



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 06:37 PM EDT

PDB ID : 7RF1  
Title : RT XFEL structure of Photosystem II averaged across all S-states at 1.89 Angstrom resolution  
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2021-07-13  
Resolution : 1.89 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)  
Refmac : 5.8.0158

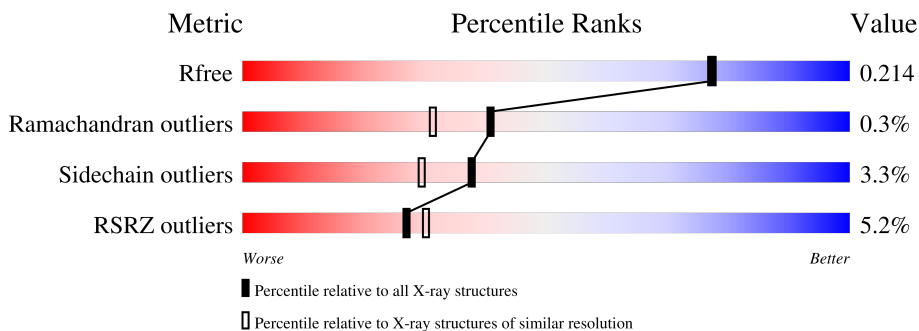
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	 97%
1	a	344	 93%
2	B	510	 97%
2	b	510	 96%

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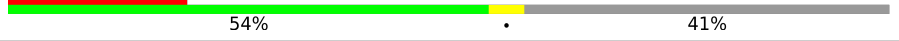




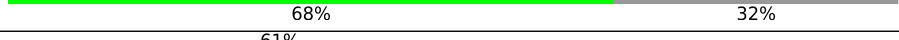

CCP4 : 7.0.044 (Gargrove)  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
3	C	461	2% 95%
3	c	461	2% 95%
4	D	352	97%
4	d	352	95%
5	E	84	8% 94%
5	e	84	14% 94%
6	F	45	7% 76% 24%
6	f	45	4% 76% 24%
7	H	66	5% 95%
7	h	66	8% 88% 8% 5%
8	I	38	5% 84% 11% 5%
8	i	38	8% 87% 8% 5%
9	J	40	10% 90% 10%
9	j	40	12% 85% 5% 10%
10	K	46	7% 78% 20%
10	k	46	7% 74% 7% 20%
11	L	37	97%
11	l	37	5% 86% 11%
12	M	36	3% 89% 8%
12	m	36	86% 11%
13	O	272	8% 85% 10%
13	o	272	7% 86% 10%
14	T	32	6% 88% 6% 6%
14	t	32	9% 91% 6%
15	U	134	% 69% 28%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	h	101	X	-	-	-
27	STE	C	528	-	-	-	X
27	STE	I	102	-	-	-	X
27	STE	i	101	-	-	-	X

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 104284 atoms, of which 51760 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	5140	1717	2518	431	459	15	0	0	0
1	a	334	5129	1714	2510	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	7878	2631	3873	666	695	13	0	5	0
2	b	505	7824	2614	3840	665	692	13	0	1	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	6775	2248	3350	571	593	13	0	2	0
3	c	451	6926	2290	3426	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	5338	1800	2621	444	461	12	0	0	0
4	d	341	5350	1804	2627	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
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	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
			557	187	282	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			557	187	282	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			

- 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	
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

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

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

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

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

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
13	O	244	Total	C	H	N	O	S	0	1	0
			3700	1168	1830	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3720	1170	1846	317	383	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2137	675	1073	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2137	675	1073	177	208	4			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
20	R	28	Total 459	C 151	H 238	N 38	O 32	0	0	0
20	r	28	Total 459	C 151	H 238	N 38	O 32	0	0	0

