



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2024 – 06:56 AM EST

PDB ID : 6DHO  
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.07 Angstrom resolution  
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.  
Deposited on : 2018-05-20  
Resolution : 2.07 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36

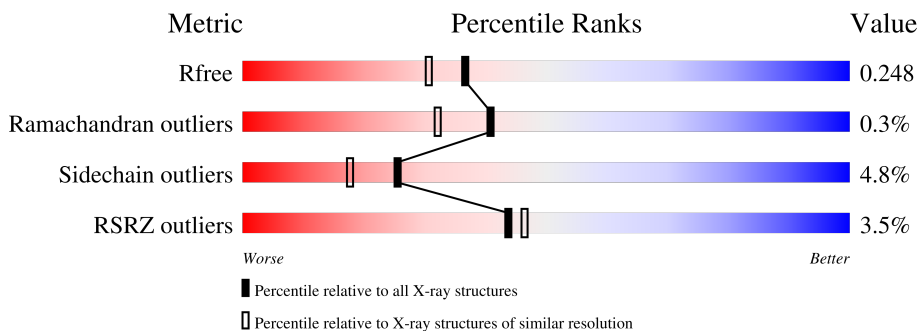
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

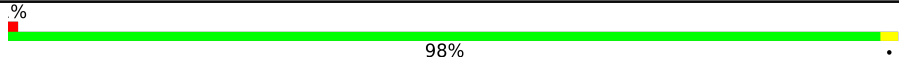
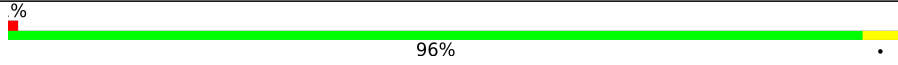
The reported resolution of this entry is 2.07 Å.

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	2684 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	 98%
1	a	334	 96%

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buster-report : 1.1.7 (2018)  
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
 Refmac : 5.8.0158  
 CCP4 : 7.0.044 (Gargrove)  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	B	505	97%
2	b	505	98%
3	C	451	96%
3	c	451	96%
4	D	341	99%
4	d	341	98%
5	E	82	89% 10%
5	e	82	96%
6	F	34	100%
6	f	34	85% 15%
7	H	65	94% 6%
7	h	65	91% 6%
8	I	36	86% 14%
8	i	36	97%
9	J	36	100%
9	j	36	94% 6%
10	K	37	89% 11%
10	k	37	89% 11%
11	L	37	97%
11	l	37	89% 8%
12	M	33	94% 6%
12	m	33	91% 6%
13	O	244	95% 5%
13	o	244	92% 7%
14	T	30	87% 10%

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Mol	Chain	Length	Quality of chain
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	a	411	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	403	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>
23	CLA	h	101	X	-	-	-

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 105756 atoms, of which 52470 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	334	6018	2010	2937	507	545	19	0	59	0
1	a	334	6006	2007	2928	507	545	19	0	59	0

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	505	7849	2631	3845	666	694	13	0	5	0
2	b	505	7789	2610	3811	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	442	6868	2282	3392	579	601	14	0	7	0
3	c	451	7017	2324	3464	596	619	14	0	8	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	341	5350	1806	2624	445	463	12	0	1	0
4	d	341	5362	1810	2630	445	465	12	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6	F	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	H	65	Total	C	H	N	O	S	0	0	0
			1030	338	523	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	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	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			516	172	261	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O	0	0	0	
			600	197	304	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
13	O	244	Total	C	H	N	O	S	0	1	0
			3730	1174	1850	317	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
14	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
14	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
17	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
20	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			
20	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

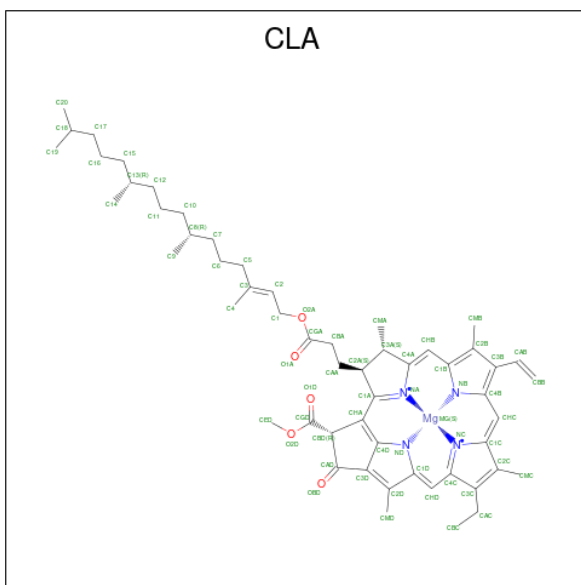
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 102 44 48 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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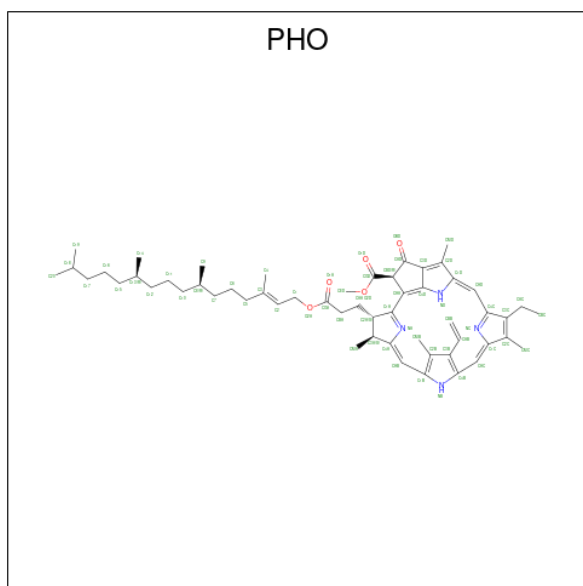
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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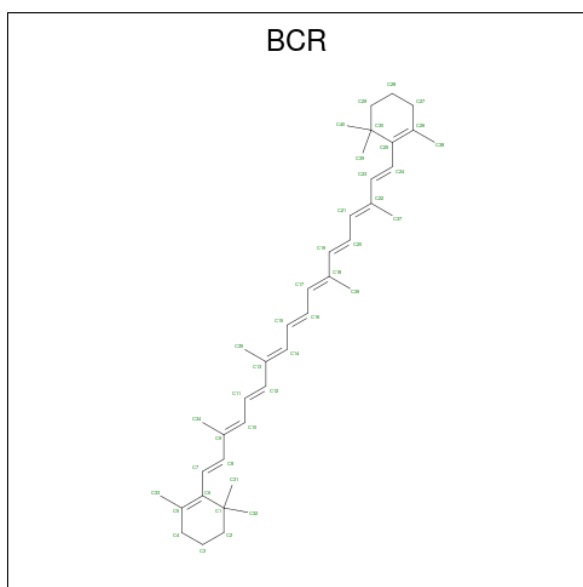
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
23	h	1	137	55	72	1	4	5	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
24	A	1	138	55	74	4	5	0	0
24	A	1	138	55	74	4	5	0	0
24	a	1	138	55	74	4	5	0	0
24	d	1	138	55	74	4	5	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	T	1	Total	C	H	0	0
			96	40	56		
25	Z	1	Total	C	H	0	0
			96	40	56		
25	a	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		

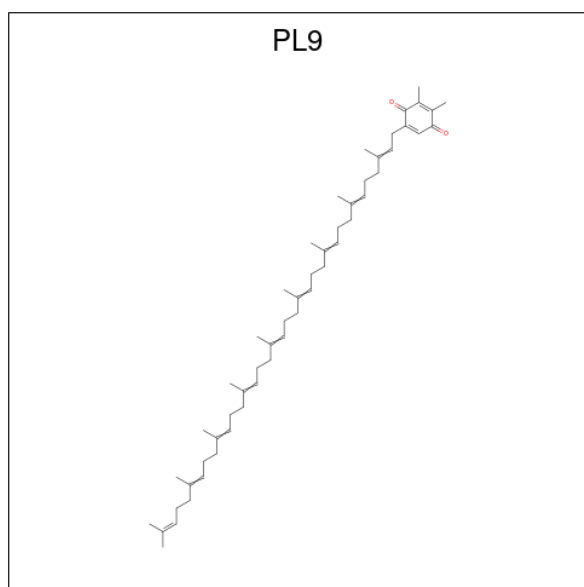
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
25	b	1	96	40	56	0	0
25	c	1	96	40	56	0	0
25	c	1	96	40	56	0	0
25	d	1	96	40	56	0	0
25	k	1	96	40	56	0	0
25	k	1	96	40	56	0	0
25	t	1	96	40	56	0	0
25	x	1	96	40	56	0	0

- Molecule 26 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:  $C_{53}H_{80}O_2$ ).



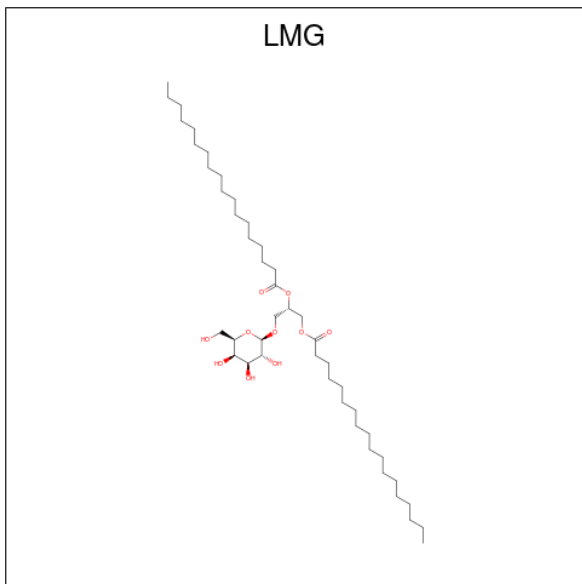
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	135	53	80	2	0	0
26	D	1	135	53	80	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



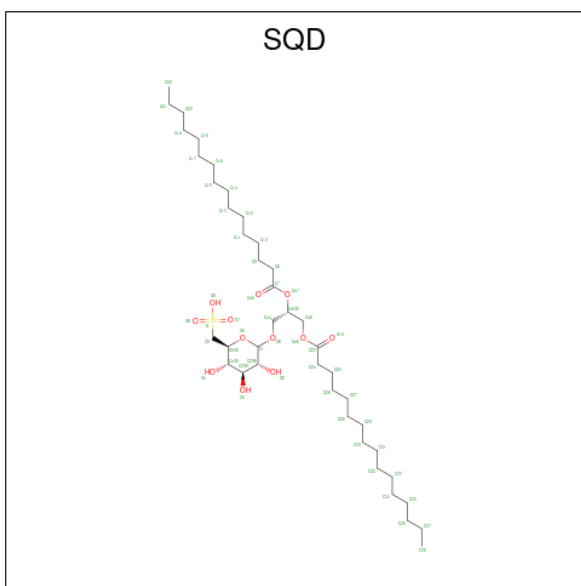
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- 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<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



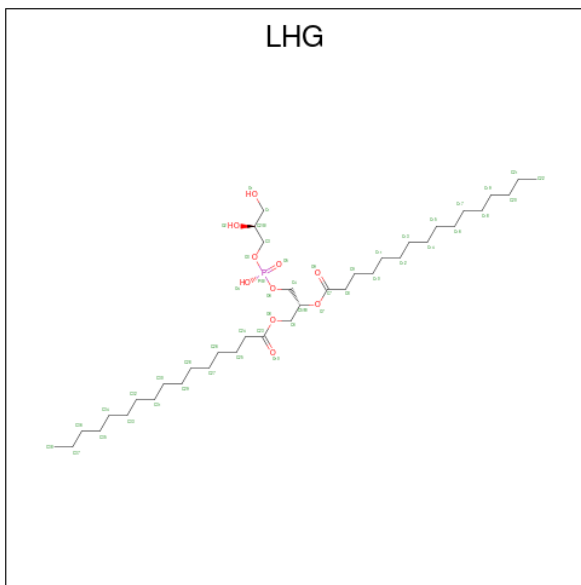
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O	0	0	
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O	0	0	
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		

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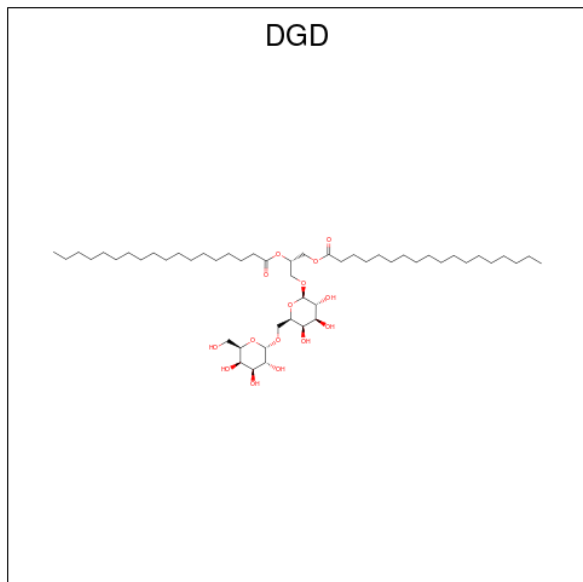
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
28	f	1	90	28	49	12	1	0	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



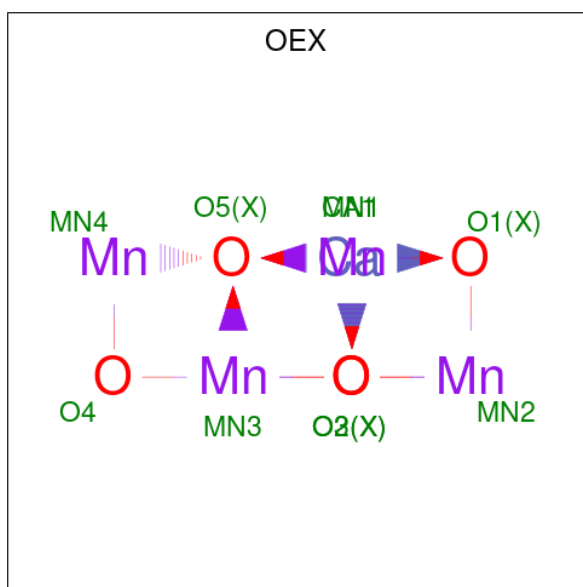
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
29	A	1	123	38	74	10	1	0	0
29	B	1	123	38	74	10	1	0	0
29	B	1	123	38	74	10	1	0	0
29	D	1	123	38	74	10	1	0	0
29	D	1	114	36	67	10	1	0	0
29	d	1	123	38	74	10	1	0	0
29	d	1	123	38	74	10	1	0	0
29	d	1	90	28	51	10	1	0	0
29	e	1	99	31	57	10	1	0	0
29	l	1	123	38	74	10	1	0	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



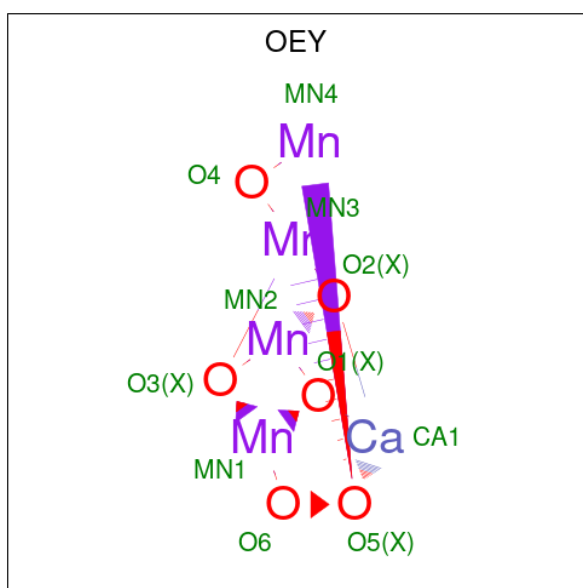
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
30	A	1	Total 162	C 51	H 96	O 15	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0
30	H	1	Total 144	C 47	H 82	O 15	0	0
30	a	1	Total 119	C 39	H 75	O 5	0	0
30	c	1	Total 144	C 47	H 82	O 15	0	0
30	c	1	Total 144	C 47	H 82	O 15	0	0
30	c	1	Total 144	C 47	H 82	O 15	0	0
30	h	1	Total 144	C 47	H 82	O 15	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $CaMn_4O_5$ ).



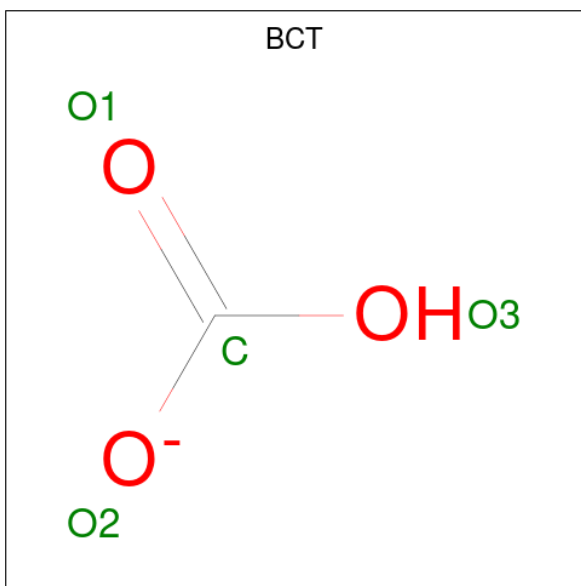
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
31	A	1	10	1	4	5	0	1
31	a	1	10	1	4	5	0	1

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
32	A	1	11	1	4	6	0	1
32	a	1	11	1	4	6	0	1

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
33	A	1	5	1	1	3	0	0
33	a	1	5	1	1	3	0	0

- Molecule 34 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

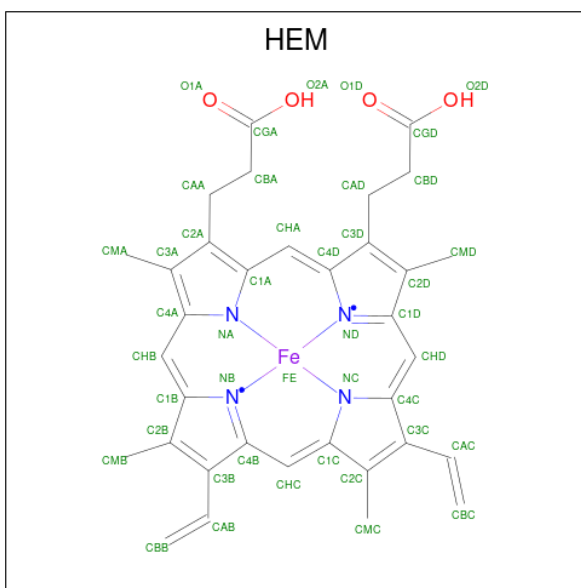
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
34	B	5	192	67	117	8	0	0
34	C	3	103	36	63	4	0	0
34	E	1	28	10	16	2	0	0
34	H	1	53	18	35		0	0
34	I	1	41	15	26		0	0
34	J	1	28	10	16	2	0	0
34	M	2	63	23	38	2	0	0
34	X	1	55	18	35	2	0	0
34	a	1	28	10	16	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	b	6	Total	C	H	O	0	0
			267	91	170	6		
34	c	2	Total	C	H	O	0	0
			83	28	51	4		
34	d	2	Total	C	H	O	0	0
			98	33	61	4		
34	j	1	Total	C	H	O	0	0
			28	10	16	2		
34	l	1	Total	C	H		0	0
			53	18	35			
34	m	1	Total	C	H	O	0	0
			28	10	16	2		
34	t	2	Total	C	H	O	0	0
			60	22	36	2		

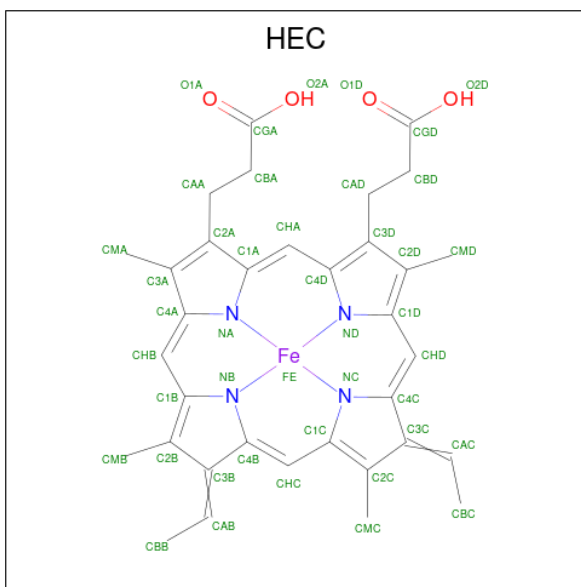
- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
35	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
36	V	1	73	34	1	30	4	4	0	0
36	v	1	73	34	1	30	4	4	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	146	Total 146	O 146	0	8
37	B	213	Total 213	O 213	0	0
37	C	193	Total 193	O 193	0	0
37	D	129	Total 129	O 129	0	0
37	E	29	Total 29	O 29	0	0
37	F	14	Total 14	O 14	0	0
37	H	29	Total 29	O 29	0	0
37	I	14	Total 14	O 14	0	0
37	J	12	Total 12	O 12	0	0
37	K	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	8	Total O 8 8	0	0
37	M	7	Total O 7 7	0	0
37	O	123	Total O 123 123	0	0
37	T	14	Total O 14 14	0	0
37	U	49	Total O 49 49	0	0
37	V	73	Total O 73 73	0	0
37	Y	3	Total O 3 3	0	0
37	X	8	Total O 8 8	0	0
37	Z	4	Total O 4 4	0	0
37	R	3	Total O 3 3	0	0
37	a	125	Total O 125 125	0	8
37	b	188	Total O 188 188	0	0
37	c	159	Total O 159 159	0	0
37	d	123	Total O 123 123	0	0
37	e	22	Total O 22 22	0	0
37	f	5	Total O 5 5	0	0
37	h	20	Total O 20 20	0	0
37	i	12	Total O 12 12	0	0
37	j	8	Total O 8 8	0	0
37	k	4	Total O 4 4	0	0
37	l	10	Total O 10 10	0	0

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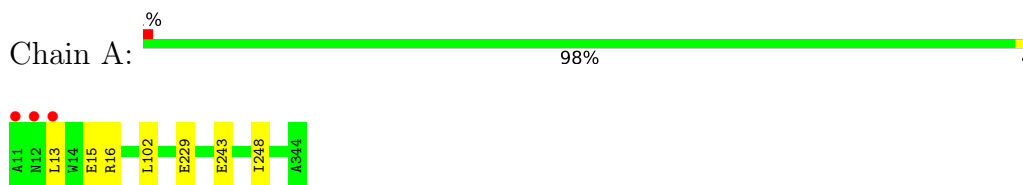
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	m	6	Total O 6 6	0	0
37	o	120	Total O 120 120	0	0
37	t	12	Total O 12 12	0	0
37	u	50	Total O 50 50	0	0
37	v	68	Total O 68 68	0	0
37	y	4	Total O 4 4	0	0
37	x	11	Total O 11 11	0	0
37	z	1	Total O 1 1	0	0
37	r	6	Total O 6 6	0	0

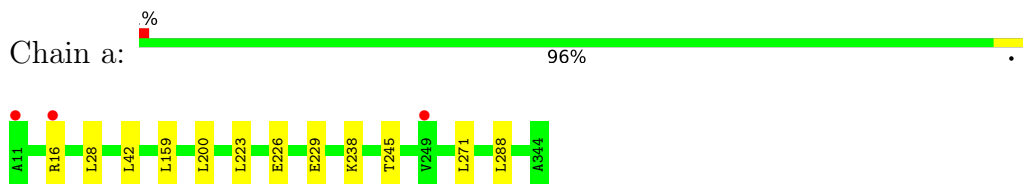
### 3 Residue-property plots [i](#)

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

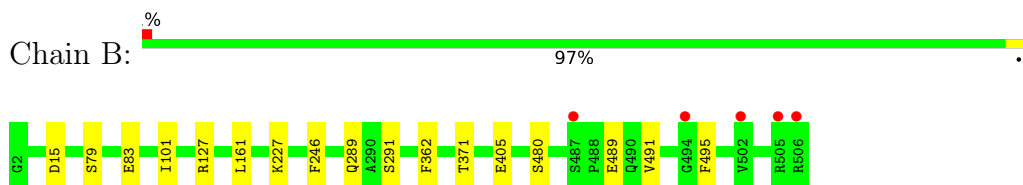
- Molecule 1: Photosystem II protein D1 1



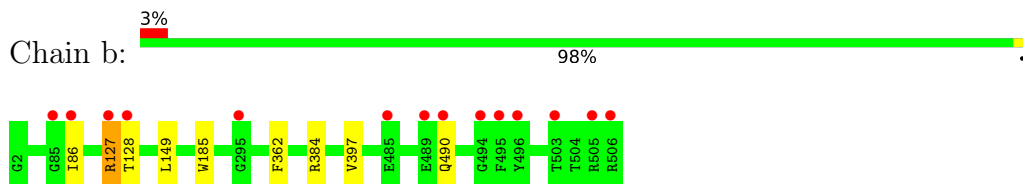
- Molecule 1: Photosystem II protein D1 1



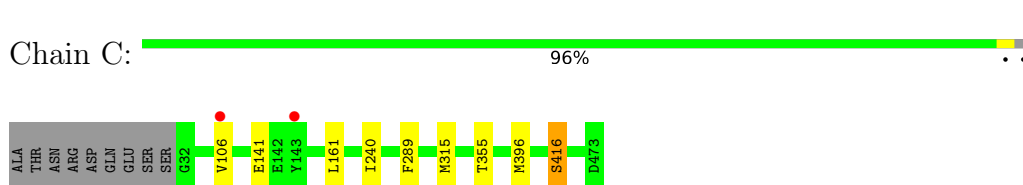
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



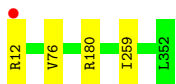
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



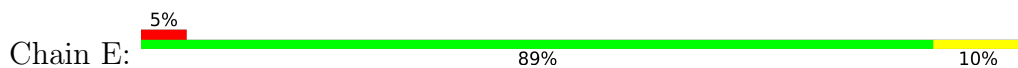
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



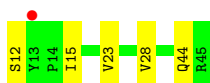
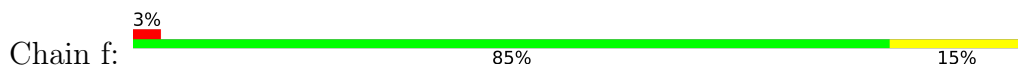
- Molecule 5: Cytochrome b559 subunit alpha



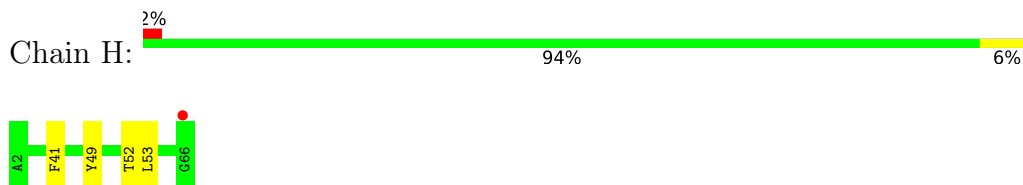
- Molecule 6: Cytochrome b559 subunit beta



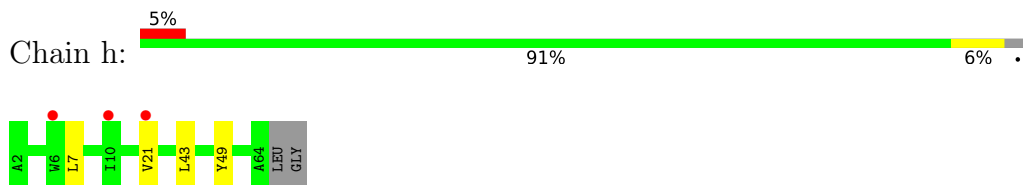
- Molecule 6: Cytochrome b559 subunit beta



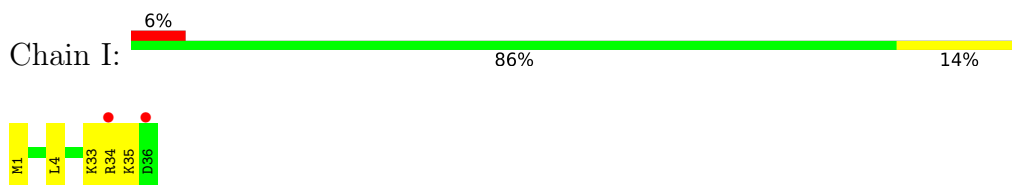
- Molecule 7: Photosystem II reaction center protein H



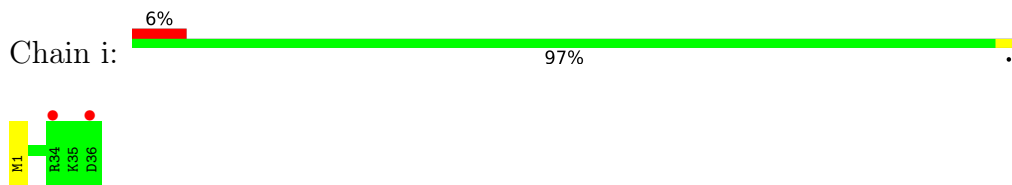
- Molecule 7: Photosystem II reaction center protein H



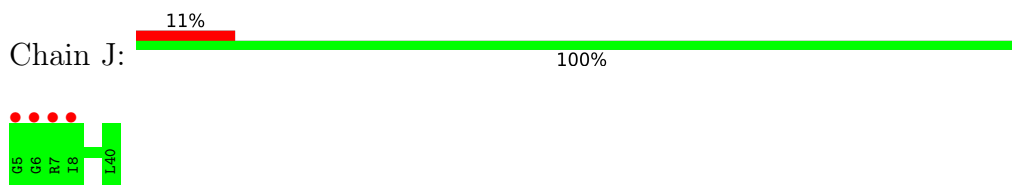
- Molecule 8: Photosystem II reaction center protein I



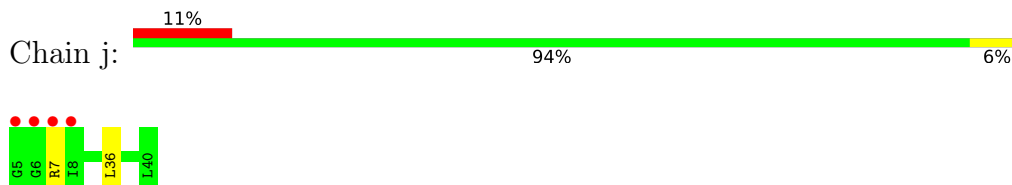
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

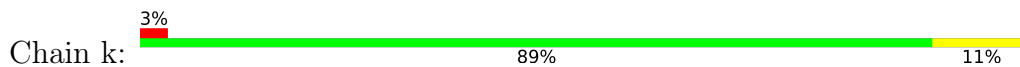


- Molecule 10: Photosystem II reaction center protein K





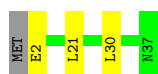
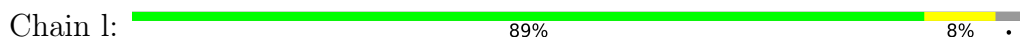
- Molecule 10: Photosystem II reaction center protein K



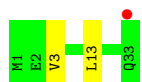
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



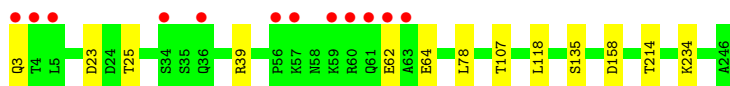
- Molecule 12: Photosystem II reaction center protein M



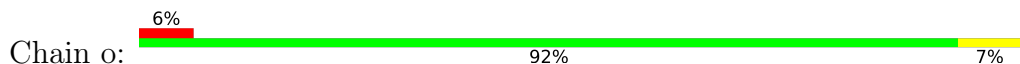
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

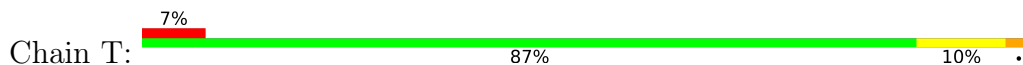


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

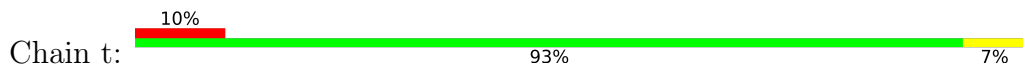




- Molecule 14: Photosystem II reaction center protein T



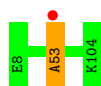
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

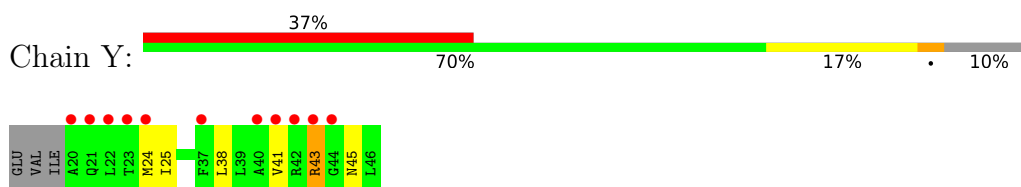


- Molecule 16: Cytochrome c-550

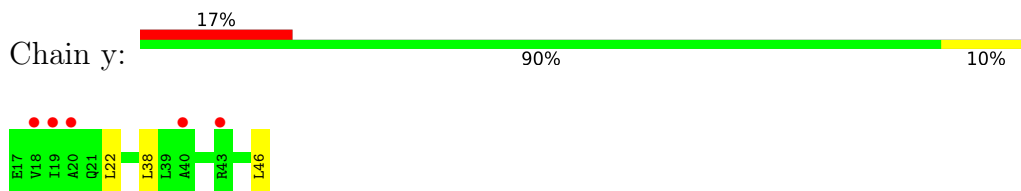


- Molecule 17: Photosystem II reaction center protein Ycf12

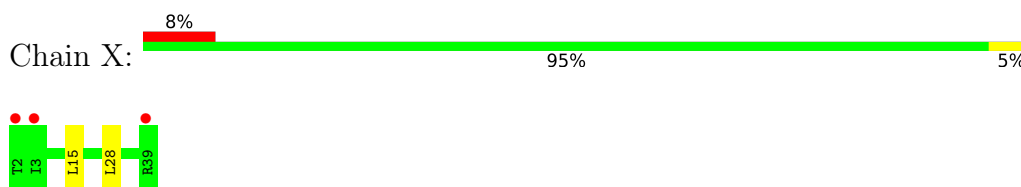




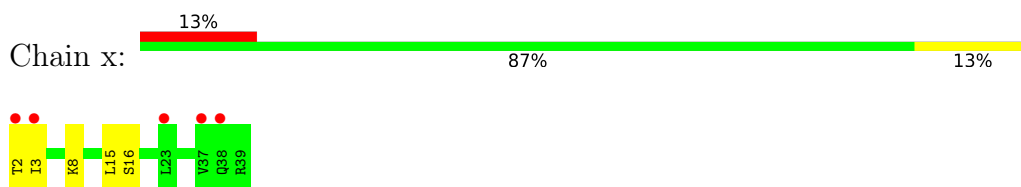
- Molecule 17: Photosystem II reaction center protein Ycf12



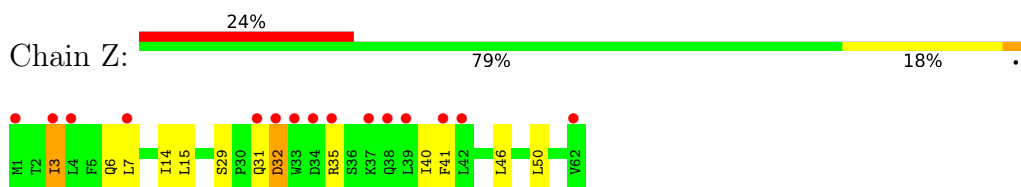
- Molecule 18: Photosystem II reaction center X protein



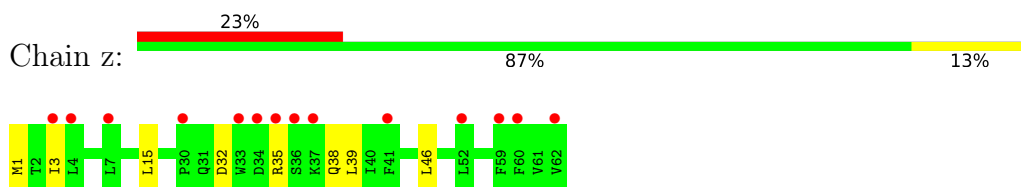
- Molecule 18: Photosystem II reaction center X protein



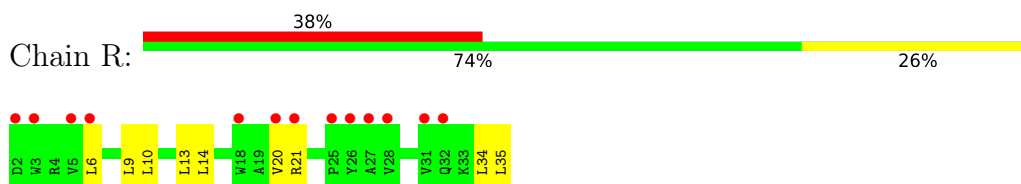
- Molecule 19: Photosystem II reaction center protein Z



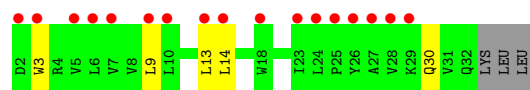
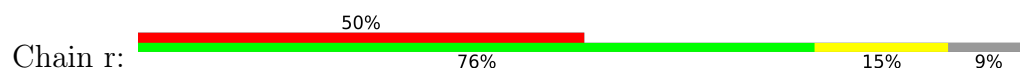
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



## ● 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, $\alpha$ , $\beta$ , $\gamma$	117.01Å 221.54Å 308.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.58 – 2.07 30.58 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.58-2.07) 87.1 (30.58-2.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.54 (at 2.06Å)	Xtrriage
Refinement program	PHENIX dev_svn	Depositor
R, $R_{free}$	0.184 , 0.247 0.184 , 0.248	Depositor DCC
$R_{free}$ test set	4294 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 71.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	105756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: CL, BCR, LMG, PL9, CLA, SQD, BCT, UNL, FE2, HEC, OEX, OEY, HEM, FME, DGD, LHG, PHO

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	0.69	0/3179	0.73	0/4331
1	a	0.65	0/3176	0.70	0/4327
2	B	0.63	0/4160	0.67	1/5668 (0.0%)
2	b	0.62	1/4118 (0.0%)	0.68	1/5611 (0.0%)
3	C	0.60	0/3593	0.66	1/4891 (0.0%)
3	c	0.59	1/3673 (0.0%)	0.67	0/4998
4	D	0.64	0/2820	0.66	0/3840
4	d	0.63	1/2829 (0.0%)	0.67	1/3852 (0.0%)
5	E	0.51	0/684	0.61	0/935
5	e	0.50	0/683	0.61	0/932
6	F	0.51	0/284	0.58	0/387
6	f	0.45	0/284	0.58	0/387
7	H	0.59	0/520	0.67	0/709
7	h	0.57	0/511	0.67	0/697
8	I	0.64	0/293	0.63	0/396
8	i	0.66	0/293	0.74	0/396
9	J	0.55	0/263	0.67	0/356
9	j	0.47	0/261	0.63	0/353
10	K	0.49	0/314	0.66	0/427
10	k	0.47	0/303	0.61	0/416
11	L	0.60	0/311	0.66	0/422
11	l	0.62	0/303	0.68	0/412
12	M	0.60	0/249	0.67	0/341
12	m	0.64	0/244	0.65	0/334
13	O	0.59	0/1914	0.73	1/2596 (0.0%)
13	o	0.56	0/1905	0.71	1/2583 (0.0%)
14	T	0.69	0/257	0.75	1/349 (0.3%)
14	t	0.69	0/255	0.62	0/346
15	U	0.53	0/785	0.65	0/1064
15	u	0.59	0/785	0.68	0/1064
16	V	0.56	0/1085	0.64	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.53	0/1085	0.64	0/1473
17	Y	0.40	0/197	0.60	0/264
17	y	0.35	0/219	0.54	0/294
18	X	0.52	0/284	0.59	0/384
18	x	0.38	0/284	0.55	0/384
19	Z	0.47	0/490	0.60	0/669
19	z	0.42	0/488	0.56	0/666
20	R	0.41	0/277	0.63	0/380
20	r	0.33	0/233	0.48	0/323
All	All	0.60	3/43891 (0.0%)	0.67	7/59730 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	u	0	1
19	Z	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	323	GLU	CB-CG	5.85	1.63	1.52
3	c	296	VAL	CB-CG1	-5.38	1.41	1.52
2	b	185	TRP	CB-CG	-5.00	1.41	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.63	123.37	118.30
2	b	384	ARG	NE-CZ-NH2	5.59	123.10	120.30
2	B	15	ASP	CB-CG-OD2	-5.55	113.30	118.30
13	O	158	ASP	CB-CG-OD1	5.45	123.21	118.30
14	T	24	ARG	NE-CZ-NH1	5.36	122.98	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	Z	32	ASP	Peptide
15	u	53	ALA	Peptide

## 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	390/334 (117%)	381 (98%)	9 (2%)	0	100	100
1	a	390/334 (117%)	382 (98%)	8 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	495 (98%)	7 (1%)	1 (0%)	47	39
3	C	447/451 (99%)	435 (97%)	11 (2%)	1 (0%)	47	39
3	c	457/451 (101%)	442 (97%)	14 (3%)	1 (0%)	47	39
4	D	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	55 (90%)	6 (10%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	J	34/36 (94%)	31 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	4	1
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	226 (93%)	16 (7%)	1 (0%)	34	25
13	o	242/244 (99%)	230 (95%)	8 (3%)	4 (2%)	9	2
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	90 (95%)	4 (4%)	1 (1%)	14	5
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	19 (76%)	4 (16%)	2 (8%)	1	0
17	y	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
18	X	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	50 (83%)	7 (12%)	3 (5%)	2	0
19	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	9	2
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	4	0
20	r	29/34 (85%)	22 (76%)	6 (21%)	1 (3%)	3	0
All	All	5365/5326 (101%)	5164 (96%)	183 (3%)	18 (0%)	41	32

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	62	GLU
3	c	416	SER
13	o	60	ARG
13	o	61	GLN

### 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	319/270 (118%)	312 (98%)	7 (2%)	52	46
1	a	318/270 (118%)	306 (96%)	12 (4%)	33	26
2	B	407/403 (101%)	390 (96%)	17 (4%)	30	23
2	b	402/403 (100%)	395 (98%)	7 (2%)	60	57
3	C	351/352 (100%)	342 (97%)	9 (3%)	46	40
3	c	360/352 (102%)	344 (96%)	16 (4%)	28	21
4	D	277/276 (100%)	273 (99%)	4 (1%)	67	64
4	d	278/276 (101%)	272 (98%)	6 (2%)	52	46
5	E	72/72 (100%)	63 (88%)	9 (12%)	4	1
5	e	71/72 (99%)	68 (96%)	3 (4%)	30	23
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	0
7	H	53/54 (98%)	49 (92%)	4 (8%)	13	6
7	h	53/54 (98%)	49 (92%)	4 (8%)	13	6
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	1
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	23/24 (96%)	21 (91%)	2 (9%)	10	4
10	K	31/30 (103%)	27 (87%)	4 (13%)	4	1
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	36
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	4
12	M	28/29 (97%)	26 (93%)	2 (7%)	14	7
12	m	28/29 (97%)	27 (96%)	1 (4%)	35	28
13	O	208/207 (100%)	197 (95%)	11 (5%)	22	14
13	o	207/207 (100%)	191 (92%)	16 (8%)	13	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	26/26 (100%)	23 (88%)	3 (12%)	5	1
14	t	25/26 (96%)	24 (96%)	1 (4%)	31	24
15	U	84/84 (100%)	81 (96%)	3 (4%)	35	28
15	u	84/84 (100%)	84 (100%)	0	100	100
16	V	117/117 (100%)	113 (97%)	4 (3%)	37	30
16	v	117/117 (100%)	110 (94%)	7 (6%)	19	11
17	Y	19/23 (83%)	14 (74%)	5 (26%)	0	0
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	1
18	X	31/31 (100%)	29 (94%)	2 (6%)	17	9
18	x	31/31 (100%)	26 (84%)	5 (16%)	2	0
19	Z	52/52 (100%)	41 (79%)	11 (21%)	1	0
19	z	51/52 (98%)	44 (86%)	7 (14%)	3	1
20	R	28/29 (97%)	20 (71%)	8 (29%)	0	0
20	r	19/29 (66%)	15 (79%)	4 (21%)	1	0
All	All	4435/4348 (102%)	4221 (95%)	214 (5%)	25	18

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	229	GLU
4	d	12	ARG
18	x	3	ILE
1	a	288	LEU
3	c	29	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	58	ASN
19	z	38	GLN
13	O	231	HIS
17	Y	21	GLN
2	b	497	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	m	1	12	8,9,10	1.02	1 (12%)	7,9,11	0.67	0
14	FME	T	1	14	8,9,10	1.11	1 (12%)	7,9,11	1.62	2 (28%)
14	FME	t	1	14	8,9,10	1.07	1 (12%)	7,9,11	1.97	1 (14%)
12	FME	M	1	12	8,9,10	0.92	0	7,9,11	1.02	0
8	FME	i	1	8	8,9,10	1.01	0	7,9,11	1.15	1 (14%)
8	FME	I	1	8	8,9,10	0.87	0	7,9,11	1.47	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
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.69	1.42	1.46
14	T	1	FME	CA-N	-2.32	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	FME	CA-N	-2.08	1.43	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.32	116.18	122.82
8	I	1	FME	CA-N-CN	-3.12	118.02	122.82
14	T	1	FME	CA-N-CN	-2.62	118.79	122.82
8	i	1	FME	C-CA-N	2.40	114.07	109.73
14	T	1	FME	O1-CN-N	-2.12	119.68	125.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
12	M	1	FME	CB-CA-N-CN
8	i	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 188 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	607	37	65,73,73	1.48	9 (13%)	76,113,113	1.46	9 (11%)
33	BCT	a	404	21	2,3,3	1.46	0	2,3,3	3.14	2 (100%)
23	CLA	h	101	37	65,73,73	1.75	11 (16%)	76,113,113	1.48	14 (18%)
27	LMG	D	406	-	51,51,55	0.98	2 (3%)	59,59,63	1.28	8 (13%)
25	BCR	k	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.22	5 (8%)
29	LHG	D	407	-	48,48,48	0.98	3 (6%)	51,54,54	1.32	7 (13%)
27	LMG	B	621	-	26,26,55	0.76	0	26,26,63	1.12	2 (7%)
23	CLA	B	606	-	65,73,73	1.87	11 (16%)	76,113,113	1.64	13 (17%)
25	BCR	B	619	-	41,41,41	1.23	3 (7%)	56,56,56	1.32	8 (14%)
30	DGD	C	515	-	63,63,67	1.40	9 (14%)	77,77,81	1.33	9 (11%)
23	CLA	c	502	-	65,73,73	1.57	9 (13%)	76,113,113	1.43	9 (11%)
23	CLA	c	505	-	65,73,73	1.57	8 (12%)	76,113,113	1.41	10 (13%)
23	CLA	b	604	-	65,73,73	1.55	10 (15%)	76,113,113	1.62	13 (17%)
23	CLA	B	609	-	65,73,73	1.67	14 (21%)	76,113,113	1.55	12 (15%)
27	LMG	b	622	-	55,55,55	1.03	3 (5%)	63,63,63	1.45	8 (12%)
27	LMG	c	523	-	49,49,55	0.89	1 (2%)	57,57,63	1.31	7 (12%)
25	BCR	k	102	-	41,41,41	0.90	1 (2%)	56,56,56	1.15	3 (5%)
23	CLA	B	616	-	60,68,73	1.60	9 (15%)	70,107,113	1.59	15 (21%)
27	LMG	c	521	-	48,48,55	1.12	6 (12%)	56,56,63	1.36	7 (12%)
23	CLA	B	614	-	65,73,73	1.52	9 (13%)	76,113,113	1.48	12 (15%)
32	OEY	a	417[B]	1,3,37	0,16,16	-	-	-	-	-
23	CLA	B	613	-	65,73,73	1.61	10 (15%)	76,113,113	1.44	8 (10%)
23	CLA	A	404	-	65,73,73	1.63	10 (15%)	76,113,113	1.48	12 (15%)
26	PL9	D	405	-	55,55,55	1.57	8 (14%)	68,69,69	1.47	11 (16%)
23	CLA	b	614	-	65,73,73	1.66	8 (12%)	76,113,113	1.36	10 (13%)
24	PHO	A	406	-	51,69,69	0.99	4 (7%)	47,99,99	1.46	8 (17%)
25	BCR	c	515	-	41,41,41	1.27	3 (7%)	56,56,56	1.44	10 (17%)
23	CLA	C	503	-	65,73,73	1.83	12 (18%)	76,113,113	1.81	13 (17%)
23	CLA	c	511	3	65,73,73	1.76	8 (12%)	76,113,113	1.38	7 (9%)
23	CLA	d	402	-	65,73,73	1.59	9 (13%)	76,113,113	1.66	8 (10%)
30	DGD	A	415	-	67,67,67	1.25	8 (11%)	81,81,81	1.48	11 (13%)
23	CLA	D	401	37	65,73,73	1.43	8 (12%)	76,113,113	1.34	9 (11%)
23	CLA	C	501	-	65,73,73	1.82	10 (15%)	76,113,113	1.42	7 (9%)
27	LMG	C	518	-	48,48,55	1.02	3 (6%)	56,56,63	1.34	8 (14%)
25	BCR	T	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.53	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	c	519	-	37,37,55	1.15	4 (10%)	45,45,63	1.26	6 (13%)
27	LMG	d	409	-	44,44,55	1.02	3 (6%)	52,52,63	1.33	7 (13%)
23	CLA	c	501	-	65,73,73	1.59	11 (16%)	76,113,113	1.67	10 (13%)
28	SQD	f	101	-	40,41,54	1.16	5 (12%)	49,52,65	1.75	9 (18%)
28	SQD	B	624	-	53,54,54	0.93	2 (3%)	62,65,65	1.83	12 (19%)
25	BCR	b	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
29	LHG	B	622	-	48,48,48	0.69	1 (2%)	51,54,54	1.12	5 (9%)
23	CLA	b	616	-	65,73,73	1.76	12 (18%)	76,113,113	1.30	4 (5%)
25	BCR	t	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.43	9 (16%)
24	PHO	a	407	-	51,69,69	1.19	6 (11%)	47,99,99	1.19	3 (6%)
23	CLA	C	508	-	65,73,73	1.42	8 (12%)	76,113,113	1.50	10 (13%)
23	CLA	c	508	-	64,72,73	1.50	8 (12%)	74,111,113	1.45	9 (12%)
23	CLA	a	406	37	65,73,73	1.83	10 (15%)	76,113,113	1.49	9 (11%)
23	CLA	c	510	-	65,73,73	1.54	9 (13%)	76,113,113	1.51	9 (11%)
25	BCR	C	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	8 (14%)
29	LHG	A	413	-	48,48,48	0.99	4 (8%)	51,54,54	1.21	2 (3%)
30	DGD	c	517	-	63,63,67	1.09	6 (9%)	77,77,81	1.41	9 (11%)
26	PL9	d	405	-	55,55,55	1.37	10 (18%)	68,69,69	1.79	20 (29%)
23	CLA	C	505	-	65,73,73	1.44	7 (10%)	76,113,113	1.20	6 (7%)
31	OEX	A	416[A]	1,3,37	0,15,15	-	-	-	-	-
25	BCR	K	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.41	9 (16%)
23	CLA	b	607	-	65,73,73	1.74	9 (13%)	76,113,113	1.67	10 (13%)
28	SQD	F	101	-	35,36,54	1.02	3 (8%)	42,45,65	1.79	9 (21%)
27	LMG	M	101	-	51,51,55	0.99	3 (5%)	59,59,63	1.50	10 (16%)
27	LMG	D	409	-	31,31,55	0.99	3 (9%)	33,33,63	1.24	3 (9%)
23	CLA	C	511	3	65,73,73	1.77	12 (18%)	76,113,113	1.63	7 (9%)
24	PHO	d	401	-	51,69,69	1.10	7 (13%)	47,99,99	1.44	7 (14%)
30	DGD	a	414	-	43,43,67	1.45	5 (11%)	45,45,81	1.49	7 (15%)
23	CLA	d	403	-	65,73,73	1.52	11 (16%)	76,113,113	1.32	11 (14%)
23	CLA	C	504	37	59,67,73	1.50	10 (16%)	68,105,113	1.30	7 (10%)
31	OEX	a	416[A]	1,3,37	0,15,15	-	-	-	-	-
28	SQD	b	601	-	48,49,54	0.95	3 (6%)	57,60,65	1.96	13 (22%)
23	CLA	B	608	-	65,73,73	1.48	10 (15%)	76,113,113	1.32	9 (11%)
23	CLA	c	513	-	65,73,73	1.50	10 (15%)	76,113,113	1.24	7 (9%)
25	BCR	Z	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	c	514	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	12 (21%)
30	DGD	c	518	-	63,63,67	1.10	6 (9%)	77,77,81	1.46	15 (19%)
25	BCR	d	404	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	5 (8%)
36	HEC	v	201	16	32,50,50	2.23	4 (12%)	24,82,82	1.46	5 (20%)
25	BCR	x	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	6 (10%)
29	LHG	d	406	-	48,48,48	0.72	0	51,54,54	1.29	6 (11%)
26	PL9	A	410	-	55,55,55	1.14	2 (3%)	68,69,69	1.69	15 (22%)
23	CLA	b	603	-	65,73,73	1.53	9 (13%)	76,113,113	1.46	11 (14%)
28	SQD	a	413	-	35,35,54	1.11	2 (5%)	37,37,65	1.39	5 (13%)
29	LHG	D	408	-	46,46,48	1.07	4 (8%)	49,52,54	1.30	5 (10%)
25	BCR	H	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.40	6 (10%)
24	PHO	A	407	-	51,69,69	1.13	5 (9%)	47,99,99	1.27	5 (10%)
23	CLA	b	605	-	65,73,73	1.49	8 (12%)	76,113,113	1.49	13 (17%)
23	CLA	B	601	37	65,73,73	1.71	7 (10%)	76,113,113	1.76	10 (13%)
23	CLA	B	612	-	65,73,73	1.44	8 (12%)	76,113,113	1.51	9 (11%)
23	CLA	C	512	-	65,73,73	1.52	9 (13%)	76,113,113	1.43	11 (14%)
29	LHG	d	407	-	48,48,48	0.78	1 (2%)	51,54,54	1.29	6 (11%)
23	CLA	b	613	-	65,73,73	1.56	9 (13%)	76,113,113	1.50	13 (17%)
25	BCR	B	617	-	41,41,41	1.19	4 (9%)	56,56,56	1.38	8 (14%)
28	SQD	a	412	-	53,54,54	0.98	4 (7%)	62,65,65	1.90	11 (17%)
30	DGD	H	102	-	63,63,67	1.32	9 (14%)	77,77,81	1.45	11 (14%)
30	DGD	C	517	-	63,63,67	1.13	8 (12%)	77,77,81	1.37	8 (10%)
25	BCR	A	409	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	6 (10%)
27	LMG	A	411	-	48,48,55	0.94	2 (4%)	56,56,63	1.39	9 (16%)
25	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	10 (17%)
23	CLA	b	615	-	65,73,73	1.60	8 (12%)	76,113,113	1.60	8 (10%)
23	CLA	B	611	-	65,73,73	1.39	10 (15%)	76,113,113	1.54	14 (18%)
29	LHG	B	623	-	48,48,48	0.86	2 (4%)	51,54,54	1.43	6 (11%)
23	CLA	C	502	-	65,73,73	1.50	8 (12%)	76,113,113	1.38	11 (14%)
32	OEY	A	417[B]	1,3,37	0,16,16	-	-	-	-	-
25	BCR	a	409	-	41,41,41	0.99	2 (4%)	56,56,56	1.34	10 (17%)
29	LHG	l	101	-	48,48,48	0.78	1 (2%)	51,54,54	1.22	5 (9%)
23	CLA	C	507	37	65,73,73	1.56	10 (15%)	76,113,113	1.54	10 (13%)
23	CLA	a	411	37	65,73,73	1.71	9 (13%)	76,113,113	1.73	11 (14%)
25	BCR	D	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	DGD	h	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.53	14 (18%)
23	CLA	c	504	37	60,68,73	1.54	9 (15%)	70,107,113	1.48	9 (12%)
23	CLA	b	611	37	65,73,73	1.43	8 (12%)	76,113,113	1.39	10 (13%)
23	CLA	B	604	-	65,73,73	1.52	7 (10%)	76,113,113	1.59	13 (17%)
27	LMG	b	623	-	21,21,55	0.83	1 (4%)	20,20,63	0.95	1 (5%)
23	CLA	D	402	-	65,73,73	1.25	10 (15%)	76,113,113	1.23	8 (10%)
29	LHG	d	408	-	38,38,48	0.88	1 (2%)	41,44,54	1.21	4 (9%)
30	DGD	C	516	-	63,63,67	1.07	4 (6%)	77,77,81	1.44	12 (15%)
23	CLA	C	506	-	65,73,73	1.69	9 (13%)	76,113,113	1.37	7 (9%)
35	HEM	e	102	6,5	41,50,50	1.45	4 (9%)	45,82,82	1.67	8 (17%)
23	CLA	c	509	-	65,73,73	1.52	7 (10%)	76,113,113	1.52	9 (11%)
23	CLA	A	405	37	65,73,73	1.52	12 (18%)	76,113,113	1.42	8 (10%)
23	CLA	D	403	-	65,73,73	1.49	12 (18%)	76,113,113	1.32	6 (7%)
33	BCT	A	418	21	2,3,3	1.08	0	2,3,3	3.47	2 (100%)
28	SQD	A	412	-	51,52,54	1.06	4 (7%)	60,63,65	2.29	15 (25%)
29	LHG	e	101	-	41,41,48	0.92	3 (7%)	44,47,54	1.37	4 (9%)
23	CLA	B	610	37	65,73,73	1.63	8 (12%)	76,113,113	1.51	9 (11%)
23	CLA	b	609	-	65,73,73	1.57	10 (15%)	76,113,113	1.49	14 (18%)
23	CLA	c	506	-	65,73,73	2.08	9 (13%)	76,113,113	1.45	13 (17%)
23	CLA	a	405	-	65,73,73	1.43	8 (12%)	76,113,113	1.53	11 (14%)
25	BCR	K	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	6 (10%)
23	CLA	C	513	-	65,73,73	1.51	10 (15%)	76,113,113	1.56	8 (10%)
23	CLA	c	507	37	65,73,73	1.54	11 (16%)	76,113,113	1.49	9 (11%)
25	BCR	b	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.40	10 (17%)
26	PL9	a	410	-	55,55,55	1.08	4 (7%)	68,69,69	1.73	12 (17%)
23	CLA	C	510	-	65,73,73	1.56	10 (15%)	76,113,113	1.34	7 (9%)
23	CLA	b	612	-	65,73,73	1.53	9 (13%)	76,113,113	1.55	12 (15%)
23	CLA	B	605	-	65,73,73	1.49	8 (12%)	76,113,113	1.41	13 (17%)
23	CLA	C	509	-	65,73,73	1.50	9 (13%)	76,113,113	1.31	7 (9%)
23	CLA	B	603	-	65,73,73	1.51	11 (16%)	76,113,113	1.31	11 (14%)
35	HEM	E	101	6,5	41,50,50	1.45	3 (7%)	45,82,82	1.37	8 (17%)
36	HEC	V	201	16	32,50,50	2.17	5 (15%)	24,82,82	1.57	6 (25%)
23	CLA	A	408	-	54,62,73	2.00	9 (16%)	62,99,113	1.65	13 (20%)
23	CLA	B	615	-	65,73,73	1.70	13 (20%)	76,113,113	1.35	7 (9%)
23	CLA	b	608	37	65,73,73	1.53	10 (15%)	76,113,113	1.33	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	a	408	-	65,73,73	1.65	9 (13%)	76,113,113	1.43	11 (14%)
28	SQD	A	414	-	38,38,54	1.04	3 (7%)	40,40,65	1.30	3 (7%)
23	CLA	b	610	-	65,73,73	1.71	10 (15%)	76,113,113	1.16	6 (7%)
25	BCR	b	620	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	9 (16%)
27	LMG	m	101	-	51,51,55	0.82	1 (1%)	59,59,63	1.54	12 (20%)
23	CLA	B	602	-	65,73,73	1.88	11 (16%)	76,113,113	1.46	12 (15%)
23	CLA	c	503	-	65,73,73	1.57	8 (12%)	76,113,113	1.65	11 (14%)
30	DGD	c	516	-	63,63,67	1.28	6 (9%)	77,77,81	1.39	12 (15%)
23	CLA	b	606	-	65,73,73	1.44	9 (13%)	76,113,113	1.58	15 (19%)
23	CLA	c	512	-	65,73,73	1.57	10 (15%)	76,113,113	1.42	11 (14%)
23	CLA	b	617	-	60,68,73	1.48	7 (11%)	70,107,113	1.48	11 (15%)

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
23	CLA	B	607	37	1/1/20/20	12/37/115/115	-
23	CLA	h	101	37	1/1/20/20	17/37/115/115	-
27	LMG	D	406	-	-	14/46/66/70	0/1/1/1
25	BCR	k	101	-	-	11/29/63/63	0/2/2/2
29	LHG	D	407	-	-	25/53/53/53	-
27	LMG	B	621	-	-	11/22/22/70	-
23	CLA	B	606	-	1/1/20/20	12/37/115/115	-
25	BCR	B	619	-	-	7/29/63/63	0/2/2/2
30	DGD	C	515	-	-	20/51/91/95	0/2/2/2
23	CLA	c	502	-	-	5/37/115/115	-
23	CLA	c	505	-	1/1/20/20	10/37/115/115	-
23	CLA	b	604	-	1/1/20/20	9/37/115/115	-
23	CLA	B	609	-	-	3/37/115/115	-
27	LMG	b	622	-	-	26/50/70/70	0/1/1/1
27	LMG	c	523	-	-	27/44/64/70	0/1/1/1
25	BCR	k	102	-	-	4/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/19/20	8/31/109/115	-
27	LMG	c	521	-	-	19/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	614	-	1/1/20/20	13/37/115/115	-
23	CLA	B	613	-	1/1/20/20	8/37/115/115	-
23	CLA	A	404	-	1/1/20/20	4/37/115/115	-
26	PL9	D	405	-	-	12/53/73/73	0/1/1/1
23	CLA	b	614	-	1/1/20/20	4/37/115/115	-
24	PHO	A	406	-	-	7/37/103/103	0/5/6/6
25	BCR	c	515	-	-	10/29/63/63	0/2/2/2
23	CLA	C	503	-	1/1/20/20	5/37/115/115	-
23	CLA	c	511	3	1/1/20/20	10/37/115/115	-
23	CLA	d	402	-	-	9/37/115/115	-
30	DGD	A	415	-	-	25/55/95/95	0/2/2/2
23	CLA	D	401	37	-	5/37/115/115	-
23	CLA	C	501	-	1/1/20/20	6/37/115/115	-
27	LMG	C	518	-	-	15/43/63/70	0/1/1/1
25	BCR	T	101	-	-	6/29/63/63	0/2/2/2
27	LMG	c	519	-	-	12/31/51/70	0/1/1/1
27	LMG	d	409	-	-	13/39/59/70	0/1/1/1
23	CLA	c	501	-	1/1/20/20	7/37/115/115	-
28	SQD	f	101	-	-	13/36/56/69	0/1/1/1
28	SQD	B	624	-	-	24/49/69/69	0/1/1/1
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
29	LHG	B	622	-	-	20/53/53/53	-
23	CLA	b	616	-	1/1/20/20	6/37/115/115	-
25	BCR	t	101	-	-	5/29/63/63	0/2/2/2
24	PHO	a	407	-	-	6/37/103/103	0/5/6/6
23	CLA	C	508	-	1/1/20/20	5/37/115/115	-
23	CLA	c	508	-	-	12/36/114/115	-
23	CLA	a	406	37	-	11/37/115/115	-
23	CLA	c	510	-	1/1/20/20	15/37/115/115	-
25	BCR	C	514	-	-	2/29/63/63	0/2/2/2
29	LHG	A	413	-	-	27/53/53/53	-
30	DGD	c	517	-	-	19/51/91/95	0/2/2/2
26	PL9	d	405	-	-	17/53/73/73	0/1/1/1
23	CLA	C	505	-	1/1/20/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	K	101	-	-	7/29/63/63	0/2/2/2
23	CLA	b	607	-	1/1/20/20	13/37/115/115	-
28	SQD	F	101	-	-	16/28/48/69	0/1/1/1
27	LMG	M	101	-	-	19/46/66/70	0/1/1/1
27	LMG	D	409	-	-	13/33/33/70	-
23	CLA	C	511	3	1/1/20/20	7/37/115/115	-
24	PHO	d	401	-	-	5/37/103/103	0/5/6/6
30	DGD	a	414	-	-	25/45/45/95	-
23	CLA	d	403	-	1/1/20/20	7/37/115/115	-
23	CLA	C	504	37	1/1/18/20	8/30/108/115	-
28	SQD	b	601	-	-	18/44/64/69	0/1/1/1
23	CLA	B	608	-	-	0/37/115/115	-
23	CLA	c	513	-	1/1/20/20	7/37/115/115	-
25	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
25	BCR	c	514	-	-	16/29/63/63	0/2/2/2
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
25	BCR	d	404	-	-	7/29/63/63	0/2/2/2
36	HEC	v	201	16	-	2/10/54/54	-
25	BCR	x	101	-	-	6/29/63/63	0/2/2/2
29	LHG	d	406	-	-	23/53/53/53	-
26	PL9	A	410	-	-	27/53/73/73	0/1/1/1
23	CLA	b	603	-	1/1/20/20	10/37/115/115	-
28	SQD	a	413	-	-	19/37/37/69	-
29	LHG	D	408	-	-	21/51/51/53	-
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	b	605	-	1/1/20/20	13/37/115/115	-
23	CLA	B	601	37	1/1/20/20	13/37/115/115	-
23	CLA	B	612	-	1/1/20/20	6/37/115/115	-
23	CLA	C	512	-	1/1/20/20	7/37/115/115	-
29	LHG	d	407	-	-	26/53/53/53	-
23	CLA	b	613	-	1/1/20/20	11/37/115/115	-
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
28	SQD	a	412	-	-	25/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	H	102	-	-	13/51/91/95	0/2/2/2
30	DGD	C	517	-	-	15/51/91/95	0/2/2/2
25	BCR	A	409	-	-	12/29/63/63	0/2/2/2
27	LMG	A	411	-	-	19/43/63/70	0/1/1/1
25	BCR	B	618	-	-	6/29/63/63	0/2/2/2
23	CLA	b	615	-	1/1/20/20	16/37/115/115	-
23	CLA	B	611	-	1/1/20/20	8/37/115/115	-
29	LHG	B	623	-	-	21/53/53/53	-
23	CLA	C	502	-	-	9/37/115/115	-
25	BCR	a	409	-	-	6/29/63/63	0/2/2/2
29	LHG	l	101	-	-	19/53/53/53	-
23	CLA	C	507	37	1/1/20/20	9/37/115/115	-
23	CLA	a	411	37	1/1/20/20	5/37/115/115	-
25	BCR	D	404	-	-	5/29/63/63	0/2/2/2
30	DGD	h	102	-	-	17/51/91/95	0/2/2/2
23	CLA	c	504	37	1/1/19/20	6/31/109/115	-
23	CLA	b	611	37	1/1/20/20	10/37/115/115	-
23	CLA	B	604	-	1/1/20/20	11/37/115/115	-
27	LMG	b	623	-	-	9/17/17/70	-
23	CLA	D	402	-	-	5/37/115/115	-
29	LHG	d	408	-	-	12/43/43/53	-
30	DGD	C	516	-	-	21/51/91/95	0/2/2/2
23	CLA	C	506	-	-	11/37/115/115	-
35	HEM	e	102	6,5	-	5/12/54/54	-
23	CLA	c	509	-	1/1/20/20	15/37/115/115	-
23	CLA	A	405	37	1/1/20/20	7/37/115/115	-
23	CLA	D	403	-	-	13/37/115/115	-
28	SQD	A	412	-	-	21/47/67/69	0/1/1/1
29	LHG	e	101	-	-	28/46/46/53	-
23	CLA	B	610	37	1/1/20/20	8/37/115/115	-
23	CLA	b	609	-	1/1/20/20	6/37/115/115	-
23	CLA	c	506	-	1/1/20/20	16/37/115/115	-
23	CLA	a	405	-	1/1/20/20	3/37/115/115	-
25	BCR	K	102	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	513	-	1/1/20/20	10/37/115/115	-
23	CLA	c	507	37	1/1/20/20	10/37/115/115	-
25	BCR	b	618	-	-	6/29/63/63	0/2/2/2
26	PL9	a	410	-	-	25/53/73/73	0/1/1/1
23	CLA	C	510	-	1/1/20/20	11/37/115/115	-
23	CLA	b	612	-	-	7/37/115/115	-
23	CLA	B	605	-	1/1/20/20	10/37/115/115	-
23	CLA	C	509	-	1/1/20/20	9/37/115/115	-
23	CLA	B	603	-	1/1/20/20	14/37/115/115	-
35	HEM	E	101	6,5	-	2/12/54/54	-
36	HEC	V	201	16	-	2/10/54/54	-
23	CLA	A	408	-	1/1/17/20	3/24/102/115	-
23	CLA	B	615	-	1/1/20/20	10/37/115/115	-
23	CLA	b	608	37	1/1/20/20	13/37/115/115	-
23	CLA	a	408	-	1/1/20/20	14/37/115/115	-
28	SQD	A	414	-	-	18/39/39/69	-
23	CLA	b	610	-	1/1/20/20	10/37/115/115	-
25	BCR	b	620	-	-	4/29/63/63	0/2/2/2
27	LMG	m	101	-	-	19/46/66/70	0/1/1/1
23	CLA	B	602	-	1/1/20/20	5/37/115/115	-
23	CLA	c	503	-	1/1/20/20	7/37/115/115	-
30	DGD	c	516	-	-	27/51/91/95	0/2/2/2
23	CLA	b	606	-	1/1/20/20	9/37/115/115	-
23	CLA	c	512	-	1/1/20/20	20/37/115/115	-
23	CLA	b	617	-	1/1/19/20	10/31/109/115	-

The worst 5 of 918 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-ND	-11.97	1.82	2.05
23	B	602	CLA	C4B-NB	9.93	1.44	1.35
23	b	614	CLA	C4B-NB	9.72	1.43	1.35
23	B	601	CLA	C4B-NB	8.67	1.42	1.35
23	C	501	CLA	C4B-NB	8.46	1.42	1.35

The worst 5 of 1303 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C4A-NA-C1A	9.88	111.15	106.71
23	C	511	CLA	C4A-NA-C1A	9.86	111.14	106.71
23	d	402	CLA	C4A-NA-C1A	9.84	111.13	106.71
23	C	503	CLA	C4A-NA-C1A	9.73	111.08	106.71
23	a	411	CLA	C4A-NA-C1A	9.62	111.03	106.71

5 of 58 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND

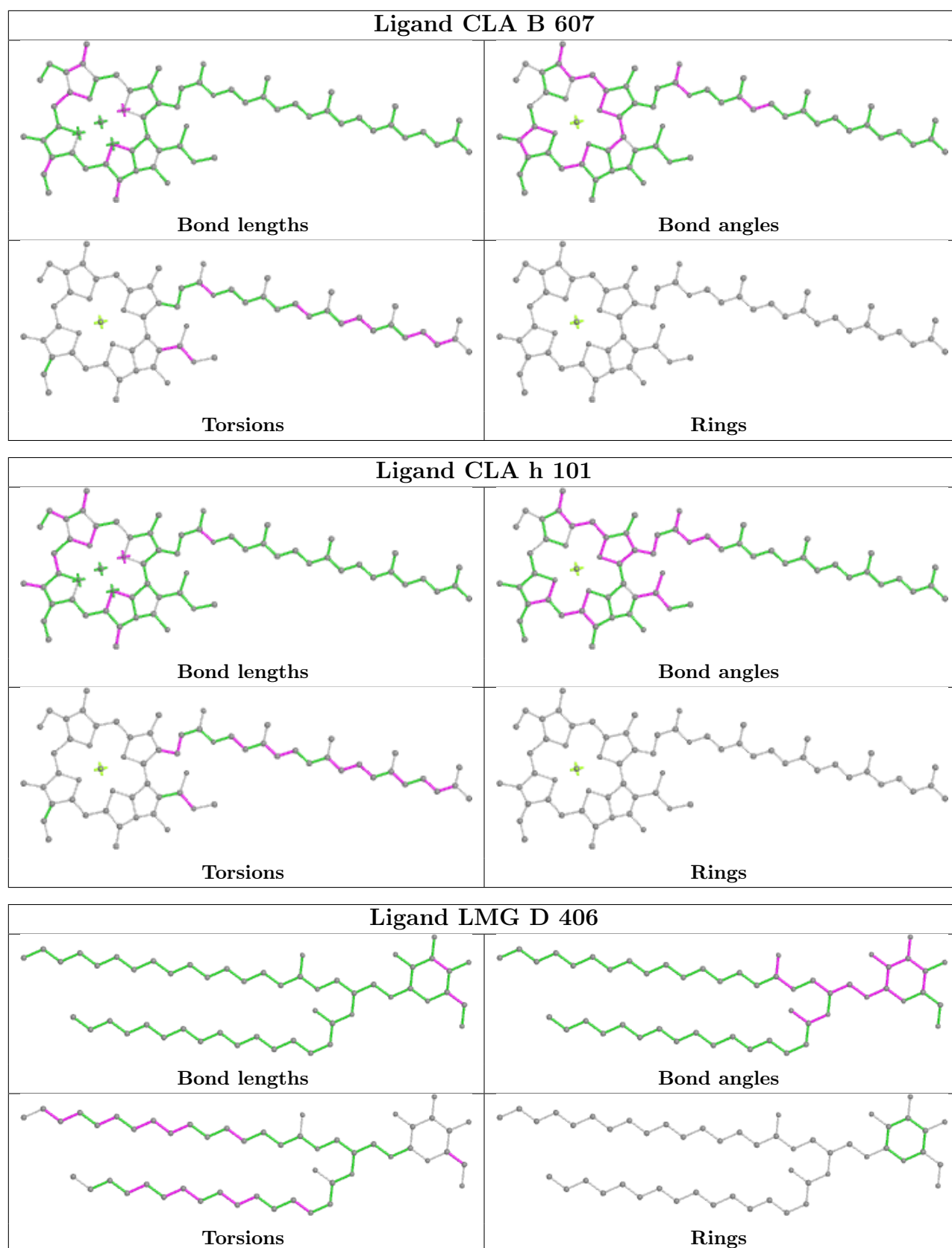
5 of 1707 torsion outliers are listed below:

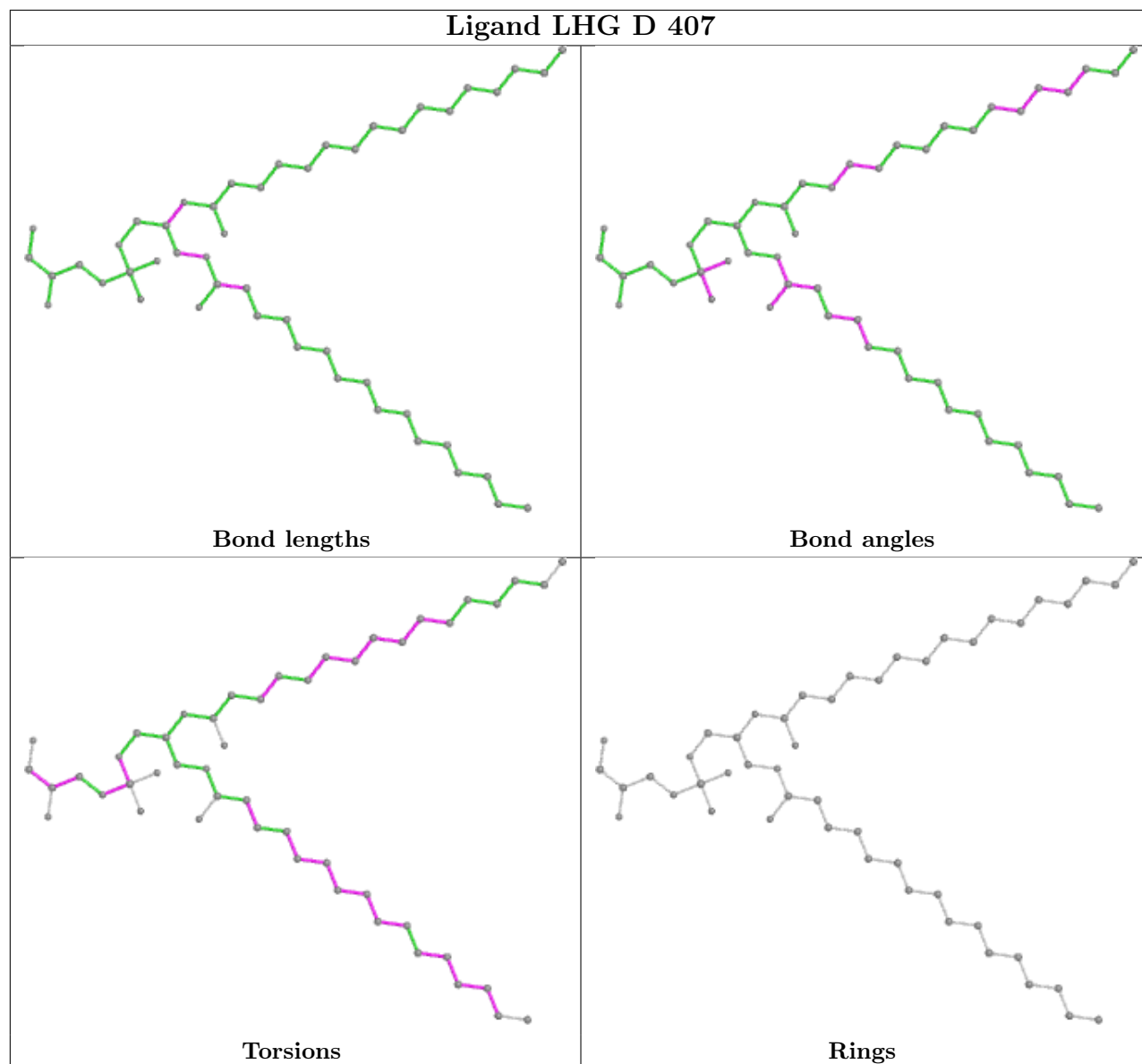
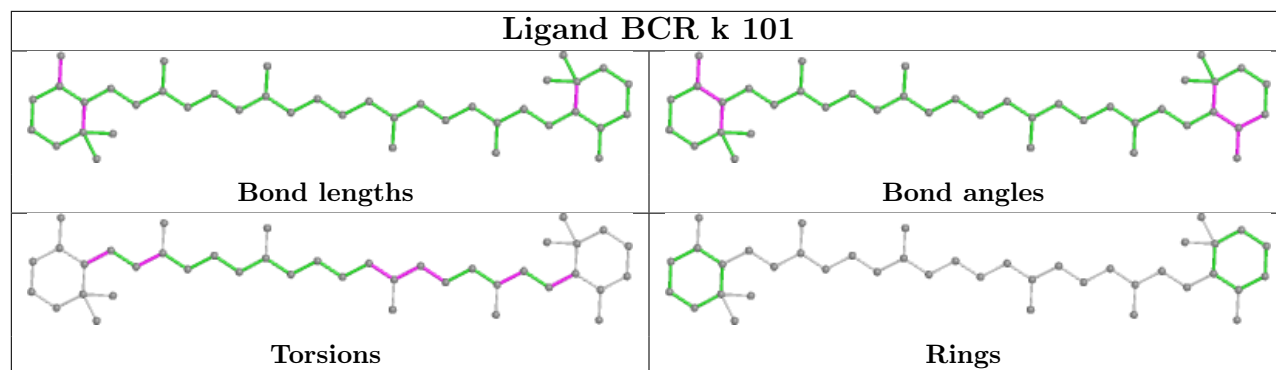
Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6

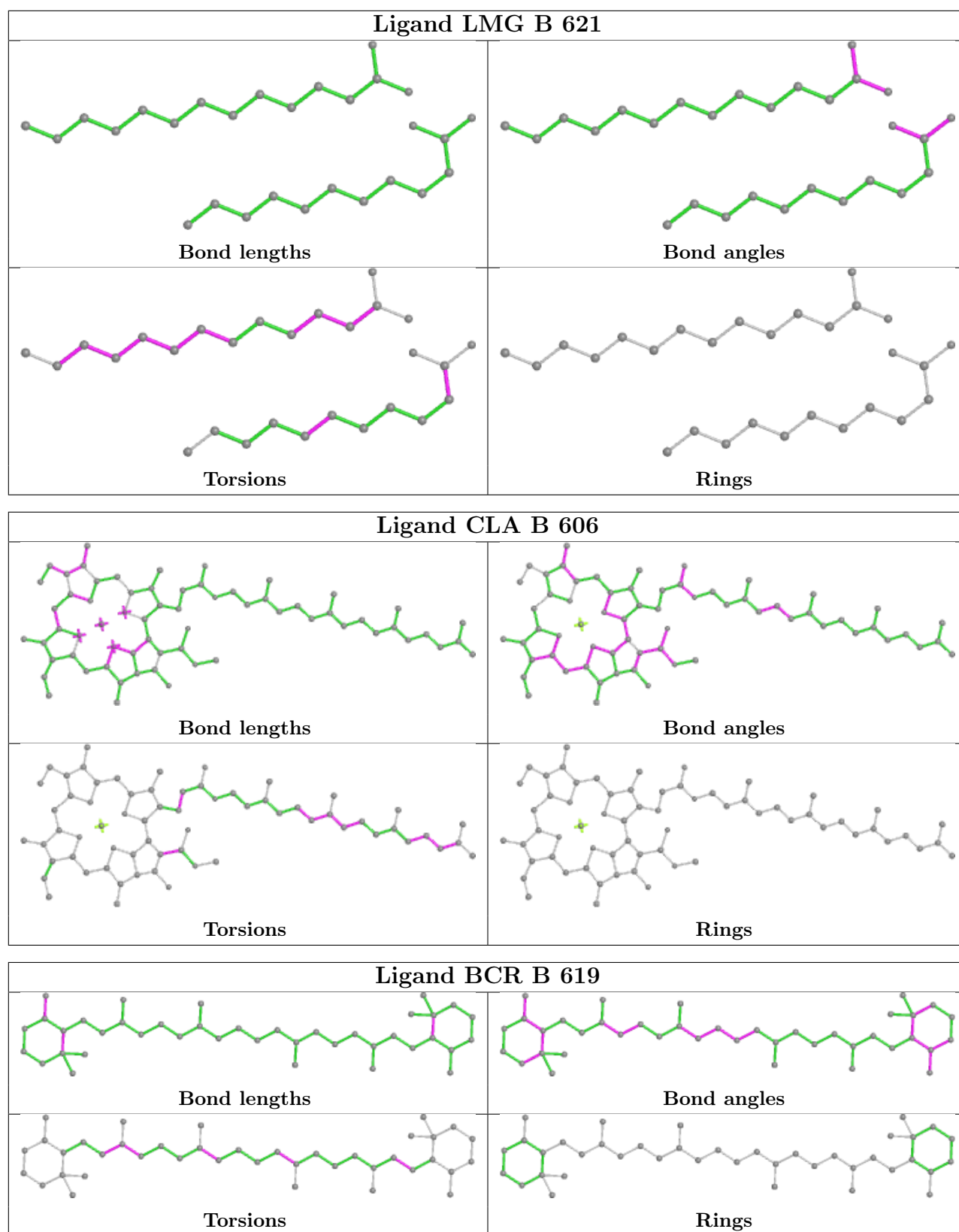
There are no ring outliers.

