



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:59 PM BST

PDB ID : 4IL6  
Title : Structure of Sr-substituted photosystem II  
Authors : Koua, F.H.M.; Umena, Y.; Kawakami, K.; Kamiya, N.; Shen, J.R.  
Deposited on : 2012-12-29  
Resolution : 2.10 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.

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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 : 2.13.1  
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) : 2.13.1

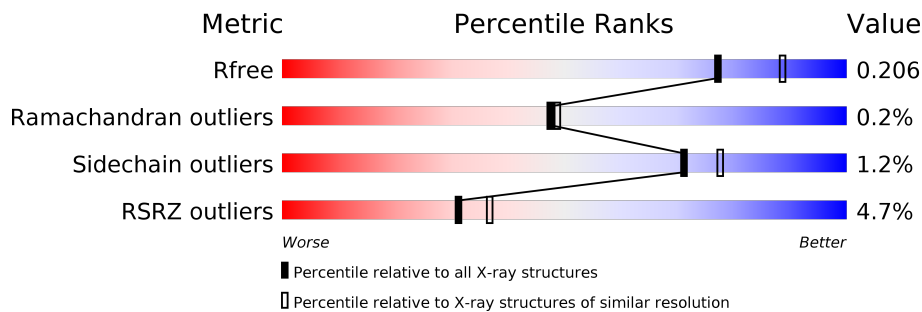
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

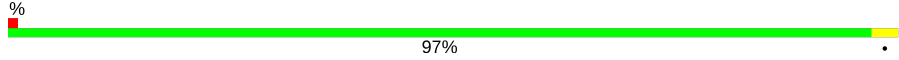
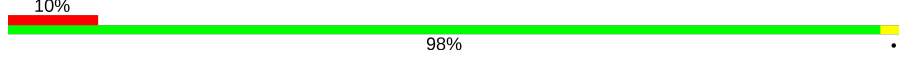
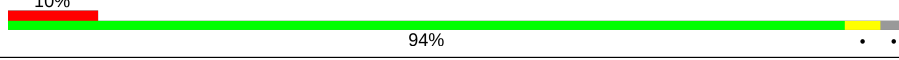
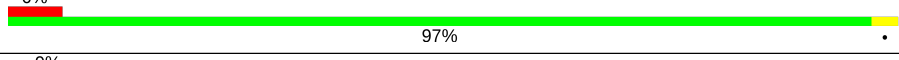

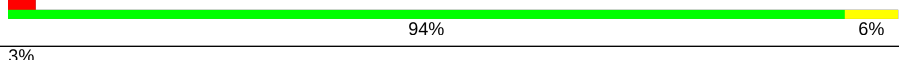
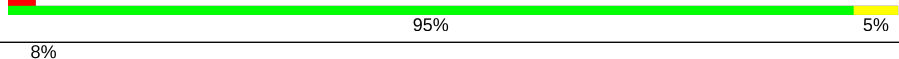
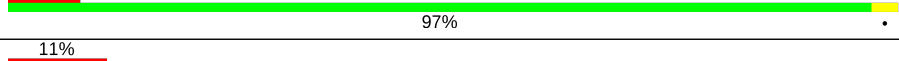
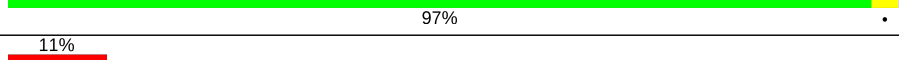
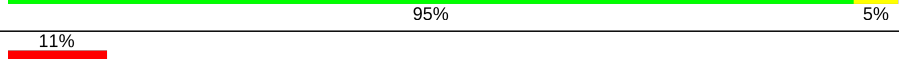
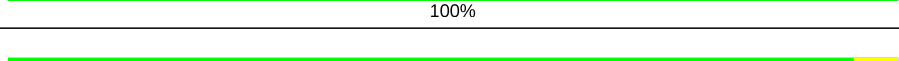
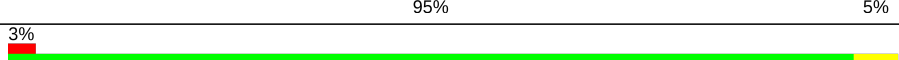
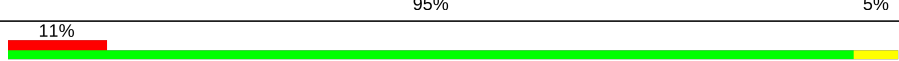
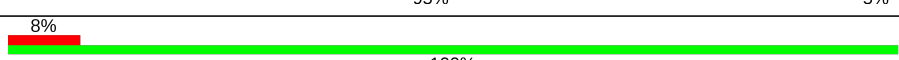
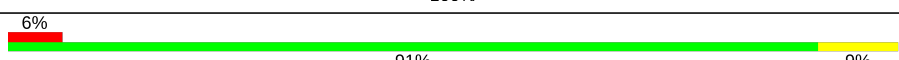
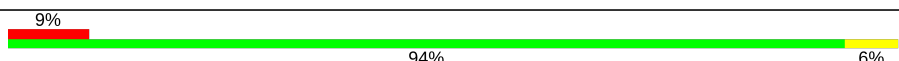
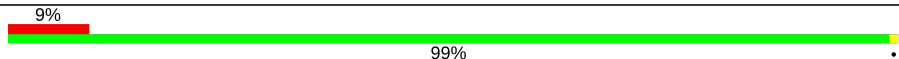
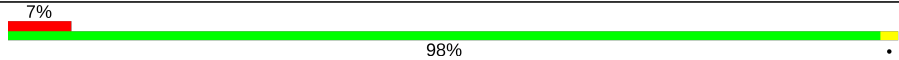
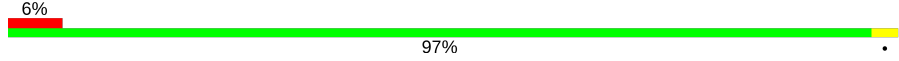
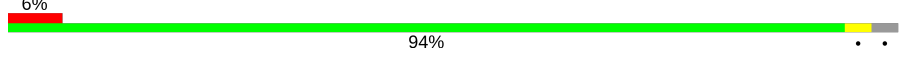
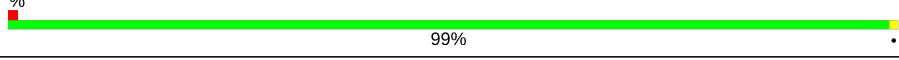
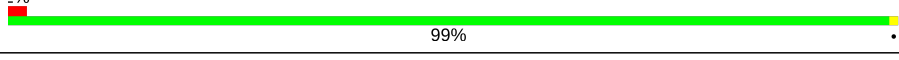
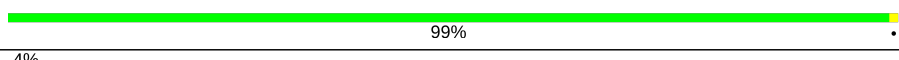
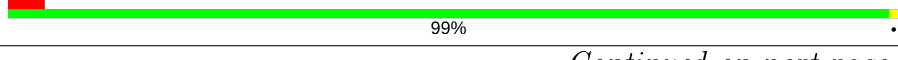

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	334	 99%
1	a	334	 99%
2	B	505	 99%
2	b	505	 98%
3	C	451	 98%
3	c	451	 97%
4	D	342	 98%

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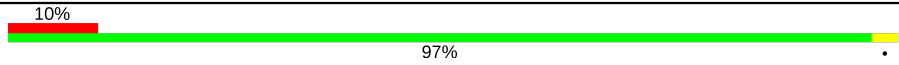
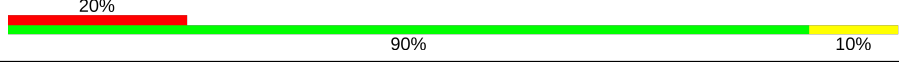
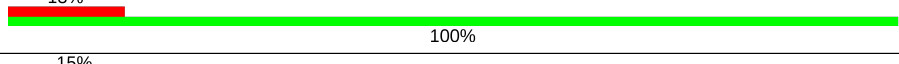
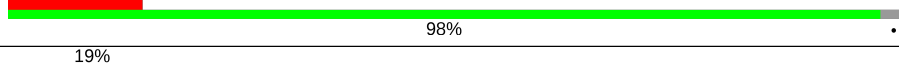
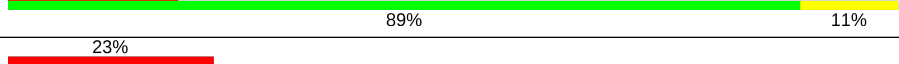

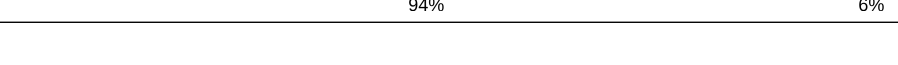


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Mol	Chain	Length	Quality of chain
4	d	342	 97%
5	E	80	 98%
5	e	80	 94%
6	F	34	 97%
6	f	34	 88%
7	H	63	 94%
7	h	63	 95%
8	I	36	 97%
8	i	36	 97%
9	J	37	 95%
9	j	37	 100%
10	K	37	 95%
10	k	37	 95%
11	L	37	 95%
11	l	37	 100%
12	M	34	 91%
12	m	34	 94%
13	O	244	 99%
13	o	244	 98%
14	T	31	 97%
14	t	31	 94%
15	U	97	 99%
15	u	97	 99%
16	V	137	 99%
16	v	137	 99%

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Mol	Chain	Length	Quality of chain
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	1005	X	-	-	-
24	CLA	A	1006	X	-	-	-
24	CLA	A	1008	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
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24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	D	406	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	J	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	d	404	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	y	101	-	X	-	-
32	LMT	A	1018	-	-	-	X
32	LMT	i	102	-	-	-	X
35	HTG	B	624	-	-	-	X

## 2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 53568 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 2643	C 1733	N 431	O 464	S 15	0	5	0
1	a	334	Total 2637	C 1729	N 431	O 462	S 15	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	Total 4040	C 2652	N 674	O 701	S 13	0	10	0
2	b	505	Total 4033	C 2646	N 676	O 698	S 13	0	9	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3500	C 2292	N 584	O 611	S 13	0	3	0
3	c	450	Total 3492	C 2287	N 583	O 609	S 13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	Total 2726	C 1805	N 445	O 464	S 12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	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	2	0
			660	431	105	124				
5	e	78	Total	C	N	O		0	0	0
			638	418	103	117				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			
9	j	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	304	202	48	53	1	0	0	0
11	l	37	304	202	48	53	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	34	274	184	40	49	1	0	1	0
12	m	34	274	184	40	49	1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	244	1883	1176	317	386	4	0	2	0
13	o	243	1868	1167	315	382	4	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	31	267	187	38	40	2	0	0	0
14	t	30	258	181	36	39	2	0	0	0

- 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
			780	495	129	156			
15	u	97	Total	C	N	O	0	1	0
			780	495	129	156			

- 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	3	0
			1081	687	179	211	4			
16	v	137	Total	C	N	O	S	0	2	0
			1076	683	177	212	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
			224	147	38	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			296	197	47	52			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

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

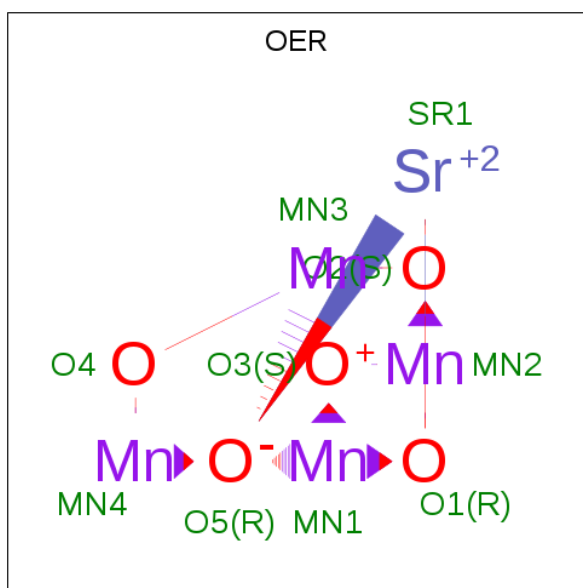
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			
19	z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			



- Molecule 21 is SR-MN4-O5 CLUSTER (three-letter code: OER) (formula:  $\text{Mn}_4\text{O}_5\text{Sr}$ ).



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

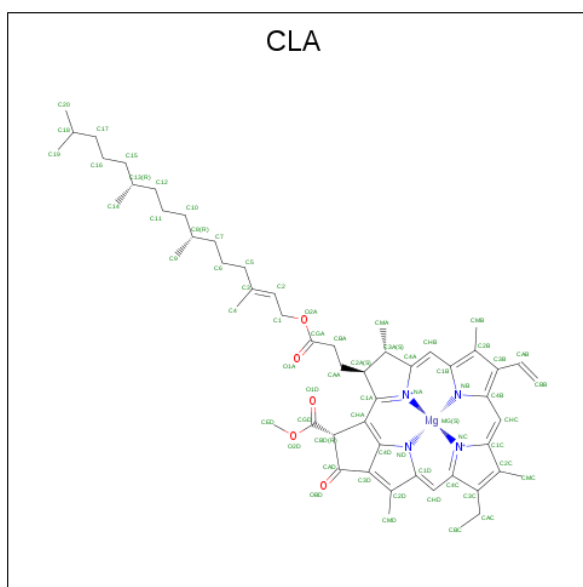
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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



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

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

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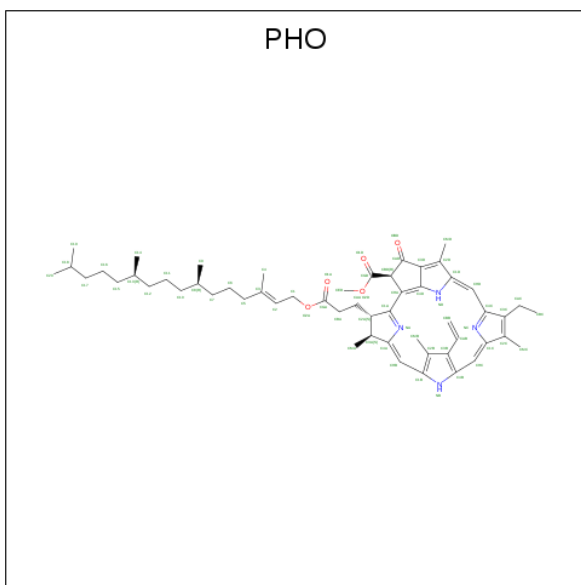
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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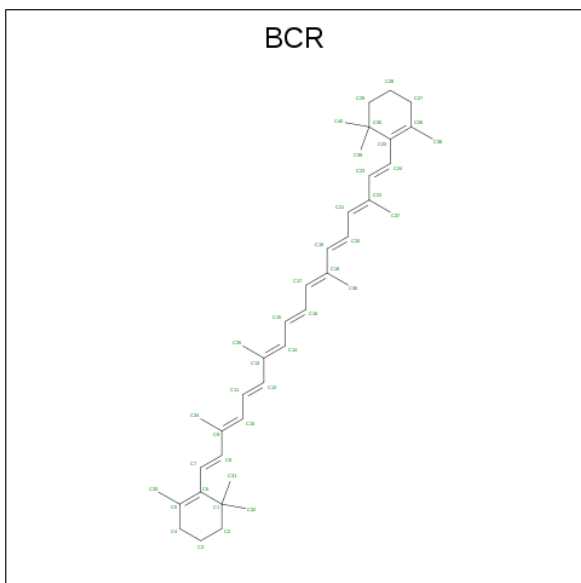
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



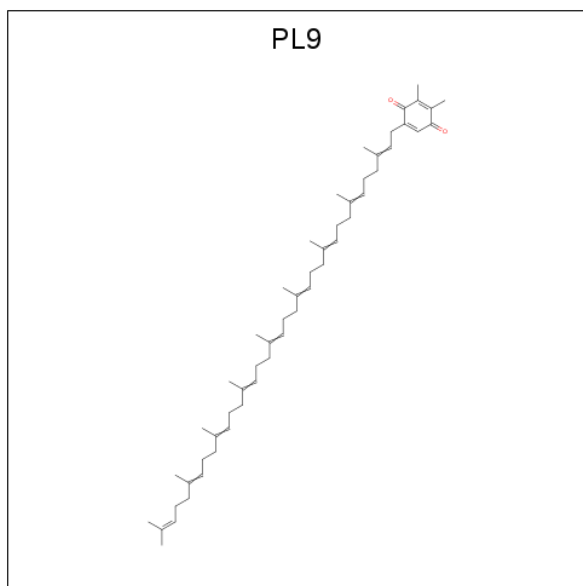
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
25	A	1	Total	64	55	4	5	0	0
25	D	1	Total	64	55	4	5	0	0
25	a	1	Total	64	55	4	5	0	0
25	a	1	Total	64	55	4	5	0	0

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



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

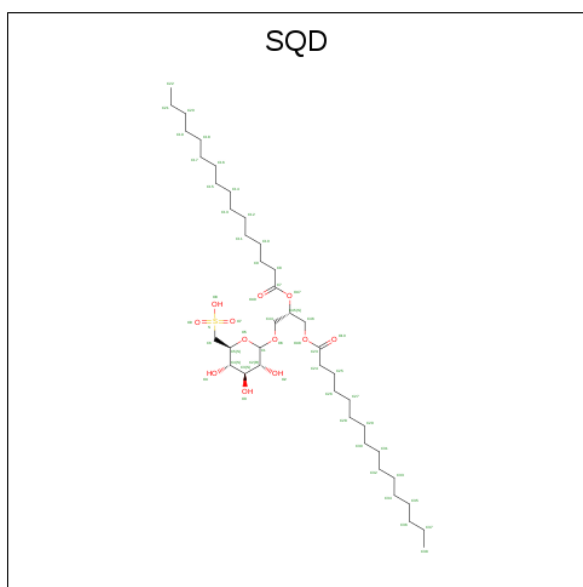
- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



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

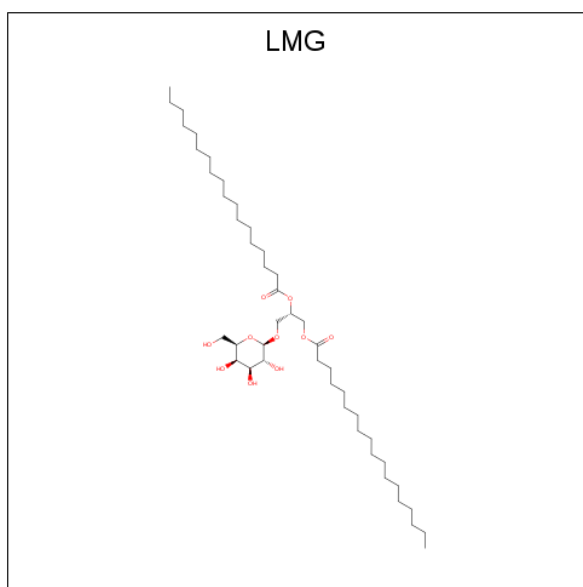
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).





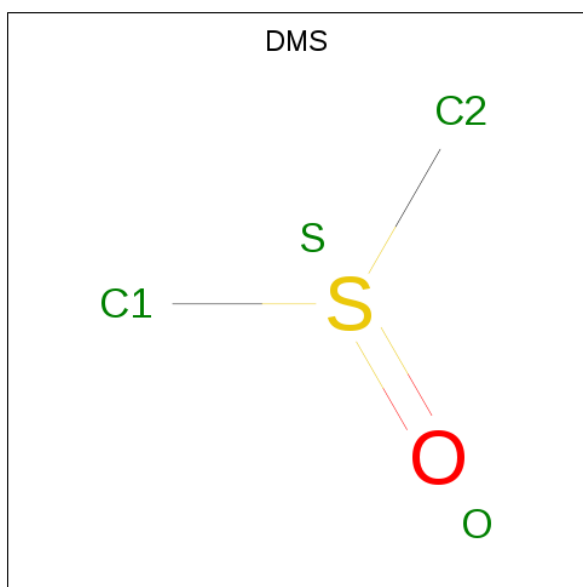
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
28	A	1	54	41	12	1	0	0
28	A	1	54	41	12	1	0	0
28	B	1	108	82	24	2	0	1
28	D	1	43	30	12	1	0	0
28	a	1	54	41	12	1	0	0
28	b	1	108	82	24	2	0	1
28	c	1	54	41	12	1	0	0
28	f	1	43	30	12	1	0	0

- Molecule 29 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
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	Z	1	Total	C	O	0	0
			51	41	10		
29	a	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	d	1	Total	C	O	0	0
			51	41	10		
29	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 30 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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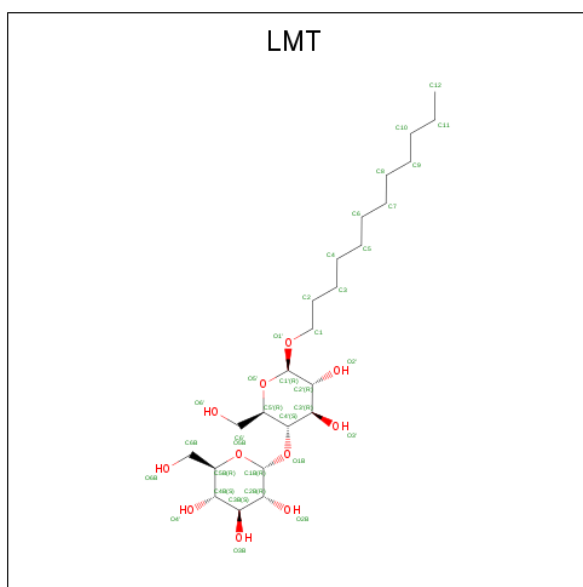
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	U	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	u	1	Total 4	C 2	O 1	S 1	0	0
30	v	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	J	1	Total C 16 16	0	0
31	i	1	Total C 16 16	0	0
31	D	2	Total C O 56 51 5	0	0
31	K	1	Total C O 34 29 5	0	0
31	y	1	Total C 16 16	0	0
31	l	1	Total C 16 16	0	0
31	B	2	Total C 32 32	0	0
31	I	2	Total C 26 26	0	0
31	c	1	Total C O 32 27 5	0	0
31	a	1	Total C O 30 25 5	0	0
31	x	1	Total C 16 16	0	0
31	A	1	Total C O 28 23 5	0	0
31	j	1	Total C 16 16	0	0
31	X	1	Total C 16 16	0	0
31	d	2	Total C O 52 47 5	0	0
31	t	1	Total C 16 16	0	0
31	Y	1	Total C 16 16	0	0
31	L	1	Total C 16 16	0	0
31	b	2	Total C 32 32	0	0

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



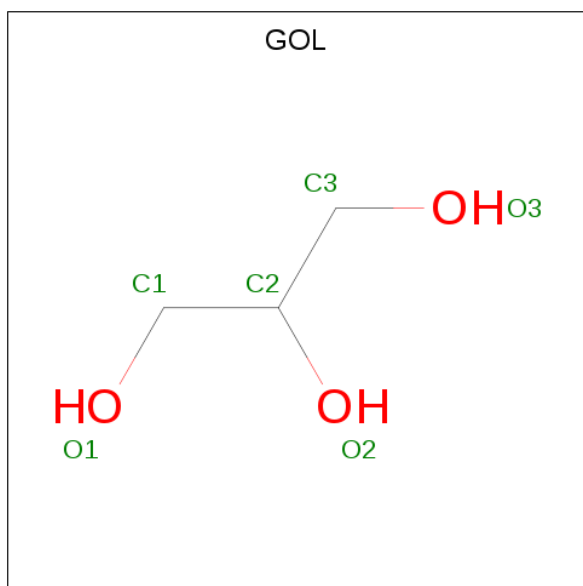
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	C	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	f	1	Total	C	O	0	0
			35	24	11		
32	i	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



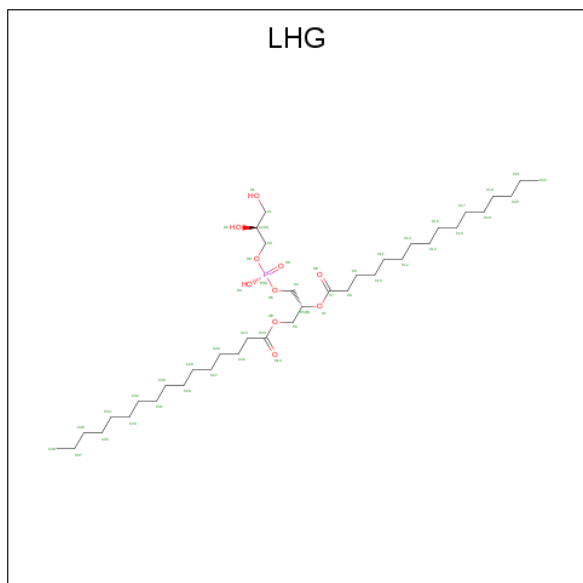
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			6	3	3		
33	B	1	Total	C	O	0	0
			6	3	3		
33	D	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	a	1	Total	C	O	0	0
			6	3	3		
33	b	1	Total	C	O	0	0
			6	3	3		
33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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	v	1	Total	C	O	0	0
			6	3	3		
33	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{76}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	b	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		

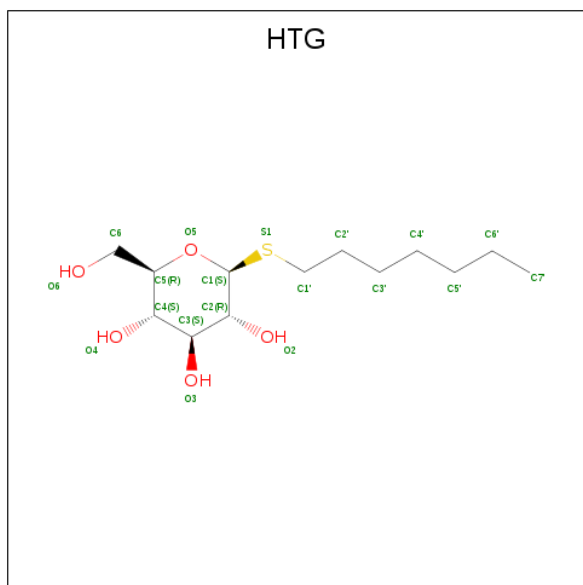
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
34	e	1	49	38	10	1	0	0

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



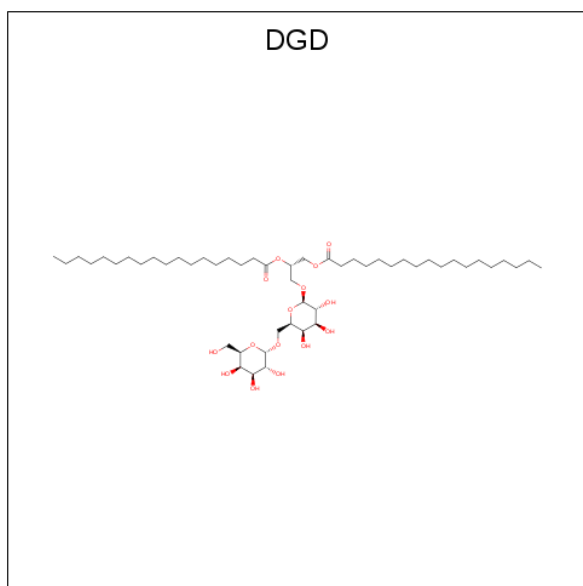
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	D	1	19	13	5	1	0	0
35	D	1	19	13	5	1	0	0
35	V	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0

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

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



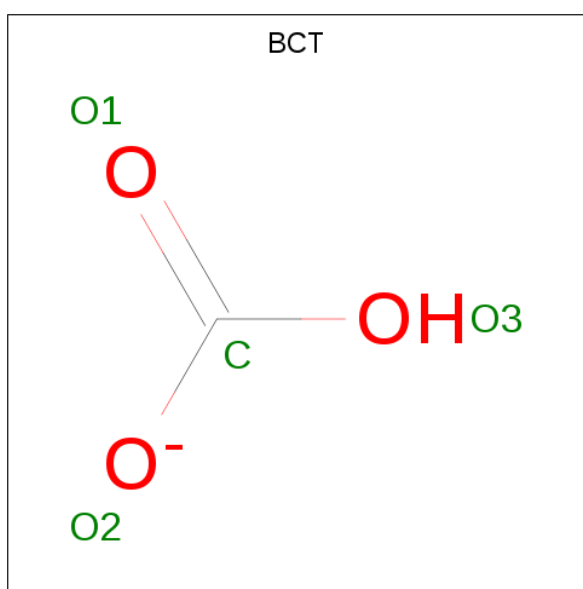
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	C	1	Total 62	C 47	O 15	0	0
36	C	1	Total 62	C 47	O 15	0	0
36	C	1	Total 62	C 47	O 15	0	0
36	H	1	Total 62	C 47	O 15	0	0

Continued on next page...

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

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	B	252	Total O 253 253	0	1
40	C	168	Total O 168 168	0	0
40	D	132	Total O 132 132	0	0
40	E	22	Total O 22 22	0	0
40	F	6	Total O 6 6	0	0
40	H	31	Total O 31 31	0	0
40	I	4	Total O 4 4	0	0
40	J	7	Total O 7 7	0	0
40	K	7	Total O 7 7	0	0
40	L	11	Total O 11 11	0	0
40	M	6	Total O 6 6	0	0
40	O	119	Total O 119 119	0	0
40	T	10	Total O 10 10	0	0
40	U	63	Total O 63 63	0	0
40	V	96	Total O 96 96	0	0
40	Y	1	Total O 1 1	0	0
40	X	8	Total O 8 8	0	0
40	Z	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	118	Total O 118 118	0	0
40	b	209	Total O 209 209	0	0

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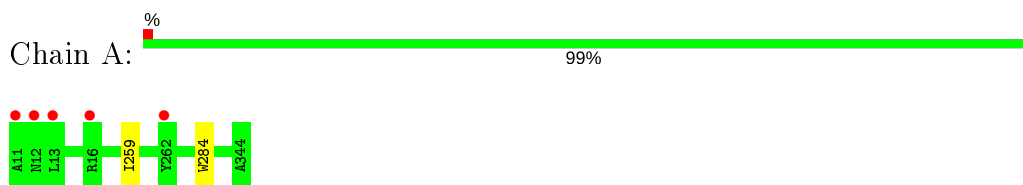
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	c	169	Total O 169 169	0	0
40	d	121	Total O 121 121	0	0
40	e	9	Total O 9 9	0	0
40	f	5	Total O 5 5	0	0
40	h	23	Total O 23 23	0	0
40	i	4	Total O 4 4	0	0
40	j	5	Total O 5 5	0	0
40	k	3	Total O 3 3	0	0
40	l	8	Total O 8 8	0	0
40	m	10	Total O 10 10	0	0
40	o	112	Total O 112 112	0	0
40	t	13	Total O 13 13	0	0
40	u	74	Total O 74 74	0	0
40	v	65	Total O 65 65	0	0
40	y	1	Total O 1 1	0	0
40	x	9	Total O 9 9	0	0

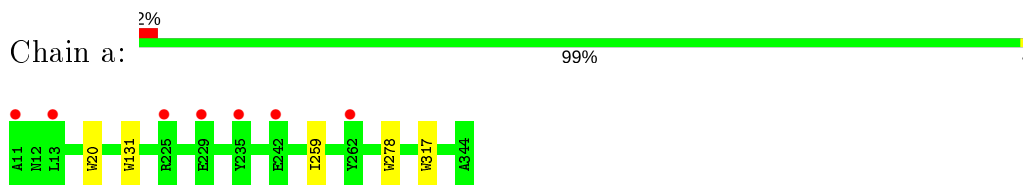
### 3 Residue-property plots [i](#)

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

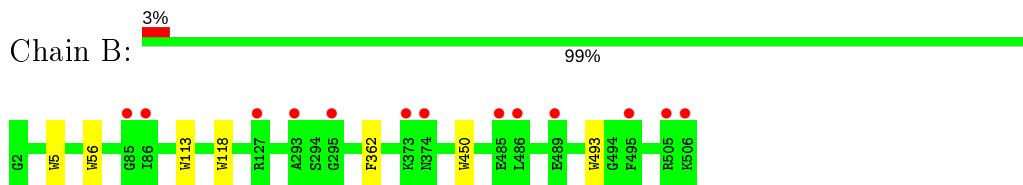
- Molecule 1: Photosystem Q(B) protein



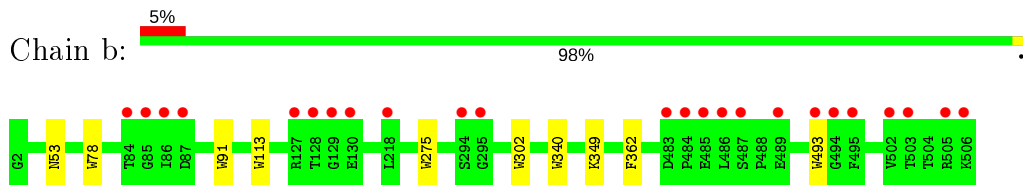
- Molecule 1: Photosystem Q(B) protein



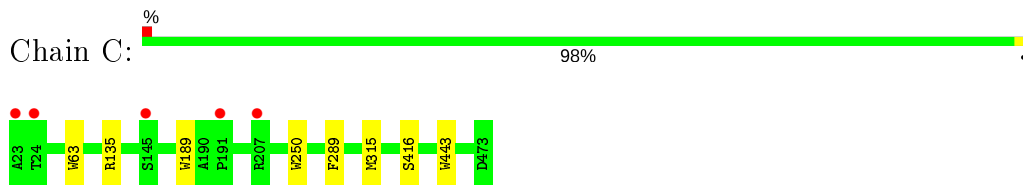
- Molecule 2: Photosystem II core light harvesting protein



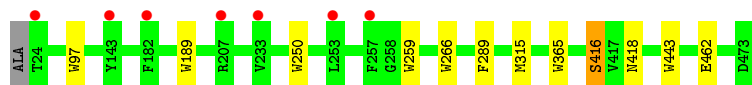
- Molecule 2: Photosystem II core light harvesting protein



- Molecule 3: Photosystem II CP43 protein



- Molecule 3: Photosystem II CP43 protein



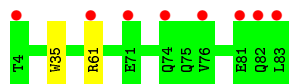
- Molecule 4: Photosystem II D2 protein



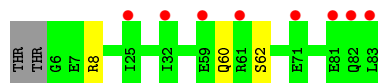
- Molecule 4: Photosystem II D2 protein



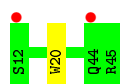
- Molecule 5: Cytochrome b559 subunit alpha



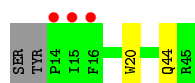
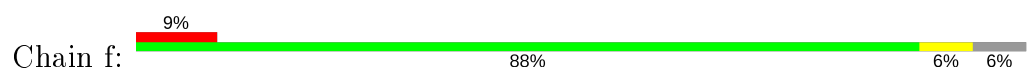
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

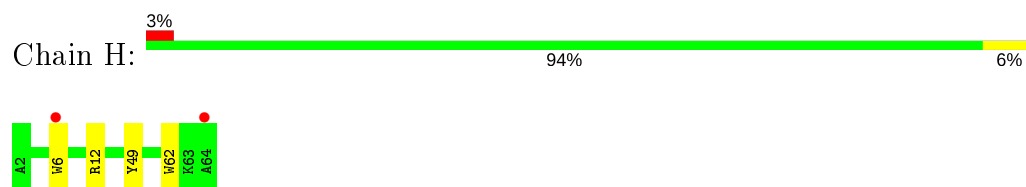


- Molecule 6: Cytochrome b559 subunit beta

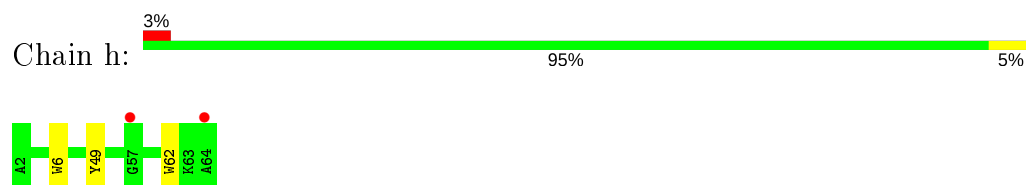




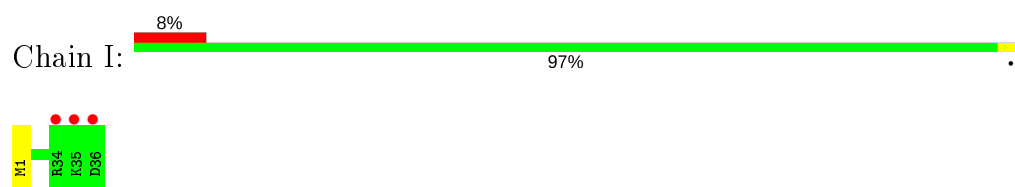
- Molecule 7: Photosystem II reaction center protein H



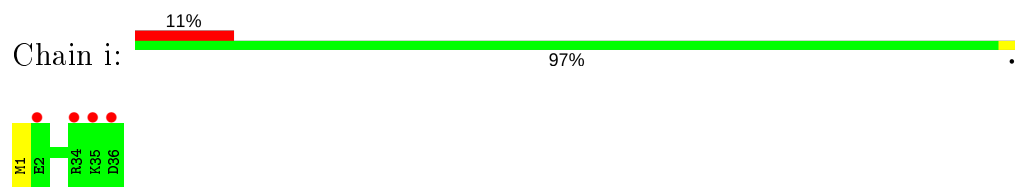
- Molecule 7: Photosystem II reaction center protein H



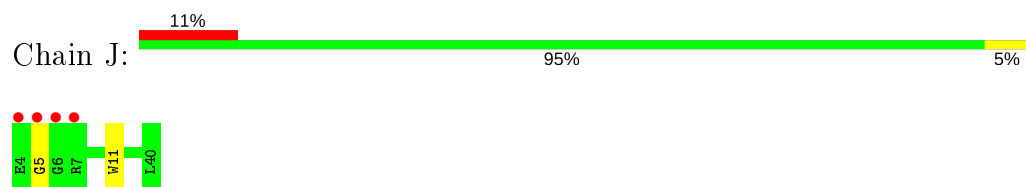
- Molecule 8: Photosystem II reaction center protein I



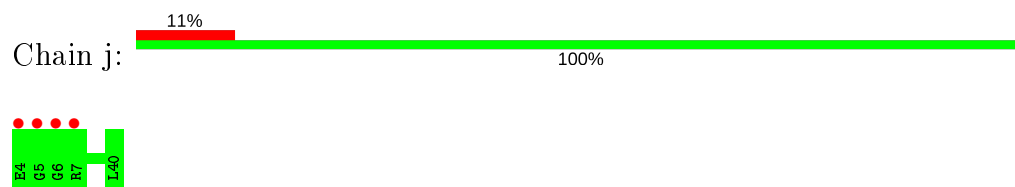
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

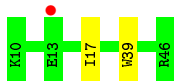


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K



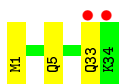
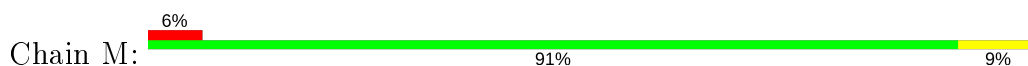
- Molecule 11: Photosystem II reaction center protein L



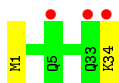
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



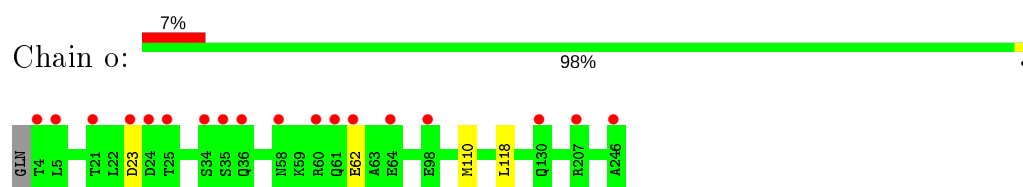
- Molecule 12: Photosystem II reaction center protein M



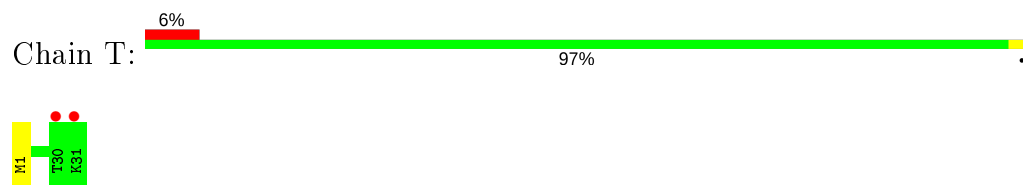
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



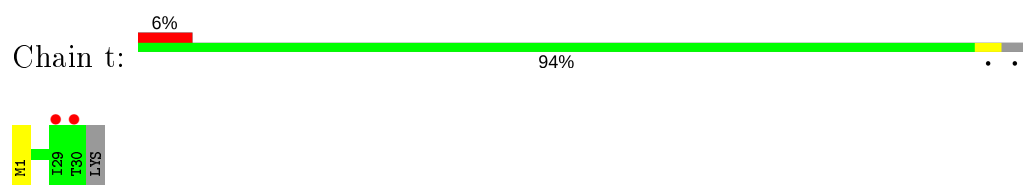
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



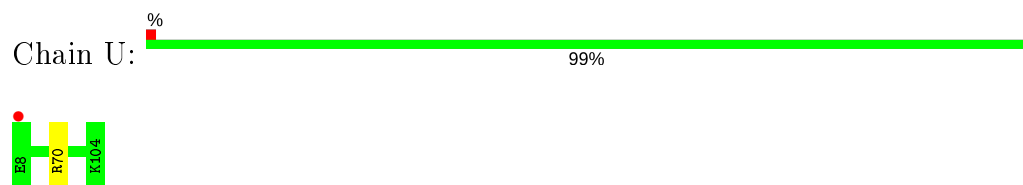
- Molecule 14: Photosystem II reaction center protein T



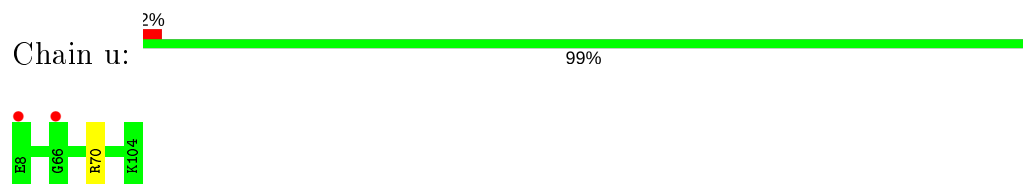
- Molecule 14: Photosystem II reaction center protein T



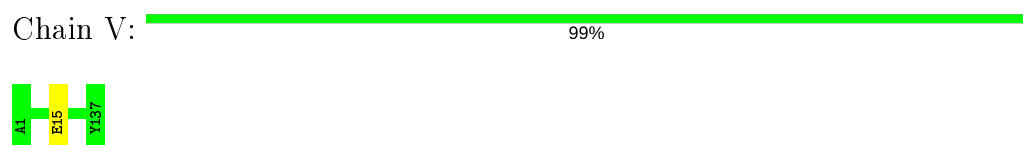
- Molecule 15: Photosystem II 12 kDa extrinsic protein



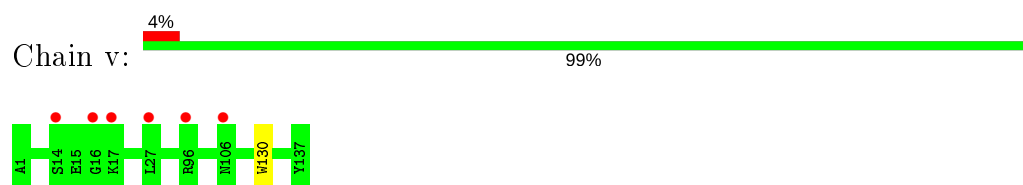
- Molecule 15: Photosystem II 12 kDa extrinsic protein



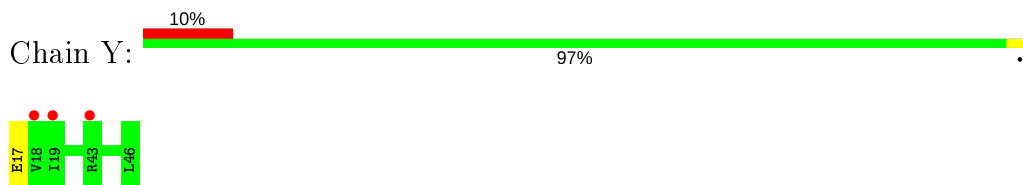
- Molecule 16: Cytochrome c-550



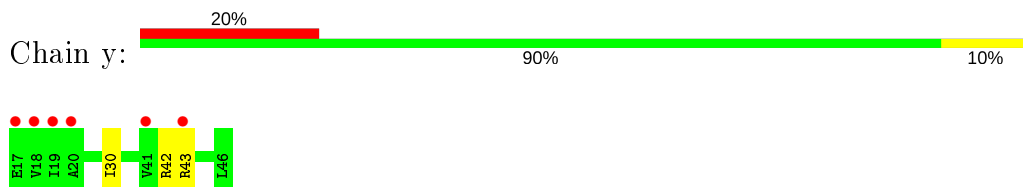
- Molecule 16: Cytochrome c-550



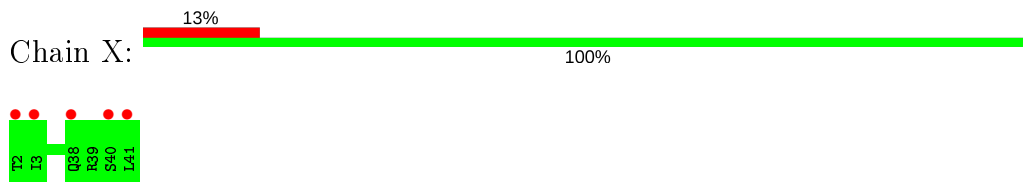
- Molecule 17: Photosystem II reaction center protein ycf12



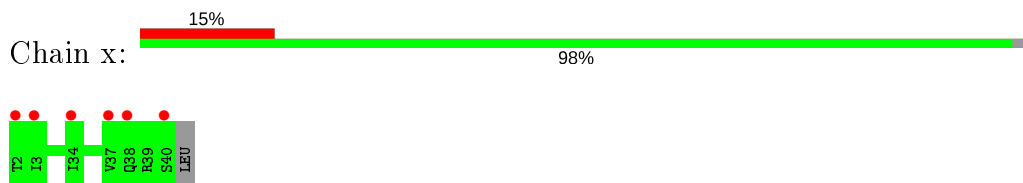
- Molecule 17: Photosystem II reaction center protein ycf12



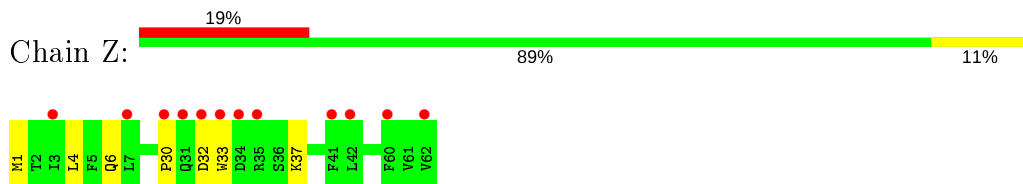
- Molecule 18: Photosystem II reaction center protein X



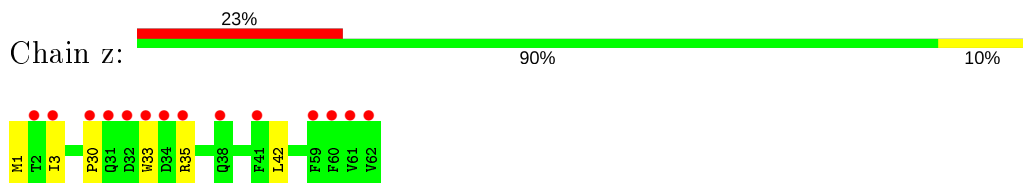
- Molecule 18: Photosystem II reaction center protein X



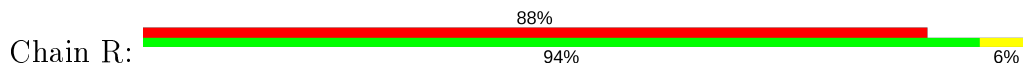
- Molecule 19: Photosystem II reaction center protein Z

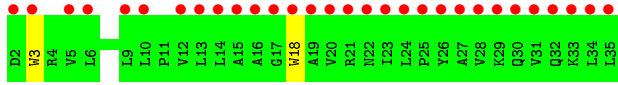


- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.86Å 228.79Å 285.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.10) 99.9 (19.96-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.176 , 0.205 0.177 , 0.206	Depositor DCC
$R_{free}$ test set	23034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	53568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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

### 5.1 Standard geometry

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

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	0.57	1/2743 (0.0%)	0.52	0/3740
1	a	0.56	4/2734 (0.1%)	0.52	0/3728
2	B	0.58	6/4210 (0.1%)	0.53	0/5731
2	b	0.58	7/4200 (0.2%)	0.52	0/5719
3	C	0.58	4/3622 (0.1%)	0.52	0/4931
3	c	0.58	7/3611 (0.2%)	0.51	0/4916
4	D	0.62	3/2821 (0.1%)	0.54	0/3844
4	d	0.60	7/2821 (0.2%)	0.53	0/3844
5	E	0.51	1/685 (0.1%)	0.51	0/936
5	e	0.49	0/657	0.49	0/897
6	F	0.57	1/284 (0.4%)	0.46	0/387
6	f	0.56	1/265 (0.4%)	0.47	0/360
7	H	0.60	2/522 (0.4%)	0.52	0/712
7	h	0.60	2/511 (0.4%)	0.53	0/697
8	I	0.34	0/293	0.42	0/396
8	i	0.35	0/293	0.44	0/396
9	J	0.54	1/272 (0.4%)	0.49	0/368
9	j	0.51	0/272	0.49	0/368
10	K	0.52	1/303 (0.3%)	0.49	0/416
10	k	0.51	1/303 (0.3%)	0.52	0/416
11	L	0.38	0/311	0.46	0/422
11	l	0.36	0/311	0.47	0/422
12	M	0.30	0/270	0.48	0/368
12	m	0.33	0/270	0.47	0/368
13	O	0.34	0/1920	0.53	0/2603
13	o	0.33	0/1902	0.52	0/2579
14	T	0.40	0/266	0.45	0/360
14	t	0.38	0/257	0.45	0/349
15	U	0.36	0/794	0.51	0/1076
15	u	0.34	0/794	0.51	0/1076
16	V	0.40	0/1111	0.49	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.40	1/1103 (0.1%)	0.48	0/1497
17	Y	0.33	0/225	0.49	0/301
17	y	0.30	0/225	0.48	0/301
18	X	0.32	0/299	0.43	0/403
18	x	0.33	0/290	0.42	0/392
19	Z	0.52	1/482 (0.2%)	0.46	0/659
19	z	0.51	1/482 (0.2%)	0.46	0/659
20	R	0.65	2/279 (0.7%)	0.52	0/383
All	All	0.53	54/43013 (0.1%)	0.51	0/58527

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	317	TRP	CD2-CE2	5.39	1.47	1.41
4	d	167	TRP	CD2-CE2	5.37	1.47	1.41
4	d	191	TRP	CD2-CE2	5.34	1.47	1.41
2	b	91	TRP	CD2-CE2	5.32	1.47	1.41
2	B	56	TRP	CD2-CE2	5.26	1.47	1.41

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	337/334 (101%)	333 (99%)	3 (1%)	1 (0%)	41 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	41	41
2	B	513/505 (102%)	505 (98%)	8 (2%)	0	100	100
2	b	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
3	C	452/451 (100%)	442 (98%)	9 (2%)	1 (0%)	47	49
3	c	450/451 (100%)	441 (98%)	8 (2%)	1 (0%)	47	49
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	333 (98%)	6 (2%)	1 (0%)	41	41
5	E	80/80 (100%)	79 (99%)	1 (1%)	0	100	100
5	e	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	59 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4	1
9	j	35/37 (95%)	35 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	240 (98%)	4 (2%)	0	100	100
13	o	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	96/97 (99%)	93 (97%)	3 (3%)	0	100	100
15	u	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
16	V	138/137 (101%)	134 (97%)	4 (3%)	0	100	100
16	v	137/137 (100%)	134 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9	4
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5296 (99%)	5151 (98%)	99 (2%)	8 (0%)	47	49

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
9	J	5	GLY
4	d	234	ALA
19	z	30	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/269 (102%)	274 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	413/403 (102%)	412 (100%)	1 (0%)	93	96
2	b	412/403 (102%)	409 (99%)	3 (1%)	84	88
3	C	355/352 (101%)	352 (99%)	3 (1%)	81	86
3	c	354/352 (101%)	349 (99%)	5 (1%)	67	73
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	79
4	d	277/277 (100%)	274 (99%)	3 (1%)	73	79
5	E	73/71 (103%)	72 (99%)	1 (1%)	67	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	69/71 (97%)	66 (96%)	3 (4%)	29	29
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	26/28 (93%)	25 (96%)	1 (4%)	33	34
7	H	54/53 (102%)	51 (94%)	3 (6%)	21	18
7	h	53/53 (100%)	52 (98%)	1 (2%)	57	63
8	I	32/32 (100%)	32 (100%)	0	100	100
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	25/25 (100%)	25 (100%)	0	100	100
9	j	25/25 (100%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	40
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	40
11	L	35/35 (100%)	33 (94%)	2 (6%)	20	18
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	31/30 (103%)	29 (94%)	2 (6%)	17	14
12	m	31/30 (103%)	30 (97%)	1 (3%)	39	41
13	O	209/207 (101%)	207 (99%)	2 (1%)	76	82
13	o	207/207 (100%)	203 (98%)	4 (2%)	57	63
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	26/27 (96%)	26 (100%)	0	100	100
15	U	85/84 (101%)	84 (99%)	1 (1%)	71	77
15	u	85/84 (101%)	84 (99%)	1 (1%)	71	77
16	V	120/117 (103%)	119 (99%)	1 (1%)	81	86
16	v	119/117 (102%)	119 (100%)	0	100	100
17	Y	23/23 (100%)	22 (96%)	1 (4%)	29	29
17	y	23/23 (100%)	20 (87%)	3 (13%)	4	2
18	X	33/33 (100%)	33 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	51/51 (100%)	47 (92%)	4 (8%)	12	9
19	z	51/51 (100%)	48 (94%)	3 (6%)	19	17
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4364/4323 (101%)	4310 (99%)	54 (1%)	71	77

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	37	LYS
3	c	416	SER
17	y	42	ARG
2	b	53	ASN
2	b	362	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	147	ASN
19	Z	58	ASN
16	v	34	GLN
16	V	34	GLN
2	B	331	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](#)

8 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	$\# Z  > 2$
19	FME	Z	1	19	8,9,10	0.60	0	7,9,11	1.97	4 (57%)
8	FME	I	1	8	8,9,10	0.54	0	7,9,11	1.30	1 (14%)
12	FME	m	1	12	8,9,10	0.50	0	7,9,11	1.58	2 (28%)
14	FME	T	1	14	8,9,10	0.55	0	7,9,11	1.84	3 (42%)
8	FME	i	1	8	8,9,10	0.51	0	7,9,11	1.35	1 (14%)
19	FME	z	1	19	8,9,10	0.48	0	7,9,11	1.73	1 (14%)

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	0.49	0	7,9,11	1.53	2 (28%)
14	FME	t	1	14	8,9,10	0.50	0	7,9,11	1.60	2 (28%)

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
19	FME	Z	1	19	-	4/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
19	FME	z	1	19	-	5/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	1	FME	CE-SD-CG	3.06	110.90	100.40
14	T	1	FME	C-CA-N	2.88	114.93	109.73
14	T	1	FME	CE-SD-CG	2.85	110.19	100.40
19	Z	1	FME	C-CA-N	2.77	114.73	109.73
19	z	1	FME	CE-SD-CG	2.74	109.81	100.40

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Z	1	FME	O1-CN-N-CA
19	Z	1	FME	N-CA-CB-CG
8	I	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	CB-CA-N-CN

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 261 ligands modelled in this entry, 24 are unknown and 10 are monoatomic - leaving 227 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
26	BCR	b	622	-	41,41,41	3.90	15 (36%)	56,56,56	8.19	36 (64%)
36	DGD	c	515	-	63,63,67	0.89	3 (4%)	77,77,81	0.89	2 (2%)
30	DMS	O	301	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
34	LHG	D	410	-	48,48,48	0.87	2 (4%)	51,54,54	0.95	4 (7%)
24	CLA	C	503	-	59,73,73	2.57	14 (23%)	67,113,113	2.09	14 (20%)
30	DMS	B	634	-	3,3,3	2.68	1 (33%)	3,3,3	0.48	0
24	CLA	B	612	-	59,73,73	2.40	14 (23%)	67,113,113	1.95	15 (22%)
32	LMT	C	520	-	36,36,36	0.52	0	47,47,47	1.01	1 (2%)
34	LHG	E	101	-	48,48,48	0.96	2 (4%)	51,54,54	0.96	3 (5%)
26	BCR	D	406	-	41,41,41	3.87	14 (34%)	56,56,56	8.13	45 (80%)
28	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.16	5 (8%)
24	CLA	c	502	-	59,73,73	2.41	15 (25%)	67,113,113	2.05	16 (23%)
24	CLA	b	618	-	59,73,73	2.44	14 (23%)	67,113,113	2.13	15 (22%)
24	CLA	b	617	-	59,73,73	2.60	15 (25%)	67,113,113	2.16	20 (29%)
33	GOL	b	632	-	5,5,5	0.22	0	5,5,5	0.28	0
24	CLA	A	1005	-	59,73,73	2.29	14 (23%)	67,113,113	1.94	13 (19%)
24	CLA	C	504	40	59,73,73	2.51	15 (25%)	67,113,113	2.10	17 (25%)
24	CLA	b	607	-	59,73,73	2.47	14 (23%)	67,113,113	2.33	13 (19%)
26	BCR	b	620	-	41,41,41	3.82	14 (34%)	56,56,56	8.09	40 (71%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	a	413	-	41,41,41	3.75	14 (34%)	56,56,56	8.51	40 (71%)
24	CLA	a	408	40	59,73,73	2.21	13 (22%)	67,113,113	1.95	16 (23%)
30	DMS	u	201	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
35	HTG	C	521	-	19,19,19	1.05	2 (10%)	23,24,24	1.23	1 (4%)
26	BCR	K	101	-	41,41,41	3.85	15 (36%)	56,56,56	8.01	41 (73%)
32	LMT	a	402	-	36,36,36	0.58	1 (2%)	47,47,47	0.86	3 (6%)
30	DMS	c	528	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
32	LMT	m	101	-	36,36,36	0.47	0	47,47,47	0.69	0
24	CLA	B	601	40	59,73,73	2.43	16 (27%)	67,113,113	2.14	17 (25%)
36	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	0.87	2 (2%)
30	DMS	O	302	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
26	BCR	B	619	-	41,41,41	3.87	15 (36%)	56,56,56	7.98	35 (62%)
24	CLA	B	611	-	59,73,73	2.52	14 (23%)	67,113,113	2.04	14 (20%)
33	GOL	v	204	-	5,5,5	0.25	0	5,5,5	0.31	0
28	SQD	c	518	-	53,54,54	1.04	3 (5%)	62,65,65	1.30	7 (11%)
35	HTG	D	413	-	19,19,19	1.05	2 (10%)	23,24,24	1.29	1 (4%)
34	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	0.92	3 (5%)
28	SQD	f	102	-	42,43,54	1.20	4 (9%)	51,54,65	1.37	7 (13%)
26	BCR	T	101	-	41,41,41	3.90	15 (36%)	56,56,56	8.04	38 (67%)
35	HTG	d	416	-	19,19,19	1.01	2 (10%)	23,24,24	1.59	1 (4%)
24	CLA	b	608	-	59,73,73	2.14	14 (23%)	67,113,113	1.94	15 (22%)
33	GOL	A	1019	-	5,5,5	0.26	0	5,5,5	0.30	0
30	DMS	c	529	-	3,3,3	2.60	1 (33%)	3,3,3	0.48	0
30	DMS	c	526	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
36	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.84	3 (3%)
26	BCR	y	101	-	41,41,41	3.91	15 (36%)	56,56,56	8.83	44 (78%)
24	CLA	b	604	40	59,73,73	2.79	15 (25%)	67,113,113	2.12	17 (25%)
32	LMT	a	416	-	36,36,36	0.50	0	47,47,47	0.76	1 (2%)
24	CLA	c	508	-	59,73,73	2.63	16 (27%)	67,113,113	2.05	16 (23%)
27	PL9	D	407	-	55,55,55	0.73	2 (3%)	68,69,69	1.43	13 (19%)
32	LMT	i	102	-	36,36,36	0.51	0	47,47,47	1.02	2 (4%)
26	BCR	t	101	-	41,41,41	3.89	15 (36%)	56,56,56	8.09	40 (71%)
33	GOL	d	417	-	5,5,5	0.32	0	5,5,5	0.17	0
36	DGD	c	516	-	63,63,67	0.92	3 (4%)	77,77,81	0.91	3 (3%)
38	HEM	V	201	16	27,50,50	2.14	6 (22%)	17,82,82	2.01	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	DMS	A	1014	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
30	DMS	C	525	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
24	CLA	C	512	-	59,73,73	3.02	14 (23%)	67,113,113	2.08	17 (25%)
29	LMG	A	1012	-	51,51,55	0.95	2 (3%)	59,59,63	0.92	2 (3%)
24	CLA	c	501	-	59,73,73	2.49	15 (25%)	67,113,113	2.14	16 (23%)
34	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	3 (5%)
35	HTG	b	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.18	2 (8%)
24	CLA	B	615	-	59,73,73	2.58	16 (27%)	67,113,113	2.20	16 (23%)
24	CLA	C	506	-	59,73,73	2.41	15 (25%)	67,113,113	2.07	14 (20%)
24	CLA	B	606	-	59,73,73	2.63	16 (27%)	67,113,113	2.20	17 (25%)
30	DMS	c	524	-	3,3,3	2.58	1 (33%)	3,3,3	0.34	0
21	OER	a	403	1,3,40	0,15,15	0.00	-	-	-	-
30	DMS	d	413	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
29	LMG	a	415	-	51,51,55	0.96	2 (3%)	59,59,63	0.97	2 (3%)
29	LMG	d	409	39	51,51,55	0.94	2 (3%)	59,59,63	0.87	2 (3%)
35	HTG	b	601	-	19,19,19	1.01	2 (10%)	23,24,24	1.36	1 (4%)
24	CLA	c	512	-	59,73,73	2.55	15 (25%)	67,113,113	2.15	17 (25%)
24	CLA	C	507	40	59,73,73	2.73	14 (23%)	67,113,113	2.29	15 (22%)
34	LHG	e	101	-	48,48,48	0.97	2 (4%)	51,54,54	0.99	2 (3%)
24	CLA	b	614	-	59,73,73	2.35	14 (23%)	67,113,113	1.94	15 (22%)
26	BCR	k	102	-	41,41,41	3.81	15 (36%)	56,56,56	8.37	37 (66%)
26	BCR	c	514	-	41,41,41	3.91	15 (36%)	56,56,56	8.73	41 (73%)
30	DMS	B	632	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
24	CLA	B	608	-	59,73,73	2.42	15 (25%)	67,113,113	2.01	15 (22%)
33	GOL	V	206	-	5,5,5	0.28	0	5,5,5	0.24	0
24	CLA	c	513	-	59,73,73	2.53	15 (25%)	67,113,113	2.00	16 (23%)
24	CLA	d	403	-	59,73,73	2.54	15 (25%)	67,113,113	1.92	16 (23%)
24	CLA	b	615	-	59,73,73	2.36	14 (23%)	67,113,113	2.10	15 (22%)
35	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.19	1 (4%)
30	DMS	a	417	-	3,3,3	2.55	1 (33%)	3,3,3	0.38	0
35	HTG	D	419	-	19,19,19	1.01	1 (5%)	23,24,24	1.55	1 (4%)
24	CLA	A	1006	40	59,73,73	2.16	14 (23%)	67,113,113	1.94	17 (25%)
36	DGD	C	515	-	63,63,67	0.87	2 (3%)	77,77,81	0.87	3 (3%)
24	CLA	b	613	40	59,73,73	2.36	14 (23%)	67,113,113	2.00	13 (19%)
32	LMT	M	101	-	36,36,36	0.48	0	47,47,47	0.89	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	503	-	59,73,73	2.71	15 (25%)	67,113,113	2.07	15 (22%)
34	LHG	b	624	-	48,48,48	0.91	2 (4%)	51,54,54	0.95	2 (3%)
30	DMS	B	626	-	3,3,3	2.54	1 (33%)	3,3,3	0.35	0
24	CLA	a	409	40	59,73,73	2.28	13 (22%)	67,113,113	1.95	15 (22%)
24	CLA	B	602	-	59,73,73	2.35	15 (25%)	67,113,113	1.99	16 (23%)
30	DMS	V	203	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
24	CLA	c	507	40	59,73,73	2.51	15 (25%)	67,113,113	2.33	17 (25%)
30	DMS	b	633	-	3,3,3	2.66	1 (33%)	3,3,3	0.65	0
27	PL9	A	1010	-	55,55,55	0.68	2 (3%)	68,69,69	1.63	17 (25%)
24	CLA	c	509	-	59,73,73	2.47	15 (25%)	67,113,113	2.14	17 (25%)
35	HTG	o	301	-	19,19,19	1.04	1 (5%)	23,24,24	1.30	1 (4%)
34	LHG	d	408	-	48,48,48	0.95	2 (4%)	51,54,54	0.94	2 (3%)
24	CLA	A	1008	-	59,73,73	2.40	15 (25%)	67,113,113	2.04	16 (23%)
38	HEM	f	101	5,6	27,50,50	2.14	6 (22%)	17,82,82	1.90	3 (17%)
24	CLA	C	510	-	59,73,73	2.29	15 (25%)	67,113,113	2.10	15 (22%)
35	HTG	b	630	-	19,19,19	1.08	2 (10%)	23,24,24	1.69	2 (8%)
29	LMG	Z	101	-	51,51,55	0.98	2 (3%)	59,59,63	0.99	2 (3%)
28	SQD	A	1016	-	53,54,54	1.04	3 (5%)	62,65,65	1.16	5 (8%)
30	DMS	C	526	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
29	LMG	c	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.06	3 (5%)
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.82	3 (3%)
33	GOL	a	420	-	5,5,5	0.28	0	5,5,5	0.27	0
33	GOL	d	415	-	5,5,5	0.28	0	5,5,5	0.33	0
24	CLA	C	508	-	59,73,73	2.46	16 (27%)	67,113,113	1.99	15 (22%)
24	CLA	B	614	-	59,73,73	2.46	15 (25%)	67,113,113	2.22	19 (28%)
29	LMG	B	622	-	51,51,55	0.98	2 (3%)	59,59,63	0.90	2 (3%)
35	HTG	b	602	-	19,19,19	1.02	2 (10%)	23,24,24	1.38	1 (4%)
24	CLA	B	607	40	59,73,73	2.44	15 (25%)	67,113,113	2.10	17 (25%)
29	LMG	D	412	39	51,51,55	0.90	2 (3%)	59,59,63	0.79	1 (1%)
28	SQD	D	408	-	42,43,54	1.17	3 (7%)	51,54,65	1.61	9 (17%)
24	CLA	b	605	-	59,73,73	2.46	15 (25%)	67,113,113	2.00	16 (23%)
34	LHG	D	411	-	48,48,48	0.94	2 (4%)	51,54,54	0.93	2 (3%)
26	BCR	d	404	-	41,41,41	3.92	15 (36%)	56,56,56	8.26	40 (71%)
24	CLA	b	612	-	59,73,73	2.69	15 (25%)	67,113,113	2.12	13 (19%)
24	CLA	c	505	-	59,73,73	2.39	15 (25%)	67,113,113	2.10	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	604	-	59,73,73	2.41	13 (22%)	67,113,113	2.22	18 (26%)
38	HEM	F	101	5,6	27,50,50	2.17	5 (18%)	17,82,82	1.83	3 (17%)
33	GOL	V	204	-	5,5,5	0.29	0	5,5,5	0.22	0
24	CLA	B	605	-	59,73,73	2.31	14 (23%)	67,113,113	2.00	16 (23%)
33	GOL	B	631	-	5,5,5	0.24	0	5,5,5	0.25	0
24	CLA	c	511	3	59,73,73	2.76	14 (23%)	67,113,113	2.11	15 (22%)
35	HTG	B	624	-	19,19,19	1.03	2 (10%)	23,24,24	1.52	1 (4%)
24	CLA	C	502	-	59,73,73	2.34	14 (23%)	67,113,113	2.04	15 (22%)
26	BCR	A	1009	-	41,41,41	3.83	14 (34%)	56,56,56	8.21	41 (73%)
24	CLA	B	613	-	59,73,73	2.27	14 (23%)	67,113,113	2.07	18 (26%)
26	BCR	J	101	-	41,41,41	3.89	14 (34%)	56,56,56	8.75	39 (69%)
24	CLA	a	407	-	59,73,73	2.23	14 (23%)	67,113,113	1.83	11 (16%)
24	CLA	C	501	-	59,73,73	2.38	15 (25%)	67,113,113	2.09	16 (23%)
21	OER	A	1001	1,3,40	0,15,15	0.00	-	-	-	-
30	DMS	B	627	-	3,3,3	2.57	1 (33%)	3,3,3	0.45	0
24	CLA	D	402	-	59,73,73	2.17	14 (23%)	67,113,113	2.14	19 (28%)
24	CLA	C	505	-	59,73,73	2.58	15 (25%)	67,113,113	2.13	13 (19%)
37	BCT	d	401	22	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	b	616	-	59,73,73	2.54	14 (23%)	67,113,113	2.10	16 (23%)
35	HTG	B	629	-	19,19,19	1.02	2 (10%)	23,24,24	1.34	1 (4%)
32	LMT	t	103	-	36,36,36	0.45	0	47,47,47	1.03	2 (4%)
30	DMS	B	633	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
24	CLA	B	610	40	59,73,73	2.22	15 (25%)	67,113,113	1.99	13 (19%)
27	PL9	a	414	-	55,55,55	0.70	2 (3%)	68,69,69	1.49	14 (20%)
32	LMT	A	1017	-	36,36,36	0.53	1 (2%)	47,47,47	0.86	1 (2%)
32	LMT	f	103	-	36,36,36	0.52	0	47,47,47	0.66	0
26	BCR	k	101	-	41,41,41	3.87	15 (36%)	56,56,56	8.62	40 (71%)
30	DMS	U	201	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
36	DGD	C	516	-	63,63,67	0.91	3 (4%)	77,77,81	0.93	4 (5%)
24	CLA	c	510	-	59,73,73	2.35	15 (25%)	67,113,113	2.03	16 (23%)
29	LMG	C	518	-	51,51,55	0.98	2 (3%)	59,59,63	0.87	2 (3%)
24	CLA	C	513	-	59,73,73	2.59	16 (27%)	67,113,113	2.04	17 (25%)
30	DMS	b	628	-	3,3,3	2.51	1 (33%)	3,3,3	0.50	0
36	DGD	c	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.82	3 (3%)
24	CLA	B	609	-	59,73,73	2.45	14 (23%)	67,113,113	2.02	14 (20%)
24	CLA	B	603	-	59,73,73	2.22	14 (23%)	67,113,113	2.15	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	611	-	59,73,73	2.38	14 (23%)	67,113,113	2.03	16 (23%)
24	CLA	b	610	40	59,73,73	2.43	15 (25%)	67,113,113	2.15	16 (23%)
24	CLA	C	511	3	59,73,73	2.64	15 (25%)	67,113,113	2.22	15 (22%)
35	HTG	B	628	-	19,19,19	1.05	2 (10%)	23,24,24	1.26	1 (4%)
33	GOL	D	418	-	5,5,5	0.29	0	5,5,5	0.31	0
32	LMT	B	623	-	36,36,36	0.48	0	47,47,47	1.00	2 (4%)
30	DMS	b	635	-	3,3,3	2.67	1 (33%)	3,3,3	0.45	0
32	LMT	b	631	-	36,36,36	0.50	0	47,47,47	0.84	2 (4%)
29	LMG	C	519	-	51,51,55	0.99	2 (3%)	59,59,63	1.06	4 (6%)
28	SQD	A	1011	-	53,54,54	1.02	3 (5%)	62,65,65	1.32	9 (14%)
24	CLA	c	504	40	59,73,73	2.53	15 (25%)	67,113,113	2.06	16 (23%)
25	PHO	A	1007	-	67,69,69	2.04	14 (20%)	85,99,99	1.86	15 (17%)
28	SQD	B	620[B]	-	53,54,54	1.02	3 (5%)	62,65,65	1.17	6 (9%)
24	CLA	b	609	-	59,73,73	2.71	16 (27%)	67,113,113	2.22	17 (25%)
33	GOL	V	207	-	5,5,5	0.24	0	5,5,5	0.35	0
28	SQD	B	620[A]	-	53,54,54	1.04	3 (5%)	62,65,65	1.10	7 (11%)
35	HTG	d	410	-	19,19,19	1.05	2 (10%)	23,24,24	1.29	1 (4%)
24	CLA	C	509	-	59,73,73	2.31	15 (25%)	67,113,113	2.14	17 (25%)
26	BCR	K	102	-	41,41,41	3.94	15 (36%)	56,56,56	8.47	39 (69%)
24	CLA	b	606	-	59,73,73	2.35	14 (23%)	67,113,113	2.07	17 (25%)
30	DMS	d	414	-	3,3,3	2.65	1 (33%)	3,3,3	0.41	0
35	HTG	V	202	-	19,19,19	0.99	2 (10%)	23,24,24	1.61	3 (13%)
29	LMG	c	519	-	51,51,55	0.98	2 (3%)	59,59,63	0.88	2 (3%)
38	HEM	v	201	16	27,50,50	2.17	6 (22%)	17,82,82	1.69	3 (17%)
28	SQD	b	623[B]	-	53,54,54	1.02	3 (5%)	62,65,65	1.12	7 (11%)
26	BCR	b	621	-	41,41,41	3.84	14 (34%)	56,56,56	8.44	42 (75%)
25	PHO	a	410	-	67,69,69	2.08	15 (22%)	85,99,99	1.84	16 (18%)
24	CLA	d	402	-	59,73,73	2.30	14 (23%)	67,113,113	1.98	15 (22%)
33	GOL	v	203	-	5,5,5	0.33	0	5,5,5	0.32	0
24	CLA	B	616	-	59,73,73	2.27	14 (23%)	67,113,113	2.09	19 (28%)
32	LMT	m	103	-	36,36,36	0.53	1 (2%)	47,47,47	0.78	1 (2%)
35	HTG	C	522	-	19,19,19	1.02	2 (10%)	23,24,24	1.91	5 (21%)
34	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
34	LHG	B	621	-	48,48,48	0.93	2 (4%)	51,54,54	0.92	2 (3%)
30	DMS	b	634	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	DMS	C	527	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
30	DMS	C	524	-	3,3,3	2.59	1 (33%)	3,3,3	0.45	0
37	BCT	D	401	22	0,3,3	0.00	-	0,3,3	0.00	-
30	DMS	v	202	-	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
30	DMS	b	629	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
30	DMS	D	417	-	3,3,3	2.68	1 (33%)	3,3,3	0.44	0
26	BCR	H	101	-	41,41,41	3.84	14 (34%)	56,56,56	8.40	42 (75%)
25	PHO	D	404	-	67,69,69	2.11	15 (22%)	85,99,99	1.90	19 (22%)
26	BCR	B	618	-	41,41,41	3.81	14 (34%)	56,56,56	8.43	41 (73%)
28	SQD	b	623[A]	-	53,54,54	1.02	3 (5%)	62,65,65	1.14	7 (11%)
32	LMT	b	625	-	36,36,36	0.51	0	47,47,47	1.20	6 (12%)
26	BCR	B	617	-	41,41,41	3.82	15 (36%)	56,56,56	8.16	37 (66%)
35	HTG	c	525	-	19,19,19	1.05	2 (10%)	23,24,24	1.18	1 (4%)
29	LMG	m	102	-	51,51,55	0.99	2 (3%)	59,59,63	1.10	4 (6%)
30	DMS	V	205	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
25	PHO	a	411	-	67,69,69	2.11	15 (22%)	85,99,99	1.93	19 (22%)
24	CLA	b	619	-	59,73,73	2.43	14 (23%)	67,113,113	2.06	15 (22%)
26	BCR	C	514	-	41,41,41	3.93	15 (36%)	56,56,56	8.28	38 (67%)
32	LMT	M	102	-	36,36,36	0.50	0	47,47,47	0.73	0
30	DMS	a	418	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
26	BCR	h	101	-	41,41,41	3.87	14 (34%)	56,56,56	8.48	42 (75%)
24	CLA	D	405	-	59,73,73	2.55	15 (25%)	67,113,113	1.96	15 (22%)
29	LMG	c	520	-	51,51,55	0.99	3 (5%)	59,59,63	1.02	3 (5%)
30	DMS	D	416	-	3,3,3	2.70	1 (33%)	3,3,3	0.75	0
27	PL9	d	405	-	55,55,55	0.73	2 (3%)	68,69,69	1.38	10 (14%)
24	CLA	D	403	40	59,73,73	2.05	13 (22%)	67,113,113	2.11	15 (22%)
32	LMT	A	1018	-	36,36,36	0.53	0	47,47,47	1.00	5 (10%)
30	DMS	c	527	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
24	CLA	a	412	-	59,73,73	2.19	14 (23%)	67,113,113	2.05	16 (23%)
30	DMS	A	1013	-	3,3,3	2.53	1 (33%)	3,3,3	0.57	0
30	DMS	C	523	-	3,3,3	2.54	1 (33%)	3,3,3	0.38	0
24	CLA	c	506	-	59,73,73	2.58	14 (23%)	67,113,113	2.09	14 (20%)

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
26	BCR	b	622	-	-	6/29/63/63	0/2/2/2
36	DGD	c	515	-	-	22/51/91/95	0/2/2/2
33	GOL	b	632	-	-	2/4/4/4	-
34	LHG	D	410	-	-	15/53/53/53	-
24	CLA	C	503	-	2/2/20/25	4/37/135/135	-
28	SQD	c	518	-	-	22/49/69/69	0/1/1/1
24	CLA	B	612	-	3/3/20/25	4/37/135/135	-
32	LMT	C	520	-	-	9/21/61/61	0/2/2/2
34	LHG	E	101	-	-	32/53/53/53	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	SQD	a	401	-	-	25/49/69/69	0/1/1/1
24	CLA	c	502	-	1/1/20/25	7/37/135/135	-
24	CLA	b	617	-	3/3/20/25	21/37/135/135	-
34	LHG	d	408	-	-	14/53/53/53	-
24	CLA	A	1005	-	3/3/20/25	1/37/135/135	-
24	CLA	C	504	40	3/3/20/25	10/37/135/135	-
24	CLA	b	607	-	3/3/20/25	5/37/135/135	-
26	BCR	b	620	-	-	5/29/63/63	0/2/2/2
26	BCR	a	413	-	-	5/29/63/63	0/2/2/2
24	CLA	a	408	40	1/1/20/25	3/37/135/135	-
35	HTG	C	521	-	-	5/10/30/30	0/1/1/1
26	BCR	K	101	-	-	9/29/63/63	0/2/2/2
32	LMT	a	402	-	-	7/21/61/61	0/2/2/2
32	LMT	m	101	-	-	0/21/61/61	0/2/2/2
24	CLA	B	601	40	3/3/20/25	14/37/135/135	-
36	DGD	C	517	-	-	10/51/91/95	0/2/2/2
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2
38	HEM	f	101	5,6	-	1/6/54/54	-
33	GOL	v	204	-	-	3/4/4/4	-
35	HTG	D	413	-	-	5/10/30/30	0/1/1/1
34	LHG	d	406	-	-	16/53/53/53	-
28	SQD	f	102	-	-	23/38/58/69	0/1/1/1
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
35	HTG	d	416	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	608	-	3/3/20/25	7/37/135/135	-
33	GOL	A	1019	-	-	2/4/4/4	-
25	PHO	a	411	-	-	5/53/103/103	0/5/6/6
36	DGD	h	102	-	-	18/51/91/95	0/2/2/2
26	BCR	y	101	-	-	11/29/63/63	0/2/2/2
24	CLA	c	510	-	3/3/20/25	11/37/135/135	-
32	LMT	a	416	-	-	8/21/61/61	0/2/2/2
24	CLA	c	508	-	2/2/20/25	14/37/135/135	-
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
32	LMT	i	102	-	-	12/21/61/61	0/2/2/2
26	BCR	t	101	-	-	5/29/63/63	0/2/2/2
33	GOL	d	417	-	-	2/4/4/4	-
36	DGD	c	516	-	-	27/51/91/95	0/2/2/2
38	HEM	V	201	16	-	0/6/54/54	-
33	GOL	B	631	-	-	0/4/4/4	-
24	CLA	B	607	40	3/3/20/25	3/37/135/135	-
29	LMG	A	1012	-	-	27/46/66/70	0/1/1/1
24	CLA	c	501	-	3/3/20/25	3/37/135/135	-
24	CLA	B	611	-	3/3/20/25	7/37/135/135	-
35	HTG	b	626	-	-	5/10/30/30	0/1/1/1
24	CLA	B	615	-	3/3/20/25	7/37/135/135	-
24	CLA	C	506	-	3/3/20/25	12/37/135/135	-
24	CLA	C	513	-	2/2/20/25	10/37/135/135	-
35	HTG	c	525	-	-	5/10/30/30	0/1/1/1
29	LMG	a	415	-	-	23/46/66/70	0/1/1/1
29	LMG	d	409	39	-	17/46/66/70	0/1/1/1
24	CLA	c	512	-	3/3/20/25	16/37/135/135	-
36	DGD	c	517	-	-	19/51/91/95	0/2/2/2
26	BCR	H	101	-	-	9/29/63/63	0/2/2/2
34	LHG	e	101	-	-	28/53/53/53	-
24	CLA	b	614	-	1/1/20/25	3/37/135/135	-
26	BCR	k	102	-	-	9/29/63/63	0/2/2/2
26	BCR	c	514	-	-	7/29/63/63	0/2/2/2
24	CLA	B	608	-	1/1/20/25	1/37/135/135	-
33	GOL	V	206	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	513	-	1/1/20/25	20/37/135/135	-
24	CLA	d	403	-	2/2/20/25	15/37/135/135	-
35	HTG	c	522	-	-	5/10/30/30	0/1/1/1
35	HTG	D	419	-	-	7/10/30/30	0/1/1/1
24	CLA	A	1006	40	2/2/20/25	11/37/135/135	-
36	DGD	C	515	-	-	26/51/91/95	0/2/2/2
24	CLA	b	613	40	3/3/20/25	5/37/135/135	-
32	LMT	M	101	-	-	9/21/61/61	0/2/2/2
24	CLA	c	503	-	1/1/20/25	3/37/135/135	-
34	LHG	b	624	-	-	20/53/53/53	-
35	HTG	V	202	-	-	6/10/30/30	0/1/1/1
24	CLA	a	409	40	2/2/20/25	8/37/135/135	-
24	CLA	B	602	-	3/3/20/25	4/37/135/135	-
24	CLA	b	605	-	3/3/20/25	5/37/135/135	-
27	PL9	A	1010	-	-	6/53/73/73	0/1/1/1
24	CLA	c	509	-	3/3/20/25	11/37/135/135	-
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1
24	CLA	A	1008	-	1/1/20/25	8/37/135/135	-
24	CLA	C	510	-	3/3/20/25	6/37/135/135	-
35	HTG	b	630	-	-	7/10/30/30	0/1/1/1
29	LMG	Z	101	-	-	27/46/66/70	0/1/1/1
28	SQD	A	1016	-	-	23/49/69/69	0/1/1/1
29	LMG	c	521	-	-	25/46/66/70	0/1/1/1
36	DGD	H	102	-	-	16/51/91/95	0/2/2/2
33	GOL	a	420	-	-	2/4/4/4	-
33	GOL	d	415	-	-	2/4/4/4	-
24	CLA	C	508	-	3/3/20/25	13/37/135/135	-
24	CLA	B	614	-	3/3/20/25	11/37/135/135	-
29	LMG	B	622	-	-	22/46/66/70	0/1/1/1
35	HTG	b	602	-	-	2/10/30/30	0/1/1/1
29	LMG	D	412	39	-	15/46/66/70	0/1/1/1
28	SQD	D	408	-	-	22/38/58/69	0/1/1/1
24	CLA	c	507	40	3/3/20/25	9/37/135/135	-
34	LHG	D	411	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	d	404	-	-	10/29/63/63	0/2/2/2
24	CLA	b	612	-	-	2/37/135/135	-
24	CLA	c	505	-	2/2/20/25	9/37/135/135	-
24	CLA	B	604	-	3/3/20/25	11/37/135/135	-
38	HEM	F	101	5,6	-	0/6/54/54	-
33	GOL	V	204	-	-	2/4/4/4	-
24	CLA	B	605	-	3/3/20/25	3/37/135/135	-
24	CLA	c	511	3	2/2/20/25	2/37/135/135	-
35	HTG	B	624	-	-	7/10/30/30	0/1/1/1
24	CLA	C	502	-	1/1/20/25	10/37/135/135	-
26	BCR	A	1009	-	-	6/29/63/63	0/2/2/2
24	CLA	B	613	-	3/3/20/25	4/37/135/135	-
26	BCR	J	101	-	-	12/29/63/63	0/2/2/2
24	CLA	a	407	-	3/3/20/25	1/37/135/135	-
24	CLA	C	501	-	3/3/20/25	6/37/135/135	-
24	CLA	b	619	-	3/3/20/25	11/37/135/135	-
24	CLA	C	505	-	1/1/20/25	8/37/135/135	-
24	CLA	b	616	-	3/3/20/25	9/37/135/135	-
35	HTG	B	629	-	-	2/10/30/30	0/1/1/1
32	LMT	t	103	-	-	16/21/61/61	0/2/2/2
24	CLA	B	610	40	3/3/20/25	9/37/135/135	-
27	PL9	a	414	-	-	5/53/73/73	0/1/1/1
24	CLA	b	606	-	3/3/20/25	8/37/135/135	-
32	LMT	f	103	-	-	15/21/61/61	0/2/2/2
26	BCR	k	101	-	-	14/29/63/63	0/2/2/2
36	DGD	C	516	-	-	23/51/91/95	0/2/2/2
24	CLA	b	615	-	3/3/20/25	9/37/135/135	-
29	LMG	C	518	-	-	20/46/66/70	0/1/1/1
24	CLA	B	606	-	3/3/20/25	10/37/135/135	-
24	CLA	C	512	-	3/3/20/25	16/37/135/135	-
24	CLA	B	609	-	2/2/20/25	1/37/135/135	-
24	CLA	B	603	-	3/3/20/25	7/37/135/135	-
24	CLA	b	611	-	1/1/20/25	1/37/135/135	-
24	CLA	b	610	40	3/3/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
33	GOL	D	418	-	-	4/4/4/4	-
32	LMT	B	623	-	-	14/21/61/61	0/2/2/2
32	LMT	b	631	-	-	10/21/61/61	0/2/2/2
29	LMG	C	519	-	-	22/46/66/70	0/1/1/1
28	SQD	A	1011	-	-	20/49/69/69	0/1/1/1
33	GOL	v	203	-	-	2/4/4/4	-
24	CLA	c	504	40	2/2/20/25	12/37/135/135	-
25	PHO	A	1007	-	-	1/53/103/103	0/5/6/6
28	SQD	B	620[B]	-	-	24/49/69/69	0/1/1/1
24	CLA	b	609	-	3/3/20/25	9/37/135/135	-
33	GOL	V	207	-	-	2/4/4/4	-
28	SQD	B	620[A]	-	-	29/49/69/69	0/1/1/1
35	HTG	d	410	-	-	4/10/30/30	0/1/1/1
24	CLA	C	509	-	3/3/20/25	7/37/135/135	-
32	LMT	A	1017	-	-	10/21/61/61	0/2/2/2
26	BCR	K	102	-	-	8/29/63/63	0/2/2/2
28	SQD	b	623[A]	-	-	22/49/69/69	0/1/1/1
29	LMG	c	519	-	-	25/46/66/70	0/1/1/1
38	HEM	v	201	16	-	0/6/54/54	-
28	SQD	b	623[B]	-	-	29/49/69/69	0/1/1/1
26	BCR	b	621	-	-	5/29/63/63	0/2/2/2
24	CLA	D	405	-	2/2/20/25	14/37/135/135	-
24	CLA	d	402	-	1/1/20/25	6/37/135/135	-
24	CLA	b	618	-	3/3/20/25	5/37/135/135	-
24	CLA	B	616	-	3/3/20/25	14/37/135/135	-
32	LMT	m	103	-	-	7/21/61/61	0/2/2/2
35	HTG	C	522	-	-	6/10/30/30	0/1/1/1
34	LHG	d	407	-	-	15/53/53/53	-
34	LHG	B	621	-	-	19/53/53/53	-
32	LMT	A	1018	-	-	13/21/61/61	0/2/2/2
34	LHG	D	409	-	-	16/53/53/53	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	C	507	40	3/3/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	D	404	-	-	6/53/103/103	0/5/6/6
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
32	LMT	b	625	-	-	11/21/61/61	0/2/2/2
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
29	LMG	m	102	-	-	22/46/66/70	0/1/1/1
24	CLA	C	511	3	2/2/20/25	7/37/135/135	-
24	CLA	D	402	-	2/2/20/25	4/37/135/135	-
26	BCR	C	514	-	-	6/29/63/63	0/2/2/2
32	LMT	M	102	-	-	6/21/61/61	0/2/2/2
26	BCR	h	101	-	-	8/29/63/63	0/2/2/2
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
27	PL9	d	405	-	-	2/53/73/73	0/1/1/1
24	CLA	D	403	40	1/1/20/25	3/37/135/135	-
24	CLA	c	506	-	3/3/20/25	13/37/135/135	-
25	PHO	a	410	-	-	4/53/103/103	0/5/6/6
24	CLA	a	412	-	1/1/20/25	14/37/135/135	-
24	CLA	b	604	40	1/1/20/25	19/37/135/135	-

The worst 5 of 1598 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	17.54	2.47	2.06
24	b	604	CLA	MG-NC	13.70	2.38	2.06
24	b	617	CLA	MG-NA	13.60	2.38	2.06
24	C	505	CLA	MG-NA	13.03	2.37	2.06
24	C	507	CLA	MG-NA	12.84	2.36	2.06

The worst 5 of 2311 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1009	BCR	C20-C21-C22	28.08	167.39	127.31
26	J	101	BCR	C16-C17-C18	28.03	167.31	127.31
26	y	101	BCR	C20-C21-C22	27.20	166.12	127.31
26	k	101	BCR	C15-C16-C17	27.02	178.83	123.47
26	c	514	BCR	C16-C17-C18	26.99	165.84	127.31

5 of 166 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	503	CLA	NC
24	C	503	CLA	NA
24	B	612	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND

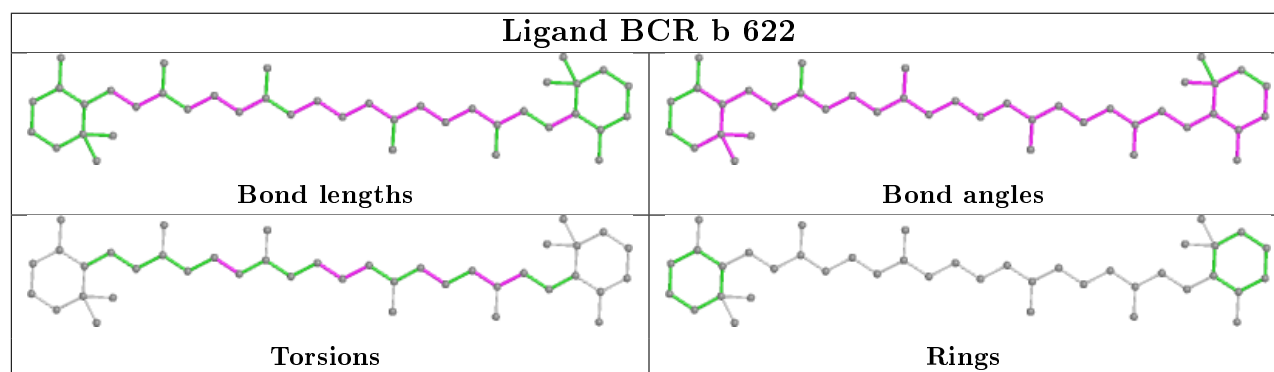
5 of 1872 torsion outliers are listed below:

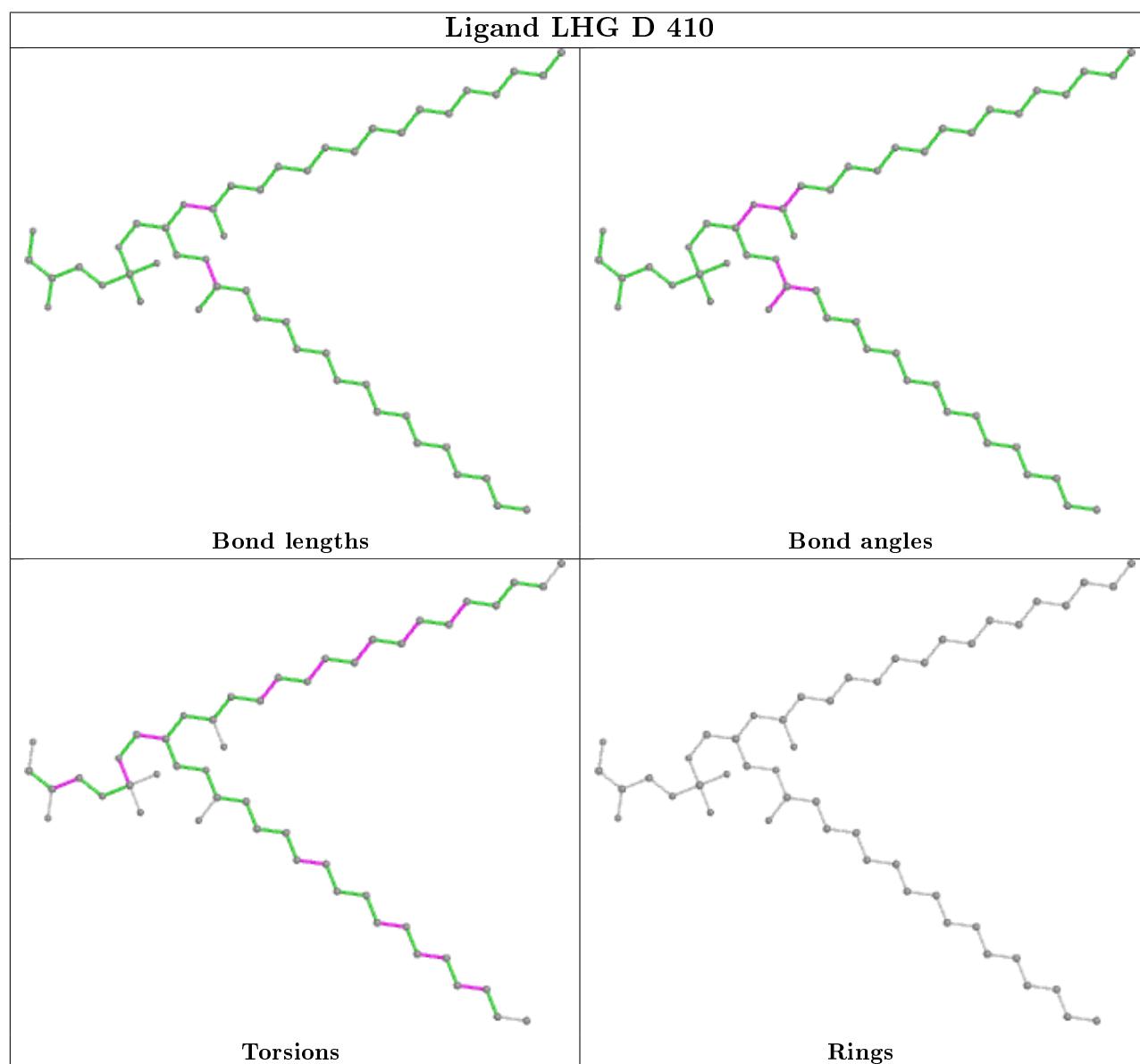
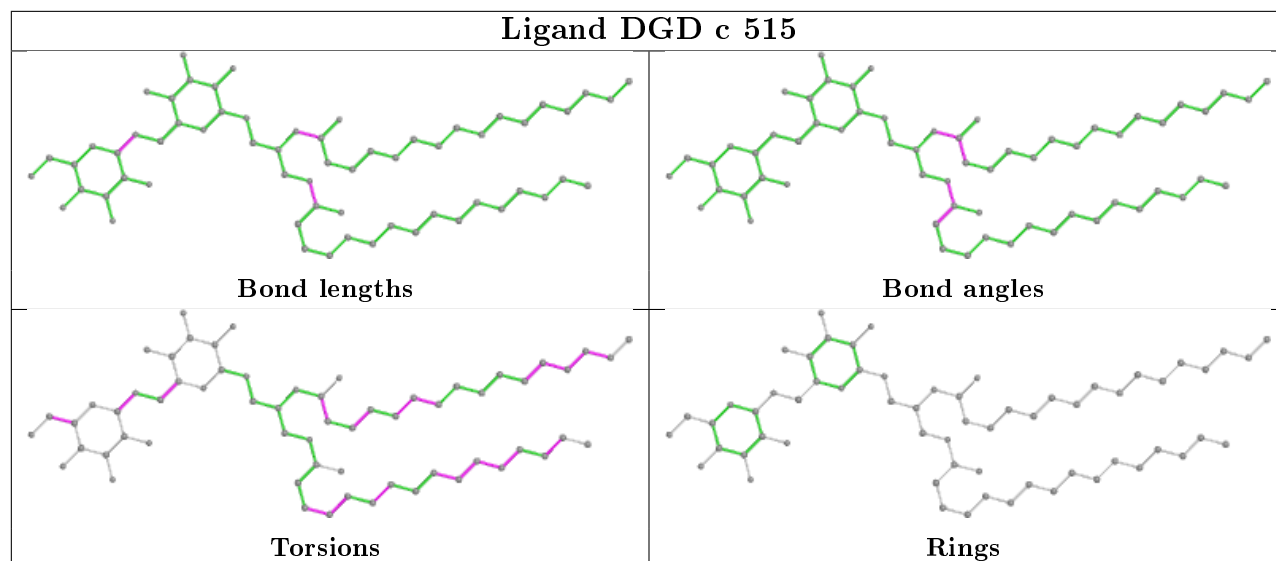
Mol	Chain	Res	Type	Atoms
26	b	622	BCR	C14-C15-C16-C17
26	b	622	BCR	C15-C16-C17-C18
34	D	410	LHG	C4-O6-P-O4
26	D	406	BCR	C37-C22-C23-C24
26	D	406	BCR	C22-C23-C24-C25

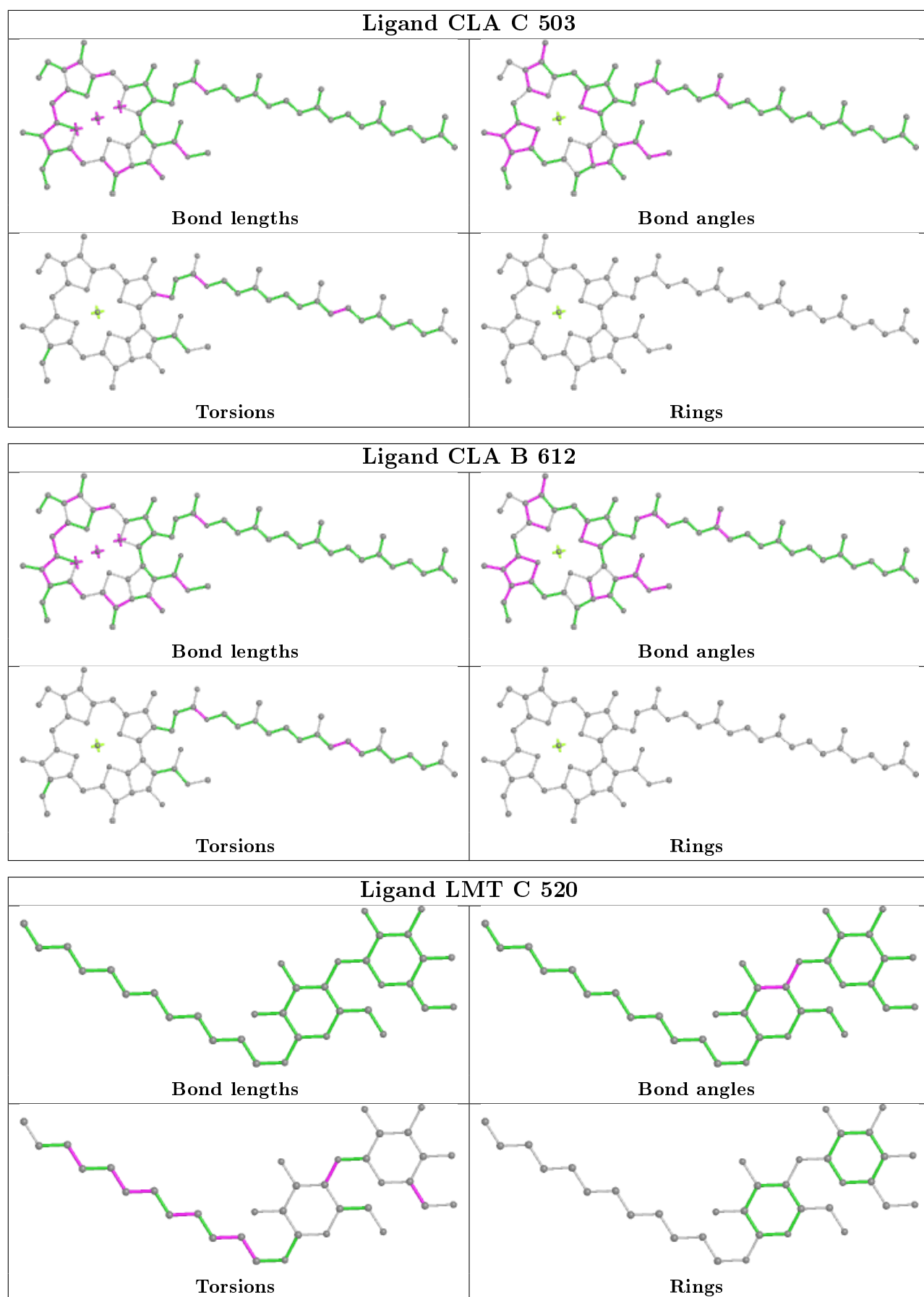
There are no ring outliers.

