



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2023 – 08:51 PM EDT

PDB ID : 6W1Q  
Title : RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 Angstrom resolution  
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2020-03-04  
Resolution : 2.27 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  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

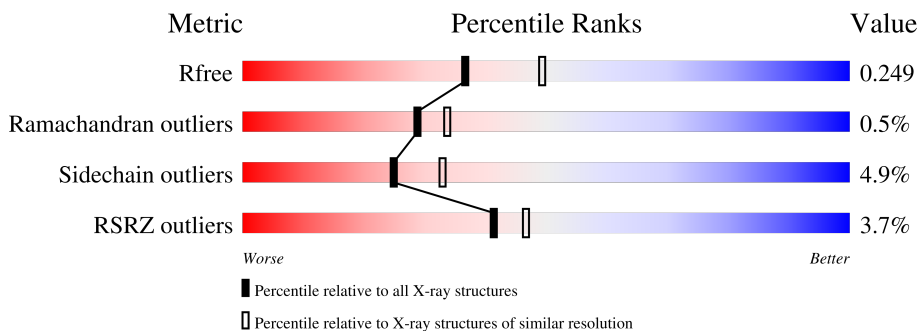
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

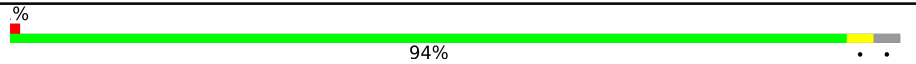
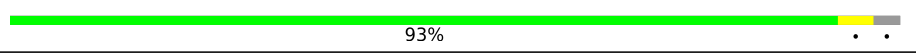
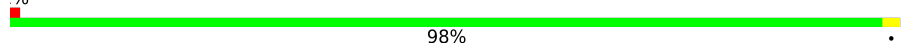
The reported resolution of this entry is 2.27 Å.

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	6980 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	 94%
1	a	344	 93%
2	B	506	 98%

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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) : 2.35.1



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Mol	Chain	Length	Quality of chain
2	b	506	3% 96%
3	C	461	2% 94%
3	c	461	2% 94%
4	D	352	94%
4	d	352	93%
5	E	84	4% 93% 5%
5	e	84	10% 93% 5%
6	F	45	76% 24%
6	f	45	2% 73% 24%
7	H	66	2% 91% 8%
7	h	66	9% 83% 12% 5%
8	I	38	3% 87% 8% 5%
8	i	38	8% 87% 8% 5%
9	J	40	8% 88% 10%
9	j	40	10% 85% 5% 10%
10	K	46	7% 76% 20%
10	k	46	65% 15% 20%
11	L	37	97%
11	l	37	8% 86% 11%
12	M	36	3% 86% 6% 8%
12	m	36	81% 8% 11%
13	O	272	4% 84% 6% 10%
13	o	272	4% 84% 6% 10%
14	R	41	27% 71% 12% 17%
14	r	41	61% 61% 15% 24%

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Mol	Chain	Length	Quality of chain
15	T	30	
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	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>
31	STE	a	412	-	-	-	X

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 103197 atoms, of which 51556 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	334	5130	1717	2508	431	459	15	0	0	0
1	a	334	5118	1714	2499	431	459	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	505	7864	2631	3859	666	695	13	0	5	0
2	b	505	7800	2610	3822	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	442	6767	2249	3341	571	593	13	0	2	0
3	c	451	6913	2290	3413	587	610	13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	D	341	5330	1800	2613	444	461	12	0	0	0
4	d	341	5342	1804	2619	444	463	12	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	H	65	Total	C	H	N	O	S	0	0	0
			1042	341	532	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
10	K	37	Total 598	C 204	H 305	N 43	O 46	0	0	0
10	k	37	Total 598	C 204	H 305	N 43	O 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	H	N	O				S
11	L	37	Total 620	C 202	H 316	N 48	O 53	S 1	0	0	0
11	l	36	Total 600	C 197	H 304	N 47	O 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	H	N	O				S
12	M	33	Total 525	C 171	H 269	N 37	O 47	S 1	0	0	0
12	m	32	Total 518	C 168	H 267	N 36	O 46	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
13	O	244	Total 3698	C 1168	H 1828	N 313	O 385	S 4	0	1	0
13	o	244	Total 3718	C 1170	H 1844	N 317	O 383	S 4	0	0	0

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
14	R	34	Total 569	C 184	H 298	N 47	O 40	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
17	V	137	Total	C	H	N	O	S	0	0	0
			2132	675	1068	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2132	675	1068	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
19	Y	27	Total 413	C 128	H 217	N 35	O 30	S 3	0	0	0
19	y	30	Total 459	C 144	H 241	N 35	O 36	S 3	0	0	0

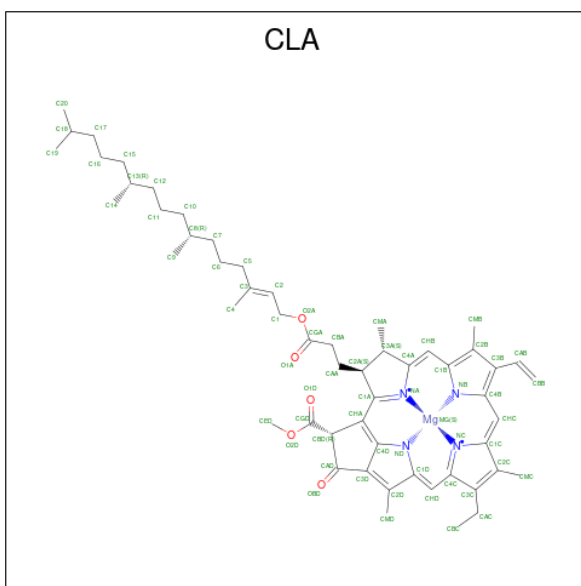
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

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

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

- Molecule 22 is 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	
22	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		

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

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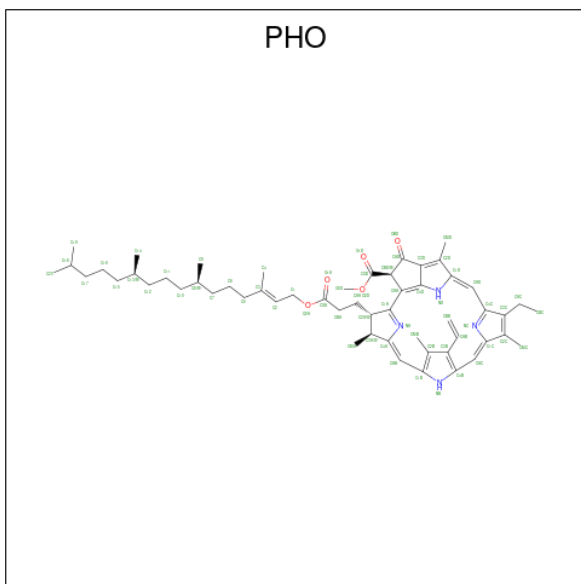
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).

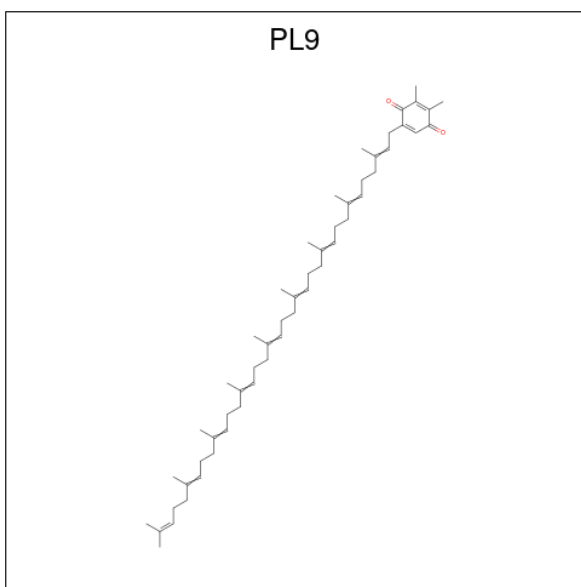


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

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

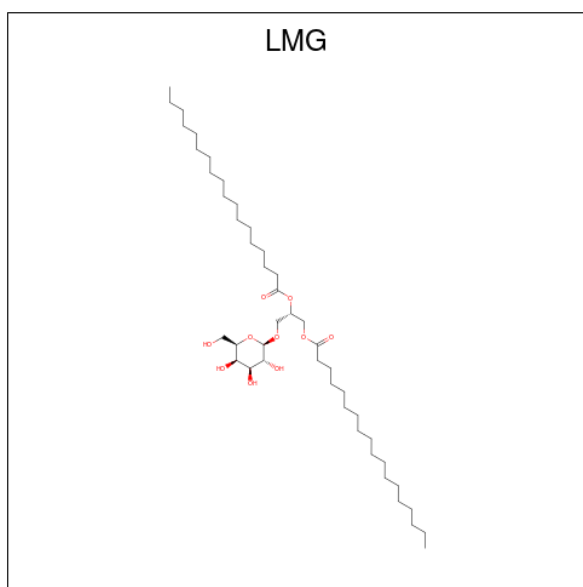
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

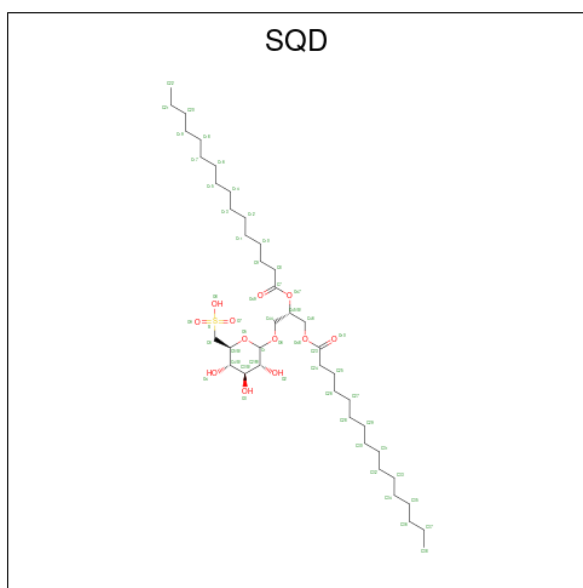
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	Total 114	C 38	H 66	O 10	0	0
26	B	1	Total 68	C 24	H 40	O 4	0	0
26	D	1	Total 120	C 41	H 69	O 10	0	0
26	D	1	Total 78	C 27	H 45	O 6	0	0
26	M	1	Total 120	C 41	H 69	O 10	0	0
26	Y	1	Total 114	C 38	H 66	O 10	0	0
26	a	1	Total 140	C 45	H 85	O 10	0	0
26	b	1	Total 141	C 45	H 86	O 10	0	0
26	c	1	Total 79	C 27	H 42	O 10	0	0
26	c	1	Total 116	C 38	H 68	O 10	0	0
26	c	1	Total 117	C 39	H 68	O 10	0	0
26	d	1	Total 101	C 34	H 57	O 10	0	0
26	m	1	Total 122	C 41	H 71	O 10	0	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY]

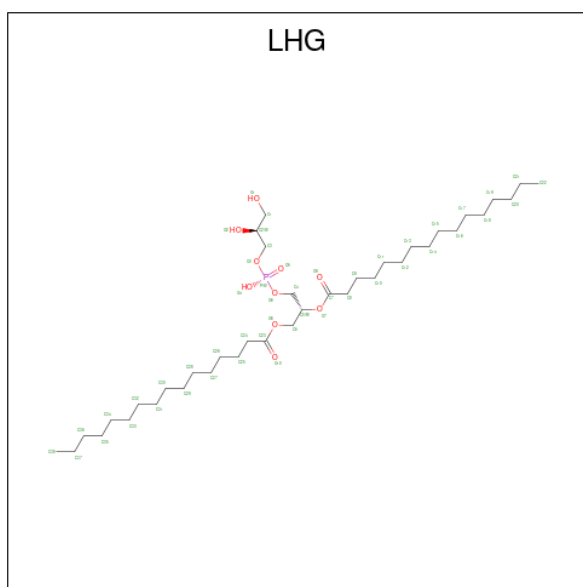
L]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			121	39	69	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
27	t	1	Total	C	H	O		0	0
			92	31	56	5			

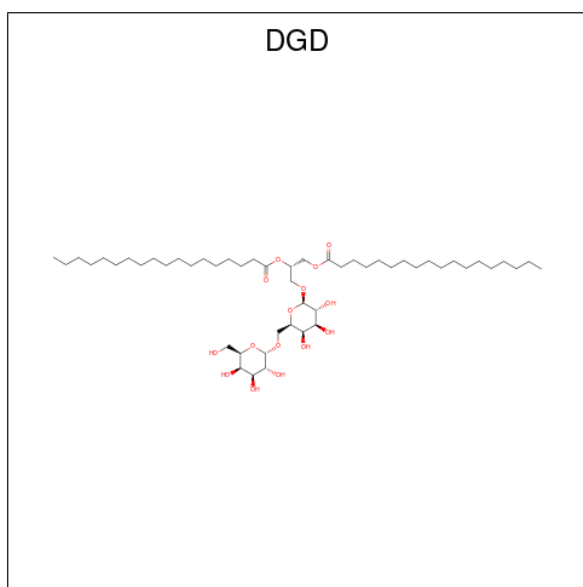
- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).





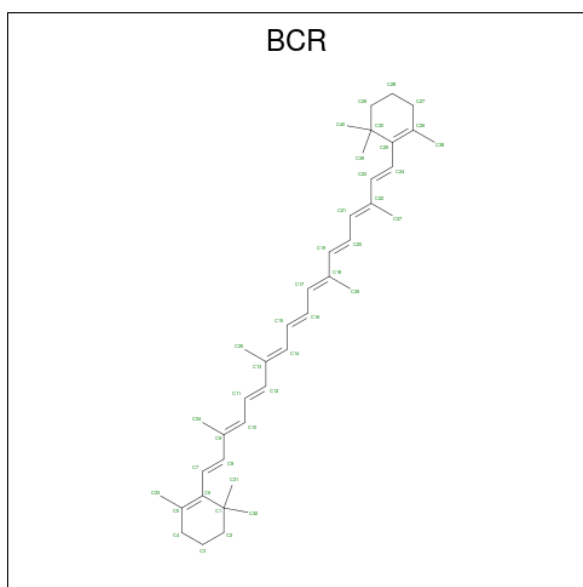
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
28	A	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	D	1	Total	C	H	O	P	0	0
			113	36	66	10	1		
28	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	b	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
29	A	1	Total	C	H	O	0	0
			160	51	94	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			141	47	79	15		
29	H	1	Total	C	H	O	0	0
			139	47	77	15		
29	c	1	Total	C	H	O	0	0
			141	47	79	15		
29	c	1	Total	C	H	O	0	0
			140	47	78	15		
29	c	1	Total	C	H	O	0	0
			139	47	77	15		
29	h	1	Total	C	H	O	0	0
			141	47	79	15		

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



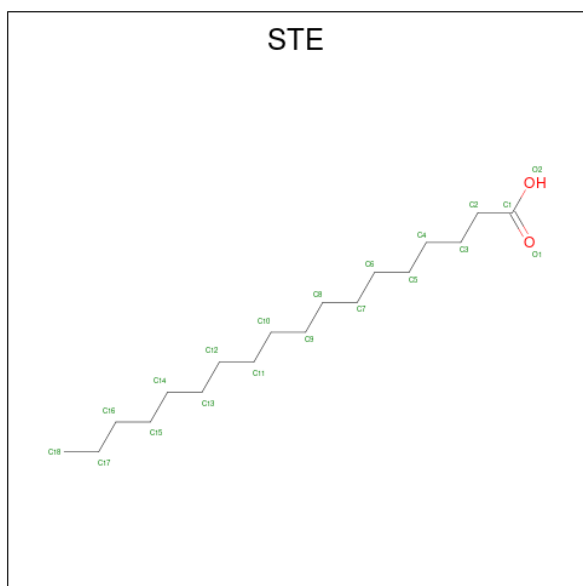
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	H	0	0
			96	40	56		
30	B	1	Total	C	H	0	0
			96	40	56		
30	B	1	Total	C	H	0	0
			96	40	56		
30	C	1	Total	C	H	0	0
			96	40	56		
30	C	1	Total	C	H	0	0
			96	40	56		
30	D	1	Total	C	H	0	0
			96	40	56		
30	H	1	Total	C	H	0	0
			96	40	56		
30	I	1	Total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

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

- Molecule 31 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			43	15	26	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		

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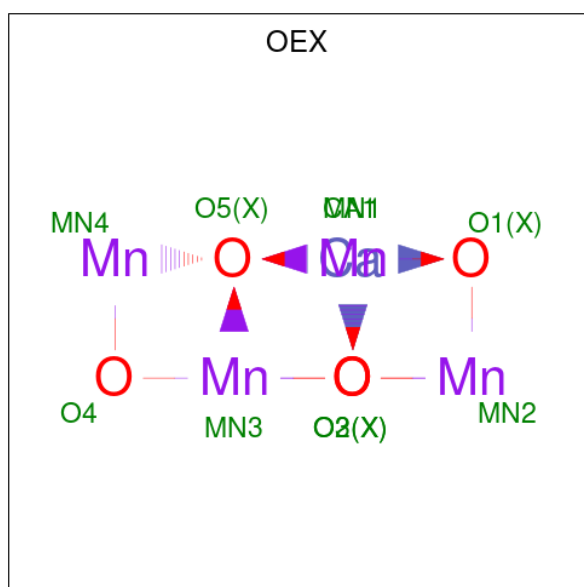
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C H 47 16 31	0	0
31	B	1	Total C H O 28 10 16 2	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	C	1	Total C H 47 16 31	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	H	1	Total C H 53 18 35	0	0
31	I	1	Total C H 41 15 26	0	0
31	J	1	Total C H O 28 10 16 2	0	0
31	L	1	Total C H O 28 10 16 2	0	0
31	M	1	Total C H O 37 13 22 2	0	0
31	M	1	Total C H 26 10 16	0	0
31	M	1	Total C H 53 18 35	0	0
31	R	1	Total C H O 28 10 16 2	0	0
31	X	1	Total C H O 55 18 35 2	0	0
31	Z	1	Total C H 20 8 12	0	0
31	a	1	Total C H O 28 10 16 2	0	0
31	a	1	Total C H 41 15 26	0	0
31	b	1	Total C H 47 16 31	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H O 40 14 24 2	0	0
31	b	1	Total C H 44 15 29	0	0

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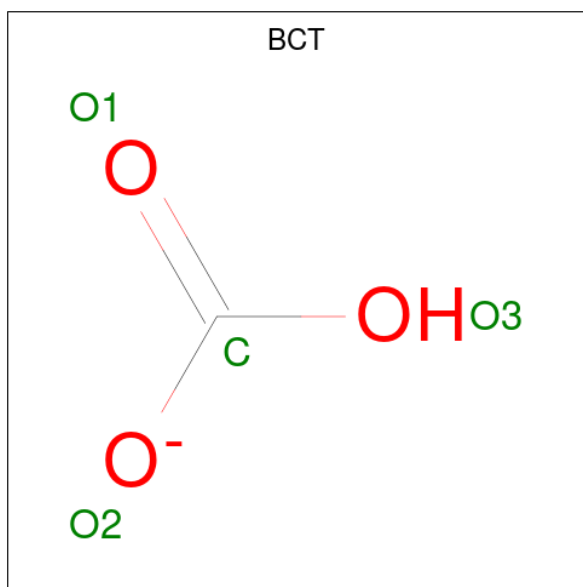
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	b	1	Total C H 41 14 27	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	j	1	Total C H O 28 10 16 2	0	0
31	k	1	Total C H O 28 10 16 2	0	0
31	t	1	Total C H O 34 12 20 2	0	0
31	t	1	Total C H 26 10 16	0	0
31	x	1	Total C H O 55 18 35 2	0	0

- Molecule 32 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



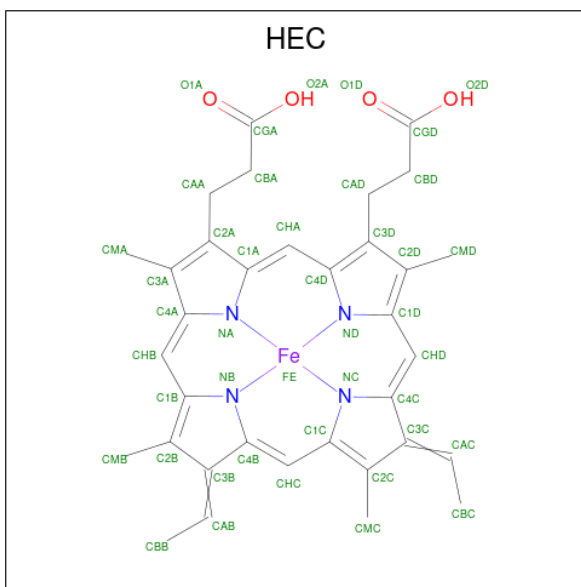
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
32	C	1	10	1	4	5	0	0
32	a	1	10	1	4	5	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
33	D	1	5	1	1	3	0	0
33	d	1	5	1	1	3	0	0

- Molecule 34 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
34	F	1	75	34	1	32	4	4	0	0
34	V	1	73	34	1	30	4	4	0	0
34	f	1	75	34	1	32	4	4	0	0
34	v	1	73	34	1	30	4	4	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	V	1	Total	Na	0	0
			1	1		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	112	Total	O	0	0
			112	112		
36	B	142	Total	O	0	0
			142	142		
36	C	125	Total	O	0	0
			125	125		
36	D	96	Total	O	0	0
			96	96		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	E	22	Total O 22 22	0	0
36	F	6	Total O 6 6	0	0
36	H	16	Total O 16 16	0	0
36	I	10	Total O 10 10	0	0
36	J	14	Total O 14 14	0	0
36	K	3	Total O 3 3	0	0
36	L	10	Total O 10 10	0	0
36	M	9	Total O 9 9	0	0
36	O	60	Total O 60 60	0	0
36	R	11	Total O 11 11	0	0
36	T	8	Total O 8 8	0	0
36	U	28	Total O 28 28	0	0
36	V	49	Total O 49 49	0	0
36	X	10	Total O 10 10	0	0
36	Y	2	Total O 2 2	0	0
36	Z	7	Total O 7 7	0	0
36	a	96	Total O 96 96	0	0
36	b	116	Total O 116 116	0	0
36	c	108	Total O 108 108	0	0
36	d	87	Total O 87 87	0	0
36	e	11	Total O 11 11	0	0

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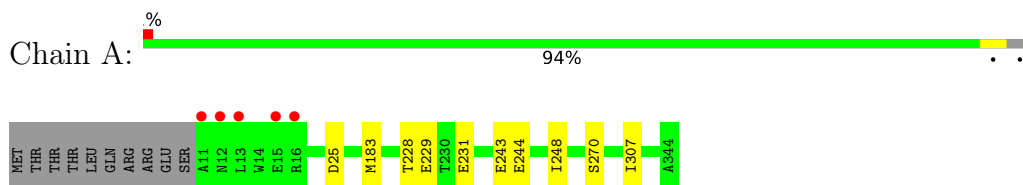
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	f	7	Total O 7 7	0	0
36	h	17	Total O 17 17	0	0
36	i	14	Total O 14 14	0	0
36	j	8	Total O 8 8	0	0
36	k	7	Total O 7 7	0	0
36	l	11	Total O 11 11	0	0
36	m	4	Total O 4 4	0	0
36	o	67	Total O 67 67	0	0
36	r	3	Total O 3 3	0	0
36	t	8	Total O 8 8	0	0
36	u	34	Total O 34 34	0	0
36	v	30	Total O 30 30	0	0
36	x	6	Total O 6 6	0	0
36	y	12	Total O 12 12	0	0
36	z	6	Total O 6 6	0	0

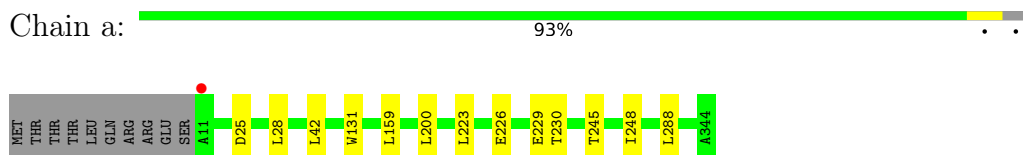
### 3 Residue-property plots [i](#)

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

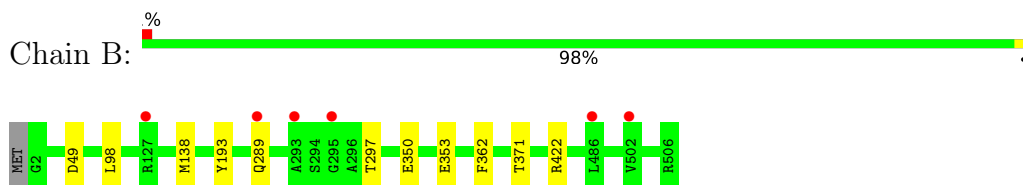
- Molecule 1: Photosystem II protein D1 1



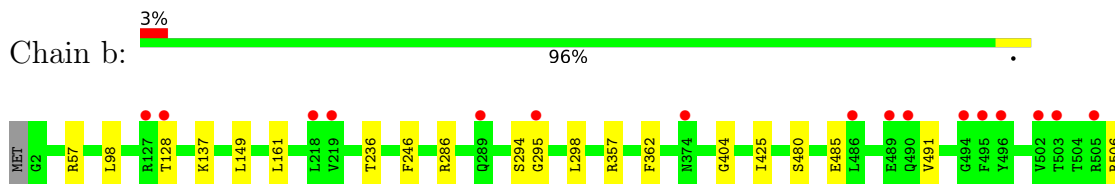
- Molecule 1: Photosystem II protein D1 1



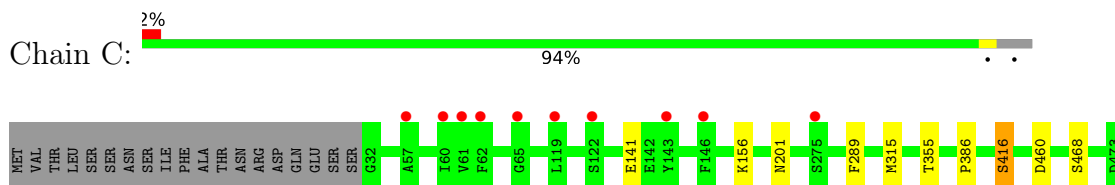
- Molecule 2: Photosystem II CP47 reaction center protein



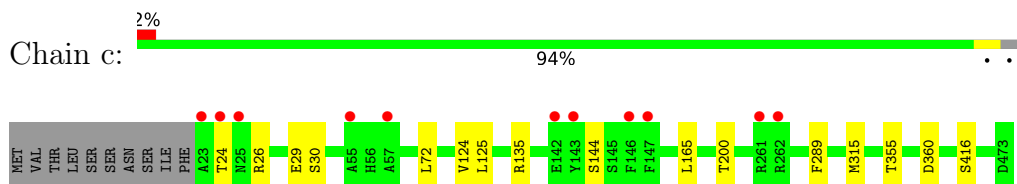
- Molecule 2: Photosystem II CP47 reaction center protein



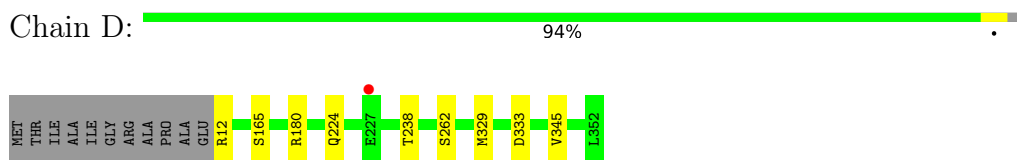
- Molecule 3: Photosystem II CP43 reaction center protein



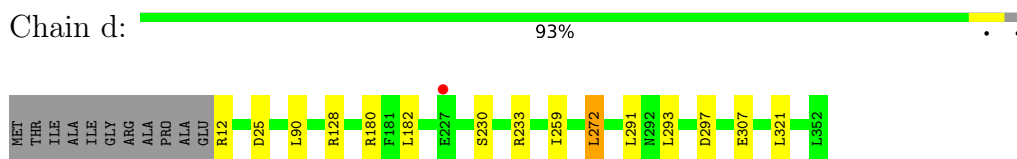
- Molecule 3: Photosystem II CP43 reaction center protein



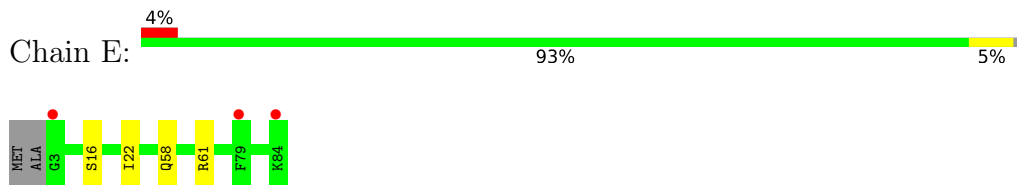
• Molecule 4: Photosystem II D2 protein



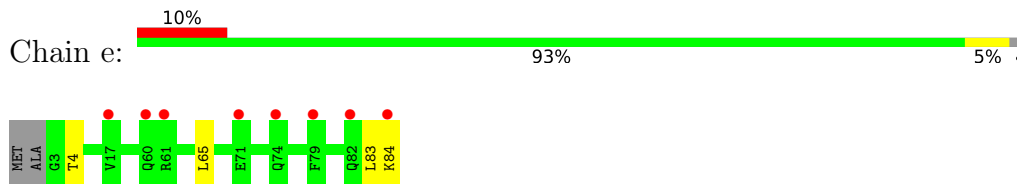
• Molecule 4: Photosystem II D2 protein



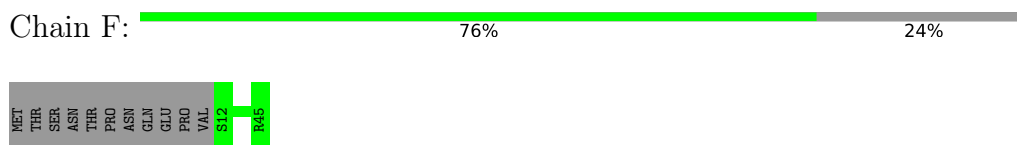
• Molecule 5: Cytochrome b559 subunit alpha



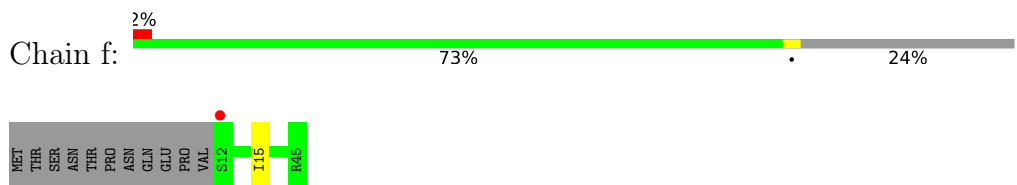
• Molecule 5: Cytochrome b559 subunit alpha



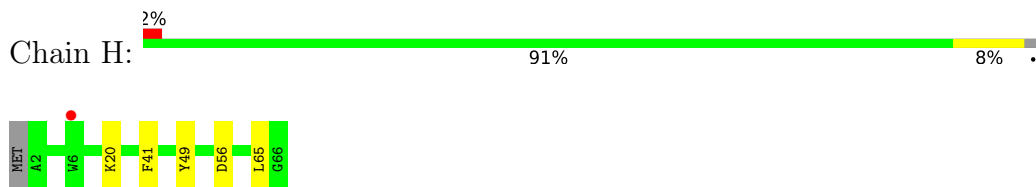
• Molecule 6: Cytochrome b559 subunit beta



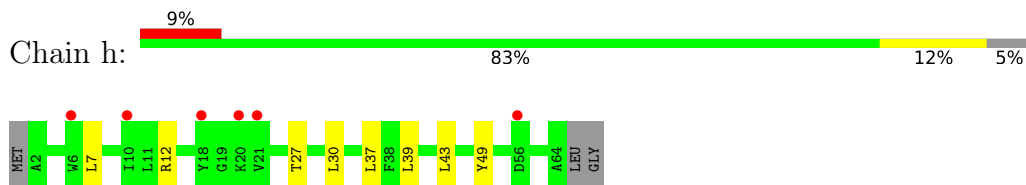
• Molecule 6: Cytochrome b559 subunit beta



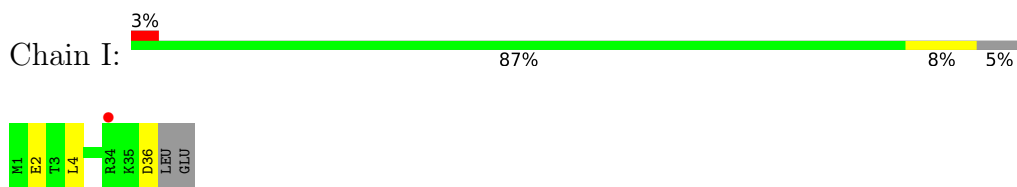
- Molecule 7: Photosystem II reaction center protein H



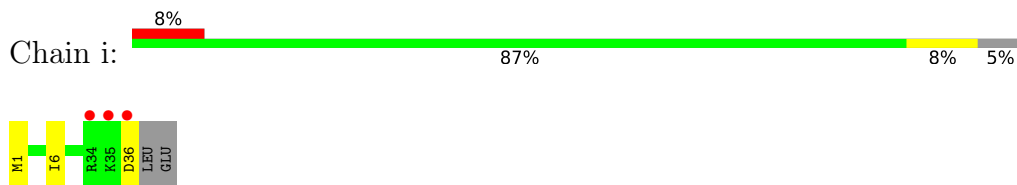
- Molecule 7: Photosystem II reaction center protein H



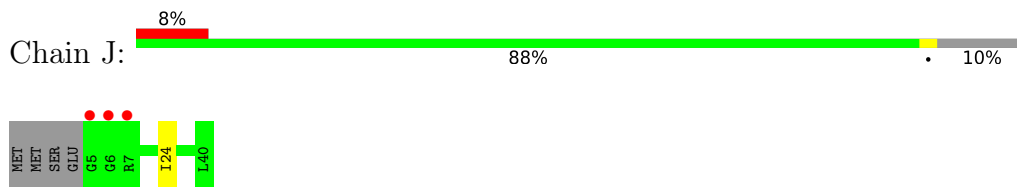
- Molecule 8: Photosystem II reaction center protein I



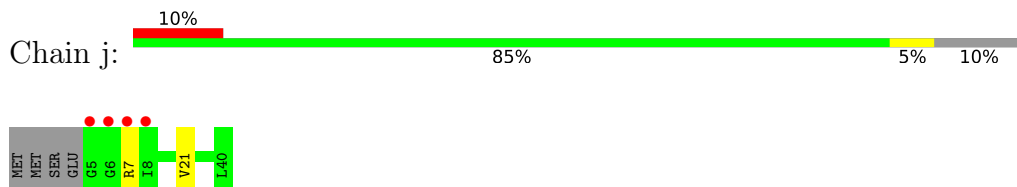
- Molecule 8: Photosystem II reaction center protein I



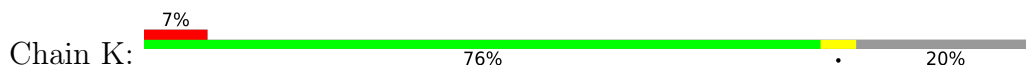
- Molecule 9: Photosystem II reaction center protein J

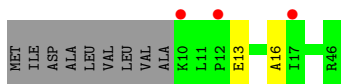


- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K





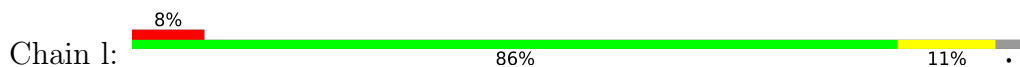
- Molecule 10: Photosystem II reaction center protein K



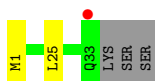
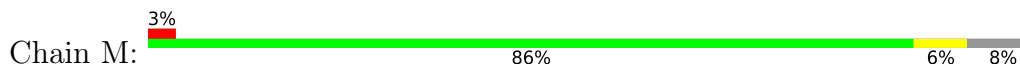
- Molecule 11: Photosystem II reaction center protein L



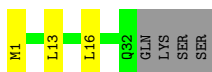
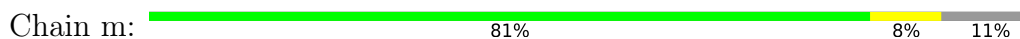
- Molecule 11: Photosystem II reaction center protein L



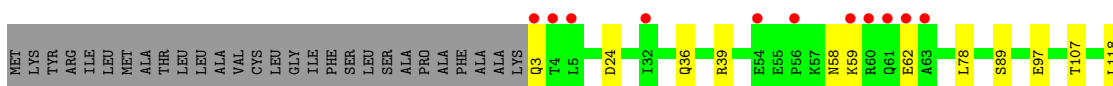
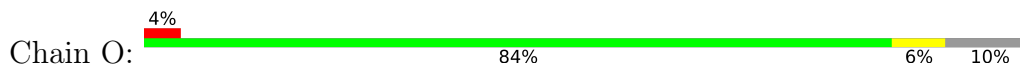
- Molecule 12: Photosystem II reaction center protein M



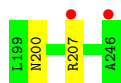
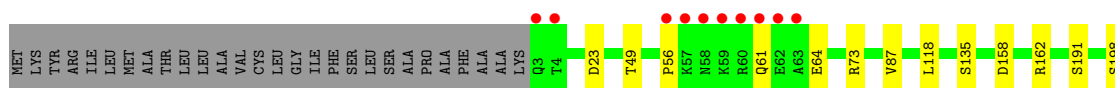
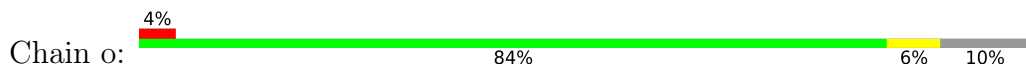
- Molecule 12: Photosystem II reaction center protein M



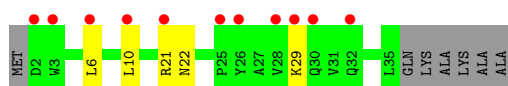
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



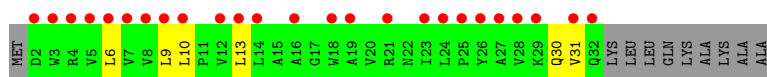
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



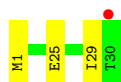
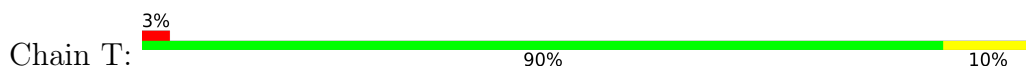
- Molecule 14: Photosystem II protein Y



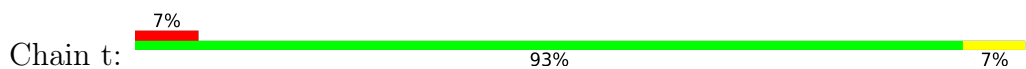
- Molecule 14: Photosystem II protein Y



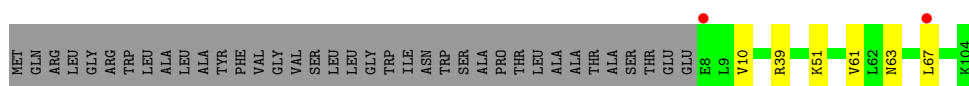
- Molecule 15: Photosystem II reaction center protein T



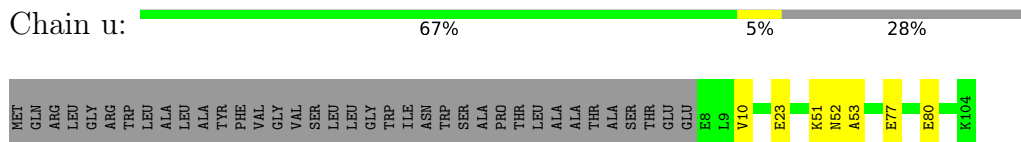
- Molecule 15: Photosystem II reaction center protein T



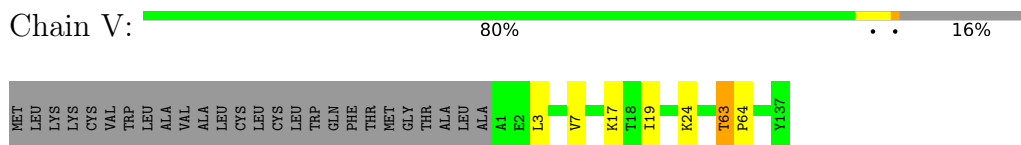
- Molecule 16: Photosystem II 12 kDa extrinsic protein



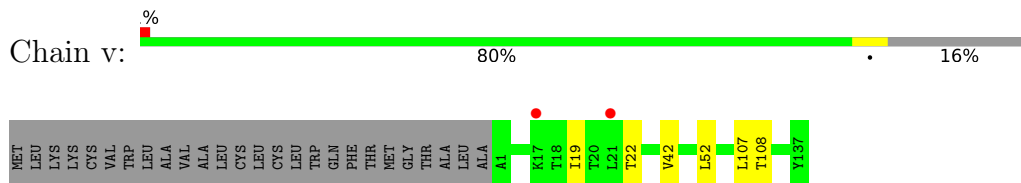
- Molecule 16: Photosystem II 12 kDa extrinsic protein



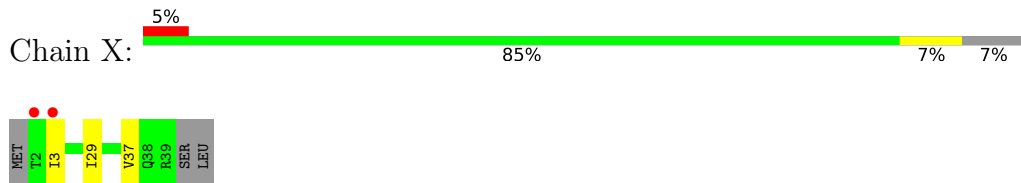
● Molecule 17: Cytochrome c-550



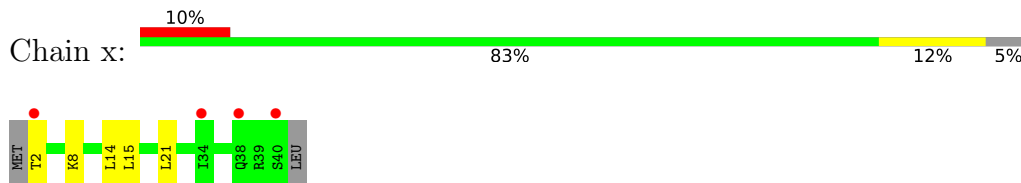
● Molecule 17: Cytochrome c-550



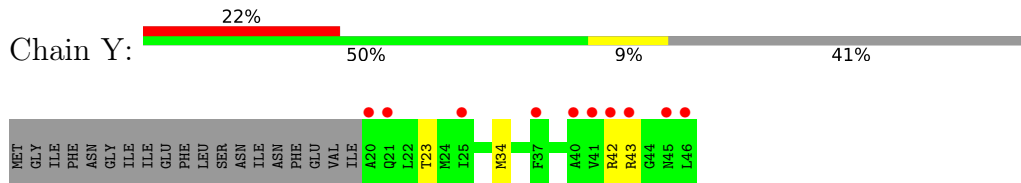
● Molecule 18: Photosystem II reaction center X protein



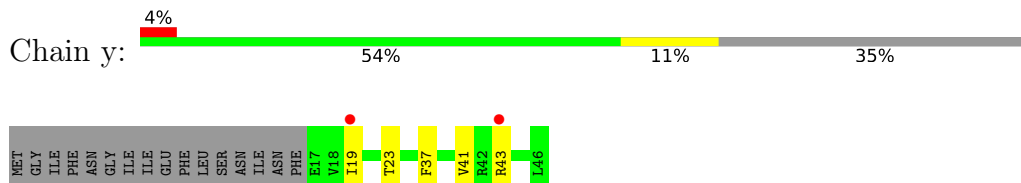
● Molecule 18: Photosystem II reaction center X protein



● Molecule 19: Photosystem II reaction center protein Ycf12

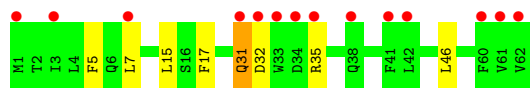
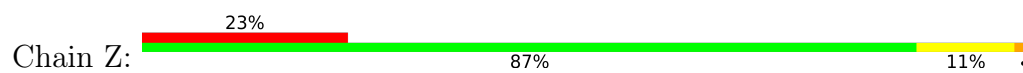


● Molecule 19: Photosystem II reaction center protein Ycf12

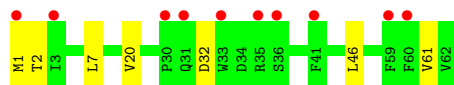
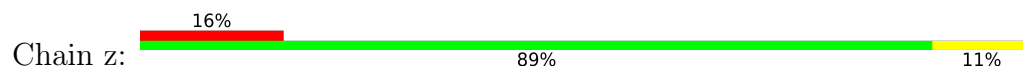




## ● Molecule 20: Photosystem II reaction center protein Z



## ● Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.3 (33.45-2.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.58 (at 2.27Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.178 , 0.249 0.178 , 0.249	Depositor DCC
$R_{free}$ test set	3275 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	103197	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.70	0/2707	0.75	2/3692 (0.1%)
1	a	0.71	0/2704	0.73	2/3688 (0.1%)
2	B	0.70	1/4161 (0.0%)	0.72	2/5669 (0.0%)
2	b	0.67	0/4118	0.72	1/5611 (0.0%)
3	C	0.67	1/3547 (0.0%)	0.72	1/4830 (0.0%)
3	c	0.64	0/3619	0.72	1/4926 (0.0%)
4	D	0.72	0/2812	0.73	2/3832 (0.1%)
4	d	0.70	0/2821	0.75	4/3844 (0.1%)
5	E	0.64	0/688	0.65	0/940
5	e	0.60	0/683	0.65	0/932
6	F	0.53	0/284	0.62	0/387
6	f	0.50	0/284	0.67	0/387
7	H	0.70	1/523 (0.2%)	0.73	0/713
7	h	0.60	0/511	0.72	0/697
8	I	0.67	0/293	0.72	0/396
8	i	0.69	0/293	0.69	0/396
9	J	0.58	0/263	0.67	0/356
9	j	0.57	0/263	0.63	0/356
10	K	0.64	0/303	0.67	0/416
10	k	0.52	0/303	0.64	0/416
11	L	0.69	0/311	0.77	0/422
11	l	0.75	0/303	0.73	0/412
12	M	0.68	0/249	0.66	0/341
12	m	0.73	0/244	0.77	0/334
13	O	0.66	0/1904	0.77	0/2585
13	o	0.69	0/1905	0.81	2/2583 (0.1%)
14	R	0.50	0/277	0.60	0/380
14	r	0.43	0/246	0.54	0/339
15	T	0.83	0/257	0.80	0/349
15	t	0.78	0/255	0.67	0/346
16	U	0.60	0/785	0.71	0/1064
16	u	0.67	0/785	0.78	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	V	0.62	0/1085	0.74	1/1473 (0.1%)
17	v	0.59	0/1085	0.71	0/1473
18	X	0.62	0/284	0.74	0/384
18	x	0.51	0/289	0.68	0/391
19	Y	0.49	0/197	0.71	0/264
19	y	0.41	0/219	0.59	0/294
20	Z	0.50	0/490	0.60	0/669
20	z	0.49	0/488	0.59	0/666
All	All	0.67	3/42838 (0.0%)	0.72	18/58317 (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	u	0	1
17	V	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-7.38	1.17	1.34
2	B	193	TYR	CD2-CE2	-6.56	1.29	1.39
7	H	41	PHE	CB-CG	-5.27	1.42	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	57	ARG	NE-CZ-NH1	-7.43	116.59	120.30
17	V	63	THR	C-N-CD	-7.34	104.45	120.60
3	C	460	ASP	CB-CG-OD1	6.72	124.35	118.30
4	d	128	ARG	NE-CZ-NH2	-6.60	117.00	120.30
13	o	162	ARG	NE-CZ-NH2	6.60	123.60	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

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Mol	Chain	Res	Type	Group
16	u	52	ASN	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
1	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
2	B	508/506 (100%)	494 (97%)	14 (3%)	0	100	100
2	b	503/506 (99%)	484 (96%)	16 (3%)	3 (1%)	25	29
3	C	442/461 (96%)	423 (96%)	18 (4%)	1 (0%)	47	57
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	47	57
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	327 (96%)	13 (4%)	0	100	100
5	E	81/84 (96%)	78 (96%)	2 (2%)	1 (1%)	13	12
5	e	80/84 (95%)	78 (98%)	1 (1%)	1 (1%)	12	11
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	28 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	4	2
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	4	2
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%)	227 (93%)	13 (5%)	3 (1%)	13	12
13	o	242/272 (89%)	224 (93%)	15 (6%)	3 (1%)	13	12
14	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
14	r	29/41 (71%)	25 (86%)	2 (7%)	2 (7%)	1	0
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	89 (94%)	5 (5%)	1 (1%)	14	14
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	25
17	v	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	25
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	3	1
19	y	28/46 (61%)	20 (71%)	6 (21%)	2 (7%)	1	0
20	Z	60/62 (97%)	56 (93%)	2 (3%)	2 (3%)	4	2
20	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	4	2
All	All	5240/5688 (92%)	5024 (96%)	189 (4%)	27 (0%)	29	34

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	58	ASN
13	O	62	GLU
17	V	64	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	262 (97%)	8 (3%)	41	54
1	a	269/280 (96%)	258 (96%)	11 (4%)	30	41
2	B	408/404 (101%)	400 (98%)	8 (2%)	55	70
2	b	402/404 (100%)	386 (96%)	16 (4%)	31	42
3	C	346/362 (96%)	338 (98%)	8 (2%)	50	65
3	c	354/362 (98%)	340 (96%)	14 (4%)	31	42
4	D	276/283 (98%)	268 (97%)	8 (3%)	42	56
4	d	277/283 (98%)	264 (95%)	13 (5%)	26	34
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	27
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	39
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	47
7	H	54/55 (98%)	50 (93%)	4 (7%)	13	16
7	h	53/55 (96%)	45 (85%)	8 (15%)	3	2
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	9
8	i	32/34 (94%)	30 (94%)	2 (6%)	18	22
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	39
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	12
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	51
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	56
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	47
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	17
13	O	206/228 (90%)	193 (94%)	13 (6%)	18	22
13	o	207/228 (91%)	197 (95%)	10 (5%)	25	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
14	r	23/33 (70%)	19 (83%)	4 (17%)	2	1
15	T	26/26 (100%)	24 (92%)	2 (8%)	13	15
15	t	25/26 (96%)	24 (96%)	1 (4%)	31	42
16	U	84/112 (75%)	78 (93%)	6 (7%)	14	17
16	u	84/112 (75%)	79 (94%)	5 (6%)	19	24
17	V	117/138 (85%)	112 (96%)	5 (4%)	29	38
17	v	117/138 (85%)	112 (96%)	5 (4%)	29	38
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	8
18	x	31/34 (91%)	26 (84%)	5 (16%)	2	2
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2	2
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	3
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	3
20	z	51/52 (98%)	46 (90%)	5 (10%)	8	8
All	All	4328/4644 (93%)	4117 (95%)	211 (5%)	25	33

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	485	GLU
4	d	307	GLU
18	x	8	LYS
3	c	26	ARG
3	c	315	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
19	Y	45	ASN
20	Z	6	GLN
13	o	130	GLN
3	c	28	GLN
13	o	61	GLN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	FME	T	1	15	8,9,10	1.11	1 (12%)	7,9,11	0.94	1 (14%)
12	FME	M	1	12	8,9,10	1.17	1 (12%)	7,9,11	1.09	1 (14%)
8	FME	I	1	8	8,9,10	1.06	0	7,9,11	0.66	0
8	FME	i	1	8	8,9,10	1.28	1 (12%)	7,9,11	1.24	1 (14%)
15	FME	t	1	15	8,9,10	1.56	1 (12%)	7,9,11	1.18	0
12	FME	m	1	12	8,9,10	0.89	0	7,9,11	1.36	1 (14%)

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
15	FME	T	1	15	-	4/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	3/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
15	FME	t	1	15	-	4/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-4.11	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.73	1.42	1.46
12	M	1	FME	CA-N	-2.62	1.42	1.46
15	T	1	FME	CA-N	-2.10	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	2.85	127.20	122.82
8	i	1	FME	CA-N-CN	-2.39	119.14	122.82
12	M	1	FME	CA-N-CN	-2.06	119.65	122.82
15	T	1	FME	CG-CB-CA	2.03	118.59	112.95

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
8	I	1	FME	N-CA-CB-CG
15	T	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, 7 are monoatomic - leaving 183 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
22	CLA	C	506	-	65,73,73	1.87	11 (16%)	76,113,113	1.44	11 (14%)
22	CLA	C	501	-	65,73,73	1.64	10 (15%)	76,113,113	1.57	10 (13%)
22	CLA	B	614	-	65,73,73	1.76	11 (16%)	76,113,113	1.50	10 (13%)
22	CLA	c	501	-	65,73,73	1.67	9 (13%)	76,113,113	1.62	10 (13%)
30	BCR	B	616	-	41,41,41	1.07	3 (7%)	56,56,56	1.40	9 (16%)
28	LHG	d	409	-	38,38,48	1.06	4 (10%)	41,44,54	1.21	5 (12%)
26	LMG	b	622	-	55,55,55	1.16	5 (9%)	63,63,63	1.45	5 (7%)
34	HEC	F	101	5,6	32,50,50	2.29	3 (9%)	24,82,82	2.02	7 (29%)
22	CLA	C	505	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	10 (13%)
22	CLA	a	405	-	65,73,73	1.65	9 (13%)	76,113,113	1.40	11 (14%)
22	CLA	c	505	-	65,73,73	1.54	7 (10%)	76,113,113	1.48	10 (13%)
31	STE	b	621	-	19,19,19	0.72	0	19,19,19	0.96	1 (5%)
22	CLA	B	609	36	65,73,73	1.55	11 (16%)	76,113,113	1.65	10 (13%)
22	CLA	B	604	-	65,73,73	1.26	5 (7%)	76,113,113	1.53	13 (17%)
22	CLA	C	509	-	65,73,73	1.55	10 (15%)	76,113,113	1.38	11 (14%)
22	CLA	D	403	-	65,73,73	1.59	8 (12%)	76,113,113	1.37	10 (13%)
30	BCR	D	406	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
22	CLA	c	509	-	65,73,73	1.55	9 (13%)	76,113,113	1.66	13 (17%)
22	CLA	C	511	3	65,73,73	1.73	11 (16%)	76,113,113	1.54	6 (7%)
30	BCR	b	618	-	41,41,41	1.46	4 (9%)	56,56,56	1.36	9 (16%)
30	BCR	H	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.24	8 (14%)
22	CLA	b	615	-	65,73,73	2.34	12 (18%)	76,113,113	1.42	8 (10%)
30	BCR	K	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.54	12 (21%)
27	SQD	t	102	-	35,35,54	1.19	3 (8%)	37,37,65	1.46	4 (10%)
31	STE	d	411	-	16,16,19	0.78	0	16,16,19	0.98	1 (6%)
22	CLA	C	510	-	65,73,73	1.56	10 (15%)	76,113,113	1.78	11 (14%)
22	CLA	c	510	-	65,73,73	1.41	7 (10%)	76,113,113	1.50	9 (11%)
30	BCR	k	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	6 (10%)
30	BCR	a	406	-	41,41,41	1.09	3 (7%)	56,56,56	1.53	12 (21%)
22	CLA	a	403	36	65,73,73	1.58	10 (15%)	76,113,113	1.48	12 (15%)
25	PL9	A	408	-	55,55,55	1.65	4 (7%)	68,69,69	1.54	15 (22%)
34	HEC	V	201	17	32,50,50	1.97	3 (9%)	24,82,82	1.89	6 (25%)
22	CLA	b	601	36	65,73,73	1.60	9 (13%)	76,113,113	1.58	11 (14%)
30	BCR	K	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	9 (16%)
33	BCT	d	402	21	2,3,3	1.20	0	2,3,3	3.06	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	507	36	65,73,73	1.44	10 (15%)	76,113,113	1.51	7 (9%)
31	STE	C	520	-	15,15,19	0.55	0	14,14,19	0.52	0
22	CLA	b	608	-	65,73,73	1.42	9 (13%)	76,113,113	1.43	12 (15%)
23	PHO	D	401	-	51,69,69	1.24	6 (11%)	47,99,99	1.36	6 (12%)
31	STE	L	103	-	11,11,19	0.75	0	11,11,19	1.68	2 (18%)
22	CLA	A	403	36	65,73,73	1.94	10 (15%)	76,113,113	1.52	13 (17%)
23	PHO	A	404	-	51,69,69	1.22	7 (13%)	47,99,99	1.43	8 (17%)
28	LHG	a	411	-	41,41,48	1.15	6 (14%)	44,47,54	1.24	4 (9%)
22	CLA	C	512	-	65,73,73	1.41	7 (10%)	76,113,113	1.57	11 (14%)
31	STE	B	624	-	15,15,19	0.47	0	14,14,19	0.84	0
22	CLA	B	607	-	65,73,73	1.60	11 (16%)	76,113,113	1.25	8 (10%)
27	SQD	D	409	-	35,36,54	1.09	4 (11%)	42,45,65	1.97	11 (26%)
22	CLA	H	101	36	65,73,73	1.80	8 (12%)	76,113,113	1.48	5 (6%)
30	BCR	b	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	9 (16%)
27	SQD	L	101	-	48,49,54	1.00	2 (4%)	57,60,65	2.32	18 (31%)
32	OEX	C	522	3,36,1	0,15,15	-	-	-	-	-
23	PHO	a	404	-	51,69,69	1.00	5 (9%)	47,99,99	1.44	8 (17%)
26	LMG	D	412	-	31,31,55	1.24	3 (9%)	33,33,63	1.11	2 (6%)
31	STE	C	521	-	11,11,19	0.66	0	11,11,19	1.44	2 (18%)
30	BCR	C	514	-	41,41,41	1.24	2 (4%)	56,56,56	1.56	12 (21%)
31	STE	Z	101	-	7,7,19	0.52	0	6,6,19	0.26	0
31	STE	b	626	-	19,19,19	0.82	0	19,19,19	0.53	0
22	CLA	b	612	-	65,73,73	1.61	9 (13%)	76,113,113	1.59	12 (15%)
25	PL9	a	409	-	55,55,55	1.13	4 (7%)	68,69,69	1.53	12 (17%)
27	SQD	f	102	-	40,41,54	1.13	4 (10%)	49,52,65	2.02	12 (24%)
28	LHG	A	411	-	48,48,48	1.01	2 (4%)	51,54,54	1.22	5 (9%)
29	DGD	H	103	-	63,63,67	1.34	9 (14%)	77,77,81	1.58	13 (16%)
26	LMG	c	521	-	49,49,55	1.13	6 (12%)	57,57,63	1.34	8 (14%)
34	HEC	v	201	17	32,50,50	2.31	5 (15%)	24,82,82	2.21	4 (16%)
26	LMG	B	620	-	26,26,55	1.38	4 (15%)	26,26,63	1.08	2 (7%)
22	CLA	B	615	-	60,68,73	1.80	13 (21%)	70,107,113	1.57	10 (14%)
22	CLA	b	613	-	65,73,73	1.47	9 (13%)	76,113,113	1.60	10 (13%)
22	CLA	b	602	-	65,73,73	1.73	11 (16%)	76,113,113	1.65	13 (17%)
30	BCR	k	102	-	41,41,41	1.04	3 (7%)	56,56,56	1.16	4 (7%)
31	STE	b	629	-	19,19,19	0.77	1 (5%)	19,19,19	0.93	0
22	CLA	a	402	-	65,73,73	1.39	9 (13%)	76,113,113	1.56	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	602	-	65,73,73	1.39	10 (15%)	76,113,113	1.58	17 (22%)
26	LMG	c	518	-	37,37,55	1.44	7 (18%)	45,45,63	1.31	5 (11%)
31	STE	b	620	-	15,15,19	0.54	0	14,14,19	0.72	0
22	CLA	B	605	-	65,73,73	1.90	10 (15%)	76,113,113	1.42	9 (11%)
22	CLA	C	502	-	65,73,73	1.50	8 (12%)	76,113,113	1.41	9 (11%)
22	CLA	c	507	36	65,73,73	1.77	12 (18%)	76,113,113	1.54	12 (15%)
31	STE	B	625	-	11,11,19	0.81	0	11,11,19	1.49	3 (27%)
29	DGD	C	518	-	63,63,67	1.11	6 (9%)	77,77,81	1.53	11 (14%)
31	STE	b	624	-	15,15,19	0.86	0	15,15,19	0.90	0
22	CLA	b	610	36	65,73,73	1.52	11 (16%)	76,113,113	1.44	12 (15%)
22	CLA	B	611	-	65,73,73	1.63	10 (15%)	76,113,113	1.46	11 (14%)
26	LMG	m	101	-	51,51,55	1.25	4 (7%)	59,59,63	1.49	8 (13%)
29	DGD	c	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.38	8 (10%)
28	LHG	L	102	-	48,48,48	0.88	2 (4%)	51,54,54	1.17	4 (7%)
29	DGD	h	101	-	63,63,67	1.03	4 (6%)	77,77,81	1.46	14 (18%)
28	LHG	D	410	-	48,48,48	0.96	3 (6%)	51,54,54	1.22	5 (9%)
22	CLA	B	610	-	65,73,73	1.66	10 (15%)	76,113,113	1.78	13 (17%)
22	CLA	b	604	-	65,73,73	1.57	7 (10%)	76,113,113	1.60	14 (18%)
30	BCR	d	406	-	41,41,41	1.08	2 (4%)	56,56,56	1.39	8 (14%)
22	CLA	d	405	-	65,73,73	1.86	14 (21%)	76,113,113	1.31	9 (11%)
26	LMG	D	408	-	51,51,55	1.18	4 (7%)	59,59,63	1.35	6 (10%)
30	BCR	x	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.47	11 (19%)
31	STE	M	104	-	17,17,19	0.41	0	16,16,19	0.85	0
22	CLA	D	405	-	65,73,73	1.84	12 (18%)	76,113,113	1.21	6 (7%)
30	BCR	c	514	-	41,41,41	1.16	3 (7%)	56,56,56	1.65	12 (21%)
22	CLA	B	603	-	65,73,73	1.47	8 (12%)	76,113,113	1.81	14 (18%)
31	STE	t	103	-	13,13,19	0.87	0	13,13,19	1.10	2 (15%)
28	LHG	D	413	-	48,48,48	1.00	3 (6%)	51,54,54	1.40	7 (13%)
30	BCR	b	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	9 (16%)
31	STE	a	412	-	11,11,19	0.81	0	11,11,19	0.95	0
29	DGD	C	516	-	63,63,67	1.37	9 (14%)	77,77,81	1.39	11 (14%)
29	DGD	c	516	-	63,63,67	1.10	7 (11%)	77,77,81	1.55	16 (20%)
31	STE	B	622	-	11,11,19	0.77	0	11,11,19	1.41	1 (9%)
27	SQD	a	410	-	53,54,54	1.04	3 (5%)	62,65,65	1.78	13 (20%)
28	LHG	D	411	-	46,46,48	1.05	3 (6%)	49,52,54	1.21	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LHG	d	408	-	48,48,48	0.77	1 (2%)	51,54,54	1.12	3 (5%)
30	BCR	t	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.44	10 (17%)
31	STE	H	104	-	17,17,19	0.46	0	16,16,19	0.64	0
22	CLA	c	506	-	65,73,73	1.79	8 (12%)	76,113,113	1.62	16 (21%)
22	CLA	c	502	-	65,73,73	1.62	11 (16%)	76,113,113	1.51	13 (17%)
27	SQD	A	410	-	51,52,54	1.12	4 (7%)	60,63,65	2.08	16 (26%)
22	CLA	b	606	-	65,73,73	2.00	12 (18%)	76,113,113	1.56	12 (15%)
33	BCT	D	402	21	2,3,3	0.96	0	2,3,3	3.91	2 (100%)
22	CLA	C	508	-	65,73,73	1.72	10 (15%)	76,113,113	1.53	14 (18%)
25	PL9	d	407	-	55,55,55	1.58	11 (20%)	68,69,69	1.52	15 (22%)
30	BCR	k	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.44	10 (17%)
31	STE	k	104	-	11,11,19	0.92	0	11,11,19	0.87	0
31	STE	t	104	-	9,9,19	0.56	0	8,8,19	0.37	0
31	STE	x	102	-	19,19,19	0.76	0	19,19,19	0.96	2 (10%)
32	OEX	a	415	3,36,1	0,15,15	-	-	-	-	-
22	CLA	c	511	3	65,73,73	1.83	7 (10%)	76,113,113	1.59	11 (14%)
22	CLA	A	405	-	54,62,73	1.62	8 (14%)	62,99,113	1.70	12 (19%)
22	CLA	b	609	-	65,73,73	1.92	12 (18%)	76,113,113	1.50	12 (15%)
22	CLA	d	403	-	65,73,73	1.72	10 (15%)	76,113,113	1.45	7 (9%)
30	BCR	T	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	4 (7%)
31	STE	X	101	-	19,19,19	0.62	0	19,19,19	1.24	2 (10%)
29	DGD	c	515	-	63,63,67	1.31	8 (12%)	77,77,81	1.45	13 (16%)
22	CLA	d	404	36	65,73,73	1.81	8 (12%)	76,113,113	1.72	15 (19%)
27	SQD	A	412	-	38,38,54	1.09	2 (5%)	40,40,65	1.44	5 (12%)
31	STE	I	102	-	14,14,19	0.66	0	13,13,19	0.40	0
26	LMG	a	414	-	55,55,55	1.50	8 (14%)	63,63,63	1.30	7 (11%)
31	STE	J	101	-	11,11,19	0.67	0	11,11,19	1.29	1 (9%)
29	DGD	C	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.39	10 (12%)
29	DGD	A	413	-	67,67,67	1.39	10 (14%)	81,81,81	1.33	14 (17%)
26	LMG	d	410	-	44,44,55	1.18	4 (9%)	52,52,63	1.26	6 (11%)
22	CLA	B	606	36	65,73,73	1.62	12 (18%)	76,113,113	1.50	8 (10%)
30	BCR	I	101	-	41,41,41	1.19	4 (9%)	56,56,56	1.57	11 (19%)
31	STE	M	102	-	14,14,19	0.90	0	14,14,19	1.02	1 (7%)
31	STE	a	413	-	14,14,19	0.46	0	13,13,19	0.66	0
34	HEC	f	101	5,6	32,50,50	2.30	4 (12%)	24,82,82	2.39	5 (20%)
30	BCR	B	618	-	41,41,41	1.22	2 (4%)	56,56,56	1.59	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	STE	R	101	-	11,11,19	0.74	0	11,11,19	1.09	1 (9%)
26	LMG	A	409	-	48,48,55	1.16	5 (10%)	56,56,63	1.42	8 (14%)
31	STE	b	627	-	9,9,19	0.57	0	8,8,19	0.44	0
22	CLA	C	513	-	65,73,73	1.55	11 (16%)	76,113,113	1.58	13 (17%)
22	CLA	b	616	-	60,68,73	1.46	7 (11%)	70,107,113	1.64	10 (14%)
22	CLA	B	612	-	65,73,73	2.23	11 (16%)	76,113,113	1.39	11 (14%)
22	CLA	C	503	-	65,73,73	1.71	10 (15%)	76,113,113	1.82	15 (19%)
22	CLA	b	603	-	65,73,73	1.76	10 (15%)	76,113,113	1.86	16 (21%)
22	CLA	c	513	-	65,73,73	1.57	7 (10%)	76,113,113	1.38	8 (10%)
25	PL9	D	407	-	55,55,55	1.58	13 (23%)	68,69,69	1.70	17 (25%)
22	CLA	c	503	-	65,73,73	1.49	9 (13%)	76,113,113	1.42	15 (19%)
30	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.44	11 (19%)
22	CLA	D	404	36	65,73,73	1.79	10 (15%)	76,113,113	1.31	10 (13%)
31	STE	M	103	-	9,9,19	0.71	0	8,8,19	0.40	0
31	STE	b	628	-	13,13,19	0.56	0	12,12,19	0.37	0
26	LMG	M	101	-	51,51,55	1.10	4 (7%)	59,59,63	1.39	8 (13%)
31	STE	j	101	-	11,11,19	1.00	1 (9%)	11,11,19	0.73	0
22	CLA	B	601	-	65,73,73	1.75	9 (13%)	76,113,113	1.48	14 (18%)
22	CLA	b	607	36	65,73,73	1.50	12 (18%)	76,113,113	1.30	7 (9%)
27	SQD	B	621	-	53,54,54	1.02	3 (5%)	62,65,65	1.93	14 (22%)
30	BCR	C	515	-	41,41,41	1.00	2 (4%)	56,56,56	1.30	9 (16%)
22	CLA	A	402	-	65,73,73	1.56	6 (9%)	76,113,113	1.69	18 (23%)
22	CLA	c	512	-	65,73,73	1.95	13 (20%)	76,113,113	1.52	12 (15%)
28	LHG	b	623	-	48,48,48	0.93	2 (4%)	51,54,54	1.24	3 (5%)
26	LMG	c	520	-	48,48,55	1.06	5 (10%)	56,56,63	1.29	7 (12%)
31	STE	b	625	-	14,14,19	0.38	0	13,13,19	0.92	0
22	CLA	b	605	-	65,73,73	1.43	11 (16%)	76,113,113	1.64	14 (18%)
28	LHG	l	101	-	48,48,48	0.90	3 (6%)	51,54,54	1.11	2 (3%)
31	STE	C	519	-	11,11,19	0.99	0	11,11,19	1.42	2 (18%)
31	STE	c	519	-	19,19,19	0.76	1 (5%)	19,19,19	0.84	0
31	STE	B	619	-	16,16,19	0.86	1 (6%)	16,16,19	0.91	0
22	CLA	B	613	-	65,73,73	1.66	6 (9%)	76,113,113	1.26	9 (11%)
23	PHO	d	401	-	51,69,69	1.13	5 (9%)	47,99,99	1.50	7 (14%)
31	STE	B	623	-	17,17,19	0.76	0	17,17,19	0.94	0
22	CLA	C	504	36	59,67,73	1.59	9 (15%)	68,105,113	1.46	9 (13%)
22	CLA	c	504	36	60,68,73	1.57	8 (13%)	70,107,113	1.43	13 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	508	-	64,72,73	1.52	7 (10%)	74,111,113	1.40	10 (13%)
26	LMG	Y	101	-	48,48,55	1.10	7 (14%)	56,56,63	1.26	6 (10%)
22	CLA	B	608	-	65,73,73	1.49	7 (10%)	76,113,113	1.51	11 (14%)
22	CLA	b	611	-	65,73,73	1.54	9 (13%)	76,113,113	1.65	17 (22%)
22	CLA	b	614	-	65,73,73	1.78	11 (16%)	76,113,113	1.53	12 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	506	-	1/1/20/20	23/37/115/115	-
22	CLA	C	501	-	1/1/20/20	5/37/115/115	-
22	CLA	B	614	-	1/1/20/20	7/37/115/115	-
22	CLA	c	501	-	1/1/20/20	5/37/115/115	-
30	BCR	B	616	-	-	8/29/63/63	0/2/2/2
28	LHG	d	409	-	-	13/43/43/53	-
26	LMG	b	622	-	-	28/50/70/70	0/1/1/1
34	HEC	F	101	5,6	-	3/10/54/54	-
22	CLA	C	505	-	1/1/20/20	9/37/115/115	-
22	CLA	a	405	-	1/1/20/20	7/37/115/115	-
22	CLA	c	505	-	1/1/20/20	14/37/115/115	-
31	STE	b	621	-	-	10/17/17/17	-
22	CLA	B	609	36	1/1/20/20	6/37/115/115	-
22	CLA	B	604	-	1/1/20/20	12/37/115/115	-
22	CLA	C	509	-	1/1/20/20	16/37/115/115	-
22	CLA	D	403	-	1/1/20/20	6/37/115/115	-
30	BCR	D	406	-	-	8/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/20/20	8/37/115/115	-
22	CLA	C	511	3	1/1/20/20	7/37/115/115	-
30	BCR	b	618	-	-	5/29/63/63	0/2/2/2
30	BCR	H	102	-	-	11/29/63/63	0/2/2/2
22	CLA	b	615	-	1/1/20/20	13/37/115/115	-
30	BCR	K	101	-	-	12/29/63/63	0/2/2/2
27	SQD	t	102	-	-	12/37/37/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	d	411	-	-	9/14/14/17	-
22	CLA	C	510	-	1/1/20/20	14/37/115/115	-
22	CLA	c	510	-	1/1/20/20	13/37/115/115	-
30	BCR	k	103	-	-	7/29/63/63	0/2/2/2
30	BCR	a	406	-	-	2/29/63/63	0/2/2/2
22	CLA	a	403	36	-	10/37/115/115	-
25	PL9	A	408	-	-	21/53/73/73	0/1/1/1
34	HEC	V	201	17	-	2/10/54/54	-
22	CLA	b	601	36	1/1/20/20	22/37/115/115	-
30	BCR	K	102	-	-	13/29/63/63	0/2/2/2
22	CLA	C	507	36	1/1/20/20	6/37/115/115	-
31	STE	C	520	-	-	4/13/13/17	-
22	CLA	b	608	-	1/1/20/20	7/37/115/115	-
23	PHO	D	401	-	-	5/37/103/103	0/5/6/6
31	STE	L	103	-	-	5/9/9/17	-
22	CLA	A	403	36	-	10/37/115/115	-
23	PHO	A	404	-	-	6/37/103/103	0/5/6/6
28	LHG	a	411	-	-	26/46/46/53	-
22	CLA	C	512	-	1/1/20/20	9/37/115/115	-
31	STE	B	624	-	-	7/13/13/17	-
22	CLA	B	607	-	1/1/20/20	8/37/115/115	-
27	SQD	D	409	-	-	14/28/48/69	0/1/1/1
22	CLA	H	101	36	1/1/20/20	20/37/115/115	-
30	BCR	b	619	-	-	3/29/63/63	0/2/2/2
27	SQD	L	101	-	-	24/44/64/69	0/1/1/1
23	PHO	a	404	-	-	3/37/103/103	0/5/6/6
26	LMG	D	412	-	-	19/33/33/70	-
31	STE	C	521	-	-	2/9/9/17	-
30	BCR	C	514	-	-	8/29/63/63	0/2/2/2
31	STE	Z	101	-	-	4/5/5/17	-
31	STE	b	626	-	-	9/17/17/17	-
22	CLA	b	612	-	1/1/20/20	7/37/115/115	-
25	PL9	a	409	-	-	26/53/73/73	0/1/1/1
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	A	411	-	-	23/53/53/53	-
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2
26	LMG	c	521	-	-	24/44/64/70	0/1/1/1
34	HEC	v	201	17	-	2/10/54/54	-
26	LMG	B	620	-	-	8/22/22/70	-
22	CLA	B	615	-	1/1/19/20	9/31/109/115	-
22	CLA	b	613	-	1/1/20/20	10/37/115/115	-
22	CLA	b	602	-	1/1/20/20	10/37/115/115	-
30	BCR	k	102	-	-	14/29/63/63	0/2/2/2
31	STE	b	629	-	-	6/17/17/17	-
22	CLA	a	402	-	-	1/37/115/115	-
22	CLA	B	602	-	1/1/20/20	12/37/115/115	-
26	LMG	c	518	-	-	12/31/51/70	0/1/1/1
31	STE	b	620	-	-	6/13/13/17	-
22	CLA	B	605	-	1/1/20/20	10/37/115/115	-
22	CLA	C	502	-	1/1/20/20	11/37/115/115	-
22	CLA	c	507	36	1/1/20/20	11/37/115/115	-
31	STE	B	625	-	-	4/9/9/17	-
29	DGD	C	518	-	-	15/51/91/95	0/2/2/2
31	STE	b	624	-	-	10/13/13/17	-
22	CLA	b	610	36	1/1/20/20	7/37/115/115	-
22	CLA	B	611	-	1/1/20/20	8/37/115/115	-
26	LMG	m	101	-	-	17/46/66/70	0/1/1/1
29	DGD	c	517	-	-	14/51/91/95	0/2/2/2
28	LHG	L	102	-	-	25/53/53/53	-
29	DGD	h	101	-	-	17/51/91/95	0/2/2/2
28	LHG	D	410	-	-	23/53/53/53	-
22	CLA	B	610	-	-	6/37/115/115	-
22	CLA	b	604	-	1/1/20/20	12/37/115/115	-
30	BCR	d	406	-	-	8/29/63/63	0/2/2/2
22	CLA	d	405	-	1/1/20/20	7/37/115/115	-
26	LMG	D	408	-	-	17/46/66/70	0/1/1/1
30	BCR	x	101	-	-	7/29/63/63	0/2/2/2
31	STE	M	104	-	-	9/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	405	-	-	12/37/115/115	-
30	BCR	c	514	-	-	7/29/63/63	0/2/2/2
22	CLA	B	603	-	1/1/20/20	14/37/115/115	-
31	STE	t	103	-	-	5/11/11/17	-
28	LHG	D	413	-	-	19/53/53/53	-
30	BCR	b	617	-	-	13/29/63/63	0/2/2/2
31	STE	a	412	-	-	4/9/9/17	-
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
29	DGD	c	516	-	-	18/51/91/95	0/2/2/2
31	STE	B	622	-	-	5/9/9/17	-
27	SQD	a	410	-	-	22/49/69/69	0/1/1/1
28	LHG	D	411	-	-	21/51/51/53	-
28	LHG	d	408	-	-	22/53/53/53	-
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	c	506	-	1/1/20/20	14/37/115/115	-
22	CLA	c	502	-	1/1/20/20	13/37/115/115	-
27	SQD	A	410	-	-	23/47/67/69	0/1/1/1
22	CLA	b	606	-	1/1/20/20	8/37/115/115	-
22	CLA	C	508	-	-	11/37/115/115	-
25	PL9	d	407	-	-	18/53/73/73	0/1/1/1
30	BCR	k	101	-	-	10/29/63/63	0/2/2/2
31	STE	k	104	-	-	5/9/9/17	-
31	STE	t	104	-	-	3/7/7/17	-
31	STE	x	102	-	-	11/17/17/17	-
22	CLA	c	511	3	1/1/20/20	9/37/115/115	-
22	CLA	A	405	-	1/1/17/20	3/24/102/115	-
22	CLA	b	609	-	1/1/20/20	8/37/115/115	-
22	CLA	d	403	-	1/1/20/20	9/37/115/115	-
30	BCR	T	101	-	-	11/29/63/63	0/2/2/2
31	STE	X	101	-	-	10/17/17/17	-
29	DGD	c	515	-	-	22/51/91/95	0/2/2/2
22	CLA	d	404	36	1/1/20/20	3/37/115/115	-
27	SQD	A	412	-	-	19/39/39/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	I	102	-	-	5/12/12/17	-
26	LMG	a	414	-	-	31/50/70/70	0/1/1/1
31	STE	J	101	-	-	5/9/9/17	-
29	DGD	C	517	-	-	22/51/91/95	0/2/2/2
29	DGD	A	413	-	-	28/55/95/95	0/2/2/2
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
22	CLA	B	606	36	1/1/20/20	18/37/115/115	-
30	BCR	I	101	-	-	7/29/63/63	0/2/2/2
31	STE	M	102	-	-	6/12/12/17	-
31	STE	a	413	-	-	9/12/12/17	-
34	HEC	f	101	5,6	-	2/10/54/54	-
30	BCR	B	618	-	-	9/29/63/63	0/2/2/2
31	STE	R	101	-	-	5/9/9/17	-
26	LMG	A	409	-	-	15/43/63/70	0/1/1/1
31	STE	b	627	-	-	5/7/7/17	-
22	CLA	C	513	-	1/1/20/20	7/37/115/115	-
22	CLA	b	616	-	1/1/19/20	6/31/109/115	-
22	CLA	B	612	-	1/1/20/20	12/37/115/115	-
22	CLA	C	503	-	1/1/20/20	5/37/115/115	-
22	CLA	b	603	-	1/1/20/20	8/37/115/115	-
22	CLA	c	513	-	1/1/20/20	10/37/115/115	-
25	PL9	D	407	-	-	14/53/73/73	0/1/1/1
22	CLA	c	503	-	-	10/37/115/115	-
30	BCR	B	617	-	-	10/29/63/63	0/2/2/2
22	CLA	D	404	36	1/1/20/20	10/37/115/115	-
31	STE	M	103	-	-	2/7/7/17	-
31	STE	b	628	-	-	7/11/11/17	-
26	LMG	M	101	-	-	17/46/66/70	0/1/1/1
31	STE	j	101	-	-	4/9/9/17	-
22	CLA	B	601	-	-	10/37/115/115	-
22	CLA	b	607	36	1/1/20/20	16/37/115/115	-
27	SQD	B	621	-	-	27/49/69/69	0/1/1/1
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
22	CLA	A	402	-	1/1/20/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	512	-	1/1/20/20	20/37/115/115	-
28	LHG	b	623	-	-	26/53/53/53	-
26	LMG	c	520	-	-	20/43/63/70	0/1/1/1
31	STE	b	625	-	-	7/12/12/17	-
22	CLA	b	605	-	1/1/20/20	13/37/115/115	-
28	LHG	l	101	-	-	18/53/53/53	-
31	STE	C	519	-	-	5/9/9/17	-
31	STE	c	519	-	-	7/17/17/17	-
31	STE	B	619	-	-	6/14/14/17	-
22	CLA	B	613	-	1/1/20/20	16/37/115/115	-
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
31	STE	B	623	-	-	11/15/15/17	-
22	CLA	C	504	36	1/1/18/20	6/30/108/115	-
22	CLA	c	504	36	1/1/19/20	7/31/109/115	-
22	CLA	c	508	-	-	13/36/114/115	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
22	CLA	B	608	-	-	7/37/115/115	-
22	CLA	b	611	-	-	9/37/115/115	-
22	CLA	b	614	-	1/1/20/20	20/37/115/115	-

The worst 5 of 984 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	MG-ND	-12.14	1.81	2.05
22	A	403	CLA	C4B-NB	11.07	1.45	1.35
22	b	615	CLA	MG-ND	-10.89	1.84	2.05
22	B	613	CLA	C4B-NB	9.31	1.43	1.35
22	B	605	CLA	MG-NA	9.19	2.28	2.06

The worst 5 of 1446 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	C4A-NA-C1A	10.34	111.35	106.71
27	L	101	SQD	O6-C1-C2	10.31	124.40	108.30
22	C	503	CLA	C4A-NA-C1A	9.87	111.14	106.71
22	C	511	CLA	C4A-NA-C1A	9.09	110.79	106.71
22	H	101	CLA	C4A-NA-C1A	9.03	110.76	106.71

5 of 59 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND

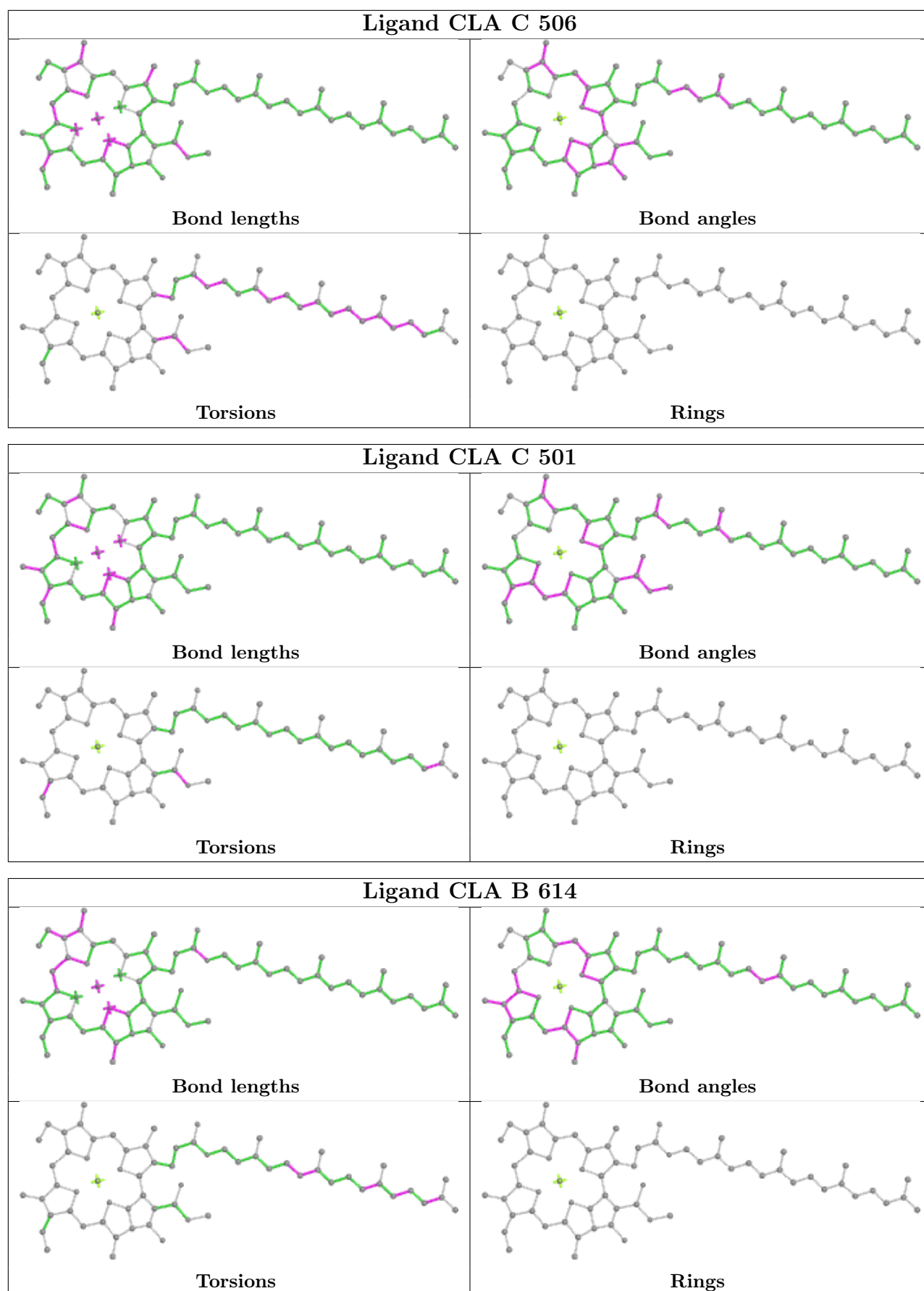
5 of 2018 torsion outliers are listed below:

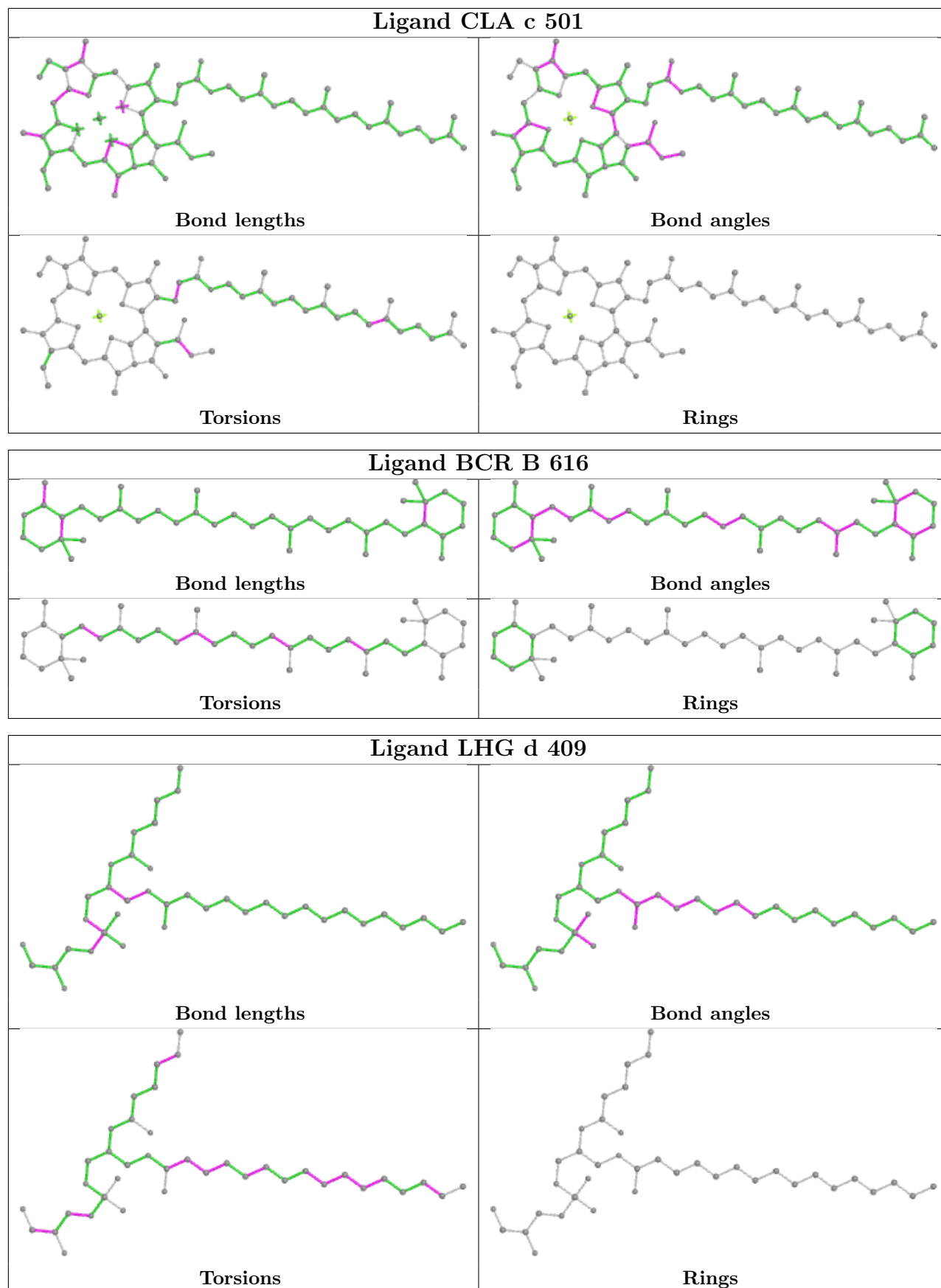
Mol	Chain	Res	Type	Atoms
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	C2-C3-C5-C6
22	B	602	CLA	C4-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6

There are no ring outliers.

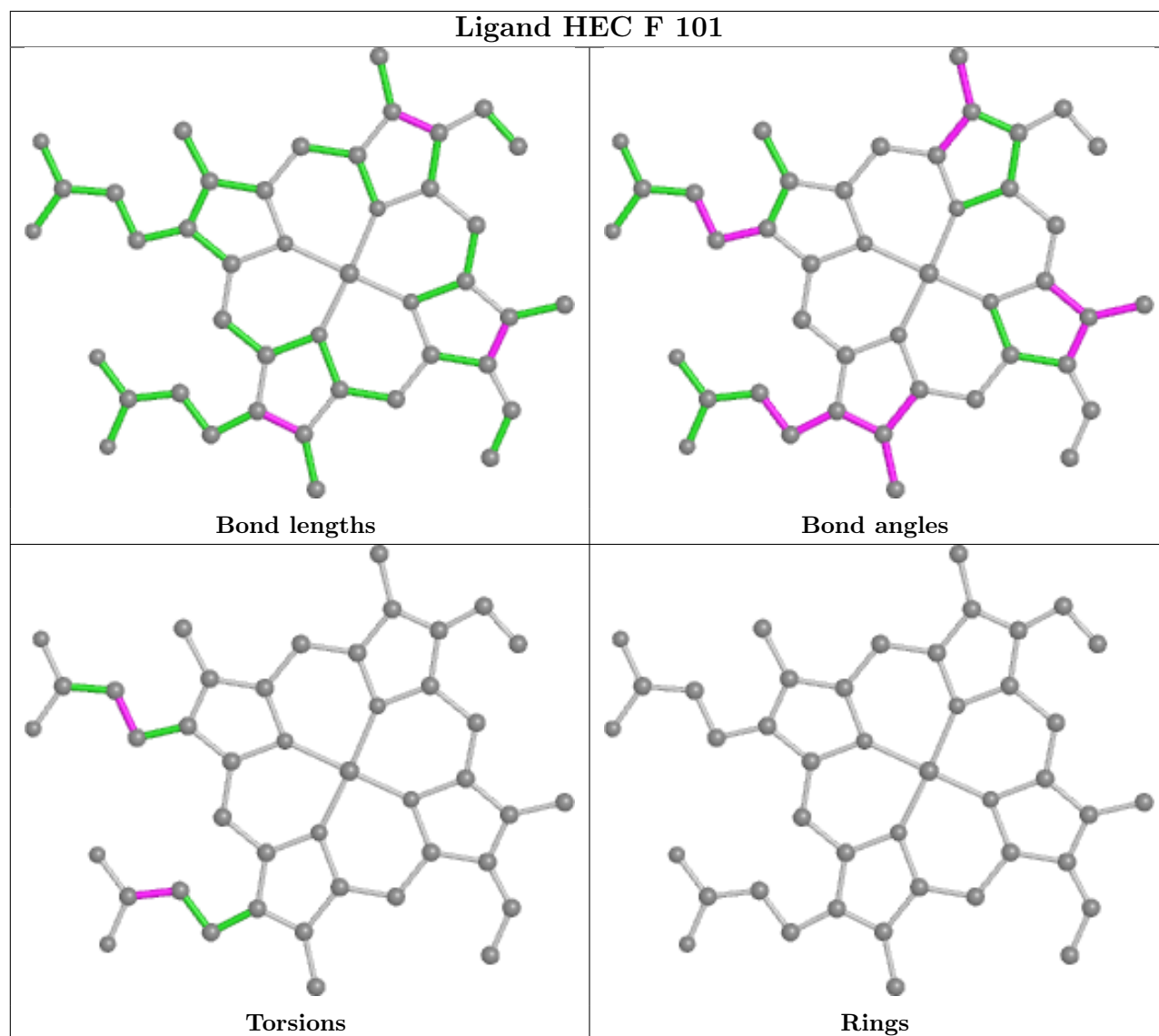
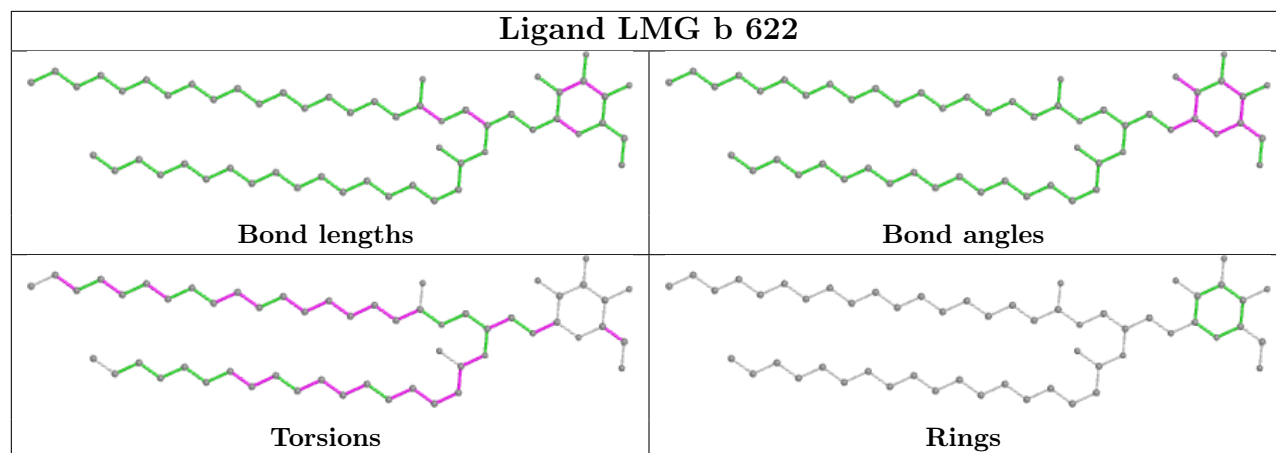
No monomer is involved in short contacts.