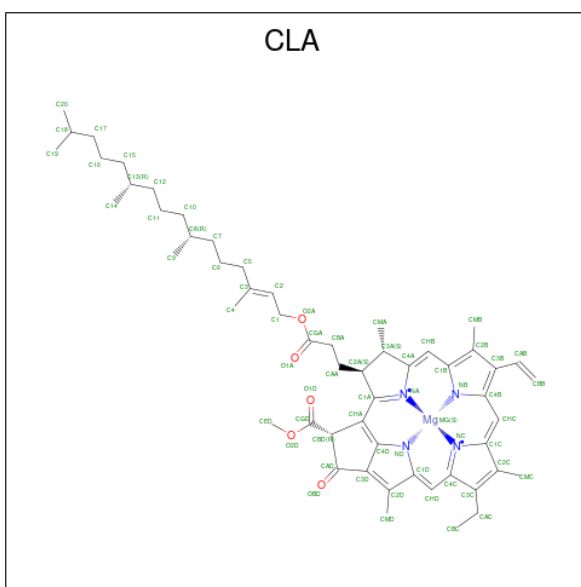
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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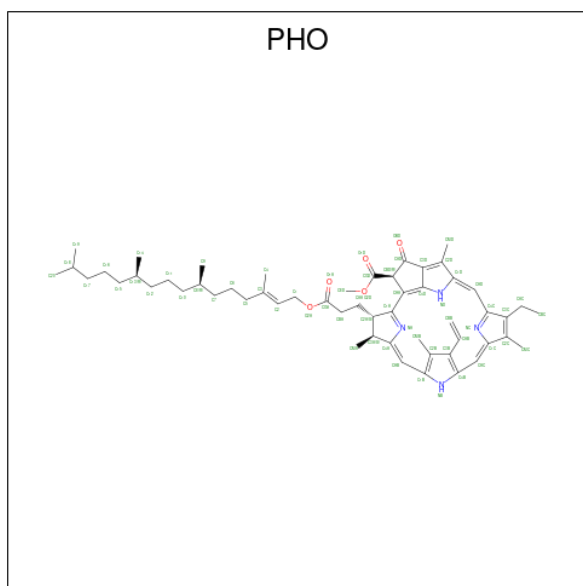
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

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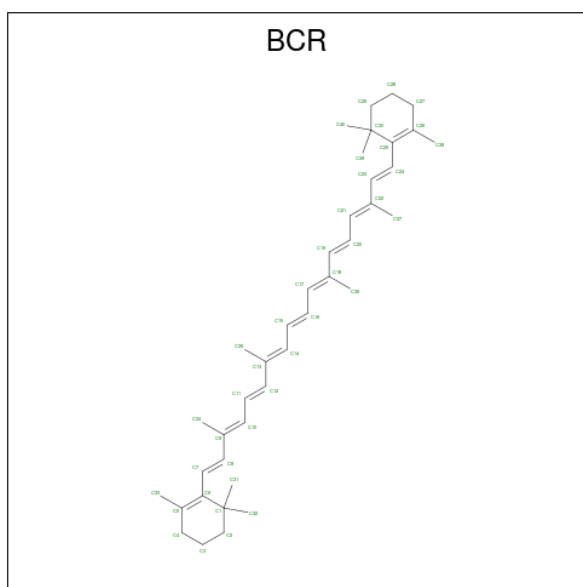
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	h	1	Total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

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



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

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



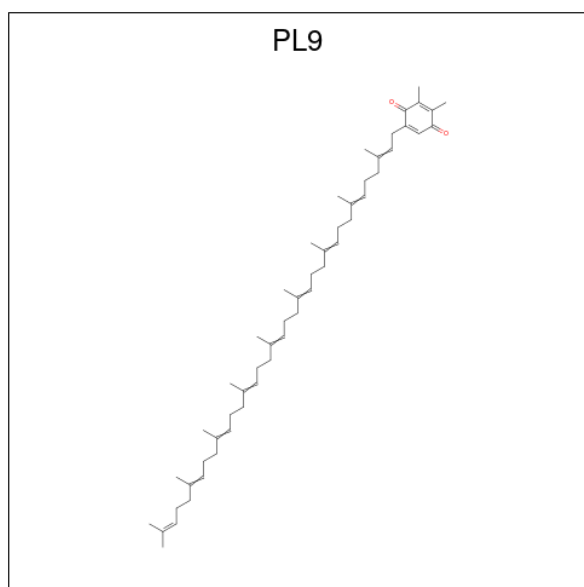
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total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