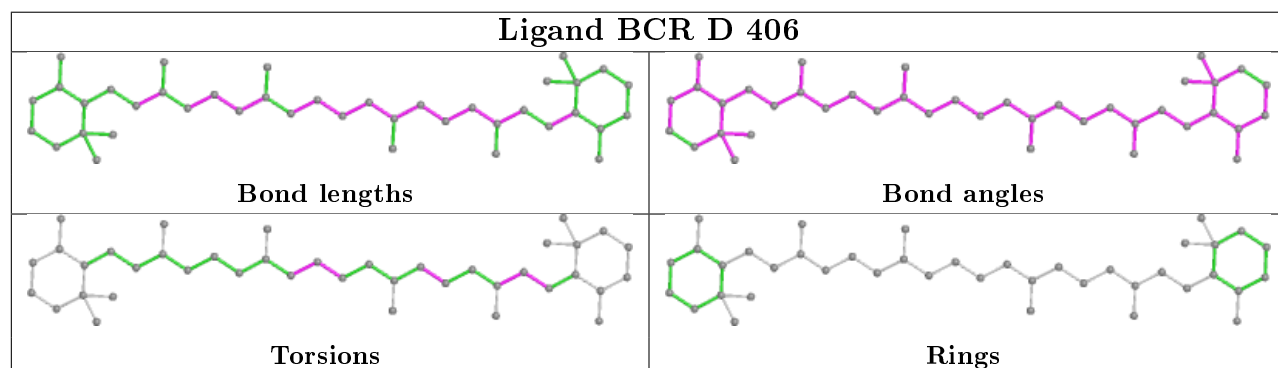
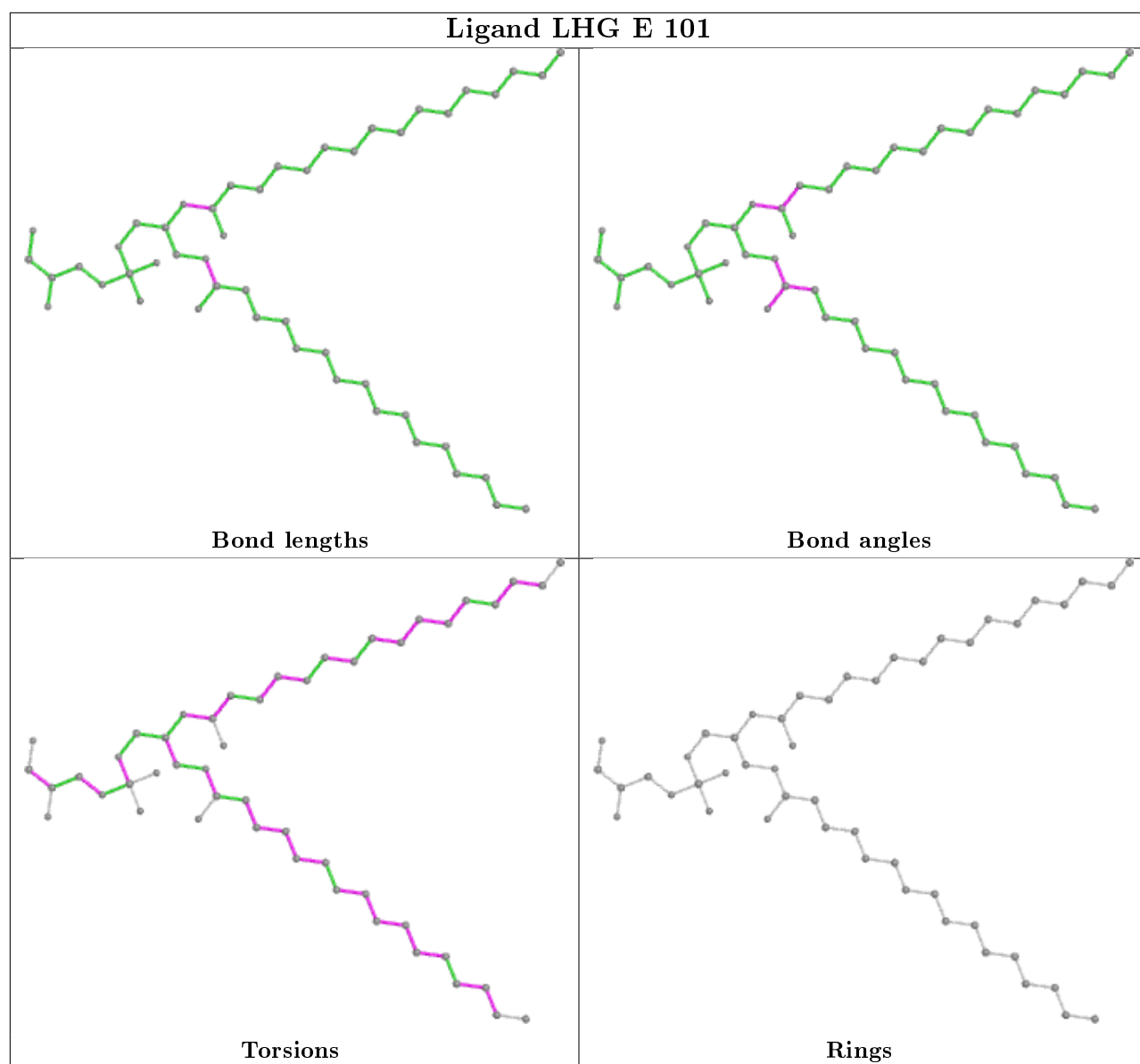
No monomer is involved in short contacts.

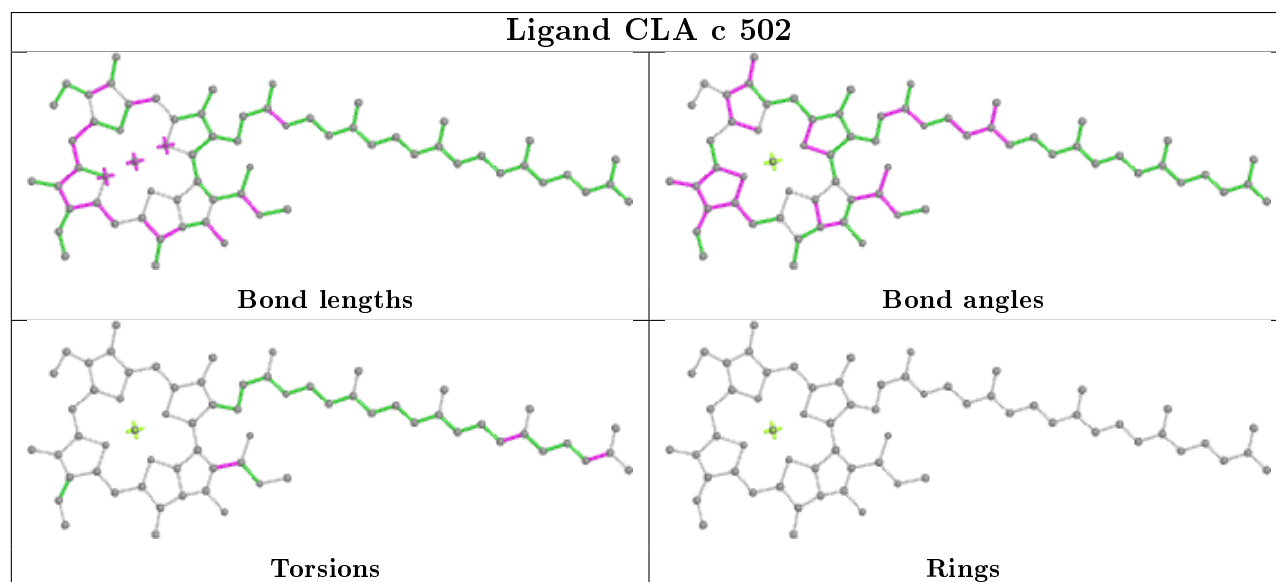
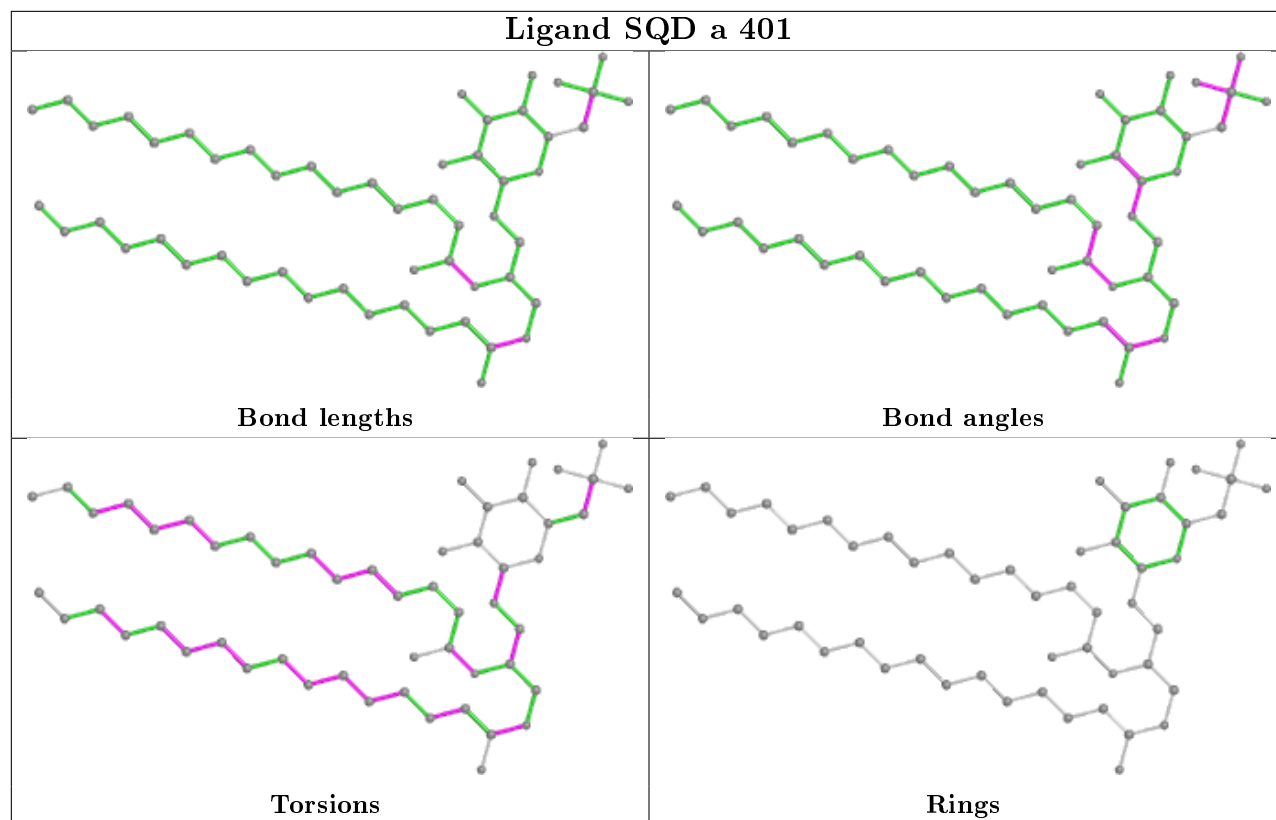
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

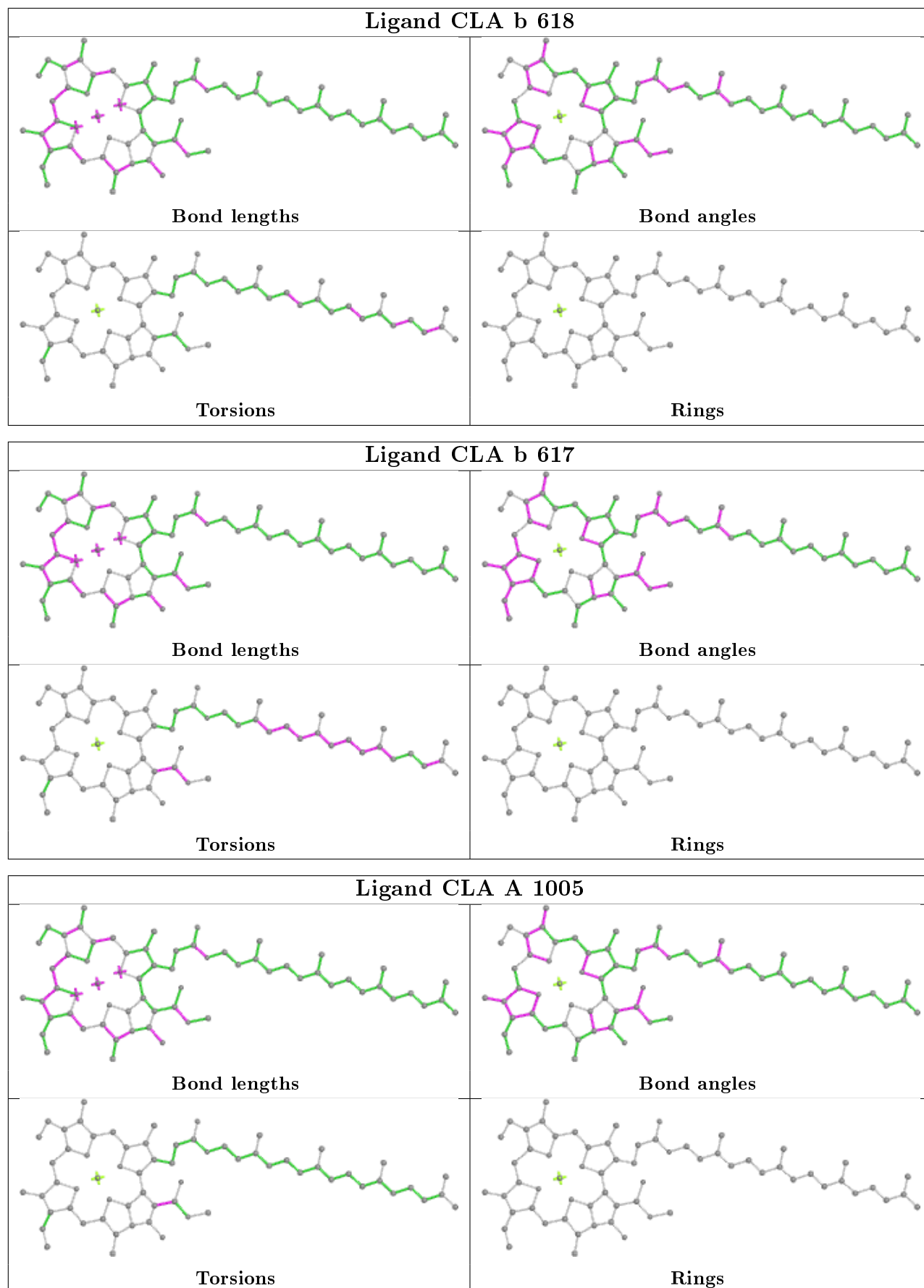




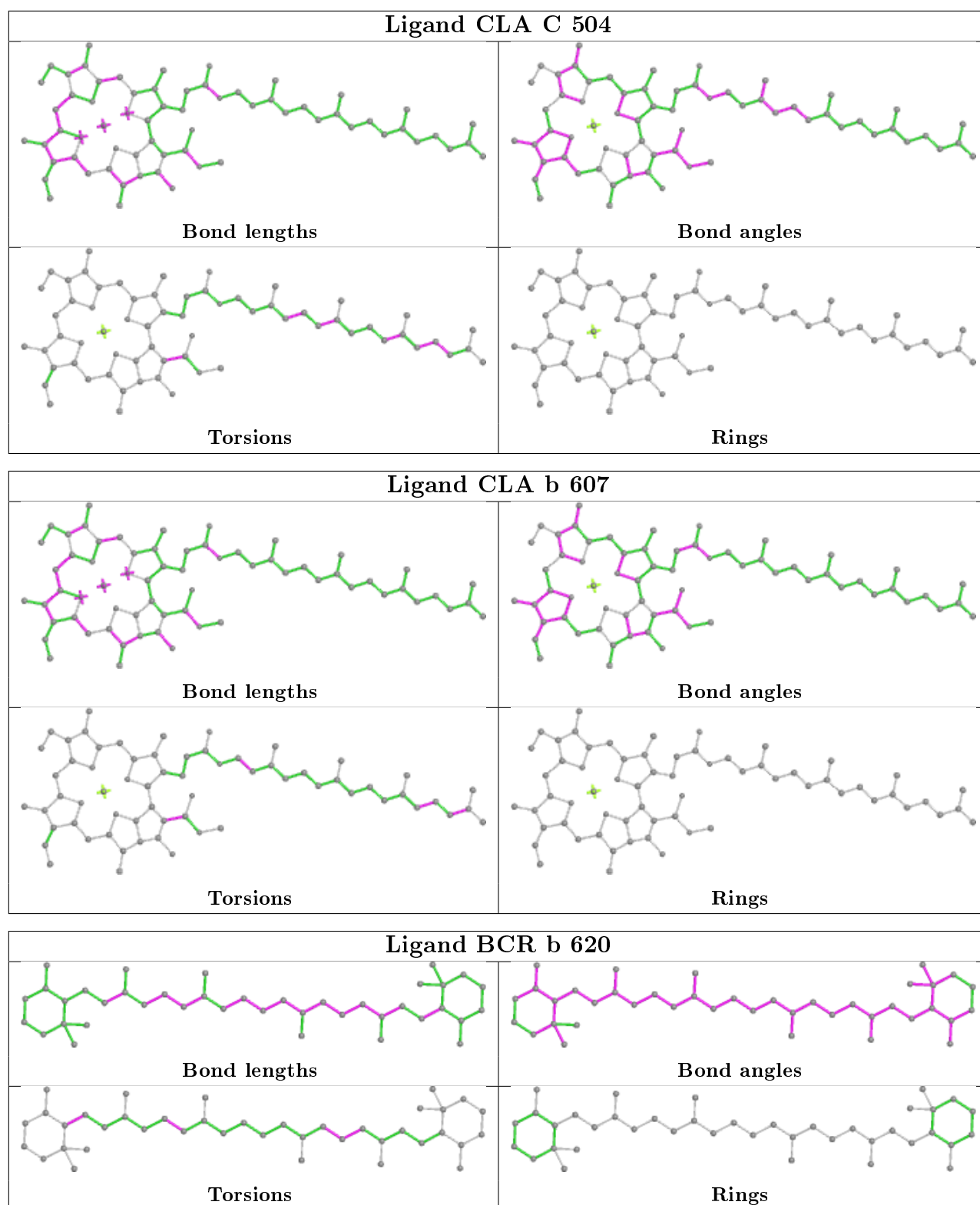


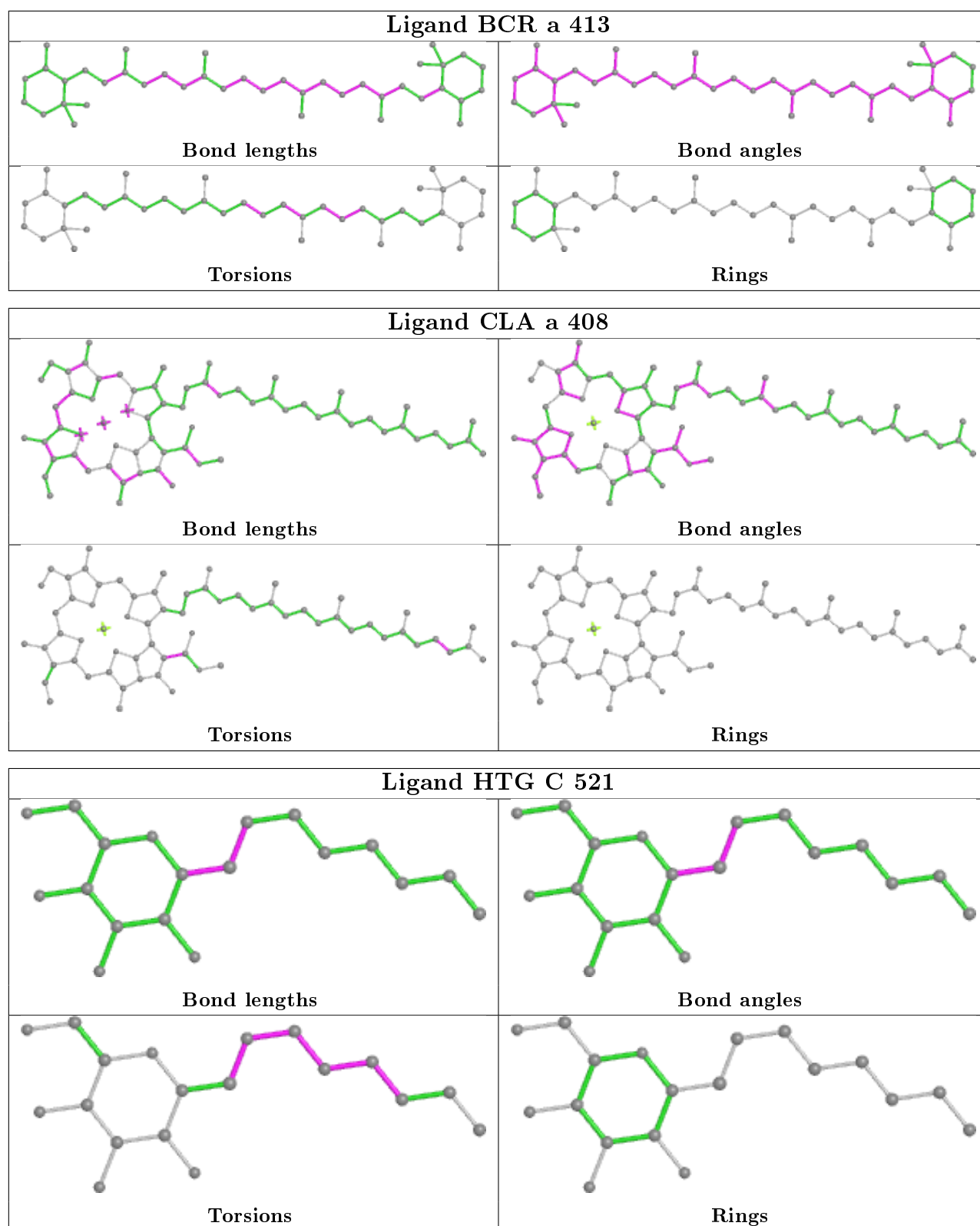


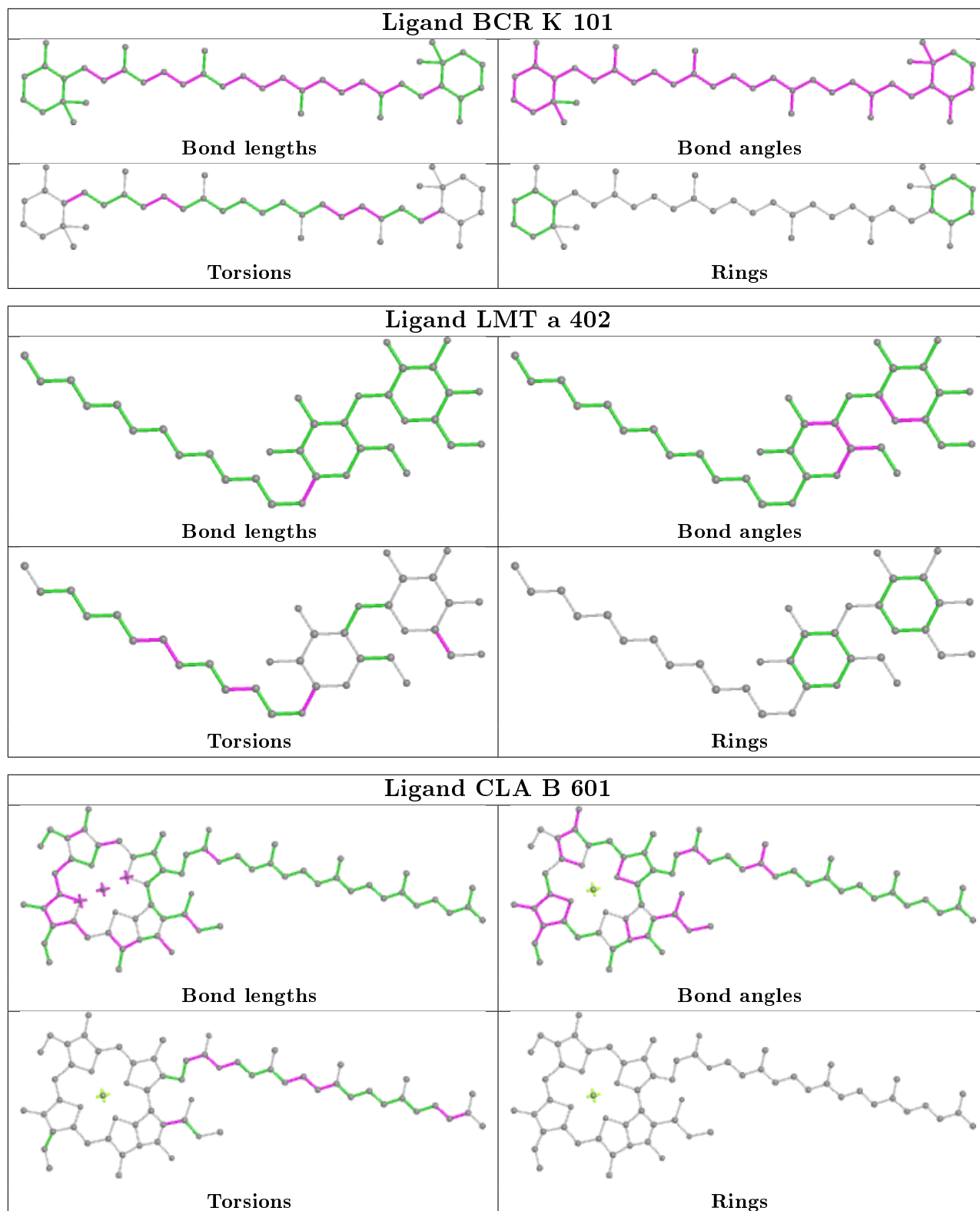


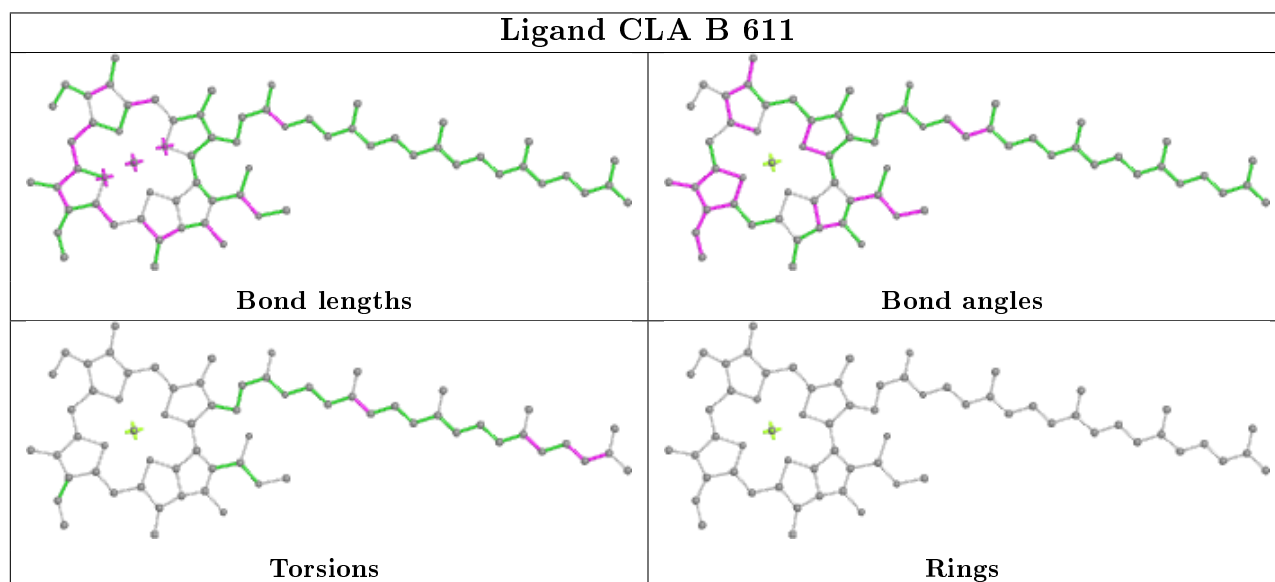
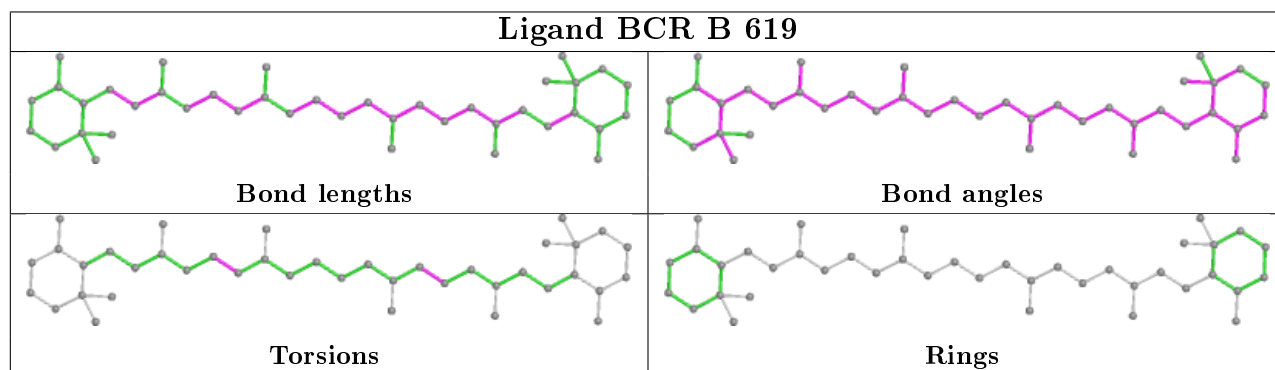
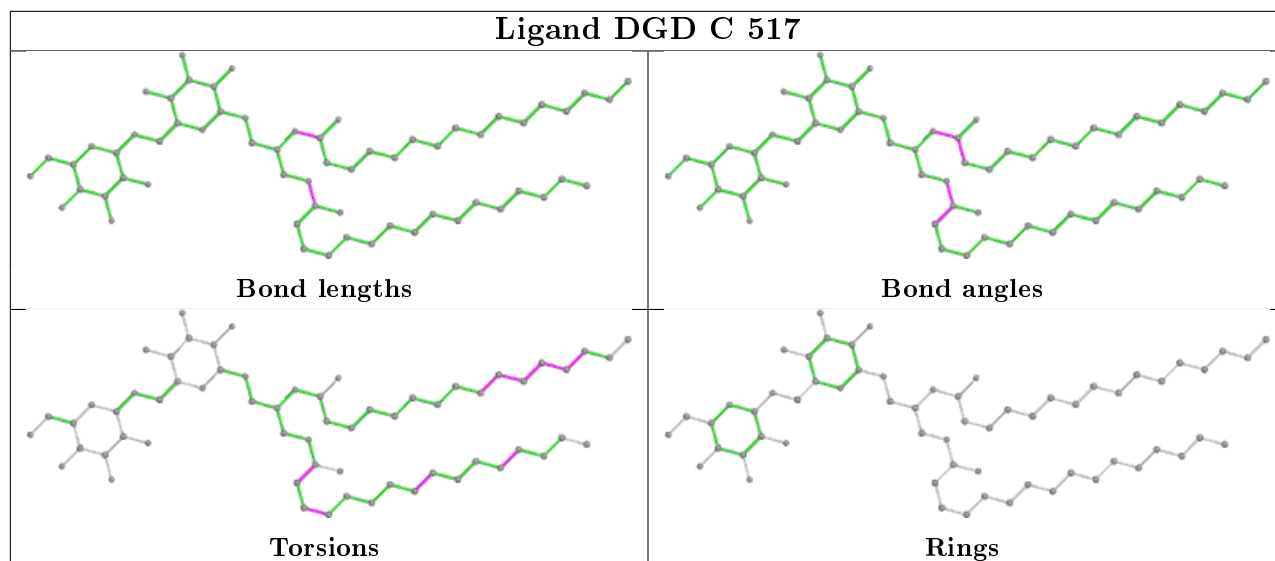


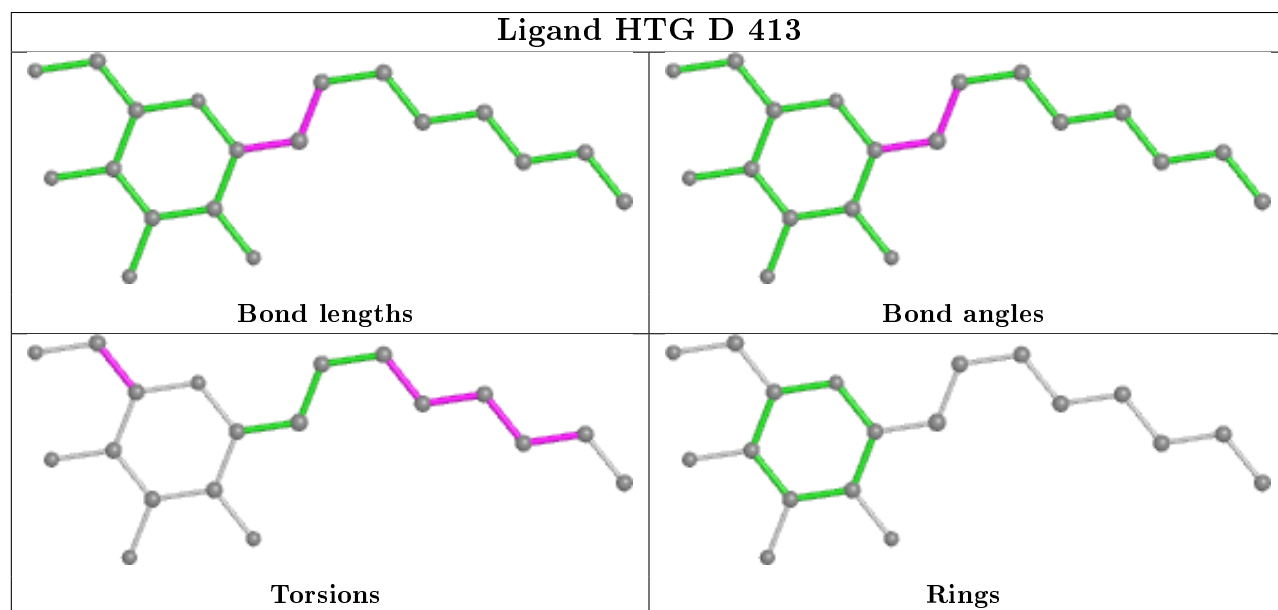
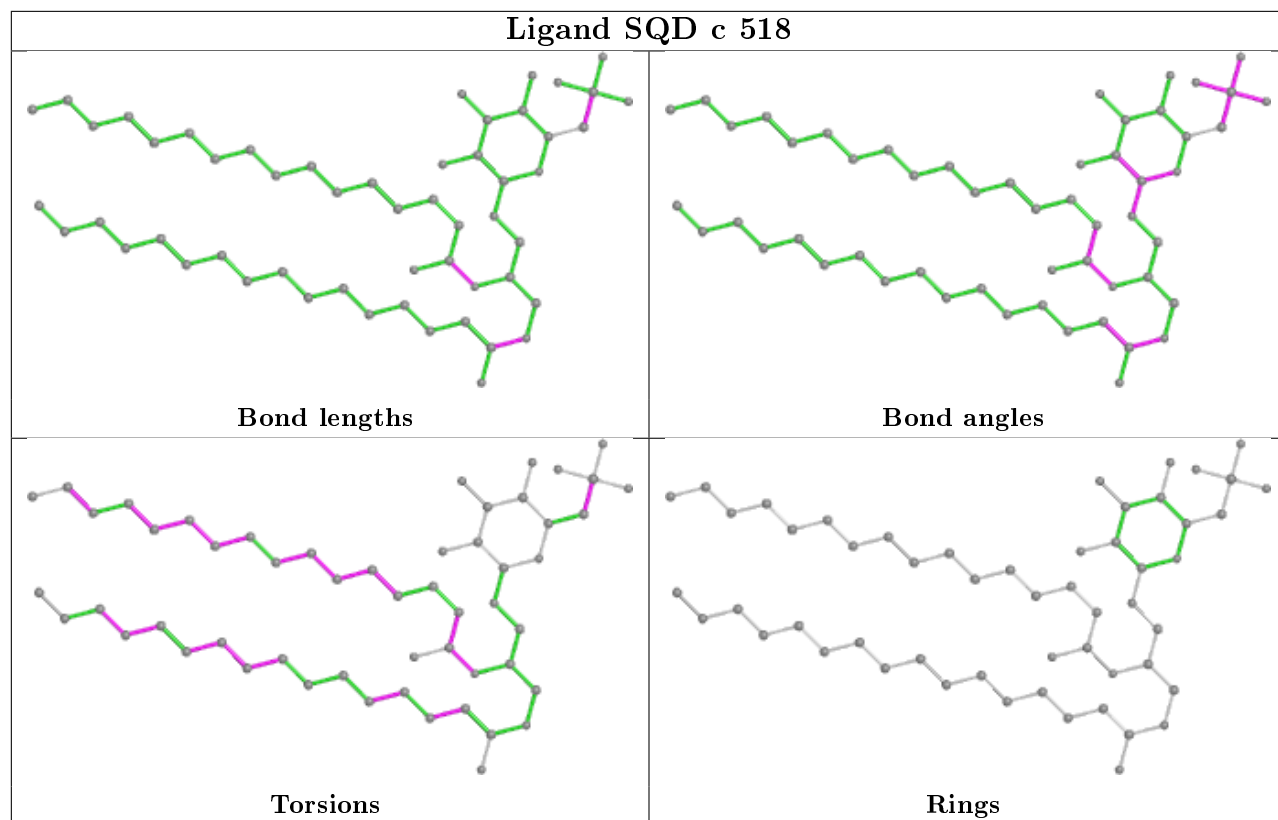


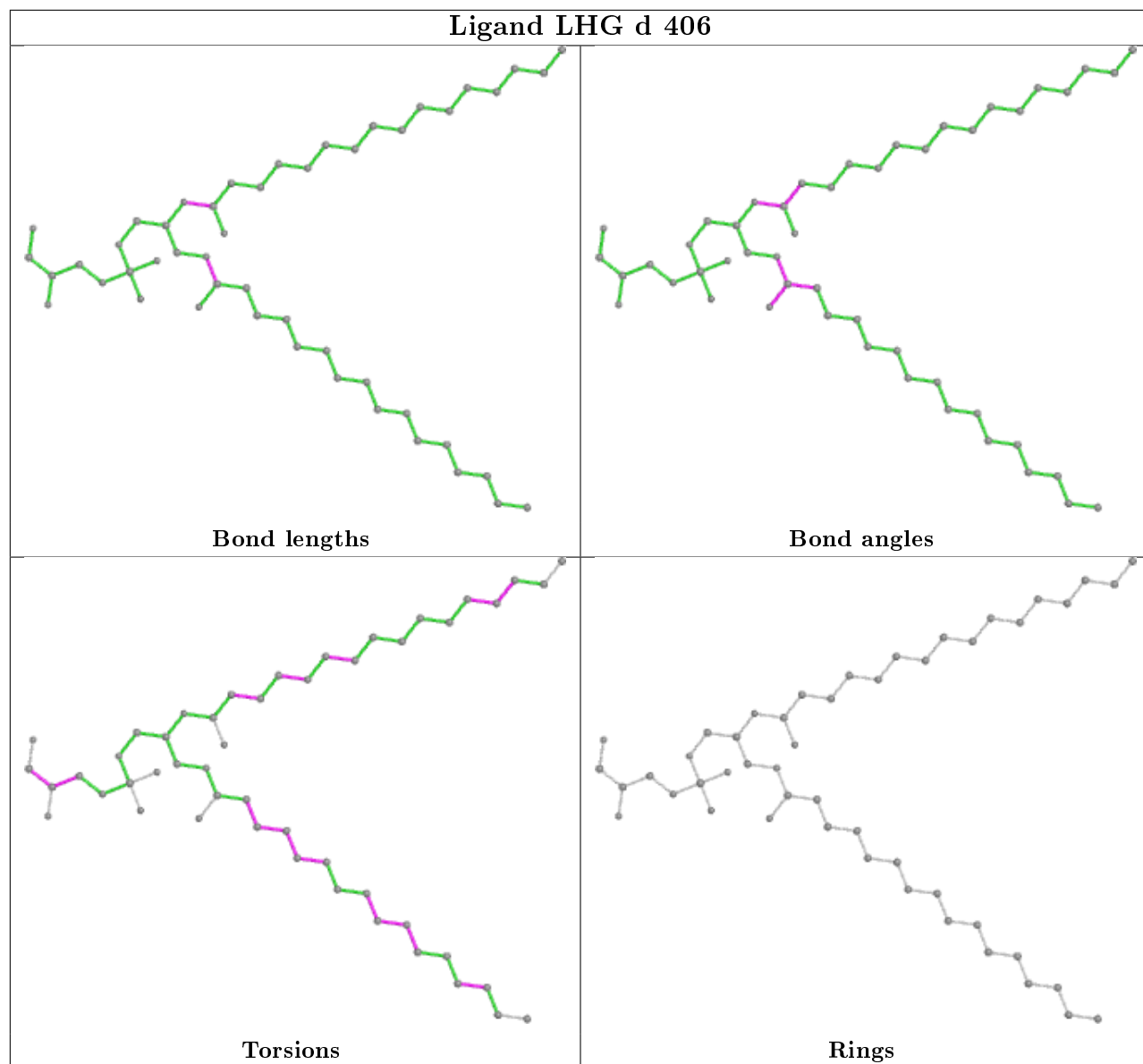


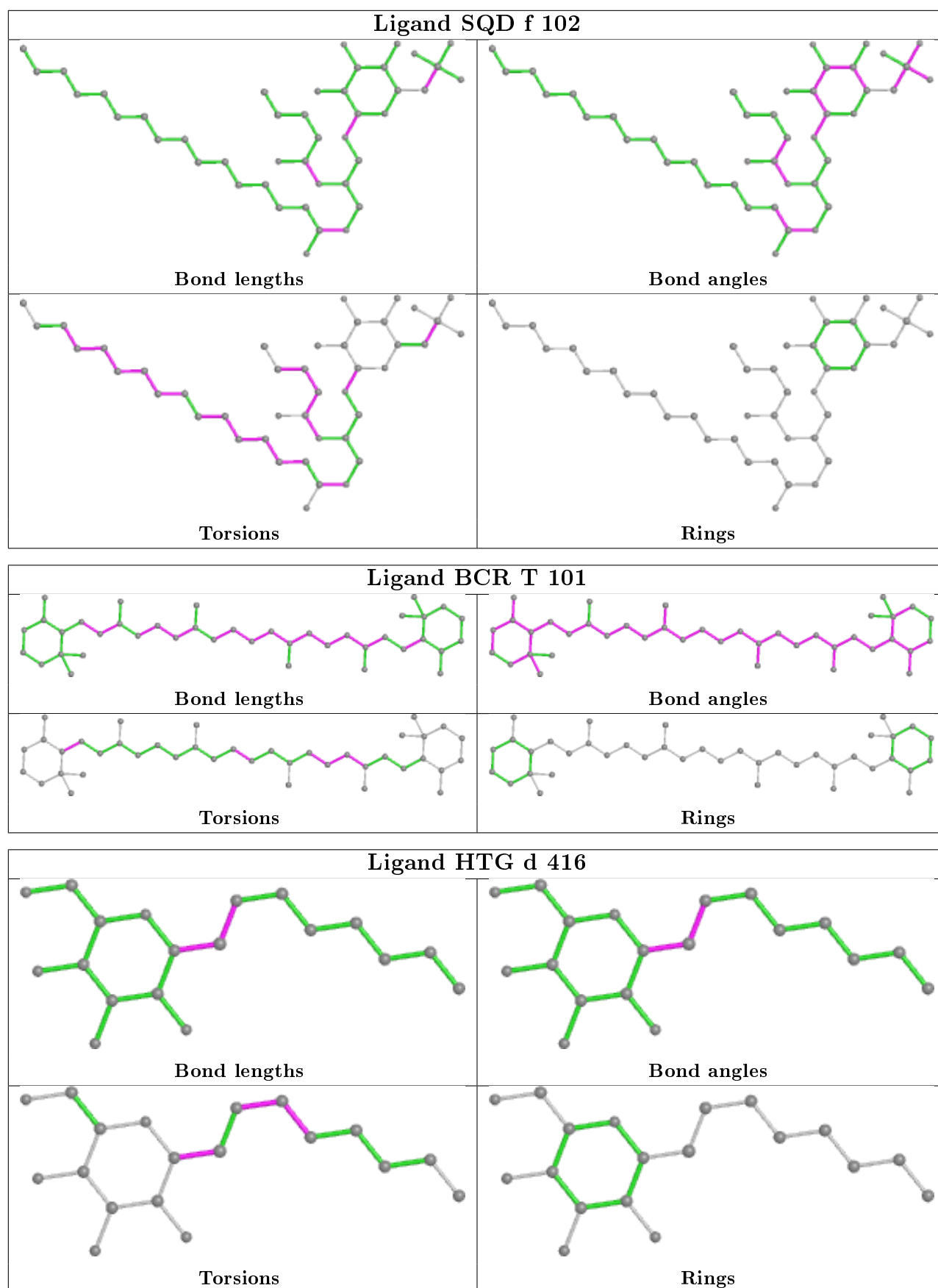


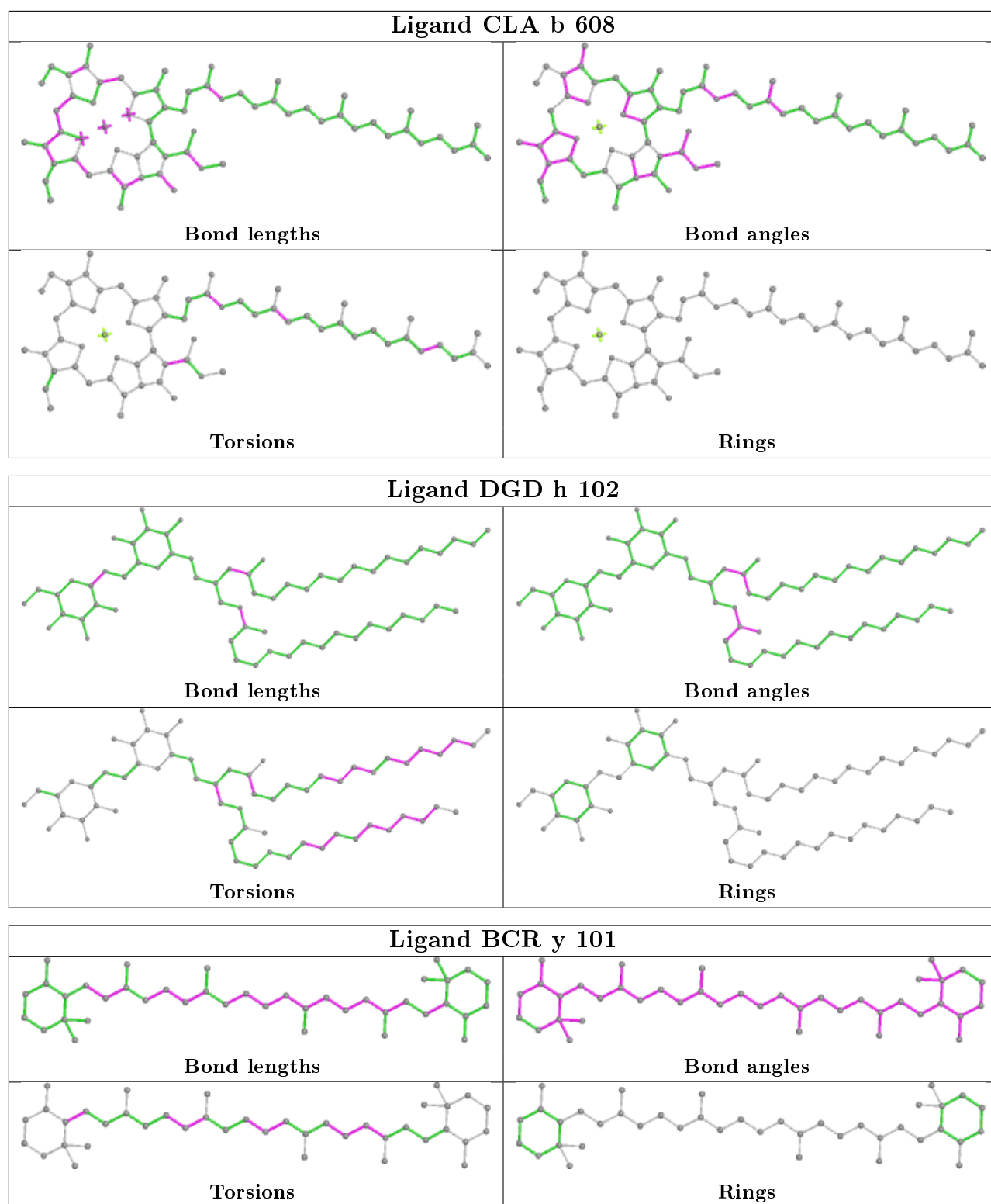




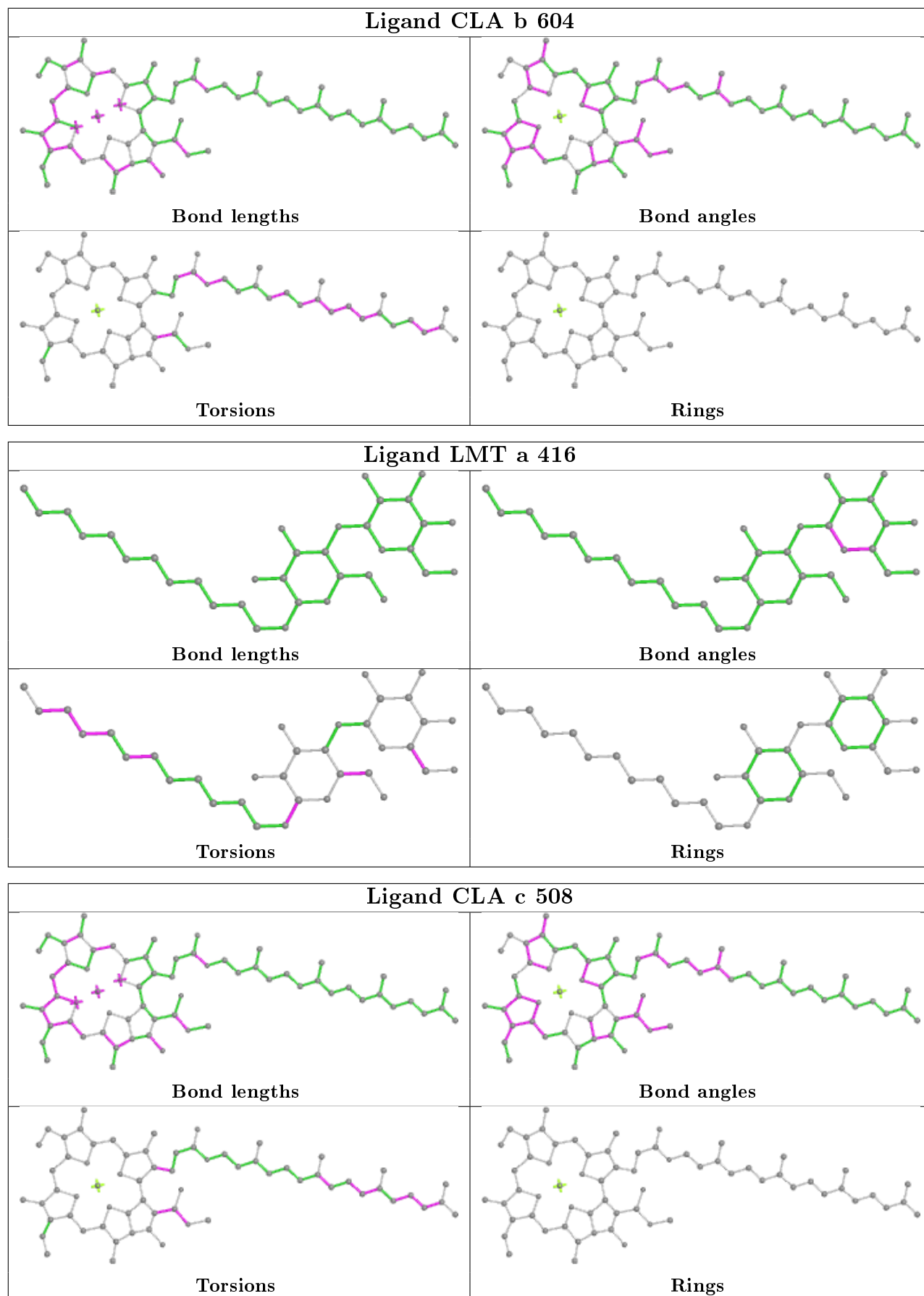


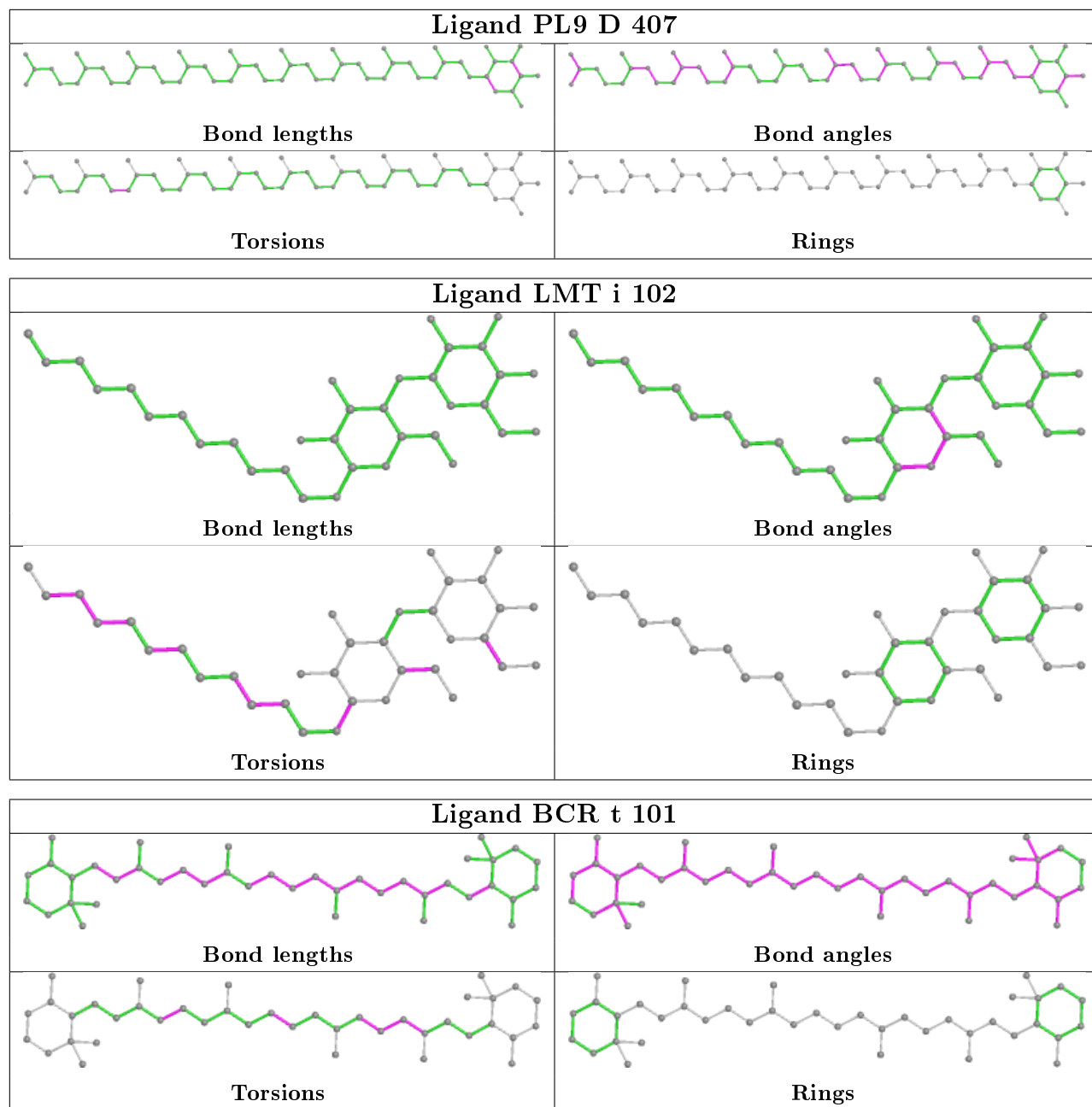


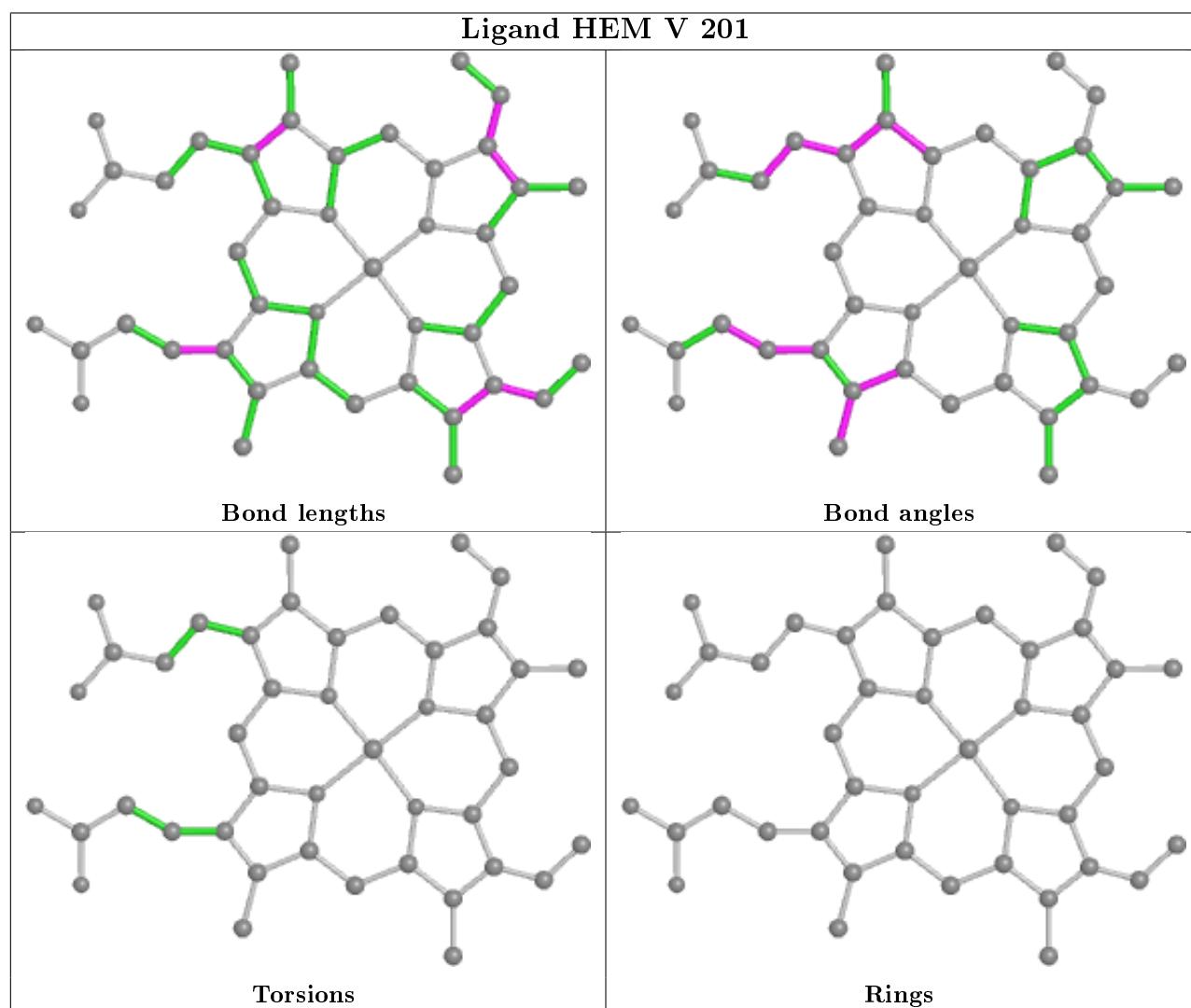
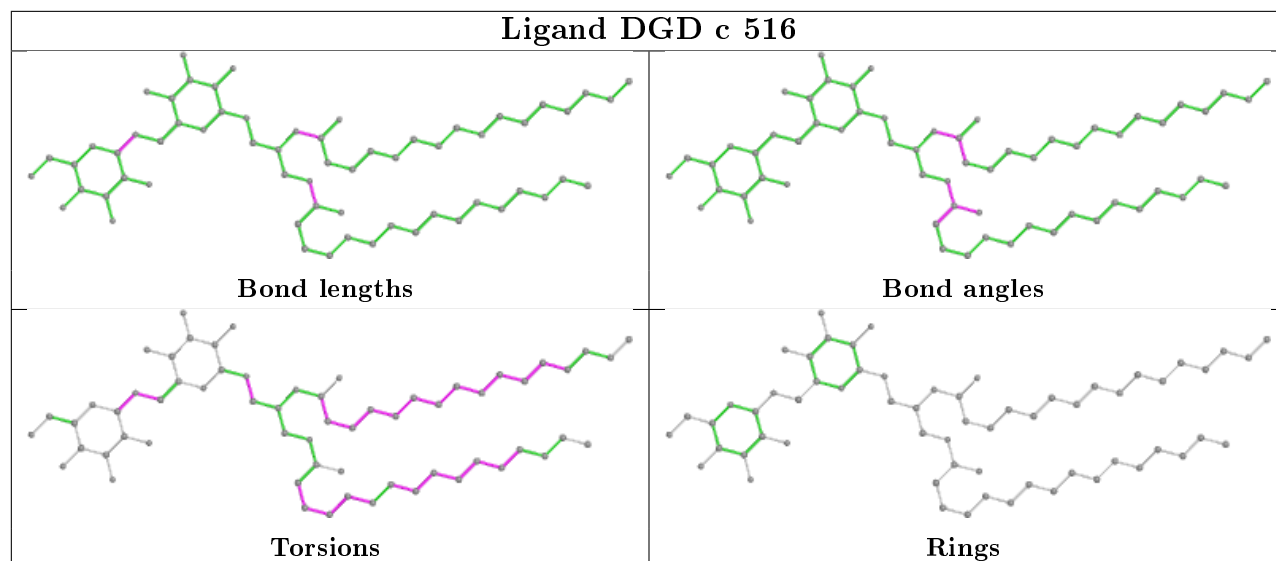


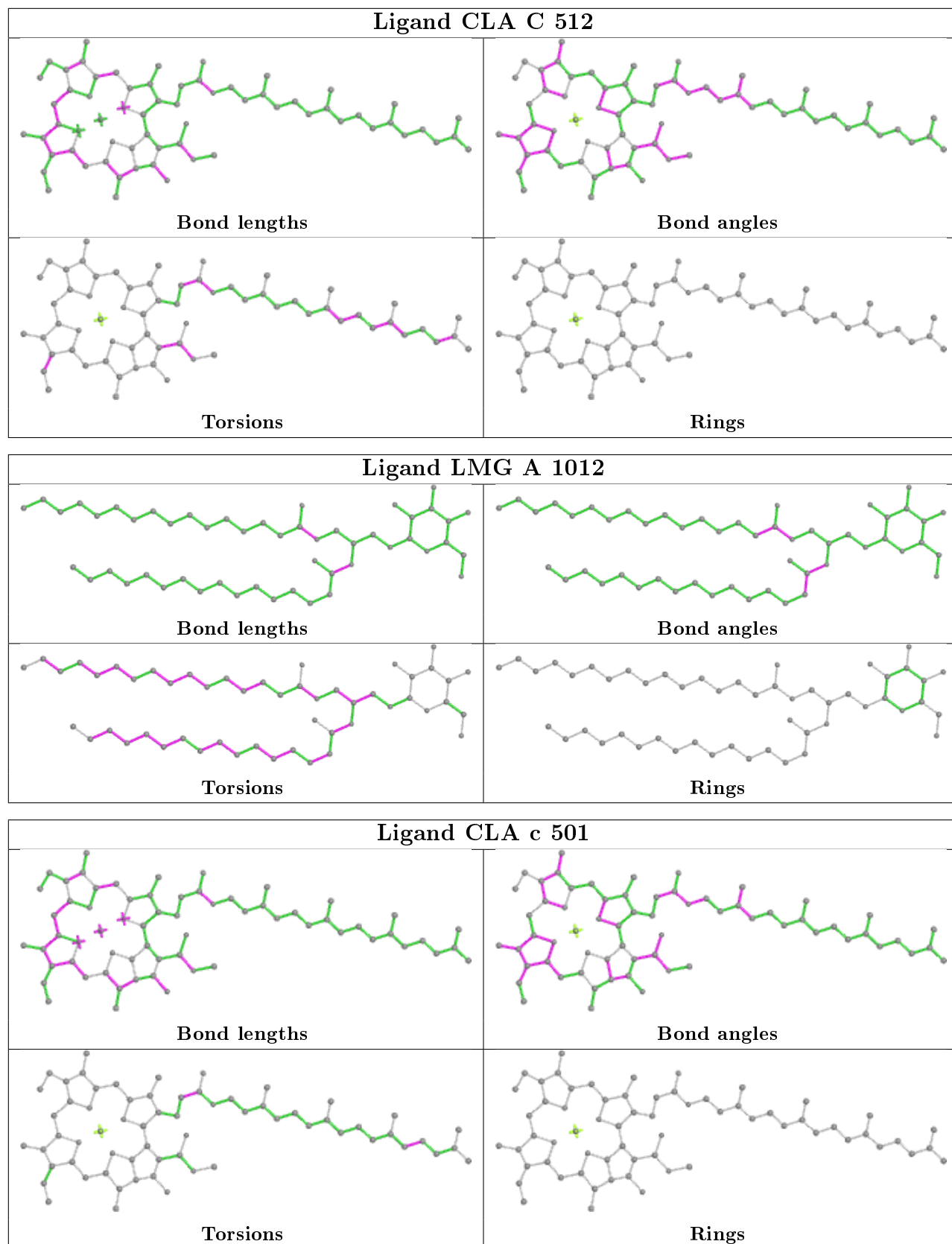


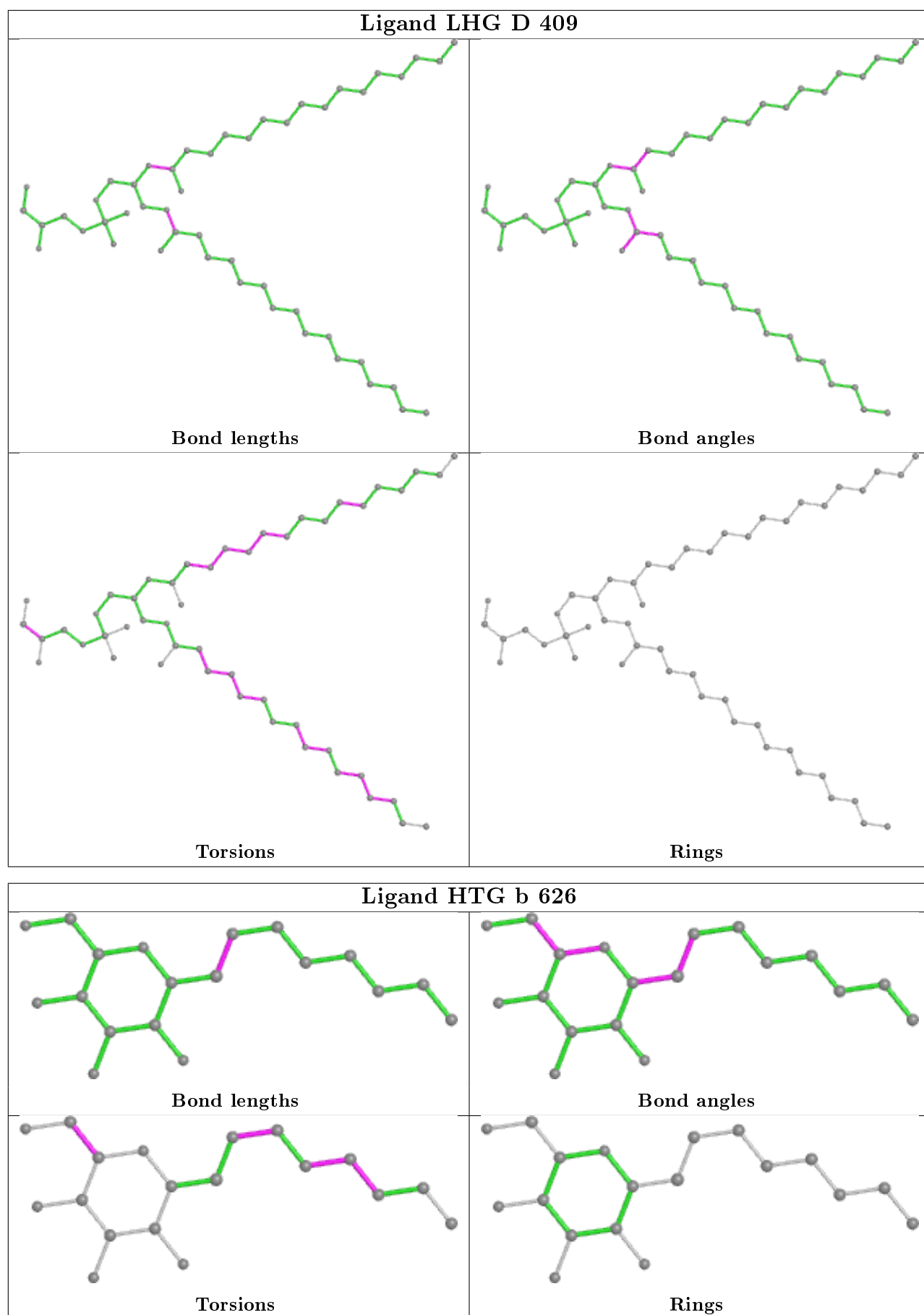


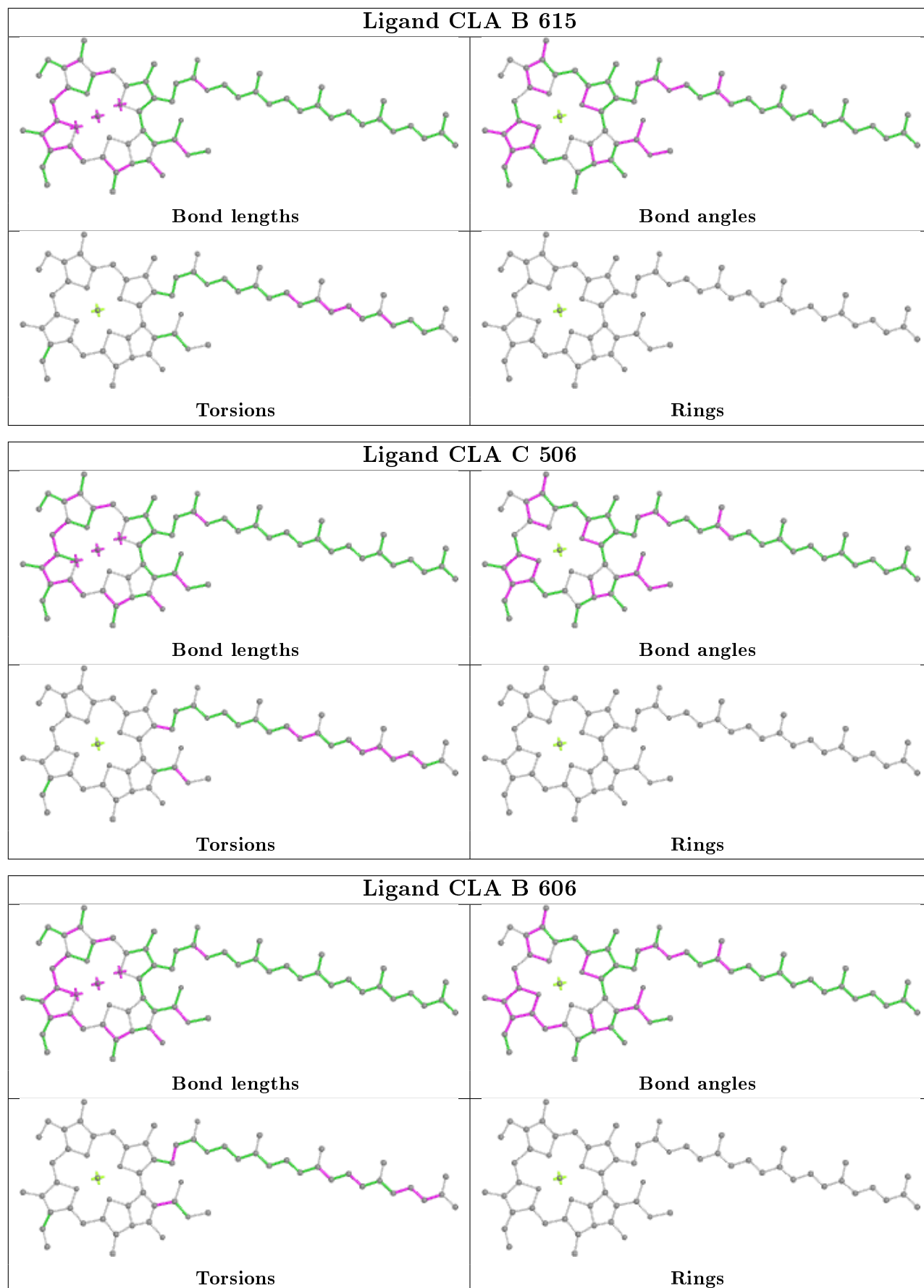


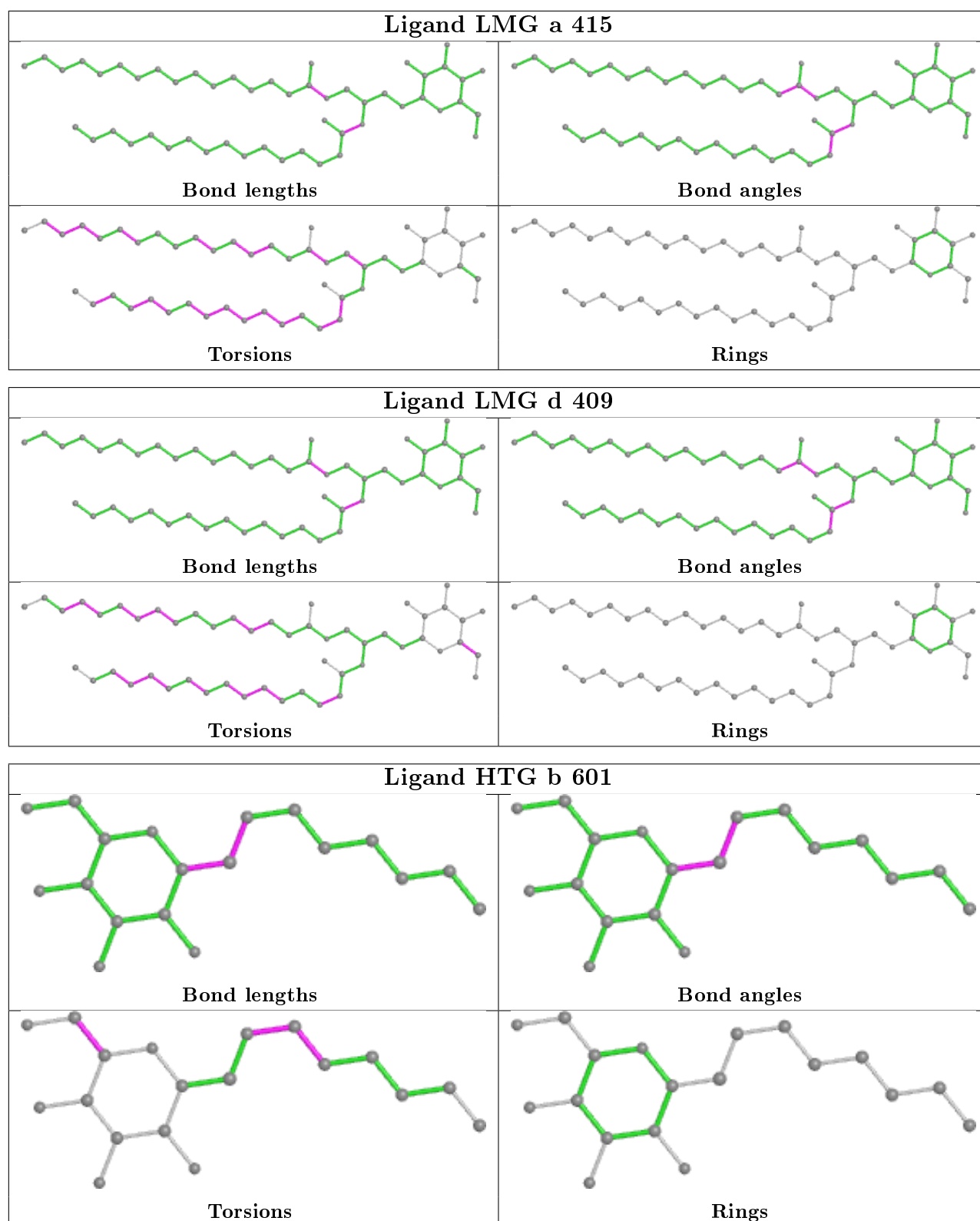


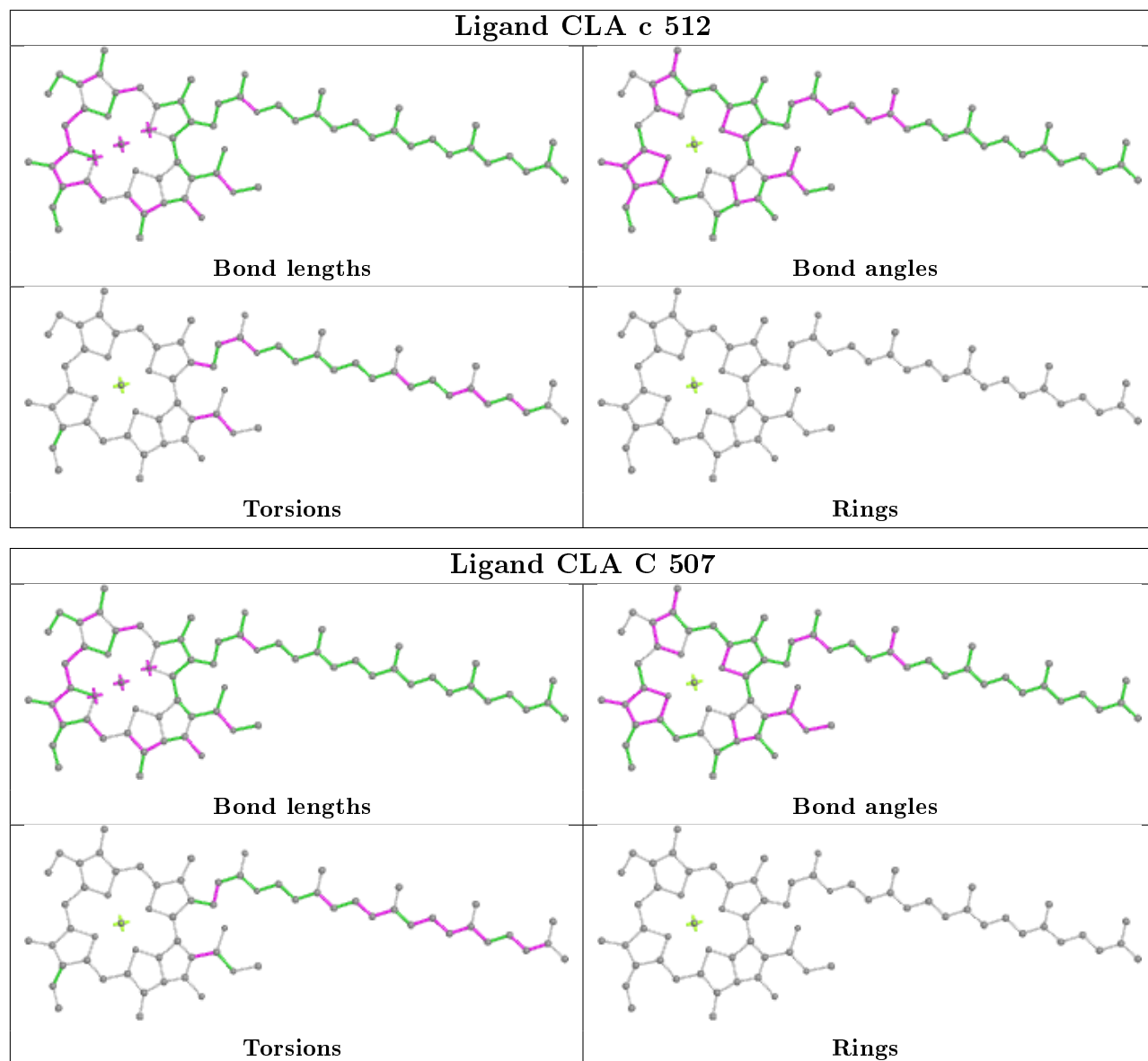




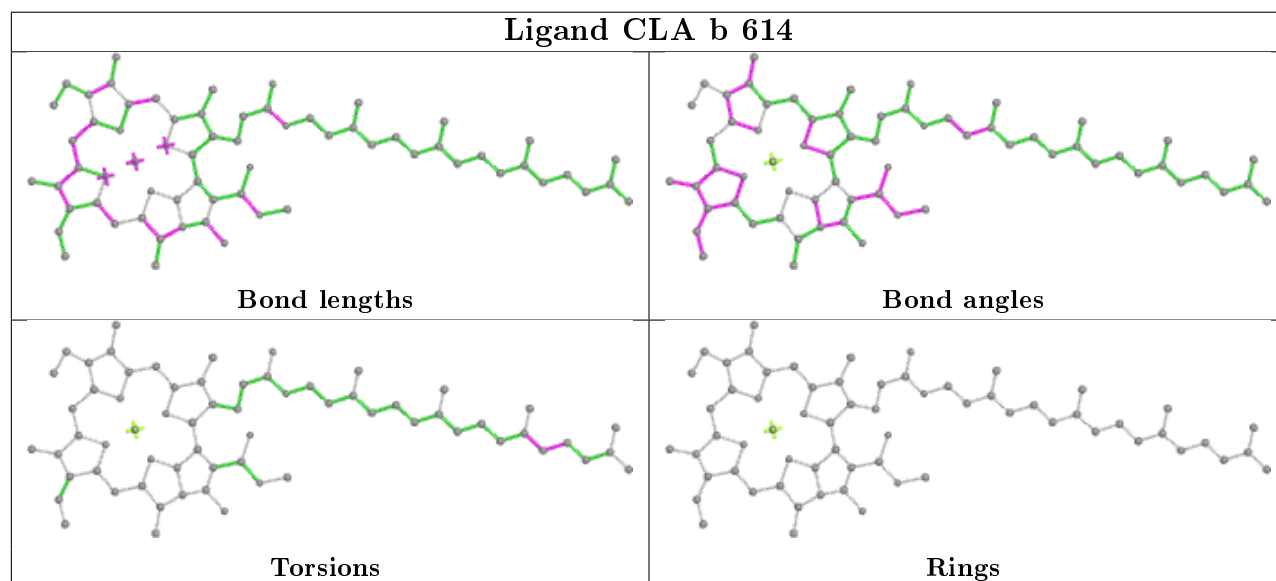
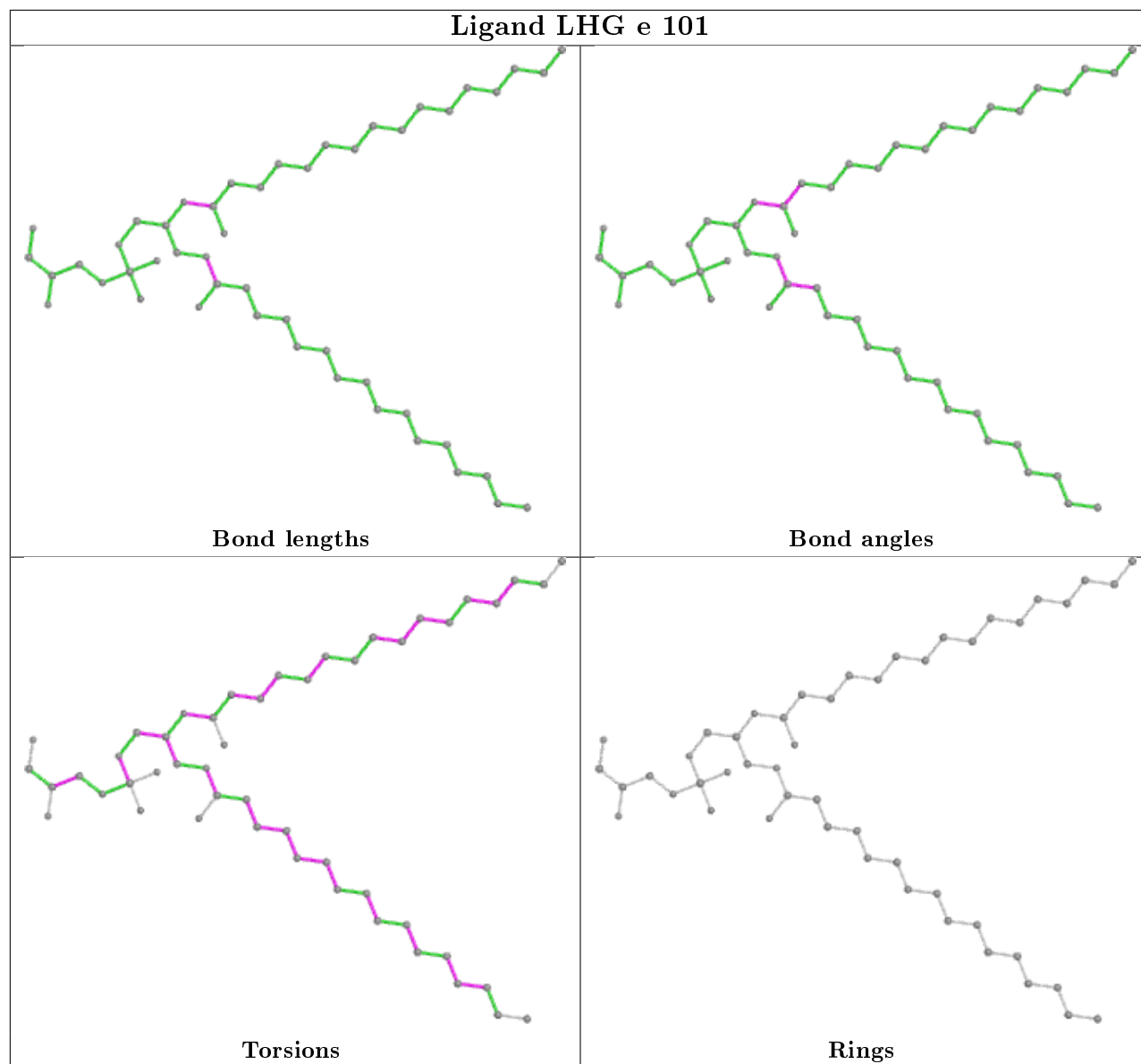