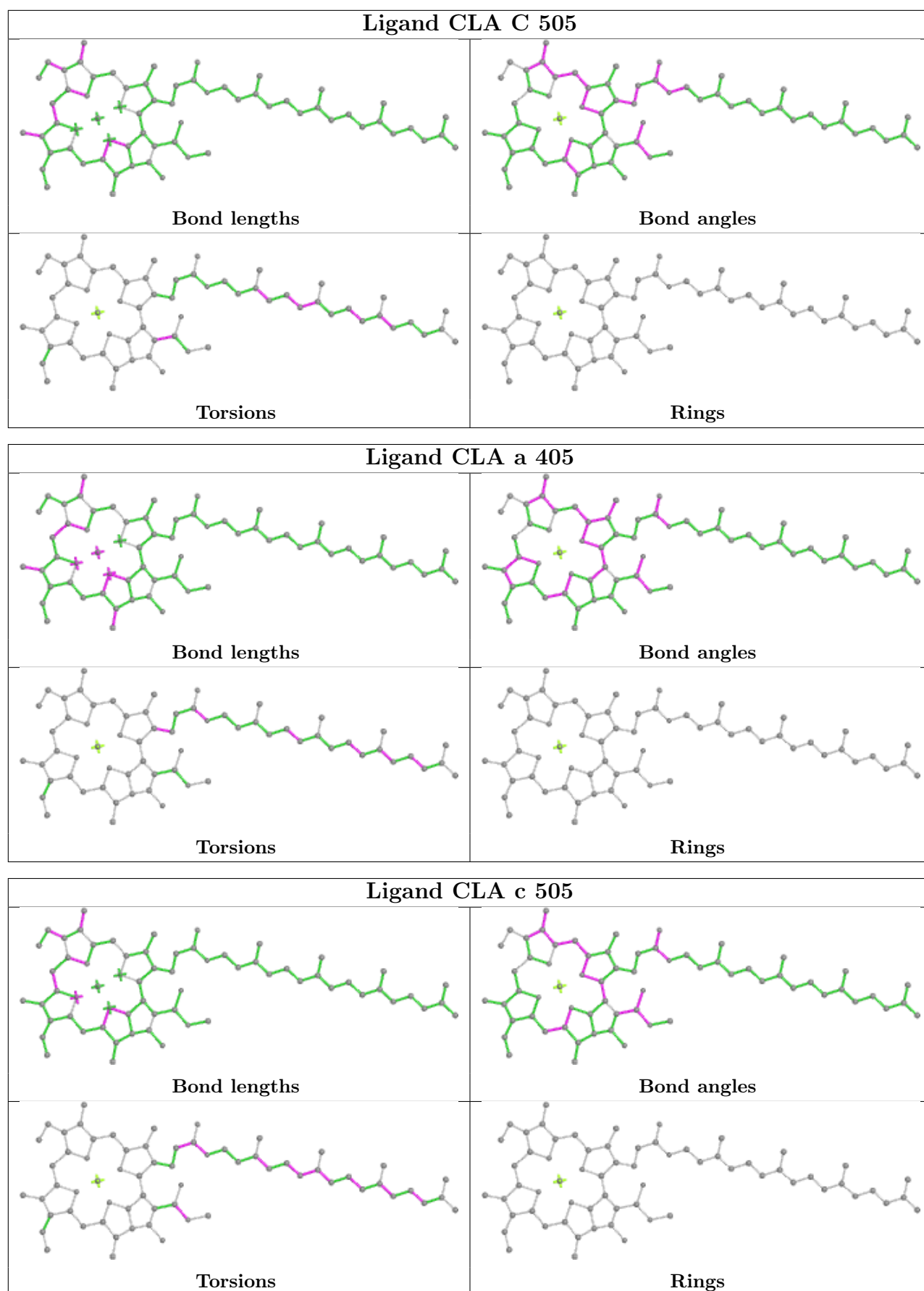
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

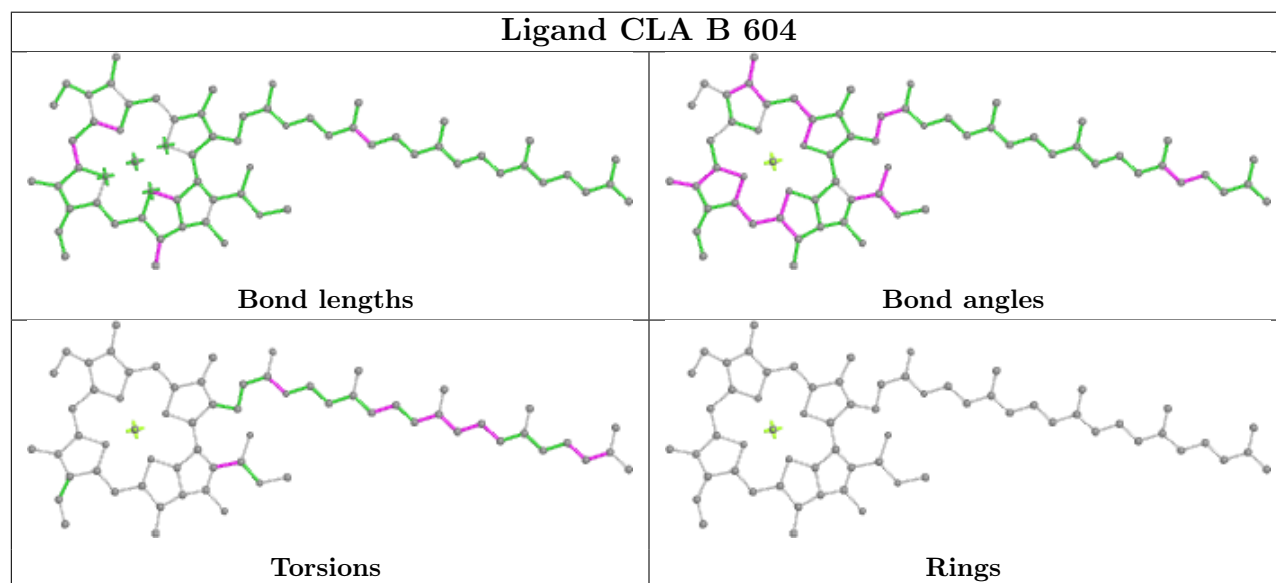
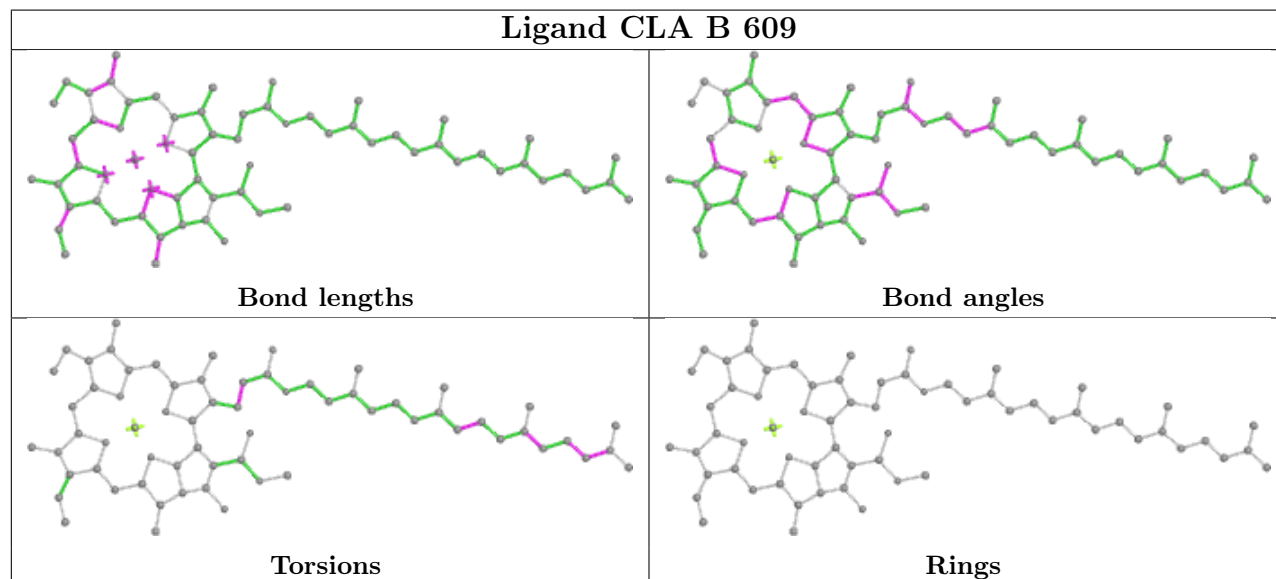
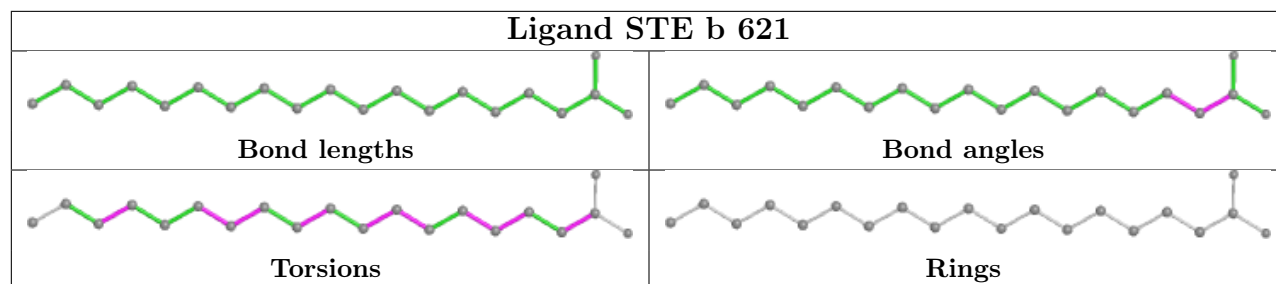


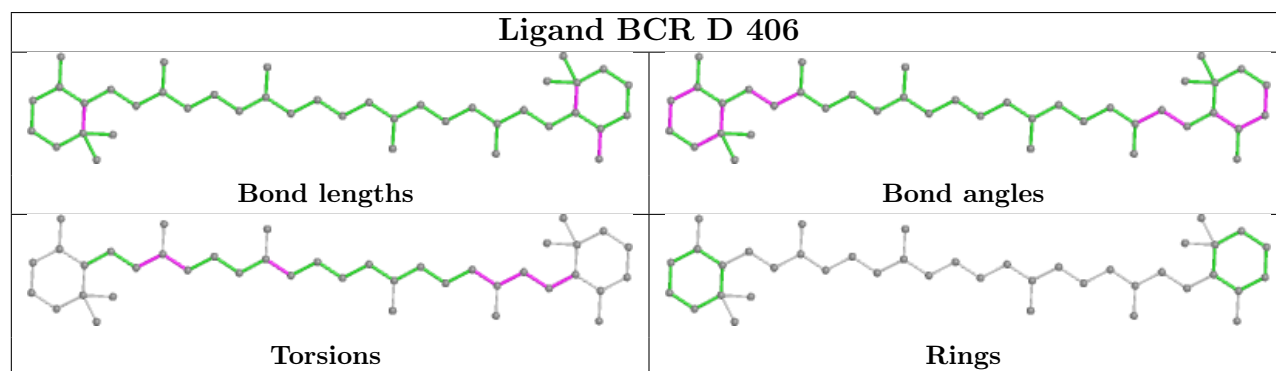
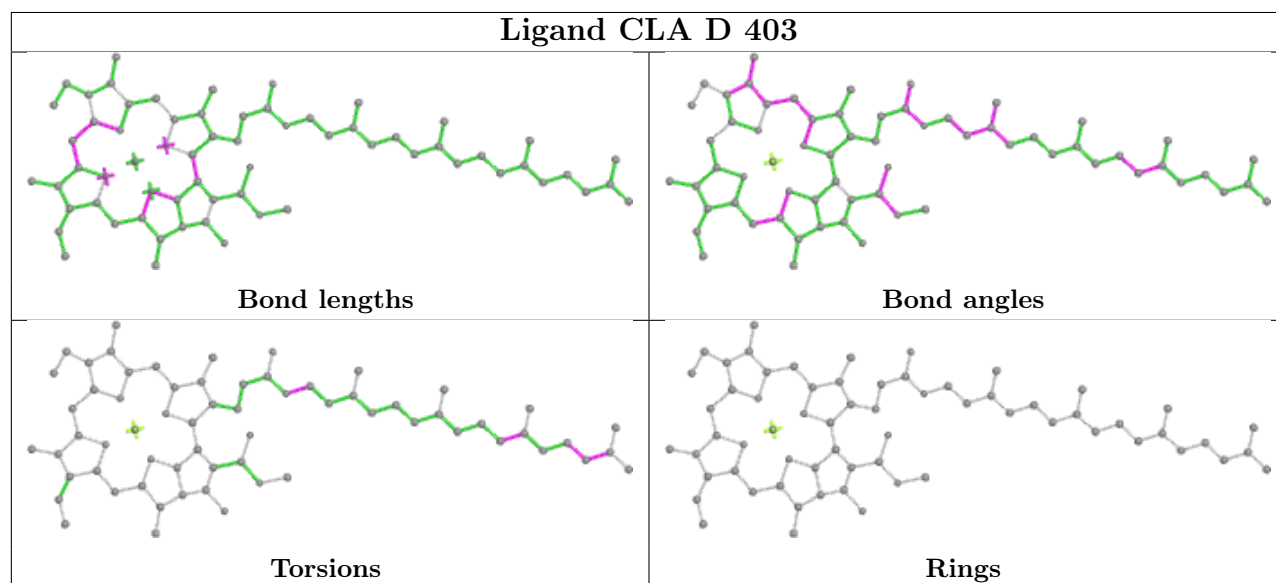
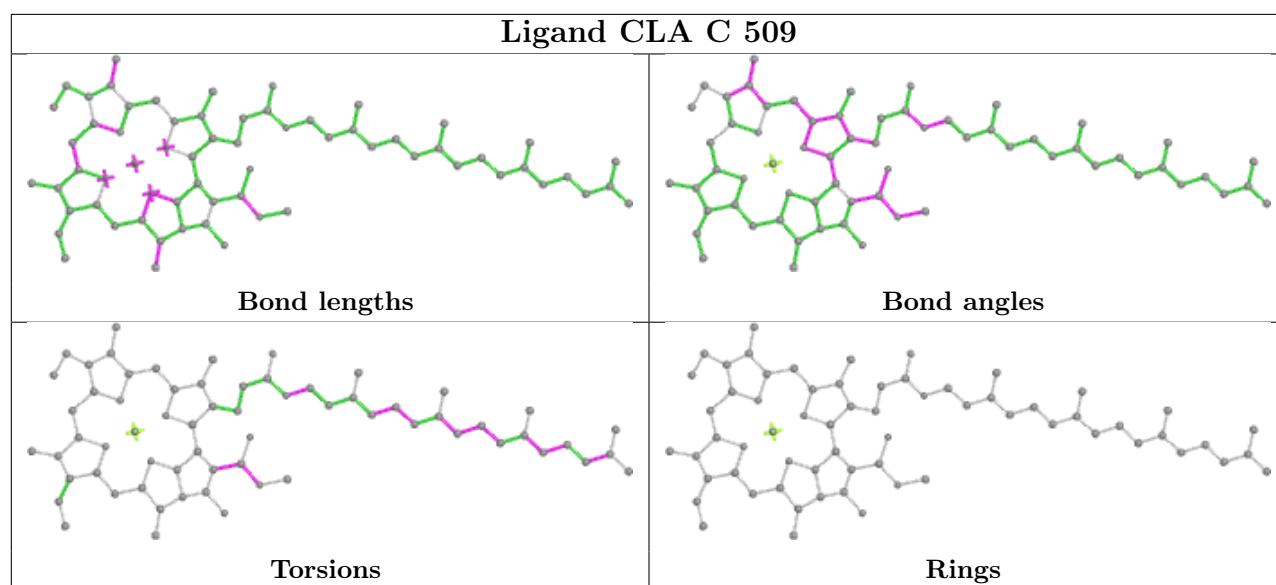


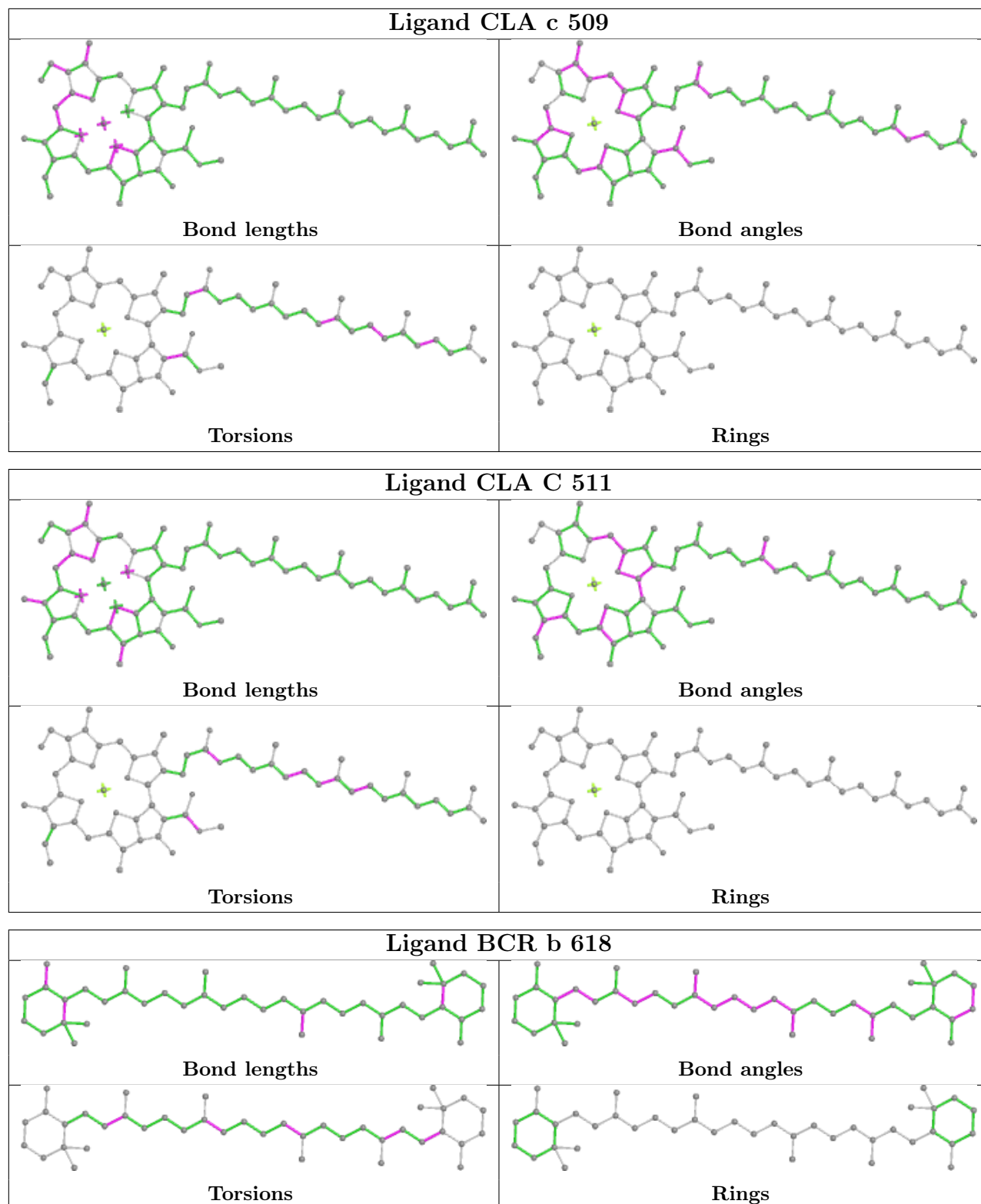


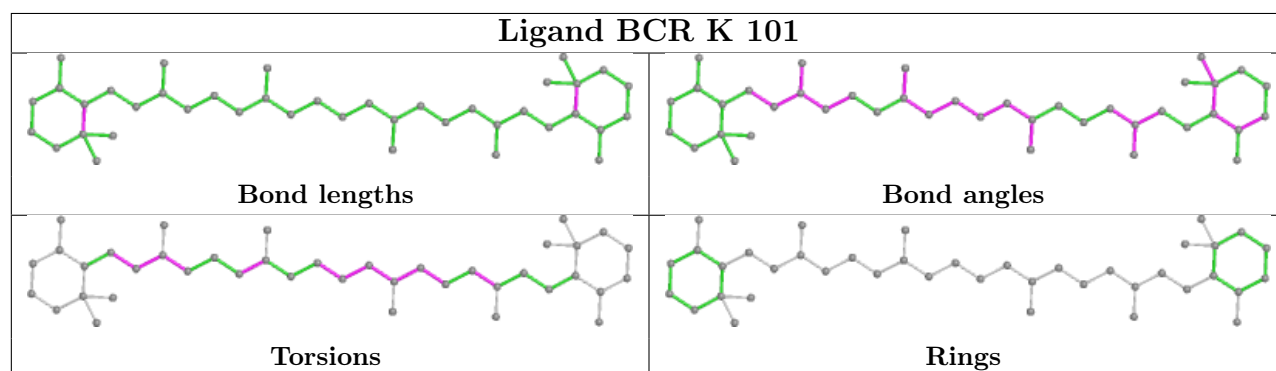
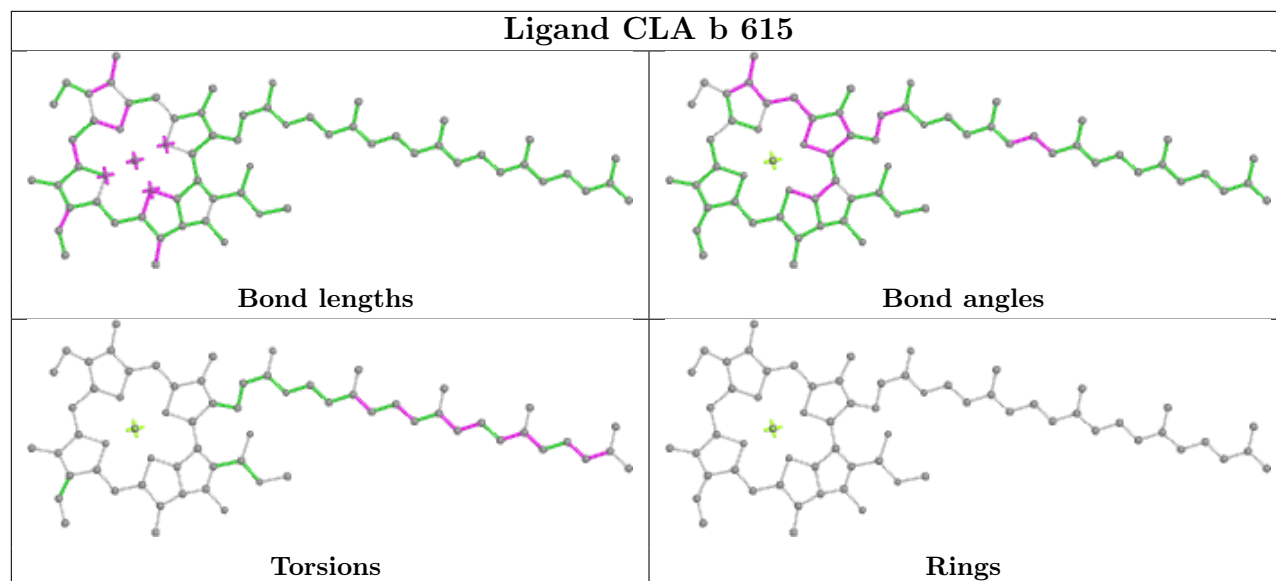
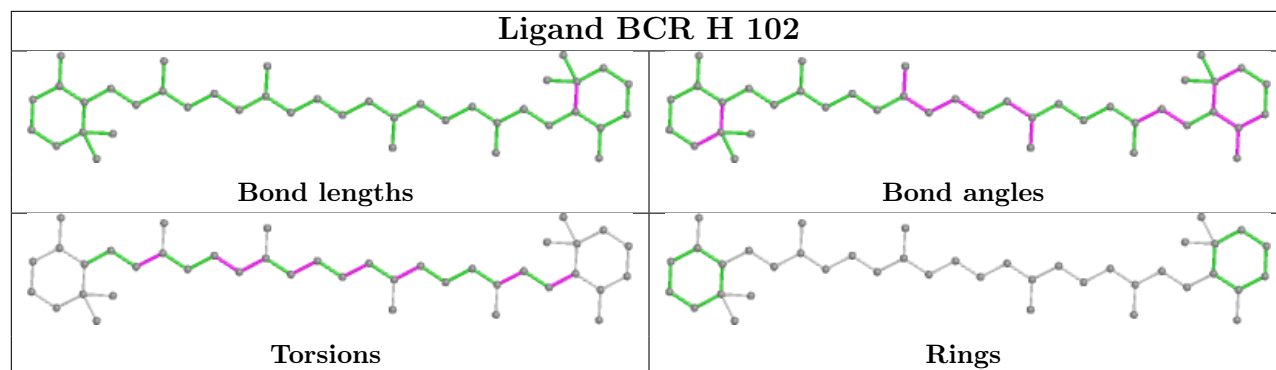


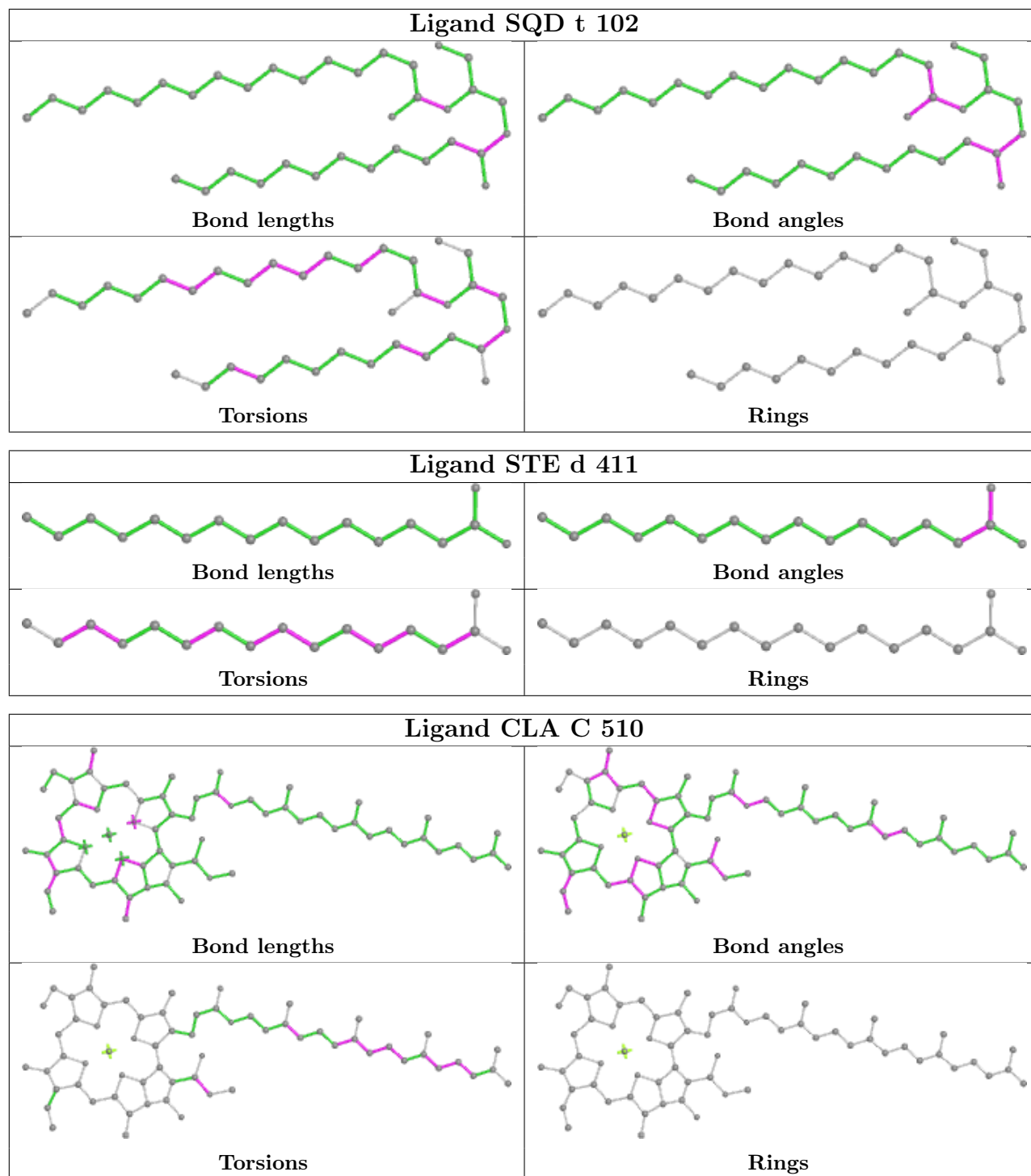


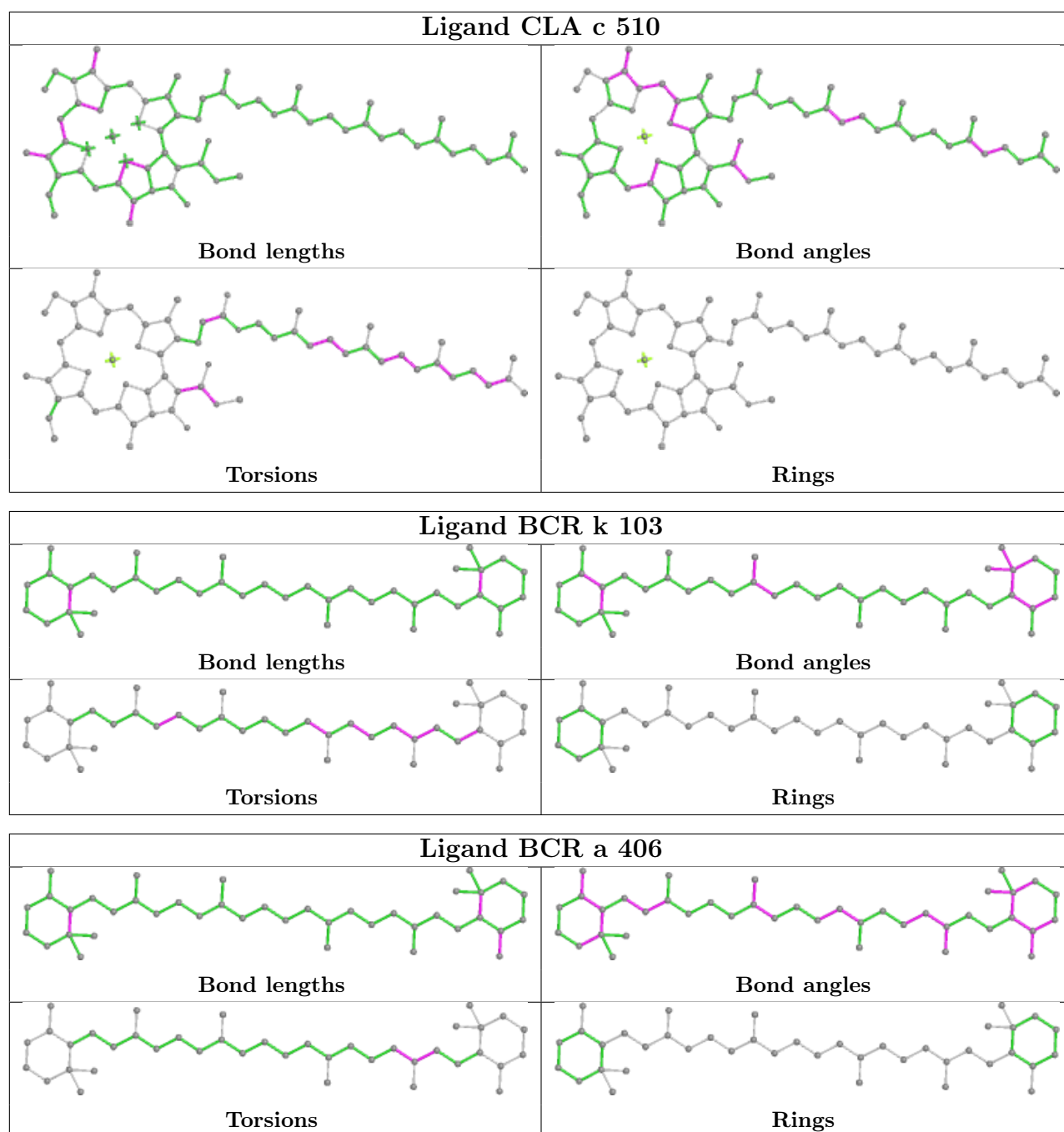




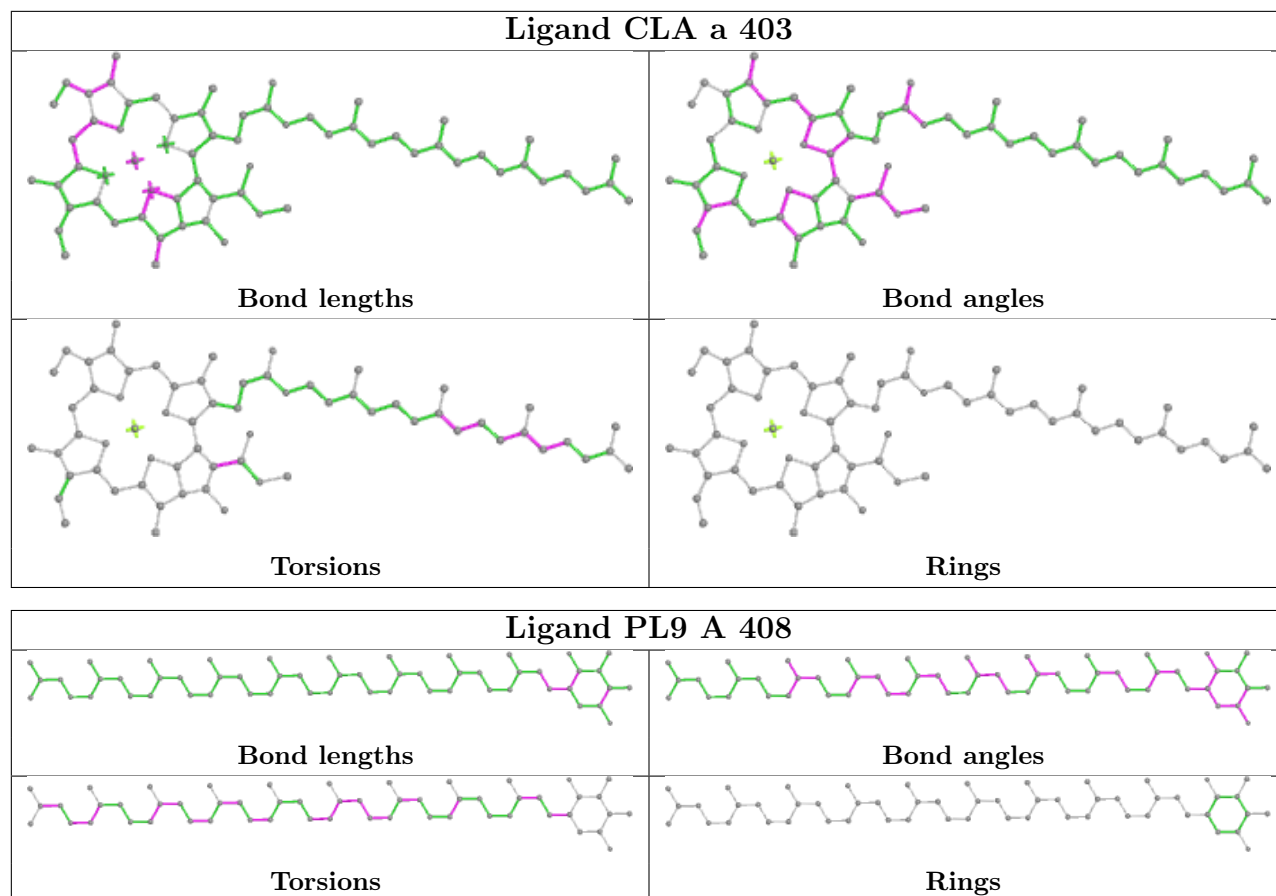


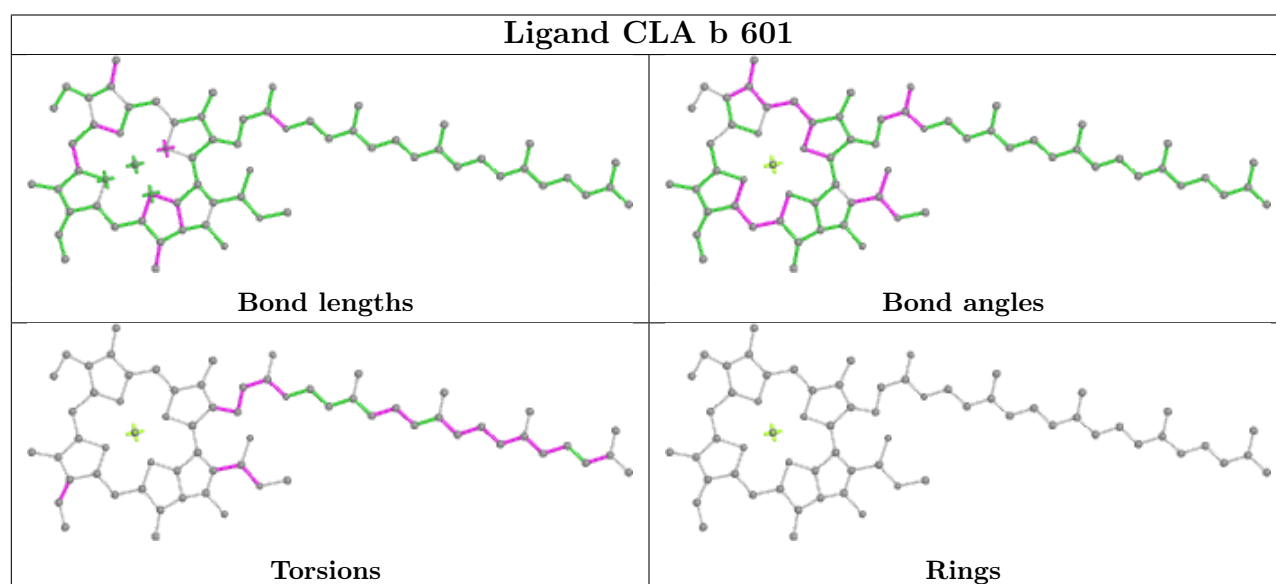
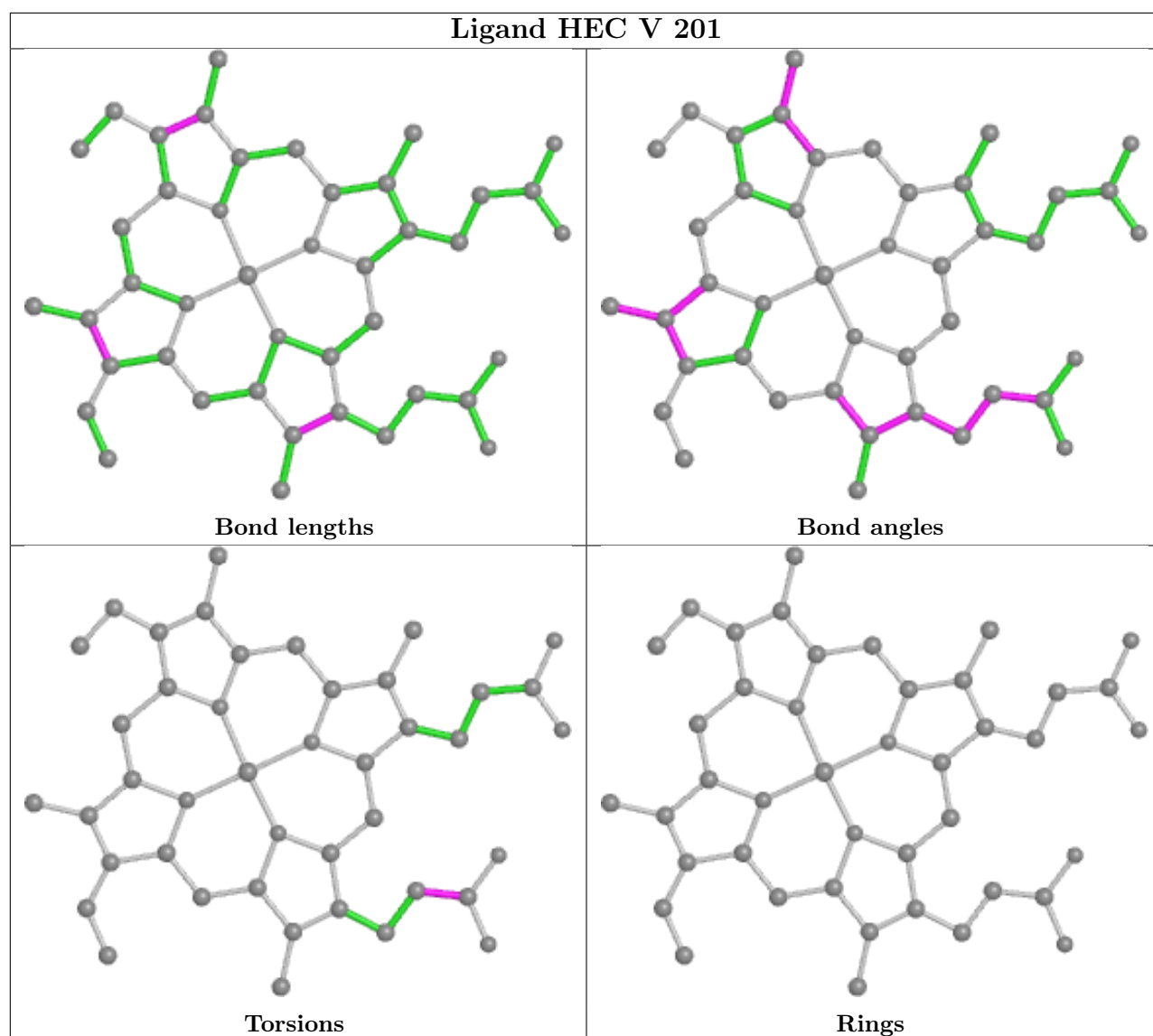


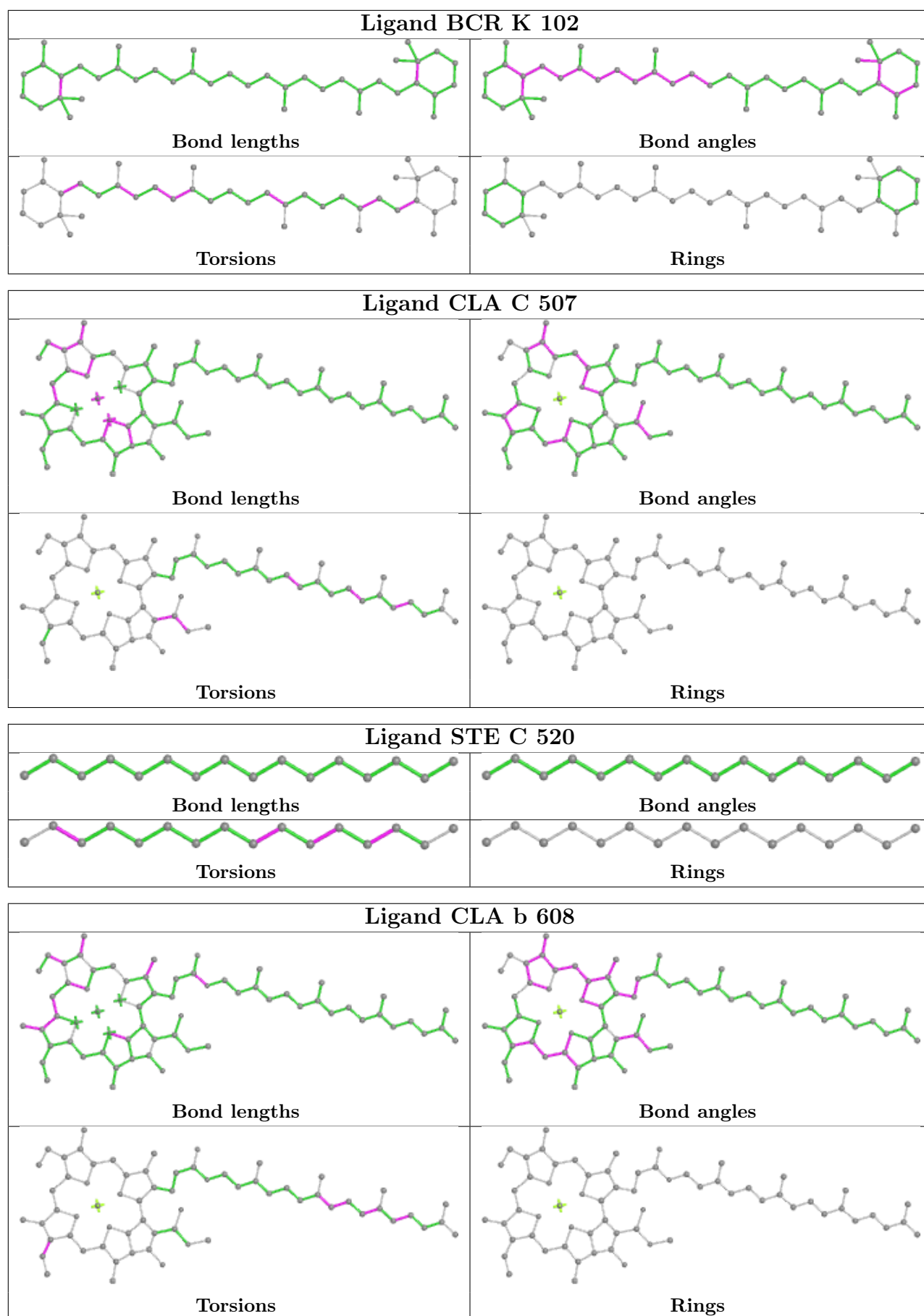


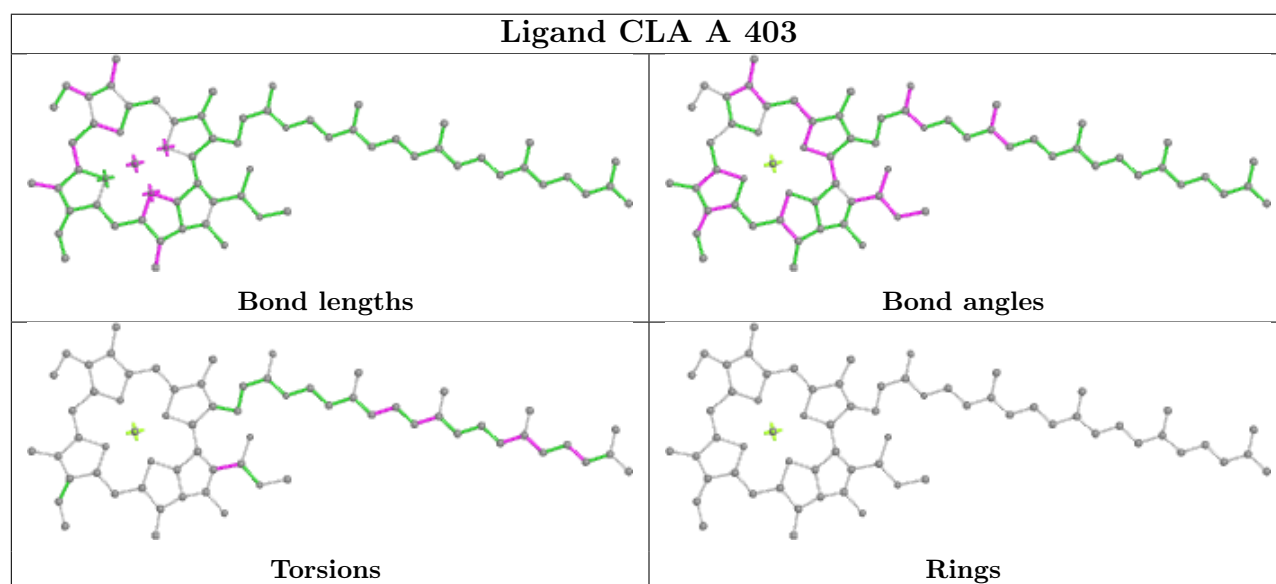
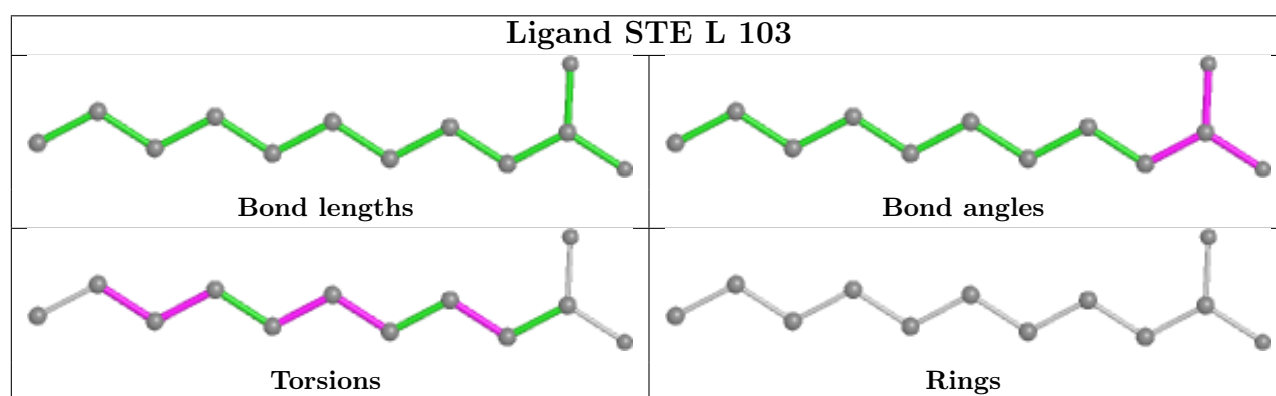
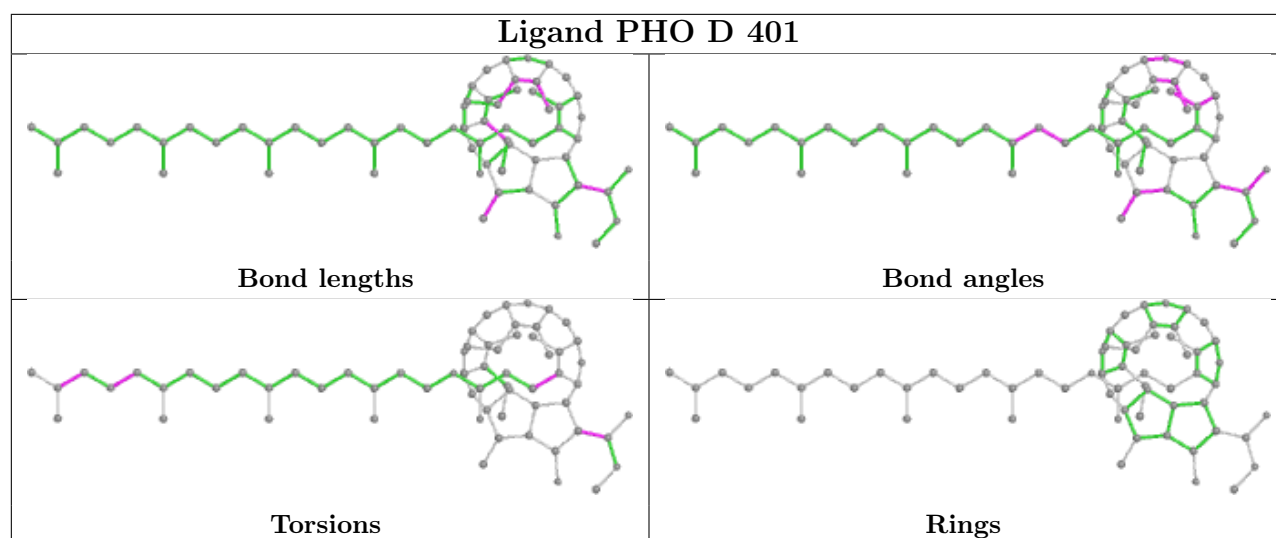


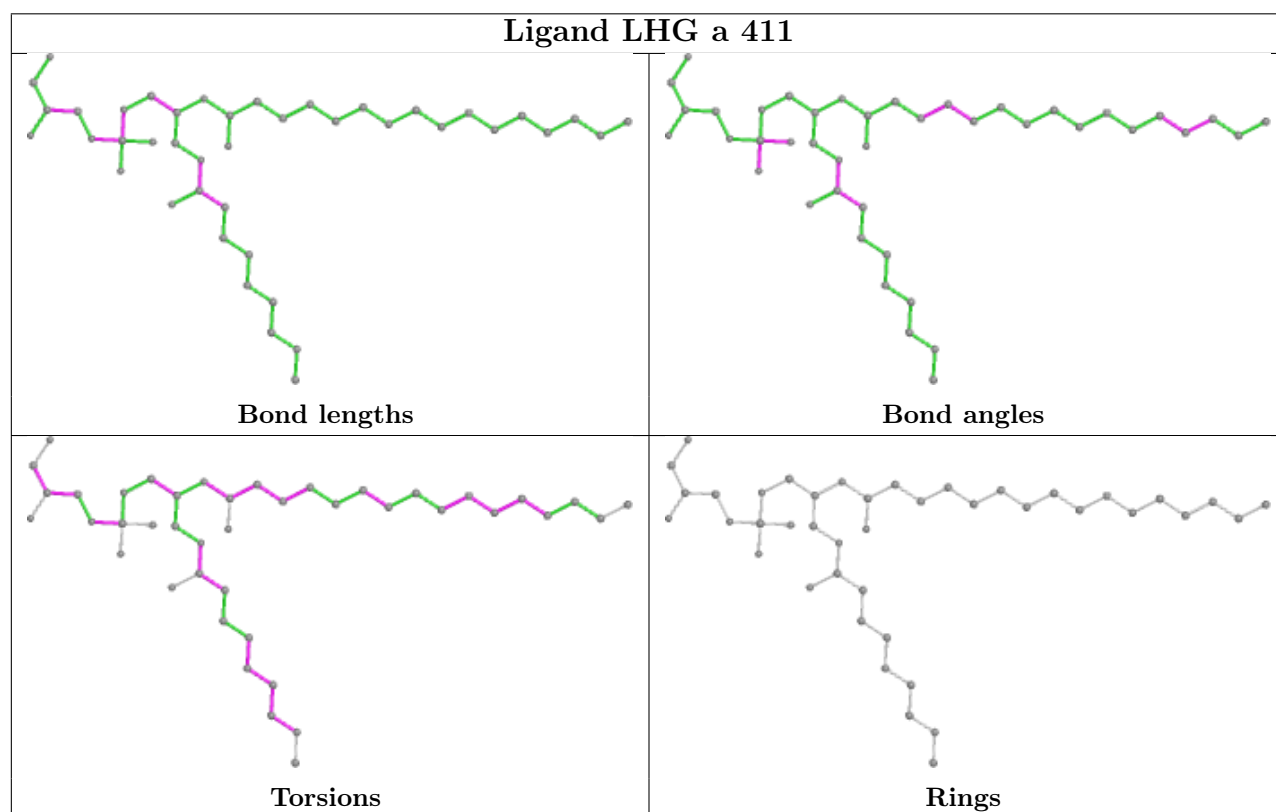
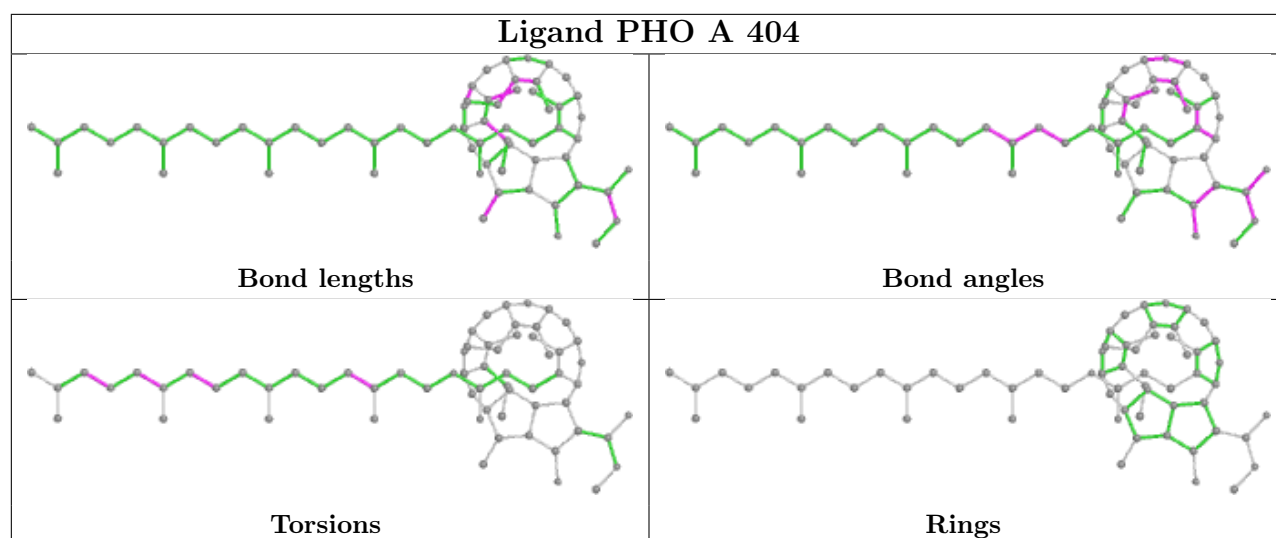


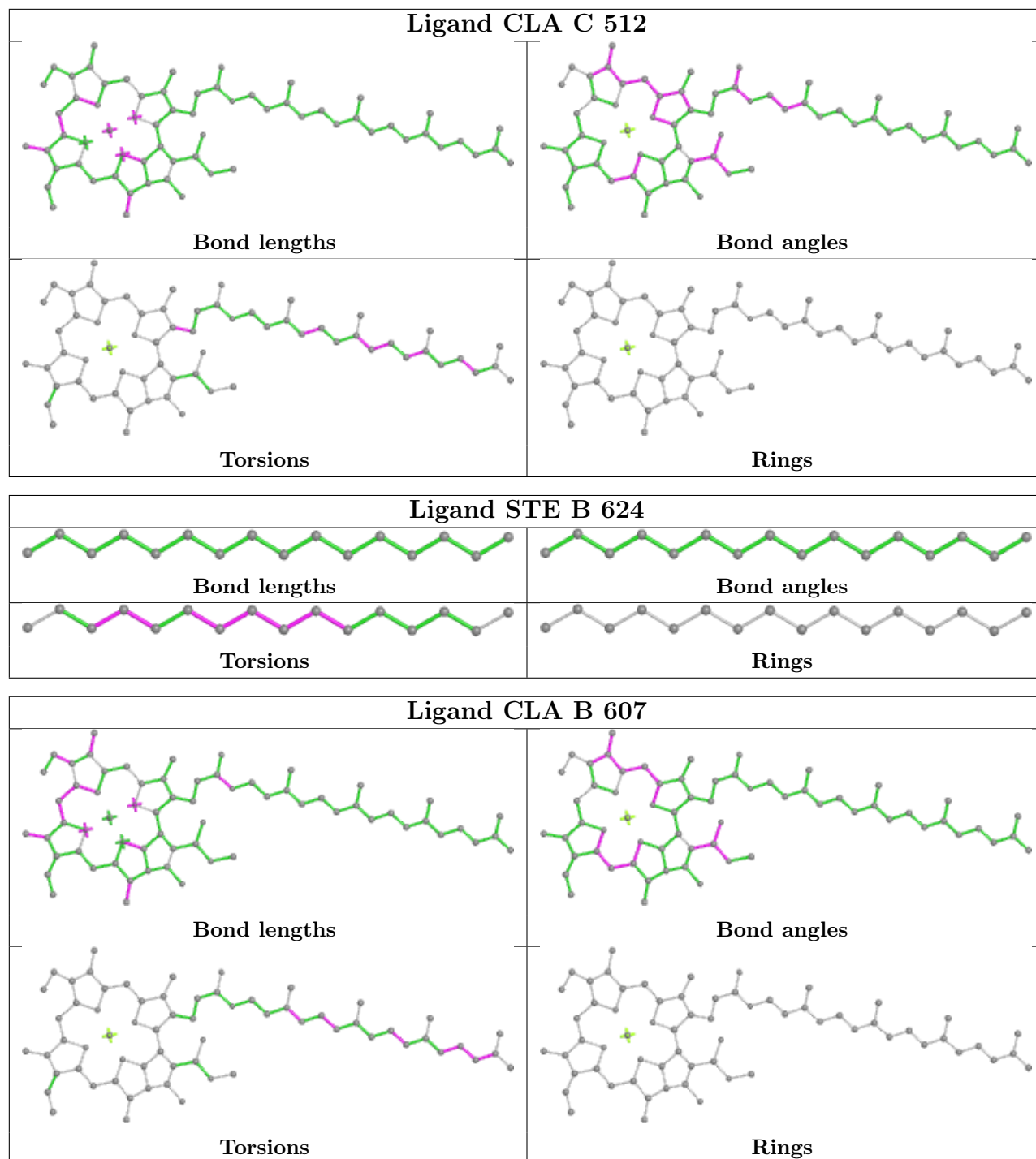


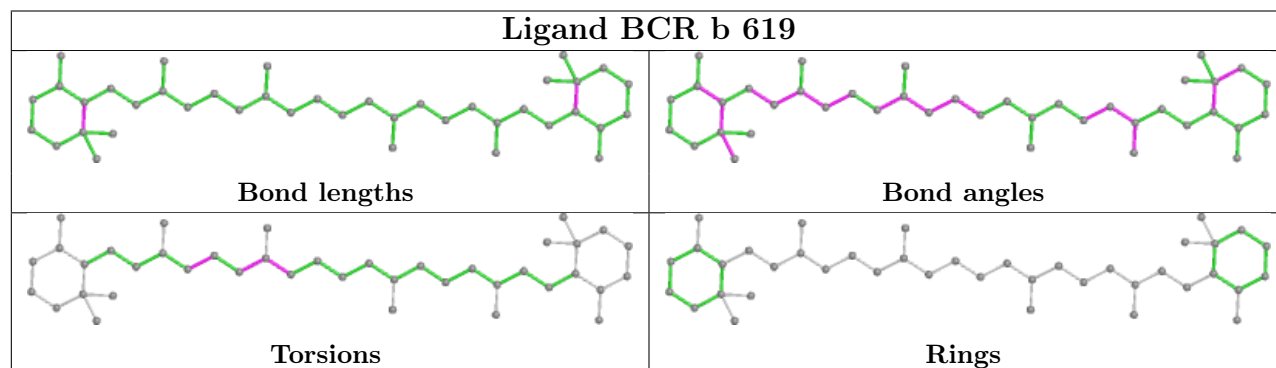
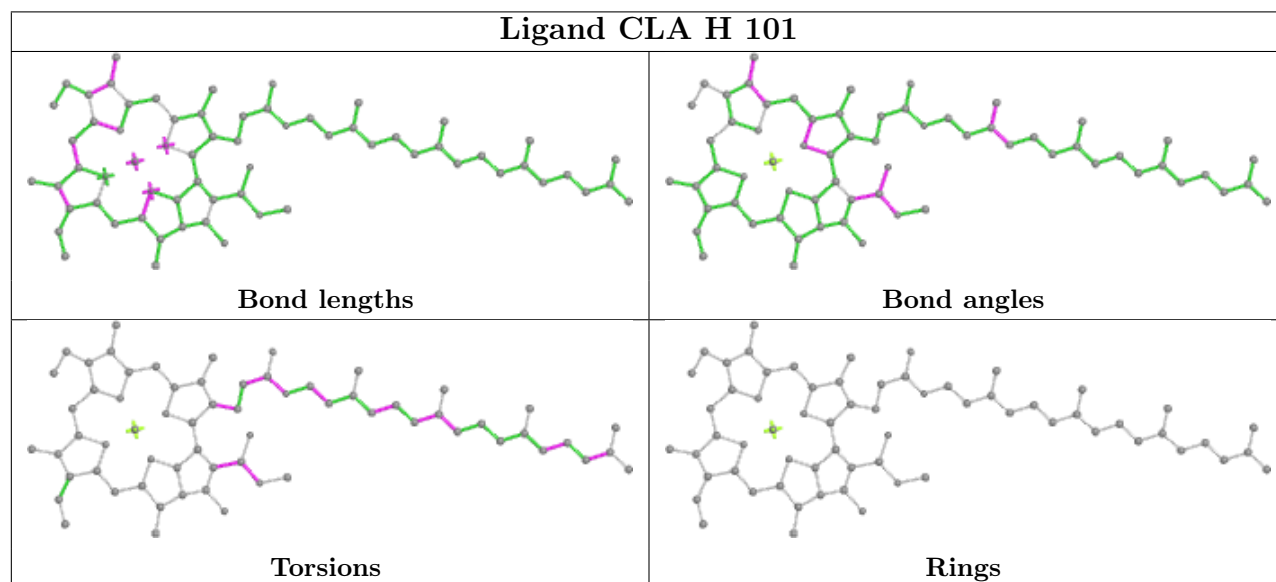
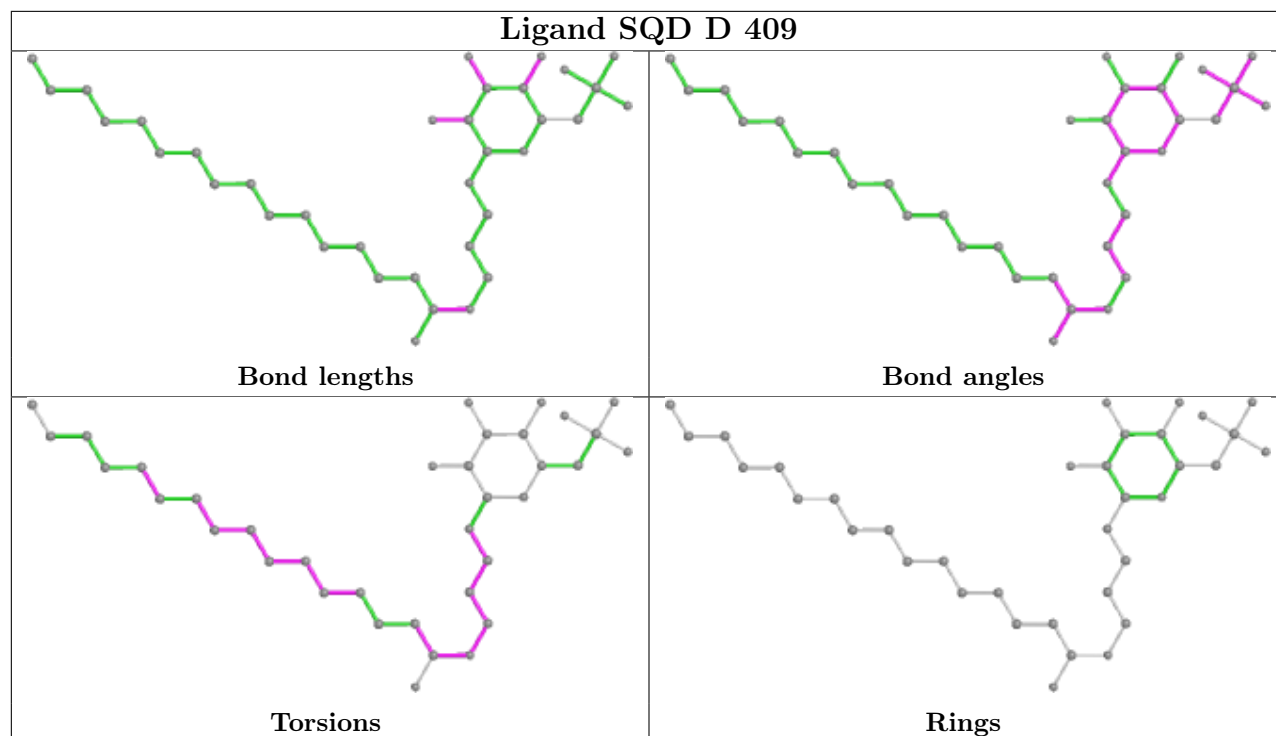


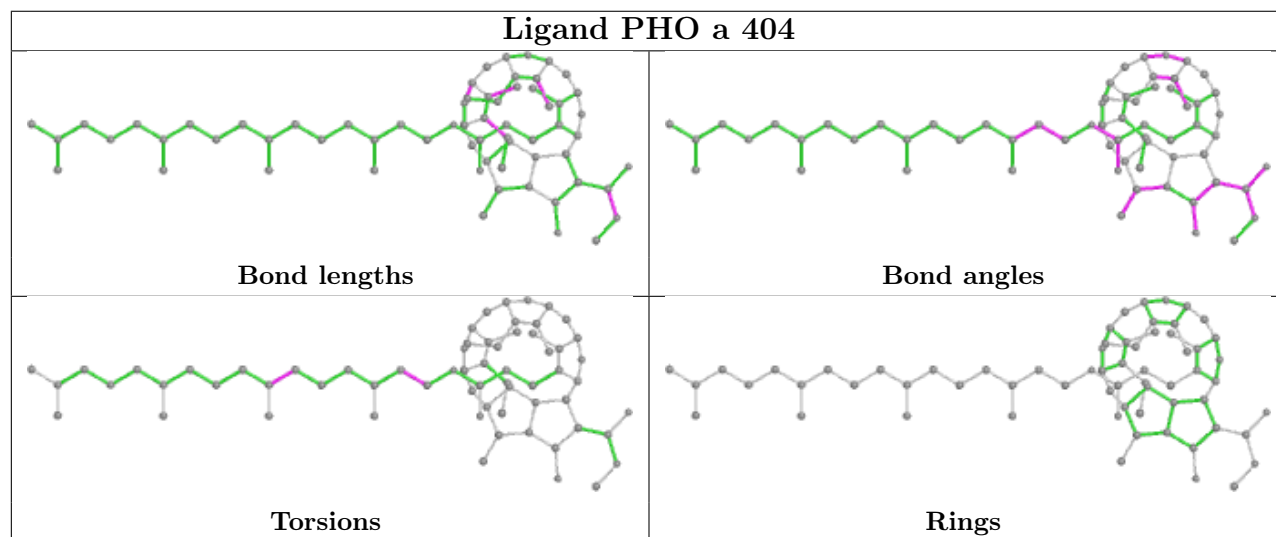
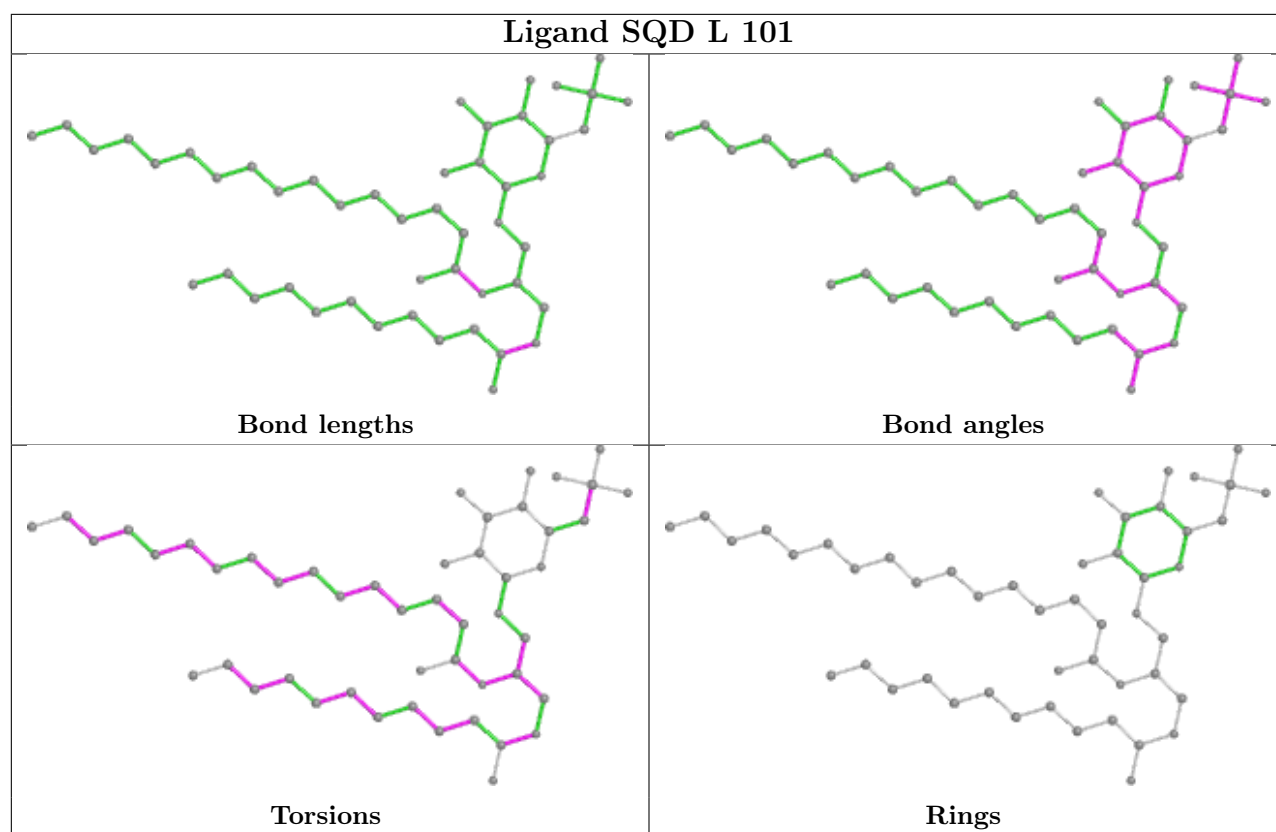




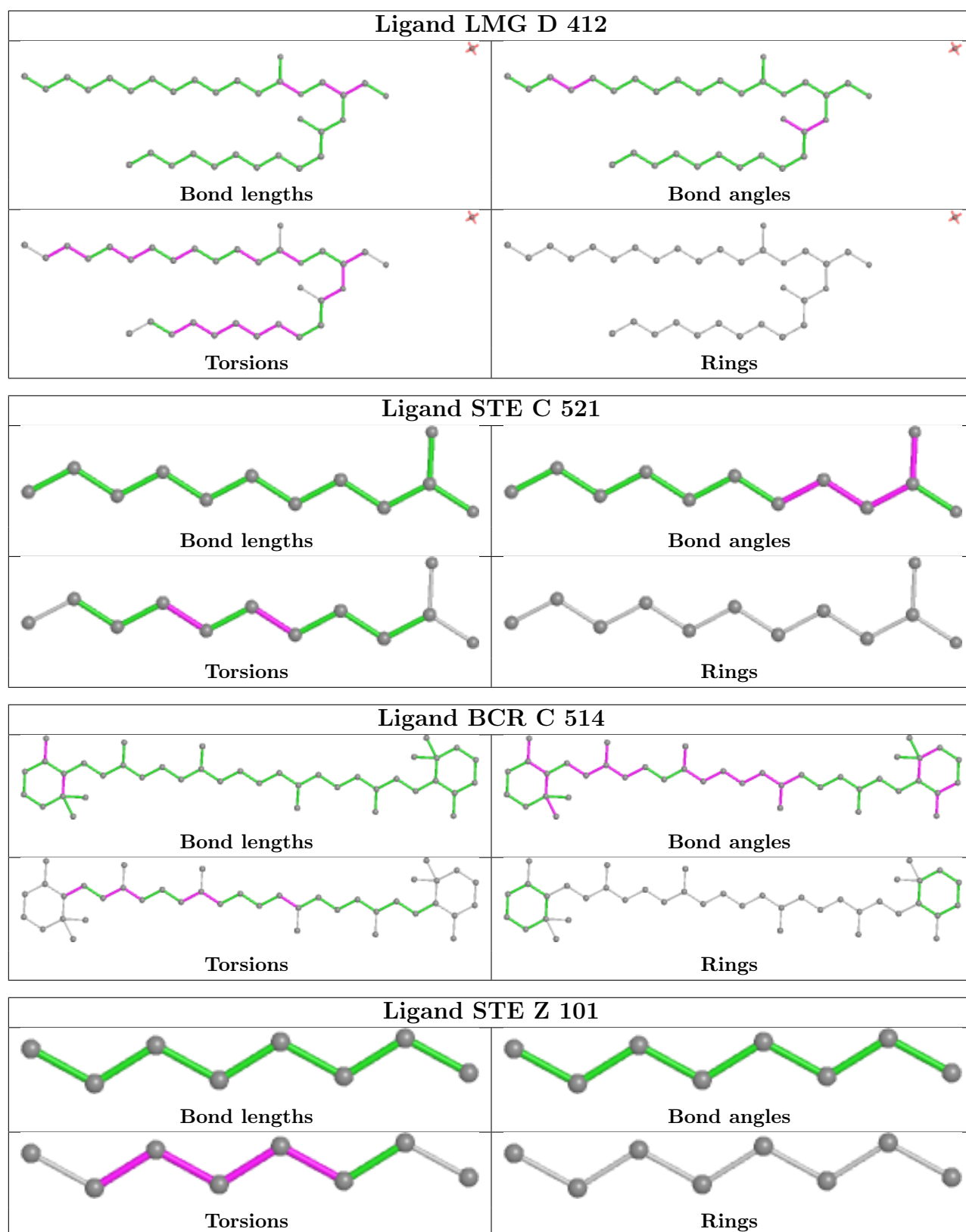


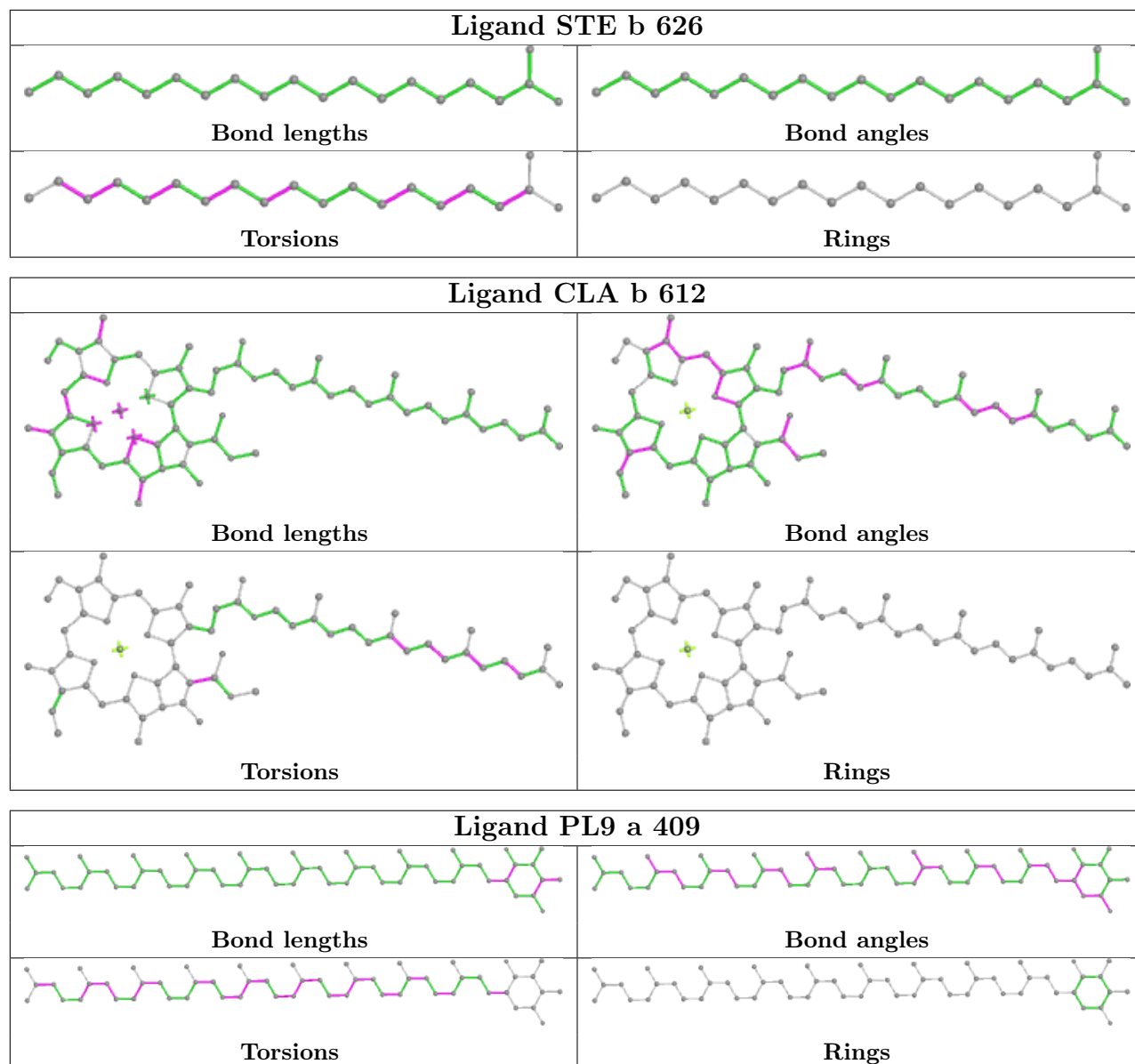


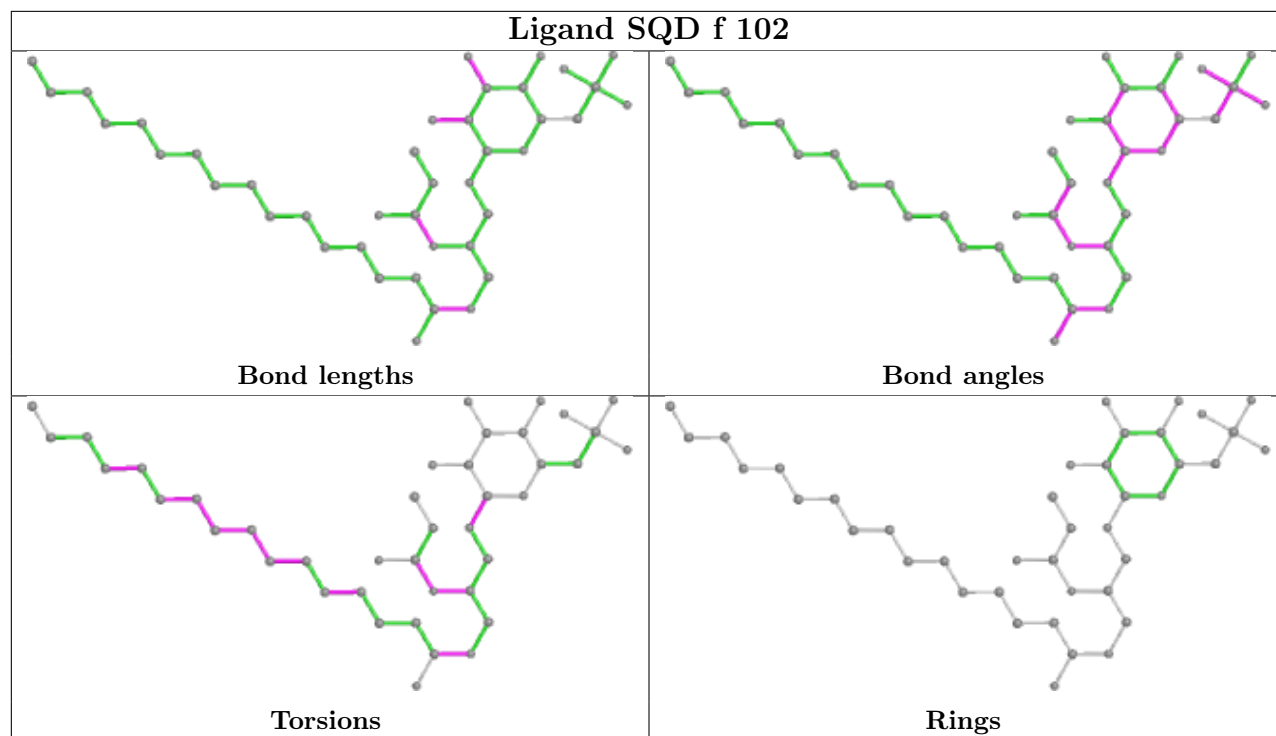


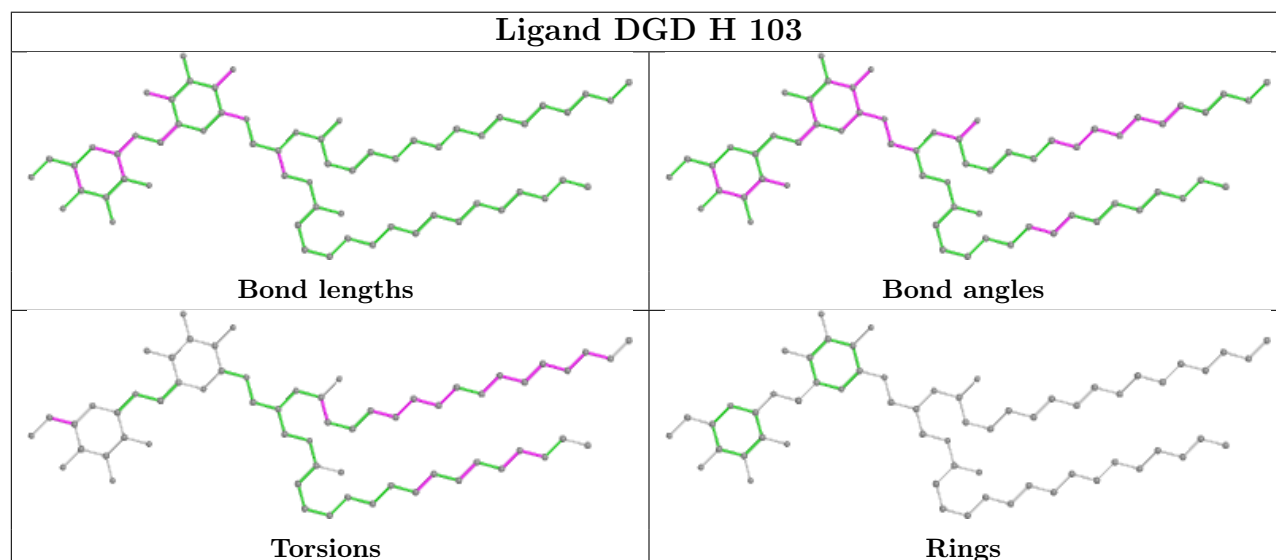
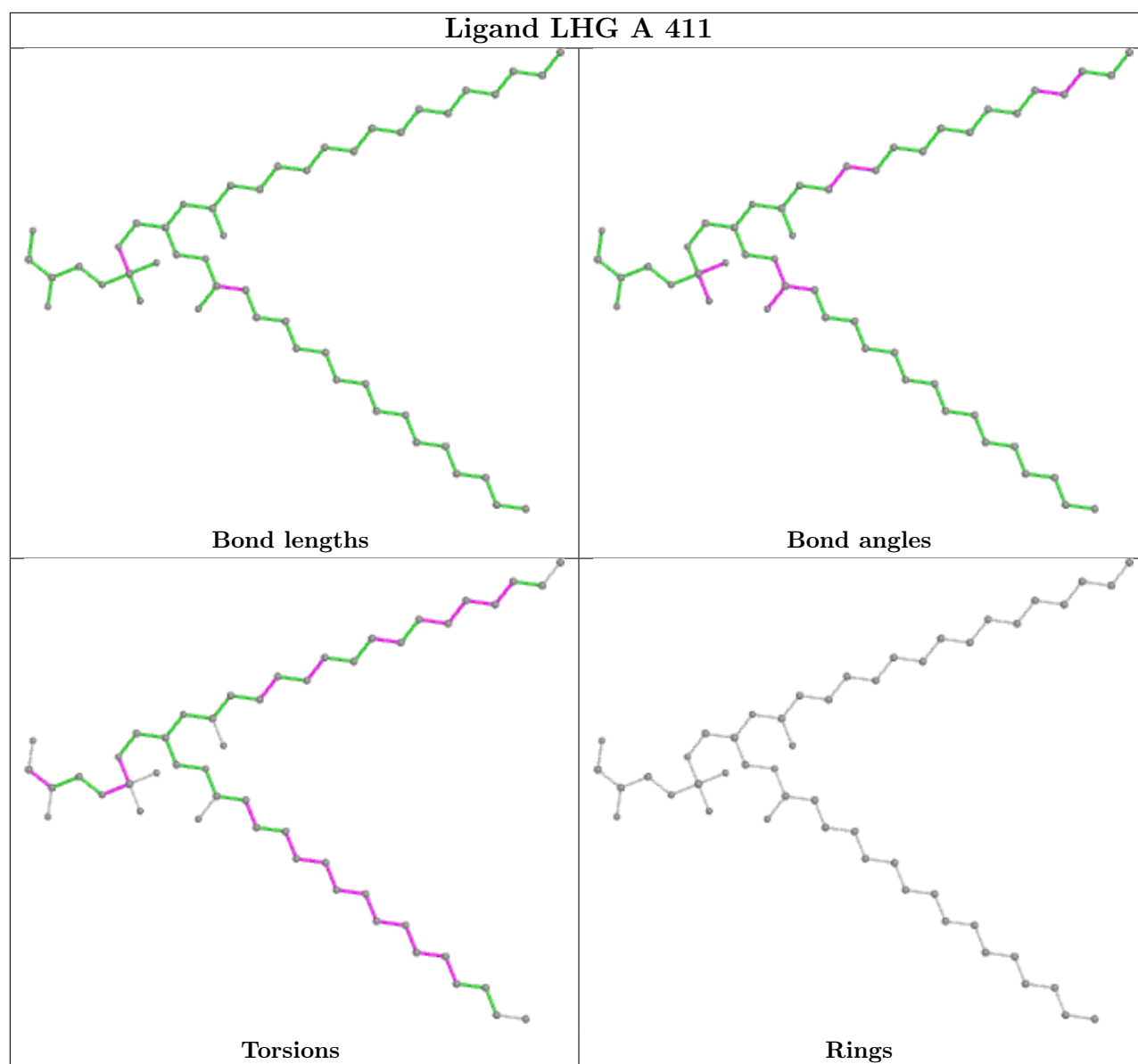


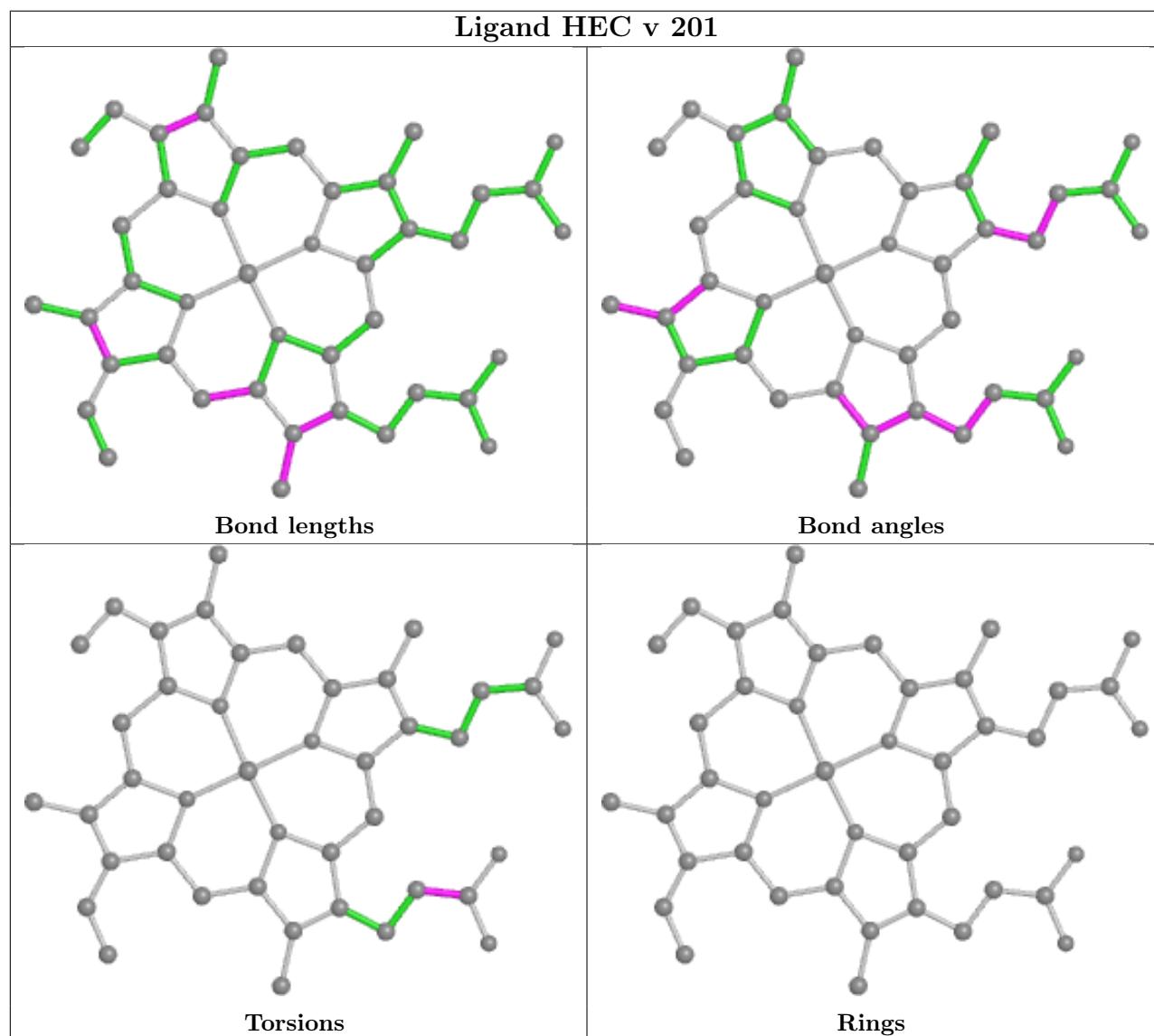
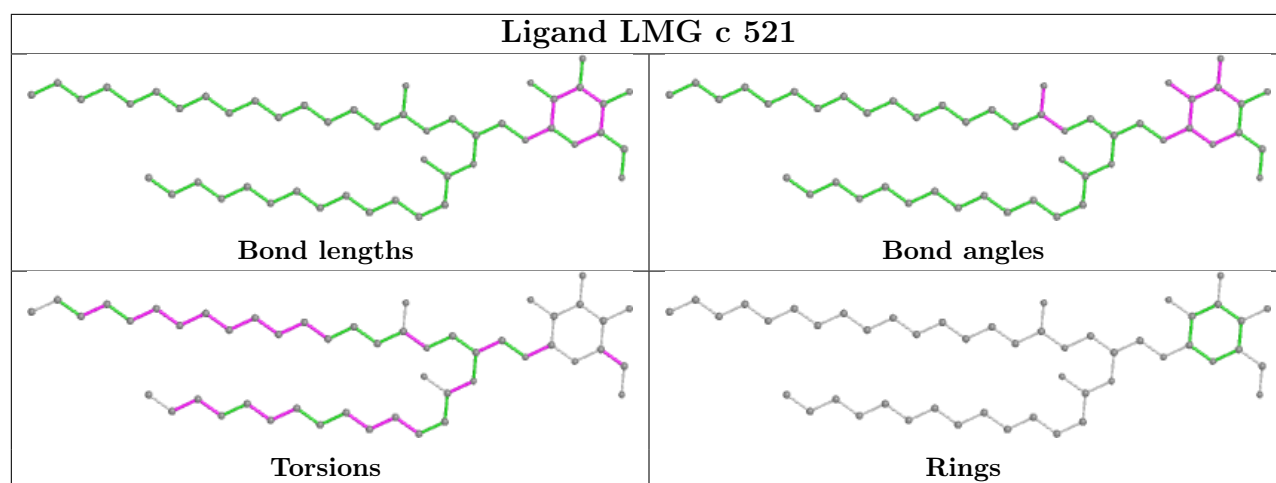