No monomer is involved in short contacts.

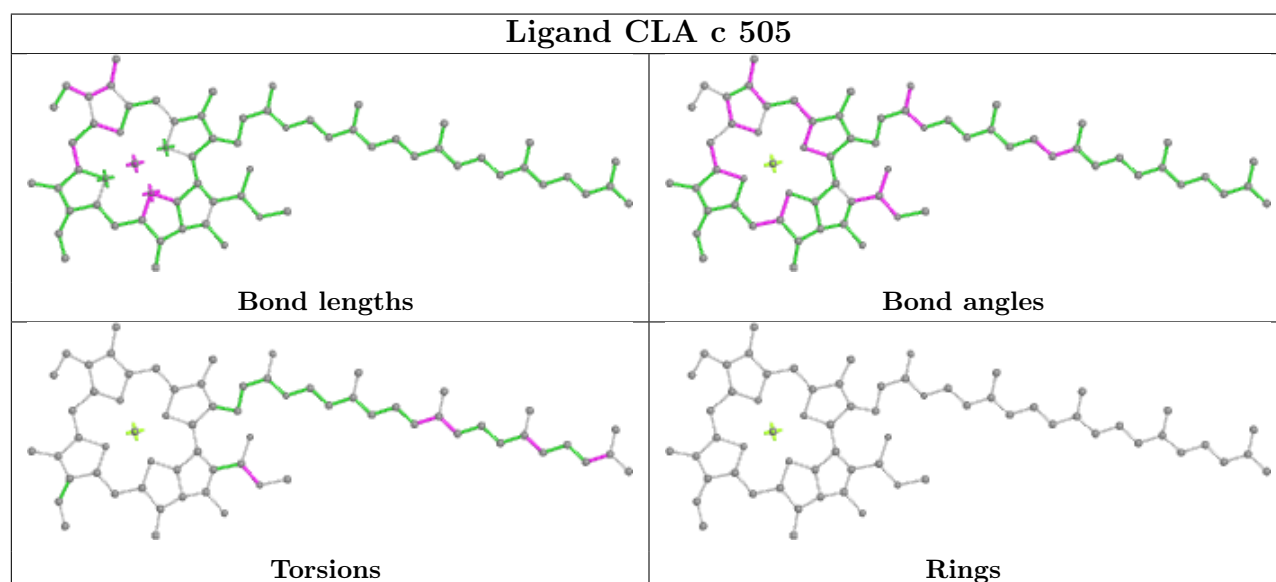
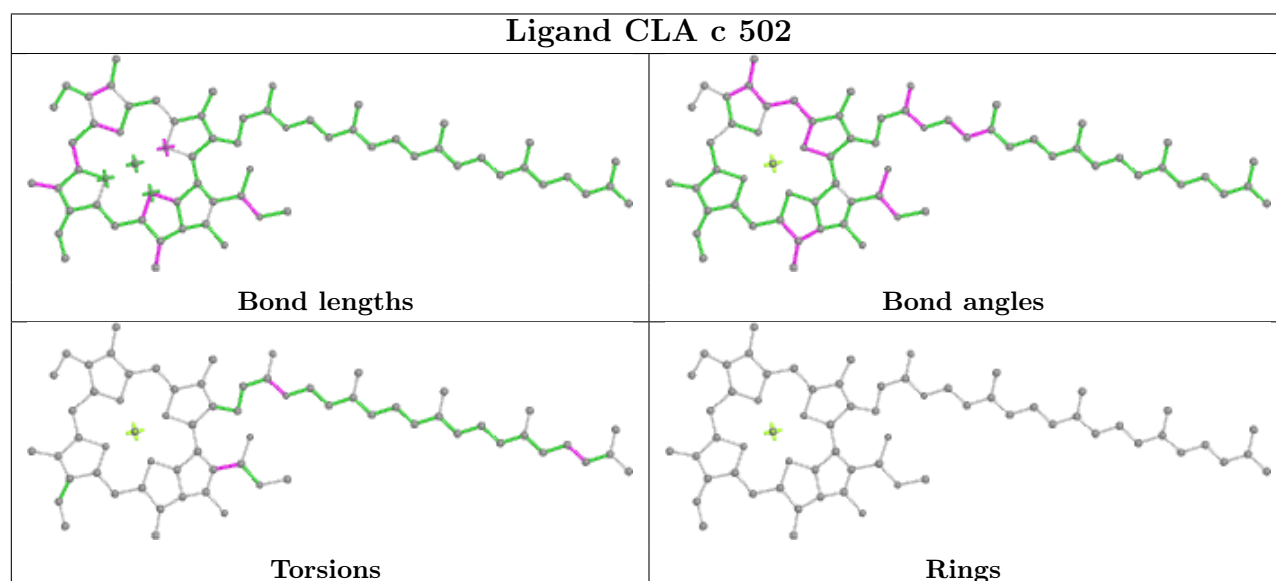
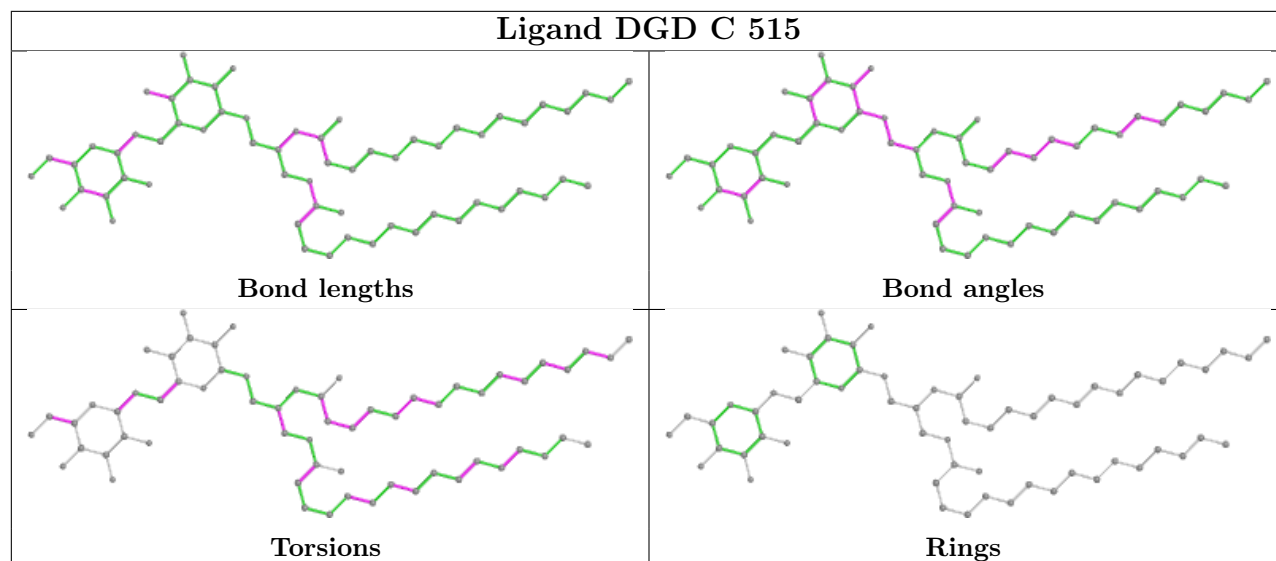
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

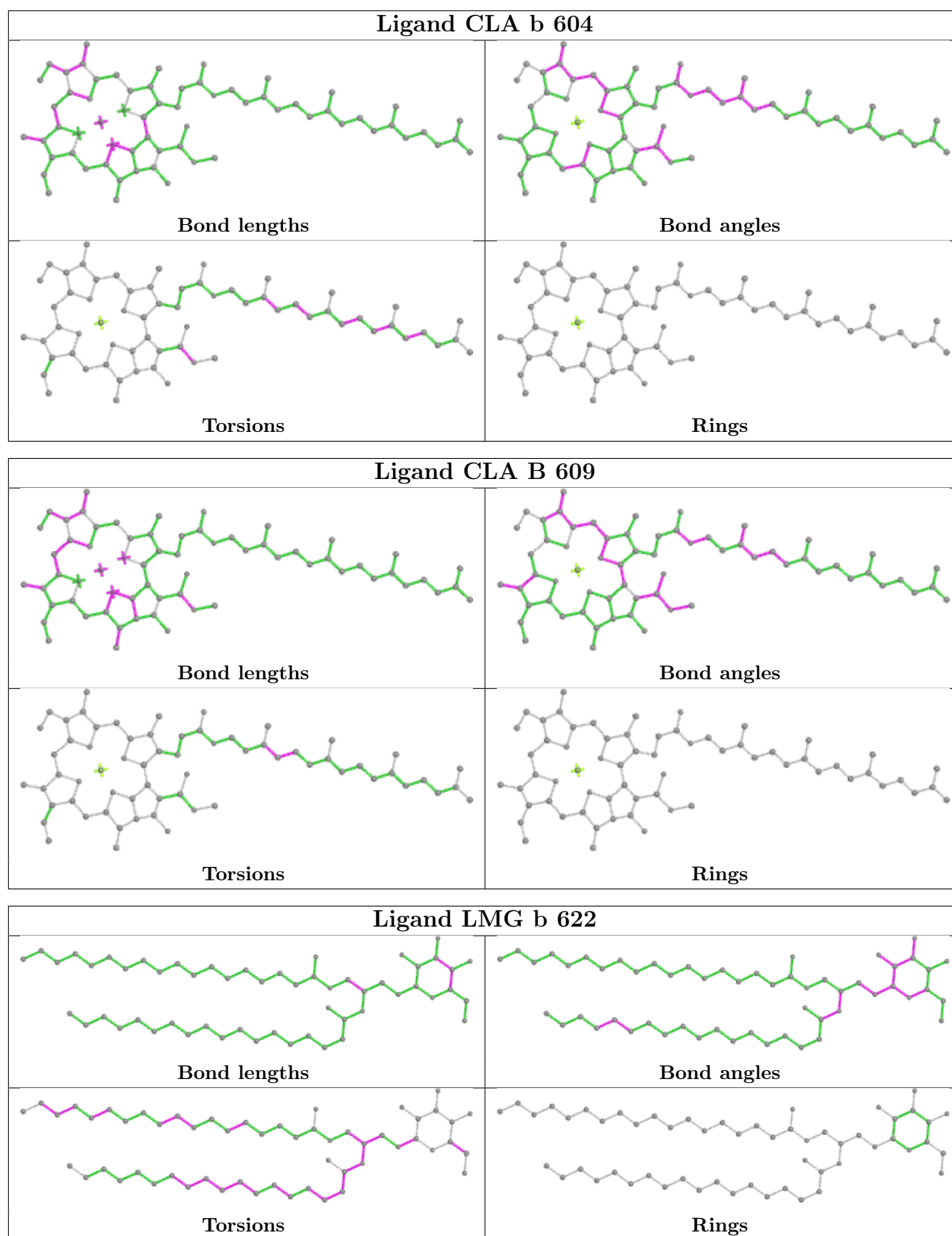


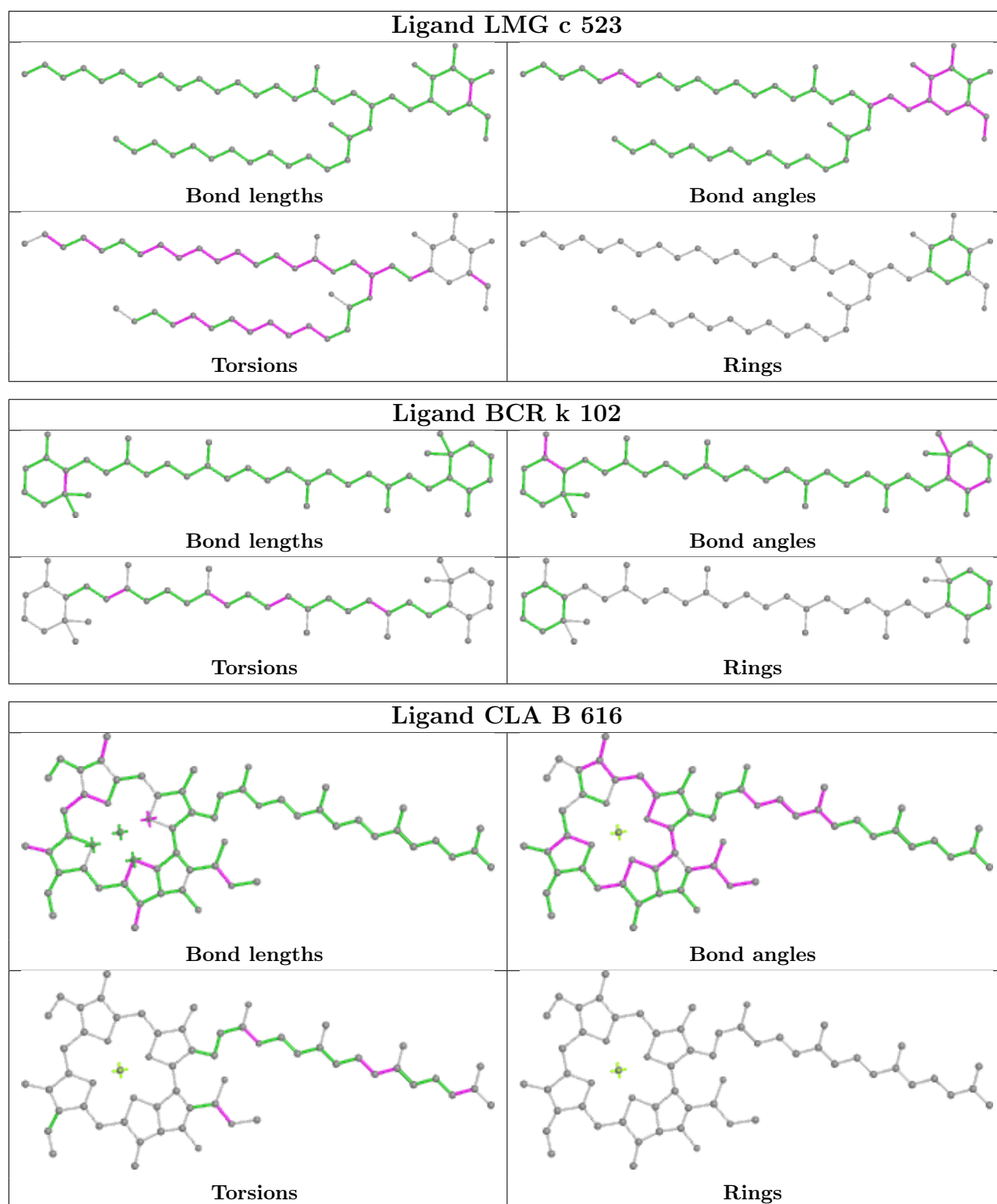


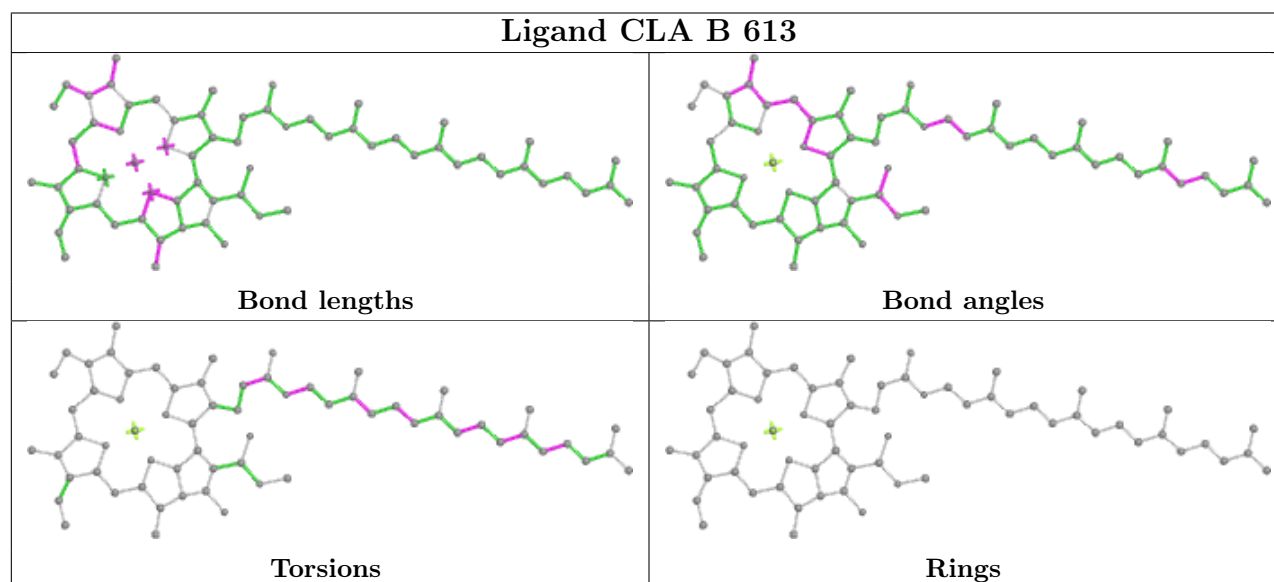
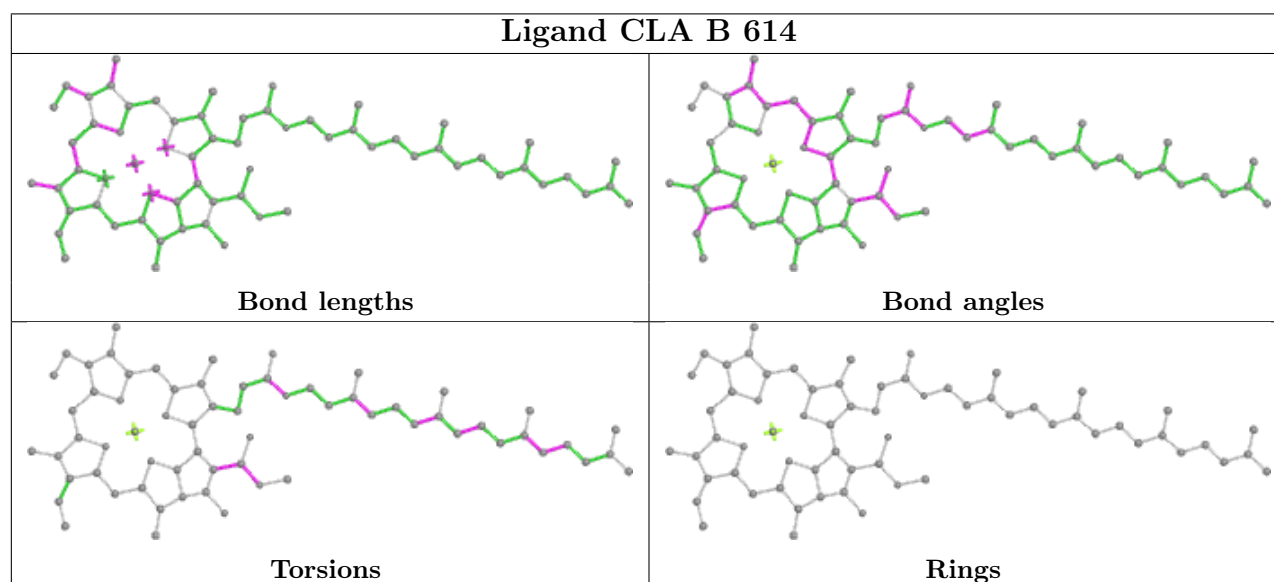
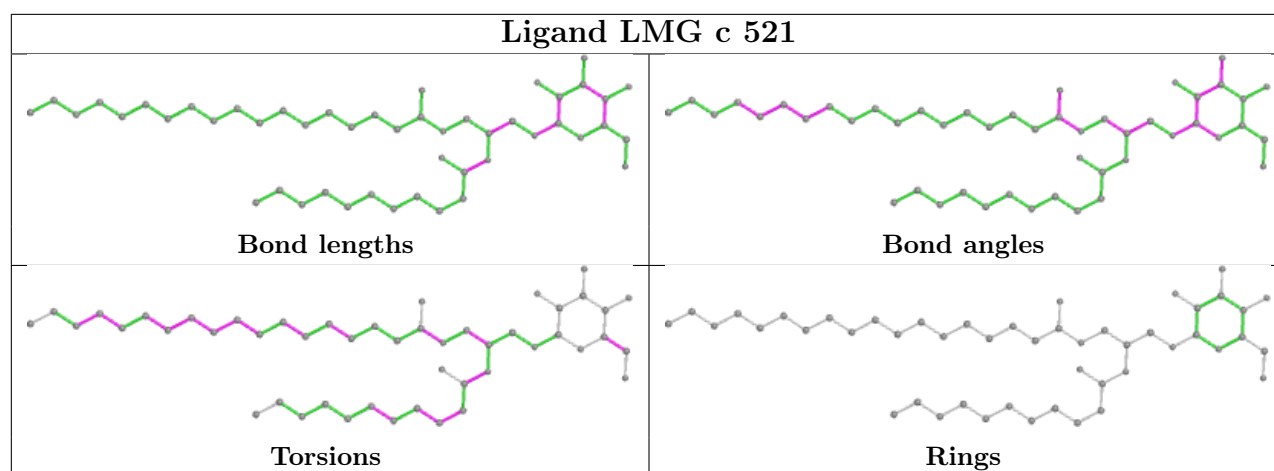


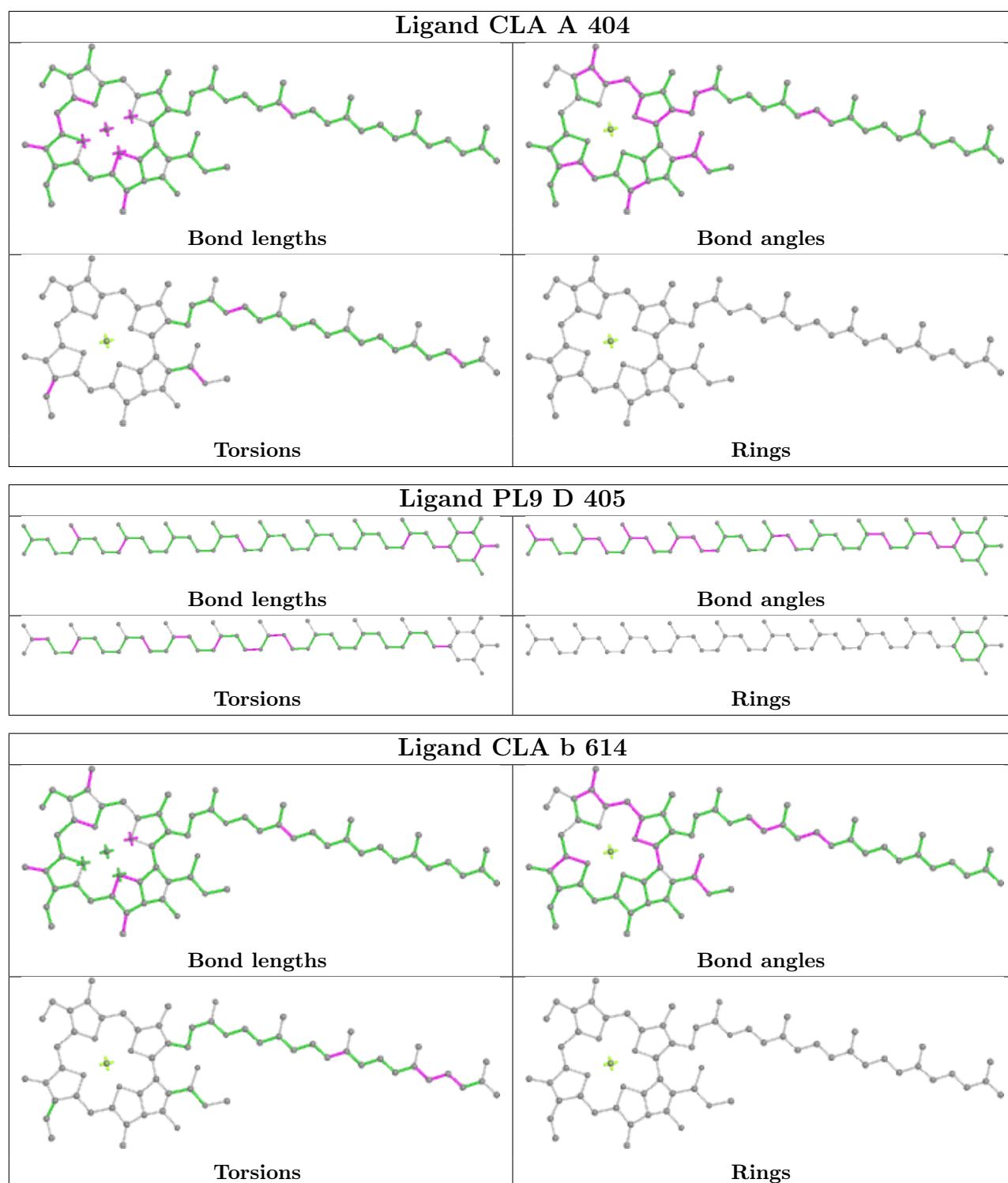


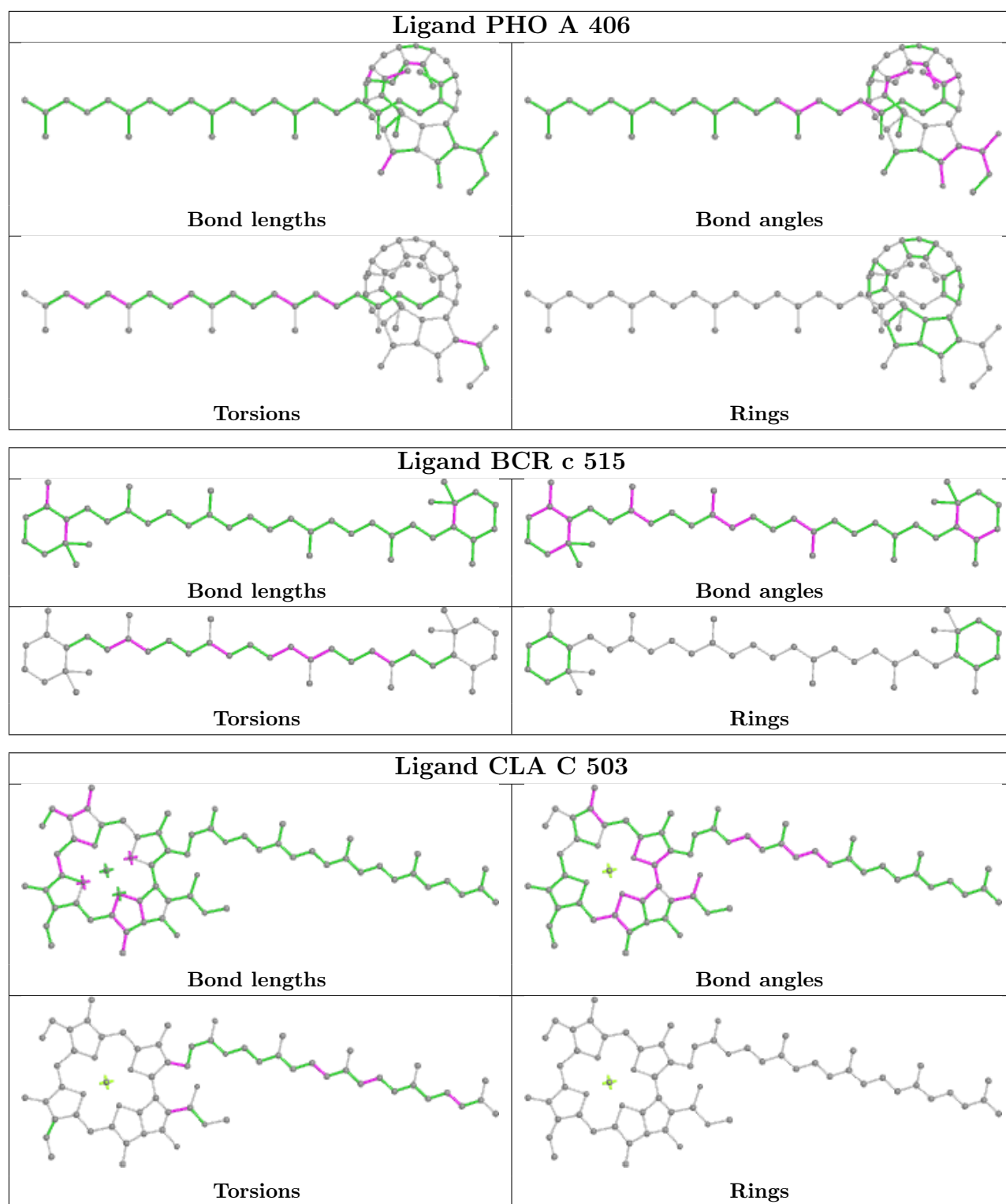


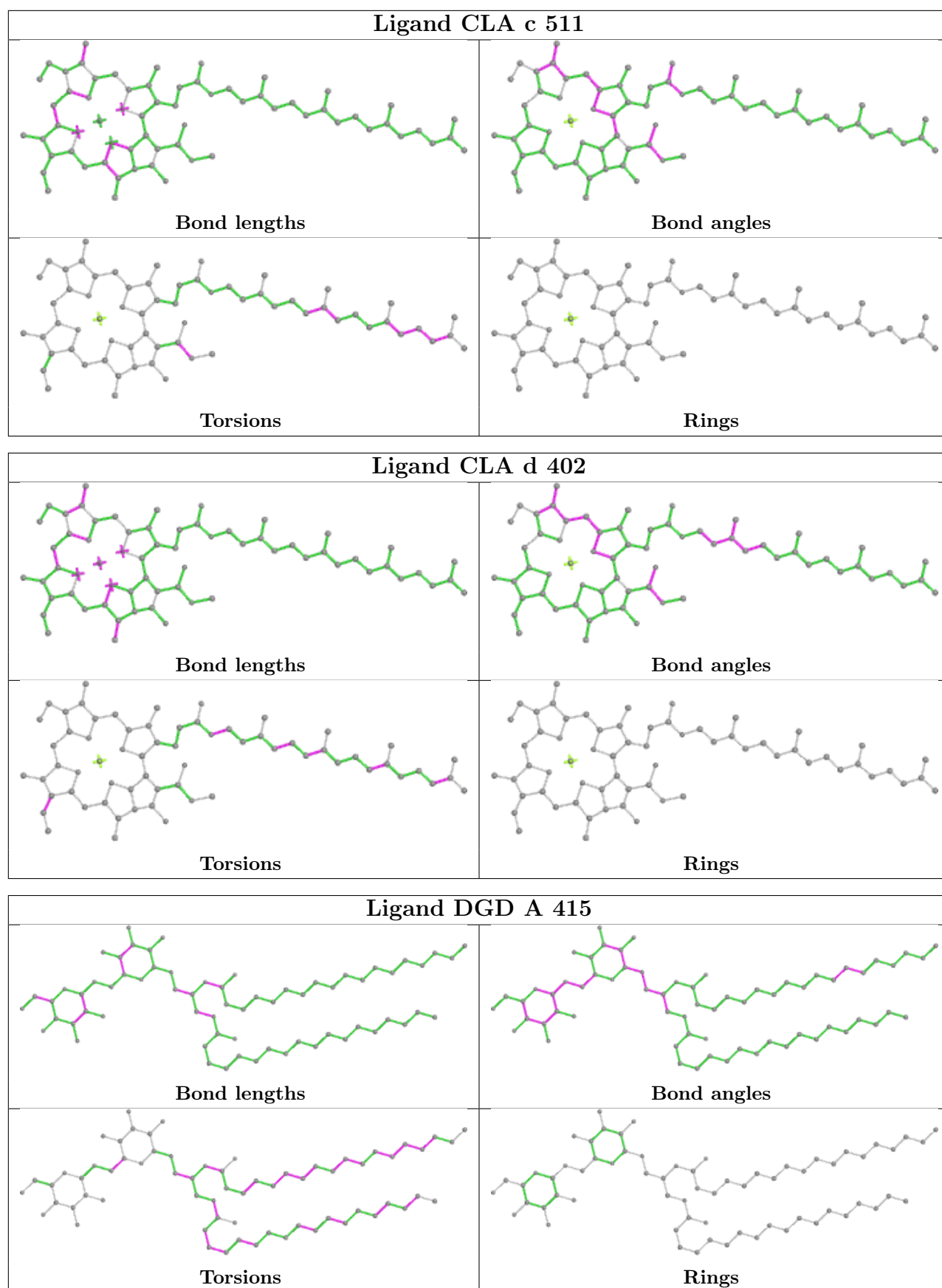


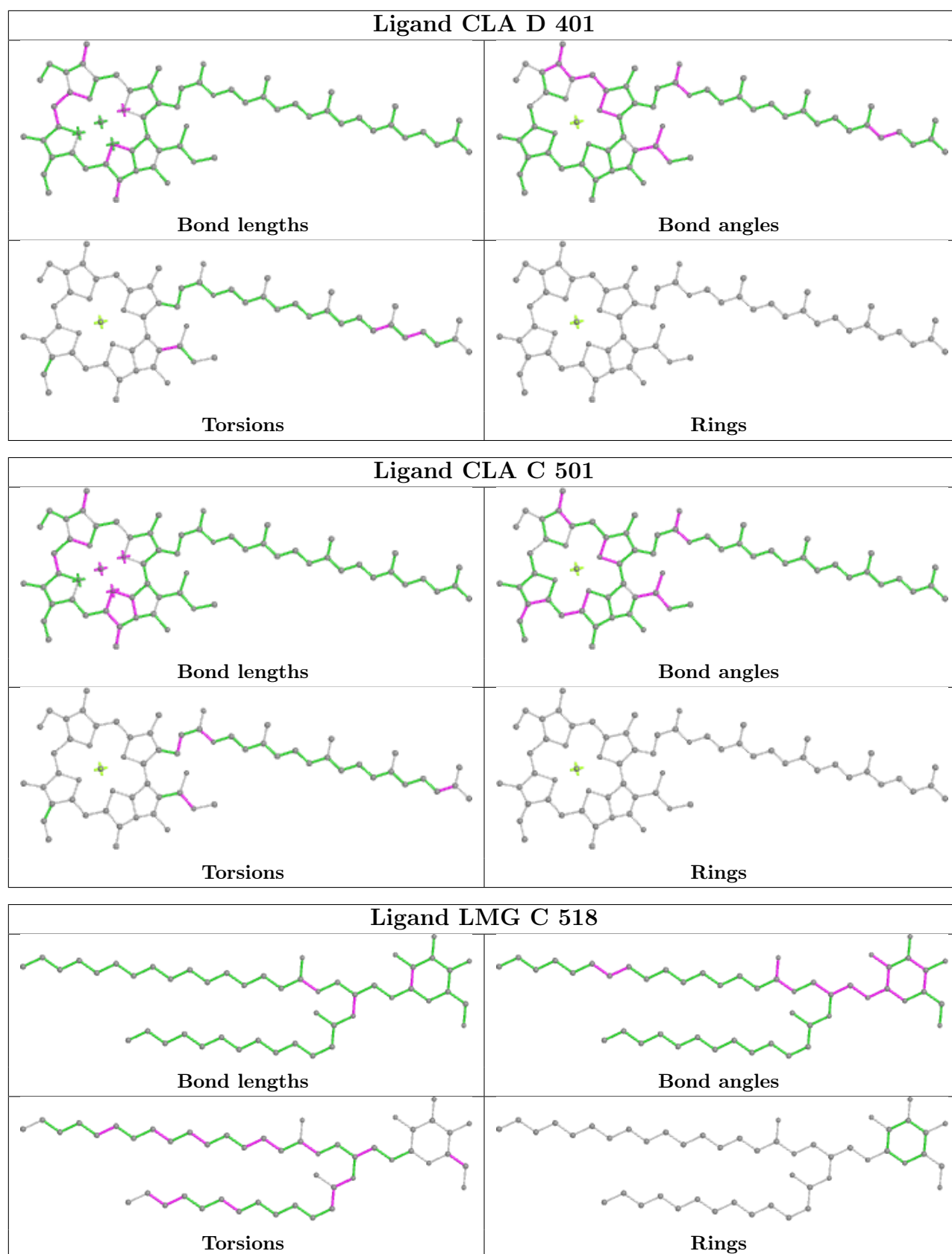




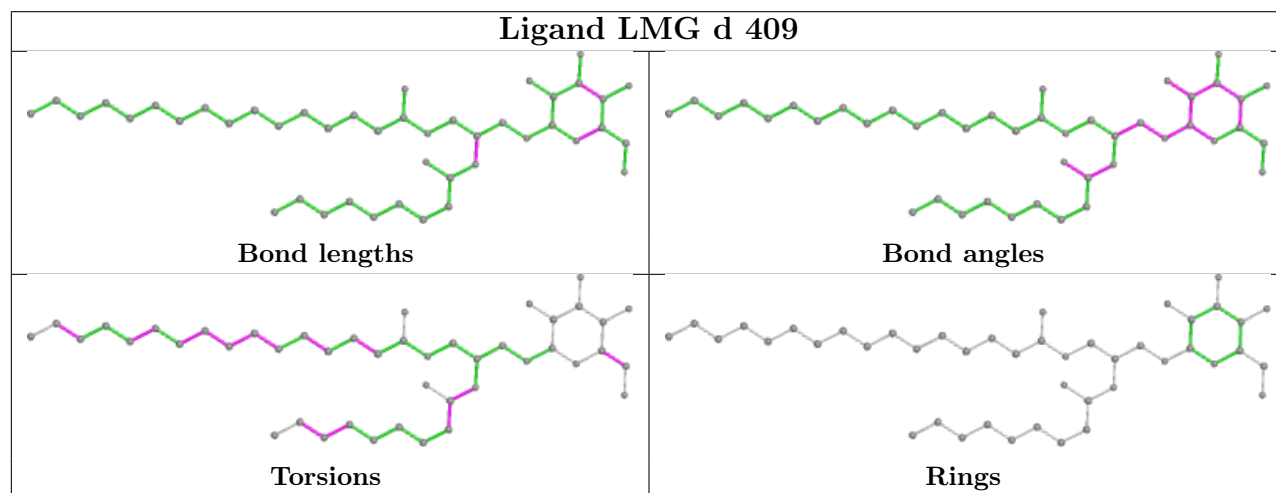
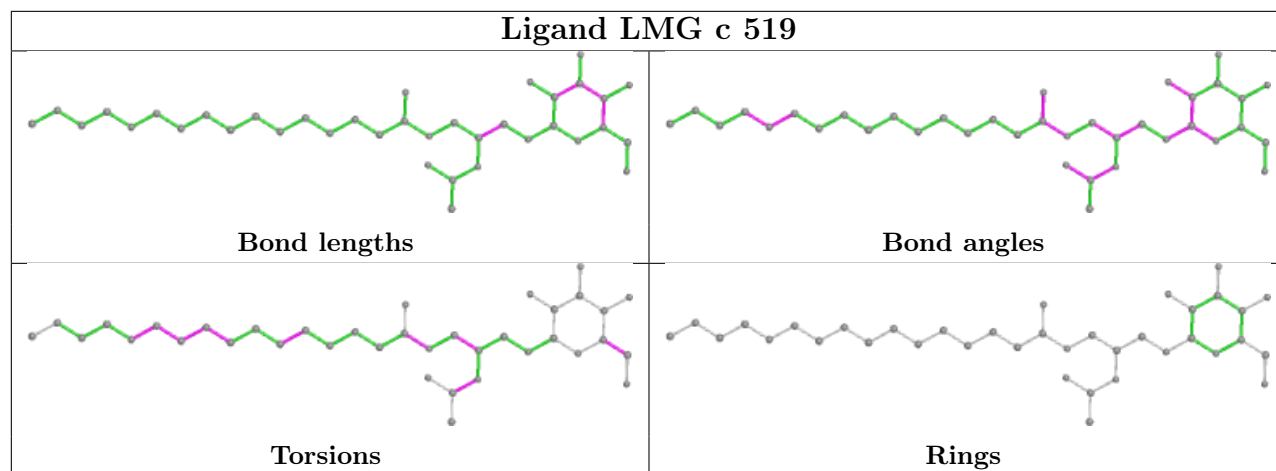
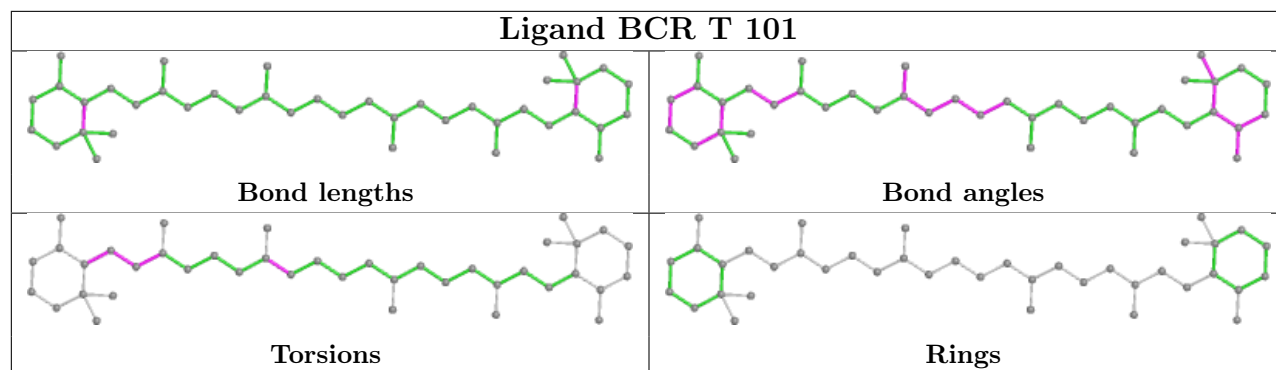


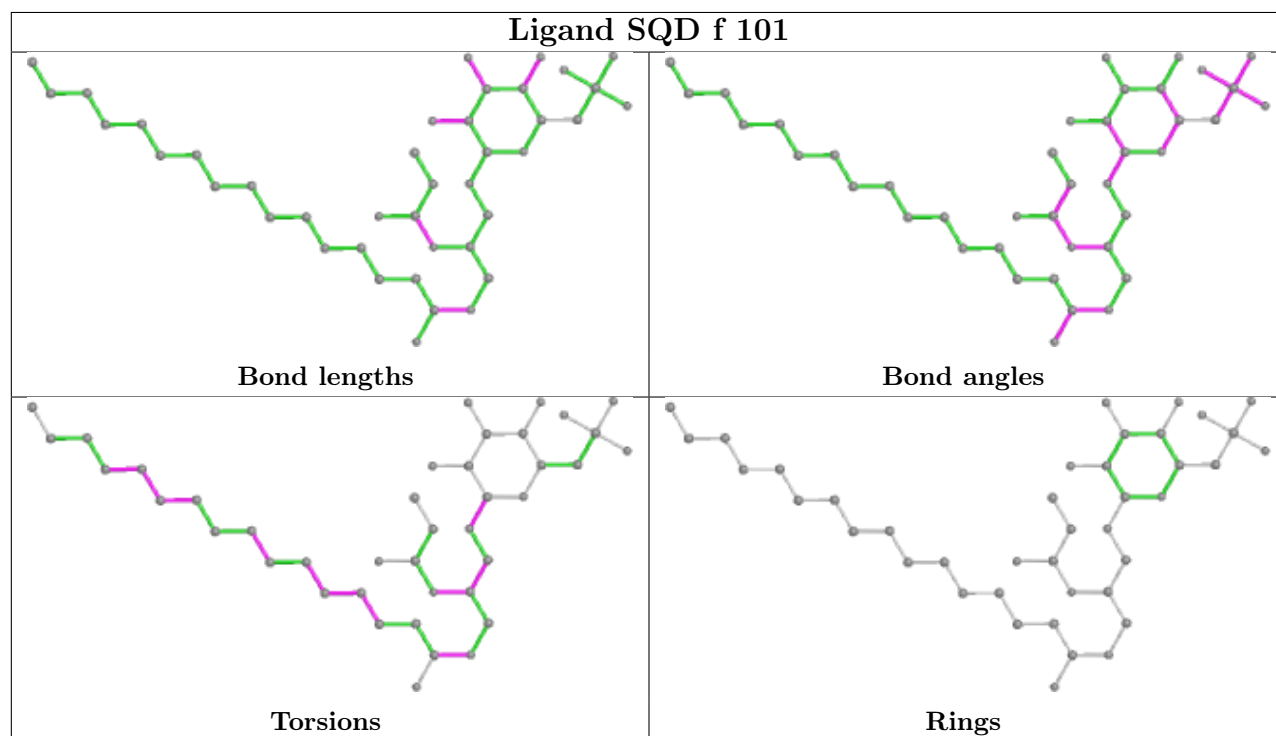
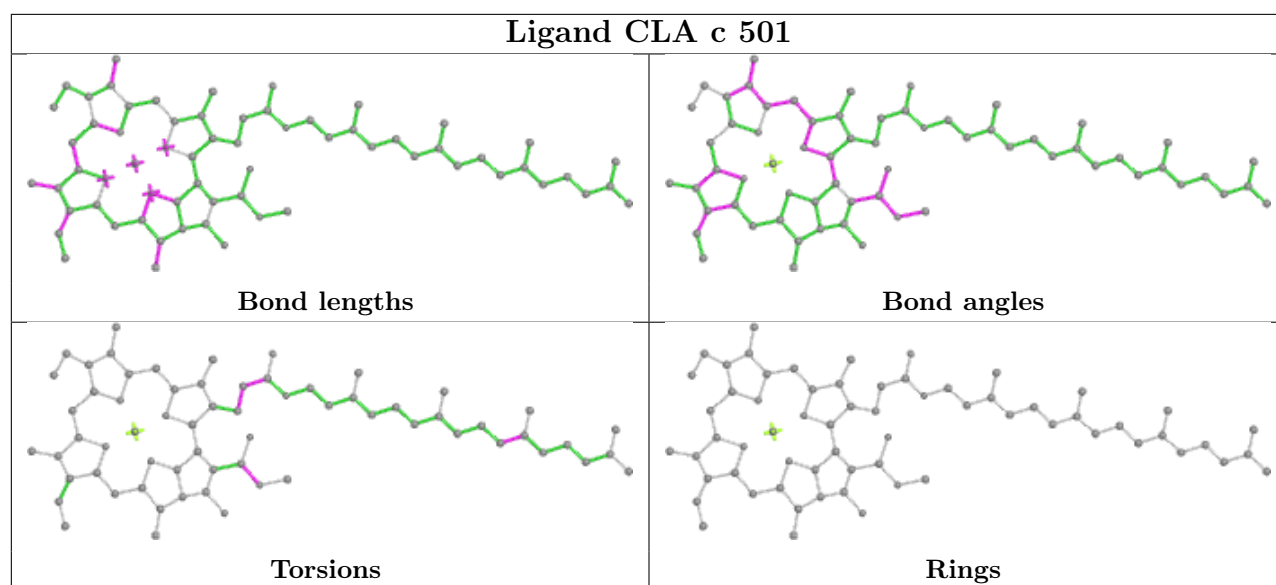


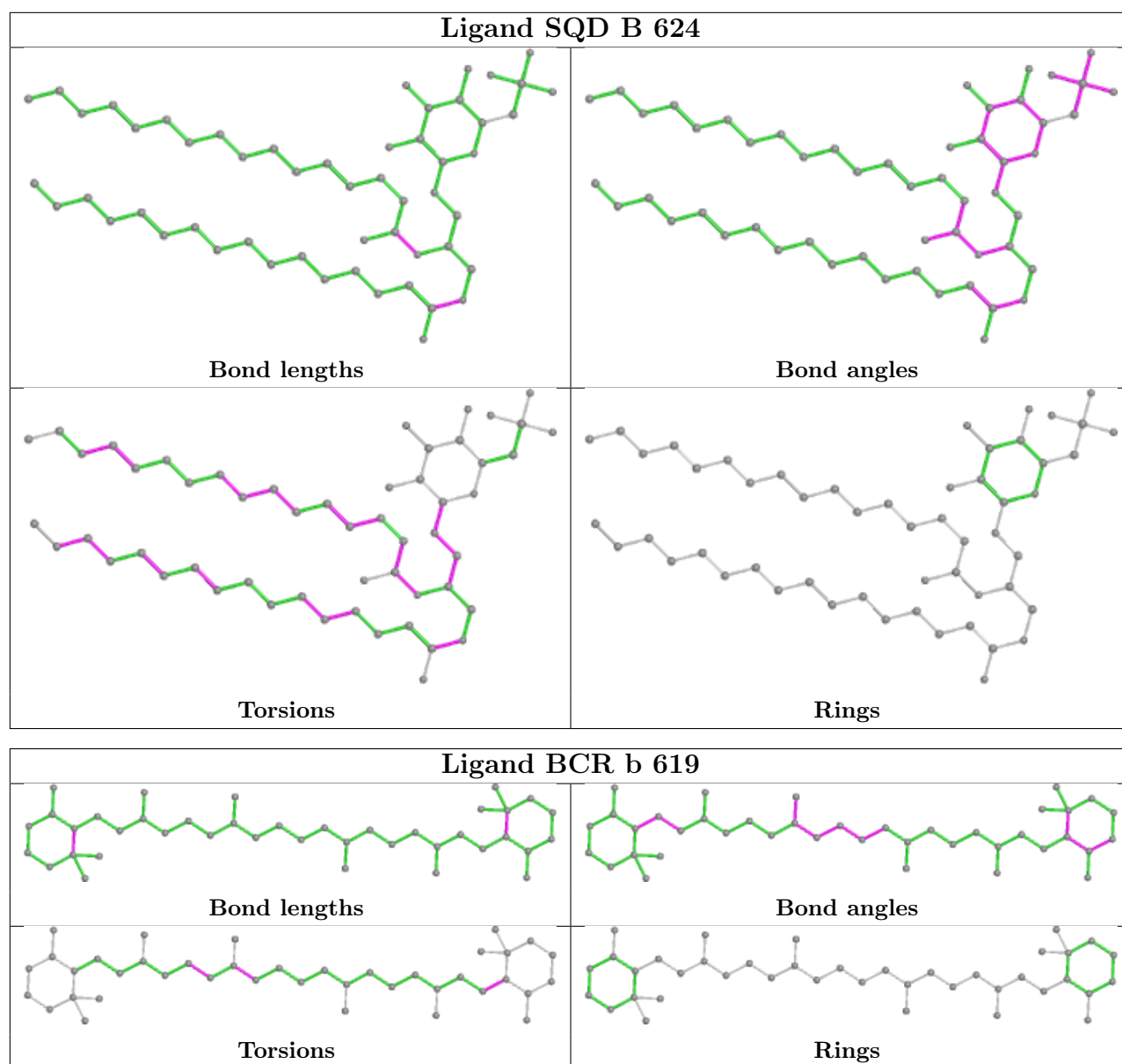


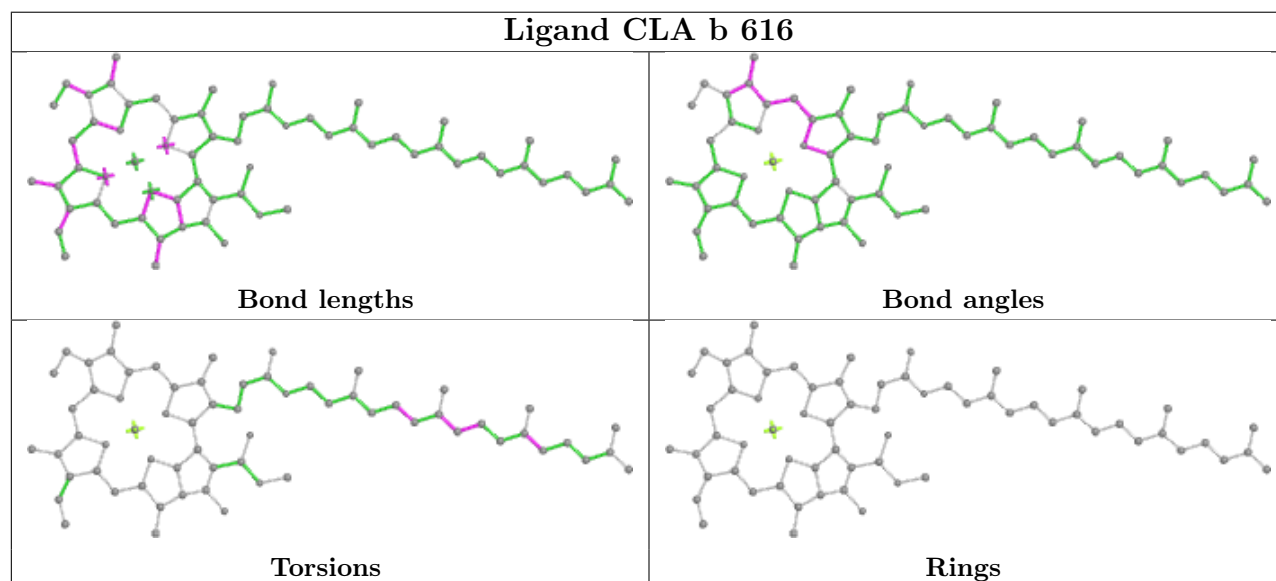
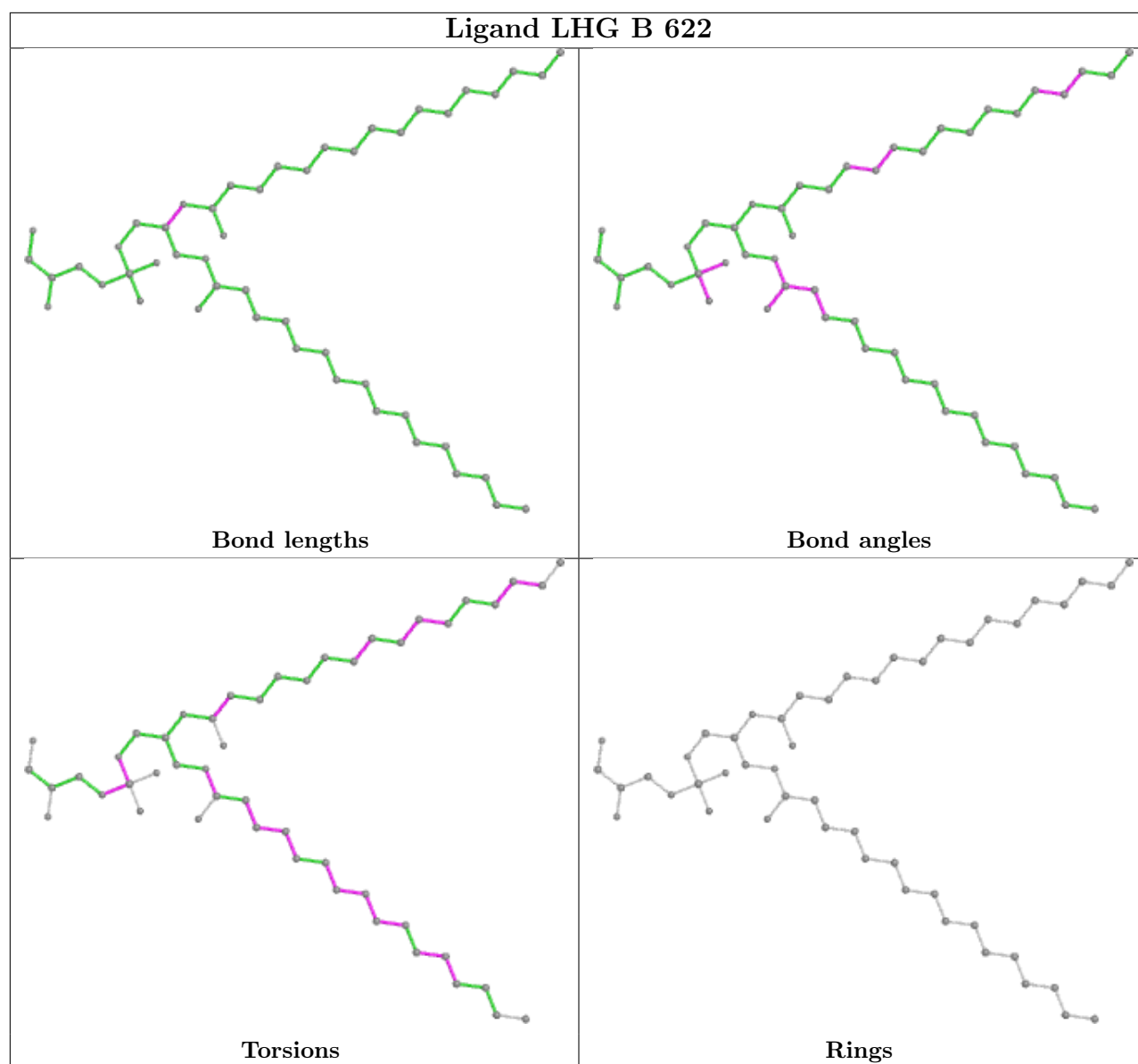


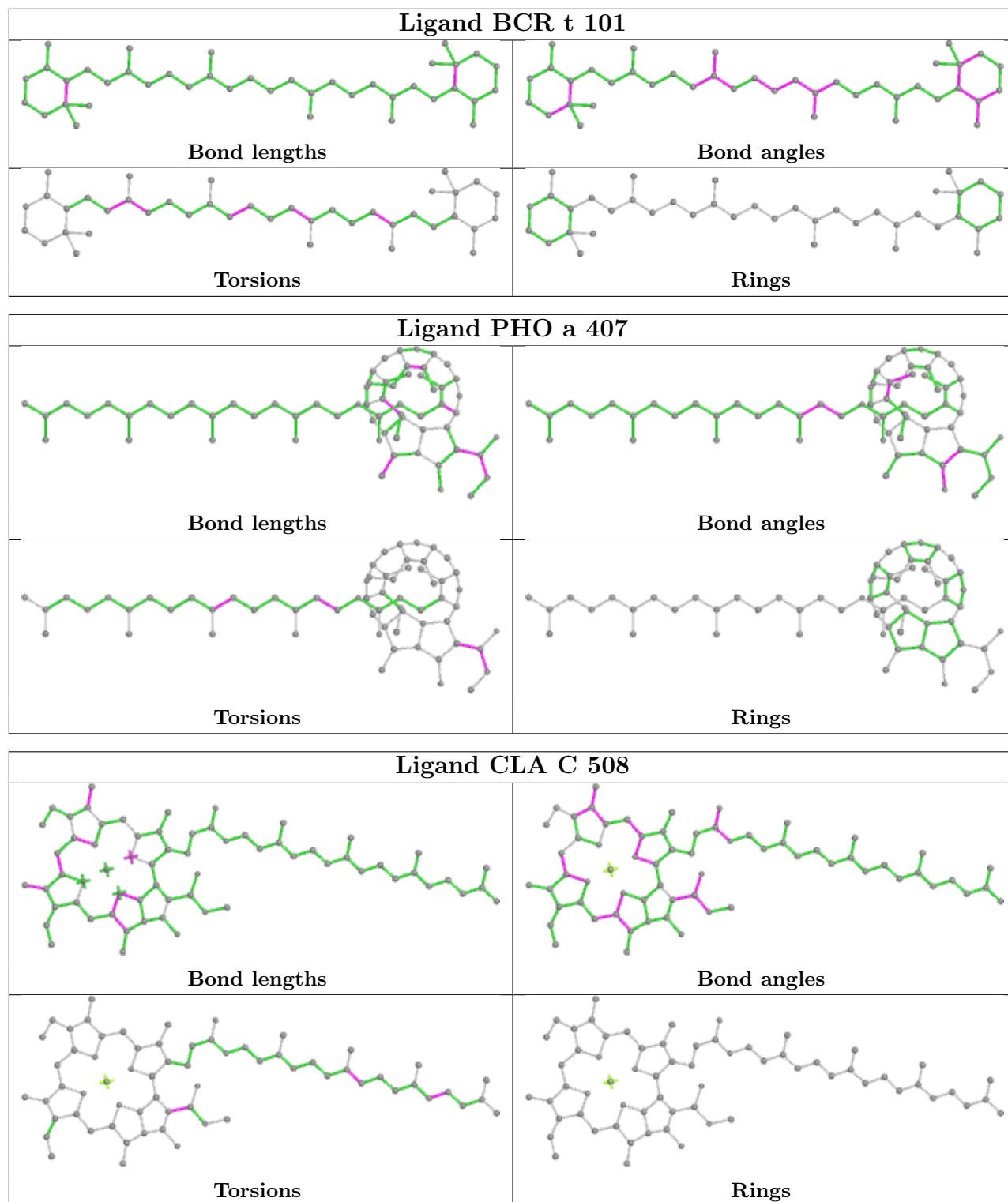


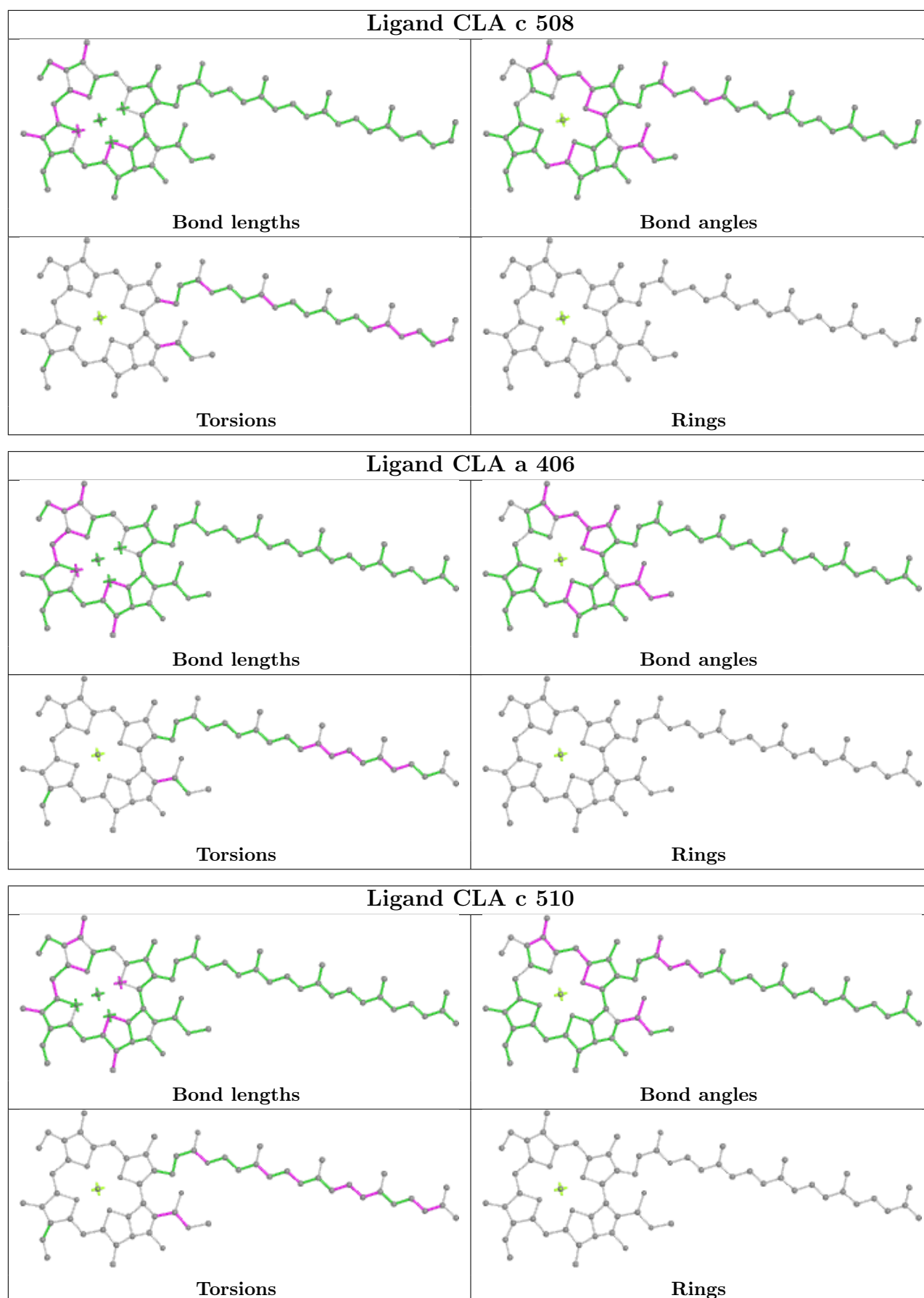


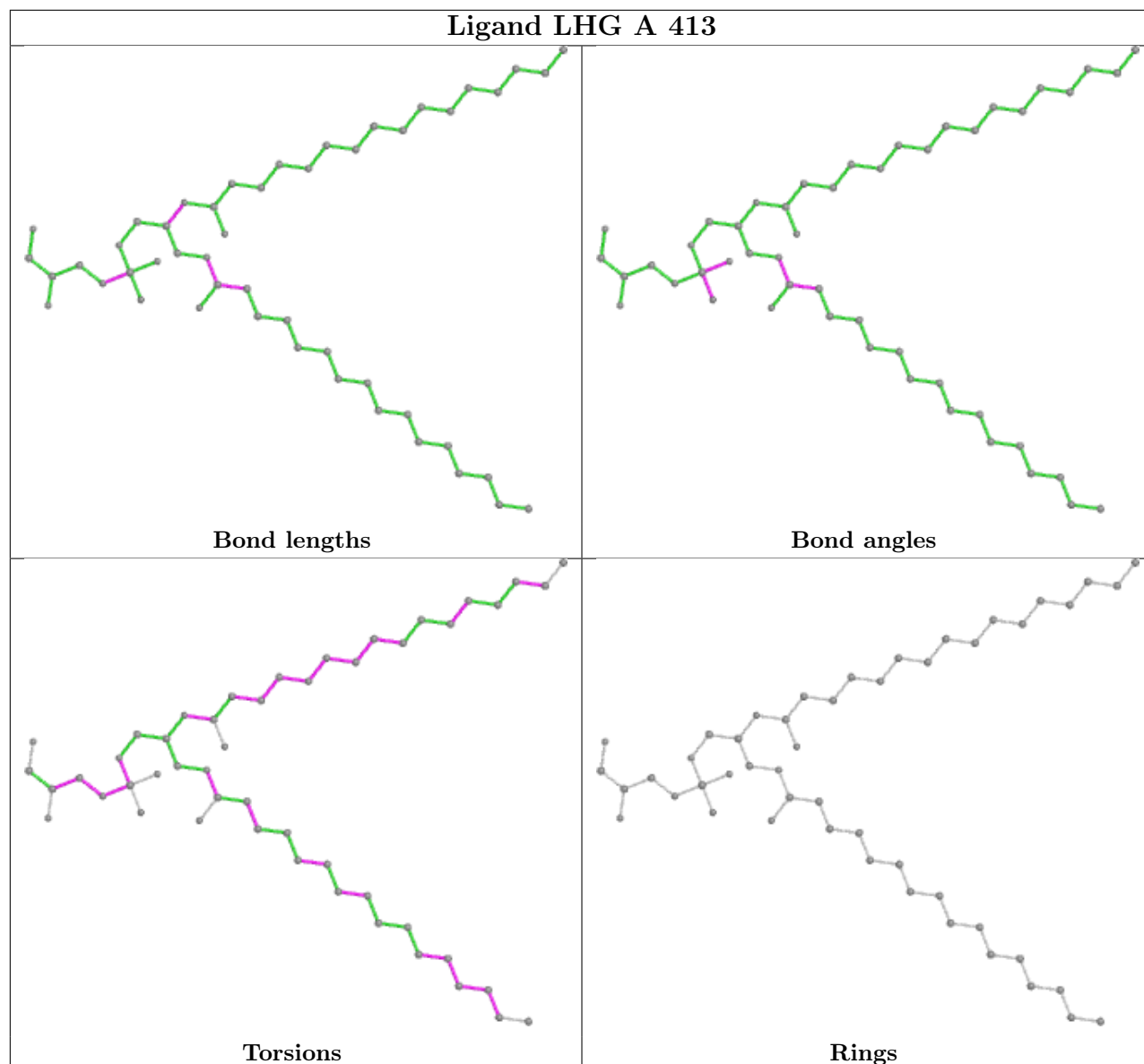
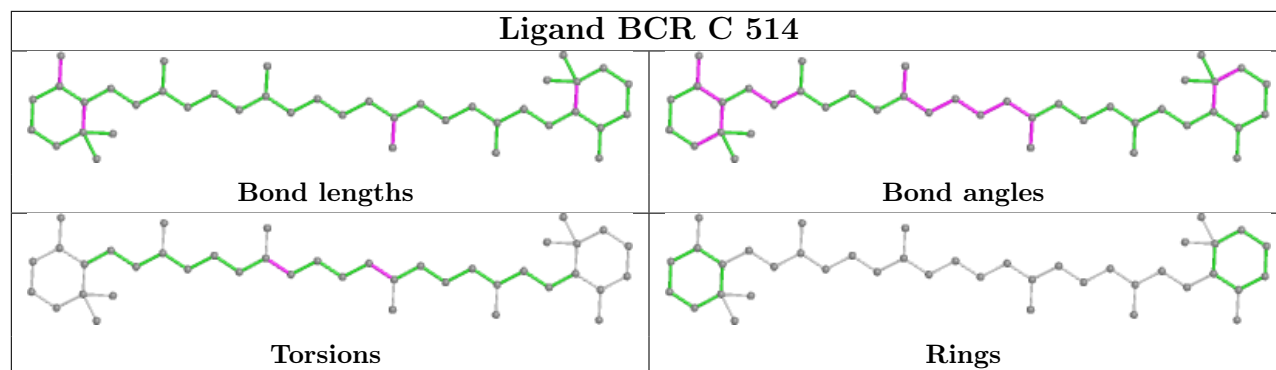


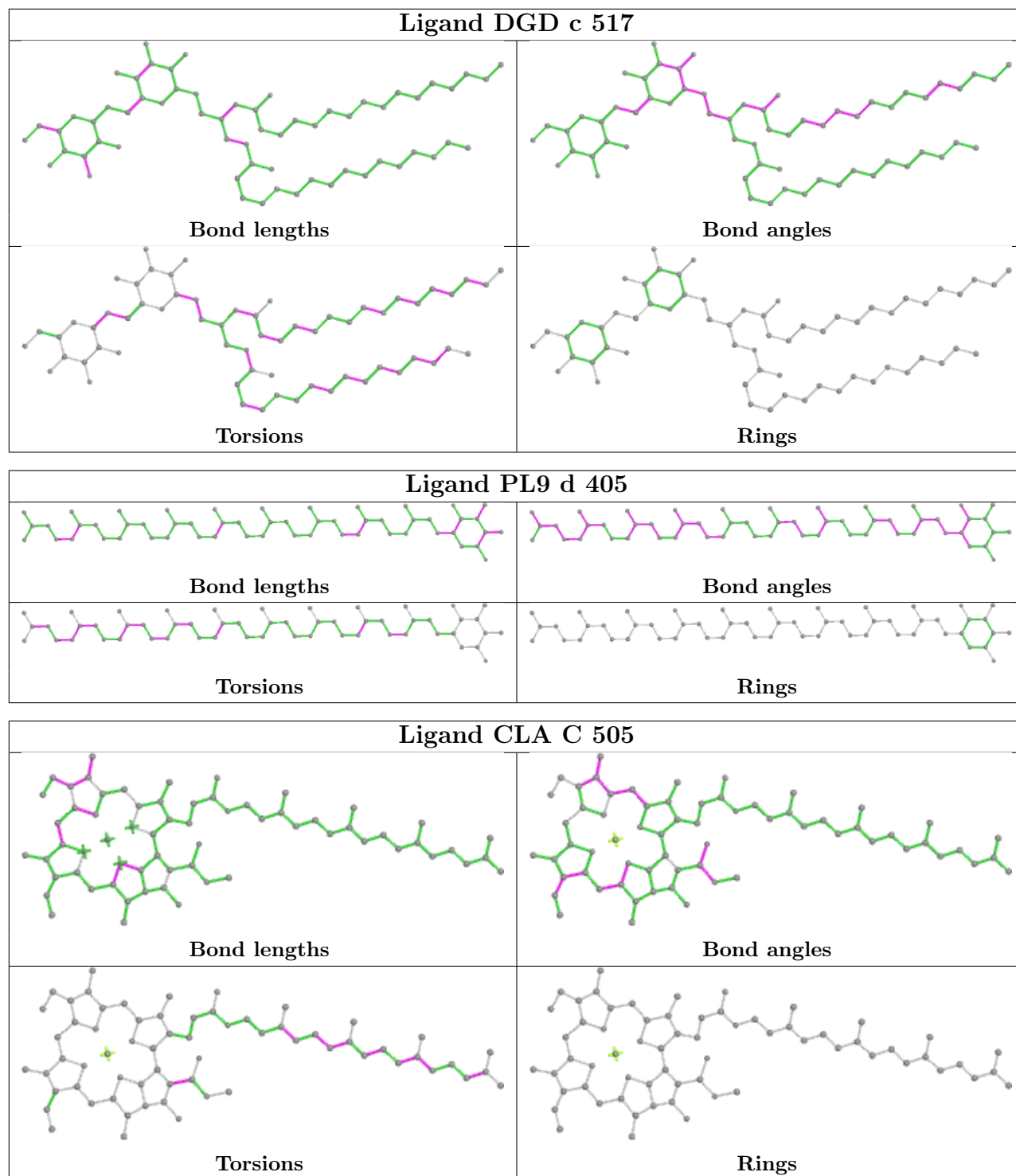




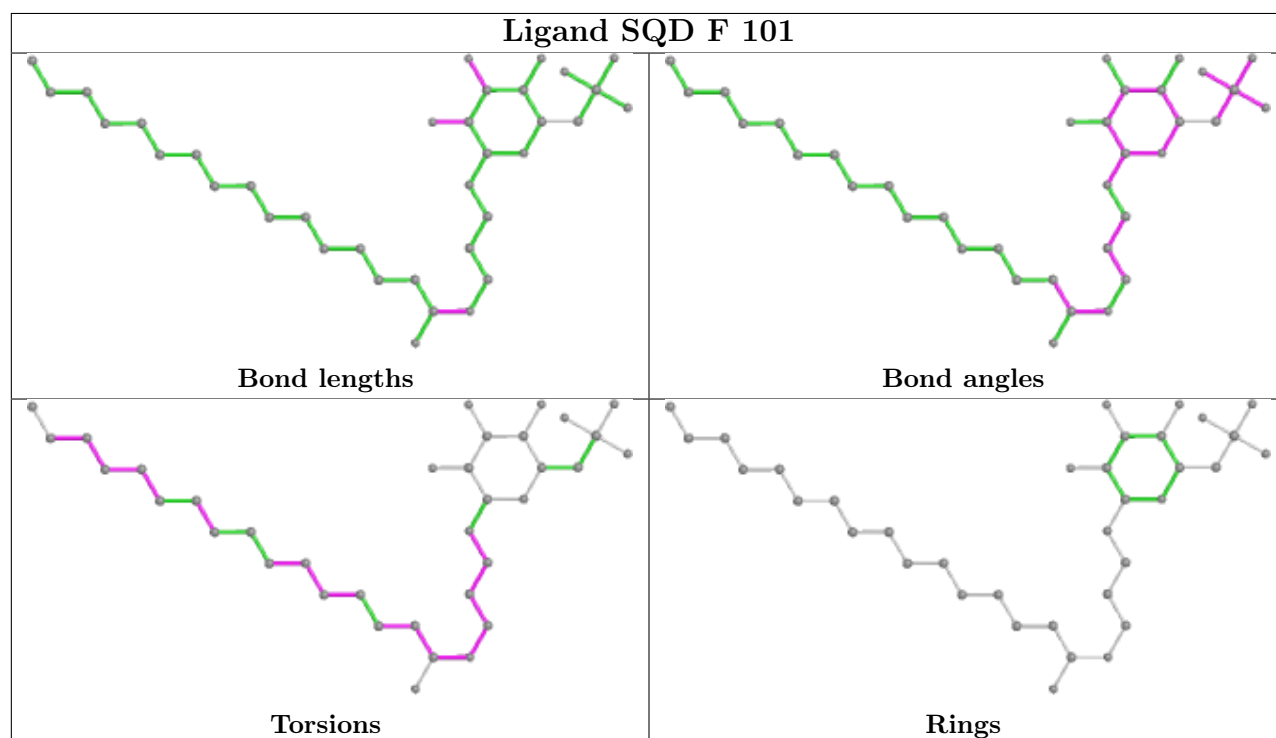
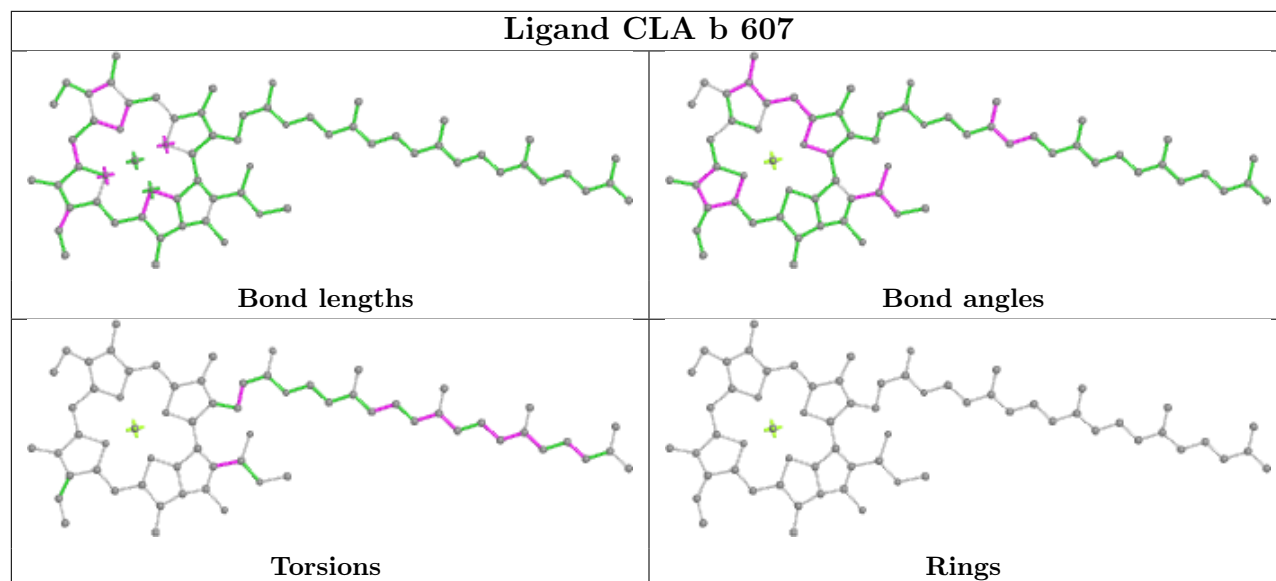
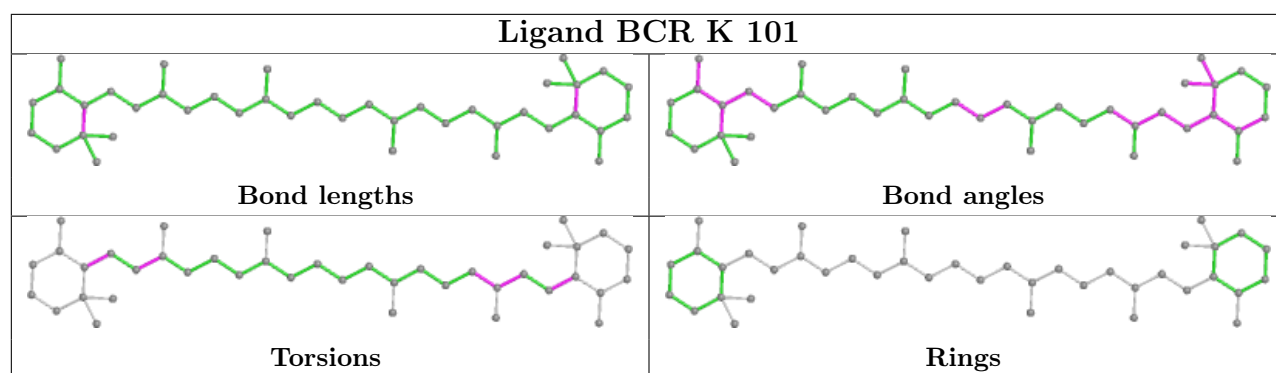