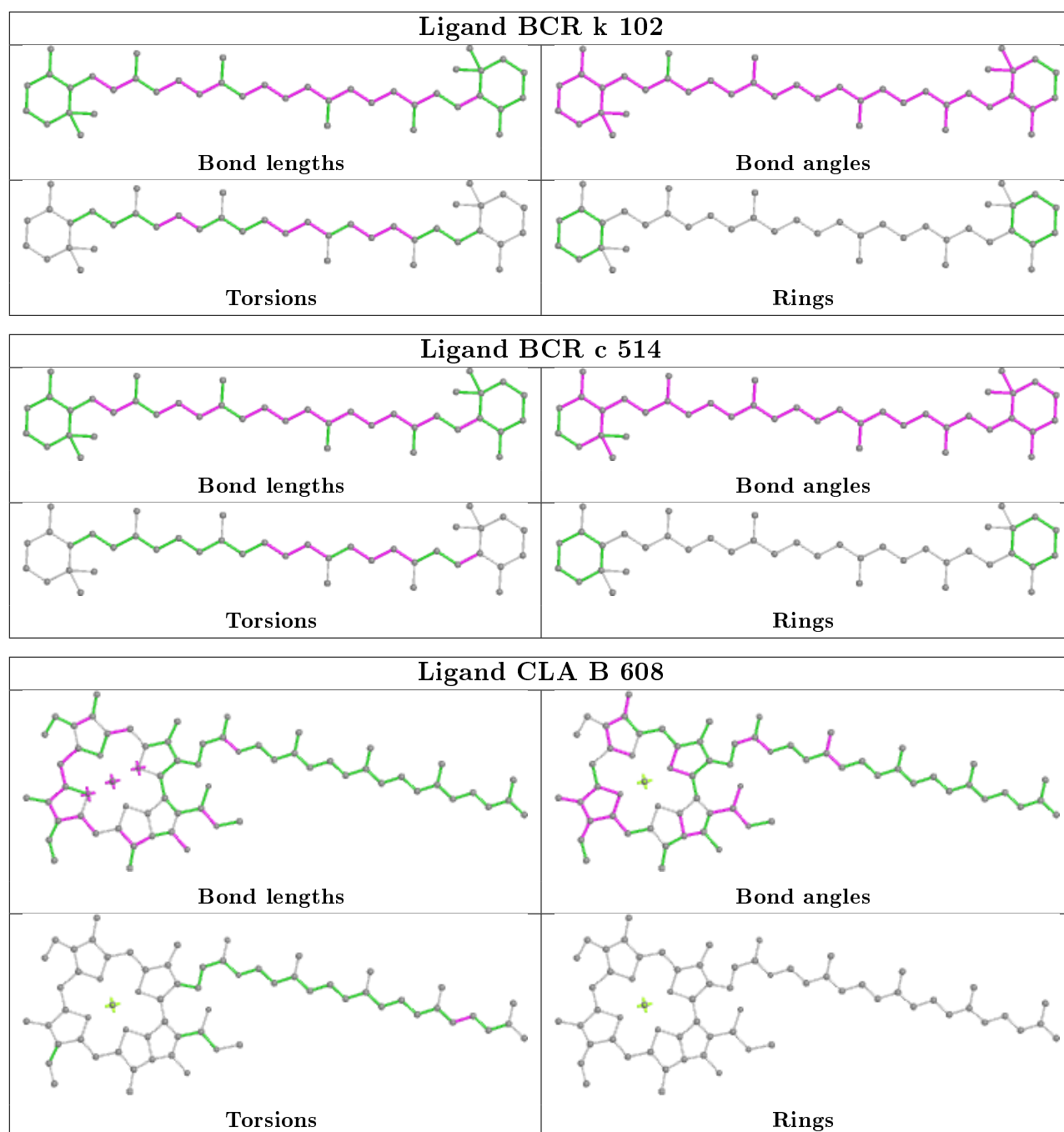


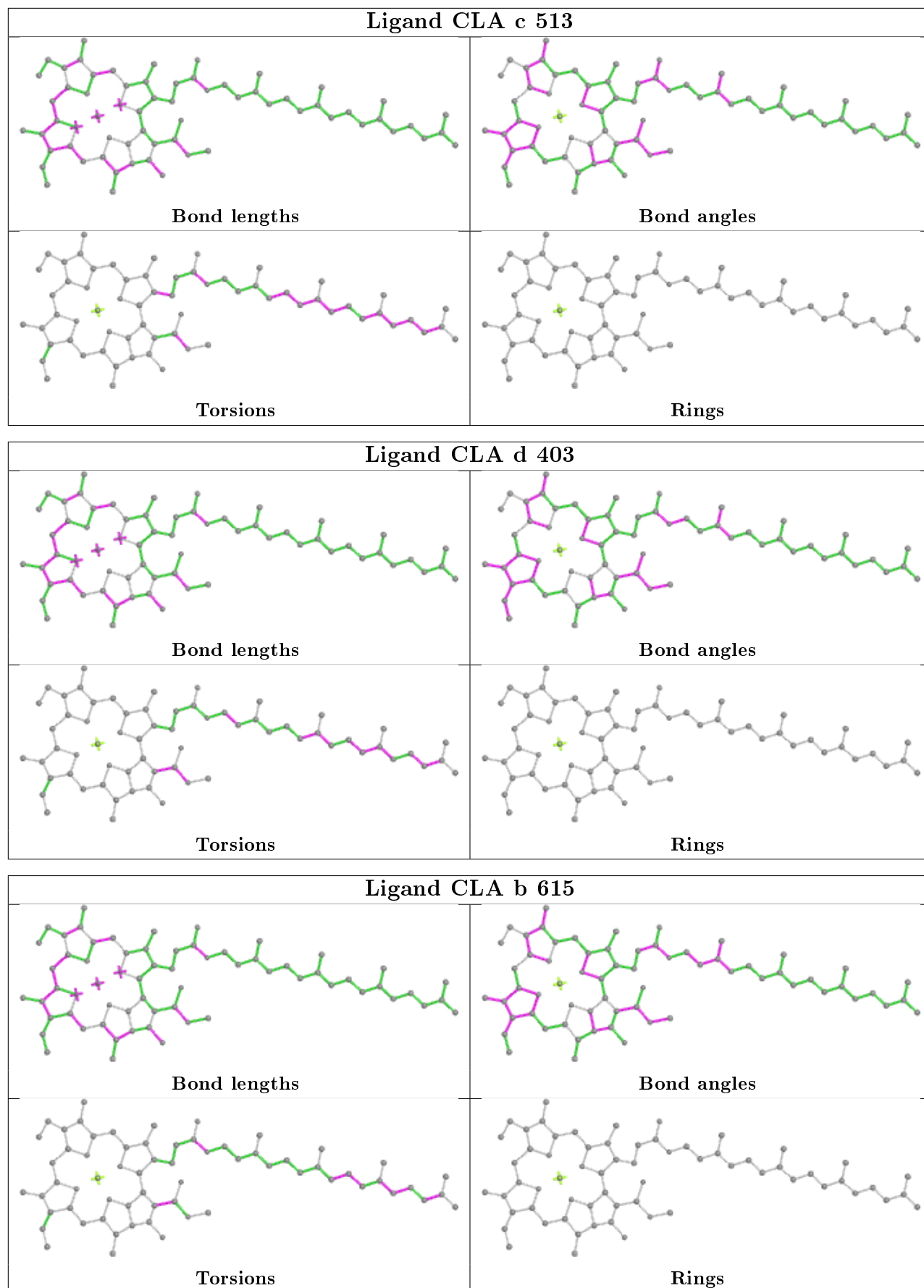


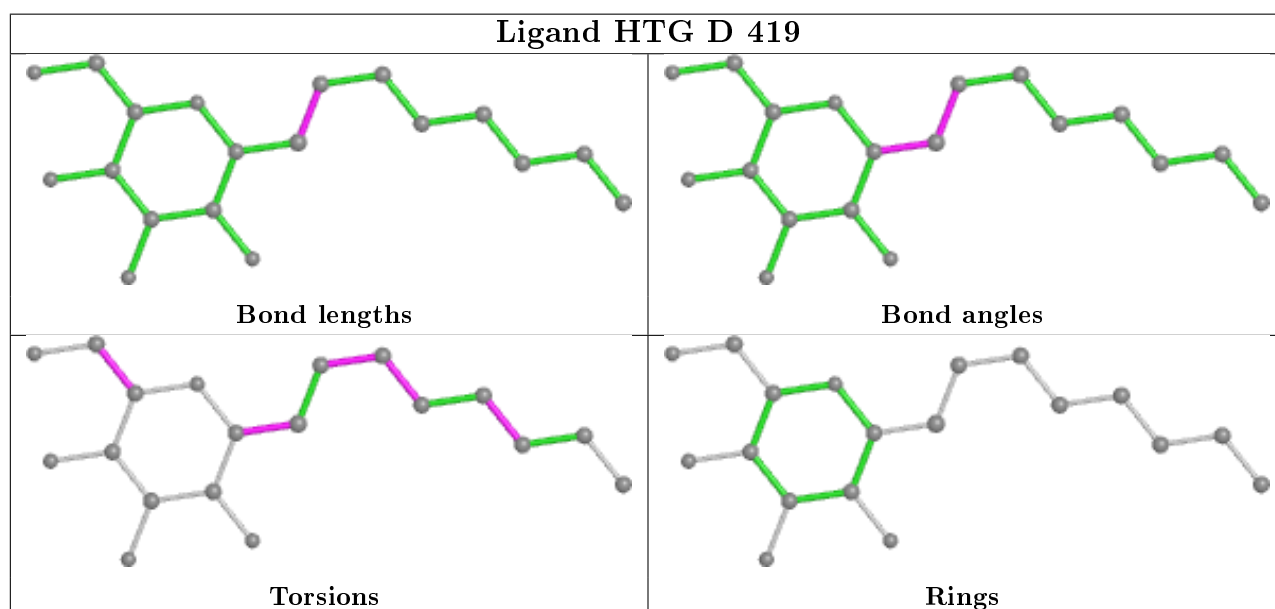
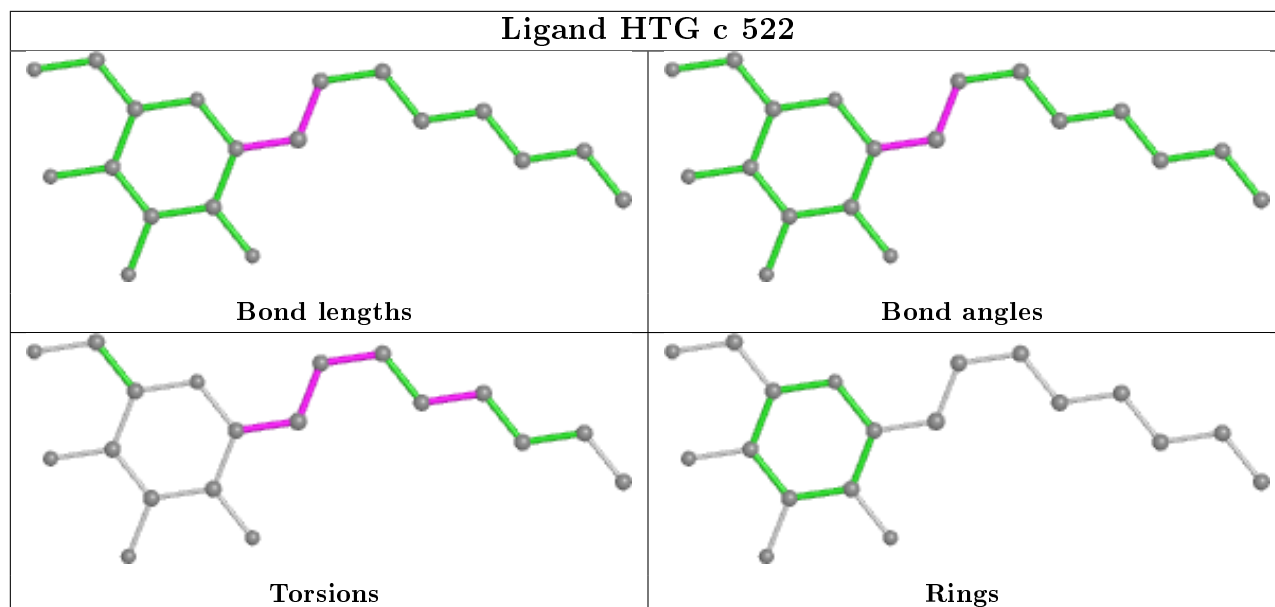


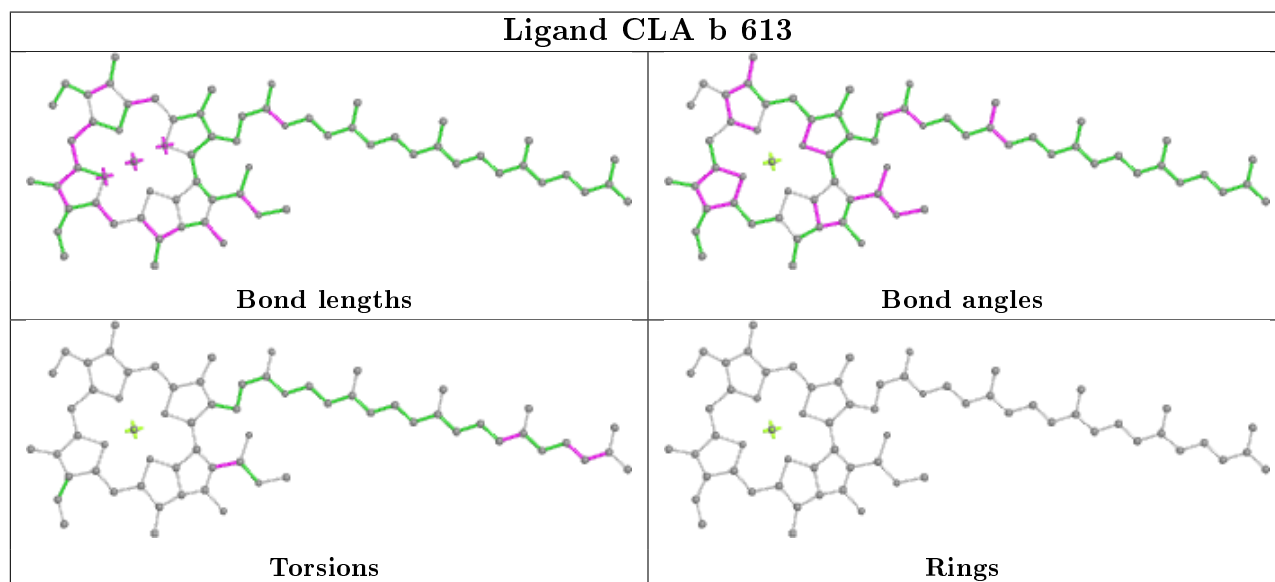
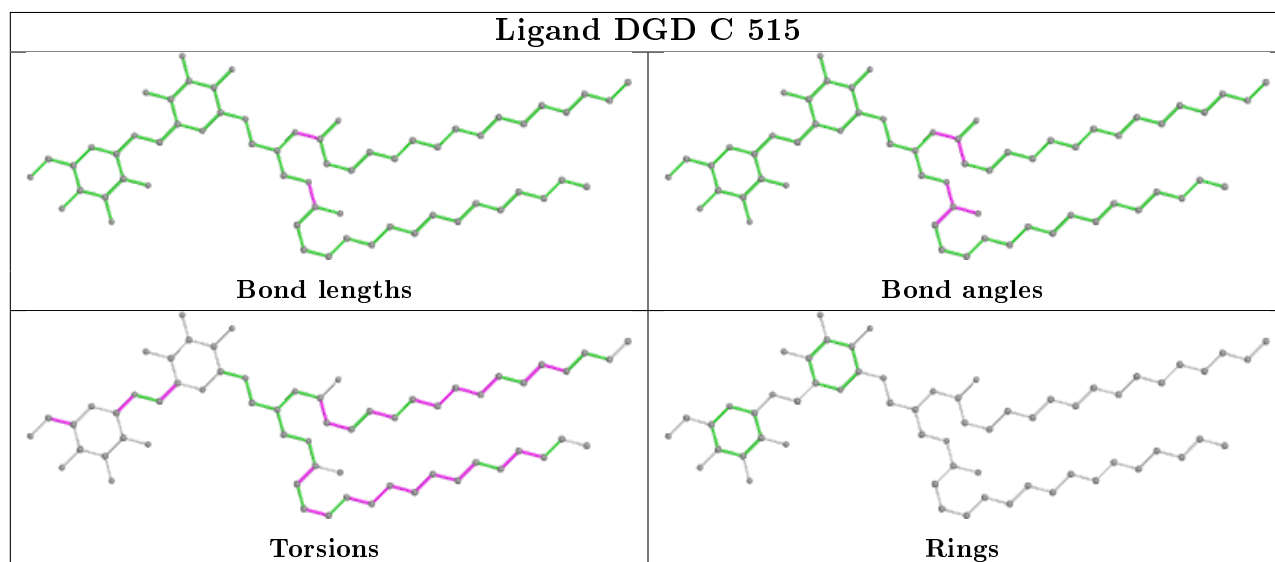
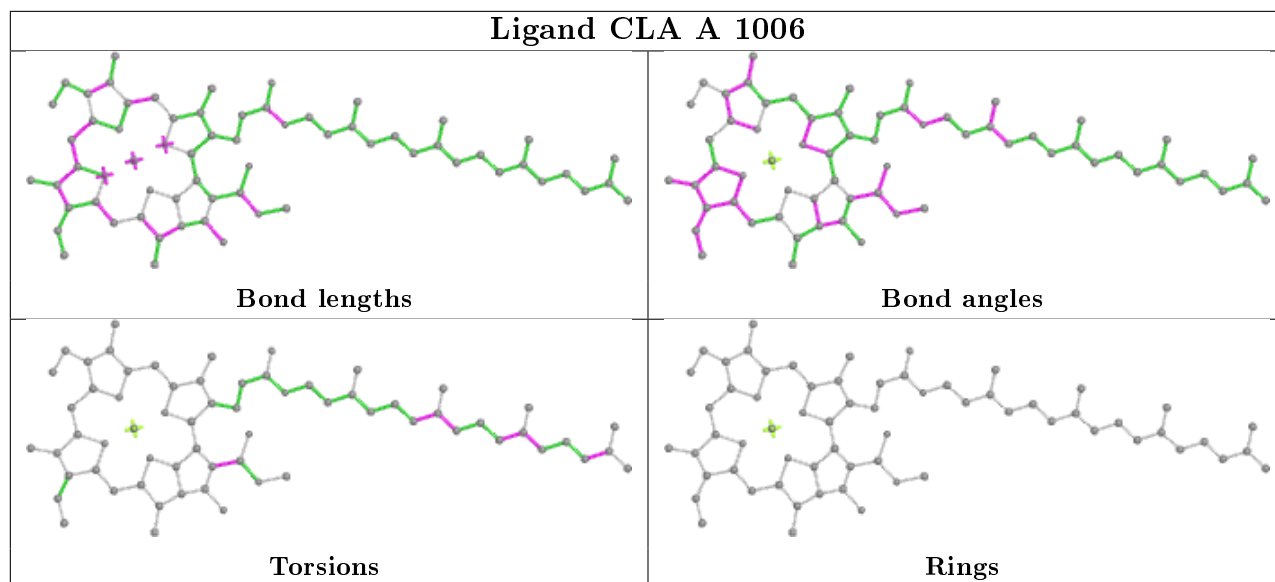


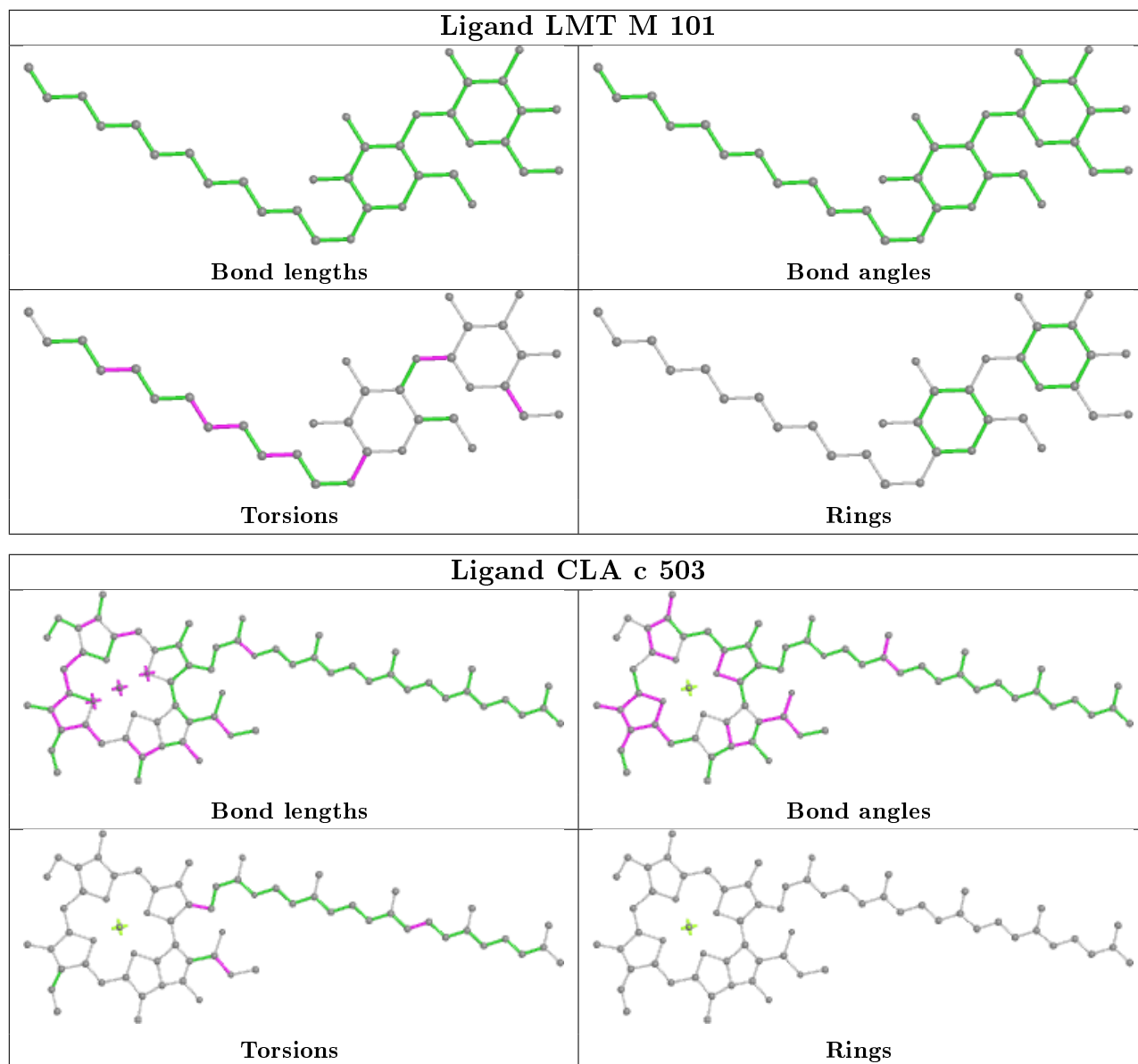


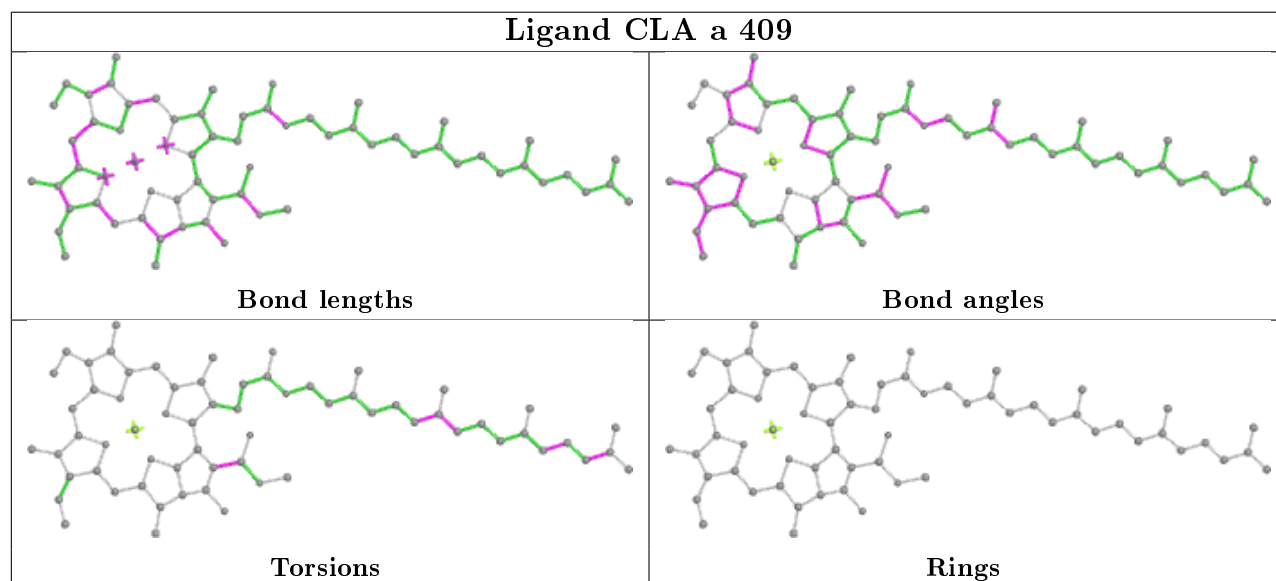
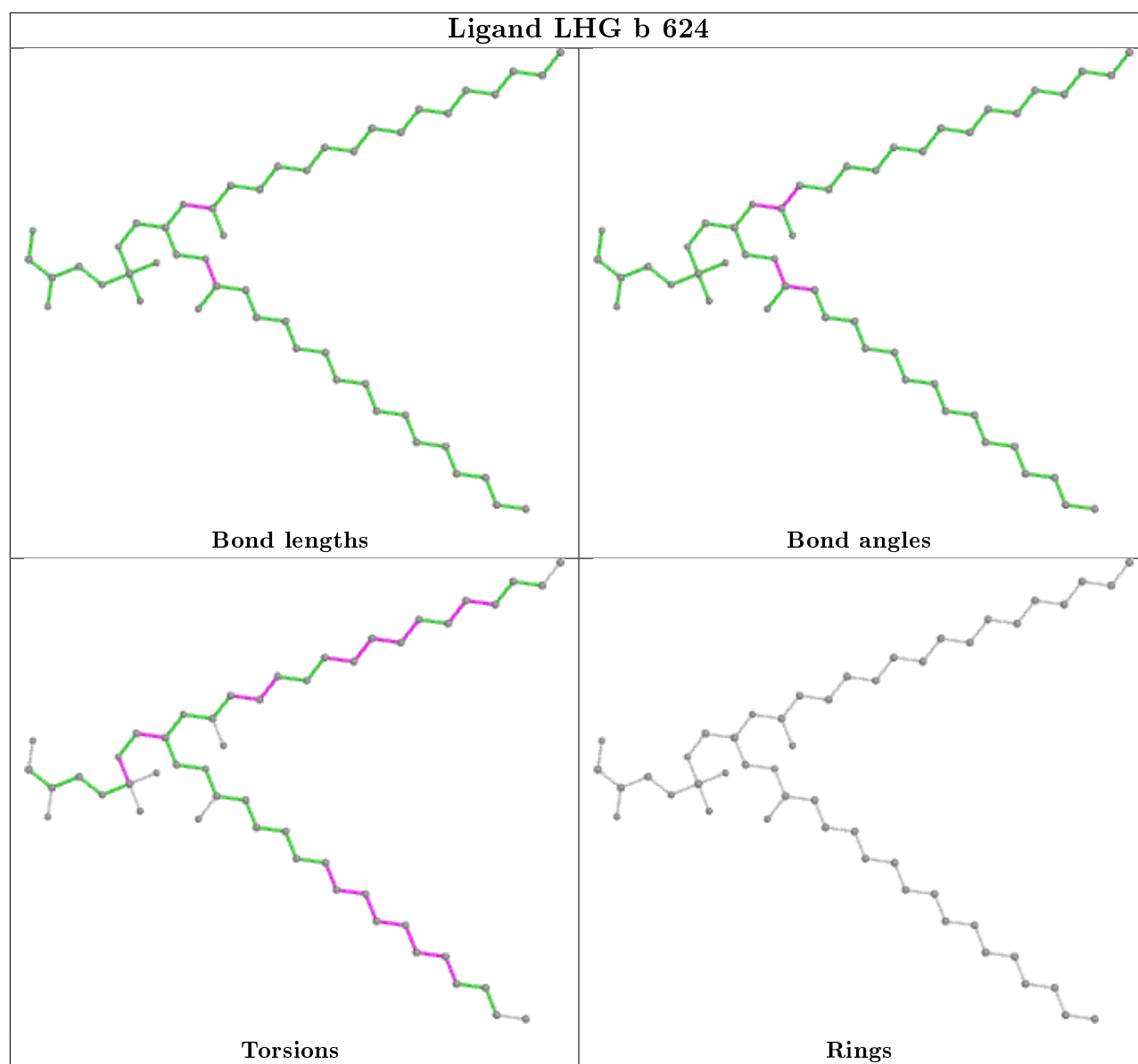


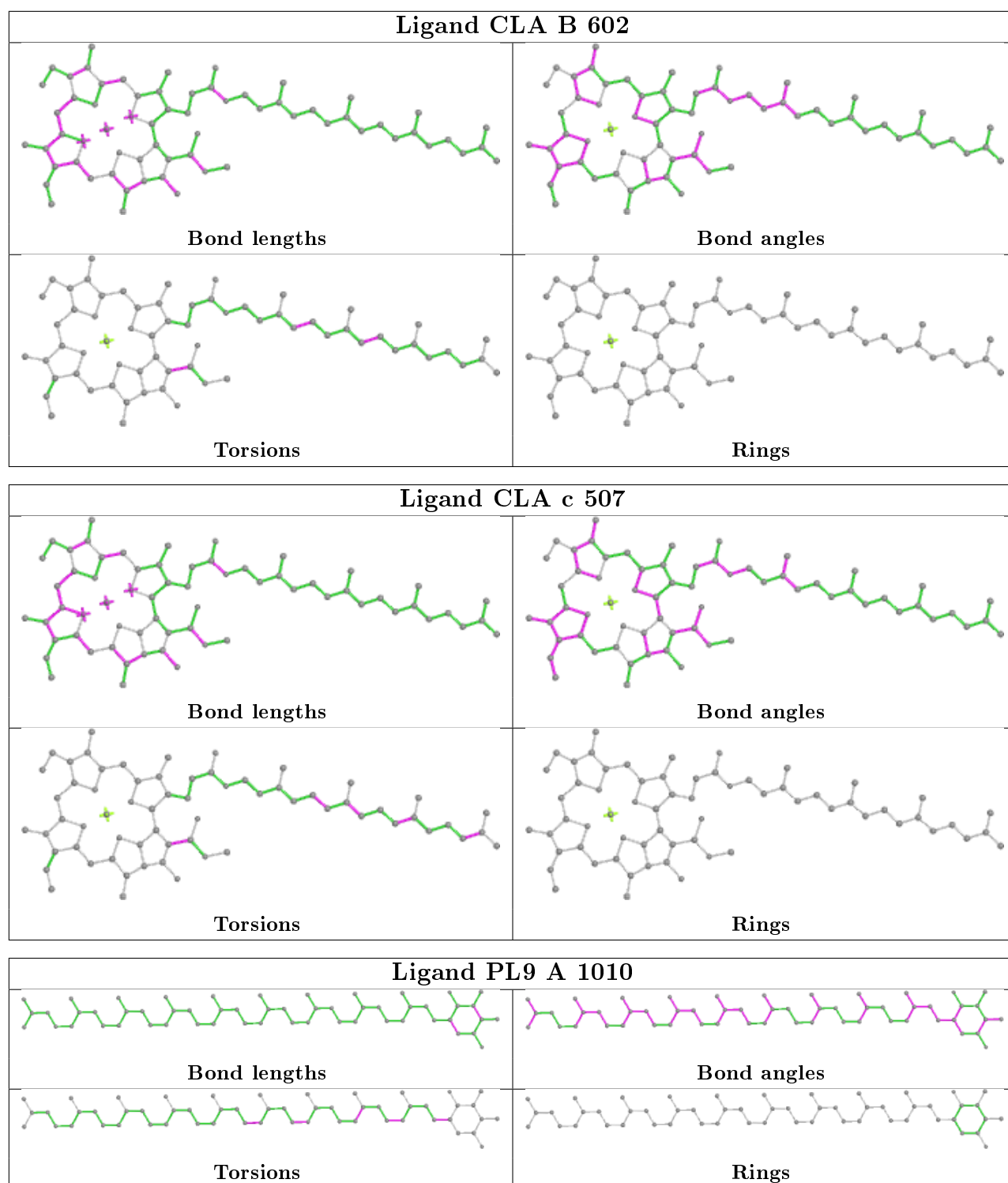




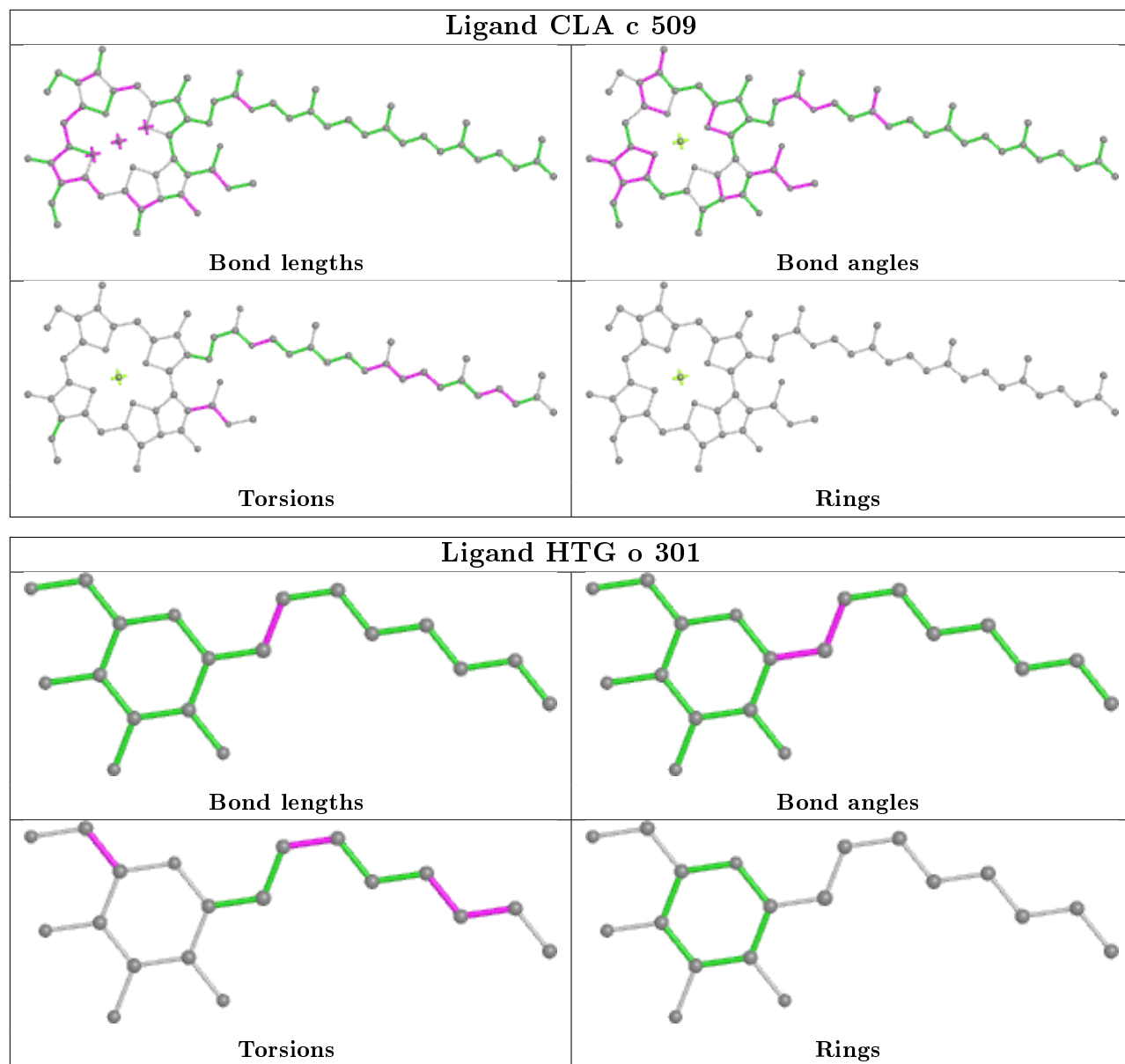


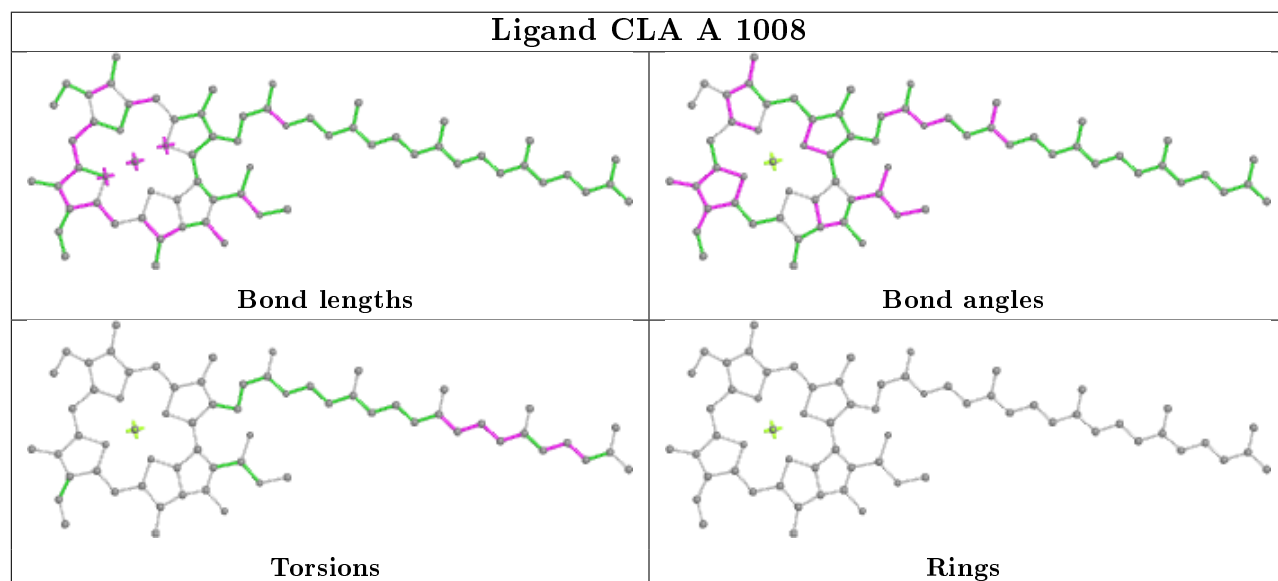
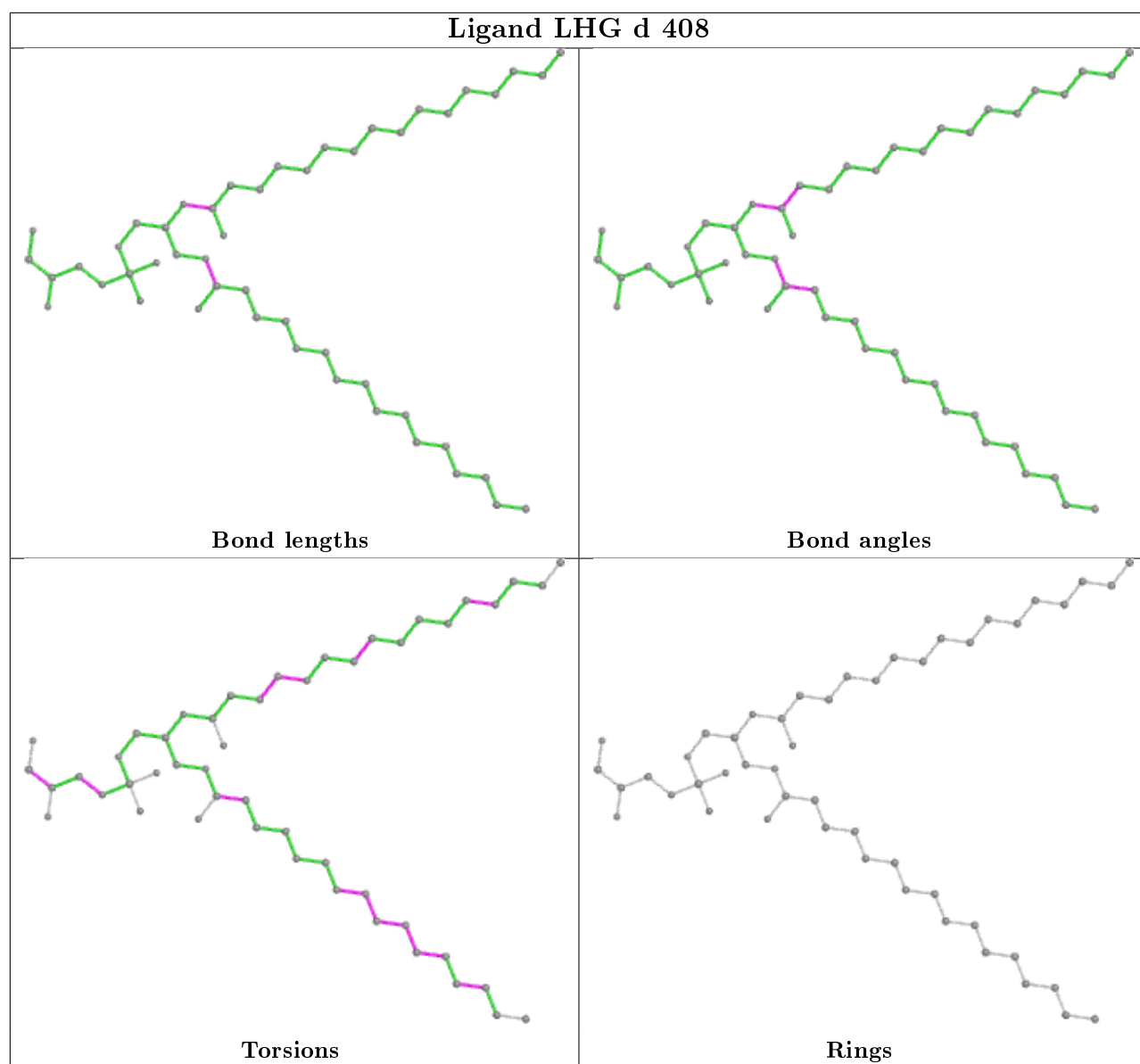


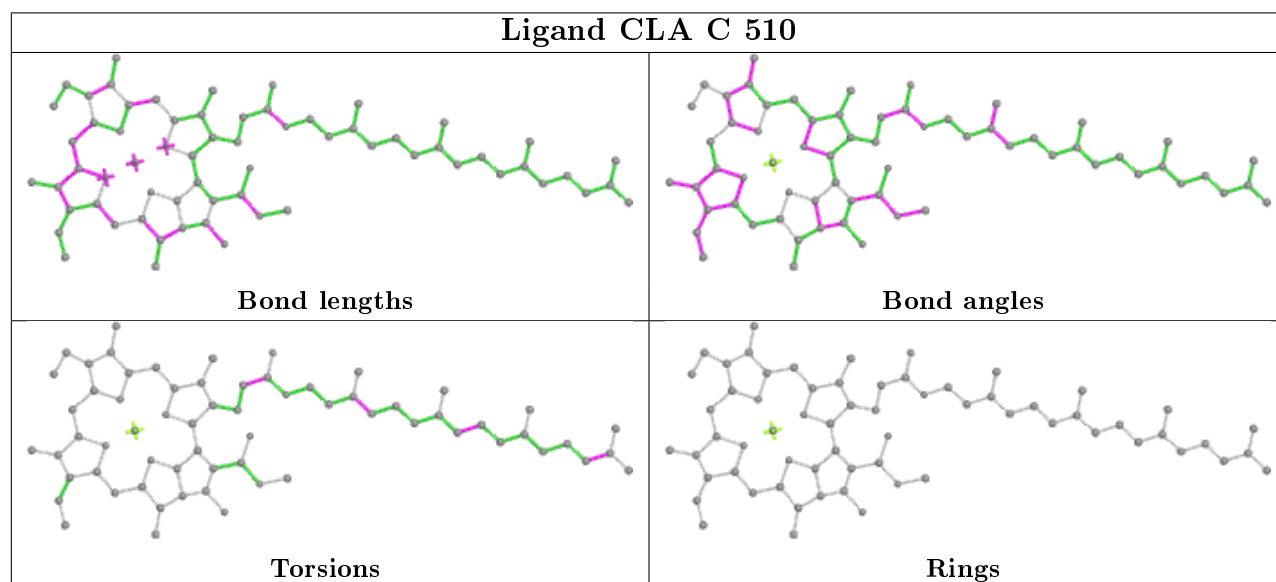
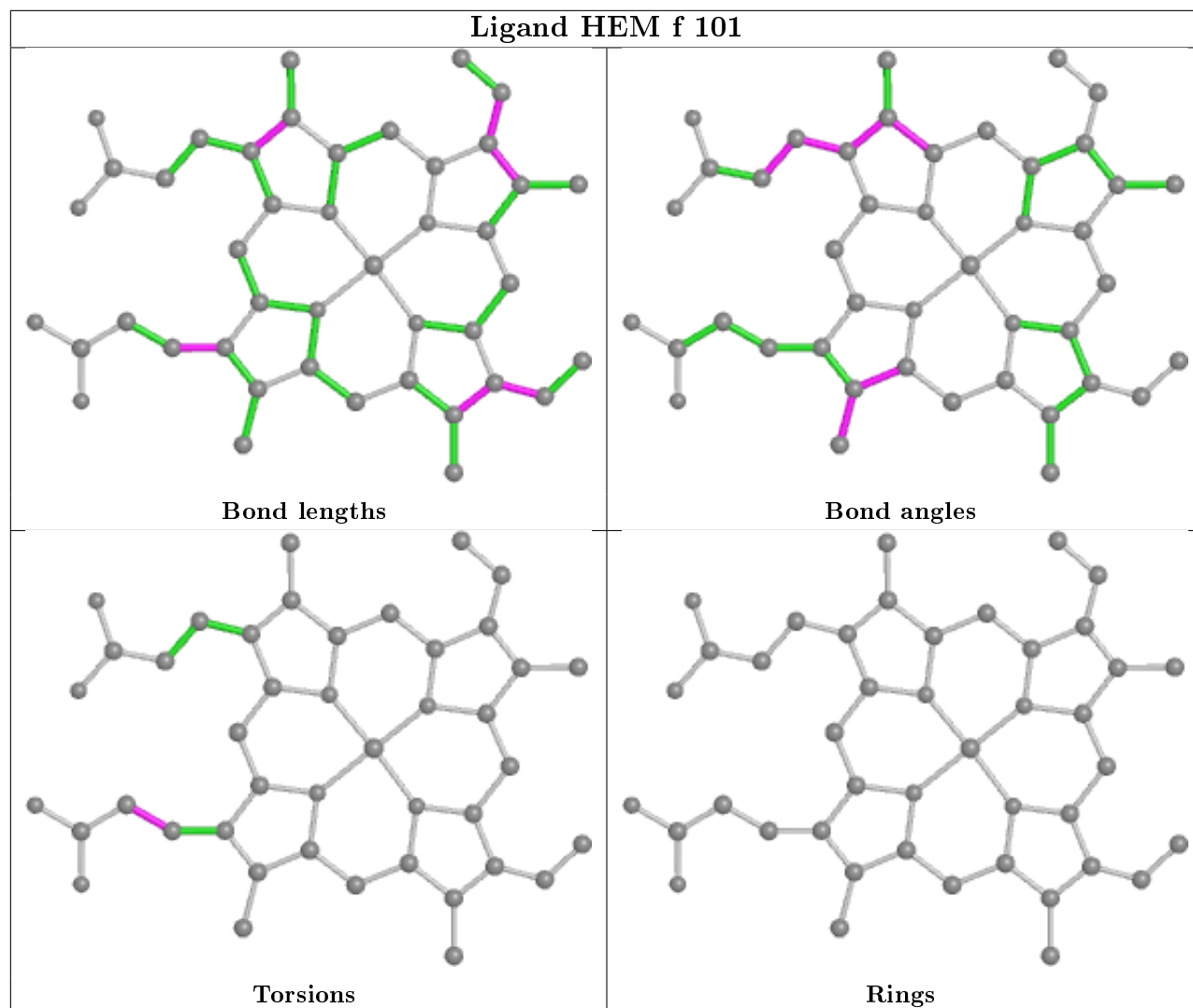


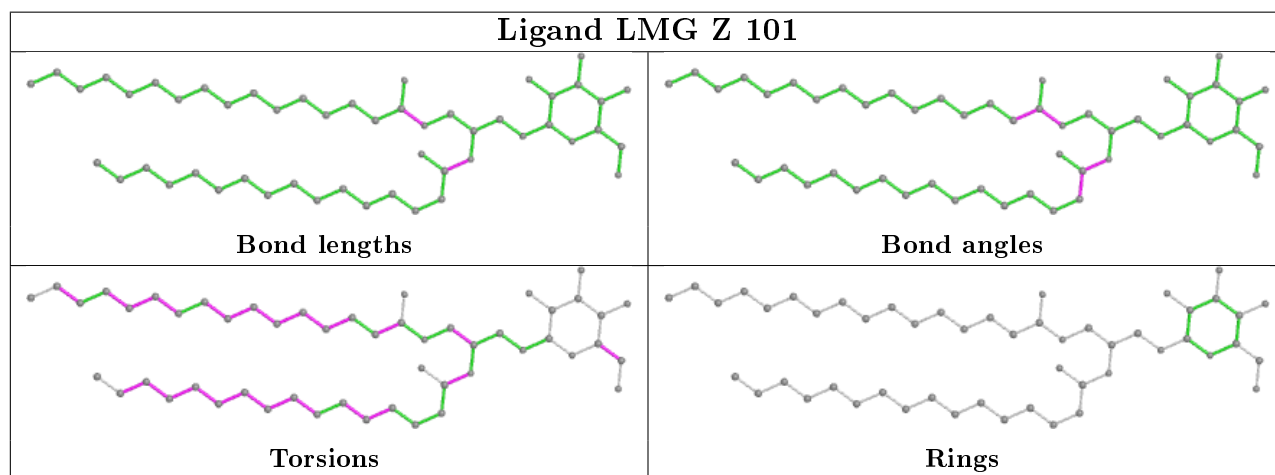
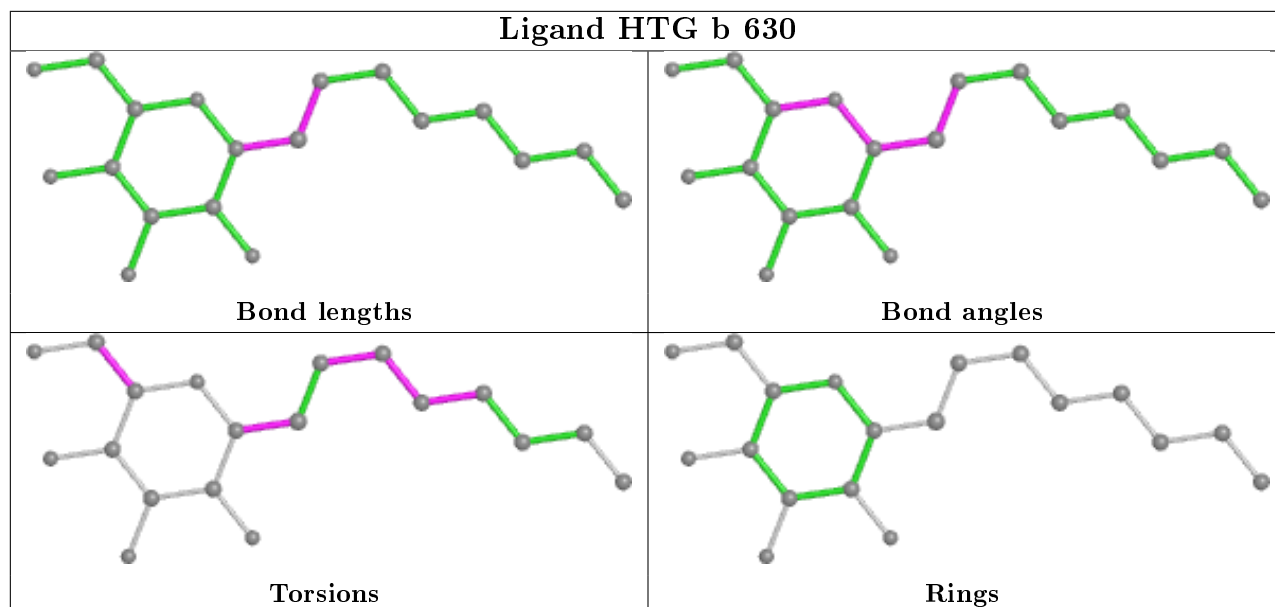


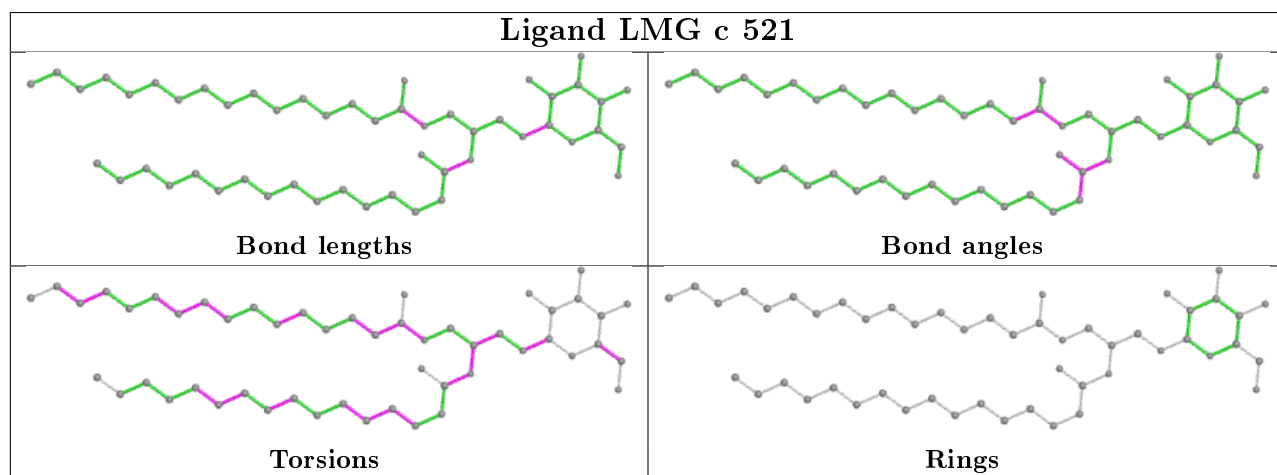
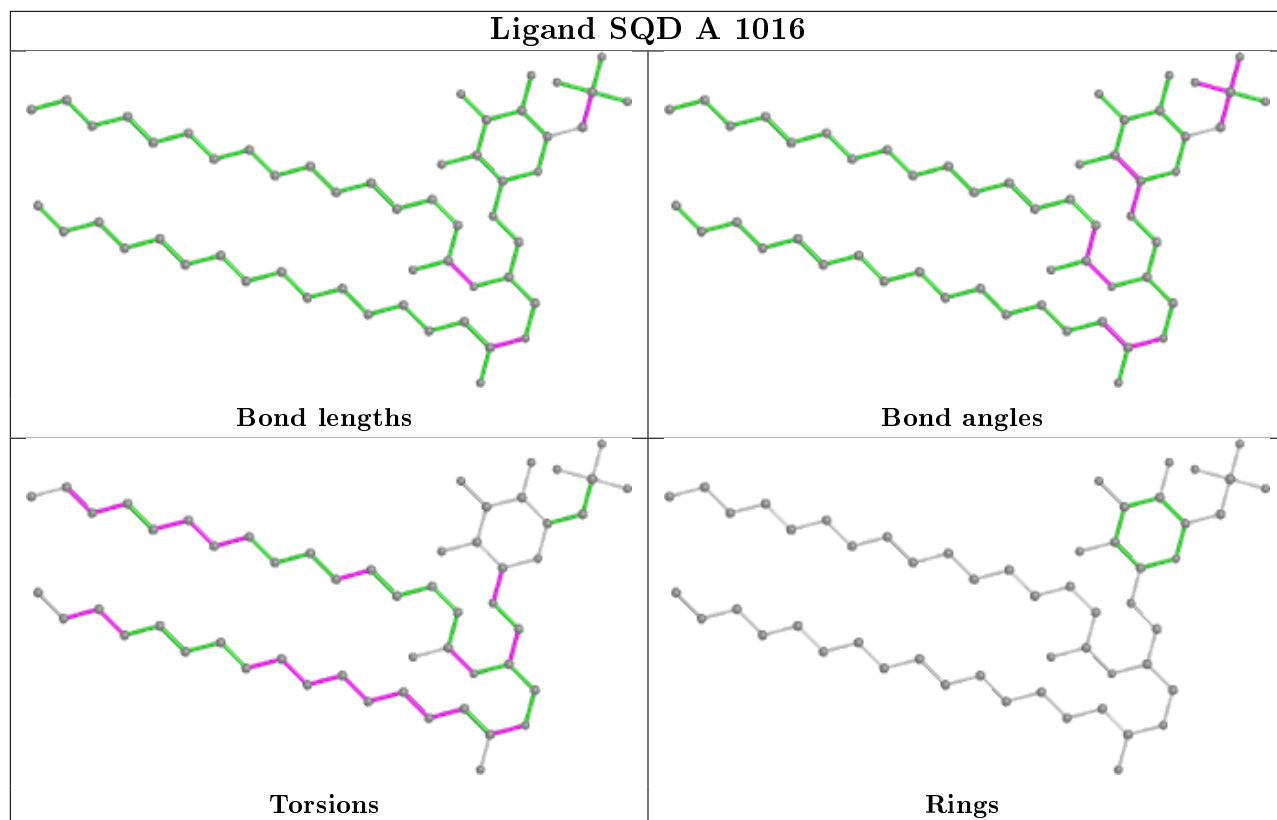


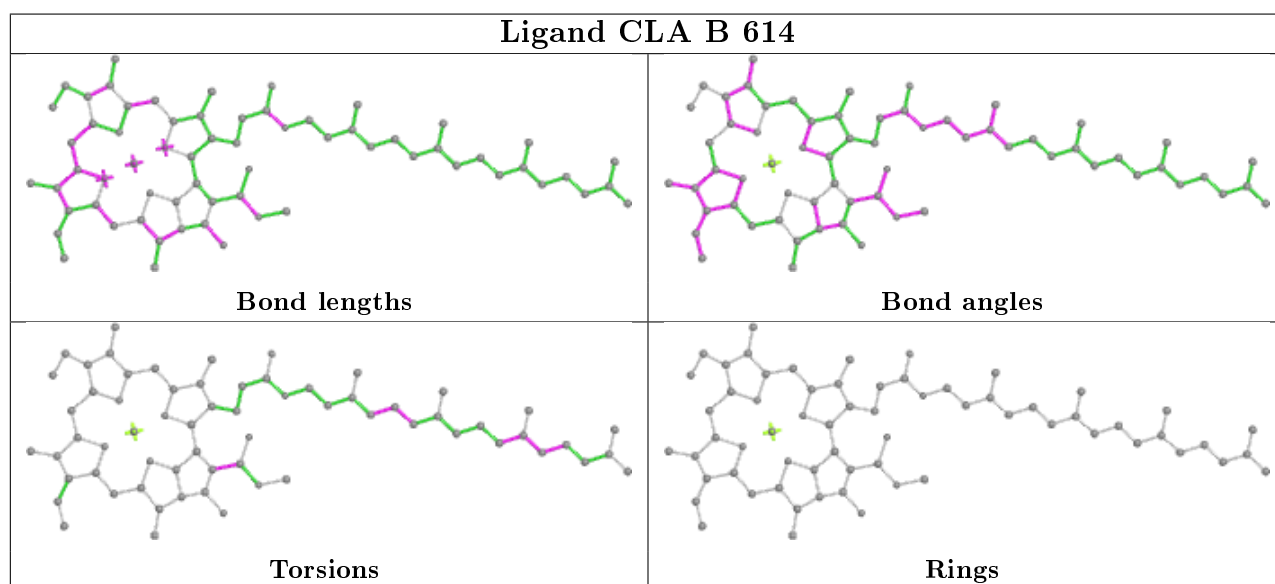
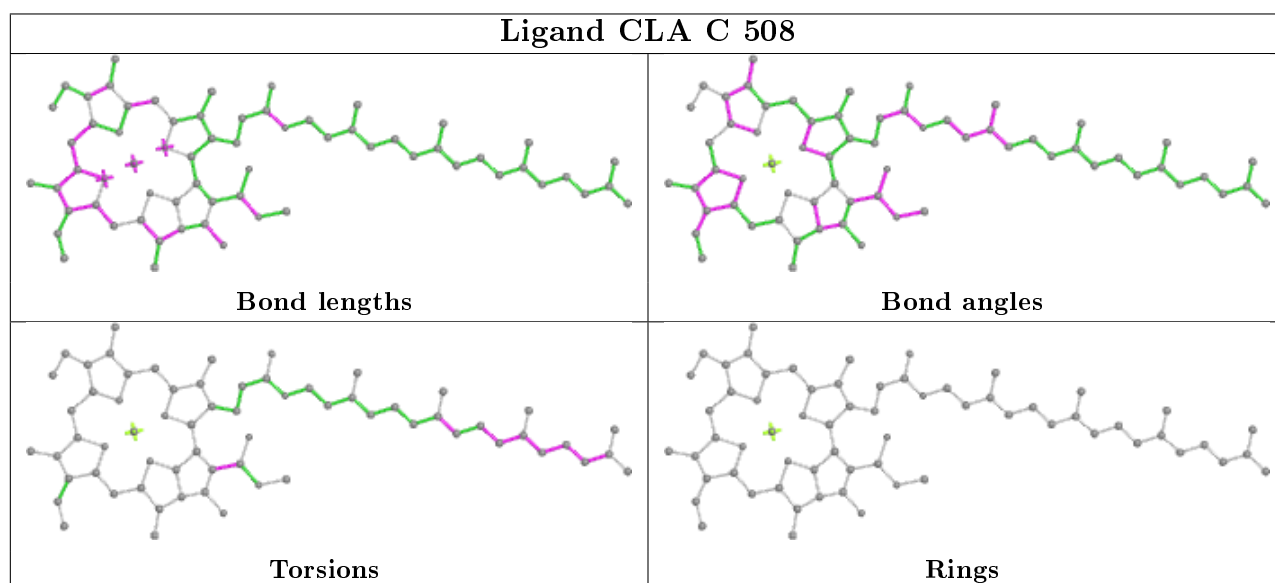
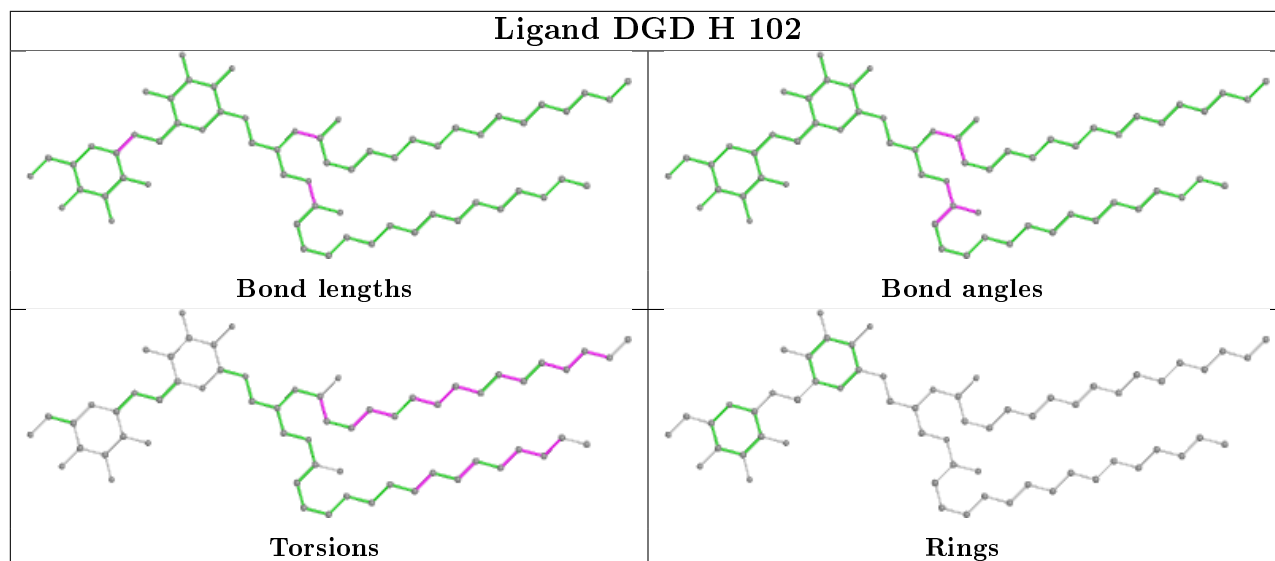


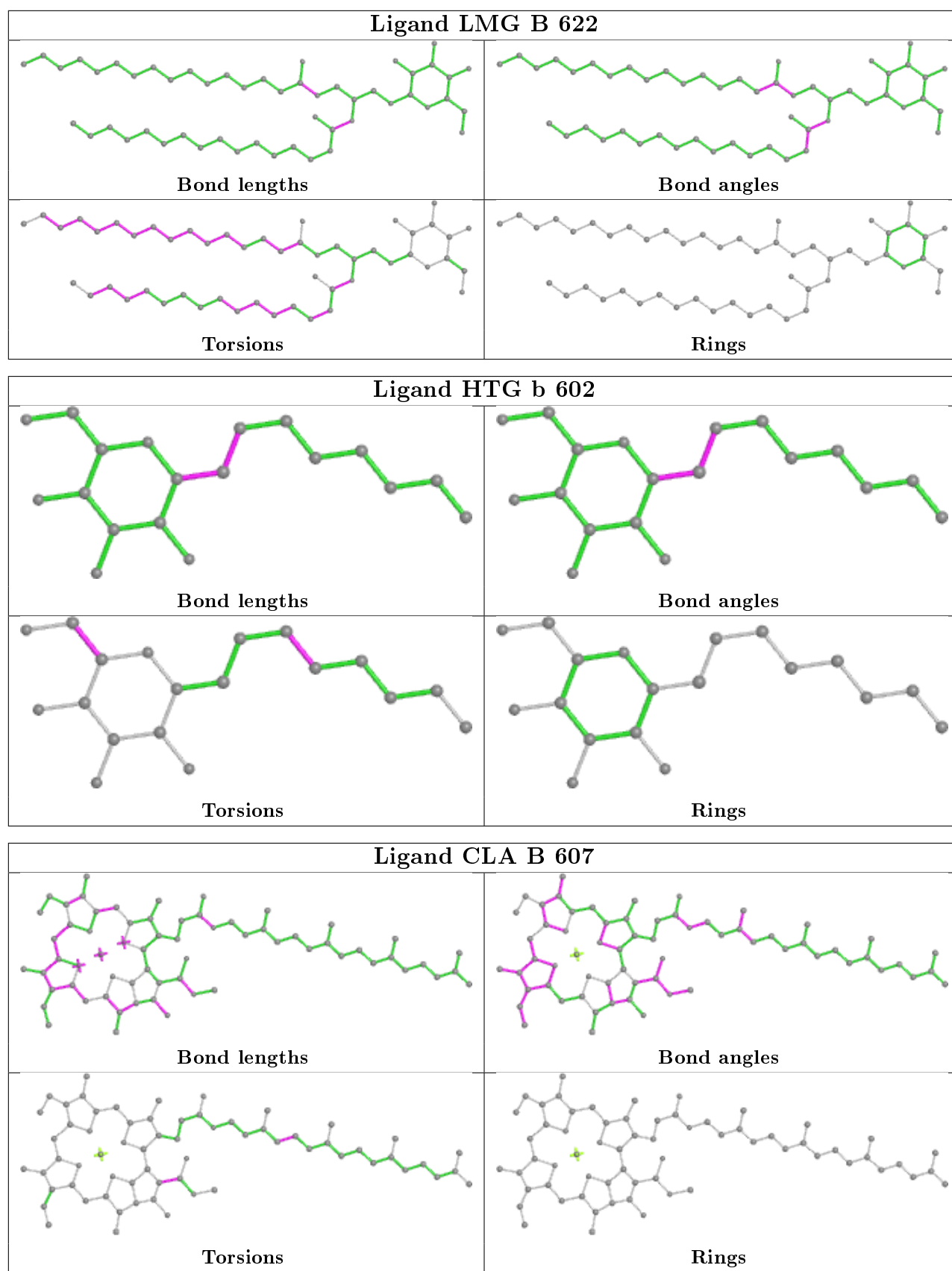


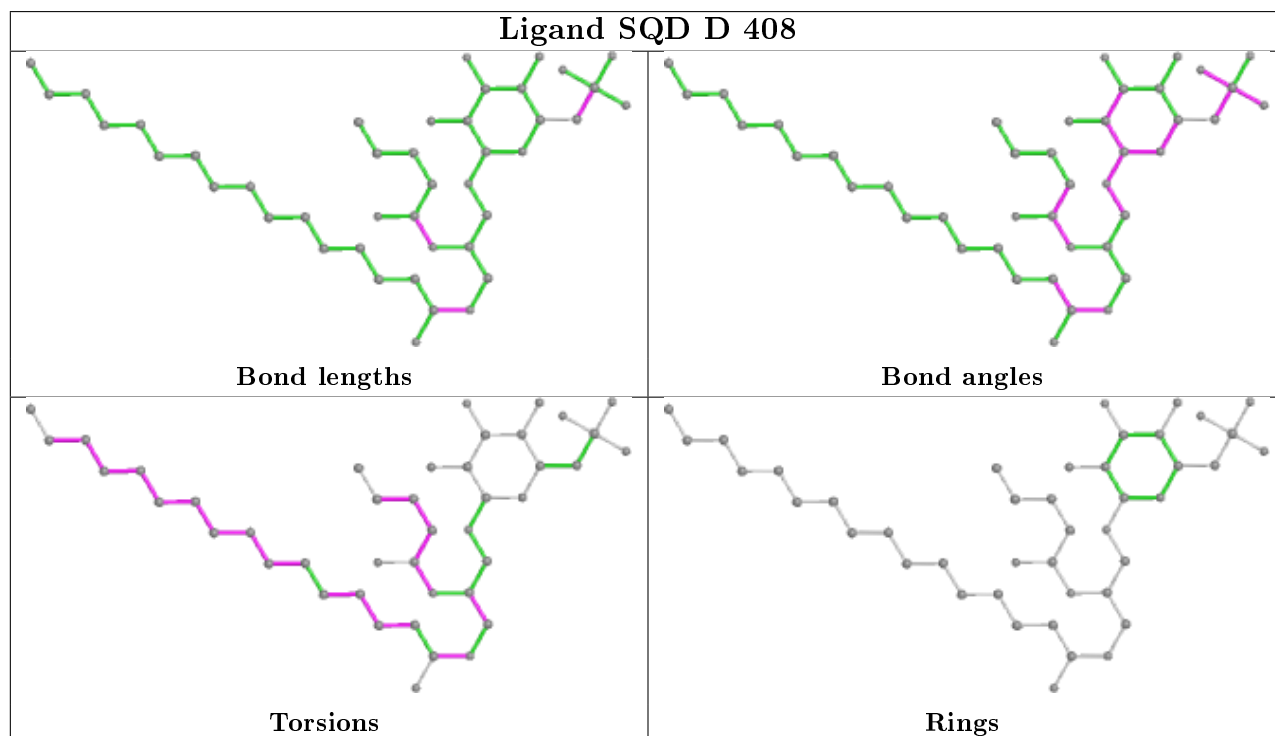
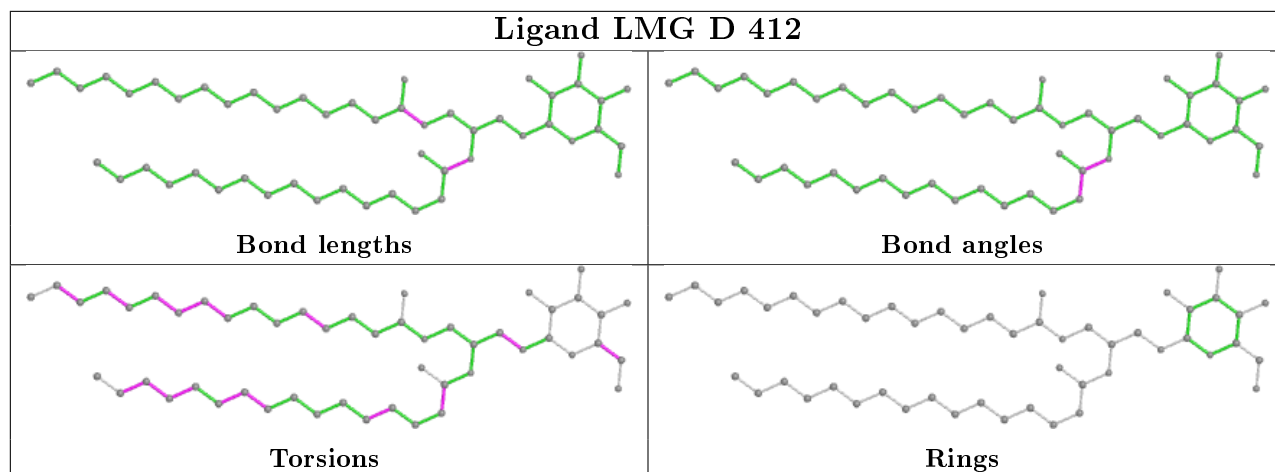




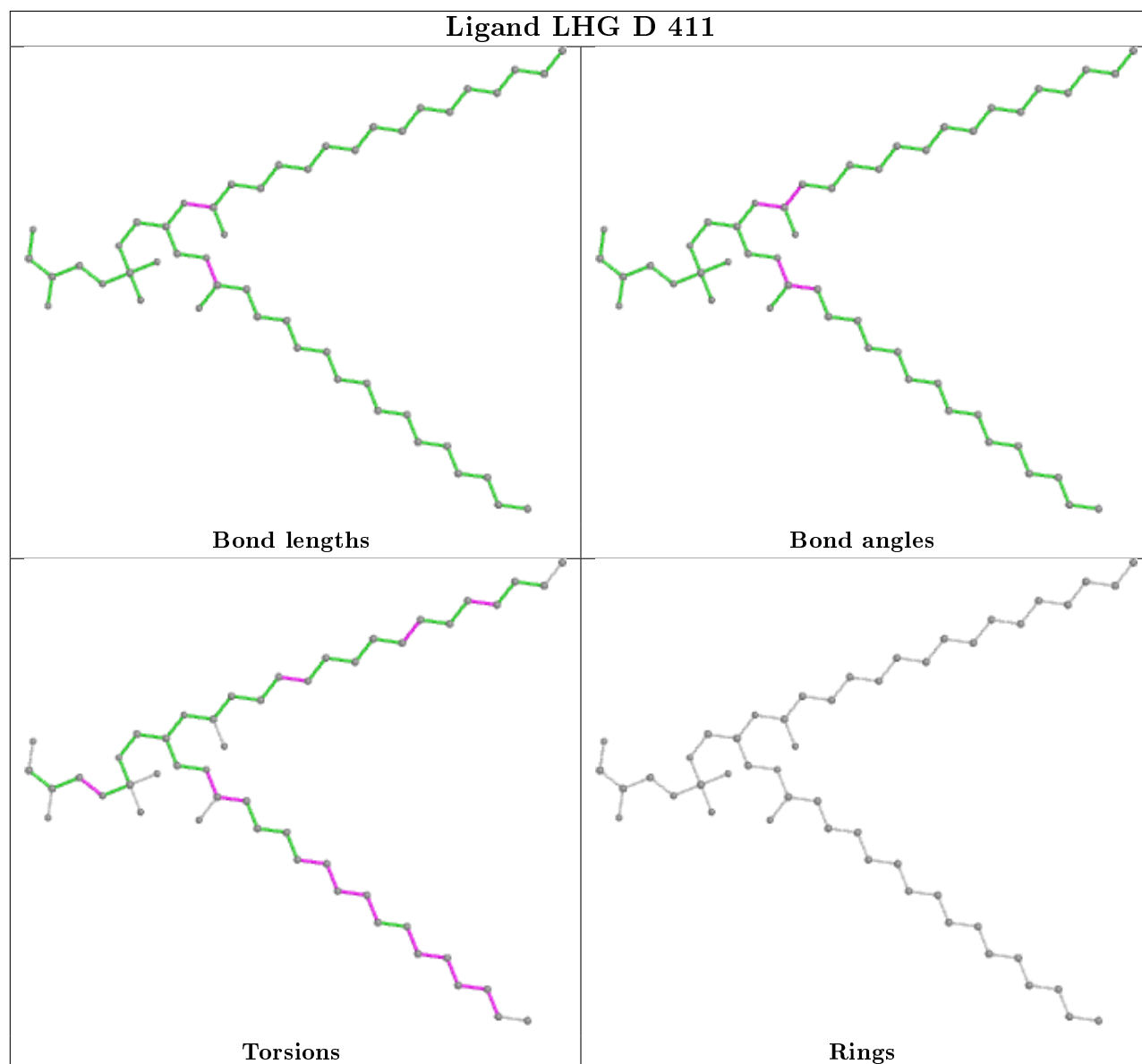
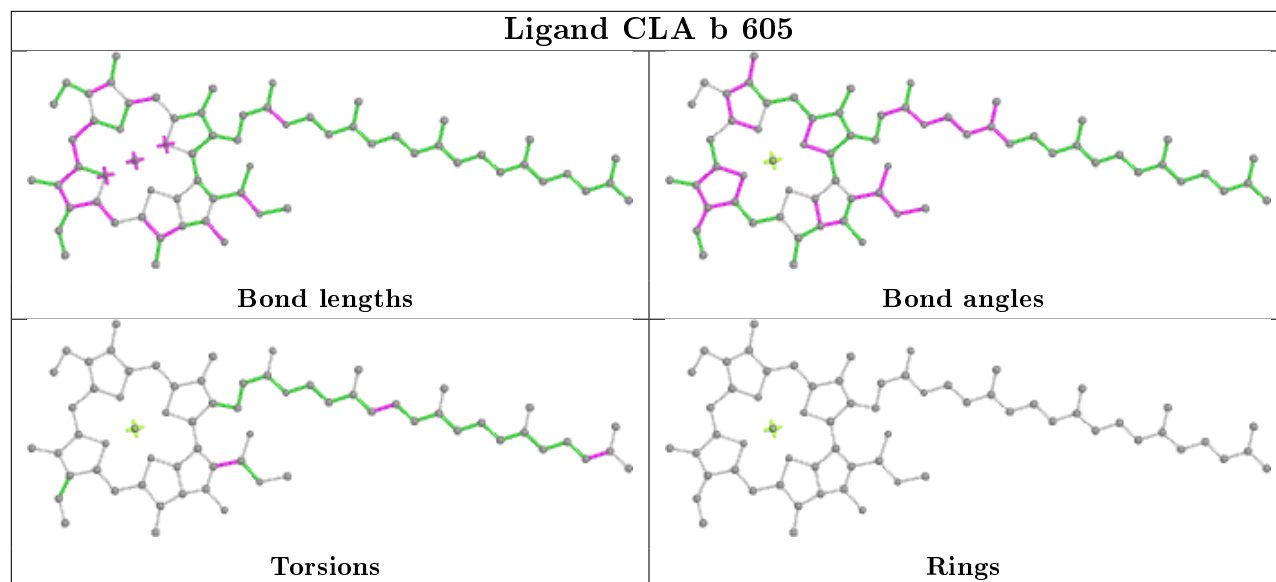


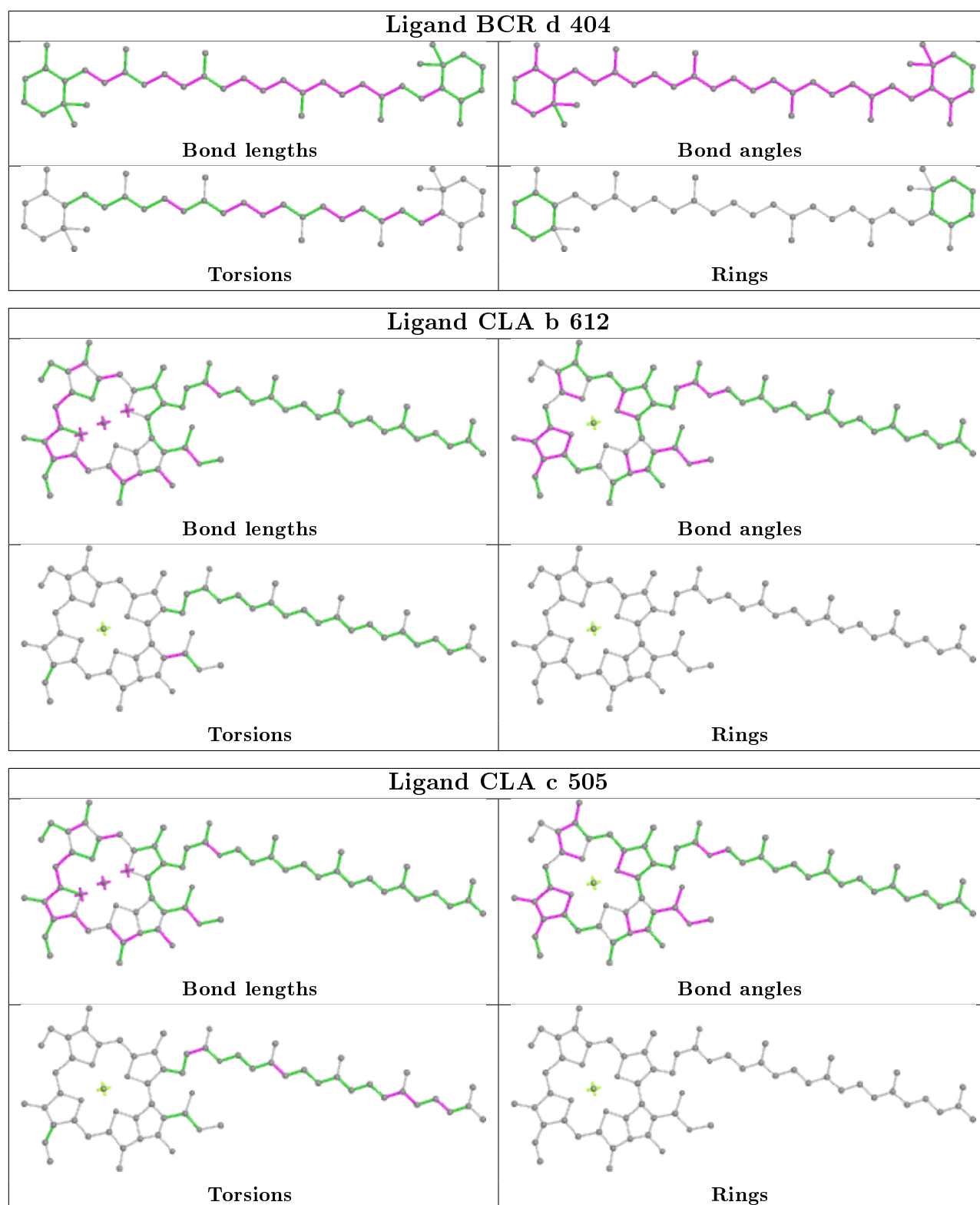


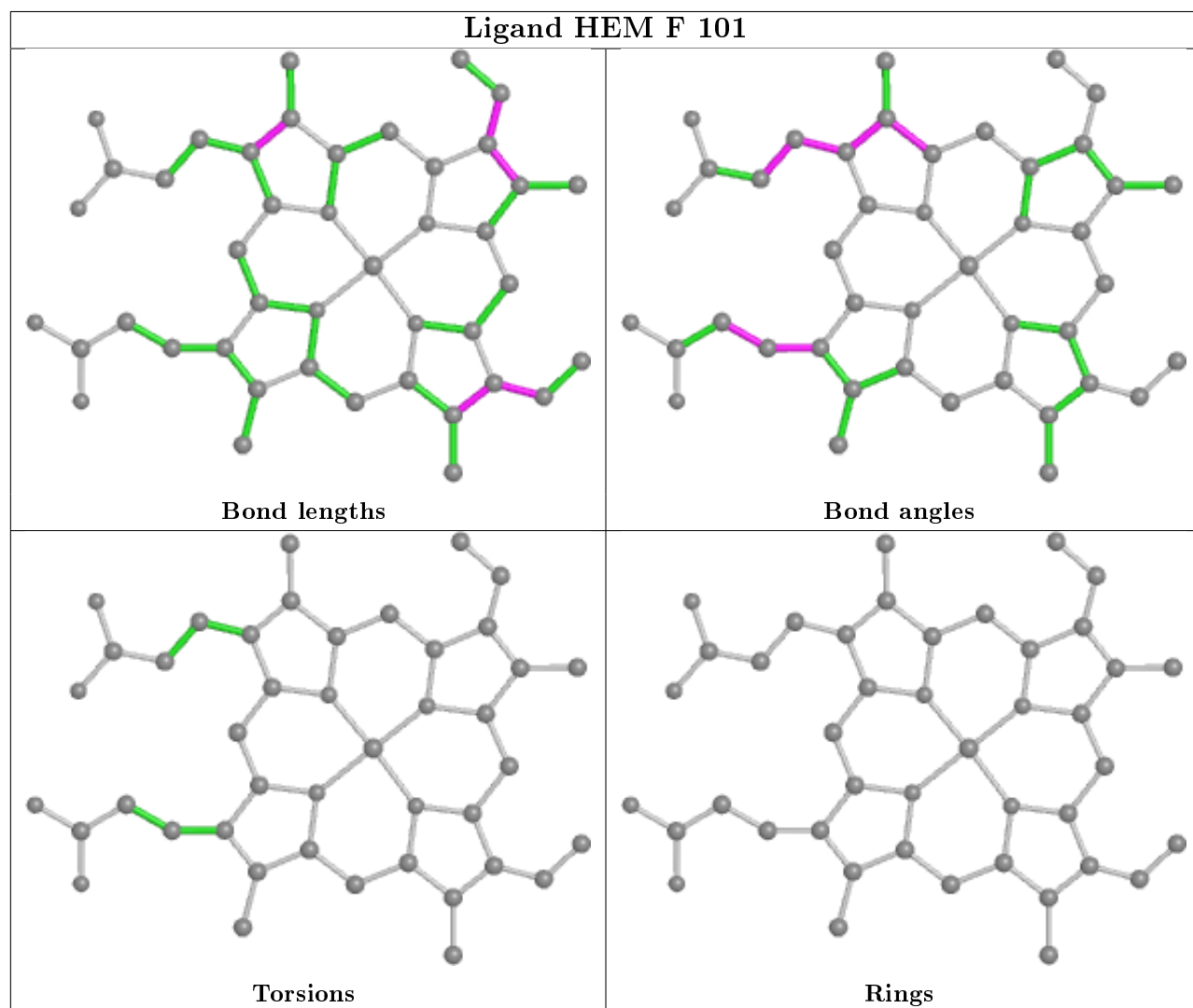
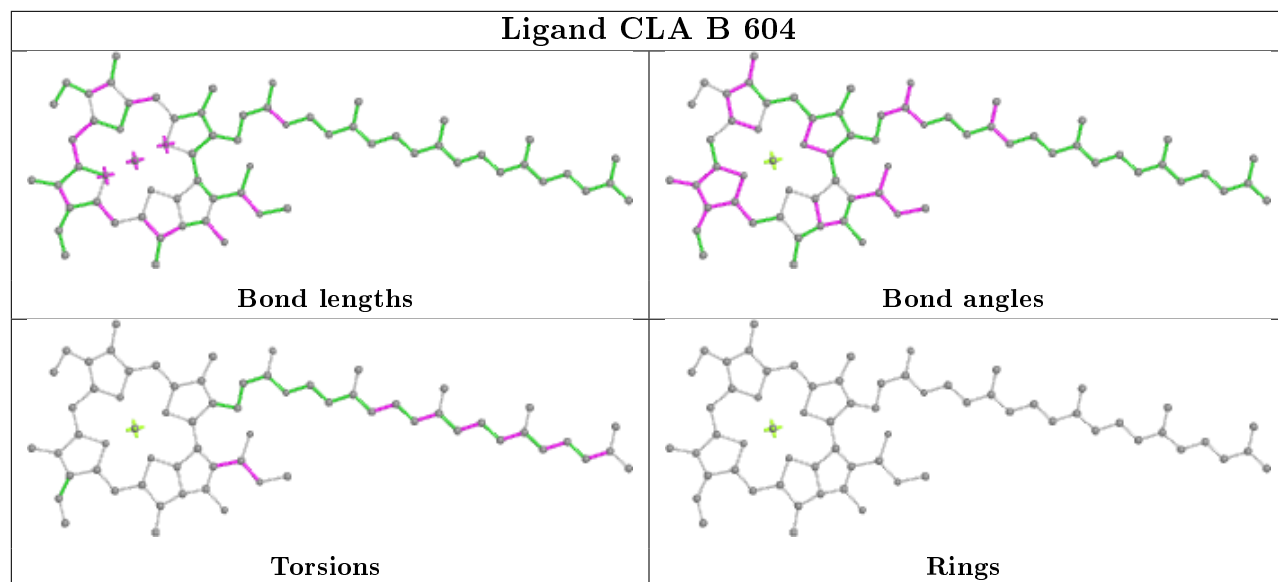


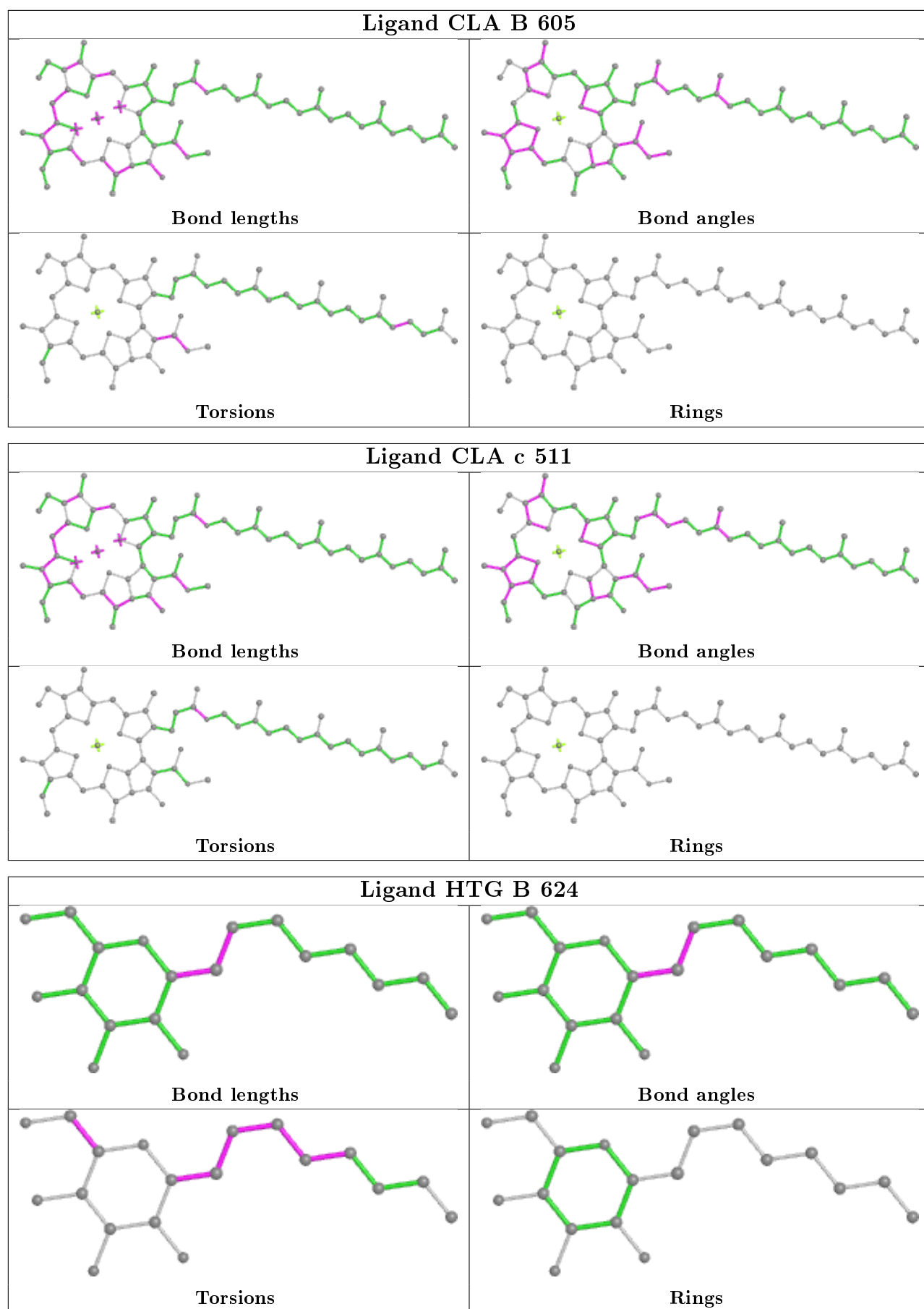


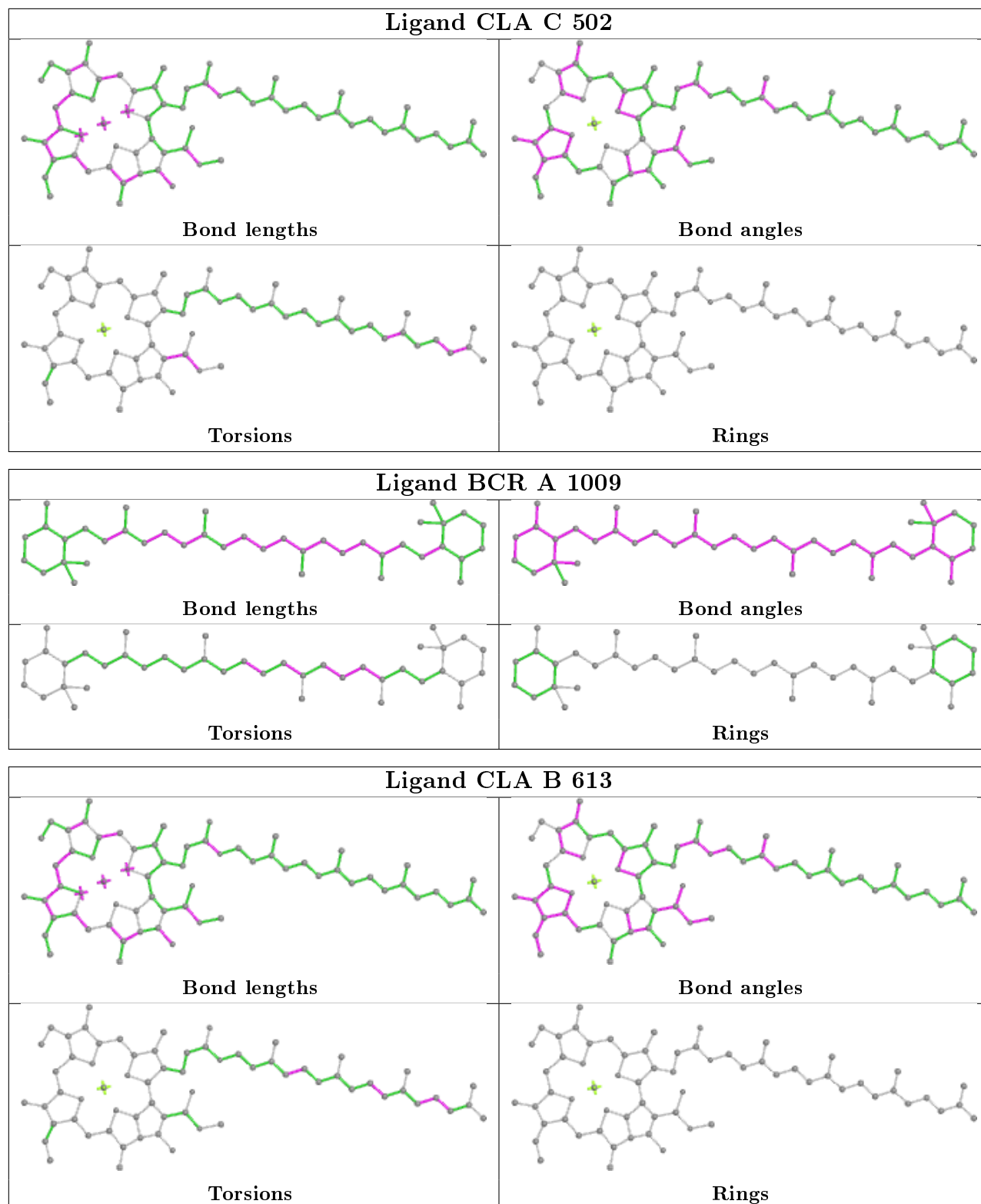


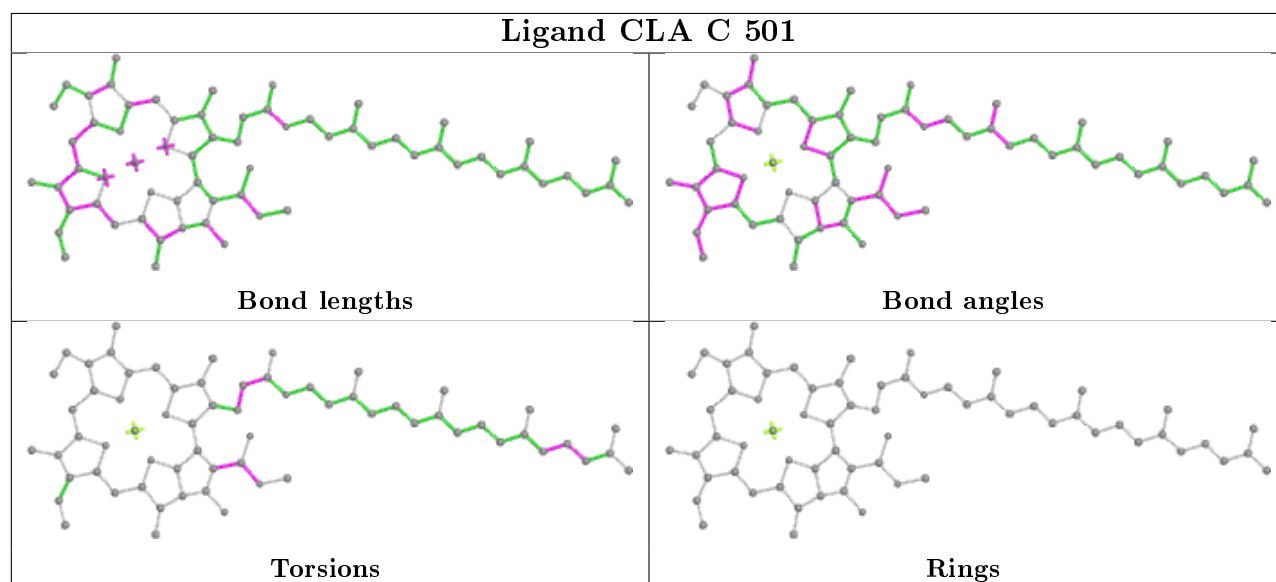
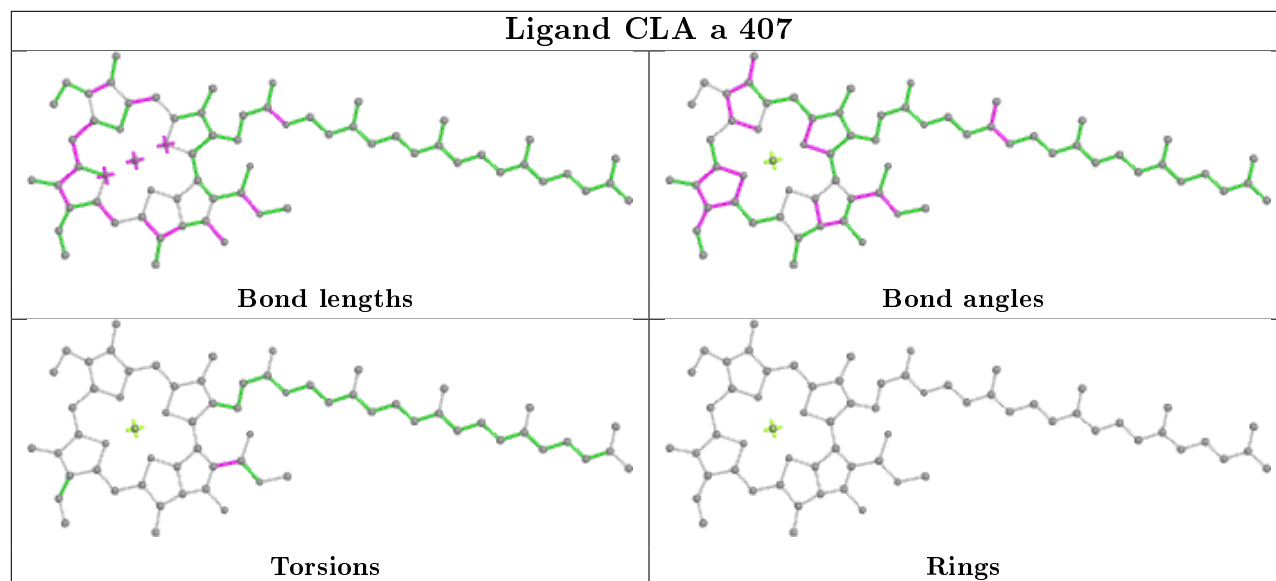
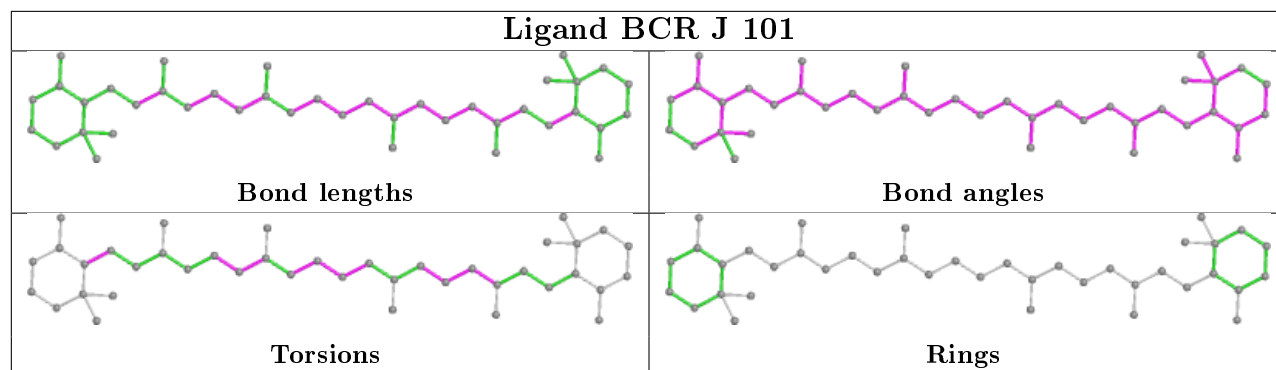


