms
23	B	603	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	611	CLA	C14-C13-C15-C16
23	B	615	CLA	CHA-CBD-CGD-O2D

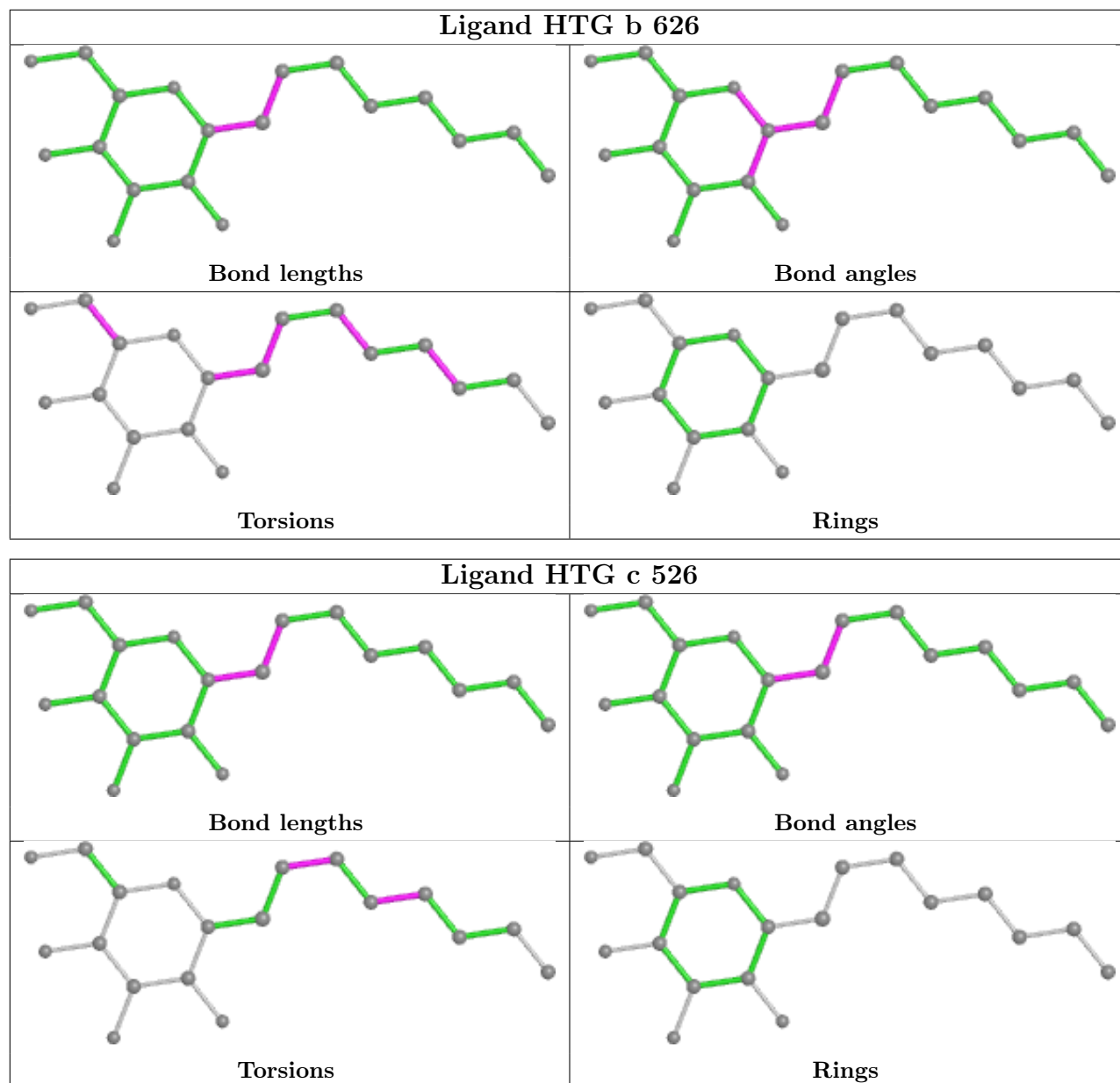
There are no ring outliers.

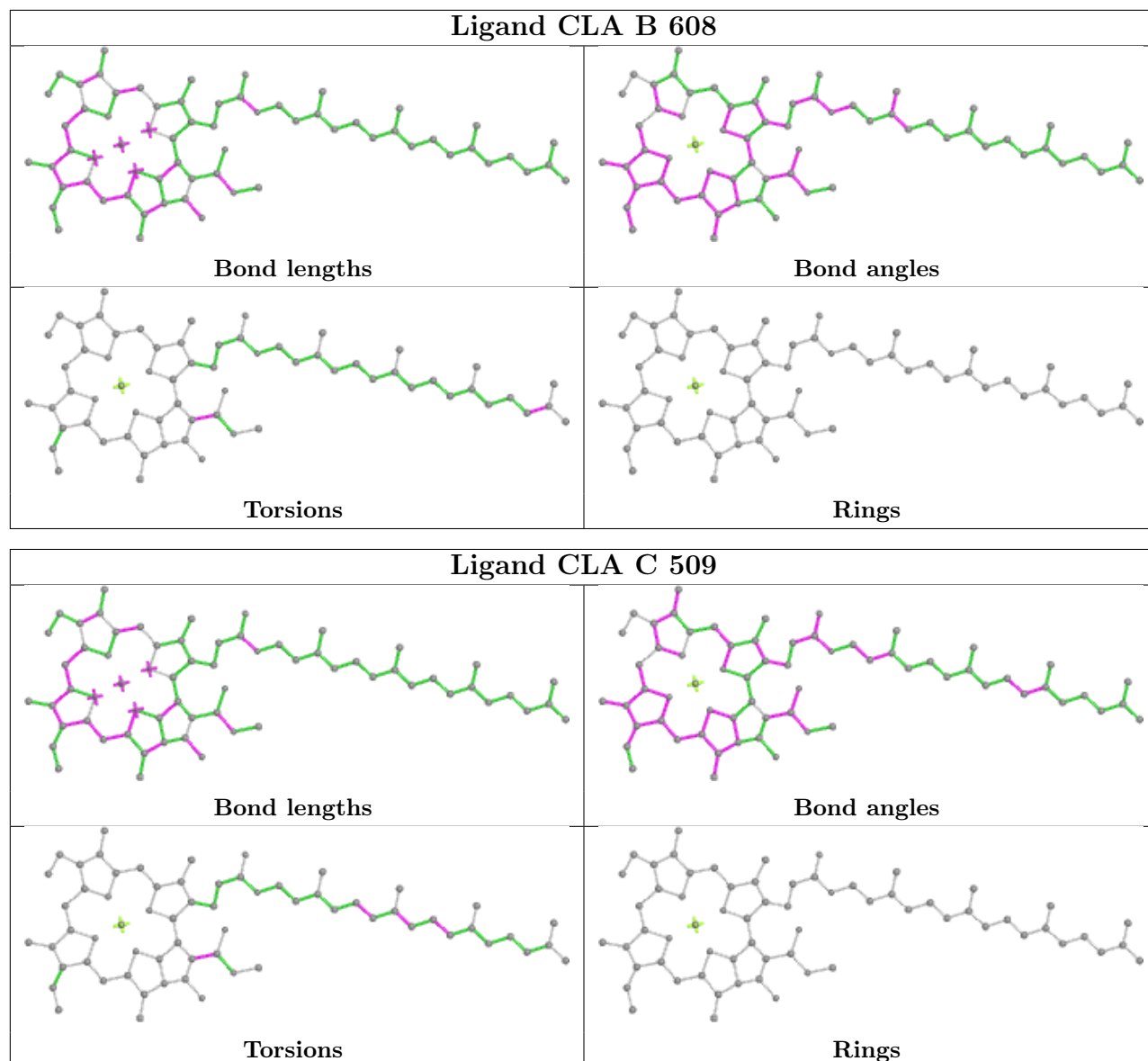
No monomer is involved in short contacts.

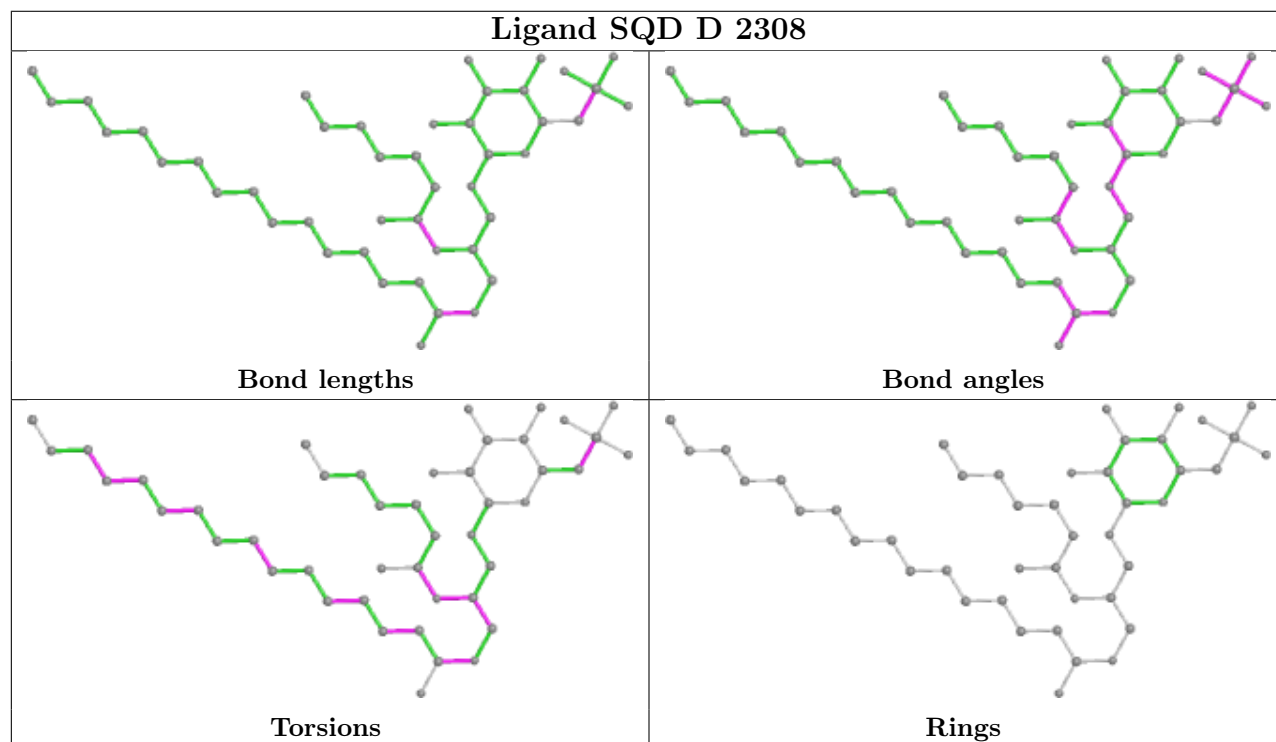
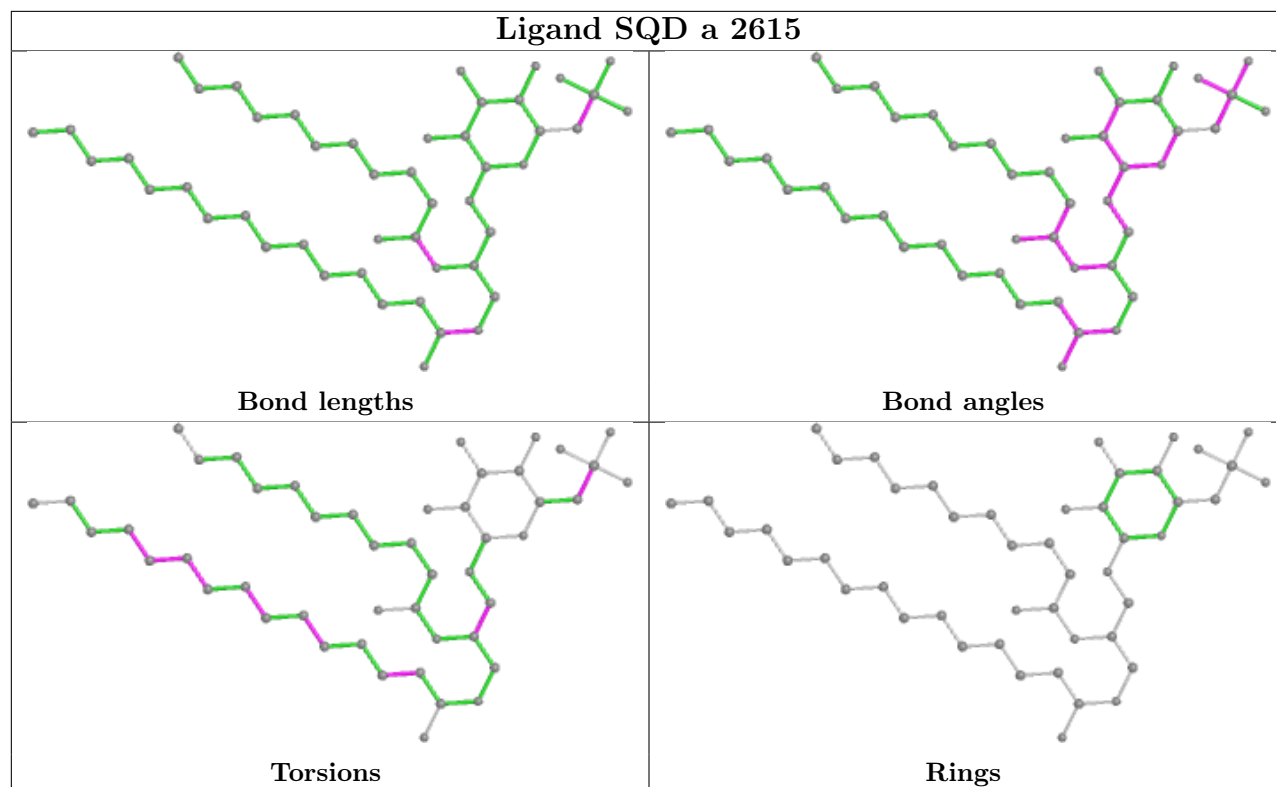
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

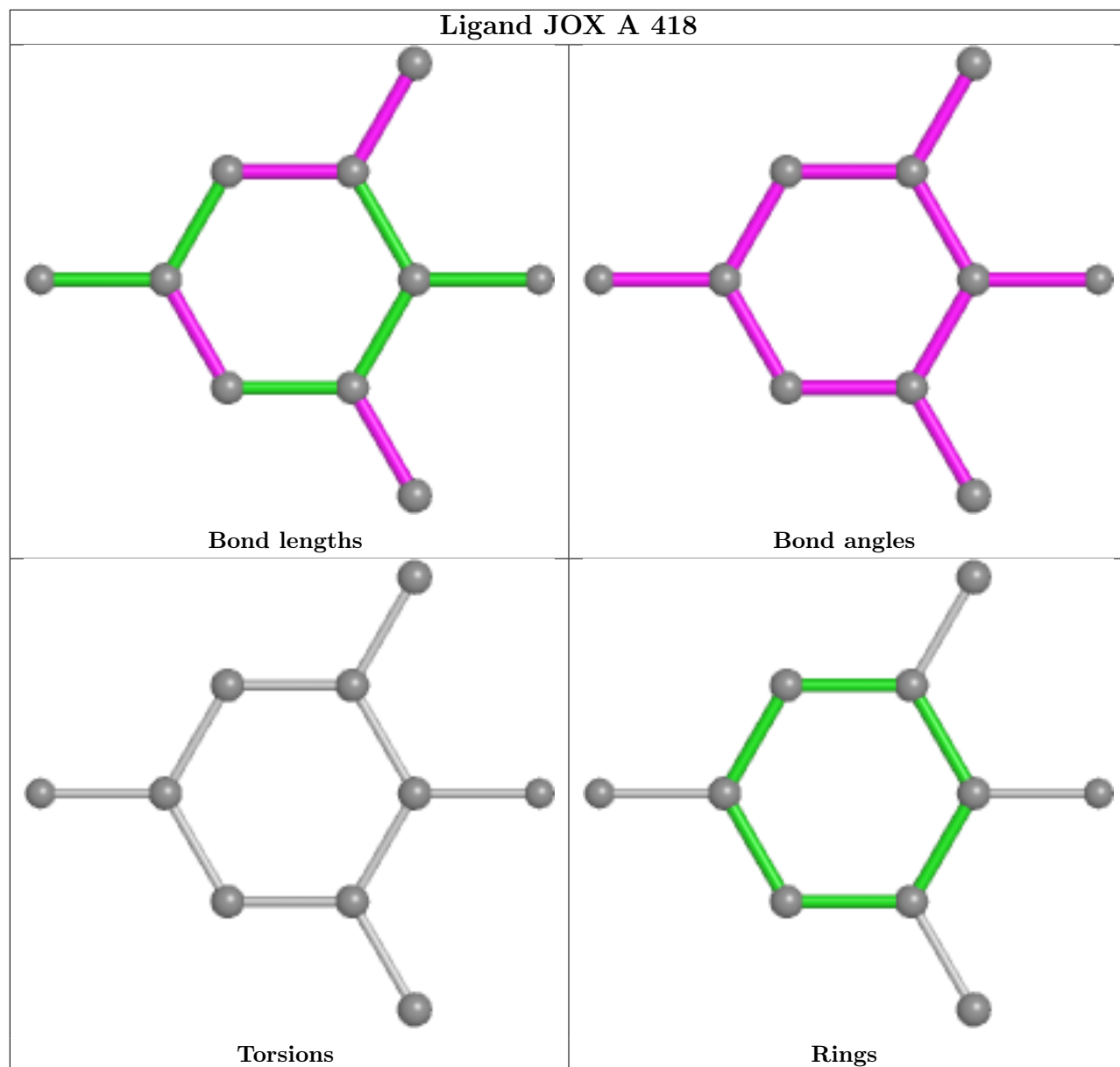
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

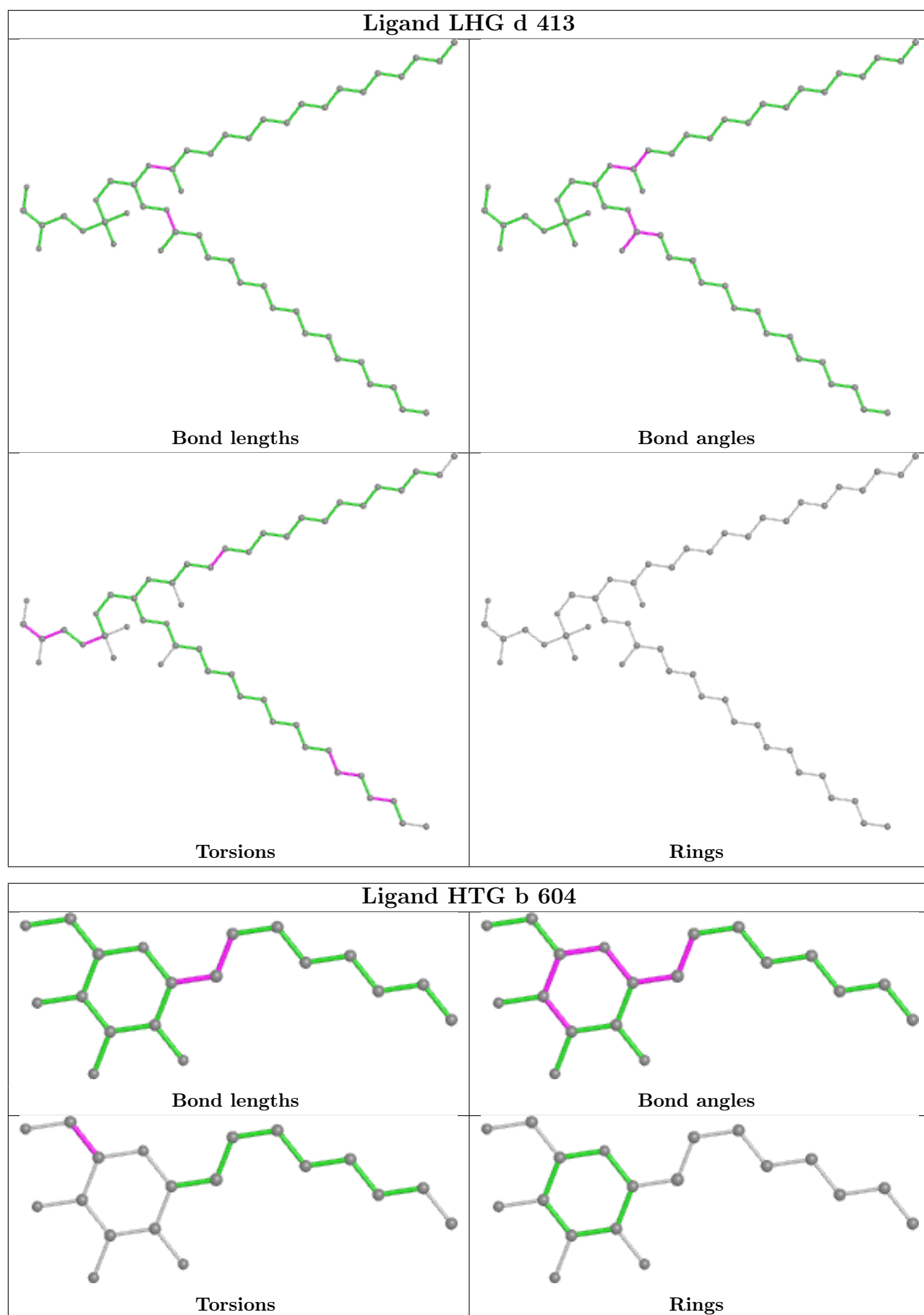




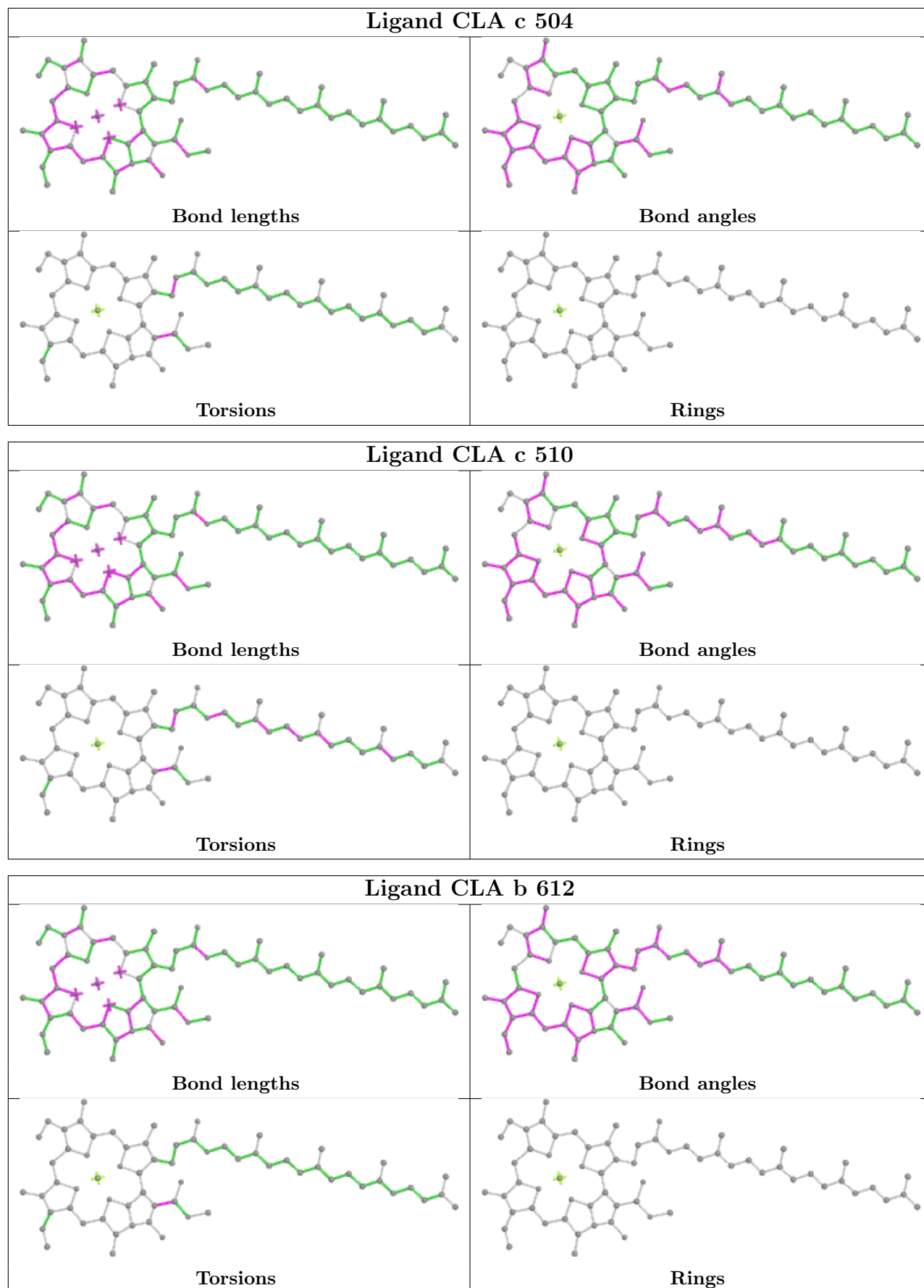


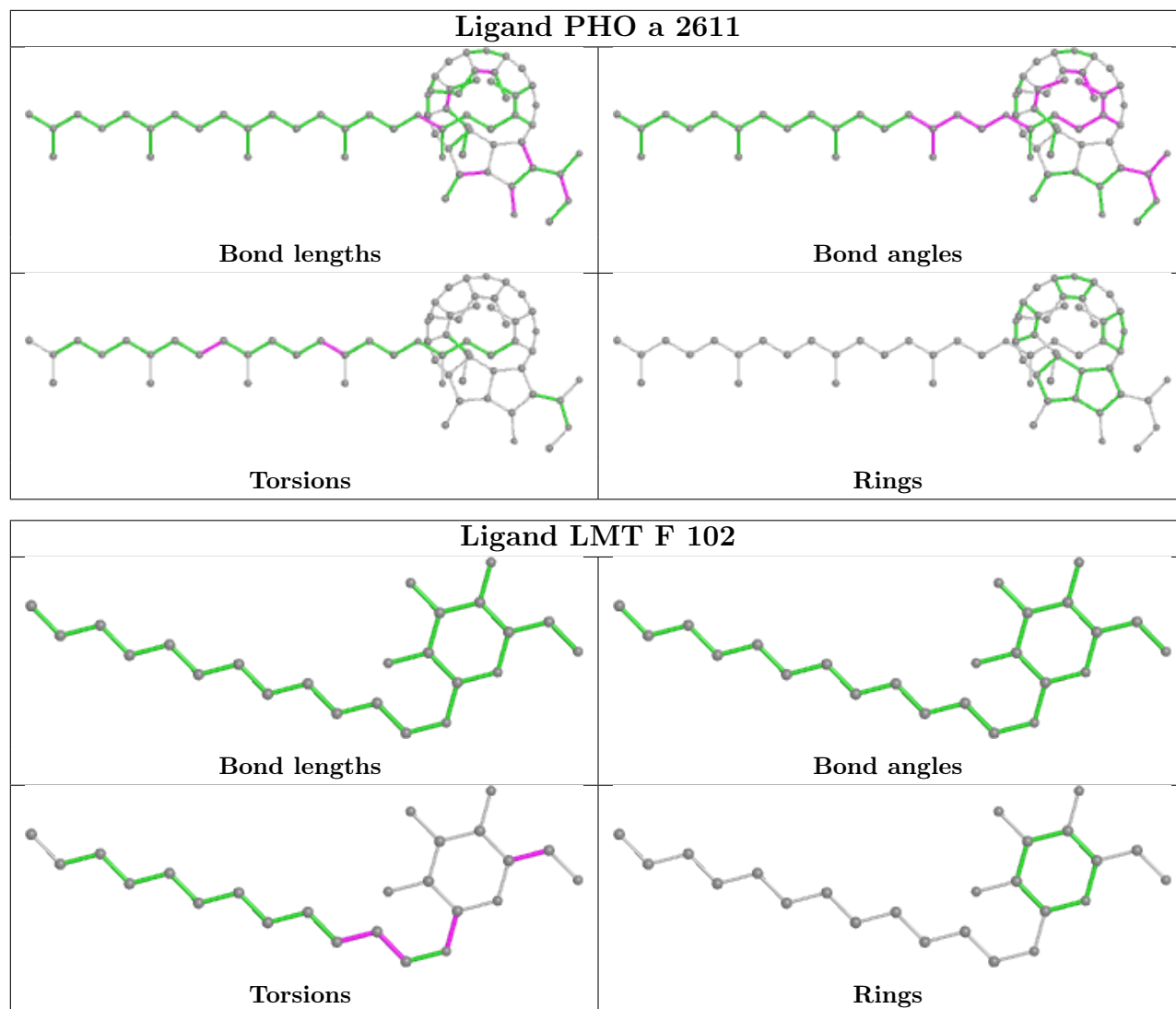


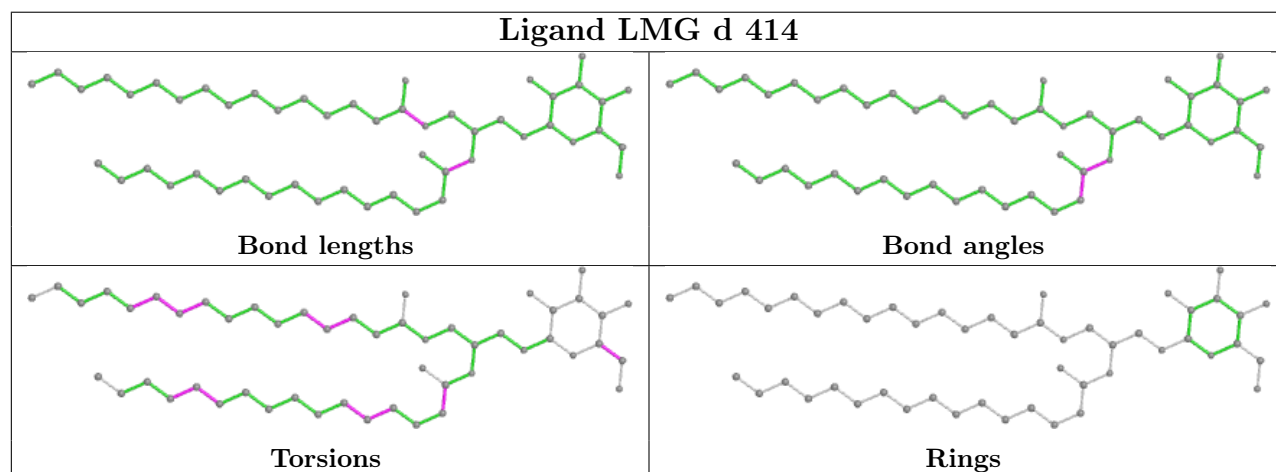
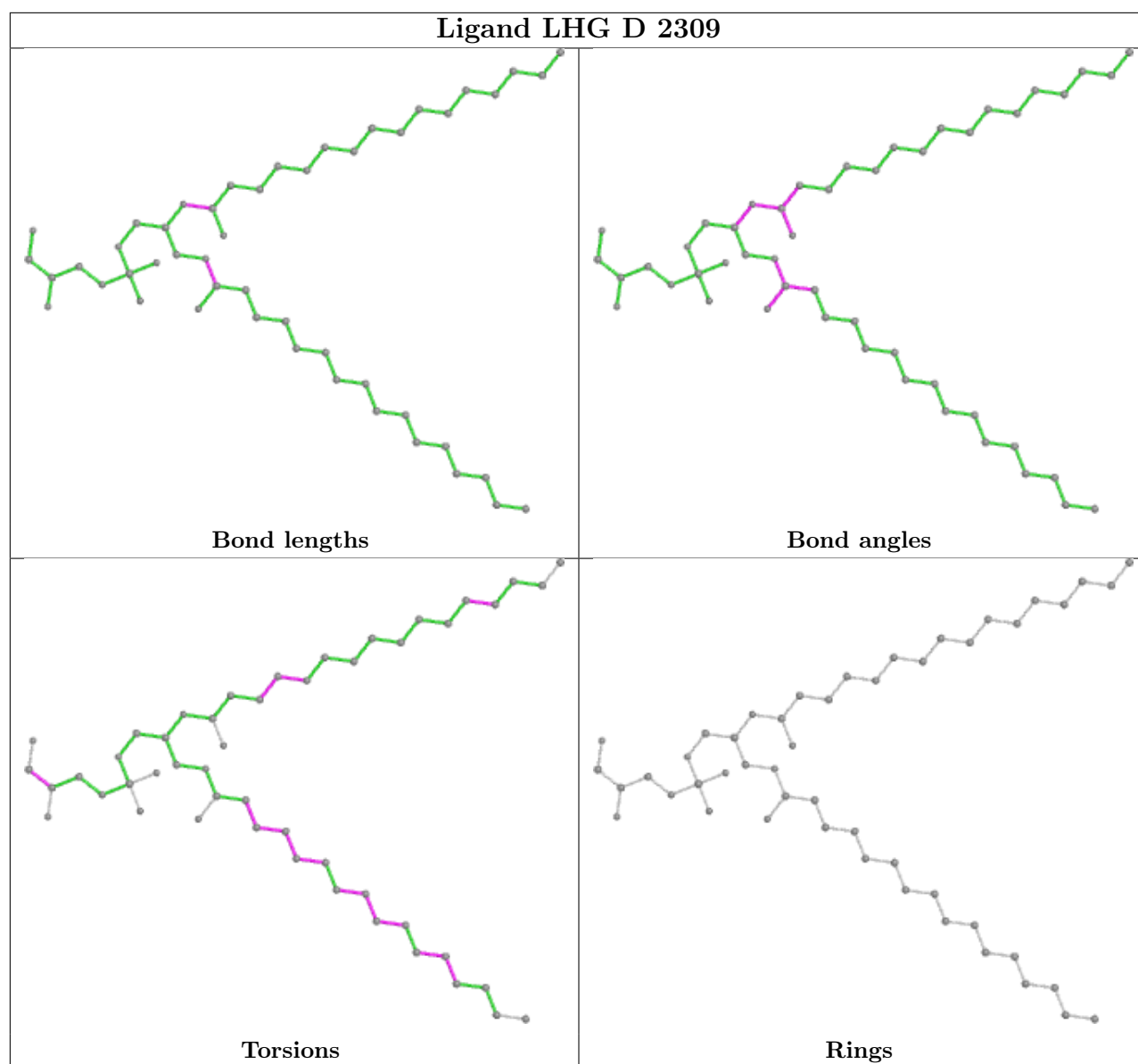


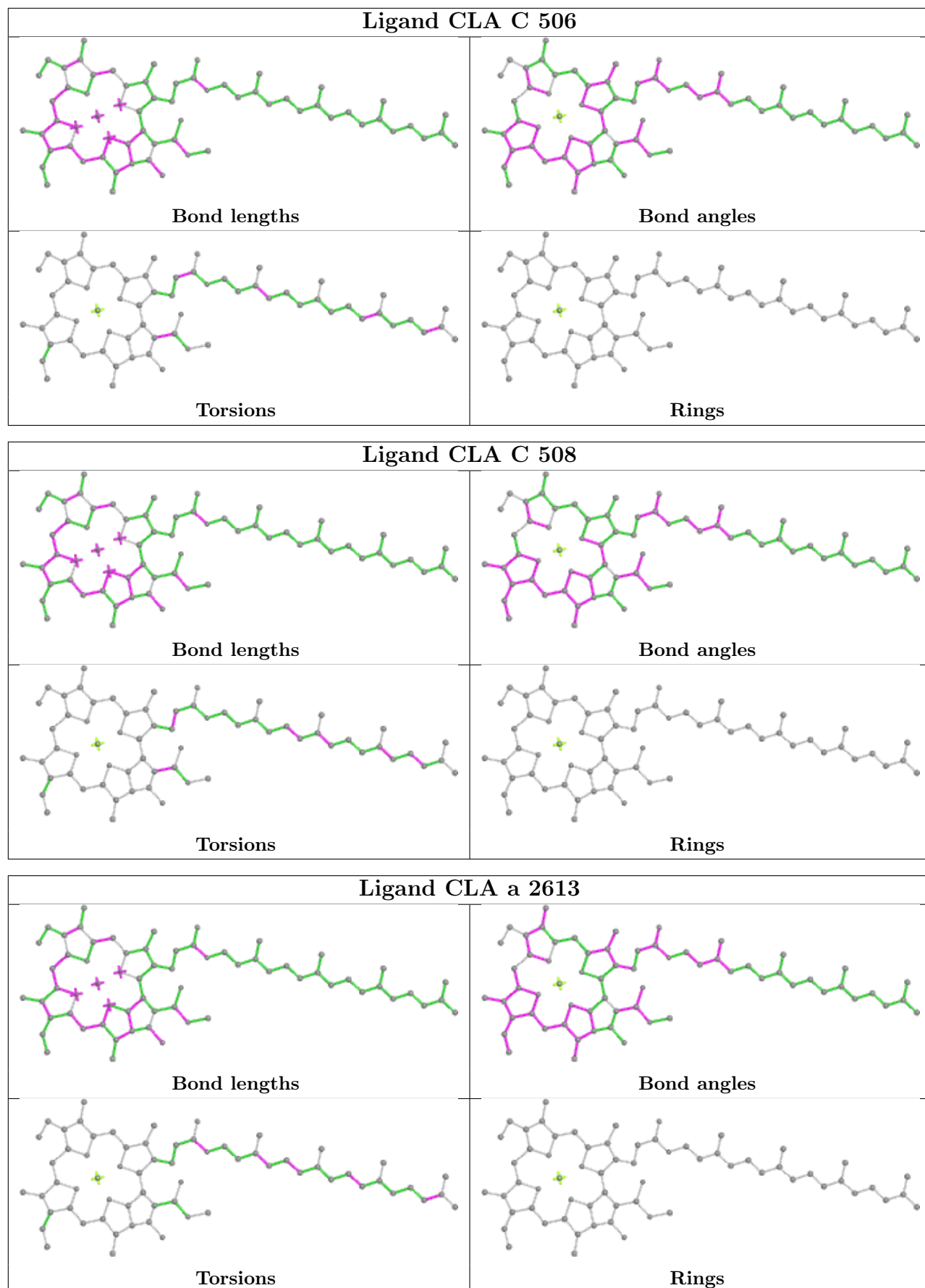


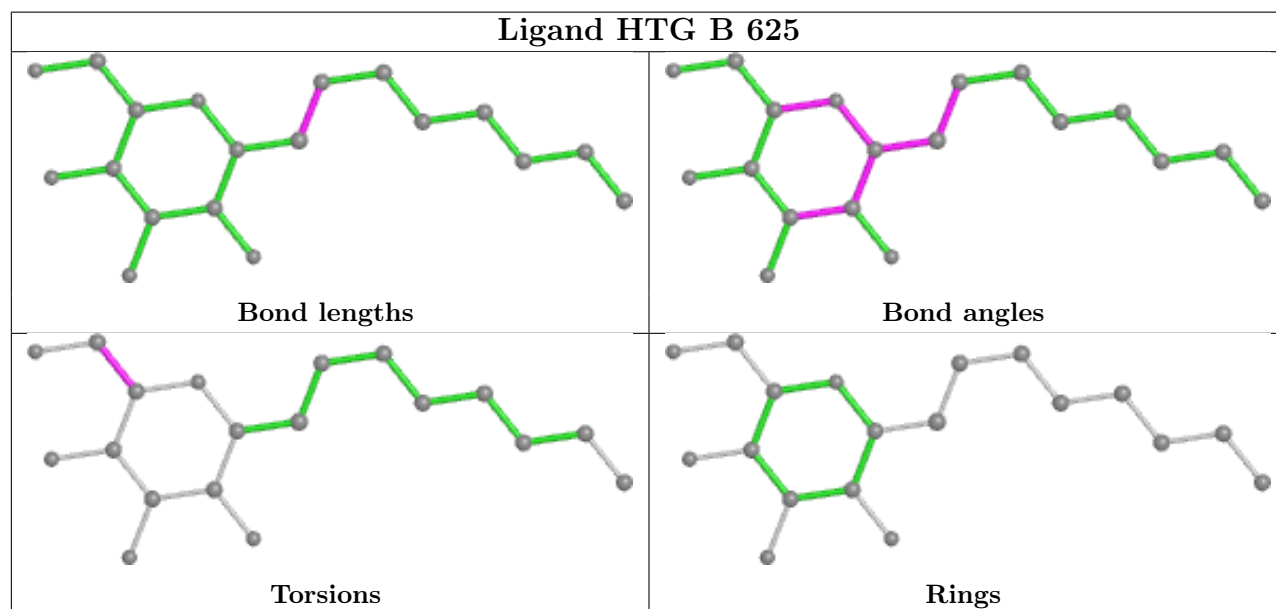
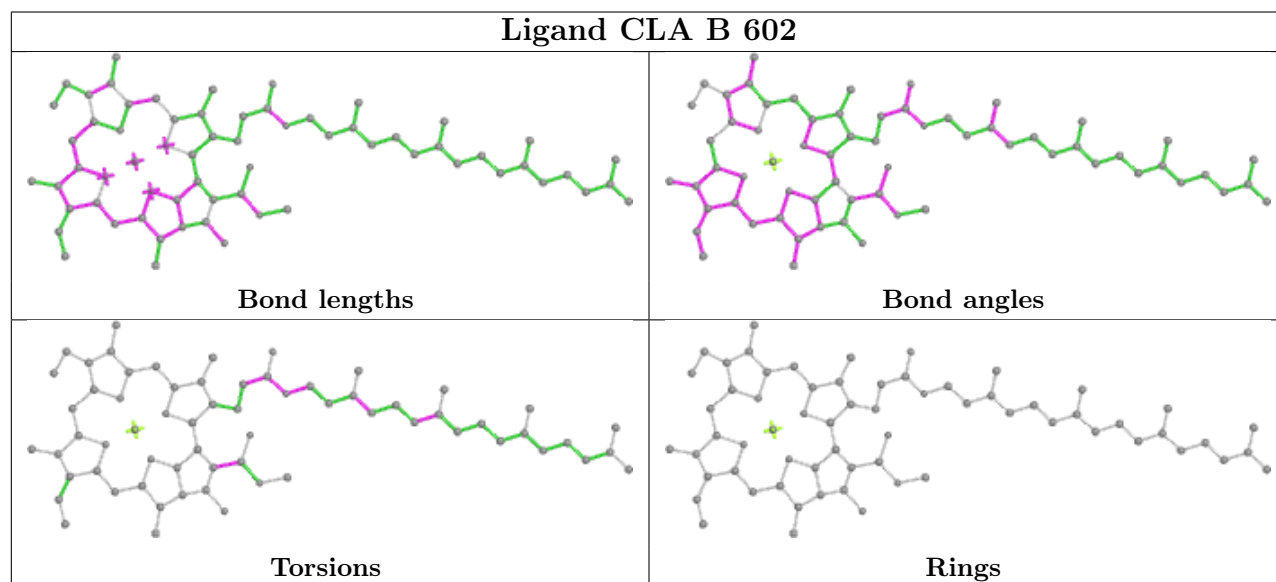
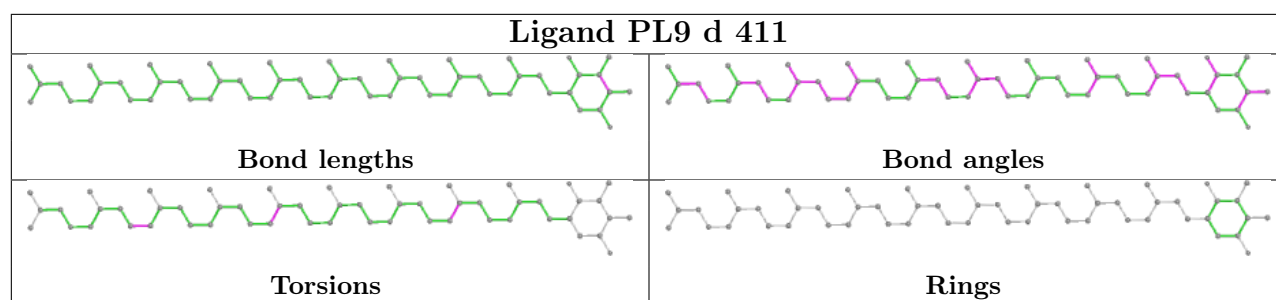


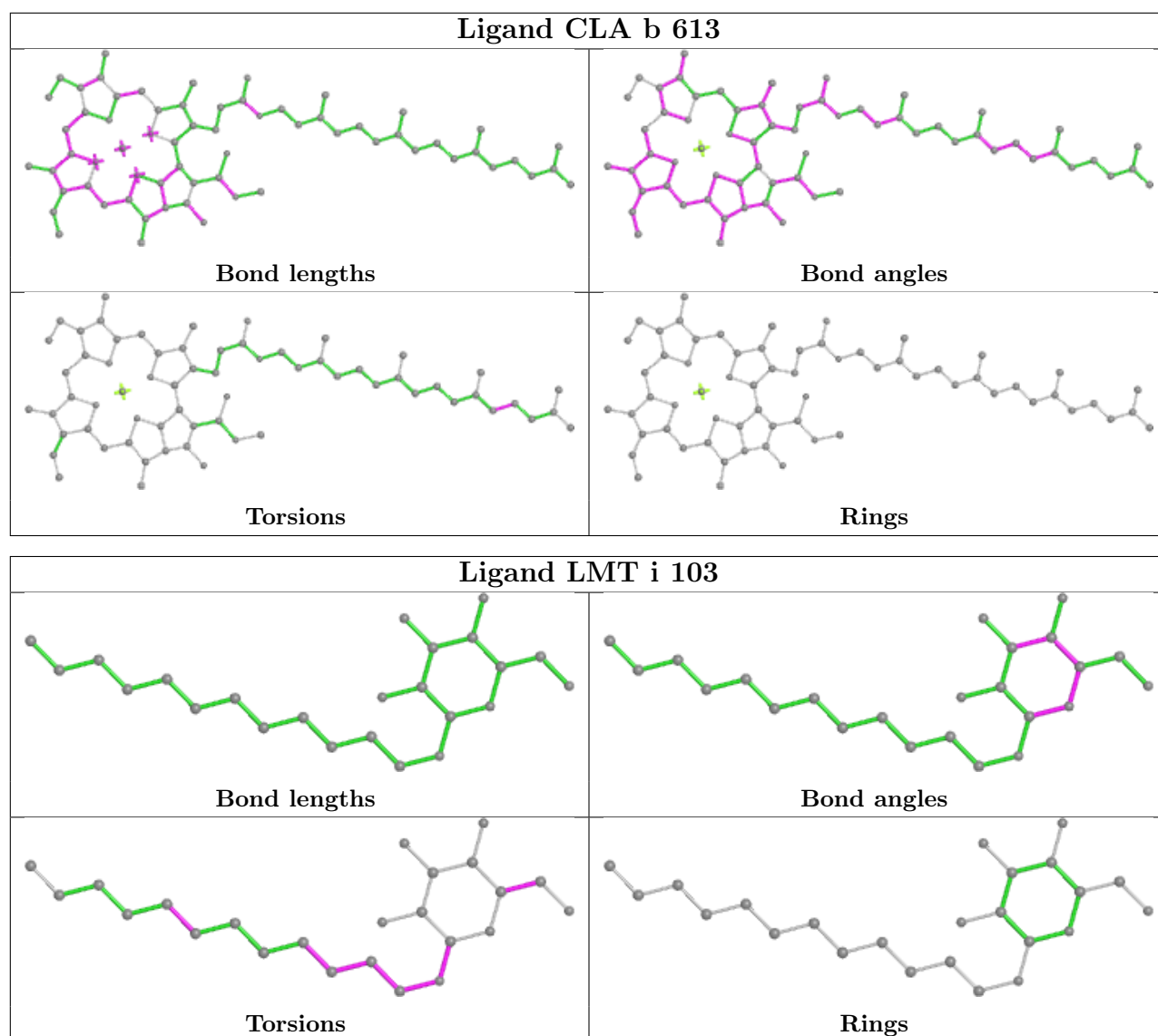


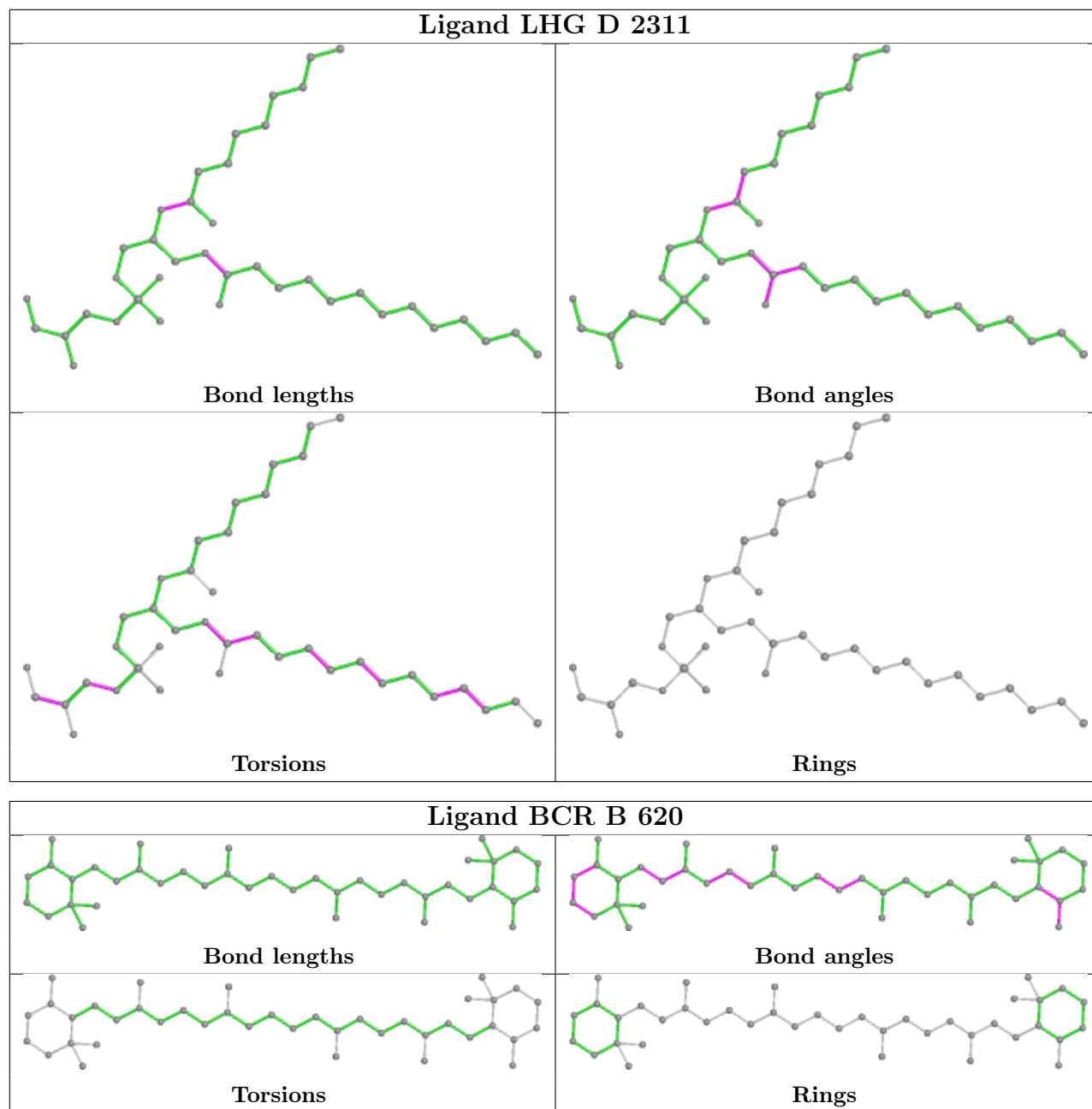


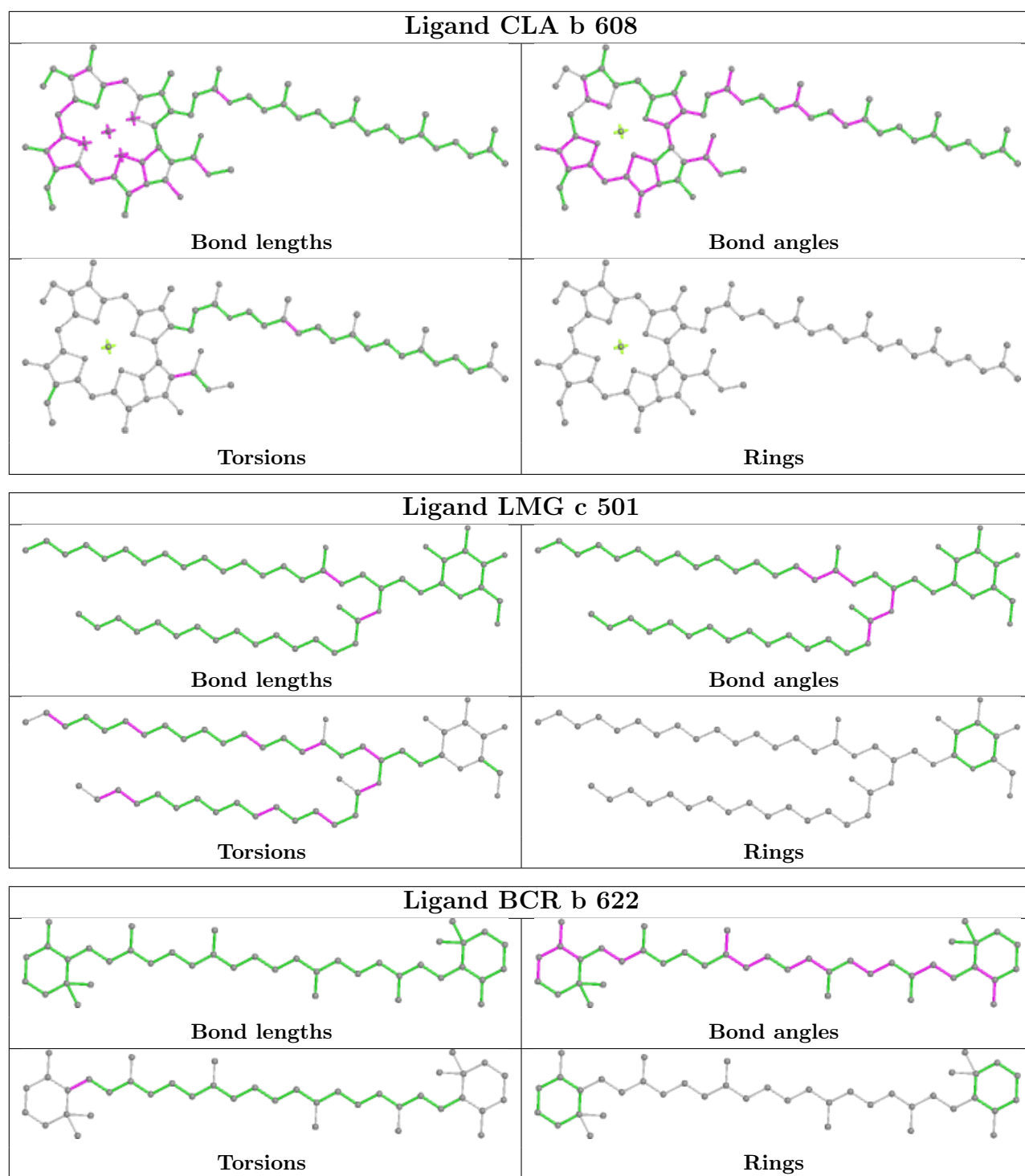




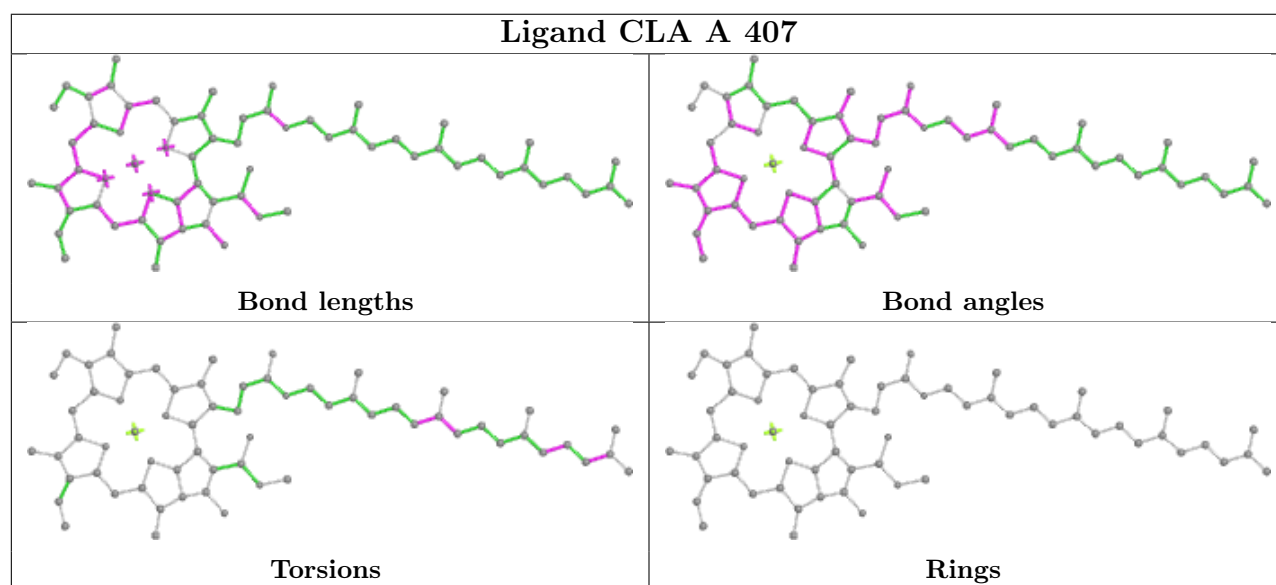
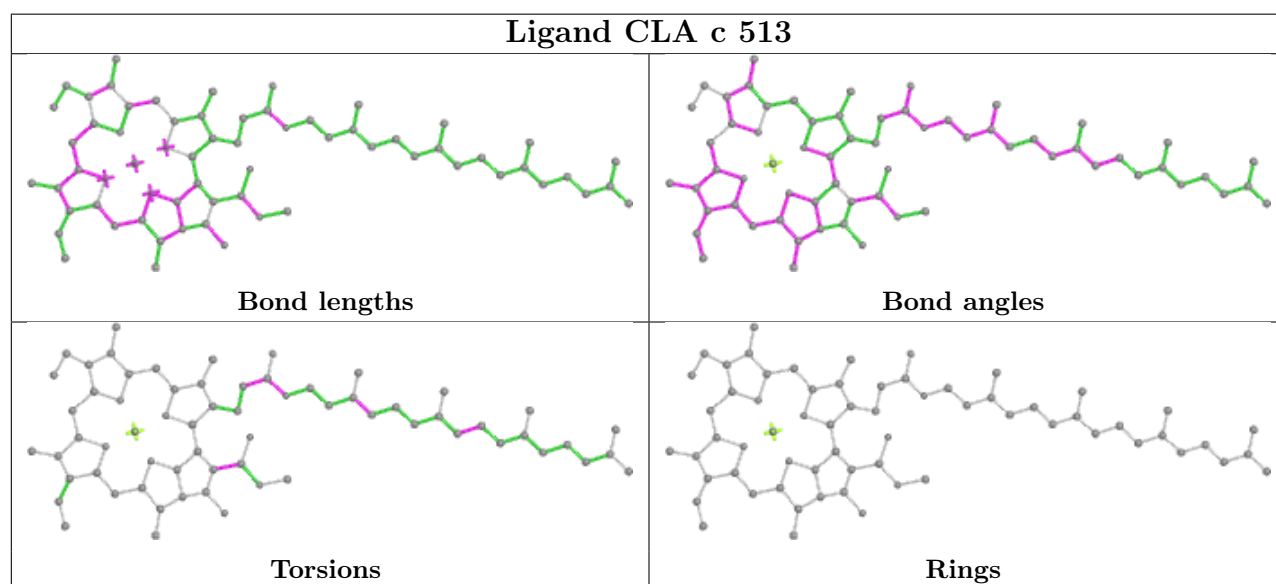
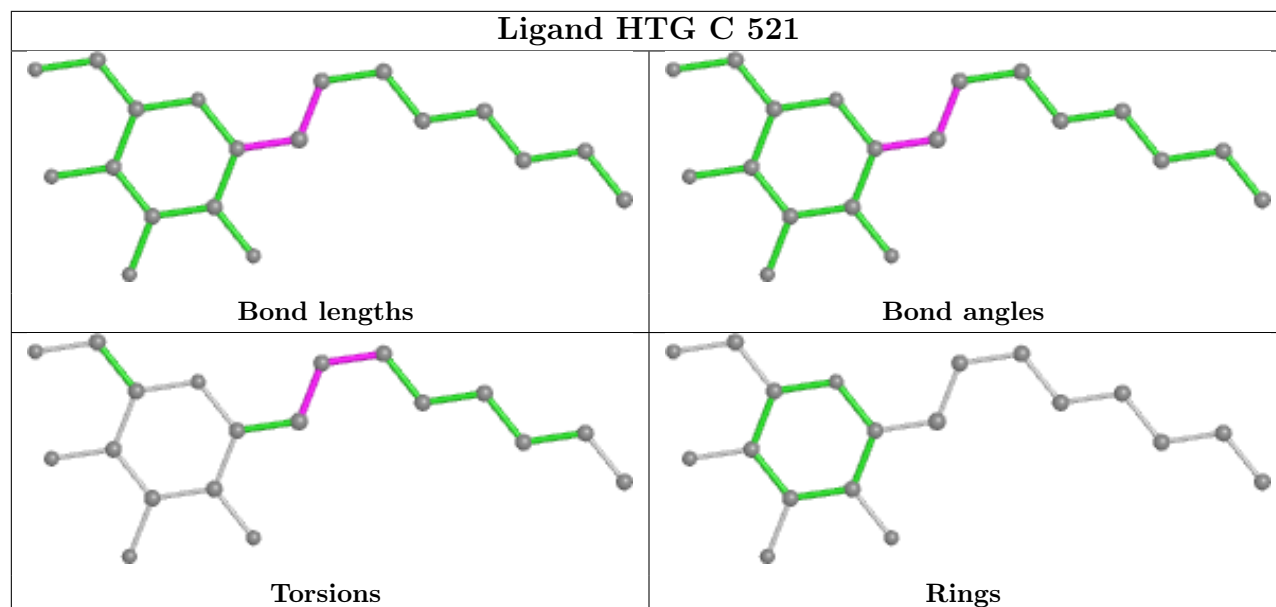


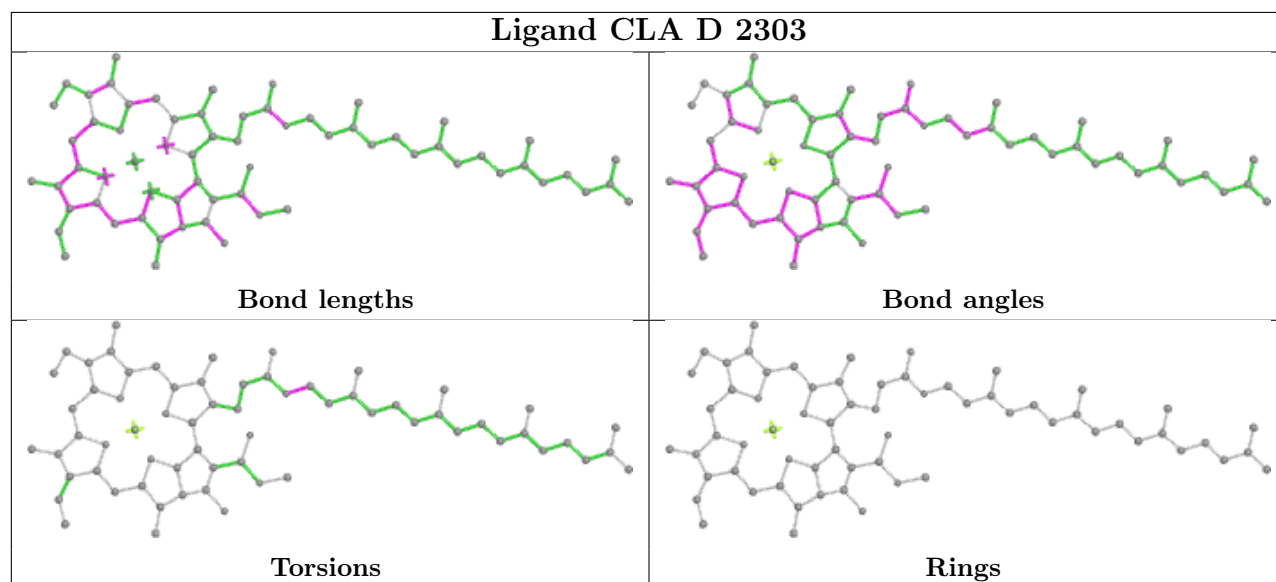
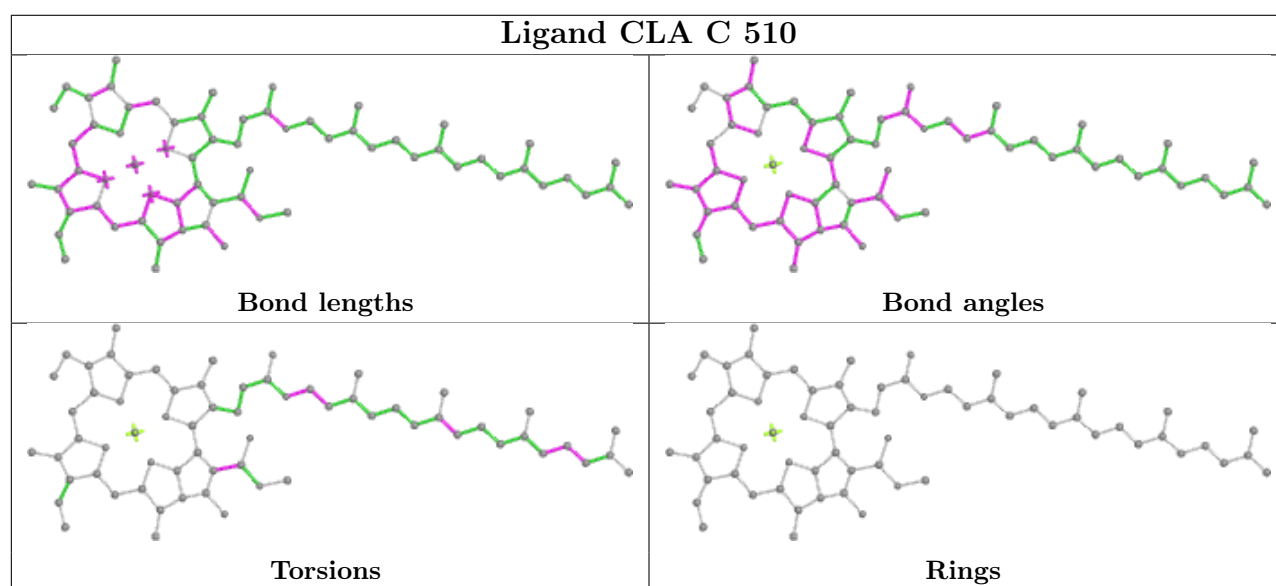
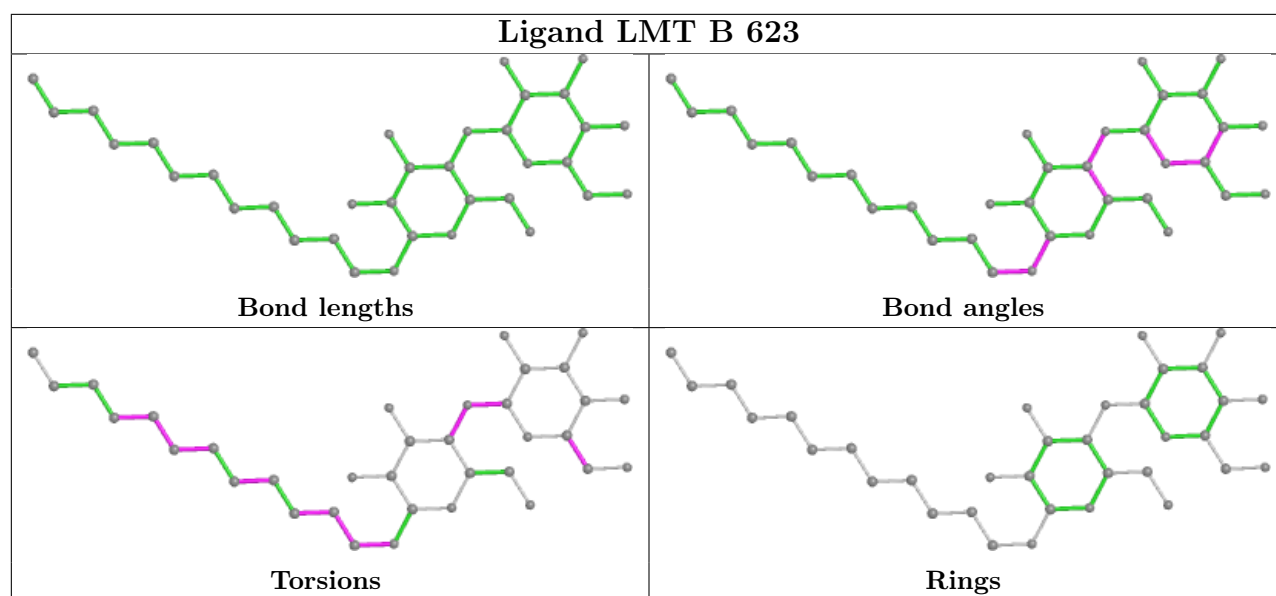


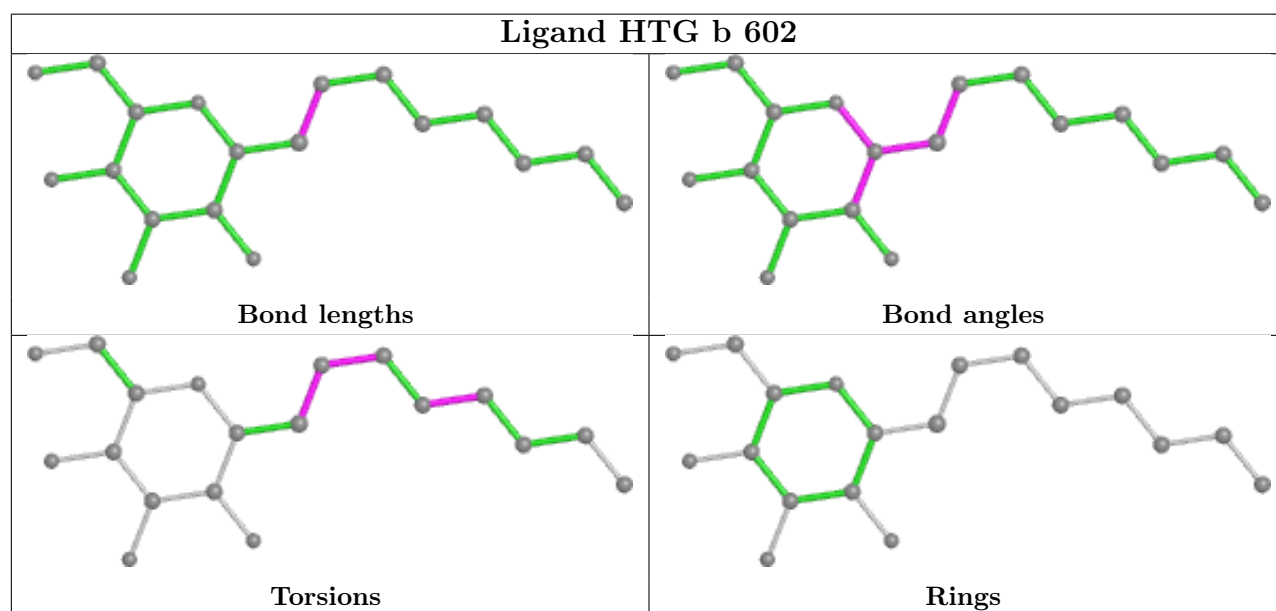
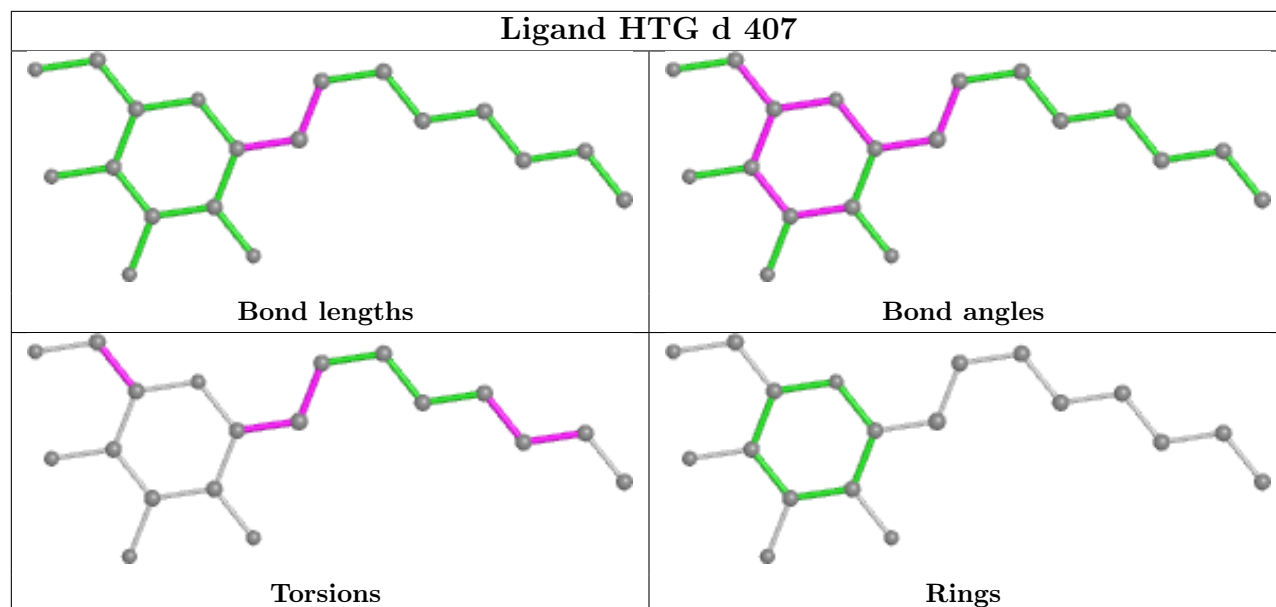


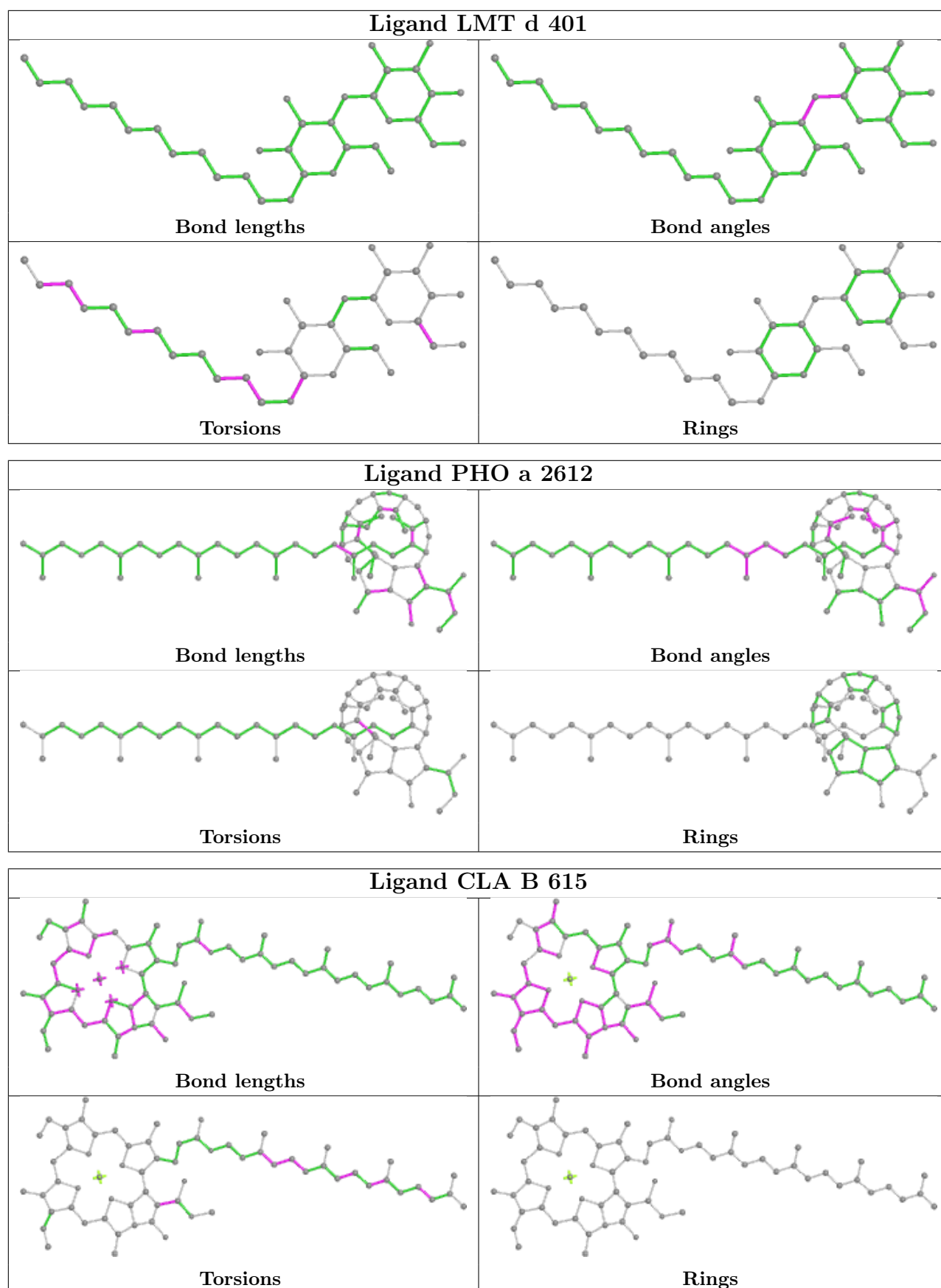


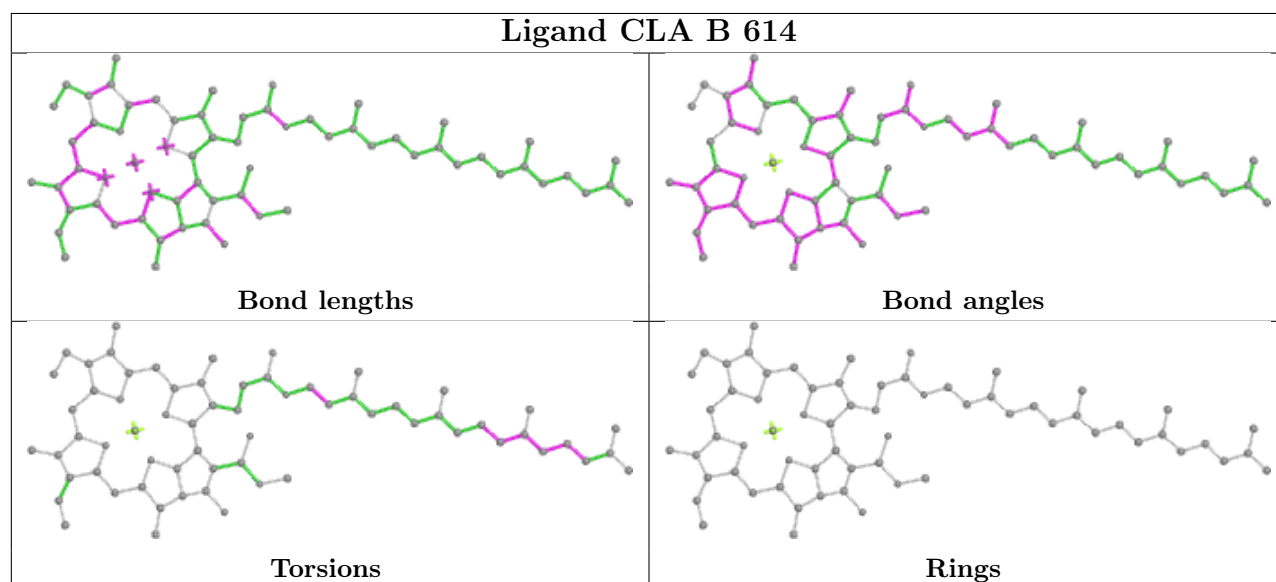
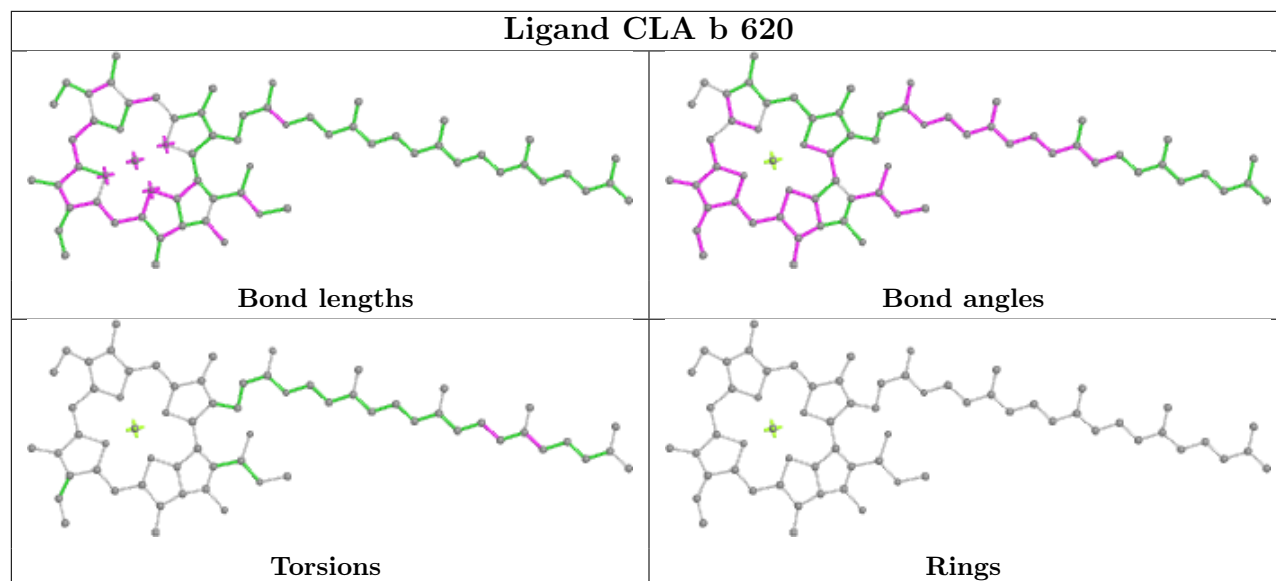
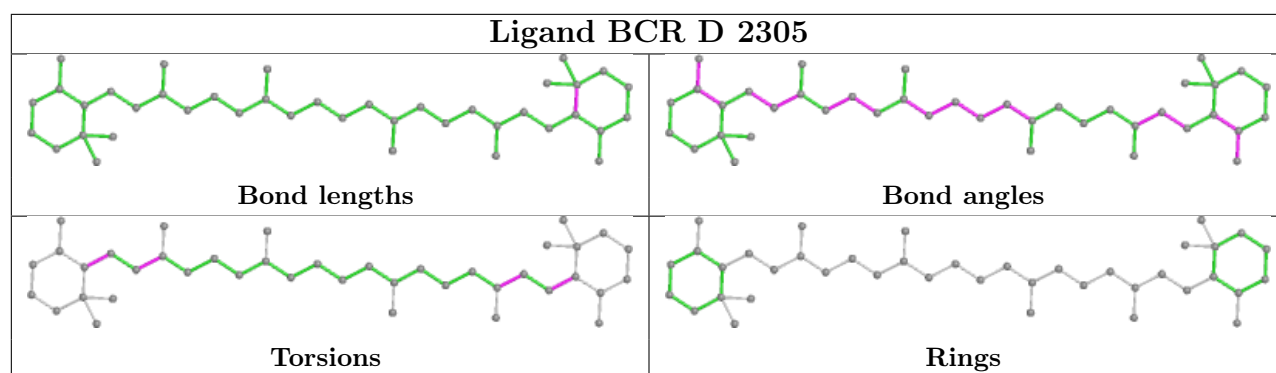