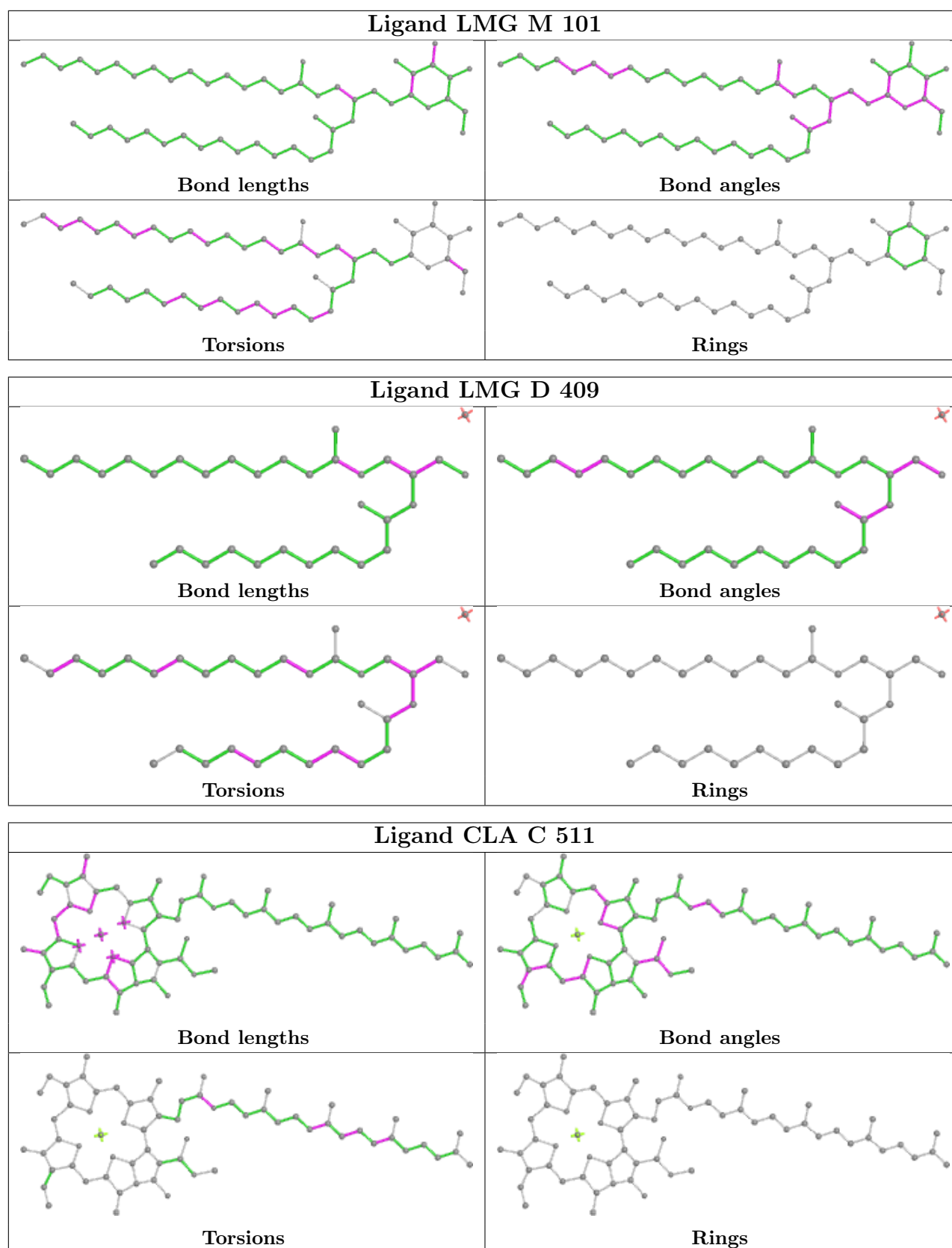


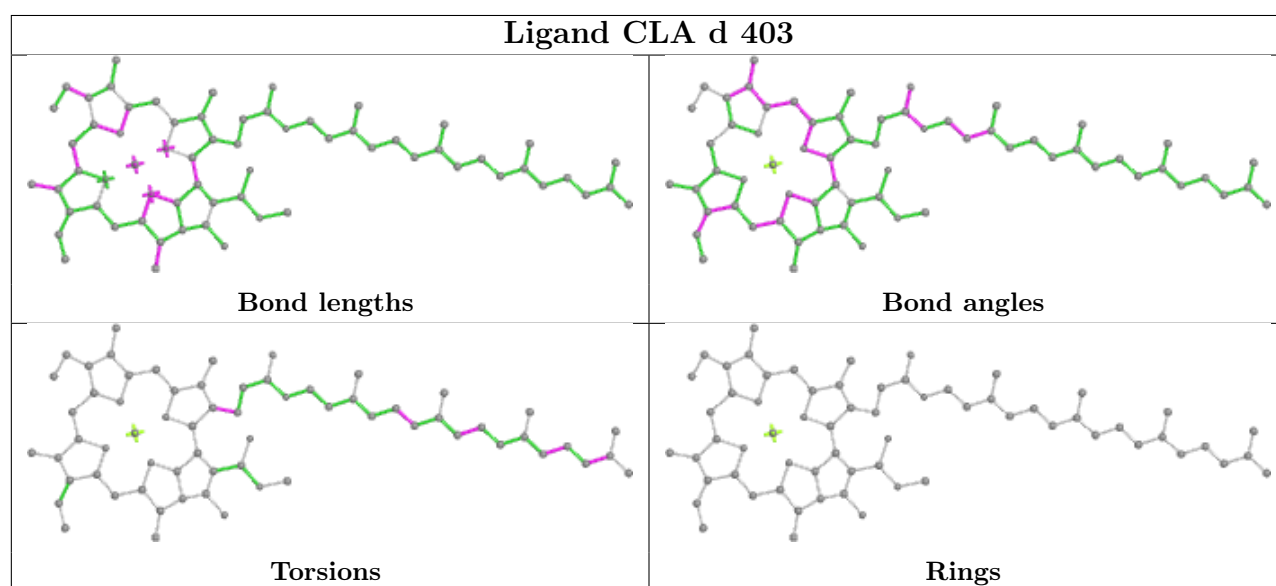
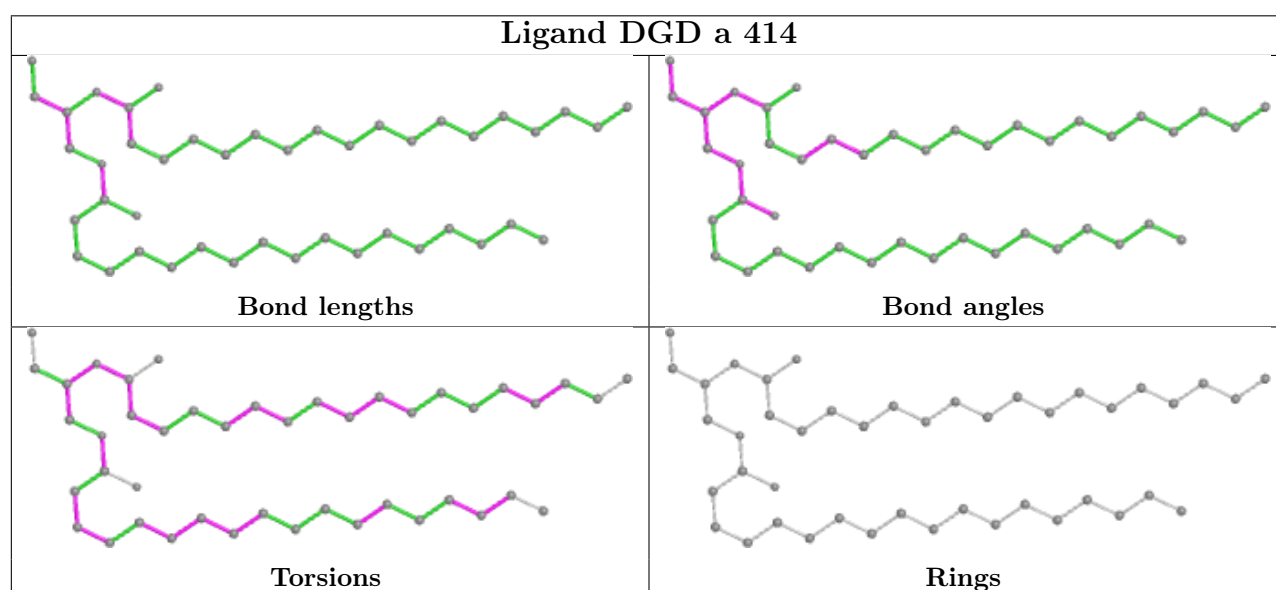
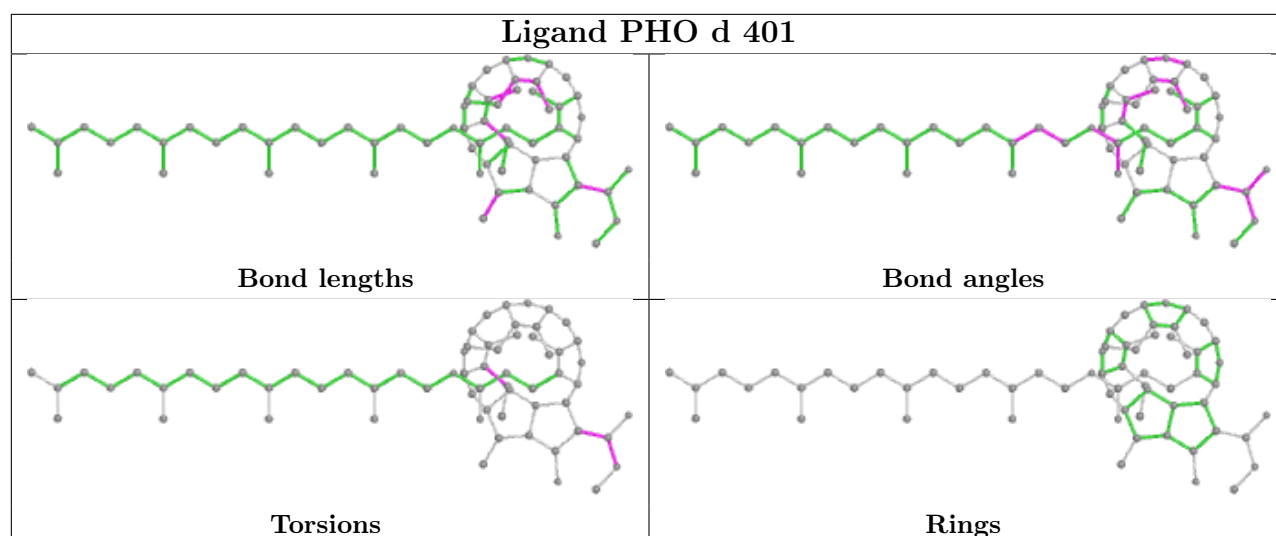


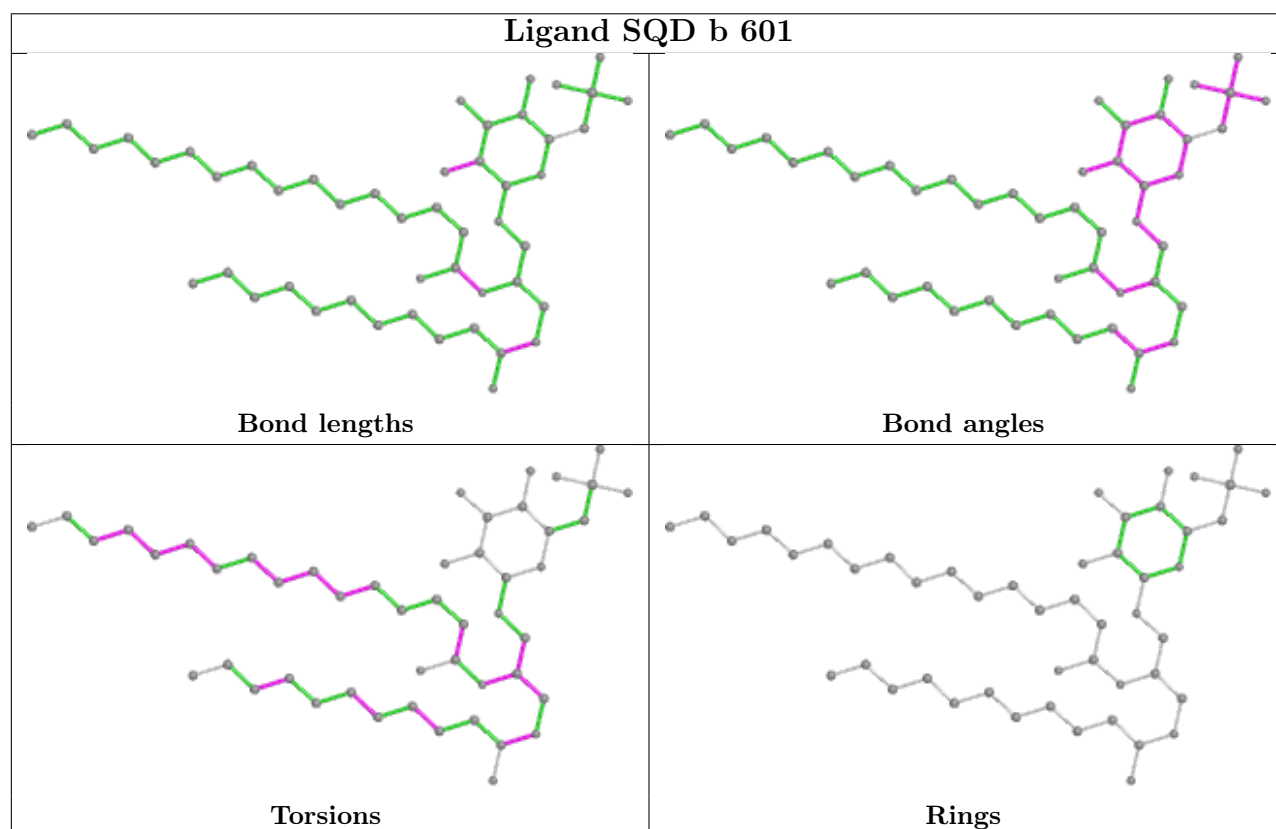
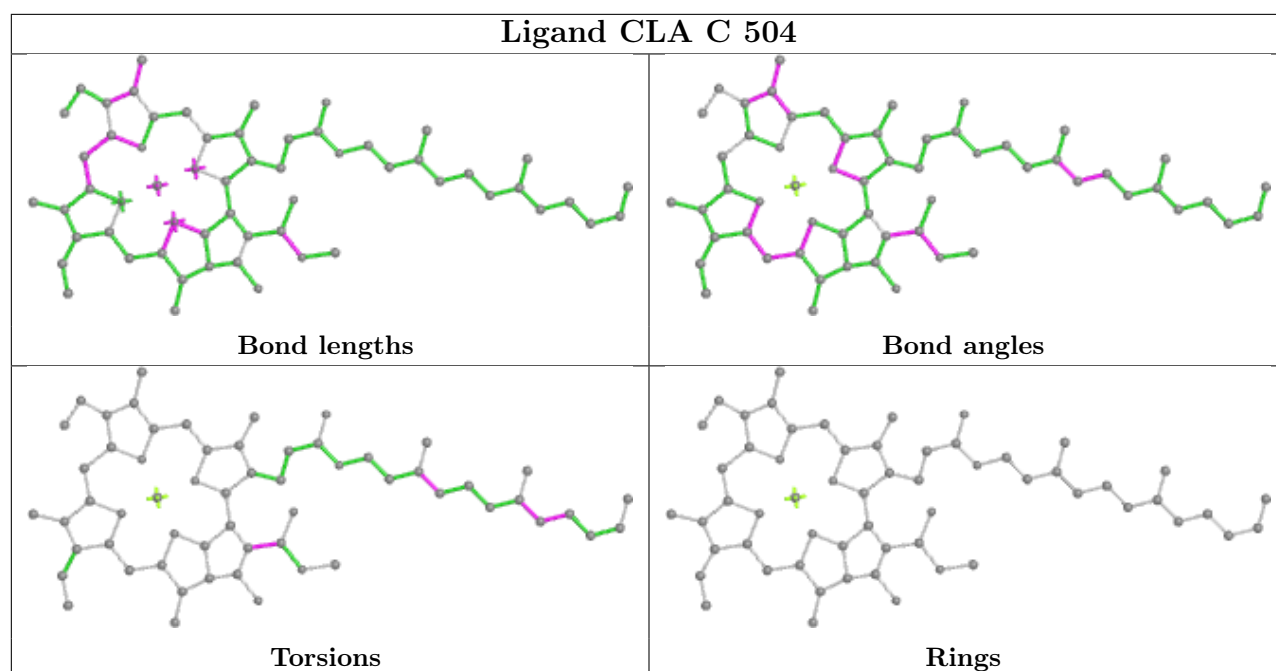


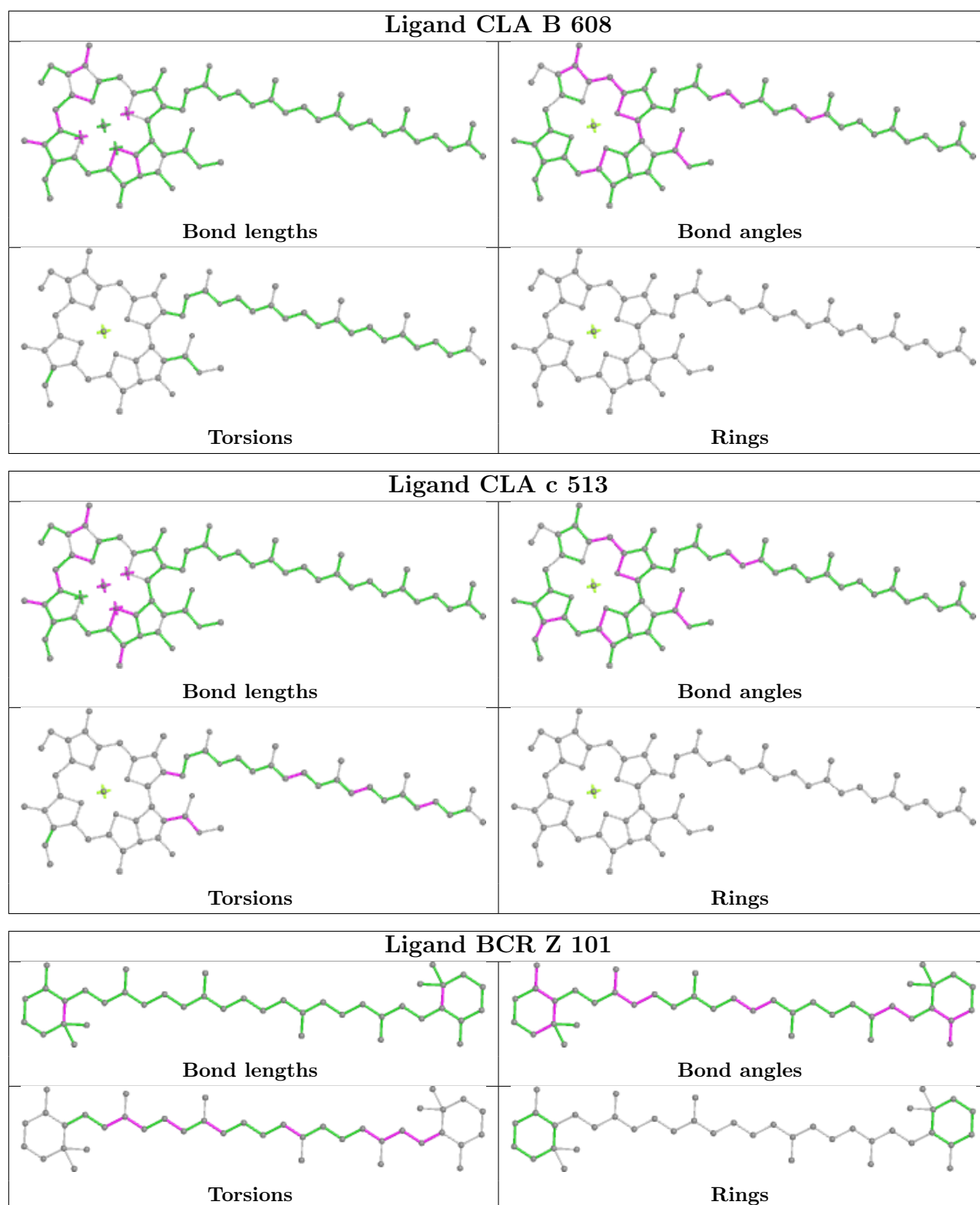


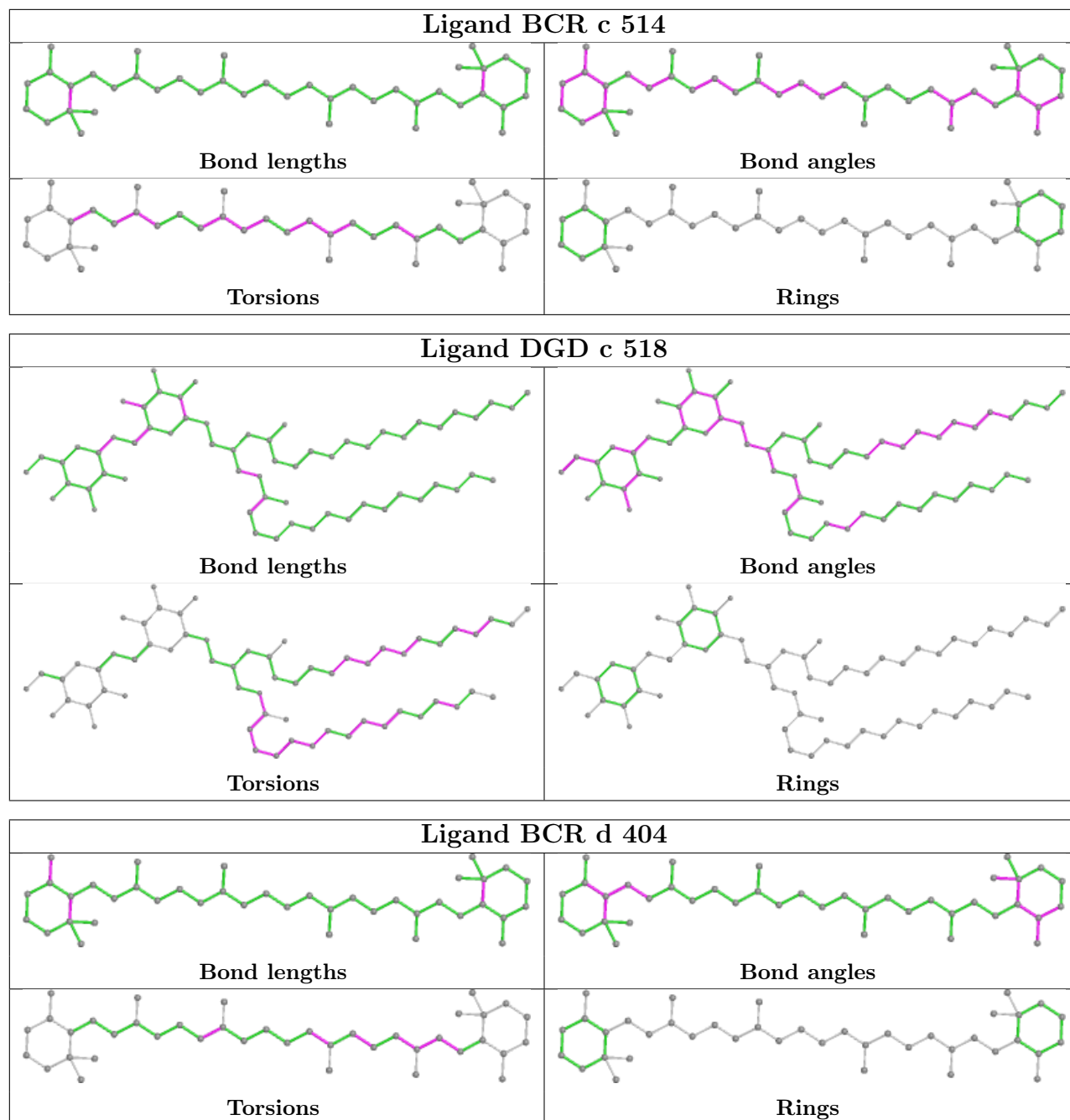


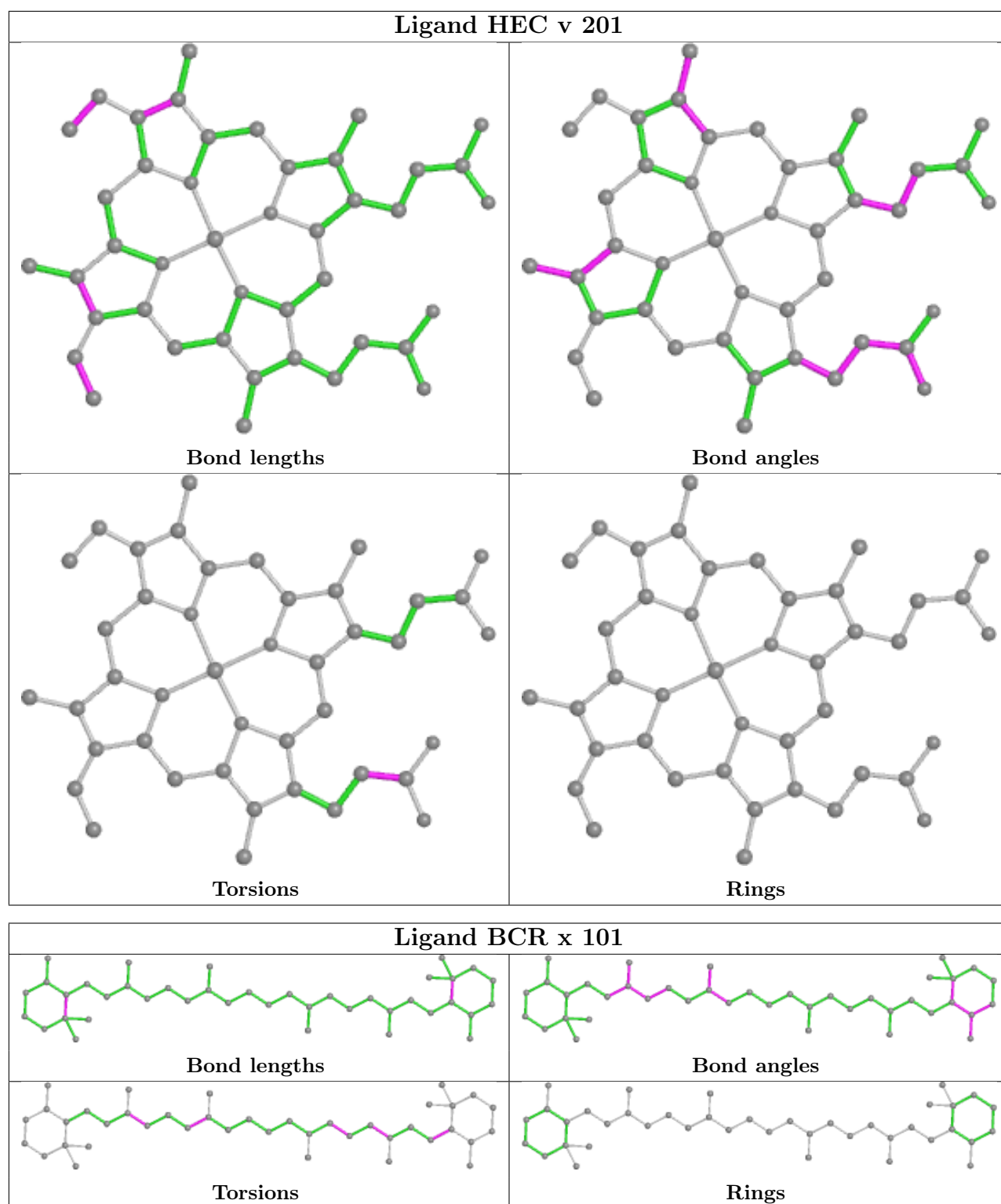


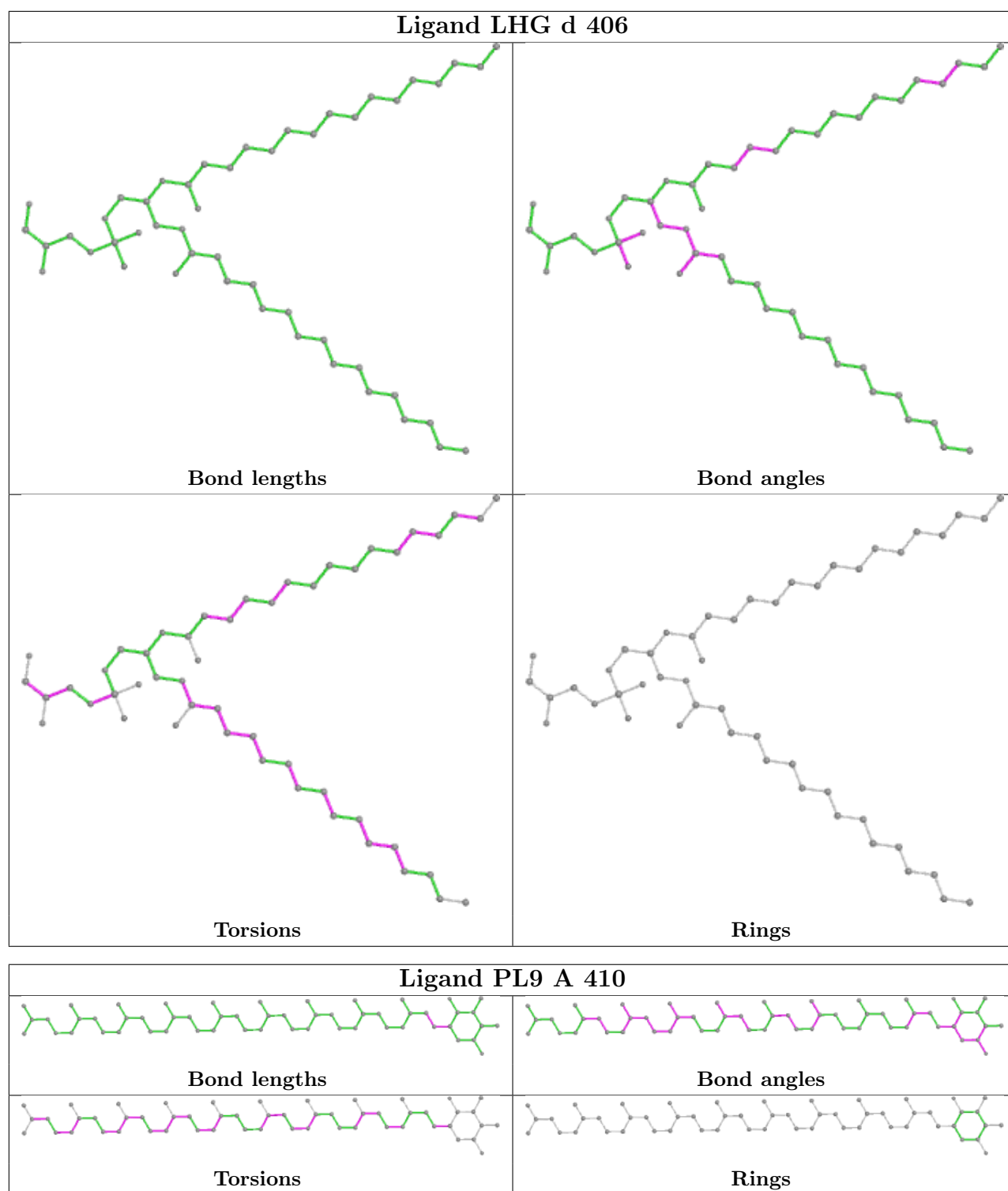




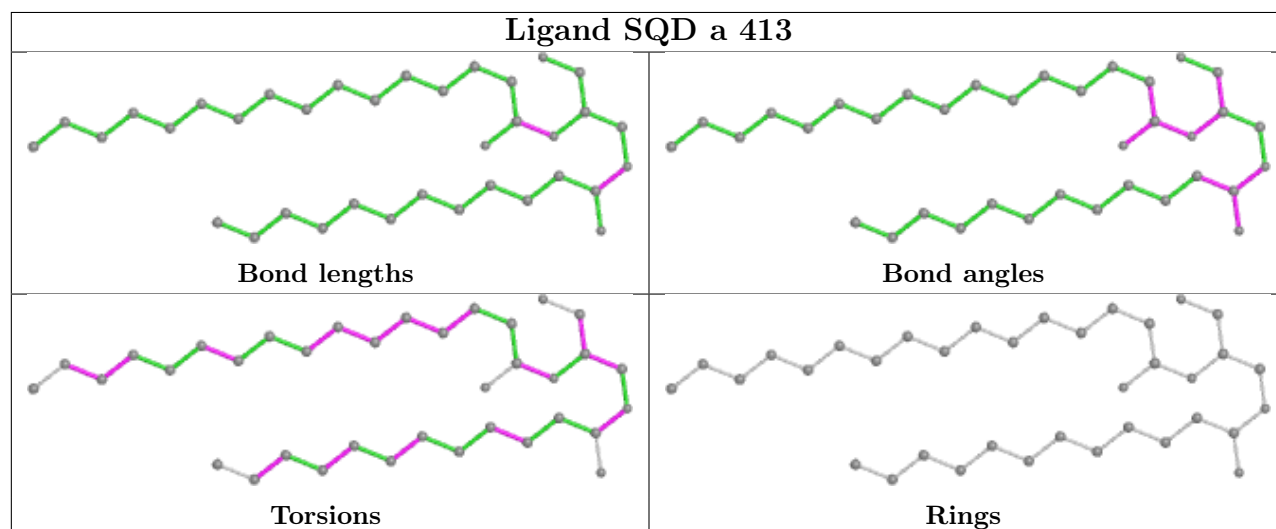
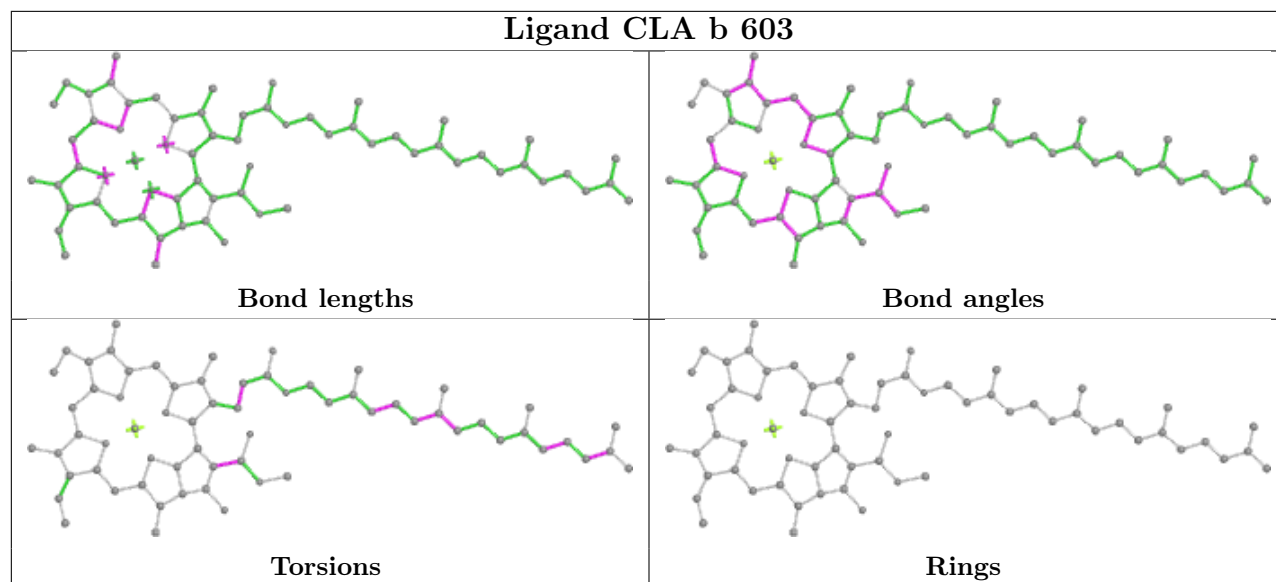


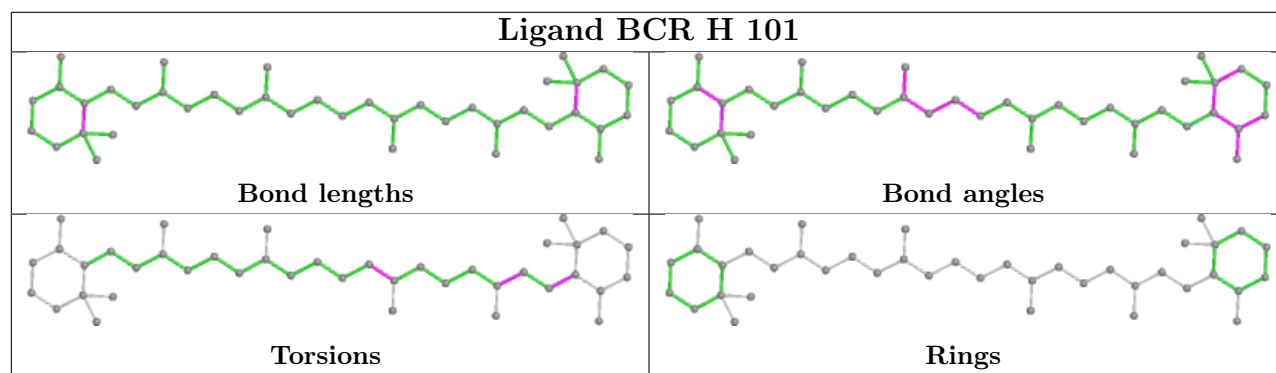
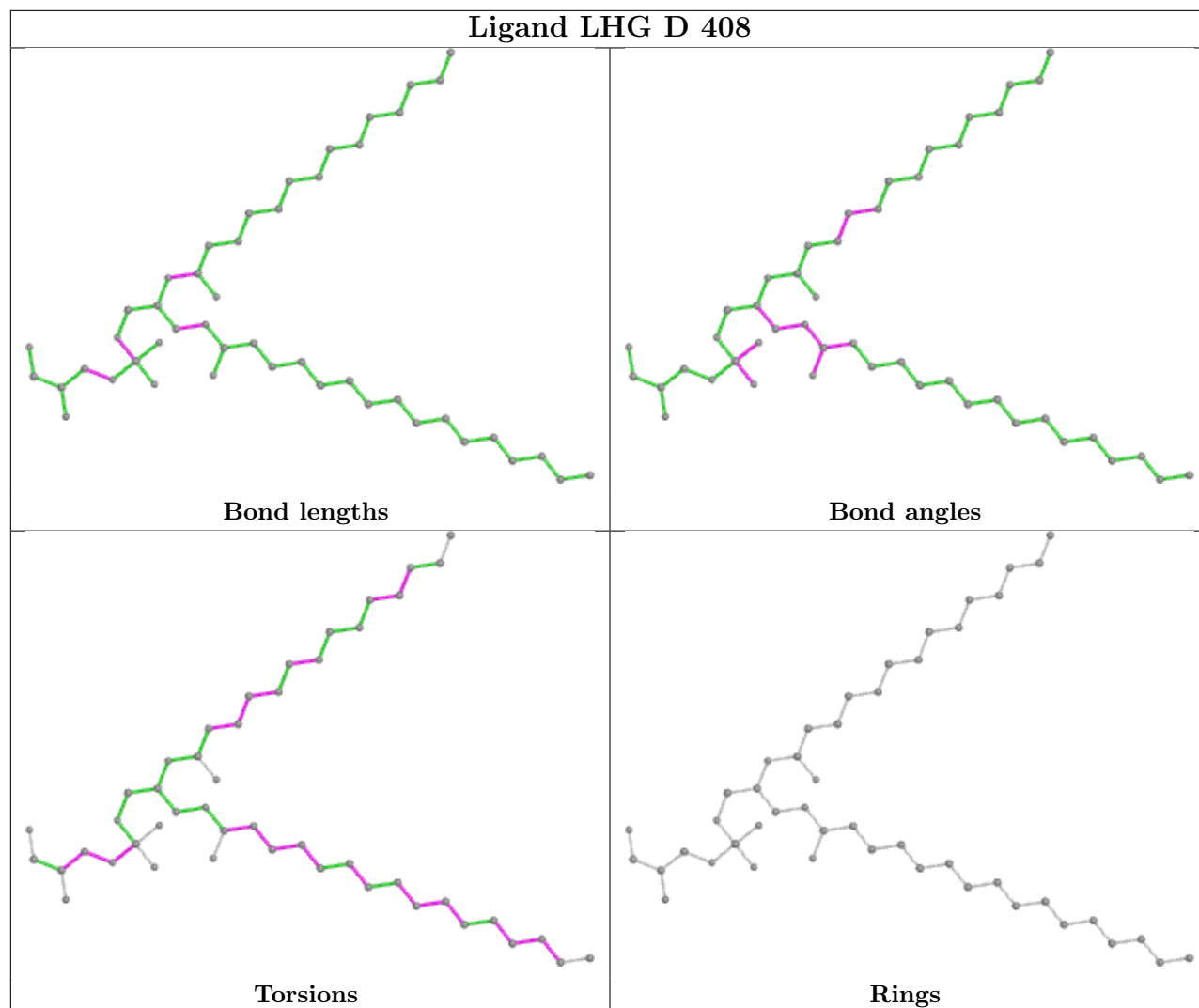


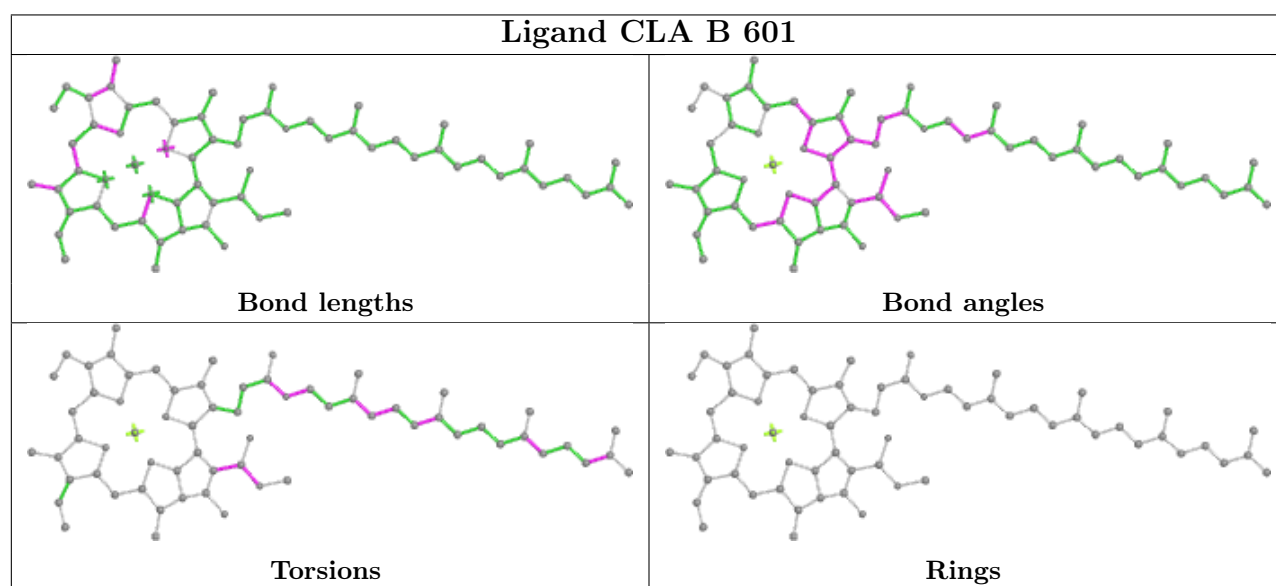
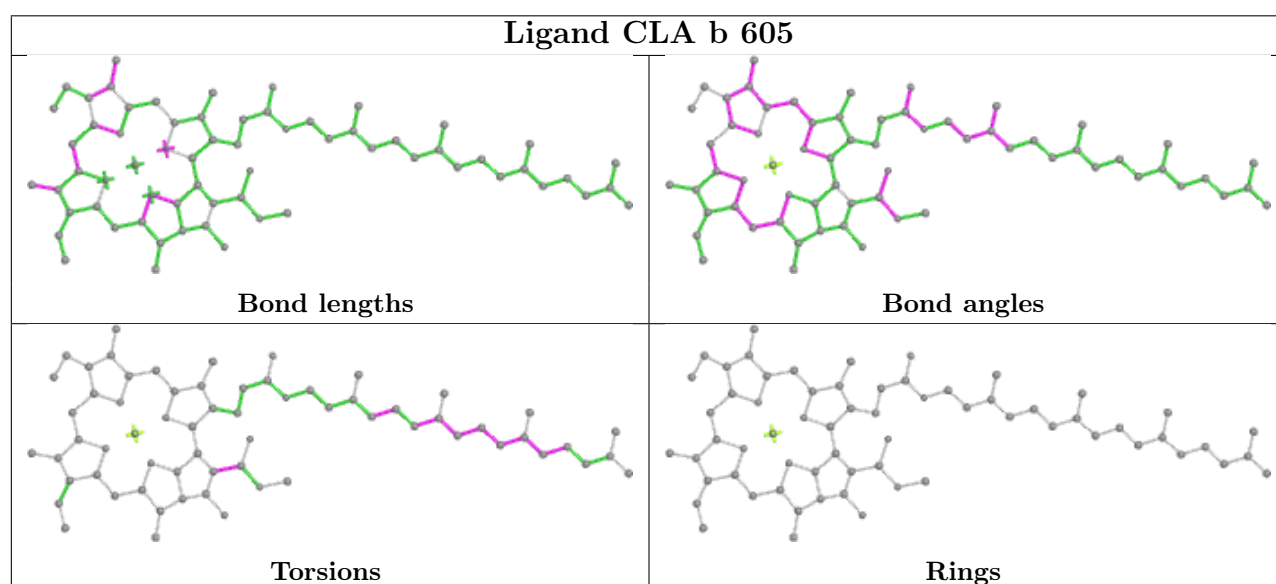
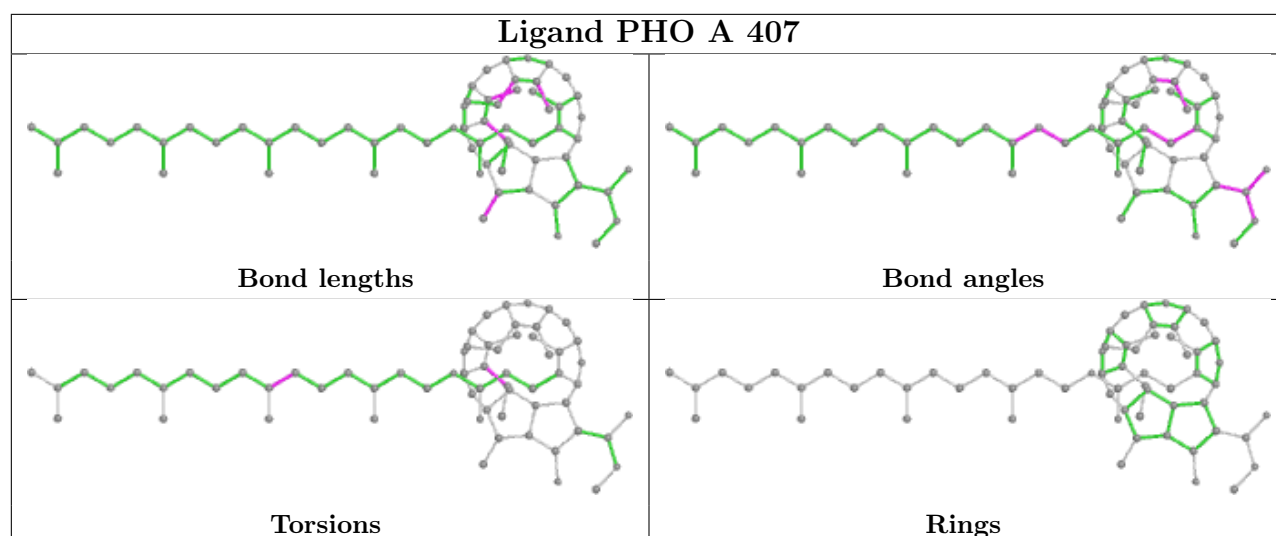


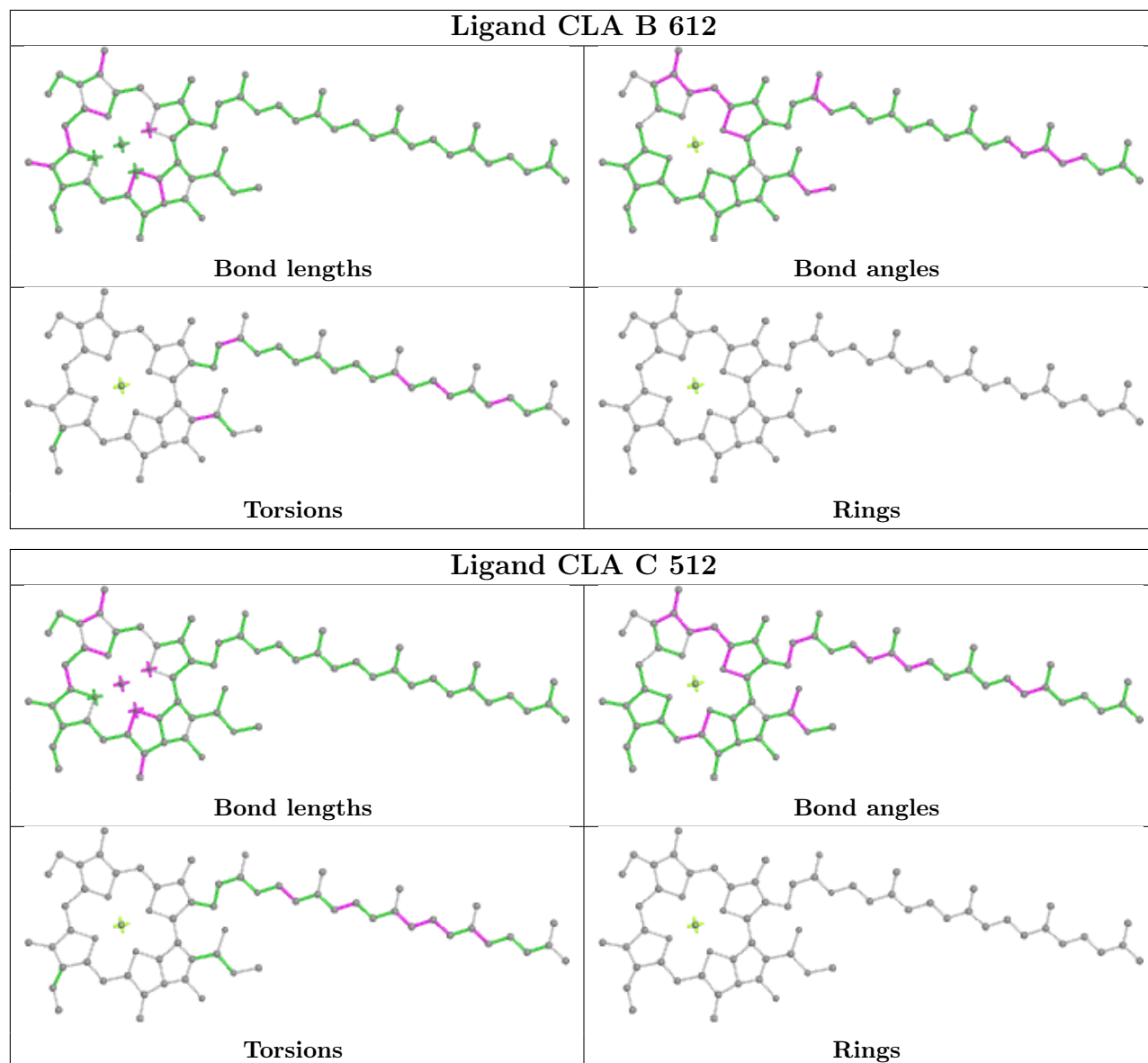


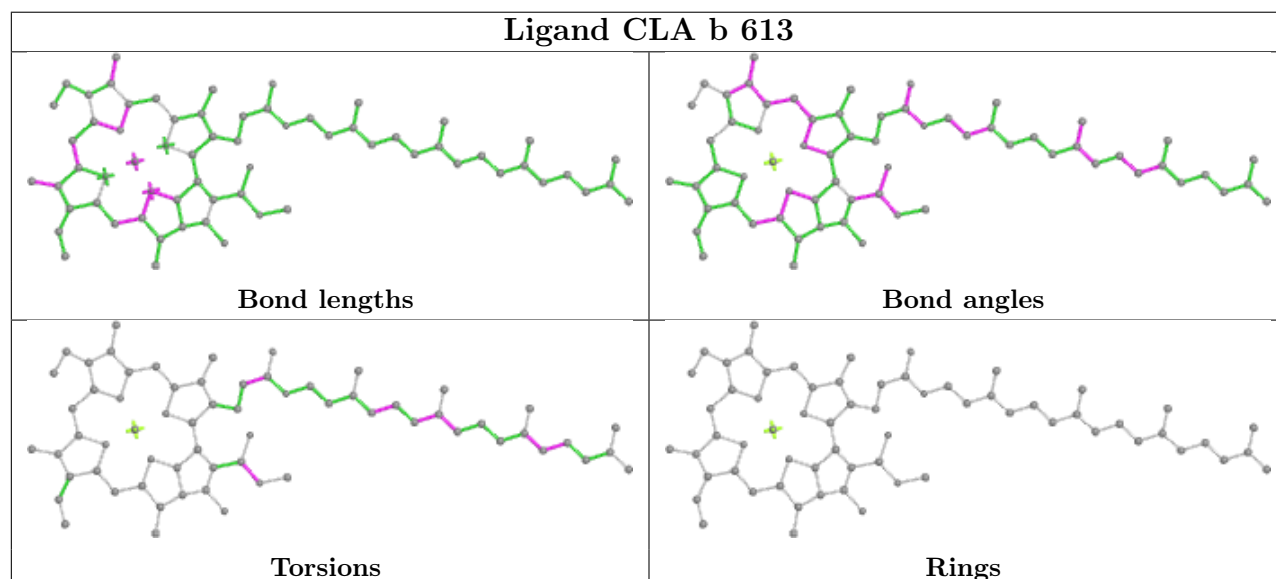
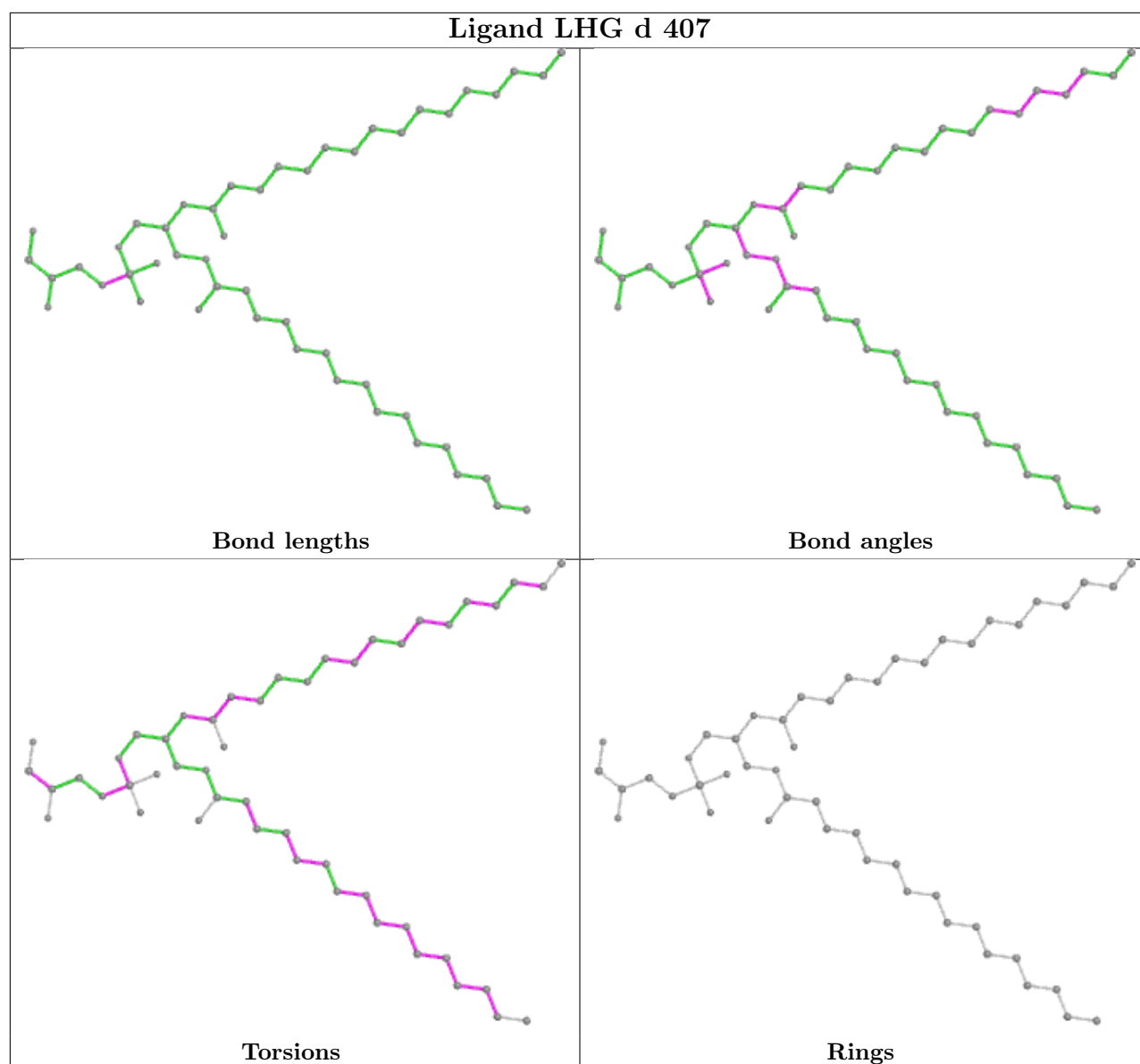


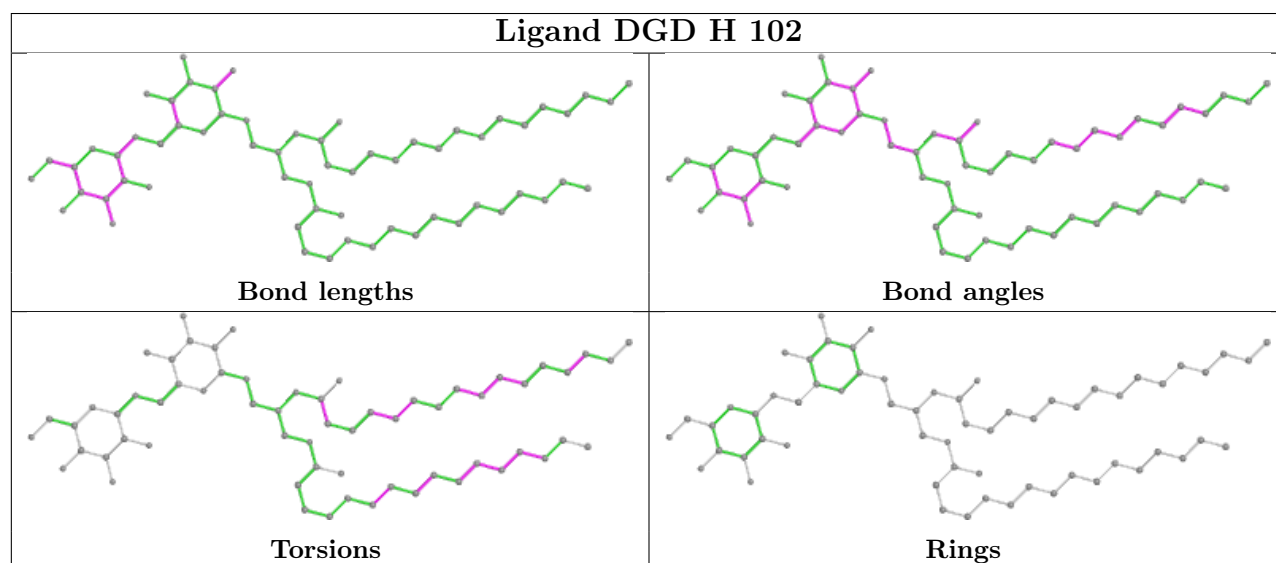
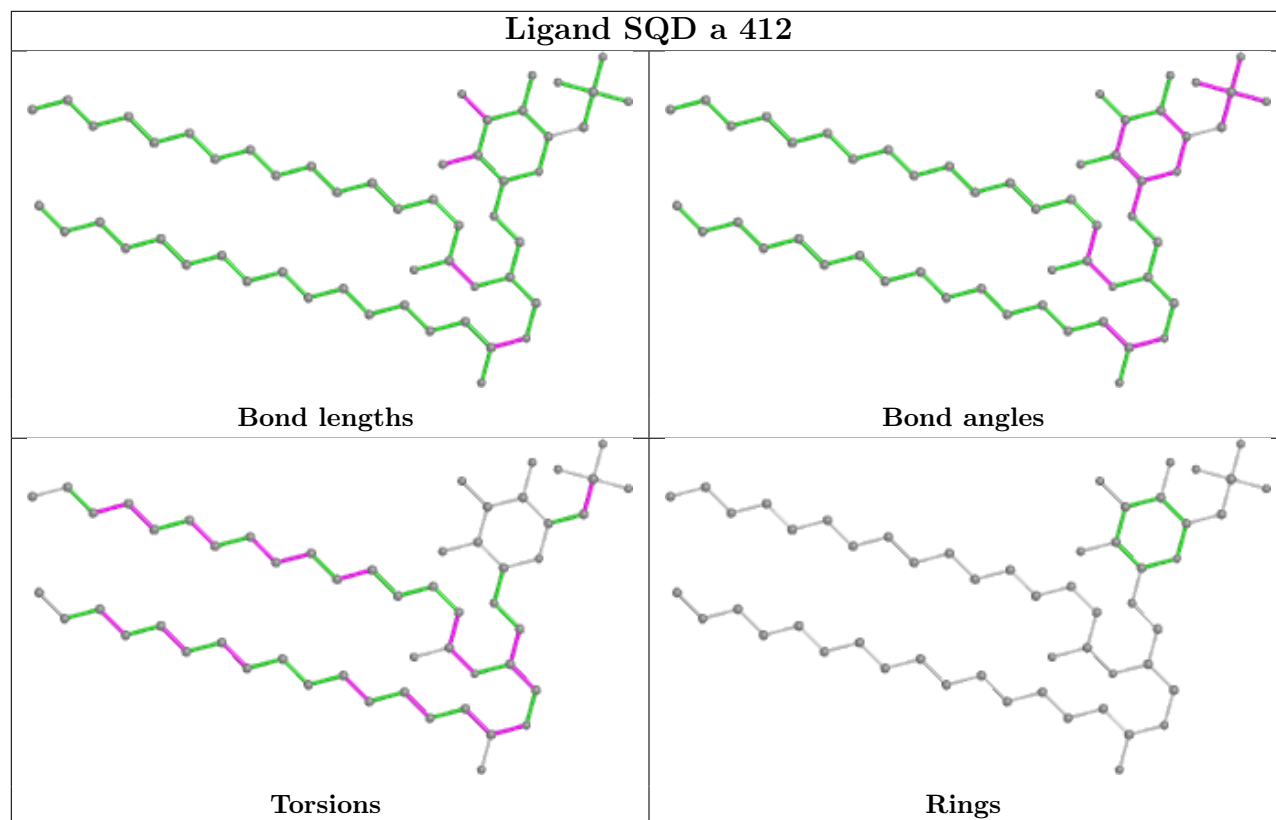
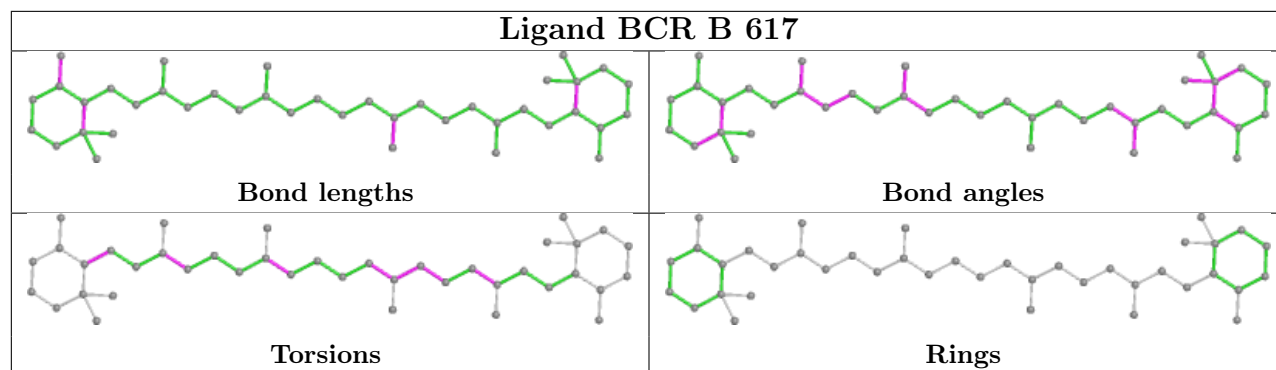


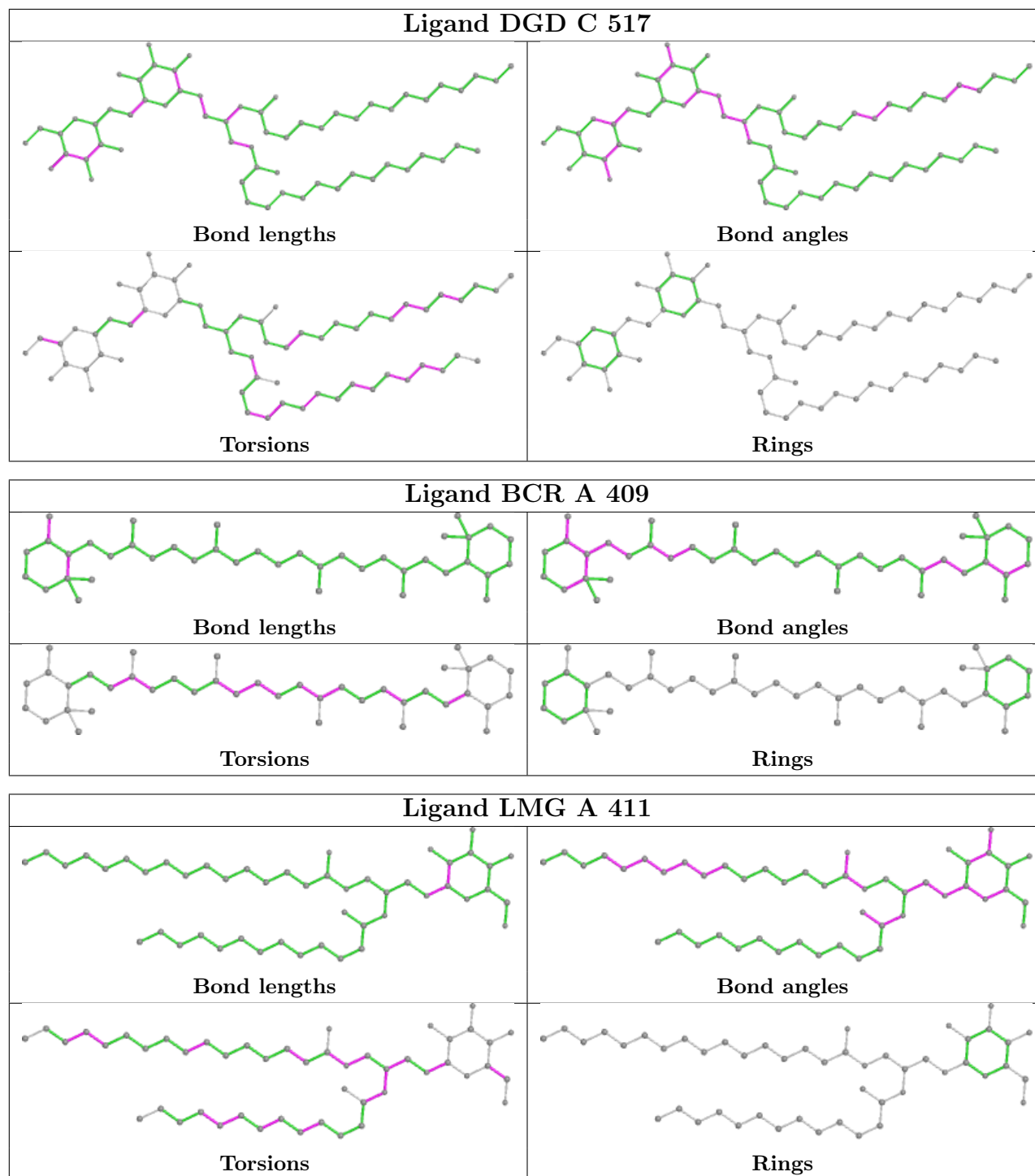


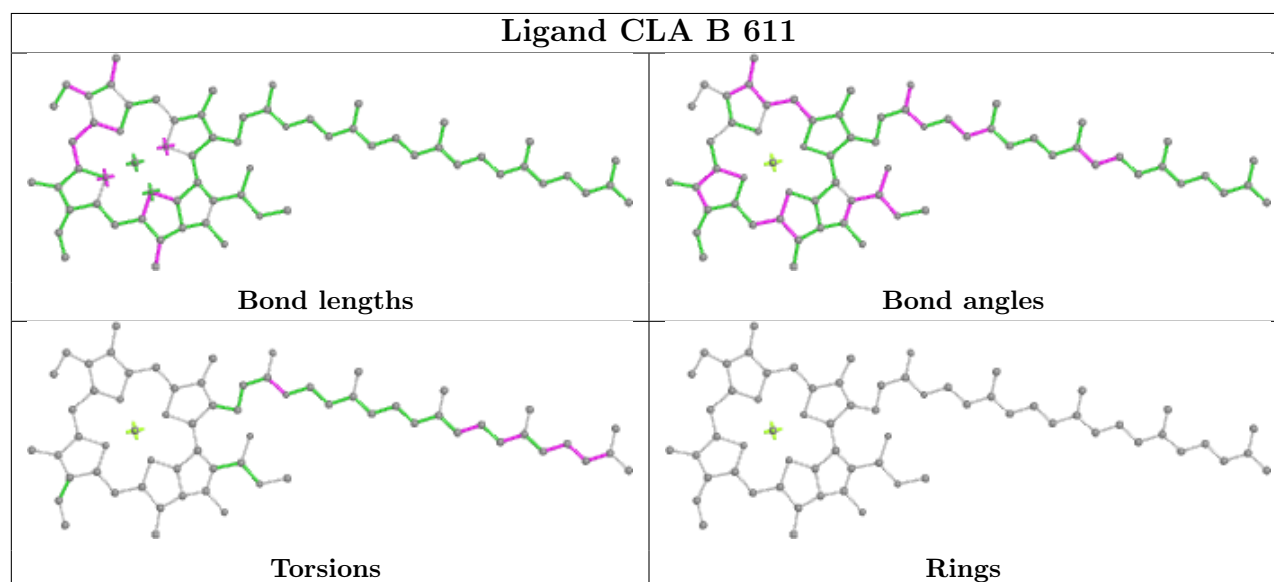
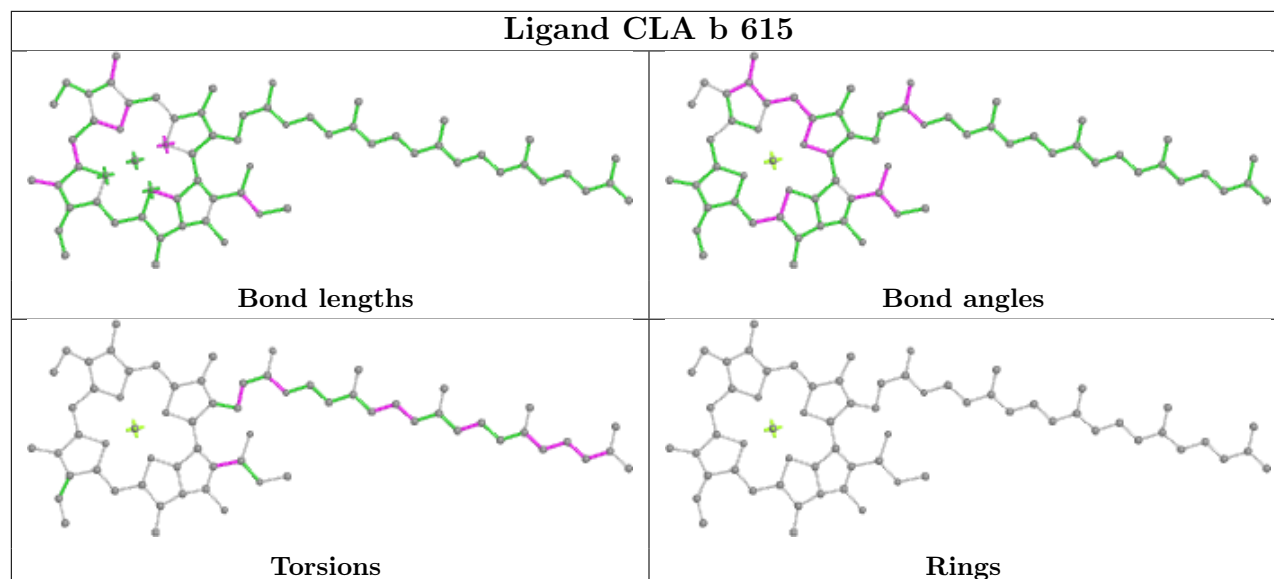
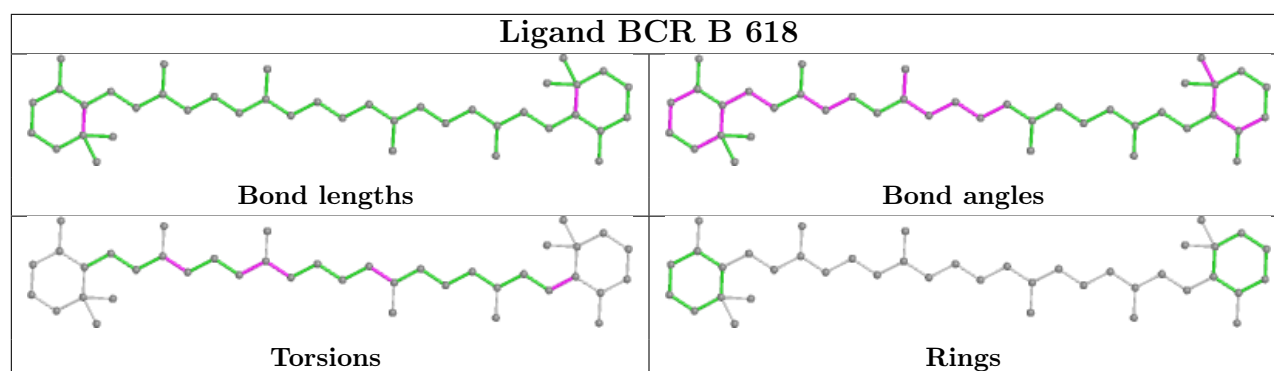




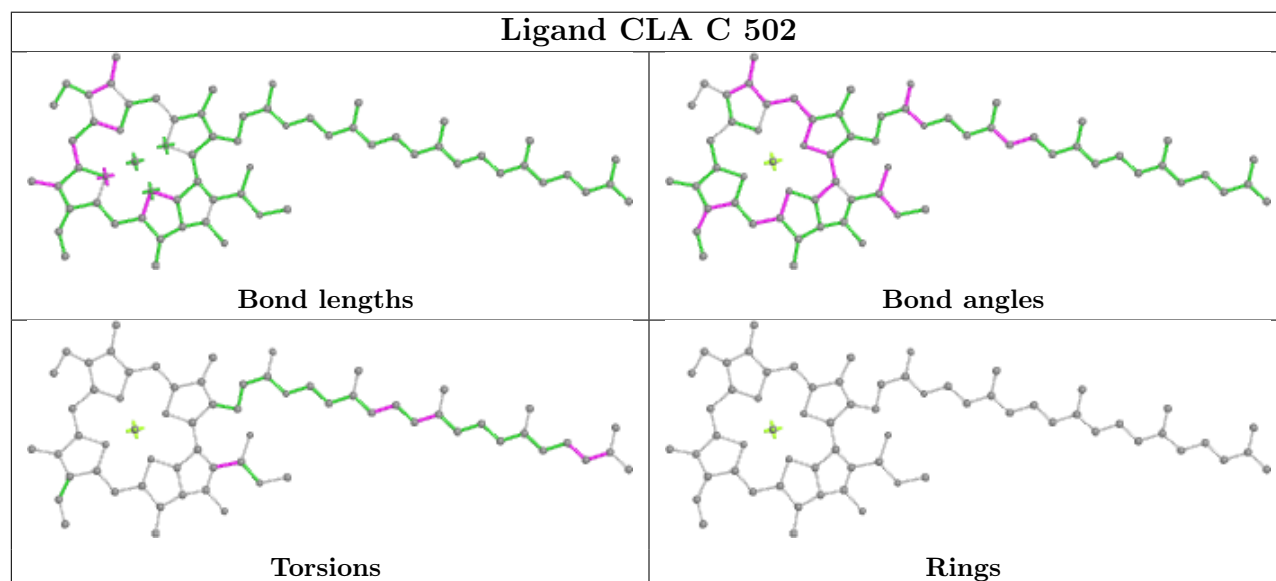
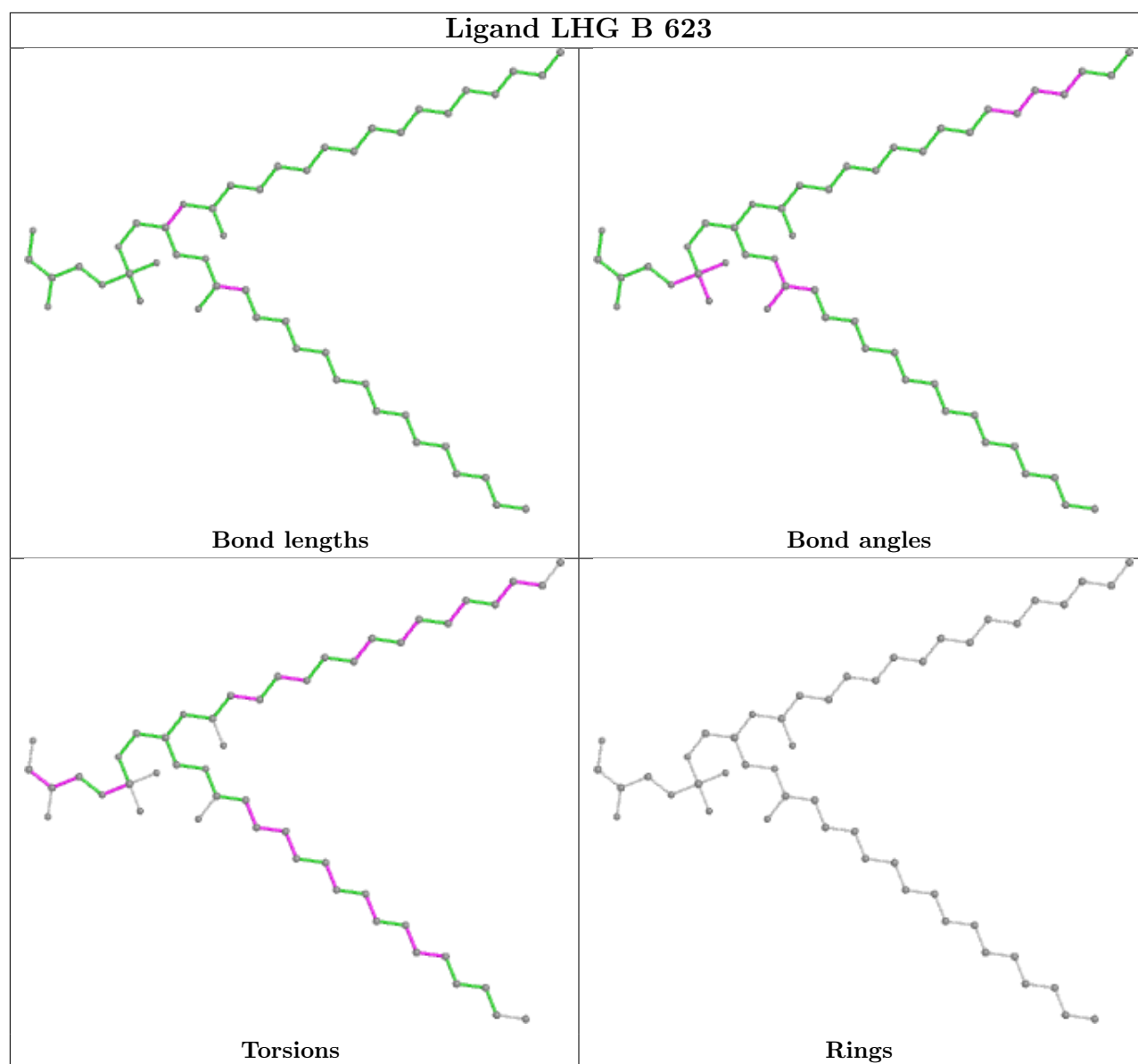