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

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



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

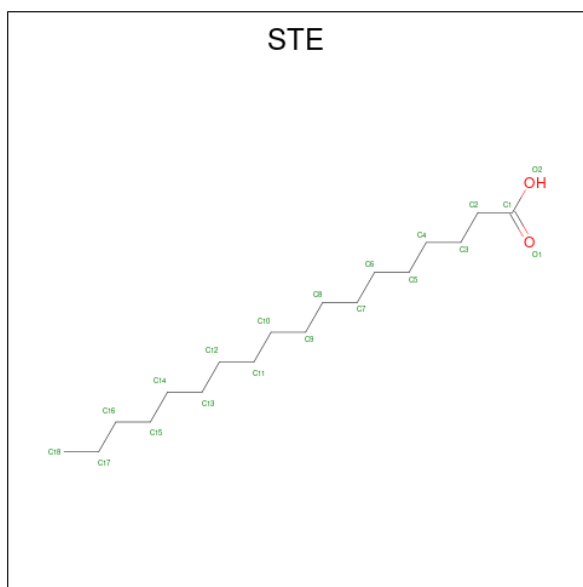
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is STEARIC ACID (three-letter code: STE) (formula:  $C_{18}H_{36}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			9	9				
27	A	1	Total	C	H	O	0	0
			8	8				
27	A	1	Total	C	H	O	0	0
			52	17	35			
27	A	1	Total	C	H	O	0	0
			11	11				
27	B	1	Total	C	H	O	0	0
			43	15	26	2		
27	B	1	Total	C	H	O	0	0
			28	10	16	2		
27	B	1	Total	C	H	O	0	0
			41	15	26			
27	C	1	Total	C	H	O	0	0
			35	12	21	2		
27	C	1	Total	C	H	O	0	0
			15	5	10			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C 7 7	0	0
27	C	1	Total C H O 28 10 16 2	0	0
27	C	1	Total C H 47 16 31	0	0
27	C	1	Total C 8 8	0	0
27	C	1	Total C 14 14	0	0
27	C	1	Total C H 43 14 29	0	0
27	D	1	Total C H O 55 18 35 2	0	0
27	D	1	Total C 9 9	0	0
27	E	1	Total C H O 28 10 16 2	0	0
27	E	1	Total C 12 12	0	0
27	E	1	Total C H O 55 18 35 2	0	0
27	H	1	Total C H 53 18 35	0	0
27	I	1	Total C H 41 15 26	0	0
27	I	1	Total C H O 45 15 28 2	0	0
27	J	1	Total C H O 28 10 16 2	0	0
27	M	1	Total C H O 37 13 22 2	0	0
27	M	1	Total C H 26 10 16	0	0
27	T	1	Total C H 46 16 30	0	0
27	Z	1	Total C H 52 17 35	0	0
27	a	1	Total C H 26 10 16	0	0
27	a	1	Total C H O 28 10 16 2	0	0

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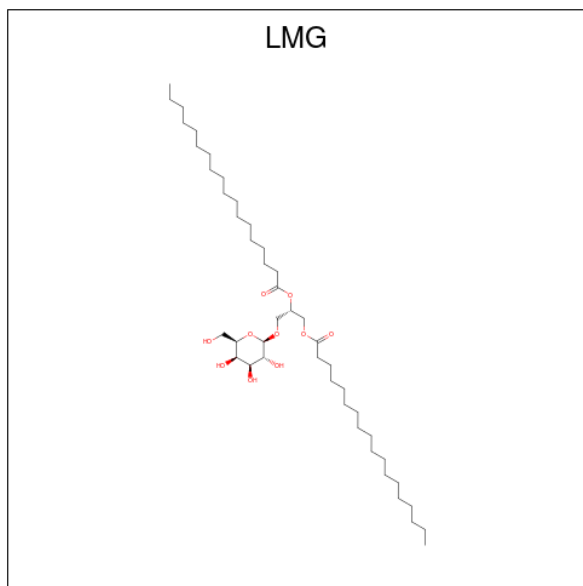
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C H O 55 18 35 2	0	0
27	b	1	Total C O 20 18 2	0	0
27	b	1	Total C H O 40 14 24 2	0	0
27	b	1	Total C H 26 10 16	0	0
27	b	1	Total C 11 11	0	0
27	c	1	Total C H 37 13 24	0	0
27	c	1	Total C H 53 18 35	0	0
27	d	1	Total C H O 43 15 26 2	0	0
27	d	1	Total C H O 28 10 16 2	0	0
27	d	1	Total C 10 10	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C 8 8	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C O 13 11 2	0	0
27	i	1	Total C O 12 10 2	0	0
27	i	1	Total C H 18 6 12	0	0
27	j	1	Total C H O 28 10 16 2	0	0
27	j	1	Total C 16 16	0	0
27	l	1	Total C H 53 18 35	0	0
27	m	1	Total C H O 28 10 16 2	0	0
27	m	1	Total C H 44 15 29	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	t	1	Total	C	H	O	0	0
			34	12	20	2		
27	t	1	Total	C	H	O	0	0
			46	16	28	2		
27	x	1	Total	C	H	O	0	0
			55	18	35	2		
27	z	1	Total	C	H		0	0
			24	9	15			