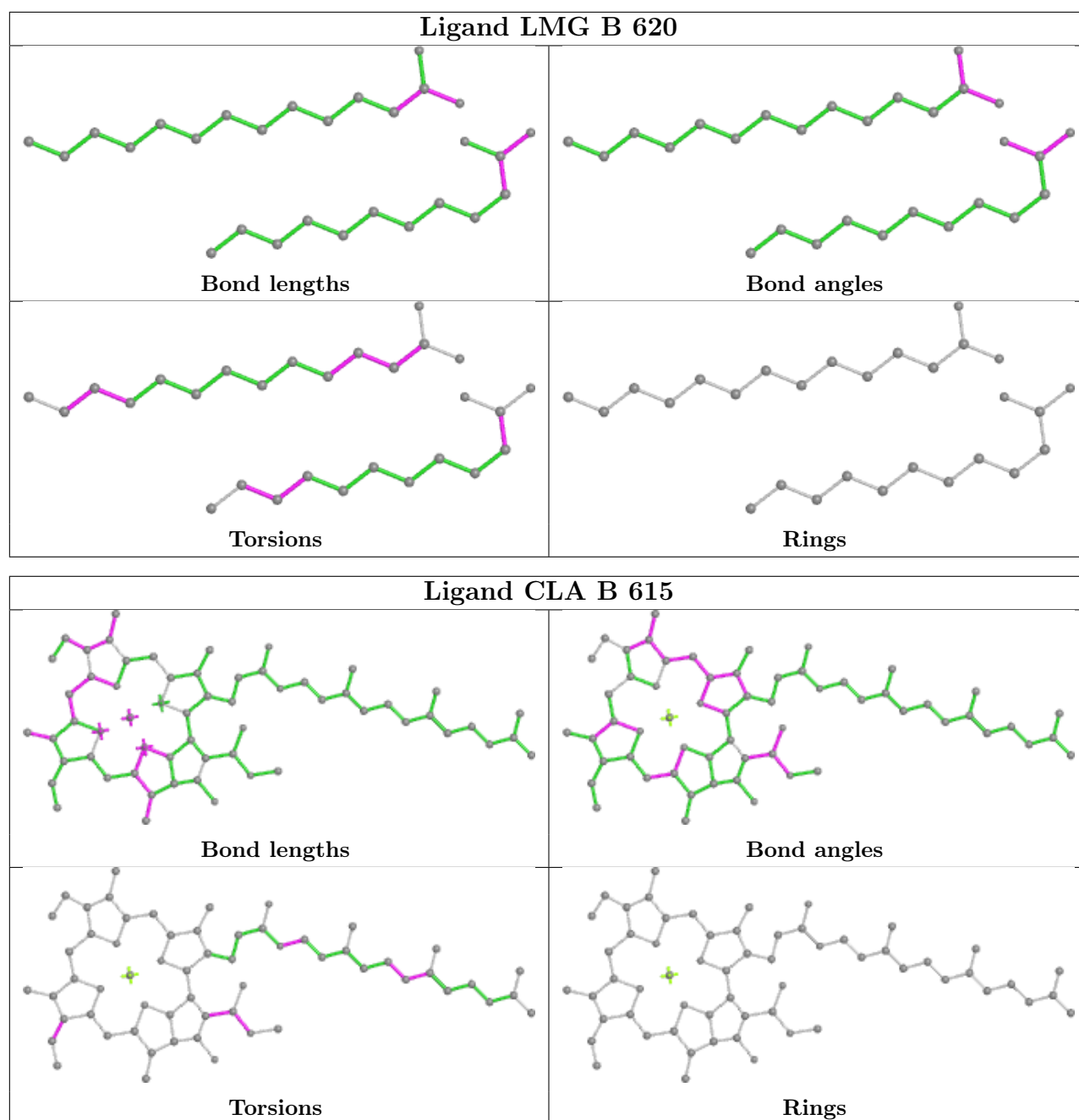


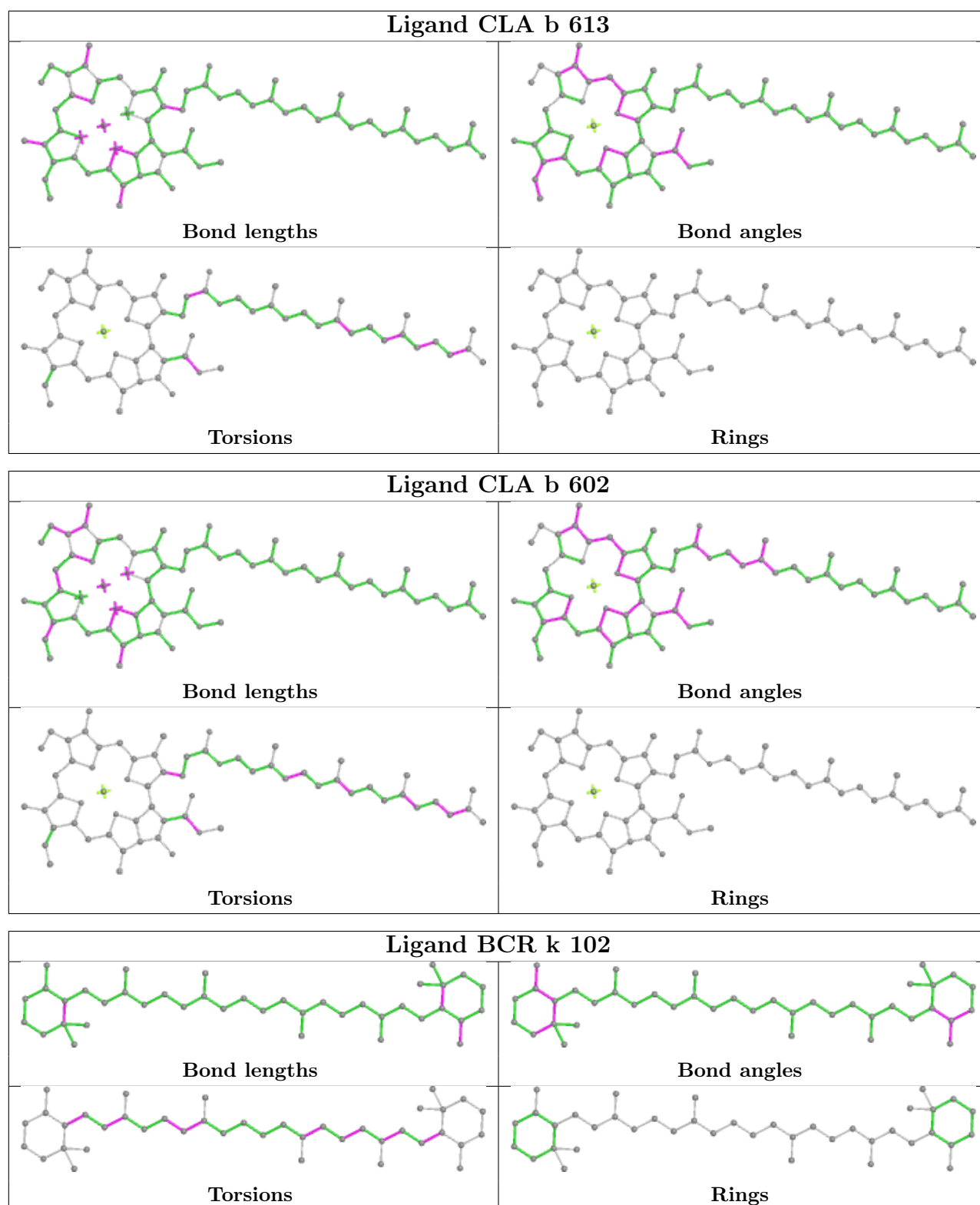


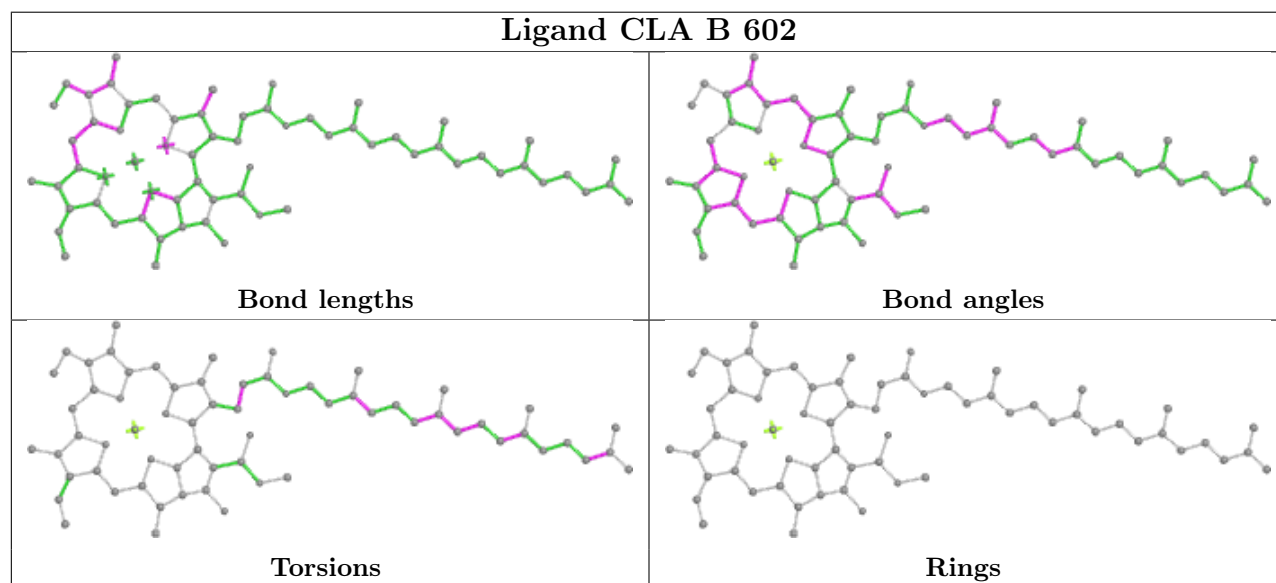
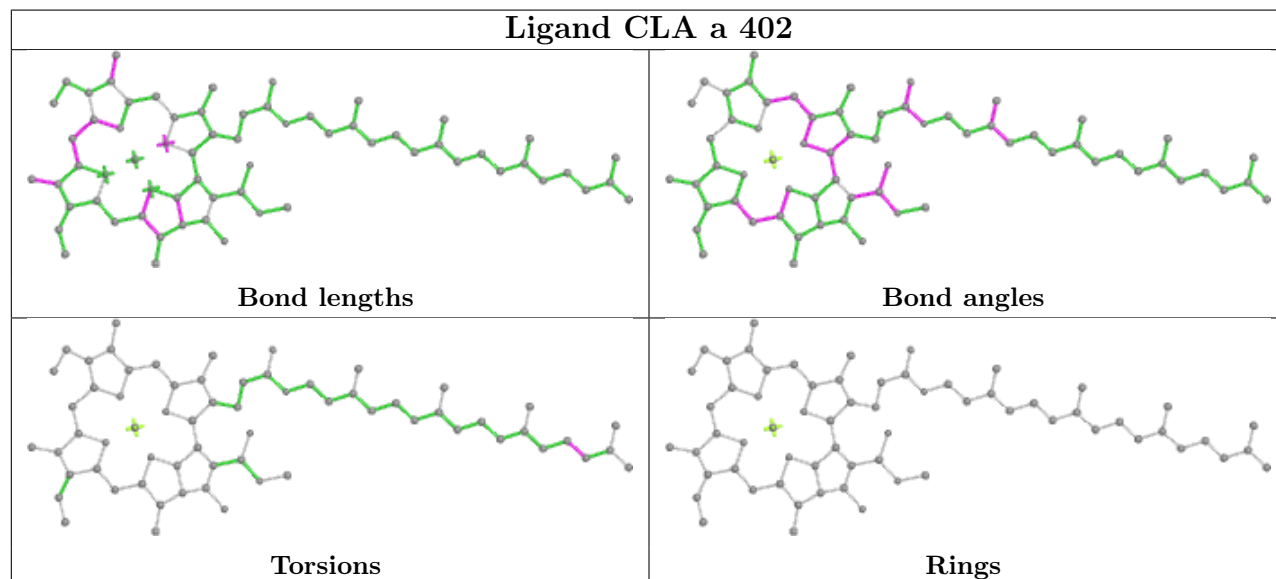
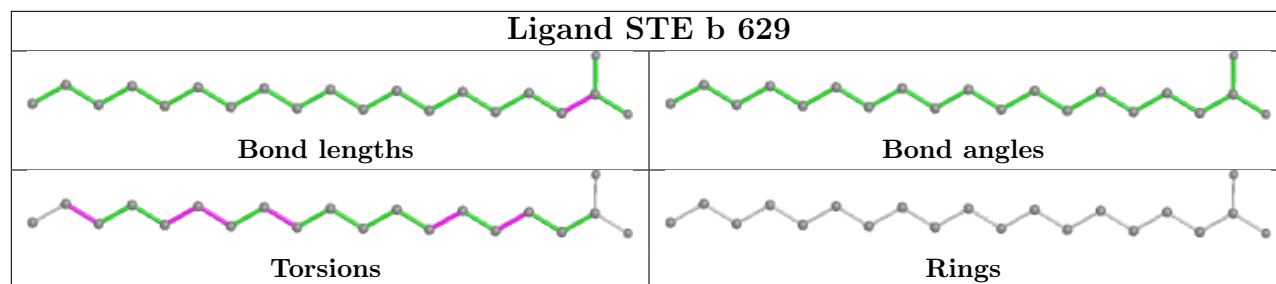




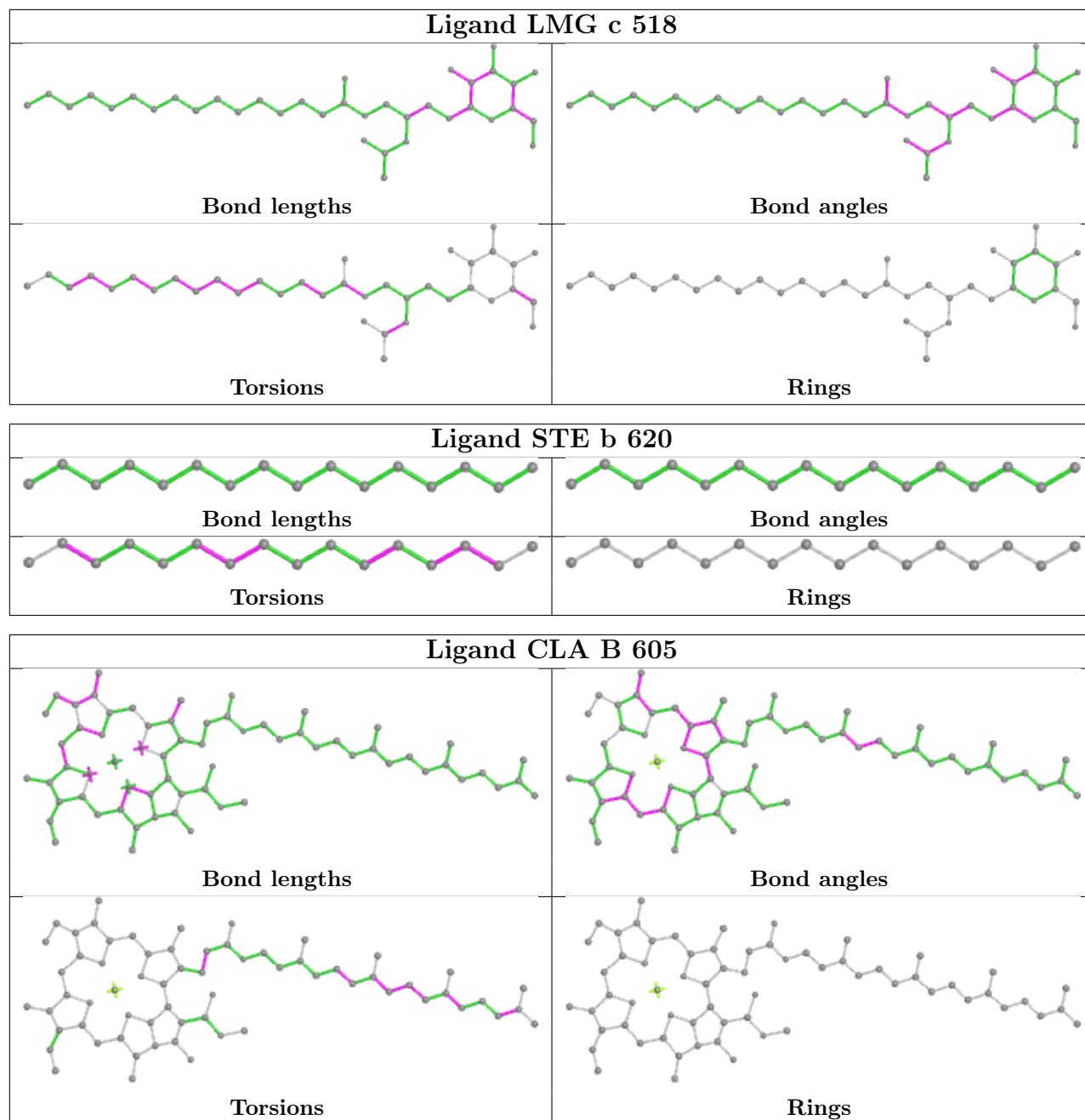


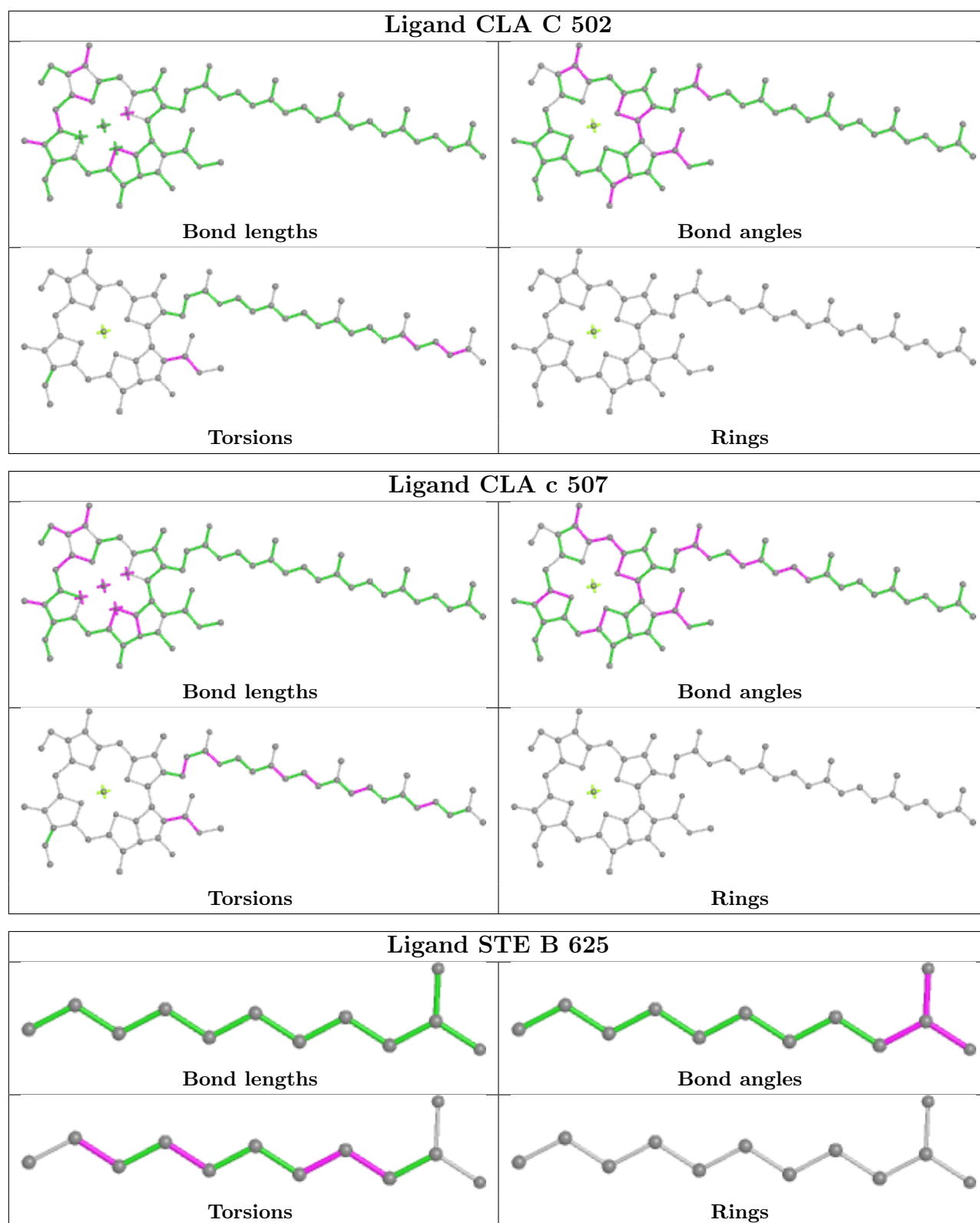


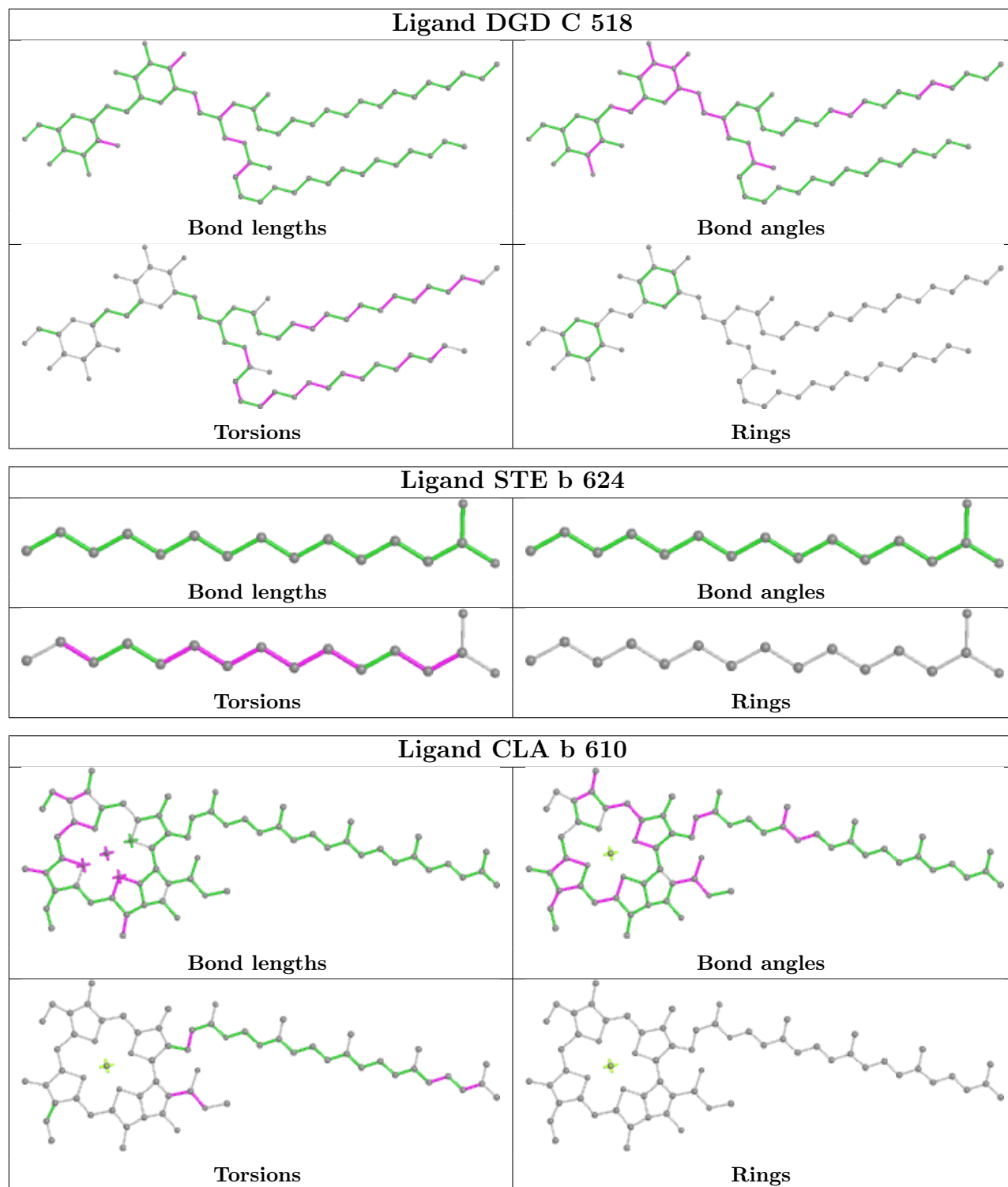


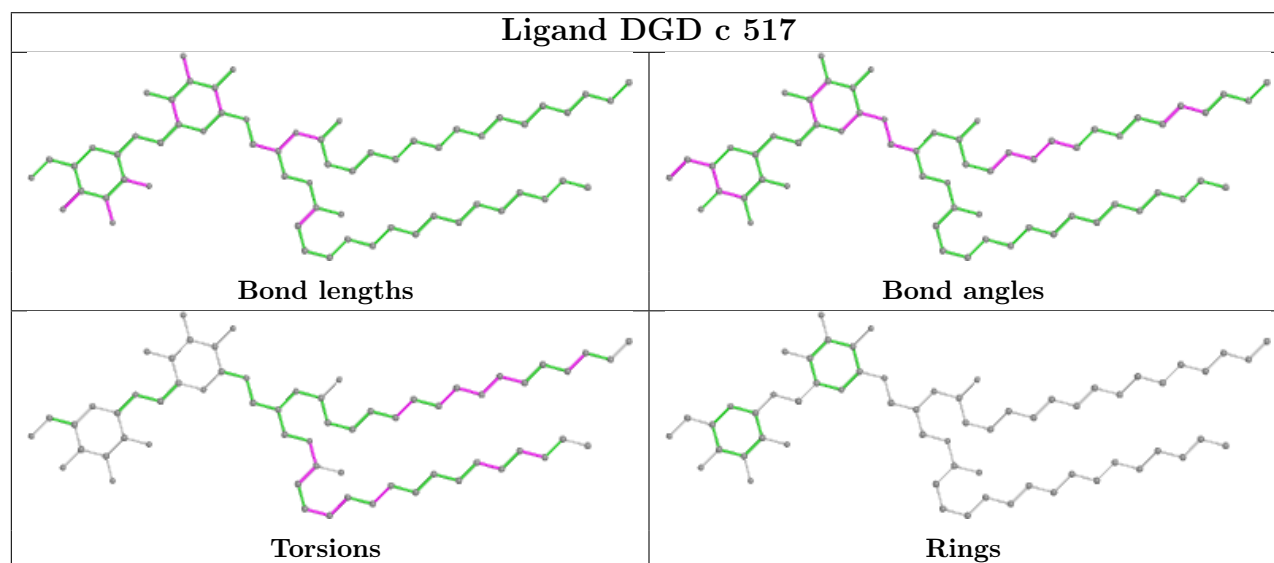
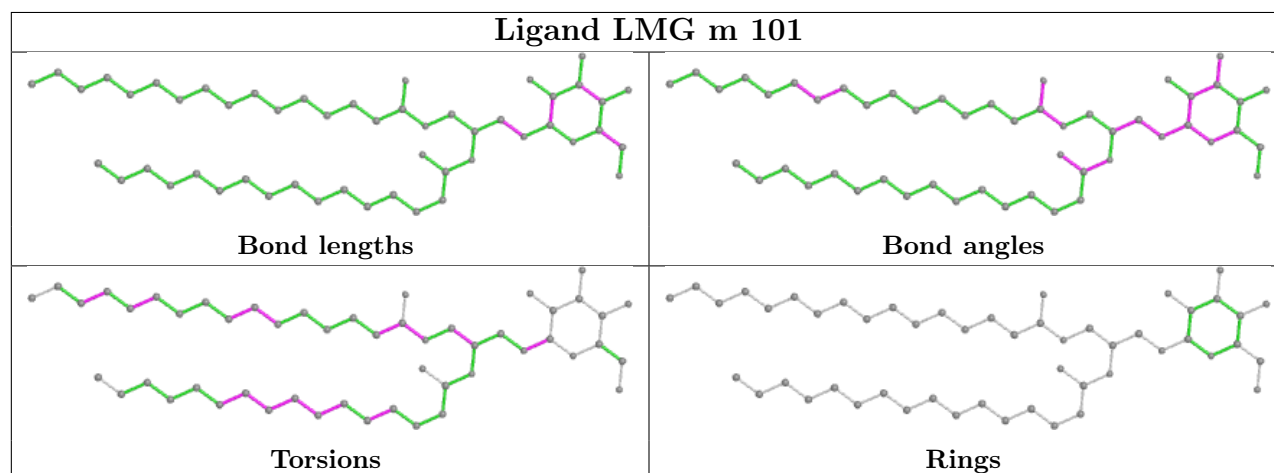
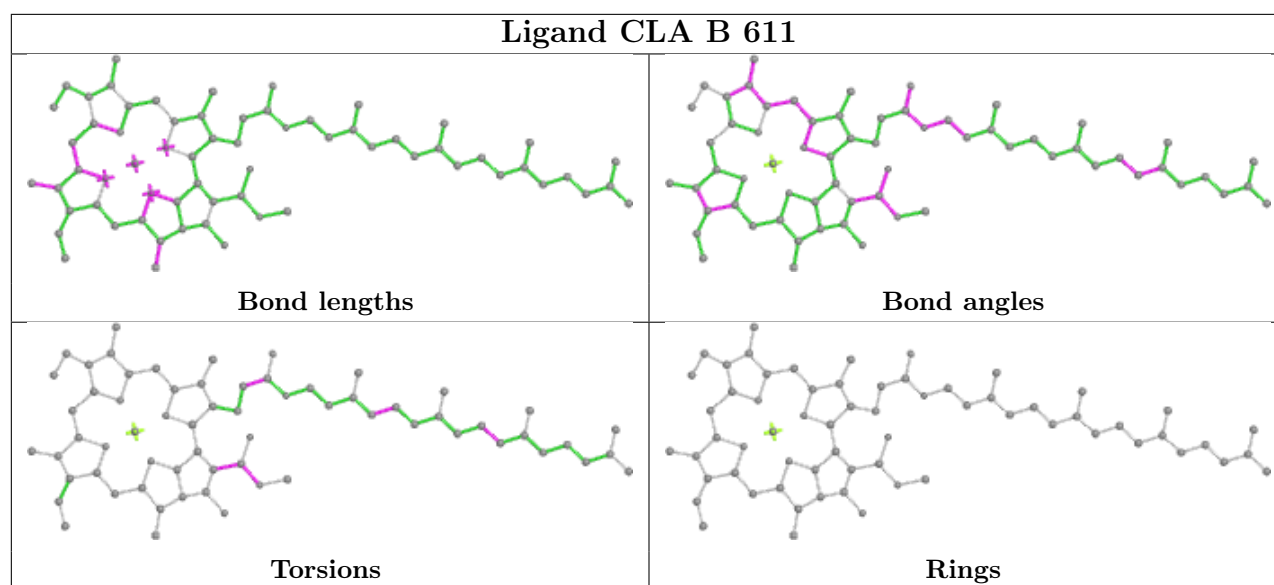


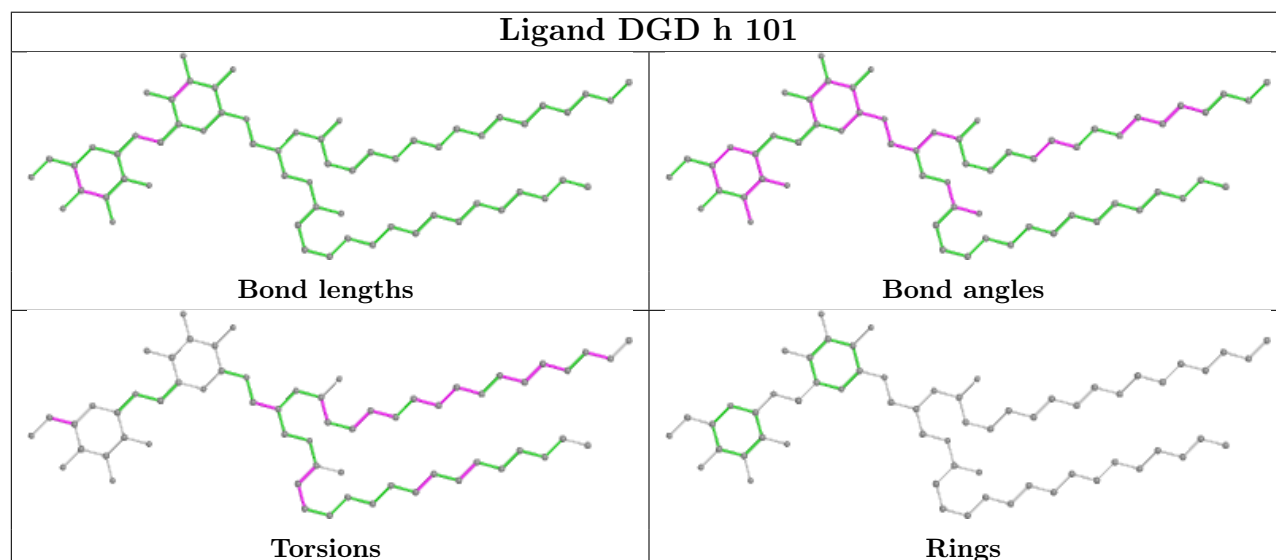
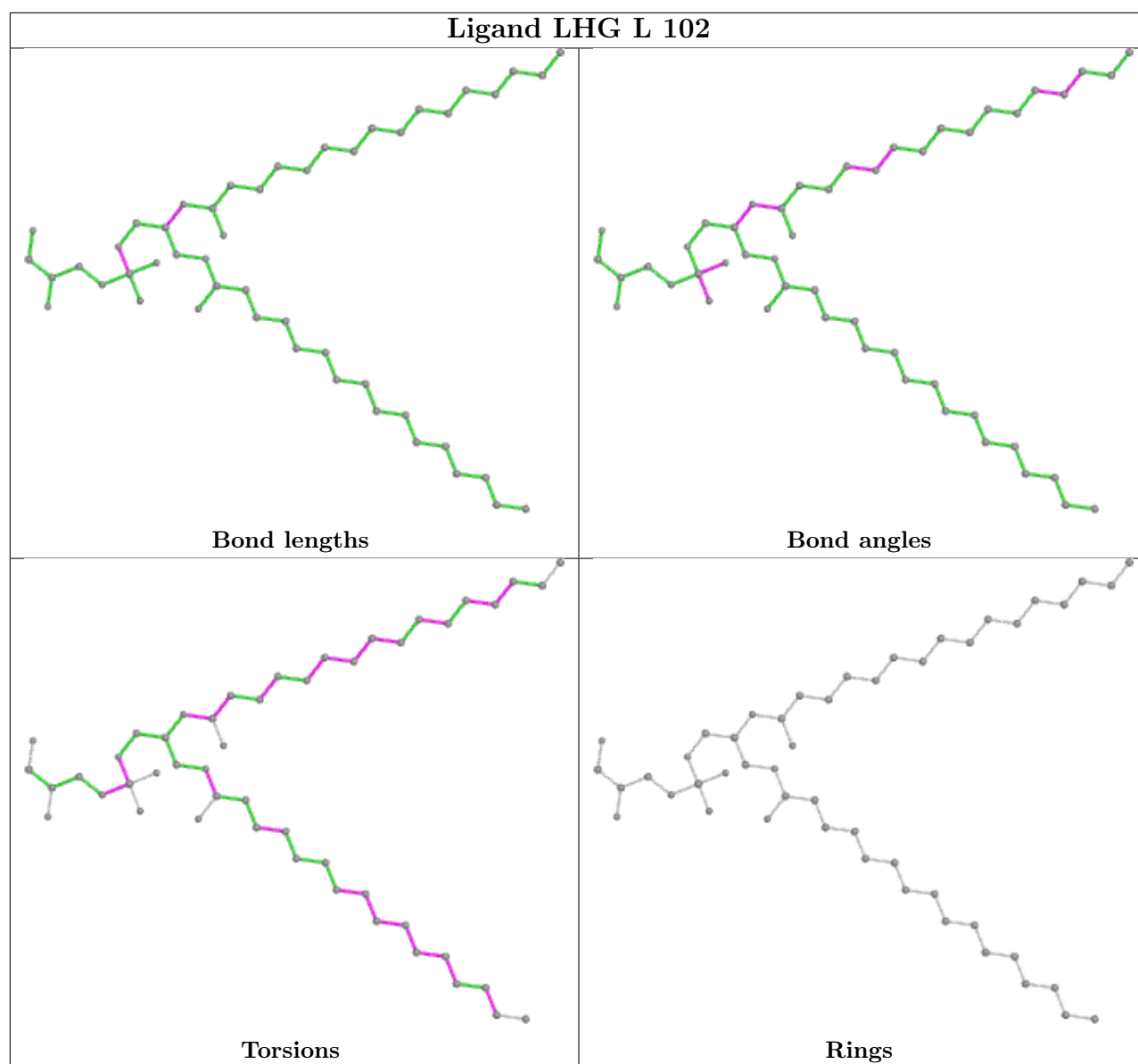


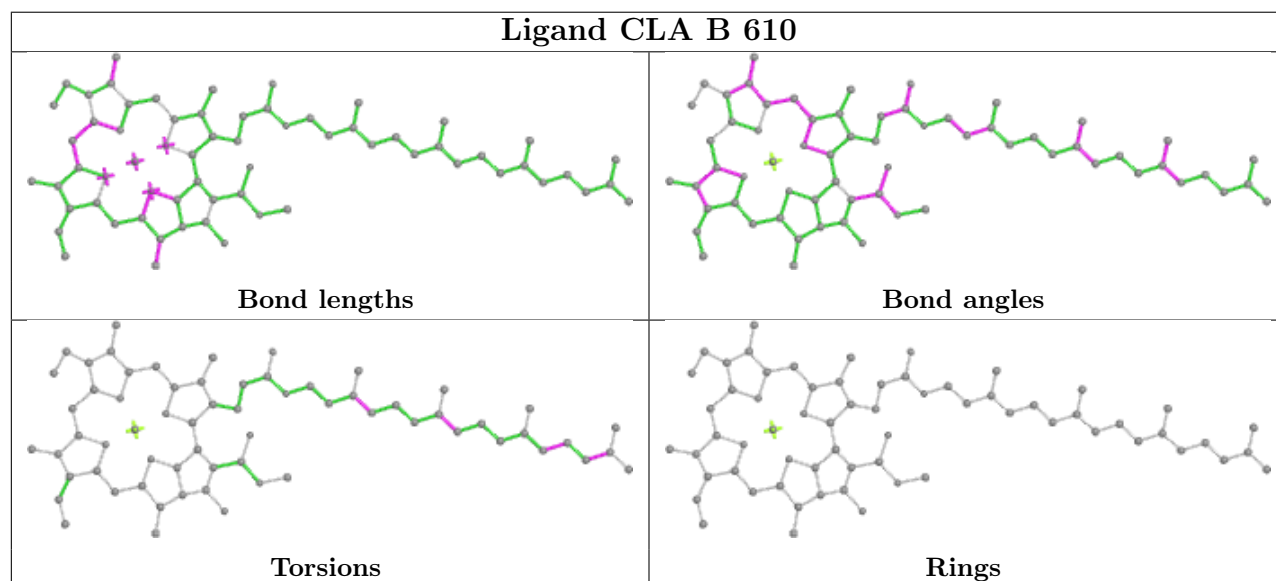
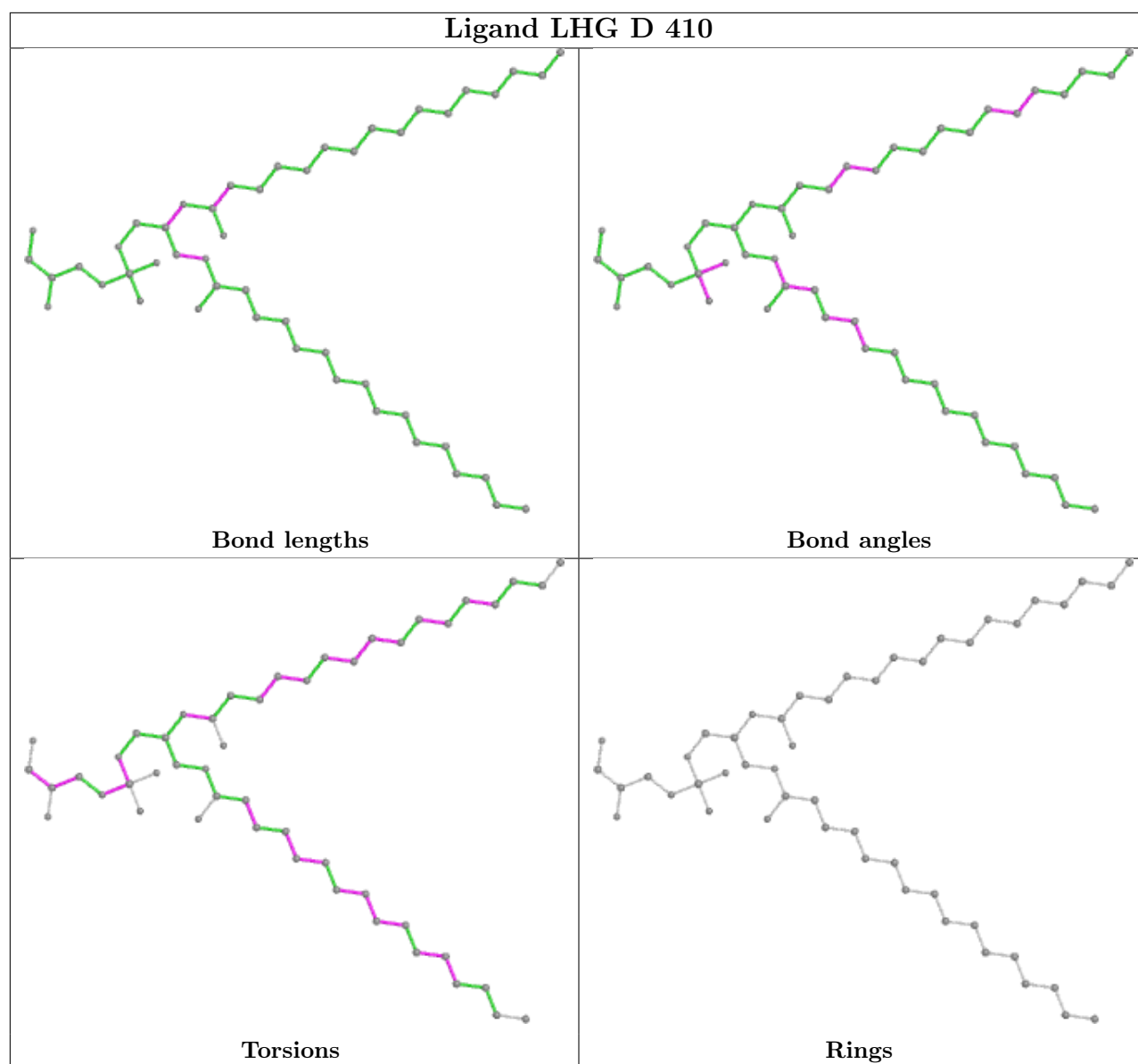


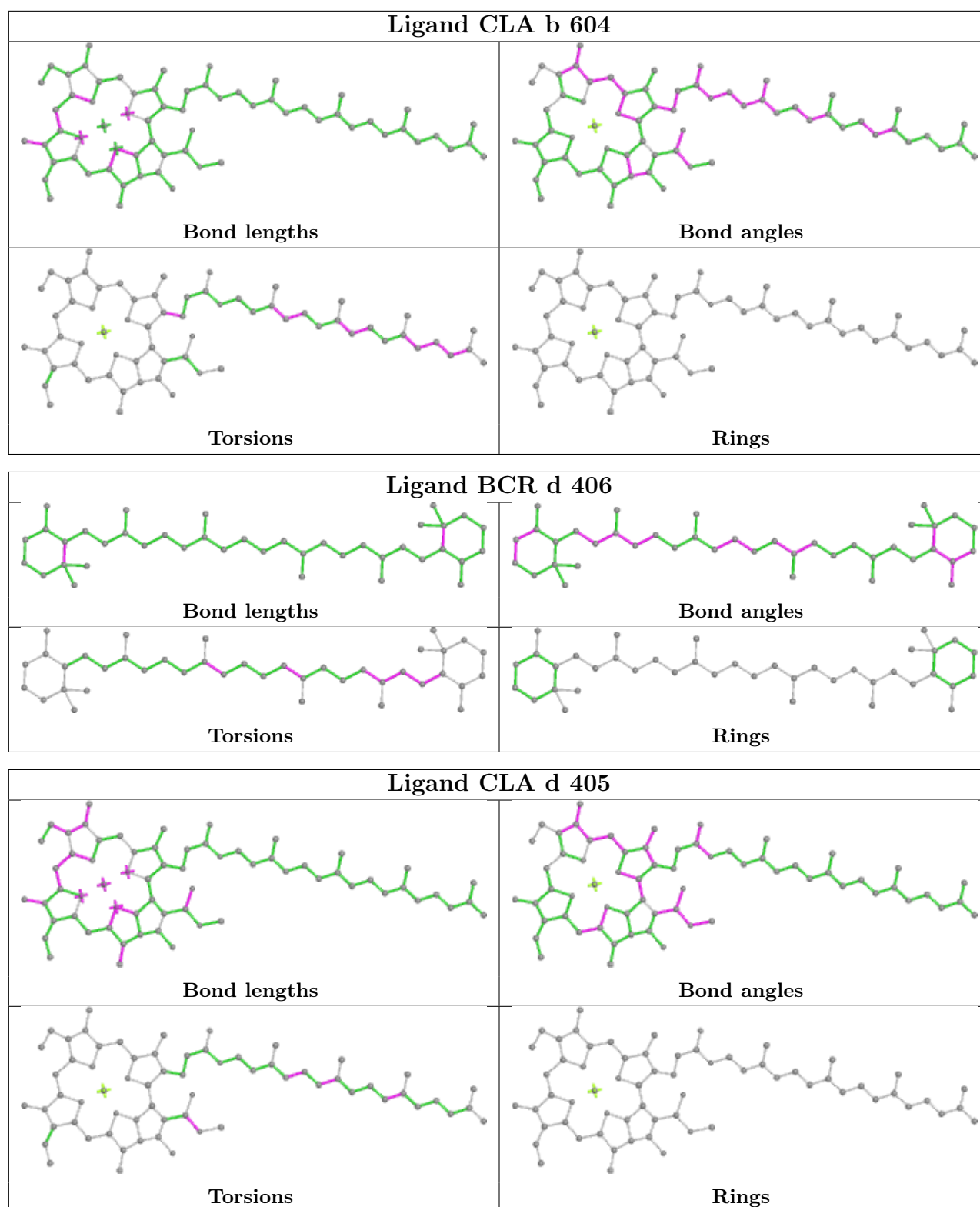


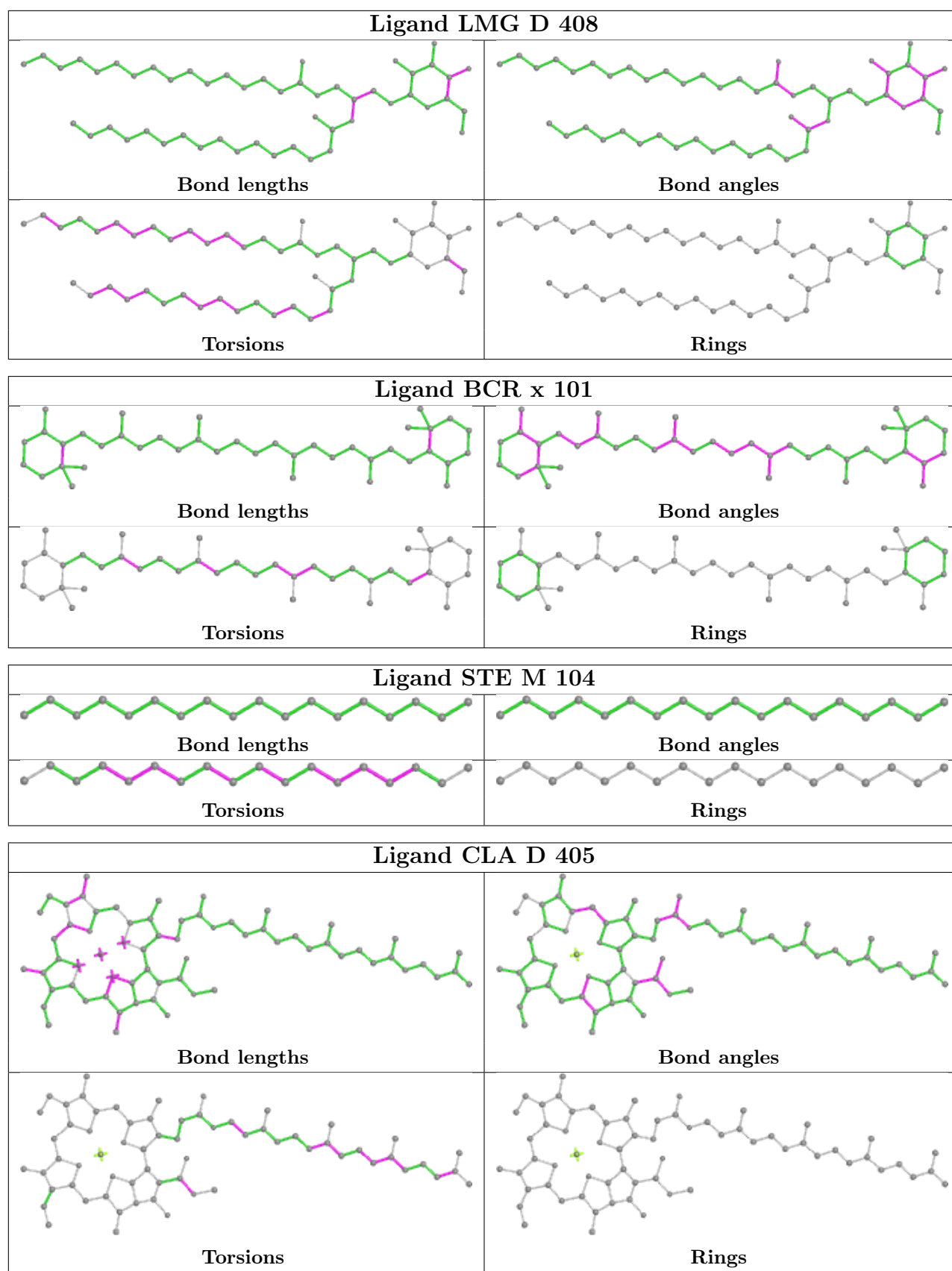




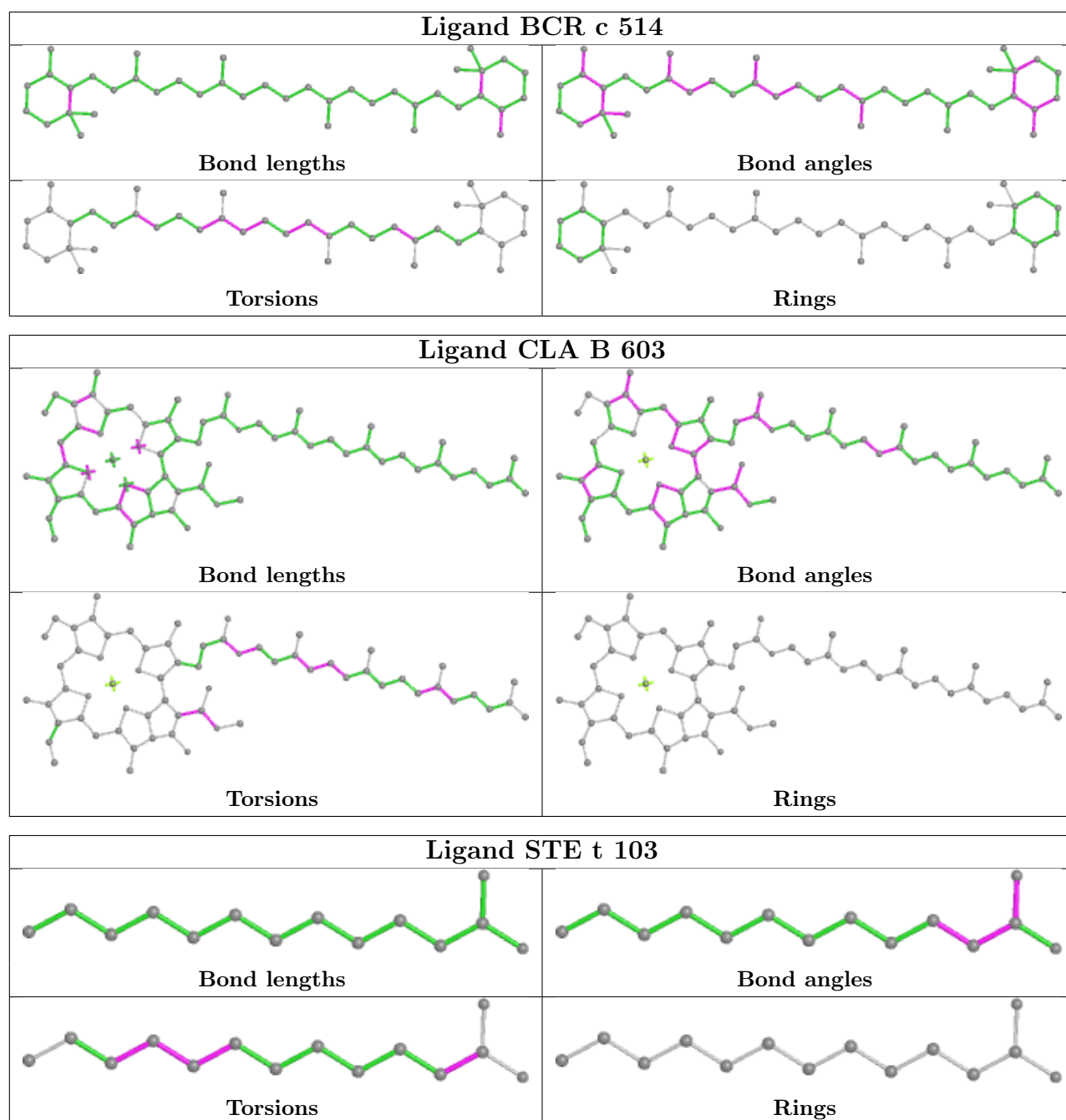


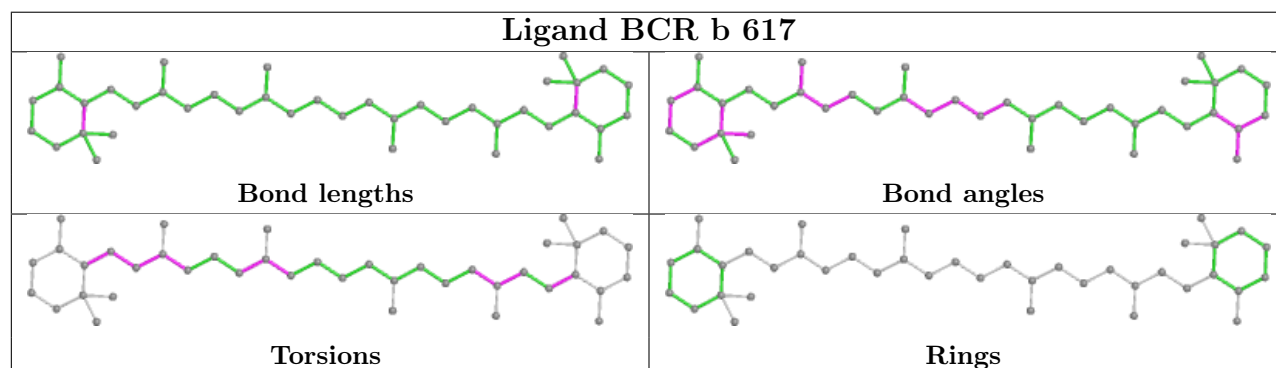
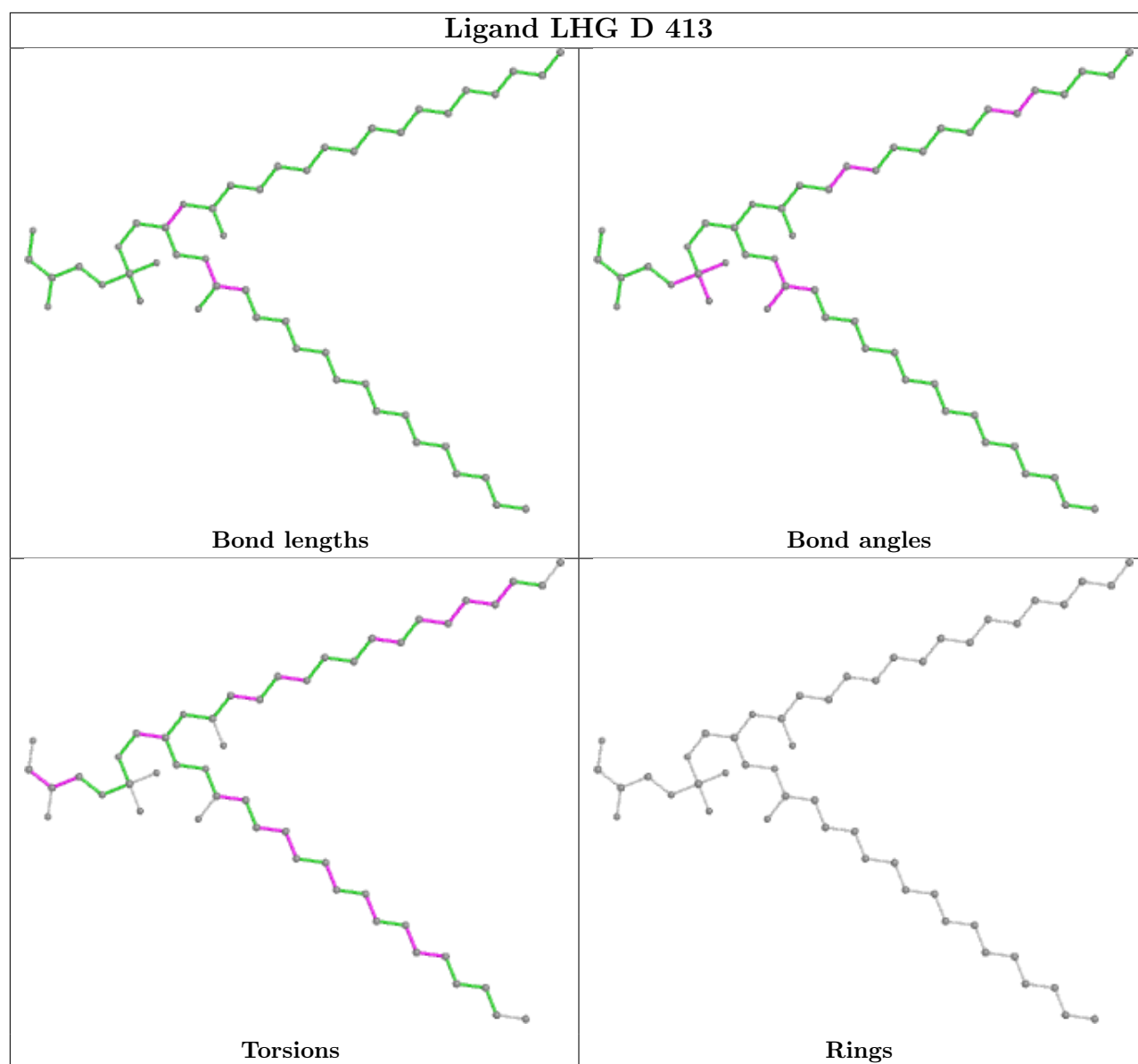


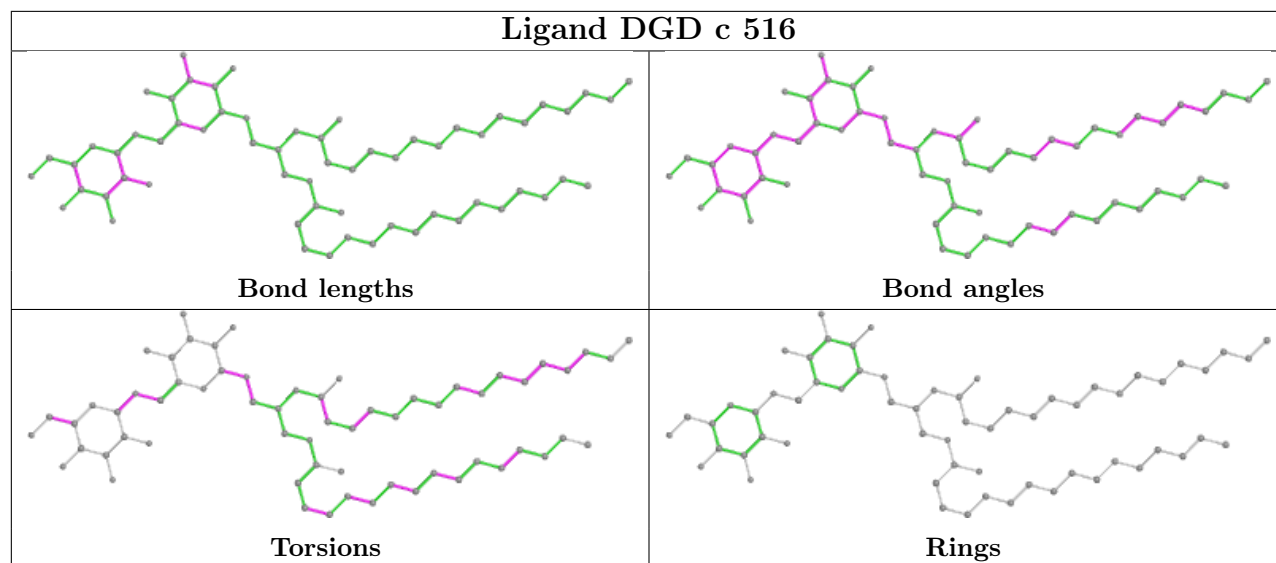
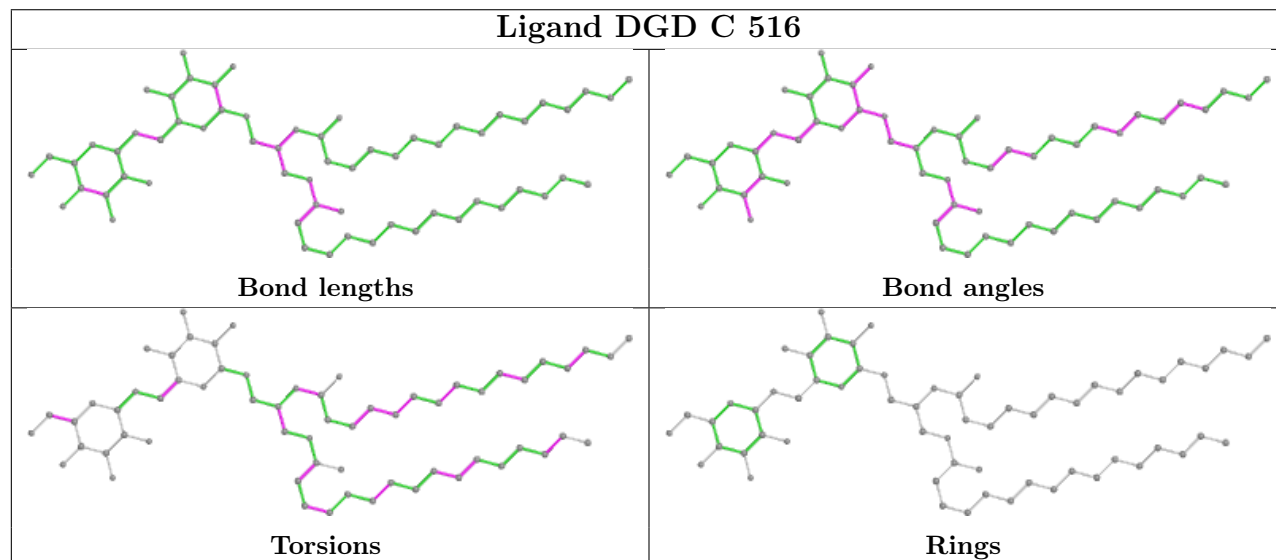
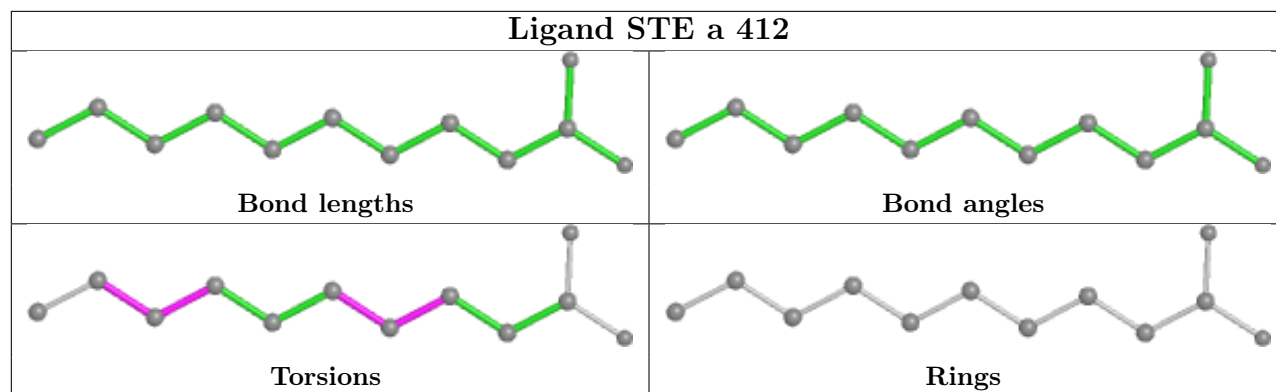


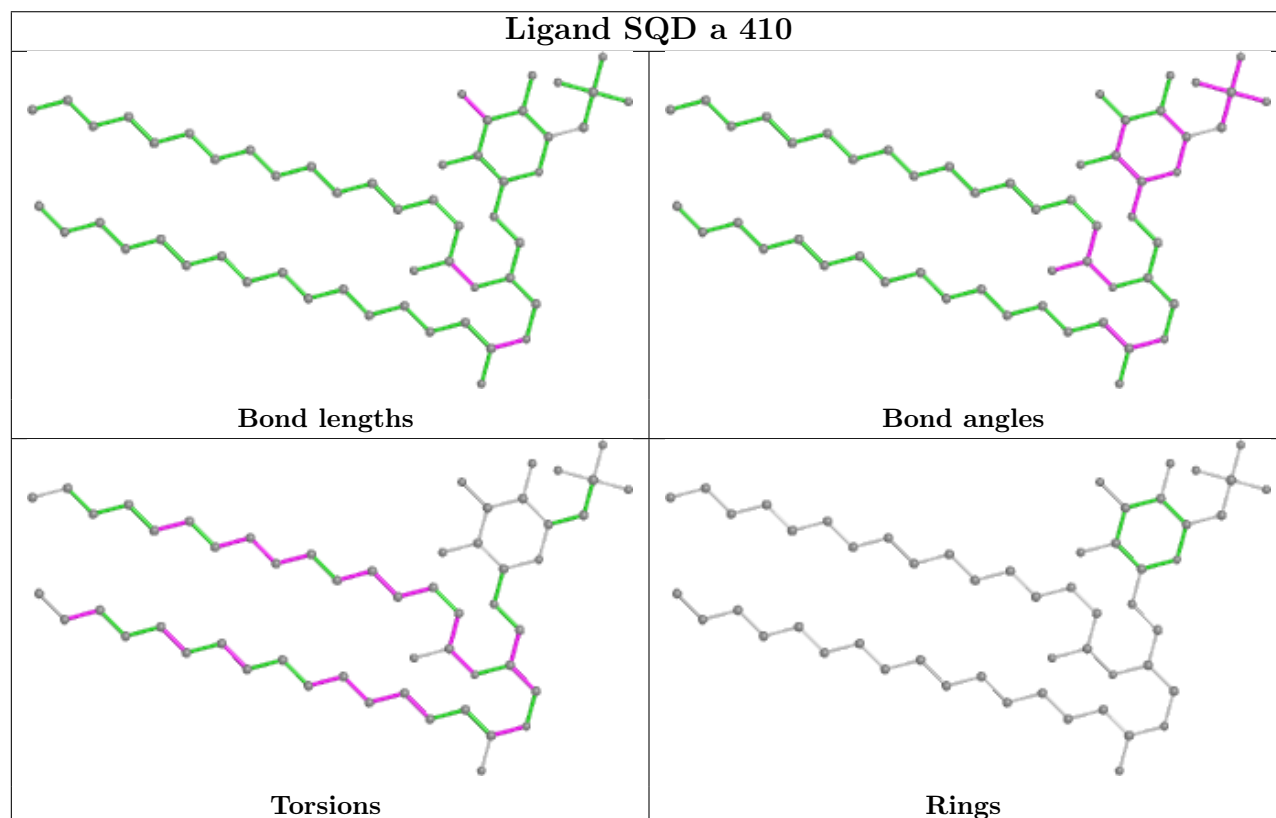
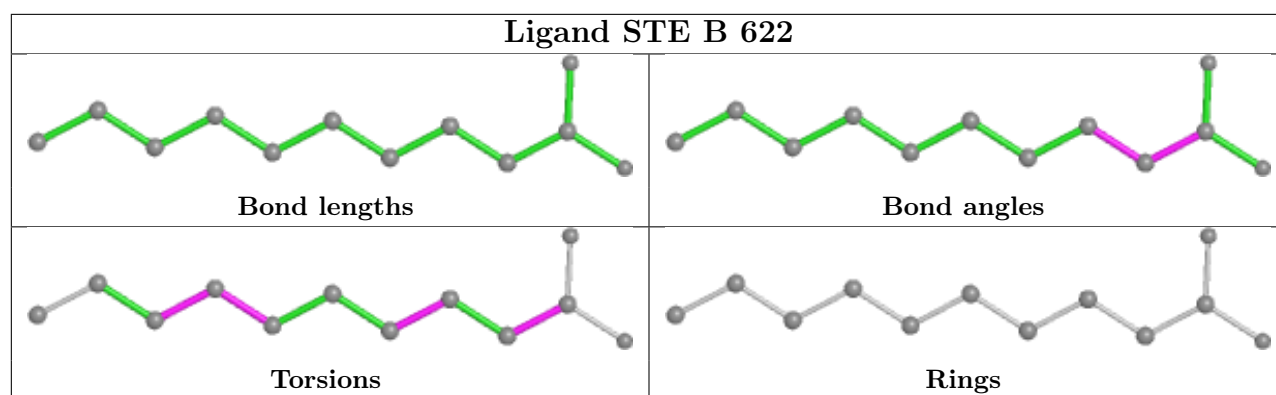


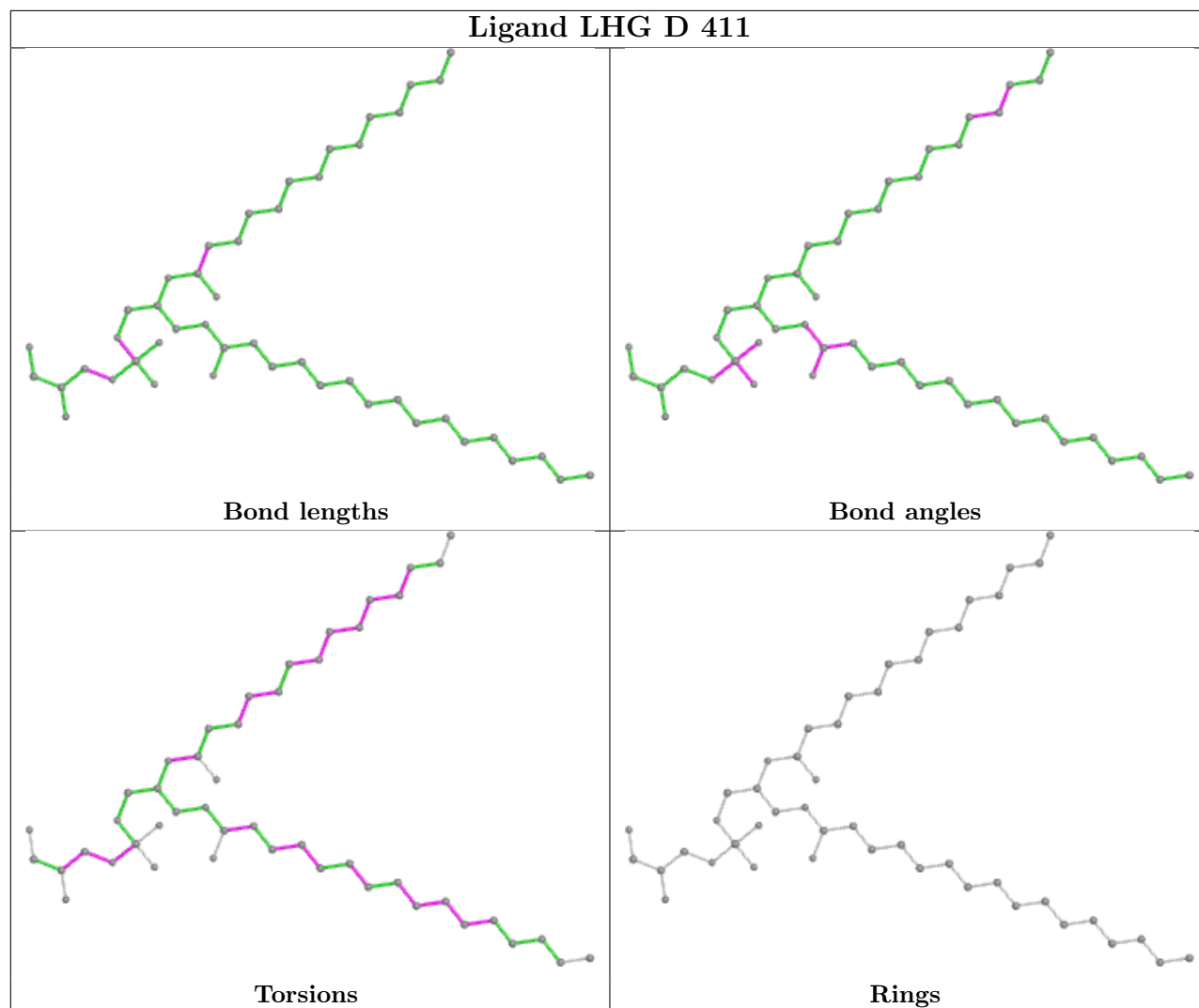


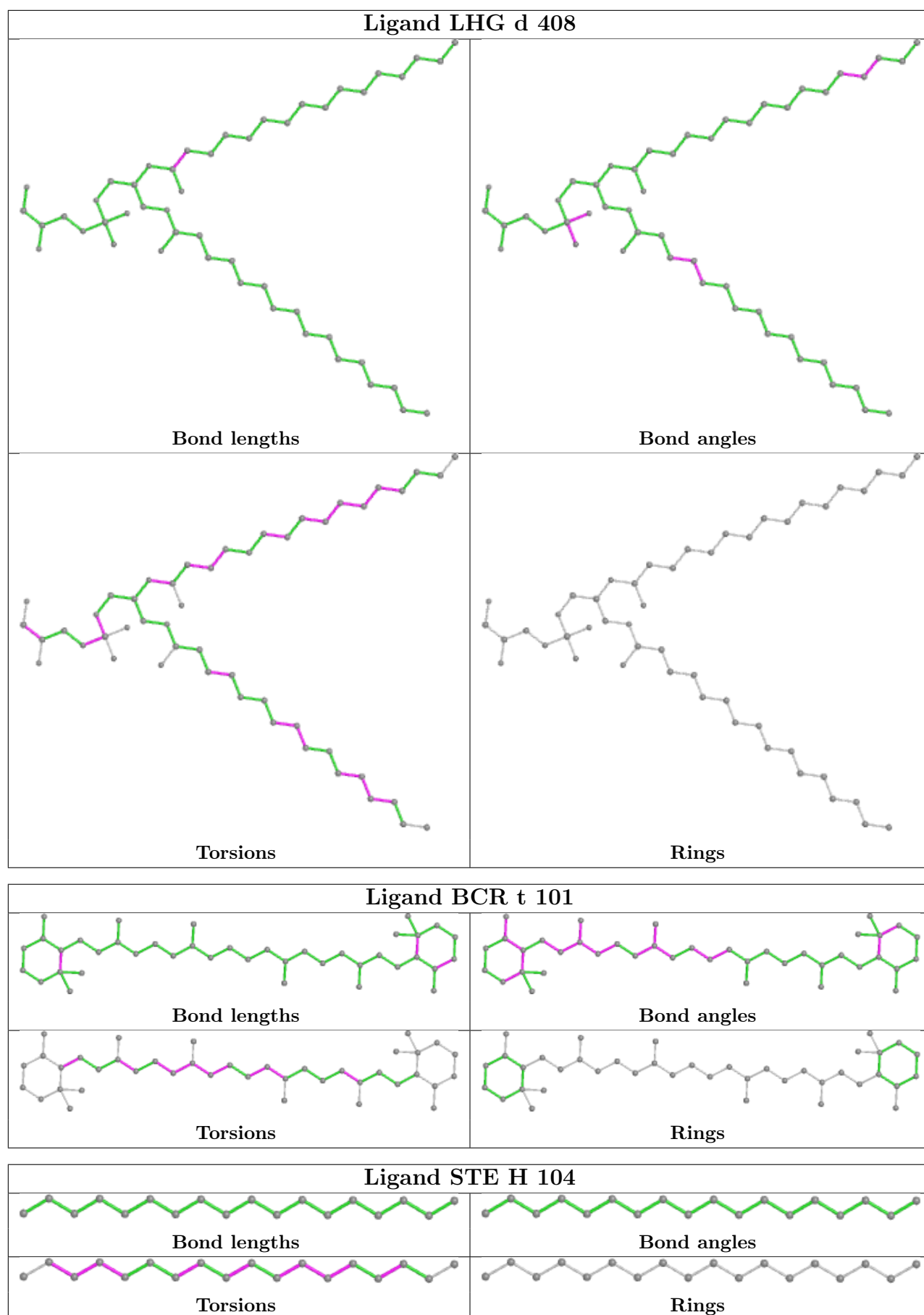


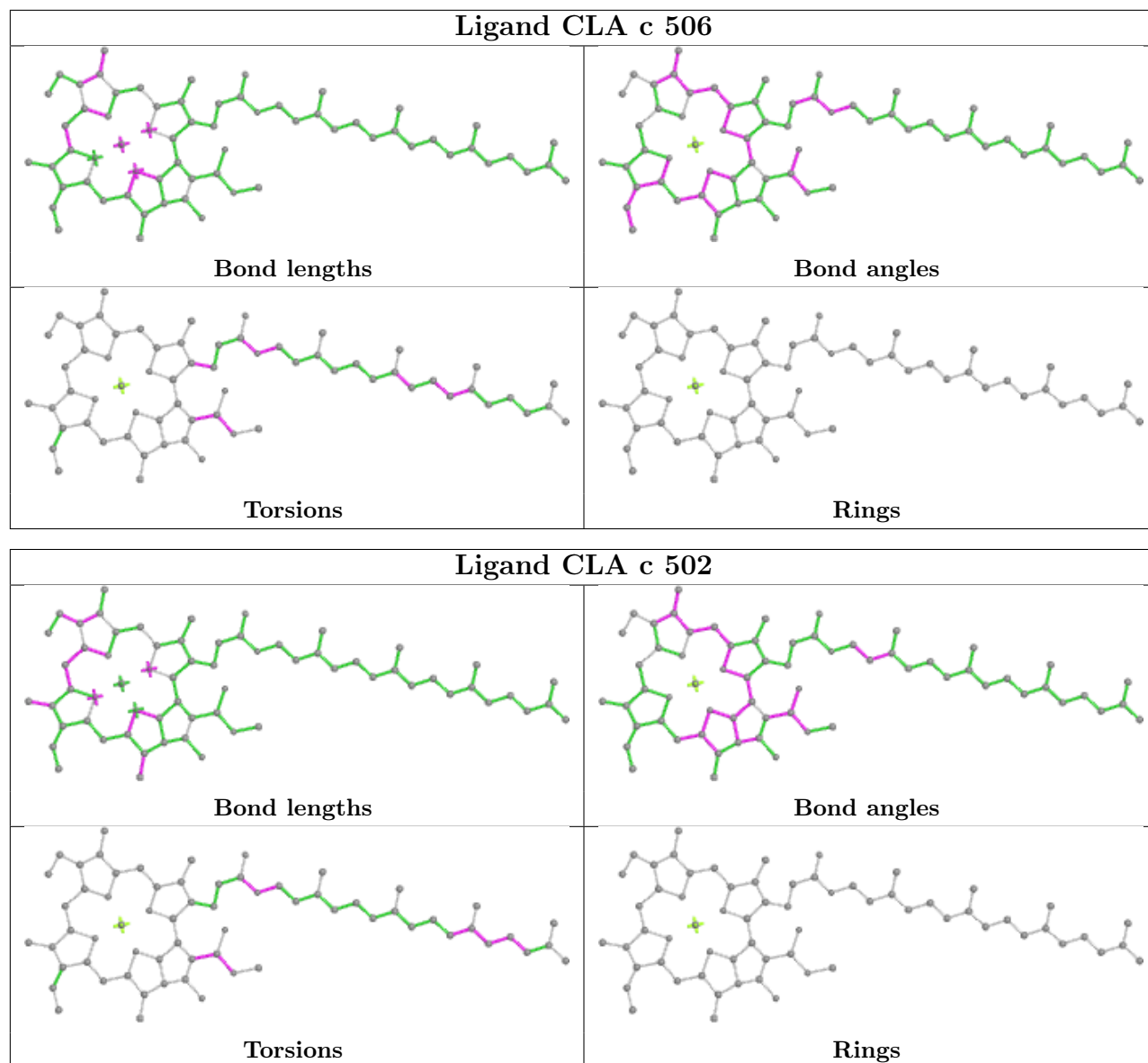


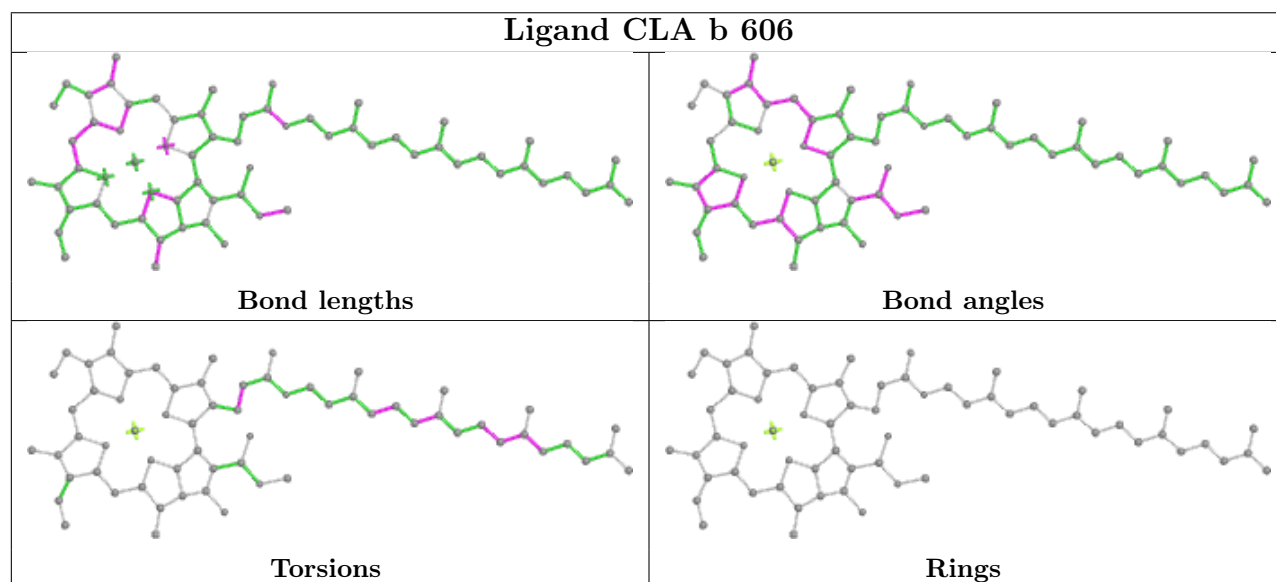
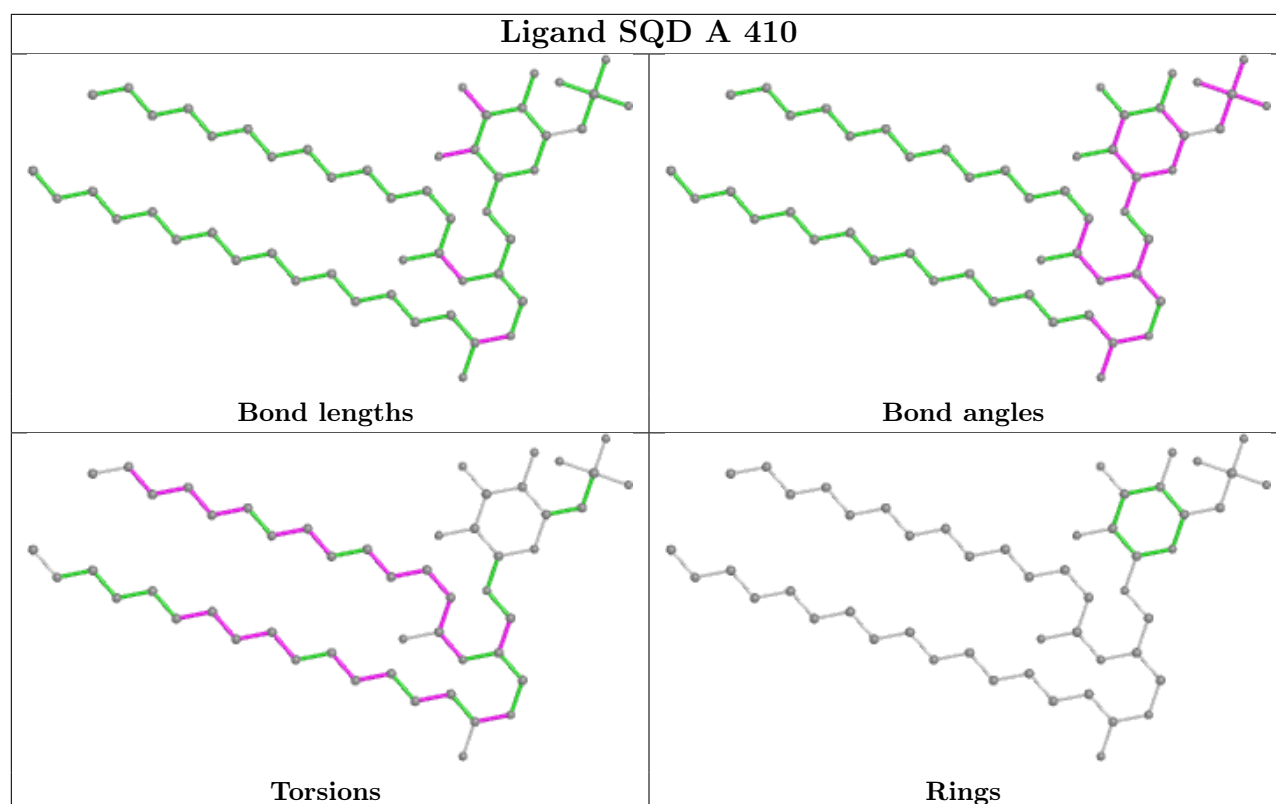