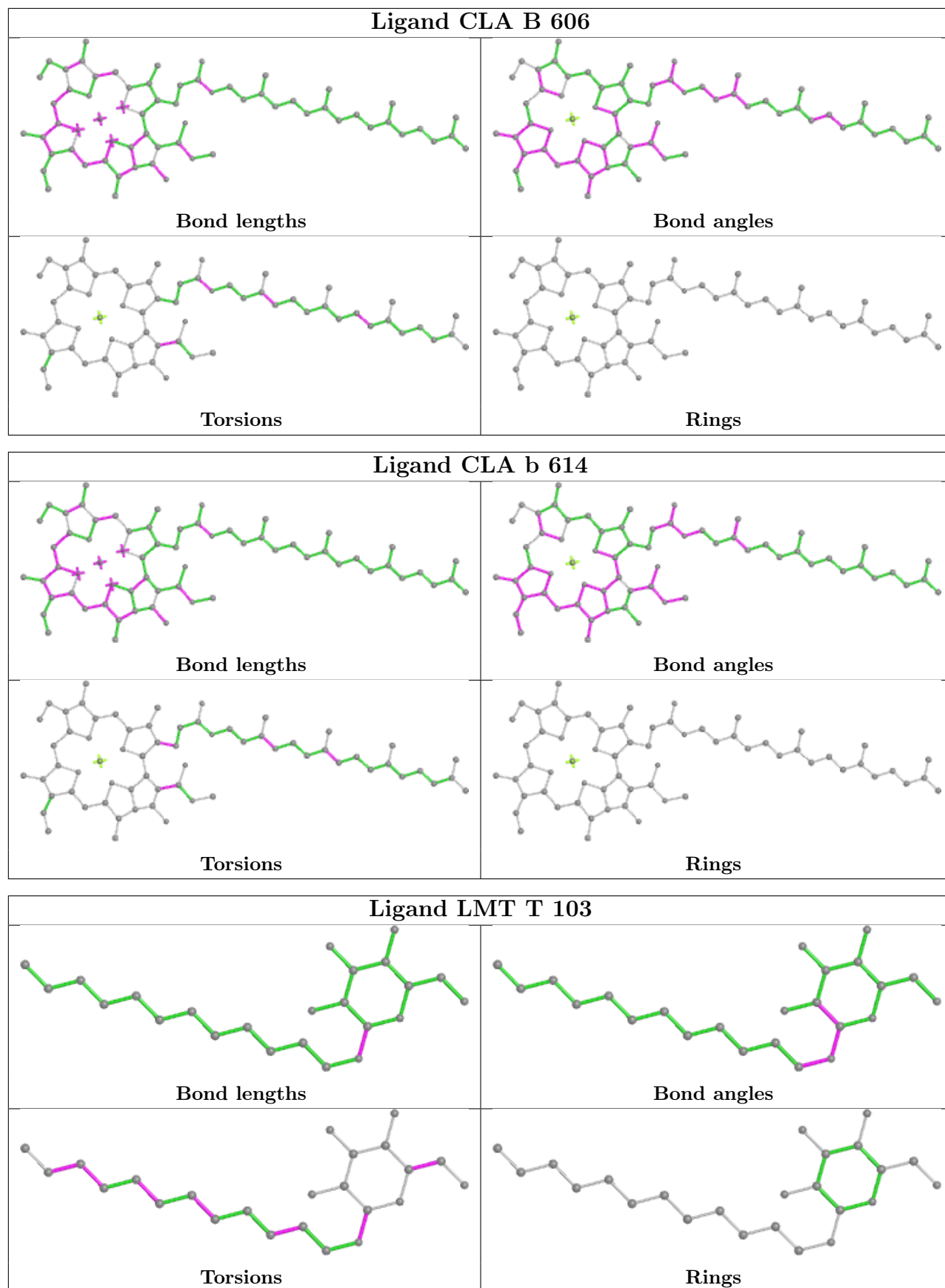


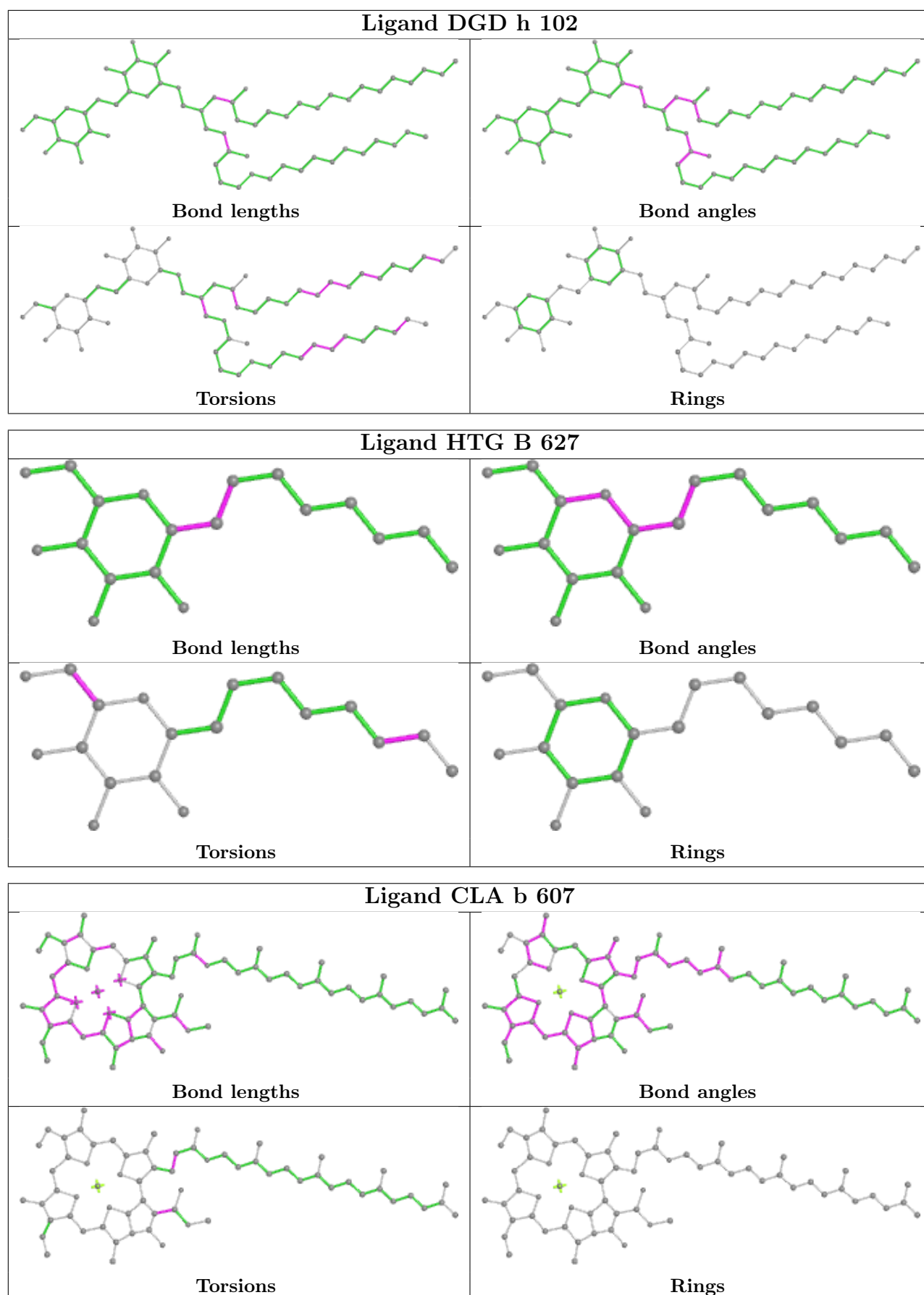


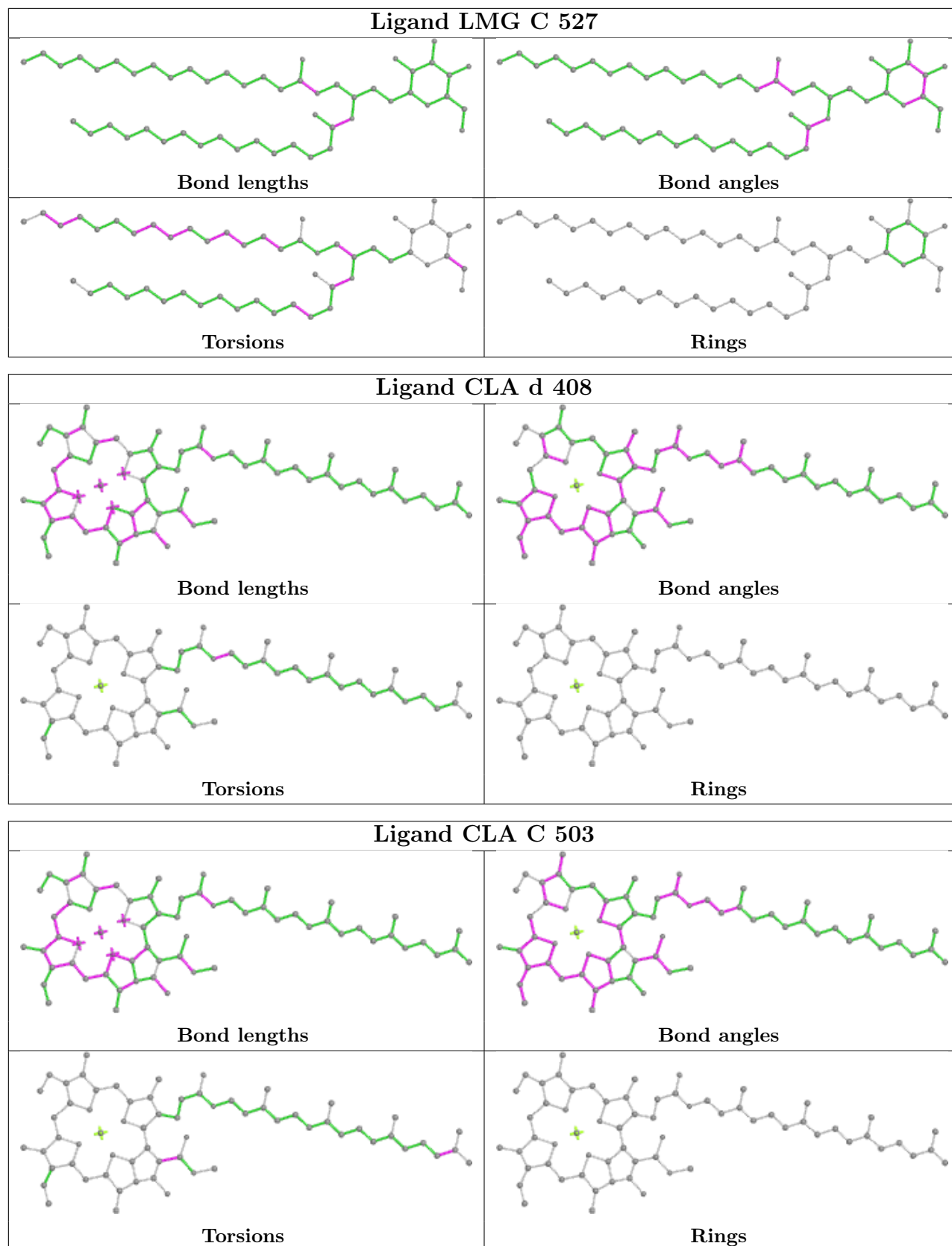




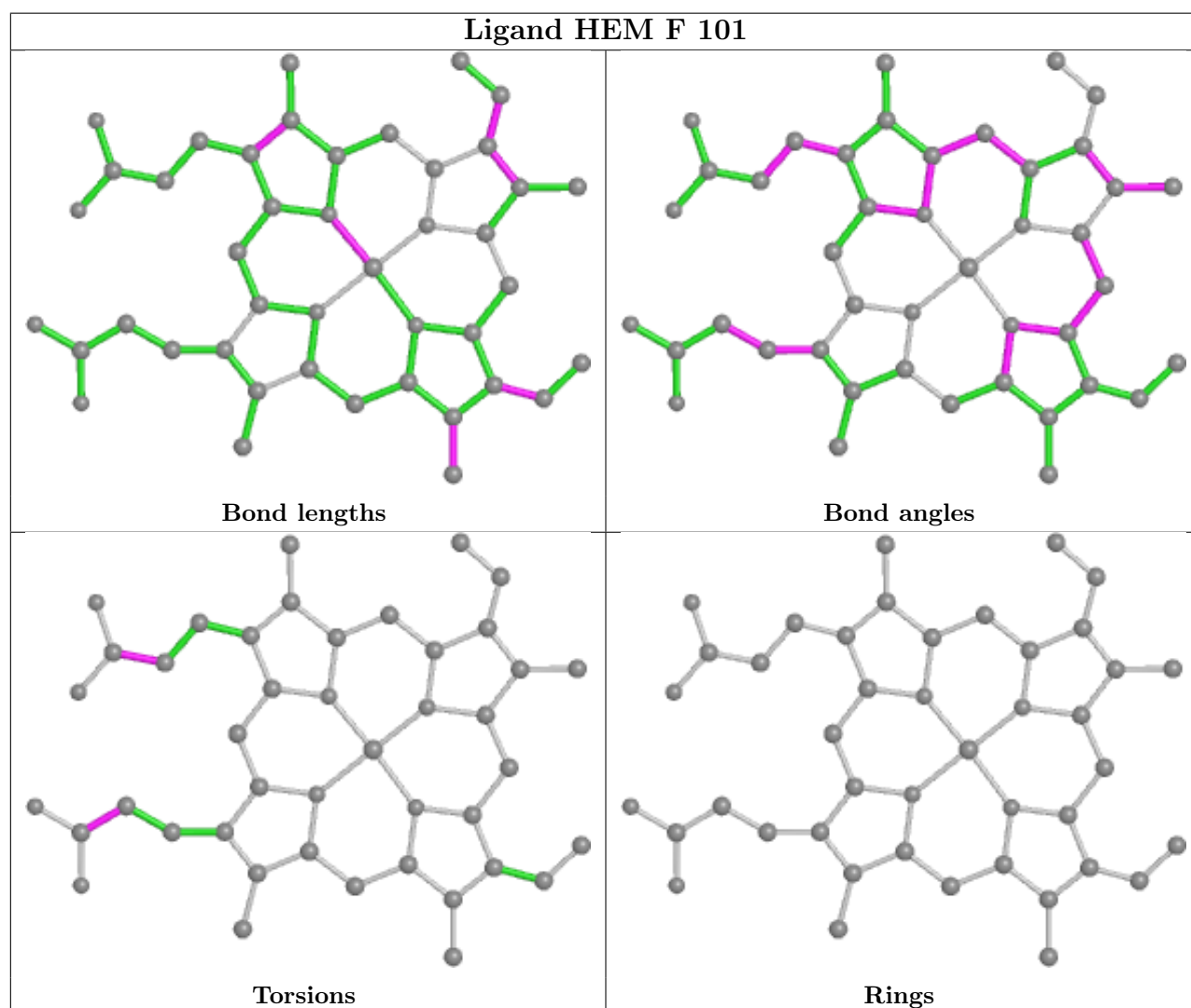
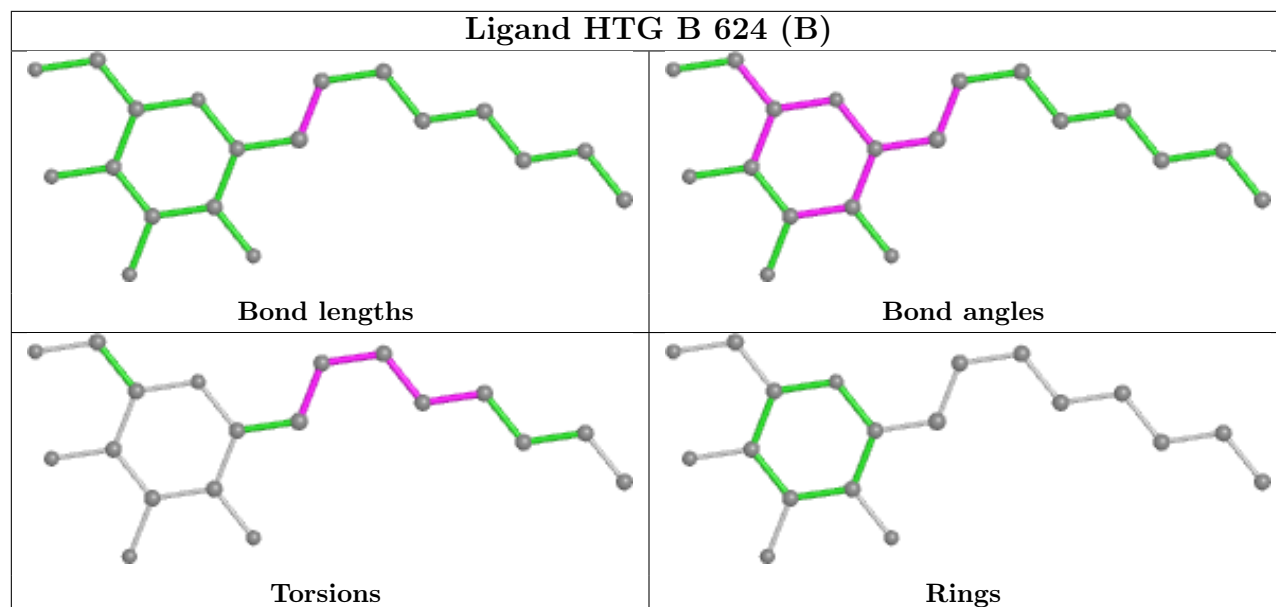


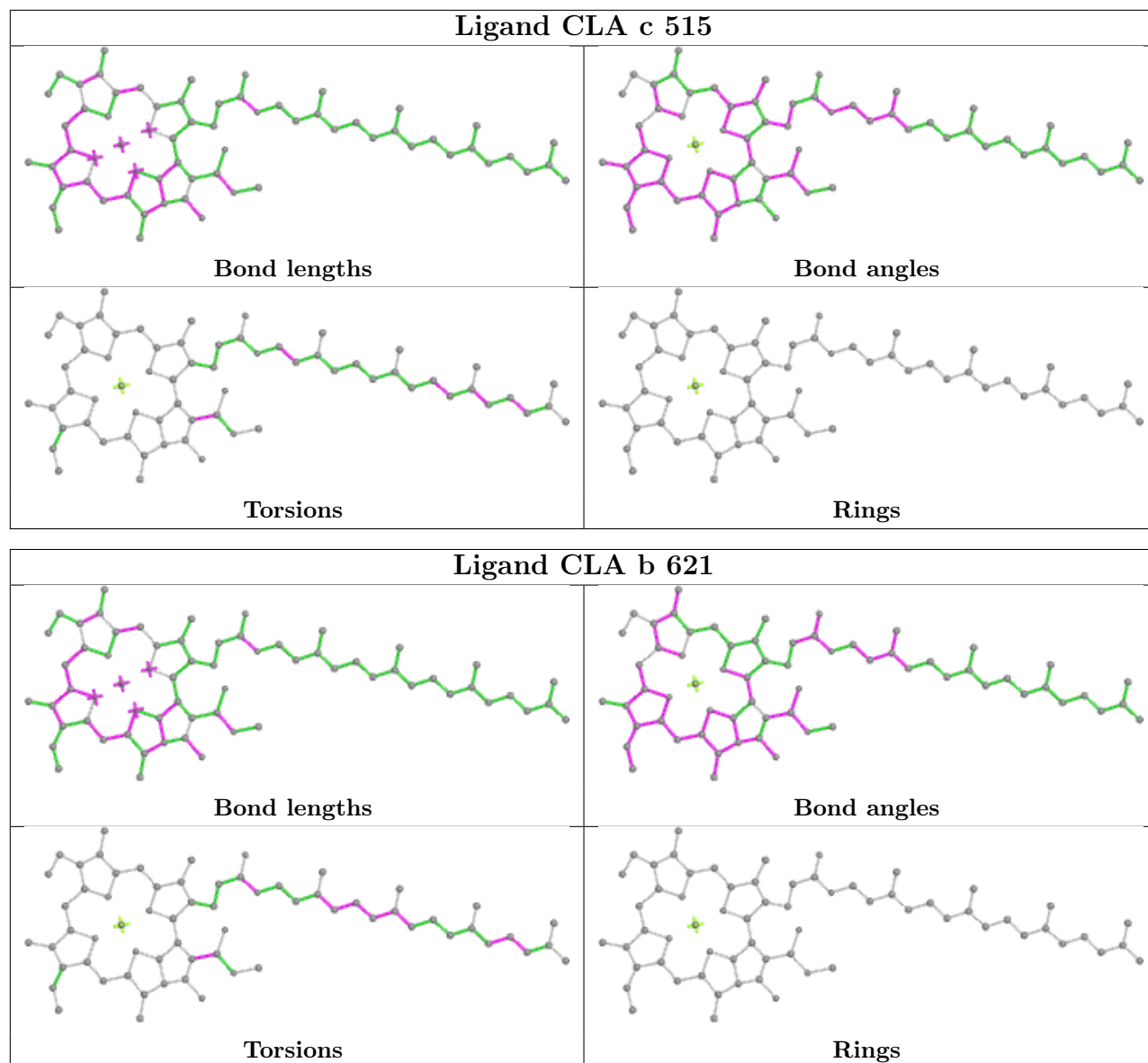


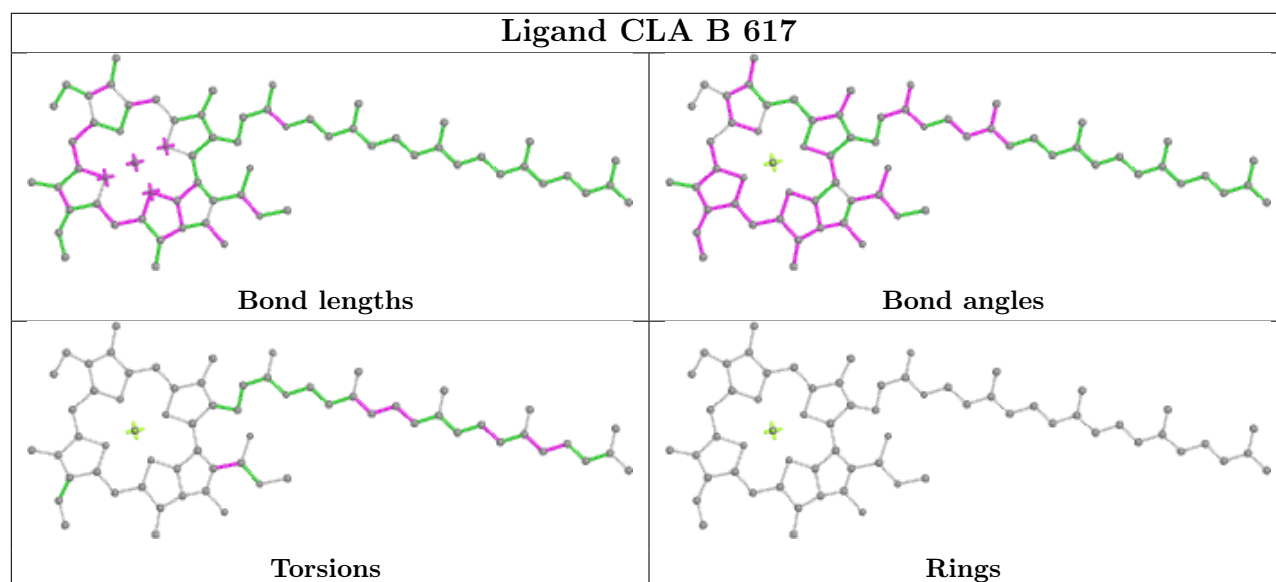
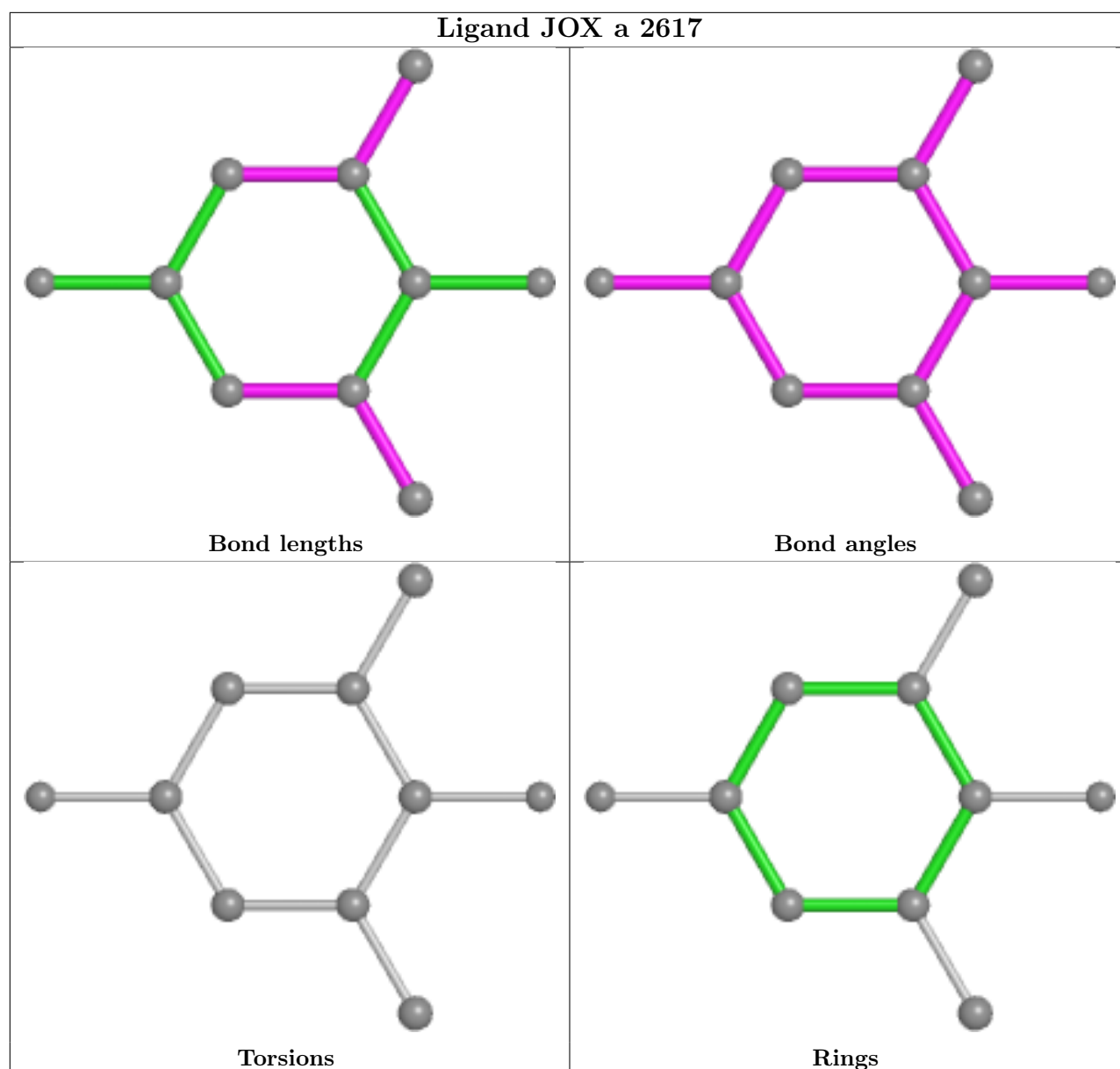


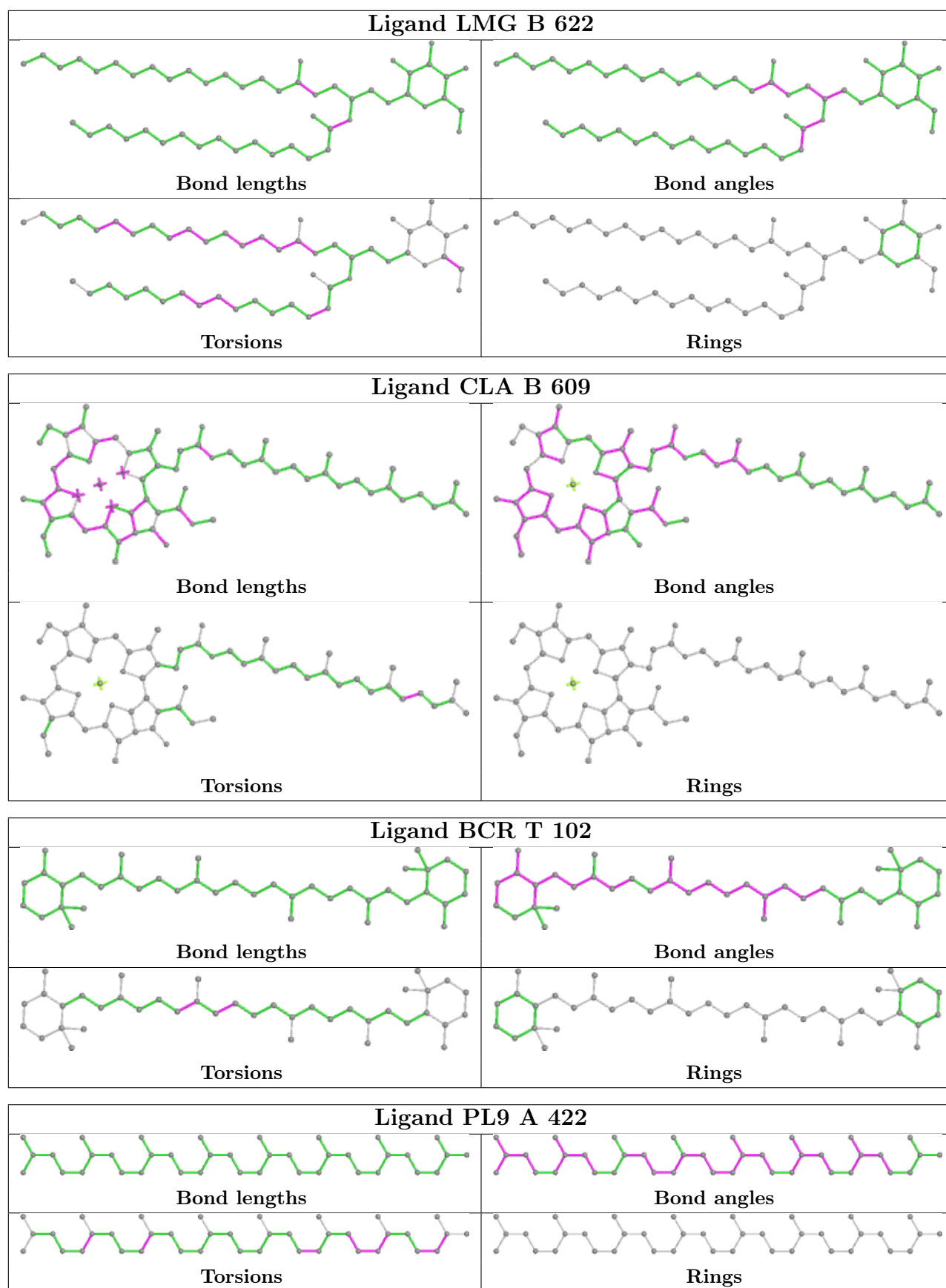


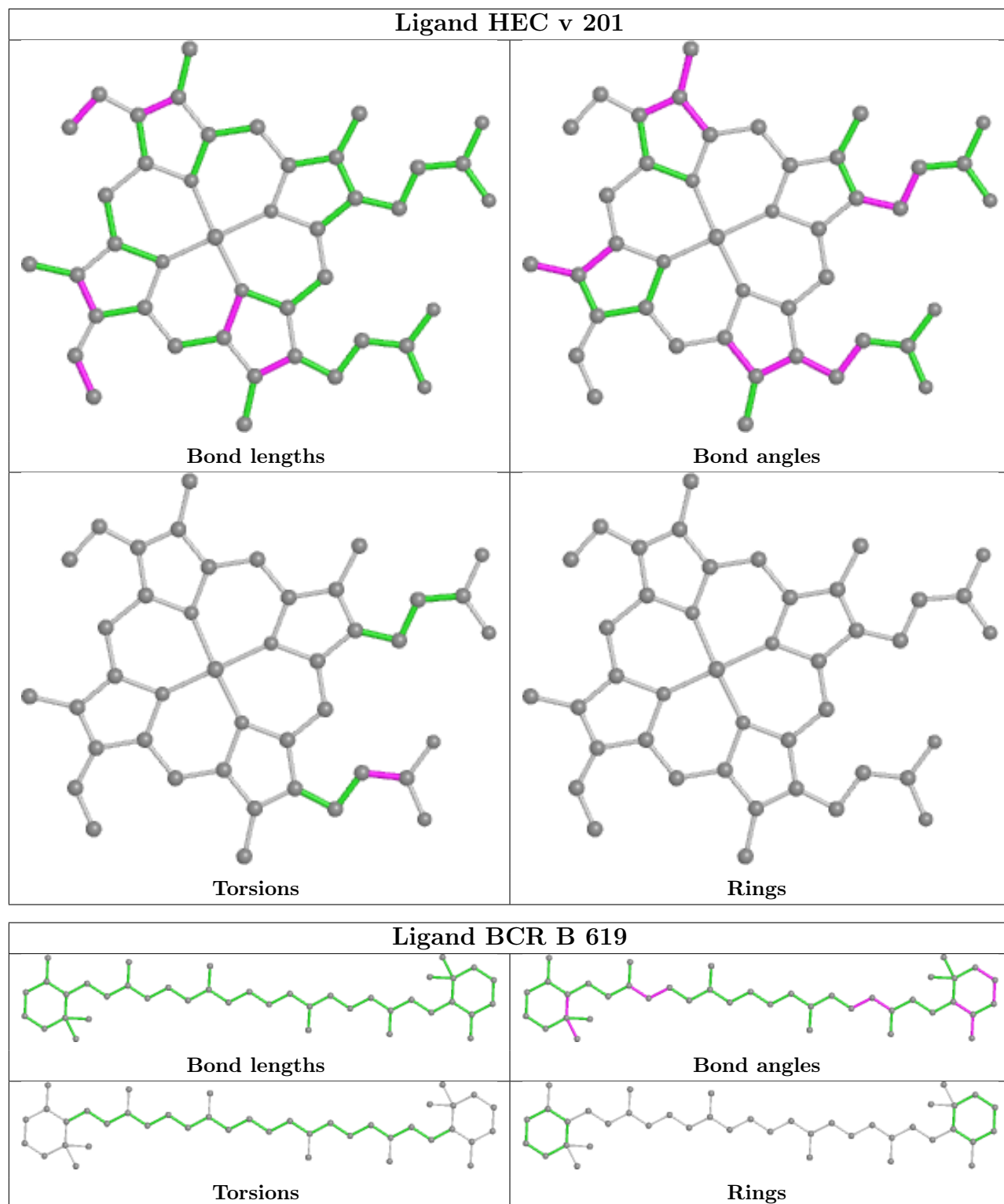


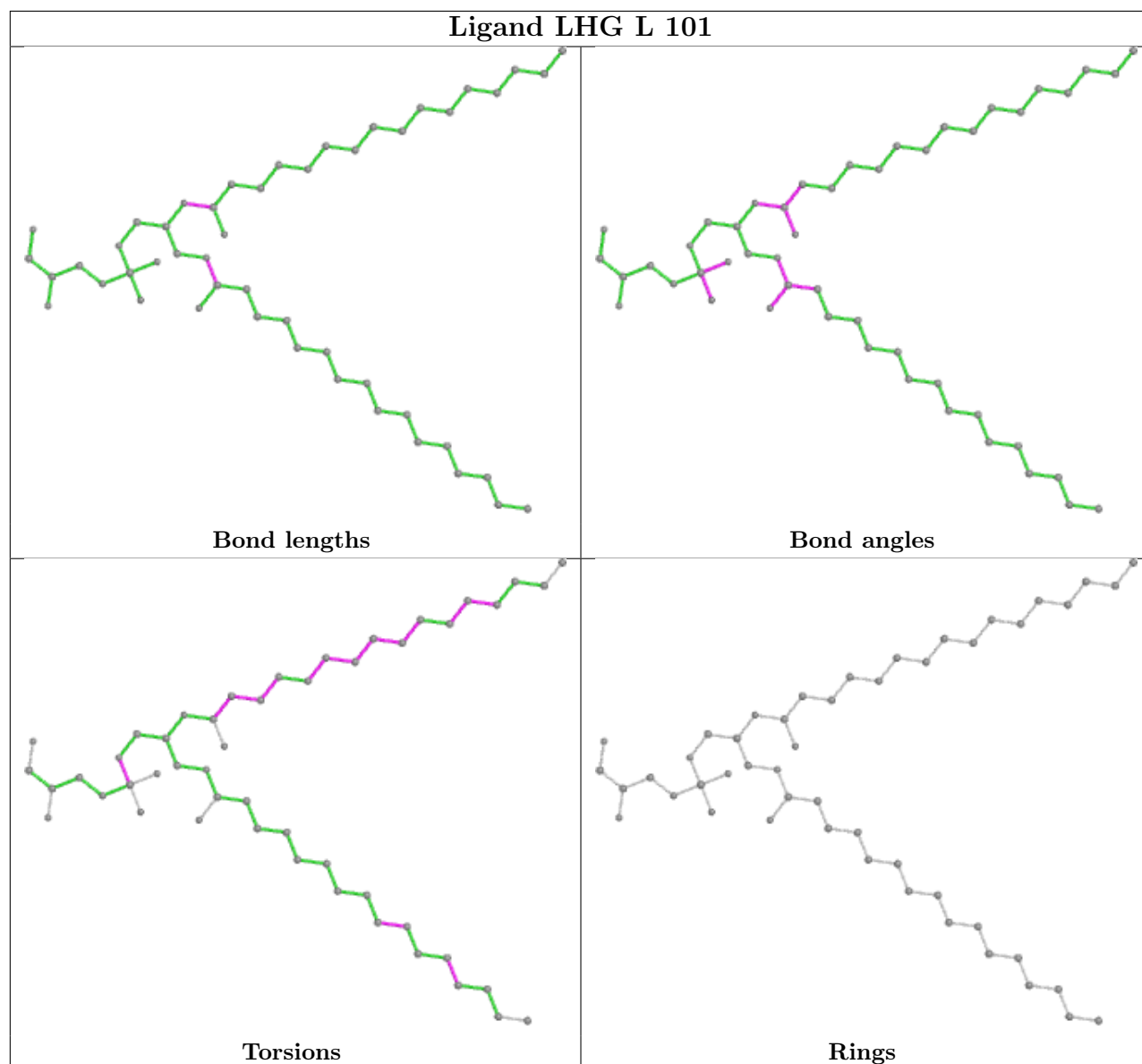
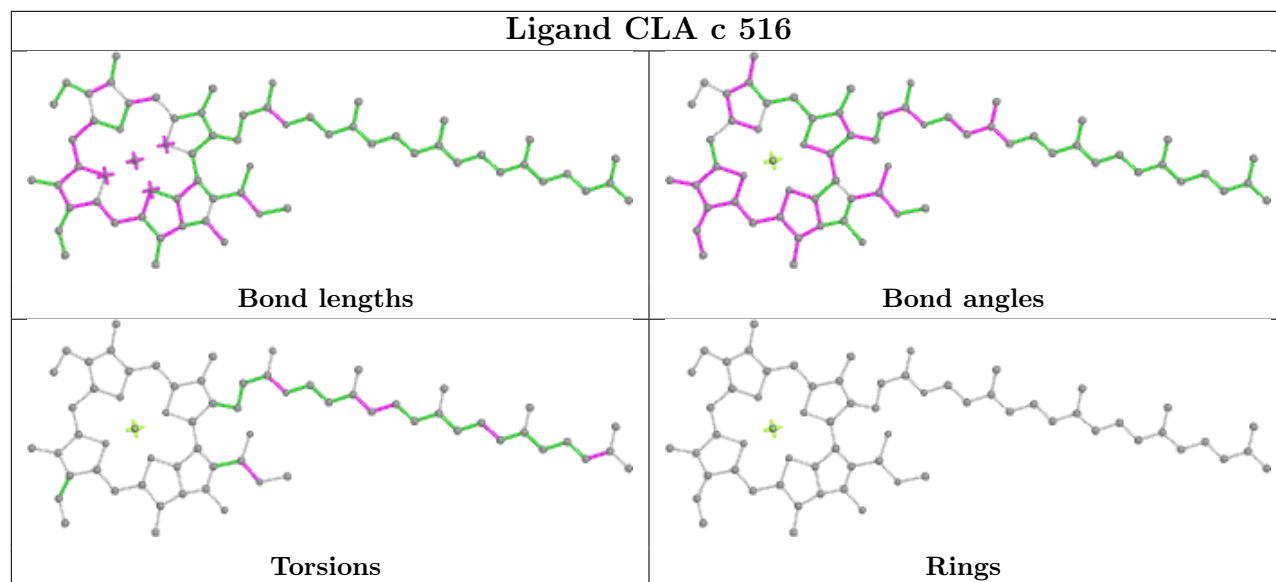


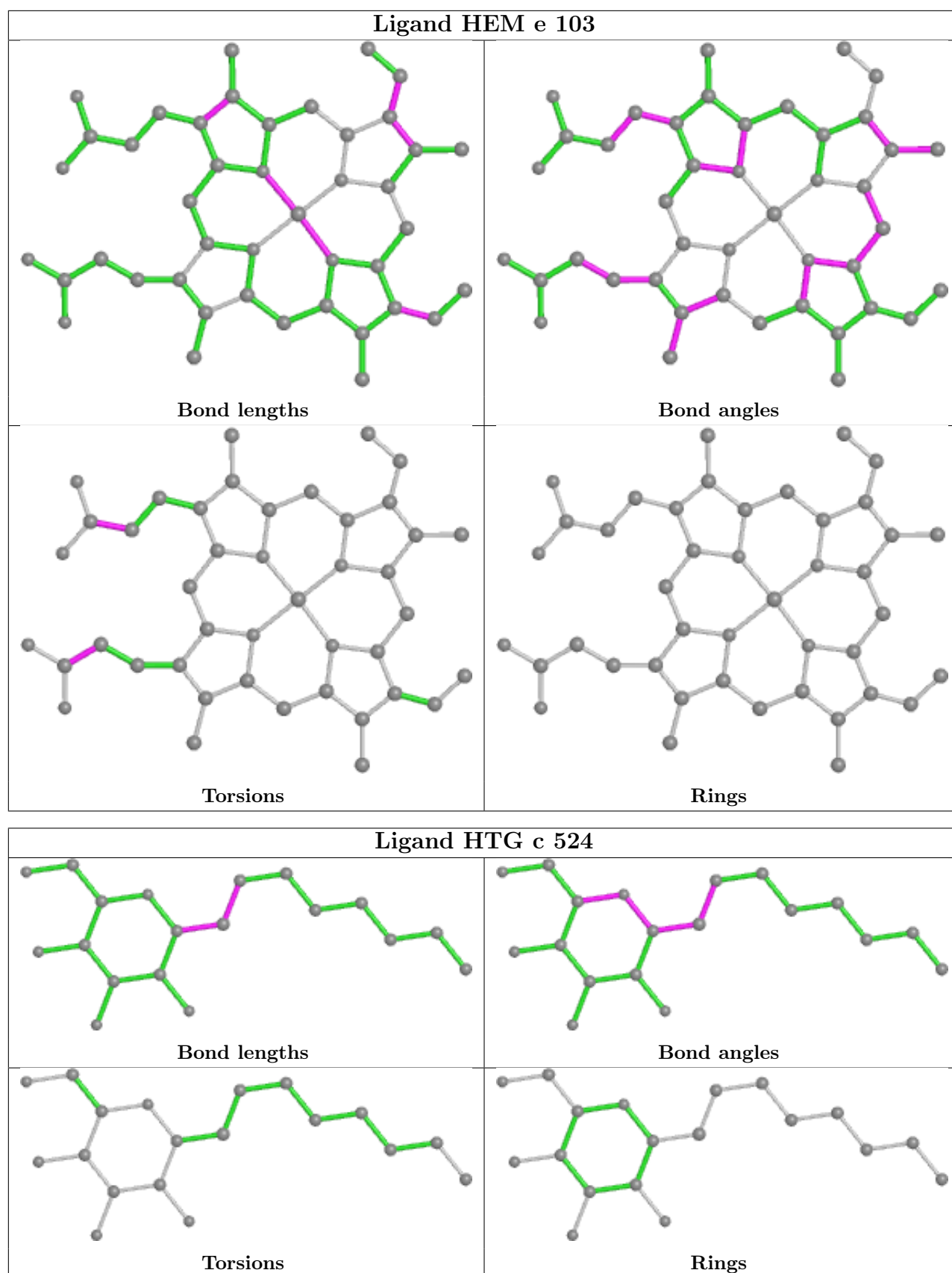


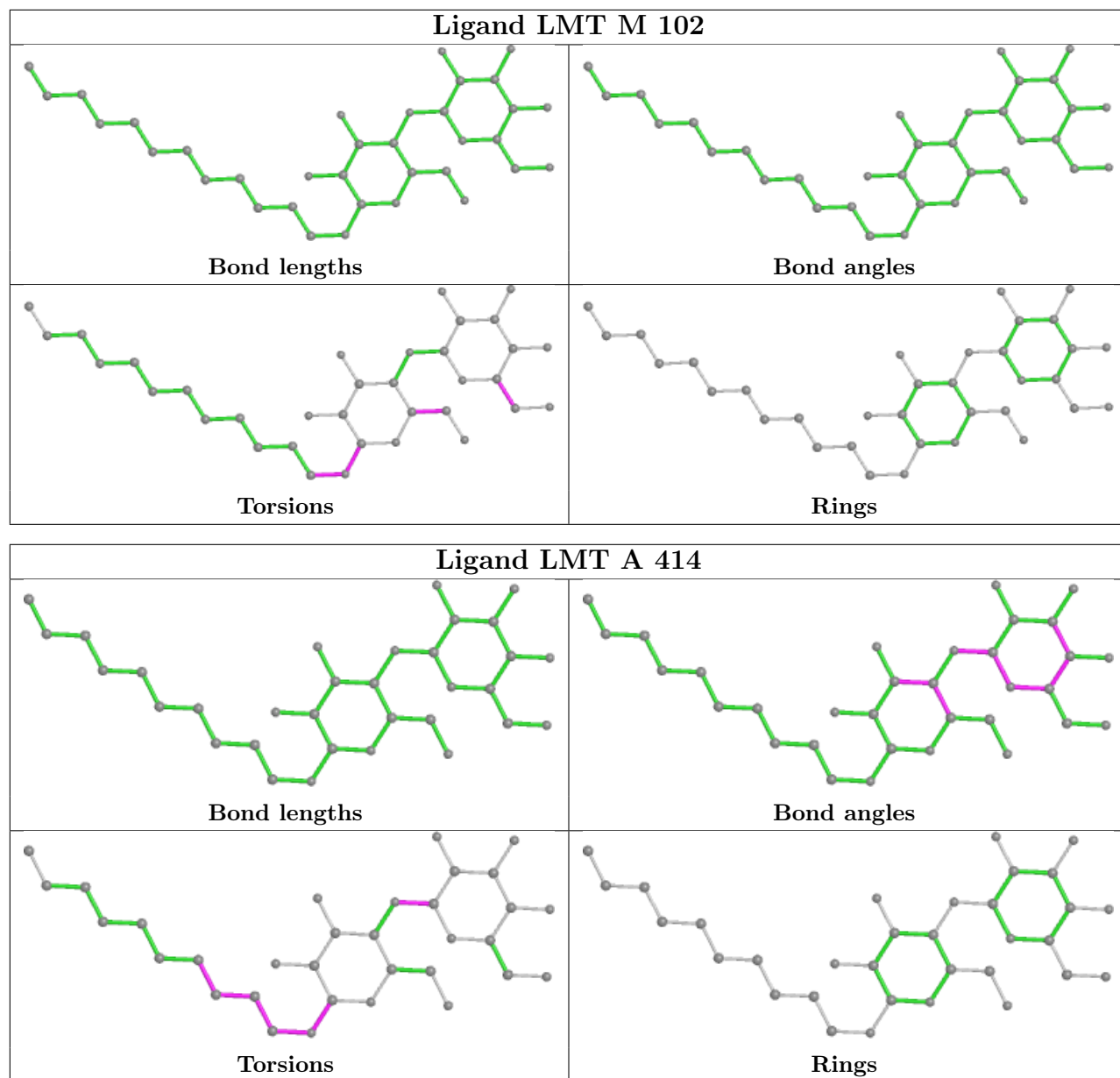




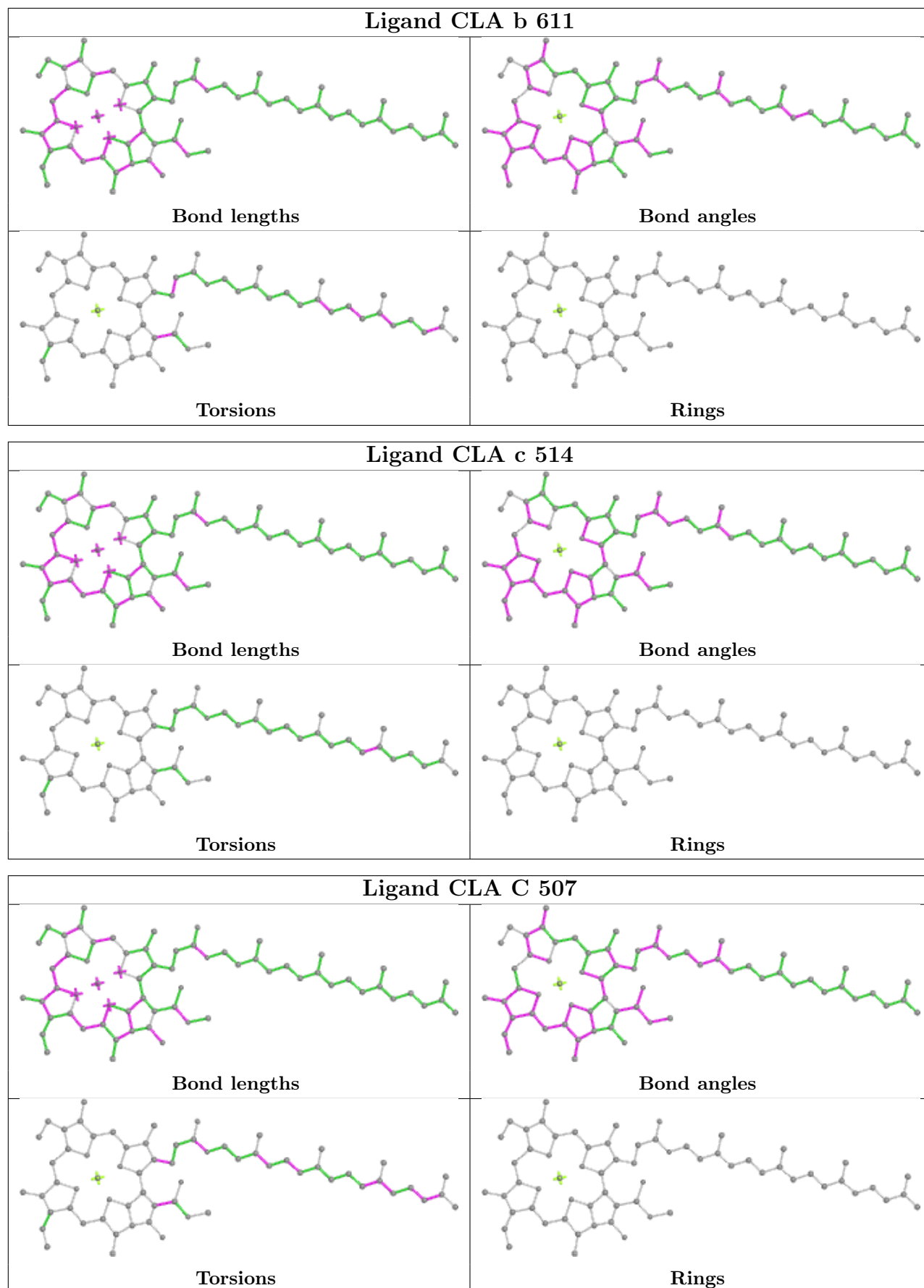


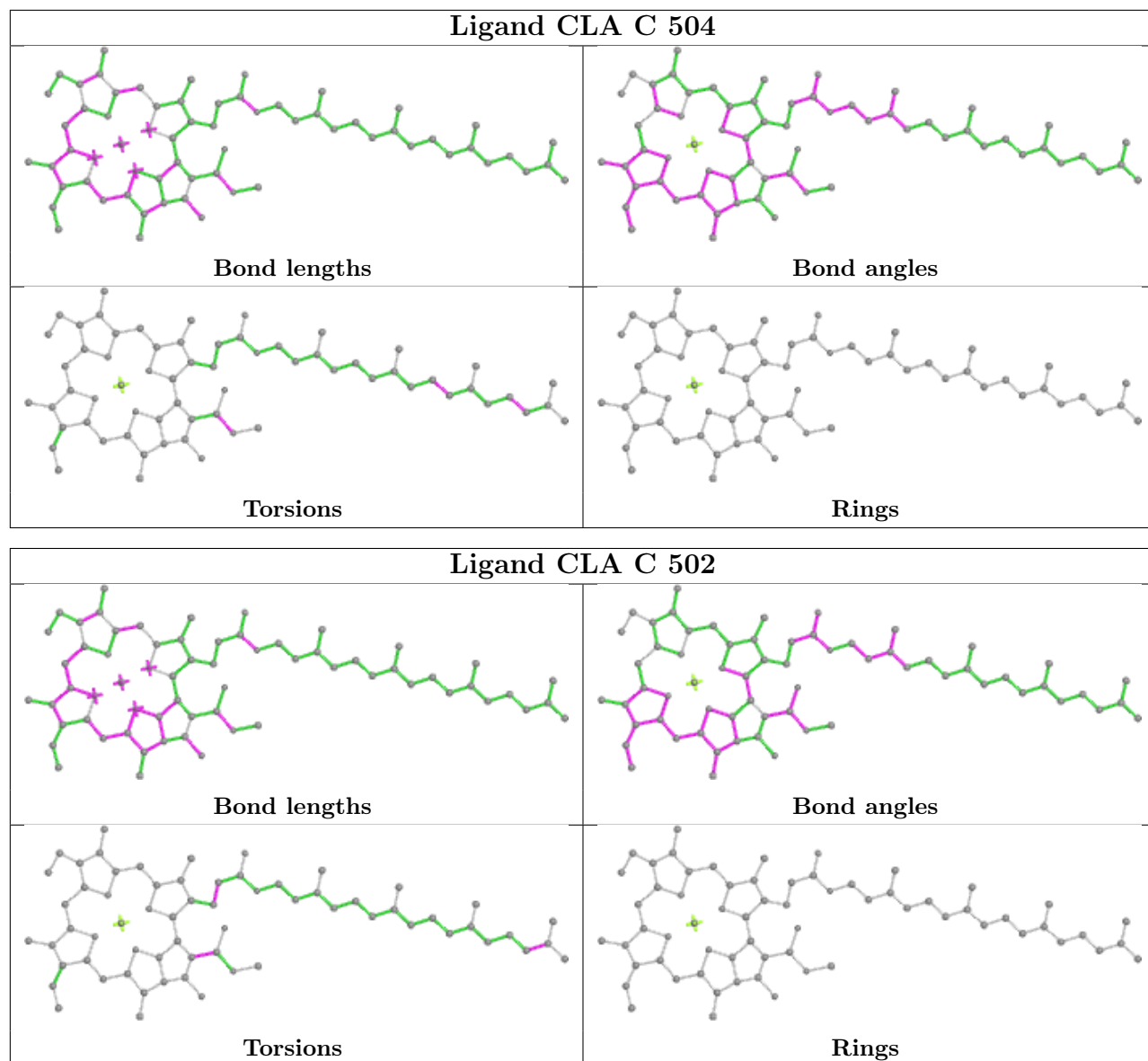


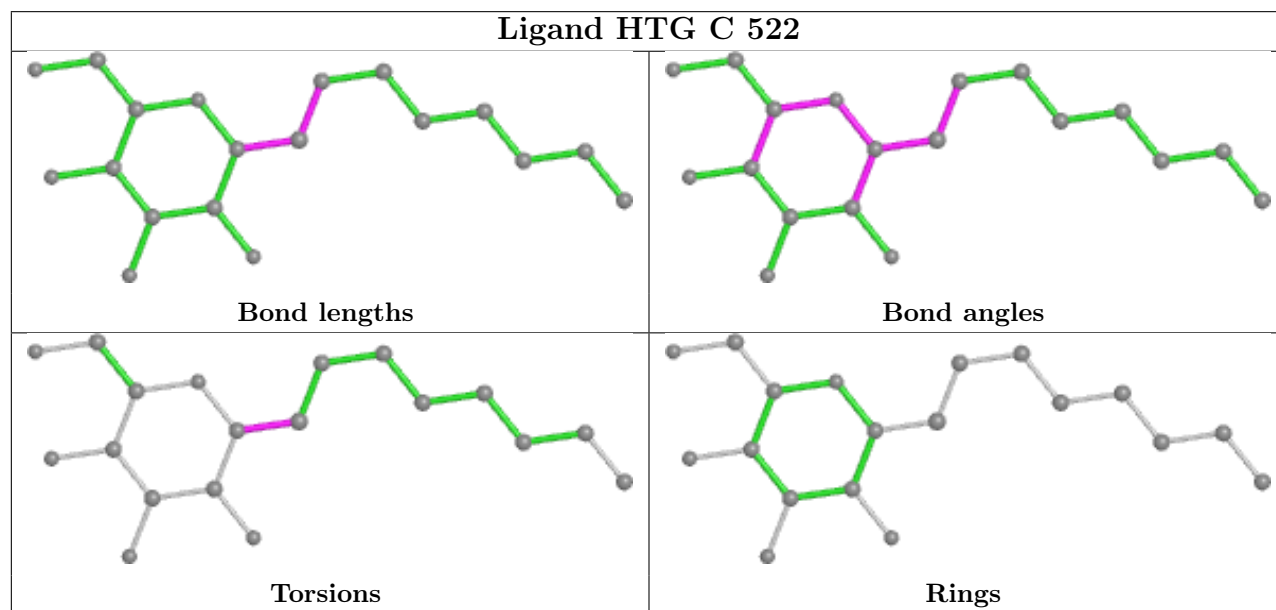
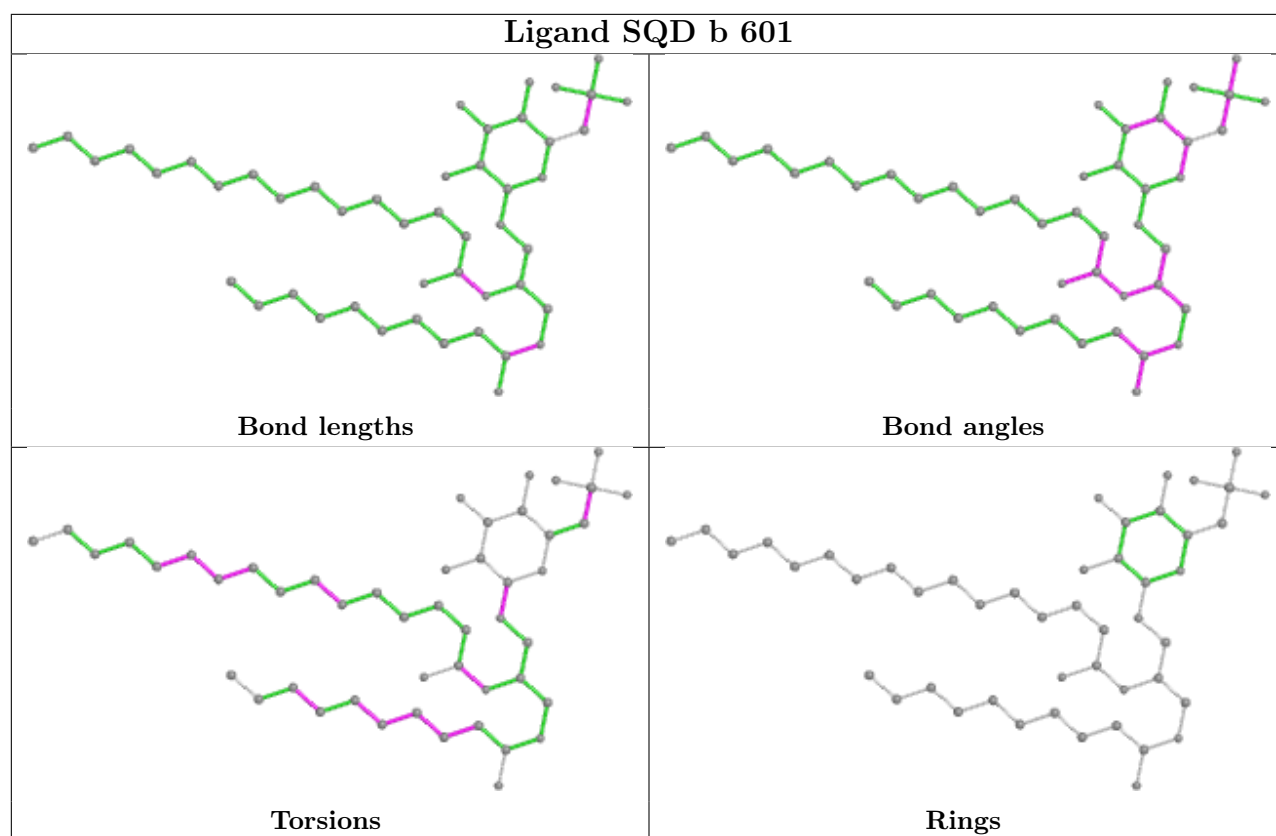


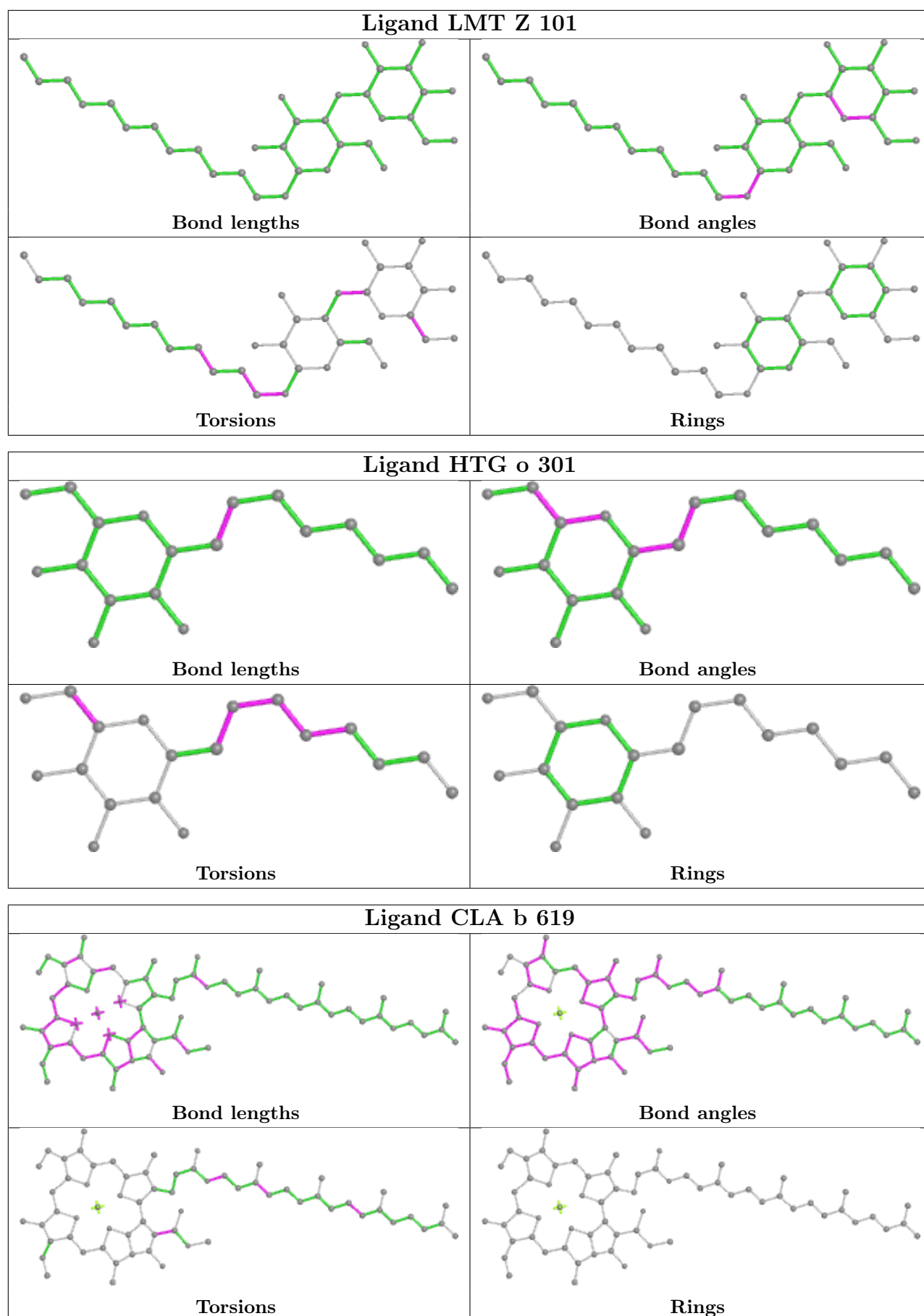


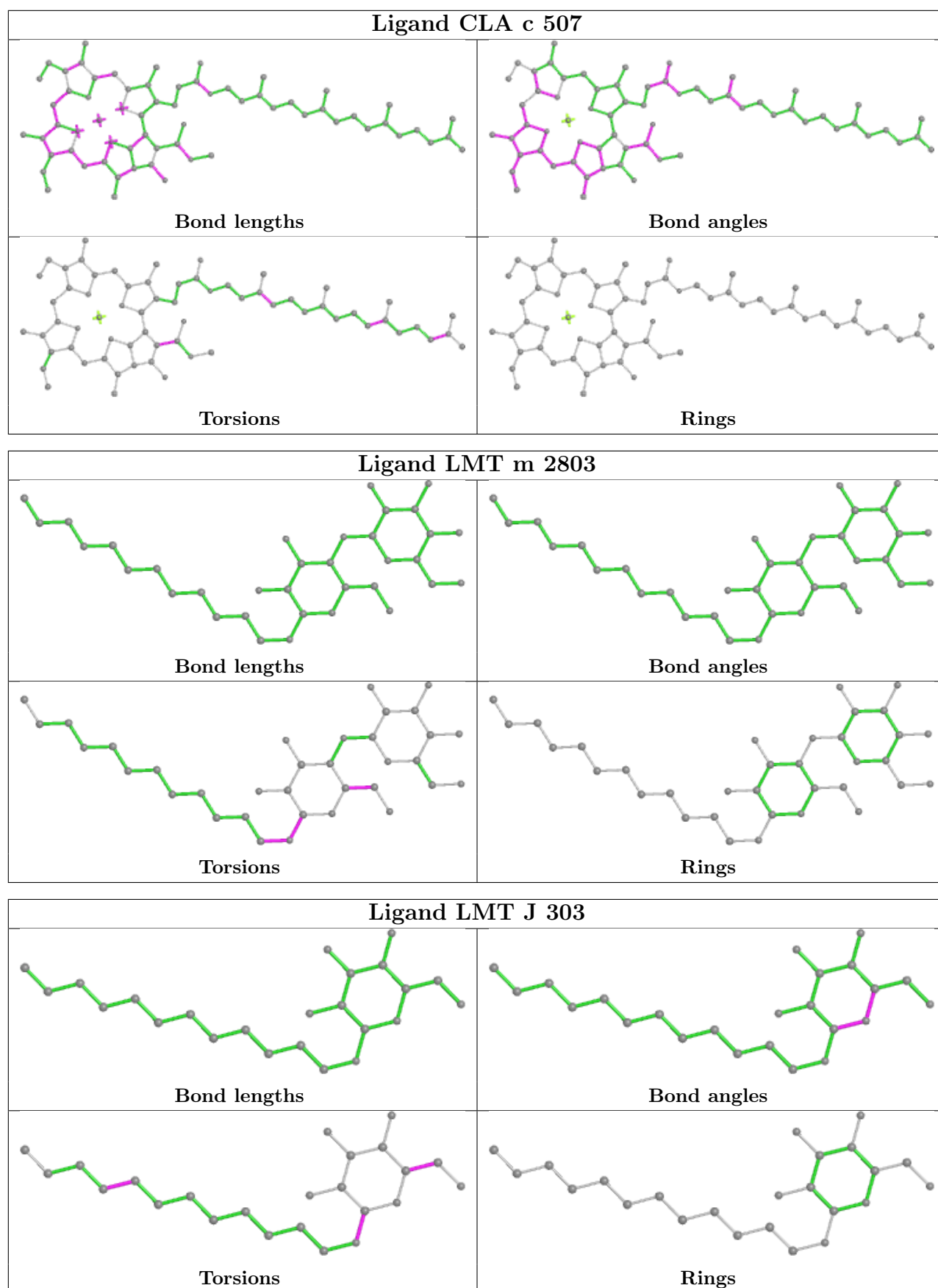


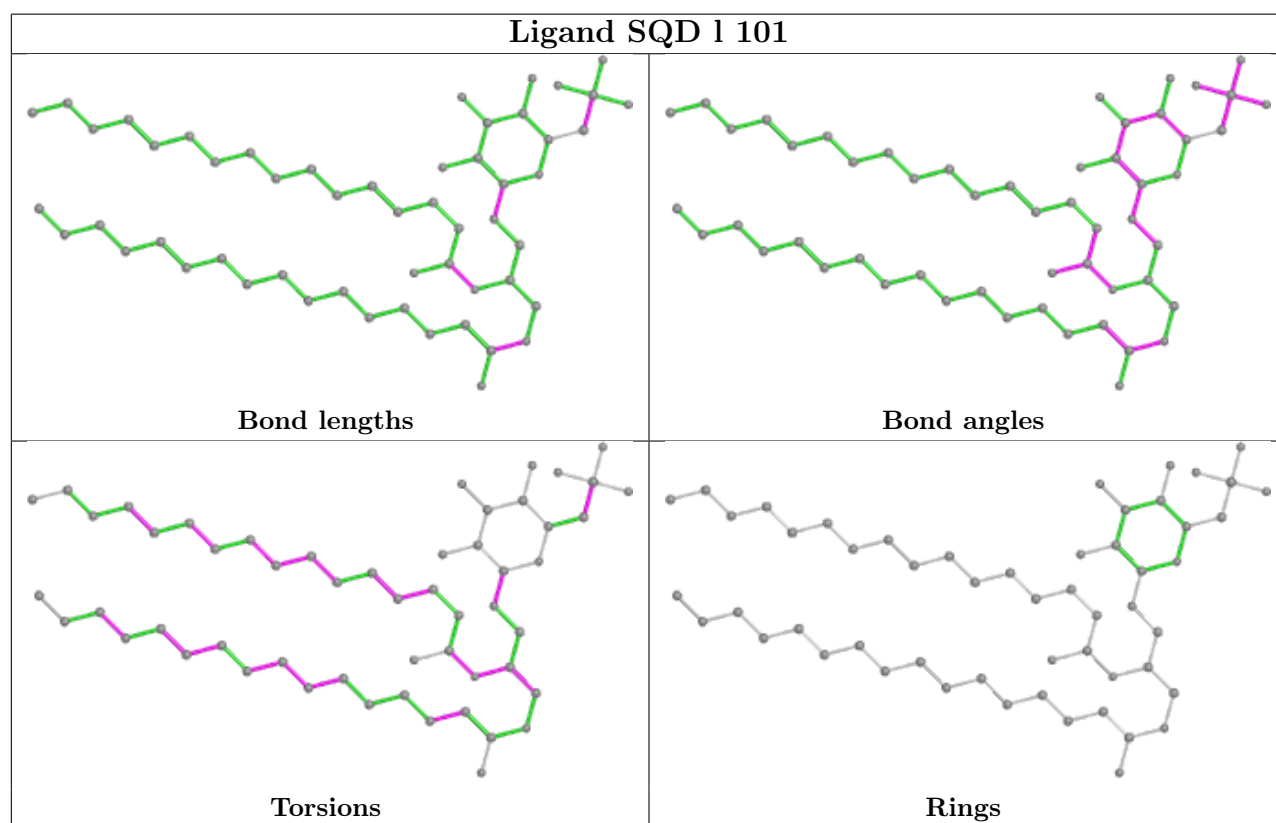
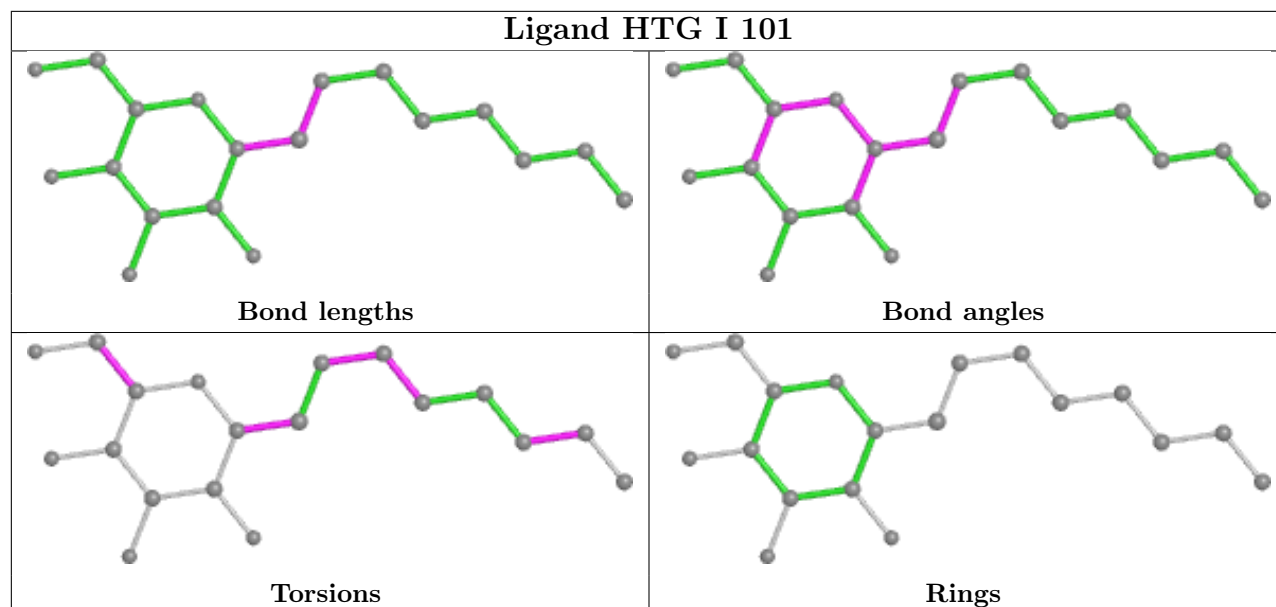


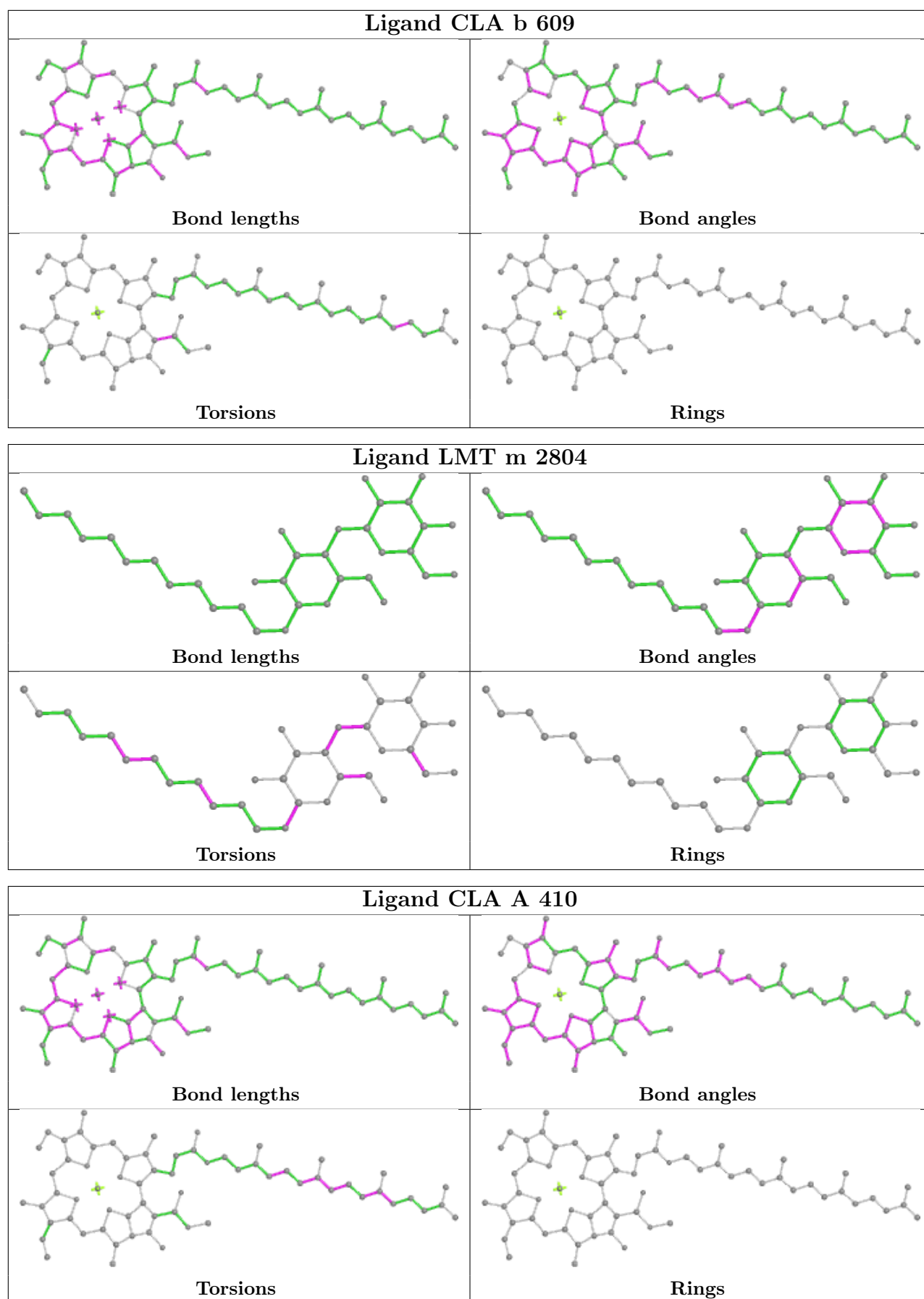


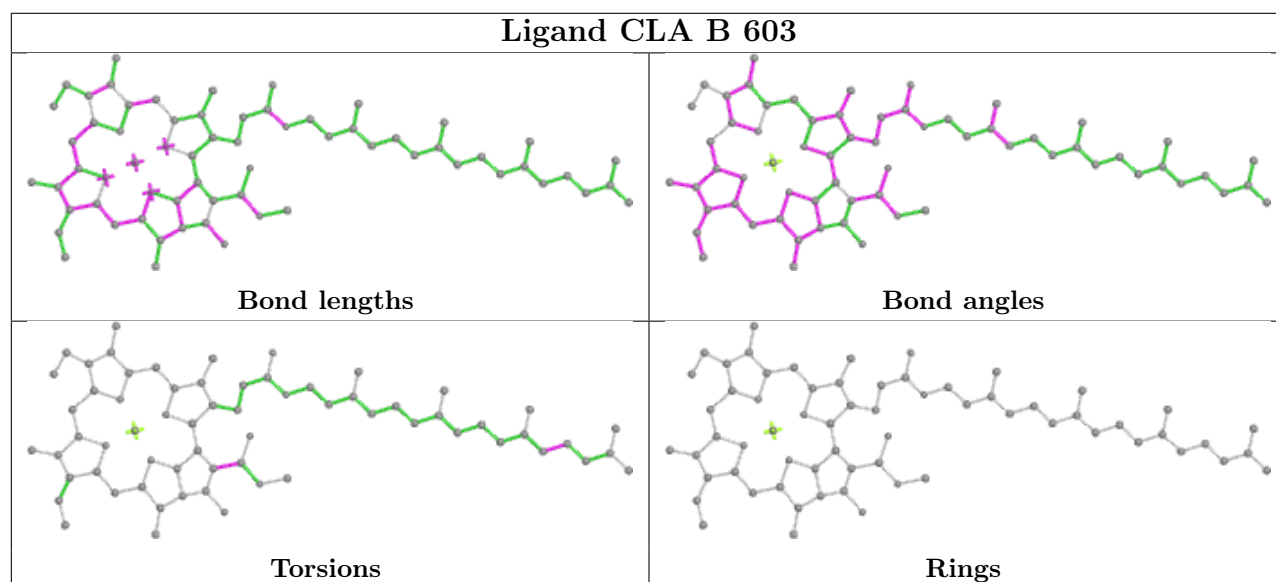
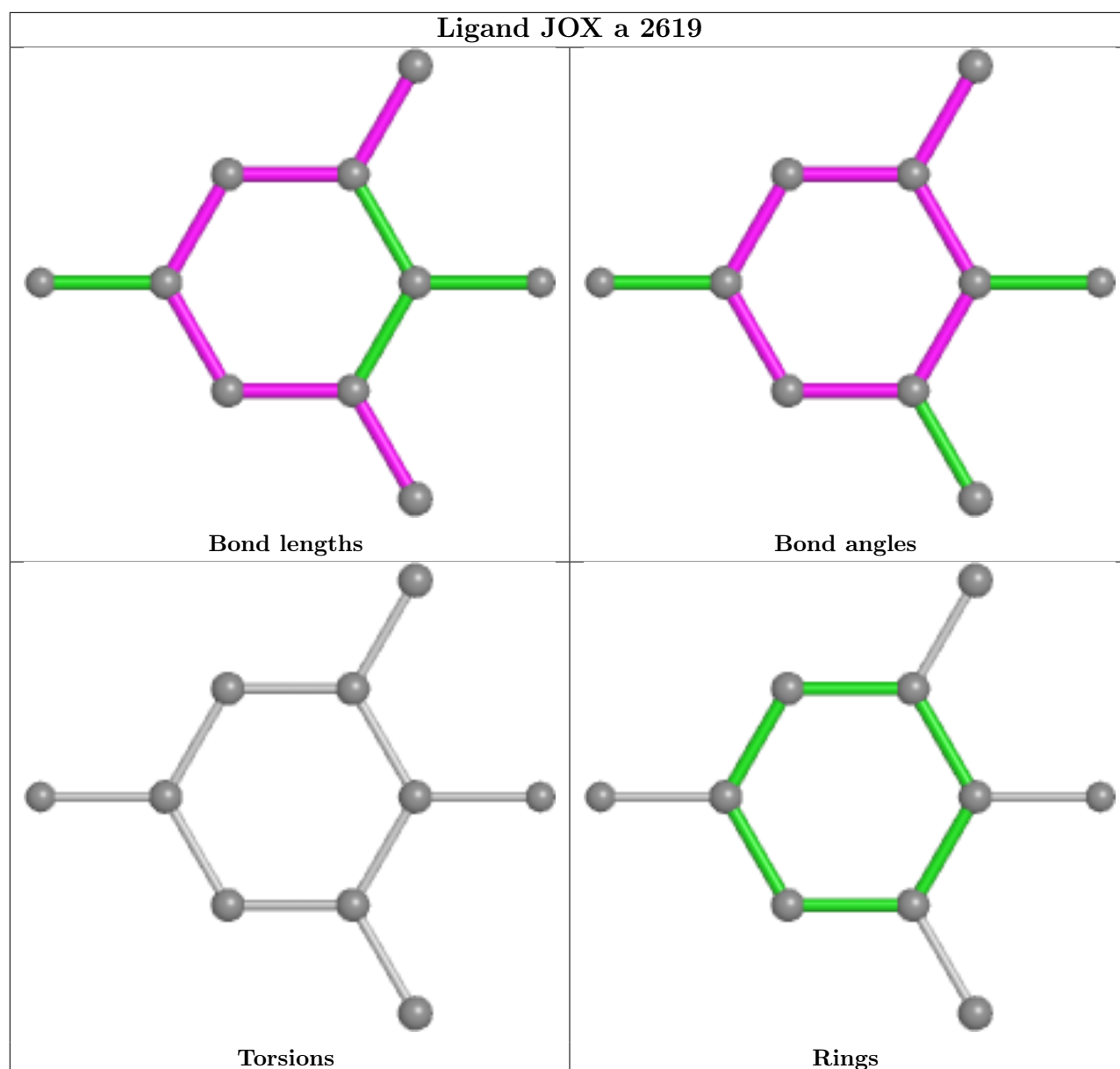




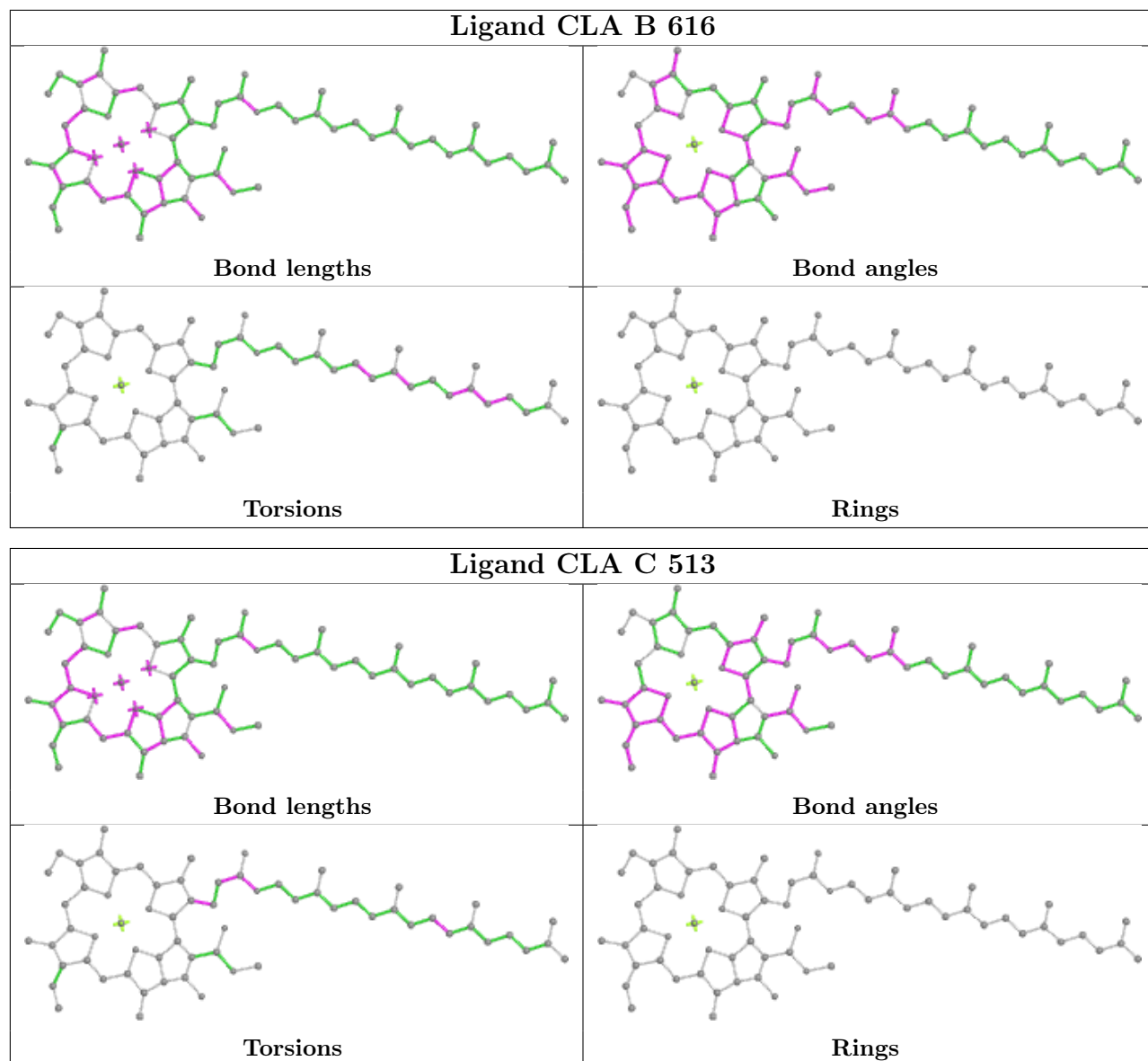


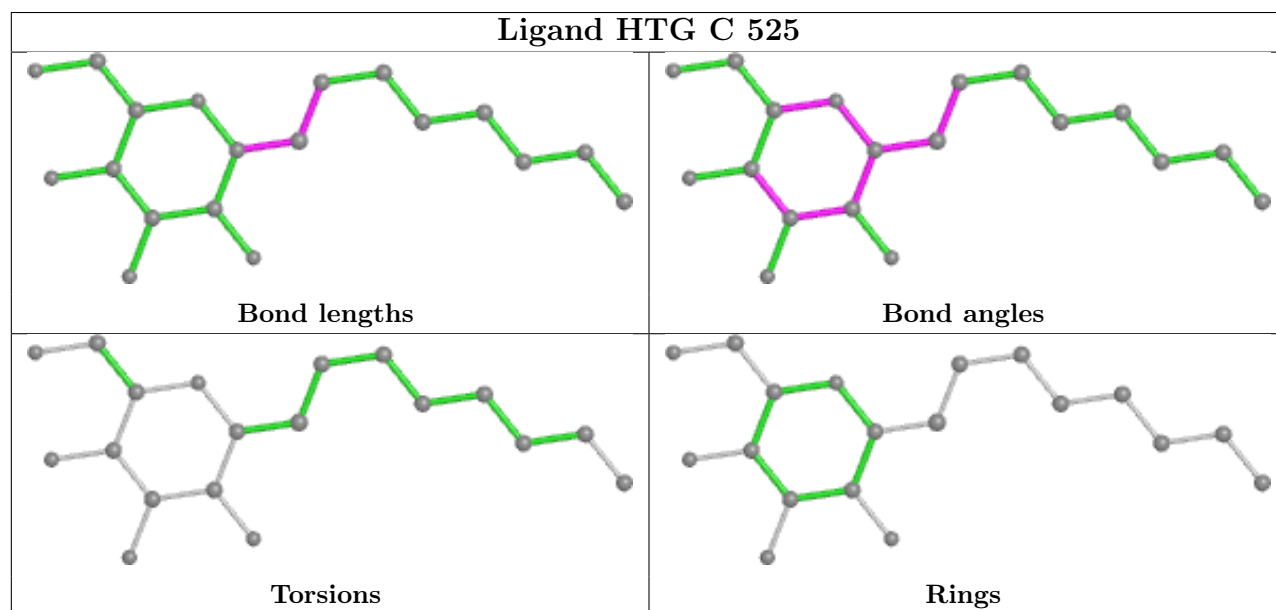
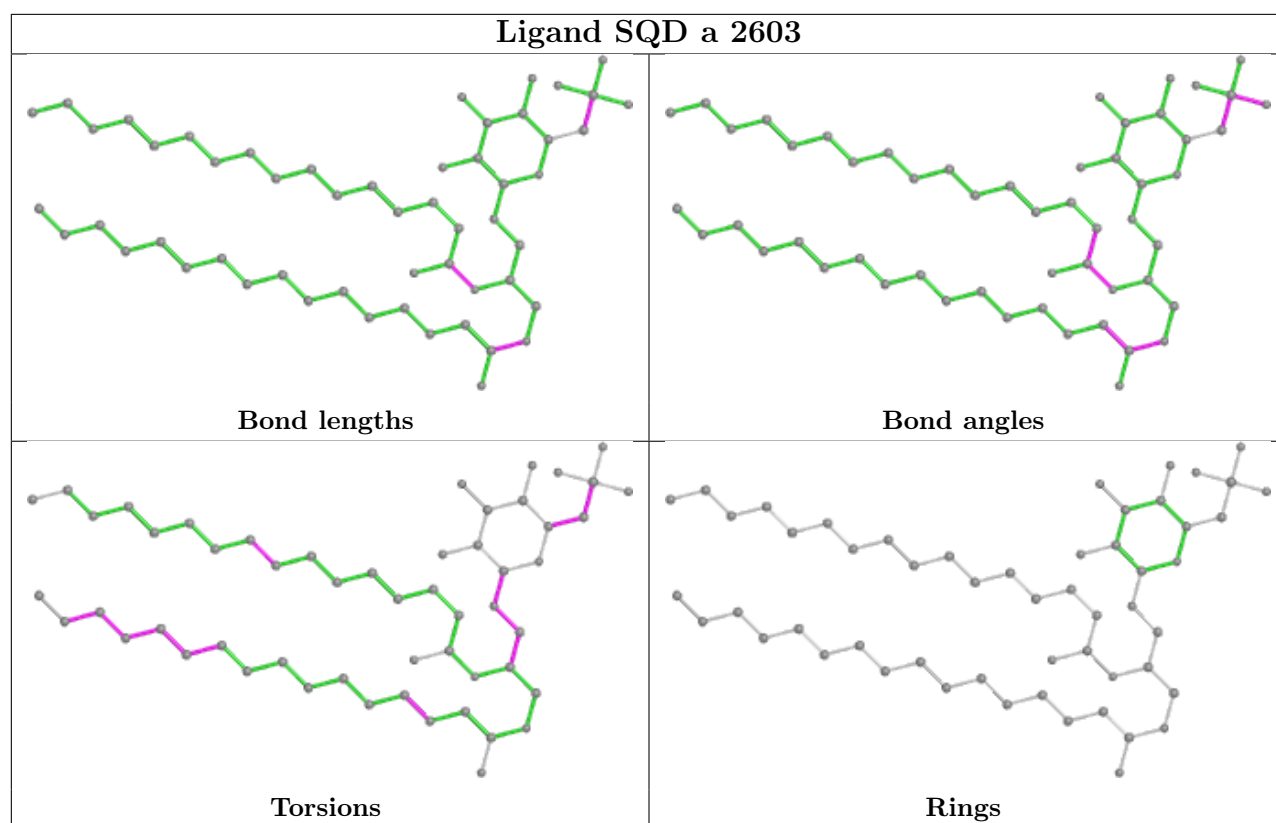