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



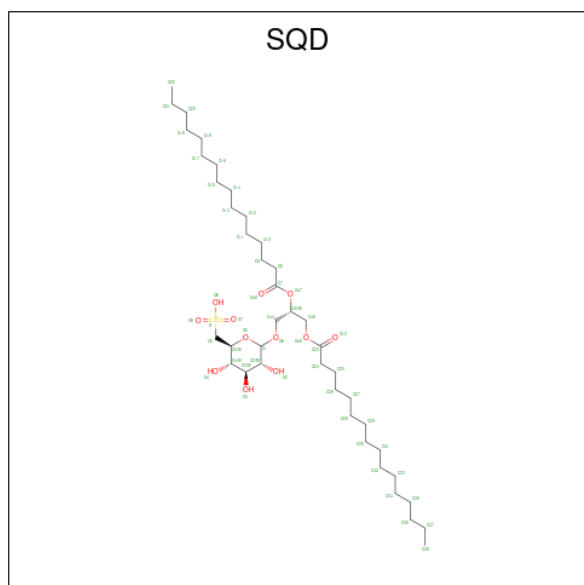
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			109	35	64	10		
28	C	1	Total	C	H	O	0	0
			83	26	47	10		
28	C	1	Total	C	H	O	0	0
			114	38	66	10		
28	D	1	Total	C	H	O	0	0
			124	40	74	10		
28	D	1	Total	C	H	O	0	0
			123	41	72	10		
28	M	1	Total	C	H	O	0	0
			123	41	72	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	a	1	Total	C	H	O	0	0
			141	45	86	10		
28	b	1	Total	C	O		0	0
			24	20	4			
28	b	1	Total	C	H	O	0	0
			123	41	72	10		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			75	25	45	5		
28	c	1	Total	C	H	O	0	0
			110	36	64	10		
28	c	1	Total	C	H	O	0	0
			117	38	69	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



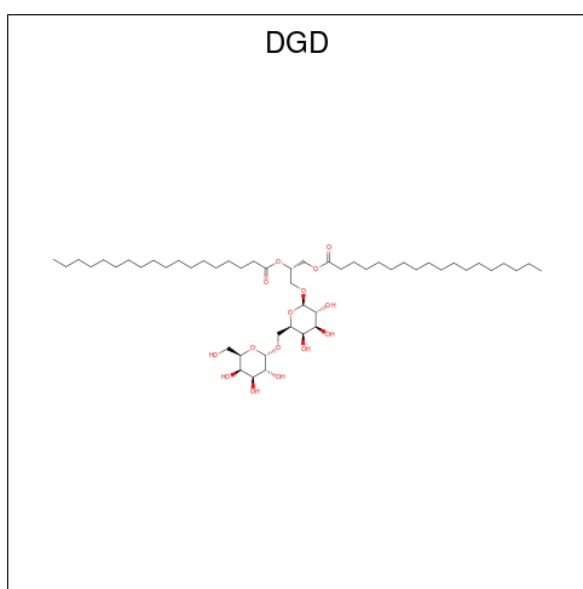
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	O	S		0	0
			54	41	12	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	O	S		0	0
			54	41	12	1			
29	b	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
29	l	1	Total	C	H	O	S	0	0
			131	41	77	12	1		