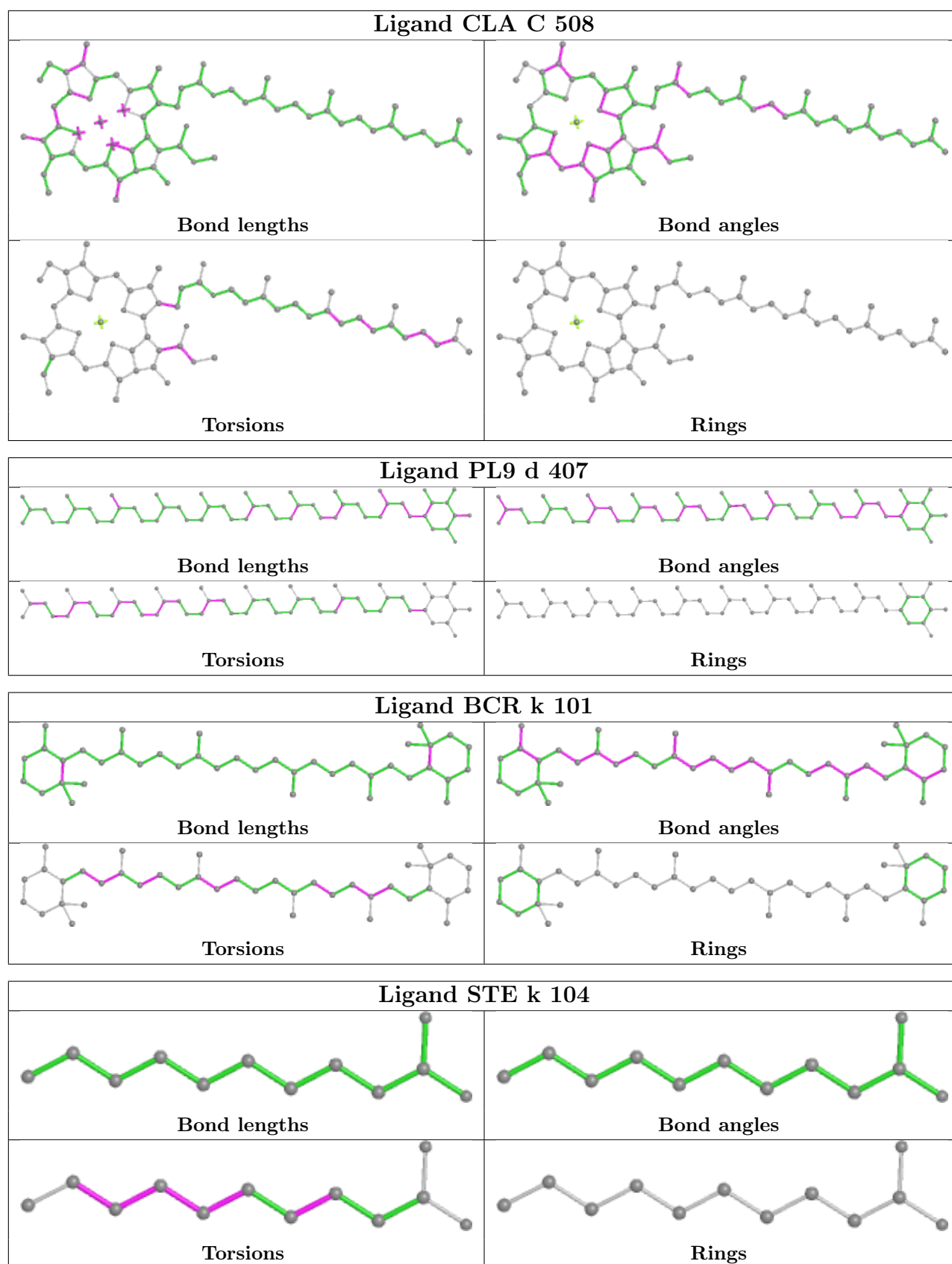


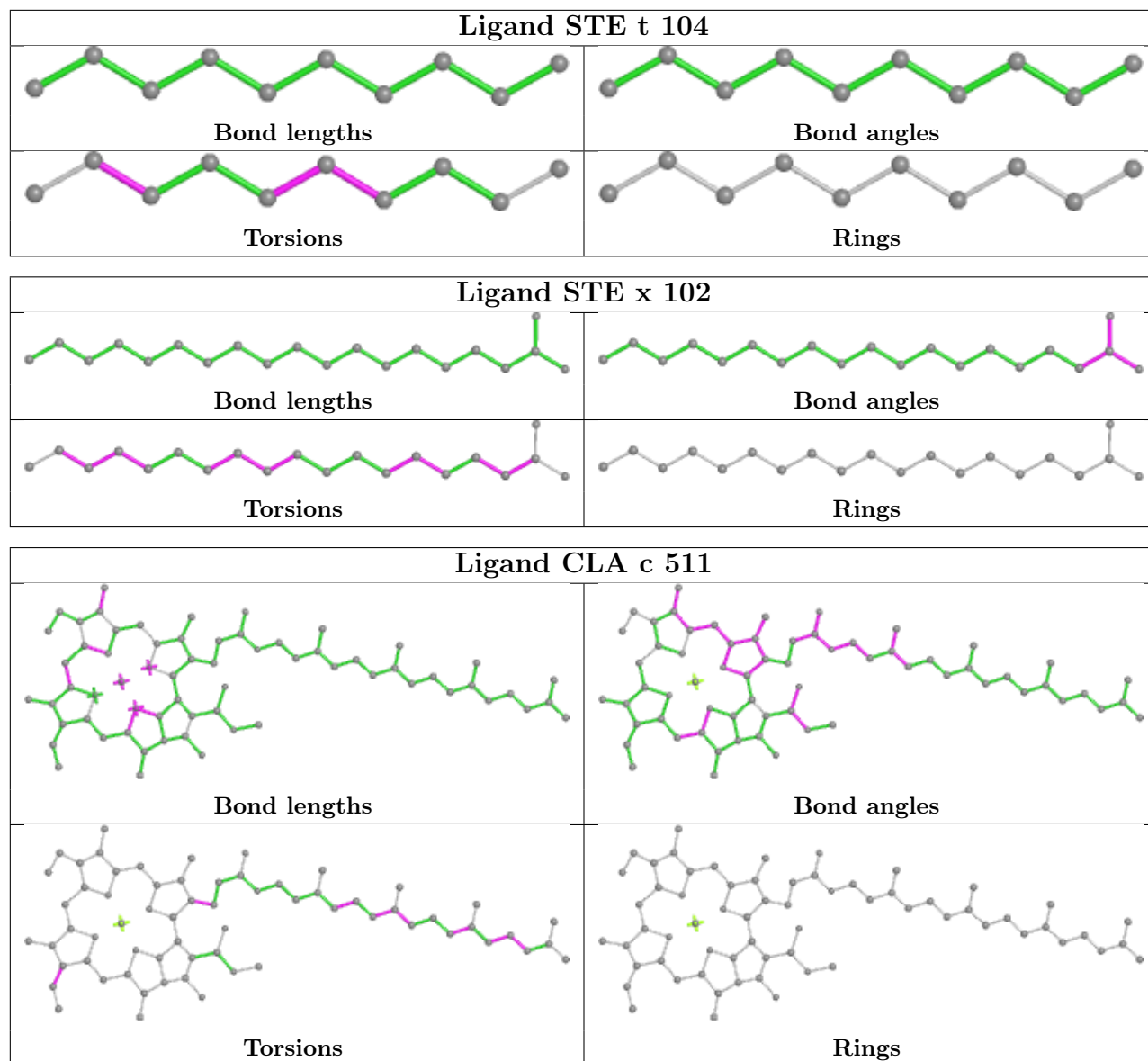


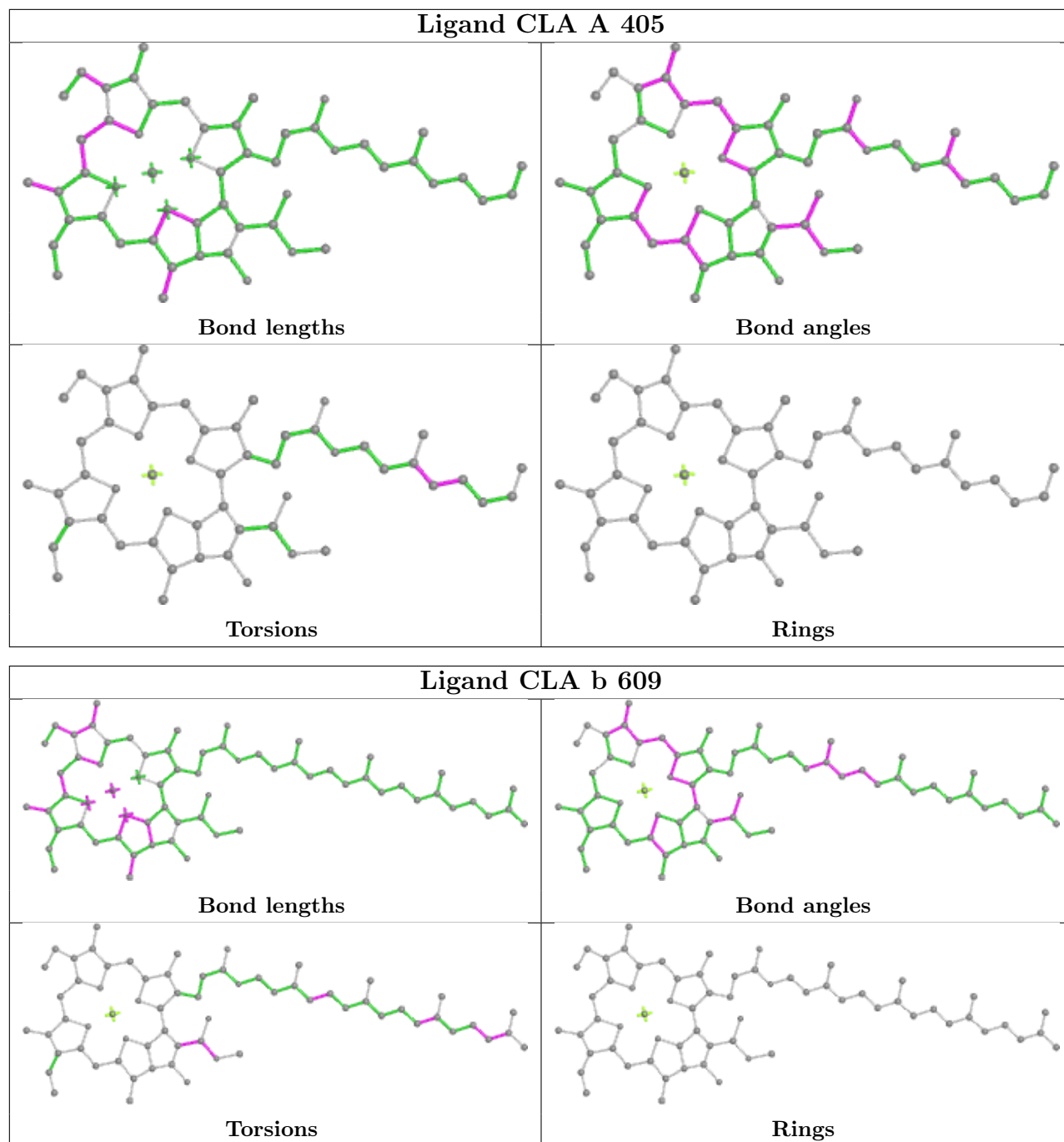


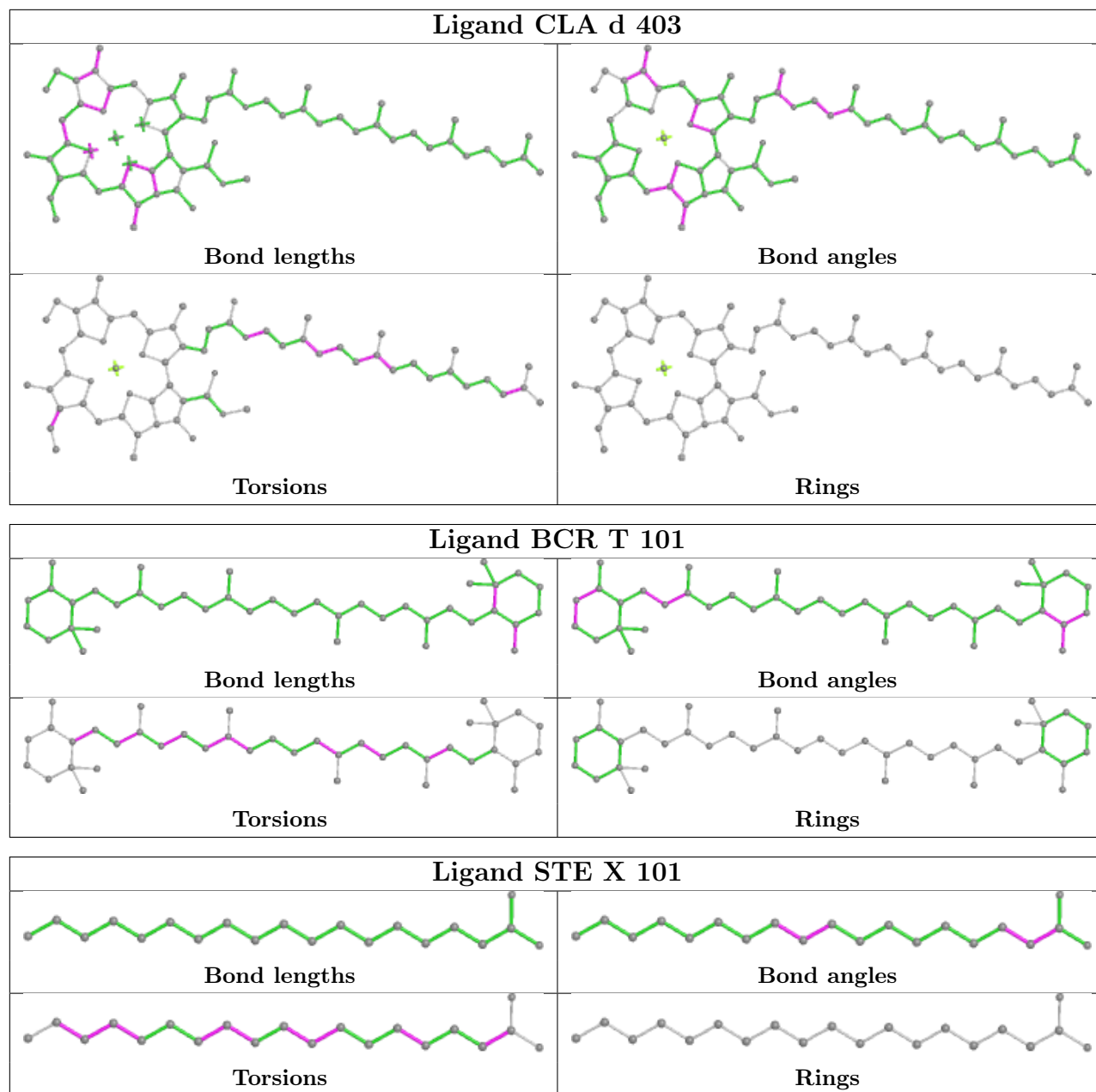


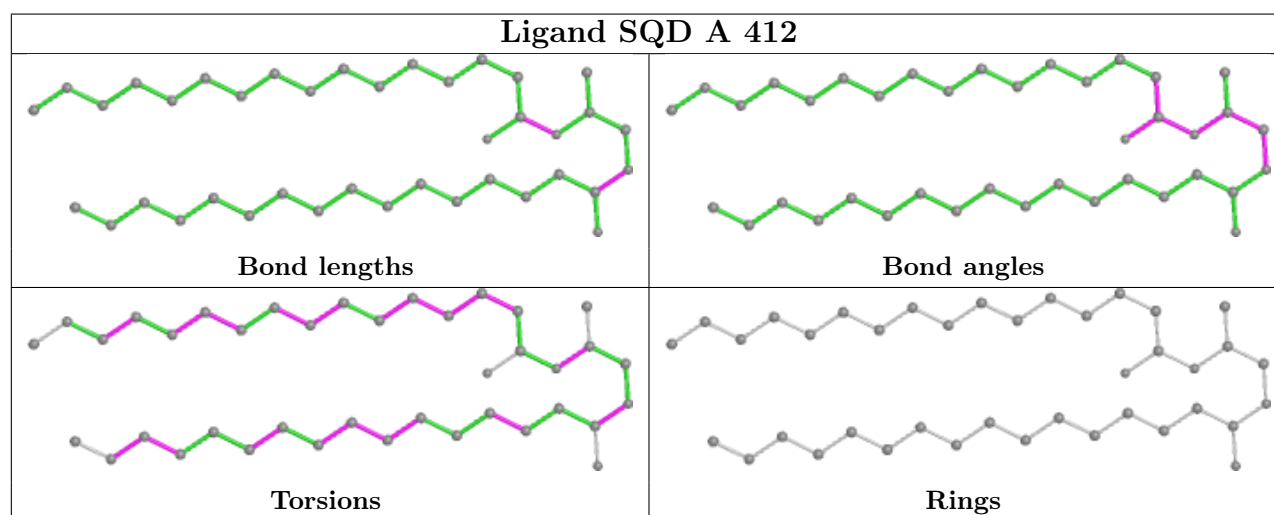
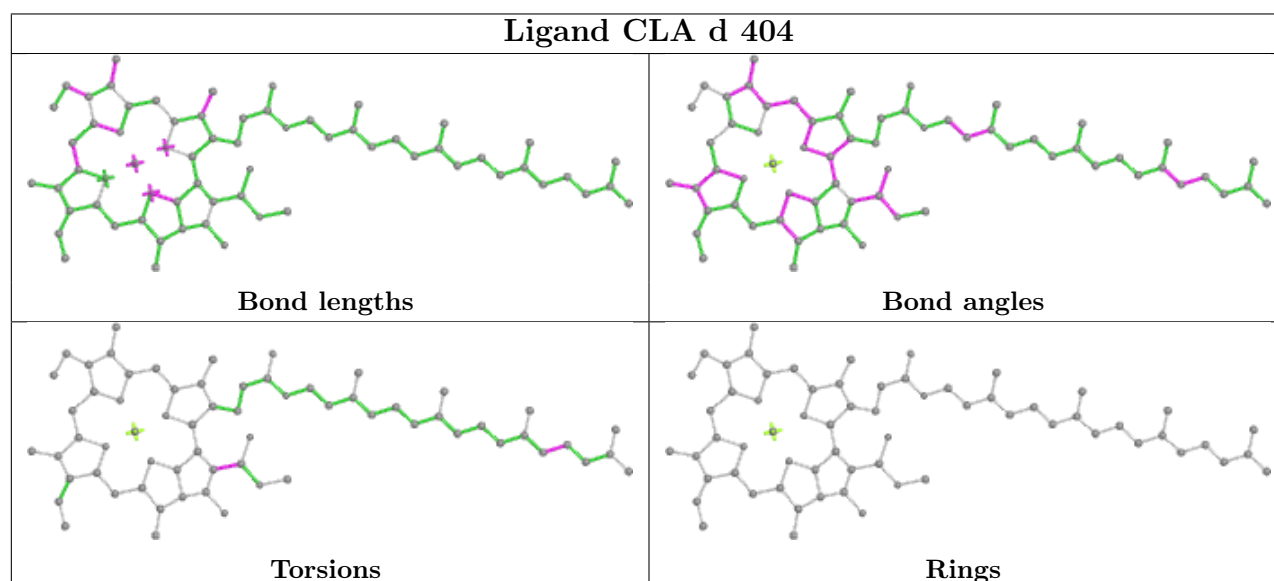
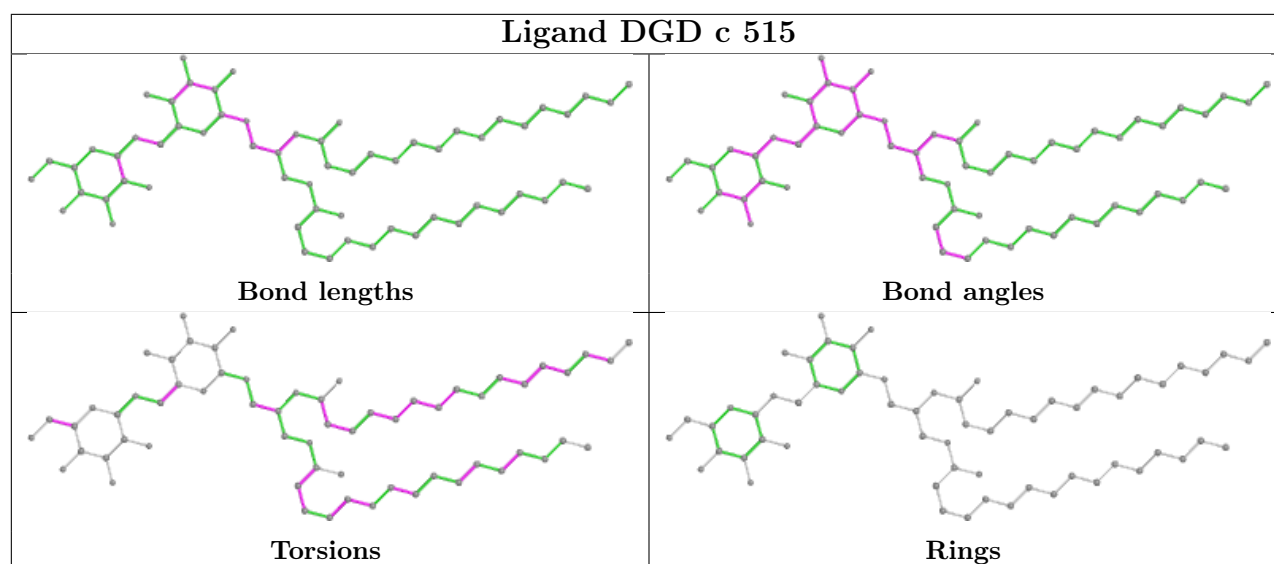


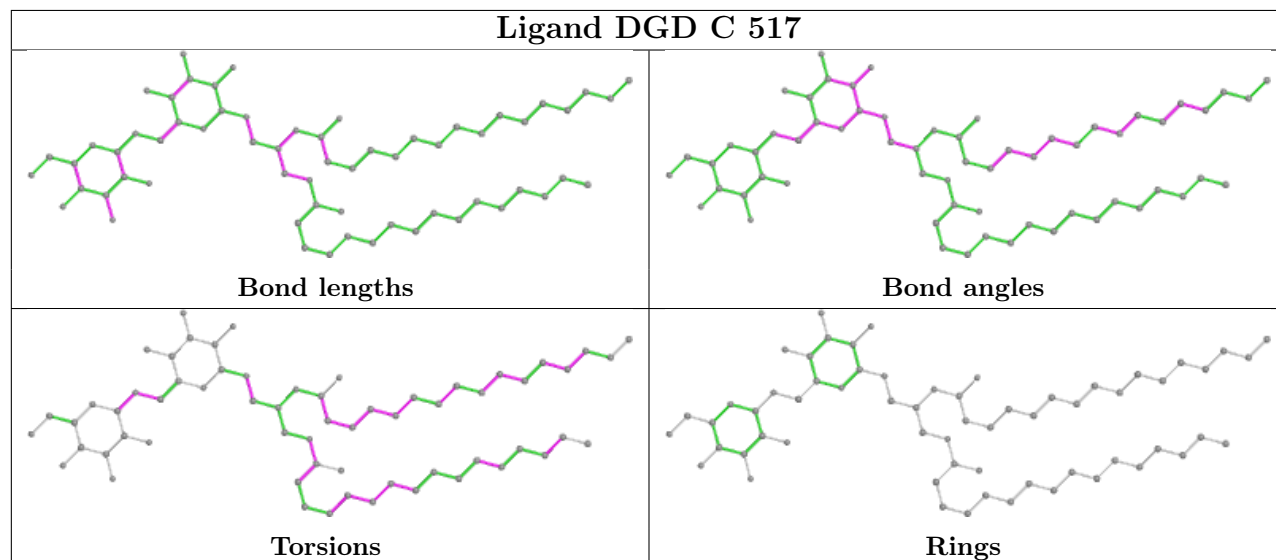
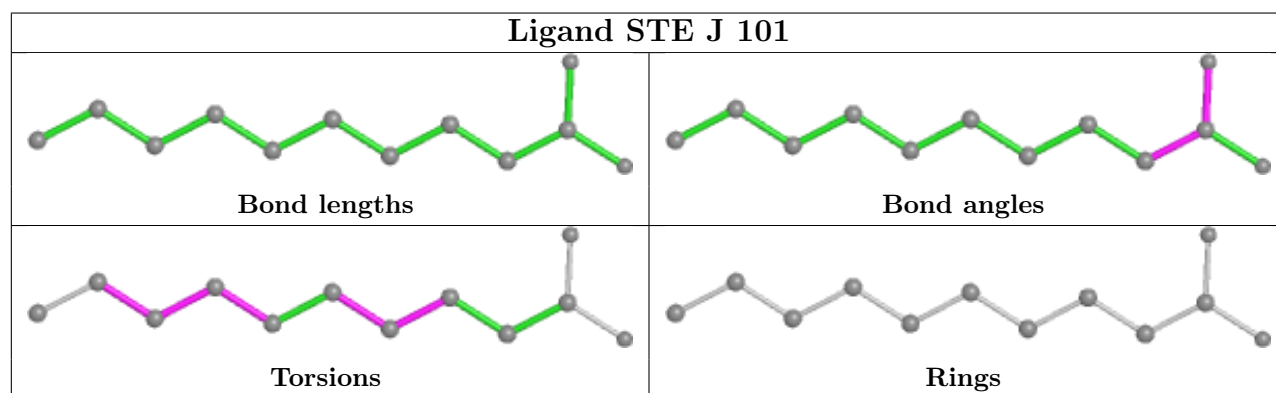
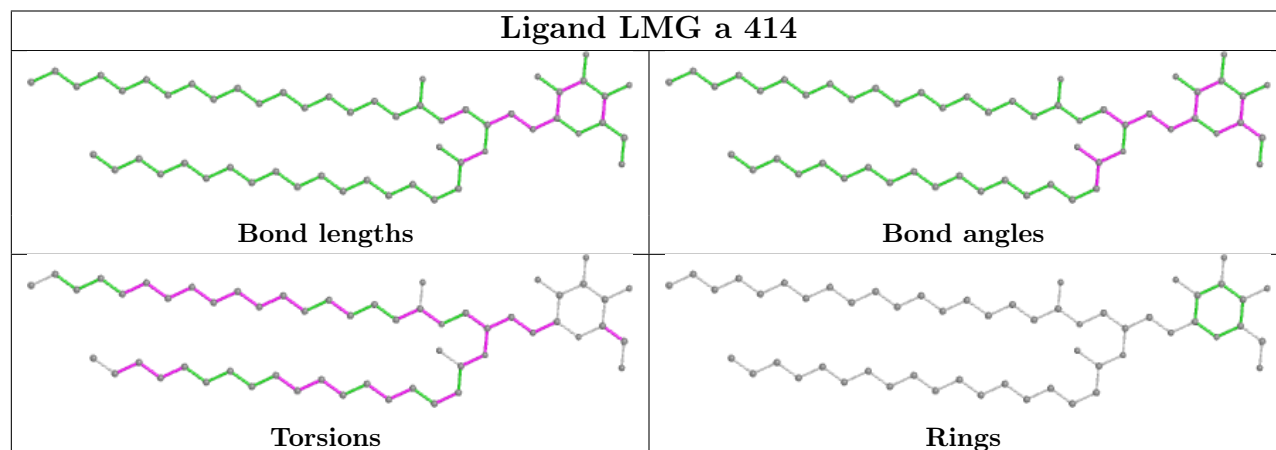
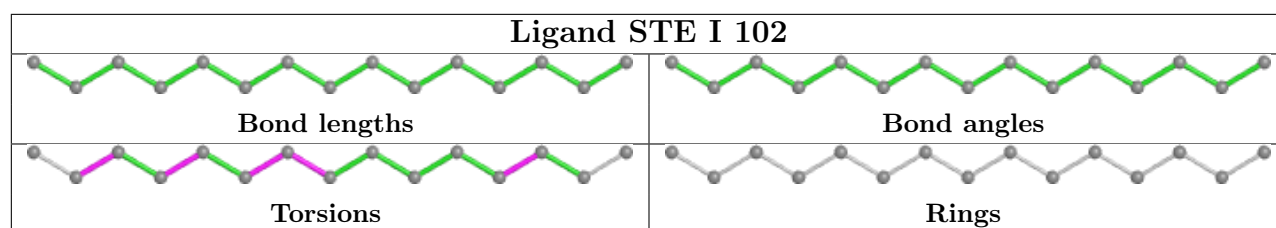


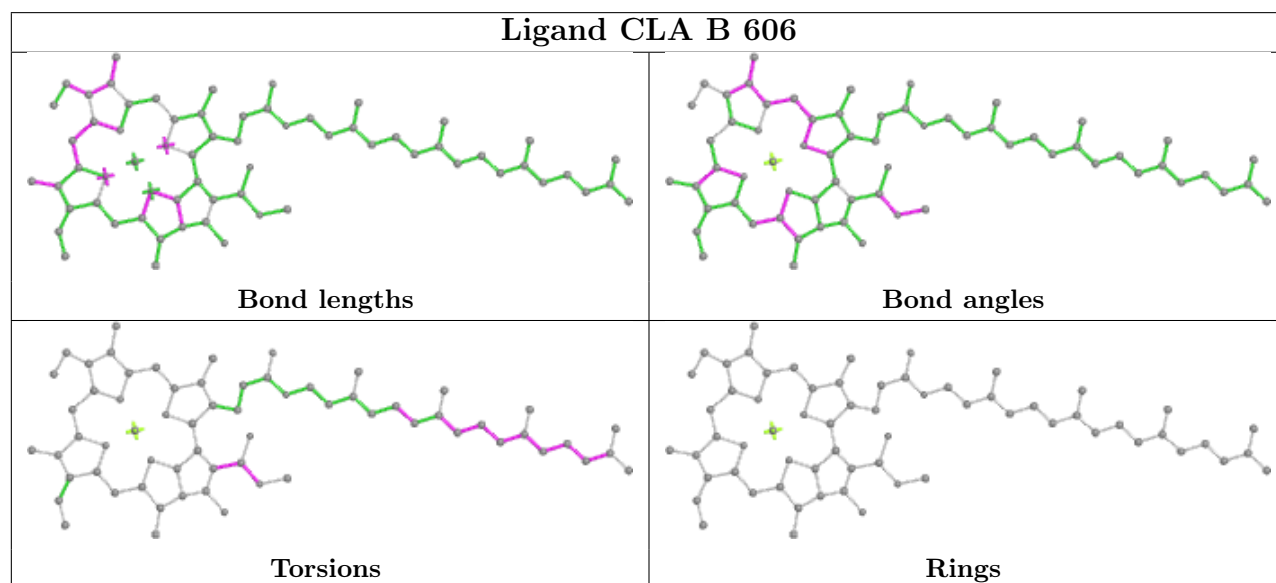
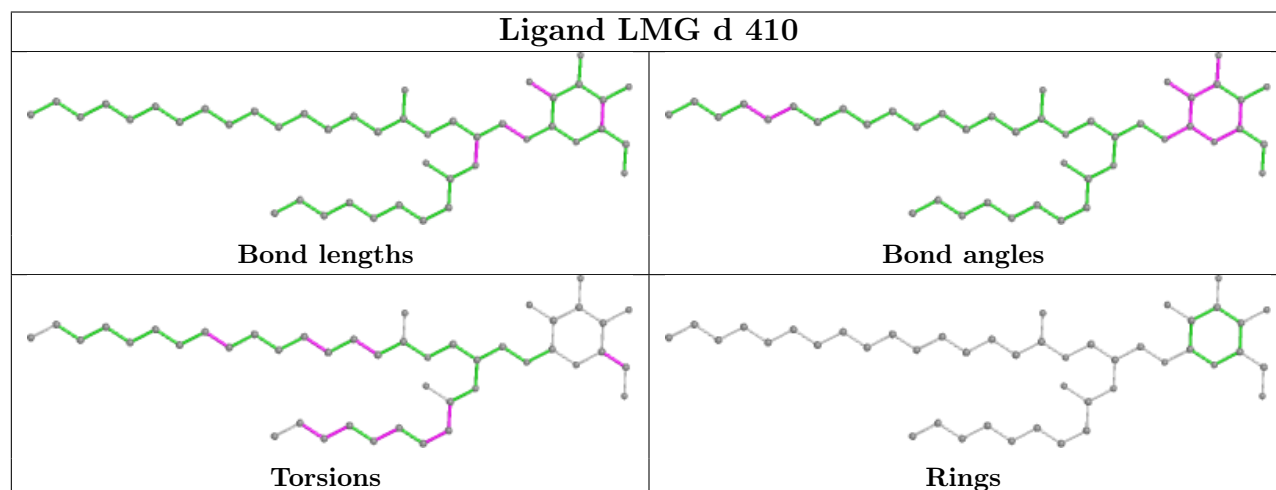
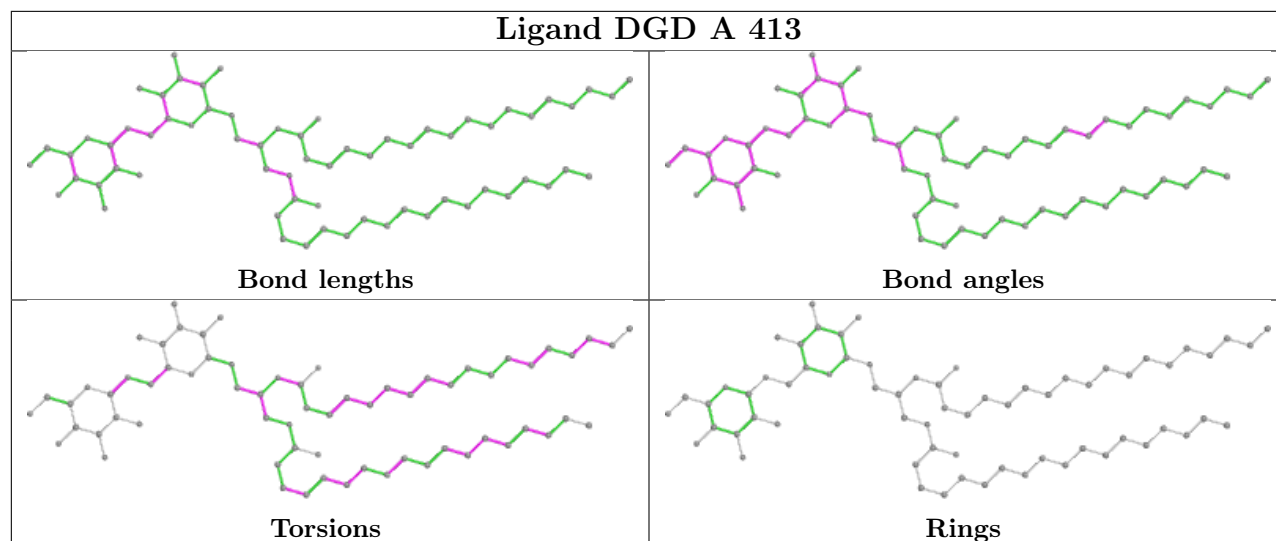


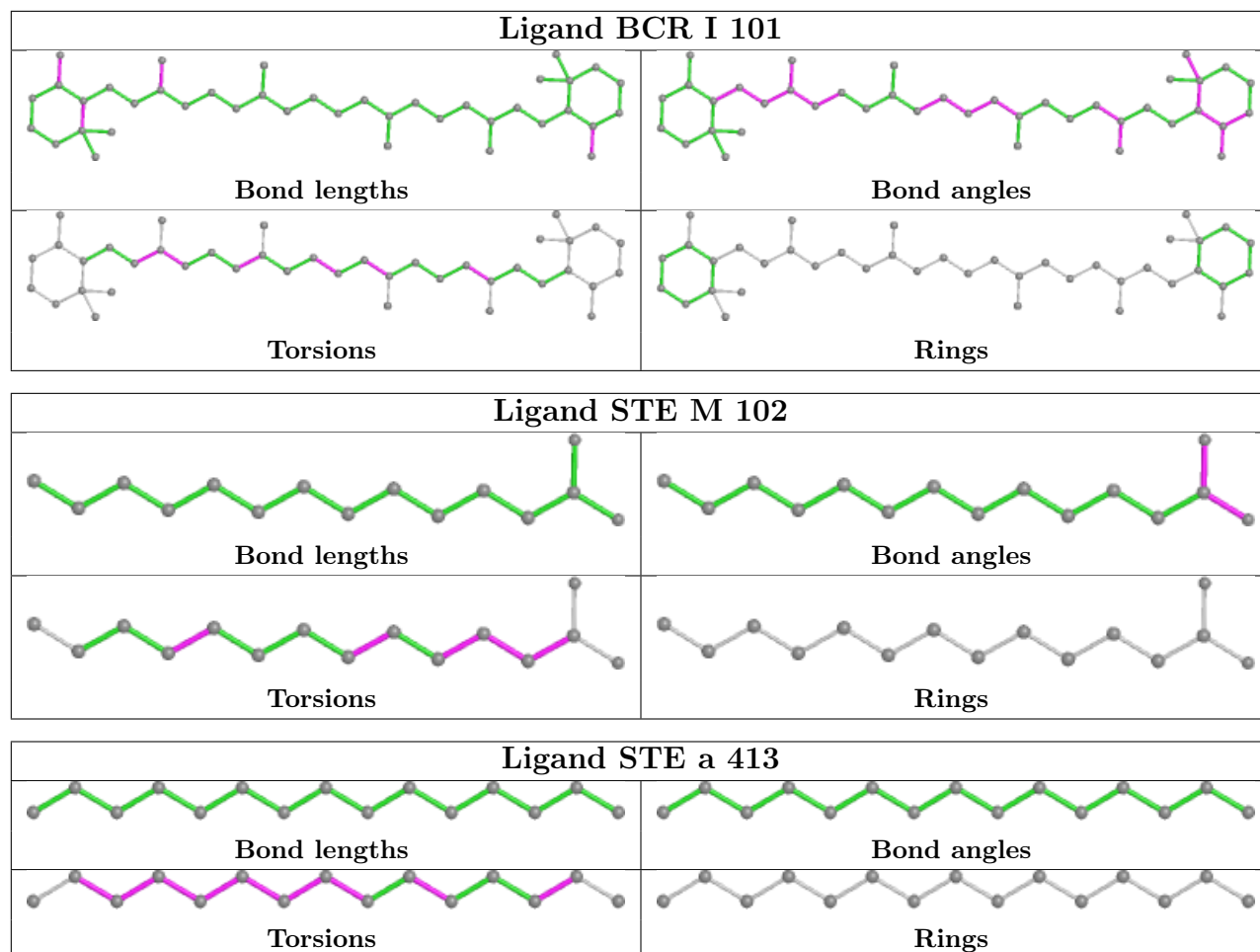




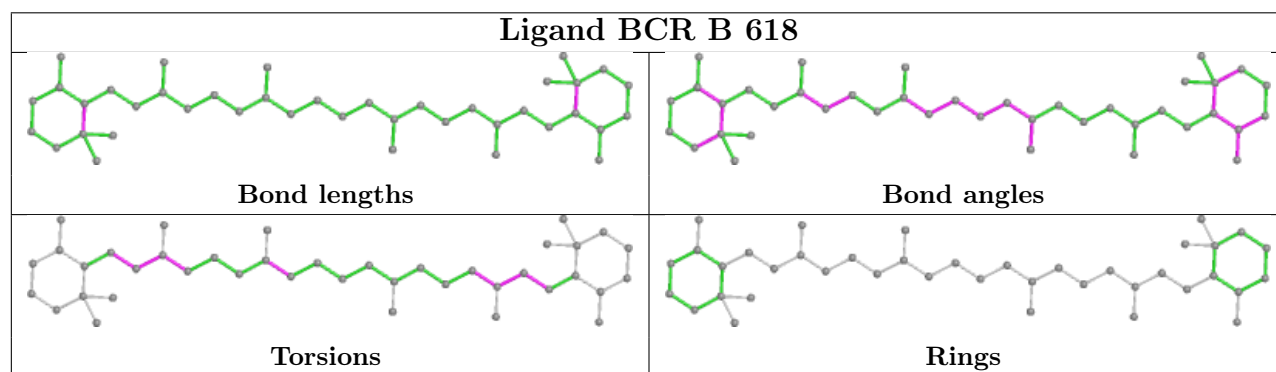
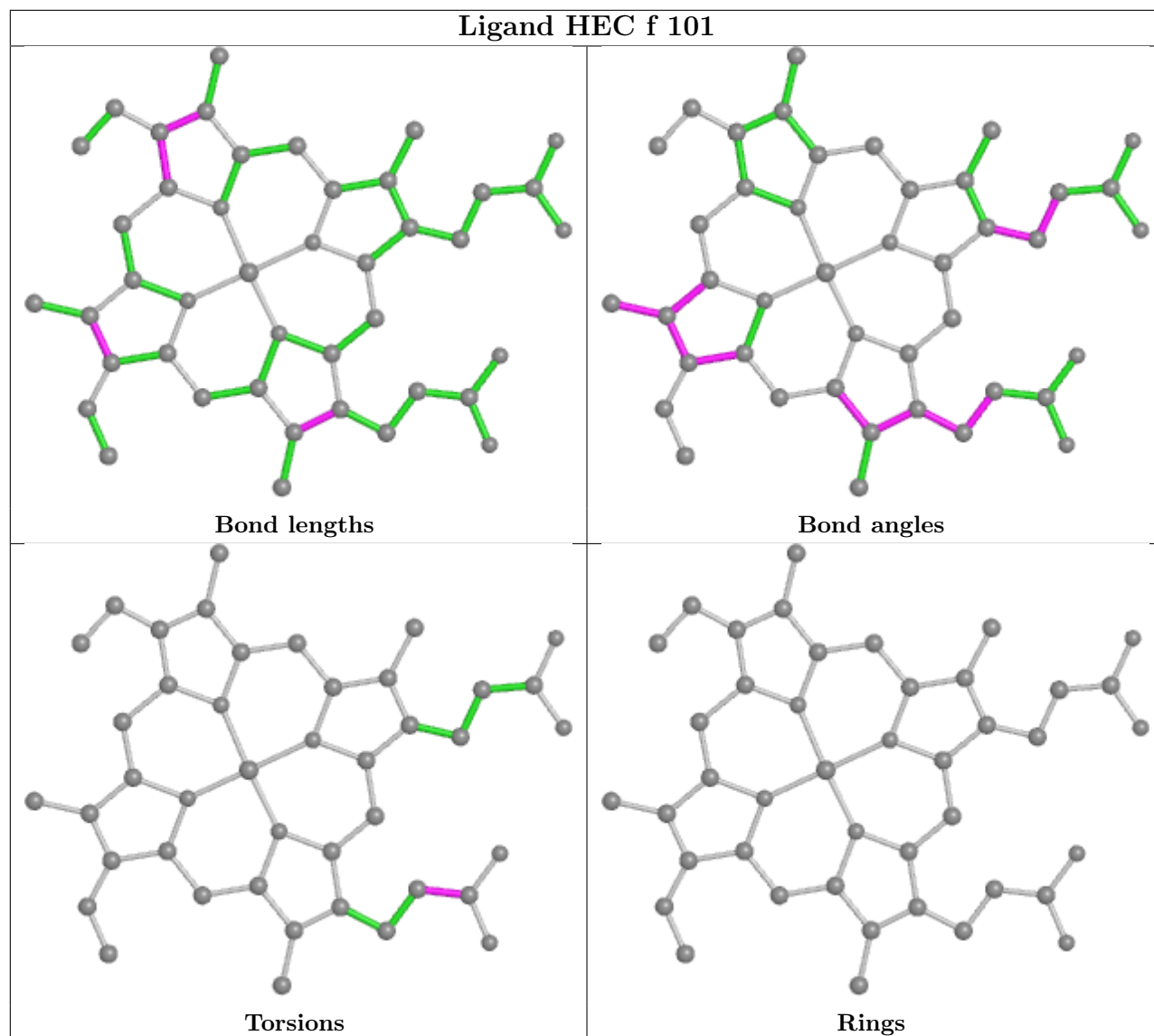


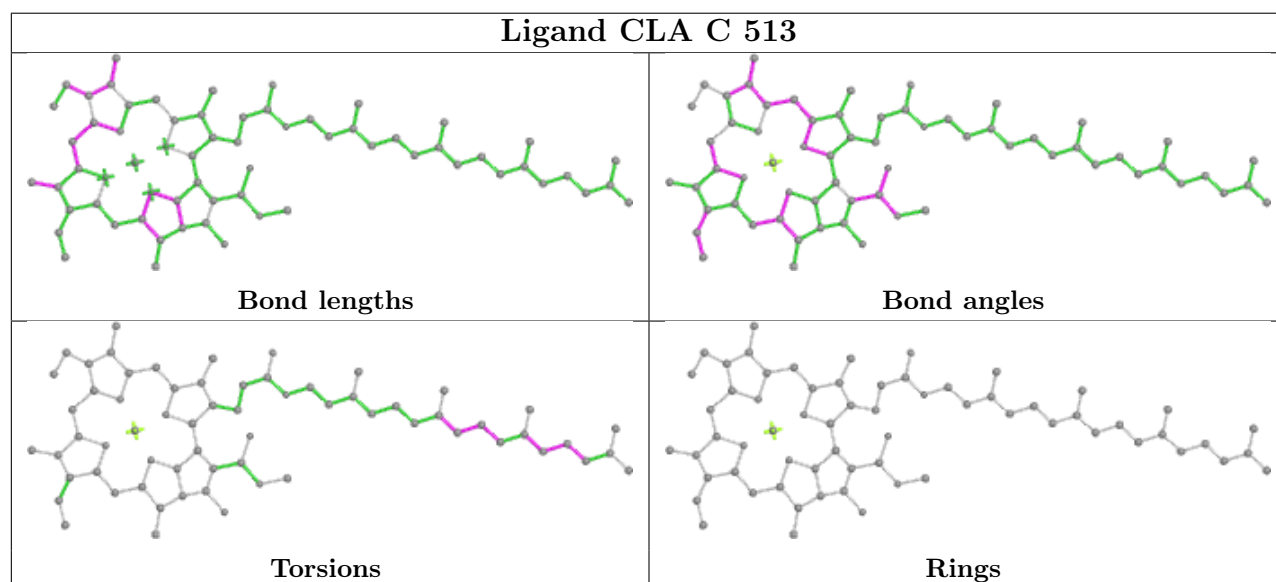
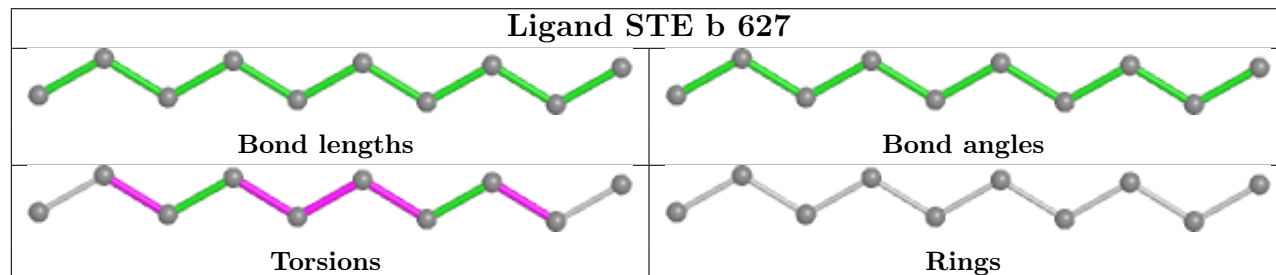
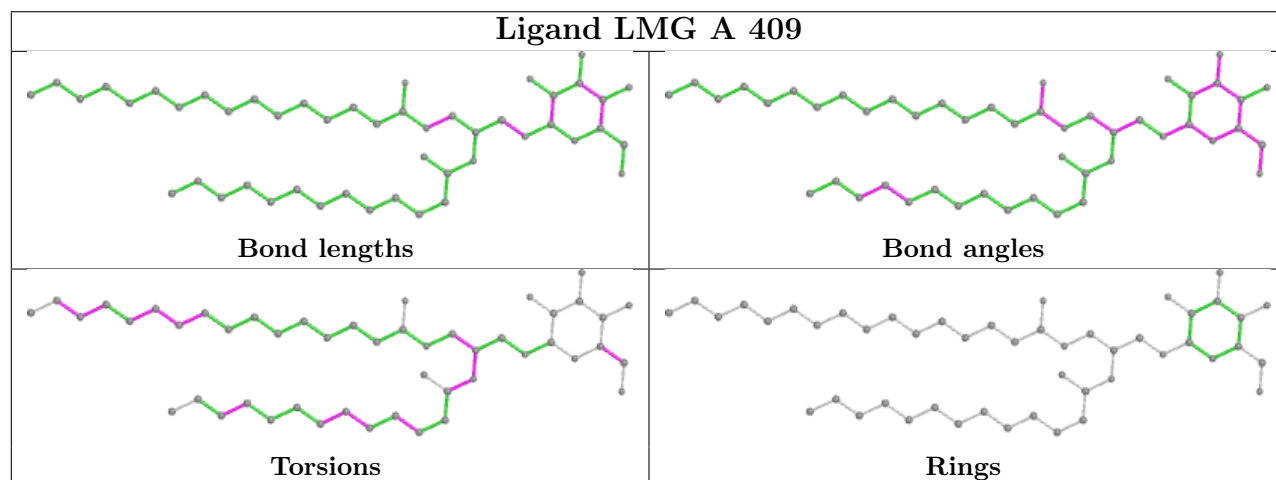
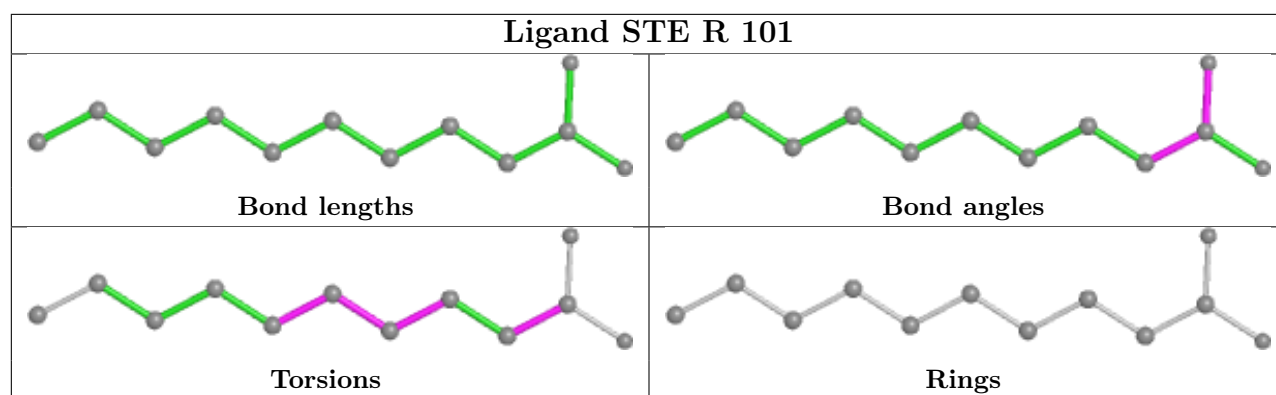


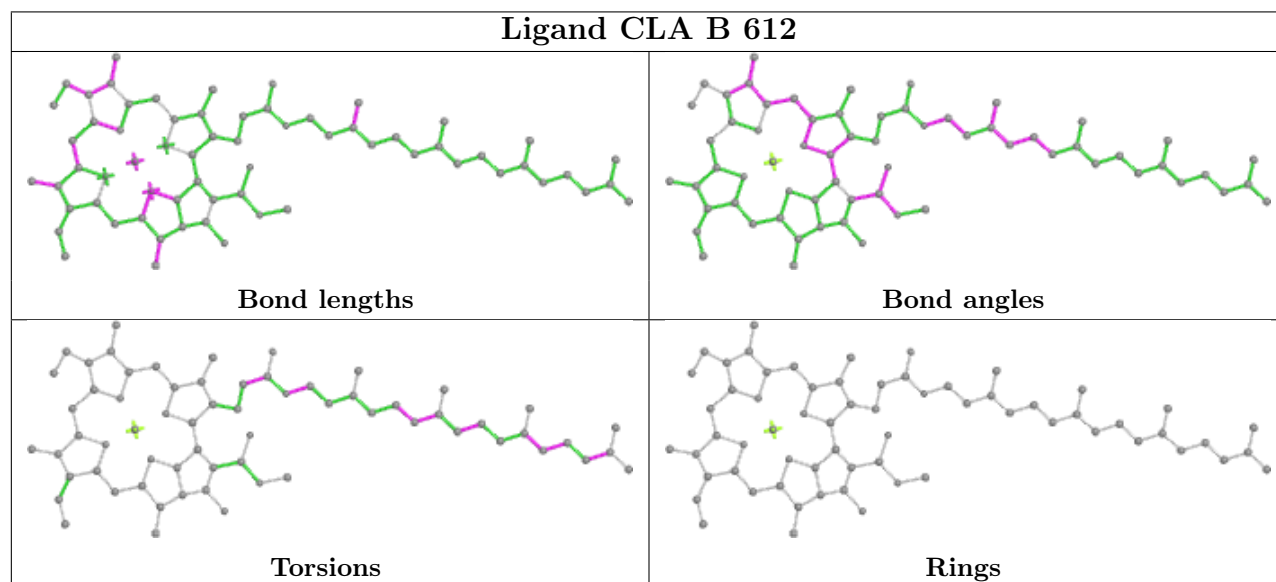
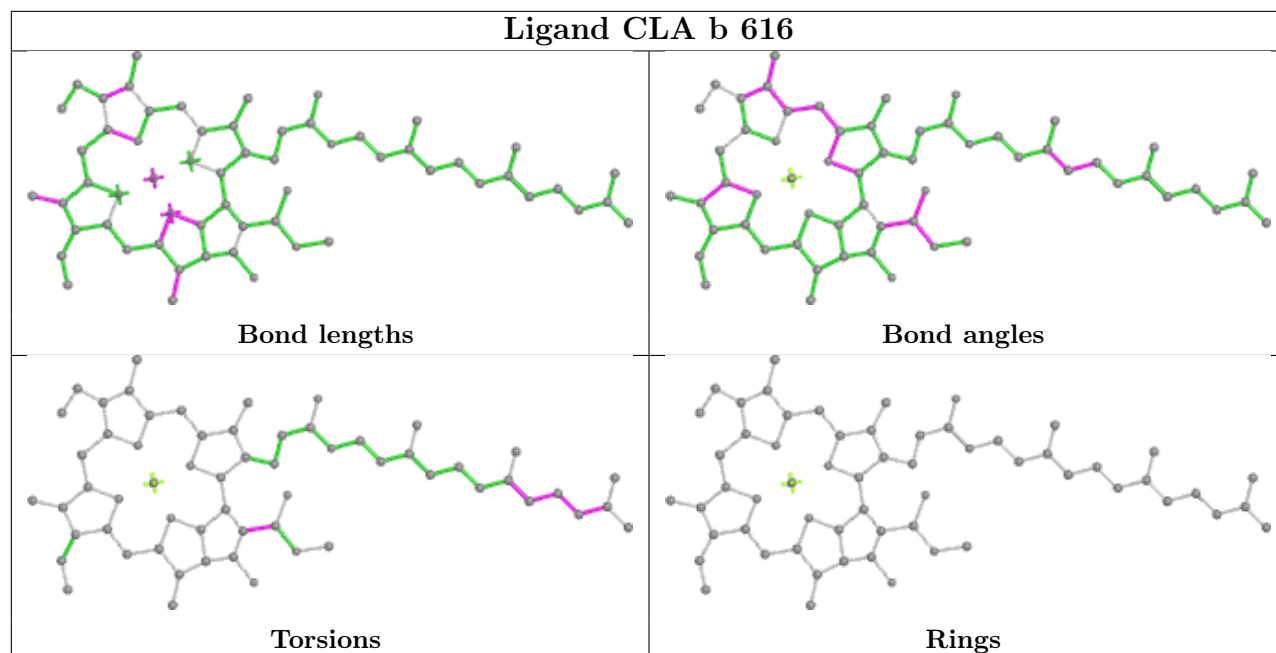


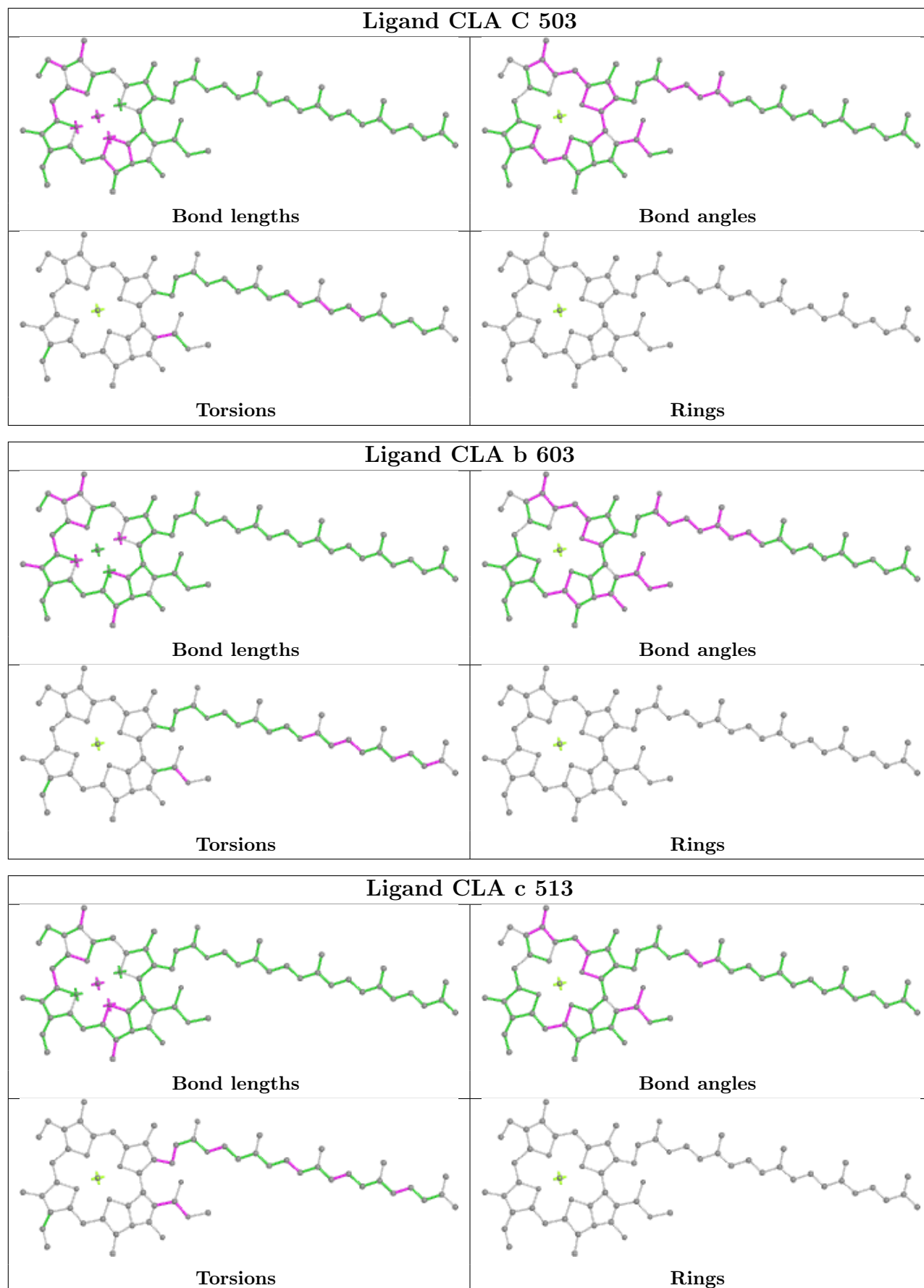


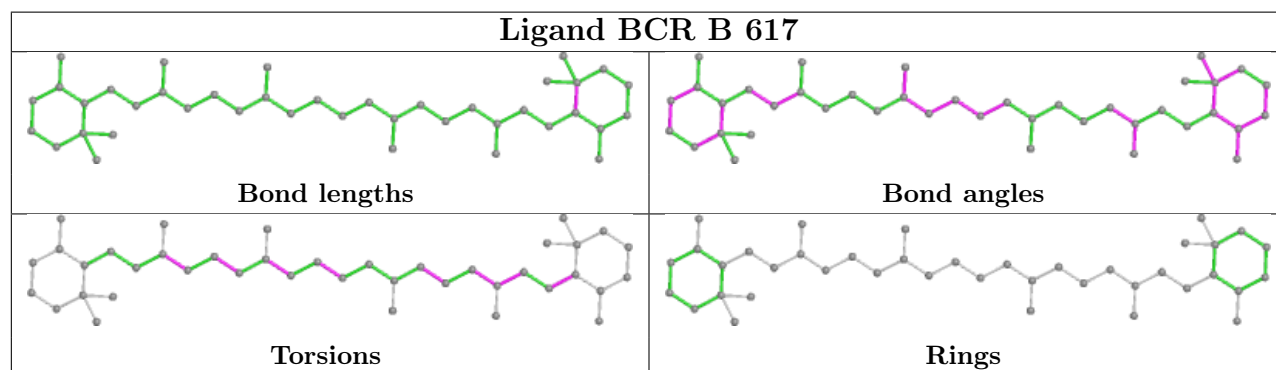
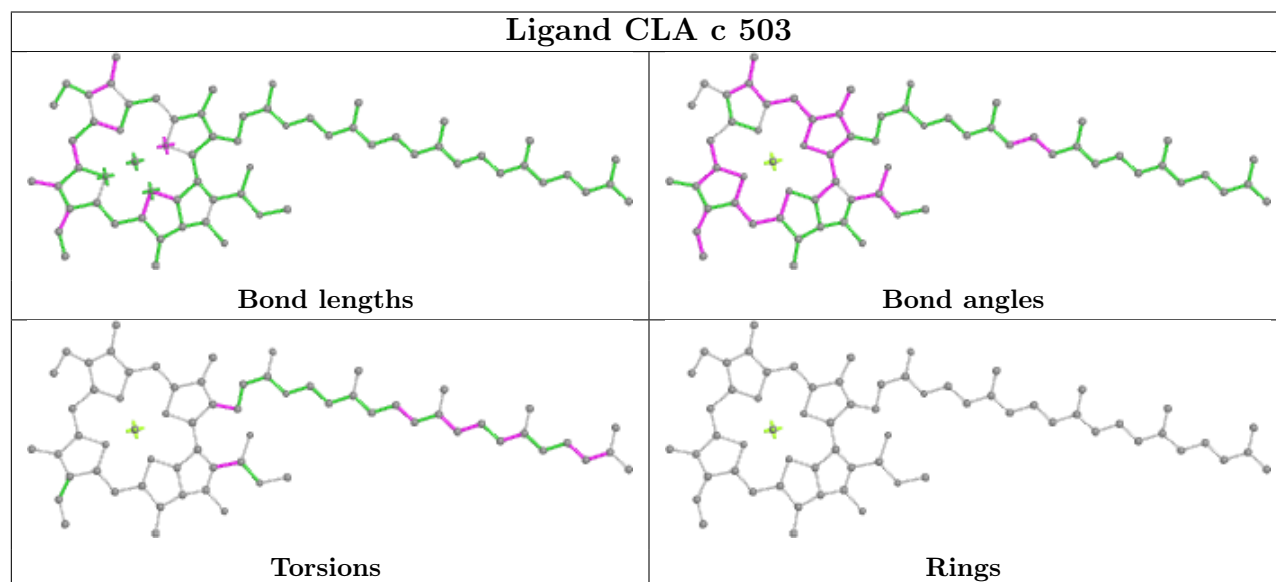
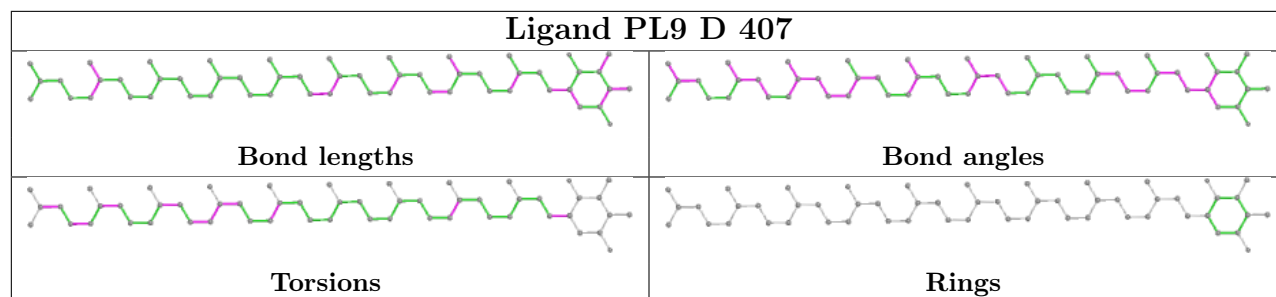


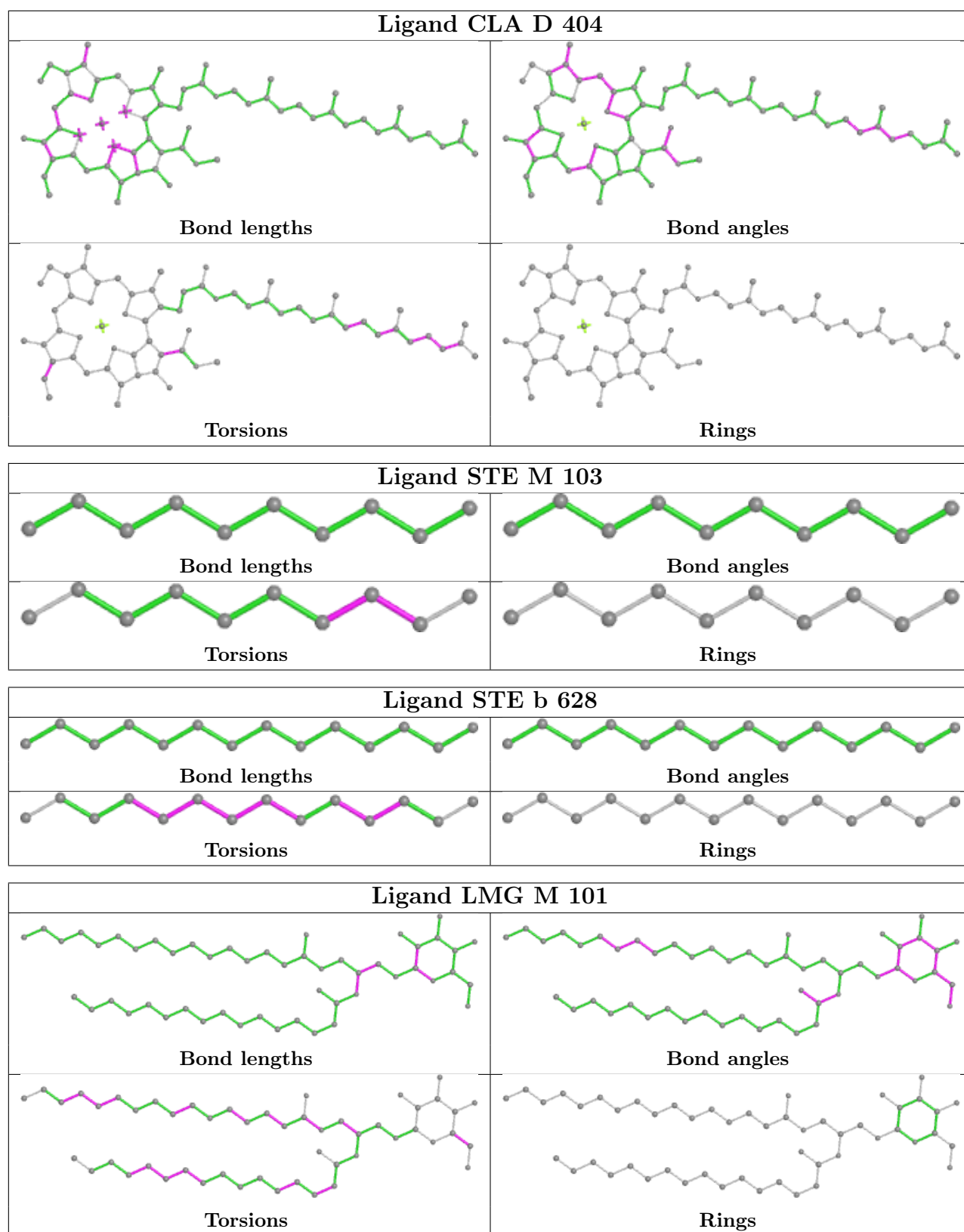


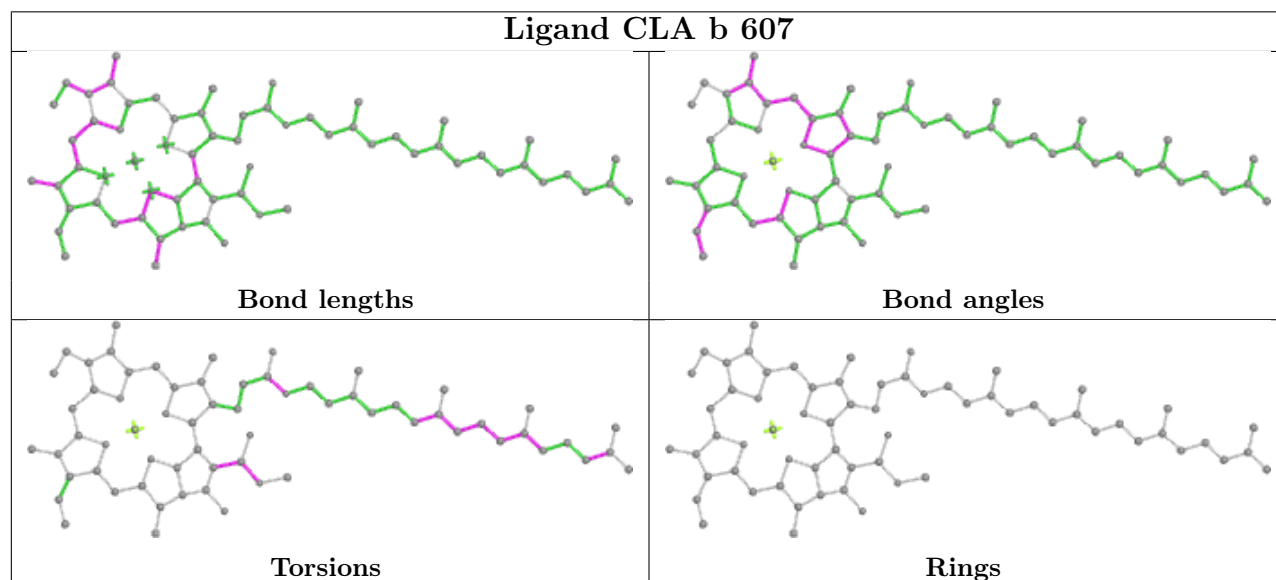
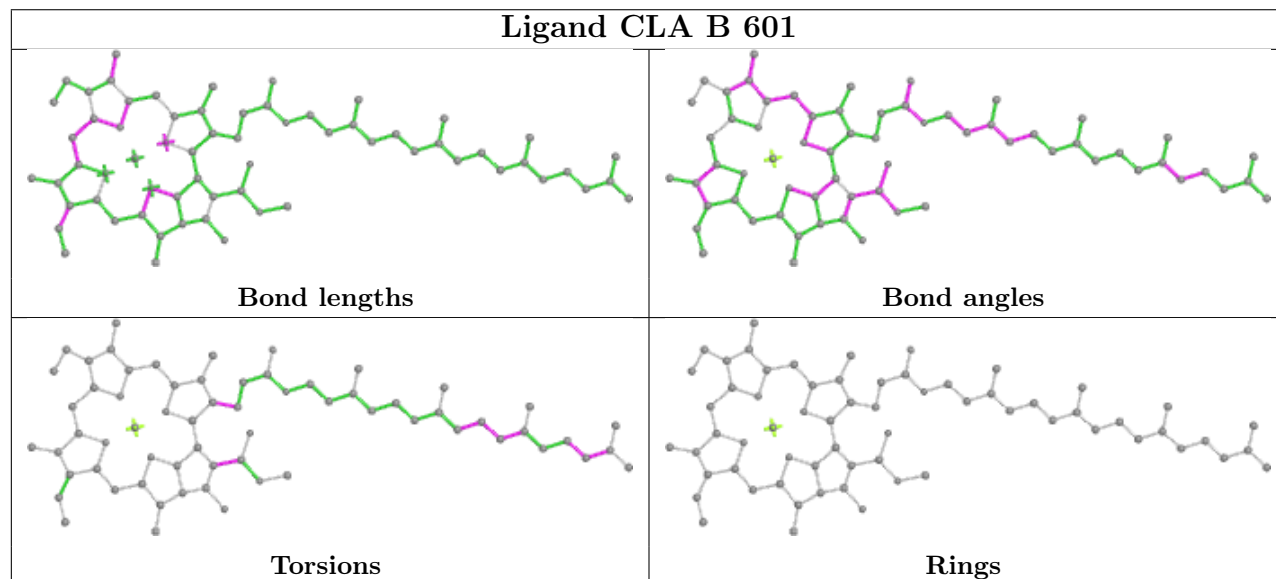
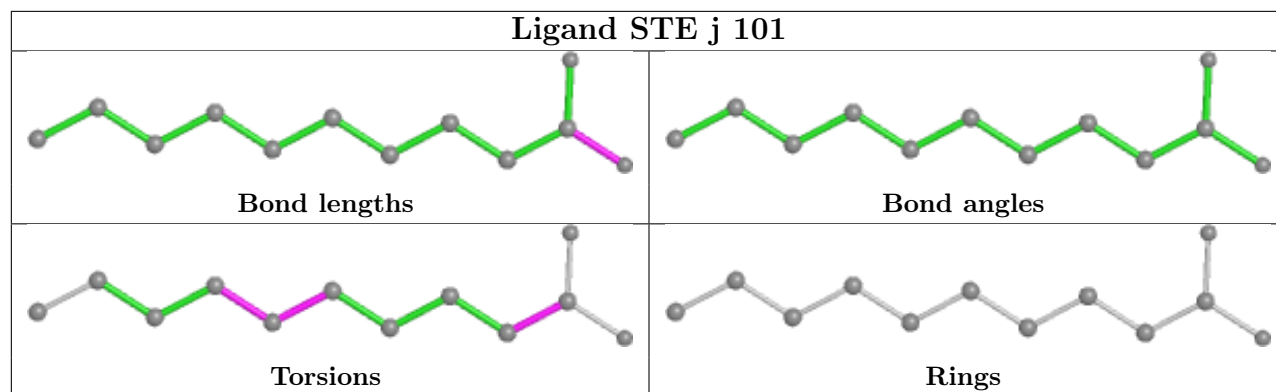


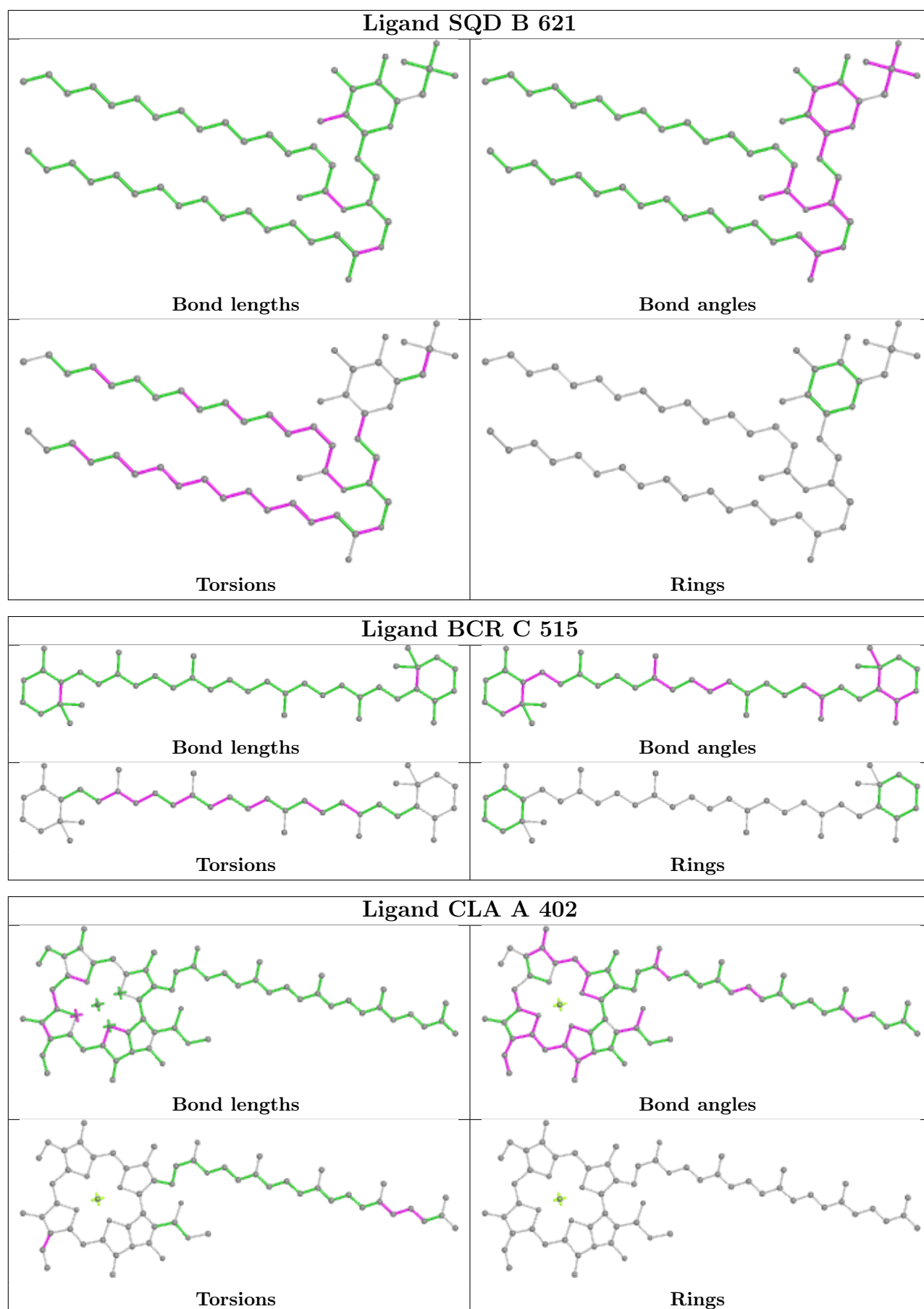




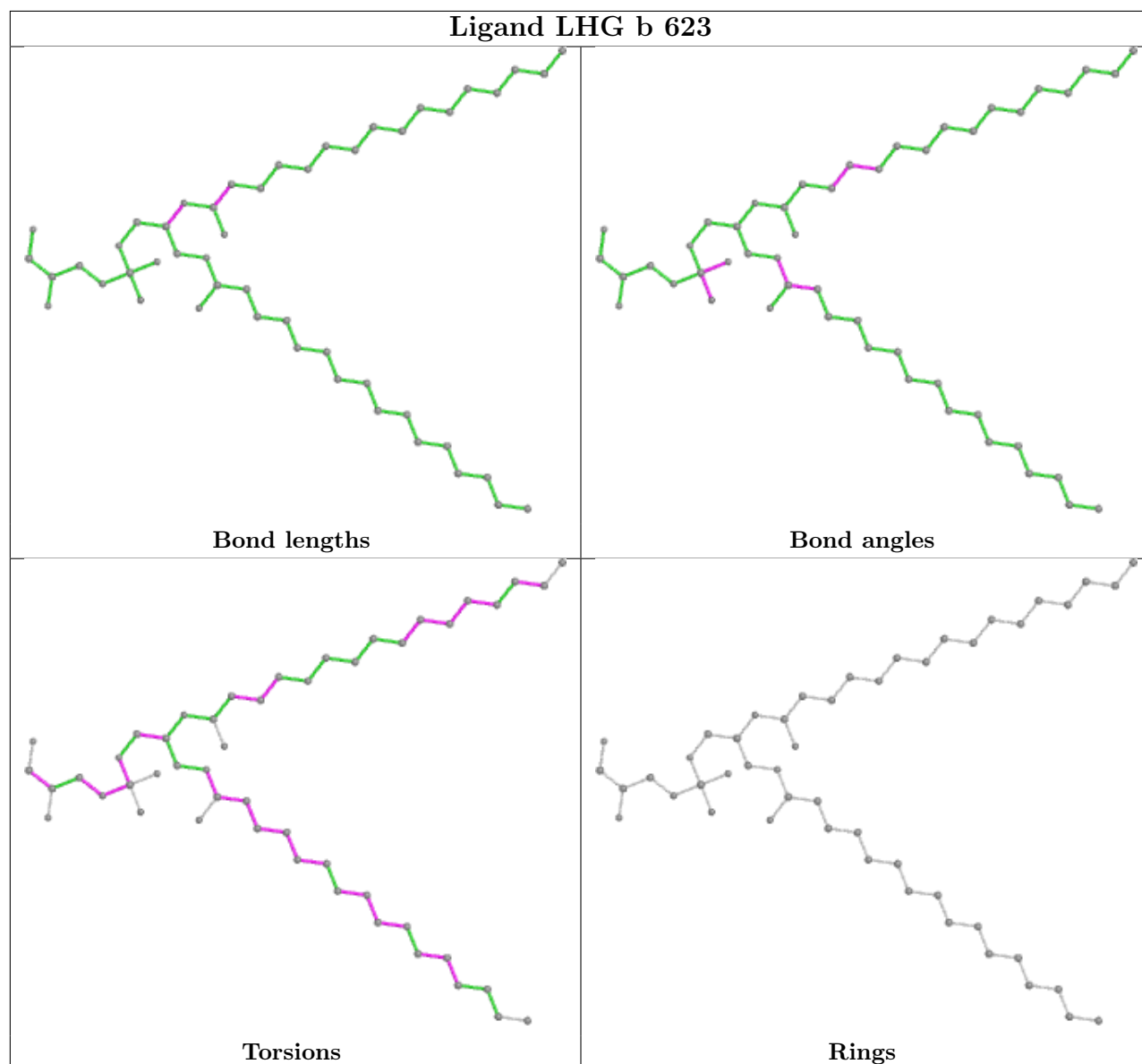
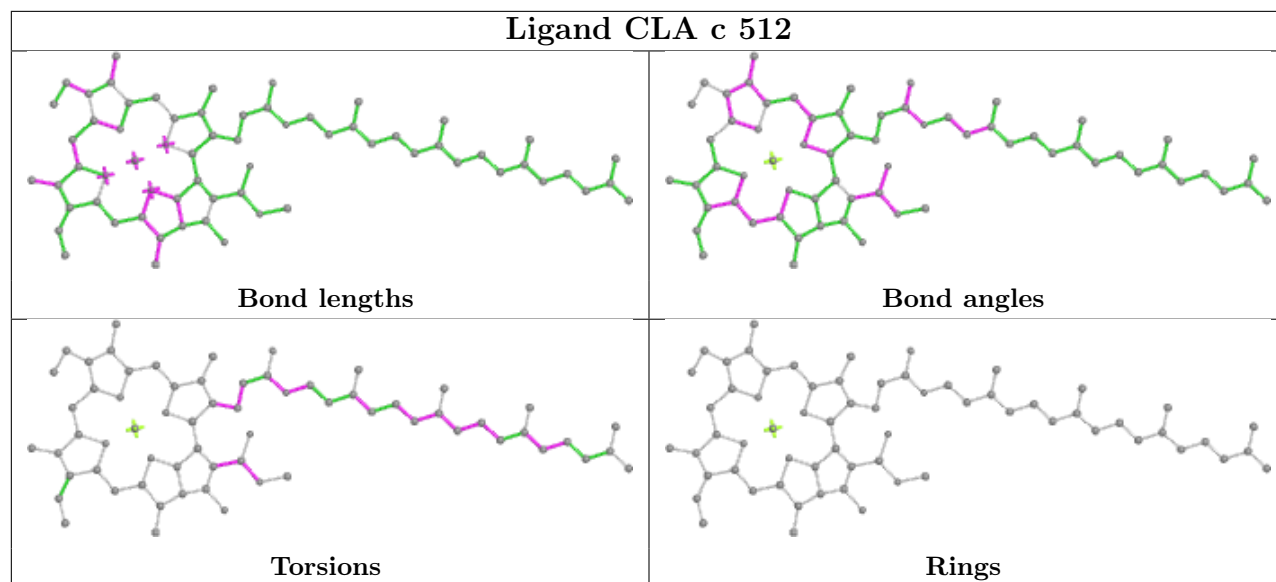


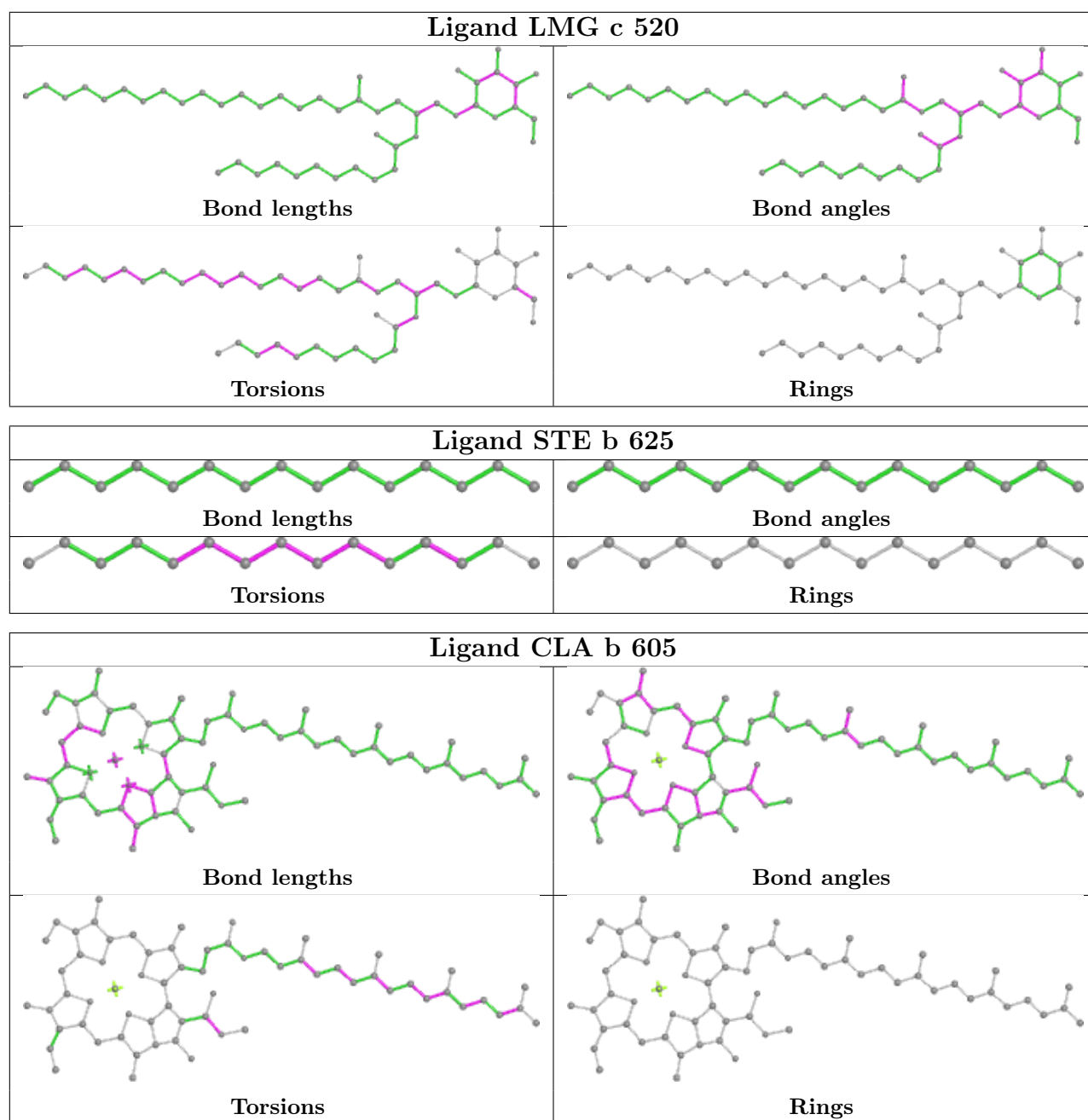


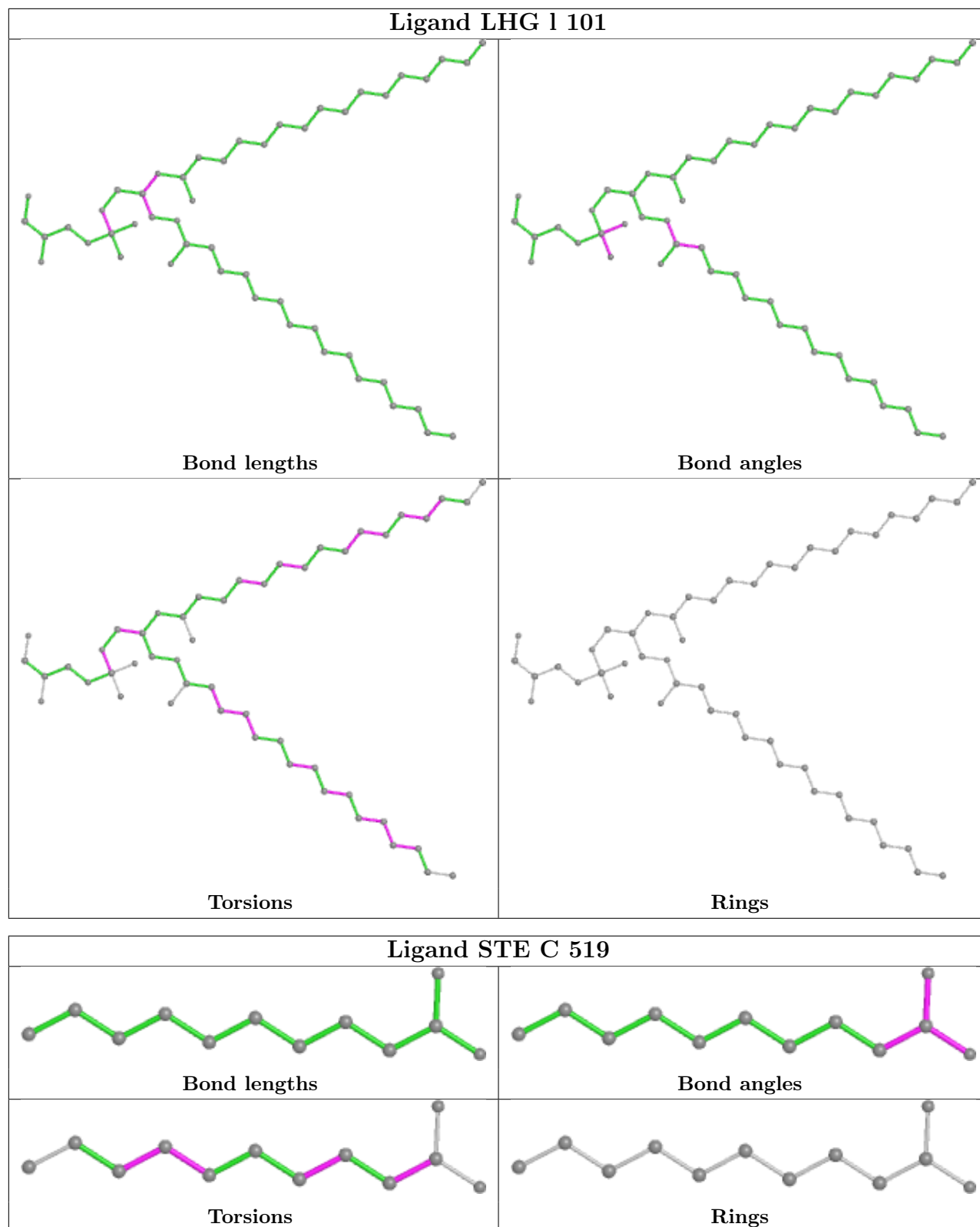


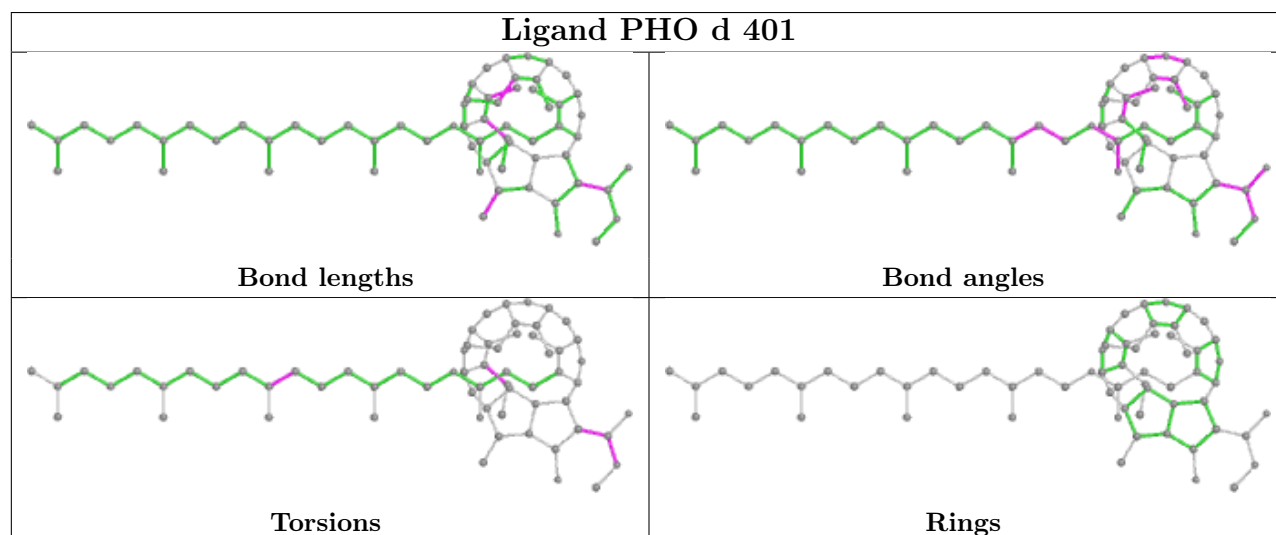
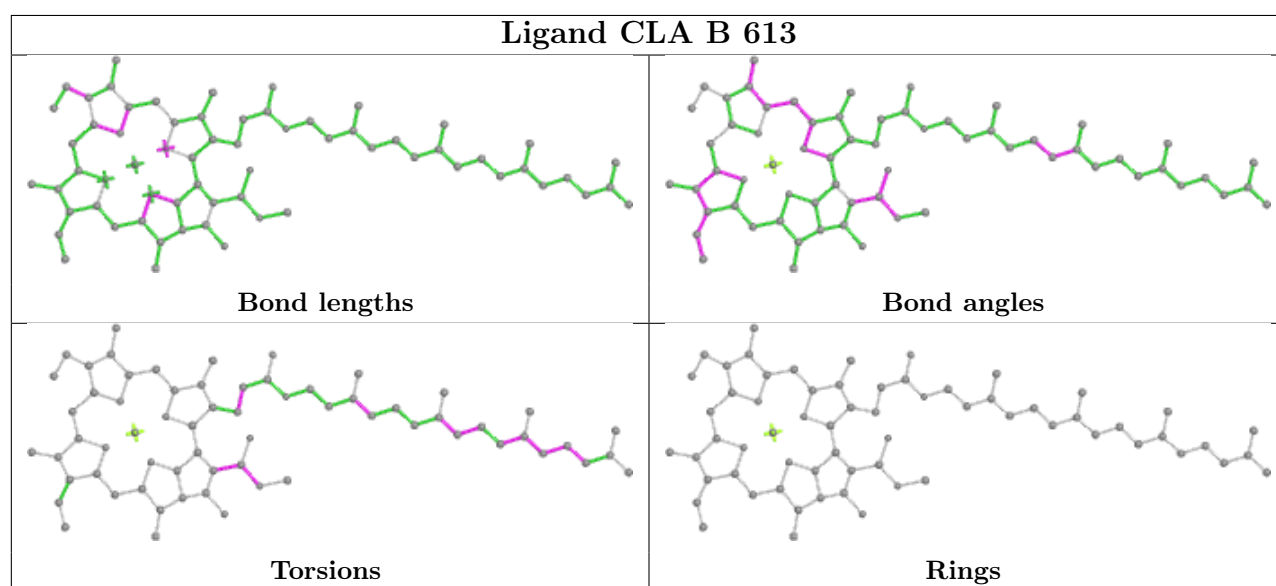
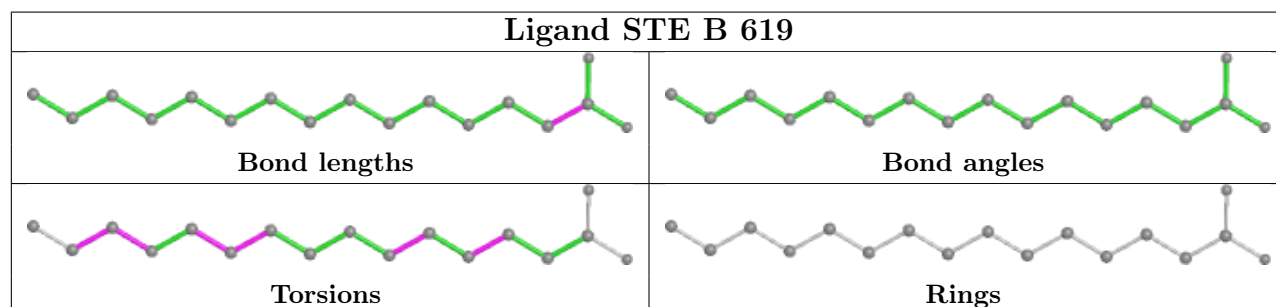
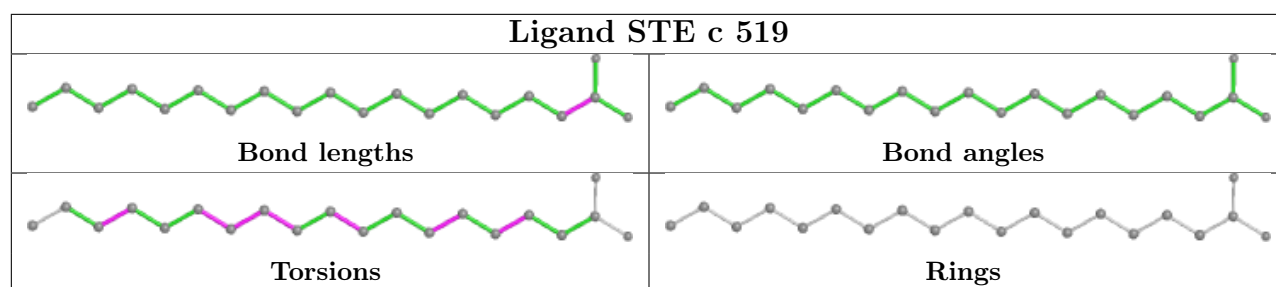


