



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2023 – 02:41 PM EDT

PDB ID : 8F4J  
Title : RT XFEL structure of Photosystem II 4000 microseconds after the third illumination at 2.00 Angstrom resolution  
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.  
Deposited on : 2022-11-10  
Resolution : 2.00 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 : 2.35

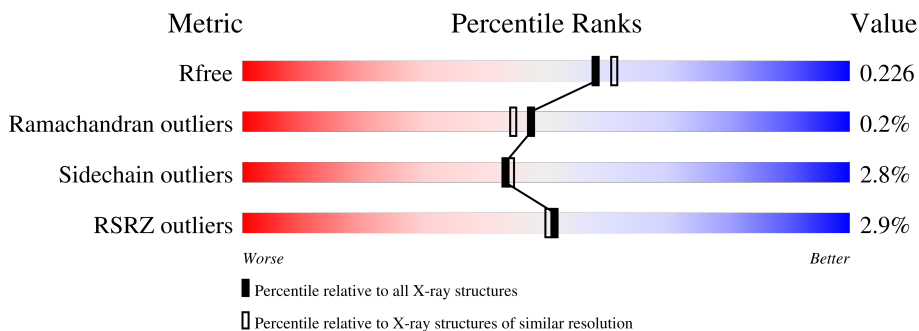
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

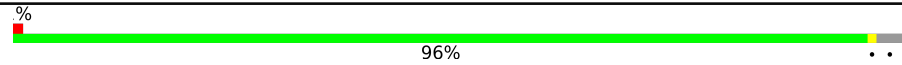
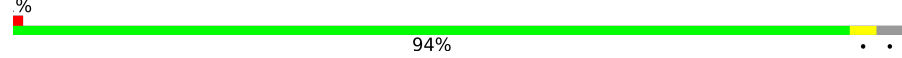
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	 96%
1	a	344	 94%

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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) : 2.35

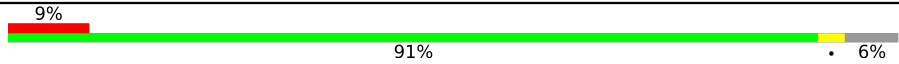

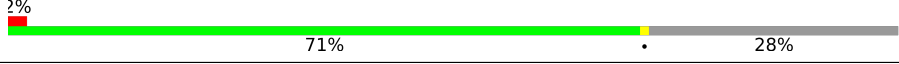
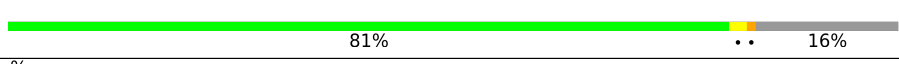

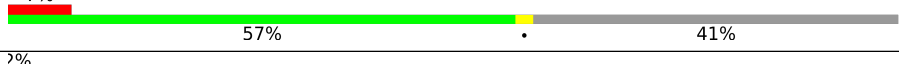

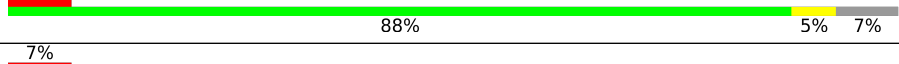
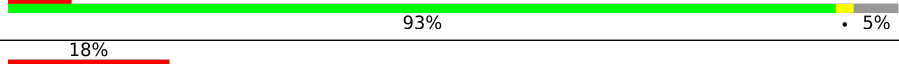
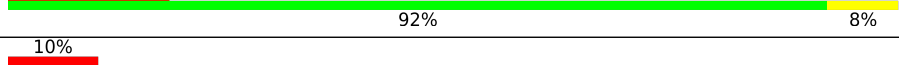
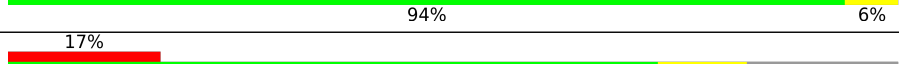
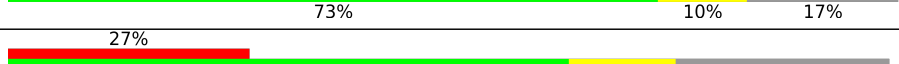



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Mol	Chain	Length	Quality of chain
2	B	510	2% 98% ..
2	b	510	2% 98% ..
3	C	461	95% ..
3	c	461	% 95% ..
4	D	352	% 96% ..
4	d	352	% 95% ..
5	E	84	8% 95% ..
5	e	84	6% 94% ..
6	F	45	4% 76% 24%
6	f	45	4% 73% 24%
7	H	66	2% 97% ..
7	h	66	2% 91% 5% 5%
8	I	38	5% 92% 5%
8	i	38	5% 89% 5% 5%
9	J	40	5% 90% 10%
9	j	40	8% 88% 10%
10	K	46	2% 76% 20%
10	k	46	76% 20%
11	L	37	5% 100%
11	l	37	5% 86% 11%
12	M	36	3% 86% 6% 8%
12	m	36	83% 6% 11%
13	O	272	6% 86% 10%
13	o	272	5% 88% 10%
14	T	32	3% 91% 6%

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	612	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	613	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
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25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	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>
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	h	101	X	-	-	-

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 54524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 3604	C 2343	N 595	O 643	S 23	0	64	0
1	a	334	Total 3601	C 2340	N 595	O 643	S 23	0	64	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	Total 4005	C 2631	N 666	O 695	S 13	0	4	0
2	b	505	Total 3978	C 2610	N 665	O 690	S 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	N	O	S			
3	C	442	Total 3592	C 2355	N 601	O 621	S 15	0	11	0
3	c	451	Total 3666	C 2396	N 617	O 638	S 15	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	Total 2745	C 1818	N 448	O 467	S 12	0	2	0
4	d	341	Total 2751	C 1822	N 448	O 469	S 12	0	3	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	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	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	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	N	O	0	0	0
			293	204	43	46			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	304	202	48	53	1	0	0	0
11	l	36	296	197	47	52		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	256	171	37	47	1	0	0	0
12	m	32	251	168	36	46	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	244	1870	1168	313	385	4	0	1	0
13	o	244	1874	1170	317	383	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	258	181	36	39	2	0	0	0
14	t	30	256	180	36	38	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	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	N	O	S	0	0	0
			196	128	35	30	3			
17	y	30	Total	C	N	O	S	0	0	0
			218	144	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	N	O	S	0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O	S	0	0	0
			286	191	46	49				

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

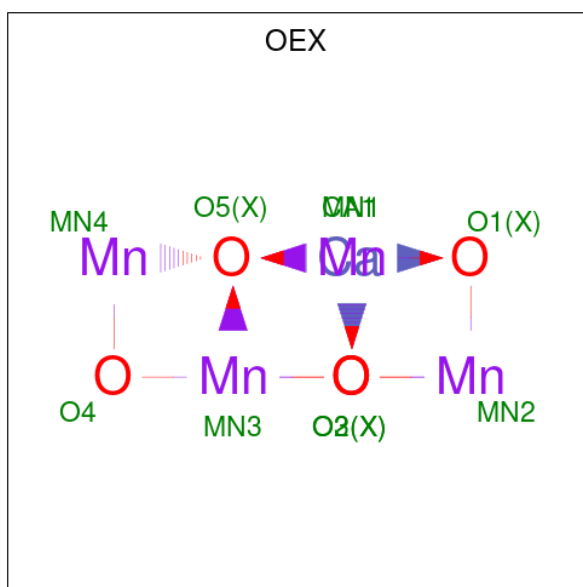
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			477	326	72	77	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O	S	0	0	0
			246	166	43	37				

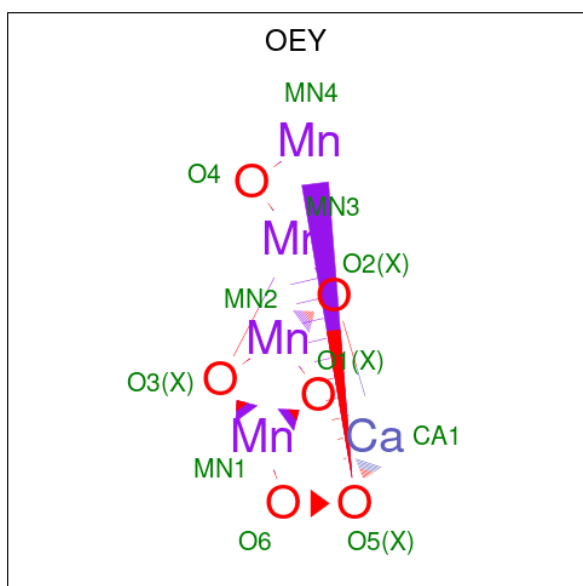
- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 22 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).



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

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

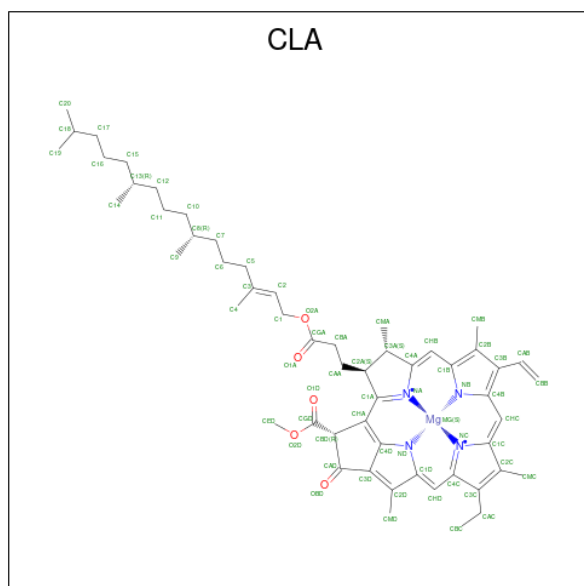
- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 25 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	
			Total	C	Mg	N			O
25	A	1	65	55	1	4	5	0	0
25	A	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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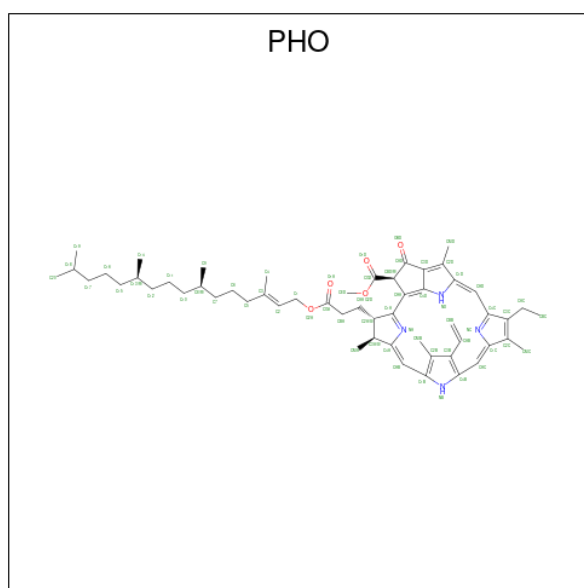
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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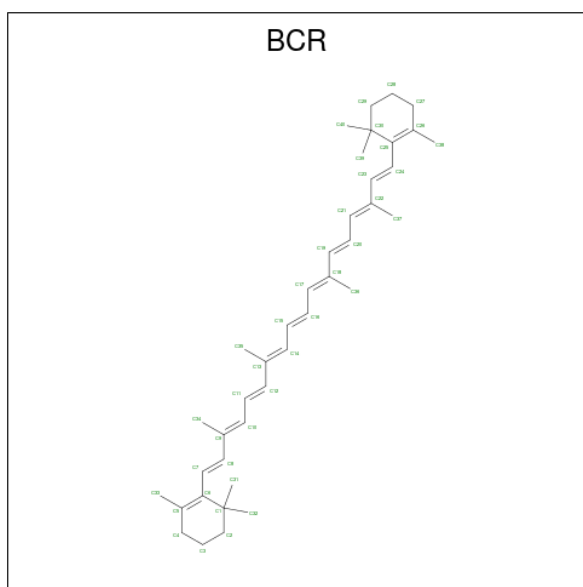
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



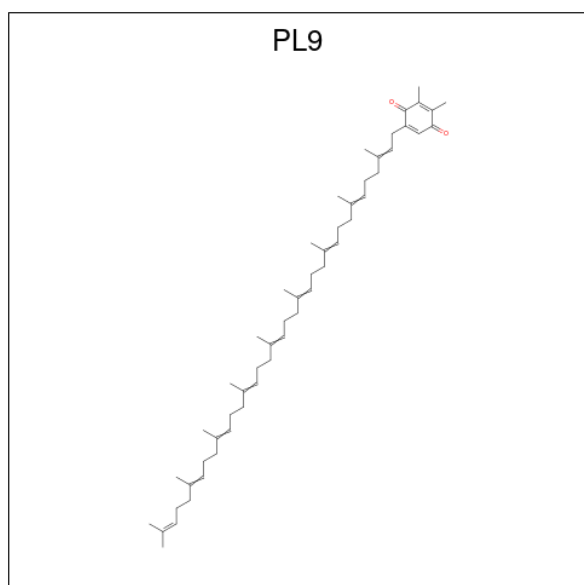
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



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

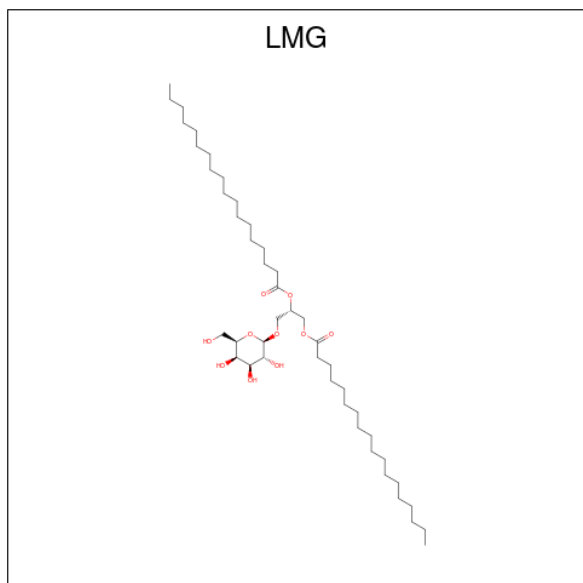
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



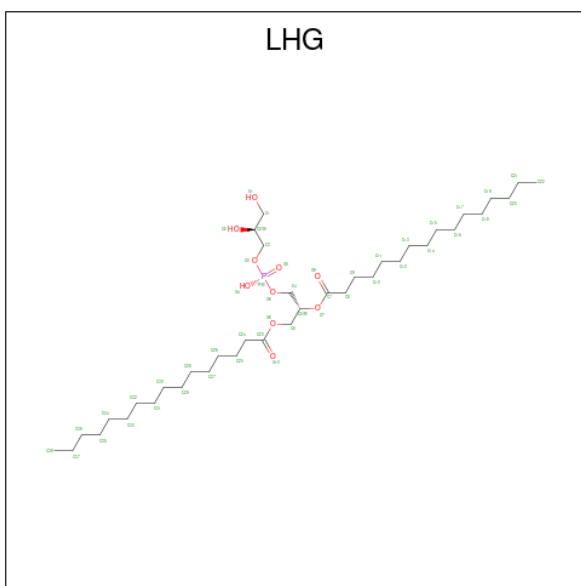
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C	O	0	0
			37	27	10		
29	c	1	Total	C	O	0	0
			48	38	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			49	39	10		
29	d	1	Total	C	O	0	0
			23	21	2		
29	d	1	Total	C	O	0	0
			44	34	10		
29	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



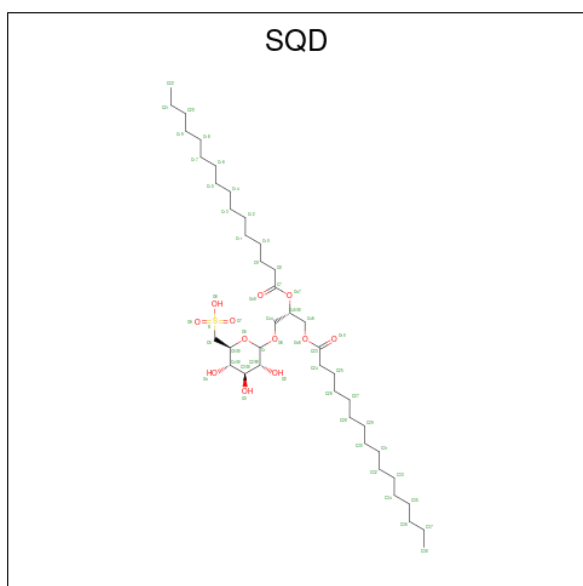
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			47	36	10	1		
30	B	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	E	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		

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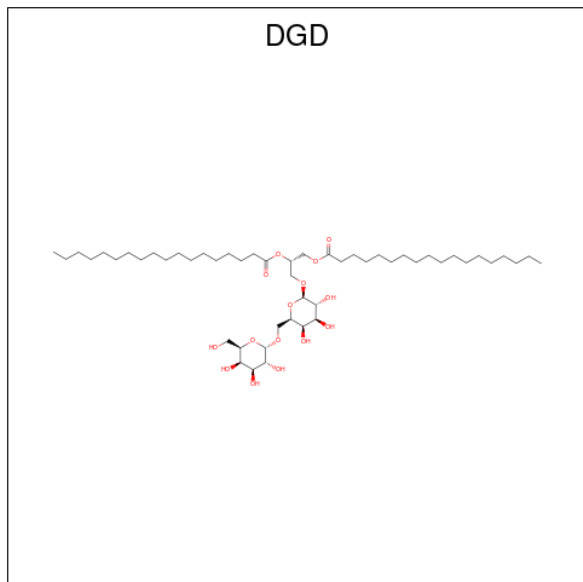
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	d	1	Total	C	O	P	0	0
			39	28	10	1		
30	e	1	Total	C	O	P	0	0
			42	31	10	1		
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 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).



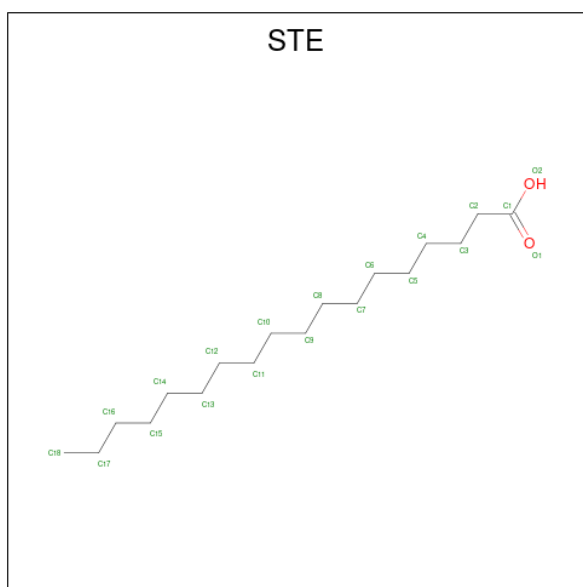
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	S	0	0
			52	39	12	1		
31	A	1	Total	C	O		0	0
			39	35	4			
31	B	1	Total	C	O	S	0	0
			54	41	12	1		
31	F	1	Total	C	O	S	0	0
			36	25	10	1		
31	a	1	Total	C	O	S	0	0
			54	41	12	1		
31	a	1	Total	C	O		0	0
			36	31	5			
31	b	1	Total	C	O	S	0	0
			49	36	12	1		
31	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			66	51	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	H	1	Total	C	O	0	0
			62	47	15		
32	a	1	Total	C	O	0	0
			44	39	5		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 33 is STEARIC ACID (three-letter code: STE) (formula:  $C_{18}H_{36}O_2$ ).



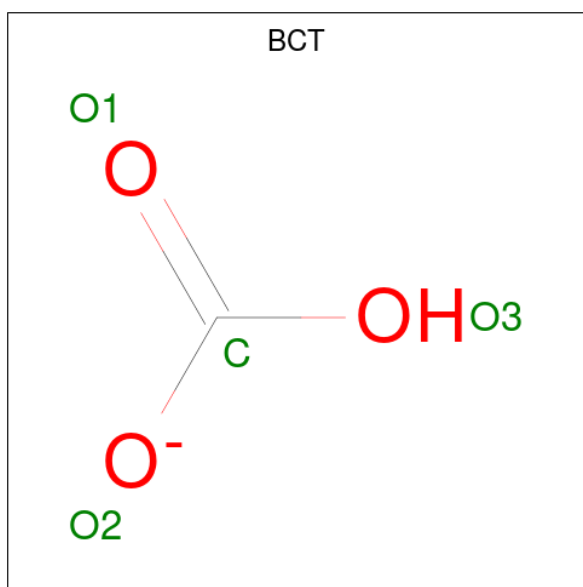
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 17 15 2	0	0
33	B	1	Total C O 12 10 2	0	0
33	B	1	Total C O 12 10 2	0	0
33	B	1	Total C 16 16	0	0
33	C	1	Total C O 12 10 2	0	0
33	C	1	Total C O 12 10 2	0	0
33	C	1	Total C 16 16	0	0
33	E	1	Total C O 12 10 2	0	0
33	H	1	Total C 18 18	0	0
33	I	1	Total C 15 15	0	0
33	J	1	Total C O 12 10 2	0	0
33	M	1	Total C O 15 13 2	0	0
33	M	1	Total C 10 10	0	0
33	X	1	Total C O 20 18 2	0	0

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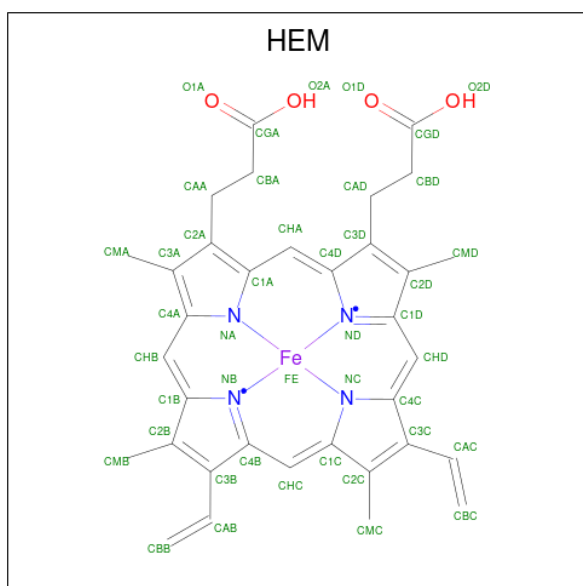
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C 16 16	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C O 16 14 2	0	0
33	b	1	Total C 15 15	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	d	1	Total C O 17 15 2	0	0
33	j	1	Total C O 12 10 2	0	0
33	k	1	Total C O 12 10 2	0	0
33	l	1	Total C 18 18	0	0
33	m	1	Total C O 12 10 2	0	0
33	t	1	Total C O 14 12 2	0	0
33	t	1	Total C 10 10	0	0
33	t	1	Total C O 18 16 2	0	0
33	x	1	Total C O 20 18 2	0	0

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	D	1	Total	C	O	0	0
			4	1	3		
34	a	1	Total	C	O	0	0
			4	1	3		

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



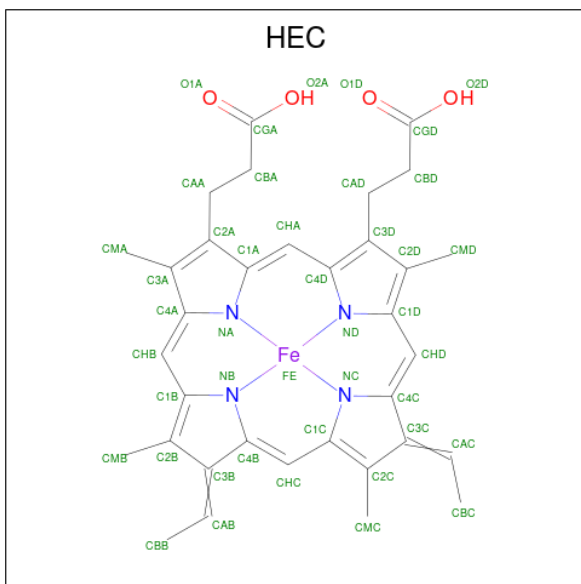
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	150	Total	O	0	4
			158	158		
37	B	214	Total	O	0	0
			214	214		
37	C	196	Total	O	0	0
			196	196		
37	D	115	Total	O	0	0
			115	115		
37	E	33	Total	O	0	0
			33	33		
37	F	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	27	Total O 27 27	0	0
37	I	20	Total O 20 20	0	0
37	J	13	Total O 13 13	0	0
37	K	5	Total O 5 5	0	0
37	L	10	Total O 10 10	0	0
37	M	7	Total O 7 7	0	0
37	O	89	Total O 89 89	0	0
37	T	9	Total O 9 9	0	0
37	U	40	Total O 40 40	0	0
37	V	61	Total O 61 61	0	0
37	X	12	Total O 12 12	0	0
37	Z	6	Total O 6 6	0	0
37	a	123	Total O 131 131	0	4
37	b	199	Total O 199 199	0	0
37	c	150	Total O 150 150	0	0
37	d	109	Total O 109 109	0	0
37	e	17	Total O 17 17	0	0
37	f	3	Total O 3 3	0	0
37	h	17	Total O 17 17	0	0
37	i	17	Total O 17 17	0	0
37	j	14	Total O 14 14	0	0

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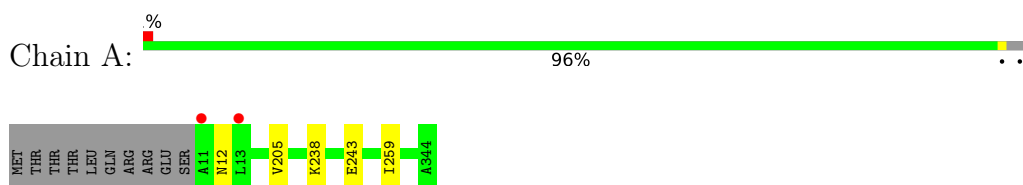
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
37	k	7	Total 7	O 7	0	0
37	l	7	Total 7	O 7	0	0
37	m	9	Total 9	O 9	0	0
37	o	85	Total 85	O 85	0	0
37	t	14	Total 14	O 14	0	0
37	u	48	Total 48	O 48	0	0
37	v	56	Total 56	O 56	0	0
37	x	10	Total 10	O 10	0	0
37	z	5	Total 5	O 5	0	0
37	r	2	Total 2	O 2	0	0

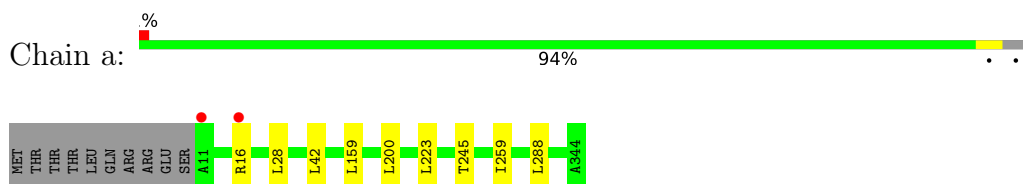
### 3 Residue-property plots [i](#)

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.

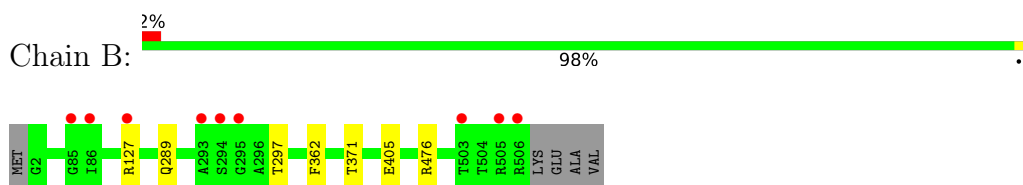
- Molecule 1: Photosystem II protein D1 1



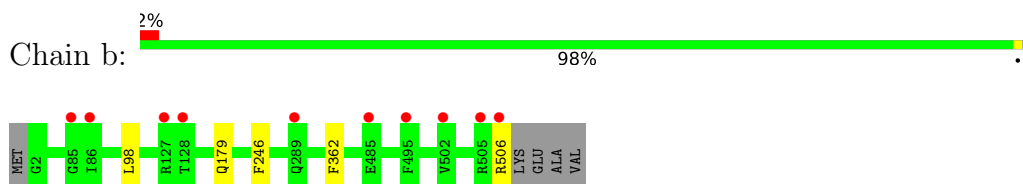
- Molecule 1: Photosystem II protein D1 1



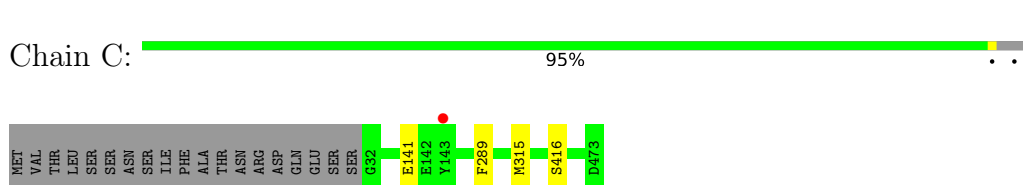
- Molecule 2: Photosystem II CP47 reaction center protein



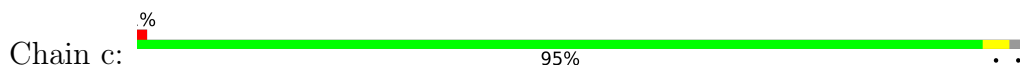
- Molecule 2: Photosystem II CP47 reaction center protein



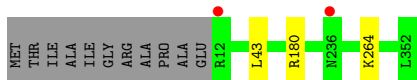
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



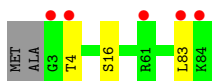
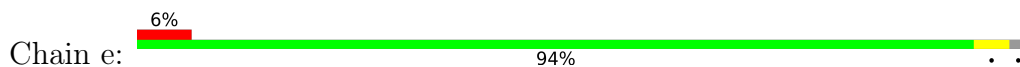
- Molecule 4: Photosystem II D2 protein



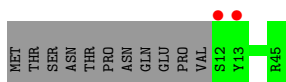
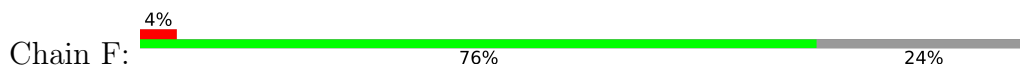
- Molecule 5: Cytochrome b559 subunit alpha



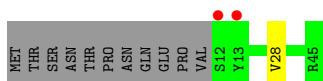
- Molecule 5: Cytochrome b559 subunit alpha



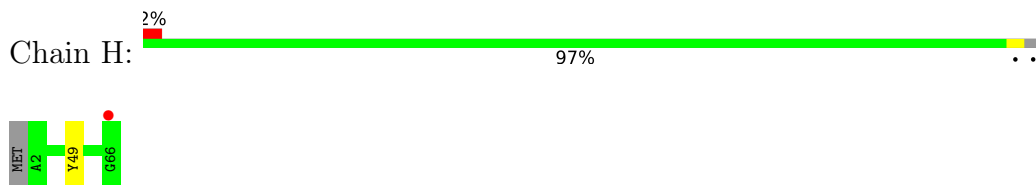
- Molecule 6: Cytochrome b559 subunit beta



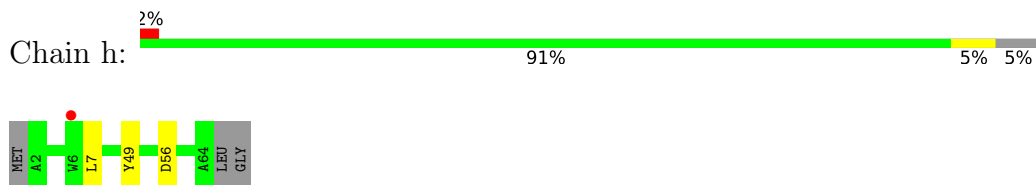
- Molecule 6: Cytochrome b559 subunit beta



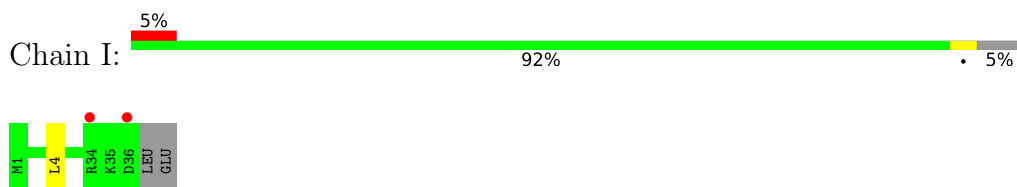
- Molecule 7: Photosystem II reaction center protein H



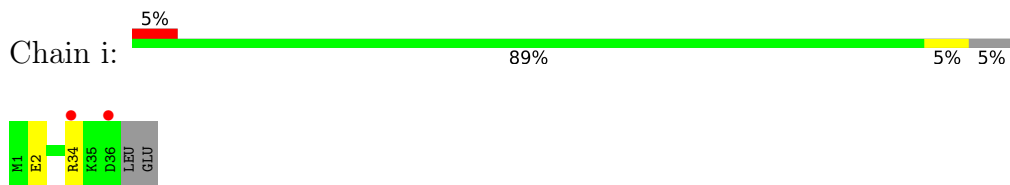
- Molecule 7: Photosystem II reaction center protein H



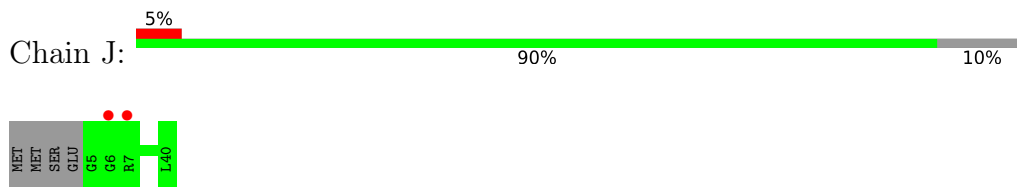
- Molecule 8: Photosystem II reaction center protein I



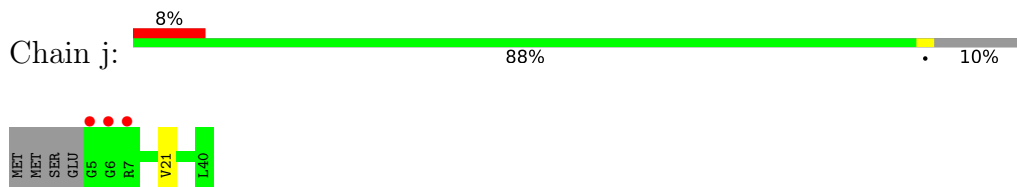
- Molecule 8: Photosystem II reaction center protein I



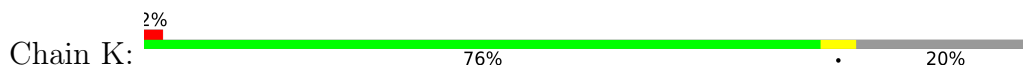
- Molecule 9: Photosystem II reaction center protein J

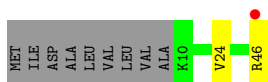


- Molecule 9: Photosystem II reaction center protein J

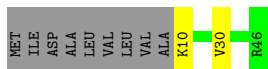
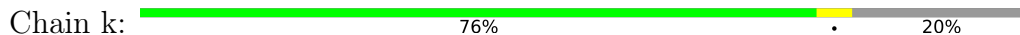


- Molecule 10: Photosystem II reaction center protein K





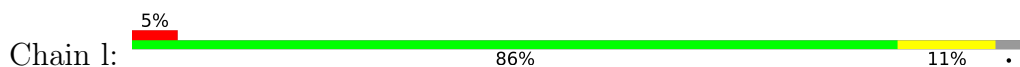
- Molecule 10: Photosystem II reaction center protein K



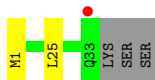
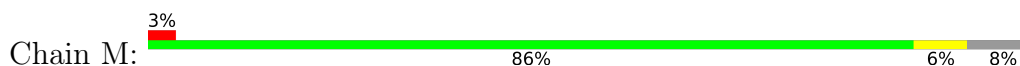
- Molecule 11: Photosystem II reaction center protein L



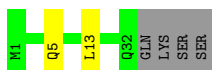
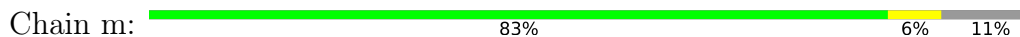
- Molecule 11: Photosystem II reaction center protein L



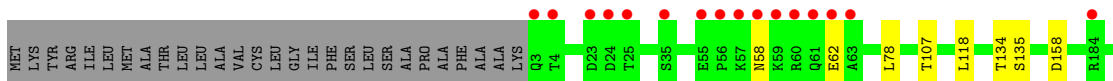
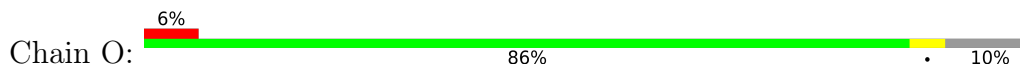
- Molecule 12: Photosystem II reaction center protein M



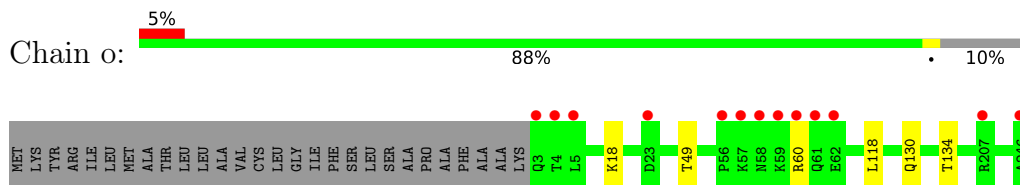
- Molecule 12: Photosystem II reaction center protein M



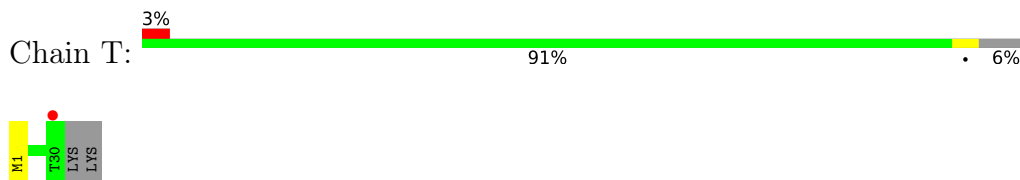
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



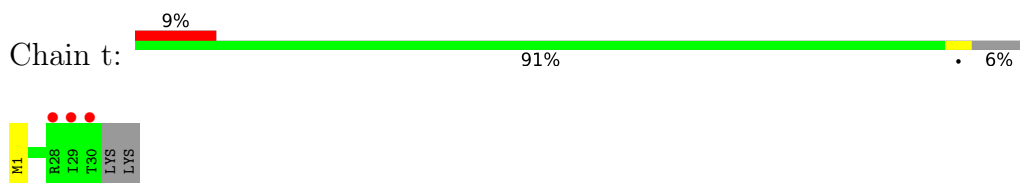
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



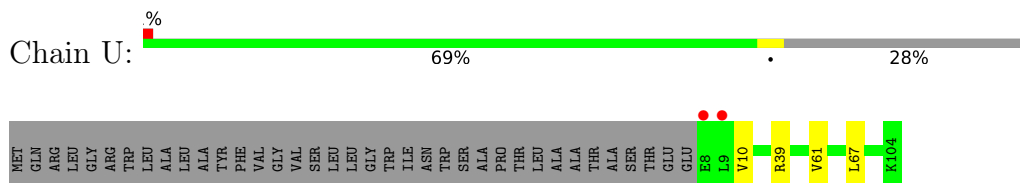
- Molecule 14: Photosystem II reaction center protein T



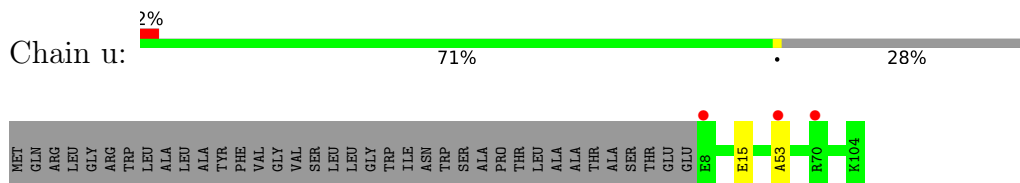
- Molecule 14: Photosystem II reaction center protein T



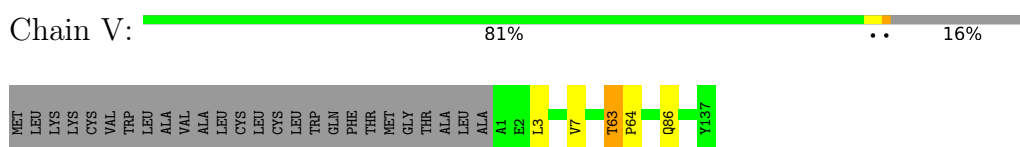
- Molecule 15: Photosystem II 12 kDa extrinsic protein



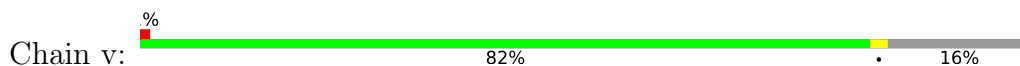
- Molecule 15: Photosystem II 12 kDa extrinsic protein

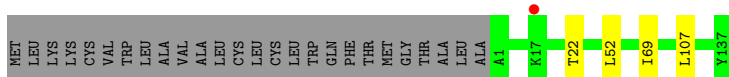


- Molecule 16: Cytochrome c-550

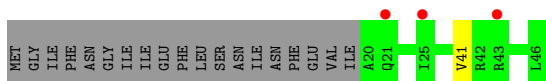


- Molecule 16: Cytochrome c-550

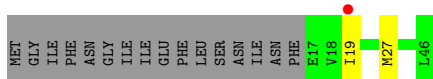




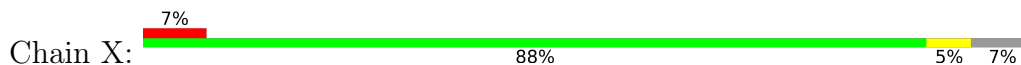
- Molecule 17: Photosystem II reaction center protein Ycf12



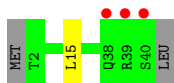
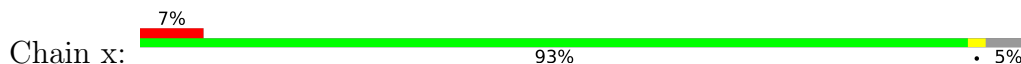
- Molecule 17: Photosystem II reaction center protein Ycf12



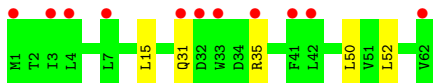
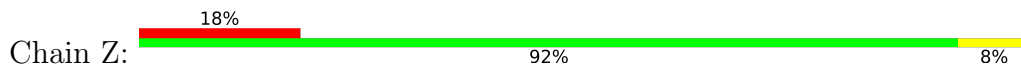
- Molecule 18: Photosystem II reaction center X protein



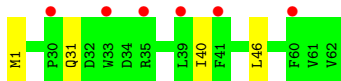
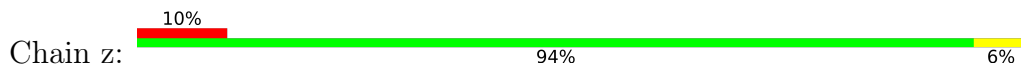
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z

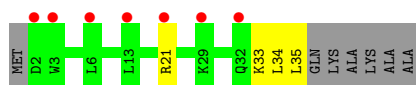
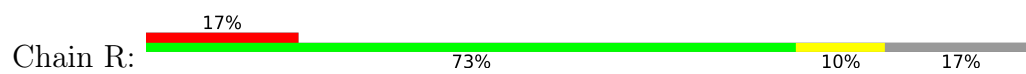


- Molecule 19: Photosystem II reaction center protein Z

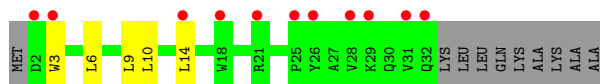


- Molecule 20: Photosystem II protein Y





- 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, $\alpha$ , $\beta$ , $\gamma$	117.34Å 222.83Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.74 – 2.00 19.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.74-2.00) 84.5 (19.74-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.33 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.182 , 0.226 0.182 , 0.226	Depositor DCC
$R_{free}$ test set	4807 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 64.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	54524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.42	0/3717	0.57	0/5060
1	a	0.39	0/3714	0.57	0/5056
2	B	0.41	0/4155	0.58	0/5661
2	b	0.40	0/4118	0.57	0/5611
3	C	0.41	0/3711	0.55	0/5051
3	c	0.39	0/3791	0.56	0/5158
4	D	0.42	0/2838	0.57	0/3862
4	d	0.42	0/2847	0.58	0/3874
5	E	0.36	0/688	0.55	0/940
5	e	0.34	0/683	0.55	0/932
6	F	0.38	0/284	0.50	0/387
6	f	0.31	0/284	0.56	0/387
7	H	0.40	0/523	0.58	0/713
7	h	0.39	0/511	0.58	0/697
8	I	0.40	0/293	0.56	0/396
8	i	0.42	0/293	0.55	0/396
9	J	0.38	0/263	0.56	0/356
9	j	0.33	0/263	0.53	0/356
10	K	0.37	0/303	0.52	0/416
10	k	0.36	0/303	0.58	0/416
11	L	0.38	0/311	0.55	0/422
11	l	0.41	0/303	0.61	0/412
12	M	0.35	0/249	0.52	0/341
12	m	0.37	0/244	0.53	0/334
13	O	0.39	0/1904	0.62	1/2585 (0.0%)
13	o	0.37	0/1905	0.62	0/2583
14	T	0.43	0/257	0.60	0/349
14	t	0.45	0/255	0.54	0/346
15	U	0.36	0/785	0.57	0/1064
15	u	0.37	0/785	0.59	0/1064
16	V	0.36	0/1085	0.58	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.34	0/1085	0.56	0/1473
17	Y	0.30	0/197	0.52	0/264
17	y	0.30	0/219	0.48	0/294
18	X	0.36	0/284	0.51	0/384
18	x	0.30	0/289	0.46	0/391
19	Z	0.32	0/490	0.49	0/669
19	z	0.30	0/488	0.42	0/666
20	R	0.32	0/277	0.52	0/380
20	r	0.31	0/252	0.53	0/347
All	All	0.39	0/45246	0.57	2/61566 (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
16	V	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	63	THR	C-N-CD	-5.42	108.69	120.60
13	O	158	ASP	CB-CG-OD1	5.13	122.92	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

## 5.2 Too-close contacts

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	458/344 (133%)	445 (97%)	12 (3%)	1 (0%)	47	44
1	a	458/344 (133%)	440 (96%)	17 (4%)	1 (0%)	47	44
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	461/461 (100%)	449 (97%)	11 (2%)	1 (0%)	47	44
3	c	471/461 (102%)	457 (97%)	13 (3%)	1 (0%)	47	44
4	D	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
4	d	342/352 (97%)	332 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	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	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	9 (4%)	3 (1%)	13	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	14	8
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	22	16
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100
20	R	32/41 (78%)	31 (97%)	0	1 (3%)	4	1
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5534/5700 (97%)	5383 (97%)	141 (2%)	10 (0%)	47	44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
13	O	62	GLU
3	c	416	SER
15	u	53	ALA

### 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	374/280 (134%)	370 (99%)	4 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	373/280 (133%)	363 (97%)	10 (3%)	44	46
2	B	407/407 (100%)	400 (98%)	7 (2%)	60	65
2	b	402/407 (99%)	397 (99%)	5 (1%)	71	76
3	C	361/362 (100%)	358 (99%)	3 (1%)	81	86
3	c	370/362 (102%)	356 (96%)	14 (4%)	33	31
4	D	278/283 (98%)	275 (99%)	3 (1%)	73	78
4	d	279/283 (99%)	272 (98%)	7 (2%)	47	49
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	27
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	27
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	34
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	50 (94%)	3 (6%)	20	16
8	I	32/34 (94%)	31 (97%)	1 (3%)	40	40
8	i	32/34 (94%)	30 (94%)	2 (6%)	18	13
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	27
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	11
10	k	30/37 (81%)	28 (93%)	2 (7%)	16	11
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	34
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	10
13	O	206/228 (90%)	200 (97%)	6 (3%)	42	43
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	43
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	80 (95%)	4 (5%)	25	22
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	76
16	V	117/138 (85%)	114 (97%)	3 (3%)	46	48
16	v	117/138 (85%)	113 (97%)	4 (3%)	37	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	19/37 (51%)	18 (95%)	1 (5%)	22	18
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	5
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	12
18	x	31/34 (91%)	30 (97%)	1 (3%)	39	38
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	5
19	z	51/52 (98%)	47 (92%)	4 (8%)	12	8
20	R	28/33 (85%)	25 (89%)	3 (11%)	6	3
20	r	25/33 (76%)	20 (80%)	5 (20%)	1	0
All	All	4572/4654 (98%)	4446 (97%)	126 (3%)	43	44

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	245	THR
16	v	22	THR
3	c	240	ILE
15	u	15	GLU
19	z	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	497	GLN
5	e	60	GLN
3	c	311	GLN
12	m	5	GLN
13	O	88	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	FME	t	1	14	8,9,10	1.12	1 (12%)	7,9,11	1.01	0
12	FME	M	1	12	8,9,10	1.02	1 (12%)	7,9,11	0.98	0
14	FME	T	1	14	8,9,10	1.04	0	7,9,11	1.01	1 (14%)
12	FME	m	1	12	8,9,10	0.92	0	7,9,11	0.81	0
8	FME	I	1	8	8,9,10	0.92	0	7,9,11	0.88	0
8	FME	i	1	8	8,9,10	1.02	0	7,9,11	0.84	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.09	1.43	1.46
14	t	1	FME	CA-N	-2.05	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.16	113.63	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	i	1	FME	O-C-CA-CB
14	t	1	FME	O-C-CA-CB
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
12	M	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 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
27	BCR	D	405	-	41,41,41	1.06	3 (7%)	56,56,56	1.16	5 (8%)
29	LMG	c	521	-	48,48,55	0.96	3 (6%)	56,56,63	1.28	7 (12%)
25	CLA	b	613	-	65,73,73	1.65	7 (10%)	76,113,113	1.32	9 (11%)
25	CLA	C	511	3	65,73,73	1.66	7 (10%)	76,113,113	1.57	6 (7%)
30	LHG	E	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.23	6 (11%)
25	CLA	B	610	37	65,73,73	1.55	9 (13%)	76,113,113	1.34	11 (14%)
25	CLA	C	504	37	59,67,73	1.53	6 (10%)	68,105,113	1.39	9 (13%)
25	CLA	B	608	-	65,73,73	1.45	8 (12%)	76,113,113	1.51	8 (10%)
25	CLA	c	509	-	65,73,73	1.51	8 (12%)	76,113,113	1.53	8 (10%)
25	CLA	b	603	-	65,73,73	1.68	7 (10%)	76,113,113	1.54	11 (14%)
27	BCR	A	610	-	41,41,41	0.94	1 (2%)	56,56,56	1.11	4 (7%)
27	BCR	a	611	-	41,41,41	0.94	2 (4%)	56,56,56	1.23	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	BCR	b	617	-	41,41,41	1.04	2 (4%)	56,56,56	1.08	5 (8%)
29	LMG	m	101	-	51,51,55	0.90	3 (5%)	59,59,63	1.47	6 (10%)
25	CLA	b	608	-	65,73,73	1.63	9 (13%)	76,113,113	1.35	7 (9%)
25	CLA	c	502	-	65,73,73	1.56	8 (12%)	76,113,113	1.36	9 (11%)
29	LMG	d	409	-	44,44,55	0.94	3 (6%)	52,52,63	1.29	7 (13%)
32	DGD	c	516	-	63,63,67	0.91	4 (6%)	77,77,81	1.39	11 (14%)
33	STE	C	521	-	15,15,19	0.37	0	14,14,19	0.79	0
33	STE	b	626	-	9,9,19	0.37	0	8,8,19	0.59	0
33	STE	t	102	-	13,13,19	0.64	0	13,13,19	1.33	2 (15%)
25	CLA	c	501	-	65,73,73	1.52	9 (13%)	76,113,113	1.50	8 (10%)
29	LMG	D	409	-	31,31,55	0.83	2 (6%)	33,33,63	1.26	3 (9%)
33	STE	t	104	-	17,17,19	0.64	0	17,17,19	1.11	1 (5%)
33	STE	B	625	-	11,11,19	0.67	0	11,11,19	1.31	2 (18%)
28	PL9	D	406	-	55,55,55	0.92	2 (3%)	68,69,69	1.75	12 (17%)
25	CLA	b	612	-	65,73,73	1.52	7 (10%)	76,113,113	1.51	11 (14%)
25	CLA	a	608	37	65,73,73	1.61	6 (9%)	76,113,113	1.43	13 (17%)
33	STE	b	625	-	19,19,19	0.58	0	19,19,19	1.08	1 (5%)
32	DGD	A	617	-	67,67,67	1.11	6 (8%)	81,81,81	1.31	9 (11%)
25	CLA	A	607	37	65,73,73	1.52	6 (9%)	76,113,113	1.48	13 (17%)
27	BCR	t	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.38	9 (16%)
25	CLA	B	611	-	65,73,73	1.52	6 (9%)	76,113,113	1.45	9 (11%)
27	BCR	k	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.05	3 (5%)
25	CLA	c	513	-	65,73,73	1.58	7 (10%)	76,113,113	1.44	12 (15%)
28	PL9	A	611	-	55,55,55	0.78	1 (1%)	68,69,69	1.50	13 (19%)
25	CLA	c	510	-	65,73,73	1.58	6 (9%)	76,113,113	1.49	9 (11%)
33	STE	C	519	-	11,11,19	0.63	0	11,11,19	1.54	1 (9%)
28	PL9	d	405	-	55,55,55	1.01	3 (5%)	68,69,69	1.63	14 (20%)
33	STE	d	410	-	16,16,19	0.60	0	16,16,19	1.30	1 (6%)
26	PHO	A	608	-	51,69,69	0.96	2 (3%)	47,99,99	1.21	5 (10%)
25	CLA	b	602	-	65,73,73	1.56	8 (12%)	76,113,113	1.40	9 (11%)
25	CLA	b	607	-	65,73,73	1.55	6 (9%)	76,113,113	1.52	10 (13%)
25	CLA	A	606	-	65,73,73	1.52	8 (12%)	76,113,113	1.32	9 (11%)
25	CLA	B	613	-	65,73,73	1.51	6 (9%)	76,113,113	1.59	11 (14%)
25	CLA	C	506	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	8 (10%)
32	DGD	C	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.35	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	LHG	B	622	-	48,48,48	0.70	1 (2%)	51,54,54	1.35	7 (13%)
33	STE	a	618	-	11,11,19	0.77	0	11,11,19	1.20	1 (9%)
36	HEC	v	201	16	32,50,50	2.05	3 (9%)	24,82,82	1.87	5 (20%)
25	CLA	B	612	-	65,73,73	1.48	6 (9%)	76,113,113	1.50	12 (15%)
27	BCR	B	617	-	41,41,41	1.00	3 (7%)	56,56,56	1.18	6 (10%)
25	CLA	b	611	-	65,73,73	1.59	8 (12%)	76,113,113	1.44	11 (14%)
25	CLA	b	615	-	60,68,73	1.52	6 (10%)	70,107,113	1.51	10 (14%)
30	LHG	d	407	-	38,38,48	0.75	1 (2%)	41,44,54	1.08	2 (4%)
31	SQD	B	623	-	53,54,54	1.54	9 (16%)	62,65,65	1.78	10 (16%)
25	CLA	c	506	-	65,73,73	1.59	8 (12%)	76,113,113	1.31	9 (11%)
33	STE	M	102	-	14,14,19	0.62	0	14,14,19	1.44	1 (7%)
21	OEX	a	601[C]	3,37,1	0,15,15	-	-	-	-	-
30	LHG	e	102	-	41,41,48	0.80	1 (2%)	44,47,54	1.28	5 (11%)
27	BCR	K	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	6 (10%)
33	STE	I	101	-	14,14,19	0.32	0	13,13,19	0.81	0
25	CLA	C	501	-	65,73,73	1.76	9 (13%)	76,113,113	1.49	9 (11%)
33	STE	m	102	-	11,11,19	0.68	0	11,11,19	1.44	2 (18%)
25	CLA	B	606	-	65,73,73	1.64	9 (13%)	76,113,113	1.56	9 (11%)
32	DGD	c	517	-	63,63,67	0.95	2 (3%)	77,77,81	1.41	9 (11%)
25	CLA	b	601	-	65,73,73	1.46	7 (10%)	76,113,113	1.54	10 (13%)
25	CLA	c	504	37	60,68,73	1.50	5 (8%)	70,107,113	1.50	9 (12%)
34	BCT	a	606	23	2,3,3	1.22	0	2,3,3	3.13	1 (50%)
33	STE	c	520	-	19,19,19	0.59	0	19,19,19	1.04	0
33	STE	M	103	-	9,9,19	0.34	0	8,8,19	0.78	0
27	BCR	b	616	-	41,41,41	0.92	3 (7%)	56,56,56	1.20	4 (7%)
32	DGD	H	102	-	63,63,67	1.21	9 (14%)	77,77,81	1.33	8 (10%)
26	PHO	D	402	-	51,69,69	0.98	3 (5%)	47,99,99	1.34	6 (12%)
32	DGD	h	103	-	63,63,67	0.95	3 (4%)	77,77,81	1.42	12 (15%)
25	CLA	C	502	-	65,73,73	1.55	7 (10%)	76,113,113	1.24	8 (10%)
32	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.37	8 (10%)
25	CLA	c	508	-	64,72,73	1.64	9 (14%)	74,111,113	1.48	9 (12%)
33	STE	j	101	-	11,11,19	0.76	0	11,11,19	1.30	2 (18%)
33	STE	B	624	-	11,11,19	0.74	0	11,11,19	1.24	0
25	CLA	C	509	-	65,73,73	1.60	10 (15%)	76,113,113	1.45	9 (11%)
35	HEM	F	101	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.45	6 (13%)
25	CLA	B	615	-	65,73,73	1.50	8 (12%)	76,113,113	1.35	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMG	A	613	-	48,48,55	0.89	3 (6%)	56,56,63	1.29	4 (7%)
33	STE	H	103	-	17,17,19	0.41	0	16,16,19	0.68	0
31	SQD	a	616	-	35,35,54	1.63	5 (14%)	37,37,65	1.42	6 (16%)
31	SQD	f	101	-	40,41,54	1.67	9 (22%)	49,52,65	1.71	10 (20%)
29	LMG	D	407	-	51,51,55	0.76	1 (1%)	59,59,63	1.34	8 (13%)
30	LHG	D	408	-	48,48,48	0.72	2 (4%)	51,54,54	1.28	6 (11%)
33	STE	B	626	-	15,15,19	0.35	0	14,14,19	0.91	0
26	PHO	d	401	-	51,69,69	0.95	2 (3%)	47,99,99	1.46	8 (17%)
35	HEM	e	101	6,5	41,50,50	1.45	5 (12%)	45,82,82	1.51	9 (20%)
22	OEY	a	602[A]	3,37,1	0,16,16	-	-	-	-	-
33	STE	t	103	-	9,9,19	0.34	0	8,8,19	0.79	0
27	BCR	C	514	-	41,41,41	1.03	2 (4%)	56,56,56	1.17	6 (10%)
25	CLA	c	503	-	65,73,73	1.66	8 (12%)	76,113,113	1.54	9 (11%)
25	CLA	b	614	-	65,73,73	1.46	8 (12%)	76,113,113	1.39	8 (10%)
27	BCR	k	102	-	41,41,41	0.99	2 (4%)	56,56,56	1.13	3 (5%)
27	BCR	c	514	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	5 (8%)
33	STE	l	102	-	17,17,19	0.33	0	16,16,19	0.89	0
26	PHO	a	609	-	51,69,69	0.92	1 (1%)	47,99,99	1.06	4 (8%)
33	STE	E	102	-	11,11,19	0.73	0	11,11,19	1.14	0
33	STE	k	103	-	11,11,19	0.74	0	11,11,19	1.09	0
25	CLA	D	403	-	65,73,73	1.57	10 (15%)	76,113,113	1.36	7 (9%)
25	CLA	B	603	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	7 (9%)
25	CLA	d	403	-	65,73,73	1.57	6 (9%)	76,113,113	1.40	7 (9%)
36	HEC	V	201	16	32,50,50	1.94	3 (9%)	24,82,82	2.10	8 (33%)
27	BCR	c	515	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	5 (8%)
27	BCR	h	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.26	5 (8%)
33	STE	X	101	-	19,19,19	0.55	0	19,19,19	1.19	1 (5%)
25	CLA	B	616	-	60,68,73	1.74	8 (13%)	70,107,113	1.47	7 (10%)
25	CLA	b	604	-	65,73,73	1.53	7 (10%)	76,113,113	1.67	12 (15%)
29	LMG	M	101	-	51,51,55	0.86	3 (5%)	59,59,63	1.44	10 (16%)
29	LMG	d	408	-	21,21,55	0.55	0	20,20,63	1.20	3 (15%)
33	STE	B	620	-	16,16,19	0.68	0	16,16,19	1.07	0
33	STE	x	101	-	19,19,19	0.69	0	19,19,19	0.98	1 (5%)
25	CLA	a	610	-	65,73,73	1.62	6 (9%)	76,113,113	1.40	11 (14%)
21	OEX	A	601[C]	3,37,1	0,15,15	-	-	-	-	-
31	SQD	b	619	-	48,49,54	1.62	9 (18%)	57,60,65	1.78	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	b	609	37	65,73,73	1.39	6 (9%)	76,113,113	1.41	9 (11%)
25	CLA	c	511	3	65,73,73	1.83	8 (12%)	76,113,113	1.53	7 (9%)
29	LMG	c	522	-	49,49,55	0.96	4 (8%)	57,57,63	1.29	4 (7%)
25	CLA	b	610	-	65,73,73	1.62	6 (9%)	76,113,113	1.45	10 (13%)
25	CLA	A	612	37	65,73,73	1.40	7 (10%)	76,113,113	1.44	9 (11%)
25	CLA	B	609	-	65,73,73	1.54	6 (9%)	76,113,113	1.44	8 (10%)
25	CLA	C	510	-	65,73,73	1.54	6 (9%)	76,113,113	1.45	9 (11%)
28	PL9	a	612	-	55,55,55	0.81	2 (3%)	68,69,69	1.59	12 (17%)
30	LHG	A	614	-	46,46,48	0.83	3 (6%)	49,52,54	1.18	6 (12%)
25	CLA	B	607	37	65,73,73	1.49	9 (13%)	76,113,113	1.43	6 (7%)
25	CLA	D	404	-	65,73,73	1.61	10 (15%)	76,113,113	1.28	10 (13%)
25	CLA	c	507	37	65,73,73	1.57	11 (16%)	76,113,113	1.52	10 (13%)
25	CLA	A	609	-	54,62,73	1.64	8 (14%)	62,99,113	1.59	9 (14%)
25	CLA	c	512	-	65,73,73	1.54	8 (12%)	76,113,113	1.43	9 (11%)
21	OEX	a	601[B]	3,37,1	0,15,15	-	-	-	-	-
27	BCR	K	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.12	2 (3%)
27	BCR	B	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.27	4 (7%)
29	LMG	c	519	-	37,37,55	1.02	2 (5%)	45,45,63	1.35	6 (13%)
25	CLA	C	508	-	65,73,73	1.55	8 (12%)	76,113,113	1.65	11 (14%)
25	CLA	a	607	-	65,73,73	1.62	8 (12%)	76,113,113	1.44	10 (13%)
27	BCR	T	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.30	5 (8%)
29	LMG	C	518	-	48,48,55	0.74	1 (2%)	56,56,63	1.31	7 (12%)
25	CLA	b	606	37	65,73,73	1.45	8 (12%)	76,113,113	1.36	6 (7%)
27	BCR	B	618	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	8 (14%)
32	DGD	C	516	-	63,63,67	1.06	5 (7%)	77,77,81	1.34	9 (11%)
25	CLA	C	512	-	65,73,73	1.59	8 (12%)	76,113,113	1.47	9 (11%)
25	CLA	B	614	-	65,73,73	1.73	9 (13%)	76,113,113	1.48	7 (9%)
27	BCR	K	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.09	5 (8%)
33	STE	b	621	-	19,19,19	0.63	0	19,19,19	0.95	0
25	CLA	B	605	-	65,73,73	1.47	5 (7%)	76,113,113	1.46	9 (11%)
25	CLA	h	101	37	65,73,73	1.70	10 (15%)	76,113,113	1.52	9 (11%)
25	CLA	b	605	-	65,73,73	1.62	6 (9%)	76,113,113	1.57	7 (9%)
31	SQD	A	615	-	51,52,54	1.54	7 (13%)	60,63,65	1.88	10 (16%)
32	DGD	C	515	-	63,63,67	1.04	5 (7%)	77,77,81	1.38	11 (14%)
29	LMG	b	622	-	55,55,55	0.81	2 (3%)	63,63,63	1.37	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	BCR	H	101	-	41,41,41	0.95	2 (4%)	56,56,56	1.19	6 (10%)
31	SQD	F	102	-	35,36,54	1.50	6 (17%)	42,45,65	2.01	10 (23%)
33	STE	C	520	-	11,11,19	0.69	0	11,11,19	1.19	1 (9%)
25	CLA	C	503	-	65,73,73	1.71	9 (13%)	76,113,113	1.68	12 (15%)
29	LMG	B	621	-	26,26,55	0.59	1 (3%)	26,26,63	1.35	2 (7%)
25	CLA	C	513	-	65,73,73	1.54	7 (10%)	76,113,113	1.50	7 (9%)
30	LHG	a	614	-	48,48,48	0.75	3 (6%)	51,54,54	1.29	7 (13%)
30	LHG	d	406	-	48,48,48	0.69	2 (4%)	51,54,54	1.19	5 (9%)
31	SQD	a	615	-	53,54,54	1.56	7 (13%)	62,65,65	1.90	10 (16%)
22	OEY	A	602[A]	3,37,1	0,16,16	-	-	-	-	-
33	STE	b	623	-	15,15,19	0.67	0	15,15,19	1.05	0
30	LHG	L	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.14	2 (3%)
25	CLA	B	602	-	65,73,73	1.59	7 (10%)	76,113,113	1.48	10 (13%)
25	CLA	B	601	37	65,73,73	1.68	8 (12%)	76,113,113	1.47	14 (18%)
25	CLA	a	613	37	65,73,73	1.67	8 (12%)	76,113,113	1.53	8 (10%)
25	CLA	C	507	37	65,73,73	1.58	8 (12%)	76,113,113	1.52	10 (13%)
32	DGD	a	617	-	43,43,67	0.79	3 (6%)	45,45,81	1.40	7 (15%)
27	BCR	d	404	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	4 (7%)
33	STE	b	620	-	15,15,19	0.37	0	14,14,19	0.83	0
34	BCT	D	401	23	2,3,3	1.16	0	2,3,3	3.25	1 (50%)
33	STE	J	101	-	11,11,19	0.77	0	11,11,19	1.20	0
27	BCR	b	618	-	41,41,41	0.93	2 (4%)	56,56,56	1.10	4 (7%)
31	SQD	A	616	-	38,38,54	1.74	5 (13%)	40,40,65	1.19	2 (5%)
25	CLA	d	402	-	65,73,73	1.43	7 (10%)	76,113,113	1.34	8 (10%)
25	CLA	B	604	-	65,73,73	1.63	7 (10%)	76,113,113	1.62	9 (11%)
30	LHG	l	101	-	48,48,48	0.57	0	51,54,54	1.20	5 (9%)
21	OEX	A	601[B]	3,37,1	0,15,15	-	-	-	-	-
25	CLA	C	505	-	65,73,73	1.56	6 (9%)	76,113,113	1.38	5 (6%)
33	STE	b	624	-	14,14,19	0.31	0	13,13,19	0.89	0
25	CLA	c	505	-	65,73,73	1.44	6 (9%)	76,113,113	1.36	7 (9%)

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
27	BCR	D	405	-	-	3/29/63/63	0/2/2/2
29	LMG	c	521	-	-	22/43/63/70	0/1/1/1
25	CLA	b	613	-	1/1/15/20	19/37/115/115	-
25	CLA	C	511	3	1/1/15/20	3/37/115/115	-
30	LHG	E	101	-	-	27/53/53/53	-
25	CLA	B	610	37	1/1/15/20	7/37/115/115	-
25	CLA	C	504	37	1/1/13/20	7/30/108/115	-
25	CLA	B	608	-	1/1/15/20	4/37/115/115	-
25	CLA	c	509	-	1/1/15/20	12/37/115/115	-
25	CLA	b	603	-	1/1/15/20	8/37/115/115	-
27	BCR	A	610	-	-	2/29/63/63	0/2/2/2
27	BCR	a	611	-	-	1/29/63/63	0/2/2/2
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
29	LMG	m	101	-	-	19/46/66/70	0/1/1/1
25	CLA	c	502	-	1/1/15/20	6/37/115/115	-
25	CLA	b	608	-	-	10/37/115/115	-
29	LMG	d	409	-	-	11/39/59/70	0/1/1/1
32	DGD	c	516	-	-	19/51/91/95	0/2/2/2
33	STE	C	521	-	-	8/13/13/17	-
33	STE	b	626	-	-	5/7/7/17	-
33	STE	t	102	-	-	4/11/11/17	-
25	CLA	c	501	-	1/1/15/20	6/37/115/115	-
29	LMG	D	409	-	-	19/33/33/70	-
33	STE	t	104	-	-	7/15/15/17	-
33	STE	B	625	-	-	4/9/9/17	-
28	PL9	D	406	-	-	12/53/73/73	0/1/1/1
25	CLA	b	612	-	1/1/15/20	4/37/115/115	-
25	CLA	a	608	37	1/1/15/20	12/37/115/115	-
33	STE	b	625	-	-	7/17/17/17	-
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2
25	CLA	A	607	37	1/1/15/20	11/37/115/115	-
27	BCR	t	101	-	-	1/29/63/63	0/2/2/2
25	CLA	B	611	-	1/1/15/20	5/37/115/115	-
27	BCR	k	101	-	-	9/29/63/63	0/2/2/2
25	CLA	c	513	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	A	611	-	-	24/53/73/73	0/1/1/1
25	CLA	c	510	-	1/1/15/20	17/37/115/115	-
33	STE	C	519	-	-	5/9/9/17	-
28	PL9	d	405	-	-	7/53/73/73	0/1/1/1
33	STE	d	410	-	-	10/14/14/17	-
26	PHO	A	608	-	-	5/37/103/103	0/5/6/6
25	CLA	b	602	-	1/1/15/20	9/37/115/115	-
25	CLA	b	607	-	-	5/37/115/115	-
25	CLA	A	606	-	1/1/15/20	4/37/115/115	-
25	CLA	B	613	-	1/1/15/20	9/37/115/115	-
25	CLA	C	506	-	1/1/15/20	10/37/115/115	-
32	DGD	C	517	-	-	17/51/91/95	0/2/2/2
30	LHG	B	622	-	-	16/53/53/53	-
33	STE	a	618	-	-	5/9/9/17	-
36	HEC	v	201	16	-	2/10/54/54	-
25	CLA	B	612	-	1/1/15/20	9/37/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	CLA	b	611	-	1/1/15/20	5/37/115/115	-
25	CLA	b	615	-	1/1/14/20	6/31/109/115	-
30	LHG	d	407	-	-	11/43/43/53	-
31	SQD	B	623	-	-	20/49/69/69	0/1/1/1
25	CLA	c	506	-	1/1/15/20	13/37/115/115	-
33	STE	M	102	-	-	6/12/12/17	-
30	LHG	e	102	-	-	25/46/46/53	-
27	BCR	K	101	-	-	12/29/63/63	0/2/2/2
33	STE	I	101	-	-	5/12/12/17	-
25	CLA	C	501	-	1/1/15/20	6/37/115/115	-
33	STE	m	102	-	-	5/9/9/17	-
25	CLA	B	606	-	1/1/15/20	9/37/115/115	-
32	DGD	c	517	-	-	19/51/91/95	0/2/2/2
25	CLA	b	601	-	1/1/15/20	9/37/115/115	-
25	CLA	c	504	37	1/1/14/20	10/31/109/115	-
33	STE	c	520	-	-	13/17/17/17	-
33	STE	M	103	-	-	3/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	616	-	-	5/29/63/63	0/2/2/2
32	DGD	H	102	-	-	16/51/91/95	0/2/2/2
26	PHO	D	402	-	-	0/37/103/103	0/5/6/6
32	DGD	h	103	-	-	18/51/91/95	0/2/2/2
25	CLA	C	502	-	1/1/15/20	10/37/115/115	-
32	DGD	c	518	-	-	19/51/91/95	0/2/2/2
25	CLA	c	508	-	-	12/36/114/115	-
33	STE	j	101	-	-	4/9/9/17	-
33	STE	B	624	-	-	8/9/9/17	-
25	CLA	C	509	-	1/1/15/20	14/37/115/115	-
35	HEM	F	101	6,5	-	2/12/54/54	-
25	CLA	B	615	-	1/1/15/20	14/37/115/115	-
29	LMG	A	613	-	-	22/43/63/70	0/1/1/1
33	STE	H	103	-	-	11/15/15/17	-
31	SQD	a	616	-	-	17/37/37/69	-
31	SQD	f	101	-	-	14/36/56/69	0/1/1/1
29	LMG	D	407	-	-	19/46/66/70	0/1/1/1
30	LHG	D	408	-	-	19/53/53/53	-
33	STE	B	626	-	-	2/13/13/17	-
26	PHO	d	401	-	-	7/37/103/103	0/5/6/6
35	HEM	e	101	6,5	-	3/12/54/54	-
33	STE	t	103	-	-	4/7/7/17	-
27	BCR	C	514	-	-	3/29/63/63	0/2/2/2
25	CLA	c	503	-	1/1/15/20	9/37/115/115	-
25	CLA	b	614	-	1/1/15/20	9/37/115/115	-
27	BCR	k	102	-	-	4/29/63/63	0/2/2/2
27	BCR	c	514	-	-	9/29/63/63	0/2/2/2
33	STE	l	102	-	-	8/15/15/17	-
26	PHO	a	609	-	-	6/37/103/103	0/5/6/6
33	STE	E	102	-	-	7/9/9/17	-
33	STE	k	103	-	-	6/9/9/17	-
25	CLA	D	403	-	1/1/15/20	4/37/115/115	-
25	CLA	B	603	-	1/1/15/20	9/37/115/115	-
25	CLA	d	403	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HEC	V	201	16	-	2/10/54/54	-
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
27	BCR	h	102	-	-	5/29/63/63	0/2/2/2
33	STE	X	101	-	-	8/17/17/17	-
25	CLA	B	616	-	1/1/14/20	13/31/109/115	-
25	CLA	b	604	-	1/1/15/20	8/37/115/115	-
29	LMG	M	101	-	-	23/46/66/70	0/1/1/1
29	LMG	d	408	-	-	11/17/17/70	-
33	STE	B	620	-	-	5/14/14/17	-
33	STE	x	101	-	-	11/17/17/17	-
25	CLA	a	610	-	1/1/15/20	10/37/115/115	-
31	SQD	b	619	-	-	21/44/64/69	0/1/1/1
25	CLA	b	609	37	1/1/15/20	4/37/115/115	-
25	CLA	c	511	3	1/1/15/20	10/37/115/115	-
29	LMG	c	522	-	-	24/44/64/70	0/1/1/1
25	CLA	b	610	-	-	6/37/115/115	-
25	CLA	A	612	37	1/1/15/20	6/37/115/115	-
25	CLA	B	609	-	-	4/37/115/115	-
25	CLA	C	510	-	1/1/15/20	15/37/115/115	-
28	PL9	a	612	-	-	13/53/73/73	0/1/1/1
30	LHG	A	614	-	-	18/51/51/53	-
25	CLA	B	607	37	1/1/15/20	8/37/115/115	-
25	CLA	D	404	-	-	11/37/115/115	-
25	CLA	c	507	37	1/1/15/20	9/37/115/115	-
25	CLA	A	609	-	1/1/12/20	2/24/102/115	-
25	CLA	c	512	-	1/1/15/20	19/37/115/115	-
27	BCR	K	103	-	-	5/29/63/63	0/2/2/2
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
29	LMG	c	519	-	-	13/31/51/70	0/1/1/1
25	CLA	a	607	-	1/1/15/20	2/37/115/115	-
25	CLA	C	508	-	-	9/37/115/115	-
27	BCR	T	101	-	-	4/29/63/63	0/2/2/2
29	LMG	C	518	-	-	18/43/63/70	0/1/1/1
25	CLA	b	606	37	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
32	DGD	C	516	-	-	17/51/91/95	0/2/2/2
25	CLA	C	512	-	1/1/15/20	13/37/115/115	-
25	CLA	B	614	-	1/1/15/20	10/37/115/115	-
27	BCR	K	102	-	-	7/29/63/63	0/2/2/2
33	STE	b	621	-	-	10/17/17/17	-
25	CLA	B	605	-	1/1/15/20	11/37/115/115	-
25	CLA	h	101	37	1/1/15/20	14/37/115/115	-
25	CLA	b	605	-	1/1/15/20	7/37/115/115	-
31	SQD	A	615	-	-	14/47/67/69	0/1/1/1
32	DGD	C	515	-	-	19/51/91/95	0/2/2/2
29	LMG	b	622	-	-	32/50/70/70	0/1/1/1
27	BCR	H	101	-	-	5/29/63/63	0/2/2/2
31	SQD	F	102	-	-	7/28/48/69	0/1/1/1
33	STE	C	520	-	-	3/9/9/17	-
25	CLA	C	503	-	1/1/15/20	5/37/115/115	-
29	LMG	B	621	-	-	7/22/22/70	-
25	CLA	C	513	-	1/1/15/20	9/37/115/115	-
30	LHG	a	614	-	-	21/53/53/53	-
30	LHG	d	406	-	-	21/53/53/53	-
31	SQD	a	615	-	-	22/49/69/69	0/1/1/1
33	STE	b	623	-	-	7/13/13/17	-
30	LHG	L	101	-	-	22/53/53/53	-
25	CLA	B	602	-	1/1/15/20	7/37/115/115	-
25	CLA	B	601	37	1/1/15/20	14/37/115/115	-
25	CLA	a	613	37	1/1/15/20	5/37/115/115	-
25	CLA	C	507	37	1/1/15/20	5/37/115/115	-
32	DGD	a	617	-	-	21/45/45/95	-
27	BCR	d	404	-	-	4/29/63/63	0/2/2/2
33	STE	b	620	-	-	8/13/13/17	-
33	STE	J	101	-	-	3/9/9/17	-
27	BCR	b	618	-	-	4/29/63/63	0/2/2/2
31	SQD	A	616	-	-	20/39/39/69	-
25	CLA	d	402	-	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	604	-	1/1/15/20	11/37/115/115	-
30	LHG	l	101	-	-	21/53/53/53	-
25	CLA	C	505	-	1/1/15/20	9/37/115/115	-
33	STE	b	624	-	-	9/12/12/17	-
25	CLA	c	505	-	1/1/15/20	12/37/115/115	-

The worst 5 of 740 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	MG-NA	8.45	2.26	2.06
25	a	610	CLA	C4B-NB	8.27	1.42	1.35
25	C	507	CLA	C4B-NB	8.24	1.42	1.35
25	h	101	CLA	C4B-NB	8.09	1.42	1.35
25	B	614	CLA	C4B-NB	8.08	1.42	1.35

The worst 5 of 1156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	9.11	110.80	106.71
25	C	511	CLA	C4A-NA-C1A	8.61	110.58	106.71
25	c	511	CLA	C4A-NA-C1A	8.59	110.57	106.71
25	b	605	CLA	C4A-NA-C1A	8.42	110.49	106.71
25	C	508	CLA	C4A-NA-C1A	8.25	110.41	106.71

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	612	CLA	ND
25	B	601	CLA	ND

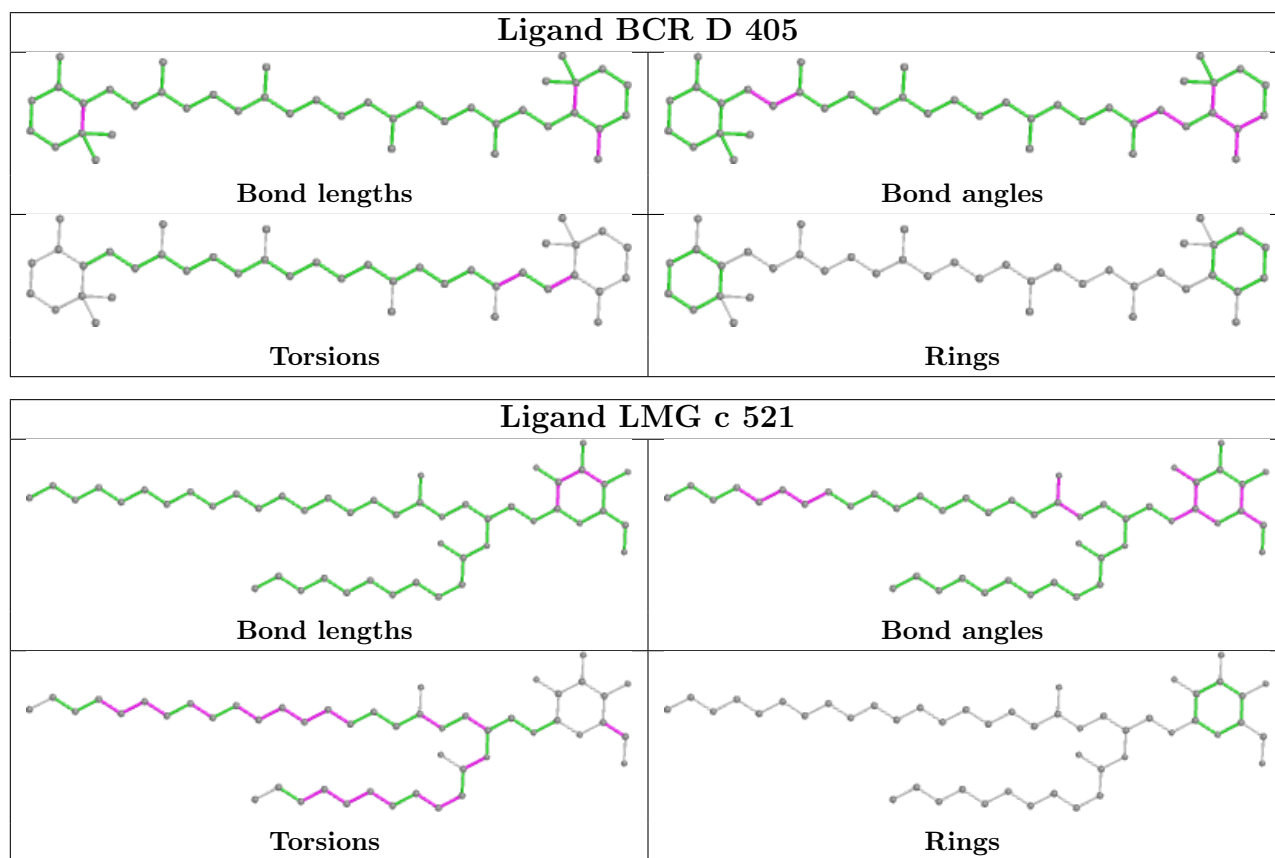
5 of 1775 torsion outliers are listed below:

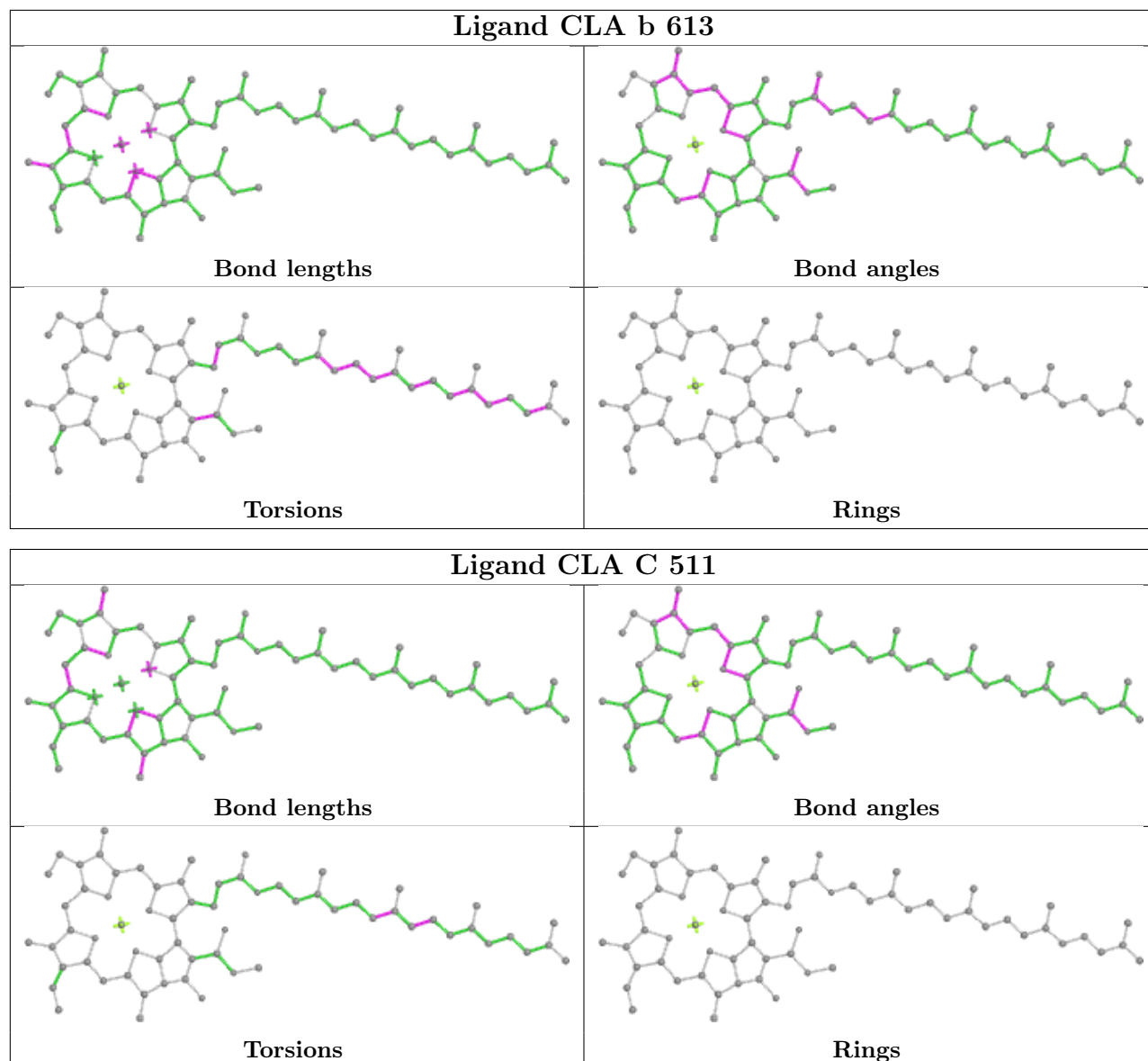
Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C14-C13-C15-C16
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	C2-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6

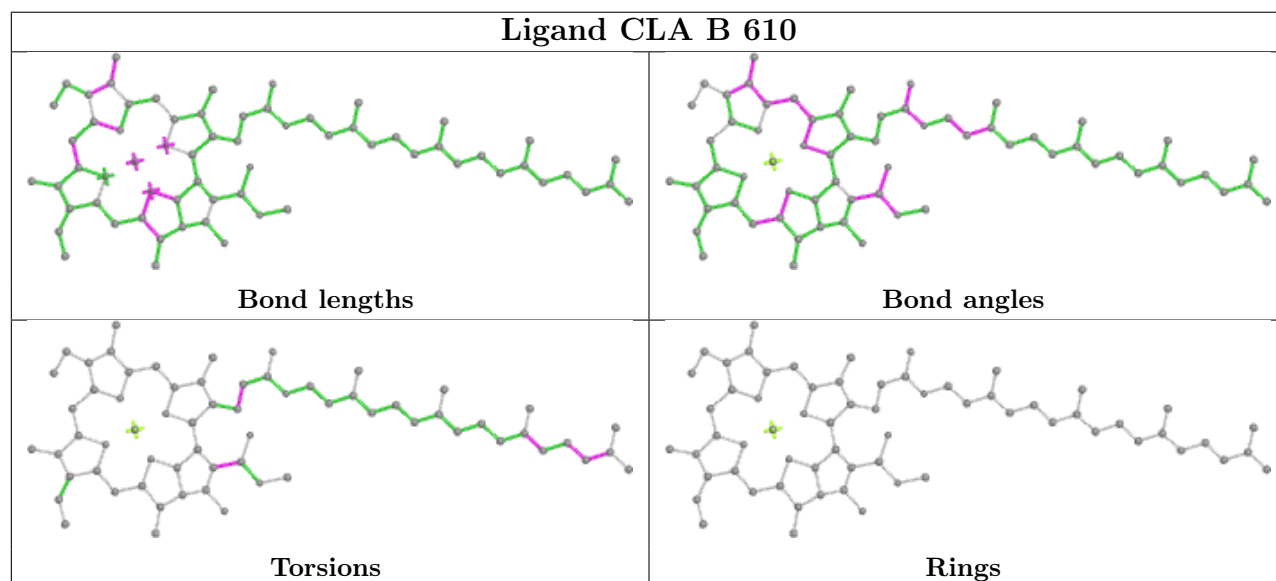
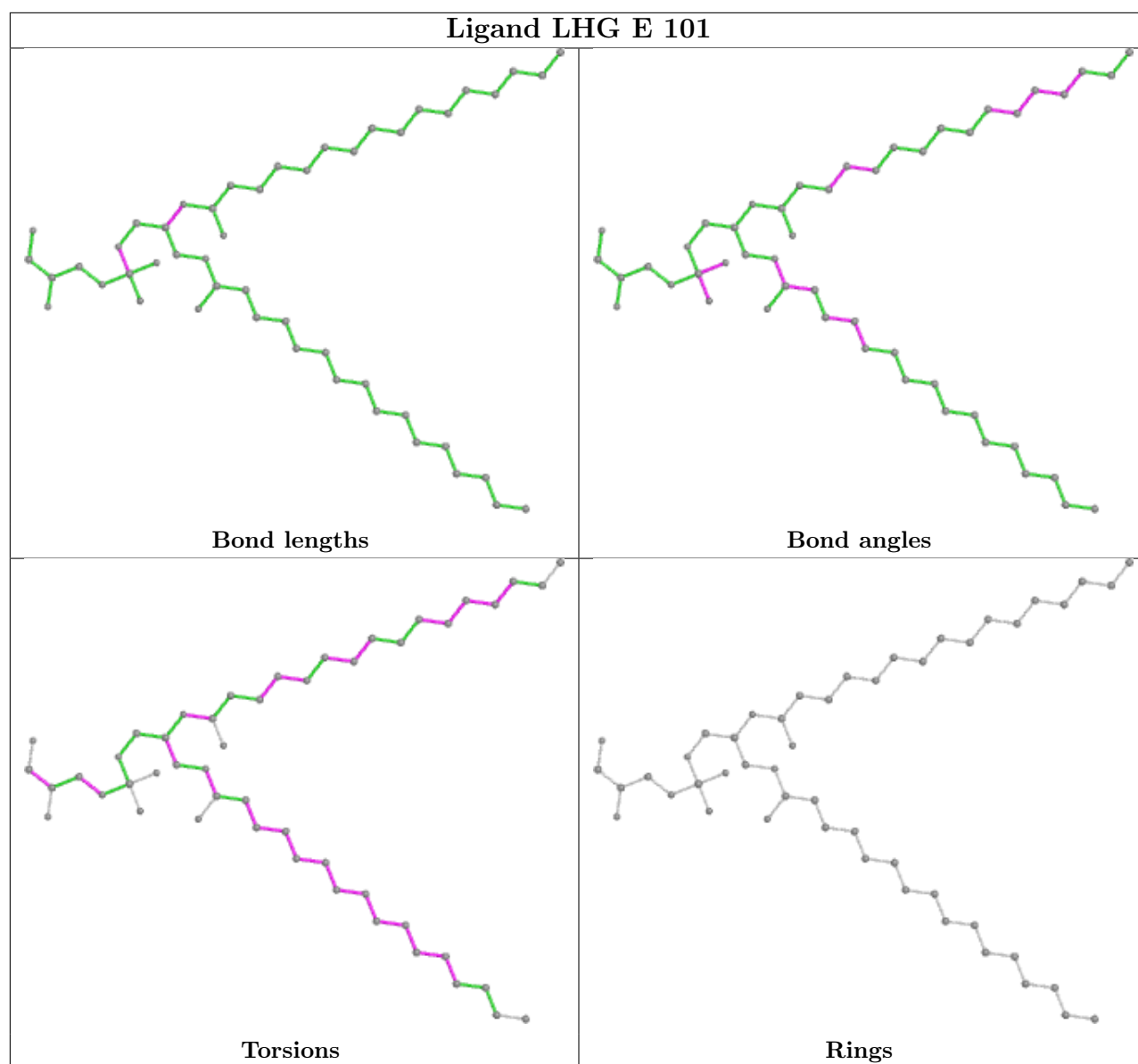
There are no ring outliers.

No monomer is involved in short contacts.