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



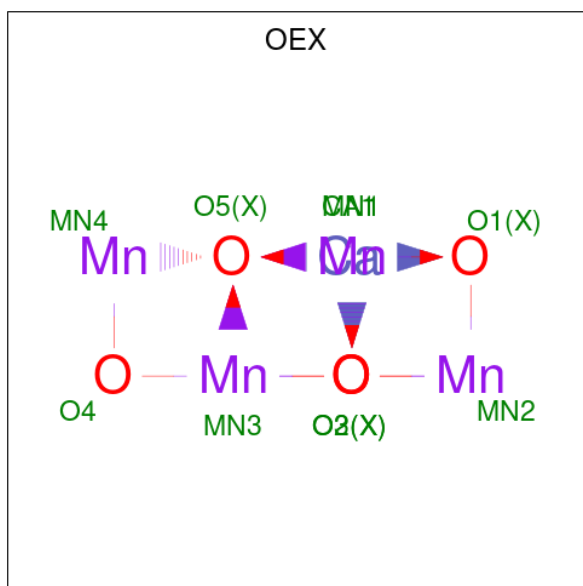
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	H	1	Total	C	H	O	0	0
			144	47	82	15		

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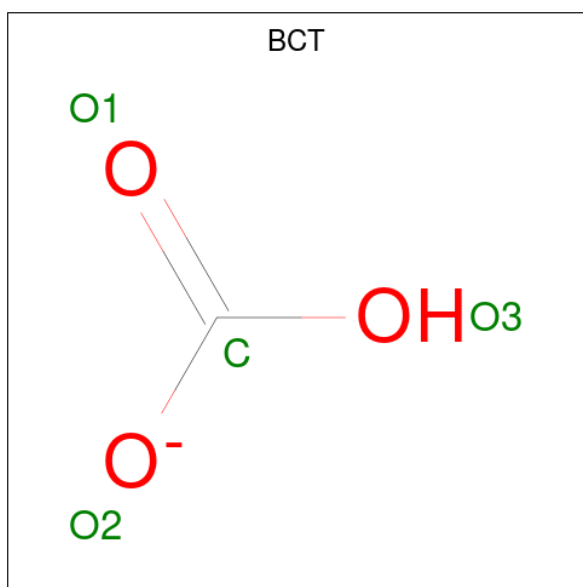
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



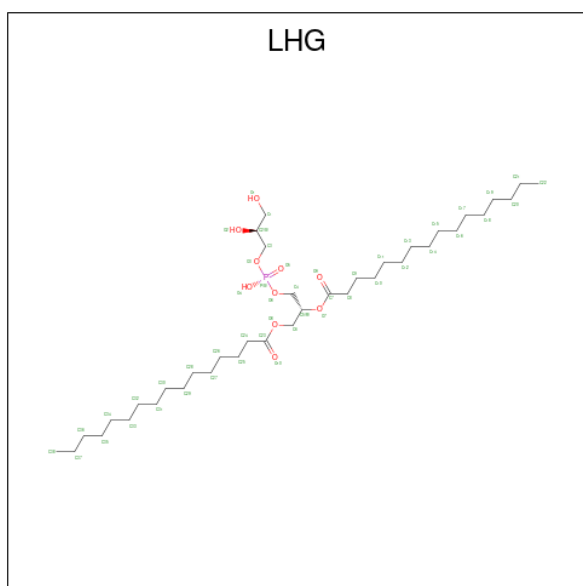
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	H	O	0	0
			5	1	1	3		
32	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