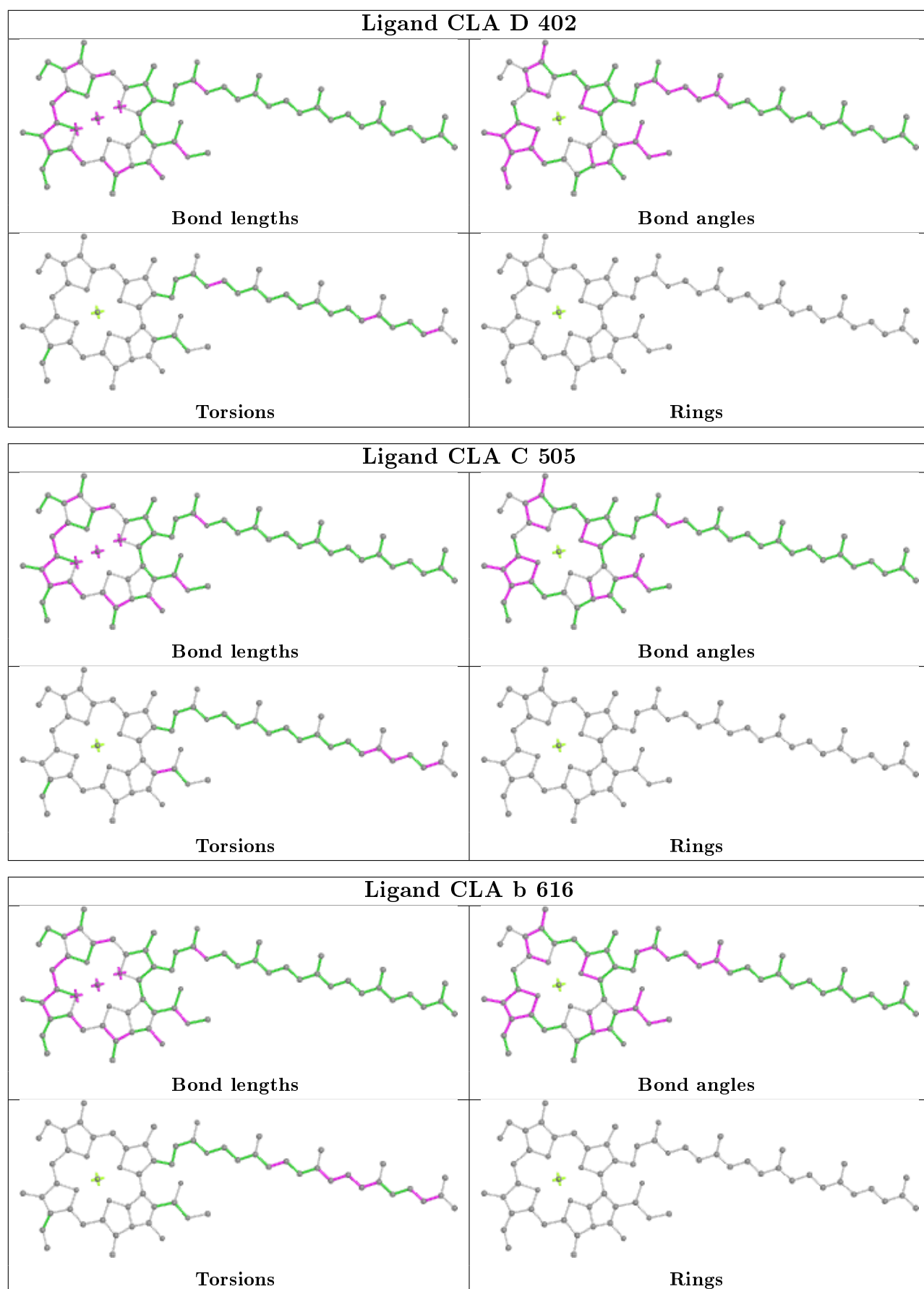


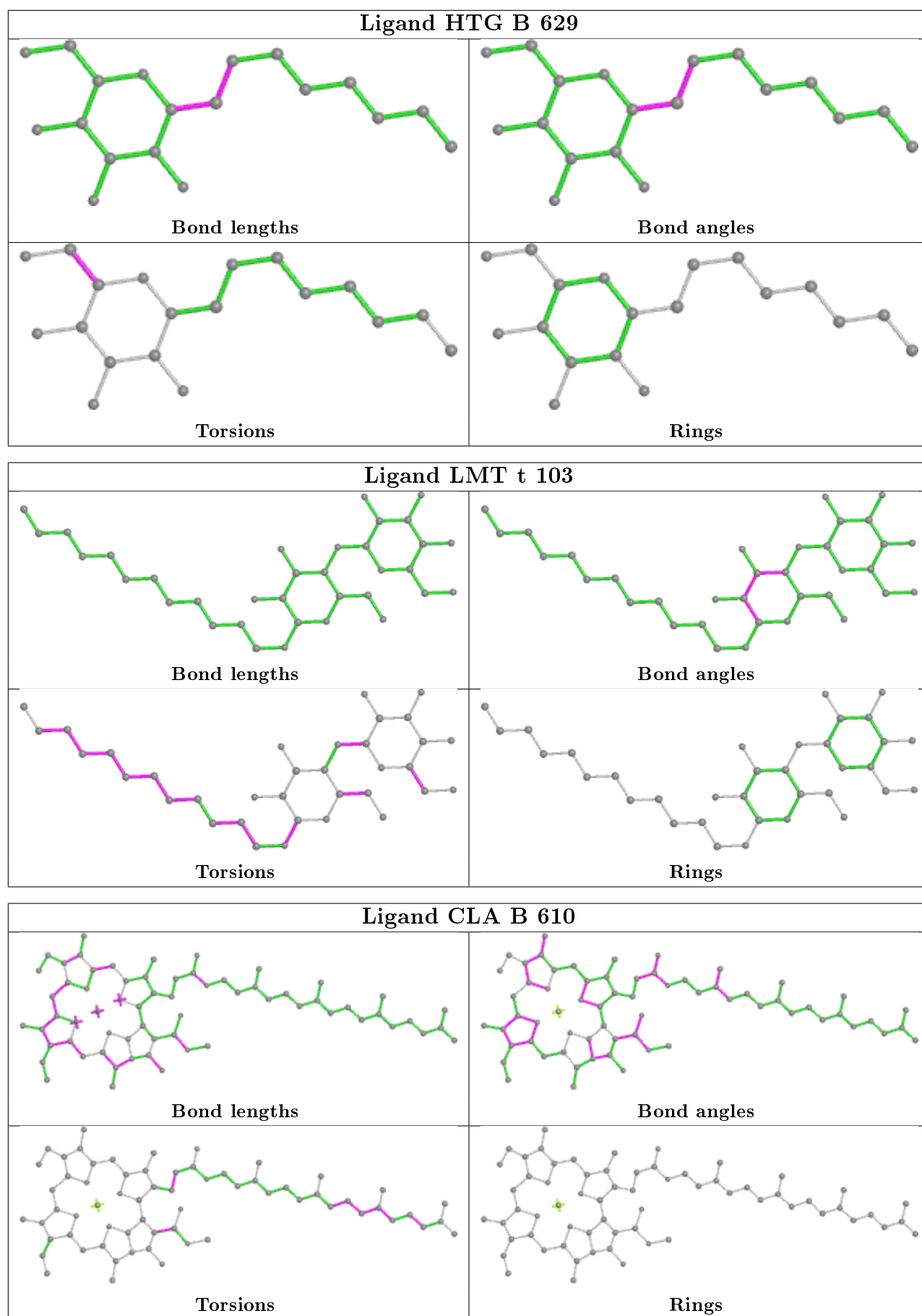




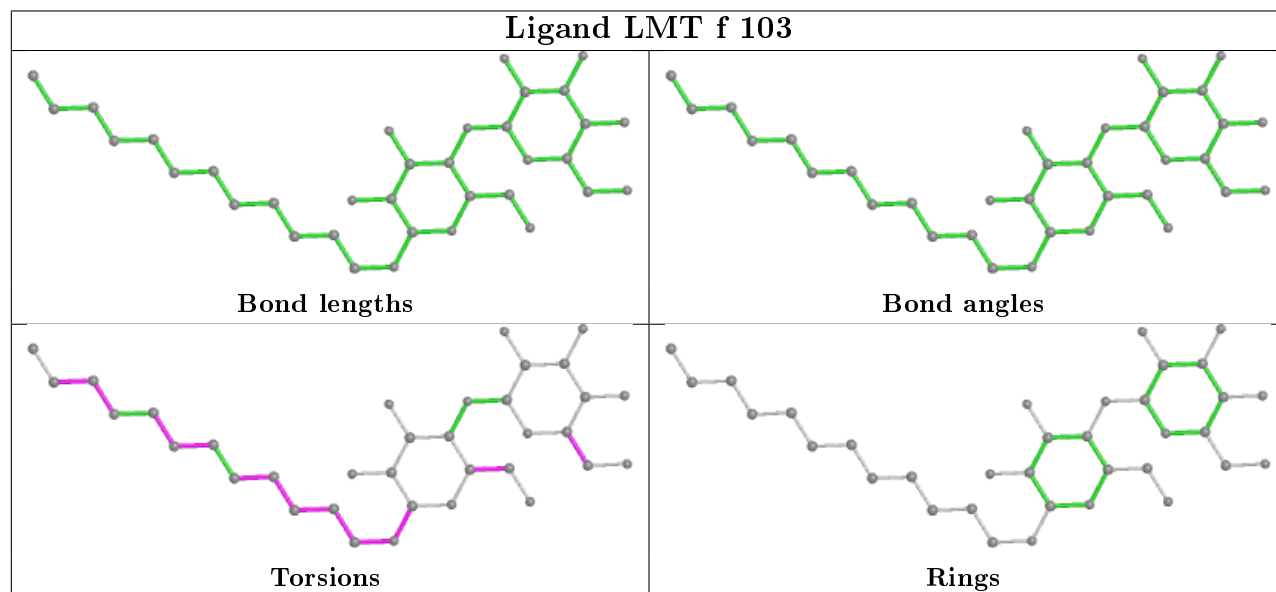
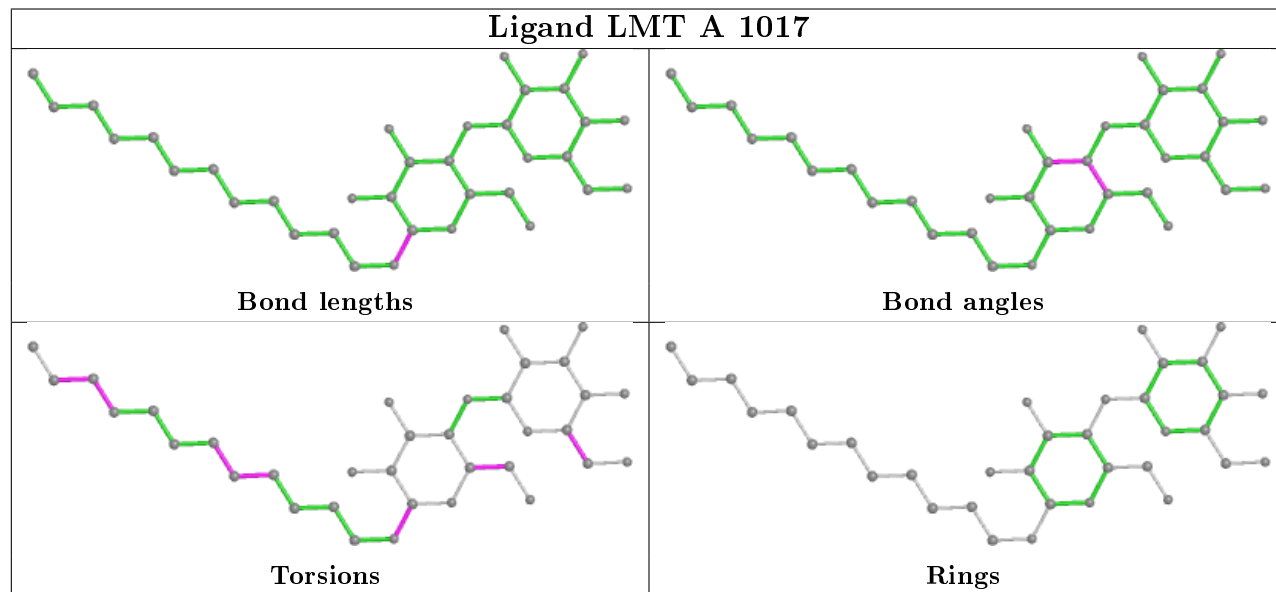
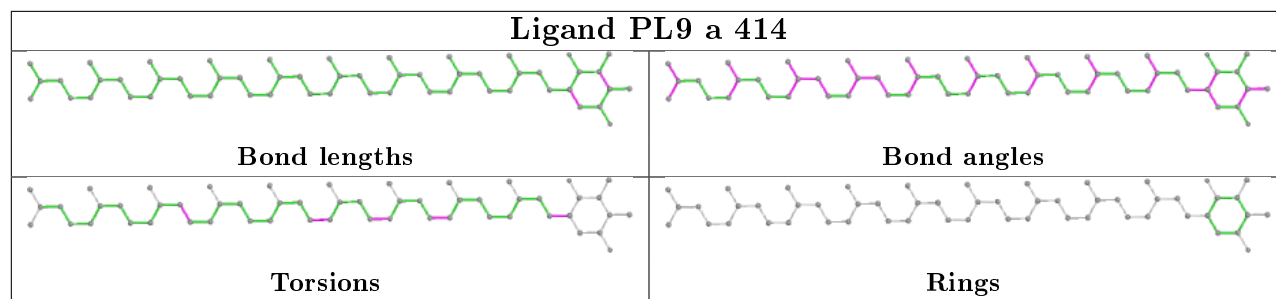


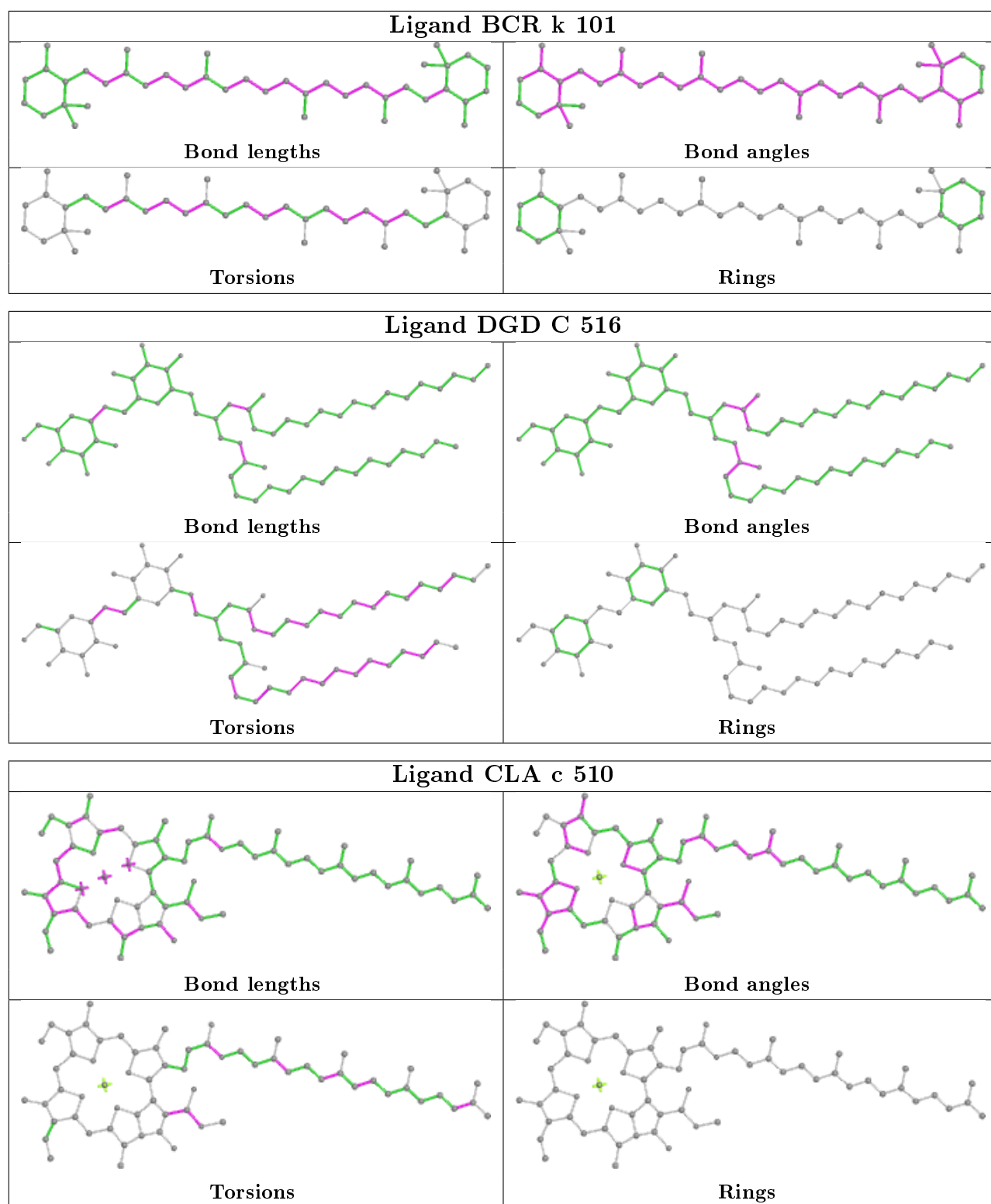


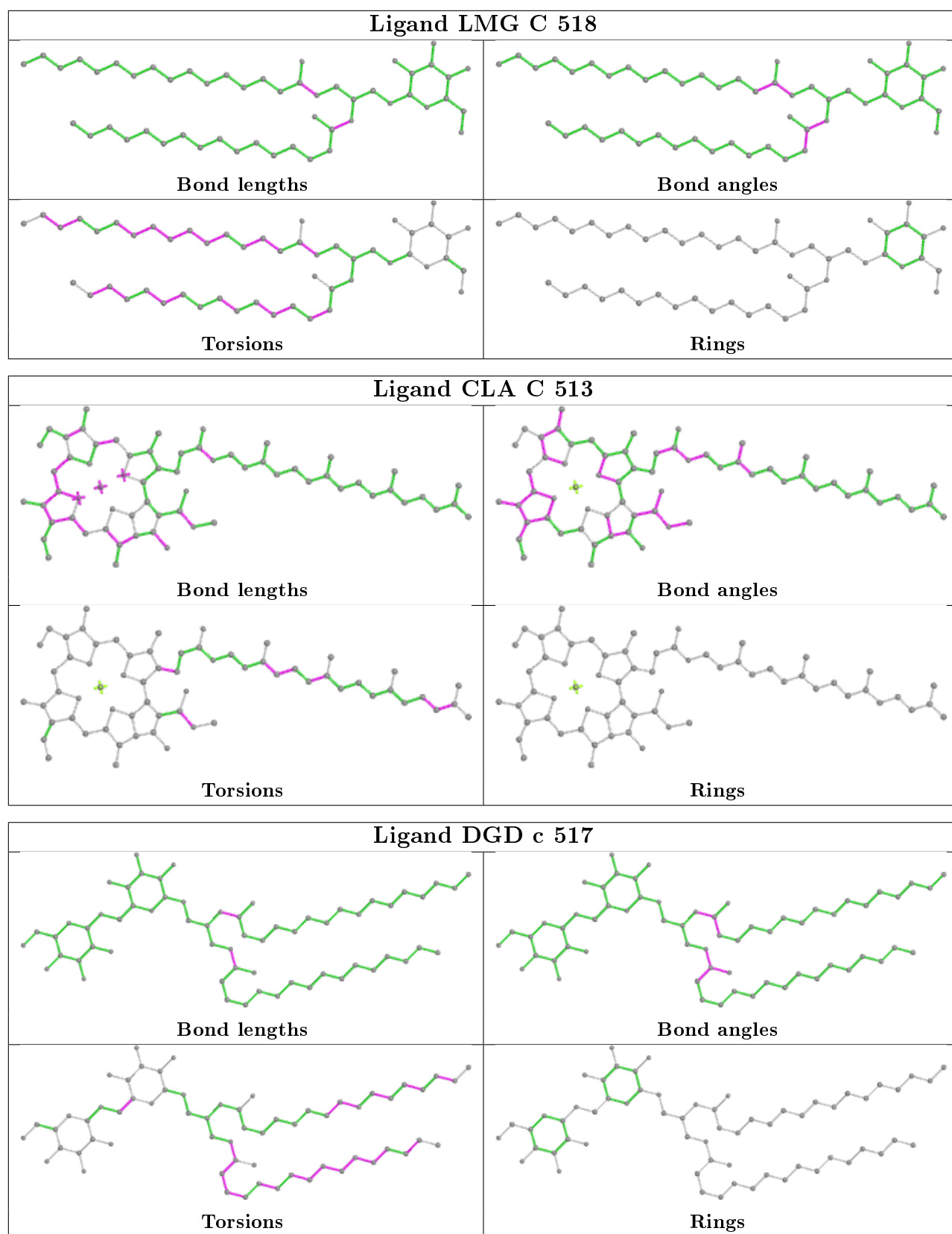


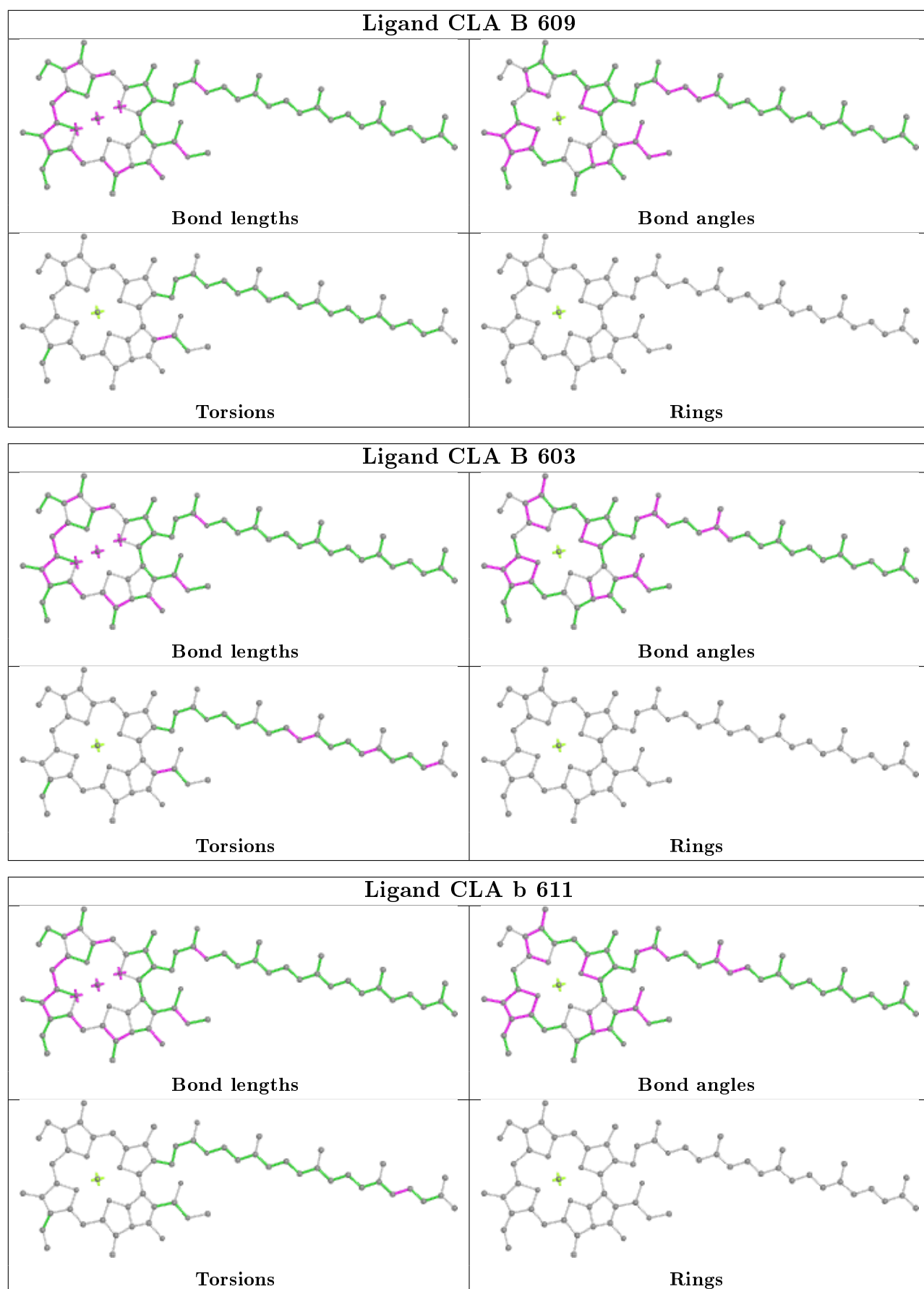


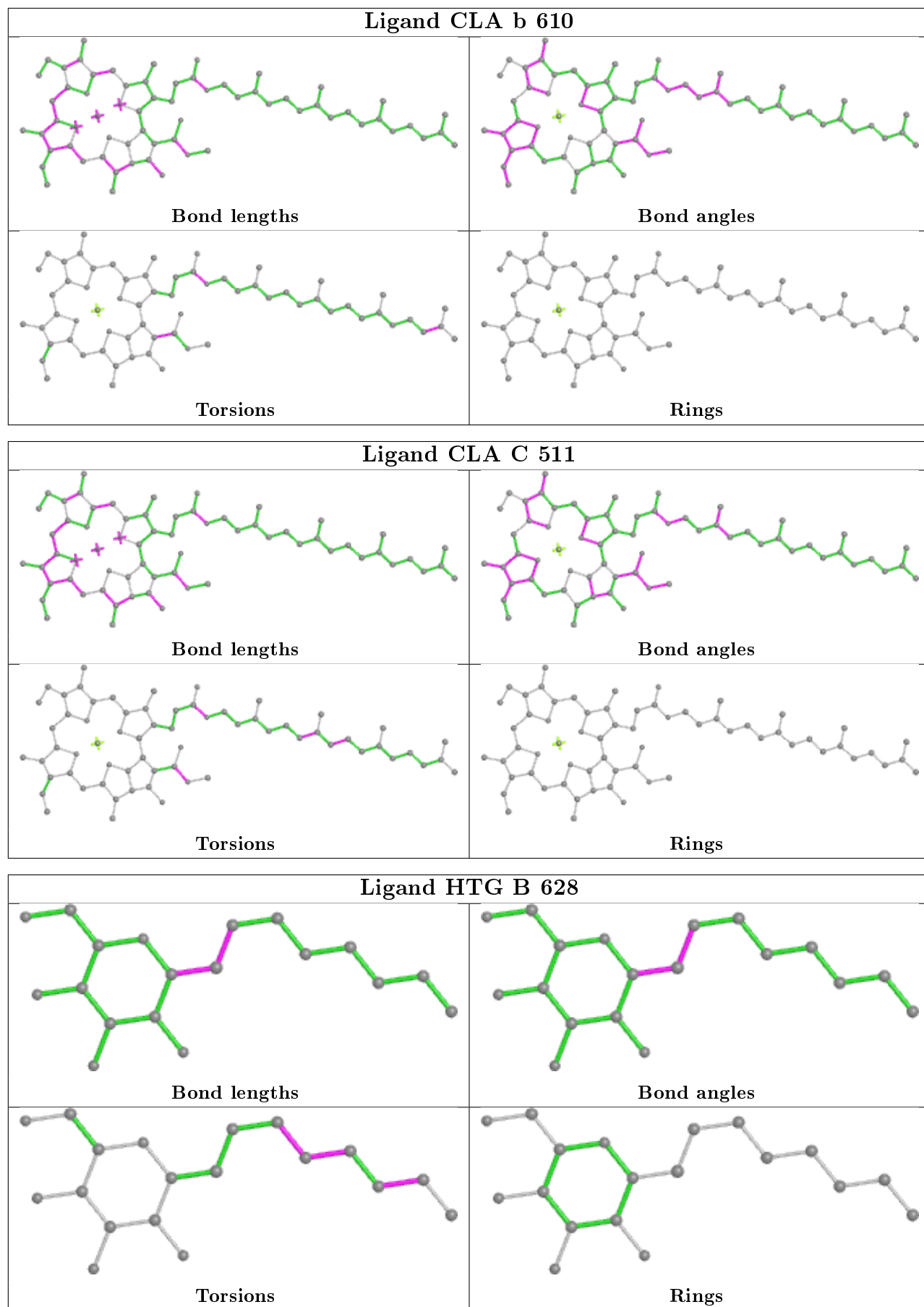


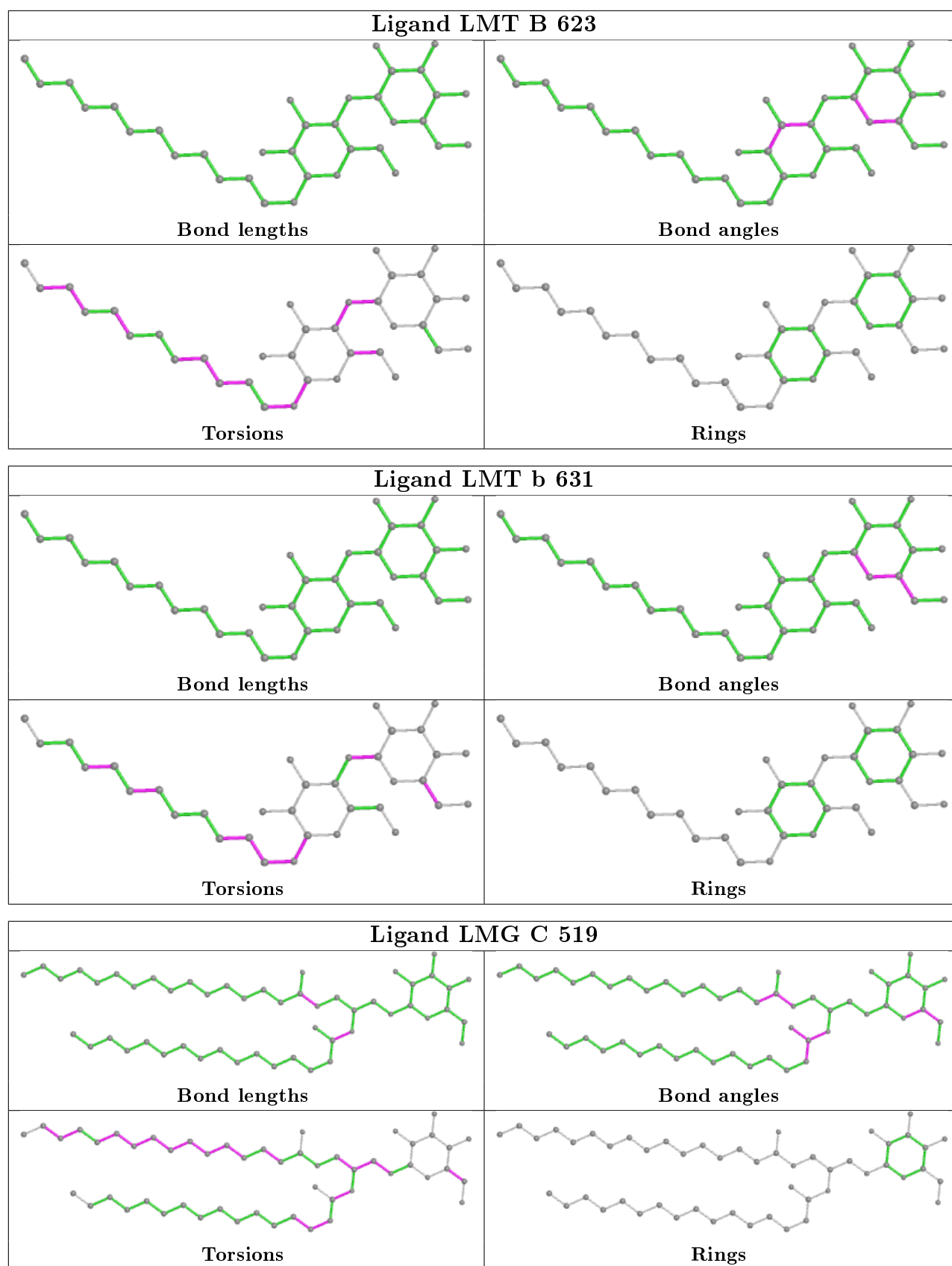


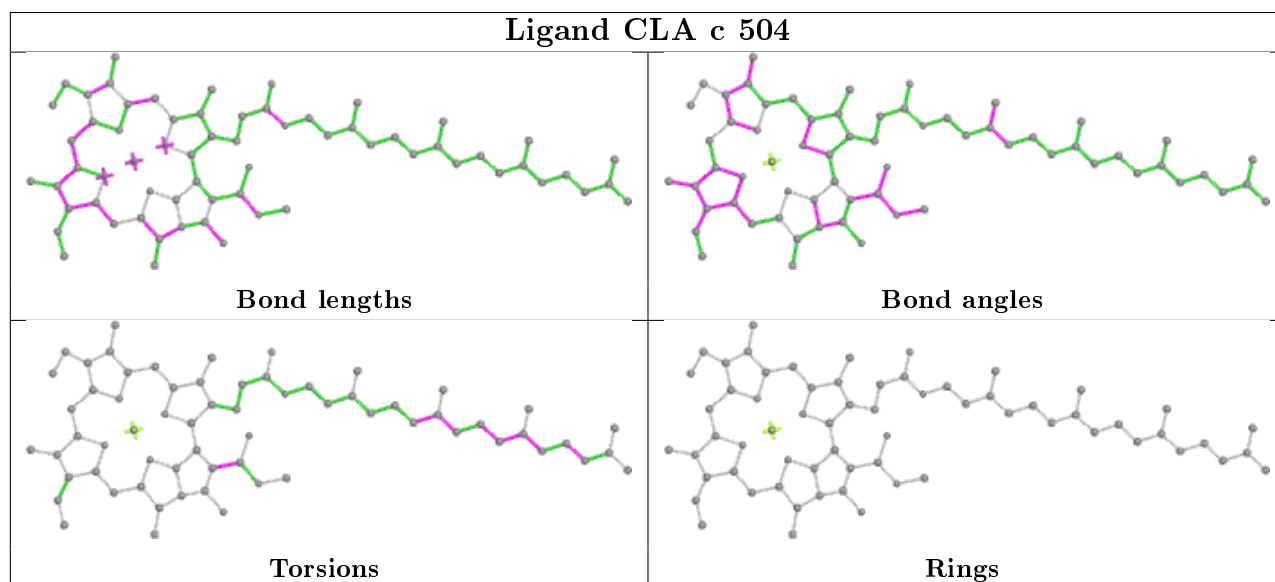
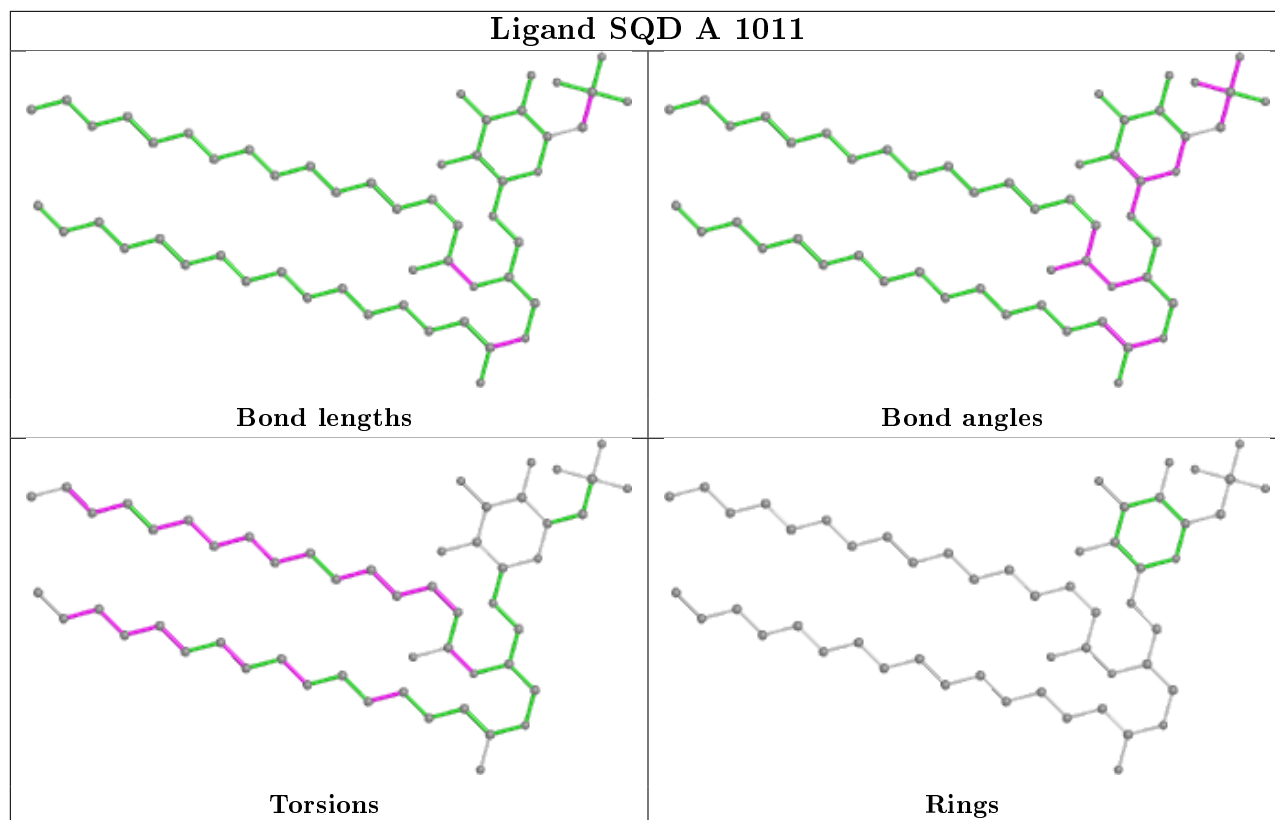


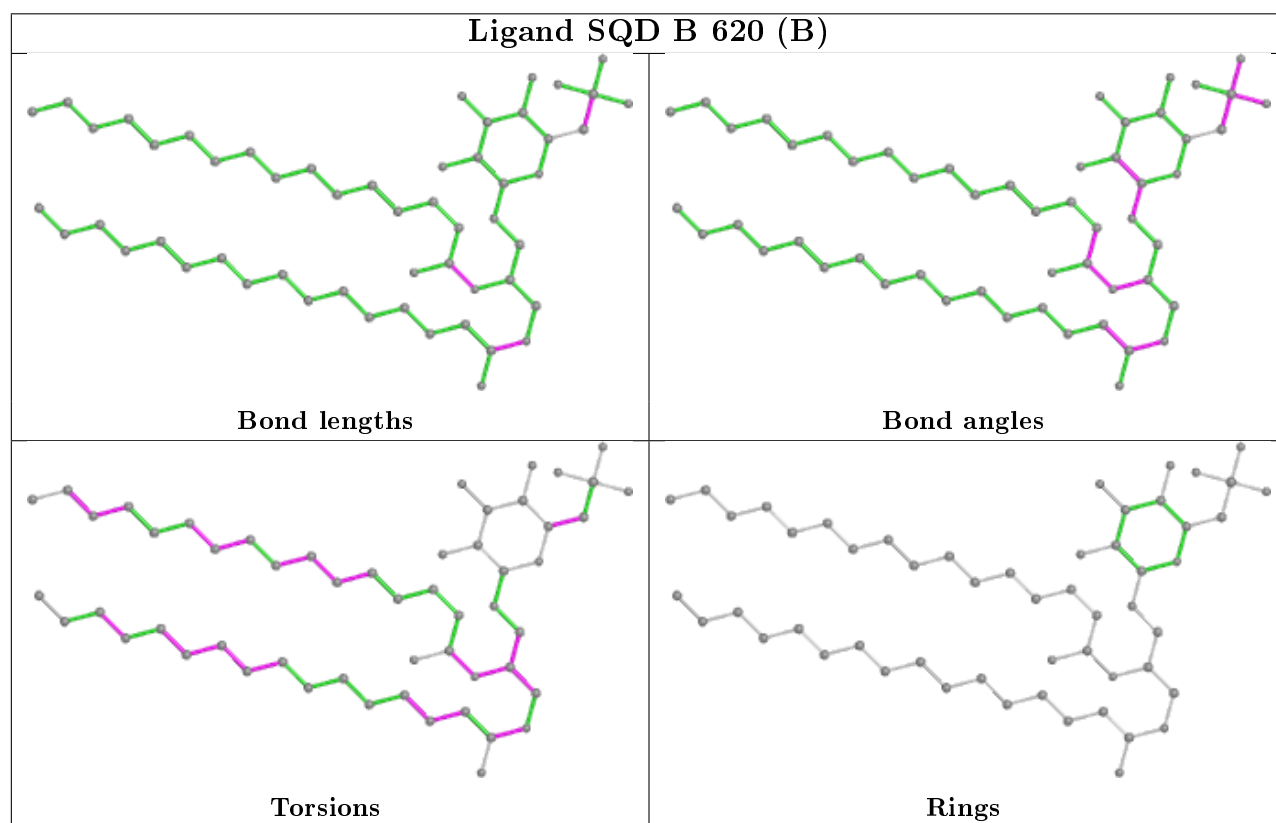
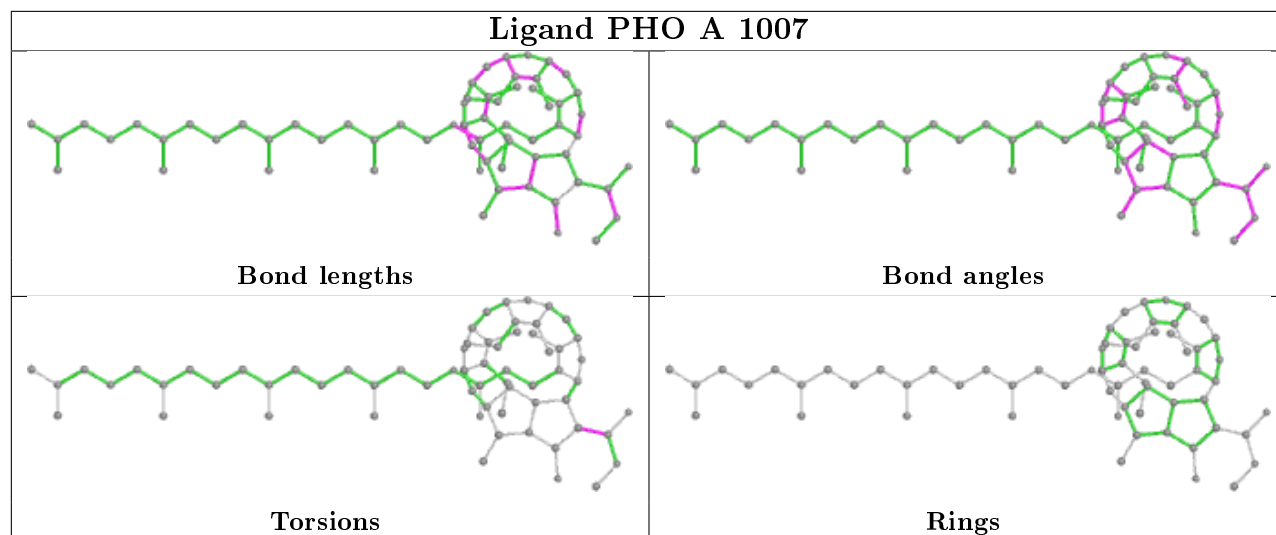




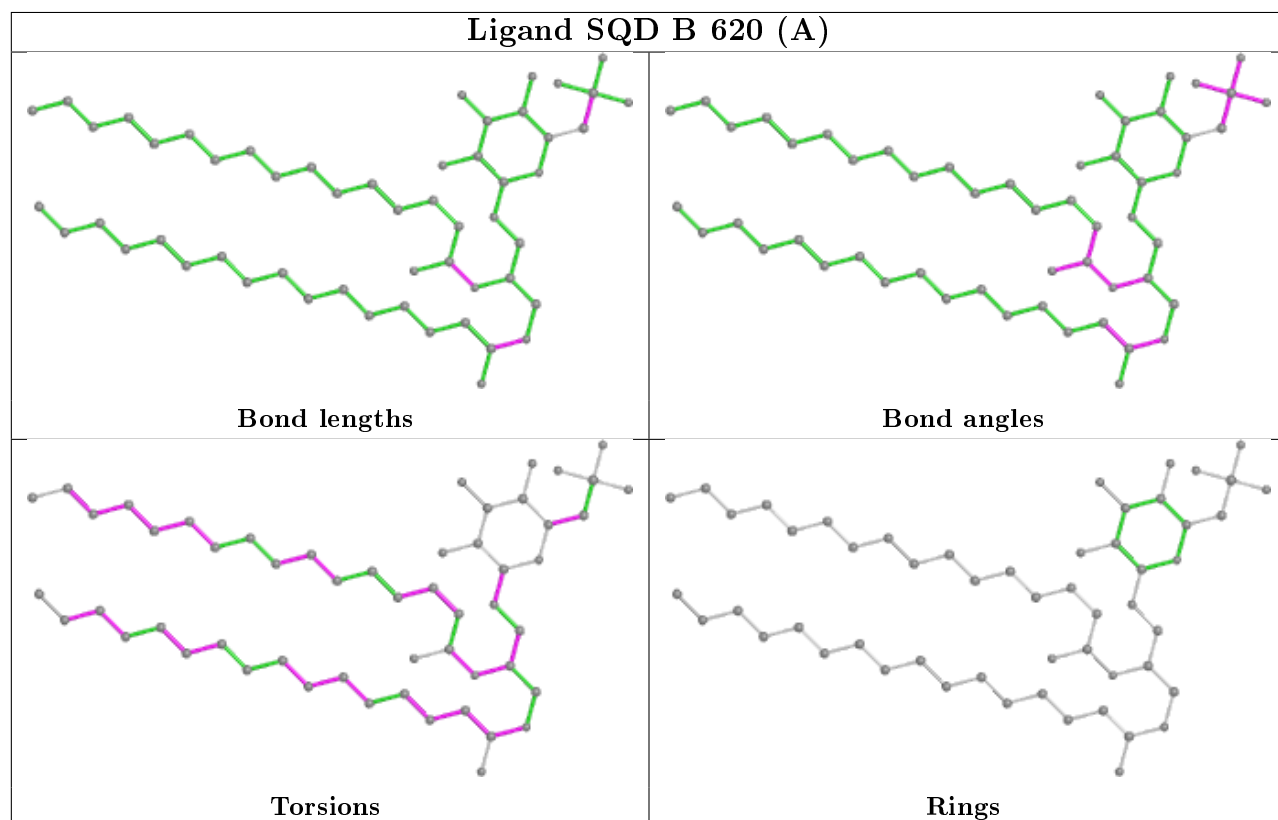
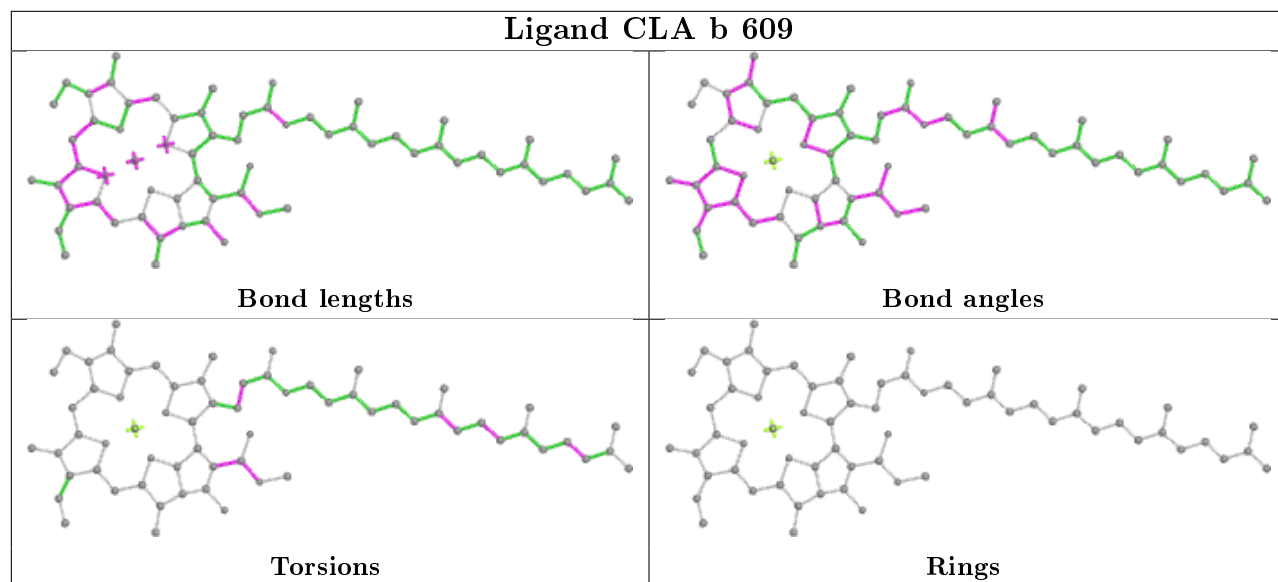


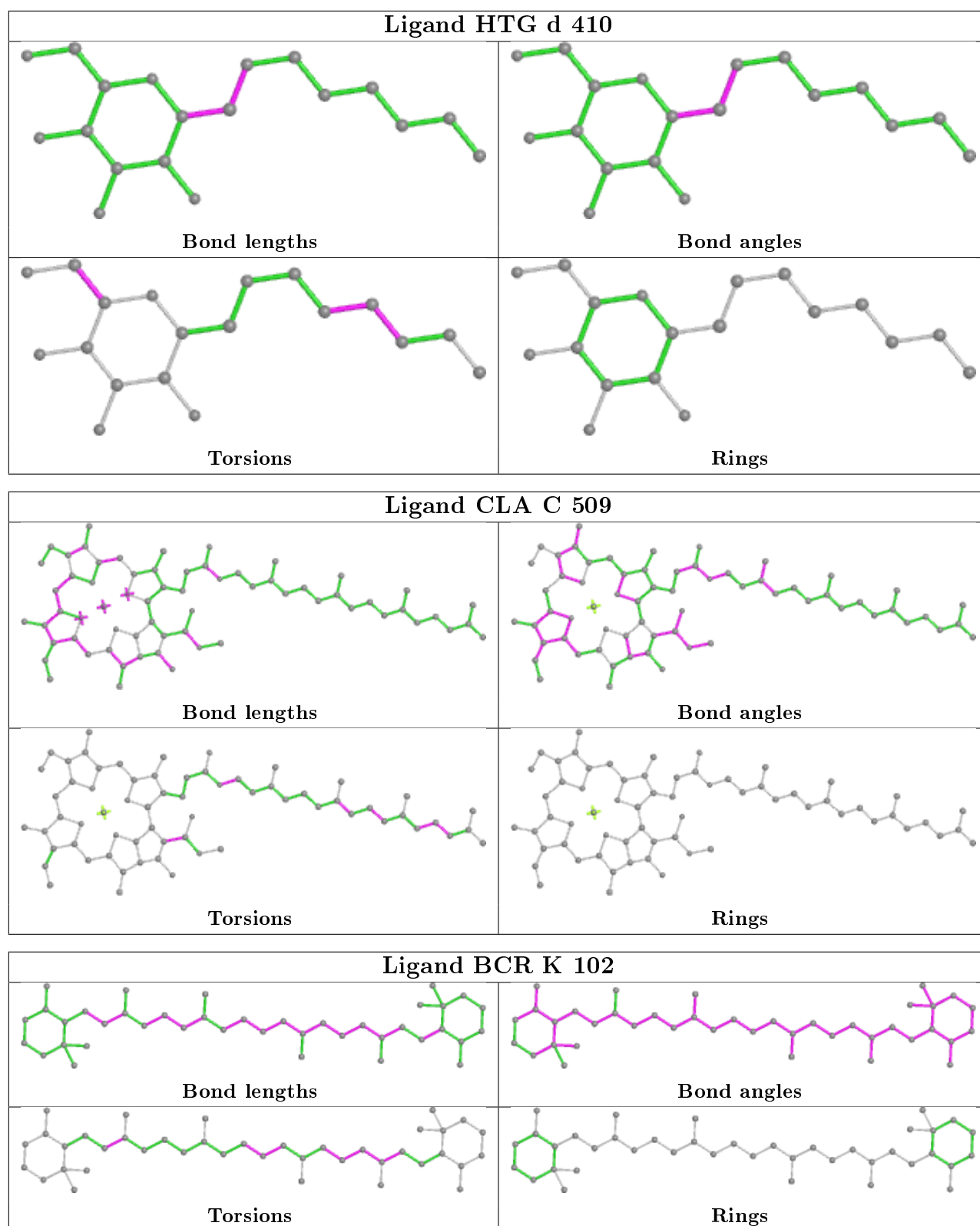


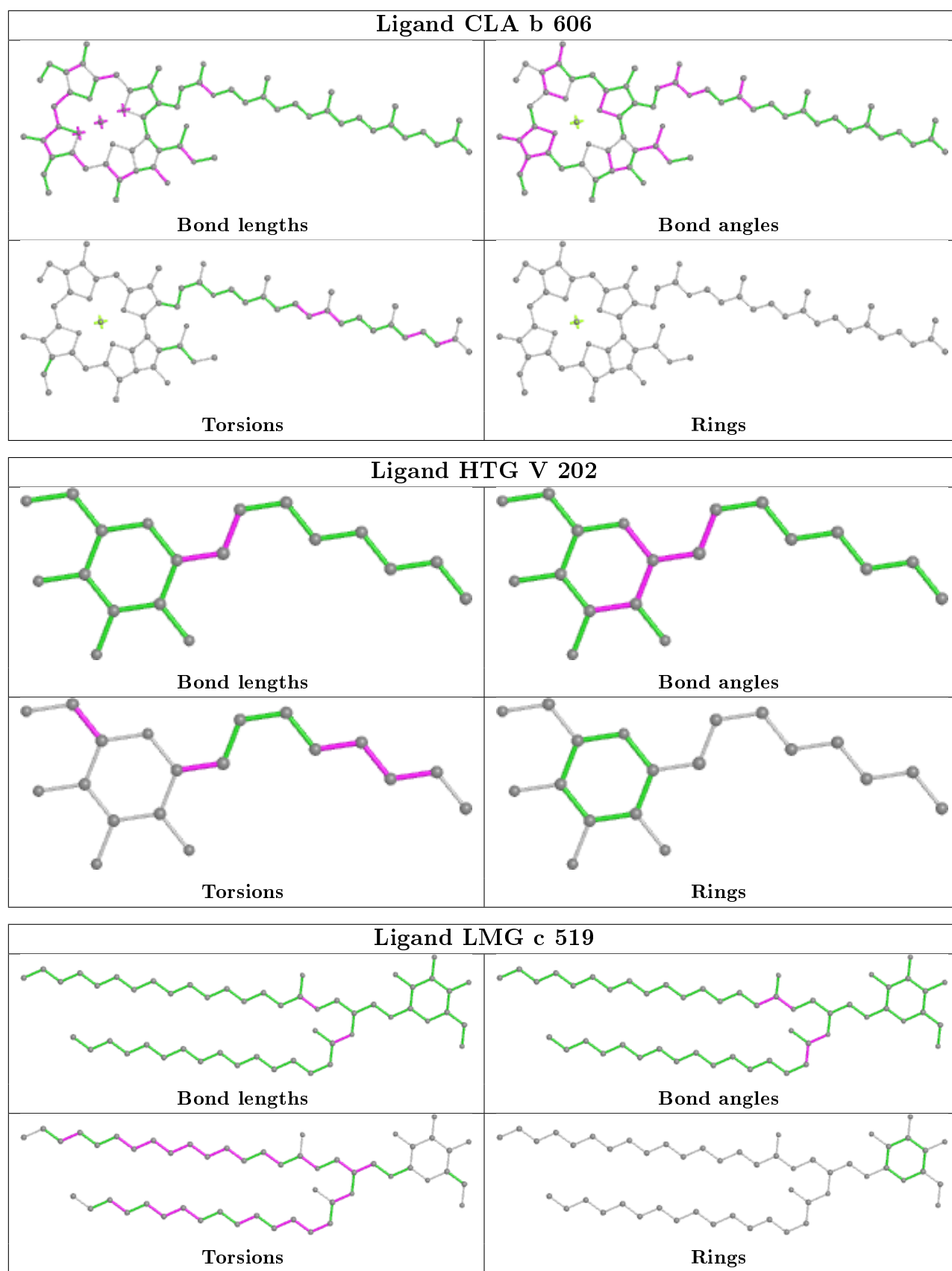


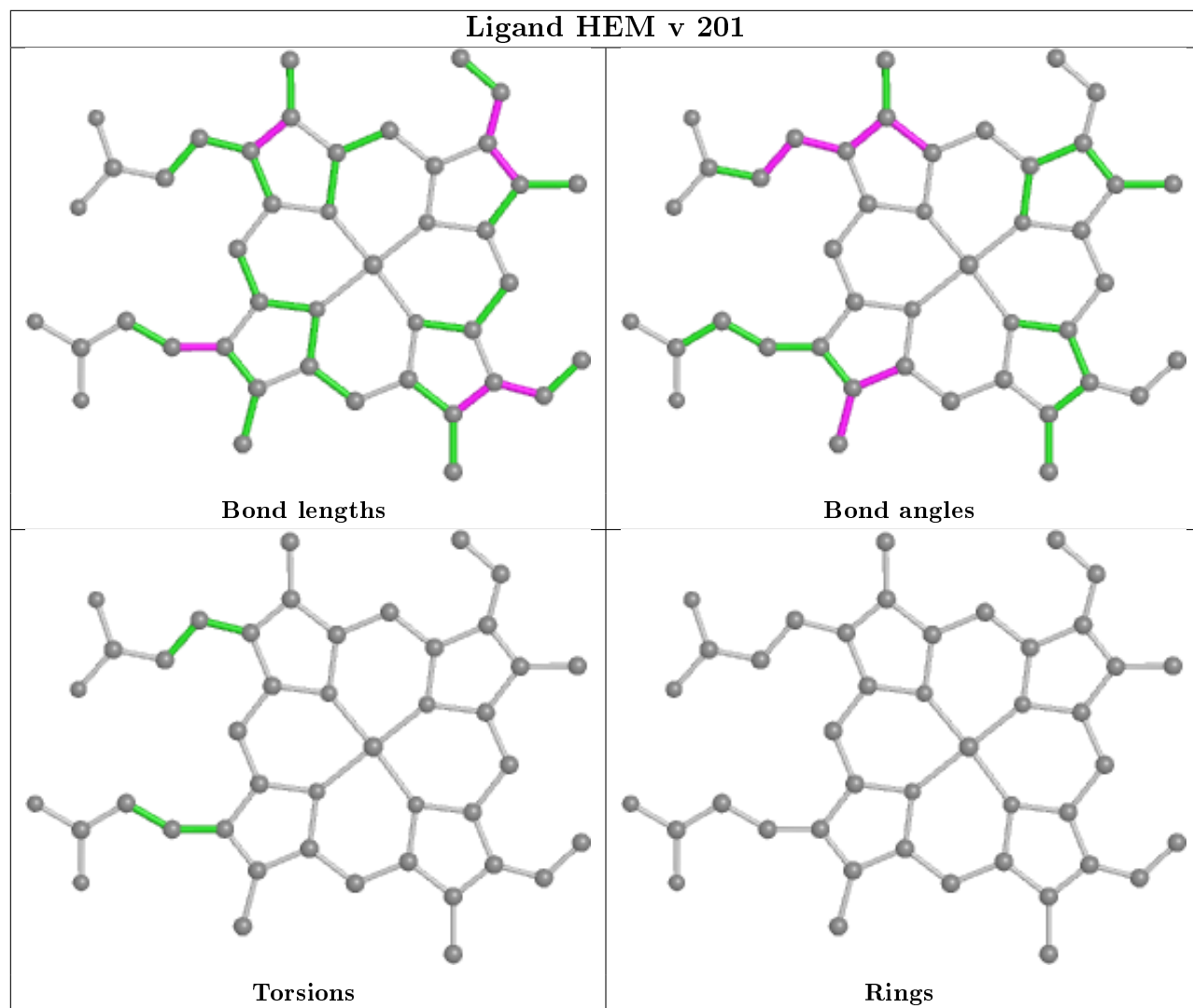


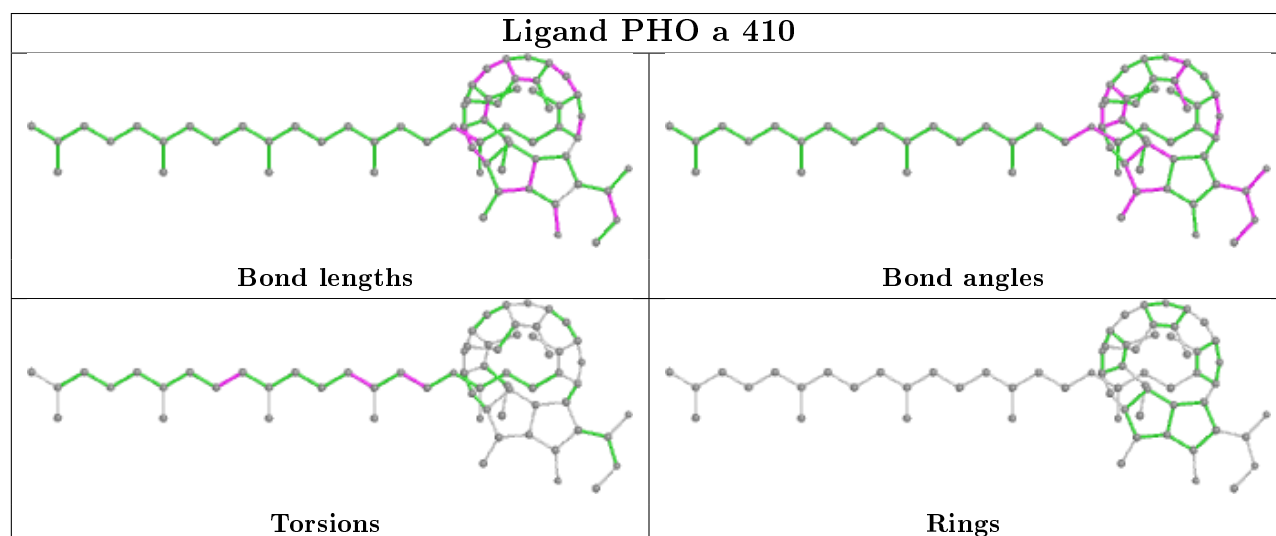
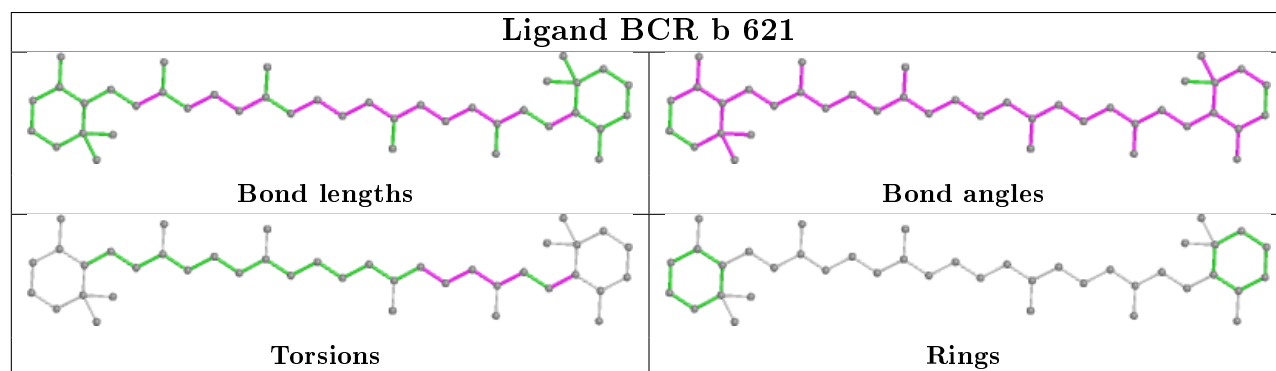
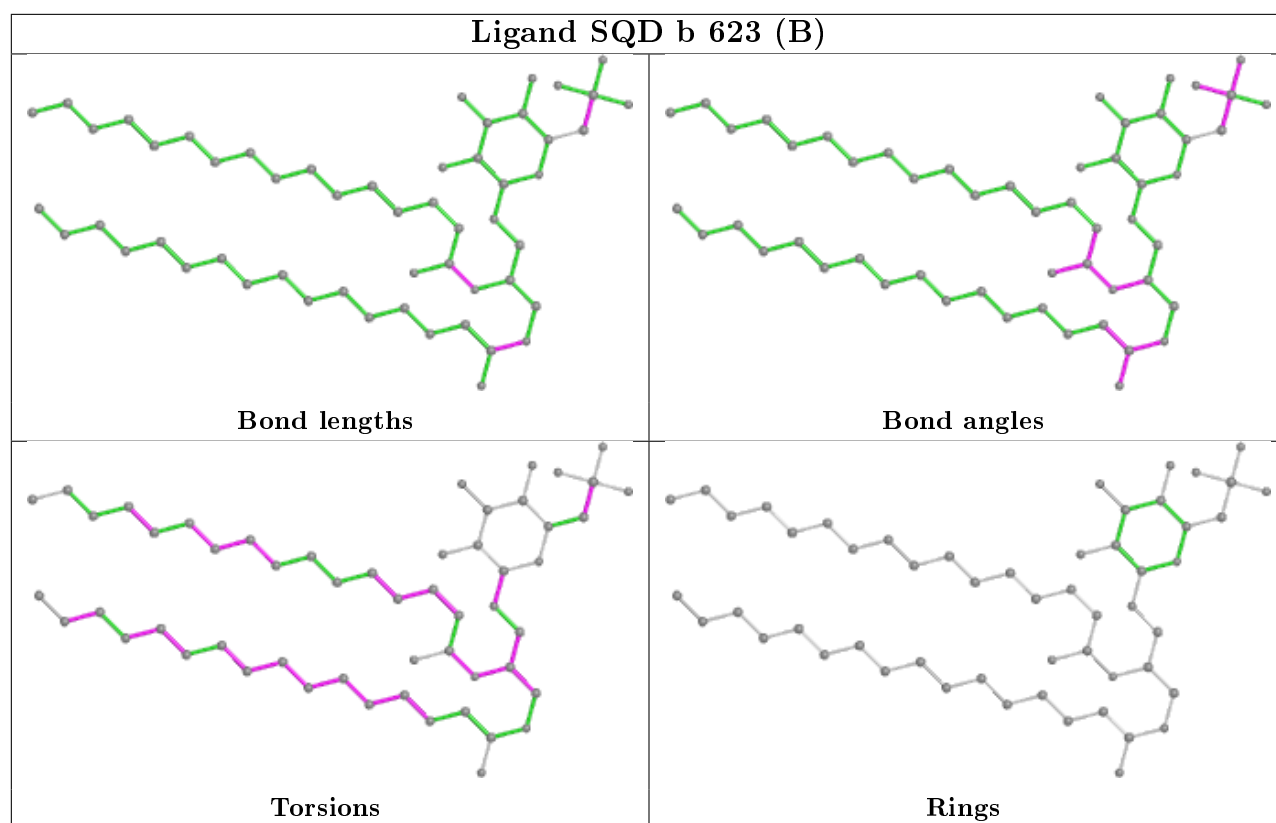


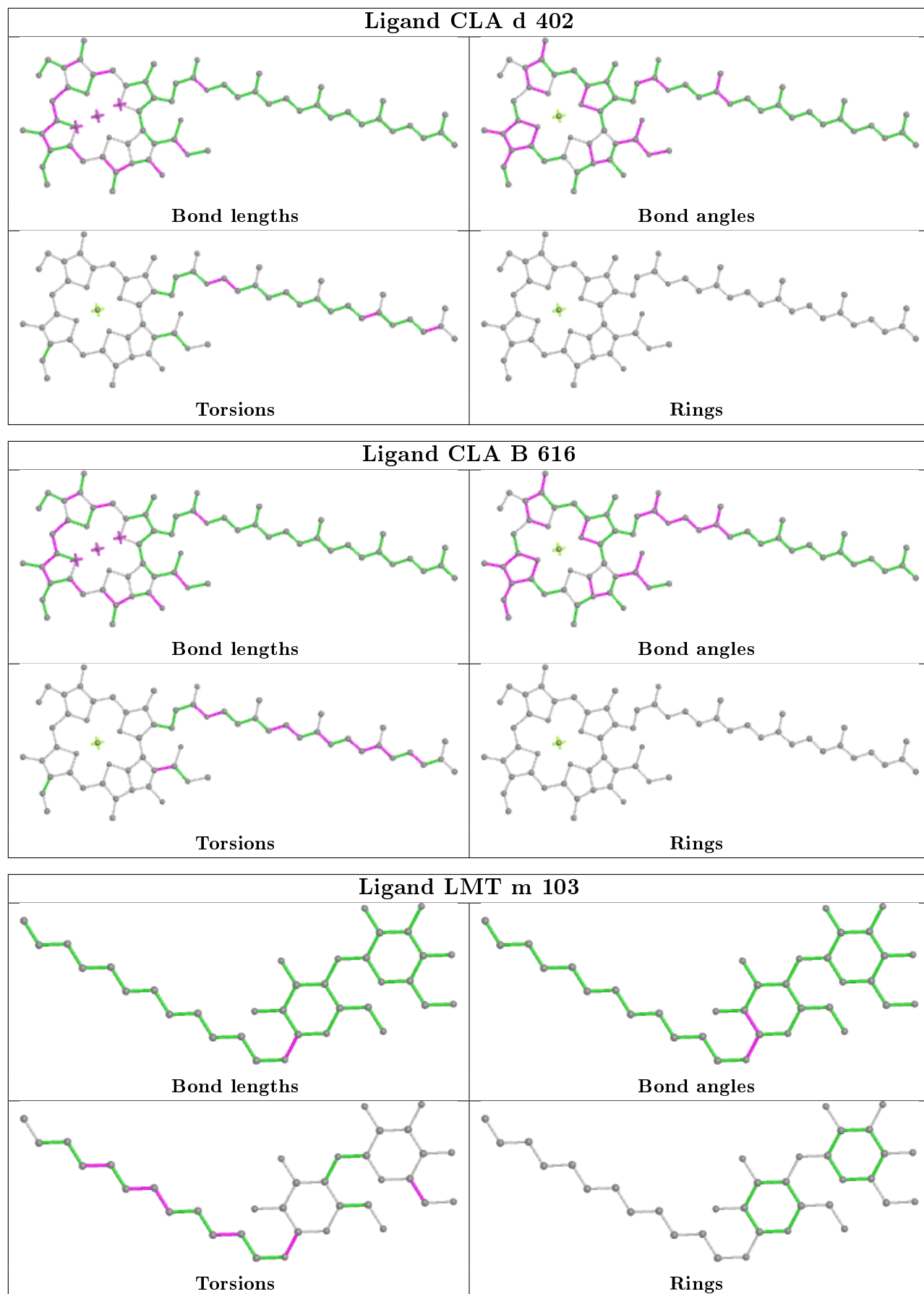


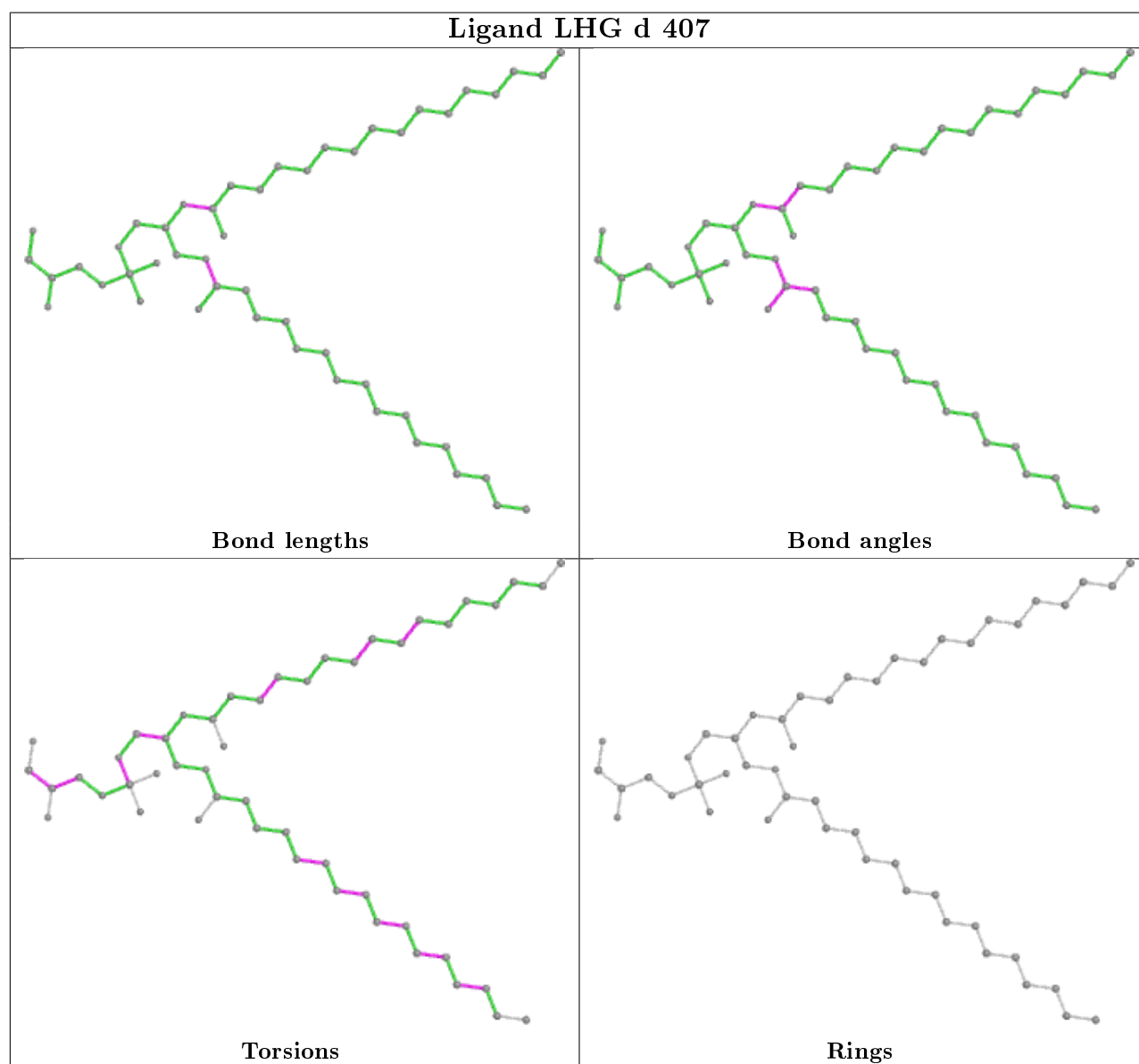
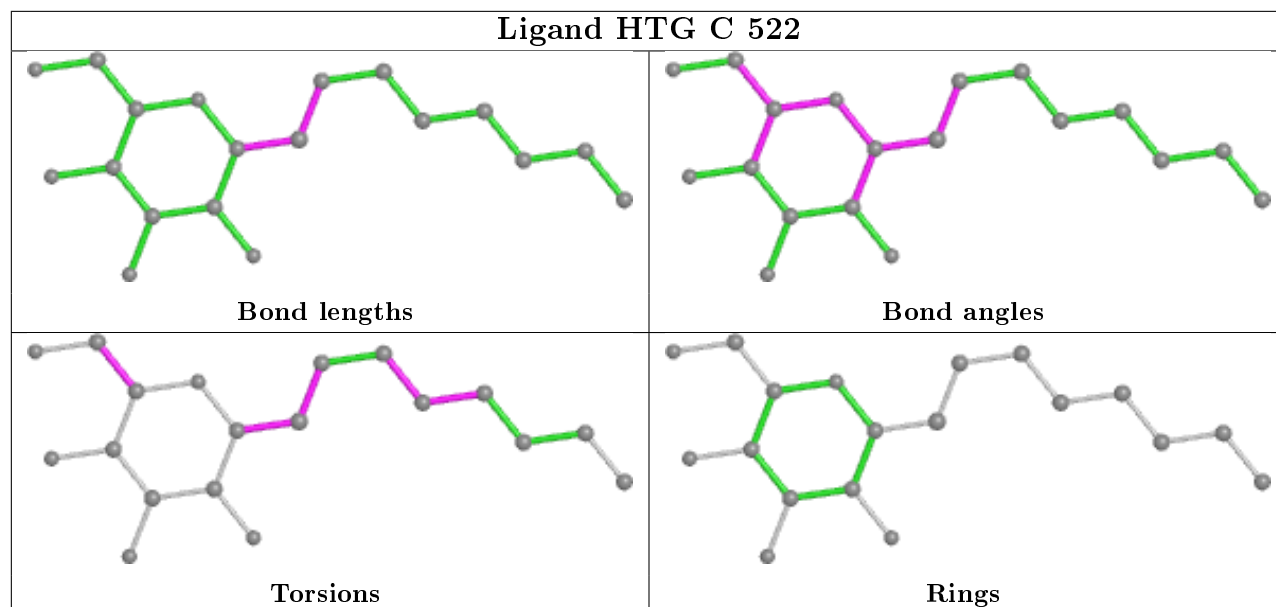


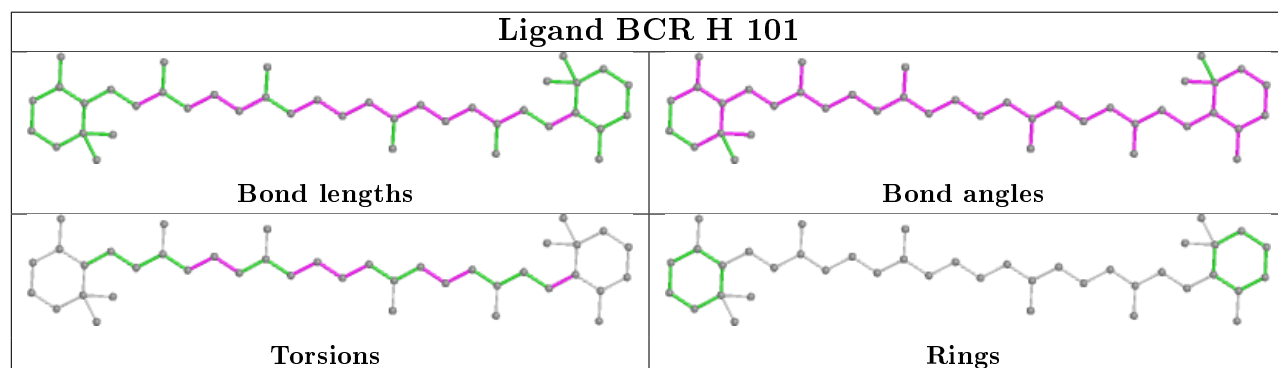
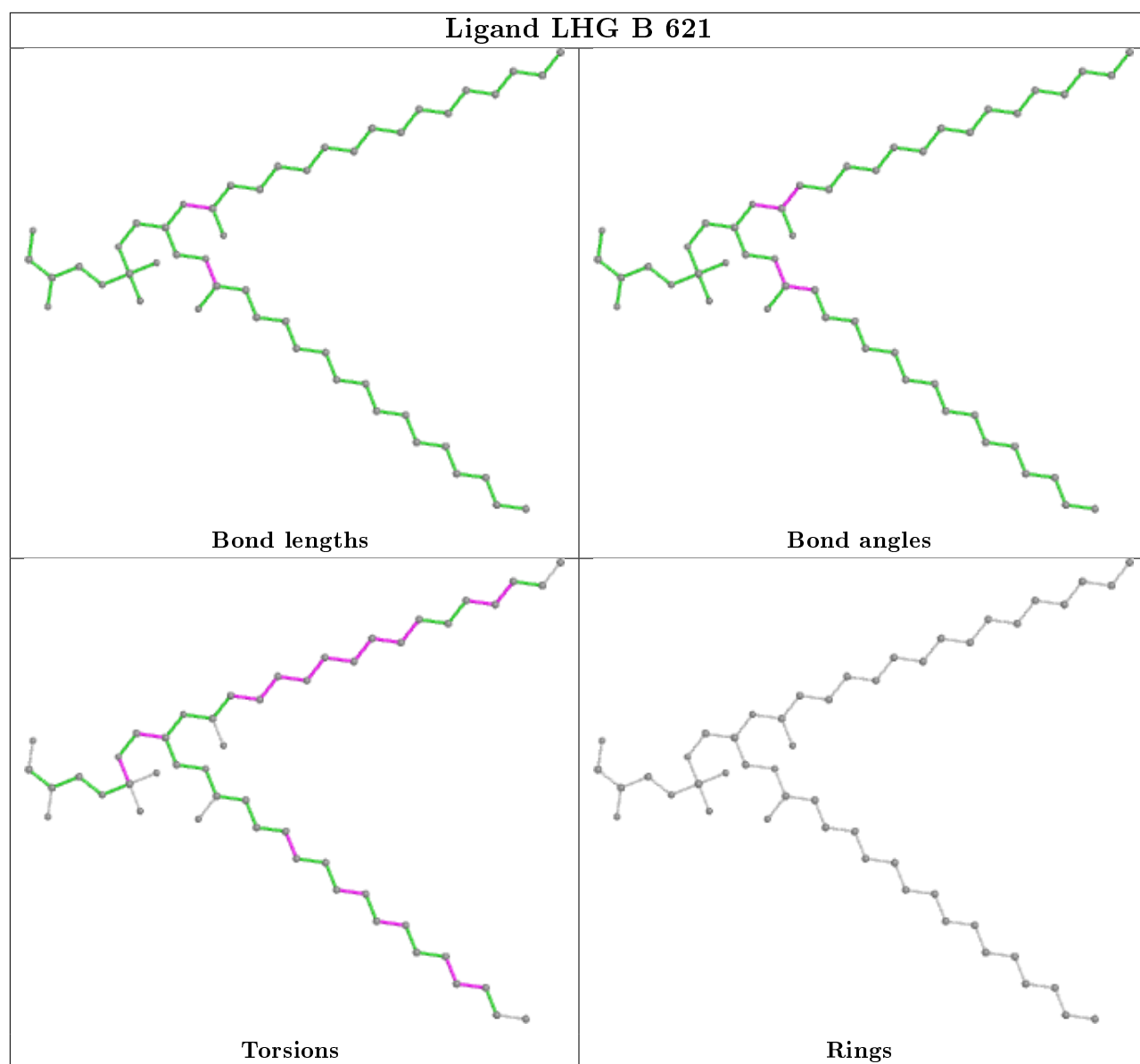