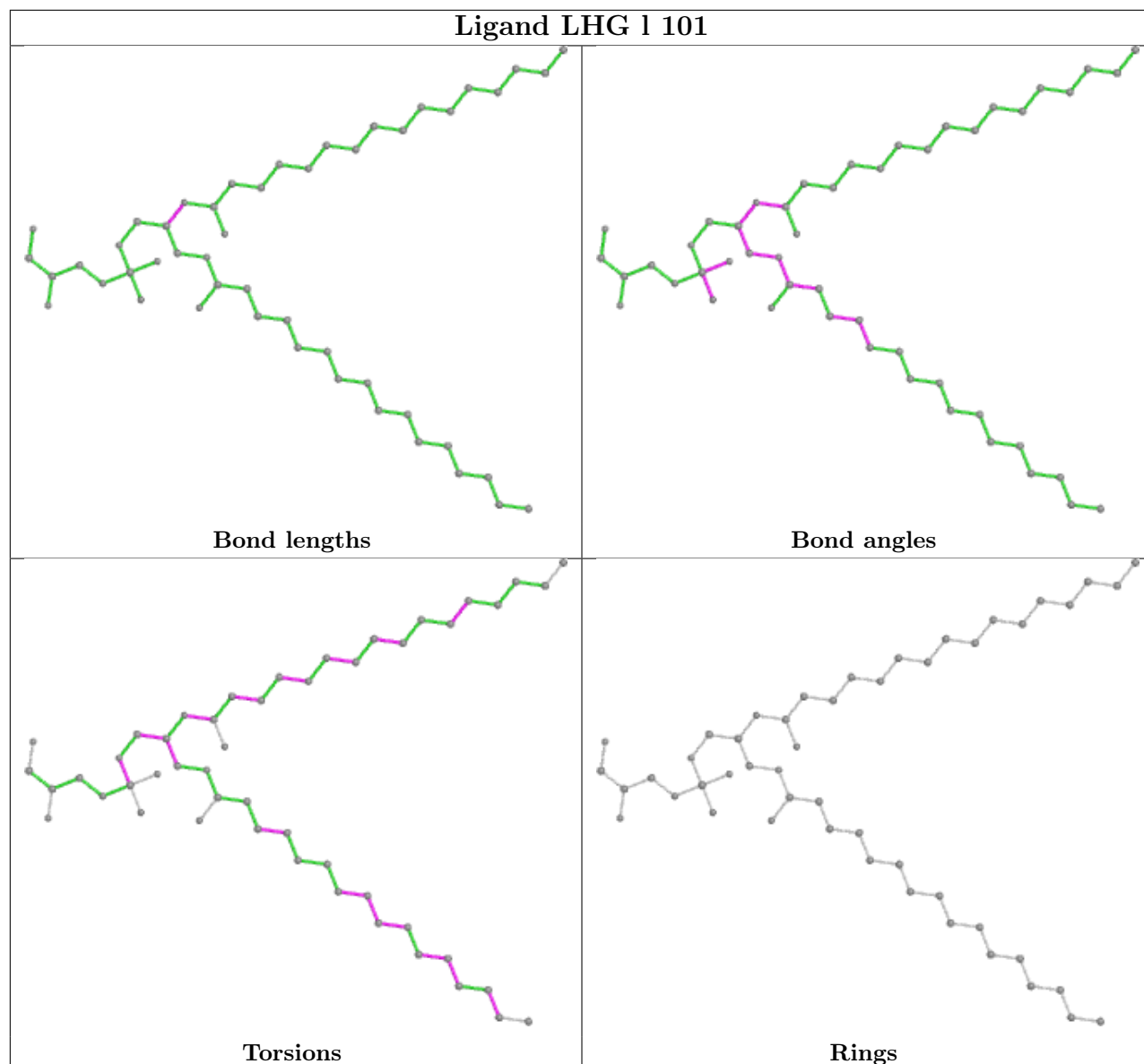
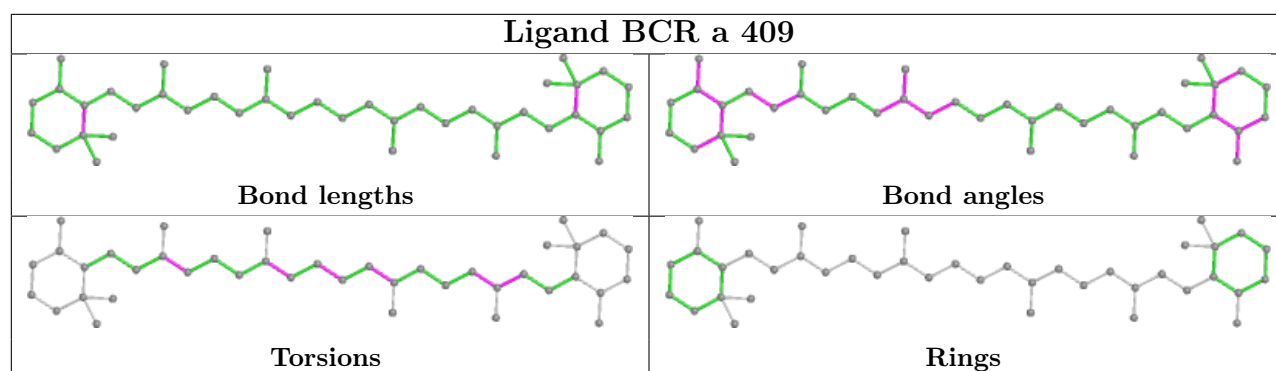


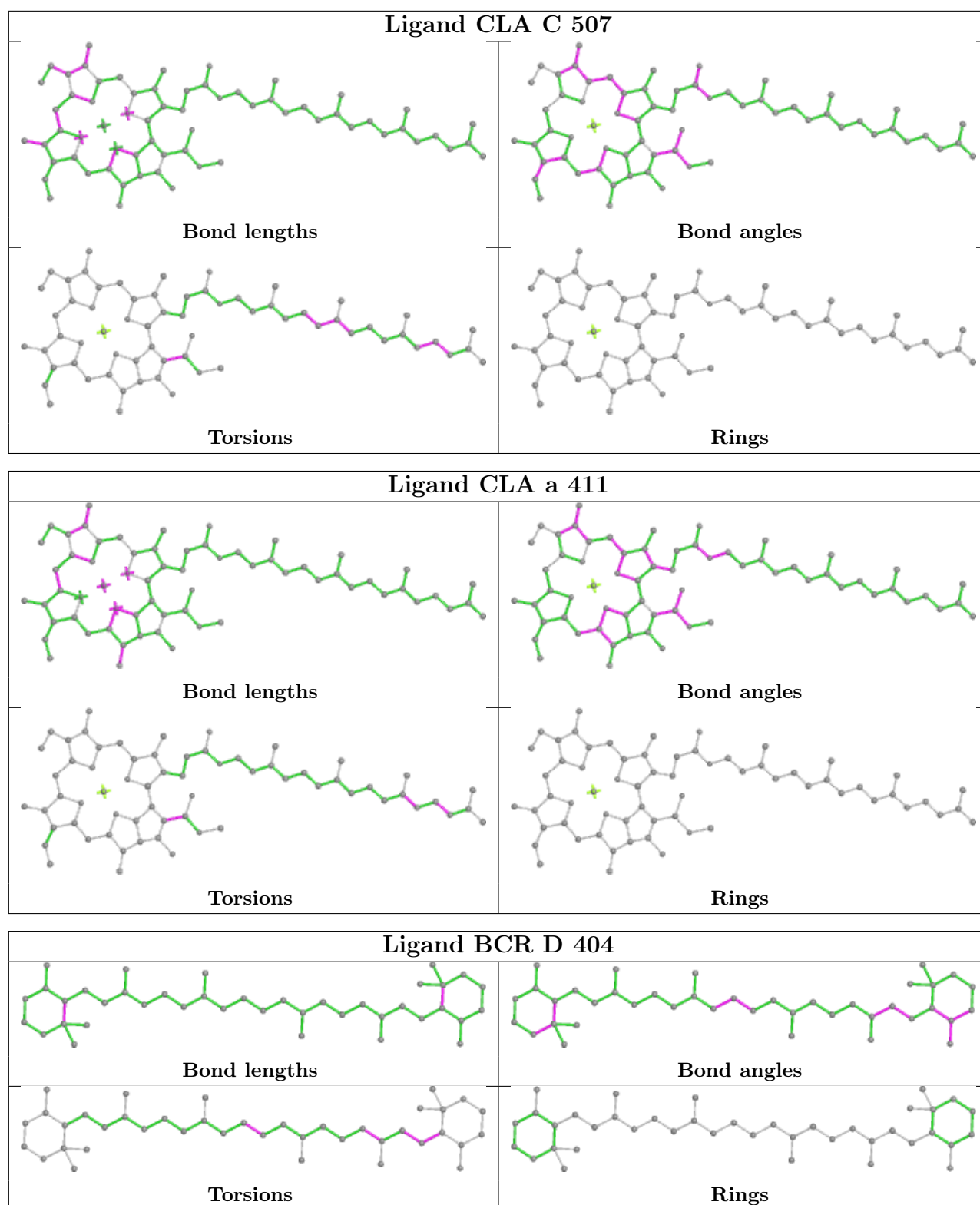


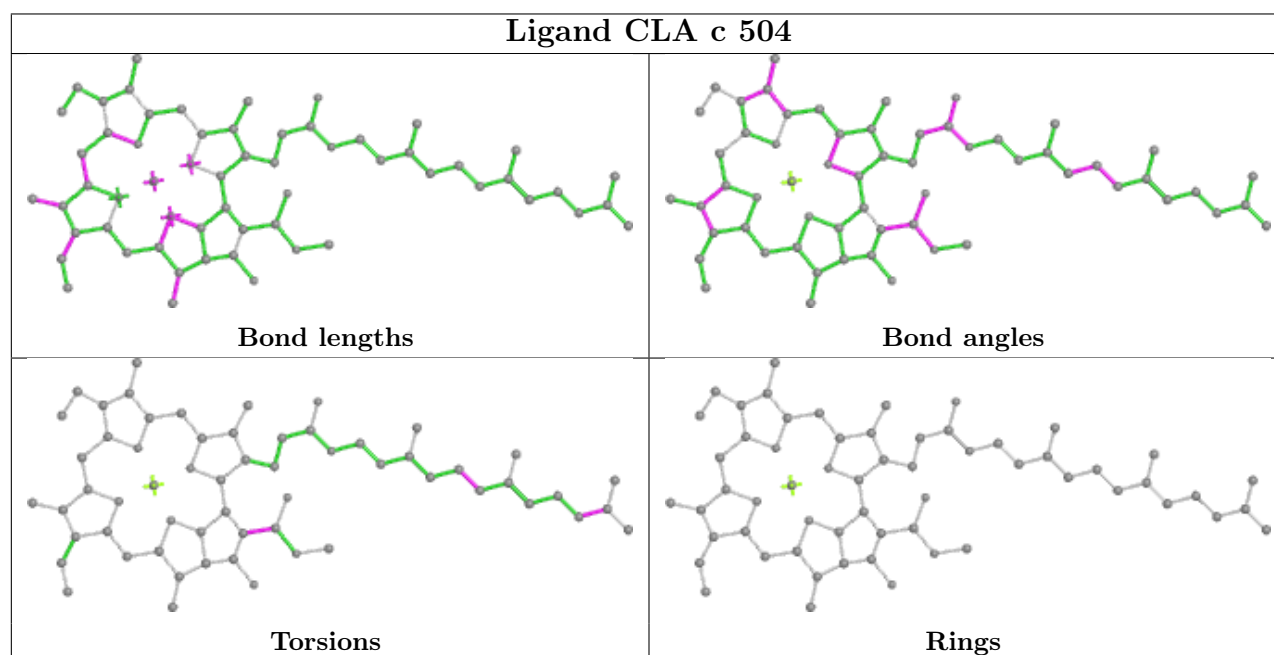
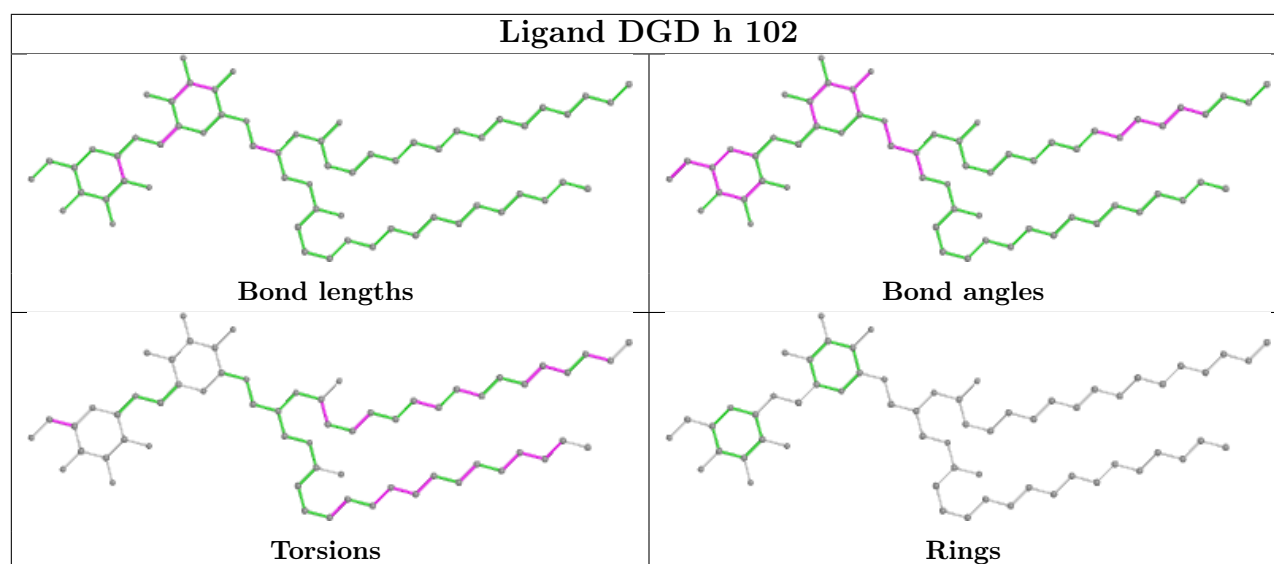


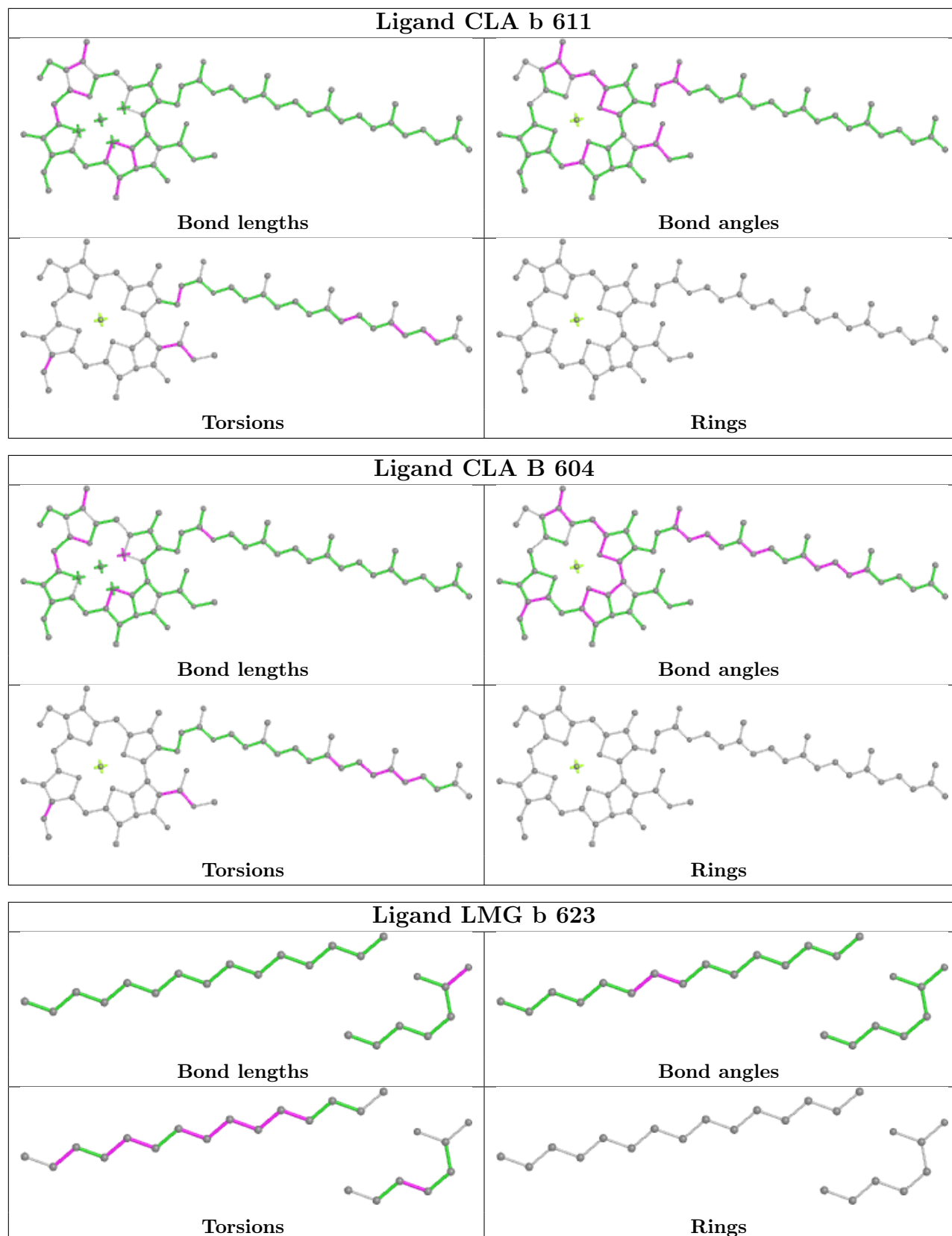


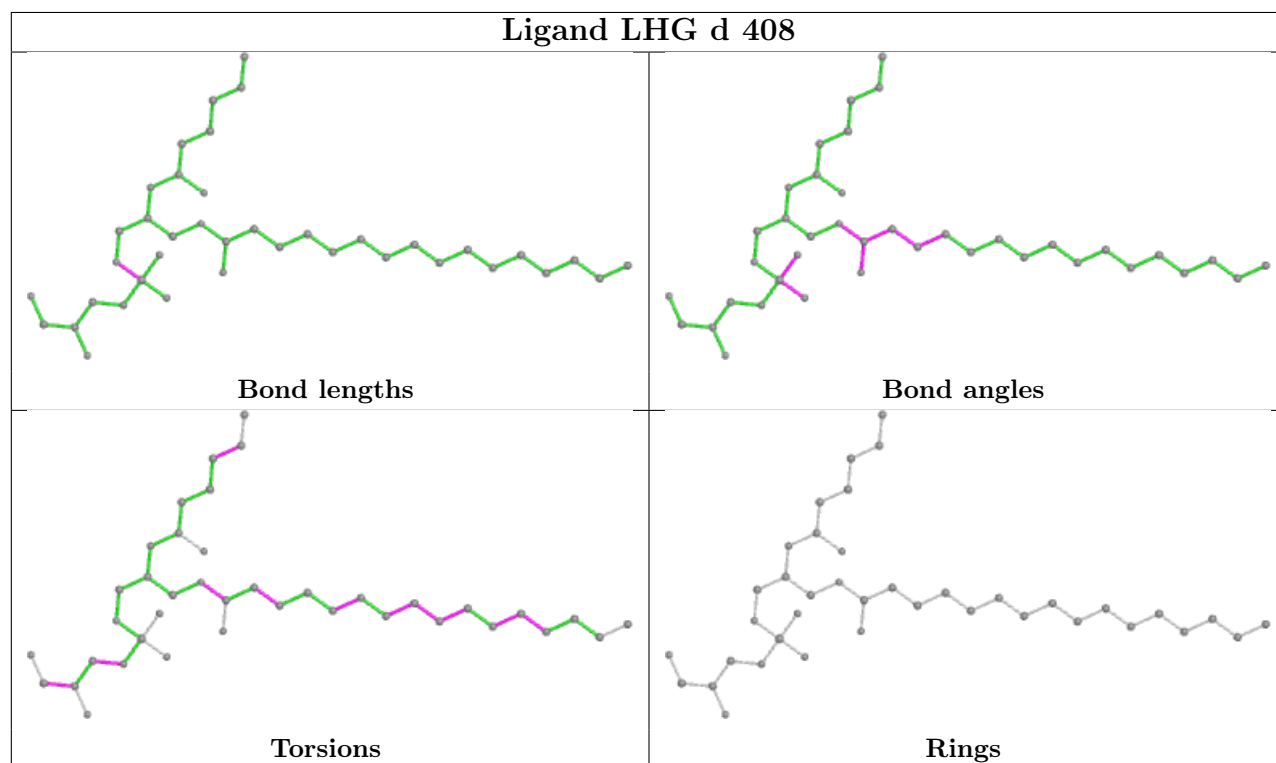
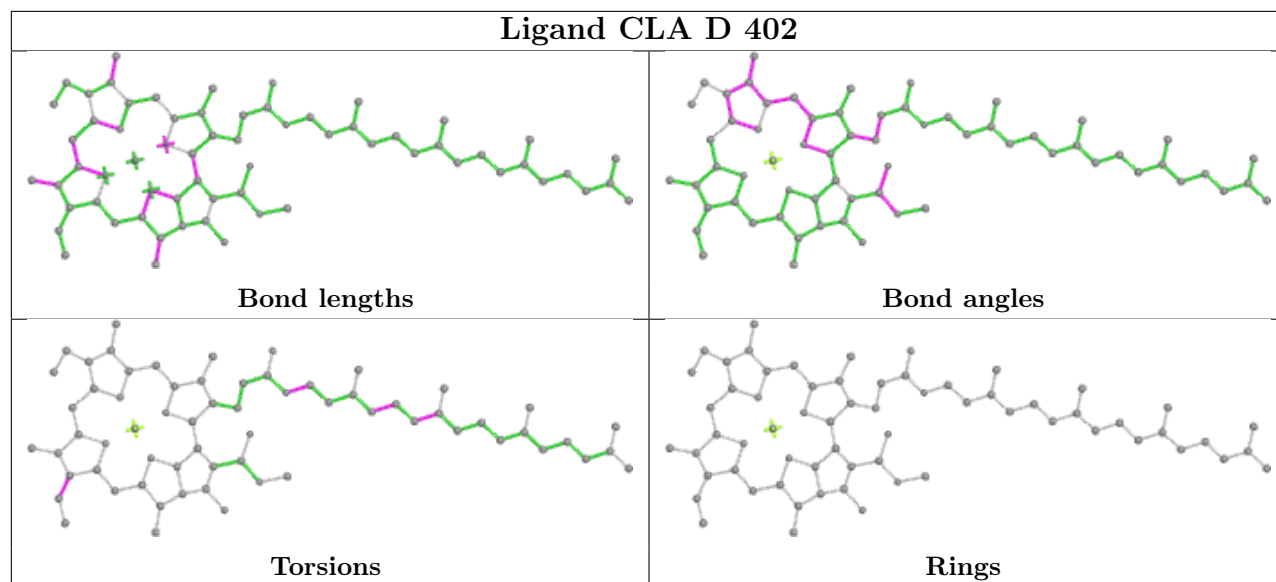


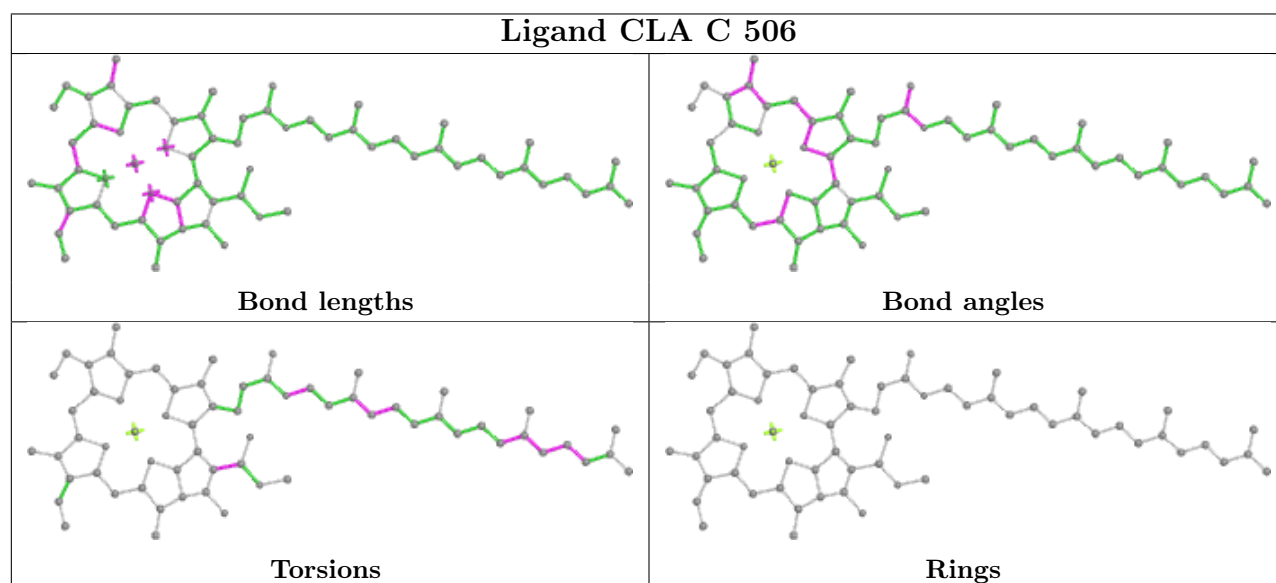
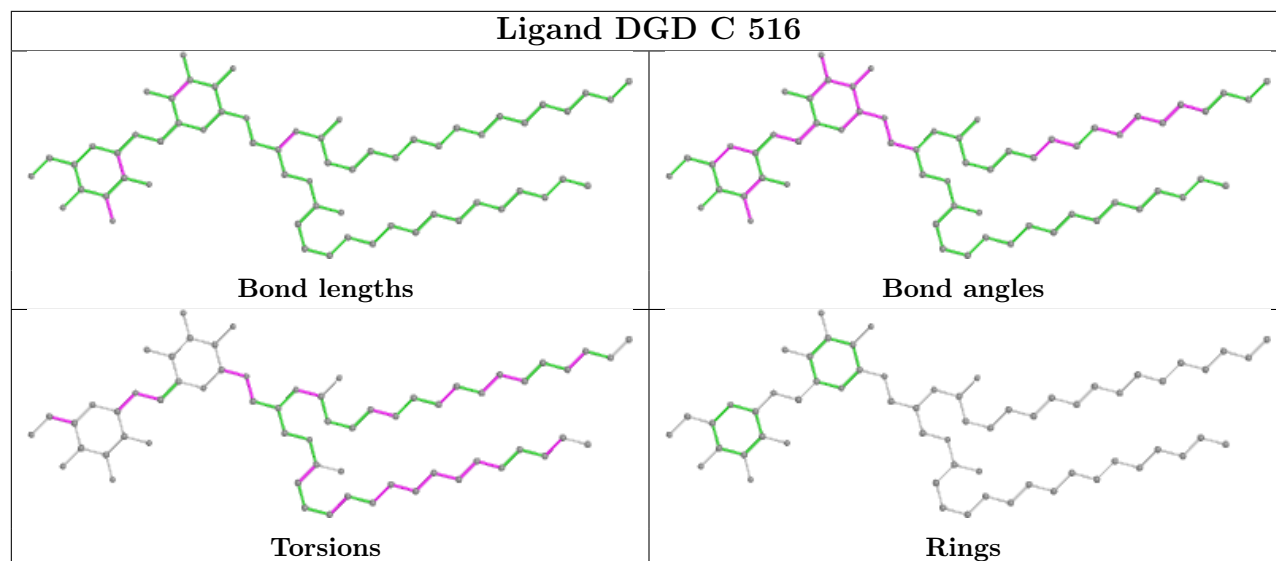


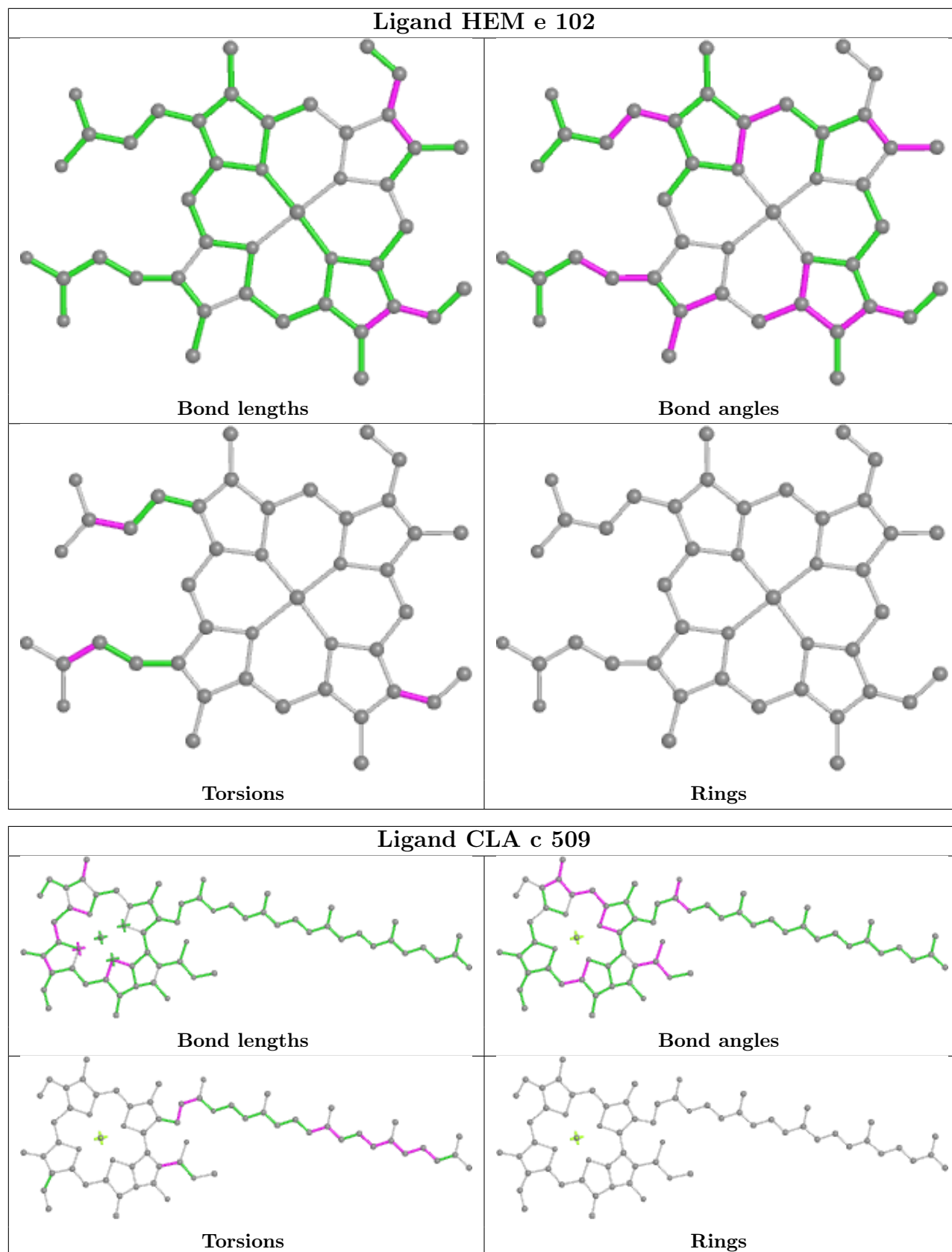




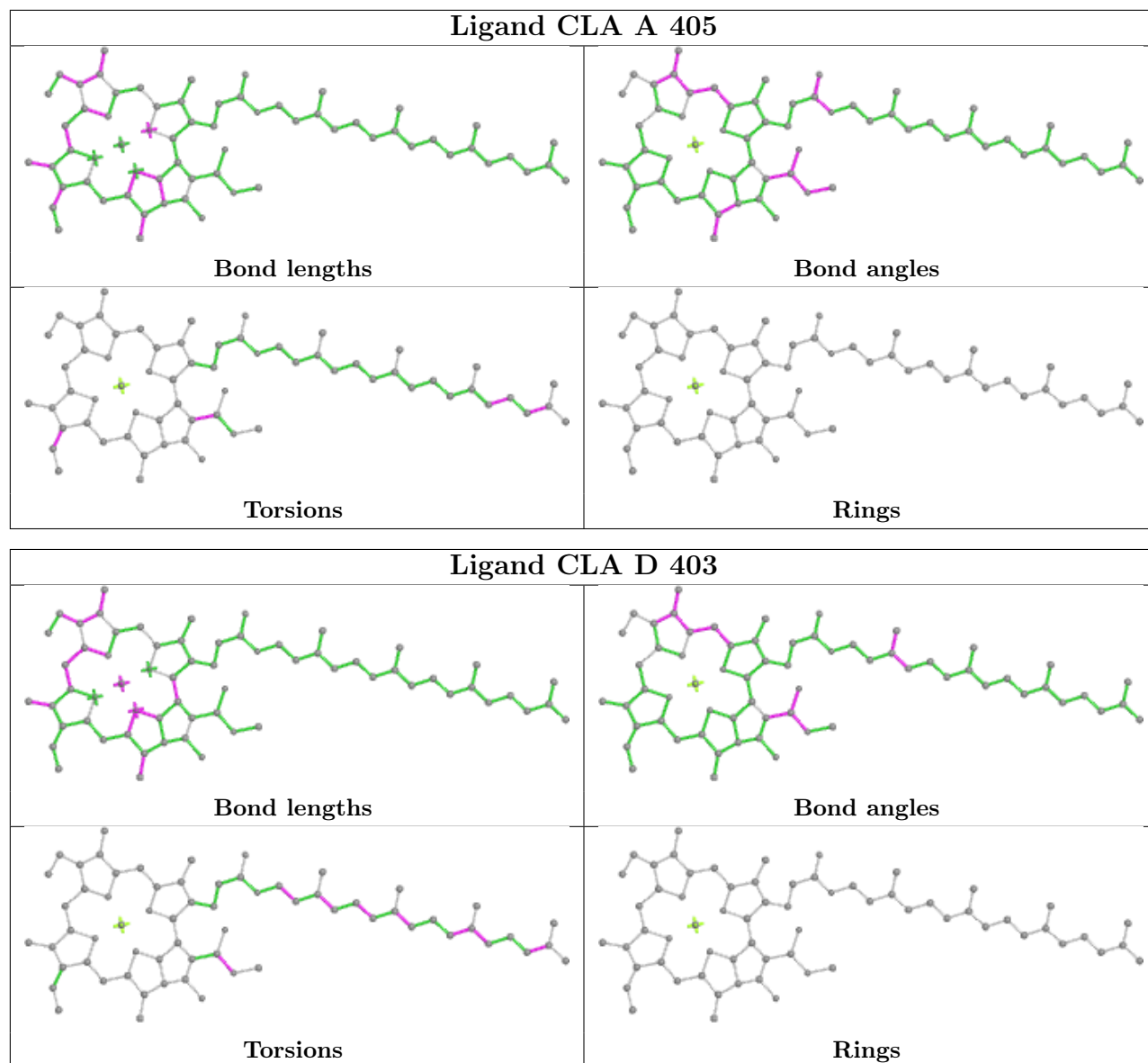


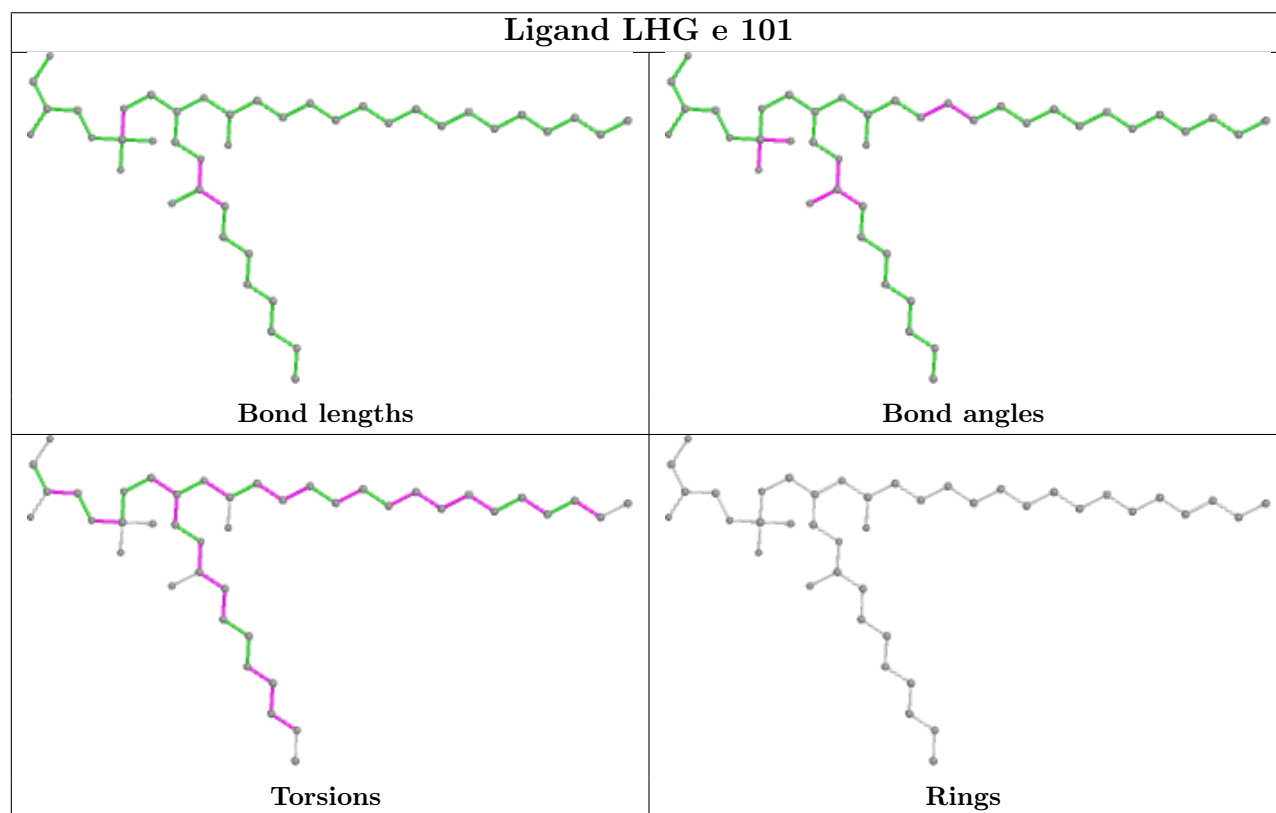
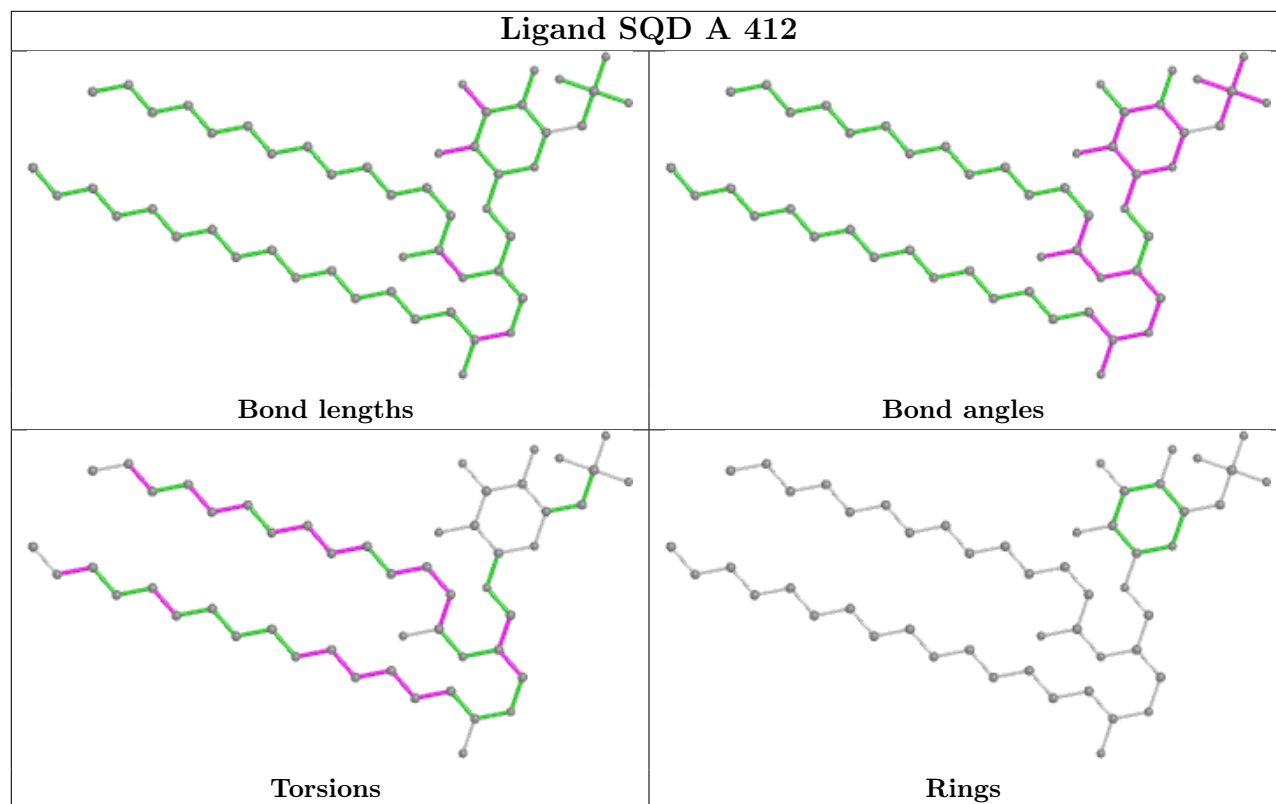


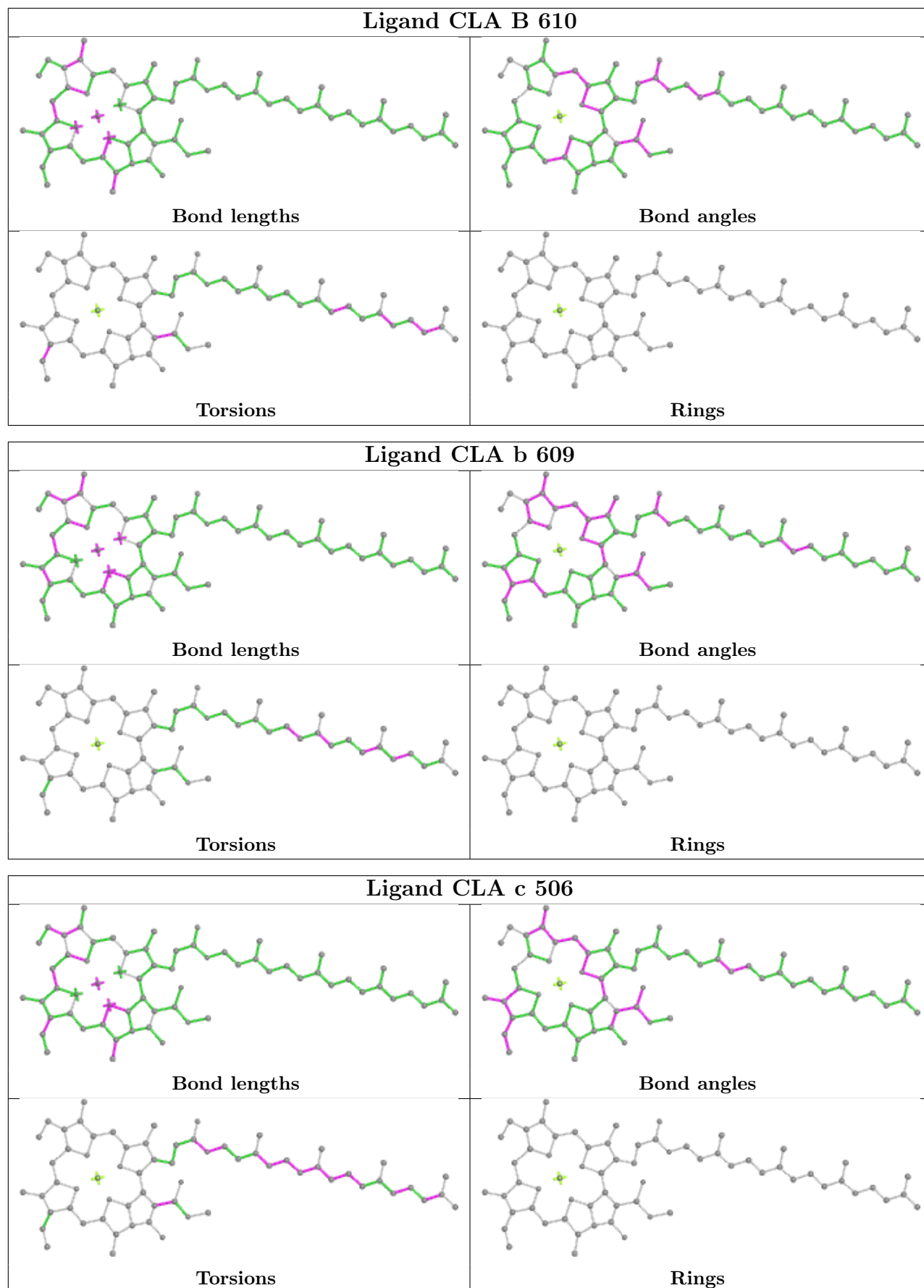


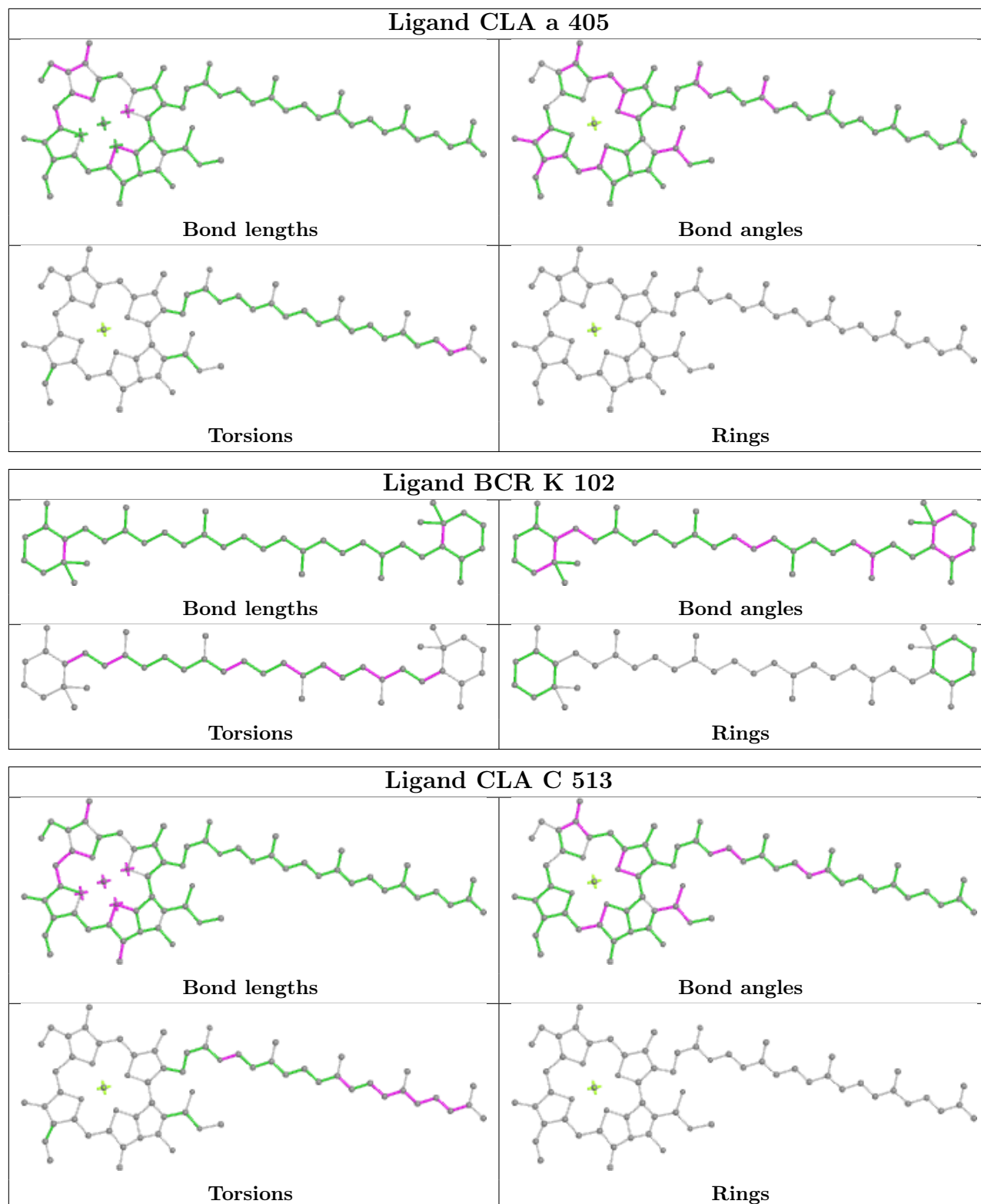


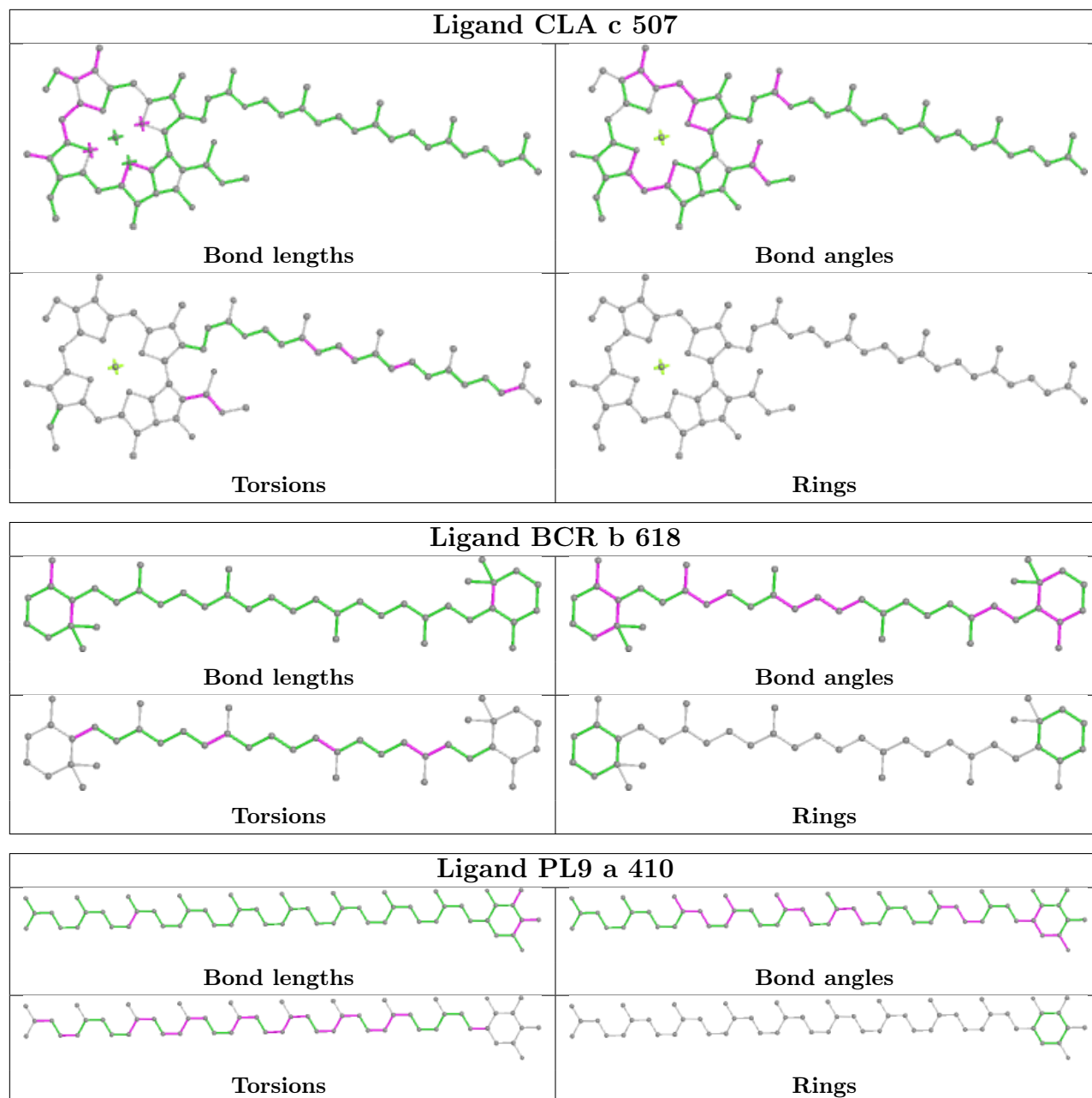


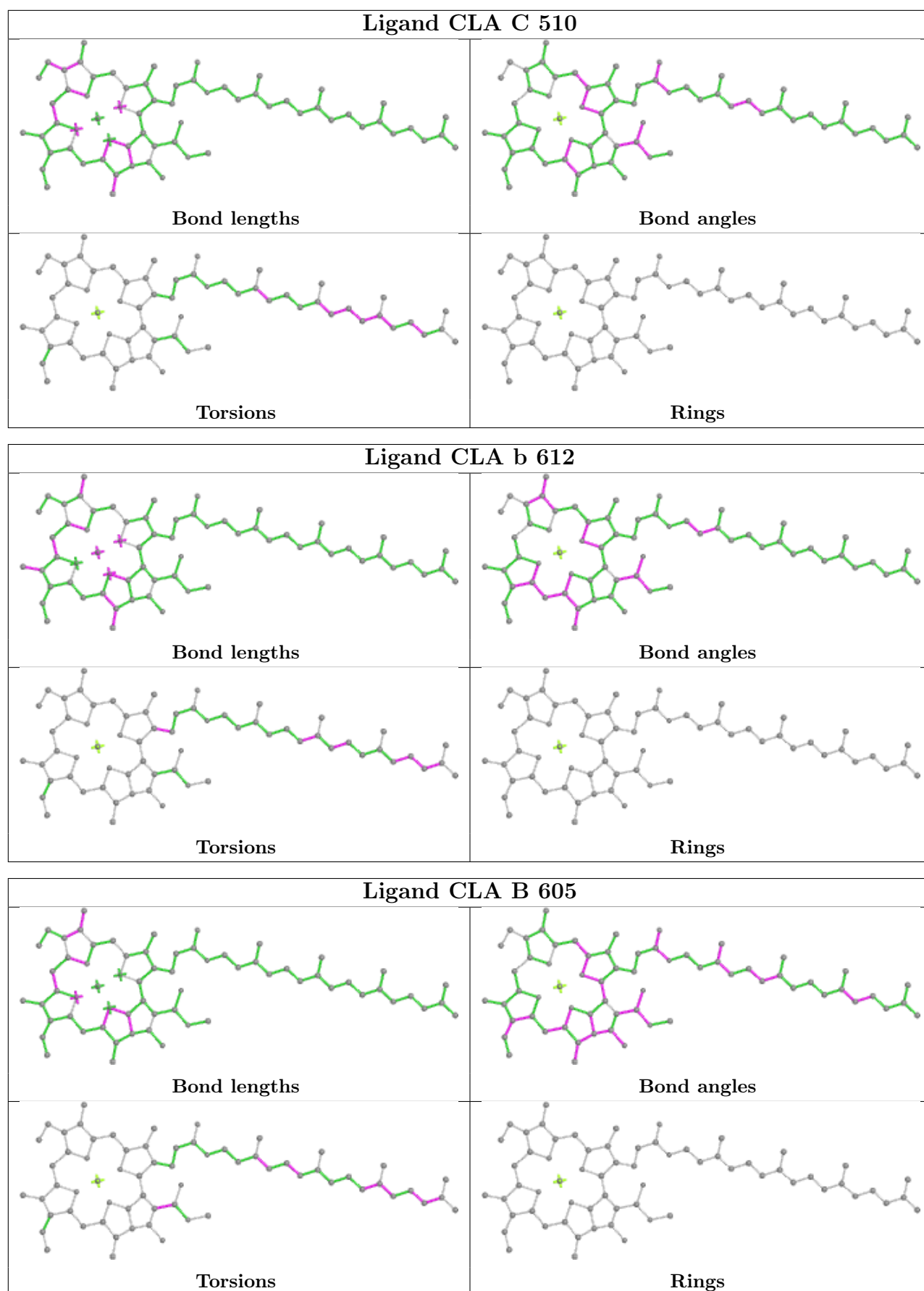


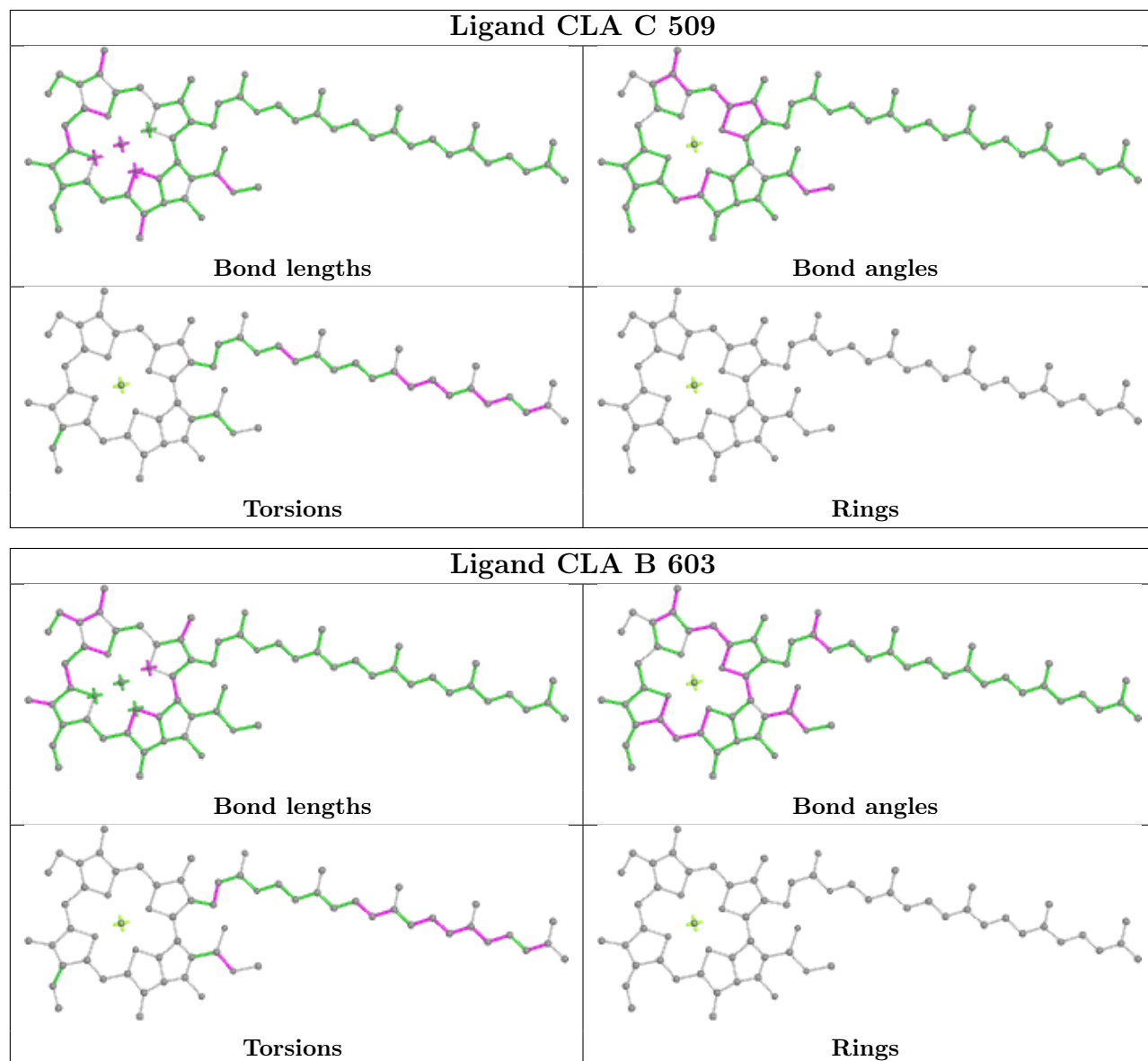


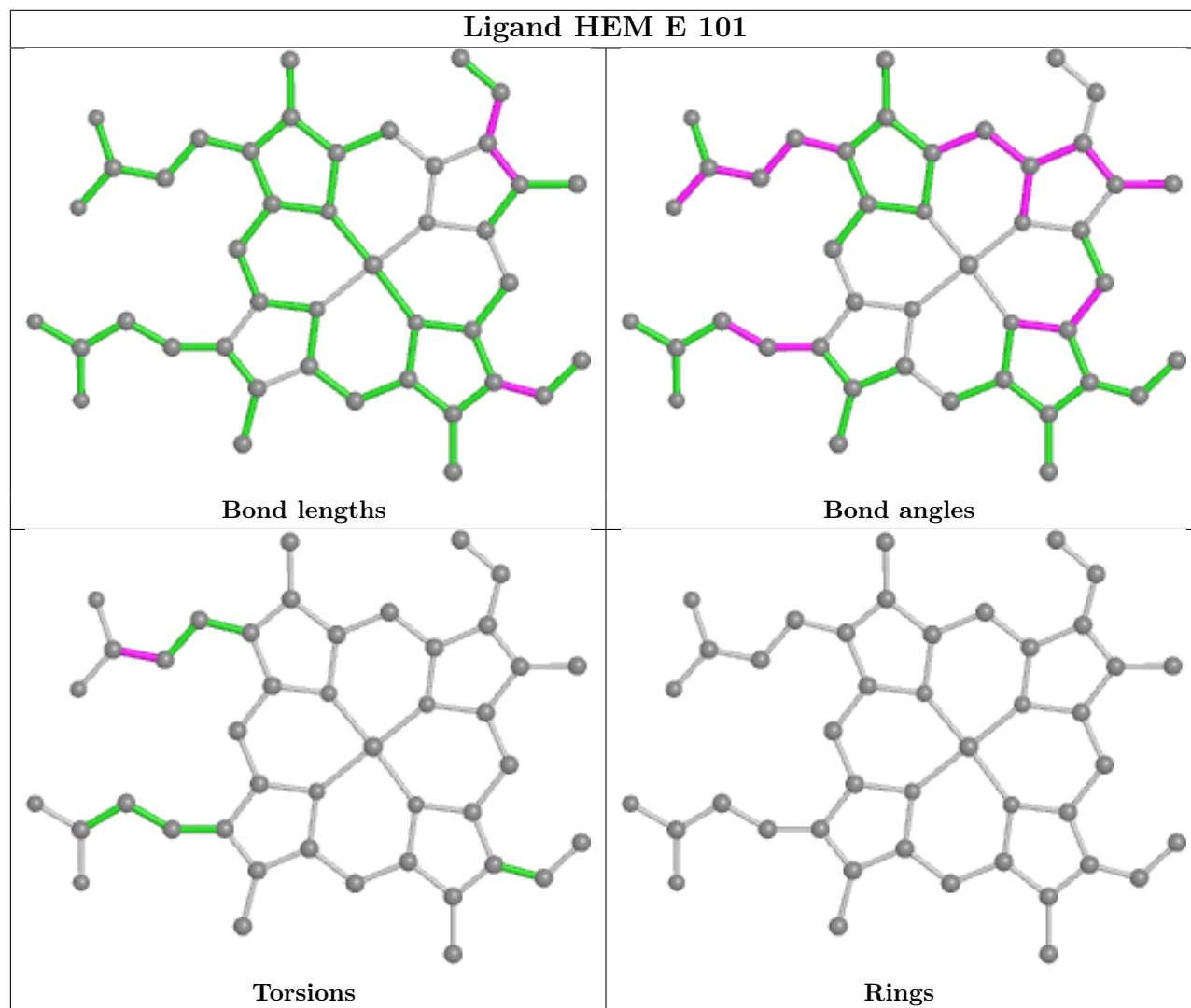




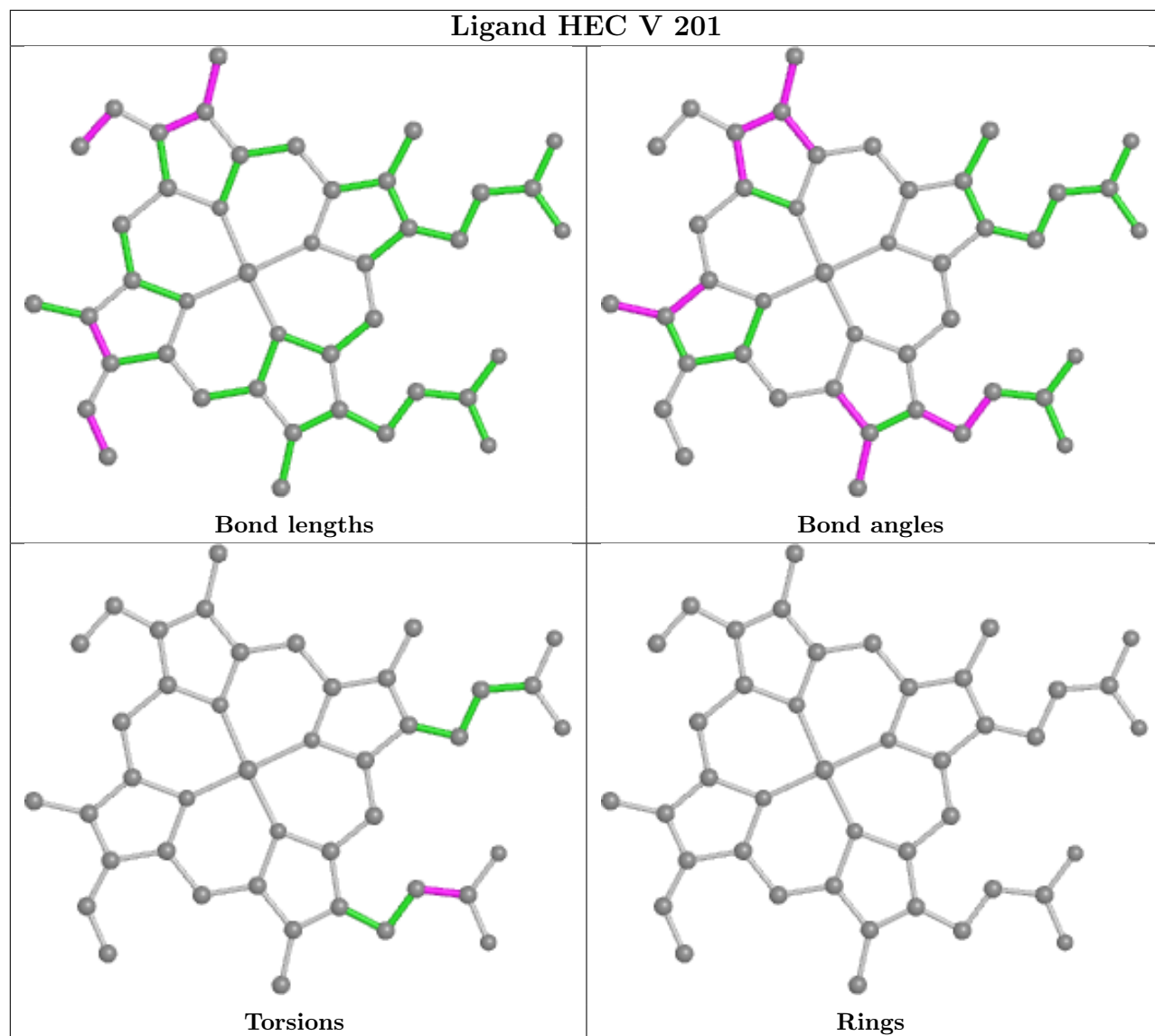


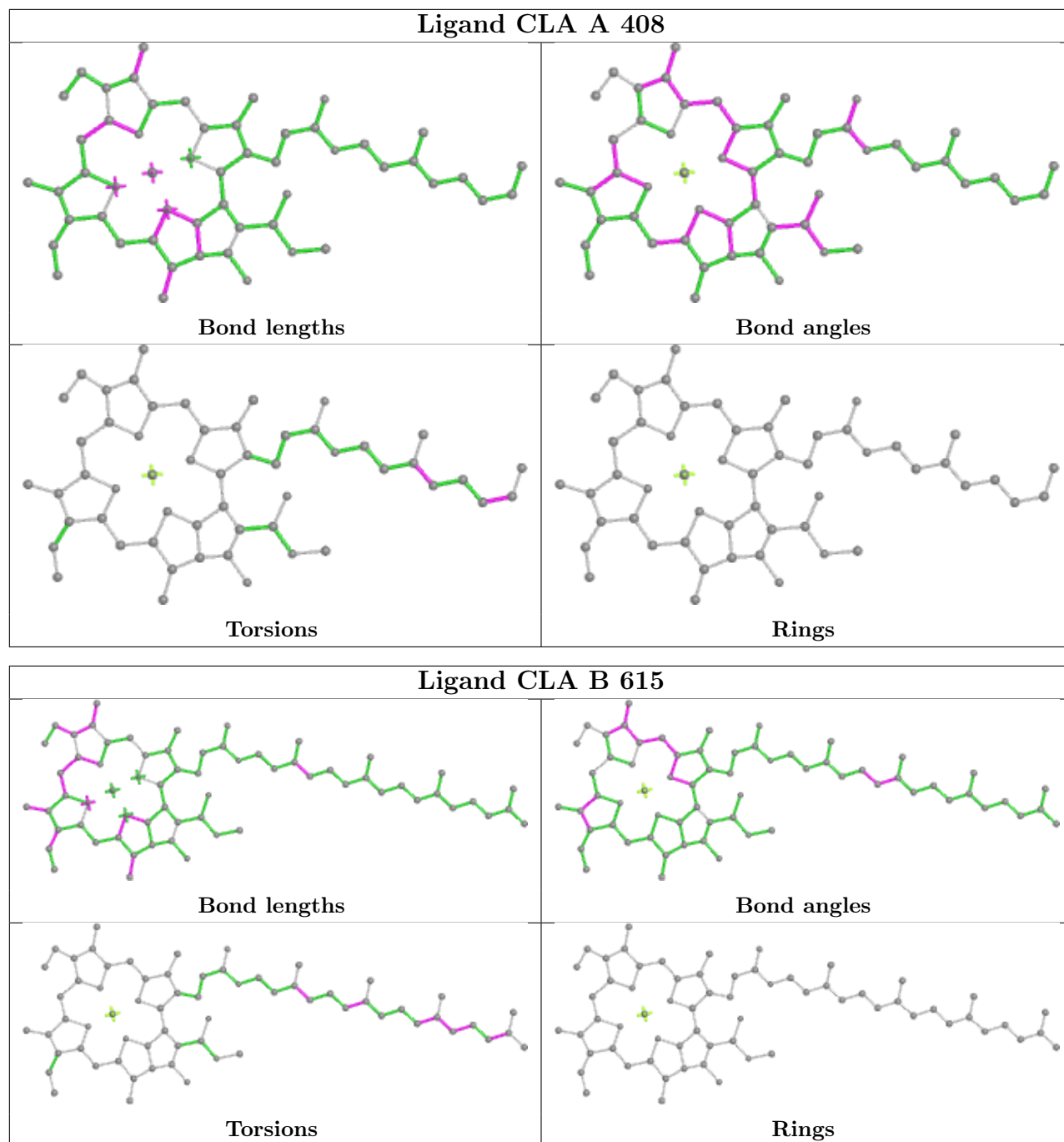


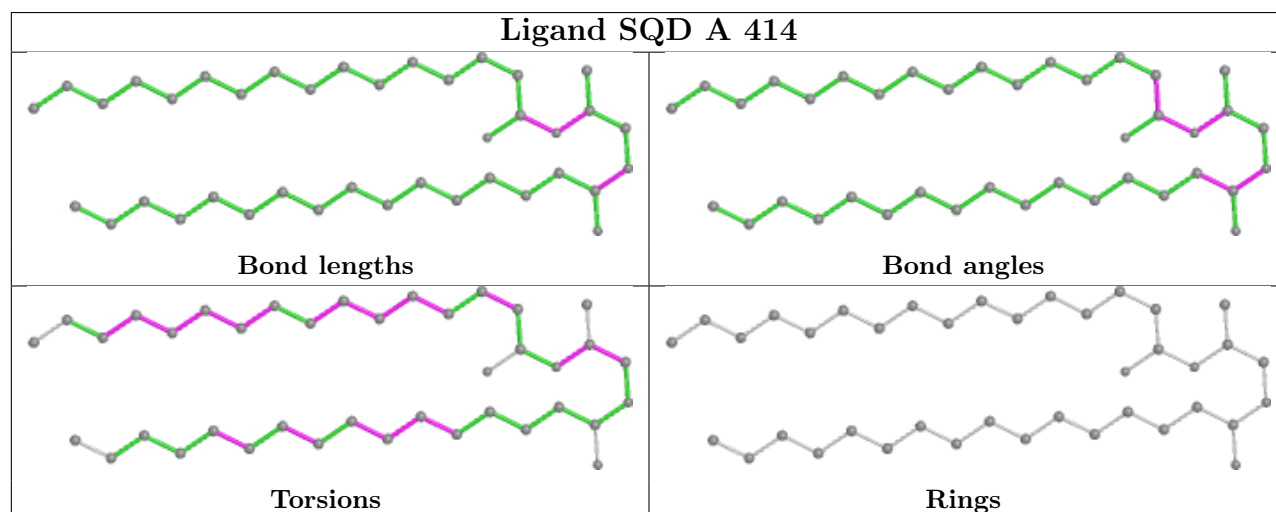
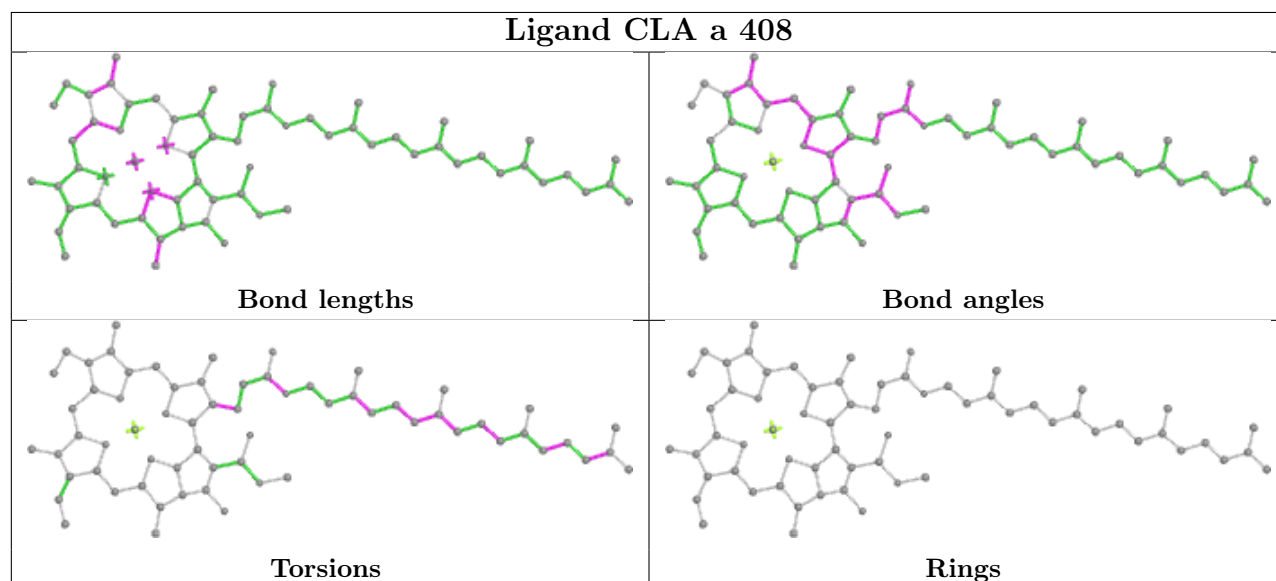
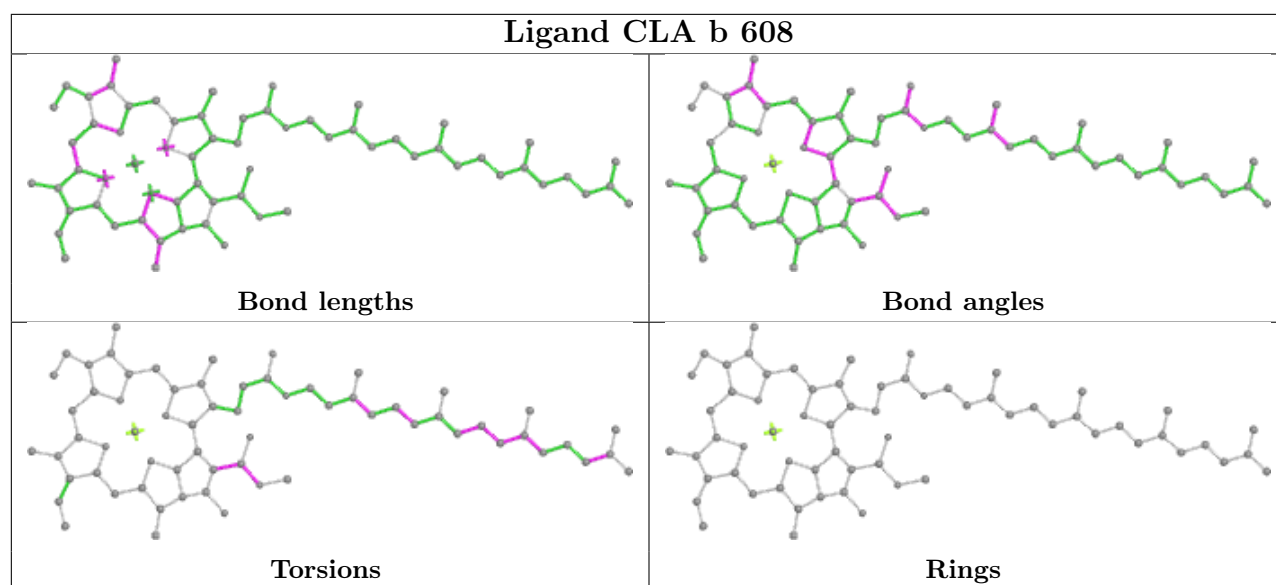