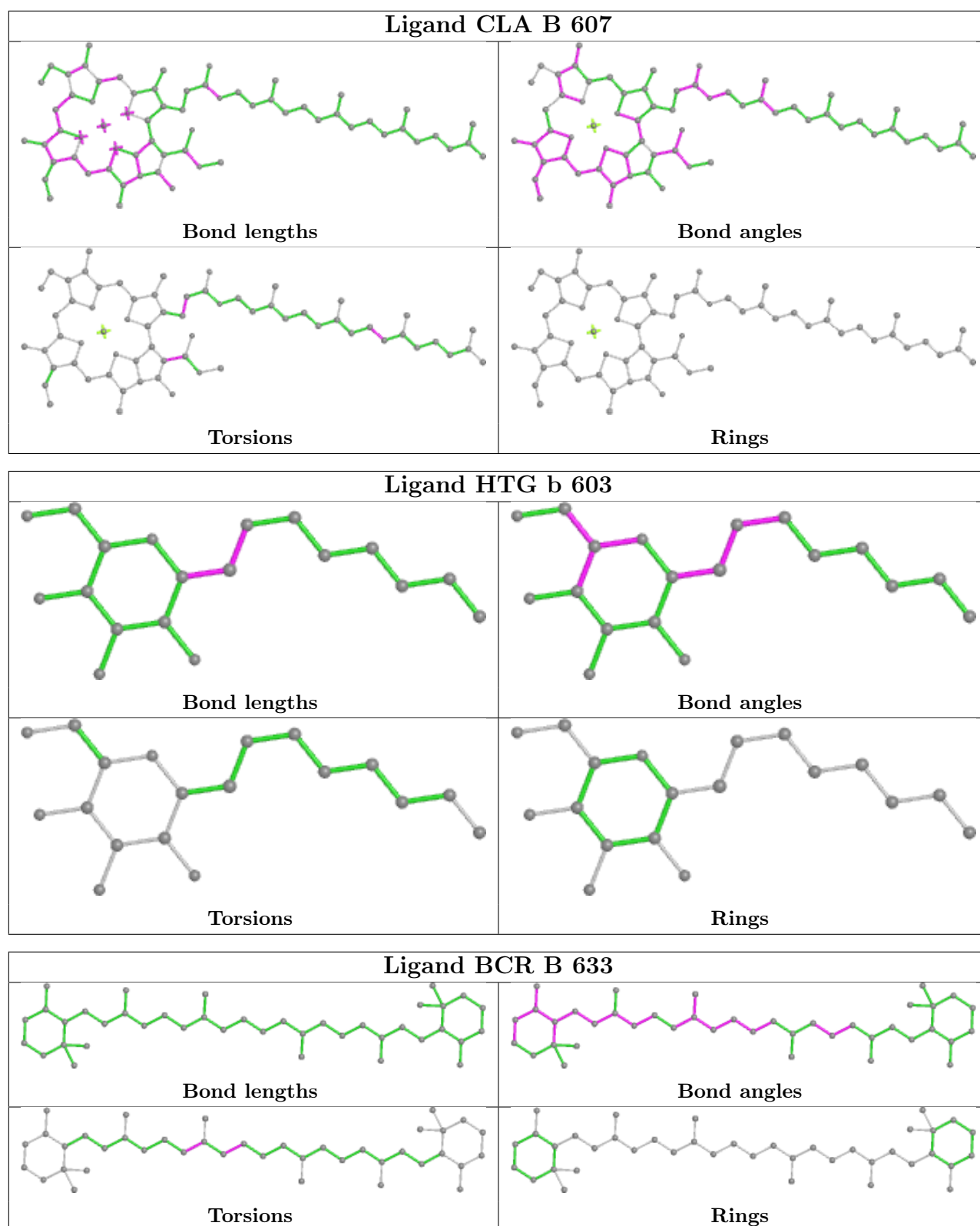


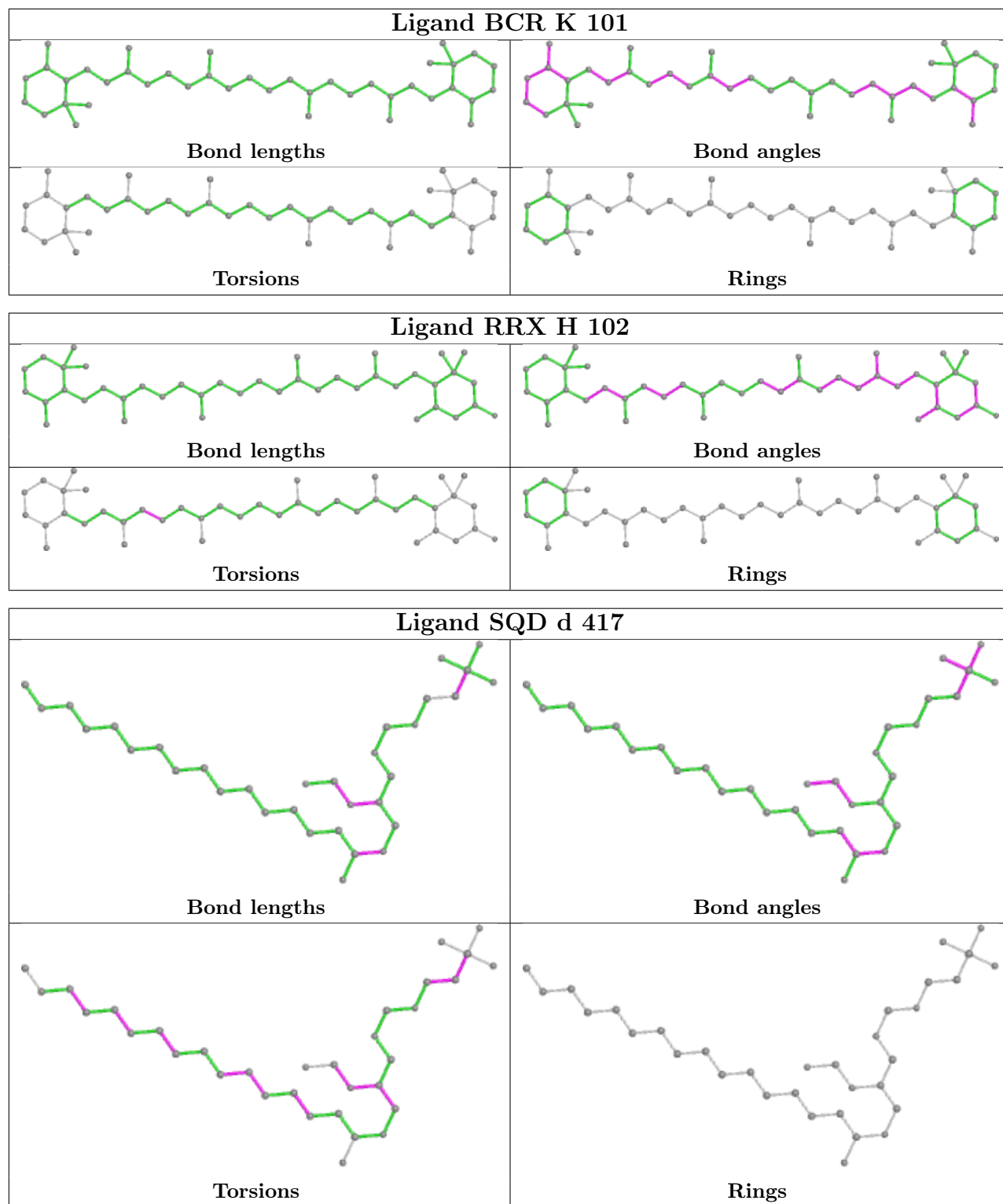


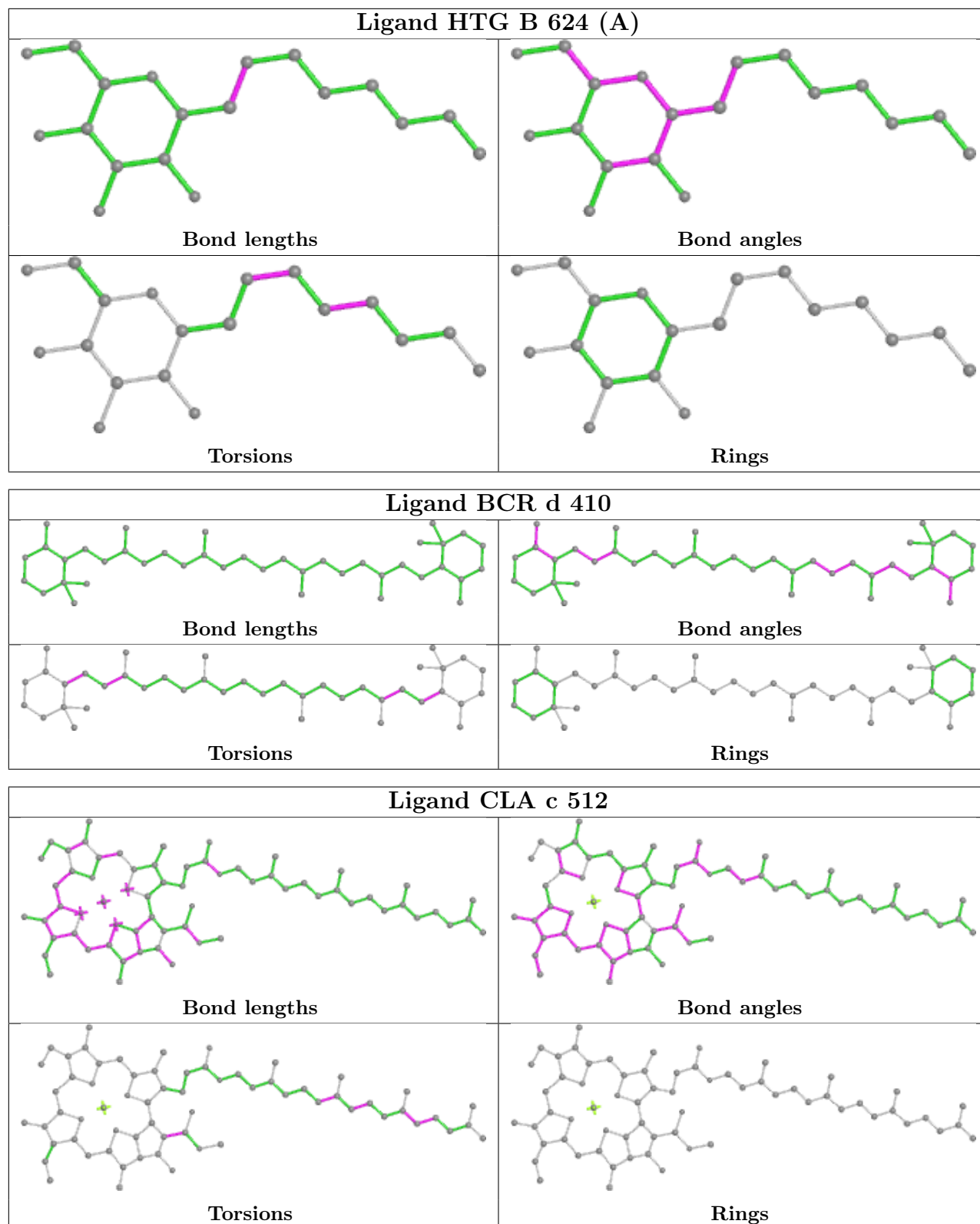


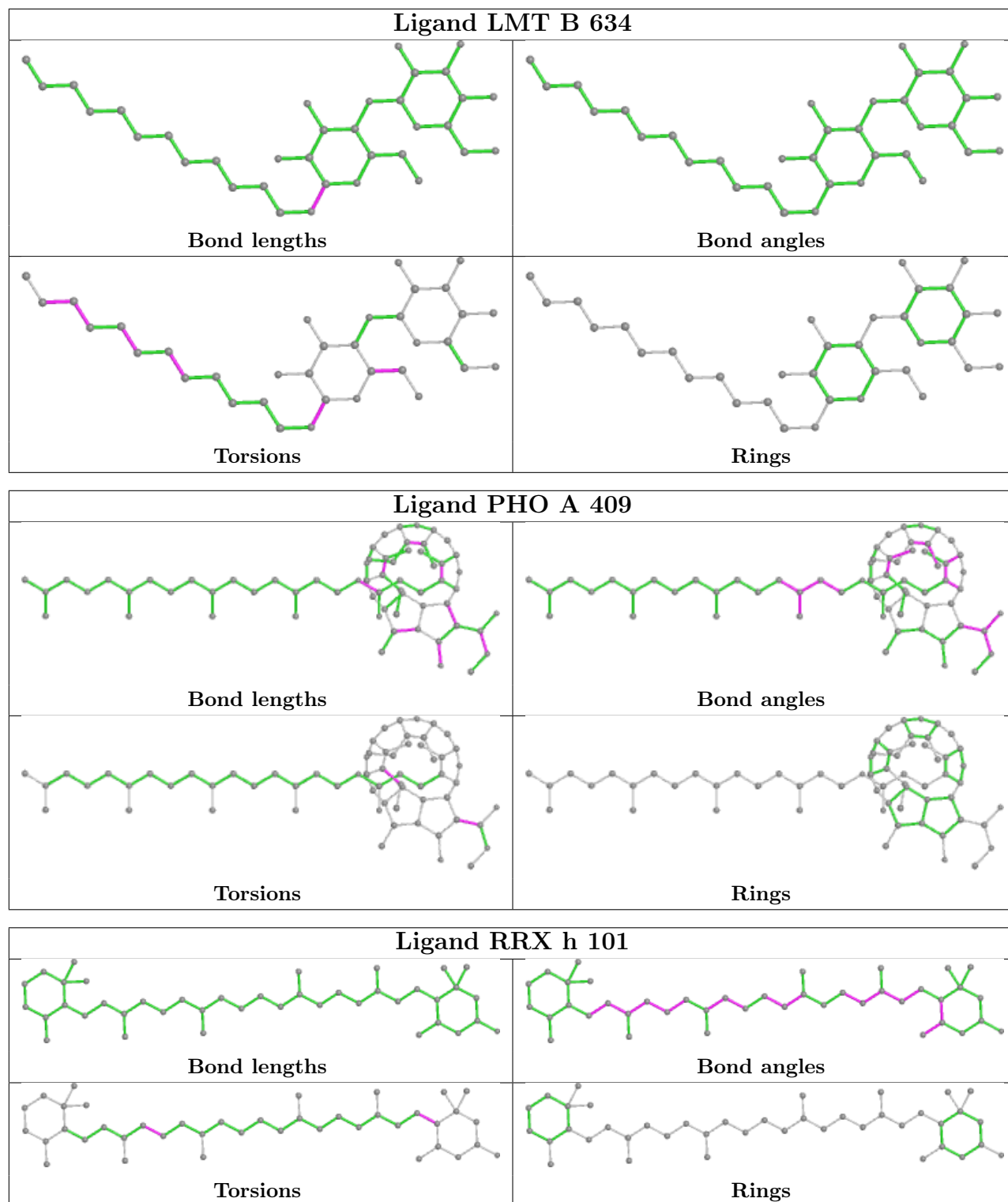


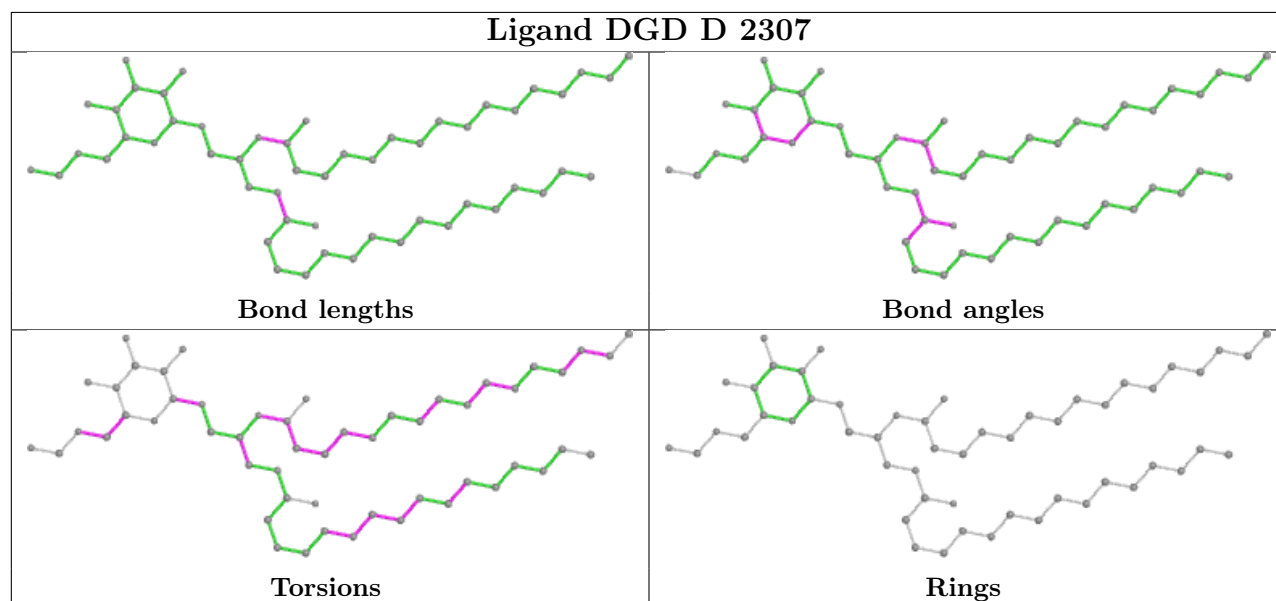
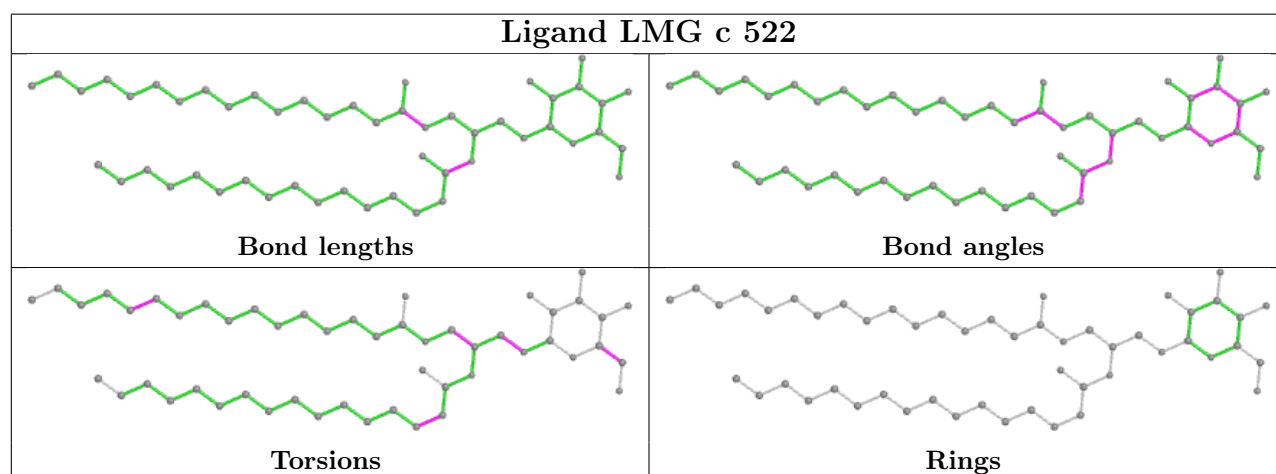
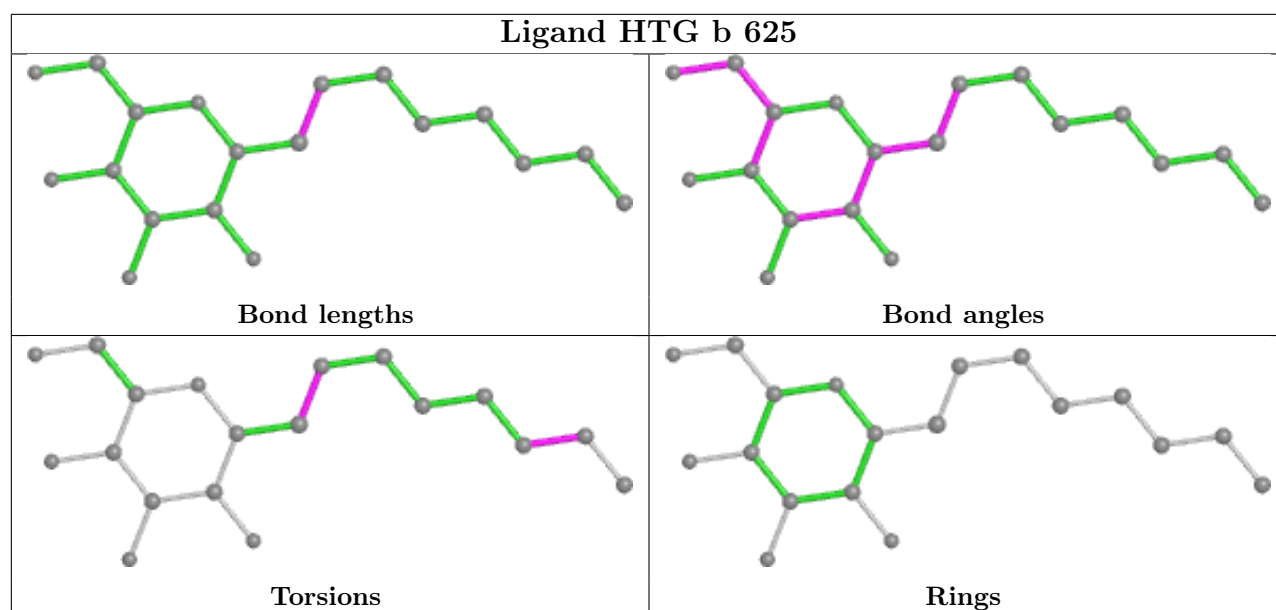


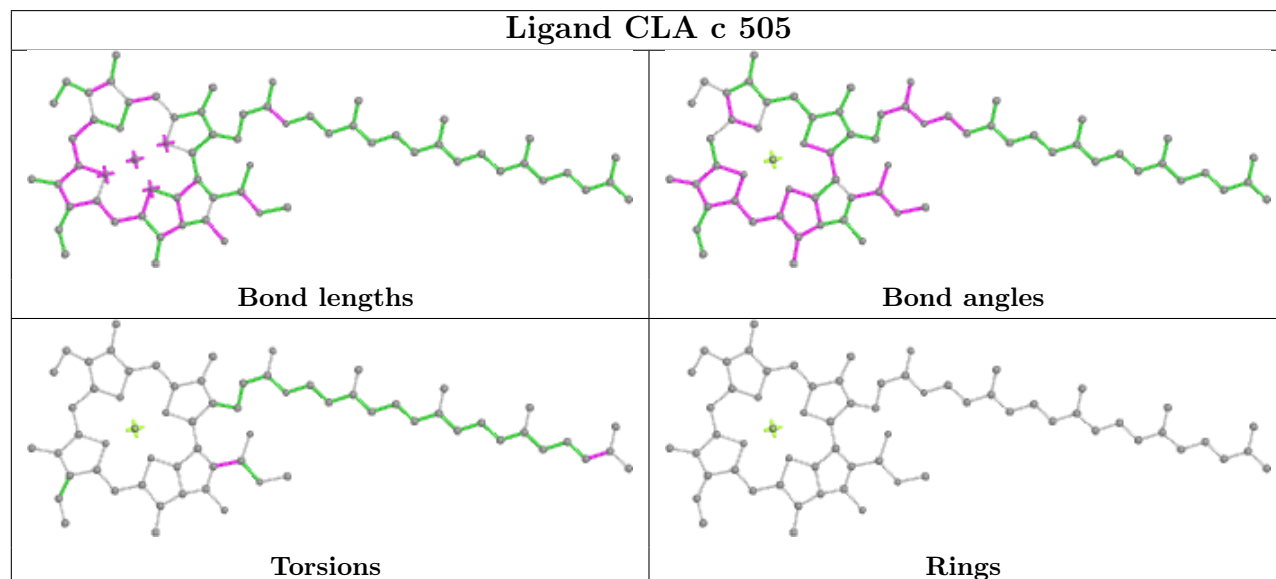
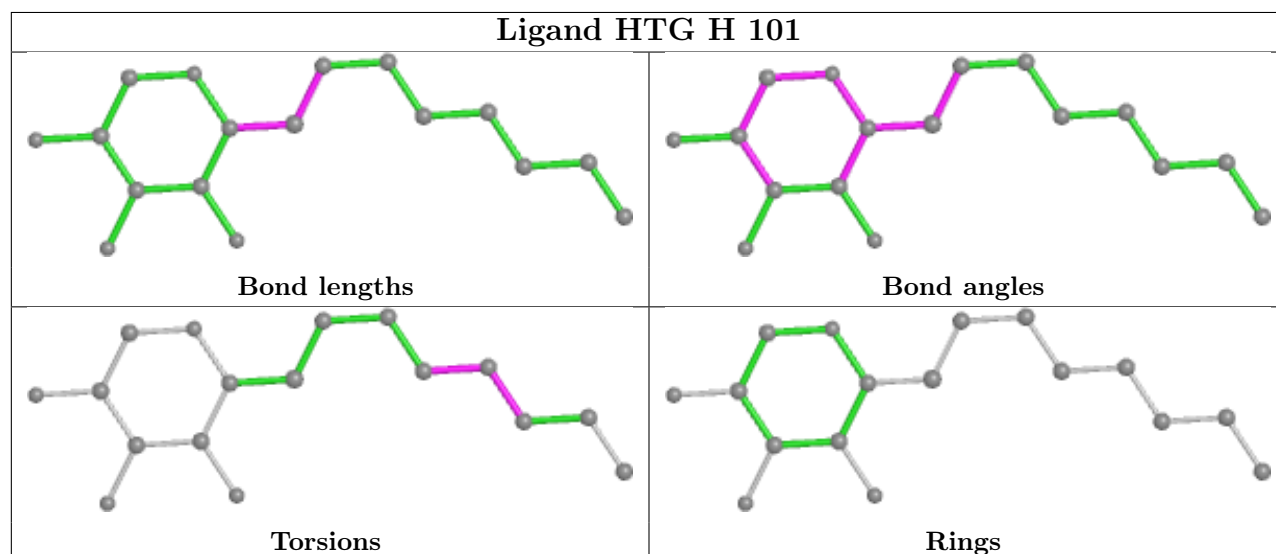
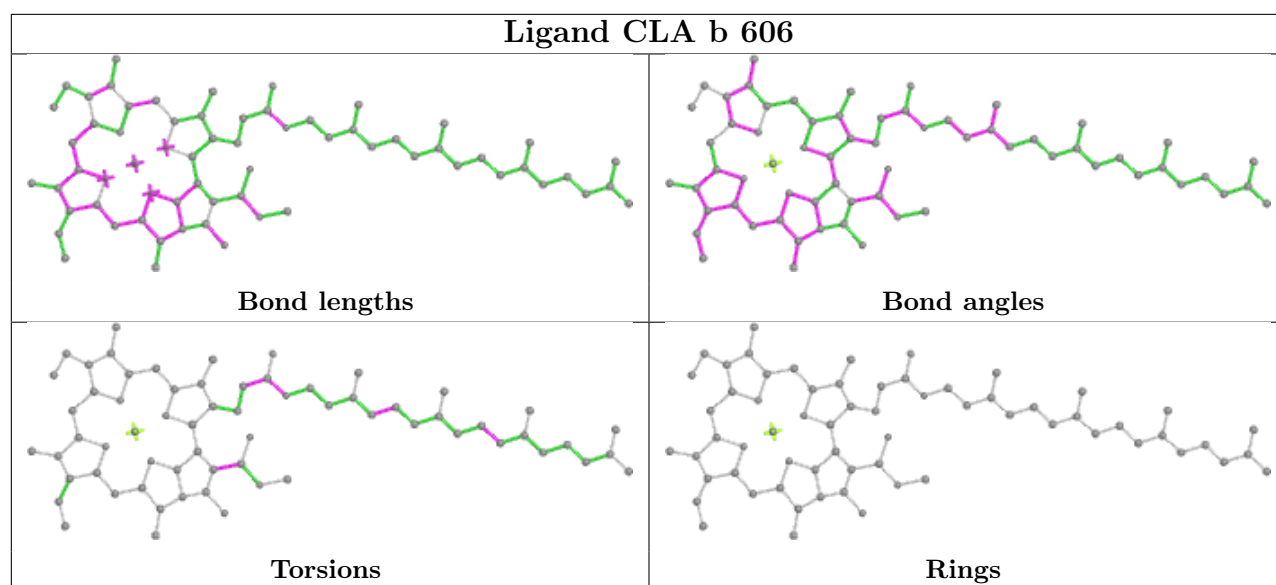




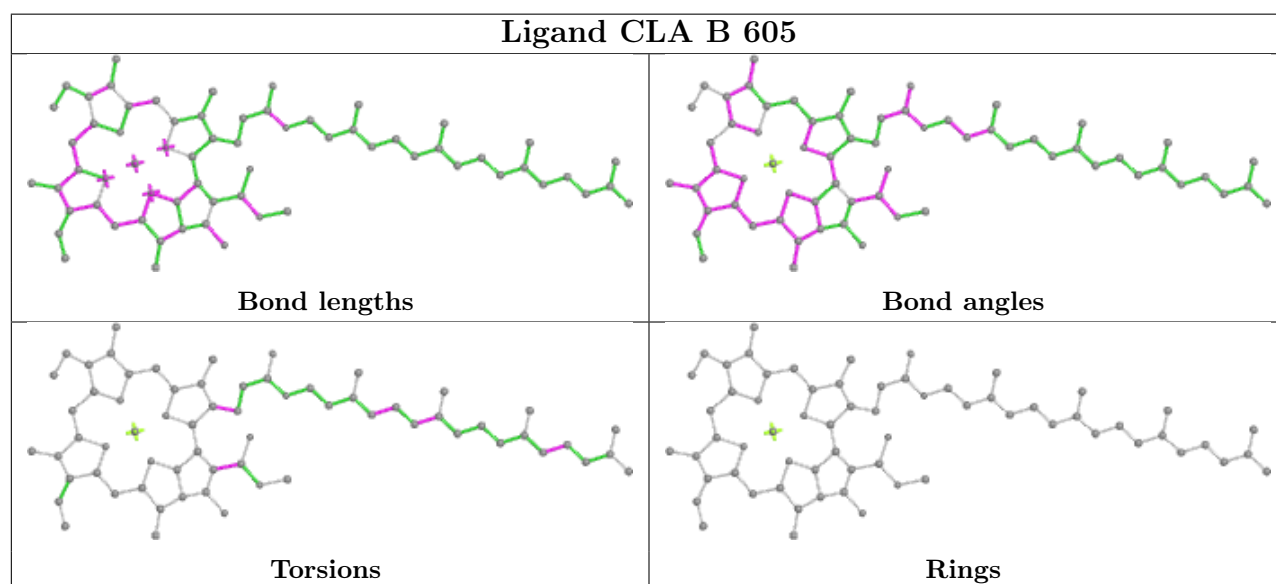
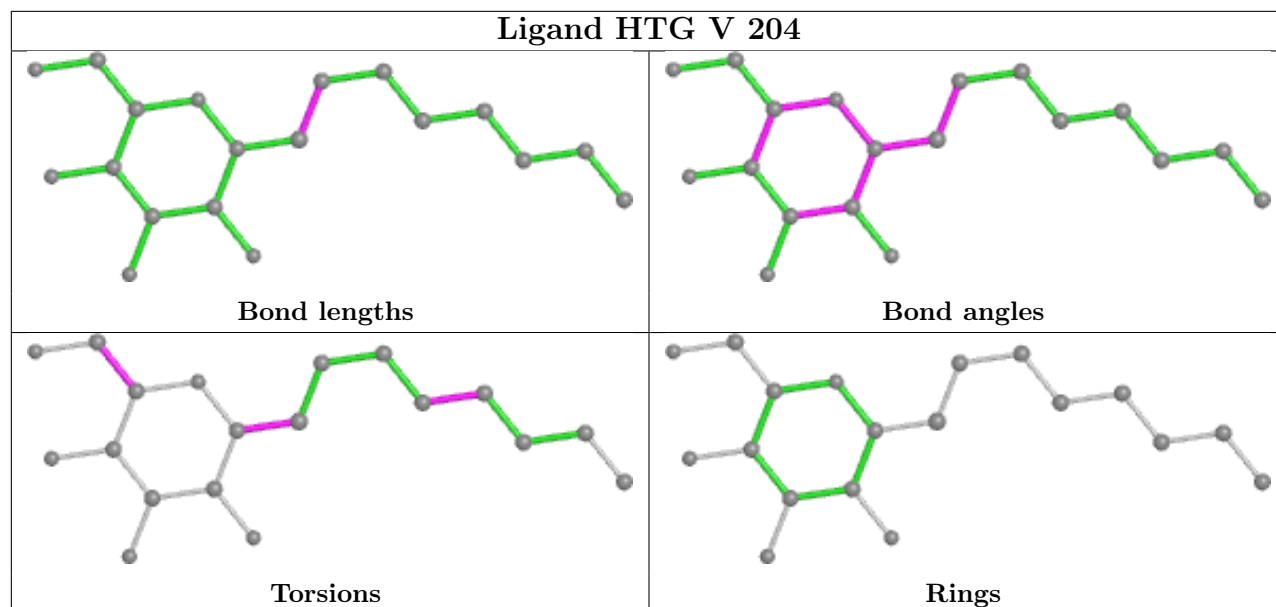


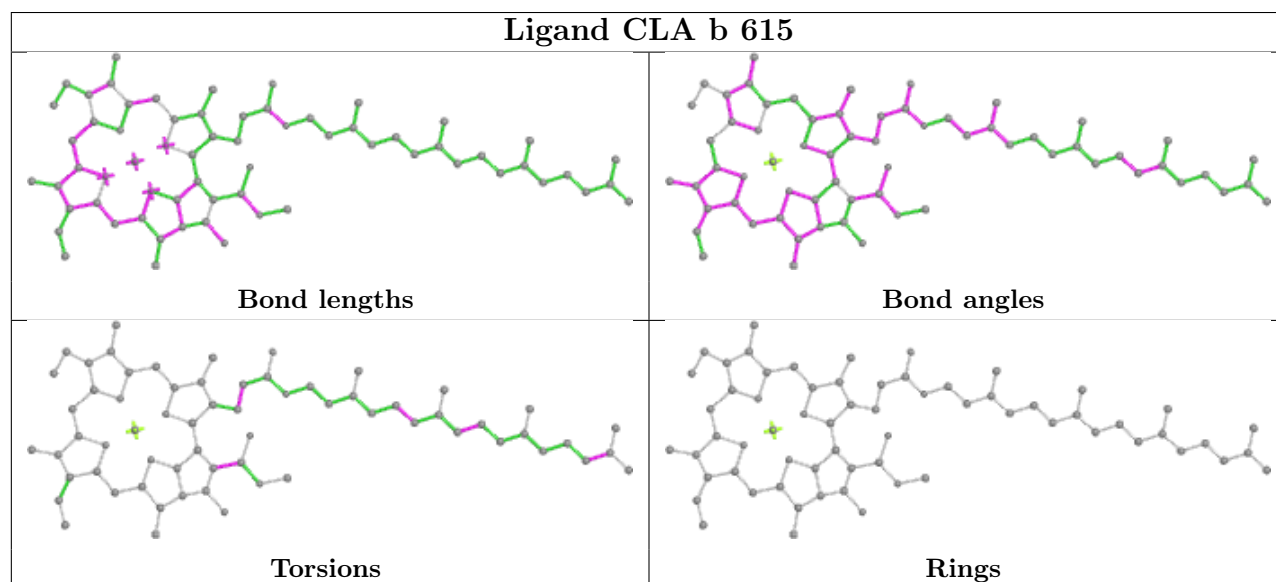
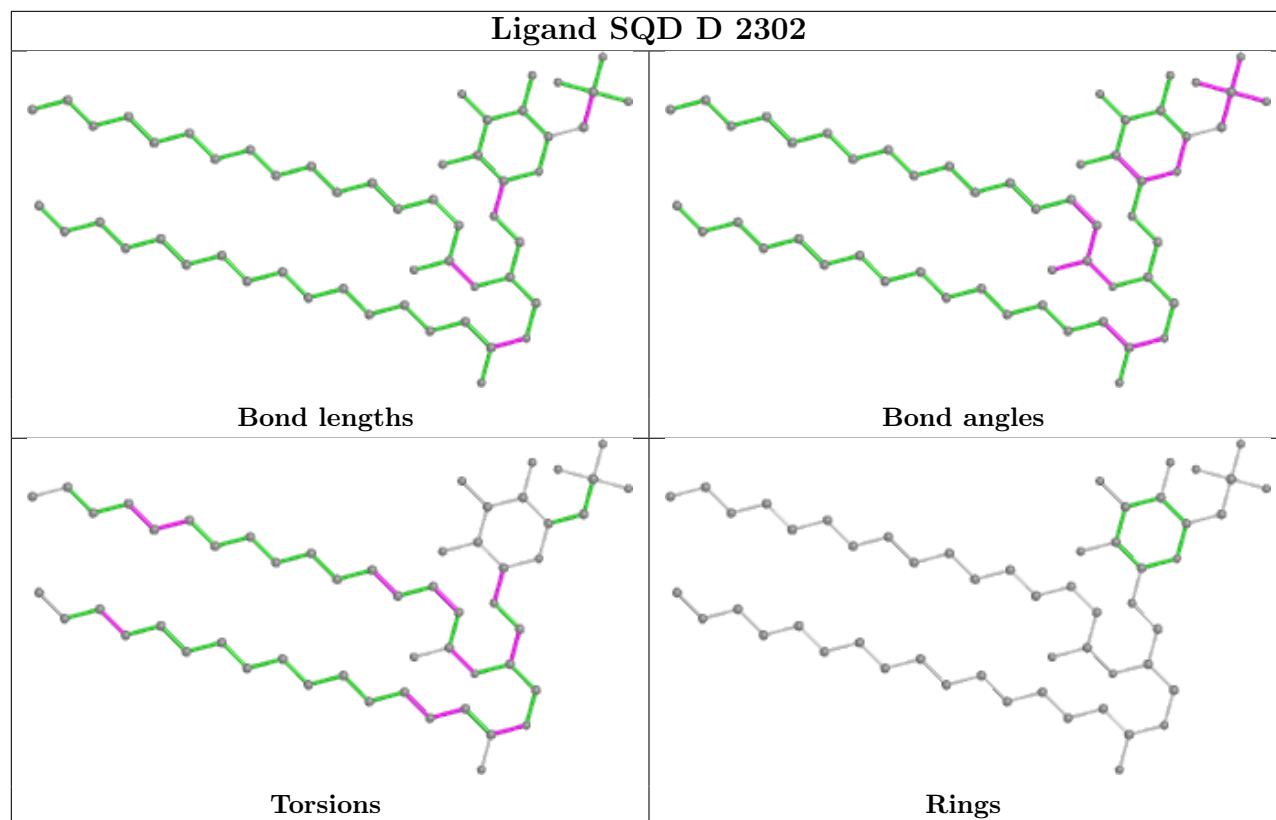


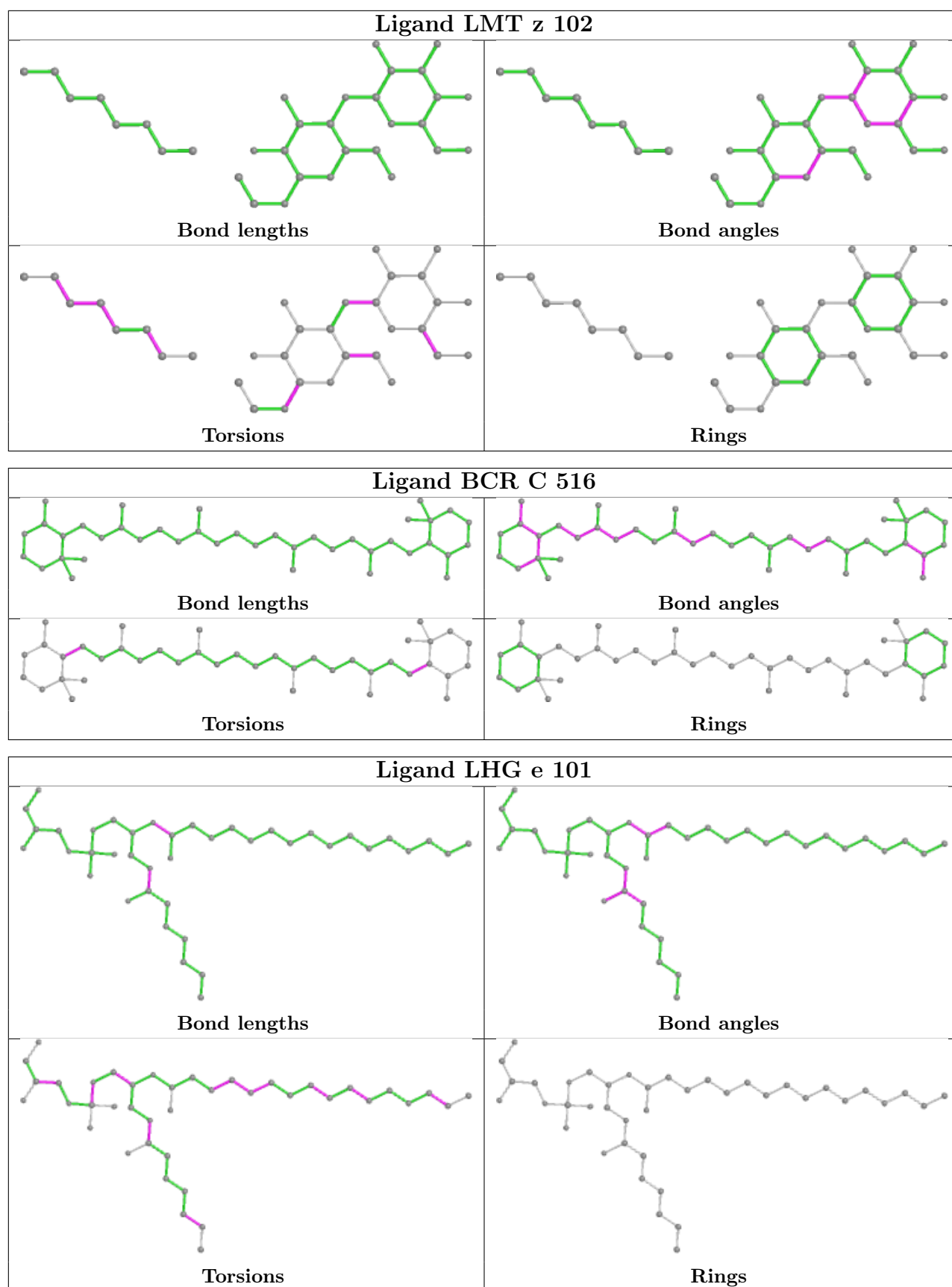


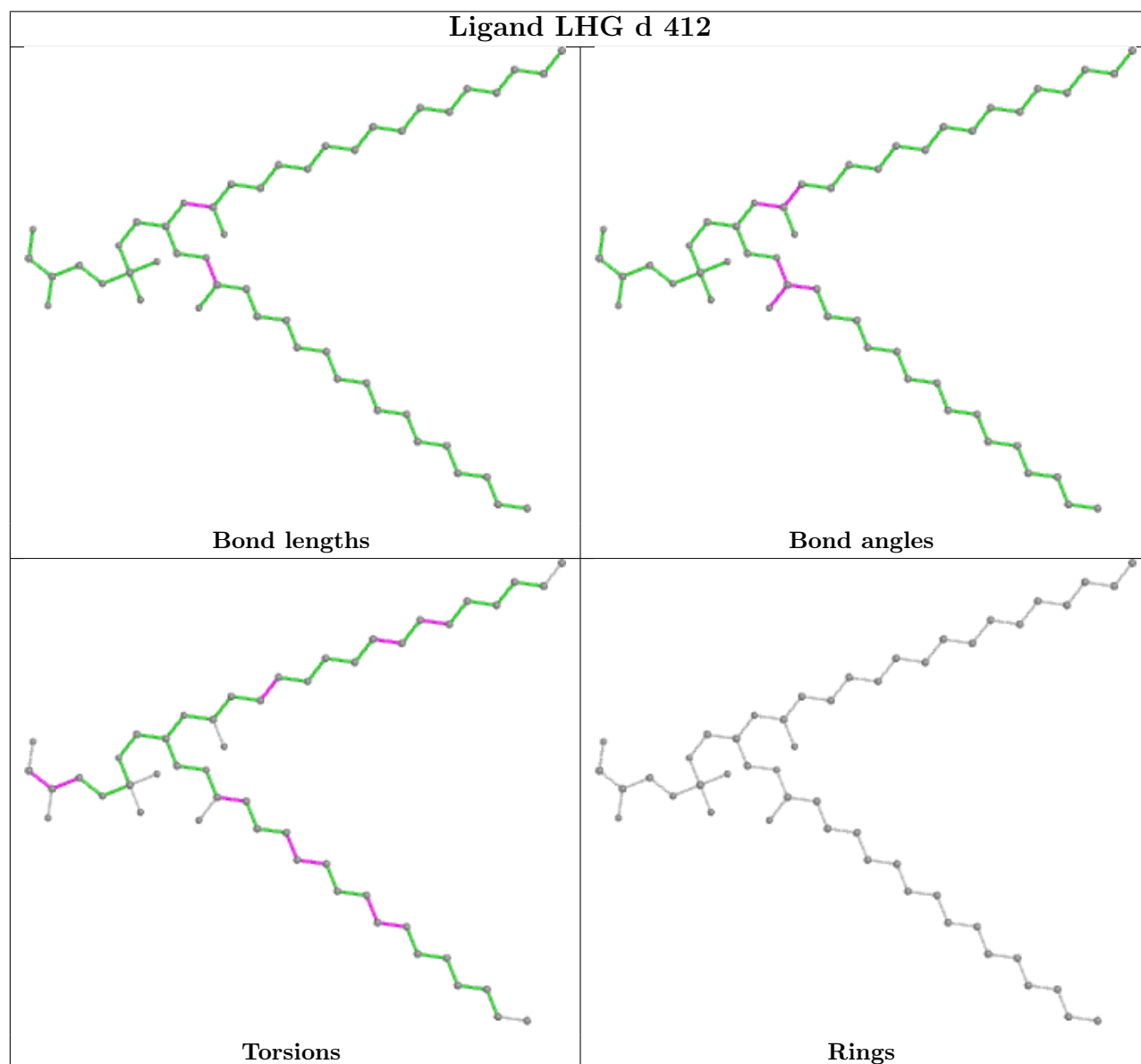
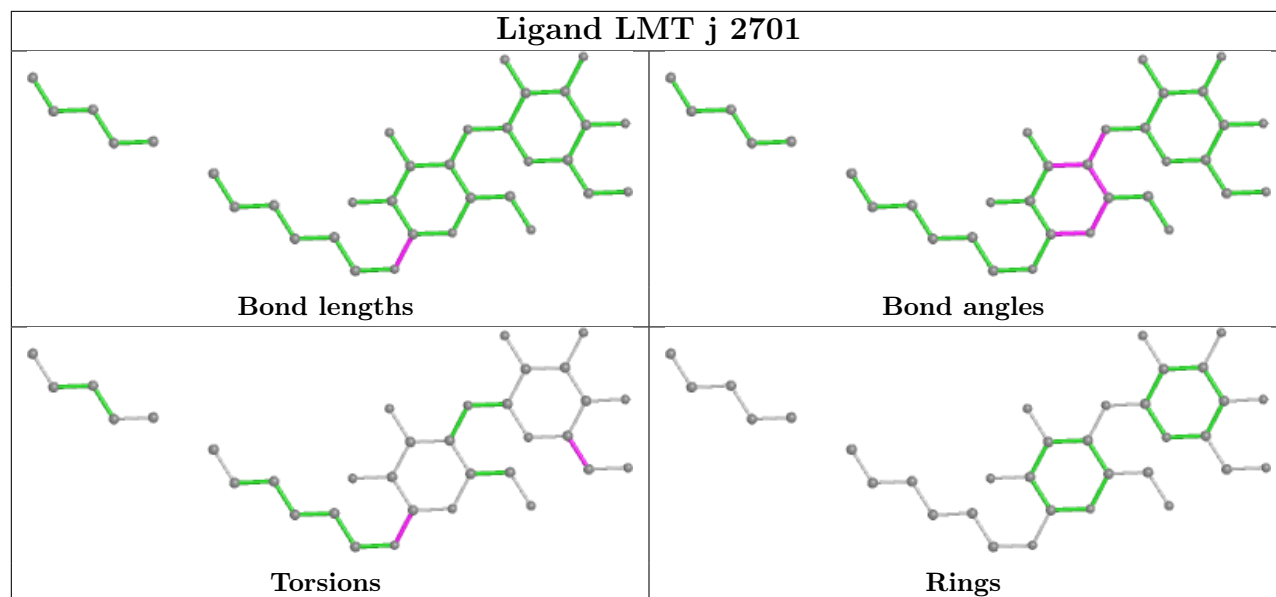


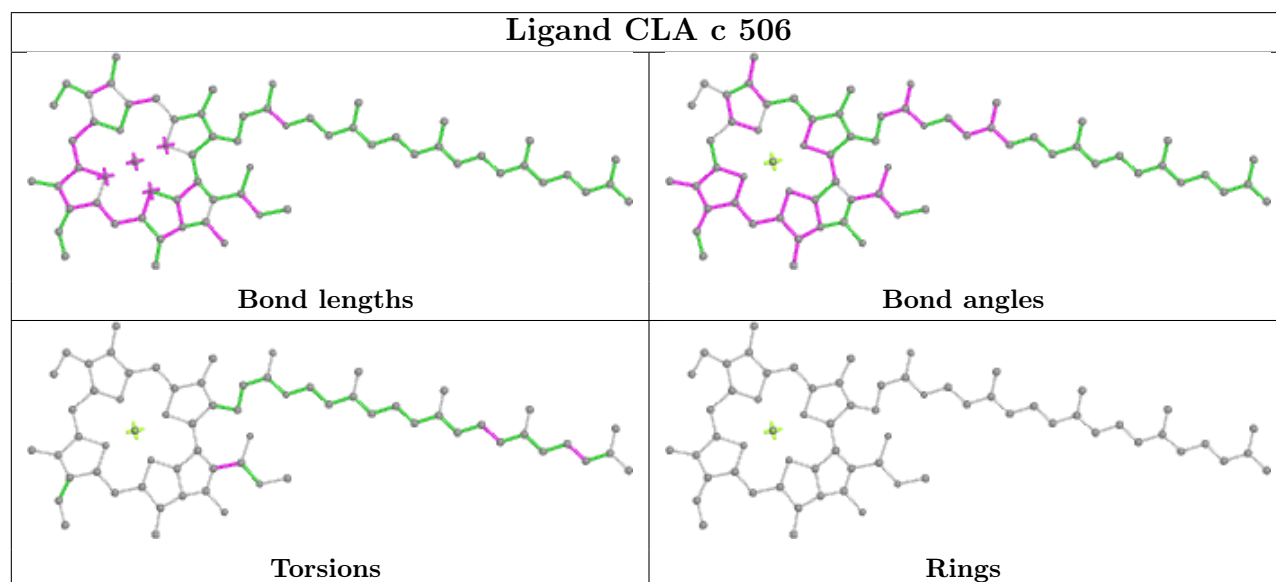
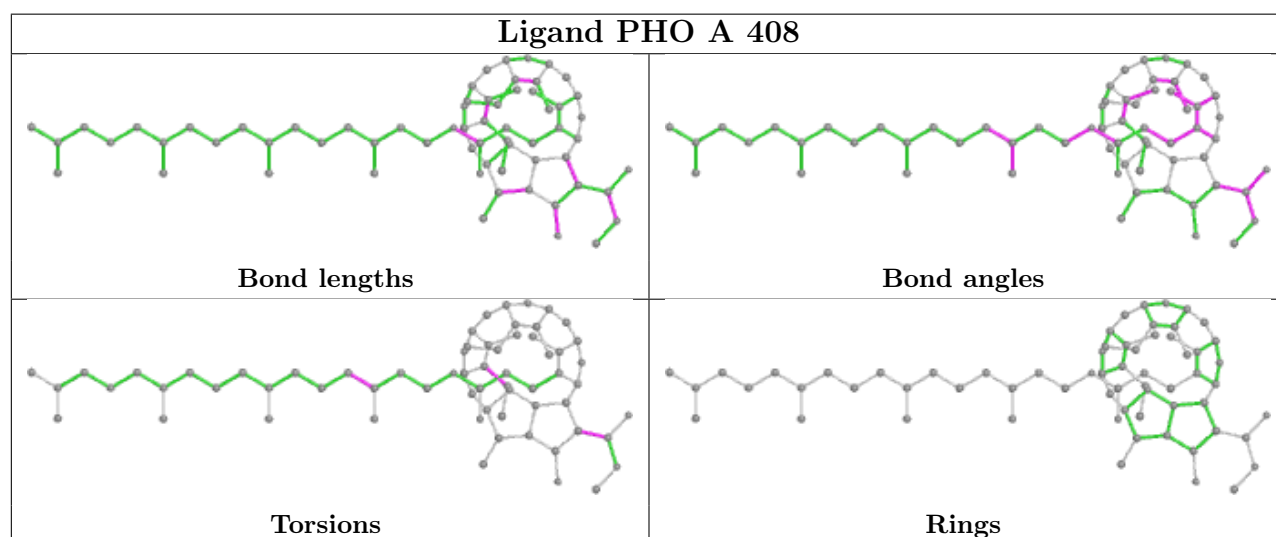
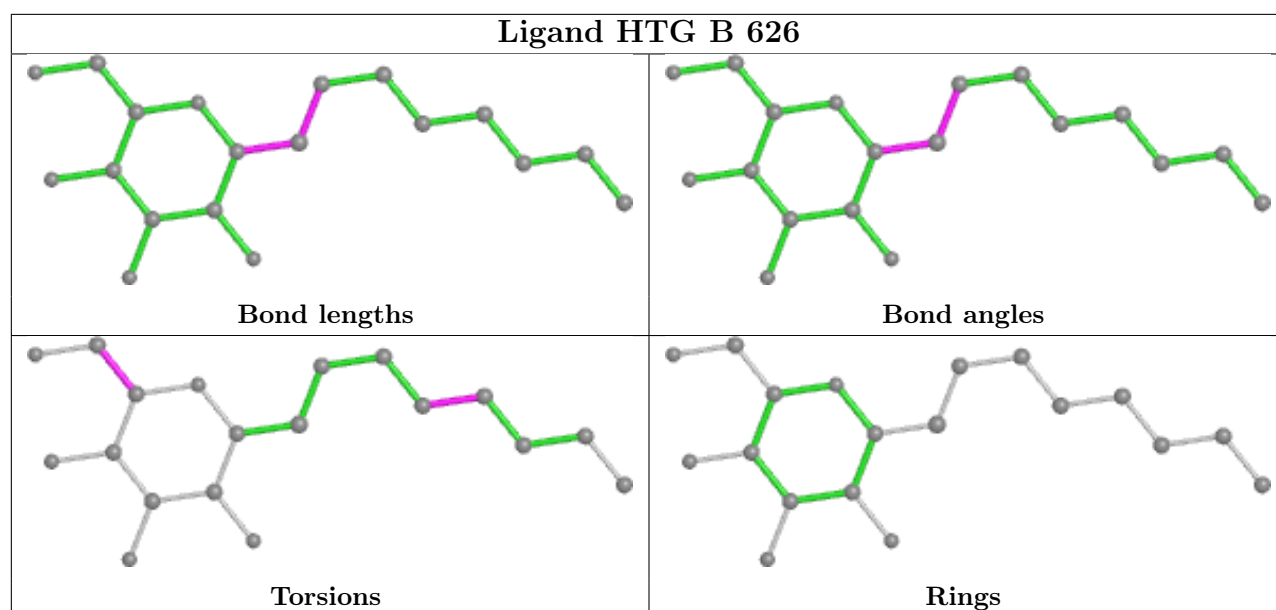


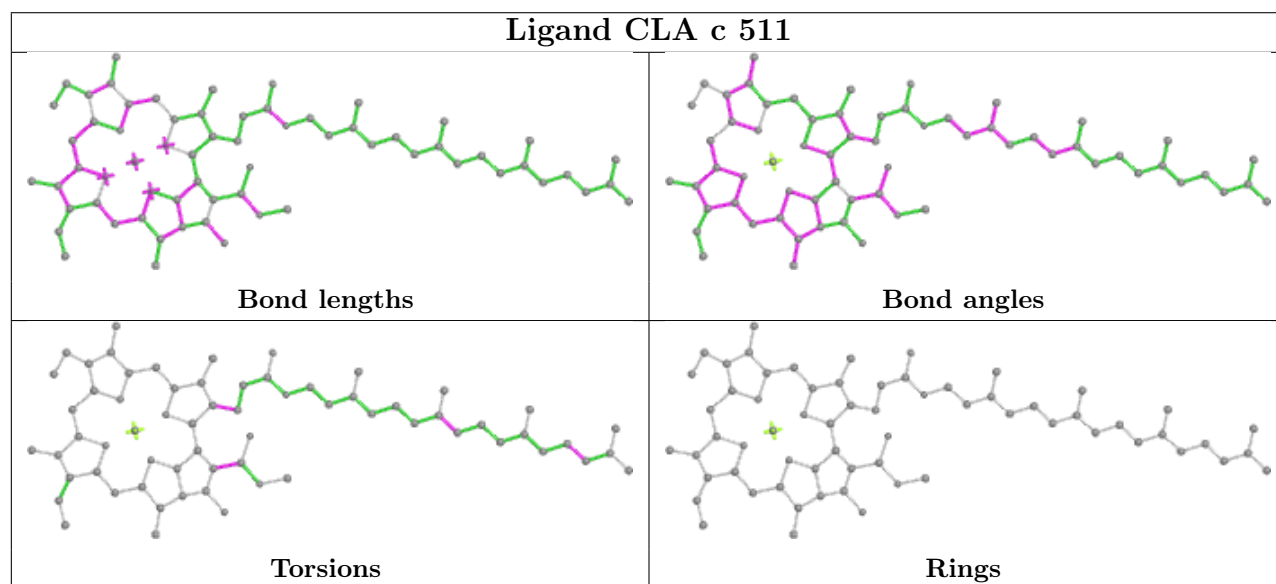
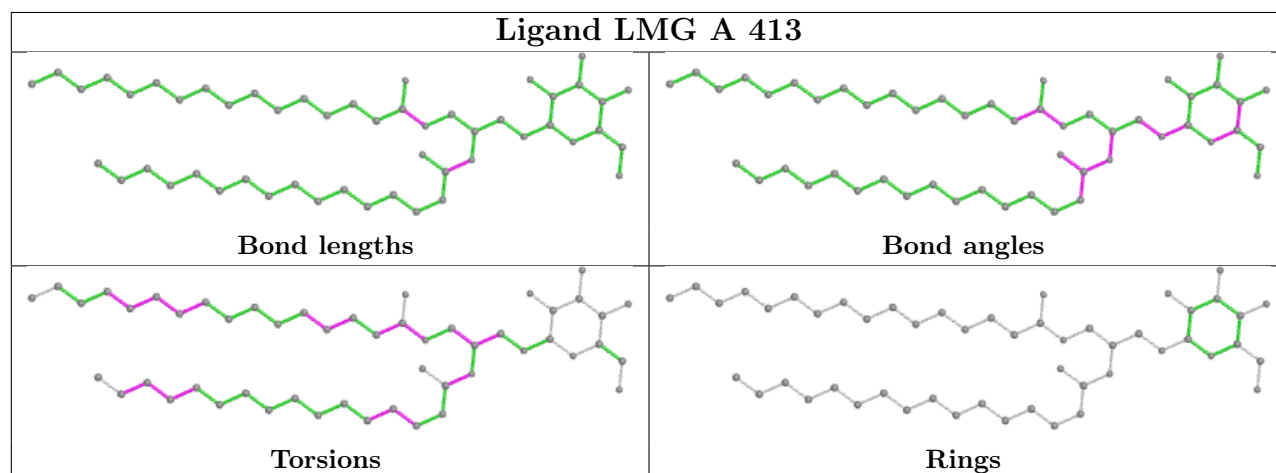
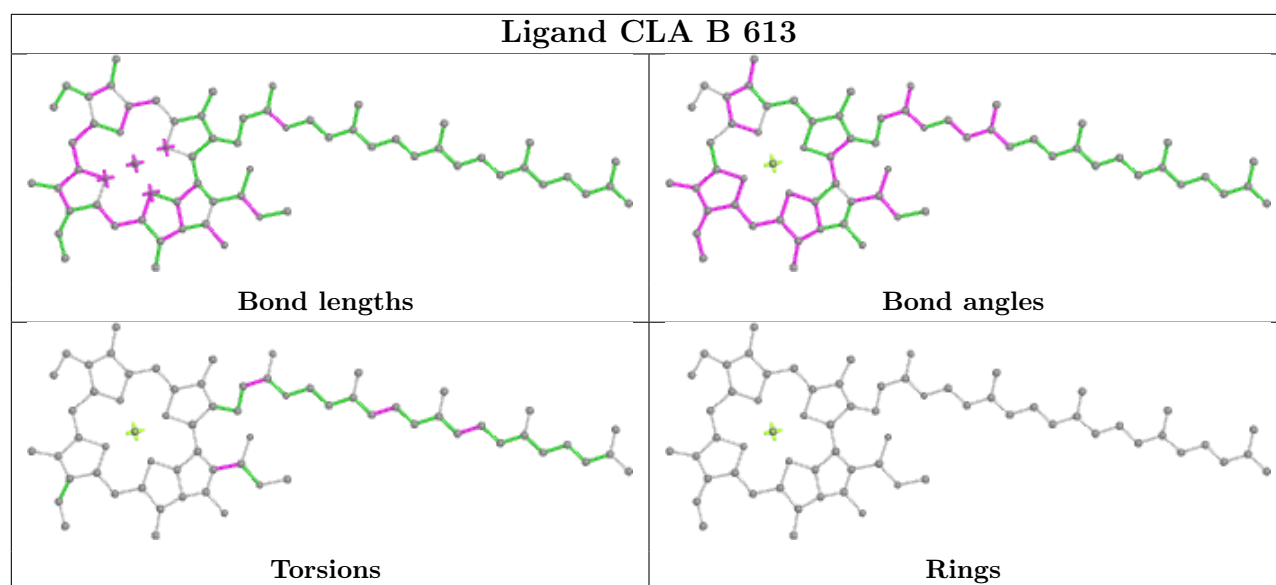


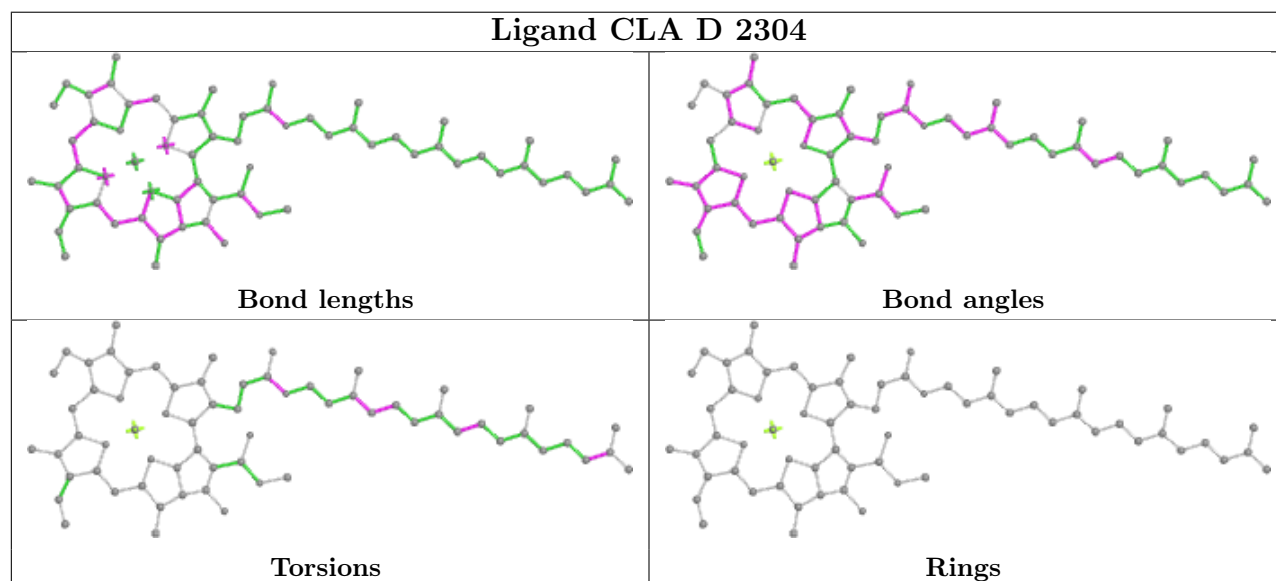
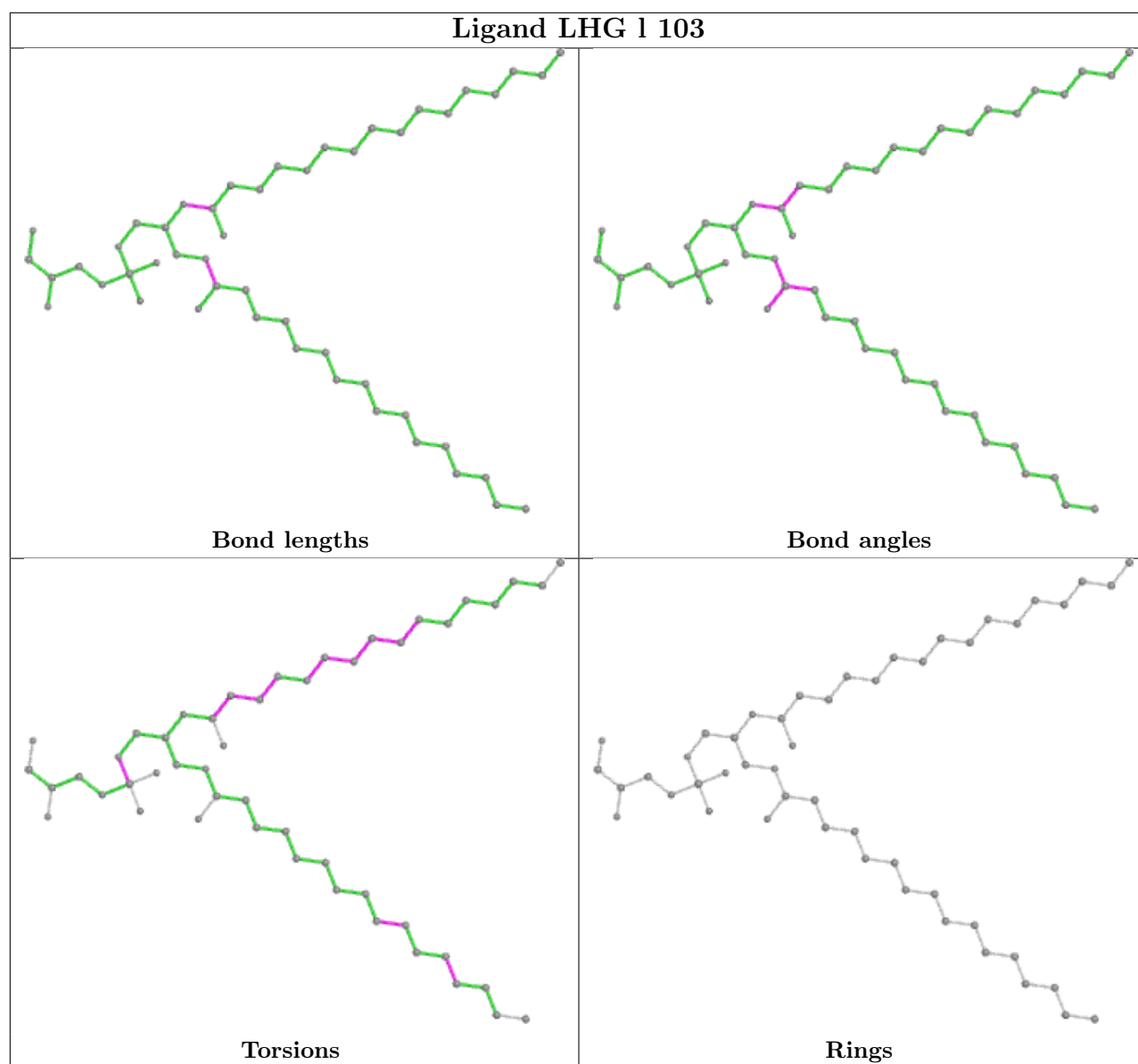


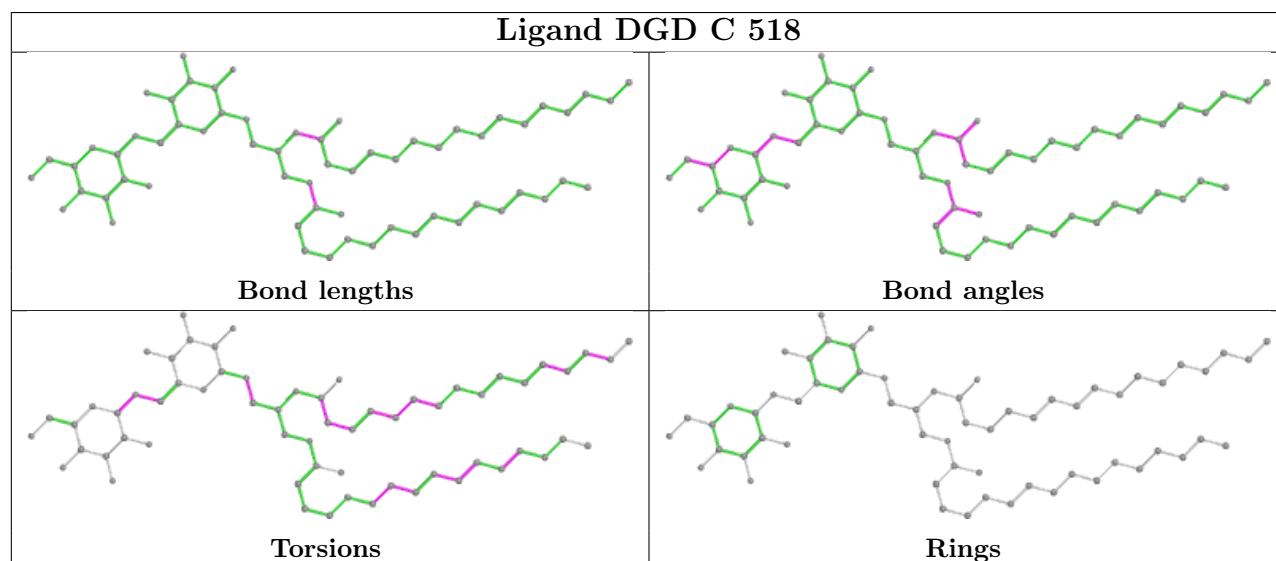
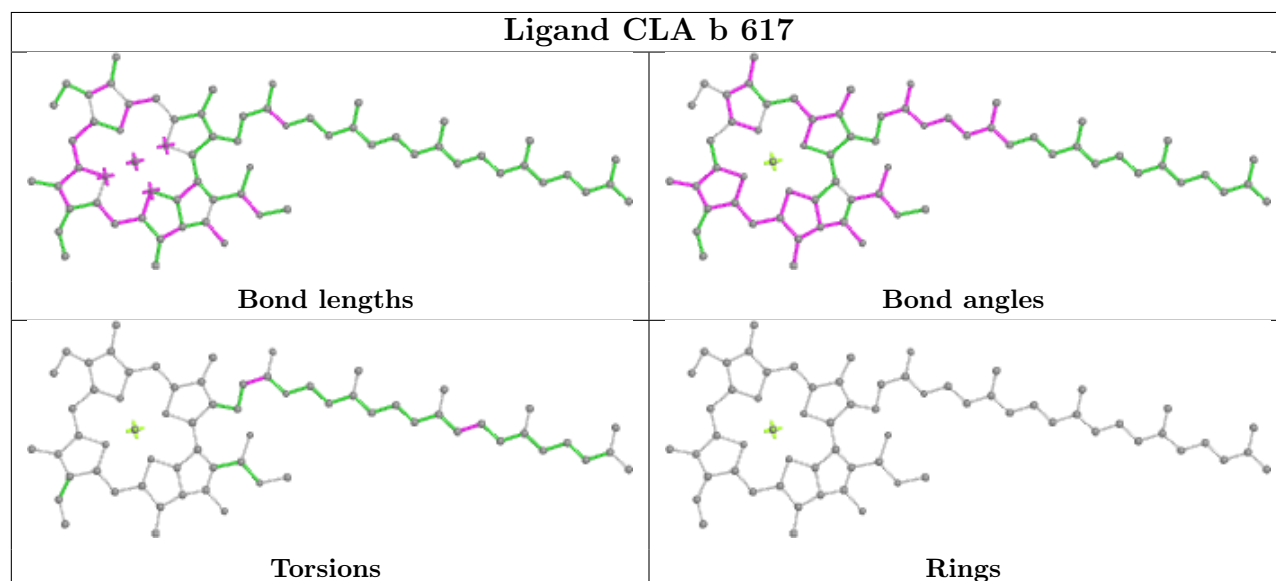
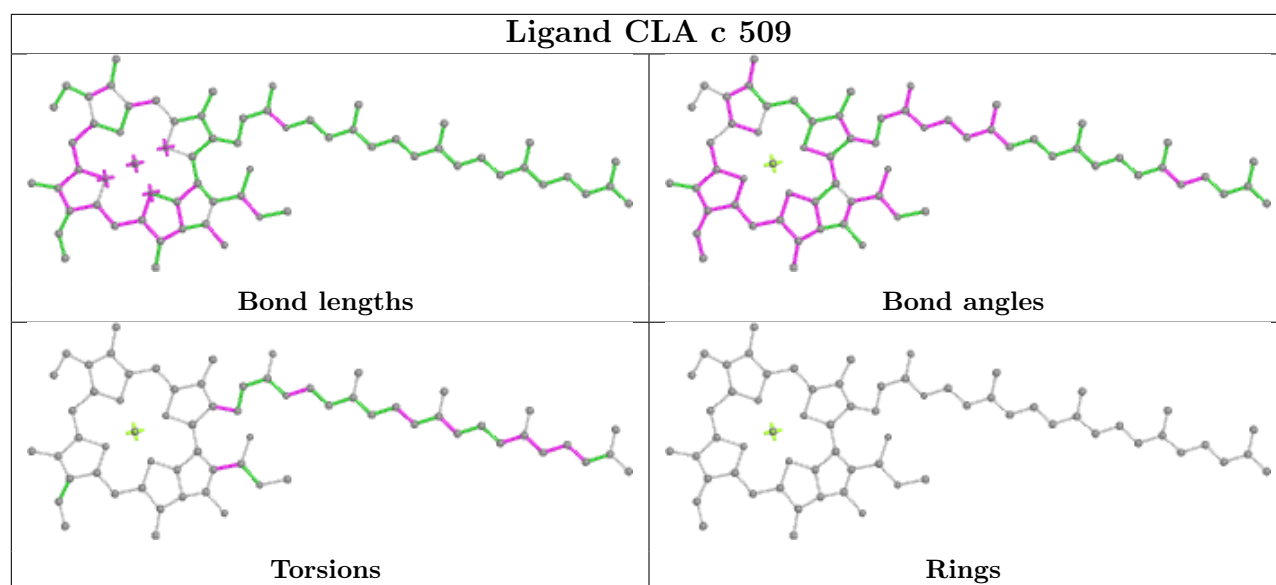




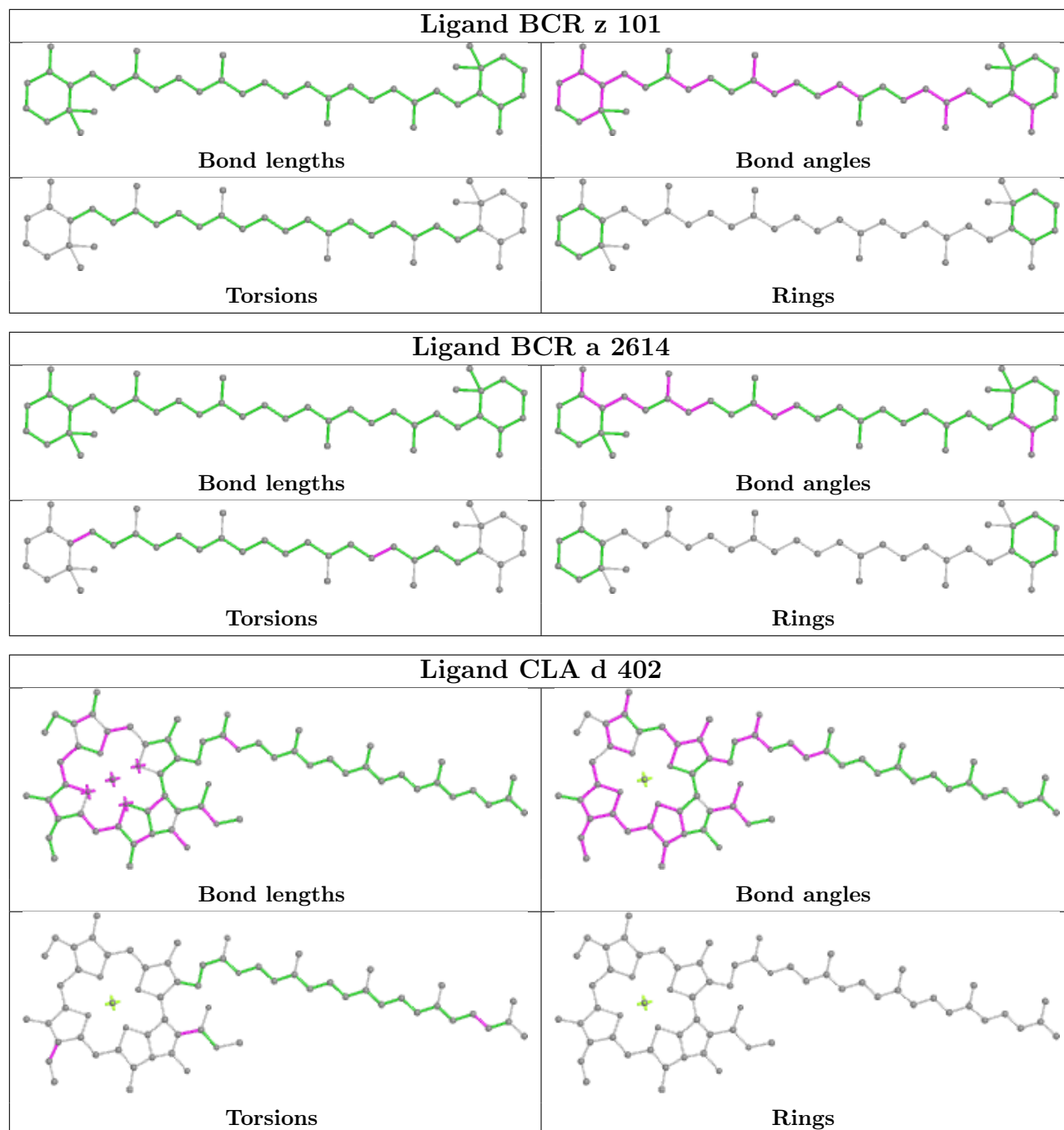


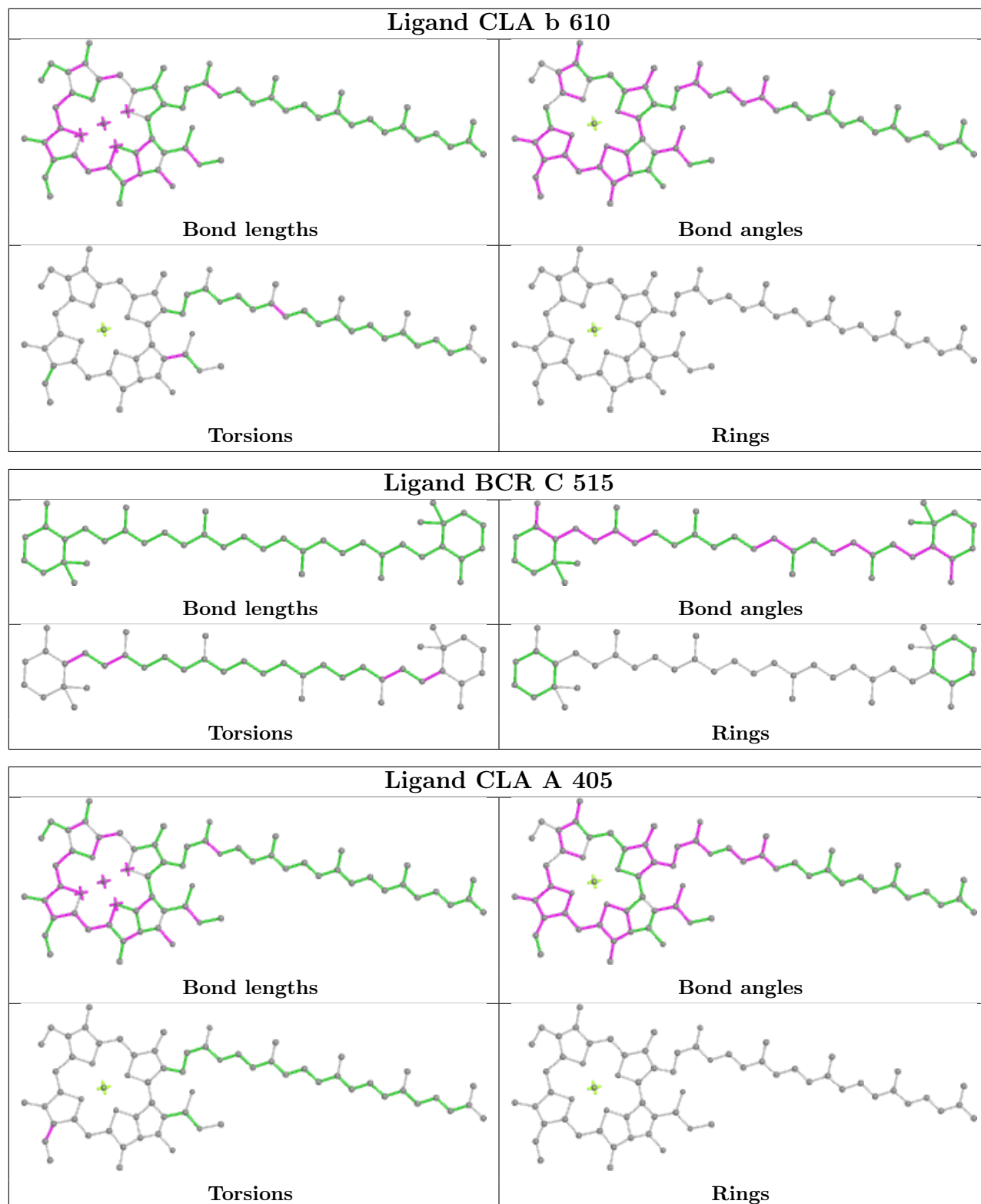


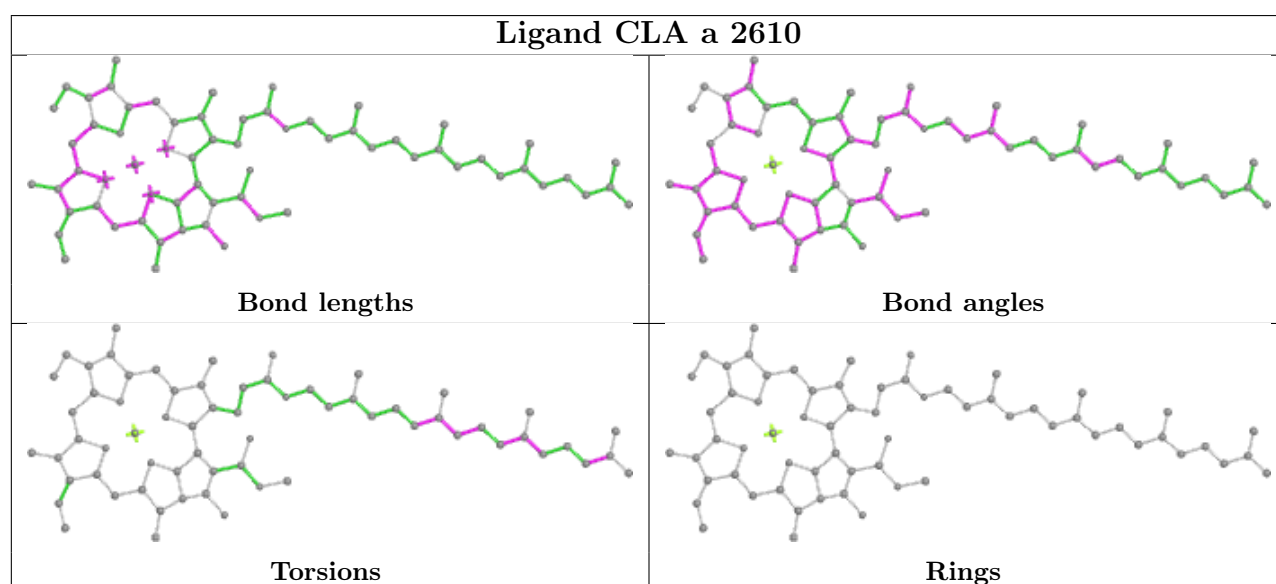
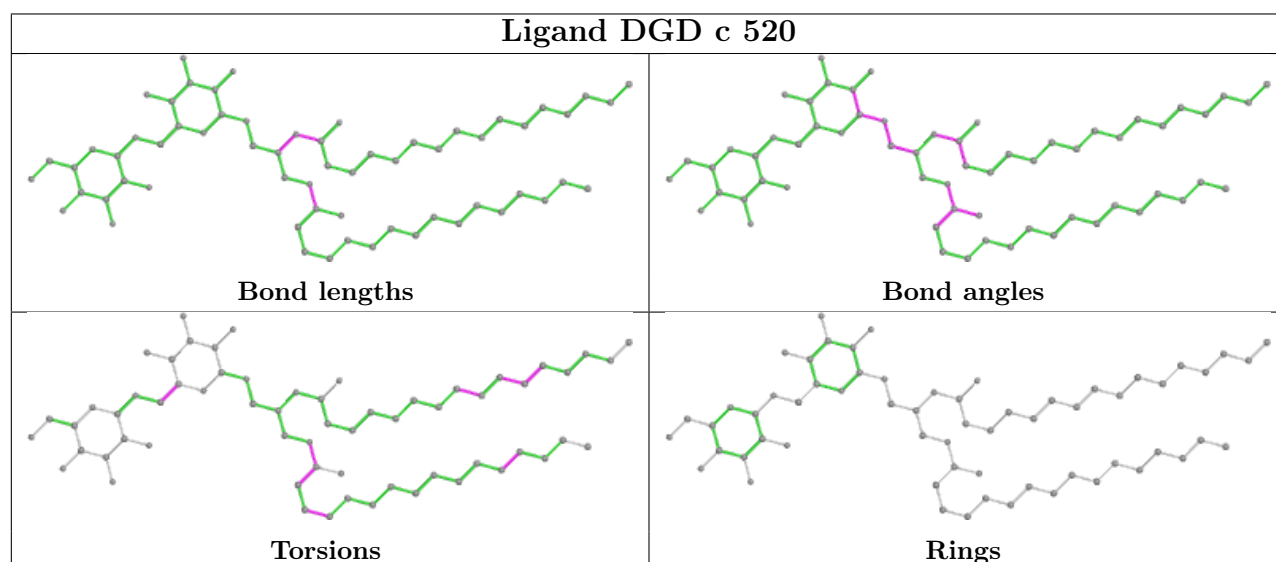
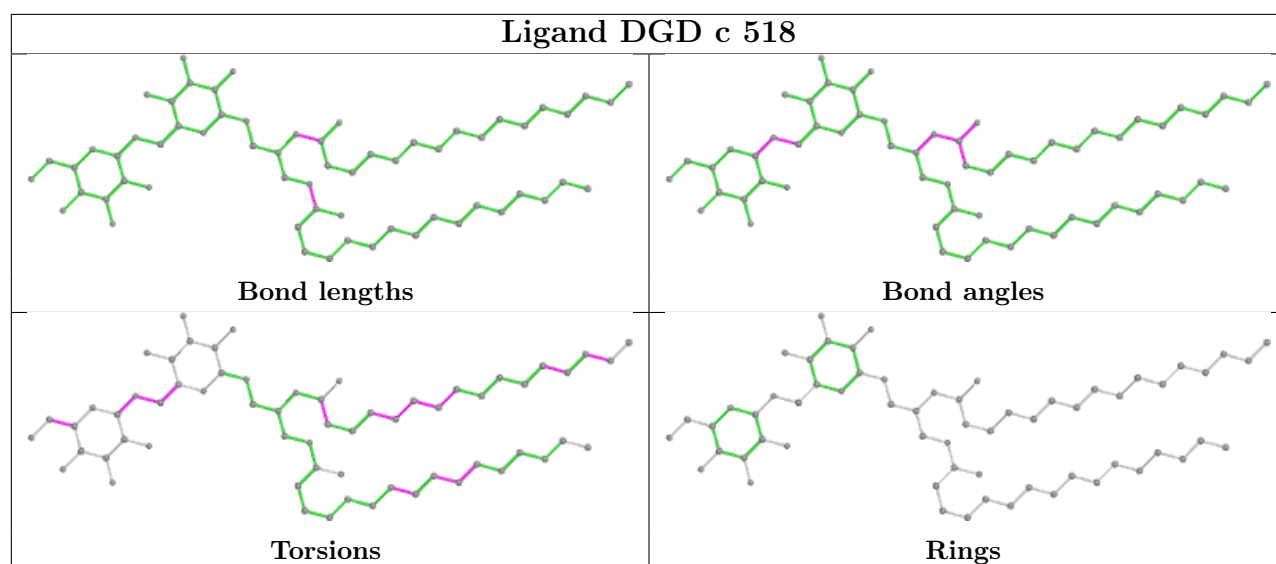


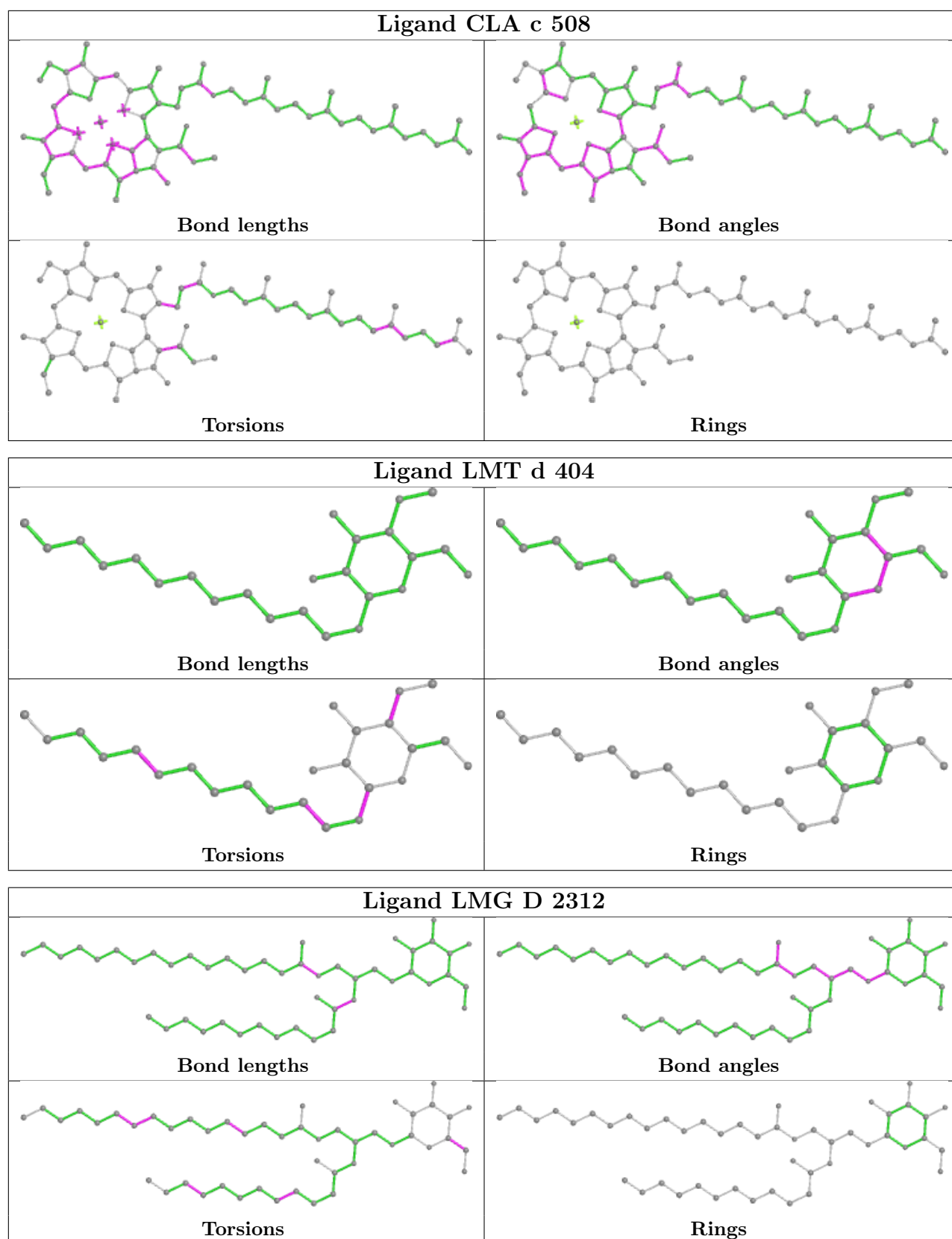


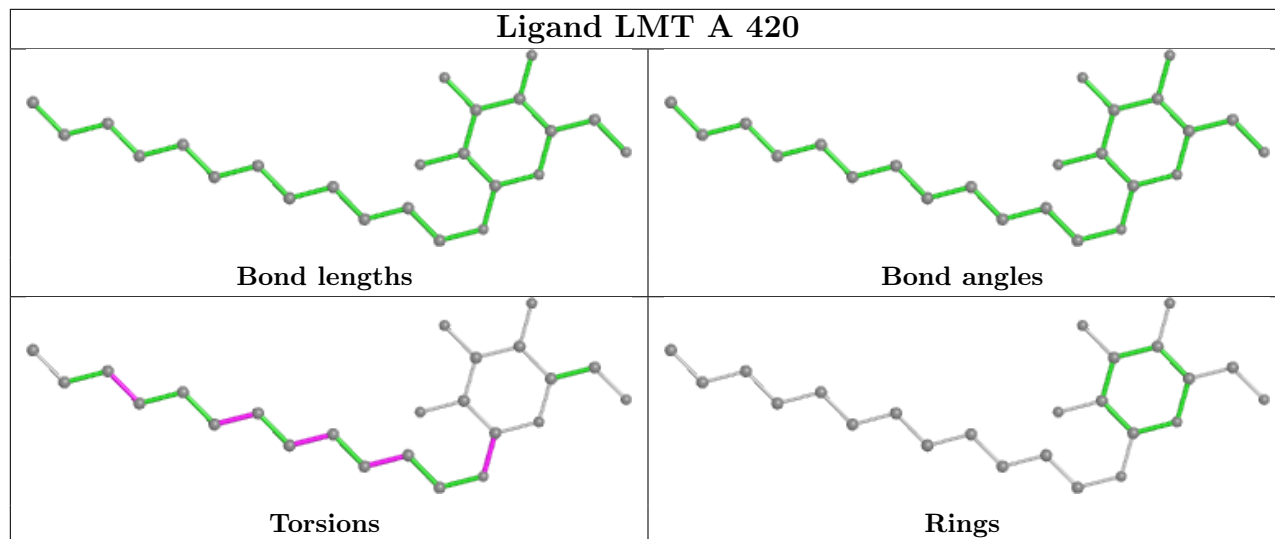
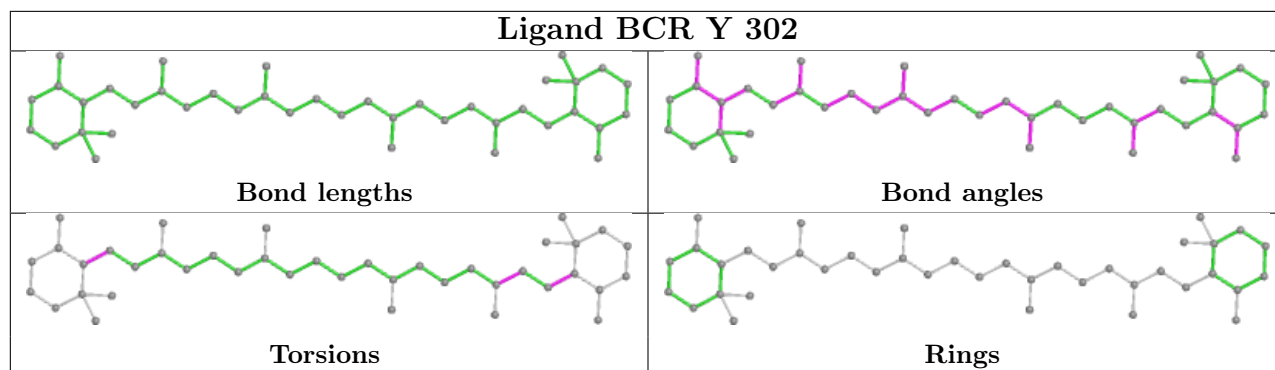