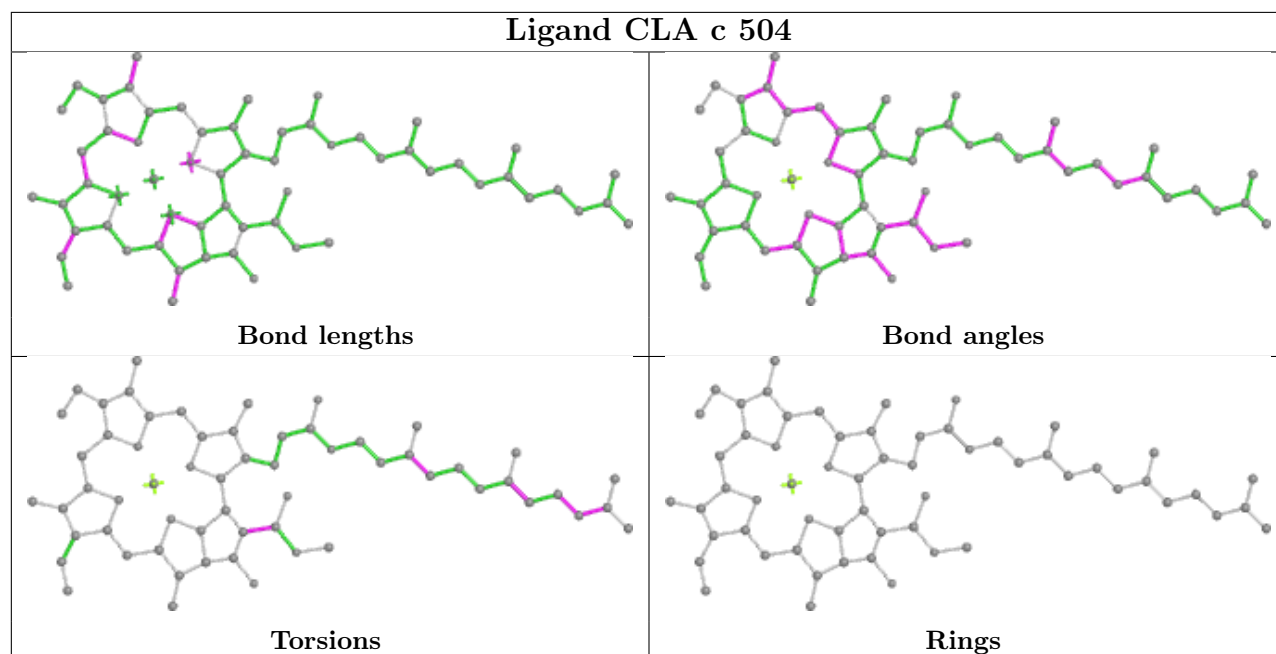
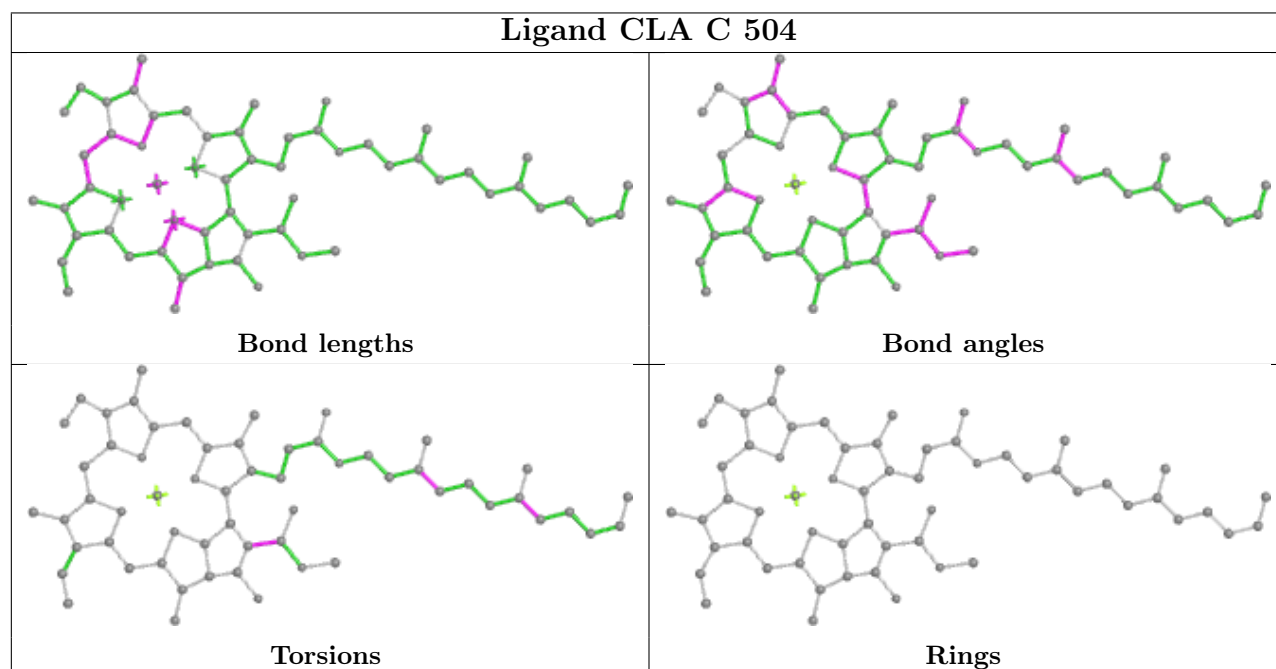
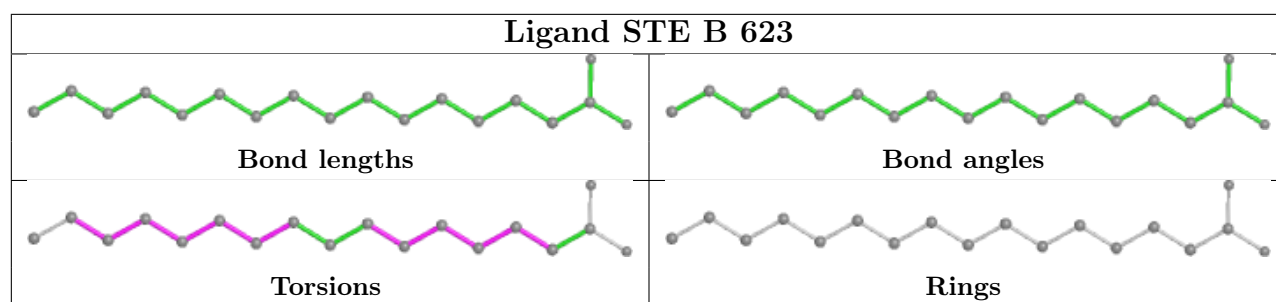


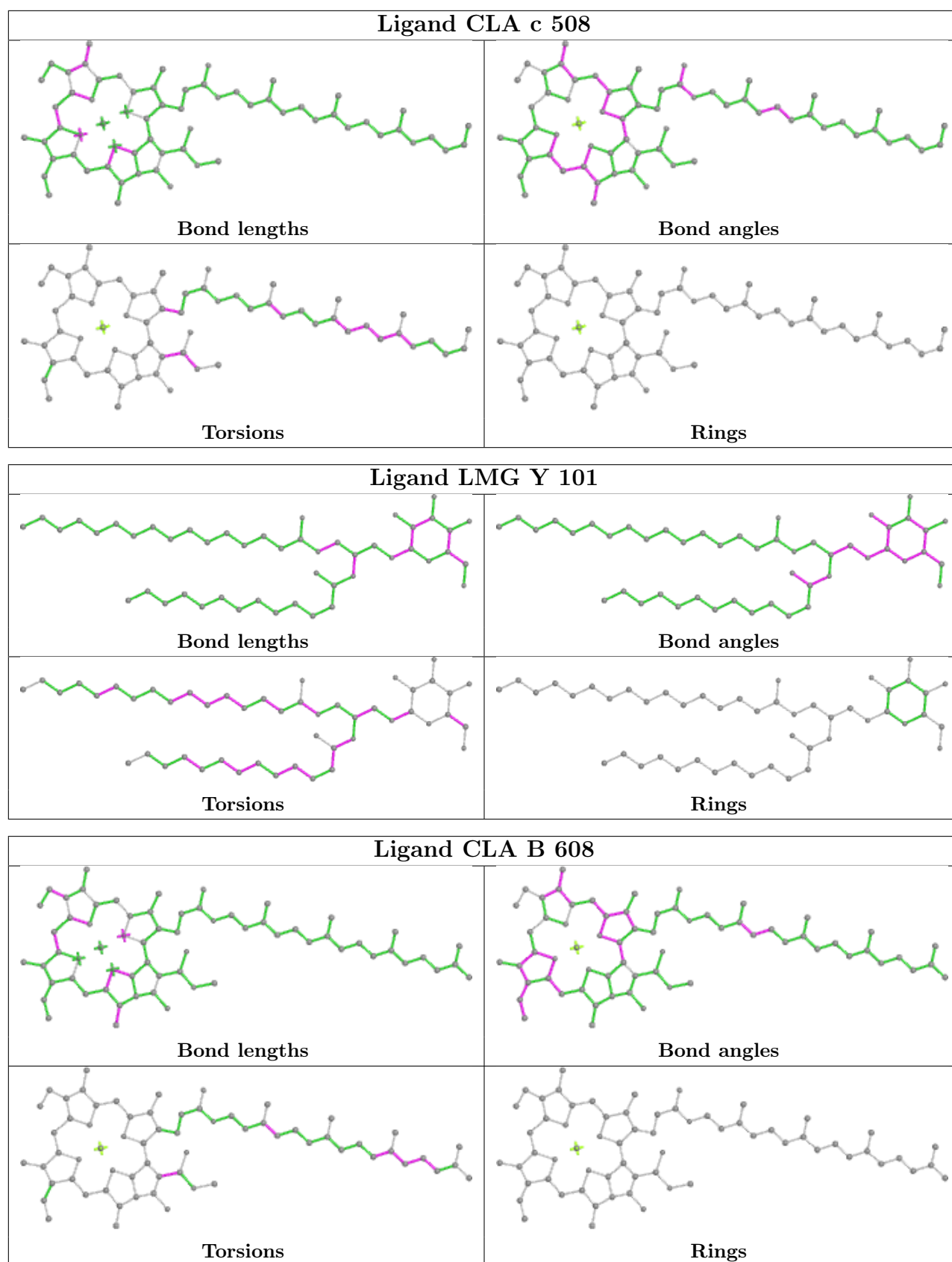


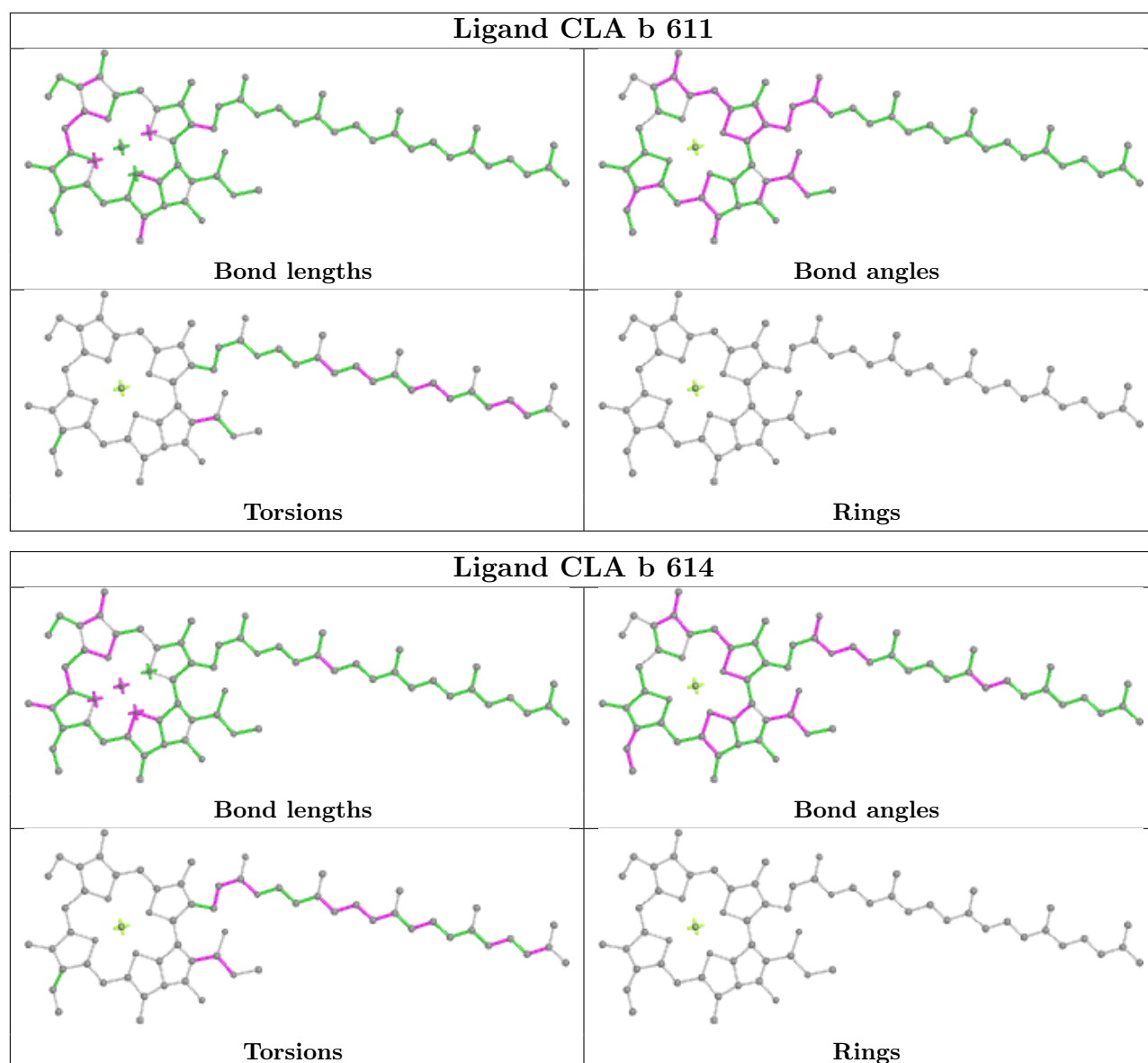












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17



## 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%)	-0.37	5 (1%) 73 78	26, 34, 53, 79	0
1	a	334/344 (97%)	-0.42	1 (0%) 94 95	27, 36, 63, 80	0
2	B	505/506 (99%)	-0.37	6 (1%) 79 82	27, 38, 68, 94	0
2	b	505/506 (99%)	-0.19	16 (3%) 47 53	29, 42, 75, 105	0
3	C	442/461 (95%)	-0.27	10 (2%) 60 66	29, 41, 59, 85	0
3	c	451/461 (97%)	-0.19	11 (2%) 59 65	31, 45, 67, 103	0
4	D	341/352 (96%)	-0.36	1 (0%) 94 95	27, 36, 54, 84	0
4	d	341/352 (96%)	-0.25	1 (0%) 94 95	27, 39, 63, 84	0
5	E	82/84 (97%)	-0.11	3 (3%) 41 47	38, 57, 76, 81	0
5	e	82/84 (97%)	0.18	8 (9%) 7 9	44, 66, 84, 88	0
6	F	34/45 (75%)	-0.49	0 100 100	40, 49, 66, 82	0
6	f	34/45 (75%)	-0.27	1 (2%) 51 57	46, 54, 79, 96	0
7	H	65/66 (98%)	-0.09	1 (1%) 73 78	36, 46, 65, 72	0
7	h	63/66 (95%)	0.23	6 (9%) 8 10	45, 56, 67, 76	0
8	I	35/38 (92%)	-0.28	1 (2%) 51 57	36, 45, 74, 84	0
8	i	35/38 (92%)	-0.09	3 (8%) 10 13	34, 46, 76, 88	0
9	J	36/40 (90%)	-0.10	3 (8%) 11 14	40, 54, 80, 89	0
9	j	36/40 (90%)	0.14	4 (11%) 5 7	44, 58, 93, 106	0
10	K	37/46 (80%)	0.09	3 (8%) 12 15	47, 58, 72, 76	0
10	k	37/46 (80%)	-0.07	0 100 100	53, 61, 77, 83	0
11	L	37/37 (100%)	-0.41	0 100 100	30, 34, 68, 78	0
11	l	36/37 (97%)	-0.34	3 (8%) 11 14	29, 36, 78, 85	0
12	M	32/36 (88%)	-0.00	1 (3%) 49 54	34, 39, 69, 76	0
12	m	31/36 (86%)	-0.05	0 100 100	32, 39, 59, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.05	12 (4%) 29 35	32, 47, 87, 132	0
13	o	244/272 (89%)	-0.21	12 (4%) 29 35	28, 46, 83, 132	0
14	R	34/41 (82%)	1.47	11 (32%) 0 0	67, 76, 92, 100	0
14	r	31/41 (75%)	3.37	25 (80%) 0 0	83, 99, 116, 127	0
15	T	29/30 (96%)	-0.48	1 (3%) 45 50	31, 36, 67, 87	0
15	t	29/30 (96%)	-0.37	2 (6%) 16 21	32, 36, 85, 92	0
16	U	97/134 (72%)	-0.20	2 (2%) 63 69	35, 49, 74, 97	0
16	u	97/134 (72%)	-0.45	0 100 100	37, 46, 64, 79	0
17	V	137/163 (84%)	-0.53	0 100 100	31, 46, 60, 84	0
17	v	137/163 (84%)	-0.22	2 (1%) 73 78	36, 52, 76, 87	0
18	X	38/41 (92%)	0.06	2 (5%) 26 31	46, 56, 77, 87	0
18	x	39/41 (95%)	0.15	4 (10%) 6 8	53, 62, 92, 107	0
19	Y	27/46 (58%)	1.15	10 (37%) 0 0	60, 79, 96, 101	0
19	y	30/46 (65%)	0.55	2 (6%) 17 22	67, 79, 92, 104	0
20	Z	62/62 (100%)	0.74	14 (22%) 0 1	59, 73, 116, 128	0
20	z	62/62 (100%)	0.77	10 (16%) 1 2	62, 79, 114, 123	0
All	All	5302/5688 (93%)	-0.18	197 (3%) 41 47	26, 43, 79, 132	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.2
14	r	14	LEU	7.1
14	r	28	VAL	6.4
20	z	33	TRP	6.3
14	r	10	LEU	6.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	FME	T	1	10/11	0.94	0.11	30,62,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	FME	t	1	10/11	0.94	0.10	33,54,70,73	0
12	FME	m	1	10/11	0.95	0.14	46,57,89,91	0
8	FME	I	1	10/11	0.96	0.20	46,62,75,90	0
12	FME	M	1	10/11	0.97	0.13	44,61,78,87	0
8	FME	i	1	10/11	0.97	0.15	45,59,72,78	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
31	STE	B	623	18/20	0.76	0.22	54,72,94,94	0
31	STE	b	626	20/20	0.76	0.24	43,74,97,100	0
31	STE	c	519	20/20	0.77	0.25	43,66,97,102	0
31	STE	x	102	20/20	0.78	0.22	51,68,91,94	0
28	LHG	a	411	42/49	0.79	0.27	66,95,118,141	0
31	STE	B	624	16/20	0.79	0.29	43,71,87,89	0
31	STE	a	412	12/20	0.79	0.42	46,79,97,98	0
31	STE	k	104	12/20	0.81	0.23	56,73,85,89	0
31	STE	b	628	14/20	0.81	0.39	57,77,110,110	0
26	LMG	D	412	33/55	0.82	0.20	36,63,101,106	0
30	BCR	H	102	40/40	0.82	0.17	35,51,67,75	0
26	LMG	c	520	48/55	0.83	0.24	35,83,112,118	0
31	STE	B	625	12/20	0.83	0.40	47,69,89,93	0
31	STE	R	101	12/20	0.83	0.29	59,80,103,104	0
22	CLA	C	512	65/65	0.84	0.19	40,61,96,105	0
31	STE	M	104	18/20	0.84	0.19	38,53,75,86	0
30	BCR	x	101	40/40	0.84	0.16	40,59,76,81	0
22	CLA	c	512	65/65	0.85	0.18	44,62,97,112	0
28	LHG	A	411	49/49	0.85	0.22	50,86,108,119	0
22	CLA	b	601	65/65	0.85	0.18	51,74,102,106	0
31	STE	b	624	16/20	0.85	0.17	53,74,88,95	0
31	STE	b	625	15/20	0.85	0.21	52,68,93,94	0
26	LMG	a	414	55/55	0.85	0.17	40,67,93,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	STE	I	102	15/20	0.85	0.17	40,58,82,84	0
31	STE	b	629	20/20	0.85	0.18	40,71,89,93	0
31	STE	J	101	12/20	0.85	0.17	51,71,80,81	0
31	STE	L	103	12/20	0.85	0.19	49,66,79,86	0
31	STE	M	103	10/20	0.85	0.16	35,56,69,69	0
27	SQD	A	412	39/54	0.86	0.20	47,69,107,111	0
31	STE	b	621	20/20	0.86	0.26	44,63,85,87	0
26	LMG	b	622	55/55	0.86	0.27	48,80,110,117	0
31	STE	B	619	17/20	0.86	0.18	37,58,76,80	0
25	PL9	a	409	55/55	0.86	0.23	42,77,102,105	0
31	STE	H	104	18/20	0.87	0.30	49,76,90,93	0
27	SQD	t	102	36/54	0.87	0.16	31,69,96,103	0
31	STE	a	413	15/20	0.87	0.17	35,65,81,92	0
25	PL9	A	408	55/55	0.88	0.22	34,70,94,98	0
22	CLA	C	513	65/65	0.88	0.20	43,65,107,118	0
29	DGD	A	413	66/66	0.88	0.14	41,65,89,95	0
22	CLA	H	101	65/65	0.88	0.17	36,70,99,108	0
30	BCR	K	102	40/40	0.88	0.14	37,57,74,74	0
27	SQD	L	101	49/54	0.88	0.16	40,66,106,121	0
31	STE	t	104	10/20	0.88	0.28	45,59,73,73	0
22	CLA	c	513	65/65	0.88	0.21	44,80,112,121	0
22	CLA	c	502	65/65	0.89	0.17	30,49,69,76	0
27	SQD	B	621	54/54	0.89	0.17	40,67,93,104	0
26	LMG	M	101	51/55	0.89	0.14	37,56,84,88	0
31	STE	C	519	12/20	0.89	0.14	41,55,68,73	0
31	STE	C	520	16/20	0.89	0.16	43,63,75,79	0
27	SQD	f	102	41/54	0.89	0.18	61,87,110,127	0
26	LMG	Y	101	48/55	0.89	0.18	54,76,95,104	0
26	LMG	c	521	49/55	0.89	0.15	32,66,98,113	0
22	CLA	a	405	65/65	0.90	0.16	20,44,90,104	0
26	LMG	c	518	37/55	0.90	0.18	49,72,93,98	0
22	CLA	c	508	64/65	0.90	0.17	36,56,98,124	0
26	LMG	A	409	48/55	0.90	0.17	36,63,86,104	0
30	BCR	d	406	40/40	0.90	0.13	30,58,103,111	0
31	STE	X	101	20/20	0.90	0.17	40,60,81,91	0
30	BCR	k	102	40/40	0.90	0.14	46,67,84,86	0
30	BCR	k	103	40/40	0.90	0.20	45,63,78,85	0
26	LMG	B	620	28/55	0.90	0.16	35,52,67,71	0
31	STE	b	627	10/20	0.91	0.29	45,58,65,68	0
31	STE	C	521	12/20	0.91	0.10	37,48,59,64	0
31	STE	b	620	16/20	0.91	0.22	42,55,83,100	0
30	BCR	k	101	40/40	0.91	0.16	48,67,82,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	STE	d	411	17/20	0.91	0.14	49,65,73,79	0
26	LMG	m	101	51/55	0.91	0.15	40,61,86,96	0
31	STE	B	622	12/20	0.91	0.09	36,57,72,72	0
26	LMG	D	408	51/55	0.91	0.20	34,66,92,114	0
26	LMG	d	410	44/55	0.92	0.15	41,61,90,108	0
22	CLA	b	616	60/65	0.92	0.15	31,48,93,99	0
22	CLA	D	405	65/65	0.92	0.15	26,50,132,139	0
22	CLA	d	405	65/65	0.92	0.15	32,56,101,116	0
31	STE	Z	101	8/20	0.92	0.14	38,65,78,78	0
27	SQD	D	409	36/54	0.92	0.17	50,78,97,114	0
29	DGD	c	517	62/66	0.92	0.17	36,64,94,109	0
31	STE	j	101	12/20	0.92	0.14	50,63,72,76	0
30	BCR	C	514	40/40	0.92	0.14	30,47,58,76	0
31	STE	t	103	14/20	0.92	0.14	41,59,67,71	0
22	CLA	B	605	65/65	0.92	0.13	29,45,82,98	0
30	BCR	K	101	40/40	0.92	0.13	45,63,82,83	0
22	CLA	c	510	65/65	0.93	0.15	36,51,66,92	0
22	CLA	c	511	65/65	0.93	0.16	41,62,80,90	0
22	CLA	B	615	60/65	0.93	0.15	23,43,96,105	0
29	DGD	c	516	62/66	0.93	0.14	36,61,97,110	0
22	CLA	C	502	65/65	0.93	0.14	29,48,70,79	0
30	BCR	B	618	40/40	0.93	0.12	24,48,68,80	0
22	CLA	C	507	65/65	0.93	0.15	25,46,67,73	0
22	CLA	C	508	65/65	0.93	0.13	29,48,112,124	0
22	CLA	b	609	65/65	0.93	0.14	31,54,74,77	0
22	CLA	b	615	65/65	0.93	0.14	27,47,67,74	0
22	CLA	C	509	65/65	0.93	0.18	31,51,68,77	0
31	STE	M	102	15/20	0.93	0.13	37,54,63,69	0
22	CLA	B	601	65/65	0.93	0.17	26,42,63,67	0
22	CLA	c	506	65/65	0.93	0.14	34,56,106,111	0
27	SQD	a	410	54/54	0.93	0.16	44,70,104,112	0
22	CLA	B	614	65/65	0.93	0.13	26,42,69,86	0
22	CLA	c	509	65/65	0.93	0.20	32,54,74,84	0
30	BCR	B	616	40/40	0.94	0.12	30,46,69,72	0
30	BCR	B	617	40/40	0.94	0.11	29,44,57,64	0
22	CLA	C	506	65/65	0.94	0.13	28,50,90,108	0
25	PL9	D	407	55/55	0.94	0.11	26,39,57,63	0
30	BCR	C	515	40/40	0.94	0.17	42,60,73,75	0
30	BCR	D	406	40/40	0.94	0.11	35,50,88,108	0
22	CLA	c	503	65/65	0.94	0.16	34,50,62,68	0
22	CLA	c	504	60/65	0.94	0.12	36,51,85,99	0
22	CLA	c	505	65/65	0.94	0.17	30,47,73,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	BCR	b	617	40/40	0.94	0.12	34,48,64,67	0
30	BCR	b	619	40/40	0.94	0.12	24,55,73,87	0
30	BCR	c	514	40/40	0.94	0.14	35,51,69,74	0
22	CLA	b	602	65/65	0.94	0.16	31,48,68,71	0
22	CLA	c	507	65/65	0.94	0.14	31,50,65,78	0
22	CLA	b	606	65/65	0.94	0.12	29,47,83,90	0
22	CLA	B	613	65/65	0.94	0.16	26,45,87,104	0
22	CLA	b	611	65/65	0.94	0.14	25,41,55,66	0
22	CLA	b	613	65/65	0.94	0.16	21,41,83,97	0
22	CLA	b	614	65/65	0.94	0.14	26,43,87,93	0
29	DGD	C	516	62/66	0.94	0.14	28,48,85,107	0
29	DGD	C	517	62/66	0.94	0.14	30,57,112,139	0
29	DGD	C	518	62/66	0.94	0.13	33,57,77,94	0
29	DGD	H	103	62/66	0.94	0.11	34,51,67,75	0
22	CLA	a	403	65/65	0.94	0.15	29,47,106,117	0
22	CLA	B	603	65/65	0.94	0.14	25,40,97,105	0
29	DGD	h	101	62/66	0.94	0.14	35,53,70,78	0
22	CLA	D	403	65/65	0.95	0.12	22,36,53,65	0
22	CLA	D	404	65/65	0.95	0.12	22,35,57,66	0
22	CLA	c	501	65/65	0.95	0.14	30,50,65,68	0
22	CLA	C	503	65/65	0.95	0.14	31,49,59,63	0
22	CLA	C	504	59/65	0.95	0.13	30,49,95,100	0
22	CLA	a	402	65/65	0.95	0.12	24,36,51,59	0
22	CLA	C	505	65/65	0.95	0.16	27,47,75,82	0
22	CLA	B	611	65/65	0.95	0.16	22,37,50,60	0
22	CLA	B	612	65/65	0.95	0.15	21,40,75,84	0
22	CLA	B	602	65/65	0.95	0.16	23,38,67,75	0
22	CLA	b	604	65/65	0.95	0.14	24,45,87,105	0
22	CLA	b	605	65/65	0.95	0.14	24,39,59,63	0
27	SQD	A	410	52/54	0.95	0.16	39,68,101,103	0
22	CLA	A	405	54/65	0.95	0.12	22,36,72,78	0
30	BCR	T	101	40/40	0.95	0.09	30,46,61,66	0
30	BCR	a	406	40/40	0.95	0.11	24,38,59,64	0
22	CLA	b	608	65/65	0.95	0.14	30,48,73,79	0
30	BCR	b	618	40/40	0.95	0.11	29,44,61,68	0
22	CLA	C	510	65/65	0.95	0.15	30,50,68,81	0
22	CLA	d	403	65/65	0.95	0.14	25,41,70,83	0
22	CLA	d	404	65/65	0.95	0.12	22,37,47,53	0
22	CLA	b	610	65/65	0.95	0.18	28,43,58,69	0
23	PHO	a	404	64/64	0.95	0.14	24,37,46,47	0
22	CLA	C	511	65/65	0.95	0.13	34,59,80,85	0
22	CLA	b	612	65/65	0.95	0.17	27,40,54,58	0

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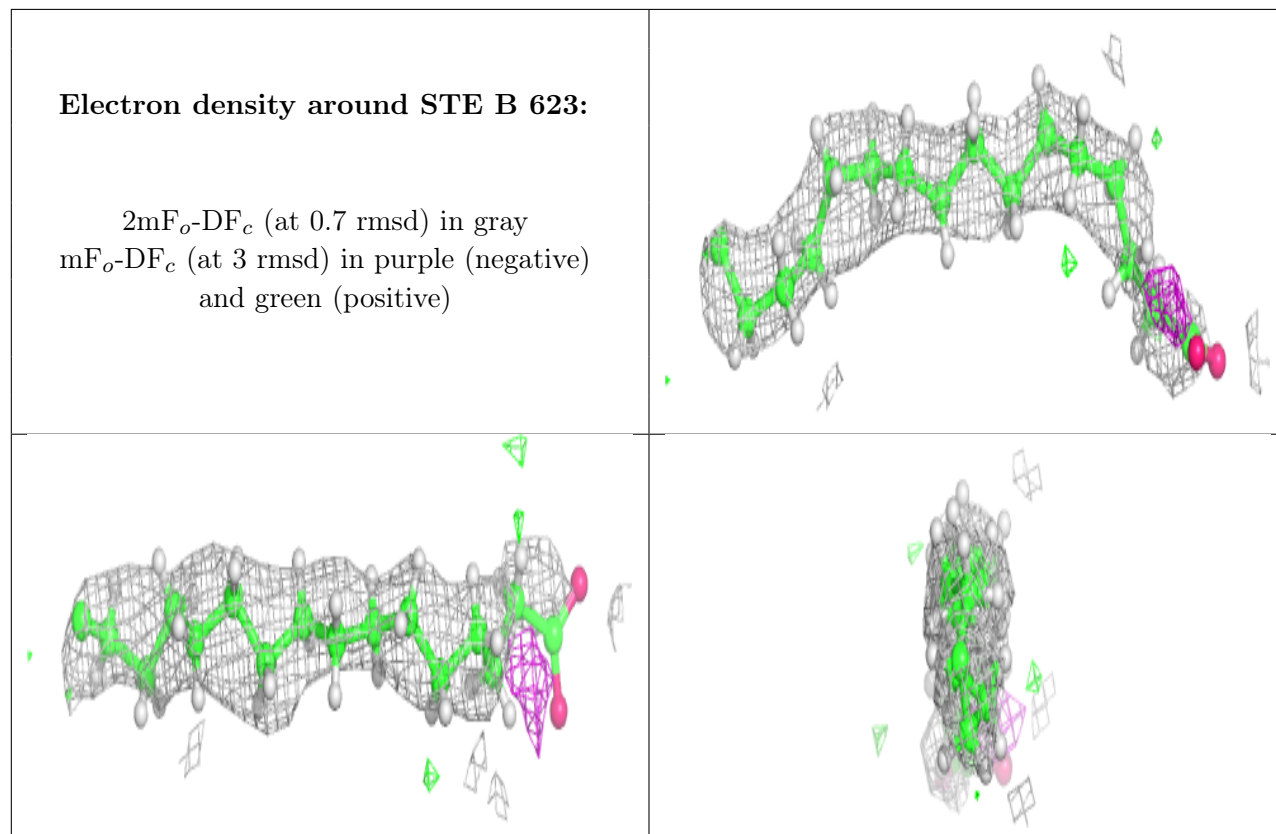
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	LHG	b	623	49/49	0.95	0.15	38,58,85,104	0
28	LHG	d	409	39/49	0.95	0.12	37,55,73,83	0
22	CLA	A	403	65/65	0.95	0.15	23,42,94,109	0
25	PL9	d	407	55/55	0.95	0.11	25,40,54,60	0
22	CLA	B	608	65/65	0.95	0.12	27,43,60,65	0
22	CLA	C	501	65/65	0.96	0.12	25,43,59,65	0
22	CLA	b	607	65/65	0.96	0.12	26,42,86,96	0
22	CLA	A	402	65/65	0.96	0.11	19,33,52,62	0
28	LHG	l	101	49/49	0.96	0.12	34,50,65,71	0
30	BCR	I	101	40/40	0.96	0.09	22,40,52,54	0
23	PHO	A	404	64/64	0.96	0.12	15,35,45,47	0
23	PHO	D	401	64/64	0.96	0.12	26,39,51,54	0
22	CLA	B	607	65/65	0.96	0.13	27,43,71,75	0
23	PHO	d	401	64/64	0.96	0.12	25,43,55,67	0
22	CLA	B	604	65/65	0.96	0.14	21,38,53,63	0
29	DGD	c	515	62/66	0.96	0.11	31,49,85,92	0
22	CLA	b	603	65/65	0.96	0.15	26,43,82,91	0
22	CLA	B	609	65/65	0.96	0.14	25,39,49,58	0
22	CLA	B	610	65/65	0.96	0.15	19,38,54,62	0
28	LHG	D	410	49/49	0.96	0.11	31,47,58,65	0
28	LHG	D	411	47/49	0.96	0.13	27,54,84,95	0
28	LHG	D	413	49/49	0.96	0.12	32,48,80,93	0
30	BCR	t	101	40/40	0.96	0.09	28,44,55,63	0
33	BCT	d	402	4/4	0.96	0.17	35,40,52,62	0
34	HEC	F	101	43/43	0.96	0.12	37,54,73,76	0
34	HEC	f	101	43/43	0.96	0.14	44,62,87,99	0
35	NA	V	202	1/1	0.96	0.22	61,61,61,61	0
28	LHG	L	102	49/49	0.97	0.10	30,47,67,80	0
24	CL	A	407	1/1	0.97	0.06	39,39,39,39	0
34	HEC	V	201	43/43	0.97	0.13	25,39,48,49	0
22	CLA	B	606	65/65	0.97	0.12	18,39,81,92	0
34	HEC	v	201	43/43	0.97	0.12	31,42,53,61	0
28	LHG	d	408	49/49	0.97	0.11	28,48,60,65	0
33	BCT	D	402	4/4	0.98	0.18	28,35,46,55	0
24	CL	a	407	1/1	0.99	0.07	34,34,34,34	0
24	CL	a	408	1/1	0.99	0.04	35,35,35,35	0
24	CL	A	406	1/1	0.99	0.09	35,35,35,35	0
32	OEX	C	522	10/10	0.99	0.14	26,33,37,38	0
32	OEX	a	415	10/10	0.99	0.13	26,34,36,40	0
21	FE2	A	401	1/1	0.99	0.10	32,32,32,32	0
21	FE2	a	401	1/1	1.00	0.07	36,36,36,36	0

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



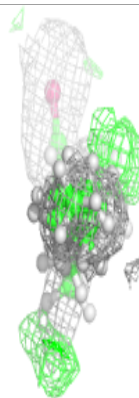
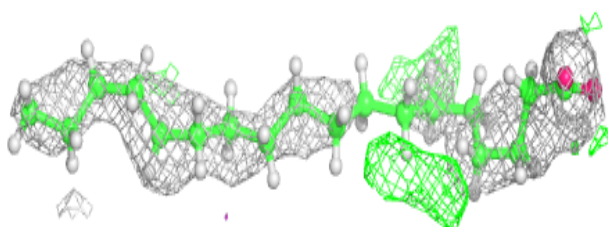
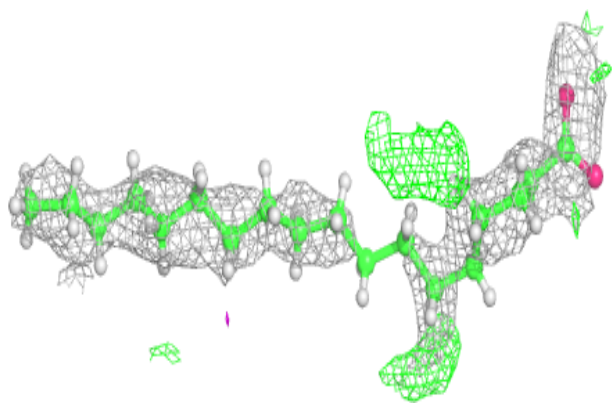
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



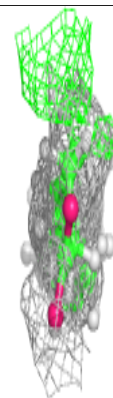
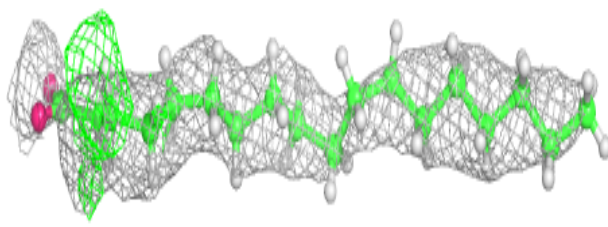
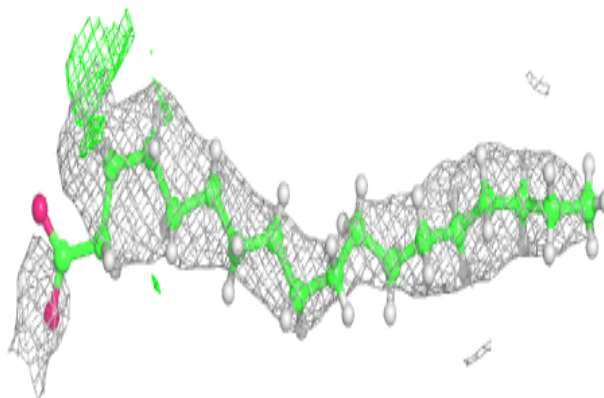


**Electron density around STE b 626:**

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

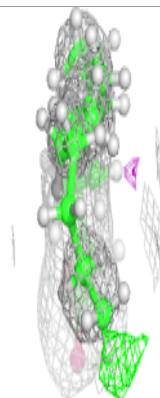
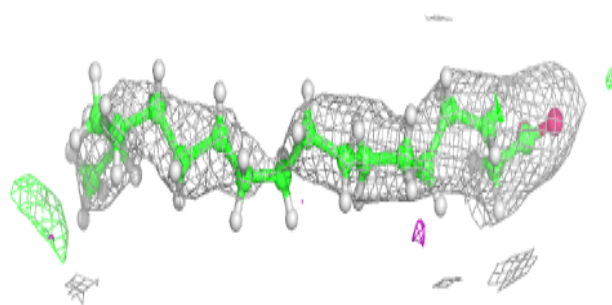
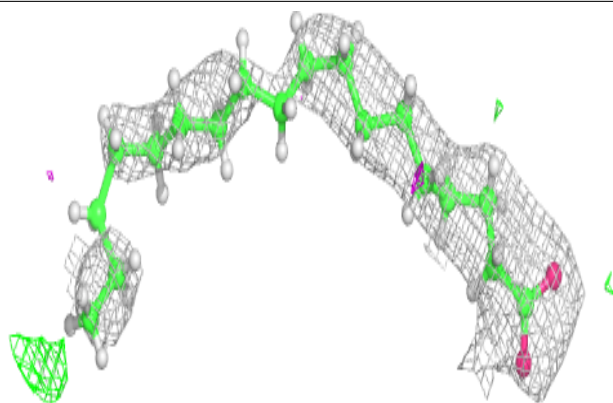
**Electron density around STE c 519:**

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

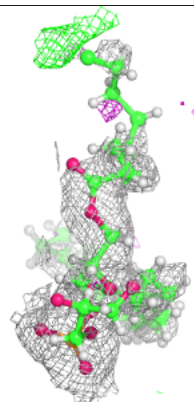
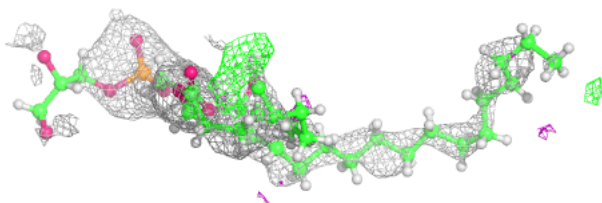
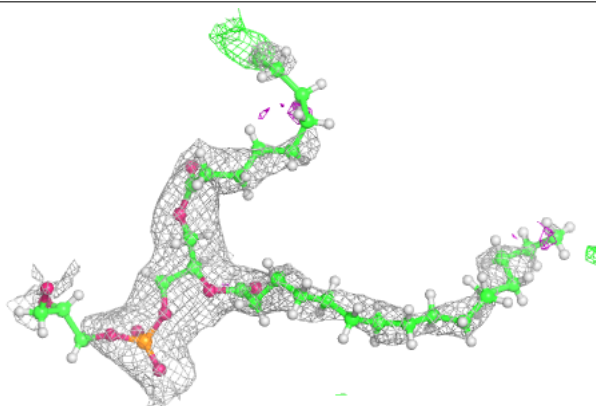


**Electron density around STE x 102:**

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

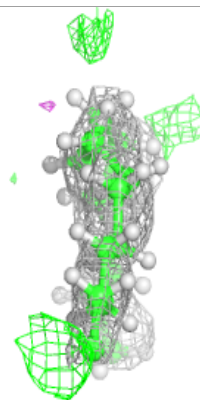
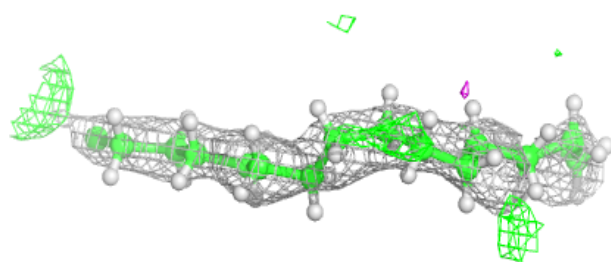
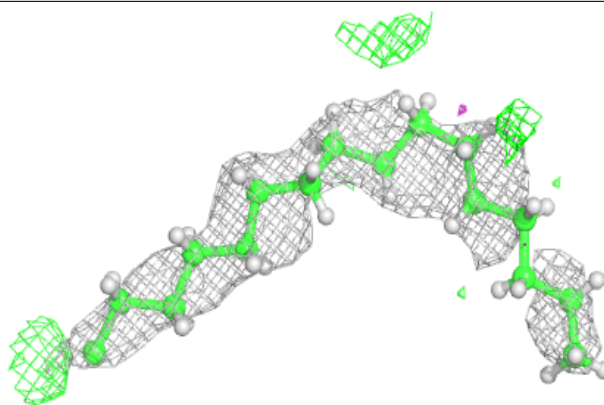
**Electron density around LHG a 411:**

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

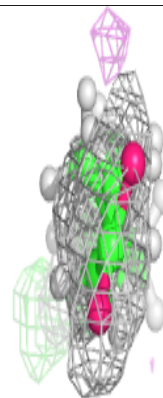
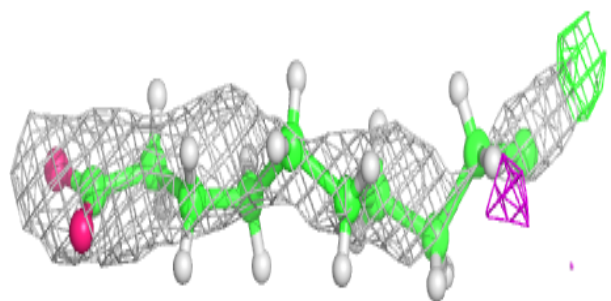
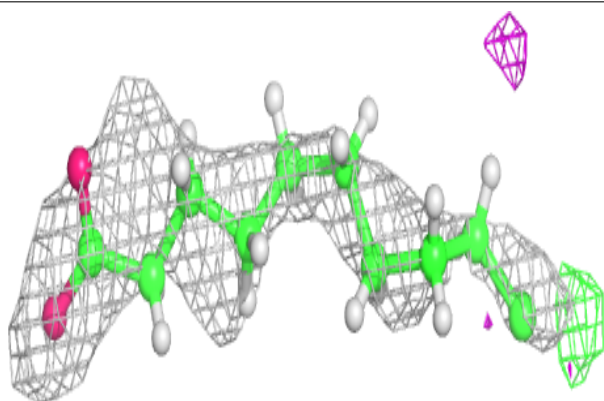


**Electron density around STE B 624:**

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

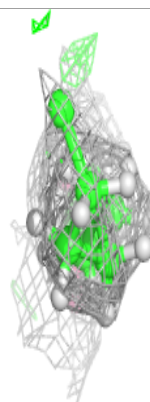
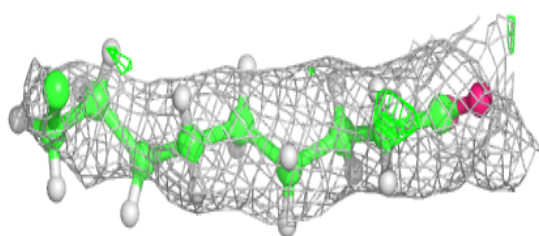
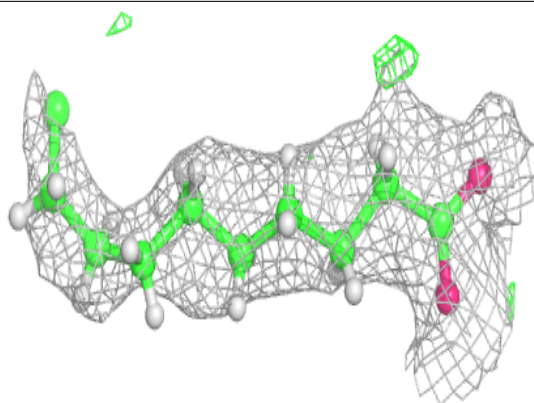
**Electron density around STE a 412:**

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

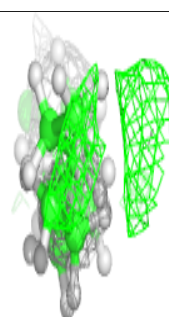
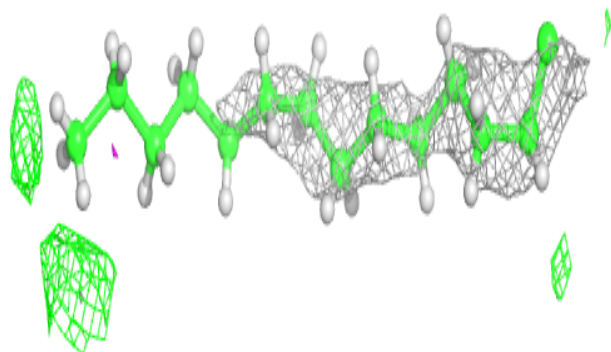
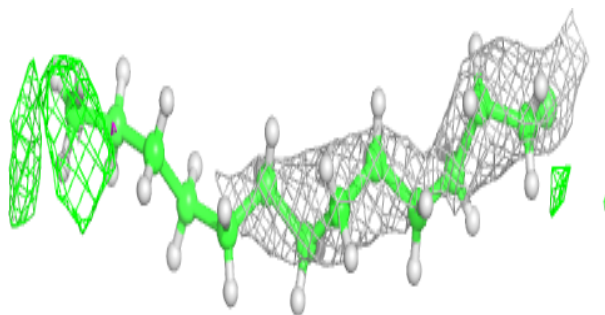


**Electron density around STE k 104:**

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

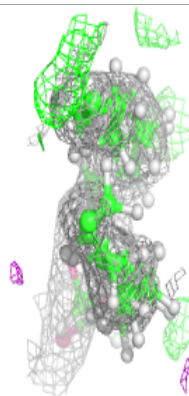
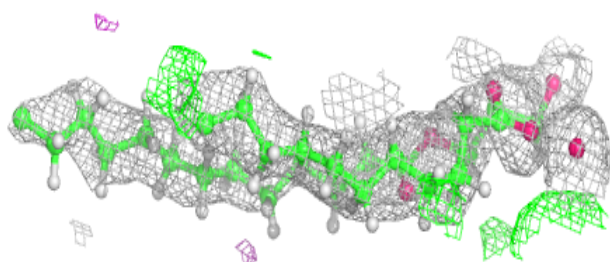
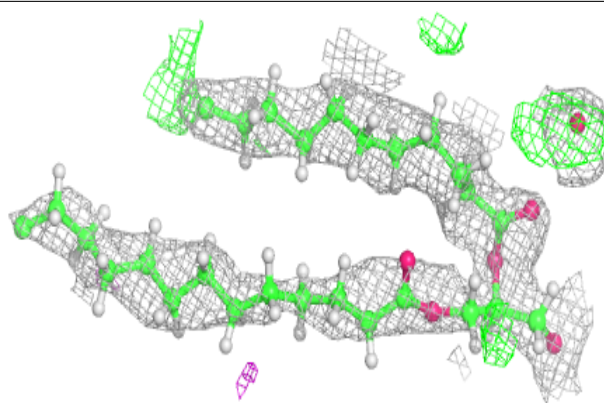
**Electron density around STE b 628:**

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

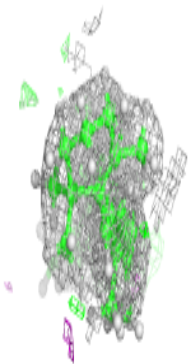
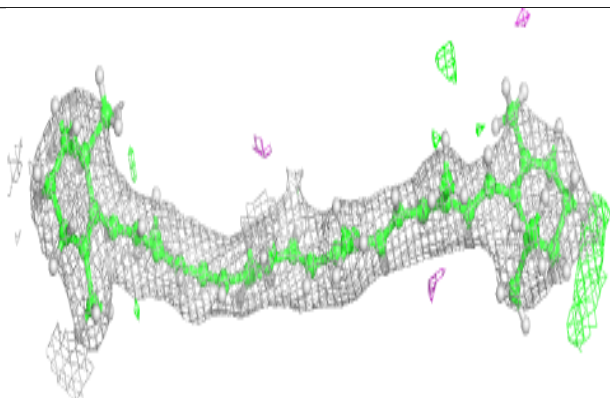
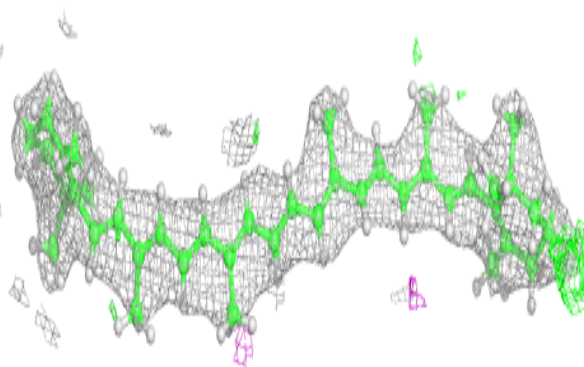


**Electron density around LMG D 412:**

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

**Electron density around BCR H 102:**

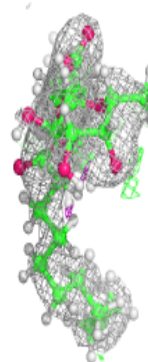
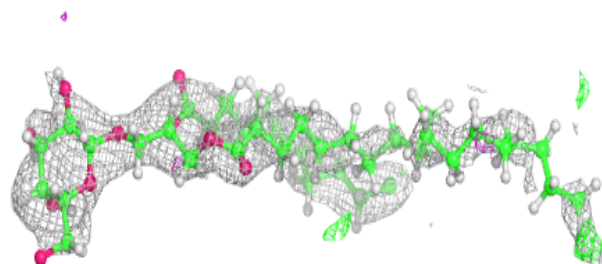
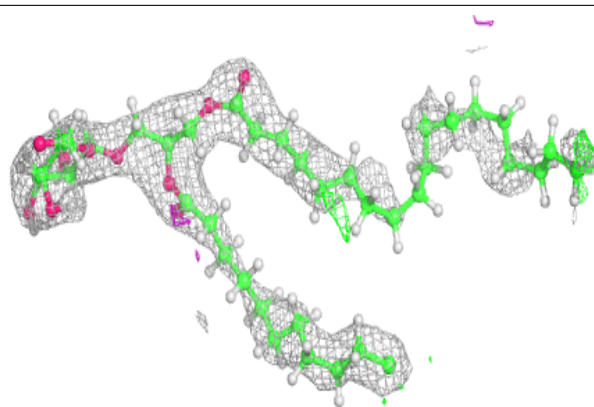
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



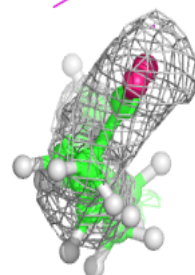
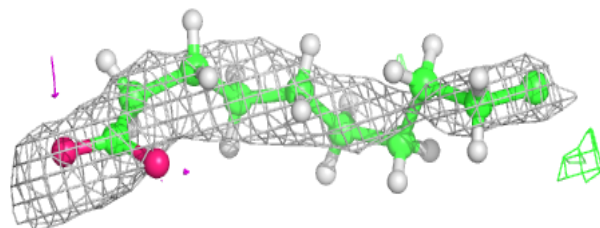
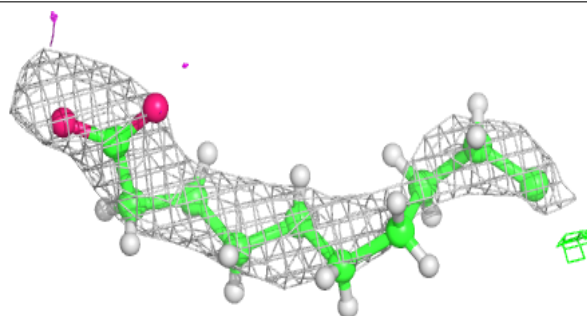


**Electron density around LMG c 520:**

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

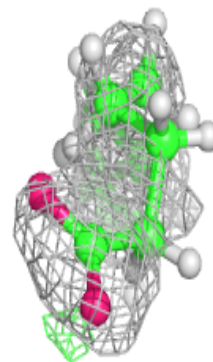
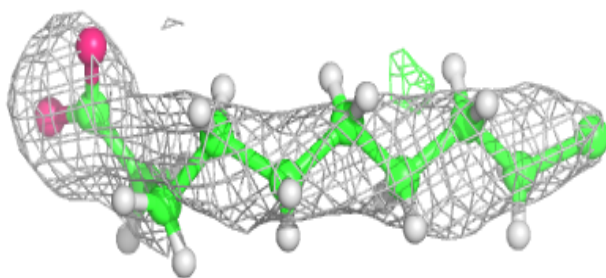
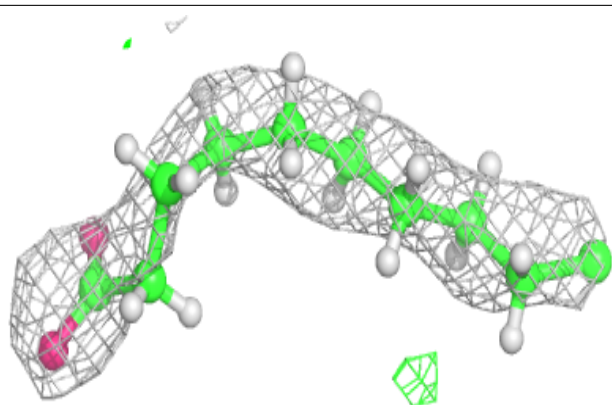
**Electron density around STE B 625:**

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



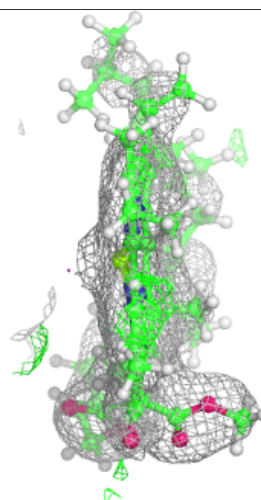
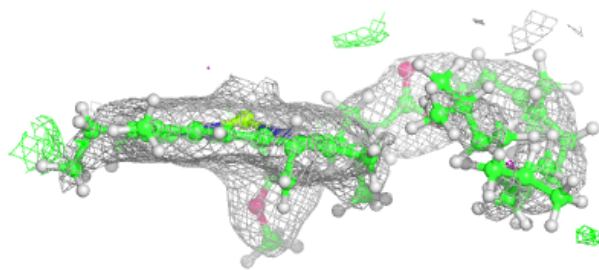
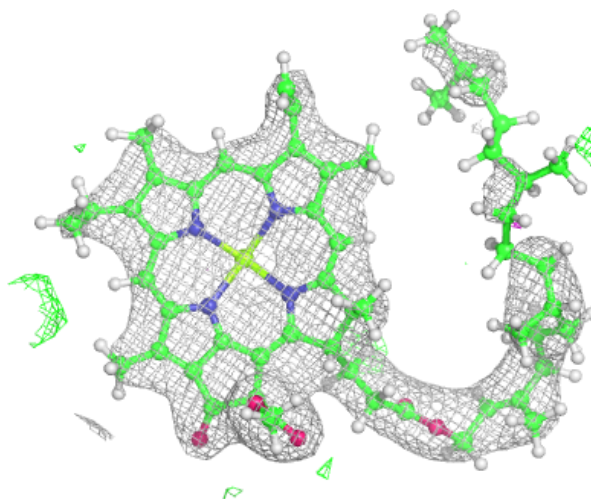
**Electron density around STE R 101:**

$2mF_o-DF_c$  (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:**

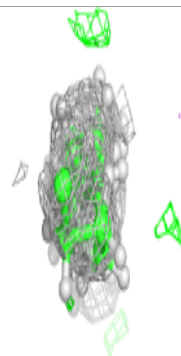
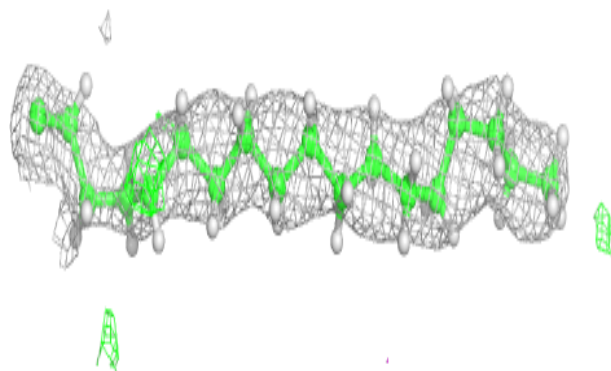
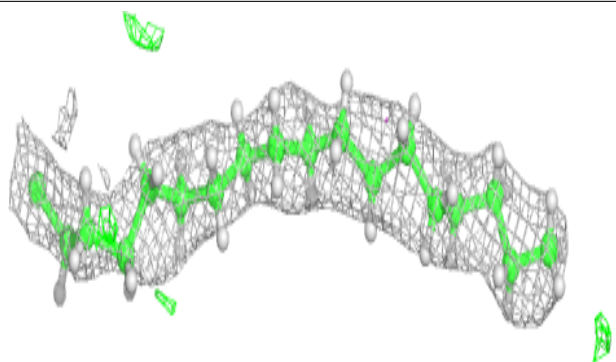
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



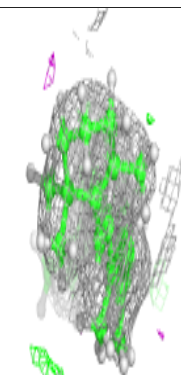
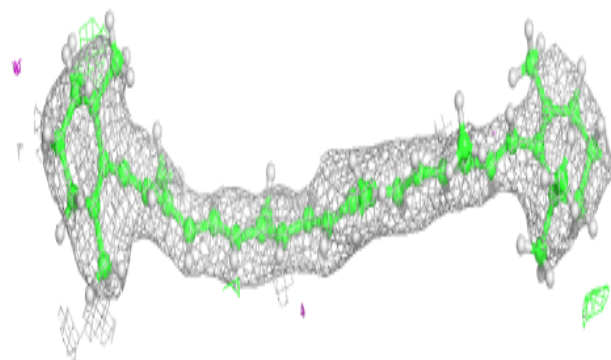
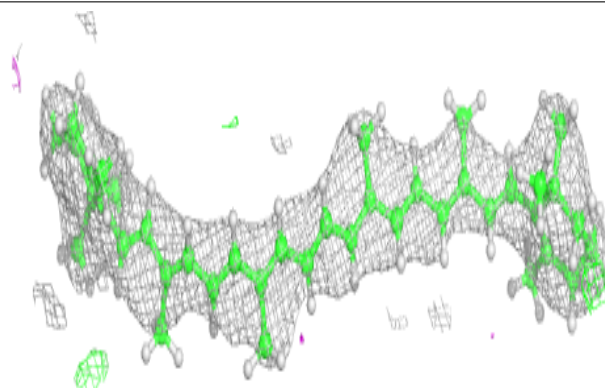


**Electron density around STE M 104:**

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

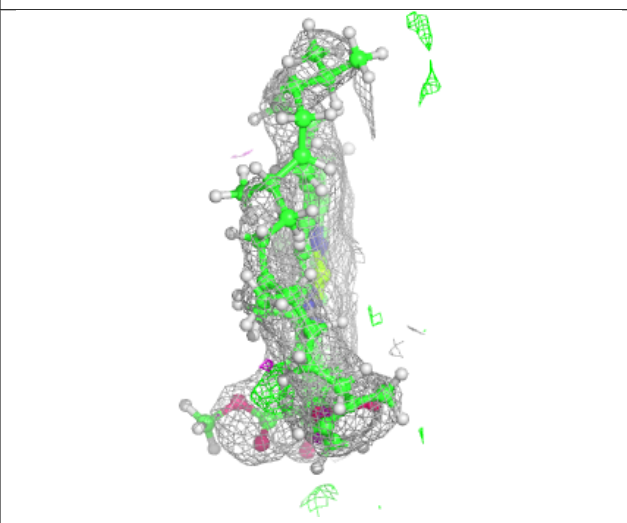
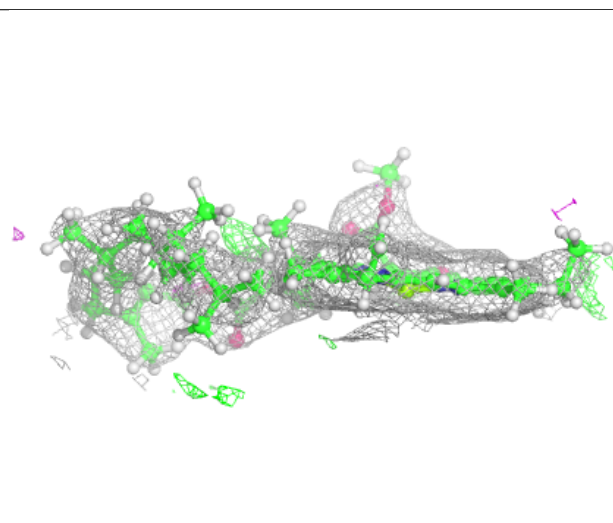
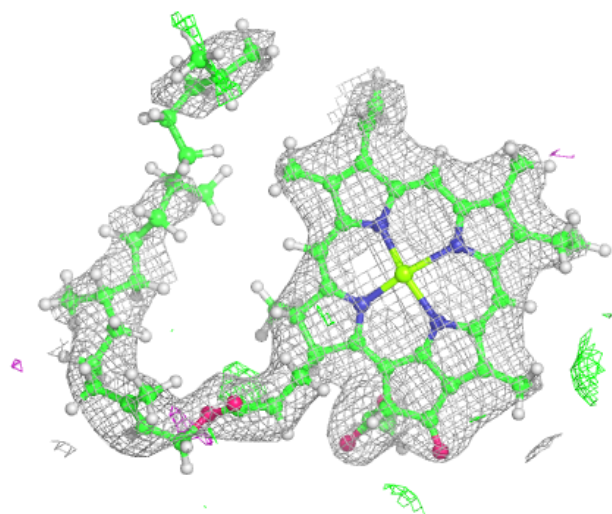
**Electron density around BCR x 101:**

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



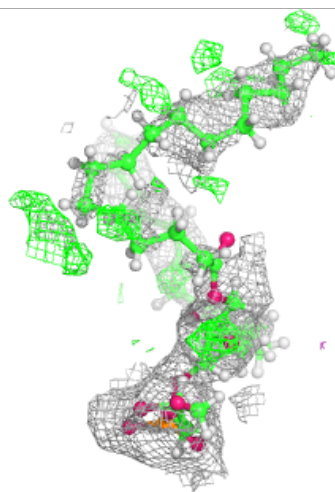
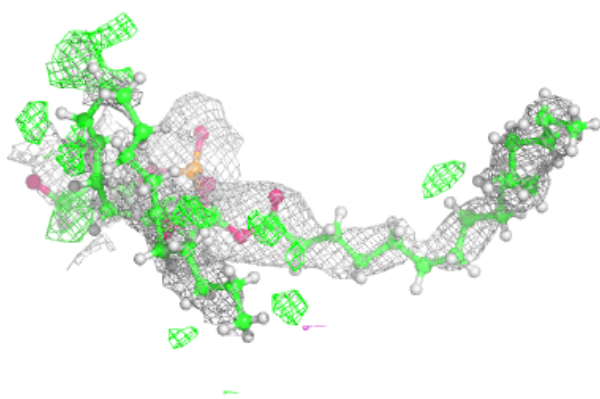
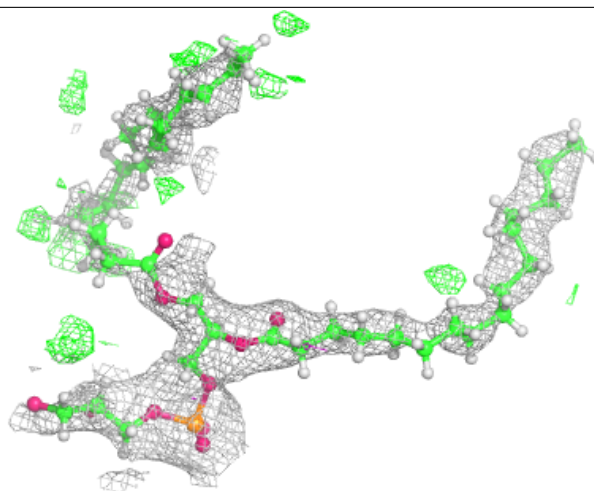
**Electron density around CLA c 512:**

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



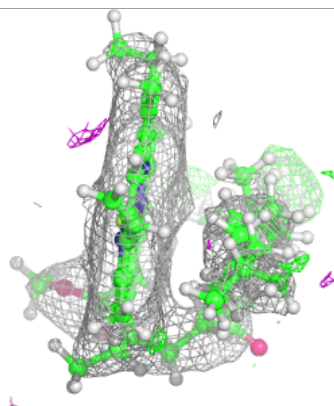
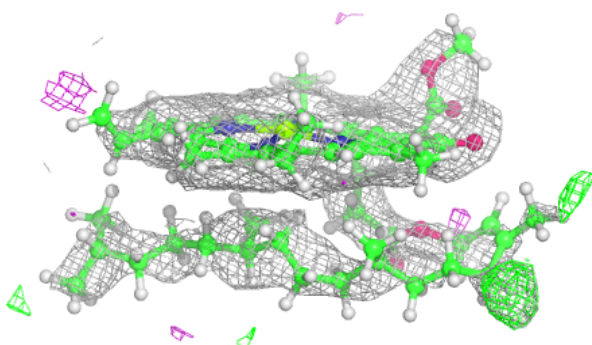
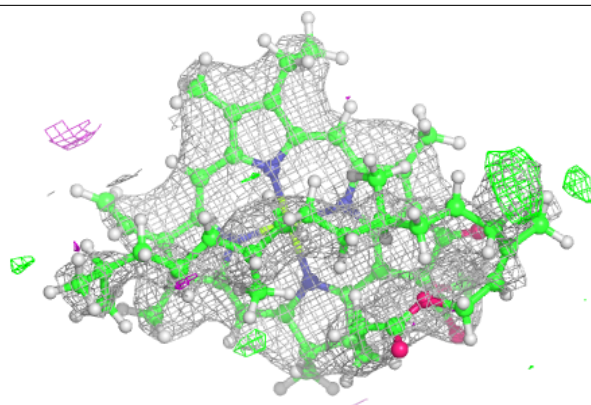
**Electron density around LHG A 411:**

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

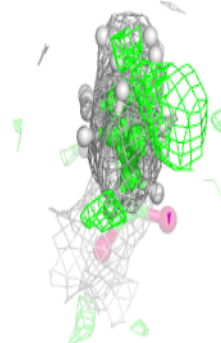
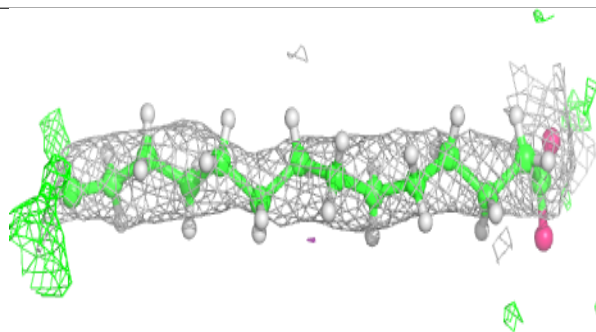
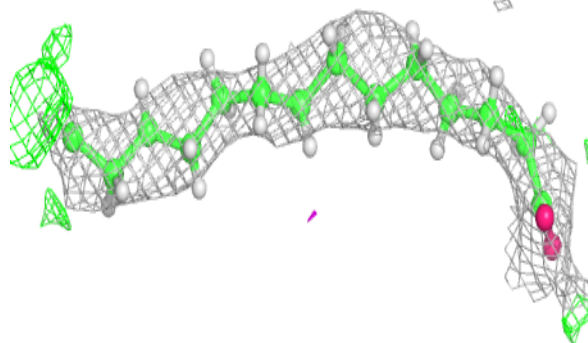


**Electron density around CLA b 601:**

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

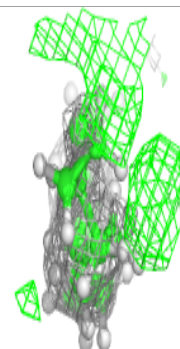
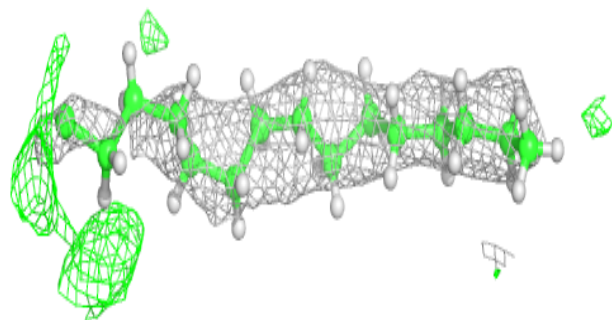
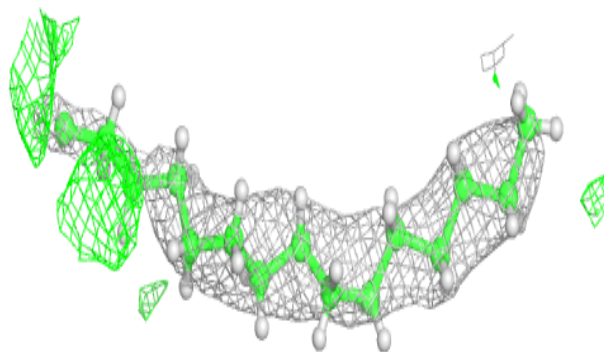
**Electron density around STE b 624:**

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

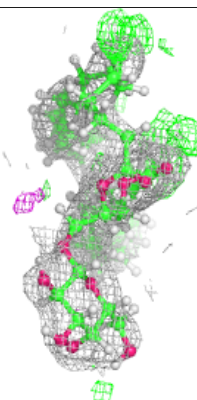
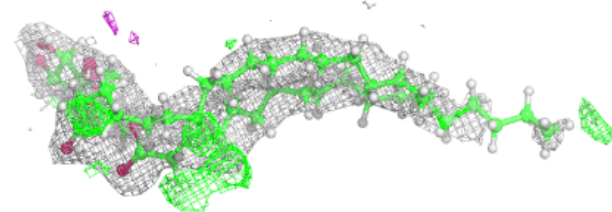
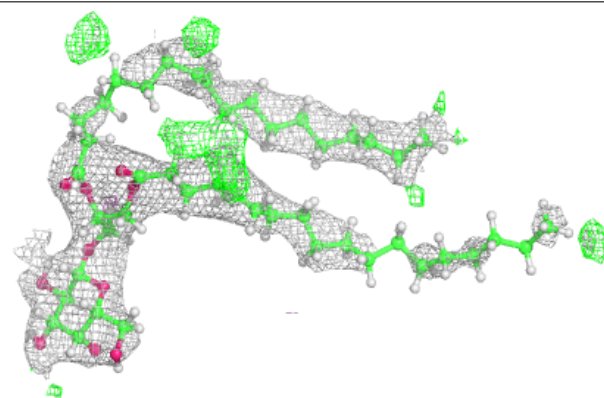


**Electron density around STE b 625:**

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

**Electron density around LMG a 414:**

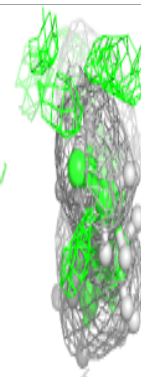
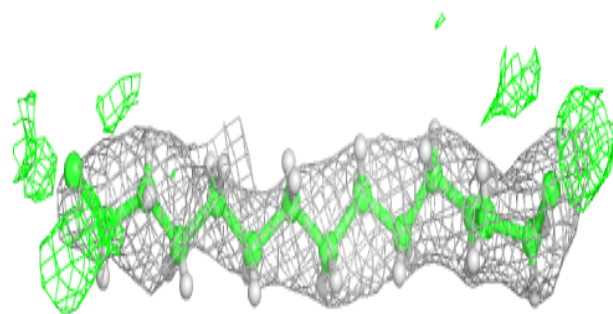
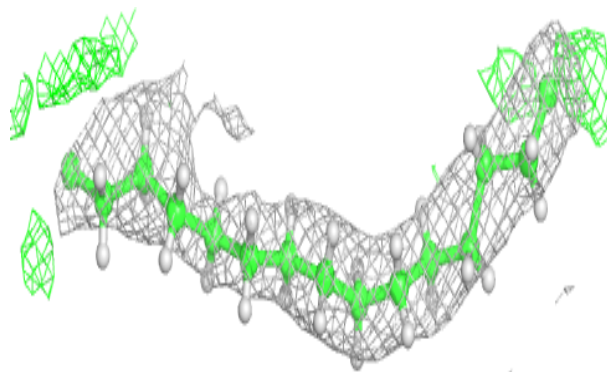
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



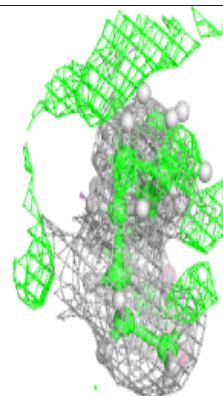
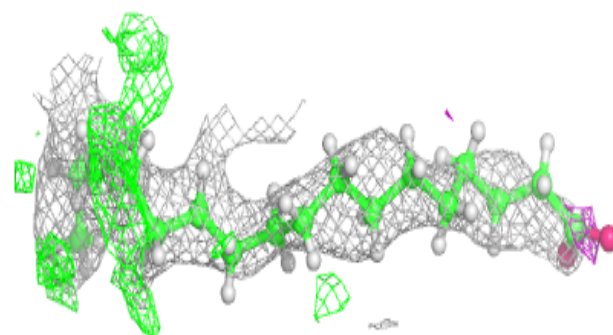
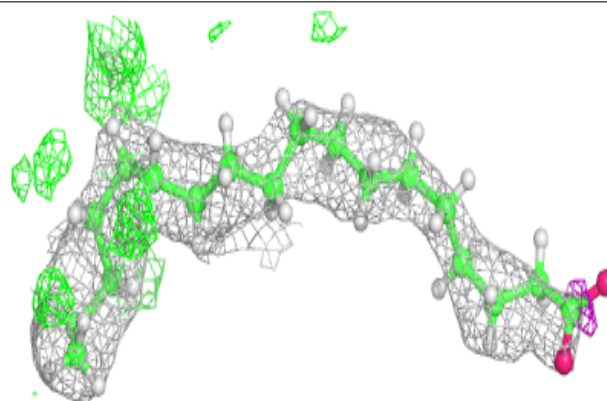


**Electron density around STE I 102:**

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

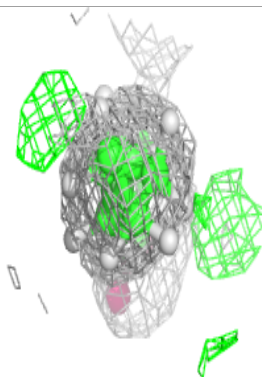
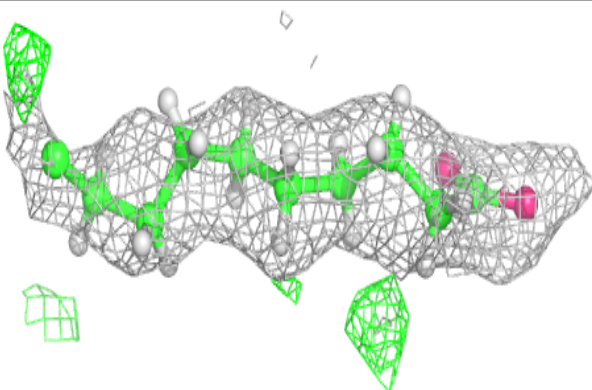
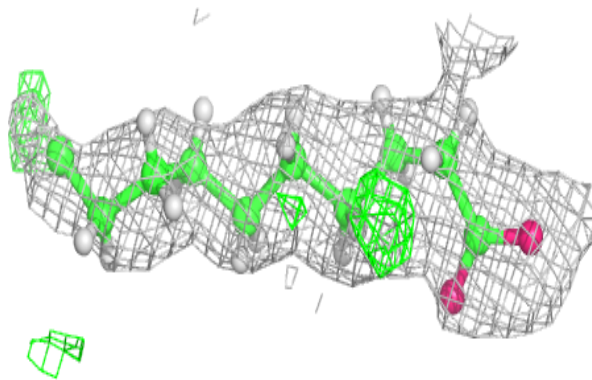
**Electron density around STE b 629:**

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

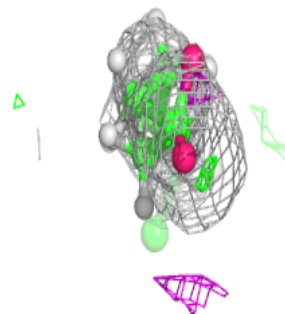
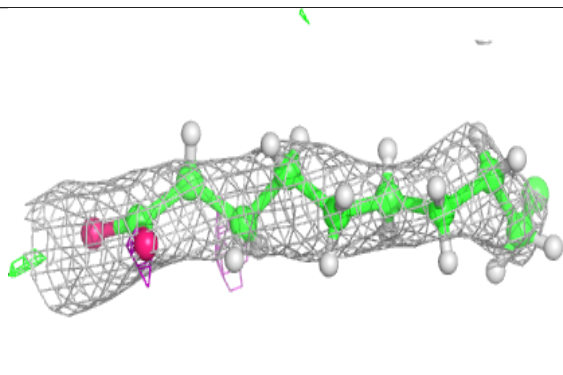
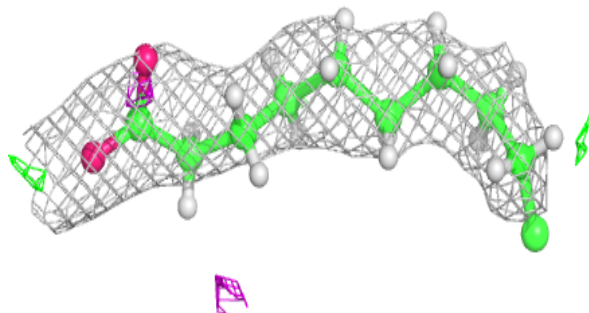


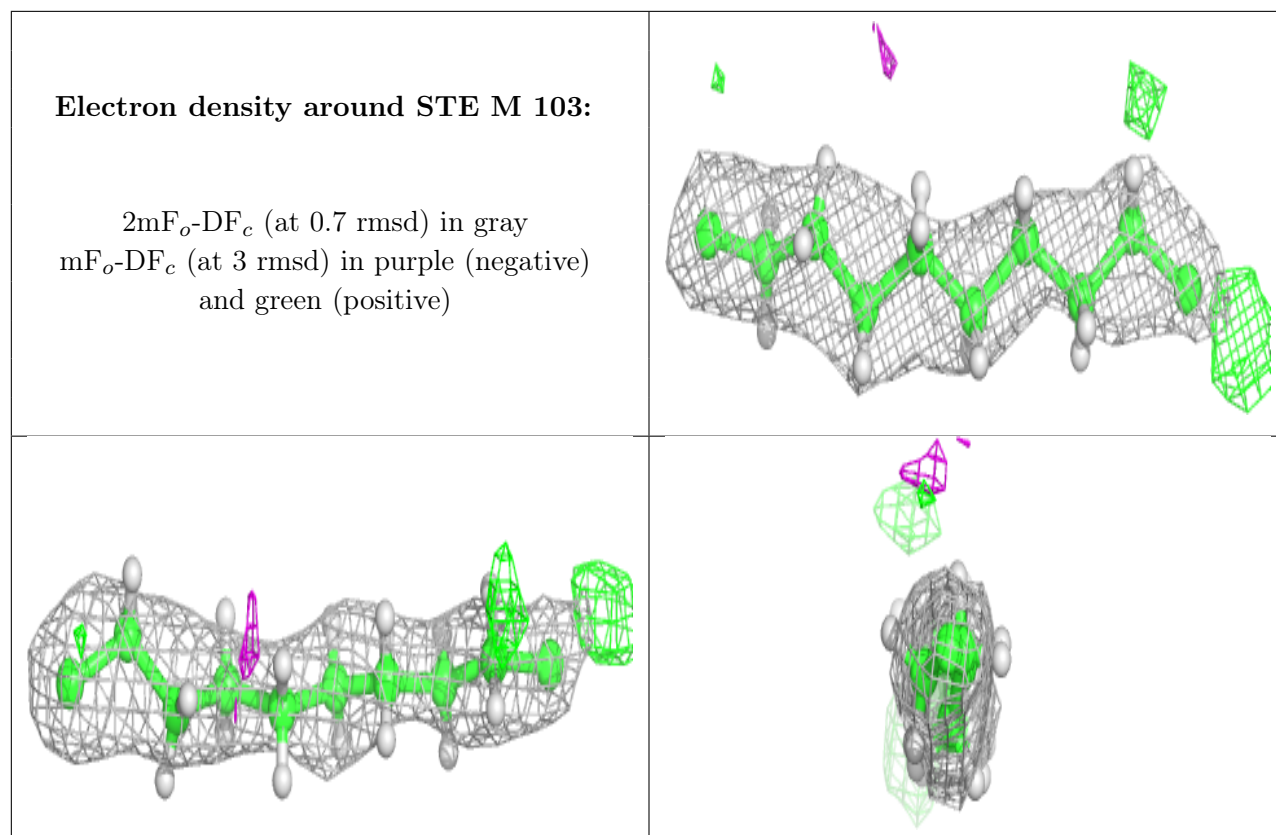
**Electron density around STE J 101:**

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

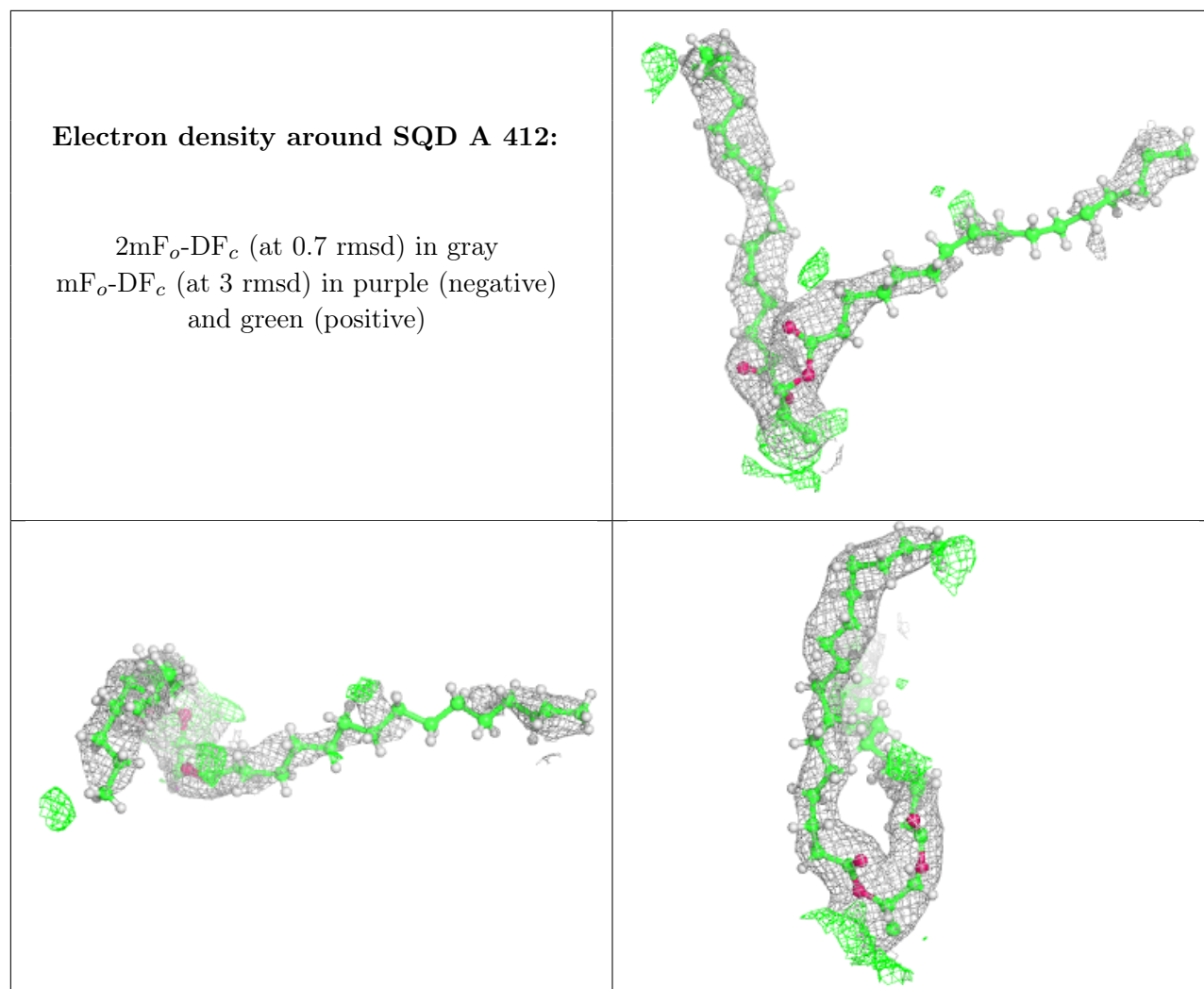
**Electron density around STE L 103:**

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



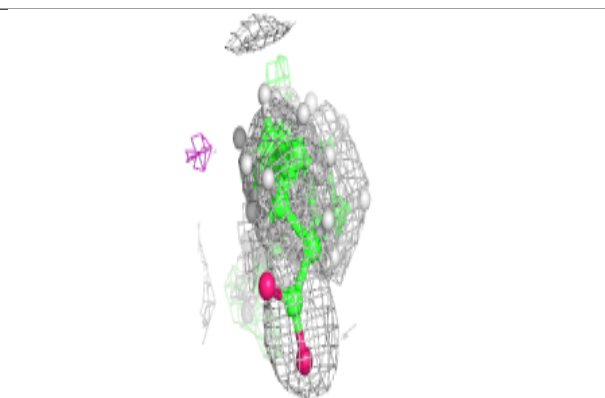
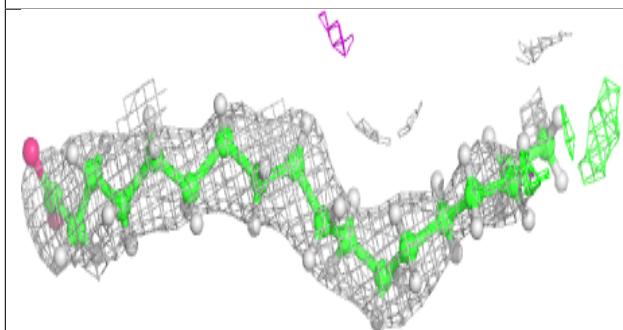
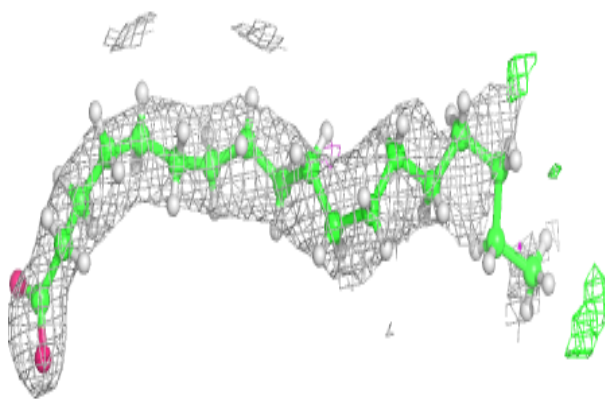




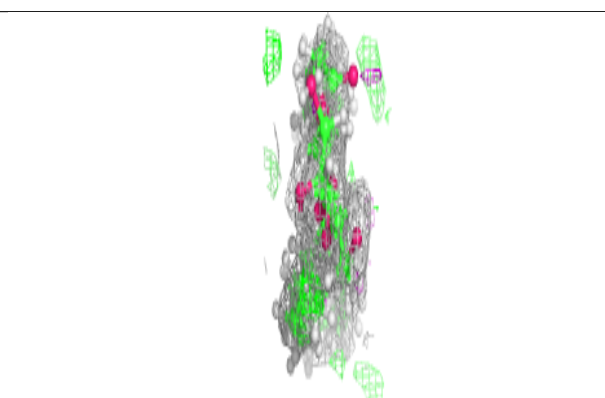
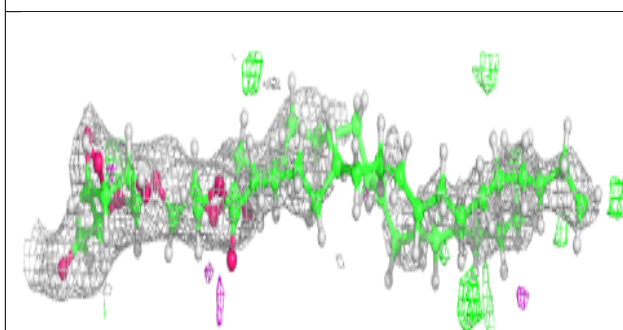
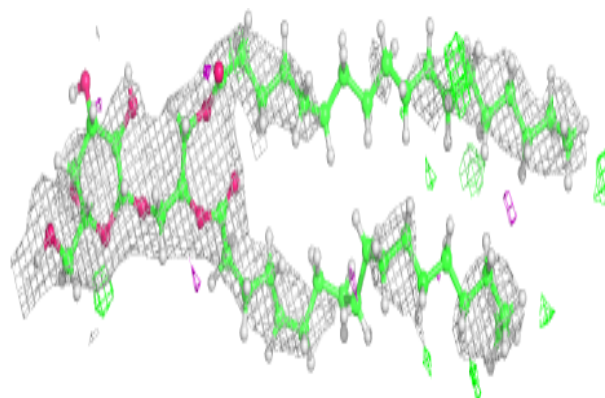


**Electron density around STE b 621:**

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

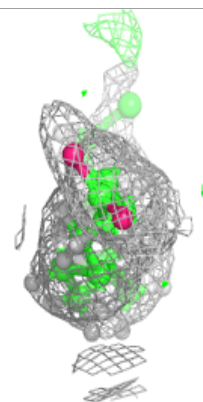
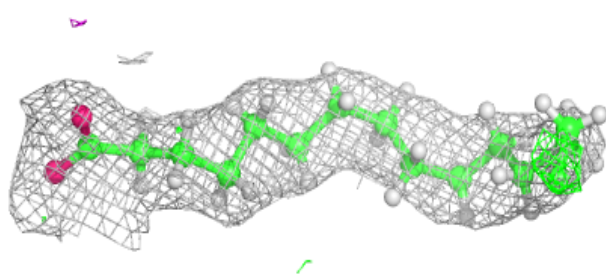
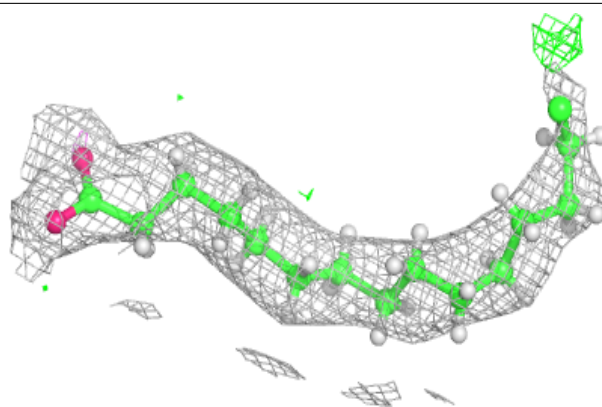
**Electron density around LMG b 622:**

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

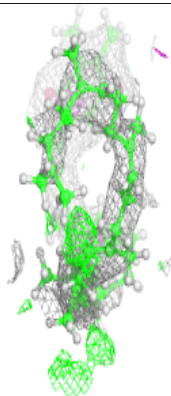
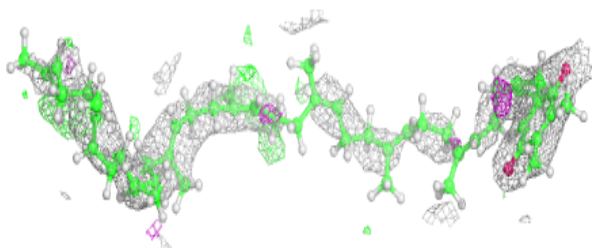
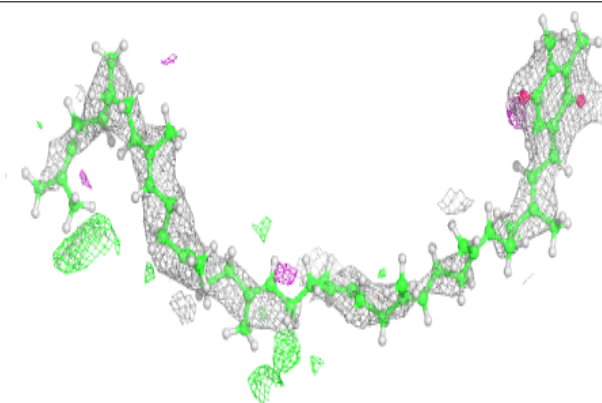