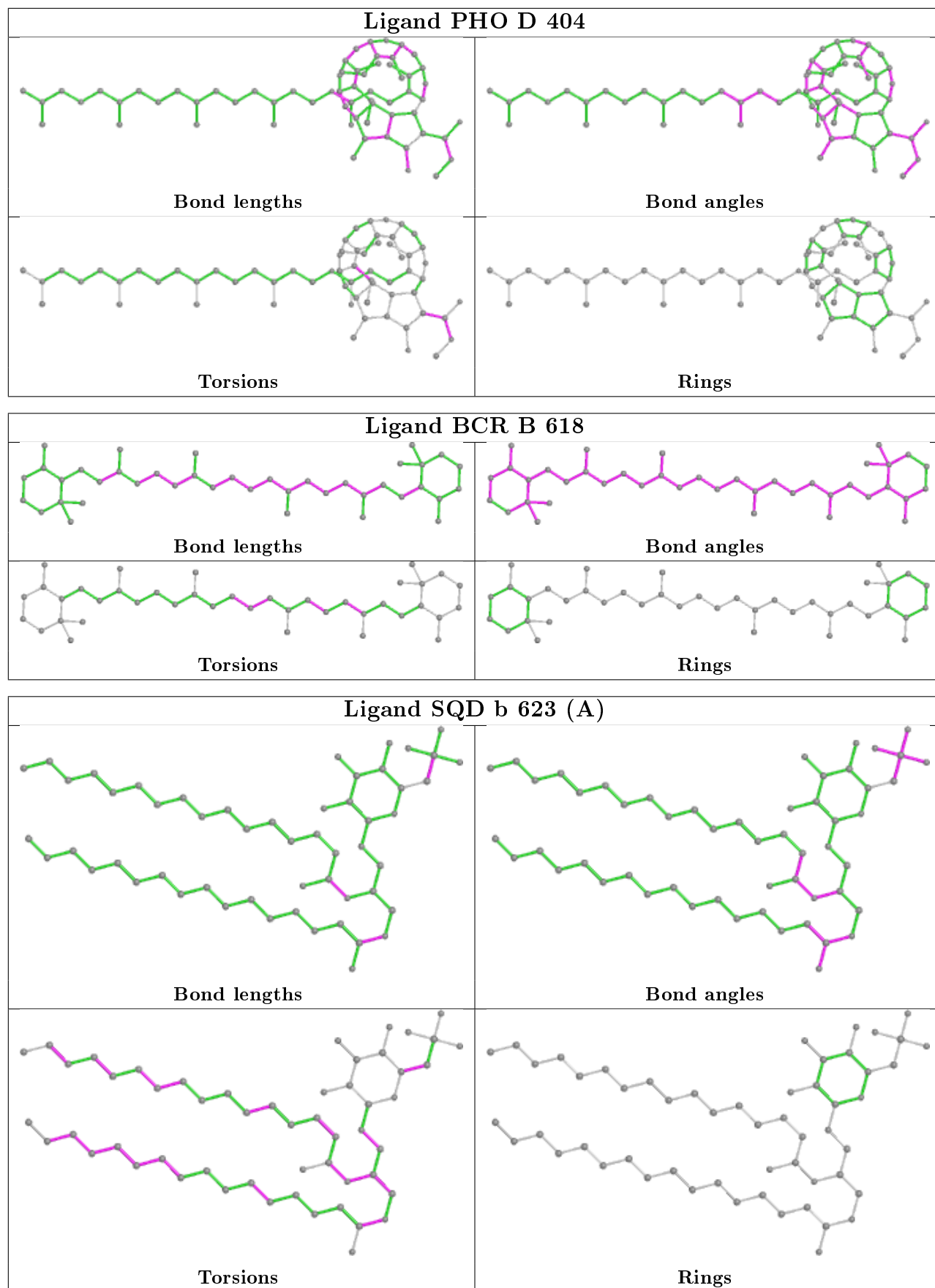


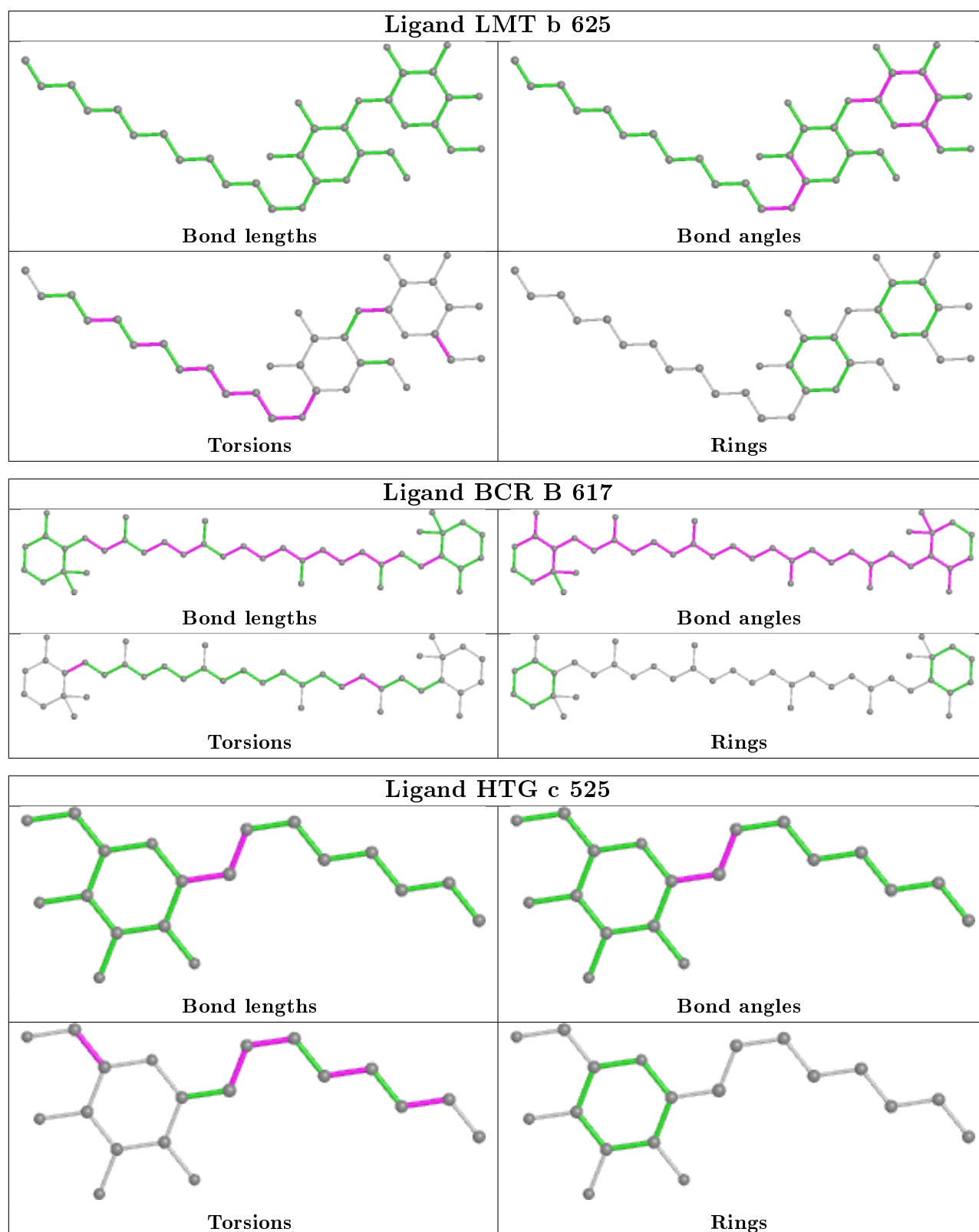


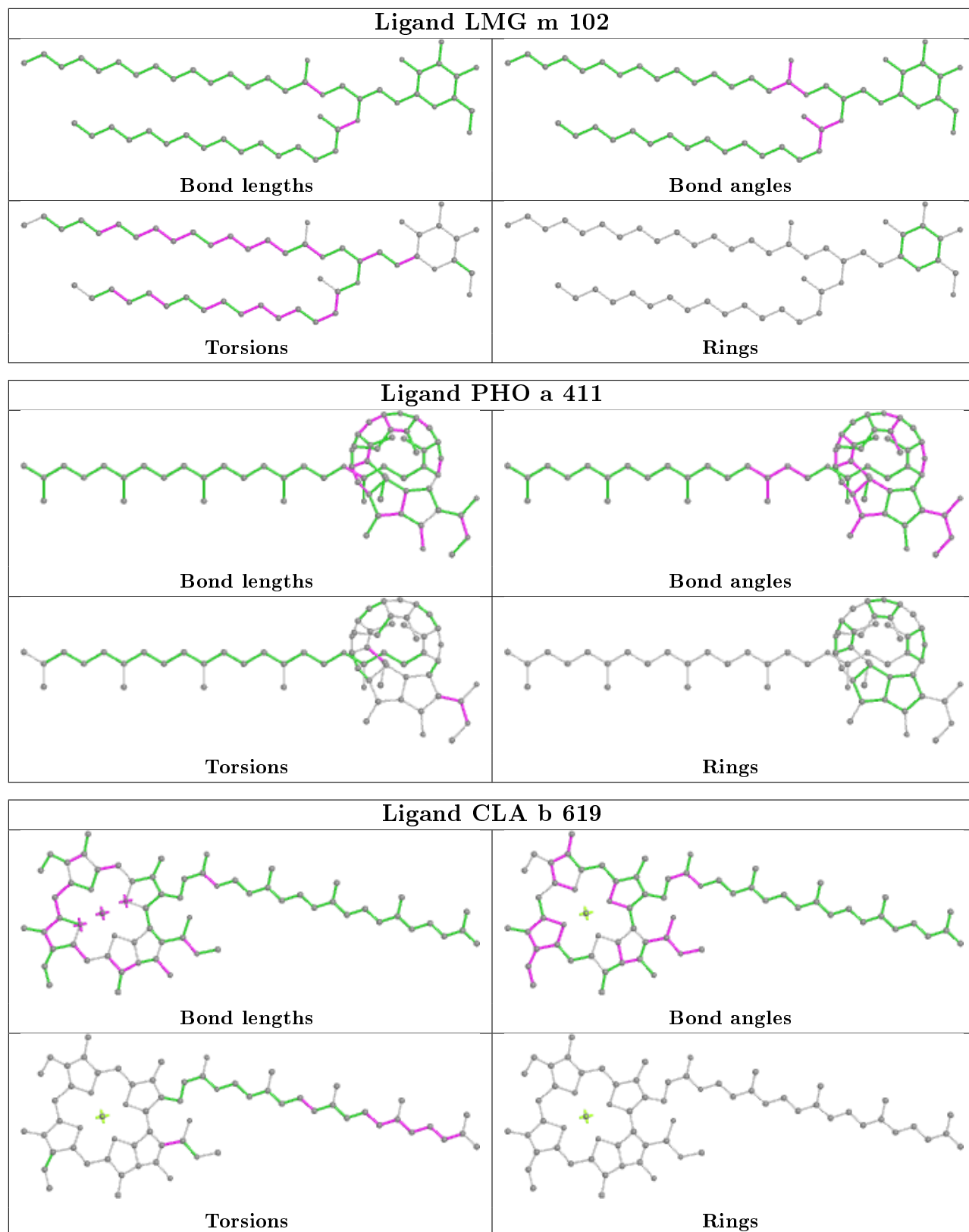


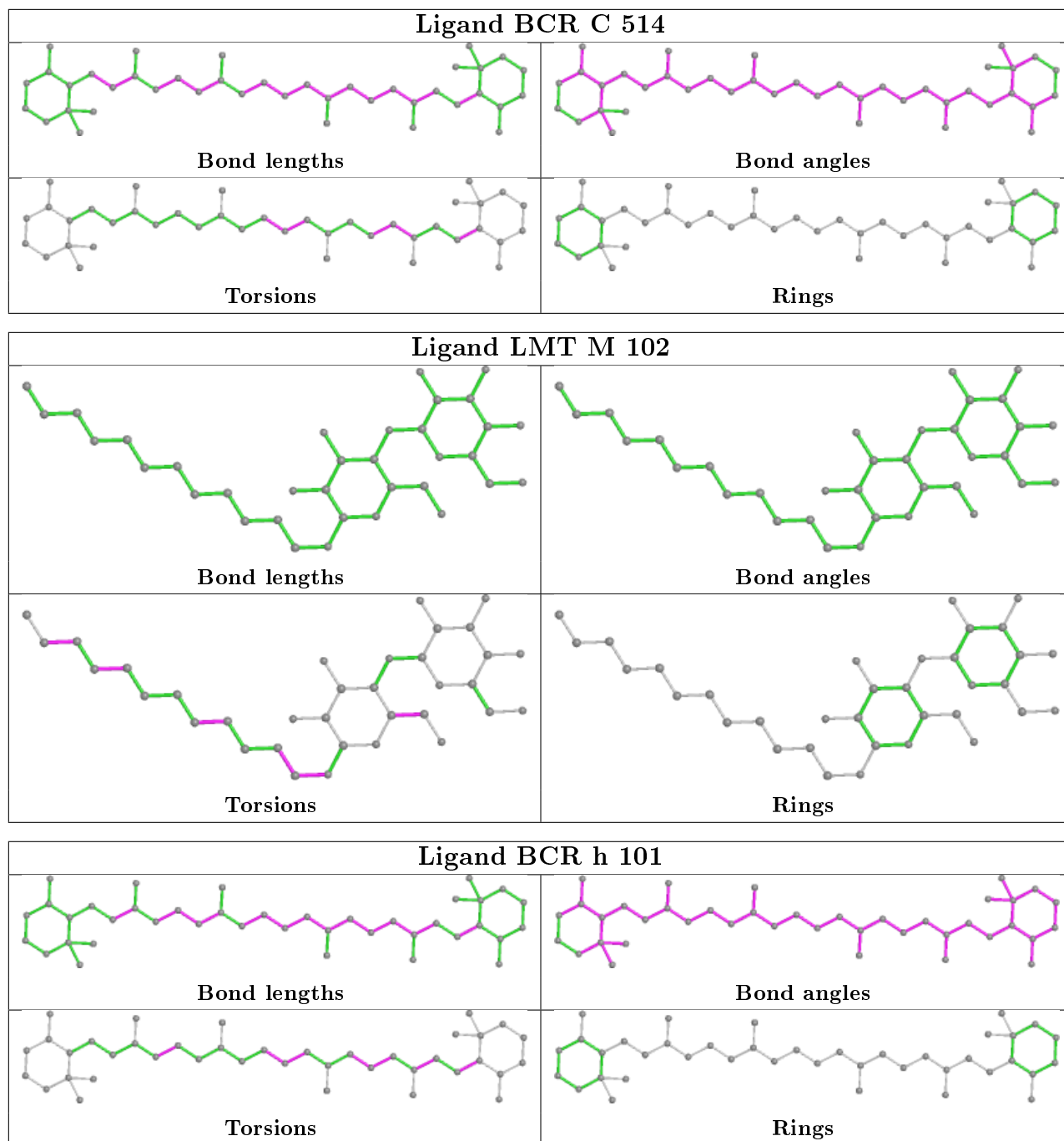


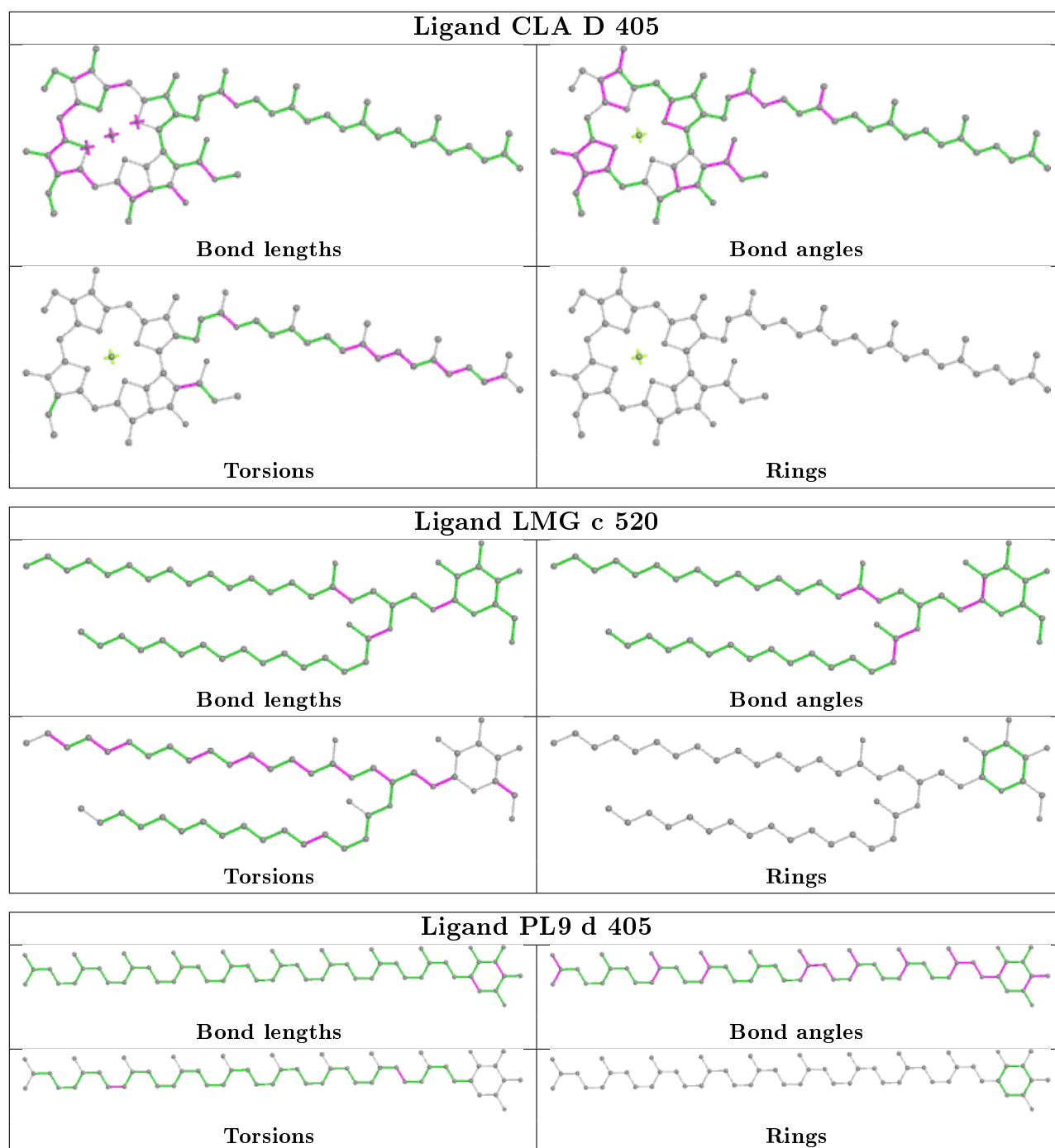


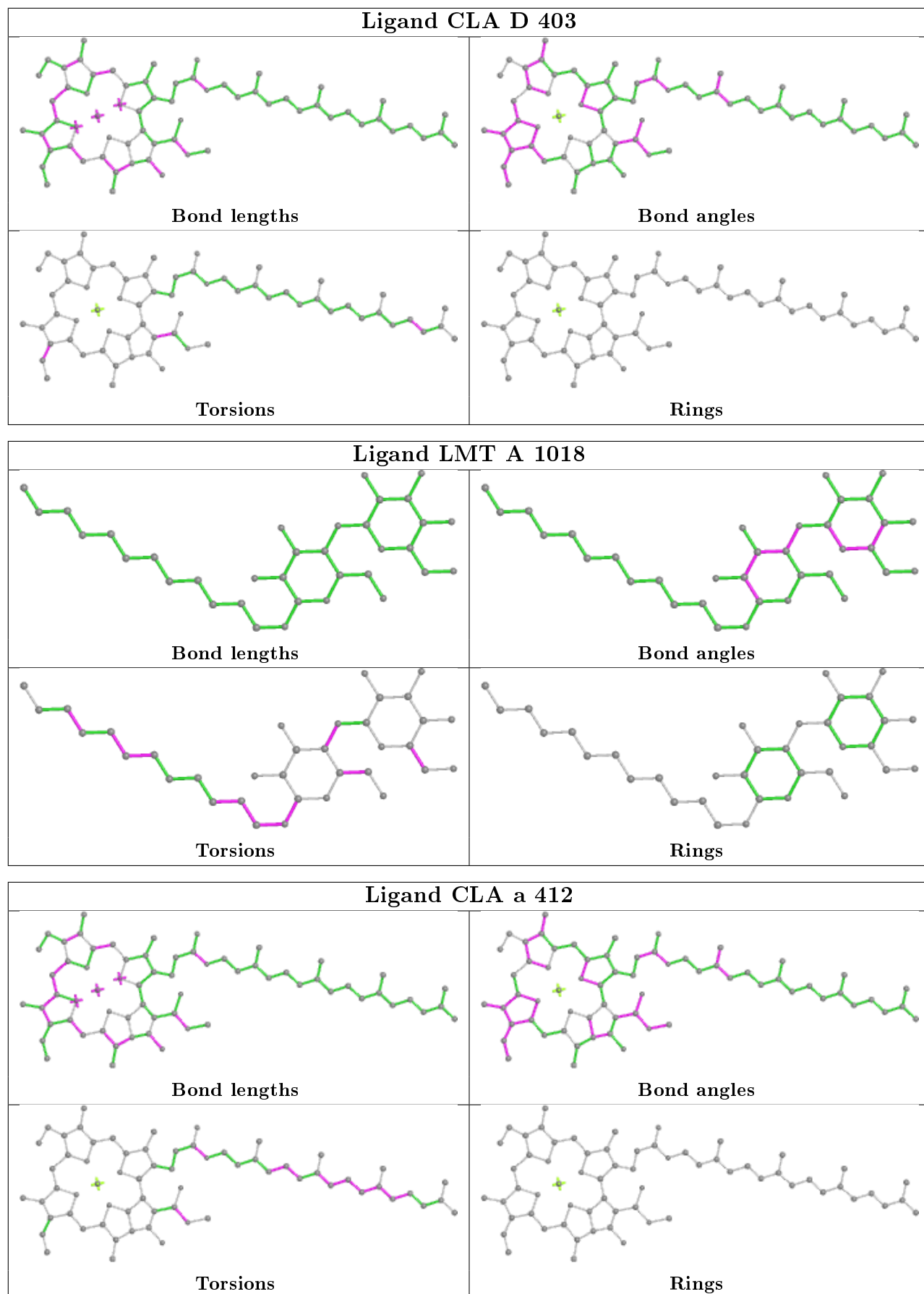


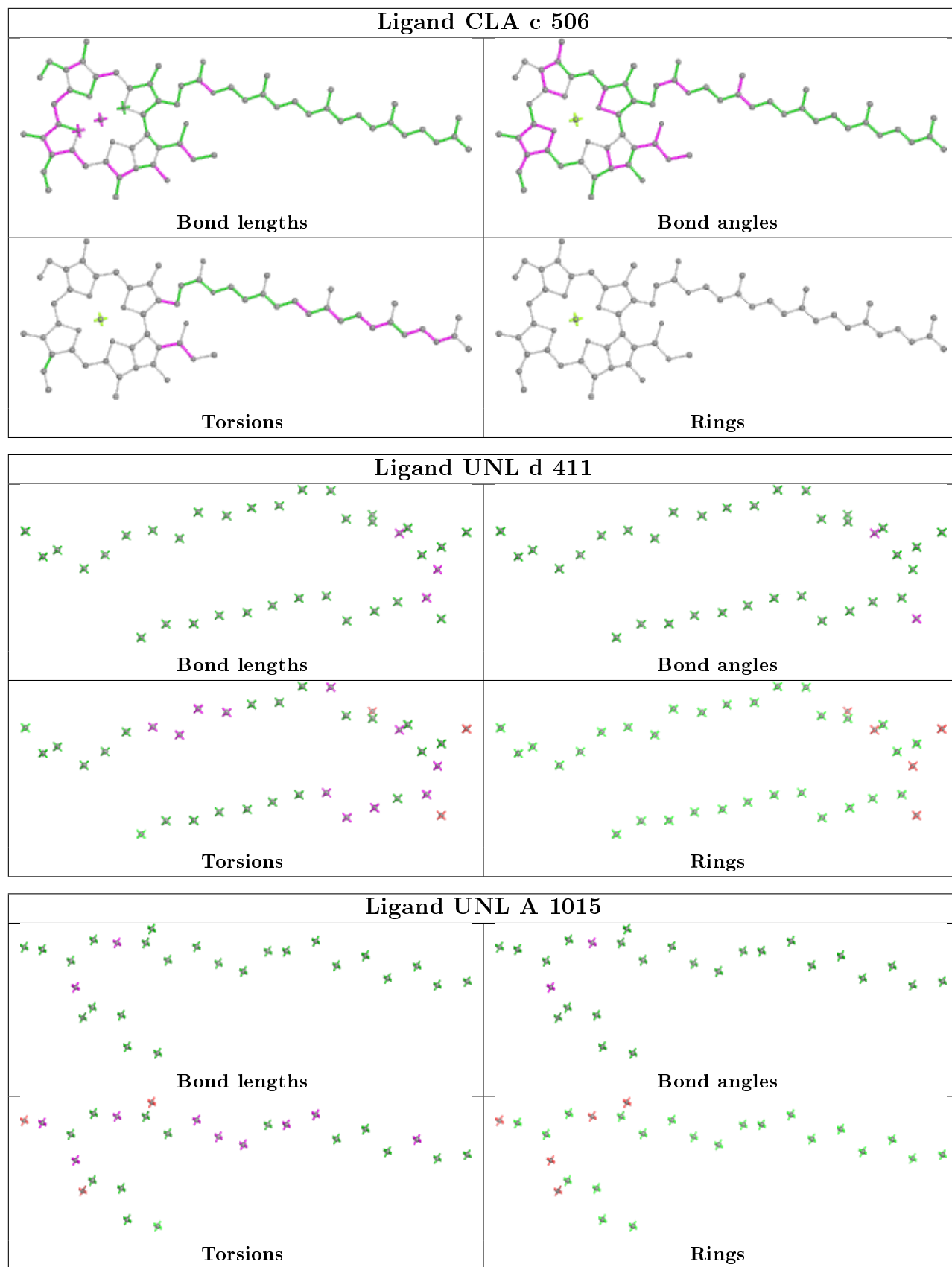


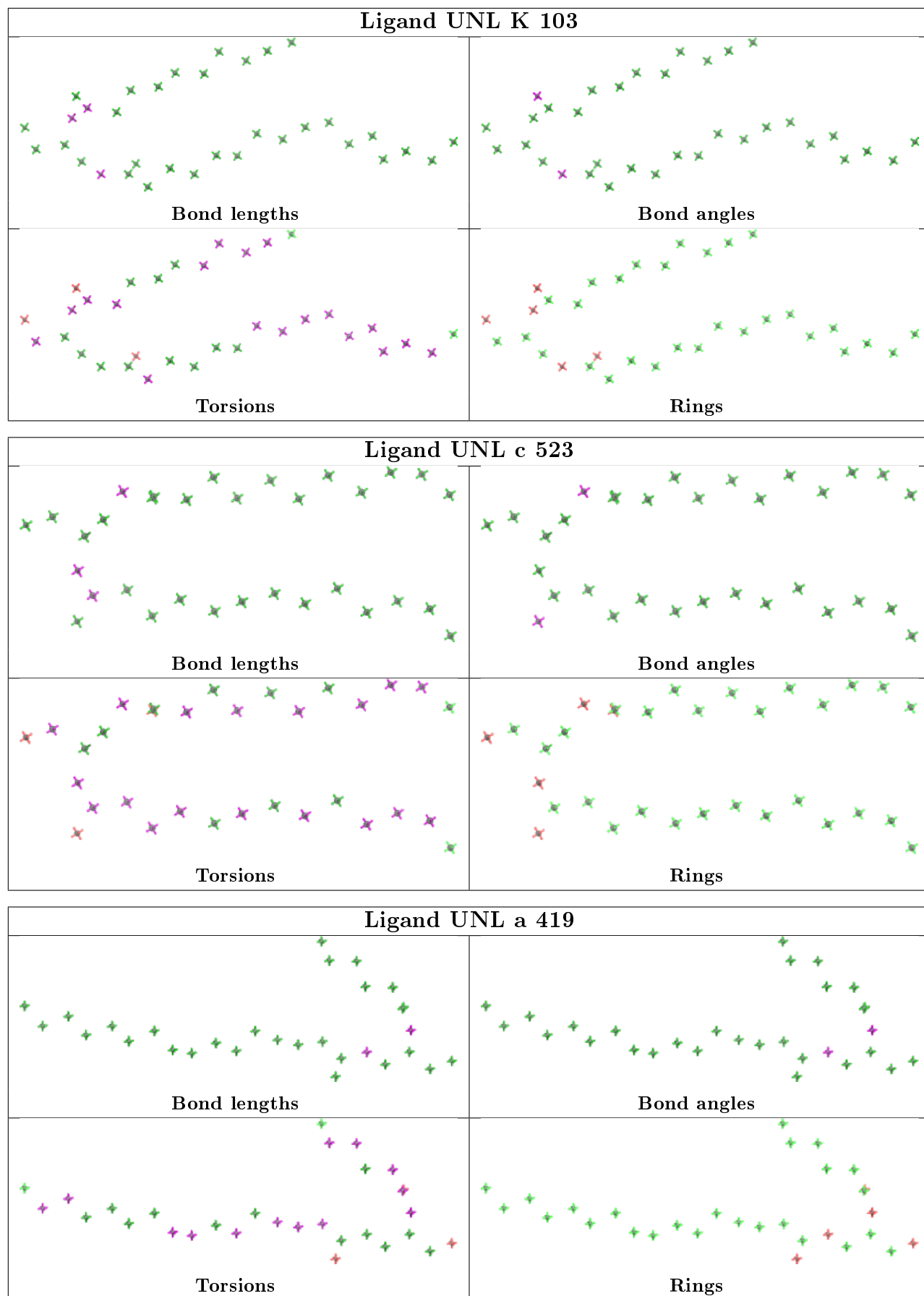




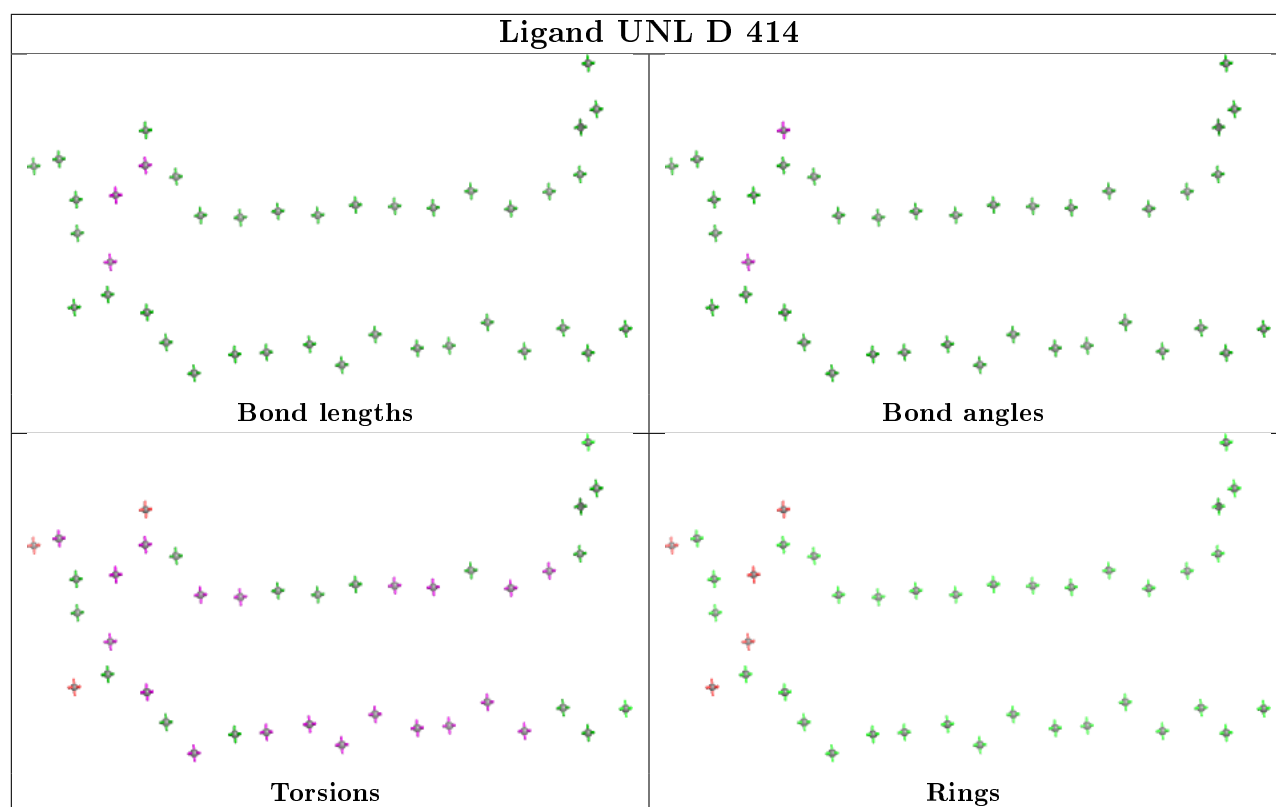












## 5.7 Other polymers [i](#)

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	334/334 (100%)	-0.72	5 (1%) 73 77	19, 25, 44, 64	0
1	a	334/334 (100%)	-0.59	7 (2%) 63 68	21, 28, 51, 72	0
2	B	505/505 (100%)	-0.52	13 (2%) 56 61	20, 29, 50, 69	0
2	b	505/505 (100%)	-0.34	24 (4%) 30 36	21, 31, 59, 88	0
3	C	451/451 (100%)	-0.54	5 (1%) 80 84	22, 33, 47, 72	0
3	c	450/451 (99%)	-0.38	7 (1%) 72 75	26, 38, 51, 68	0
4	D	342/342 (100%)	-0.70	4 (1%) 79 82	18, 26, 39, 88	0
4	d	342/342 (100%)	-0.66	4 (1%) 79 82	21, 29, 46, 80	0
5	E	80/80 (100%)	0.22	8 (10%) 7 9	29, 43, 65, 74	0
5	e	78/80 (97%)	0.51	8 (10%) 6 8	35, 47, 68, 75	0
6	F	34/34 (100%)	-0.36	2 (5%) 22 27	29, 34, 55, 67	0
6	f	32/34 (94%)	-0.04	3 (9%) 8 11	33, 40, 69, 78	0
7	H	63/63 (100%)	-0.21	2 (3%) 47 54	27, 36, 45, 54	0
7	h	63/63 (100%)	-0.14	2 (3%) 47 54	30, 39, 49, 56	0
8	I	35/36 (97%)	-0.04	3 (8%) 10 13	32, 37, 71, 87	0
8	i	35/36 (97%)	0.01	4 (11%) 5 6	32, 37, 71, 92	0
9	J	37/37 (100%)	-0.12	4 (10%) 5 7	28, 37, 84, 92	0
9	j	37/37 (100%)	0.15	4 (10%) 5 7	33, 44, 68, 75	0
10	K	37/37 (100%)	-0.54	0 100 100	33, 38, 50, 52	0
10	k	37/37 (100%)	-0.05	1 (2%) 54 60	38, 44, 61, 71	0
11	L	37/37 (100%)	-0.34	4 (10%) 5 7	21, 24, 57, 73	0
11	l	37/37 (100%)	-0.25	3 (8%) 12 15	22, 25, 63, 88	0
12	M	33/34 (97%)	-0.29	2 (6%) 21 26	24, 27, 51, 76	0
12	m	33/34 (97%)	-0.35	3 (9%) 9 12	25, 29, 52, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/244 (100%)	0.07	21 (8%) 10 13	20, 37, 68, 88	0
13	o	243/244 (99%)	0.02	18 (7%) 14 18	24, 38, 68, 78	0
14	T	30/31 (96%)	-0.26	2 (6%) 17 22	22, 27, 56, 84	0
14	t	29/31 (93%)	-0.33	2 (6%) 16 21	23, 27, 53, 66	0
15	U	97/97 (100%)	-0.33	1 (1%) 82 85	25, 31, 48, 66	0
15	u	97/97 (100%)	-0.37	2 (2%) 63 68	28, 32, 42, 71	0
16	V	137/137 (100%)	-0.57	0 100 100	24, 30, 43, 62	0
16	v	137/137 (100%)	-0.12	6 (4%) 34 40	30, 40, 57, 66	0
17	Y	30/30 (100%)	0.45	3 (10%) 7 9	40, 47, 58, 63	0
17	y	30/30 (100%)	0.63	6 (20%) 1 1	45, 56, 69, 75	0
18	X	40/40 (100%)	0.20	5 (12%) 3 5	33, 40, 65, 80	0
18	x	39/40 (97%)	0.37	6 (15%) 2 2	38, 47, 76, 83	0
19	Z	61/62 (98%)	0.52	12 (19%) 1 1	37, 45, 77, 86	0
19	z	61/62 (98%)	1.01	14 (22%) 0 0	49, 59, 90, 96	0
20	R	34/34 (100%)	3.95	30 (88%) 0 0	71, 86, 100, 101	0
All	All	5280/5296 (99%)	-0.32	250 (4%) 31 37	18, 33, 61, 101	0

The worst 5 of 250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	8.7
19	z	62	VAL	8.1
18	x	2	THR	7.5
3	C	23	ALA	7.4
20	R	18	TRP	7.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.71	0.34	87,91,94,95	0
19	FME	Z	1	10/11	0.75	0.23	69,71,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	t	1	10/11	0.89	0.14	28,30,46,49	0
12	FME	M	1	10/11	0.91	0.12	33,36,43,49	0
12	FME	m	1	10/11	0.92	0.12	35,38,49,54	0
14	FME	T	1	10/11	0.95	0.09	27,29,44,46	0
8	FME	i	1	10/11	0.96	0.08	36,38,40,40	0
8	FME	I	1	10/11	0.97	0.07	34,39,40,40	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
32	LMT	i	102	35/35	0.22	0.41	52,88,111,111	0
32	LMT	A	1018	35/35	0.24	0.44	51,93,113,116	0
31	UNL	b	603	16/-	0.45	0.36	64,67,71,71	0
33	GOL	D	418	6/6	0.46	0.31	70,72,73,74	0
29	LMG	Z	101	51/55	0.48	0.35	47,77,104,110	0
32	LMT	a	402	35/35	0.50	0.32	52,65,69,70	0
32	LMT	m	103	35/35	0.52	0.29	55,90,100,101	0
32	LMT	t	103	35/35	0.53	0.30	46,75,96,99	0
35	HTG	B	624	19/19	0.53	0.41	58,86,92,92	0
32	LMT	b	625	35/35	0.53	0.29	52,82,103,104	0
35	HTG	B	629	19/19	0.53	0.28	52,86,90,90	0
35	HTG	D	413	19/19	0.54	0.31	69,80,85,86	0
35	HTG	c	525	19/19	0.55	0.36	76,90,95,96	0
29	LMG	c	521	51/55	0.56	0.30	53,81,93,97	0
32	LMT	M	101	35/35	0.56	0.29	52,85,95,97	0
35	HTG	d	410	19/19	0.57	0.32	74,84,91,91	0
32	LMT	f	103	35/35	0.58	0.35	71,92,104,104	0
31	UNL	K	103	34/-	0.58	0.23	57,76,82,83	0
31	UNL	Y	101	16/-	0.58	0.28	66,68,70,70	0
35	HTG	b	602	19/19	0.58	0.26	60,89,94,94	0
32	LMT	b	631	35/35	0.59	0.28	40,74,94,96	0
35	HTG	b	630	19/19	0.59	0.35	66,83,88,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	GOL	d	417	6/6	0.60	0.26	58,61,62,62	0
31	UNL	A	1015	28/-	0.61	0.27	62,73,78,78	0
30	DMS	b	635	4/4	0.61	0.29	66,70,72,74	0
34	LHG	e	101	49/49	0.61	0.31	66,97,101,102	0
35	HTG	D	419	19/19	0.62	0.27	59,79,83,84	0
31	UNL	a	419	30/-	0.62	0.29	62,74,87,89	0
32	LMT	A	1017	35/35	0.62	0.31	54,72,75,80	0
31	UNL	c	523	32/-	0.64	0.30	63,75,84,87	0
31	UNL	D	414	40/-	0.64	0.24	48,58,72,73	0
31	UNL	d	411	36/-	0.65	0.21	46,56,78,79	0
34	LHG	E	101	49/49	0.67	0.26	51,77,83,85	0
35	HTG	d	416	19/19	0.68	0.33	70,92,94,96	0
31	UNL	j	101	16/-	0.68	0.16	58,60,62,63	0
33	GOL	d	415	6/6	0.69	0.20	63,66,66,67	0
32	LMT	B	623	35/35	0.69	0.24	48,65,71,72	0
31	UNL	i	101	16/-	0.69	0.22	55,57,62,62	0
29	LMG	c	520	51/55	0.69	0.26	42,74,84,89	0
33	GOL	V	204	6/6	0.70	0.34	57,58,59,60	0
30	DMS	b	634	4/4	0.70	0.24	61,63,65,68	0
33	GOL	b	632	6/6	0.70	0.26	51,56,61,63	0
31	UNL	y	102	16/-	0.72	0.20	63,65,67,67	0
32	LMT	m	101	35/35	0.73	0.20	38,51,56,57	0
32	LMT	M	102	35/35	0.73	0.20	39,58,64,66	0
29	LMG	C	519	51/55	0.73	0.28	38,74,84,85	0
30	DMS	O	301	4/4	0.73	0.30	72,73,75,76	0
31	UNL	t	102	16/-	0.74	0.18	68,72,74,74	0
28	SQD	b	623[B]	54/54	0.75	0.25	49,57,77,80	54
33	GOL	v	204	6/6	0.75	0.24	74,75,76,76	0
28	SQD	b	623[A]	54/54	0.75	0.25	41,53,70,71	54
33	GOL	V	207	6/6	0.76	0.19	60,63,64,64	0
32	LMT	C	520	35/35	0.77	0.27	68,75,79,79	0
35	HTG	B	628	19/19	0.77	0.20	45,68,72,74	0
31	UNL	J	102	16/-	0.78	0.16	50,52,58,59	0
31	UNL	x	101	16/-	0.78	0.17	41,45,59,60	0
28	SQD	B	620[A]	54/54	0.79	0.24	42,56,75,76	54
30	DMS	B	633	4/4	0.79	0.24	67,69,70,75	0
28	SQD	B	620[B]	54/54	0.79	0.24	40,54,66,66	54
28	SQD	f	102	43/54	0.79	0.28	61,80,89,91	0
29	LMG	c	519	51/55	0.80	0.18	45,62,77,80	0
27	PL9	a	414	55/55	0.80	0.21	53,63,77,78	0
32	LMT	a	416	35/35	0.80	0.32	73,75,79,79	0
35	HTG	C	522	19/19	0.80	0.26	65,75,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
31	UNL	l	101	16/-	0.80	0.21	49,58,68,69	0
33	GOL	v	203	6/6	0.80	0.20	48,52,53,53	0
31	UNL	b	627	16/-	0.80	0.12	47,48,50,50	0
31	UNL	B	630	16/-	0.81	0.24	53,56,60,60	0
35	HTG	o	301	19/19	0.81	0.18	47,49,53,53	0
31	UNL	I	101	13/-	0.81	0.27	54,56,56,57	0
29	LMG	a	415	51/55	0.81	0.17	50,60,70,71	0
35	HTG	V	202	19/19	0.81	0.30	56,63,77,77	0
35	HTG	c	522	19/19	0.81	0.28	82,85,89,90	0
35	HTG	b	626	19/19	0.82	0.17	43,48,51,51	0
28	SQD	A	1016	54/54	0.82	0.17	46,60,72,73	0
27	PL9	A	1010	55/55	0.83	0.19	43,55,72,72	0
30	DMS	c	528	4/4	0.83	0.21	83,85,86,88	0
29	LMG	A	1012	51/55	0.83	0.17	49,56,67,71	0
31	UNL	L	101	16/-	0.83	0.21	53,56,63,63	0
29	LMG	C	518	51/55	0.83	0.18	36,62,70,70	0
30	DMS	a	418	4/4	0.84	0.20	62,63,66,69	0
28	SQD	a	401	54/54	0.84	0.16	42,60,74,76	0
24	CLA	B	601	65/65	0.84	0.16	34,42,66,69	0
35	HTG	C	521	19/19	0.84	0.22	69,71,74,75	0
33	GOL	V	206	6/6	0.84	0.30	53,56,57,58	0
24	CLA	b	604	65/65	0.84	0.17	40,48,69,70	0
31	UNL	B	625	16/-	0.85	0.13	44,46,52,54	0
31	UNL	X	101	16/-	0.85	0.14	39,43,51,51	0
26	BCR	K	102	40/40	0.85	0.12	39,49,52,52	0
31	UNL	I	102	13/-	0.85	0.14	55,57,60,60	0
24	CLA	c	513	65/65	0.86	0.16	45,54,69,70	0
24	CLA	C	513	65/65	0.86	0.15	41,48,66,68	0
29	LMG	B	622	51/55	0.86	0.14	38,47,58,64	0
29	LMG	m	102	51/55	0.87	0.13	35,49,57,59	0
33	GOL	A	1019	6/6	0.87	0.20	60,61,62,62	0
26	BCR	k	102	40/40	0.87	0.14	48,54,64,66	0
30	DMS	C	525	4/4	0.87	0.24	71,73,73,74	0
29	LMG	d	409	51/55	0.87	0.16	33,42,72,76	0
30	DMS	b	633	4/4	0.87	0.15	55,55,56,62	0
24	CLA	b	619	65/65	0.88	0.15	31,35,80,81	0
30	DMS	C	527	4/4	0.88	0.26	75,75,77,80	0
24	CLA	C	512	65/65	0.88	0.13	39,42,71,72	0
30	DMS	d	413	4/4	0.88	0.21	57,62,62,63	0
30	DMS	c	527	4/4	0.88	0.25	65,65,66,66	0
24	CLA	c	506	65/65	0.88	0.15	38,40,78,81	0
30	DMS	V	205	4/4	0.89	0.17	61,62,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	GOL	B	631	6/6	0.89	0.24	56,57,60,62	0
35	HTG	b	601	19/19	0.89	0.14	44,60,67,67	0
31	UNL	d	412	16/-	0.89	0.18	48,53,62,63	0
26	BCR	d	404	40/40	0.89	0.11	31,36,59,59	0
31	UNL	D	415	16/-	0.89	0.13	39,42,48,49	0
24	CLA	B	616	65/65	0.89	0.16	27,31,79,80	0
24	CLA	d	403	65/65	0.89	0.14	31,34,76,77	0
36	DGD	c	516	62/66	0.90	0.12	36,42,75,79	0
29	LMG	D	412	51/55	0.90	0.15	27,38,77,78	0
26	BCR	D	406	40/40	0.90	0.11	28,32,50,51	0
28	SQD	c	518	54/54	0.90	0.14	41,59,74,76	0
26	BCR	h	101	40/40	0.90	0.12	32,39,47,48	0
30	DMS	D	417	4/4	0.91	0.19	57,58,62,64	0
33	GOL	a	420	6/6	0.91	0.15	53,56,57,59	0
30	DMS	U	201	4/4	0.91	0.19	56,56,58,58	0
30	DMS	A	1014	4/4	0.91	0.20	54,54,55,61	0
24	CLA	c	512	65/65	0.91	0.12	42,46,65,67	0
26	BCR	K	101	40/40	0.91	0.13	32,35,37,38	0
30	DMS	B	634	4/4	0.91	0.27	54,57,59,59	0
30	DMS	C	526	4/4	0.91	0.18	71,71,72,72	0
28	SQD	D	408	43/54	0.91	0.18	41,67,74,76	0
28	SQD	A	1011	54/54	0.91	0.15	43,57,69,69	0
26	BCR	c	514	40/40	0.91	0.11	34,41,43,44	0
36	DGD	h	102	62/66	0.91	0.11	32,38,46,48	0
24	CLA	b	609	65/65	0.91	0.12	29,32,65,68	0
30	DMS	D	416	4/4	0.91	0.26	55,55,56,59	0
26	BCR	B	618	40/40	0.92	0.09	27,32,41,41	0
24	CLA	C	506	65/65	0.92	0.11	36,43,73,76	0
26	BCR	J	101	40/40	0.92	0.10	35,37,41,41	0
36	DGD	c	517	62/66	0.92	0.12	29,38,64,73	0
24	CLA	B	606	65/65	0.92	0.12	27,30,51,53	0
24	CLA	D	405	65/65	0.92	0.12	28,30,70,71	0
36	DGD	C	516	62/66	0.92	0.10	28,36,70,72	0
26	BCR	a	413	40/40	0.93	0.09	24,30,34,34	0
26	BCR	y	101	40/40	0.93	0.09	40,44,46,47	0
26	BCR	H	101	40/40	0.93	0.09	27,36,42,42	0
26	BCR	t	101	40/40	0.93	0.09	26,39,46,47	0
26	BCR	A	1009	40/40	0.93	0.10	25,29,32,32	0
34	LHG	d	408	49/49	0.93	0.15	32,41,72,74	0
24	CLA	A	1008	65/65	0.93	0.13	25,27,79,81	0
39	MG	K	104	1/1	0.93	0.07	48,48,48,48	0
36	DGD	H	102	62/66	0.93	0.11	27,34,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	DGD	c	515	62/66	0.93	0.12	28,38,69,71	0
24	CLA	c	508	65/65	0.93	0.10	32,35,65,72	0
26	BCR	k	101	40/40	0.93	0.12	36,45,47,48	0
30	DMS	u	201	4/4	0.93	0.24	56,57,57,59	0
24	CLA	a	412	65/65	0.93	0.15	26,28,90,92	0
24	CLA	b	612	65/65	0.93	0.13	30,34,37,38	0
24	CLA	C	507	65/65	0.94	0.11	34,37,51,53	0
34	LHG	d	406	49/49	0.94	0.13	38,41,46,46	0
24	CLA	C	508	65/65	0.94	0.10	28,31,65,70	0
36	DGD	C	517	62/66	0.94	0.10	24,33,62,69	0
24	CLA	a	409	65/65	0.94	0.12	24,26,85,90	0
26	BCR	C	514	40/40	0.94	0.11	31,38,41,41	0
24	CLA	C	505	65/65	0.94	0.10	32,35,44,48	0
24	CLA	c	507	65/65	0.94	0.12	33,34,50,51	0
26	BCR	b	621	40/40	0.94	0.08	28,31,41,42	0
30	DMS	O	302	4/4	0.94	0.27	58,59,62,62	0
26	BCR	B	619	40/40	0.94	0.08	31,34,42,43	0
39	MG	j	102	1/1	0.94	0.06	37,37,37,37	0
24	CLA	c	504	65/65	0.94	0.10	32,35,57,59	0
24	CLA	C	504	65/65	0.94	0.10	27,30,55,57	0
26	BCR	b	622	40/40	0.94	0.09	33,36,40,41	0
36	DGD	C	515	62/66	0.94	0.11	27,36,63,64	0
34	LHG	D	409	49/49	0.94	0.11	35,38,43,45	0
24	CLA	b	605	65/65	0.95	0.10	29,32,37,37	0
30	DMS	v	202	4/4	0.95	0.14	55,56,58,58	0
34	LHG	D	411	49/49	0.95	0.14	29,38,73,76	0
24	CLA	B	615	65/65	0.95	0.10	27,28,44,46	0
30	DMS	c	529	4/4	0.95	0.21	51,51,53,54	0
24	CLA	c	505	65/65	0.95	0.10	34,36,48,48	0
26	BCR	B	617	40/40	0.95	0.08	28,30,33,33	0
25	PHO	a	411	64/64	0.95	0.11	24,30,35,36	0
24	CLA	C	511	65/65	0.95	0.10	29,35,40,42	0
24	CLA	c	503	65/65	0.95	0.09	33,39,42,44	0
27	PL9	D	407	55/55	0.95	0.09	21,25,32,33	0
38	HEM	f	101	43/43	0.95	0.12	42,44,57,63	0
24	CLA	b	615	65/65	0.95	0.08	25,28,32,35	0
24	CLA	B	609	65/65	0.95	0.11	28,31,33,35	0
26	BCR	T	101	40/40	0.95	0.08	27,37,42,43	0
24	CLA	c	511	65/65	0.95	0.10	36,39,43,46	0
24	CLA	B	614	65/65	0.95	0.10	24,27,67,68	0
27	PL9	d	405	55/55	0.95	0.09	21,27,32,33	0
24	CLA	c	501	65/65	0.95	0.10	35,36,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	CLA	A	1006	65/65	0.95	0.10	22,23,66,69	0
34	LHG	d	407	49/49	0.95	0.11	26,31,40,45	0
30	DMS	c	526	4/4	0.95	0.19	73,74,74,75	0
24	CLA	b	613	65/65	0.95	0.10	28,31,38,40	0
24	CLA	b	611	65/65	0.96	0.08	26,28,38,39	0
24	CLA	b	610	65/65	0.96	0.08	23,25,34,35	0
30	DMS	V	203	4/4	0.96	0.15	50,51,51,52	0
24	CLA	c	502	65/65	0.96	0.09	28,31,50,51	0
24	CLA	C	501	65/65	0.96	0.08	31,35,41,42	0
30	DMS	C	524	4/4	0.96	0.17	40,41,41,42	0
38	HEM	F	101	43/43	0.96	0.11	39,41,44,46	0
30	DMS	b	629	4/4	0.96	0.11	48,49,52,53	0
24	CLA	C	503	65/65	0.96	0.08	28,33,36,38	0
37	BCT	d	401	4/4	0.96	0.09	40,40,41,42	0
26	BCR	b	620	40/40	0.96	0.09	28,34,35,35	0
24	CLA	b	607	65/65	0.96	0.09	24,26,50,51	0
24	CLA	B	604	65/65	0.96	0.10	22,24,53,55	0
24	CLA	c	509	65/65	0.96	0.11	33,35,50,51	0
24	CLA	B	610	65/65	0.96	0.09	24,26,34,36	0
24	CLA	b	608	65/65	0.96	0.10	24,26,35,35	0
34	LHG	D	410	49/49	0.96	0.11	26,30,38,41	0
24	CLA	C	509	65/65	0.96	0.10	28,31,52,53	0
24	CLA	b	617	65/65	0.96	0.10	24,28,67,68	0
24	CLA	B	607	65/65	0.96	0.09	20,22,36,37	0
30	DMS	d	414	4/4	0.96	0.11	58,59,59,60	0
34	LHG	b	624	49/49	0.96	0.09	27,32,48,53	0
24	CLA	c	510	65/65	0.96	0.09	33,35,41,43	0
24	CLA	b	614	65/65	0.96	0.09	24,26,40,41	0
24	CLA	B	605	65/65	0.96	0.10	23,26,31,32	0
24	CLA	B	602	65/65	0.96	0.09	25,27,34,35	0
24	CLA	b	618	65/65	0.96	0.08	30,32,44,46	0
25	PHO	D	404	64/64	0.96	0.09	22,25,29,30	0
24	CLA	C	502	65/65	0.96	0.09	26,28,42,44	0
25	PHO	a	410	64/64	0.97	0.08	22,24,29,31	0
24	CLA	B	611	65/65	0.97	0.09	22,24,36,37	0
24	CLA	a	408	65/65	0.97	0.08	20,23,31,34	0
39	MG	k	103	1/1	0.97	0.05	45,45,45,45	0
24	CLA	B	613	65/65	0.97	0.08	23,25,49,53	0
38	HEM	v	201	43/43	0.97	0.10	31,32,36,37	0
24	CLA	A	1005	65/65	0.97	0.10	17,20,29,33	0
24	CLA	a	407	65/65	0.97	0.10	21,23,30,35	0
30	DMS	a	417	4/4	0.97	0.09	31,32,33,33	0

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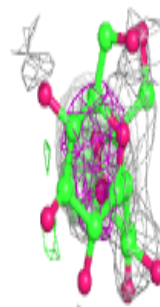
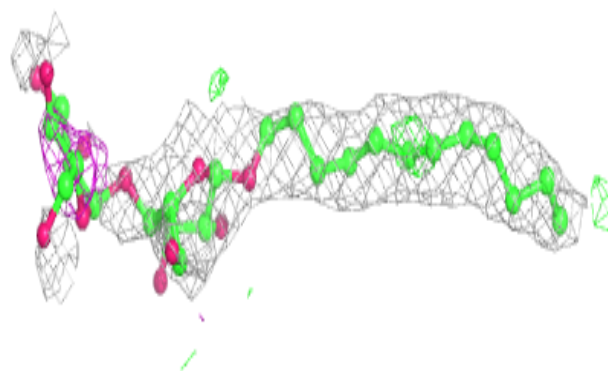
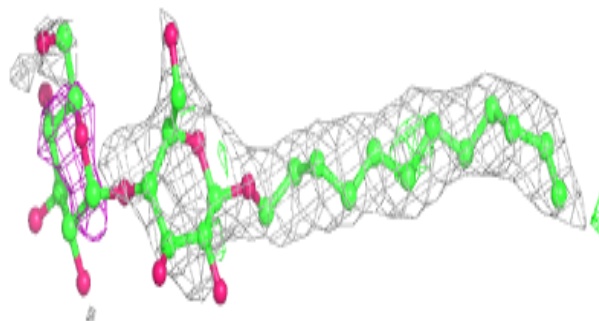
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	CLA	d	402	65/65	0.97	0.10	21,23,39,43	0
30	DMS	B	627	4/4	0.97	0.10	41,41,42,44	0
24	CLA	D	402	65/65	0.97	0.09	17,20,35,37	0
24	CLA	b	606	65/65	0.97	0.09	26,29,35,39	0
25	PHO	A	1007	64/64	0.97	0.08	21,24,26,28	0
30	DMS	B	632	4/4	0.97	0.18	57,58,60,61	0
34	LHG	B	621	49/49	0.97	0.09	26,32,45,49	0
24	CLA	B	608	65/65	0.97	0.08	25,27,31,31	0
24	CLA	D	403	65/65	0.97	0.07	18,20,29,33	0
24	CLA	C	510	65/65	0.97	0.09	27,31,38,39	0
24	CLA	b	616	65/65	0.97	0.09	25,25,50,52	0
24	CLA	B	612	65/65	0.97	0.09	24,26,30,31	0
37	BCT	D	401	4/4	0.97	0.16	37,38,38,41	0
24	CLA	B	603	65/65	0.97	0.08	25,26,32,34	0
38	HEM	V	201	43/43	0.98	0.12	25,26,28,29	0
39	MG	J	103	1/1	0.98	0.04	32,32,32,32	0
30	DMS	c	524	4/4	0.98	0.18	43,43,43,43	0
30	DMS	b	628	4/4	0.98	0.07	30,31,31,32	0
30	DMS	A	1013	4/4	0.98	0.09	29,29,30,31	0
30	DMS	B	626	4/4	0.98	0.07	25,26,26,27	0
23	CL	A	1003	1/1	0.99	0.03	25,25,25,25	0
30	DMS	C	523	4/4	0.99	0.10	36,37,38,38	0
23	CL	a	405	1/1	0.99	0.03	26,26,26,26	0
21	OER	A	1001	10/10	1.00	0.06	24,25,28,28	1
21	OER	a	403	10/10	1.00	0.05	27,28,29,31	1
23	CL	A	1004	1/1	1.00	0.02	22,22,22,22	0
22	FE2	a	404	1/1	1.00	0.05	29,29,29,29	0
22	FE2	A	1002	1/1	1.00	0.03	29,29,29,29	0
23	CL	a	406	1/1	1.00	0.05	27,27,27,27	0

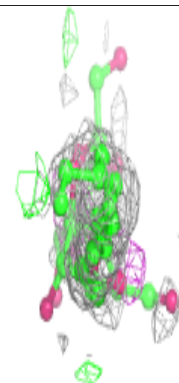
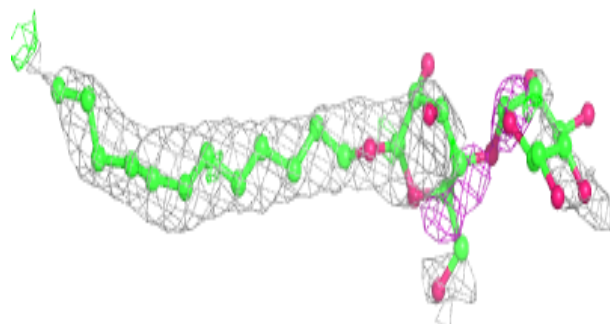
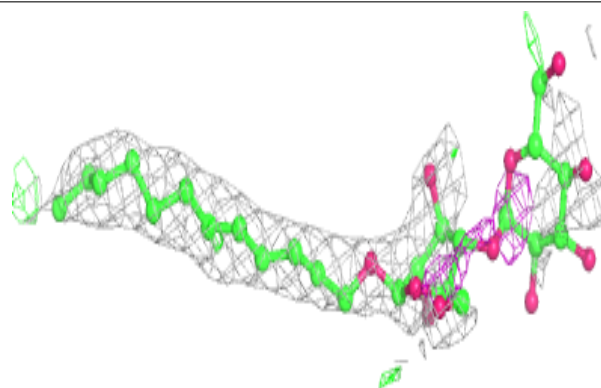
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT 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)

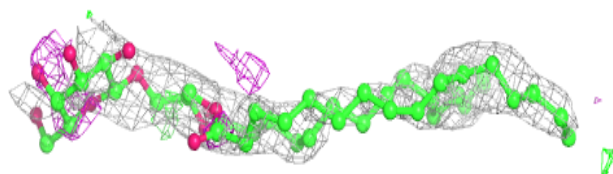
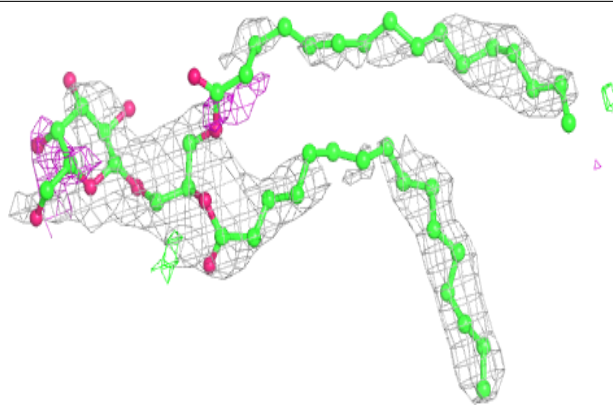
**Electron density around LMT A 1018:**

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

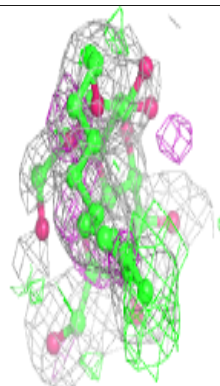
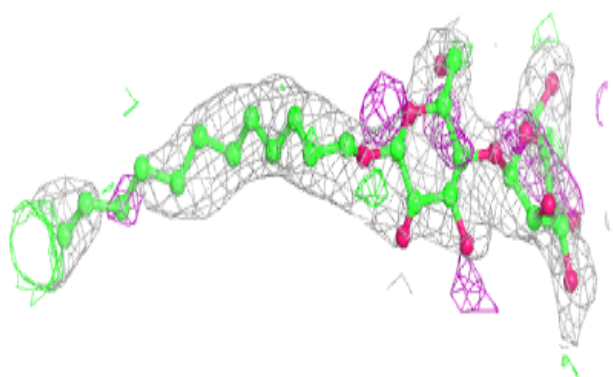
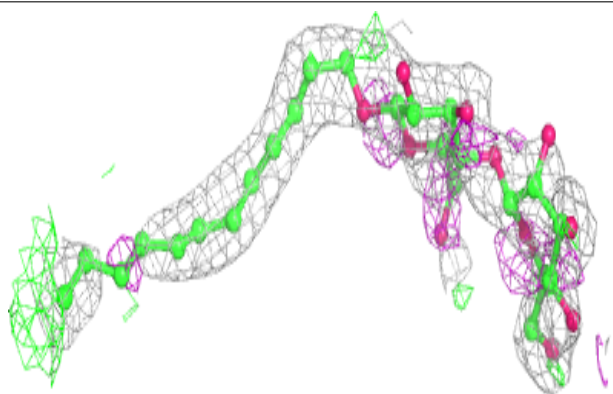


**Electron density around LMG Z 101:**

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

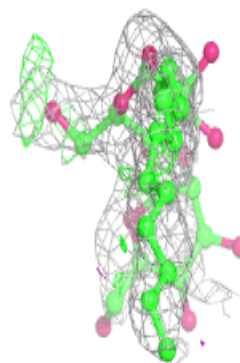
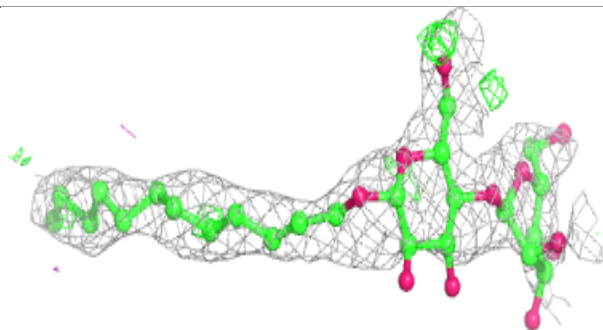
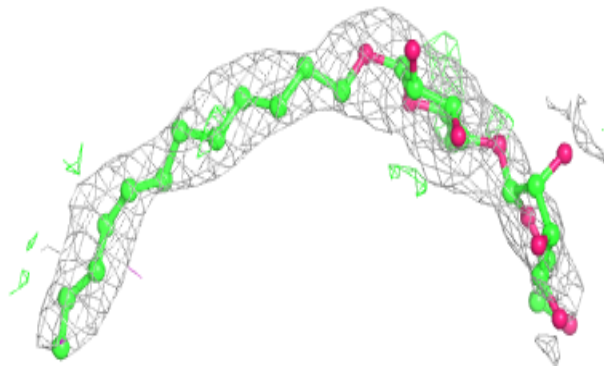
**Electron density around LMT a 402:**

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

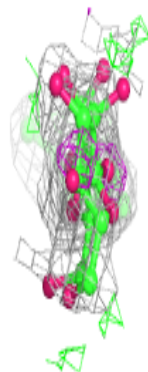
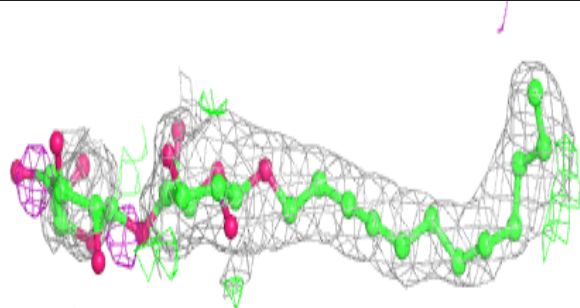
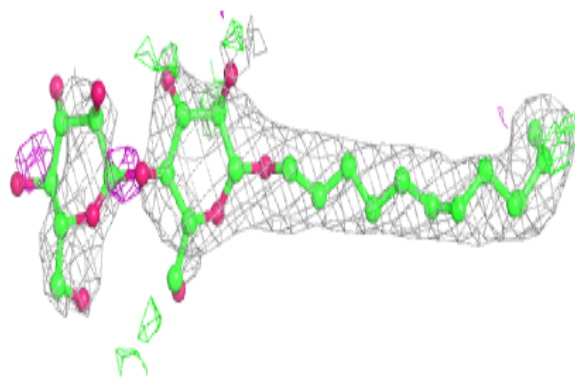


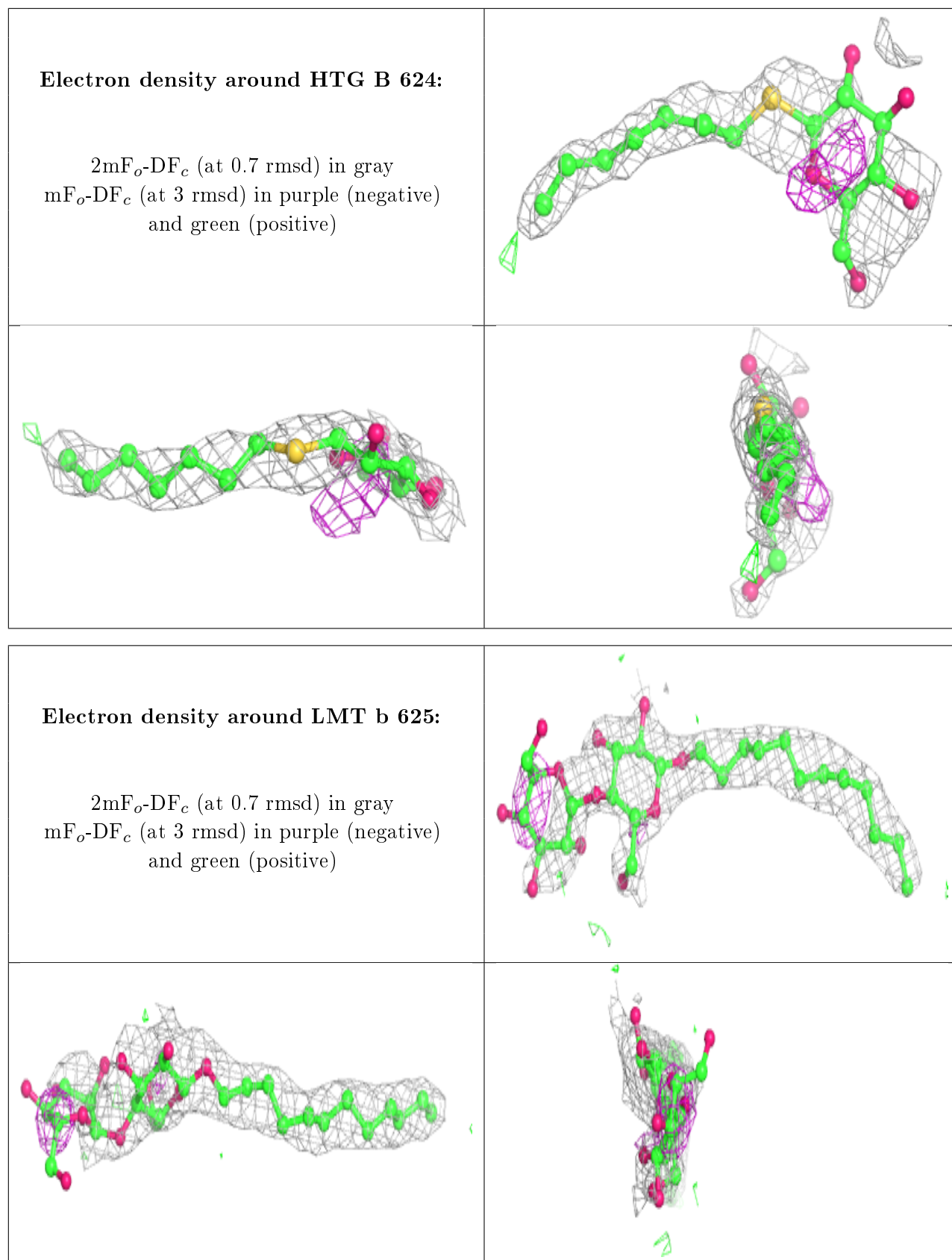
**Electron density around LMT m 103:**

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

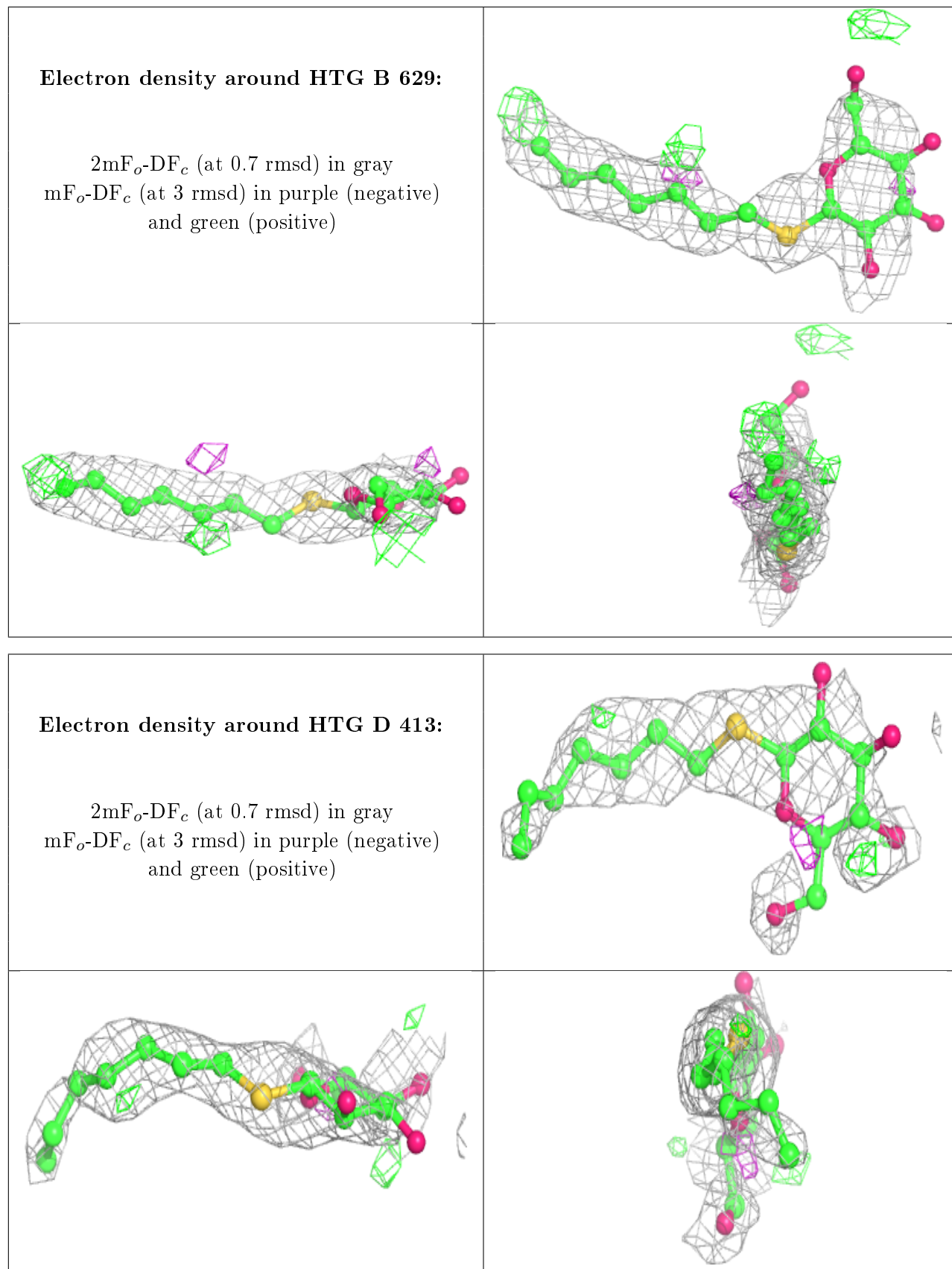
**Electron density around LMT t 103:**

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



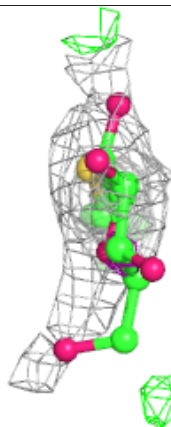
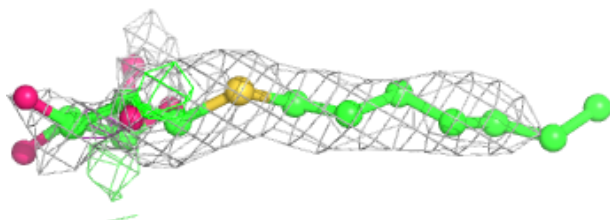
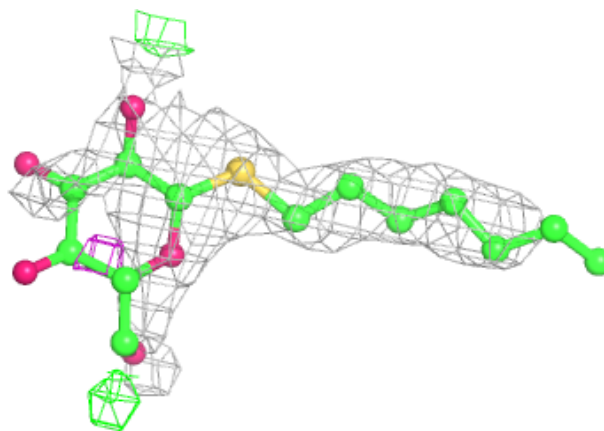




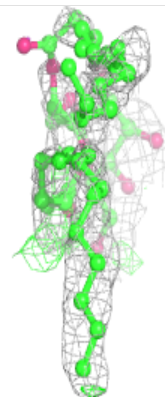
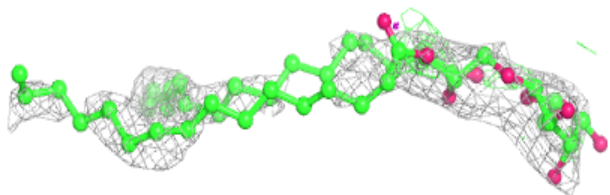
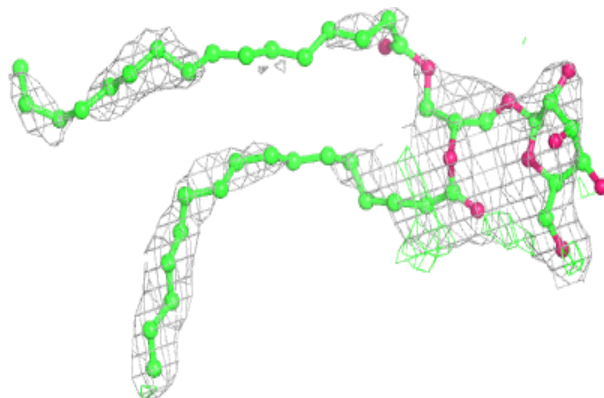


**Electron density around HTG c 525:**

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

**Electron density around LMG c 521:**

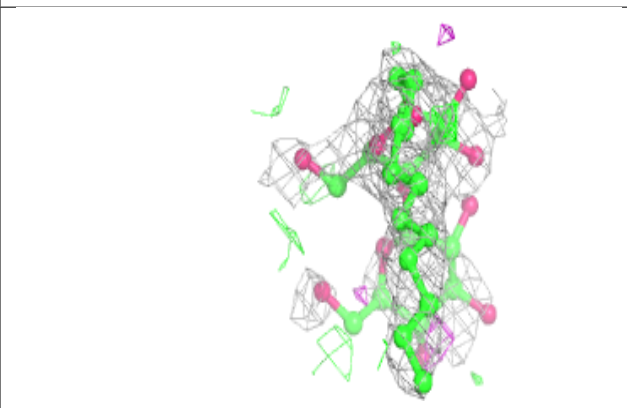
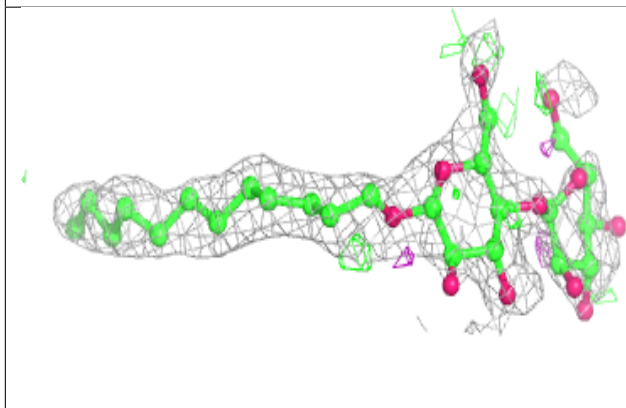
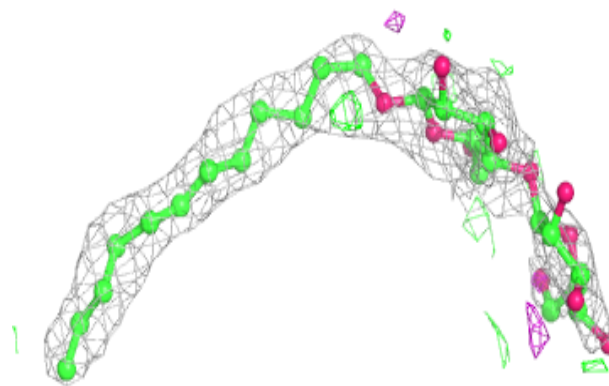
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



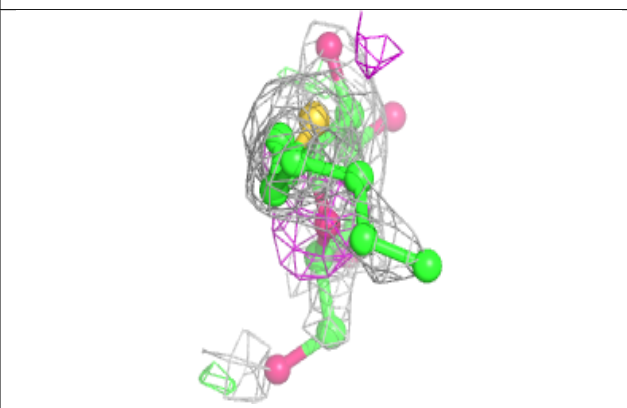
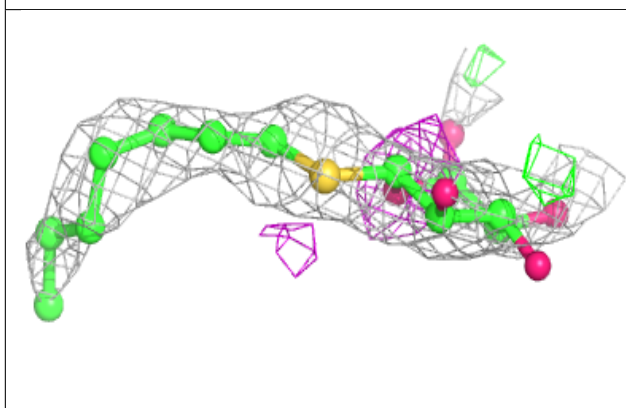
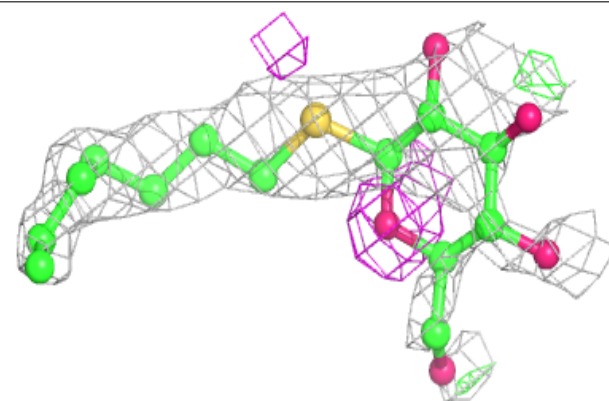


**Electron density around LMT M 101:**

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

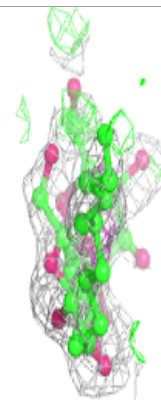
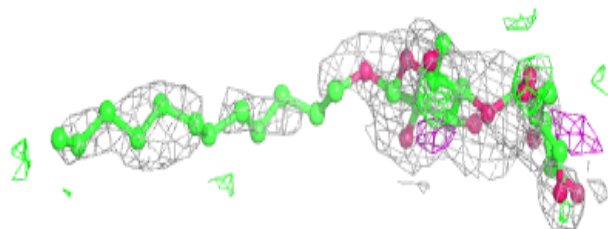
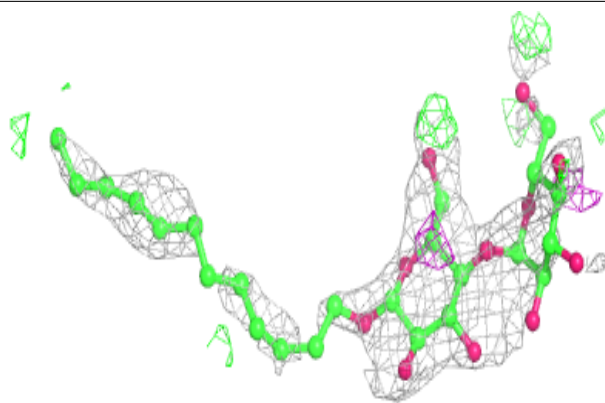
**Electron density around HTG d 410:**

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

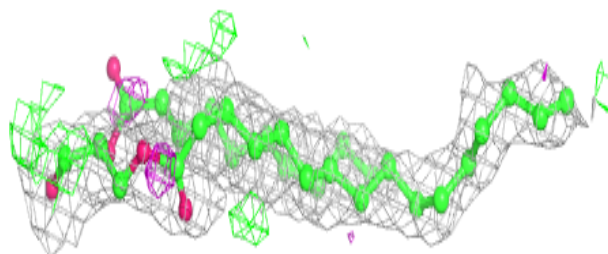
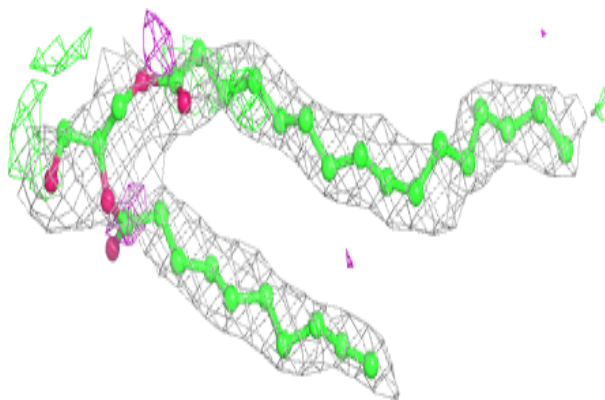


**Electron density around LMT f 103:**

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

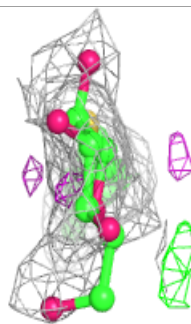
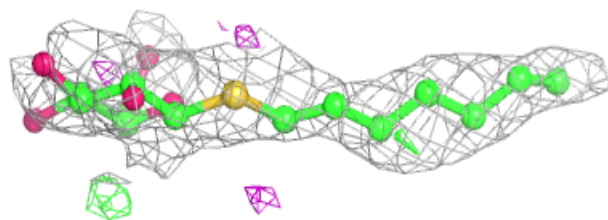
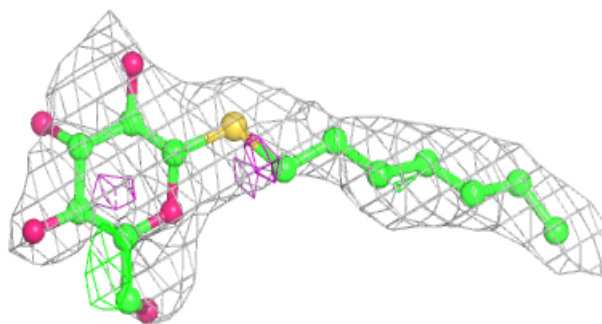
**Electron density around UNL K 103:**

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

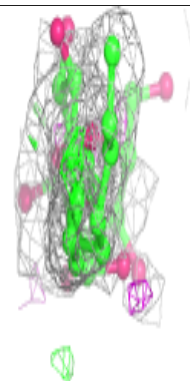
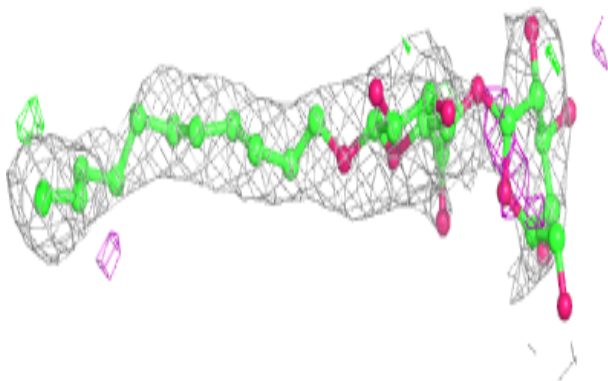
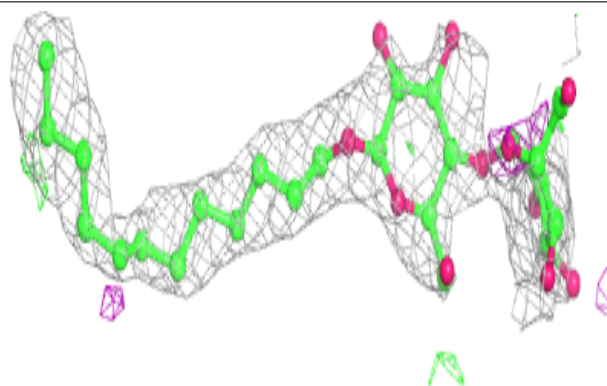


**Electron density around HTG b 602:**

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

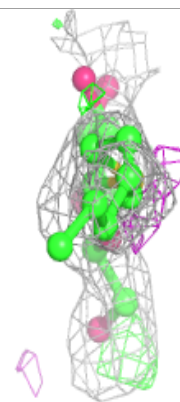
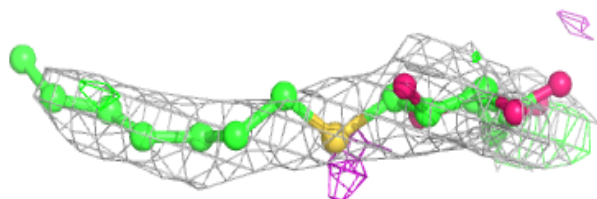
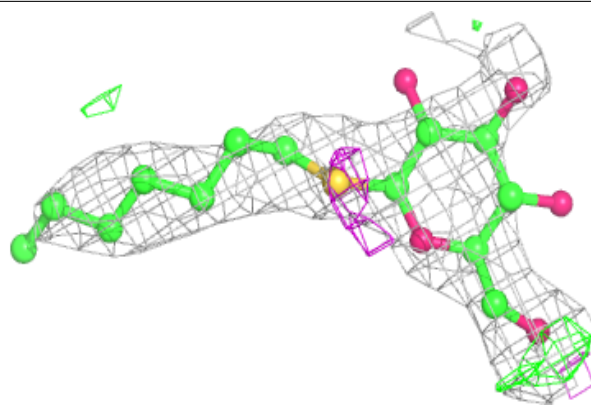
**Electron density around LMT b 631:**

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

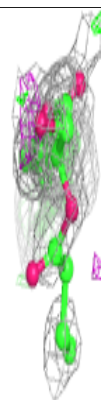
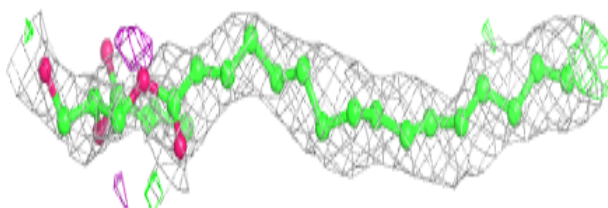
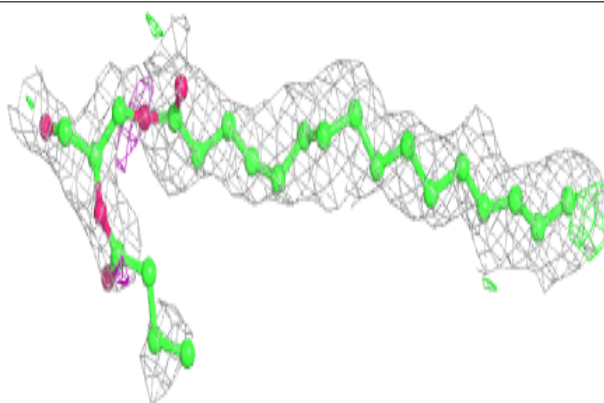


**Electron density around HTG b 630:**

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

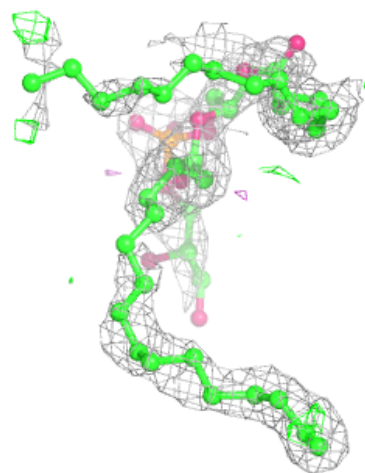
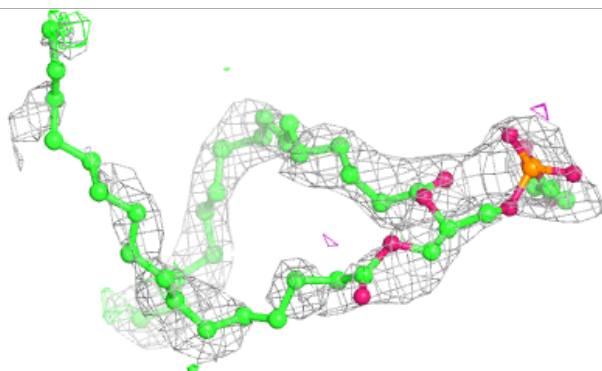
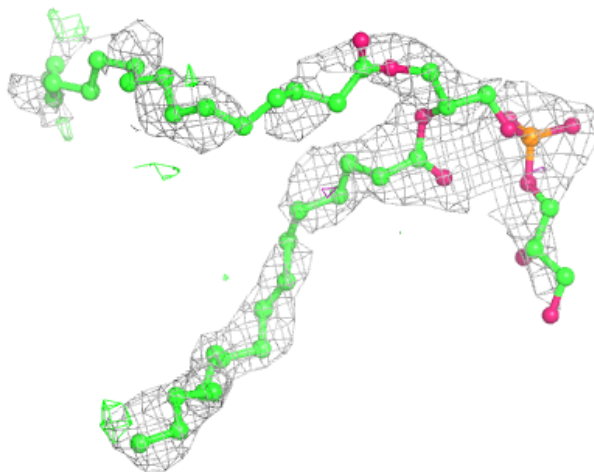
**Electron density around UNL A 1015:**

$2mF_o-DF_c$  (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:**

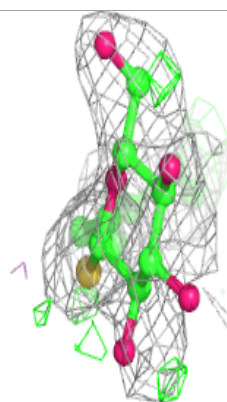
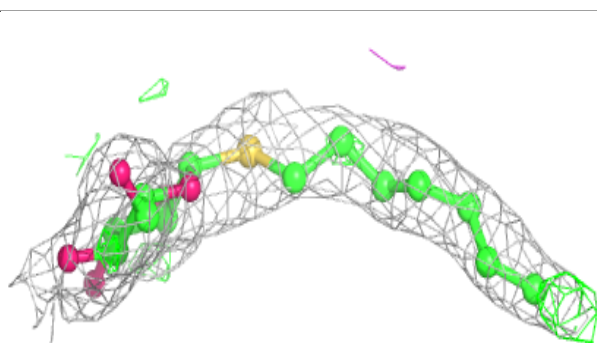
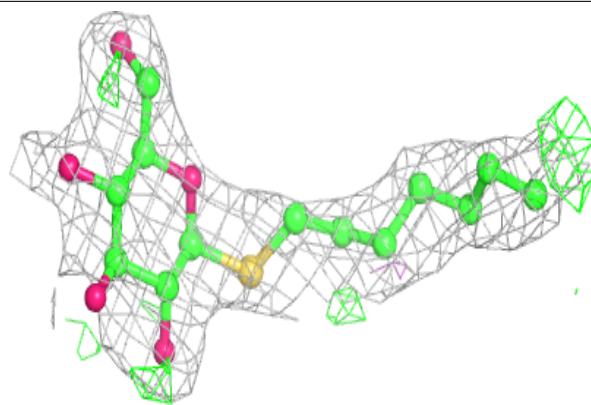
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



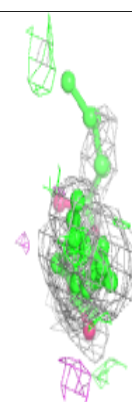
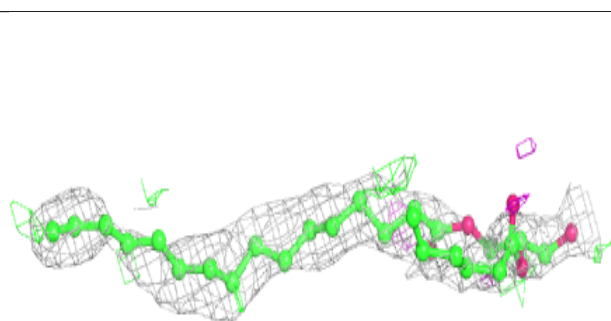
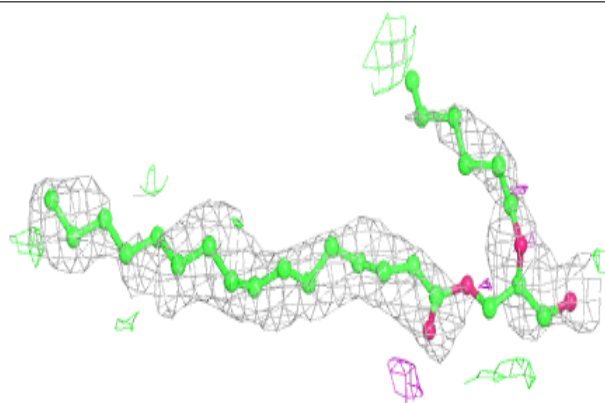


**Electron density around HTG D 419:**

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

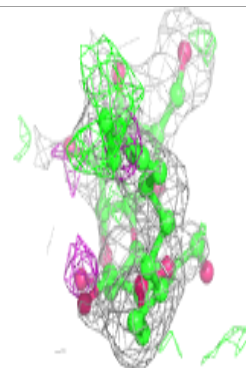
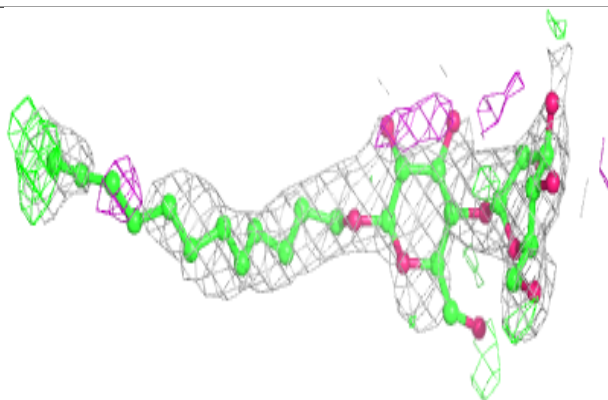
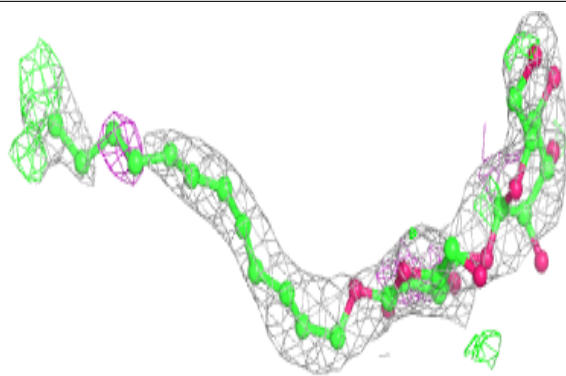
**Electron density around UNL a 419:**

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

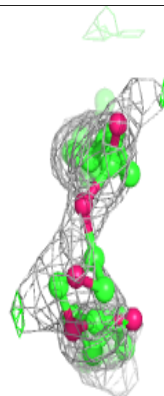
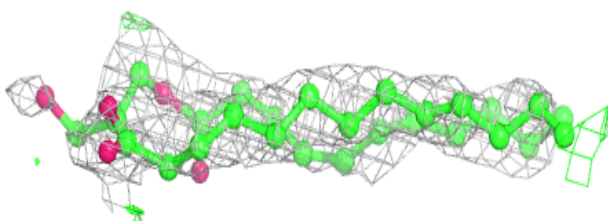
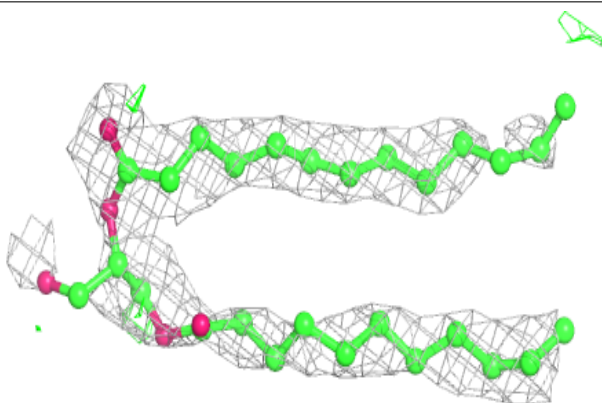


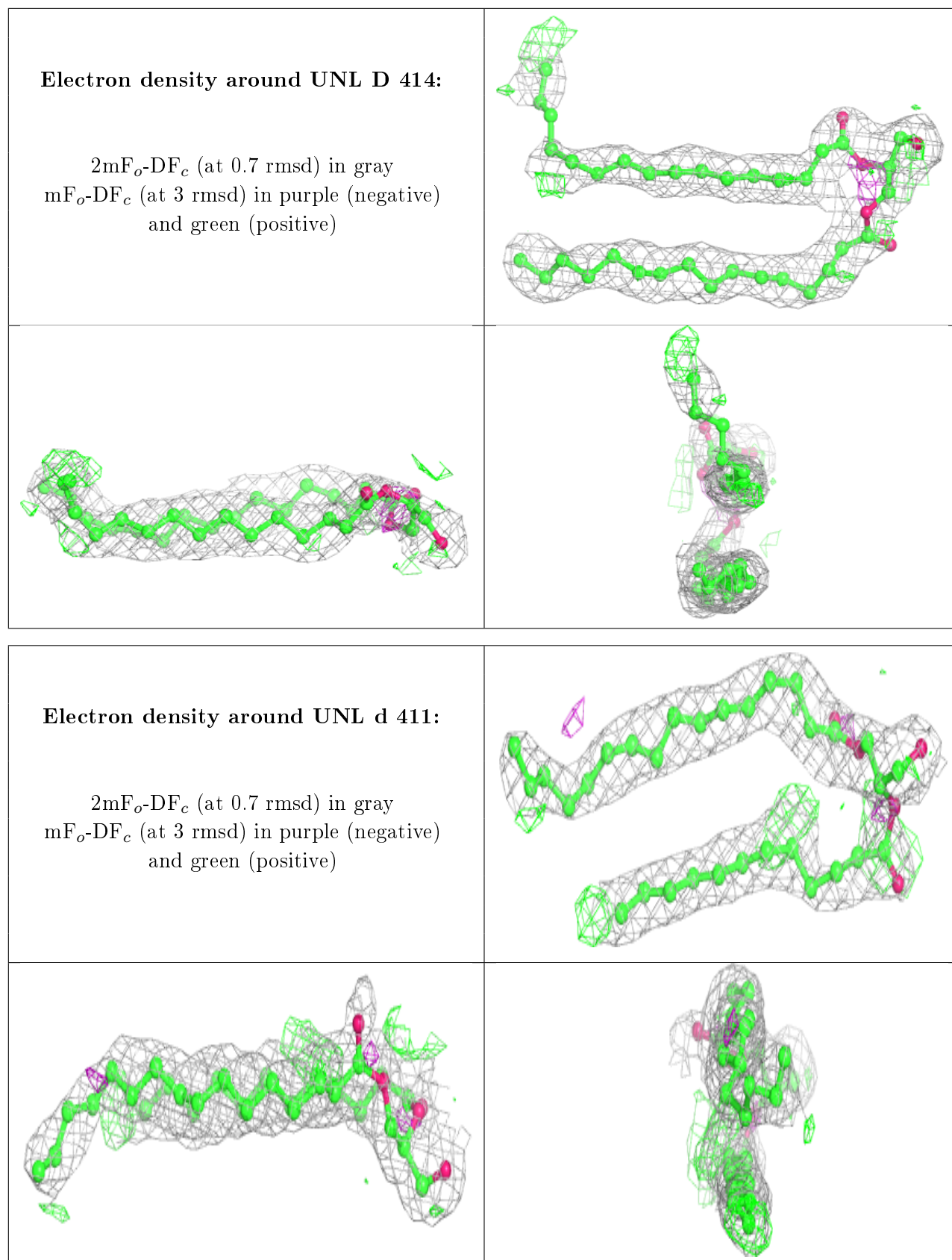
**Electron density around LMT A 1017:**

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

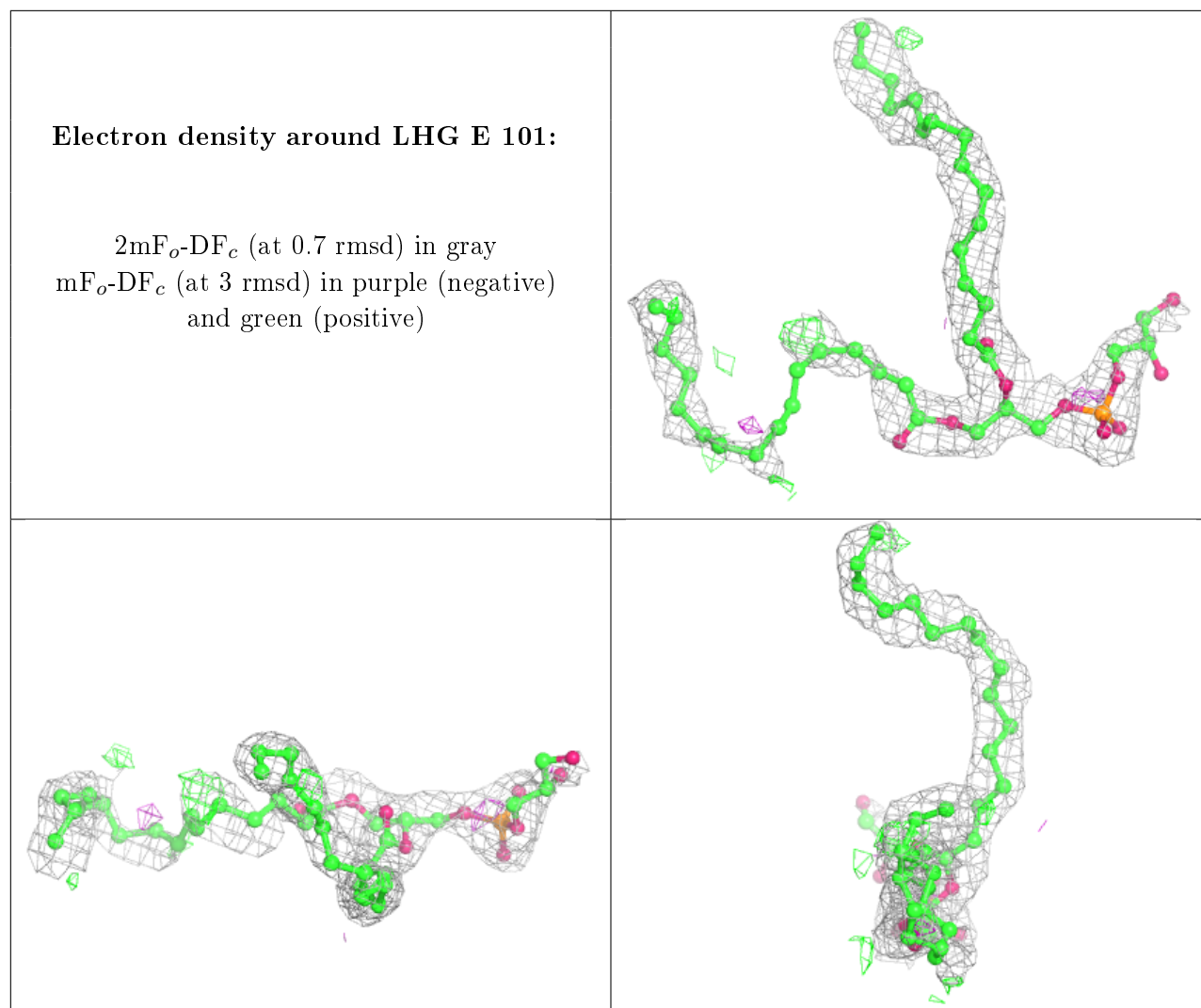
**Electron density around UNL c 523:**

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



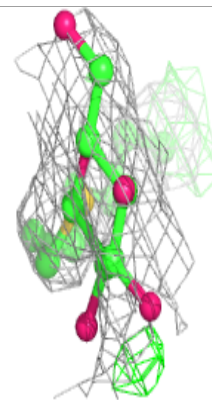
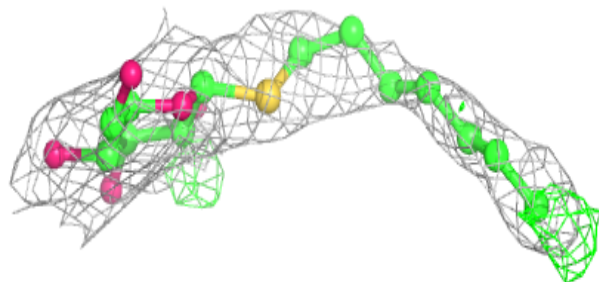
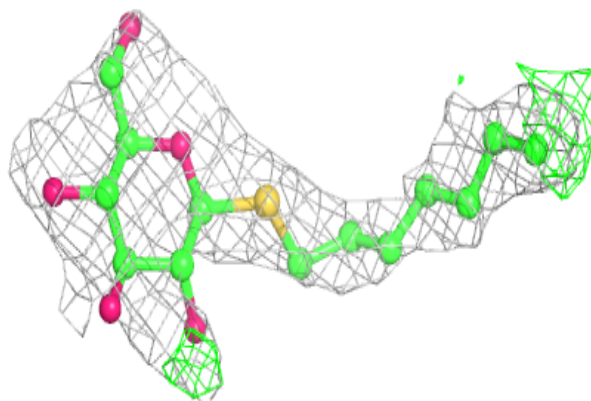