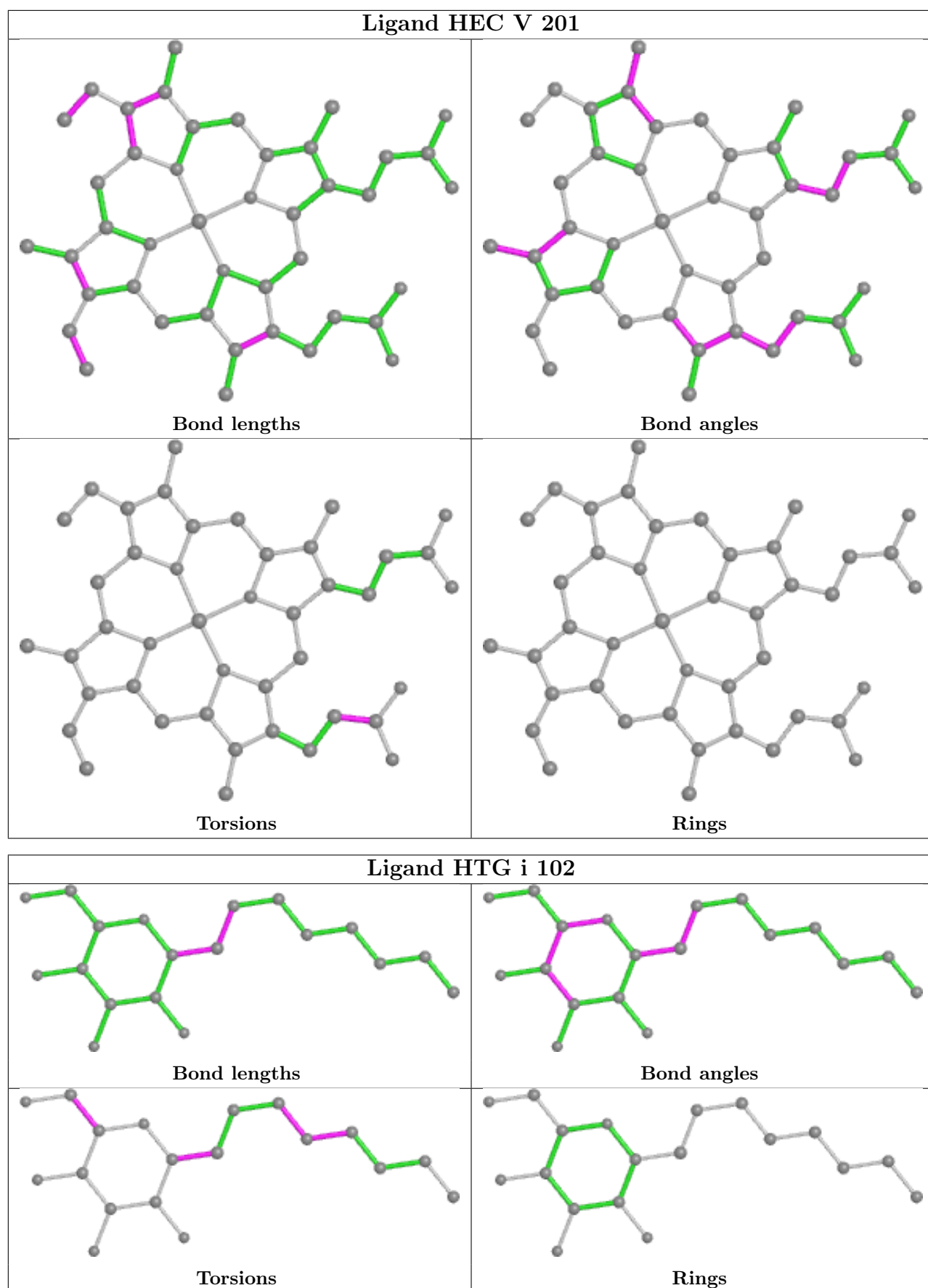


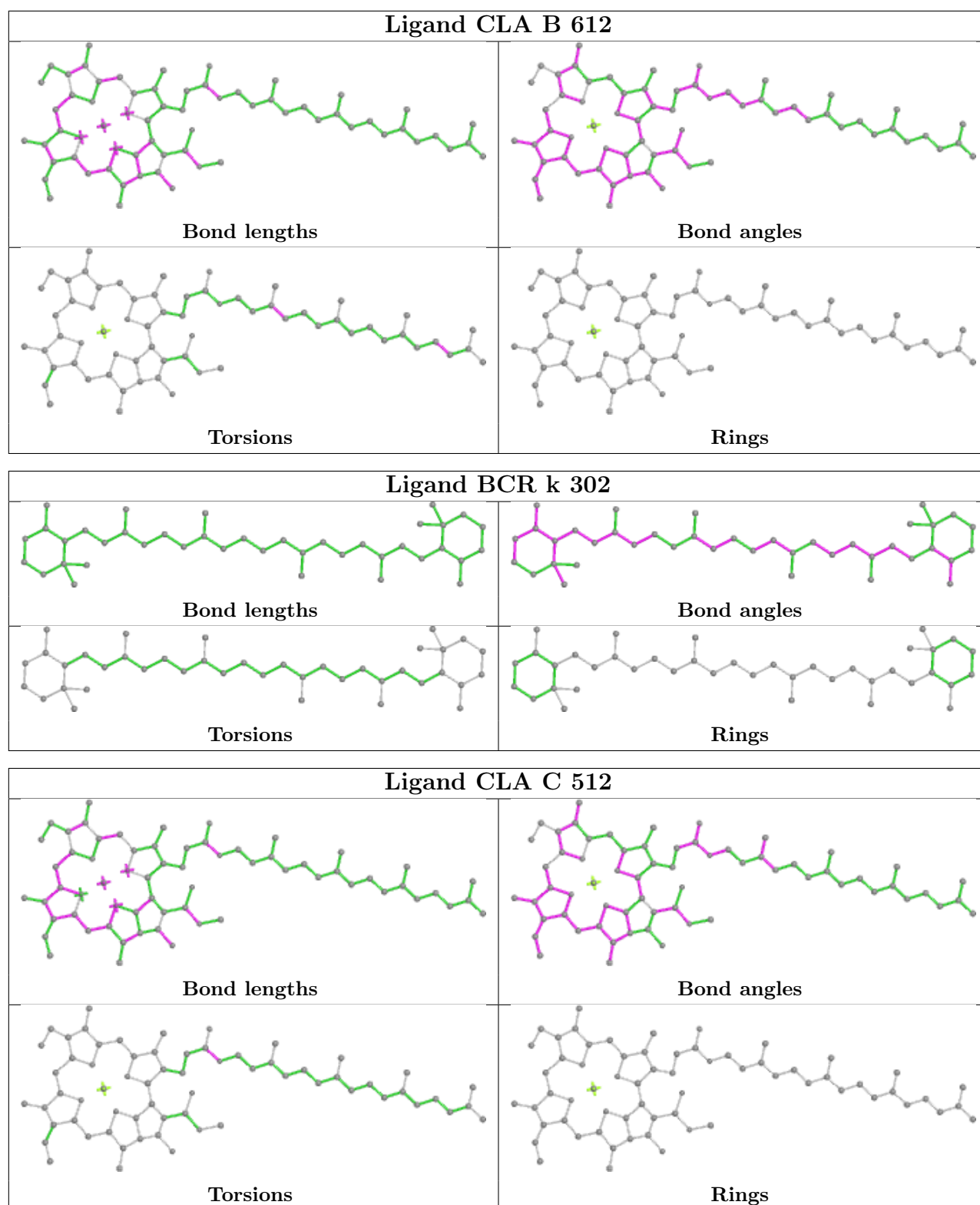


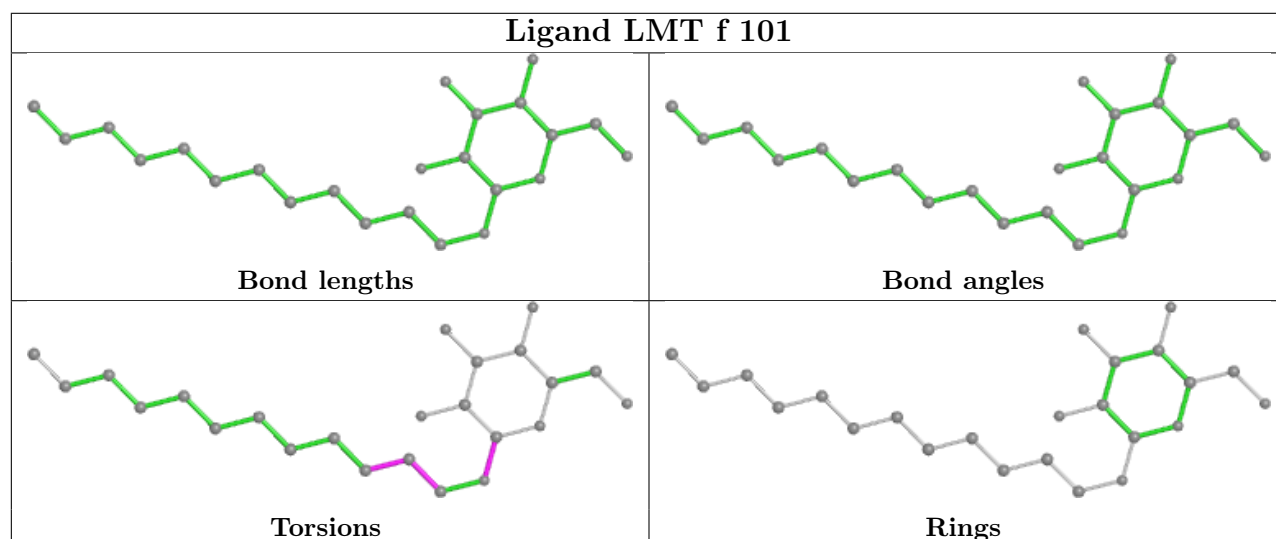
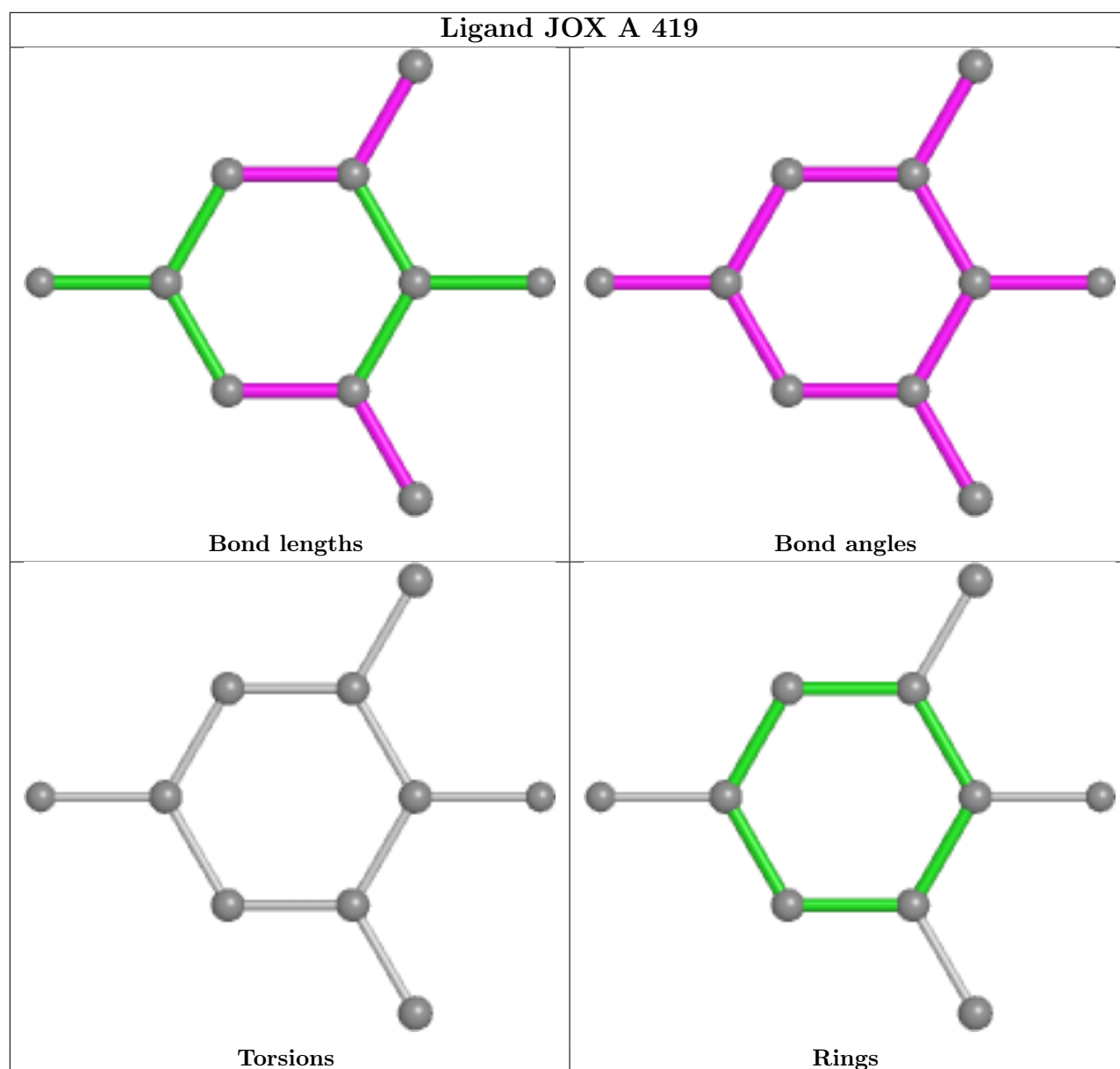




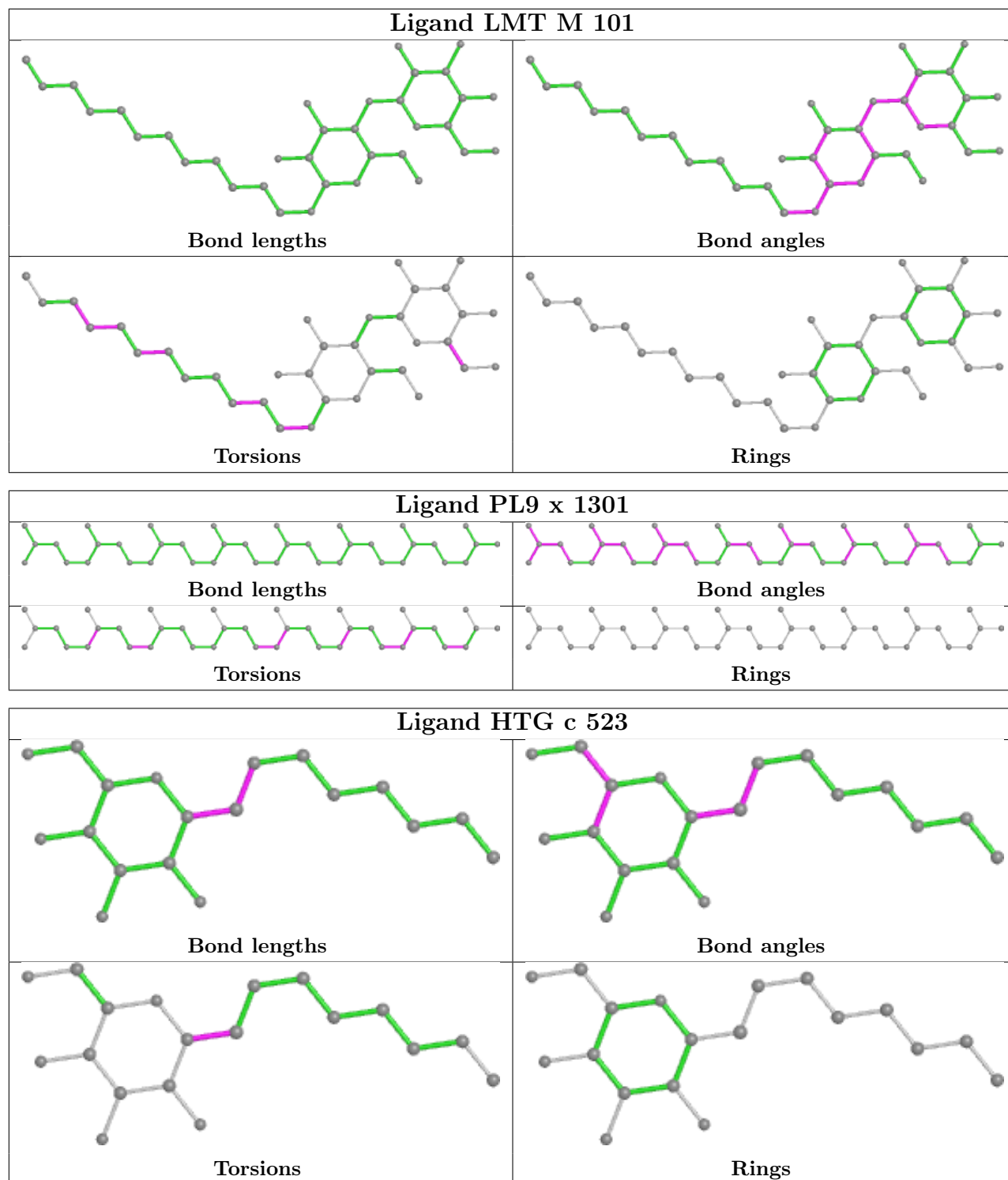


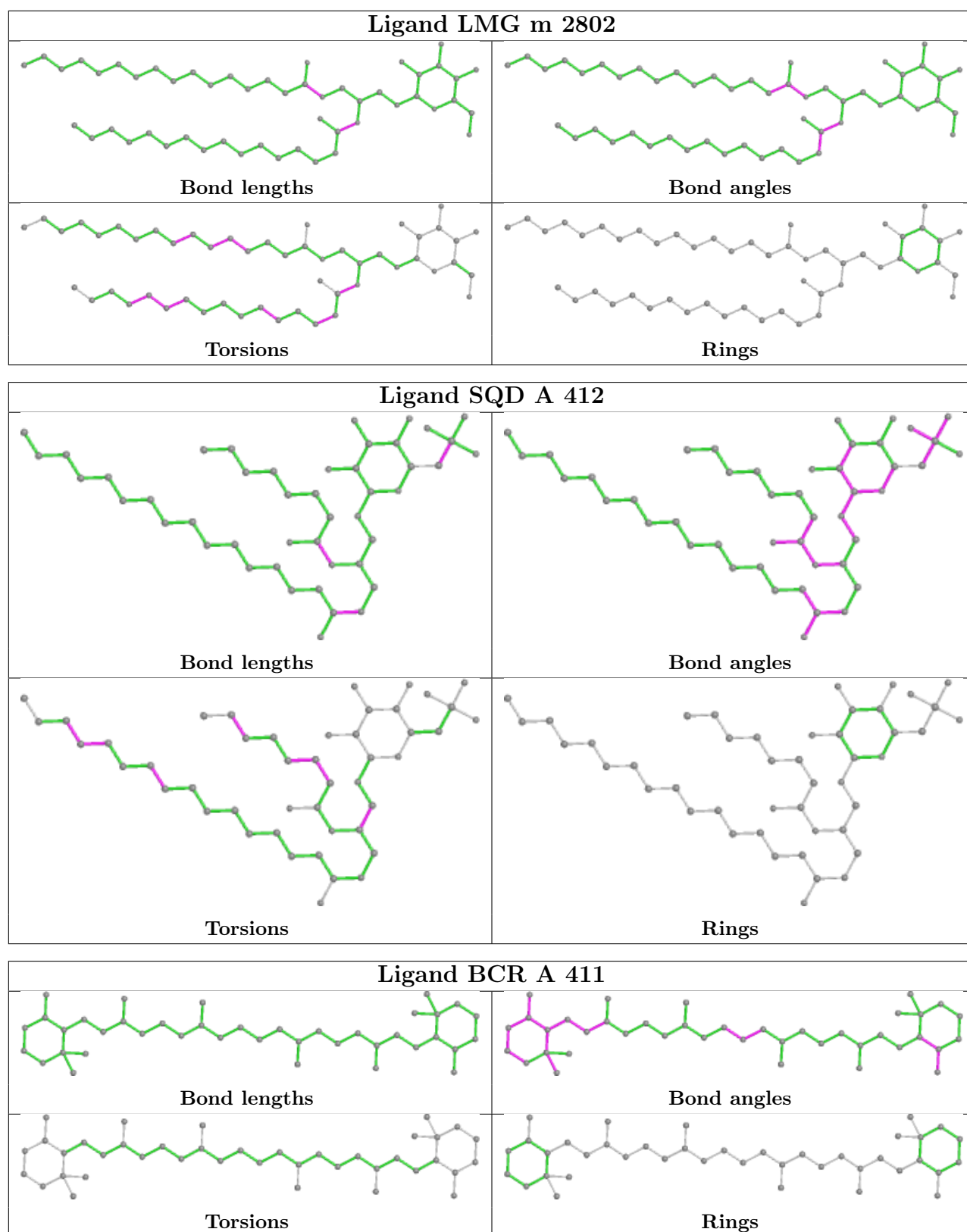


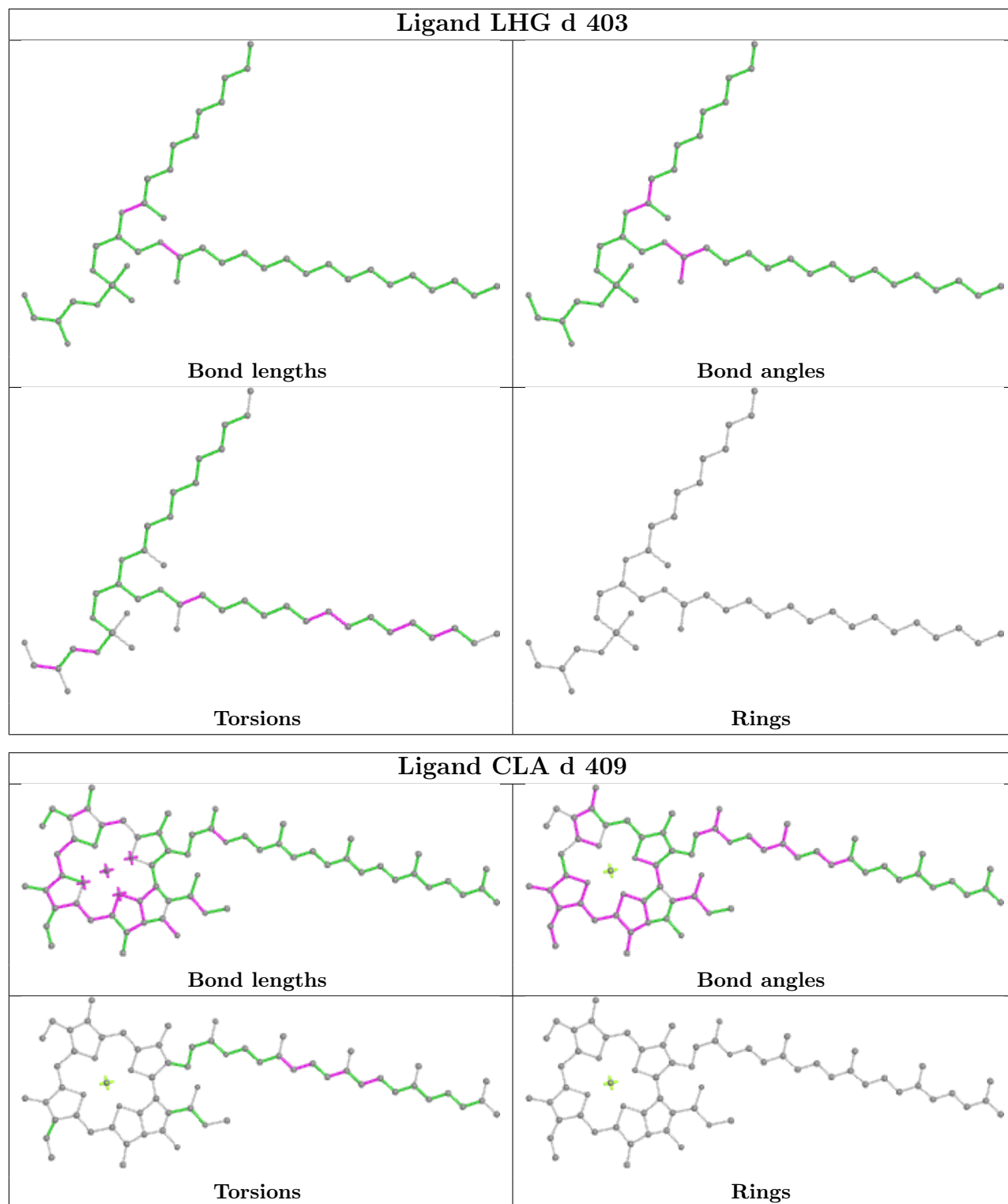


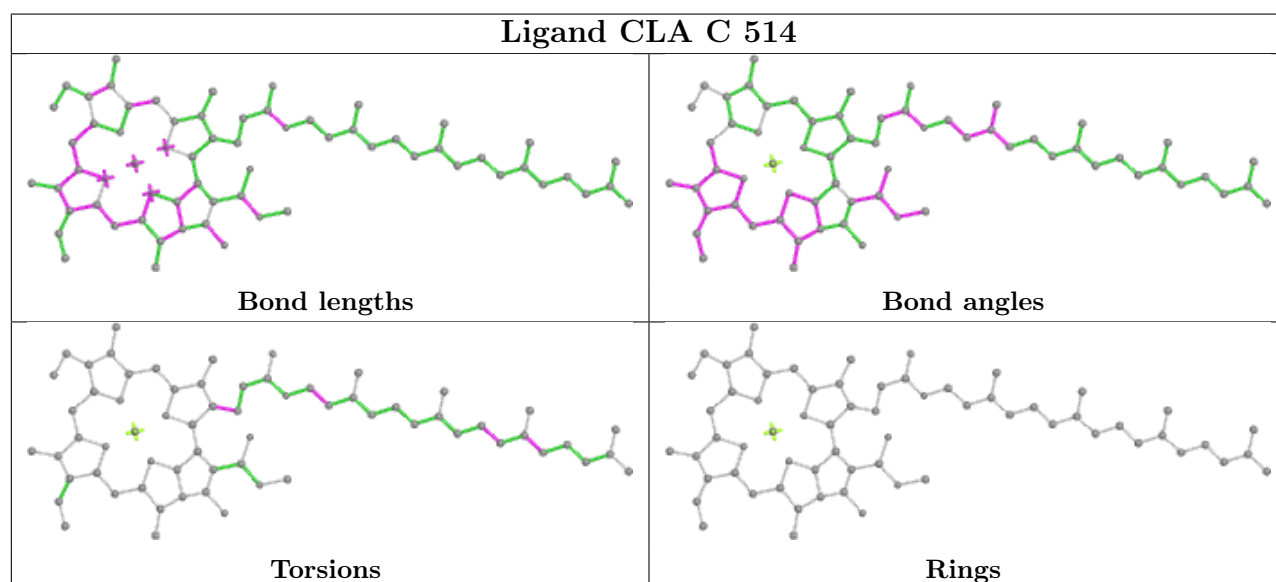
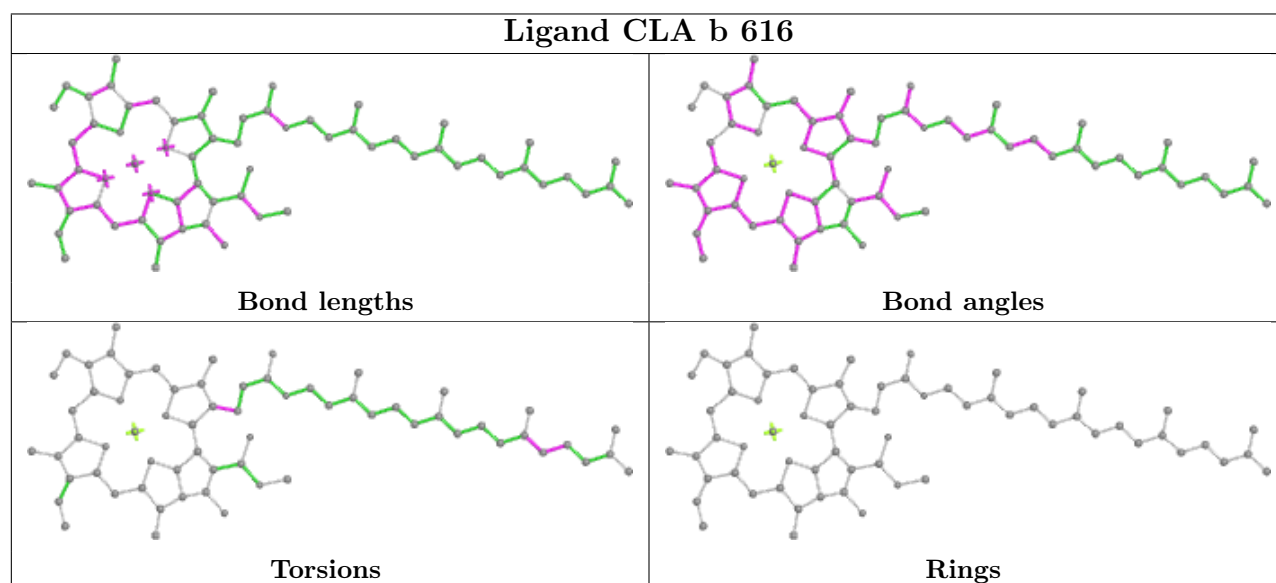
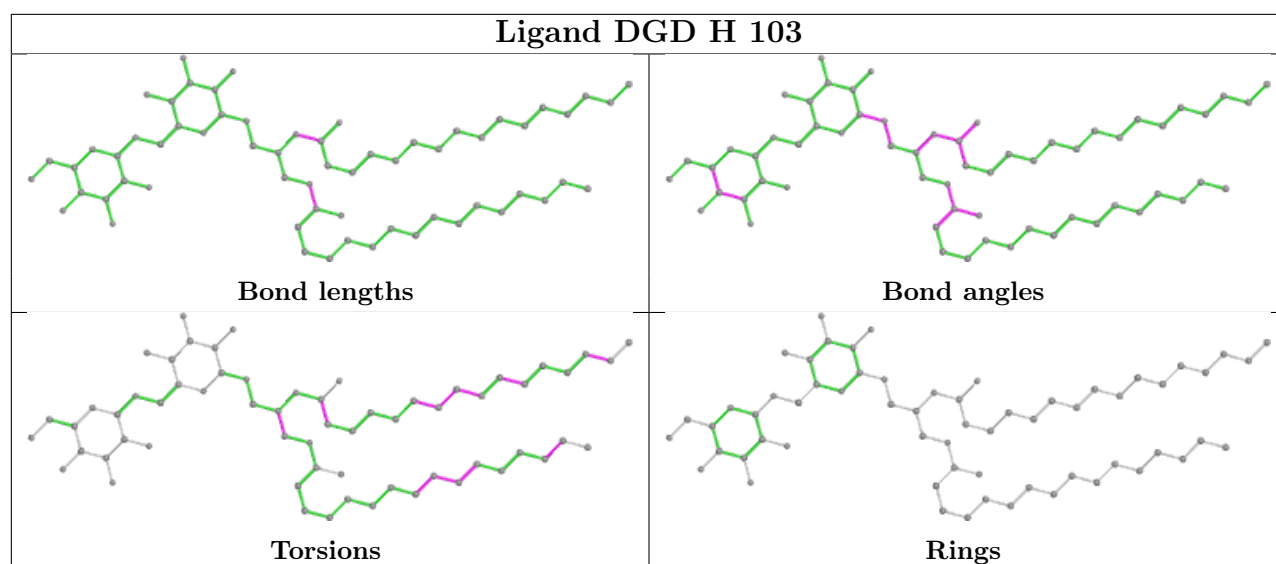


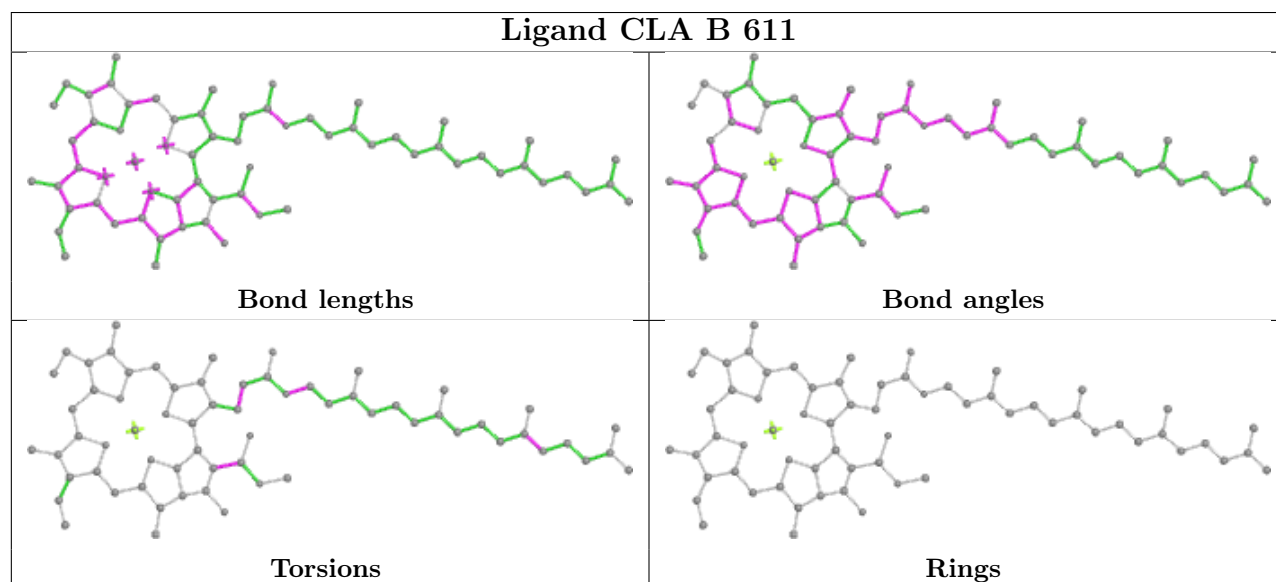
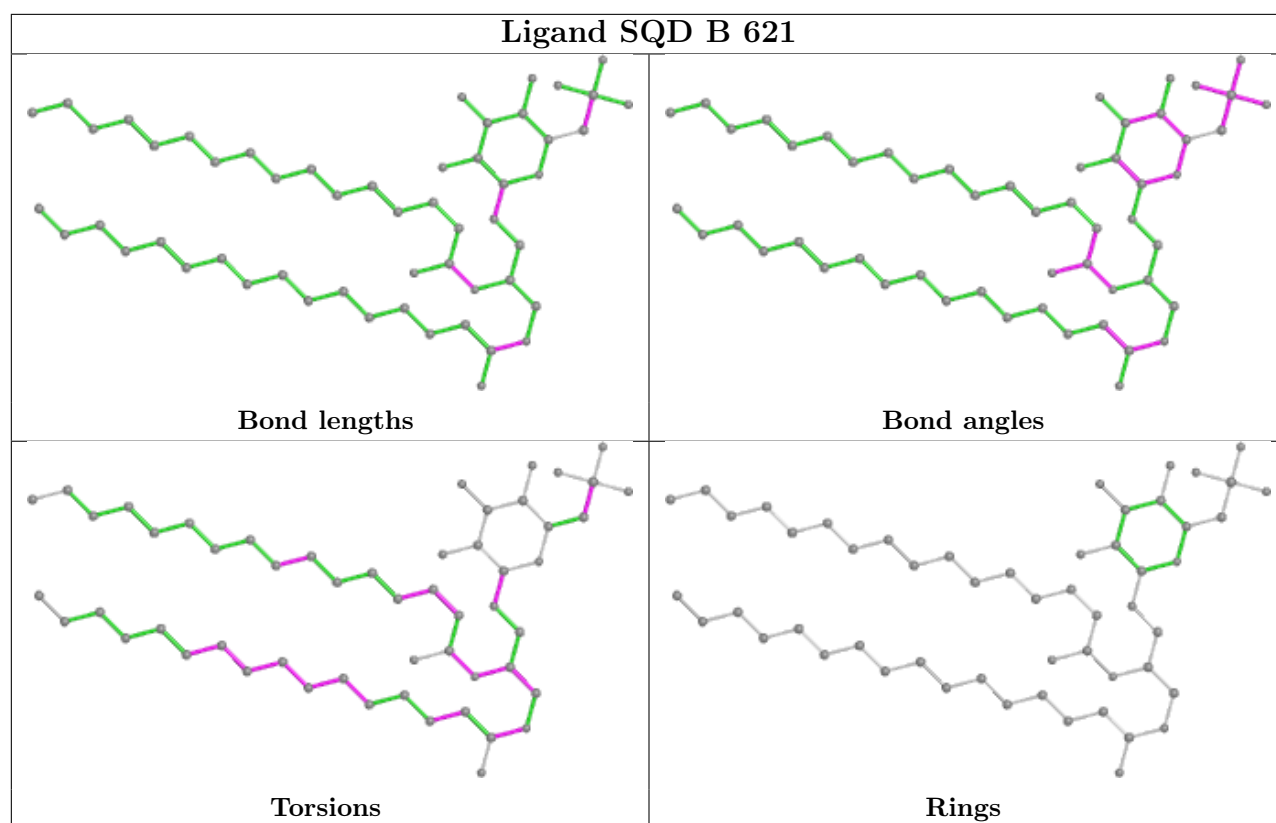


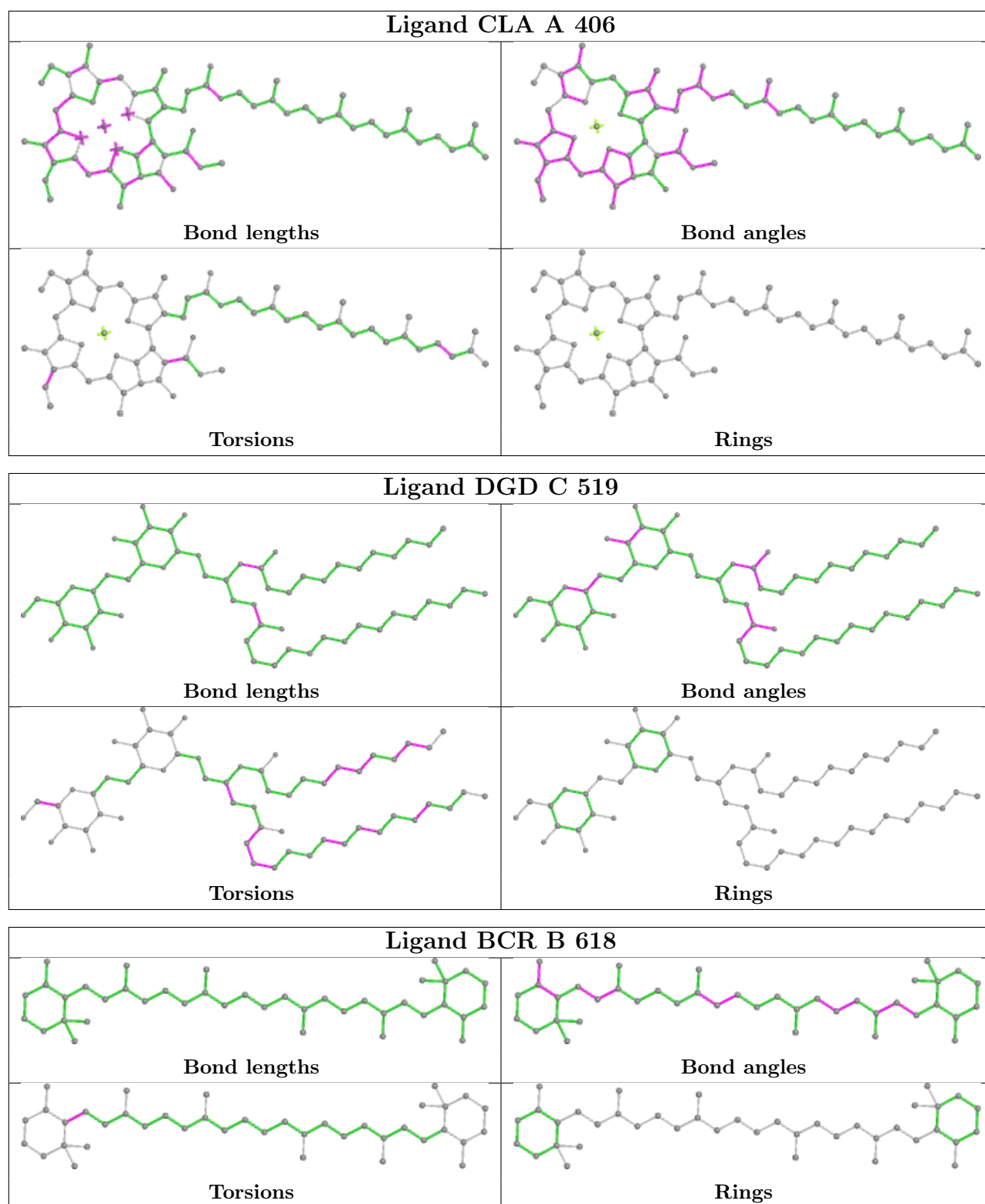


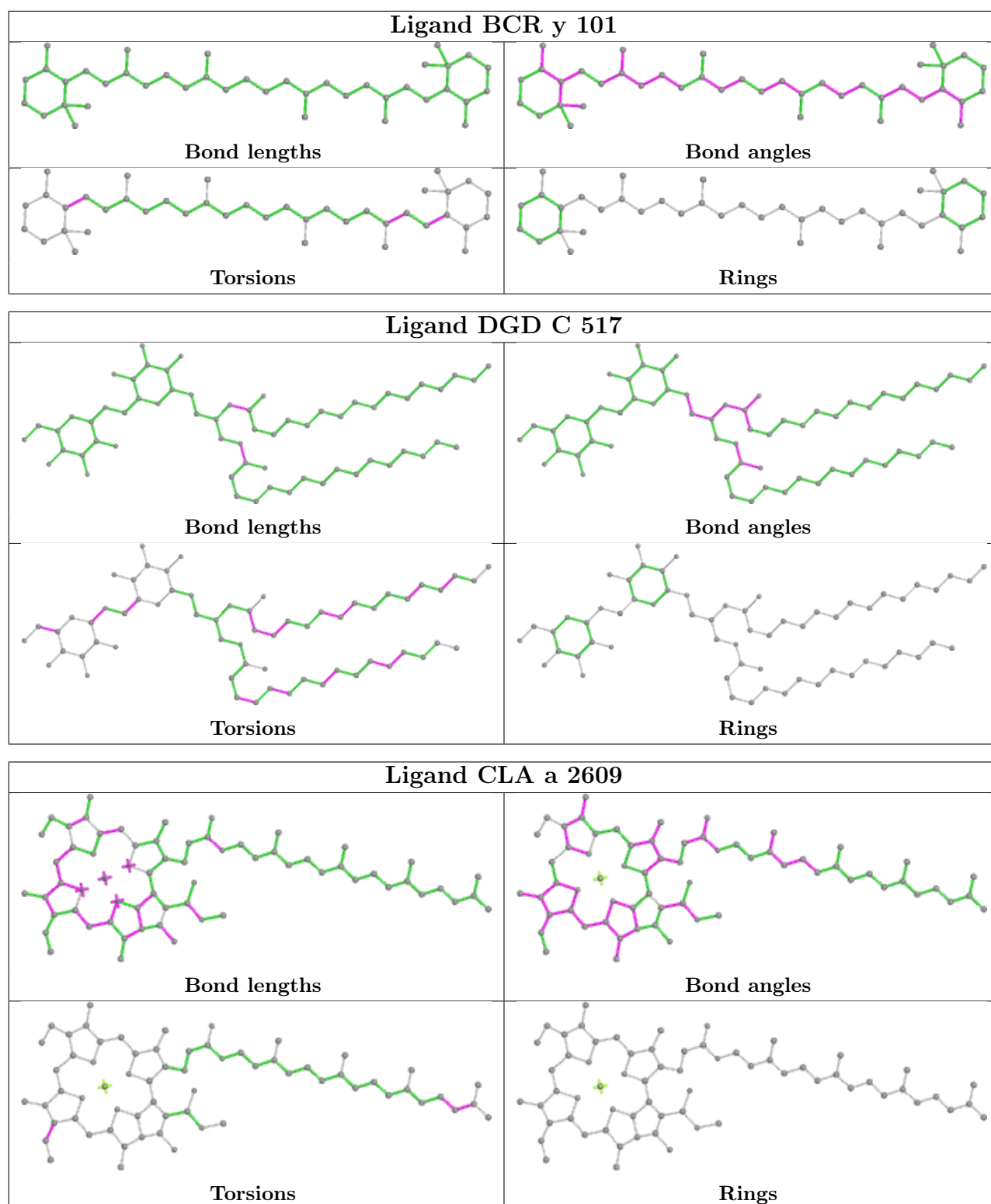


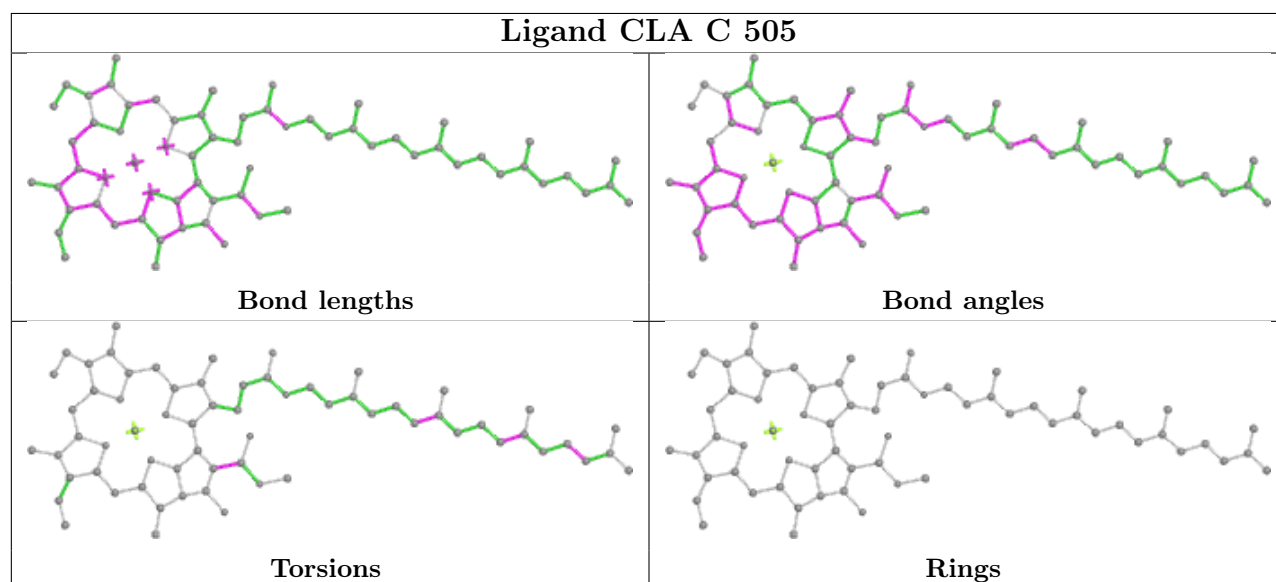
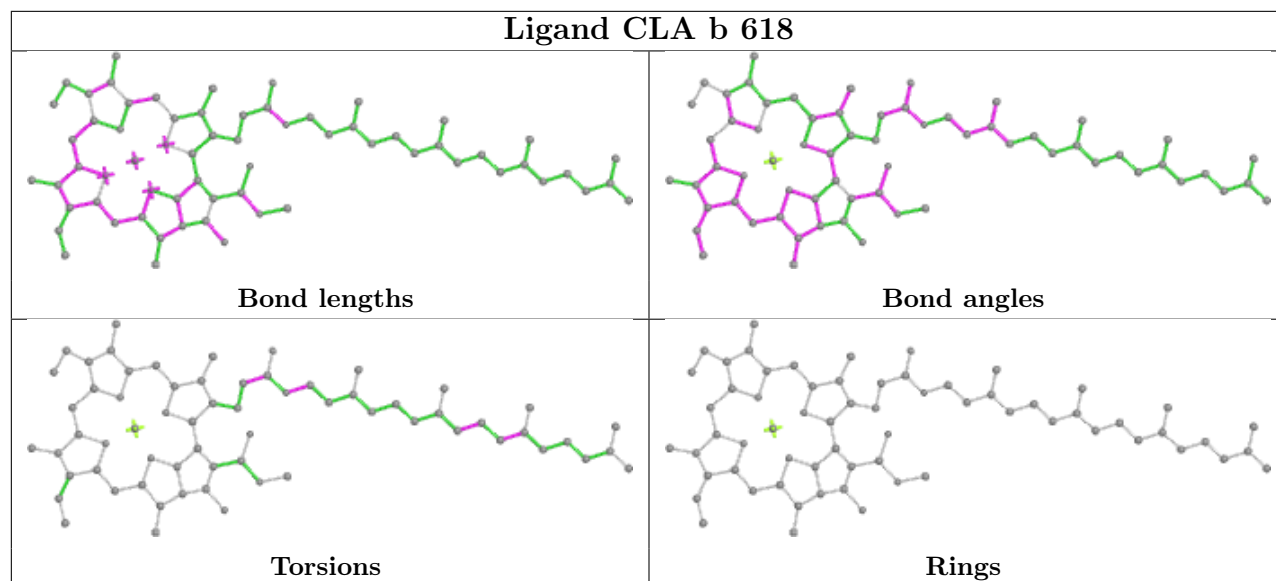
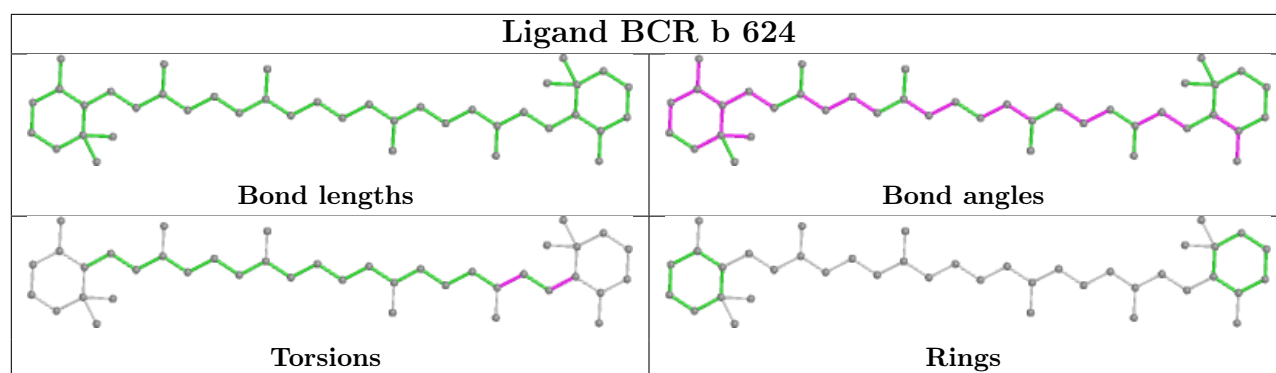




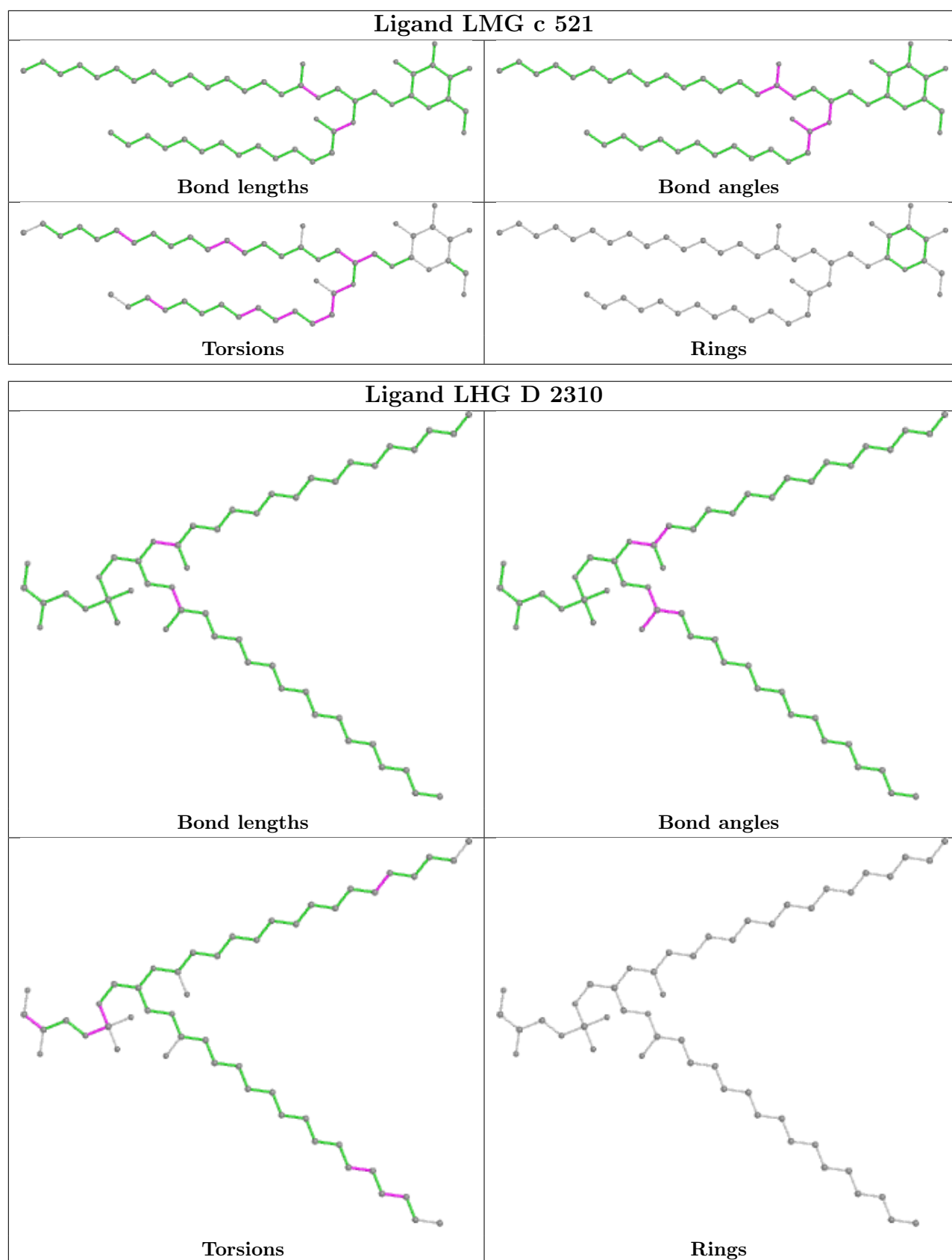


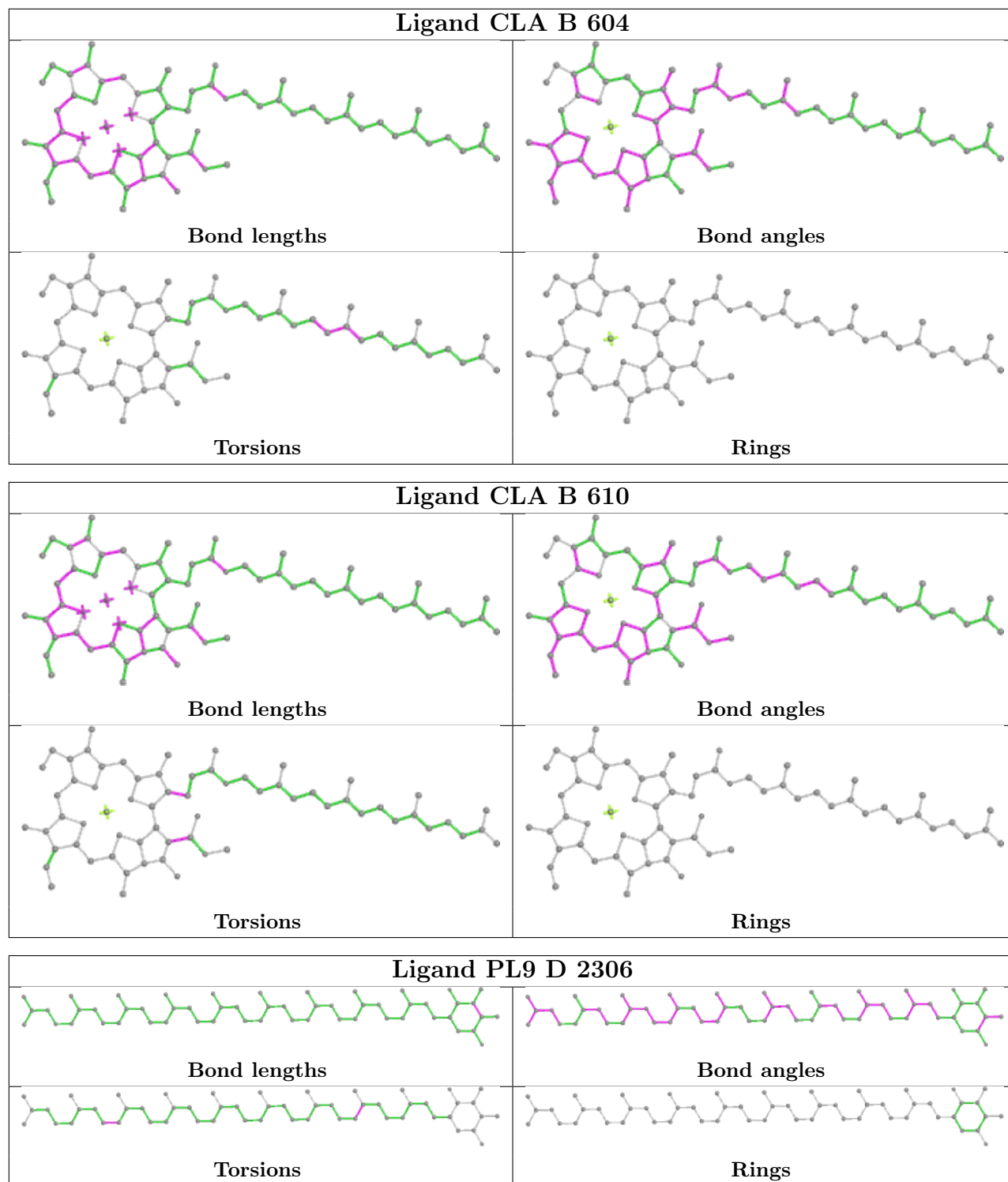


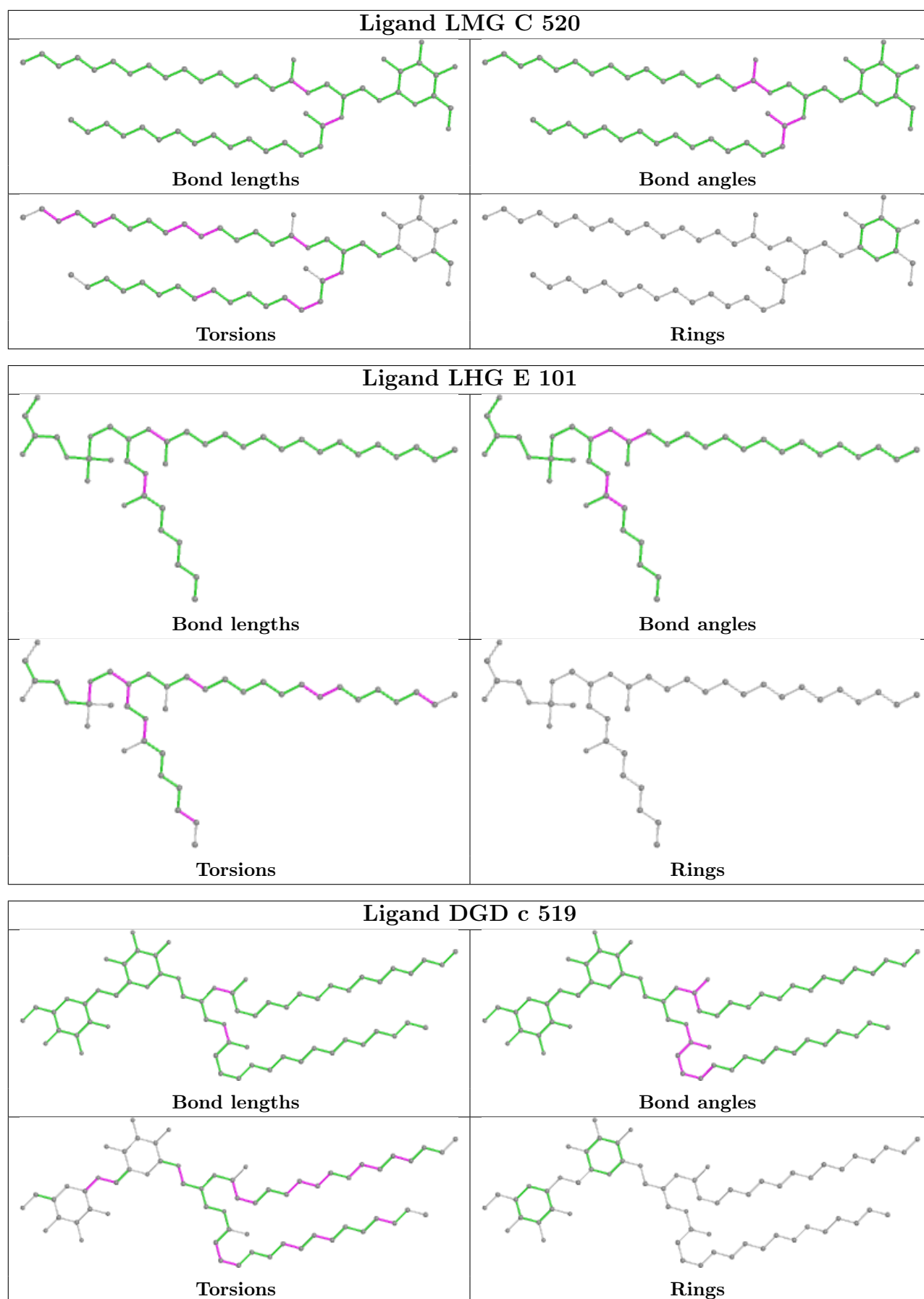


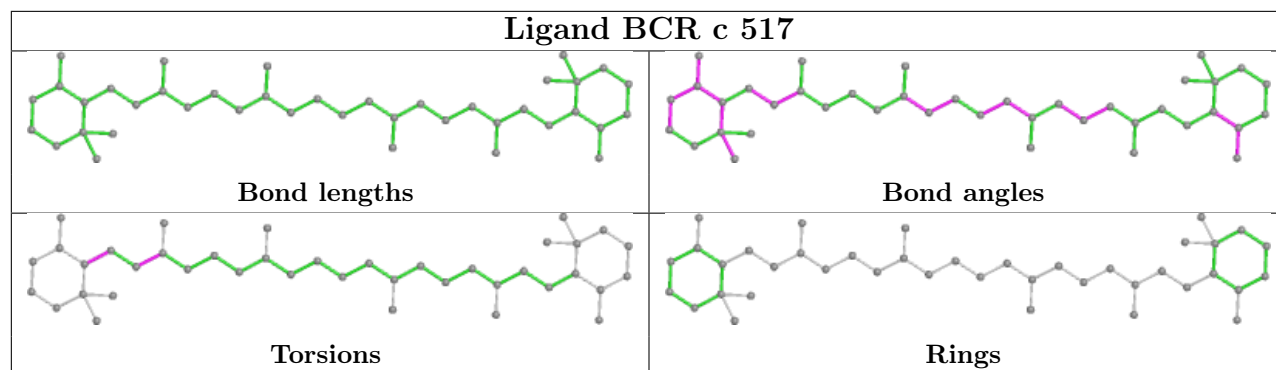












## 5.7 Other polymers [i](#)

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%)	-0.07	9 (2%) 54 63	38, 46, 86, 139	0
1	a	334/344 (97%)	0.25	26 (7%) 13 18	39, 47, 88, 143	1 (0%)
2	B	505/505 (100%)	0.12	51 (10%) 7 10	39, 52, 92, 138	0
2	b	483/505 (95%)	-0.06	33 (6%) 17 24	40, 53, 83, 143	0
3	C	451/455 (99%)	-0.00	29 (6%) 19 26	41, 59, 83, 164	0
3	c	455/455 (100%)	0.20	33 (7%) 15 21	45, 61, 81, 136	0
4	D	340/342 (99%)	-0.22	6 (1%) 68 75	37, 49, 75, 113	0
4	d	341/342 (99%)	-0.15	11 (3%) 47 56	38, 50, 77, 138	0
5	E	80/83 (96%)	0.90	22 (27%) 0 0	50, 77, 128, 144	0
5	e	79/83 (95%)	0.96	14 (17%) 1 1	56, 78, 124, 137	0
6	F	34/44 (77%)	0.04	5 (14%) 2 3	52, 64, 114, 124	0
6	f	32/44 (72%)	0.05	2 (6%) 20 27	53, 66, 119, 132	0
7	H	63/63 (100%)	0.23	5 (7%) 12 17	53, 69, 85, 111	0
7	h	63/63 (100%)	0.76	17 (26%) 0 0	56, 72, 89, 117	0
8	I	31/38 (81%)	0.35	6 (19%) 1 1	53, 71, 146, 152	0
8	i	31/38 (81%)	0.94	6 (19%) 1 1	51, 67, 129, 137	0
9	J	36/40 (90%)	-0.27	2 (5%) 24 33	48, 67, 111, 135	0
9	j	39/40 (97%)	0.14	5 (12%) 3 5	55, 68, 131, 162	0
10	K	37/37 (100%)	-0.37	1 (2%) 54 63	59, 68, 84, 92	0
10	k	37/37 (100%)	0.07	3 (8%) 12 16	58, 69, 95, 114	0
11	L	37/37 (100%)	-0.24	4 (10%) 5 8	38, 45, 88, 153	0
11	l	36/37 (97%)	0.00	1 (2%) 53 62	40, 46, 102, 158	0
12	M	32/36 (88%)	-0.50	1 (3%) 49 58	43, 48, 72, 106	0
12	m	33/36 (91%)	0.15	2 (6%) 21 28	41, 49, 100, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/244 (100%)	0.34	32 (13%) 3 4	38, 60, 104, 154	0
13	o	243/244 (99%)	0.21	33 (13%) 3 3	41, 60, 108, 162	0
14	T	29/32 (90%)	-0.20	1 (3%) 45 53	39, 46, 82, 150	0
14	t	29/32 (90%)	0.27	2 (6%) 16 23	40, 46, 80, 129	0
15	U	97/104 (93%)	-0.17	3 (3%) 49 58	46, 55, 86, 105	0
15	u	97/104 (93%)	-0.45	1 (1%) 82 86	49, 58, 80, 136	0
16	V	137/137 (100%)	-0.21	3 (2%) 62 69	45, 54, 80, 100	0
16	v	137/137 (100%)	0.43	22 (16%) 1 2	50, 66, 91, 110	0
17	Y	30/30 (100%)	1.18	7 (23%) 0 0	70, 83, 113, 124	0
17	y	30/30 (100%)	0.93	5 (16%) 1 2	75, 88, 105, 136	0
18	X	38/40 (95%)	1.56	18 (47%) 0 0	66, 79, 111, 122	0
18	x	35/40 (87%)	1.17	11 (31%) 0 0	71, 80, 122, 134	0
19	Z	61/62 (98%)	1.53	23 (37%) 0 0	66, 81, 124, 140	0
19	z	60/62 (96%)	1.89	27 (45%) 0 0	75, 88, 132, 159	0
All	All	5210/5346 (97%)	0.14	482 (9%) 8 13	37, 56, 98, 164	1 (0%)

The worst 5 of 482 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	3	GLN	9.7
2	B	486	LEU	7.9
1	A	11	ALA	7.7
18	x	2	THR	7.1
19	z	4	LEU	6.2

## 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
19	FME	Z	1	10/11	0.91	0.25	96,112,117,118	0
19	FME	z	1	10/11	0.91	0.34	114,129,141,143	0
8	FME	I	1	10/11	0.96	0.10	49,59,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	HSK	d	336[A]	10/12	0.96	0.12	51,56,59,60	7
4	HSK	d	336[B]	11/12	0.96	0.12	51,56,59,62	8
12	FME	M	1	10/11	0.96	0.11	48,56,80,81	0
12	FME	m	1	10/11	0.97	0.08	43,57,81,84	0
14	FME	t	1	10/11	0.97	0.07	46,51,77,79	0
14	FME	T	1	10/11	0.97	0.06	48,54,84,88	0
4	HSK	D	336[A]	10/12	0.98	0.10	49,51,51,51	7
4	HSK	D	336[B]	11/12	0.98	0.10	50,51,51,51	8
8	FME	i	1	10/11	0.98	0.11	52,60,62,64	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
41	MG	K	102	1/1	0.33	0.15	85,85,85,85	0
37	DGD	D	2307	53/66	0.37	0.36	96,121,171,177	0
38	LHG	e	101	40/49	0.40	0.38	93,156,201,202	0
34	DMS	c	546	4/4	0.44	0.23	151,153,154,154	0
29	GOL	E	104	6/6	0.47	0.23	124,126,128,129	0
30	UNL	j	2702	16/-	0.47	0.47	89,96,108,111	0
30	UNL	k	301	16/-	0.49	0.25	89,109,125,126	0
29	GOL	c	529	6/6	0.50	0.17	124,131,132,133	0
28	LMT	m	2804	35/35	0.51	0.31	79,146,162,166	0
34	DMS	c	547	4/4	0.53	0.46	132,138,140,141	0
29	GOL	b	631	6/6	0.53	0.26	84,100,106,106	0
29	GOL	v	204	6/6	0.53	0.41	92,115,115,123	0
30	UNL	A	416	28/-	0.53	0.29	93,104,133,143	0
28	LMT	j	2701	34/35	0.54	0.24	79,145,158,159	0
28	LMT	d	404	25/35	0.54	0.30	91,129,162,164	0
28	LMT	M	101	35/35	0.55	0.31	84,157,181,181	0
30	UNL	D	2313	12/-	0.57	0.40	93,112,114,115	0
34	DMS	b	638	4/4	0.58	0.36	159,163,163,165	0
28	LMT	M	102	35/35	0.59	0.26	59,106,136,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	I	102	40/-	0.59	0.35	101,119,151,152	0
30	UNL	c	527	12/-	0.59	0.38	104,113,125,126	0
30	UNL	i	101	19/-	0.59	0.41	88,112,144,146	0
29	GOL	d	416	6/6	0.59	0.15	129,131,132,133	0
30	UNL	B	629	15/-	0.59	0.57	90,105,111,112	0
28	LMT	B	634	35/35	0.60	0.32	55,133,160,162	0
38	LHG	E	101	40/49	0.60	0.35	94,137,163,165	0
29	GOL	B	630	6/6	0.61	0.20	94,104,109,117	0
34	DMS	c	549	4/4	0.62	0.27	124,126,128,128	0
29	GOL	O	305	6/6	0.63	0.26	70,91,97,105	0
30	UNL	Y	301	12/-	0.63	0.22	114,116,120,121	0
29	GOL	o	303	6/6	0.63	0.17	71,83,104,109	0
34	DMS	O	311	4/4	0.63	0.42	130,135,136,138	0
34	DMS	B	640	4/4	0.64	0.43	154,155,156,157	0
27	LMG	C	527	51/55	0.65	0.31	71,123,148,152	0
34	DMS	a	2620	4/4	0.65	0.45	142,146,149,151	0
29	GOL	u	501	6/6	0.66	0.21	84,92,98,102	0
36	HTG	i	102	19/19	0.66	0.23	68,143,157,158	0
30	UNL	a	2616	27/-	0.66	0.42	86,103,140,149	0
28	LMT	m	2803	35/35	0.67	0.27	61,101,118,121	0
34	DMS	T	104	4/4	0.67	0.33	156,160,160,161	0
26	SQD	D	2302	54/54	0.67	0.25	75,106,174,176	0
36	HTG	b	626	19/19	0.68	0.18	98,151,158,158	0
29	GOL	O	304	6/6	0.68	0.25	86,101,103,106	0
30	UNL	b	627	15/-	0.68	0.36	90,97,113,114	0
30	UNL	b	628	10/-	0.68	0.34	94,111,114,116	0
28	LMT	d	401	35/35	0.68	0.26	63,106,125,130	0
29	GOL	c	530	6/6	0.68	0.18	79,107,118,124	0
28	LMT	J	303	24/35	0.69	0.25	80,95,144,147	0
34	DMS	o	309	4/4	0.69	0.44	131,139,139,141	0
40	RRX	h	101	41/41	0.69	0.23	56,81,103,119	0
36	HTG	B	627	19/19	0.69	0.25	67,130,145,148	0
30	UNL	x	1302	18/-	0.70	0.20	76,86,120,124	0
29	GOL	c	531	6/6	0.70	0.16	116,118,119,120	0
30	UNL	C	501	40/-	0.70	0.37	102,120,136,139	0
29	GOL	B	632	6/6	0.71	0.26	87,96,98,101	0
36	HTG	c	526	19/19	0.71	0.27	120,165,175,175	0
34	DMS	X	101	4/4	0.71	0.25	172,174,175,175	0
28	LMT	F	102	24/35	0.71	0.35	114,127,159,161	0
34	DMS	b	643	4/4	0.72	0.35	125,131,133,136	0
36	HTG	B	625	19/19	0.72	0.42	77,130,138,140	19
30	UNL	b	632	10/-	0.72	0.26	83,93,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	D	2314	18/-	0.72	0.21	67,79,113,117	0
28	LMT	Z	101	35/35	0.72	0.27	68,142,184,187	0
36	HTG	d	407	19/19	0.72	0.41	102,133,146,148	0
29	GOL	V	203	6/6	0.73	0.14	98,111,118,123	0
36	HTG	B	624[A]	19/19	0.73	0.32	56,72,85,87	19
36	HTG	c	524	19/19	0.73	0.45	62,108,119,121	19
36	HTG	B	624[B]	19/19	0.73	0.32	57,72,86,88	19
33	PL9	A	422	39/55	0.73	0.38	88,101,124,127	0
36	HTG	d	415	19/19	0.73	0.23	80,117,124,125	19
36	HTG	C	522	19/19	0.74	0.46	88,124,137,140	0
34	DMS	c	542	4/4	0.74	0.25	148,149,150,151	0
34	DMS	b	642	4/4	0.74	0.32	153,154,156,159	0
30	UNL	C	523	10/-	0.74	0.24	99,101,107,112	0
29	GOL	U	501	6/6	0.75	0.25	105,111,113,115	0
29	GOL	O	302	6/6	0.75	0.12	78,82,87,91	0
26	SQD	a	2603	54/54	0.75	0.21	55,89,136,138	0
30	UNL	B	628	18/-	0.75	0.26	85,96,116,117	0
28	LMT	A	414	33/35	0.75	0.26	72,117,128,135	0
30	UNL	T	101	13/-	0.75	0.67	93,100,107,107	0
36	HTG	C	525	19/19	0.75	0.33	91,137,156,156	0
34	DMS	U	504	4/4	0.75	0.18	119,124,127,129	0
30	UNL	B	631	32/-	0.75	0.18	66,97,116,117	0
28	LMT	f	101	24/35	0.76	0.43	102,124,156,160	0
27	LMG	c	522	51/55	0.76	0.29	65,117,127,130	0
28	LMT	A	420	24/35	0.76	0.19	63,104,142,148	0
36	HTG	I	101	19/19	0.76	0.22	83,126,141,145	0
34	DMS	H	104	4/4	0.76	0.31	129,131,133,133	0
34	DMS	B	637	4/4	0.77	0.17	121,124,125,126	0
34	DMS	c	541	4/4	0.77	0.48	121,128,129,132	0
36	HTG	b	625	19/19	0.77	0.31	58,83,106,108	0
28	LMT	T	103	24/35	0.77	0.24	58,91,129,132	0
28	LMT	i	103	24/35	0.77	0.18	67,119,153,155	0
27	LMG	m	2802	51/55	0.77	0.26	56,81,98,107	0
30	UNL	J	304	5/-	0.77	0.34	97,98,103,104	0
33	PL9	x	1301	39/55	0.78	0.22	94,113,131,132	0
34	DMS	A	429	4/4	0.78	0.37	128,129,130,132	0
34	DMS	V	207	4/4	0.78	0.30	137,139,141,141	0
36	HTG	b	604	19/19	0.78	0.17	79,131,144,147	0
26	SQD	b	601	48/54	0.79	0.22	66,96,152,156	0
29	GOL	v	202	6/6	0.79	0.14	113,114,116,118	0
28	LMT	B	623	35/35	0.79	0.23	89,122,148,149	0
34	DMS	A	430	4/4	0.79	0.22	115,127,127,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	a	2601	15/-	0.79	0.33	79,86,93,96	0
30	UNL	c	502	36/-	0.79	0.25	91,115,128,130	0
31	JOX	A	419	10/10	0.80	0.19	60,69,76,78	0
30	UNL	d	405	37/-	0.80	0.20	74,101,137,137	0
28	LMT	z	102	33/35	0.80	0.22	80,141,156,157	0
34	DMS	o	310	4/4	0.80	0.34	144,147,149,149	0
30	UNL	A	423	9/-	0.80	0.47	84,89,93,94	0
27	LMG	c	501	51/55	0.80	0.23	67,90,101,105	0
40	RRX	H	102	41/41	0.80	0.20	48,75,95,100	0
34	DMS	B	635	4/4	0.80	0.20	130,132,133,133	0
26	SQD	B	621	54/54	0.80	0.21	60,92,128,131	0
29	GOL	D	2301	6/6	0.81	0.22	87,93,100,104	0
26	SQD	l	101	54/54	0.81	0.22	59,88,126,130	0
29	GOL	J	301	6/6	0.81	0.49	100,103,110,111	0
30	UNL	E	103	9/-	0.81	0.37	75,83,107,110	0
36	HTG	H	101	17/19	0.81	0.33	109,127,151,151	0
34	DMS	C	537	4/4	0.81	0.30	143,143,144,146	0
34	DMS	a	2624	4/4	0.81	0.47	79,105,106,109	0
29	GOL	U	502	6/6	0.81	0.24	73,82,89,97	0
27	LMG	B	622	51/55	0.81	0.22	57,81,98,100	0
34	DMS	O	319	4/4	0.81	0.34	131,134,135,136	0
37	DGD	h	102	62/66	0.82	0.21	52,71,117,119	0
30	UNL	b	630	21/-	0.82	0.16	56,79,122,124	0
34	DMS	B	646	4/4	0.82	0.30	94,96,102,107	0
34	DMS	b	637	4/4	0.82	0.25	89,107,109,112	0
34	DMS	O	314	4/4	0.82	0.51	117,121,126,133	0
27	LMG	C	520	51/55	0.82	0.21	59,91,107,114	0
29	GOL	C	524	6/6	0.83	0.14	101,110,113,118	0
30	UNL	c	528	5/-	0.83	0.30	87,89,97,97	0
34	DMS	O	306	4/4	0.83	0.32	146,150,150,153	0
29	GOL	a	2602	6/6	0.83	0.25	64,79,91,91	0
34	DMS	c	538	4/4	0.83	0.35	136,137,139,141	0
34	DMS	B	645	4/4	0.83	0.37	124,125,125,127	0
30	UNL	E	102	6/-	0.83	0.18	83,87,87,89	0
30	UNL	t	101	8/-	0.84	0.54	75,84,103,103	0
34	DMS	v	214	4/4	0.84	0.50	131,135,135,136	0
30	UNL	e	102	15/-	0.84	0.30	74,93,101,101	0
30	UNL	b	629	8/-	0.84	0.31	72,94,106,108	0
34	DMS	O	309	4/4	0.84	0.38	117,118,118,120	0
34	DMS	O	318	4/4	0.85	0.23	115,117,119,126	0
34	DMS	o	306	4/4	0.85	0.23	118,119,124,125	0
34	DMS	c	532	4/4	0.86	0.13	87,89,96,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	DMS	O	308	4/4	0.86	0.43	124,127,127,132	0
34	DMS	c	540	4/4	0.86	0.20	111,115,116,117	0
36	HTG	B	626	19/19	0.86	0.14	64,93,111,116	0
34	DMS	B	643	4/4	0.86	0.35	99,101,107,111	0
34	DMS	A	425	4/4	0.86	0.50	152,153,153,155	0
34	DMS	v	212	4/4	0.86	0.19	133,135,138,138	0
30	UNL	c	525	6/-	0.86	0.14	95,97,98,101	0
34	DMS	B	642	4/4	0.87	0.31	95,106,108,114	0
30	UNL	m	2801	15/-	0.87	0.21	68,85,119,123	0
29	GOL	v	203	6/6	0.87	0.15	81,87,91,92	0
25	BCR	k	302	40/40	0.87	0.15	53,64,78,79	0
26	SQD	D	2308	45/54	0.87	0.38	92,119,145,154	0
34	DMS	D	2317	4/4	0.88	0.21	99,105,106,109	0
34	DMS	d	420	4/4	0.88	0.46	121,122,123,124	0
34	DMS	d	422	4/4	0.88	0.43	118,121,124,128	0
34	DMS	b	640	4/4	0.88	0.33	110,112,115,117	0
34	DMS	D	2320	4/4	0.88	0.23	144,144,144,147	0
27	LMG	A	413	51/55	0.88	0.20	64,82,106,110	0
34	DMS	v	210	4/4	0.88	0.28	137,140,140,143	0
34	DMS	v	211	4/4	0.88	0.15	120,122,123,123	0
31	JOX	A	418	10/10	0.88	0.10	65,87,88,94	0
34	DMS	c	537	4/4	0.88	0.23	116,122,123,125	0
27	LMG	c	521	49/55	0.88	0.18	60,94,118,121	0
37	DGD	H	103	62/66	0.88	0.25	51,69,100,104	0
34	DMS	V	212	4/4	0.88	0.20	98,111,112,115	0
34	DMS	B	647	4/4	0.88	0.18	105,106,112,112	0
34	DMS	C	534	4/4	0.88	0.16	141,141,143,143	0
34	DMS	c	544	4/4	0.88	0.16	105,110,113,115	0
34	DMS	O	313	4/4	0.88	0.33	103,110,110,111	0
23	CLA	B	610	65/65	0.88	0.14	47,58,69,73	0
36	HTG	b	603	19/19	0.89	0.15	70,89,107,110	0
34	DMS	o	316	4/4	0.89	0.48	85,101,104,108	0
34	DMS	t	102	4/4	0.89	0.23	129,132,137,137	0
34	DMS	u	502	4/4	0.89	0.24	127,129,129,131	0
36	HTG	c	523	19/19	0.89	0.25	99,121,130,133	0
34	DMS	C	535	4/4	0.89	0.18	109,109,110,112	0
34	DMS	C	536	4/4	0.89	0.16	134,137,138,140	0
34	DMS	V	202	4/4	0.89	0.18	115,124,124,124	0
23	CLA	c	515	65/65	0.89	0.17	60,71,101,105	0
34	DMS	c	548	4/4	0.89	0.20	123,130,130,130	0
34	DMS	V	211	4/4	0.89	0.59	109,112,114,114	0
25	BCR	a	2614	40/40	0.89	0.14	38,48,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	DMS	V	213	4/4	0.89	0.20	115,118,119,120	0
34	DMS	d	423	4/4	0.89	0.25	133,137,137,140	0
30	UNL	l	102	16/-	0.89	0.25	67,90,115,121	0
34	DMS	A	428	4/4	0.89	0.18	118,118,118,120	0
23	CLA	C	514	65/65	0.89	0.23	66,78,111,115	0
34	DMS	o	315	4/4	0.89	0.29	135,137,138,138	0
37	DGD	C	518	62/66	0.90	0.16	48,63,101,111	0
34	DMS	c	545	4/4	0.90	0.22	123,124,125,127	0
34	DMS	O	315	4/4	0.90	0.35	107,114,115,121	0
34	DMS	o	308	4/4	0.90	0.34	127,131,133,135	0
38	LHG	D	2309	49/49	0.90	0.21	50,63,78,81	0
34	DMS	O	317	4/4	0.90	0.23	114,115,117,120	0
34	DMS	b	641	4/4	0.90	0.20	75,76,78,84	4
29	GOL	A	417	6/6	0.90	0.12	110,113,118,126	0
34	DMS	C	531	4/4	0.90	0.16	98,102,103,107	0
29	GOL	A	415	6/6	0.90	0.27	72,80,92,93	0
34	DMS	l	104	4/4	0.91	0.15	134,136,139,140	0
34	DMS	b	635	4/4	0.91	0.20	98,102,105,109	0
34	DMS	T	105	4/4	0.91	0.34	124,129,130,130	0
30	UNL	D	2315	18/-	0.91	0.24	65,90,111,113	0
34	DMS	A	426	4/4	0.91	0.19	94,103,103,114	0
34	DMS	o	311	4/4	0.91	0.28	86,101,102,104	0
30	UNL	d	406	18/-	0.91	0.23	70,93,104,106	0
23	CLA	B	602	65/65	0.91	0.30	58,83,121,131	0
34	DMS	O	316	4/4	0.91	0.21	107,108,109,110	0
29	GOL	b	644	6/6	0.91	0.39	75,97,105,105	0
34	DMS	v	208	4/4	0.91	0.18	125,126,127,129	0
23	CLA	c	506	65/65	0.91	0.21	47,60,66,82	0
38	LHG	l	103	49/49	0.91	0.20	46,57,79,86	0
26	SQD	d	417	33/54	0.91	0.18	100,120,146,151	0
29	GOL	a	2618	6/6	0.91	0.11	107,112,115,116	0
34	DMS	v	213	4/4	0.91	0.20	119,119,119,123	0
23	CLA	b	606	65/65	0.92	0.31	66,88,129,133	0
23	CLA	b	620	65/65	0.92	0.12	47,57,88,90	0
38	LHG	d	412	49/49	0.92	0.28	55,66,79,85	0
23	CLA	C	504	65/65	0.92	0.15	47,58,66,80	0
34	DMS	V	206	4/4	0.92	0.42	81,98,100,101	0
34	DMS	o	314	4/4	0.92	0.21	112,113,117,118	0
23	CLA	B	603	65/65	0.92	0.17	41,54,70,76	0
36	HTG	V	204	19/19	0.92	0.21	71,95,125,126	0
34	DMS	V	208	4/4	0.93	0.34	99,108,109,113	0
25	BCR	T	102	40/40	0.93	0.16	44,56,82,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	615	65/65	0.93	0.13	49,56,63,67	0
23	CLA	C	507	65/65	0.93	0.14	57,81,109,112	0
34	DMS	c	539	4/4	0.93	0.21	110,112,114,119	0
34	DMS	o	307	4/4	0.93	0.23	104,107,109,111	0
31	JOX	a	2617	10/10	0.93	0.11	64,69,89,91	0
36	HTG	o	301	19/19	0.93	0.13	62,70,85,87	0
31	JOX	a	2619	10/10	0.93	0.18	46,49,54,56	10
23	CLA	c	505	65/65	0.93	0.24	45,54,70,78	0
23	CLA	D	2304	65/65	0.93	0.14	49,58,128,136	0
37	DGD	c	519	62/66	0.93	0.19	52,65,112,125	0
36	HTG	C	521	19/19	0.93	0.24	108,112,121,121	0
34	DMS	O	307	4/4	0.93	0.15	98,107,107,110	0
23	CLA	C	510	65/65	0.93	0.15	53,63,84,88	0
25	BCR	B	619	40/40	0.93	0.20	45,55,76,79	0
25	BCR	B	633	40/40	0.93	0.17	46,62,78,79	0
25	BCR	C	515	40/40	0.93	0.13	55,78,88,89	0
34	DMS	u	504	4/4	0.93	0.31	74,90,95,98	0
34	DMS	d	418	4/4	0.93	0.30	98,99,100,111	0
34	DMS	v	209	4/4	0.93	0.46	82,93,96,102	0
41	MG	k	303	1/1	0.93	0.07	91,91,91,91	0
34	DMS	B	641	4/4	0.94	0.21	93,102,102,104	0
34	DMS	o	305	4/4	0.94	0.33	117,117,119,120	0
23	CLA	b	614	65/65	0.94	0.11	52,63,74,86	0
23	CLA	C	508	65/65	0.94	0.12	51,64,83,84	0
23	CLA	b	619	65/65	0.94	0.19	41,49,109,113	0
36	HTG	b	602	19/19	0.94	0.11	56,64,79,79	0
25	BCR	C	516	40/40	0.94	0.12	54,66,87,91	0
23	CLA	B	615	65/65	0.94	0.16	40,49,105,113	0
34	DMS	C	530	4/4	0.94	0.15	115,117,118,123	0
34	DMS	o	313	4/4	0.94	0.37	100,102,103,111	0
23	CLA	B	617	65/65	0.94	0.15	49,59,122,126	0
34	DMS	c	534	4/4	0.94	0.16	142,143,143,144	0
25	BCR	b	623	40/40	0.94	0.21	43,57,74,79	0
34	DMS	U	503	4/4	0.94	0.38	118,119,119,120	0
33	PL9	d	411	55/55	0.94	0.16	37,46,56,65	0
34	DMS	u	503	4/4	0.94	0.14	81,101,102,103	0
34	DMS	U	505	4/4	0.94	0.13	66,72,89,105	0
25	BCR	d	410	40/40	0.94	0.11	54,61,83,86	0
23	CLA	B	607	65/65	0.94	0.11	40,52,83,91	0
34	DMS	c	543	4/4	0.94	0.20	116,121,122,123	0
37	DGD	c	518	62/66	0.94	0.18	43,57,106,110	0
25	BCR	y	101	40/40	0.94	0.10	53,65,71,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	DMS	A	427	4/4	0.94	0.33	103,106,107,108	0
34	DMS	V	209	4/4	0.94	0.26	81,89,95,100	0
29	GOL	O	303	6/6	0.94	0.19	96,106,114,114	0
35	CA	b	605	1/1	0.94	0.06	72,72,72,72	0
26	SQD	A	412	46/54	0.94	0.16	76,88,106,108	0
27	LMG	d	414	51/55	0.94	0.12	54,69,105,109	0
23	CLA	c	510	65/65	0.94	0.12	48,62,75,83	0
23	CLA	B	611	65/65	0.94	0.21	47,55,67,72	0
34	DMS	a	2621	4/4	0.94	0.14	115,115,116,118	0
24	PHO	A	409	64/64	0.94	0.17	41,49,58,61	0
34	DMS	C	528	4/4	0.95	0.12	110,114,115,117	0
23	CLA	b	612	65/65	0.95	0.14	34,44,63,67	0
23	CLA	c	516	65/65	0.95	0.18	61,79,103,108	0
23	CLA	d	409	65/65	0.95	0.11	54,61,126,133	0
24	PHO	A	408	64/64	0.95	0.12	35,43,49,52	0
26	SQD	a	2615	48/54	0.95	0.13	66,86,112,114	0
23	CLA	C	513	65/65	0.95	0.11	62,75,115,122	0
25	BCR	B	618	40/40	0.95	0.17	43,51,57,60	0
34	DMS	D	2319	4/4	0.95	0.27	104,105,107,118	0
23	CLA	B	616	65/65	0.95	0.12	43,55,83,95	0
33	PL9	D	2306	55/55	0.95	0.10	38,47,55,64	0
34	DMS	b	636	4/4	0.95	0.24	101,102,104,106	0
23	CLA	b	616	65/65	0.95	0.22	40,47,68,73	0
23	CLA	D	2303	65/65	0.95	0.14	33,42,62,72	0
23	CLA	C	509	65/65	0.95	0.14	46,56,115,132	0
25	BCR	K	101	40/40	0.95	0.10	57,64,69,70	0
34	DMS	O	310	4/4	0.95	0.18	103,103,103,108	0
27	LMG	D	2312	47/55	0.95	0.18	48,59,97,100	0
34	DMS	O	312	4/4	0.95	0.31	108,109,110,113	0
23	CLA	b	621	65/65	0.95	0.15	48,61,128,132	0
25	BCR	Y	302	40/40	0.95	0.09	55,64,70,71	0
23	CLA	c	504	65/65	0.95	0.12	45,59,72,83	0
25	BCR	b	622	40/40	0.95	0.20	44,54,66,68	0
29	GOL	C	526	6/6	0.95	0.18	65,81,89,93	0
34	DMS	B	639	4/4	0.95	0.12	84,84,91,92	0
23	CLA	B	612	65/65	0.95	0.20	39,47,66,70	0
38	LHG	d	403	43/49	0.95	0.16	46,59,91,96	0
25	BCR	b	624	40/40	0.95	0.11	48,61,76,76	0
38	LHG	d	413	49/49	0.95	0.17	40,49,71,73	0
25	BCR	c	517	40/40	0.95	0.10	52,66,87,89	0
23	CLA	b	609	65/65	0.95	0.23	37,46,85,92	0
34	DMS	B	644	4/4	0.95	0.26	82,82,86,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	c	509	65/65	0.95	0.11	57,76,111,115	0
23	CLA	b	611	65/65	0.95	0.10	47,53,90,96	0
41	MG	j	2703	1/1	0.95	0.19	60,60,60,60	0
23	CLA	c	514	65/65	0.95	0.12	55,65,73,75	0
34	DMS	C	529	4/4	0.96	0.19	94,101,101,102	0
34	DMS	a	2623	4/4	0.96	0.15	100,107,108,111	0
34	DMS	v	206	4/4	0.96	0.09	84,102,103,104	0
34	DMS	v	207	4/4	0.96	0.20	107,110,111,114	0
23	CLA	C	512	65/65	0.96	0.08	55,63,74,81	0
23	CLA	C	502	65/65	0.96	0.17	48,58,75,83	0
23	CLA	b	617	65/65	0.96	0.21	41,49,56,58	0
25	BCR	z	101	40/40	0.96	0.17	68,78,93,97	0
23	CLA	C	503	65/65	0.96	0.19	41,53,70,76	0
34	DMS	b	639	4/4	0.96	0.09	93,96,97,98	0
37	DGD	C	519	58/66	0.96	0.14	43,53,79,93	0
23	CLA	A	410	65/65	0.96	0.11	41,50,123,127	0
25	BCR	B	620	40/40	0.96	0.09	50,56,67,71	0
35	CA	o	302	1/1	0.96	0.07	74,74,74,74	0
23	CLA	C	505	65/65	0.96	0.14	45,54,89,93	0
37	DGD	c	520	62/66	0.96	0.15	47,59,86,95	0
23	CLA	a	2613	65/65	0.96	0.13	39,48,130,137	0
23	CLA	B	613	65/65	0.96	0.21	39,46,56,61	0
38	LHG	D	2310	49/49	0.96	0.13	45,52,69,85	0
25	BCR	D	2305	40/40	0.96	0.19	50,60,85,86	0
38	LHG	L	101	49/49	0.96	0.12	46,57,73,76	0
34	DMS	c	536	4/4	0.96	0.26	64,74,76,78	0
23	CLA	b	607	65/65	0.96	0.12	48,57,69,76	0
23	CLA	c	508	65/65	0.96	0.12	49,57,80,86	0
34	DMS	o	312	4/4	0.96	0.23	95,98,101,105	0
23	CLA	b	608	65/65	0.96	0.14	40,52,71,75	0
23	CLA	B	608	65/65	0.96	0.15	34,44,61,73	0
23	CLA	c	511	65/65	0.96	0.23	46,56,114,137	0
23	CLA	B	604	65/65	0.96	0.21	42,51,66,72	0
23	CLA	B	605	65/65	0.96	0.26	37,44,85,94	0
23	CLA	C	511	65/65	0.96	0.16	47,56,68,78	0
24	PHO	a	2611	64/64	0.97	0.14	38,42,49,57	0
24	PHO	a	2612	64/64	0.97	0.15	39,49,59,65	0
25	BCR	A	411	40/40	0.97	0.13	38,48,58,62	0
23	CLA	A	407	65/65	0.97	0.15	36,47,109,115	0
23	CLA	C	506	65/65	0.97	0.14	51,59,80,81	0
23	CLA	b	618	65/65	0.97	0.26	40,46,93,96	0
23	CLA	b	610	65/65	0.97	0.15	39,49,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	DMS	d	419	4/4	0.97	0.18	92,94,98,106	0
23	CLA	c	512	65/65	0.97	0.24	51,59,89,100	0
34	DMS	d	421	4/4	0.97	0.13	75,89,94,98	0
38	LHG	D	2311	39/49	0.97	0.11	51,59,92,97	0
23	CLA	c	513	65/65	0.97	0.26	46,57,68,79	0
23	CLA	a	2610	65/65	0.97	0.19	38,46,116,121	0
23	CLA	B	614	65/65	0.97	0.21	37,45,91,99	0
23	CLA	b	613	65/65	0.97	0.13	41,53,72,77	0
23	CLA	d	402	65/65	0.97	0.15	35,41,50,62	0
23	CLA	B	606	65/65	0.97	0.23	37,47,62,64	0
34	DMS	D	2316	4/4	0.97	0.12	65,77,86,90	0
39	HEM	F	101	43/43	0.97	0.13	61,71,100,119	0
34	DMS	a	2622	4/4	0.97	0.46	105,107,110,115	0
23	CLA	B	609	65/65	0.97	0.19	45,54,73,79	0
23	CLA	c	507	65/65	0.97	0.20	46,56,91,95	0
34	DMS	b	634	4/4	0.97	0.21	81,86,88,92	0
37	DGD	C	517	62/66	0.97	0.20	42,55,109,112	0
23	CLA	d	408	65/65	0.98	0.18	31,42,60,71	0
35	CA	c	503	1/1	0.98	0.03	73,73,73,73	0
34	DMS	D	2318	4/4	0.98	0.25	82,85,90,92	0
23	CLA	a	2609	65/65	0.98	0.18	35,41,55,69	0
23	CLA	A	406	65/65	0.98	0.09	34,41,51,63	0
34	DMS	C	532	4/4	0.98	0.11	67,68,73,74	0
34	DMS	V	205	4/4	0.98	0.15	67,74,74,77	0
29	GOL	B	648	6/6	0.98	0.08	54,74,84,89	0
34	DMS	c	533	4/4	0.98	0.12	59,63,63,65	0
23	CLA	A	405	65/65	0.98	0.12	33,41,55,77	0
34	DMS	c	535	4/4	0.98	0.25	108,108,110,114	0
34	DMS	B	638	4/4	0.98	0.16	61,68,73,82	0
39	HEM	e	103	43/43	0.98	0.13	65,76,109,133	0
32	BCT	A	421	4/4	0.98	0.07	59,60,65,75	0
34	DMS	V	210	4/4	0.98	0.41	101,105,108,111	0
41	MG	J	302	1/1	0.98	0.10	58,58,58,58	0
32	BCT	a	2608	4/4	0.98	0.16	56,61,66,74	0
35	CA	B	601	1/1	0.98	0.04	68,68,68,68	0
35	CA	O	301	1/1	0.98	0.14	77,77,77,77	0
42	HEC	V	201	43/43	0.98	0.07	41,46,52,56	0
42	HEC	v	201	43/43	0.98	0.11	49,56,62,69	0
22	CL	A	403	1/1	0.99	0.05	46,46,46,46	0
34	DMS	A	424	4/4	0.99	0.12	48,50,52,59	0
34	DMS	B	636	4/4	0.99	0.13	43,47,47,59	0
34	DMS	C	533	4/4	0.99	0.09	61,64,65,66	0