**Electron density around STE B 619:**

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

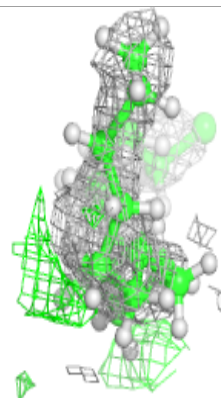
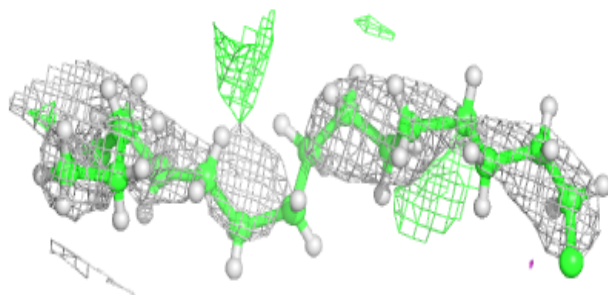
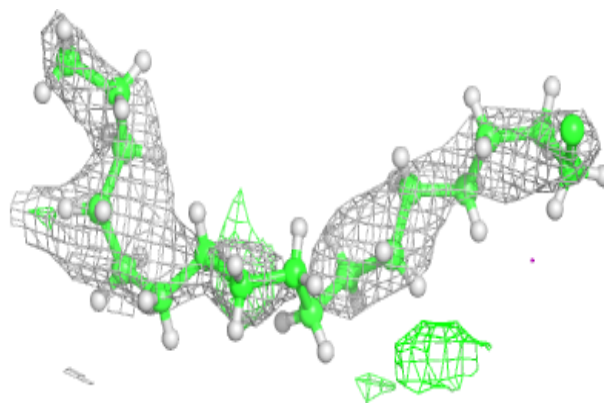
**Electron density around PL9 a 409:**

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



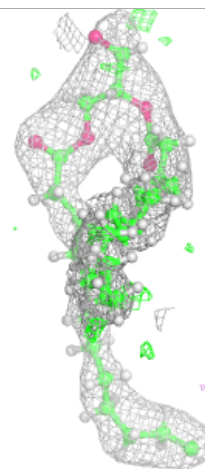
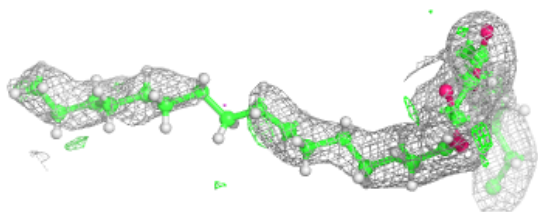
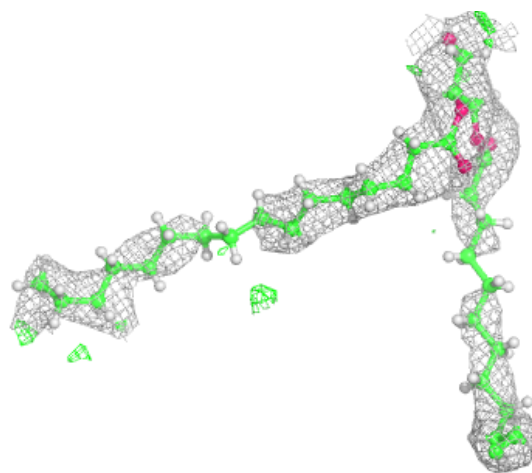
**Electron density around STE H 104:**

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



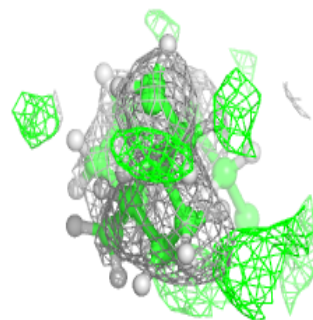
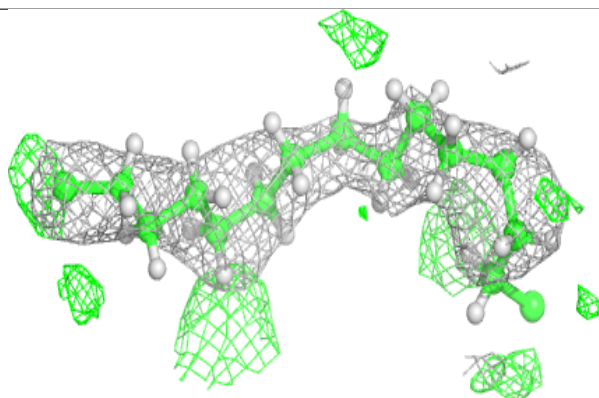
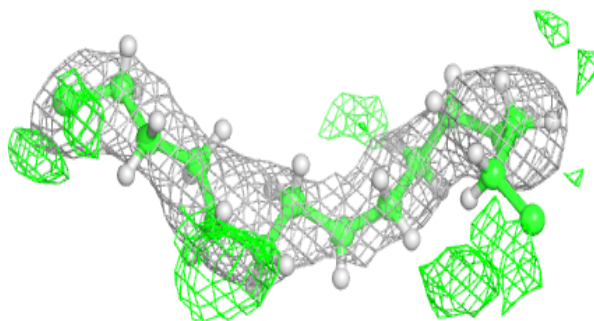
**Electron density around SQD † 102:**

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

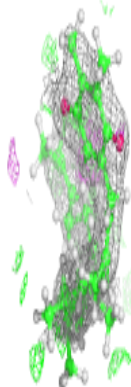
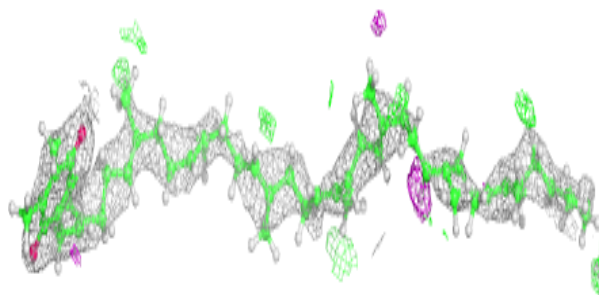
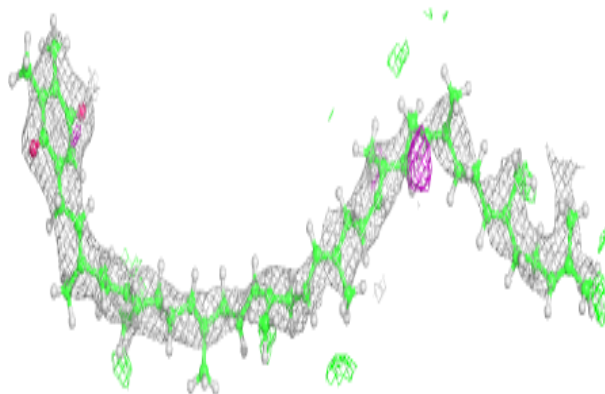


**Electron density around STE a 413:**

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

**Electron density around PL9 A 408:**

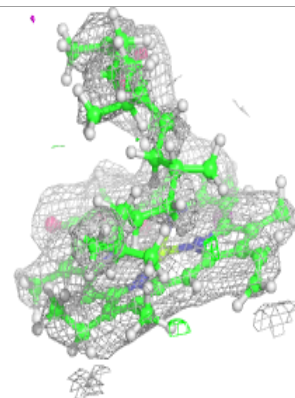
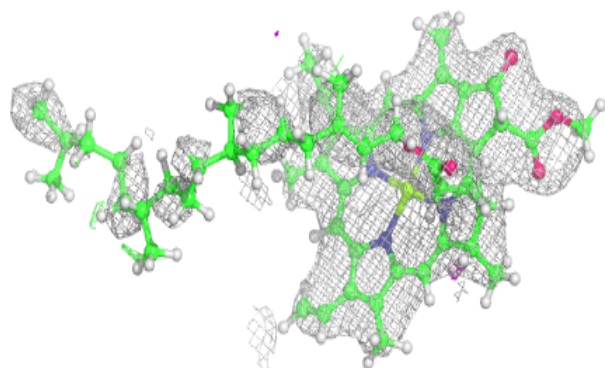
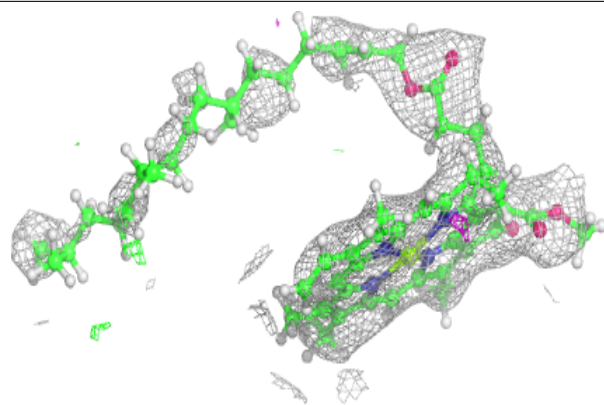
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



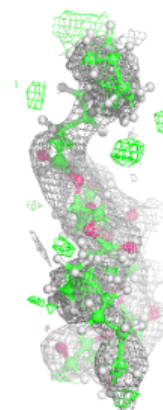
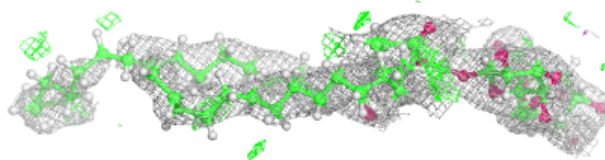
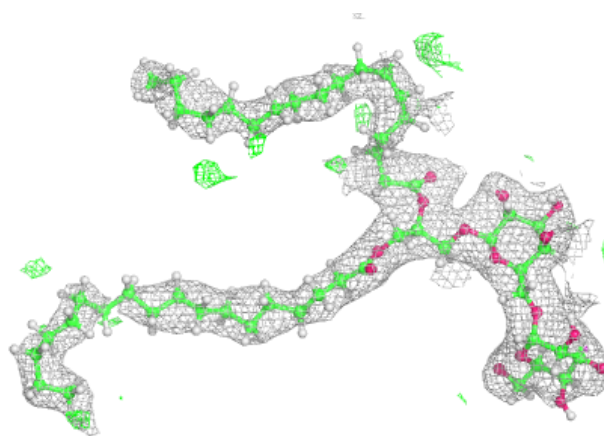


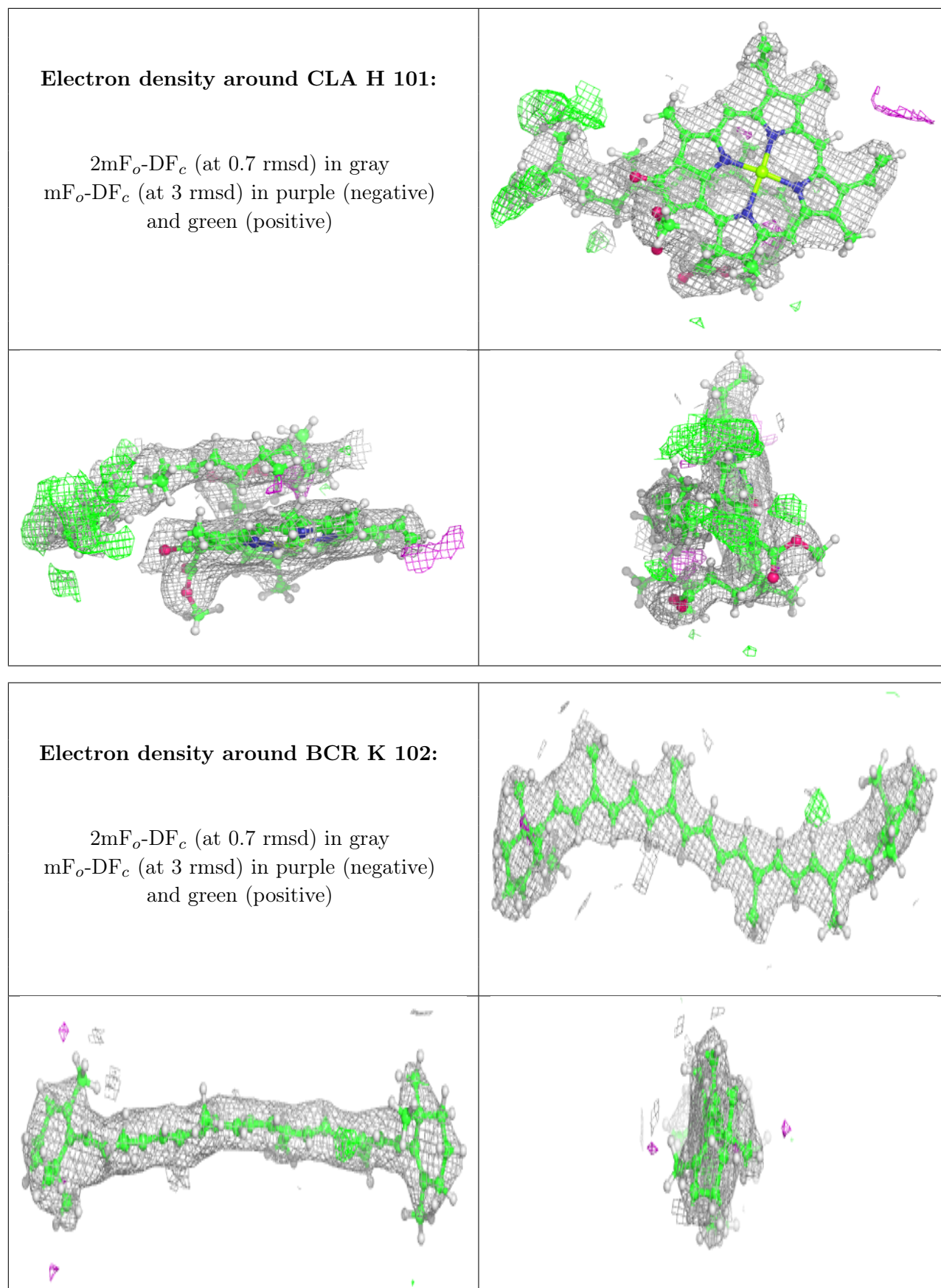
**Electron density around CLA C 513:**

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

**Electron density around DGD A 413:**

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

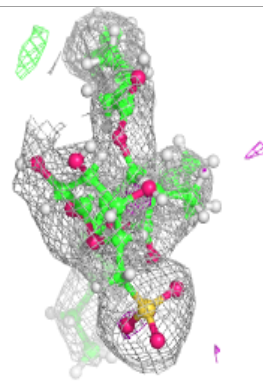
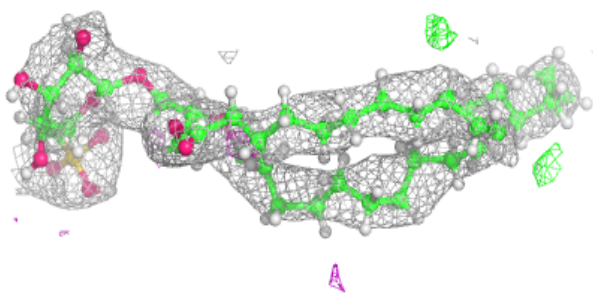
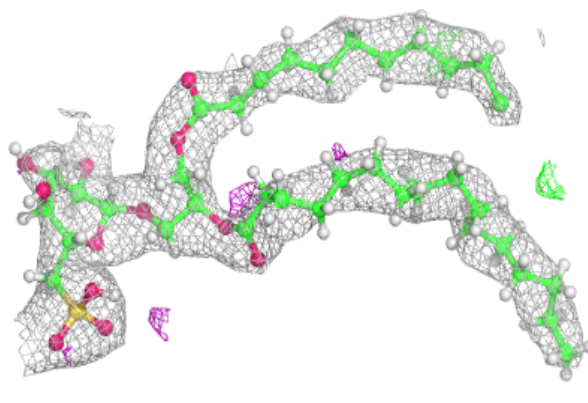




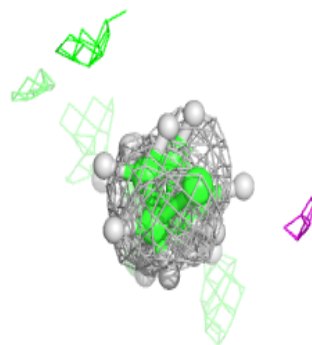
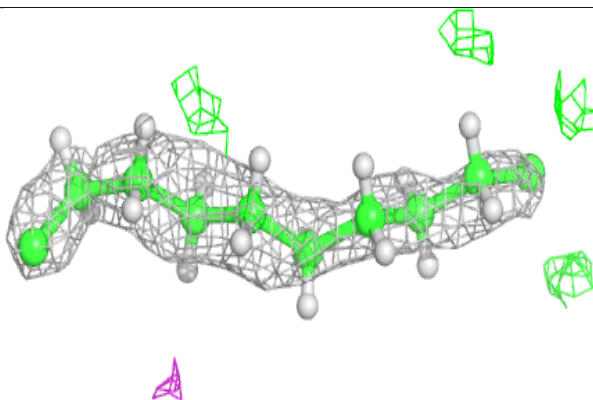
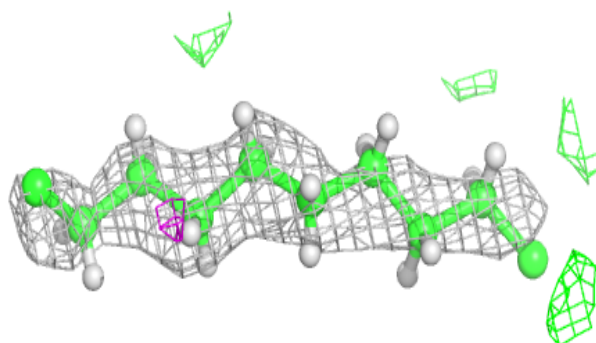


**Electron density around SQD L 101:**

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

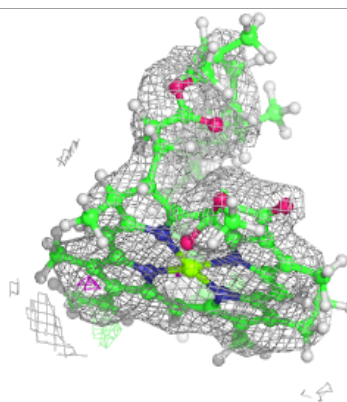
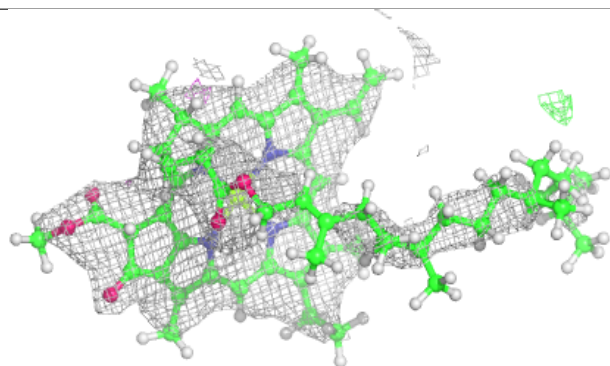
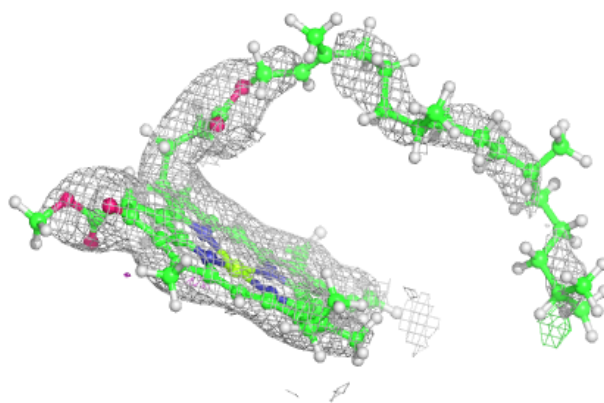
**Electron density around STE t 104:**

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

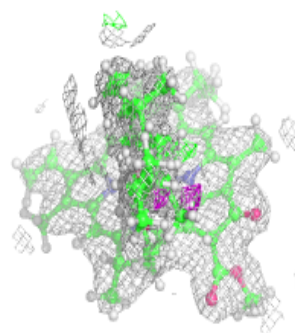
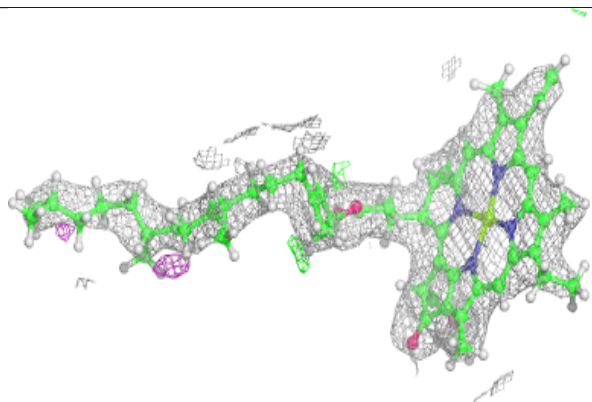
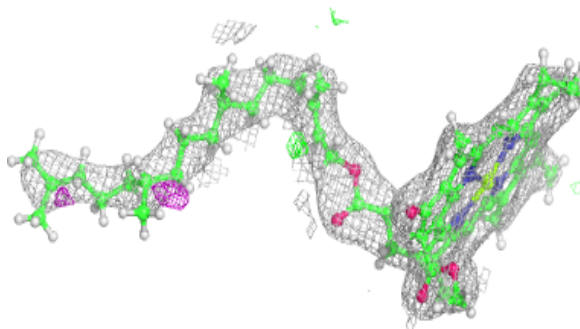


**Electron density around CLA c 513:**

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

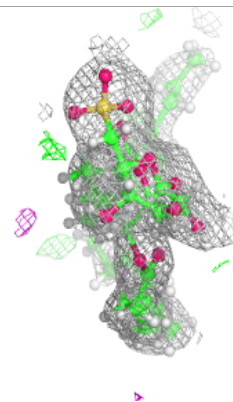
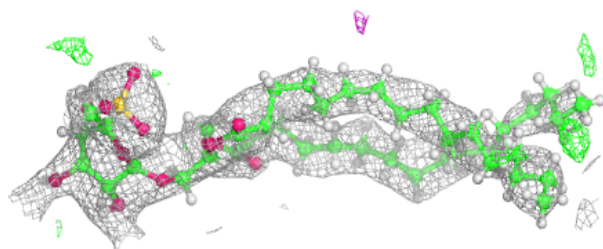
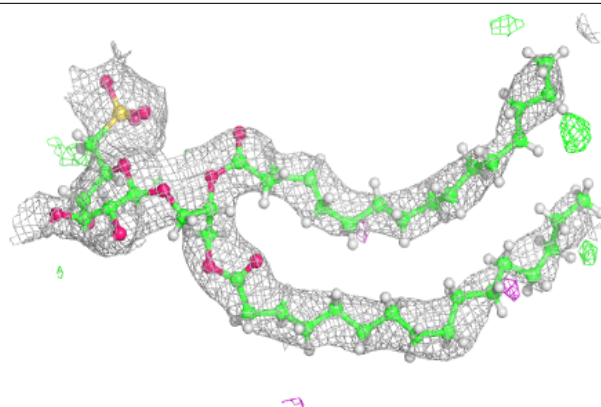
**Electron density around CLA c 502:**

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

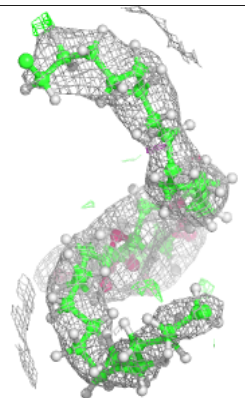
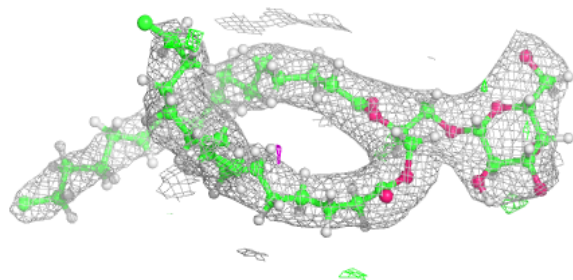
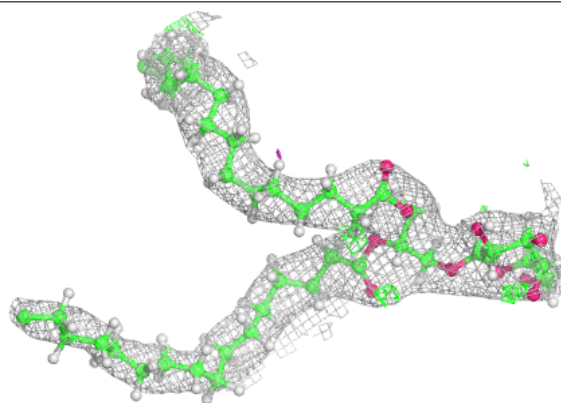


**Electron density around SQD B 621:**

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

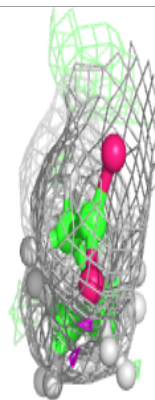
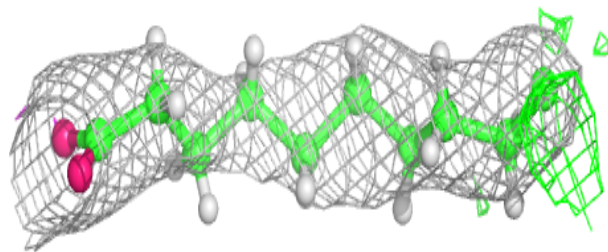
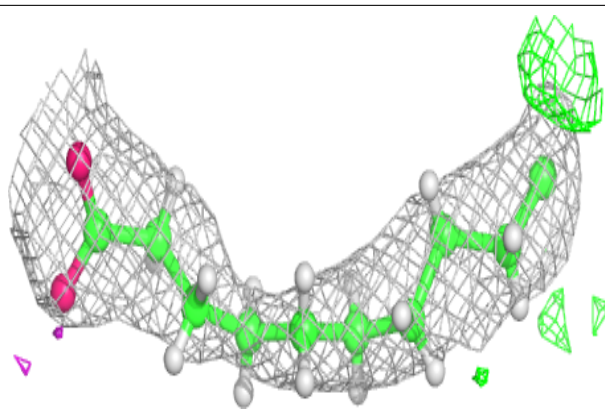
**Electron density around LMG M 101:**

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

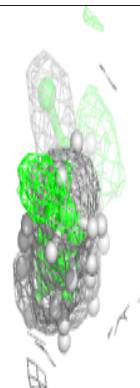
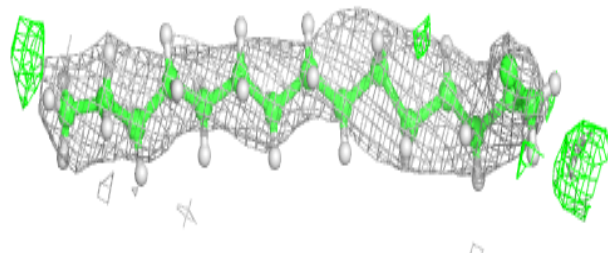
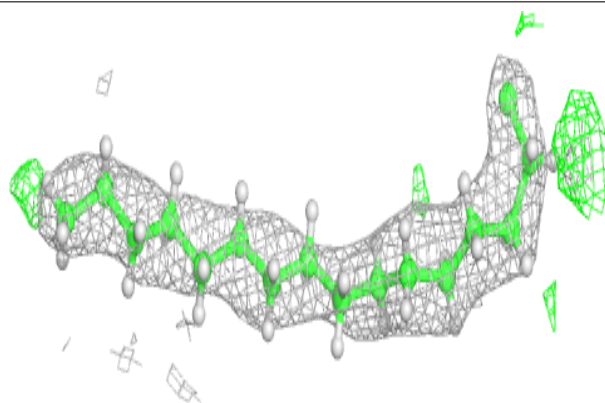


**Electron density around STE C 519:**

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

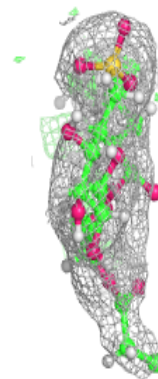
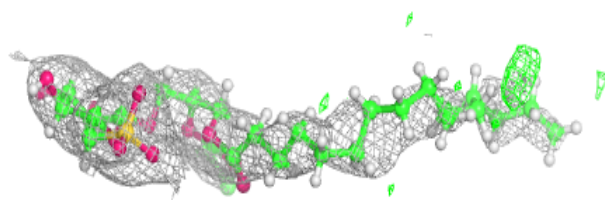
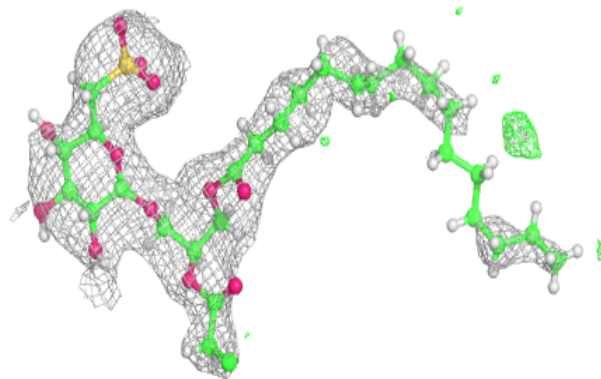
**Electron density around STE C 520:**

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



**Electron density around SQD f 102:**

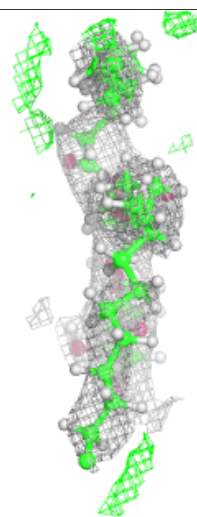
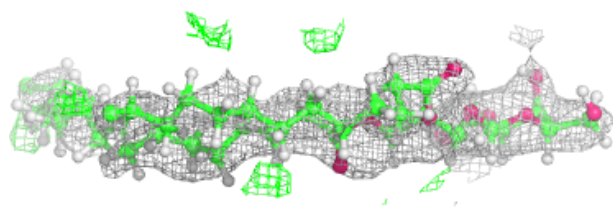
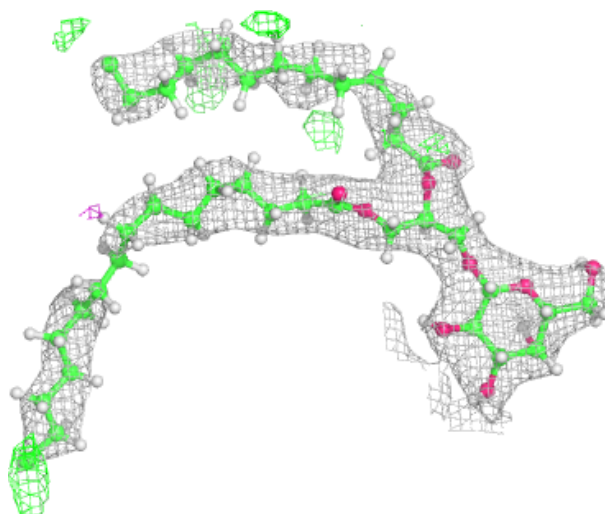
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





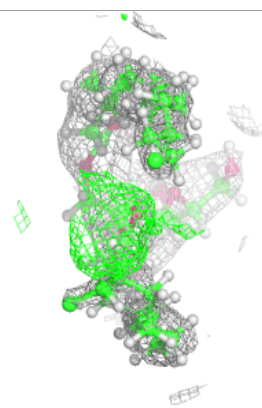
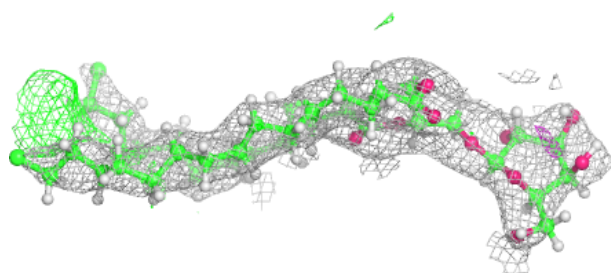
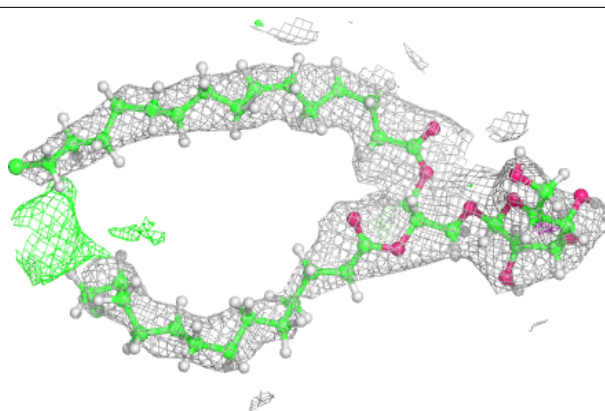
**Electron density around LMG Y 101:**

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



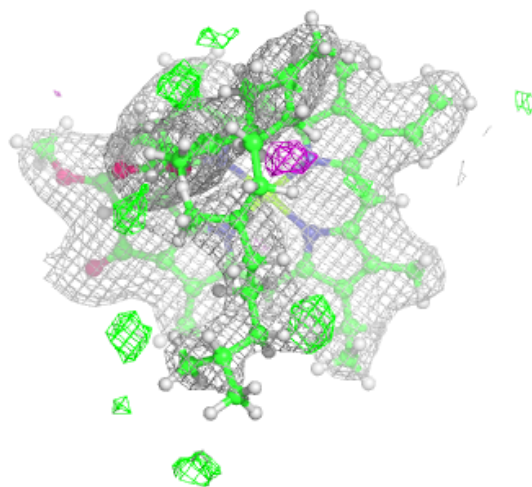
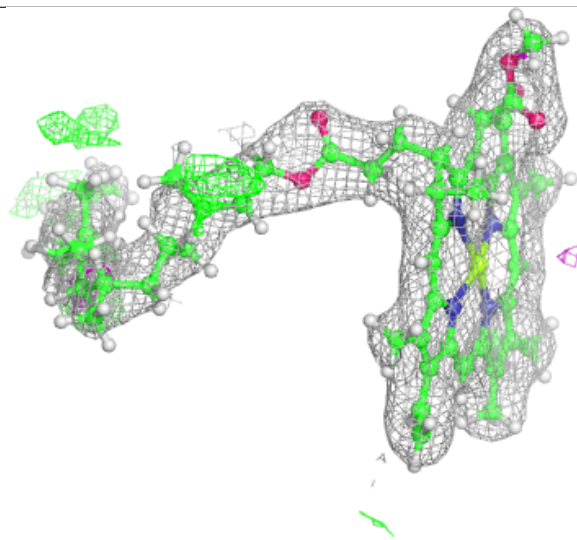
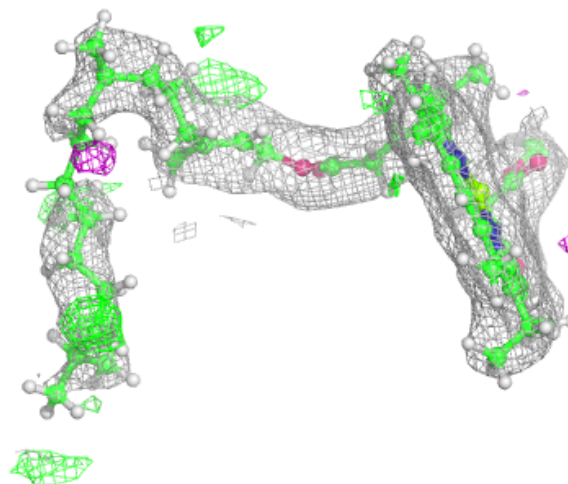
**Electron density around LMG c 521:**

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



**Electron density around CLA a 405:**

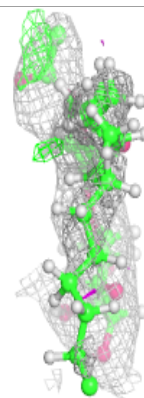
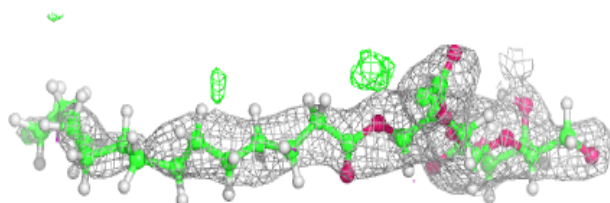
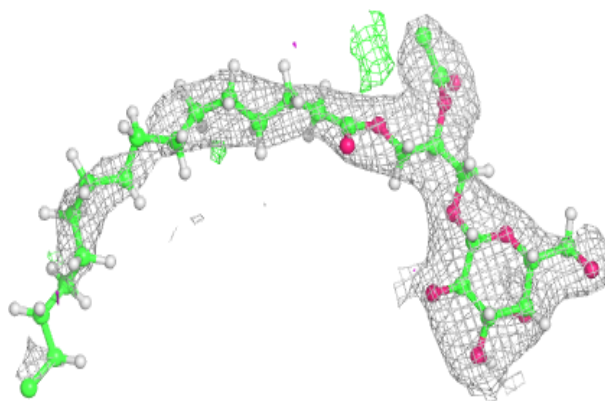
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



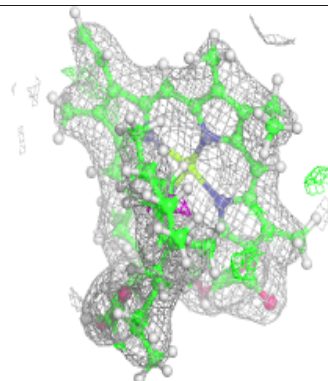
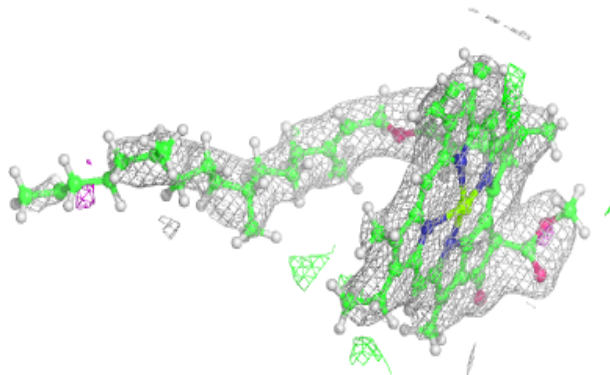
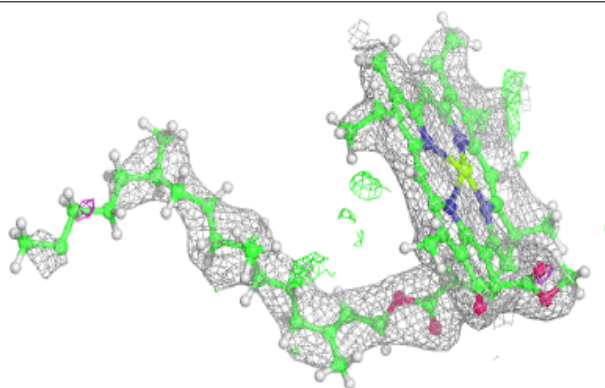


**Electron density around LMG c 518:**

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

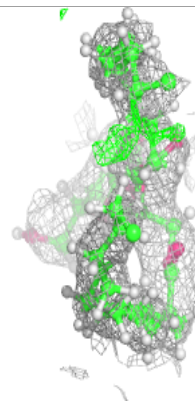
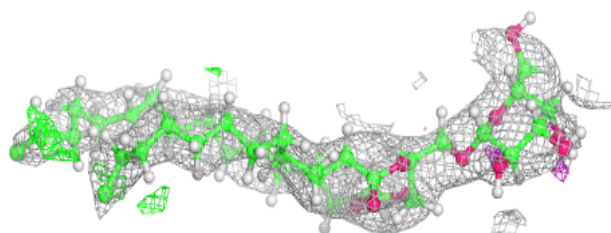
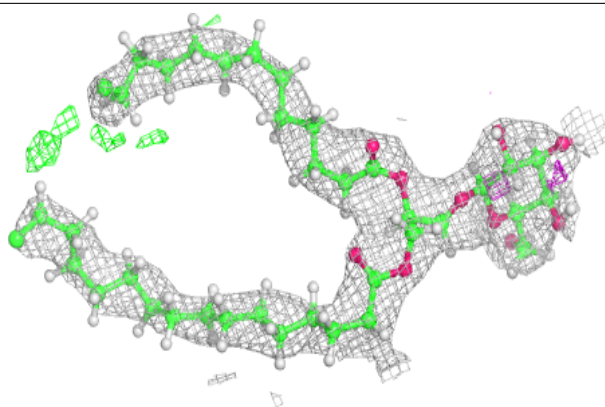
**Electron density around CLA c 508:**

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

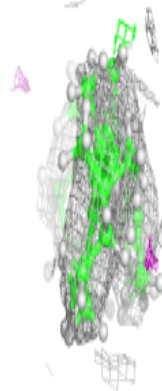
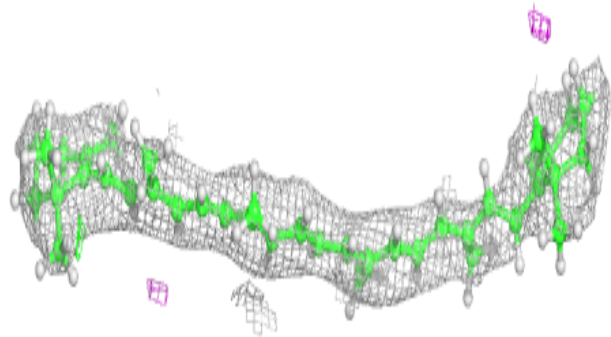
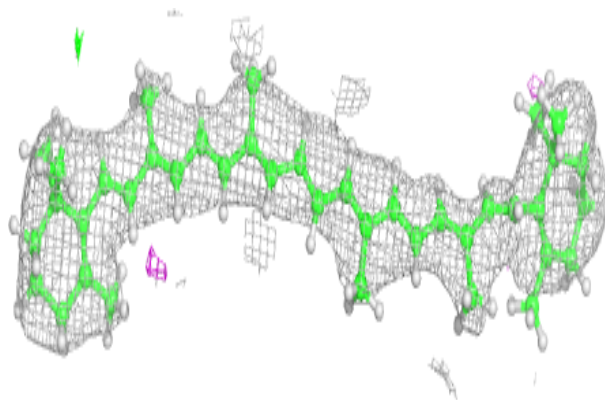


**Electron density around LMG A 409:**

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

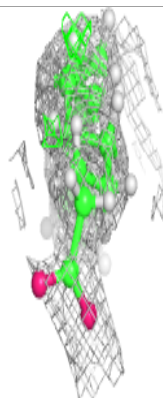
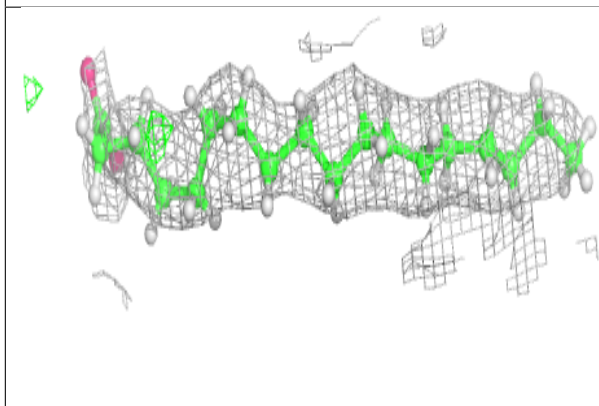
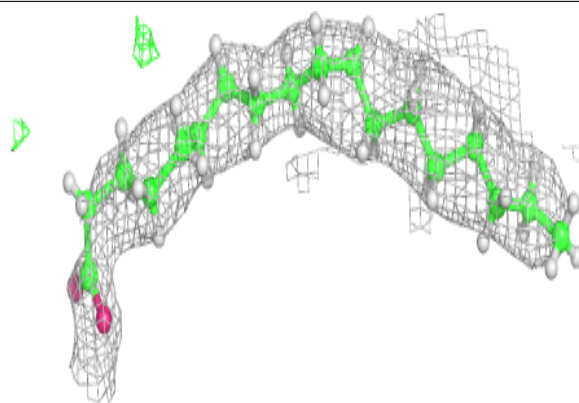
**Electron density around BCR d 406:**

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

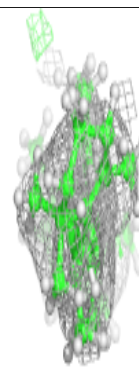
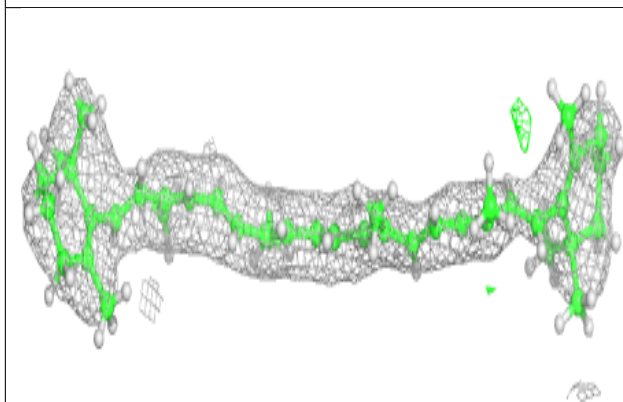
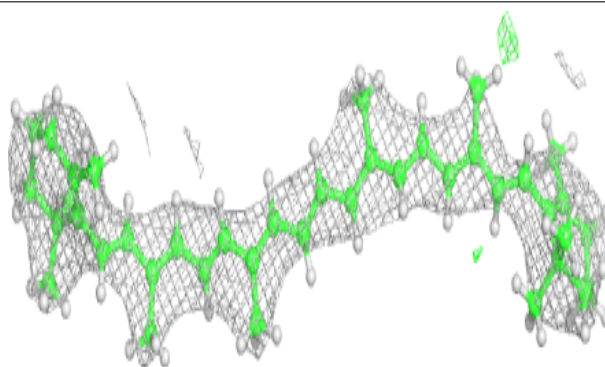


**Electron density around STE X 101:**

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

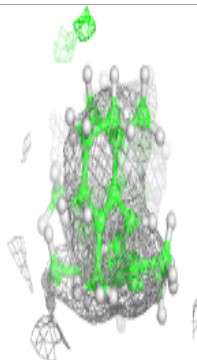
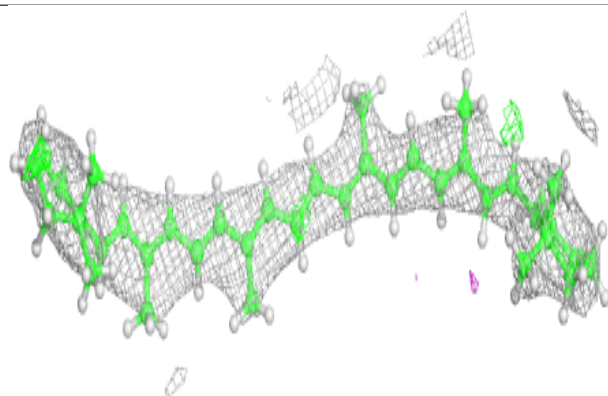
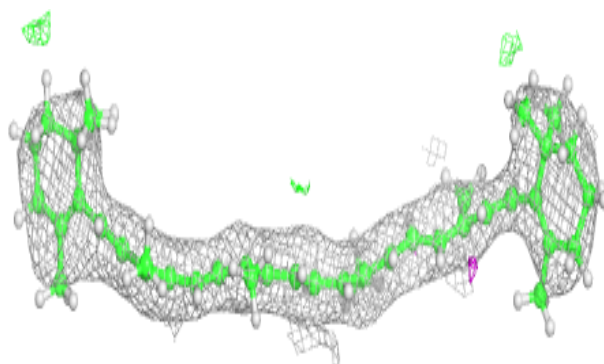
**Electron density around BCR k 102:**

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

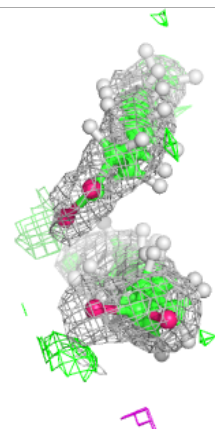
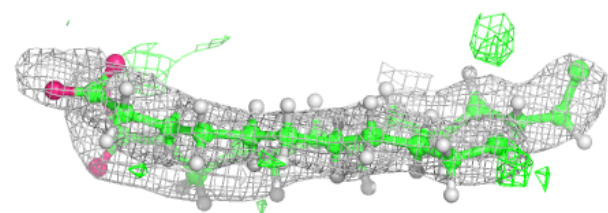
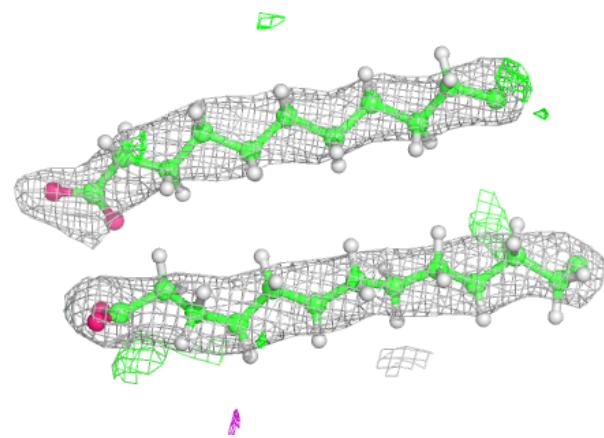


**Electron density around BCR k 103:**

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

**Electron density around LMG B 620:**

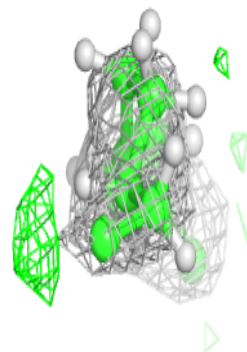
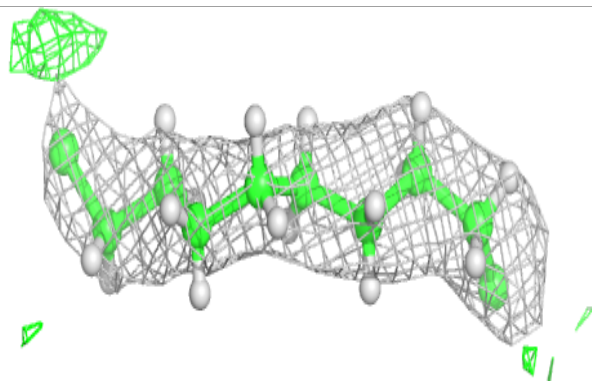
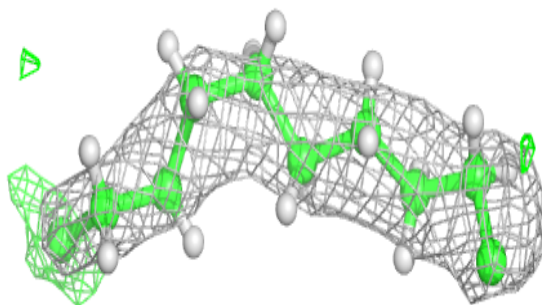
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



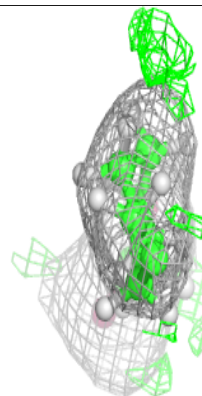
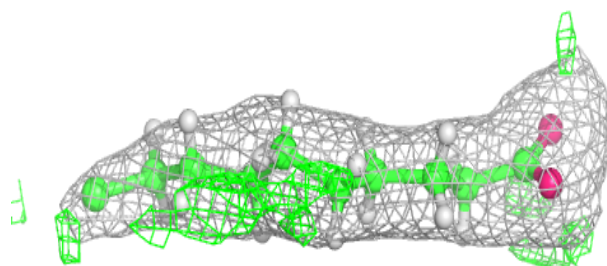
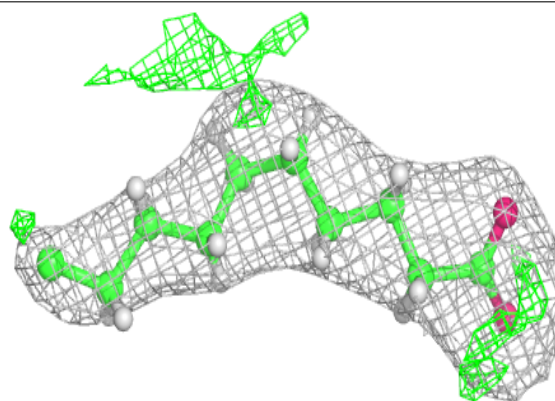


**Electron density around STE b 627:**

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

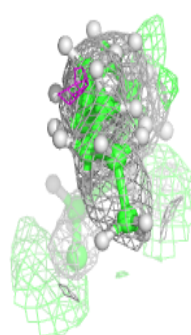
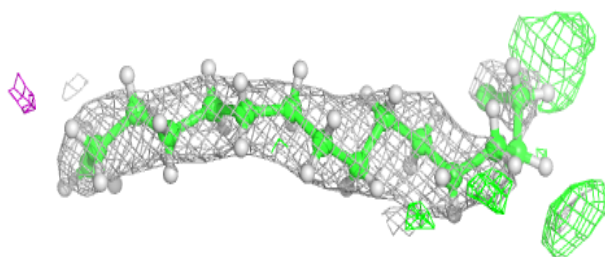
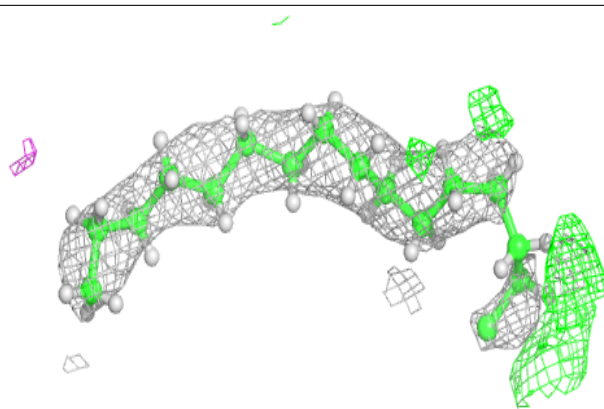
**Electron density around STE C 521:**

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

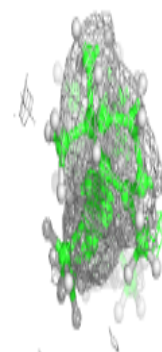
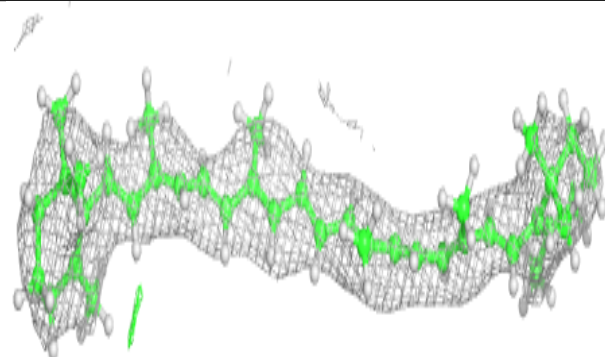
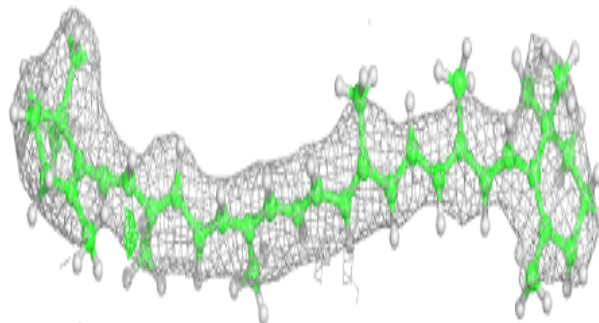


**Electron density around STE b 620:**

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

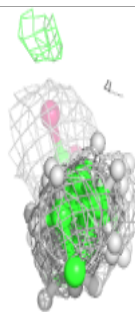
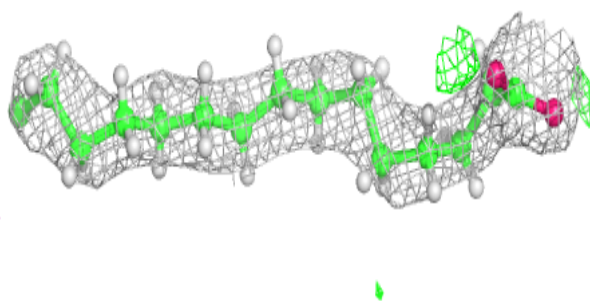
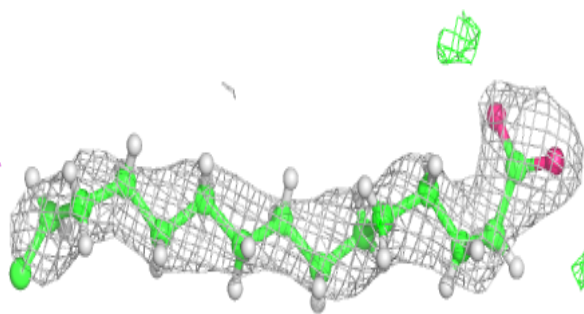
**Electron density around BCR k 101:**

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

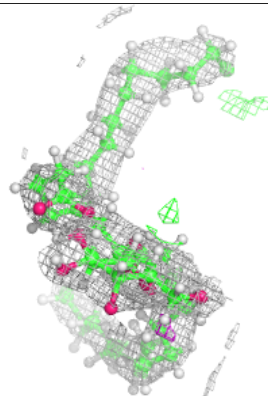
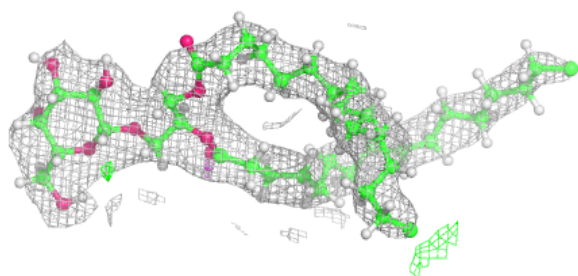
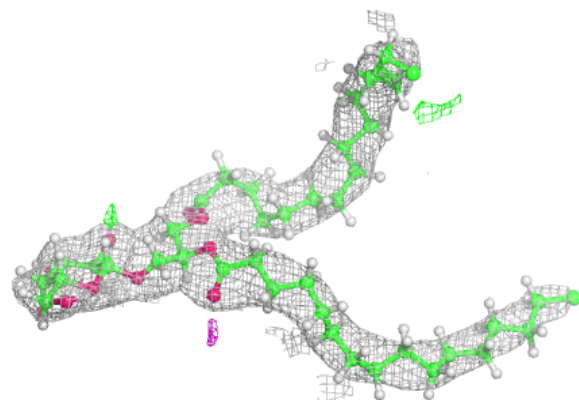


**Electron density around STE d 411:**

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

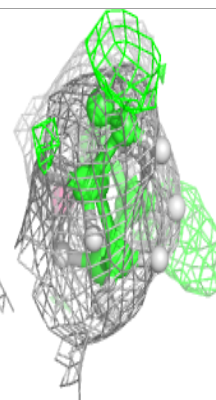
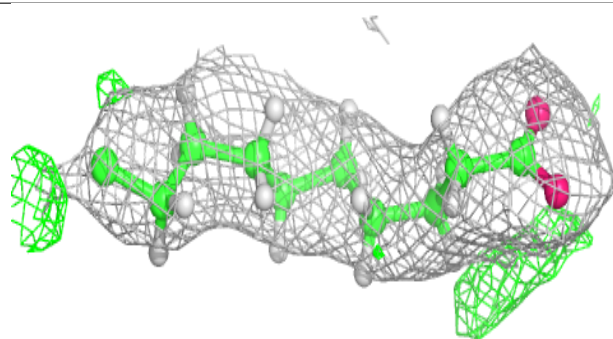
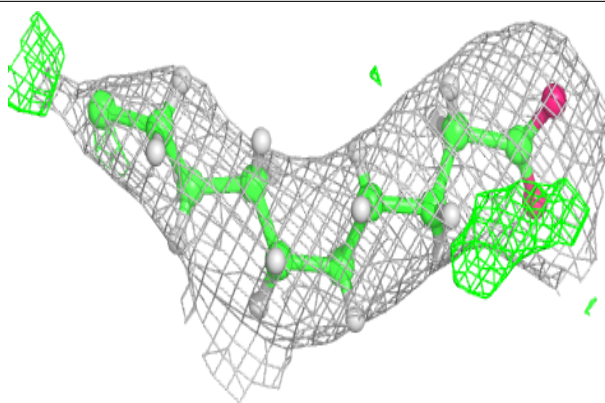
**Electron density around LMG m 101:**

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

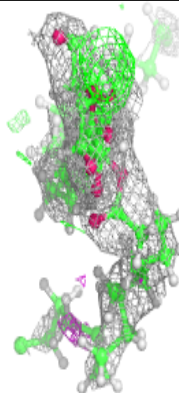
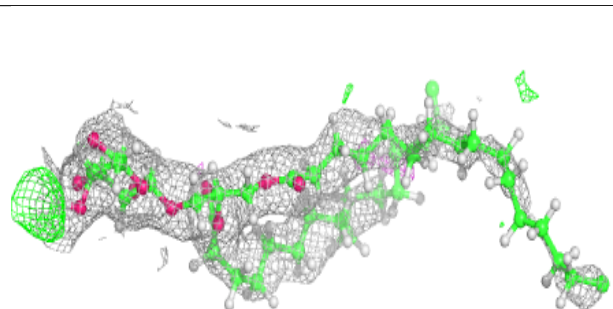
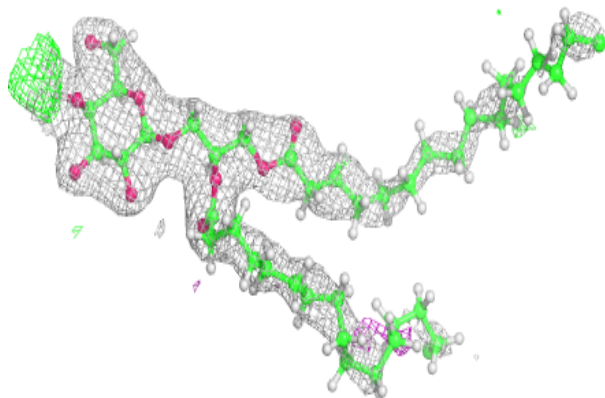


**Electron density around STE B 622:**

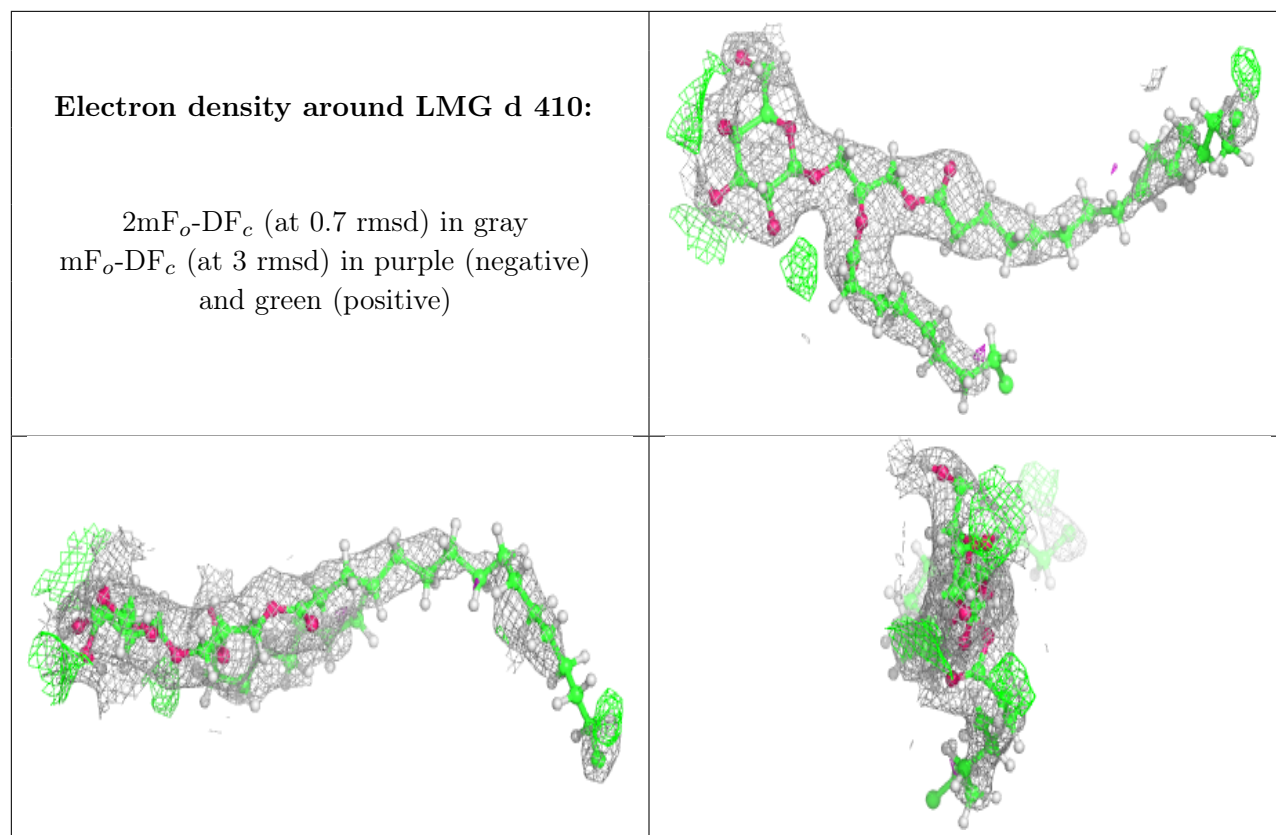
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMG D 408:**

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

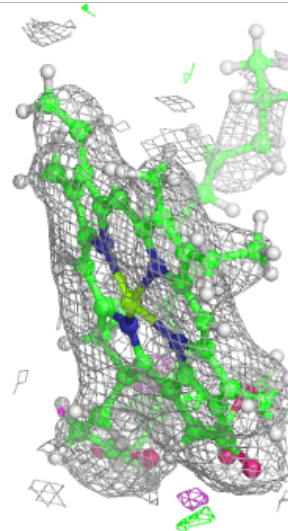
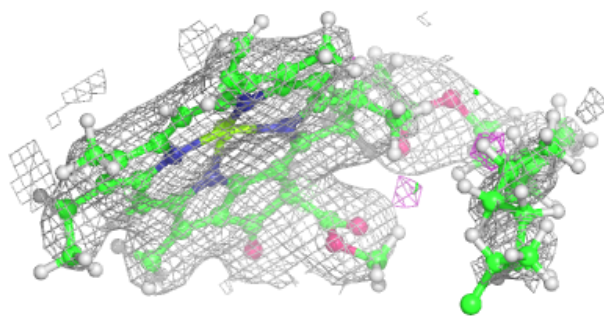
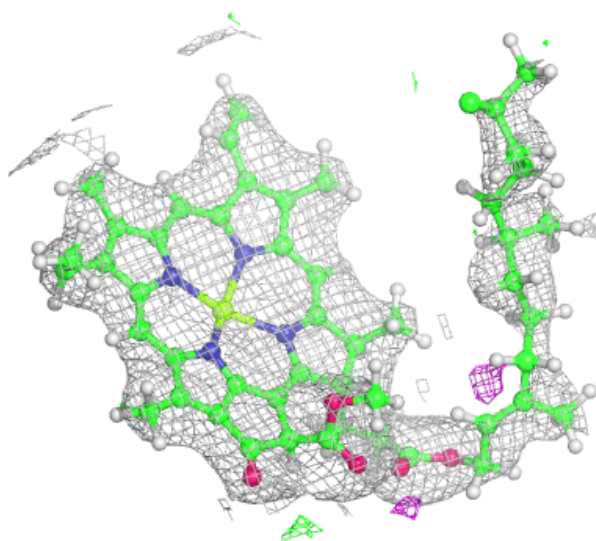






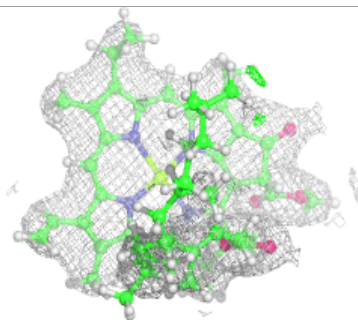
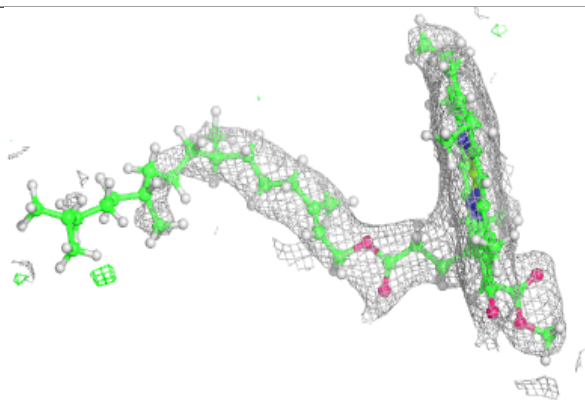
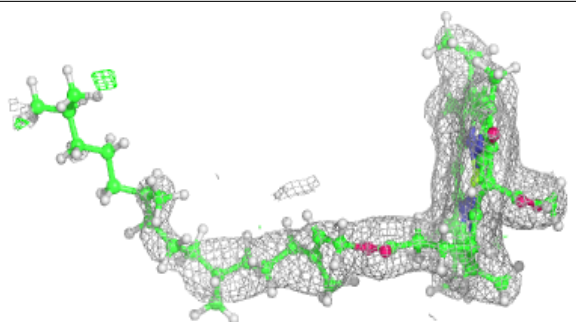
**Electron density around CLA b 616:**

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

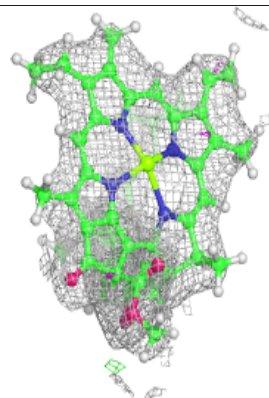
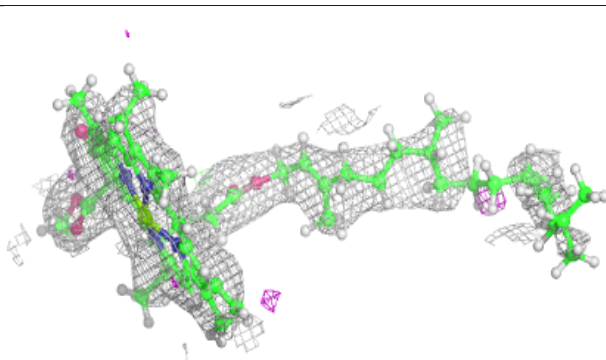
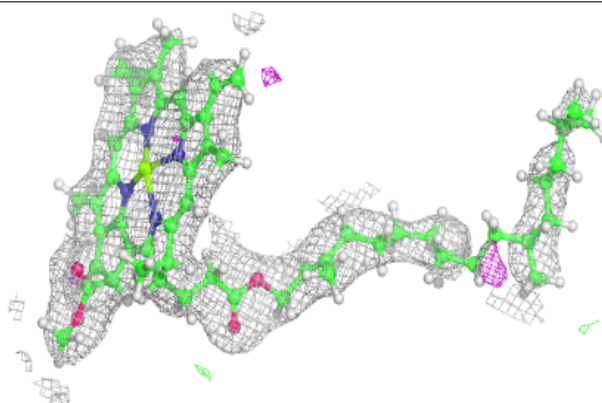


**Electron density around CLA D 405:**

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

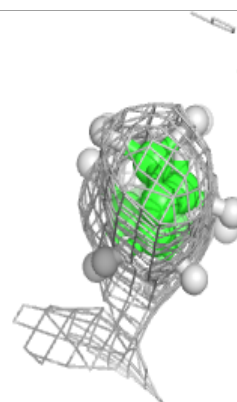
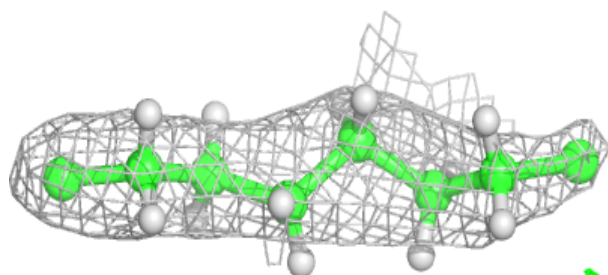
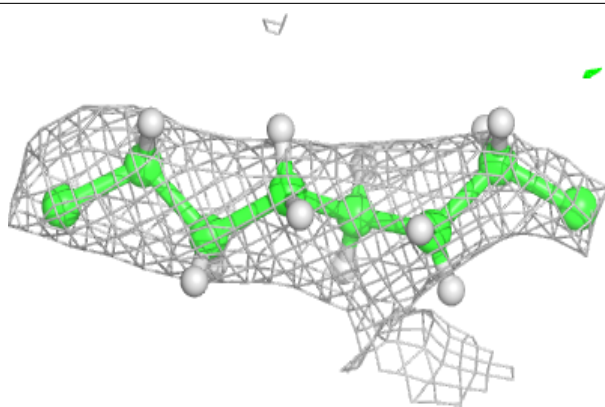
**Electron density around CLA d 405:**

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

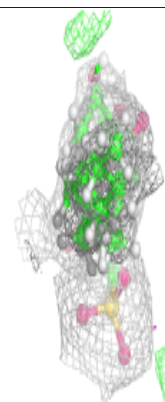
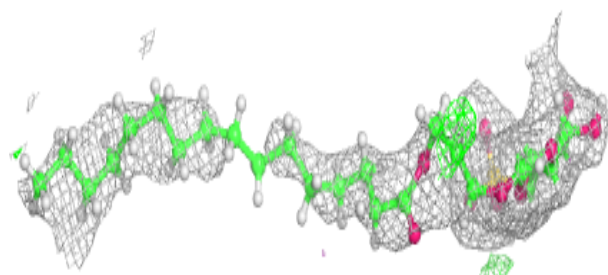
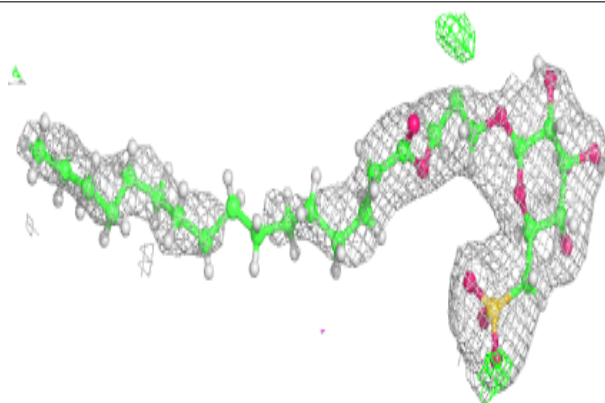


**Electron density around STE Z 101:**

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

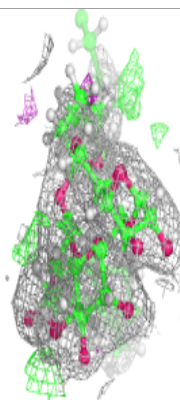
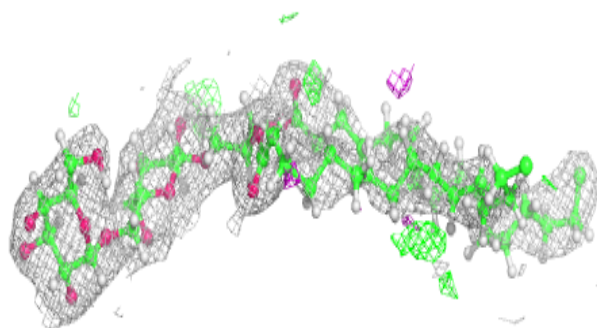
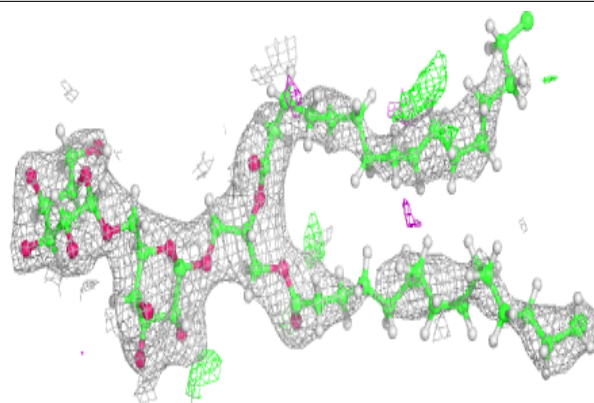
**Electron density around SQD D 409:**

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

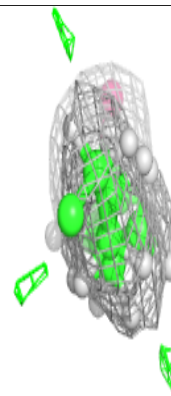
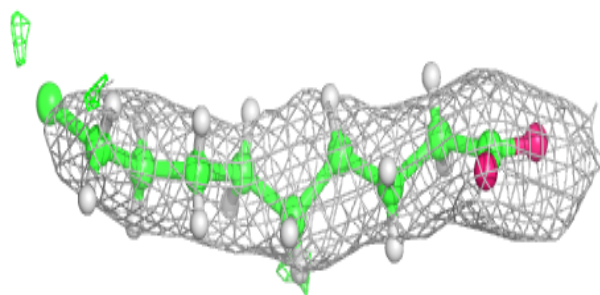
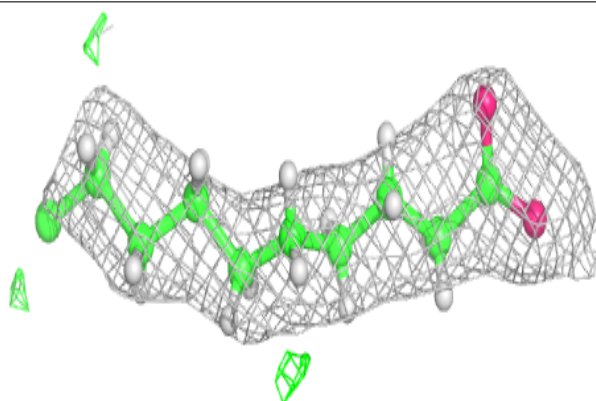


**Electron density around DGD c 517:**

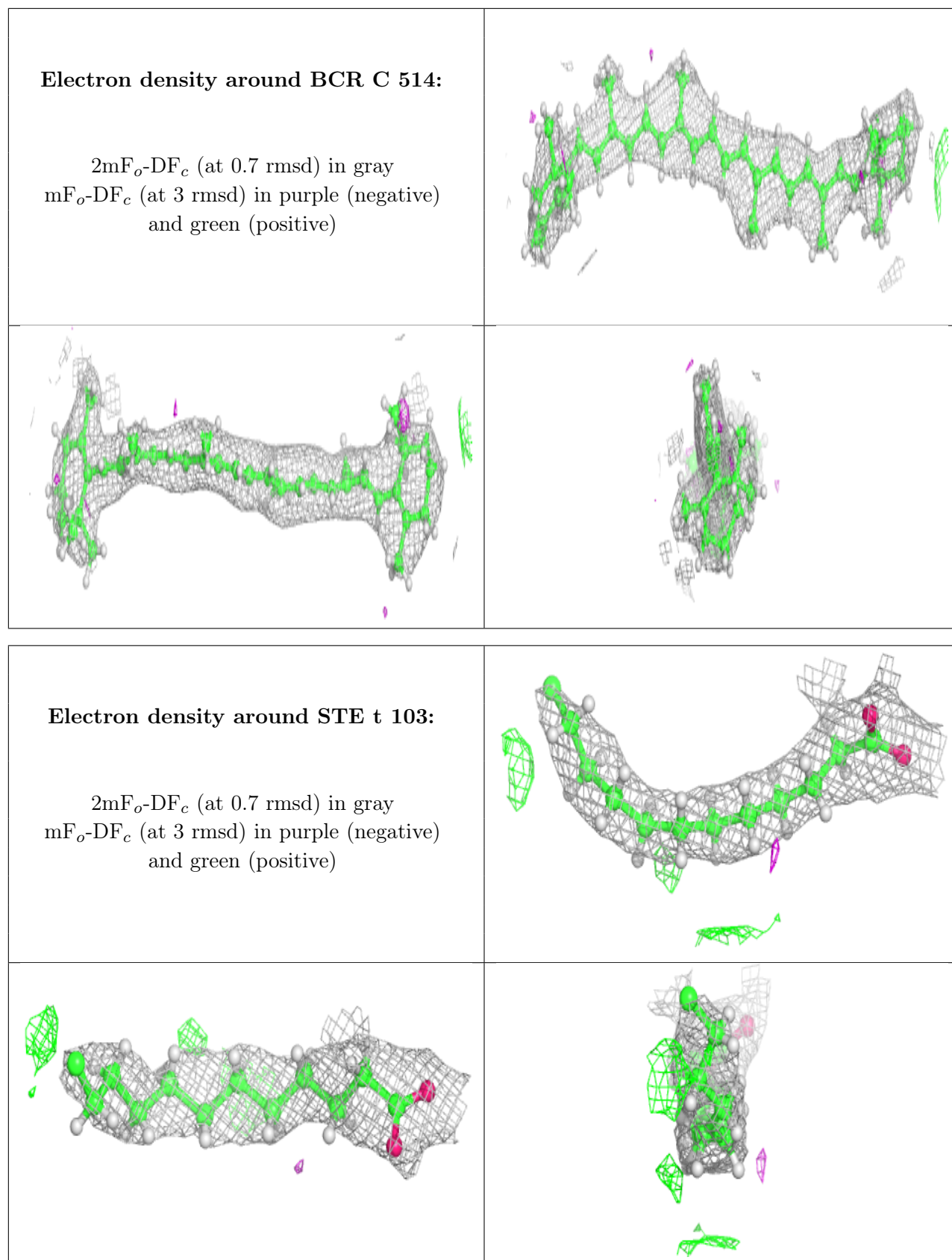
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

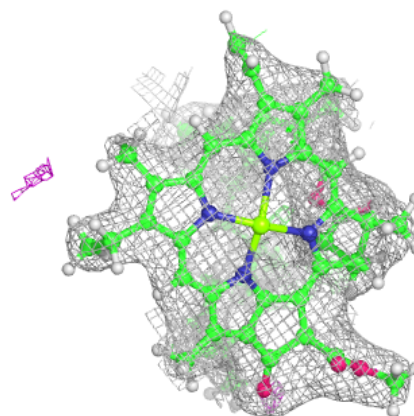
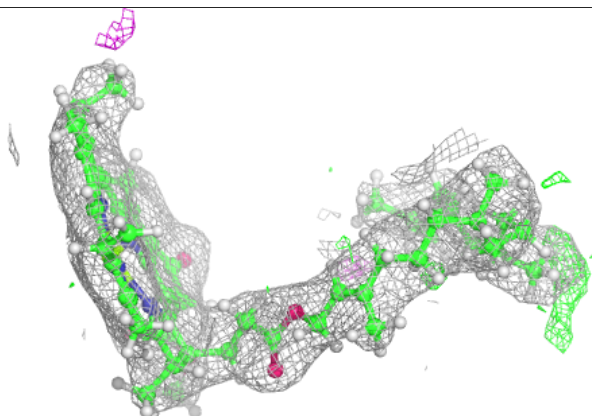
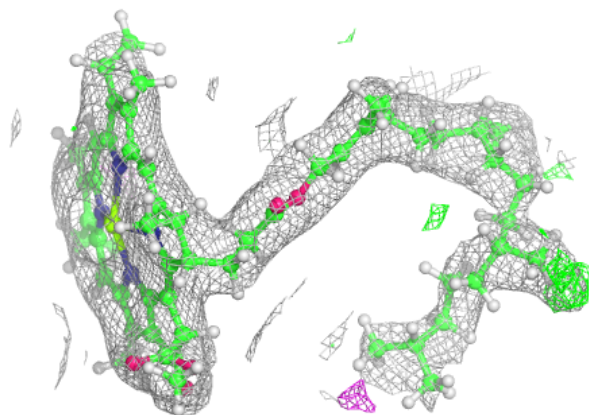




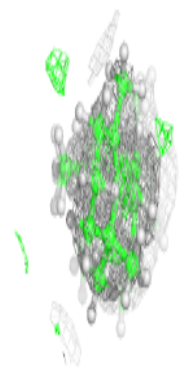
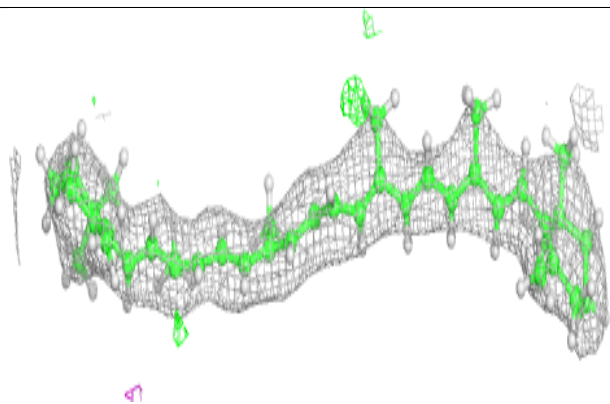
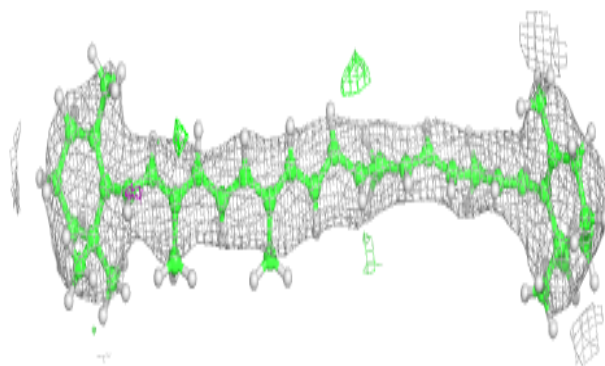


**Electron density around CLA B 605:**

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

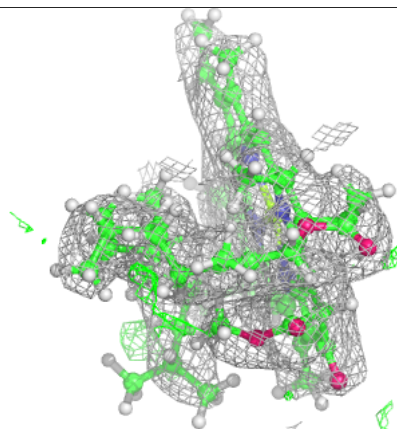
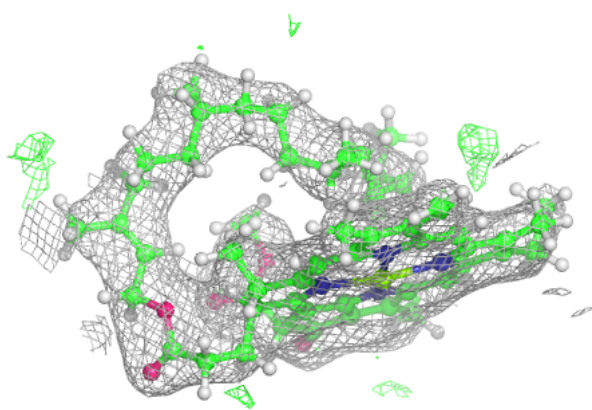
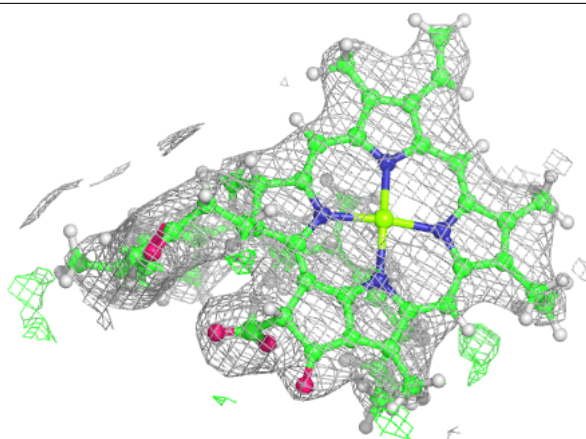
**Electron density around BCR K 101:**

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

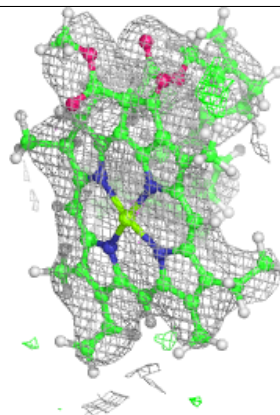
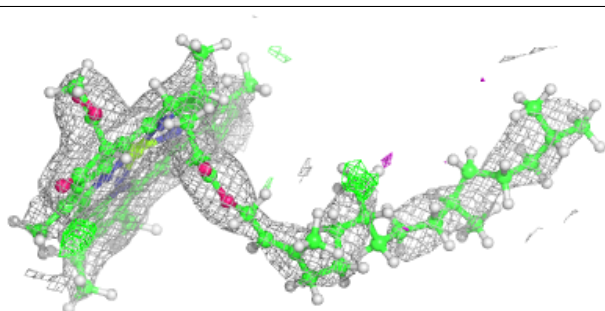
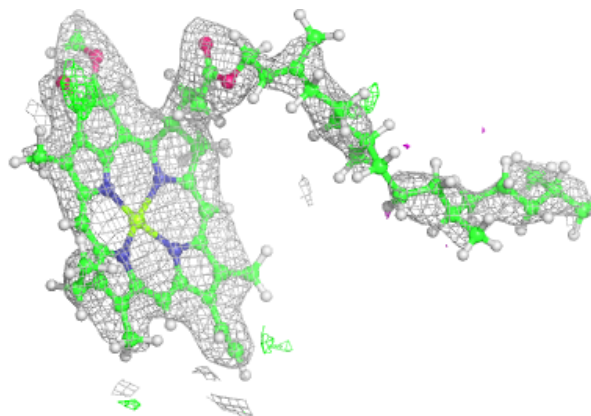


**Electron density around CLA c 510:**

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

**Electron density around CLA c 511:**

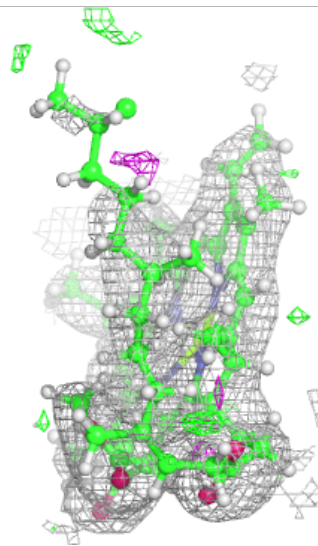
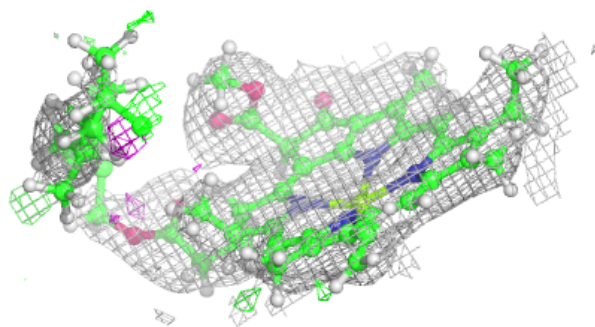
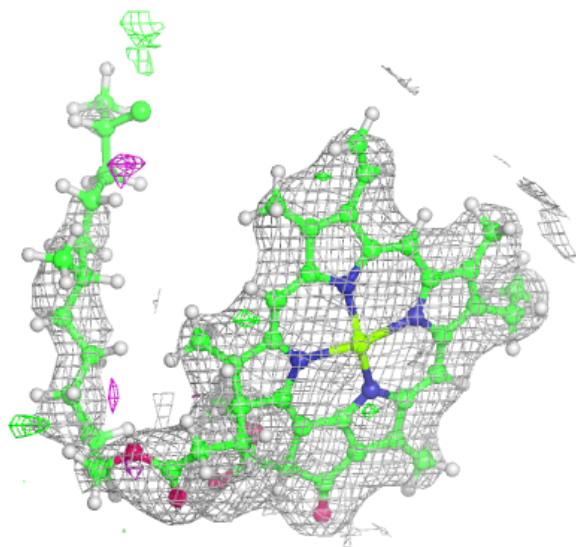
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





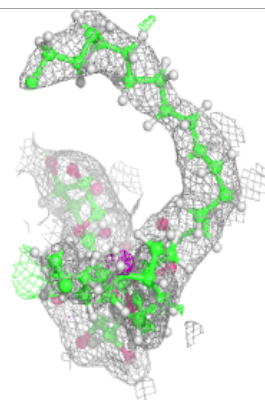
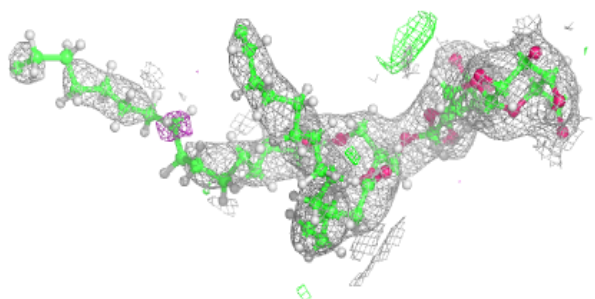
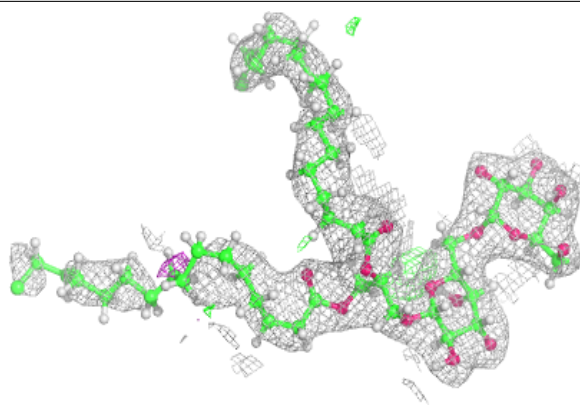
**Electron density around CLA B 615:**