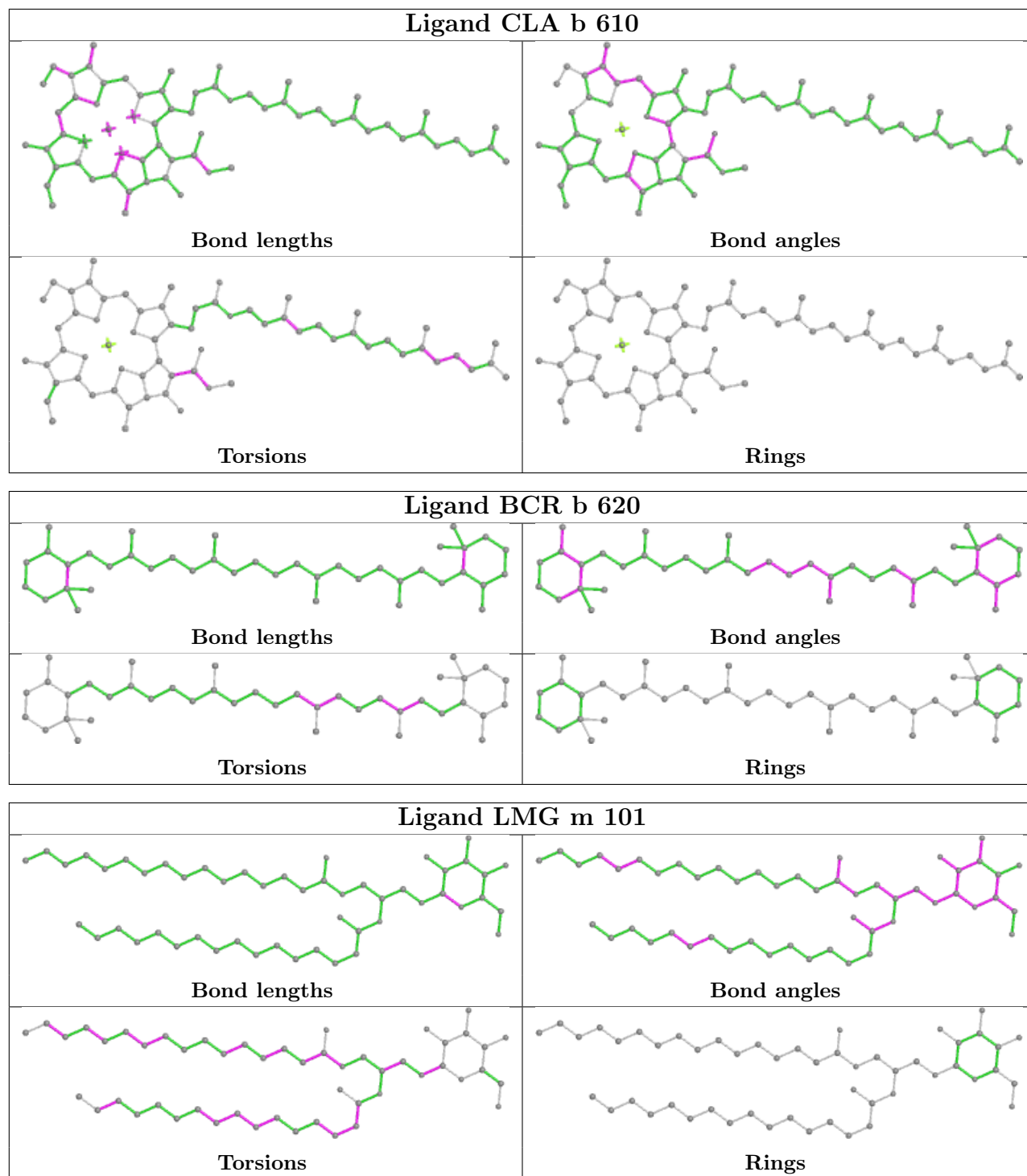


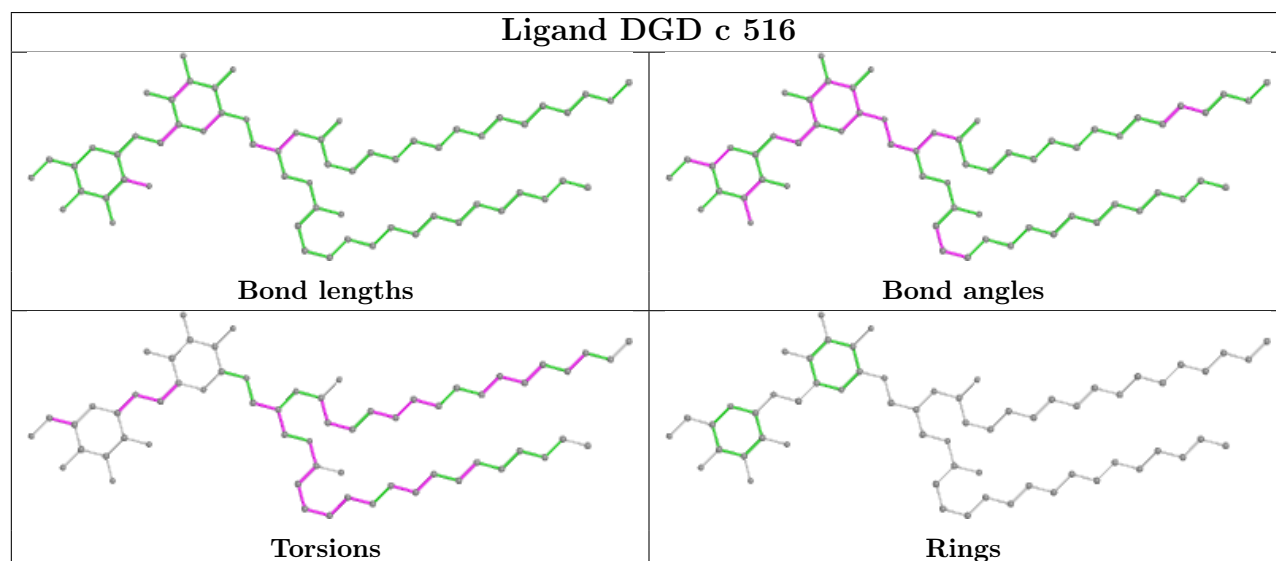
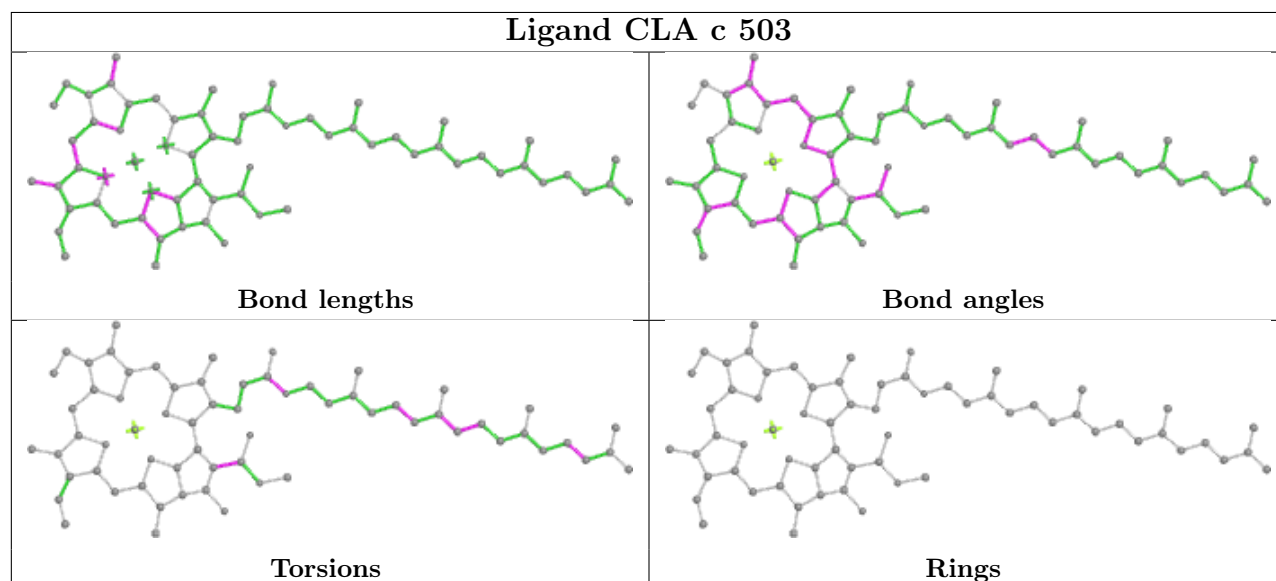
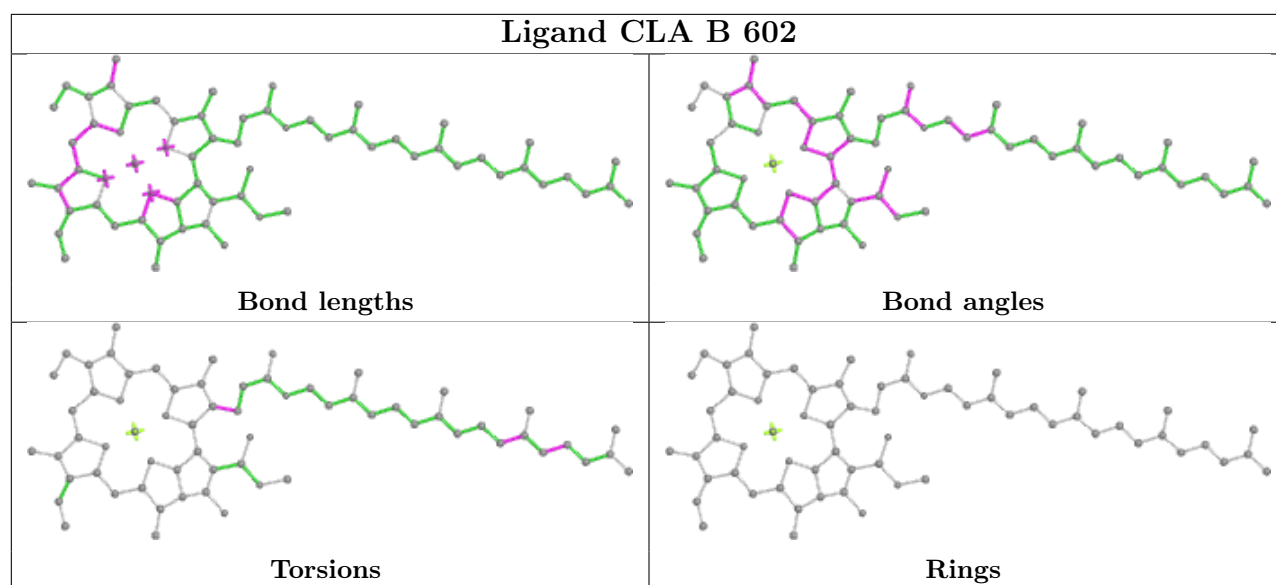


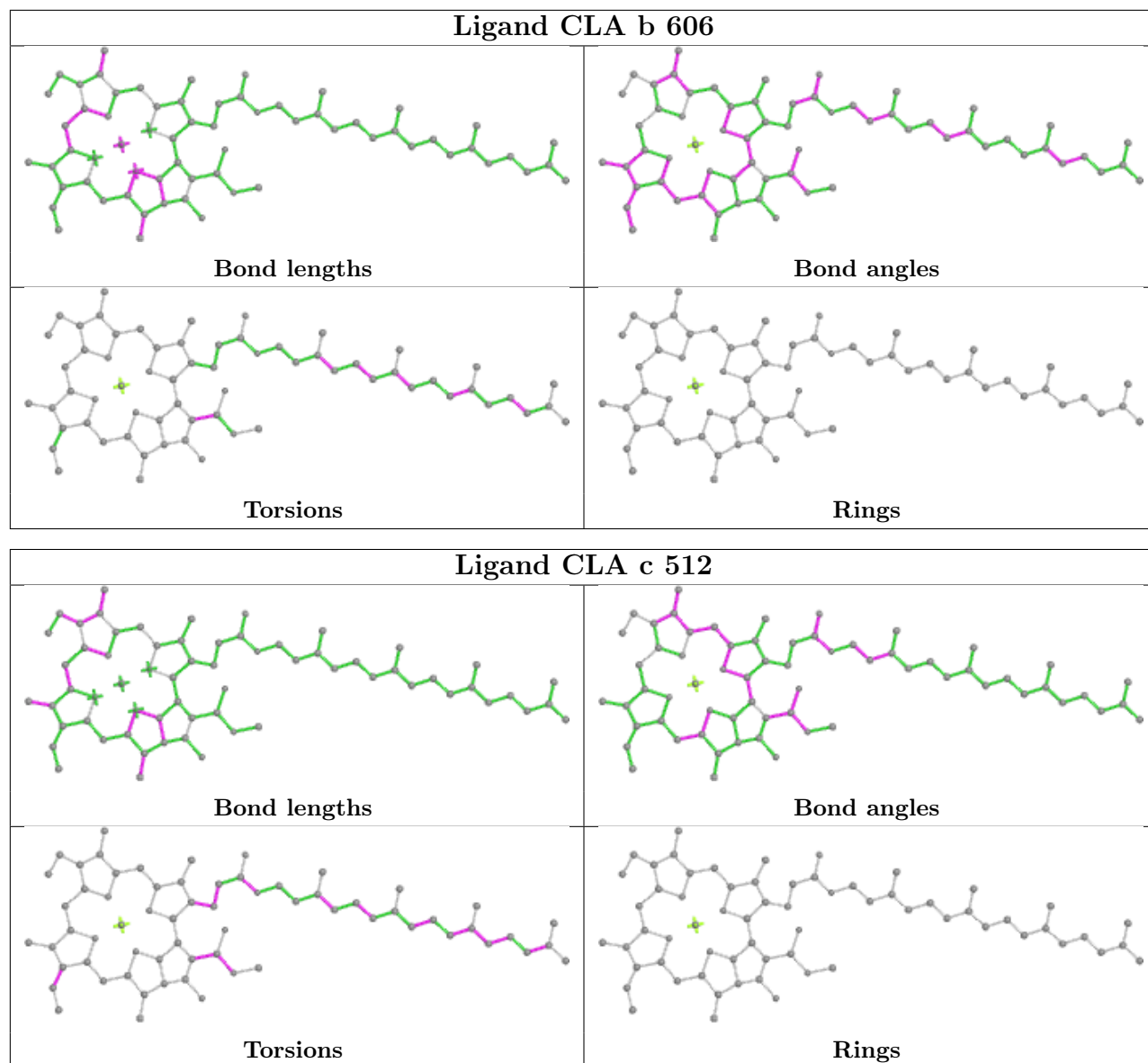


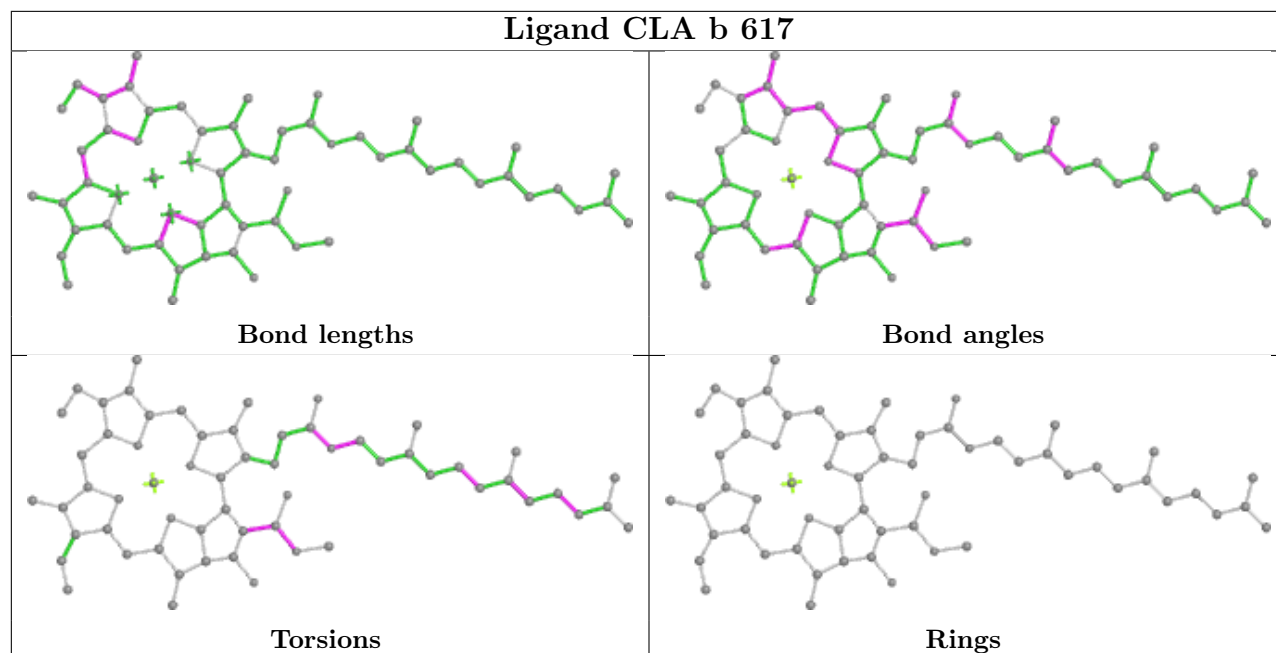












## 5.7 Other polymers [\(i\)](#)

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%)	-0.48	3 (0%) 84 85	19, 28, 48, 74	0
1	a	334/334 (100%)	-0.45	3 (0%) 84 85	21, 30, 59, 80	0
2	B	505/505 (100%)	-0.43	5 (0%) 82 83	21, 31, 61, 96	0
2	b	505/505 (100%)	-0.31	14 (2%) 53 56	19, 35, 74, 106	0
3	C	442/451 (98%)	-0.36	2 (0%) 91 91	24, 35, 53, 76	0
3	c	451/451 (100%)	-0.31	5 (1%) 80 81	24, 38, 61, 96	0
4	D	341/341 (100%)	-0.40	1 (0%) 94 94	21, 29, 48, 89	0
4	d	341/341 (100%)	-0.35	3 (0%) 84 85	23, 33, 58, 82	0
5	E	81/82 (98%)	0.14	4 (4%) 29 30	31, 50, 69, 85	0
5	e	82/82 (100%)	0.22	5 (6%) 21 21	38, 59, 80, 92	0
6	F	34/34 (100%)	-0.41	1 (2%) 51 54	34, 42, 61, 82	0
6	f	34/34 (100%)	-0.19	1 (2%) 51 54	41, 50, 73, 87	0
7	H	65/65 (100%)	-0.11	1 (1%) 73 75	33, 39, 57, 77	0
7	h	63/65 (96%)	0.17	3 (4%) 30 31	38, 47, 61, 70	0
8	I	35/36 (97%)	-0.35	2 (5%) 23 24	30, 37, 72, 79	0
8	i	35/36 (97%)	-0.16	2 (5%) 23 24	31, 38, 70, 80	0
9	J	36/36 (100%)	0.12	4 (11%) 5 5	35, 48, 76, 93	0
9	j	36/36 (100%)	0.23	4 (11%) 5 5	38, 51, 85, 92	0
10	K	37/37 (100%)	-0.21	0 100 100	40, 51, 68, 72	0
10	k	37/37 (100%)	0.12	1 (2%) 54 57	44, 55, 72, 84	0
11	L	37/37 (100%)	-0.41	0 100 100	23, 29, 67, 69	0
11	l	36/37 (97%)	-0.35	0 100 100	24, 29, 73, 81	0
12	M	32/33 (96%)	-0.31	1 (3%) 49 52	26, 32, 60, 73	0
12	m	31/33 (93%)	-0.28	0 100 100	26, 31, 50, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/244 (100%)	-0.12	12 (4%) 29 30	21, 40, 84, 142	0
13	o	244/244 (100%)	-0.14	14 (5%) 23 24	24, 39, 80, 131	0
14	T	29/30 (96%)	-0.62	2 (6%) 16 17	24, 31, 58, 71	0
14	t	29/30 (96%)	-0.44	3 (10%) 6 6	23, 31, 78, 92	0
15	U	97/97 (100%)	-0.23	3 (3%) 49 52	31, 42, 68, 95	0
15	u	97/97 (100%)	-0.47	1 (1%) 82 83	28, 38, 57, 90	0
16	V	137/137 (100%)	-0.57	0 100 100	27, 39, 56, 83	0
16	v	137/137 (100%)	-0.26	1 (0%) 87 88	33, 46, 66, 78	0
17	Y	27/30 (90%)	1.79	11 (40%) 0 0	53, 74, 115, 119	0
17	y	30/30 (100%)	0.78	5 (16%) 1 1	59, 73, 90, 105	0
18	X	38/38 (100%)	0.15	3 (7%) 12 13	38, 48, 74, 78	0
18	x	38/38 (100%)	0.50	5 (13%) 3 2	46, 56, 87, 99	0
19	Z	62/62 (100%)	0.60	15 (24%) 0 0	48, 66, 110, 124	0
19	z	62/62 (100%)	0.98	14 (22%) 0 0	53, 69, 107, 122	0
20	R	34/34 (100%)	1.82	13 (38%) 0 0	59, 70, 89, 97	0
20	r	31/34 (91%)	2.38	17 (54%) 0 0	71, 85, 98, 104	0
All	All	5300/5326 (99%)	-0.23	184 (3%) 44 46	19, 37, 74, 142	0

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	59	LYS	9.8
17	Y	20	ALA	8.4
19	z	33	TRP	7.4
13	o	3	GLN	7.3
13	o	58	ASN	7.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	FME	i	1	10/11	0.95	0.13	35,48,60,64	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	0.95	0.09	29,37,64,69	0
12	FME	M	1	10/11	0.96	0.13	34,48,63,68	0
14	FME	T	1	10/11	0.96	0.10	27,44,65,71	0
12	FME	m	1	10/11	0.97	0.12	31,46,65,72	0
8	FME	I	1	10/11	0.97	0.13	35,54,65,68	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
34	UNL	a	415	28/-	0.70	0.27	39,66,77,79	0
34	UNL	E	102	28/-	0.72	0.29	52,79,91,94	0
34	UNL	H	103	53/-	0.73	0.22	43,73,86,90	0
34	UNL	c	520	55/-	0.77	0.17	39,61,79,86	0
27	LMG	b	623	23/55	0.78	0.24	43,70,95,98	0
34	UNL	c	522	28/-	0.78	0.19	46,66,88,93	0
29	LHG	A	413	49/49	0.79	0.24	51,85,125,130	0
26	PL9	A	410	55/55	0.81	0.24	39,62,83,94	135
34	UNL	B	627	28/-	0.81	0.39	42,64,86,91	0
34	UNL	C	521	47/-	0.81	0.13	37,56,73,74	0
28	SQD	a	413	36/54	0.81	0.15	31,67,87,96	0
34	UNL	b	624	40/-	0.82	0.18	46,63,83,85	0
34	UNL	b	626	55/-	0.82	0.17	44,61,77,81	0
23	CLA	h	101	65/65	0.82	0.16	45,69,93,104	0
27	LMG	D	409	33/55	0.82	0.17	32,54,107,111	0
34	UNL	t	103	26/-	0.82	0.17	42,64,76,81	0
30	DGD	A	415	66/66	0.83	0.19	45,68,93,108	0
25	BCR	x	101	40/40	0.83	0.15	35,57,76,82	0
34	UNL	B	628	47/-	0.83	0.24	47,65,78,89	0
27	LMG	c	521	48/55	0.83	0.24	44,77,121,128	0
34	UNL	B	626	46/-	0.85	0.14	44,64,84,93	0
28	SQD	f	101	41/54	0.85	0.22	54,87,117,125	0
26	PL9	a	410	55/55	0.85	0.22	36,67,91,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	LHG	e	101	42/49	0.85	0.27	57,87,116,139	0
28	SQD	b	601	49/54	0.85	0.14	38,60,102,112	0
34	UNL	d	411	55/-	0.85	0.19	42,58,72,73	0
34	UNL	m	102	28/-	0.85	0.14	42,59,73,78	0
30	DGD	a	414	44/66	0.85	0.16	36,58,84,92	0
34	UNL	X	101	55/-	0.86	0.20	34,49,75,79	0
23	CLA	c	512	65/65	0.86	0.14	40,58,97,107	0
25	BCR	k	101	40/40	0.86	0.12	39,65,81,83	0
34	UNL	l	102	53/-	0.86	0.16	33,50,87,91	0
27	LMG	b	622	55/55	0.86	0.27	35,73,101,104	0
34	UNL	b	627	26/-	0.86	0.21	42,58,69,74	0
34	UNL	b	621	55/-	0.87	0.21	39,57,86,91	0
34	UNL	j	101	28/-	0.87	0.13	42,56,67,67	0
34	UNL	B	620	43/-	0.87	0.11	34,51,68,74	0
34	UNL	I	101	41/-	0.87	0.13	37,53,75,79	0
34	UNL	d	410	43/-	0.87	0.16	39,58,70,78	0
27	LMG	A	411	48/55	0.88	0.17	37,62,78,103	0
23	CLA	c	513	65/65	0.88	0.20	47,72,109,114	0
27	LMG	c	519	37/55	0.88	0.17	44,70,88,97	0
23	CLA	C	513	65/65	0.89	0.16	45,68,95,101	0
27	LMG	c	523	49/55	0.89	0.13	32,56,87,111	0
28	SQD	B	624	54/54	0.89	0.13	39,58,90,100	0
27	LMG	C	518	48/55	0.89	0.14	43,72,96,103	0
23	CLA	C	512	65/65	0.89	0.15	33,56,102,109	0
34	UNL	t	102	34/-	0.89	0.14	35,50,58,65	0
34	UNL	b	602	47/-	0.89	0.15	35,50,64,73	0
34	UNL	M	102	37/-	0.90	0.12	26,45,54,69	0
23	CLA	a	408	65/65	0.90	0.14	16,36,95,107	0
28	SQD	A	414	39/54	0.90	0.19	36,69,93,99	0
23	CLA	b	617	60/65	0.90	0.14	28,44,105,113	0
25	BCR	H	101	40/40	0.90	0.10	31,47,57,62	0
25	BCR	K	101	40/40	0.90	0.12	36,53,73,79	0
34	UNL	b	625	44/-	0.90	0.16	34,58,80,84	0
23	CLA	B	616	60/65	0.90	0.16	23,41,93,102	0
34	UNL	J	101	28/-	0.90	0.15	52,64,78,86	0
27	LMG	m	101	51/55	0.91	0.11	30,51,81,97	0
27	LMG	M	101	51/55	0.91	0.11	25,47,72,84	0
25	BCR	D	404	40/40	0.91	0.12	25,46,103,108	0
34	UNL	B	625	28/-	0.91	0.09	31,46,69,70	0
23	CLA	B	601	65/65	0.91	0.13	32,61,99,105	0
25	BCR	c	514	40/40	0.92	0.17	40,59,77,79	0
23	CLA	b	616	65/65	0.92	0.13	26,39,62,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
27	LMG	B	621	28/55	0.92	0.14	31,47,60,70	0
23	CLA	D	403	65/65	0.92	0.14	23,40,121,137	0
28	SQD	a	412	54/54	0.92	0.14	34,69,91,95	0
25	BCR	Z	101	40/40	0.92	0.12	34,57,72,75	0
30	DGD	h	102	62/66	0.92	0.12	33,52,65,70	0
30	DGD	H	102	62/66	0.93	0.10	30,49,61,74	0
23	CLA	d	403	65/65	0.93	0.12	29,49,97,109	0
23	CLA	C	505	65/65	0.93	0.17	25,43,73,83	0
25	BCR	C	514	40/40	0.93	0.10	27,39,54,59	0
23	CLA	c	502	65/65	0.93	0.12	27,43,65,69	0
23	CLA	c	503	65/65	0.93	0.14	32,45,56,62	0
23	CLA	c	508	64/65	0.93	0.13	30,45,93,113	0
27	LMG	D	406	51/55	0.93	0.15	26,56,89,97	0
23	CLA	c	510	65/65	0.93	0.13	33,50,69,76	0
25	BCR	b	619	40/40	0.93	0.09	27,39,55,58	0
23	CLA	B	615	65/65	0.93	0.12	24,36,70,87	0
25	BCR	d	404	40/40	0.93	0.10	36,54,90,102	0
23	CLA	B	606	65/65	0.93	0.10	21,35,73,83	0
30	DGD	C	515	62/66	0.93	0.13	21,40,86,103	0
34	UNL	M	103	26/-	0.93	0.16	24,49,57,63	0
30	DGD	C	516	62/66	0.93	0.11	30,54,108,129	0
25	BCR	B	617	40/40	0.94	0.10	26,40,54,56	0
25	BCR	B	618	40/40	0.94	0.09	23,39,54,56	0
23	CLA	C	510	65/65	0.94	0.12	29,46,75,87	0
23	CLA	C	503	65/65	0.94	0.11	29,42,52,55	0
34	UNL	C	519	28/-	0.94	0.09	34,46,55,56	0
34	UNL	C	520	28/-	0.94	0.09	42,51,64,65	0
23	CLA	C	502	65/65	0.94	0.11	24,44,56,64	0
23	CLA	C	506	65/65	0.94	0.11	27,42,95,110	0
25	BCR	K	102	40/40	0.94	0.15	34,58,73,76	0
27	LMG	d	409	44/55	0.94	0.11	31,58,89,105	0
25	BCR	T	101	40/40	0.94	0.09	27,40,60,62	0
23	CLA	c	504	60/65	0.94	0.12	30,44,86,93	0
25	BCR	b	618	40/40	0.94	0.10	22,43,54,58	0
28	SQD	F	101	36/54	0.94	0.14	41,71,87,95	0
23	CLA	c	505	65/65	0.94	0.14	23,43,68,72	0
23	CLA	c	506	65/65	0.94	0.13	28,51,111,120	0
23	CLA	c	507	65/65	0.94	0.14	21,43,62,66	0
23	CLA	a	406	65/65	0.94	0.11	24,40,100,112	0
25	BCR	k	102	40/40	0.94	0.15	37,57,66,73	0
29	LHG	d	408	39/49	0.94	0.11	26,47,73,78	0
23	CLA	c	509	65/65	0.94	0.17	30,48,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	CLA	C	507	65/65	0.94	0.12	23,40,57,62	0
26	PL9	D	405	55/55	0.94	0.12	17,32,48,52	0
23	CLA	c	511	65/65	0.94	0.14	34,57,74,76	0
23	CLA	b	605	65/65	0.94	0.15	21,34,88,99	0
23	CLA	b	607	65/65	0.94	0.10	24,40,74,83	0
30	DGD	c	517	62/66	0.94	0.09	31,52,86,96	0
30	DGD	c	518	62/66	0.94	0.10	29,52,82,94	0
23	CLA	b	610	65/65	0.94	0.11	30,46,71,89	0
23	CLA	b	615	65/65	0.94	0.14	20,37,81,97	0
25	BCR	c	515	40/40	0.95	0.11	31,48,64,72	0
28	SQD	A	412	52/54	0.95	0.14	32,61,93,101	0
23	CLA	b	614	65/65	0.95	0.12	18,32,77,84	0
23	CLA	A	405	65/65	0.95	0.11	18,34,99,118	0
23	CLA	C	511	65/65	0.95	0.10	35,51,67,69	0
25	BCR	t	101	40/40	0.95	0.07	25,36,53,61	0
24	PHO	a	407	64/64	0.95	0.11	22,31,40,48	0
25	BCR	A	409	40/40	0.95	0.09	24,34,43,47	0
23	CLA	B	604	65/65	0.95	0.11	18,31,79,87	0
23	CLA	A	408	54/65	0.95	0.12	16,30,74,77	0
29	LHG	D	408	47/49	0.95	0.10	26,46,84,100	0
29	LHG	d	406	49/49	0.95	0.12	36,52,82,94	0
26	PL9	d	405	55/55	0.95	0.10	21,35,44,47	0
25	BCR	B	619	40/40	0.95	0.09	27,42,65,78	0
29	LHG	l	101	49/49	0.95	0.11	29,48,59,64	0
23	CLA	D	402	65/65	0.95	0.11	15,32,58,67	0
23	CLA	B	609	65/65	0.95	0.10	24,35,57,66	0
23	CLA	B	610	65/65	0.95	0.14	16,31,44,48	0
30	DGD	C	517	62/66	0.95	0.09	23,45,82,93	0
23	CLA	B	612	65/65	0.95	0.14	21,32,46,51	0
23	CLA	b	603	65/65	0.95	0.15	26,42,73,83	0
30	DGD	c	516	62/66	0.95	0.10	21,43,78,84	0
23	CLA	B	614	65/65	0.95	0.14	21,38,83,95	0
23	CLA	C	508	65/65	0.95	0.12	23,41,119,127	0
23	CLA	C	509	65/65	0.95	0.14	26,45,65,79	0
23	CLA	b	611	65/65	0.95	0.13	24,38,51,57	0
25	BCR	b	620	40/40	0.95	0.10	28,47,61,67	0
23	CLA	b	613	65/65	0.95	0.15	20,34,49,55	0
29	LHG	B	623	49/49	0.96	0.11	25,44,76,87	0
23	CLA	b	604	65/65	0.96	0.12	18,37,70,77	0
23	CLA	B	605	65/65	0.96	0.14	18,30,44,46	0
29	LHG	d	407	49/49	0.96	0.11	24,44,61,72	0
23	CLA	b	606	65/65	0.96	0.11	21,35,52,57	0

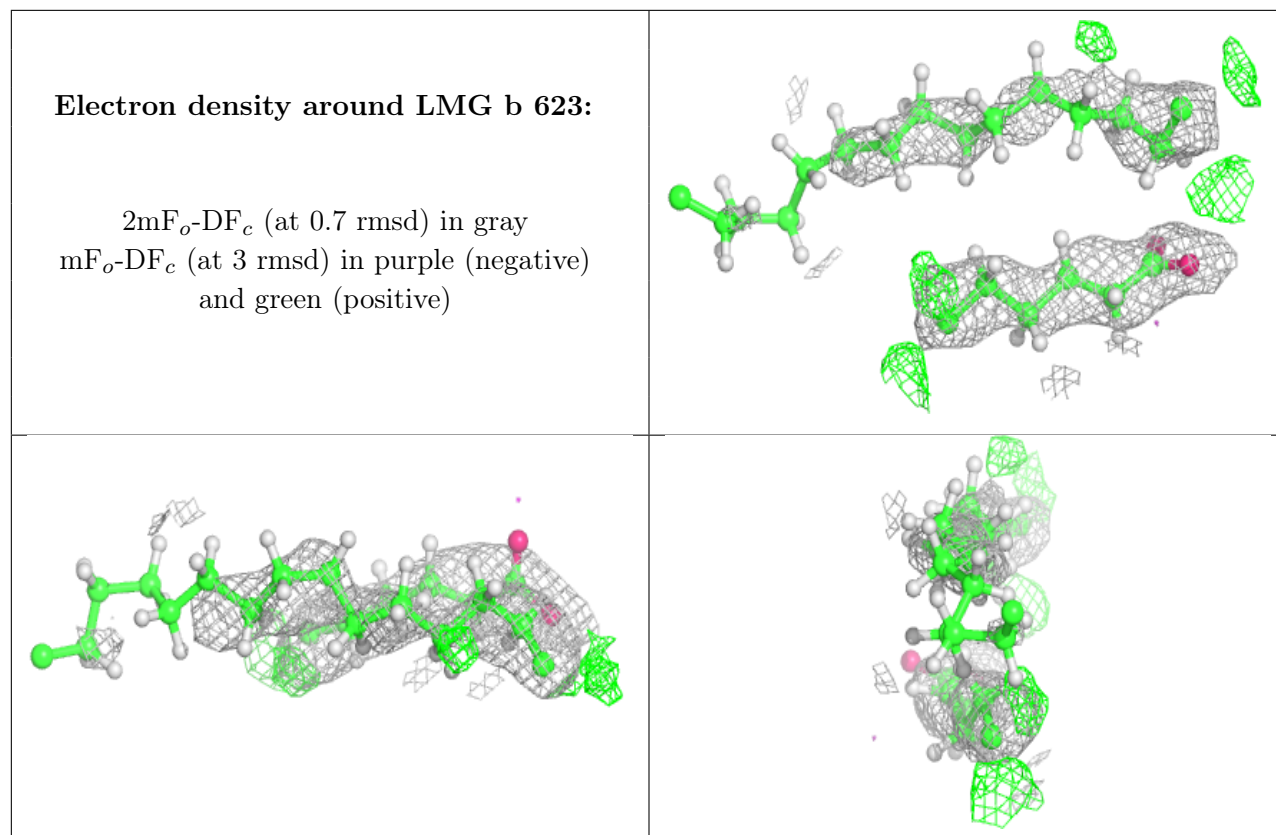
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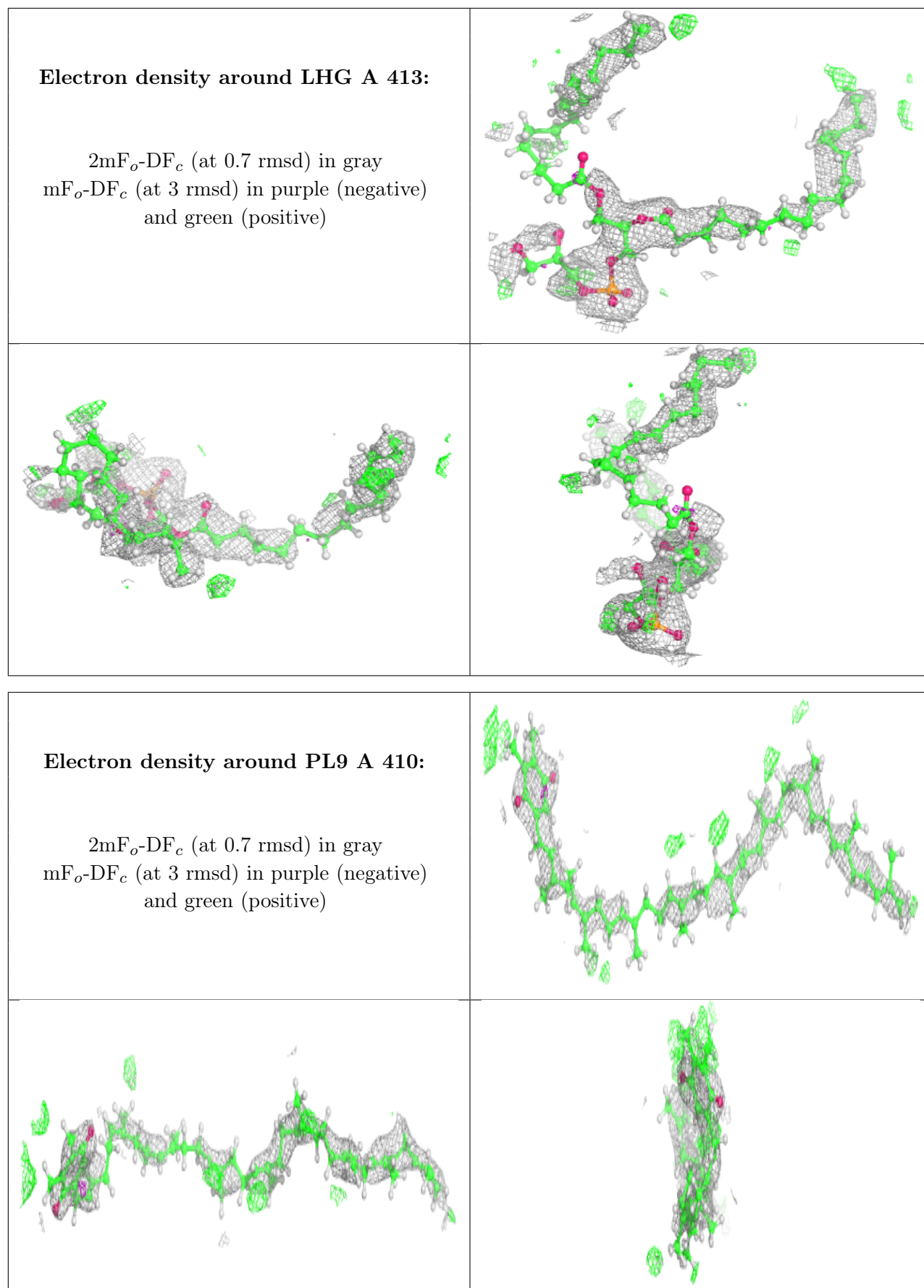
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	CLA	C	504	59/65	0.96	0.13	24,44,83,93	0
23	CLA	b	608	65/65	0.96	0.11	18,35,66,74	0
23	CLA	b	609	65/65	0.96	0.12	24,41,70,74	0
23	CLA	B	613	65/65	0.96	0.11	13,30,63,74	0
25	BCR	a	409	40/40	0.96	0.08	22,33,42,46	0
23	CLA	D	401	65/65	0.96	0.11	18,29,53,61	0
23	CLA	b	612	65/65	0.96	0.10	20,33,51,57	0
23	CLA	B	602	65/65	0.96	0.11	22,36,61,63	0
23	CLA	d	402	65/65	0.96	0.10	19,33,64,73	0
23	CLA	B	607	65/65	0.96	0.10	14,33,65,72	0
23	CLA	a	405	65/65	0.96	0.09	17,29,50,61	0
24	PHO	A	406	64/64	0.96	0.10	15,28,37,41	0
24	PHO	A	407	64/64	0.96	0.08	22,32,44,50	0
23	CLA	B	603	65/65	0.96	0.12	16,32,70,72	0
24	PHO	d	401	64/64	0.96	0.10	27,38,50,59	0
23	CLA	C	501	65/65	0.96	0.11	18,34,52,58	0
23	CLA	c	501	65/65	0.96	0.12	25,39,52,59	0
23	CLA	a	411	65/65	0.96	0.10	17,31,44,50	0
23	CLA	A	404	65/65	0.96	0.10	17,27,47,57	0
35	HEM	E	101	43/43	0.96	0.12	35,50,67,72	0
35	HEM	e	102	43/43	0.96	0.11	43,57,78,80	0
29	LHG	B	622	49/49	0.97	0.11	26,42,57,74	0
23	CLA	B	608	65/65	0.97	0.10	19,35,56,61	0
29	LHG	D	407	49/49	0.97	0.10	21,41,54,68	0
23	CLA	B	611	65/65	0.97	0.11	17,30,46,53	0
36	HEC	v	201	43/43	0.97	0.12	27,35,51,54	0
31	OEX	A	416[A]	10/10	0.98	0.10	21,30,34,35	10
36	HEC	V	201	43/43	0.98	0.12	24,31,41,41	0
33	BCT	a	404	4/4	0.98	0.13	23,23,41,49	0
22	CL	A	403	1/1	0.99	0.03	24,24,24,24	0
22	CL	a	402	1/1	0.99	0.04	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.04	27,27,27,27	0
21	FE2	a	401	1/1	0.99	0.07	35,35,35,35	0
22	CL	A	402	1/1	0.99	0.10	29,29,29,29	0
31	OEX	a	416[A]	10/10	0.99	0.11	25,31,34,35	10
32	OEY	A	417[B]	11/11	0.99	0.10	22,26,29,30	11
32	OEY	a	417[B]	11/11	0.99	0.11	22,28,30,30	11
33	BCT	A	418	4/4	0.99	0.17	26,33,39,47	0
21	FE2	A	401	1/1	1.00	0.09	30,30,30,30	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.

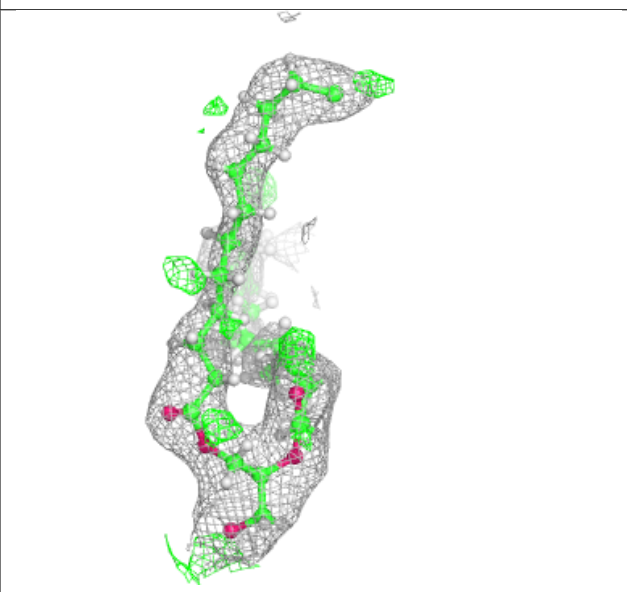
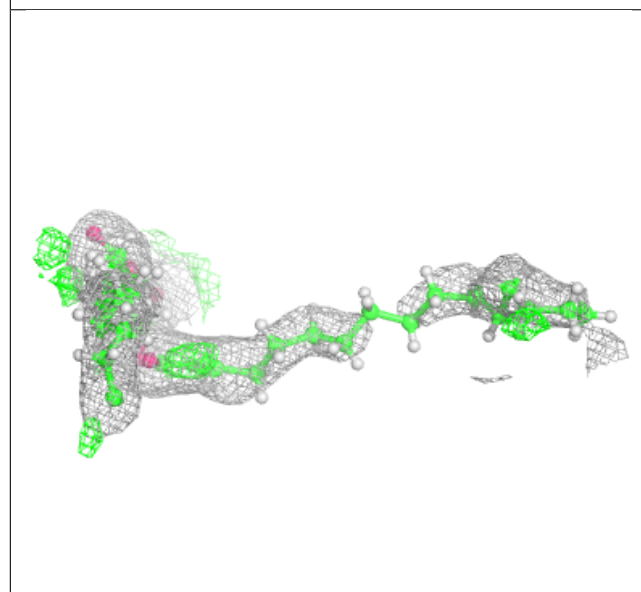
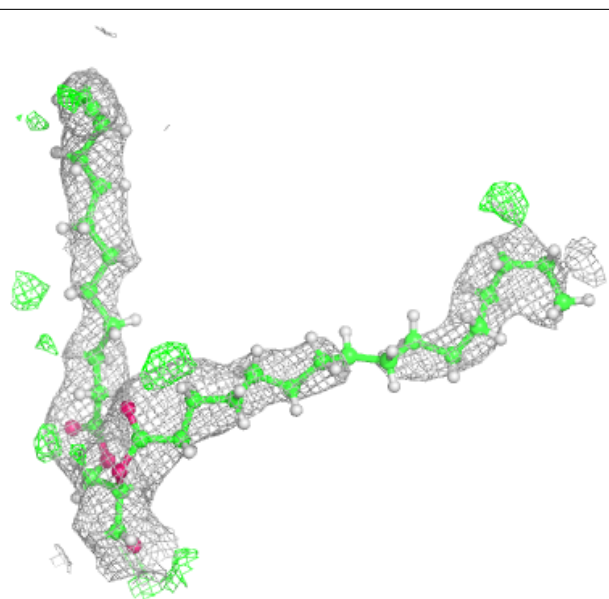






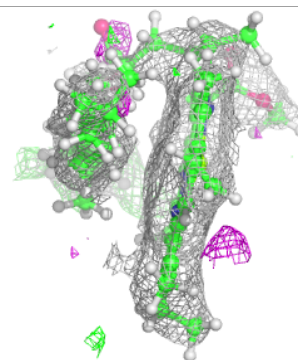
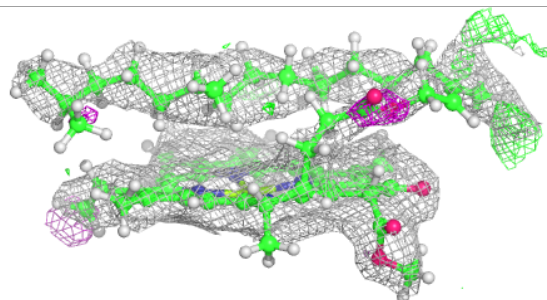
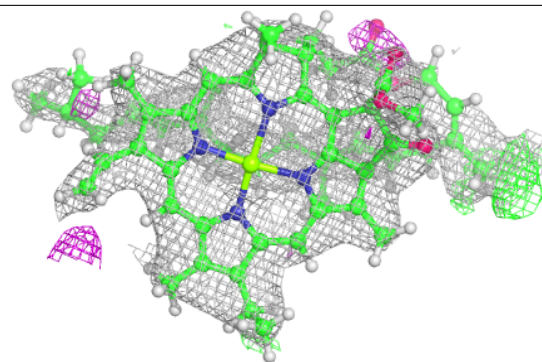
**Electron density around SQD a 413:**

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

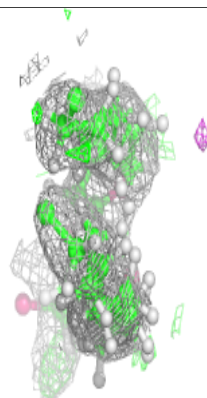
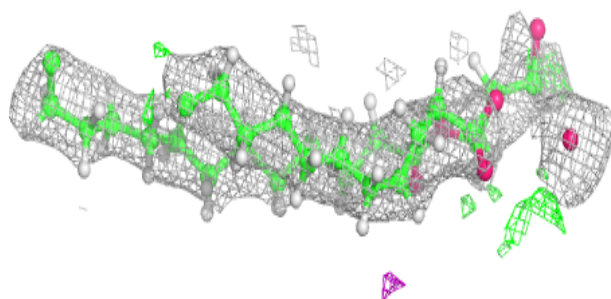
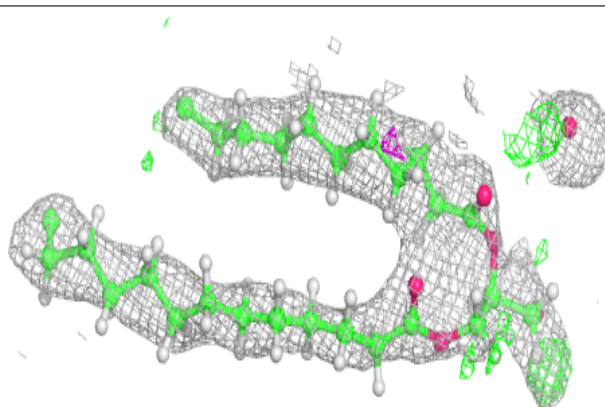


**Electron density around CLA h 101:**

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

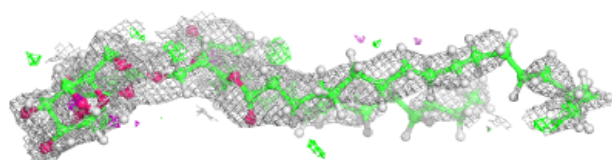
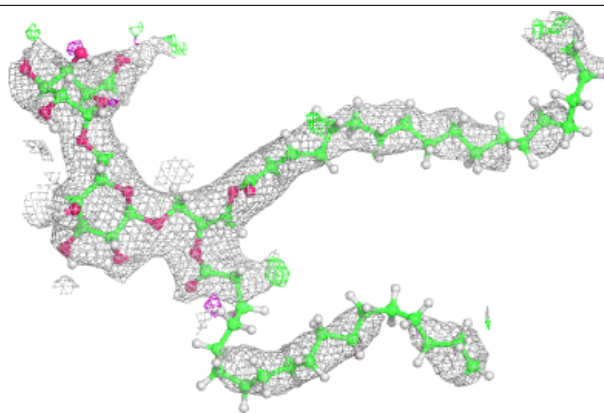
**Electron density around LMG D 409:**

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

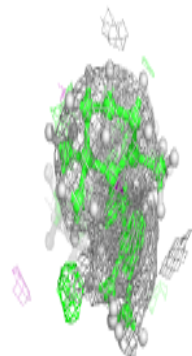
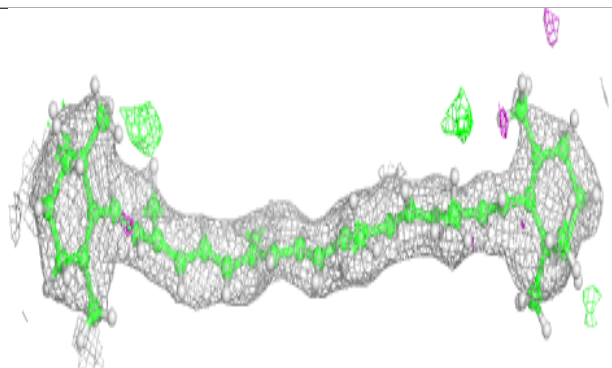
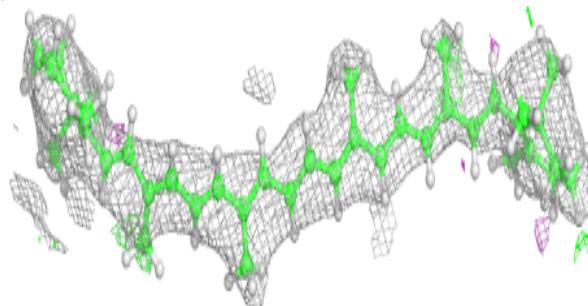


**Electron density around DGD A 415:**

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

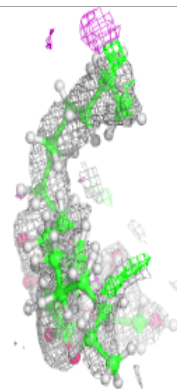
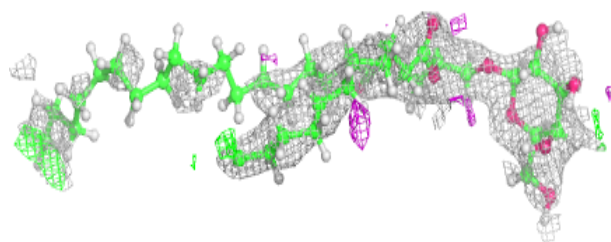
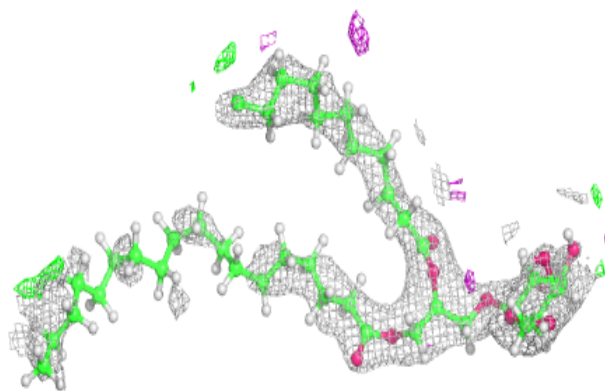
**Electron density around BCR x 101:**

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

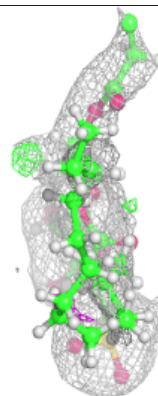
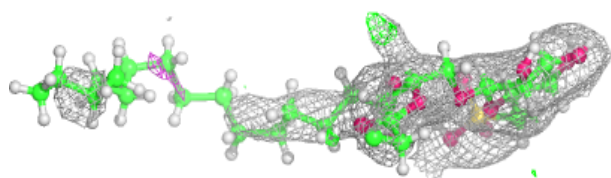
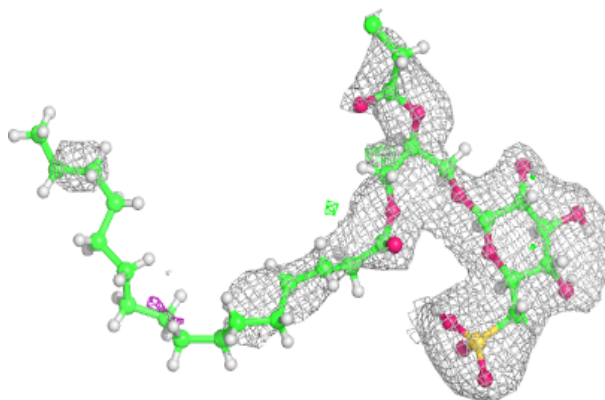


**Electron density around LMG c 521:**

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

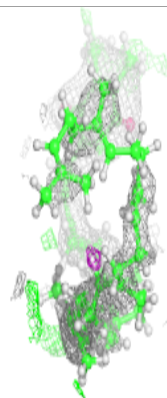
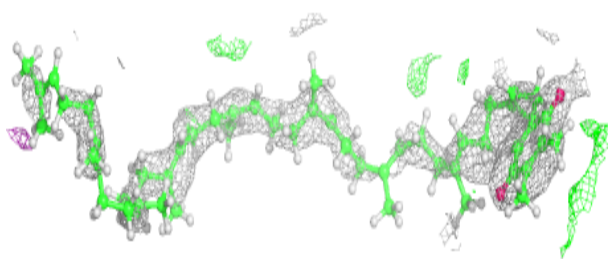
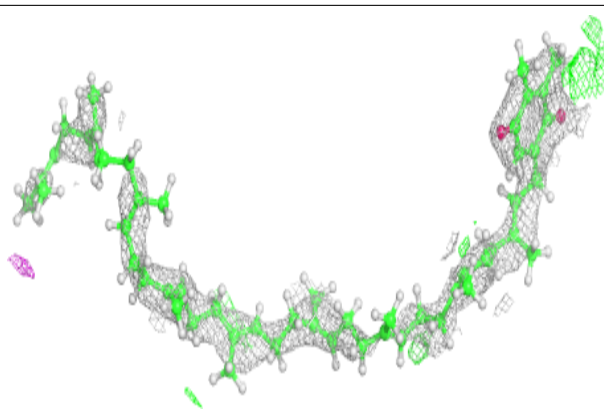
**Electron density around SQD f 101:**

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

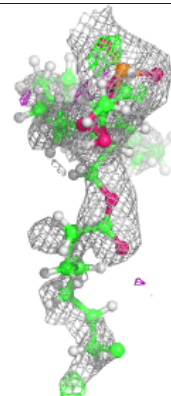
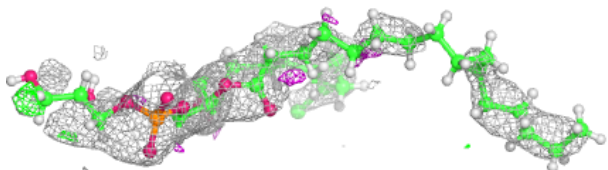
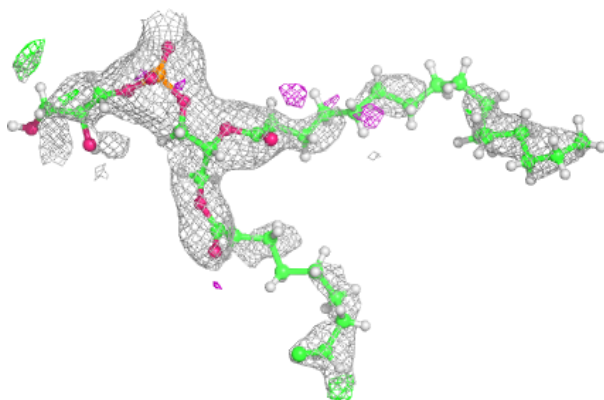


**Electron density around PL9 a 410:**

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

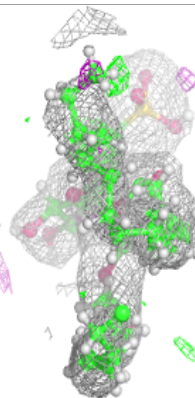
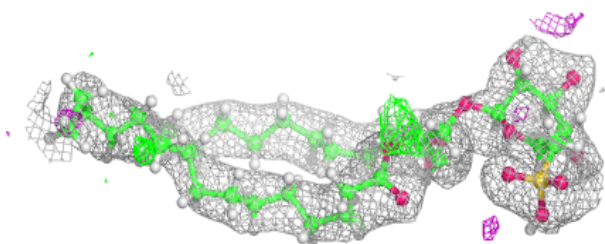
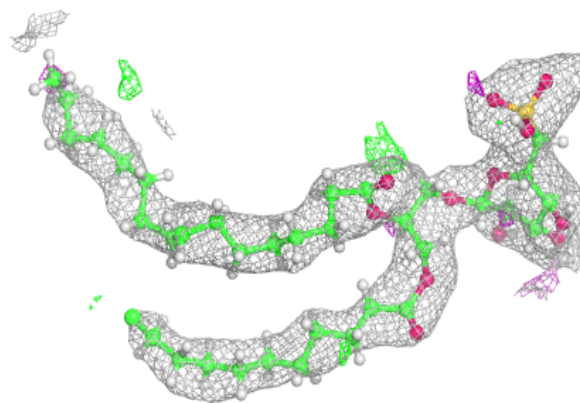
**Electron density around LHG e 101:**

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

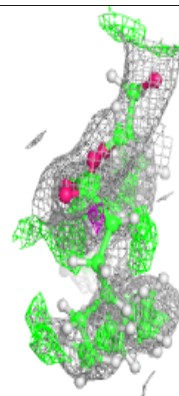
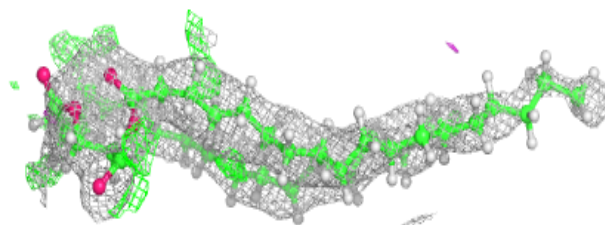
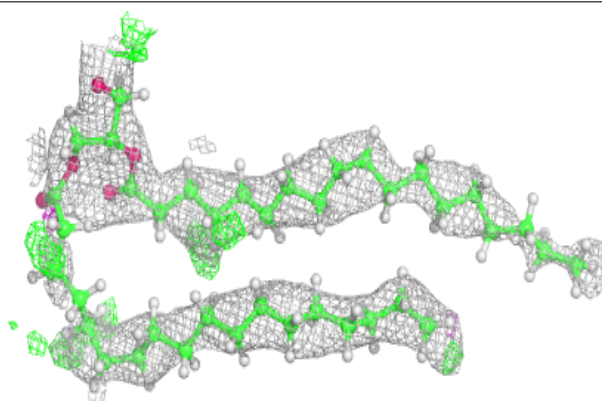


**Electron density around SQD b 601:**

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

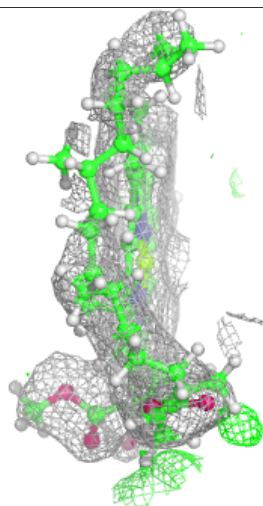
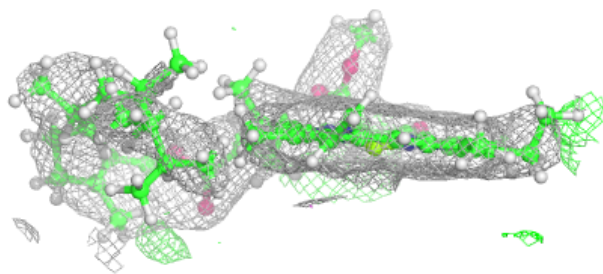
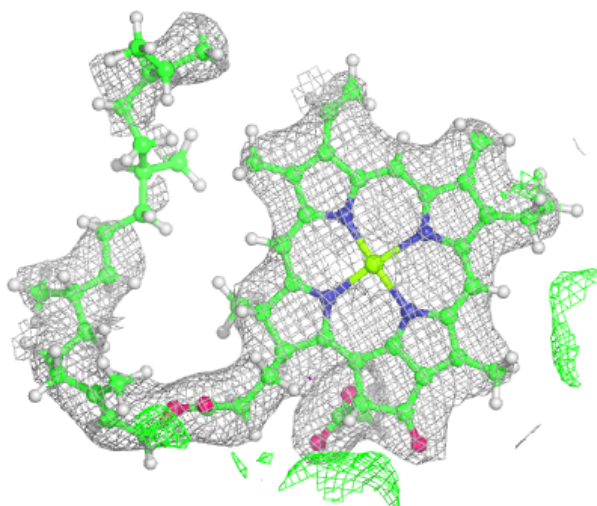
**Electron density around DGD a 414:**

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



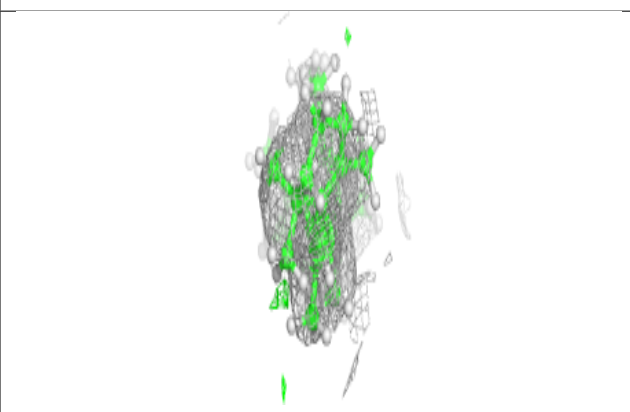
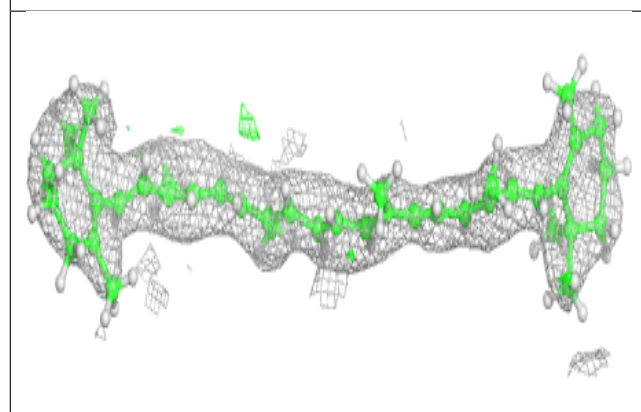
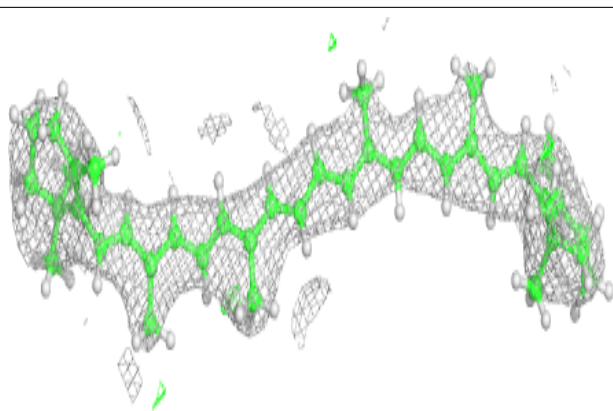
**Electron density around CLA c 512:**

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

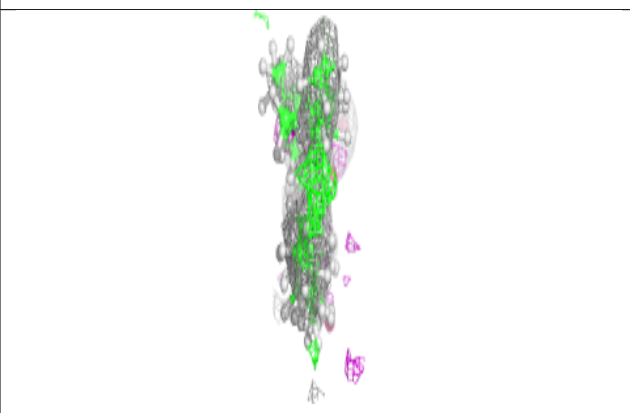
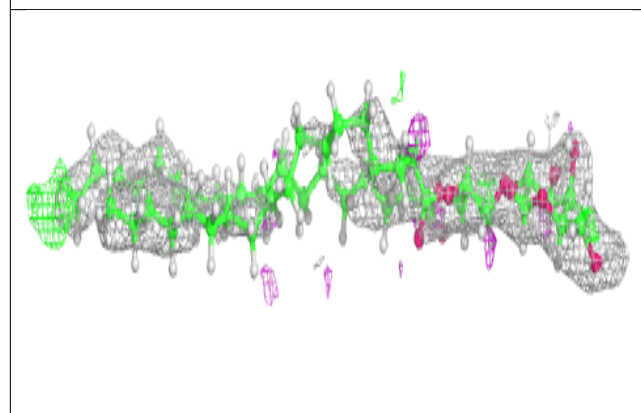
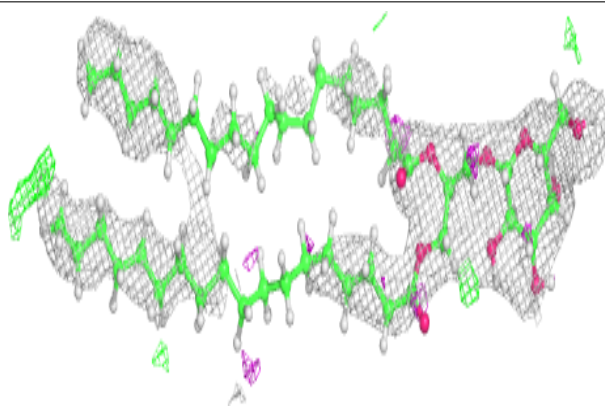


**Electron density around BCR k 101:**

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

**Electron density around LMG b 622:**

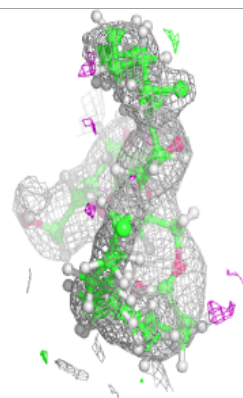
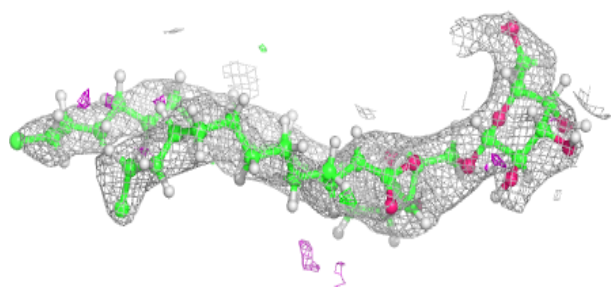
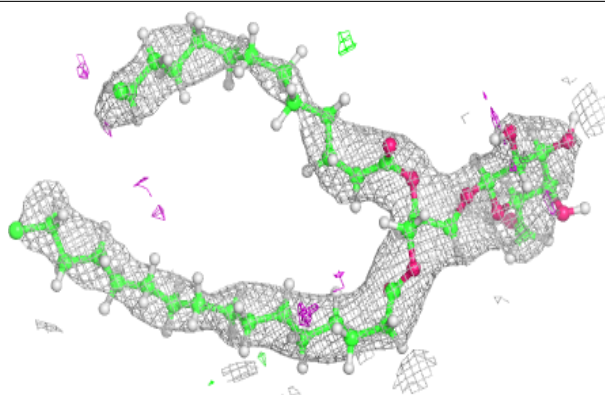
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



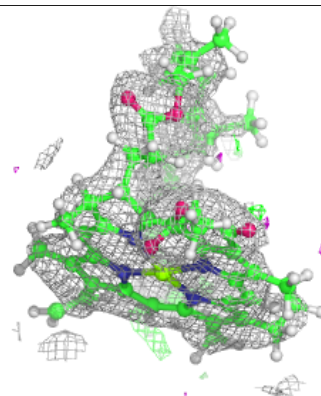
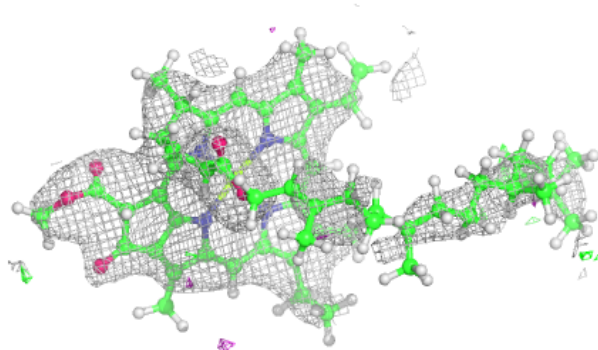
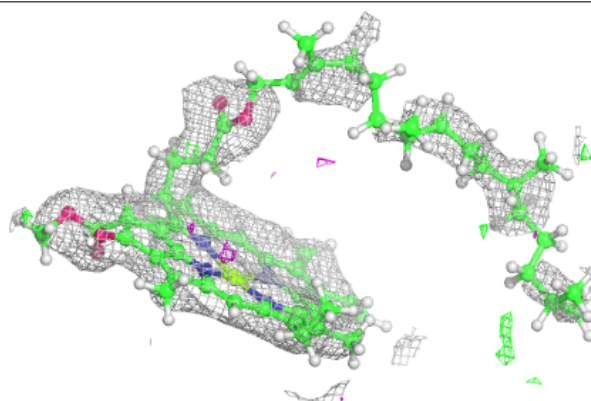


**Electron density around LMG A 411:**

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

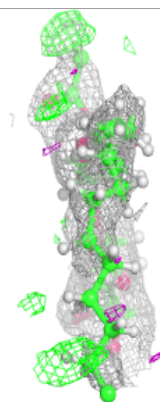
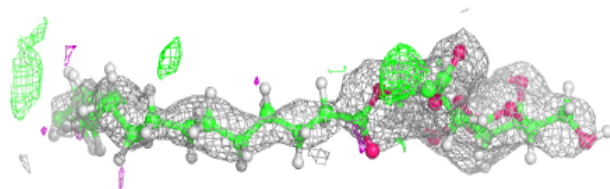
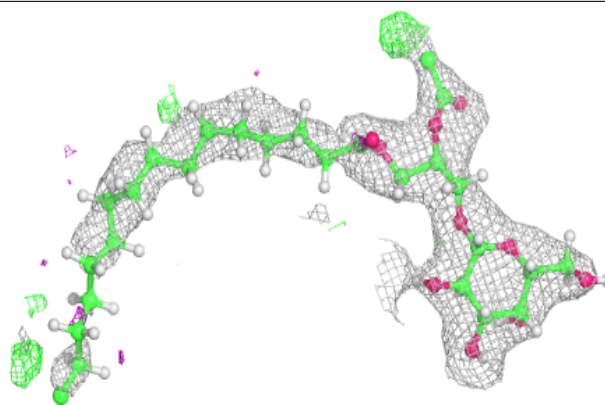
**Electron density around CLA c 513:**

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

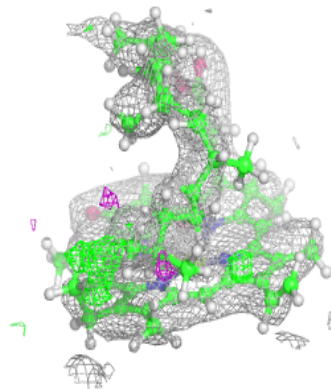
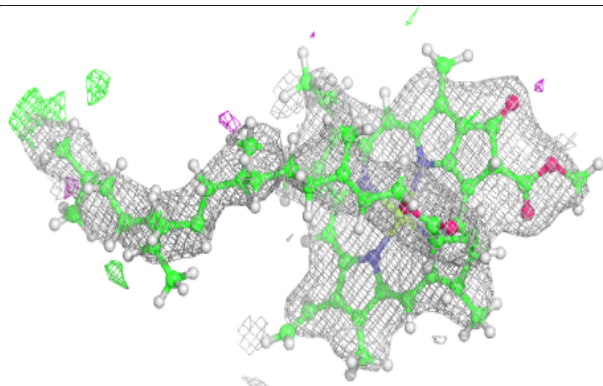
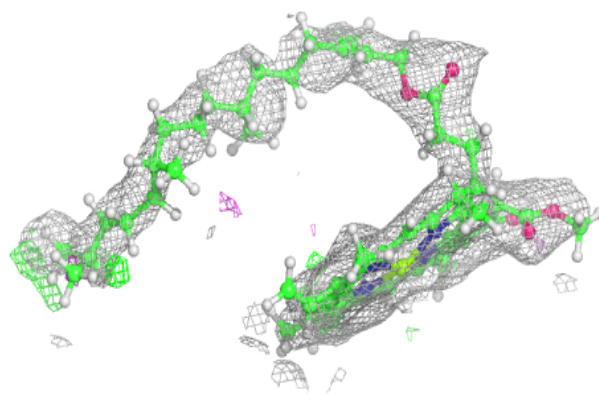


**Electron density around LMG c 519:**

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

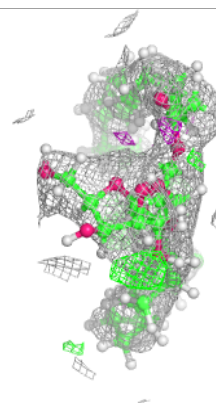
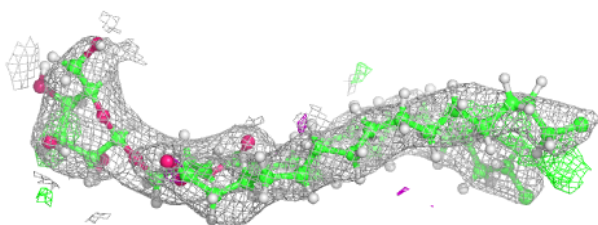
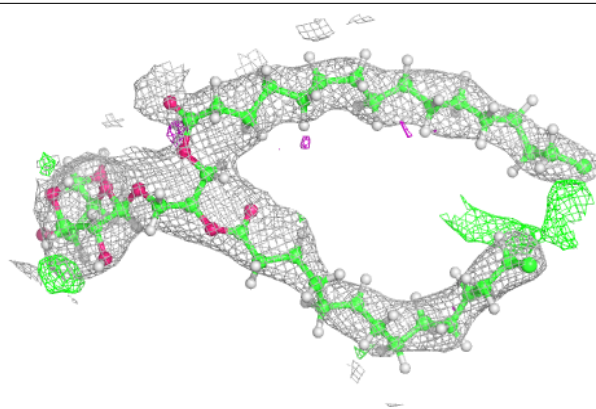
**Electron density around CLA C 513:**

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

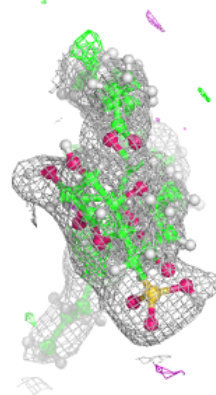
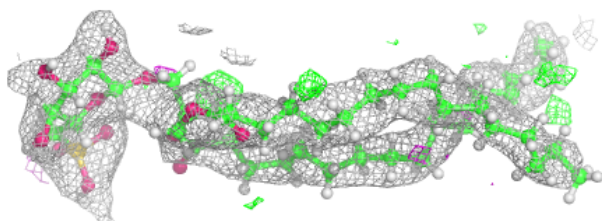
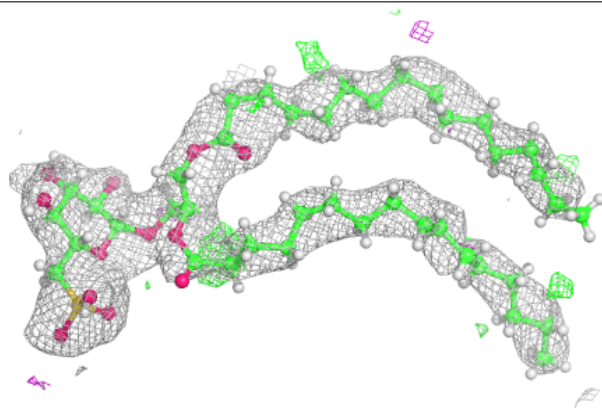


**Electron density around LMG c 523:**

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

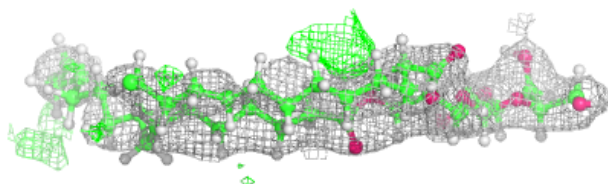
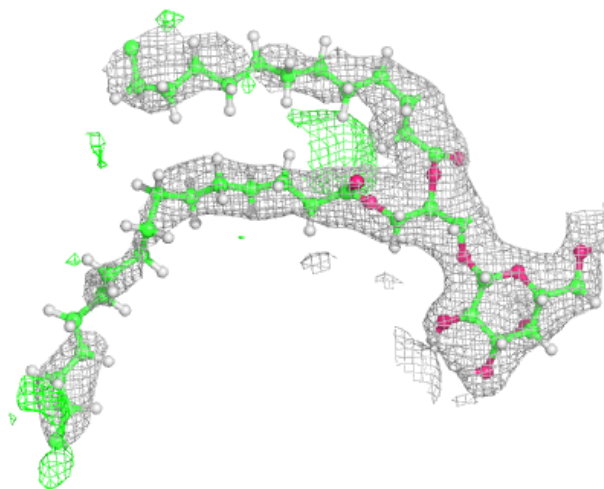
**Electron density around SQD B 624:**

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



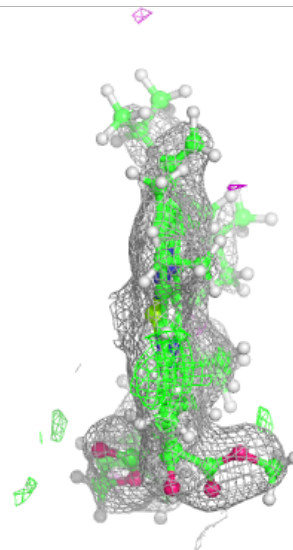
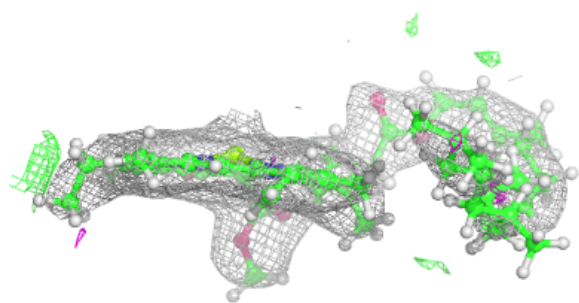
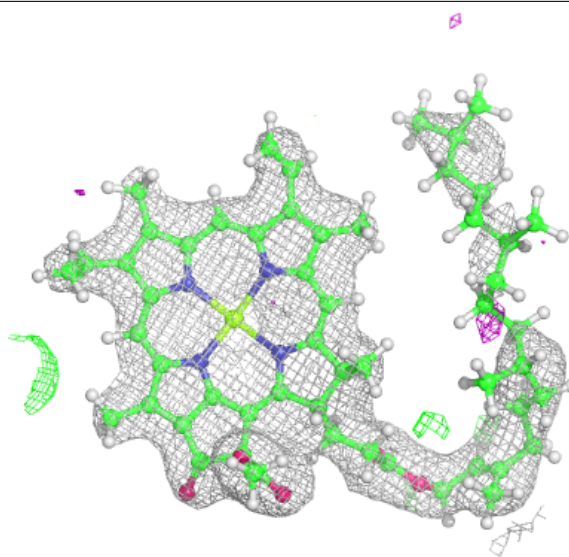
**Electron density around LMG C 518:**

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



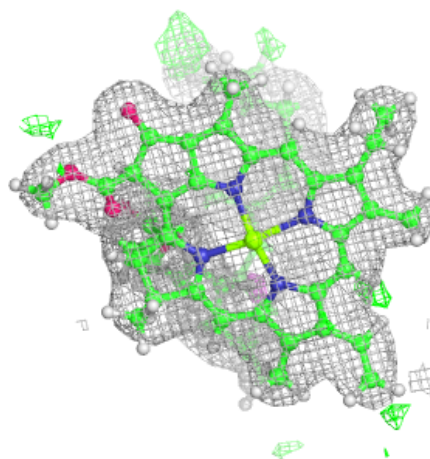
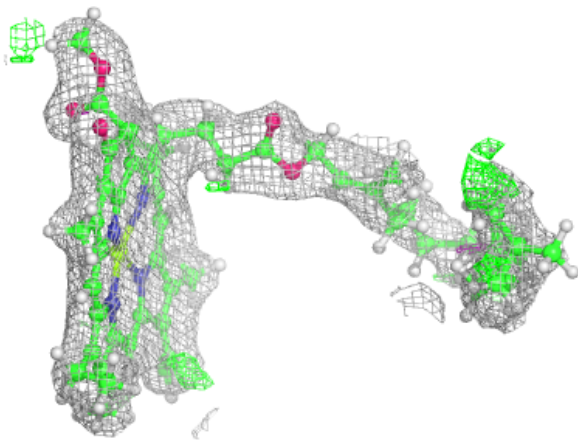
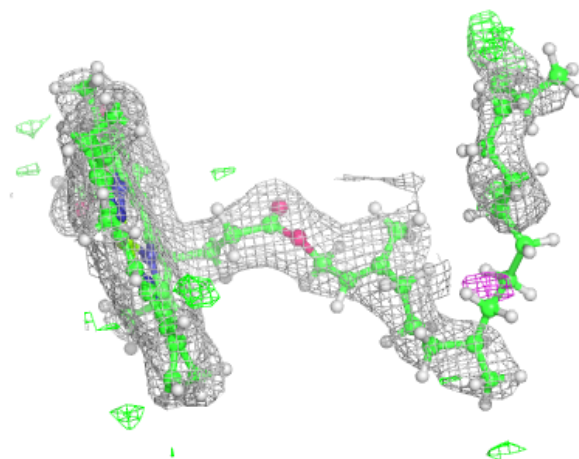
**Electron density around CLA C 512:**