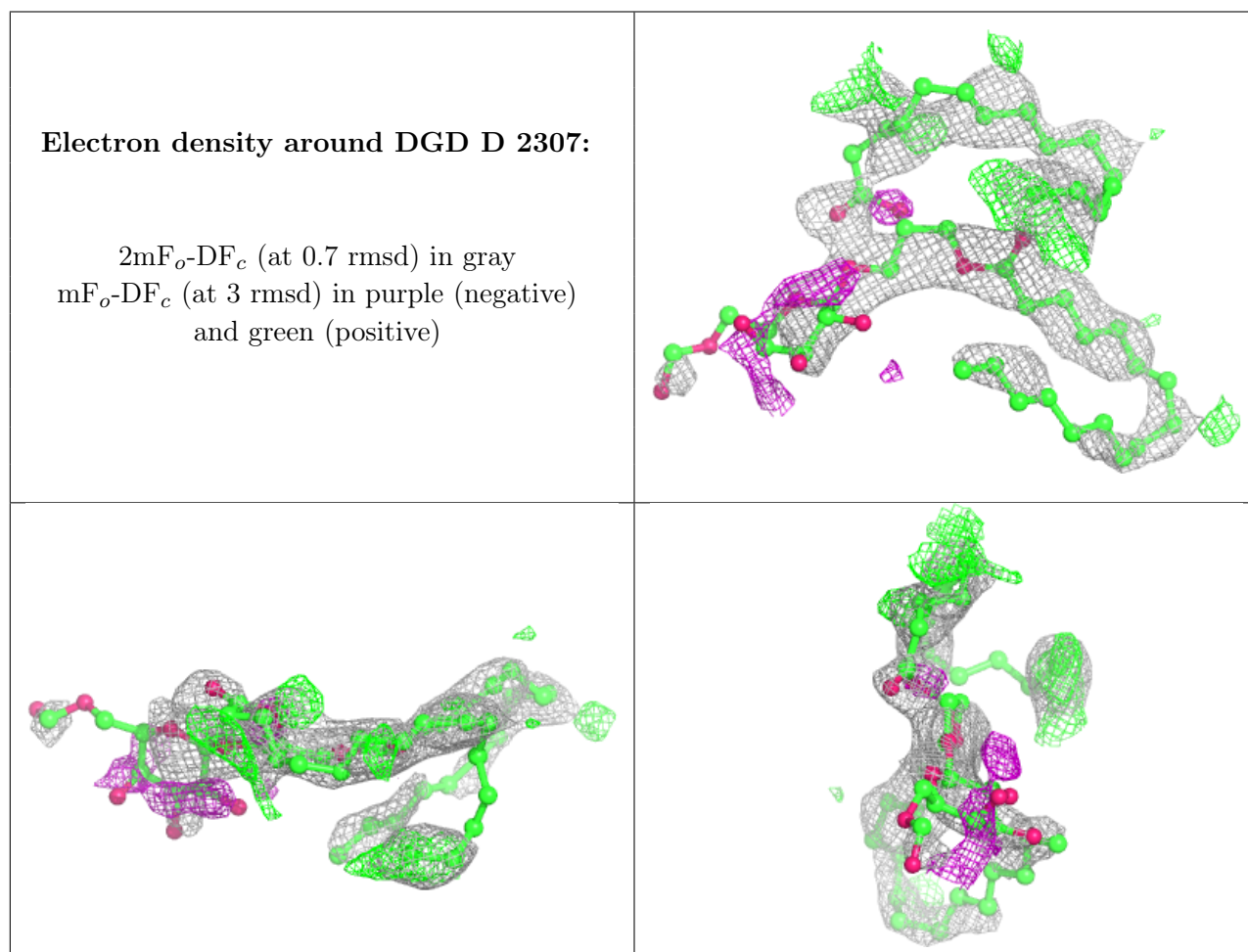
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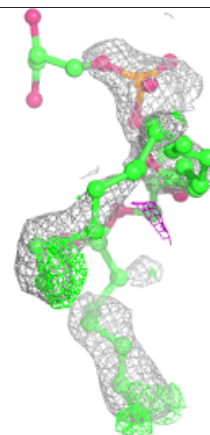
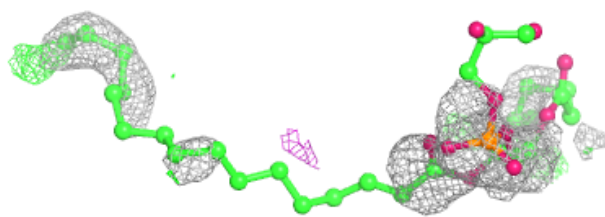
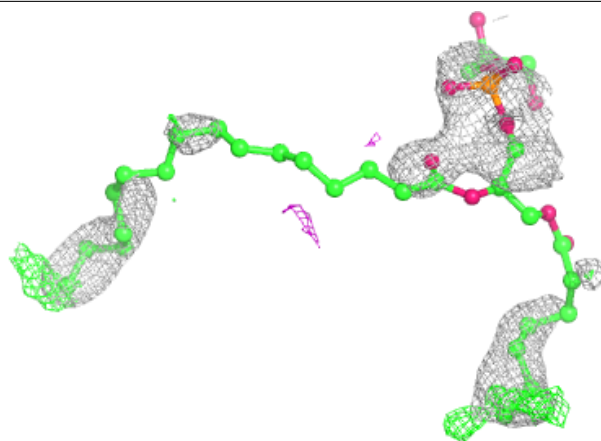
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	DMS	b	633	4/4	0.99	0.12	45,50,52,61	0
34	DMS	v	205	4/4	0.99	0.14	75,77,83,86	0
22	CL	A	404	1/1	0.99	0.10	43,43,43,43	0
22	CL	a	2606	1/1	0.99	0.04	48,48,48,48	0
20	OEX	A	401	10/10	0.99	0.12	41,46,50,52	0
20	OEX	a	2604	10/10	0.99	0.10	41,46,51,52	0
21	FE2	A	402	1/1	0.99	0.05	54,54,54,54	0
34	DMS	o	304	4/4	0.99	0.11	43,53,55,59	0
22	CL	a	2607	1/1	1.00	0.16	46,46,46,46	0
21	FE2	a	2605	1/1	1.00	0.07	52,52,52,52	0

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

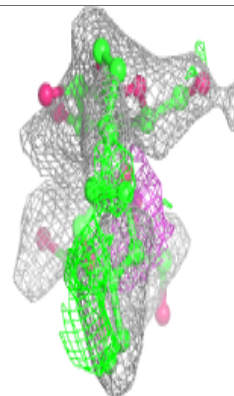
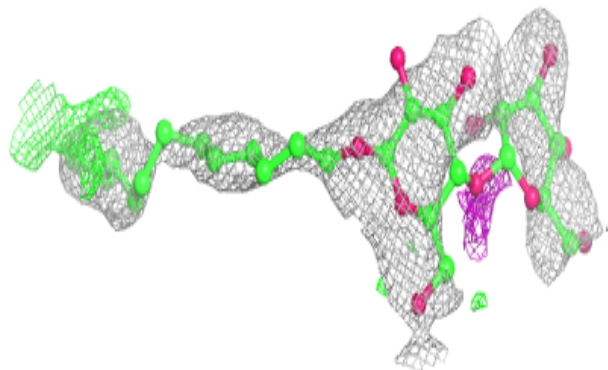
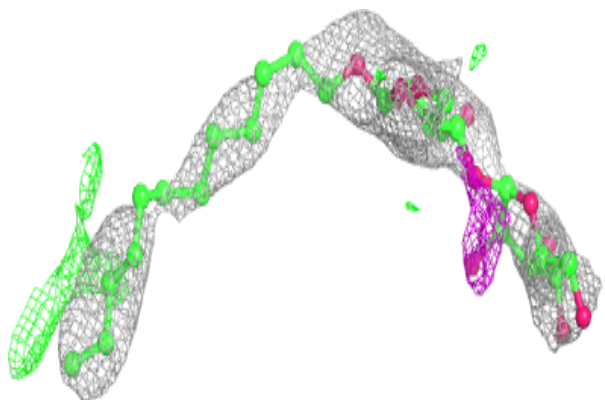


**Electron density around LHG e 101:**

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

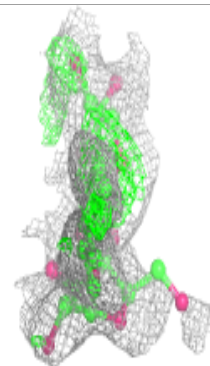
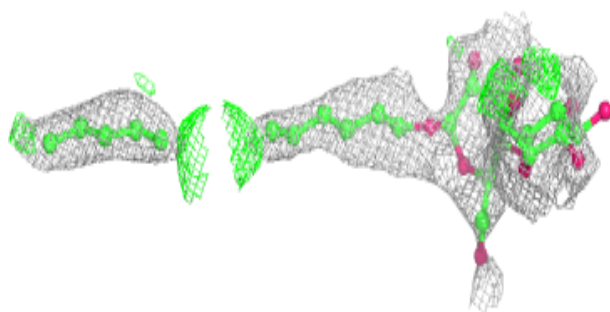
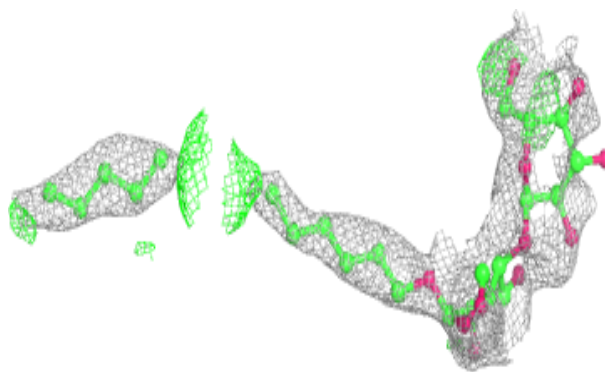
**Electron density around LMT m 2804:**

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

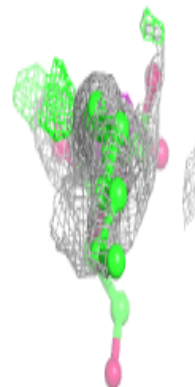
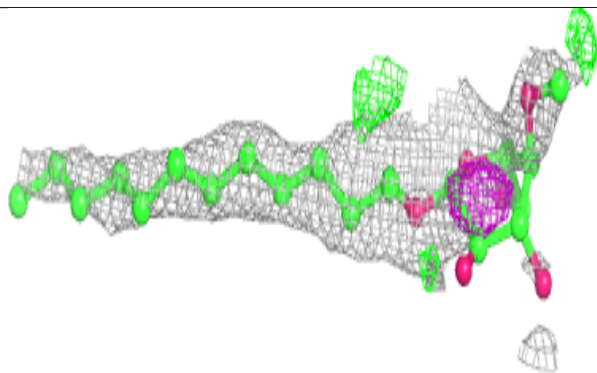
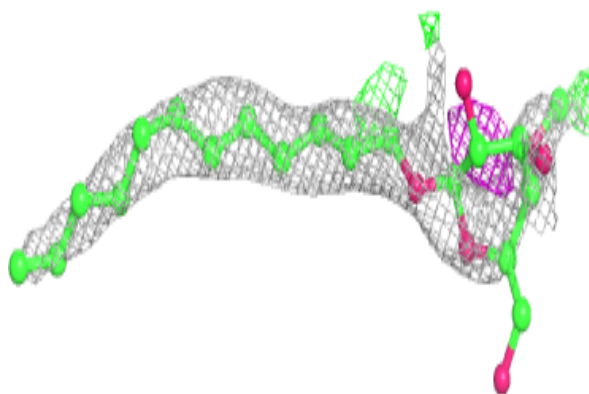


**Electron density around LMT j 2701:**

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

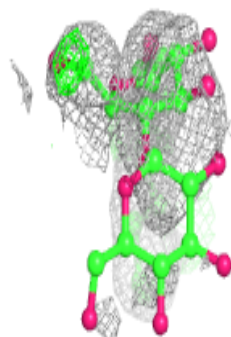
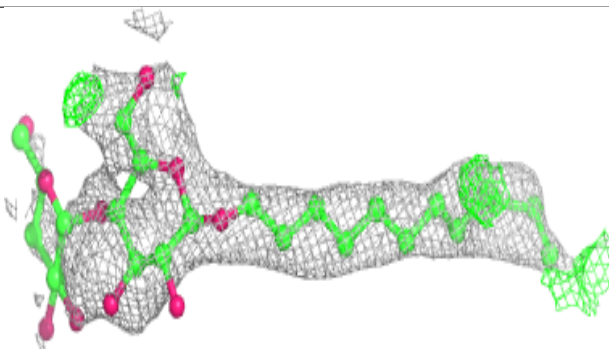
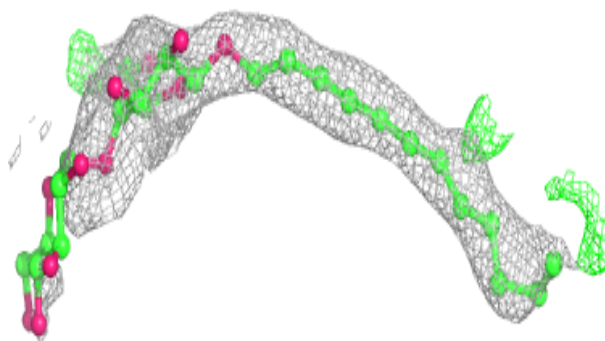
**Electron density around LMT d 404:**

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

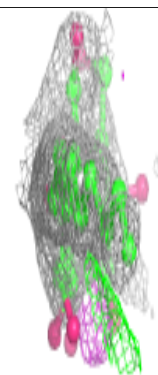
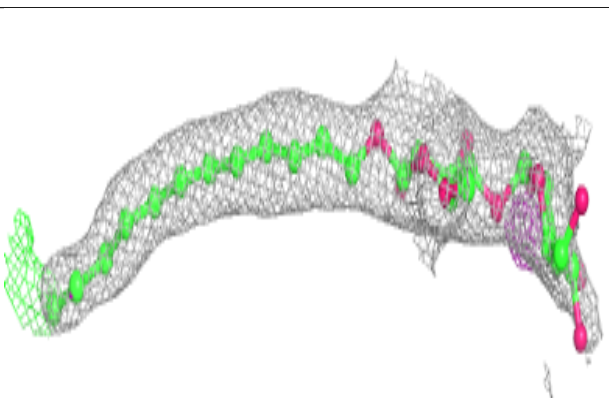
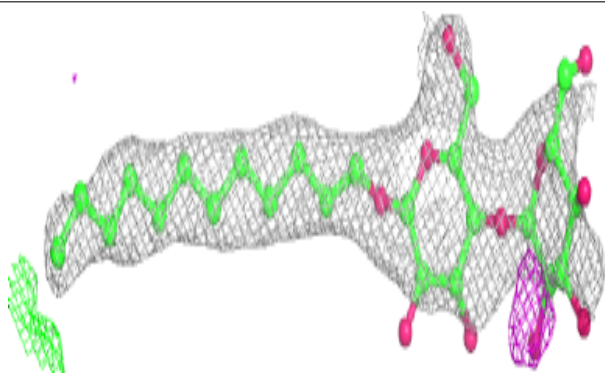


**Electron density around LMT M 101:**

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

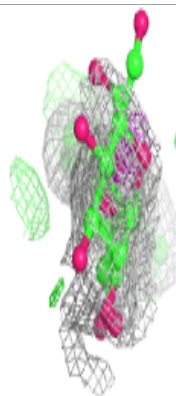
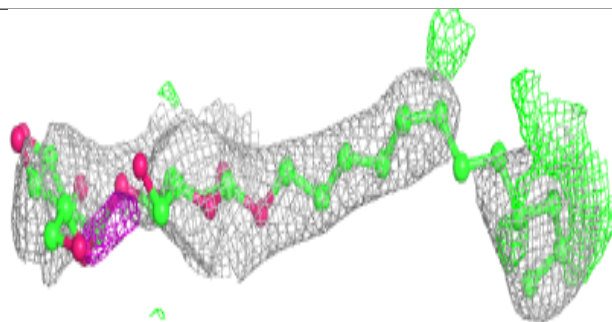
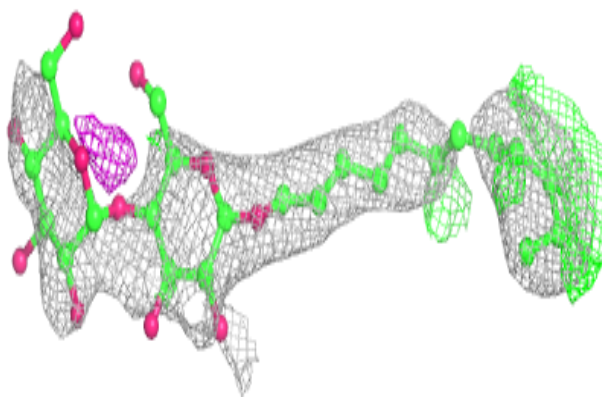
**Electron density around LMT M 102:**

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

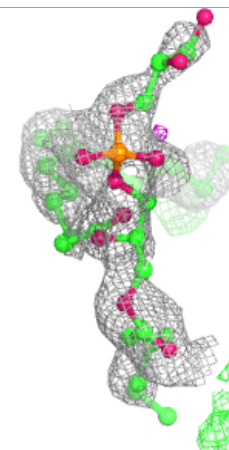
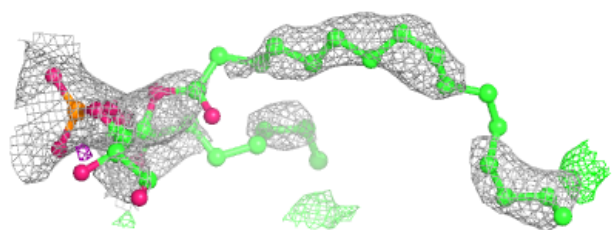
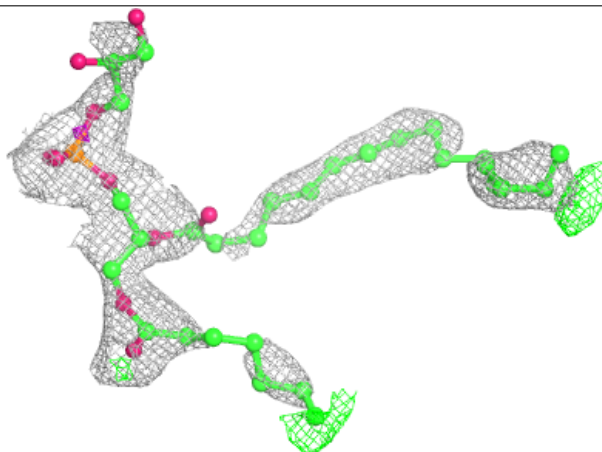


**Electron density around LMT B 634:**

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

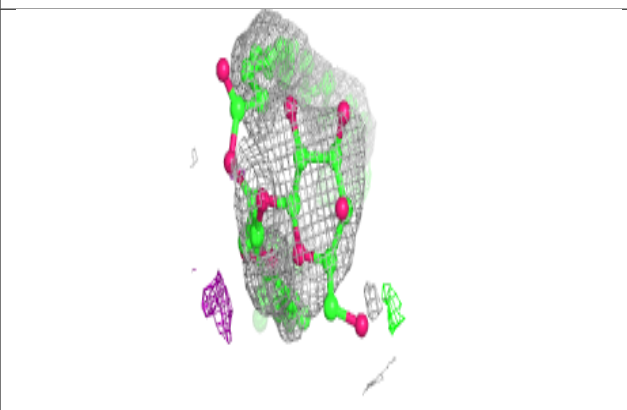
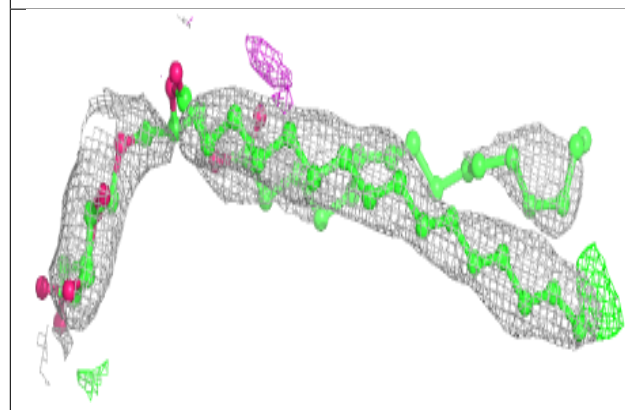
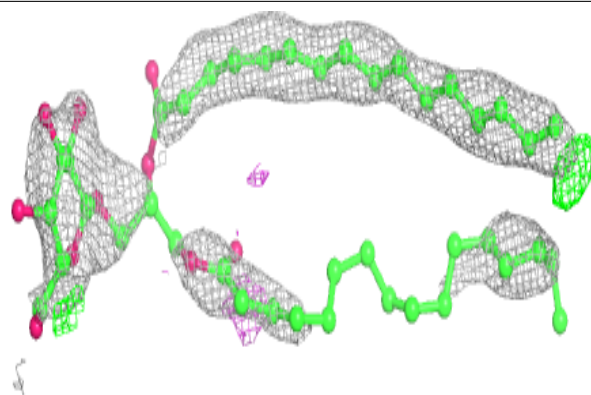
**Electron density around LHG E 101:**

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

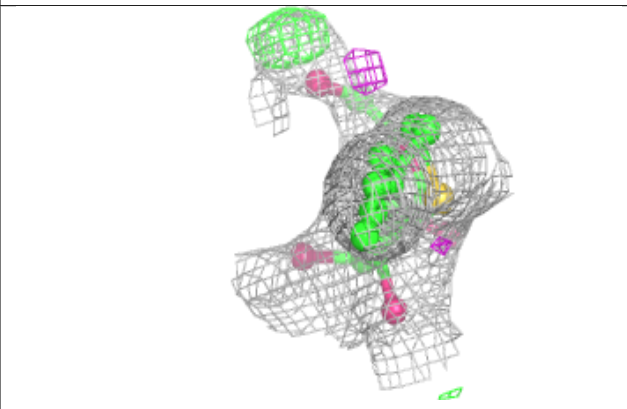
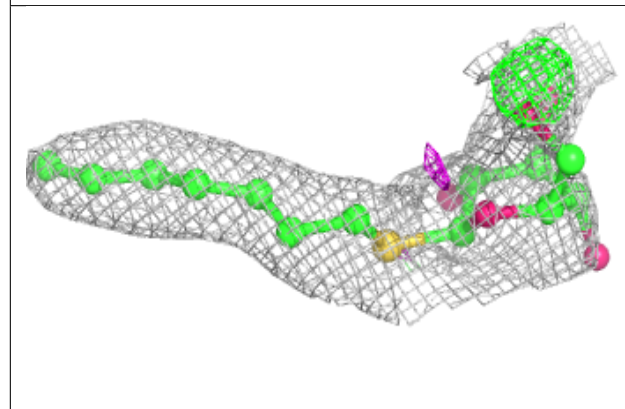
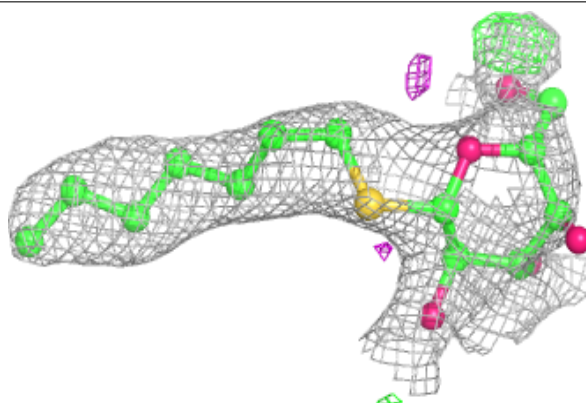


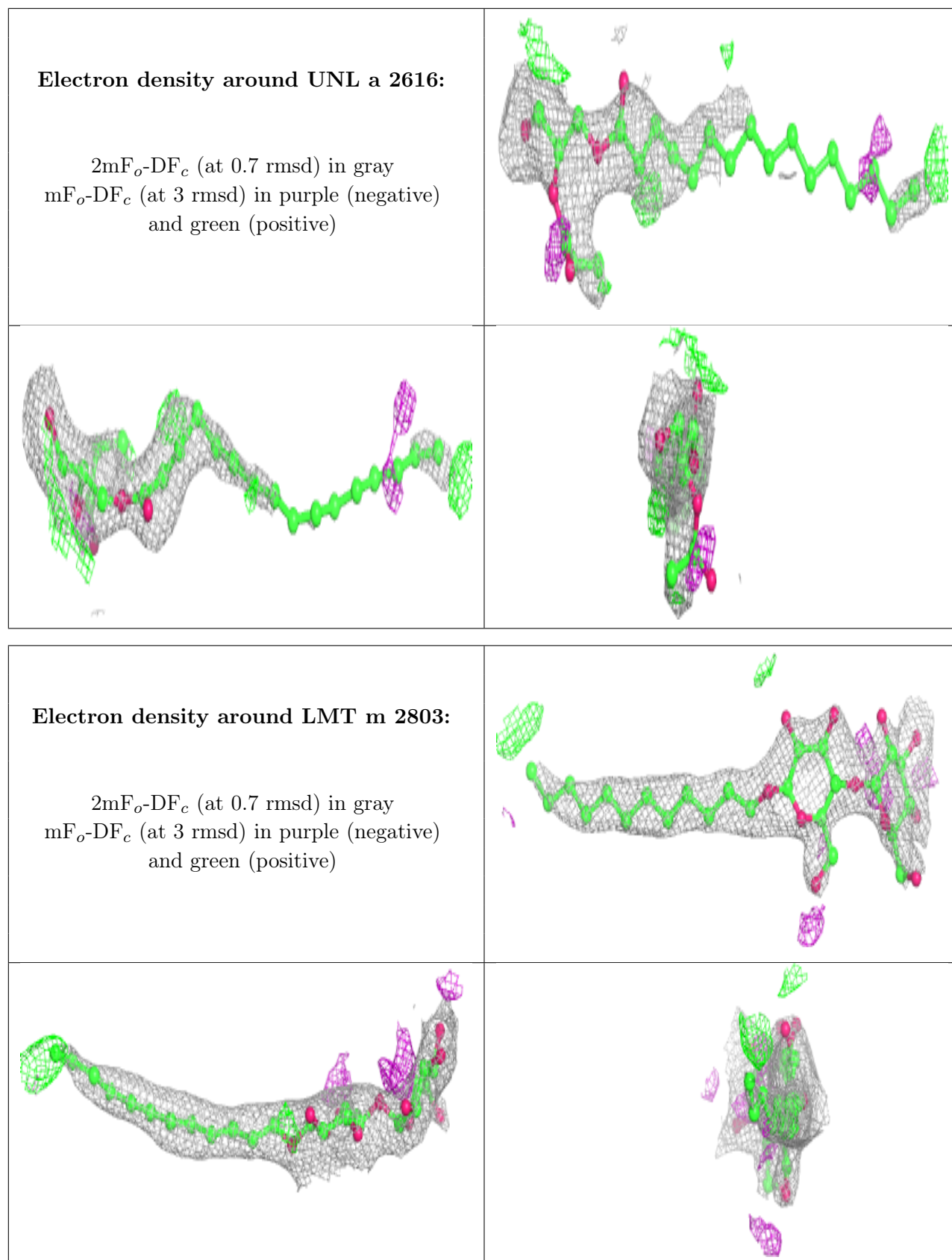
**Electron density around LMG C 527:**

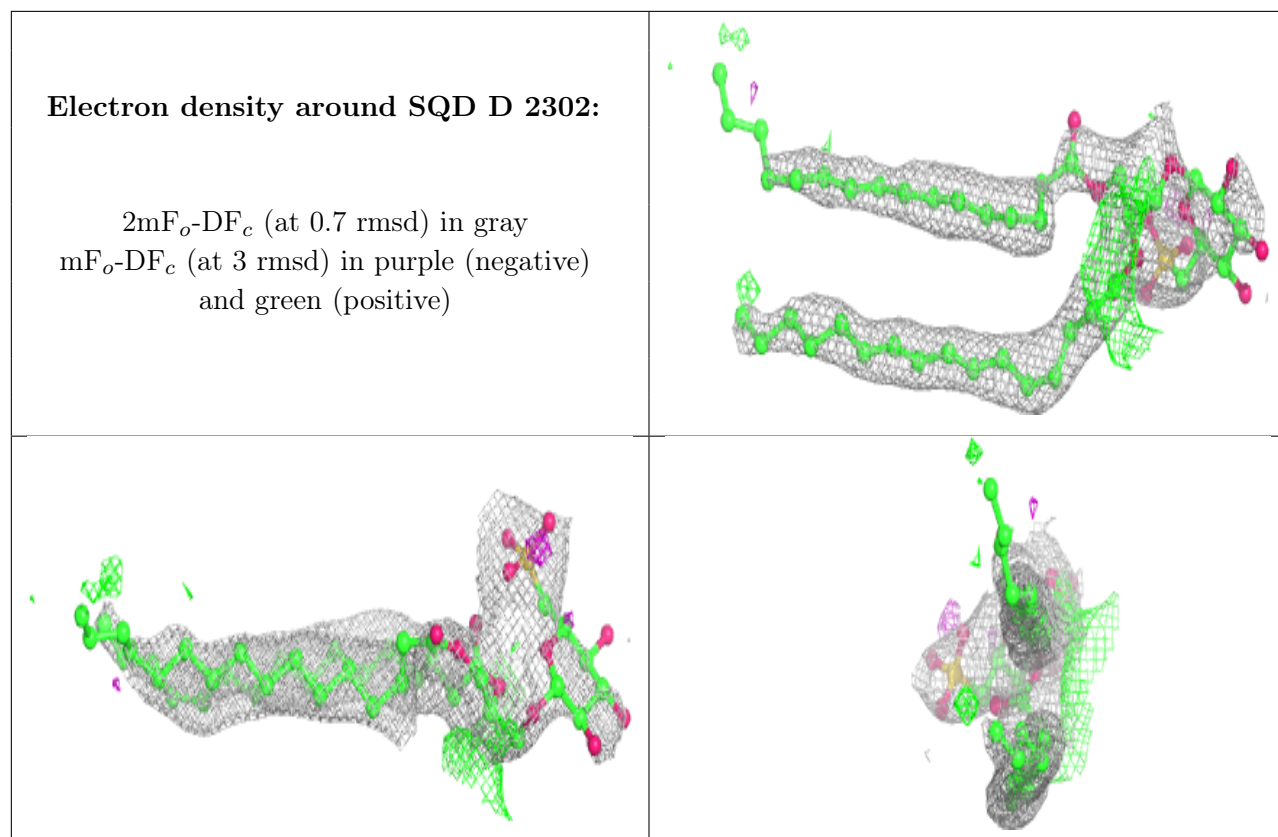
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HTG i 102:**

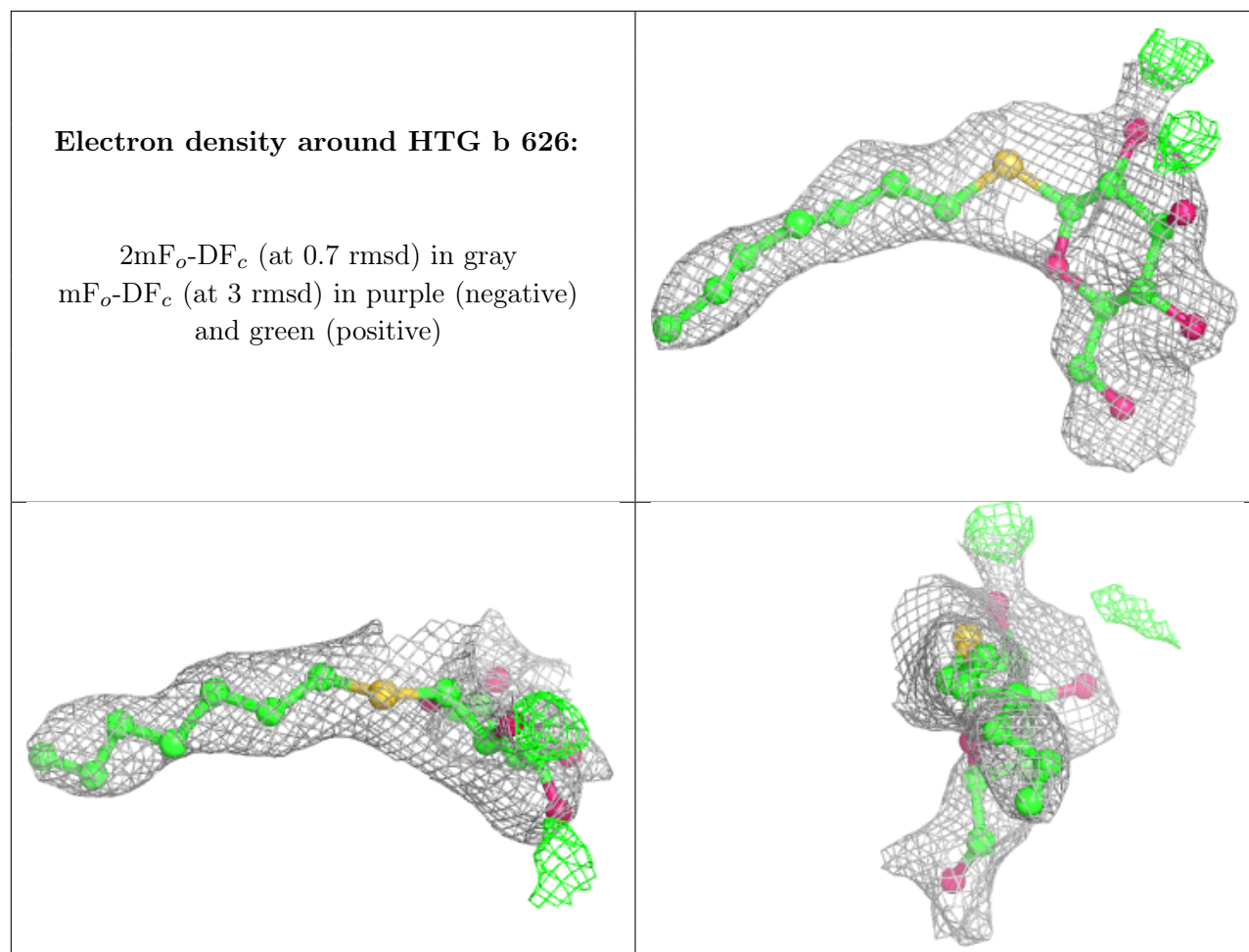
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





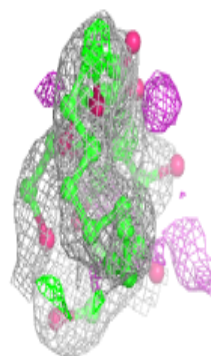
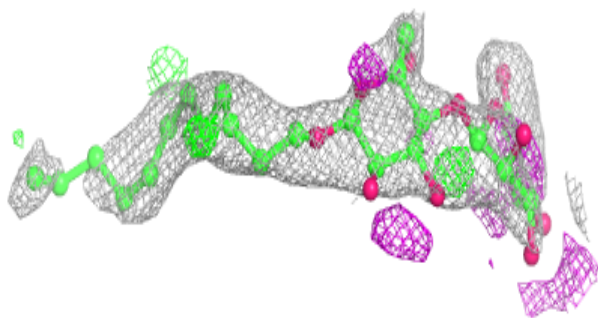
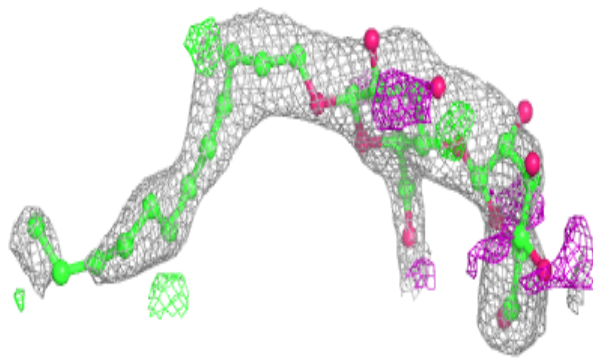




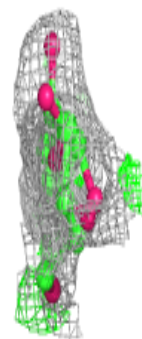
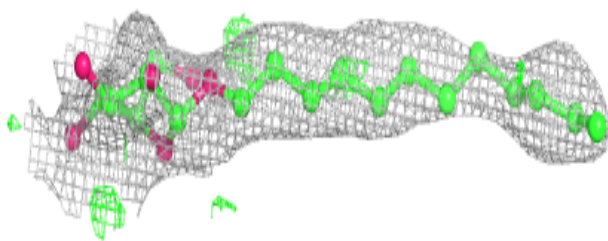
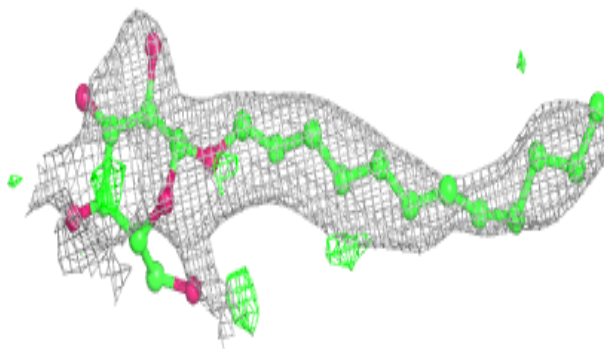


**Electron density around LMT d 401:**

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

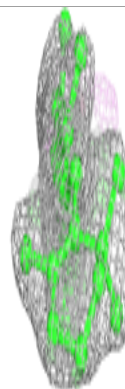
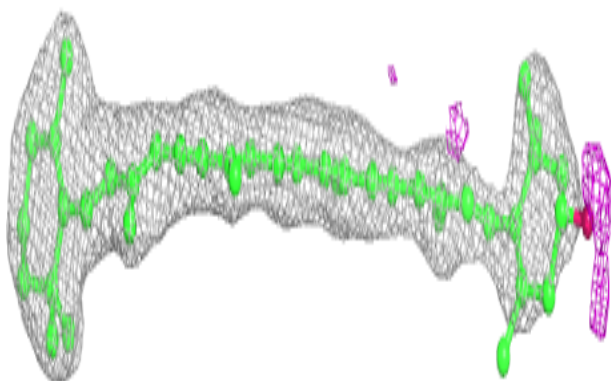
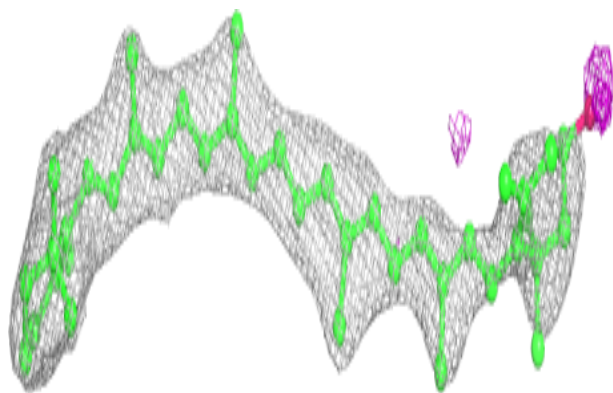
**Electron density around LMT J 303:**

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

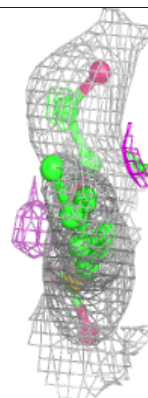
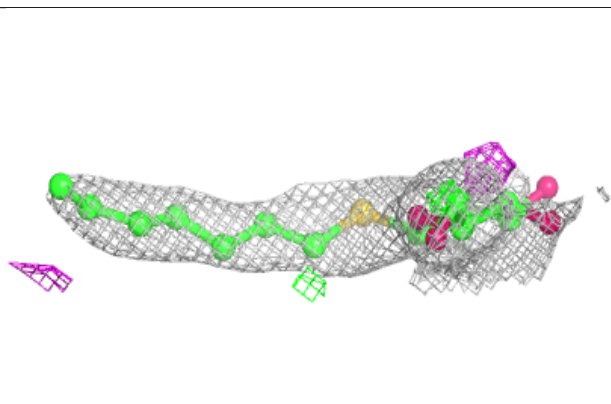
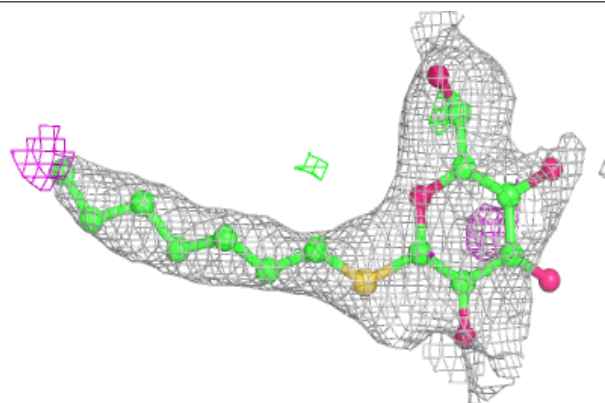


**Electron density around RRX h 101:**

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

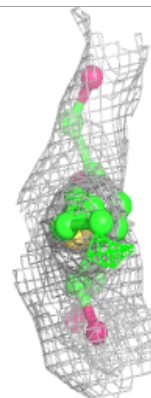
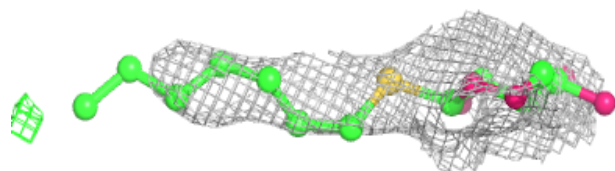
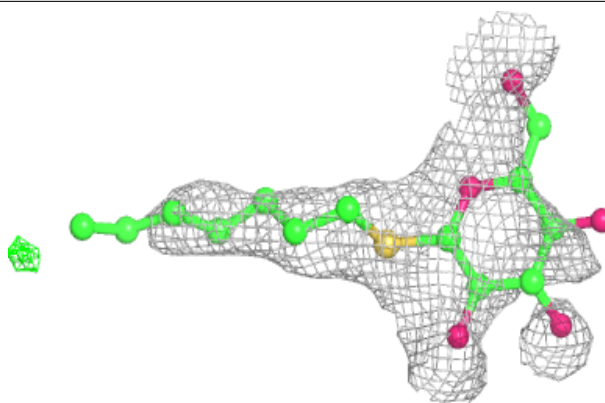
**Electron density around HTG B 627:**

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

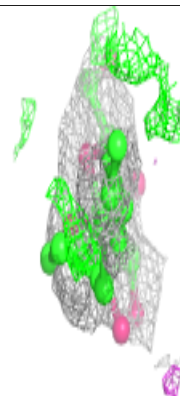
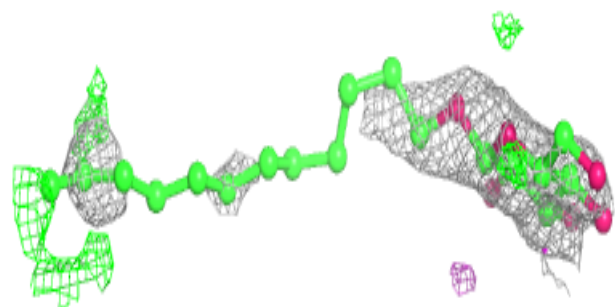
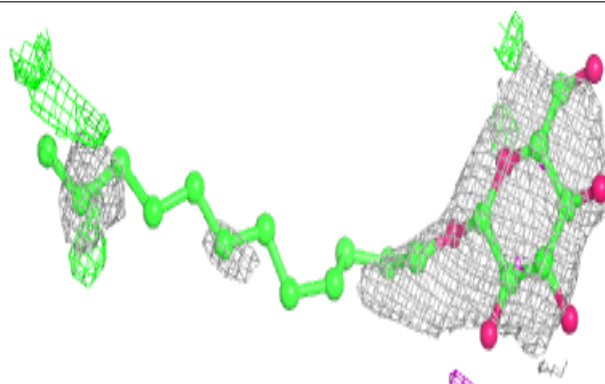


**Electron density around HTG c 526:**

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

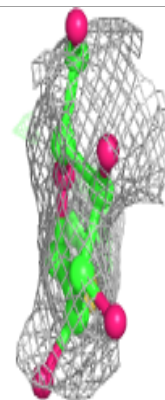
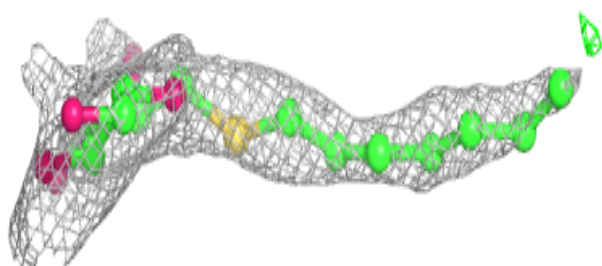
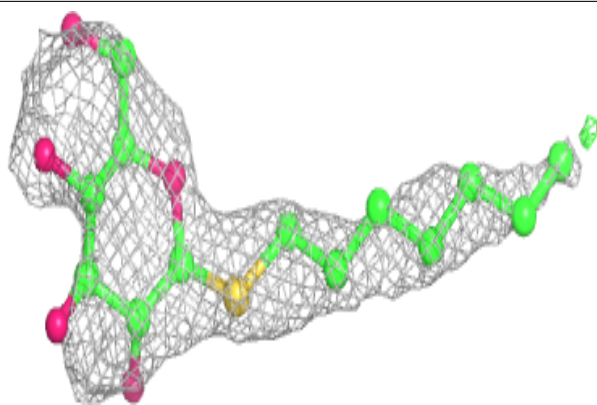
**Electron density around LMT F 102:**

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

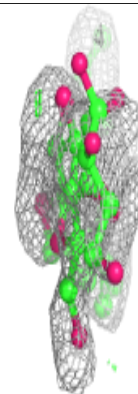
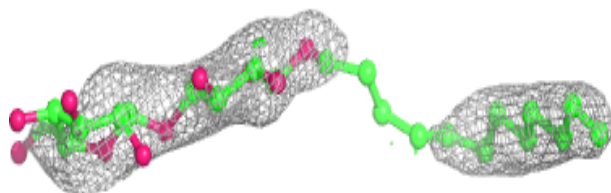
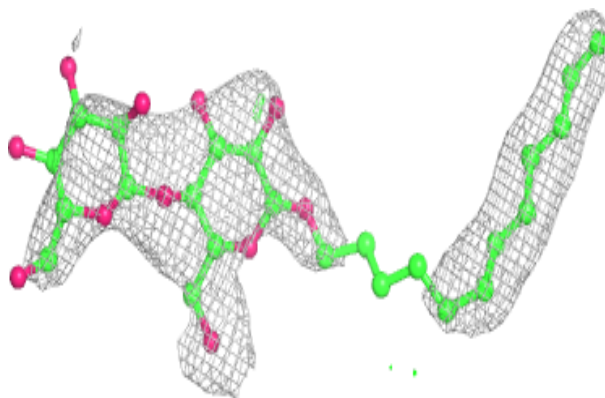


**Electron density around HTG B 625:**

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

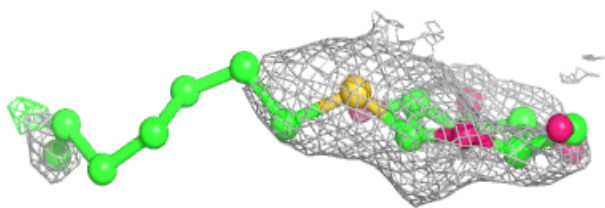
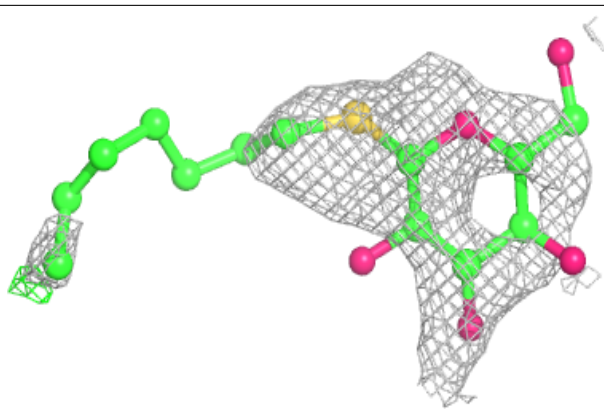
**Electron density around LMT Z 101:**

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

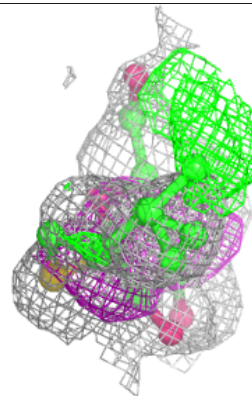
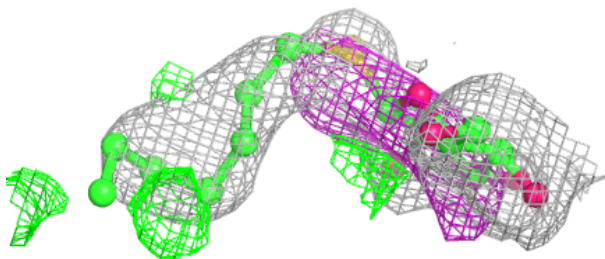
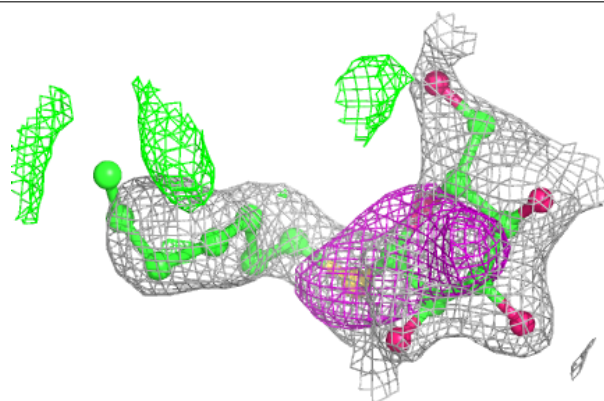


**Electron density around HTG d 407:**

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

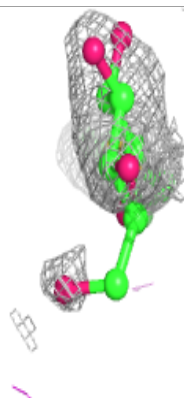
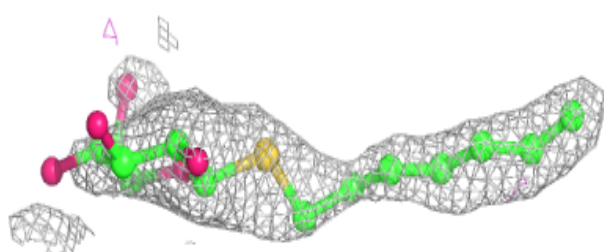
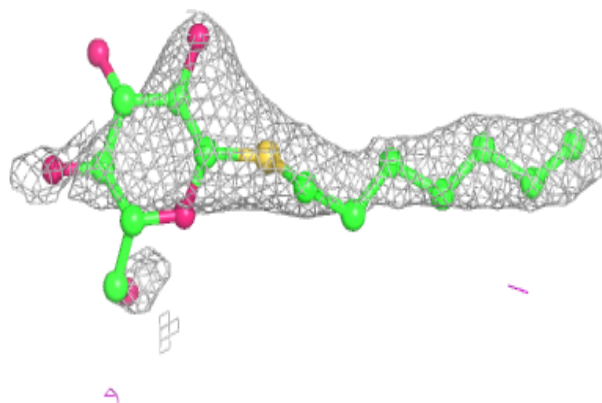
**Electron density around HTG B 624 (A):**

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

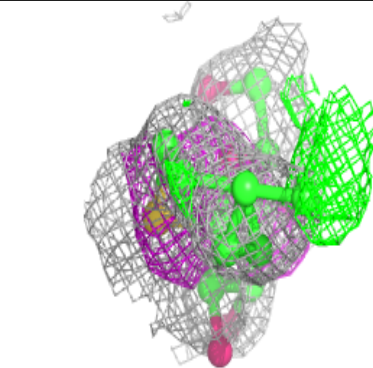
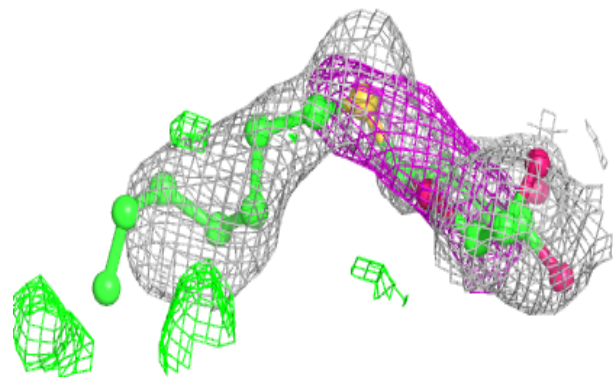
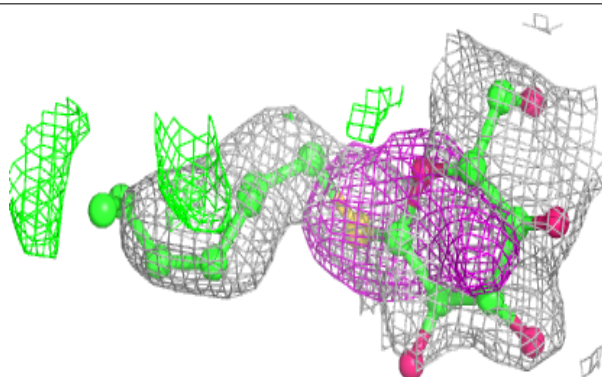


**Electron density around HTG c 524:**

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

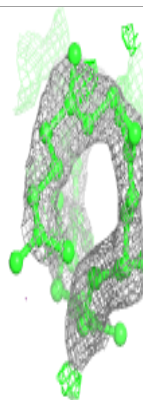
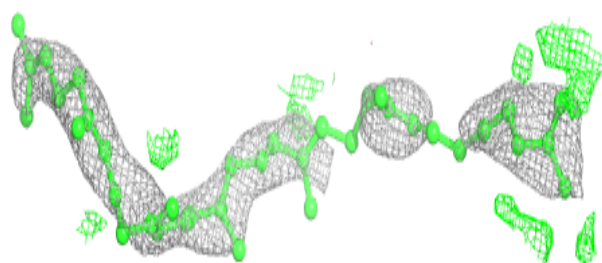
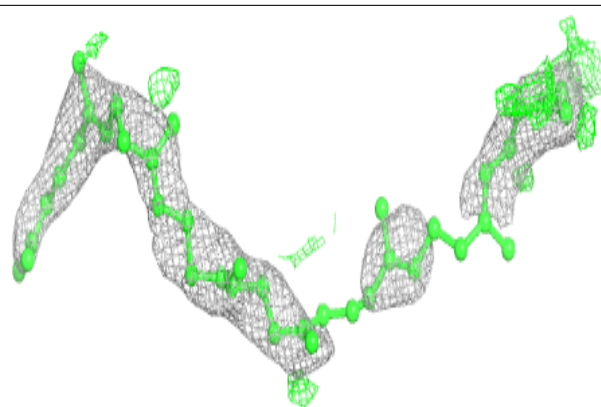
**Electron density around HTG B 624 (B):**

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

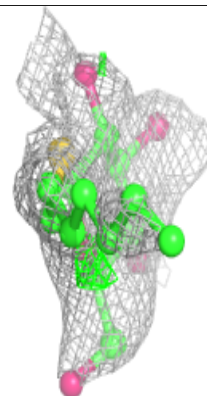
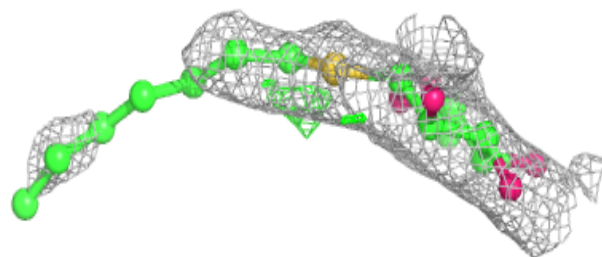
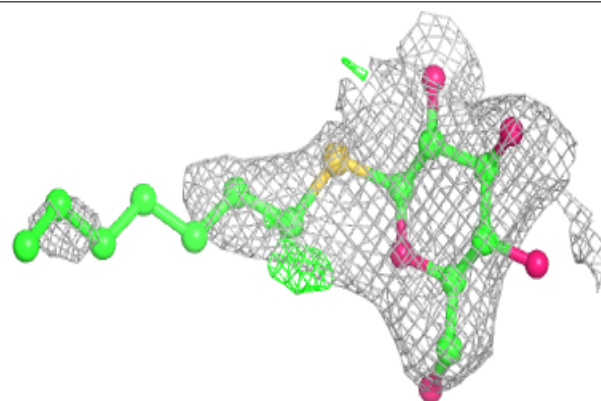


**Electron density around PL9 A 422:**

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

**Electron density around HTG d 415:**

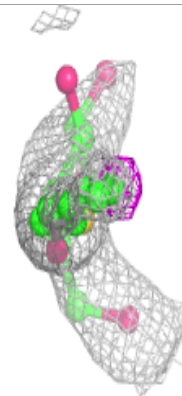
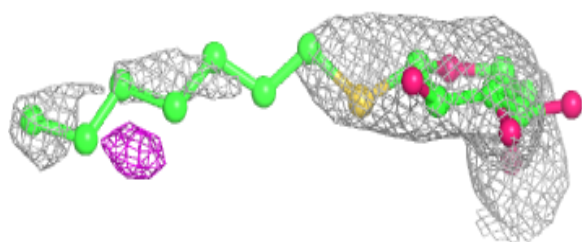
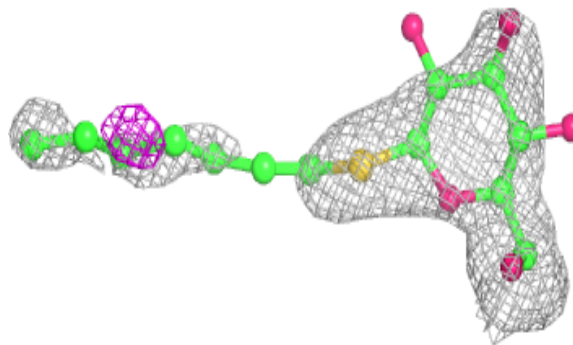
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



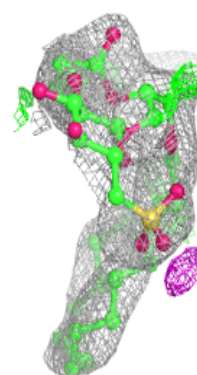
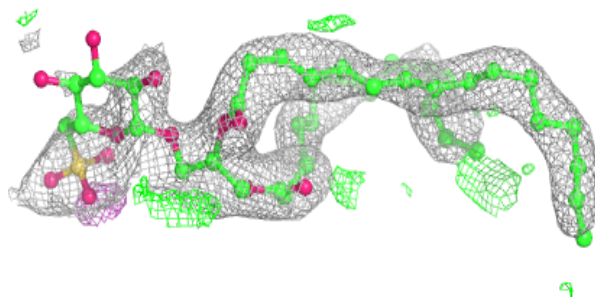
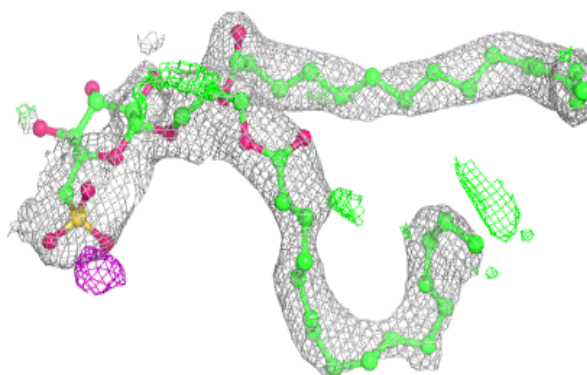


**Electron density around HTG C 522:**

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

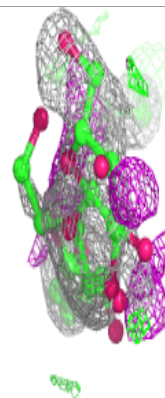
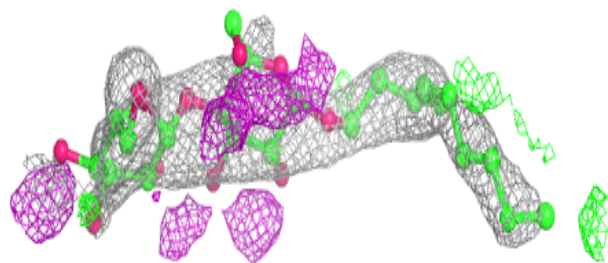
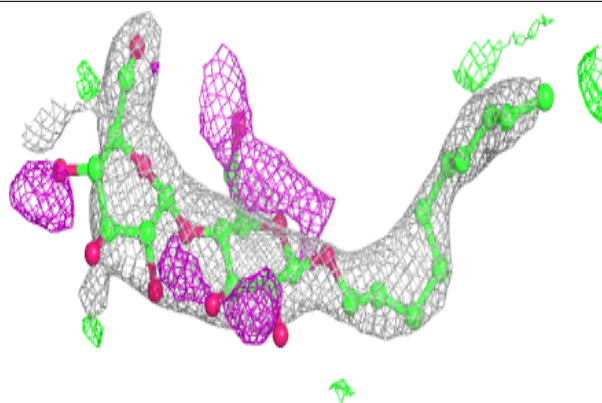
**Electron density around SQD a 2603:**

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

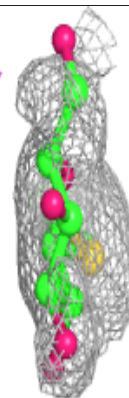
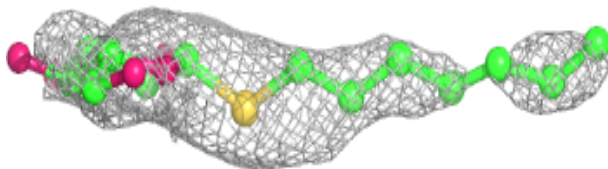
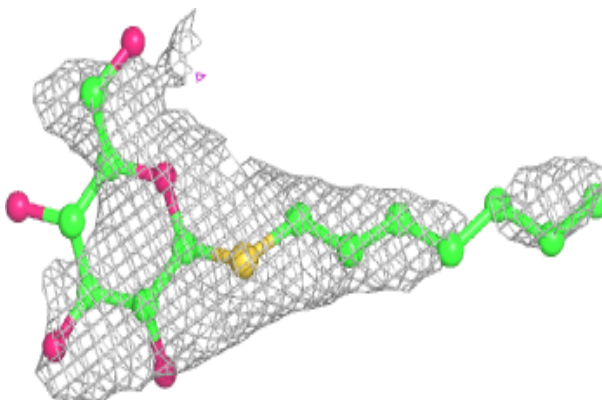


**Electron density around LMT A 414:**

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

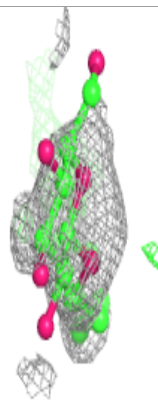
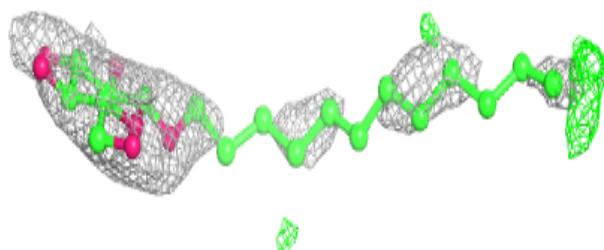
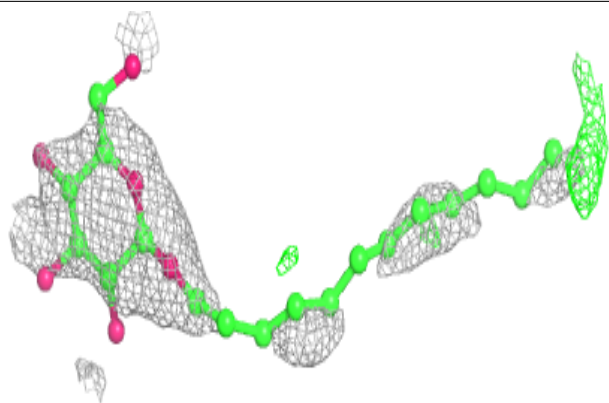
**Electron density around HTG C 525:**

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

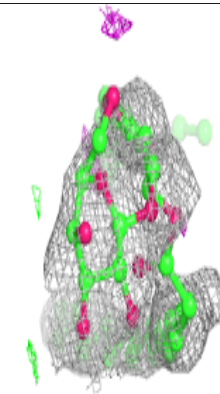
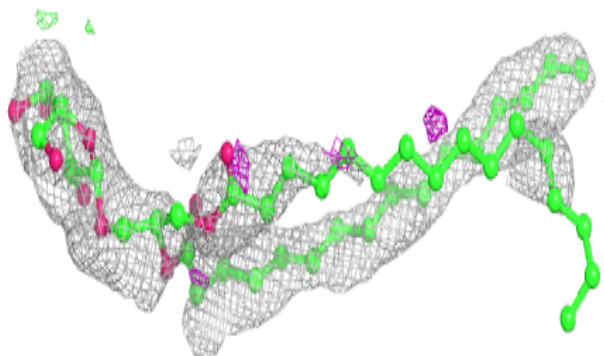
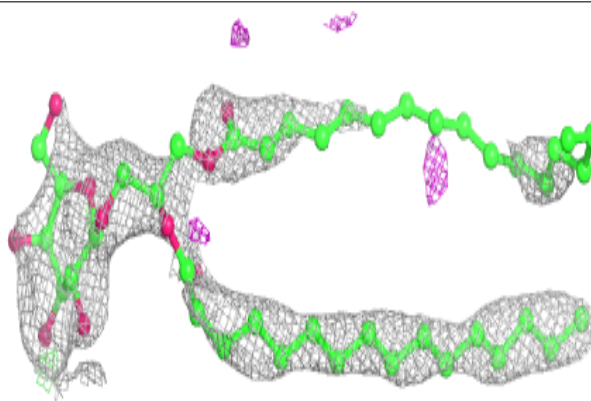


**Electron density around LMT f 101:**

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

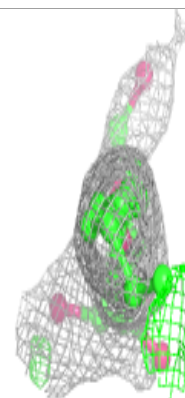
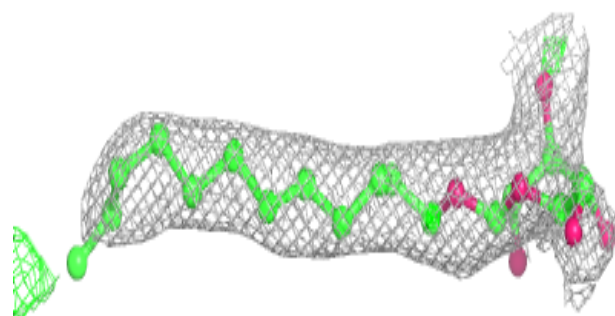
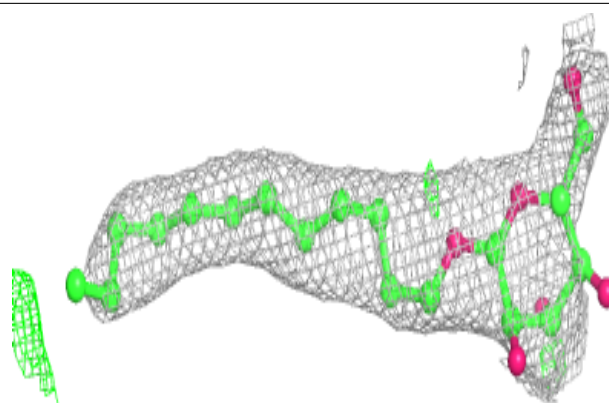
**Electron density around LMG c 522:**

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

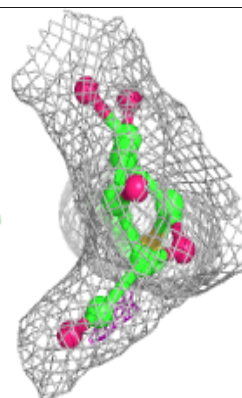
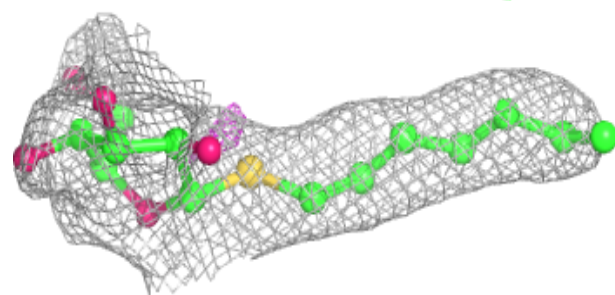
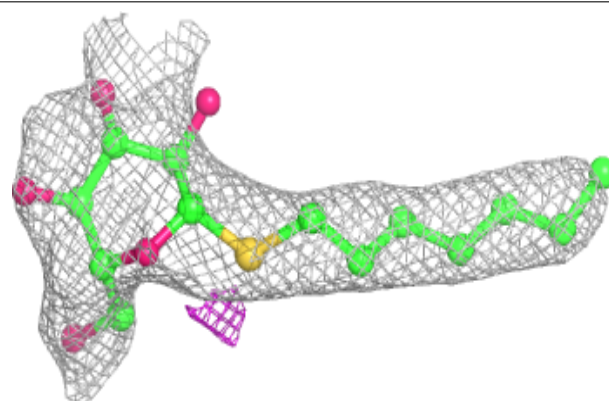


**Electron density around LMT A 420:**

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

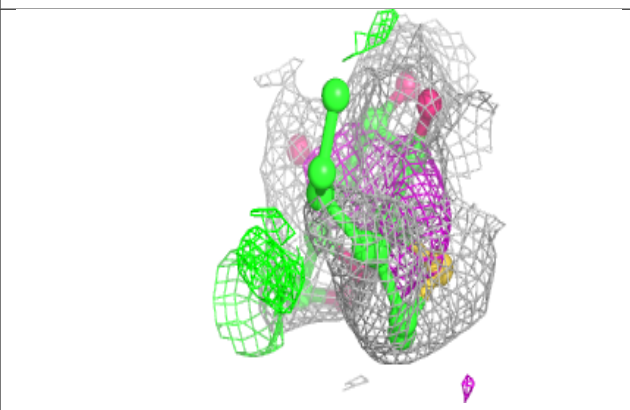
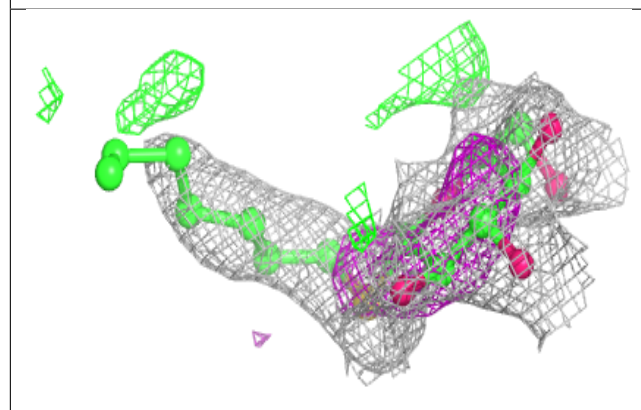
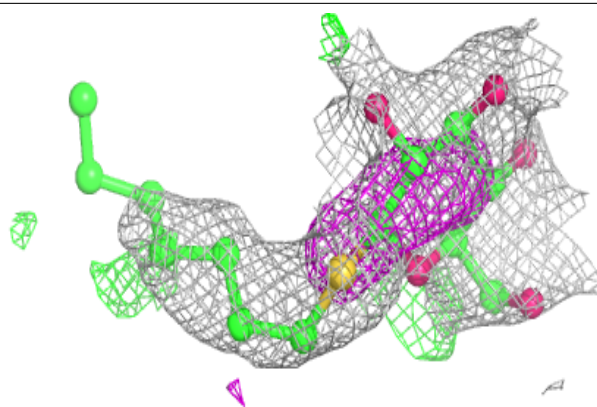
**Electron density around HTG I 101:**

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

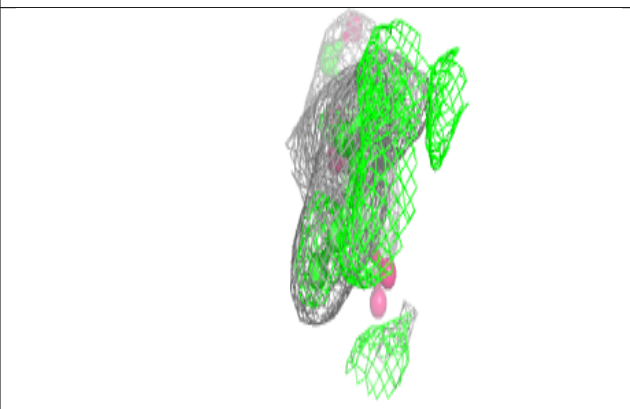
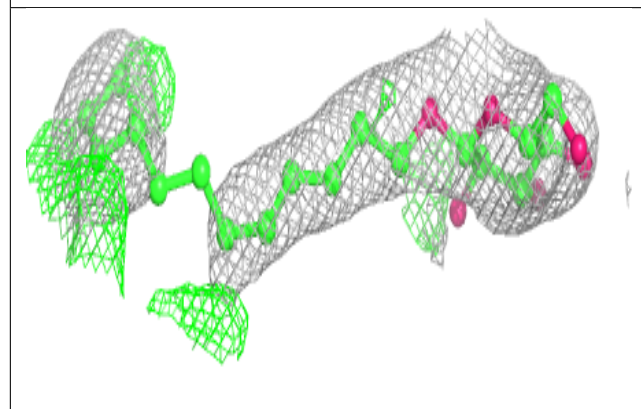
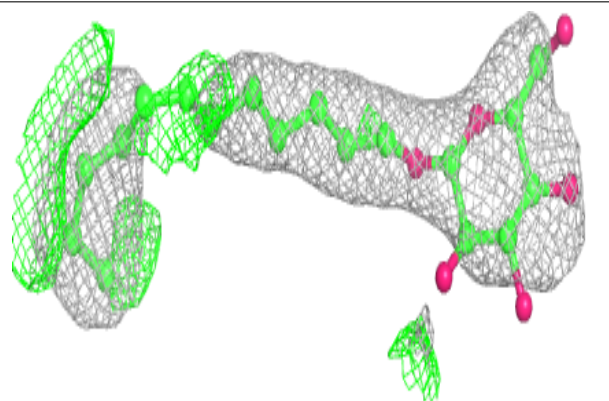


**Electron density around HTG b 625:**

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

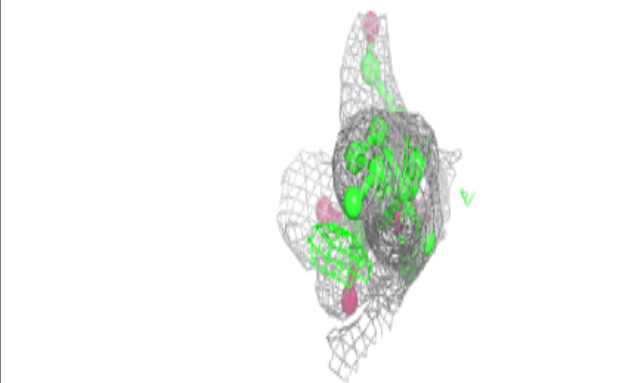
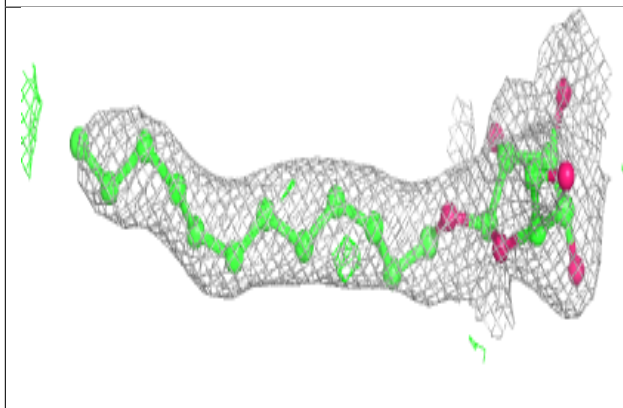
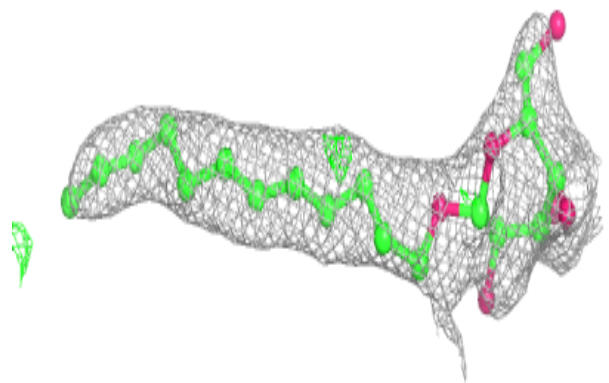
**Electron density around LMT T 103:**

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

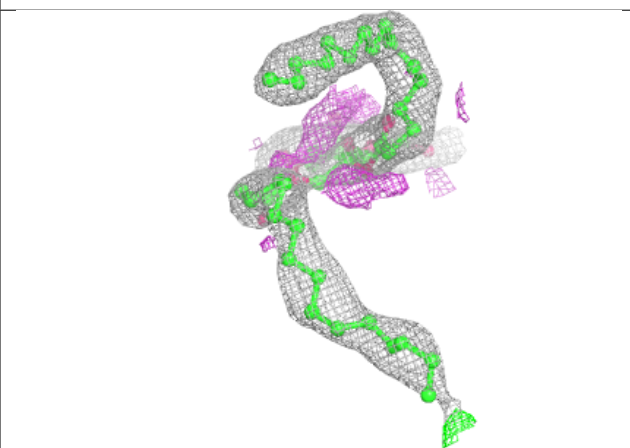
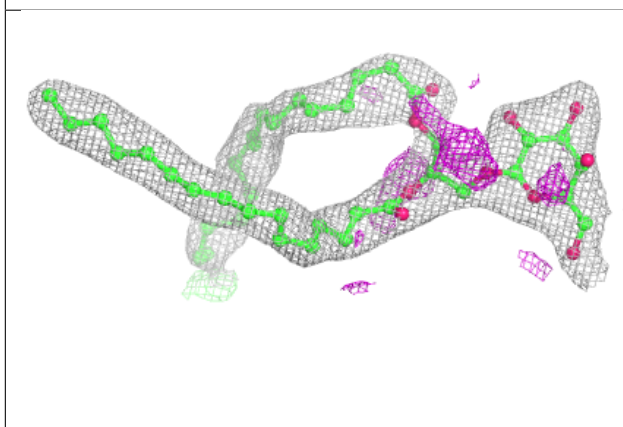
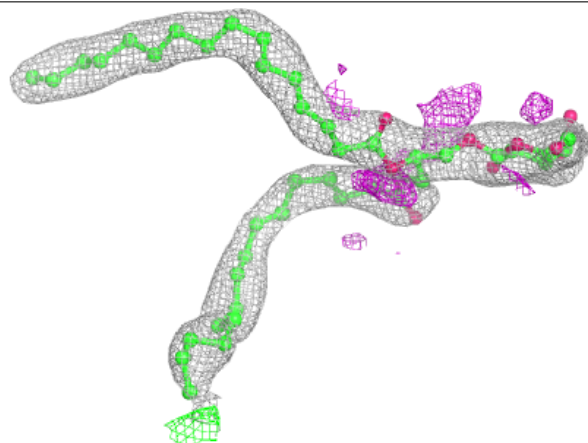


**Electron density around LMT i 103:**

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

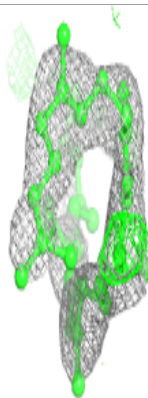
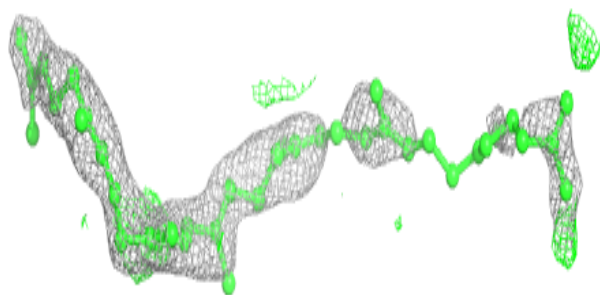
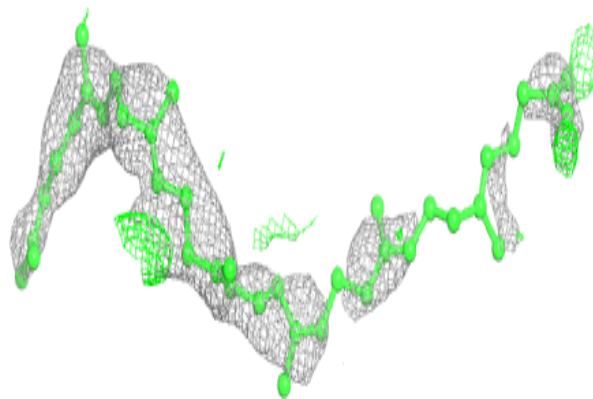
**Electron density around LMG m 2802:**

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

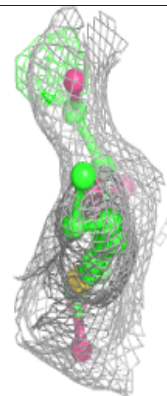
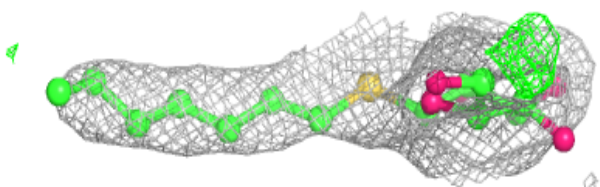
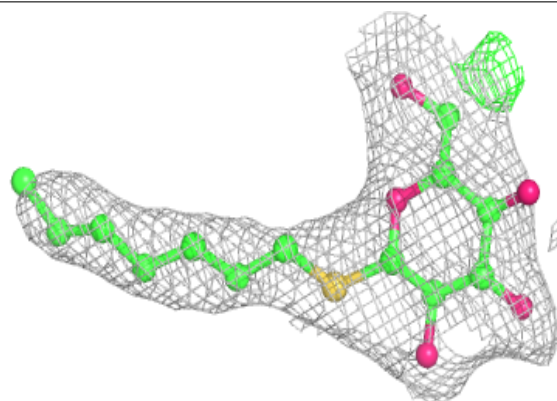


**Electron density around PL9 x 1301:**

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

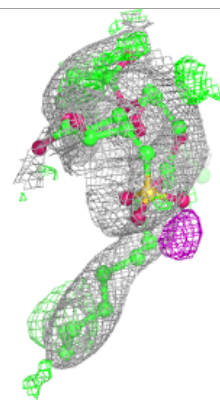
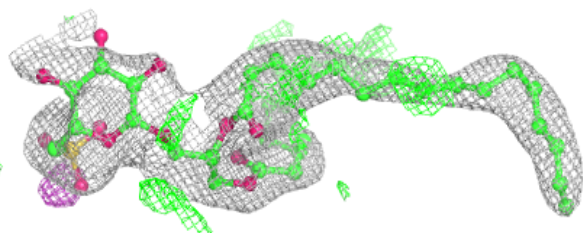
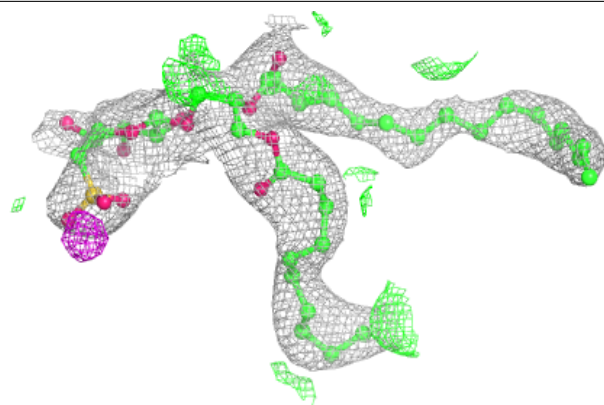
**Electron density around HTG b 604:**

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

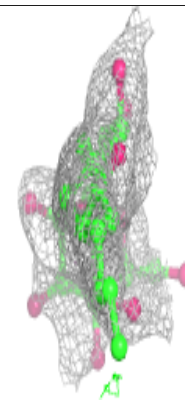
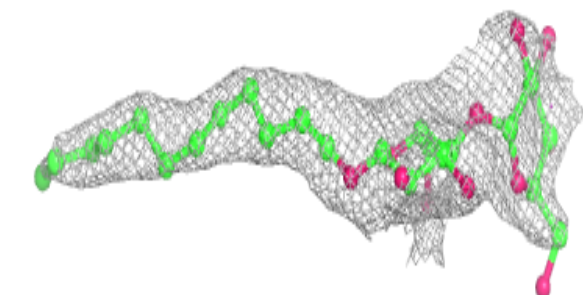
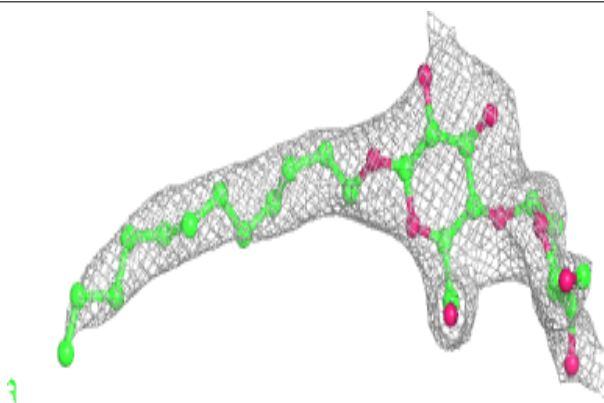


**Electron density around SQD b 601:**

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

**Electron density around LMT B 623:**

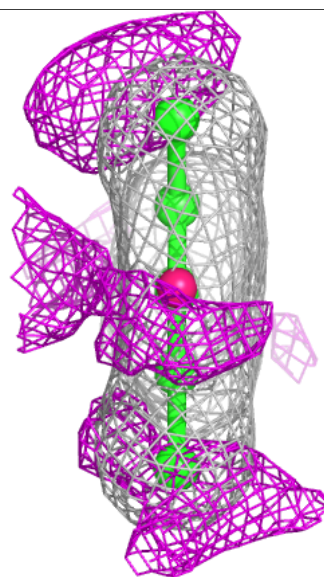
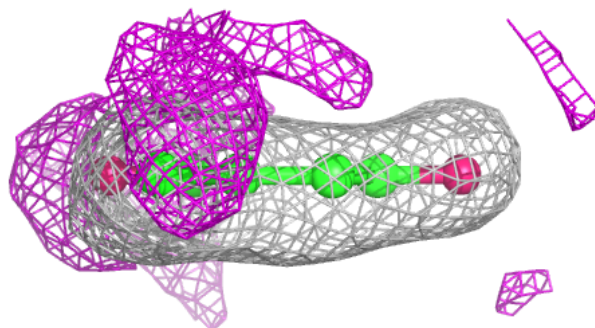
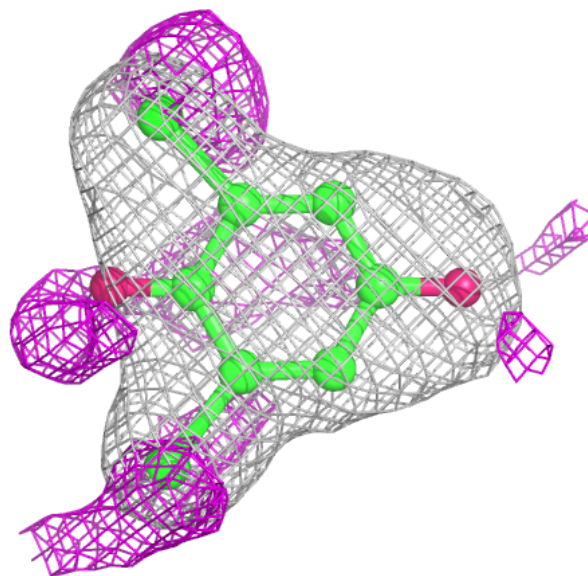
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