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

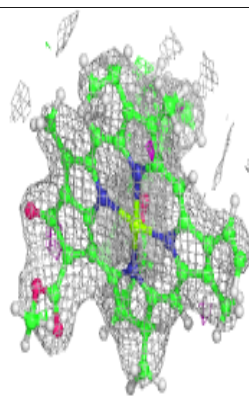
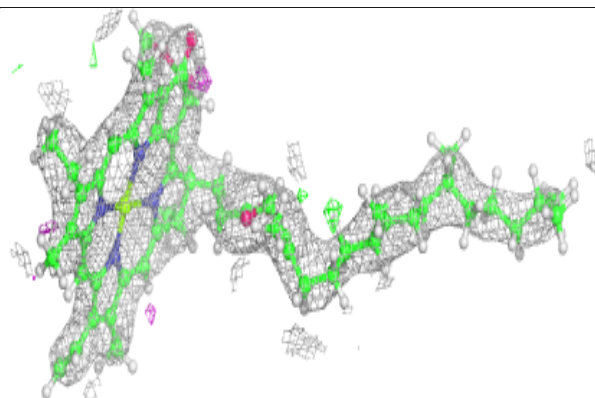
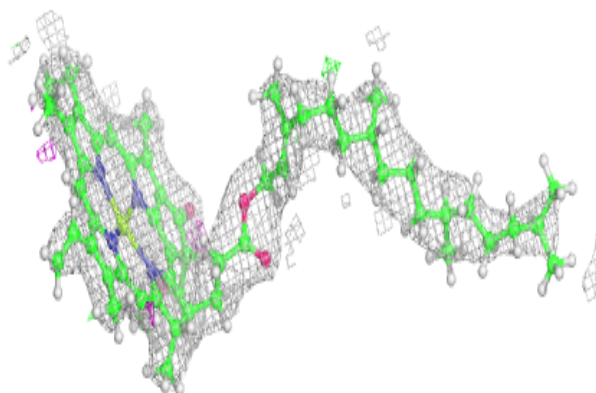


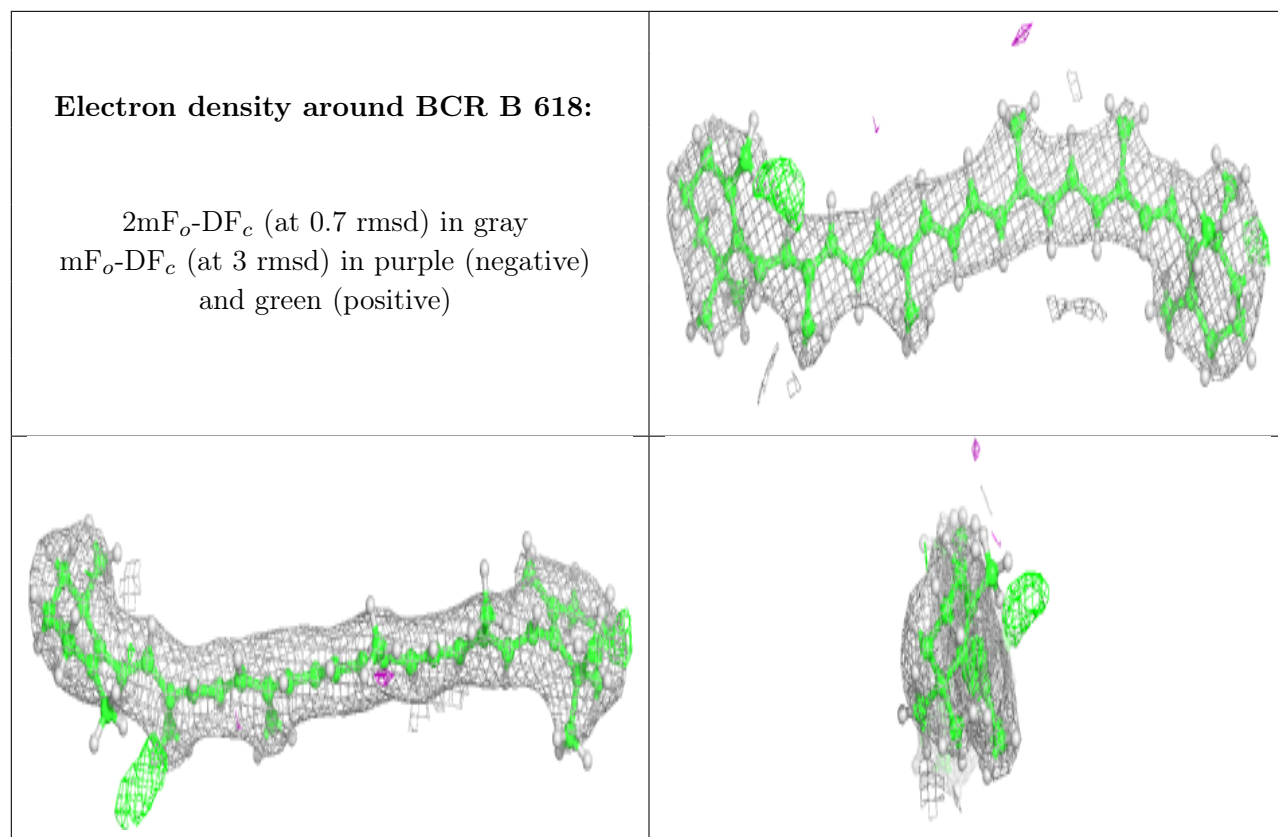
**Electron density around DGD c 516:**

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

**Electron density around CLA C 502:**

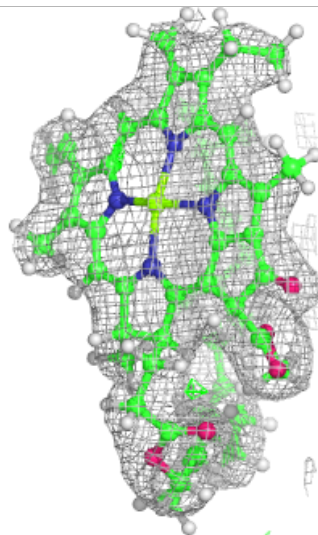
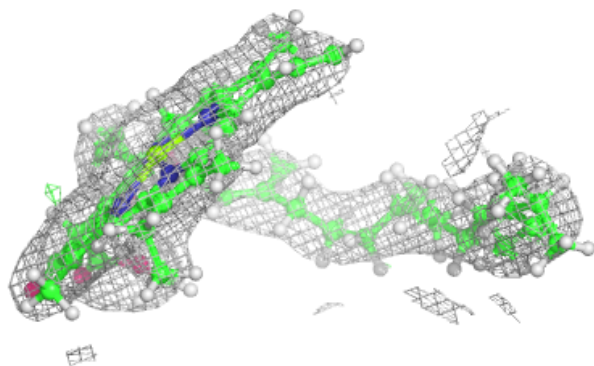
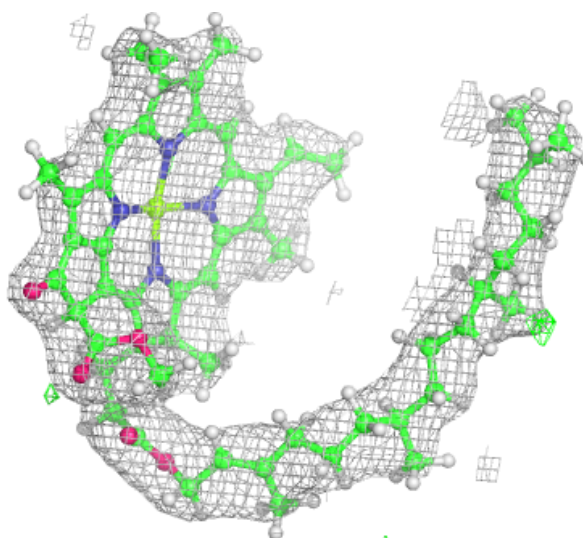
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





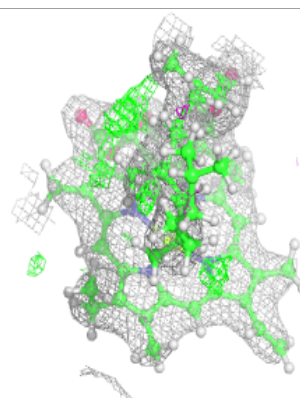
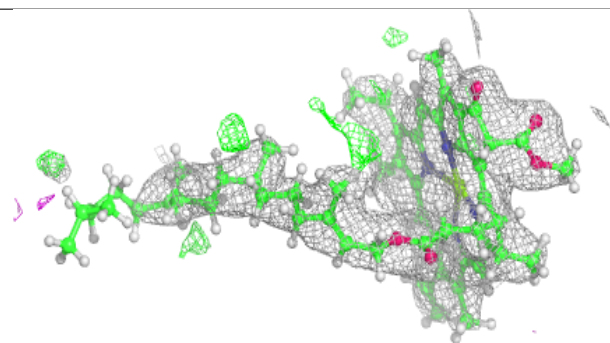
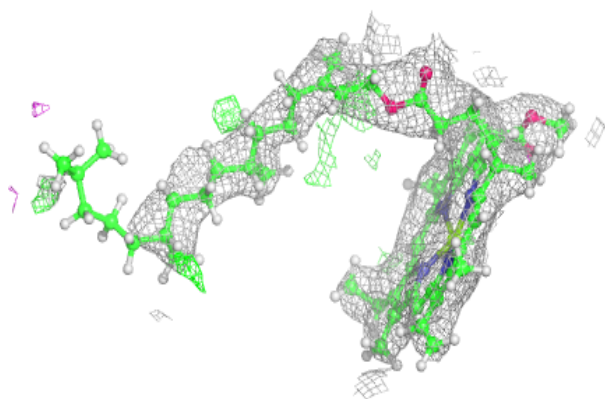
**Electron density around CLA C 507:**

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

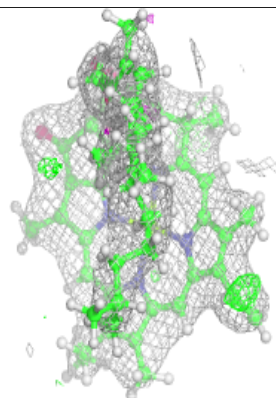
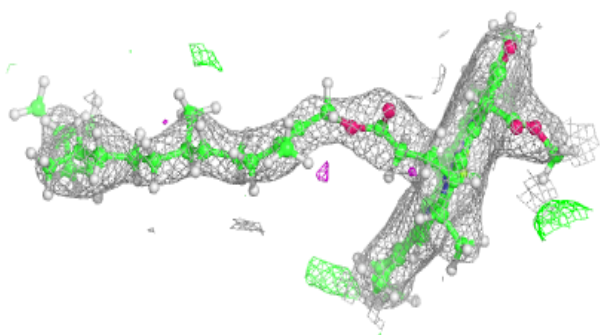
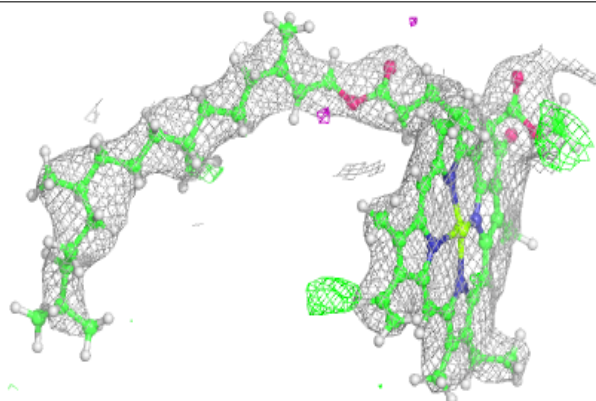


**Electron density around CLA C 508:**

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

**Electron density around CLA b 609:**

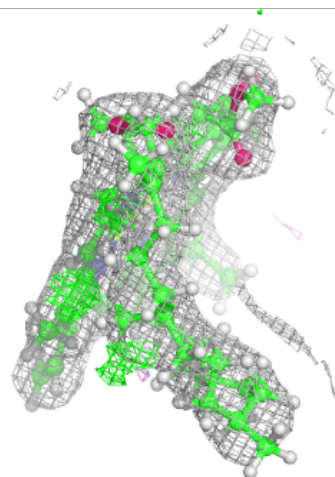
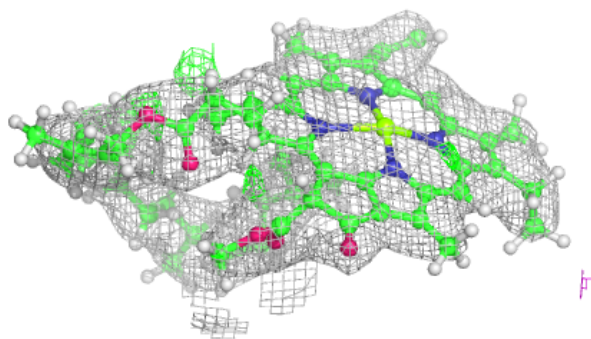
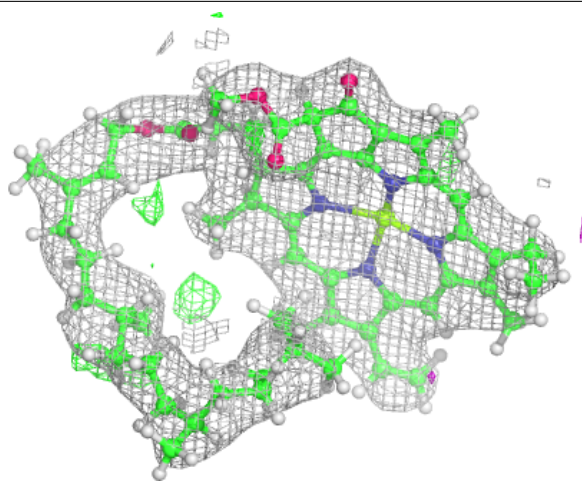
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





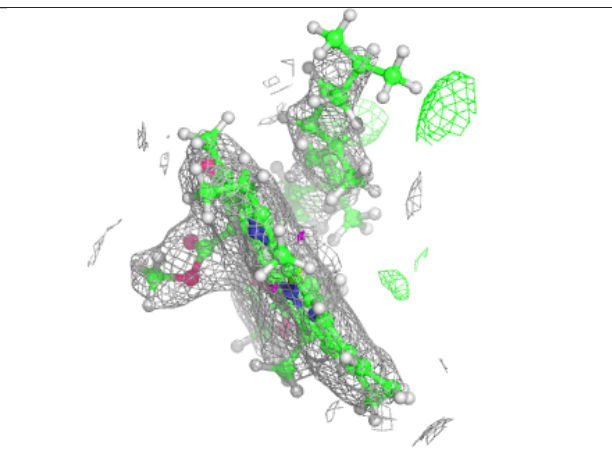
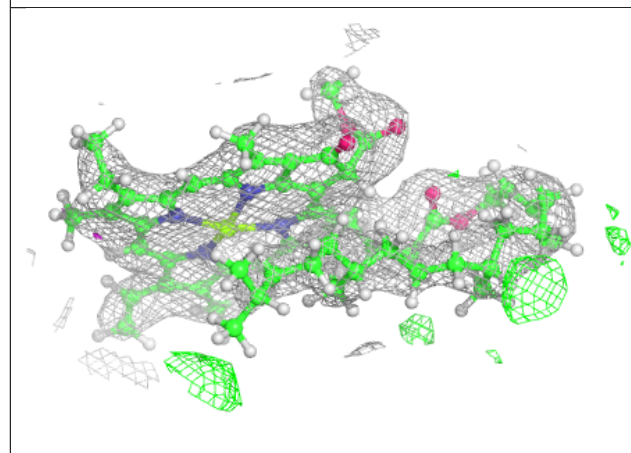
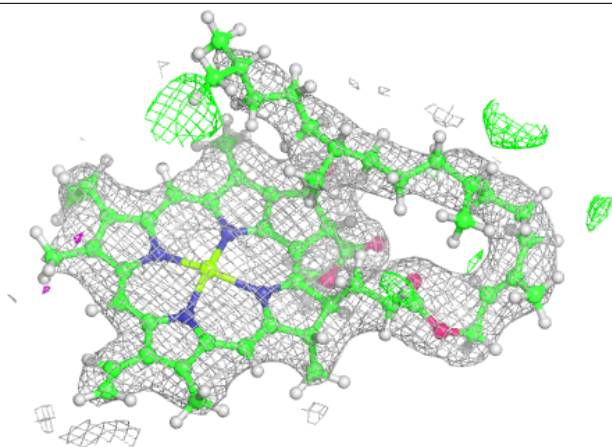
**Electron density around CLA b 615:**

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

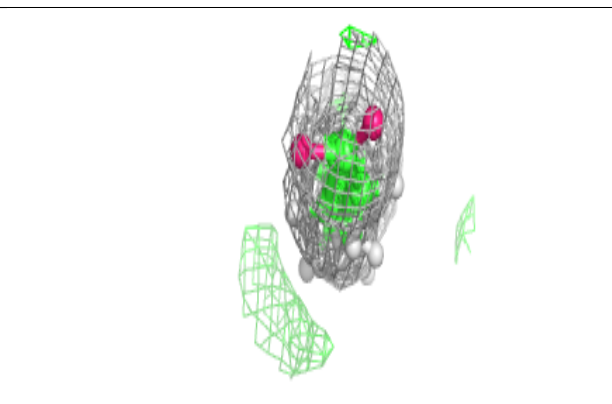
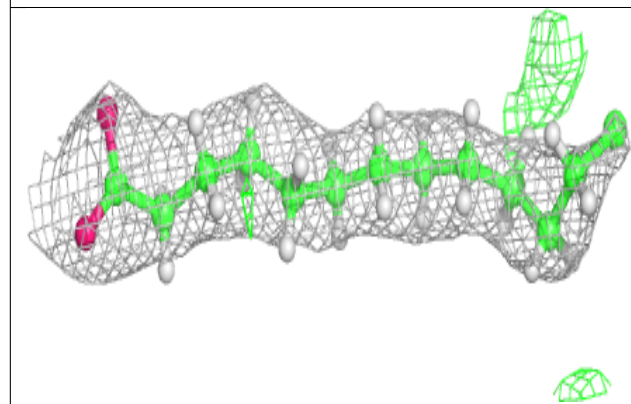
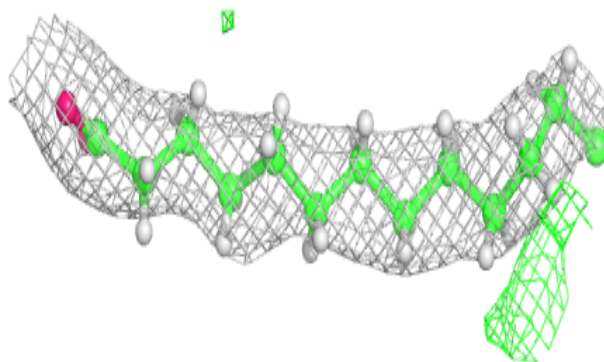


**Electron density around CLA C 509:**

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

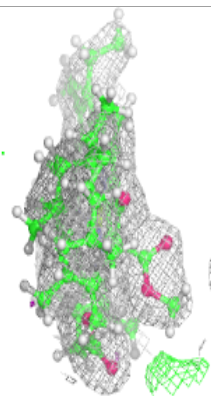
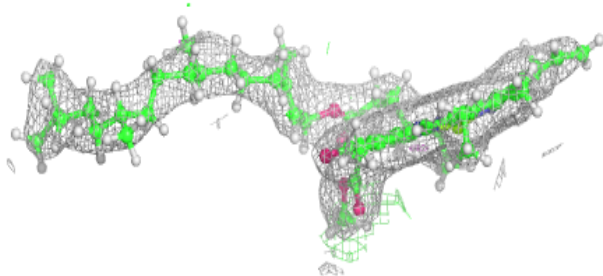
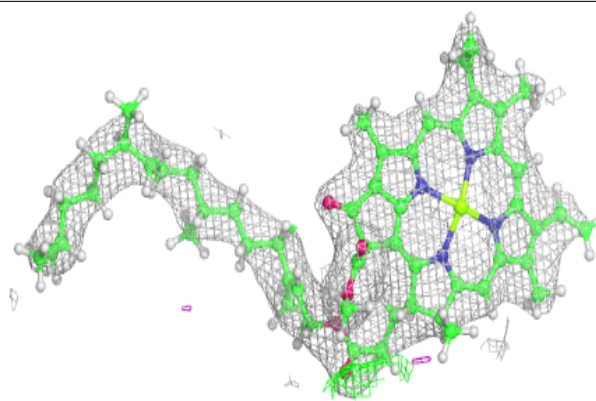
**Electron density around STE M 102:**

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



**Electron density around CLA B 601:**

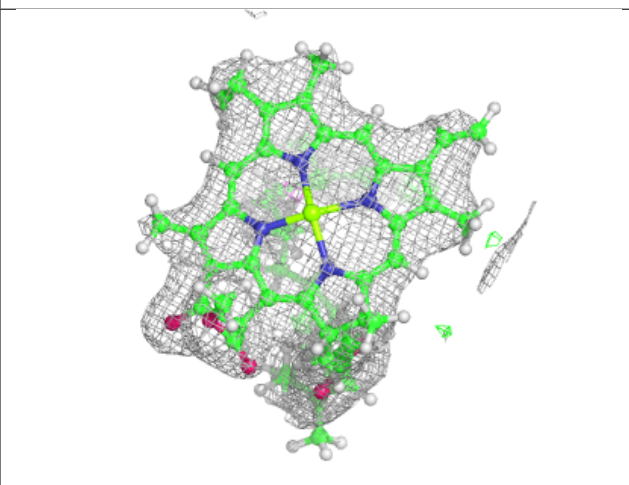
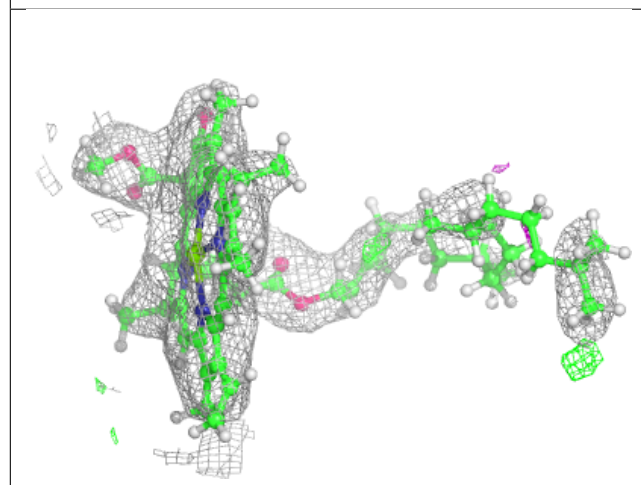
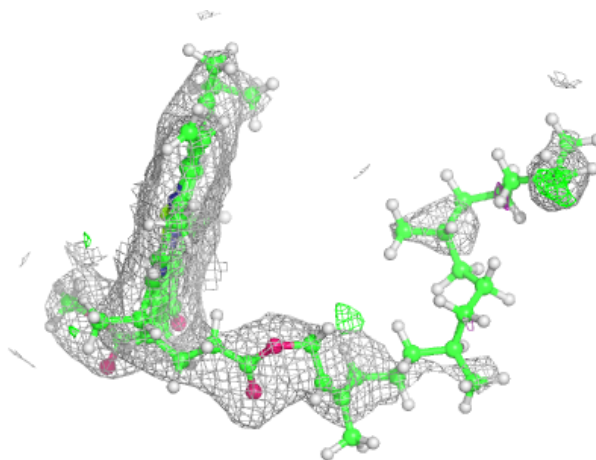
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





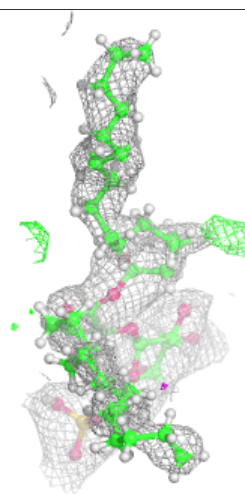
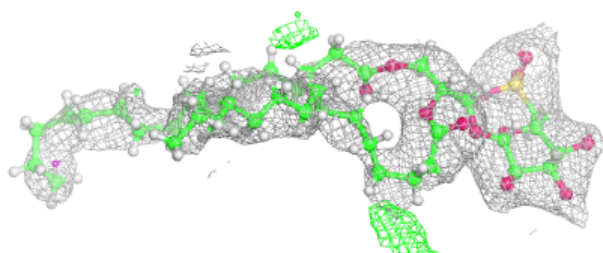
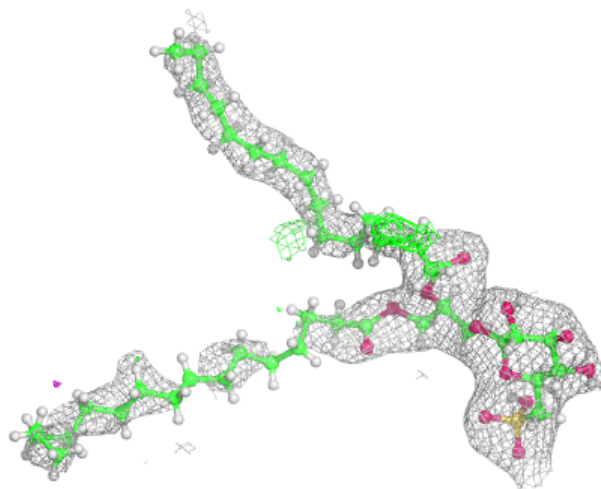
**Electron density around CLA c 506:**

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



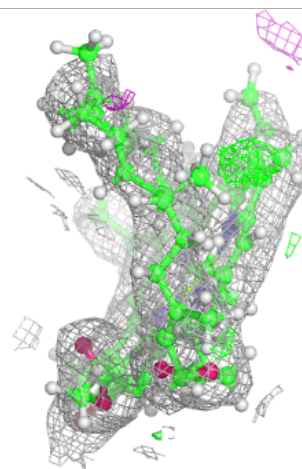
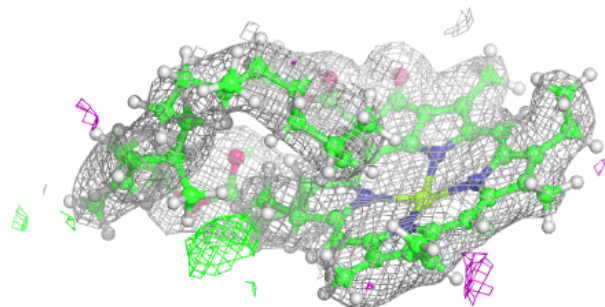
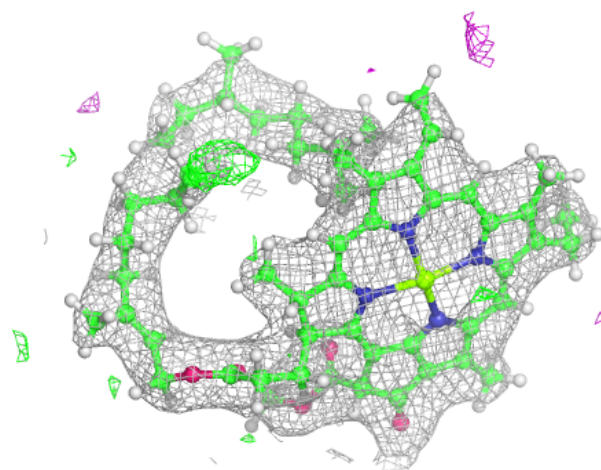
**Electron density around SQD a 410:**

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



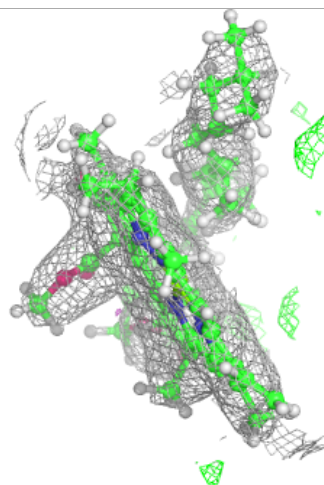
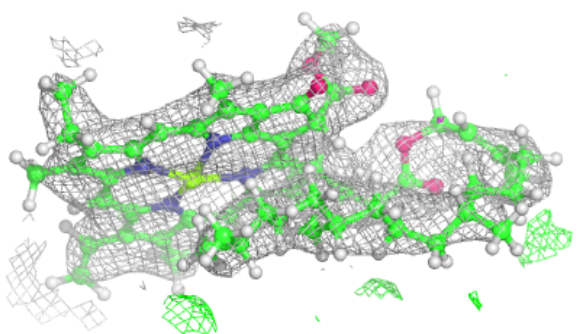
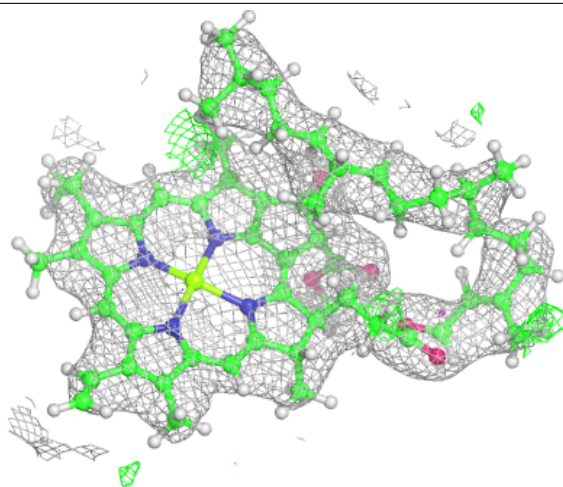
**Electron density around CLA B 614:**

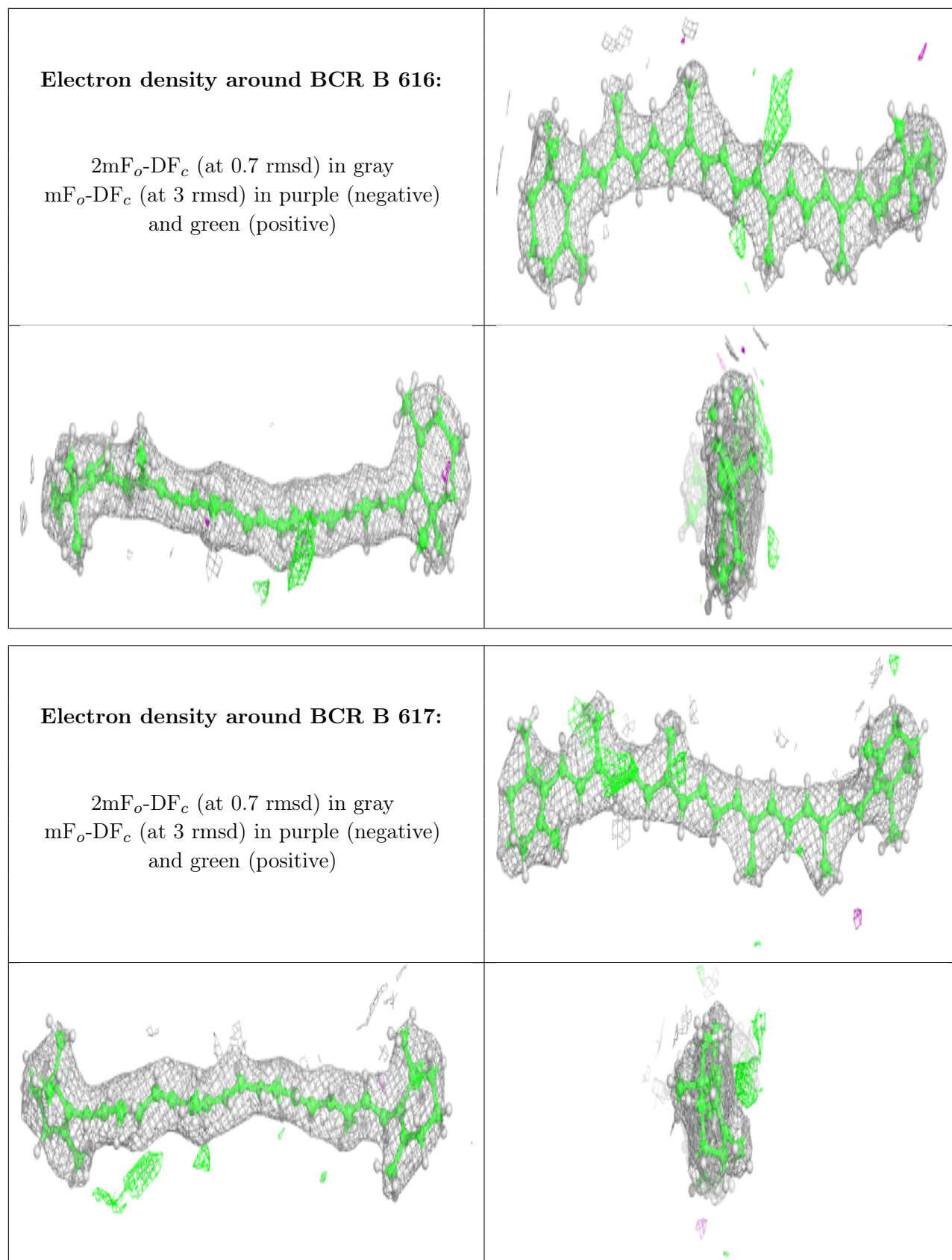
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 509:**

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

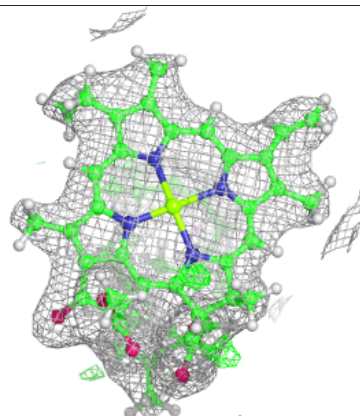
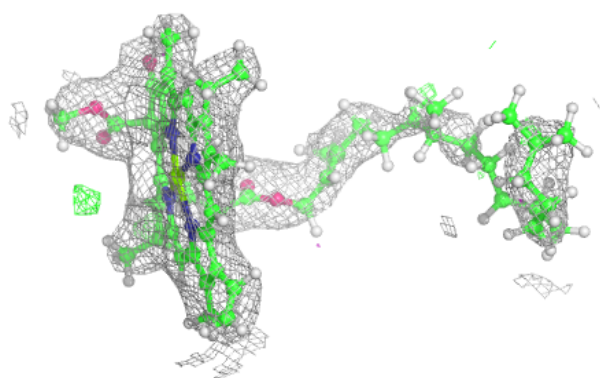
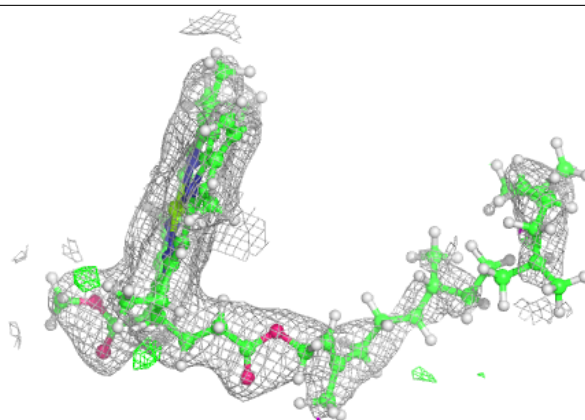




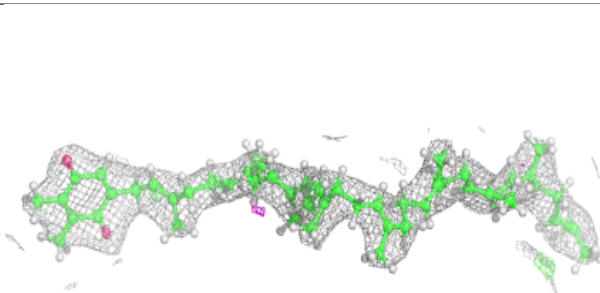
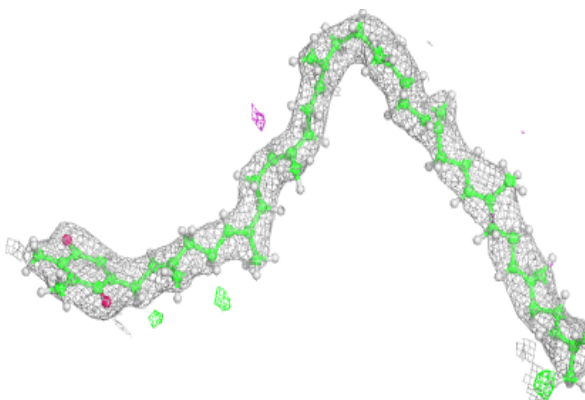


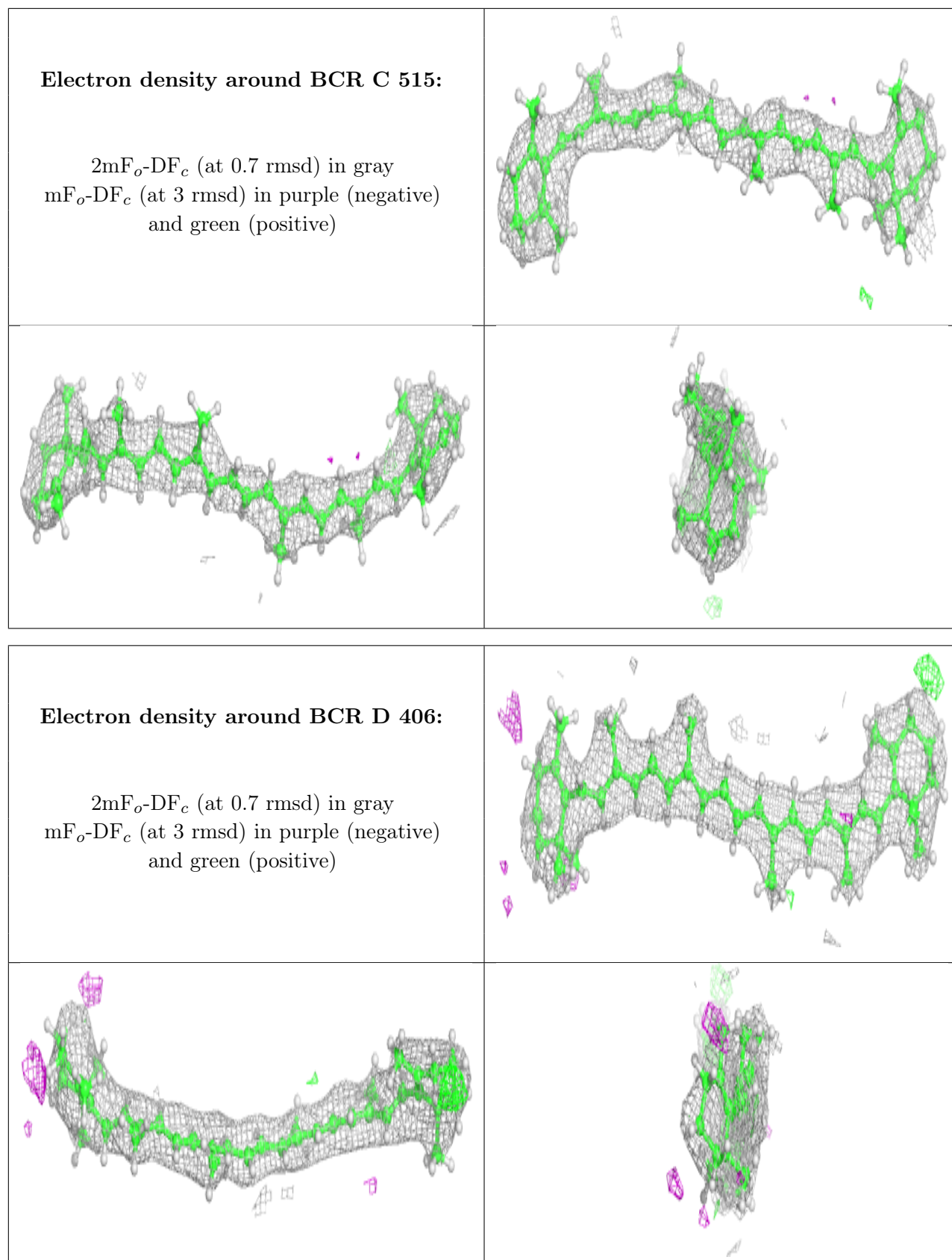
**Electron density around CLA C 506:**

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

**Electron density around PL9 D 407:**

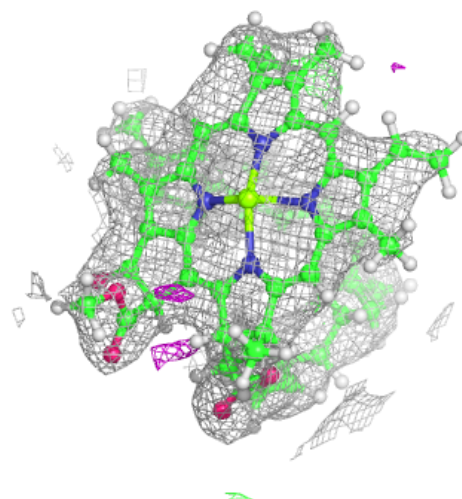
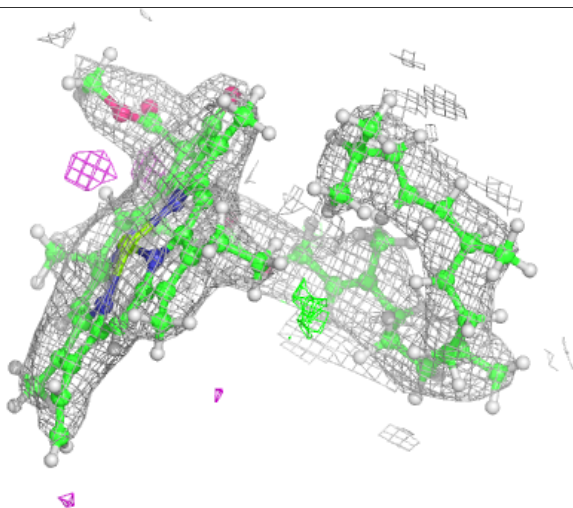
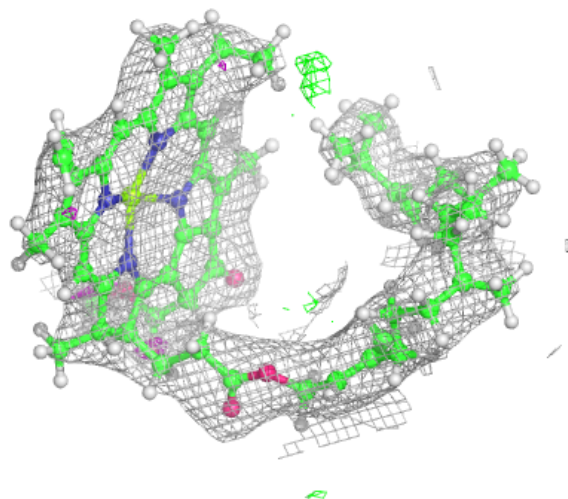
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA c 503:**

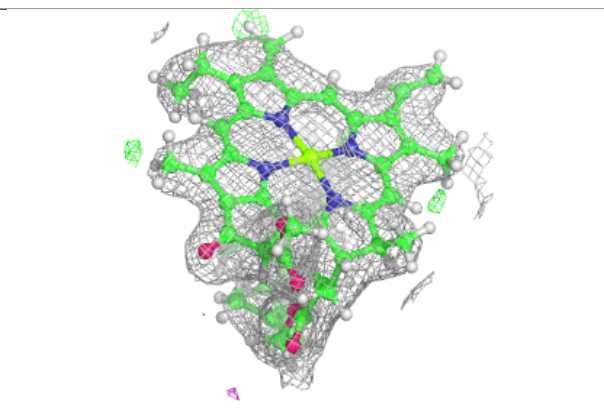
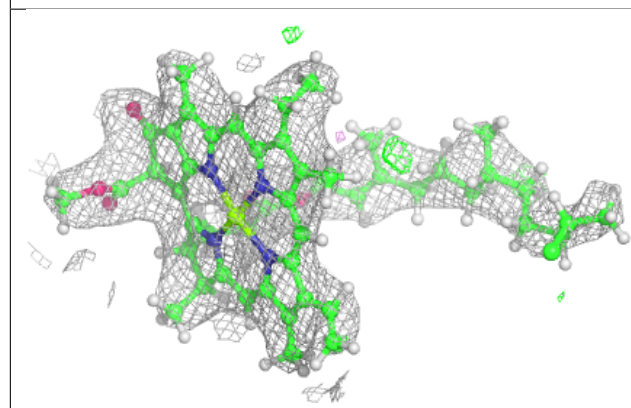
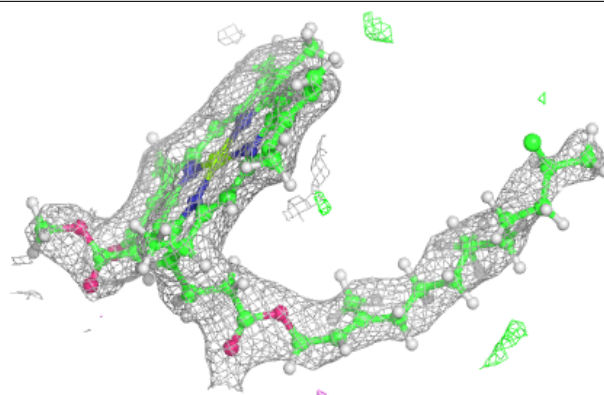
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



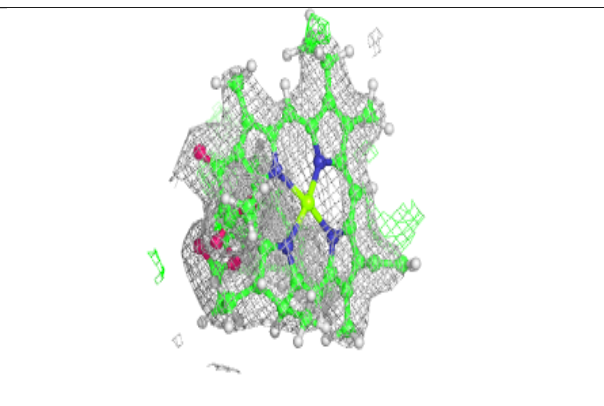
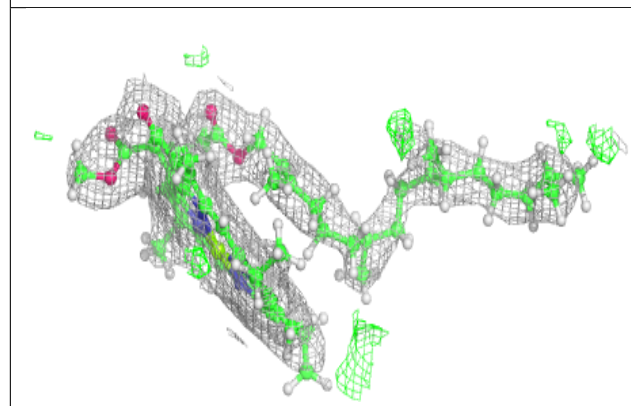
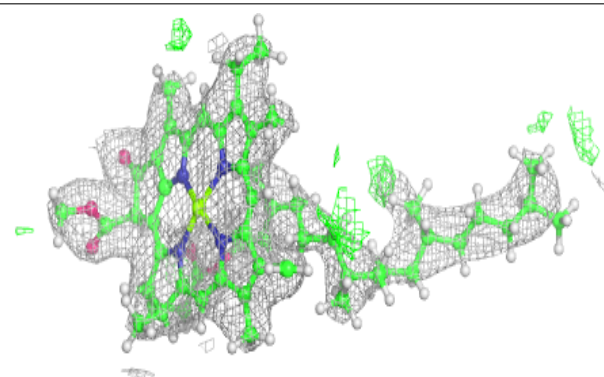


**Electron density around CLA c 504:**

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

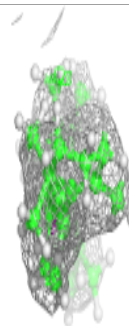
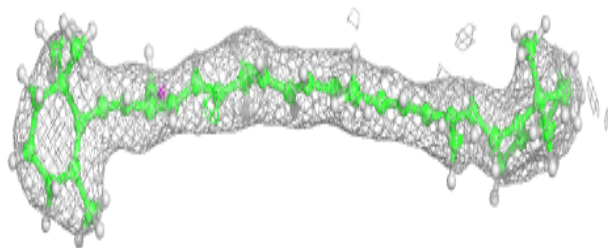
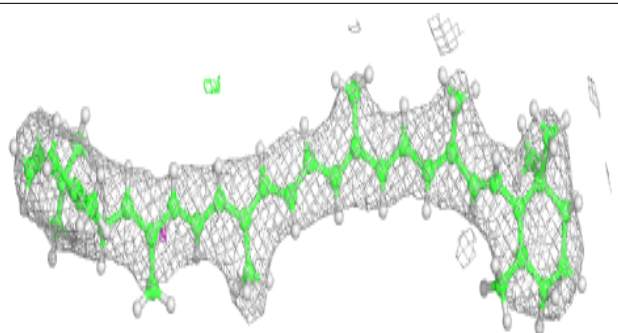
**Electron density around CLA c 505:**

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

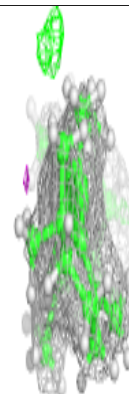
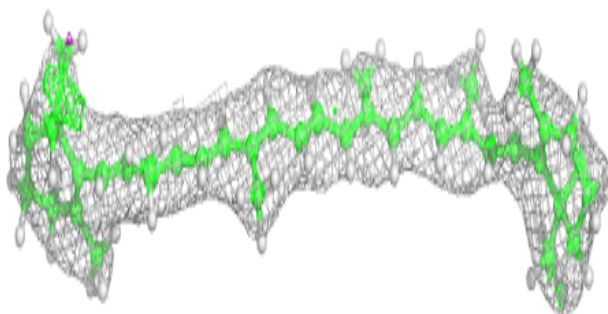
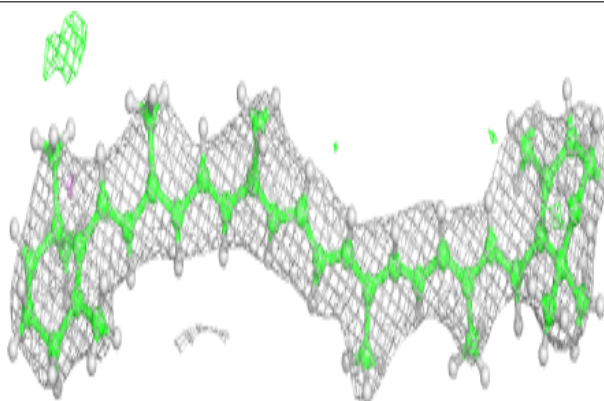


**Electron density around BCR b 617:**

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

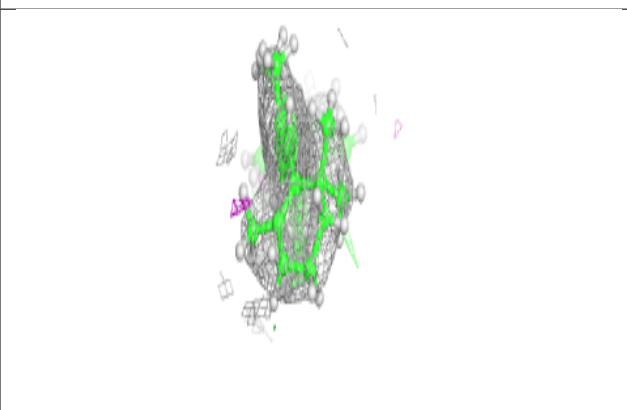
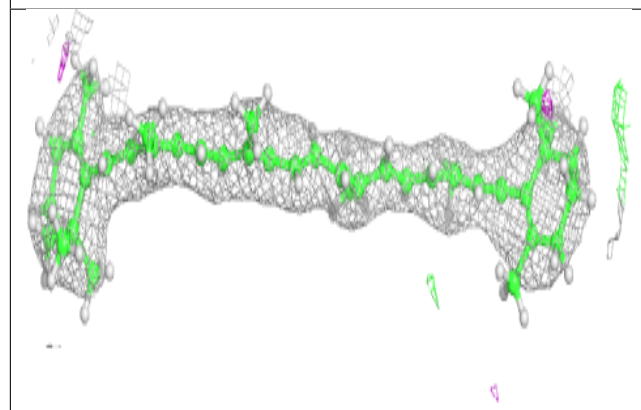
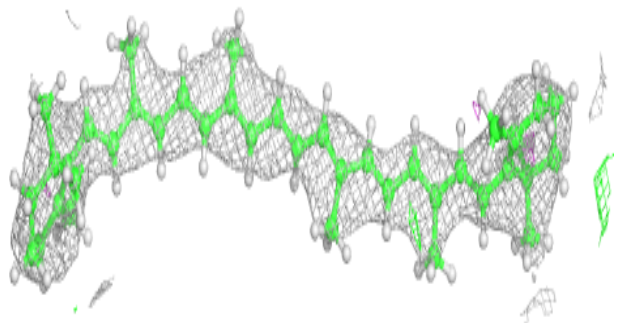
**Electron density around BCR b 619:**

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

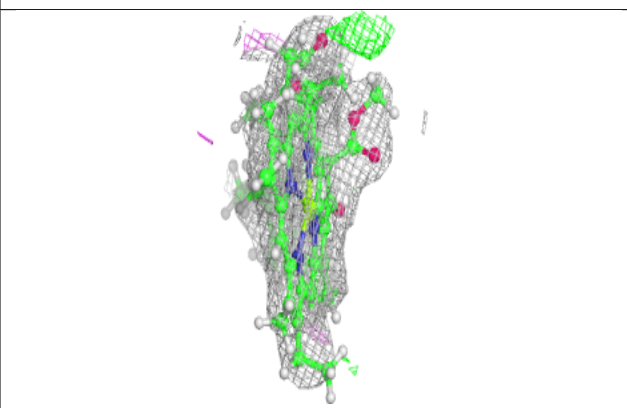
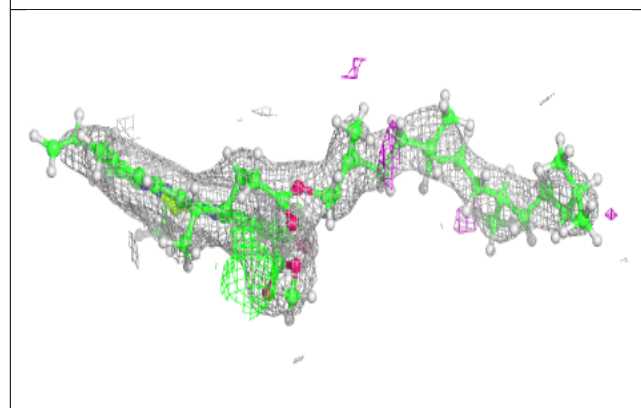
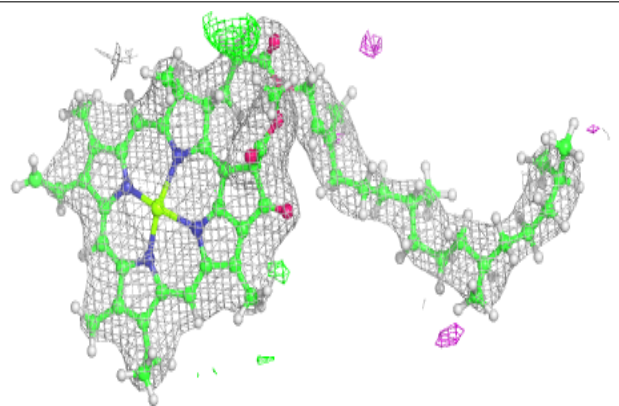


**Electron density around BCR c 514:**

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

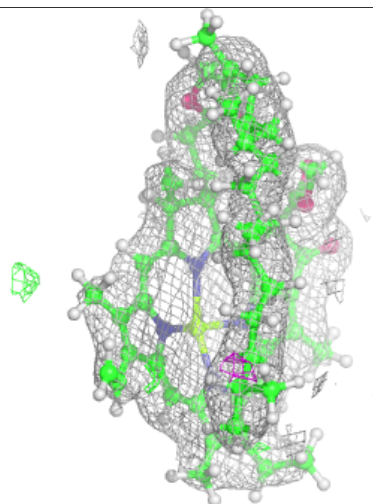
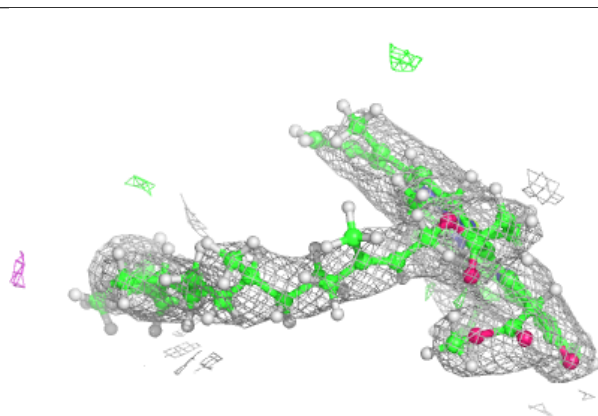
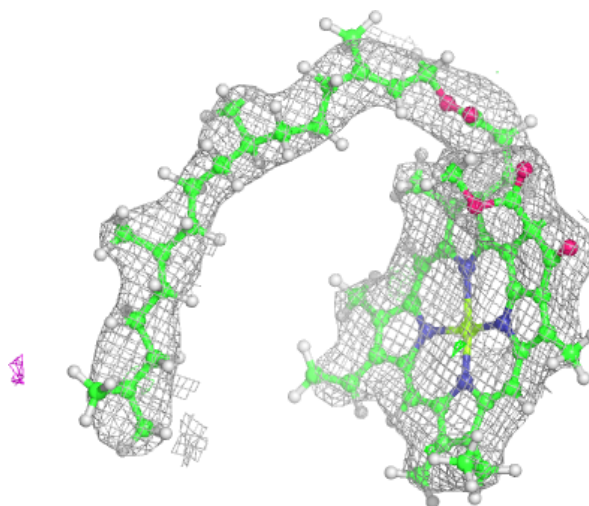
**Electron density around CLA b 602:**

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



**Electron density around CLA c 507:**

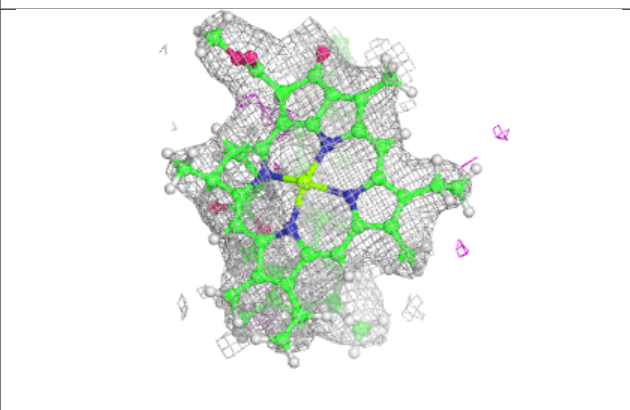
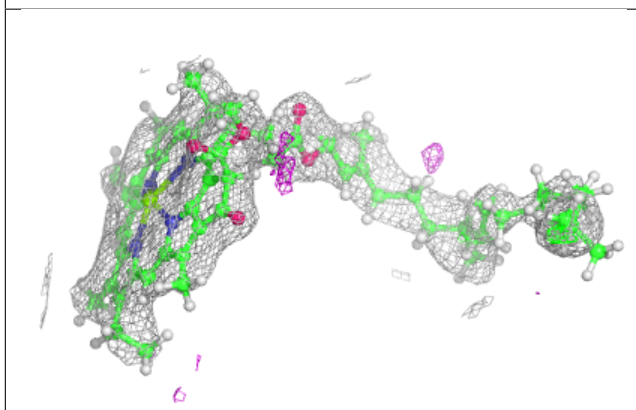
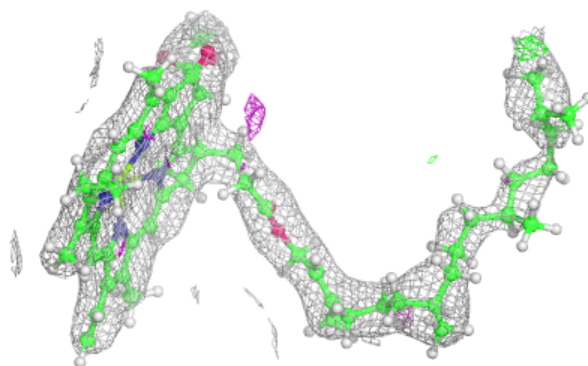
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



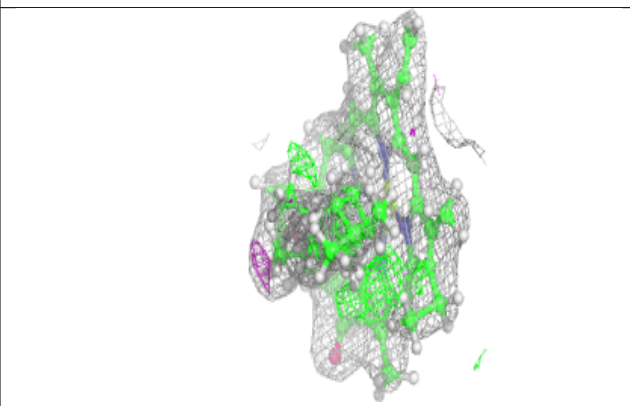
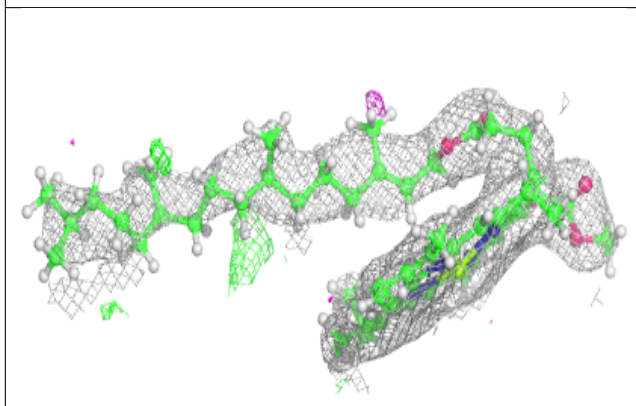
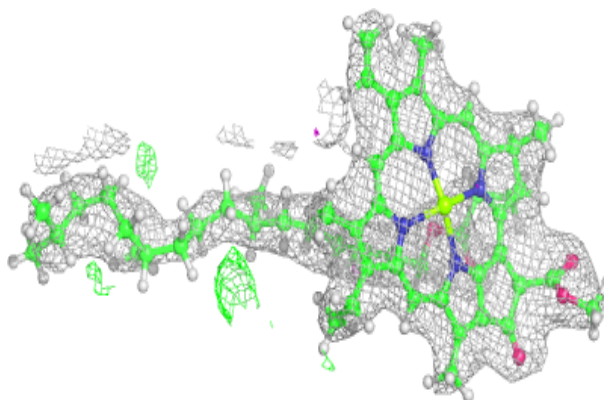


**Electron density around CLA b 606:**

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

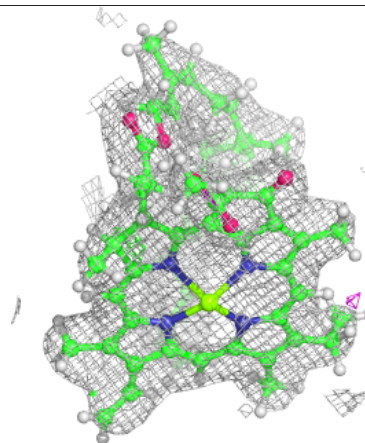
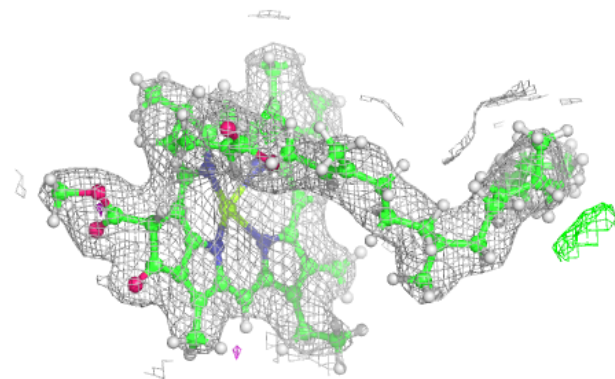
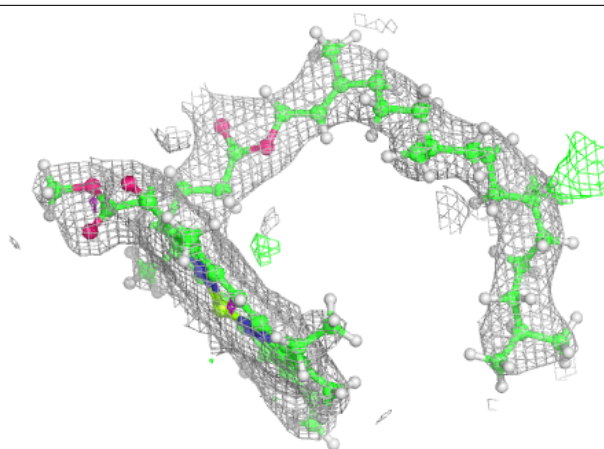
**Electron density around CLA B 613:**

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



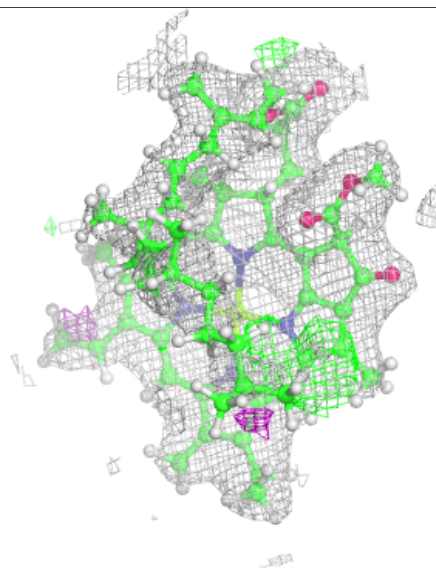
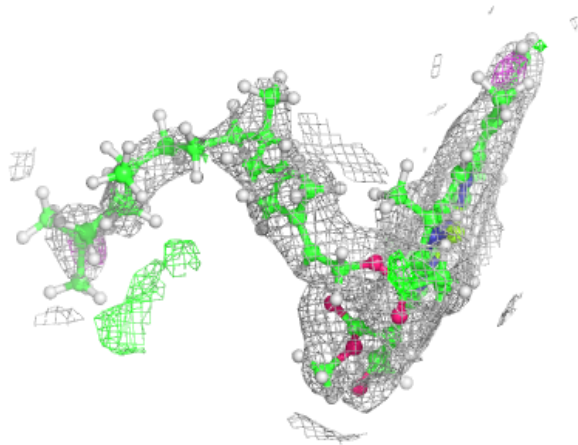
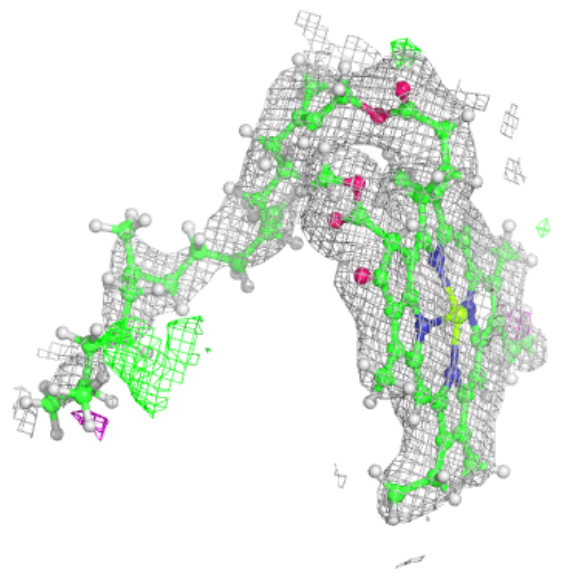
**Electron density around CLA b 611:**

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



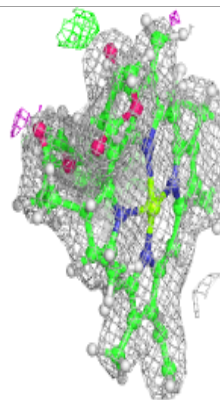
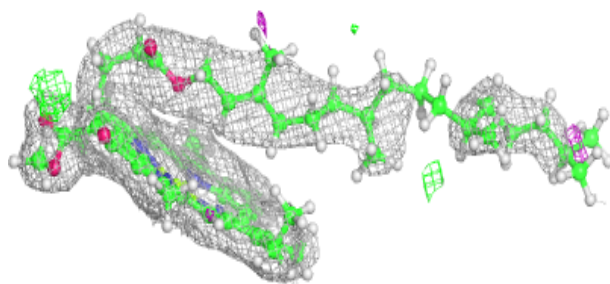
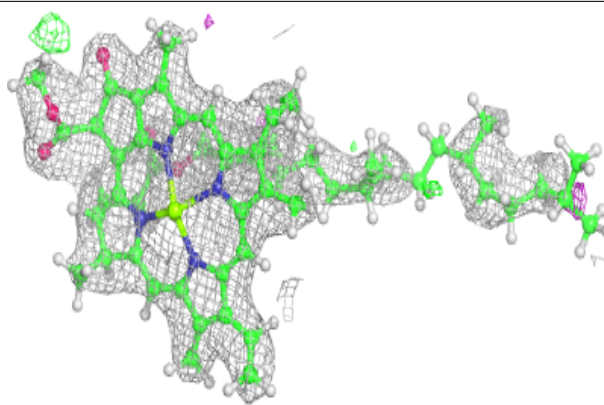
**Electron density around CLA b 613:**

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

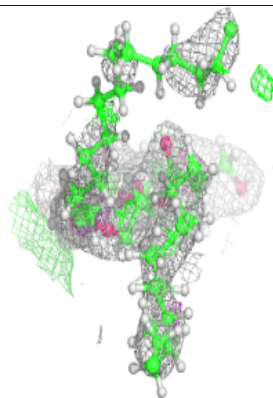
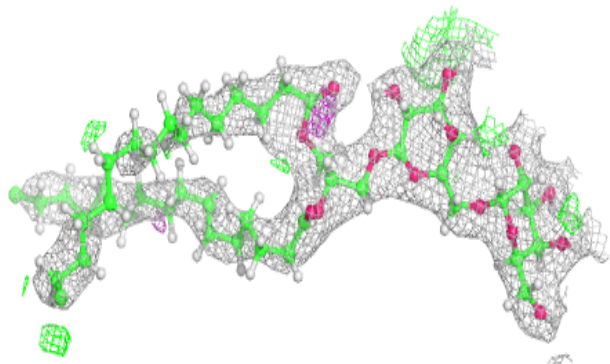
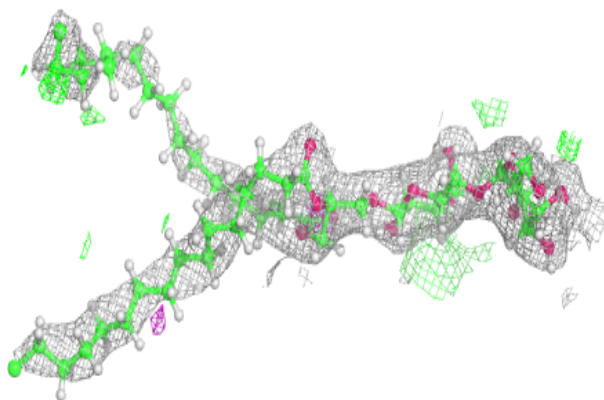


**Electron density around CLA b 614:**

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

**Electron density around DGD C 516:**

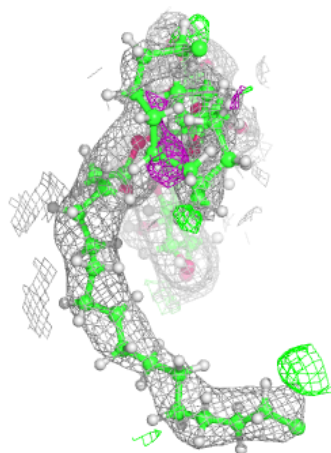
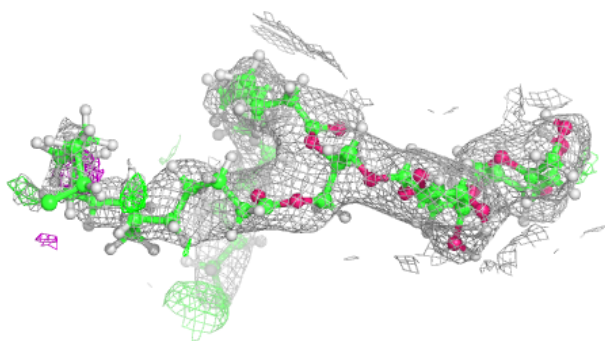
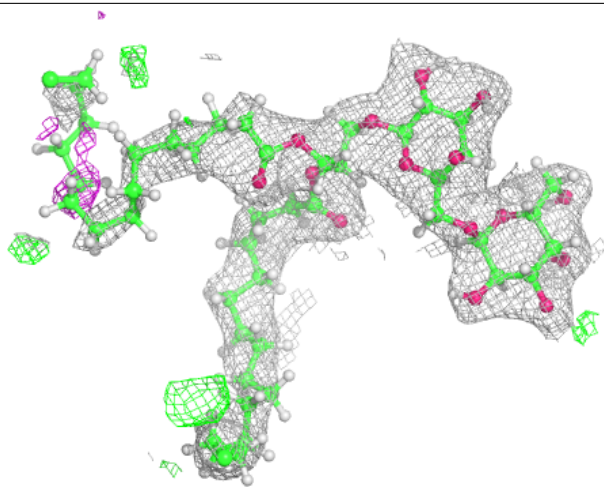
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





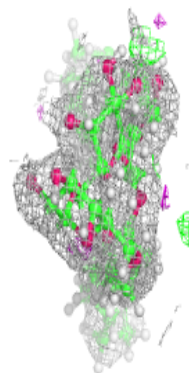
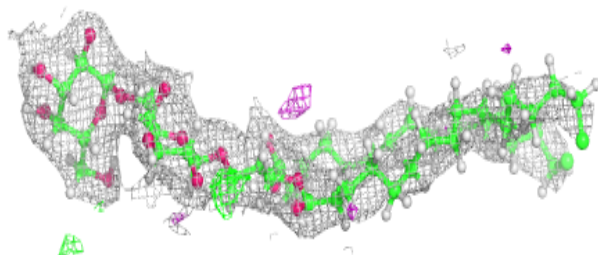
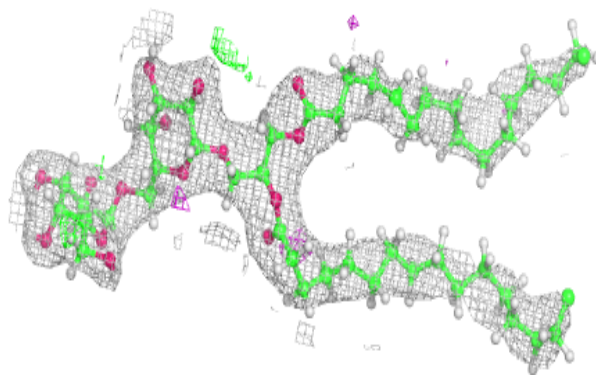
**Electron density around DGD C 517:**

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

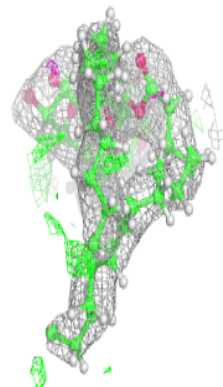
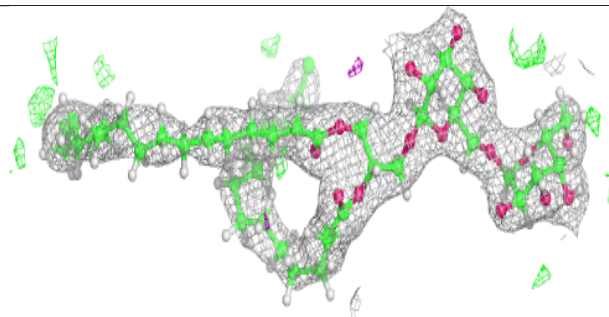
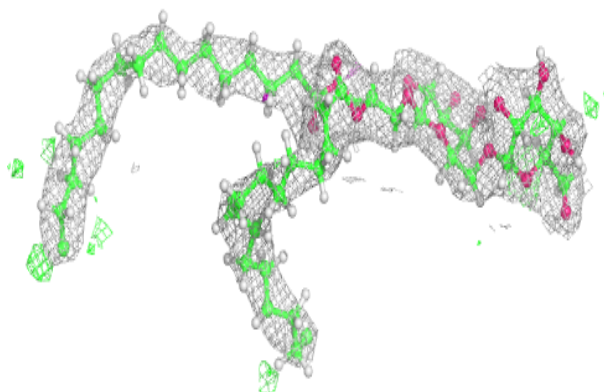


**Electron density around DGD C 518:**

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

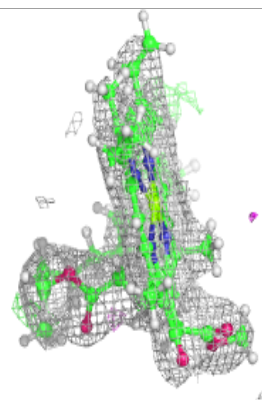
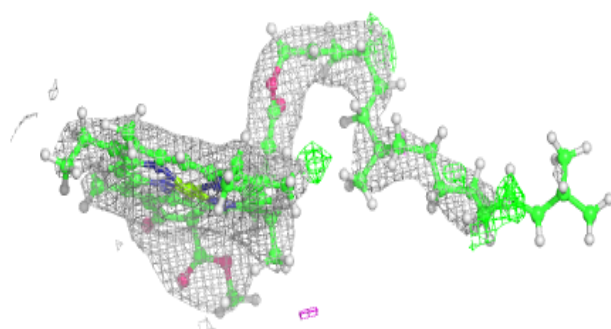
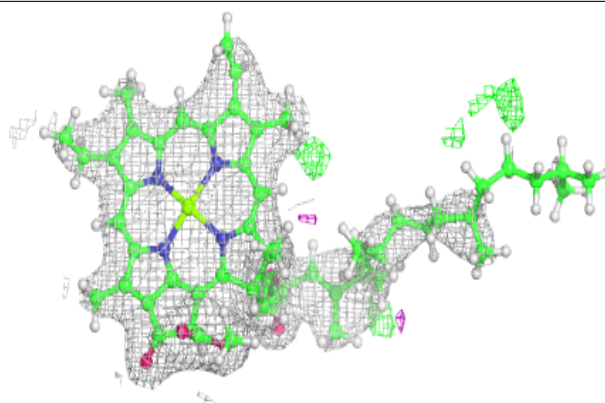
**Electron density around DGD H 103:**

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

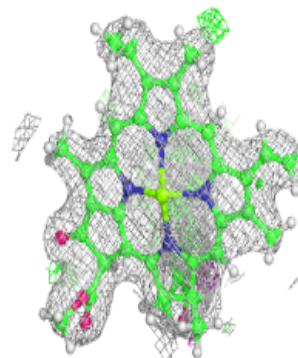
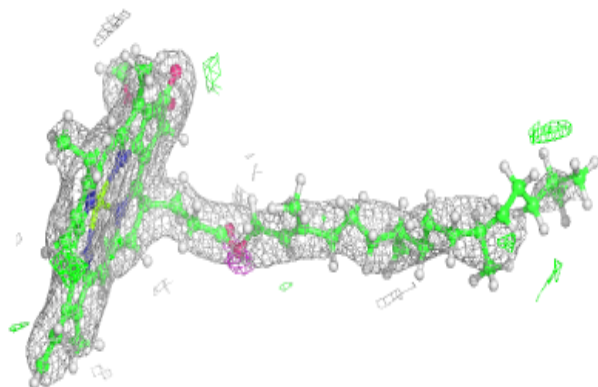
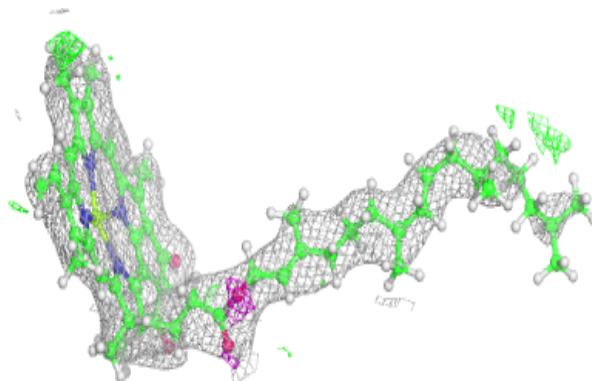


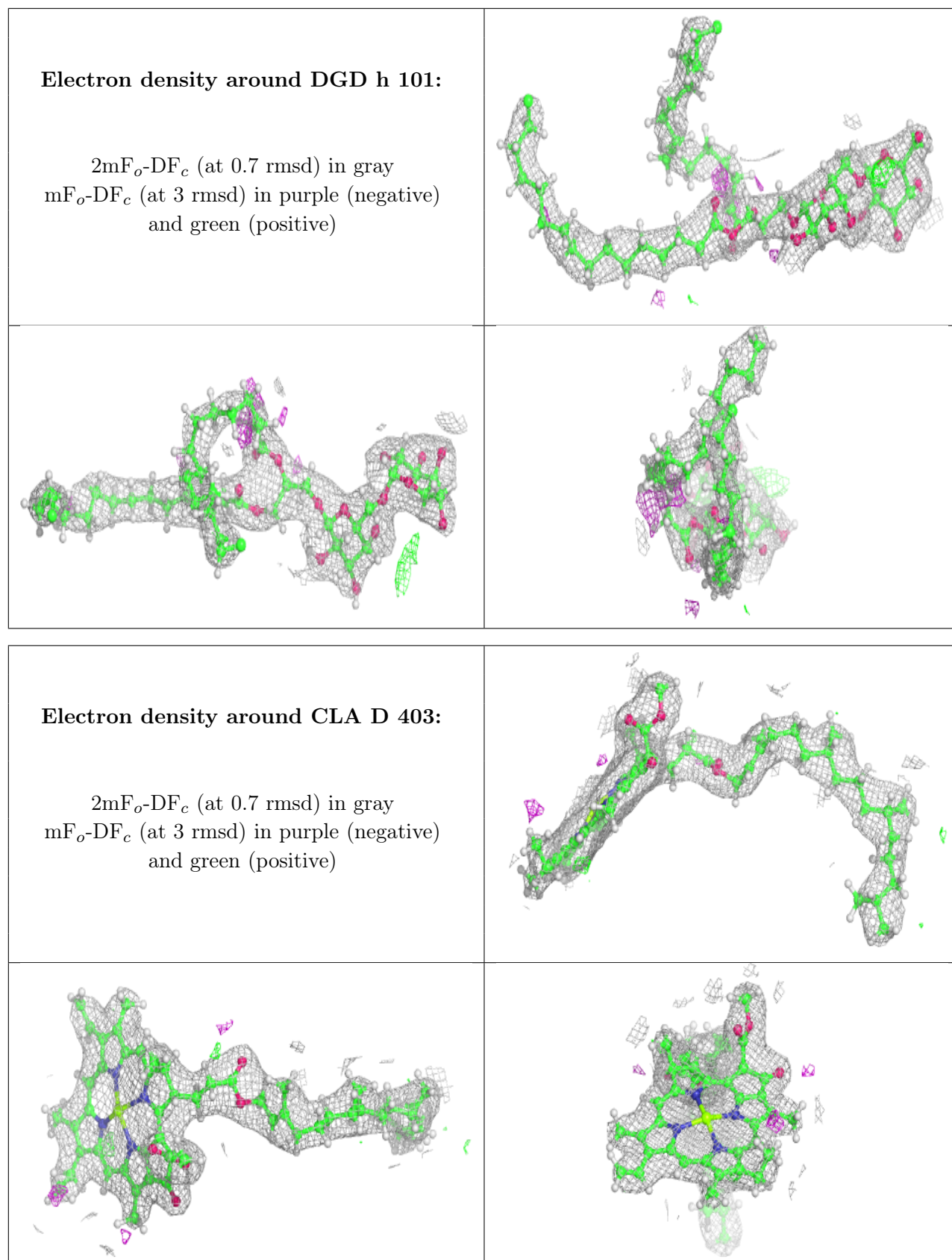
**Electron density around CLA a 403:**

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

**Electron density around CLA B 603:**

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

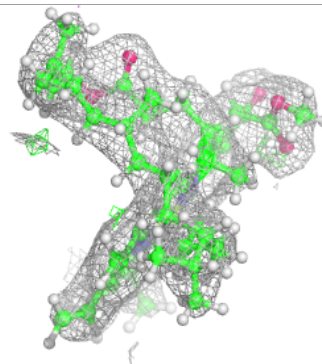
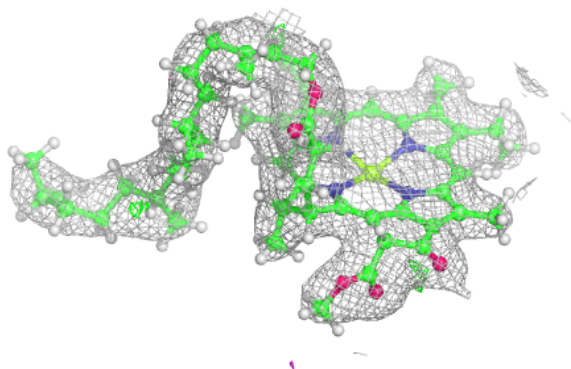
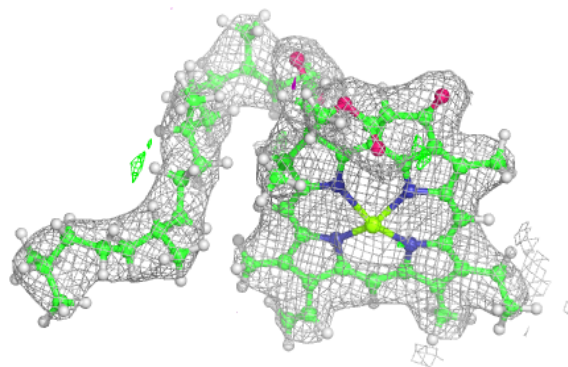




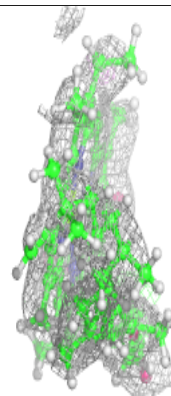
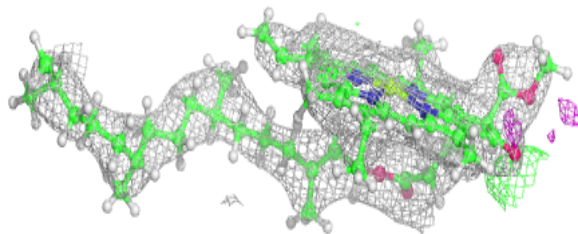
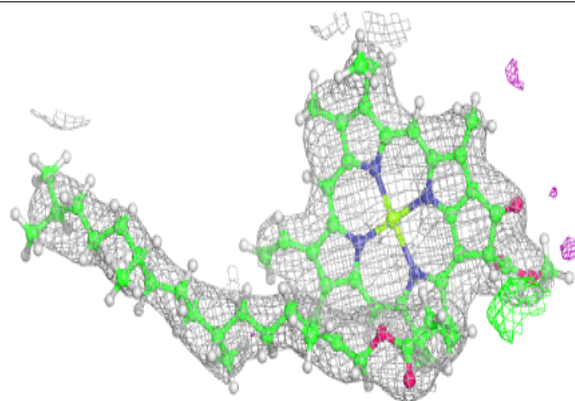


**Electron density around CLA D 404:**

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

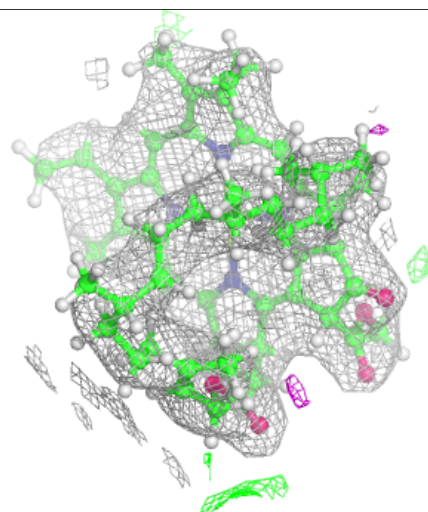
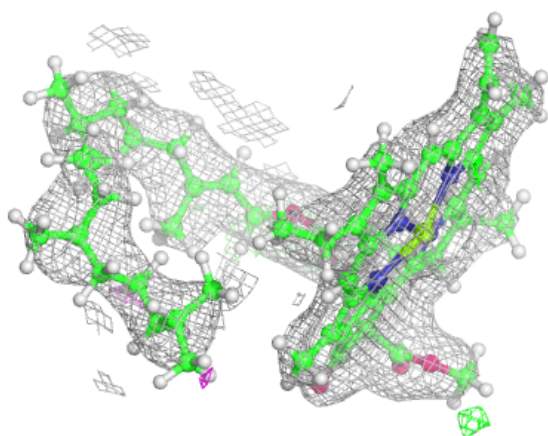
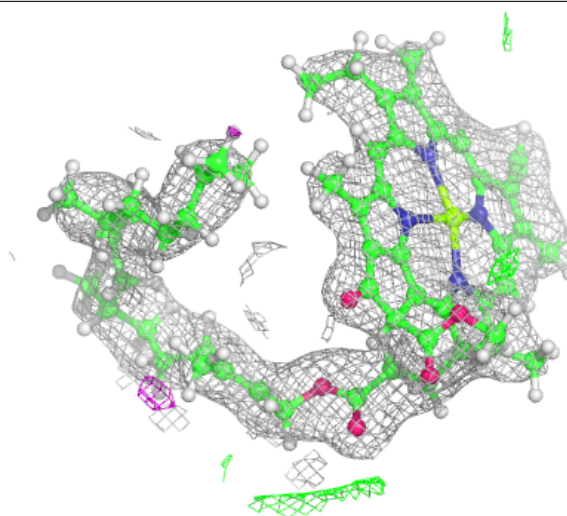
**Electron density around CLA c 501:**

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



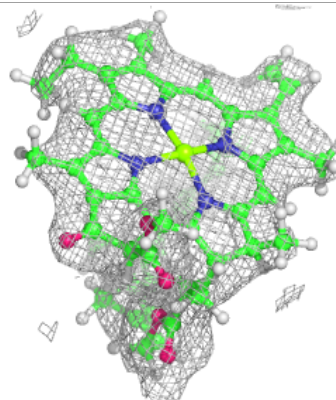
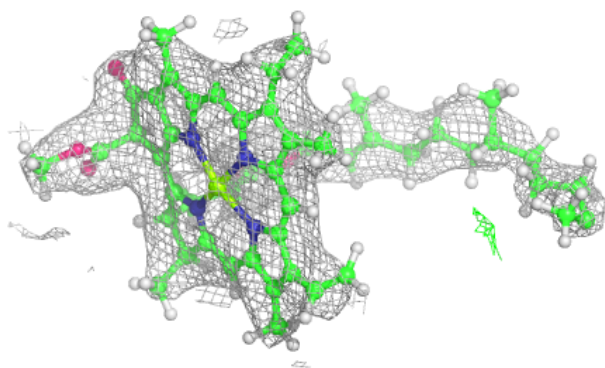
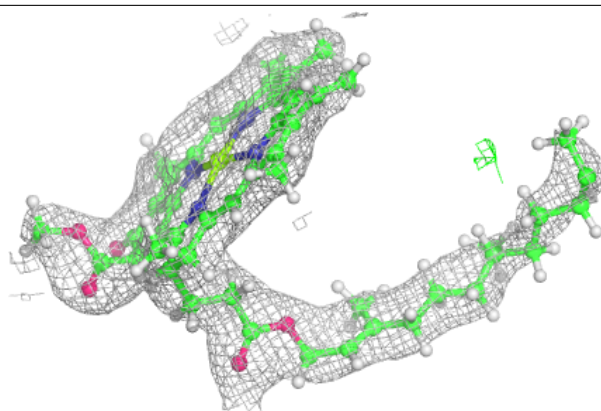
**Electron density around CLA C 503:**

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

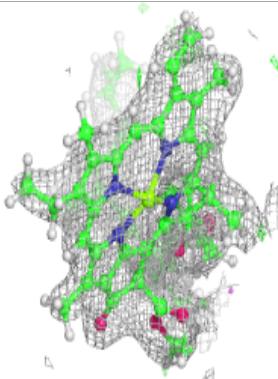
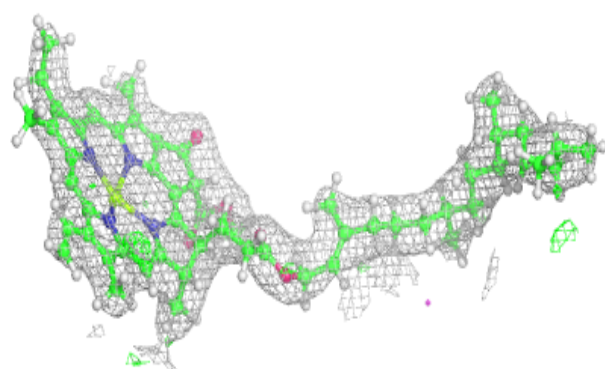
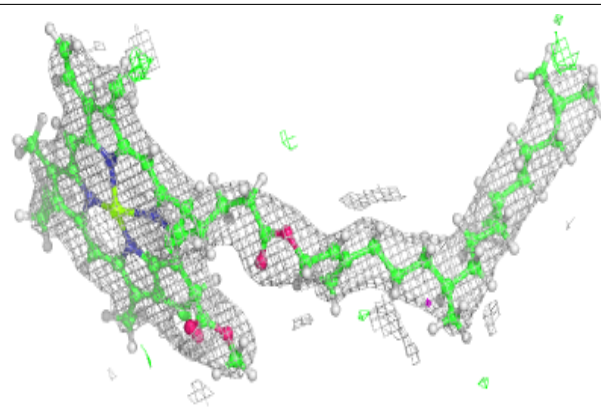


**Electron density around CLA C 504:**

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

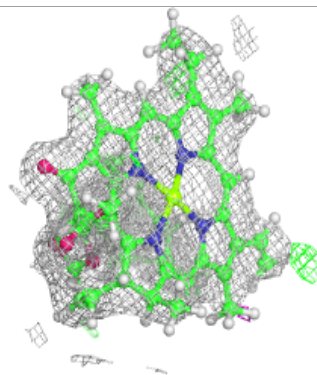
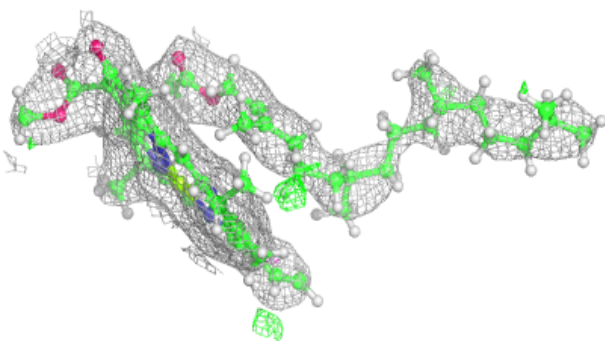
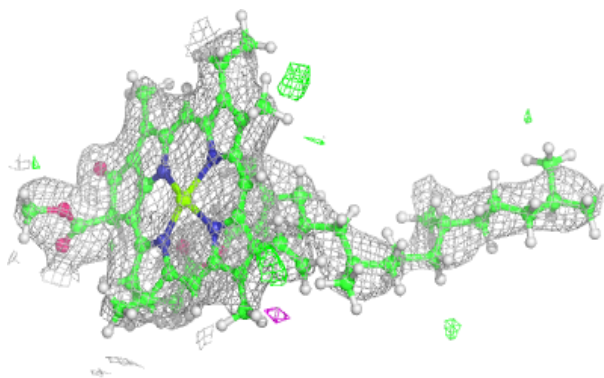
**Electron density around CLA a 402:**