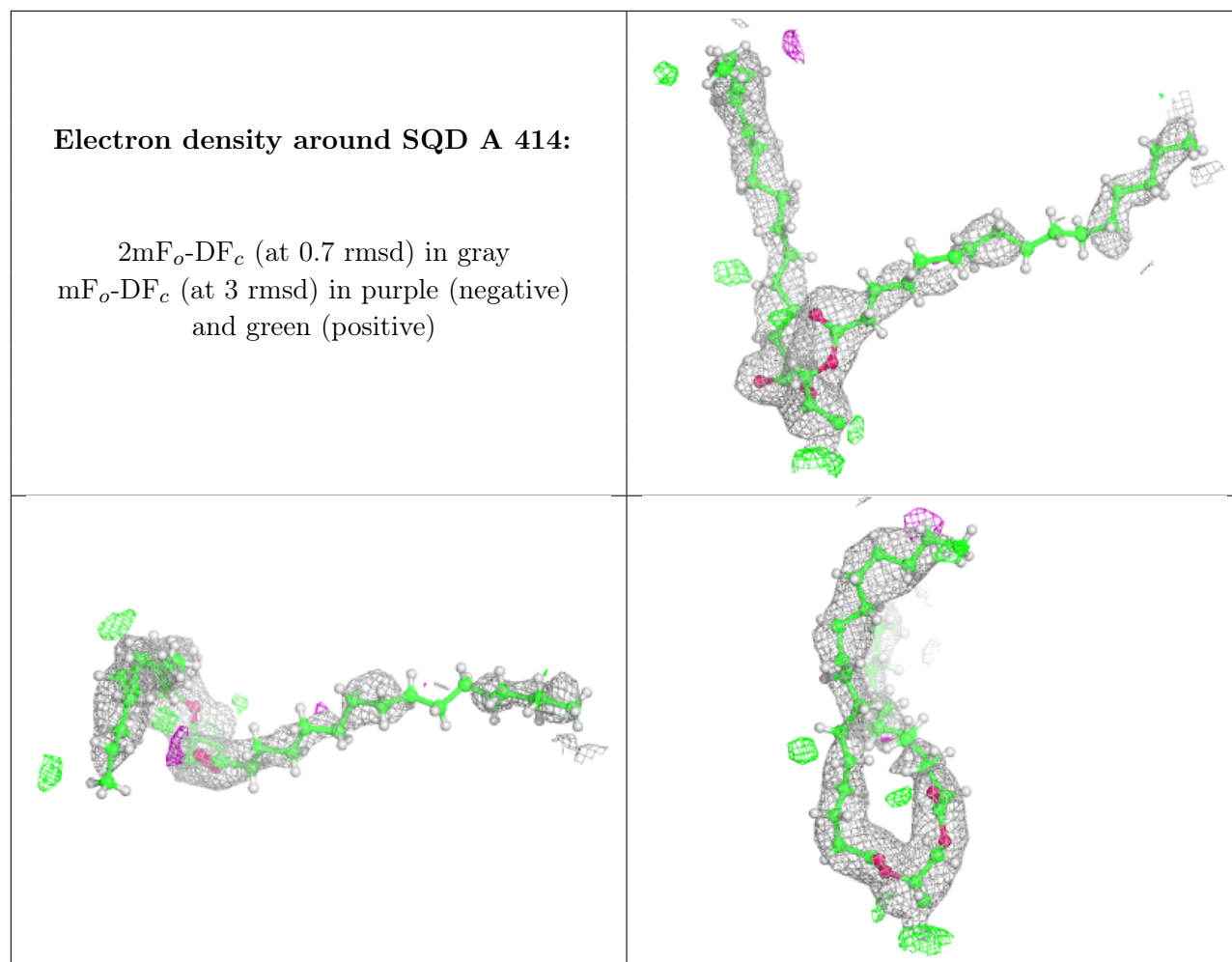
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA a 408:**

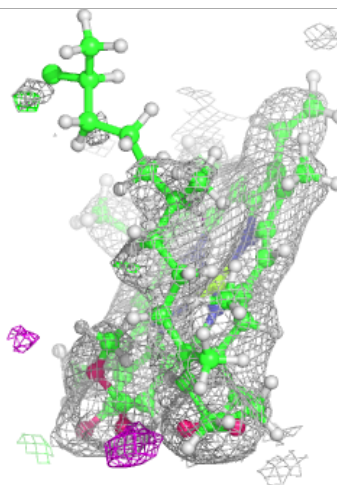
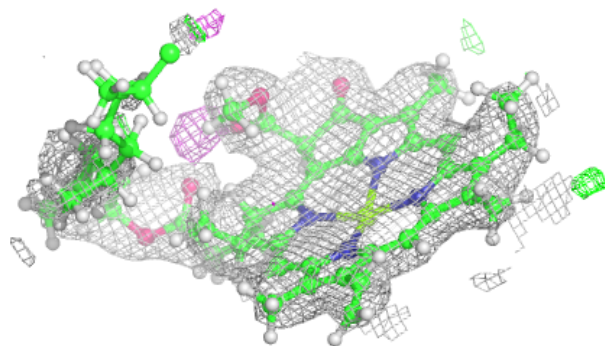
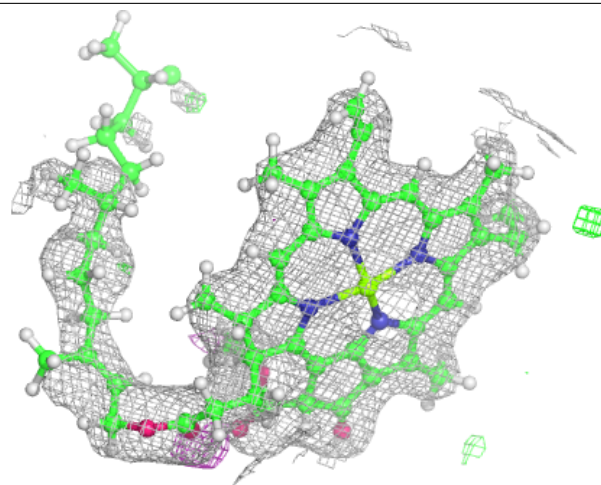
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA b 617:**

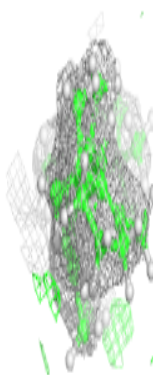
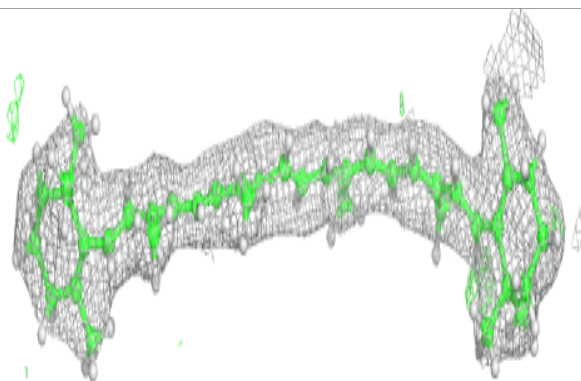
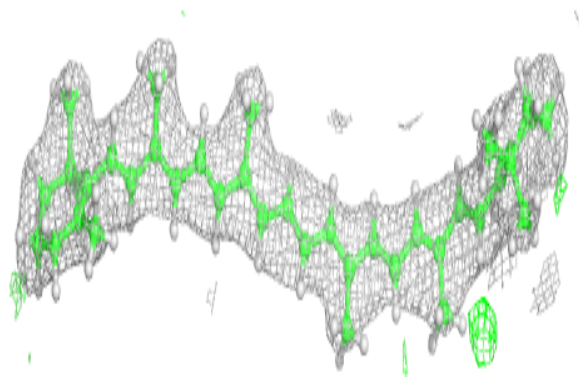
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



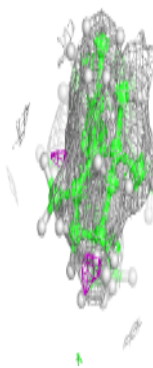
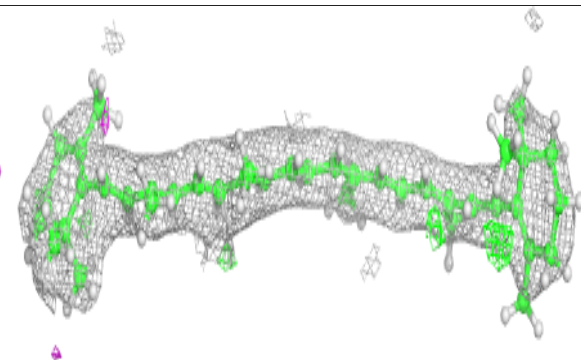
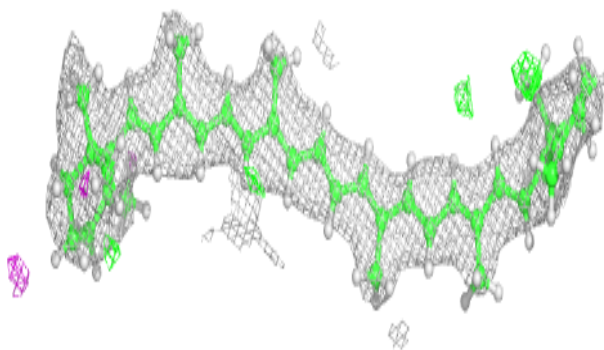


**Electron density around BCR H 101:**

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

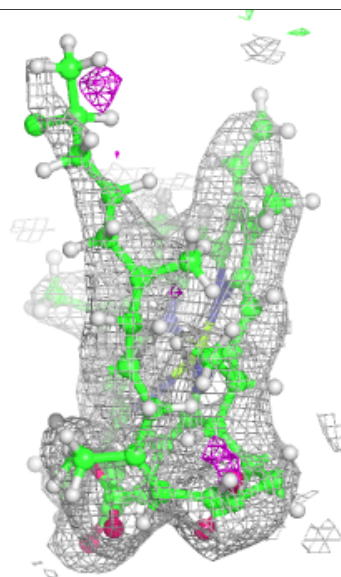
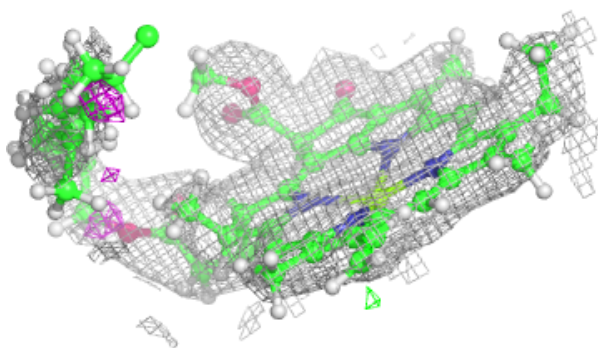
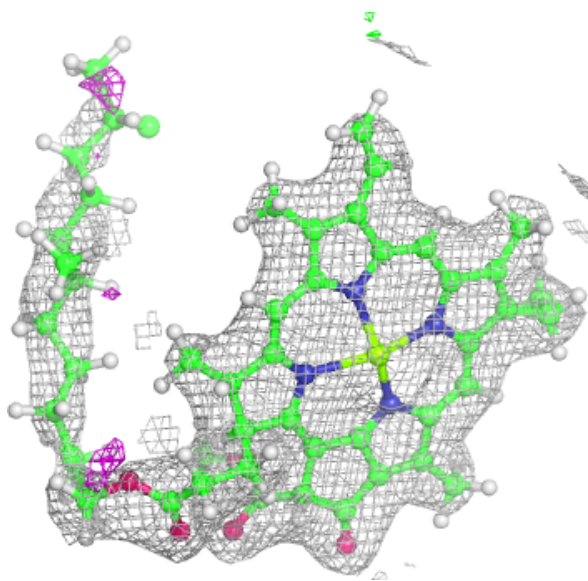
**Electron density around BCR K 101:**

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



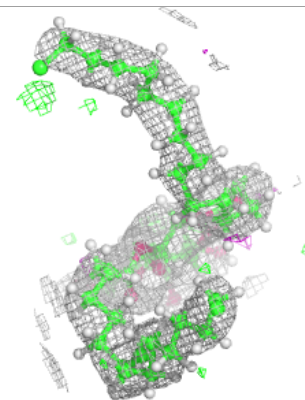
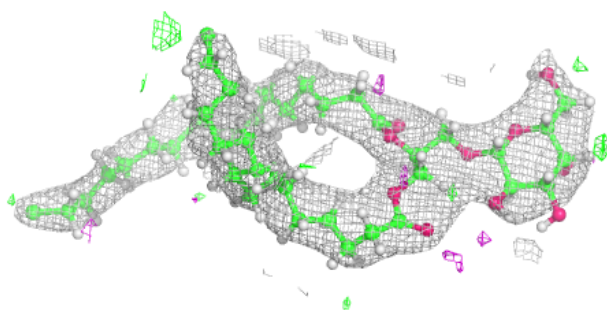
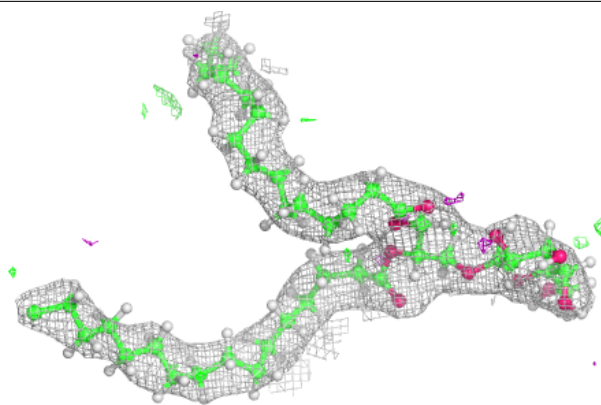
**Electron density around CLA B 616:**

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

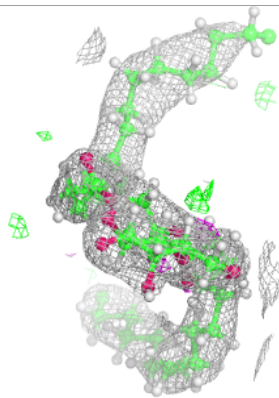
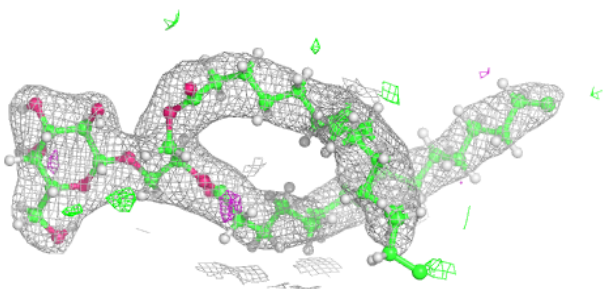
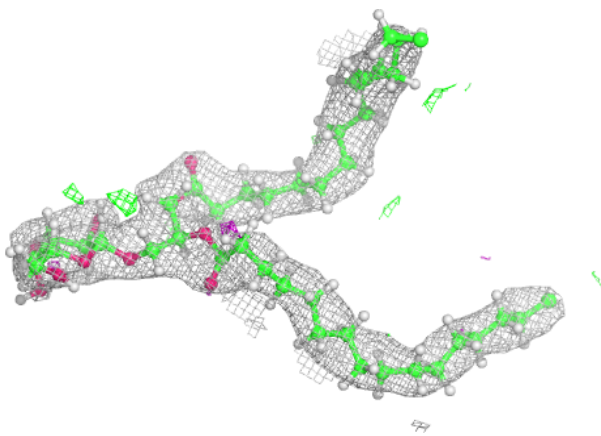


**Electron density around LMG m 101:**

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

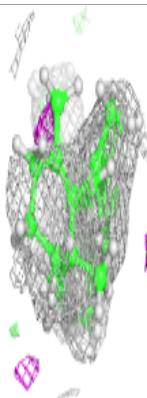
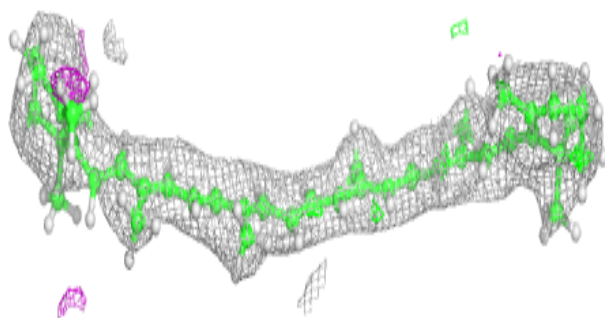
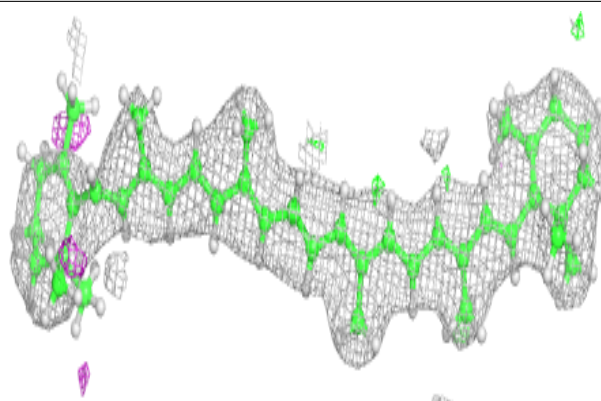
**Electron density around LMG M 101:**

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

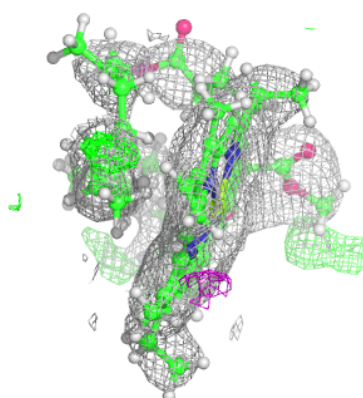
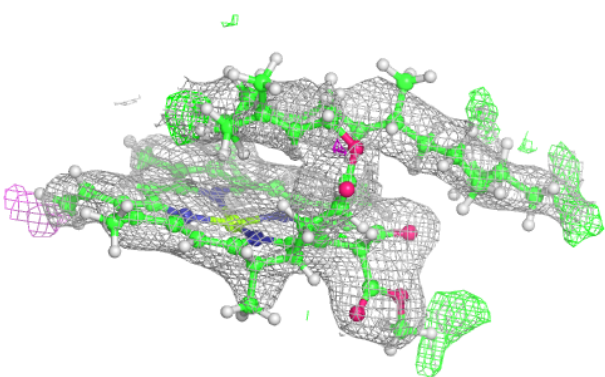
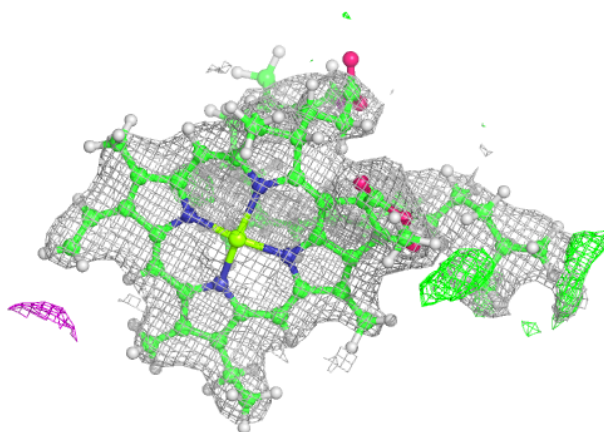


**Electron density around BCR D 404:**

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

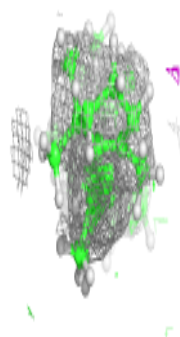
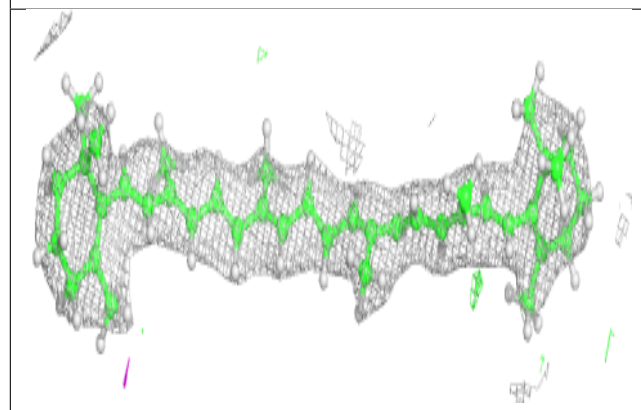
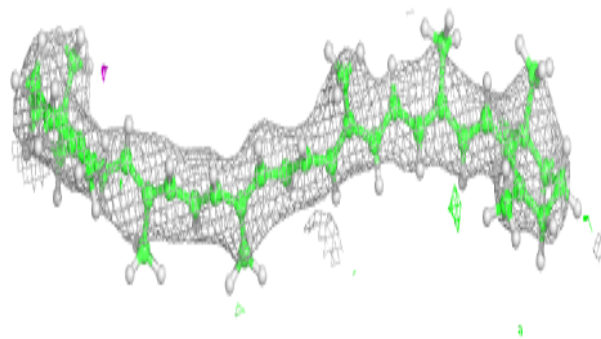
**Electron density around CLA B 601:**

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



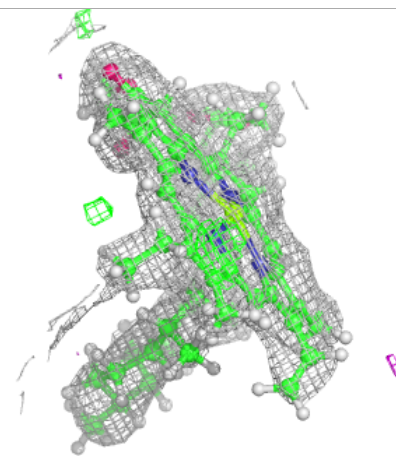
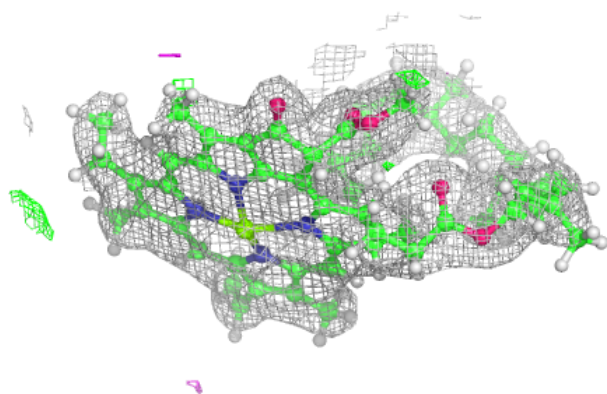
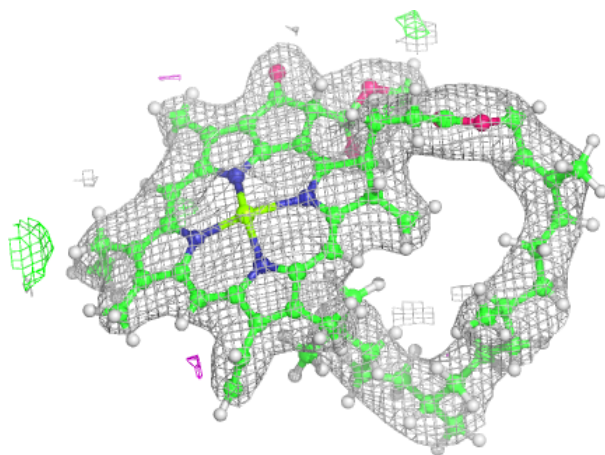
**Electron density around BCR c 514:**

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



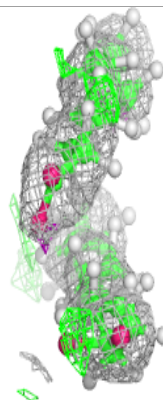
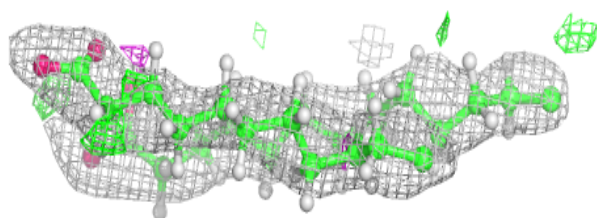
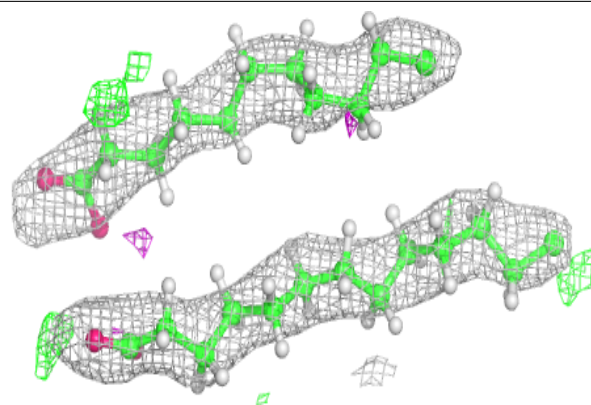
**Electron density around CLA b 616:**

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

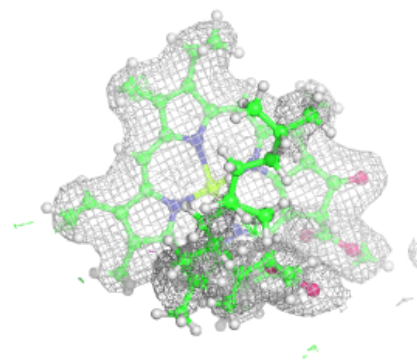
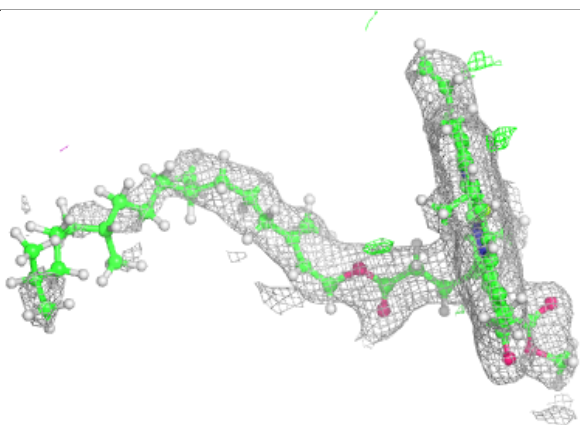
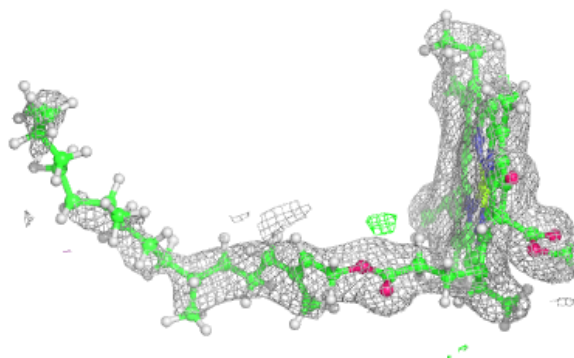


**Electron density around LMG B 621:**

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

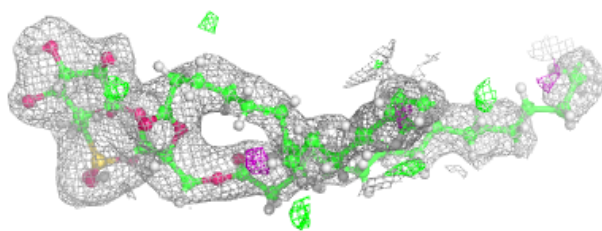
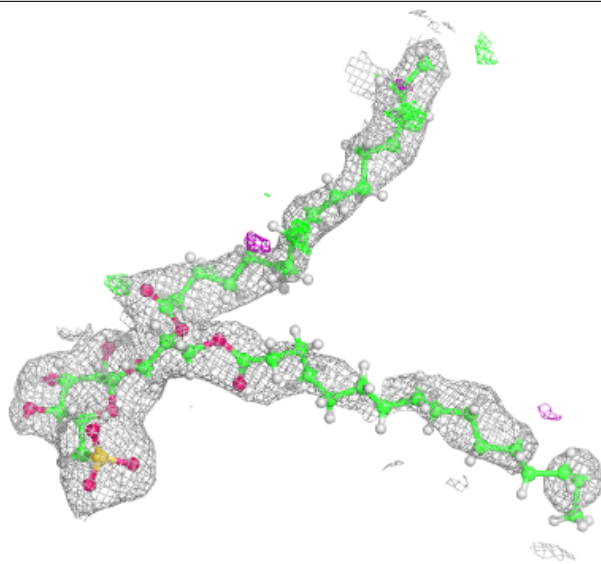
**Electron density around CLA D 403:**

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



**Electron density around SQD a 412:**

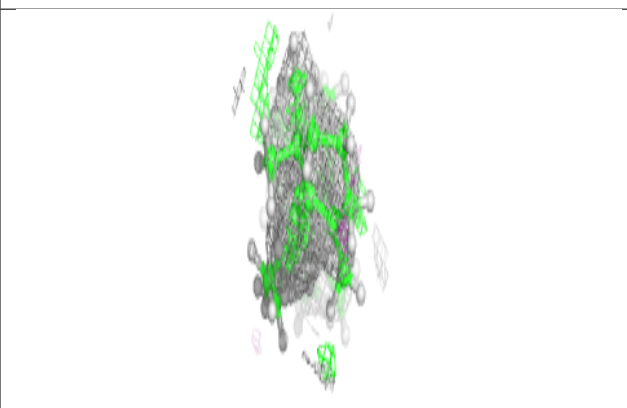
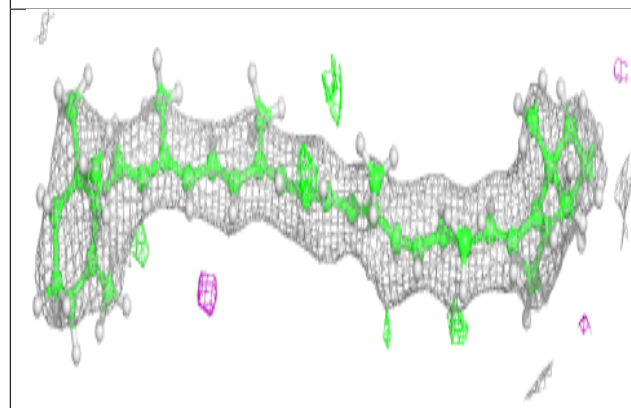
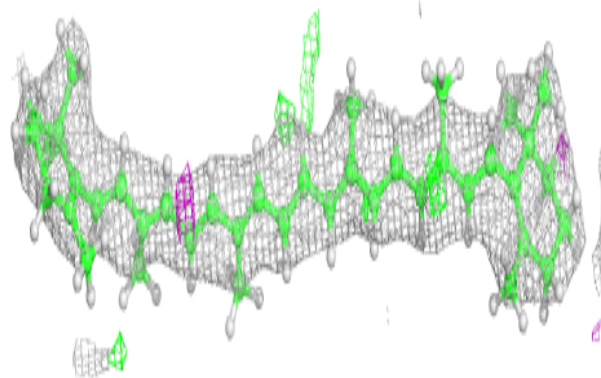
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



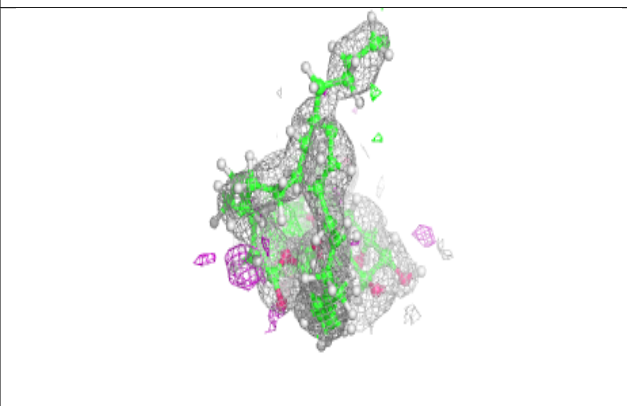
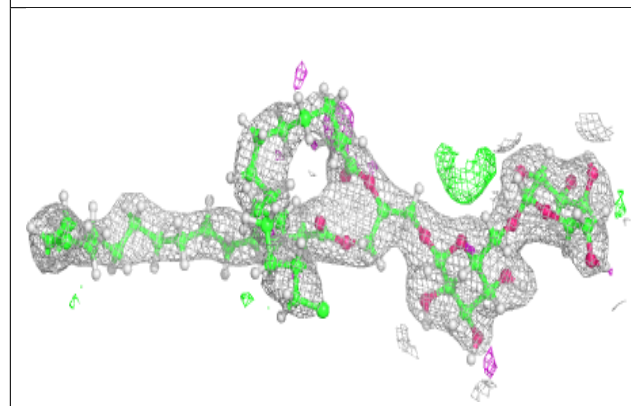
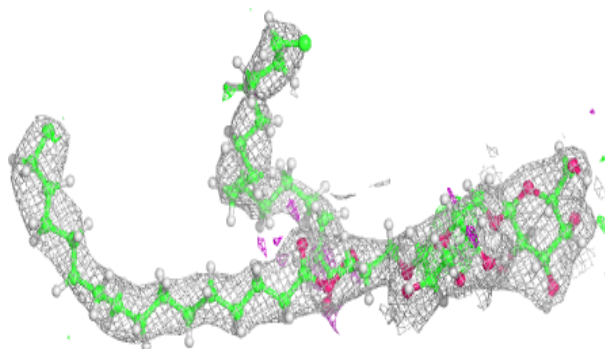


**Electron density around BCR Z 101:**

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

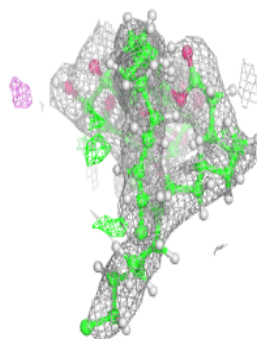
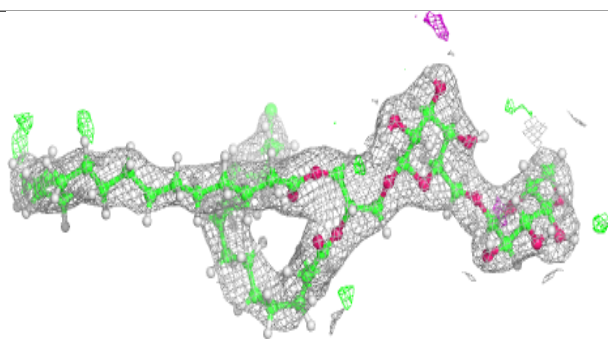
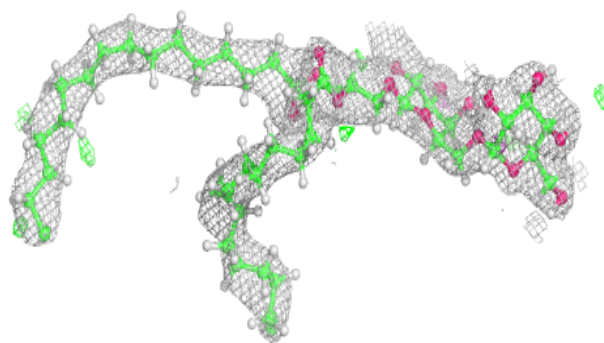
**Electron density around DGD h 102:**

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

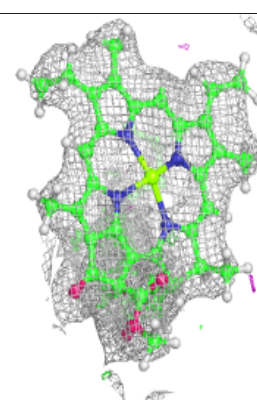
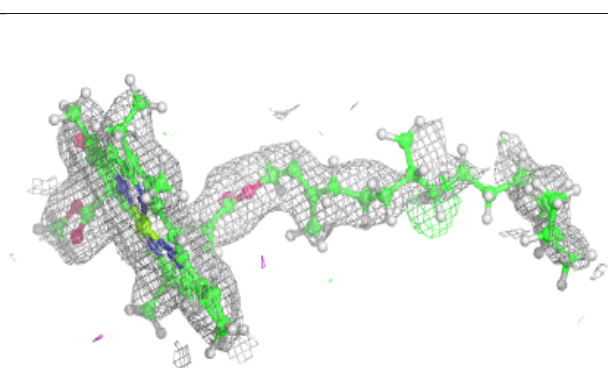
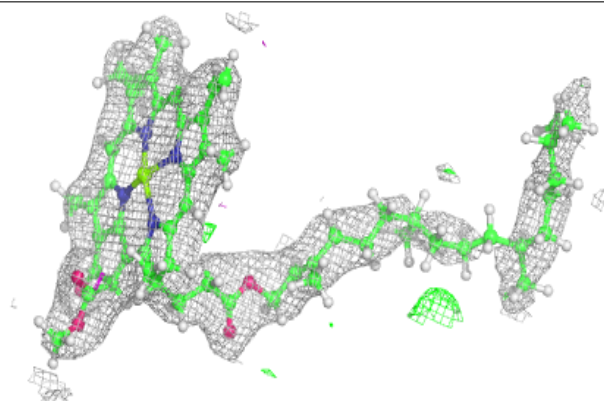


**Electron density around DGD H 102:**

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

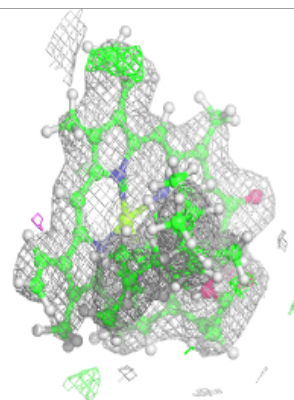
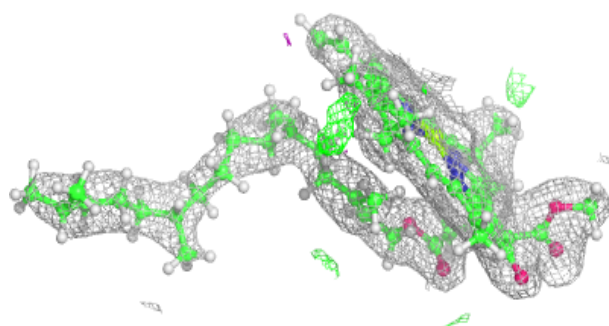
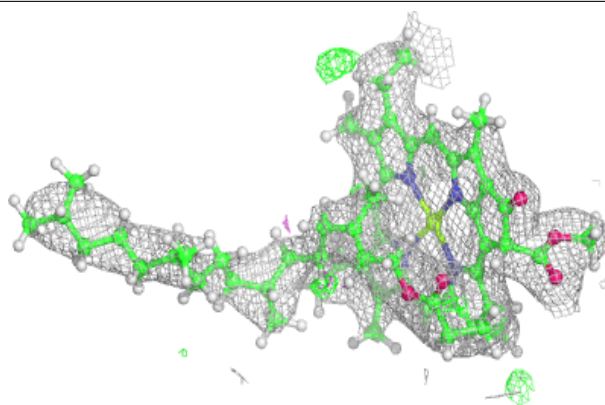
**Electron density around CLA d 403:**

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

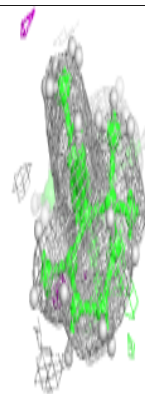
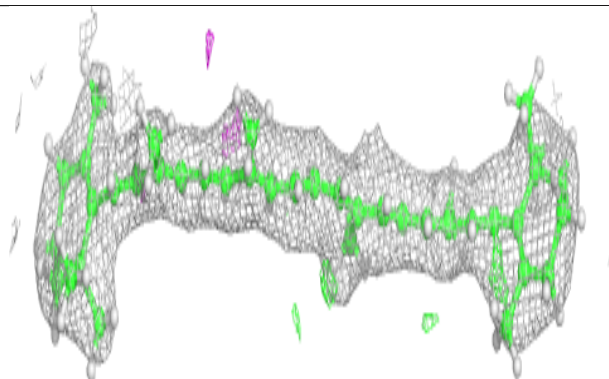
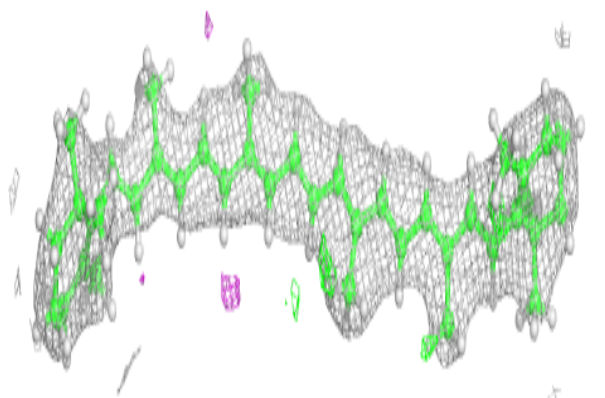


**Electron density around CLA C 505:**

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

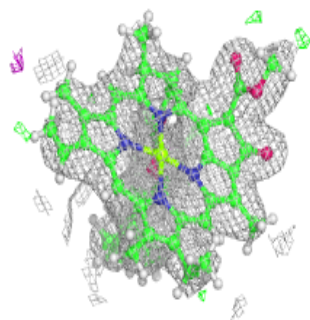
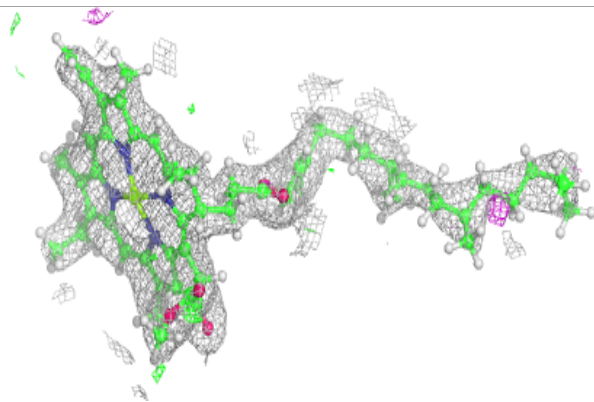
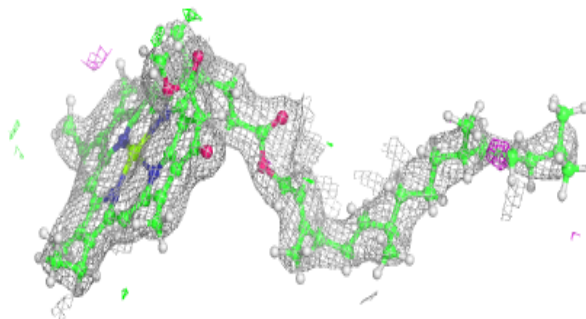
**Electron density around BCR C 514:**

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



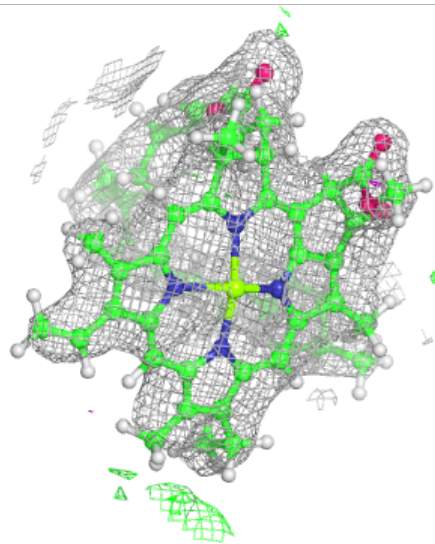
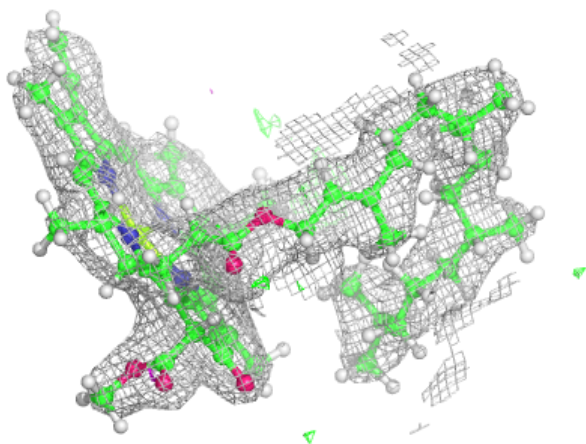
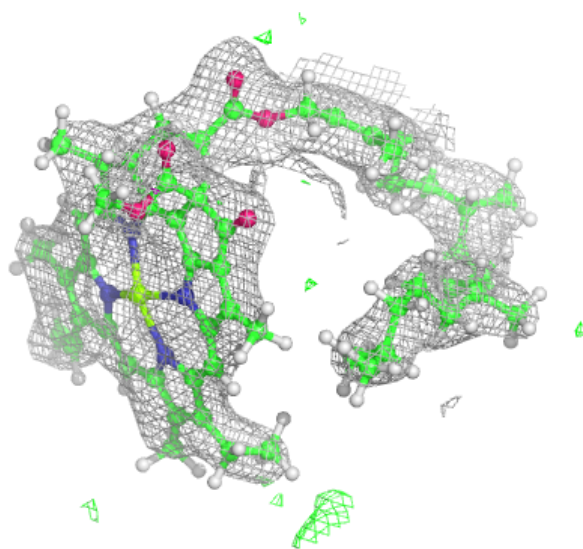
**Electron density around CLA c 502:**

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



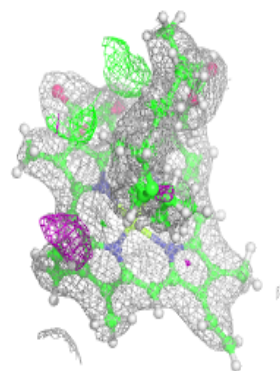
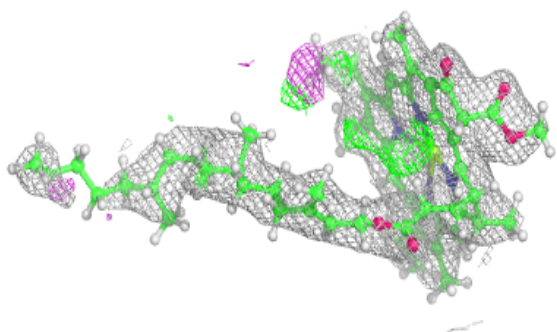
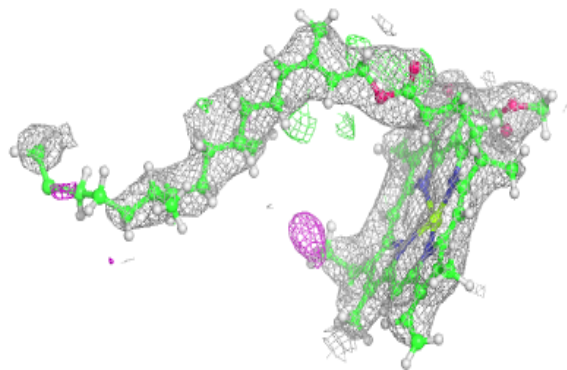
**Electron density around CLA c 503:**

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

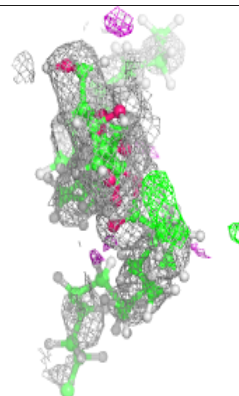
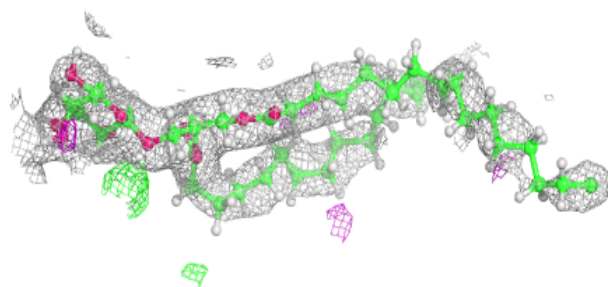
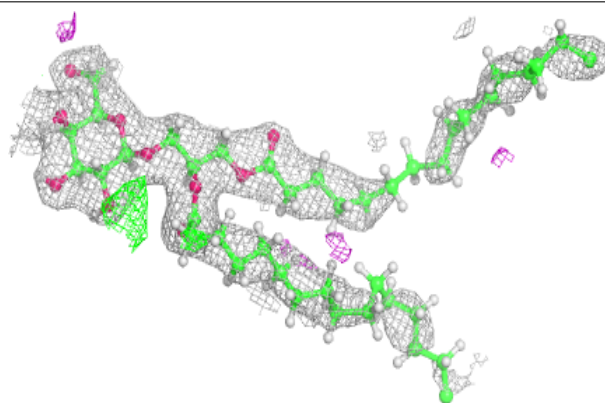


**Electron density around CLA c 508:**

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

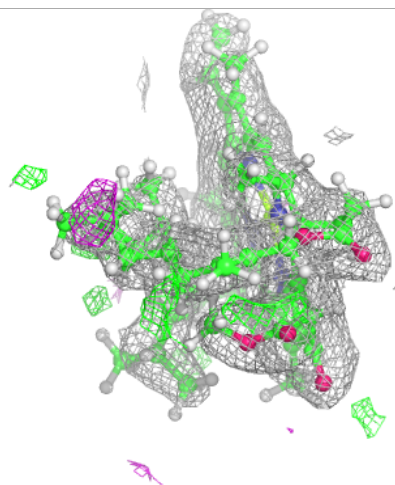
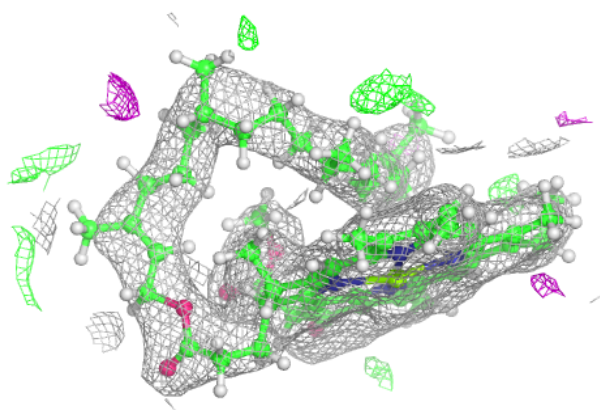
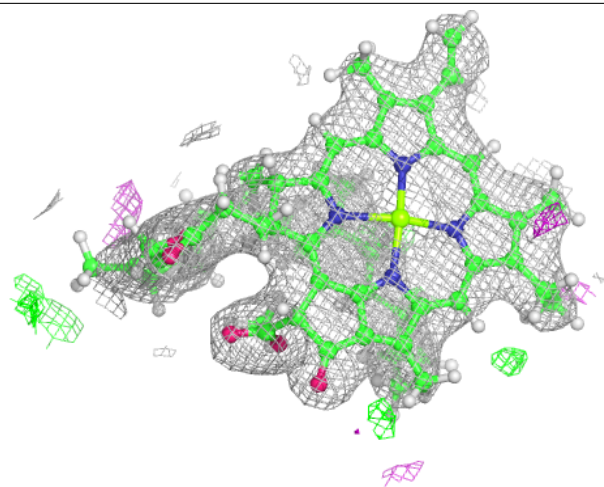
**Electron density around LMG D 406:**

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



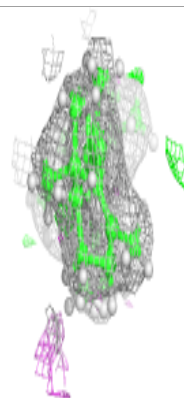
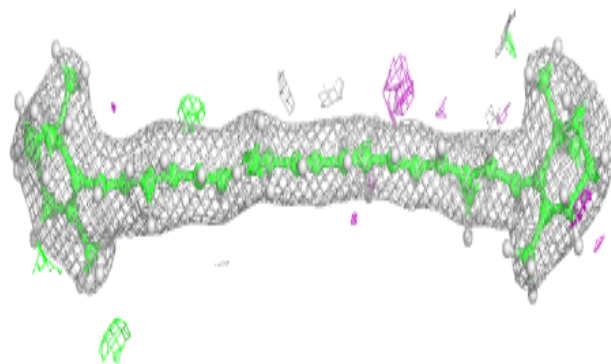
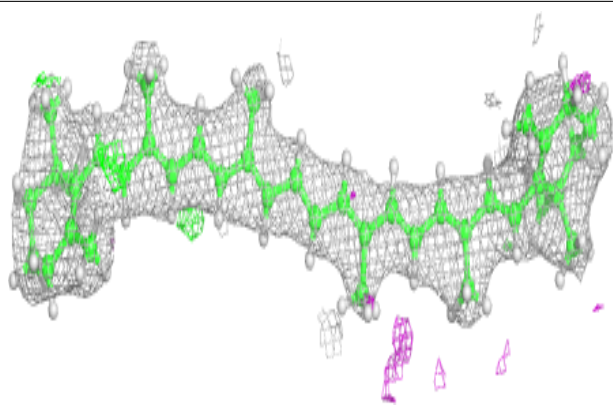
**Electron density around CLA c 510:**

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

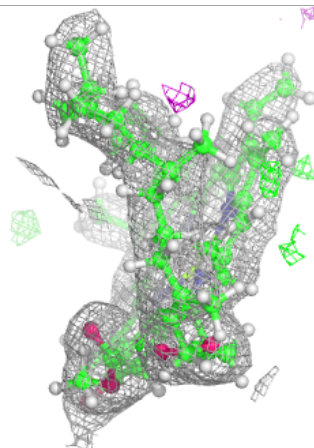
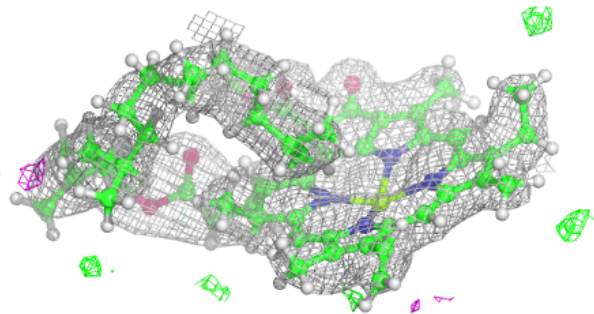
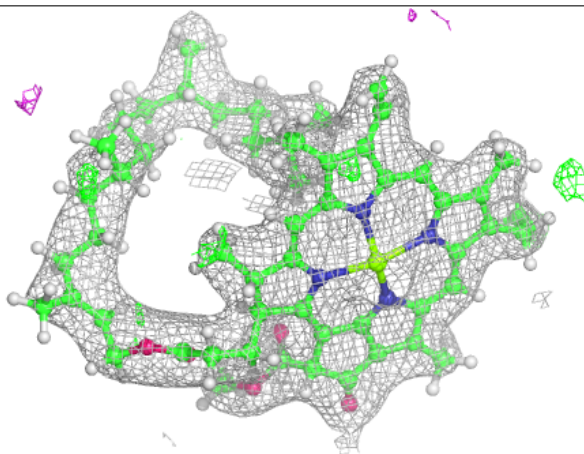


**Electron density around BCR b 619:**

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

**Electron density around CLA B 615:**

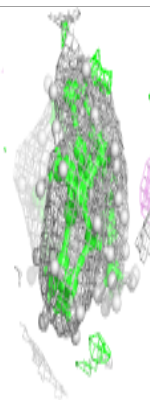
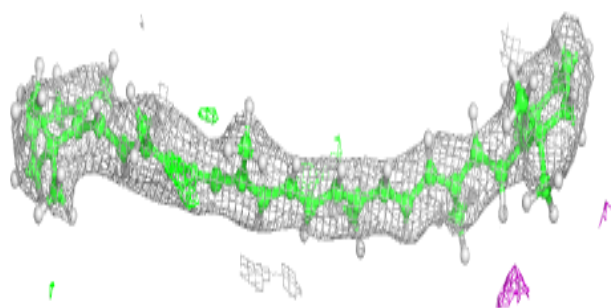
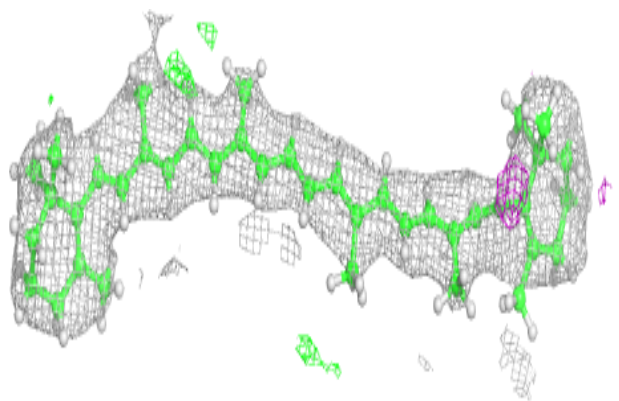
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



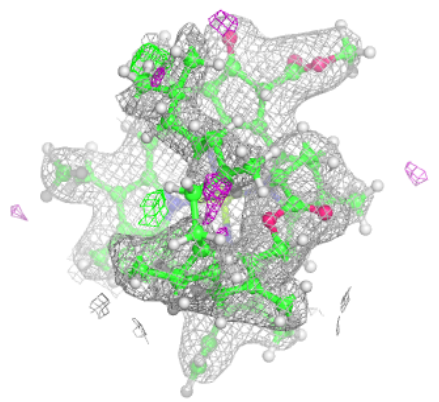
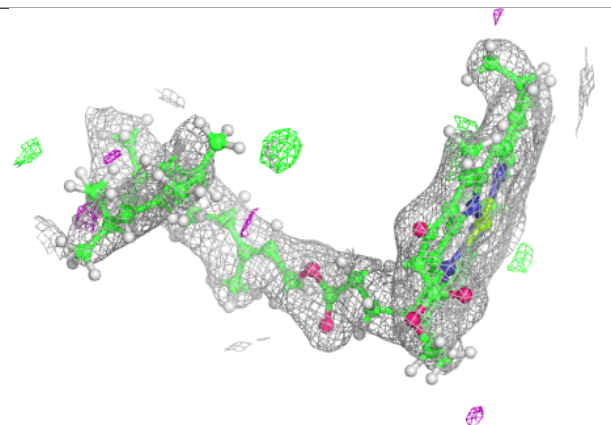
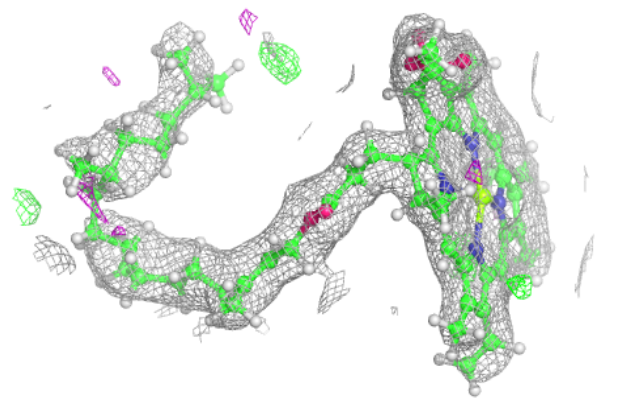


**Electron density around BCR d 404:**

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

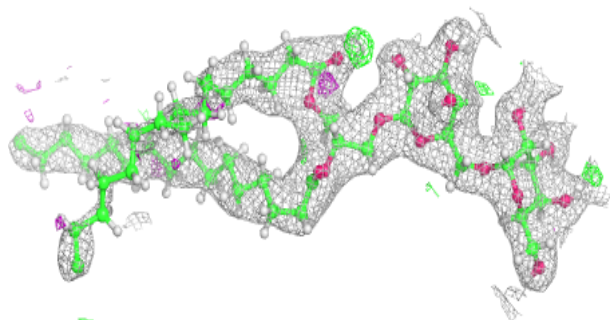
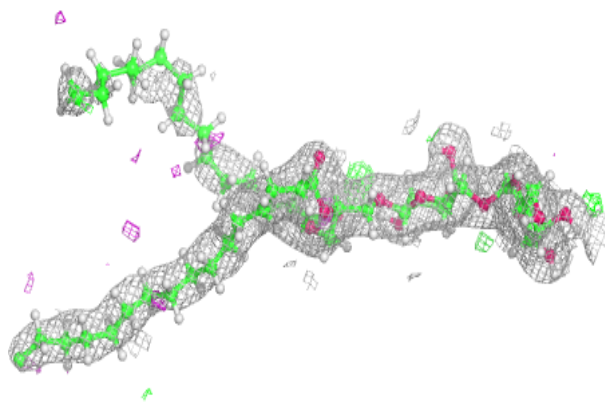
**Electron density around CLA B 606:**

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

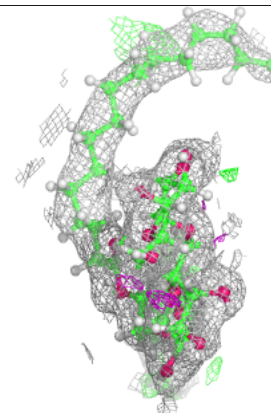
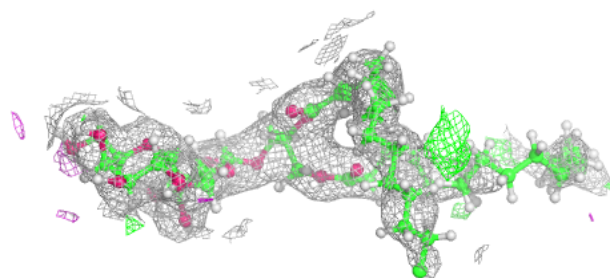
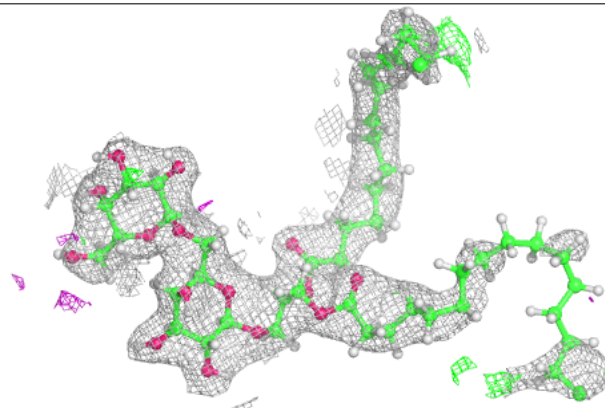


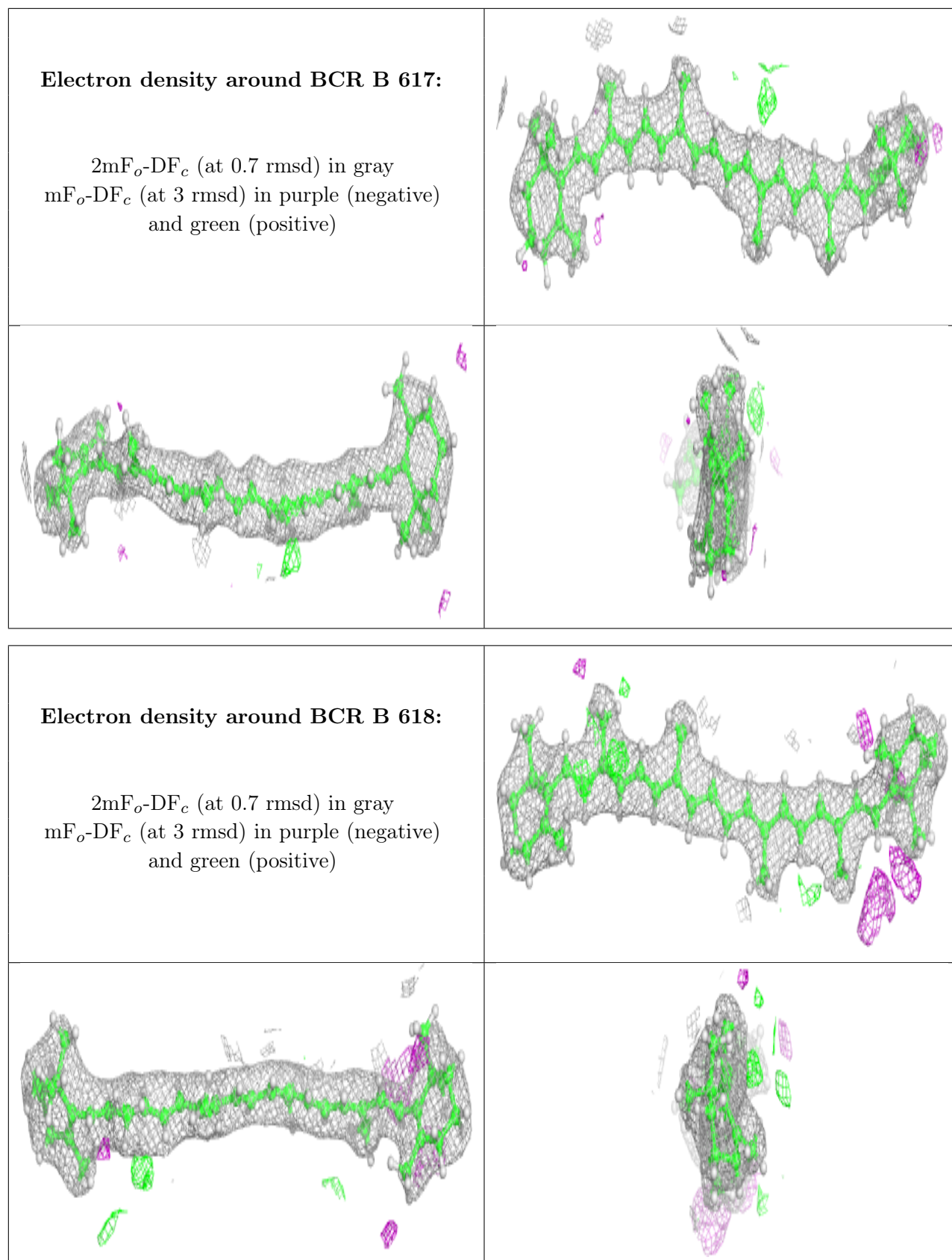
**Electron density around DGD C 515:**

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

**Electron density around DGD C 516:**

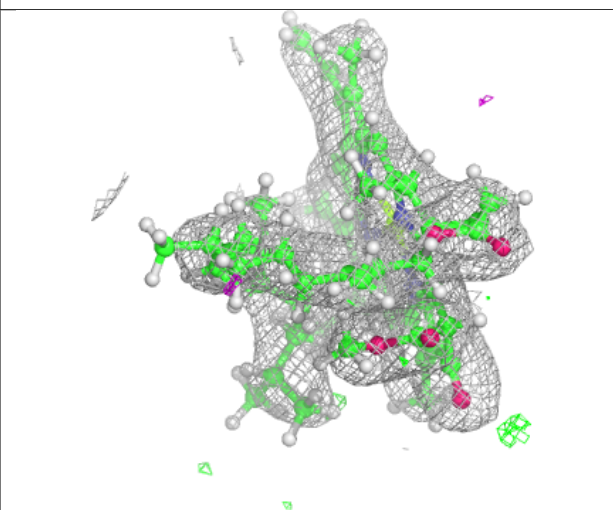
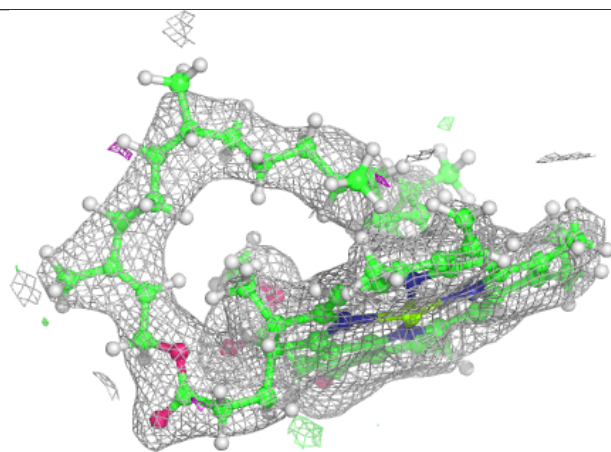
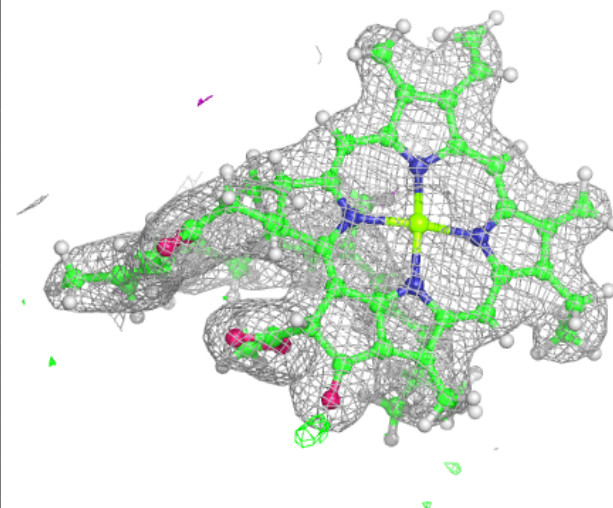
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





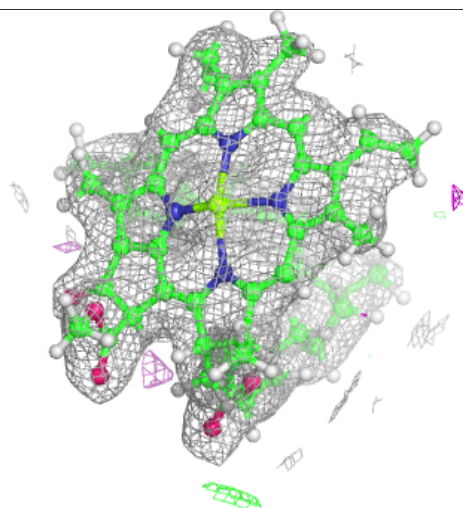
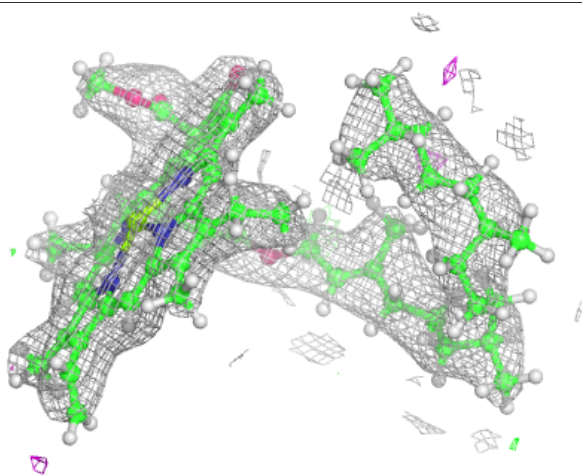
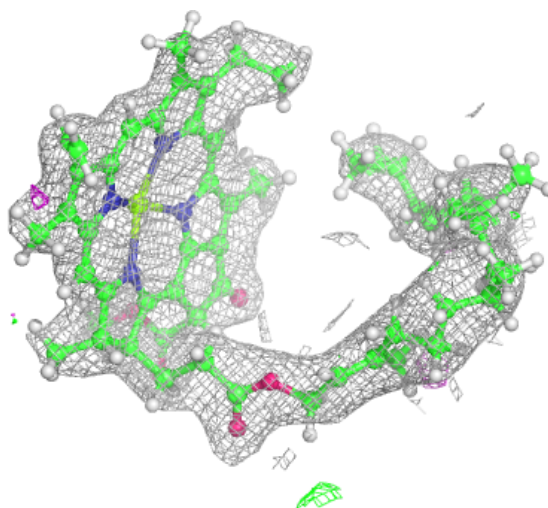
**Electron density around CLA C 510:**

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



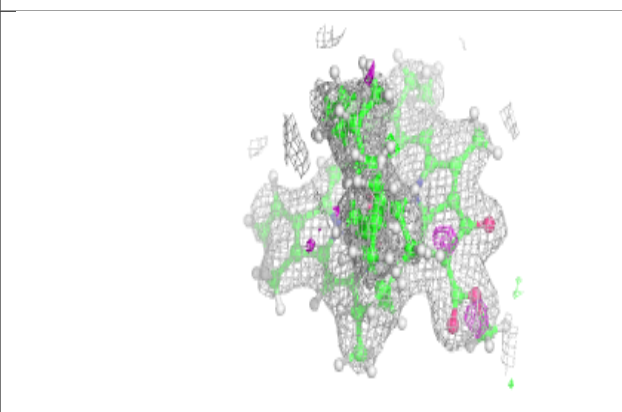
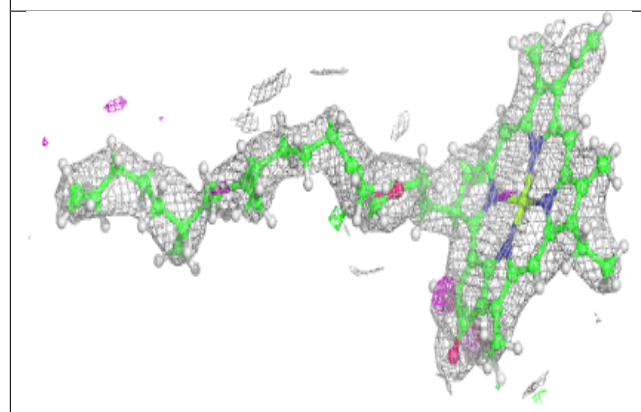
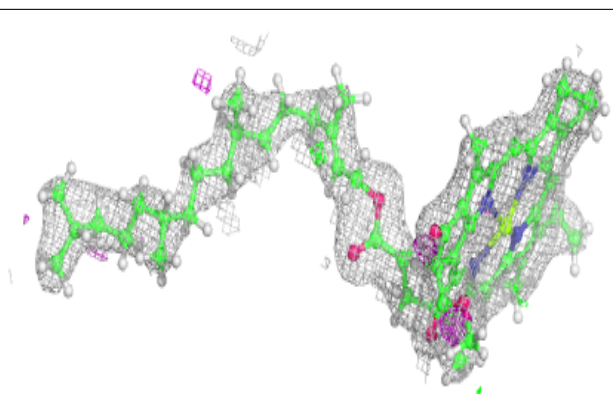
**Electron density around CLA C 503:**

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

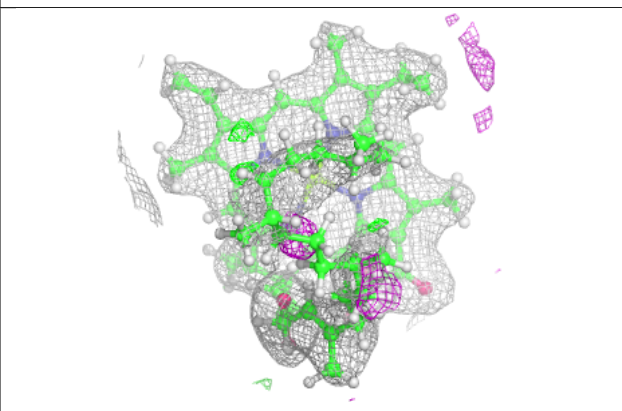
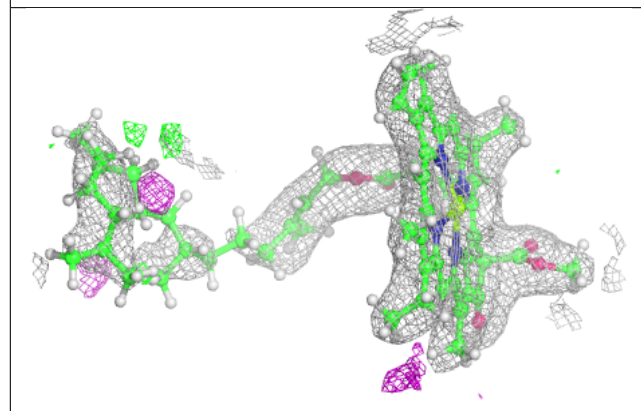
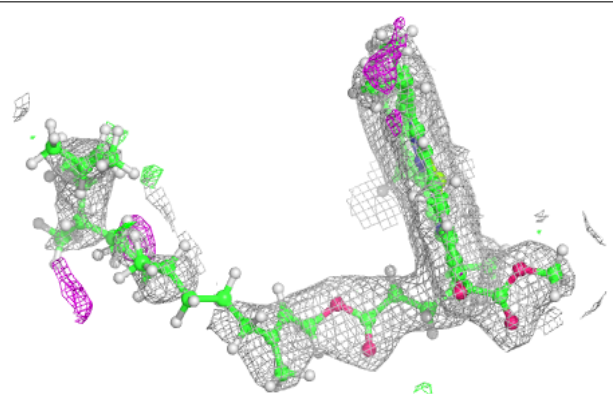


**Electron density around CLA C 502:**

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

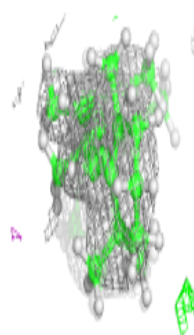
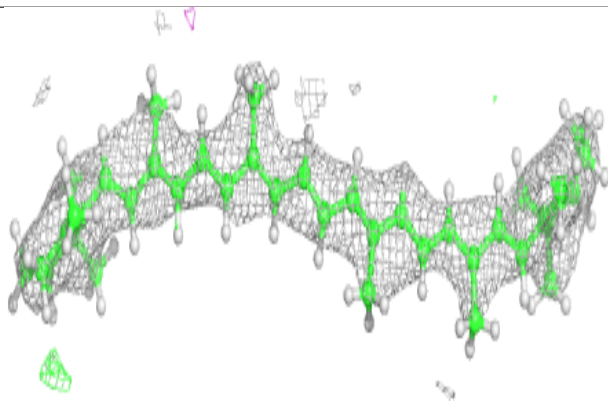
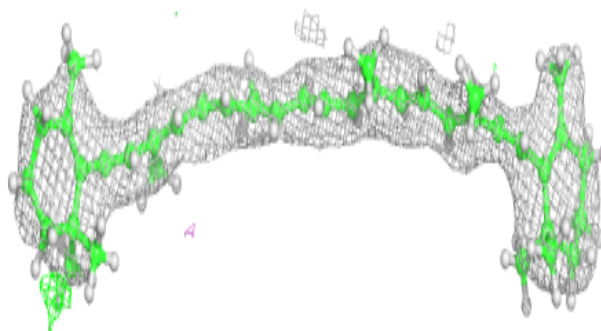
**Electron density around CLA C 506:**

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

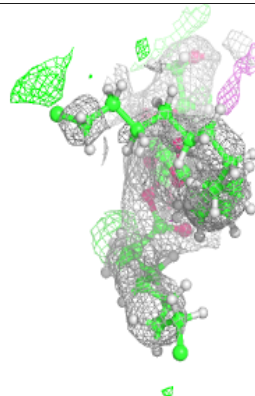
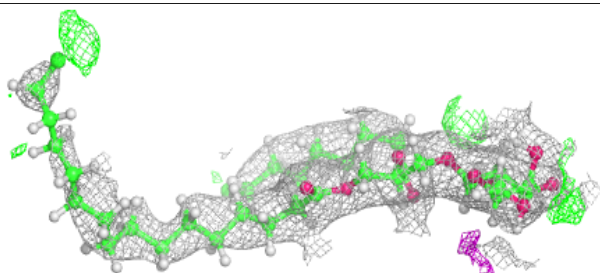
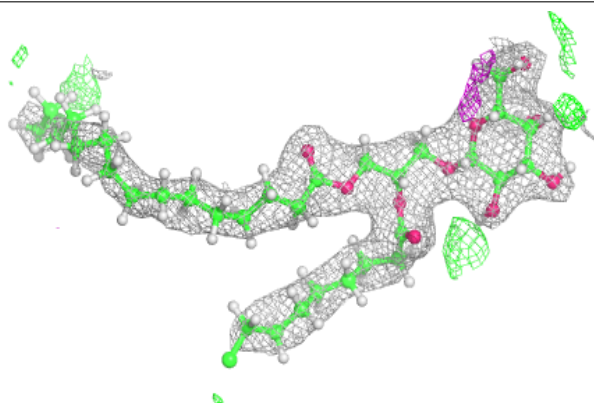