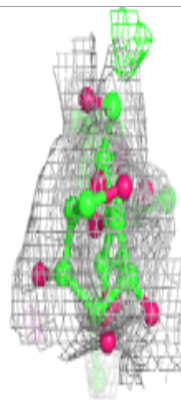
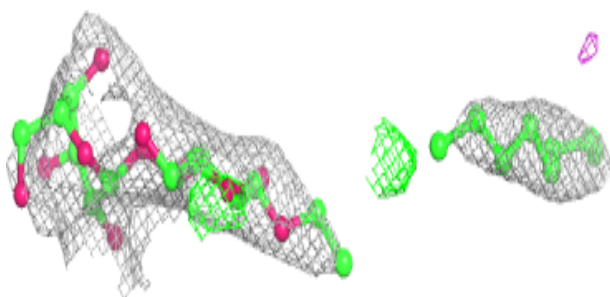
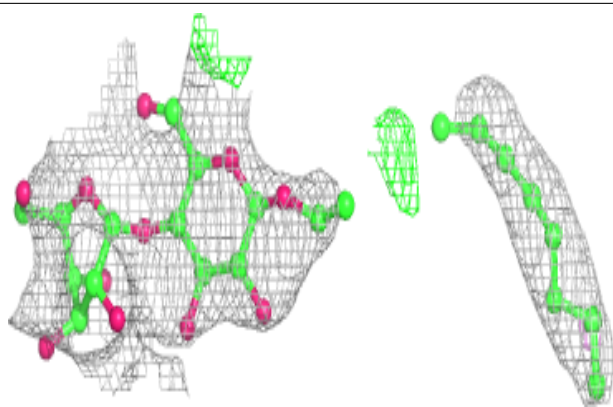
**Electron density around JOX A 419:**

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

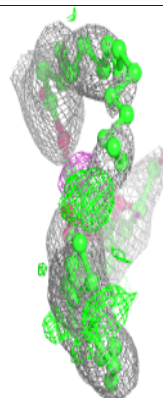
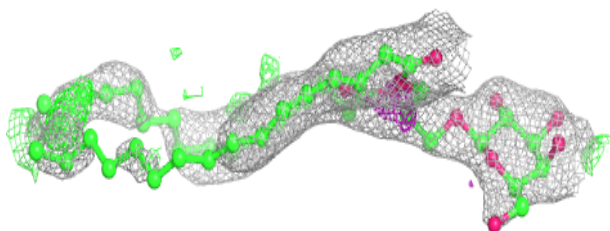
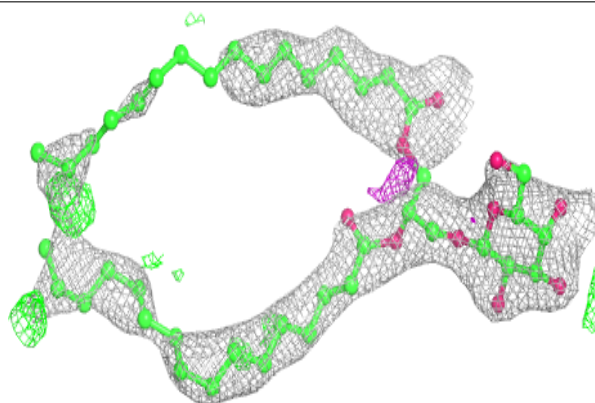


**Electron density around LMT z 102:**

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

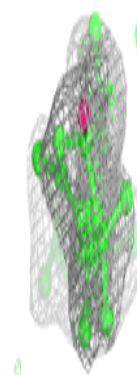
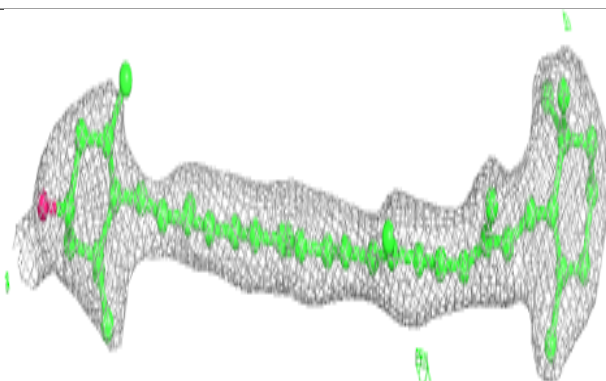
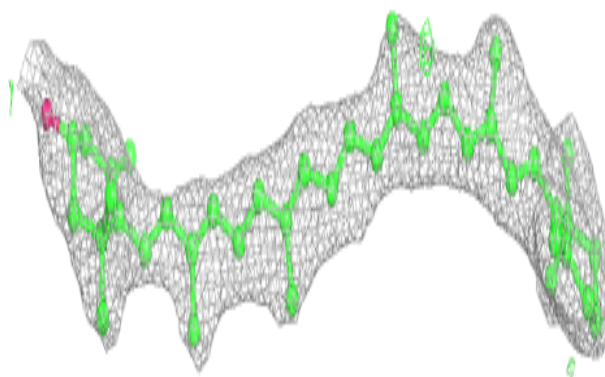
**Electron density around LMG c 501:**

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

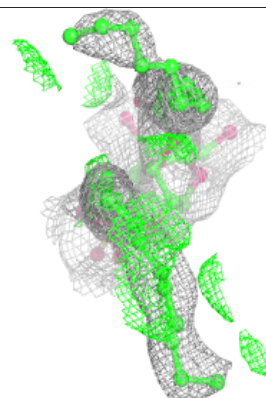
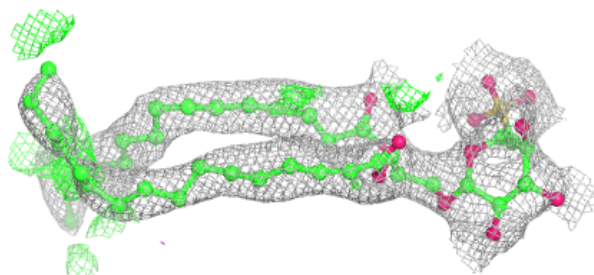
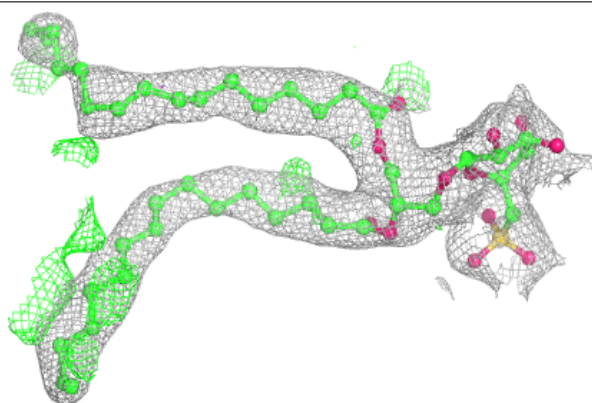


**Electron density around RRX H 102:**

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

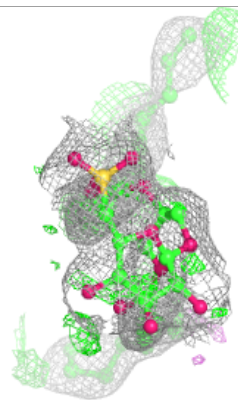
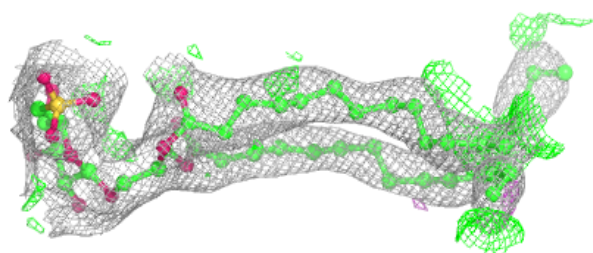
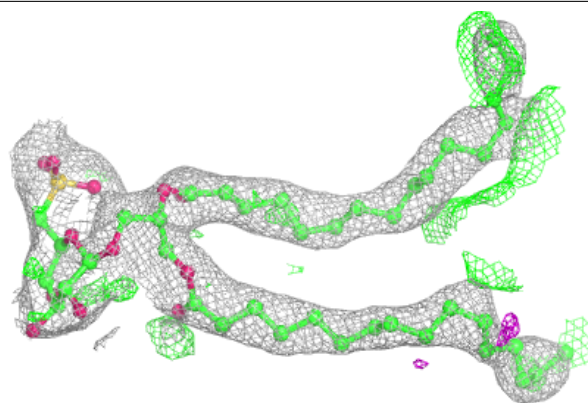
**Electron density around SQD B 621:**

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

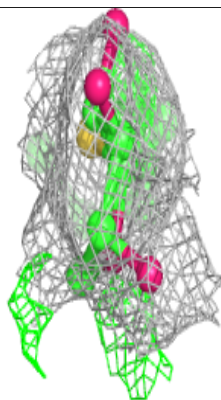
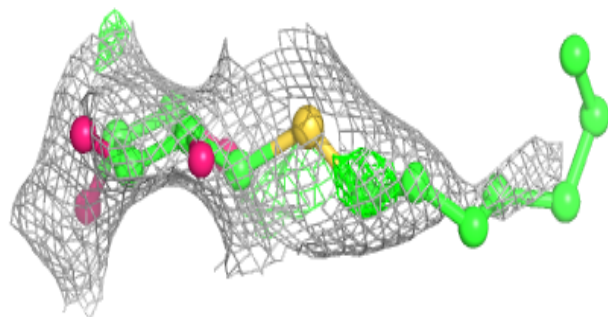
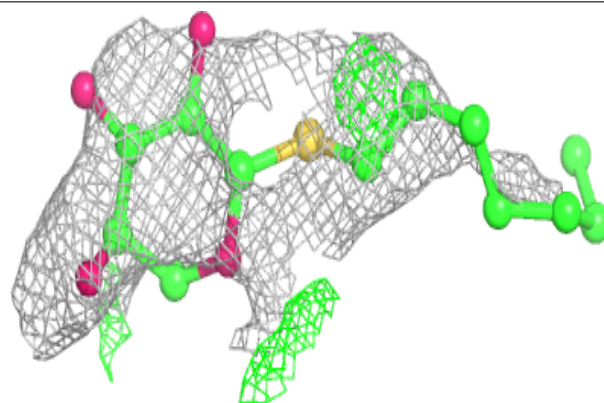


**Electron density around SQD 1 101:**

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

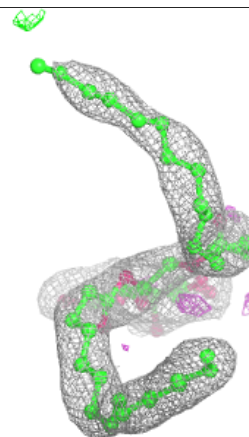
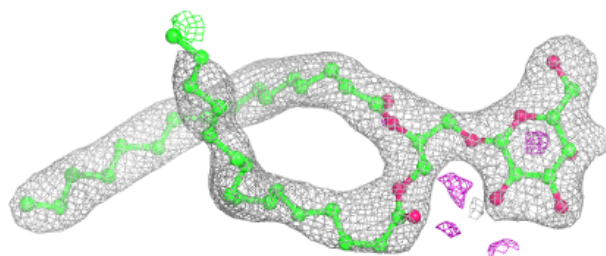
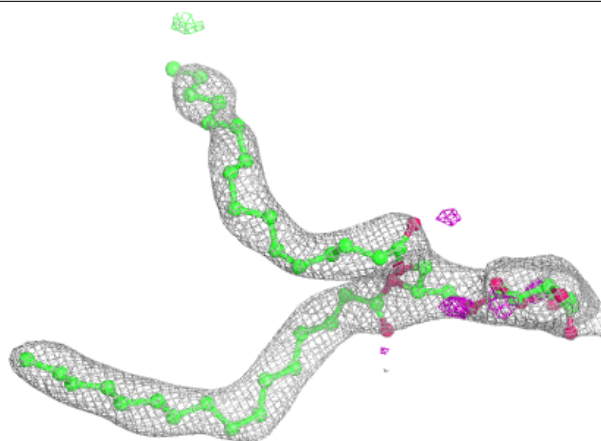
**Electron density around HTG H 101:**

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

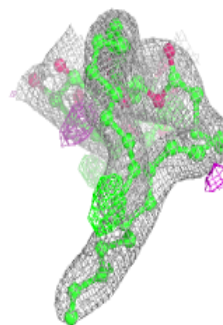
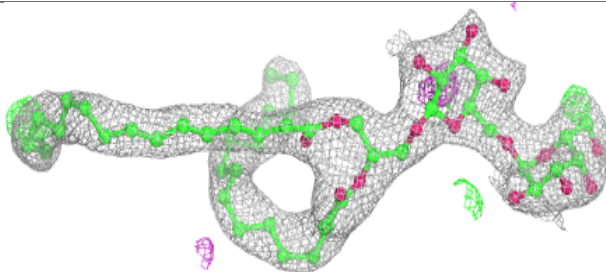
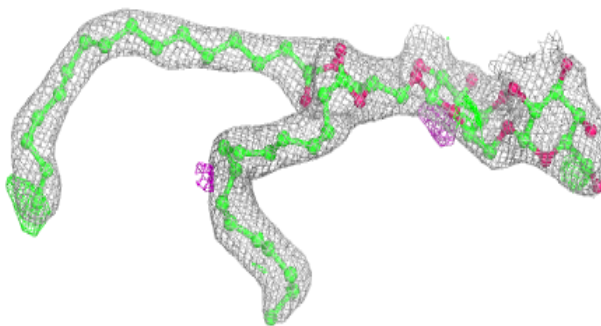


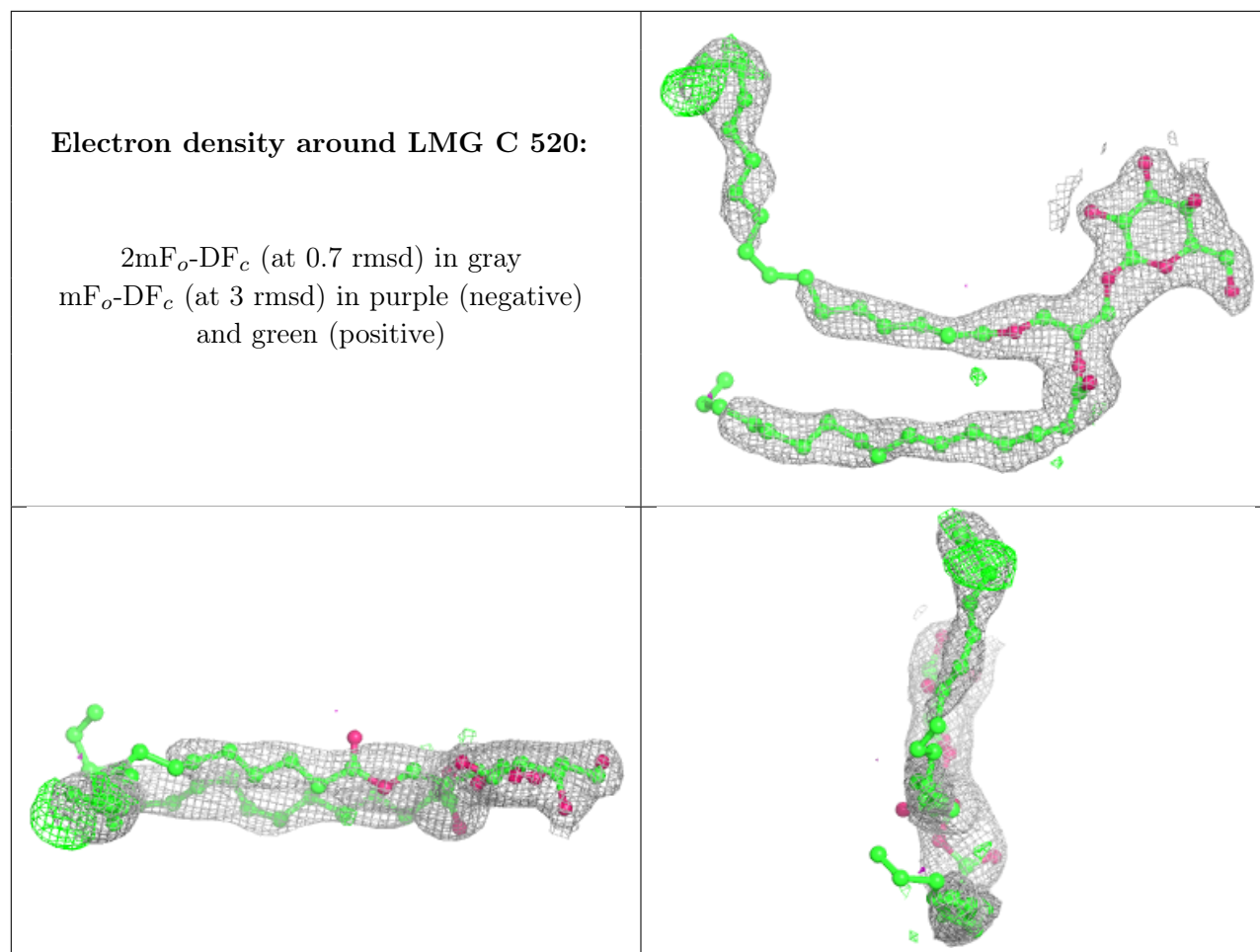
**Electron density around LMG B 622:**

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

**Electron density around DGD h 102:**

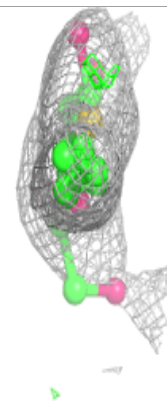
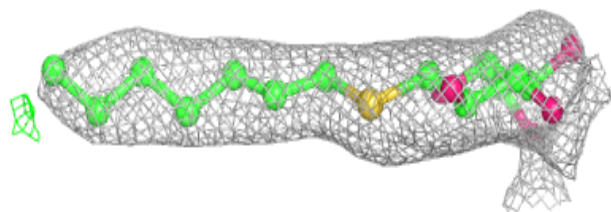
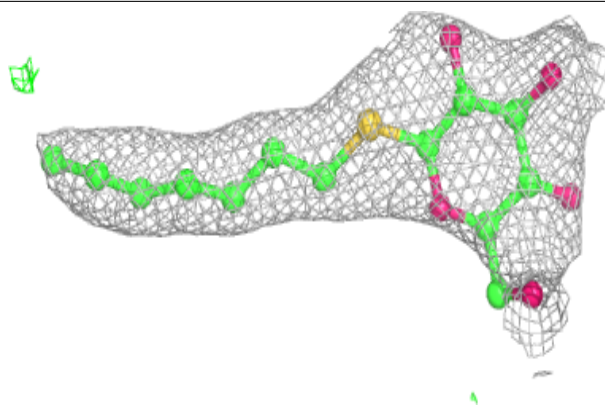
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



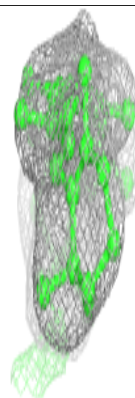
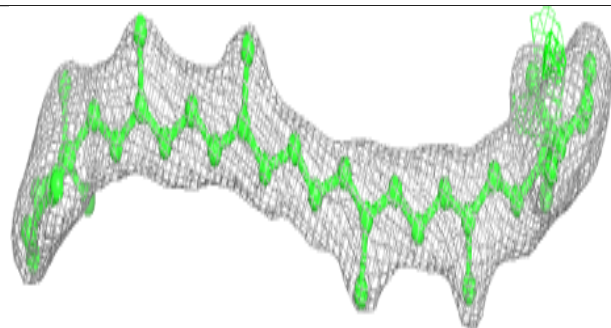
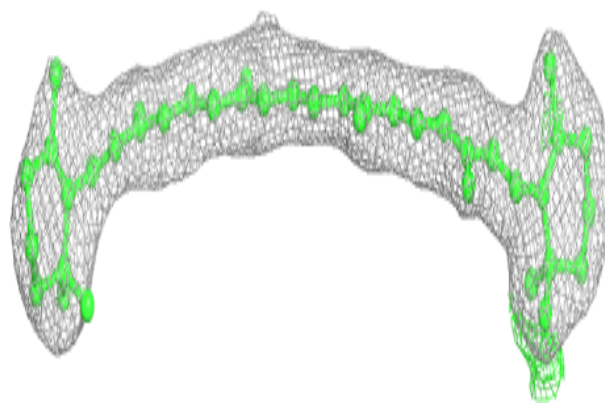


**Electron density around HTG B 626:**

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

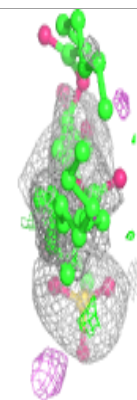
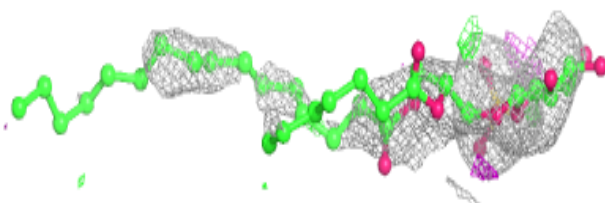
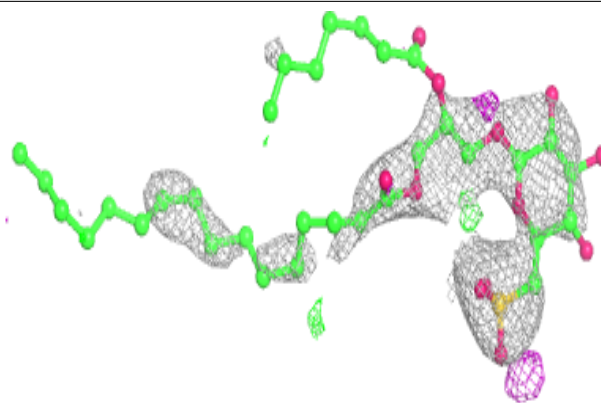
**Electron density around BCR k 302:**

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

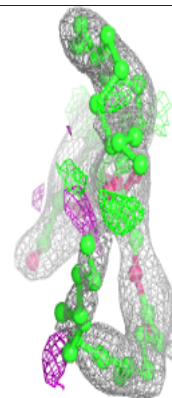
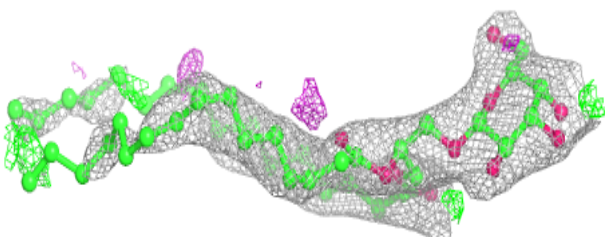
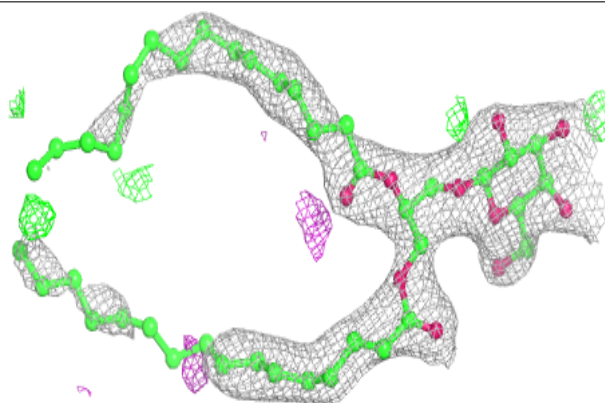


**Electron density around SQD D 2308:**

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

**Electron density around LMG A 413:**

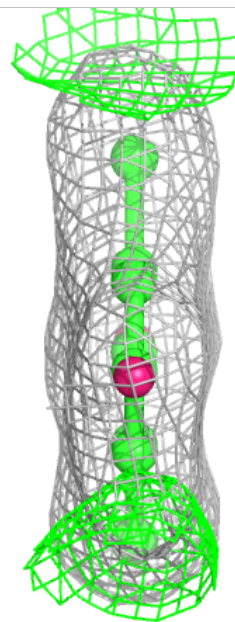
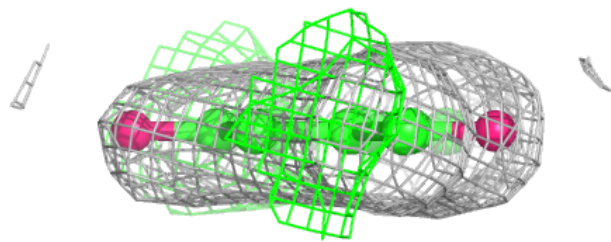
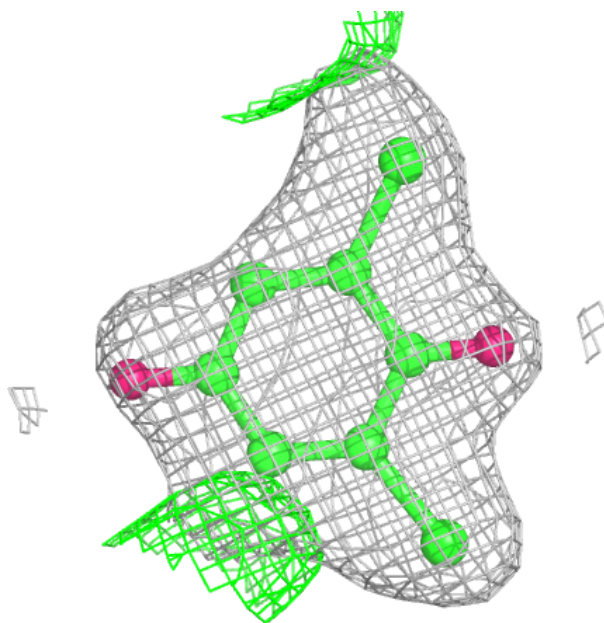
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





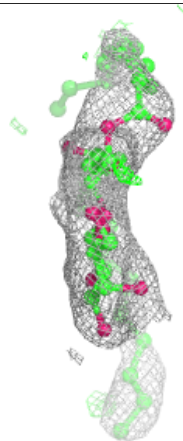
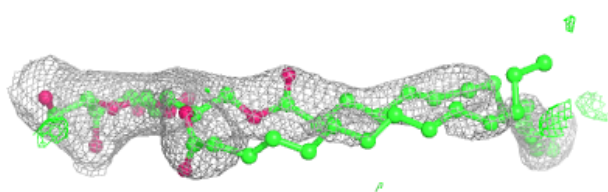
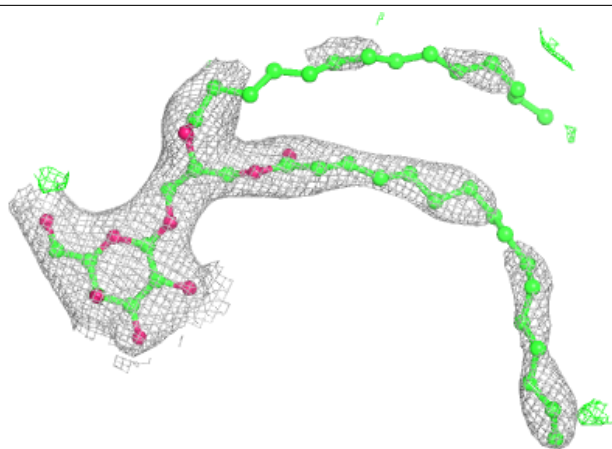
**Electron density around JOX A 418:**

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

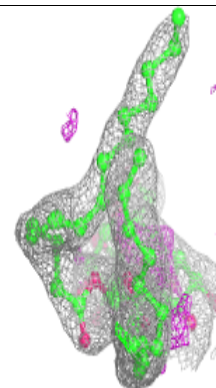
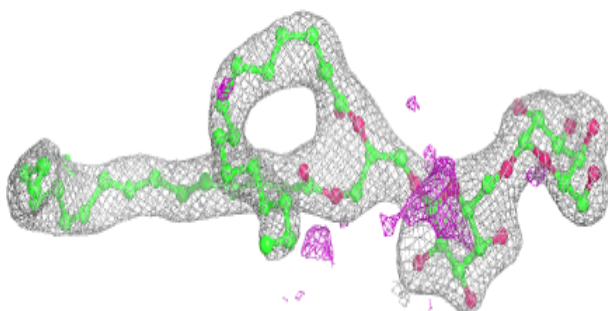
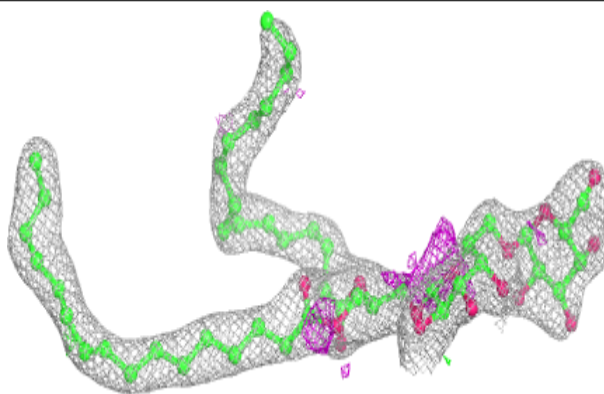


**Electron density around LMG c 521:**

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

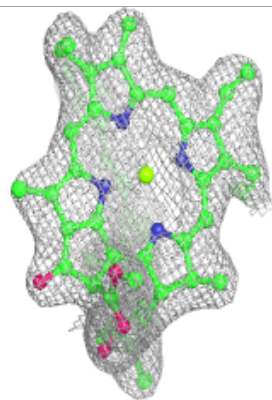
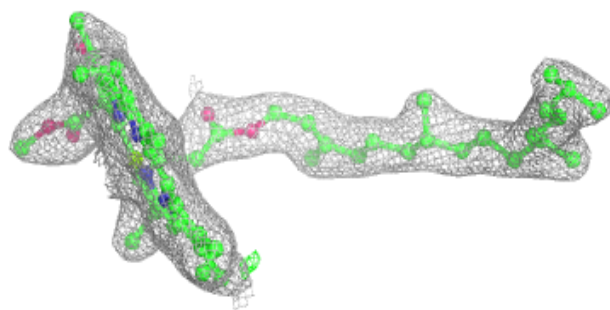
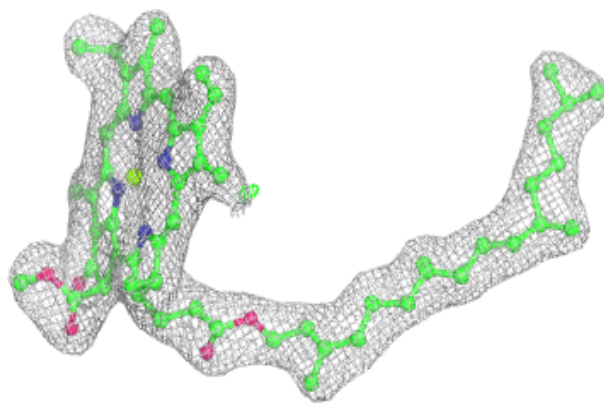
**Electron density around DGD H 103:**

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

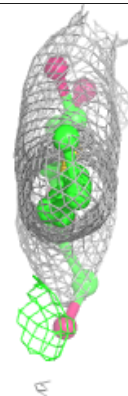
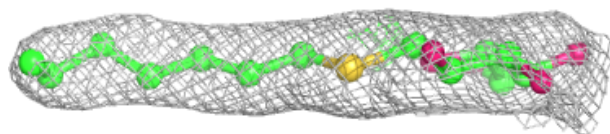
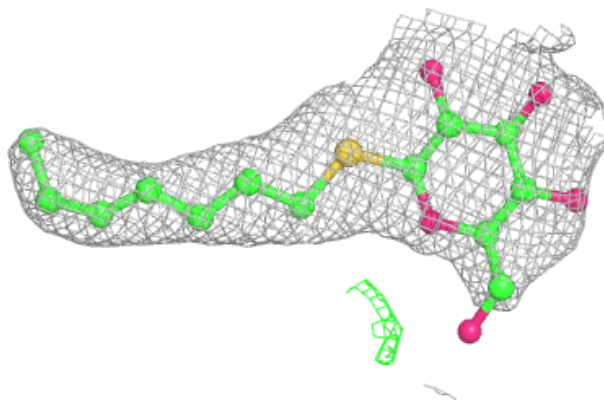


**Electron density around CLA B 610:**

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

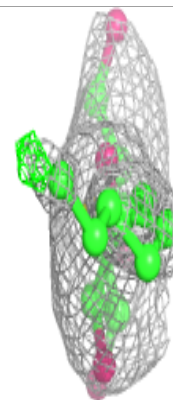
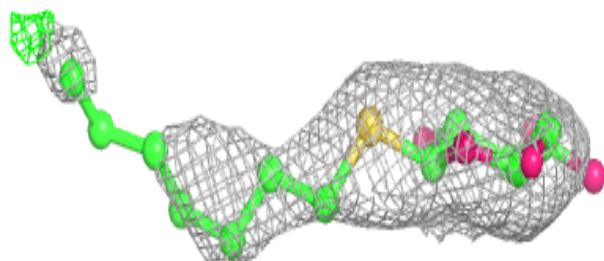
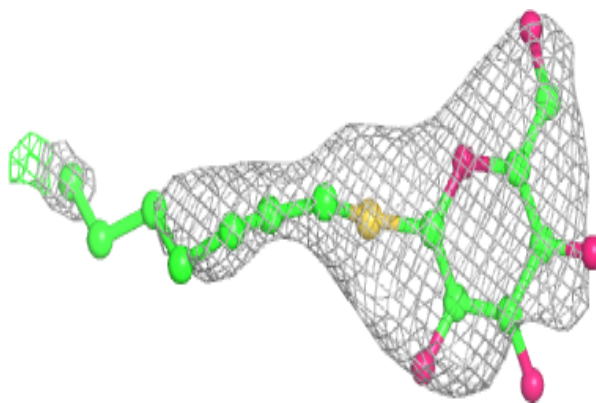
**Electron density around HTG b 603:**

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



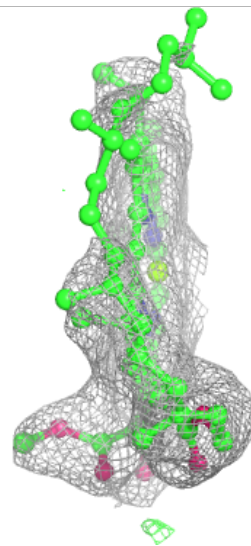
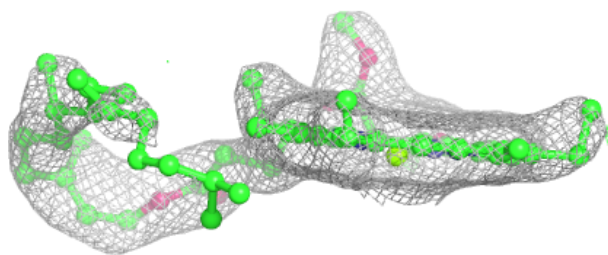
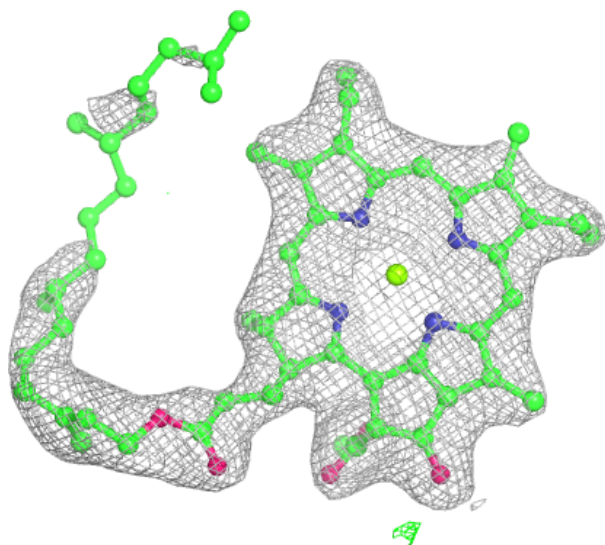
**Electron density around HTG c 523:**

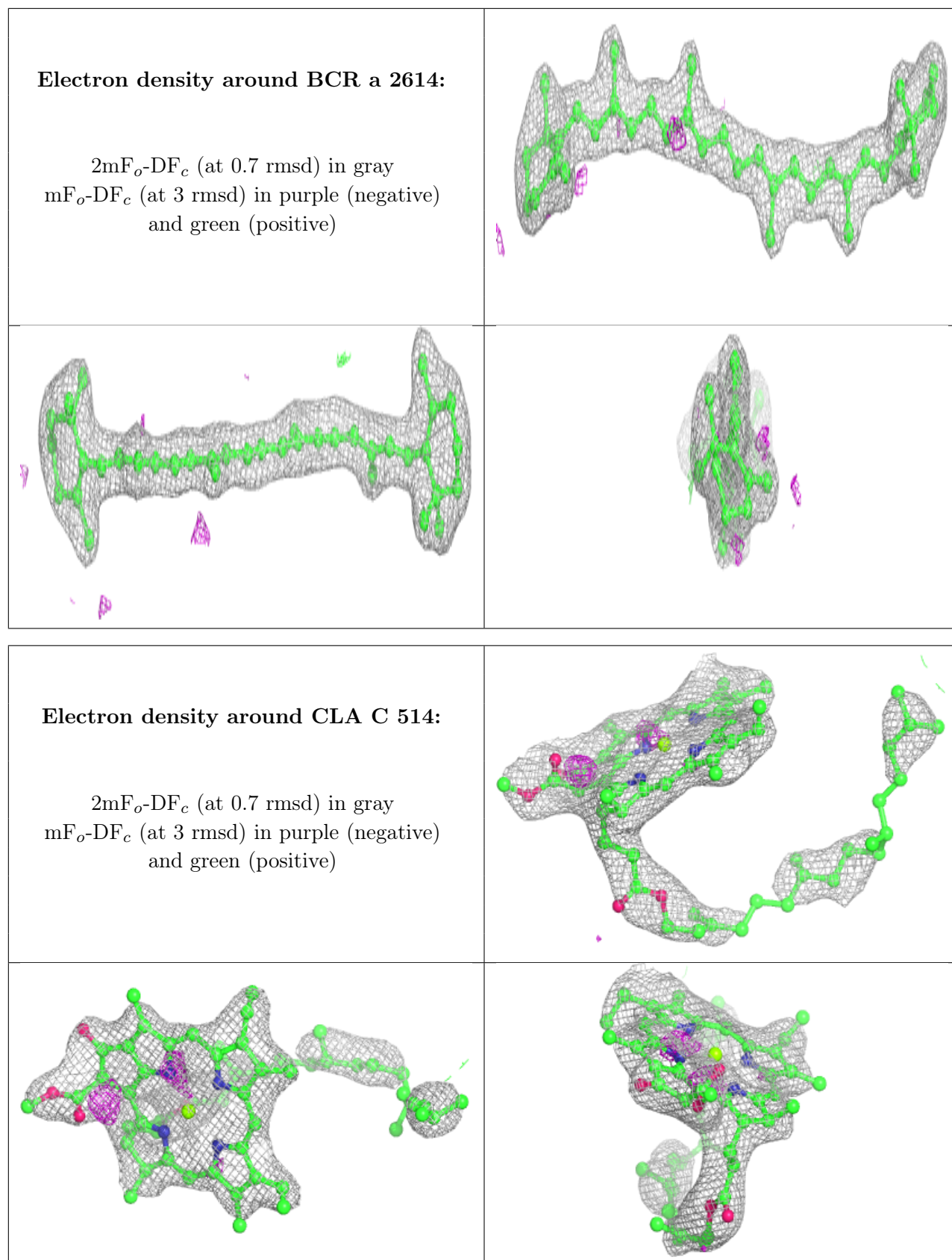
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 515:**

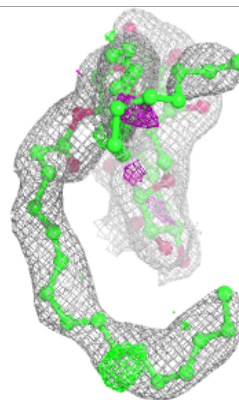
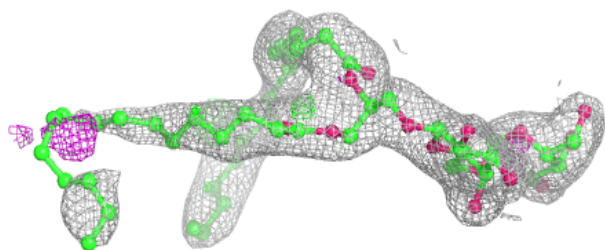
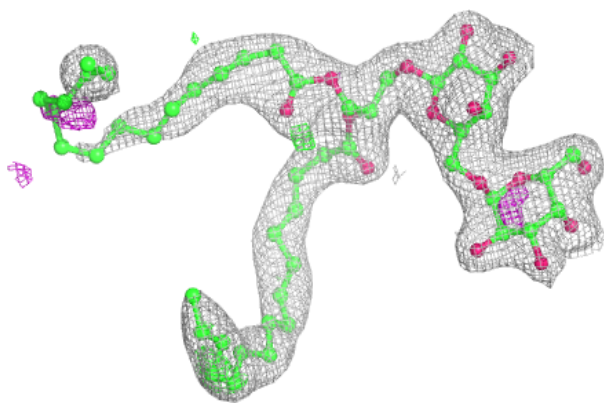
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



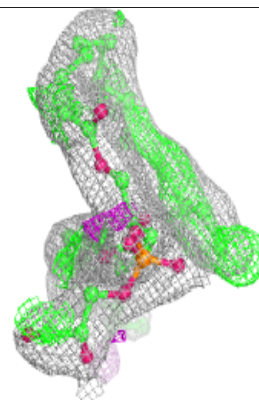
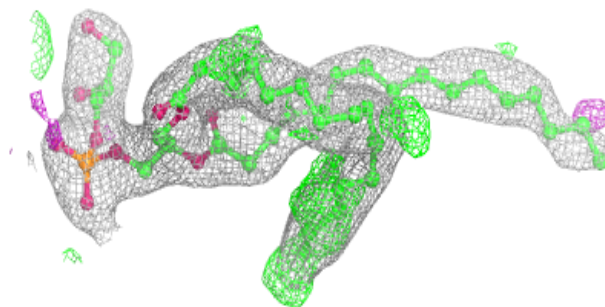
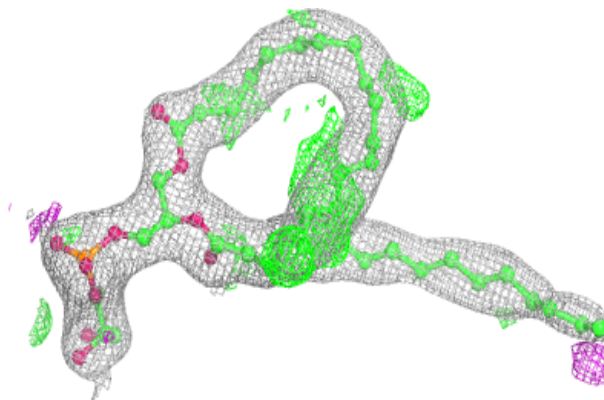


**Electron density around DGD C 518:**

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

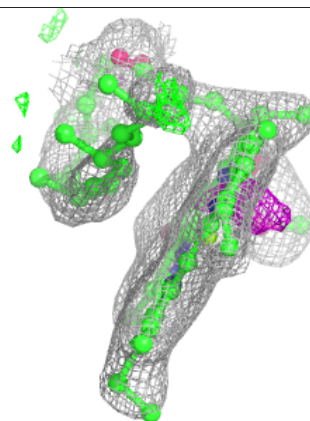
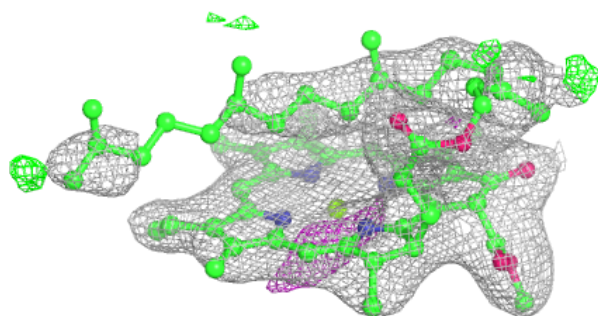
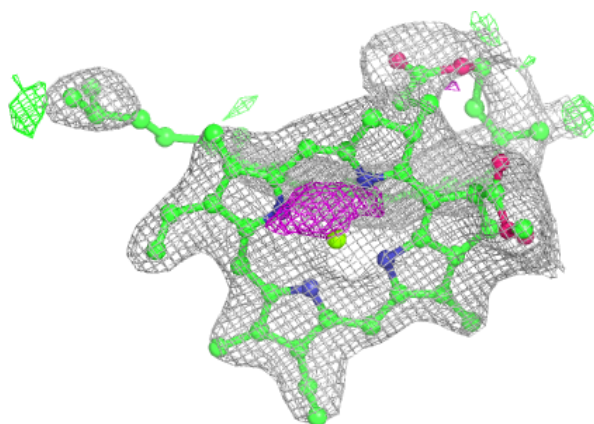
**Electron density around LHG D 2309:**

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



**Electron density around CLA B 602:**

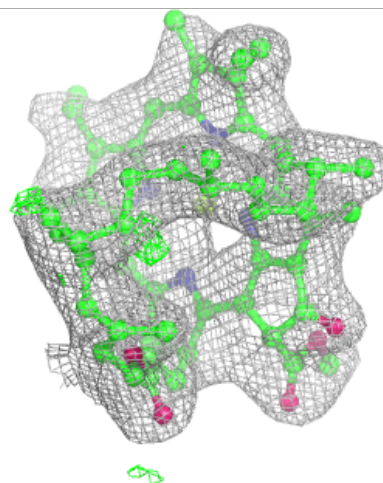
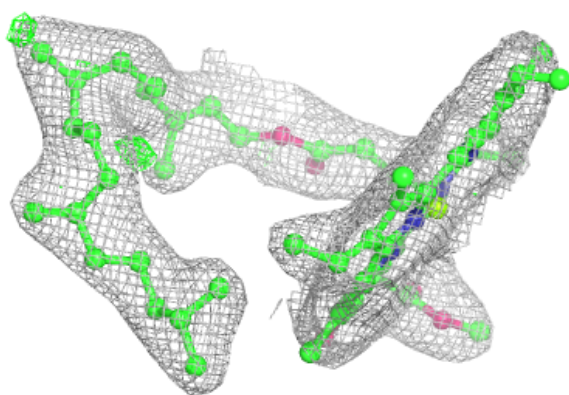
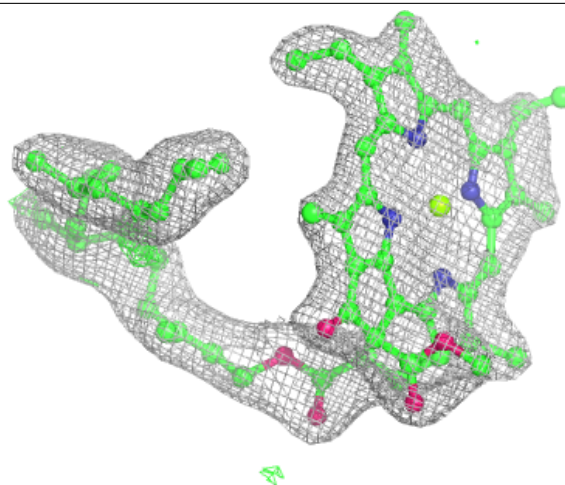
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





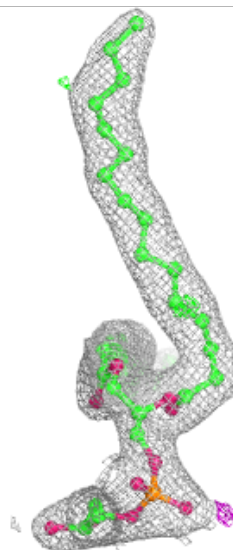
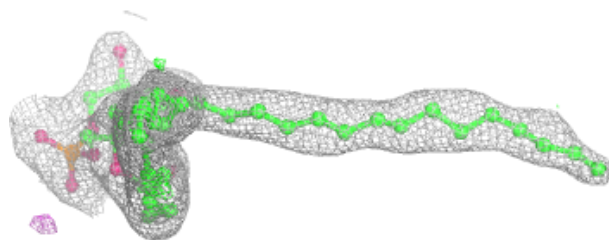
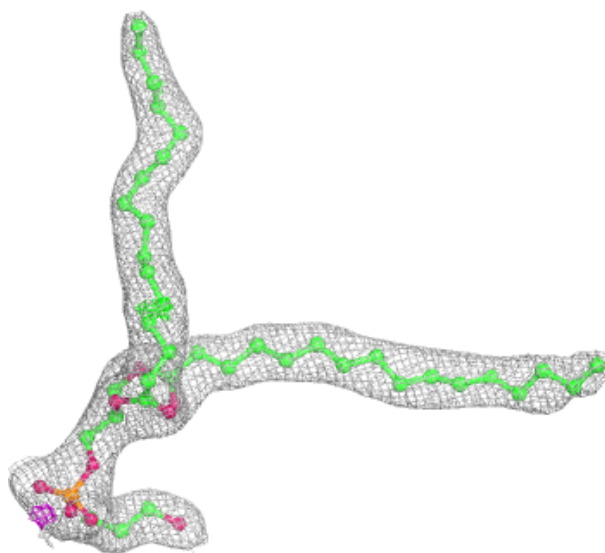
**Electron density around CLA c 506:**

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



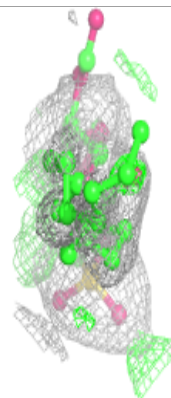
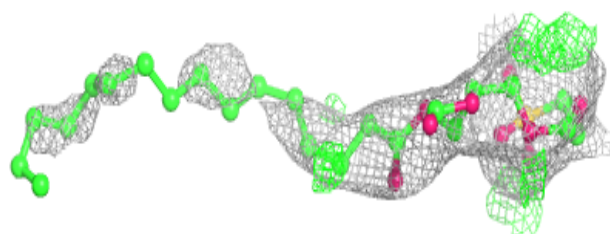
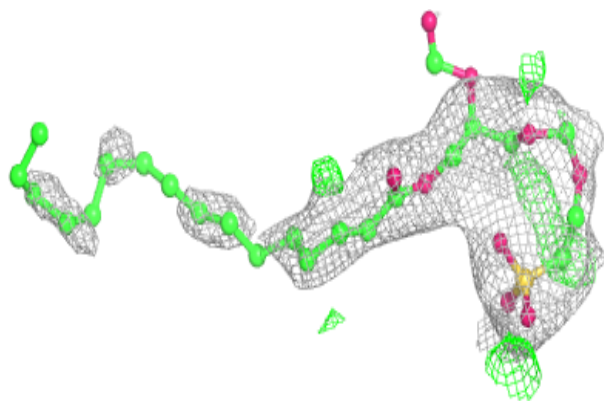
**Electron density around LHG 1 103:**

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

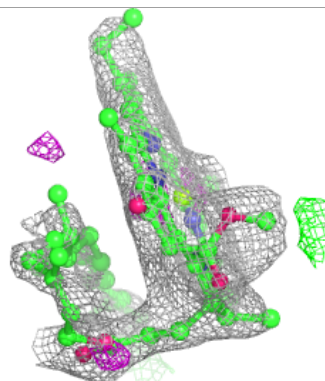
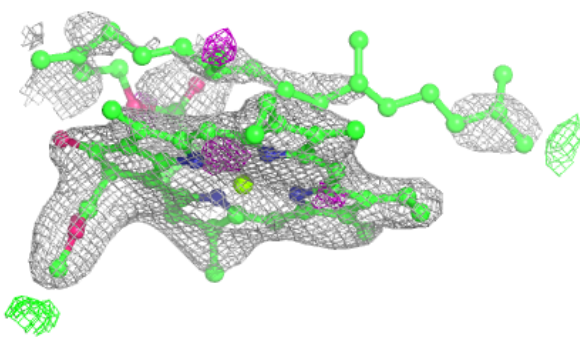
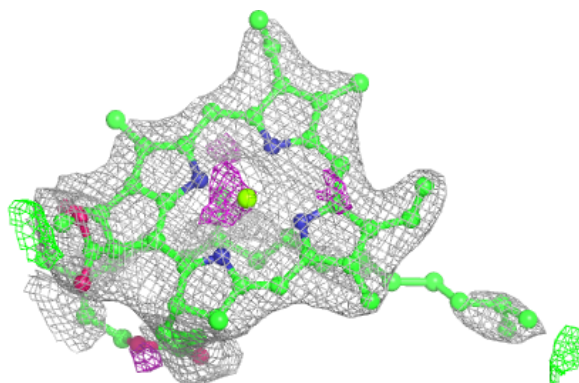


**Electron density around SQD d 417:**

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

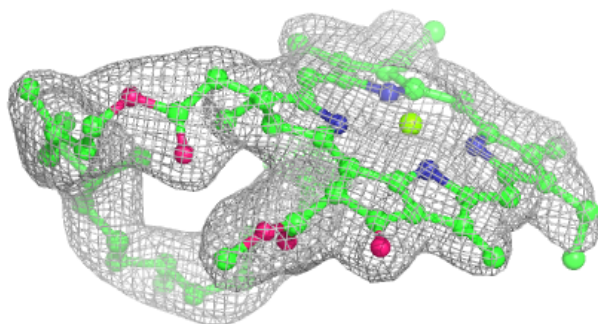
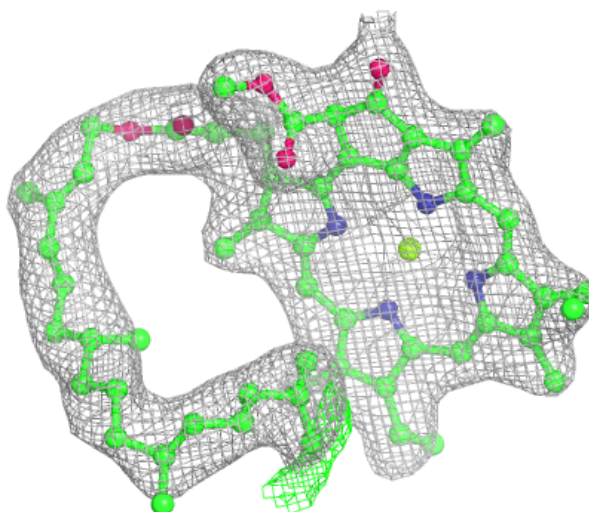
**Electron density around CLA b 606:**

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



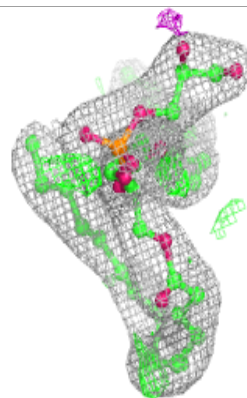
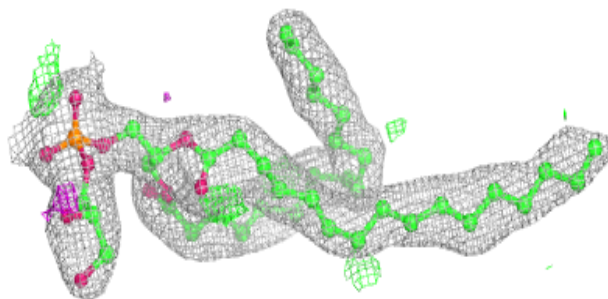
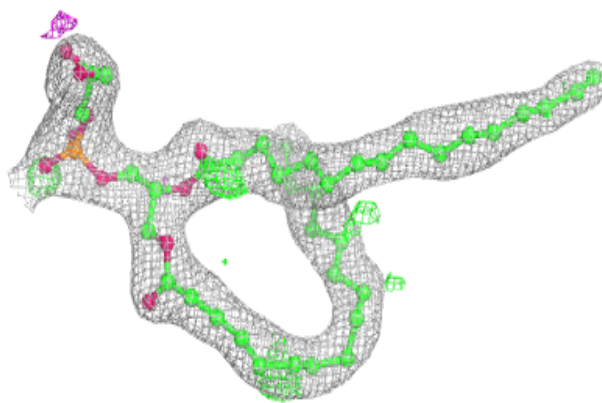
**Electron density around CLA b 620:**

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



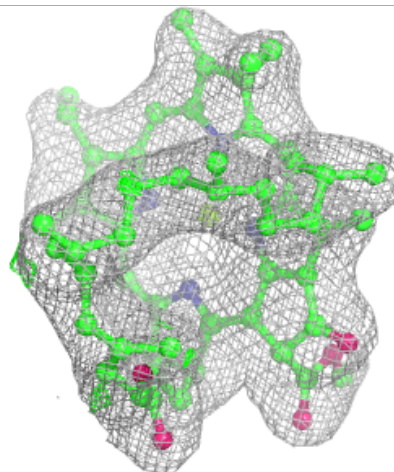
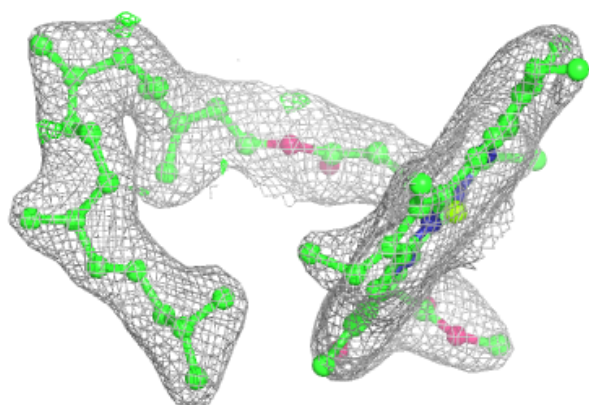
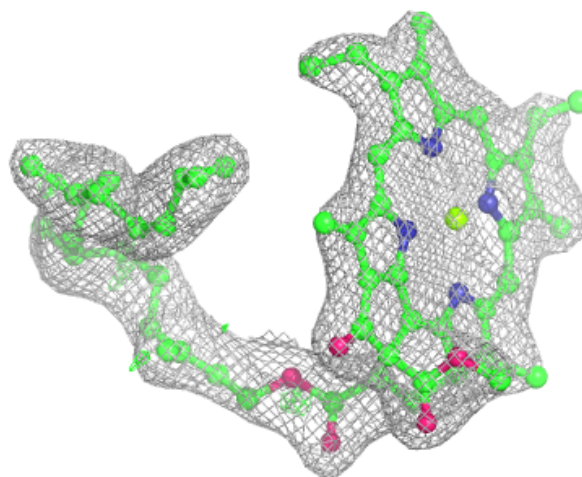
**Electron density around LHG d 412:**

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



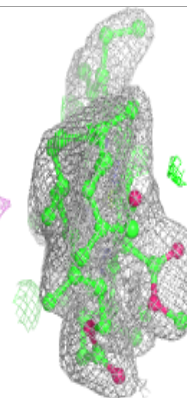
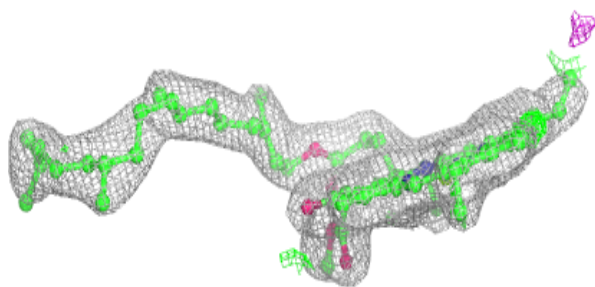
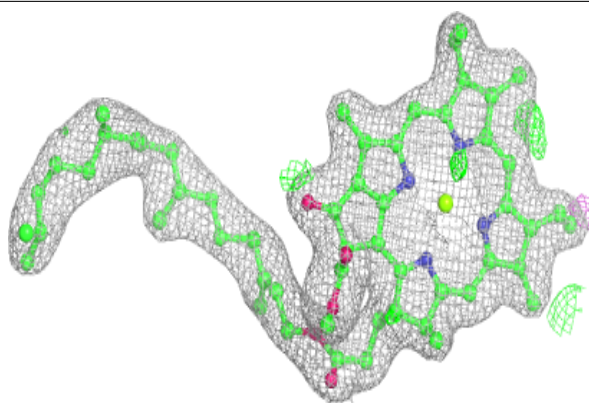
**Electron density around CLA C 504:**

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

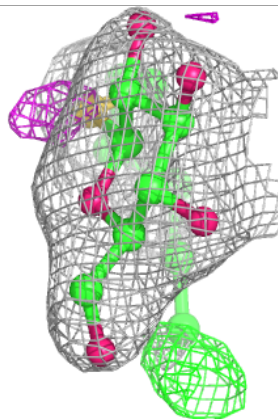
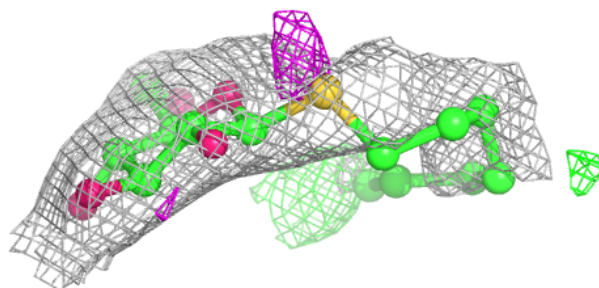
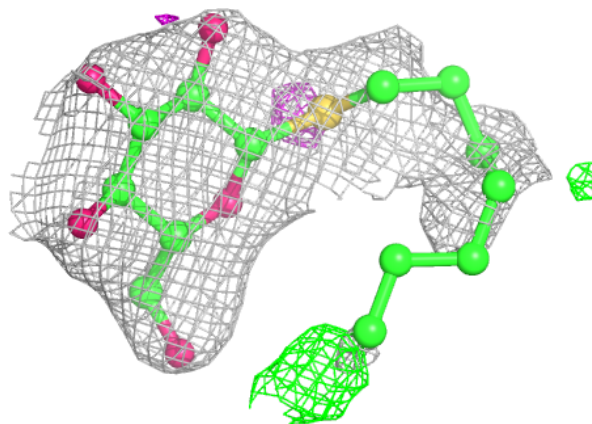


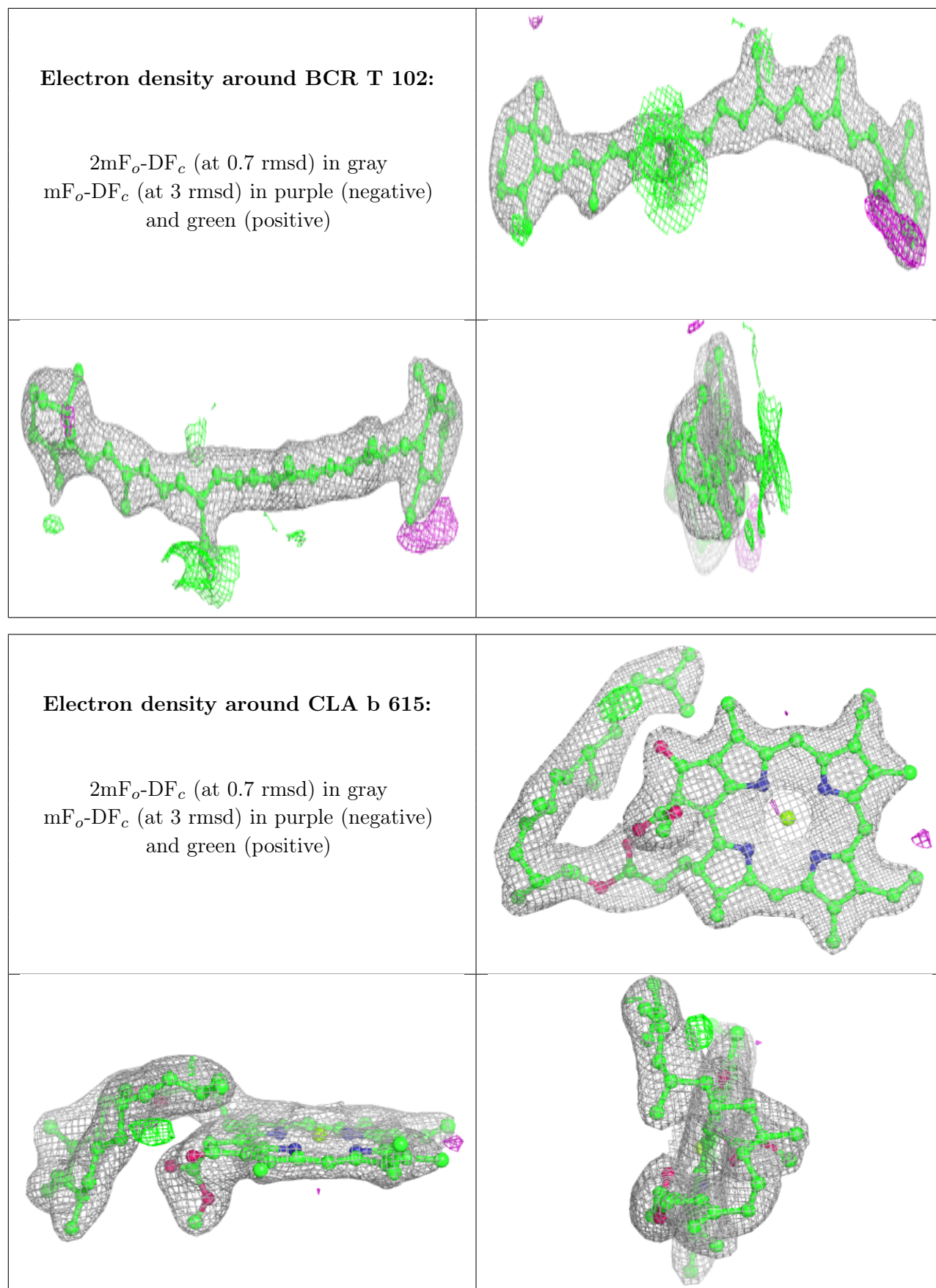
**Electron density around CLA B 603:**

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

**Electron density around HTG V 204:**

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

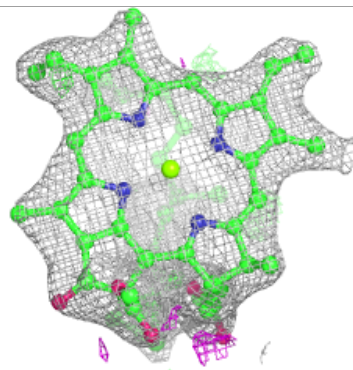
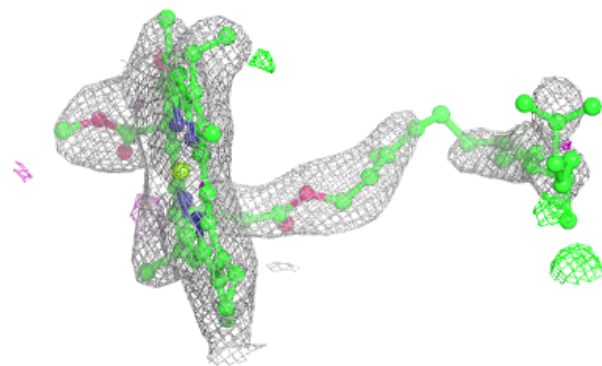
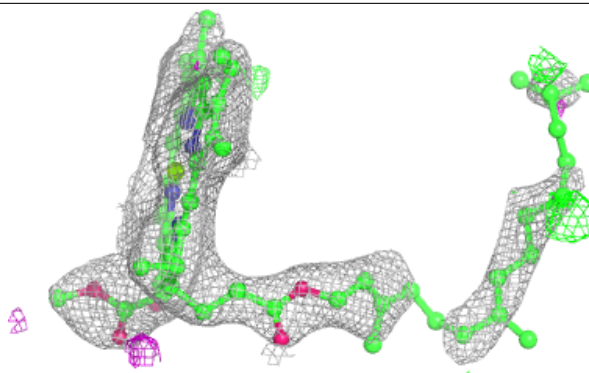






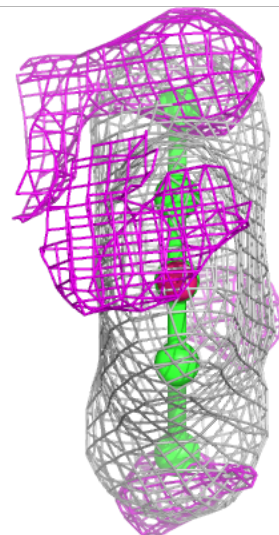
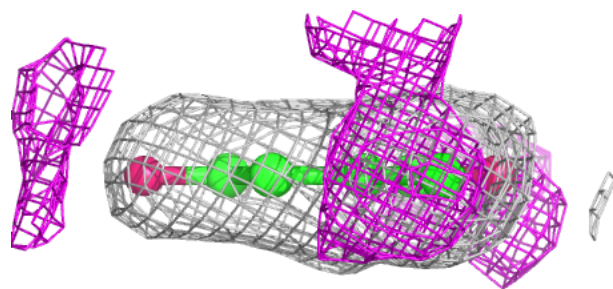
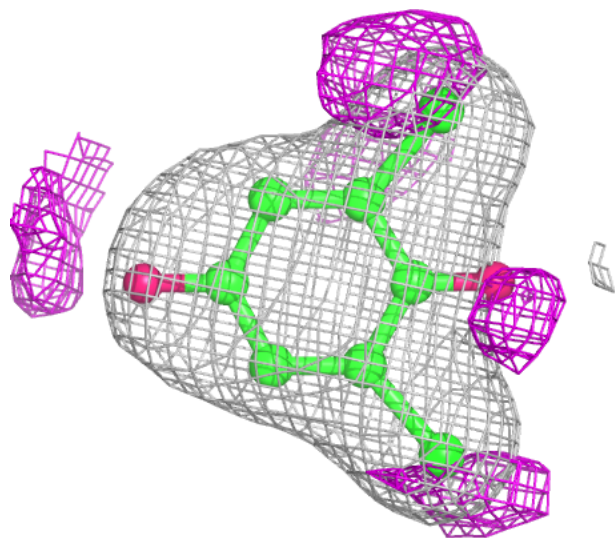
**Electron density around CLA C 507:**

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



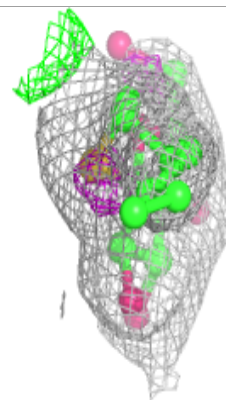
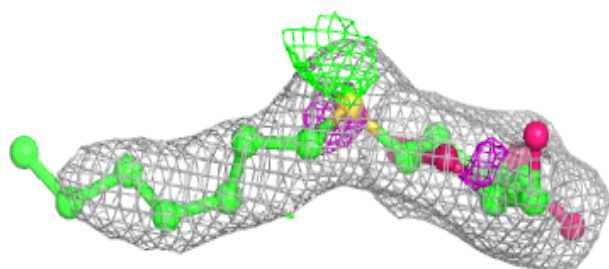
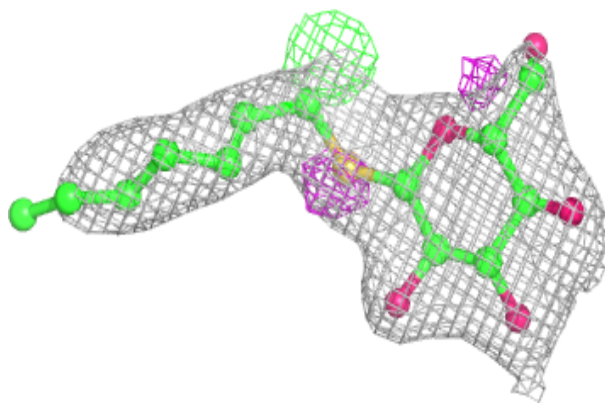
**Electron density around JOX a 2617:**

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



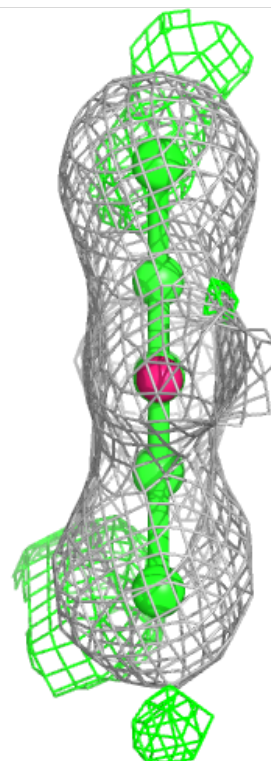
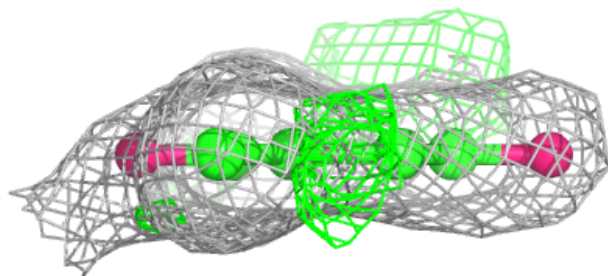
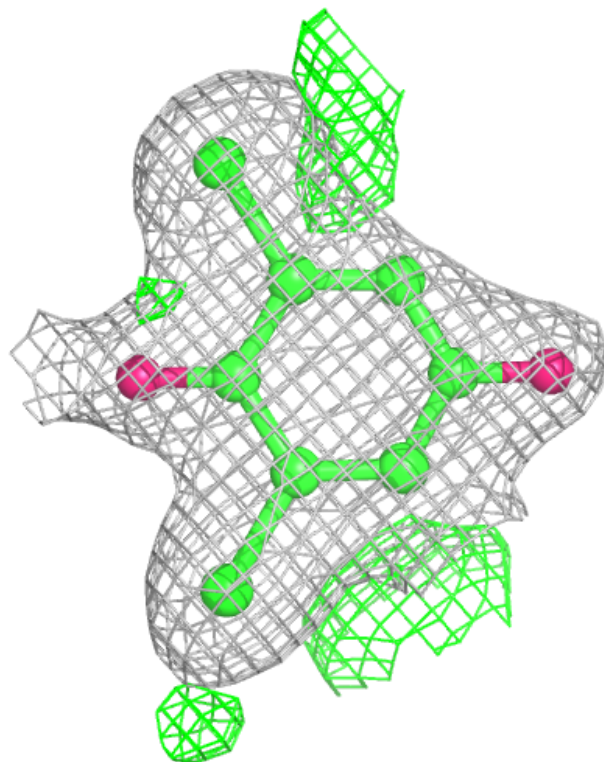
**Electron density around HTG o 301:**

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



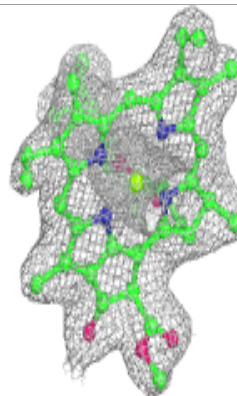
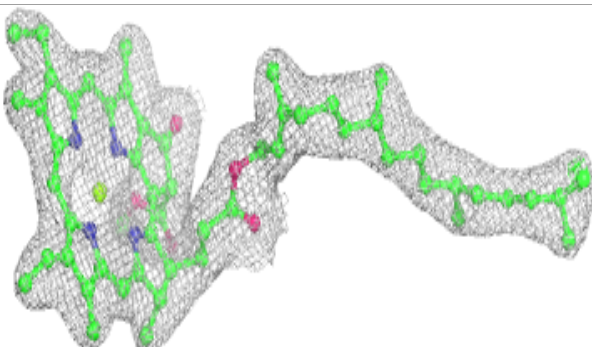
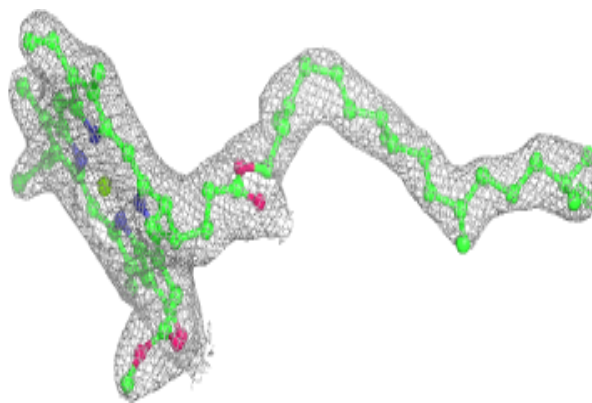
**Electron density around JOX a 2619:**

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

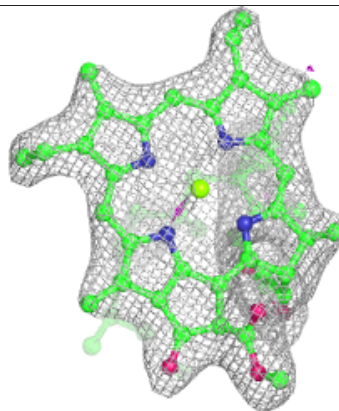
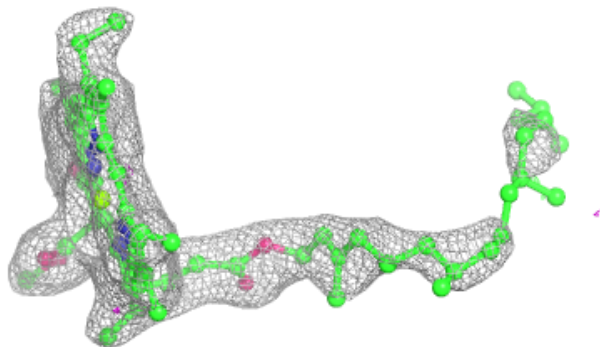
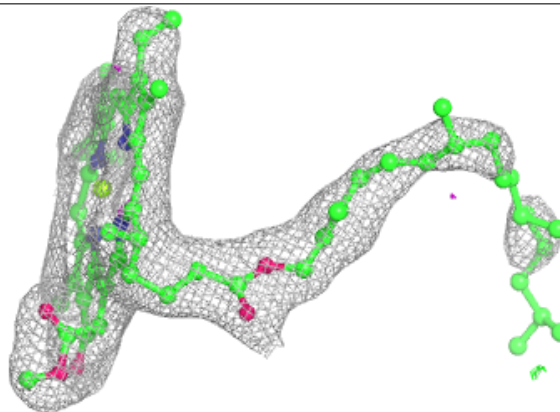


**Electron density around CLA c 505:**

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

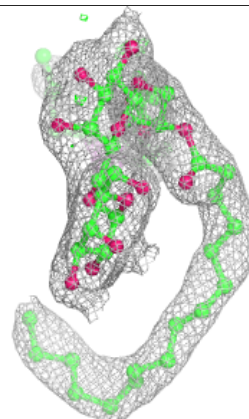
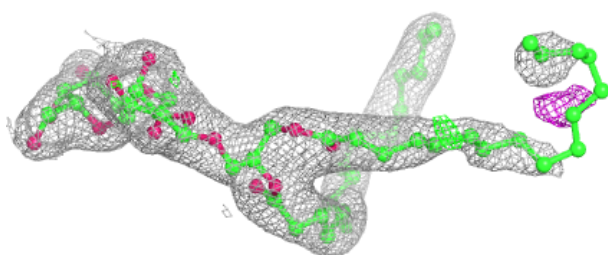
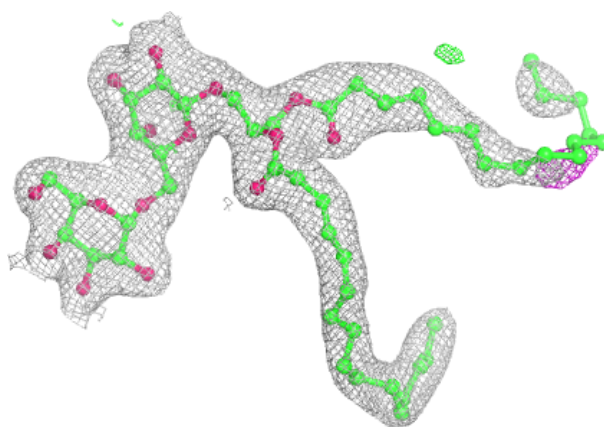
**Electron density around CLA D 2304:**

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

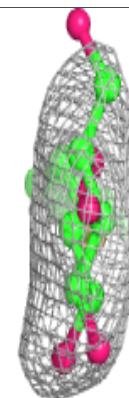
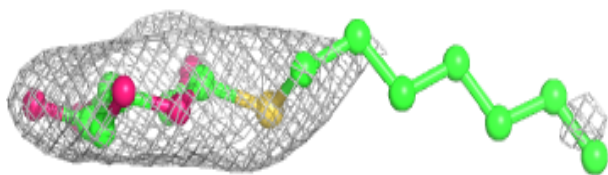
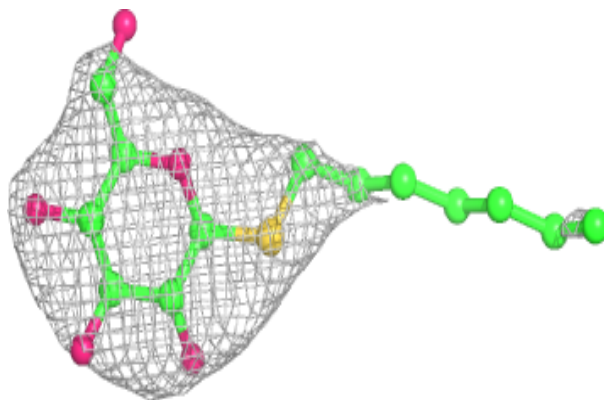


**Electron density around DGD c 519:**

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

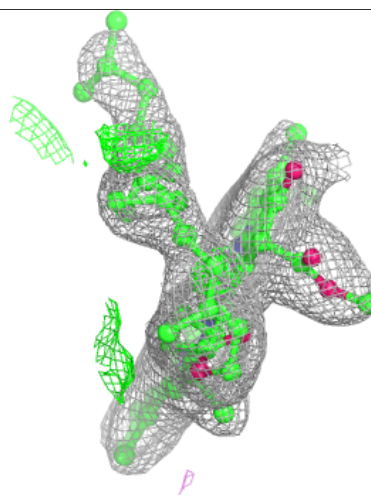
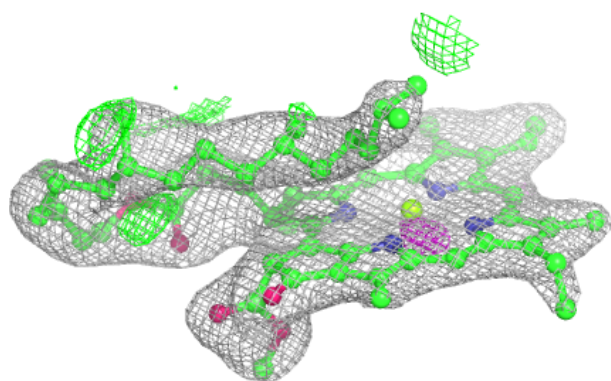
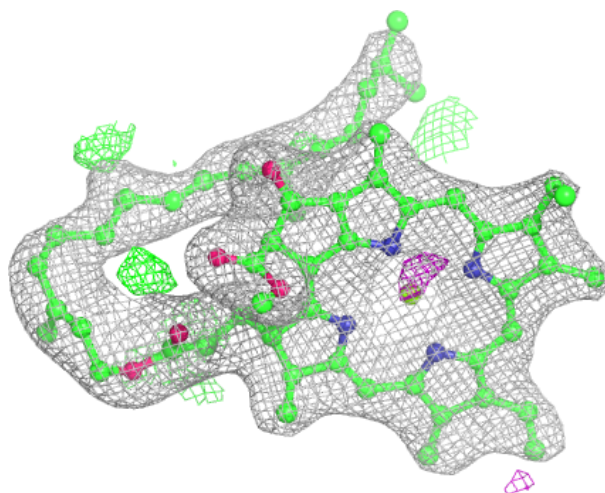
**Electron density around HTG C 521:**

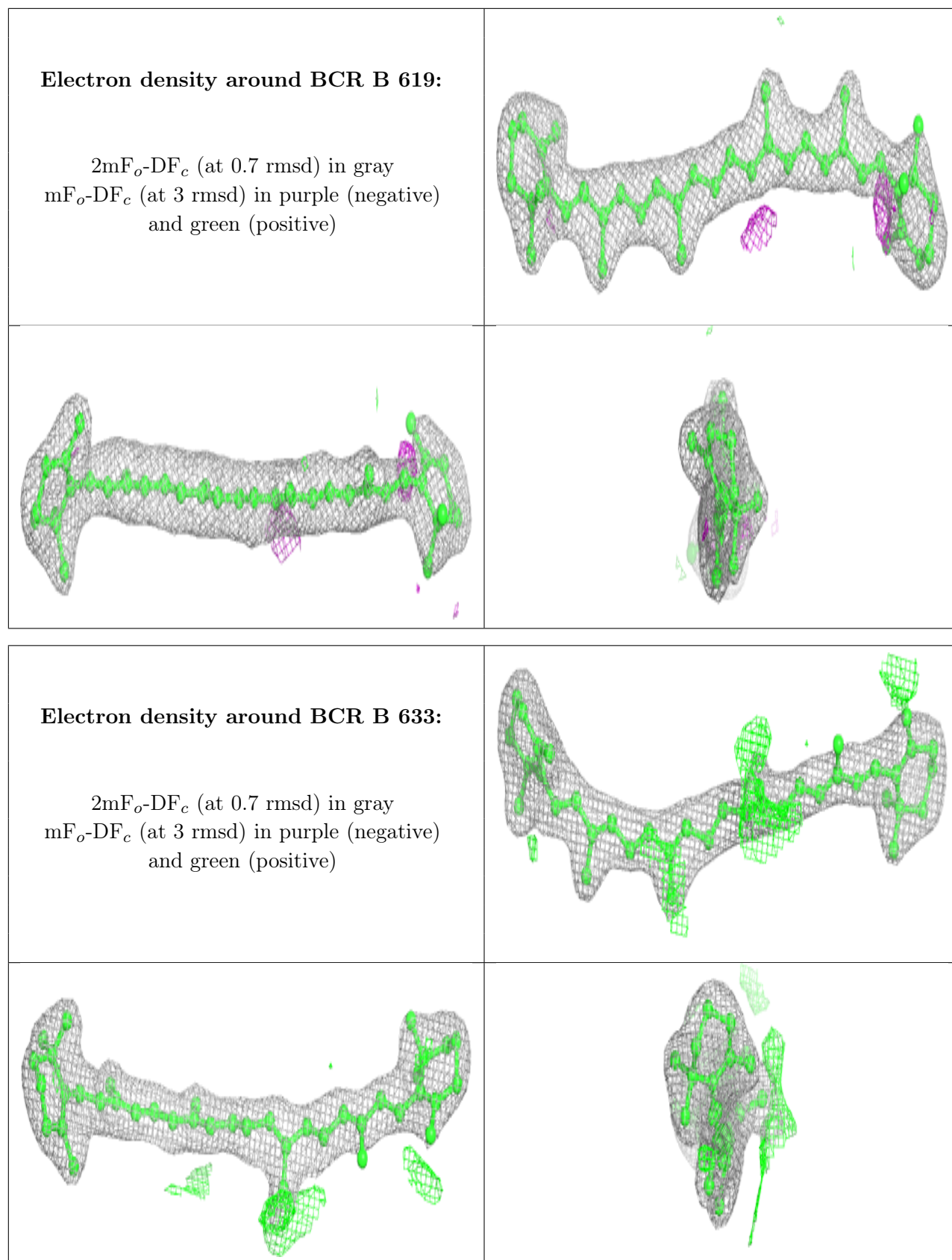
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



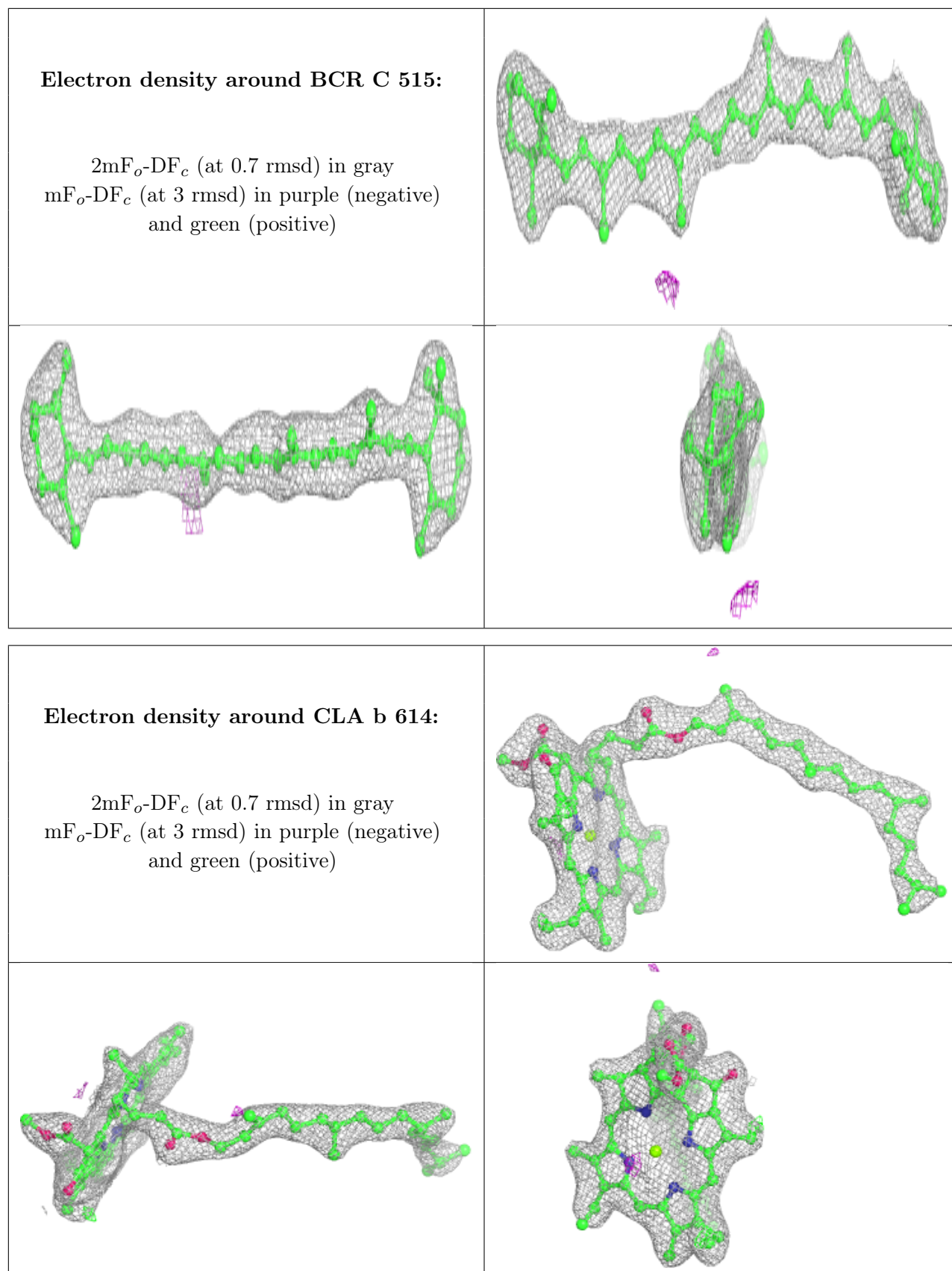
**Electron density around CLA C 510:**

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



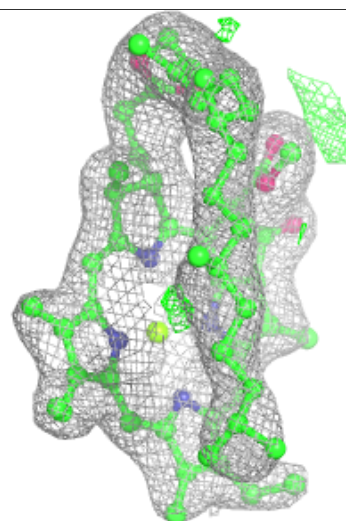
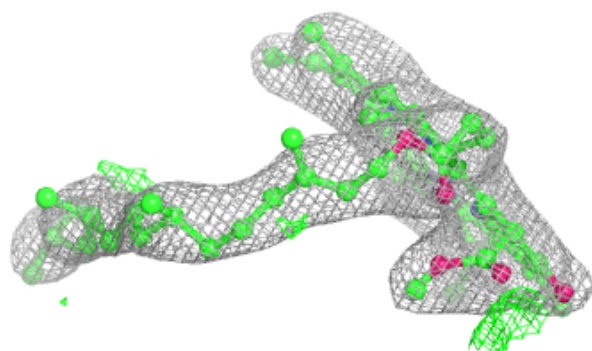
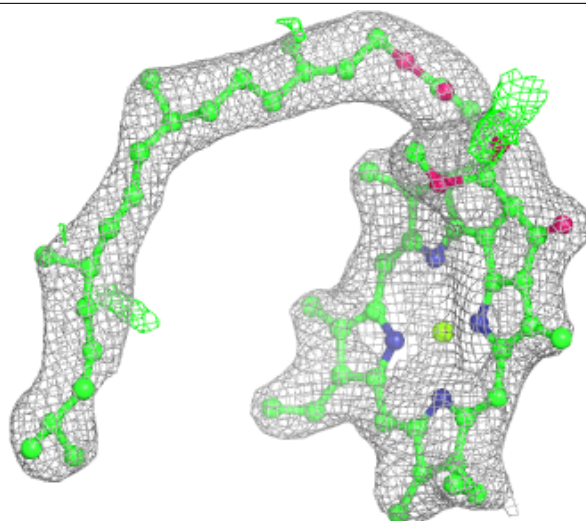