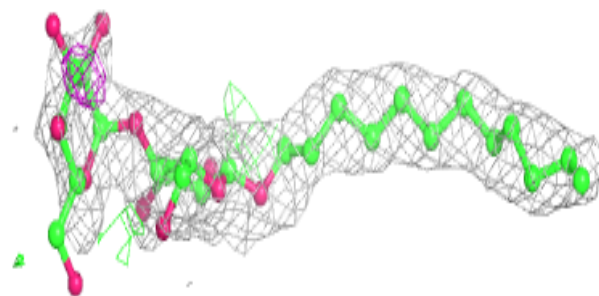
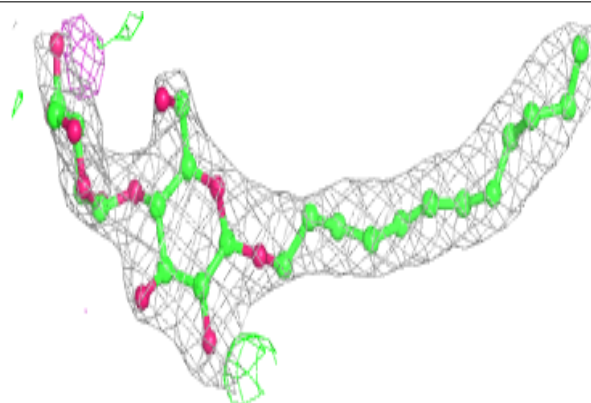


**Electron density around HTG d 416:**

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

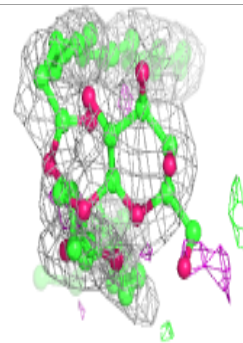
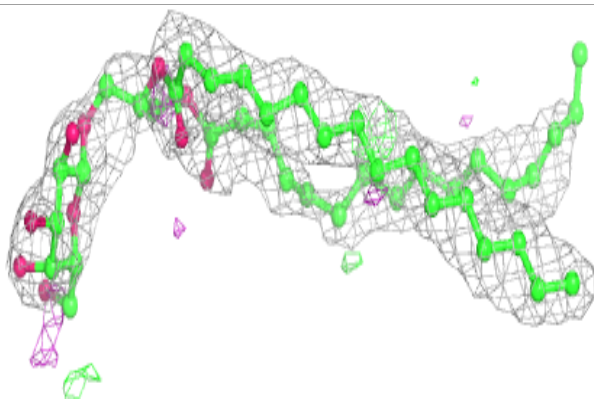
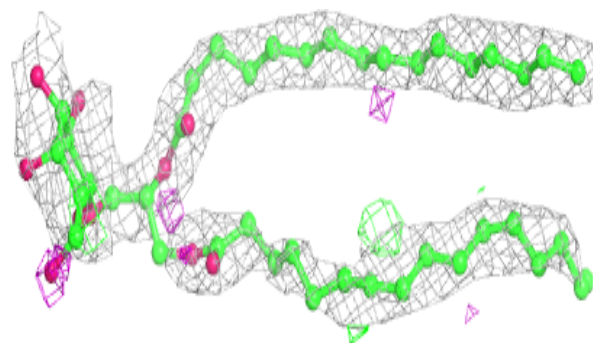
**Electron density around LMT B 623:**

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

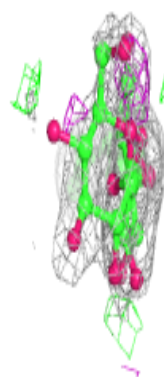
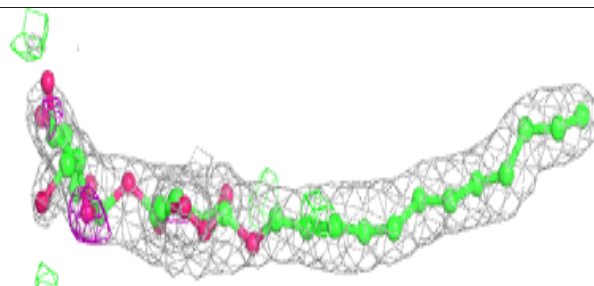
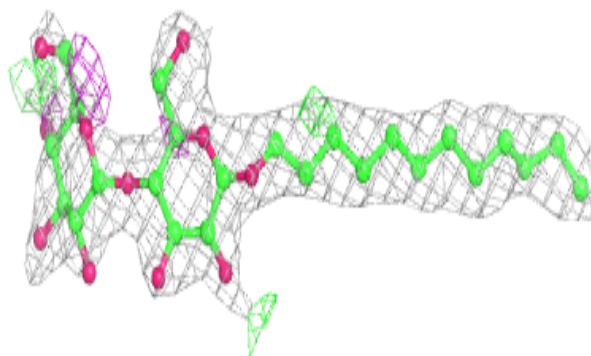


**Electron density around LMG c 520:**

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

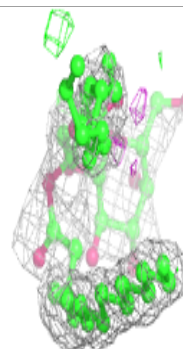
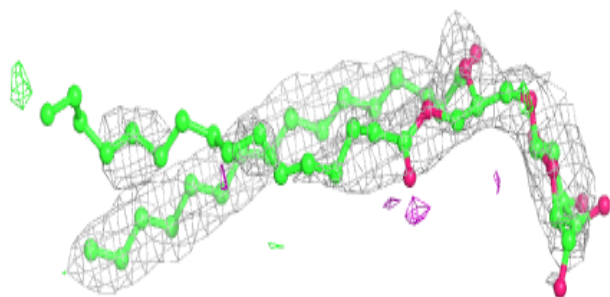
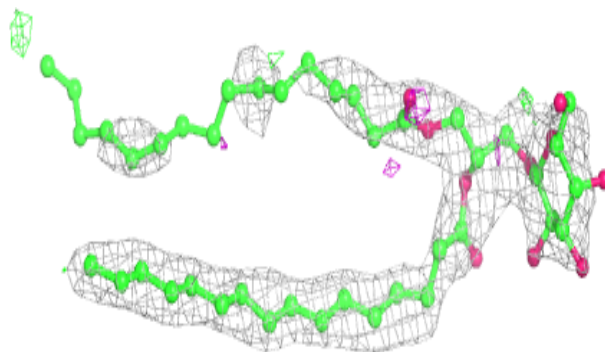
**Electron density around LMT M 102:**

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

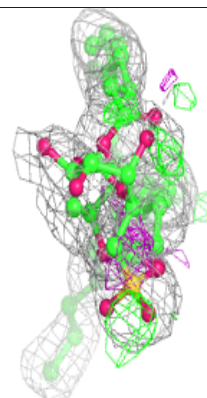
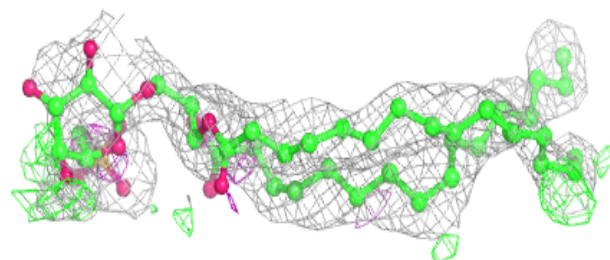
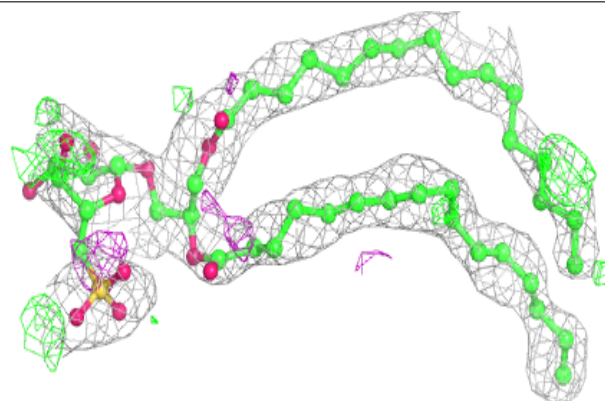


**Electron density around LMG C 519:**

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

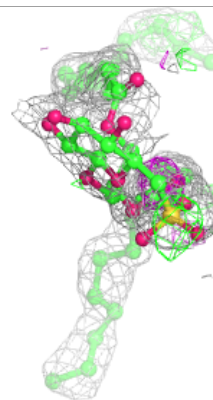
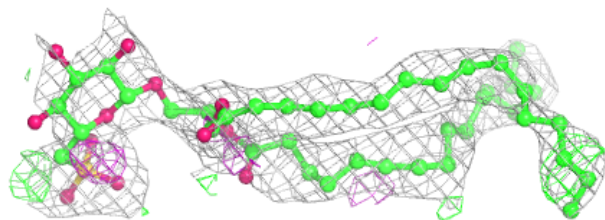
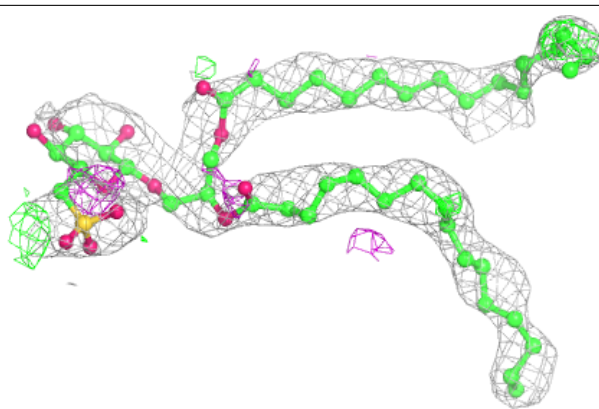
**Electron density around SQD b 623 (B):**

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

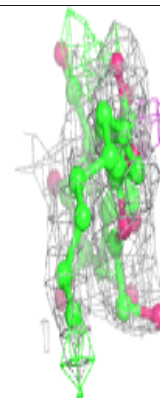
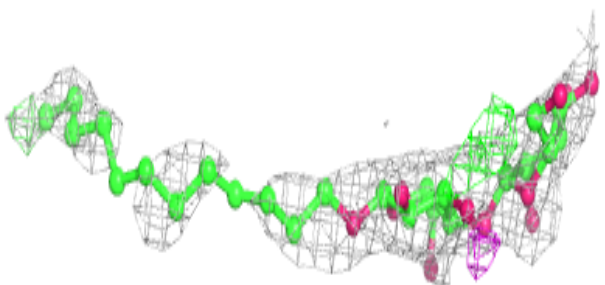
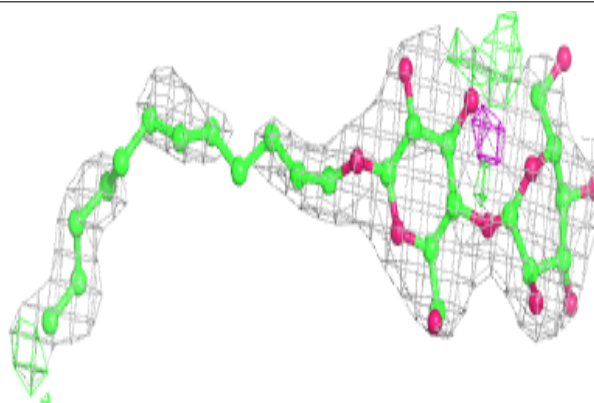


**Electron density around SQD b 623 (A):**

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

**Electron density around LMT C 520:**

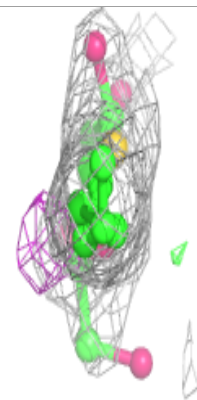
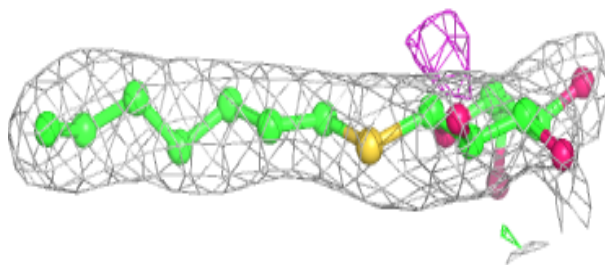
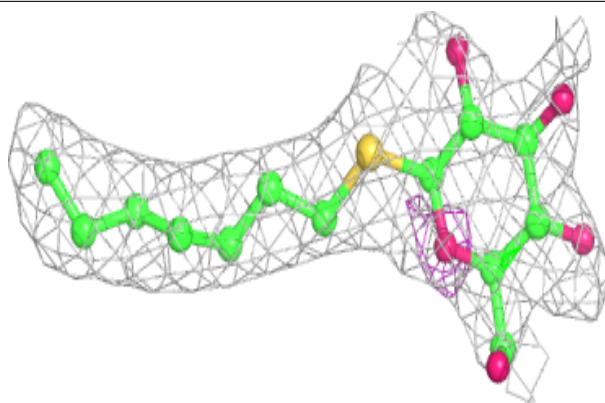
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



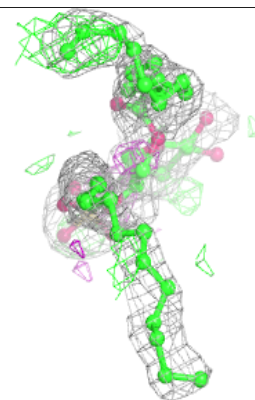
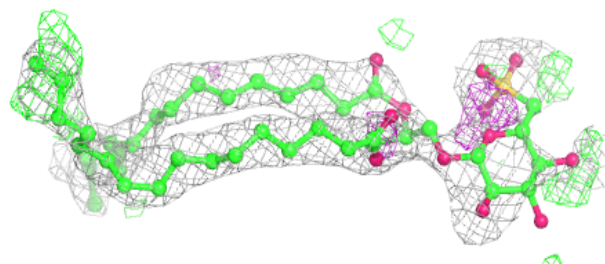
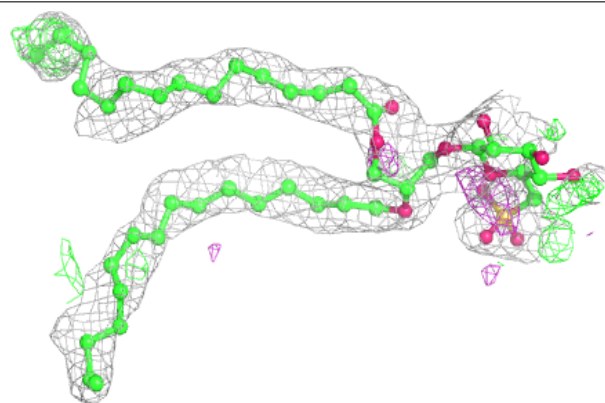


**Electron density around HTG B 628:**

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

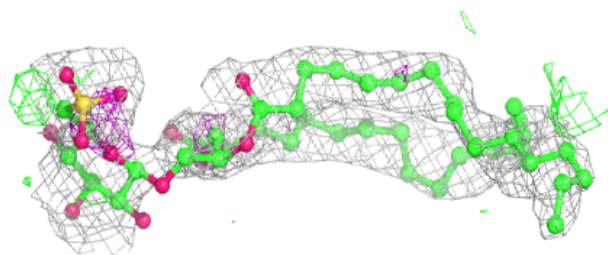
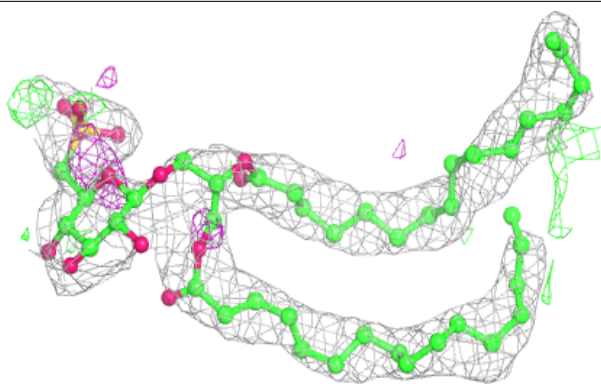
**Electron density around SQD B 620 (A):**

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

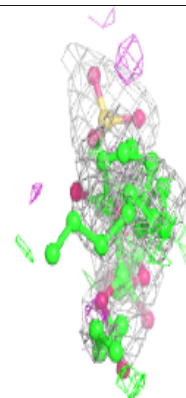
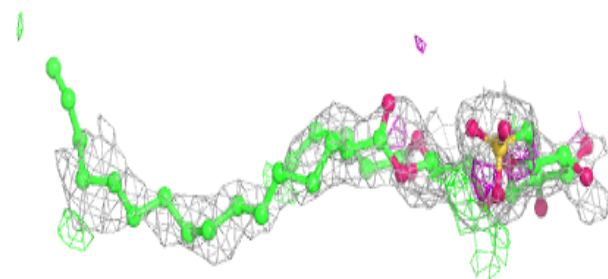
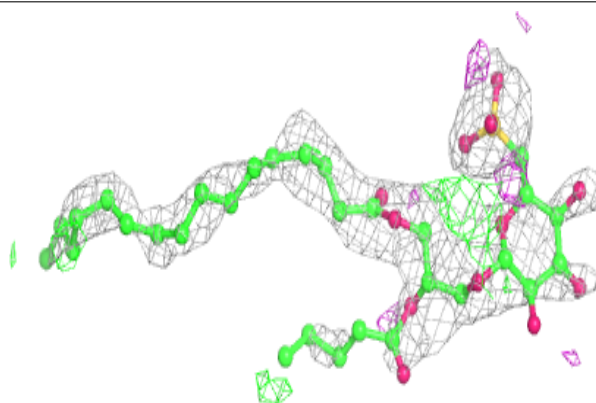


**Electron density around SQD B 620 (B):**

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

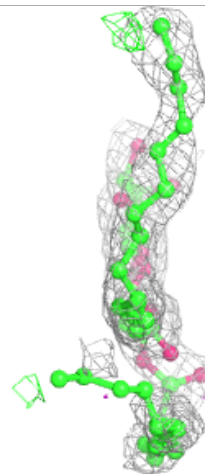
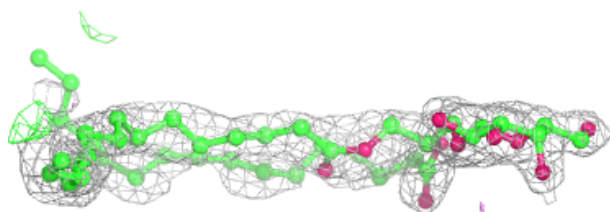
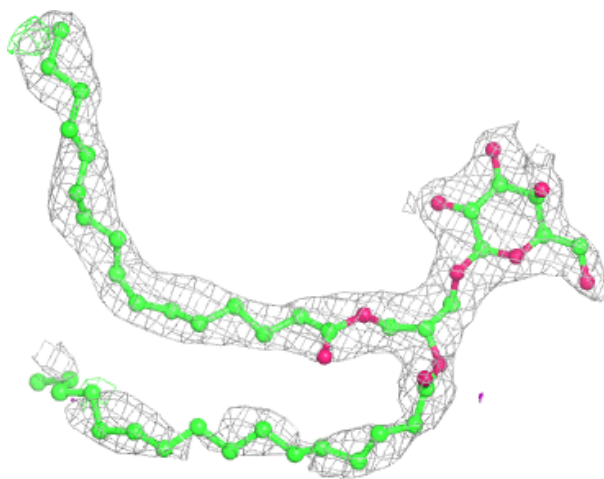
**Electron density around SQD f 102:**

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



**Electron density around LMG c 519:**

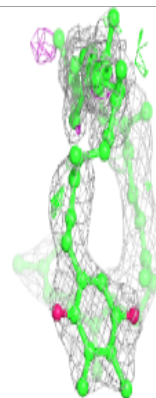
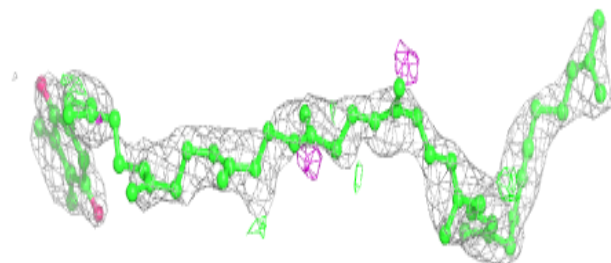
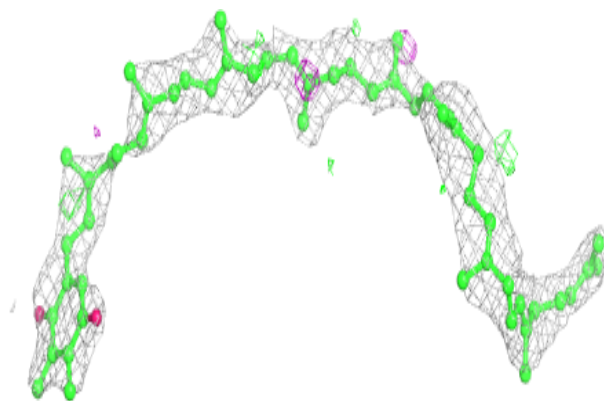
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



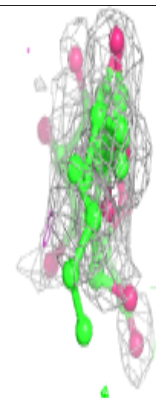
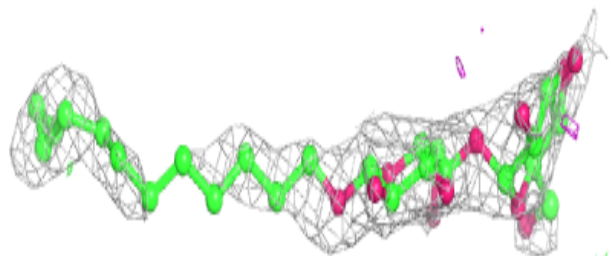
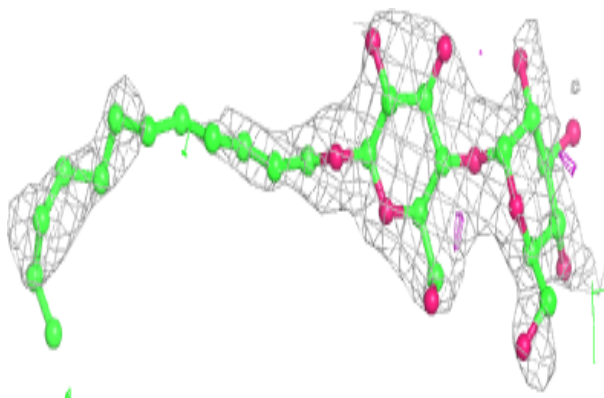


**Electron density around PL9 a 414:**

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

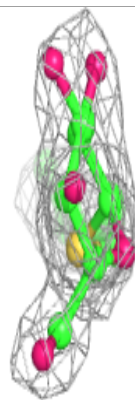
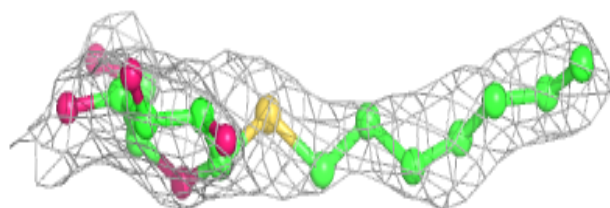
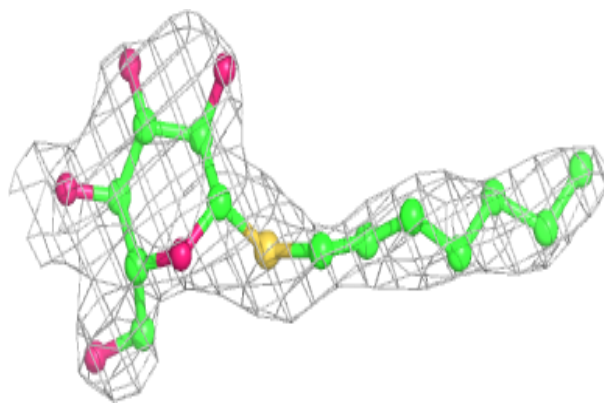
**Electron density around LMT a 416:**

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

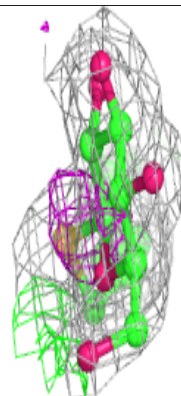
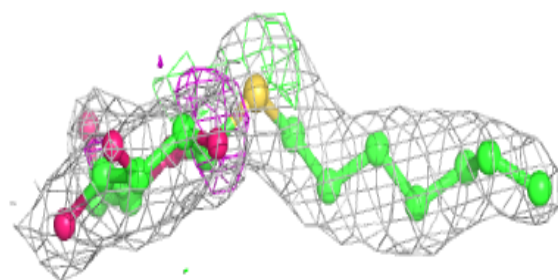
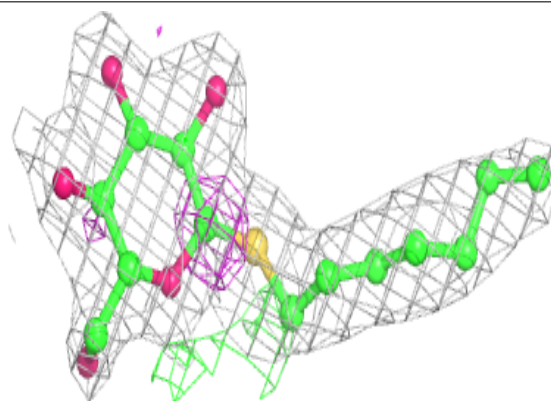


**Electron density around HTG C 522:**

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

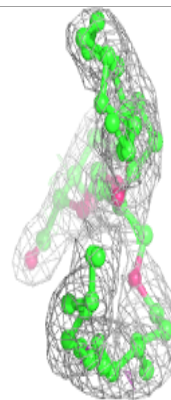
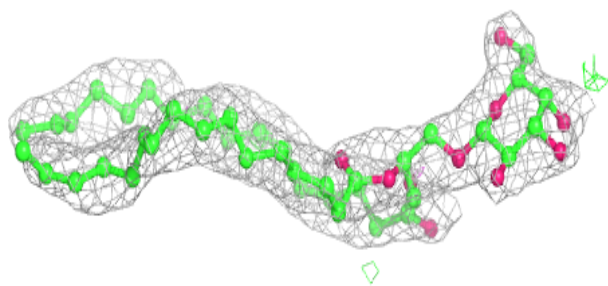
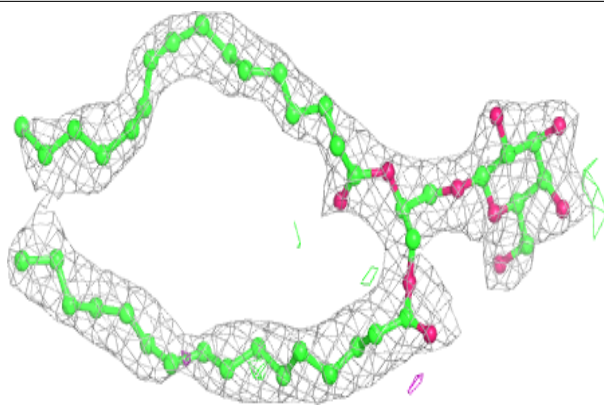
**Electron density around HTG o 301:**

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

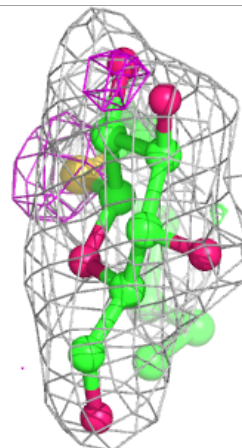
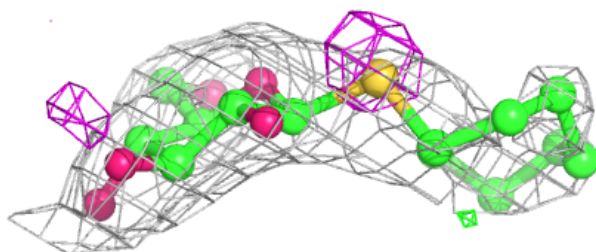
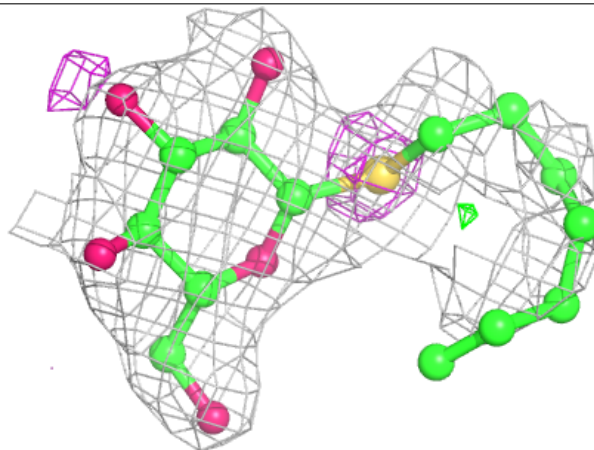


**Electron density around LMG a 415:**

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

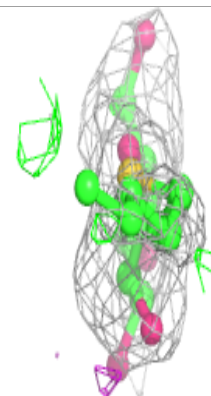
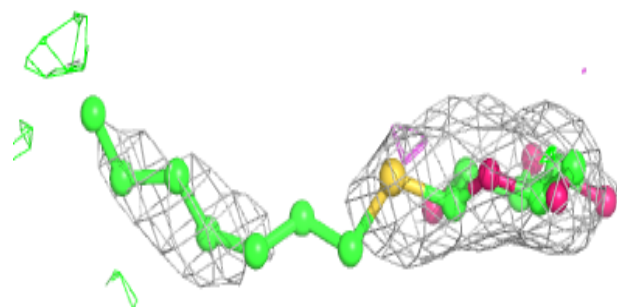
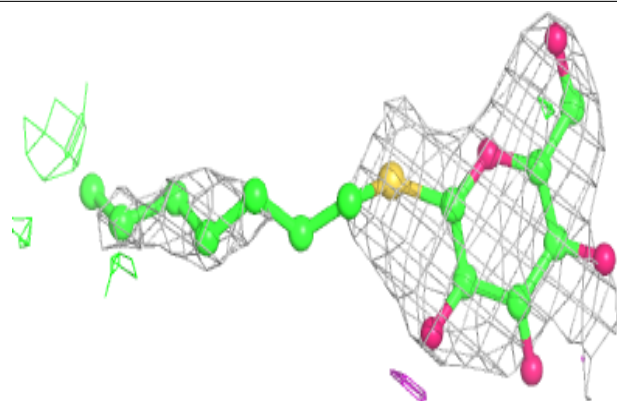
**Electron density around HTG V 202:**

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

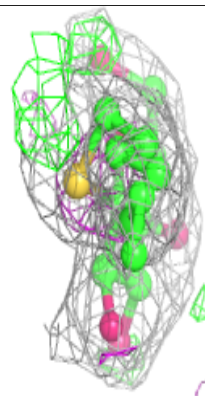
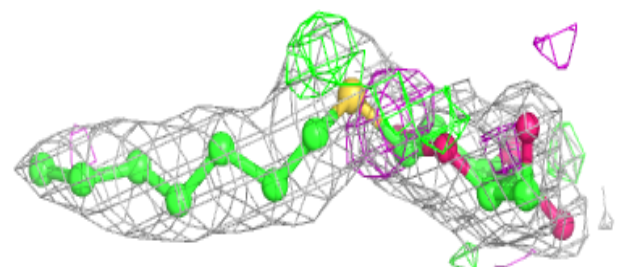
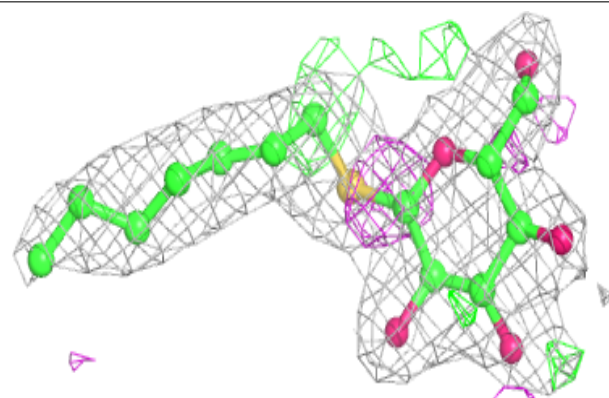


**Electron density around HTG c 522:**

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

**Electron density around HTG b 626:**

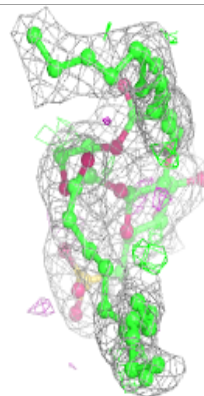
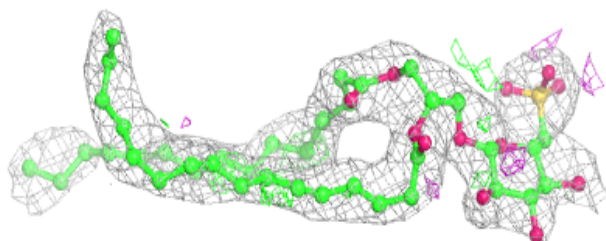
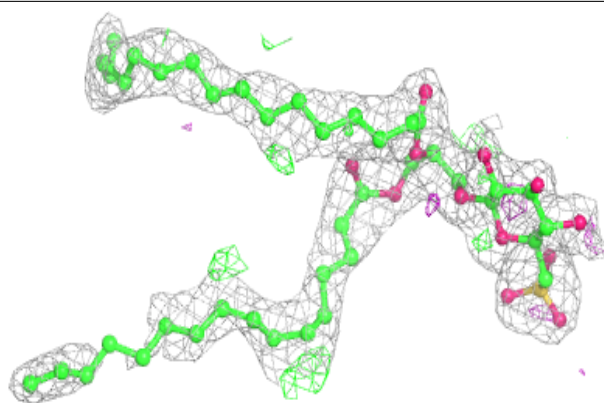
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



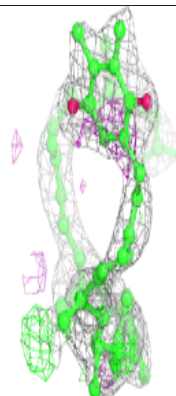
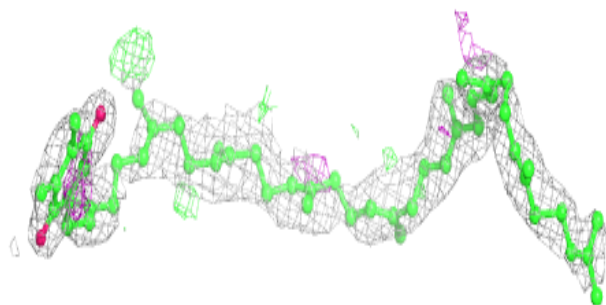
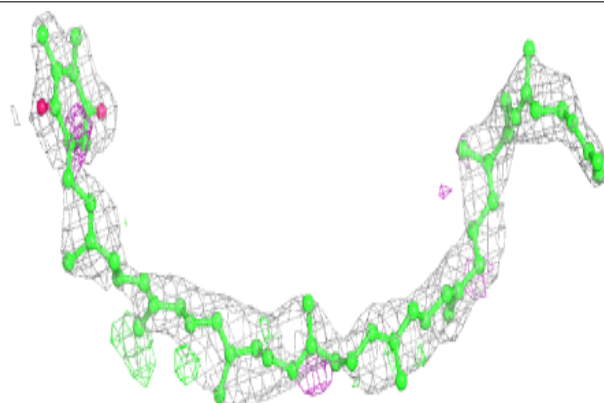


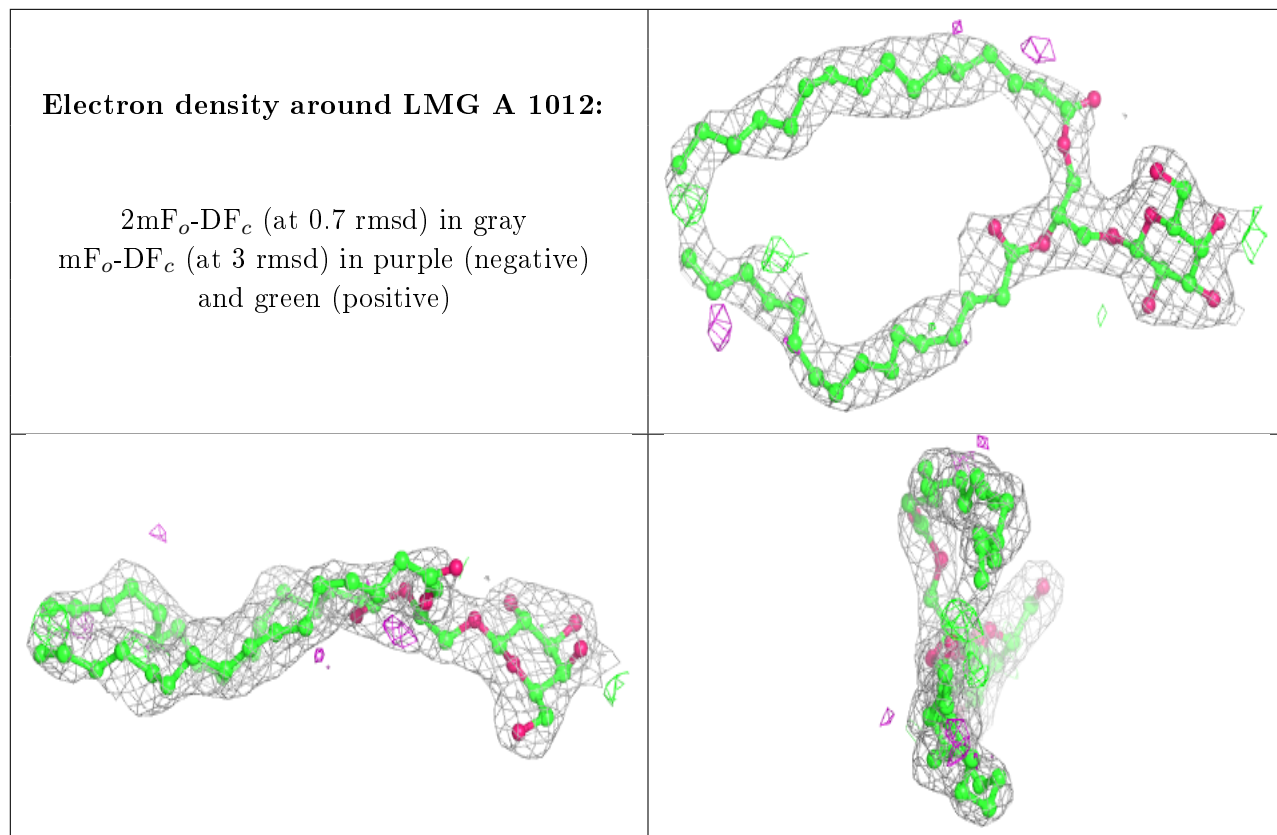
**Electron density around SQD A 1016:**

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

**Electron density around PL9 A 1010:**

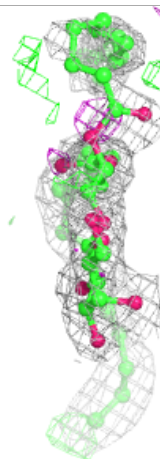
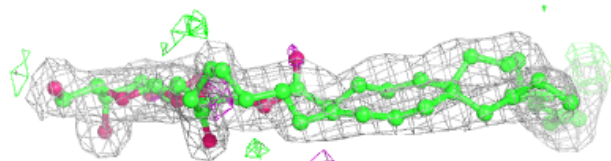
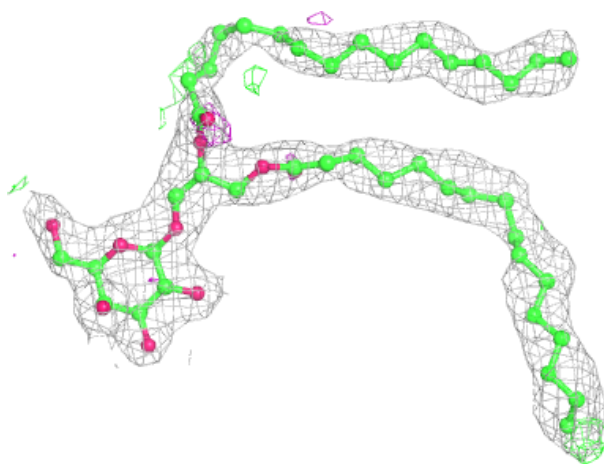
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





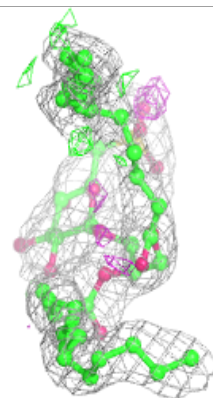
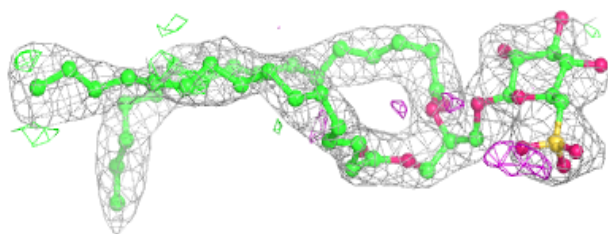
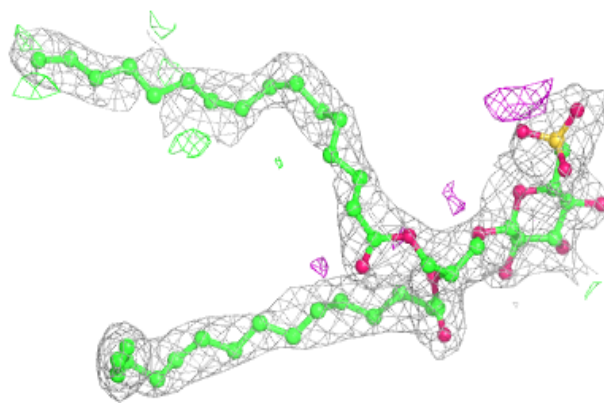
**Electron density around LMG C 518:**

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



**Electron density around SQD a 401:**

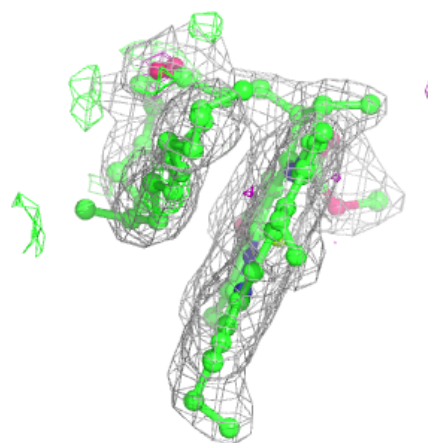
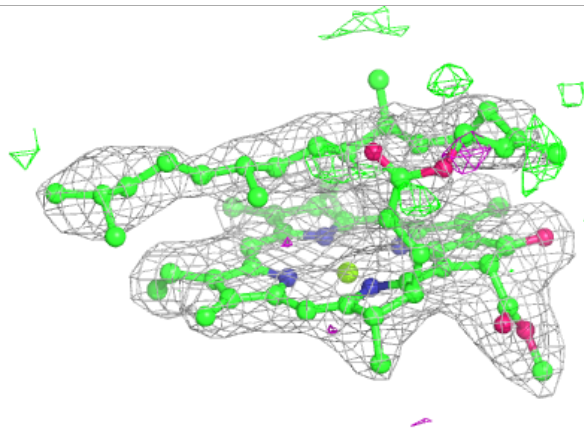
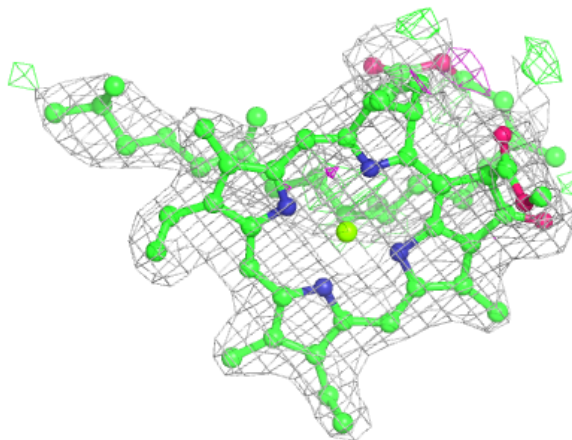
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

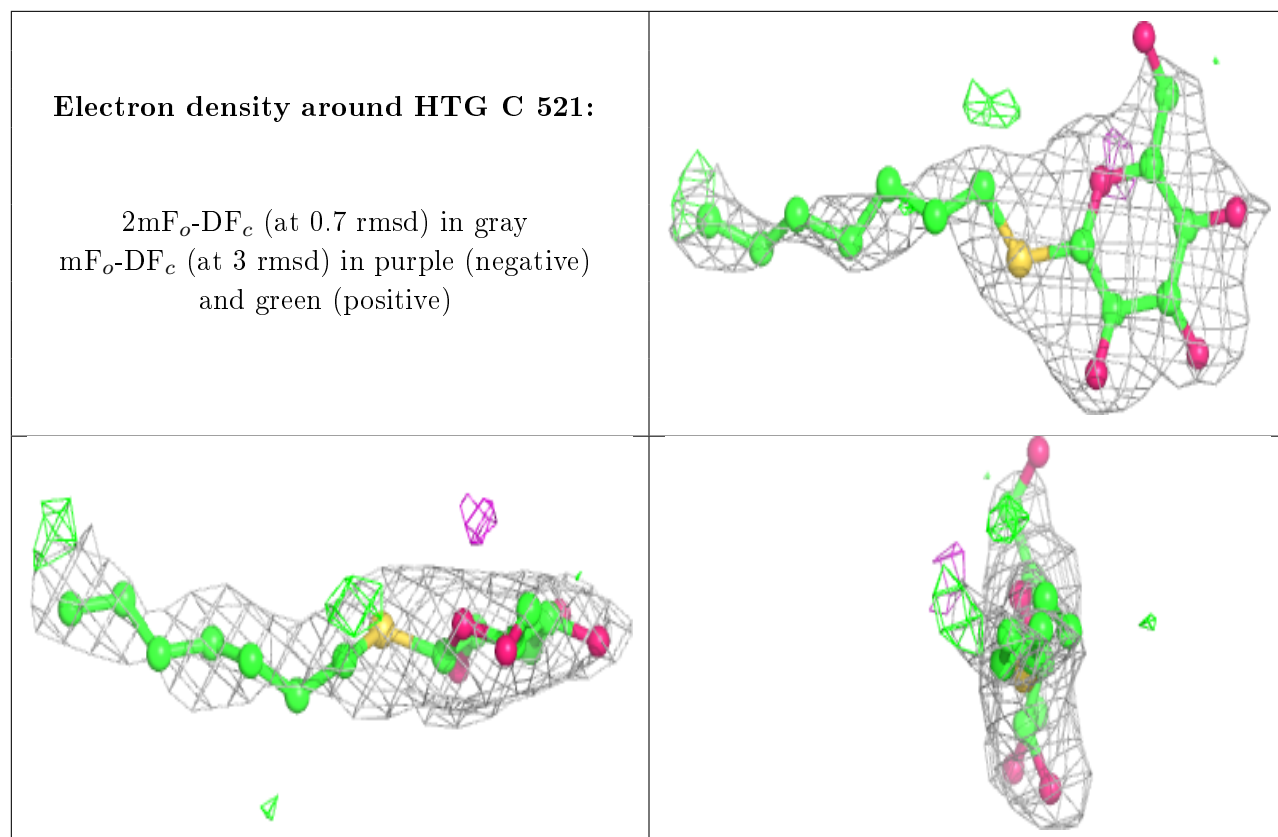




**Electron density around CLA B 601:**

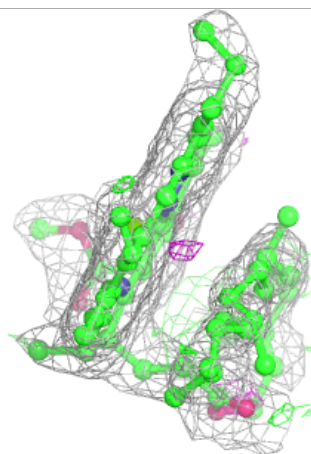
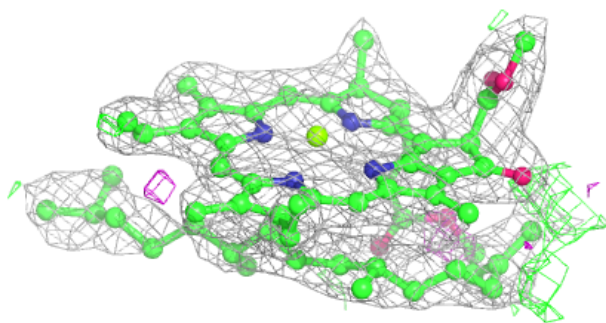
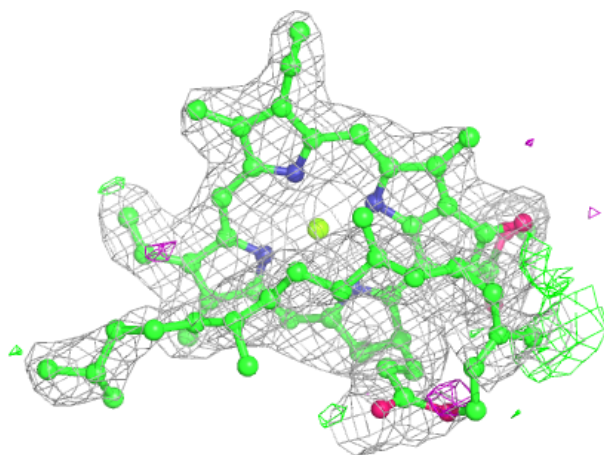
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





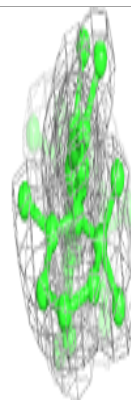
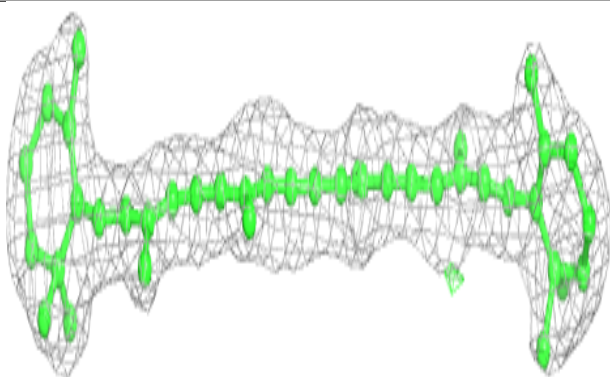
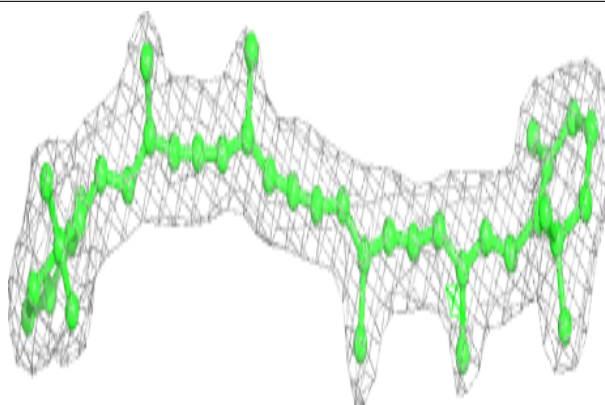
**Electron density around CLA b 604:**

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

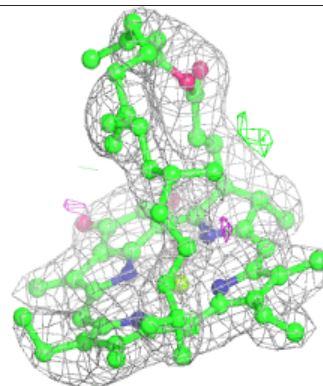
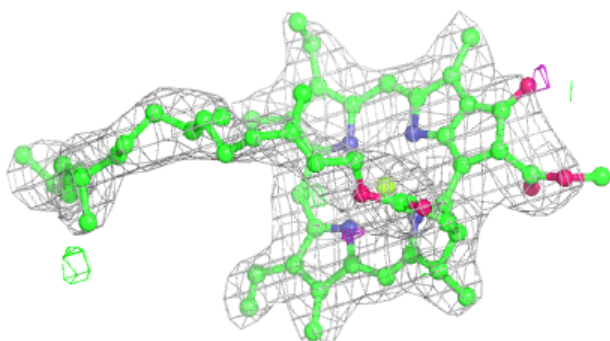
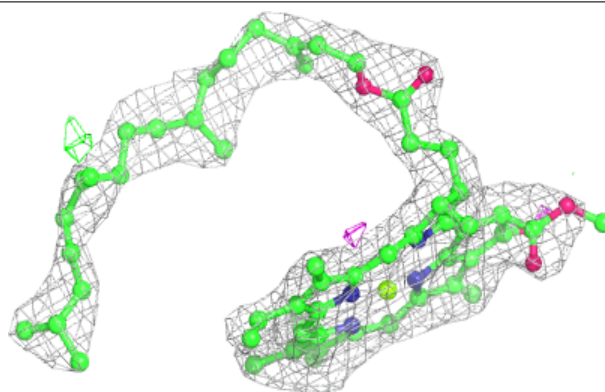


**Electron density around BCR K 102:**

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

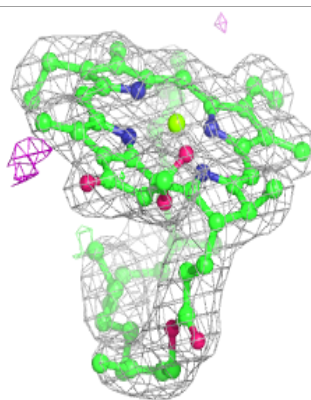
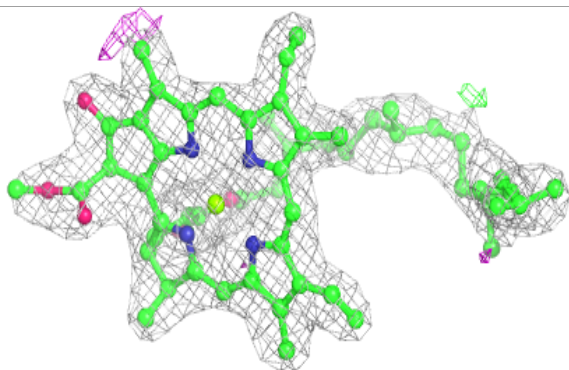
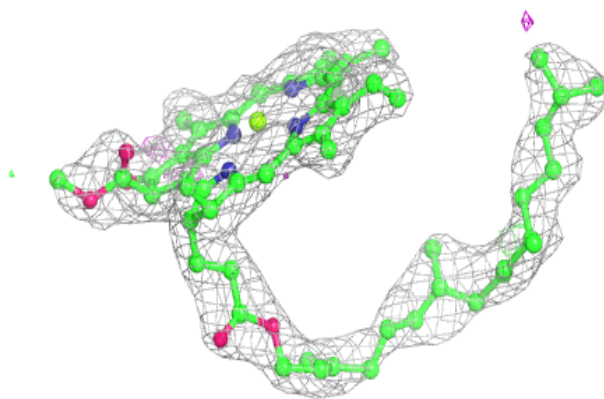
**Electron density around CLA c 513:**

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

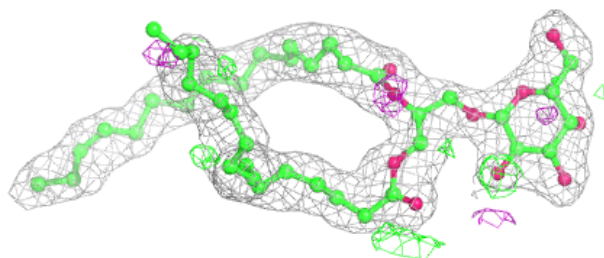
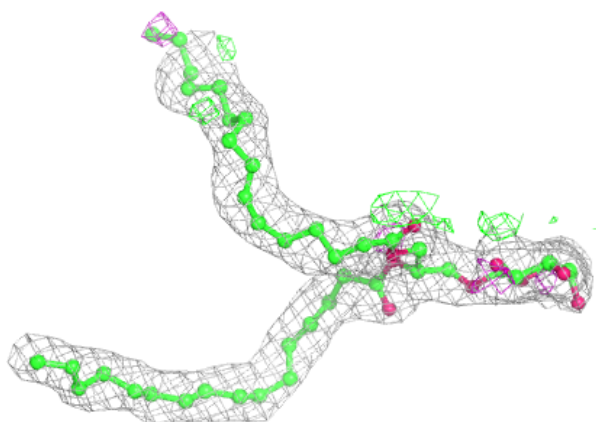


**Electron density around CLA C 513:**

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

**Electron density around LMG B 622:**

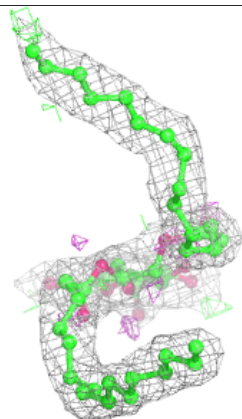
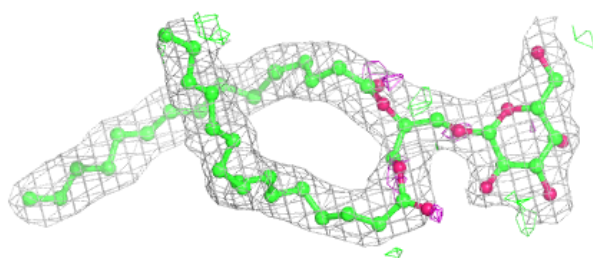
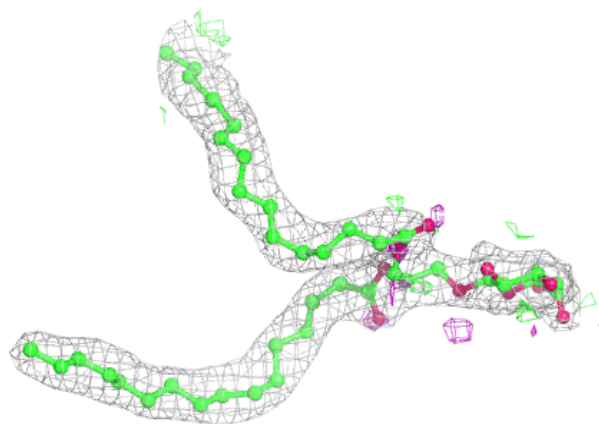
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



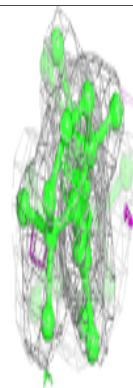
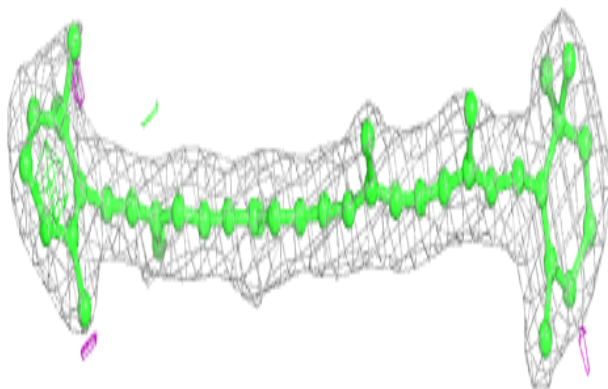
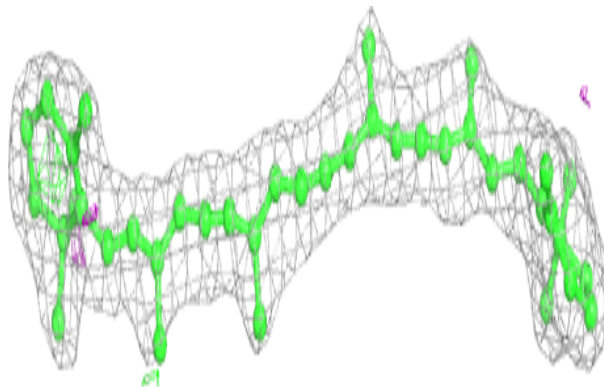


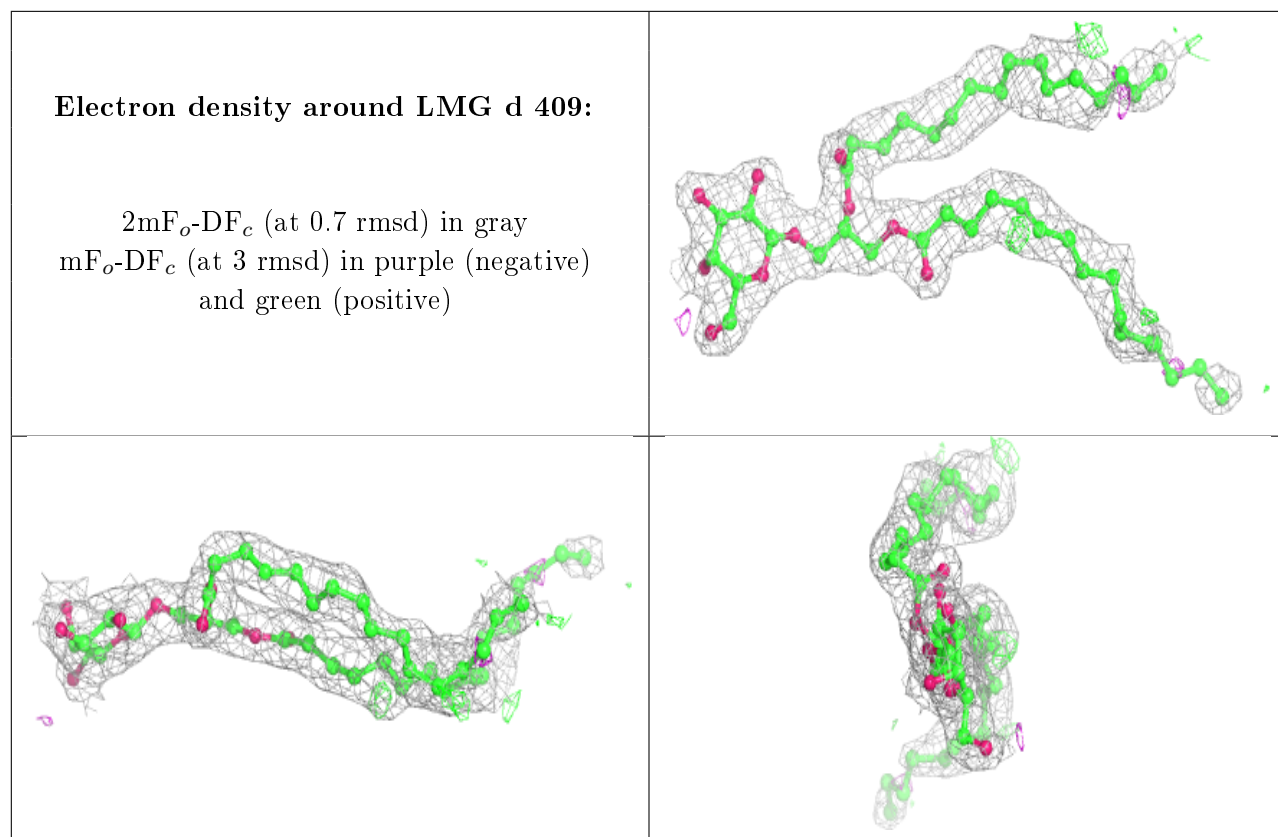
**Electron density around LMG m 102:**

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

**Electron density around BCR k 102:**

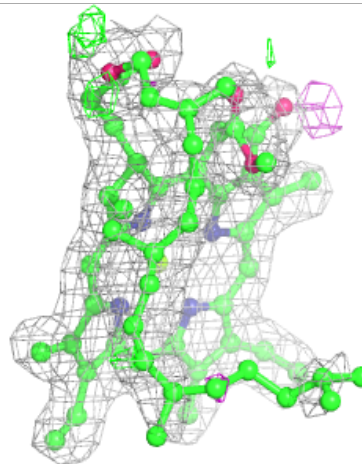
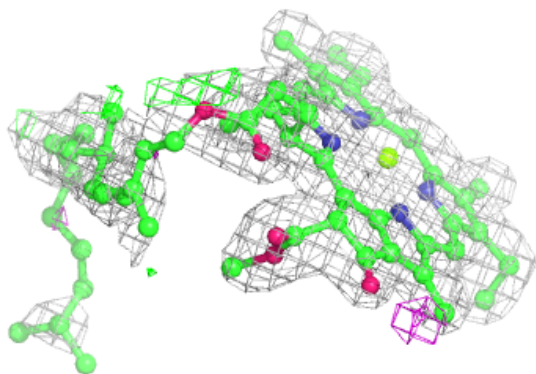
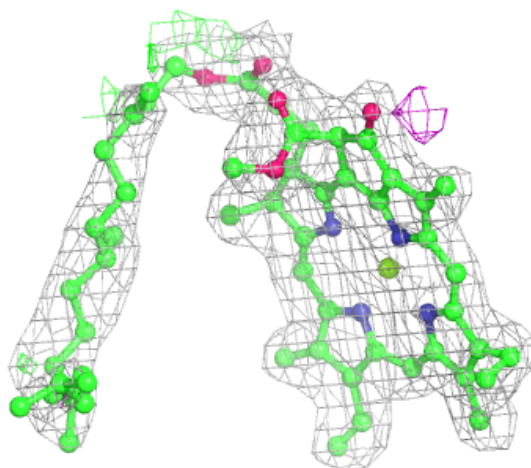
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA b 619:**

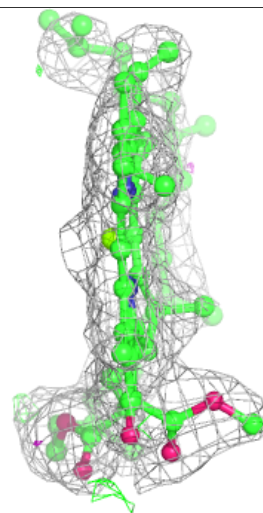
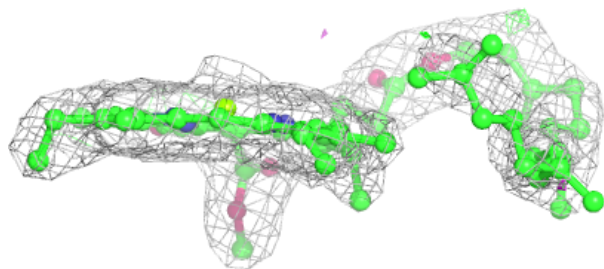
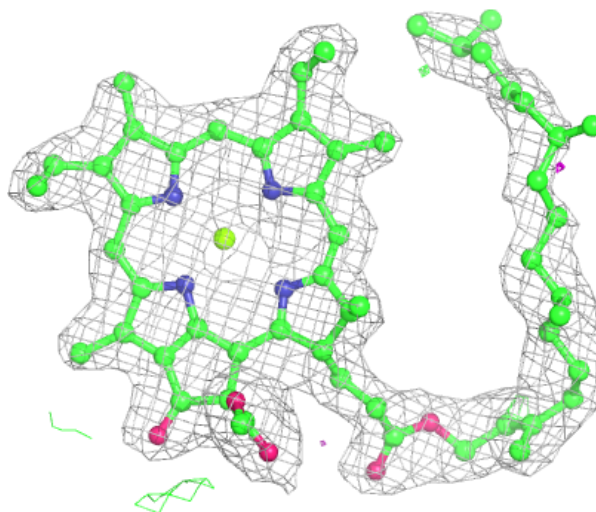
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





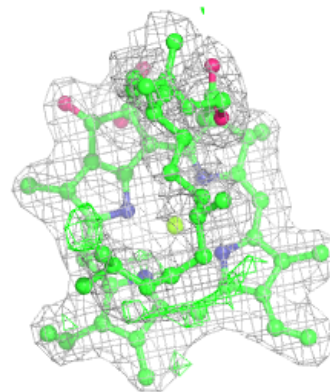
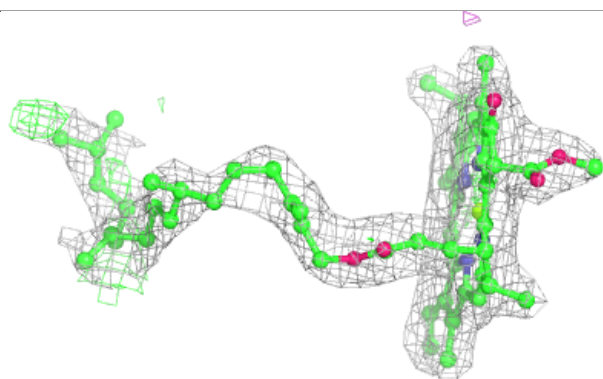
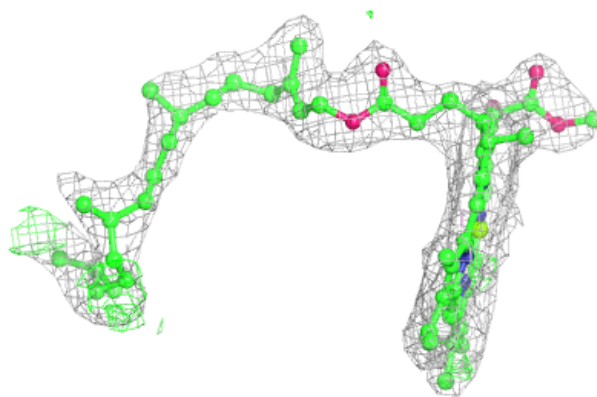
**Electron density around CLA C 512:**

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

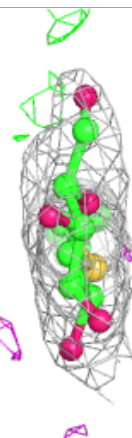
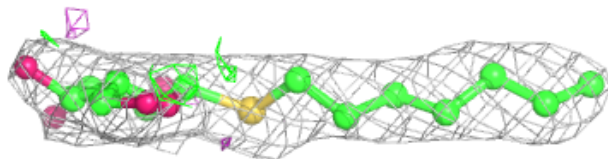
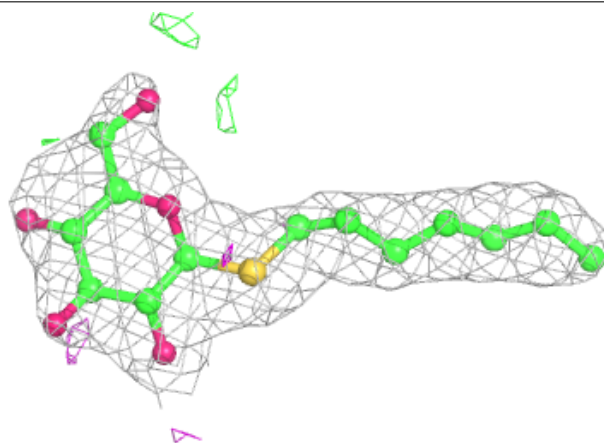


**Electron density around CLA c 506:**

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

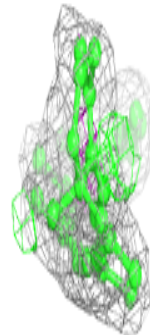
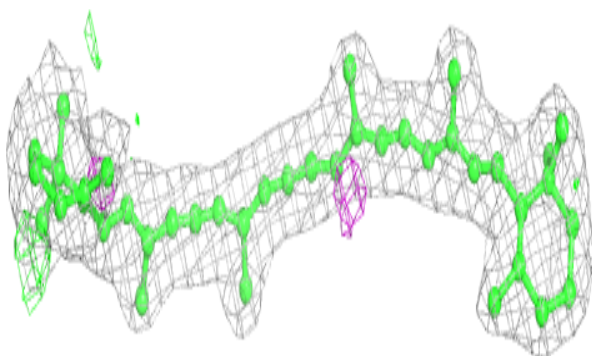
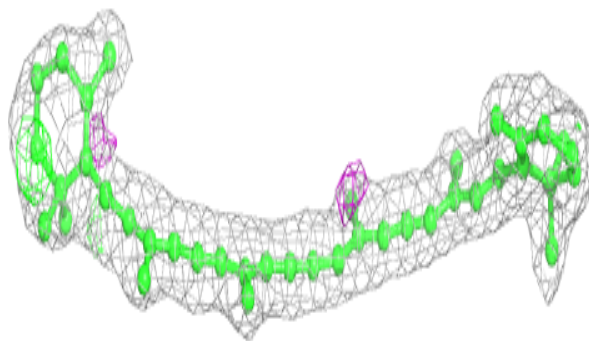
**Electron density around HTG b 601:**

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



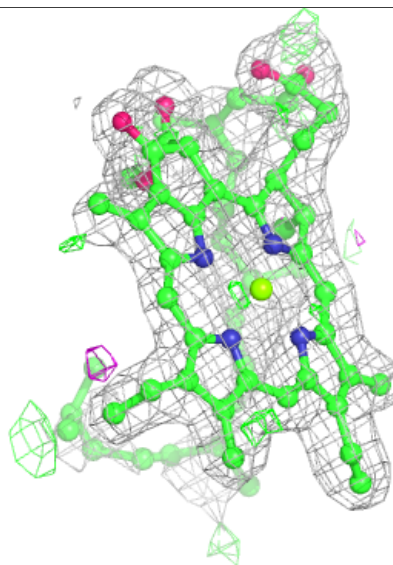
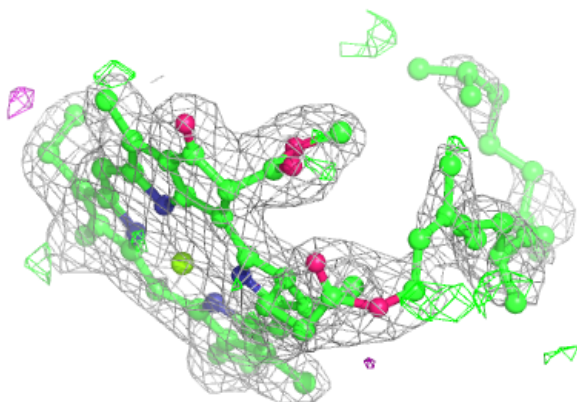
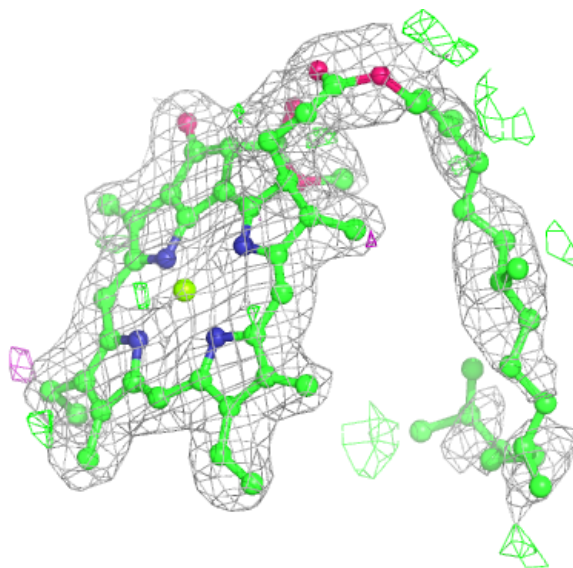
**Electron density around BCR d 404:**

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



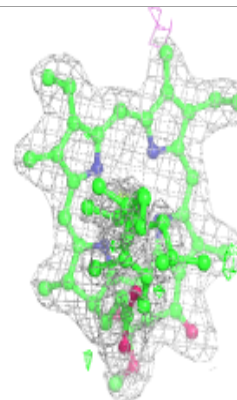
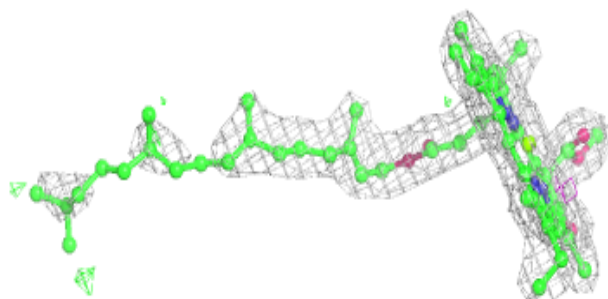
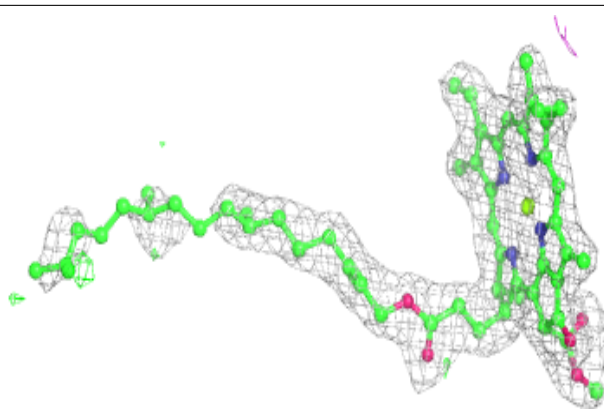
**Electron density around CLA B 616:**

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

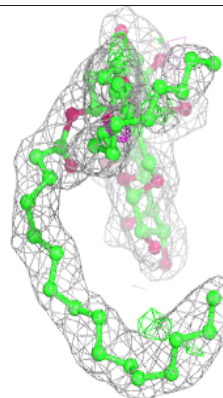
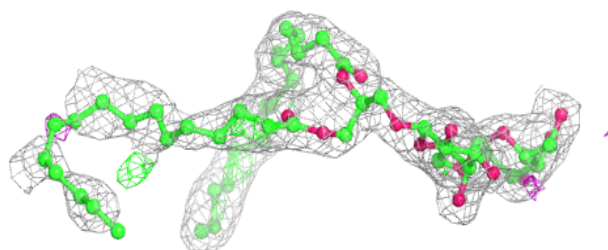
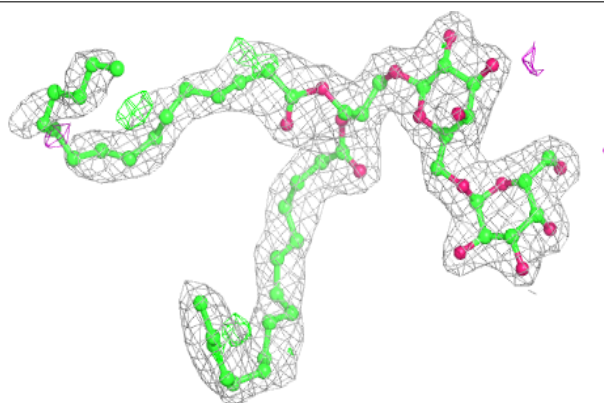


**Electron density around CLA d 403:**

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

**Electron density around DGD c 516:**

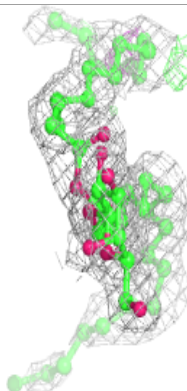
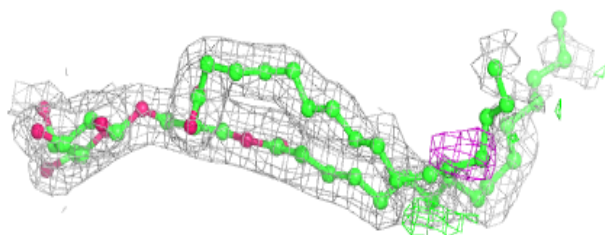
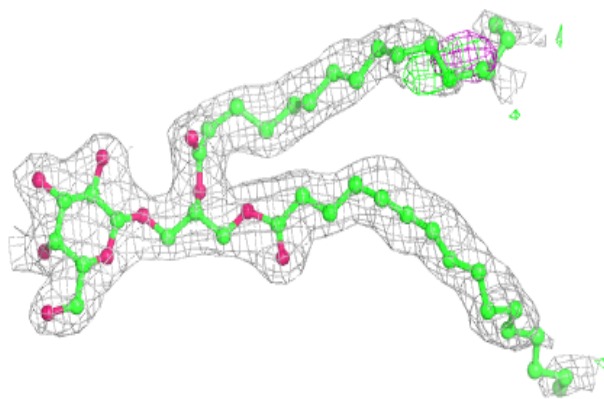
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



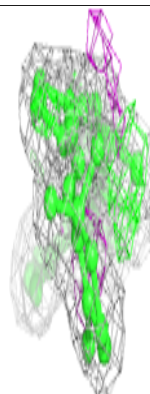
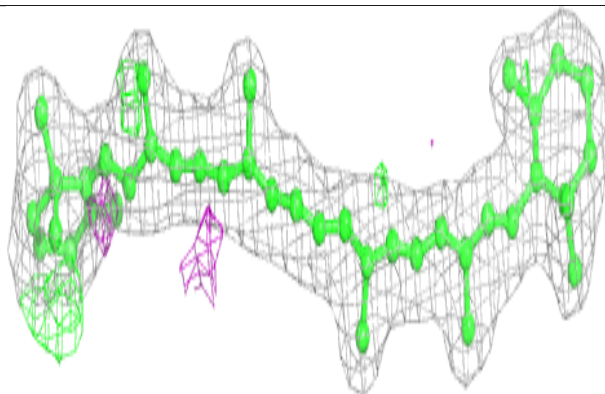
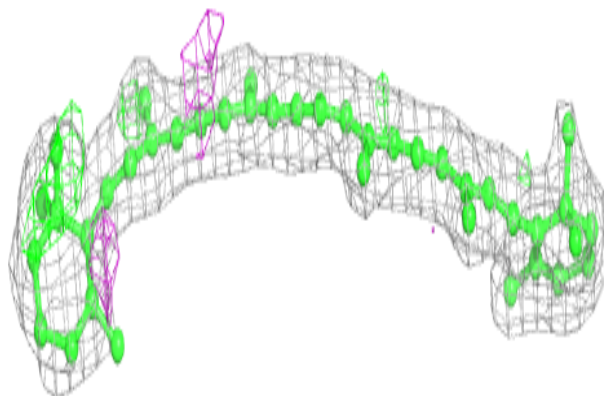


**Electron density around LMG D 412:**

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

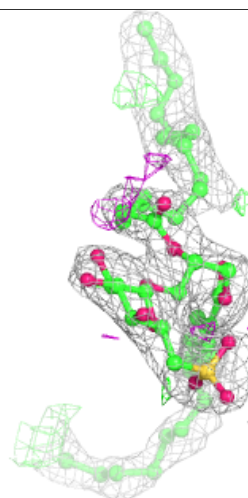
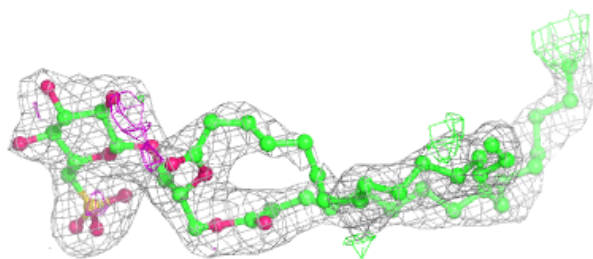
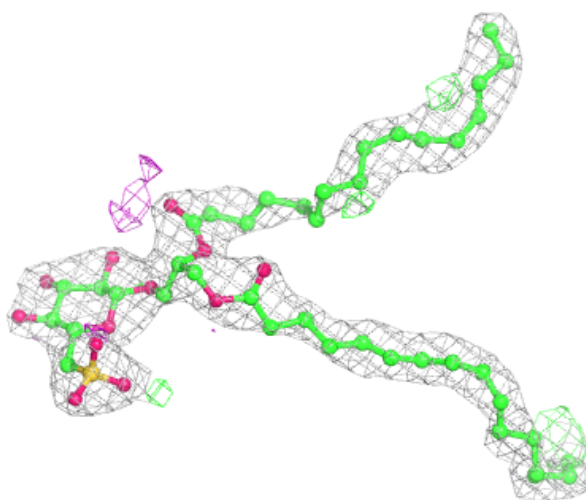
**Electron density around BCR D 406:**

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



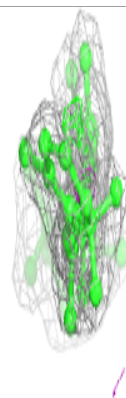
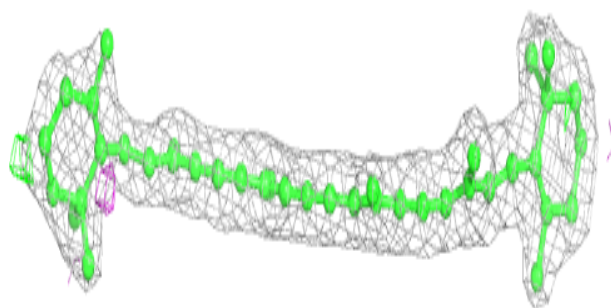
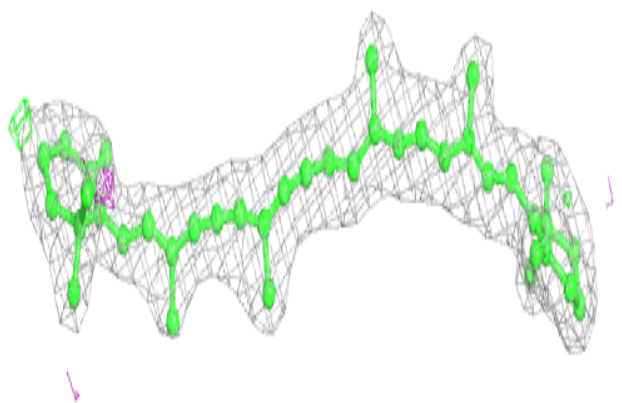
**Electron density around SQD c 518:**

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



**Electron density around BCR h 101:**

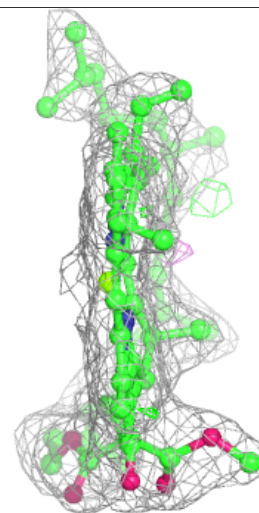
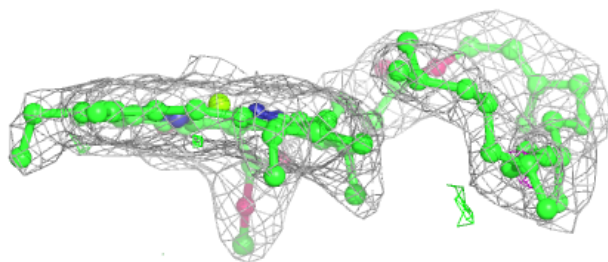
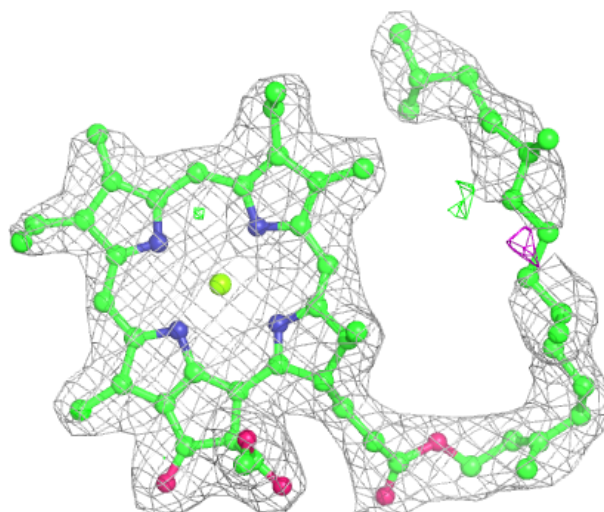
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





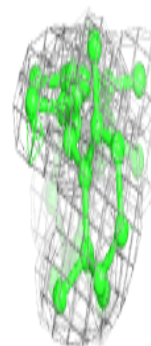
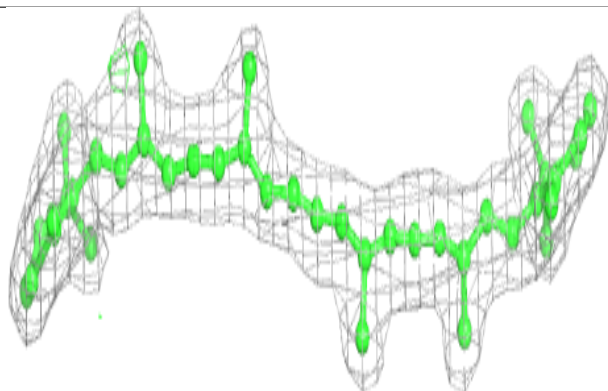
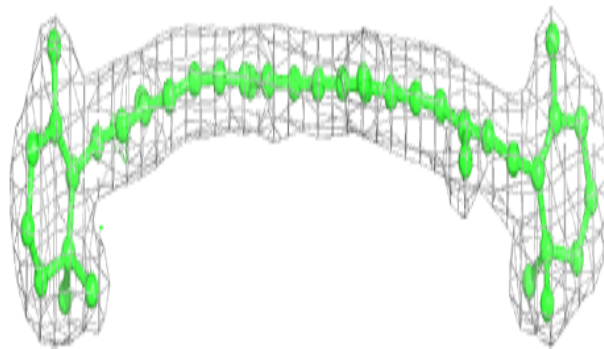
**Electron density around CLA c 512:**

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

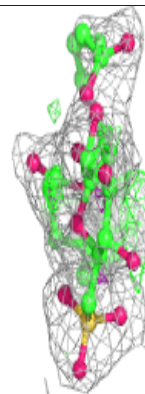
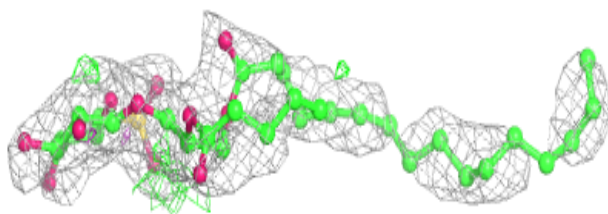
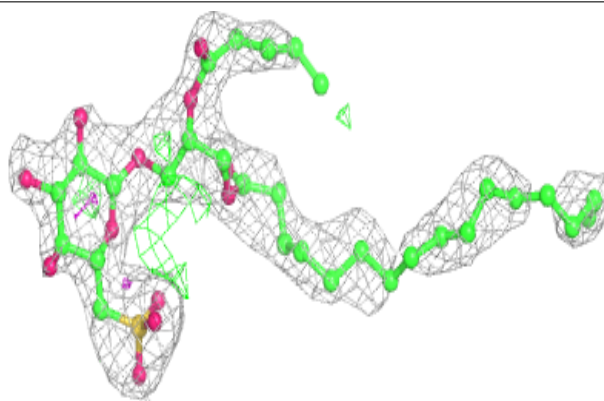


**Electron density around BCR K 101:**

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

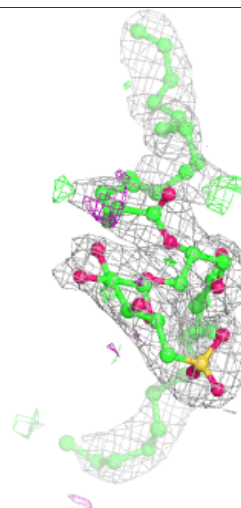
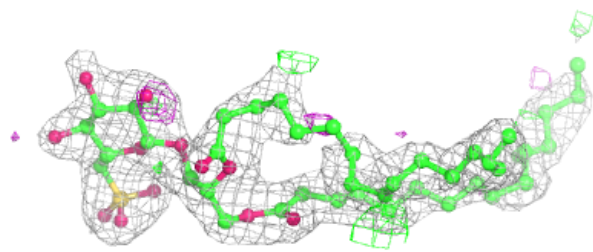
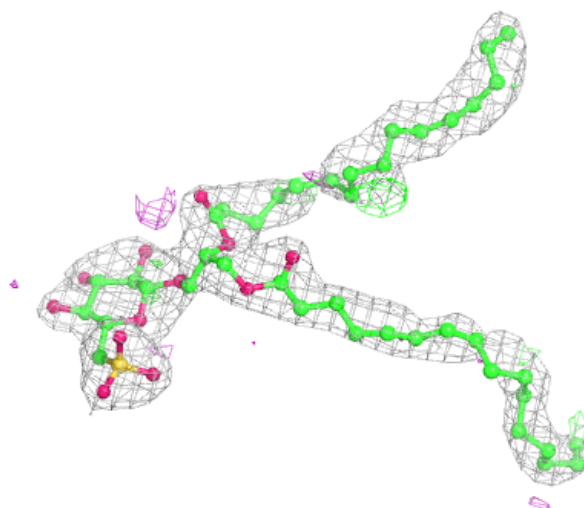
**Electron density around SQD D 408:**

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



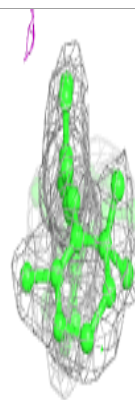
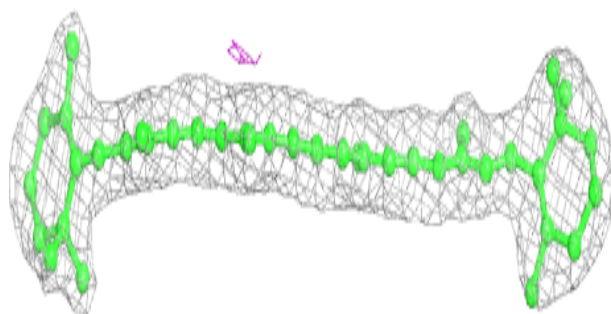
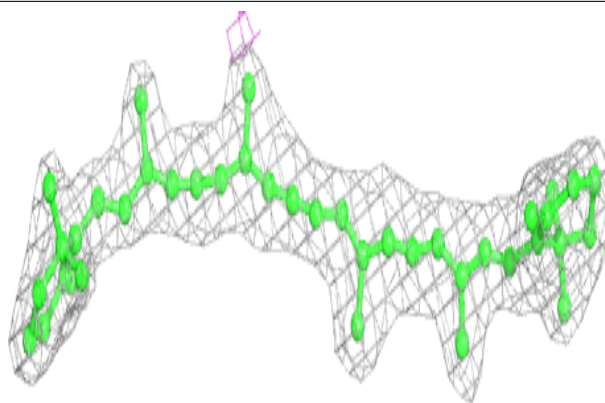
**Electron density around SQD A 1011:**

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

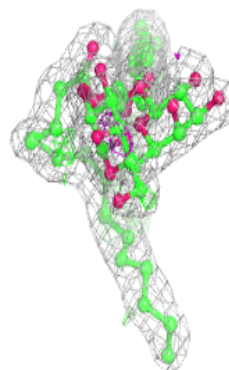
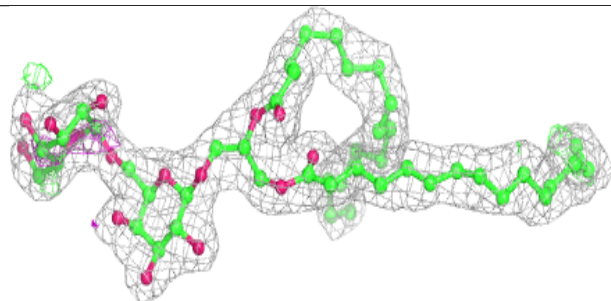
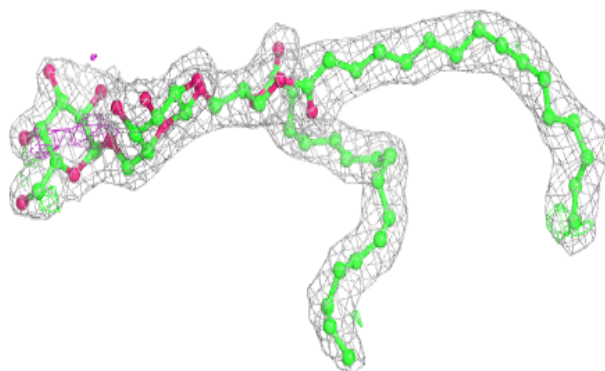