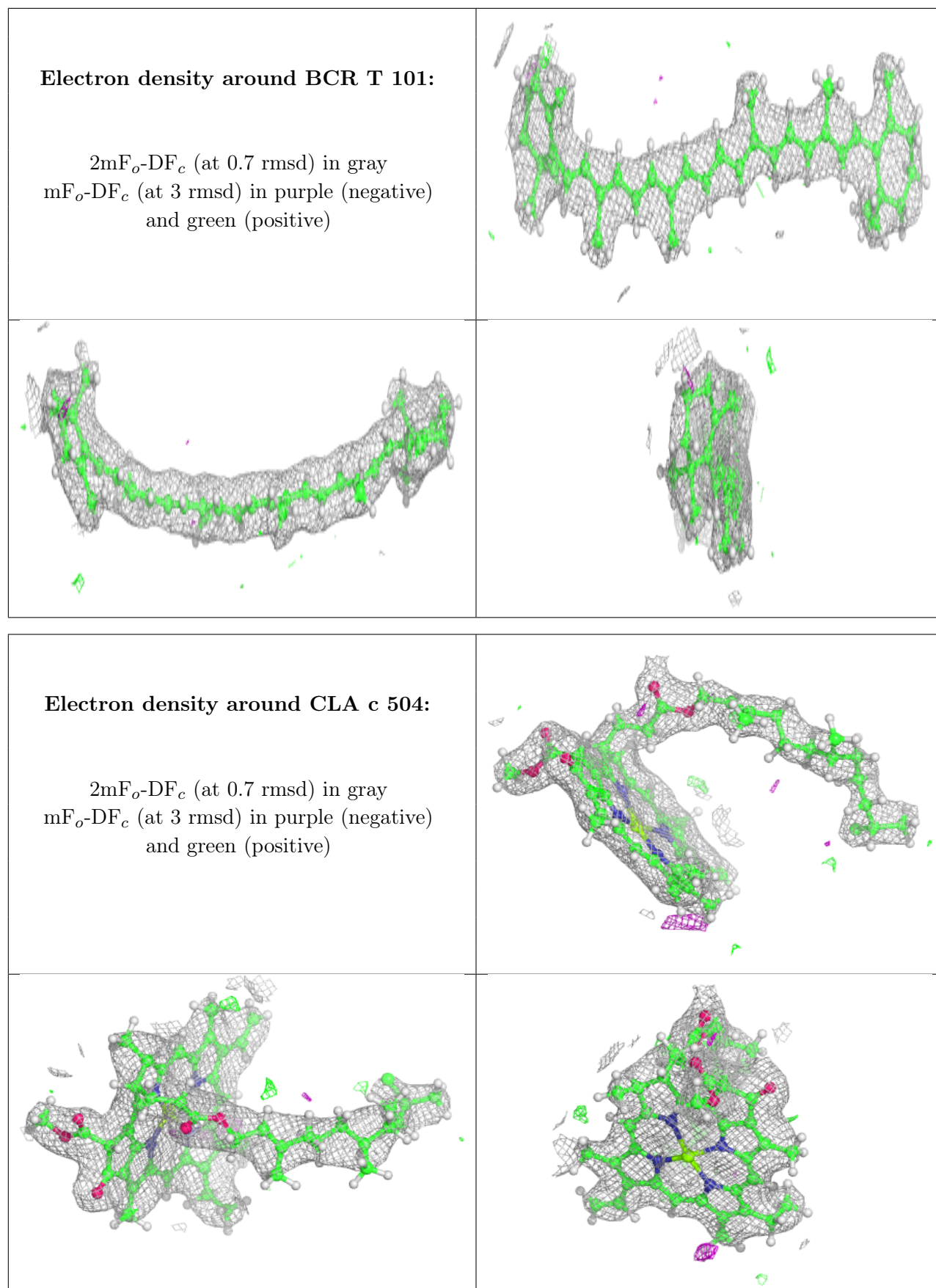
**Electron density around BCR K 102:**

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

**Electron density around LMG d 409:**

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

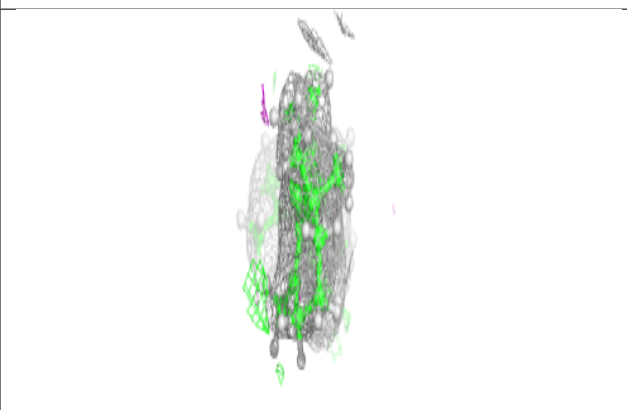
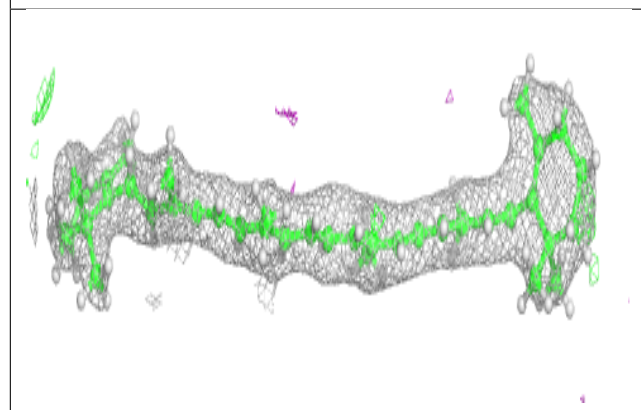
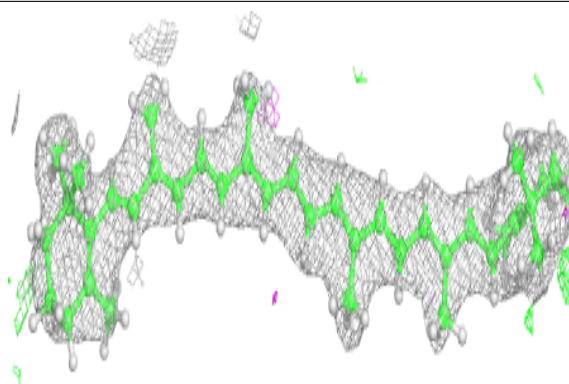




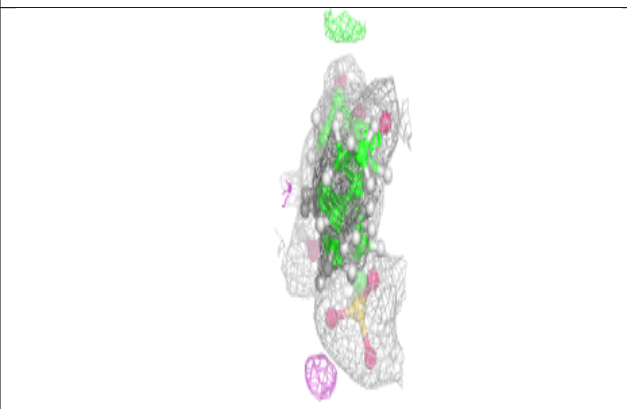
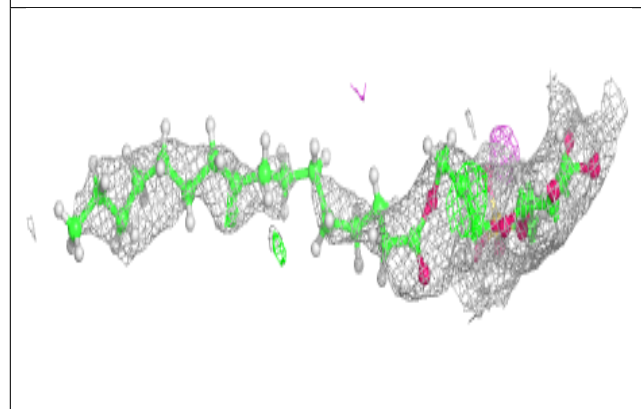
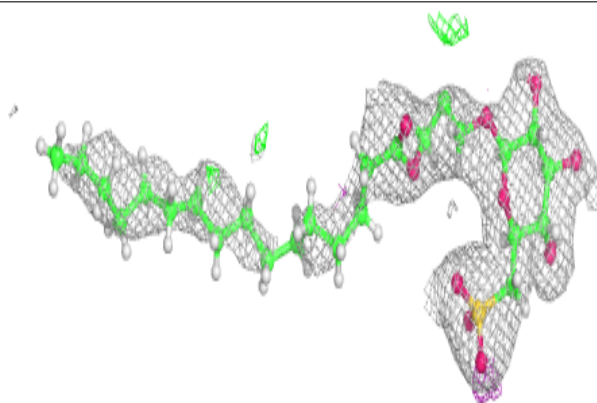


**Electron density around BCR b 618:**

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

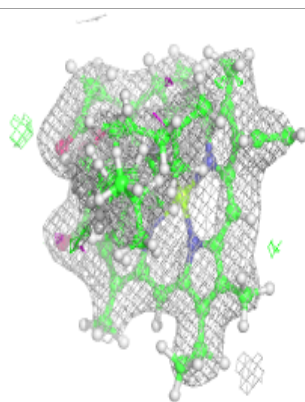
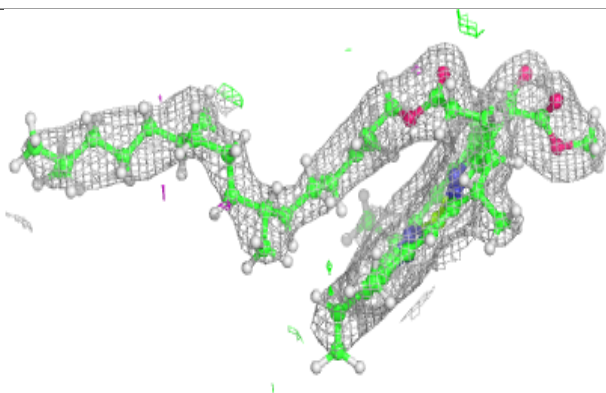
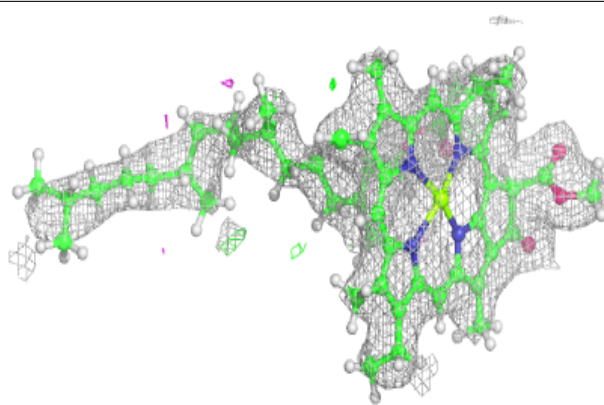
**Electron density around SQD F 101:**

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

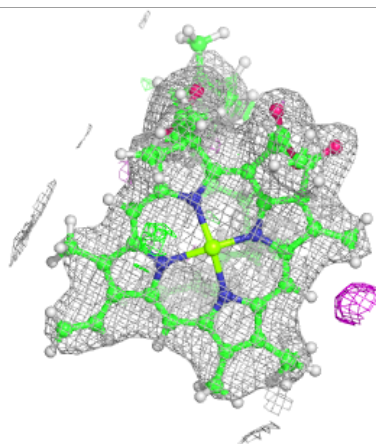
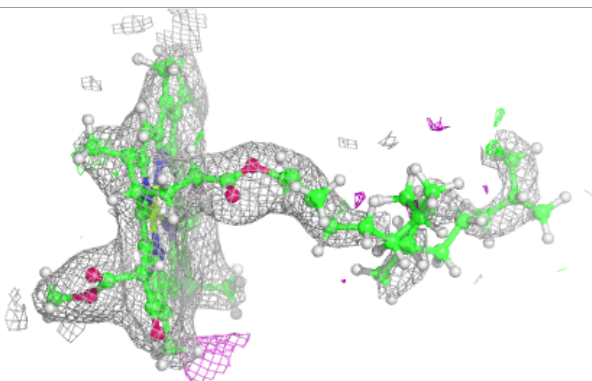
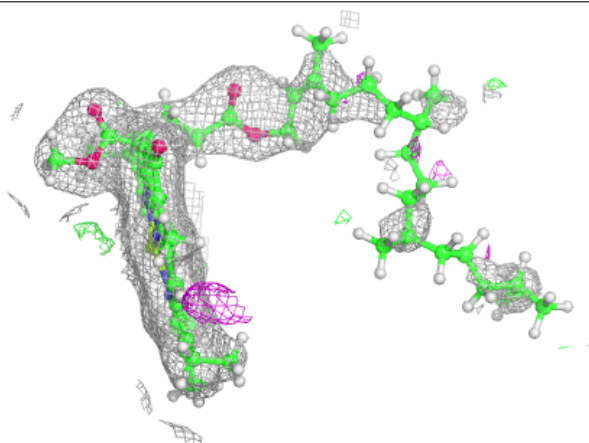


**Electron density around CLA c 505:**

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

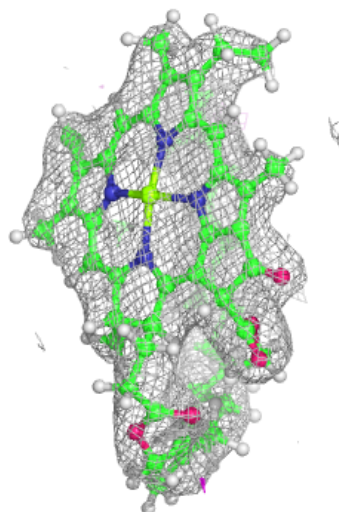
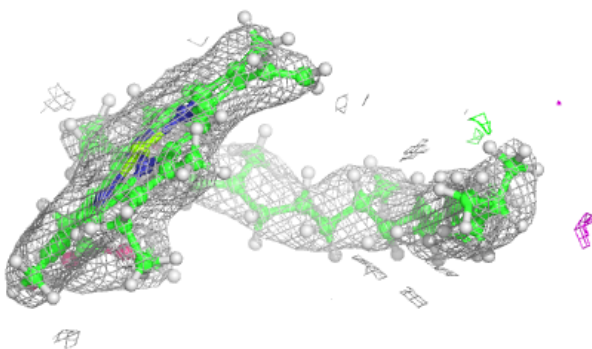
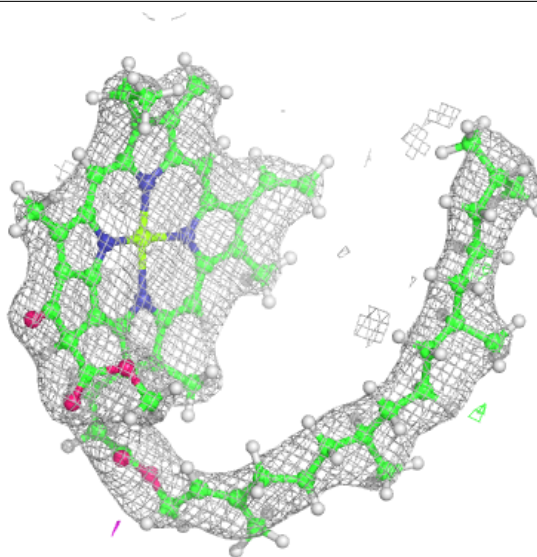
**Electron density around CLA c 506:**

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



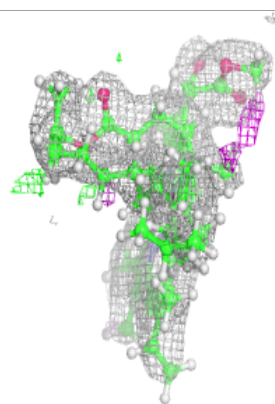
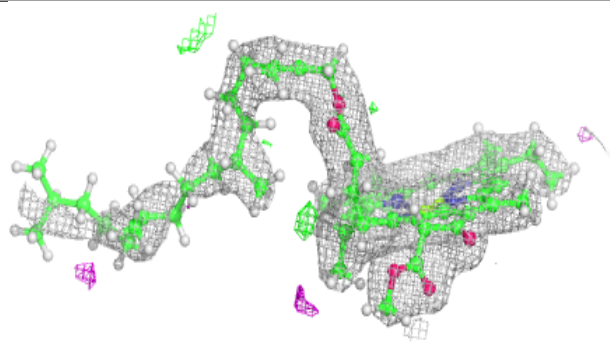
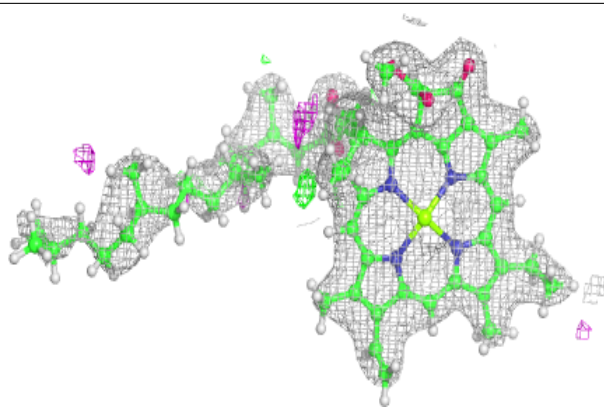
**Electron density around CLA c 507:**

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

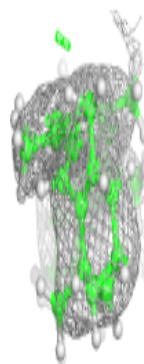
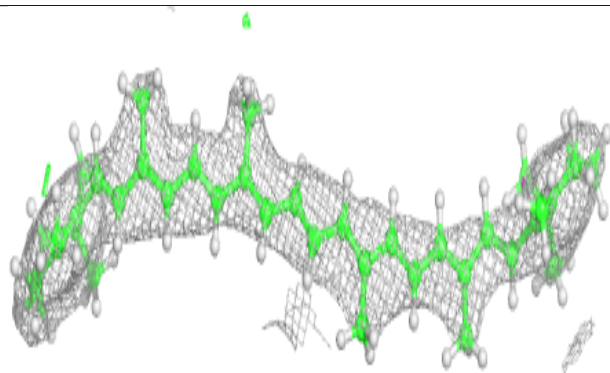
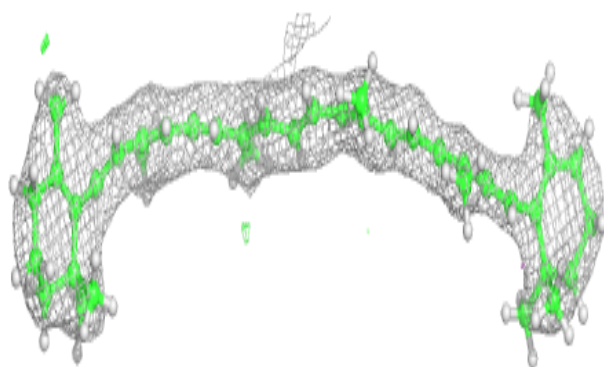


**Electron density around CLA a 406:**

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

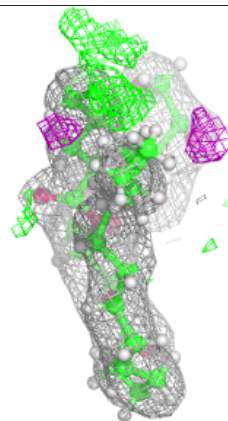
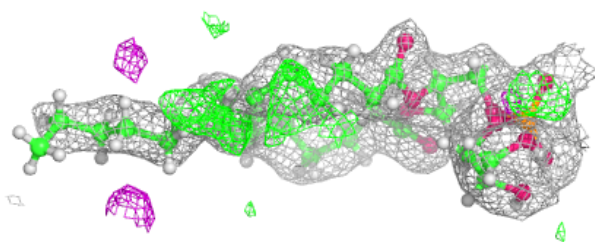
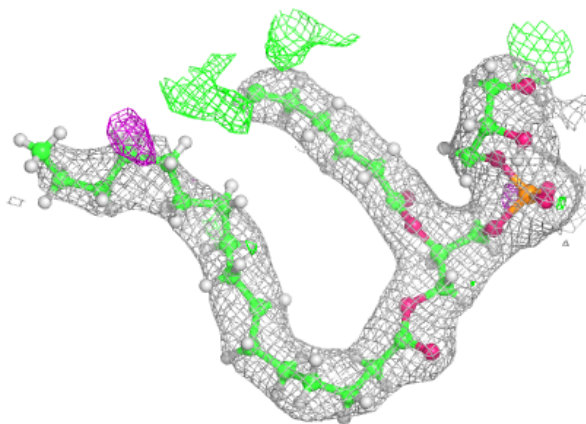
**Electron density around BCR k 102:**

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



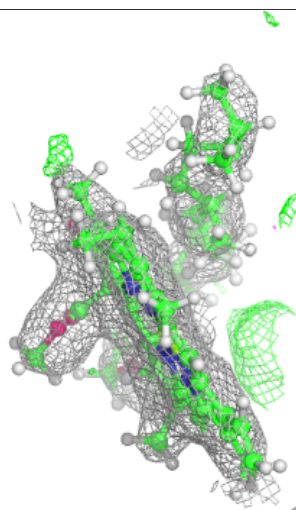
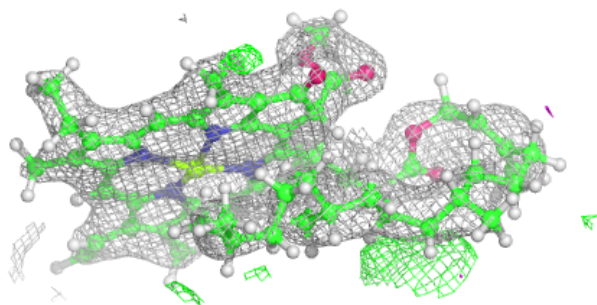
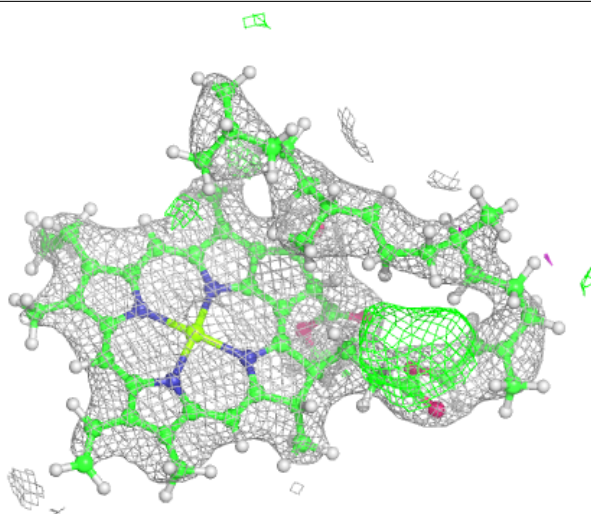
**Electron density around LHG d 408:**

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



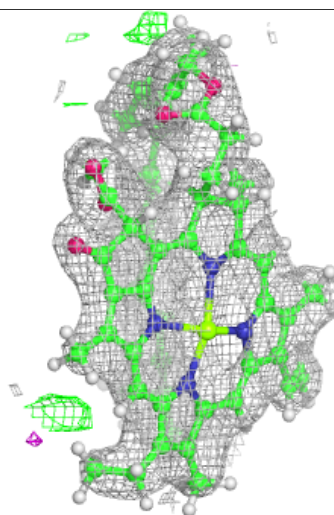
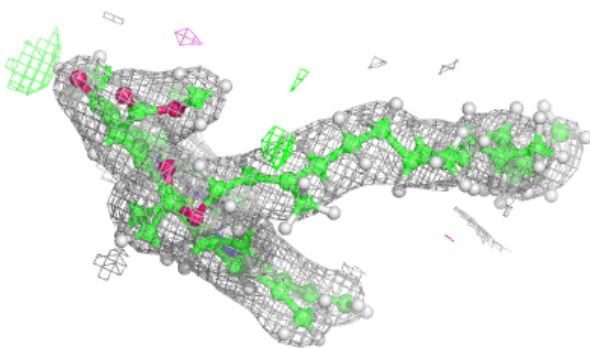
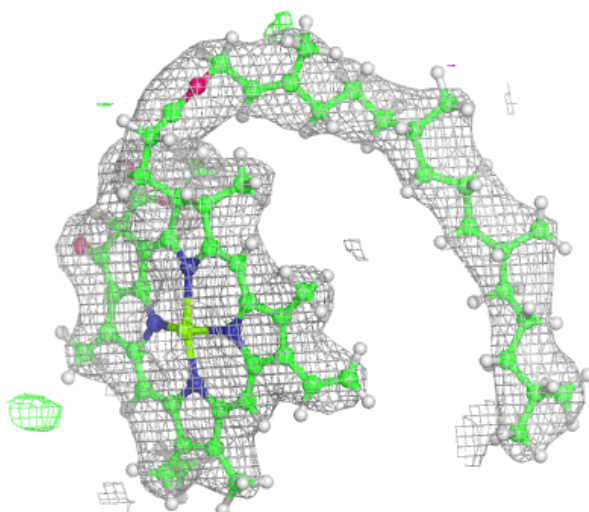
**Electron density around CLA c 509:**

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



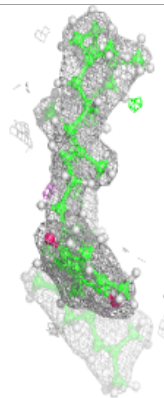
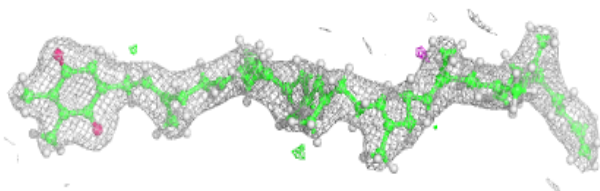
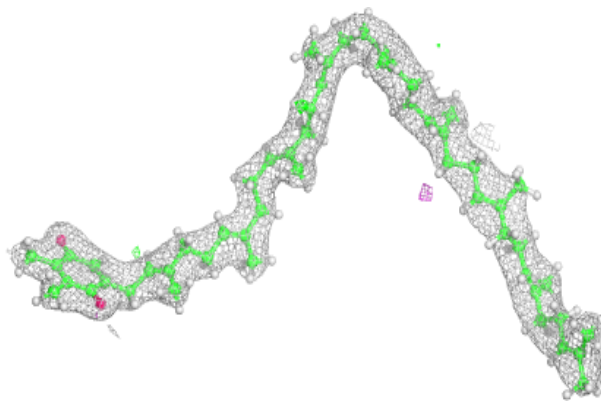
**Electron density around CLA C 507:**

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



**Electron density around PL9 D 405:**

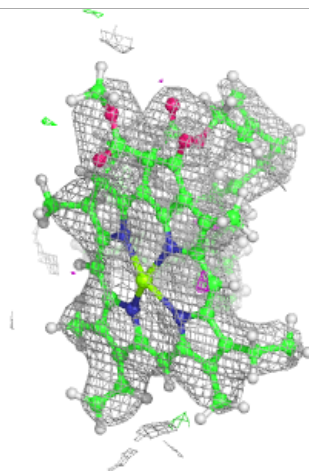
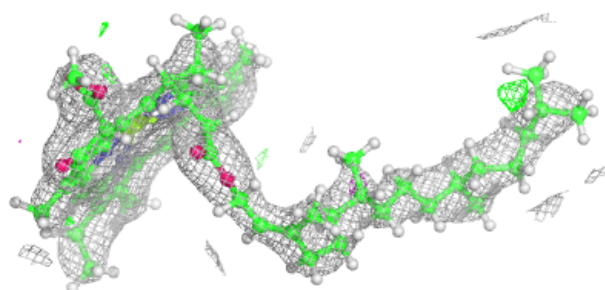
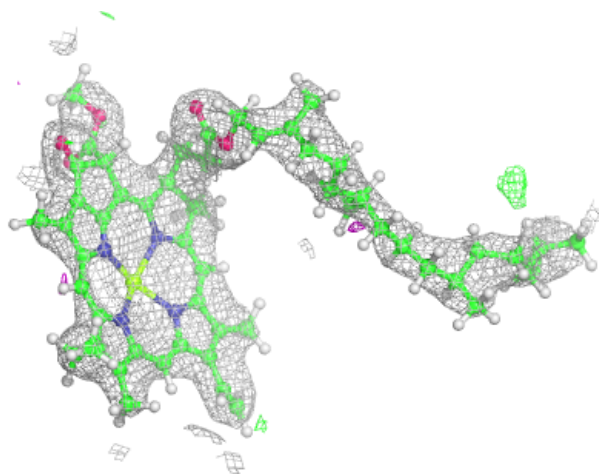
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





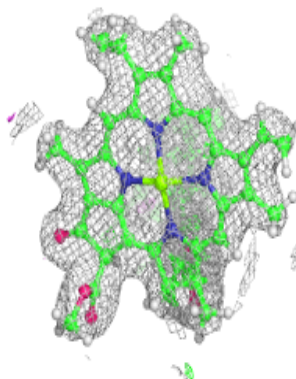
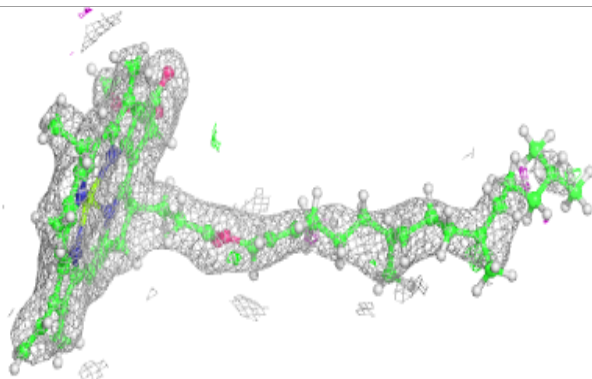
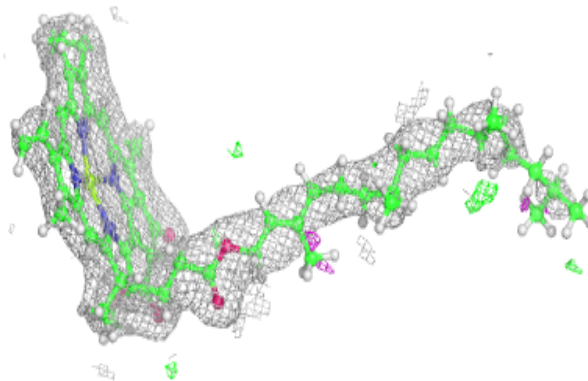
**Electron density around CLA c 511:**

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

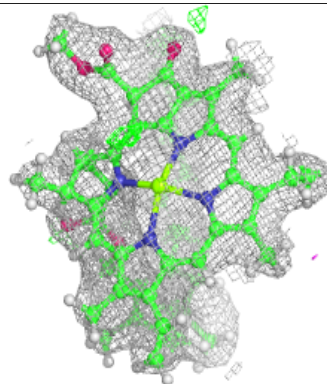
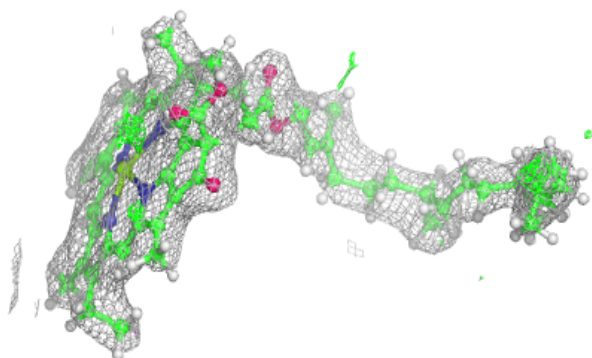
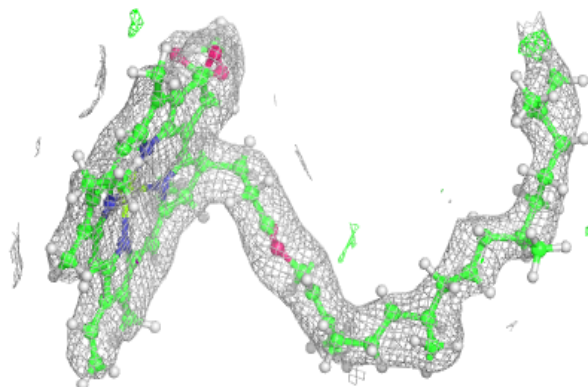


**Electron density around CLA b 605:**

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

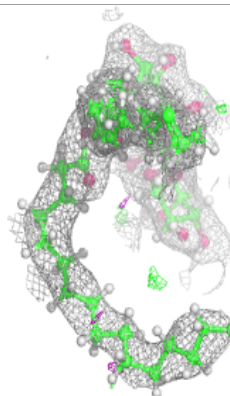
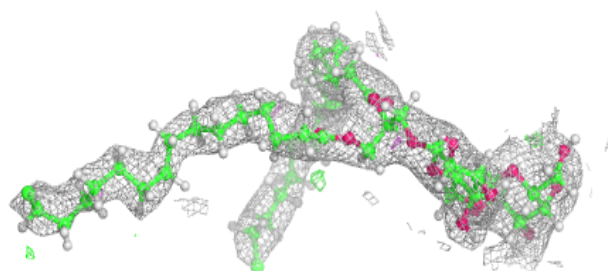
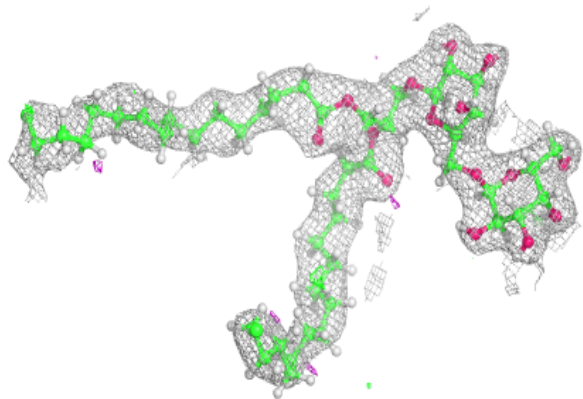
**Electron density around CLA b 607:**

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

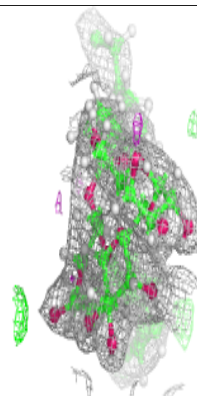
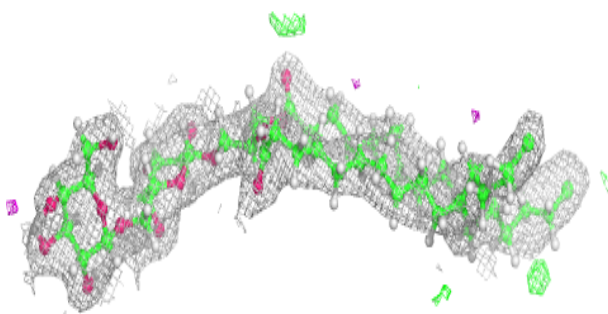
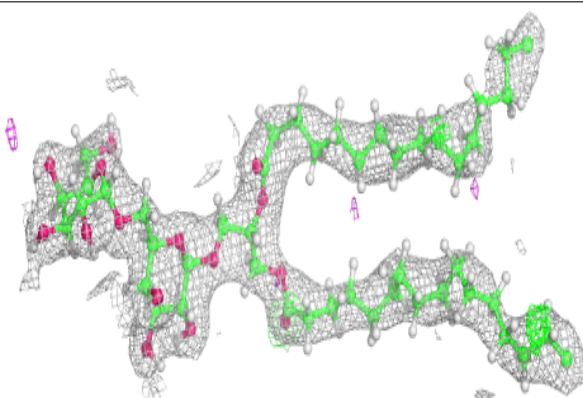


**Electron density around DGD c 517:**

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

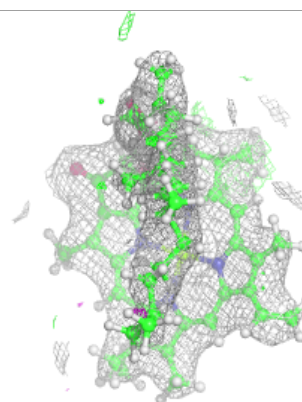
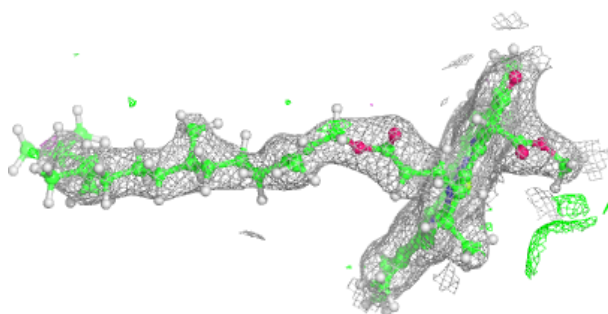
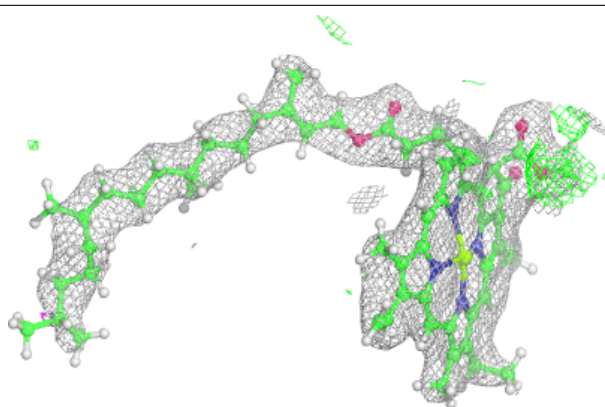
**Electron density around DGD c 518:**

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

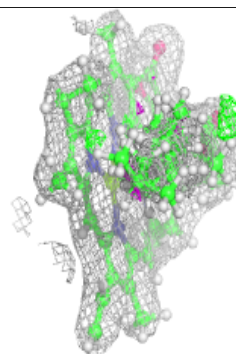
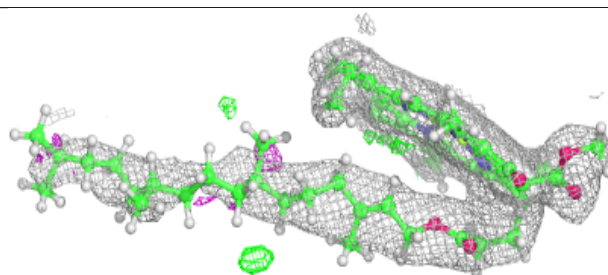
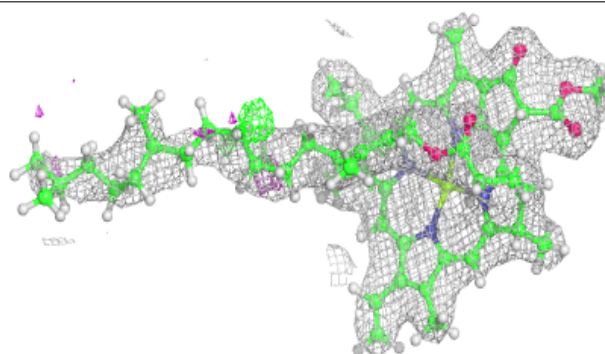


**Electron density around CLA b 610:**

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

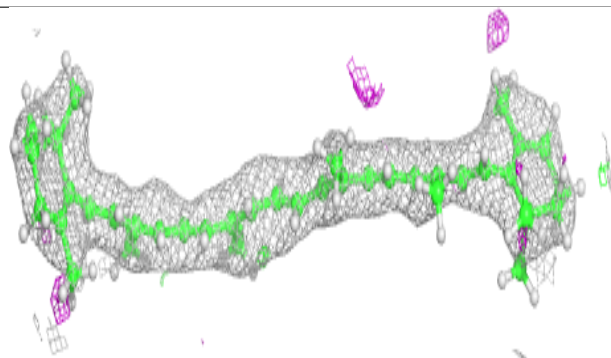
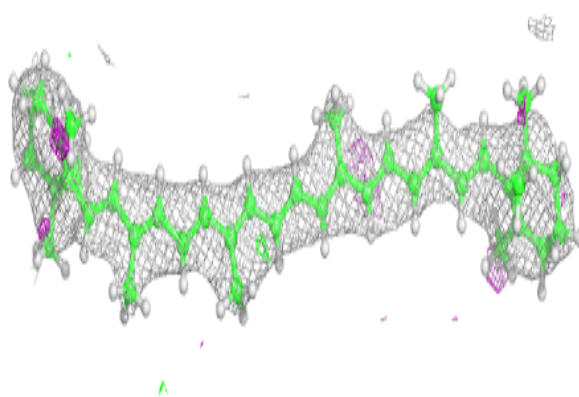
**Electron density around CLA b 615:**

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



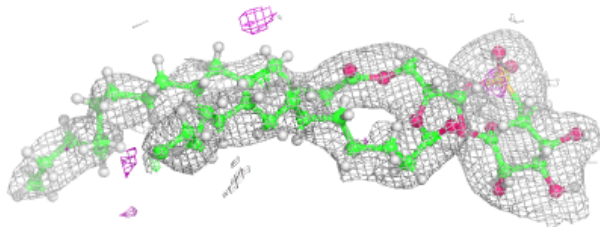
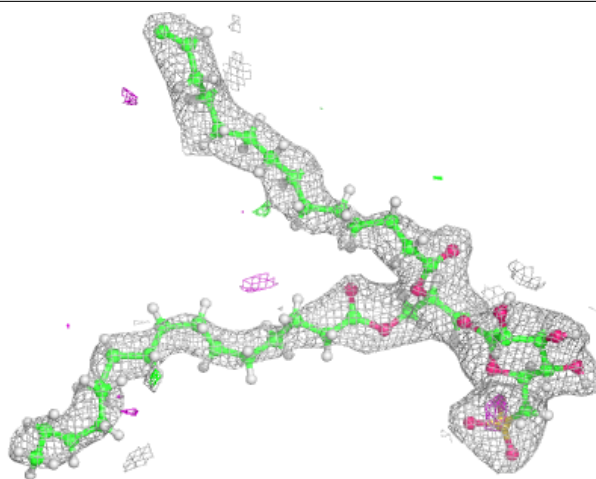
**Electron density around BCR c 515:**

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



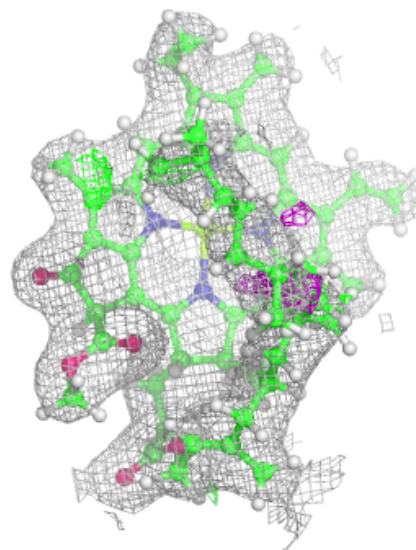
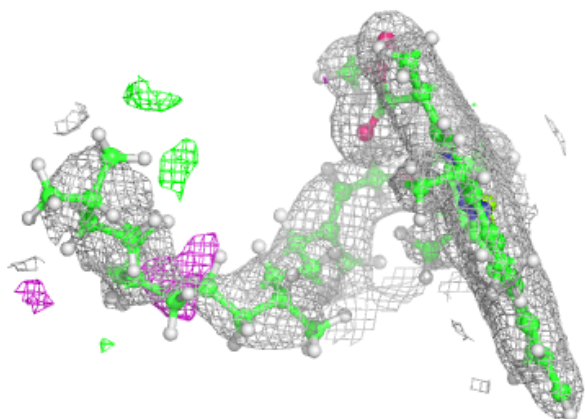
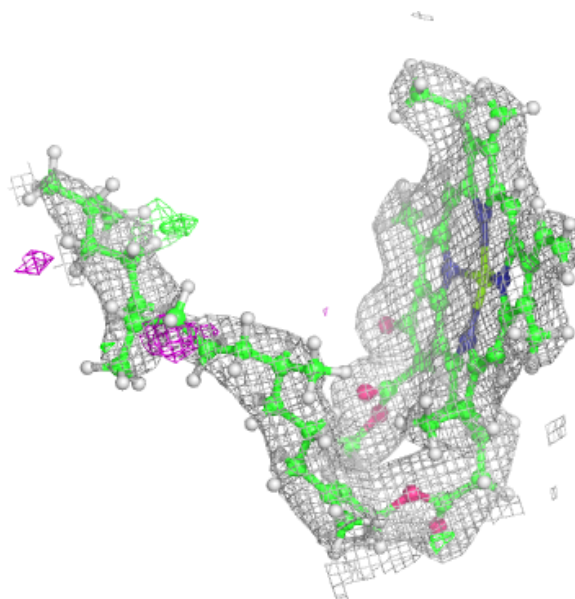
**Electron density around SQD A 412:**

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



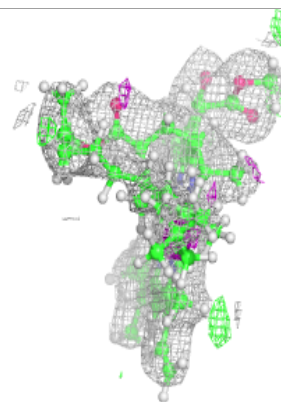
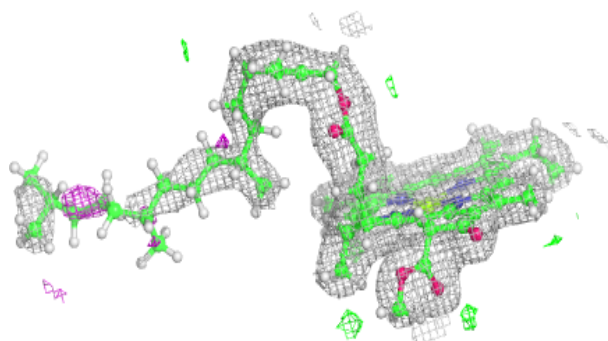
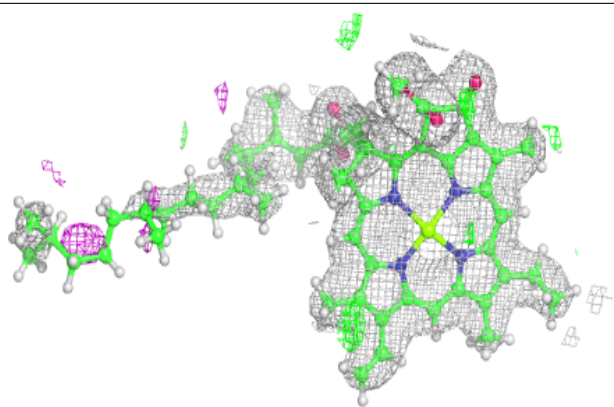
**Electron density around CLA b 614:**

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

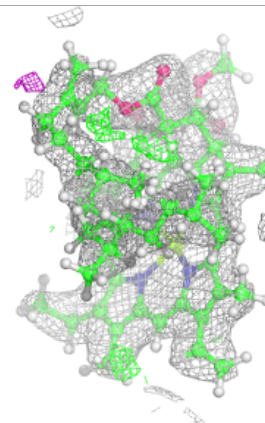
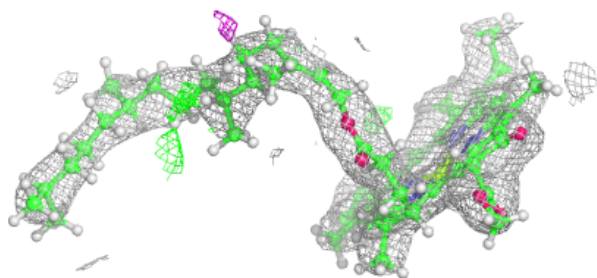
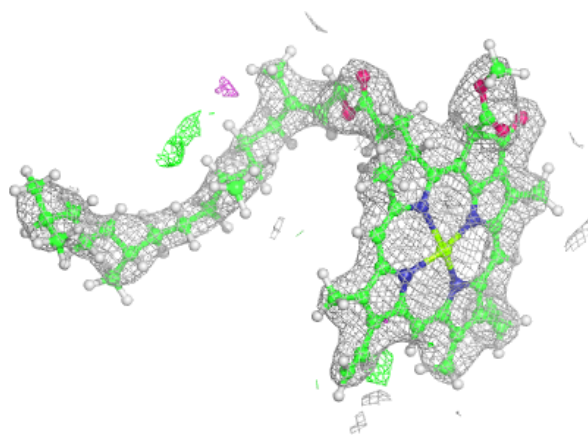


**Electron density around CLA A 405:**

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

**Electron density around CLA C 511:**

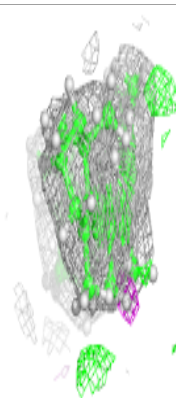
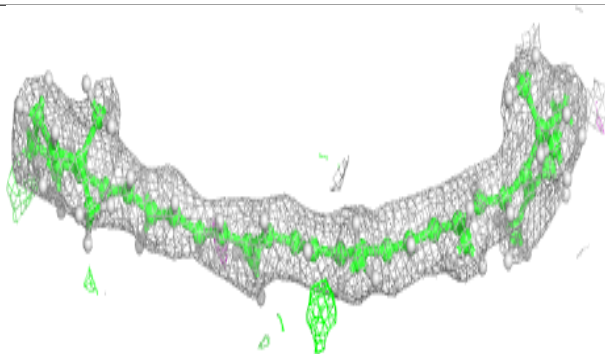
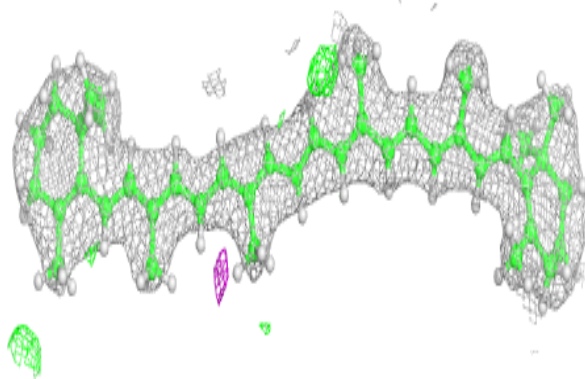
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





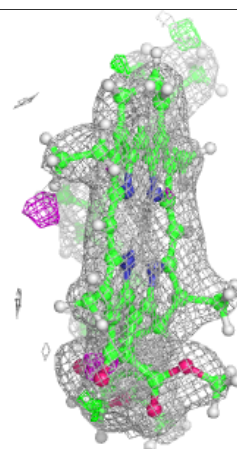
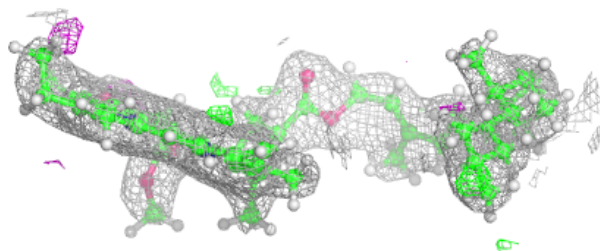
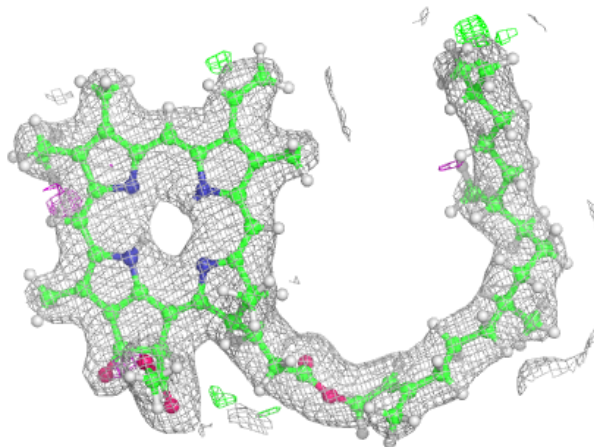
**Electron density around BCR t 101:**

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



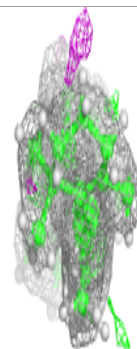
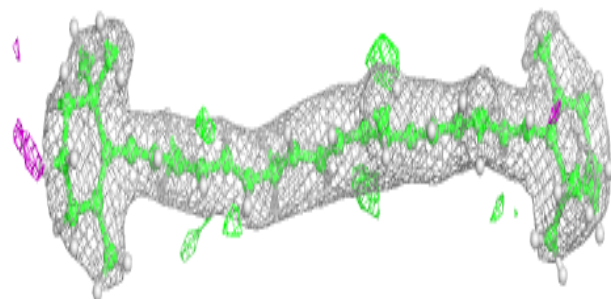
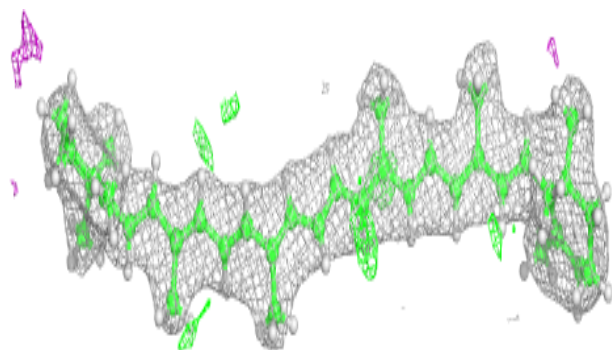
**Electron density around PHO a 407:**

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

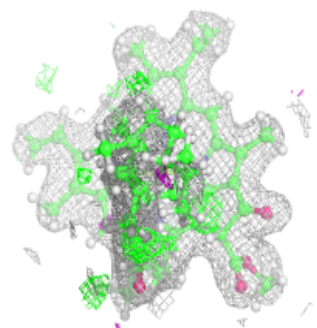
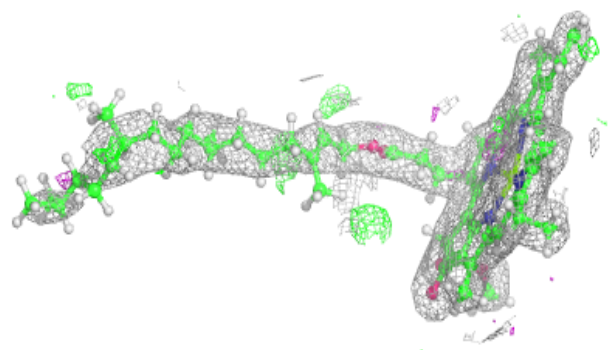
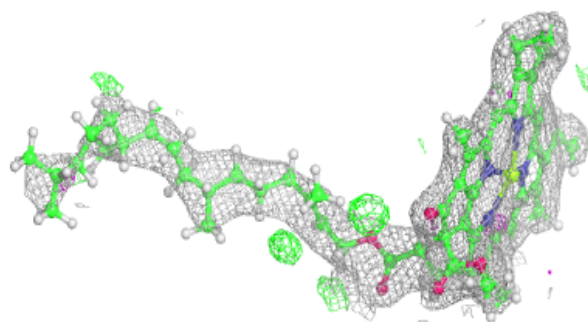


**Electron density around BCR A 409:**

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

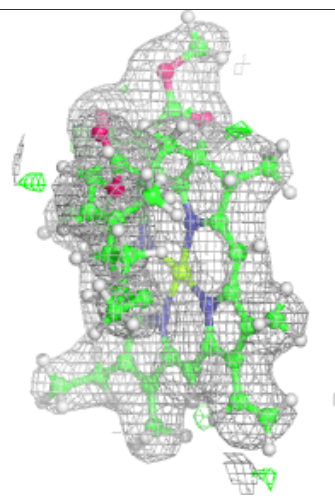
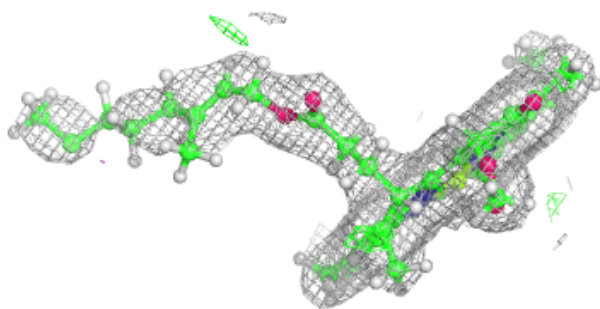
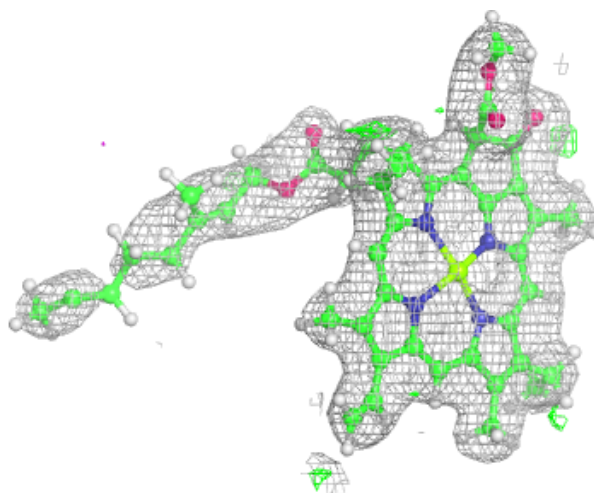
**Electron density around CLA B 604:**

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



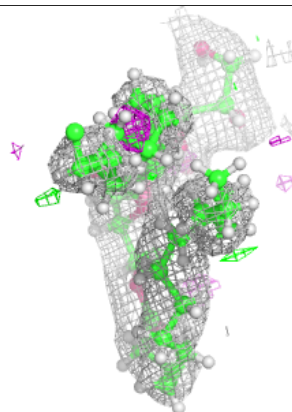
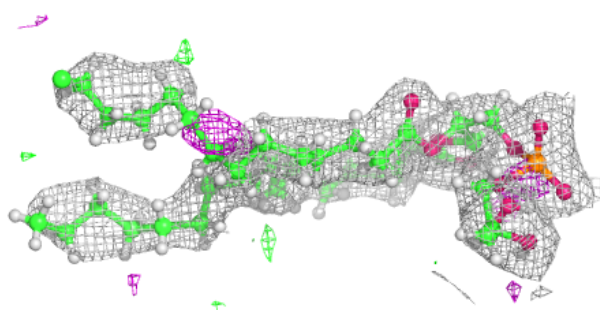
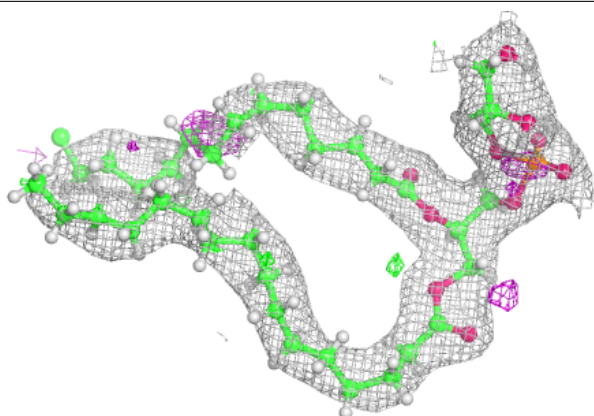
**Electron density around CLA A 408:**

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

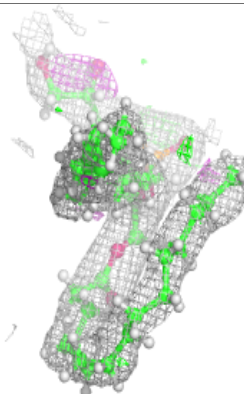
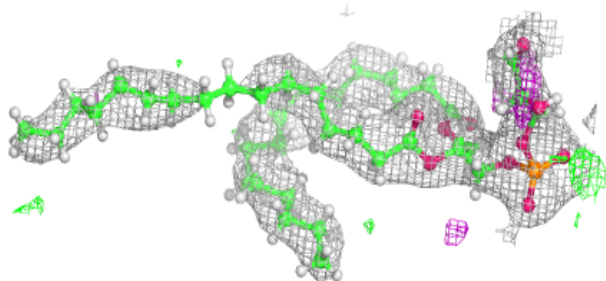
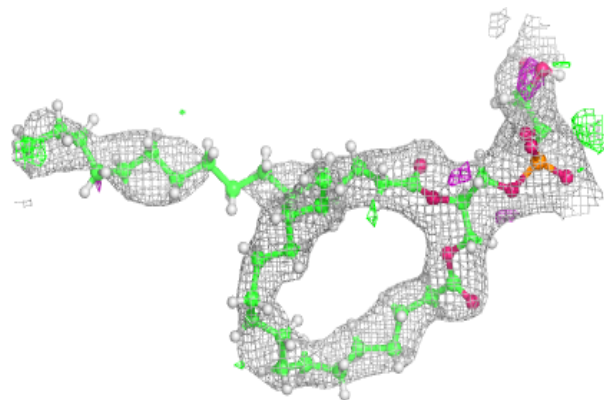


**Electron density around LHG D 408:**

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

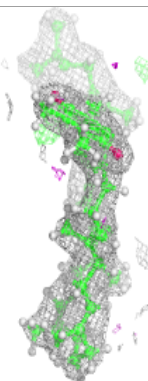
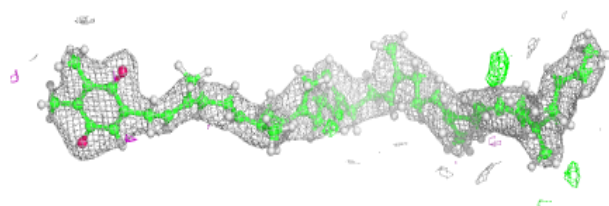
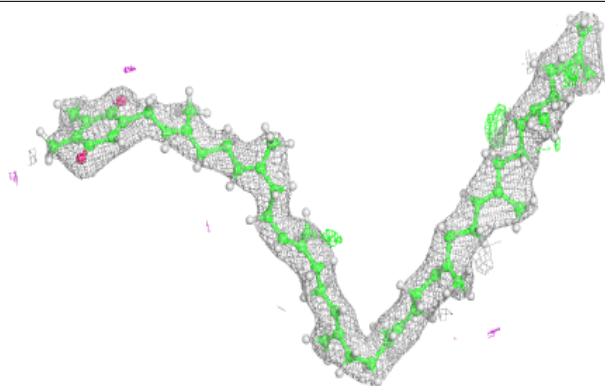
**Electron density around LHG d 406:**

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

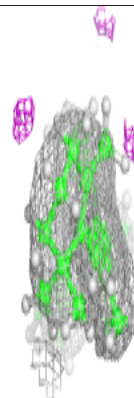
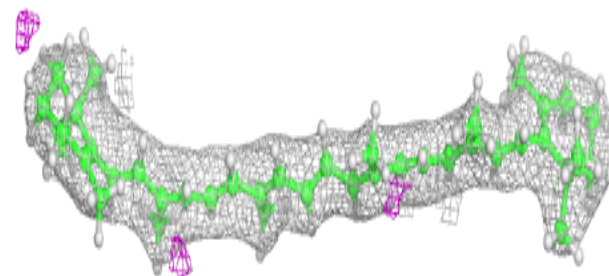
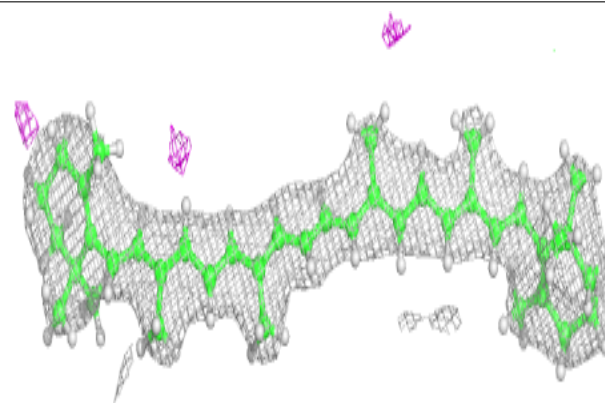


**Electron density around PL9 d 405:**

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

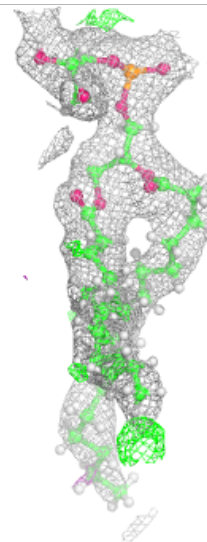
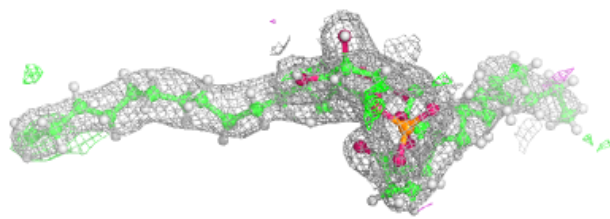
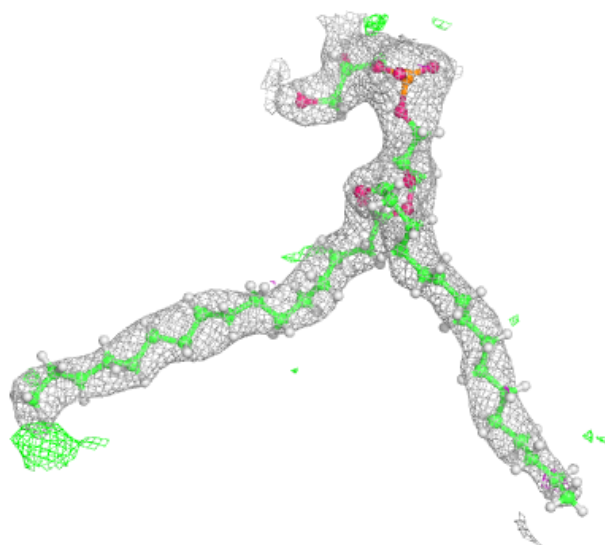
**Electron density around BCR B 619:**

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



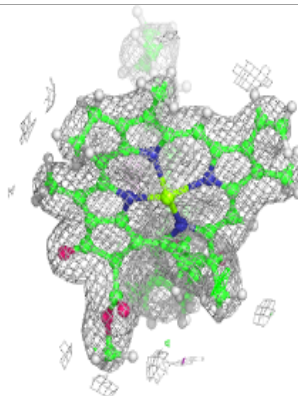
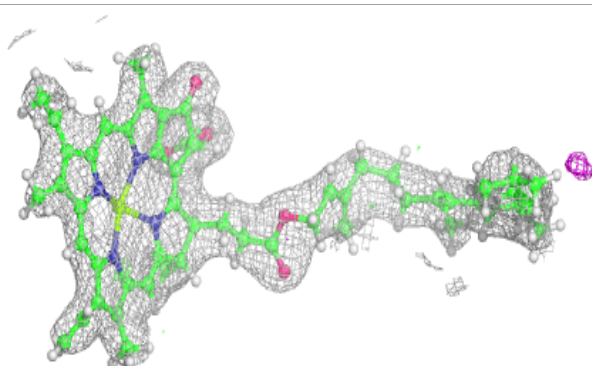
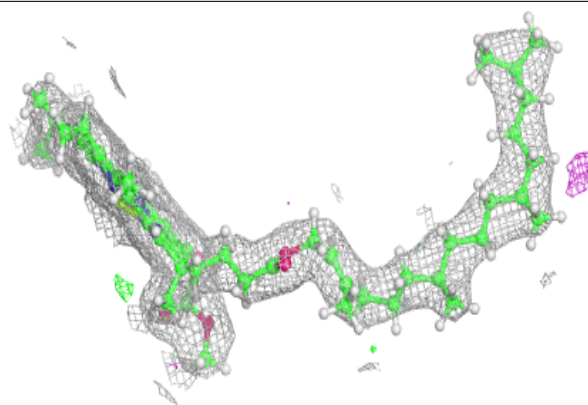
**Electron density around LHG 1 101:**

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

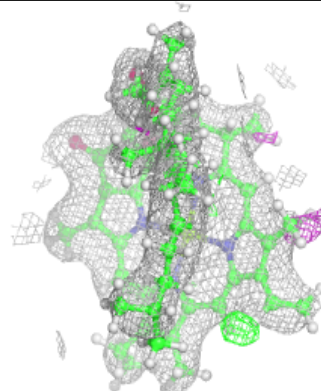
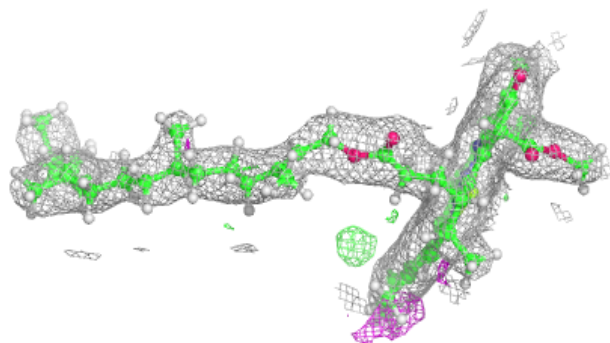
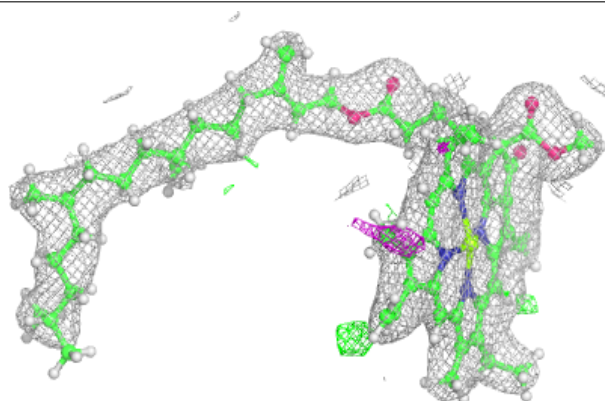


**Electron density around CLA D 402:**

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

**Electron density around CLA B 609:**

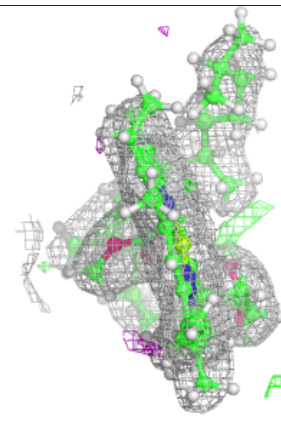
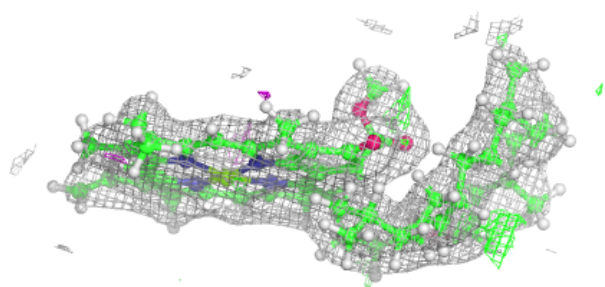
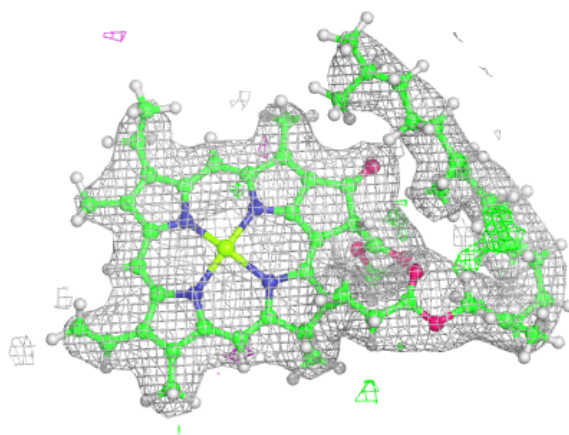
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



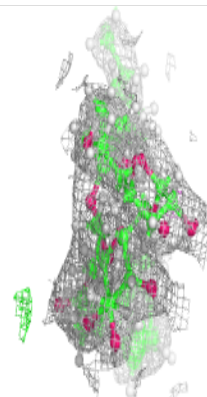
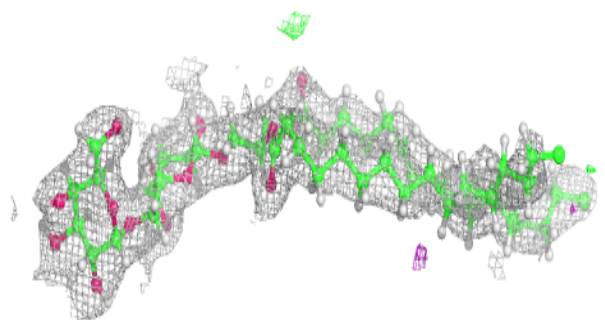
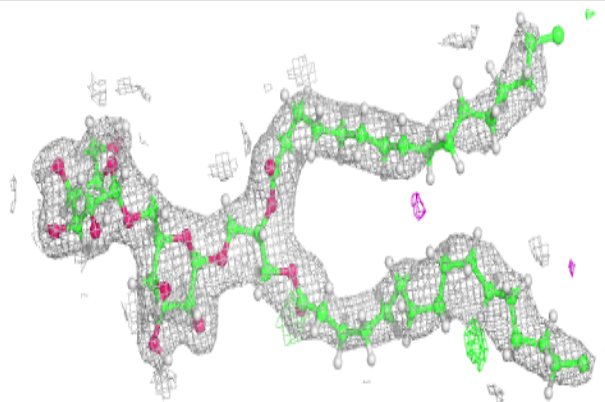


**Electron density around CLA B 610:**

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

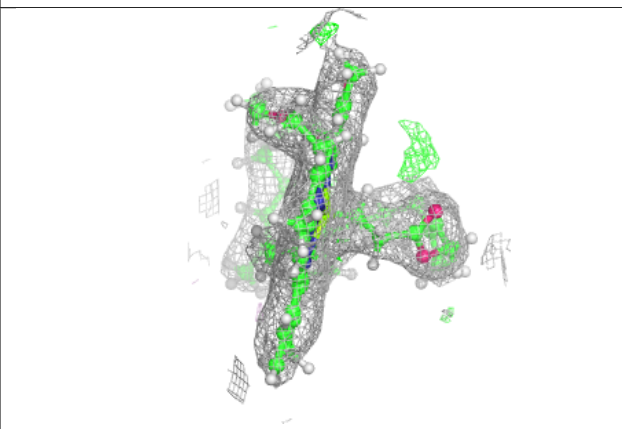
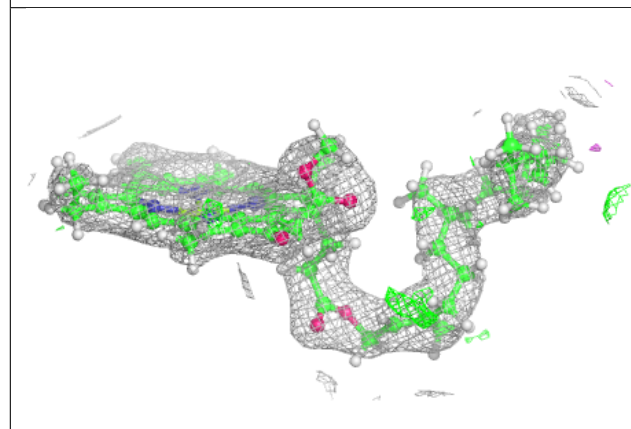
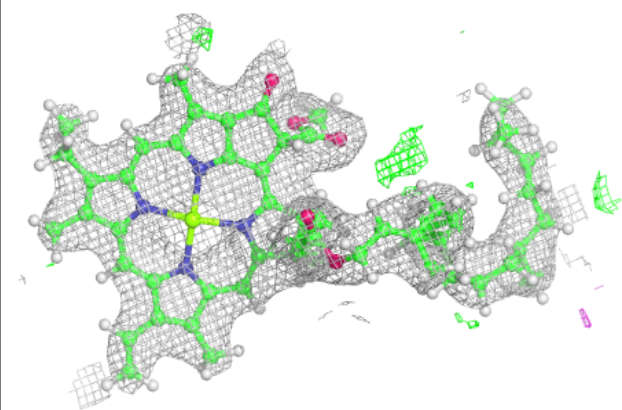
**Electron density around DGD C 517:**

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

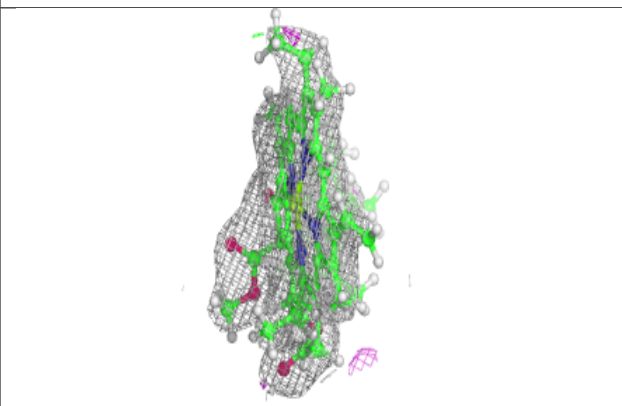
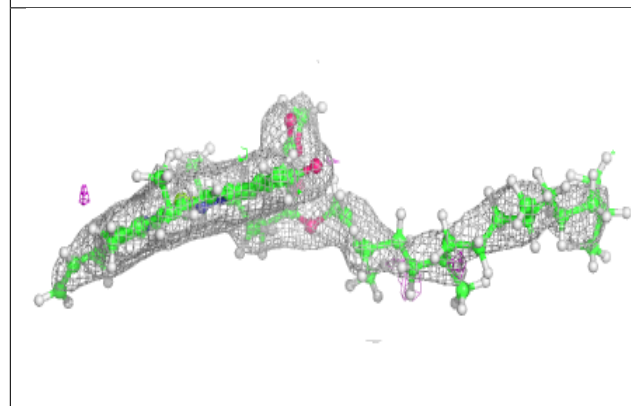
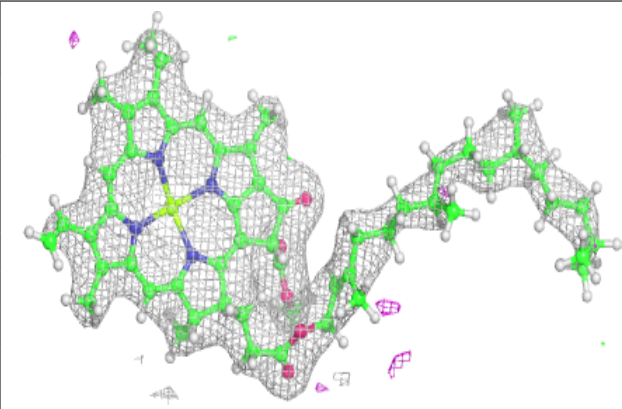


**Electron density around CLA B 612:**

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

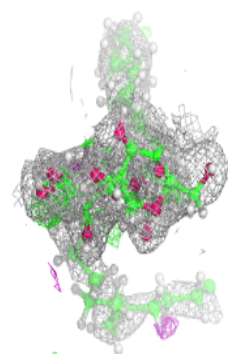
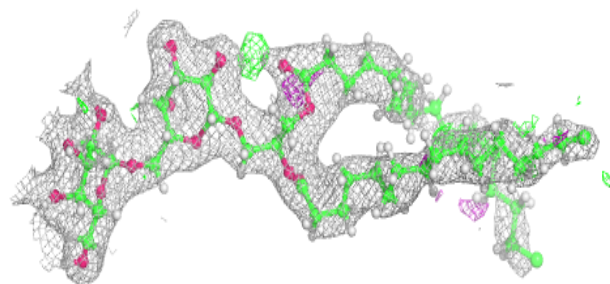
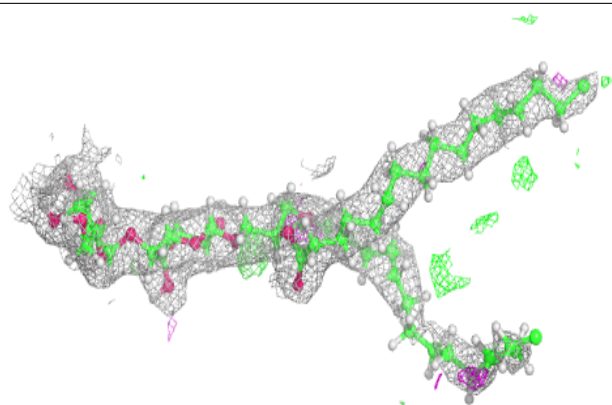
**Electron density around CLA b 603:**

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

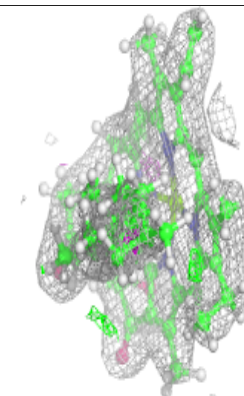
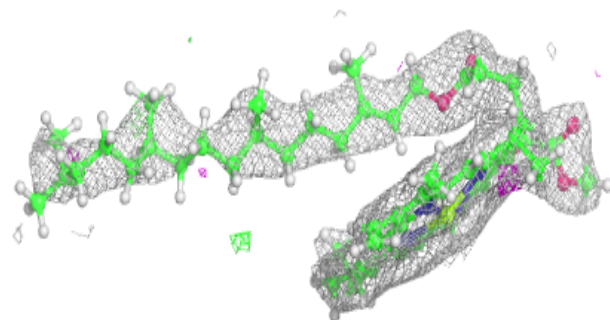
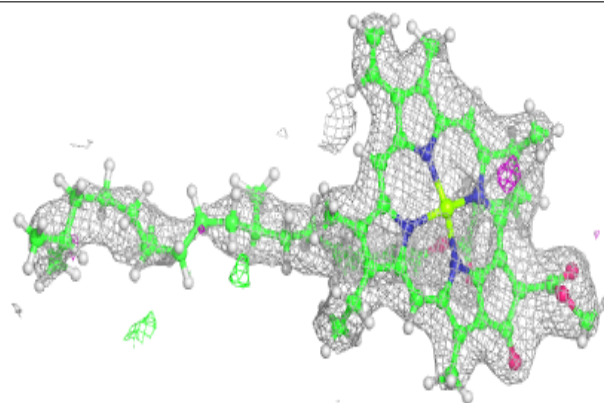