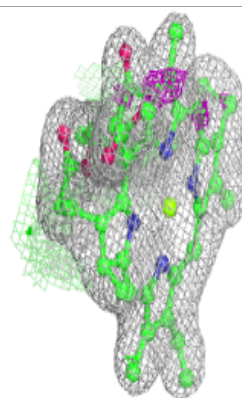
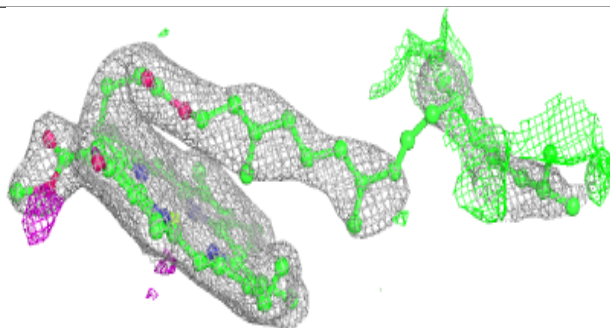
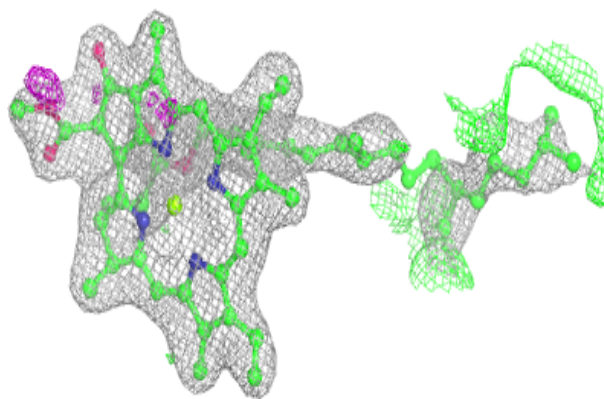
**Electron density around CLA C 508:**

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

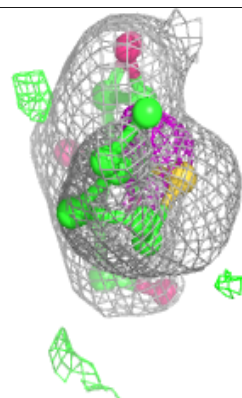
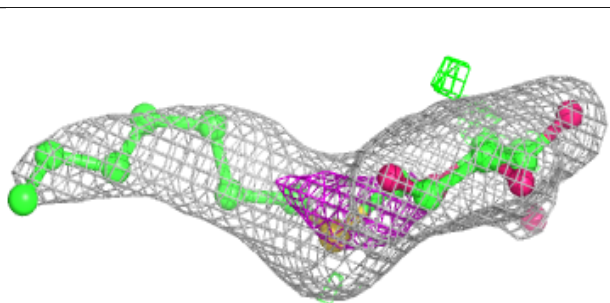
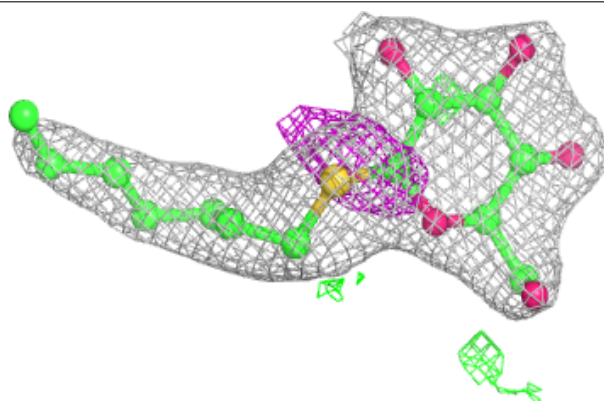


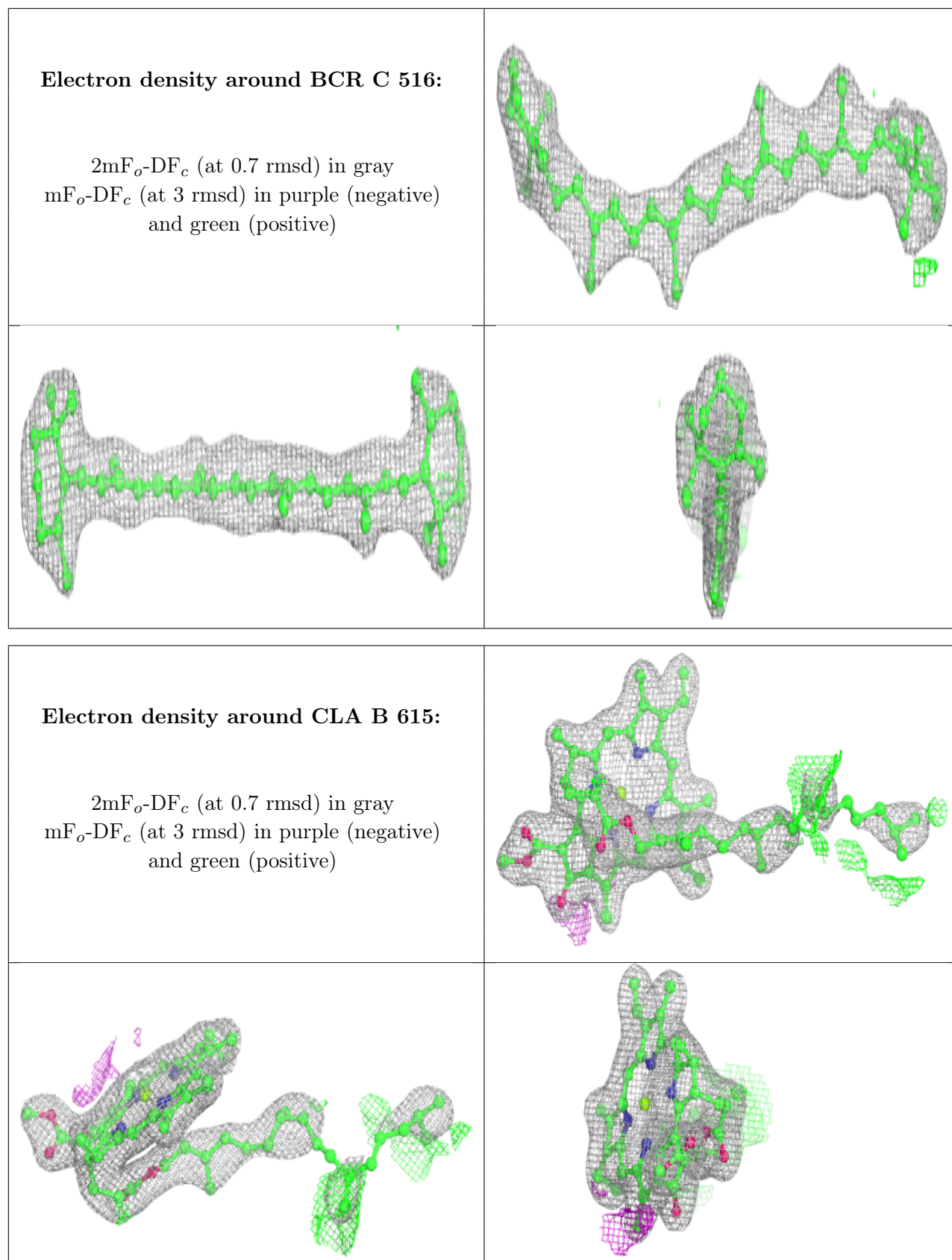
**Electron density around CLA b 619:**

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

**Electron density around HTG b 602:**

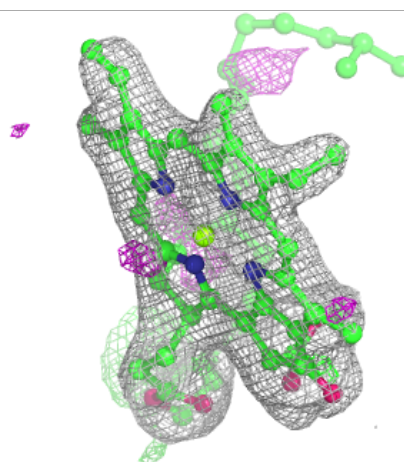
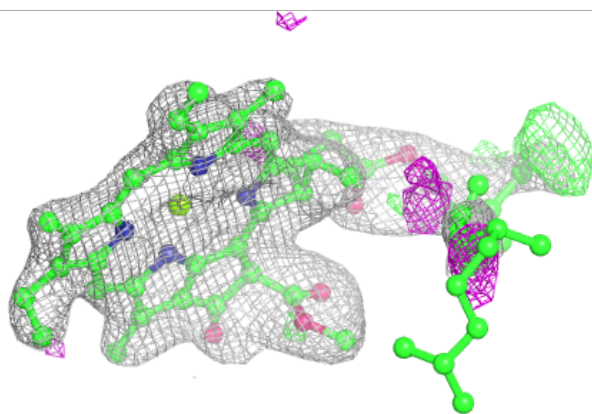
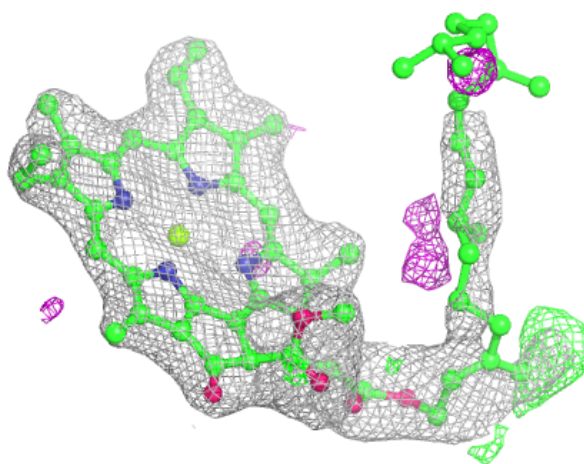
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





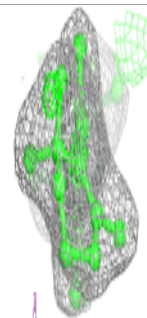
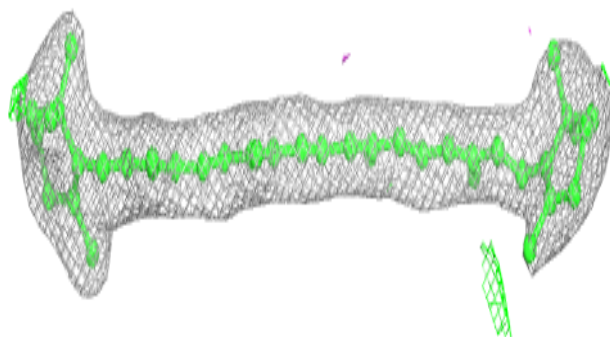
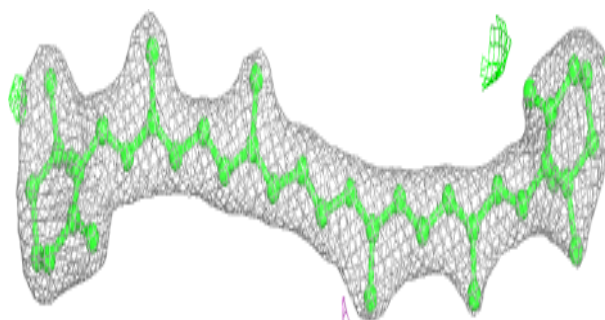
**Electron density around CLA B 617:**

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

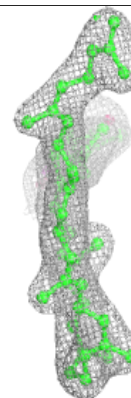
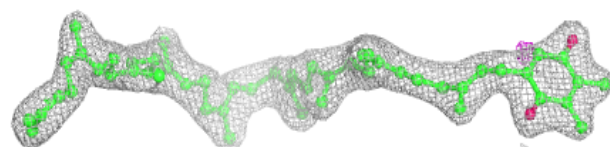
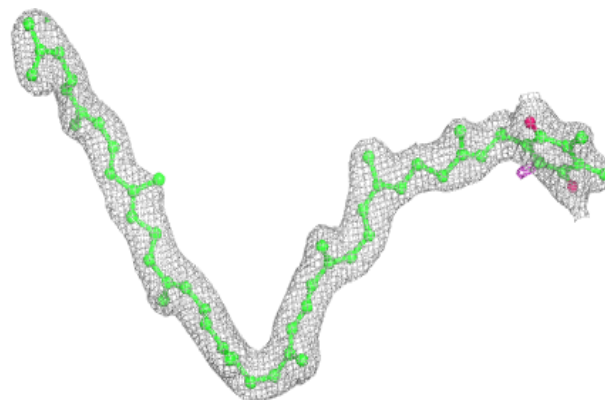


**Electron density around BCR b 623:**

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

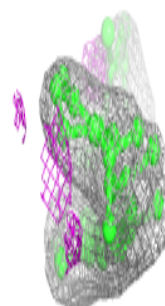
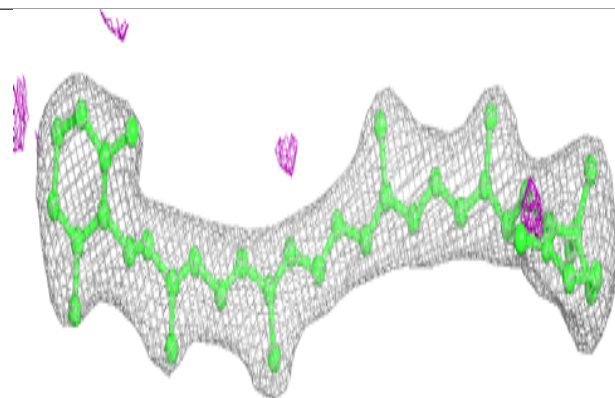
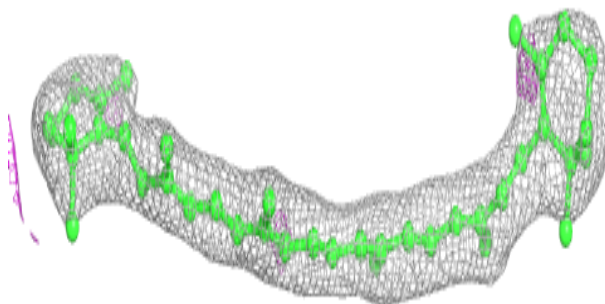
**Electron density around PL9 d 411:**

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



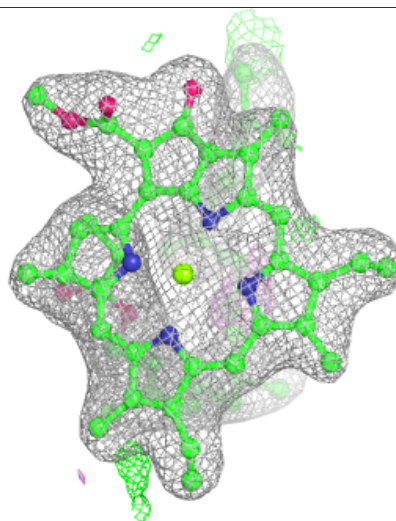
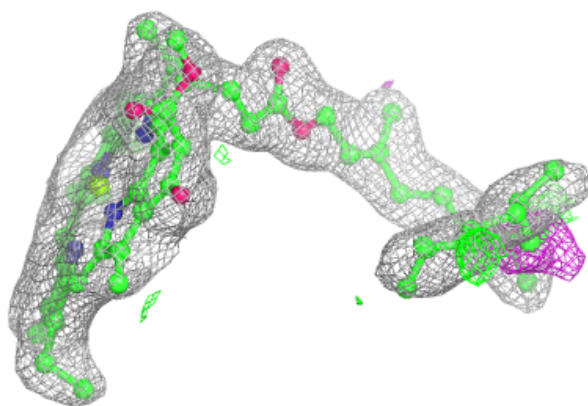
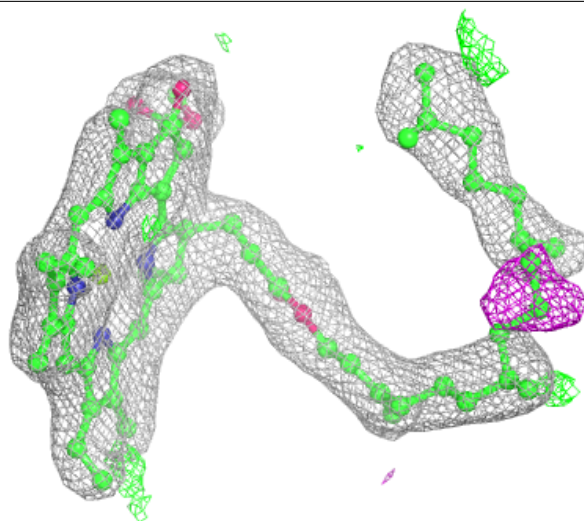
**Electron density around BCR d 410:**

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



**Electron density around CLA B 607:**

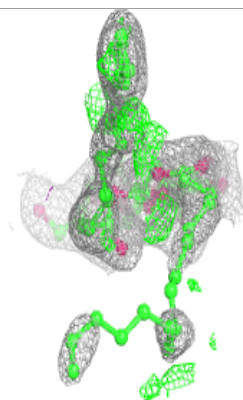
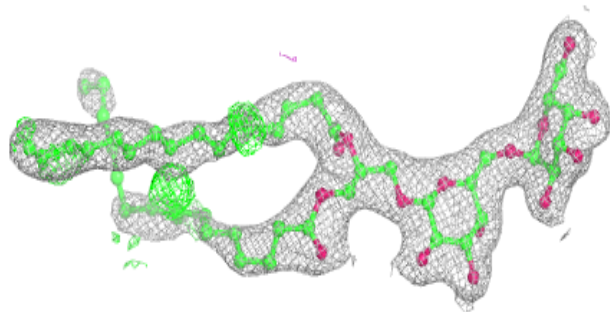
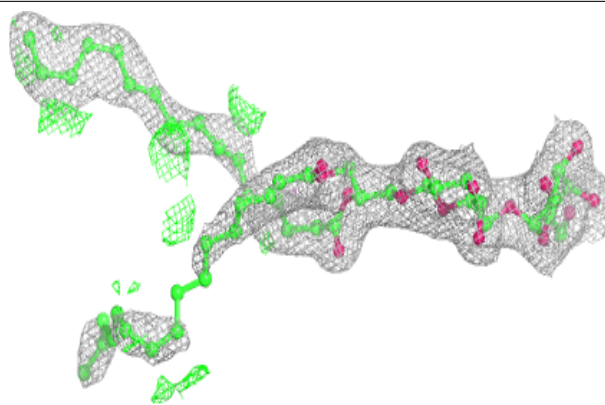
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



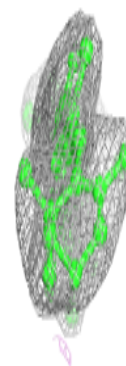
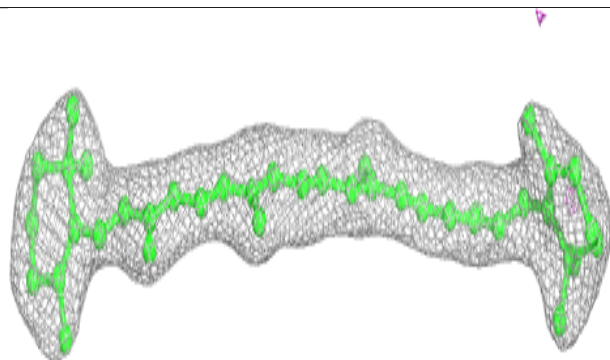
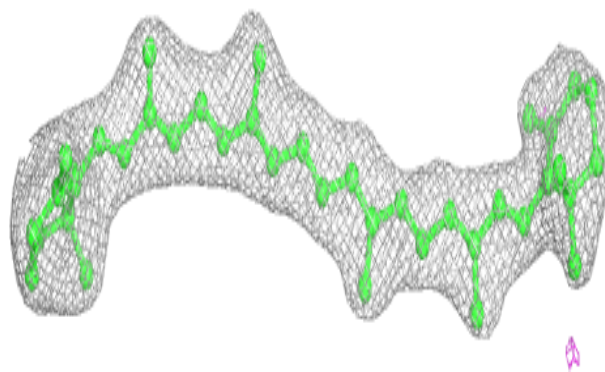


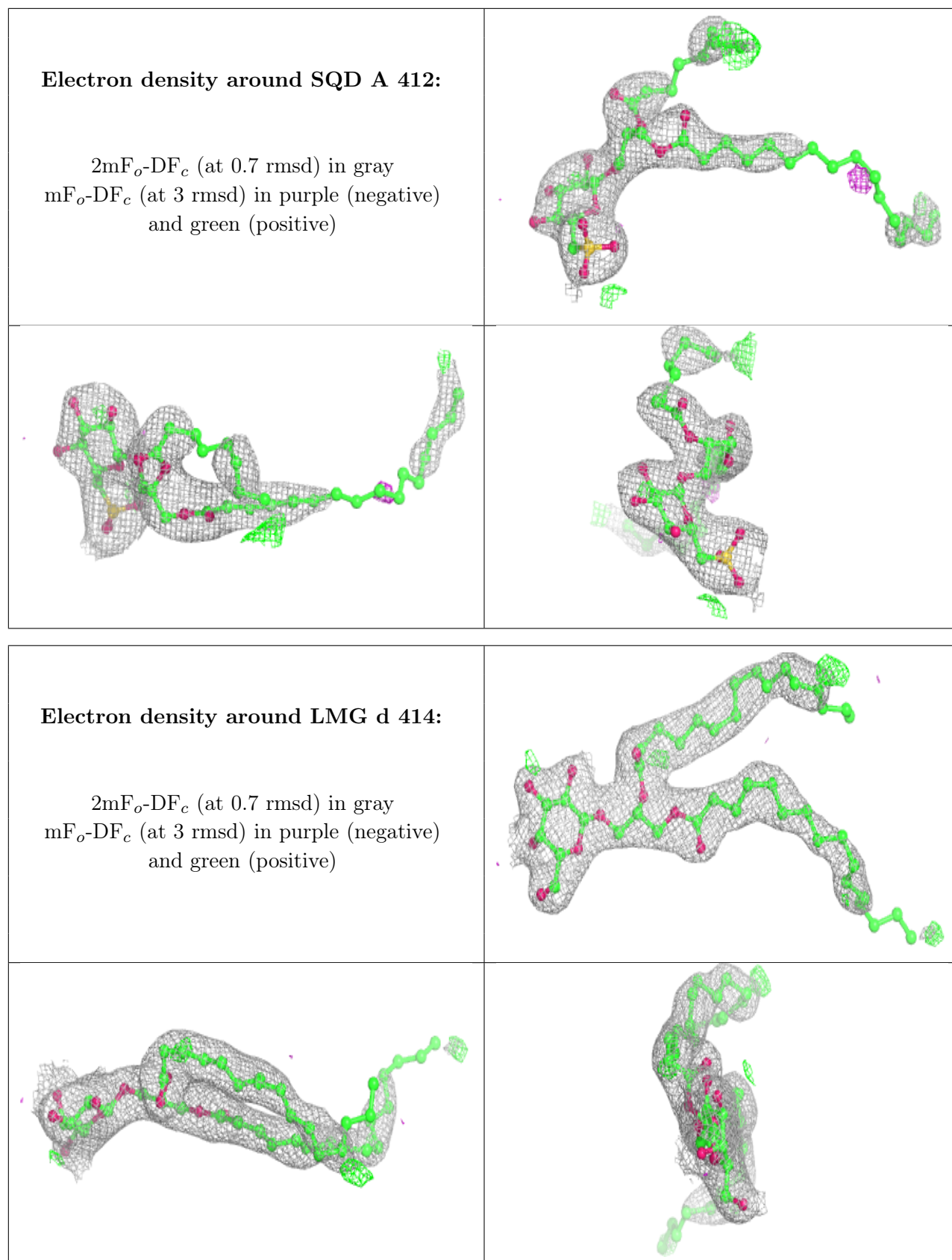
**Electron density around DGD c 518:**

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

**Electron density around BCR y 101:**

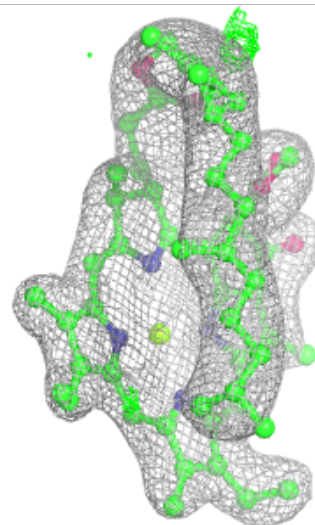
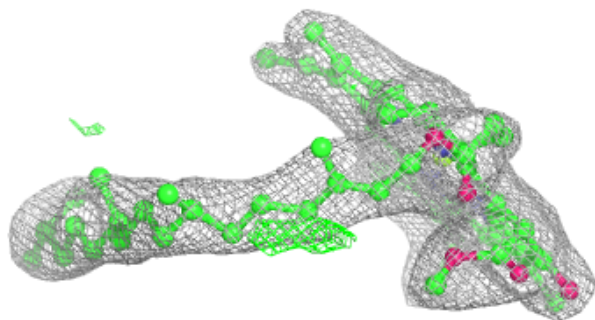
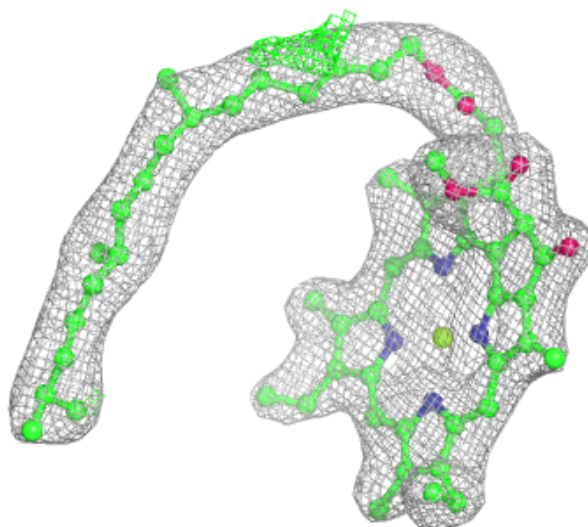
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





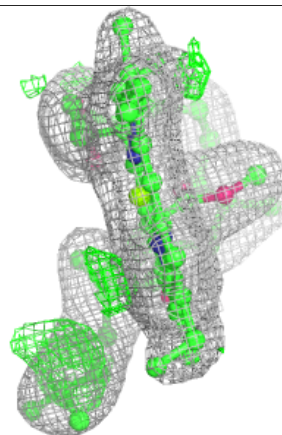
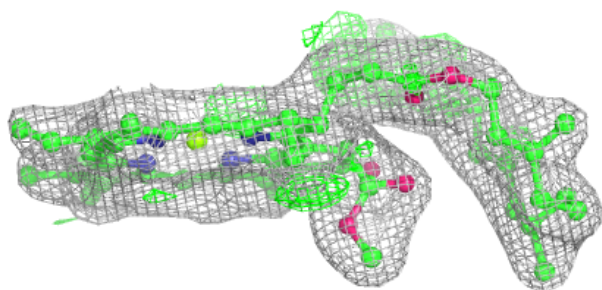
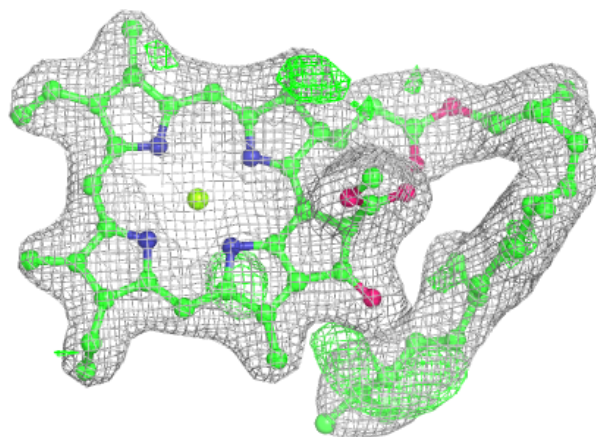
**Electron density around CLA c 510:**

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



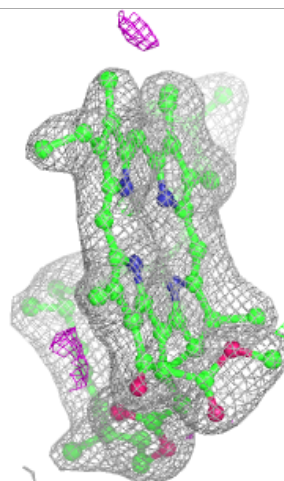
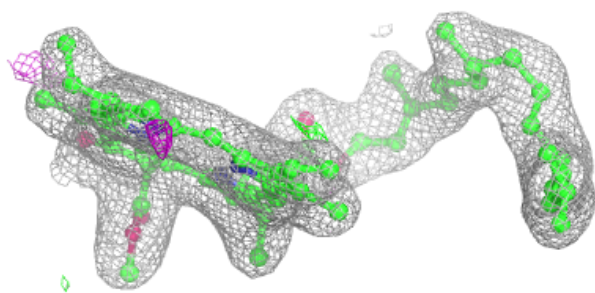
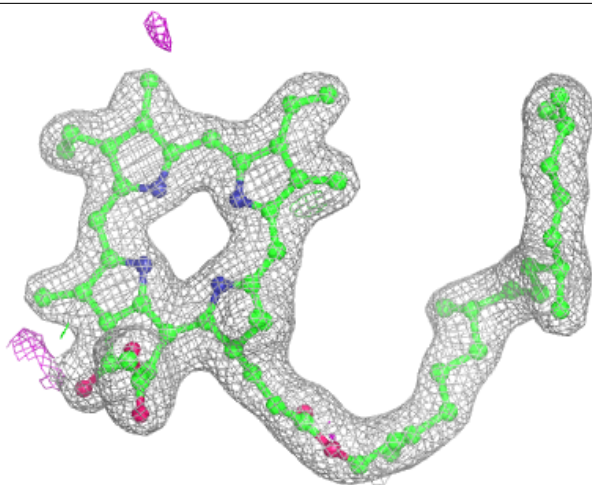
**Electron density around CLA B 611:**

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



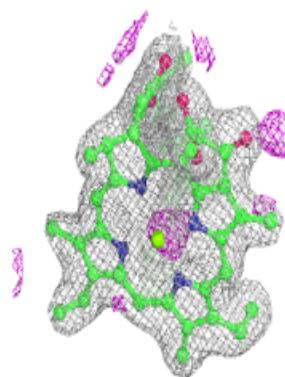
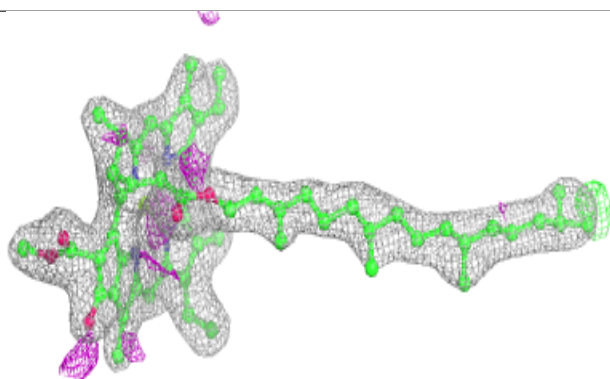
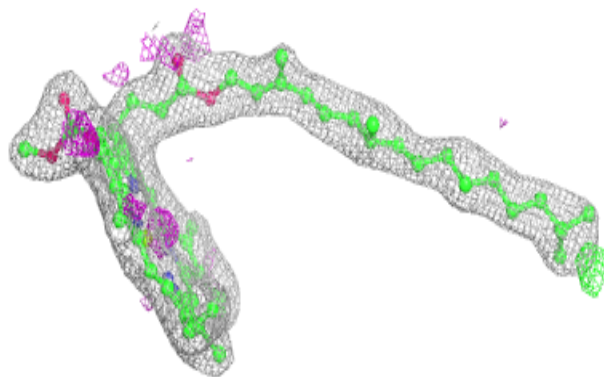
**Electron density around PHO A 409:**

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

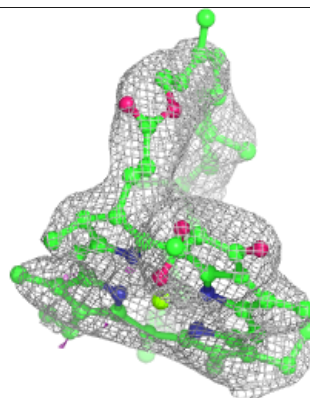
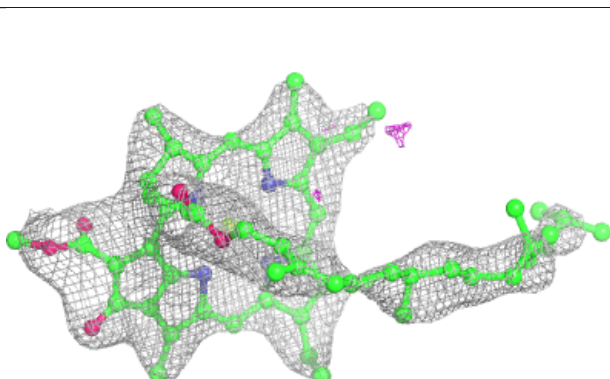
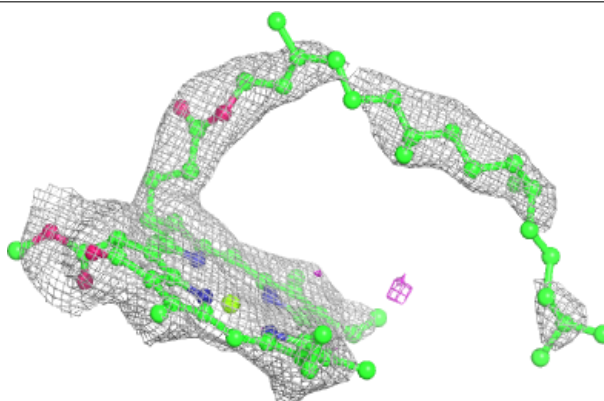


**Electron density around CLA b 612:**

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

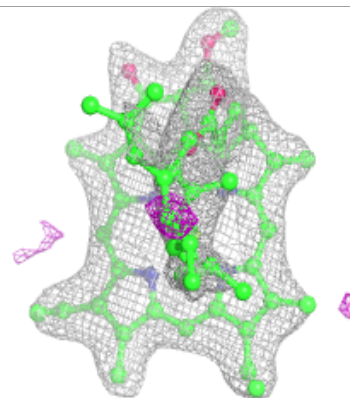
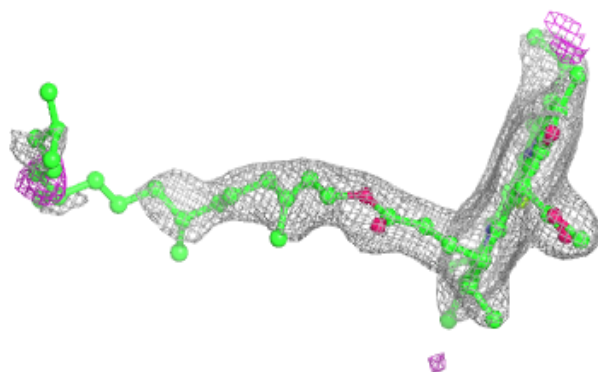
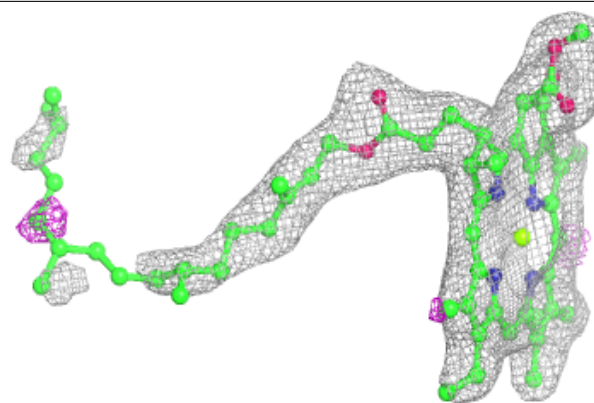
**Electron density around CLA c 516:**

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



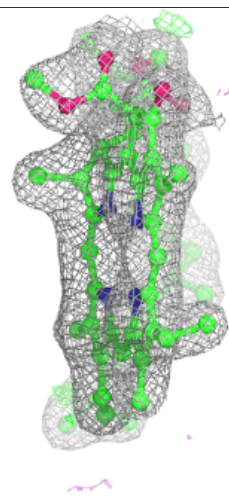
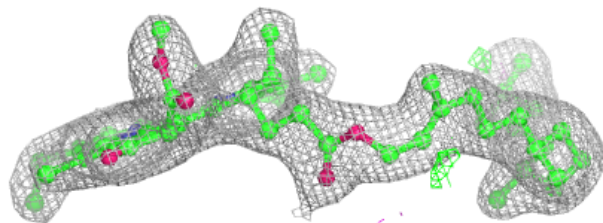
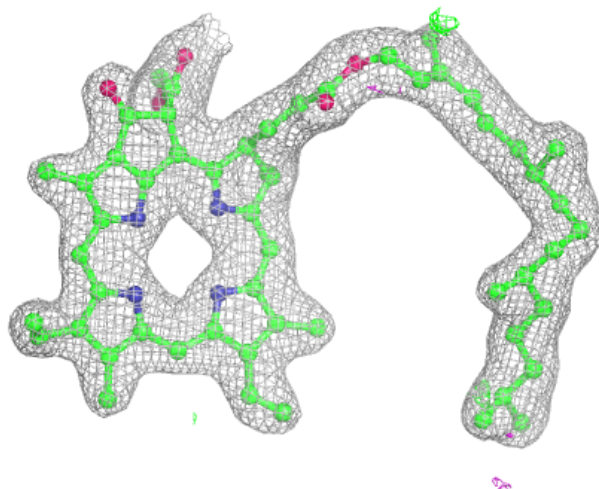
**Electron density around CLA d 409:**

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

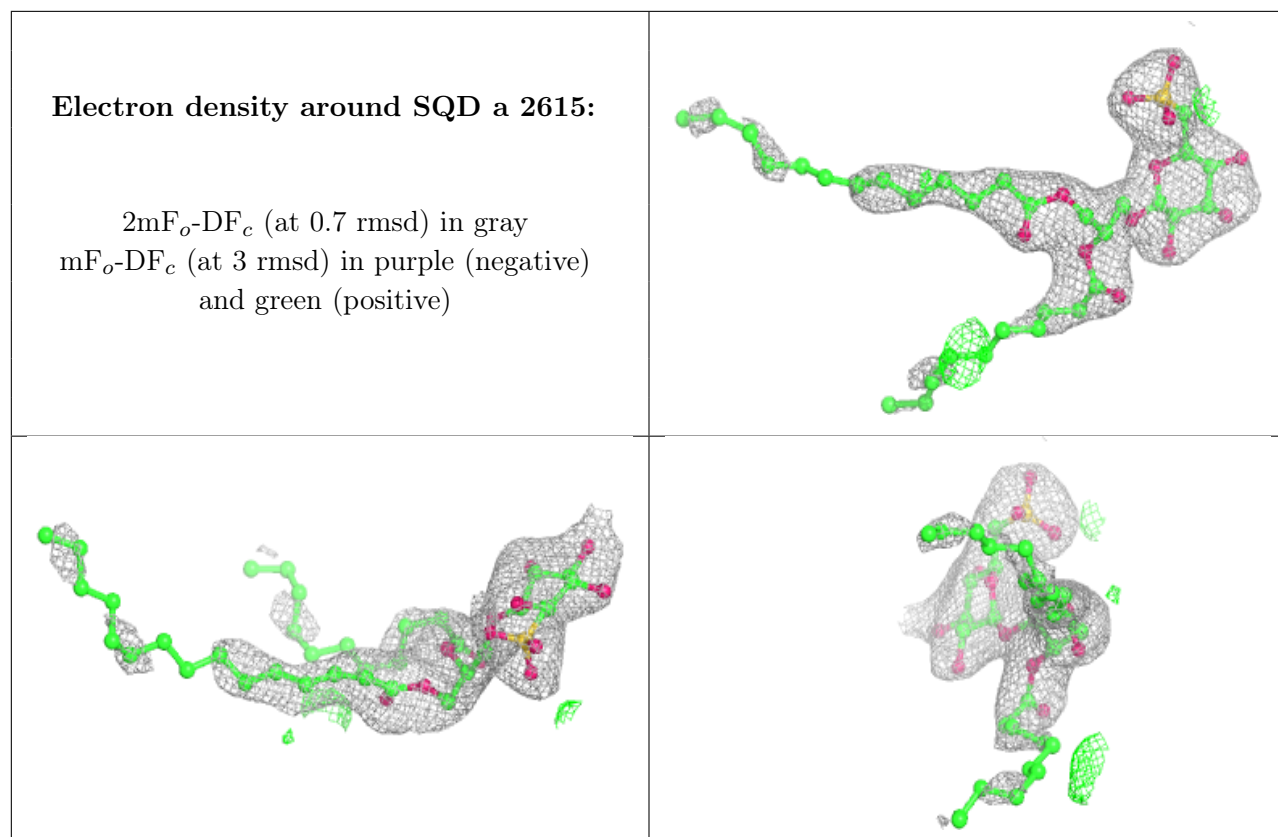


**Electron density around PHO A 408:**

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

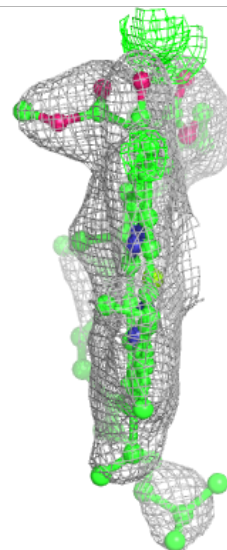
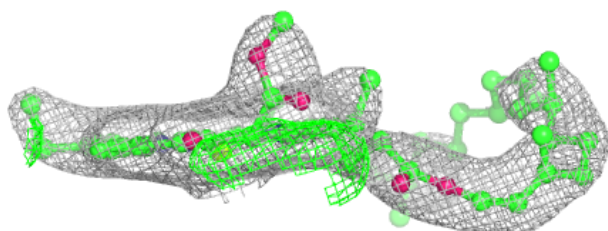
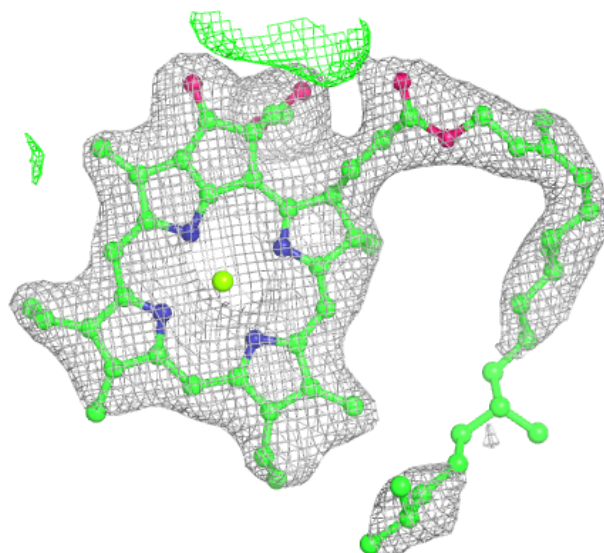


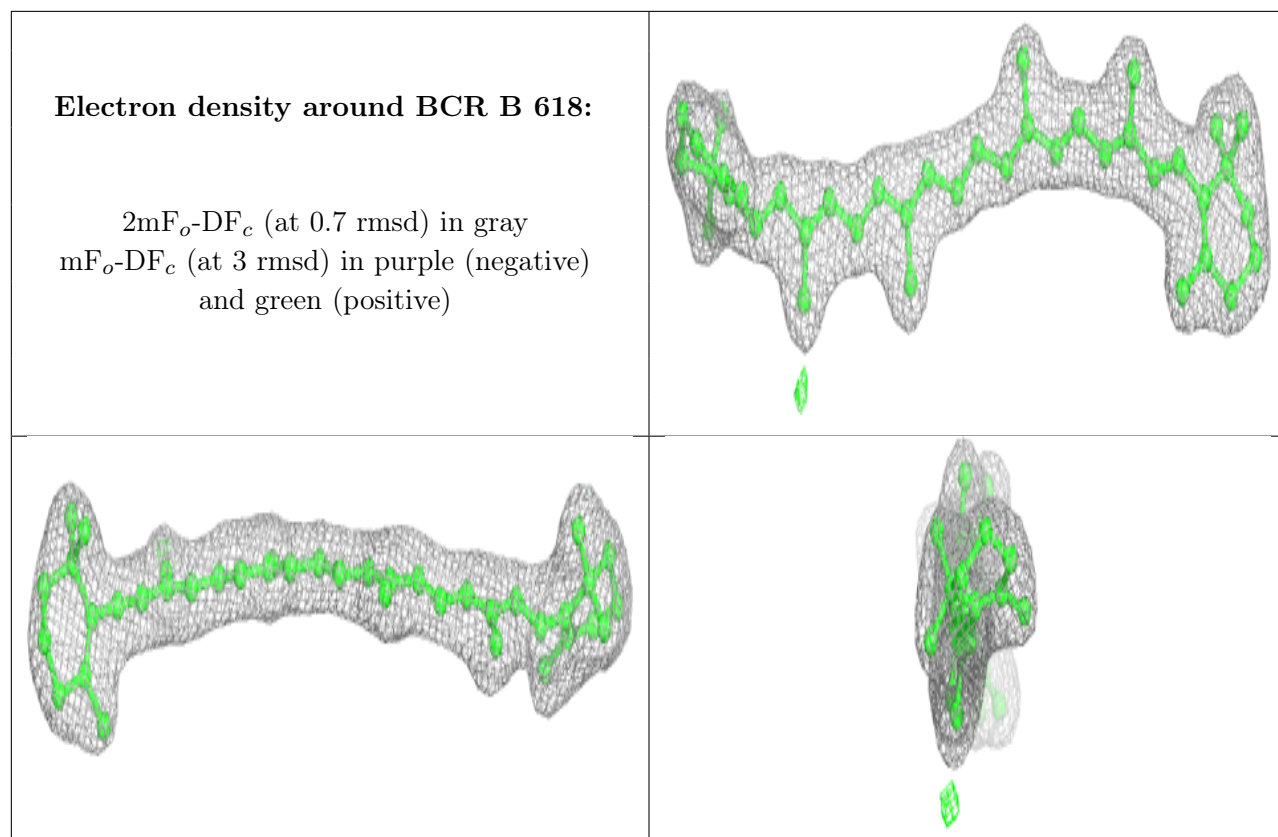




**Electron density around CLA C 513:**

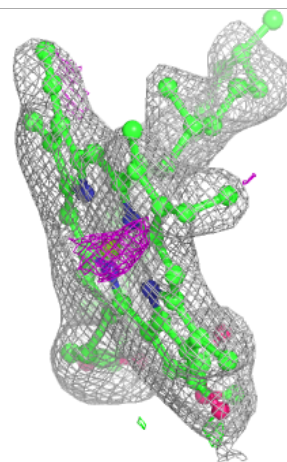
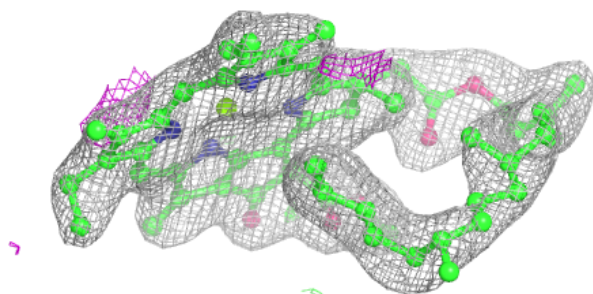
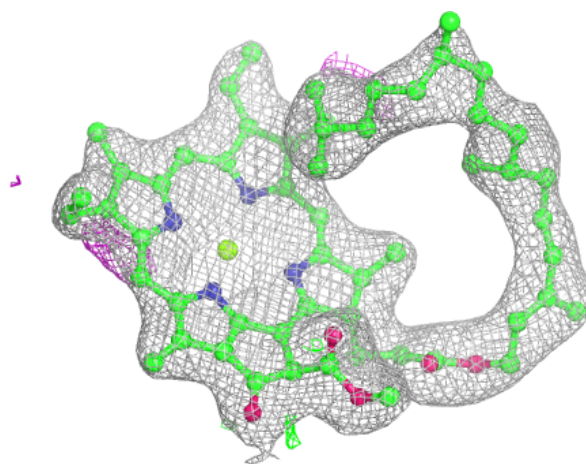
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

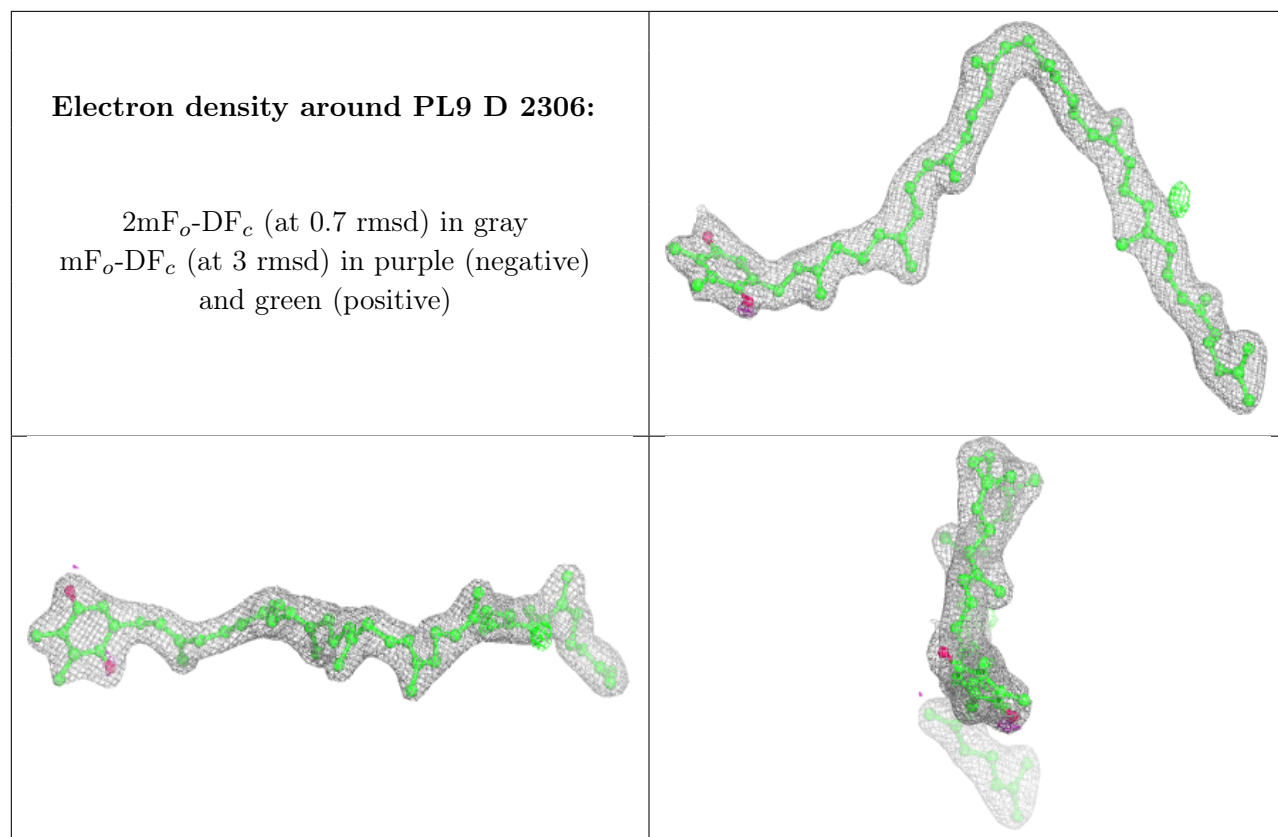




**Electron density around CLA B 616:**

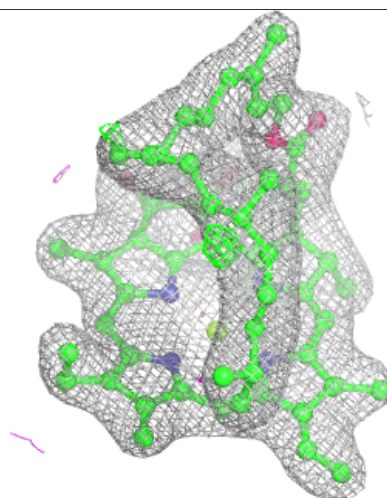
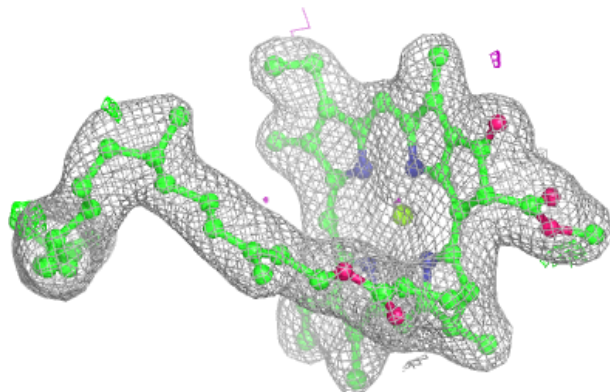
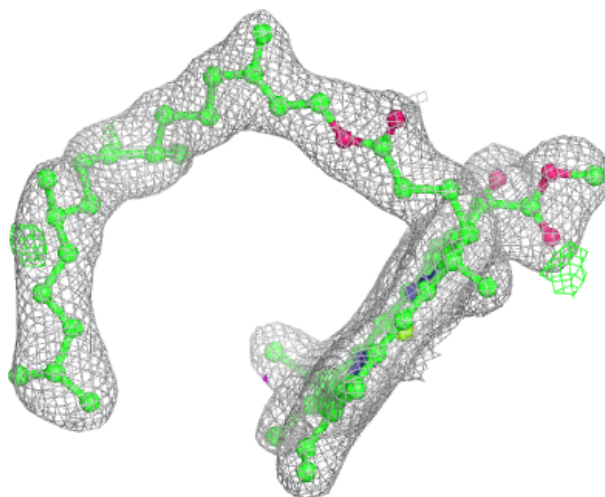
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





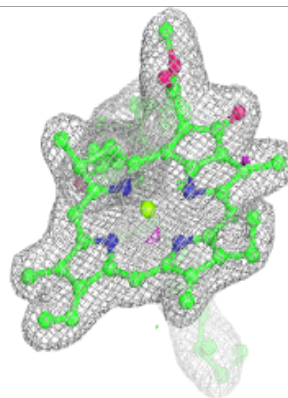
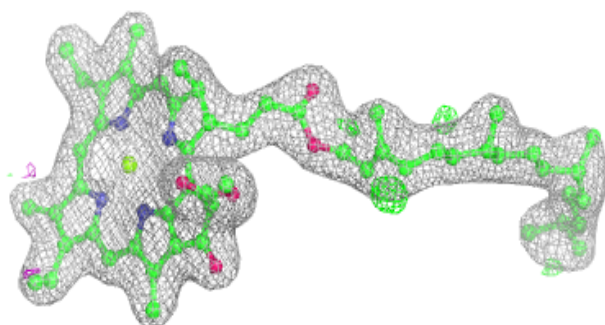
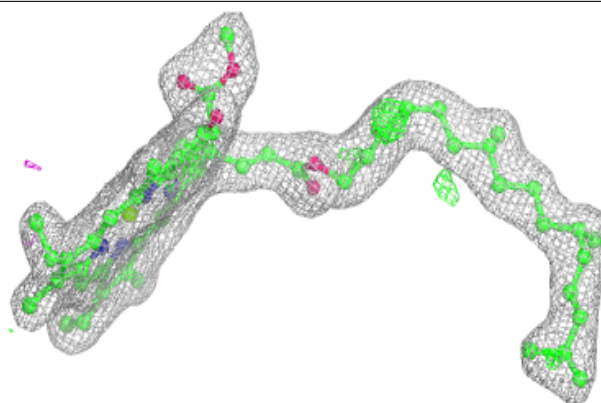
**Electron density around CLA b 616:**

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

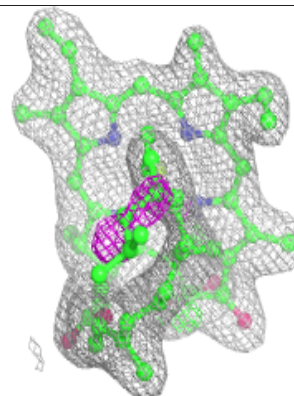
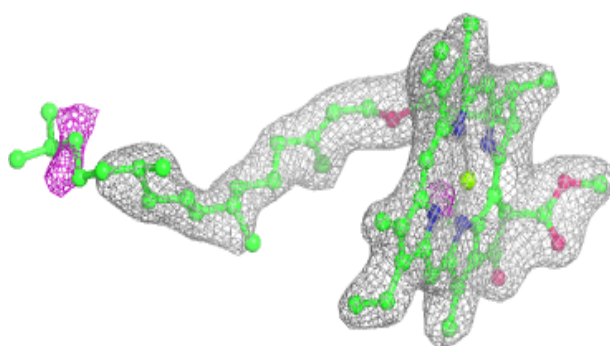
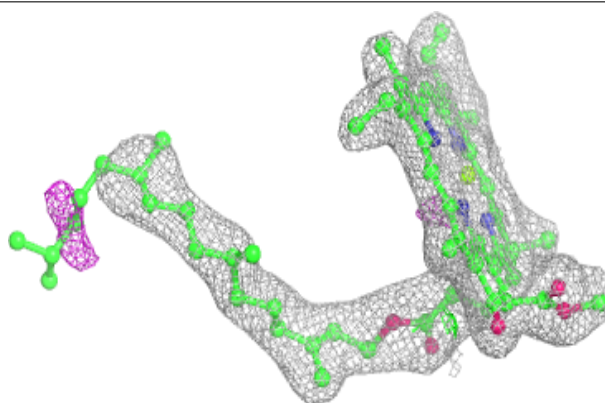


**Electron density around CLA D 2303:**

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

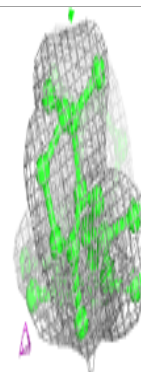
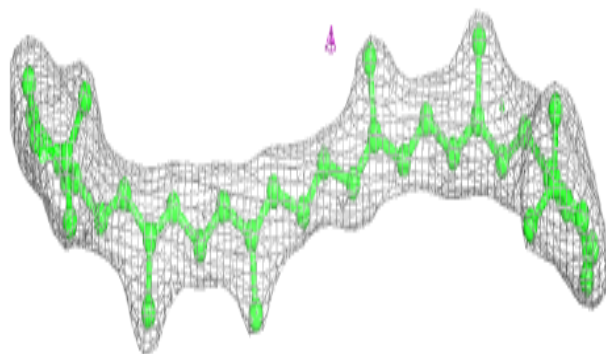
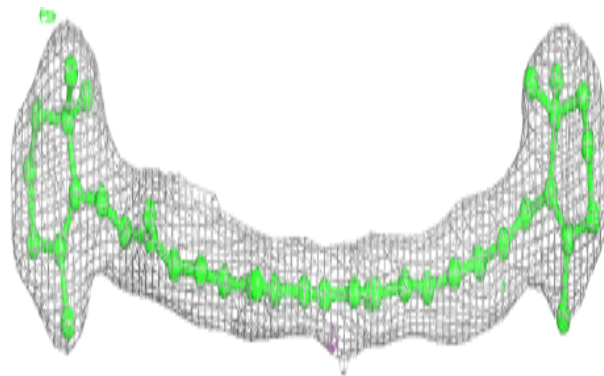
**Electron density around CLA C 509:**

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

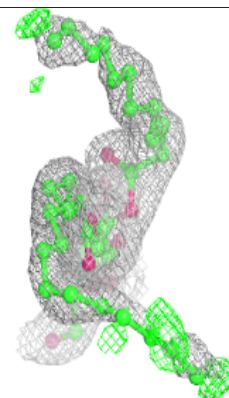
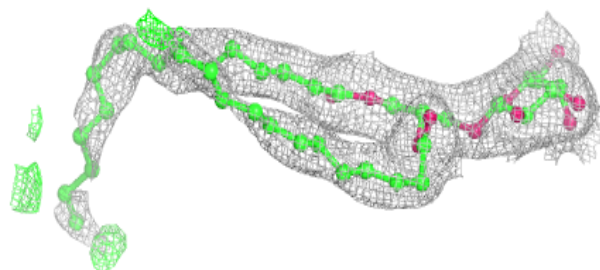
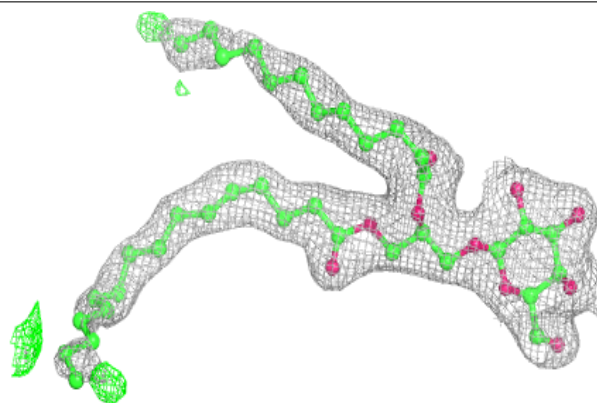


**Electron density around BCR K 101:**

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

**Electron density around LMG D 2312:**

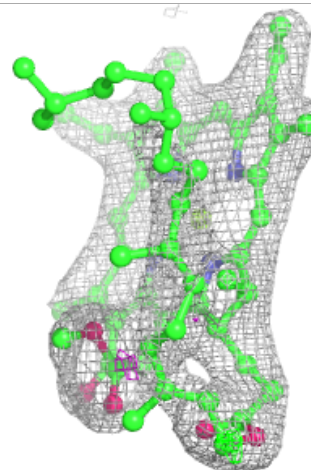
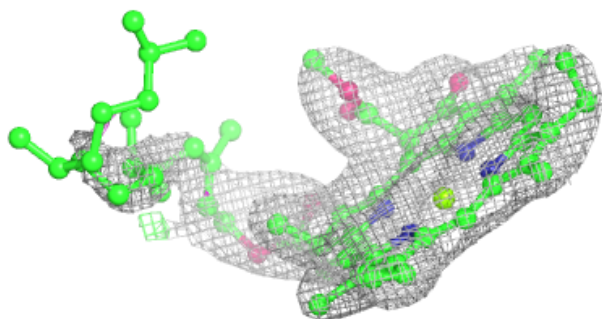
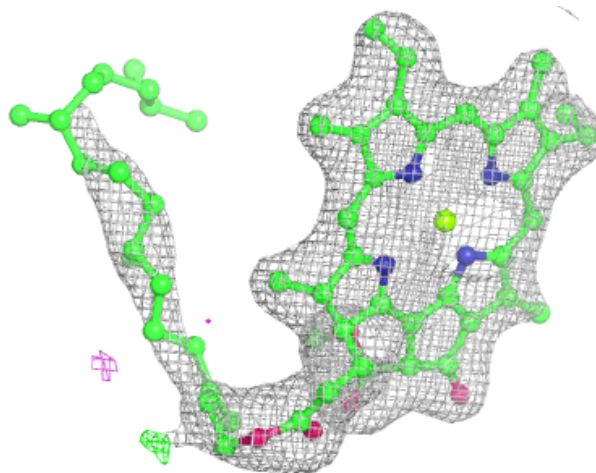
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

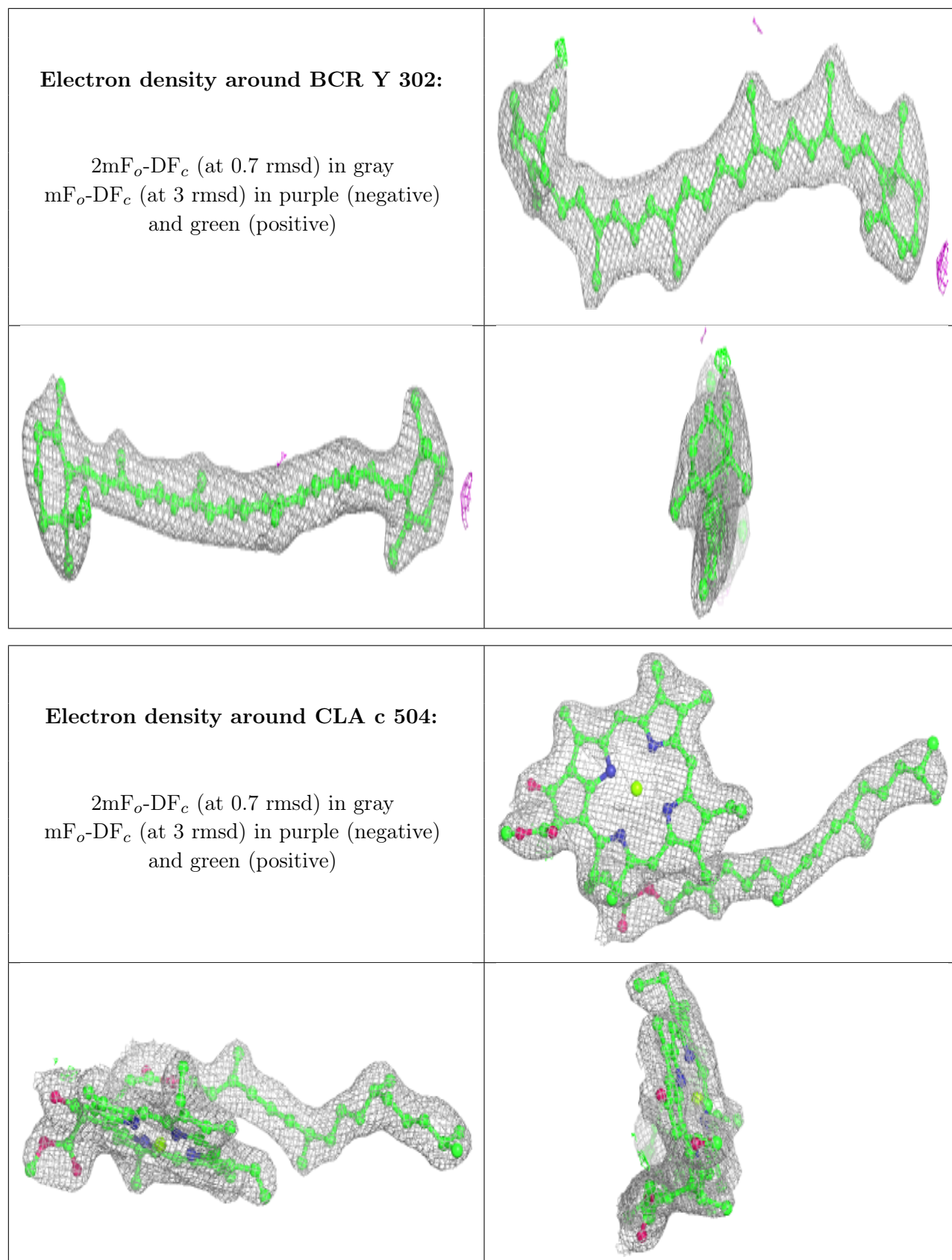


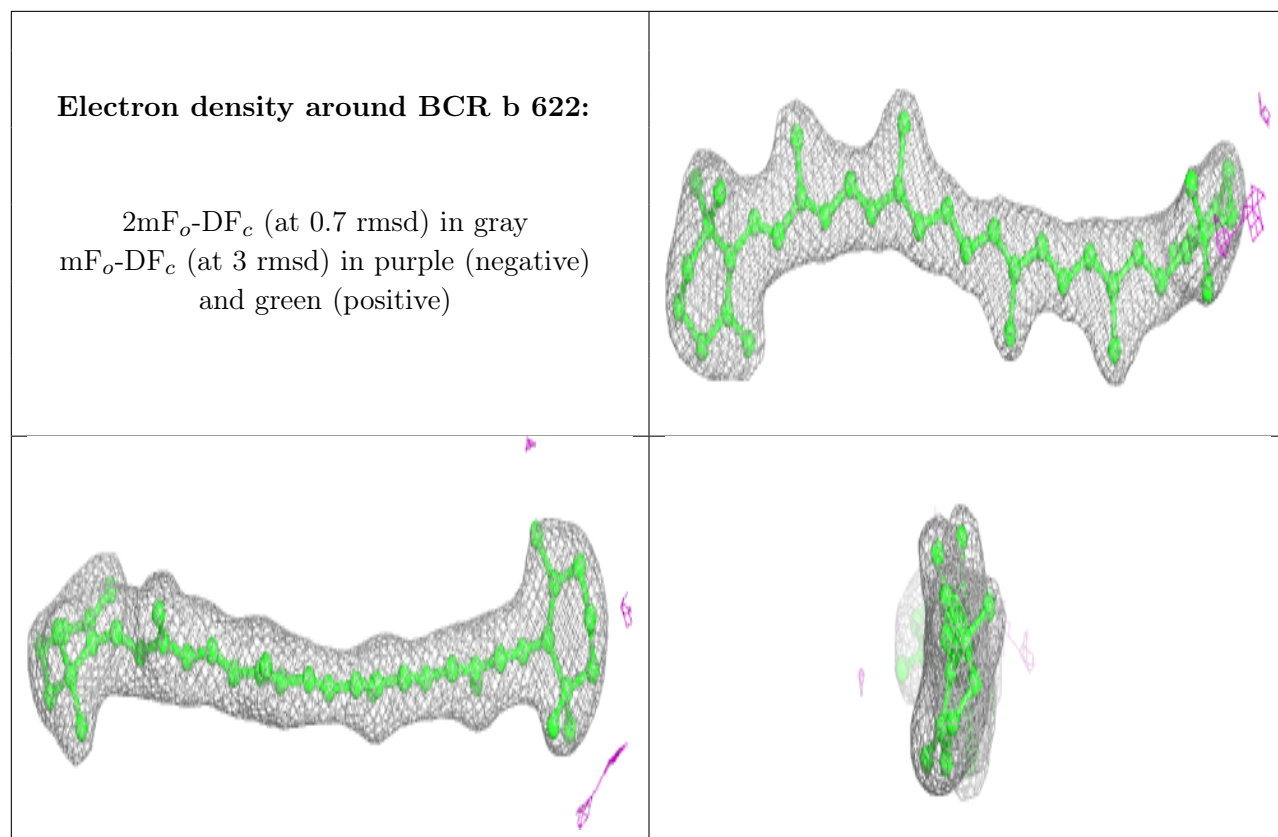


**Electron density around CLA b 621:**

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

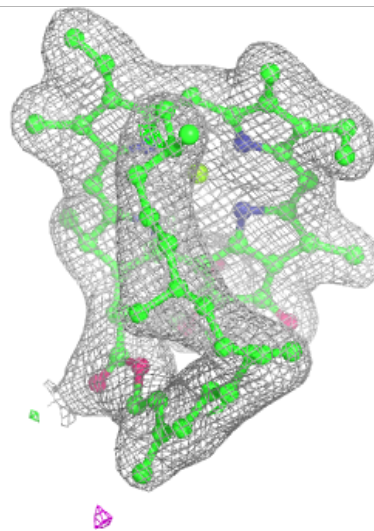
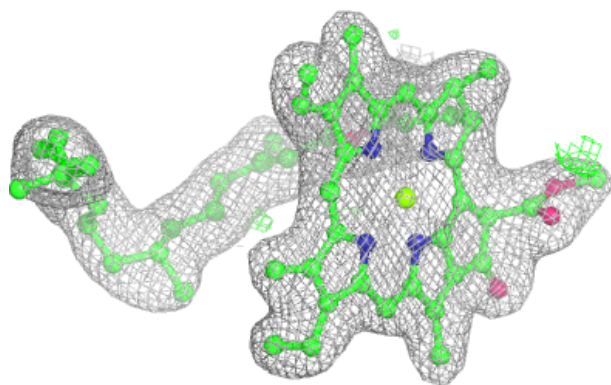
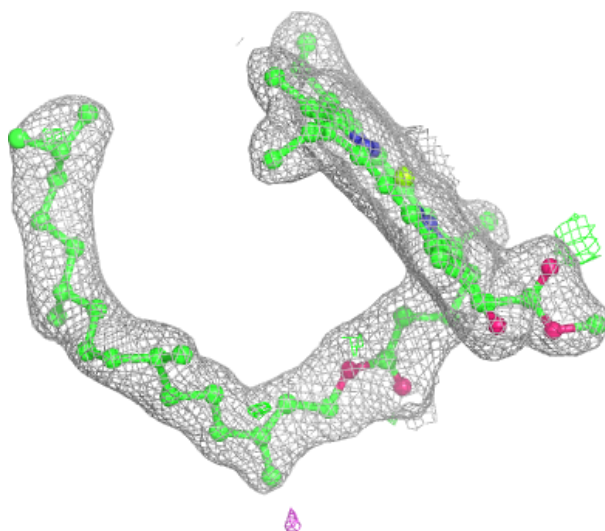






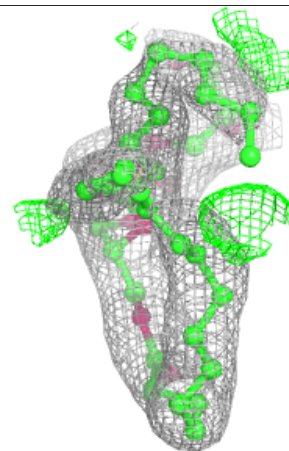
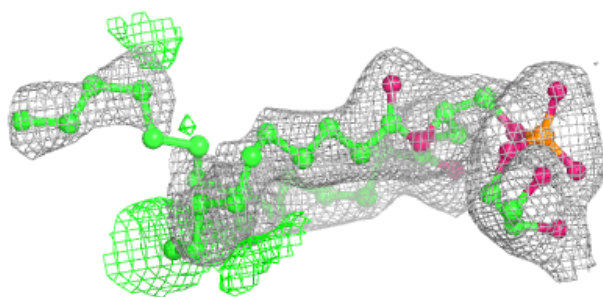
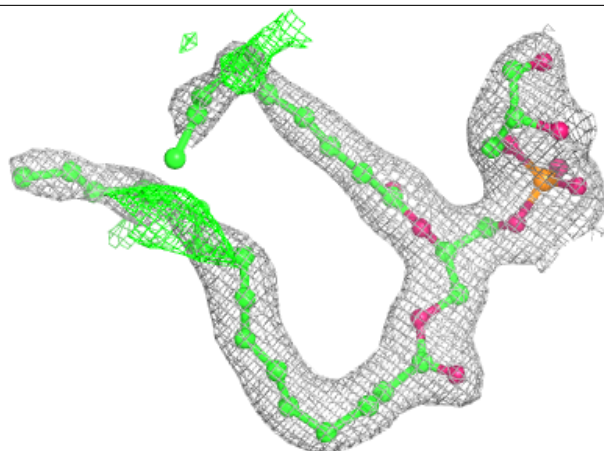
**Electron density around CLA B 612:**

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

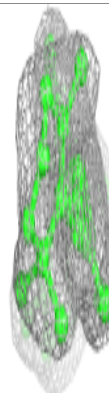
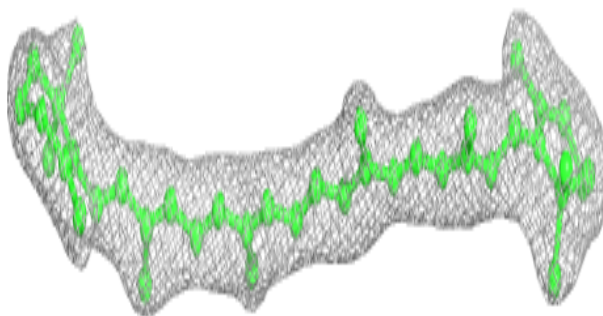
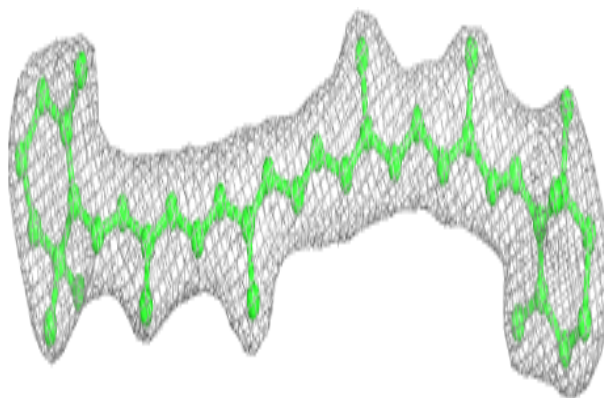


**Electron density around LHG d 403:**

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

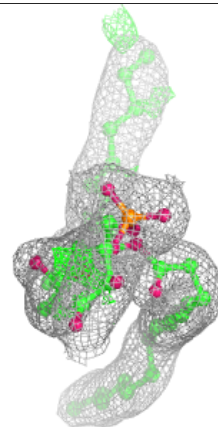
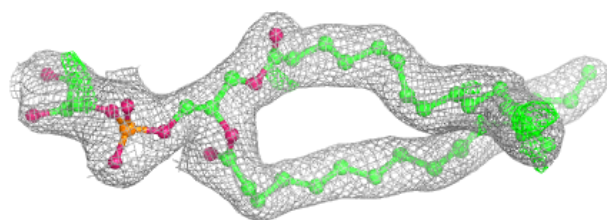
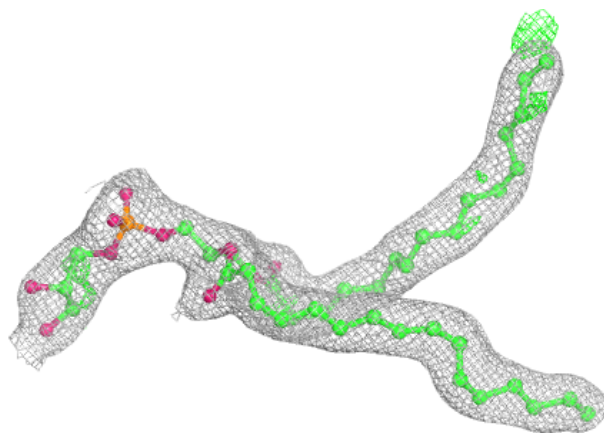
**Electron density around BCR b 624:**

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

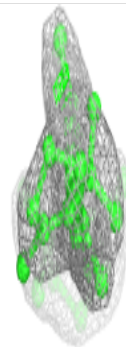
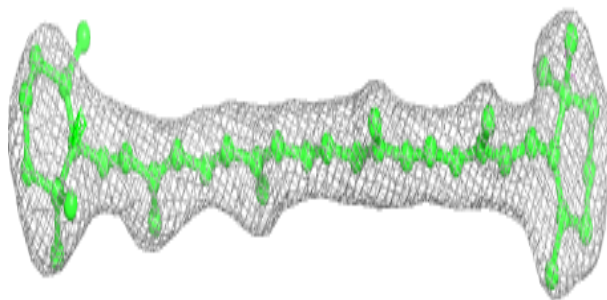
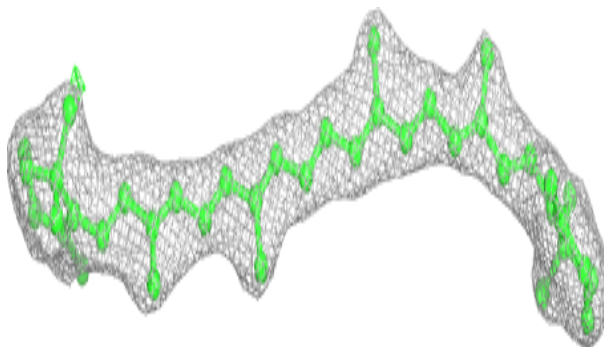


**Electron density around LHG d 413:**

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

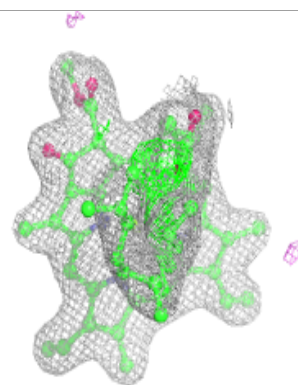
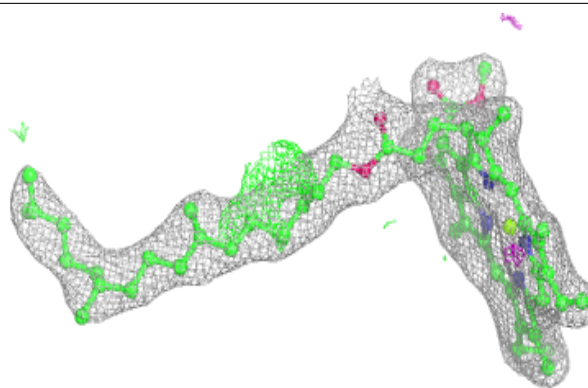
**Electron density around BCR c 517:**

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

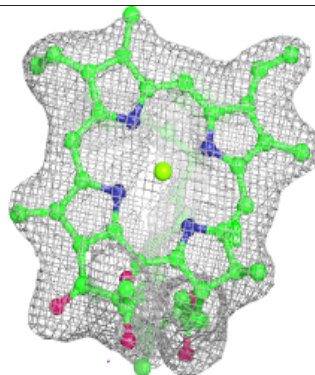
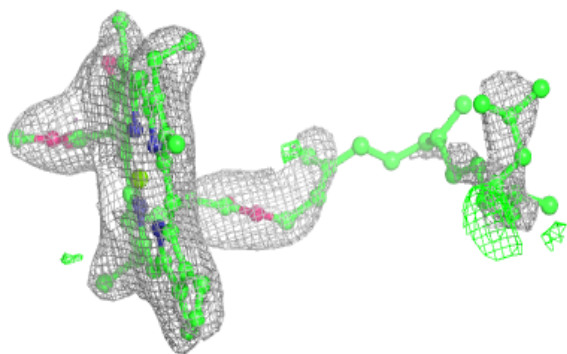
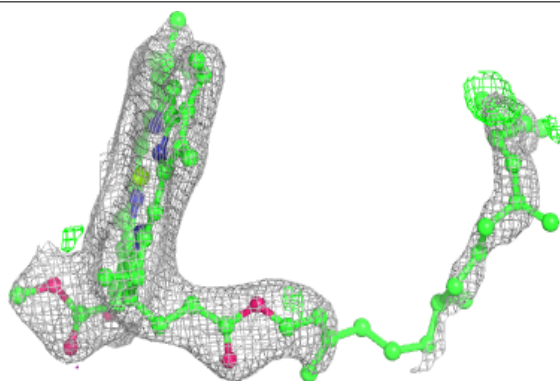


**Electron density around CLA b 609:**

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

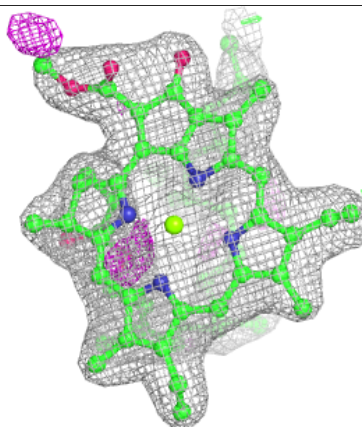
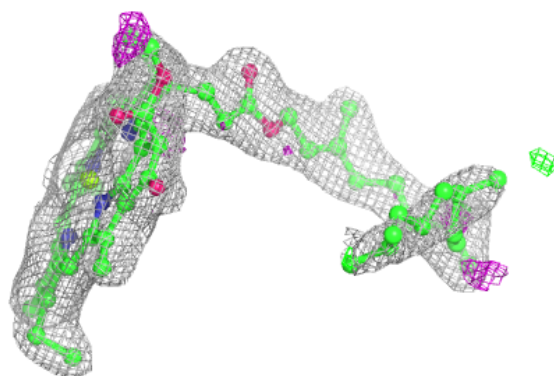
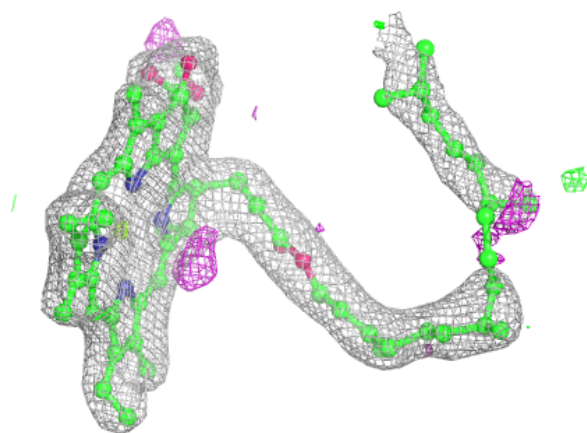
**Electron density around CLA c 509:**

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

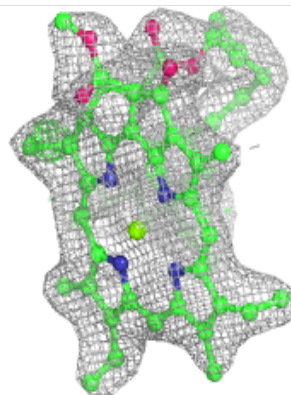
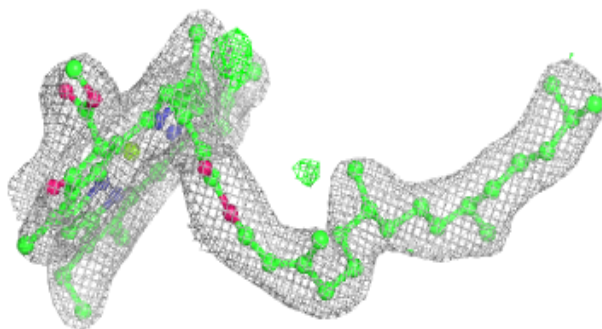
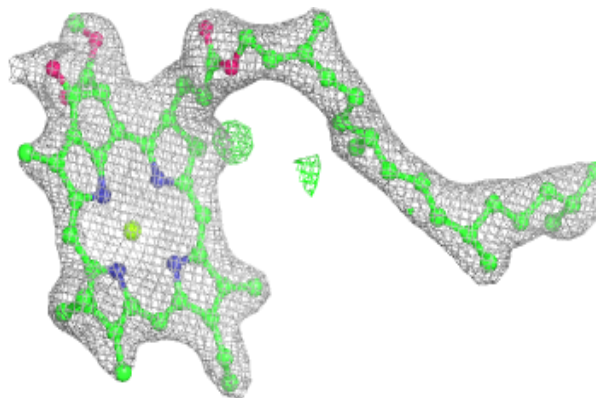


**Electron density around CLA b 611:**

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

**Electron density around CLA c 514:**

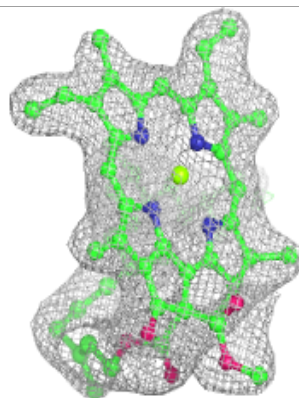
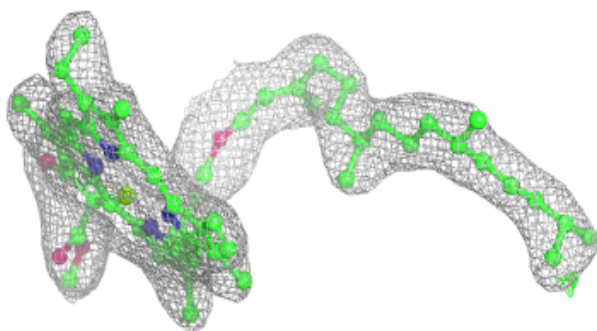
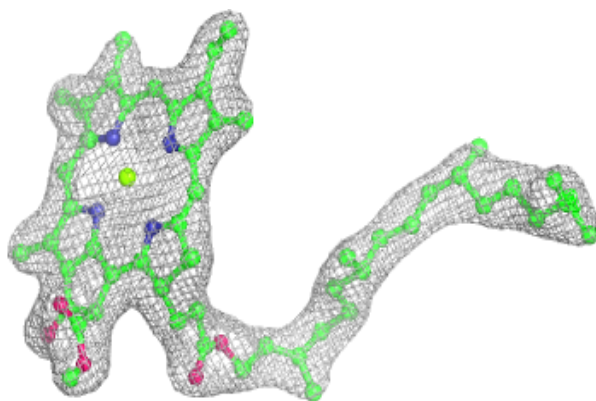
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



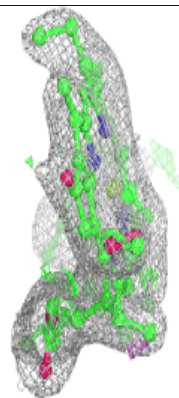
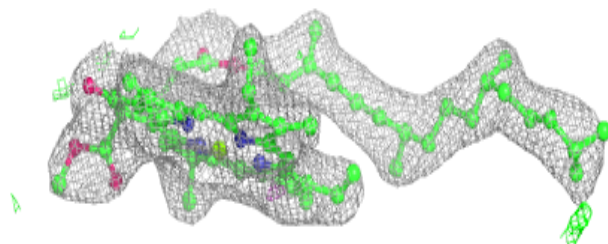
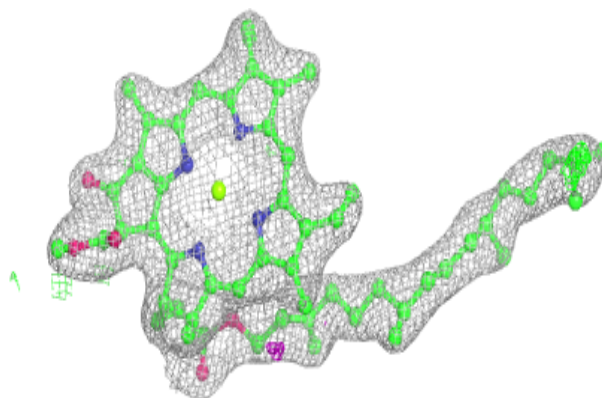


**Electron density around CLA C 512:**

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

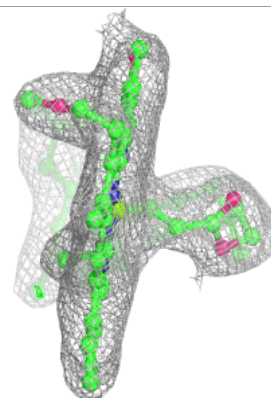
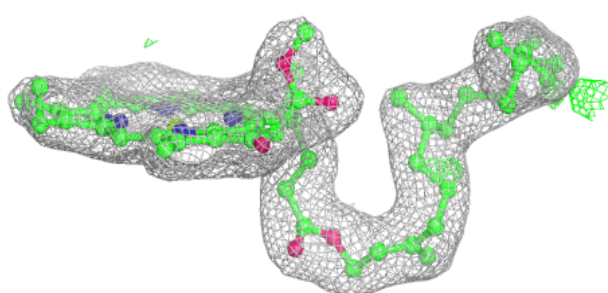
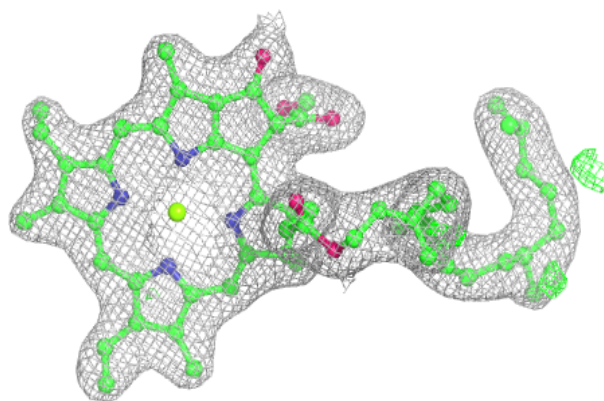
**Electron density around CLA C 502:**