**Electron density around BCR c 514:**

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

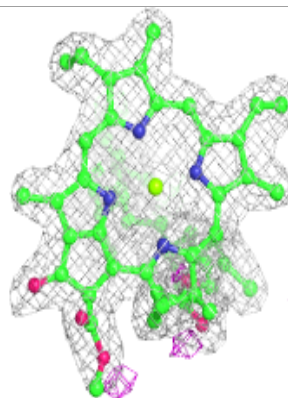
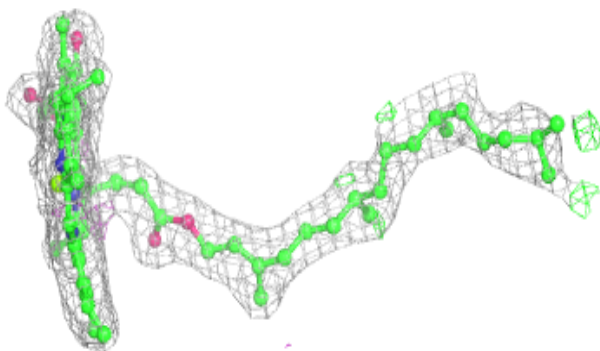
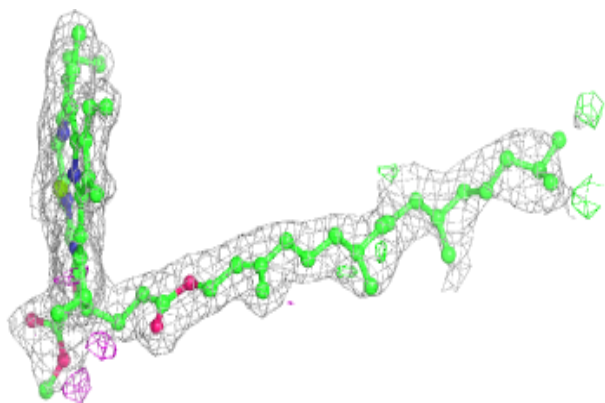
**Electron density around DGD h 102:**

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

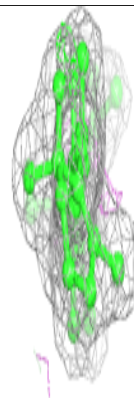
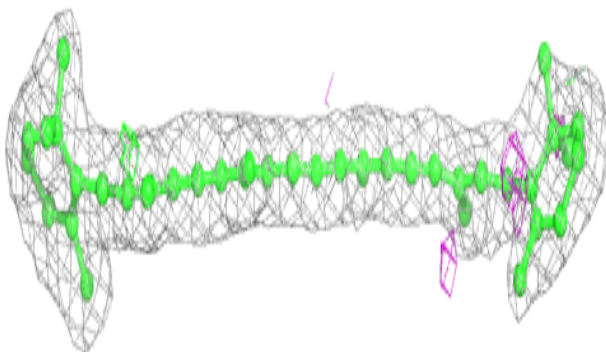
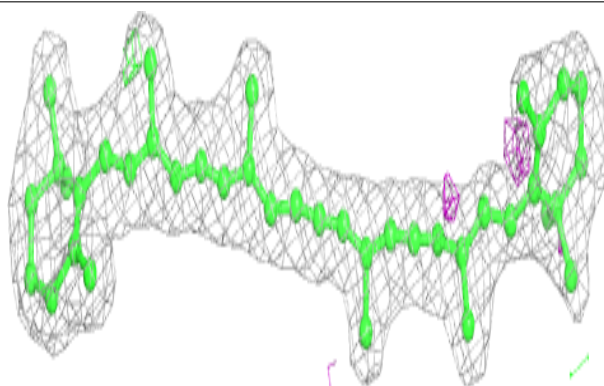


**Electron density around CLA b 609:**

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

**Electron density around BCR B 618:**

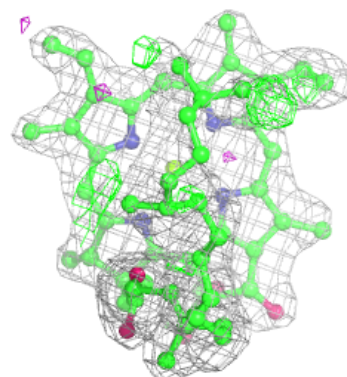
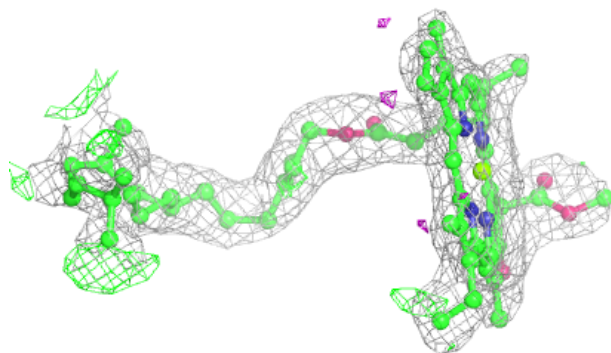
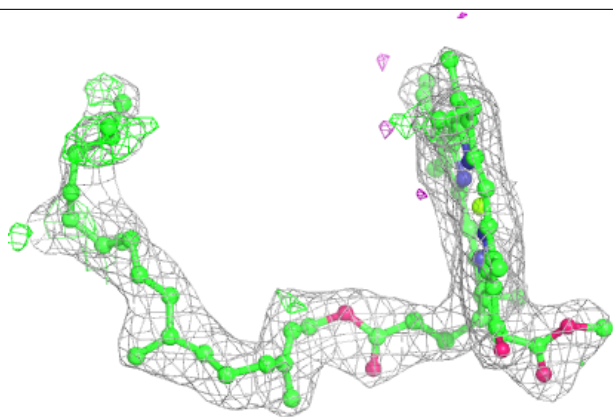
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



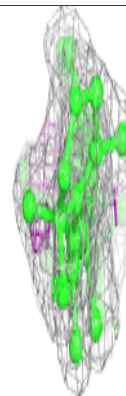
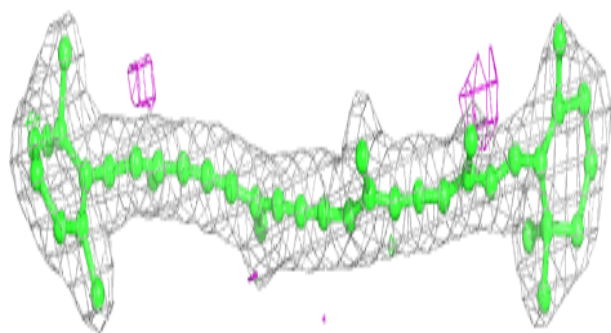
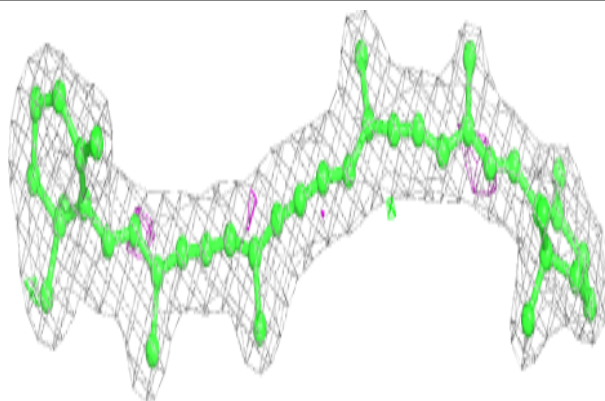


**Electron density around CLA C 506:**

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

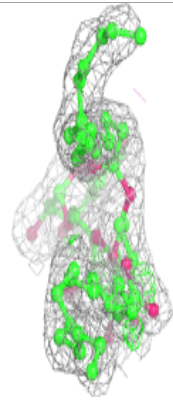
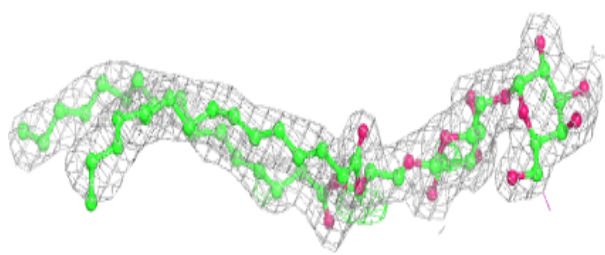
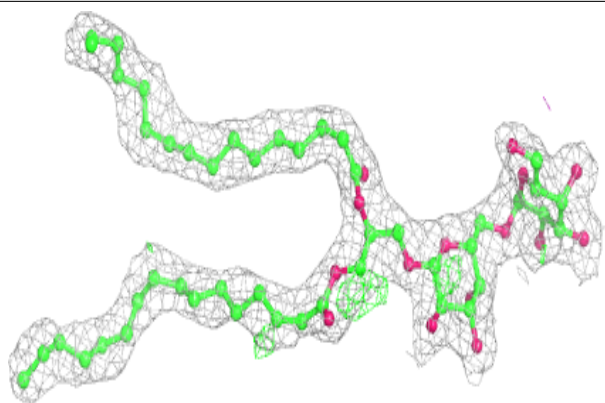
**Electron density around BCR J 101:**

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

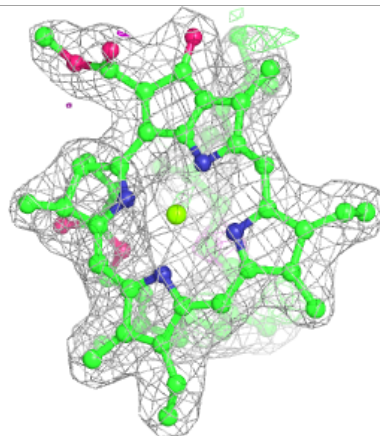
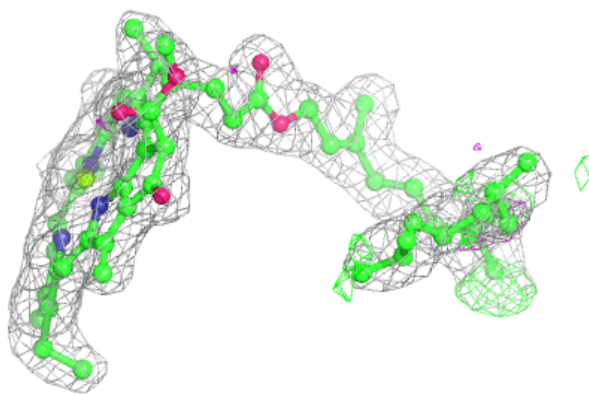
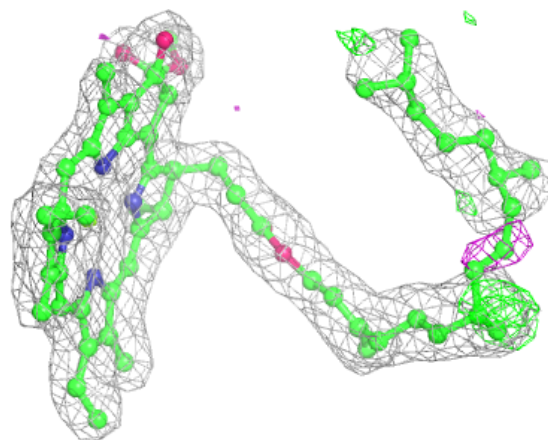


**Electron density around DGD c 517:**

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

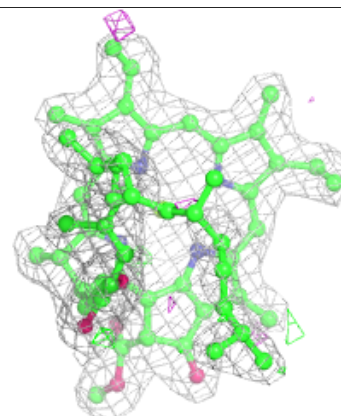
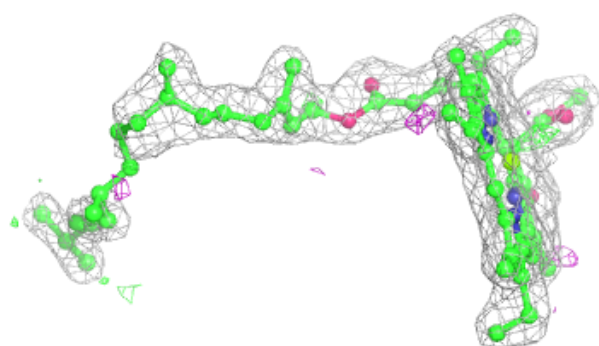
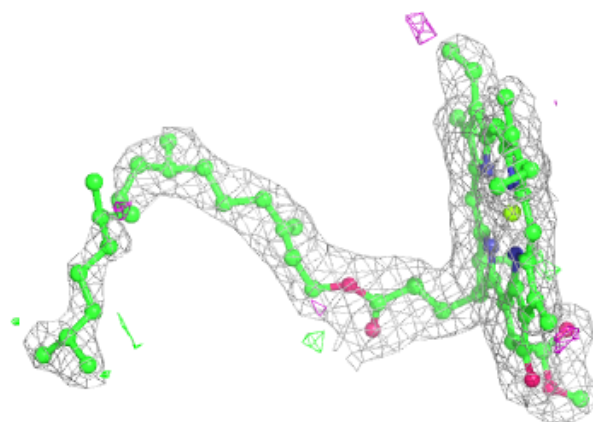
**Electron density around CLA B 606:**

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

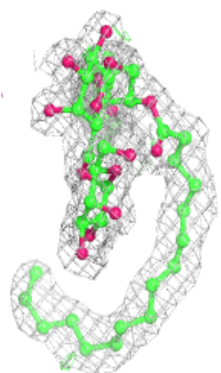
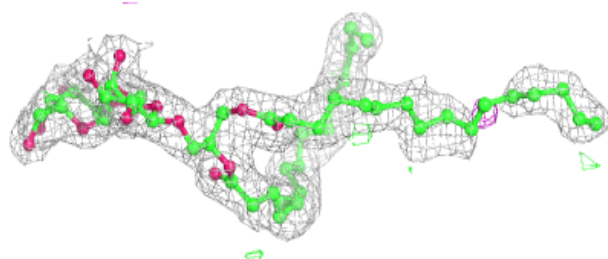
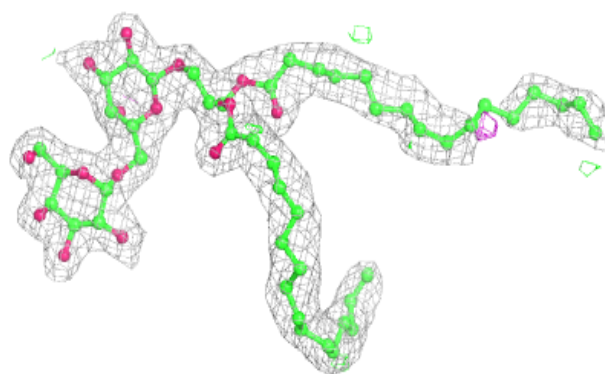


**Electron density around CLA D 405:**

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

**Electron density around DGD C 516:**

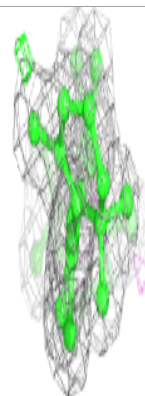
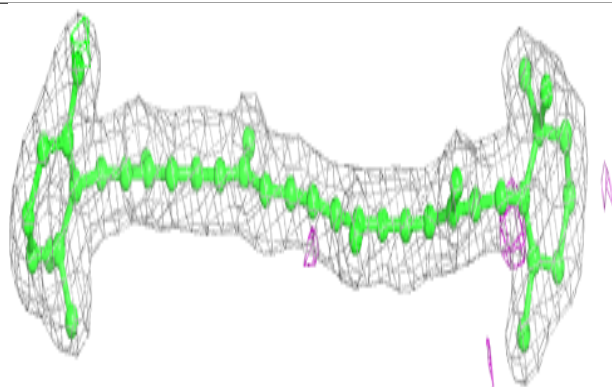
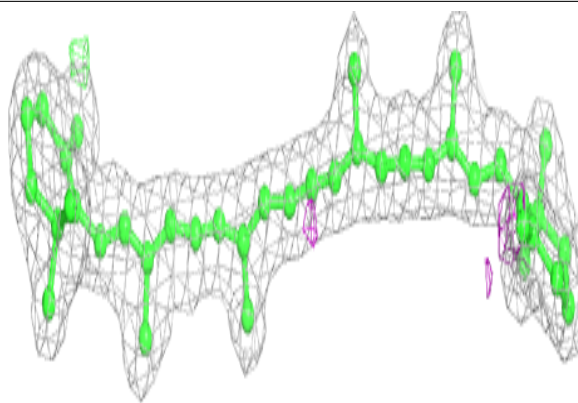
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



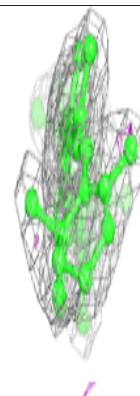
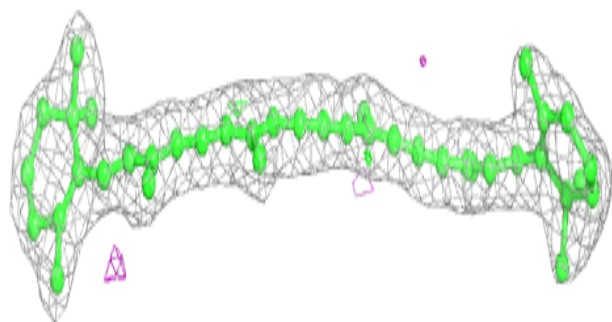
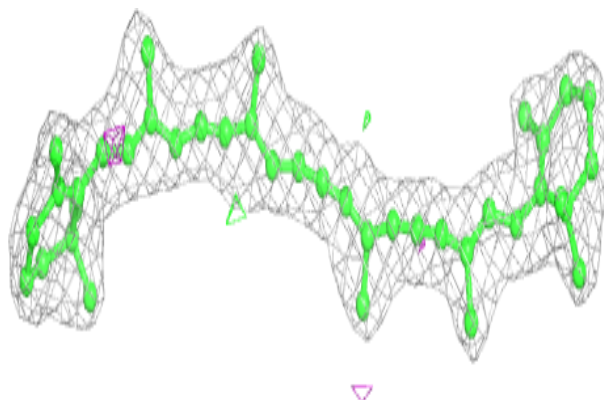


**Electron density around BCR a 413:**

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

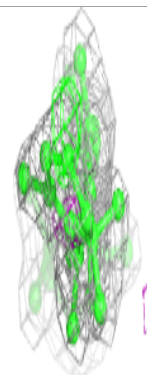
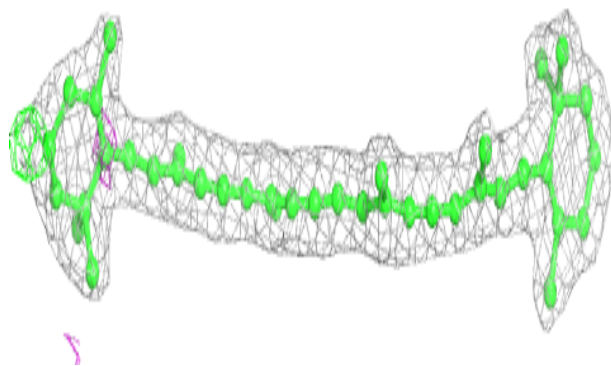
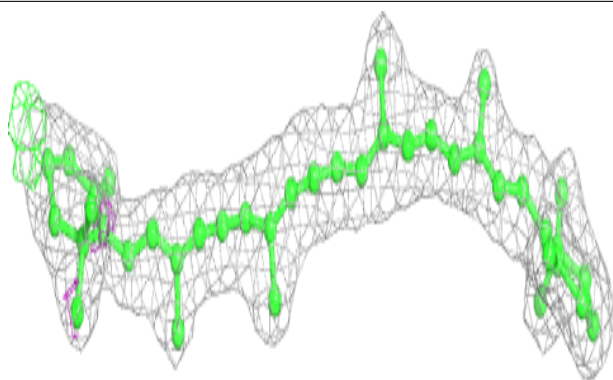
**Electron density around BCR y 101:**

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

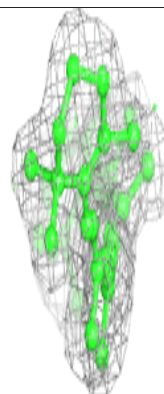
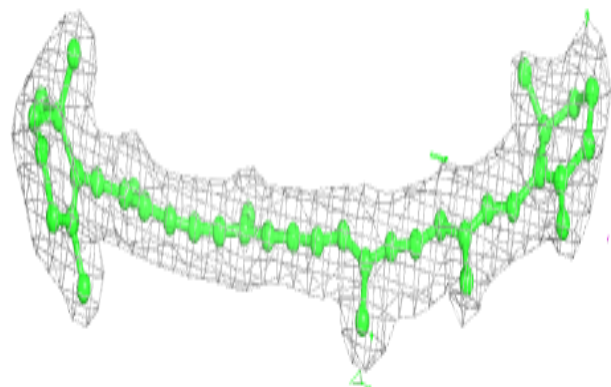
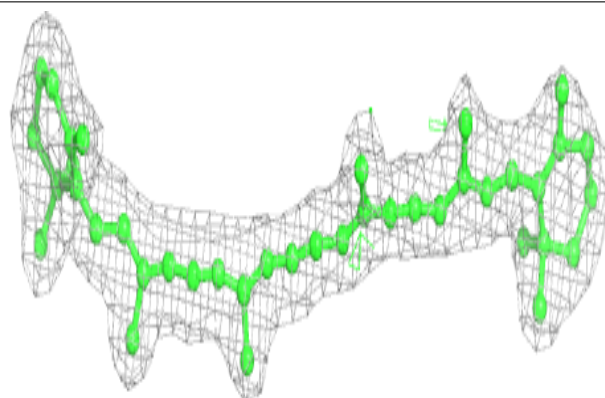


**Electron density around BCR H 101:**

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

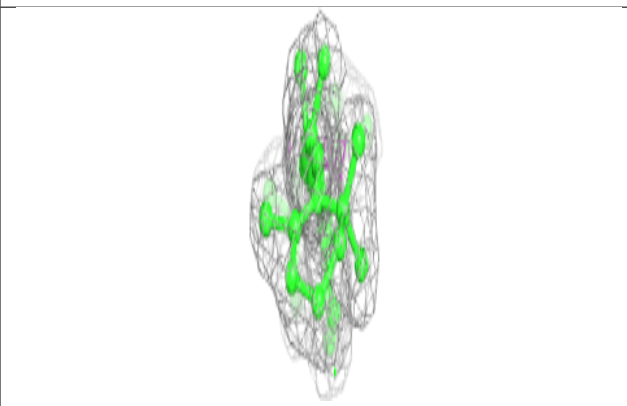
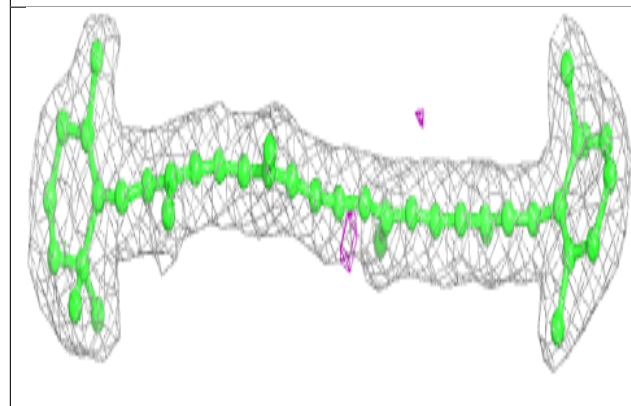
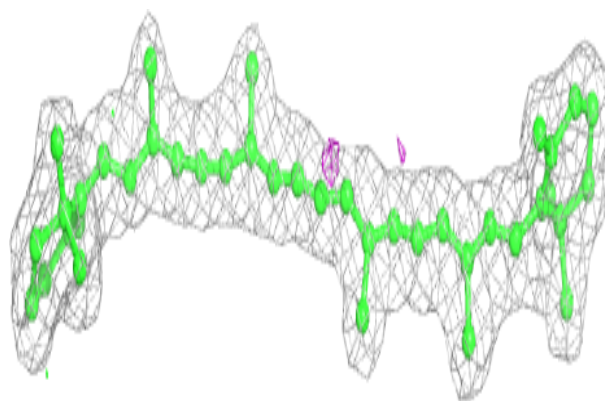
**Electron density around BCR t 101:**

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

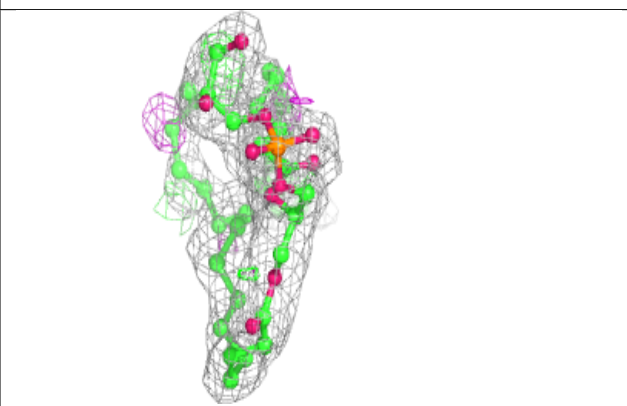
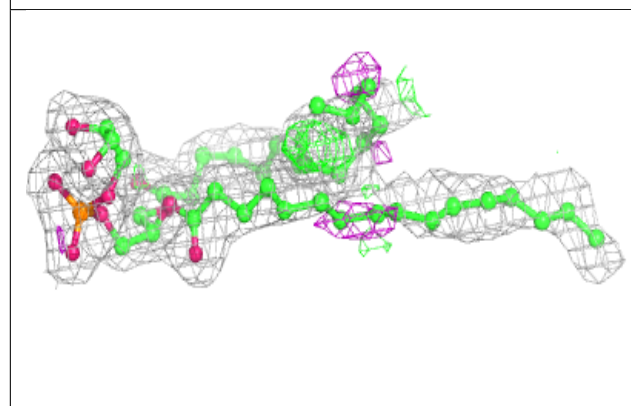
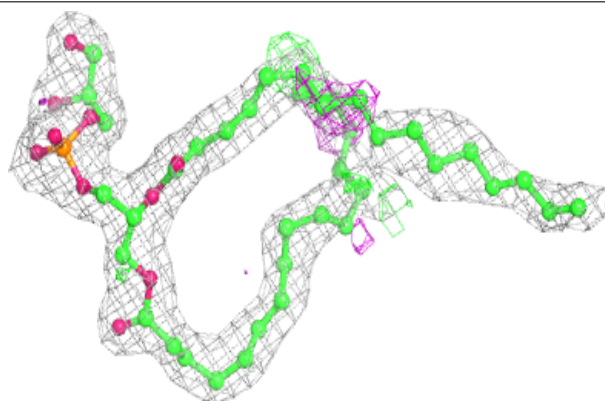


**Electron density around BCR A 1009:**

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

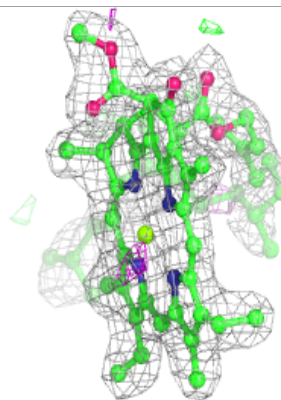
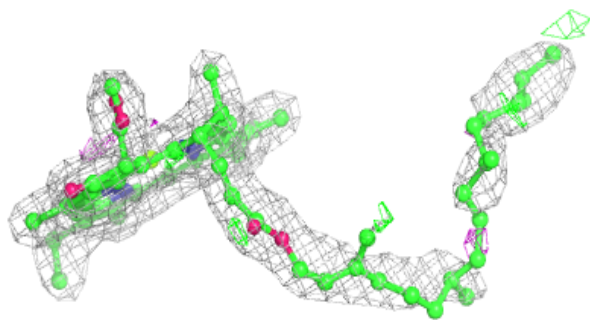
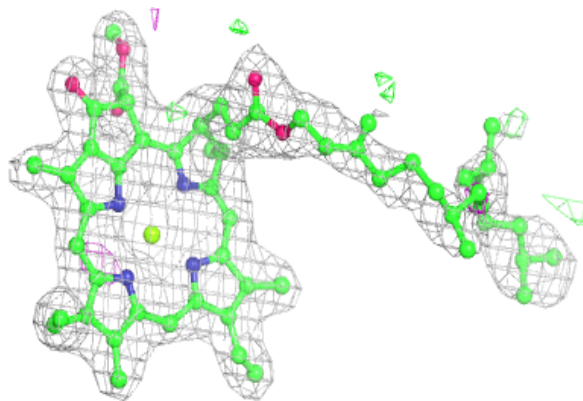
**Electron density around LHG d 408:**

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

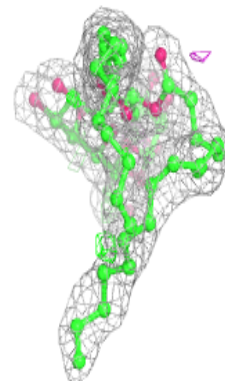
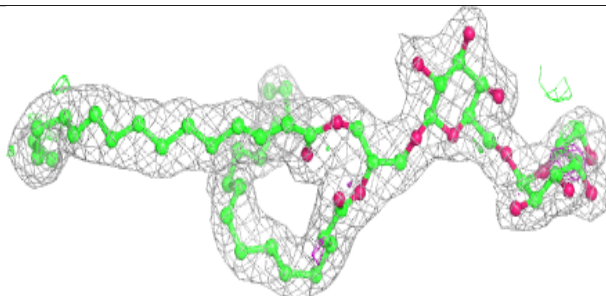
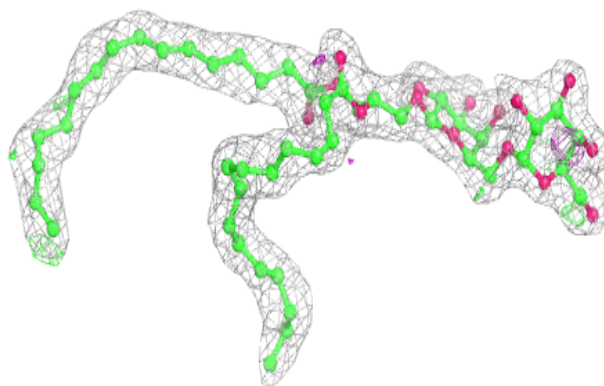


**Electron density around CLA A 1008:**

$2mF_o-DF_c$  (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:**

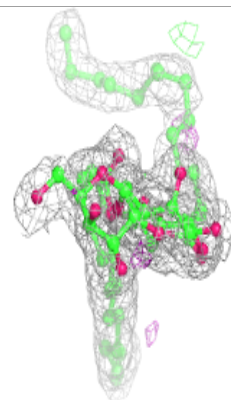
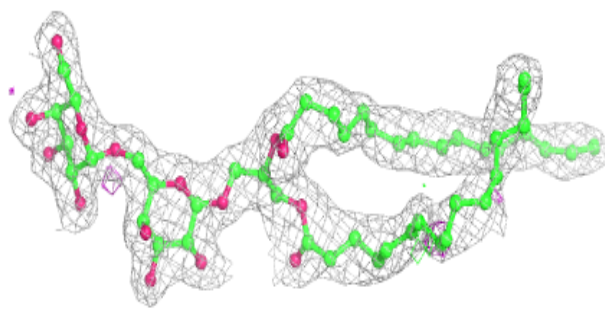
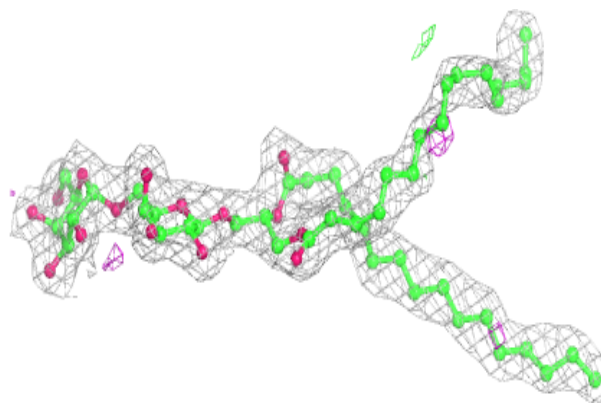
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



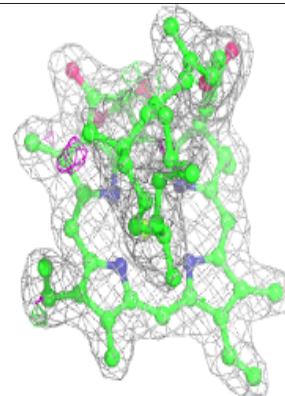
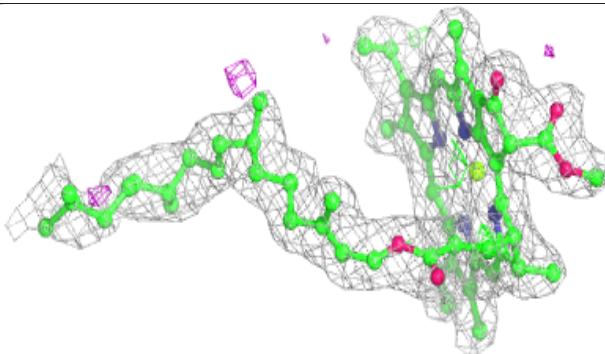
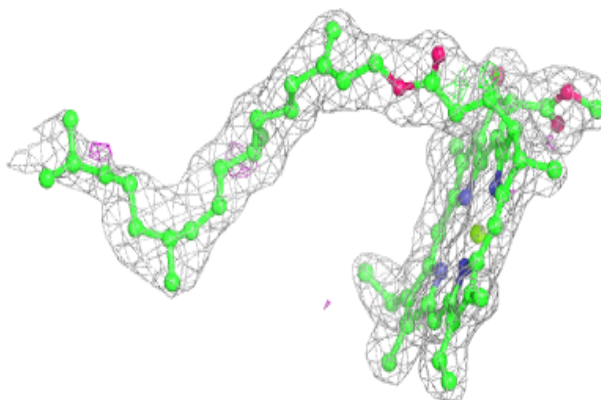


**Electron density around DGD c 515:**

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

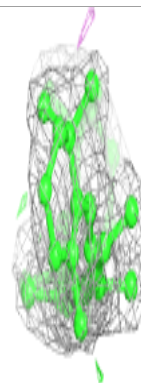
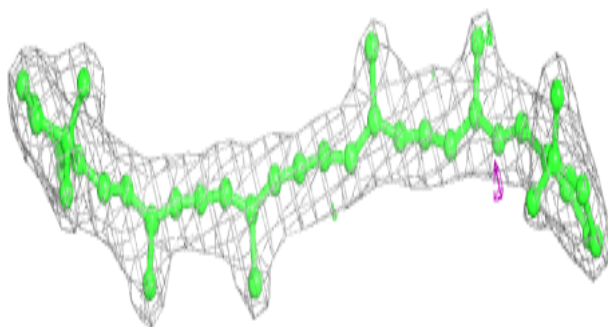
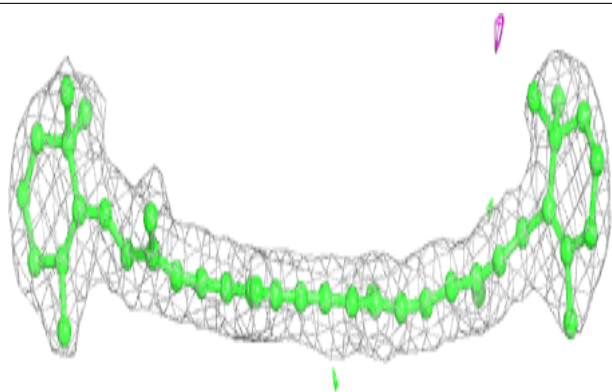
**Electron density around CLA c 508:**

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

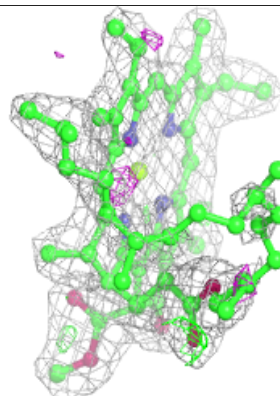
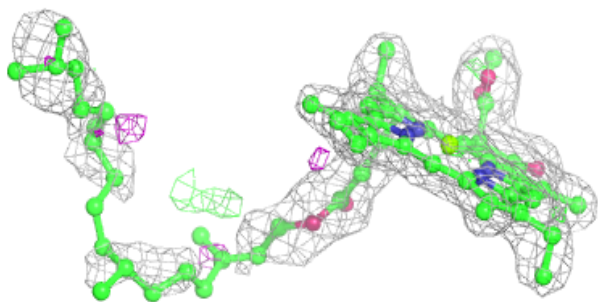
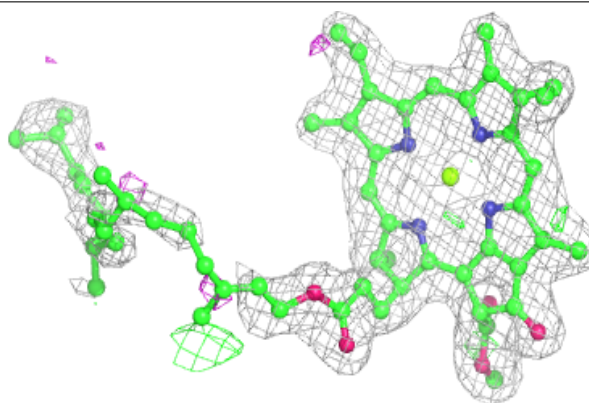


**Electron density around BCR k 101:**

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

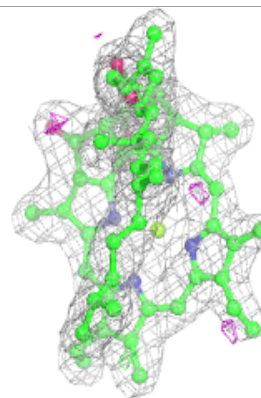
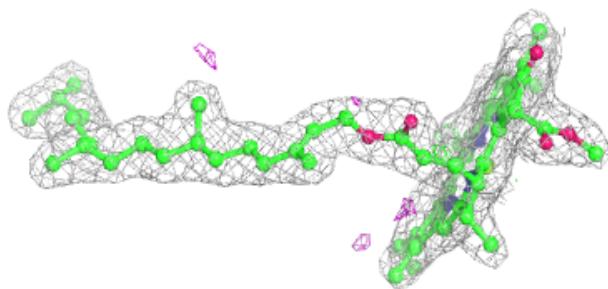
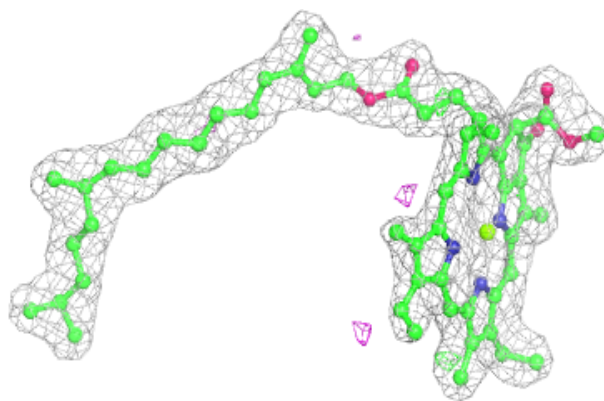
**Electron density around CLA a 412:**

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



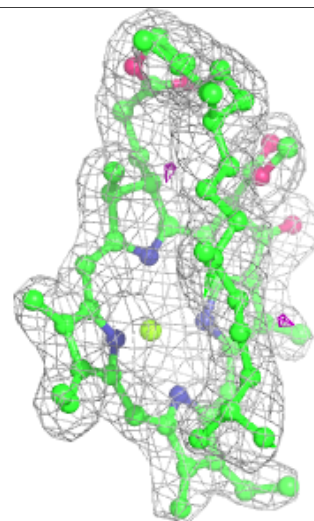
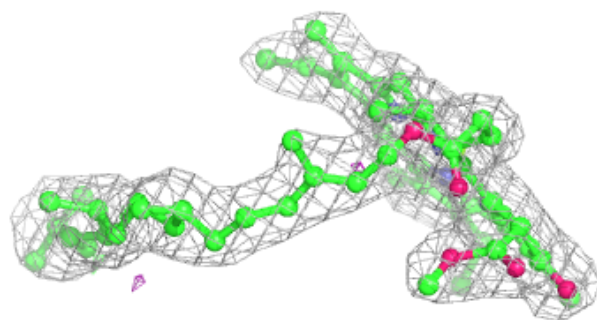
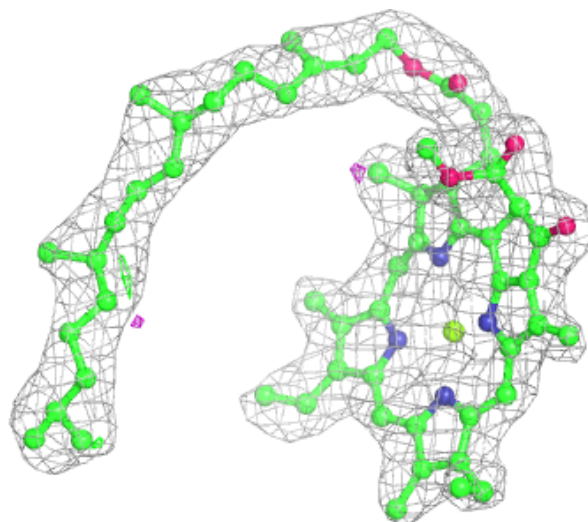
**Electron density around CLA b 612:**

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



**Electron density around CLA C 507:**

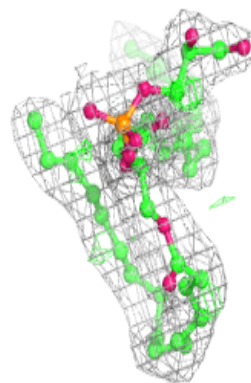
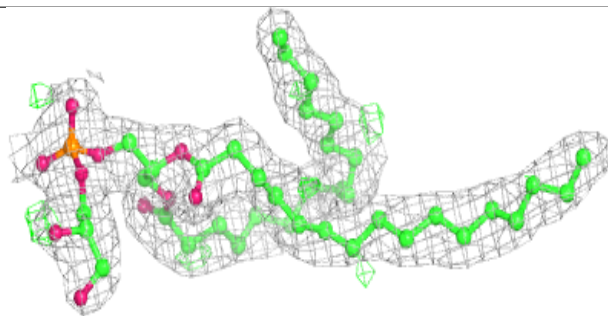
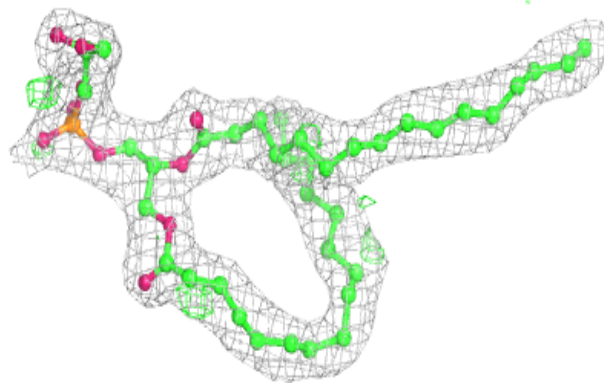
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



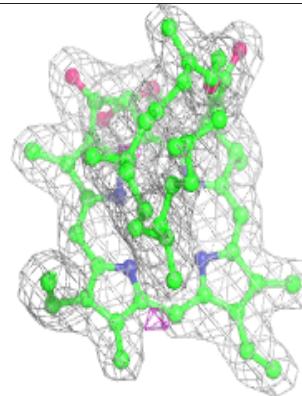
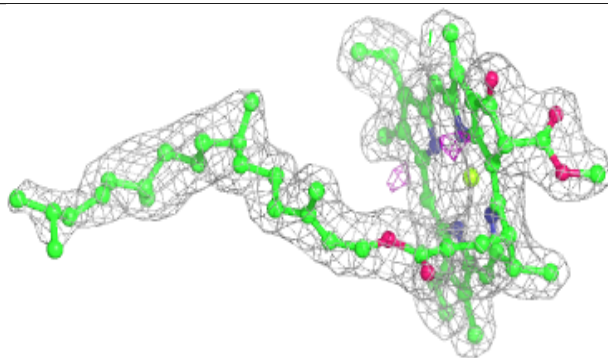
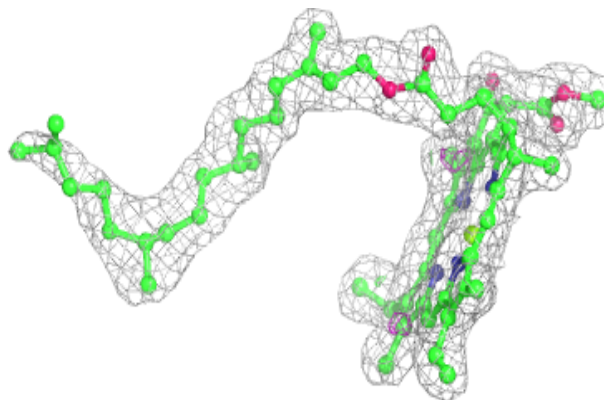


**Electron density around LHG d 406:**

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

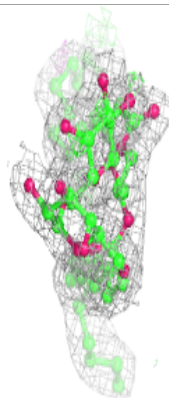
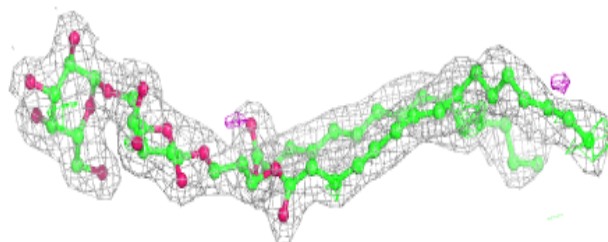
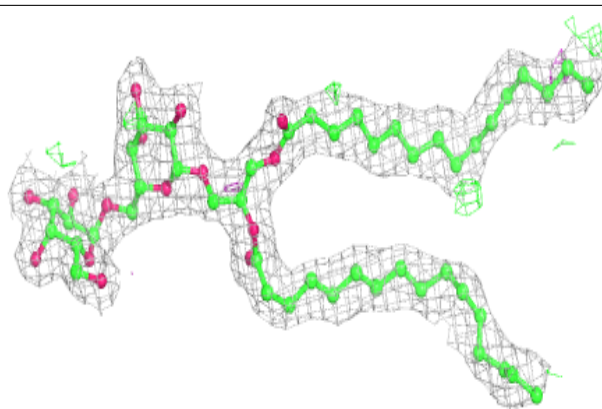
**Electron density around CLA C 508:**

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

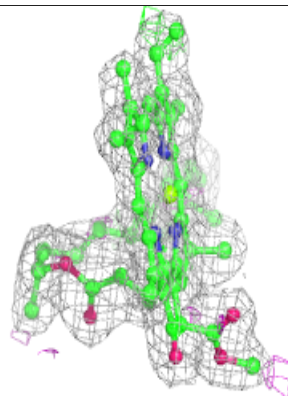
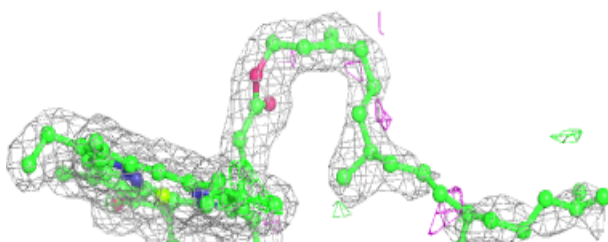
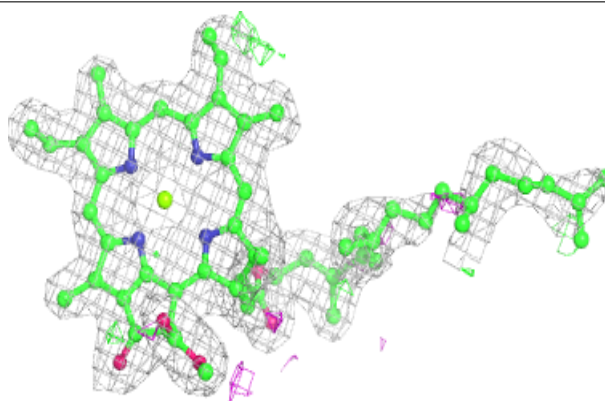


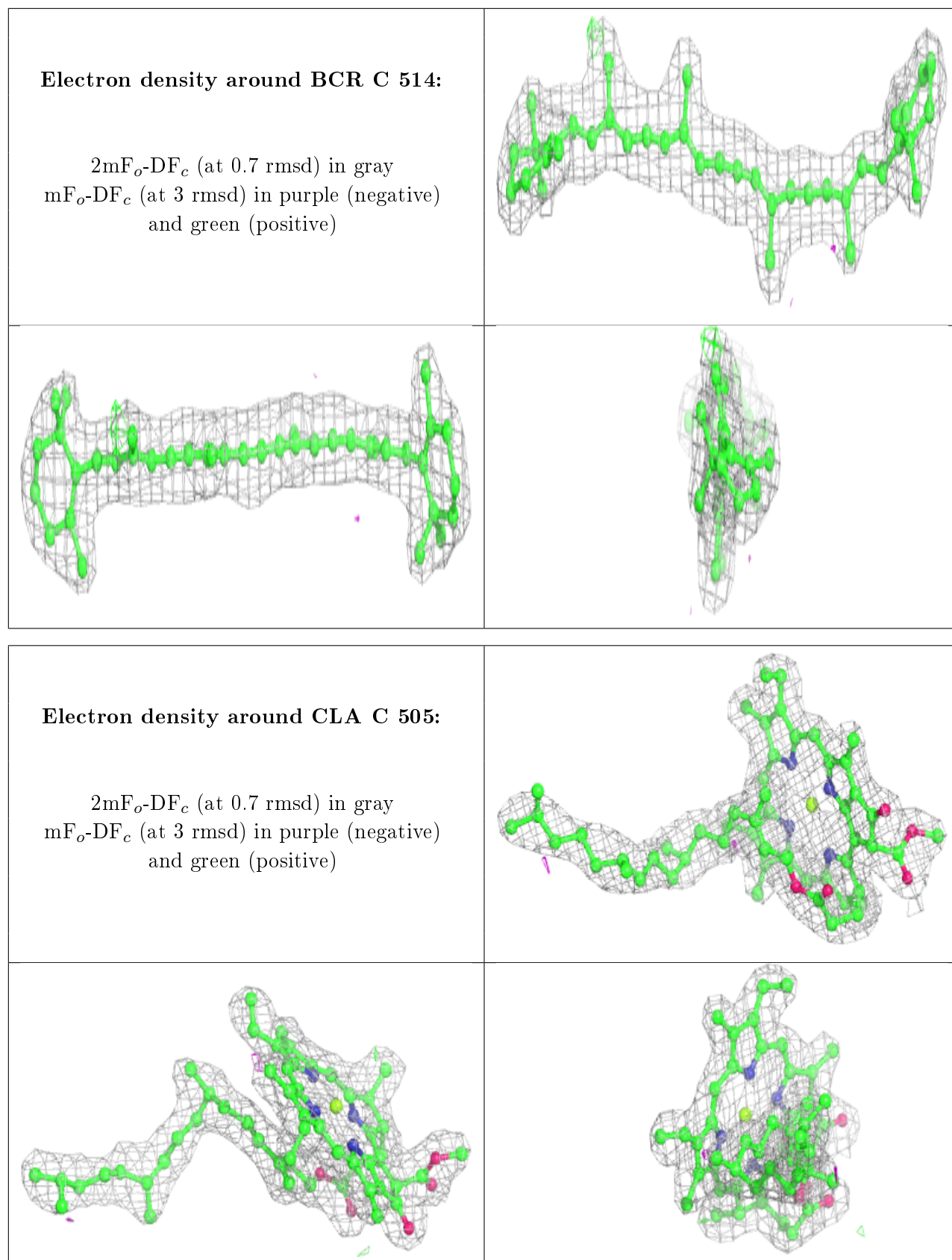
**Electron density around DGD C 517:**

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

**Electron density around CLA a 409:**

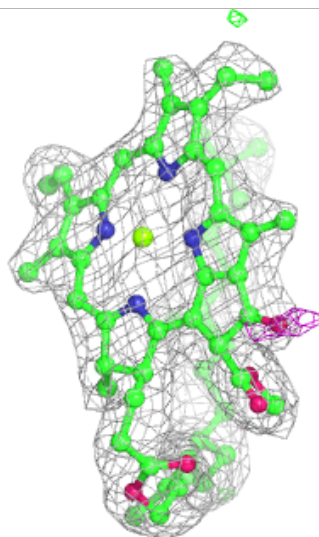
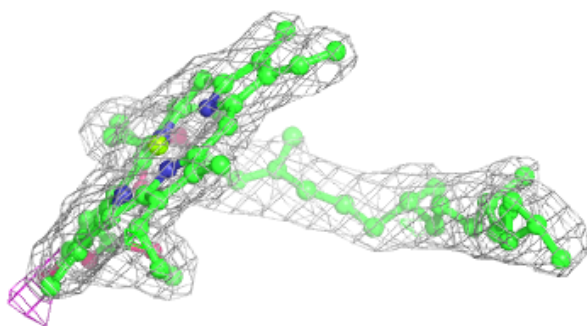
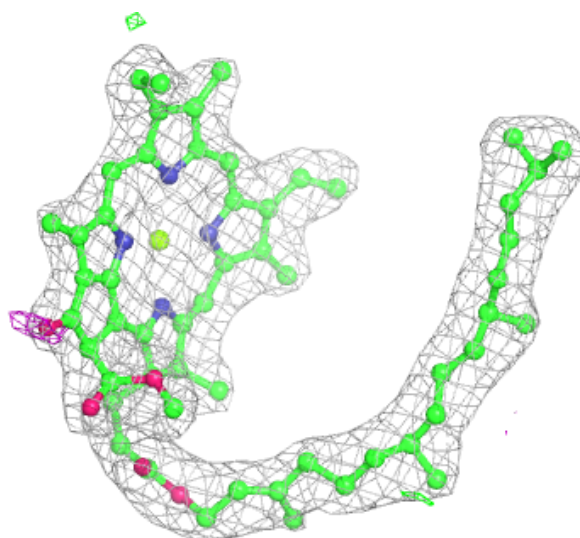
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA c 507:**

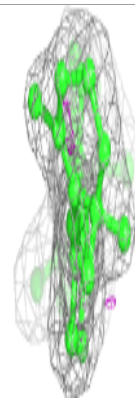
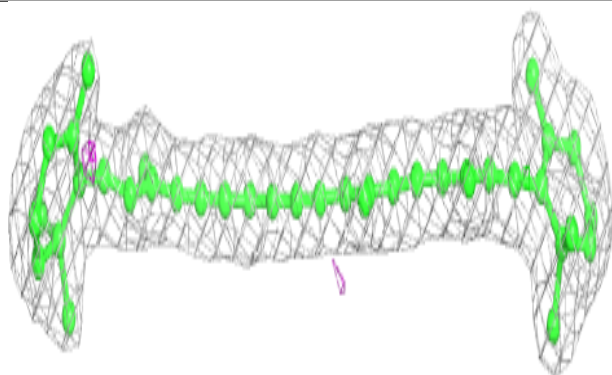
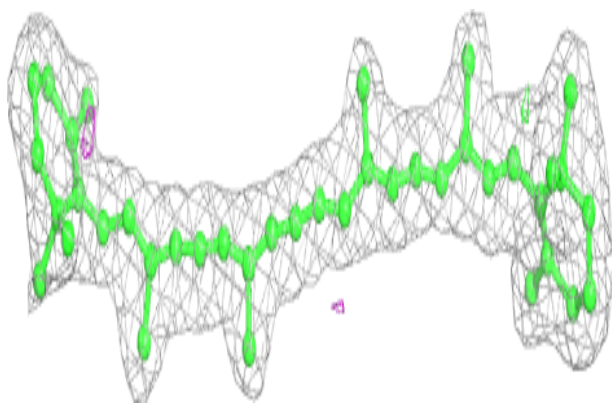
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



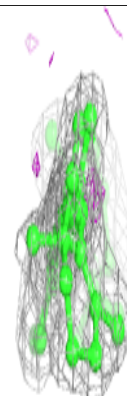
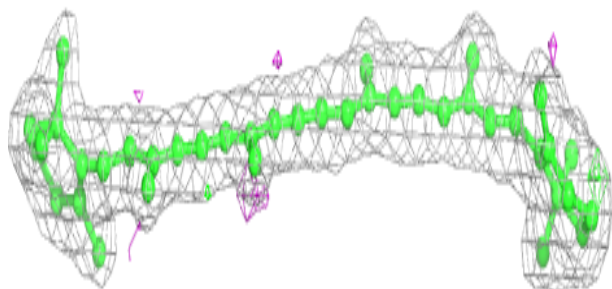
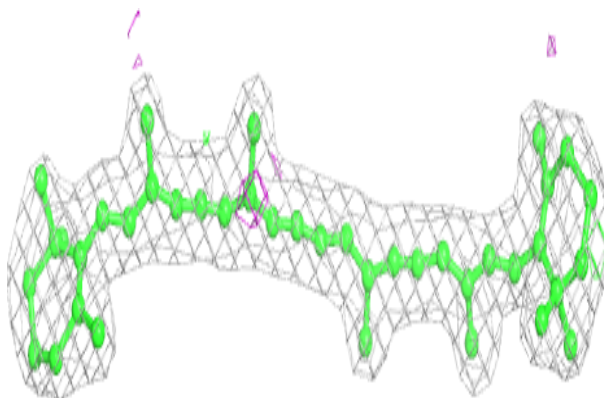


**Electron density around BCR b 621:**

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

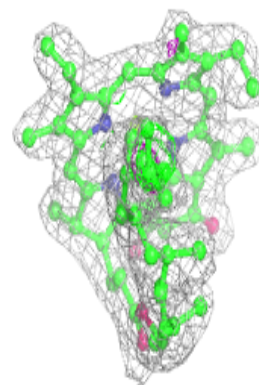
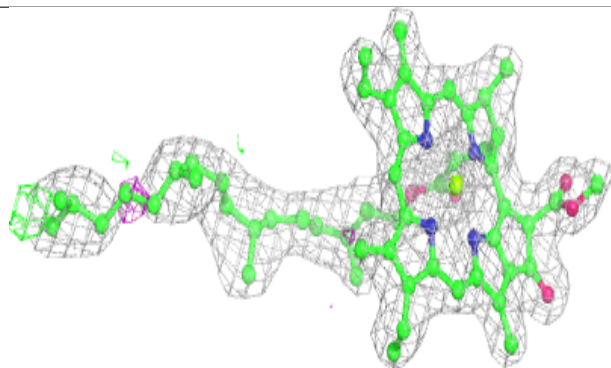
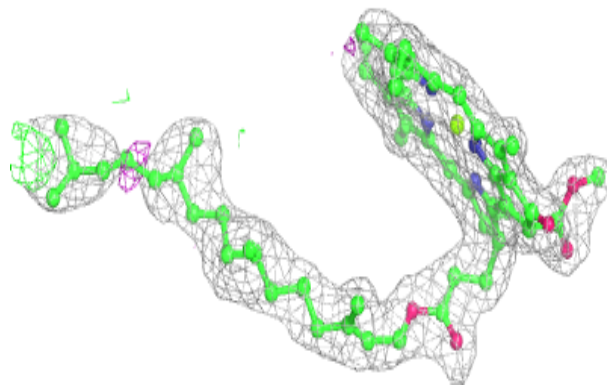
**Electron density around BCR B 619:**

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

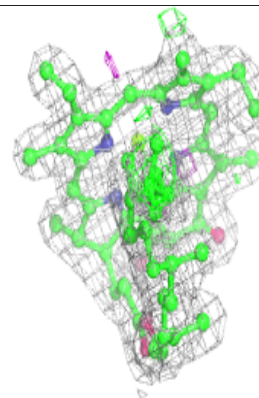
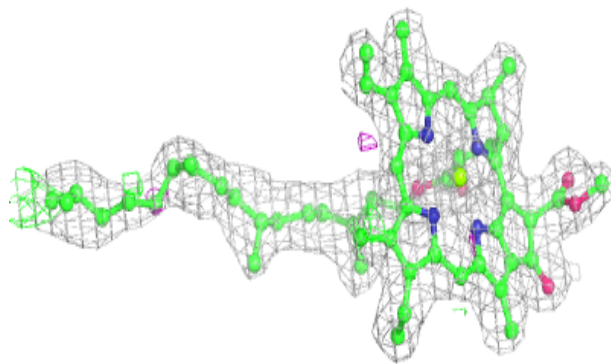
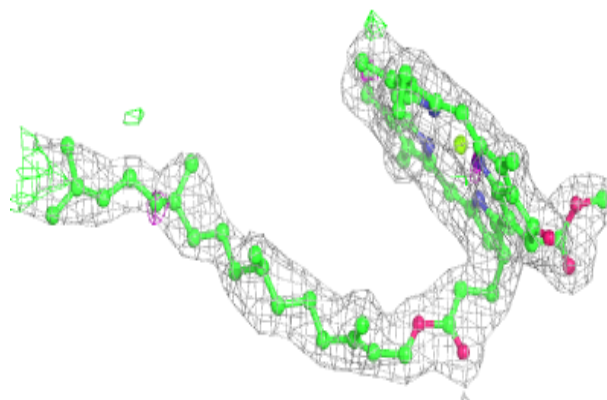


**Electron density around CLA c 504:**

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

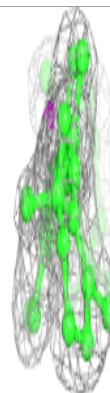
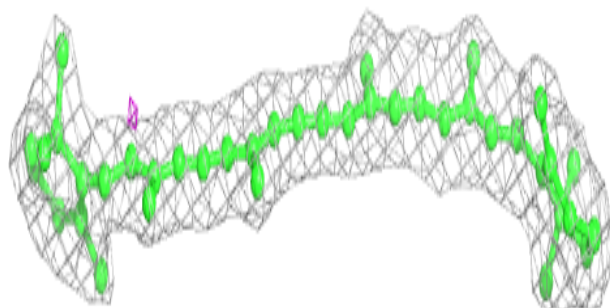
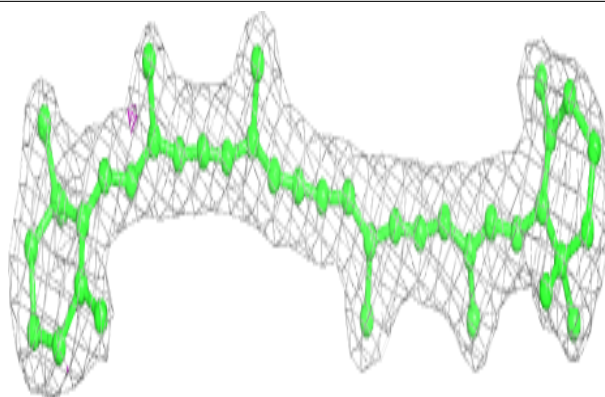
**Electron density around CLA C 504:**

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

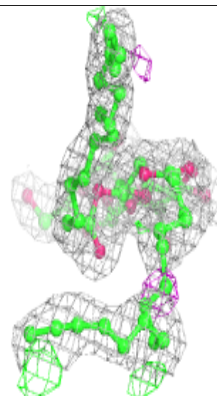
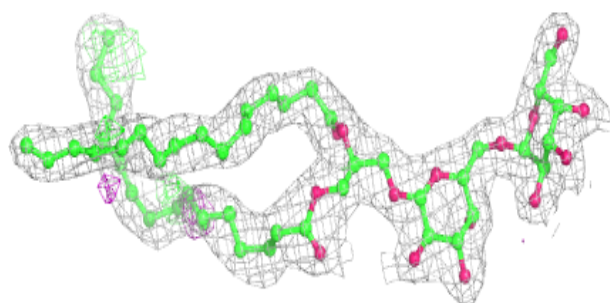
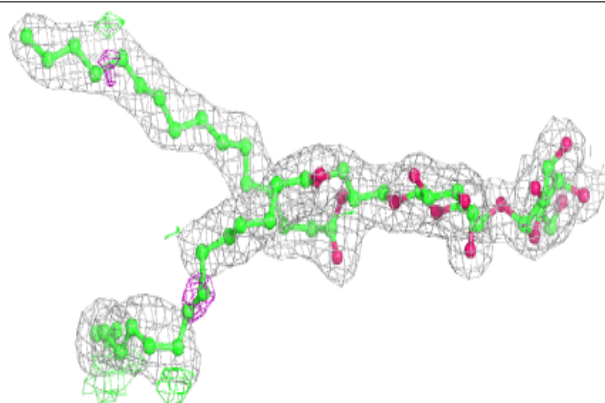


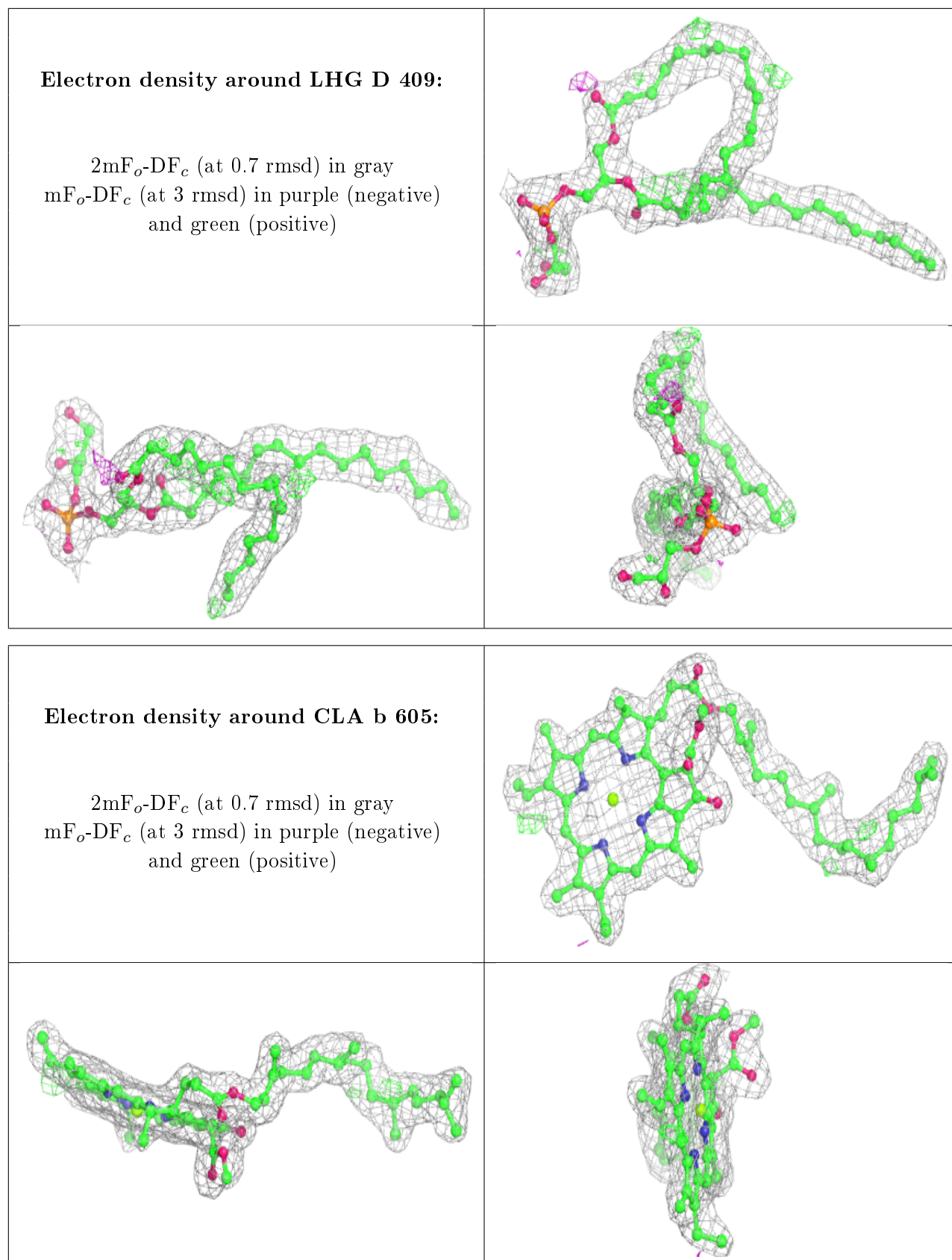
**Electron density around BCR b 622:**

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

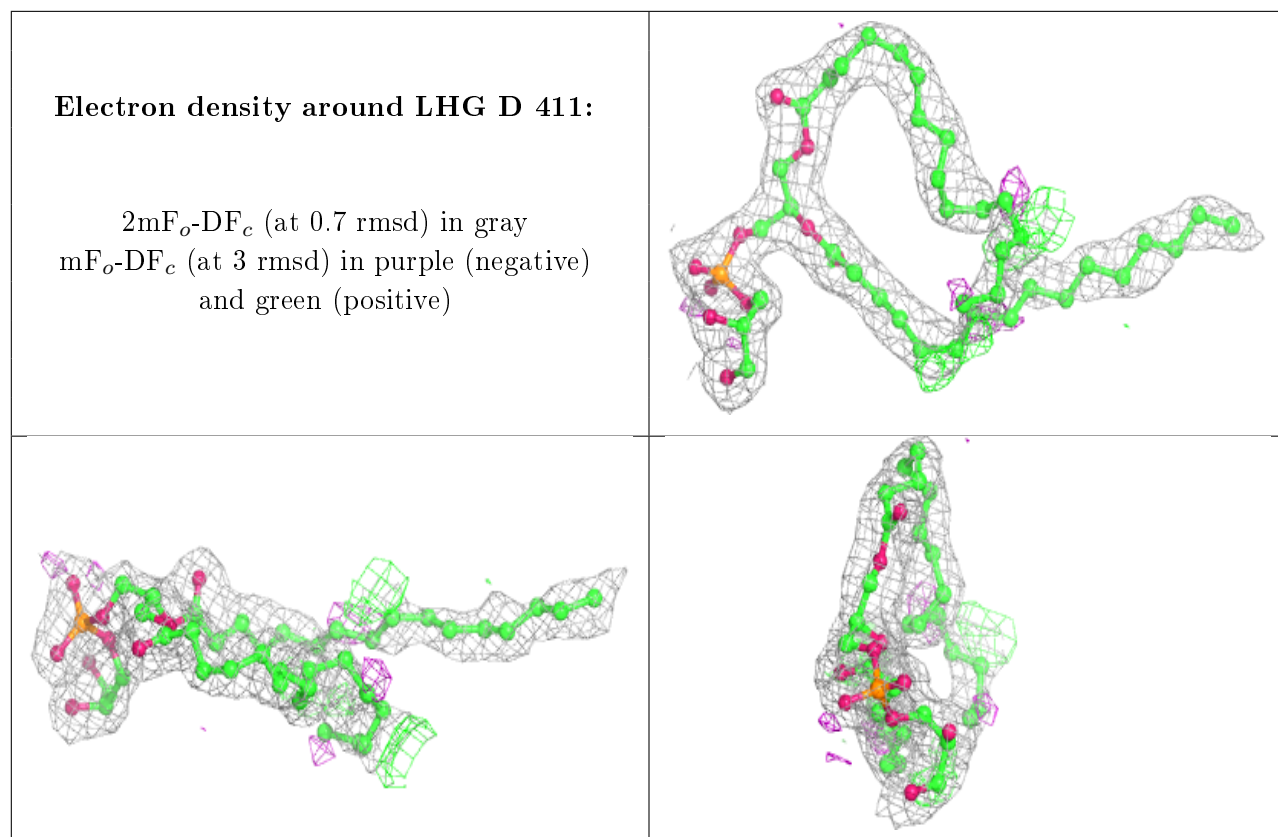
**Electron density around DGD C 515:**

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



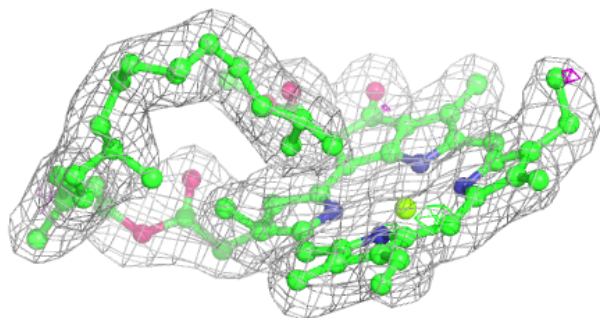
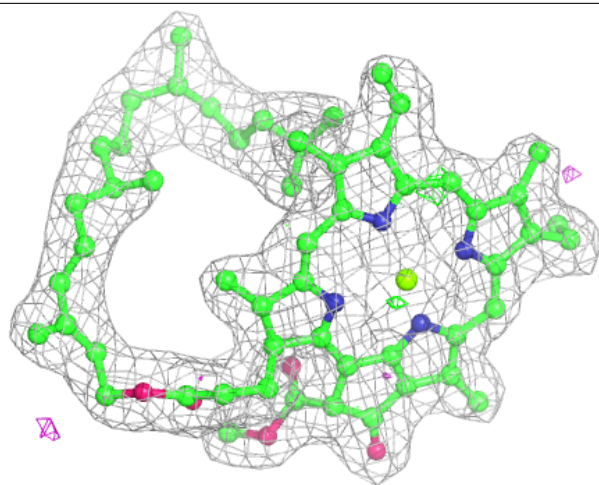






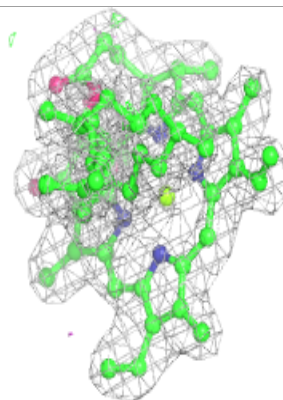
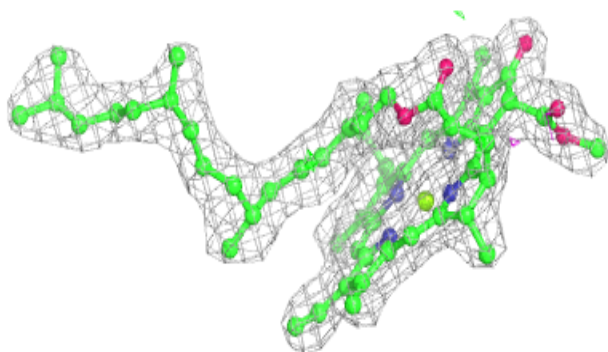
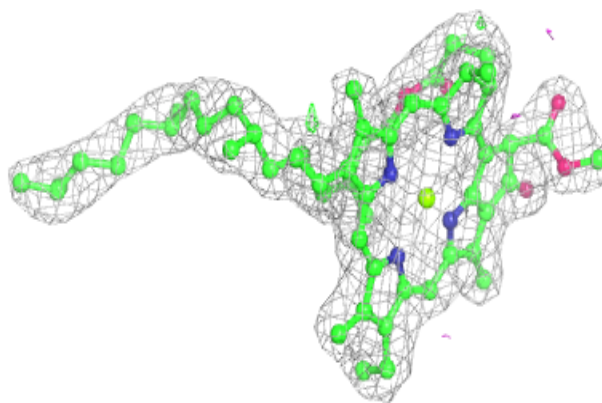
**Electron density around CLA B 615:**

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

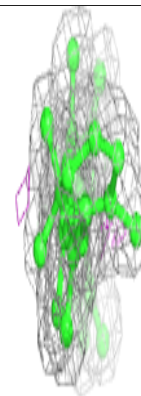
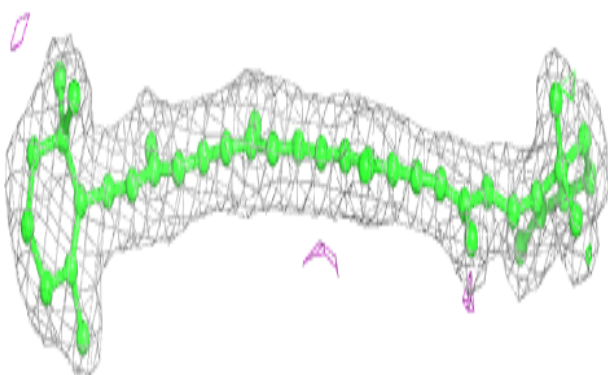
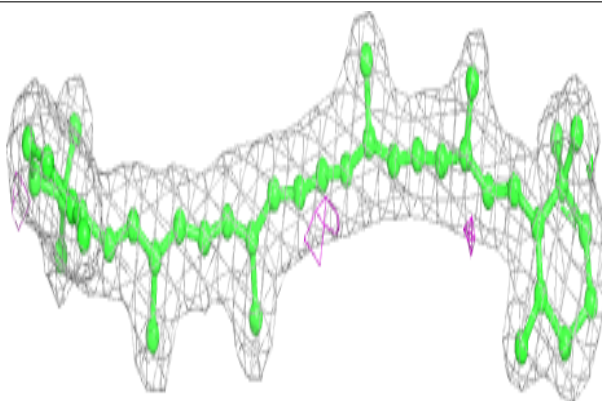


**Electron density around CLA c 505:**

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

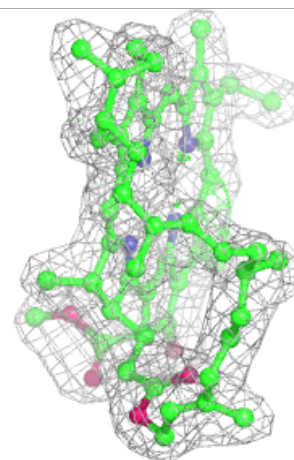
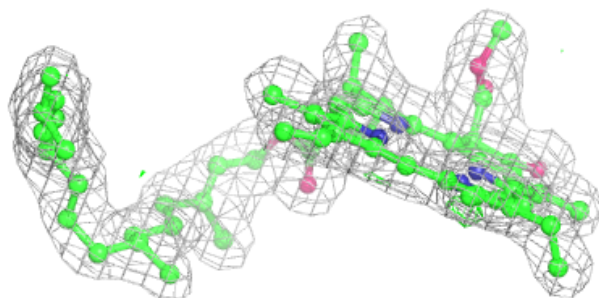
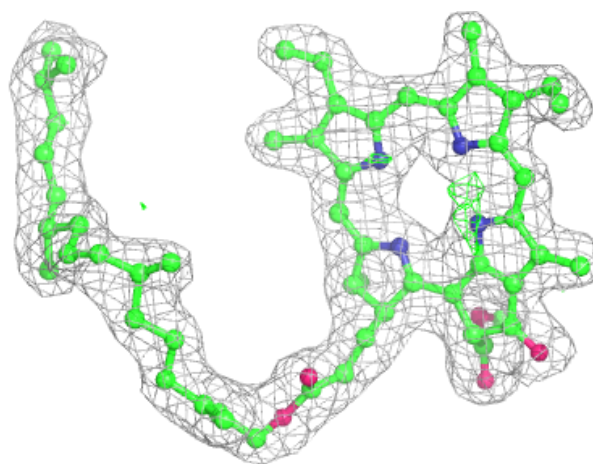
**Electron density around BCR B 617:**

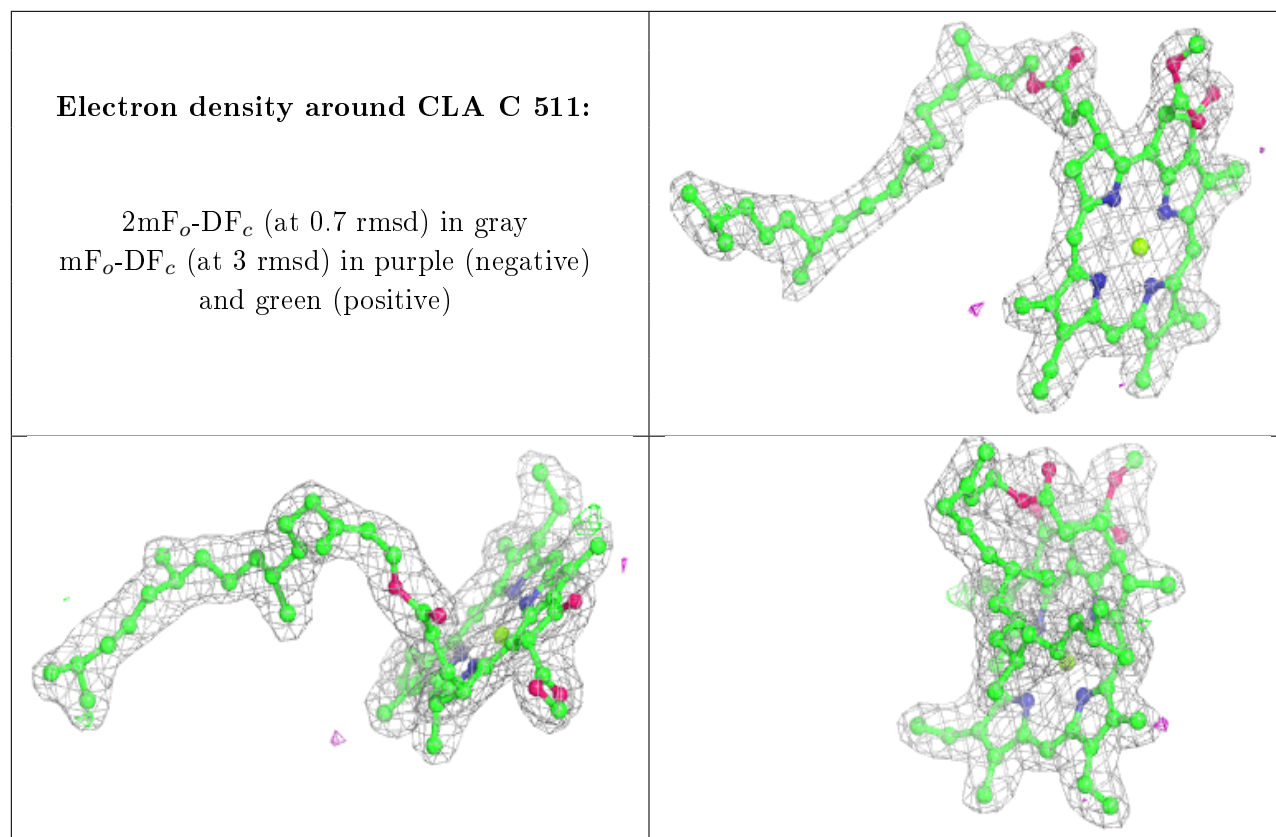
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO a 411:**

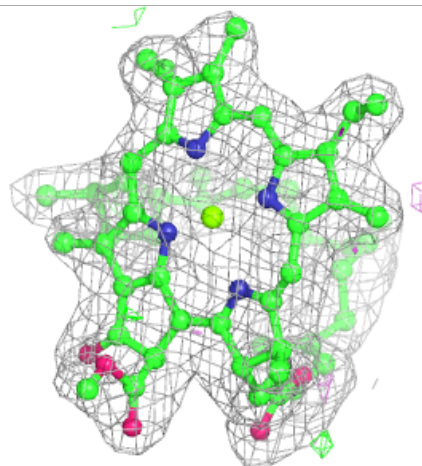
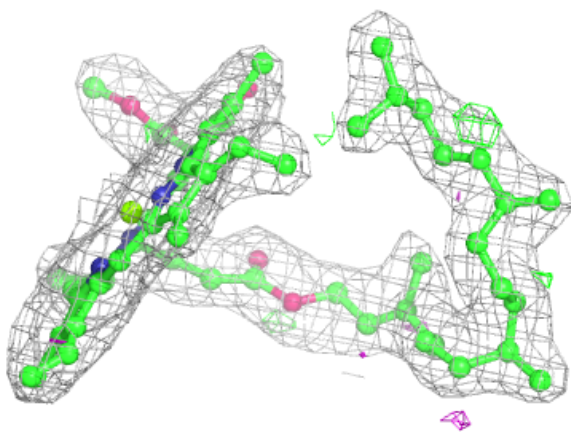
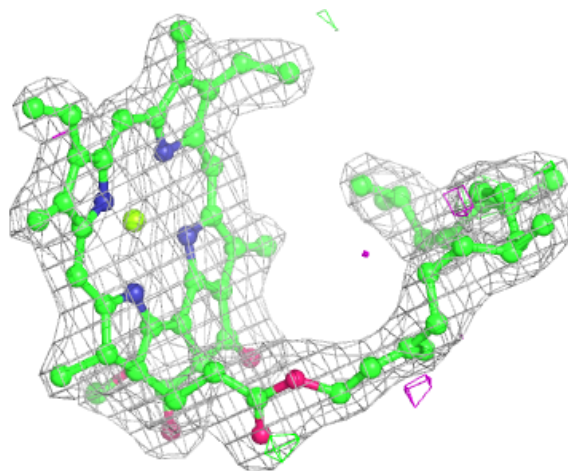
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA c 503:**

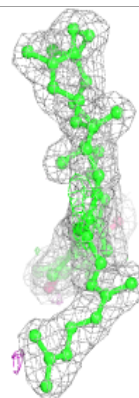
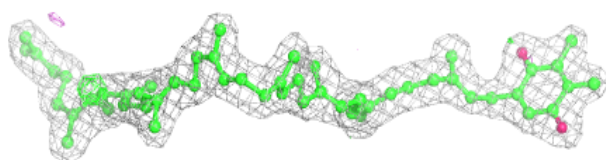
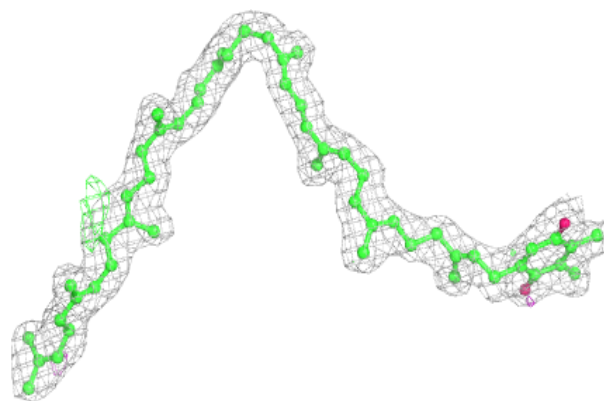
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





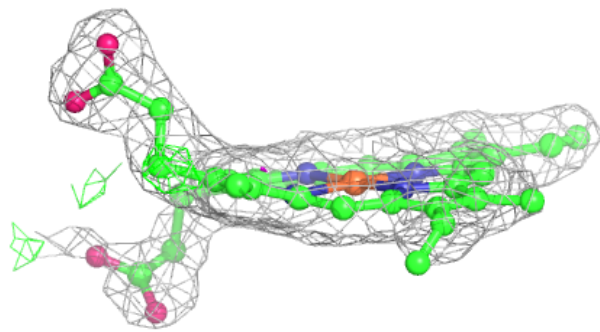
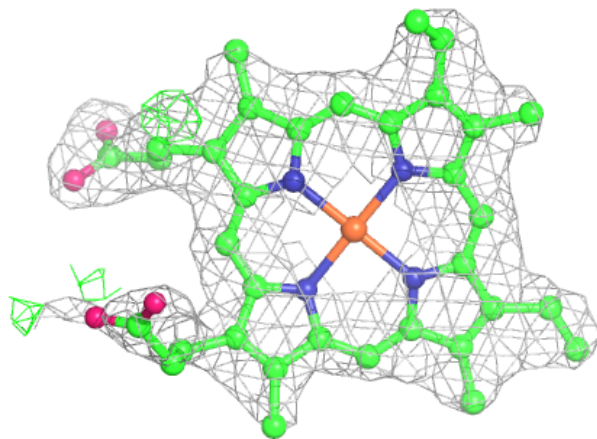
**Electron density around PL9 D 407:**

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



**Electron density around HEM f 101:**

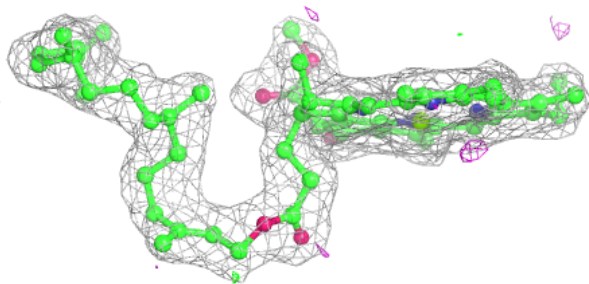
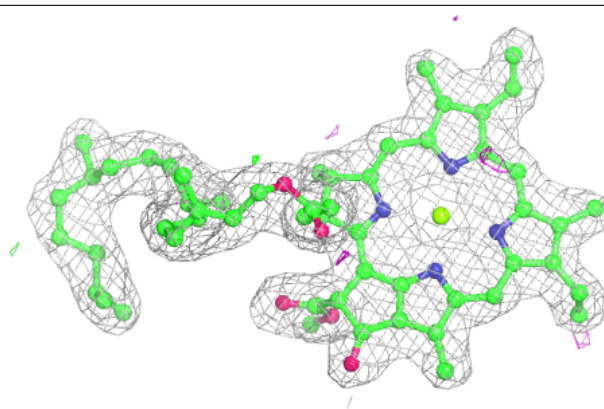
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



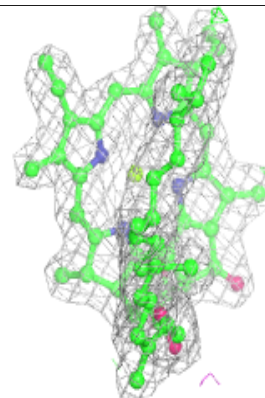
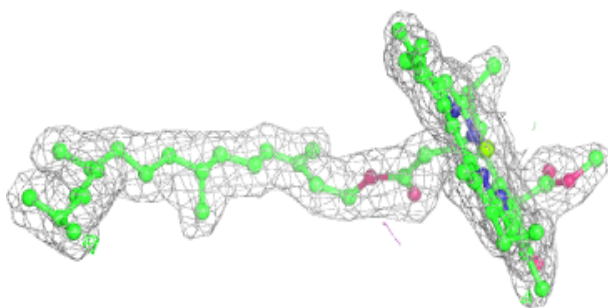
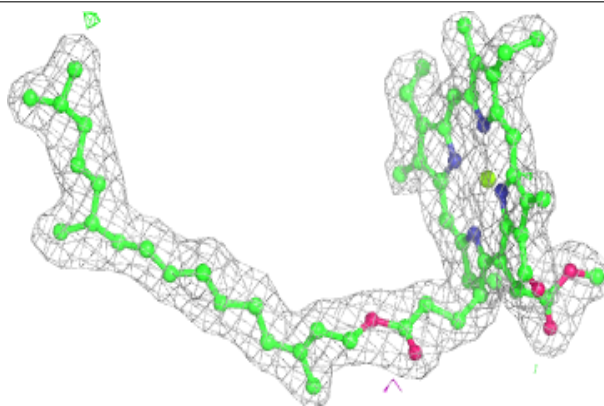


**Electron density around CLA b 615:**

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

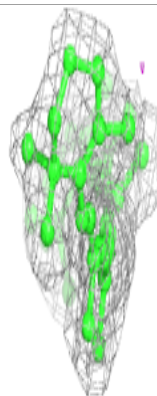
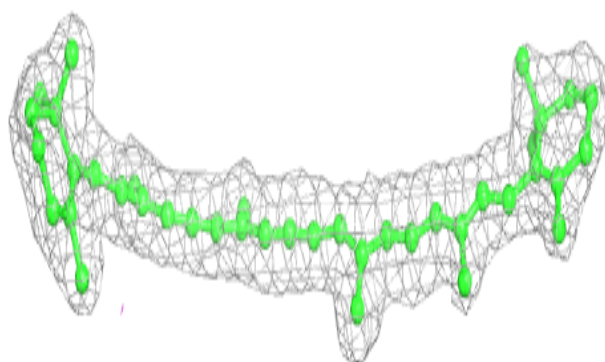
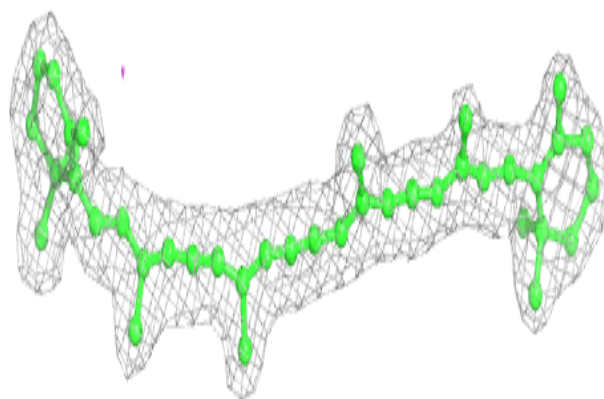
**Electron density around CLA B 609:**

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

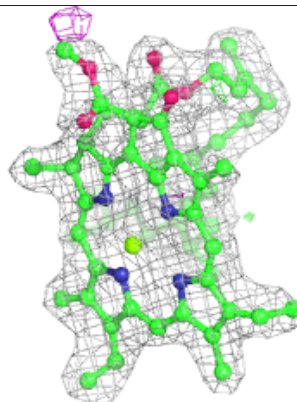
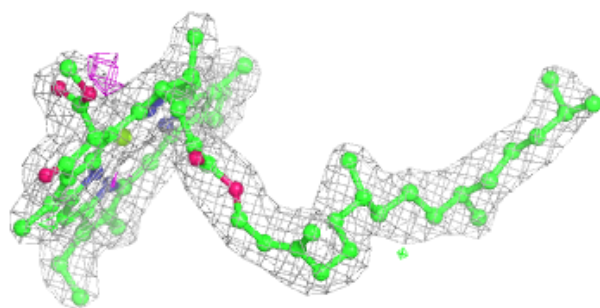
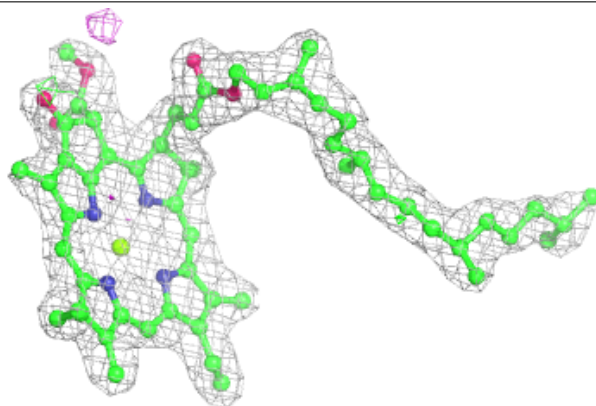


**Electron density around BCR T 101:**

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

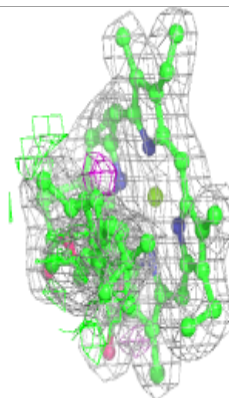
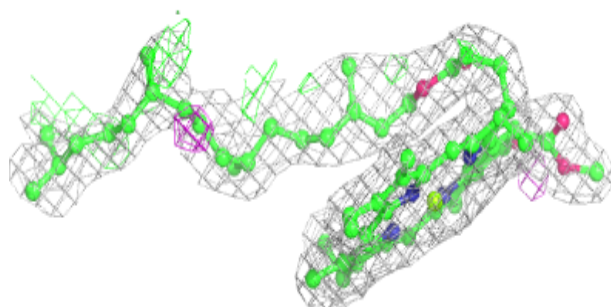
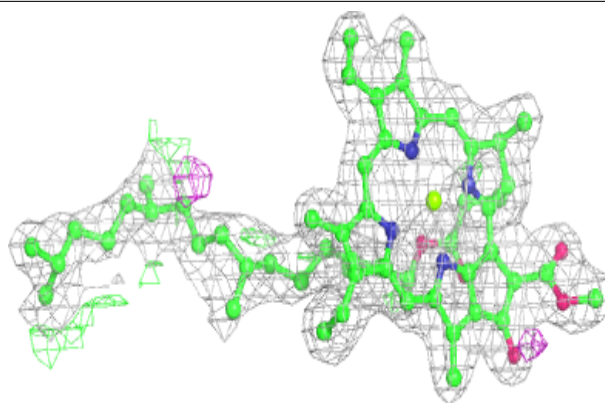
**Electron density around CLA c 511:**

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

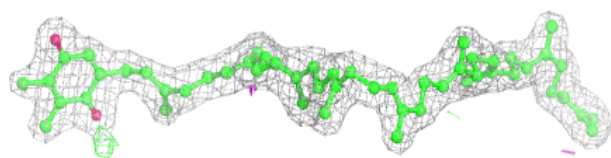
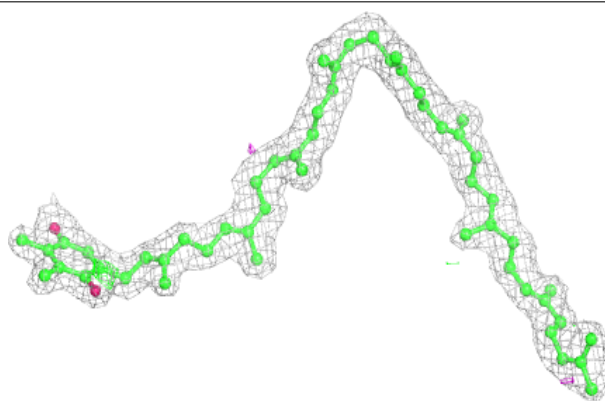