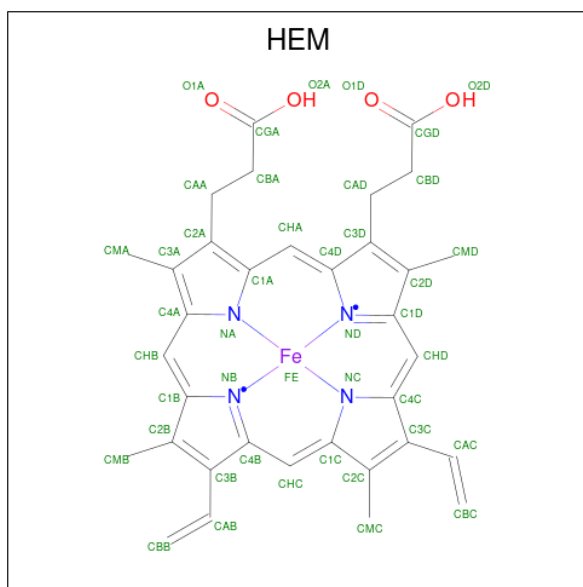
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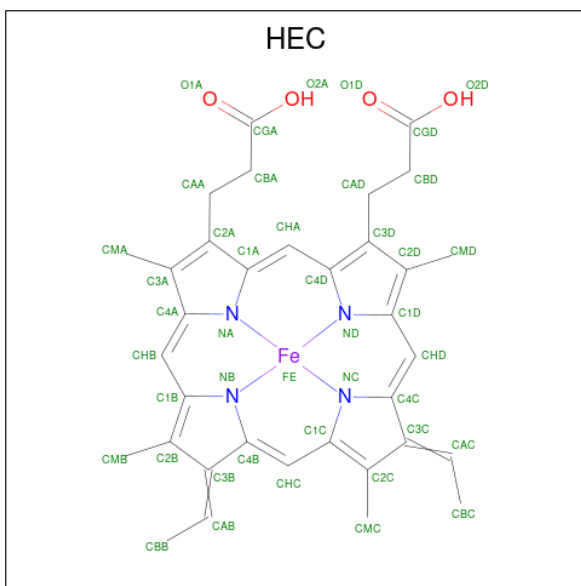
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	a	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	202	Total	O	0	0
			202	202		
36	C	180	Total	O	0	0
			180	180		
36	D	137	Total	O	0	0
			137	137		
36	E	20	Total	O	0	0
			20	20		
36	F	11	Total	O	0	0
			11	11		
36	H	26	Total	O	0	0
			26	26		
36	I	9	Total	O	0	0
			9	9		
36	J	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	K	4	Total O 4 4	0	0
36	L	10	Total O 10 10	0	0
36	M	7	Total O 7 7	0	0
36	O	104	Total O 104 104	0	0
36	T	9	Total O 9 9	0	0
36	U	45	Total O 45 45	0	0
36	V	82	Total O 82 82	0	0
36	Y	1	Total O 1 1	0	0
36	X	12	Total O 12 12	0	0
36	a	115	Total O 115 115	0	0
36	b	200	Total O 200 200	0	0
36	c	171	Total O 171 171	0	0
36	d	125	Total O 125 125	0	0
36	e	10	Total O 10 10	0	0
36	f	10	Total O 10 10	0	0
36	h	23	Total O 23 23	0	0
36	i	5	Total O 5 5	0	0
36	j	6	Total O 6 6	0	0
36	k	5	Total O 5 5	0	0
36	l	15	Total O 15 15	0	0
36	m	7	Total O 7 7	0	0

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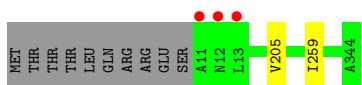
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
36	o	110	Total 110	O 110	0	0
36	t	12	Total 12	O 12	0	0
36	u	61	Total 61	O 61	0	0
36	v	59	Total 59	O 59	0	0
36	y	2	Total 2	O 2	0	0
36	x	7	Total 7	O 7	0	0
36	z	1	Total 1	O 1	0	0

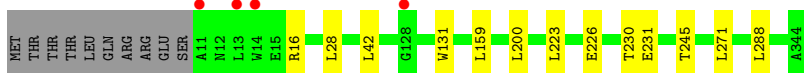
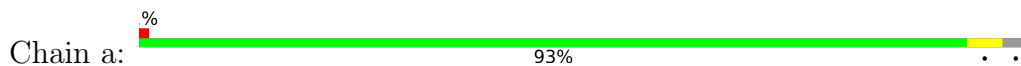
### 3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1



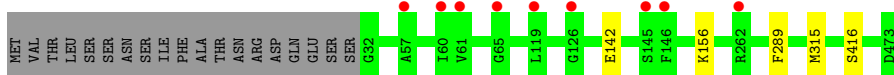
- Molecule 2: Photosystem II CP47 reaction center protein