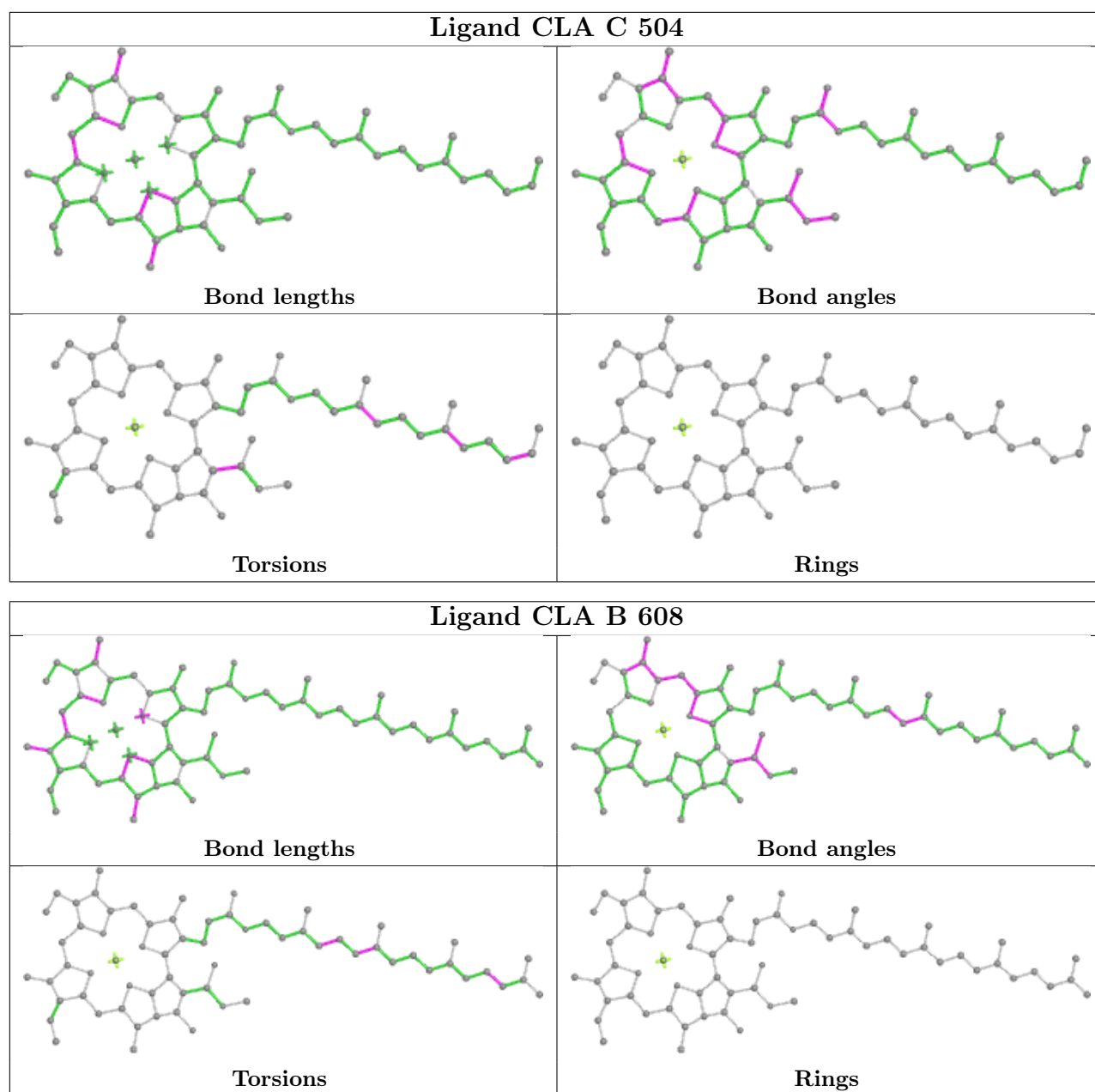
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

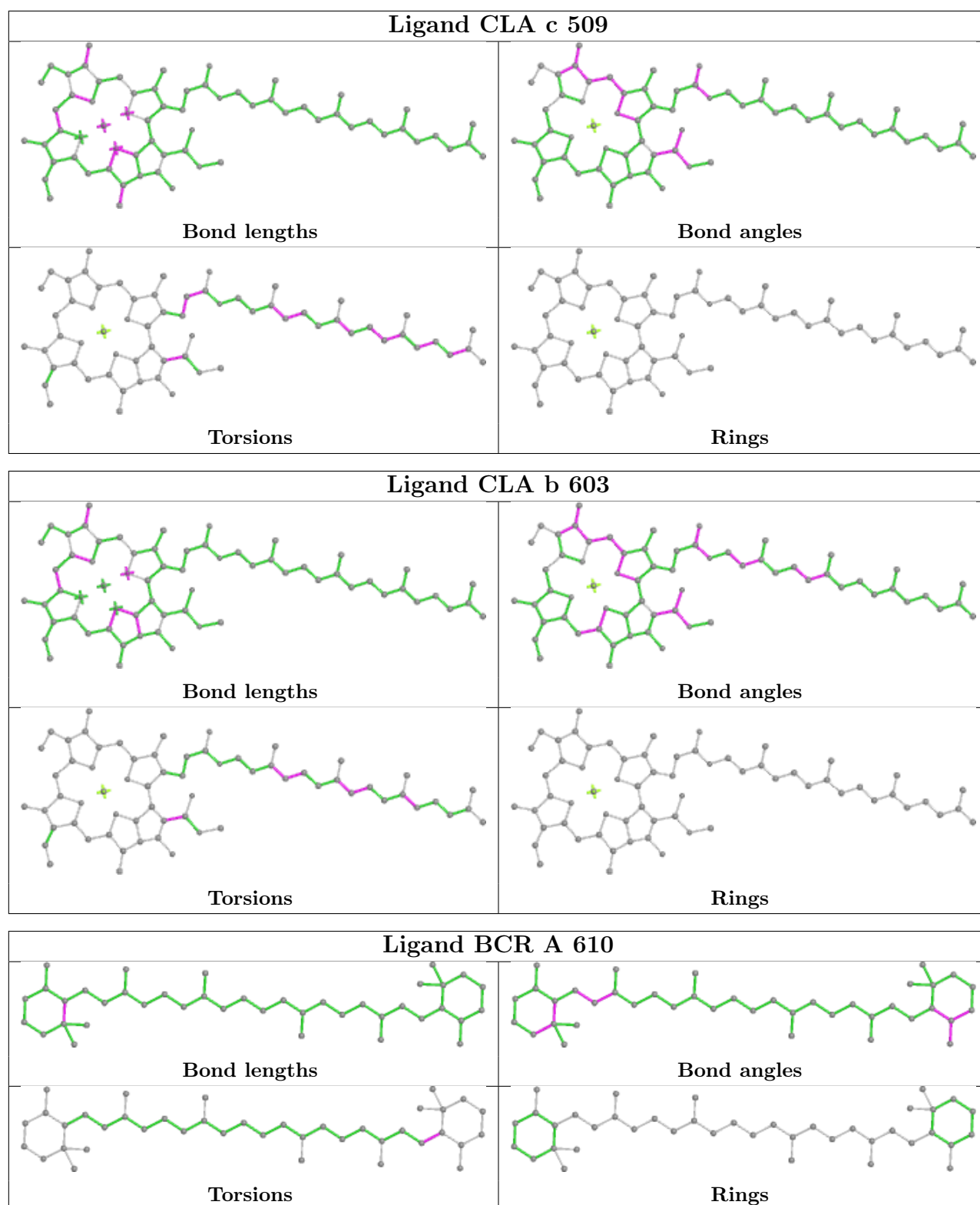


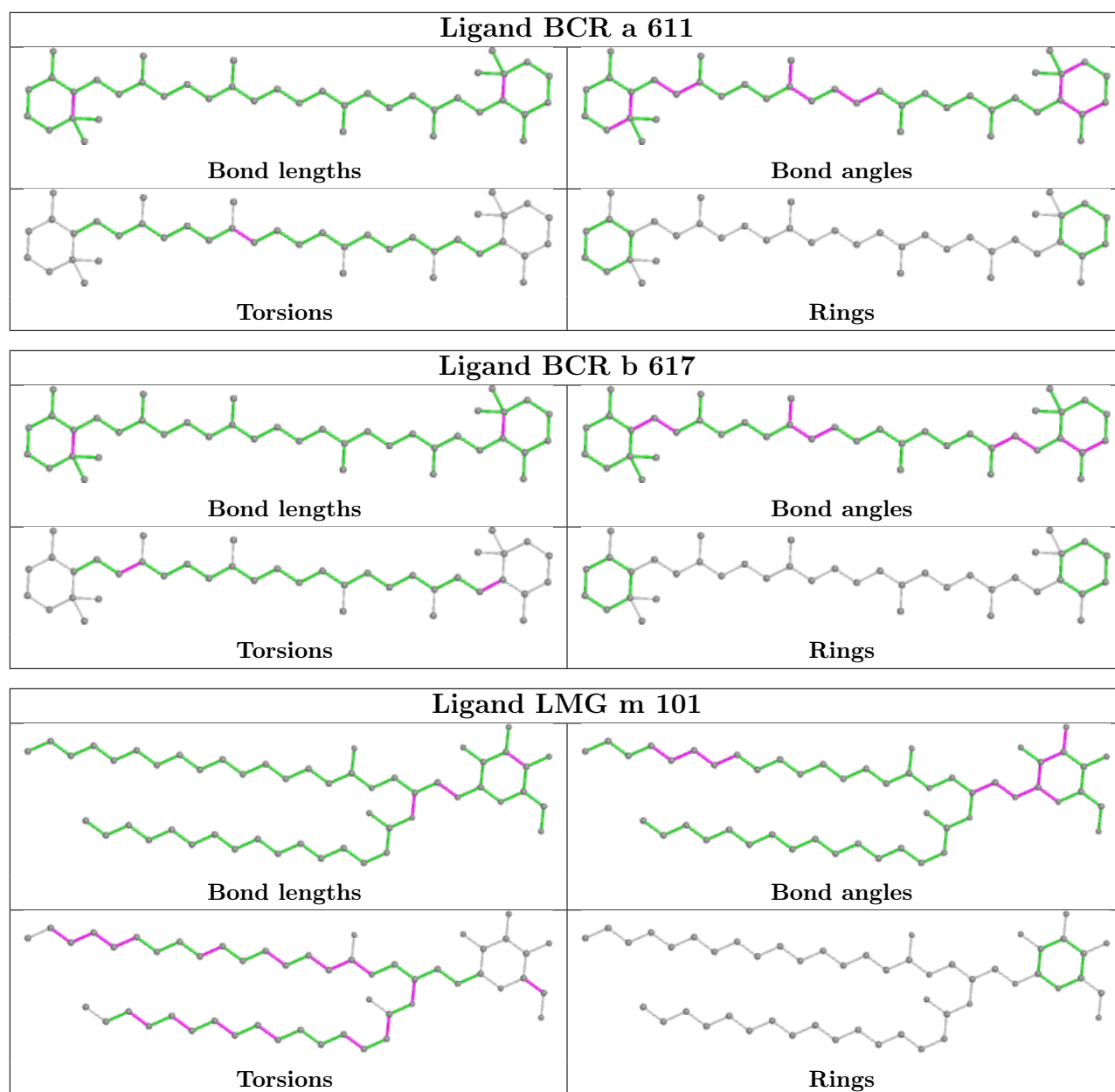


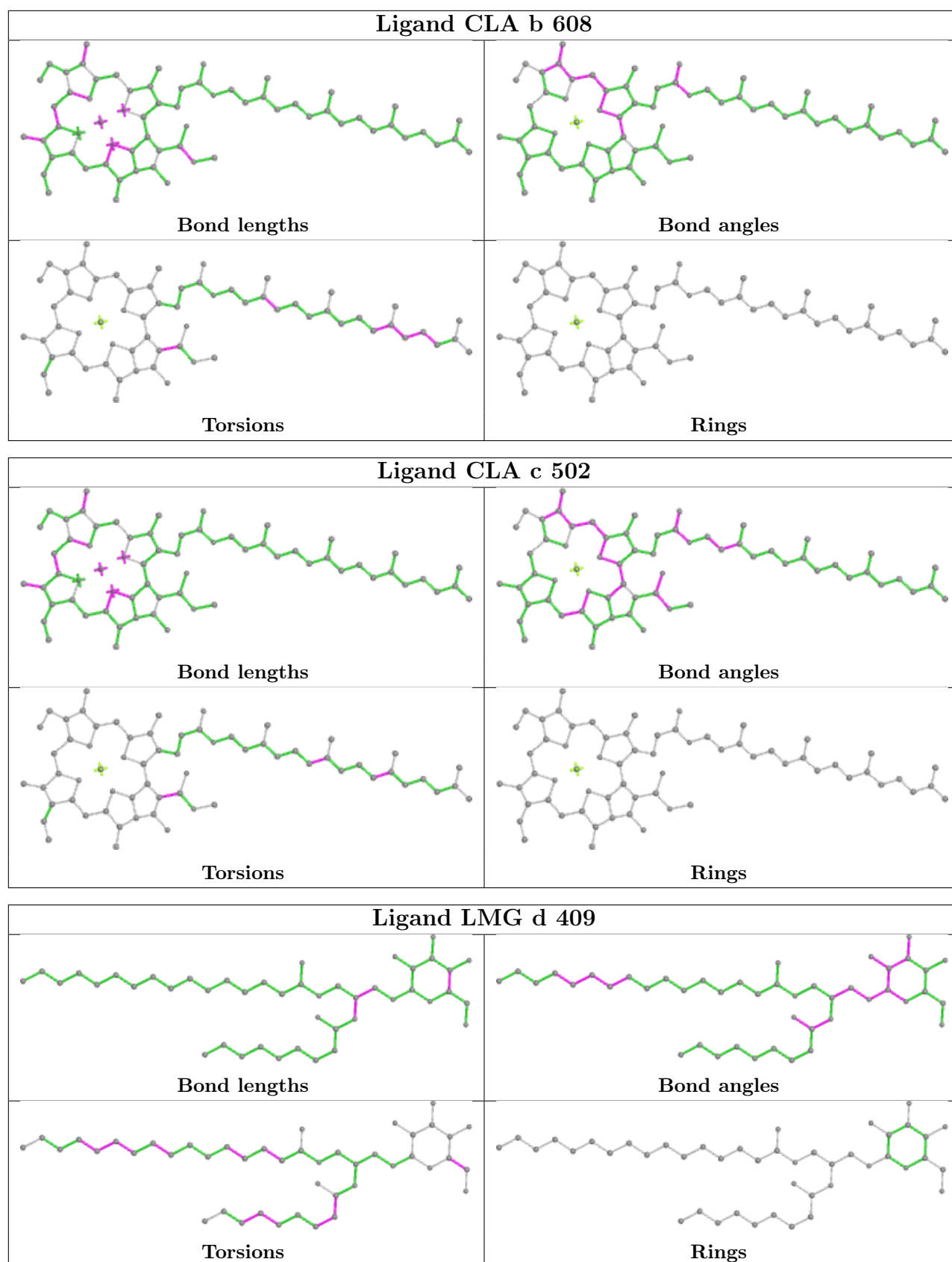


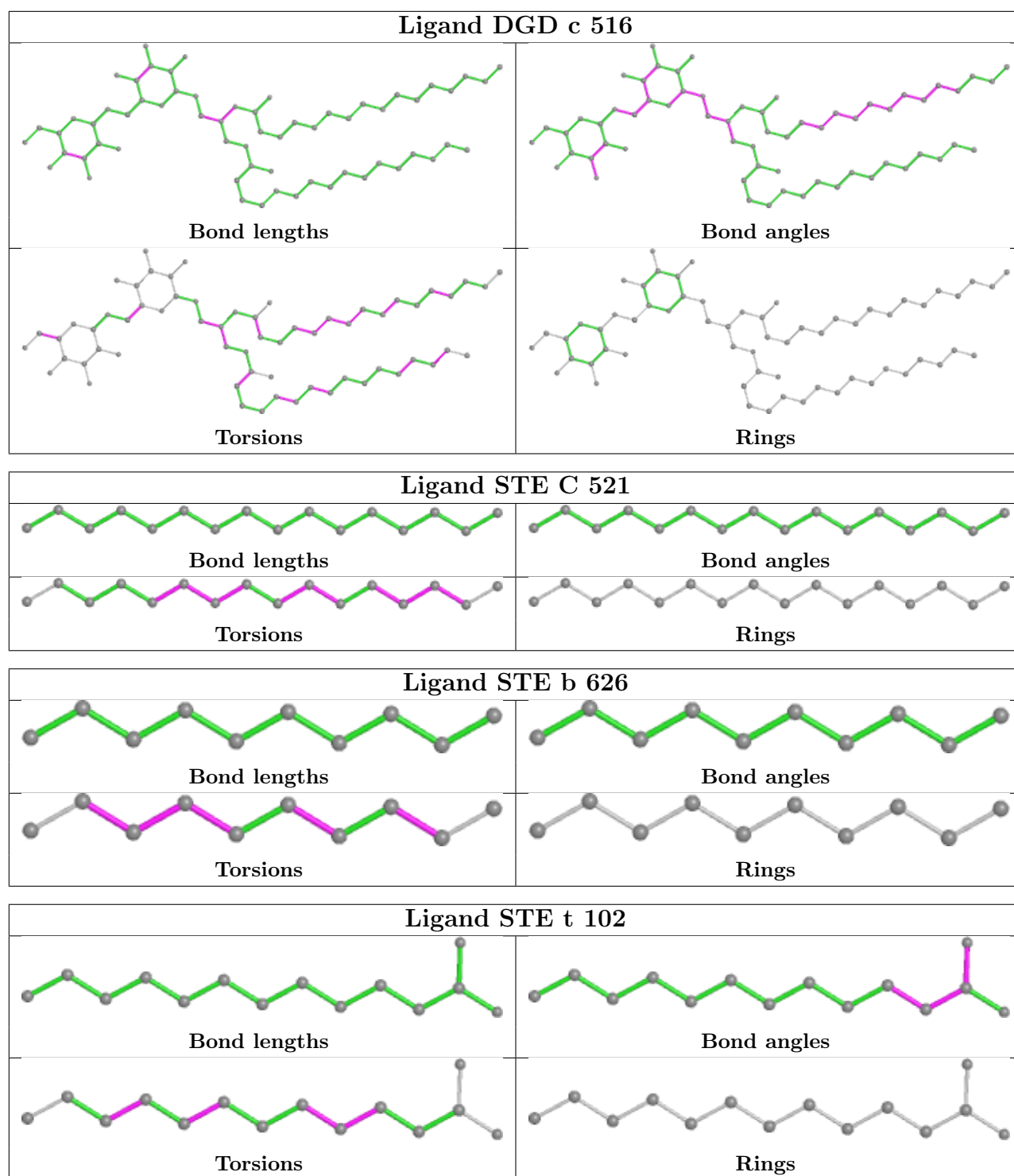


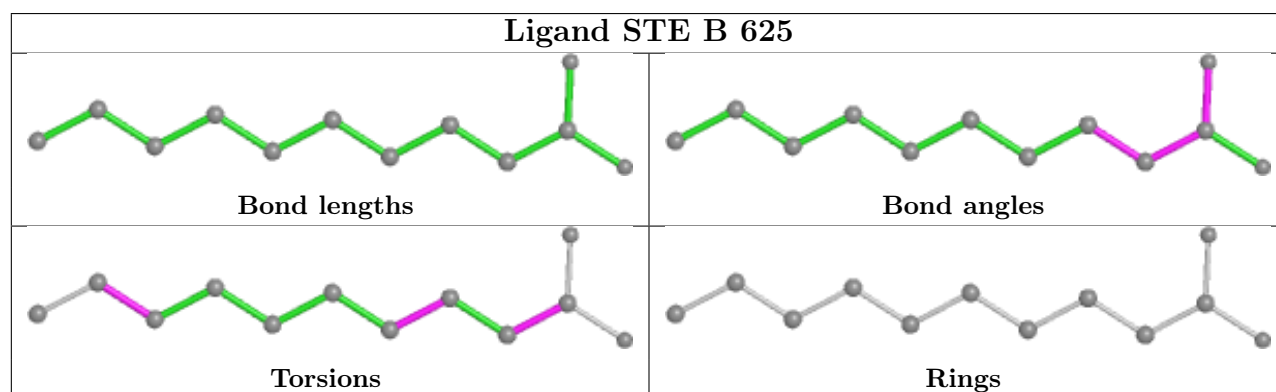
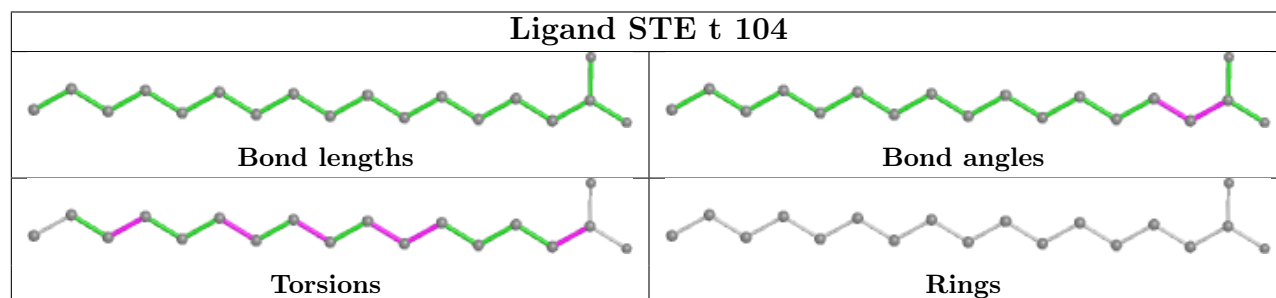
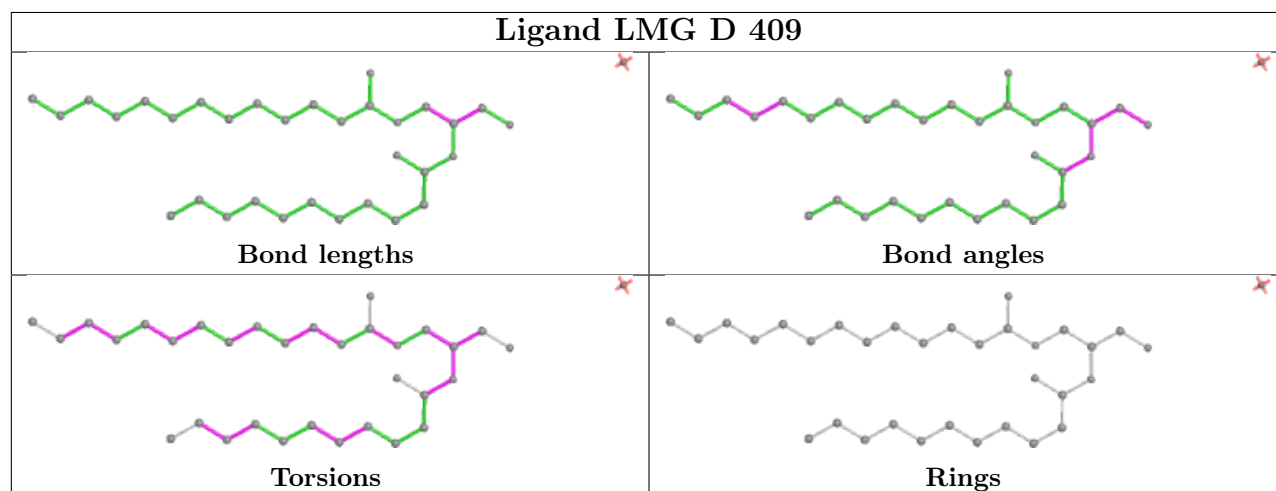
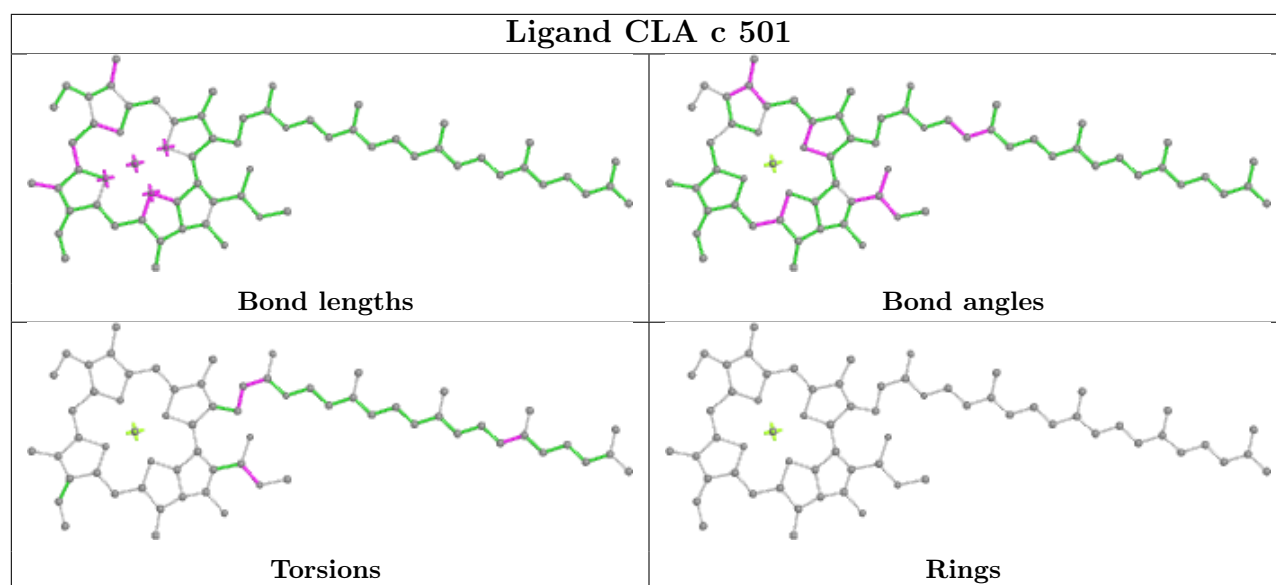


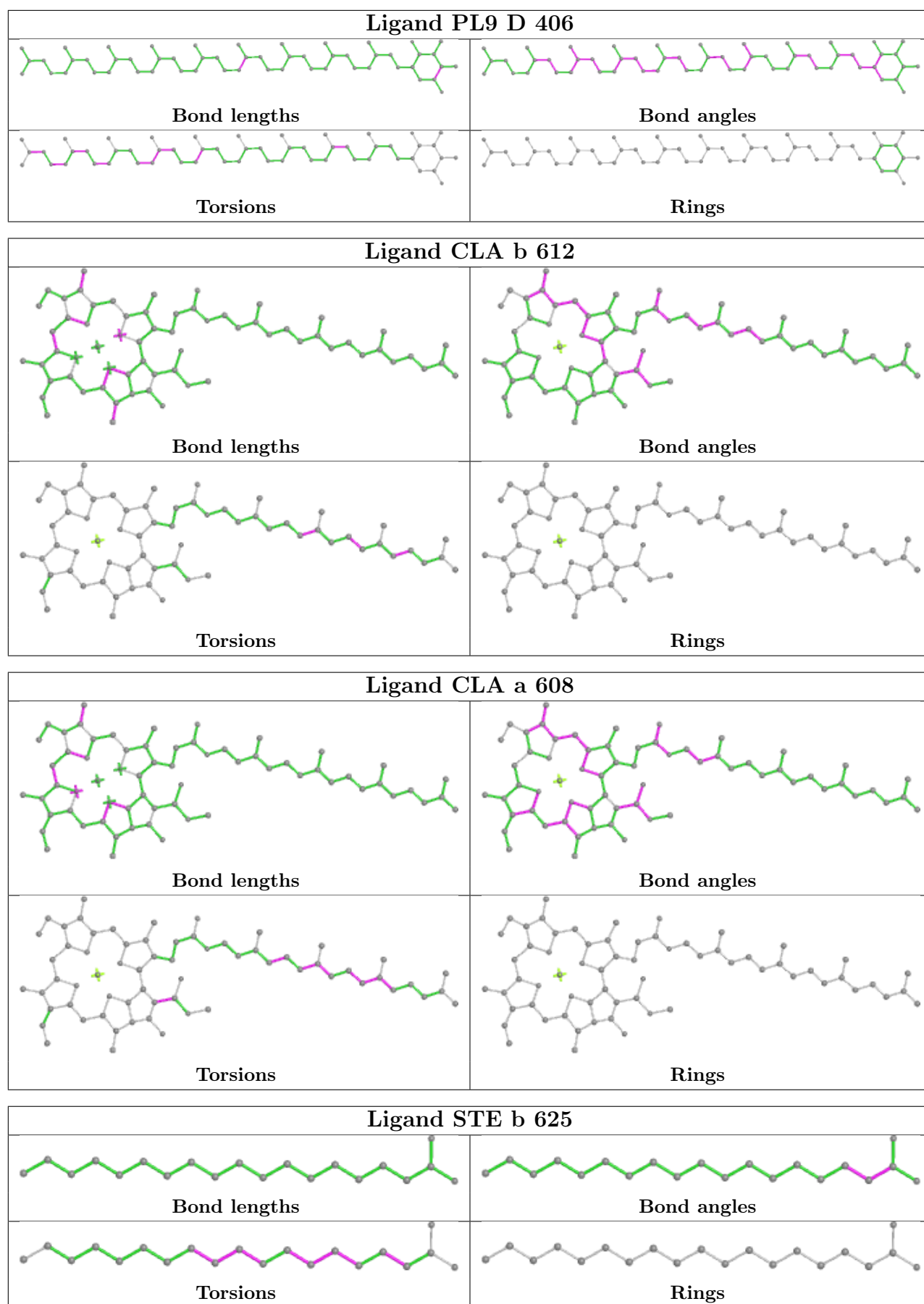


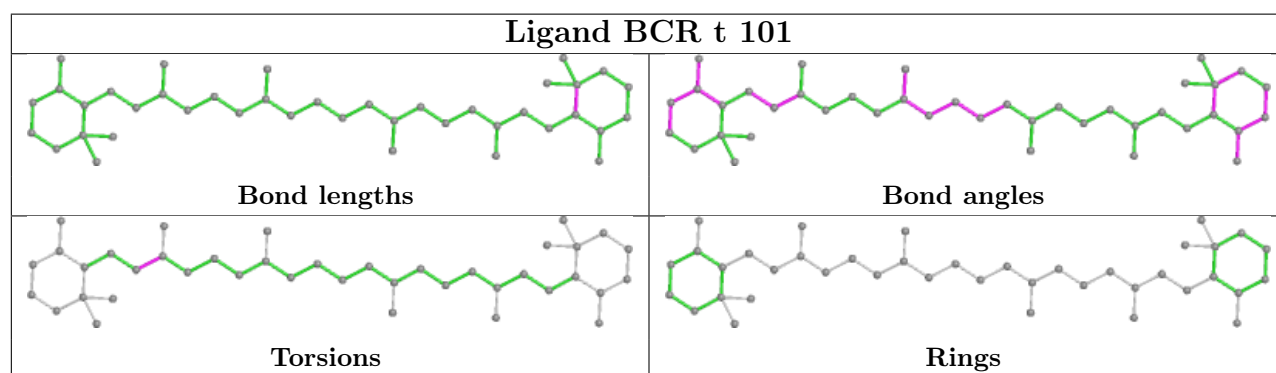
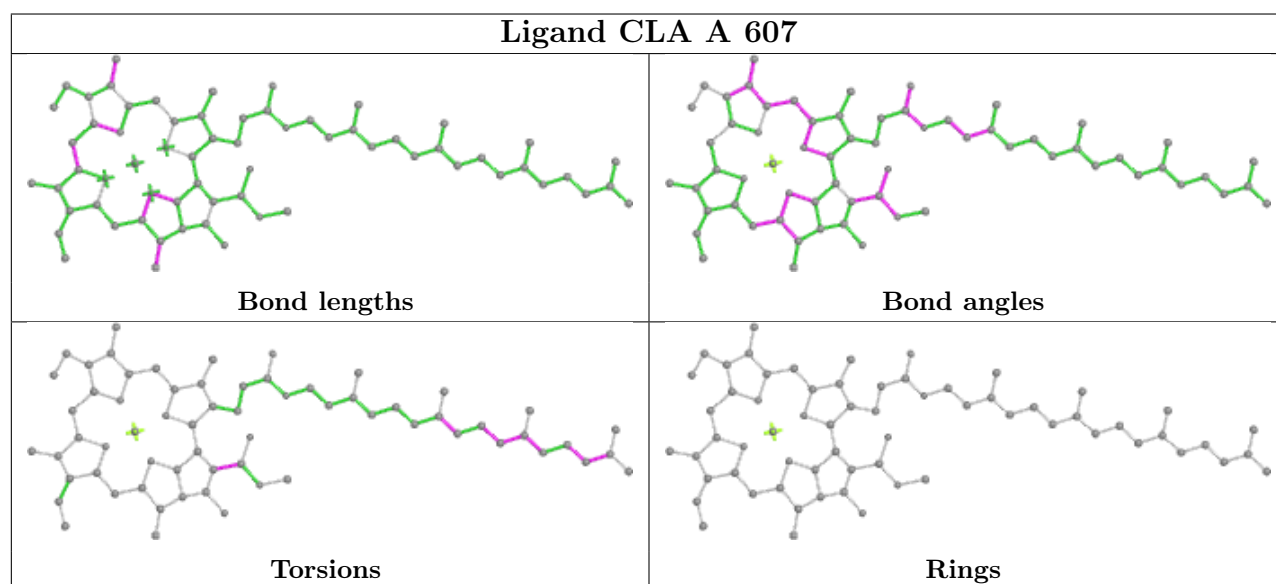
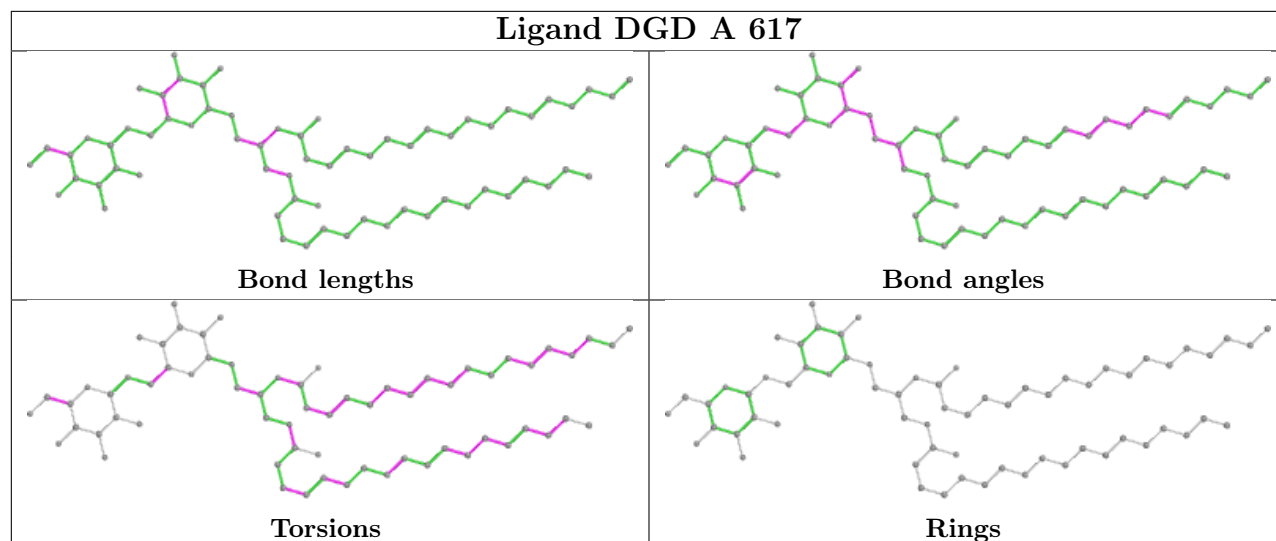




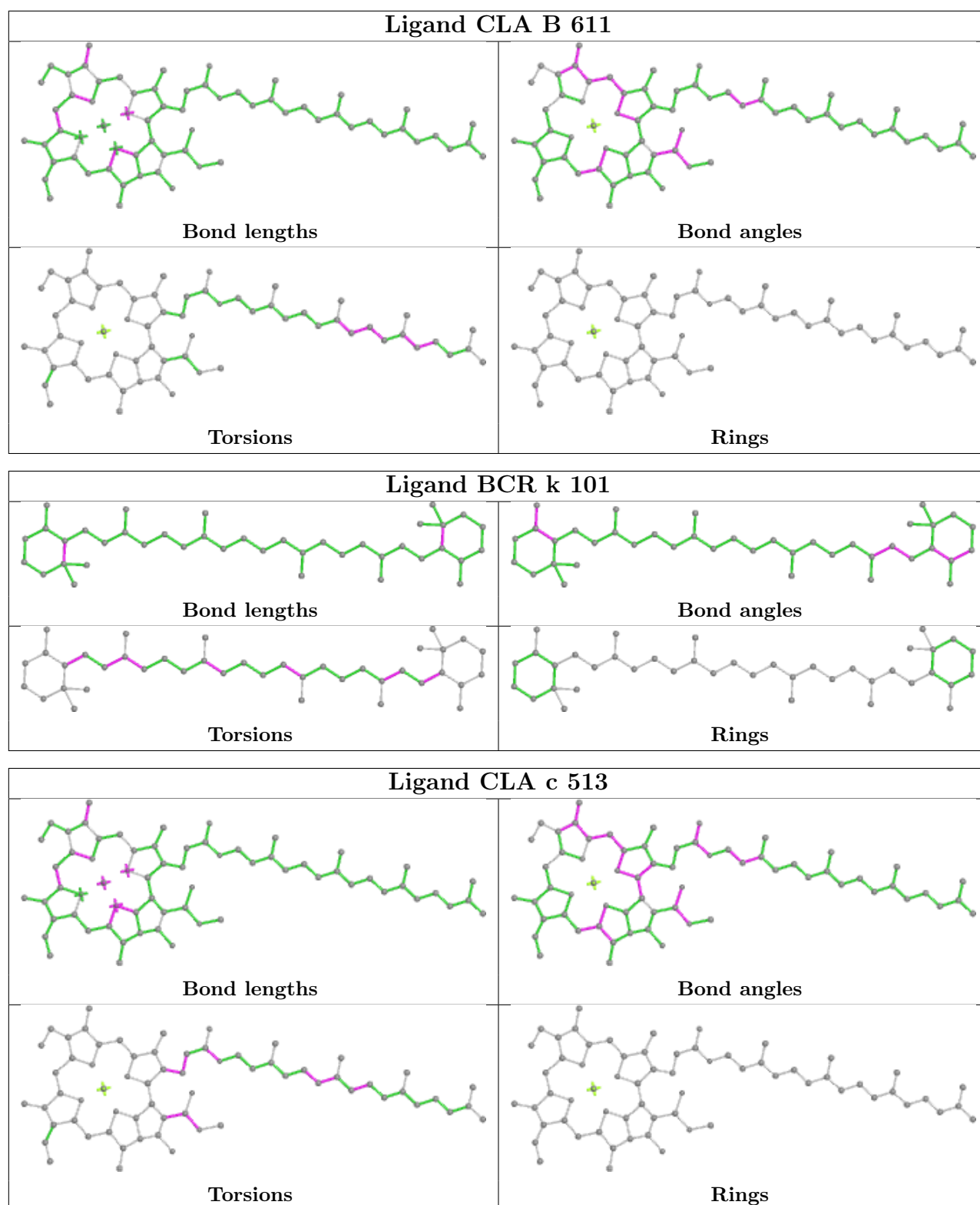


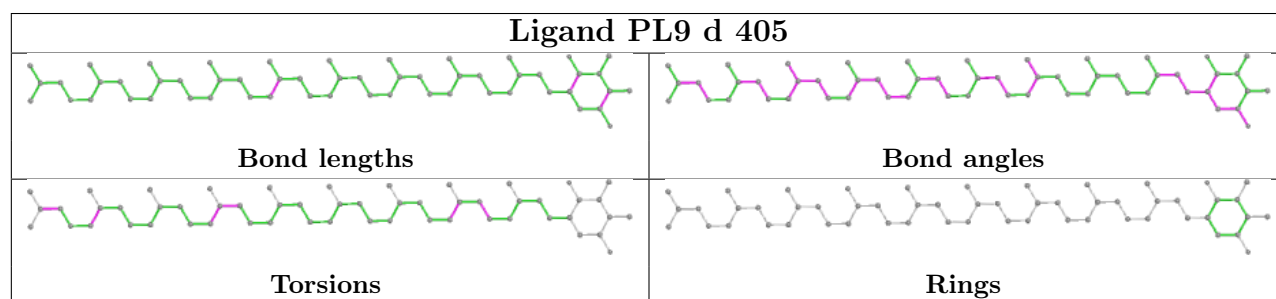
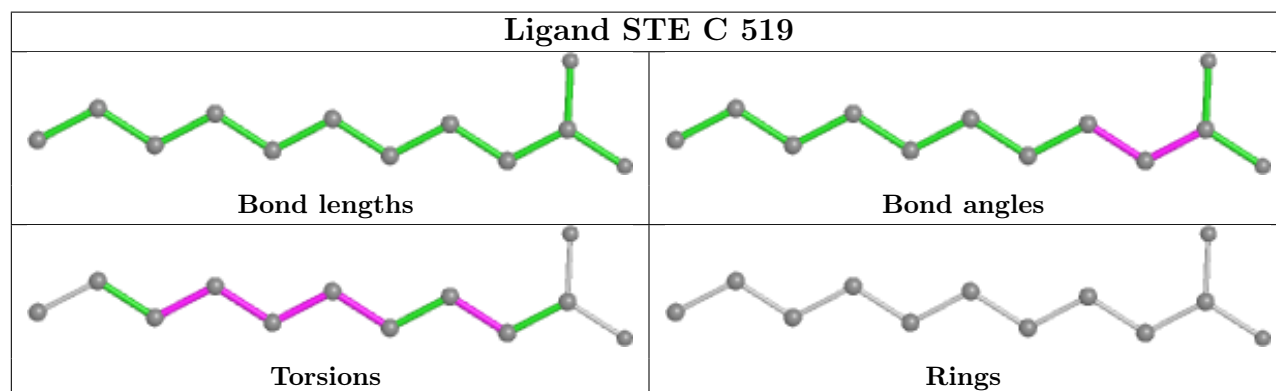
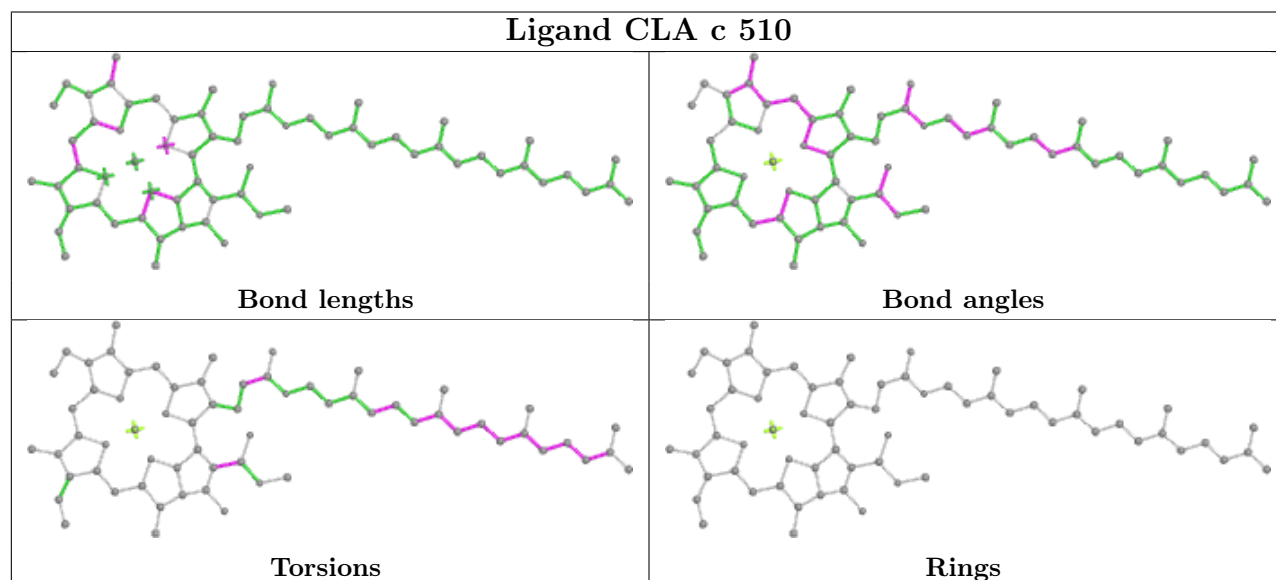
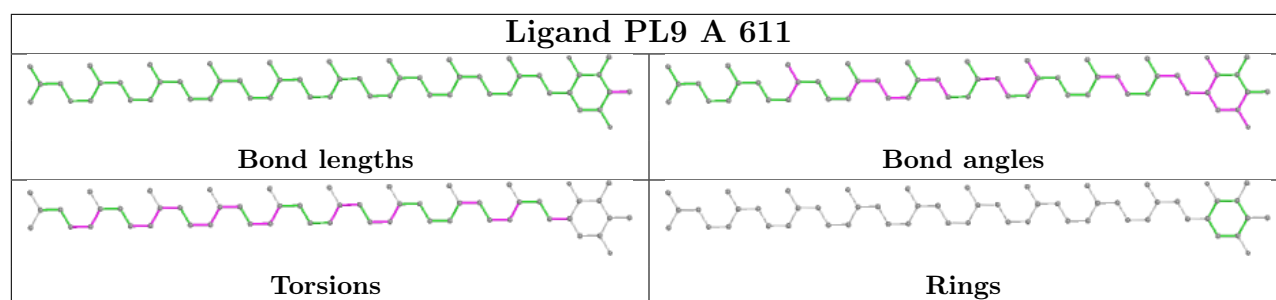


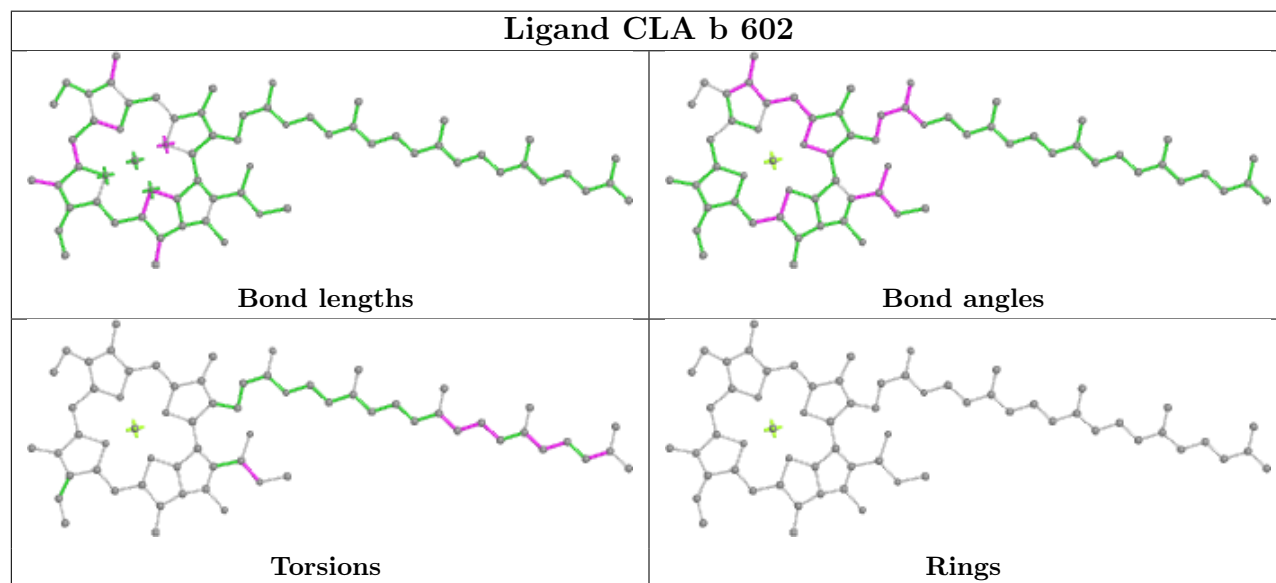
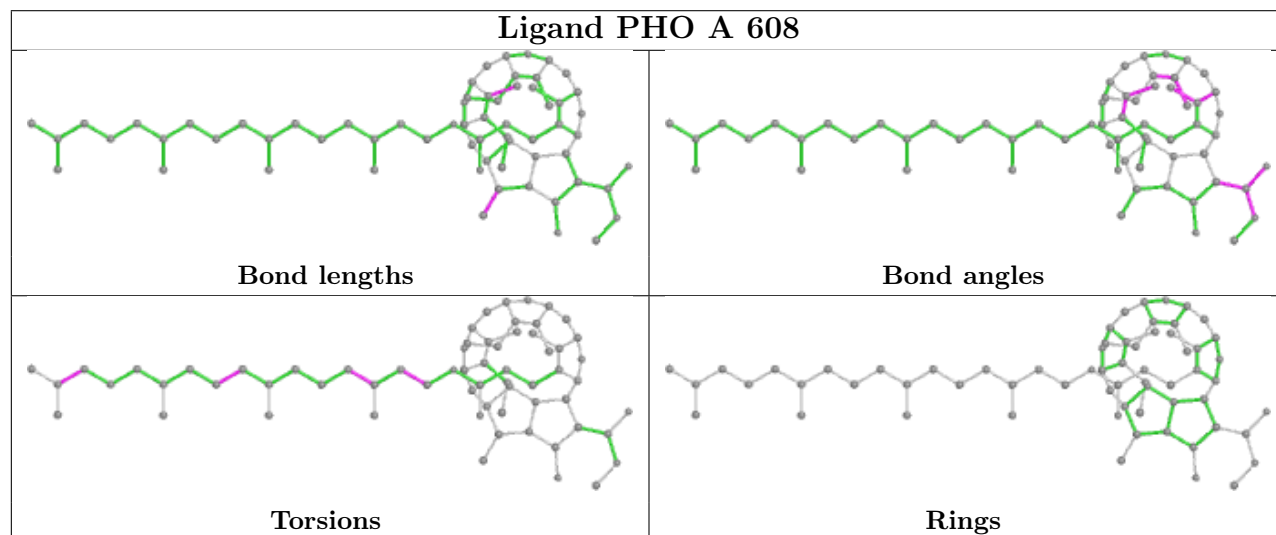
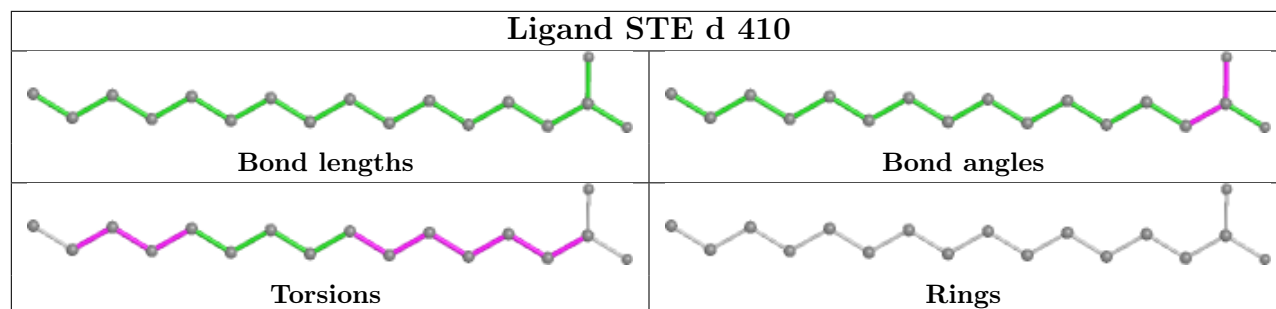


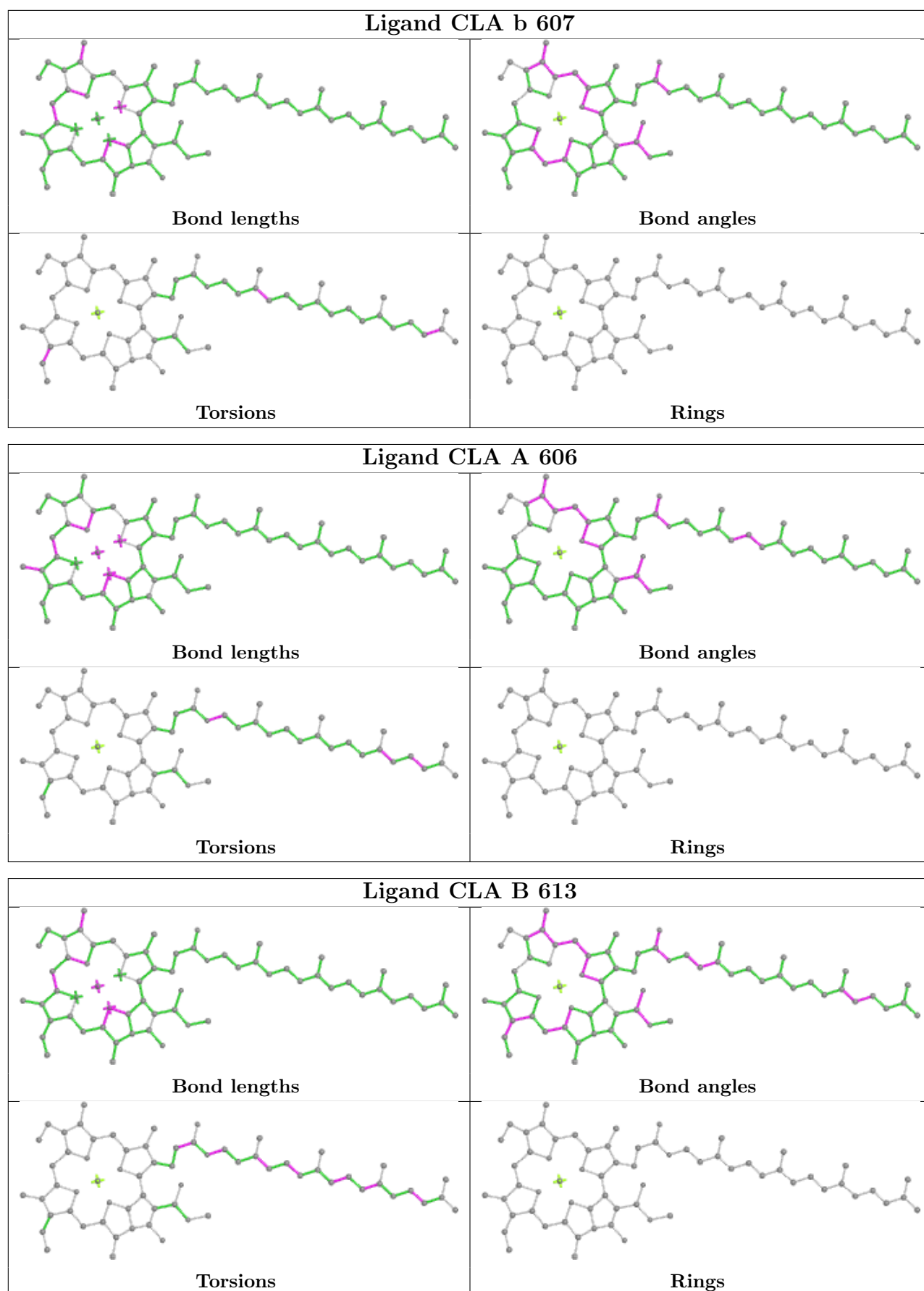


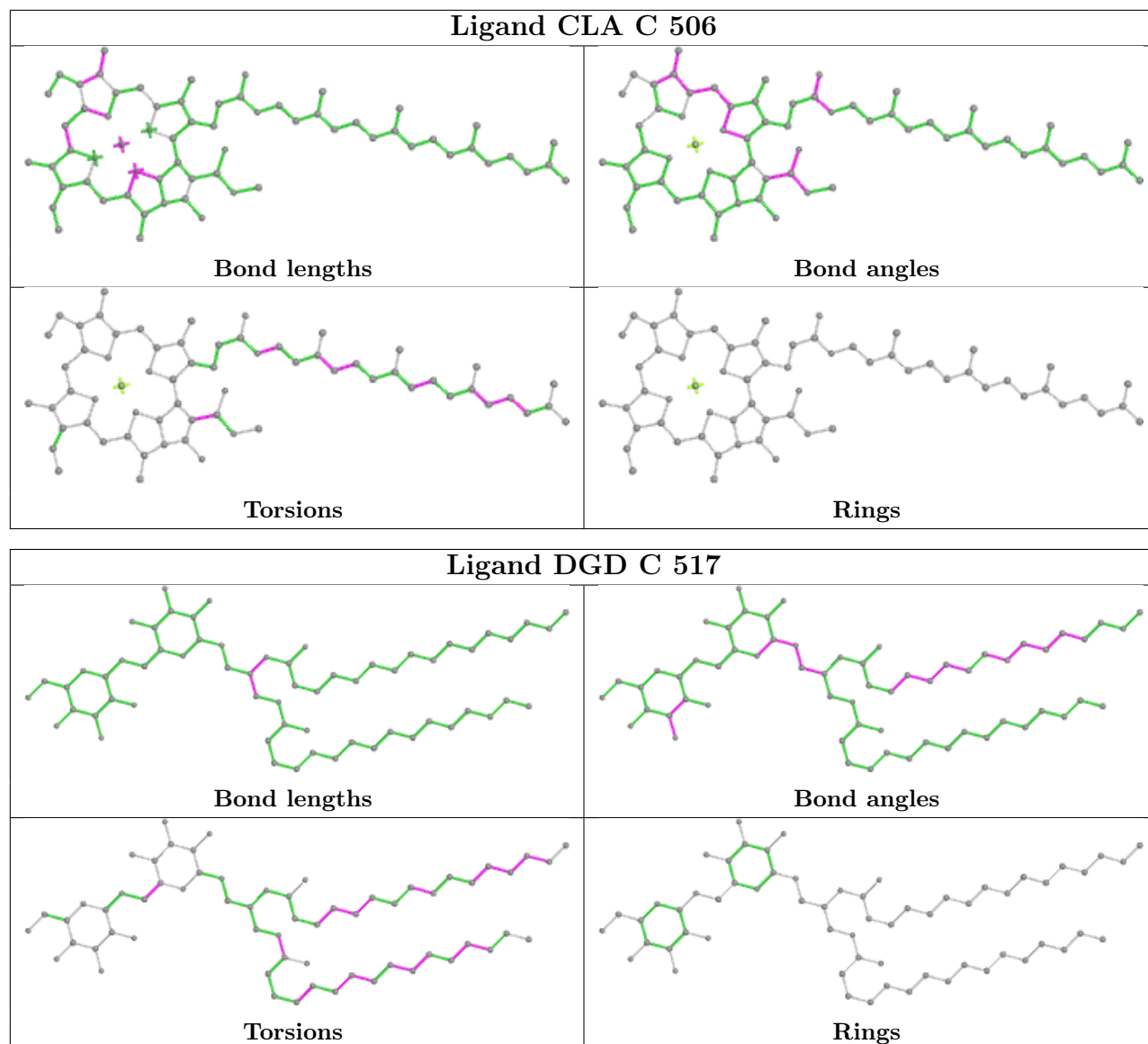


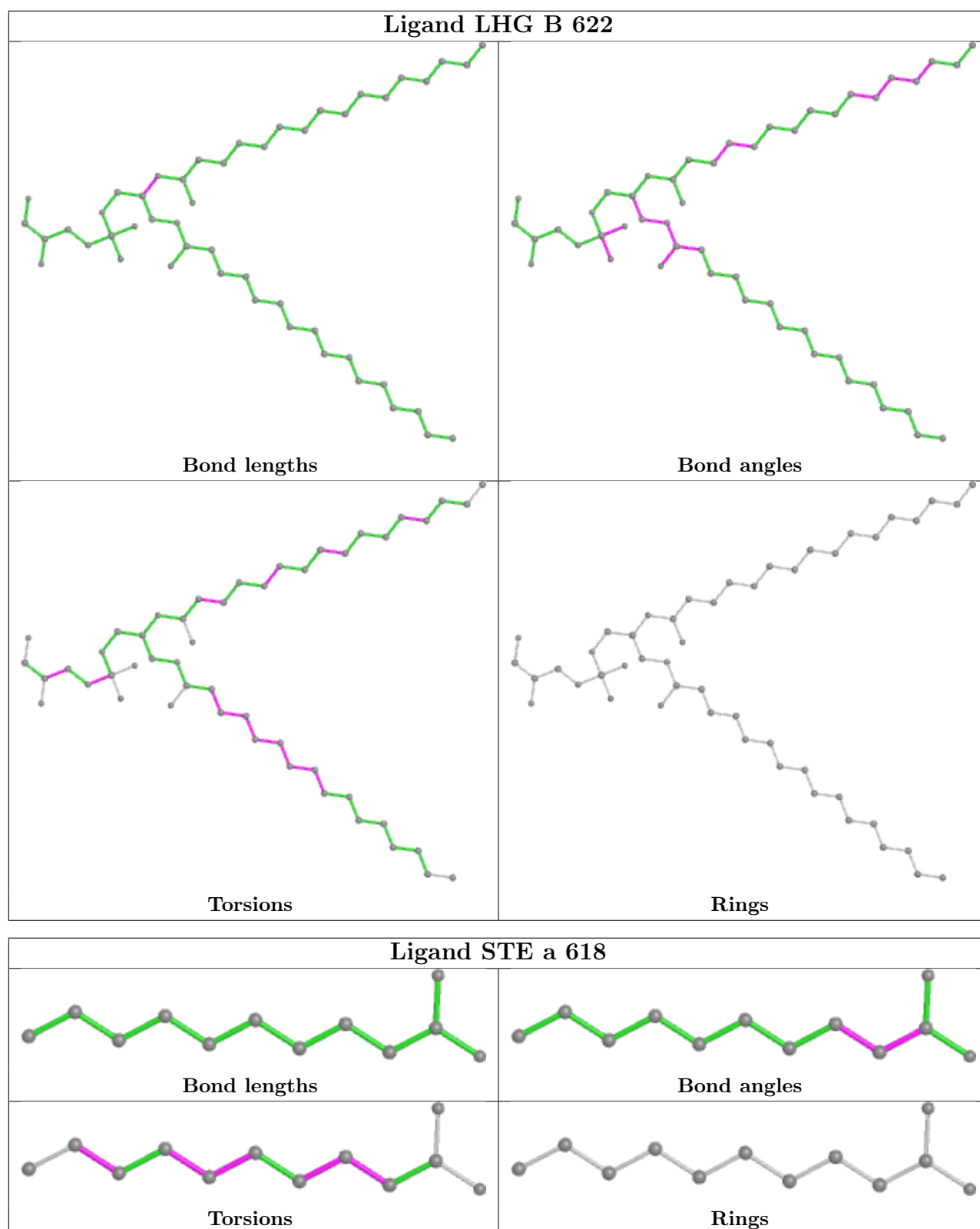


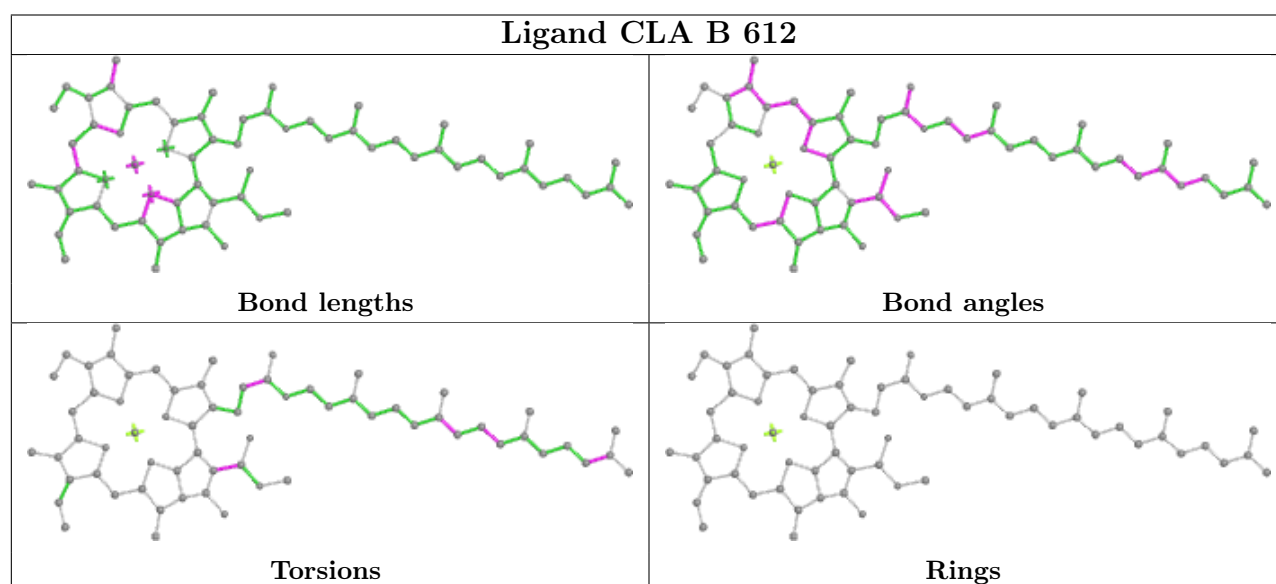
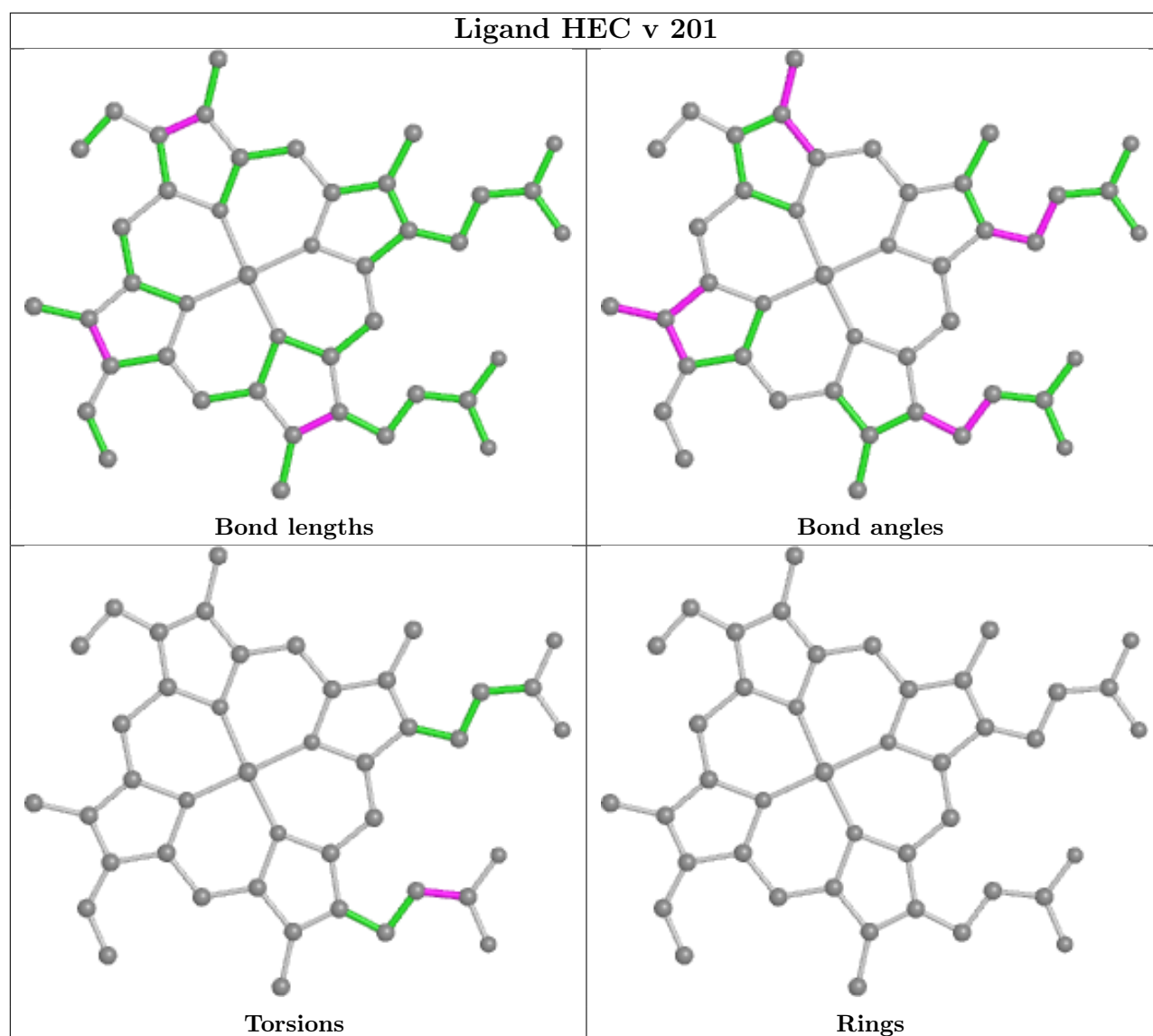


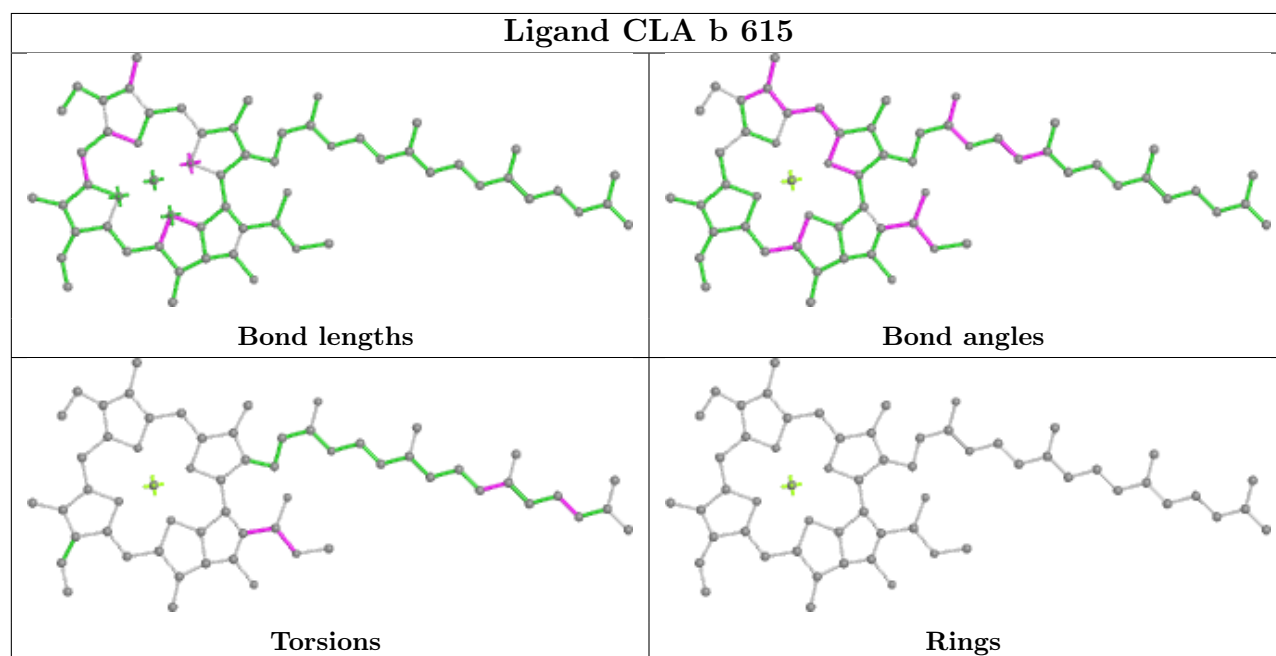
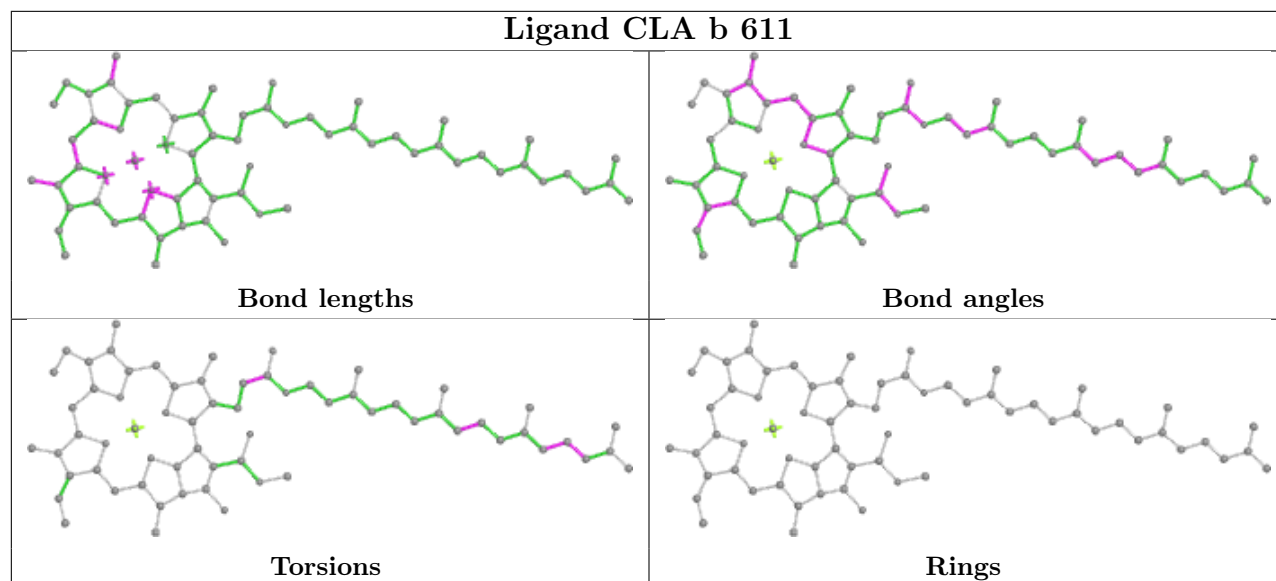
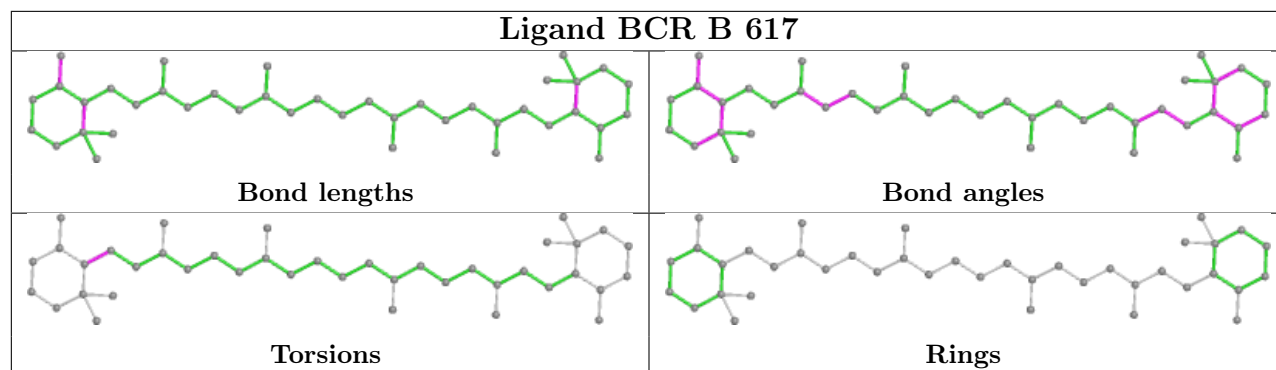




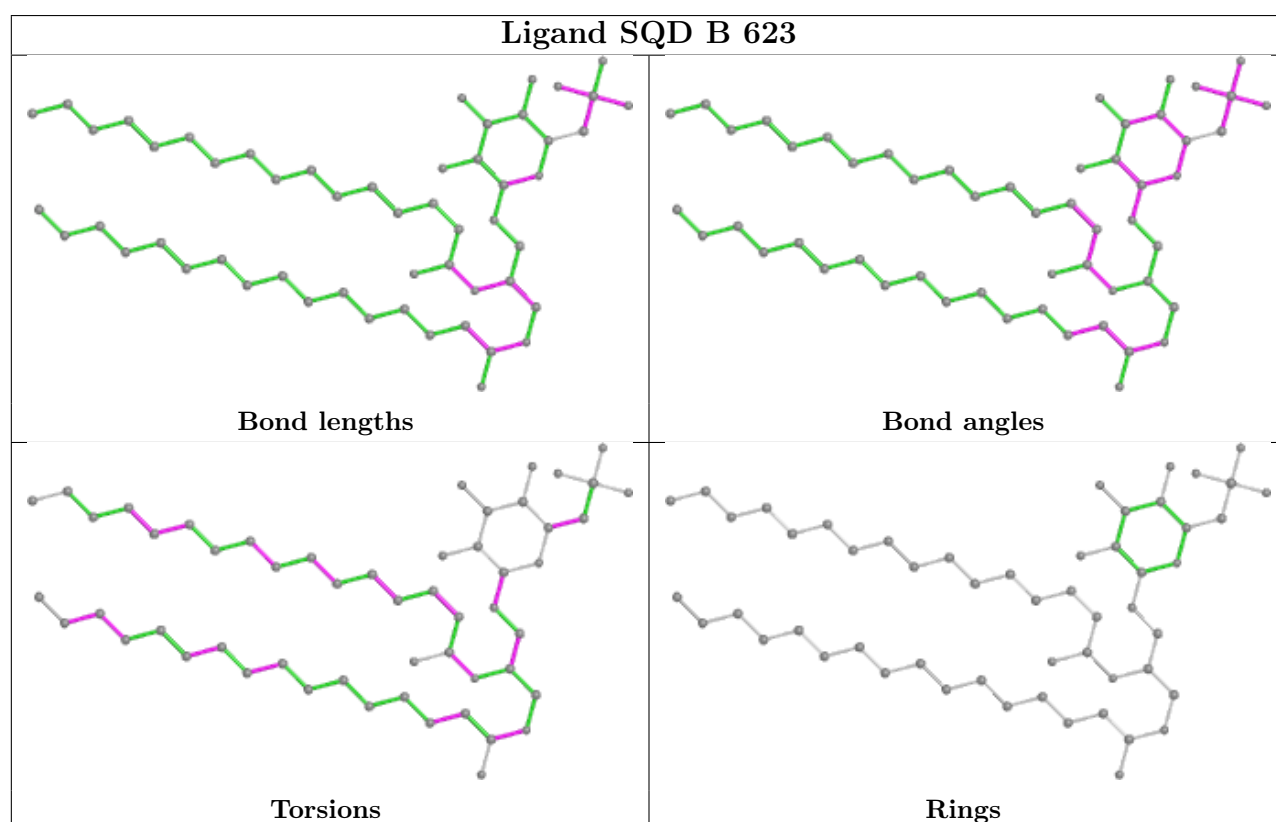
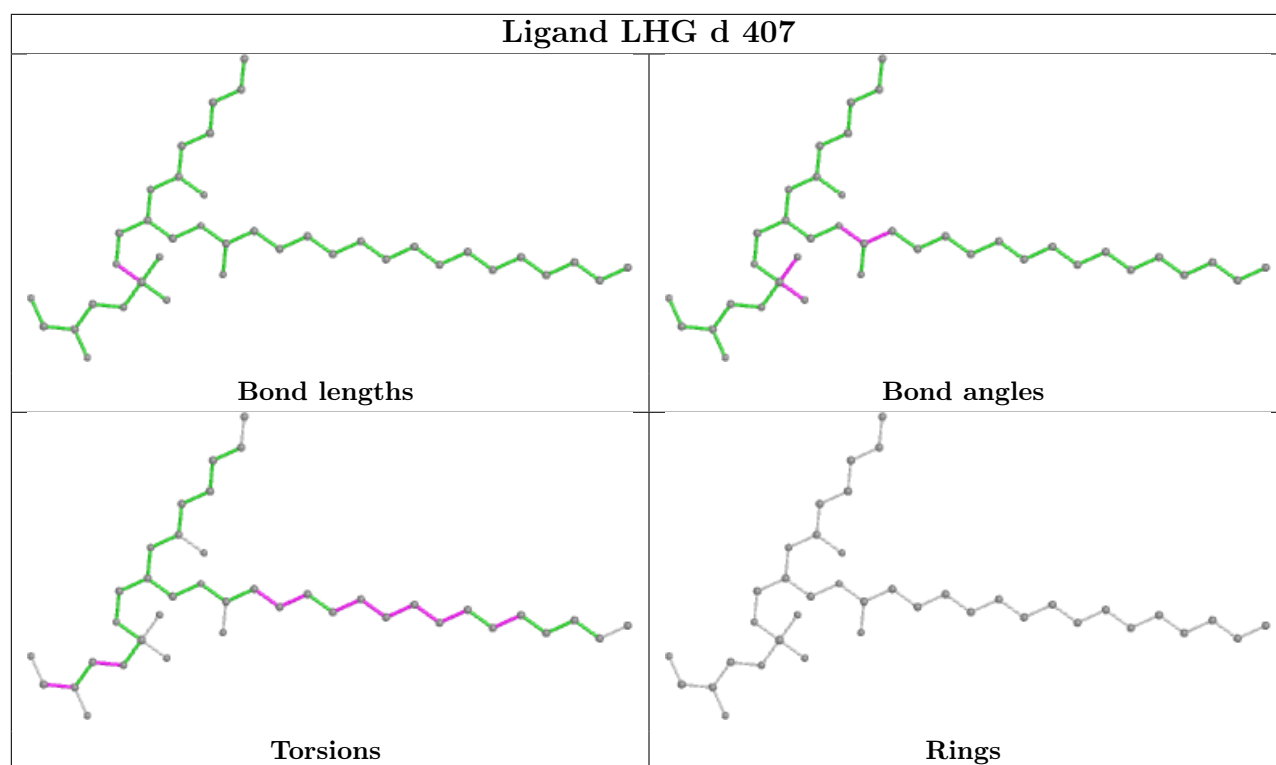


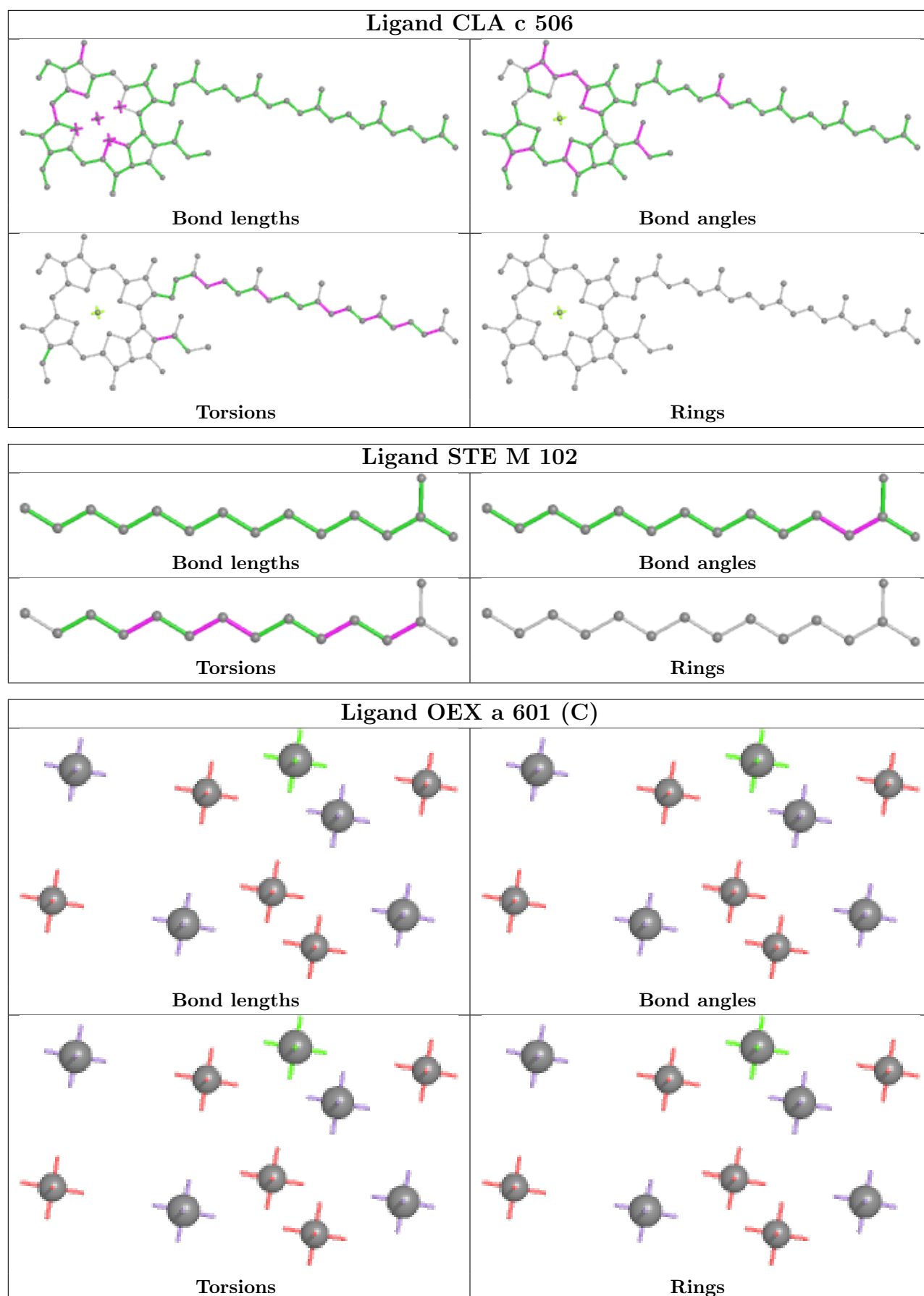


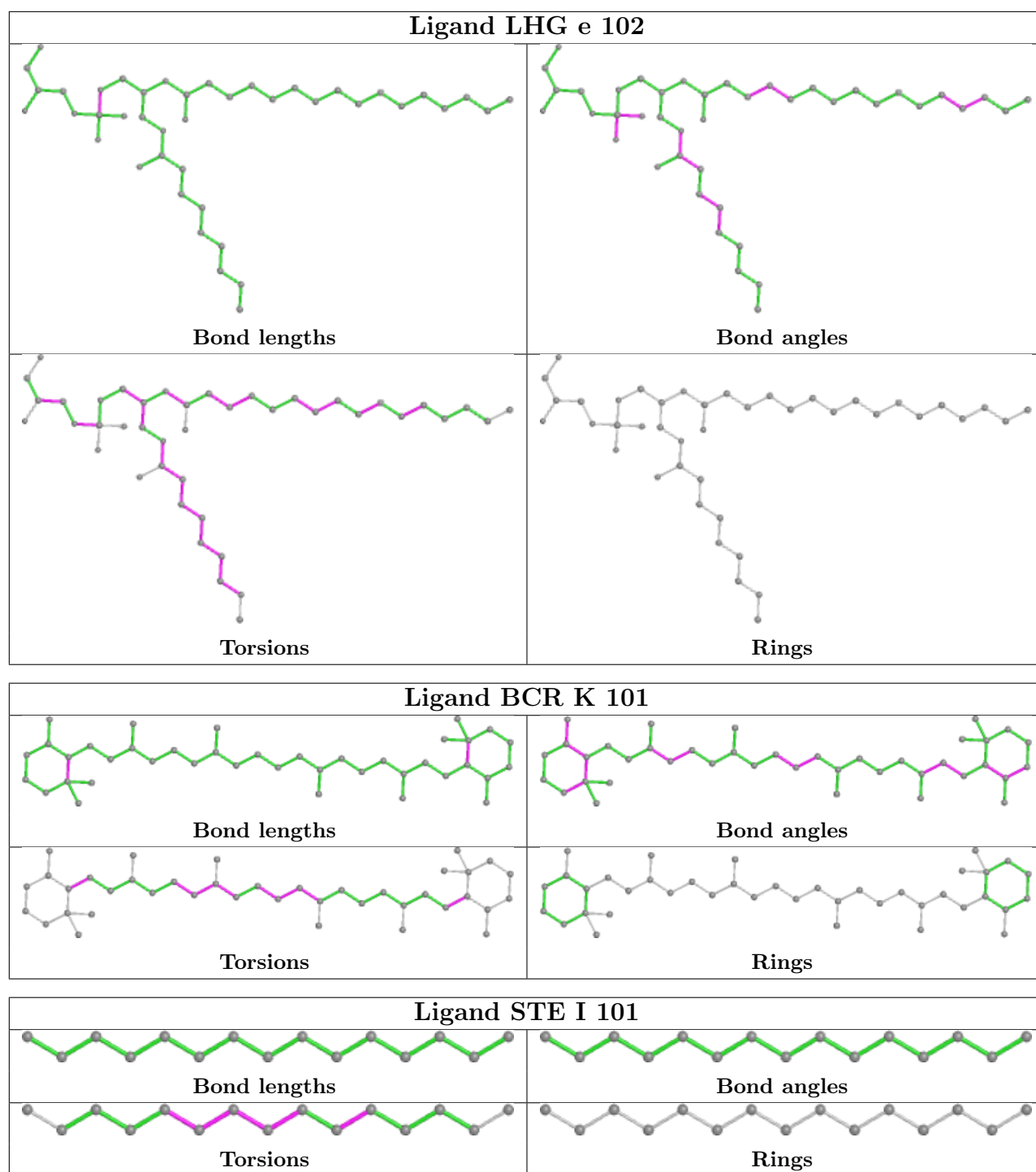


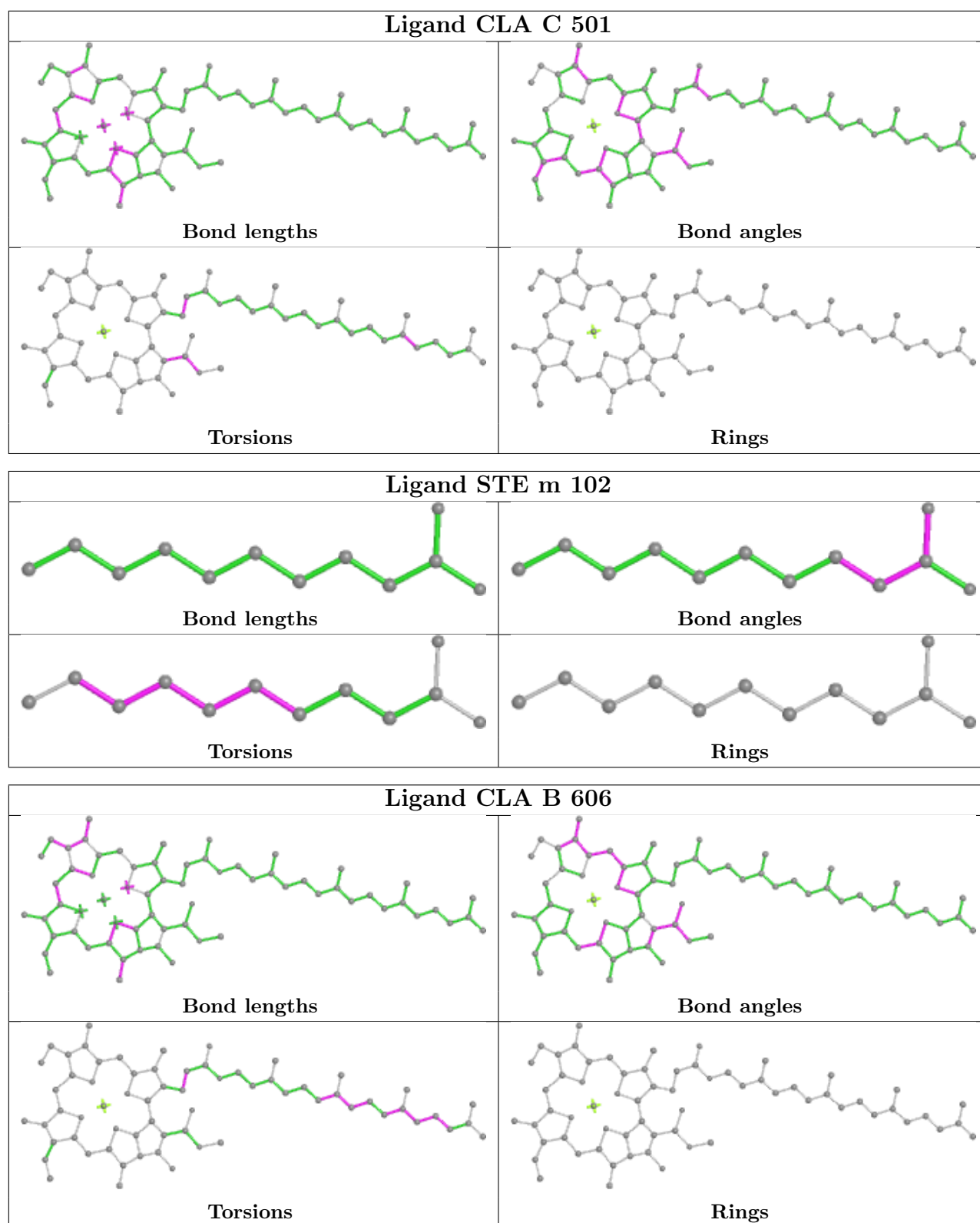


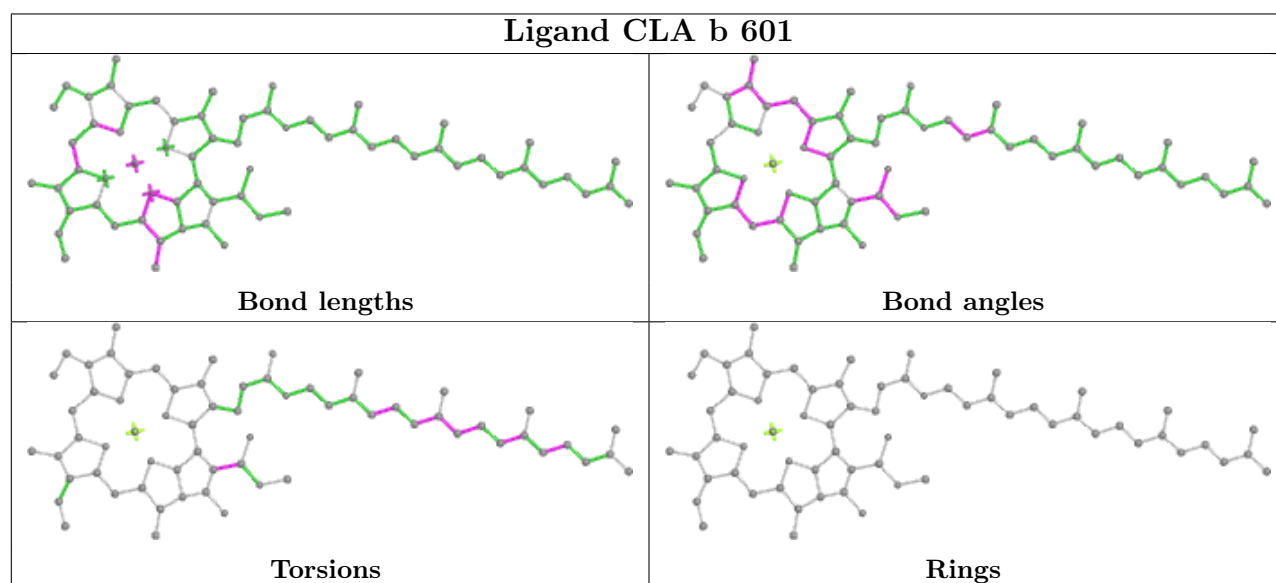
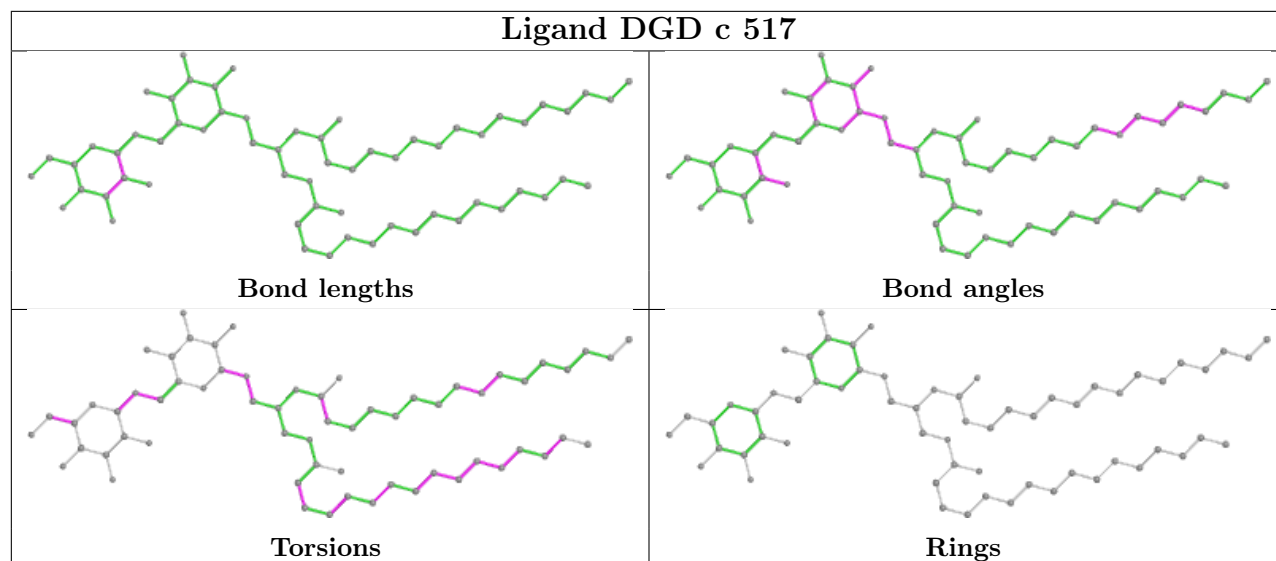