**Electron density around CLA B 614:**

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

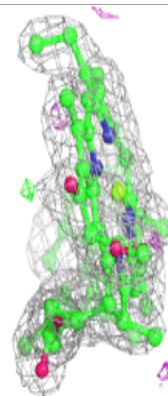
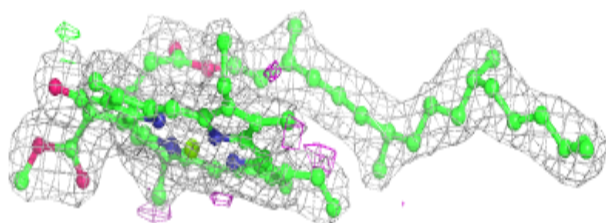
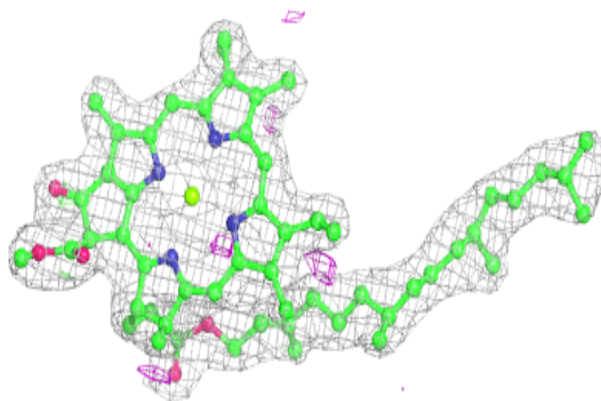
**Electron density around PL9 d 405:**

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

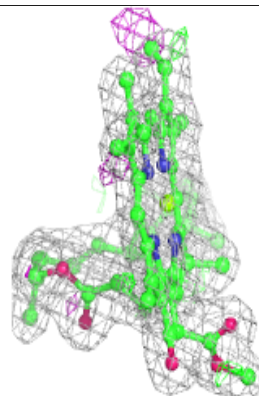
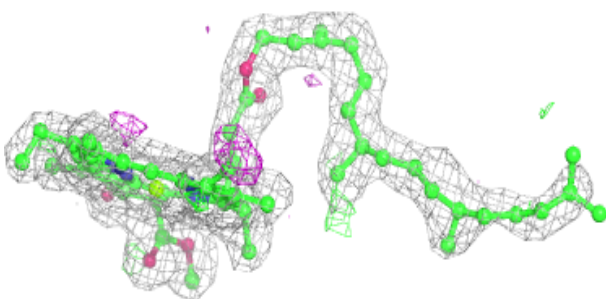
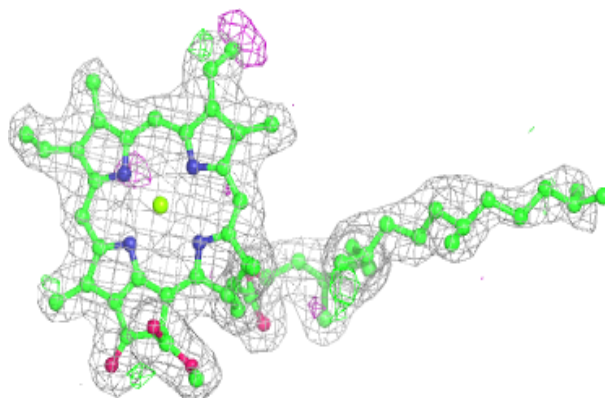


**Electron density around CLA c 501:**

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

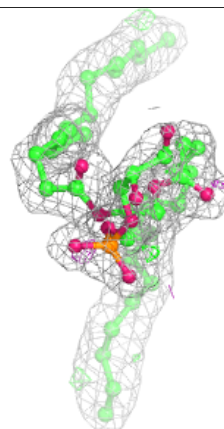
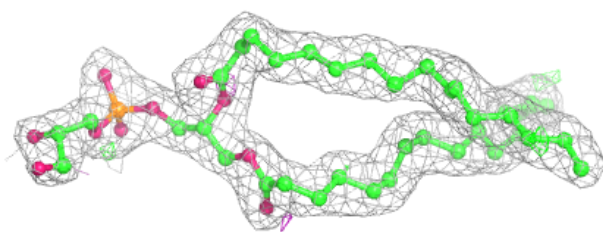
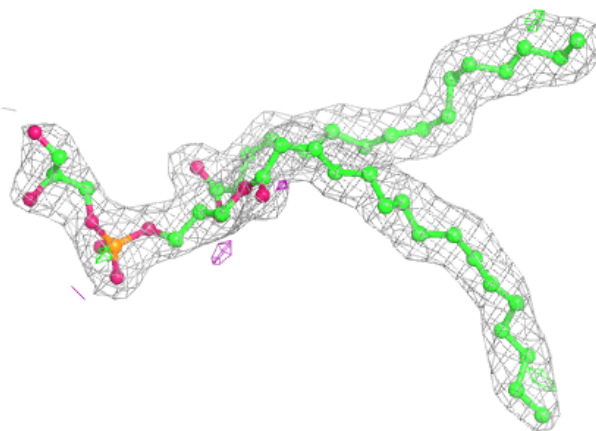
**Electron density around CLA A 1006:**

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



**Electron density around LHG d 407:**

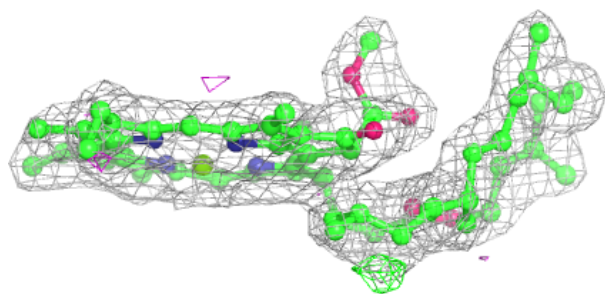
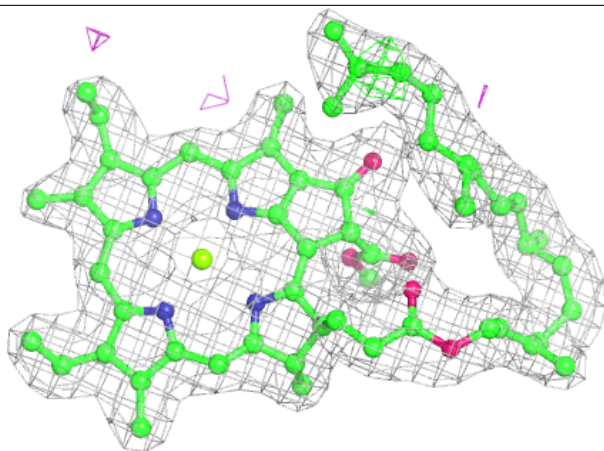
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



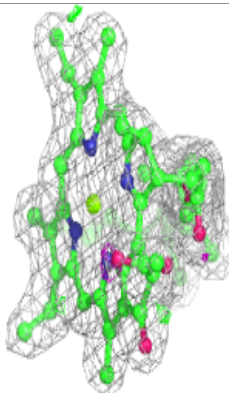
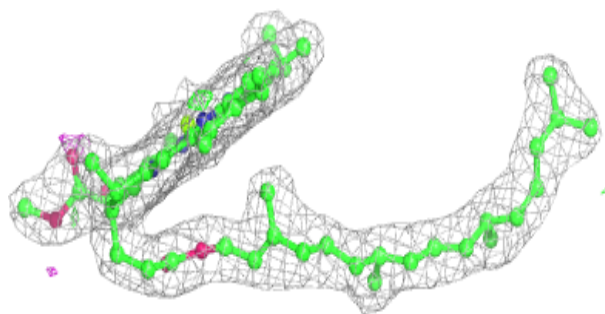
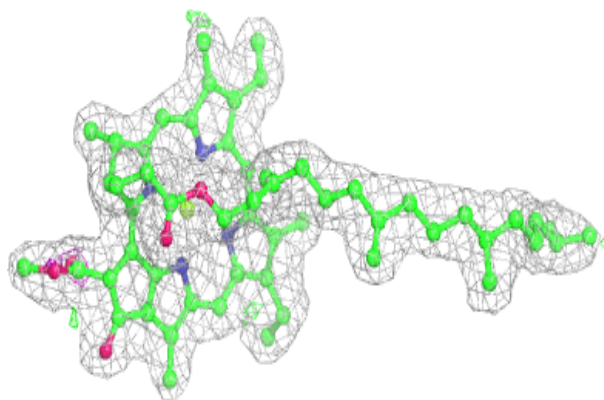


**Electron density around CLA b 613:**

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

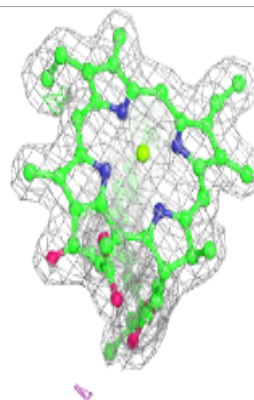
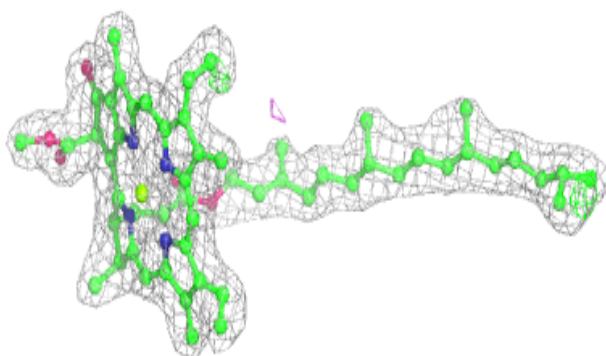
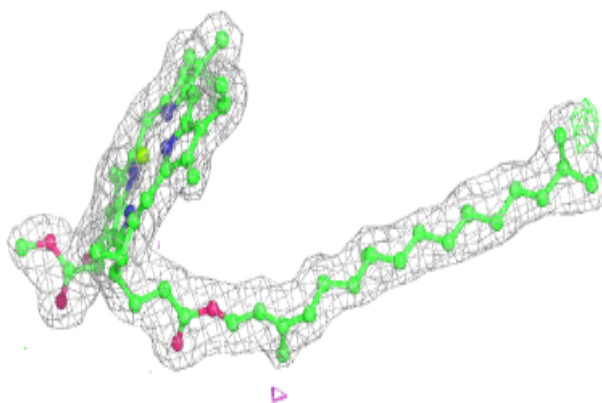
**Electron density around CLA b 611:**

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

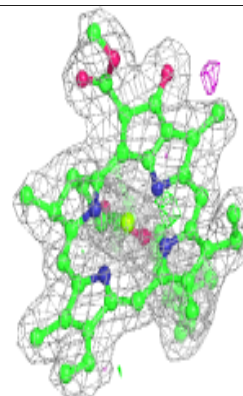
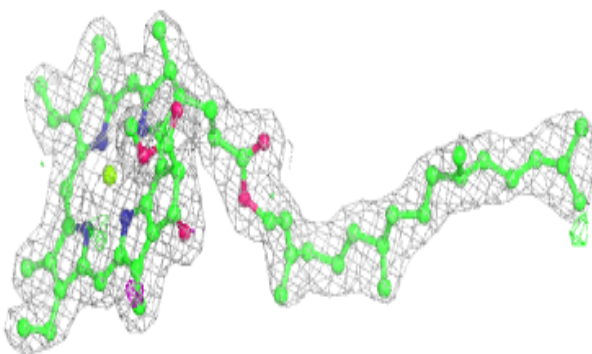
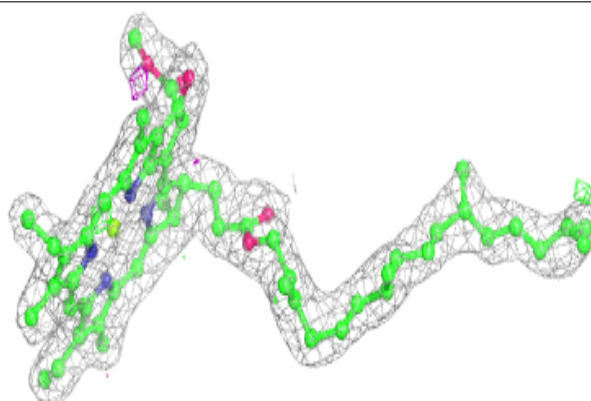


**Electron density around CLA b 610:**

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

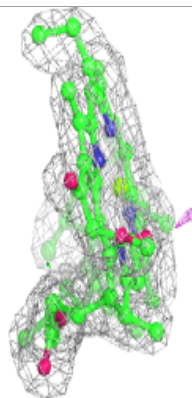
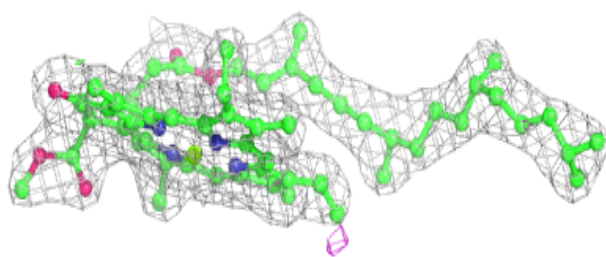
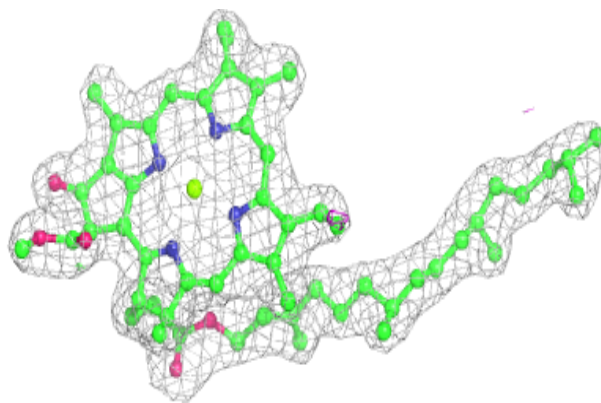
**Electron density around CLA c 502:**

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

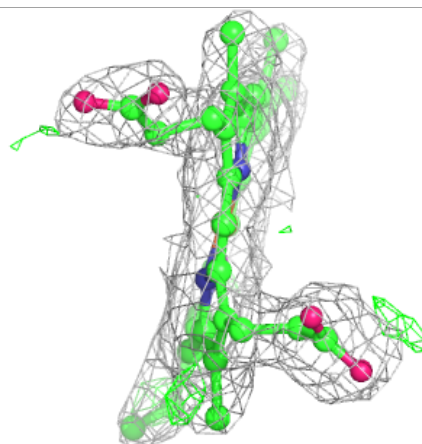
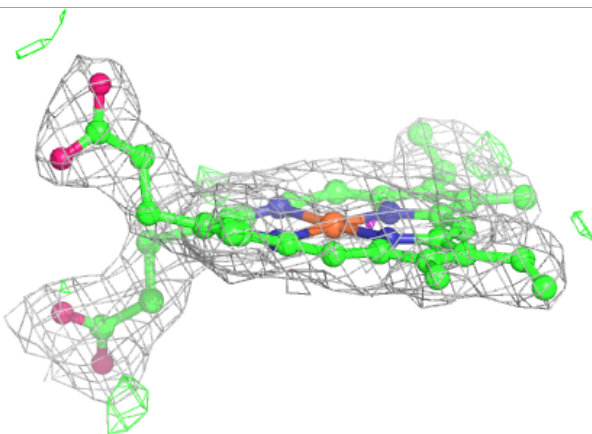
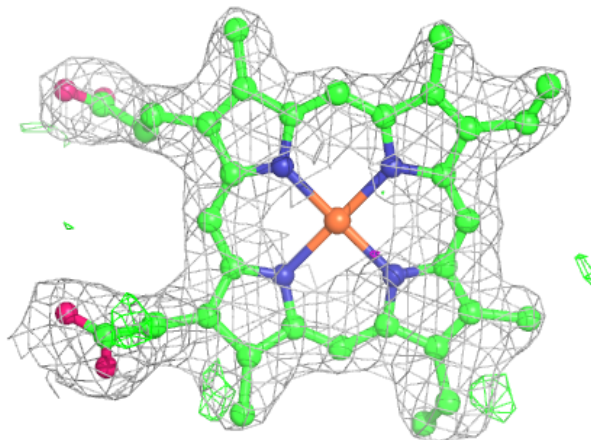


**Electron density around CLA C 501:**

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

**Electron density around HEM F 101:**

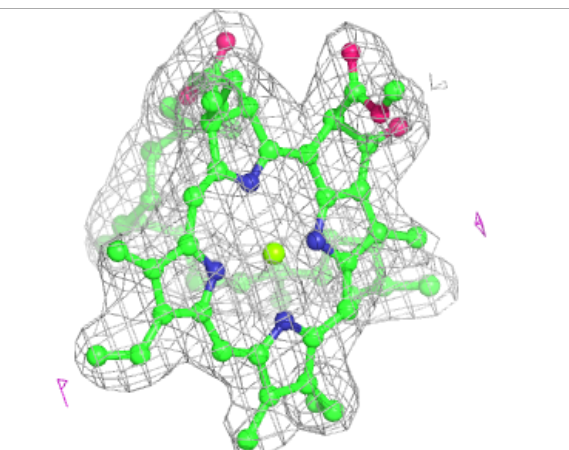
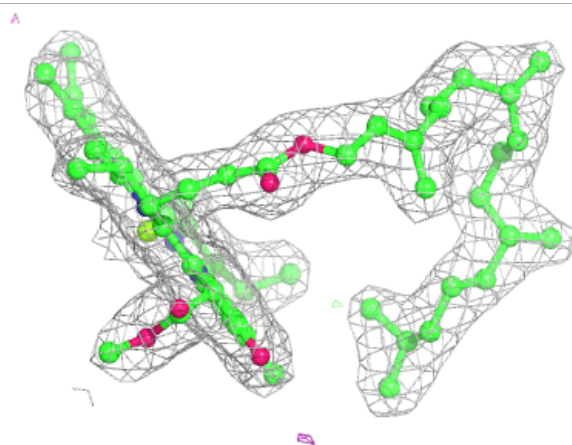
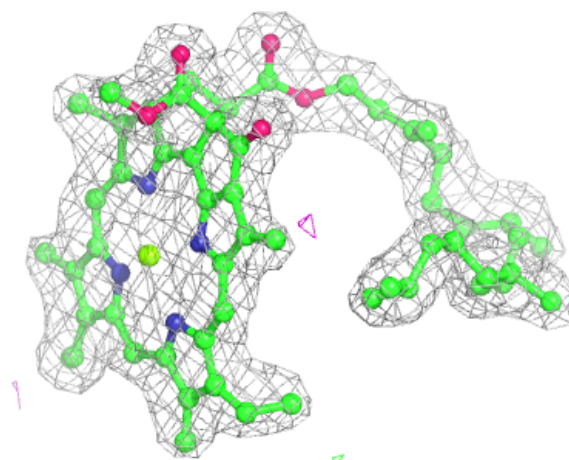
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





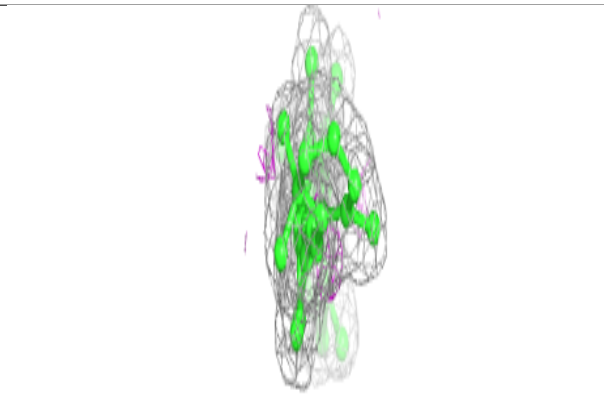
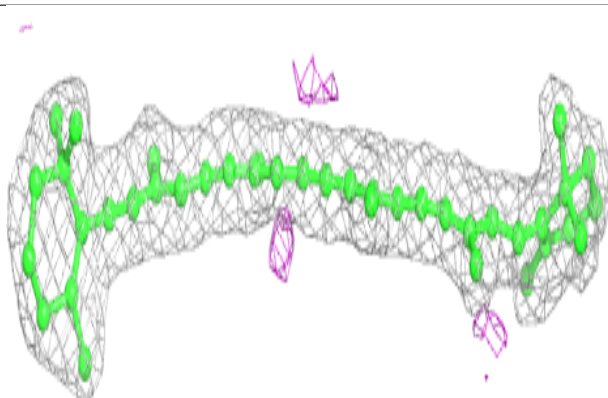
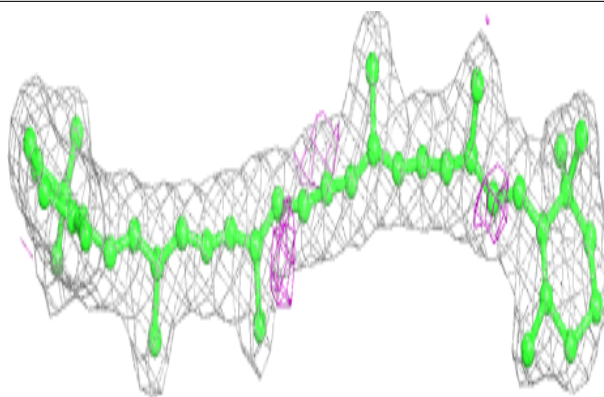
**Electron density around CLA C 503:**

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

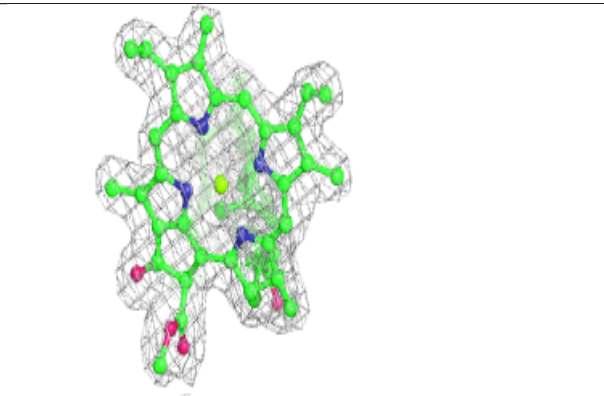
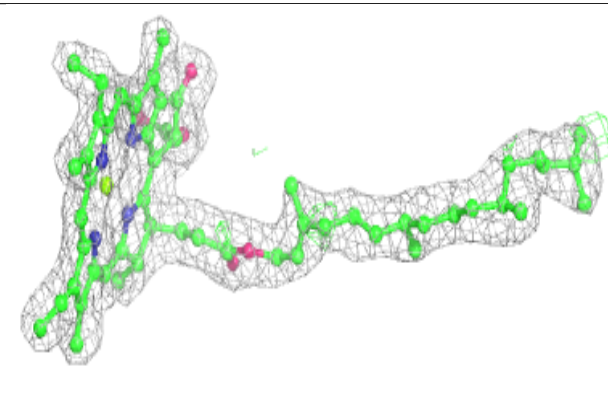
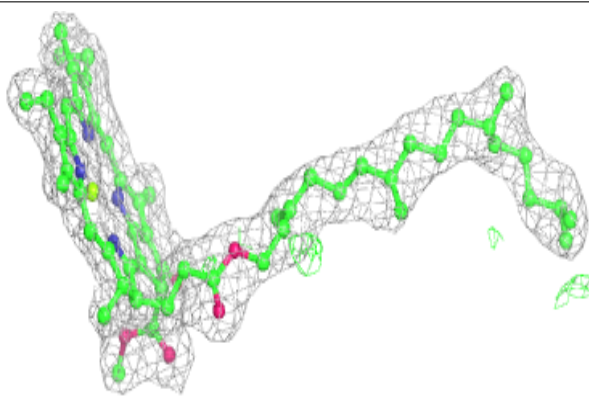


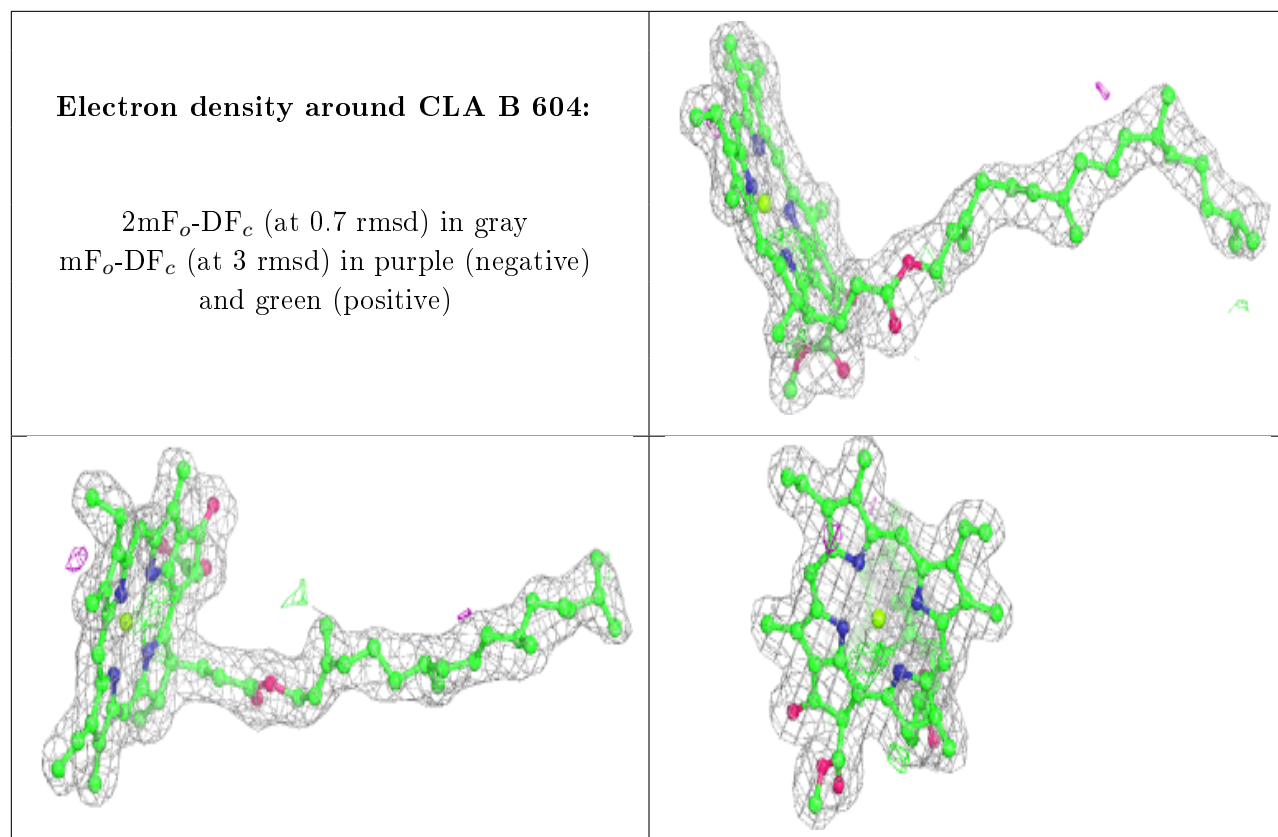
**Electron density around BCR b 620:**

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

**Electron density around CLA b 607:**

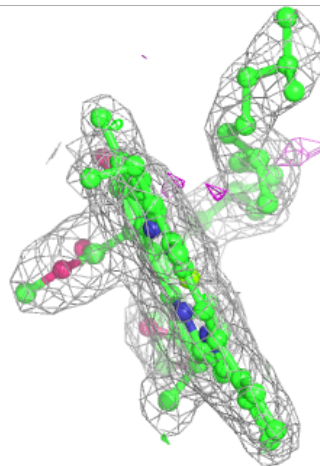
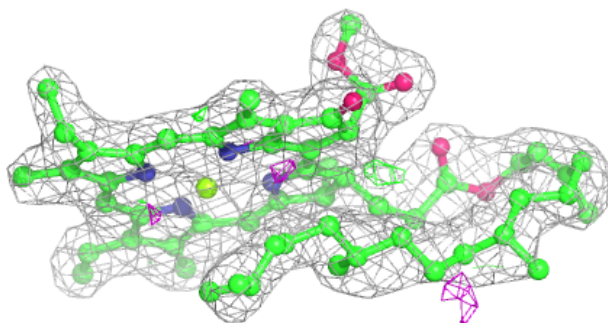
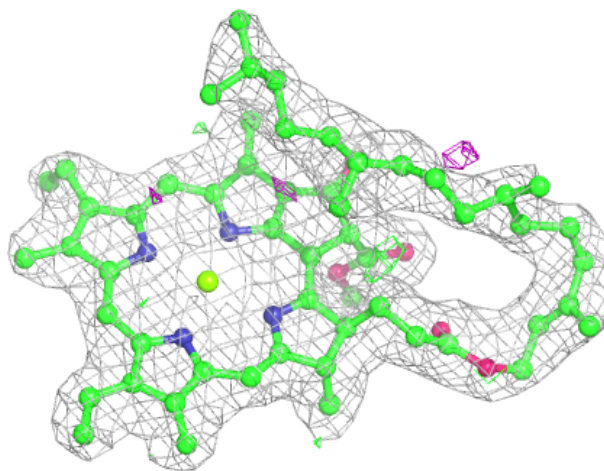
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





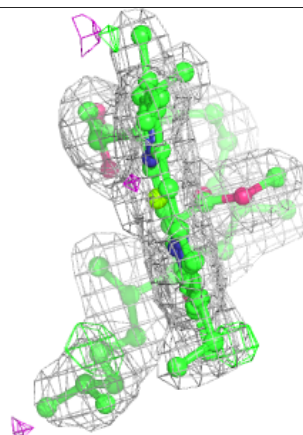
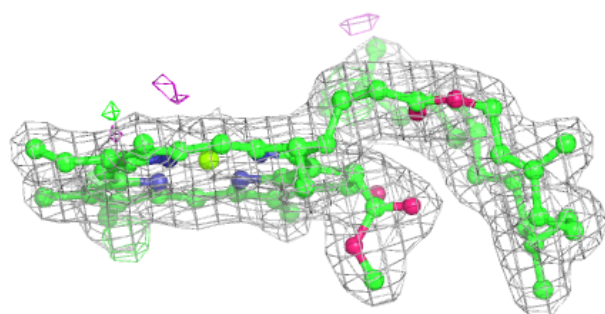
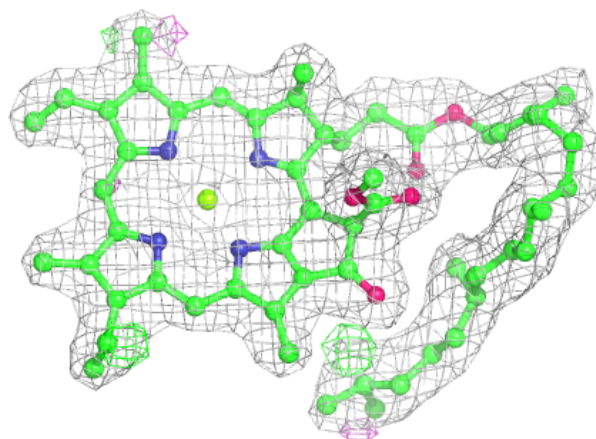
**Electron density around CLA c 509:**

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

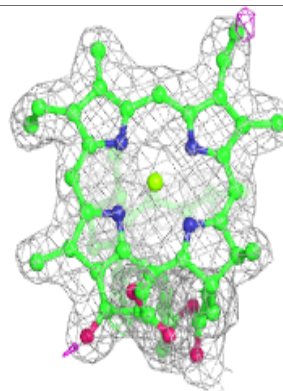
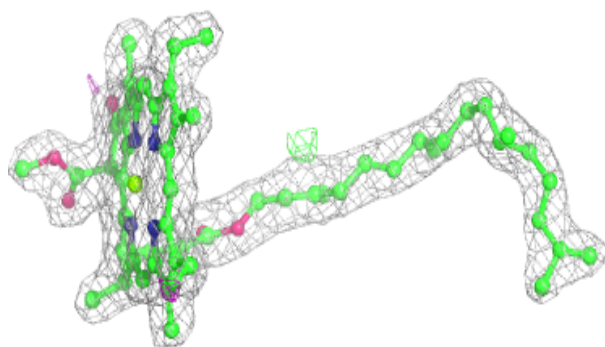
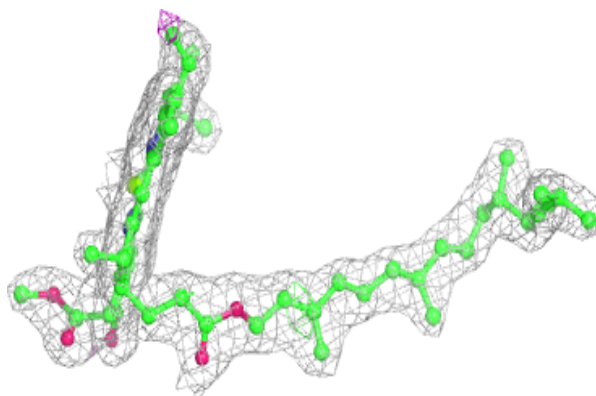


**Electron density around CLA B 610:**

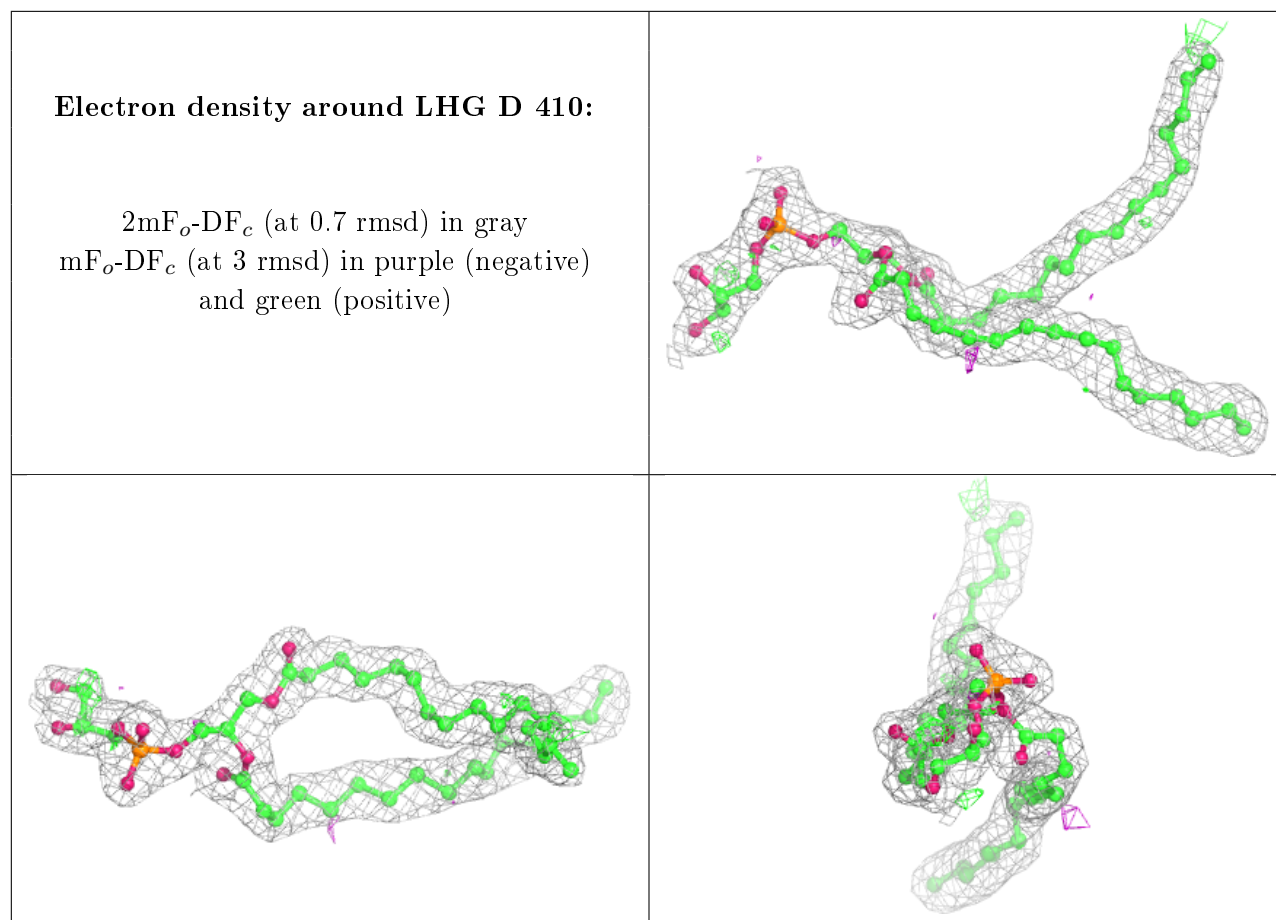
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA b 608:**

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

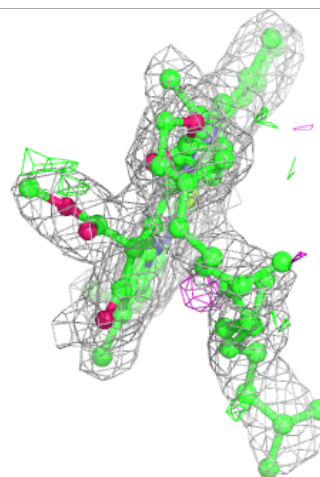
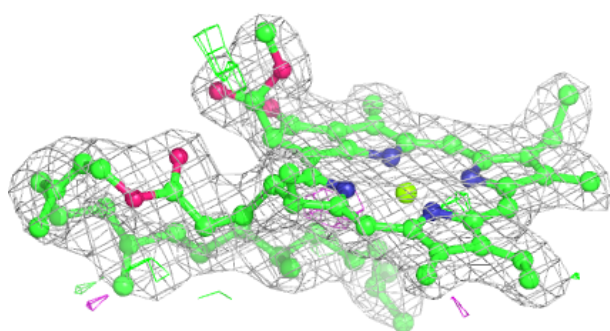
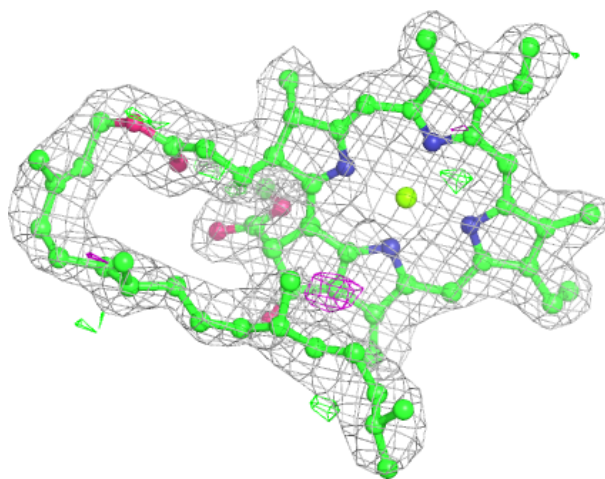






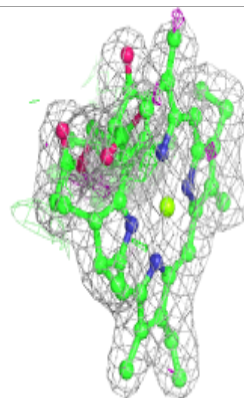
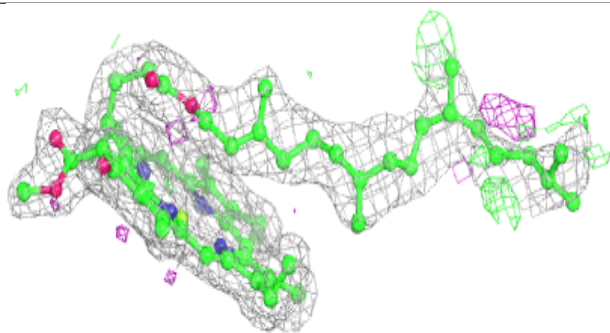
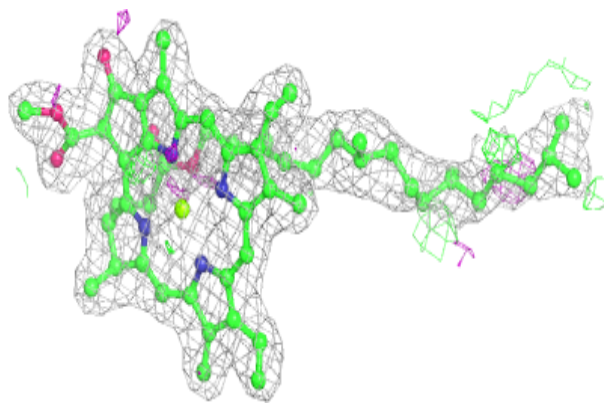
**Electron density around CLA C 509:**

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

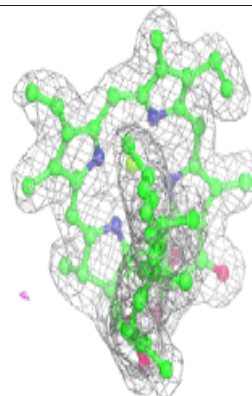
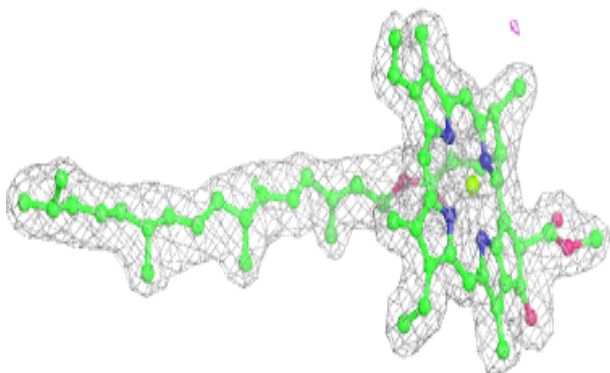
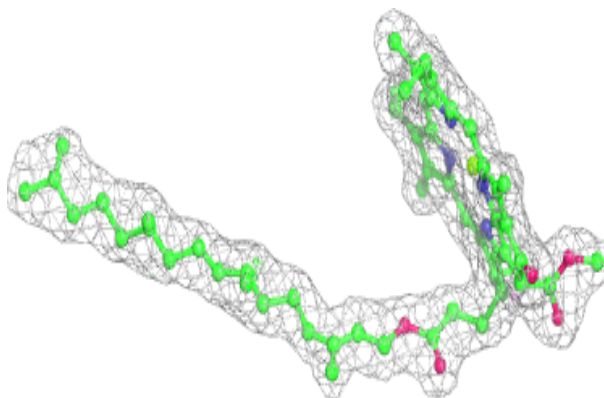


**Electron density around CLA b 617:**

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

**Electron density around CLA B 607:**

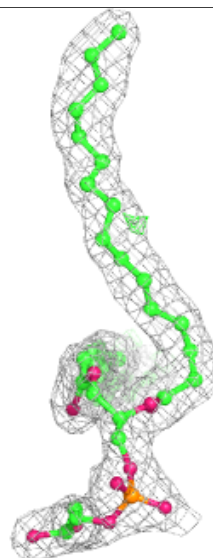
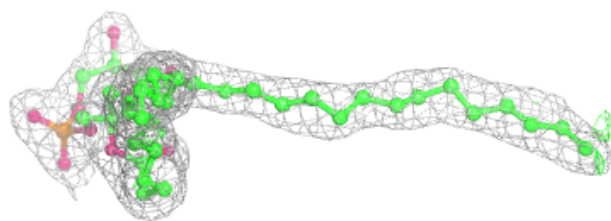
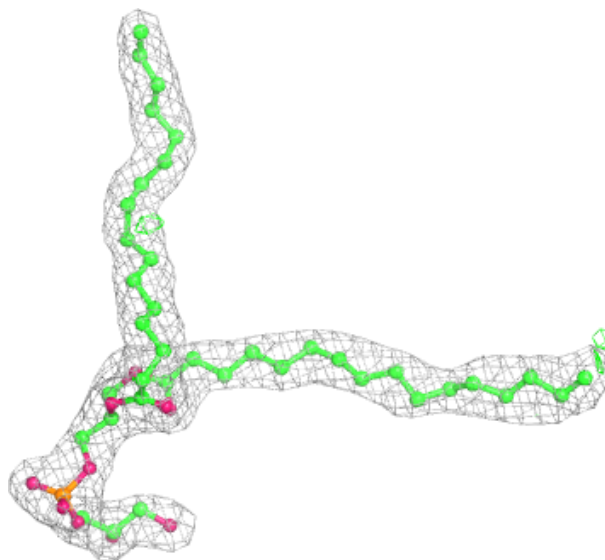
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





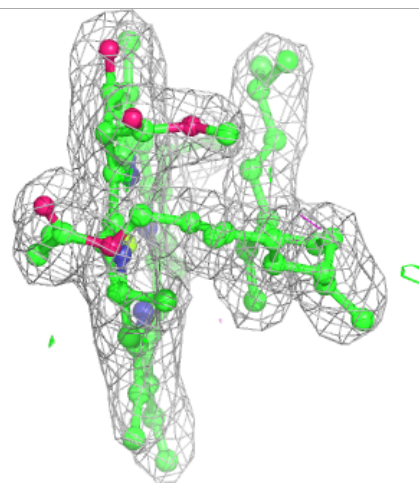
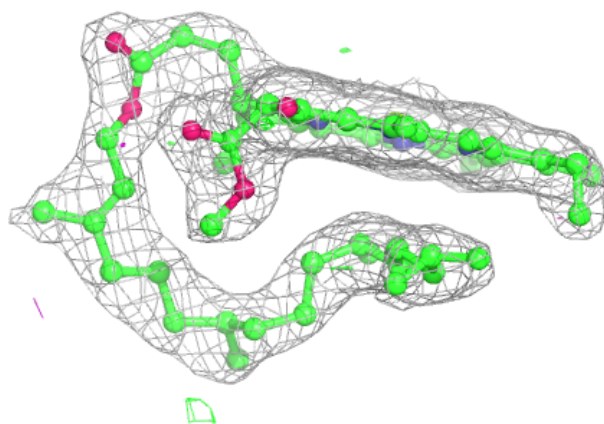
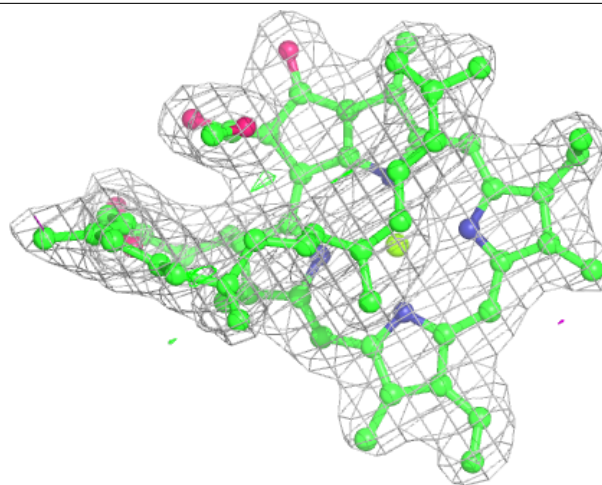
**Electron density around LHG b 624:**

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



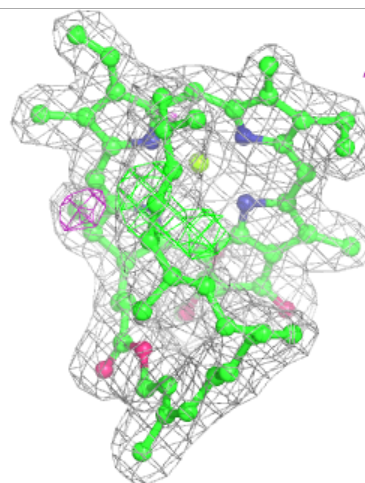
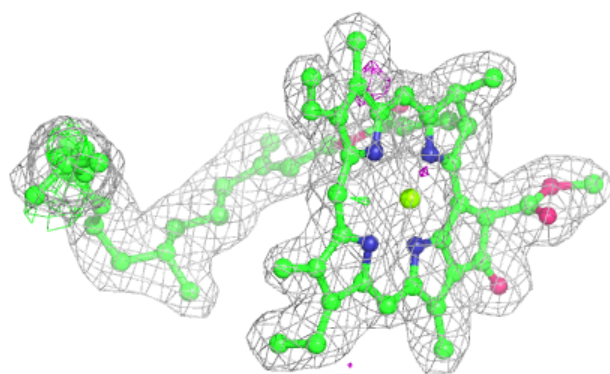
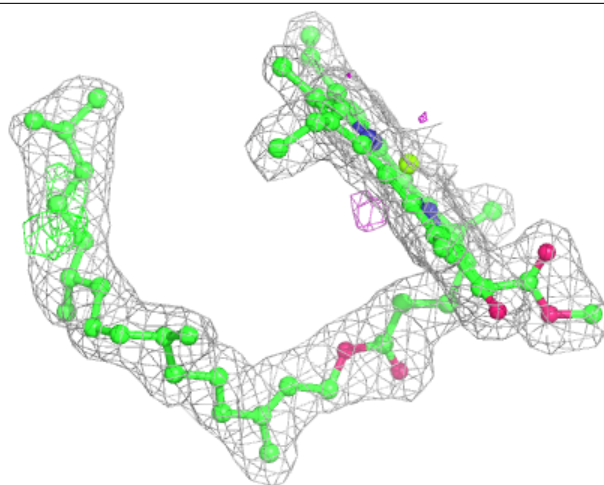
**Electron density around CLA c 510:**

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



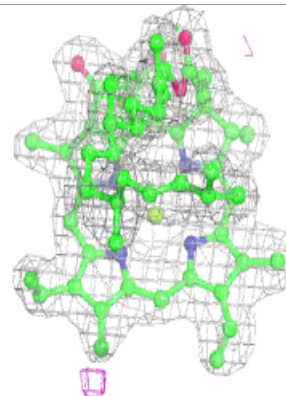
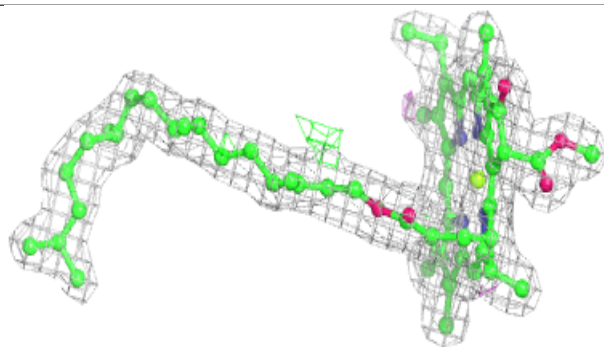
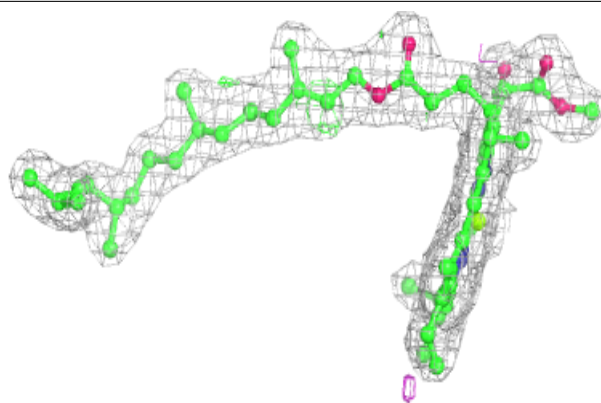
**Electron density around CLA b 614:**

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

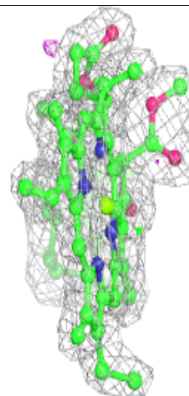
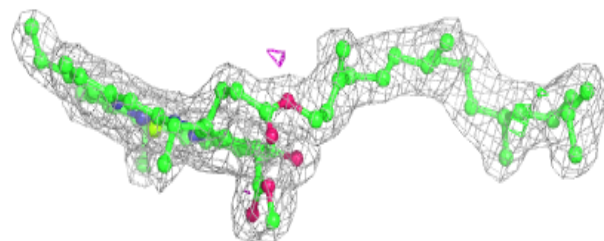
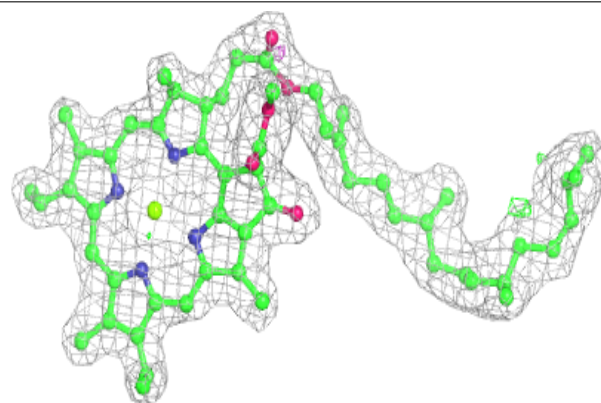


**Electron density around CLA B 605:**

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

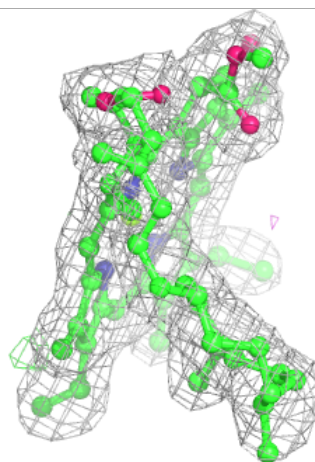
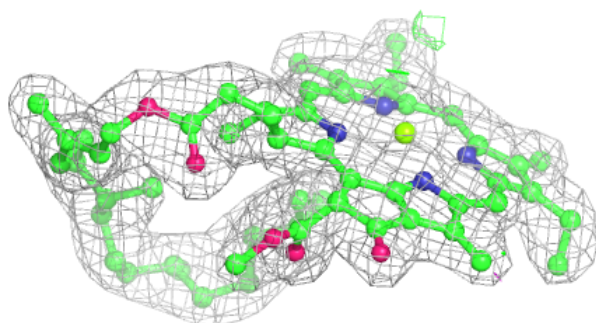
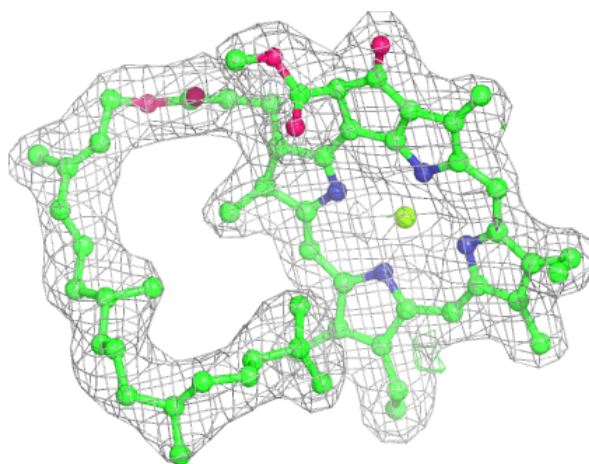
**Electron density around CLA B 602:**

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



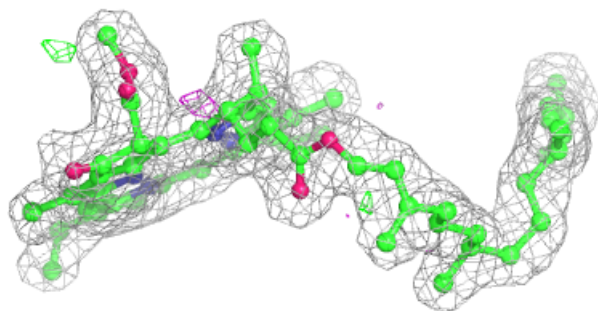
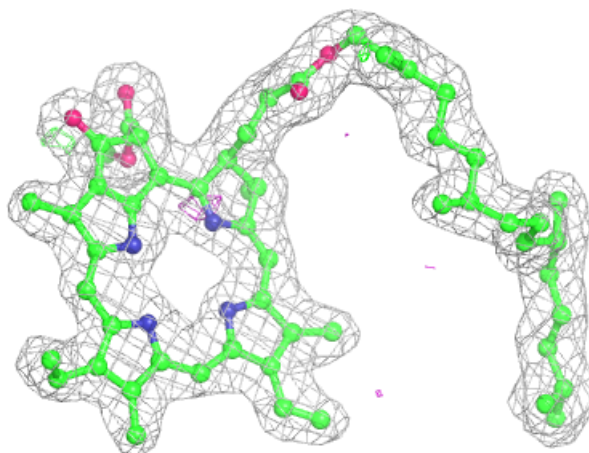
**Electron density around CLA b 618:**

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



**Electron density around PHO D 404:**

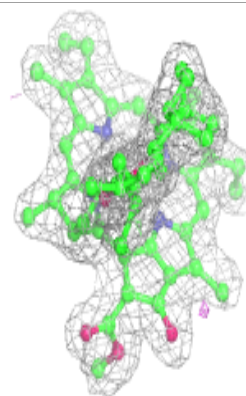
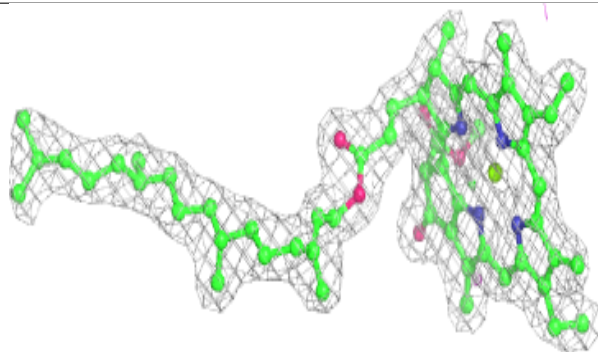
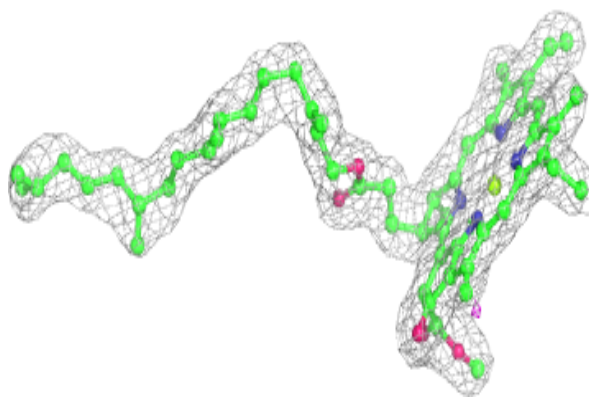
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



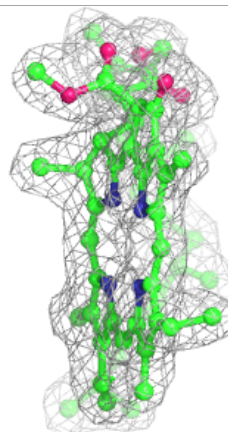
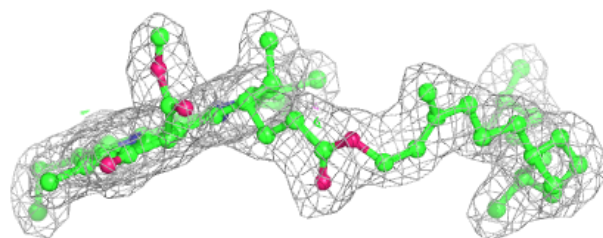
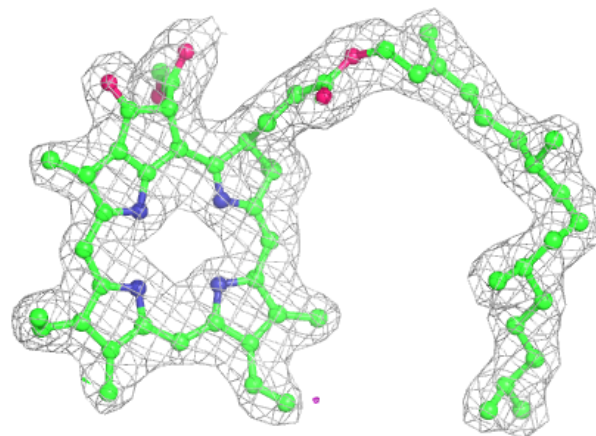


**Electron density around CLA C 502:**

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

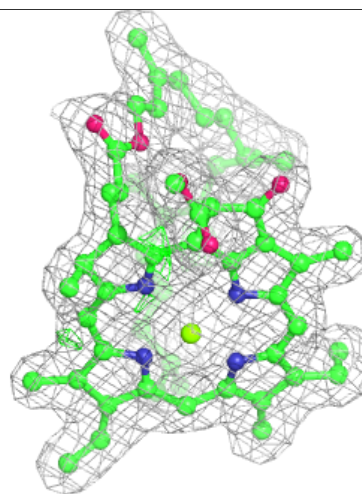
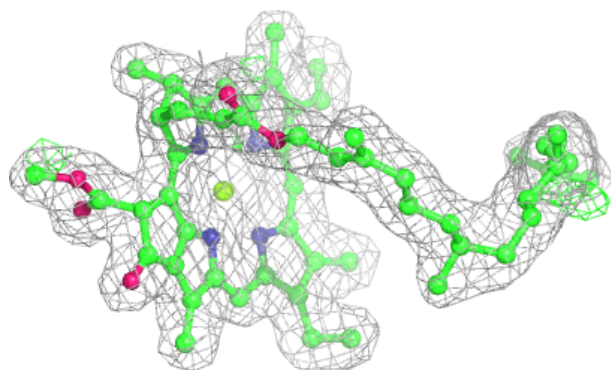
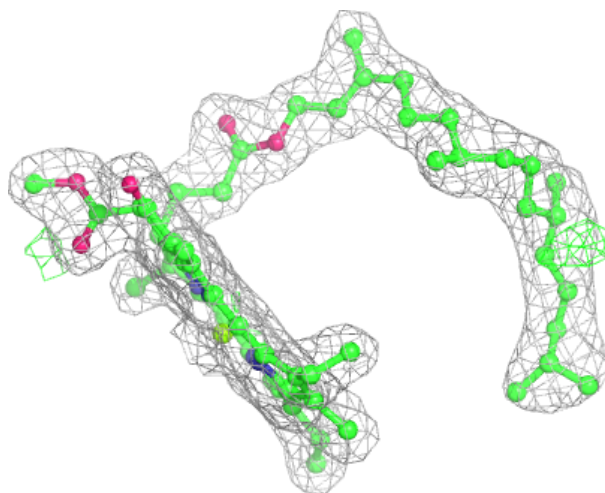
**Electron density around PHO a 410:**

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



**Electron density around CLA B 611:**

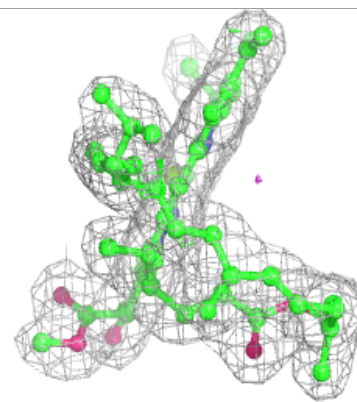
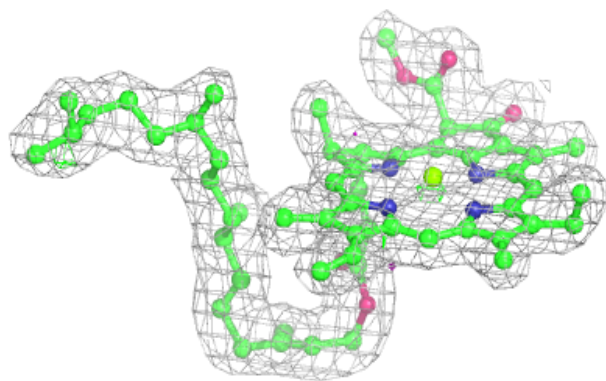
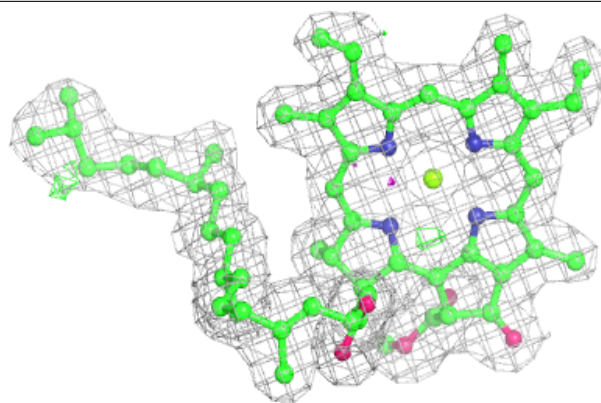
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





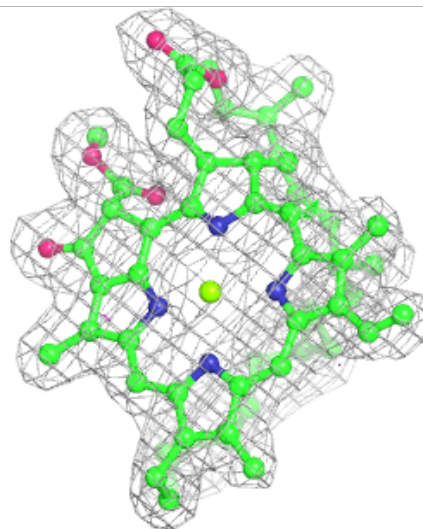
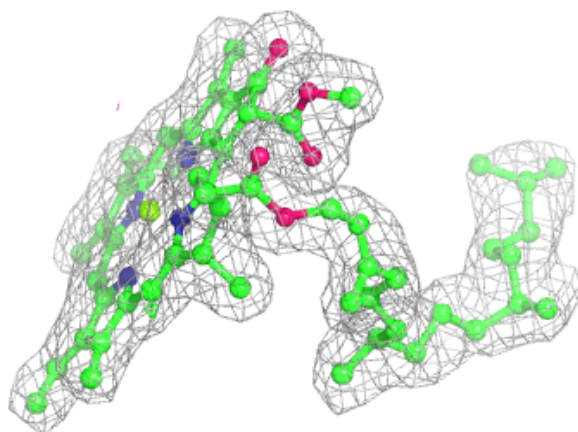
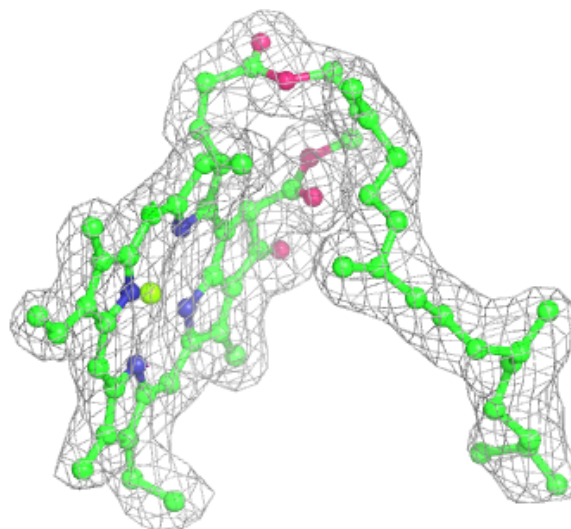
**Electron density around CLA a 408:**

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



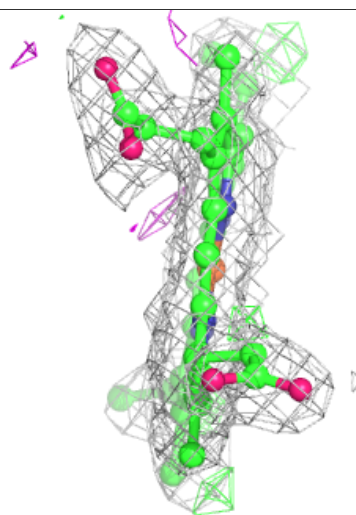
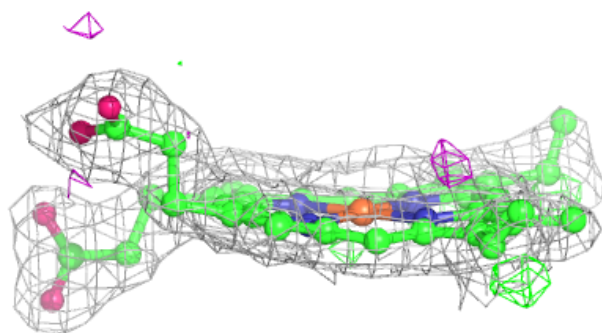
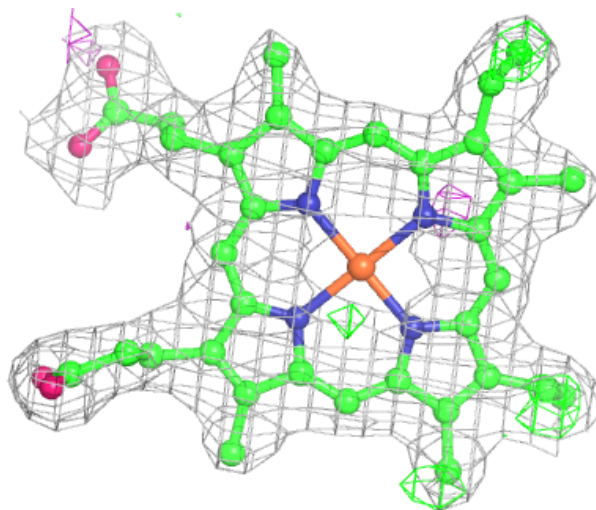
**Electron density around CLA B 613:**

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



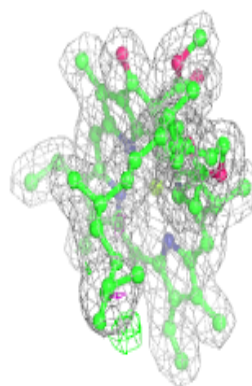
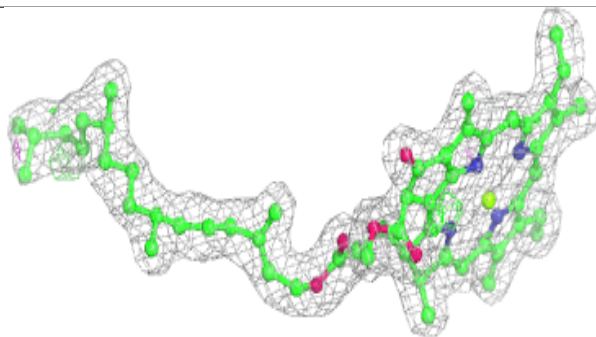
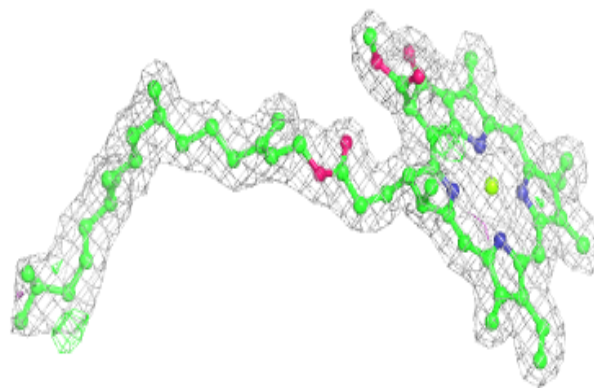
**Electron density around HEM v 201:**

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

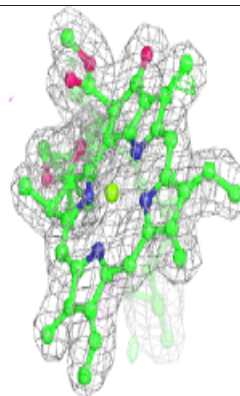
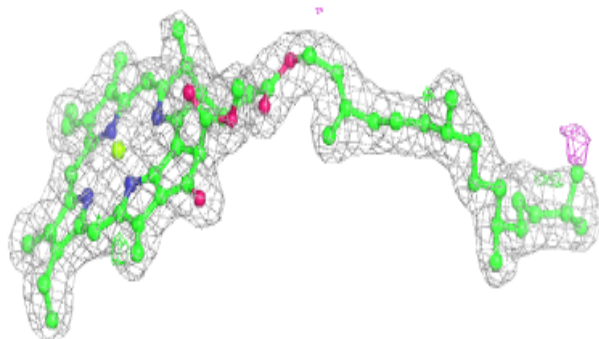
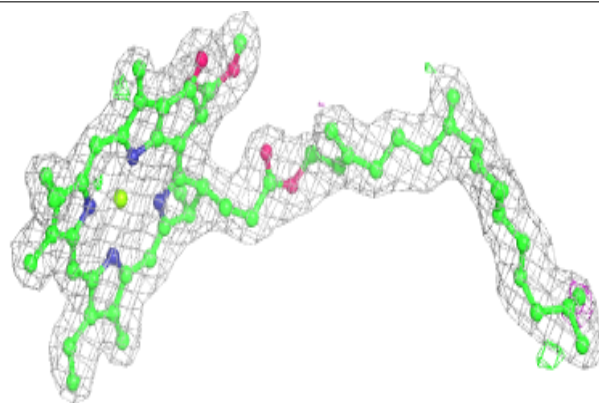


**Electron density around CLA A 1005:**

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

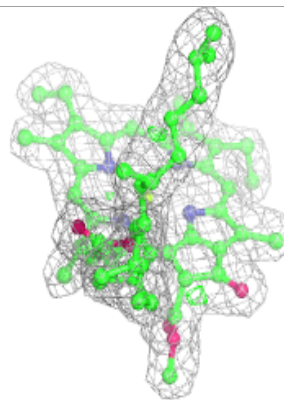
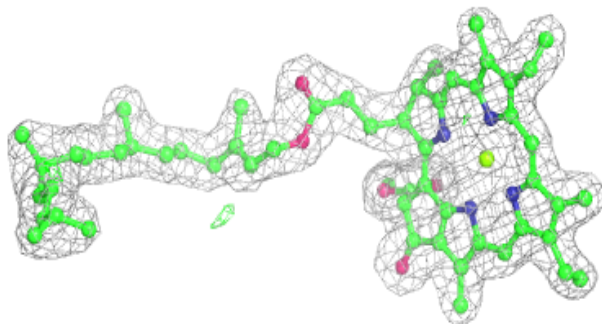
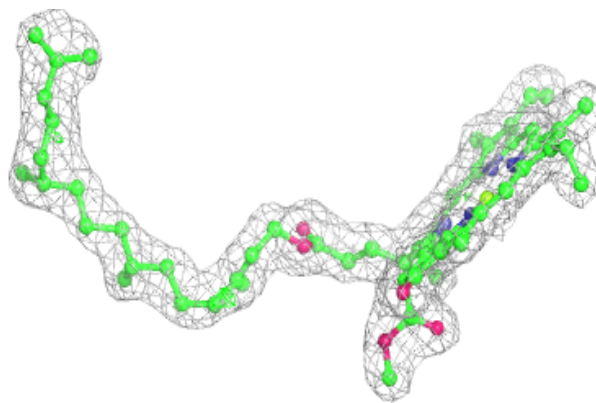
**Electron density around CLA a 407:**

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

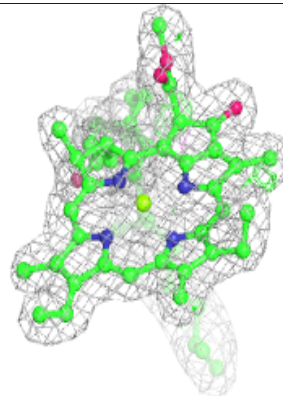
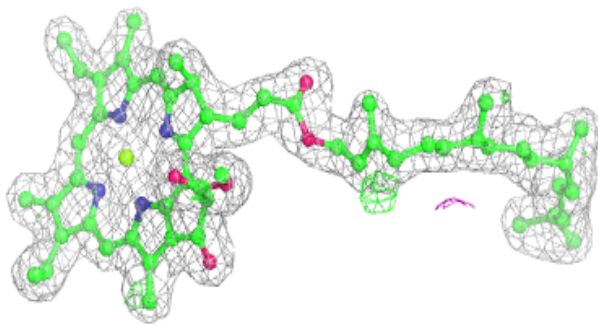
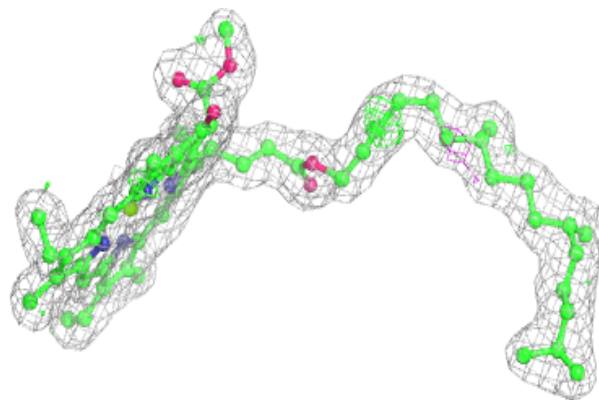


**Electron density around CLA d 402:**

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

**Electron density around CLA D 402:**

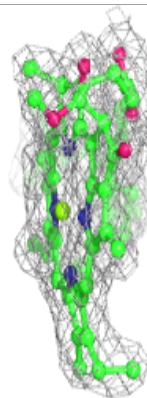
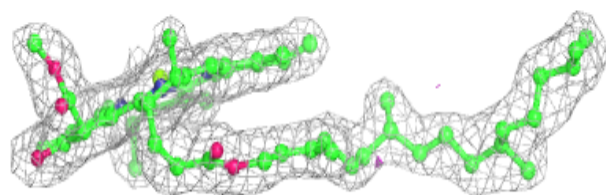
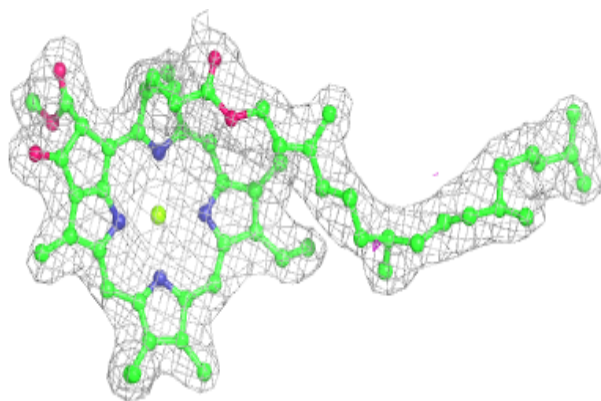
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



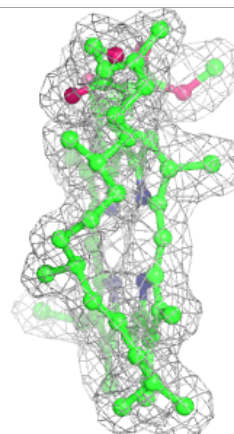
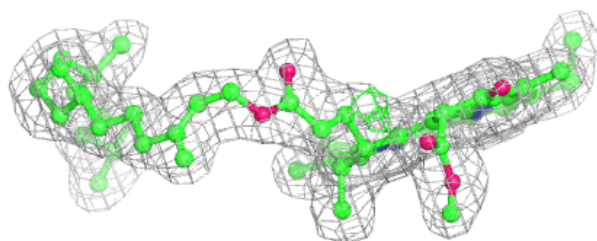
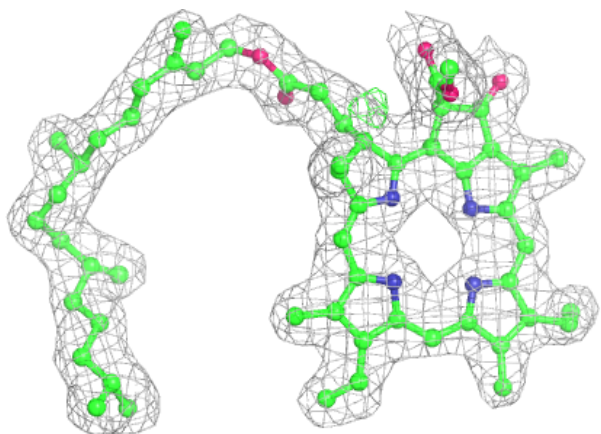


**Electron density around CLA b 606:**

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

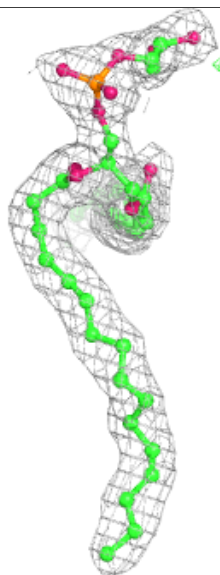
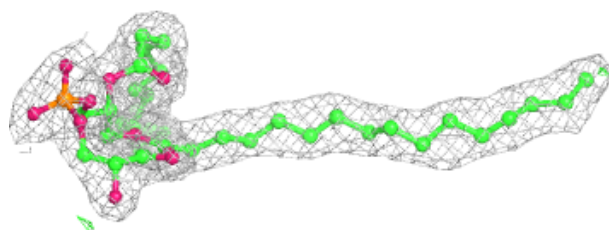
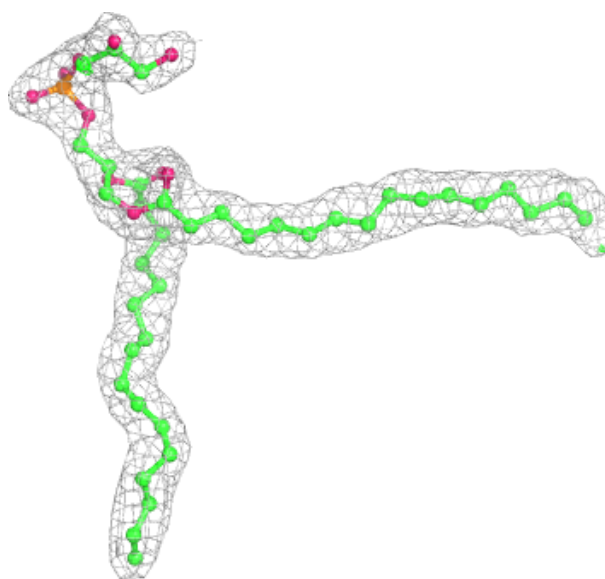
**Electron density around PHO A 1007:**

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



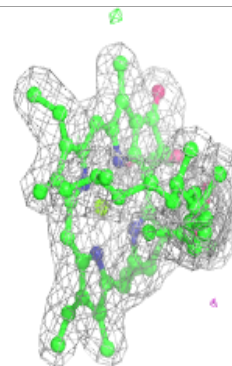
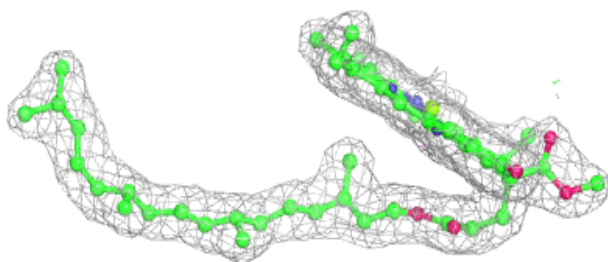
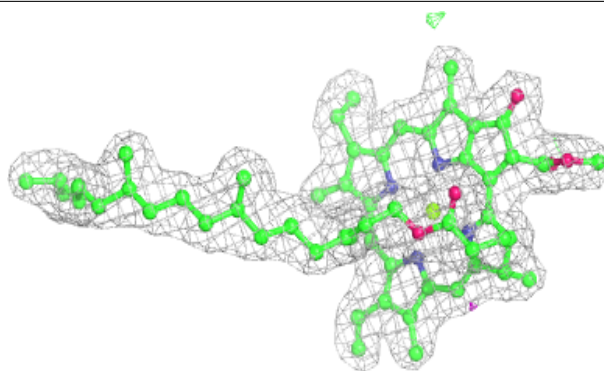
**Electron density around LHG B 621:**

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

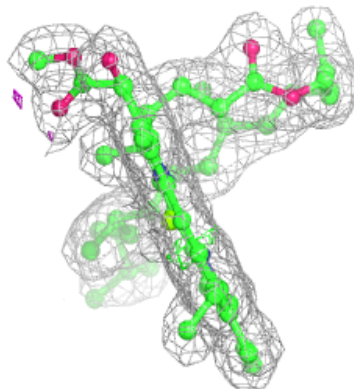
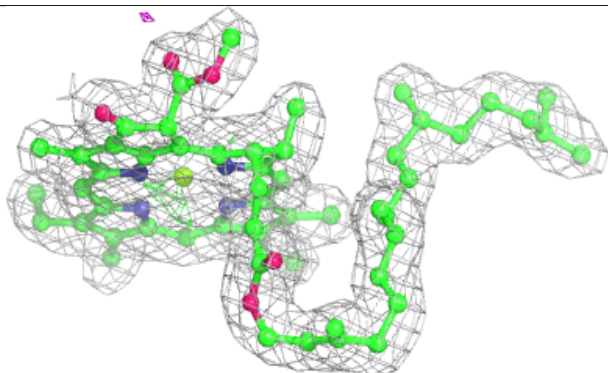
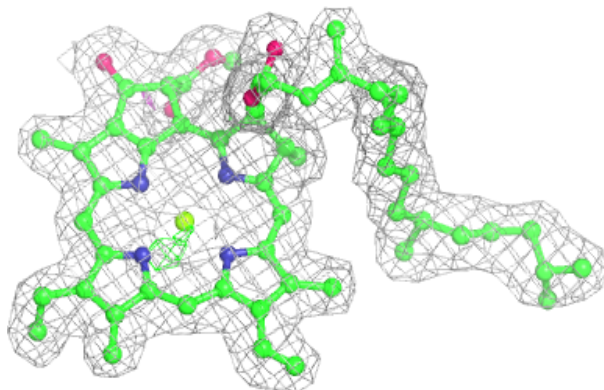


**Electron density around CLA B 608:**

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

**Electron density around CLA D 403:**

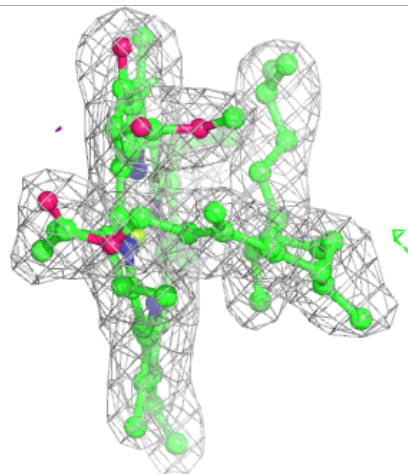
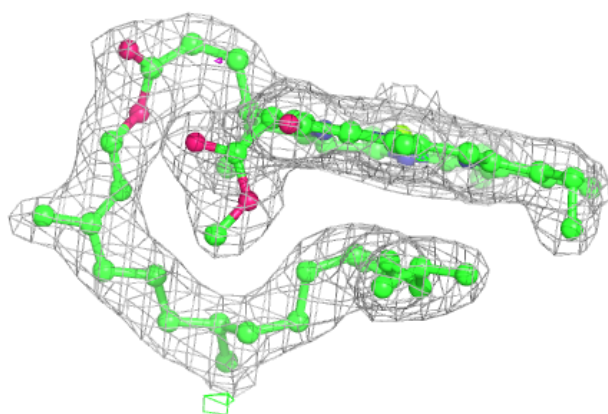
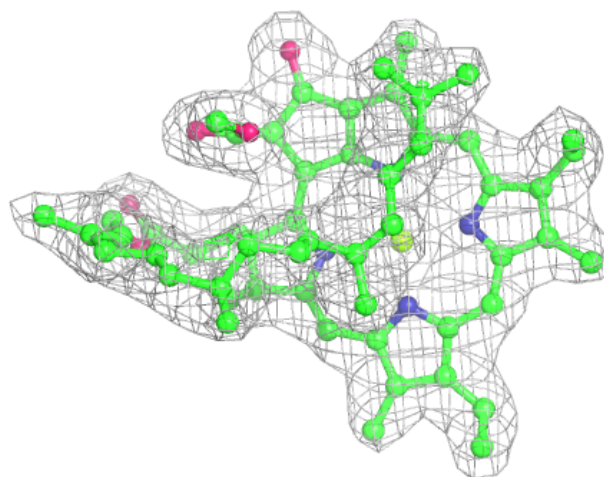
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





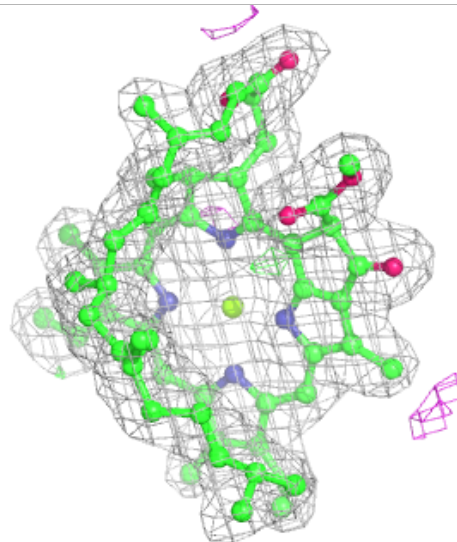
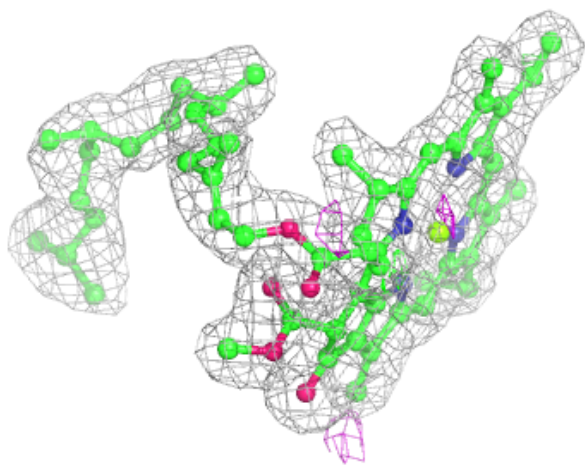
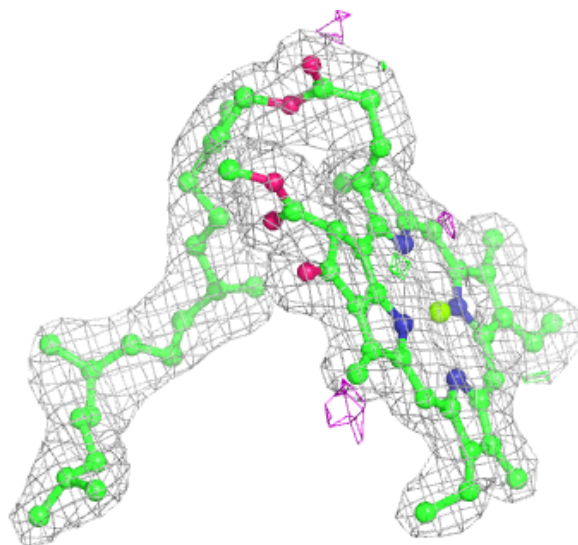
**Electron density around CLA C 510:**

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



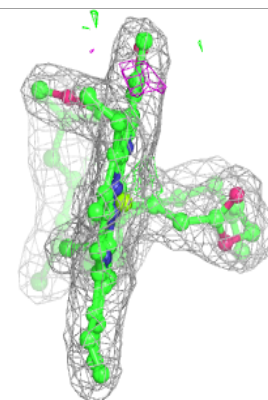
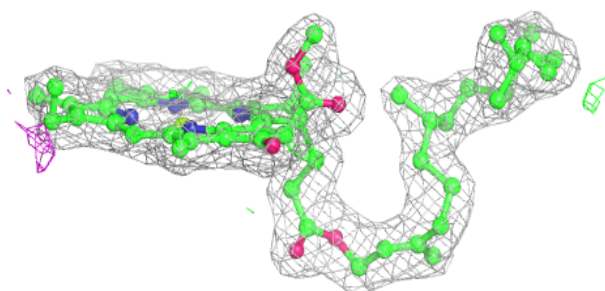
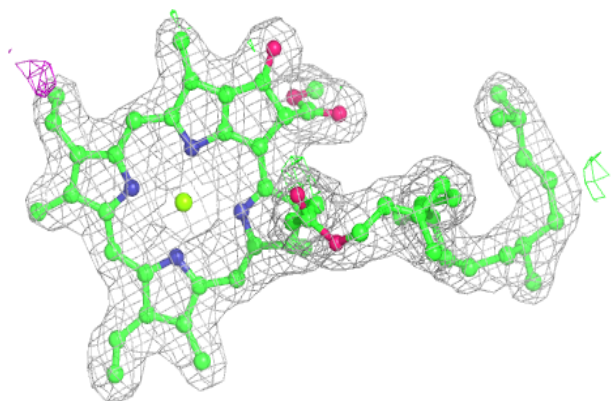
**Electron density around CLA b 616:**

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

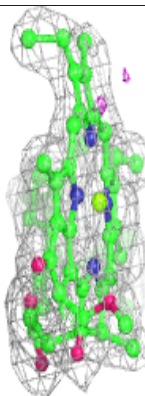
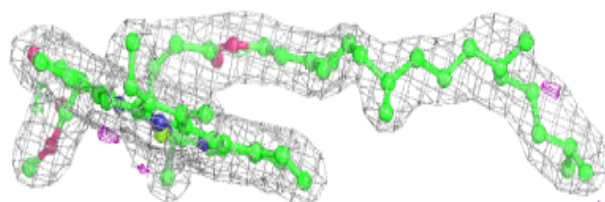
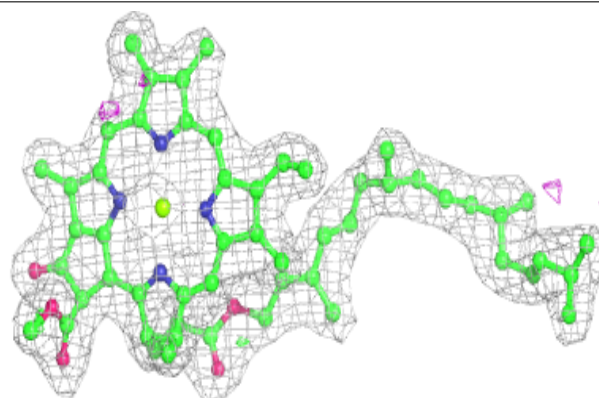


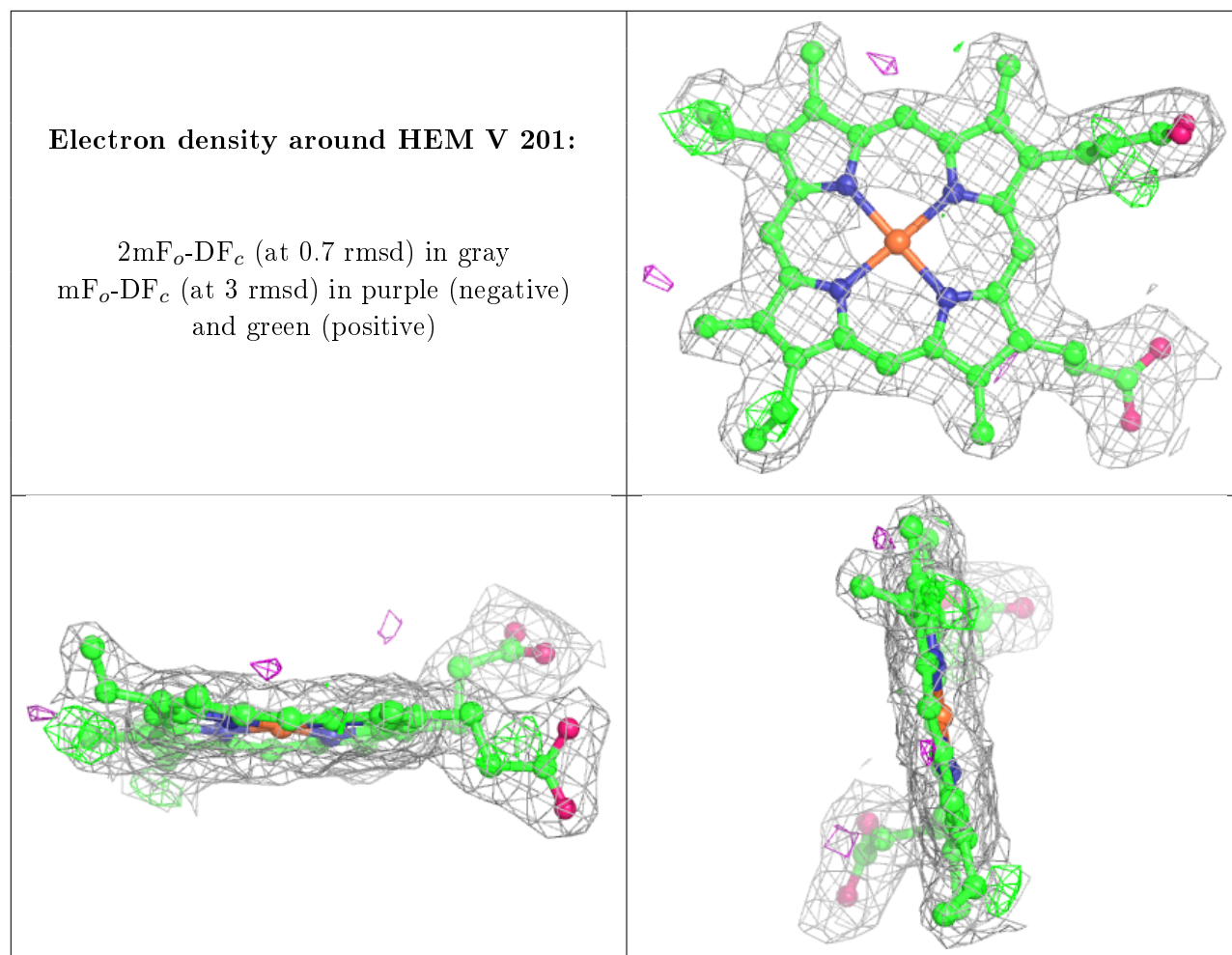
**Electron density around CLA B 612:**

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

**Electron density around CLA B 603:**

$2mF_o-DF_c$  (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.