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

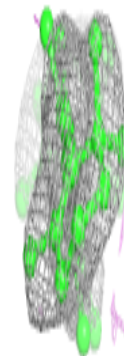
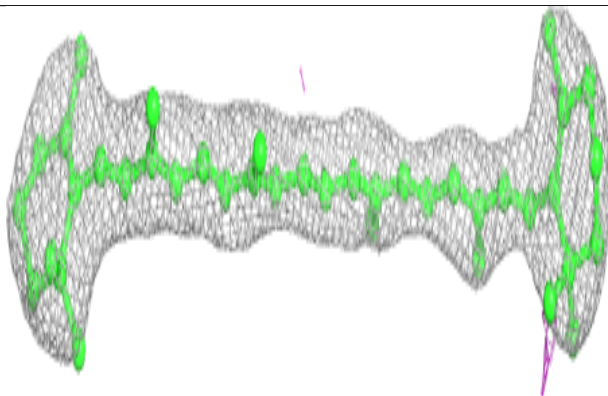
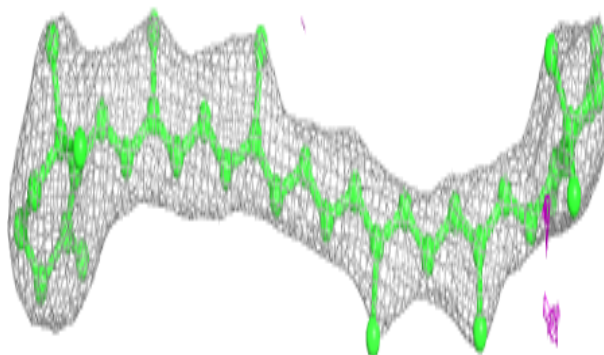


**Electron density around CLA b 617:**

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

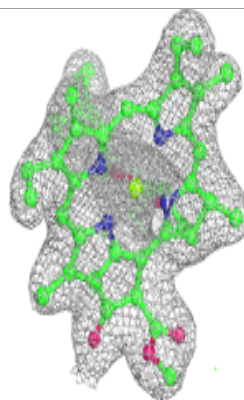
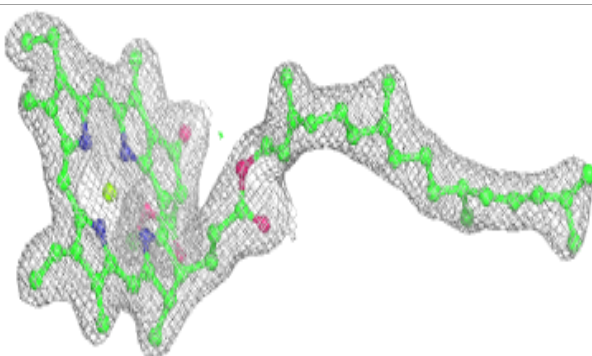
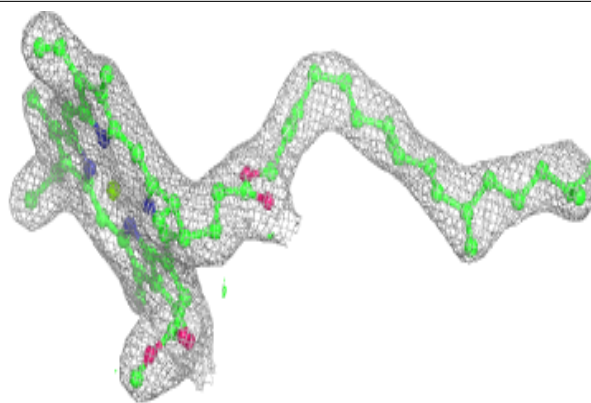
**Electron density around BCR z 101:**

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

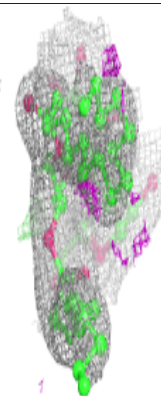
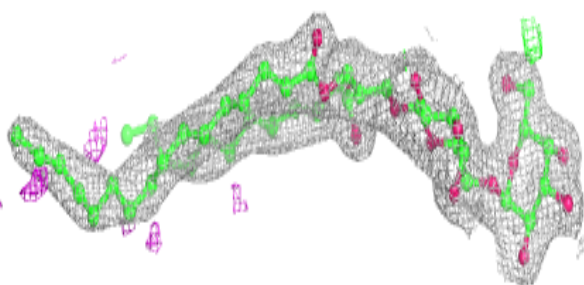
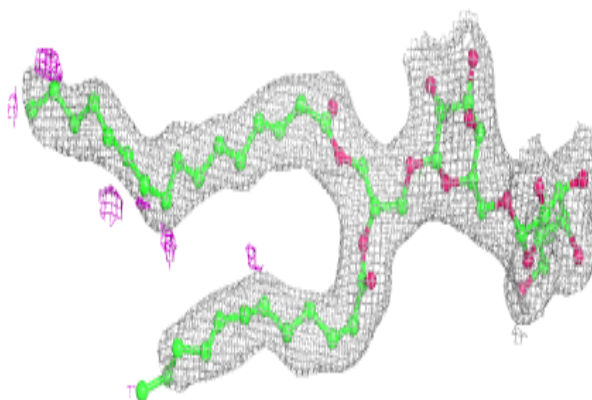


**Electron density around CLA C 503:**

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

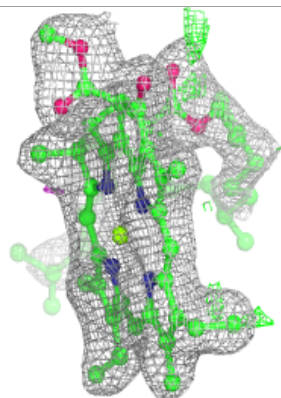
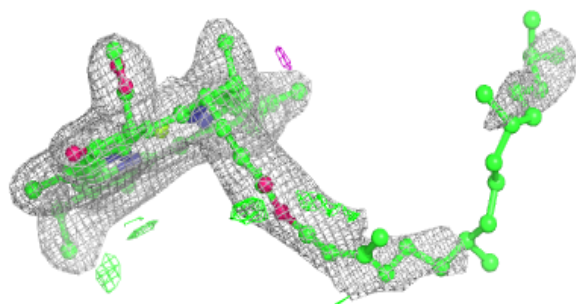
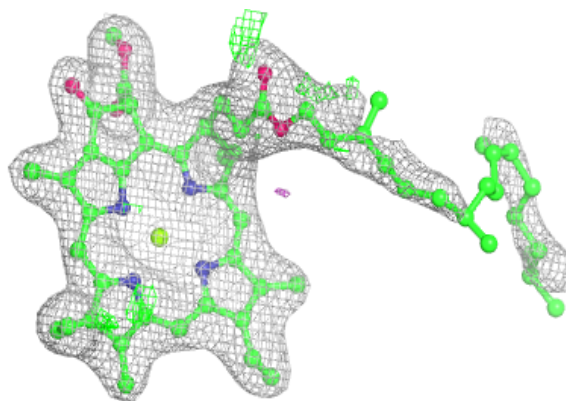
**Electron density around DGD C 519:**

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

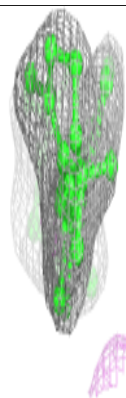
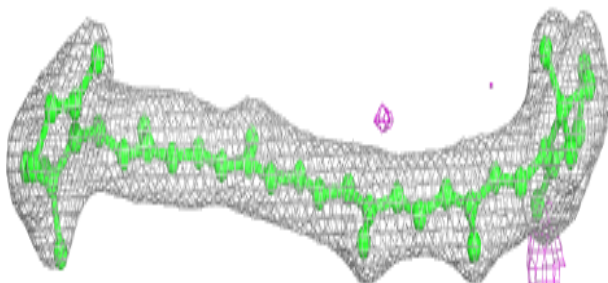
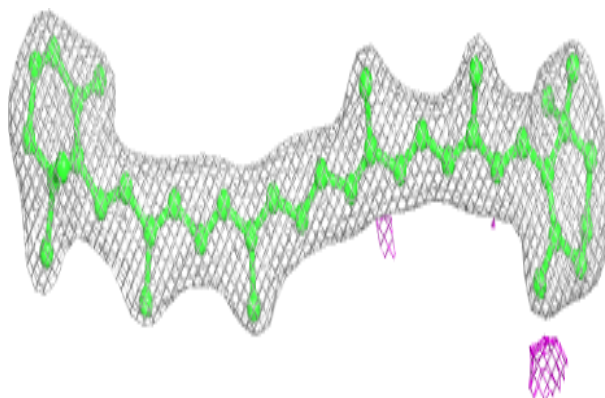


**Electron density around CLA A 410:**

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

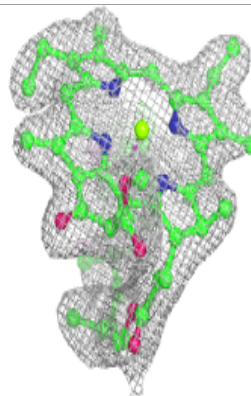
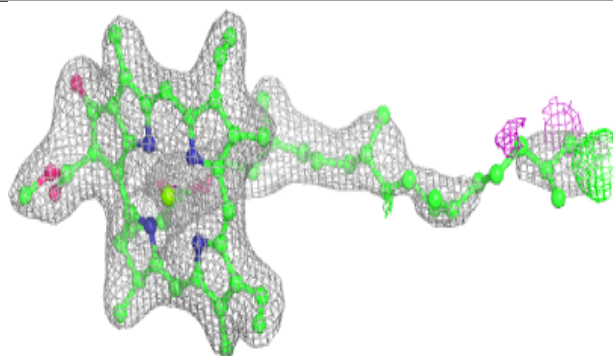
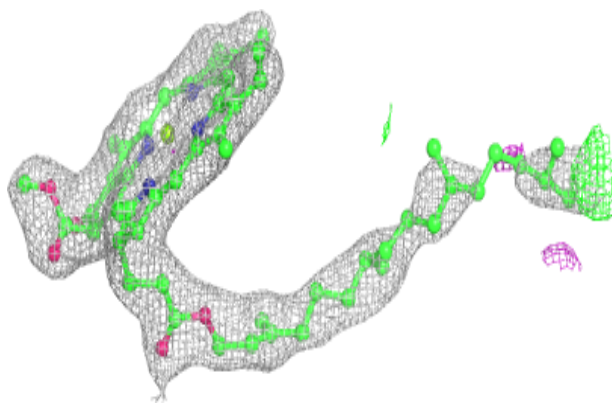
**Electron density around BCR B 620:**

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

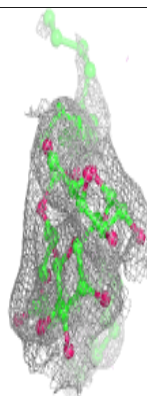
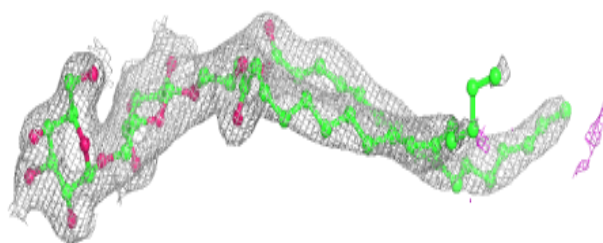
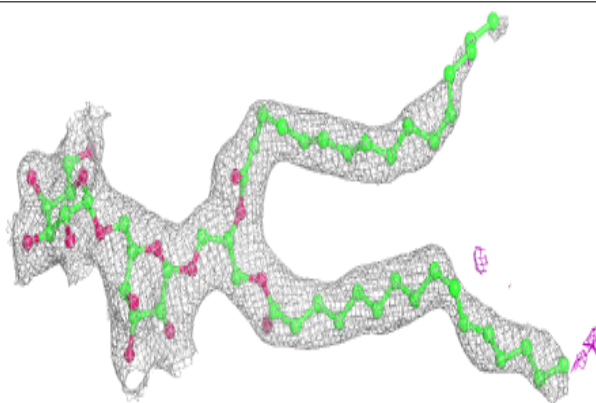


**Electron density around CLA C 505:**

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

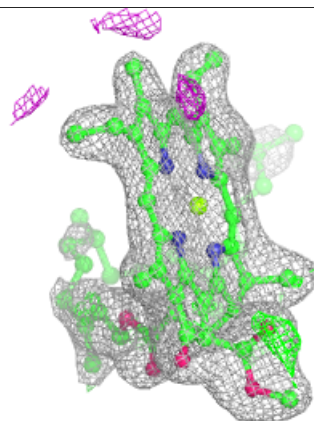
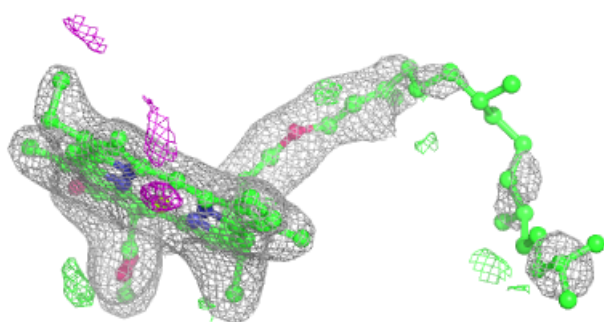
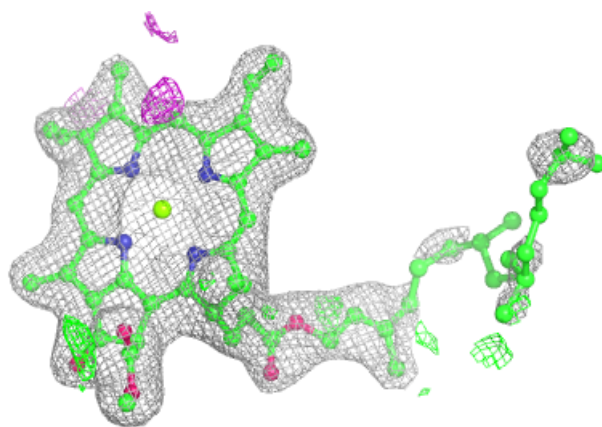
**Electron density around DGD c 520:**

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

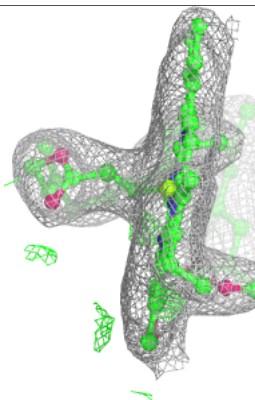
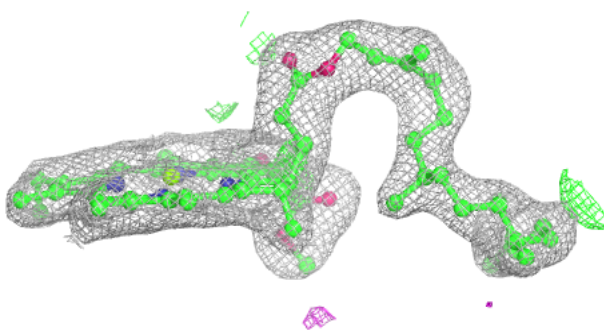
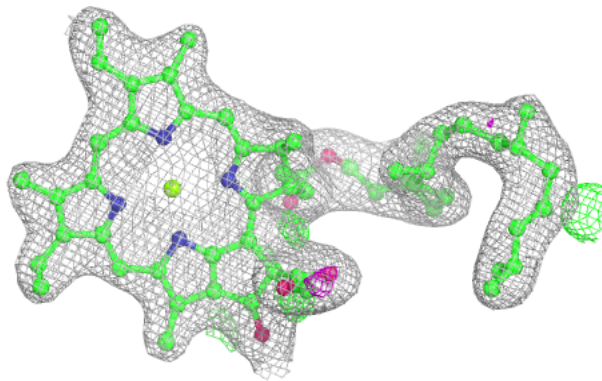


**Electron density around CLA a 2613:**

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

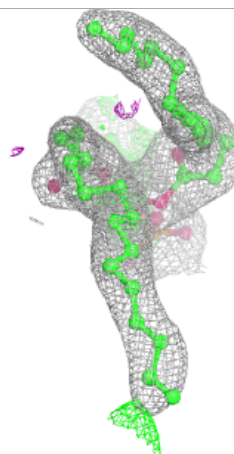
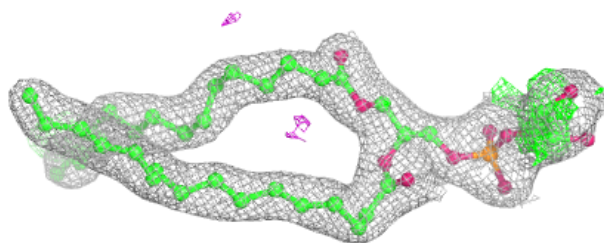
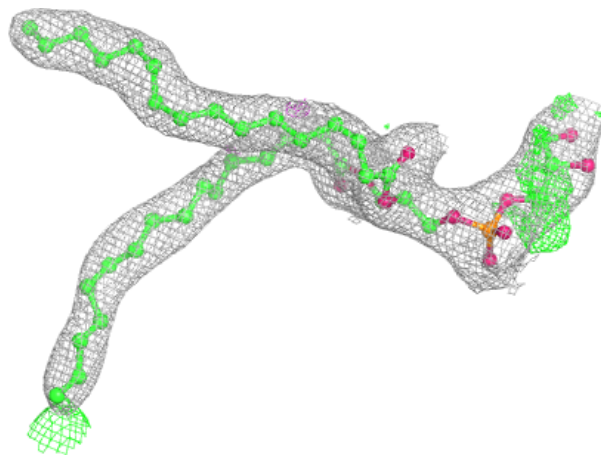
**Electron density around CLA B 613:**

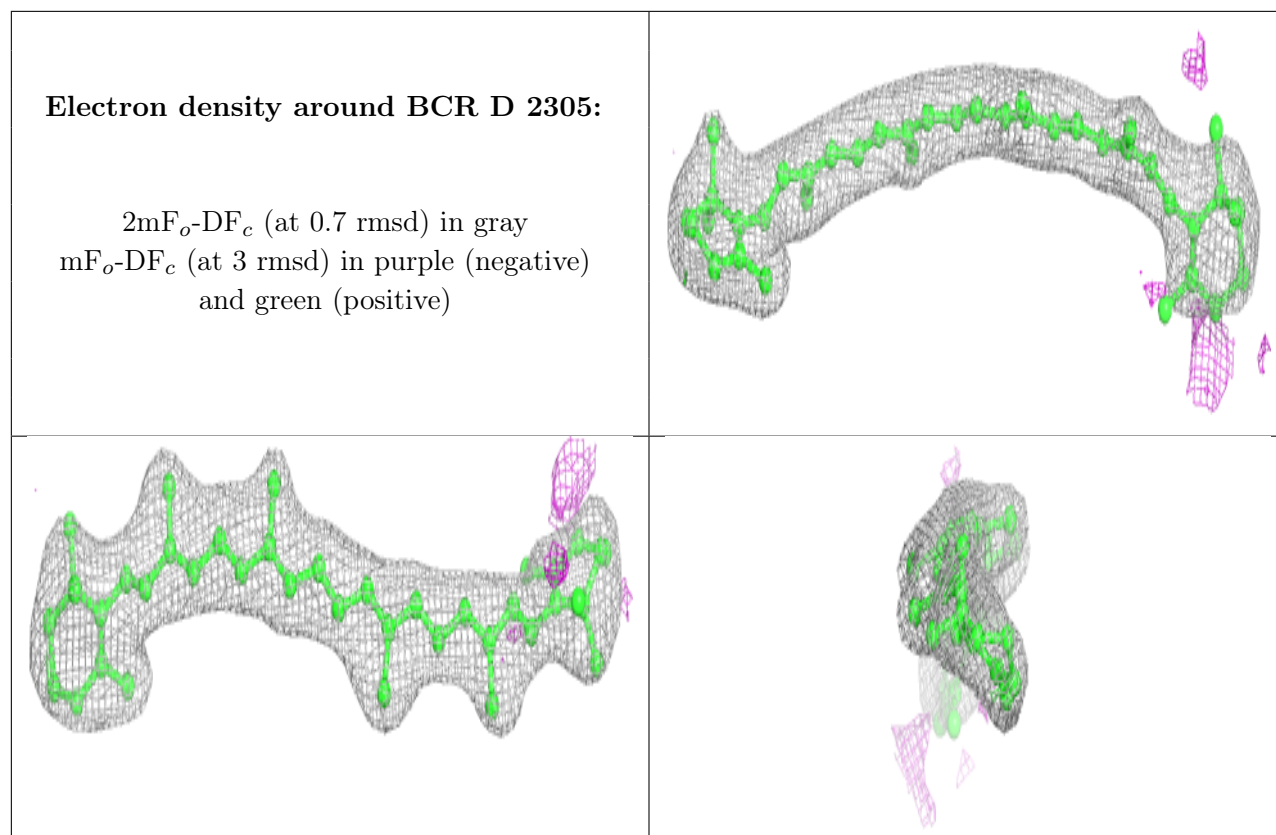
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG D 2310:**

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

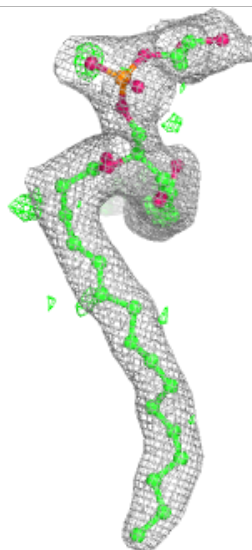
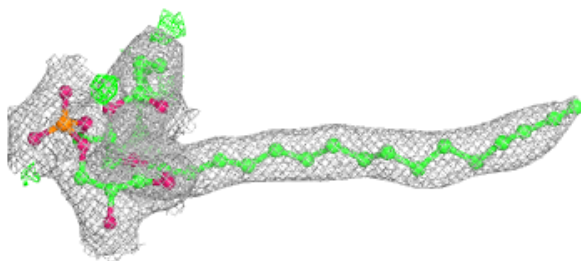






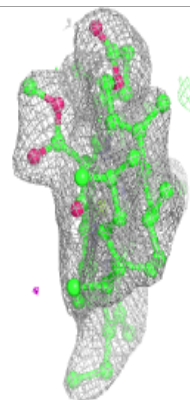
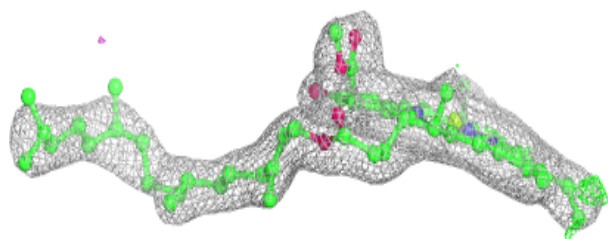
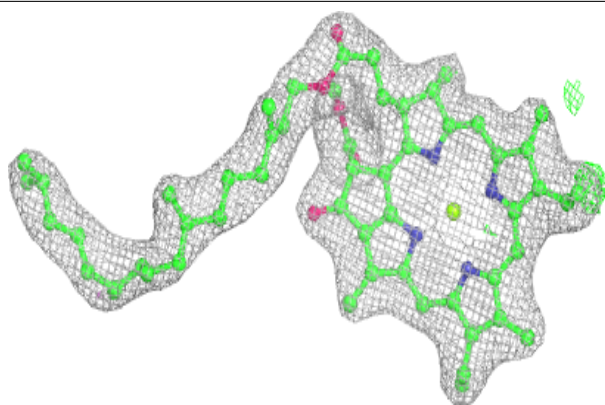
**Electron density around LHG L 101:**

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

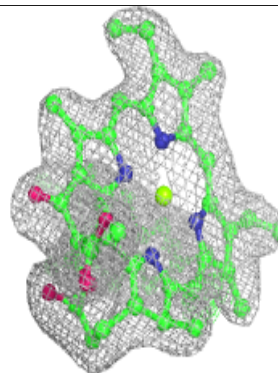
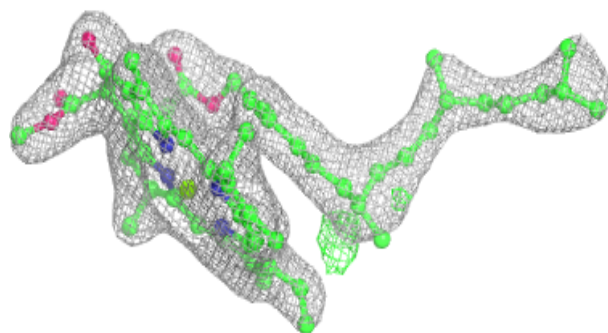
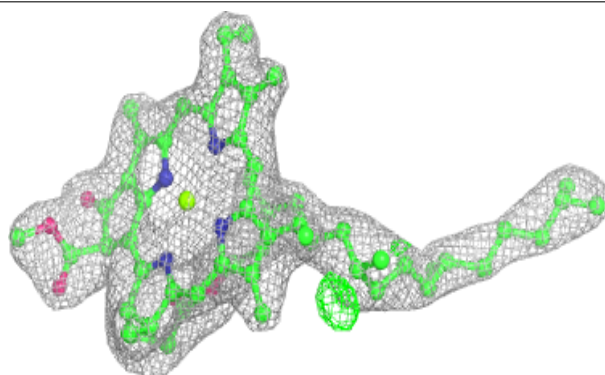


**Electron density around CLA b 607:**

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

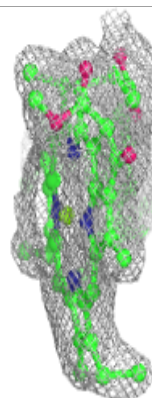
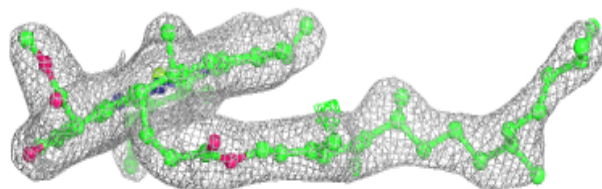
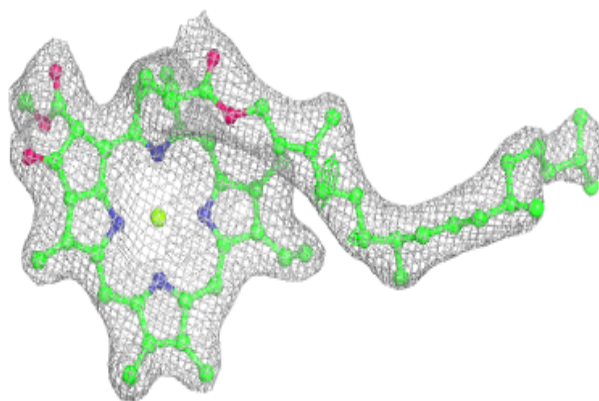
**Electron density around CLA c 508:**

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

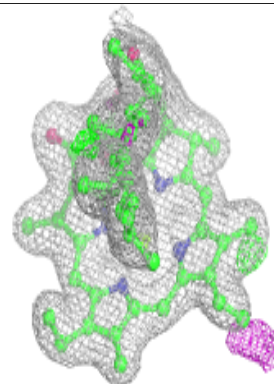
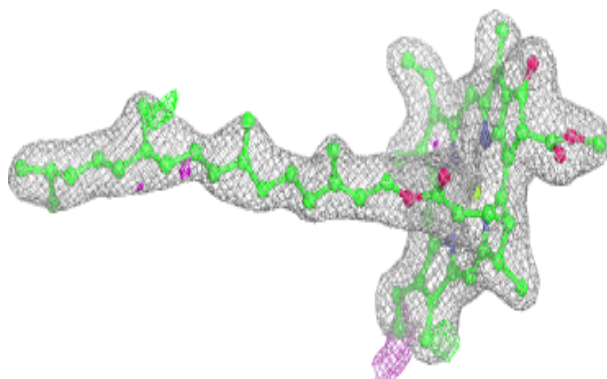
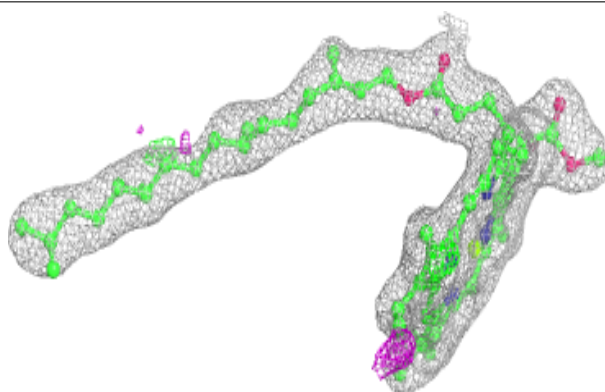


**Electron density around CLA b 608:**

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

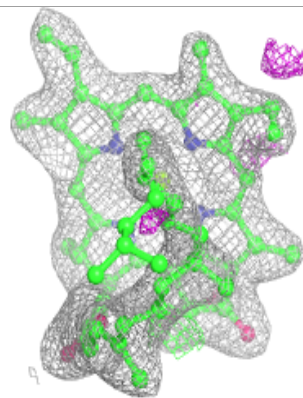
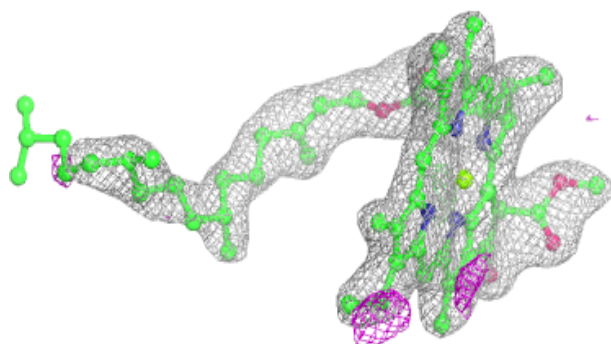
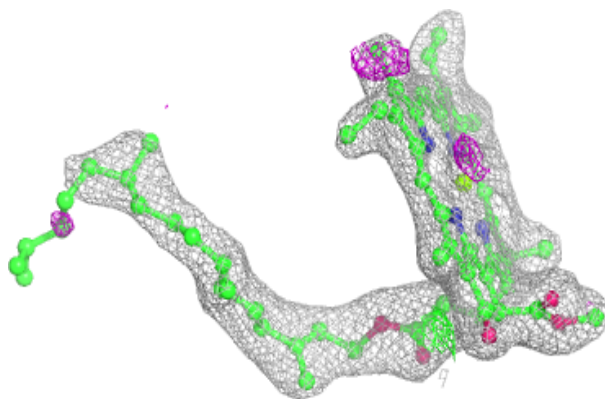
**Electron density around CLA B 608:**

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

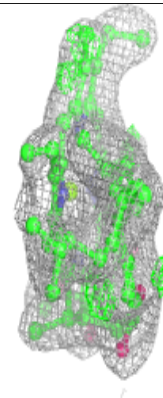
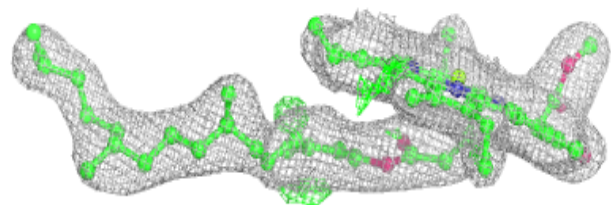
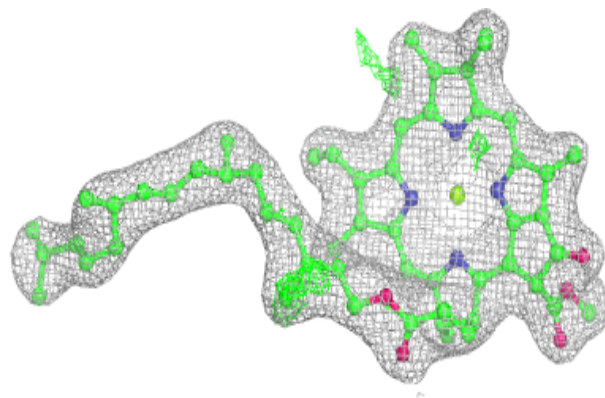


**Electron density around CLA c 511:**

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

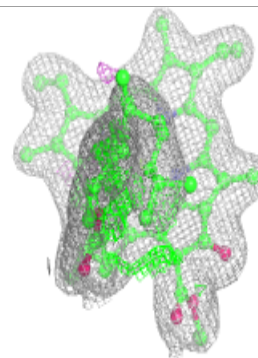
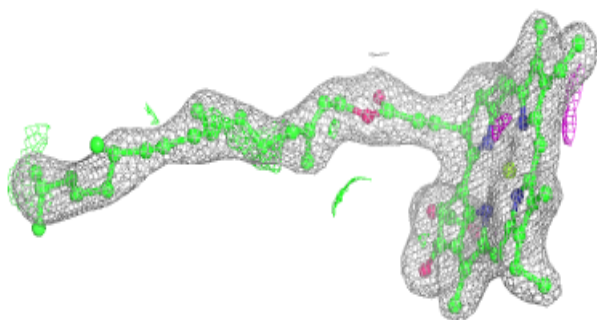
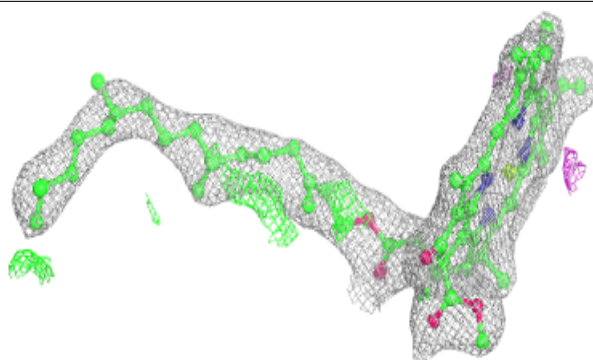
**Electron density around CLA B 604:**

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

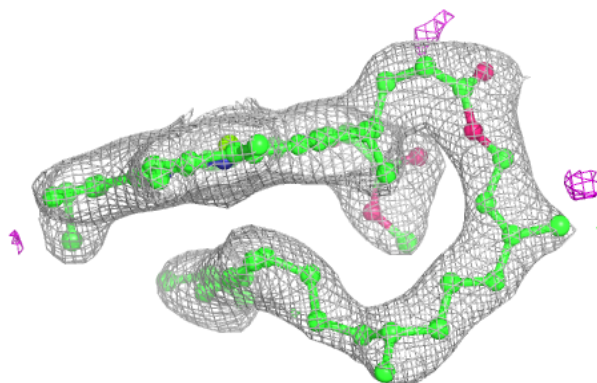
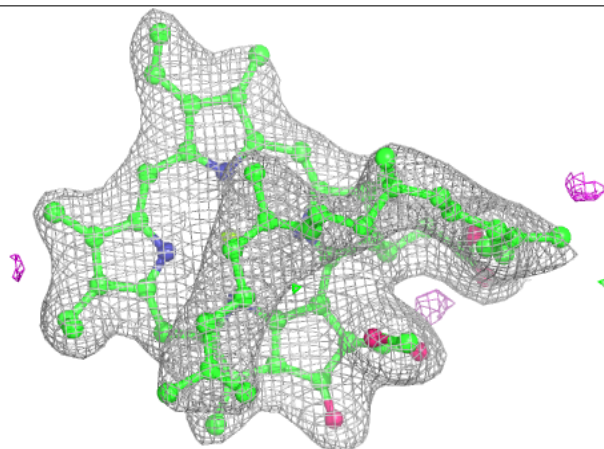


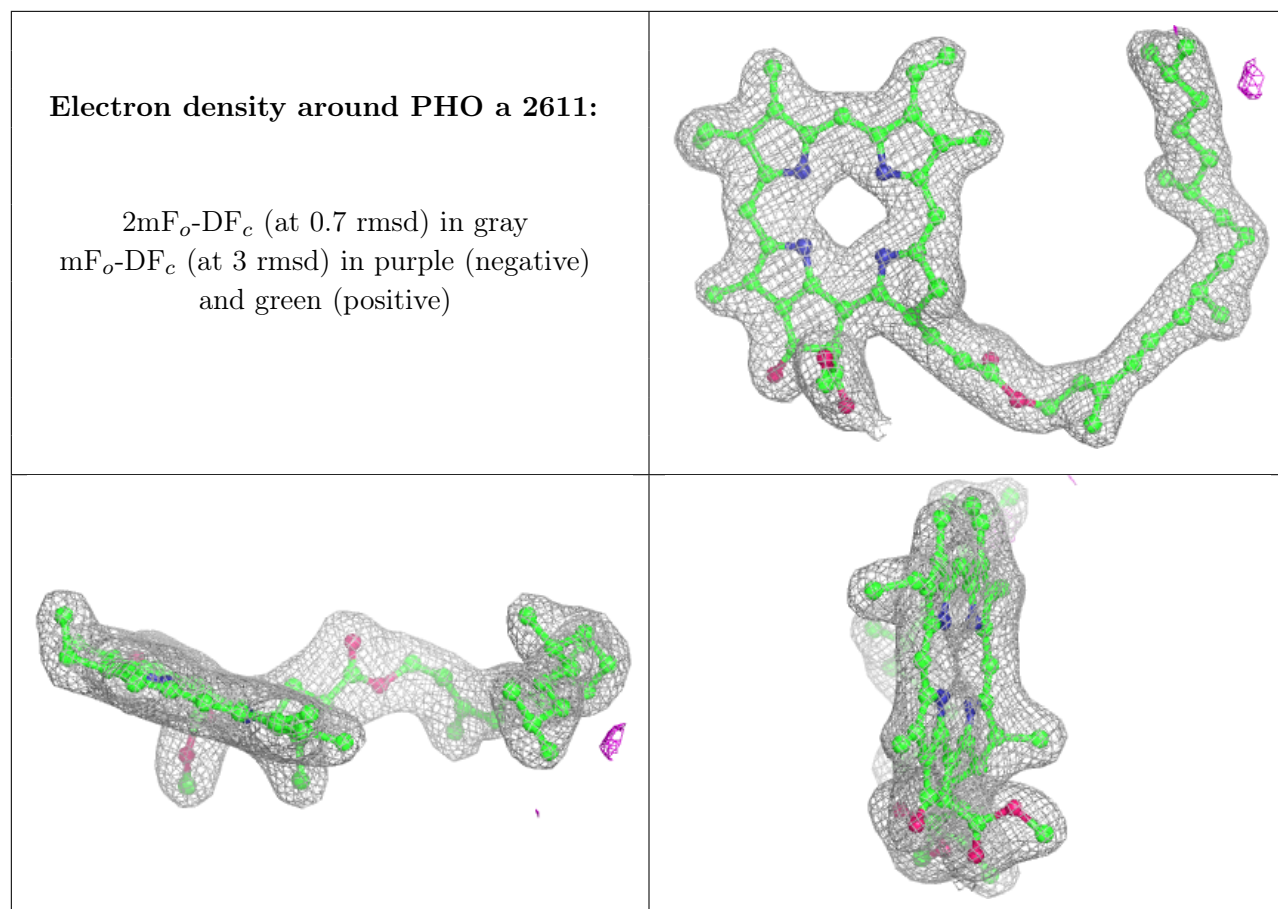
**Electron density around CLA B 605:**

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

**Electron density around CLA C 511:**

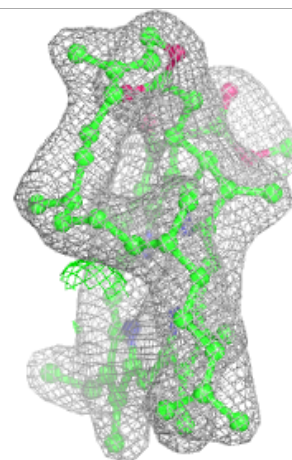
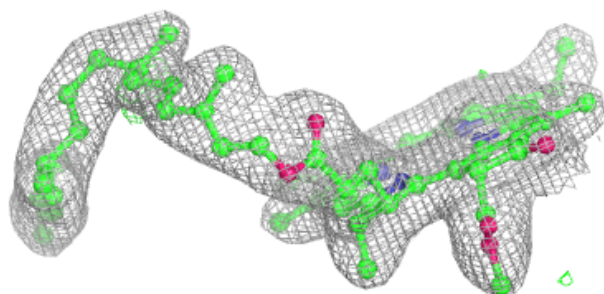
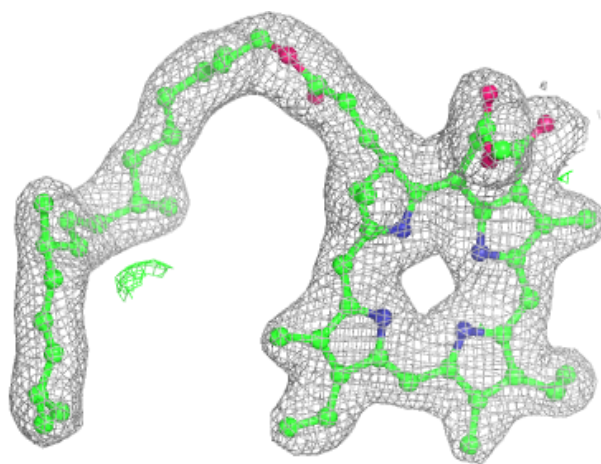
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

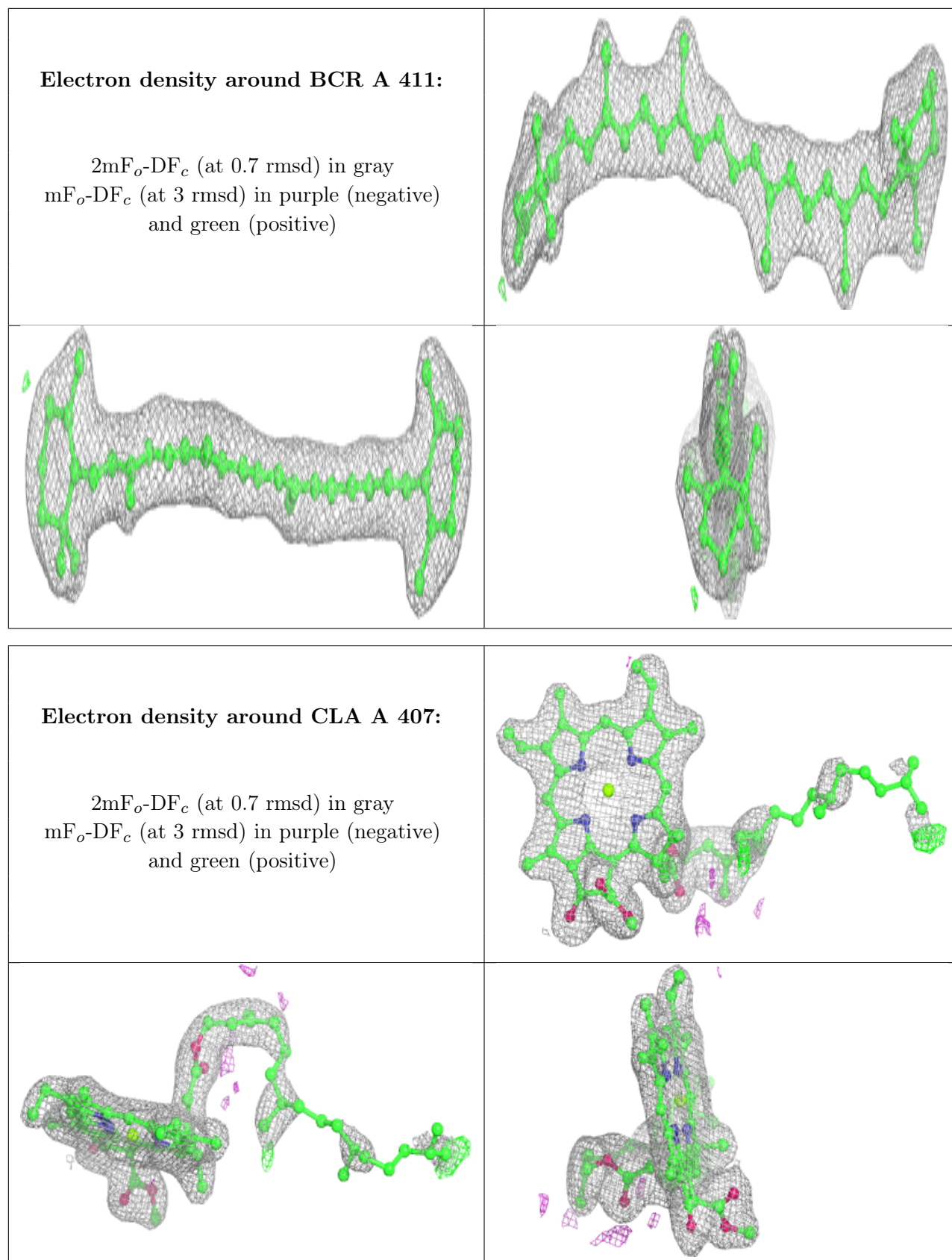




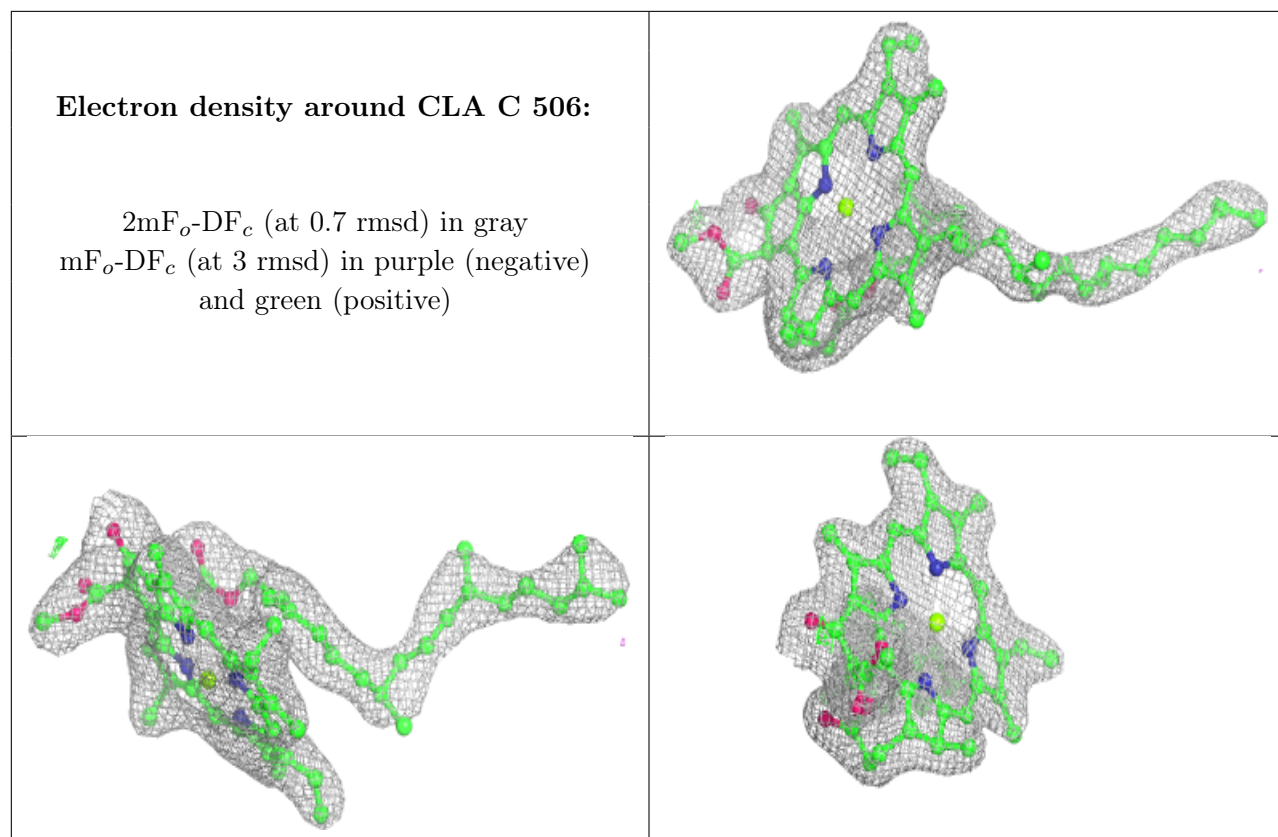
**Electron density around PHO a 2612:**

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



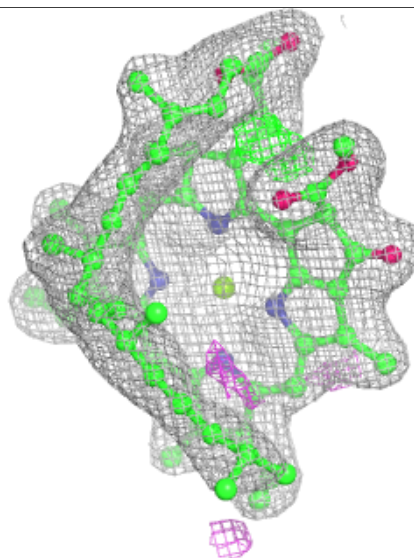
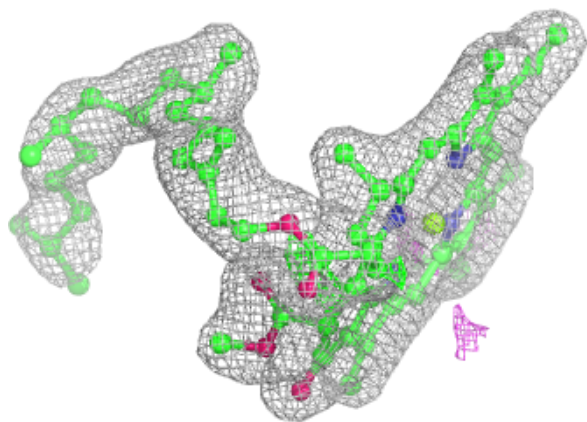
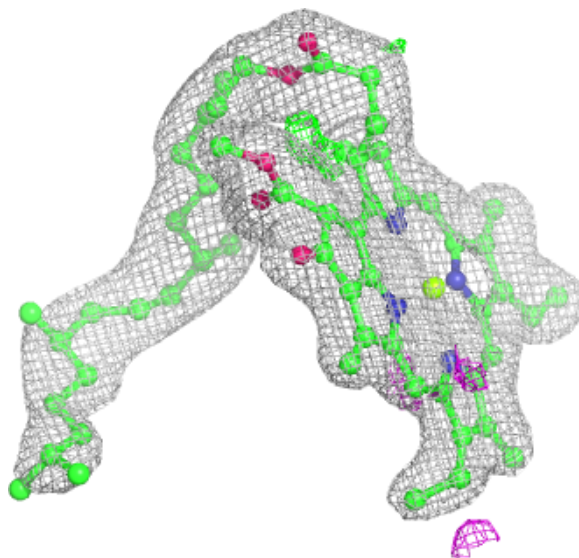






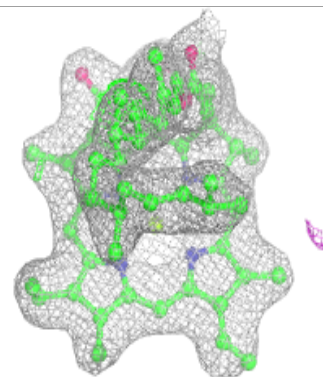
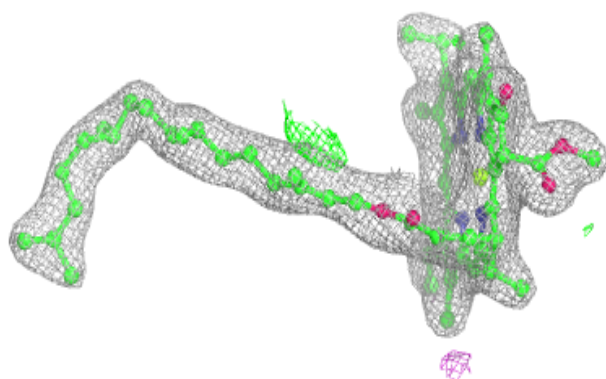
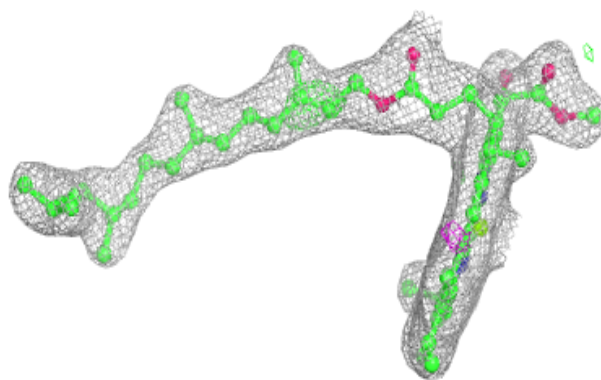
**Electron density around CLA b 618:**

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

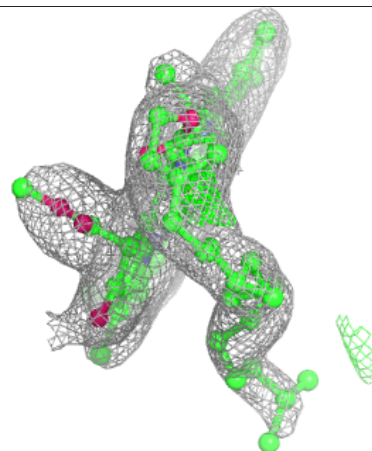
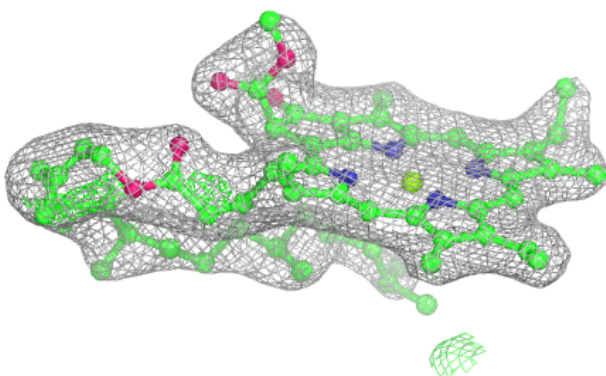
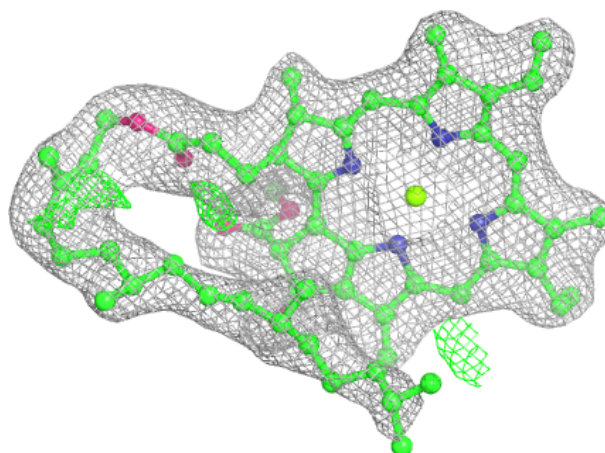


**Electron density around CLA b 610:**

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

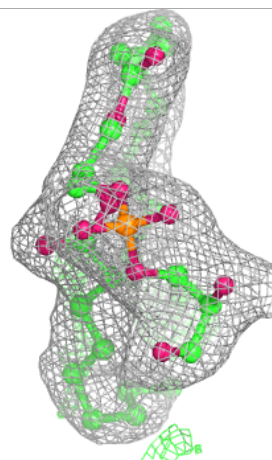
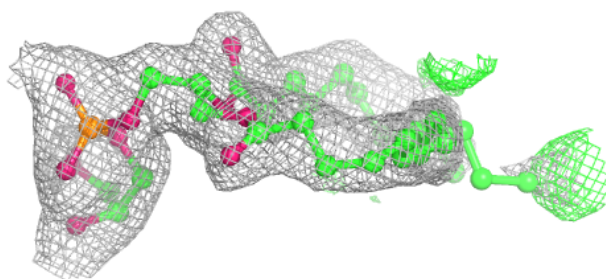
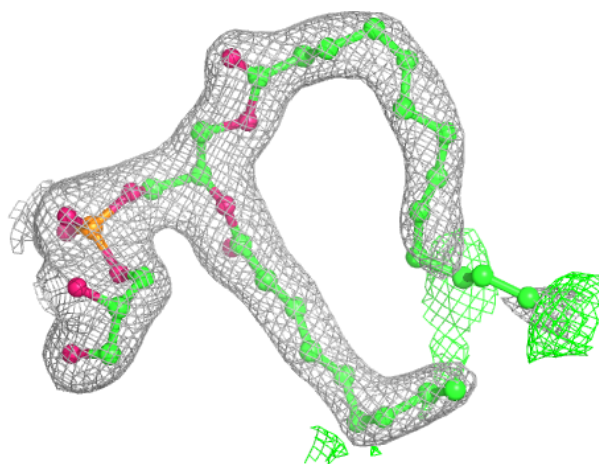
**Electron density around CLA c 512:**

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



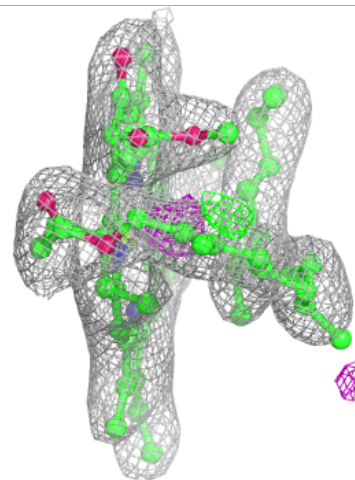
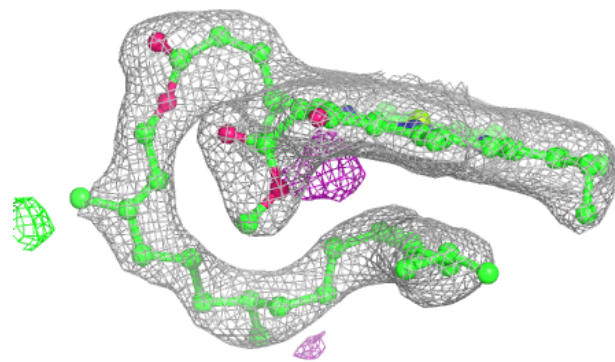
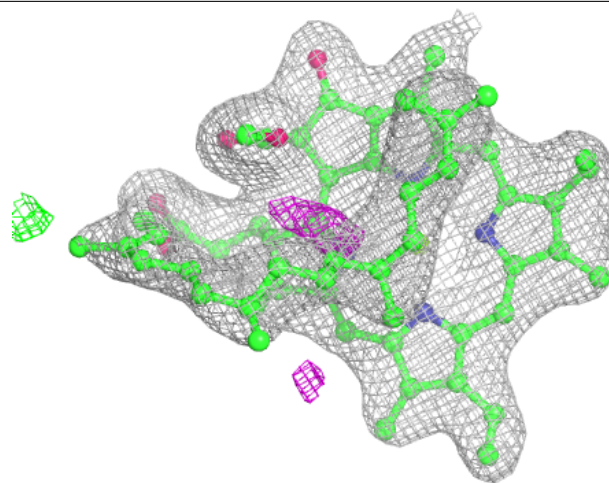
**Electron density around LHG D 2311:**

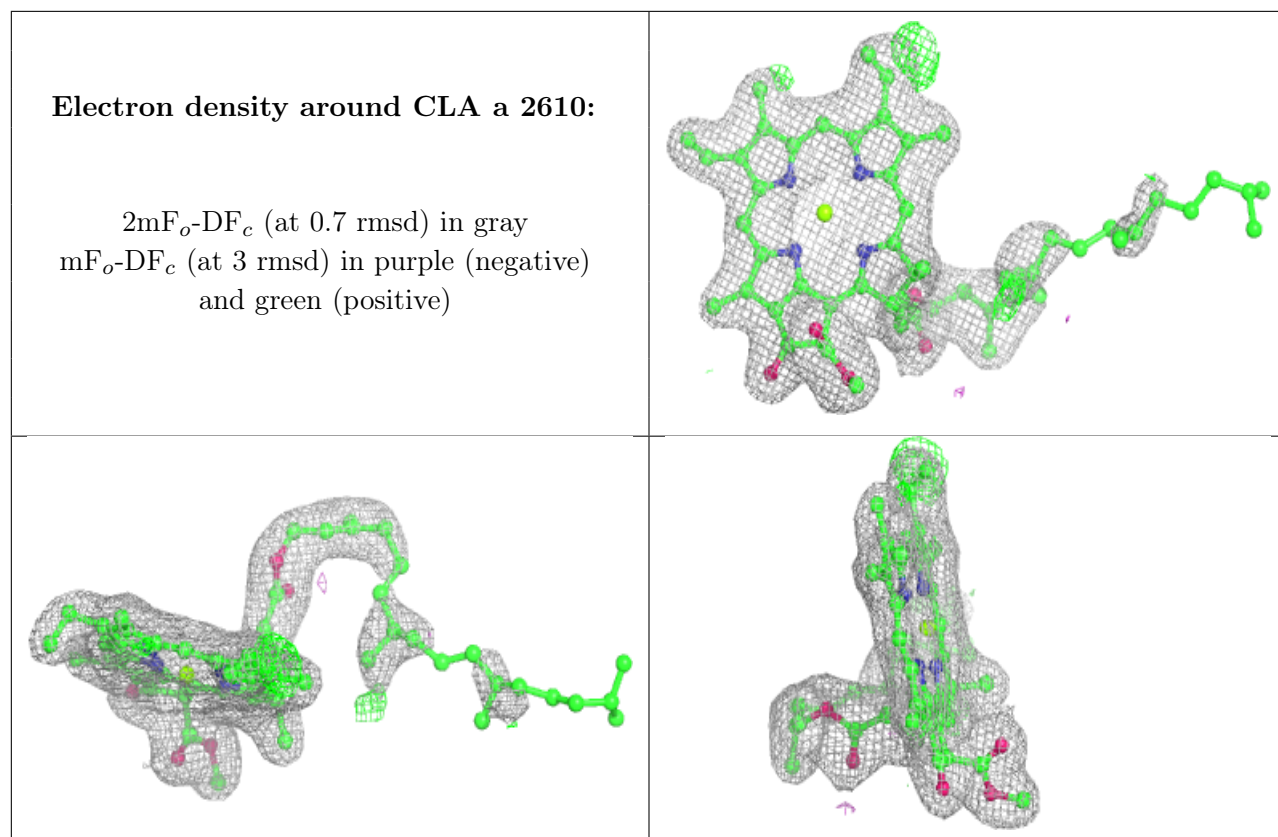
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 513:**

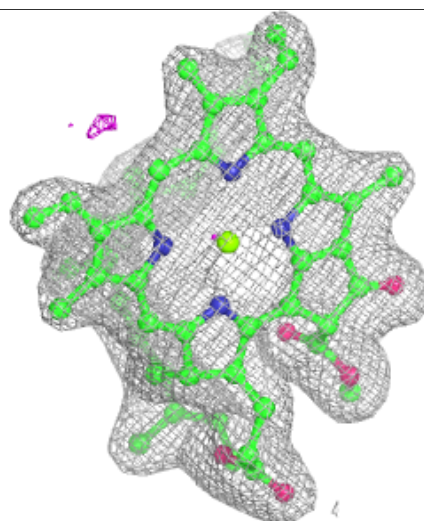
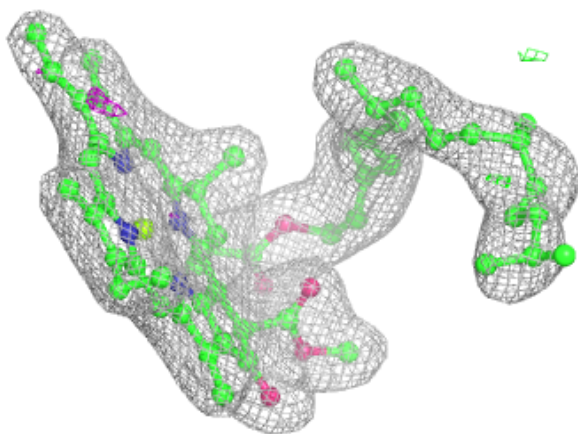
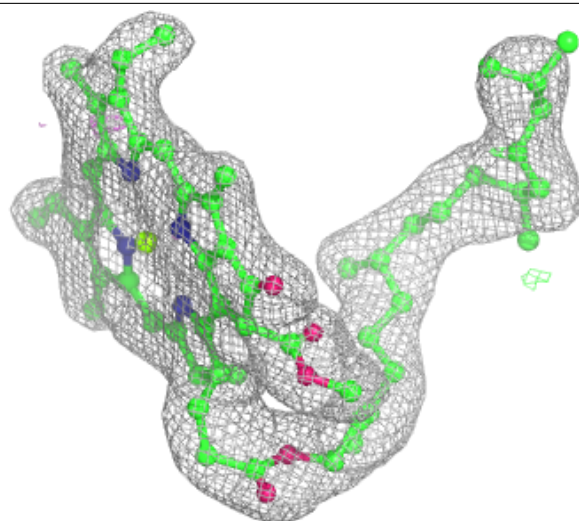
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





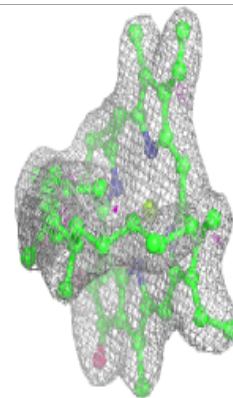
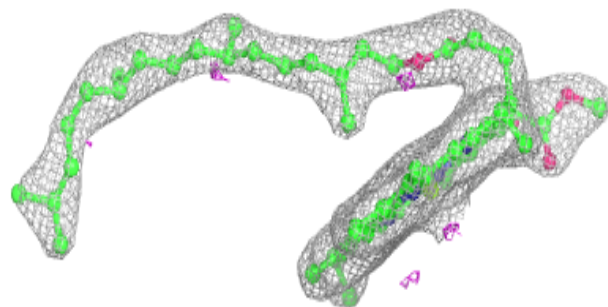
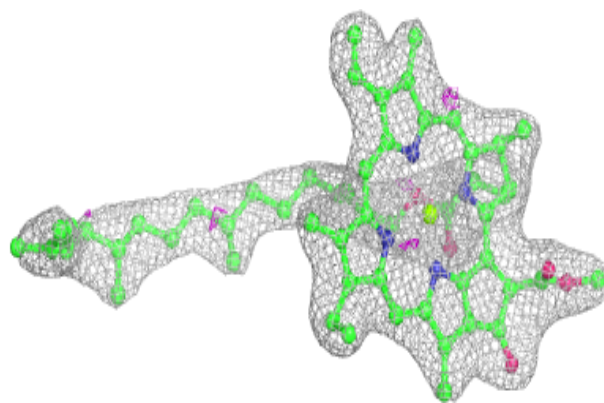
**Electron density around CLA B 614:**

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

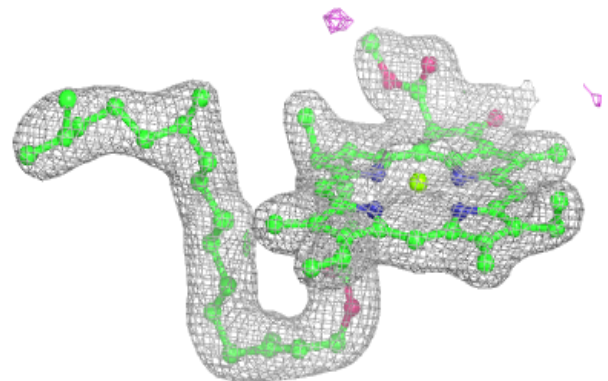
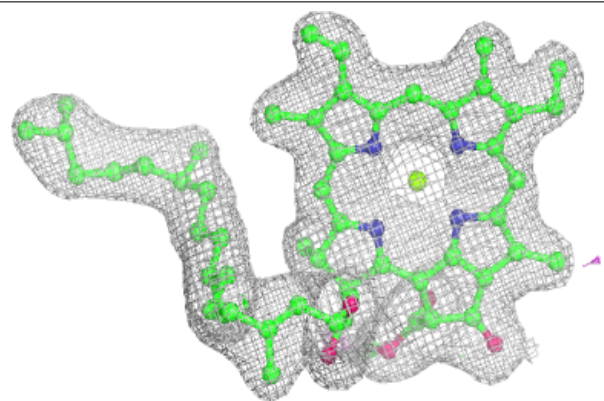


**Electron density around CLA b 613:**

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

**Electron density around CLA d 402:**

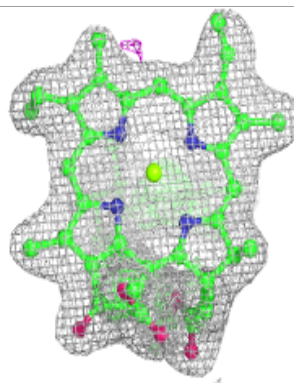
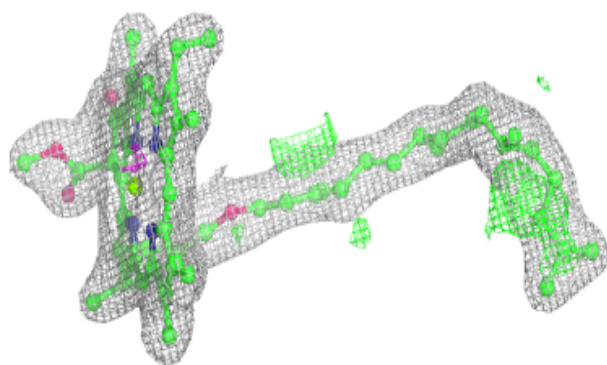
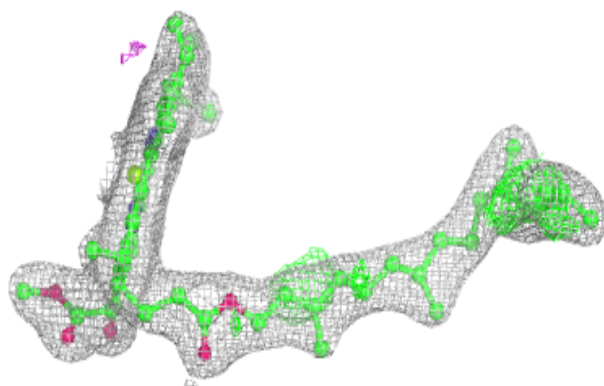
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



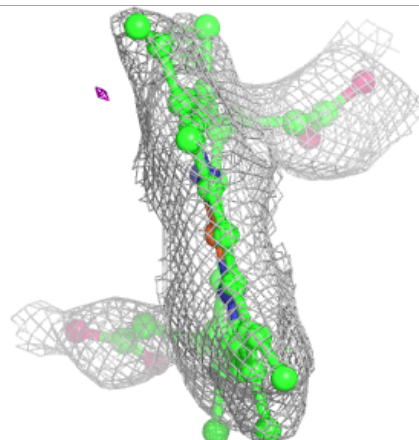
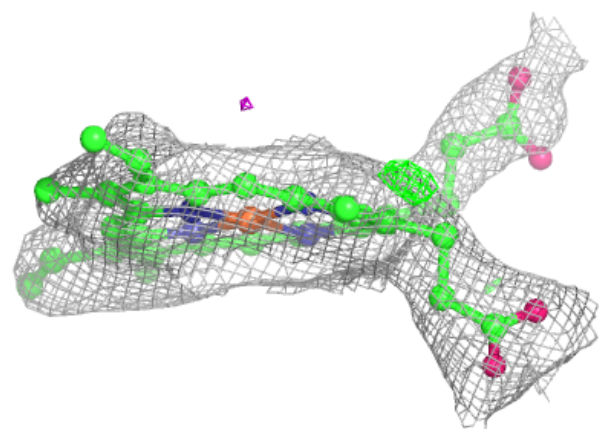
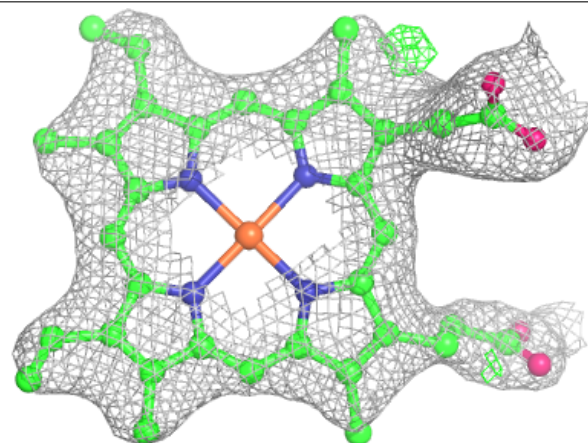


**Electron density around CLA B 606:**

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

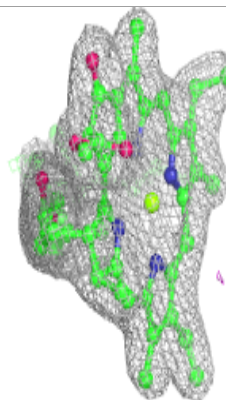
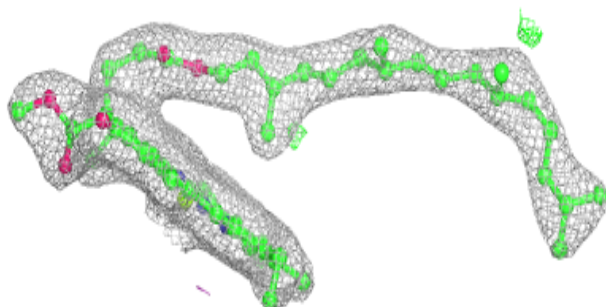
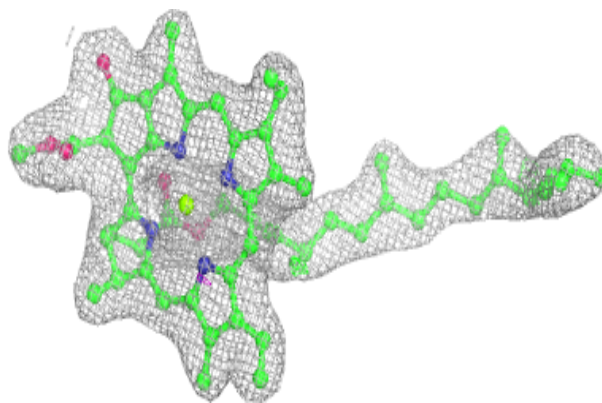
**Electron density around HEM F 101:**

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

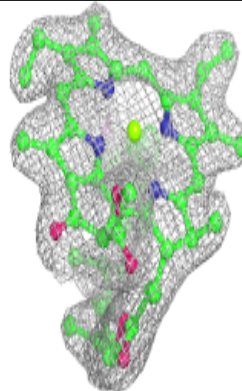
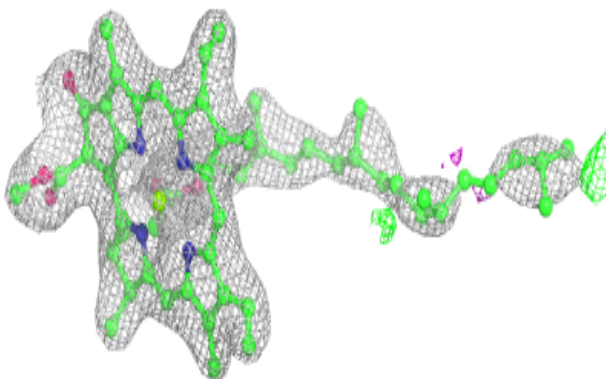
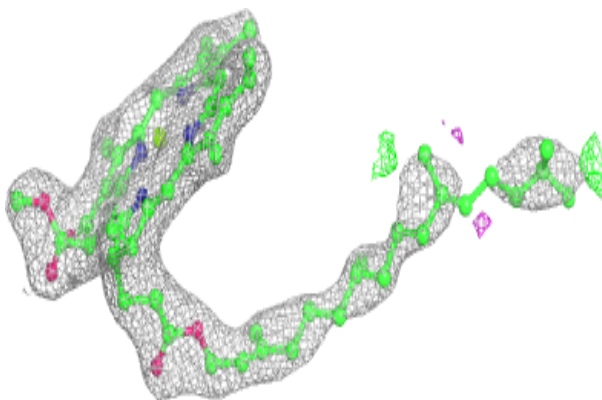


**Electron density around CLA B 609:**

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

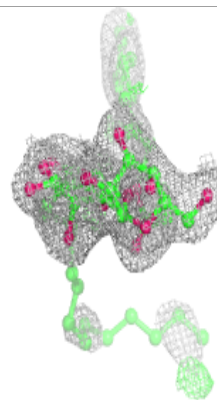
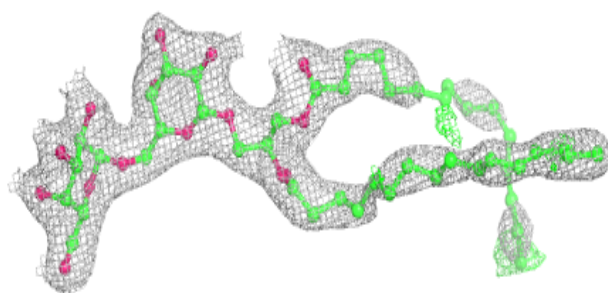
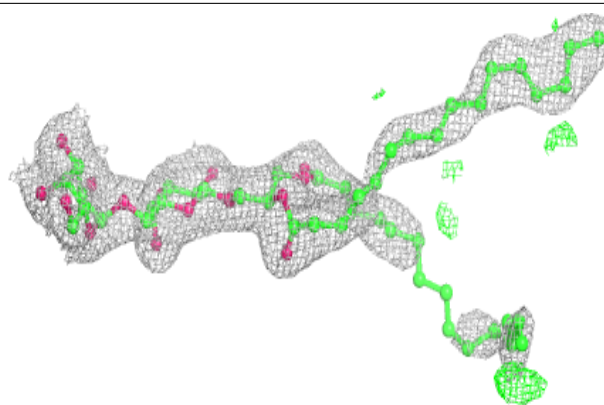
**Electron density around CLA c 507:**

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

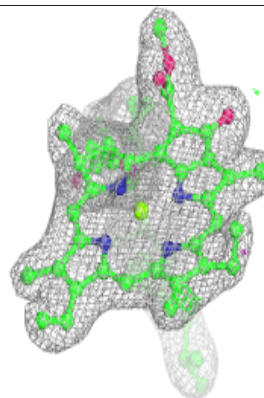
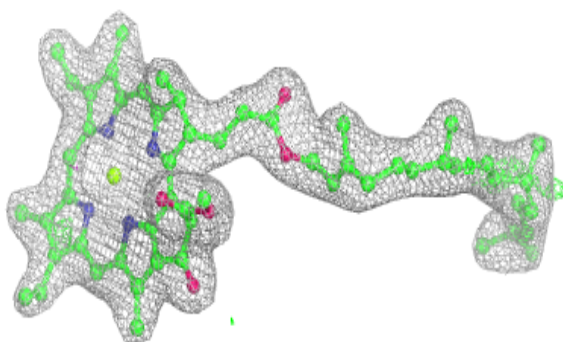
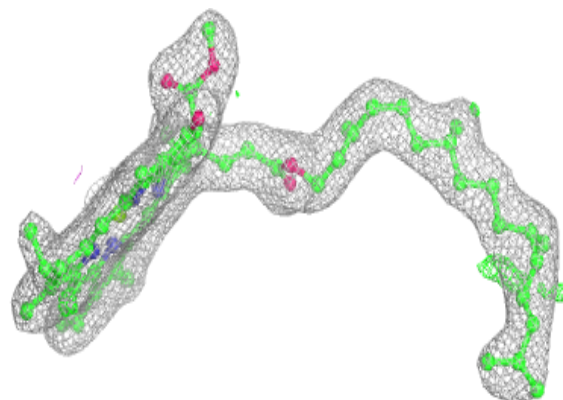


**Electron density around DGD C 517:**

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

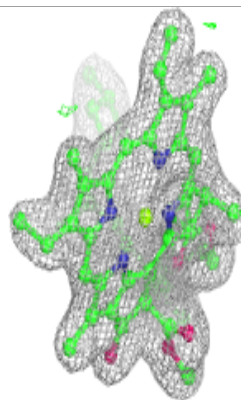
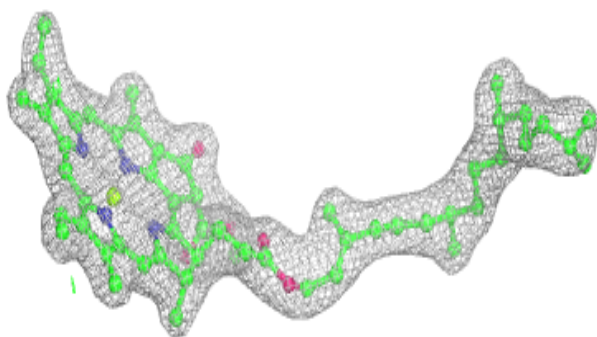
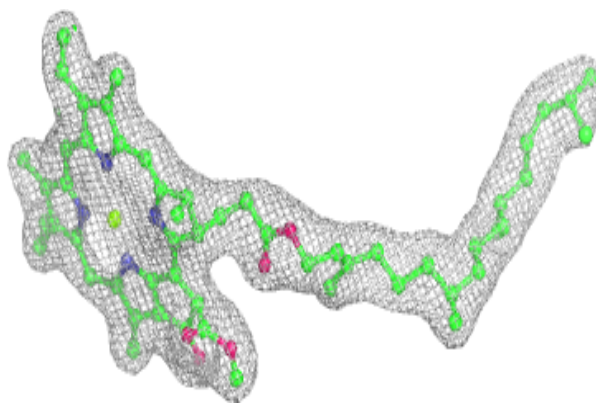
**Electron density around CLA d 408:**

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

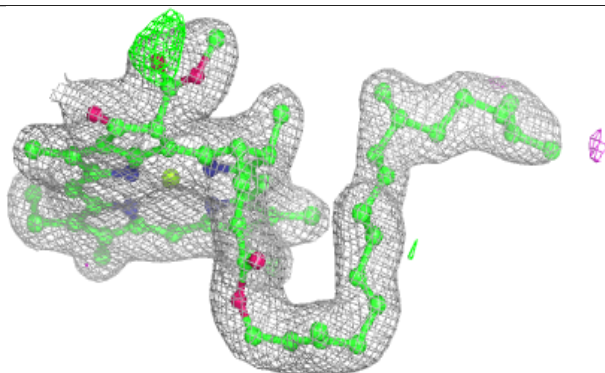
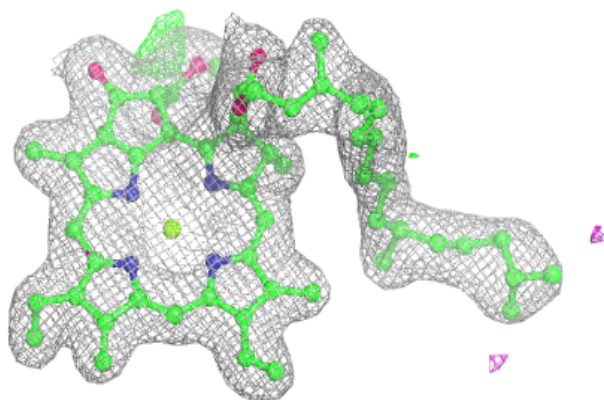


**Electron density around CLA a 2609:**

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

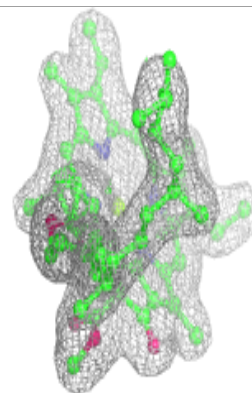
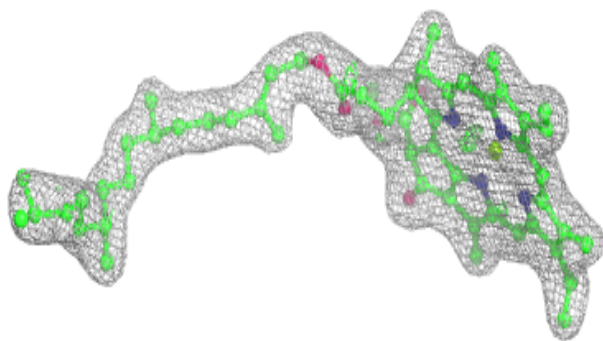
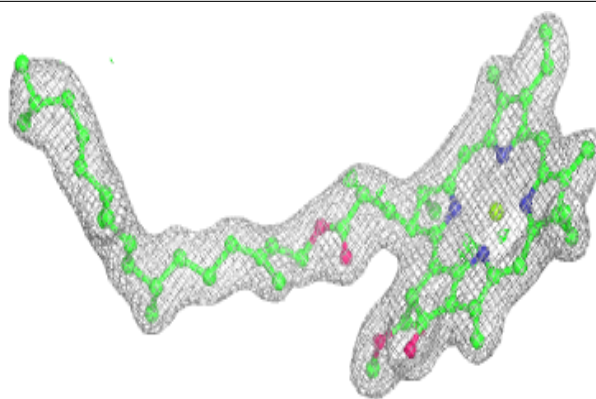
**Electron density around CLA A 406:**

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

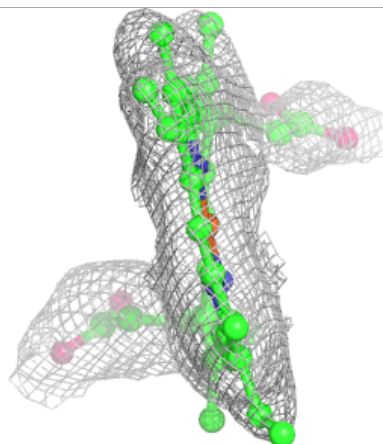
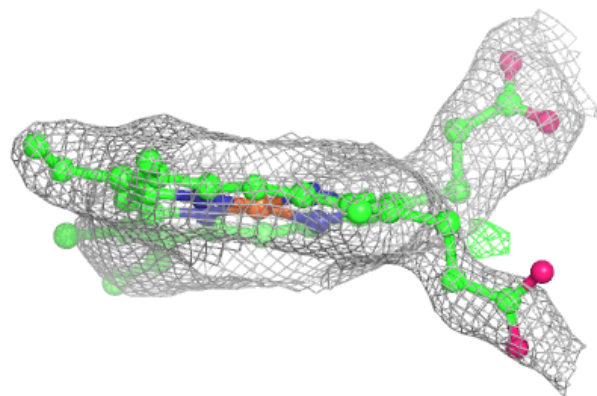
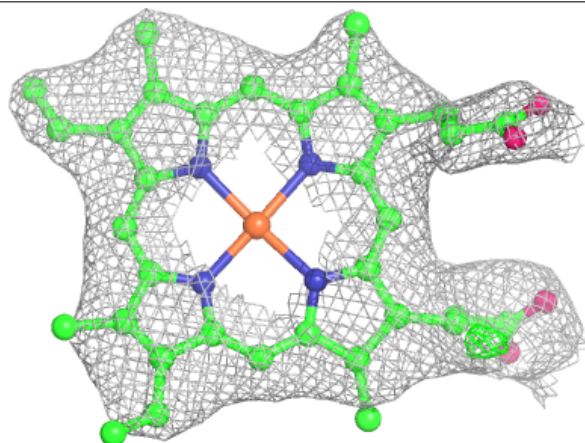


**Electron density around CLA A 405:**

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

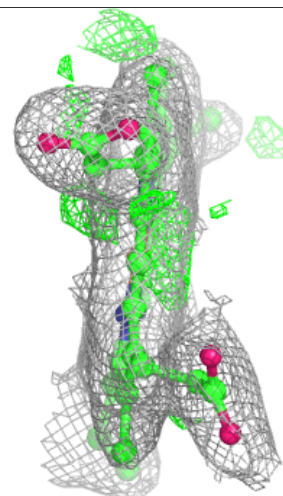
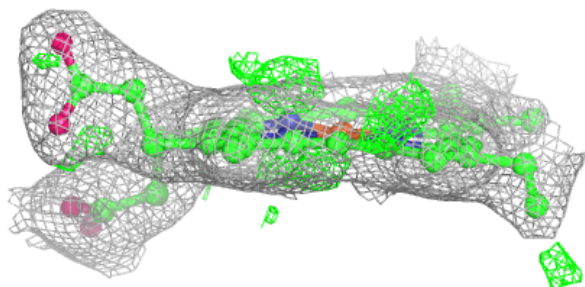
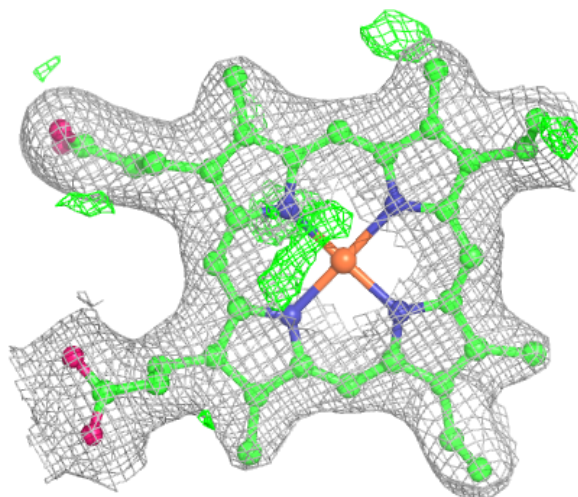
**Electron density around HEM e 103:**

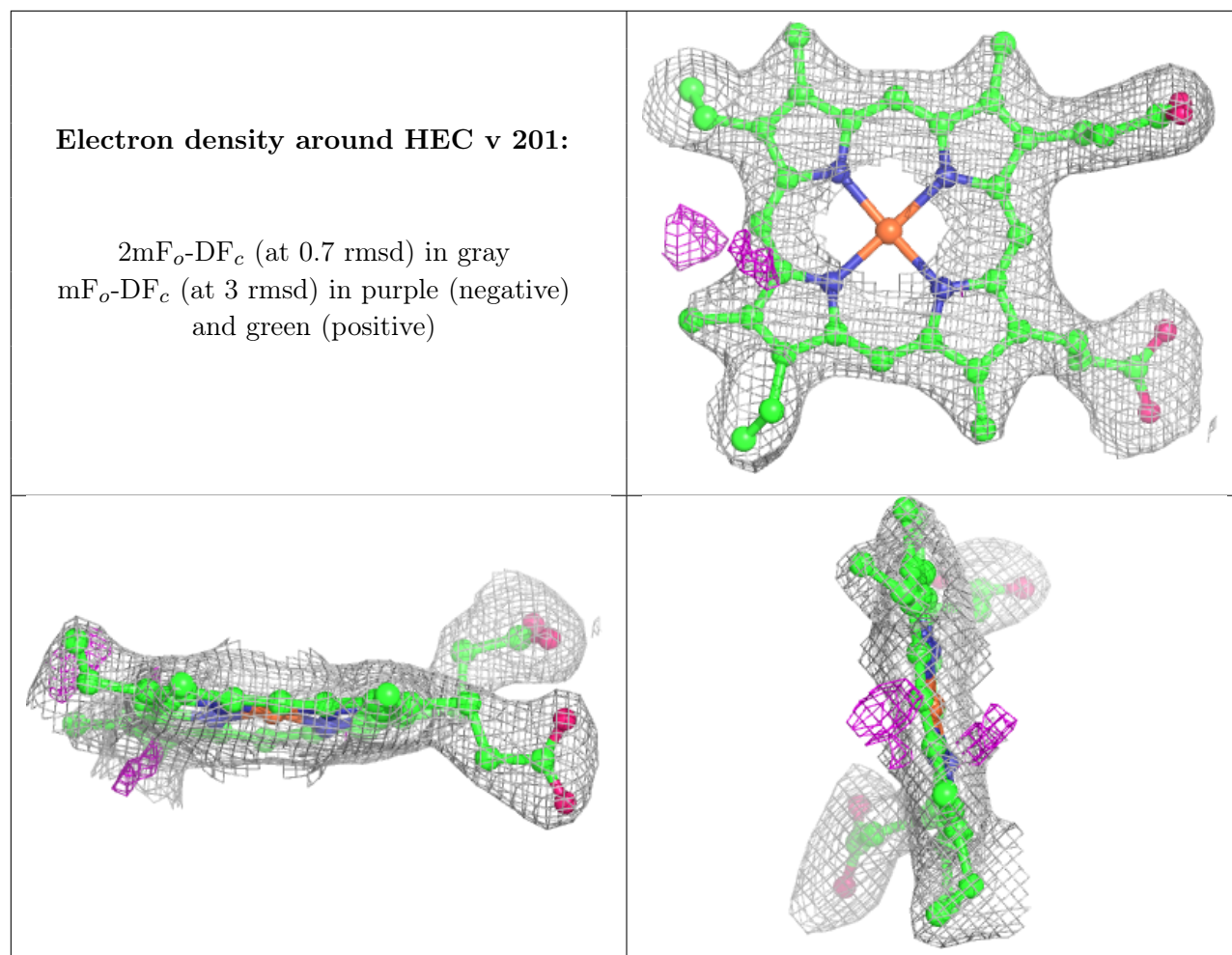
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC V 201:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.