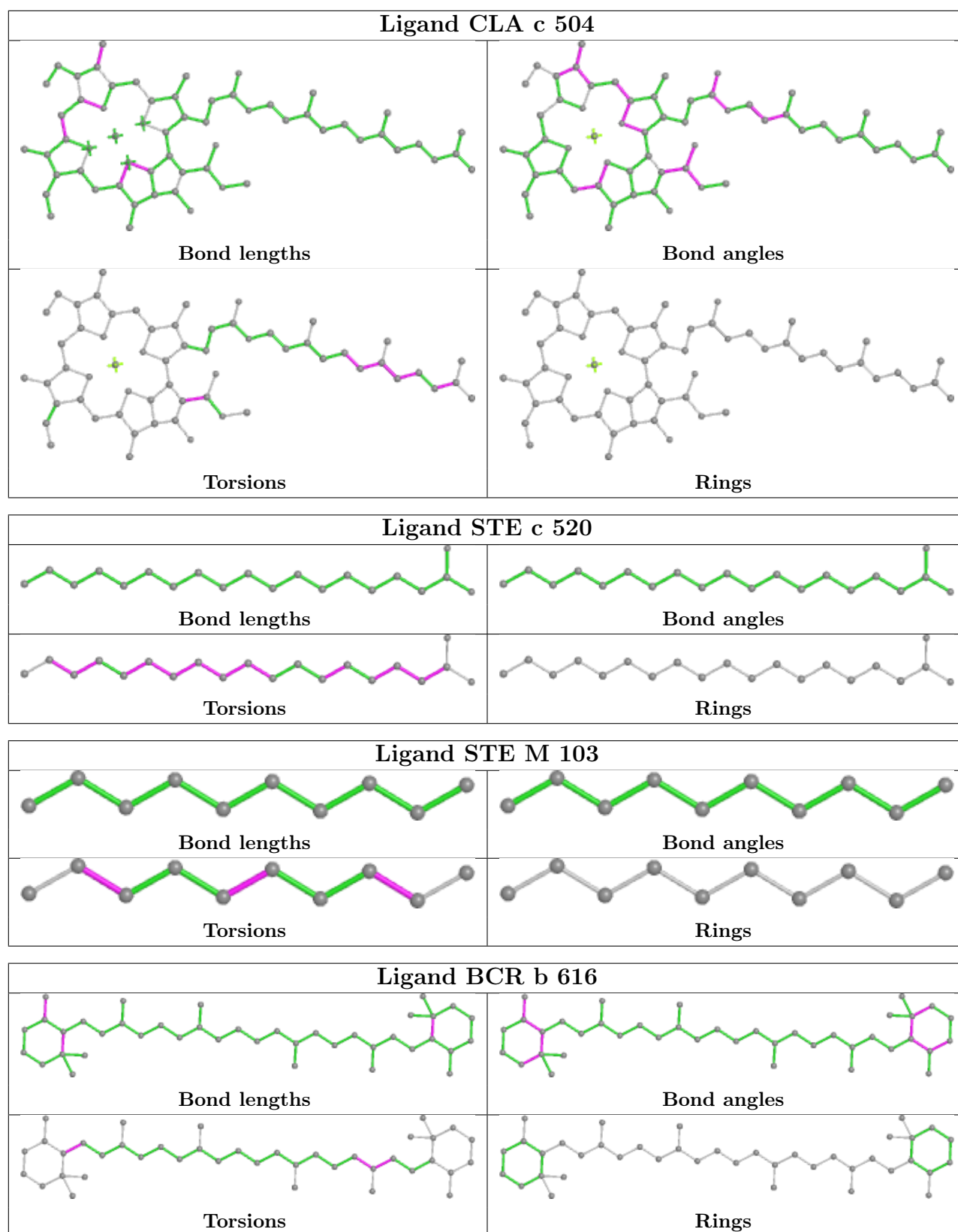


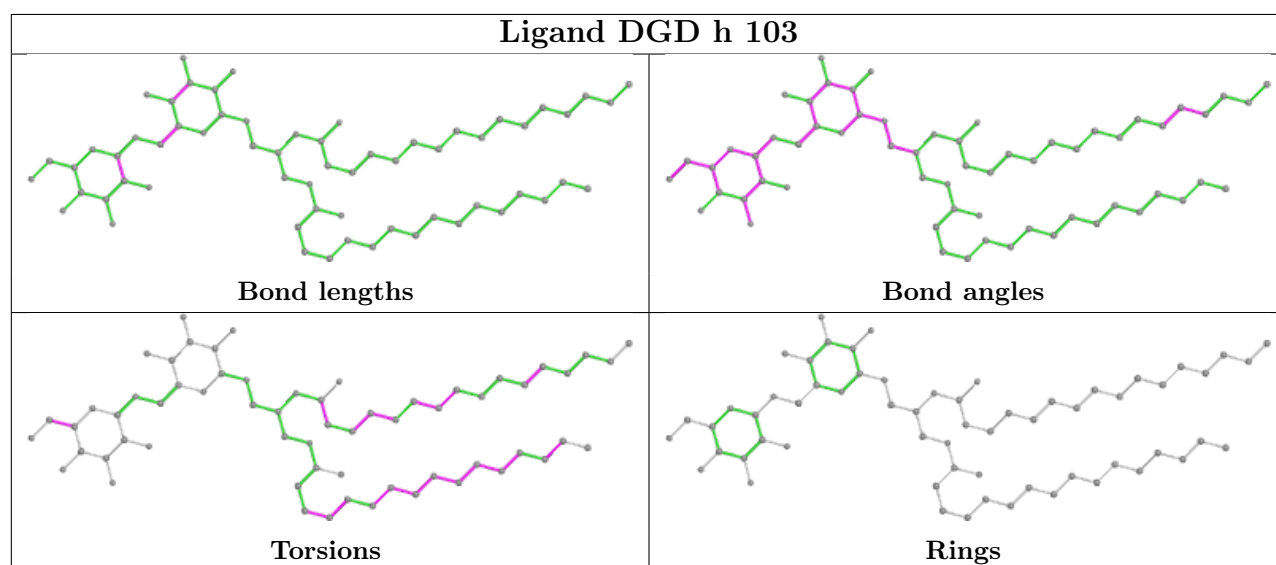
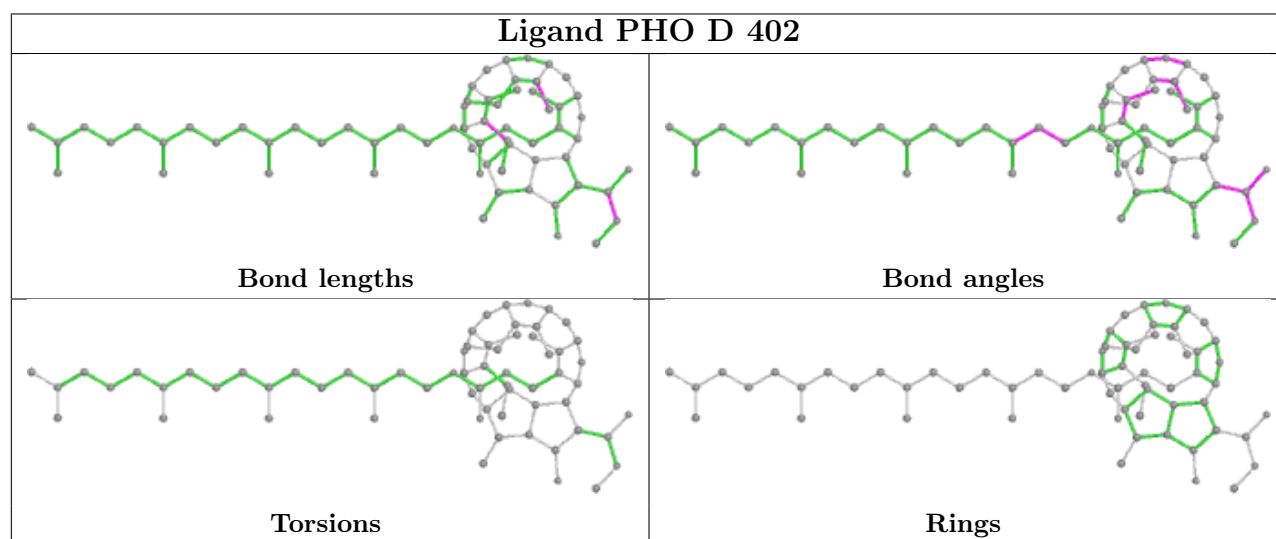
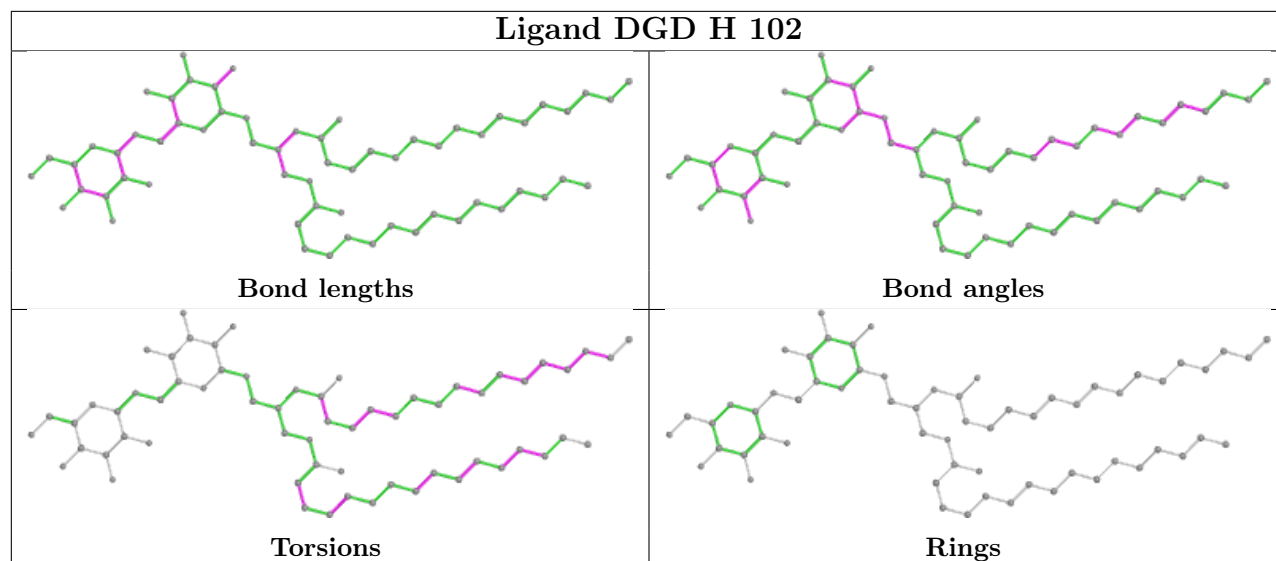


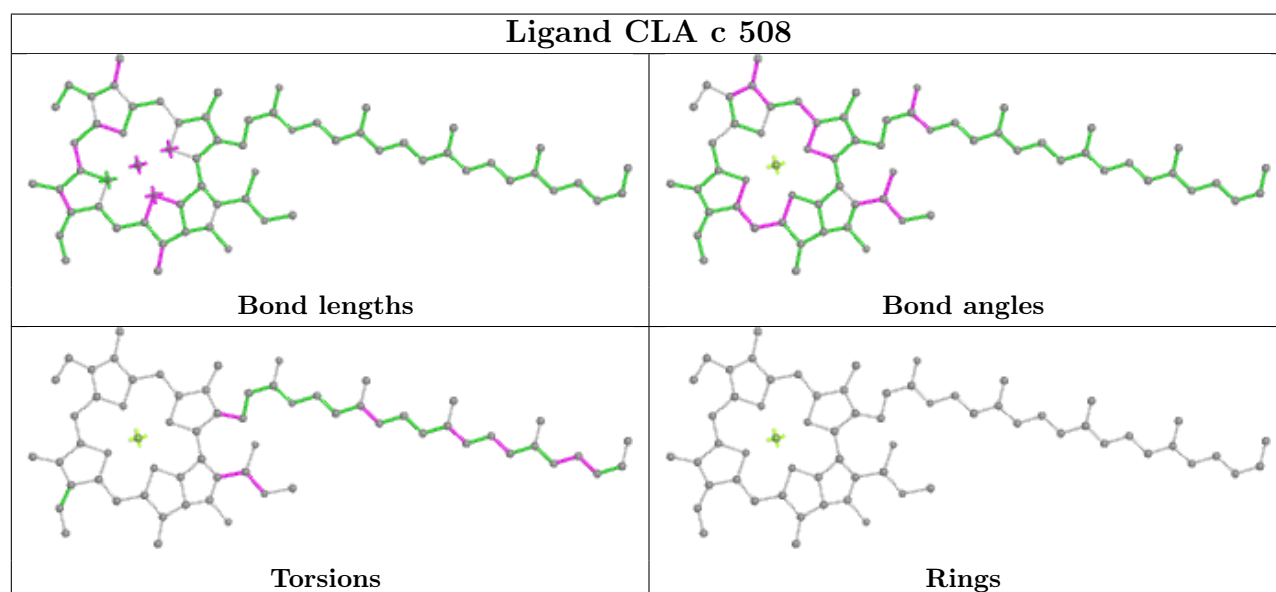
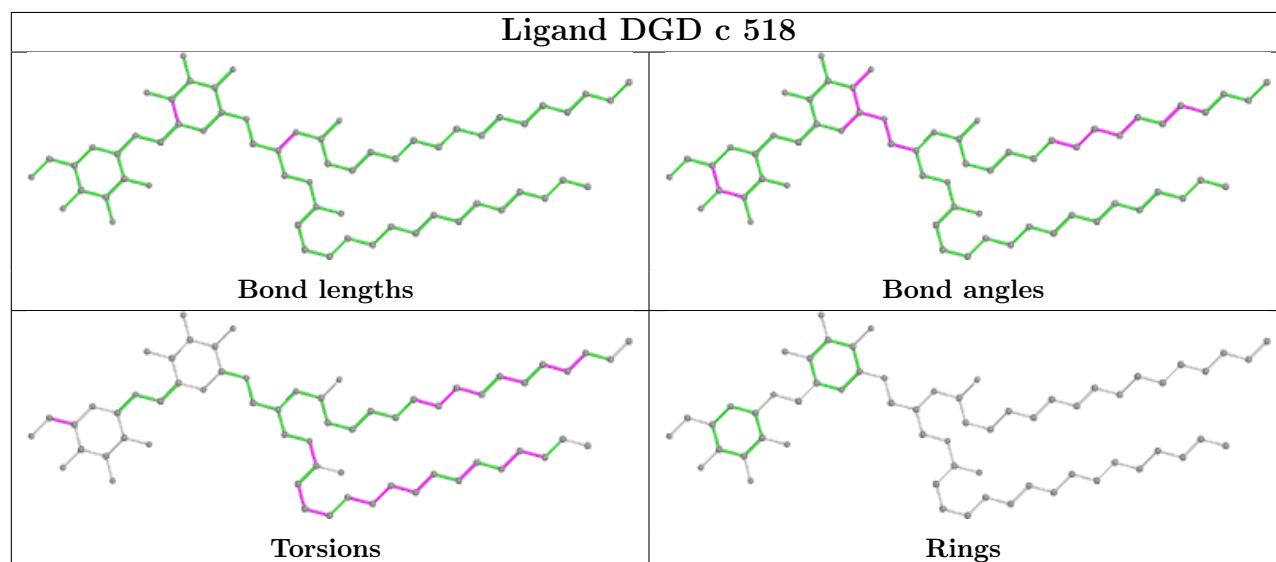
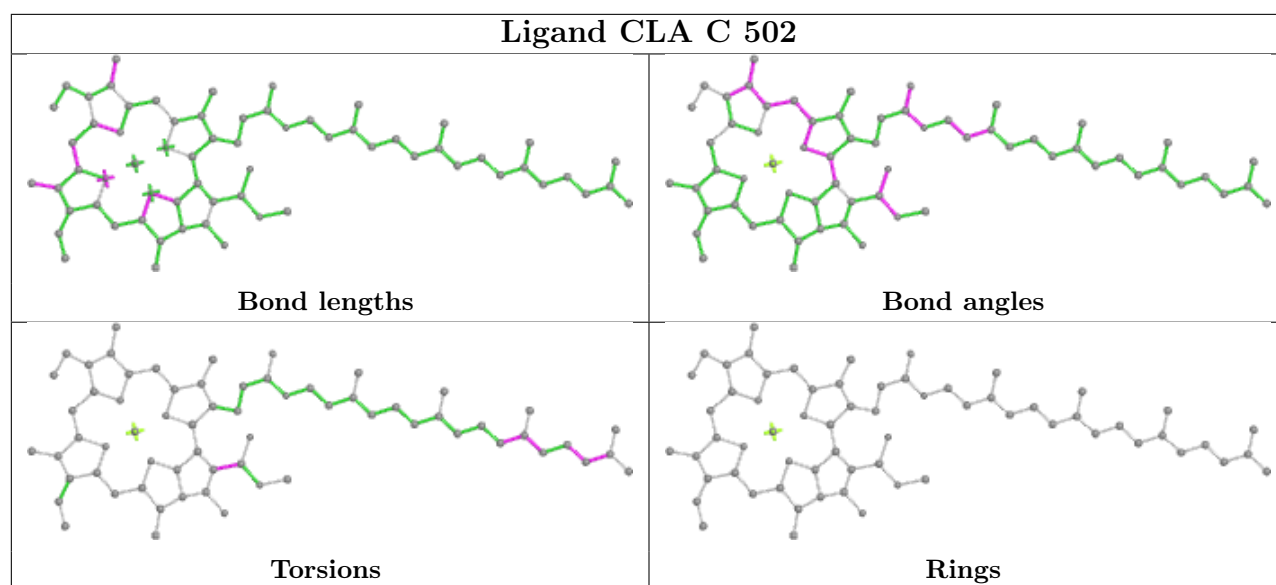




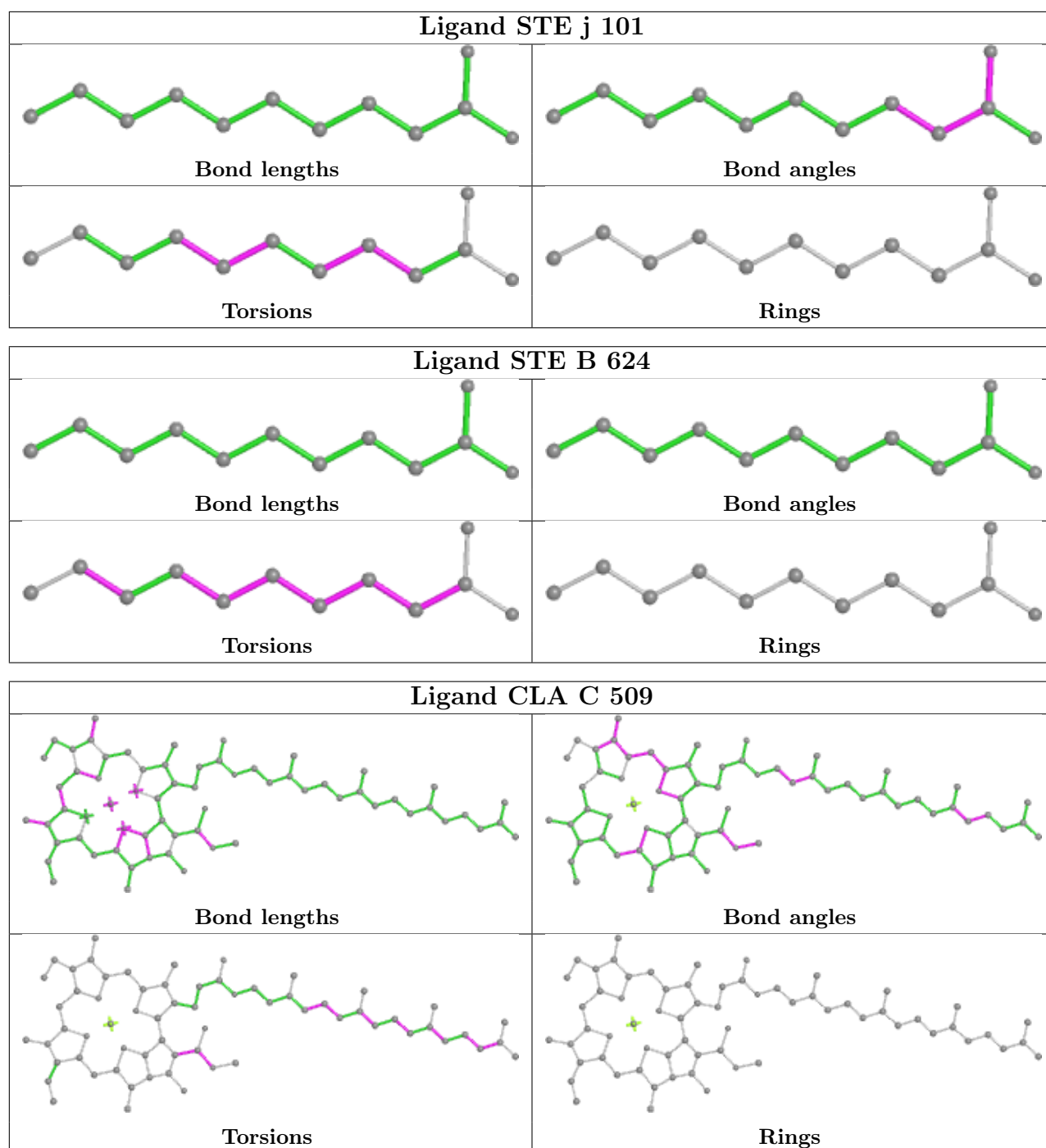


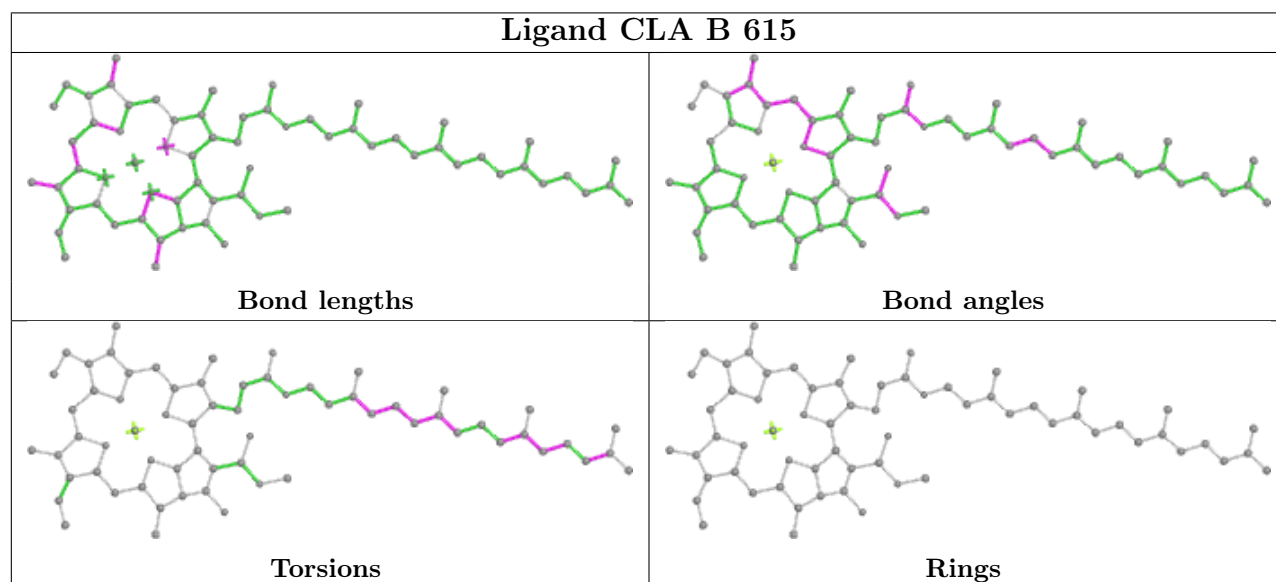
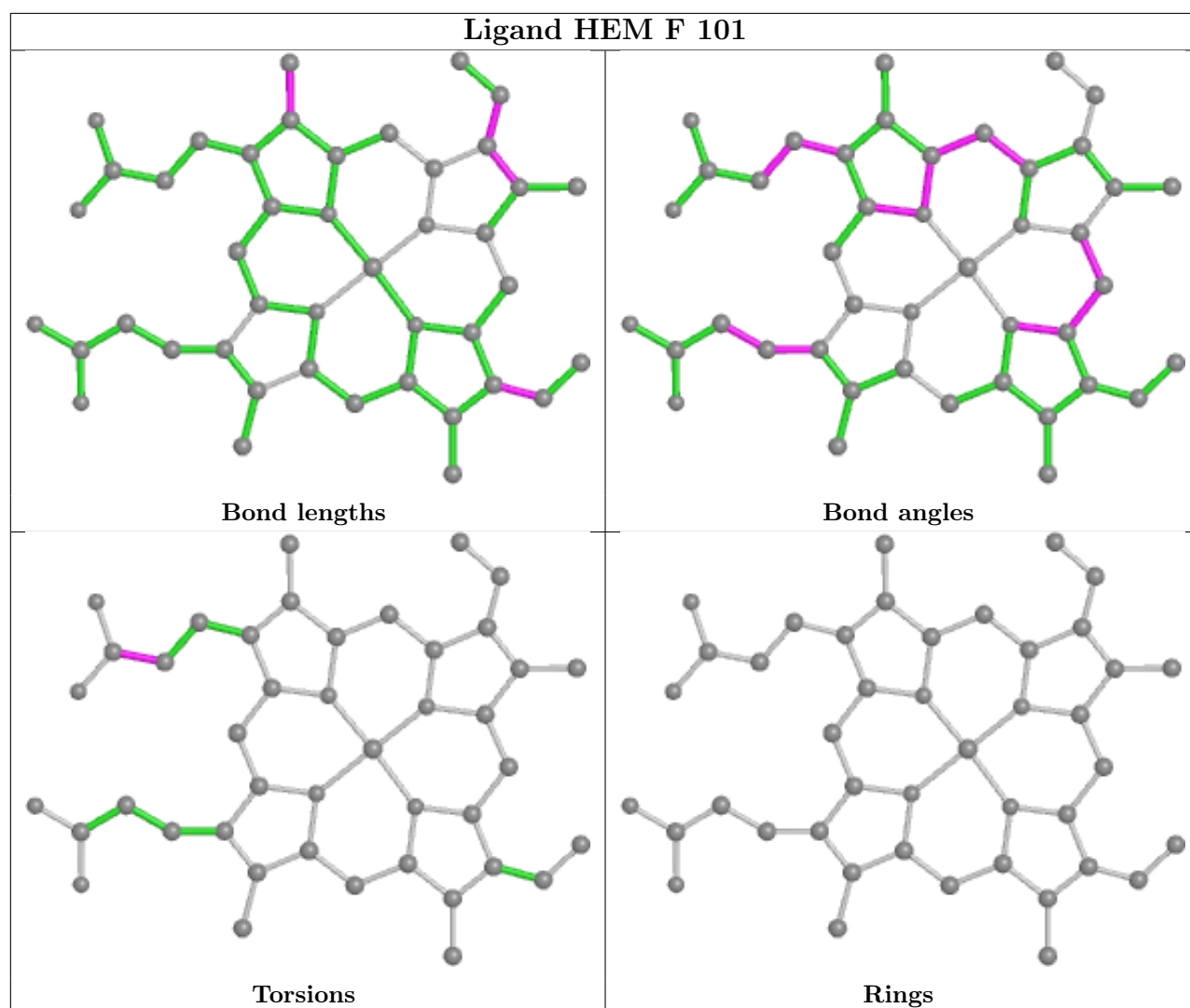


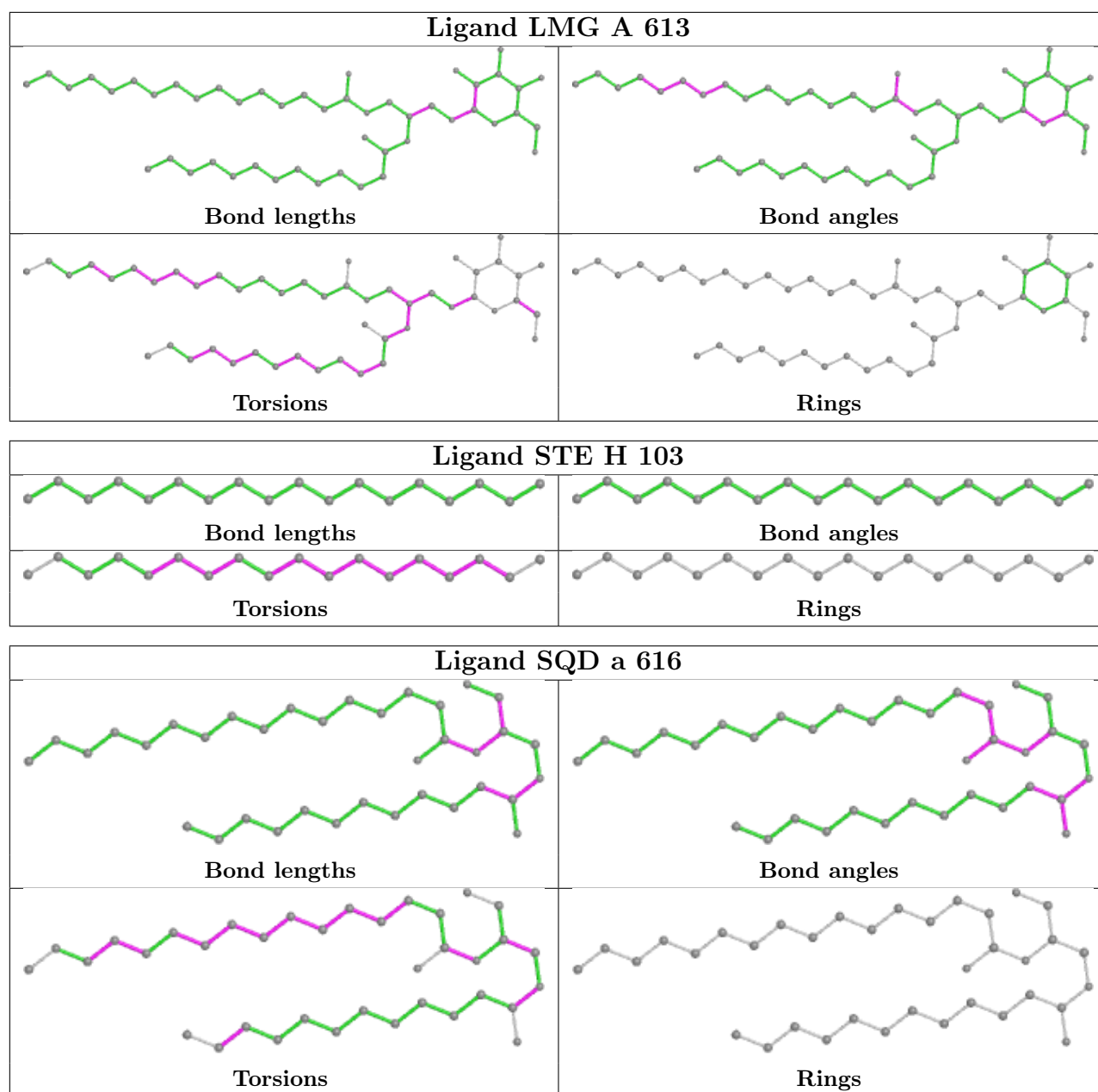


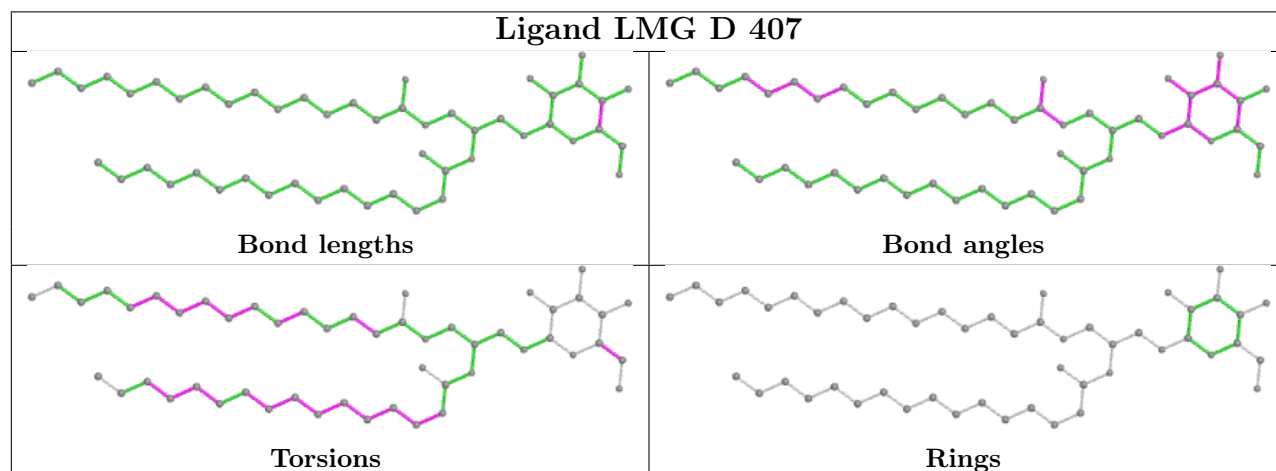
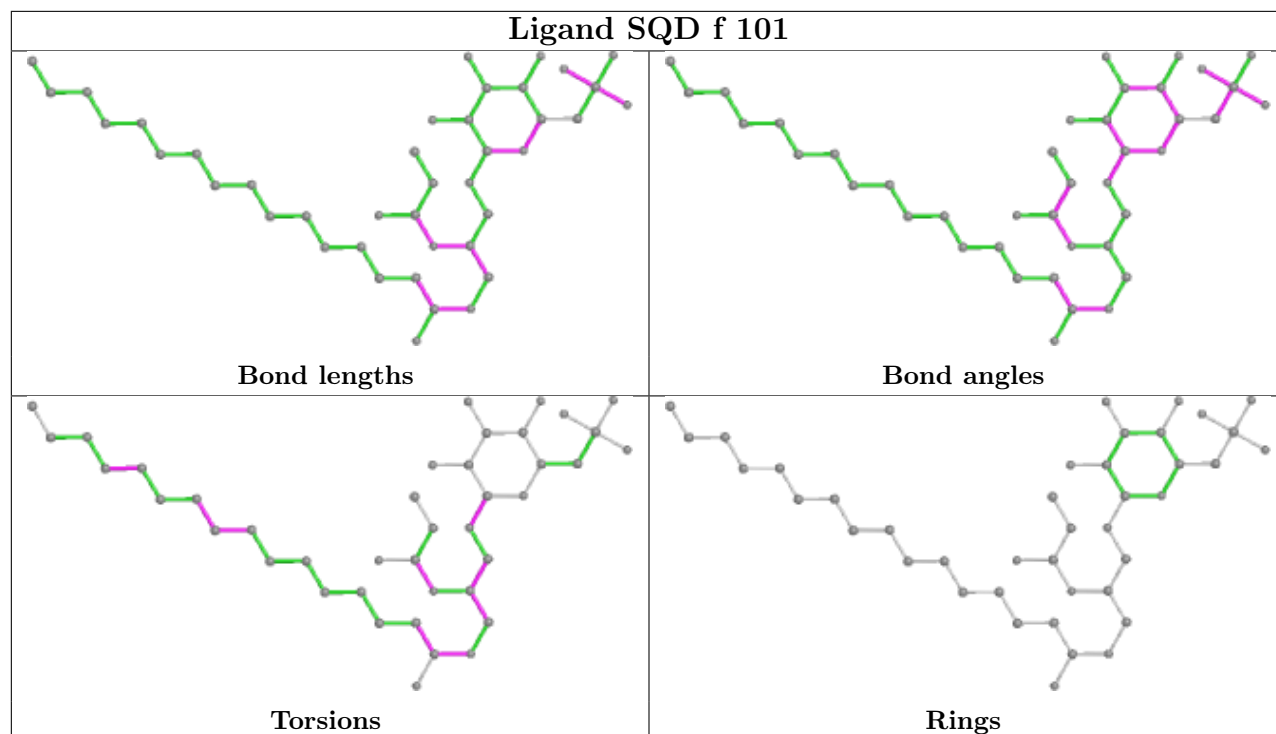


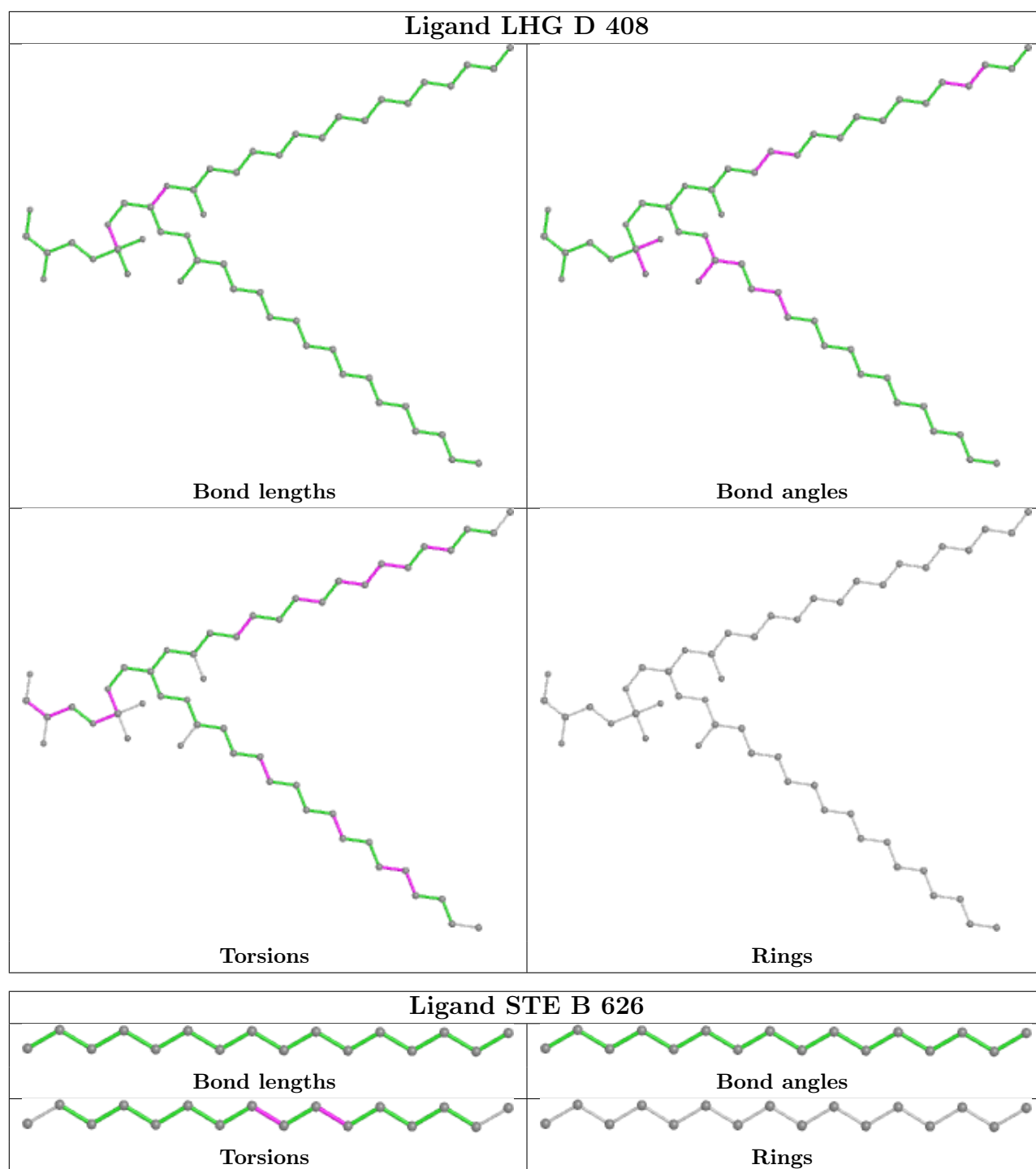


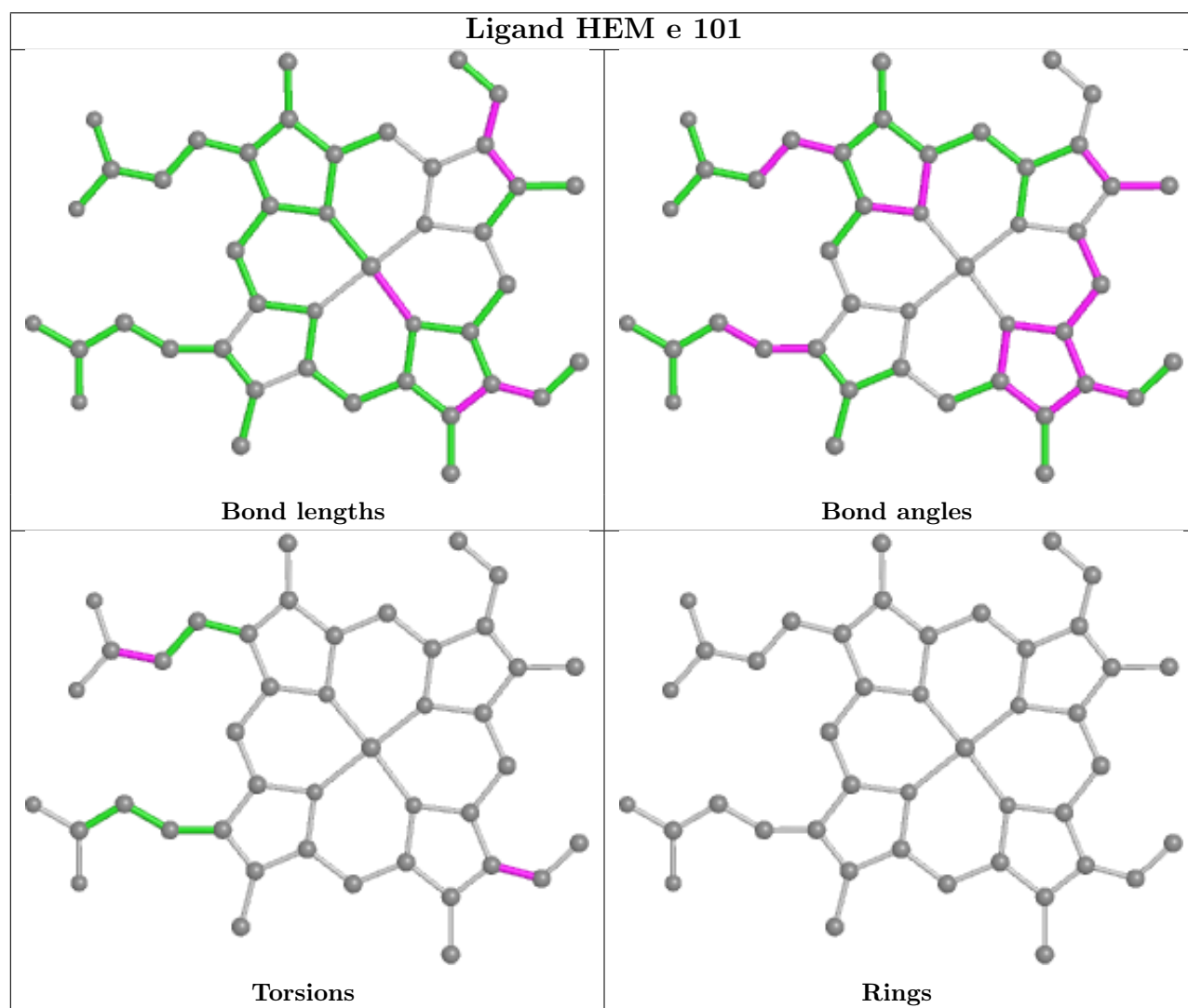
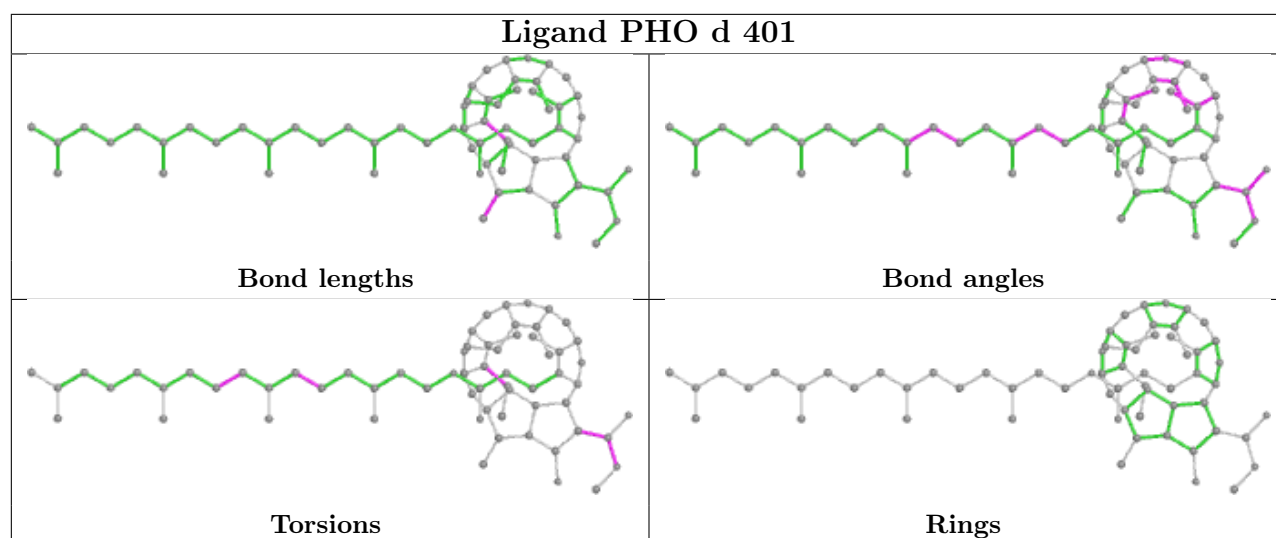


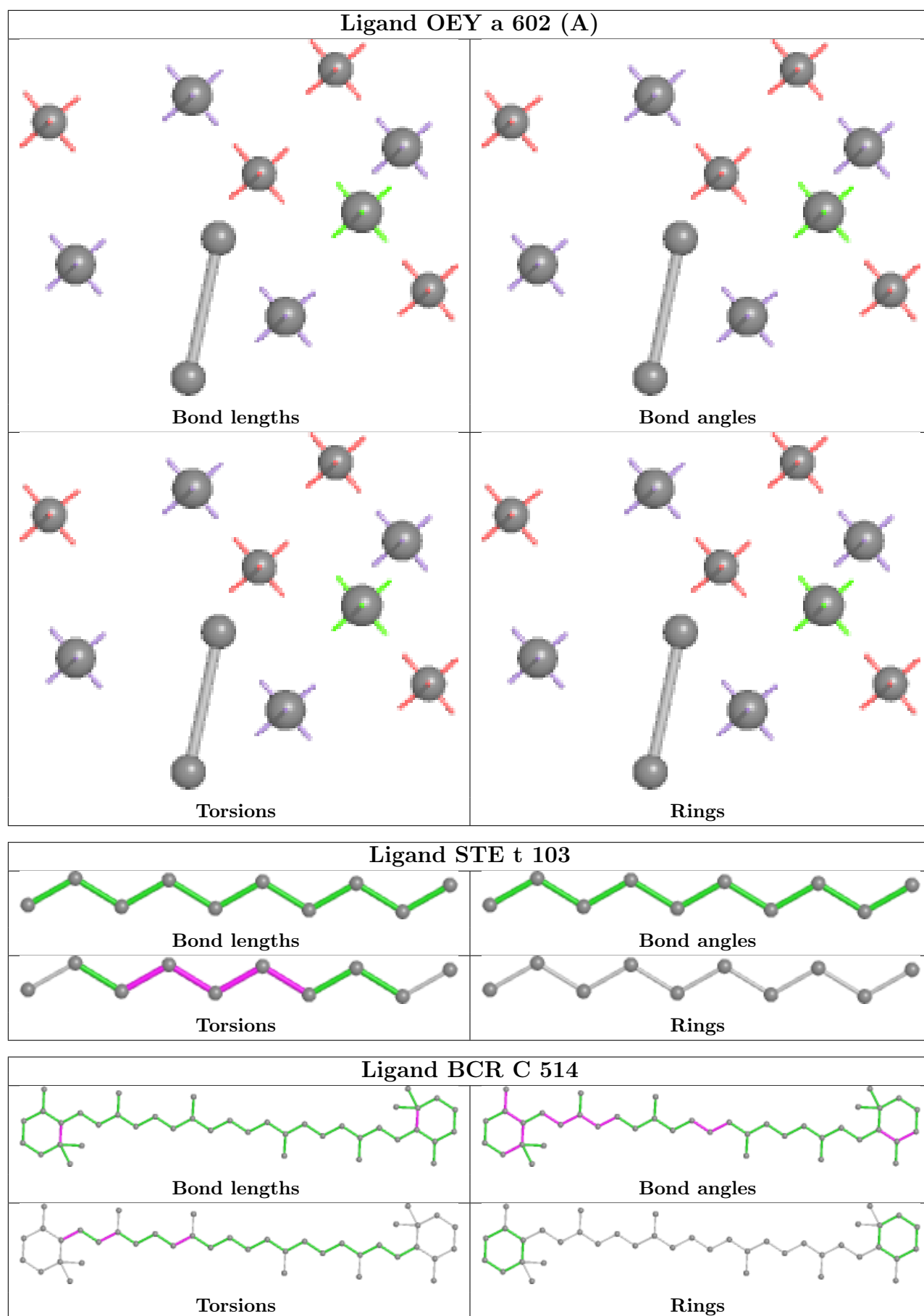


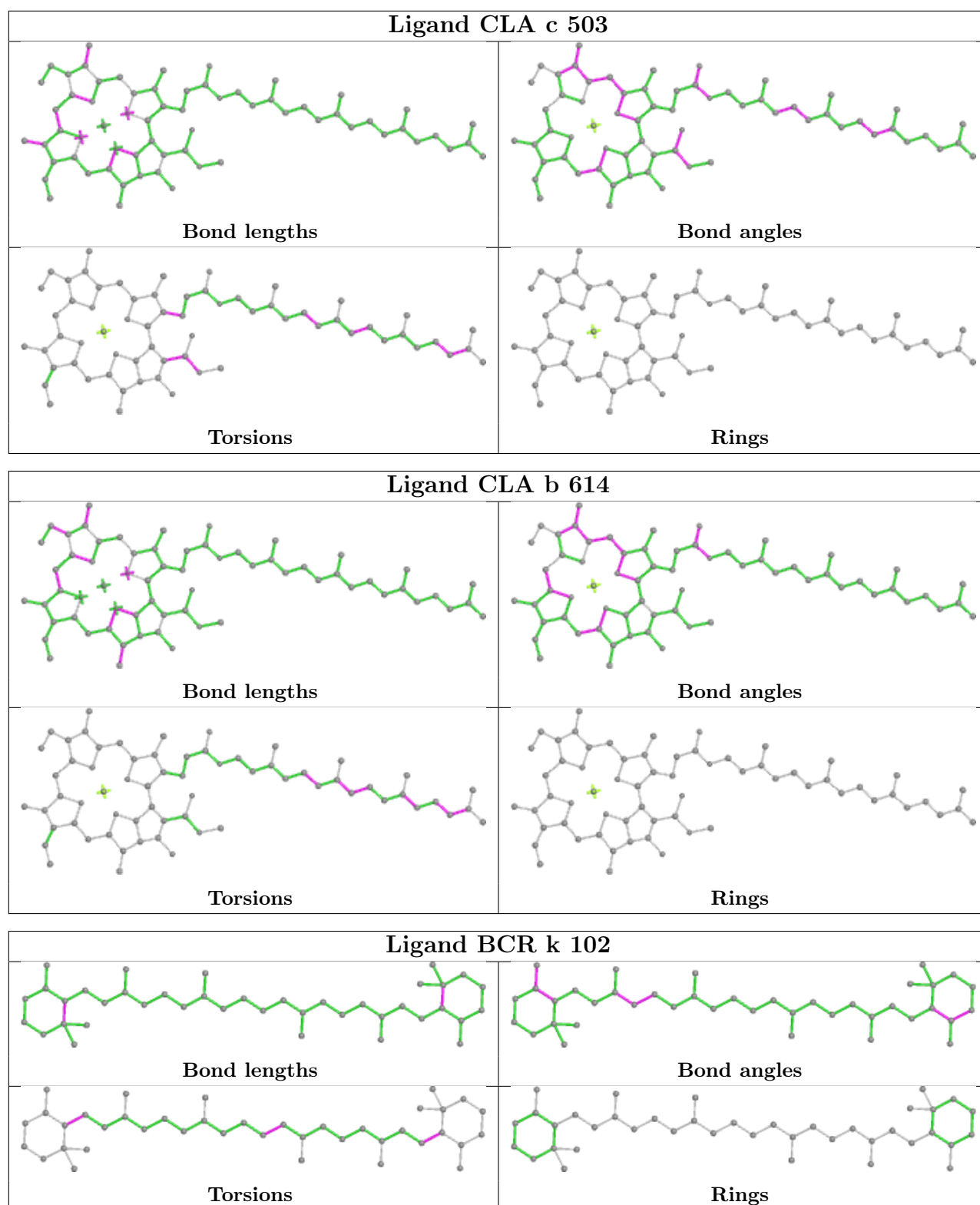




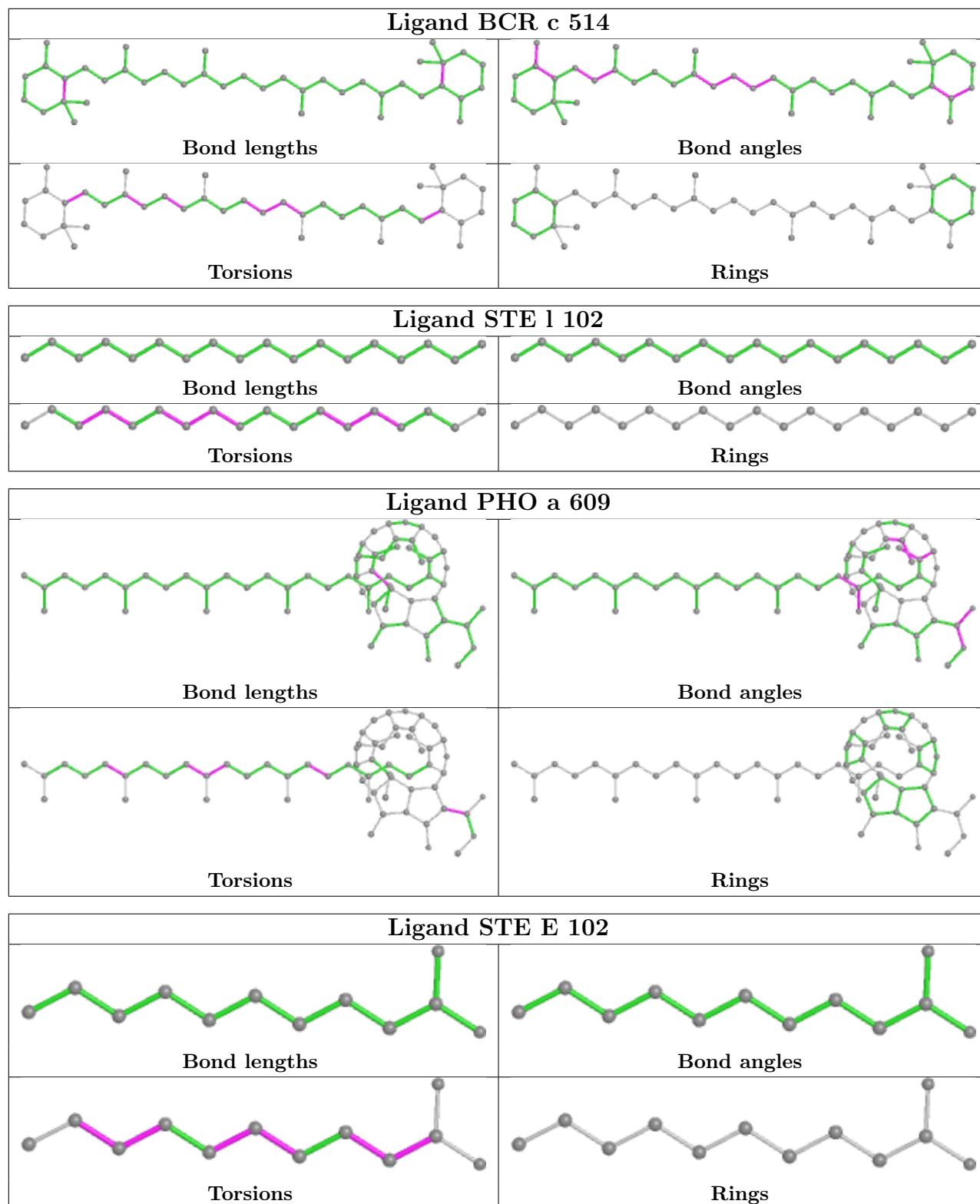


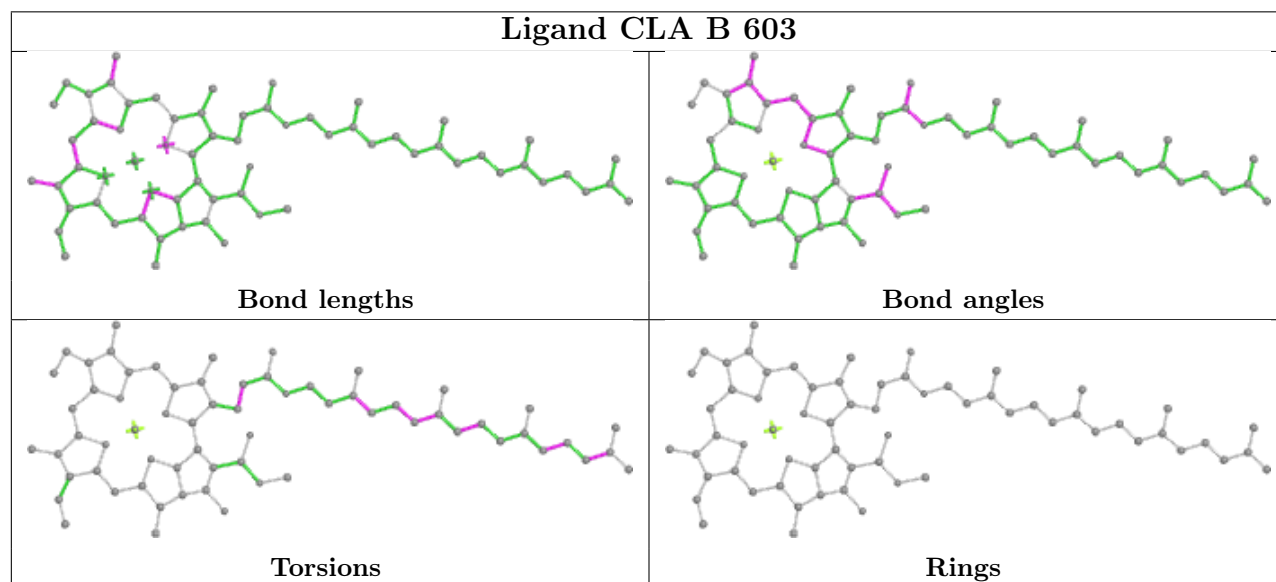
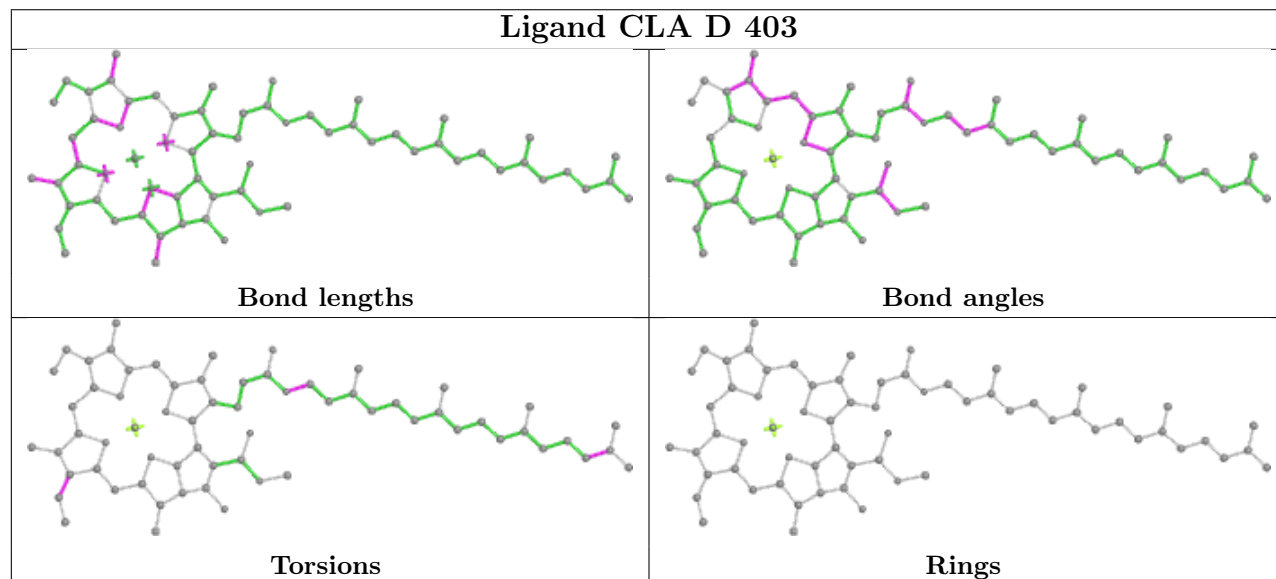
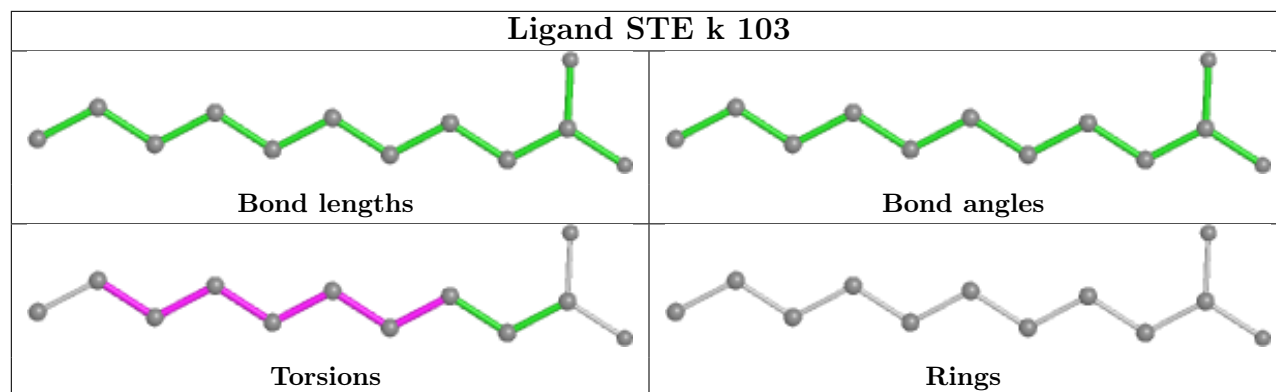


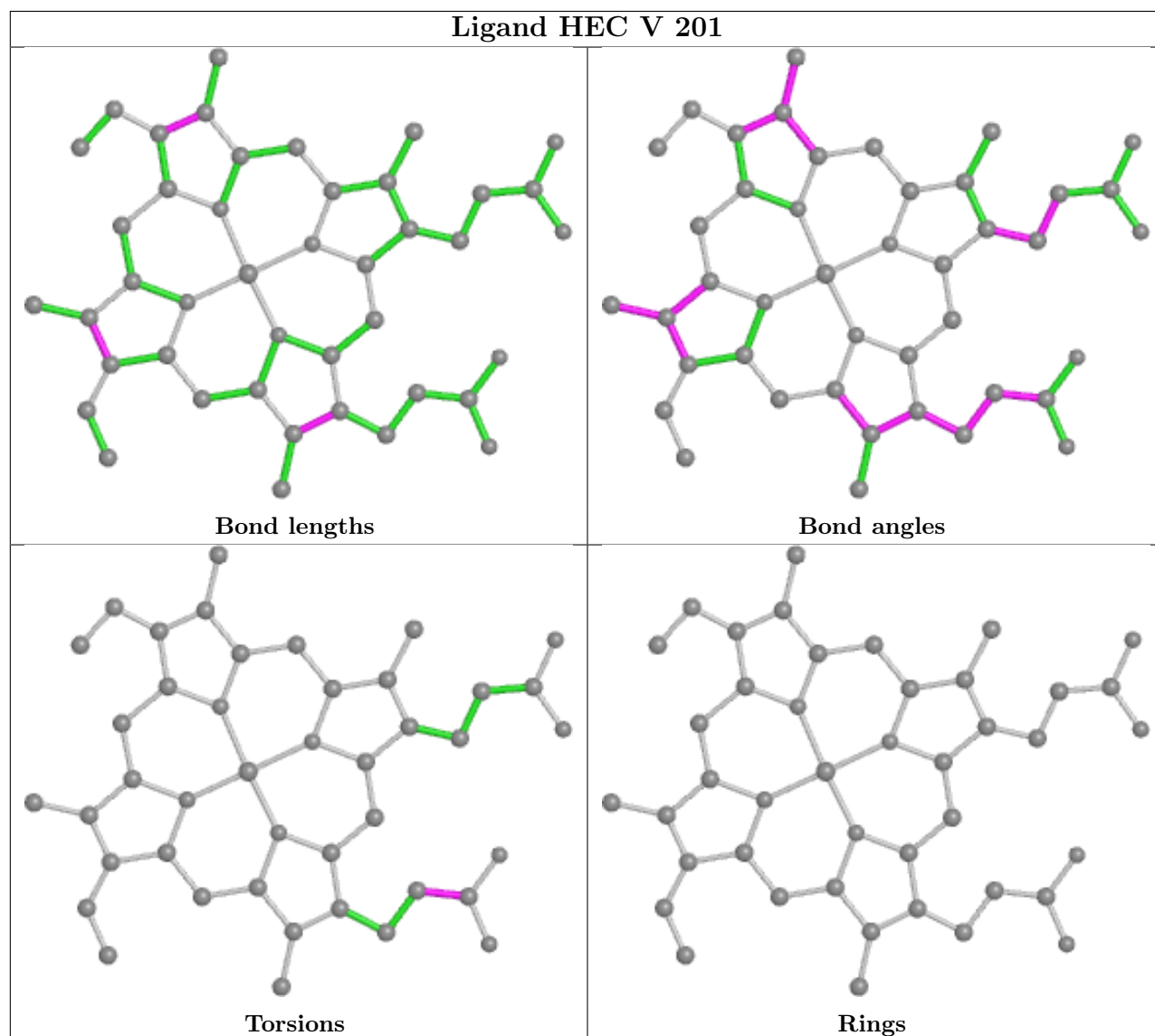
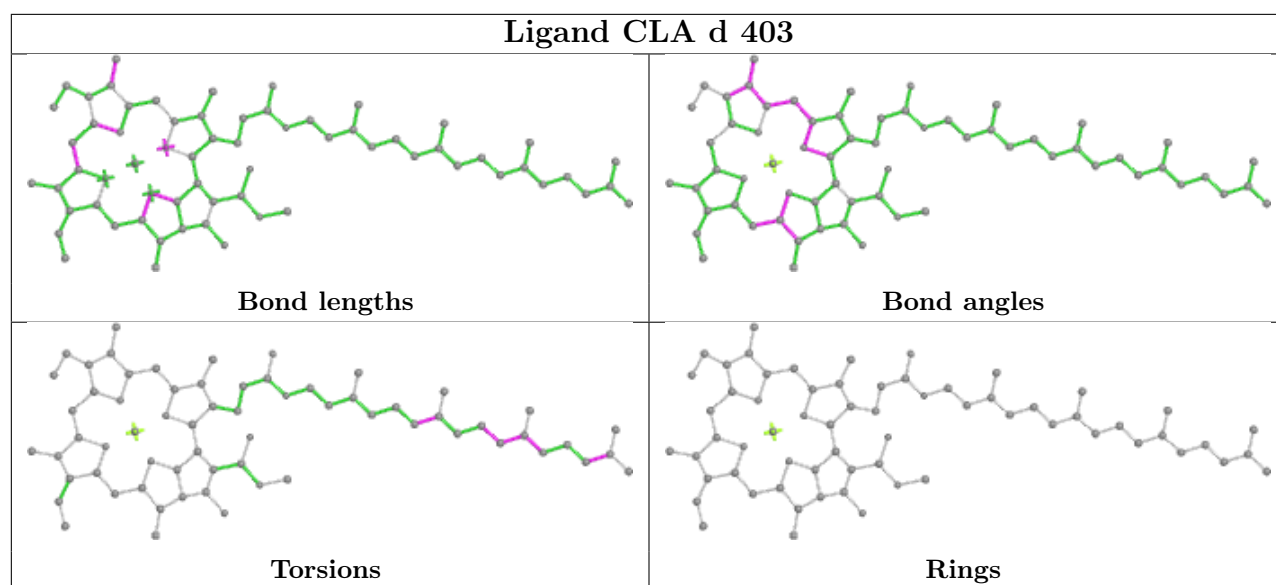


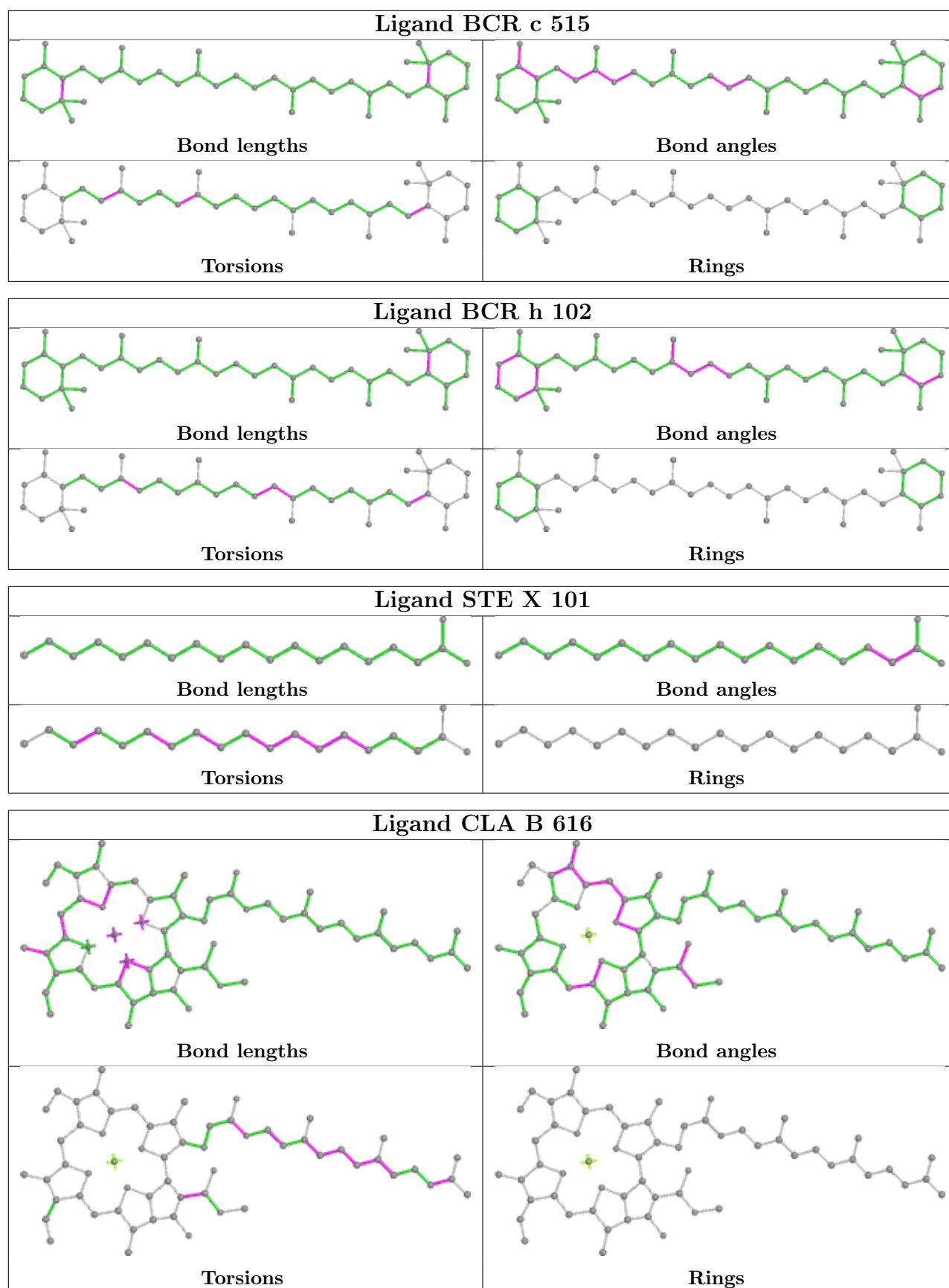


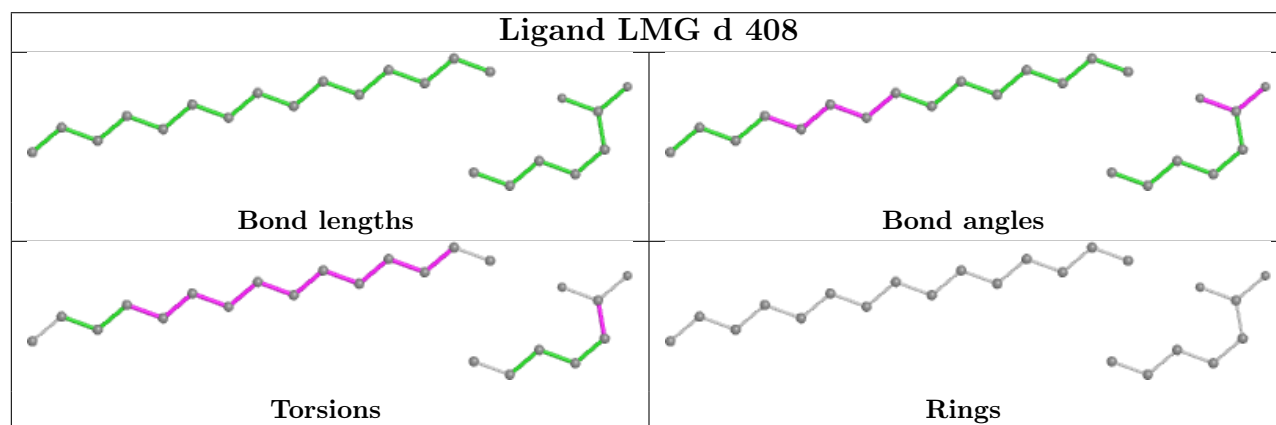
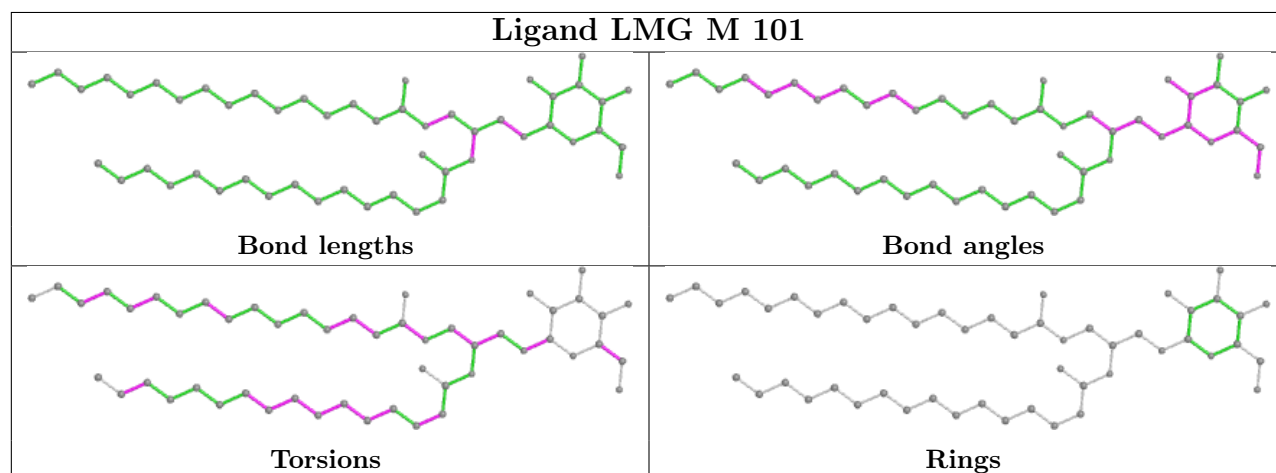
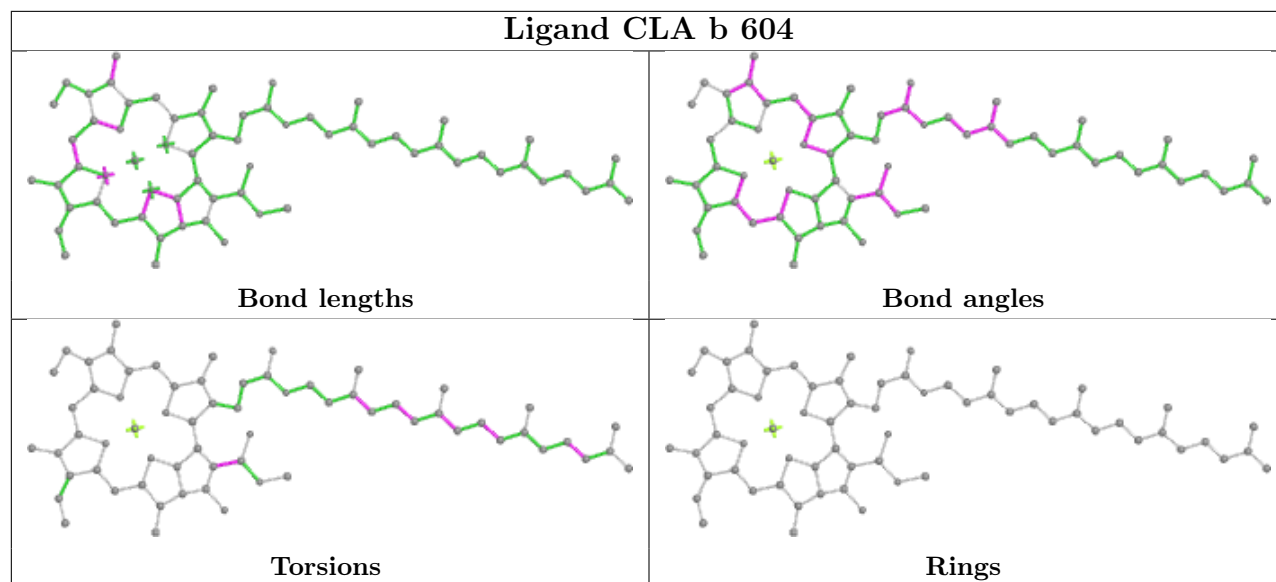


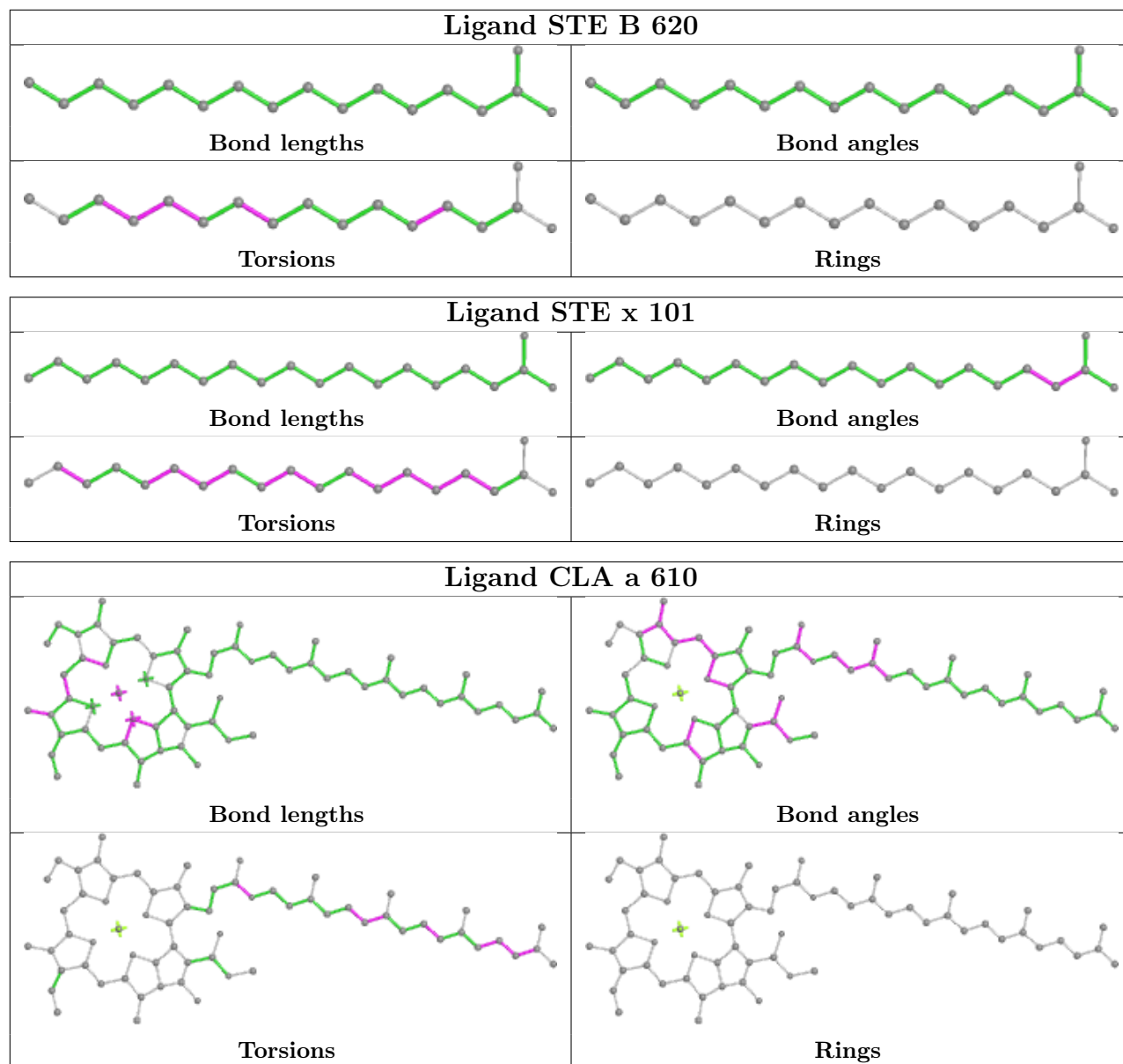


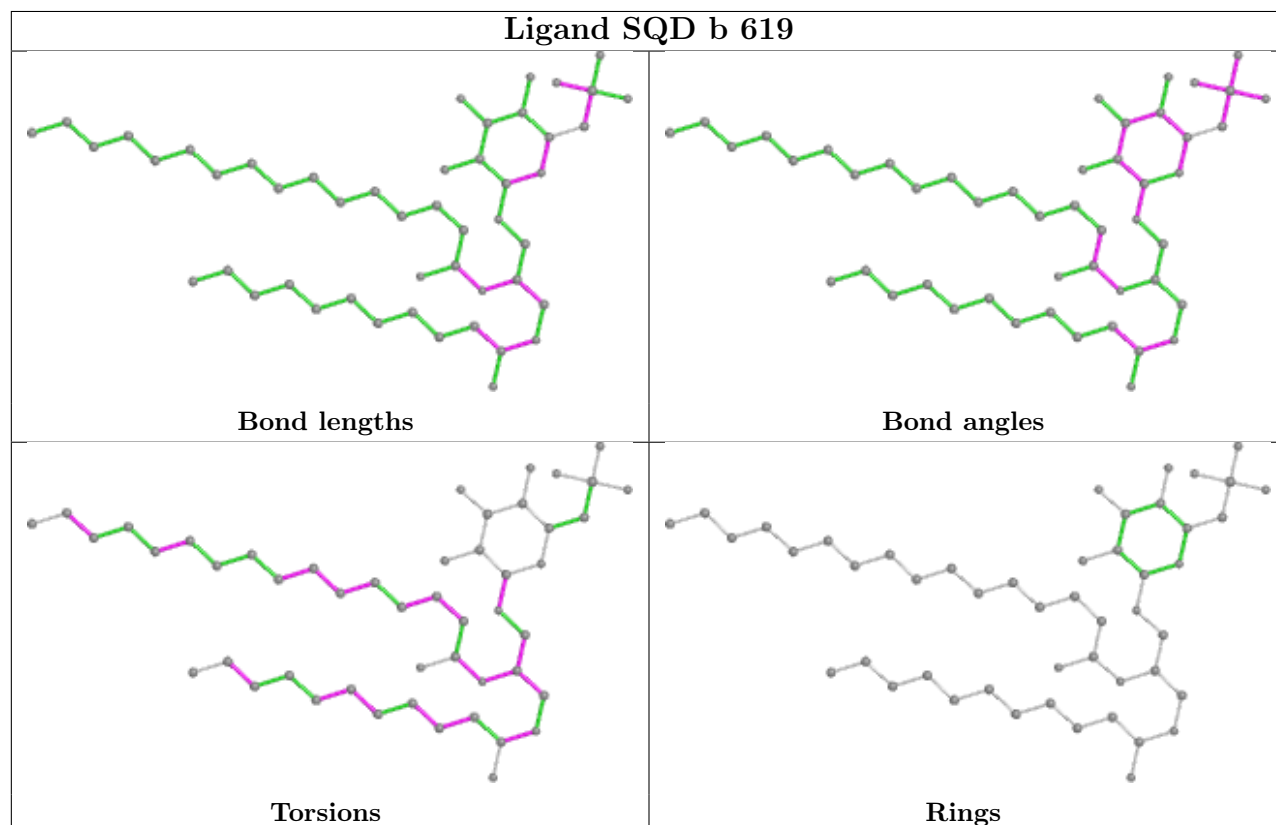
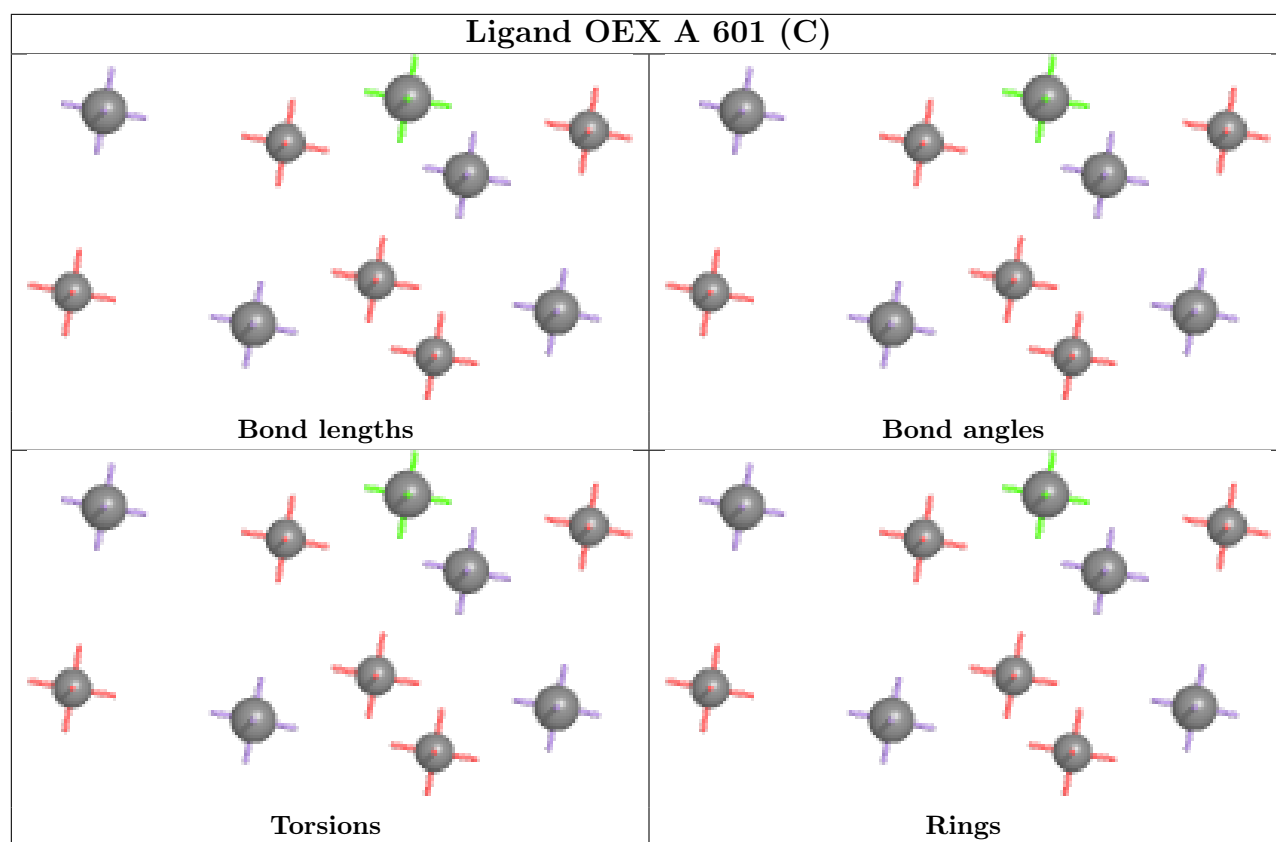