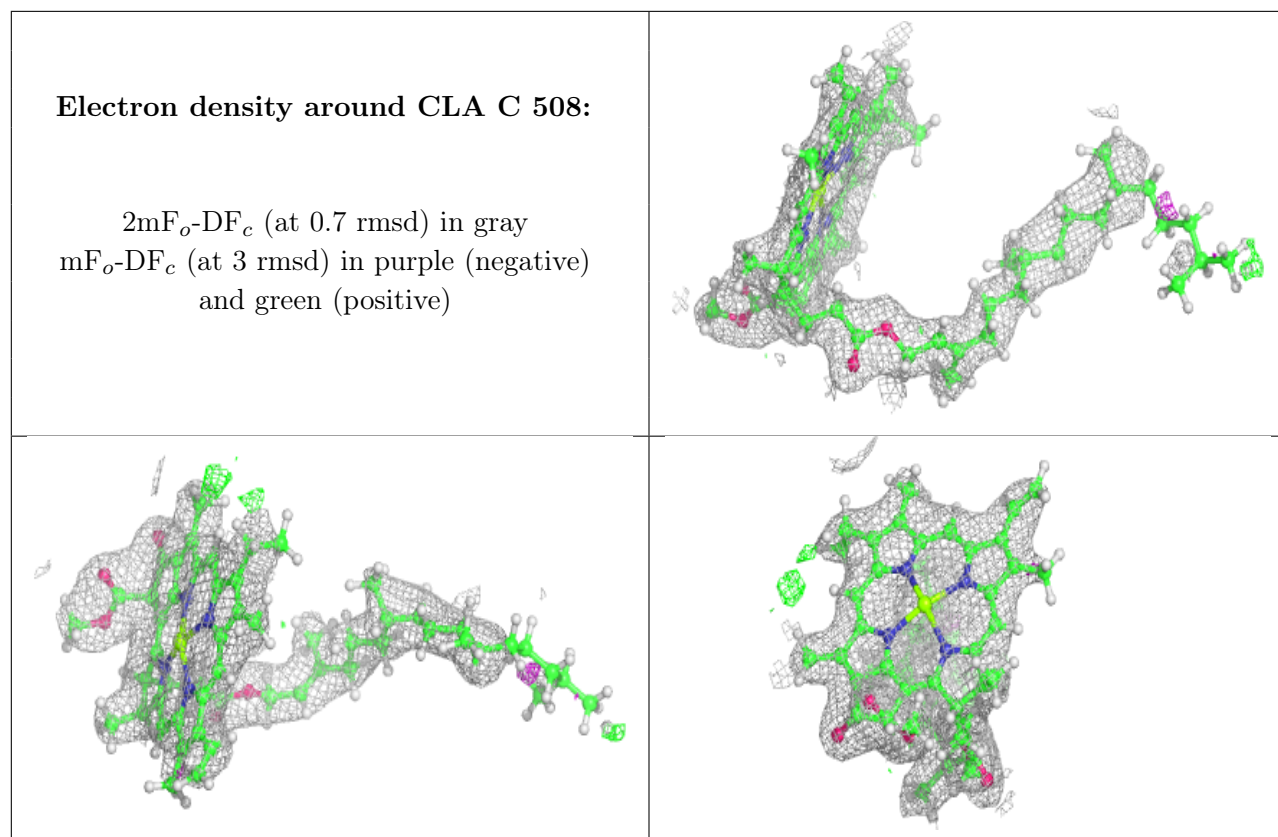
**Electron density around DGD c 516:**

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

**Electron density around CLA B 614:**

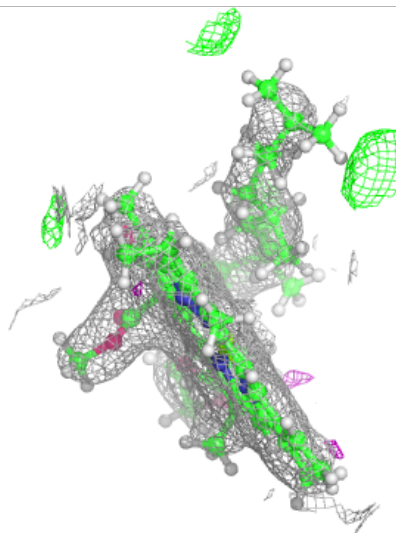
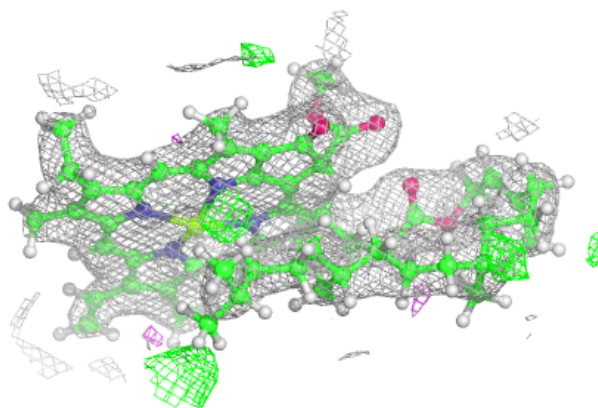
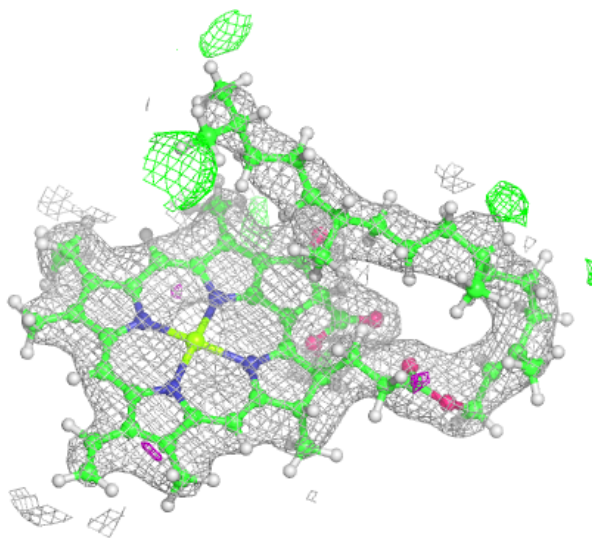
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





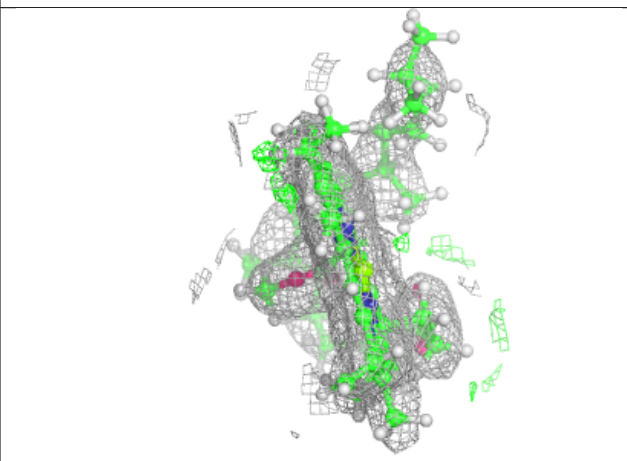
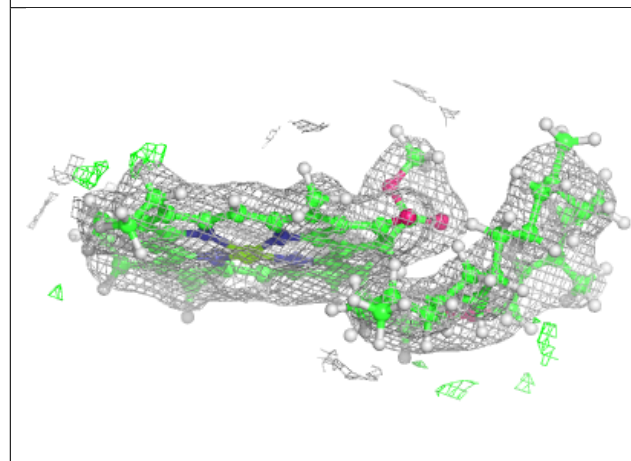
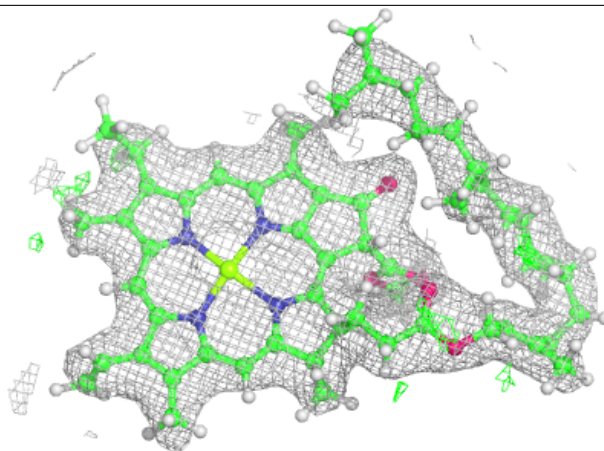
**Electron density around CLA C 509:**

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

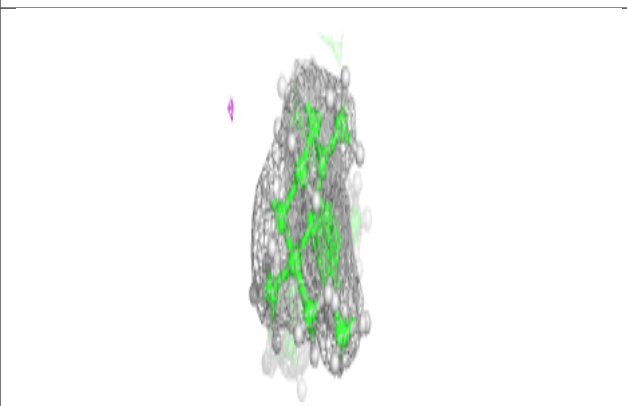
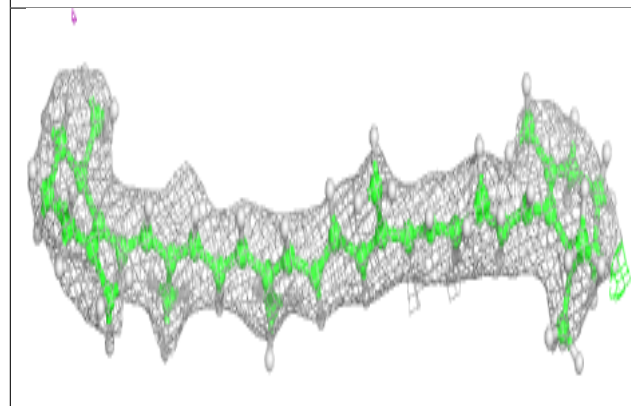
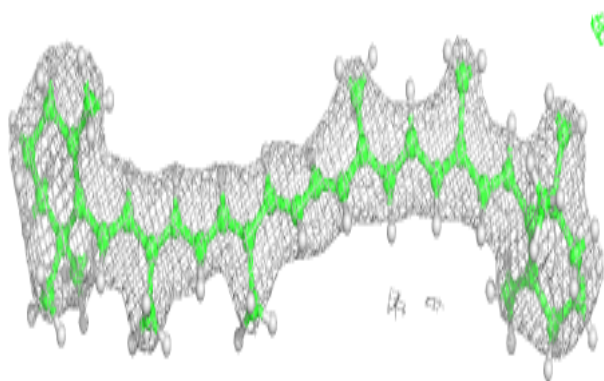


**Electron density around CLA b 611:**

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

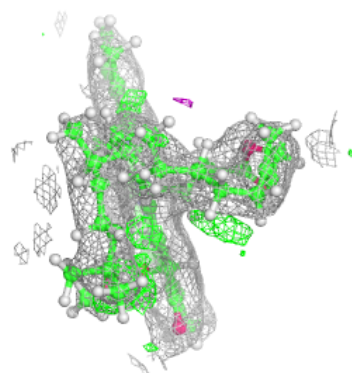
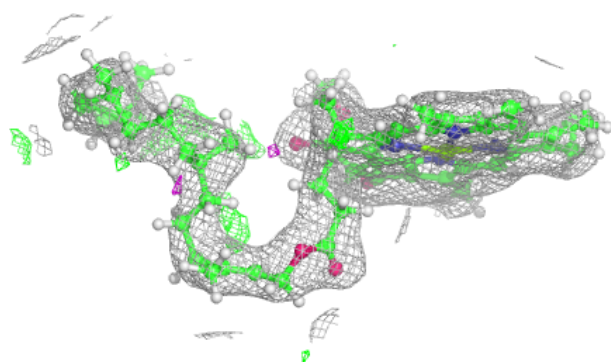
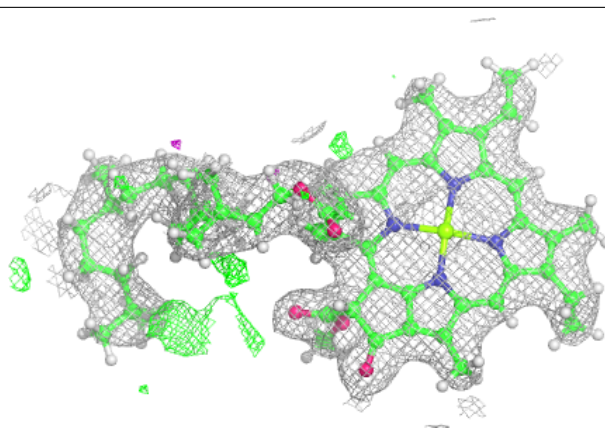
**Electron density around BCR b 620:**

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

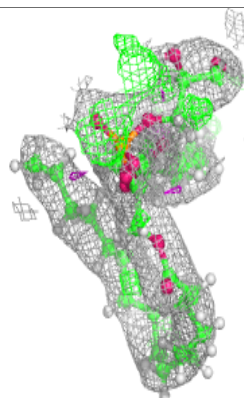
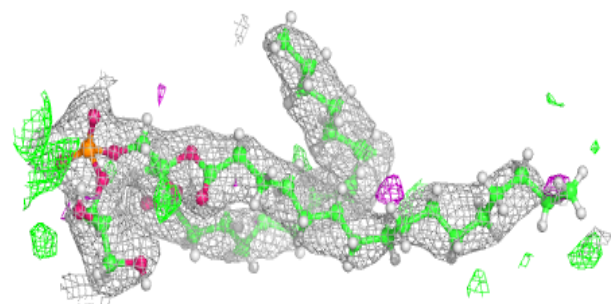
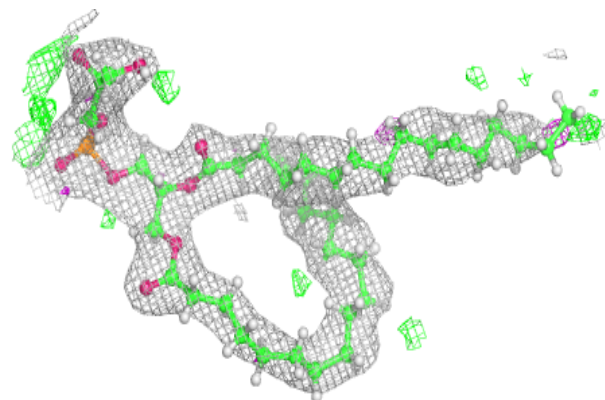


**Electron density around CLA b 613:**

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

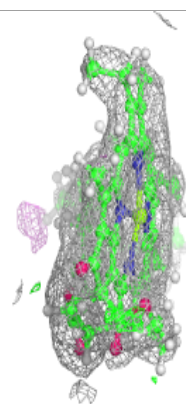
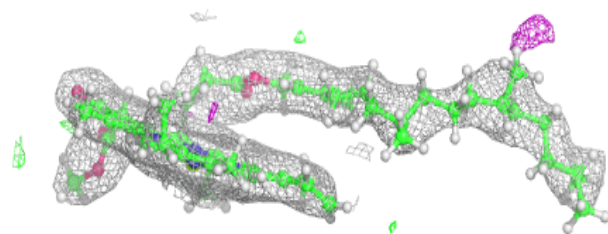
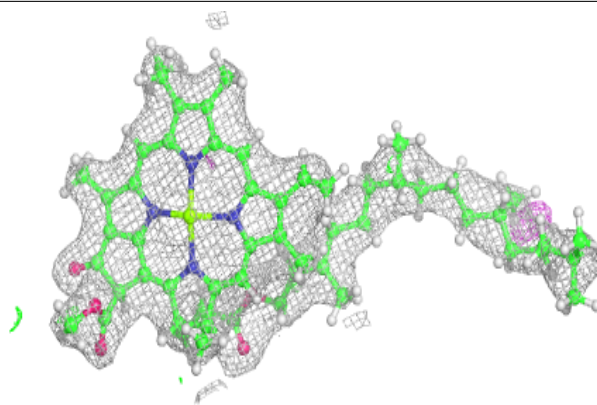
**Electron density around LHG B 623:**

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

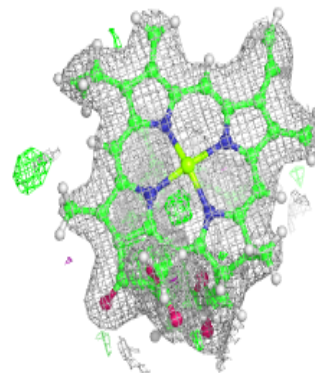
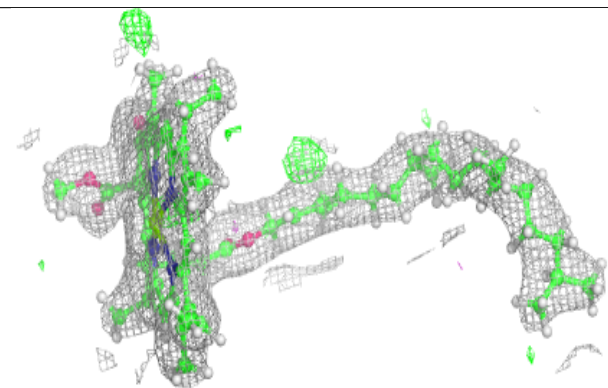
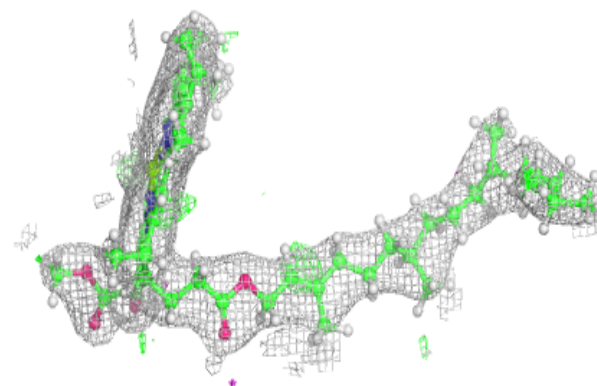


**Electron density around CLA b 604:**

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

**Electron density around CLA B 605:**

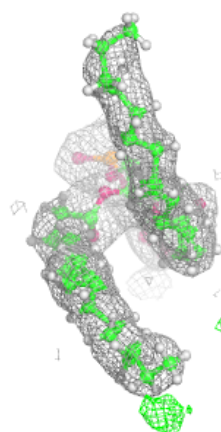
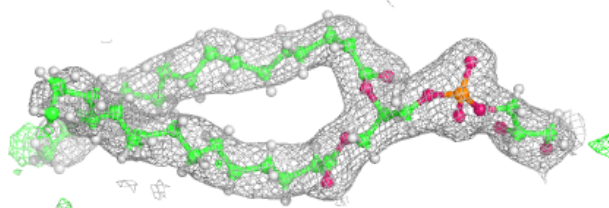
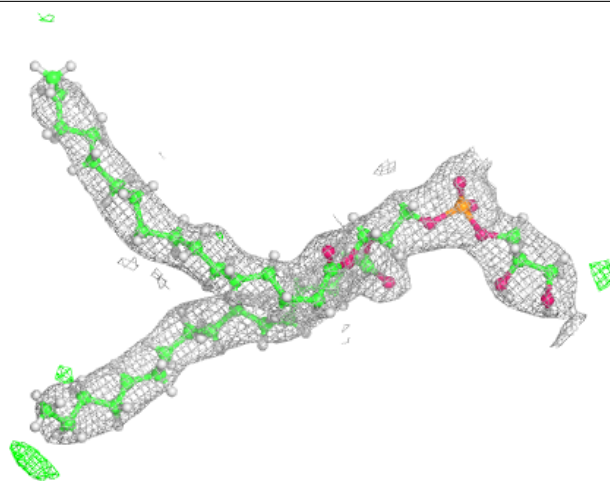
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





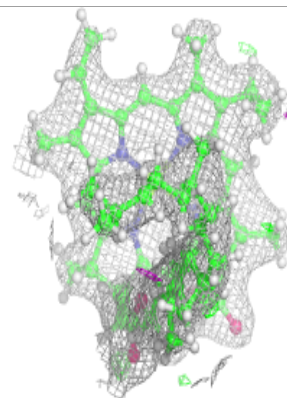
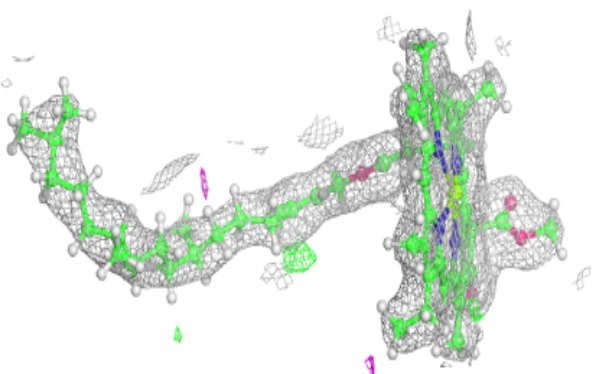
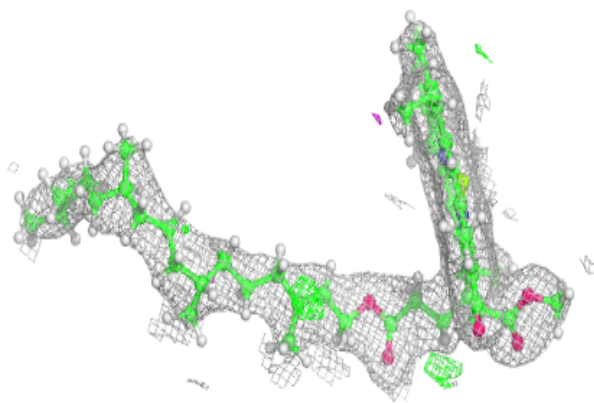
**Electron density around LHG d 407:**

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

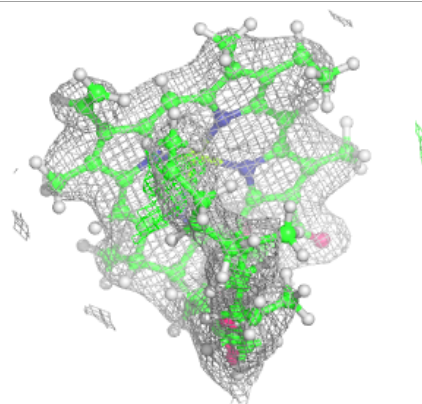
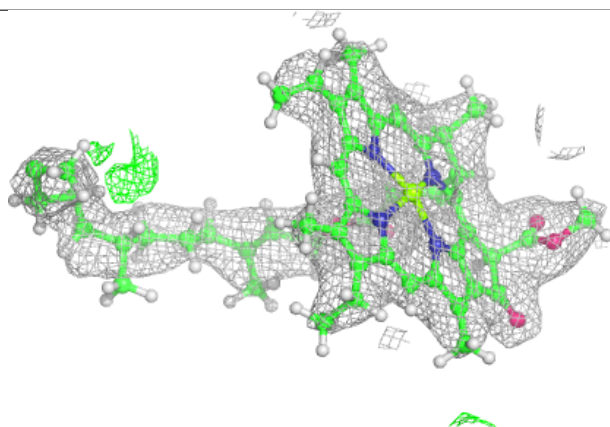
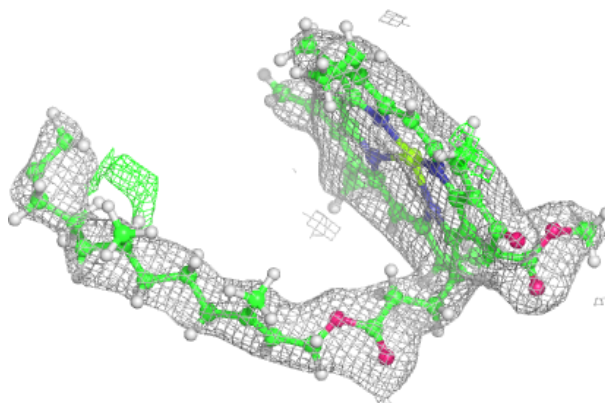


**Electron density around CLA b 606:**

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

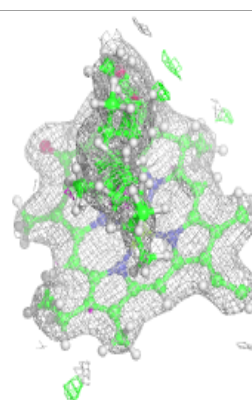
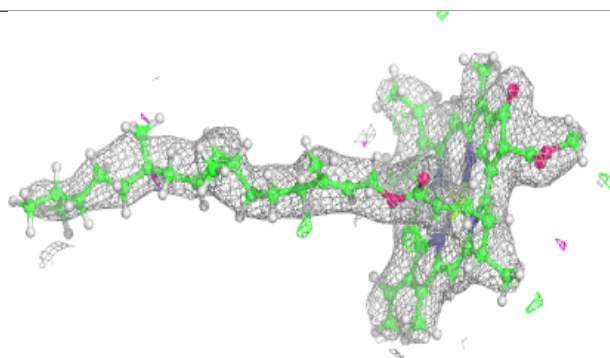
**Electron density around CLA C 504:**

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

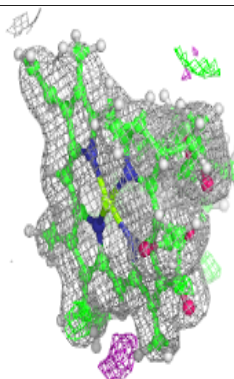
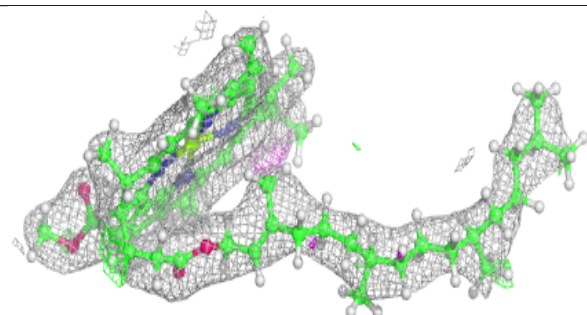
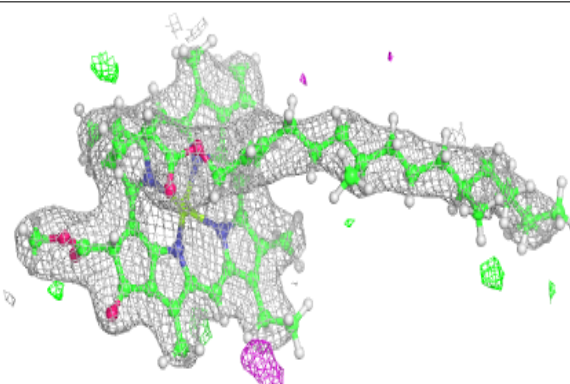


**Electron density around CLA b 608:**

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

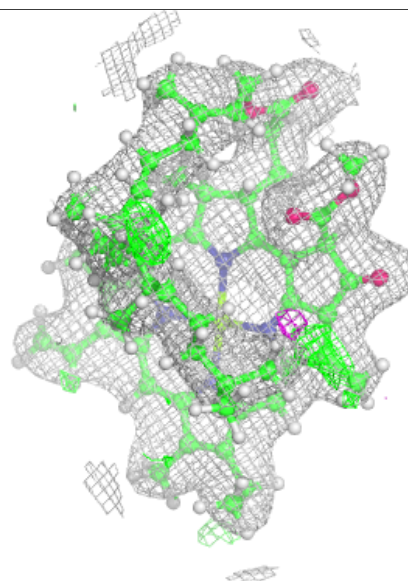
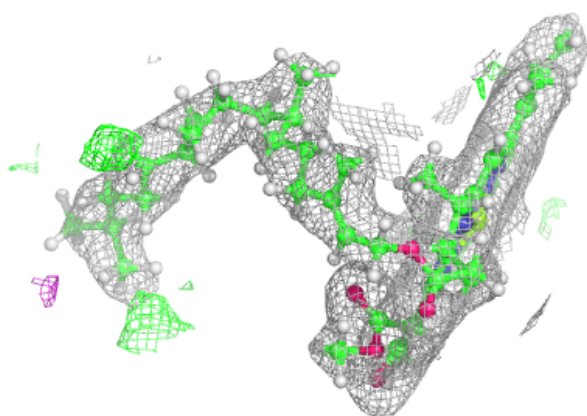
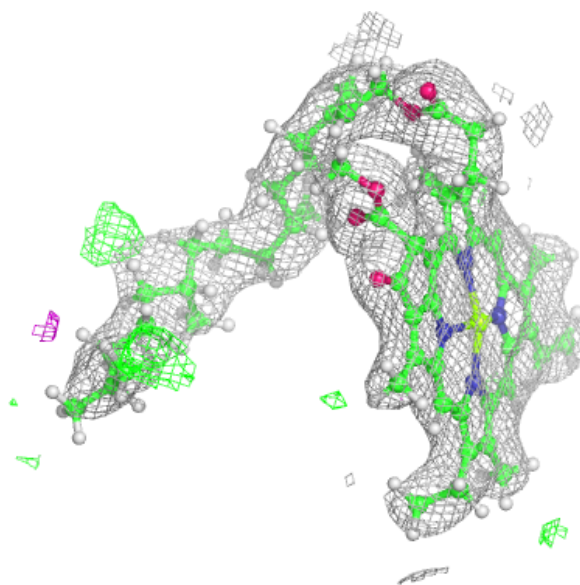
**Electron density around CLA b 609:**

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



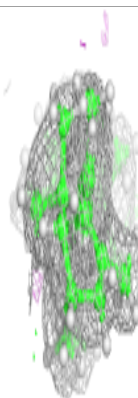
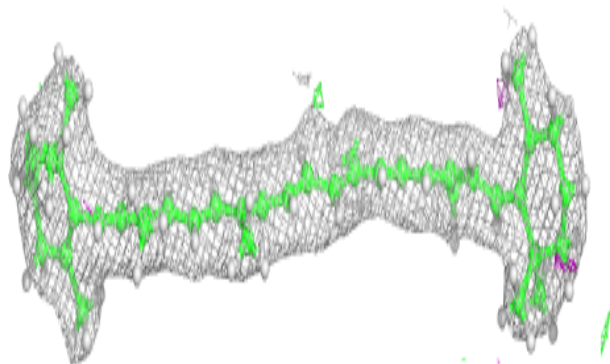
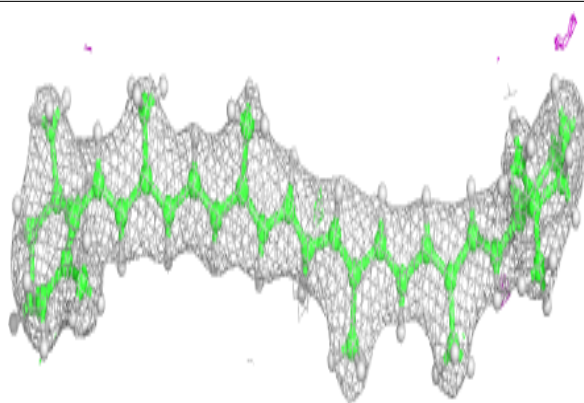
**Electron density around CLA B 613:**

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

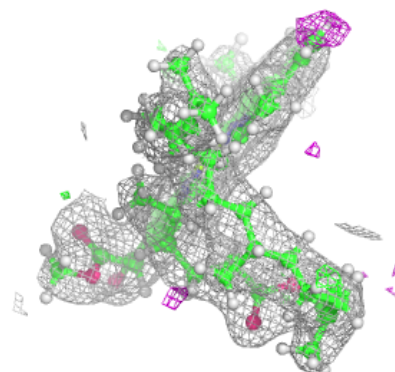
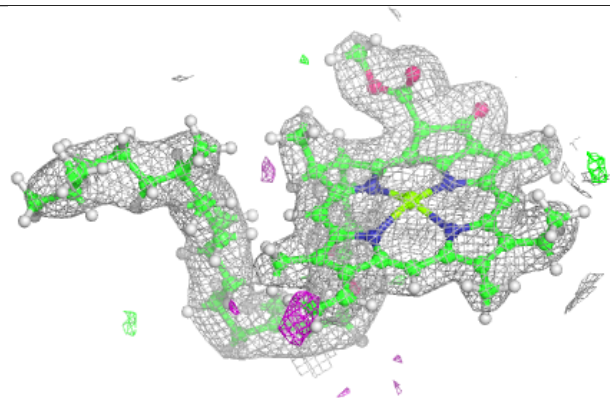
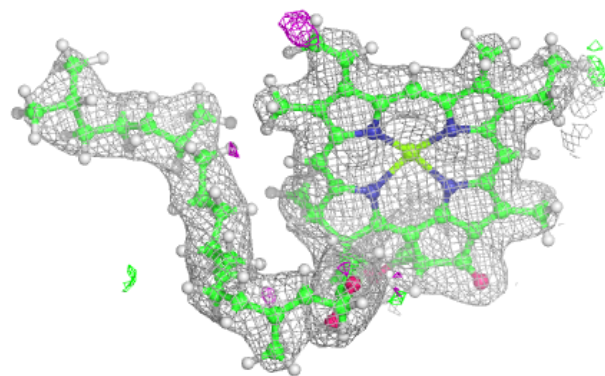


**Electron density around BCR a 409:**

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

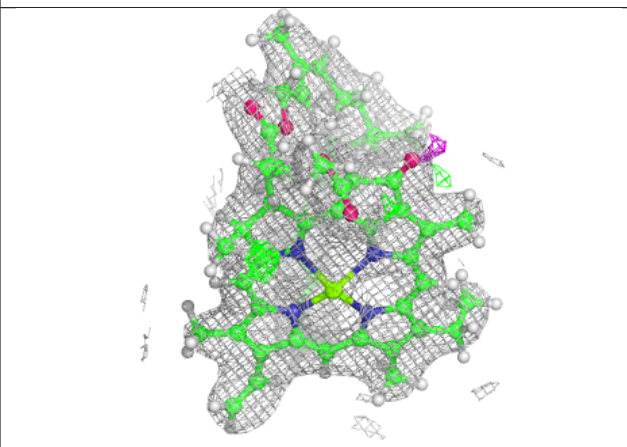
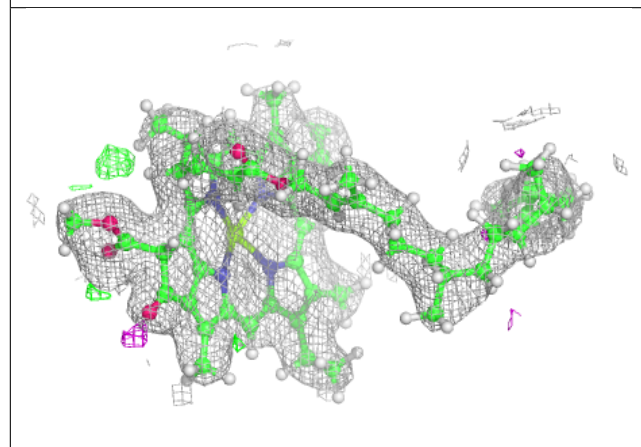
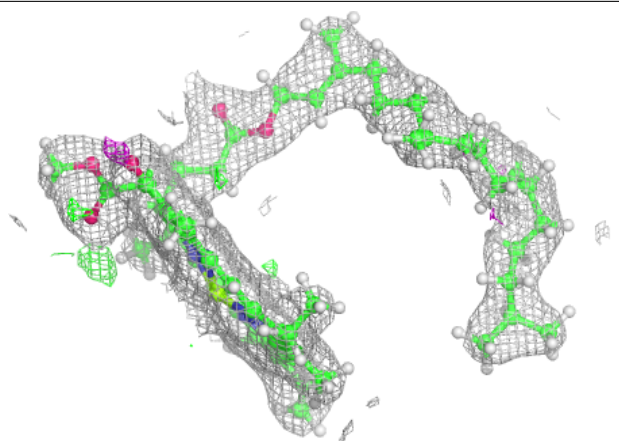
**Electron density around CLA D 401:**

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

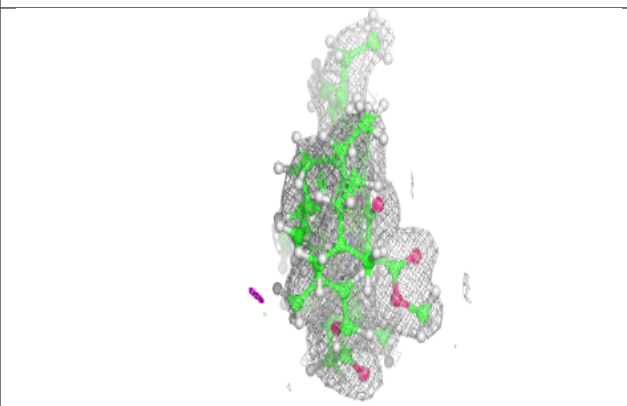
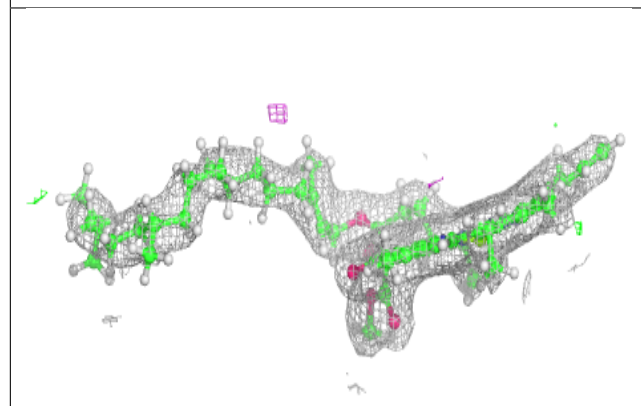
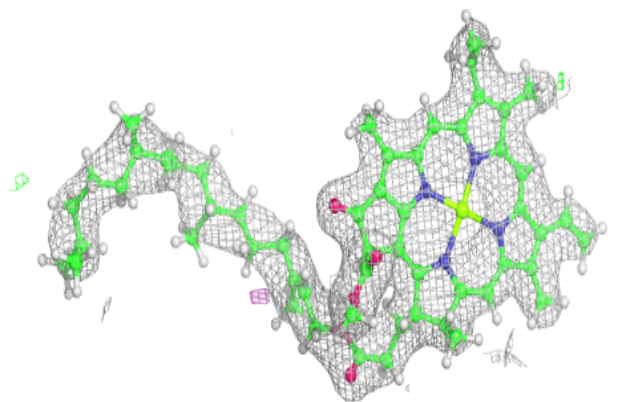


**Electron density around CLA b 612:**

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

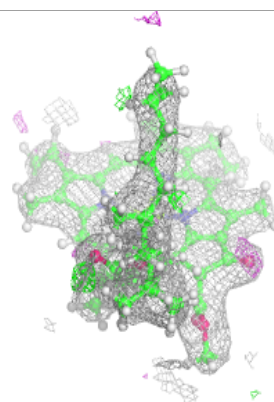
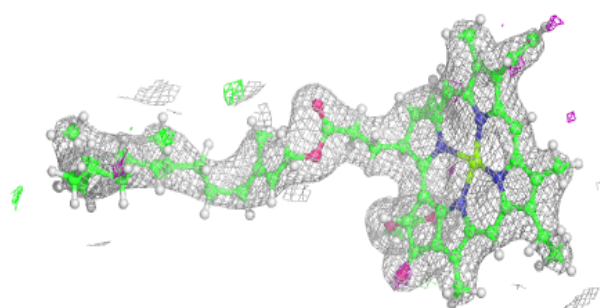
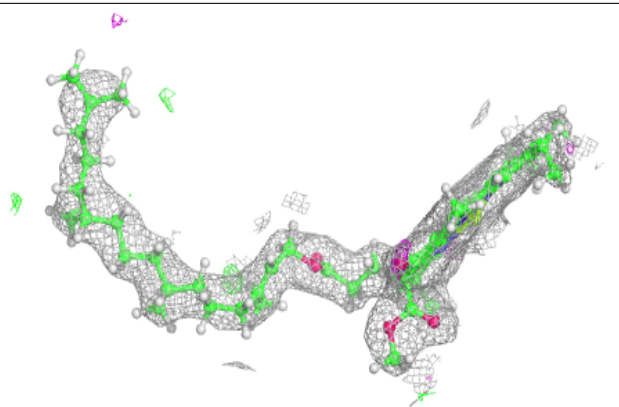
**Electron density around CLA B 602:**

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

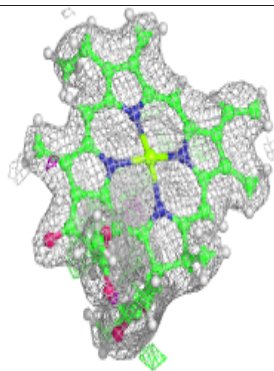
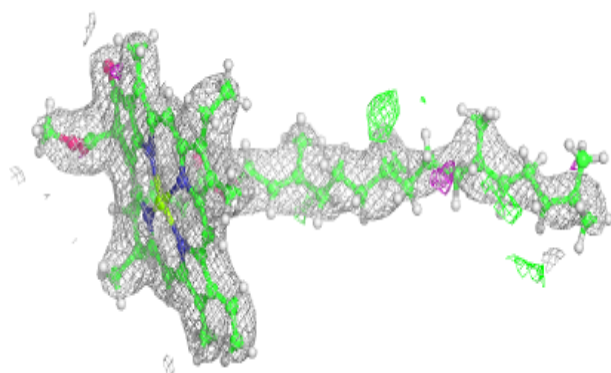
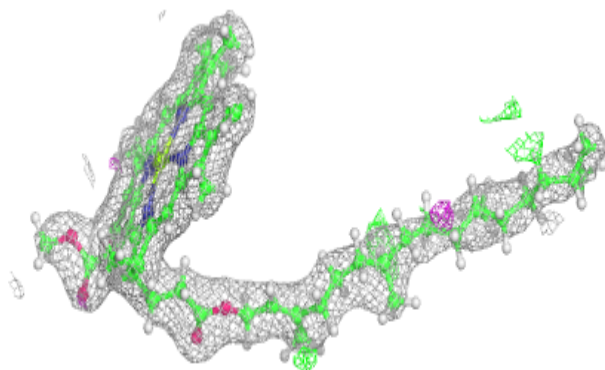


**Electron density around CLA d 402:**

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

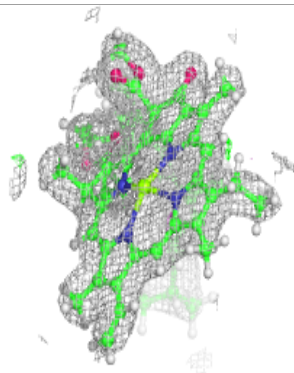
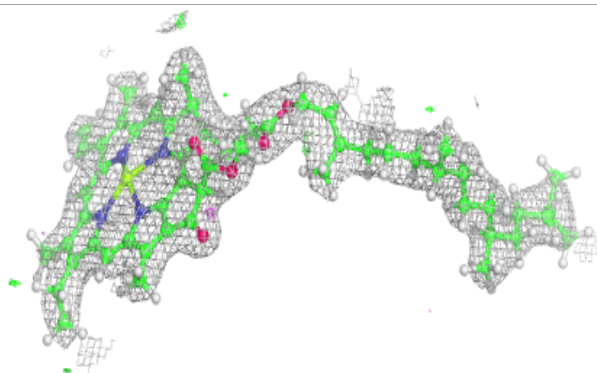
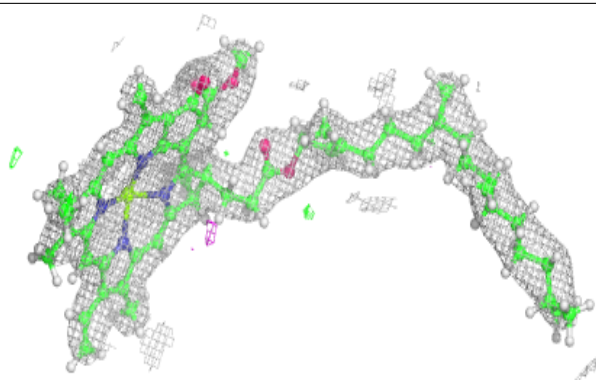
**Electron density around CLA B 607:**

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

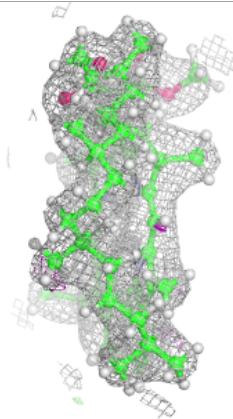
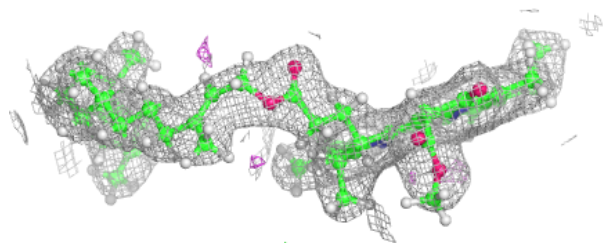
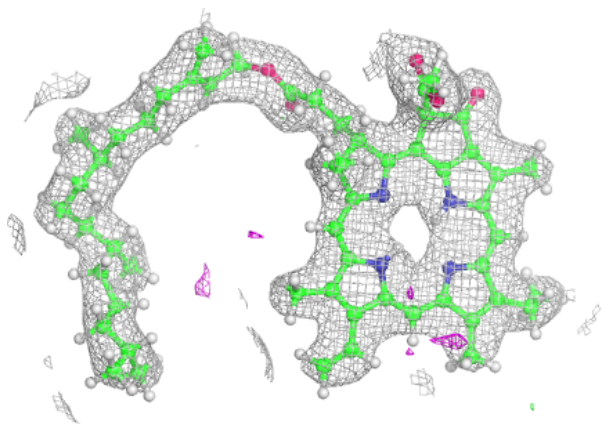


**Electron density around CLA a 405:**

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

**Electron density around PHO A 406:**

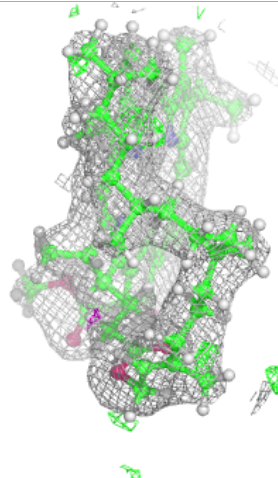
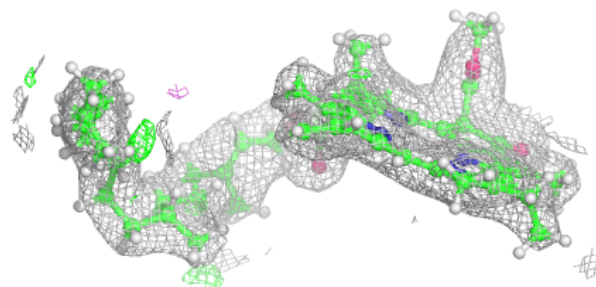
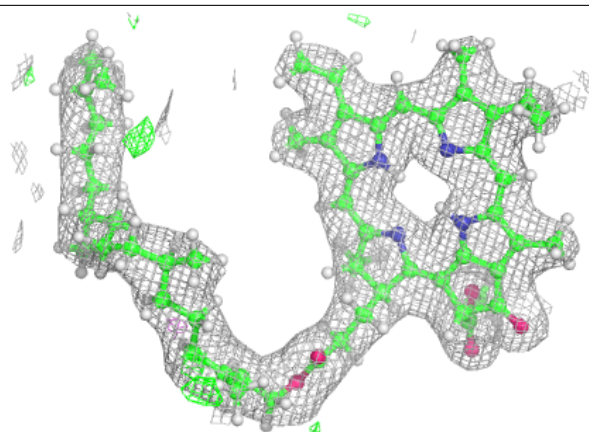
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

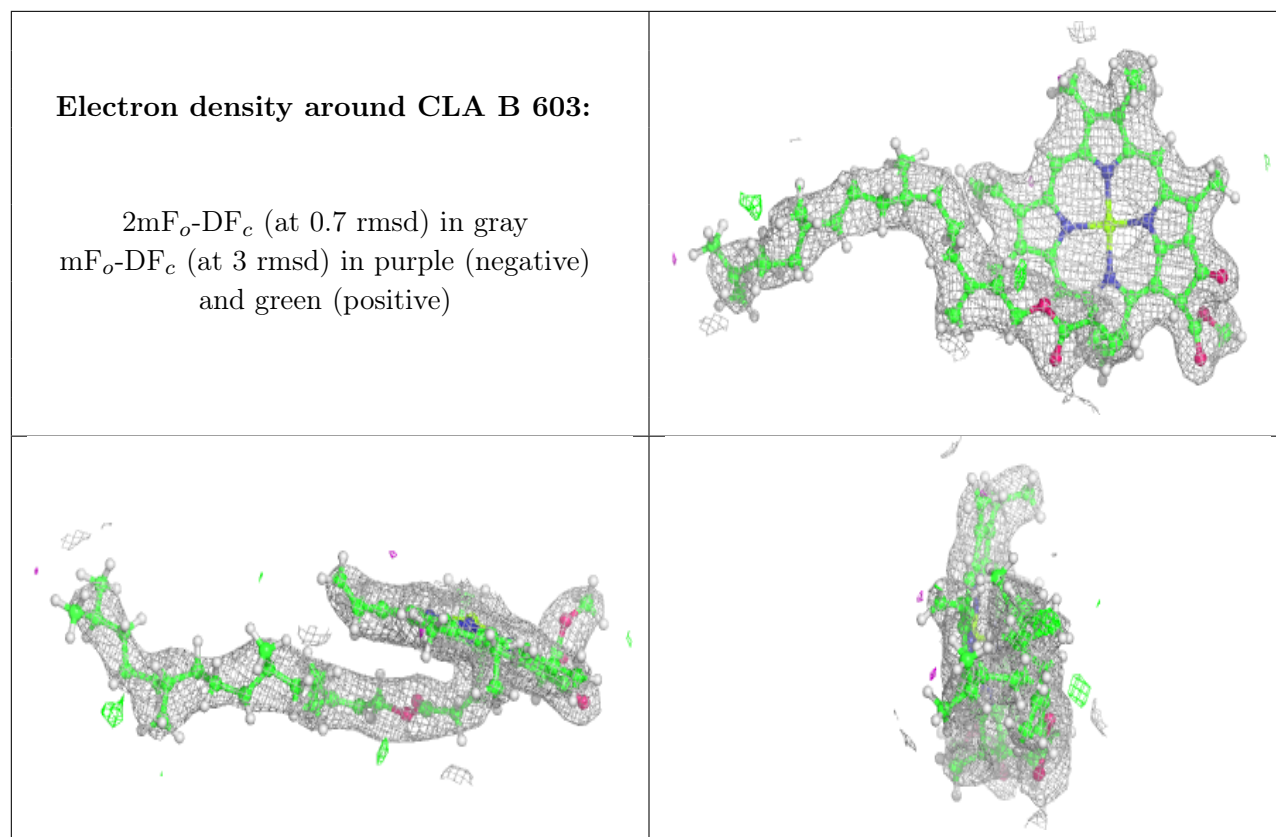




**Electron density around PHO A 407:**

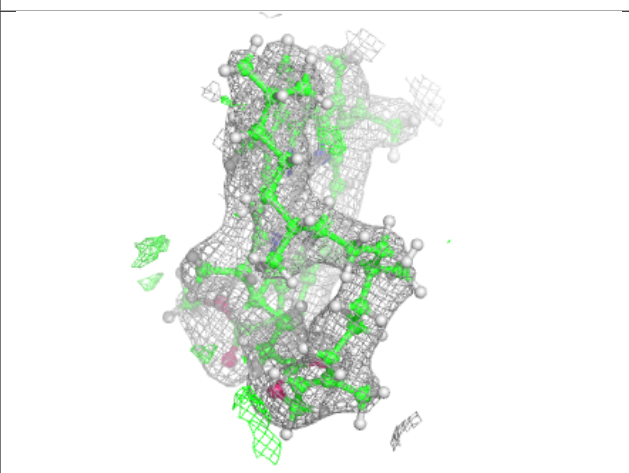
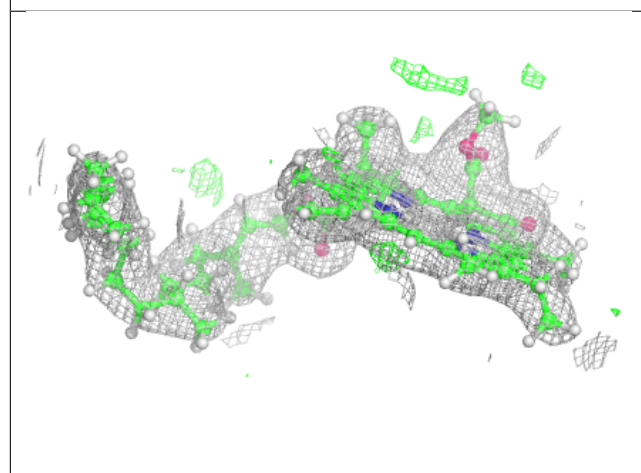
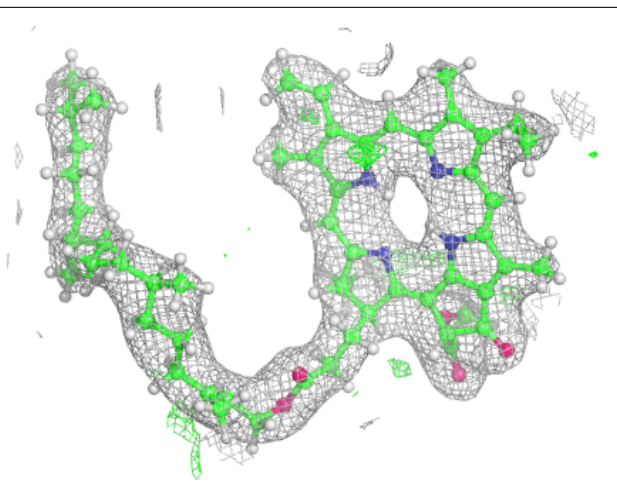
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





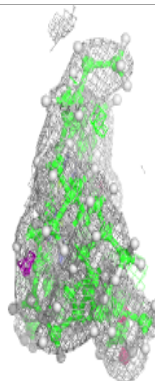
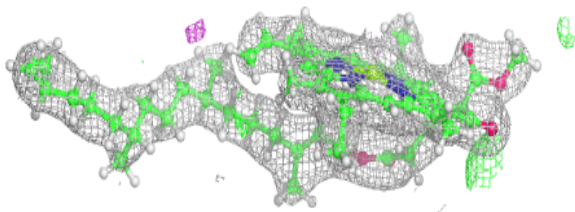
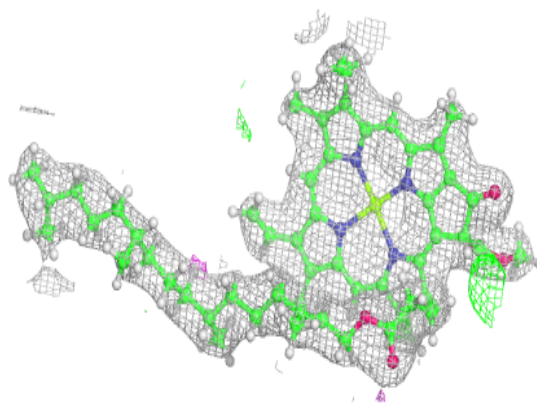
**Electron density around PHO d 401:**

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

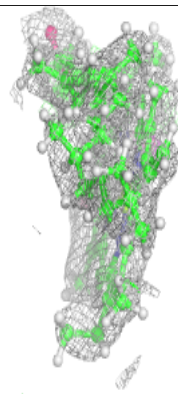
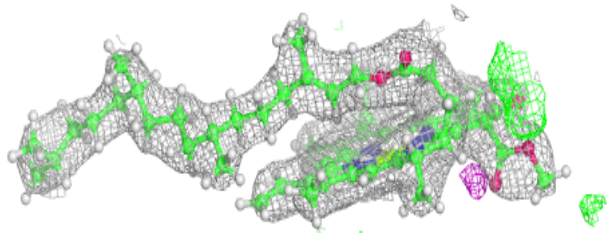
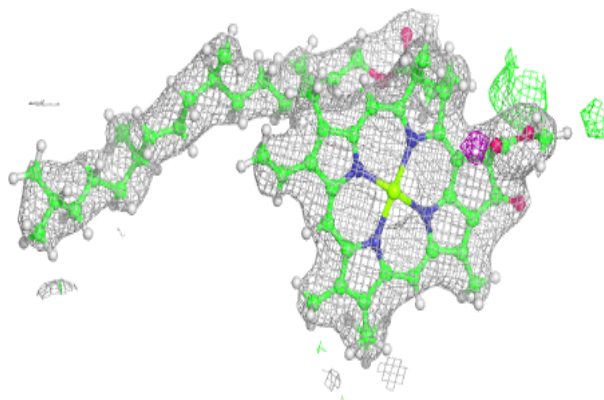


**Electron density around CLA C 501:**

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

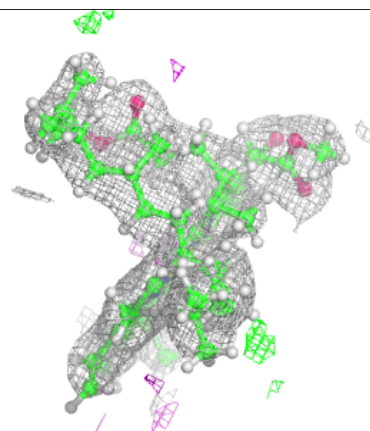
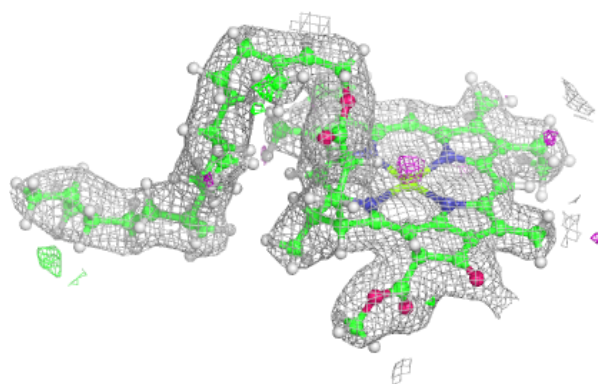
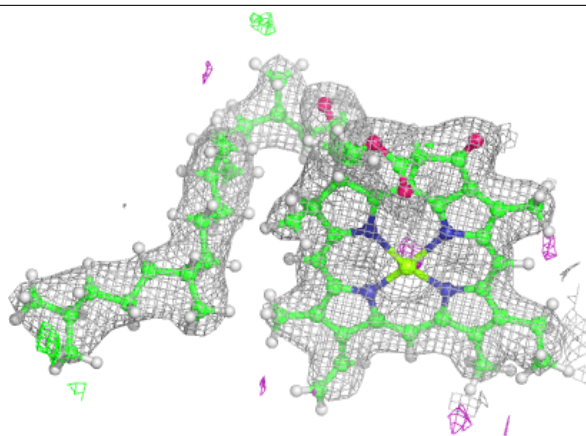
**Electron density around CLA c 501:**

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

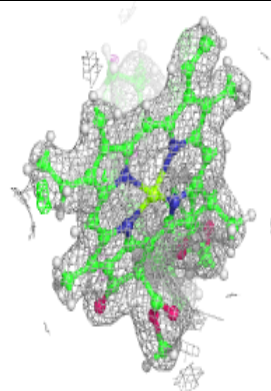
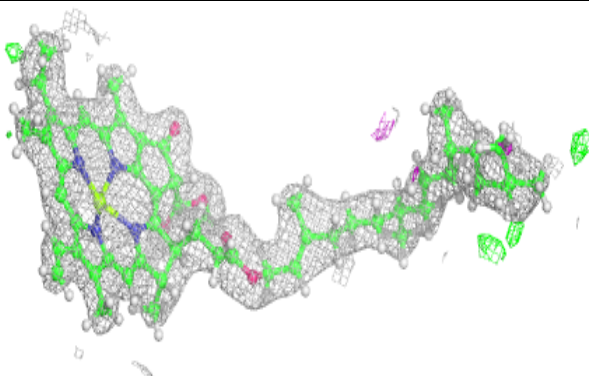
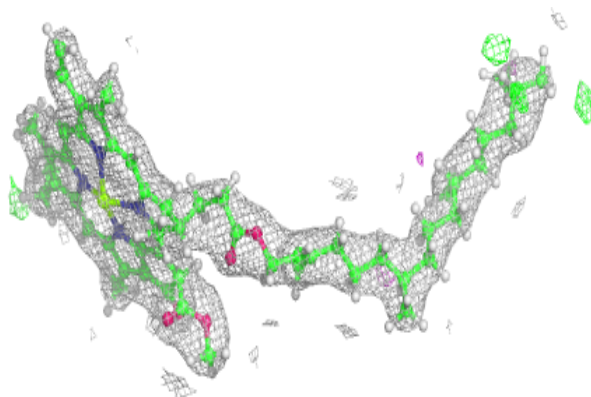


**Electron density around CLA a 411:**

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

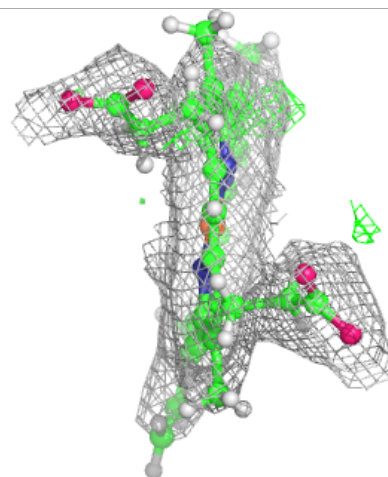
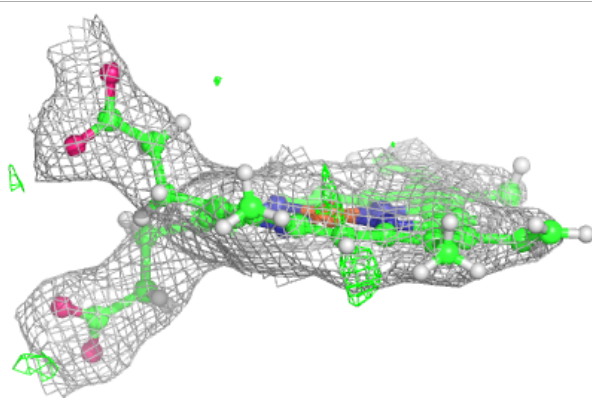
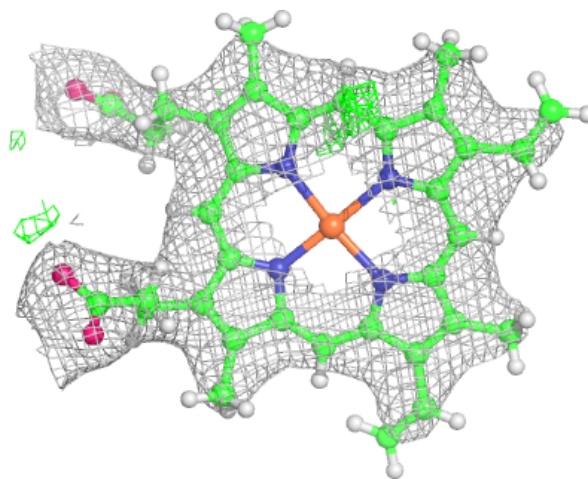
**Electron density around CLA A 404:**

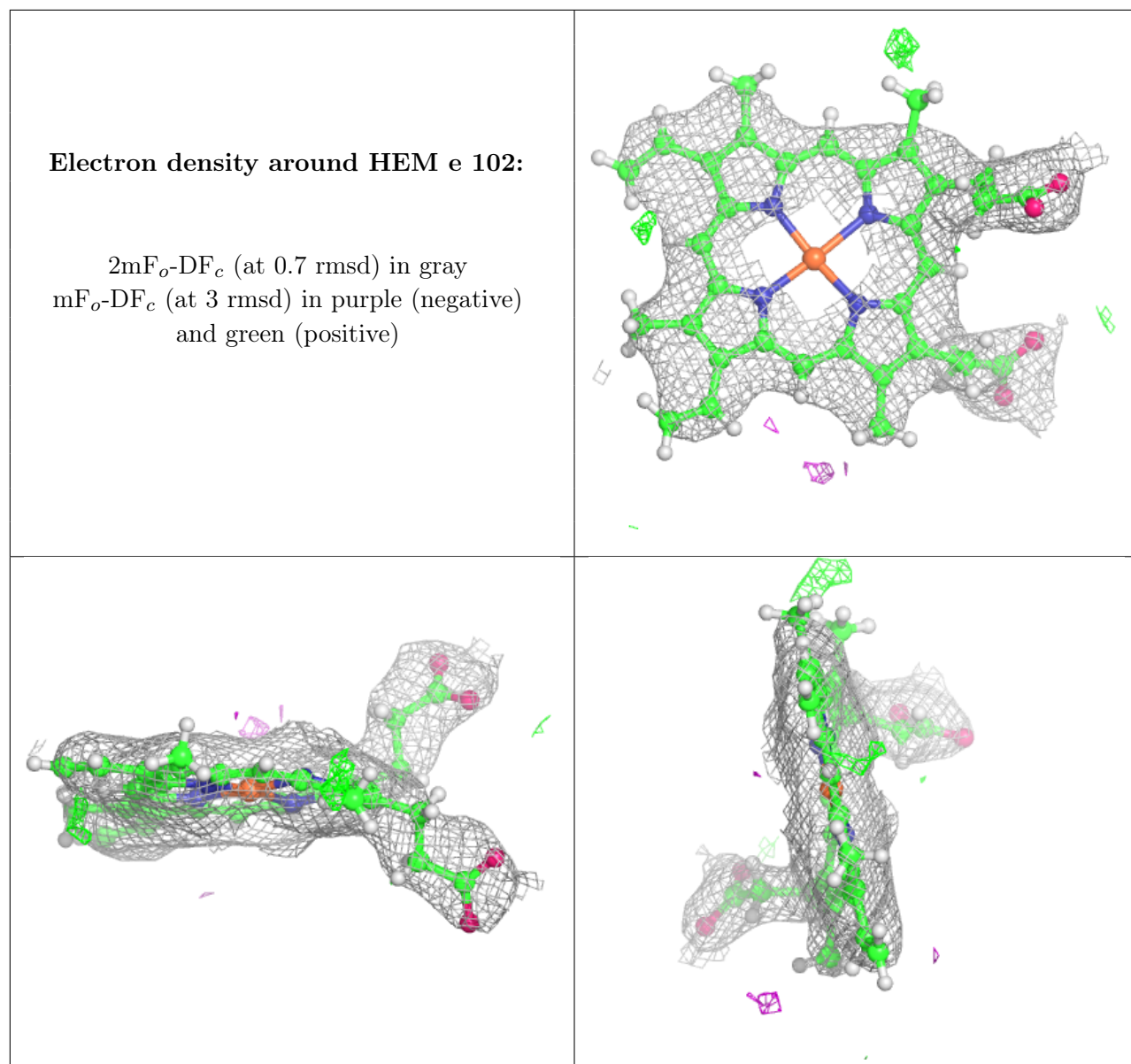
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

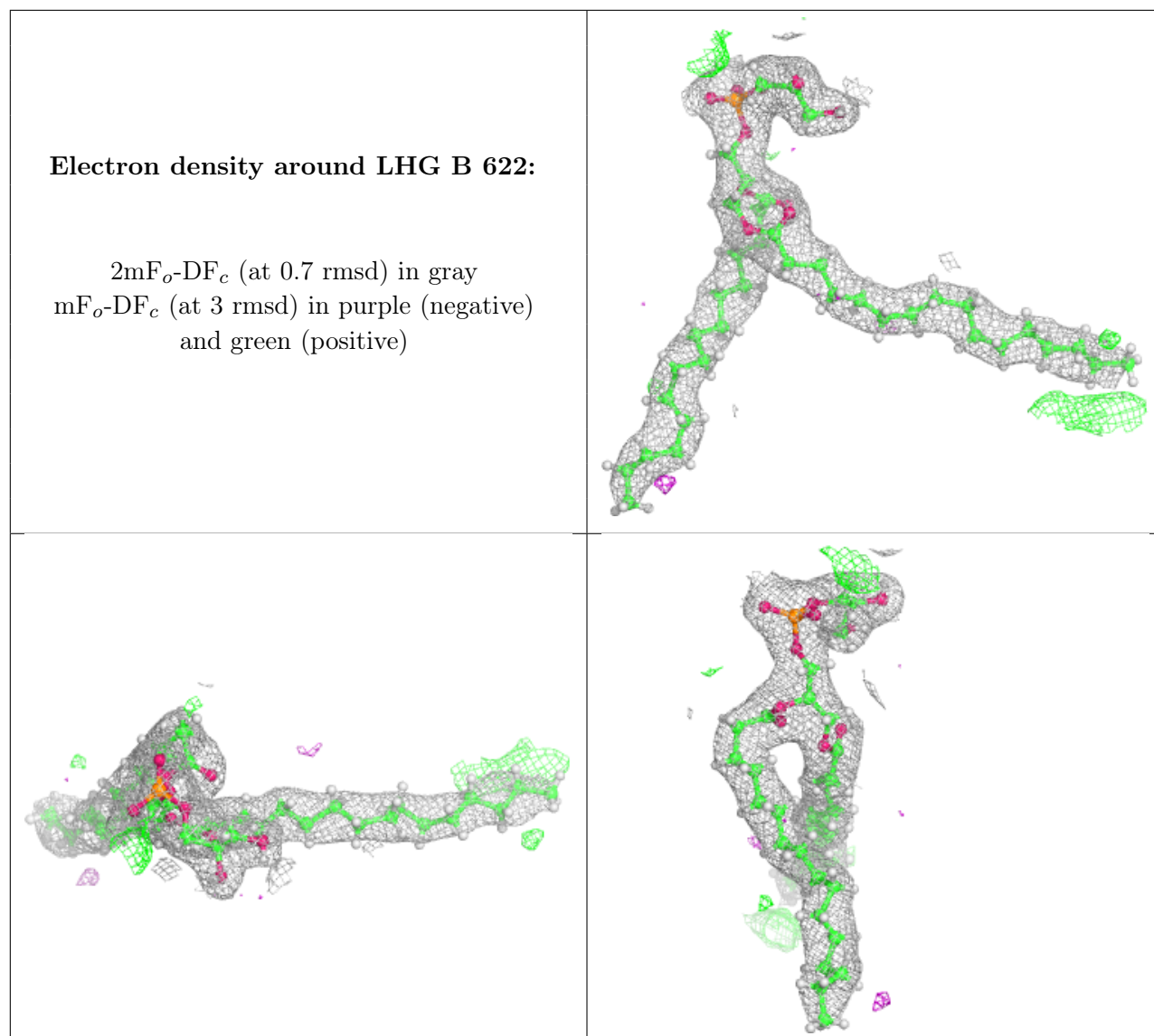


**Electron density around HEM E 101:**

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



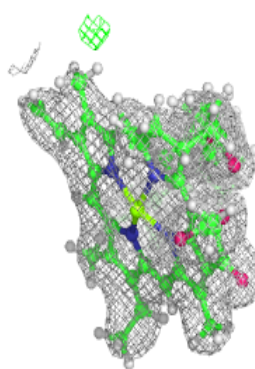
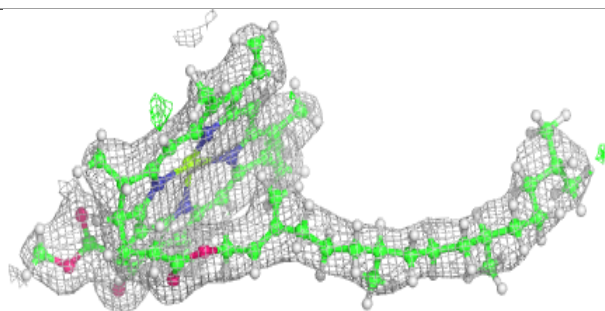
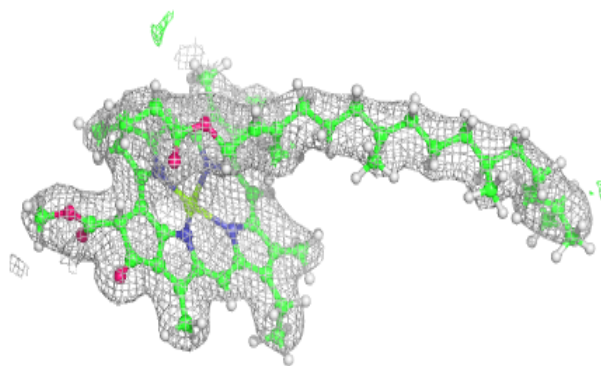




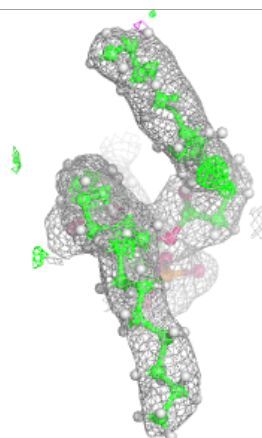
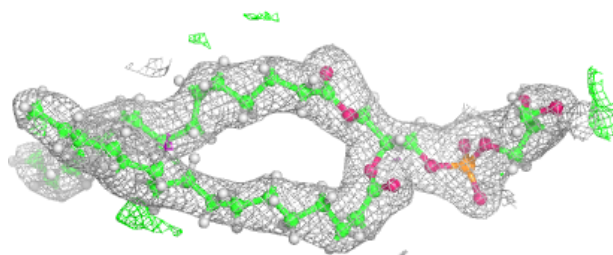
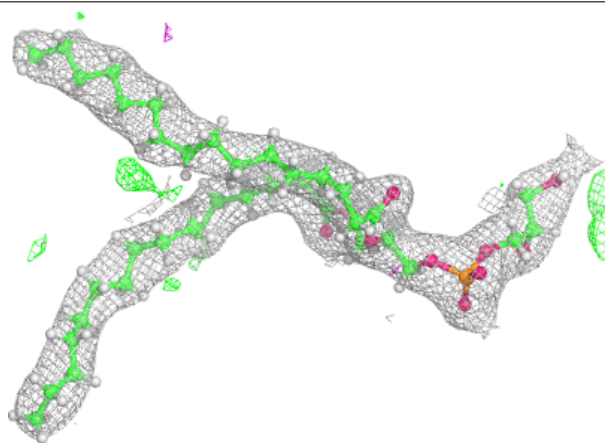


**Electron density around CLA B 608:**

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

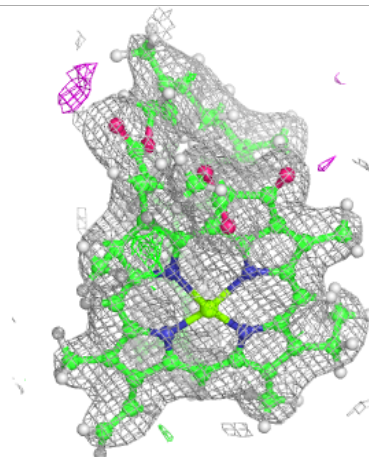
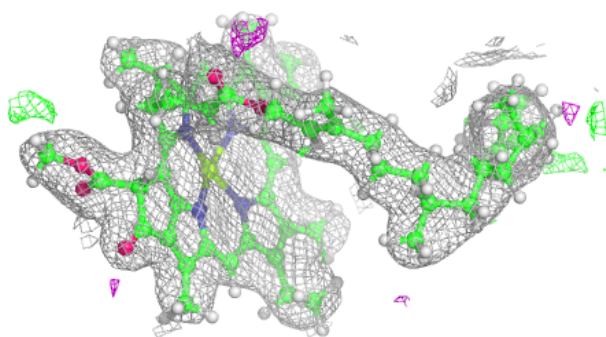
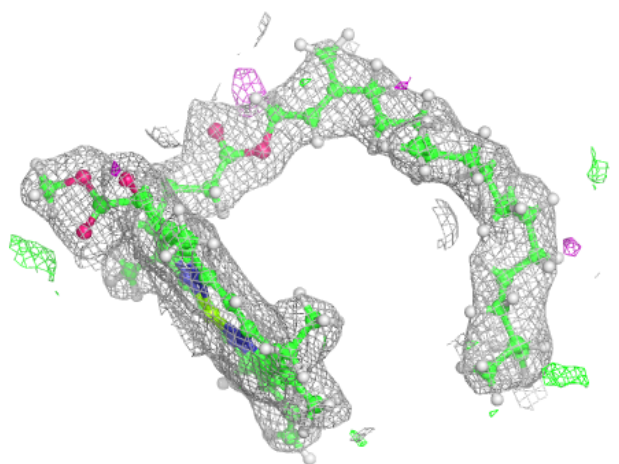
**Electron density around LHG D 407:**

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



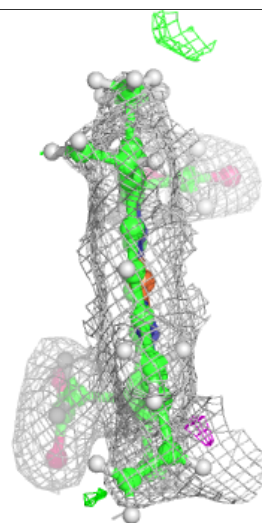
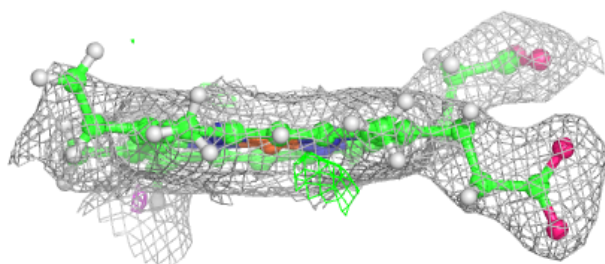
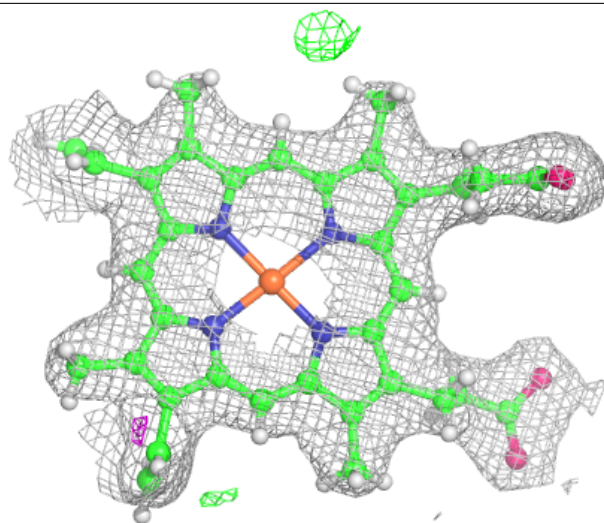
**Electron density around CLA B 611:**

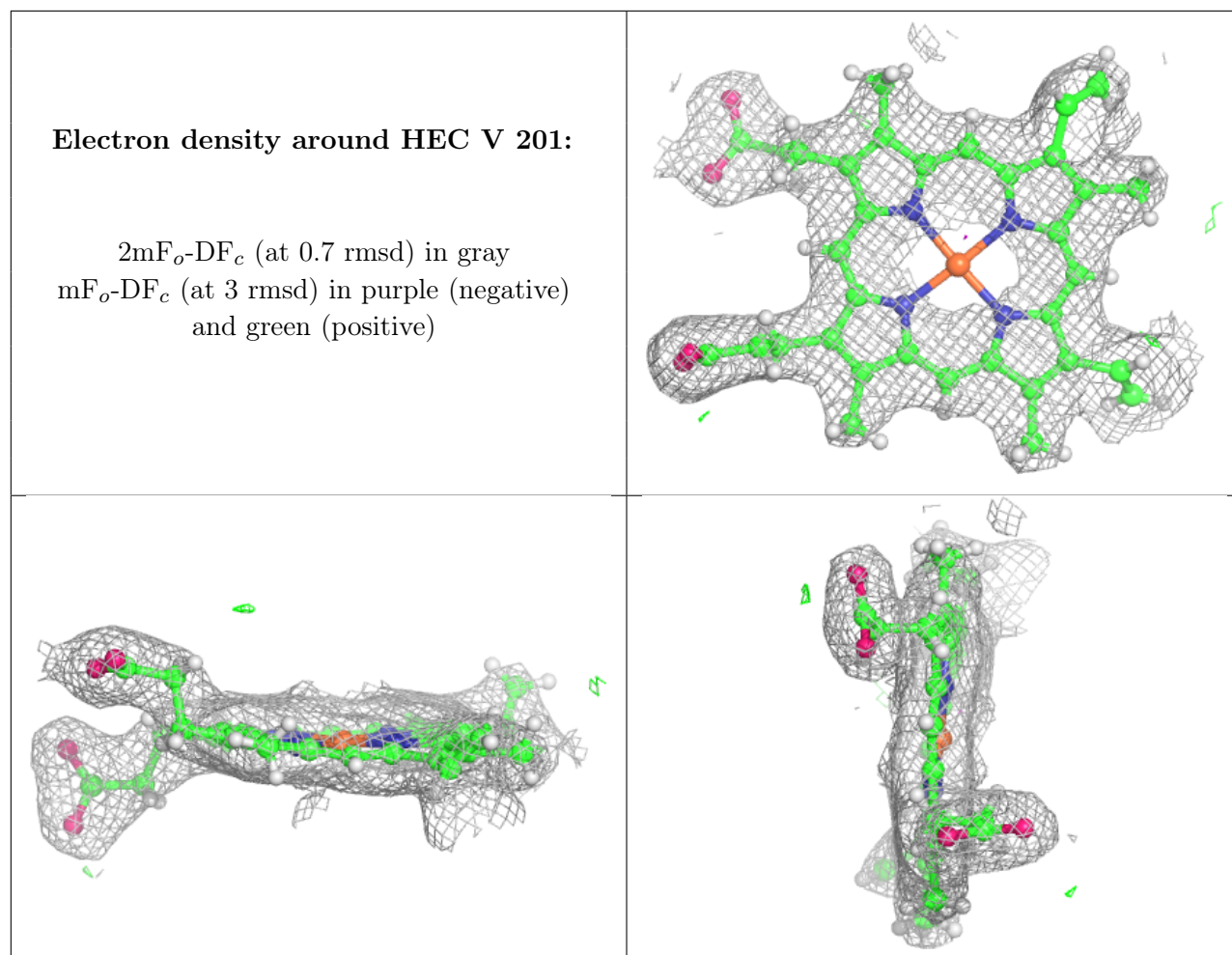
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC v 201:**

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





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.