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

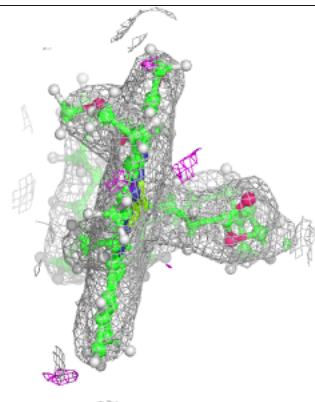
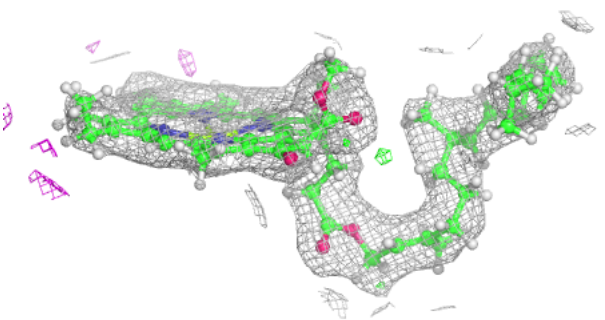
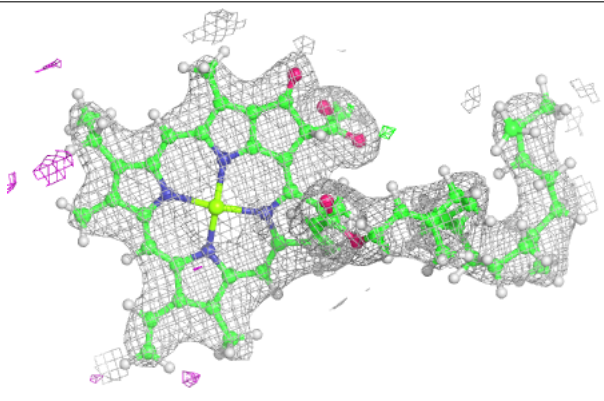


**Electron density around CLA C 505:**

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

**Electron density around CLA B 611:**

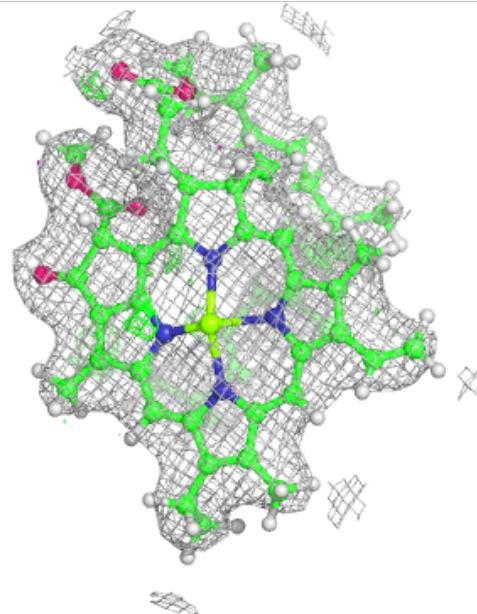
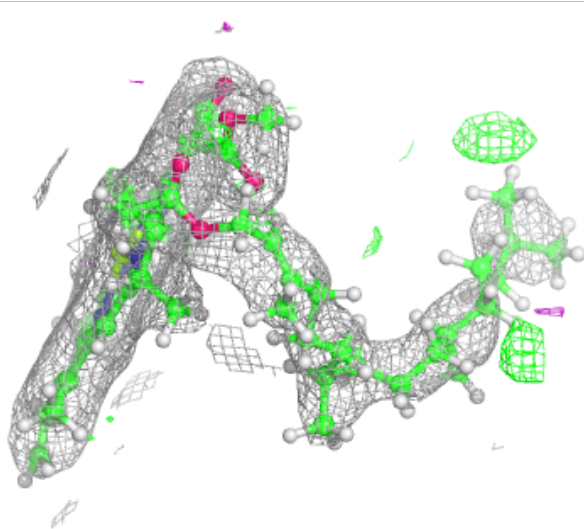
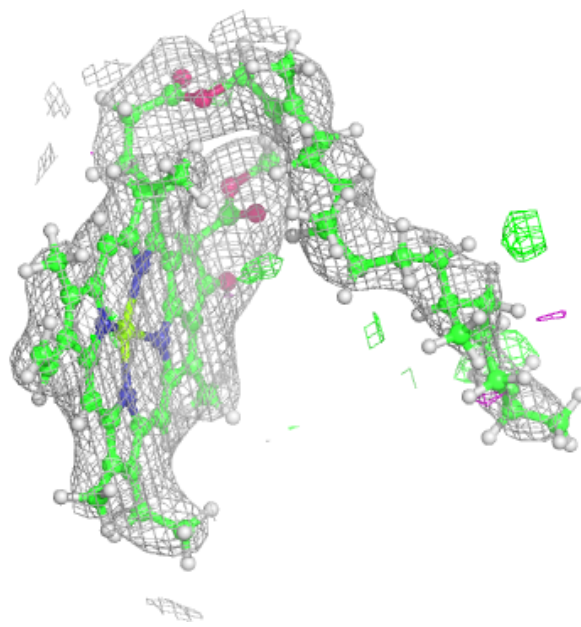
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





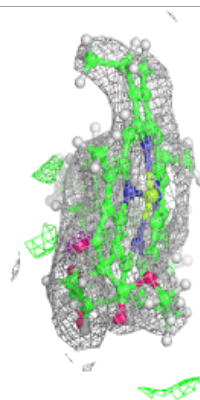
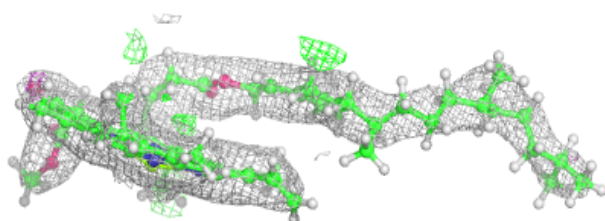
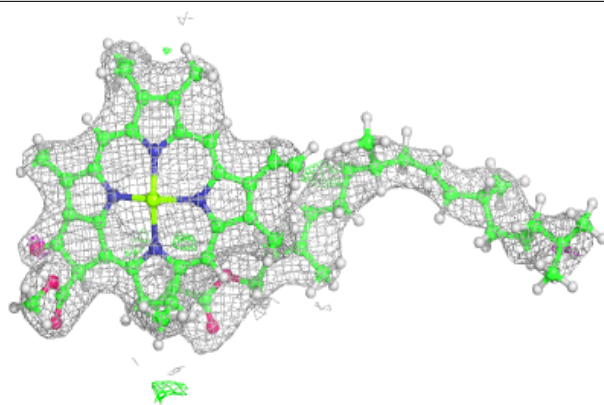
**Electron density around CLA B 612:**

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

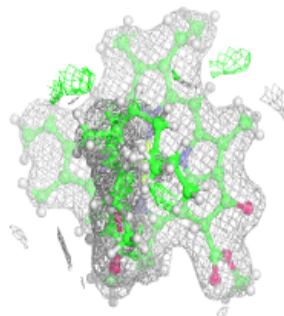
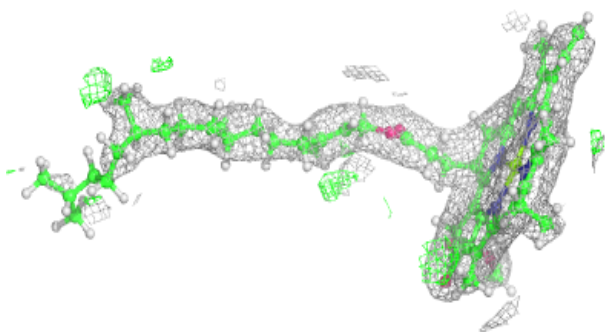
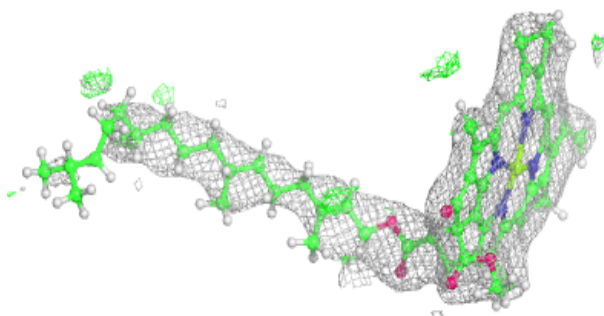


**Electron density around CLA B 602:**

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

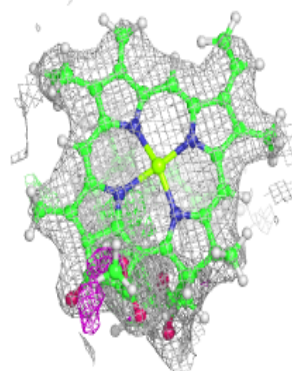
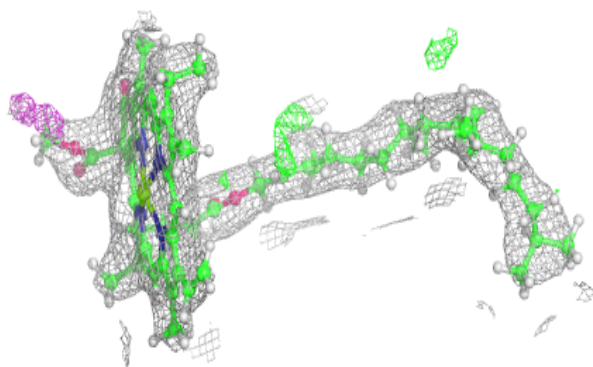
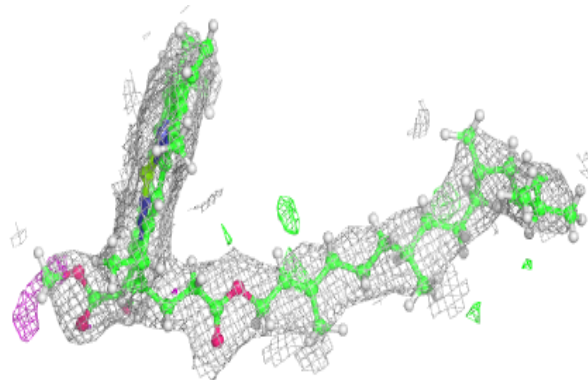
**Electron density around CLA b 604:**

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

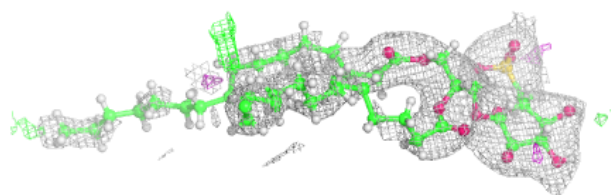
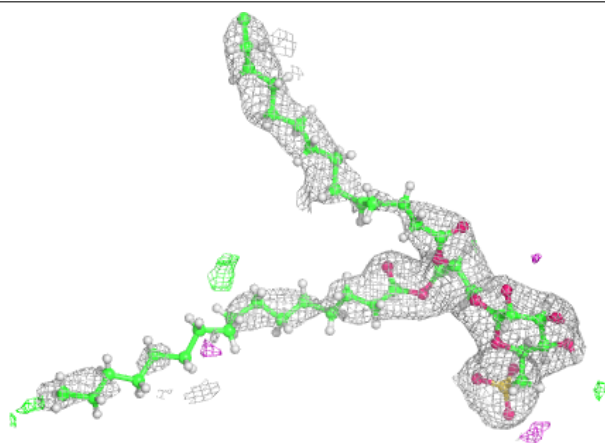


**Electron density around CLA b 605:**

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

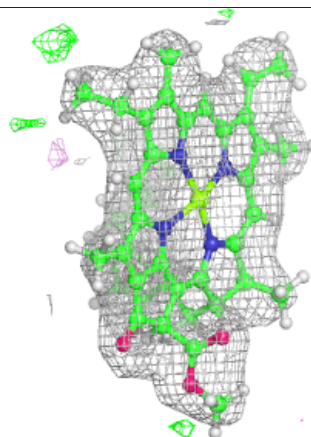
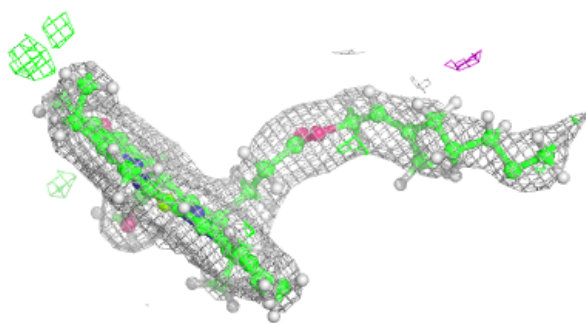
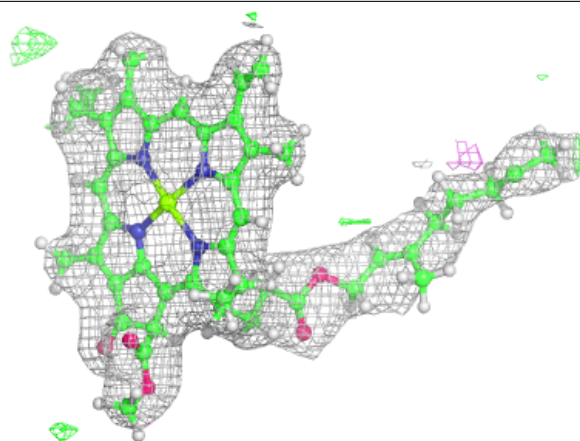
**Electron density around SQD A 410:**

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

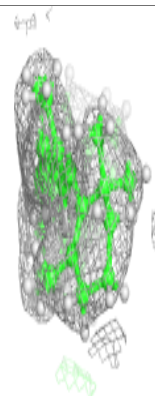
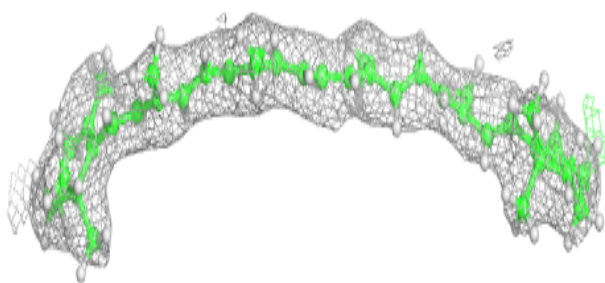
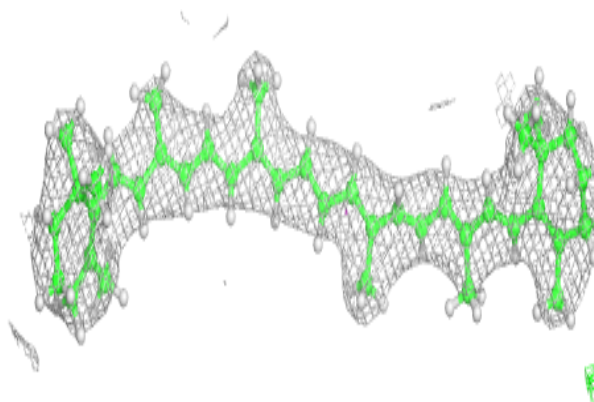


**Electron density around CLA A 405:**

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

**Electron density around BCR T 101:**

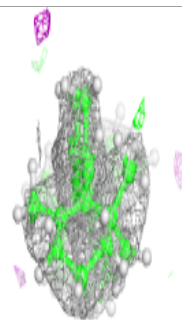
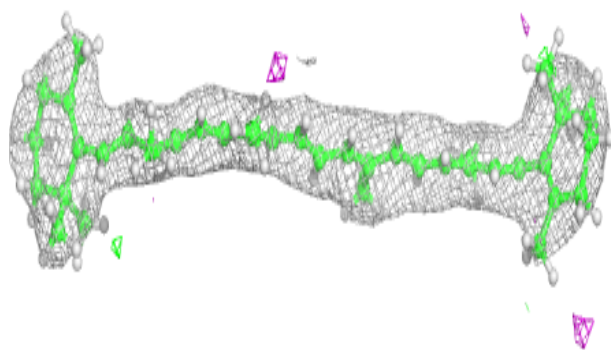
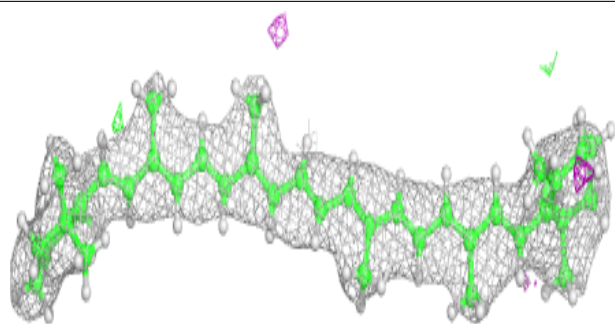
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



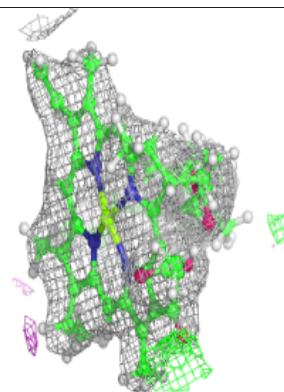
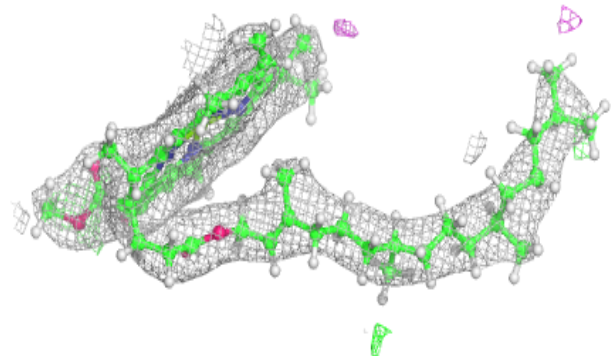
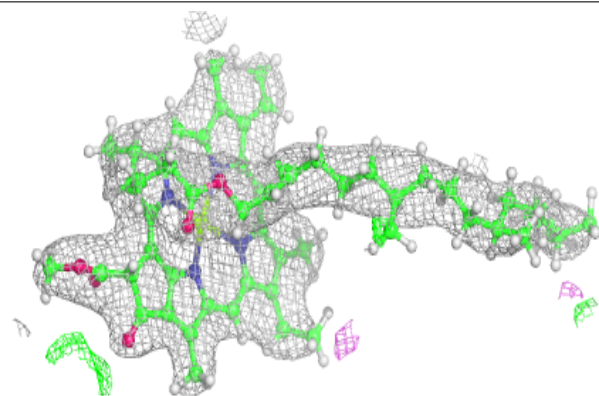


**Electron density around BCR a 406:**

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

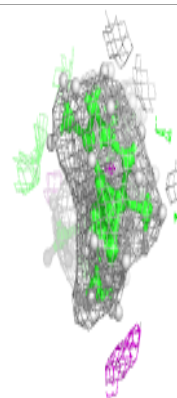
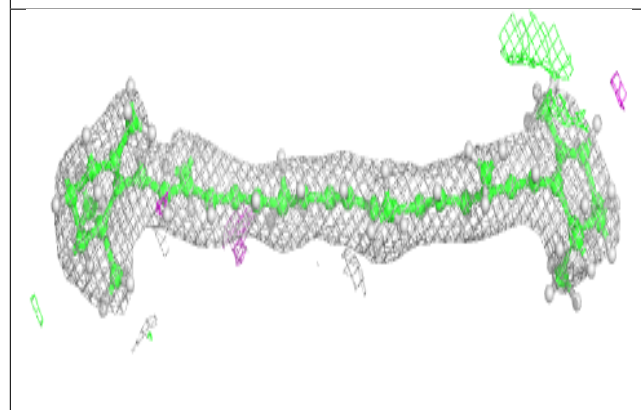
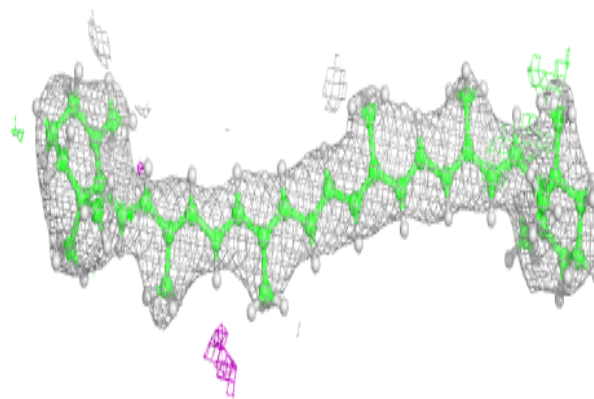
**Electron density around CLA b 608:**

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



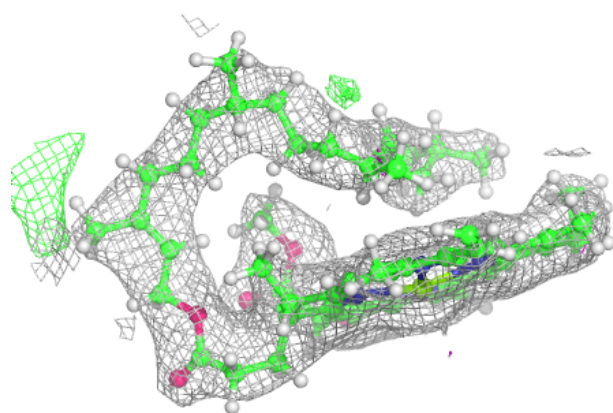
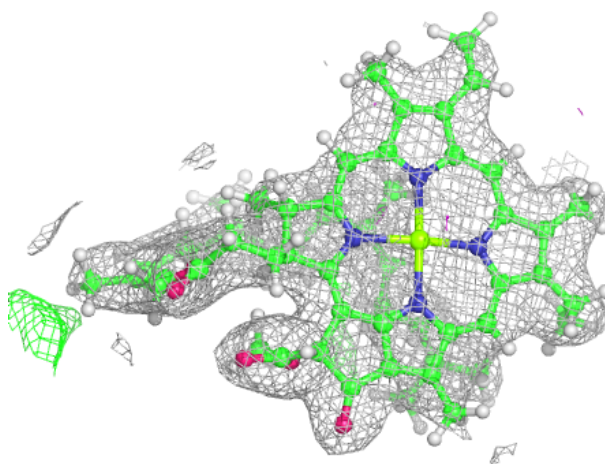
**Electron density around BCR b 618:**

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



**Electron density around CLA C 510:**

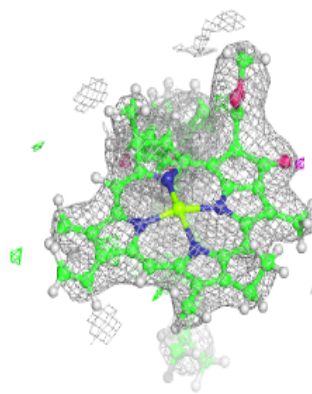
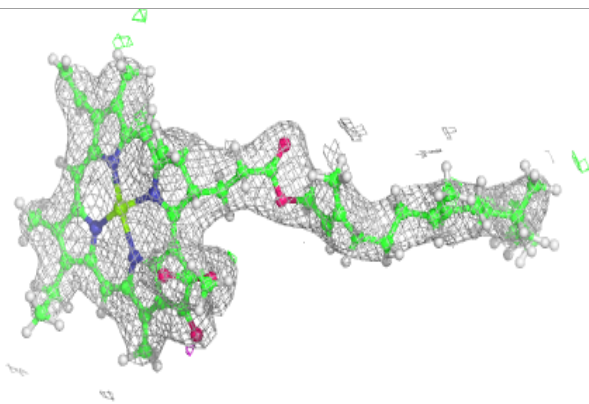
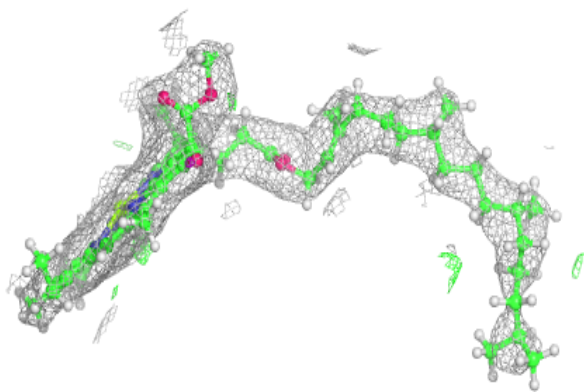
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



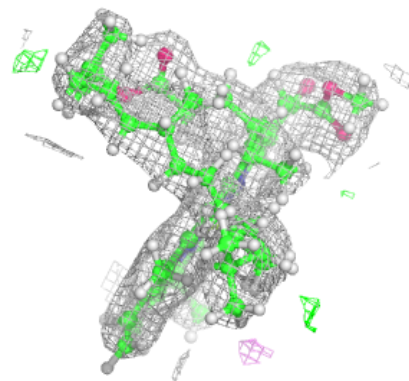
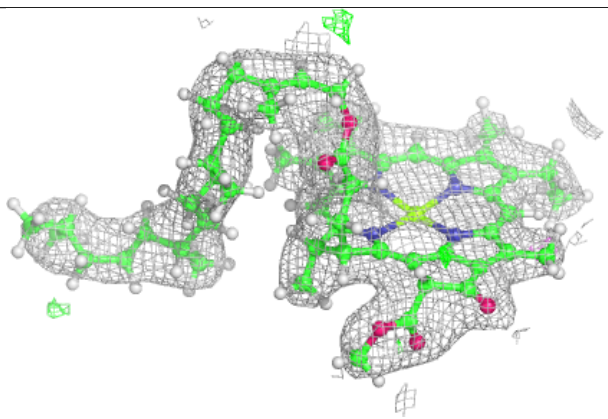
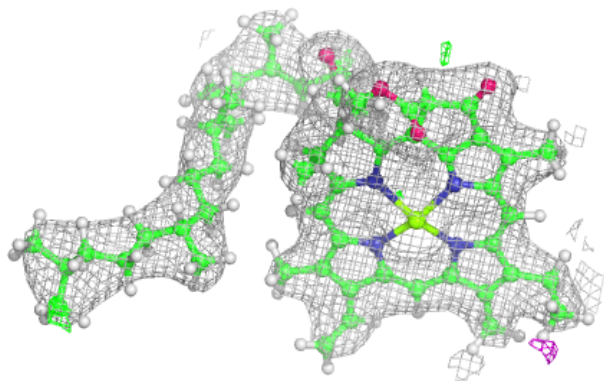


**Electron density around CLA d 403:**

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

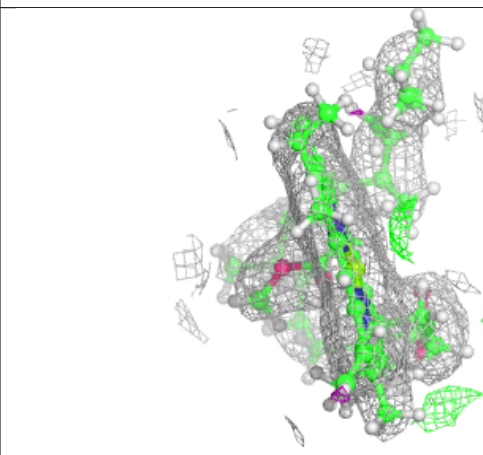
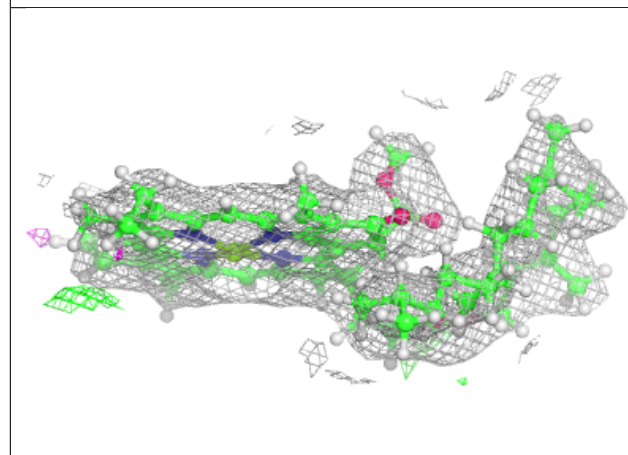
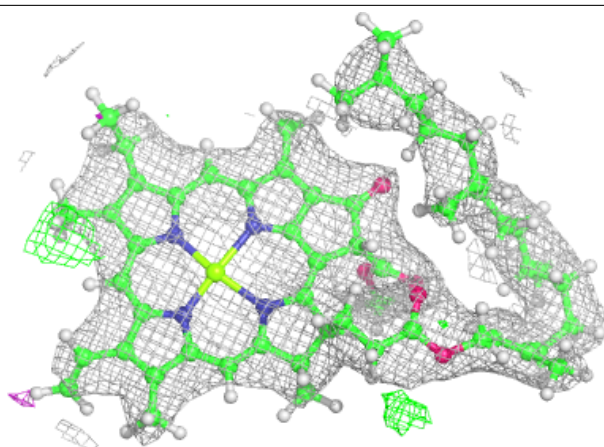
**Electron density around CLA d 404:**

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



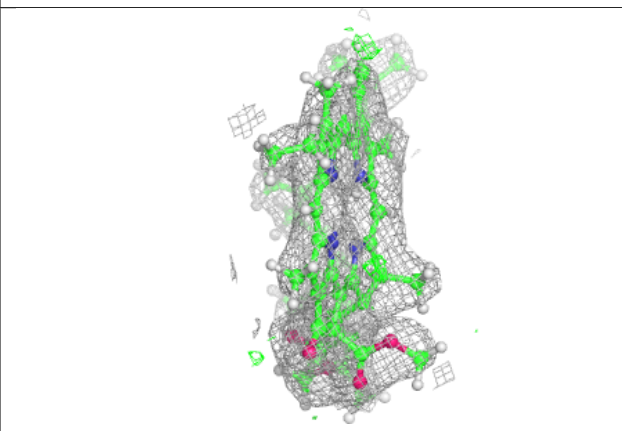
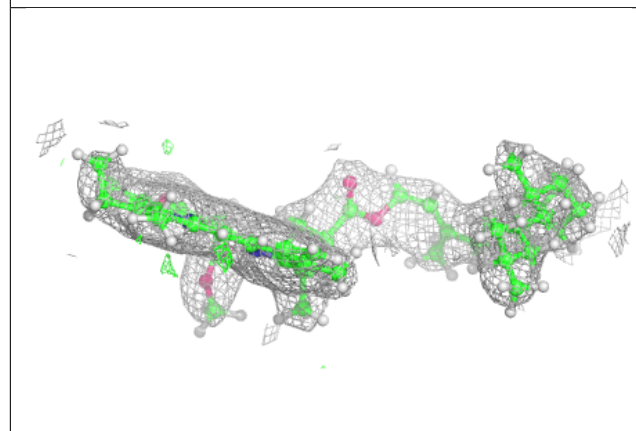
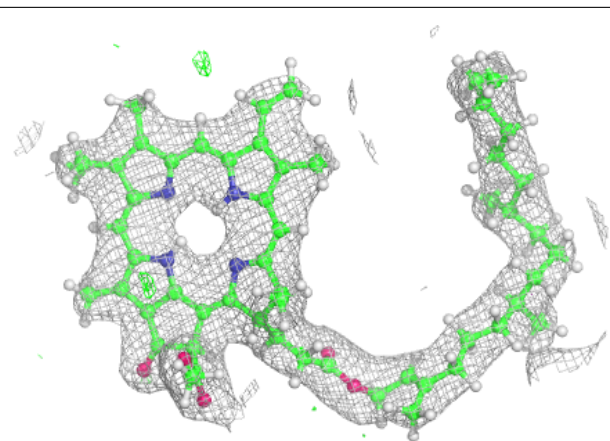
**Electron density around CLA b 610:**

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

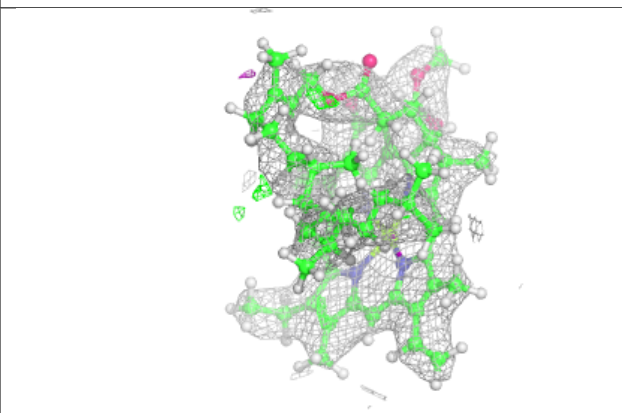
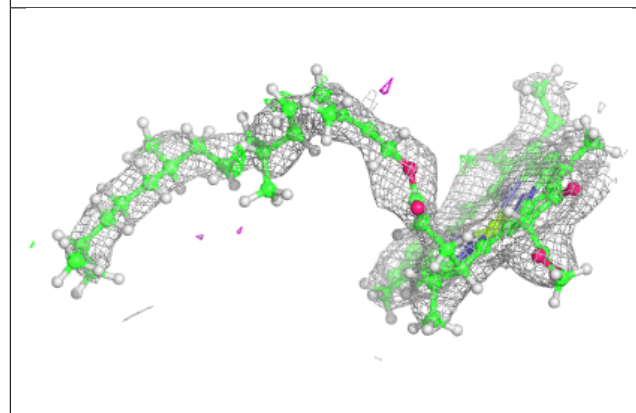
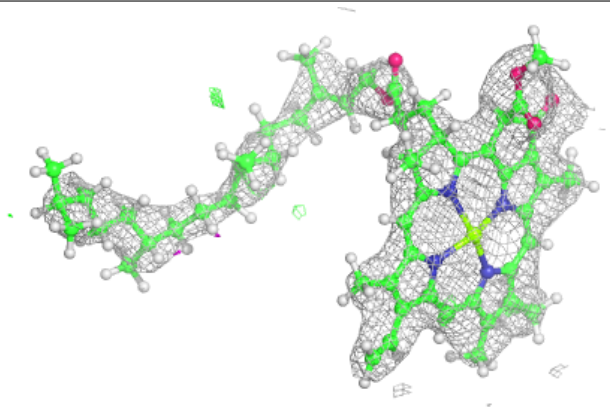


**Electron density around PHO a 404:**

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

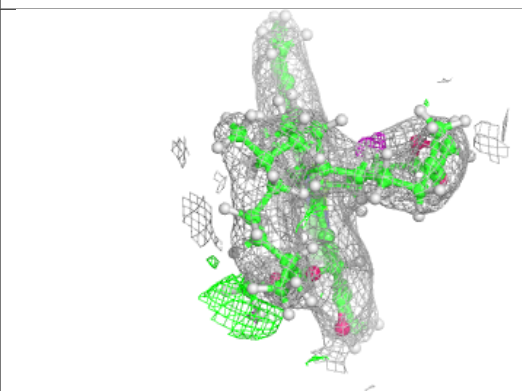
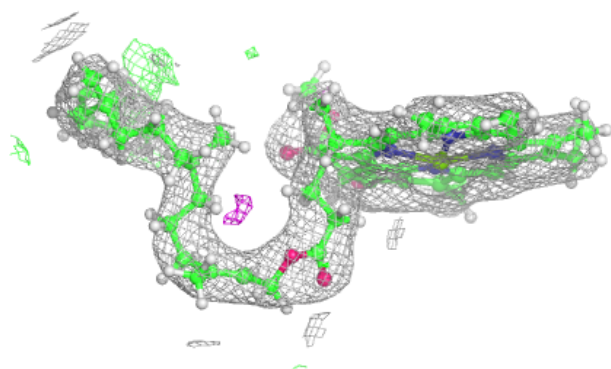
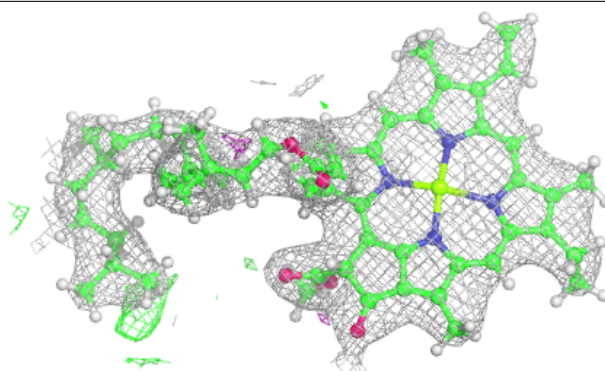
**Electron density around CLA C 511:**

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

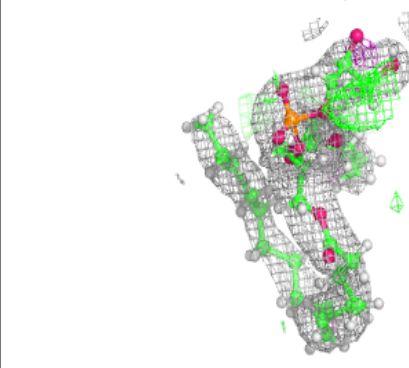
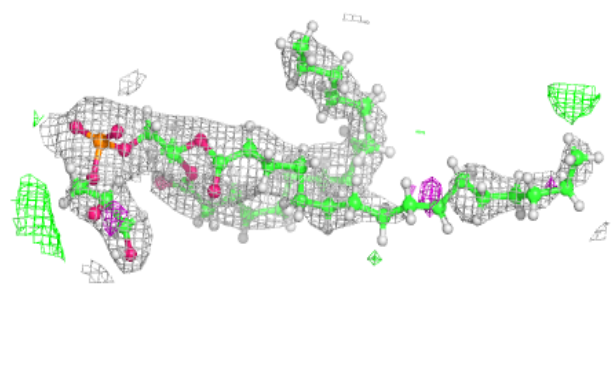
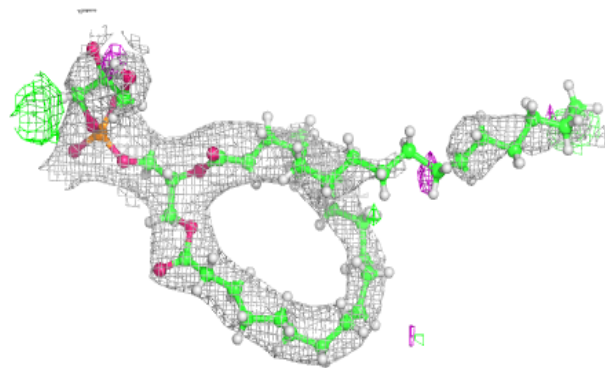


**Electron density around CLA b 612:**

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

**Electron density around LHG b 623:**

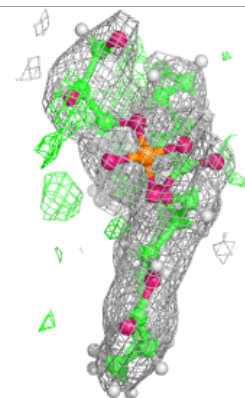
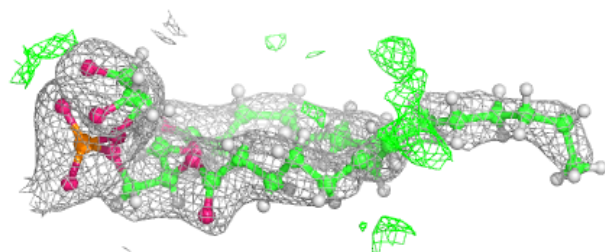
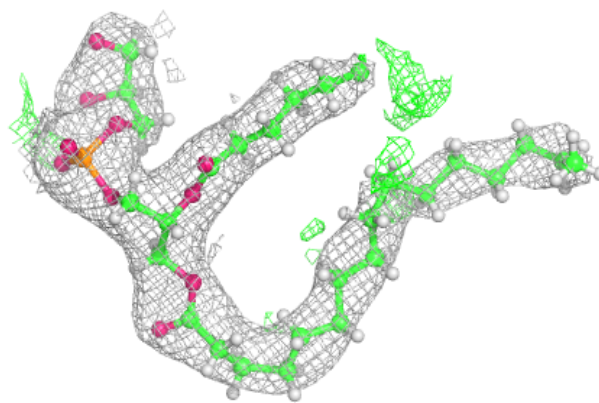
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



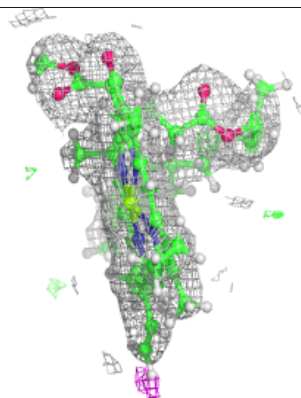
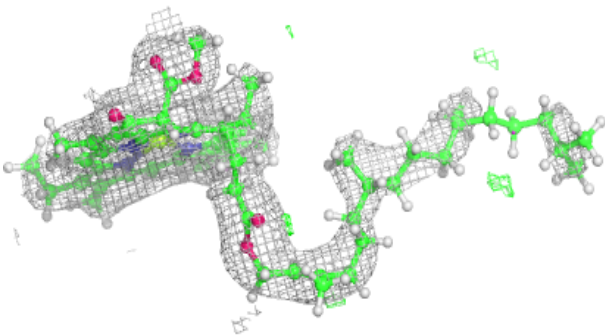
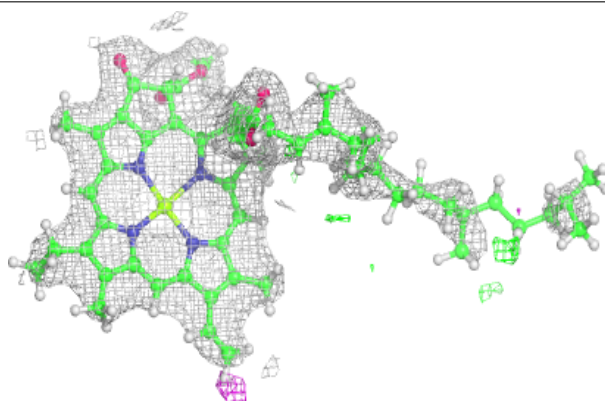


**Electron density around LHG d 409:**

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

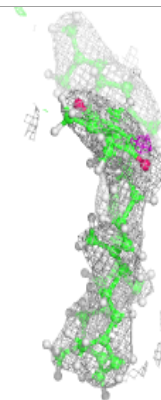
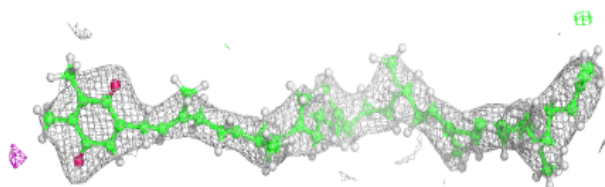
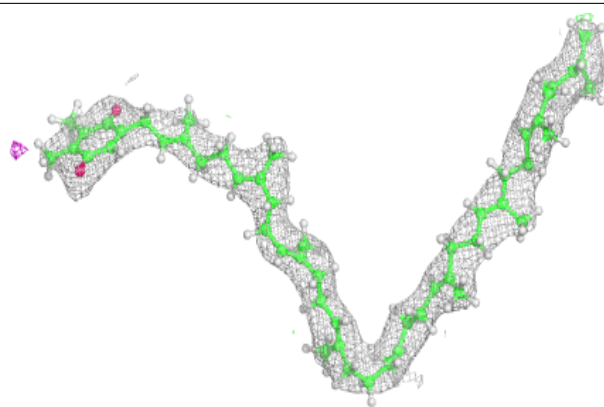
**Electron density around CLA A 403:**

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

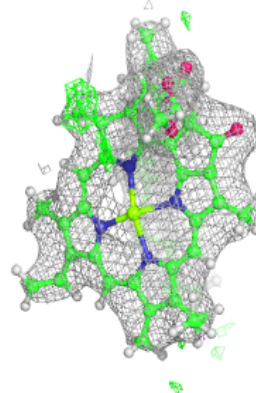
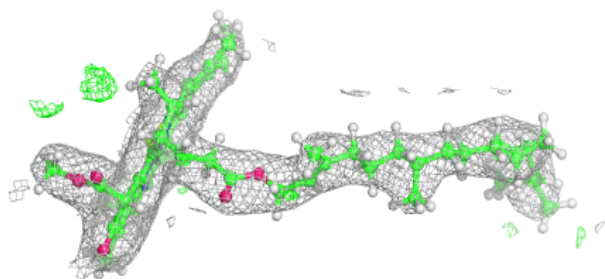
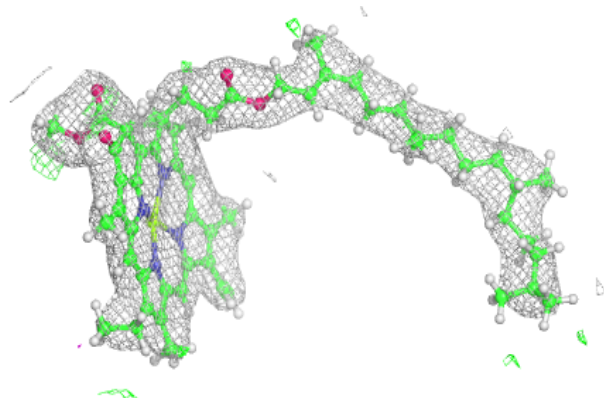


**Electron density around PL9 d 407:**

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

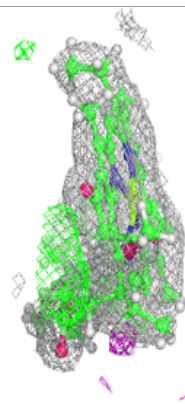
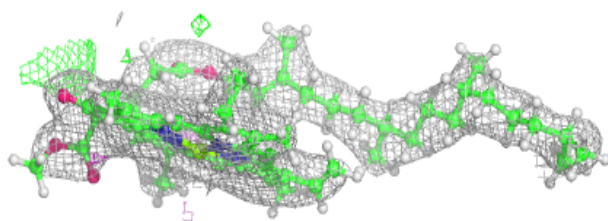
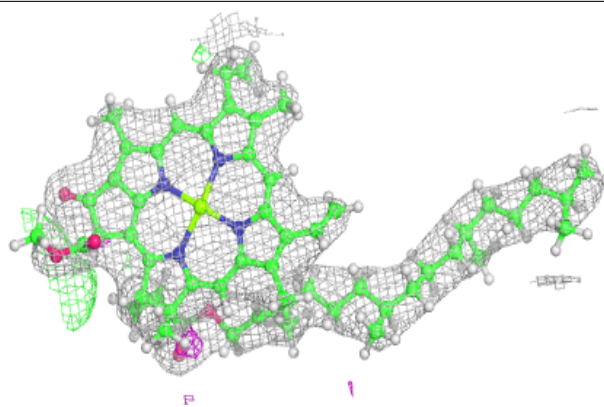
**Electron density around CLA B 608:**

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

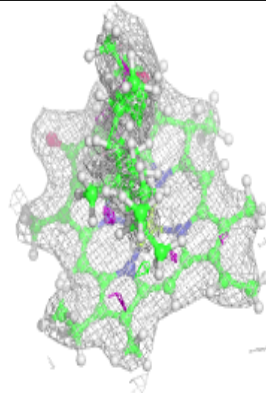
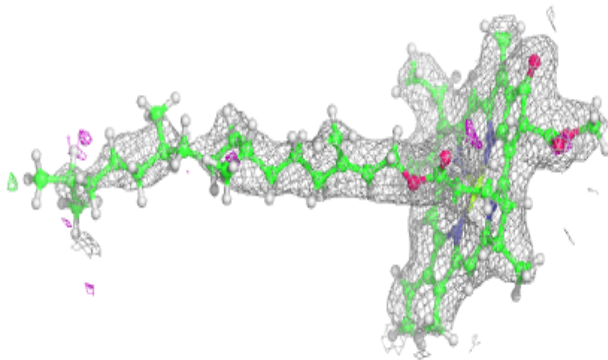
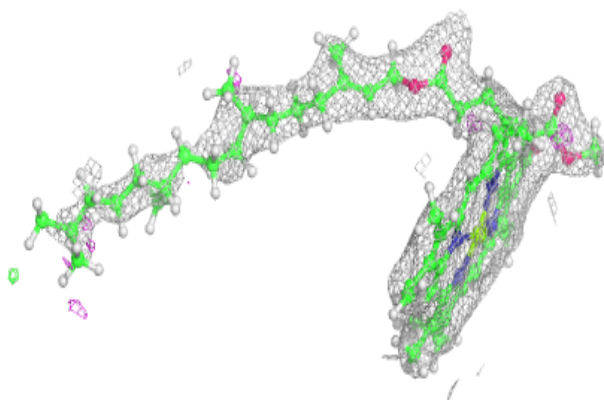


**Electron density around CLA C 501:**

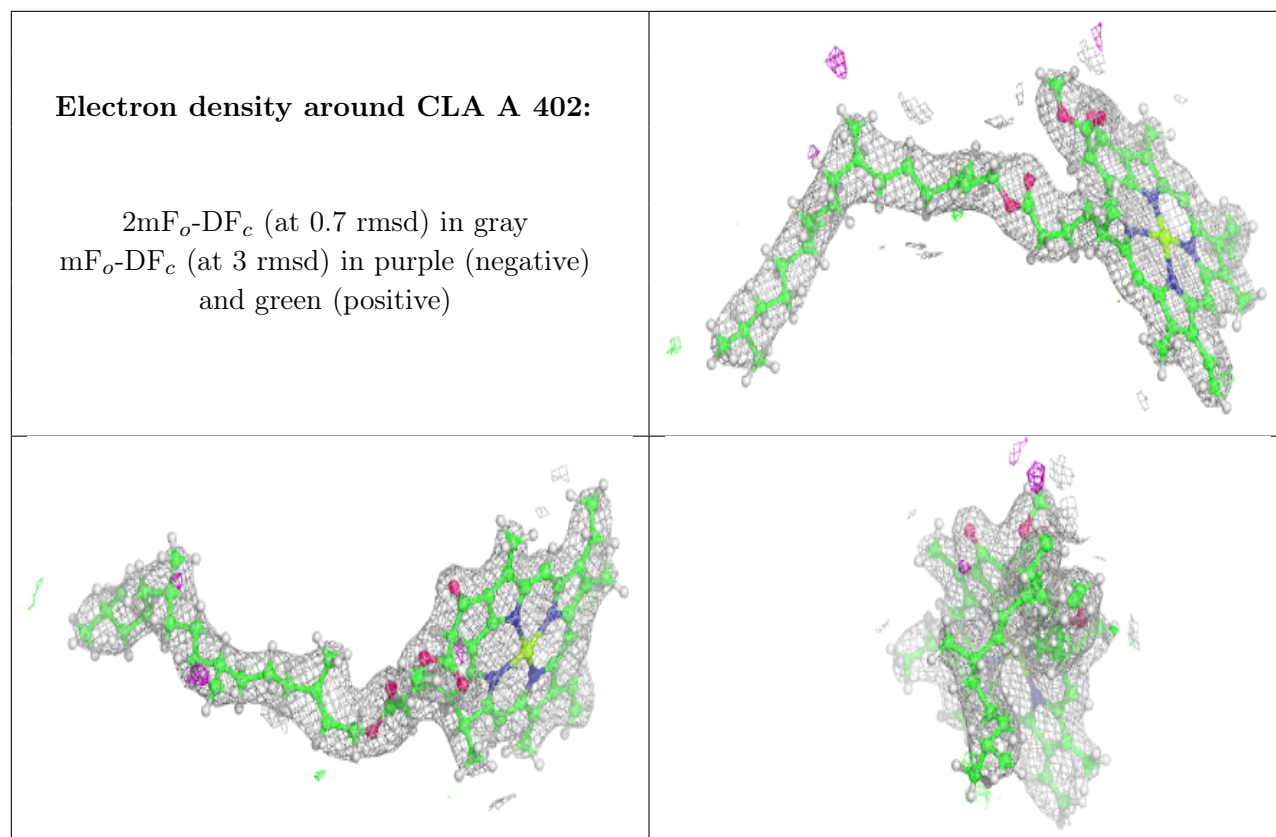
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA b 607:**

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

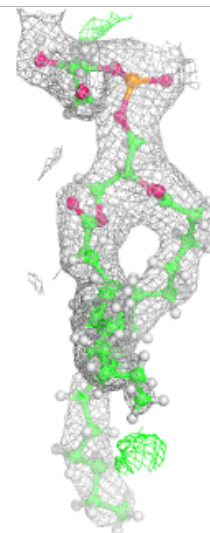
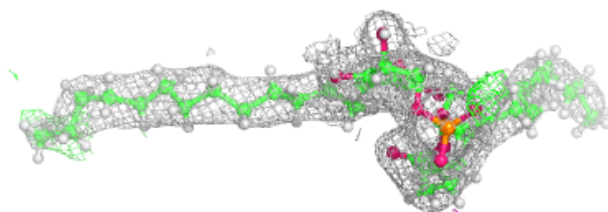
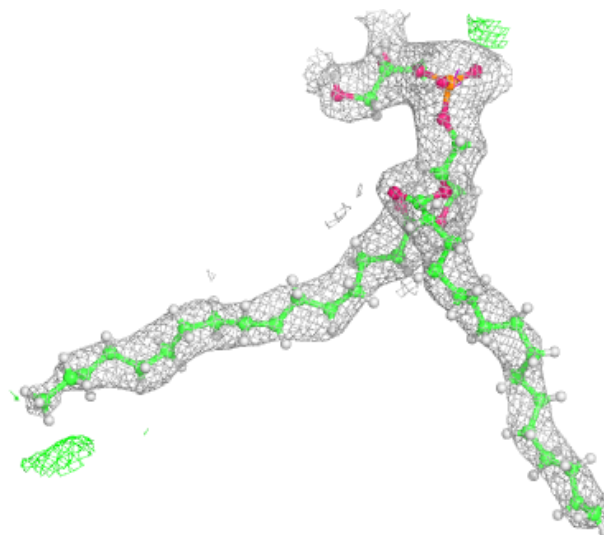






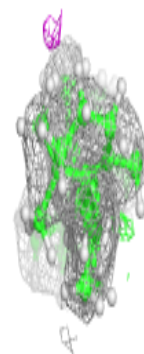
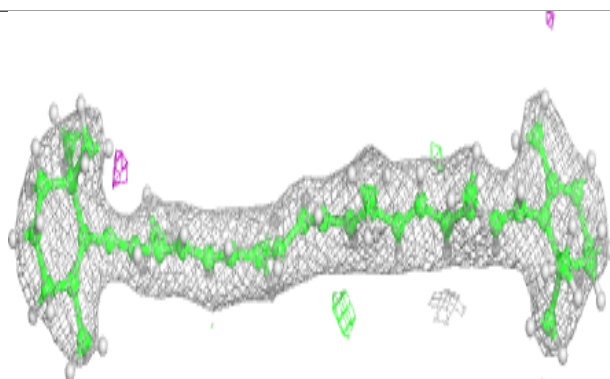
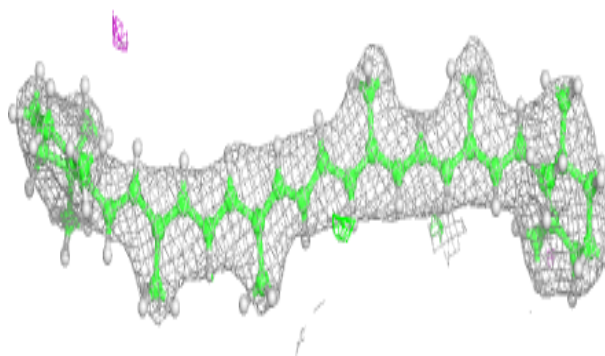
**Electron density around LHG 1 101:**

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

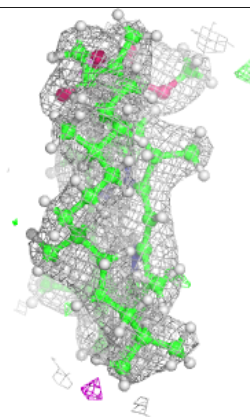
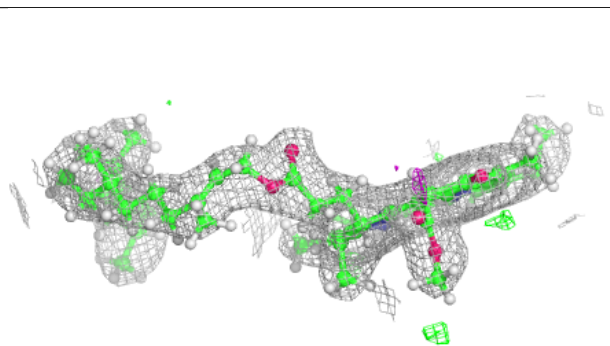
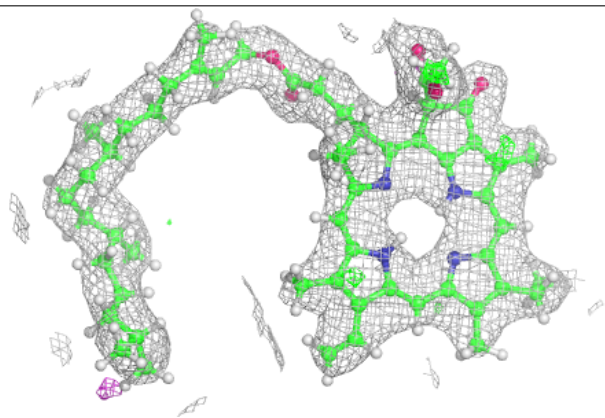


**Electron density around BCR I 101:**

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

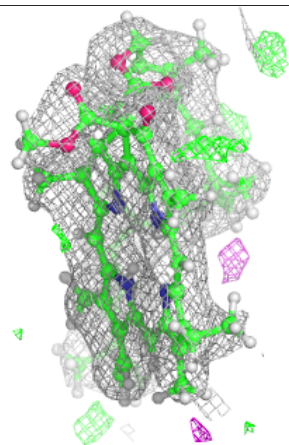
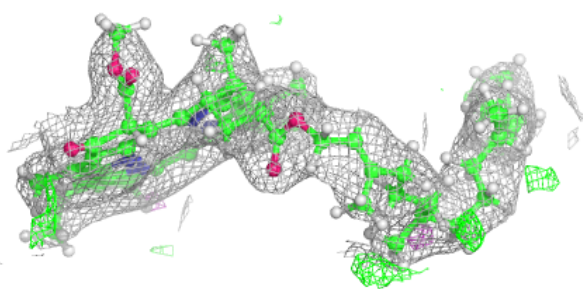
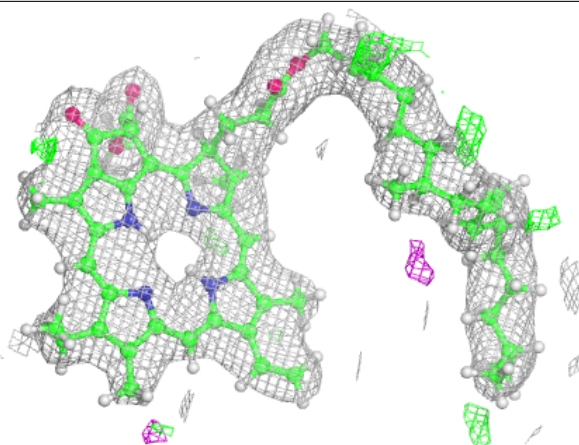
**Electron density around PHO A 404:**

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

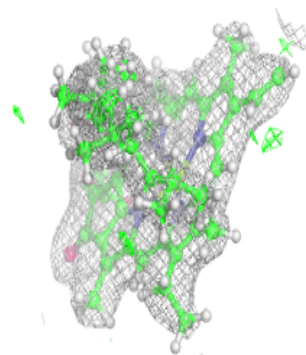
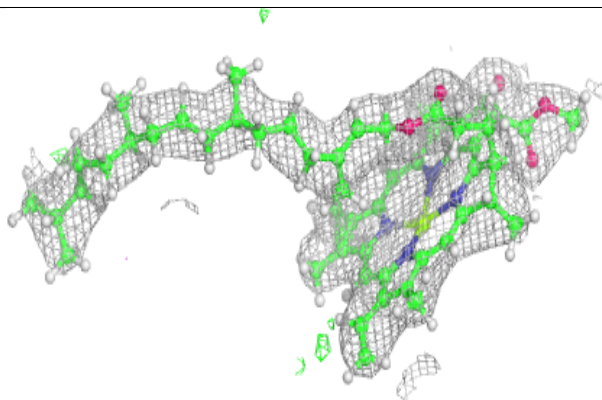
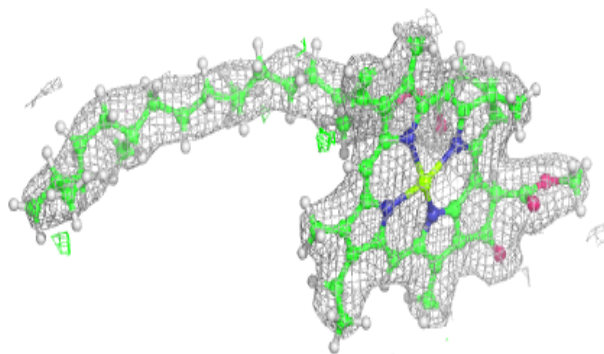


**Electron density around PHO D 401:**

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

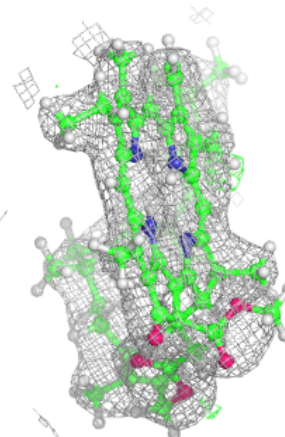
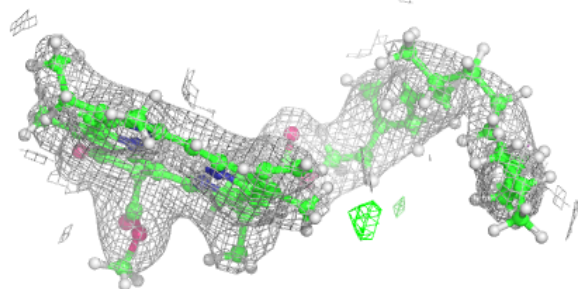
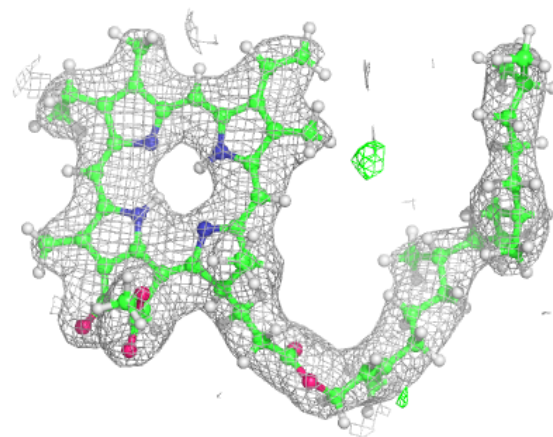
**Electron density around CLA B 607:**

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



**Electron density around PHO d 401:**

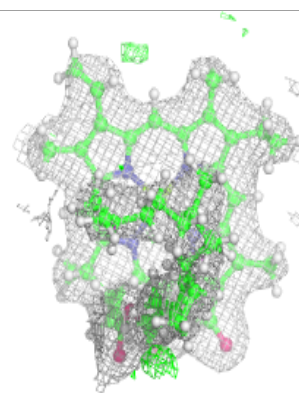
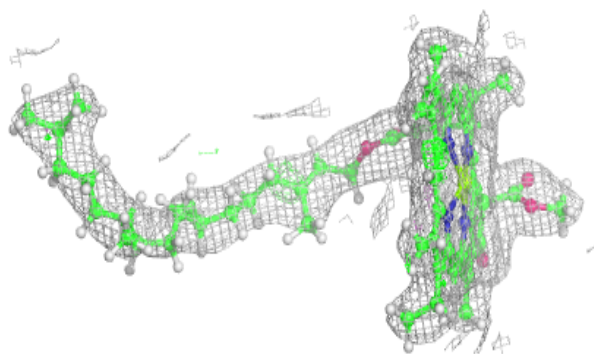
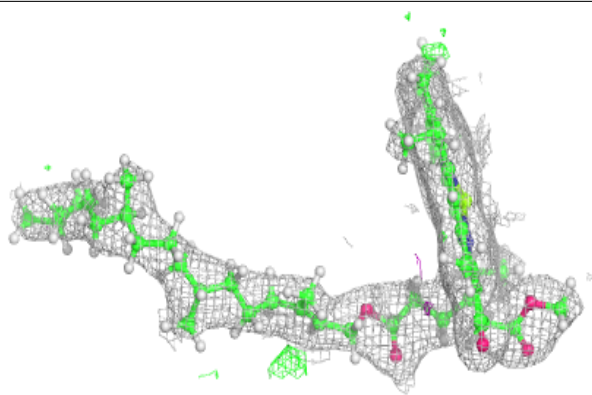
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



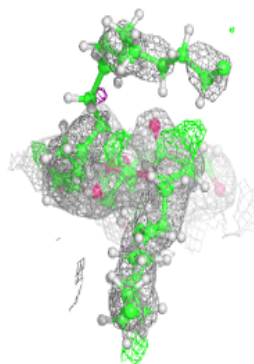
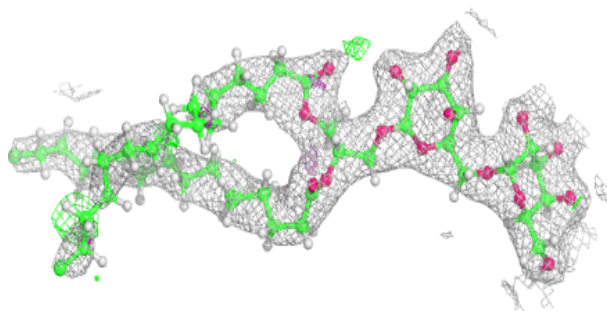
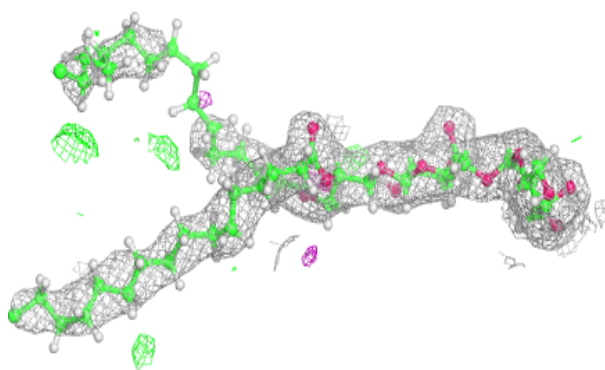


**Electron density around CLA B 604:**

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

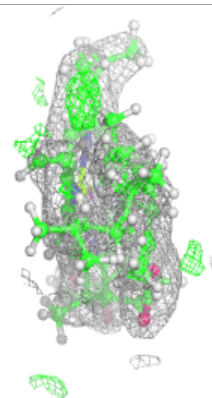
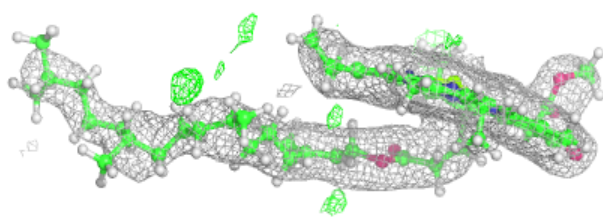
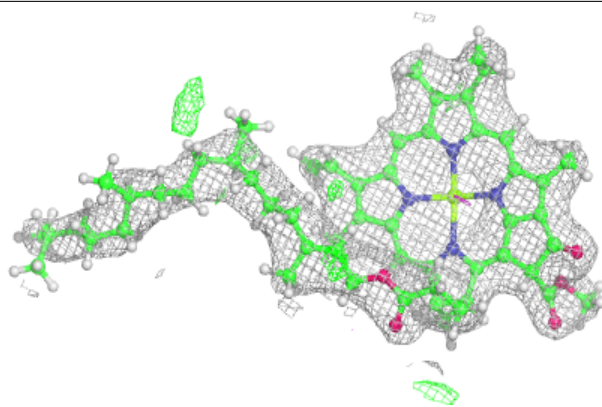
**Electron density around DGD c 515:**

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

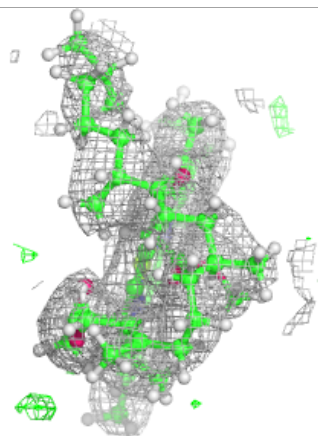
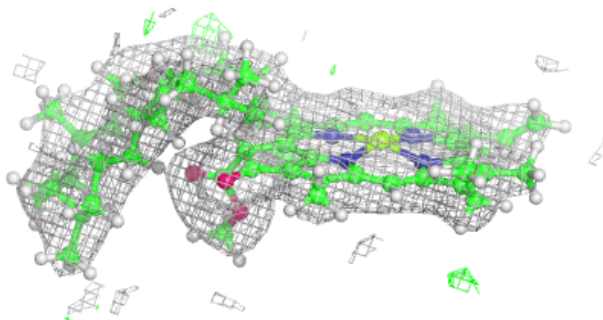
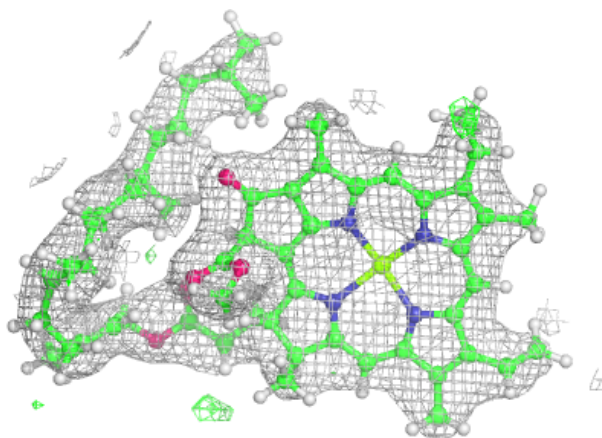


**Electron density around CLA b 603:**

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

**Electron density around CLA B 609:**

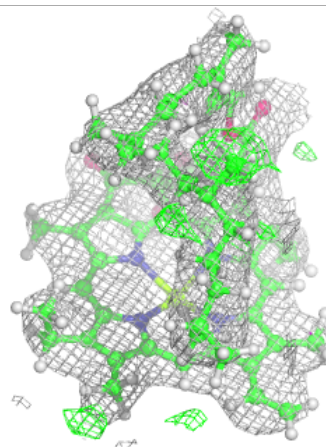
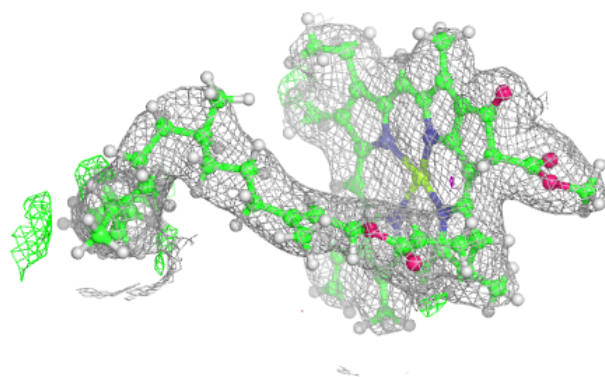
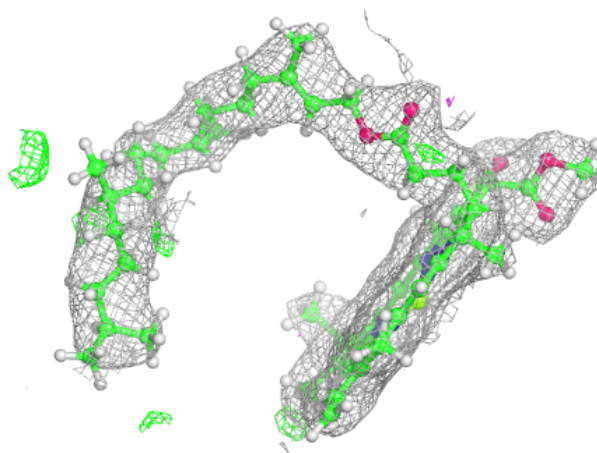
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





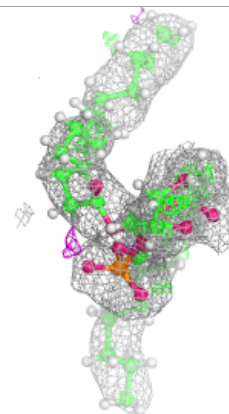
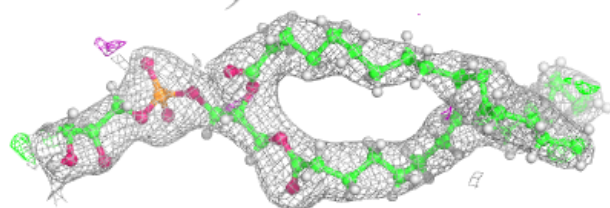
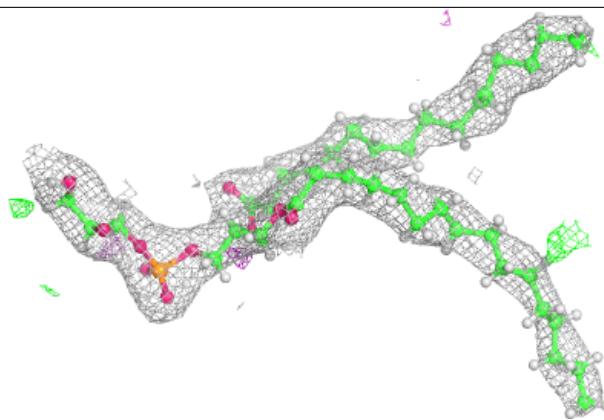
**Electron density around CLA B 610:**

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

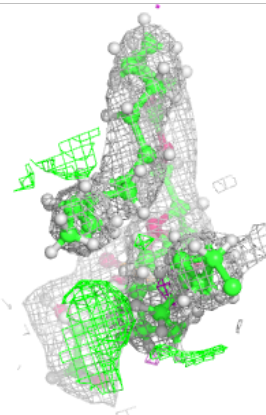
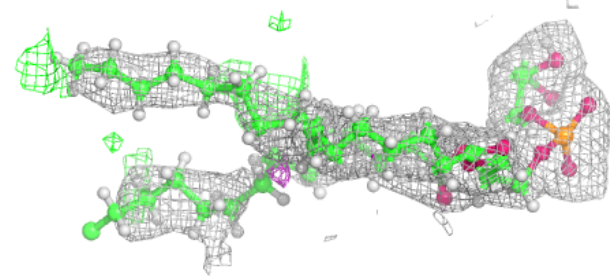
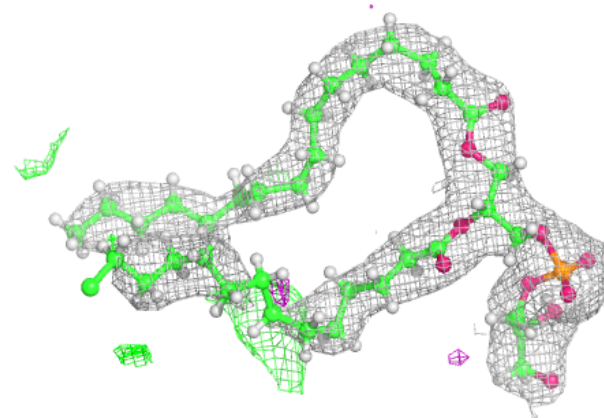


**Electron density around LHG D 410:**

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

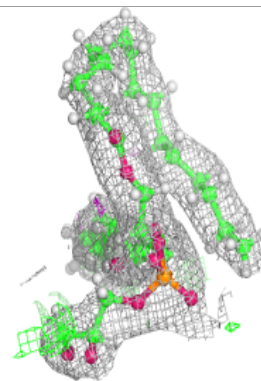
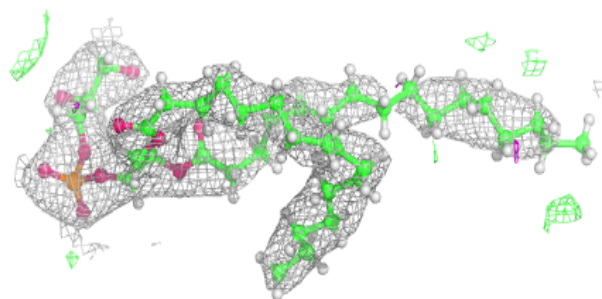
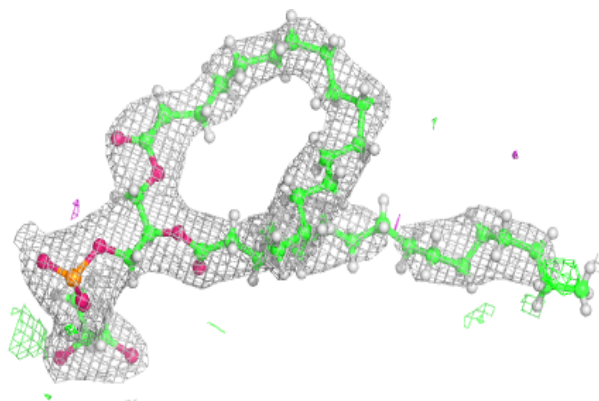
**Electron density around LHG D 411:**

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

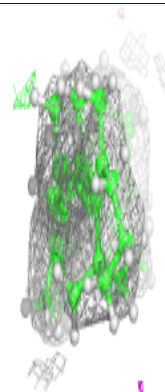
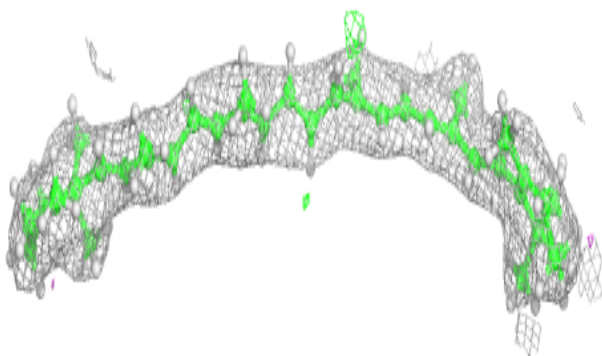
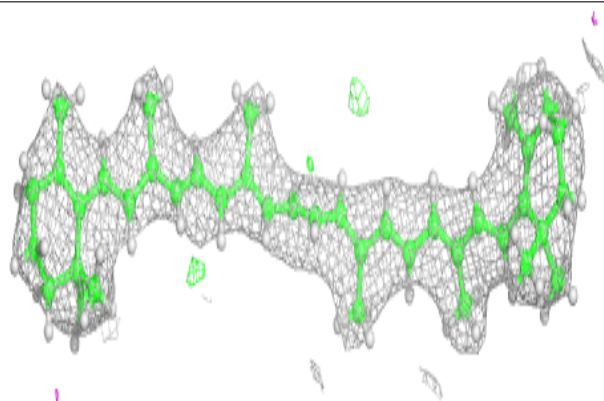


**Electron density around LHG D 413:**

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

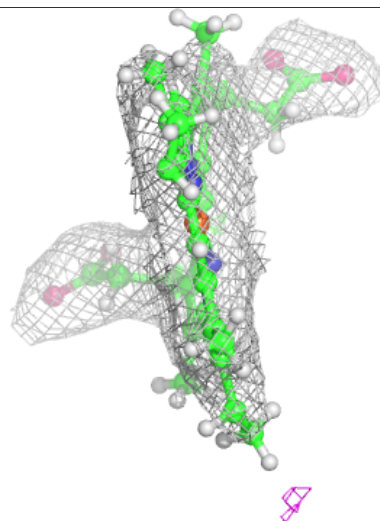
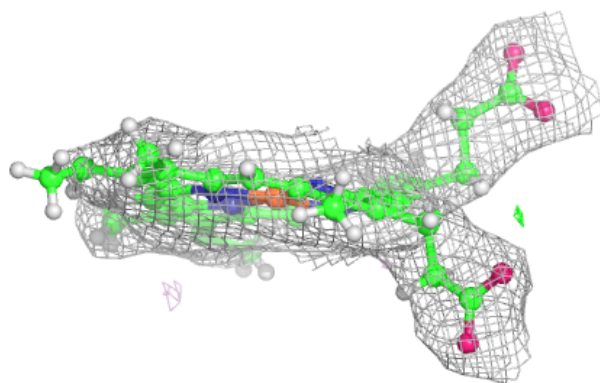
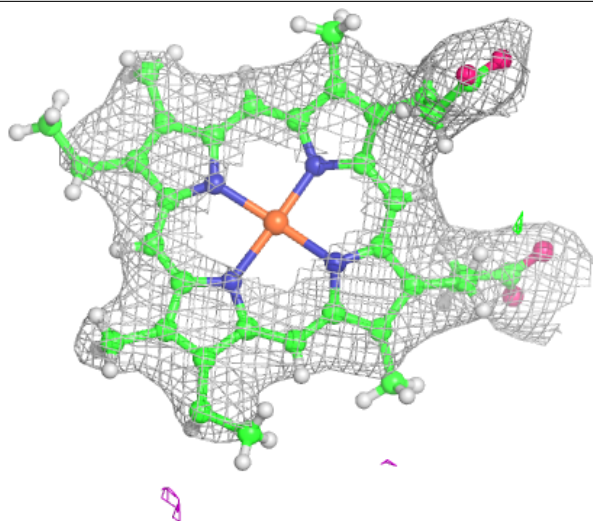
**Electron density around BCR t 101:**

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



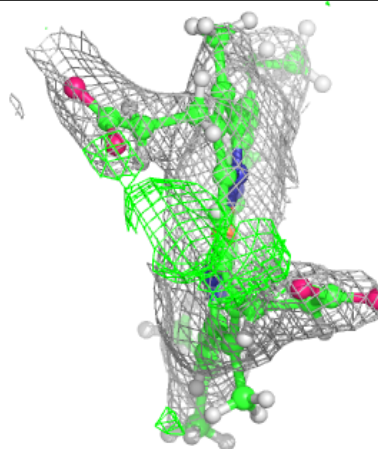
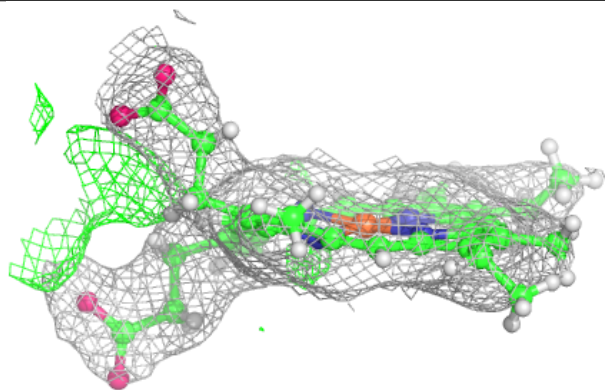
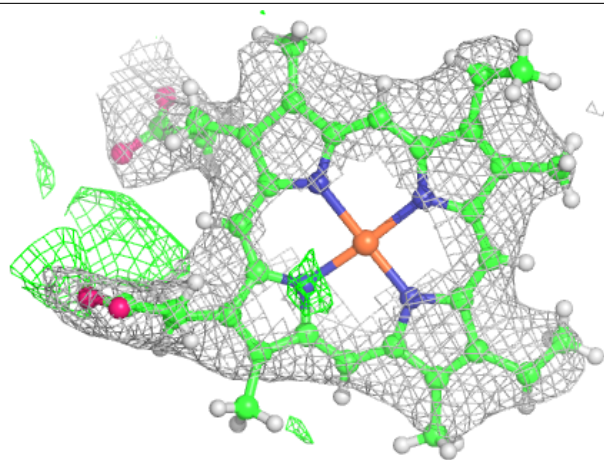
**Electron density around HEC F 101:**

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



**Electron density around HEC f 101:**

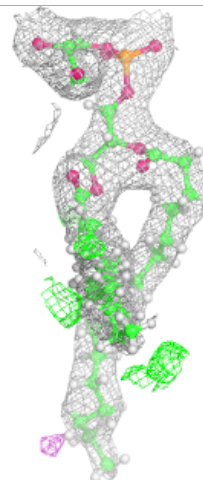
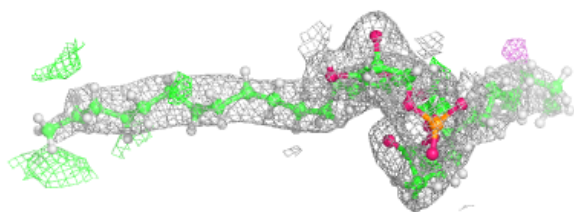
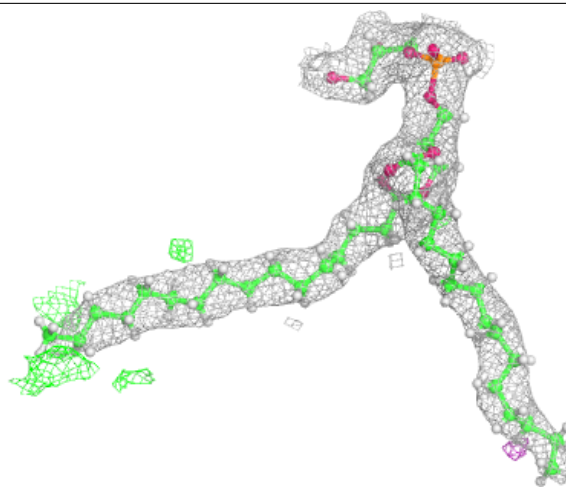
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





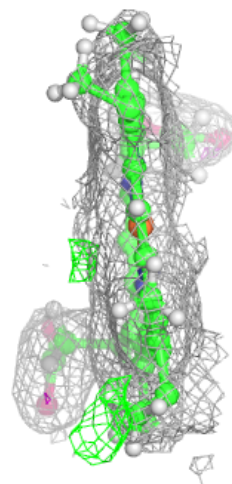
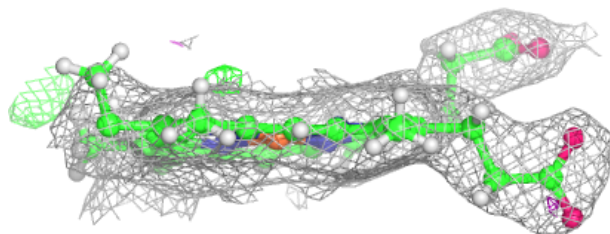
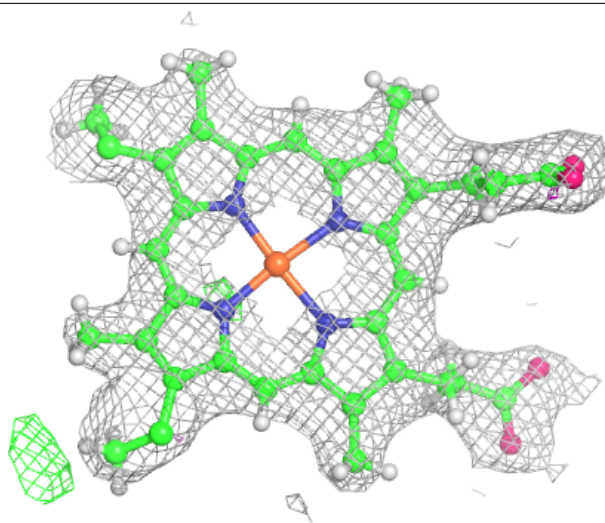
**Electron density around LHG L 102:**

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



**Electron density around HEC V 201:**

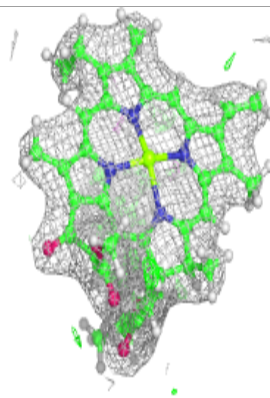
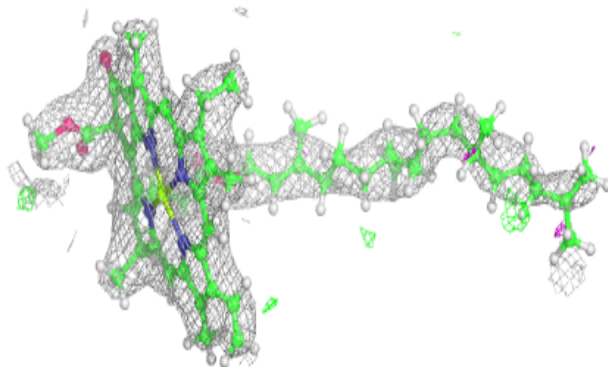
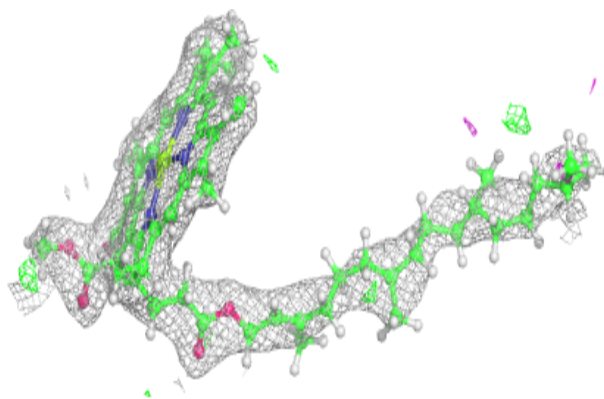
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





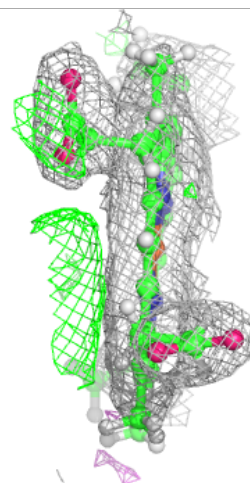
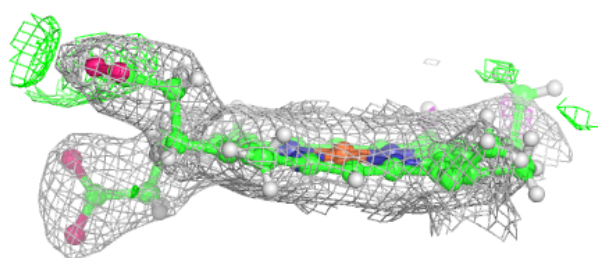
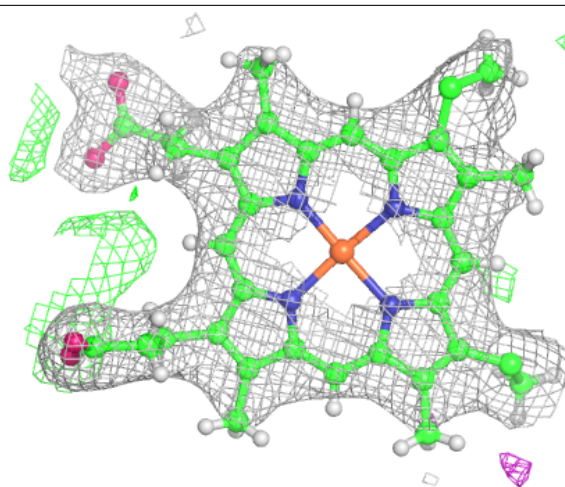
**Electron density around CLA B 606:**

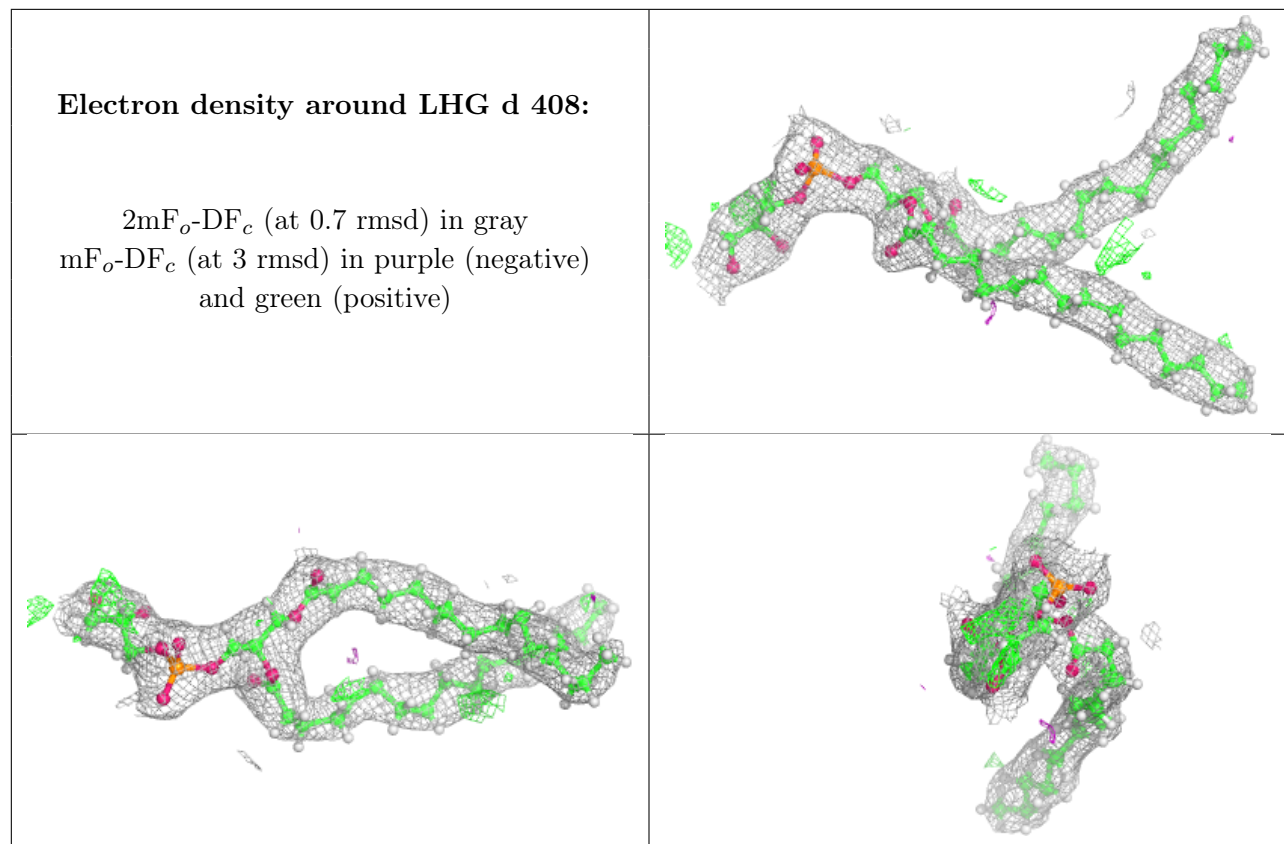
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC v 201:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.