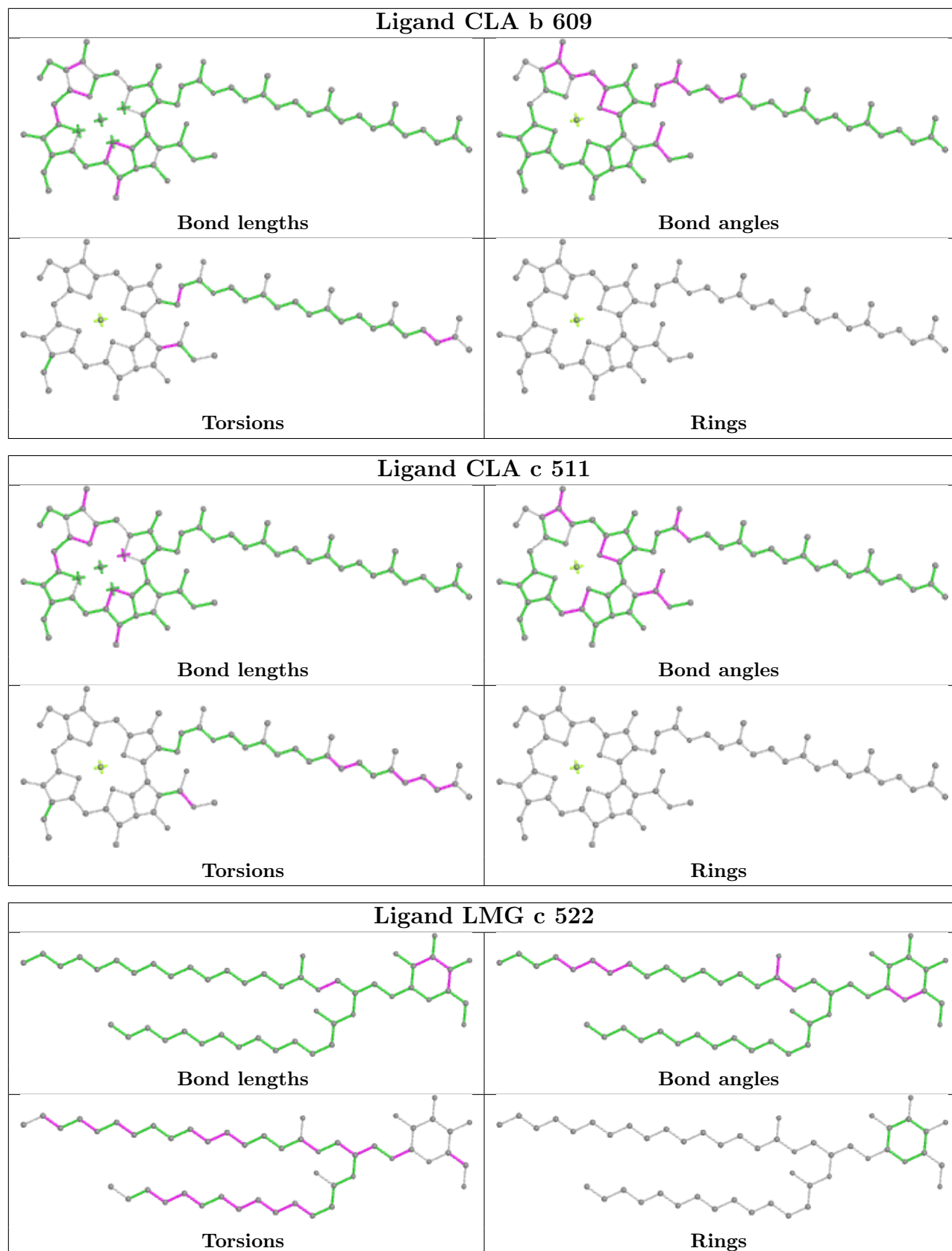




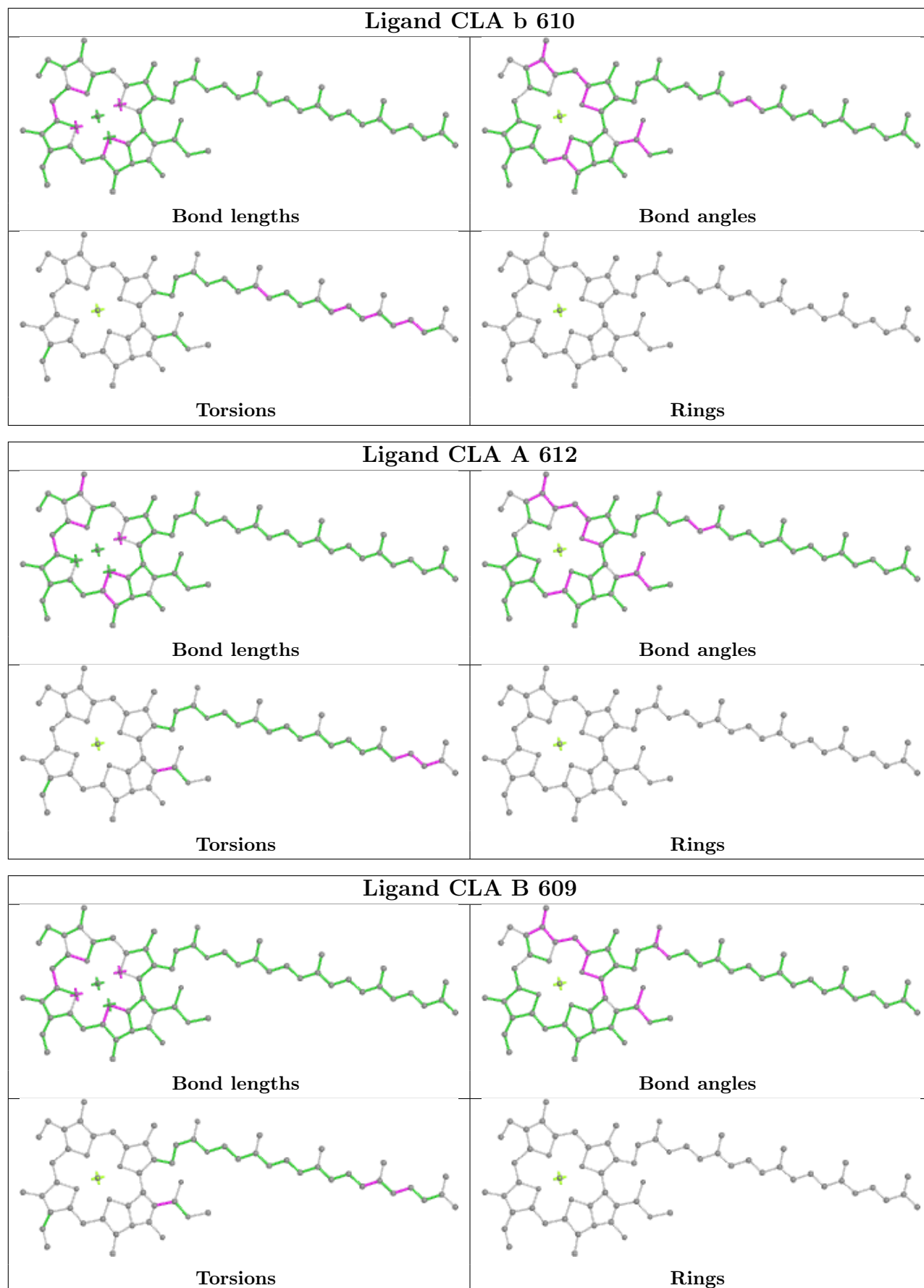


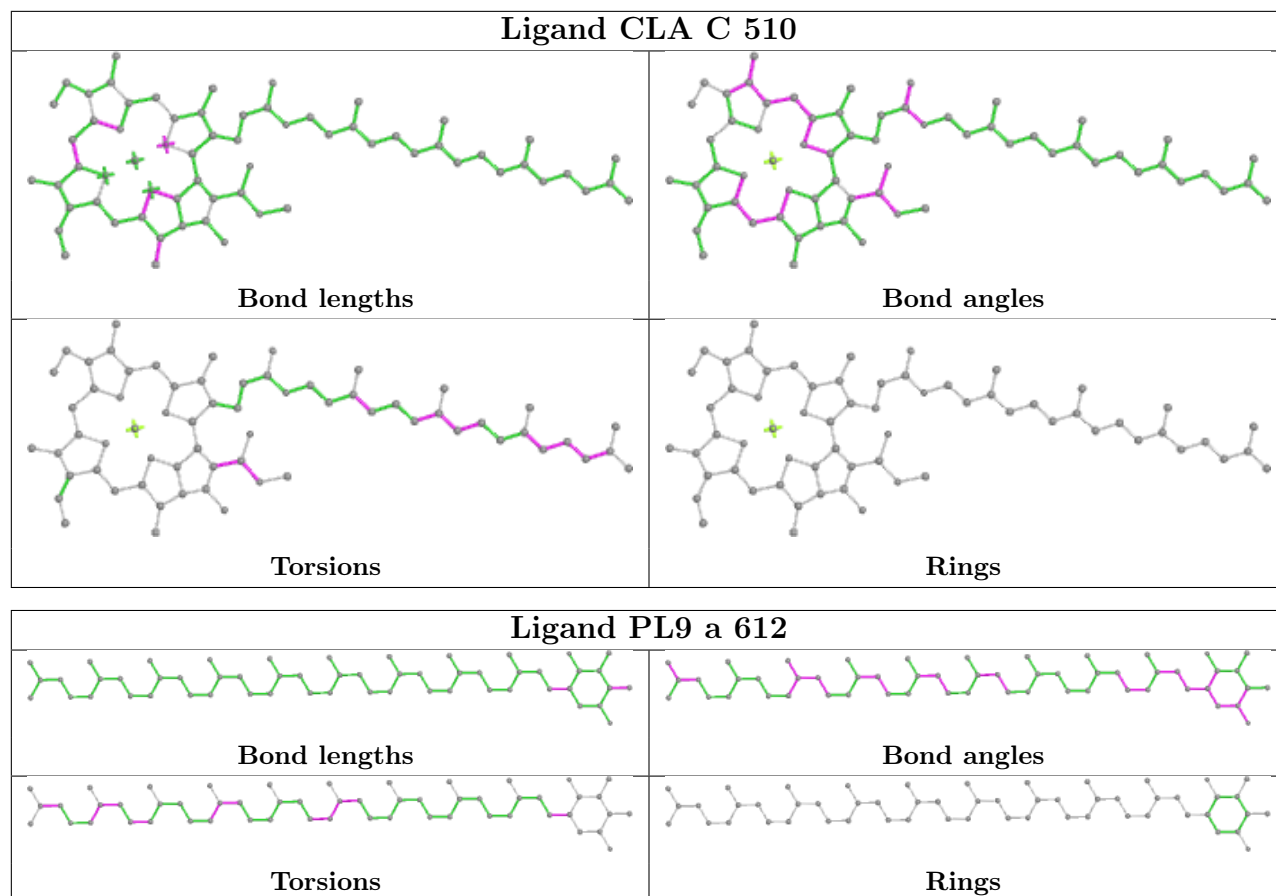


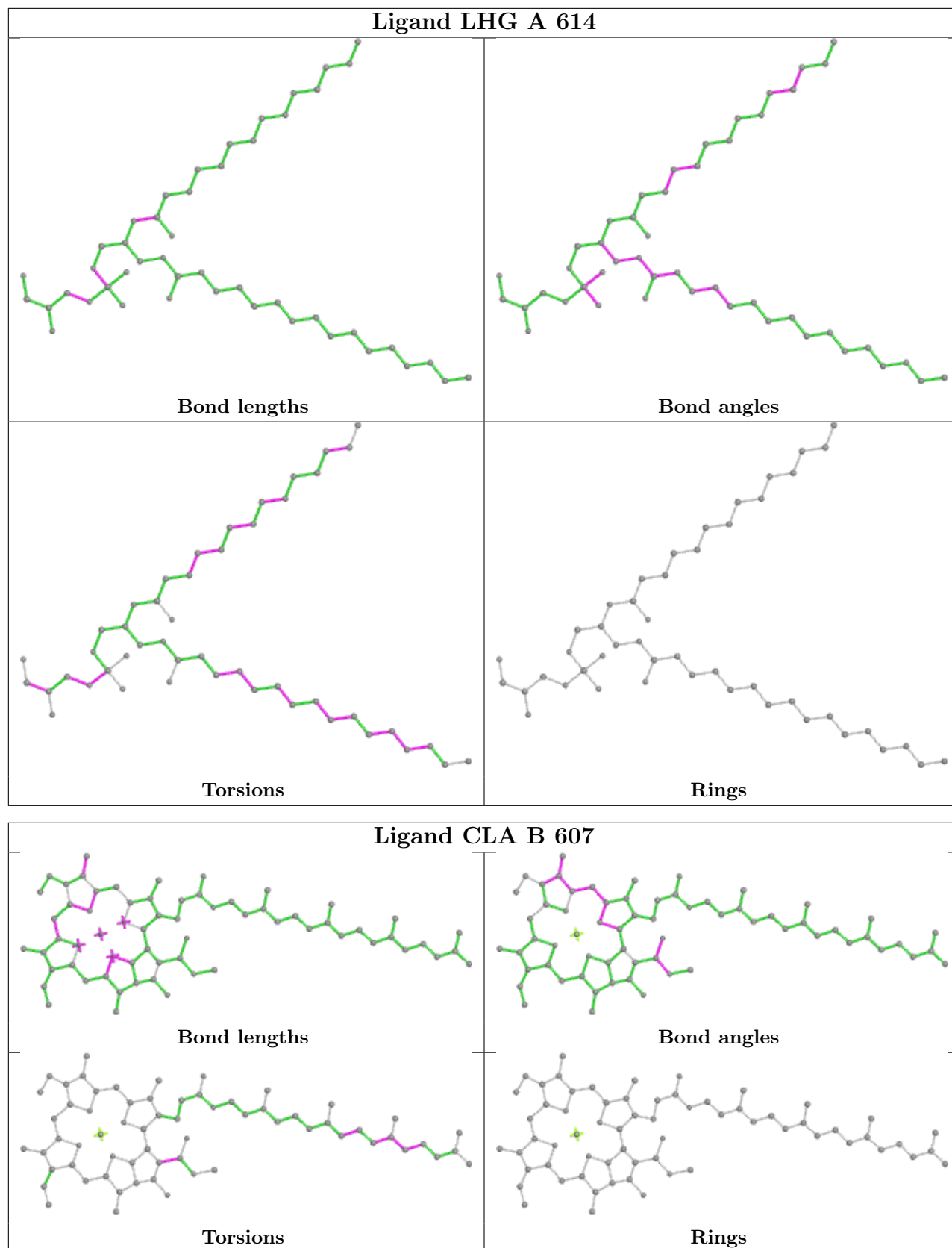


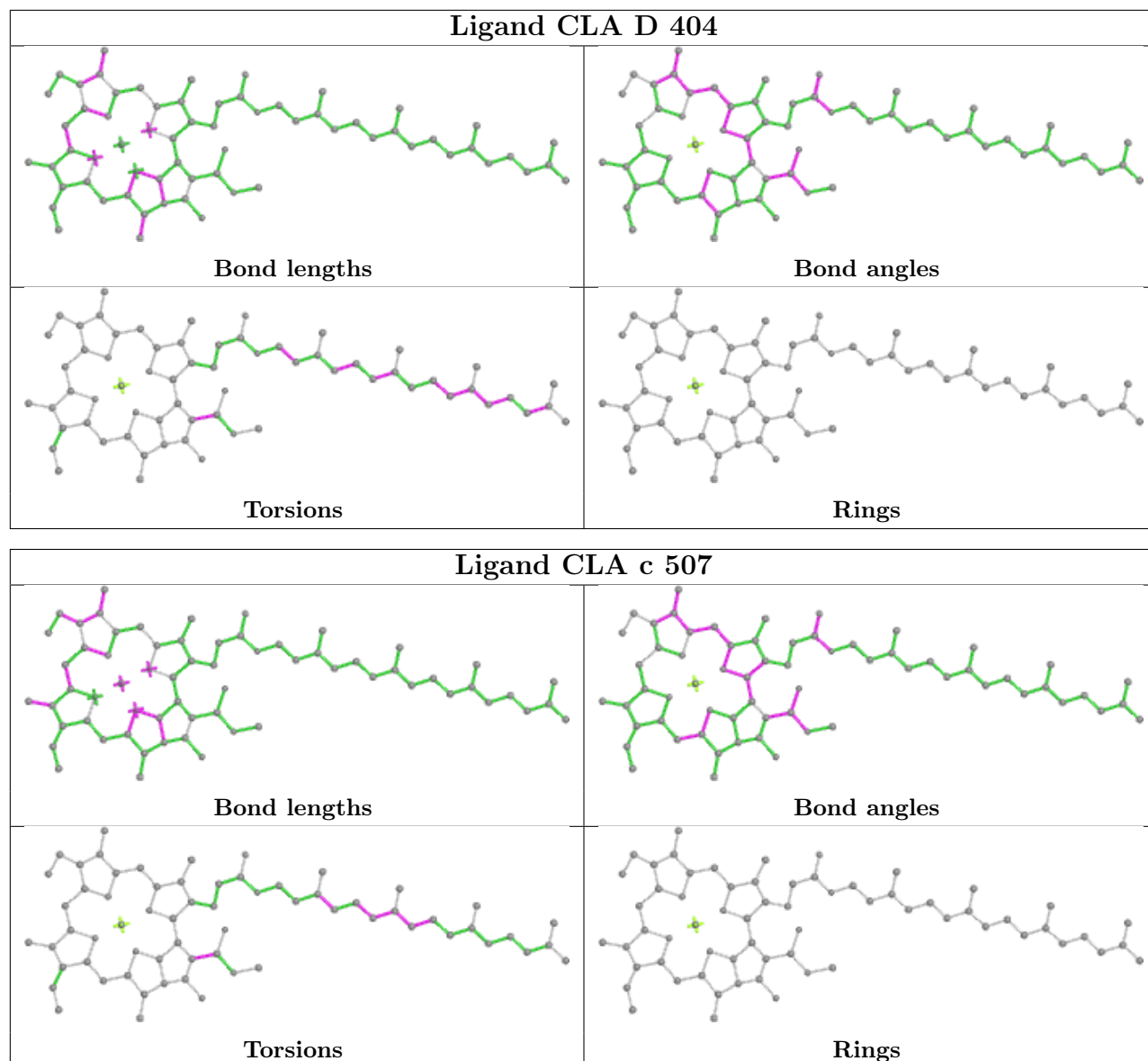


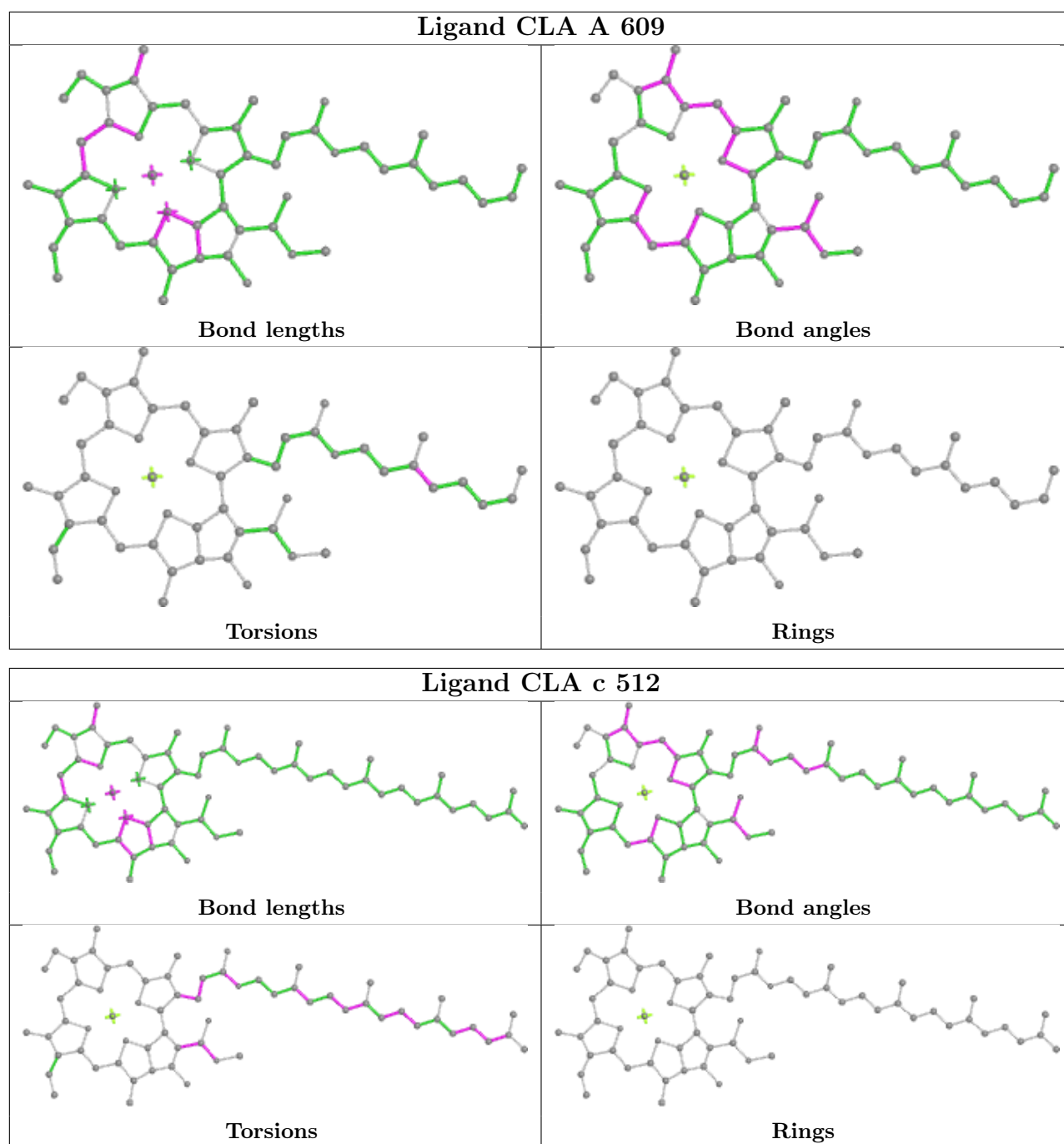


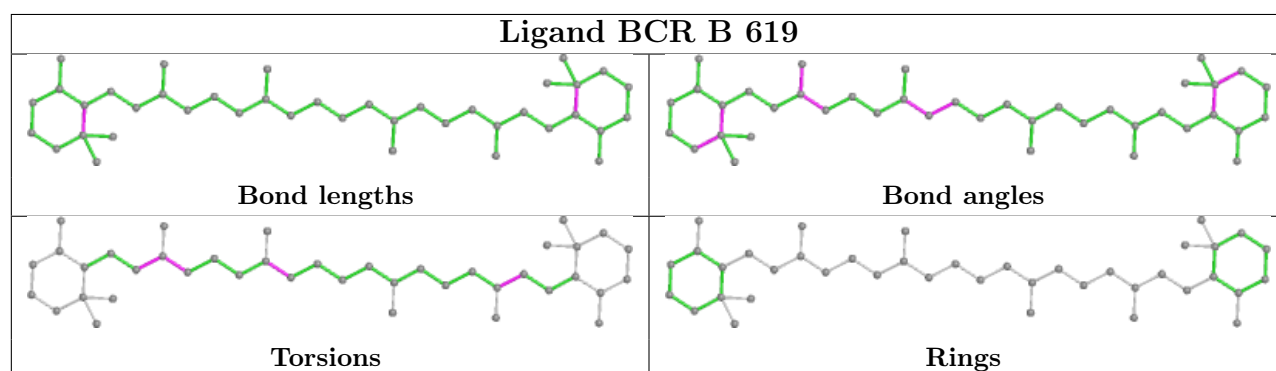
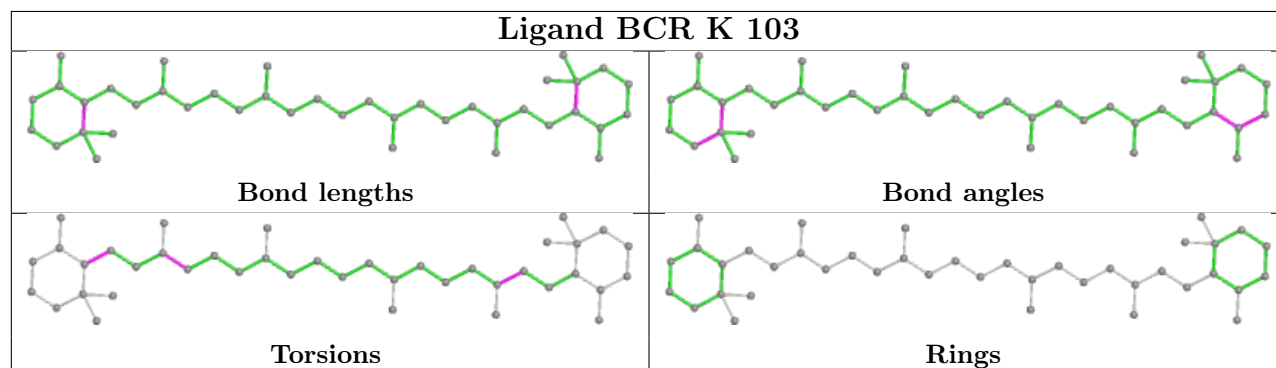
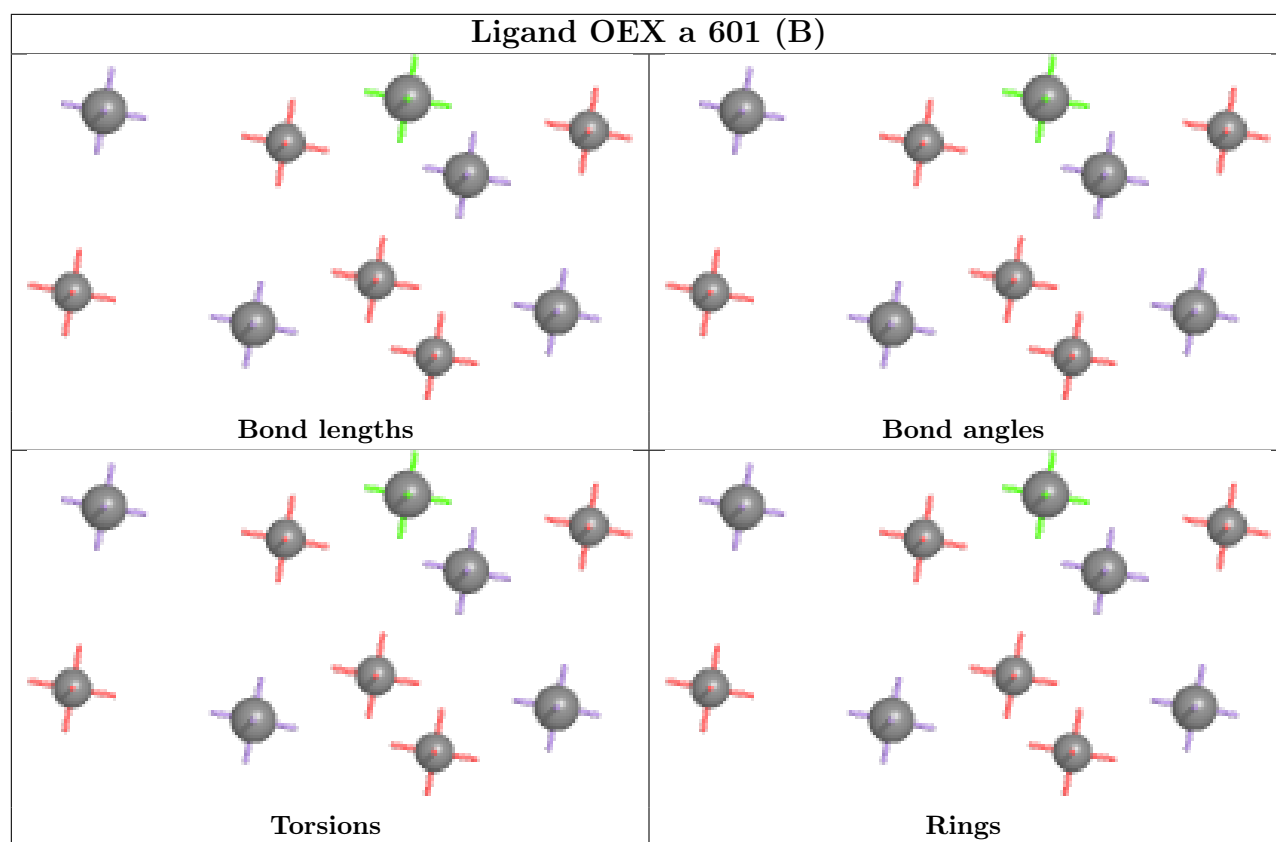


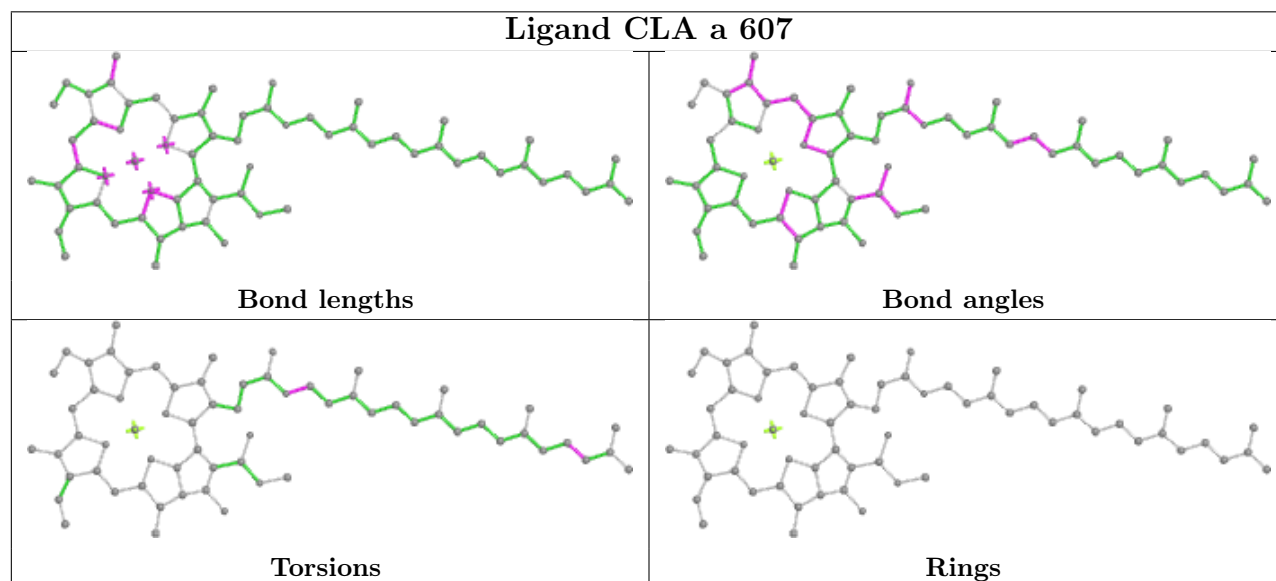
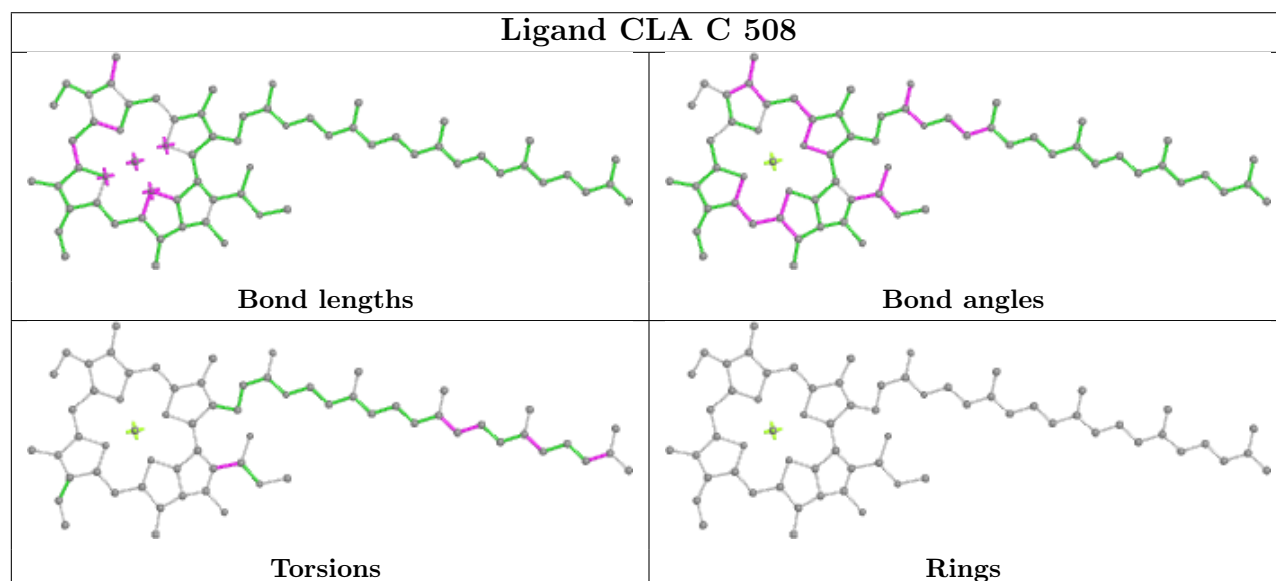
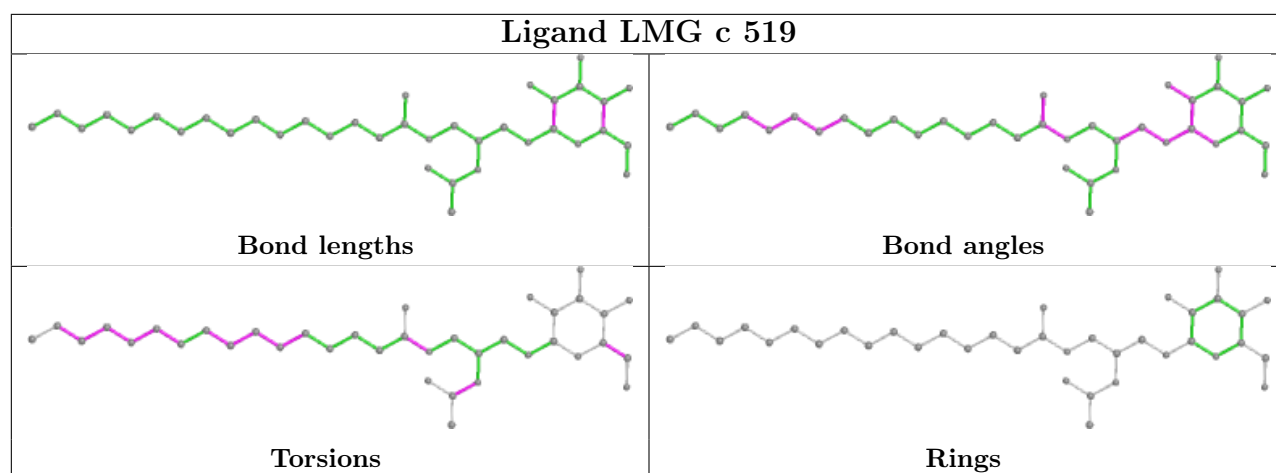


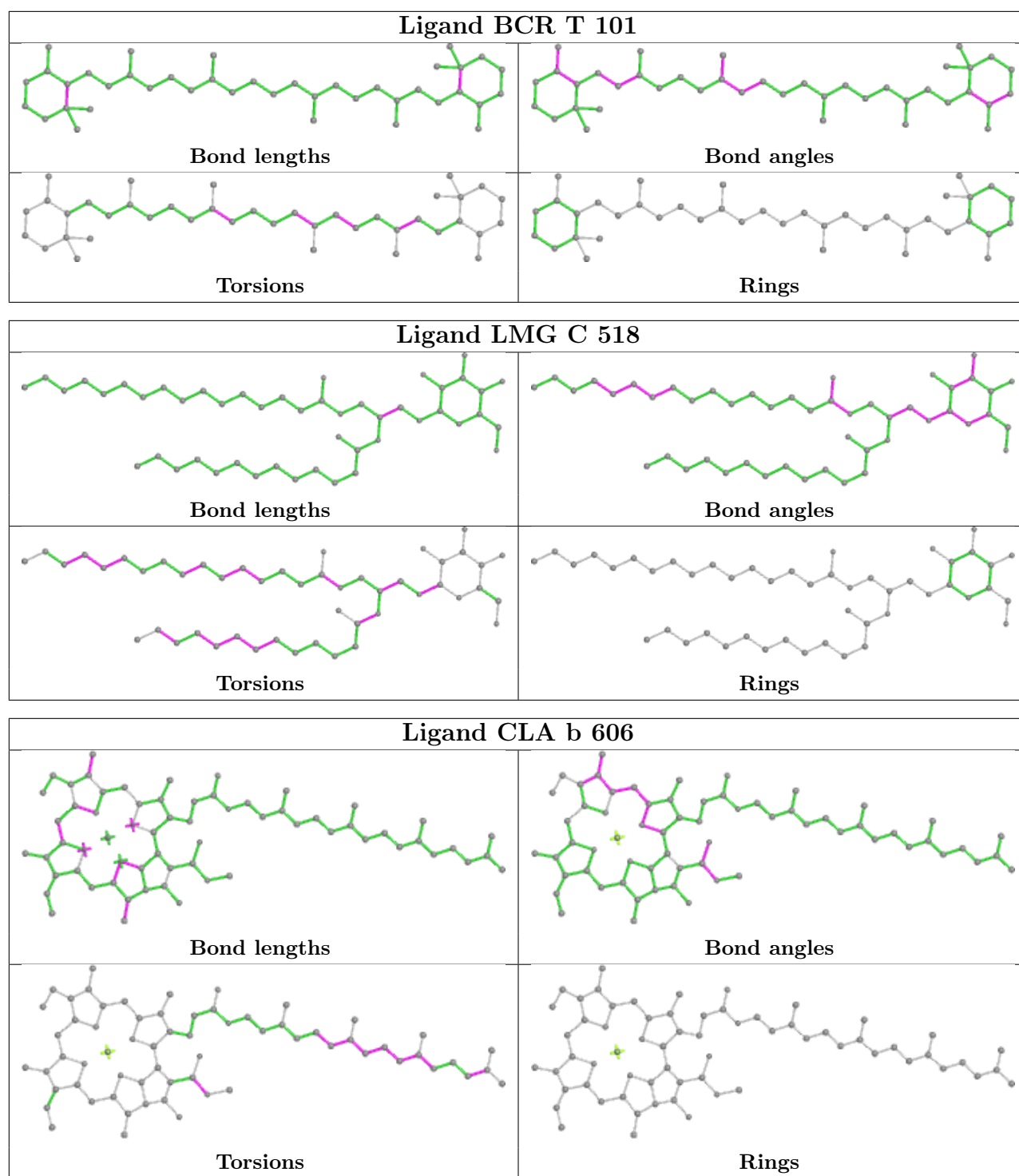




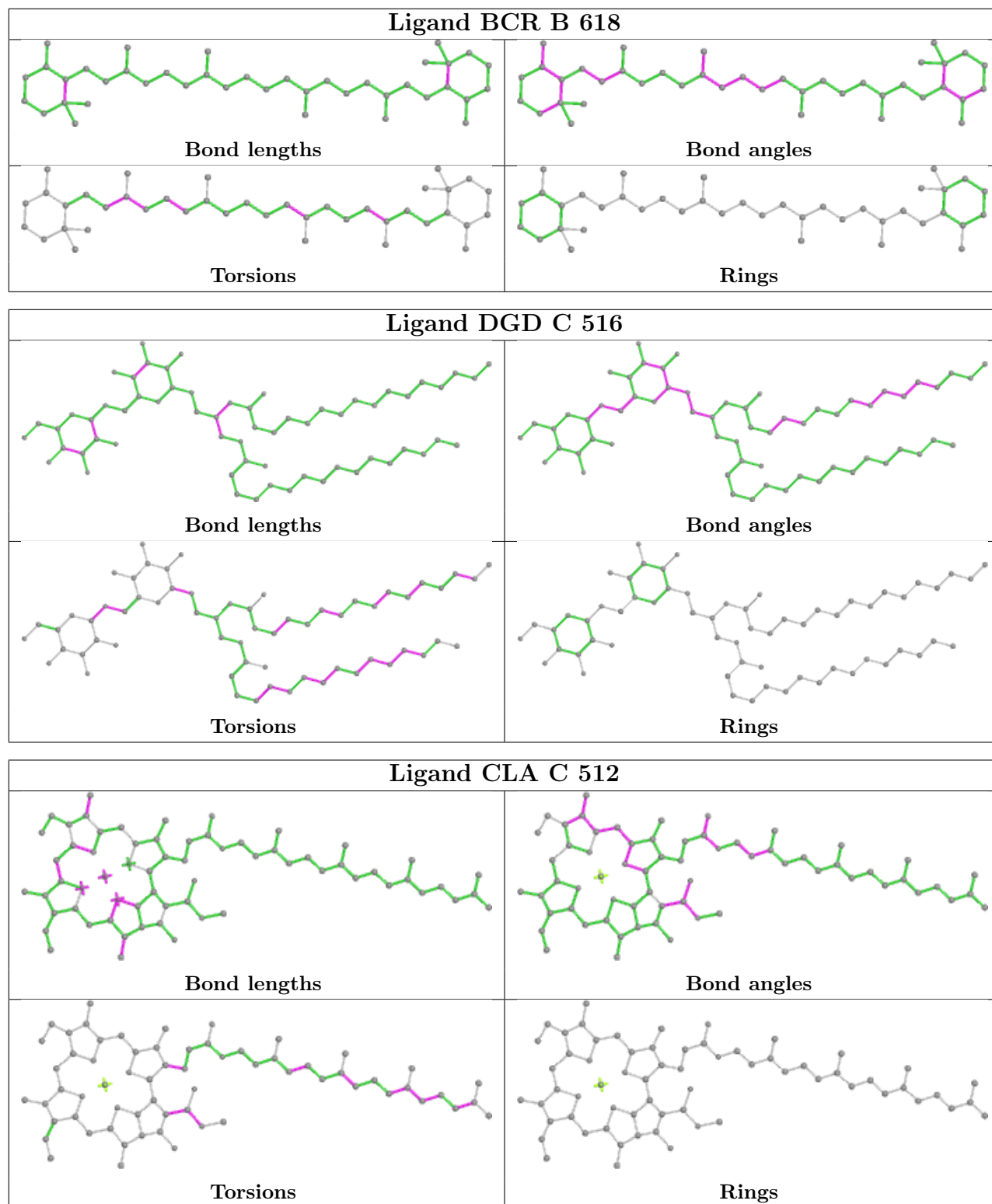


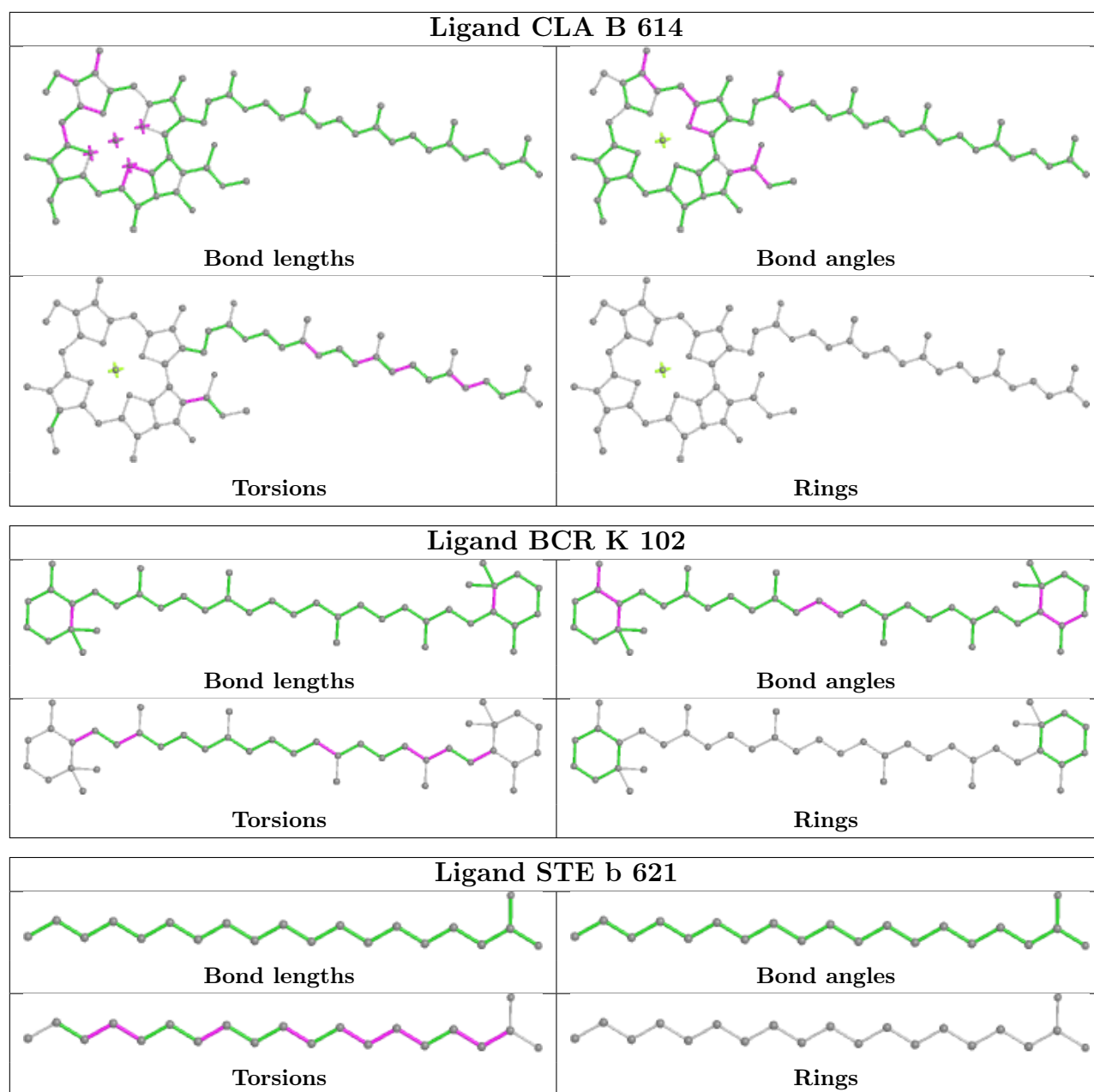


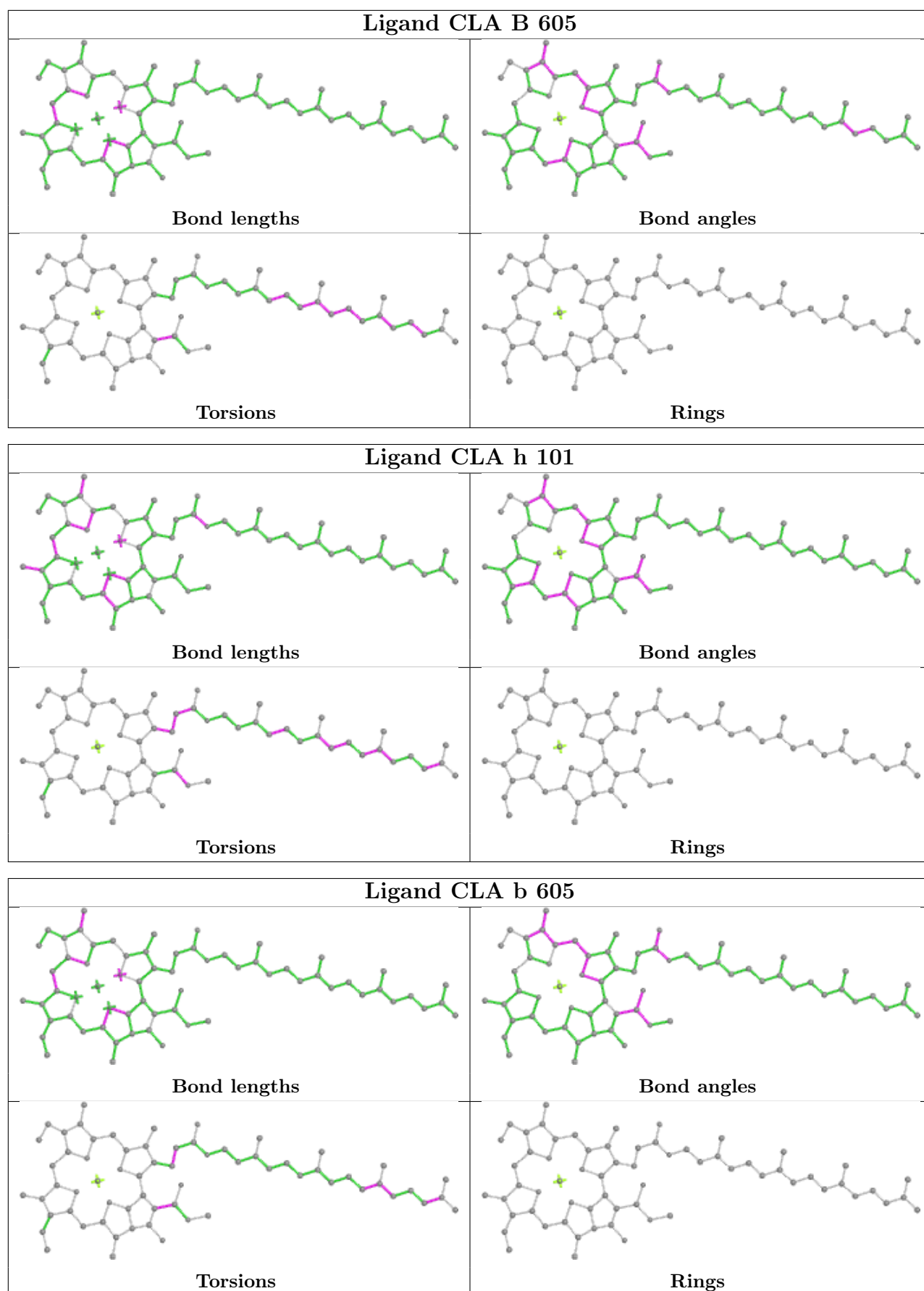


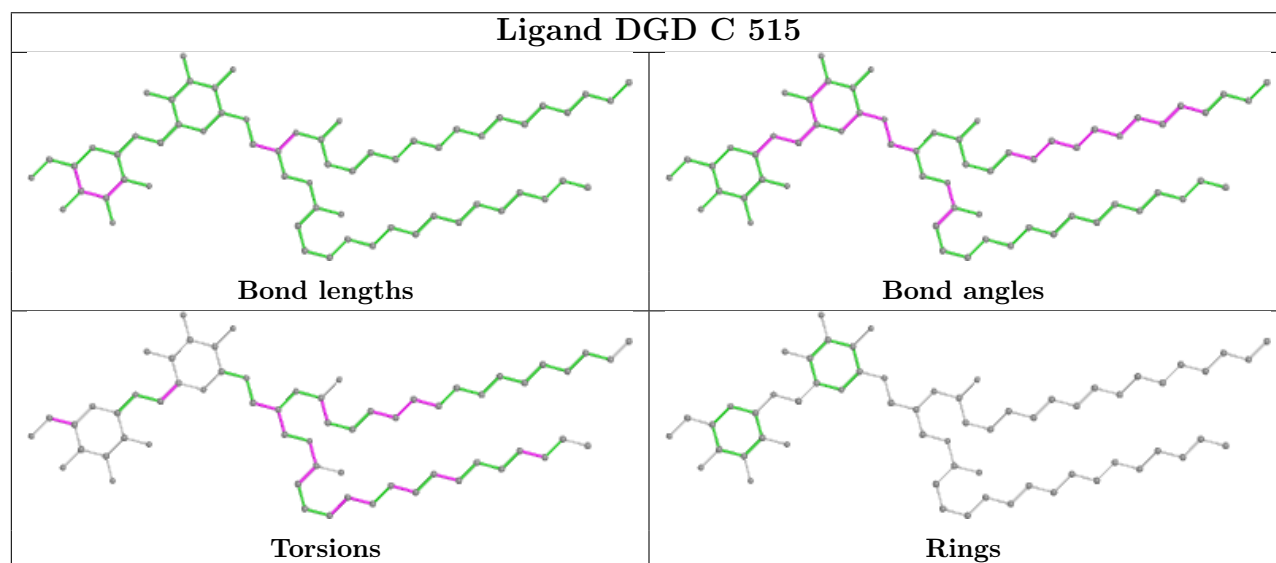
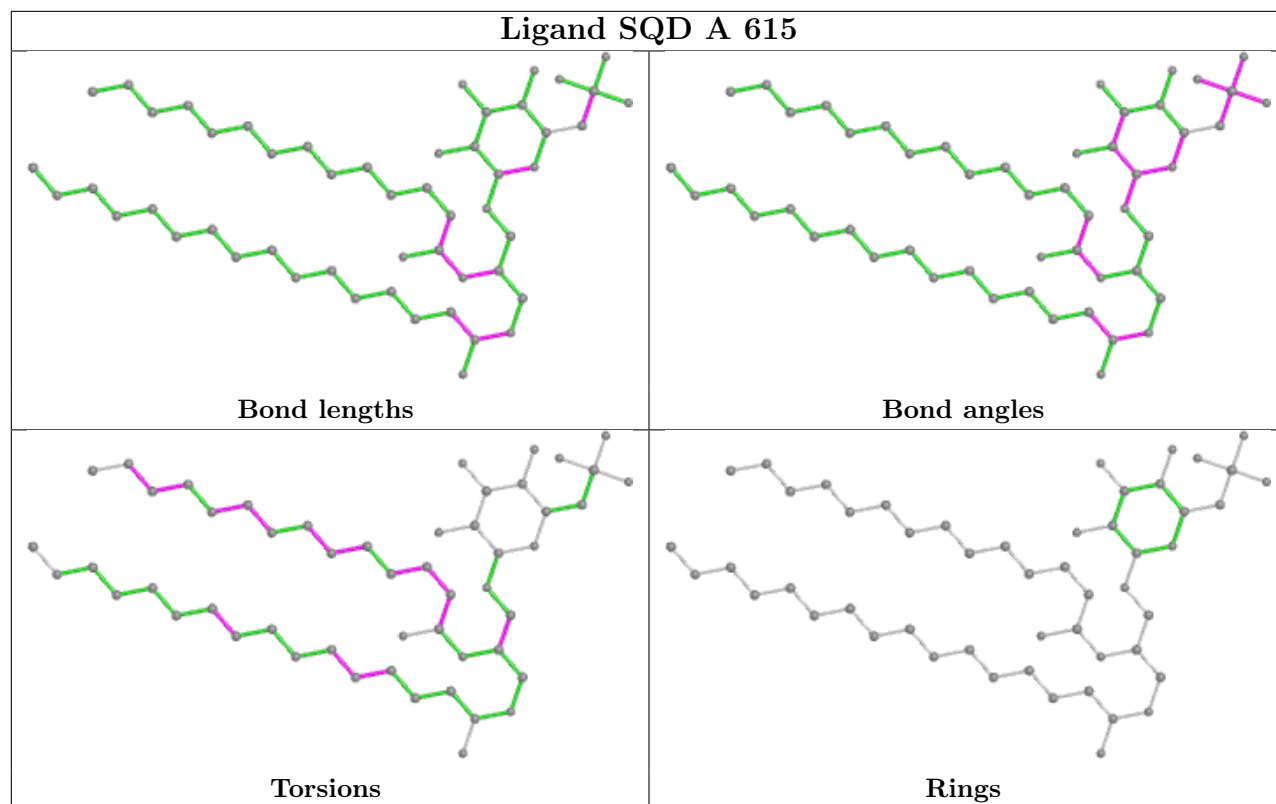


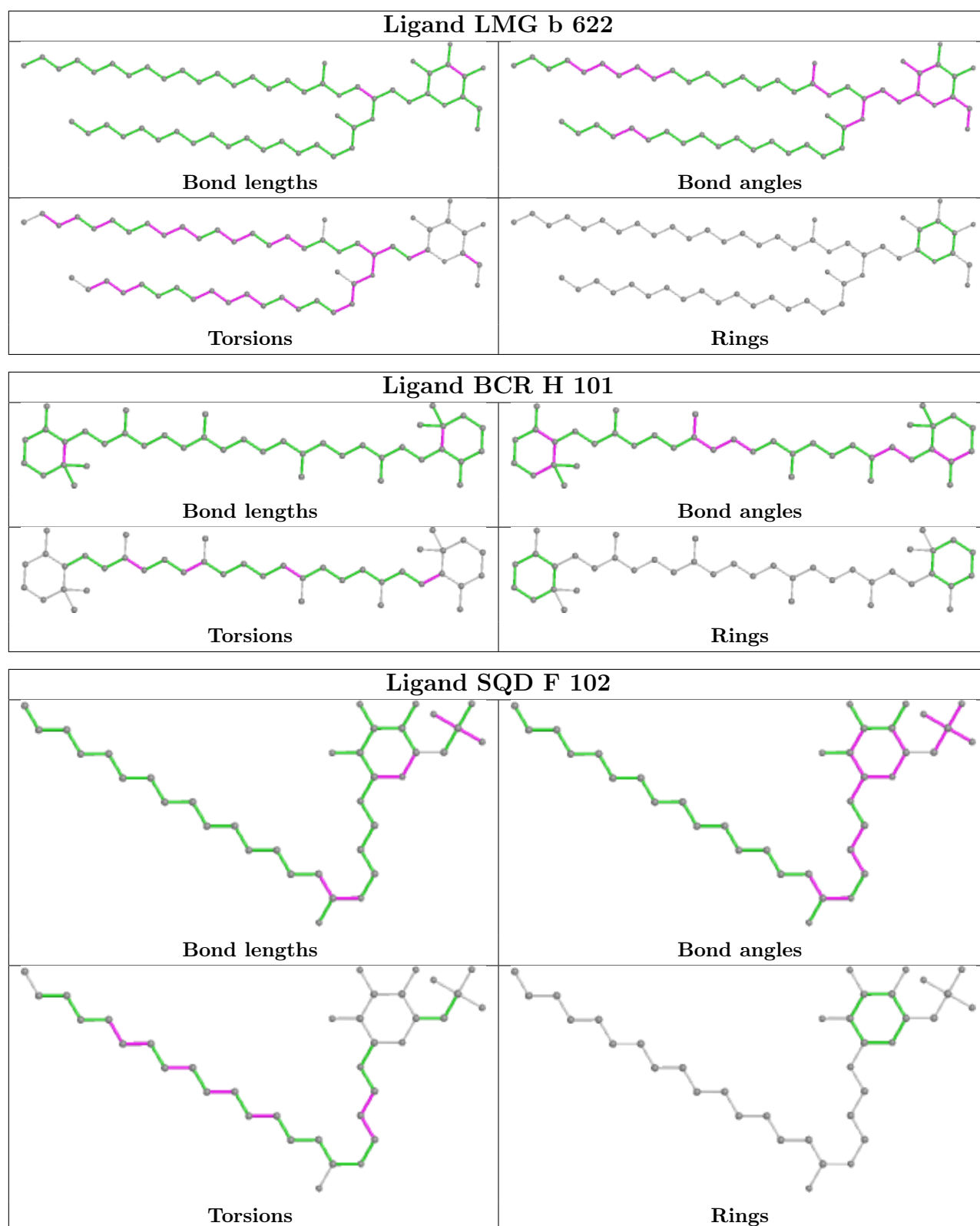


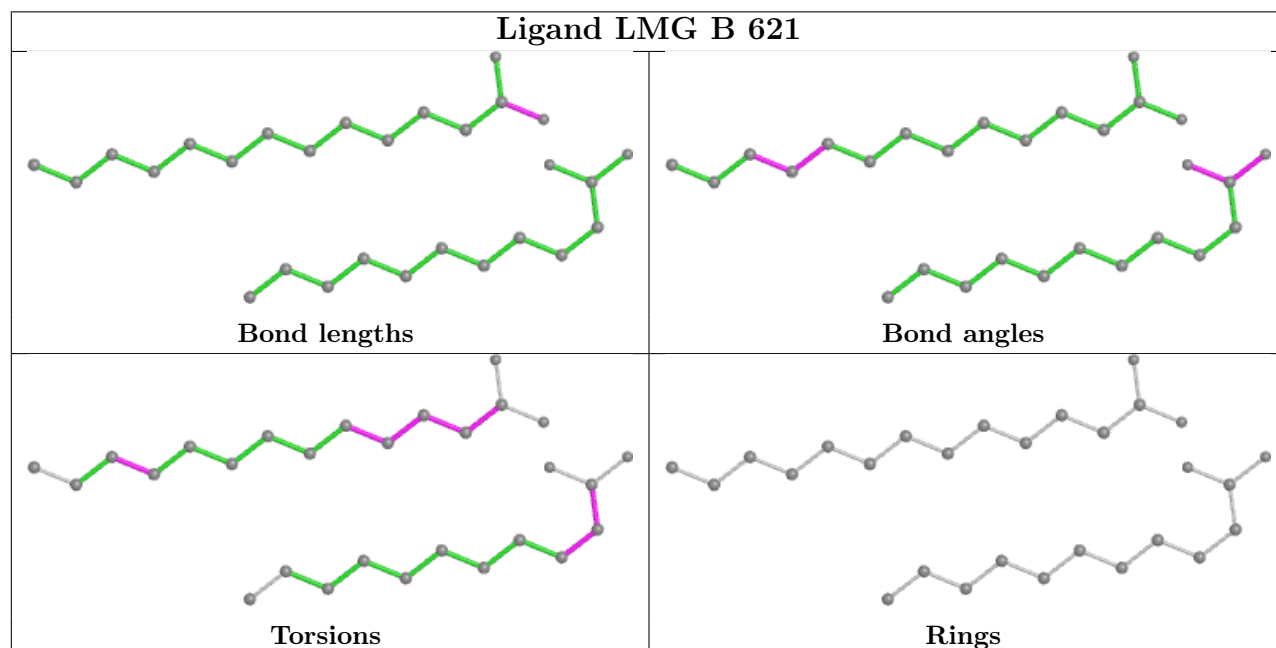
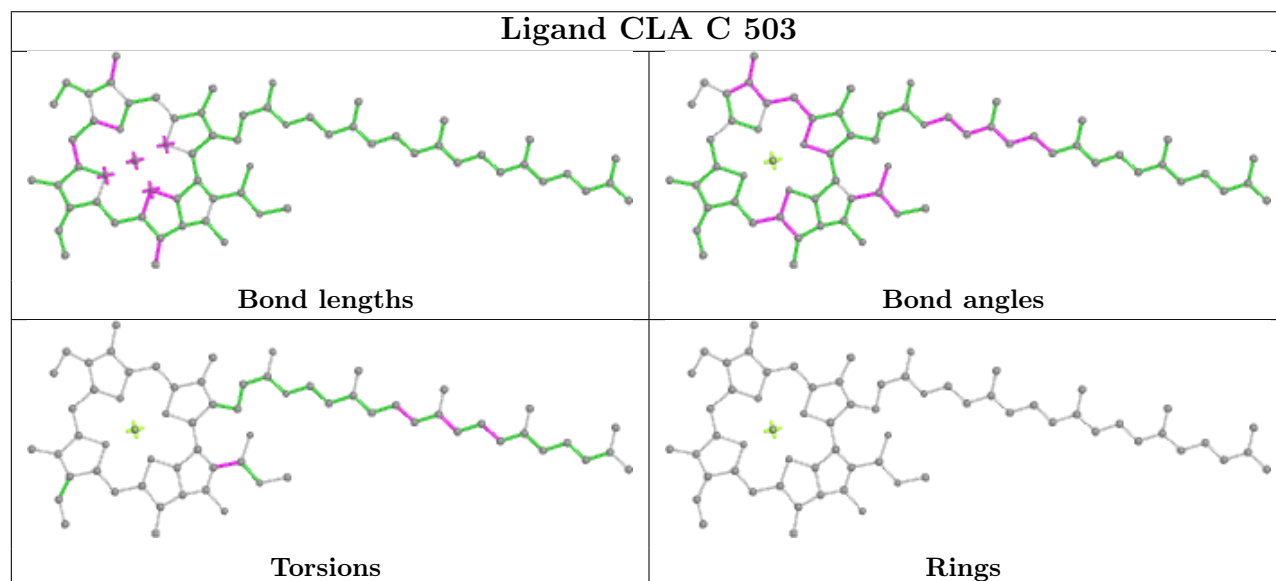
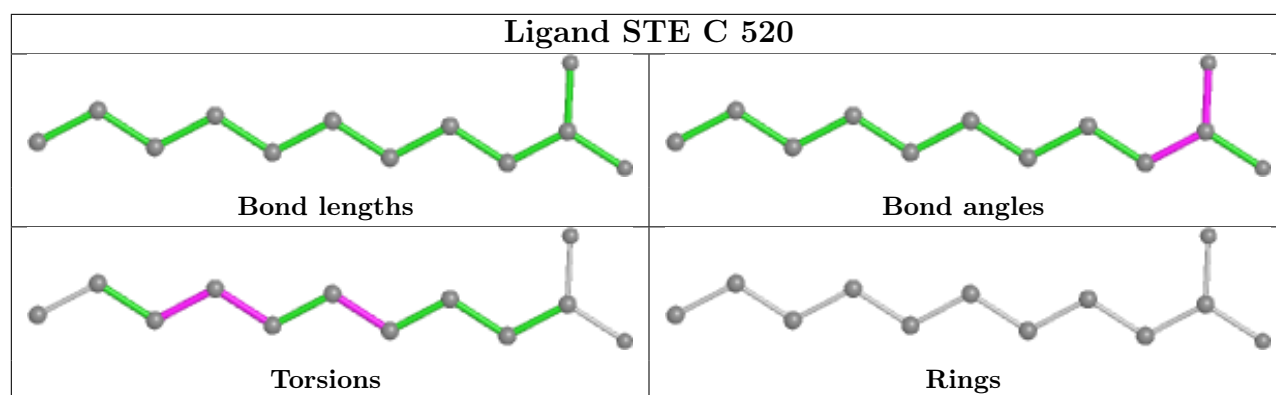


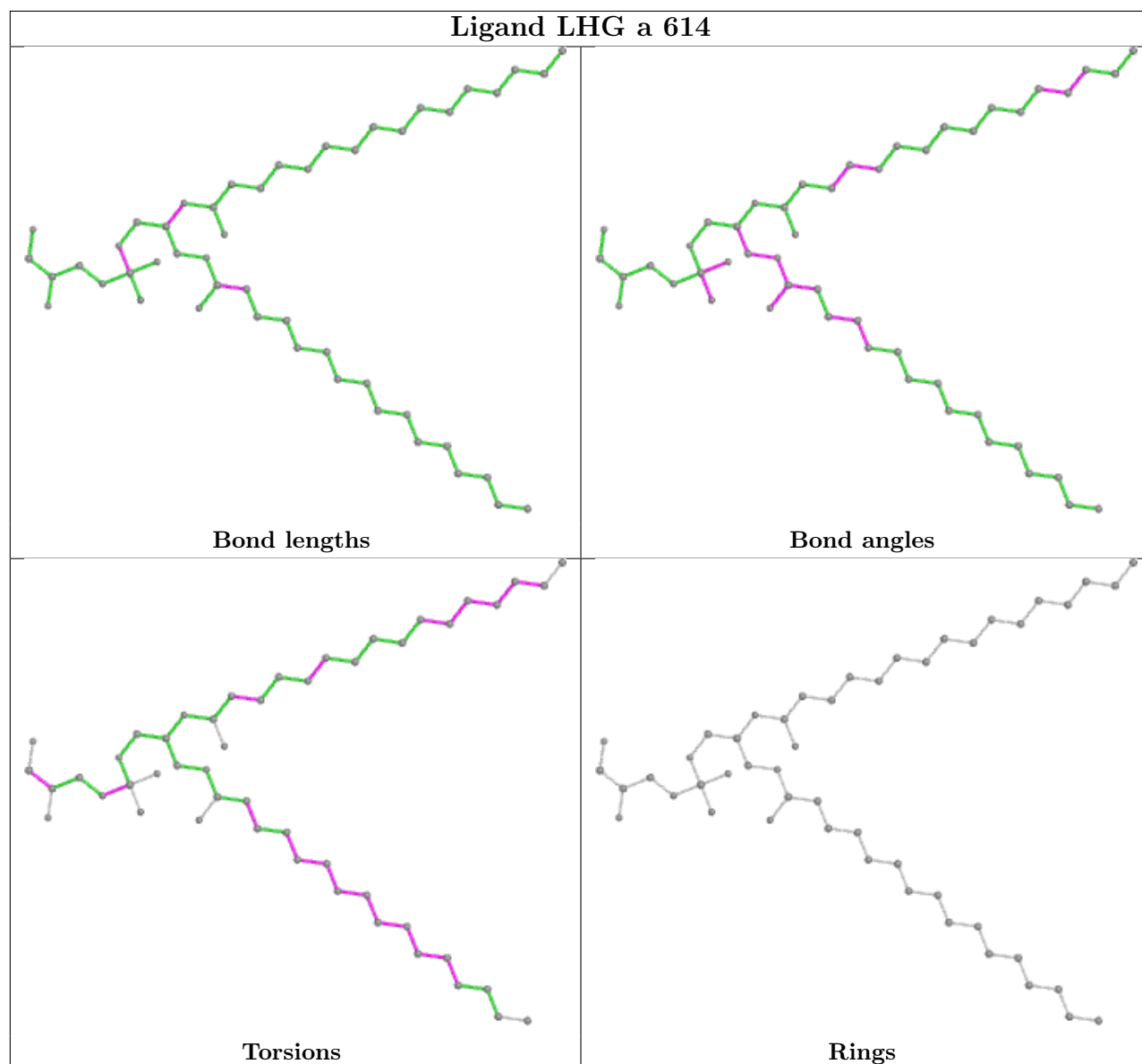
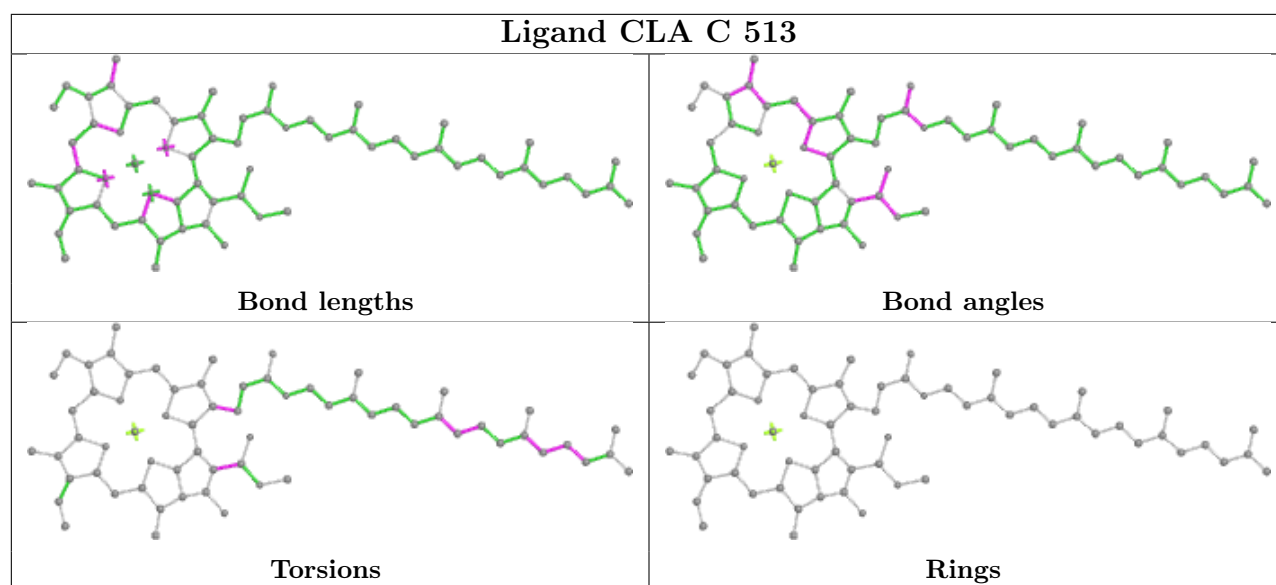


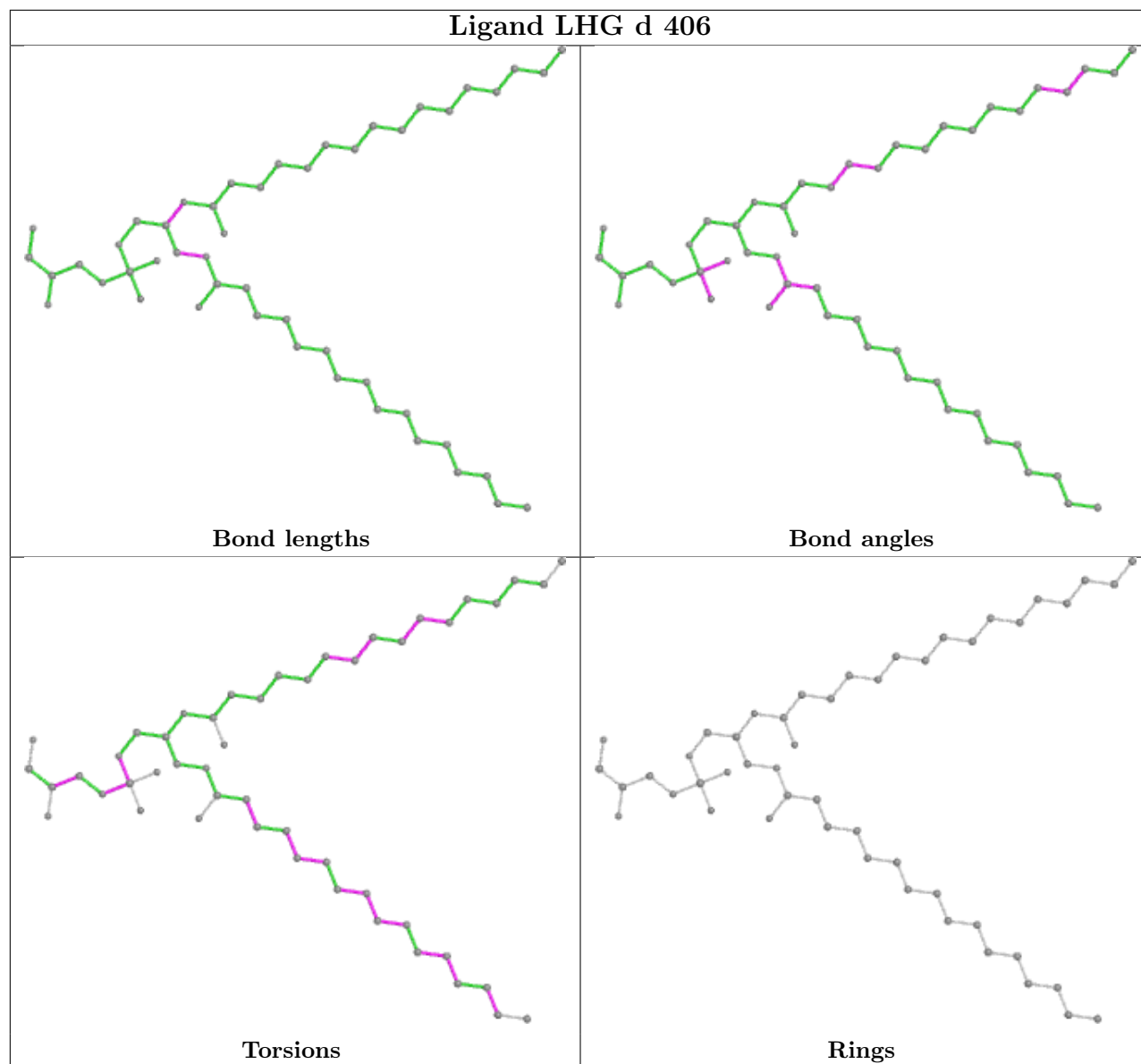




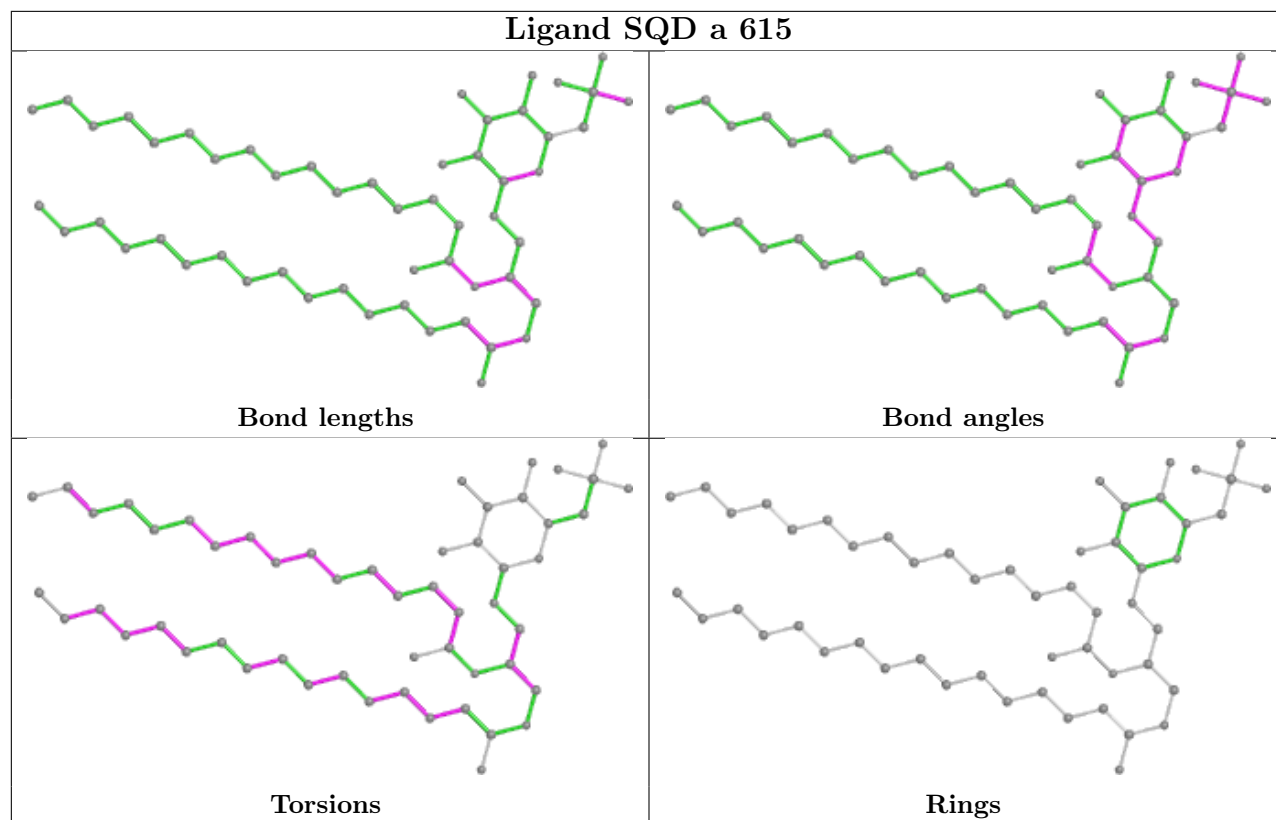


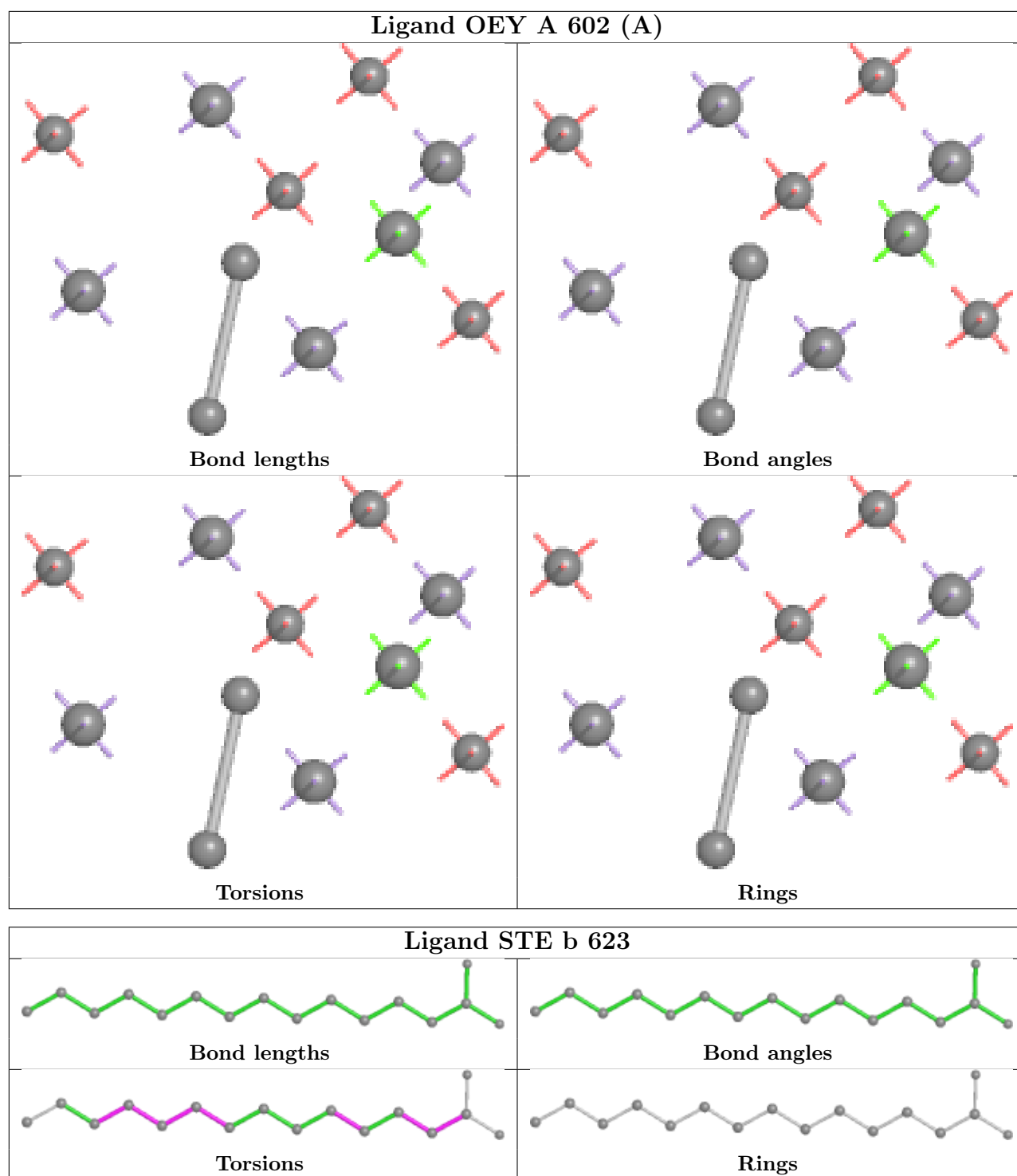


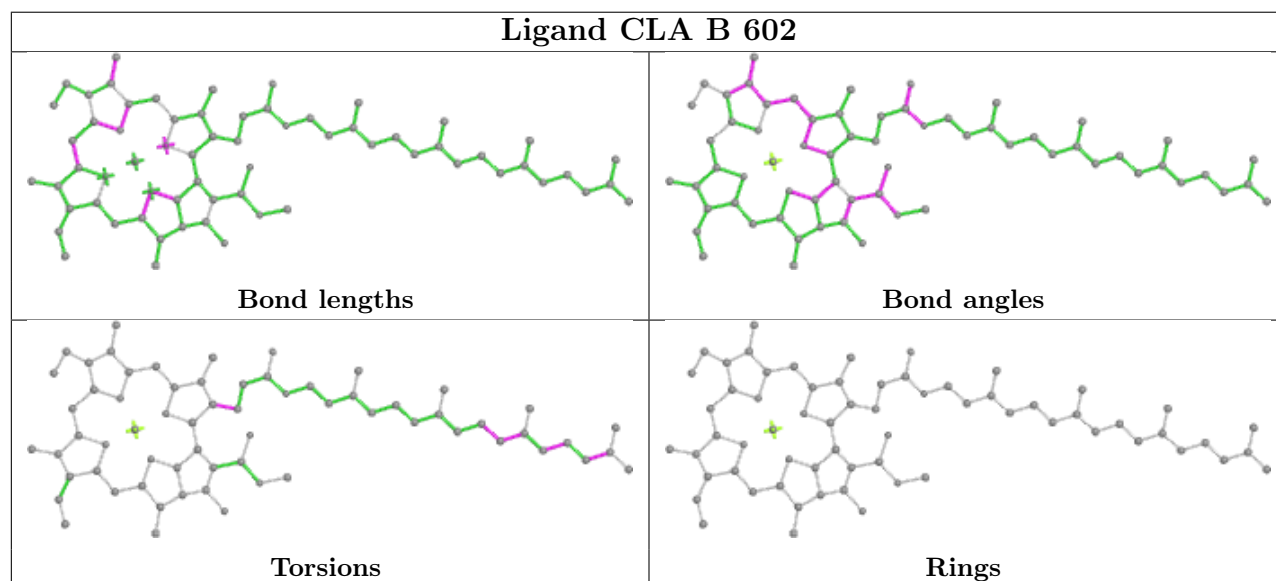
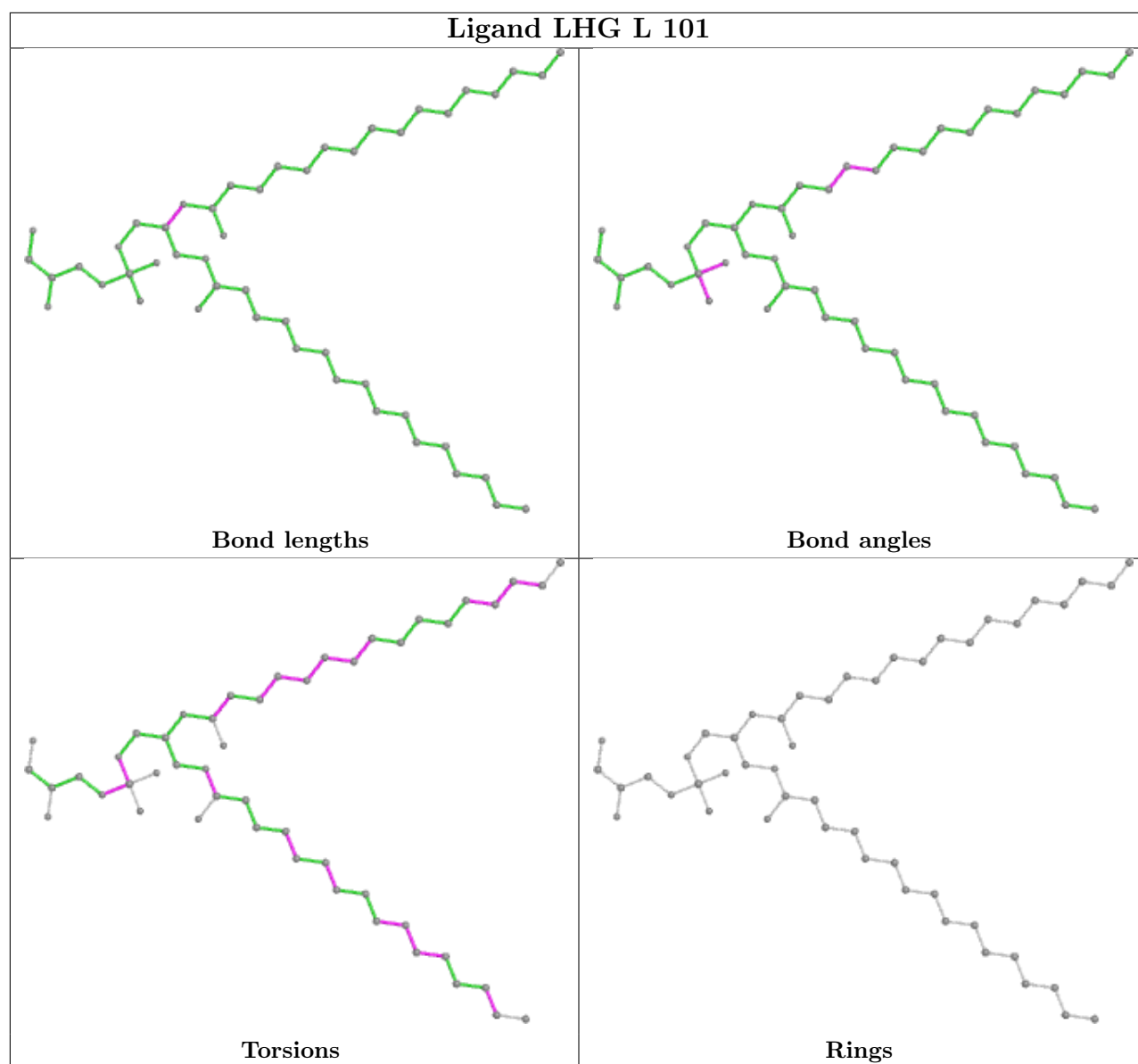


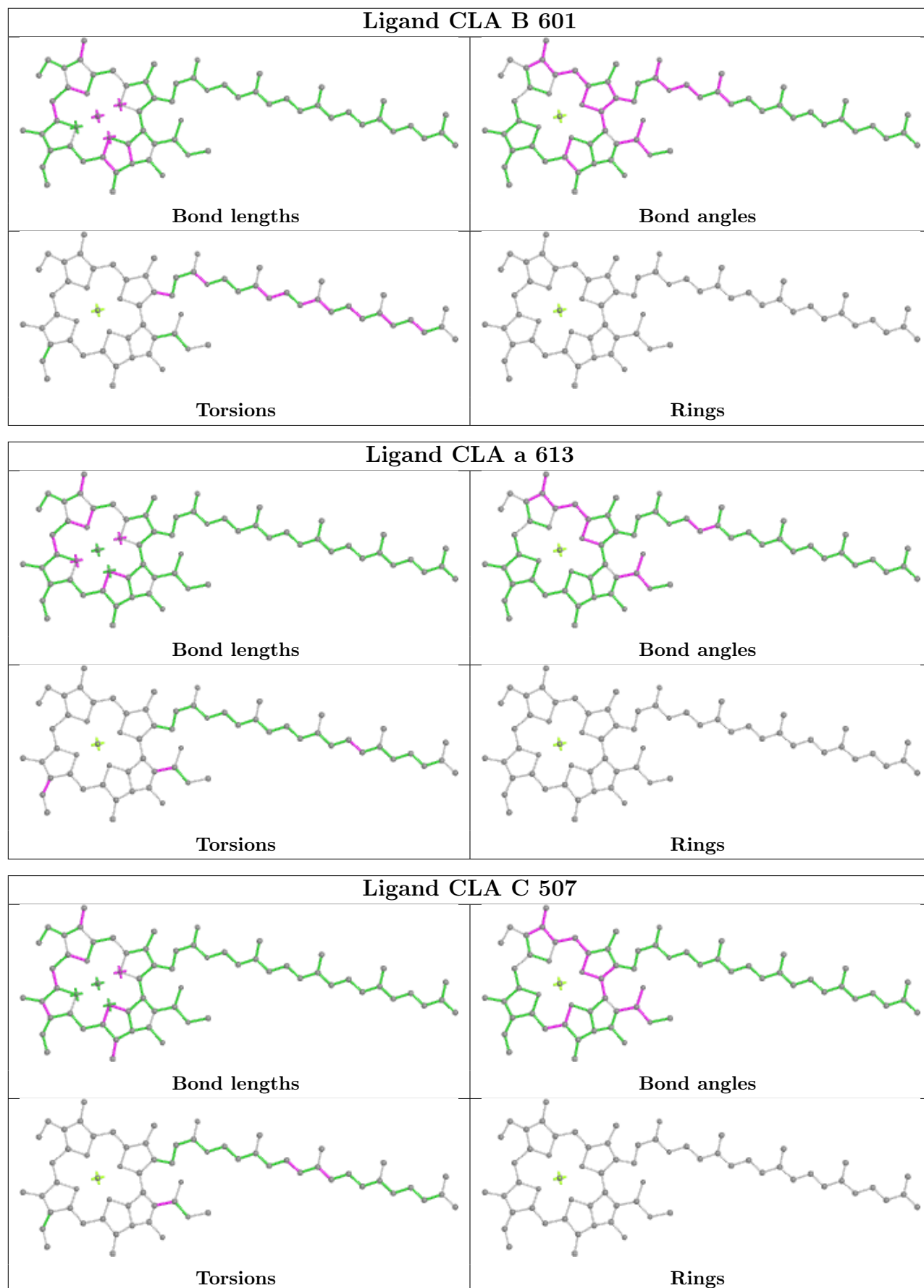


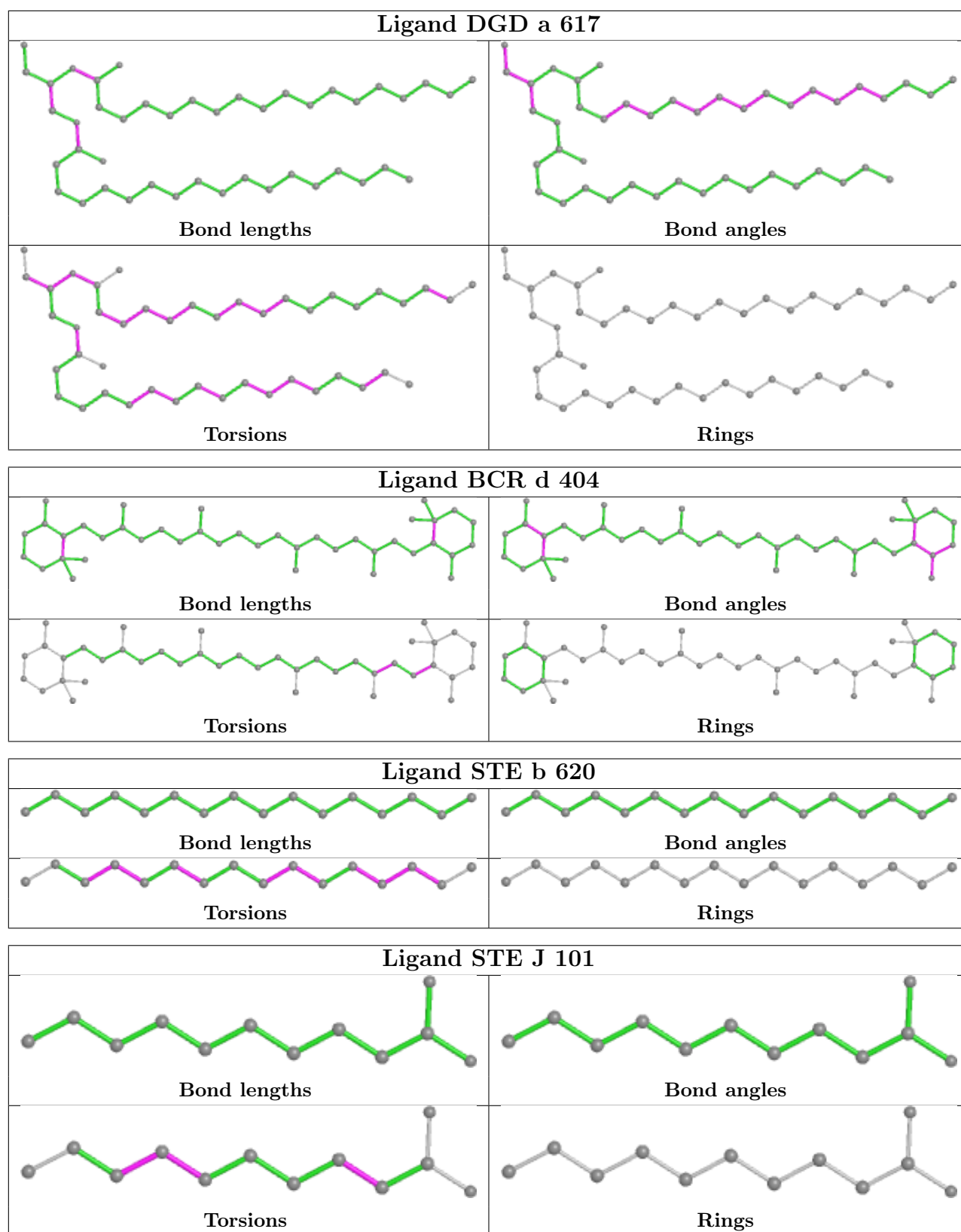


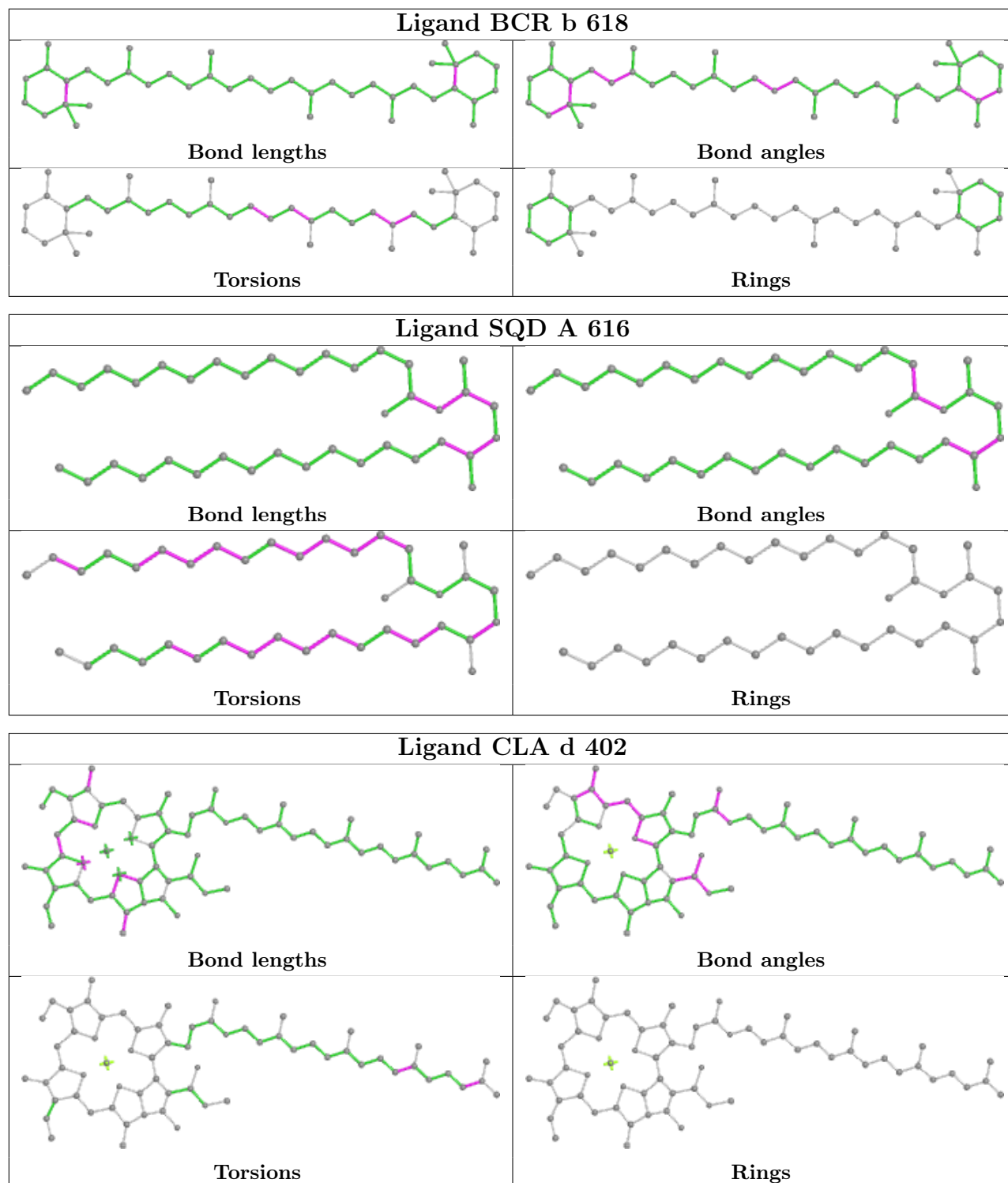


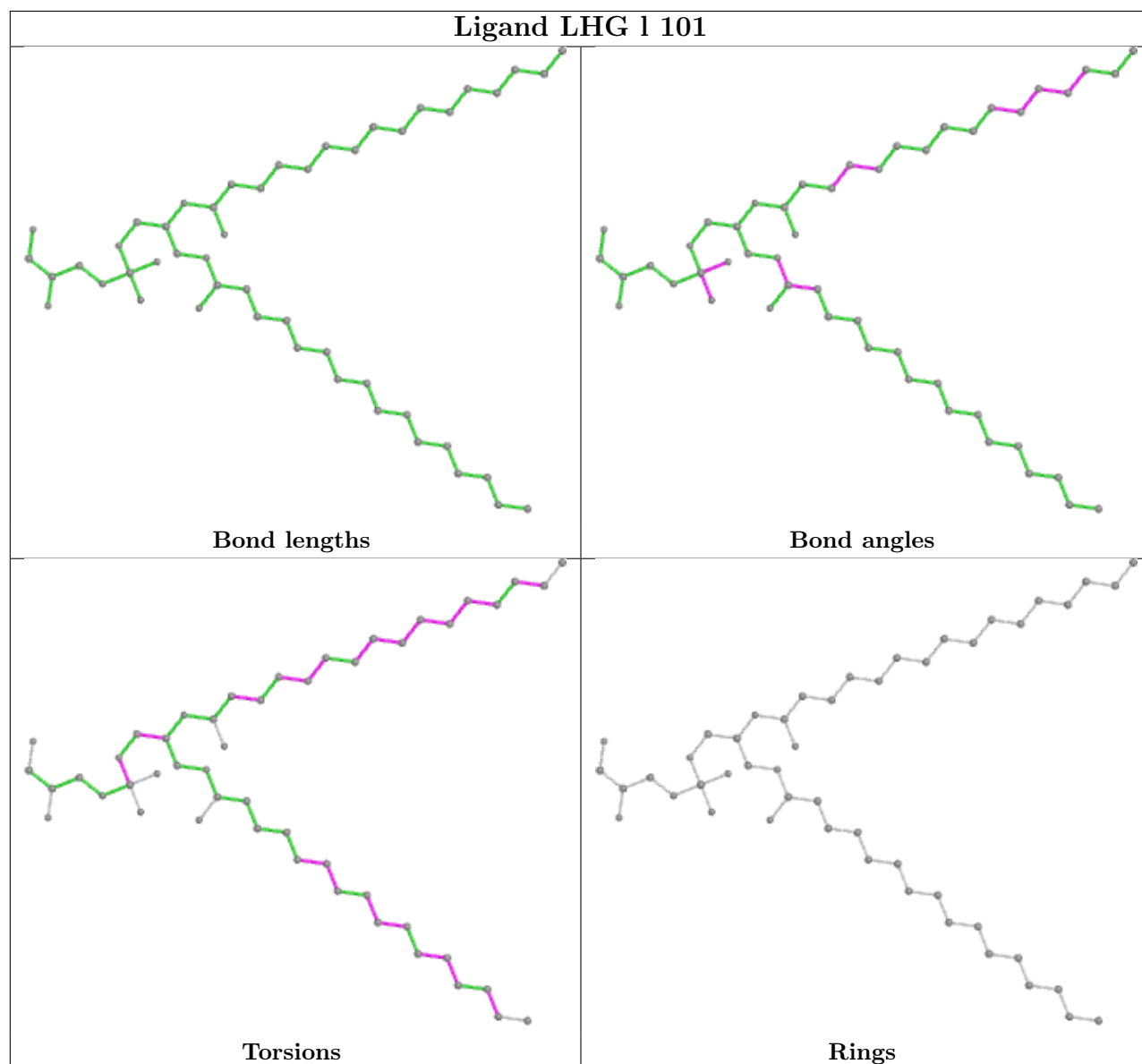
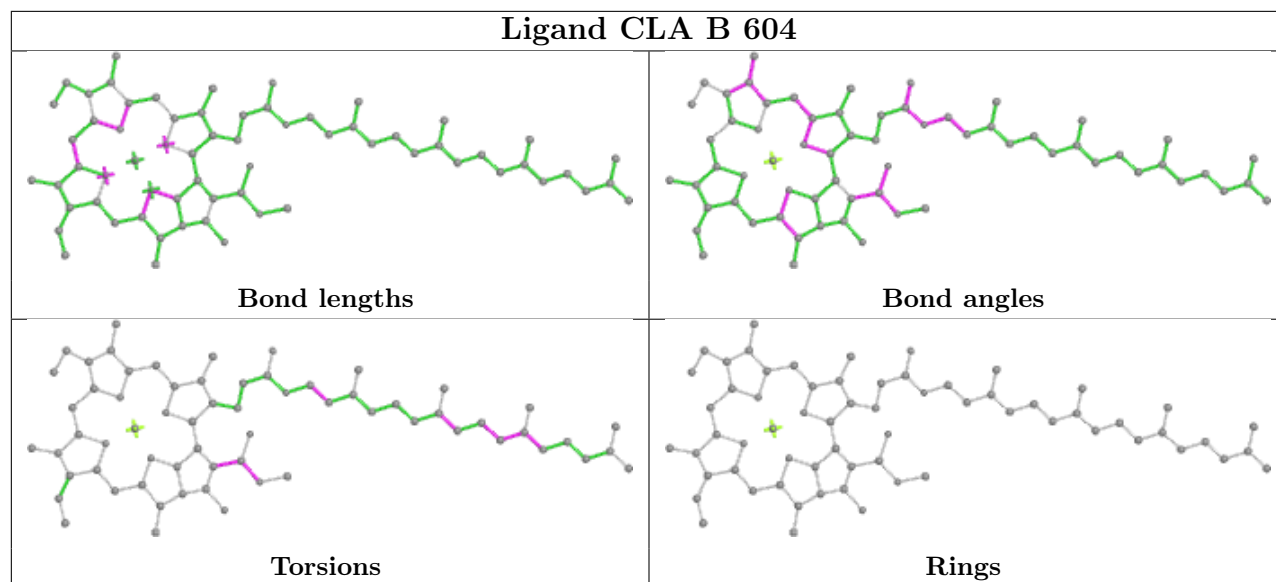


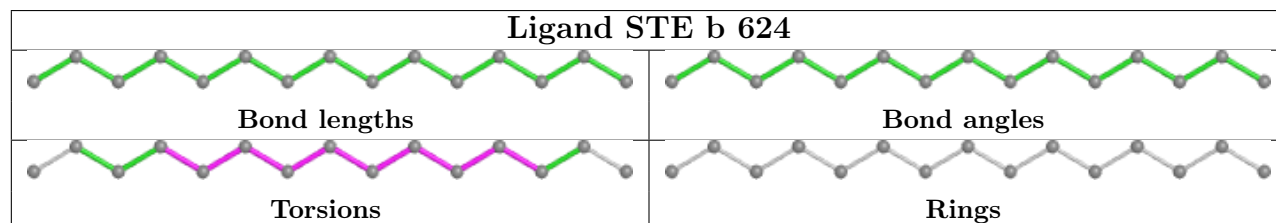
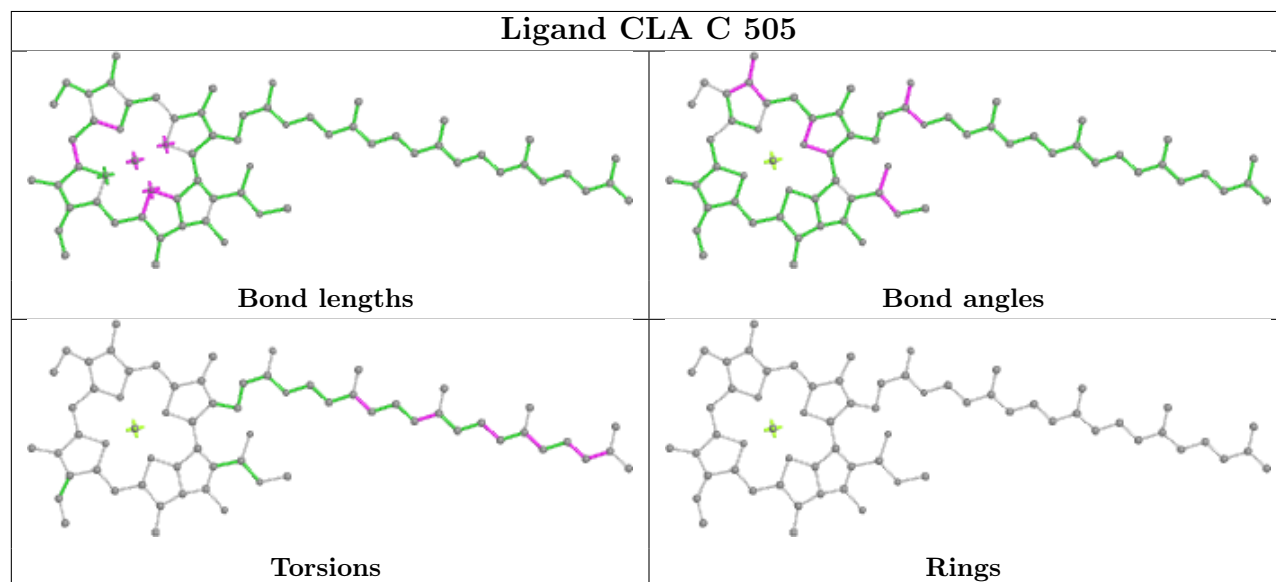
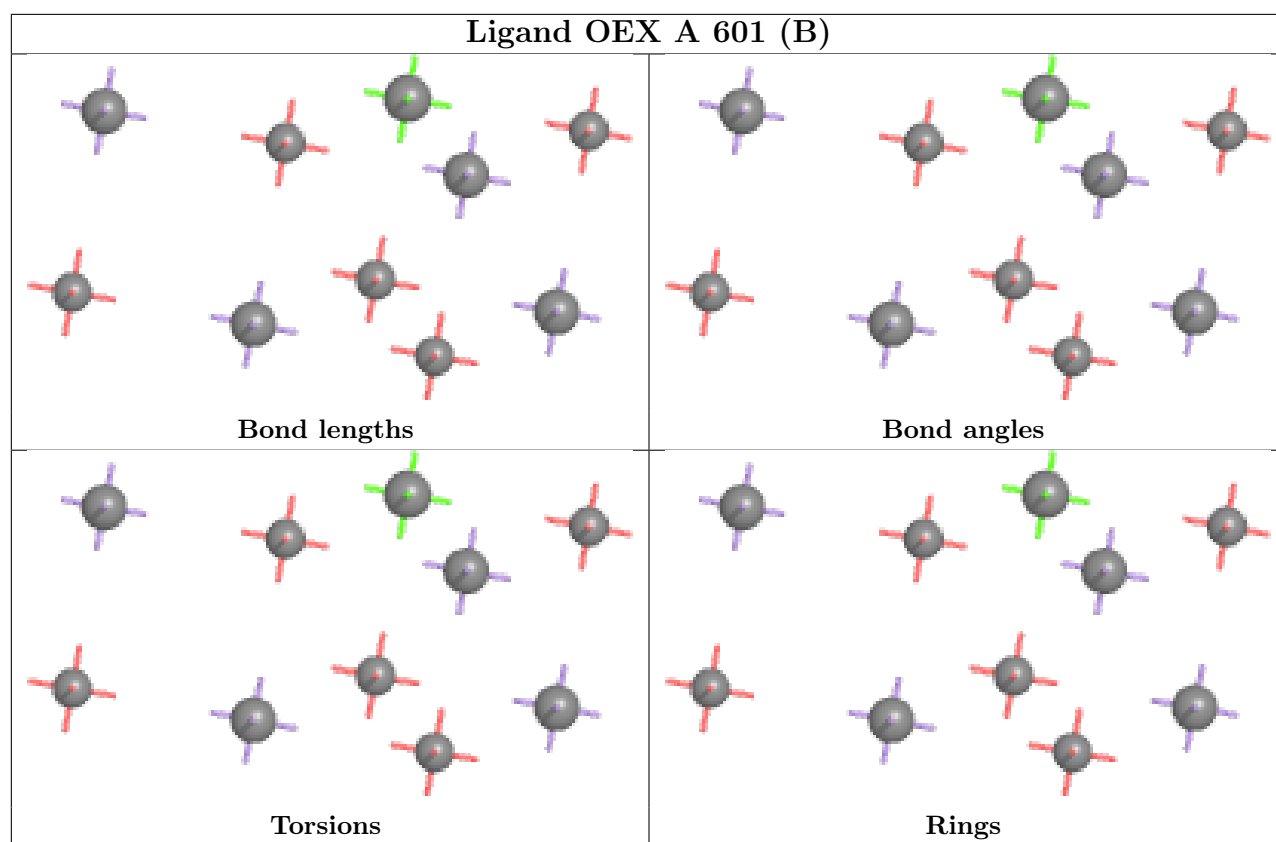




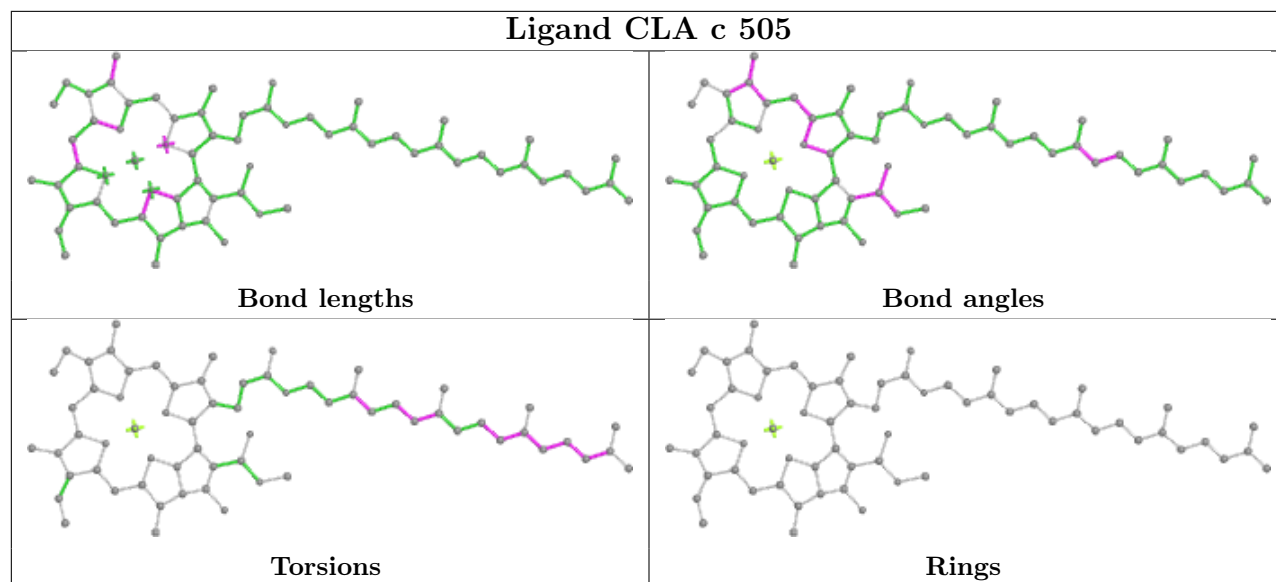












## 5.7 Other polymers [i](#)

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	334/344 (97%)	-0.57	2 (0%) 89 88	23, 28, 47, 76	0
1	a	334/344 (97%)	-0.50	2 (0%) 89 88	23, 30, 56, 76	0
2	B	505/510 (99%)	-0.46	9 (1%) 68 66	24, 33, 60, 90	0
2	b	505/510 (99%)	-0.36	10 (1%) 65 63	25, 35, 68, 105	0
3	C	442/461 (95%)	-0.52	1 (0%) 95 94	24, 35, 50, 70	0
3	c	451/461 (97%)	-0.42	6 (1%) 77 76	26, 39, 57, 91	0
4	D	341/352 (96%)	-0.58	2 (0%) 89 88	23, 30, 45, 78	0
4	d	341/352 (96%)	-0.49	3 (0%) 84 83	24, 33, 57, 82	0
5	E	82/84 (97%)	0.16	7 (8%) 10 10	33, 49, 67, 83	0
5	e	82/84 (97%)	0.23	5 (6%) 21 20	37, 56, 76, 82	0
6	F	34/45 (75%)	-0.13	2 (5%) 22 21	35, 41, 58, 88	0
6	f	34/45 (75%)	0.01	2 (5%) 22 21	39, 48, 74, 88	0
7	H	65/66 (98%)	-0.18	1 (1%) 73 72	32, 40, 54, 68	0
7	h	63/66 (95%)	-0.11	1 (1%) 72 70	39, 49, 60, 63	0
8	I	35/38 (92%)	-0.39	2 (5%) 23 23	32, 38, 62, 81	0
8	i	35/38 (92%)	-0.34	2 (5%) 23 23	31, 39, 67, 81	0
9	J	36/40 (90%)	-0.14	2 (5%) 24 23	33, 46, 71, 84	0
9	j	36/40 (90%)	0.24	3 (8%) 11 10	38, 52, 83, 93	0
10	K	37/46 (80%)	-0.05	1 (2%) 54 53	40, 47, 62, 70	0
10	k	37/46 (80%)	-0.09	0 100 100	46, 51, 66, 78	0
11	L	37/37 (100%)	-0.40	2 (5%) 25 24	24, 28, 60, 64	0
11	l	36/37 (97%)	-0.33	2 (5%) 24 23	26, 31, 63, 87	0
12	M	32/36 (88%)	-0.39	1 (3%) 49 48	27, 33, 57, 70	0
12	m	31/36 (86%)	-0.32	0 100 100	28, 32, 50, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.00	17 (6%) 16 15	25, 41, 77, 126	0
13	o	244/272 (89%)	-0.11	13 (5%) 26 25	26, 39, 78, 115	0
14	T	29/32 (90%)	-0.38	1 (3%) 45 44	26, 30, 54, 67	0
14	t	29/32 (90%)	-0.18	3 (10%) 6 6	26, 31, 67, 81	0
15	U	97/134 (72%)	-0.27	2 (2%) 63 62	30, 41, 66, 89	0
15	u	97/134 (72%)	-0.30	3 (3%) 49 48	31, 39, 55, 85	0
16	V	137/163 (84%)	-0.46	0 100 100	29, 38, 55, 71	0
16	v	137/163 (84%)	-0.27	1 (0%) 87 87	33, 44, 63, 75	0
17	Y	27/46 (58%)	0.71	3 (11%) 5 4	49, 66, 76, 85	0
17	y	30/46 (65%)	0.48	1 (3%) 46 45	56, 68, 77, 93	0
18	X	38/41 (92%)	-0.08	3 (7%) 12 11	39, 48, 65, 74	0
18	x	39/41 (95%)	0.40	3 (7%) 13 12	47, 60, 80, 92	0
19	Z	62/62 (100%)	0.67	11 (17%) 1 1	52, 63, 101, 111	0
19	z	62/62 (100%)	0.53	6 (9%) 7 7	55, 64, 100, 109	0
20	R	34/41 (82%)	0.96	7 (20%) 1 0	57, 66, 78, 84	0
20	r	31/41 (75%)	1.75	11 (35%) 0 0	68, 80, 97, 101	0
All	All	5302/5700 (93%)	-0.30	153 (2%) 51 50	23, 37, 69, 126	0

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	3	GLN	8.6
13	o	58	ASN	8.0
13	O	4	THR	7.2
6	F	12	SER	7.2
13	O	62	GLU	7.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.92	0.14	35,47,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	FME	T	1	10/11	0.94	0.11	34,39,49,63	0
14	FME	t	1	10/11	0.94	0.08	30,38,53,58	0
8	FME	I	1	10/11	0.95	0.10	39,44,52,53	0
12	FME	m	1	10/11	0.96	0.15	32,46,60,66	0
8	FME	i	1	10/11	0.97	0.15	37,46,50,53	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( $\text{\AA}^2$ )	Q<0.9
33	STE	a	618	12/20	0.65	0.24	49,63,71,74	0
29	LMG	c	521	48/55	0.70	0.26	48,66,83,91	0
30	LHG	E	101	49/49	0.71	0.26	43,73,89,90	0
33	STE	H	103	18/20	0.72	0.23	56,69,71,71	0
33	STE	B	620	17/20	0.72	0.18	32,46,61,64	0
33	STE	X	101	20/20	0.74	0.22	35,44,63,75	0
33	STE	k	103	12/20	0.74	0.29	55,65,72,77	0
33	STE	b	623	16/20	0.76	0.15	52,57,74,79	0
33	STE	t	104	18/20	0.76	0.18	45,52,78,78	0
33	STE	B	626	16/20	0.77	0.22	47,54,60,64	0
31	SQD	a	616	36/54	0.78	0.17	37,52,65,73	0
33	STE	c	520	20/20	0.78	0.15	40,51,78,80	0
29	LMG	b	622	55/55	0.79	0.26	51,63,76,78	0
33	STE	b	621	20/20	0.79	0.22	38,50,67,71	0
32	DGD	a	617	44/66	0.80	0.16	36,49,71,74	0
29	LMG	d	408	23/55	0.80	0.18	48,61,69,73	0
33	STE	B	625	12/20	0.80	0.26	51,56,71,74	0
33	STE	E	102	12/20	0.81	0.24	58,68,81,81	0
29	LMG	D	409	33/55	0.82	0.15	32,50,67,78	0
28	PL9	A	611	55/55	0.82	0.24	39,56,70,72	0
33	STE	t	102	14/20	0.82	0.14	41,45,59,59	0
33	STE	b	625	20/20	0.82	0.19	46,55,62,63	0
33	STE	C	519	12/20	0.83	0.18	38,43,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	LHG	e	102	42/49	0.83	0.30	60,76,86,97	0
29	LMG	A	613	48/55	0.83	0.17	36,54,67,76	0
28	PL9	a	612	55/55	0.83	0.21	41,61,74,80	0
33	STE	b	624	15/20	0.84	0.16	45,51,65,66	0
29	LMG	c	522	49/55	0.84	0.16	37,50,75,84	0
25	CLA	h	101	65/65	0.84	0.17	46,62,82,86	0
31	SQD	A	616	39/54	0.85	0.16	41,51,73,74	0
33	STE	b	626	10/20	0.85	0.17	43,51,58,60	0
32	DGD	A	617	66/66	0.85	0.17	47,56,65,72	0
31	SQD	B	623	54/54	0.86	0.16	36,59,78,86	0
33	STE	t	103	10/20	0.86	0.15	46,50,56,60	0
33	STE	m	102	12/20	0.86	0.15	46,56,66,66	0
33	STE	x	101	20/20	0.86	0.18	41,50,59,62	0
31	SQD	f	101	41/54	0.87	0.18	57,75,85,87	0
25	CLA	c	512	65/65	0.87	0.16	44,52,73,80	0
25	CLA	b	615	60/65	0.87	0.15	30,39,77,82	0
27	BCR	D	405	40/40	0.87	0.13	28,38,67,71	0
33	STE	B	624	12/20	0.87	0.15	41,48,59,60	0
29	LMG	B	621	28/55	0.87	0.13	35,47,57,65	0
29	LMG	D	407	51/55	0.87	0.18	31,44,68,69	0
31	SQD	b	619	49/54	0.87	0.16	40,55,78,82	0
33	STE	j	101	12/20	0.88	0.13	47,53,56,56	0
33	STE	C	520	12/20	0.88	0.17	45,52,59,59	0
33	STE	l	102	18/20	0.88	0.15	37,44,64,64	0
29	LMG	c	519	37/55	0.88	0.19	43,57,66,68	0
29	LMG	m	101	51/55	0.88	0.12	34,48,59,63	0
33	STE	J	101	12/20	0.88	0.13	45,52,59,63	0
25	CLA	c	513	65/65	0.88	0.17	41,55,78,82	0
25	CLA	C	513	65/65	0.88	0.15	38,50,72,76	0
27	BCR	c	514	40/40	0.89	0.13	44,50,57,58	0
29	LMG	M	101	51/55	0.89	0.13	33,47,59,63	0
25	CLA	B	601	65/65	0.89	0.14	31,52,75,81	0
33	STE	b	620	16/20	0.89	0.13	34,46,57,58	0
29	LMG	C	518	48/55	0.89	0.16	39,58,70,76	0
25	CLA	B	616	60/65	0.89	0.15	24,32,66,70	0
31	SQD	F	102	36/54	0.90	0.17	44,61,69,70	0
25	CLA	c	506	65/65	0.90	0.13	33,41,71,75	0
33	STE	I	101	15/20	0.90	0.13	40,50,60,63	0
33	STE	d	410	17/20	0.91	0.13	43,48,62,62	0
25	CLA	C	506	65/65	0.91	0.12	27,37,69,71	0
25	CLA	C	512	65/65	0.91	0.14	34,44,75,80	0
25	CLA	B	606	65/65	0.91	0.12	22,32,58,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	BCR	d	404	40/40	0.91	0.15	38,47,72,79	0
25	CLA	D	404	65/65	0.91	0.14	25,32,81,91	0
29	LMG	d	409	44/55	0.91	0.14	37,44,66,73	0
33	STE	M	103	10/20	0.91	0.14	41,45,51,57	0
25	CLA	d	403	65/65	0.91	0.13	30,39,72,76	0
33	STE	C	521	16/20	0.92	0.10	34,43,57,57	0
27	BCR	k	101	40/40	0.92	0.11	44,52,60,62	0
32	DGD	H	102	62/66	0.92	0.12	32,41,48,52	0
25	CLA	a	610	65/65	0.92	0.14	22,28,65,69	0
32	DGD	h	103	62/66	0.92	0.13	38,43,53,57	0
27	BCR	K	102	40/40	0.92	0.10	37,45,55,58	0
25	CLA	b	605	65/65	0.93	0.11	28,36,59,62	0
25	CLA	b	608	65/65	0.93	0.14	30,39,55,68	0
27	BCR	h	102	40/40	0.93	0.11	37,49,62,64	0
27	BCR	K	103	40/40	0.93	0.13	32,43,51,57	0
31	SQD	a	615	54/54	0.93	0.15	37,54,68,70	0
27	BCR	b	618	40/40	0.93	0.11	31,43,56,59	0
25	CLA	B	604	65/65	0.94	0.11	22,28,57,61	0
25	CLA	B	609	65/65	0.94	0.12	26,34,50,54	0
33	STE	M	102	15/20	0.94	0.09	38,44,55,64	0
27	BCR	T	101	40/40	0.94	0.09	29,35,43,46	0
27	BCR	b	617	40/40	0.94	0.09	26,34,43,46	0
25	CLA	c	508	64/65	0.94	0.10	32,38,69,88	0
32	DGD	C	516	62/66	0.94	0.10	32,42,80,88	0
32	DGD	C	517	62/66	0.94	0.10	25,39,64,71	0
25	CLA	a	608	65/65	0.94	0.11	26,35,73,78	0
25	CLA	C	508	65/65	0.94	0.10	29,34,74,85	0
32	DGD	c	517	62/66	0.94	0.10	34,44,72,76	0
32	DGD	c	518	62/66	0.94	0.11	30,42,65,70	0
25	CLA	C	511	65/65	0.94	0.11	27,42,51,56	0
25	CLA	B	614	65/65	0.94	0.11	22,32,62,69	0
27	BCR	k	102	40/40	0.94	0.12	38,47,55,58	0
27	BCR	B	618	40/40	0.94	0.08	26,34,40,43	0
30	LHG	a	614	49/49	0.94	0.11	30,46,60,63	0
27	BCR	B	619	40/40	0.94	0.09	28,38,50,53	0
31	SQD	A	615	52/54	0.94	0.14	34,48,69,73	0
25	CLA	b	613	65/65	0.94	0.11	27,35,63,67	0
27	BCR	H	101	40/40	0.94	0.10	31,41,51,53	0
27	BCR	K	101	40/40	0.94	0.10	38,47,54,56	0
30	LHG	B	622	49/49	0.95	0.11	29,39,54,57	0
27	BCR	c	515	40/40	0.95	0.10	29,42,50,53	0
25	CLA	d	402	65/65	0.95	0.10	23,29,49,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	b	609	65/65	0.95	0.11	28,34,41,48	0
30	LHG	l	101	49/49	0.95	0.10	30,39,48,54	0
25	CLA	A	607	65/65	0.95	0.10	24,29,76,83	0
27	BCR	A	610	40/40	0.95	0.08	24,31,41,42	0
27	BCR	t	101	40/40	0.95	0.08	25,32,45,47	0
27	BCR	B	617	40/40	0.95	0.09	25,33,42,43	0
25	CLA	b	614	65/65	0.95	0.10	28,36,51,59	0
28	PL9	d	405	55/55	0.95	0.10	22,31,38,39	0
25	CLA	C	503	65/65	0.95	0.08	30,36,41,46	0
27	BCR	C	514	40/40	0.95	0.10	29,36,46,48	0
25	CLA	c	501	65/65	0.95	0.10	28,35,43,49	0
32	DGD	C	515	62/66	0.95	0.09	25,33,65,72	0
25	CLA	c	502	65/65	0.95	0.10	26,34,51,56	0
25	CLA	c	503	65/65	0.95	0.10	31,39,45,49	0
25	CLA	b	601	65/65	0.95	0.11	30,37,51,53	0
25	CLA	c	507	65/65	0.95	0.11	28,37,49,52	0
32	DGD	c	516	62/66	0.95	0.10	25,35,58,68	0
25	CLA	b	603	65/65	0.95	0.10	22,31,64,72	0
27	BCR	a	611	40/40	0.95	0.08	23,31,42,44	0
27	BCR	b	616	40/40	0.95	0.09	27,37,42,45	0
25	CLA	c	511	65/65	0.95	0.11	40,47,57,62	0
25	CLA	B	602	65/65	0.95	0.10	26,32,48,53	0
25	CLA	A	609	54/65	0.95	0.12	20,26,54,60	0
30	LHG	A	614	47/49	0.95	0.11	27,38,64,73	0
25	CLA	B	608	65/65	0.96	0.09	25,30,46,51	0
25	CLA	b	610	65/65	0.96	0.09	22,31,46,52	0
25	CLA	b	611	65/65	0.96	0.09	21,30,42,45	0
25	CLA	b	612	65/65	0.96	0.09	20,28,59,63	0
25	CLA	C	507	65/65	0.96	0.10	26,33,46,51	0
25	CLA	B	603	65/65	0.96	0.09	22,27,51,59	0
25	CLA	C	509	65/65	0.96	0.10	27,35,49,53	0
25	CLA	C	510	65/65	0.96	0.09	29,36,47,53	0
25	CLA	B	610	65/65	0.96	0.09	22,30,36,40	0
25	CLA	B	611	65/65	0.96	0.09	21,28,40,42	0
25	CLA	c	504	60/65	0.96	0.09	29,37,64,68	0
25	CLA	c	505	65/65	0.96	0.09	27,36,54,57	0
25	CLA	B	612	65/65	0.96	0.09	21,28,38,41	0
25	CLA	D	403	65/65	0.96	0.09	20,25,45,51	0
25	CLA	B	613	65/65	0.96	0.09	21,27,54,65	0
25	CLA	c	509	65/65	0.96	0.10	32,39,53,57	0
25	CLA	c	510	65/65	0.96	0.10	29,41,50,54	0
25	CLA	a	607	65/65	0.96	0.09	22,27,37,44	0

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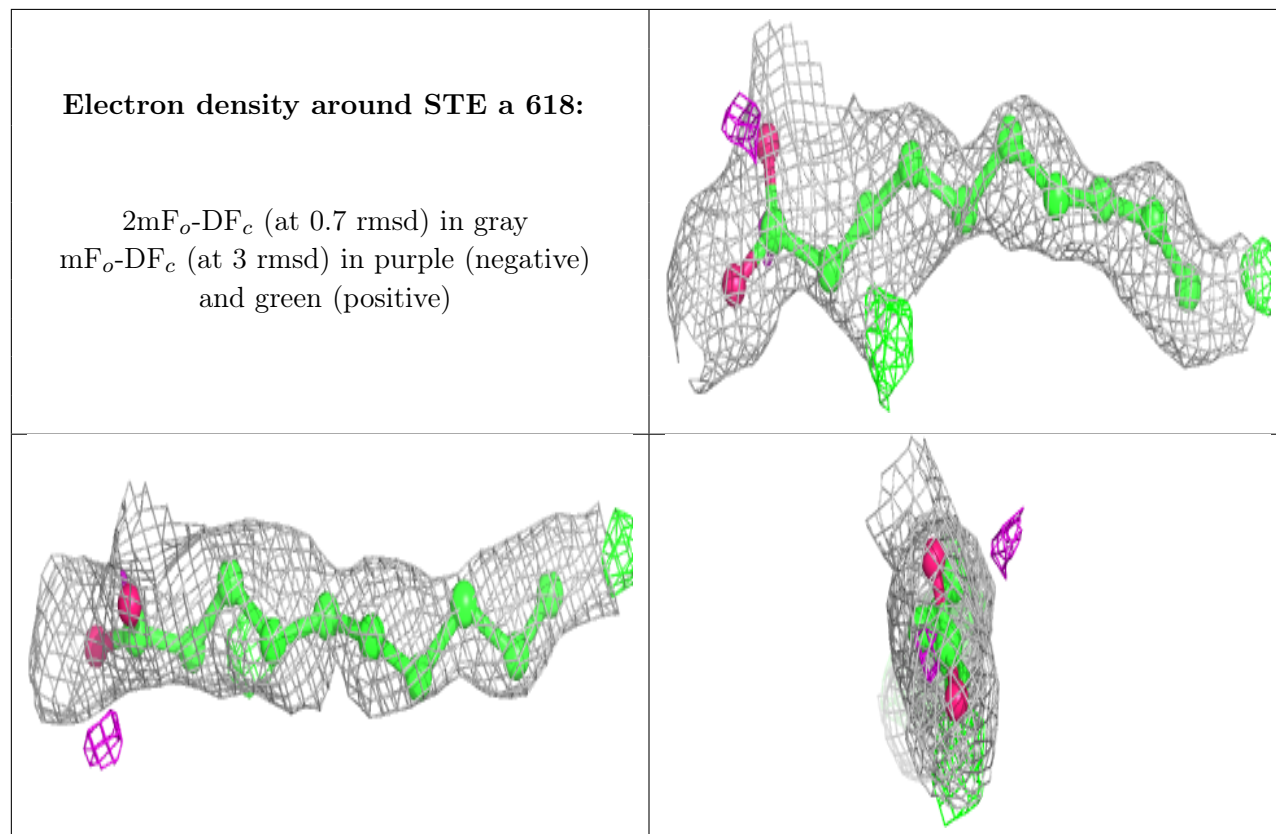
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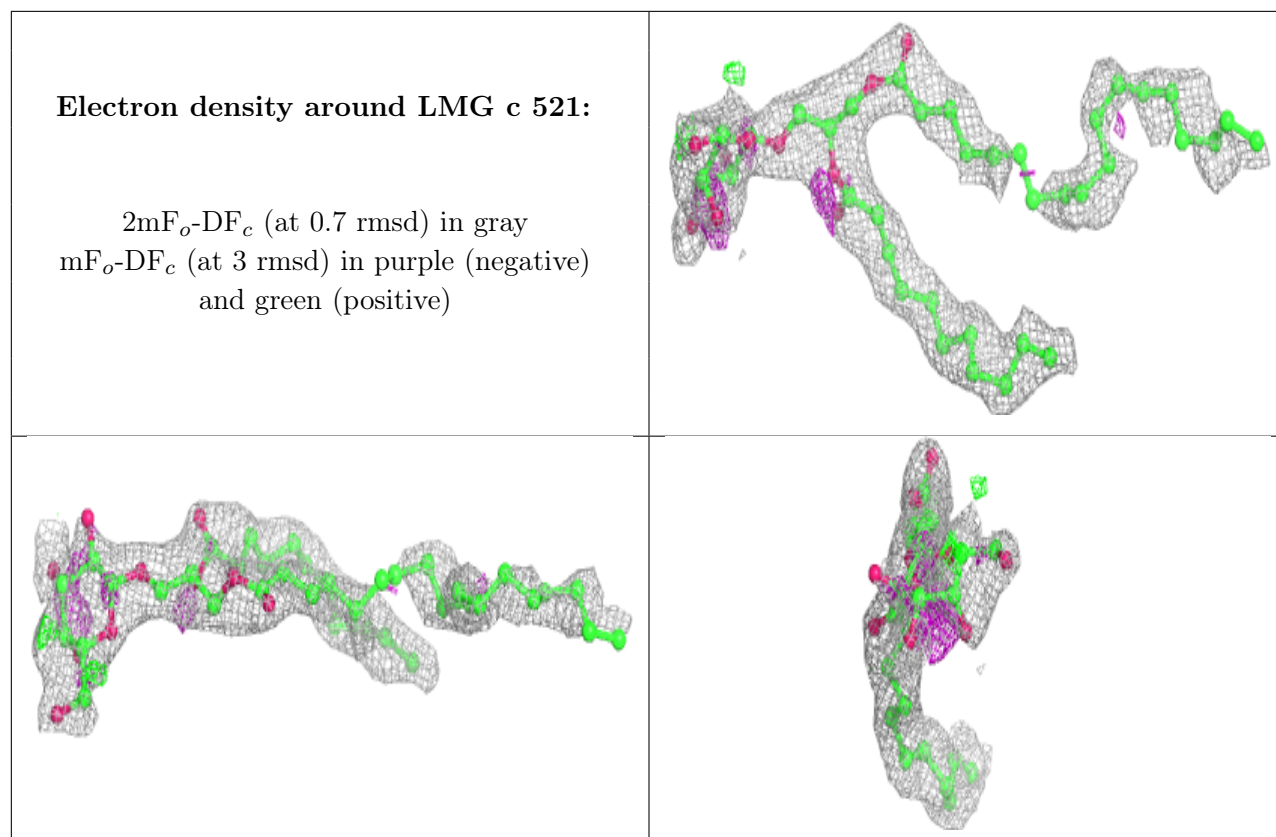
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
25	CLA	A	606	65/65	0.96	0.09	18,24,35,45	0
28	PL9	D	406	55/55	0.96	0.08	21,28,36,40	0
25	CLA	B	615	65/65	0.96	0.08	25,32,49,54	0
25	CLA	A	612	65/65	0.96	0.08	17,25,39,45	0
25	CLA	b	602	65/65	0.96	0.10	24,31,52,61	0
25	CLA	C	502	65/65	0.96	0.08	27,32,44,50	0
26	PHO	a	609	64/64	0.96	0.09	21,28,33,38	0
26	PHO	d	401	64/64	0.96	0.09	23,34,40,44	0
25	CLA	B	607	65/65	0.96	0.09	19,26,51,53	0
25	CLA	b	606	65/65	0.96	0.10	23,30,55,59	0
25	CLA	b	607	65/65	0.96	0.09	29,36,52,56	0
25	CLA	C	505	65/65	0.96	0.09	25,33,55,61	0
35	HEM	F	101	43/43	0.96	0.14	38,43,51,63	0
35	HEM	e	101	43/43	0.96	0.13	46,55,66,78	0
30	LHG	d	406	49/49	0.97	0.10	29,36,42,51	0
30	LHG	d	407	39/49	0.97	0.08	31,40,56,62	0
25	CLA	a	613	65/65	0.97	0.08	19,27,38,43	0
25	CLA	C	504	59/65	0.97	0.08	29,35,63,69	0
26	PHO	A	608	64/64	0.97	0.08	18,25,32,36	0
26	PHO	D	402	64/64	0.97	0.09	20,29,34,37	0
25	CLA	B	605	65/65	0.97	0.10	22,28,38,40	0
30	LHG	D	408	49/49	0.97	0.09	27,34,44,48	0
25	CLA	C	501	65/65	0.97	0.09	26,30,40,44	0
34	BCT	D	401	4/4	0.97	0.16	35,36,39,40	0
34	BCT	a	606	4/4	0.97	0.11	30,36,40,46	0
30	LHG	L	101	49/49	0.97	0.10	29,36,47,53	0
25	CLA	b	604	65/65	0.97	0.09	22,30,40,44	0
36	HEC	V	201	43/43	0.97	0.11	23,30,38,42	0
21	OEX	A	601[C]	10/10	0.98	0.10	22,25,28,28	10
21	OEX	A	601[B]	10/10	0.98	0.10	25,29,33,33	10
36	HEC	v	201	43/43	0.98	0.10	28,33,37,43	0
22	OEY	A	602[A]	11/11	0.99	0.10	26,29,32,32	11
22	OEY	a	602[A]	11/11	0.99	0.09	28,30,34,34	11
23	FE2	a	603	1/1	0.99	0.04	34,34,34,34	0
24	CL	A	604	1/1	0.99	0.03	28,28,28,28	0
24	CL	A	605	1/1	0.99	0.05	29,29,29,29	0
24	CL	a	604	1/1	0.99	0.09	27,27,27,27	0
21	OEX	a	601[B]	10/10	0.99	0.09	26,29,32,32	10
21	OEX	a	601[C]	10/10	0.99	0.09	21,23,25,25	10
23	FE2	A	603	1/1	1.00	0.02	30,30,30,30	0
24	CL	a	605	1/1	1.00	0.06	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all



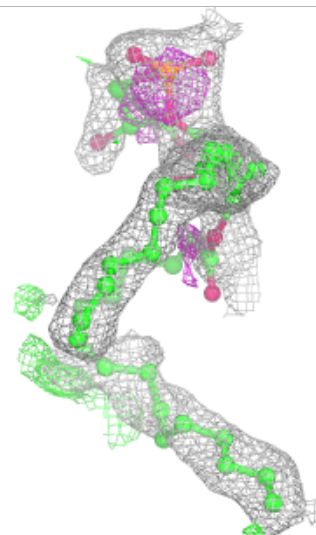
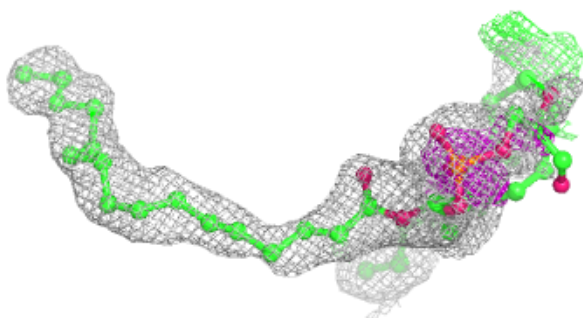
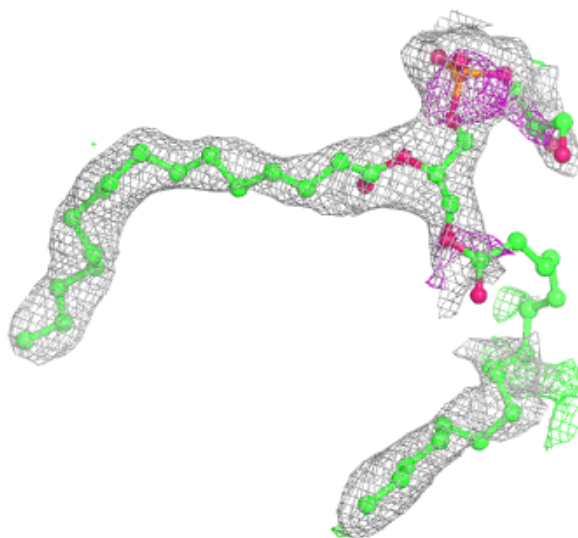
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





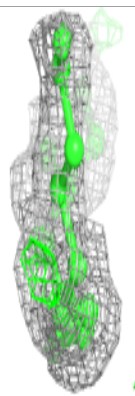
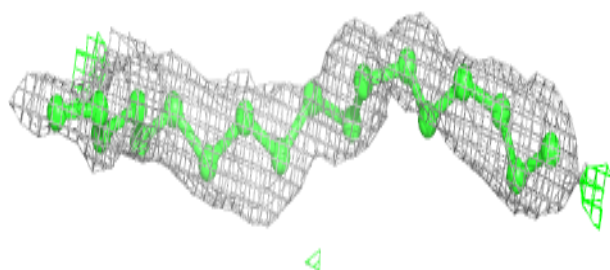
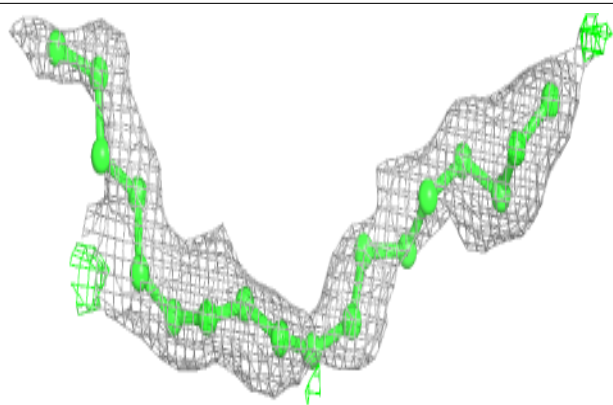
**Electron density around LHG E 101:**

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

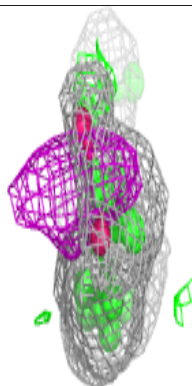
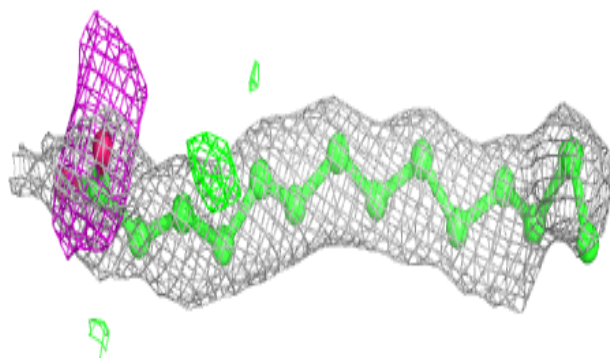
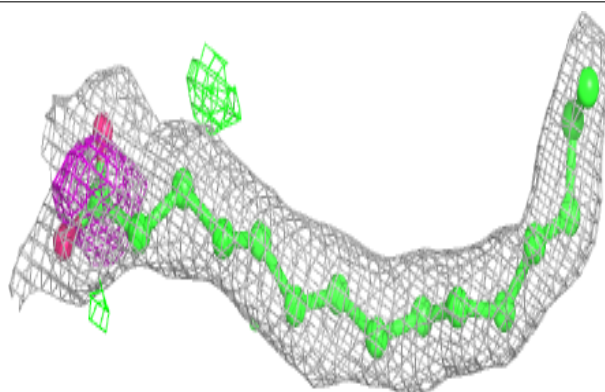


**Electron density around STE H 103:**

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

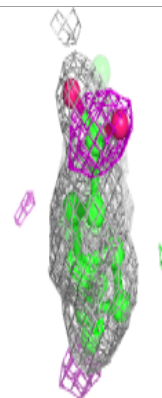
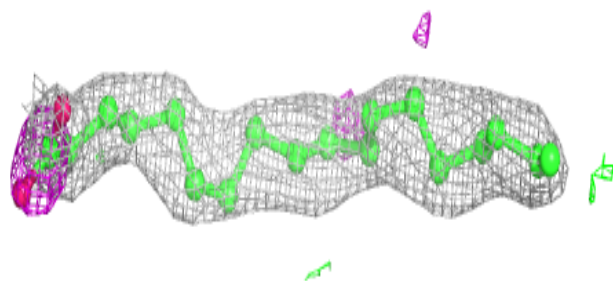
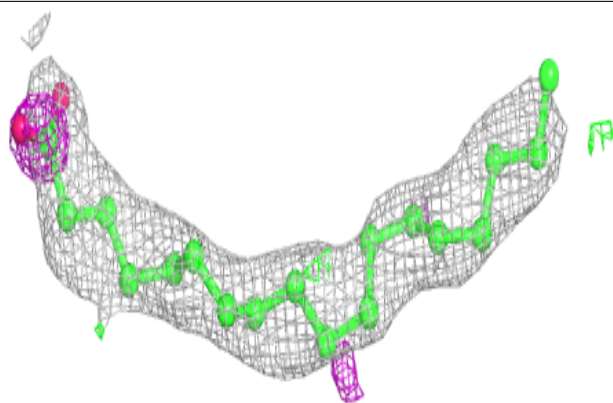
**Electron density around STE B 620:**

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

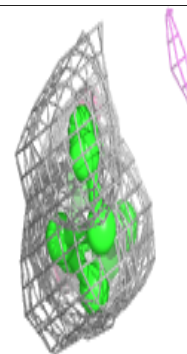
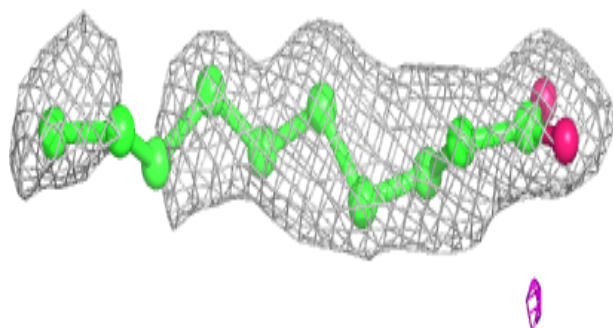
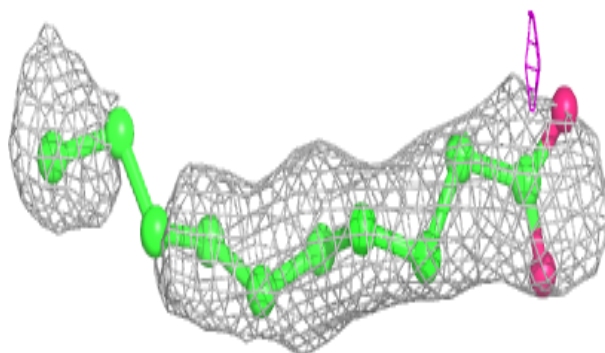


**Electron density around STE X 101:**

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

**Electron density around STE k 103:**

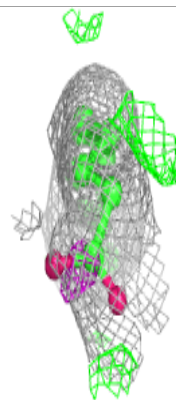
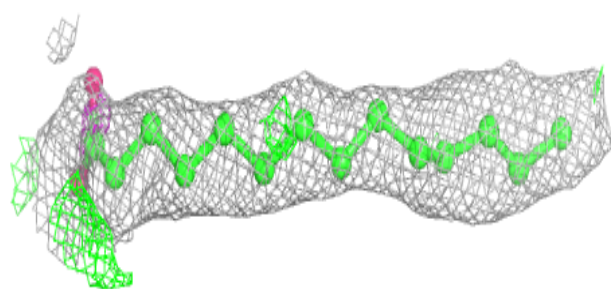
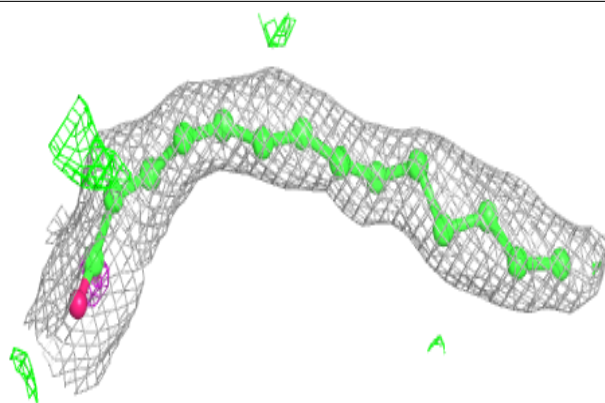
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



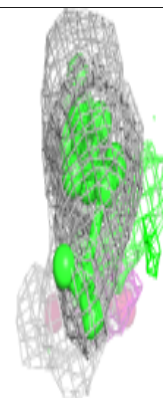
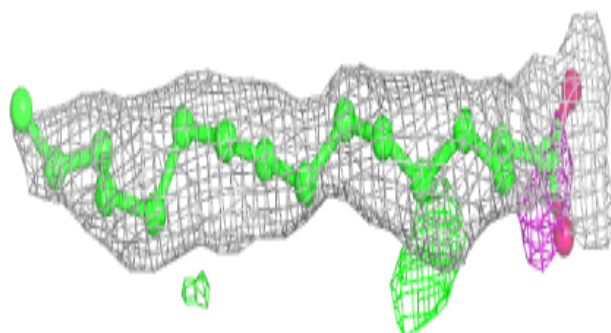
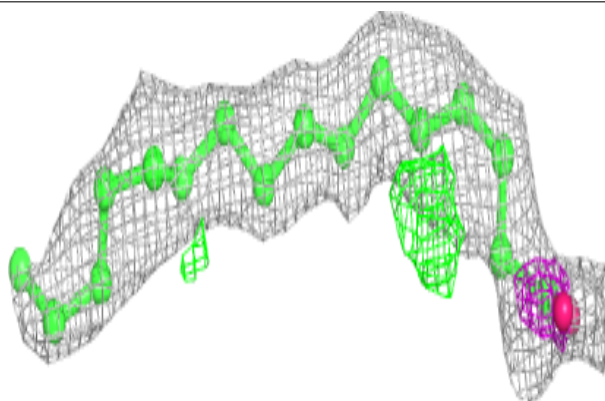


**Electron density around STE b 623:**

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

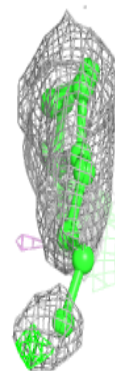
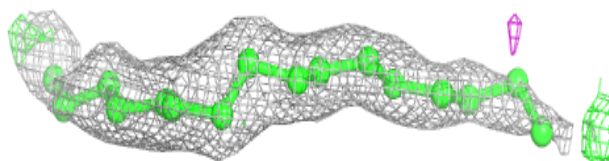
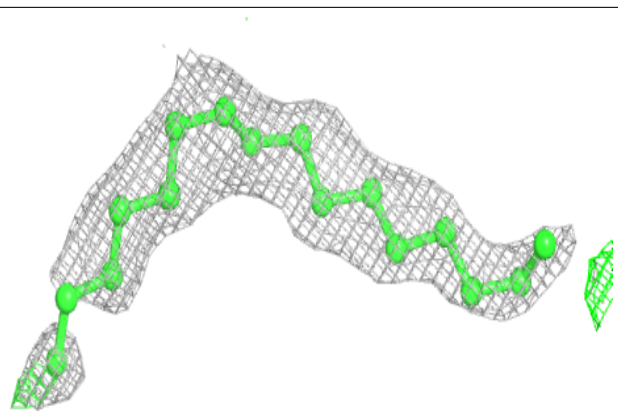
**Electron density around STE t 104:**

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



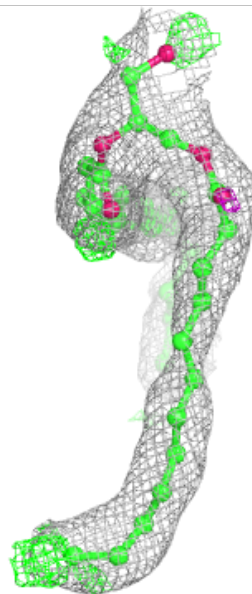
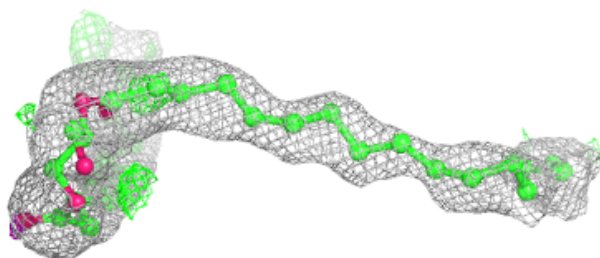
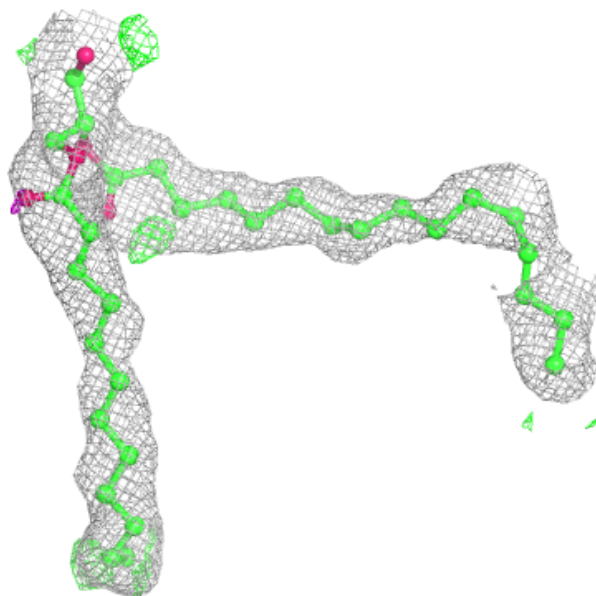
**Electron density around STE B 626:**

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



**Electron density around SQD a 616:**

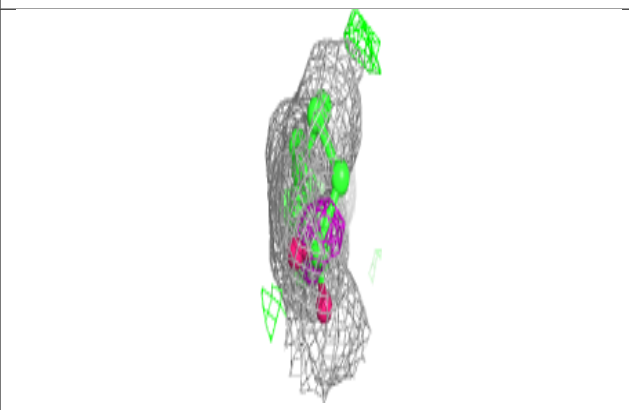
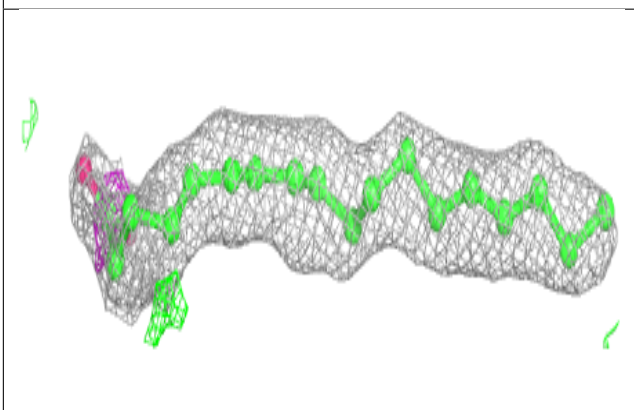
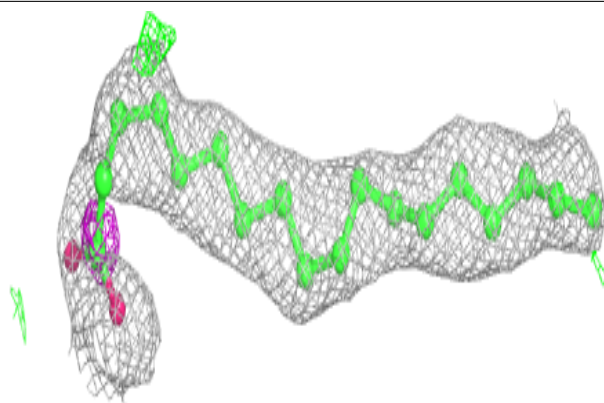
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



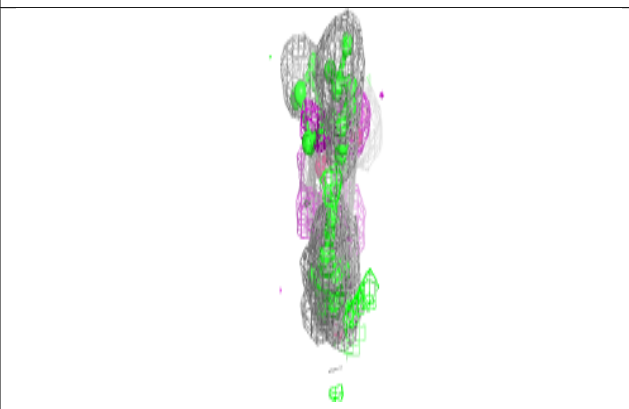
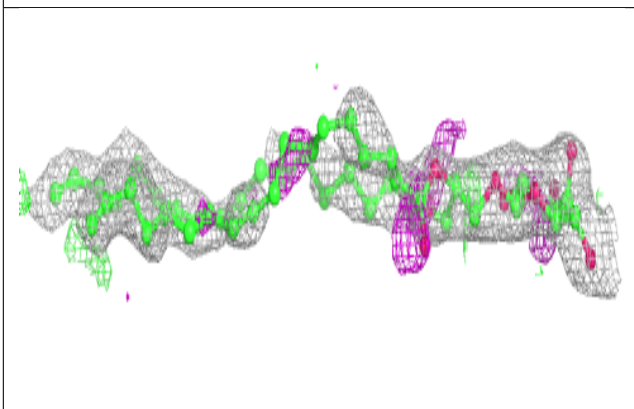
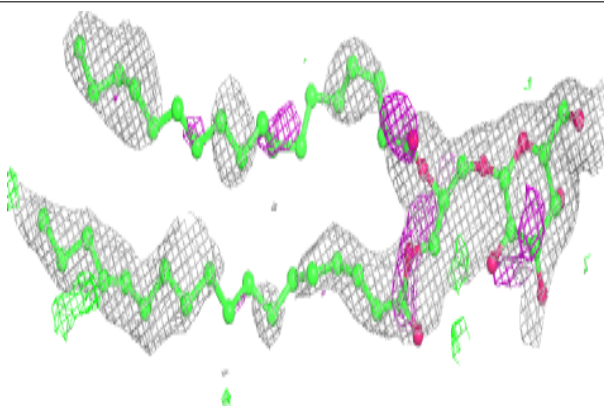


**Electron density around STE c 520:**

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

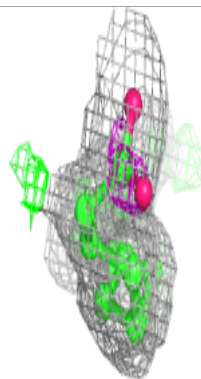
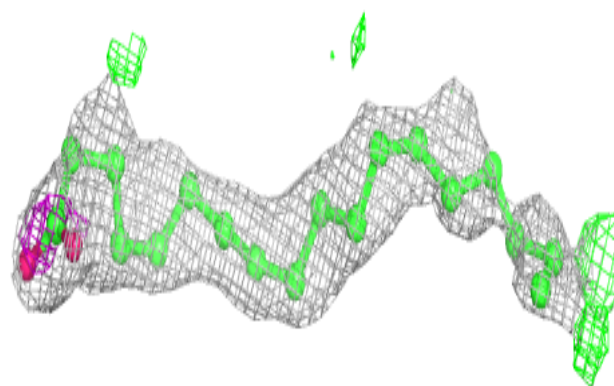
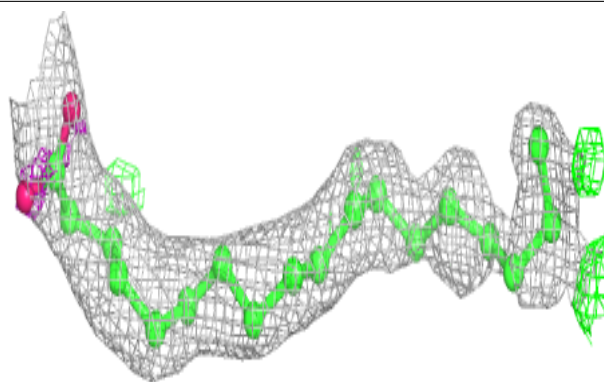
**Electron density around LMG b 622:**

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

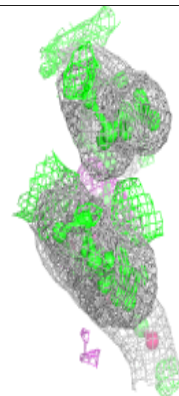
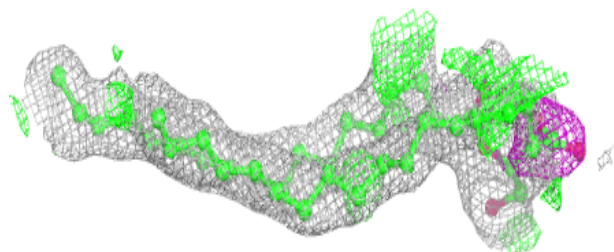
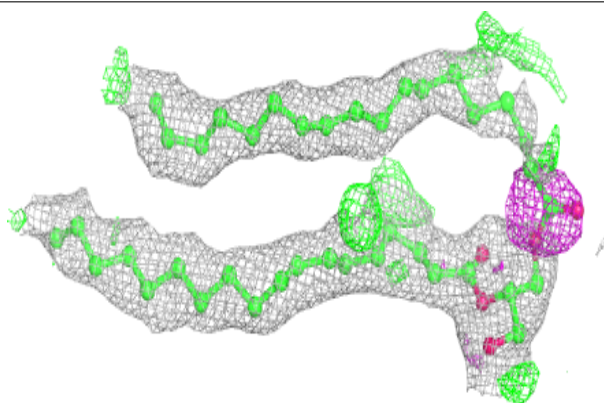


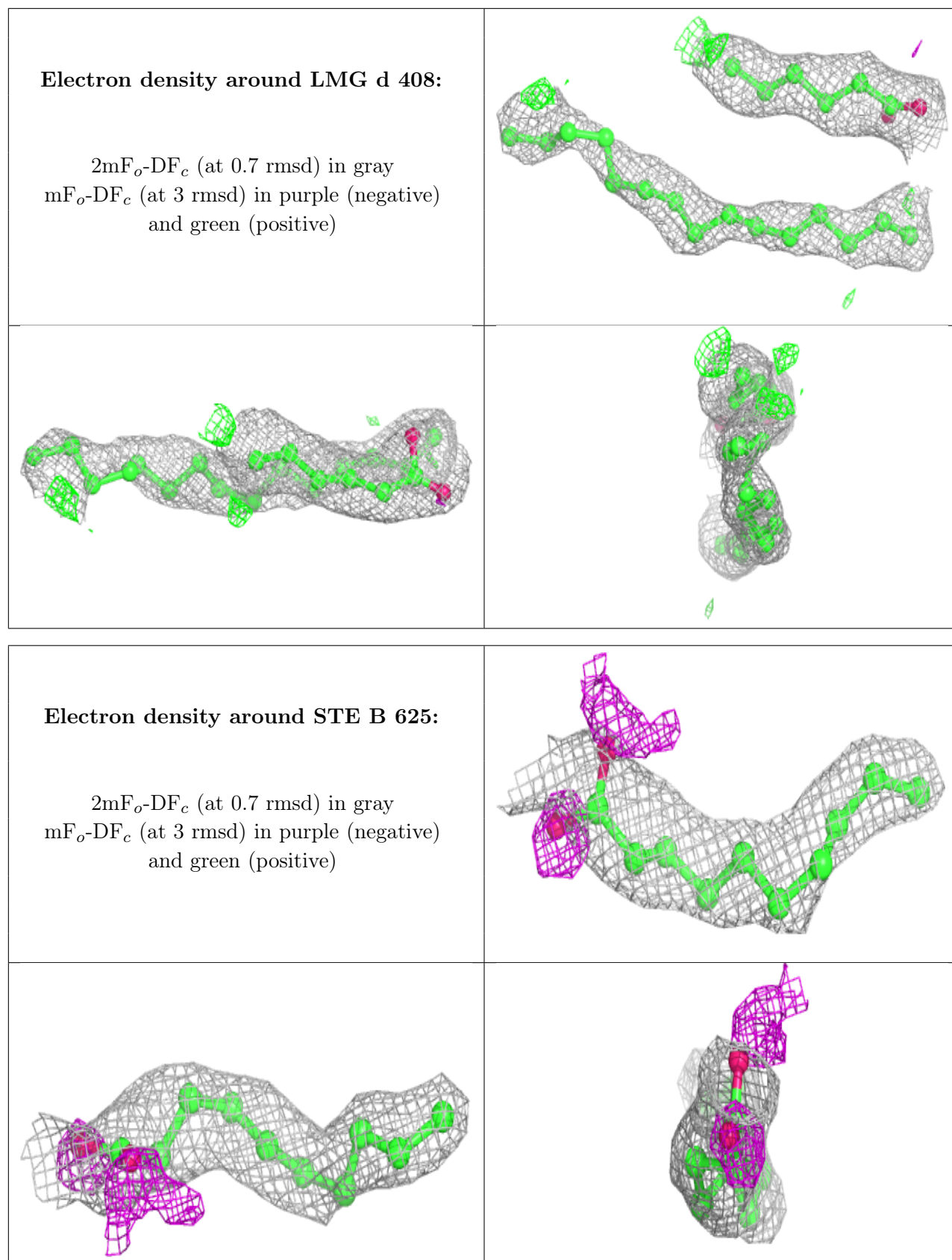
**Electron density around STE b 621:**

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

**Electron density around DGD a 617:**

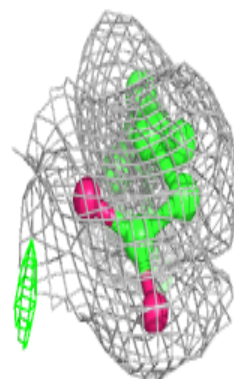
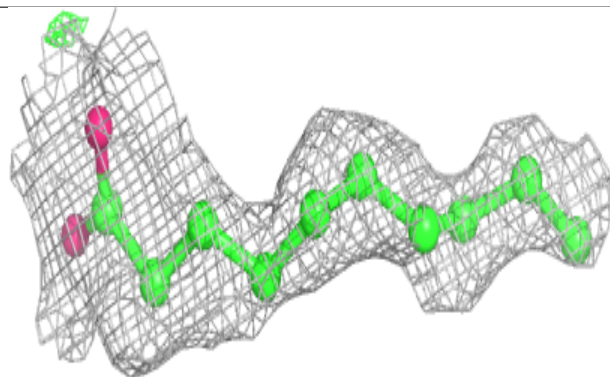
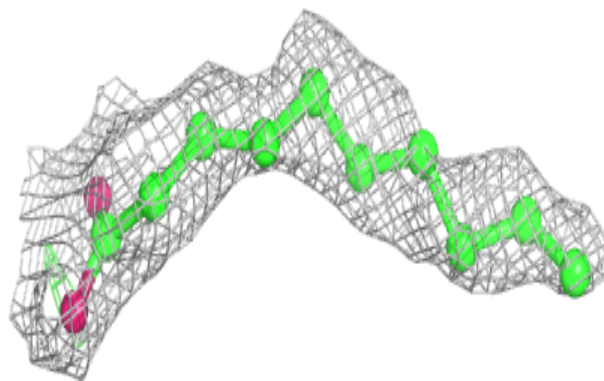
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



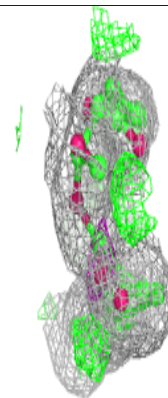
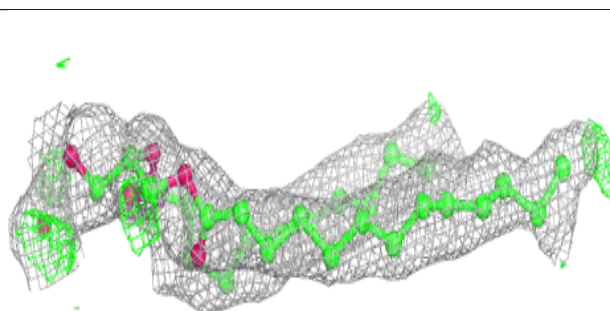
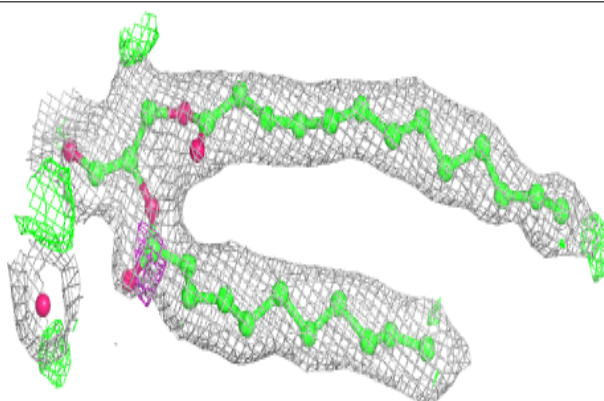


**Electron density around STE E 102:**

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

**Electron density around LMG D 409:**

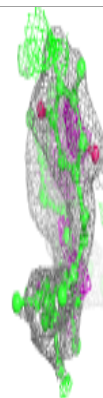
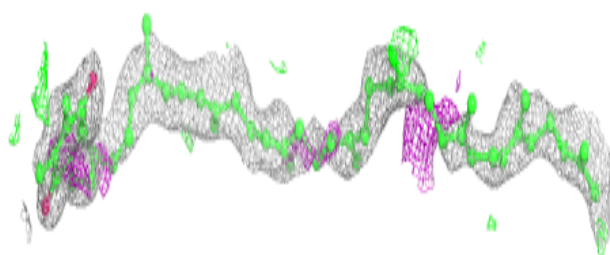
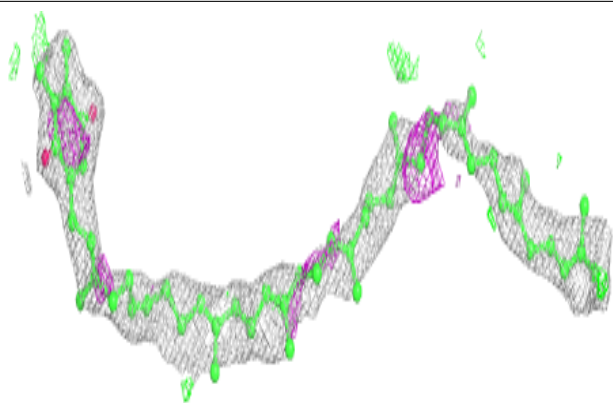
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



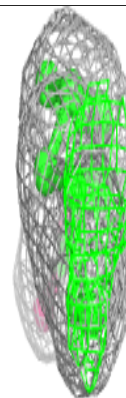
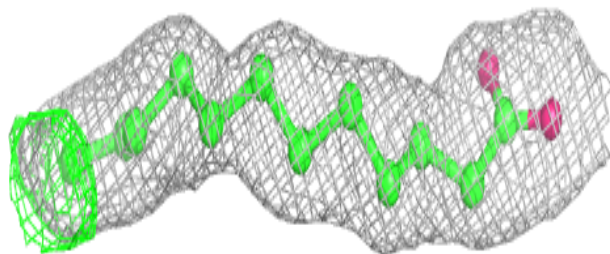
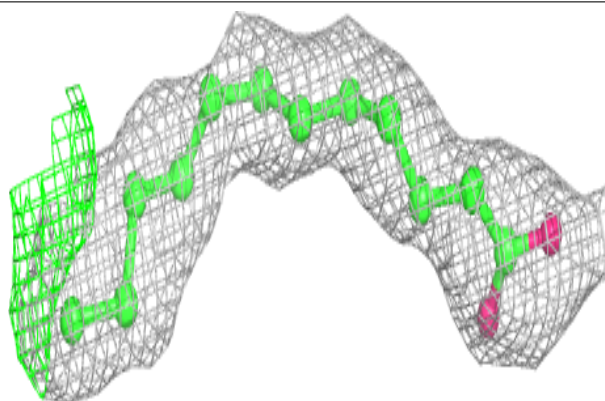


**Electron density around PL9 A 611:**

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

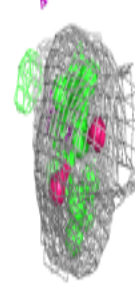
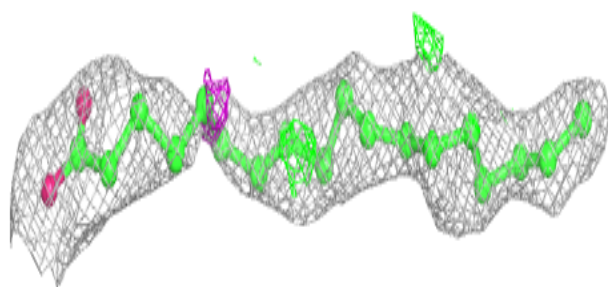
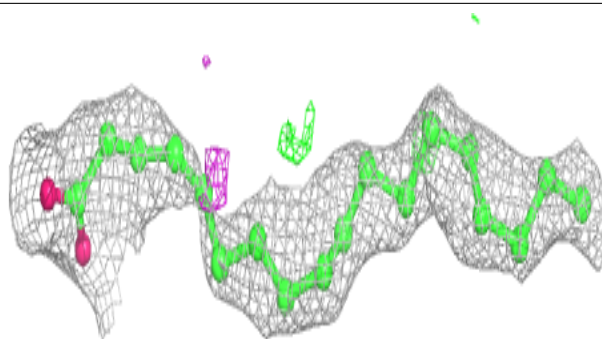
**Electron density around STE t 102:**

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

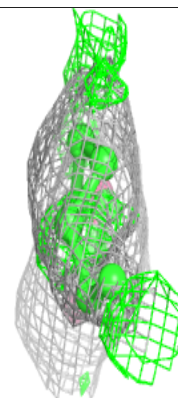
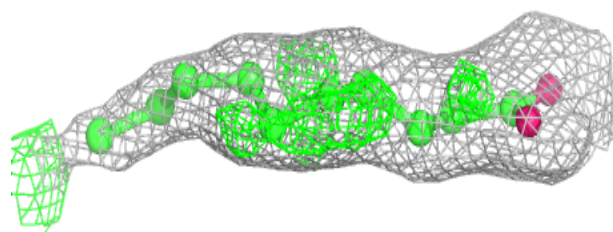
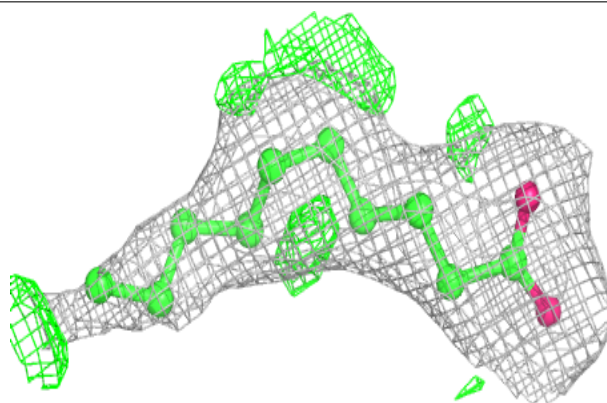


**Electron density around STE b 625:**

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

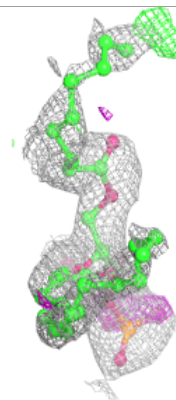
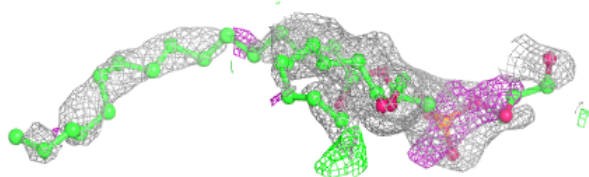
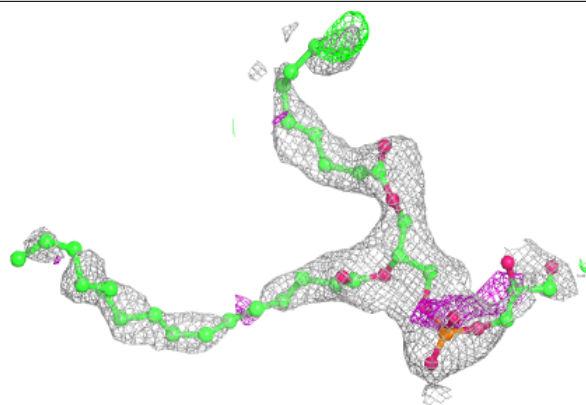
**Electron density around STE C 519:**

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

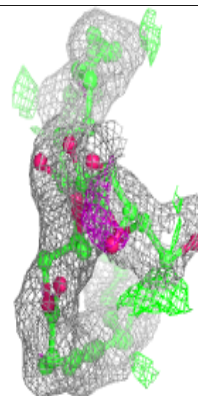
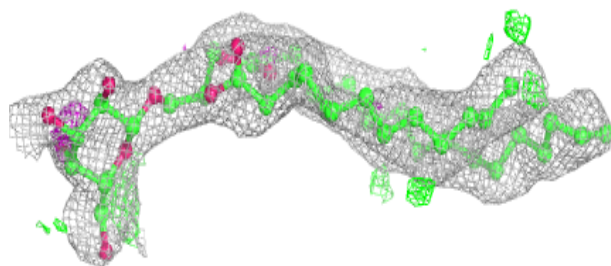
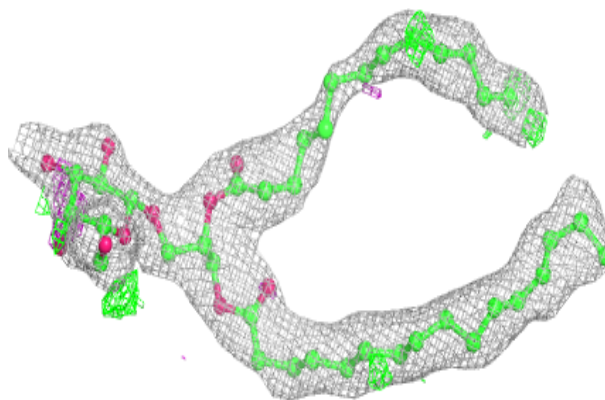


**Electron density around LHG e 102:**

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

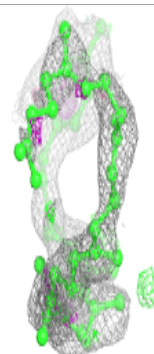
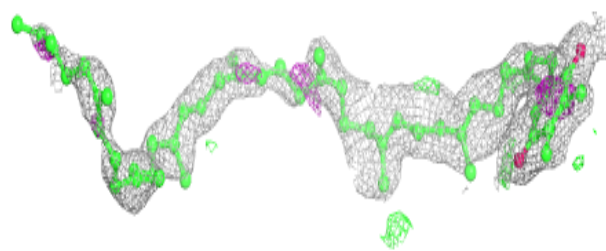
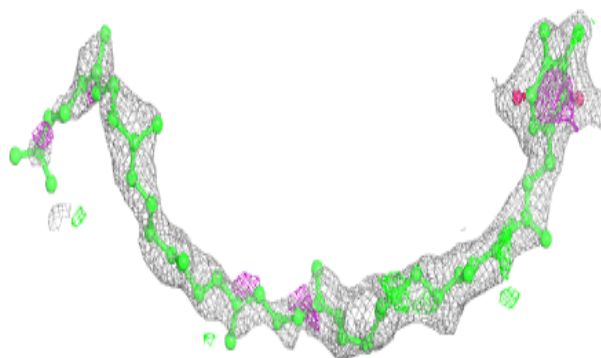
**Electron density around LMG A 613:**

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

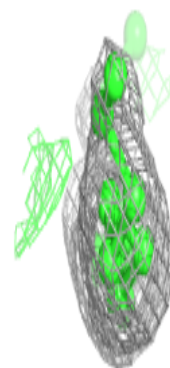
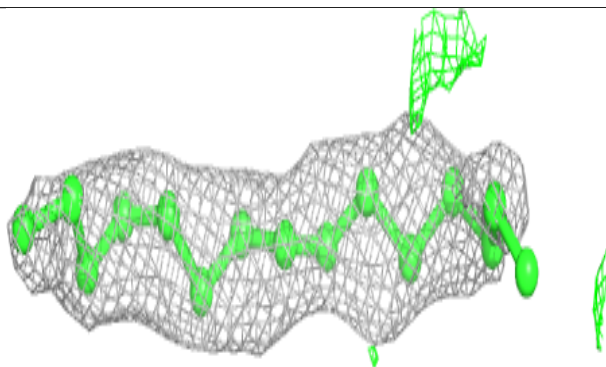
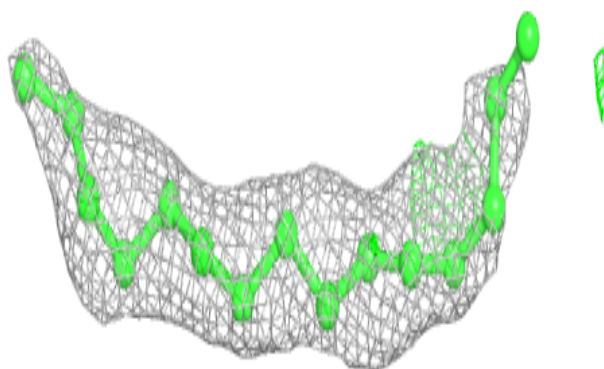


**Electron density around PL9 a 612:**

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

**Electron density around STE b 624:**

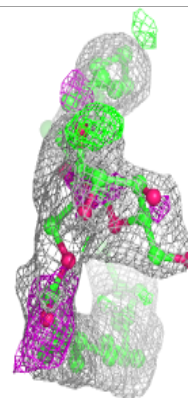
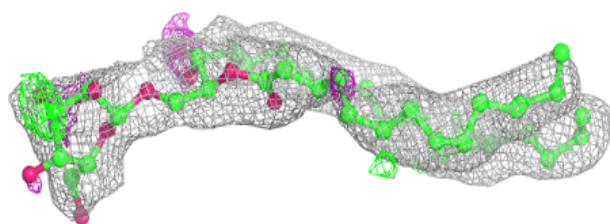
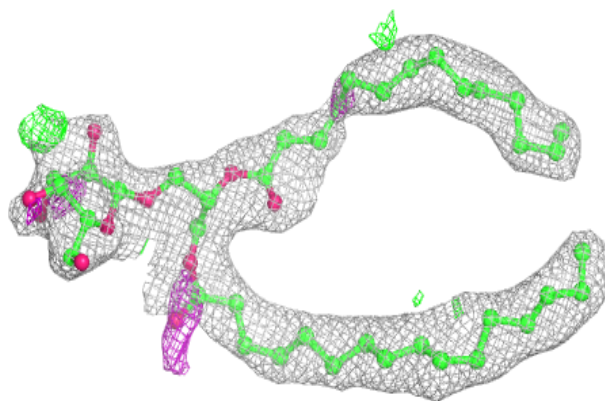
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



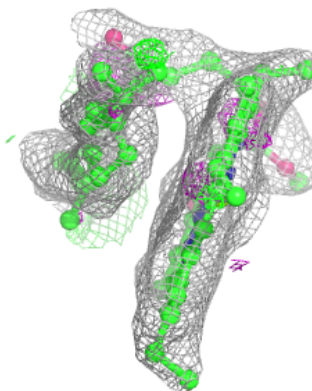
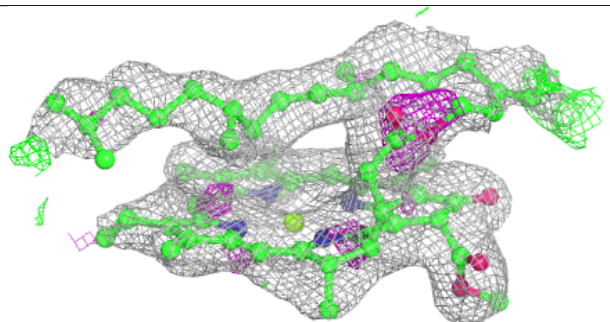
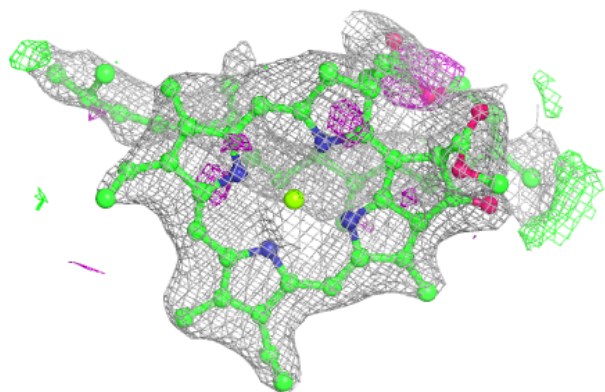


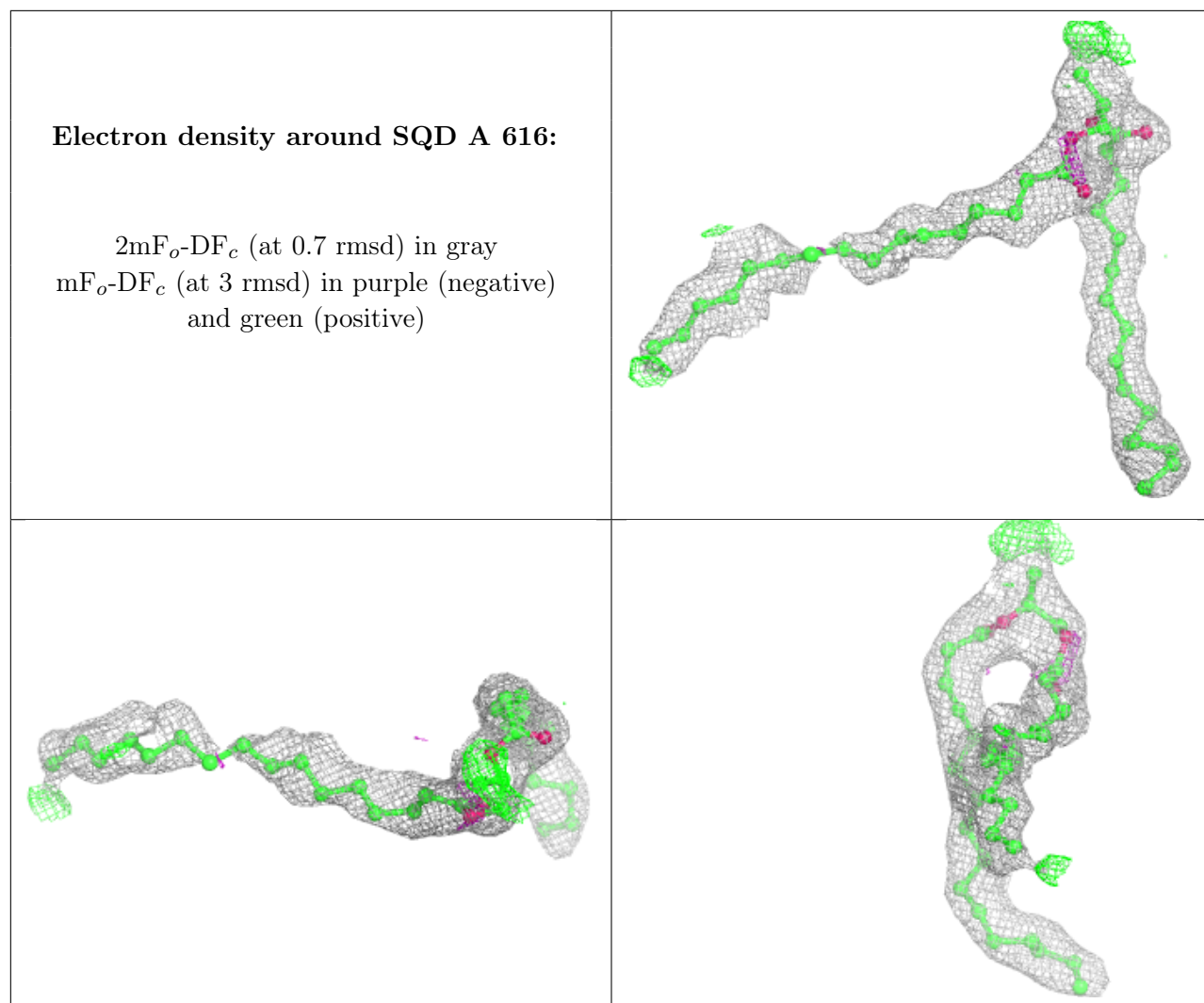
**Electron density around LMG c 522:**

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

**Electron density around CLA h 101:**

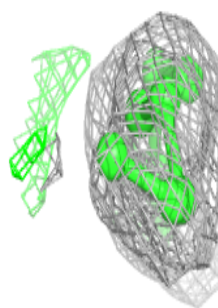
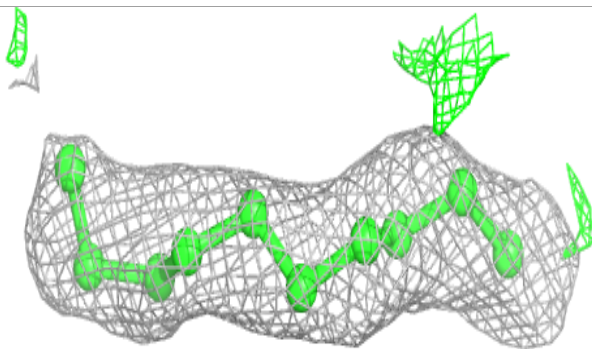
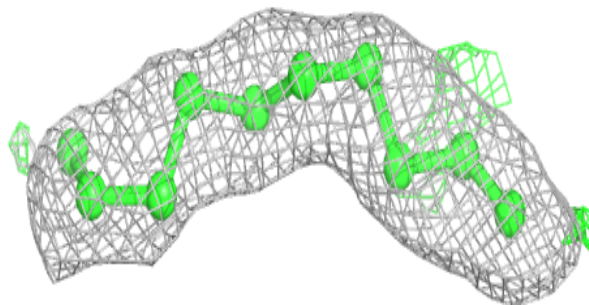
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



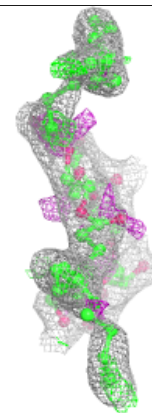
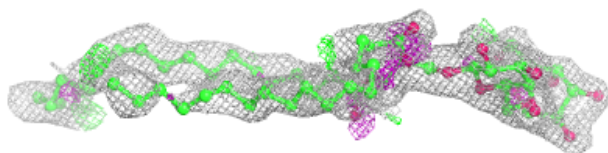
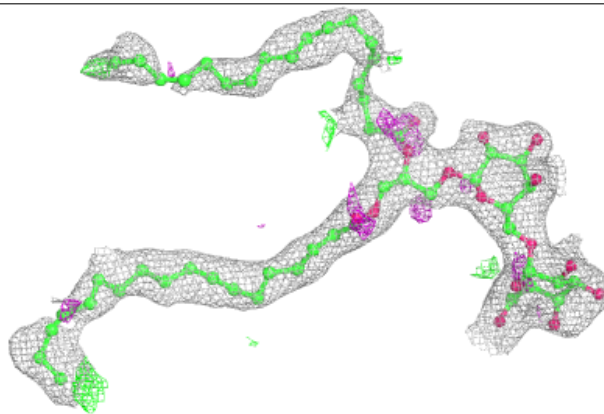


**Electron density around STE b 626:**

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

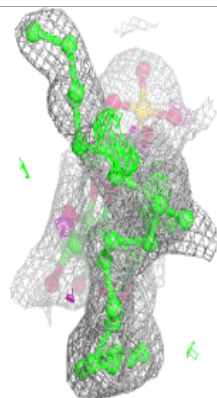
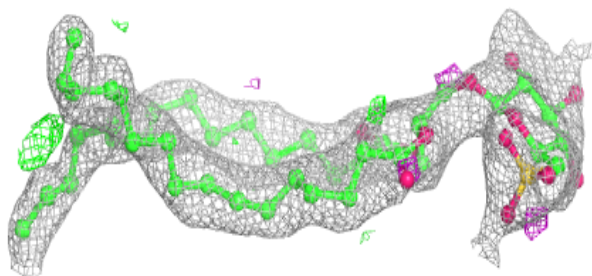
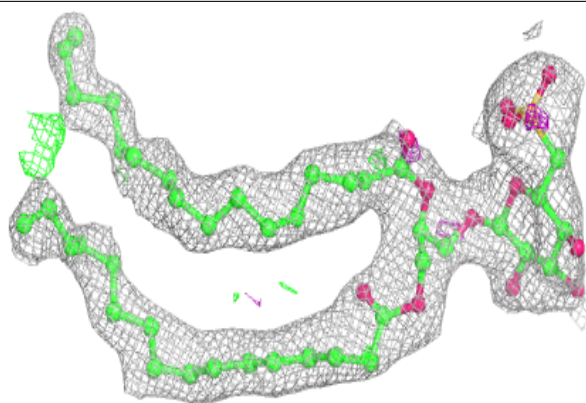
**Electron density around DGD A 617:**

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

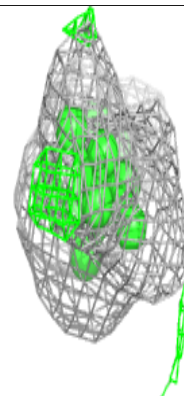
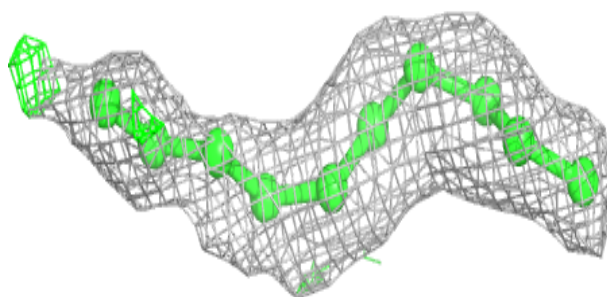
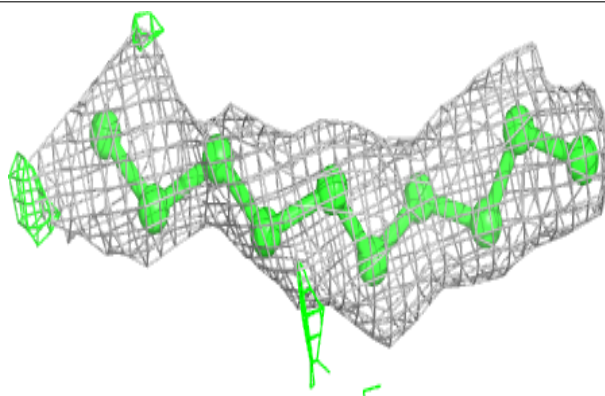


**Electron density around SQD B 623:**

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

**Electron density around STE t 103:**

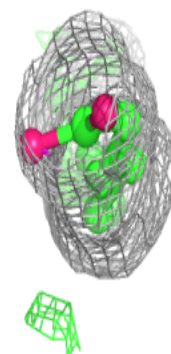
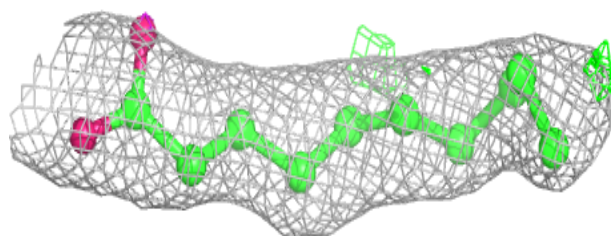
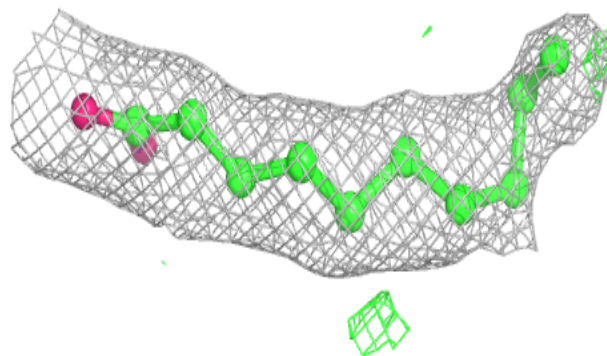
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



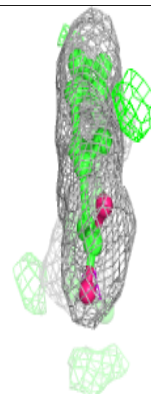
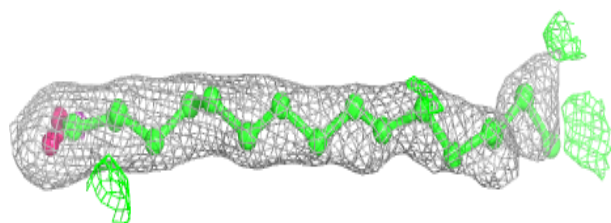
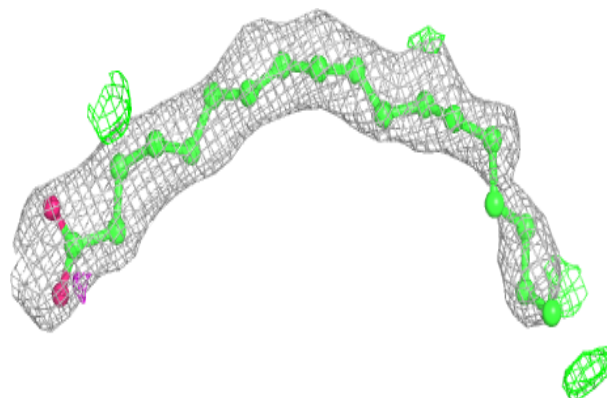


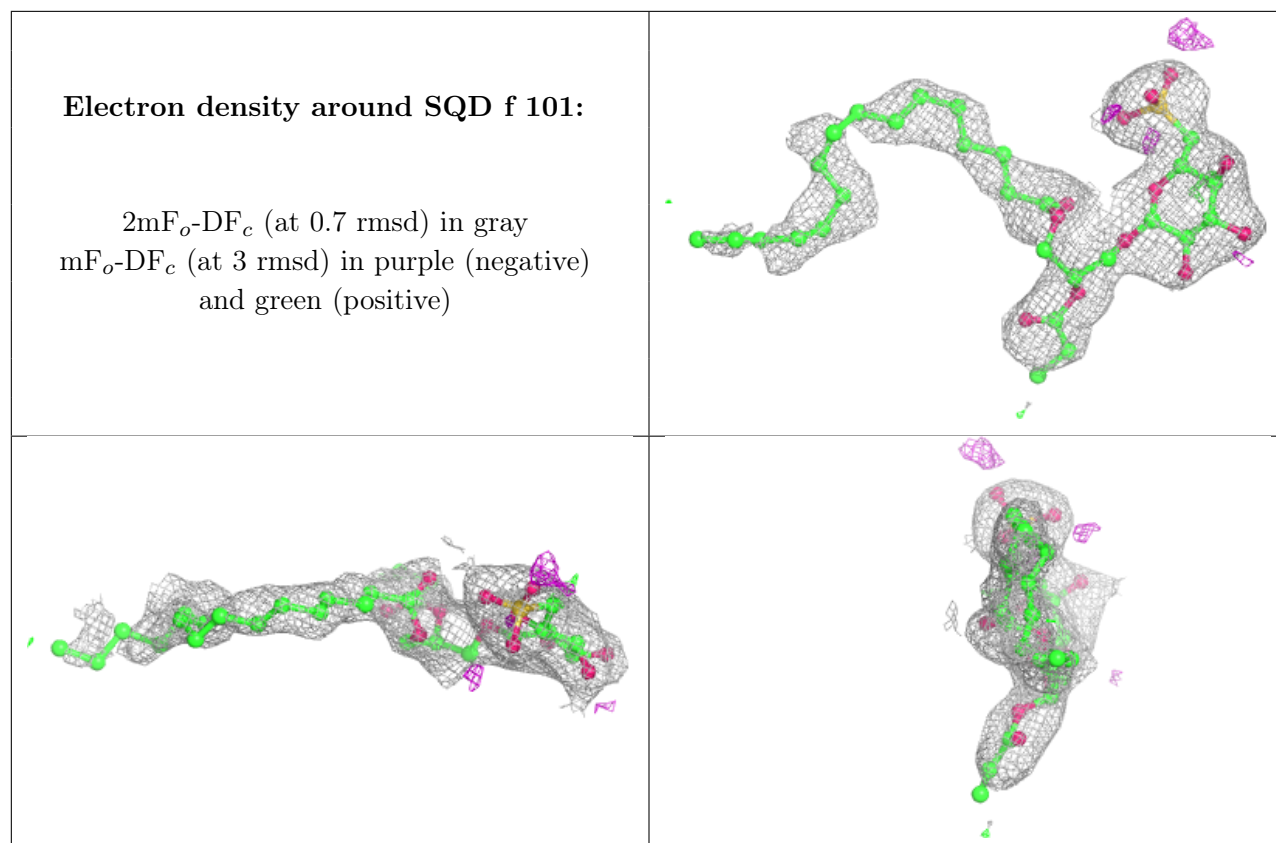
**Electron density around STE m 102:**

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

**Electron density around STE x 101:**

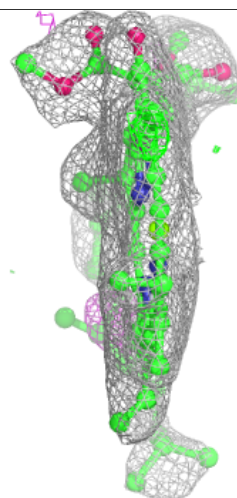
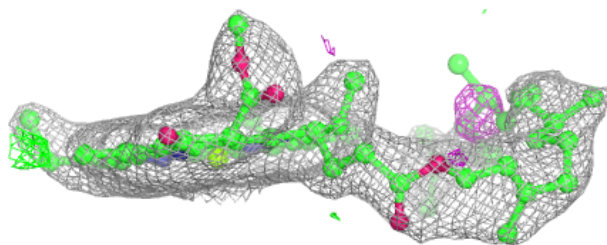
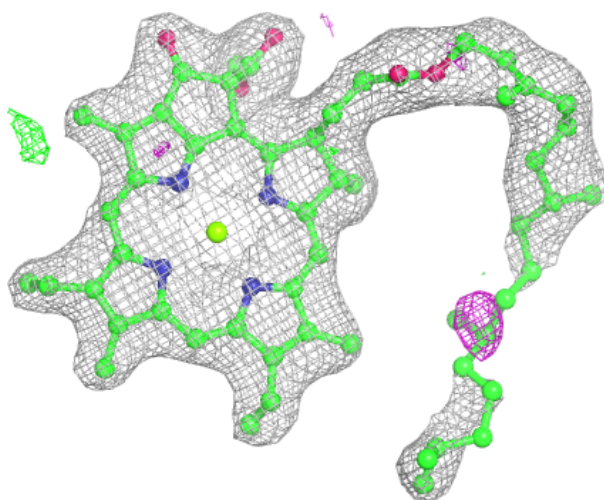
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





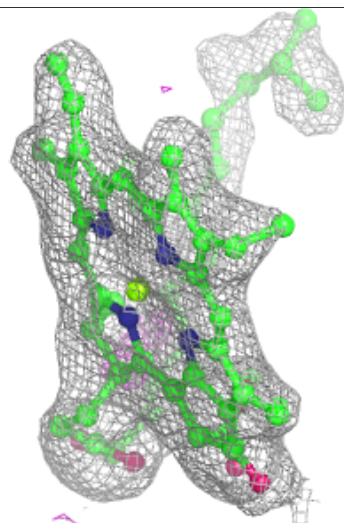
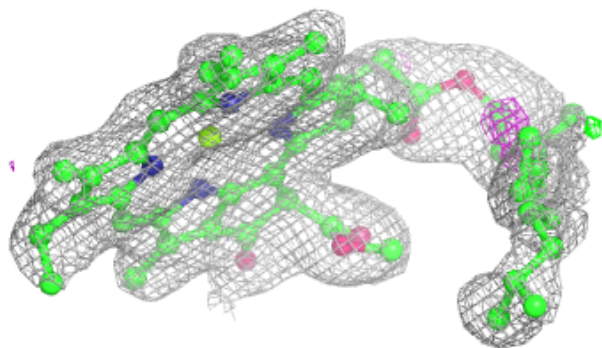
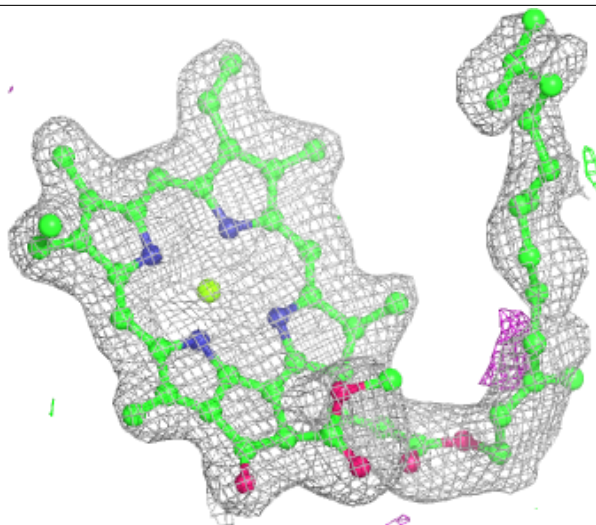
**Electron density around CLA c 512:**

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



**Electron density around CLA b 615:**

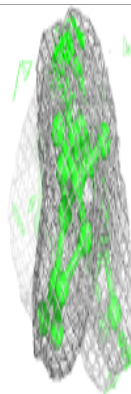
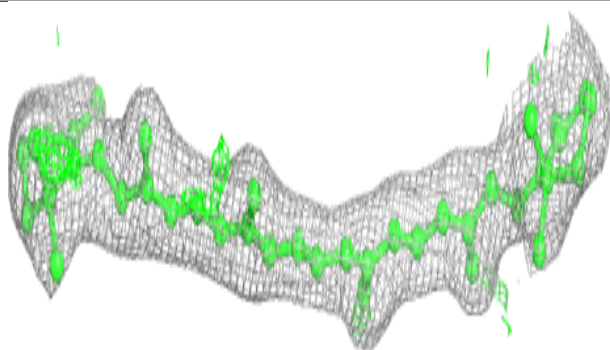
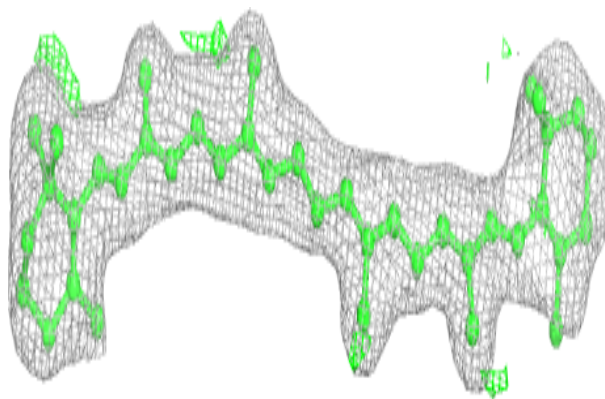
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



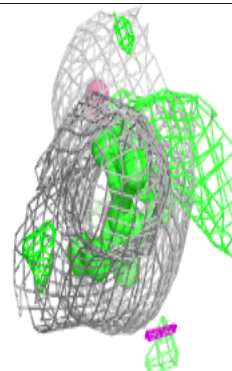
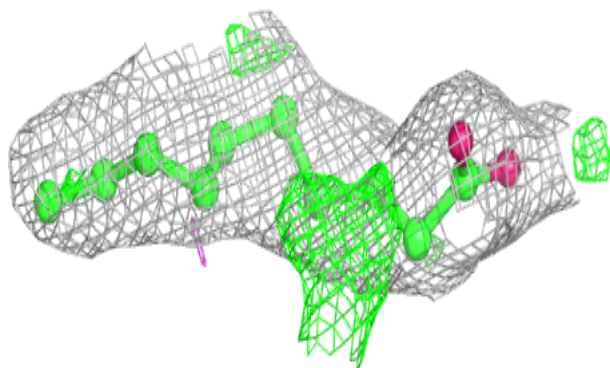
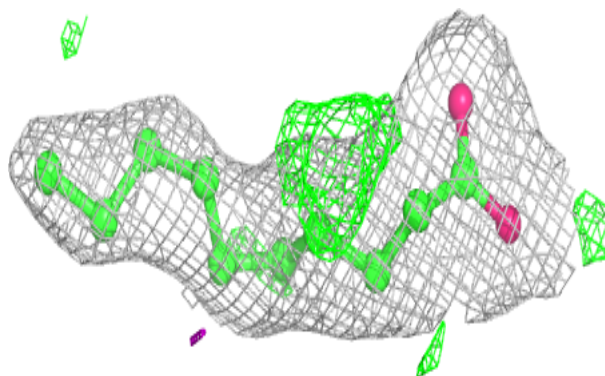


**Electron density around BCR D 405:**

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

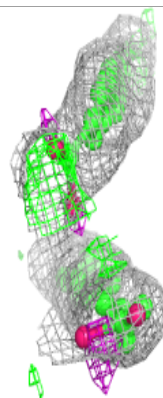
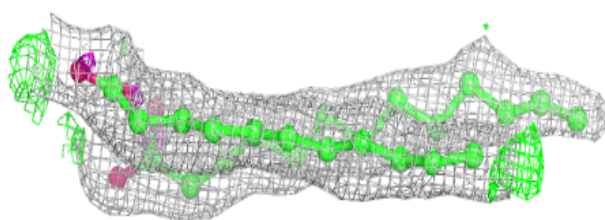
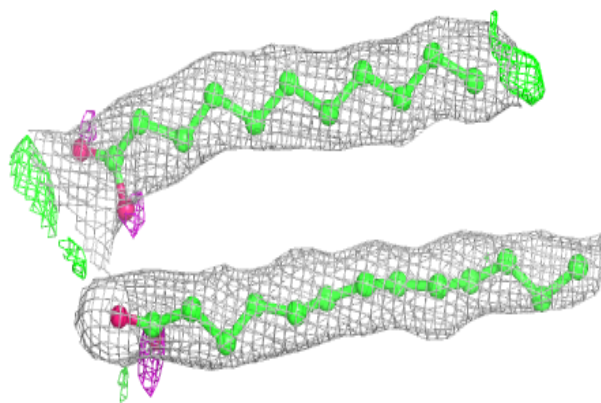
**Electron density around STE B 624:**

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

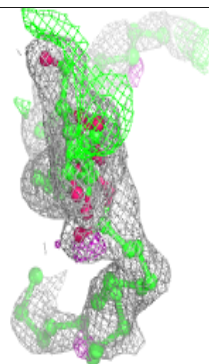
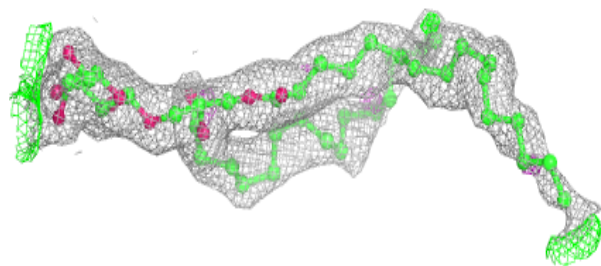
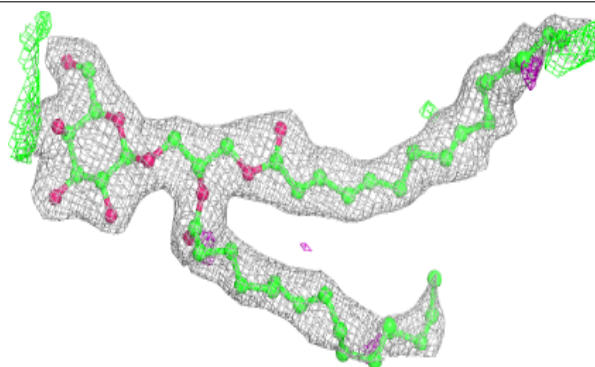


**Electron density around LMG B 621:**

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

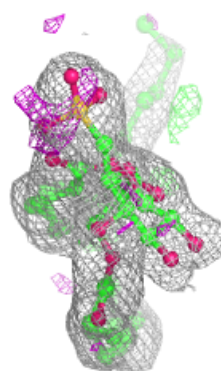
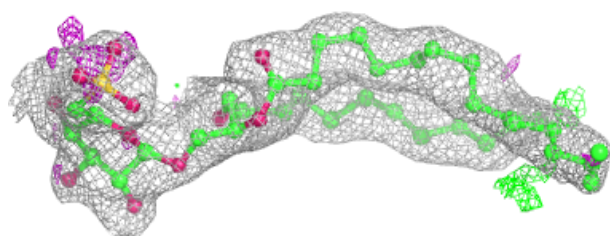
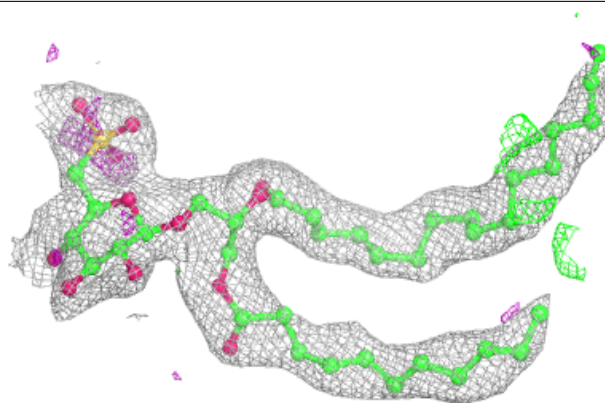
**Electron density around LMG D 407:**

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

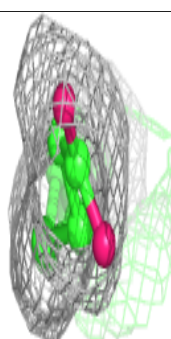
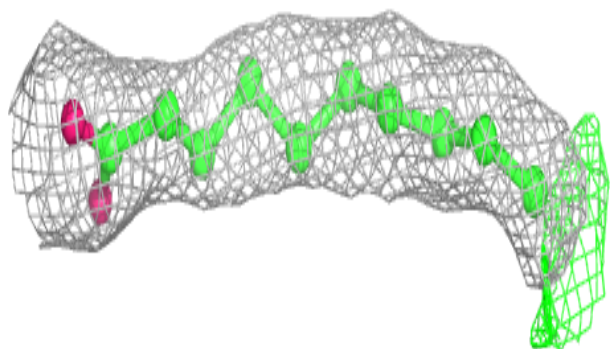
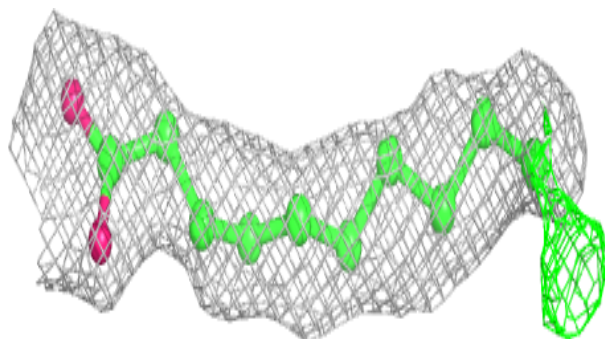


**Electron density around SQD b 619:**

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

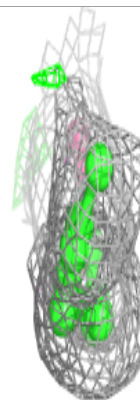
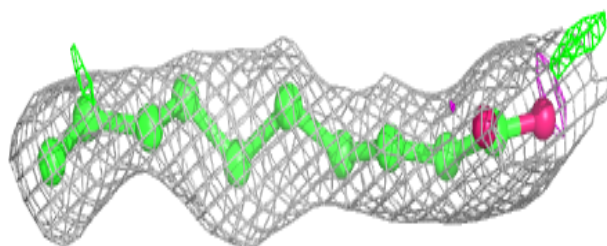
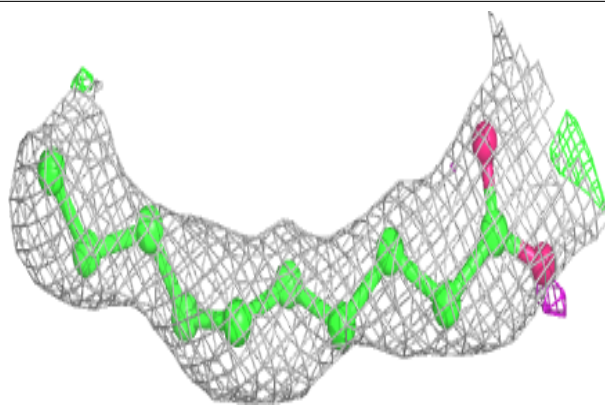
**Electron density around STE j 101:**

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

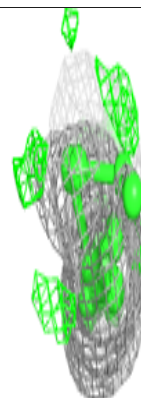
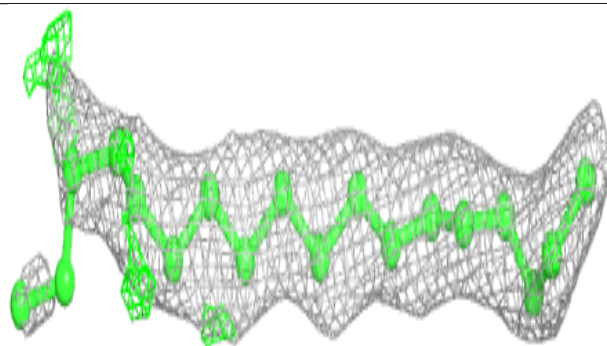
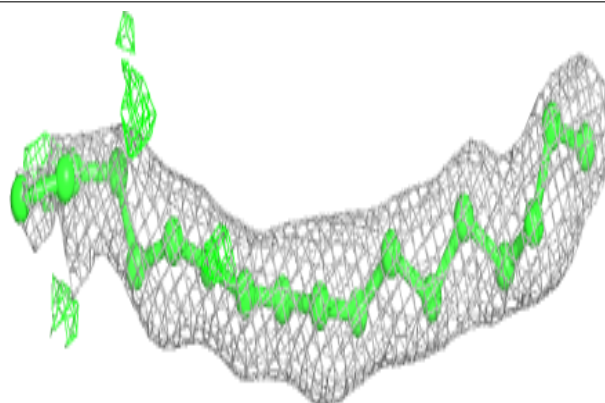


**Electron density around STE C 520:**

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

**Electron density around STE I 102:**

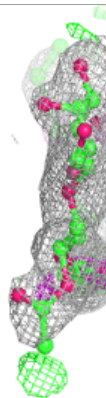
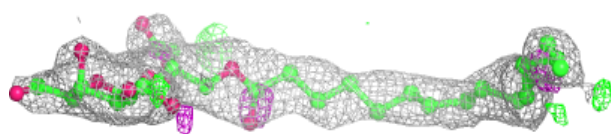
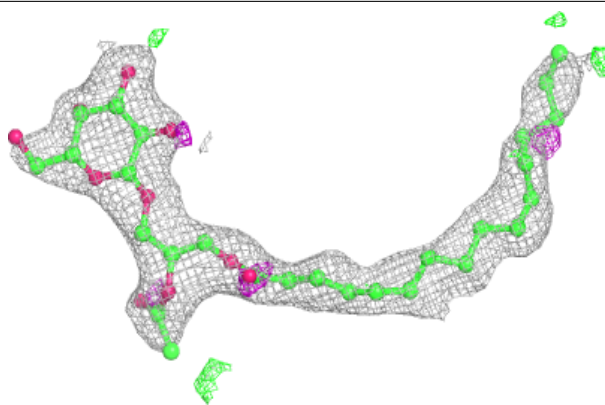
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



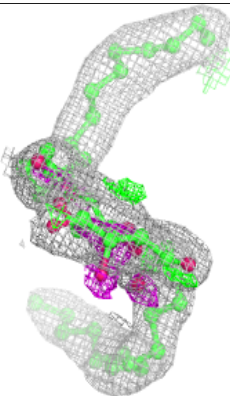
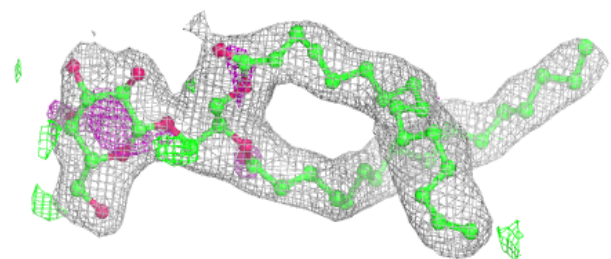
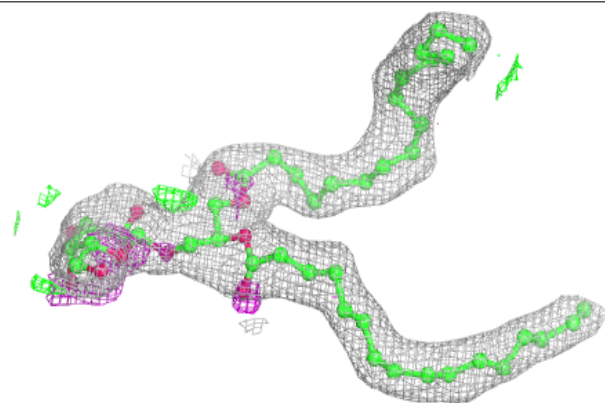


**Electron density around LMG c 519:**

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

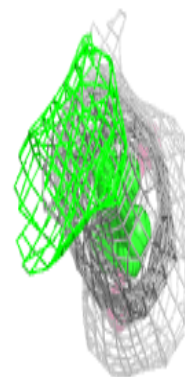
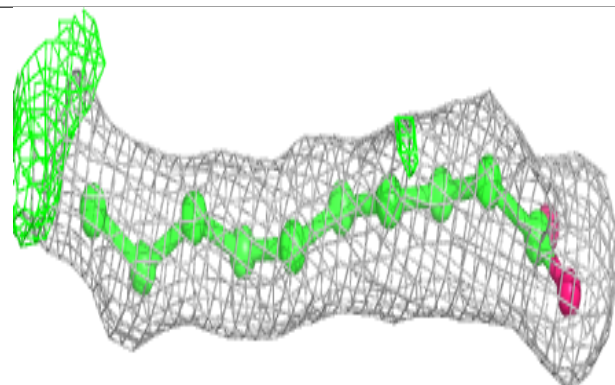
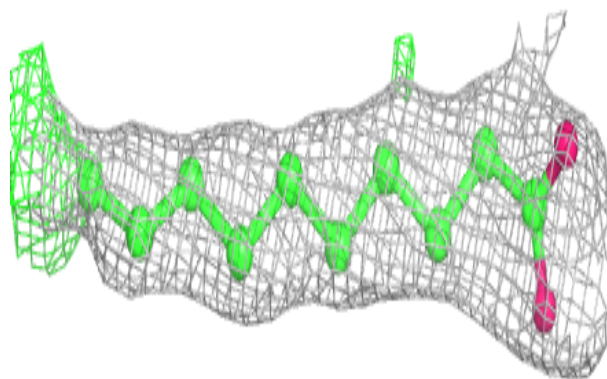
**Electron density around LMG m 101:**

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

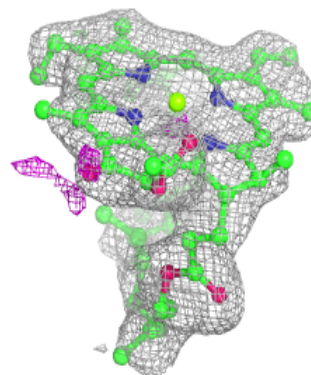
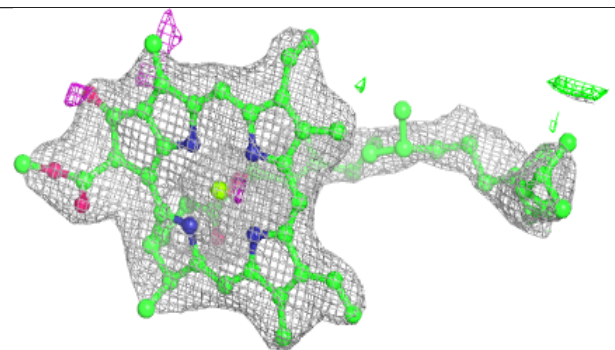
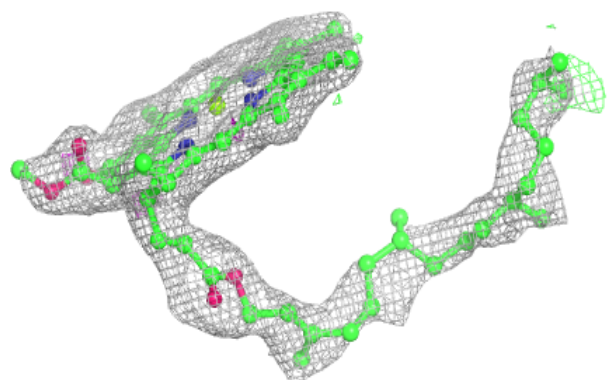


**Electron density around STE J 101:**

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

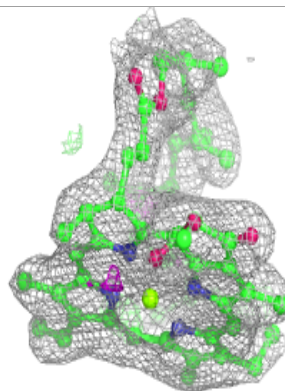
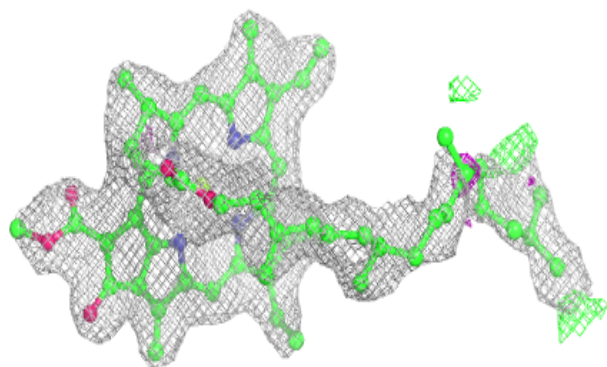
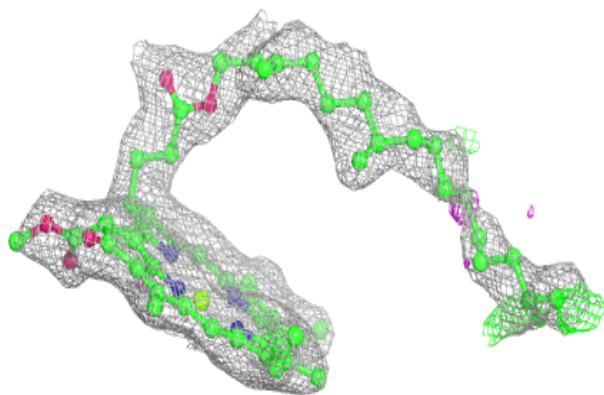
**Electron density around CLA c 513:**

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

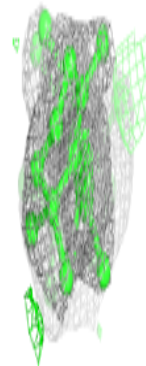
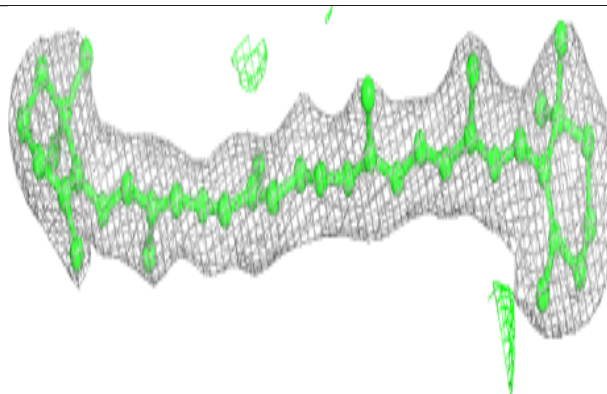
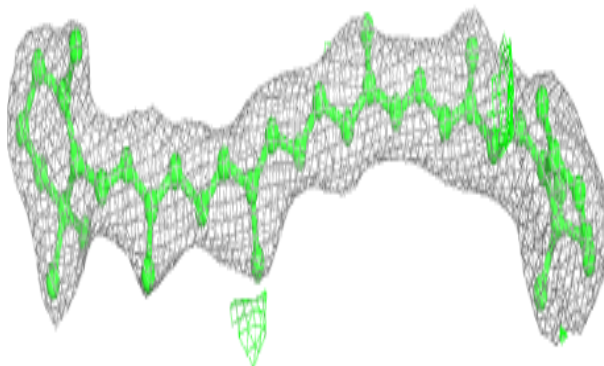


**Electron density around CLA C 513:**

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

**Electron density around BCR c 514:**

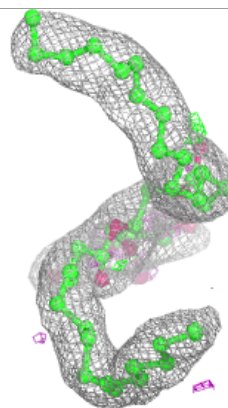
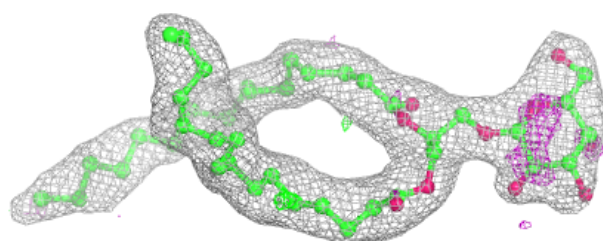
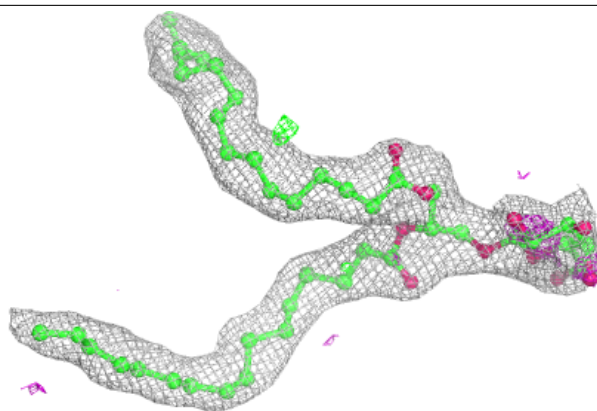
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



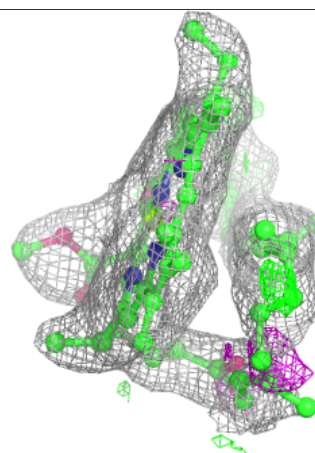
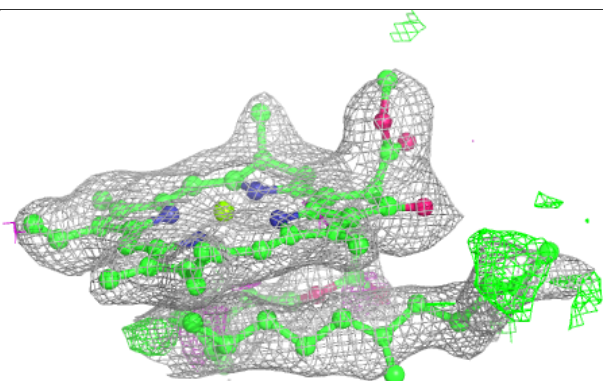
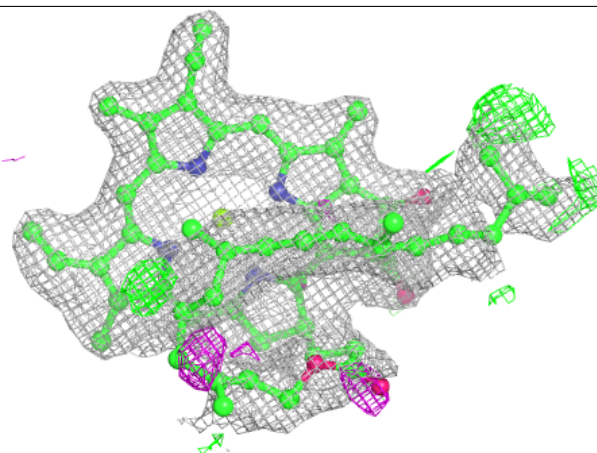


**Electron density around LMG M 101:**

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

**Electron density around CLA B 601:**

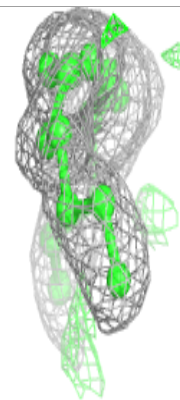
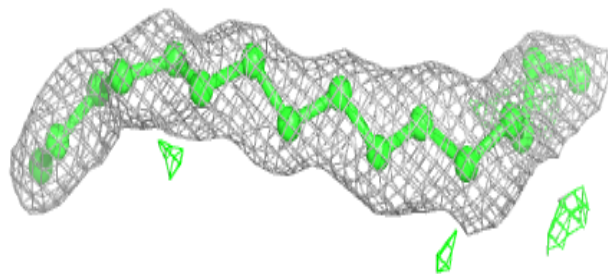
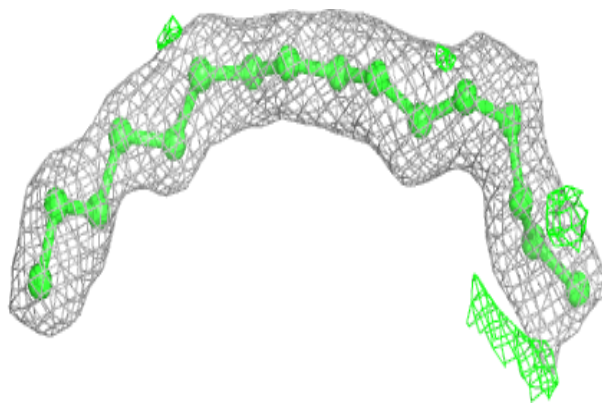
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



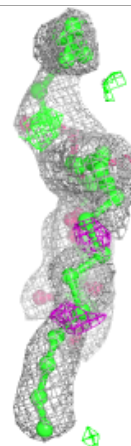
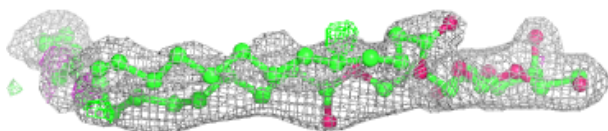
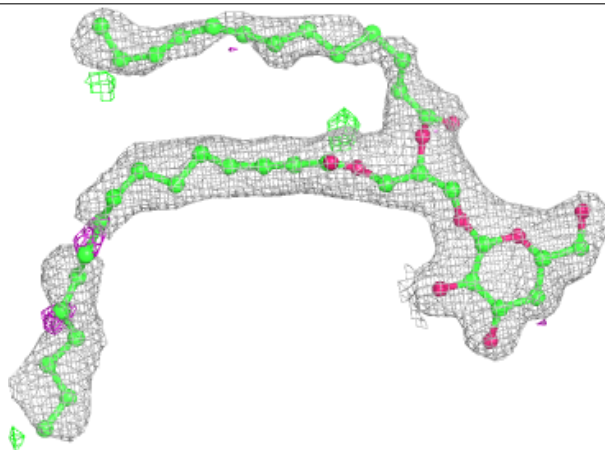


**Electron density around STE b 620:**

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

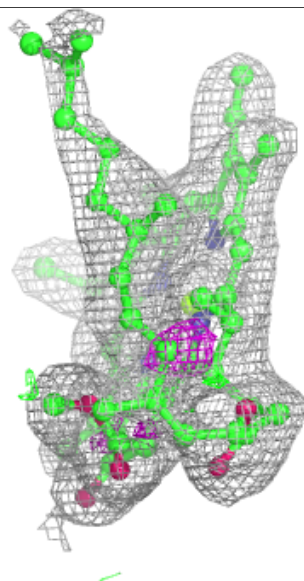
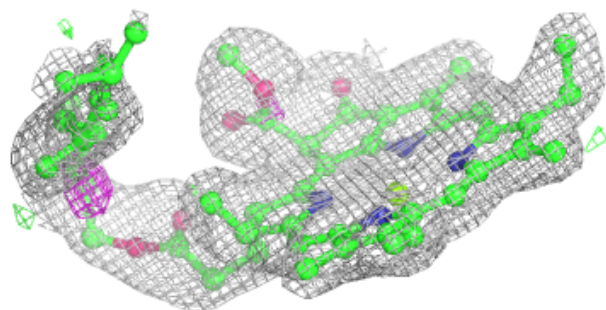
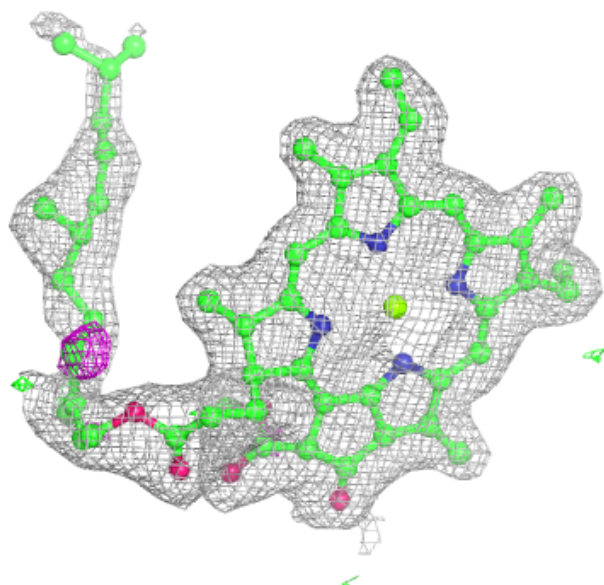
**Electron density around LMG C 518:**

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



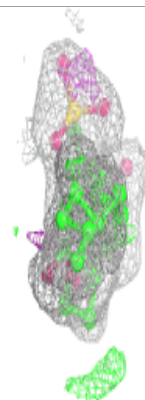
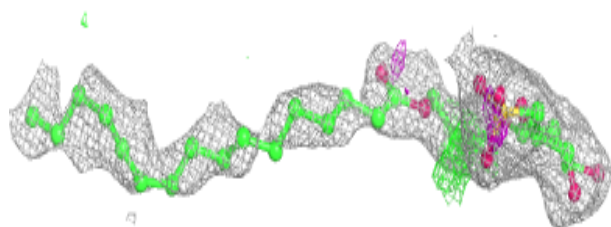
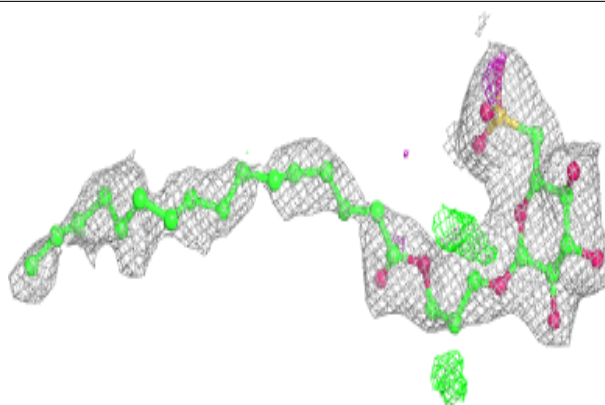
**Electron density around CLA B 616:**

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

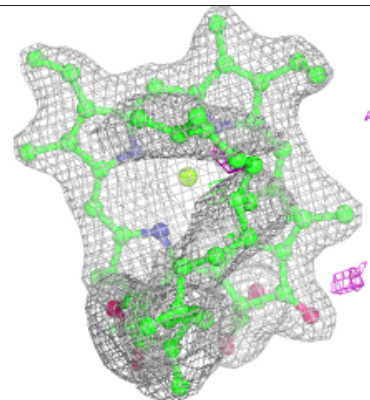
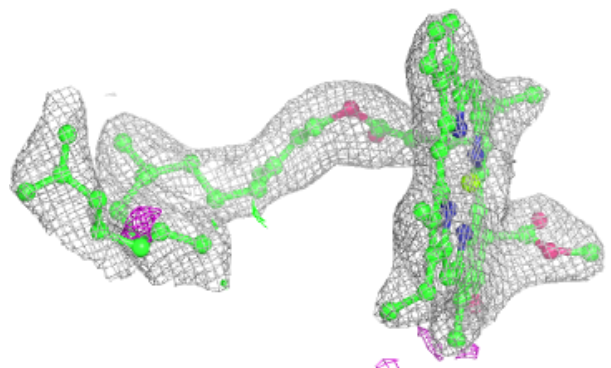
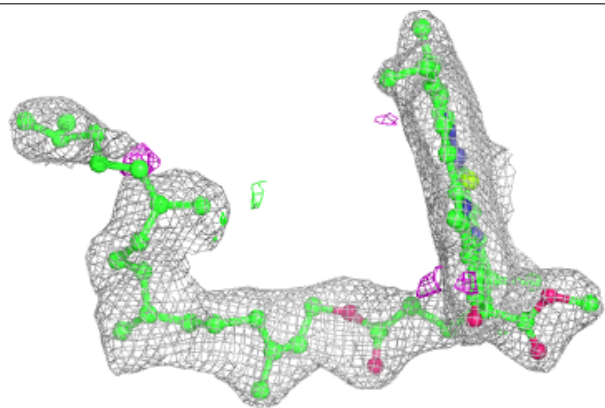


**Electron density around SQD F 102:**

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

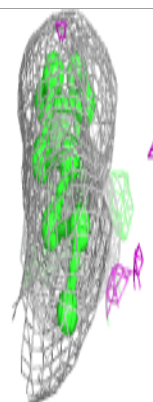
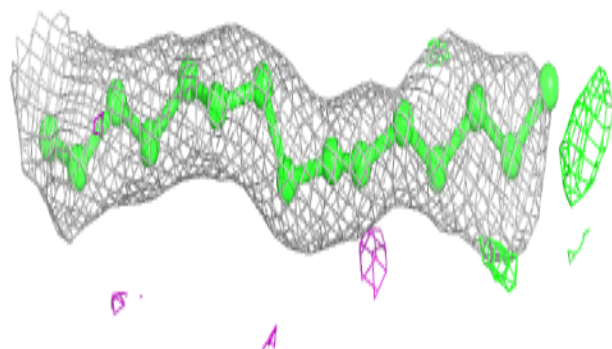
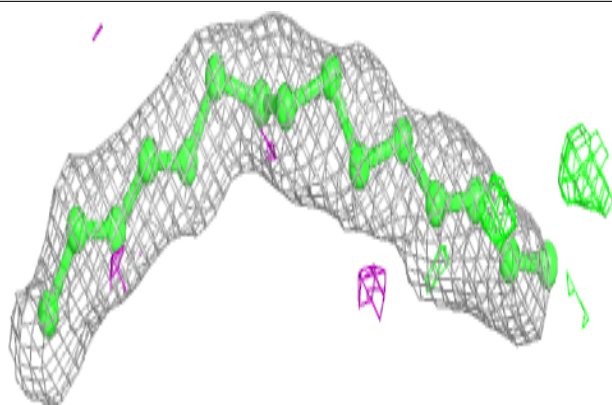
**Electron density around CLA c 506:**

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

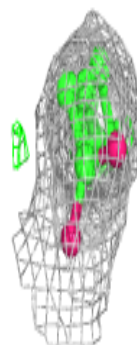
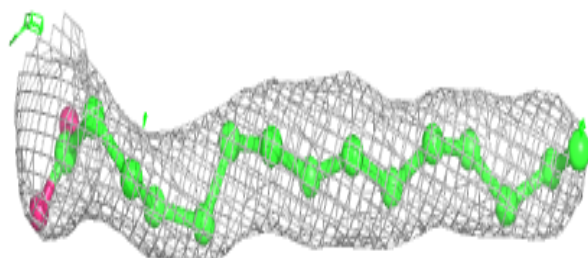
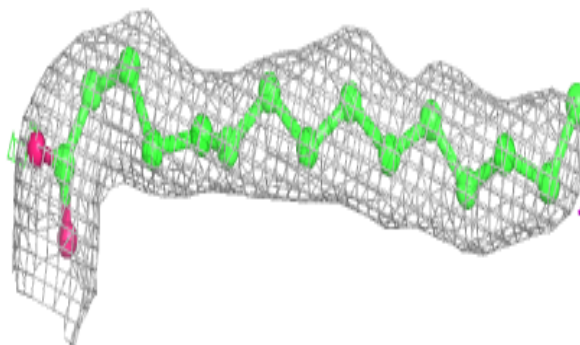


**Electron density around STE I 101:**

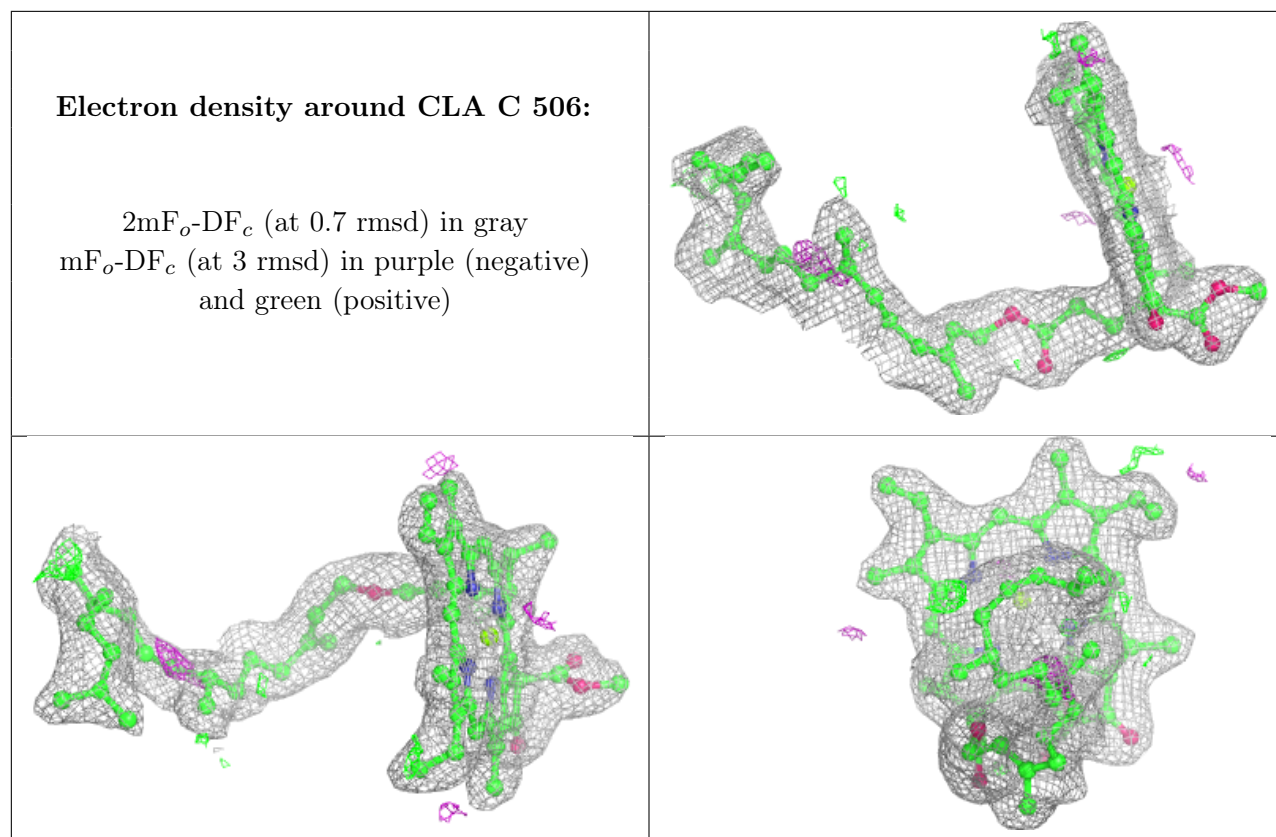
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around STE d 410:**

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

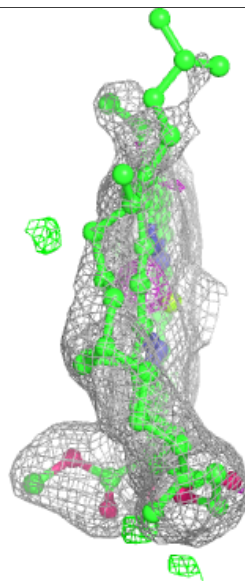
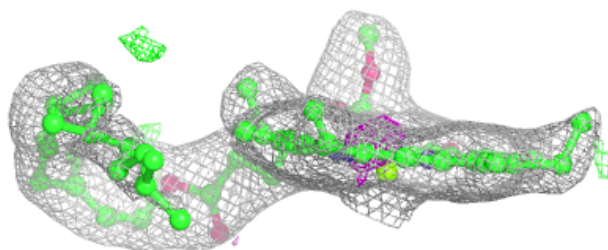
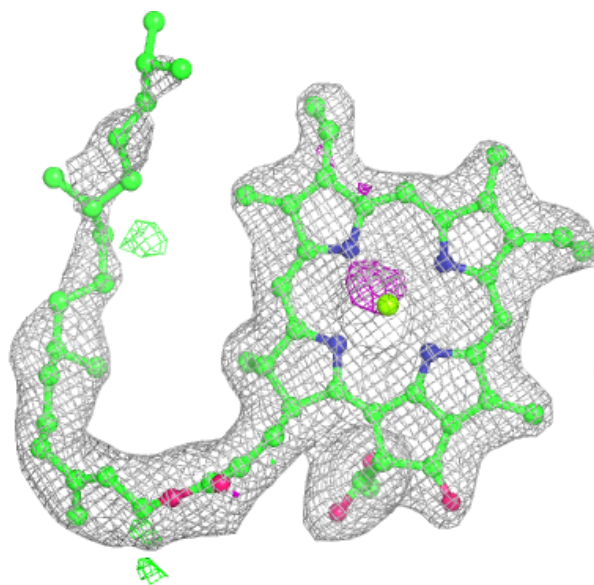






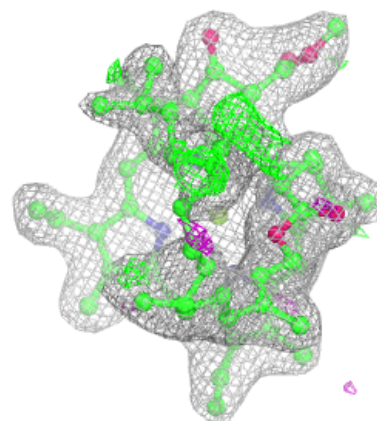
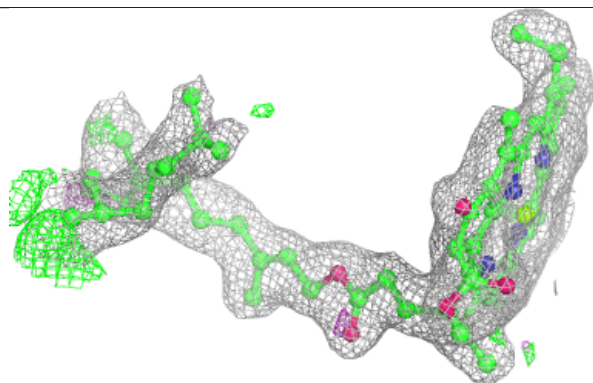
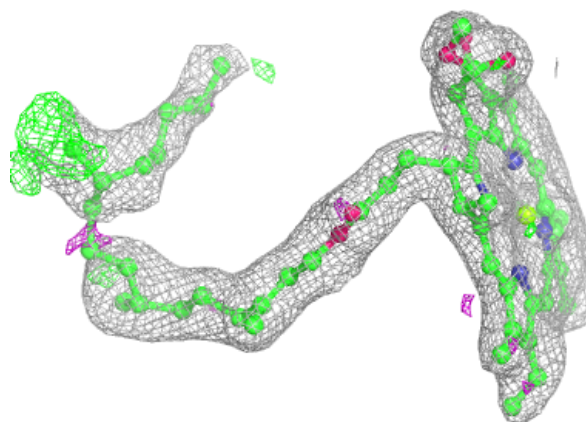
**Electron density around CLA C 512:**

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

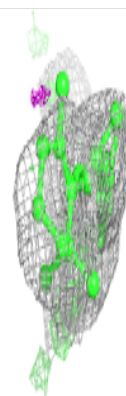
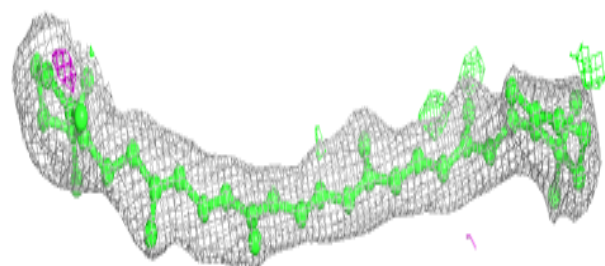
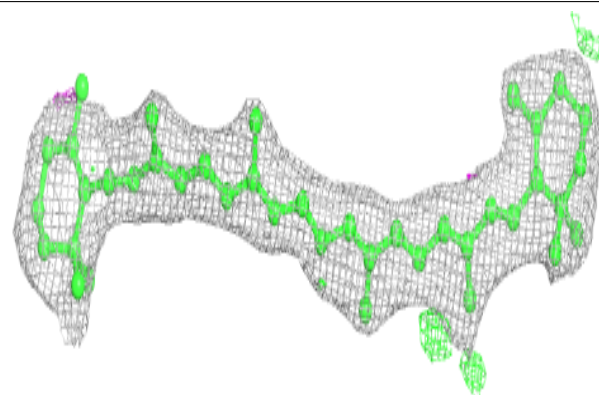


**Electron density around CLA B 606:**

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

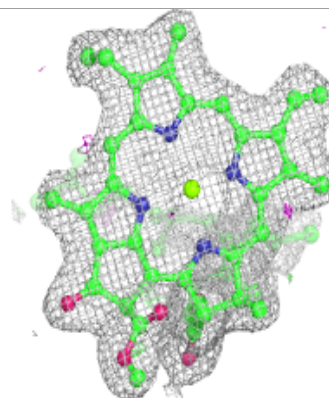
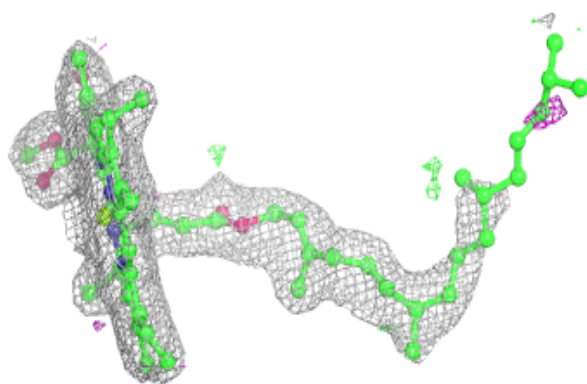
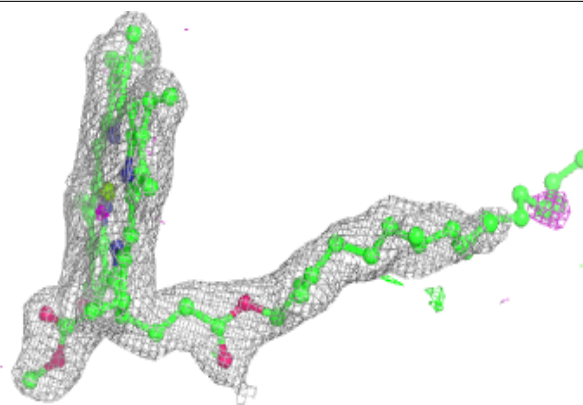
**Electron density around BCR d 404:**

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

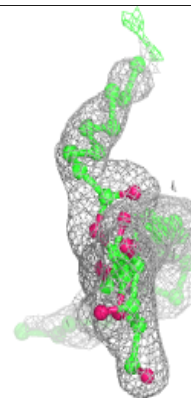
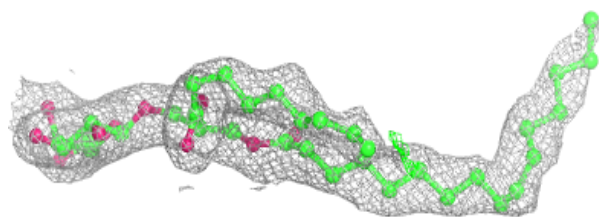
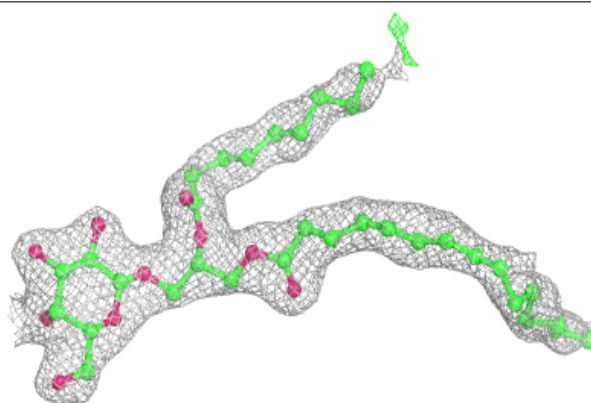


**Electron density around CLA D 404:**

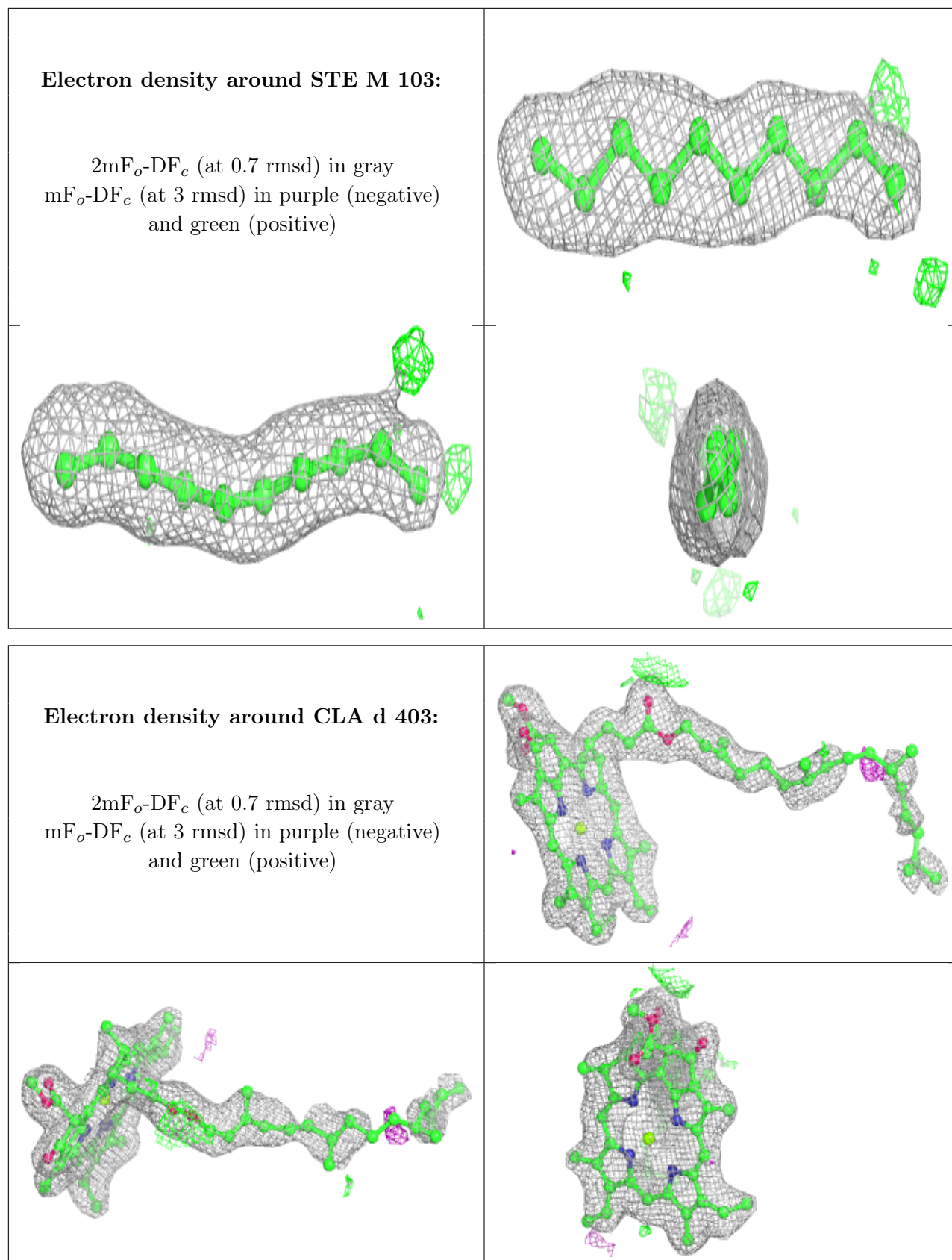
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

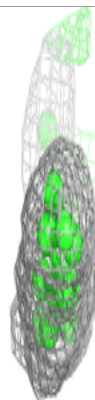
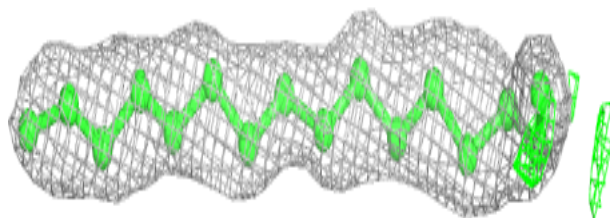
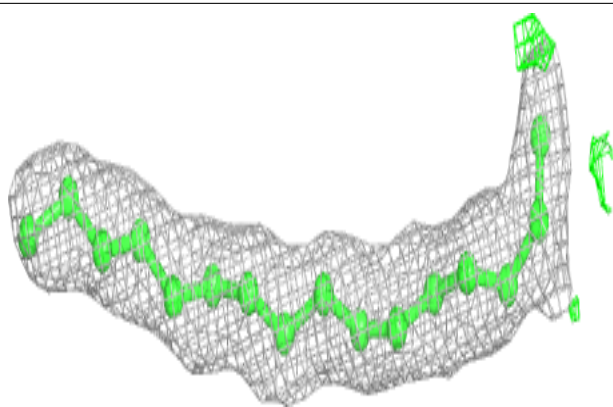




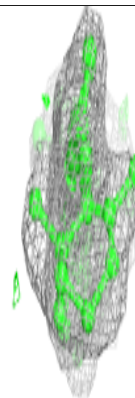
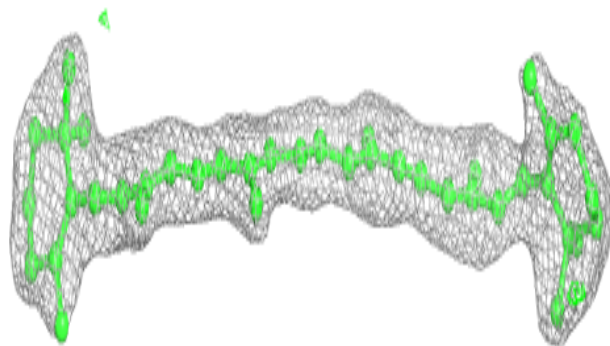
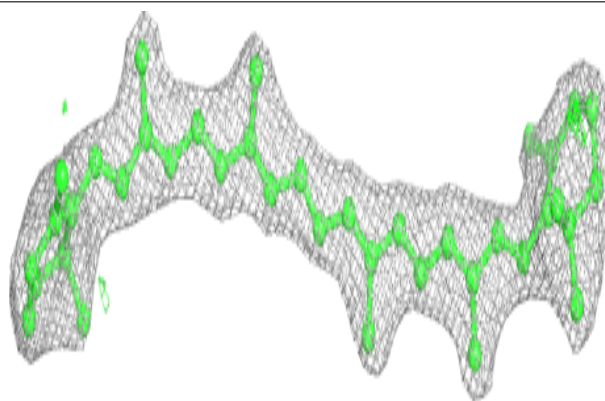


**Electron density around STE C 521:**

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

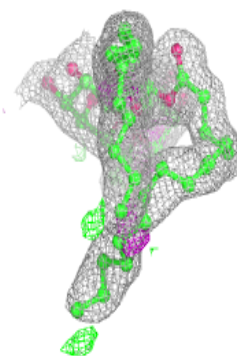
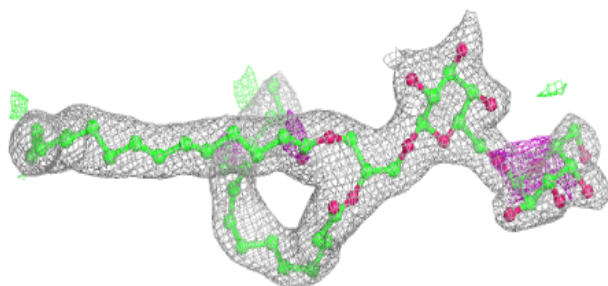
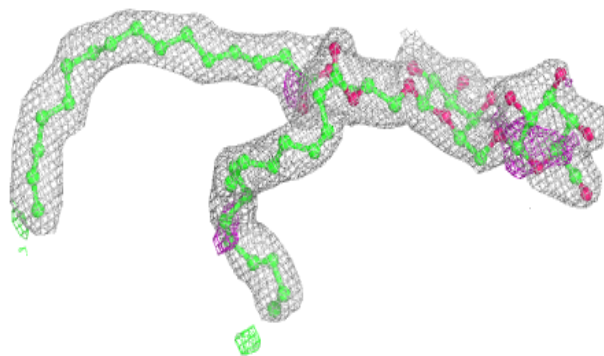
**Electron density around BCR k 101:**

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

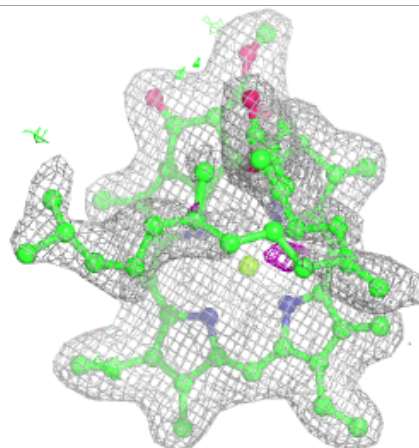
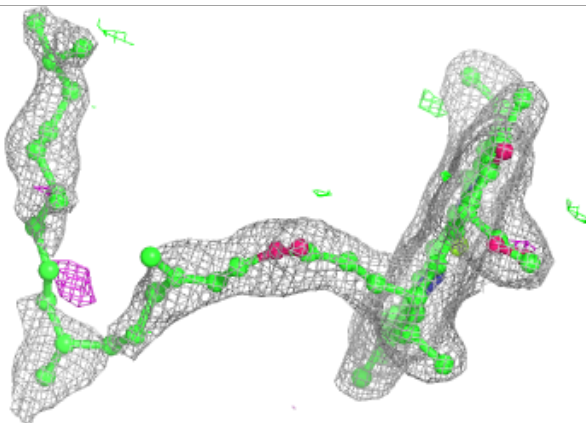
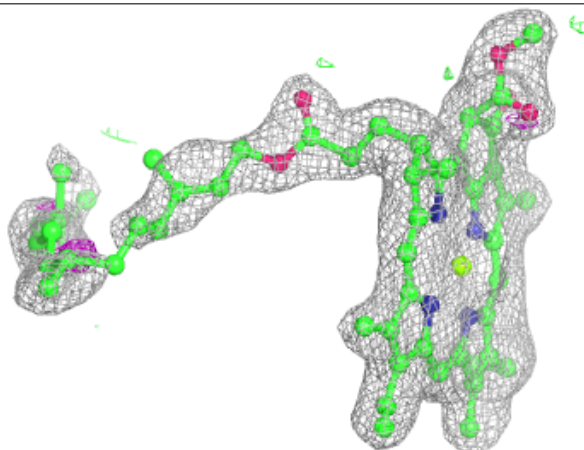


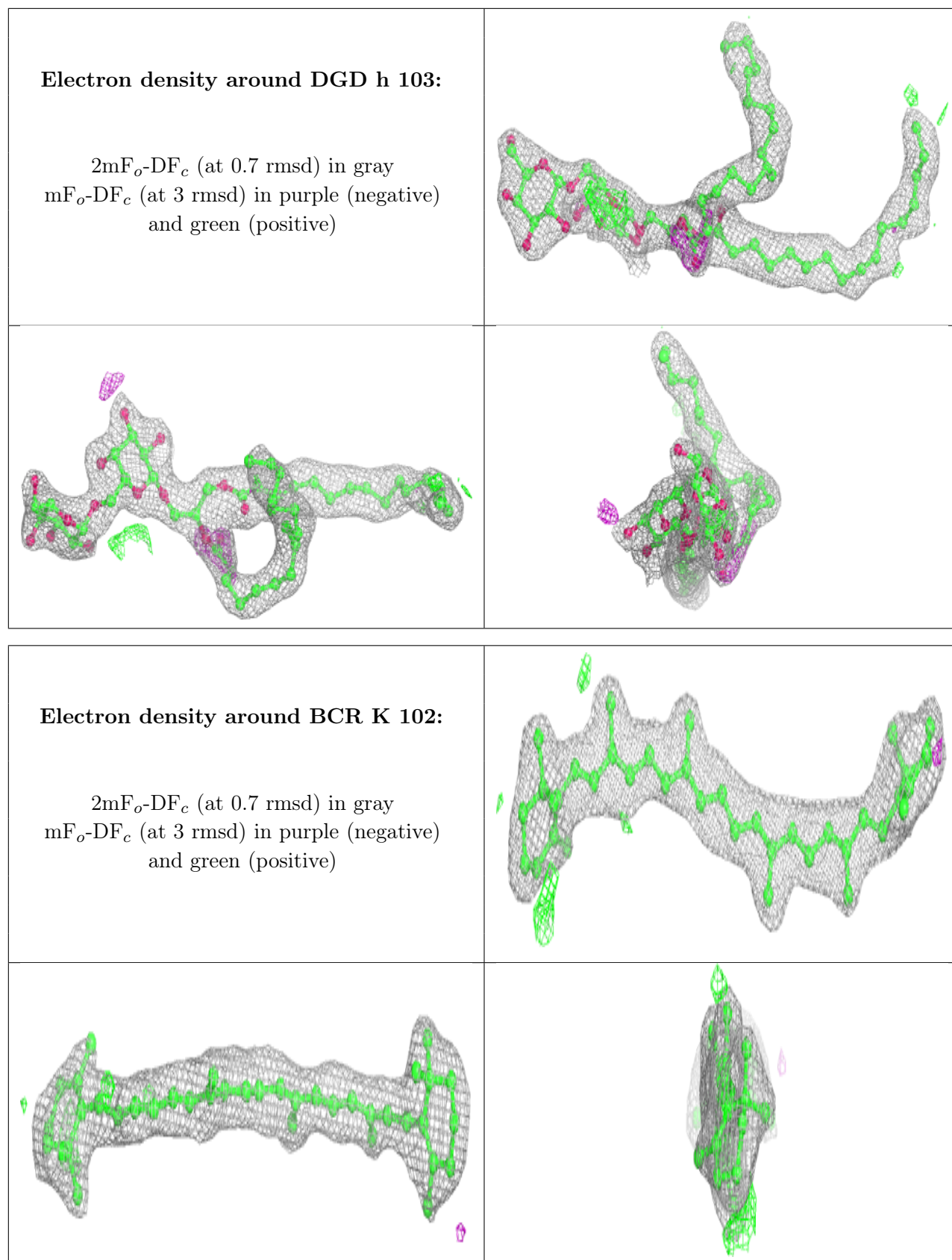
**Electron density around DGD H 102:**

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

**Electron density around CLA a 610:**

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

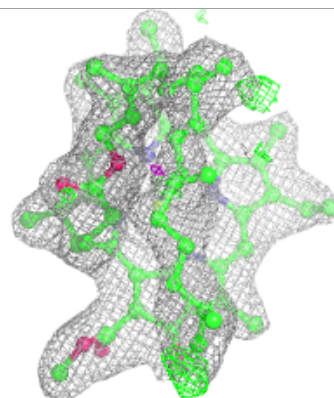
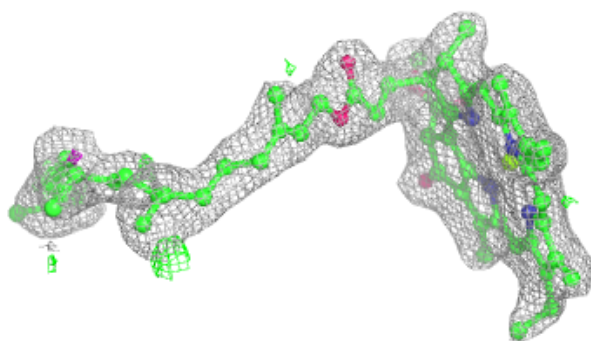
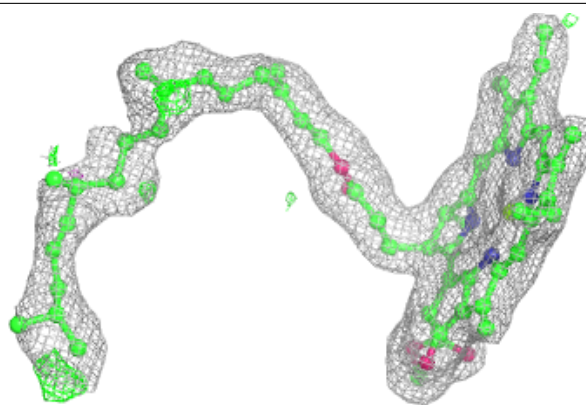




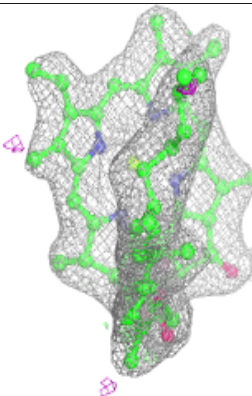
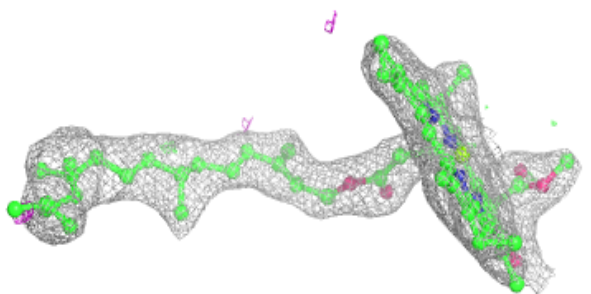
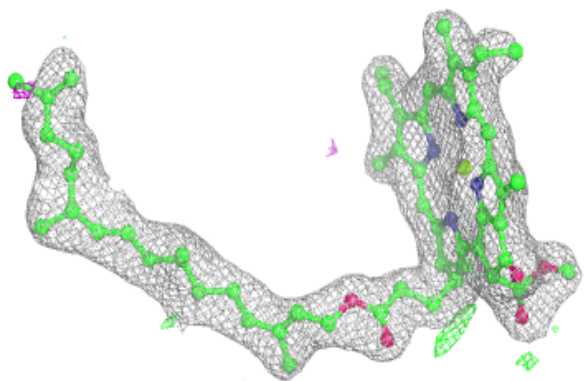


**Electron density around CLA b 605:**

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

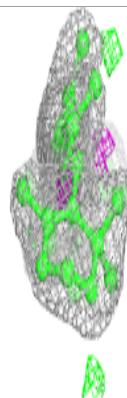
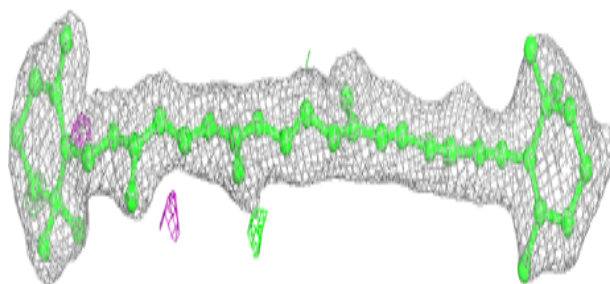
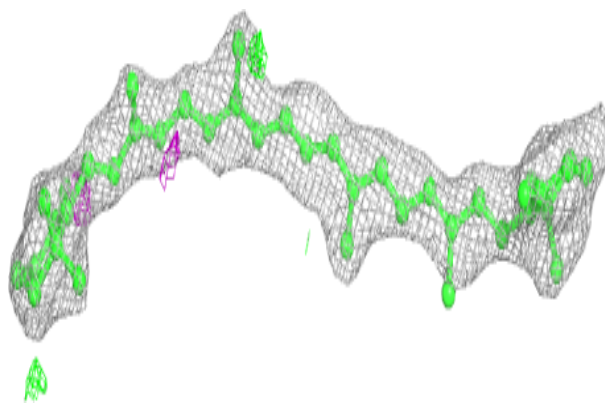
**Electron density around CLA b 608:**

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

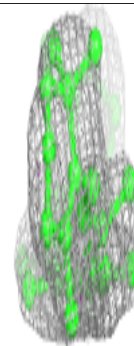
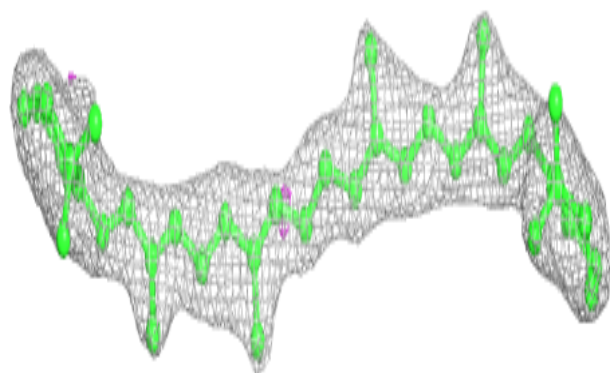
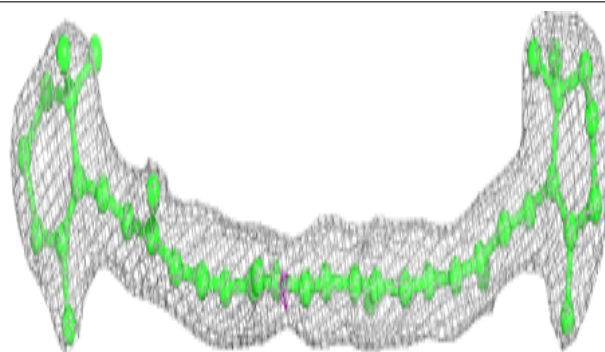


**Electron density around BCR h 102:**

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

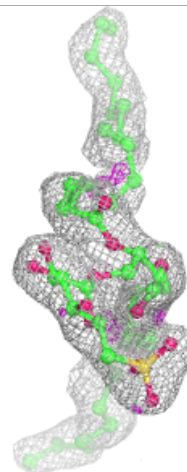
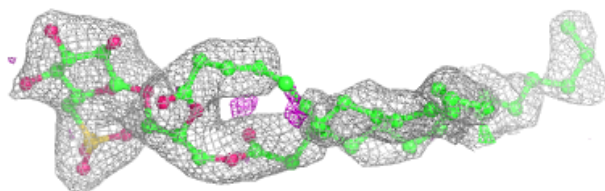
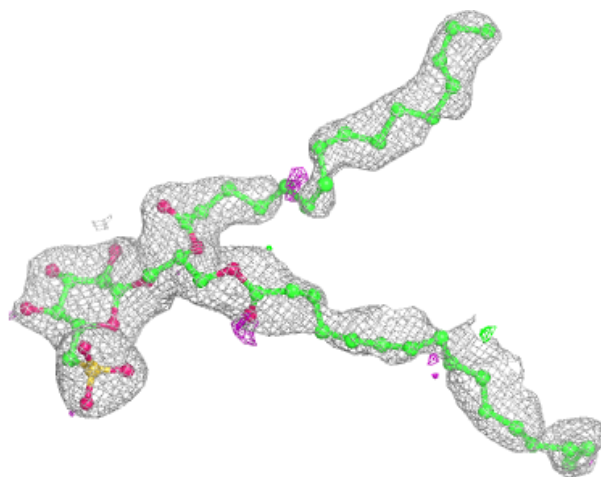
**Electron density around BCR K 103:**

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



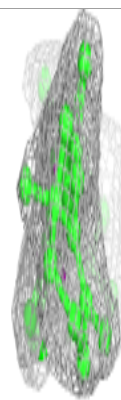
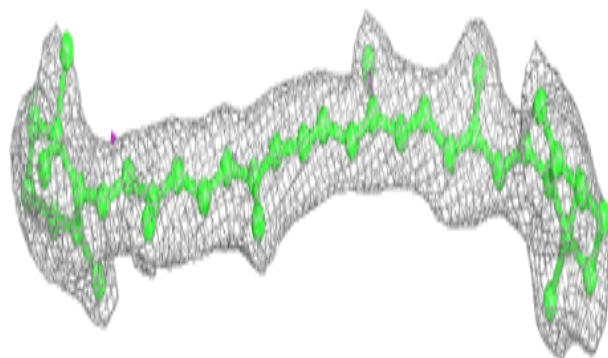
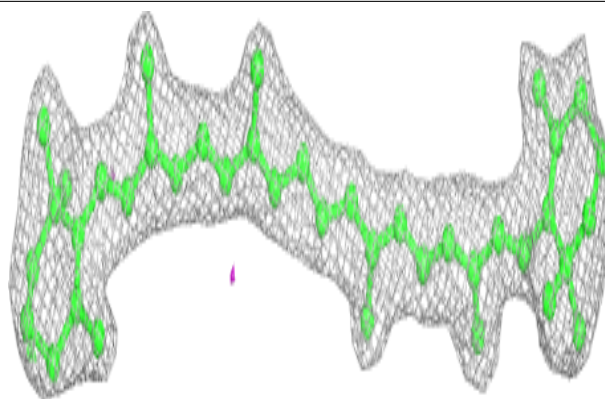
**Electron density around SQD a 615:**

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

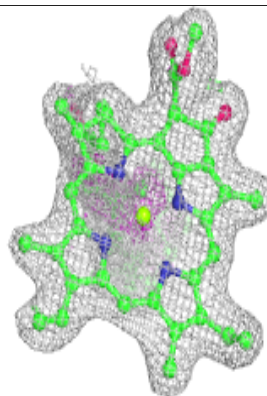
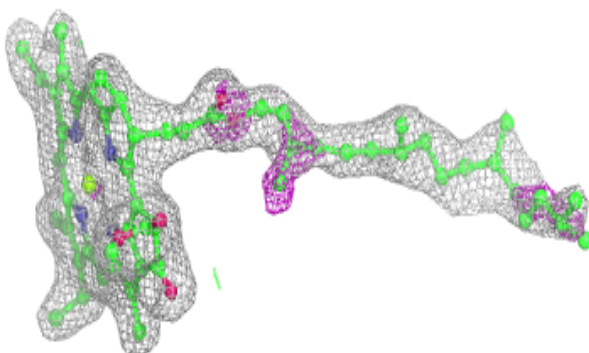
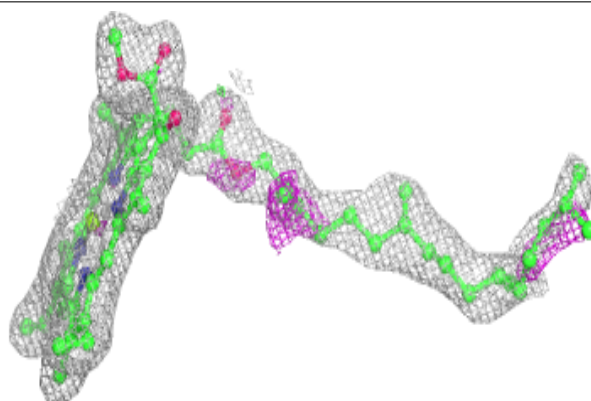


**Electron density around BCR b 618:**

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

**Electron density around CLA B 604:**

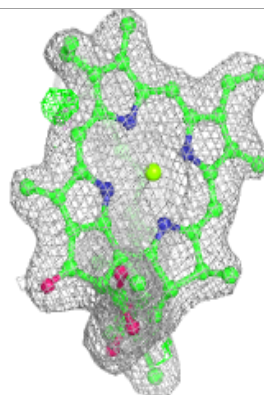
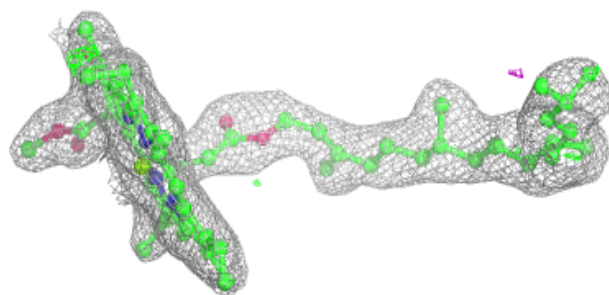
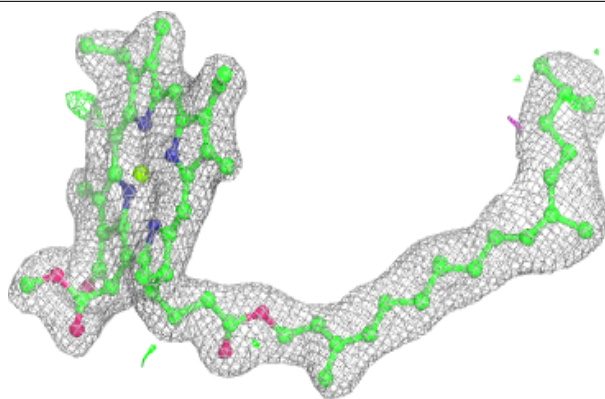
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



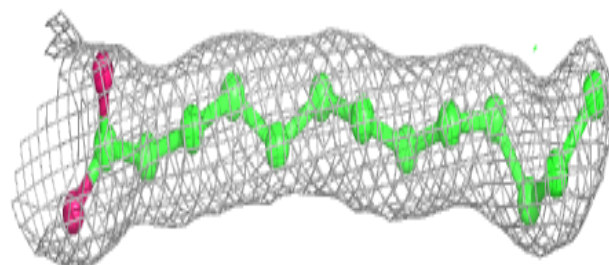
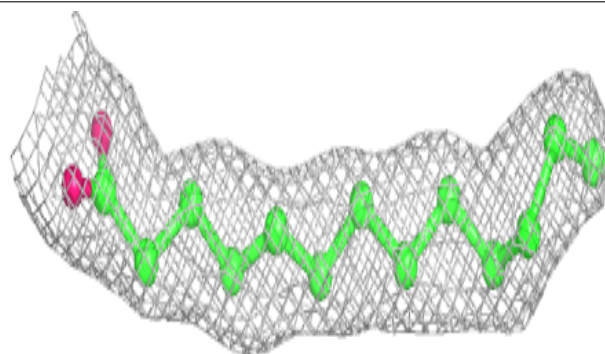


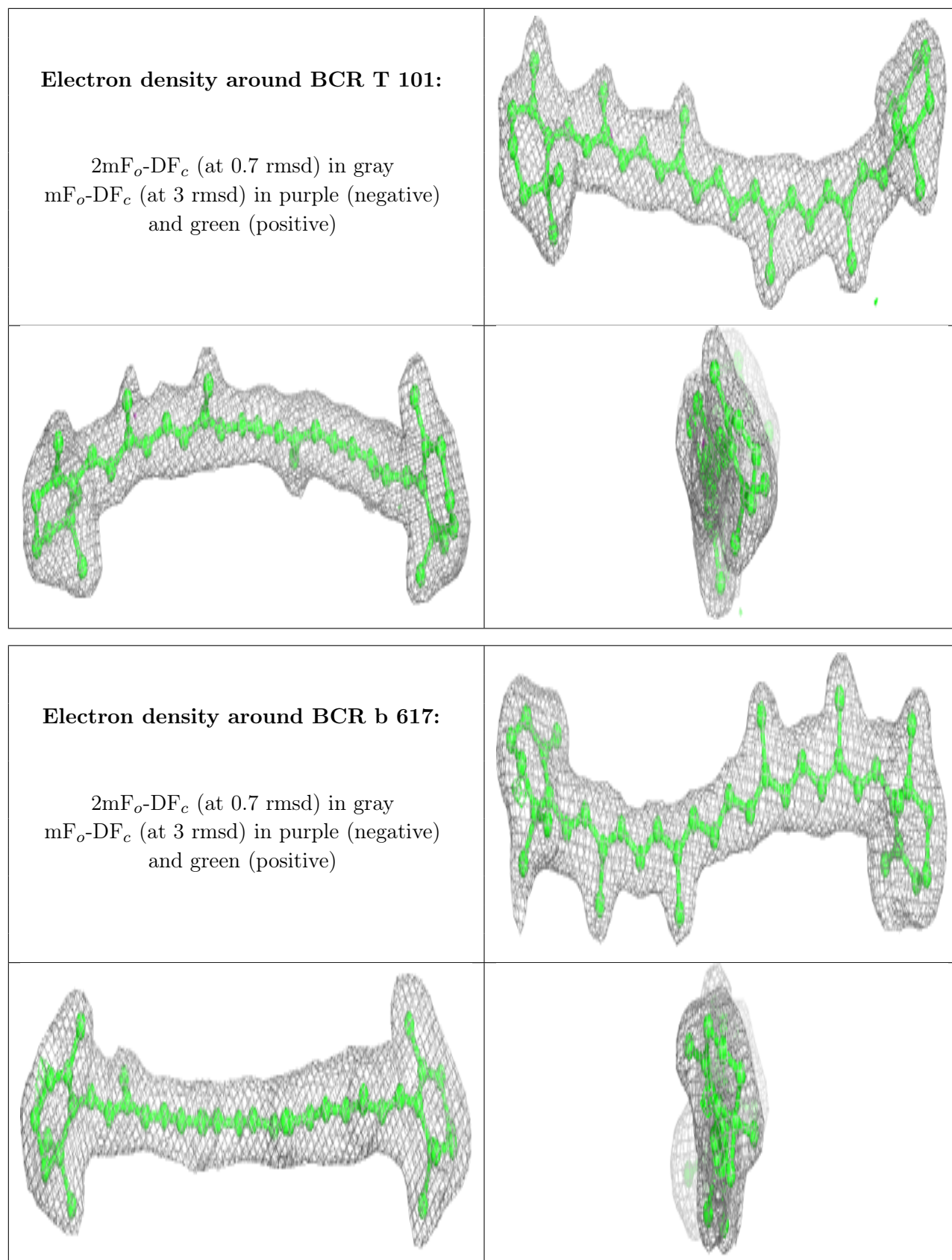
**Electron density around CLA B 609:**

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

**Electron density around STE M 102:**

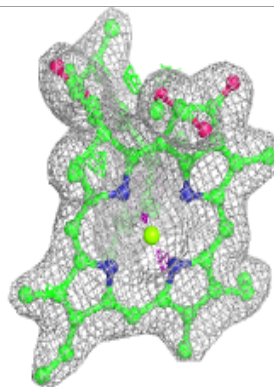
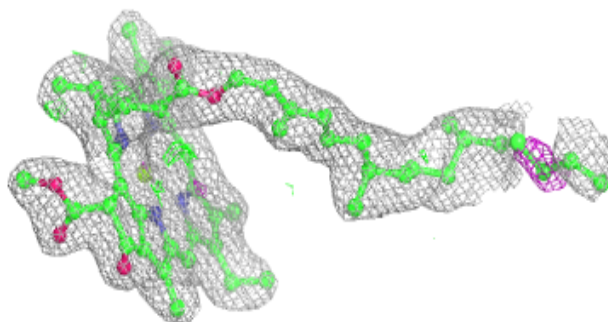
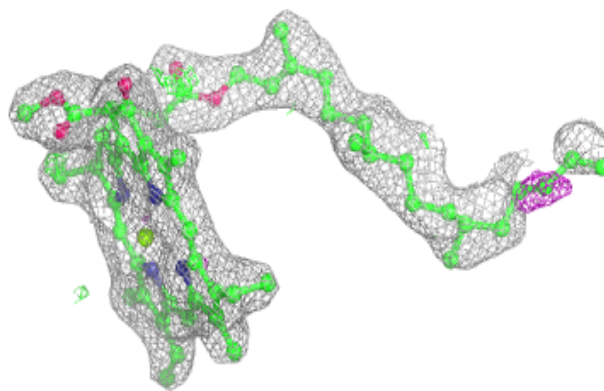
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



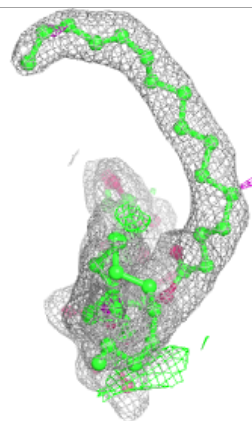
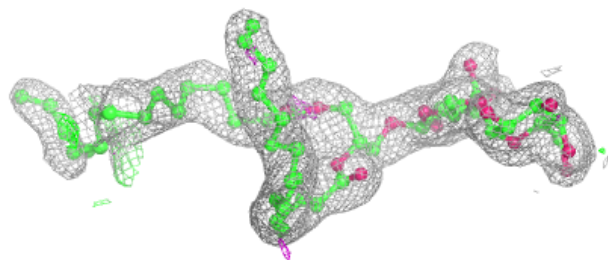
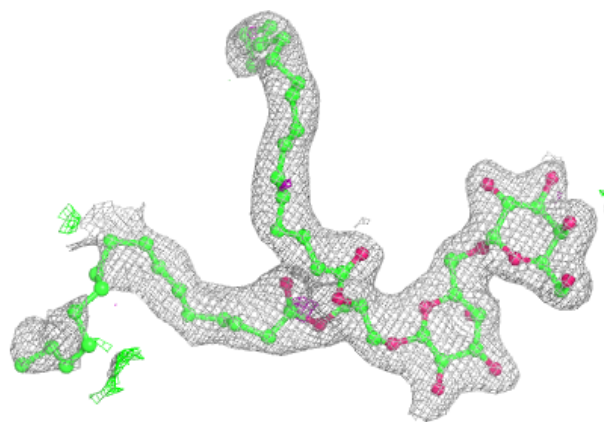


**Electron density around CLA c 508:**

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

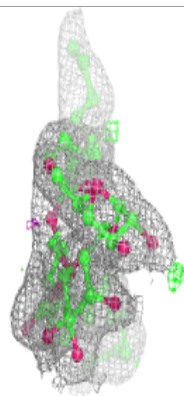
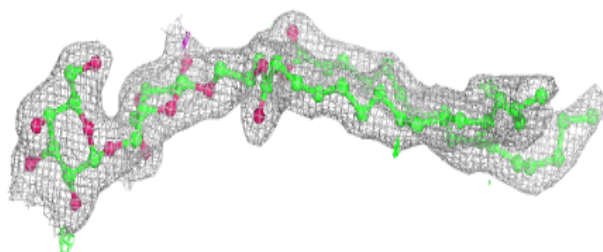
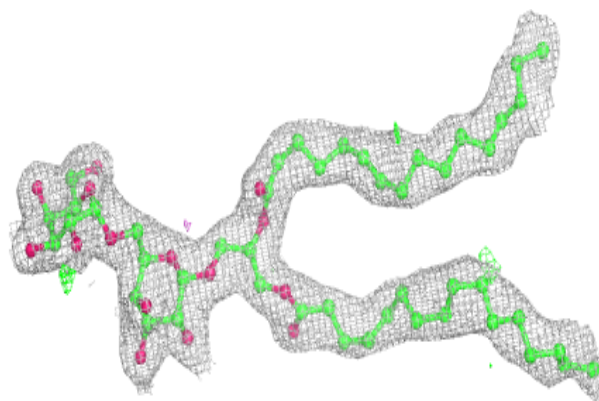
**Electron density around DGD C 516:**

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

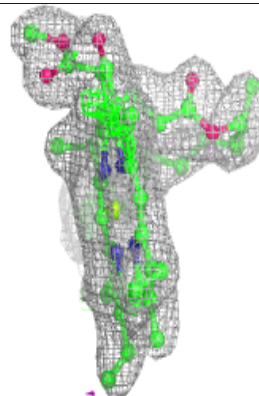
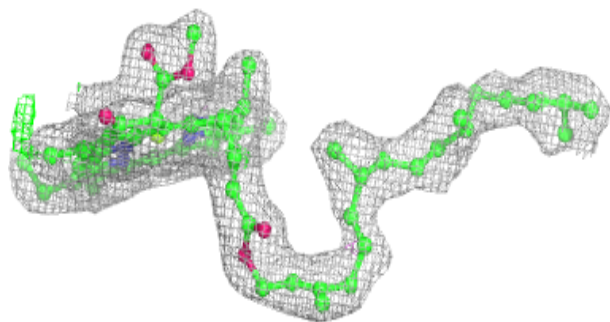
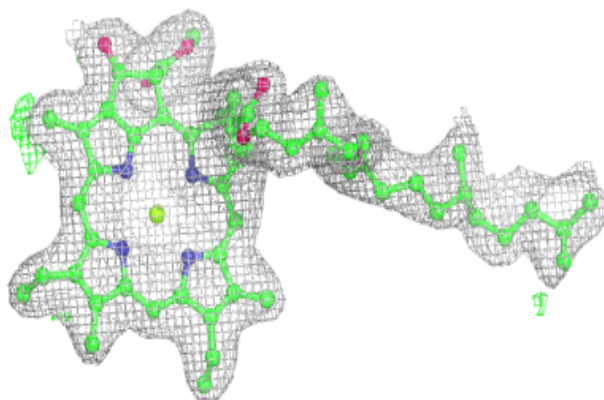


**Electron density around DGD C 517:**

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

**Electron density around CLA a 608:**

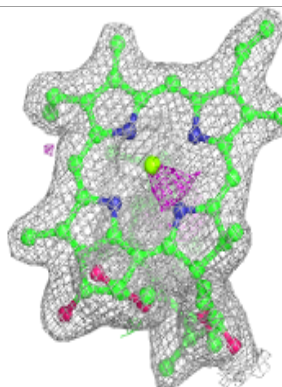
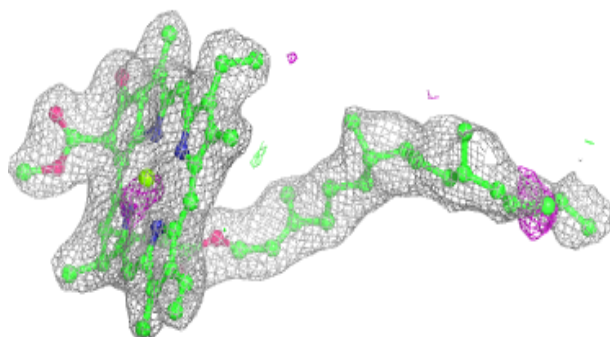
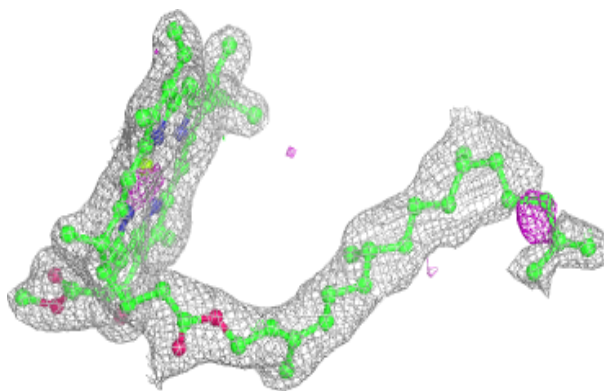
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



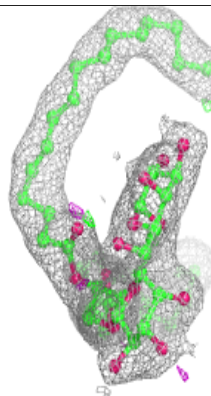
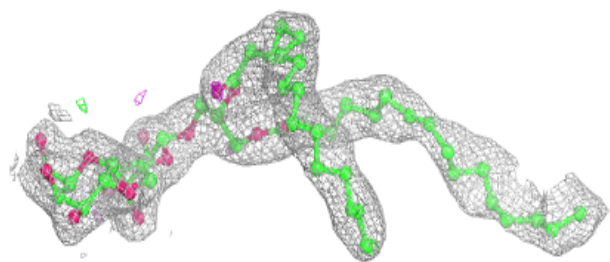
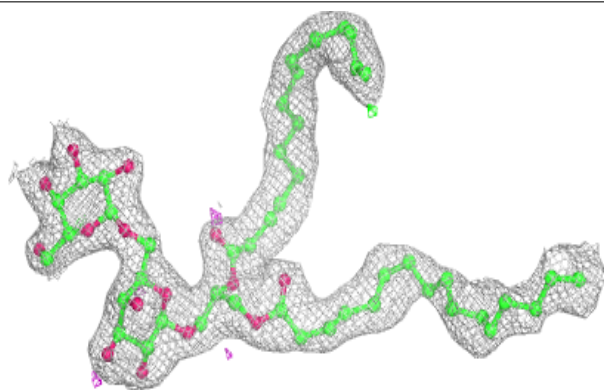


**Electron density around CLA C 508:**

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

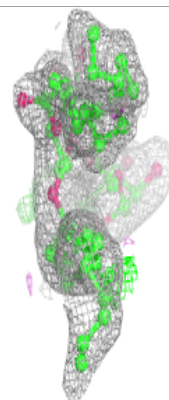
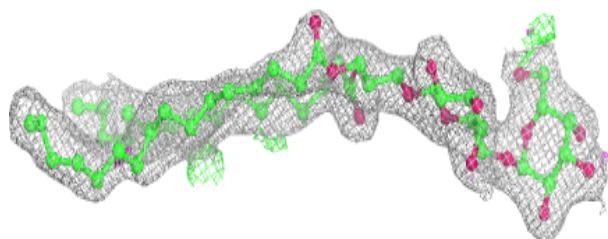
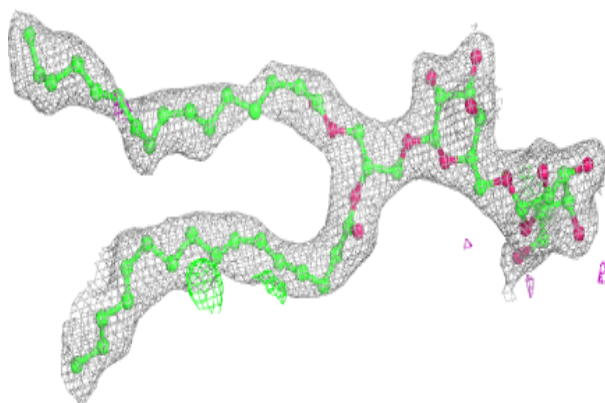
**Electron density around DGD c 517:**

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

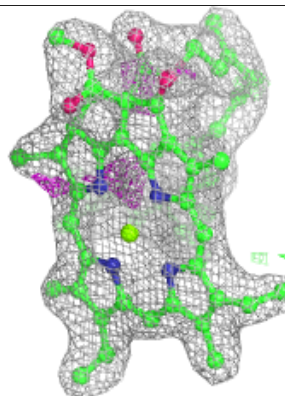
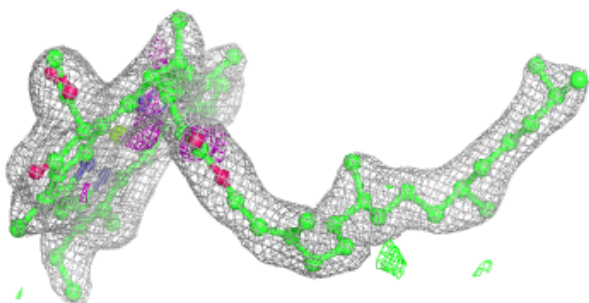
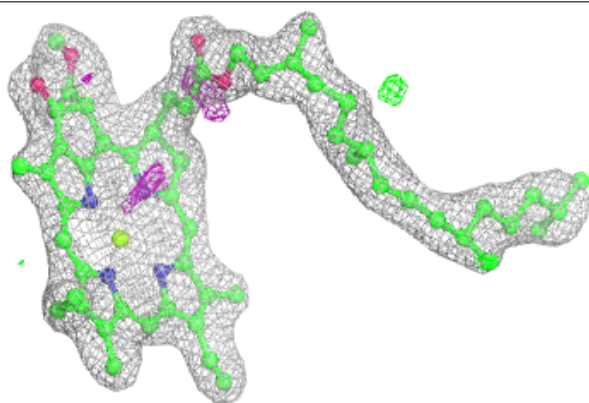


**Electron density around DGD c 518:**

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

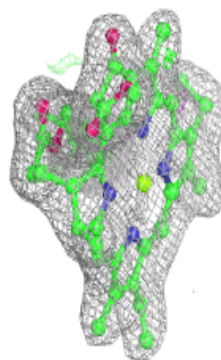
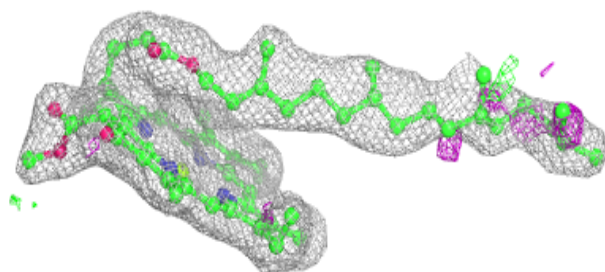
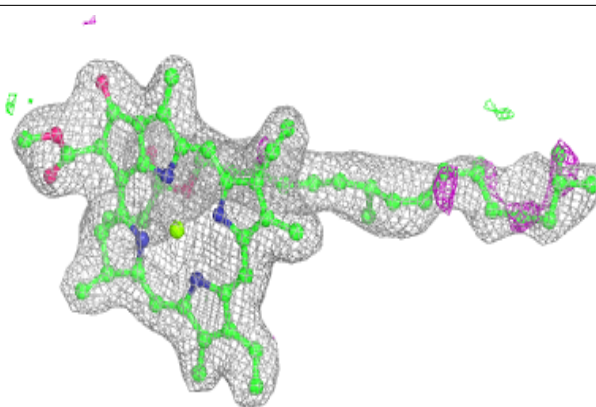
**Electron density around CLA C 511:**

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

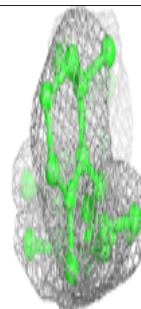
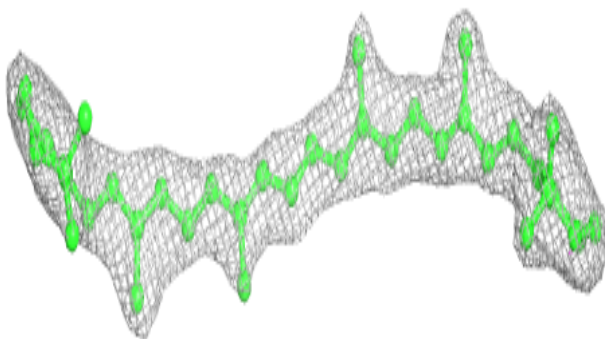
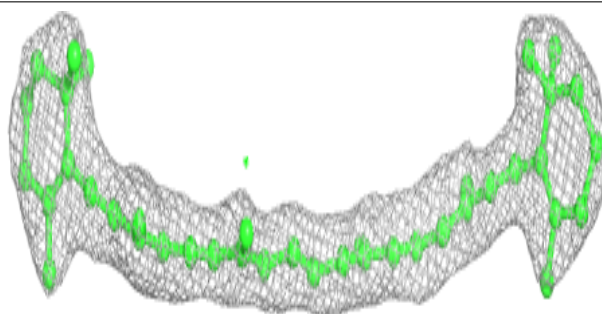


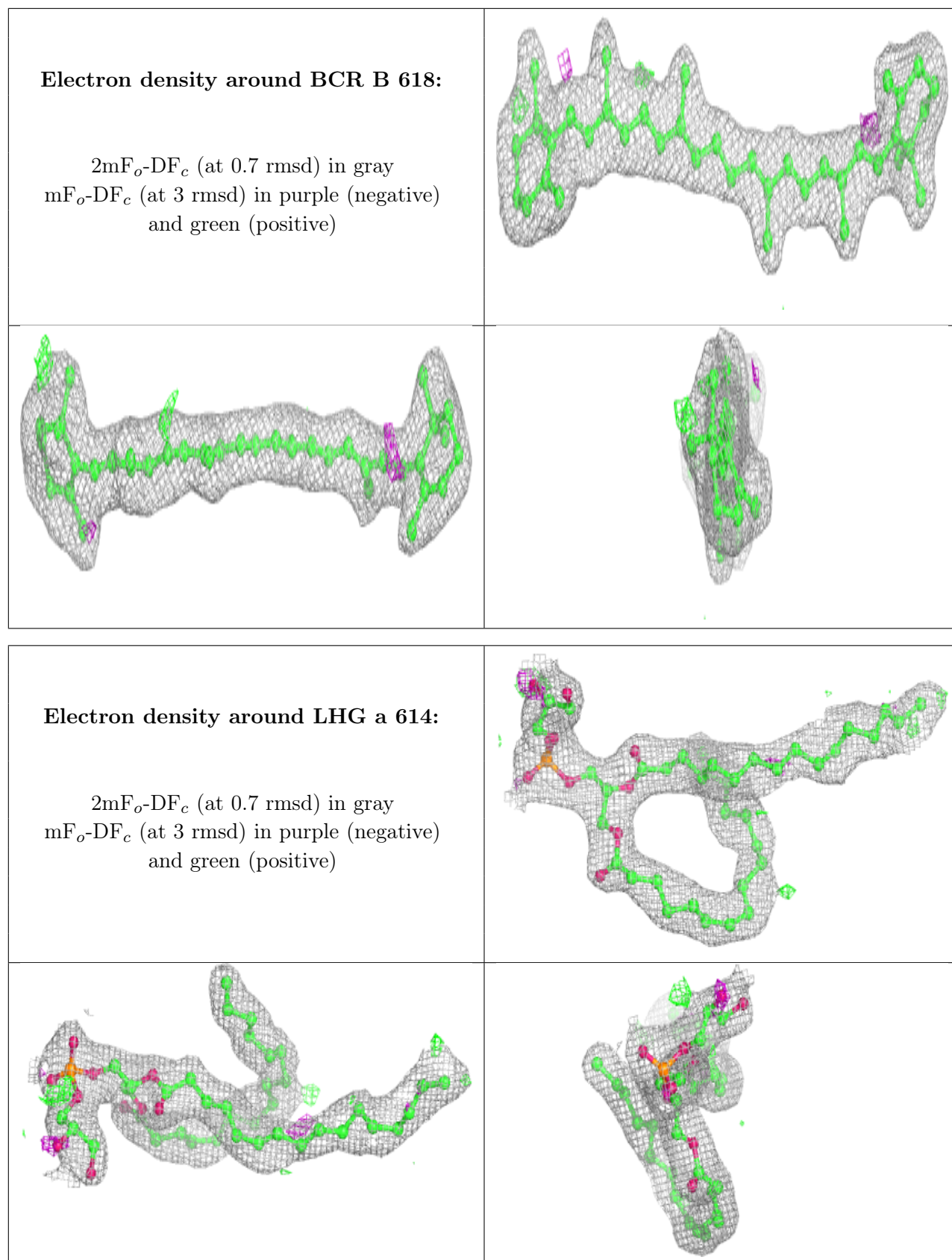
**Electron density around CLA B 614:**

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

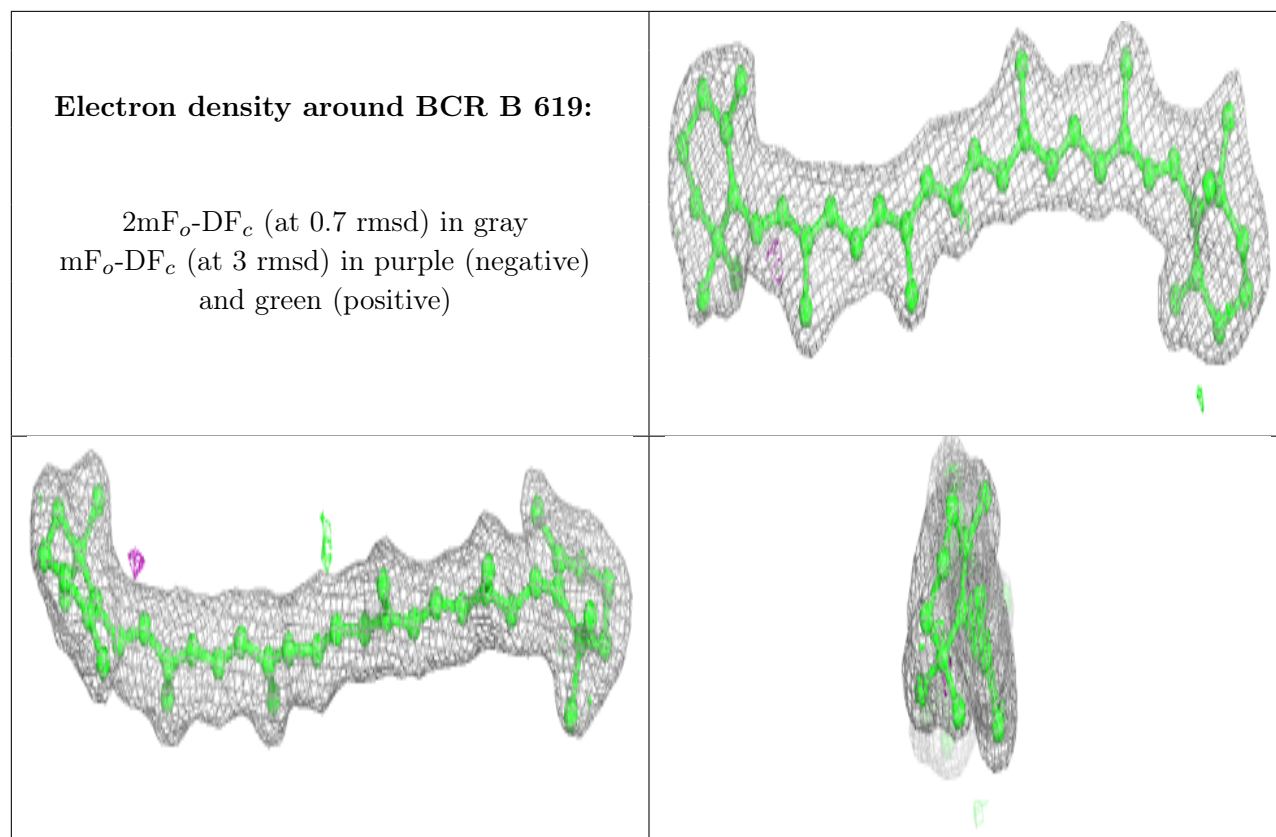
**Electron density around BCR k 102:**

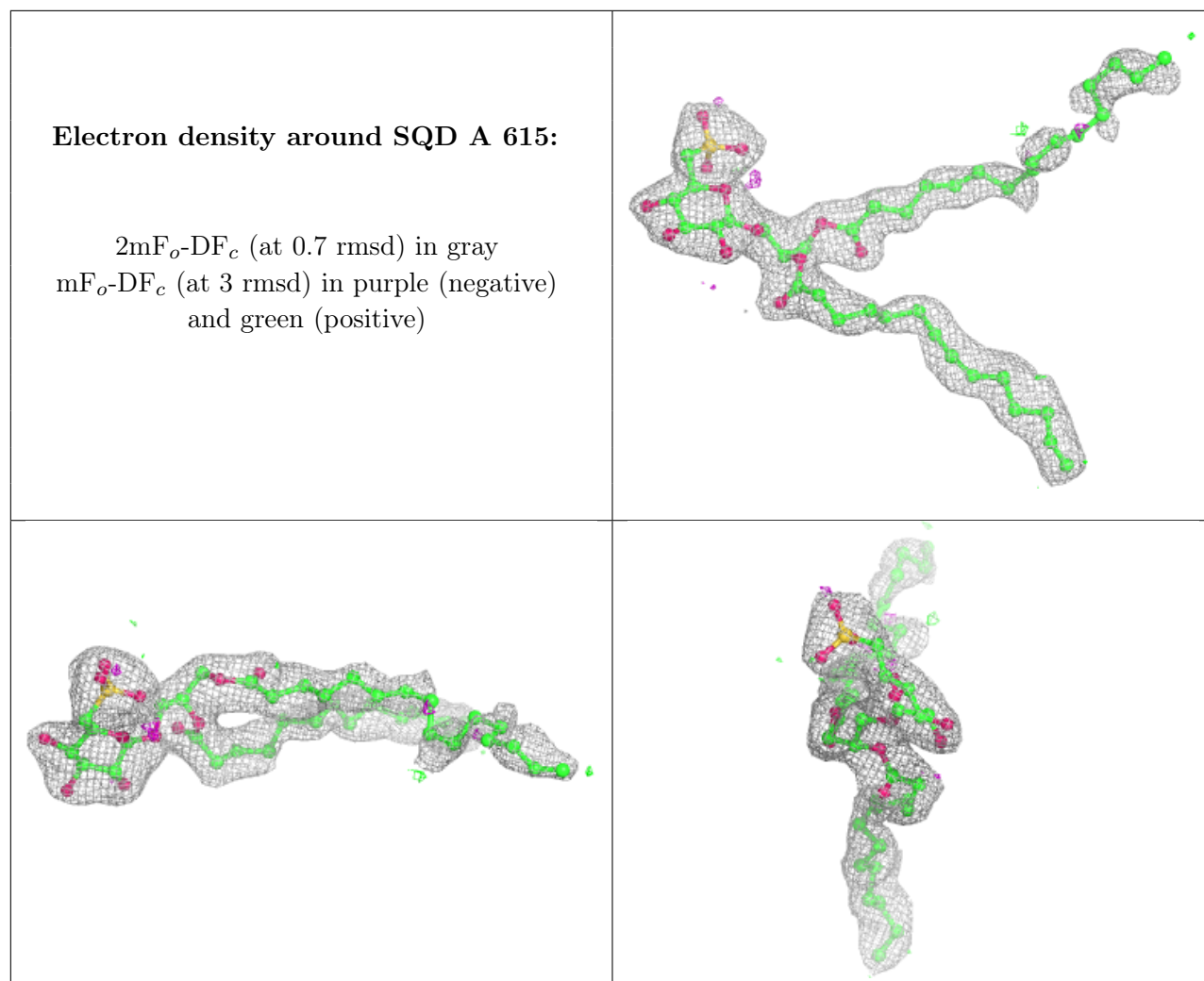
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





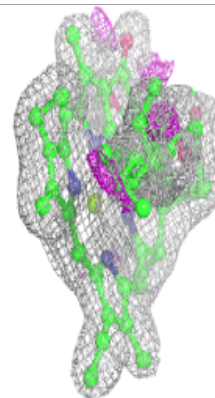
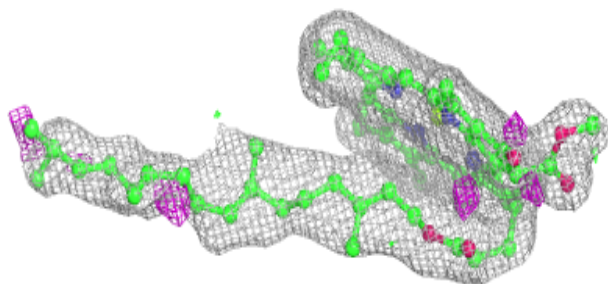
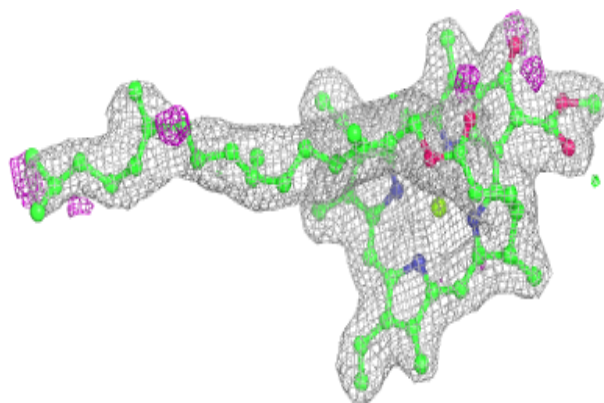




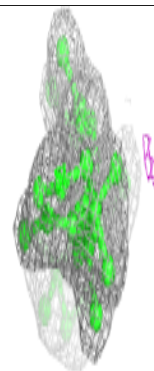
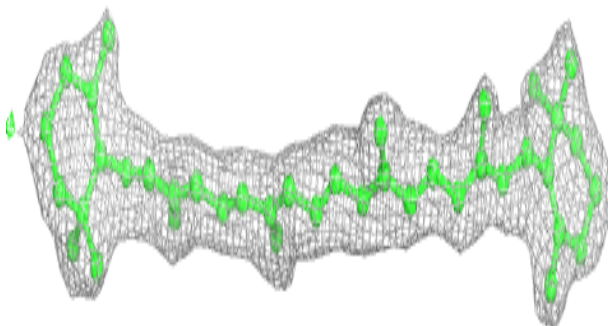
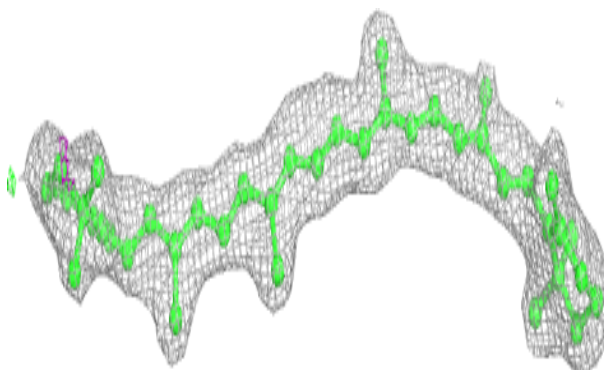


**Electron density around CLA b 613:**

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

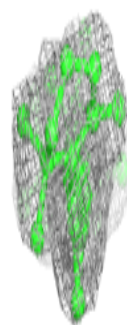
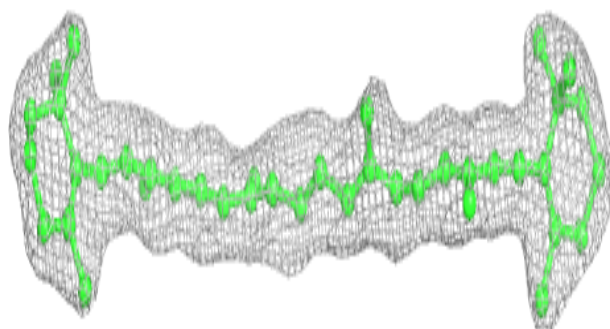
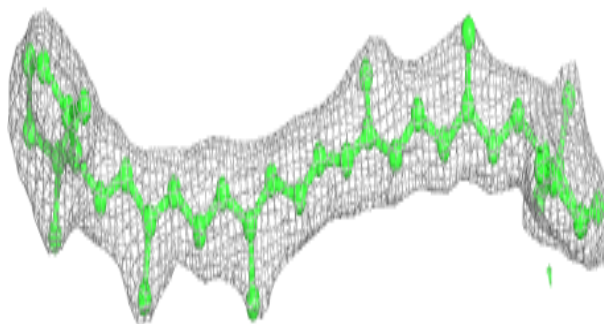
**Electron density around BCR H 101:**

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

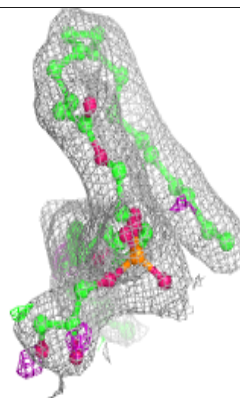
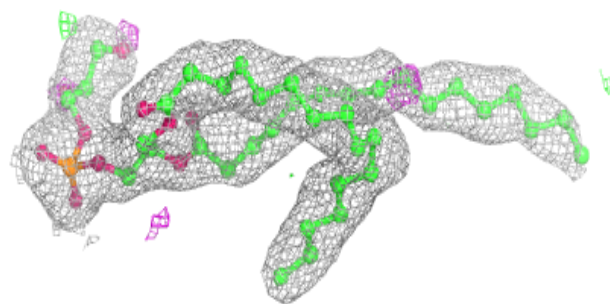
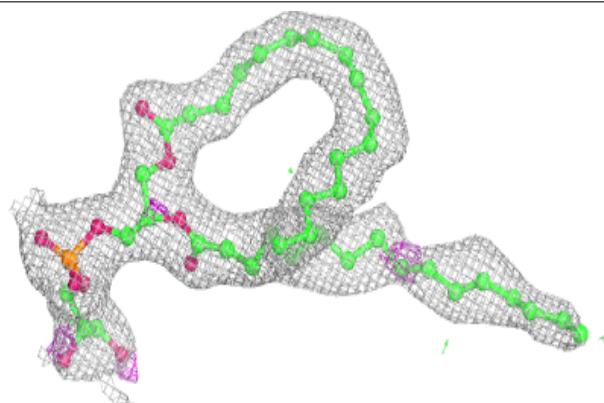


**Electron density around BCR K 101:**

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

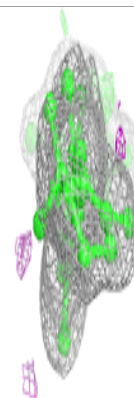
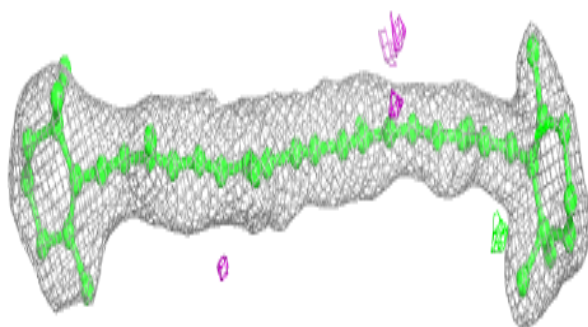
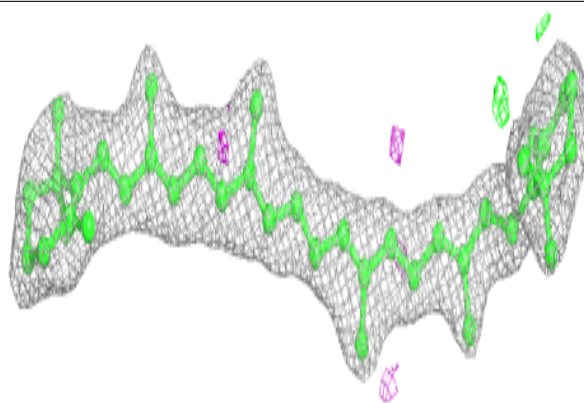
**Electron density around LHG B 622:**

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

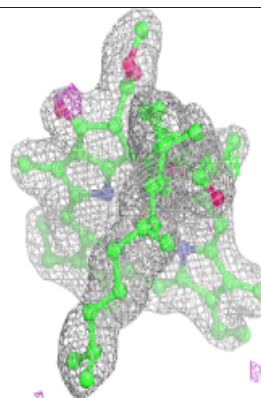
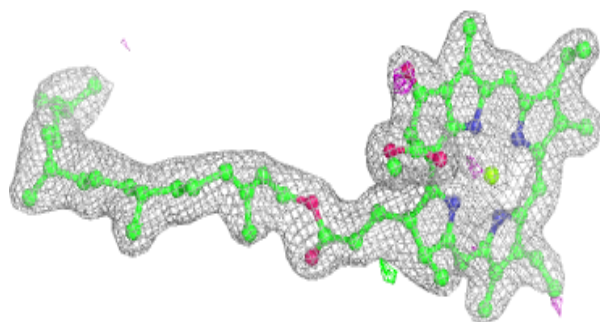
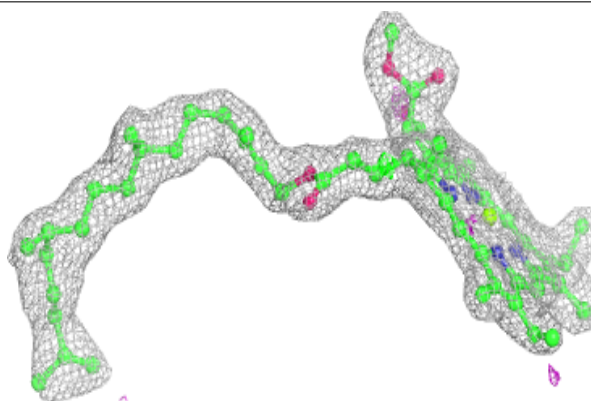


**Electron density around BCR c 515:**

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

**Electron density around CLA d 402:**

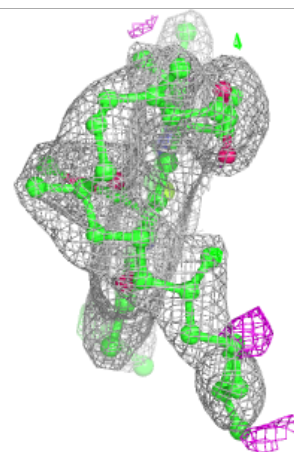
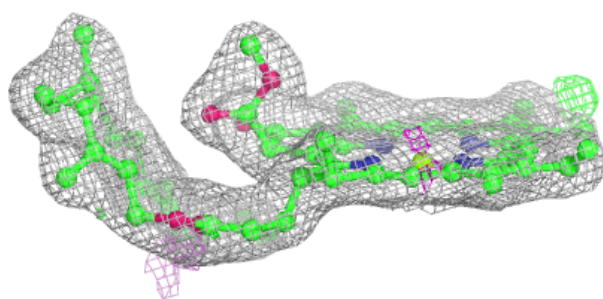
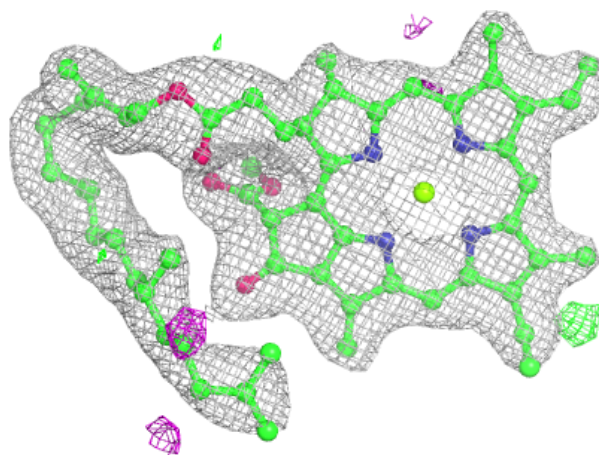
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





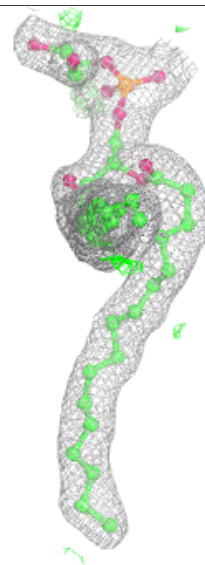
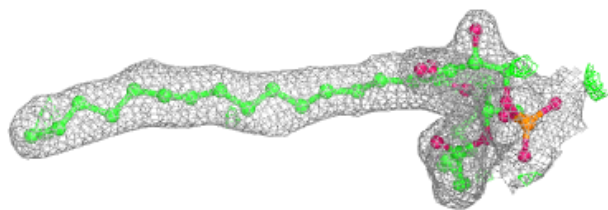
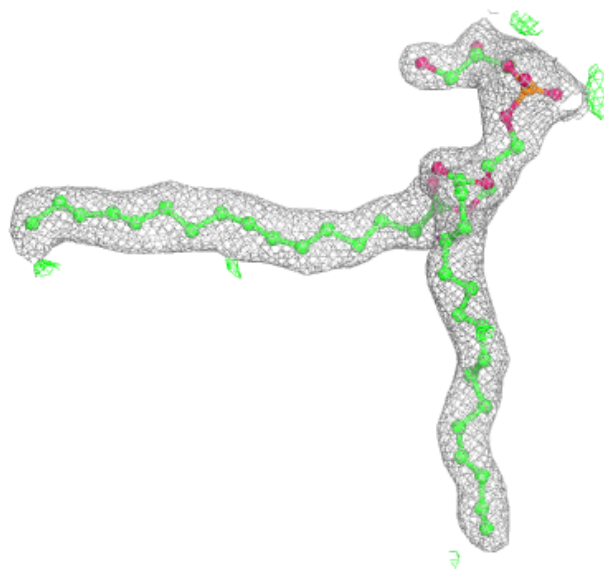
**Electron density around CLA b 609:**

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



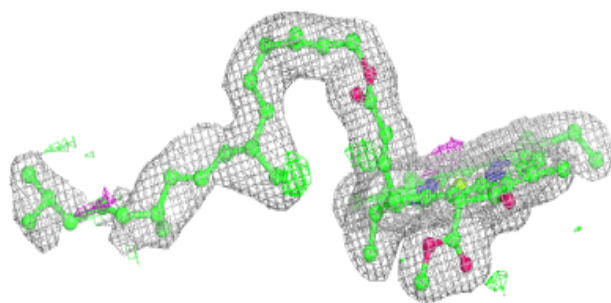
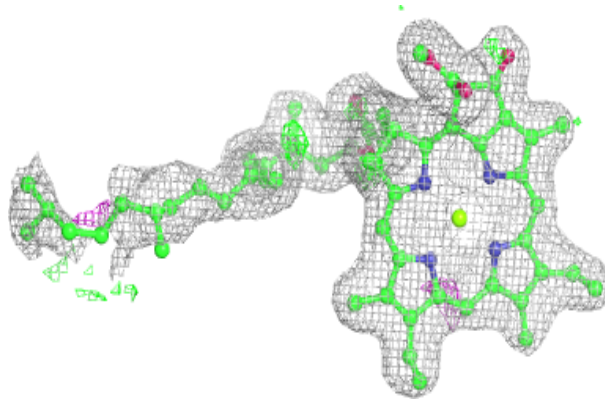
**Electron density around LHG 1 101:**

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

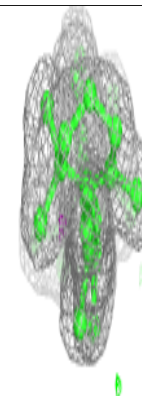
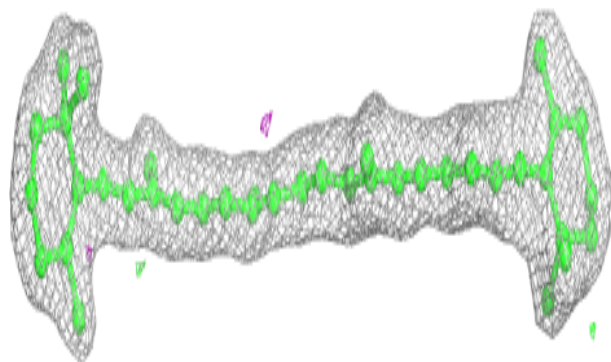
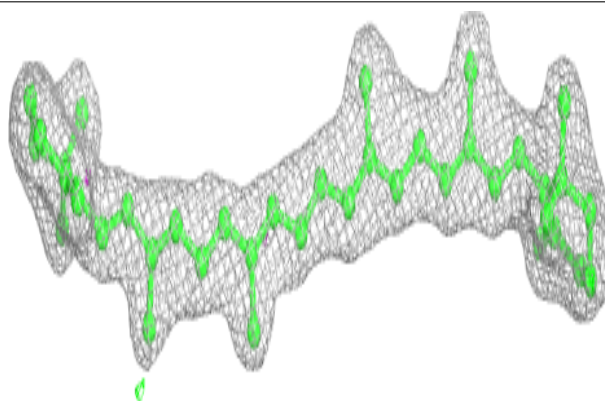


**Electron density around CLA A 607:**

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

**Electron density around BCR A 610:**

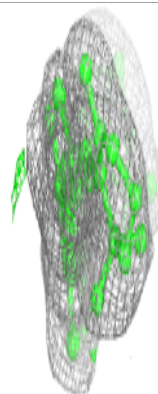
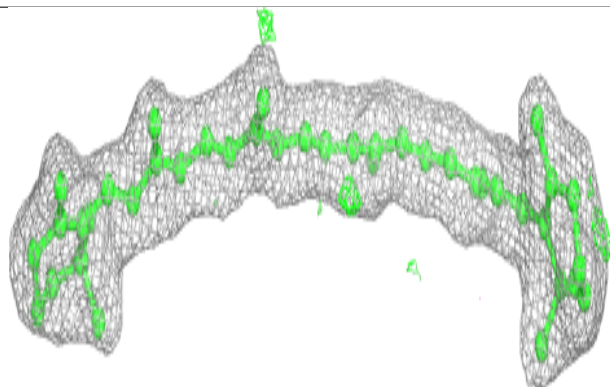
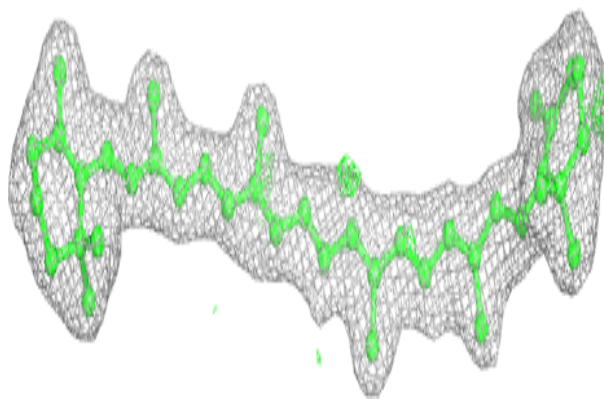
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



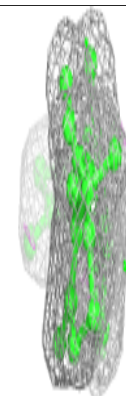
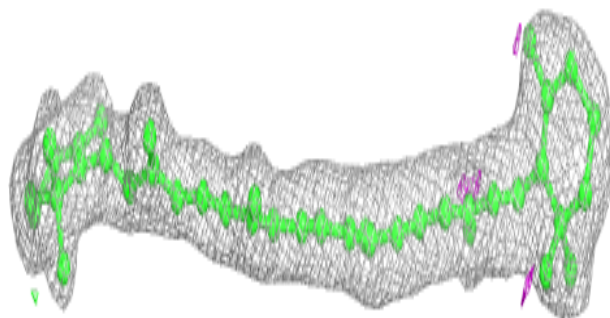
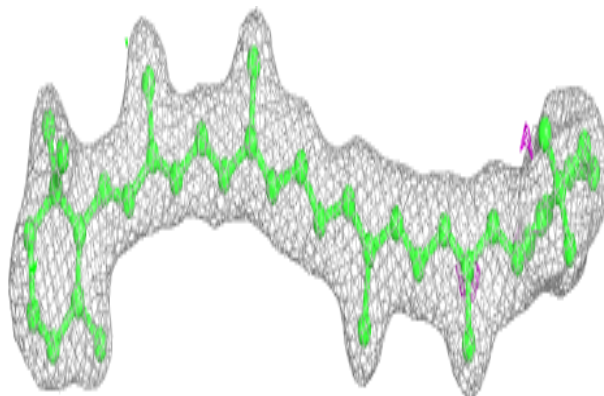


**Electron density around BCR t 101:**

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

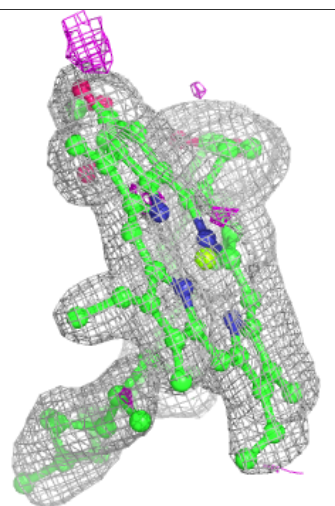
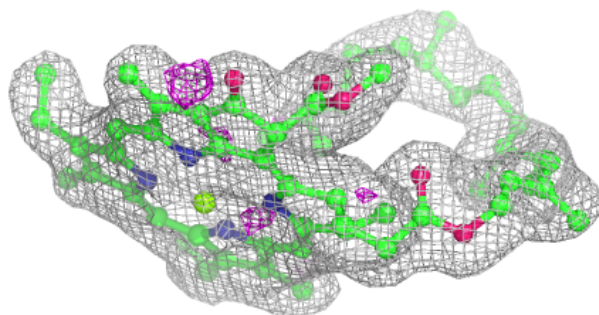
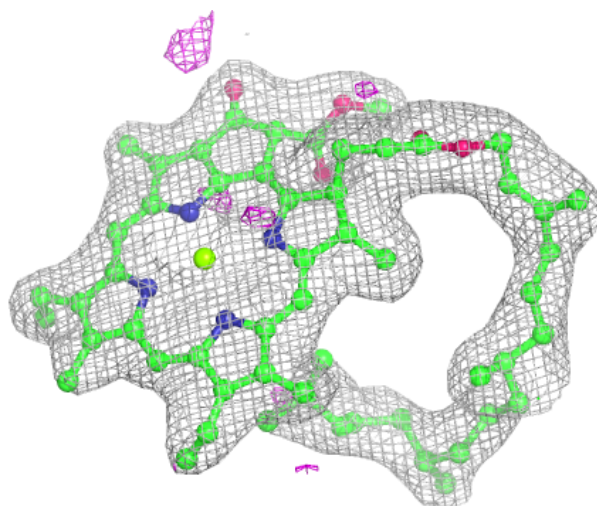
**Electron density around BCR B 617:**

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



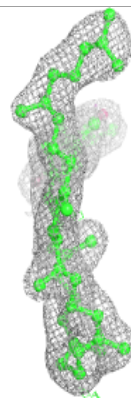
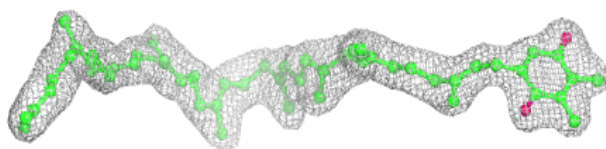
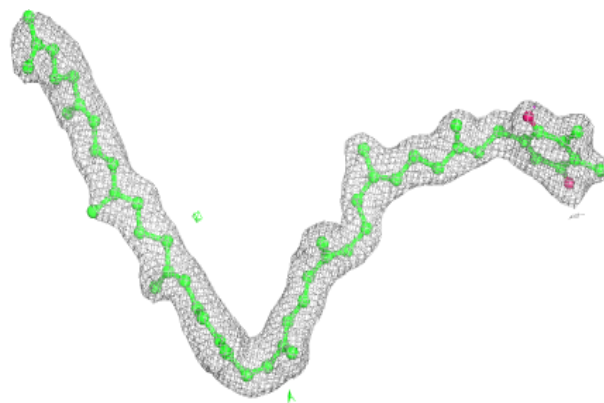
**Electron density around CLA b 614:**

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



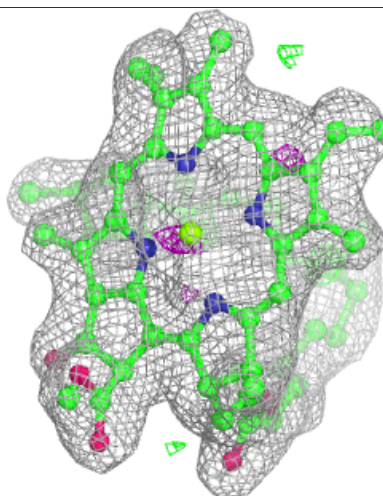
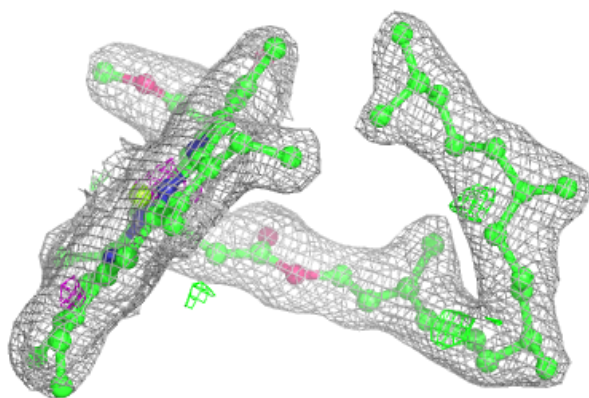
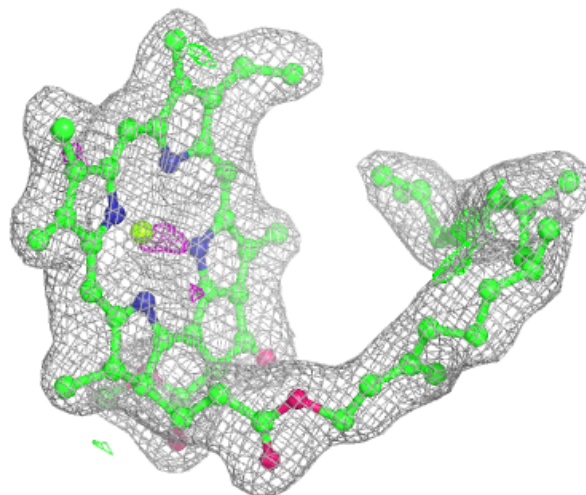
**Electron density around PL9 d 405:**

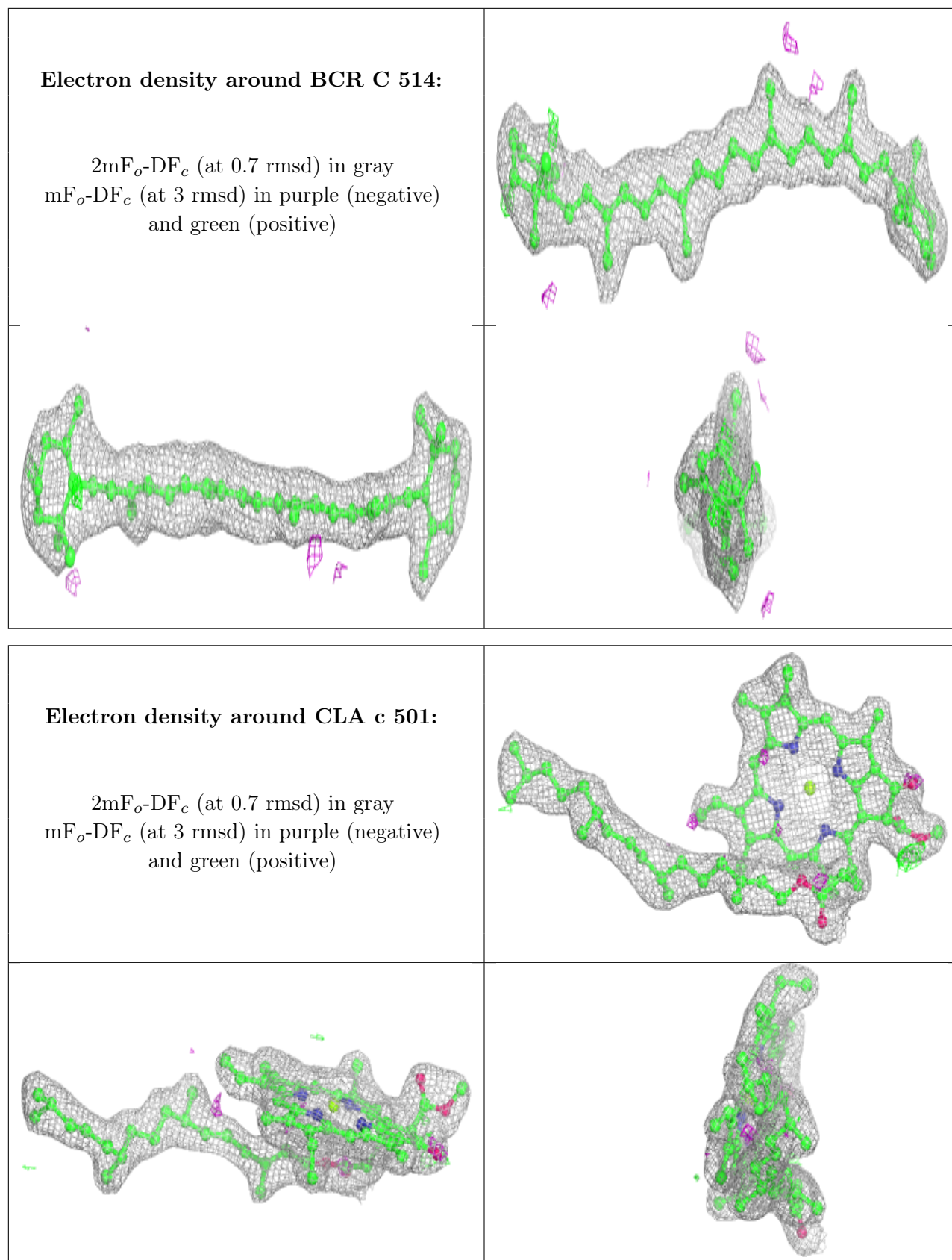
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C 503:**

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

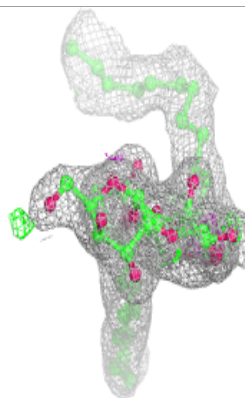
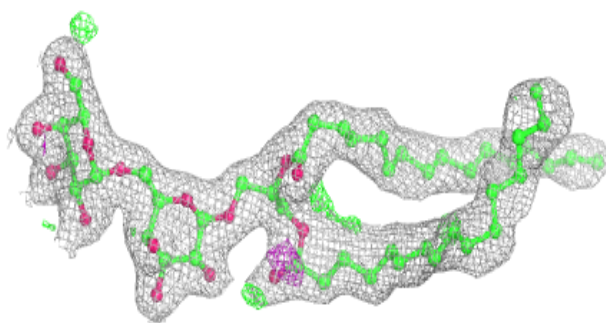
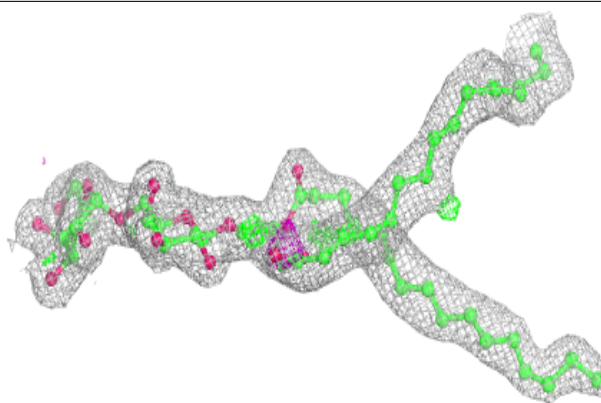




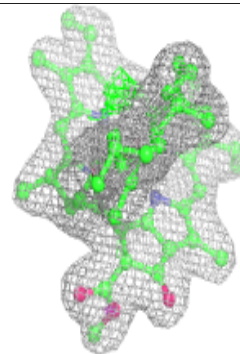
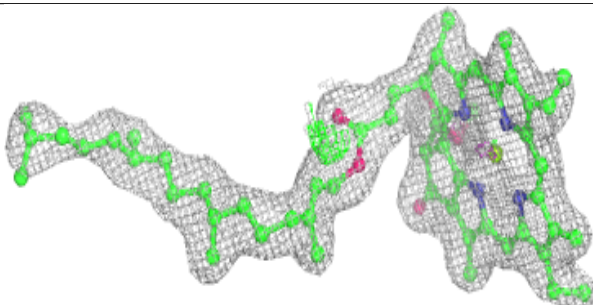
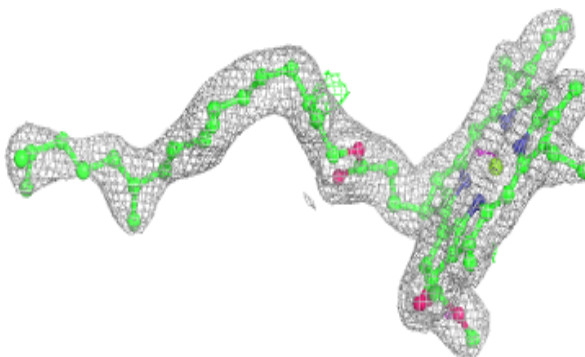


**Electron density around DGD C 515:**

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

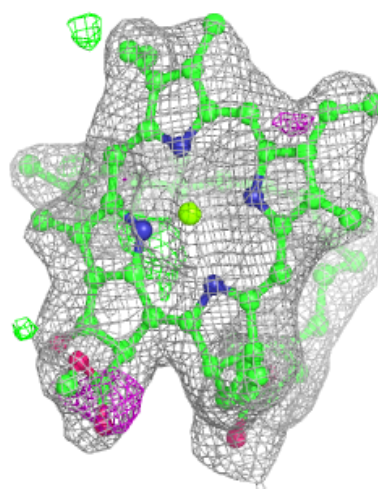
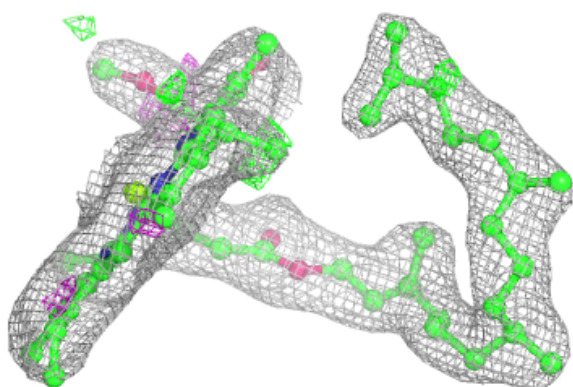
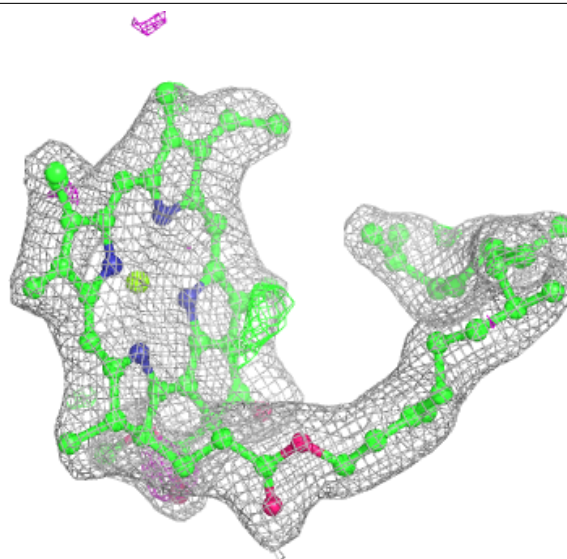
**Electron density around CLA c 502:**

$2mF_o-DF_c$  (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:**

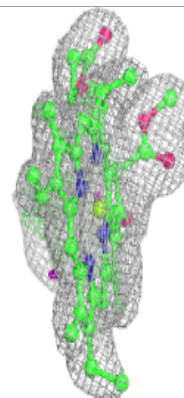
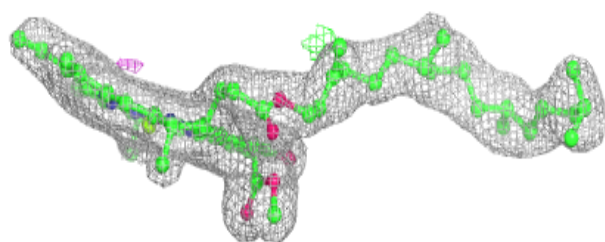
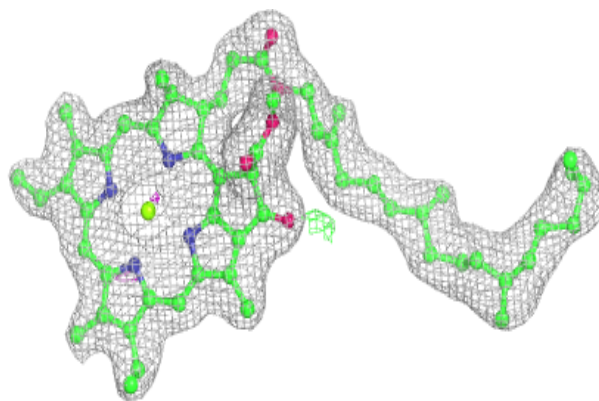
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





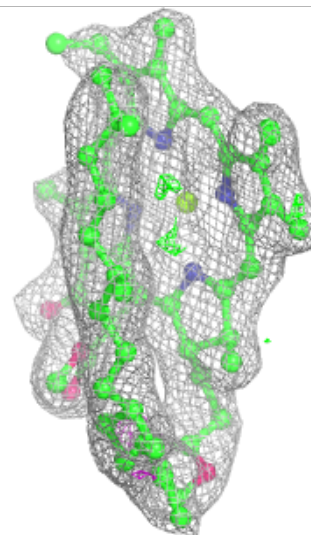
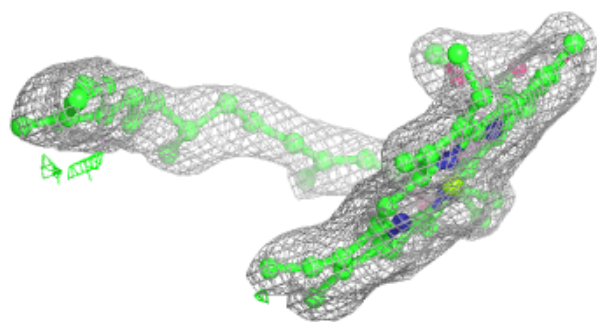
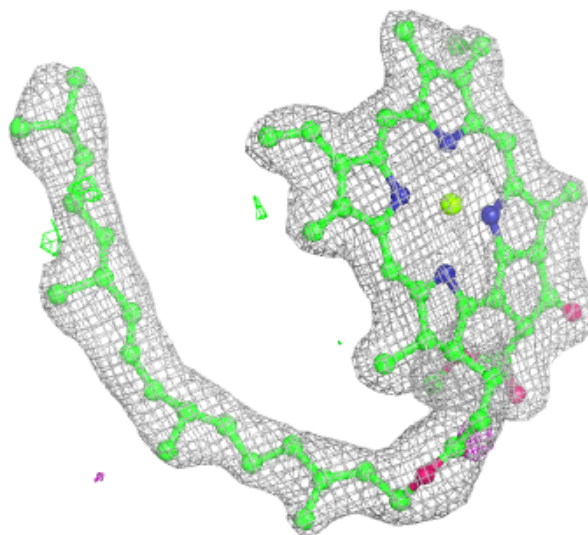
**Electron density around CLA b 601:**

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



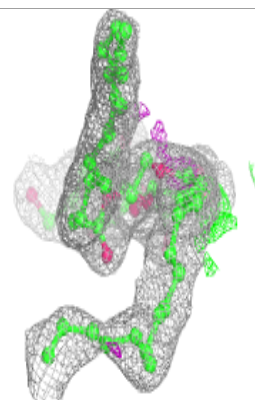
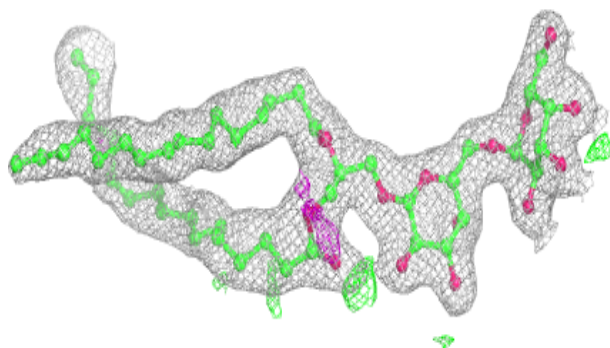
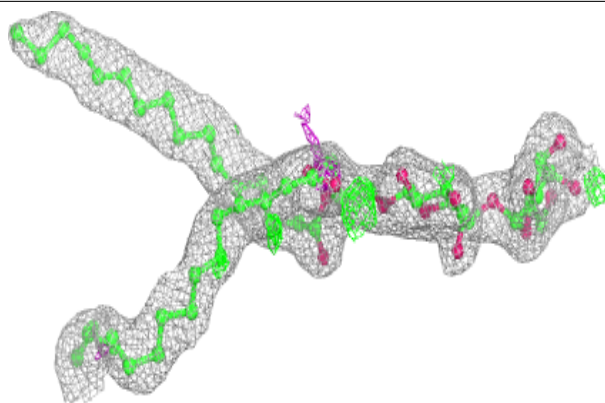
**Electron density around CLA c 507:**

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

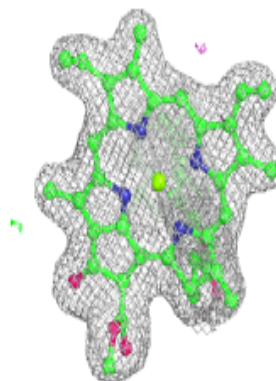
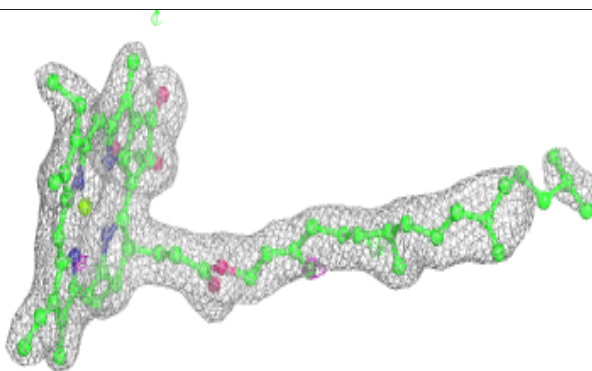
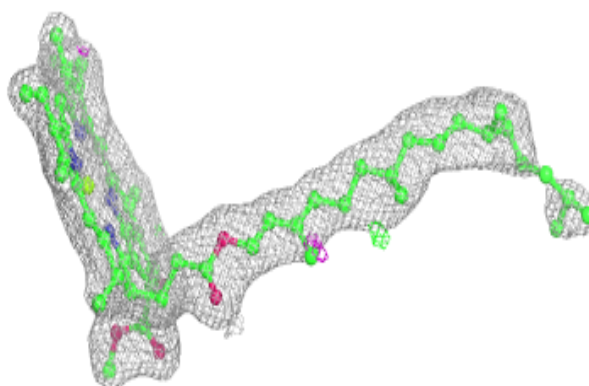


**Electron density around DGD c 516:**

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

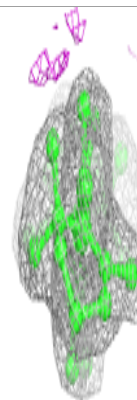
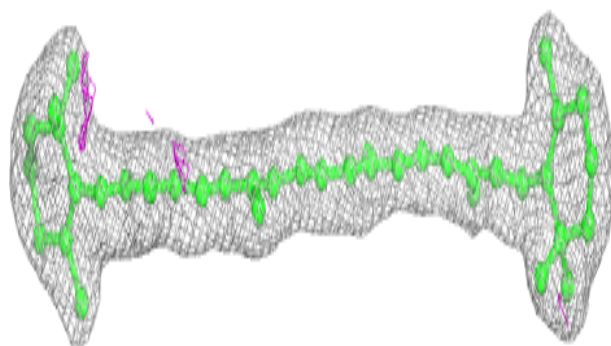
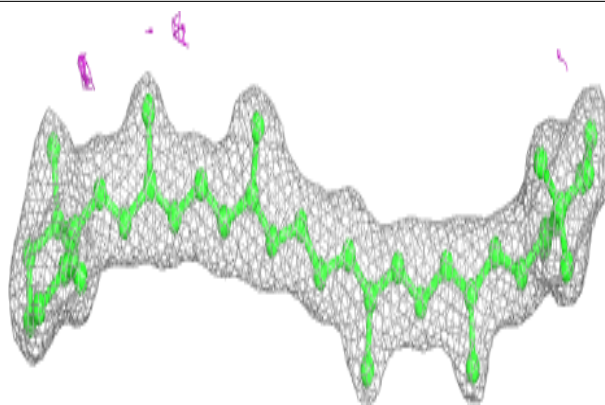
**Electron density around CLA b 603:**

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

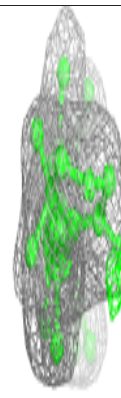
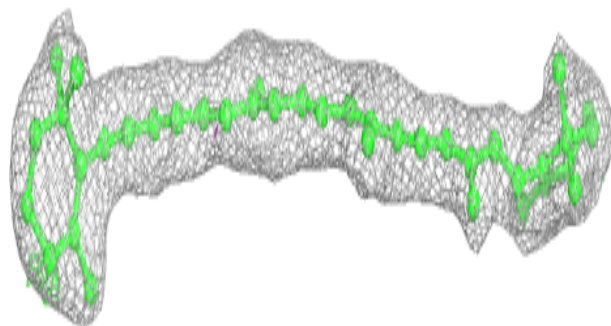
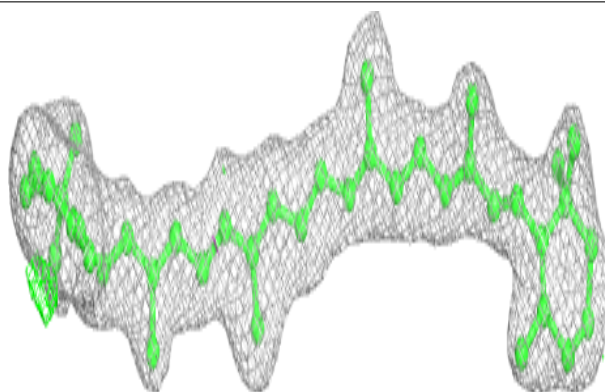


**Electron density around BCR a 611:**

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

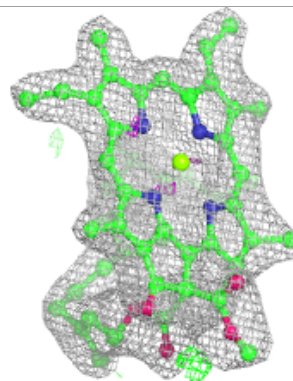
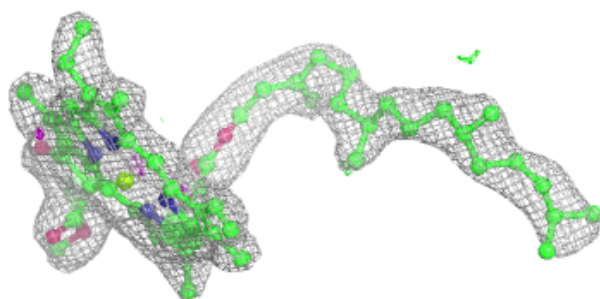
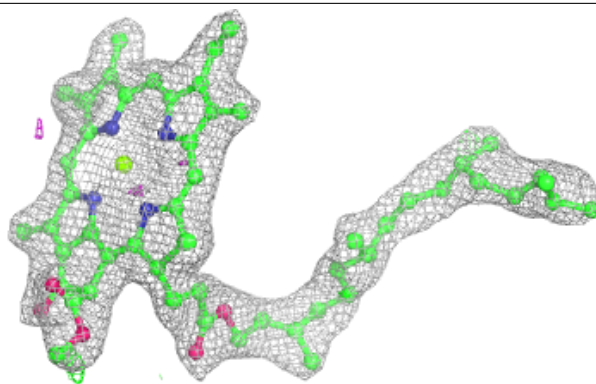
**Electron density around BCR b 616:**

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

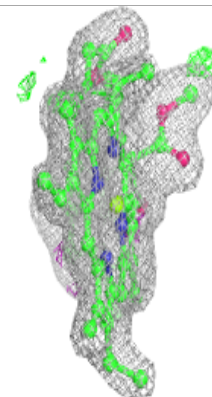
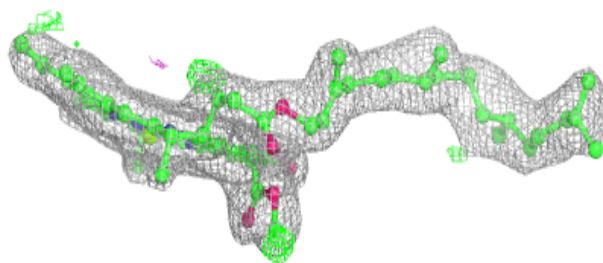
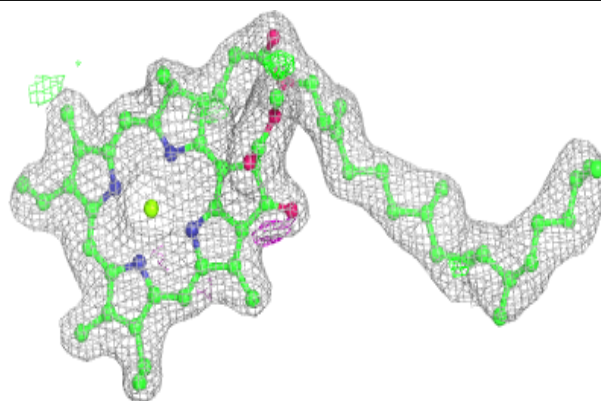


**Electron density around CLA c 511:**

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

**Electron density around CLA B 602:**

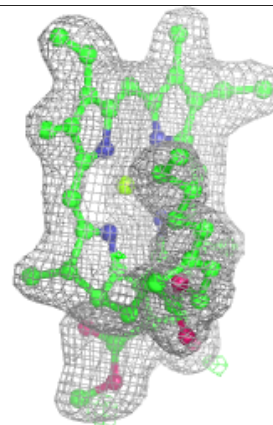
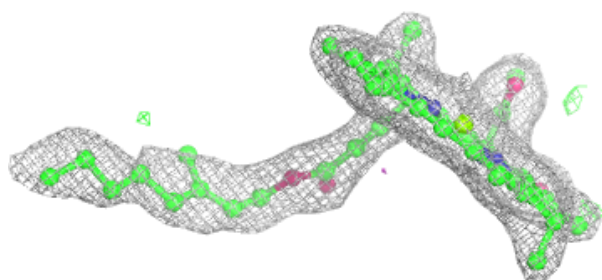
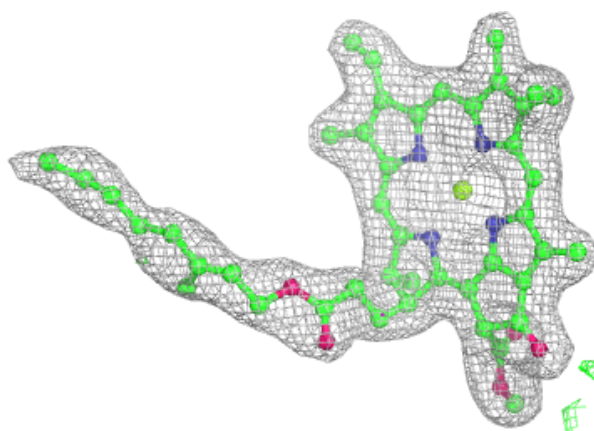
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



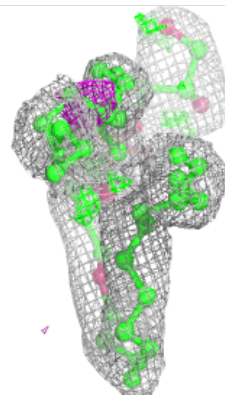
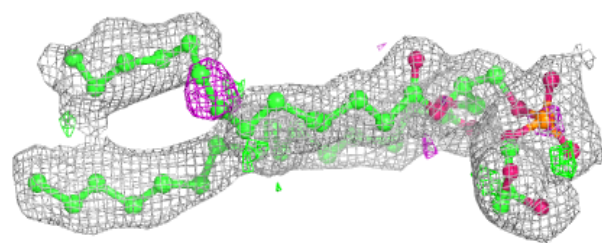
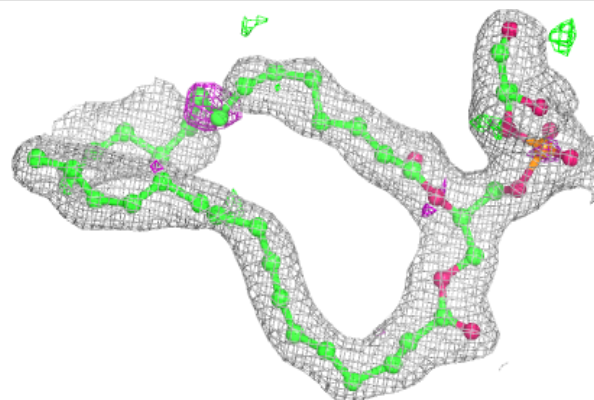


**Electron density around CLA A 609:**

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

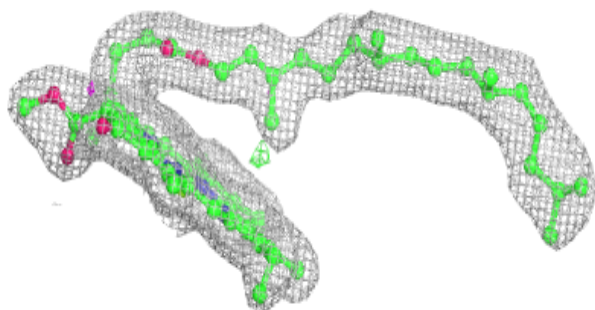
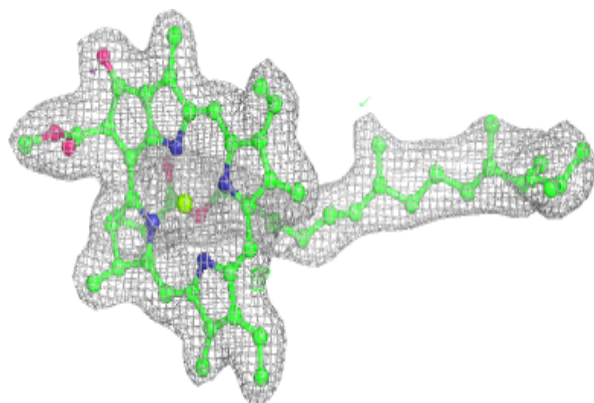
**Electron density around LHG A 614:**

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



**Electron density around CLA B 608:**

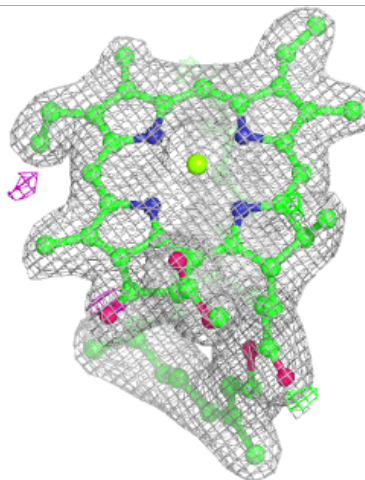
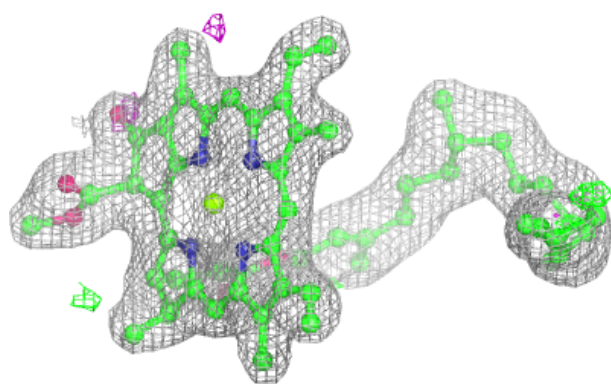
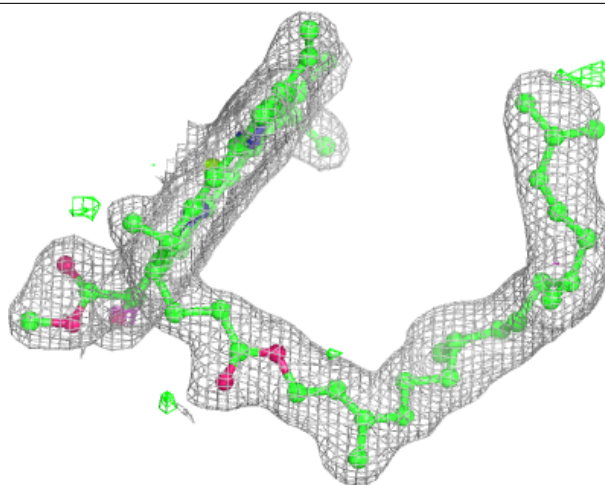
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





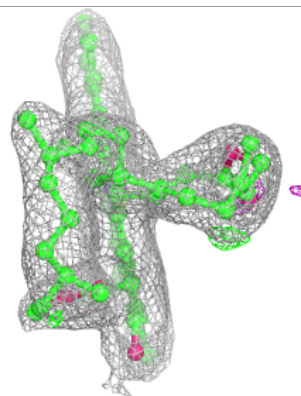
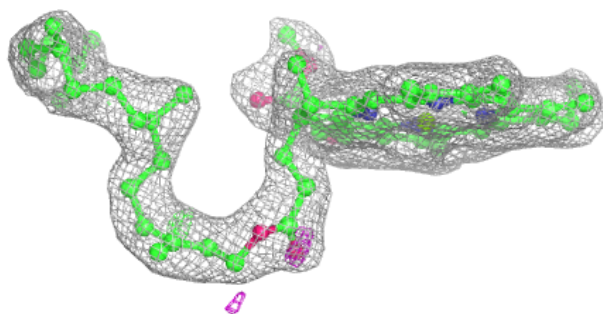
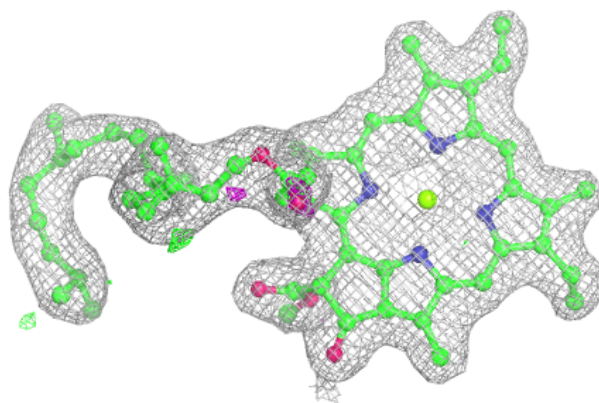
**Electron density around CLA b 610:**

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



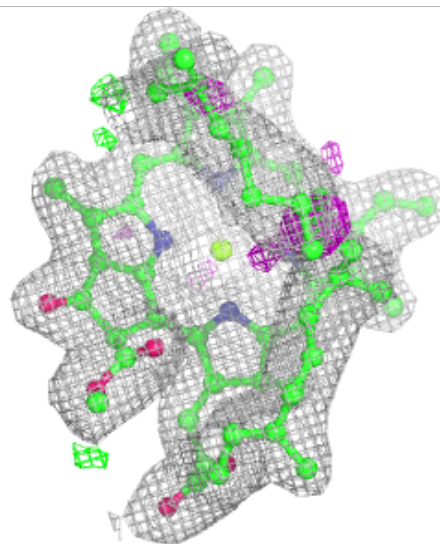
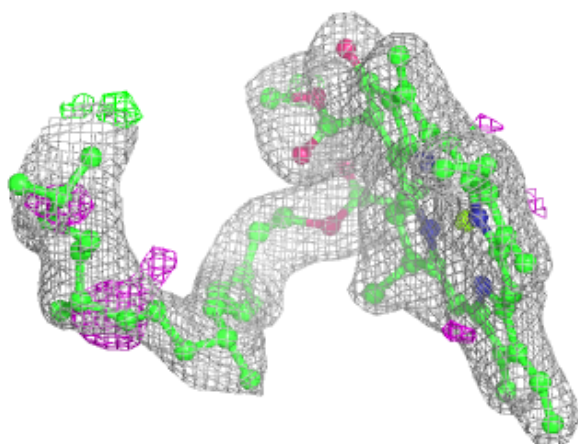
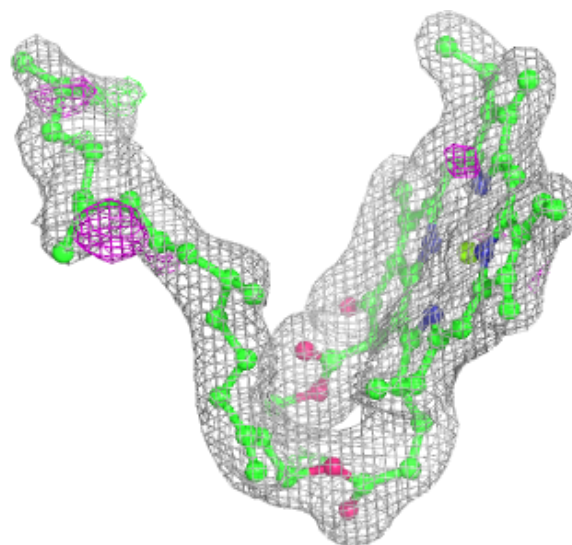
**Electron density around CLA b 611:**

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



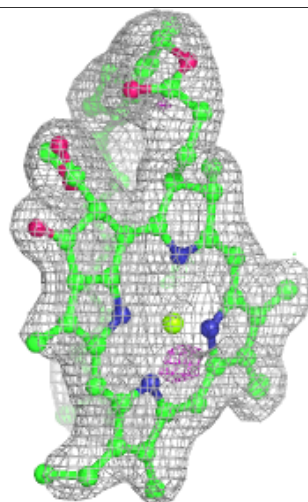
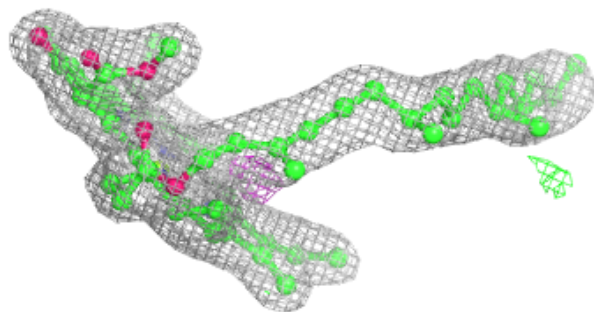
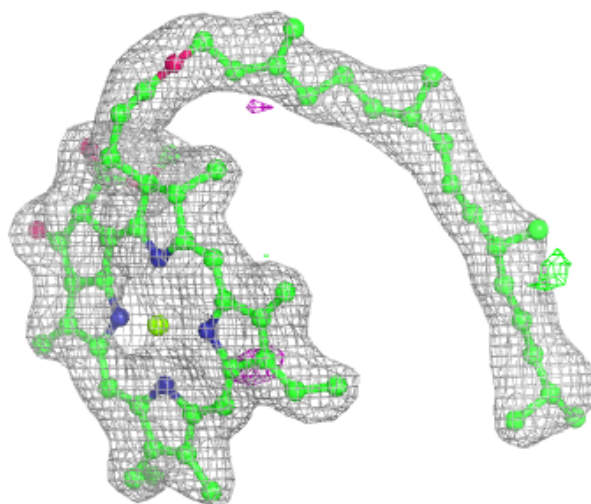
**Electron density around CLA b 612:**

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



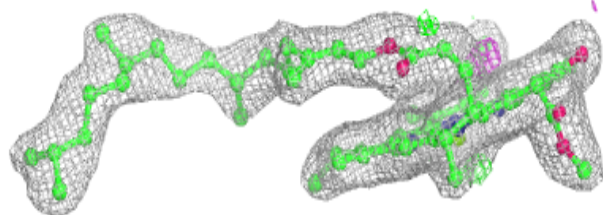
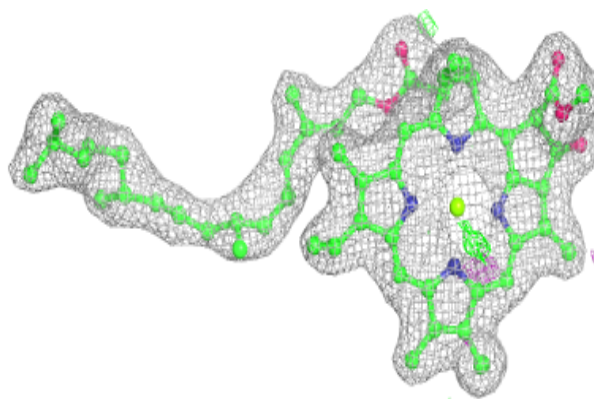
**Electron density around CLA C 507:**

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

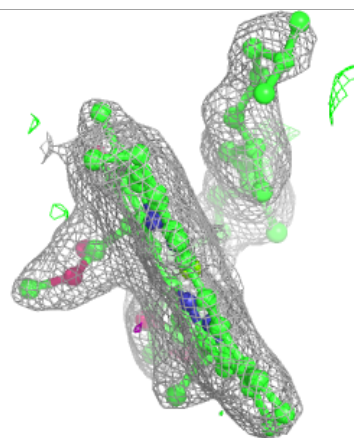
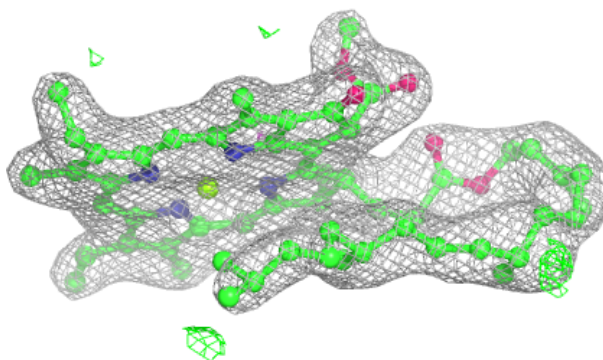
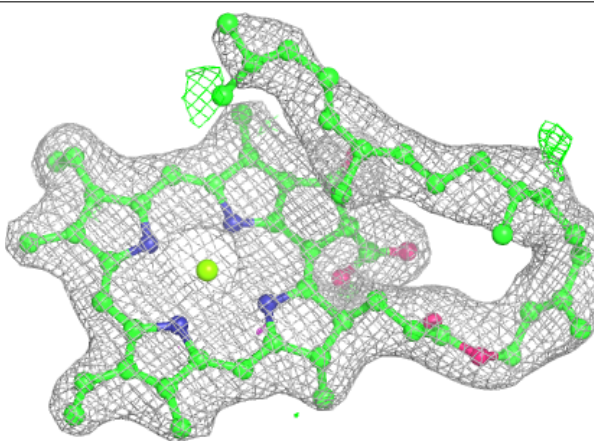


**Electron density around CLA B 603:**

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

**Electron density around CLA C 509:**

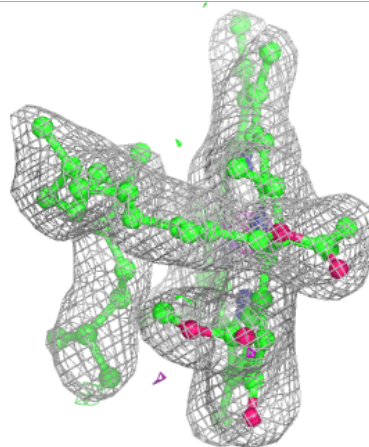
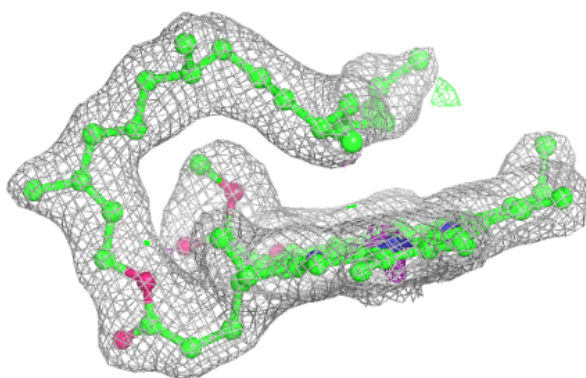
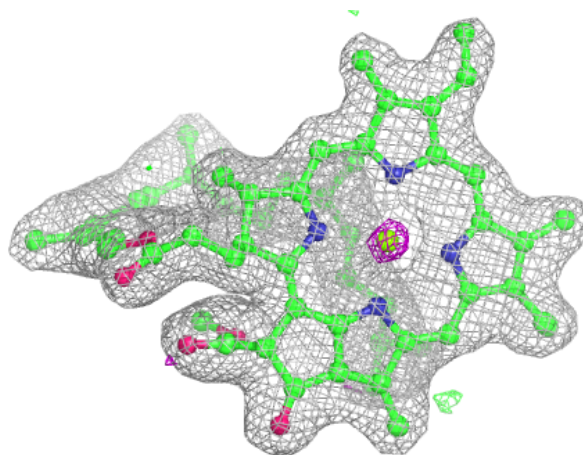
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





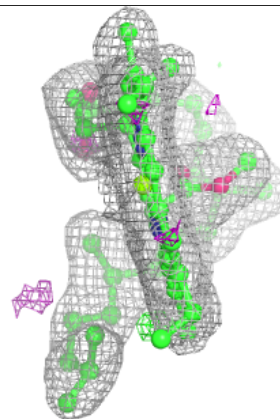
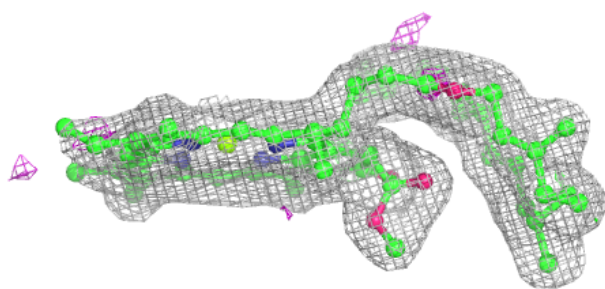
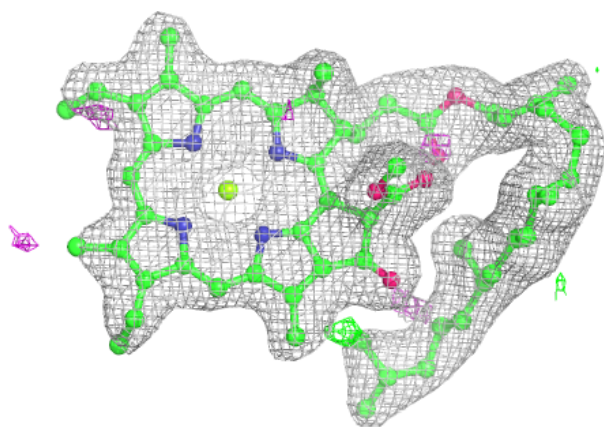
**Electron density around CLA C 510:**

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



**Electron density around CLA B 610:**

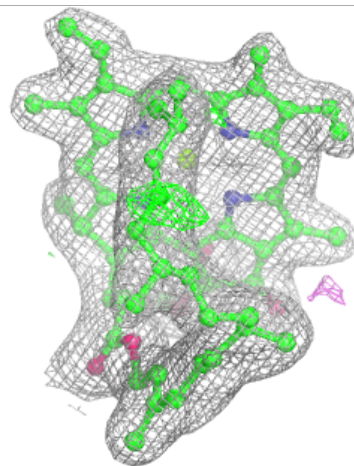
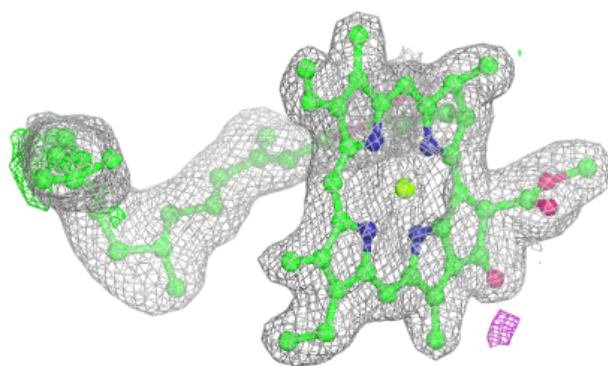
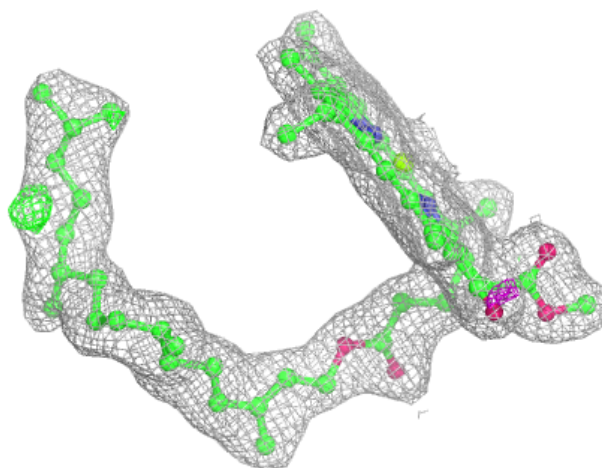
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





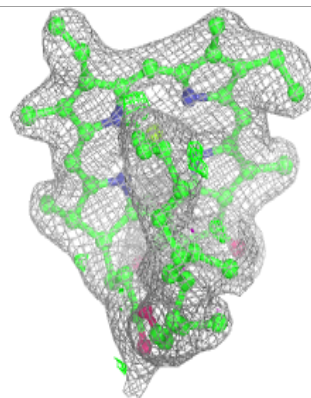
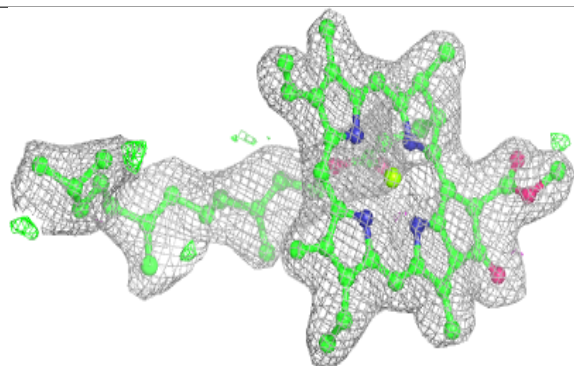
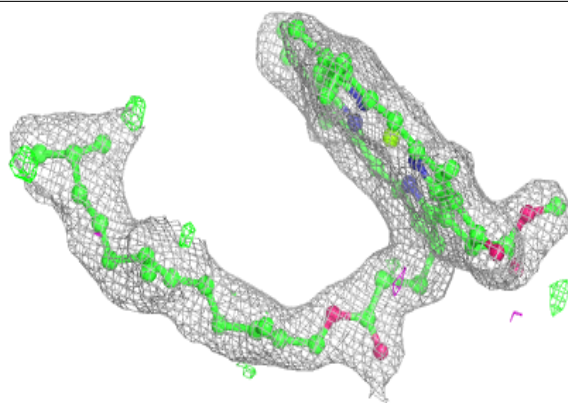
**Electron density around CLA B 611:**

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

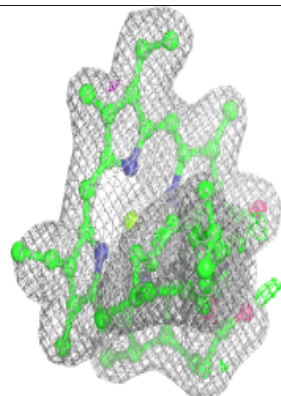
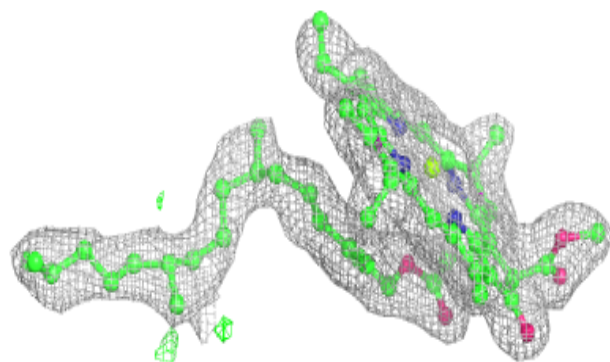
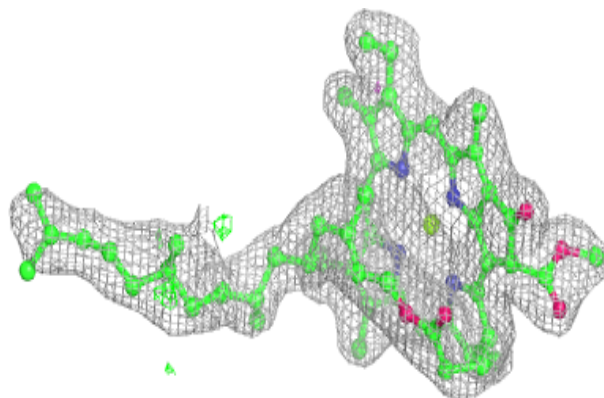


**Electron density around CLA c 504:**

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

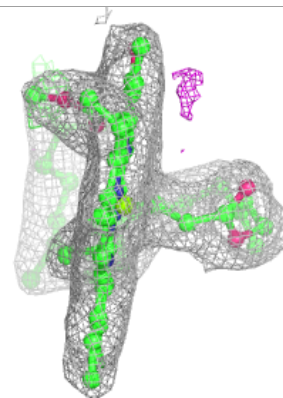
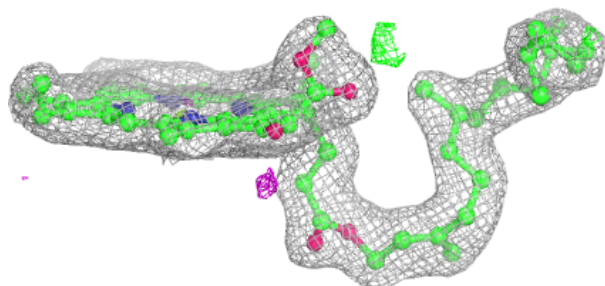
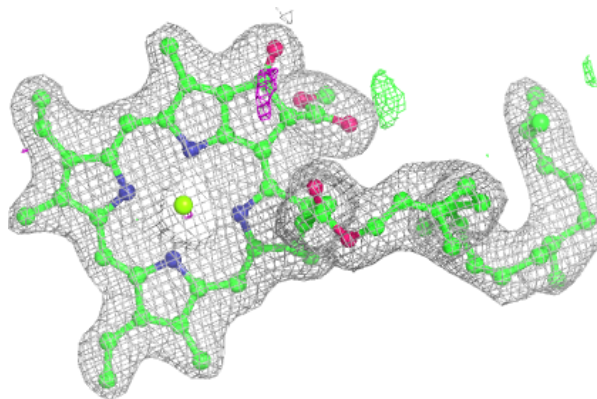
**Electron density around CLA c 505:**

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

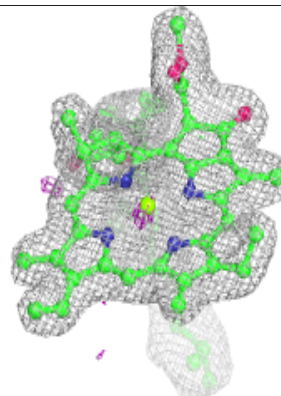
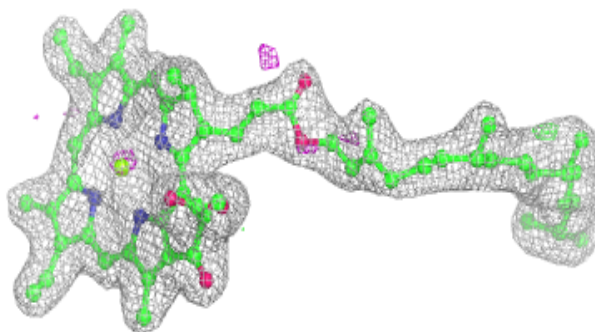
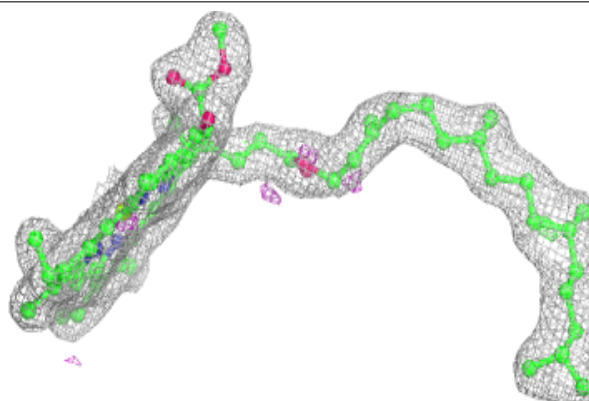


**Electron density around CLA B 612:**

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

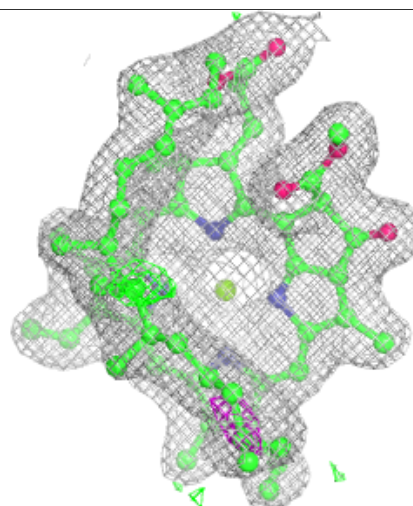
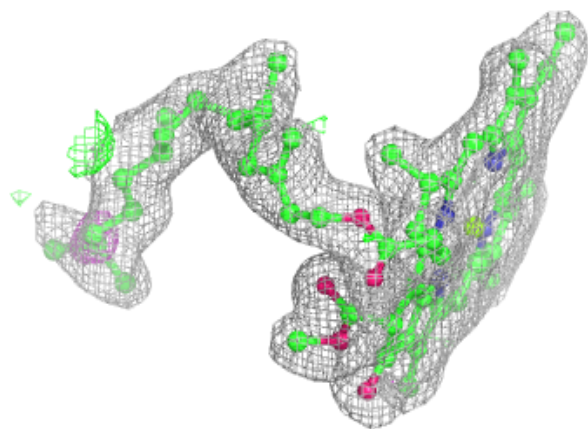
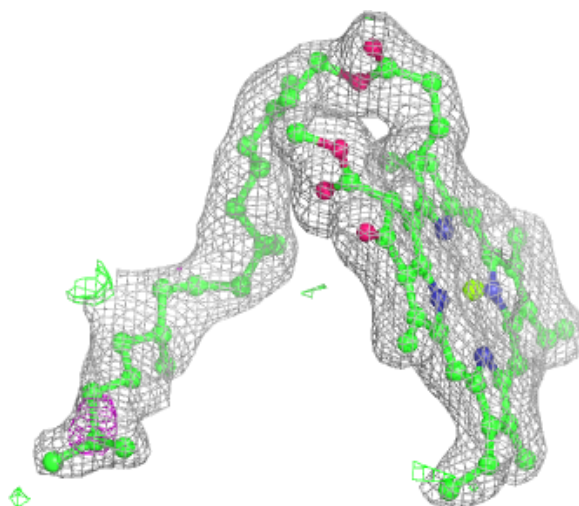
**Electron density around CLA D 403:**

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



**Electron density around CLA B 613:**

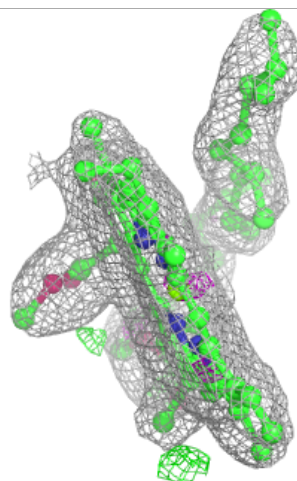
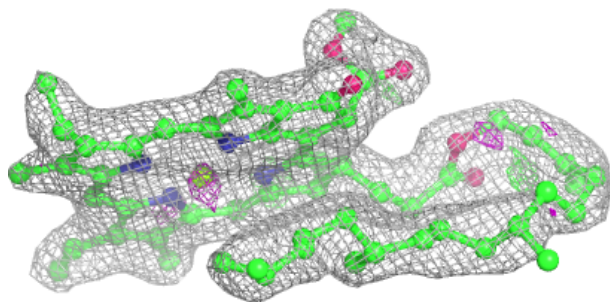
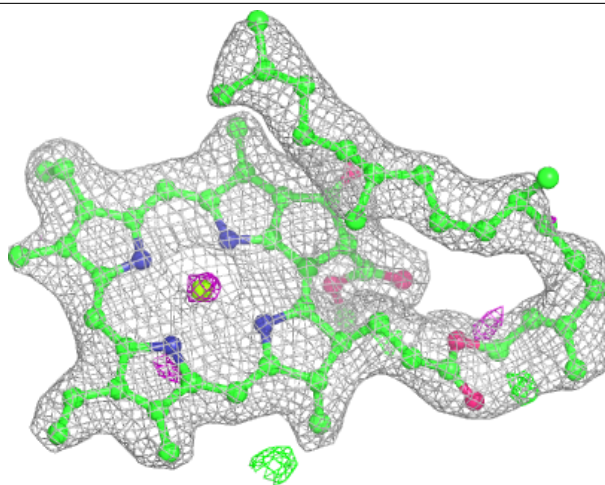
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





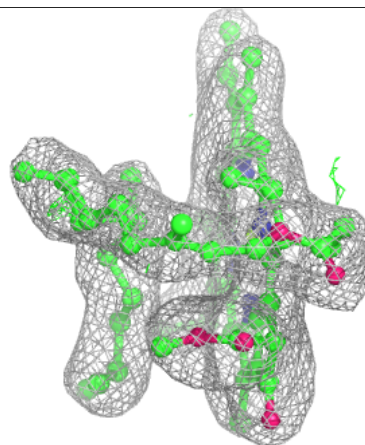
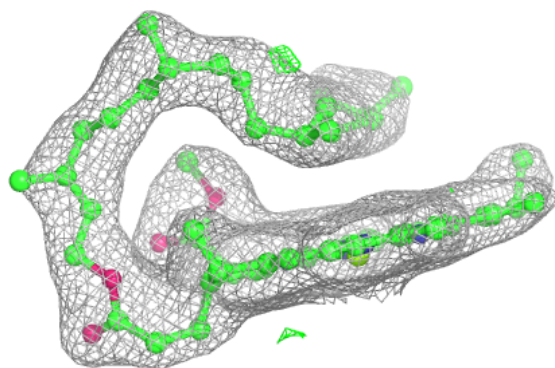
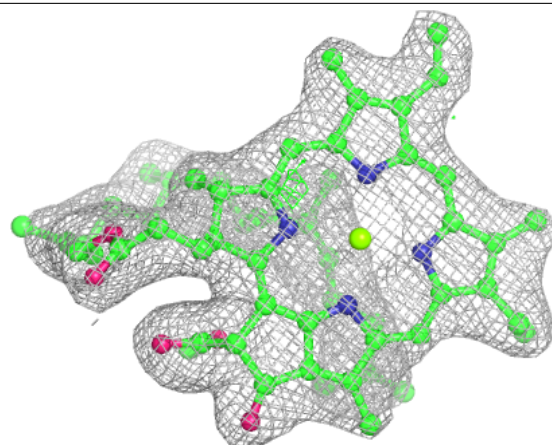
**Electron density around CLA c 509:**

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

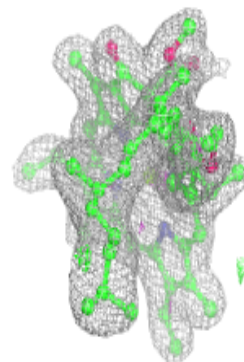
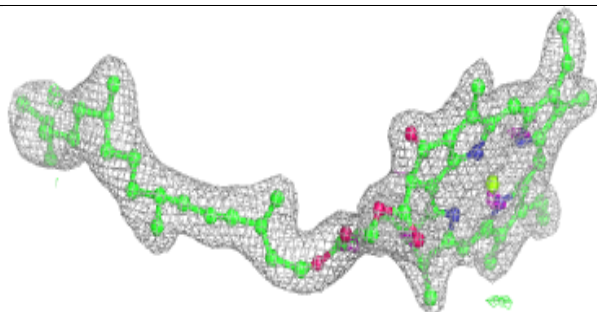
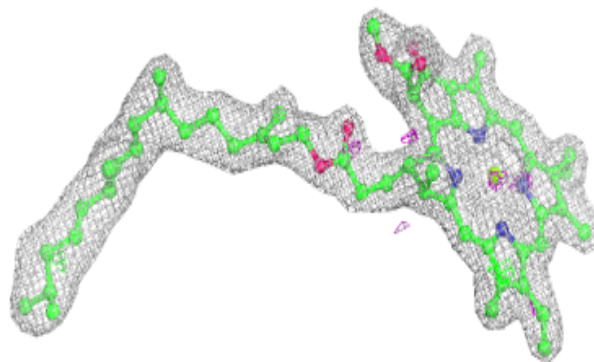


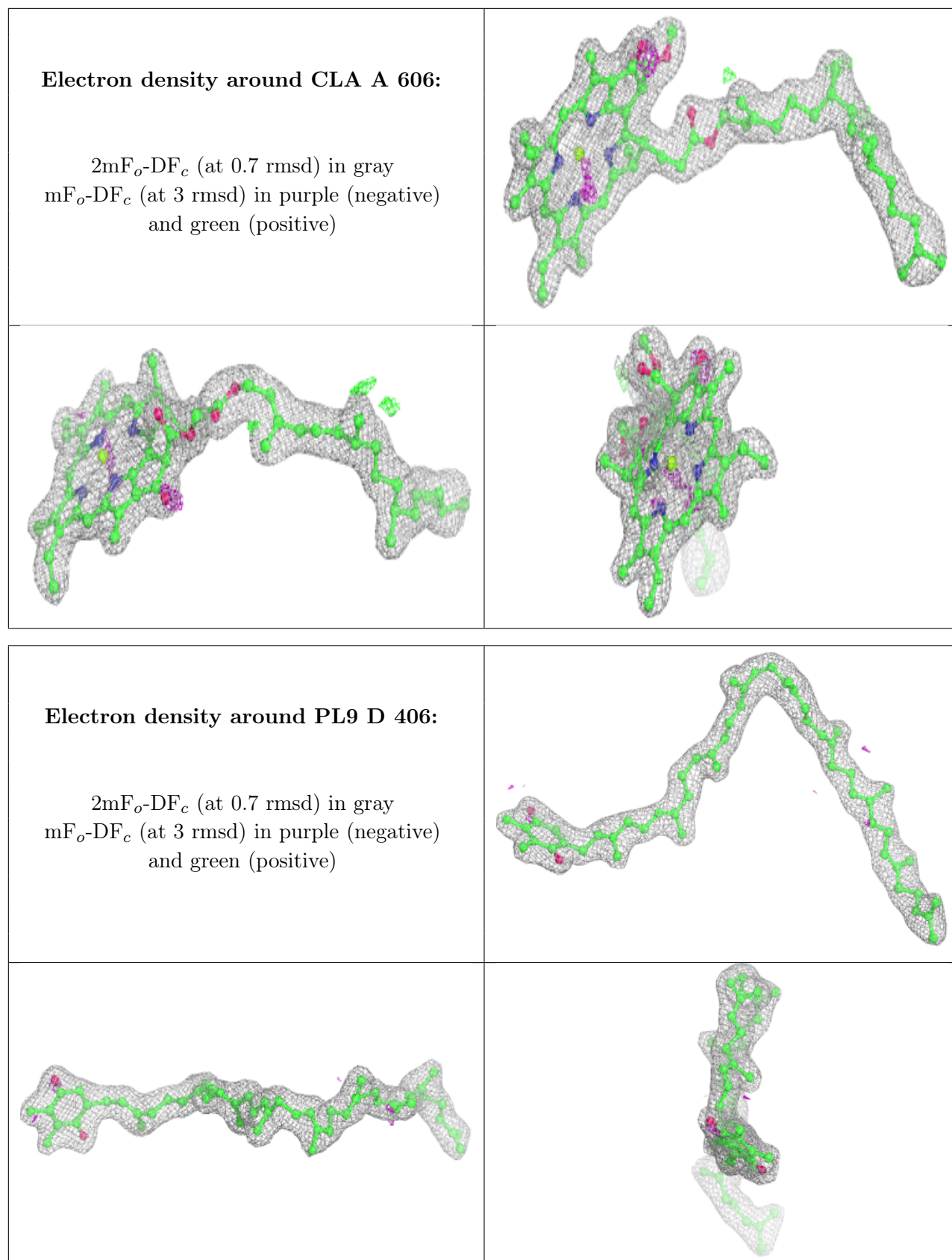
**Electron density around CLA c 510:**

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

**Electron density around CLA a 607:**

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

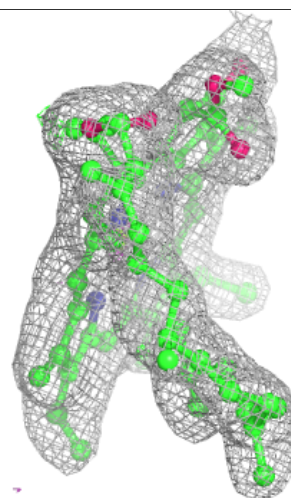
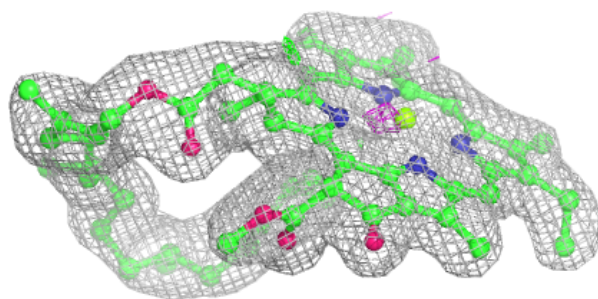
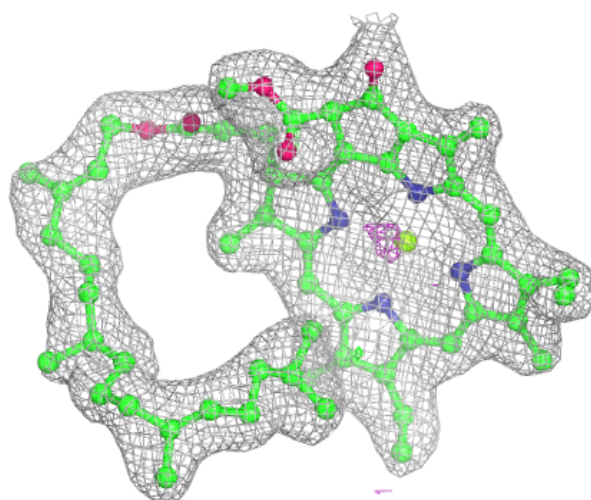






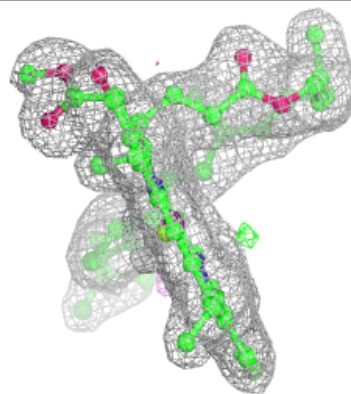
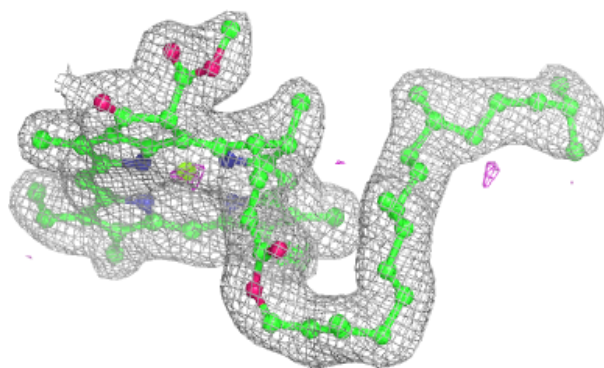
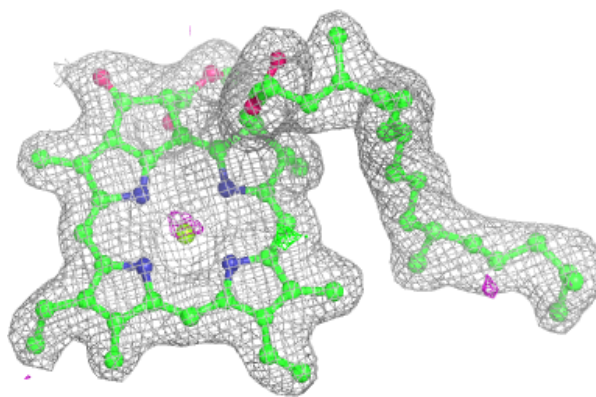
**Electron density around CLA B 615:**

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

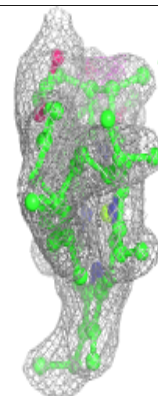
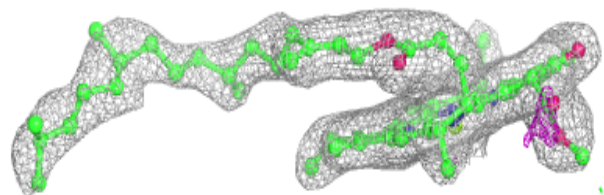
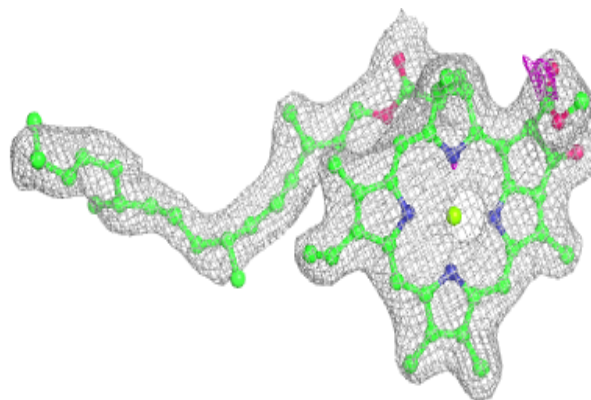


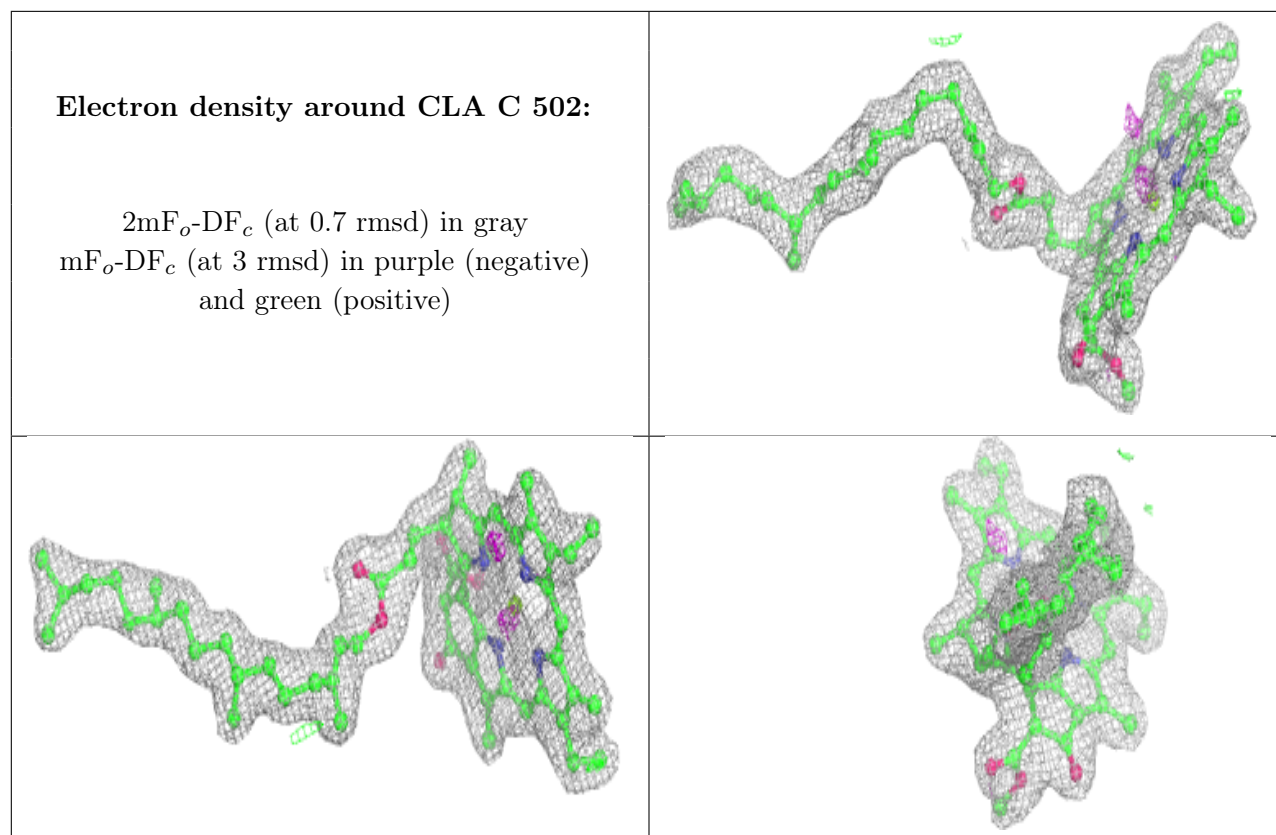
**Electron density around CLA A 612:**

$2mF_o-DF_c$  (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:**

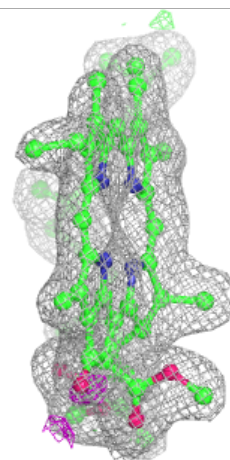
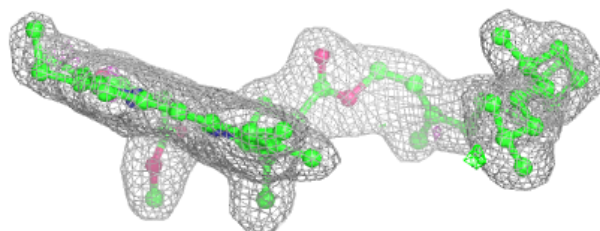
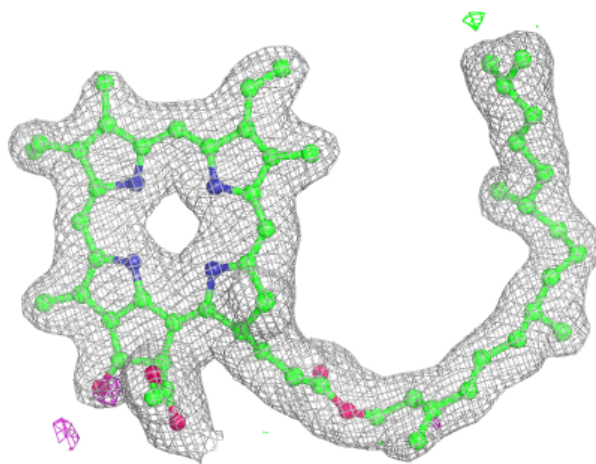
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PHO a 609:**

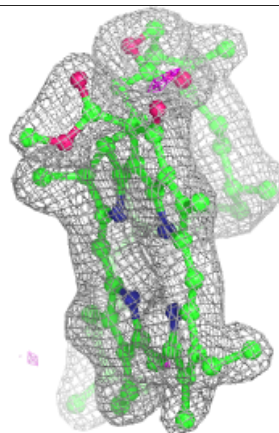
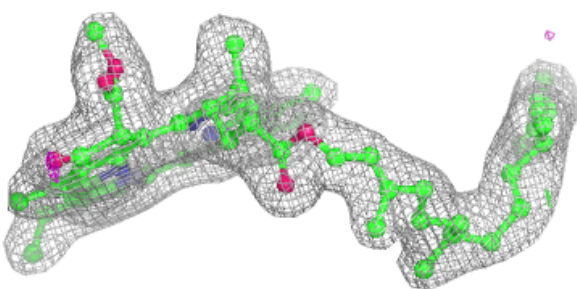
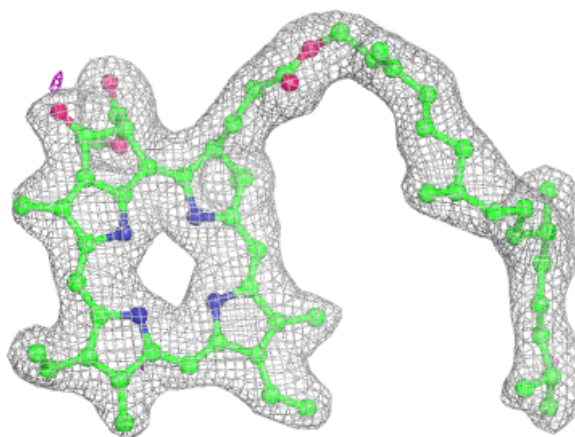
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



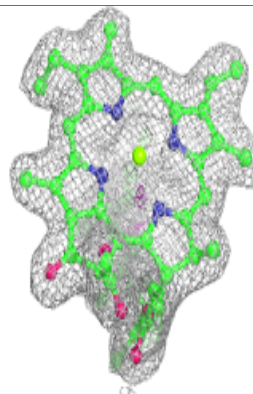
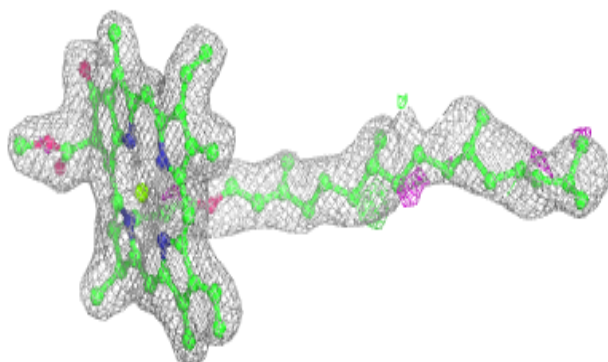
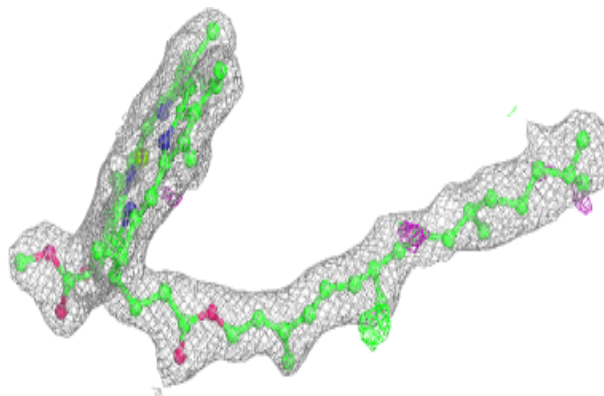


**Electron density around PHO d 401:**

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

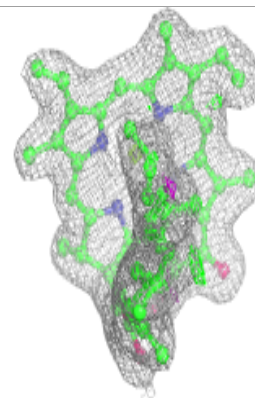
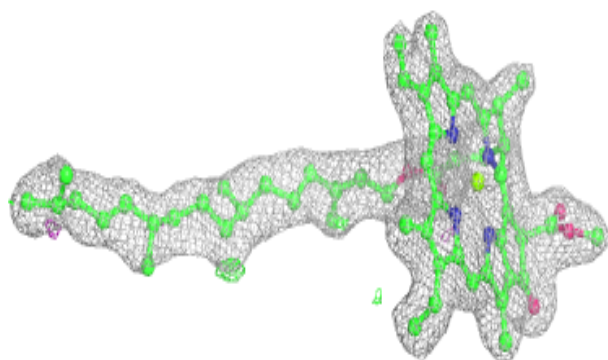
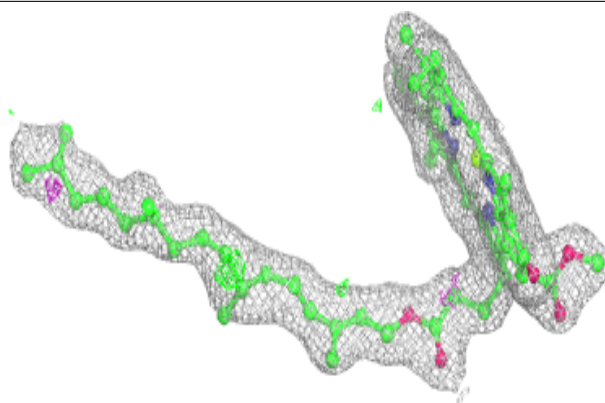
**Electron density around CLA B 607:**

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

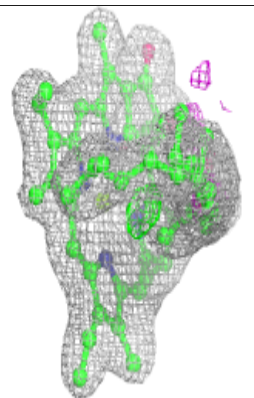
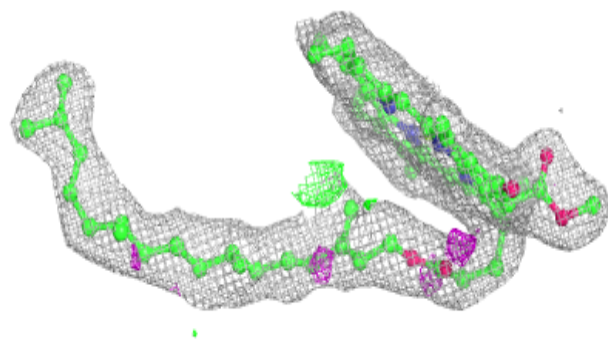
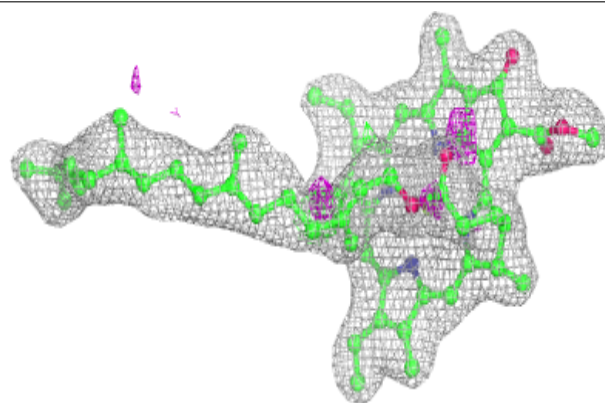


**Electron density around CLA b 606:**

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

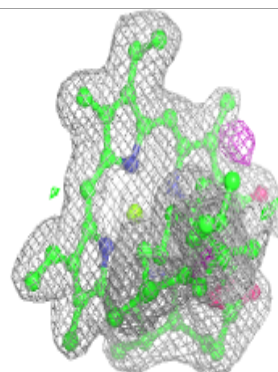
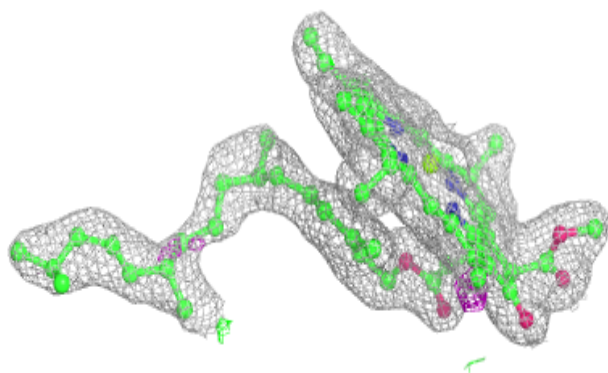
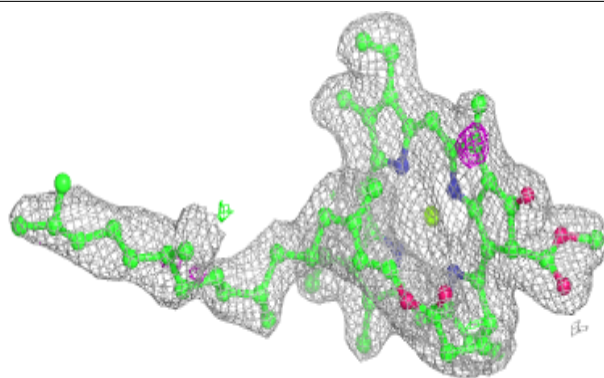
**Electron density around CLA b 607:**

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

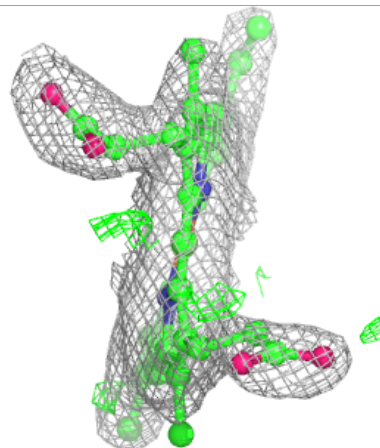
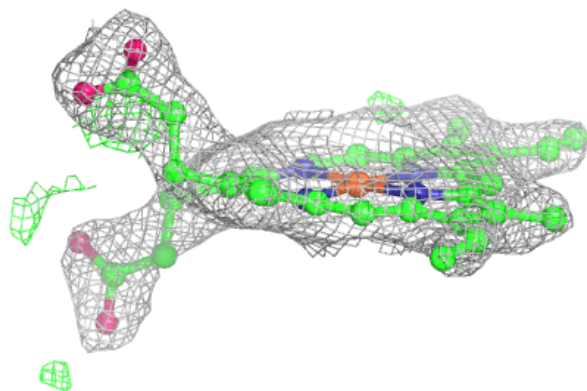
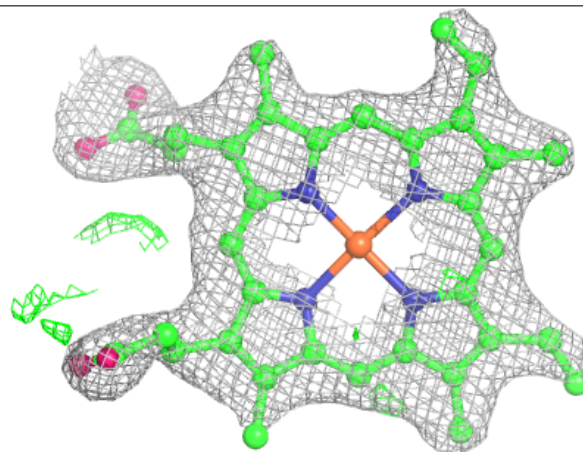


**Electron density around CLA C 505:**

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

**Electron density around HEM F 101:**

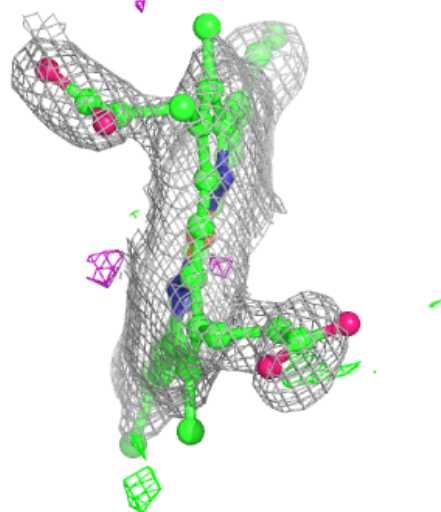
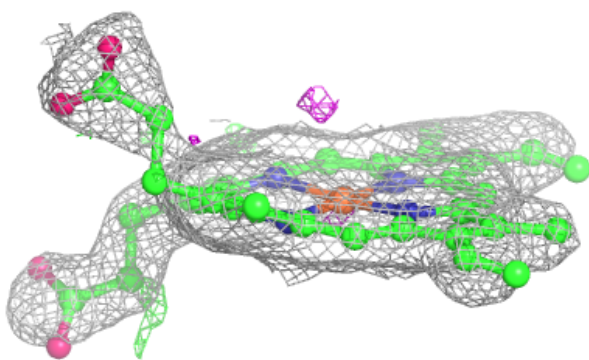
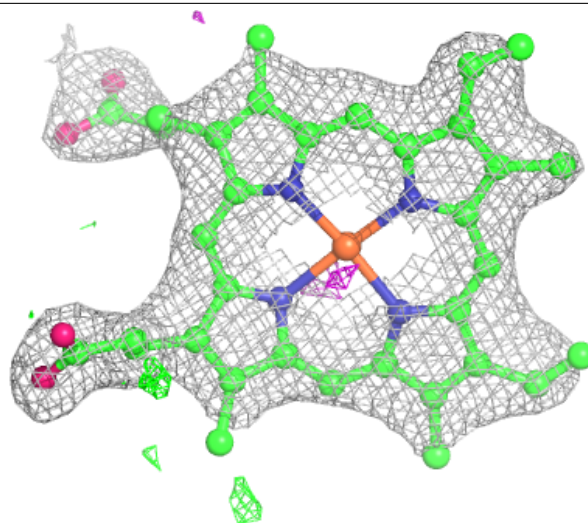
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





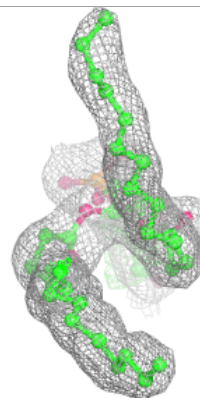
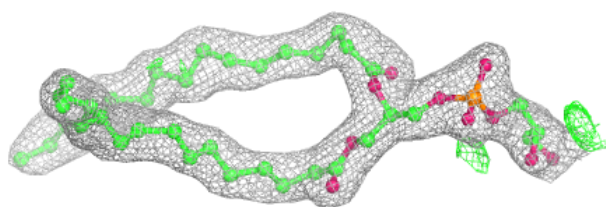
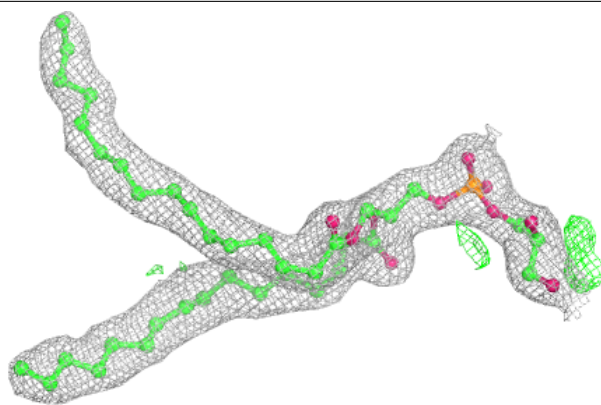
**Electron density around HEM e 101:**

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

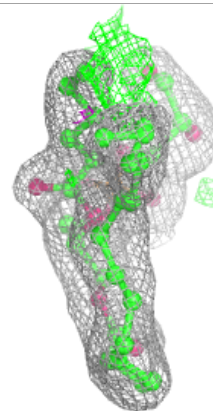
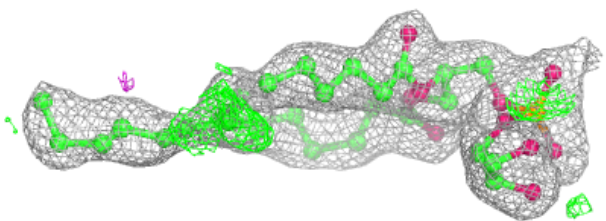
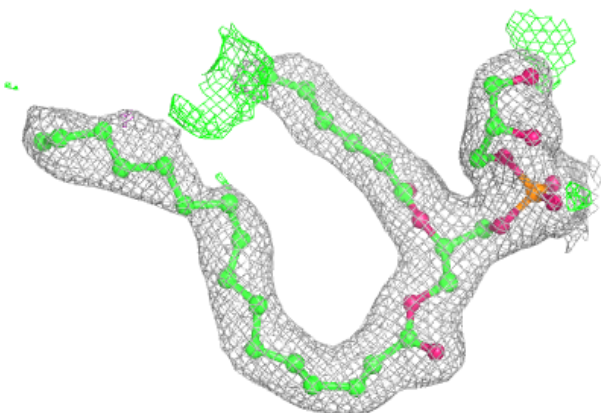


**Electron density around LHG d 406:**

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

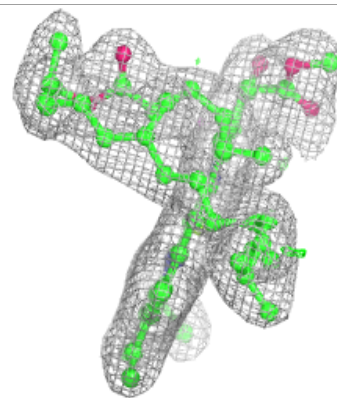
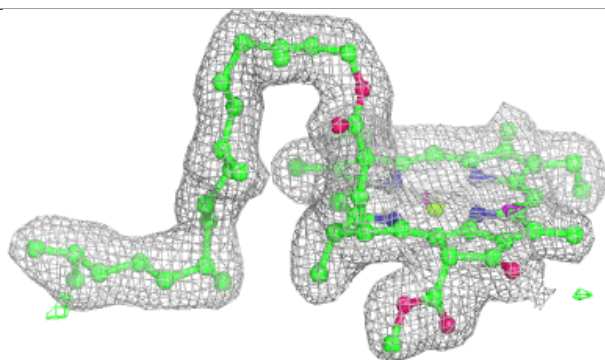
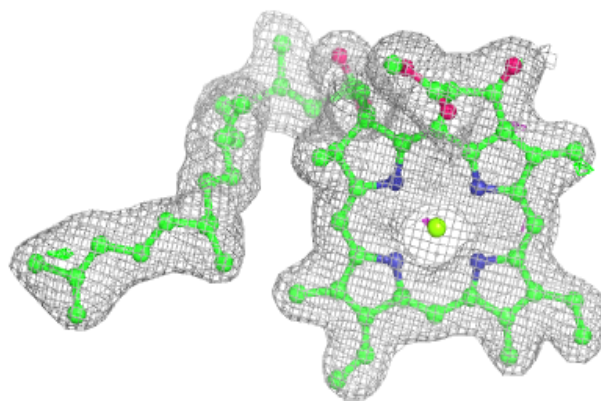
**Electron density around LHG d 407:**

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

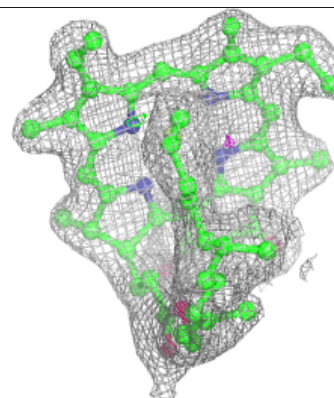
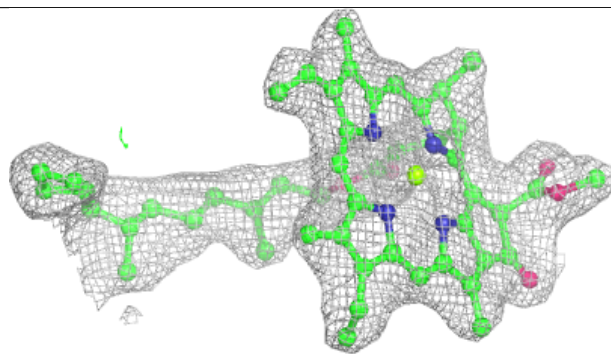
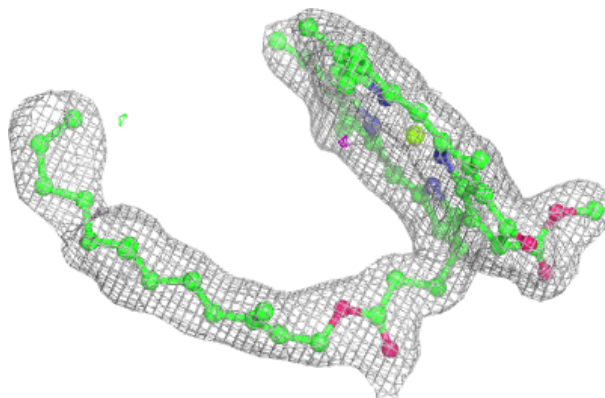


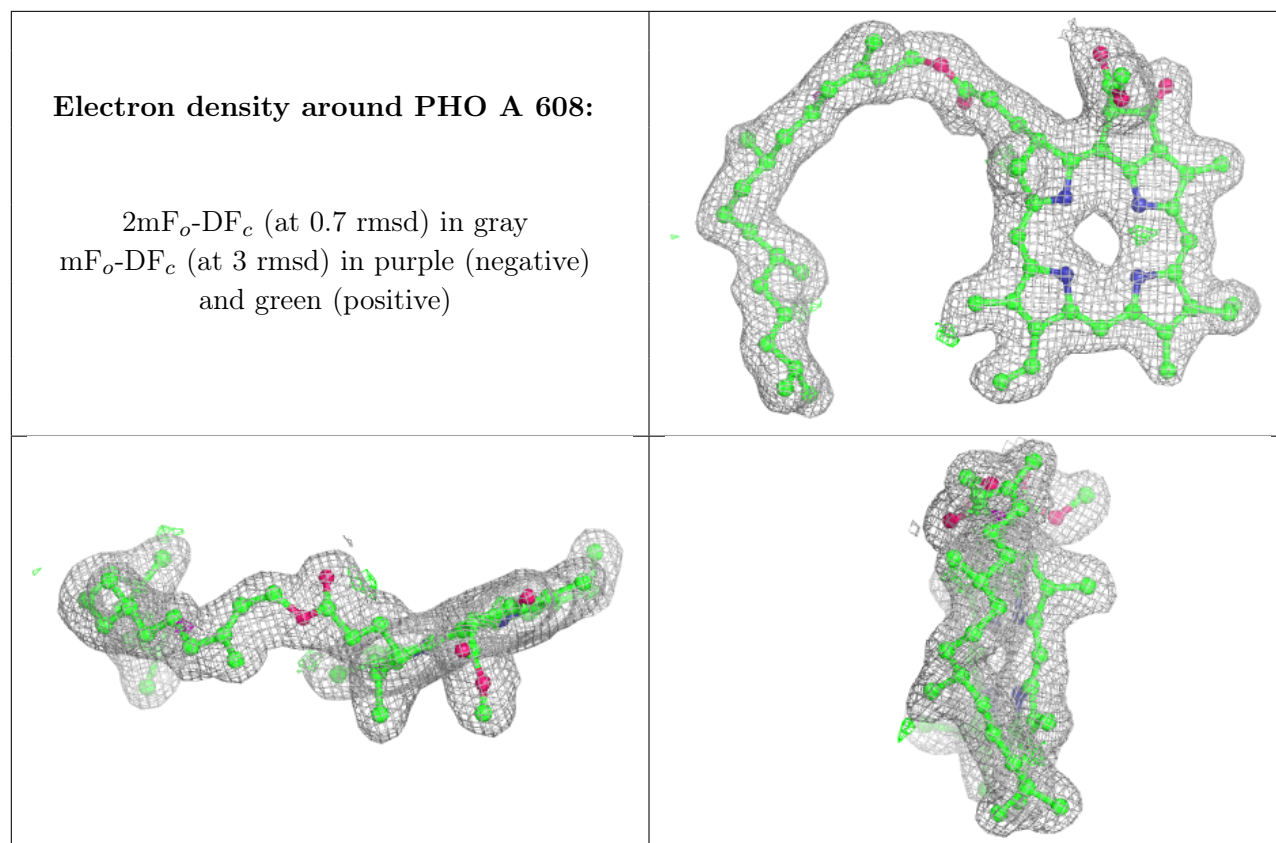
**Electron density around CLA a 613:**

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

**Electron density around CLA 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)

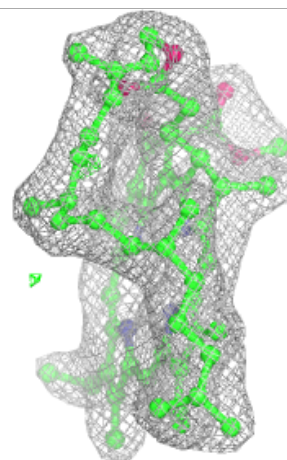
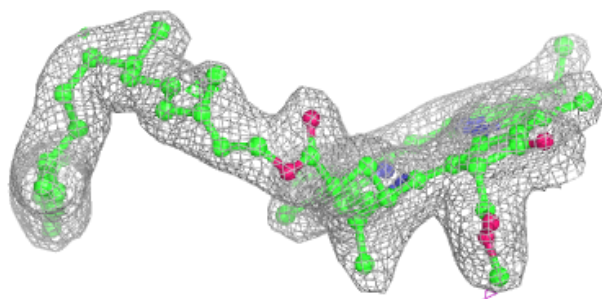
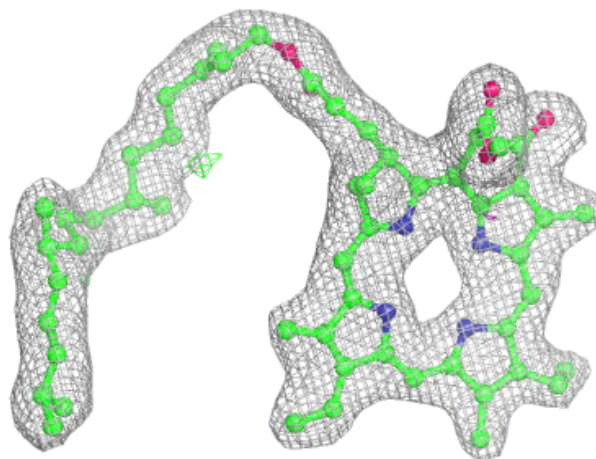






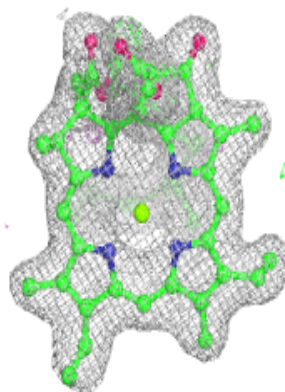
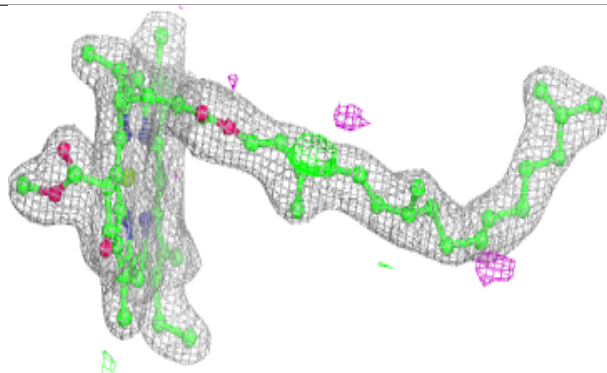
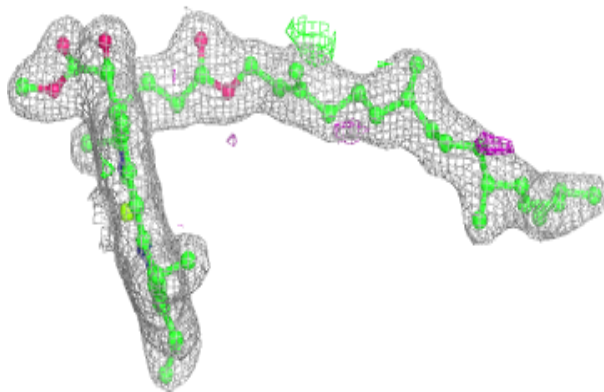
**Electron density around PHO D 402:**

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

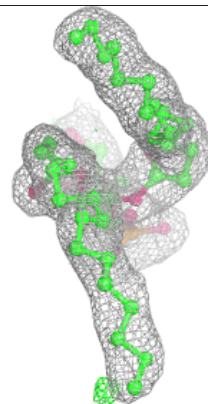
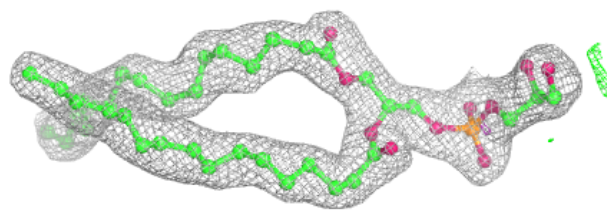
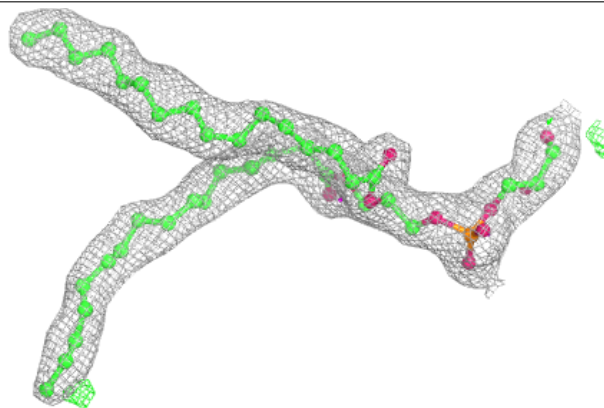


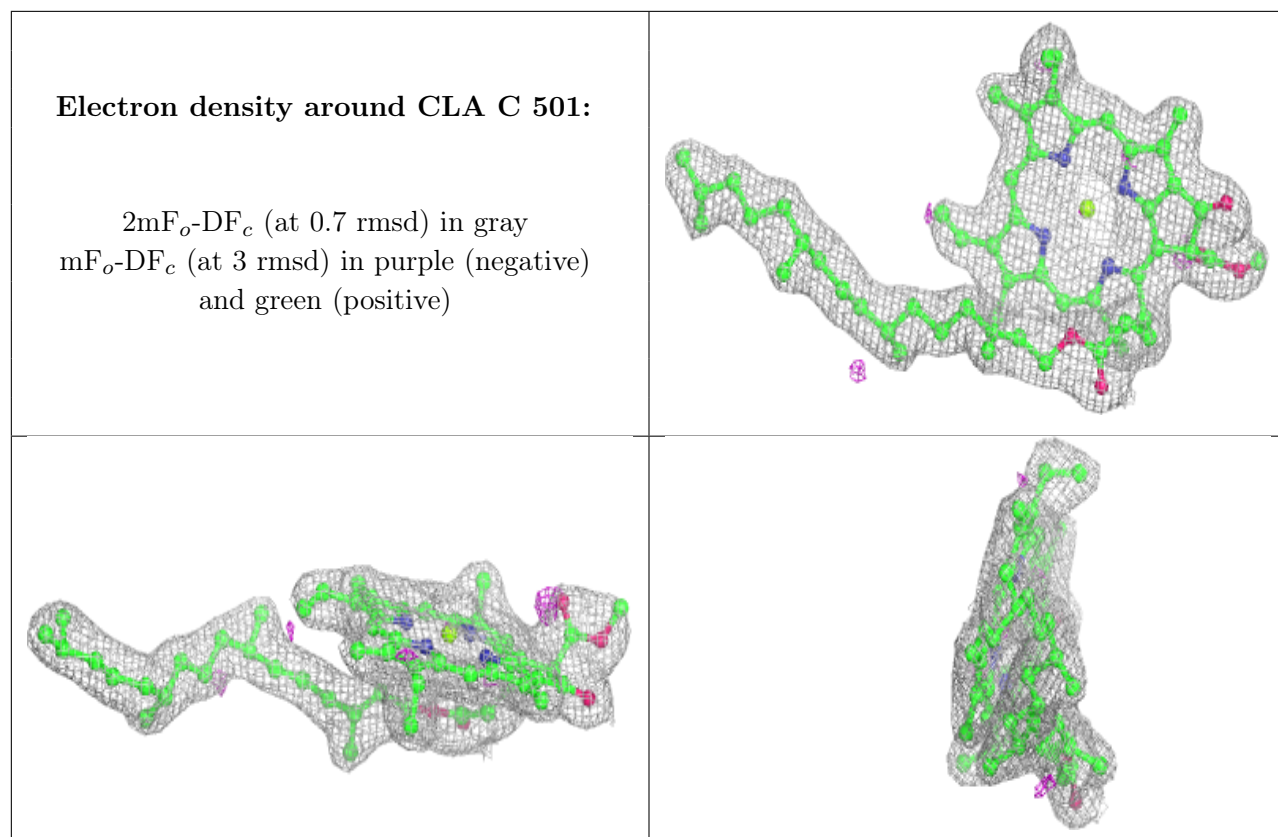
**Electron density around CLA B 605:**

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

**Electron density around LHG D 408:**

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

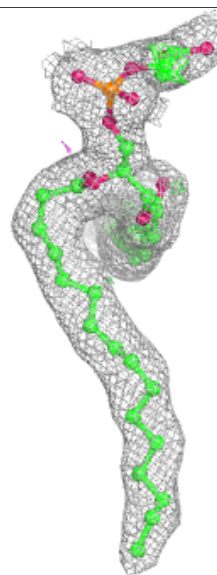
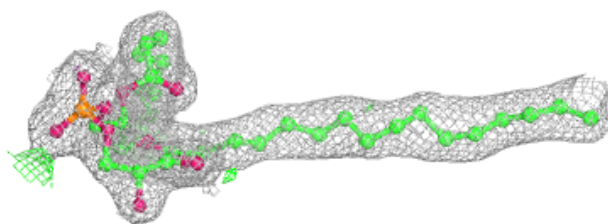
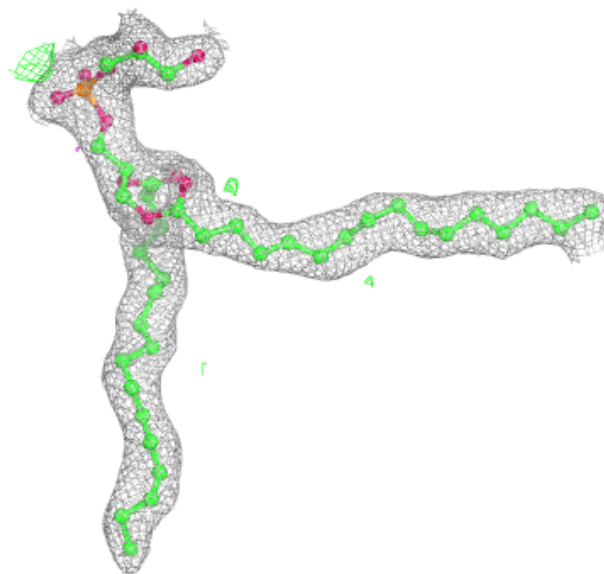






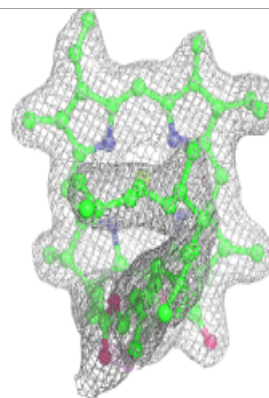
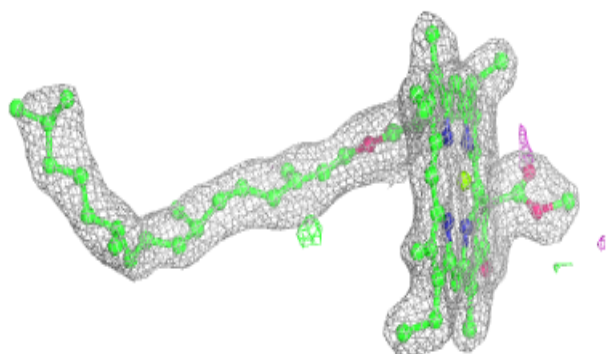
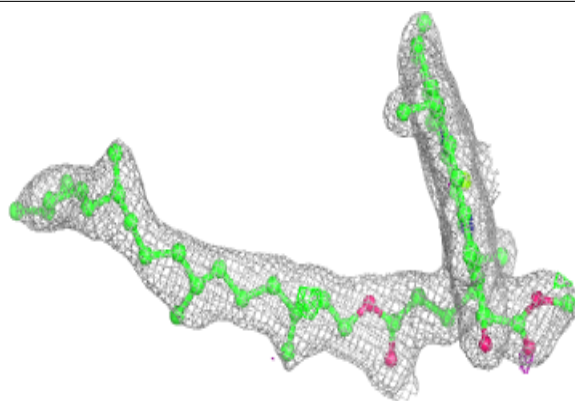
**Electron density around LHG L 101:**

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

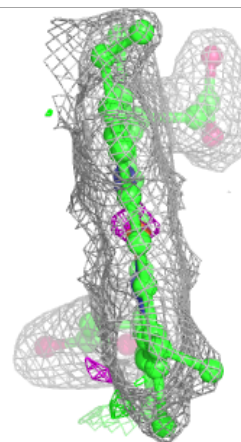
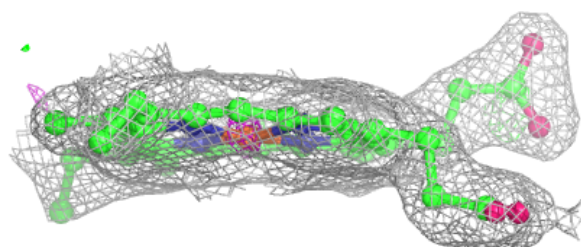
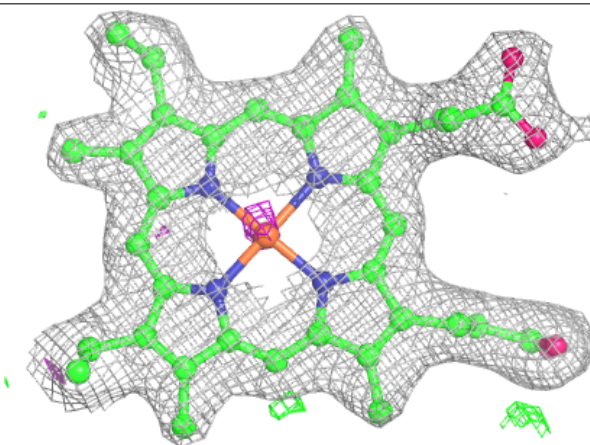


**Electron density around CLA b 604:**

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

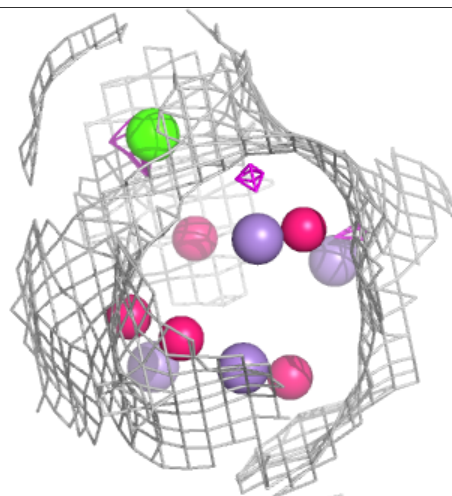
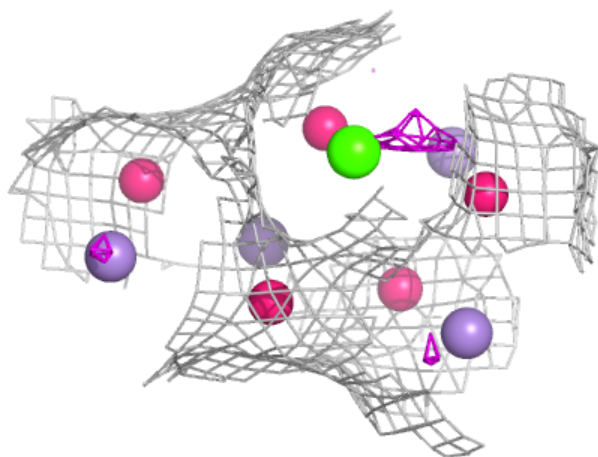
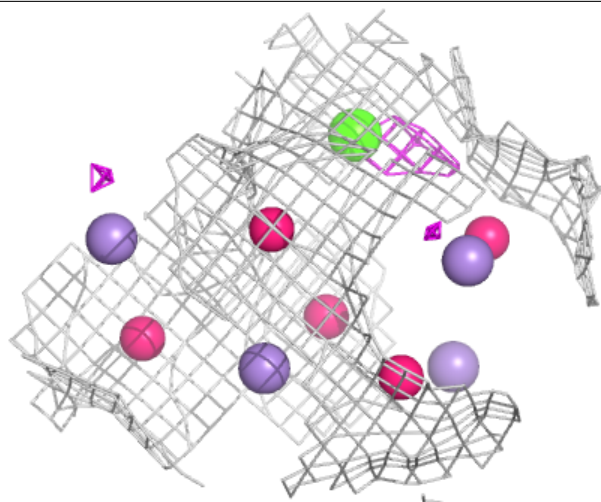
**Electron density around HEC V 201:**

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



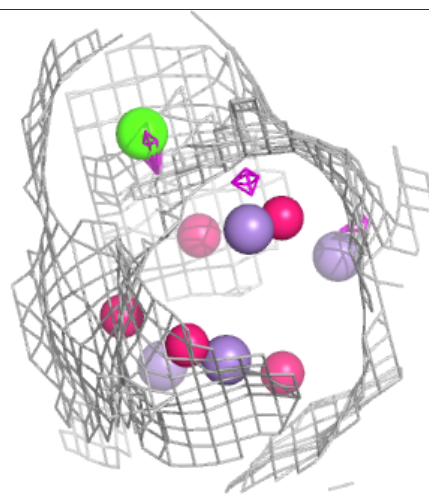
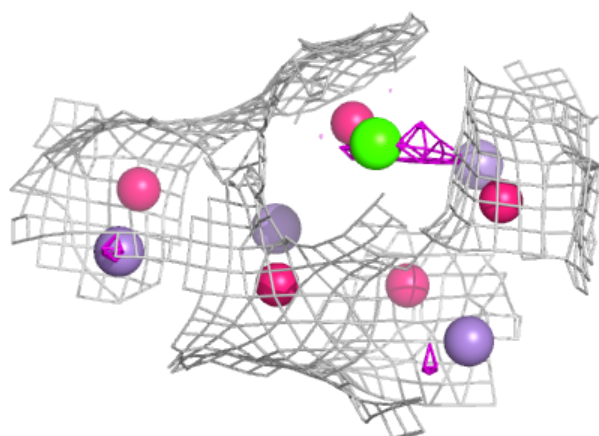
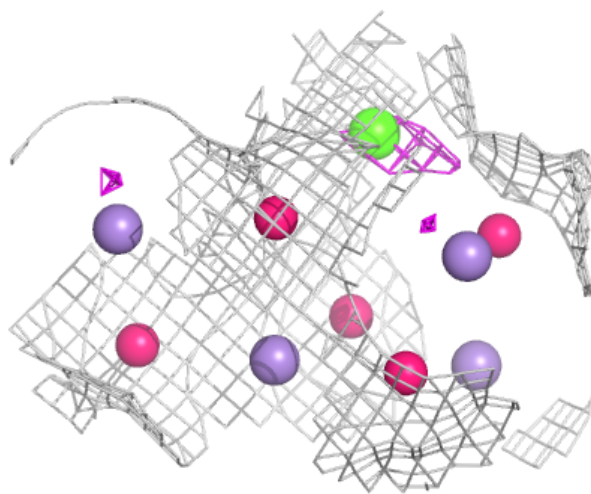
**Electron density around OEX A 601 (C):**

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



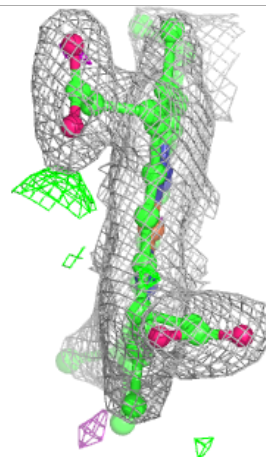
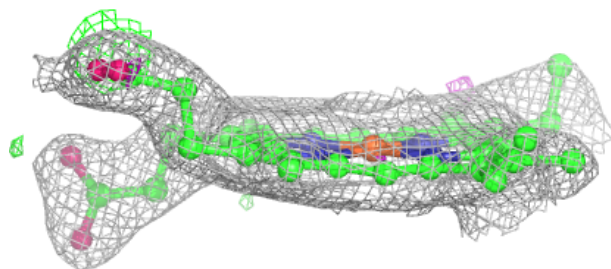
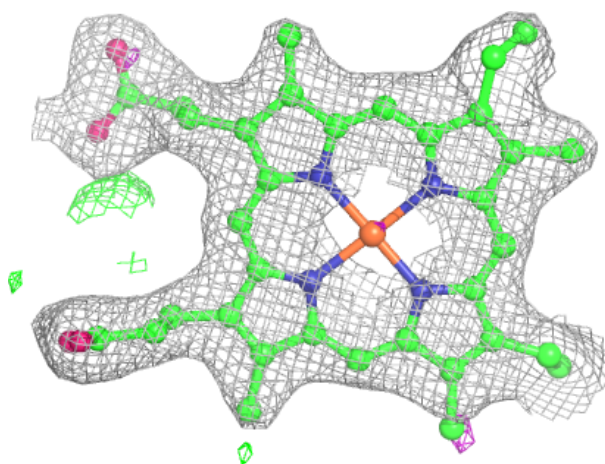
**Electron density around OEX A 601 (B):**

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



**Electron density around HEC v 201:**

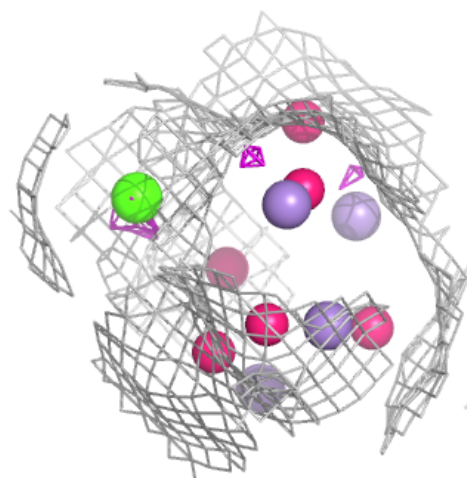
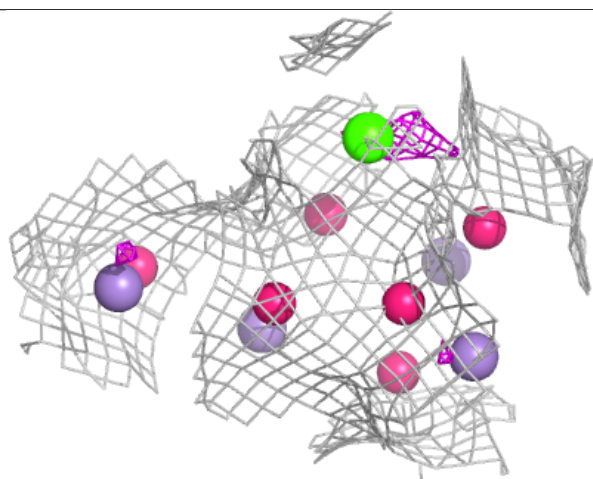
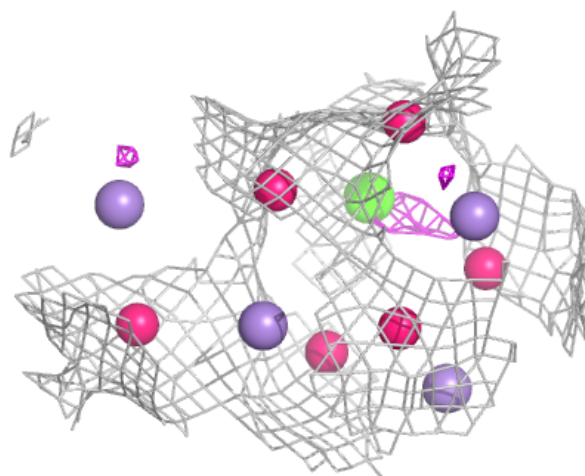
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





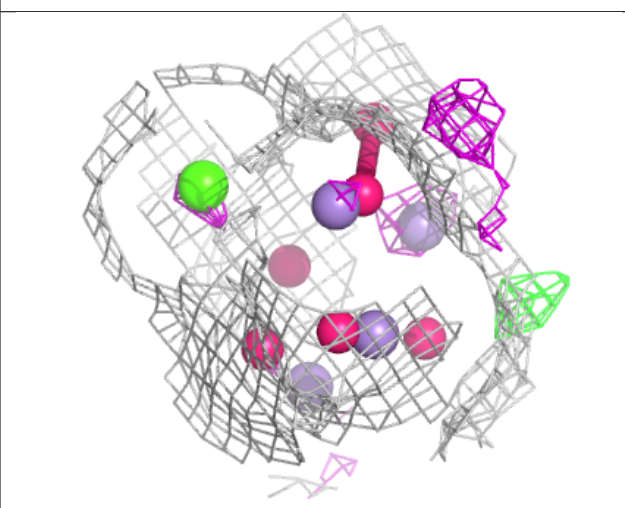
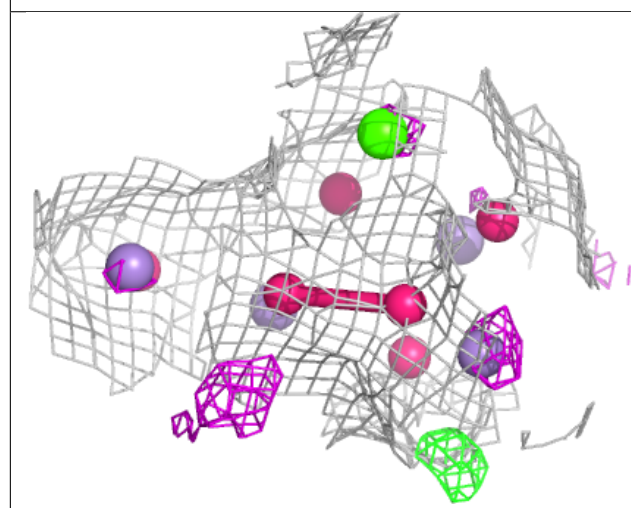
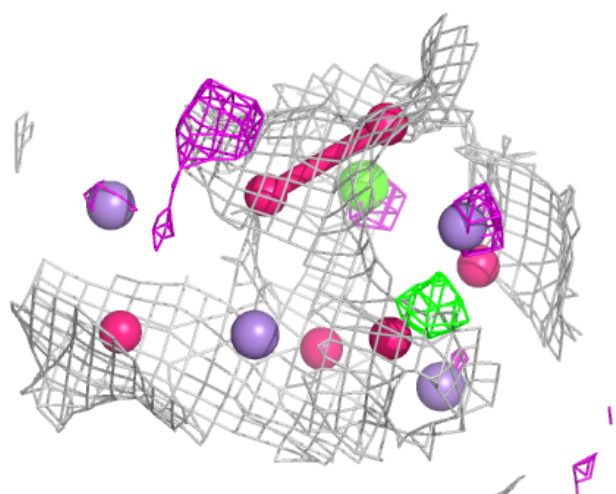
**Electron density around OEY A 602 (A):**

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



**Electron density around OEY a 602 (A):**

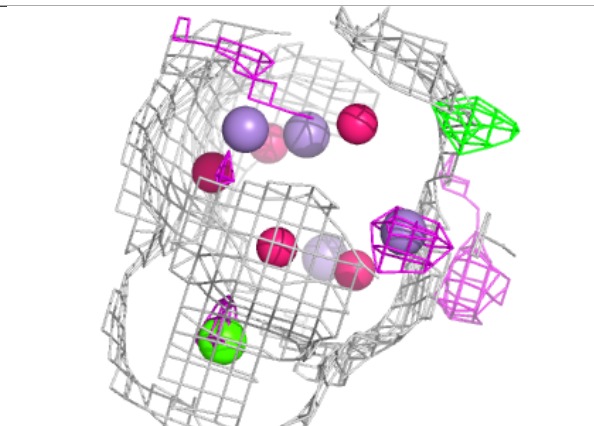
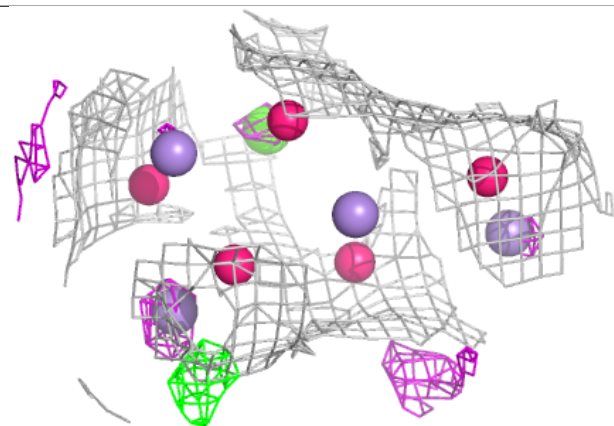
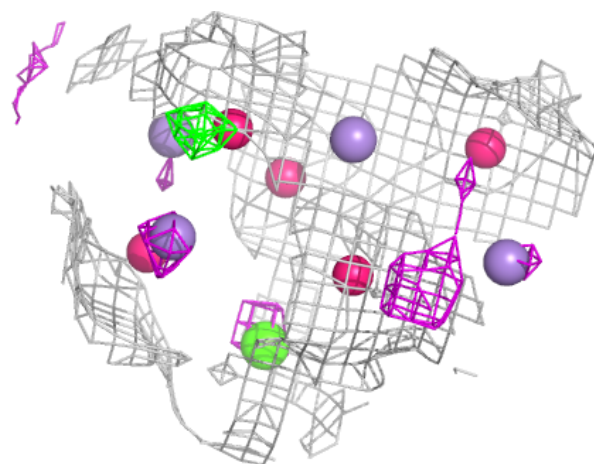
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





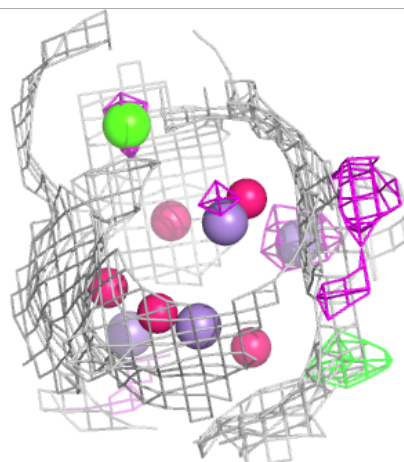
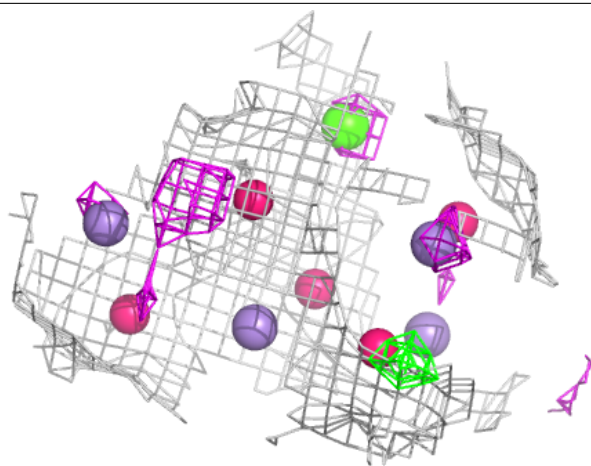
**Electron density around OEX a 601 (B):**

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



**Electron density around OEX a 601 (C):**

$2mF_o-DF_c$  (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.