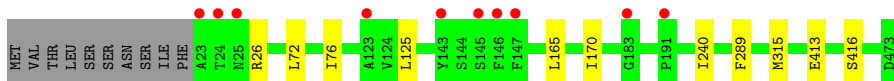
- Molecule 2: Photosystem II CP47 reaction center protein



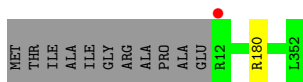
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



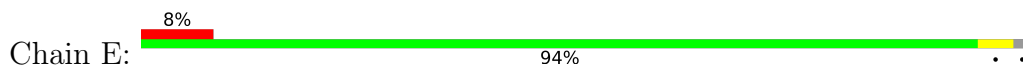
- Molecule 4: Photosystem II D2 protein



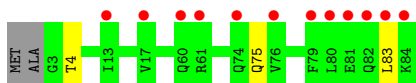
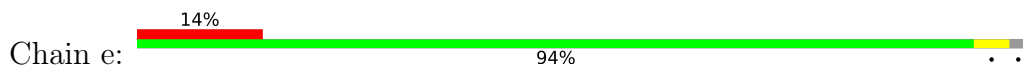
- Molecule 4: Photosystem II D2 protein



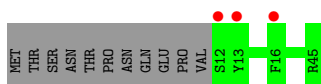
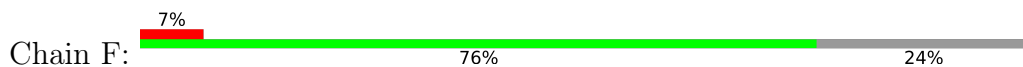
- Molecule 5: Cytochrome b559 subunit alpha



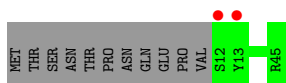
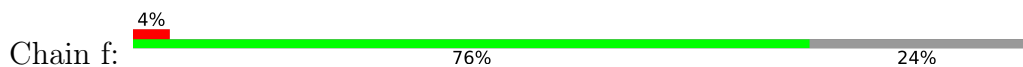
- Molecule 5: Cytochrome b559 subunit alpha



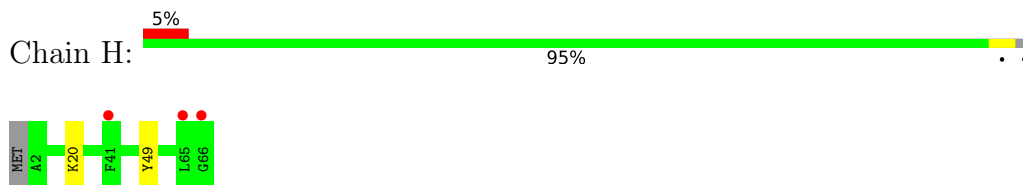
- Molecule 6: Cytochrome b559 subunit beta



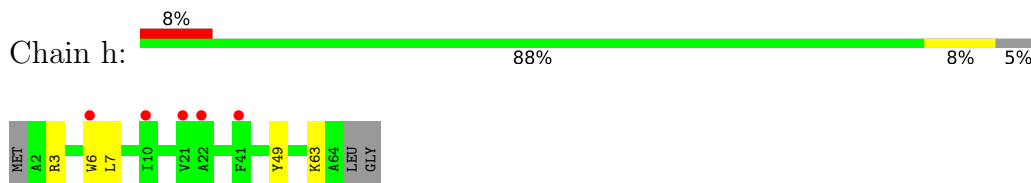
- Molecule 6: Cytochrome b559 subunit beta



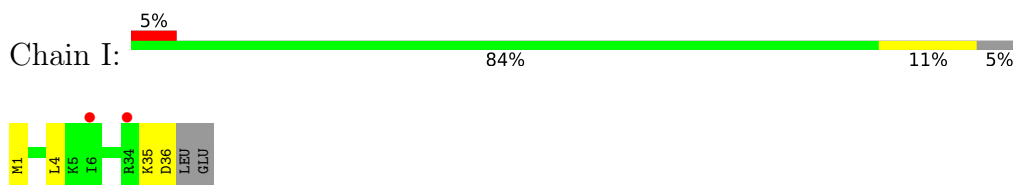
- Molecule 7: Photosystem II reaction center protein H



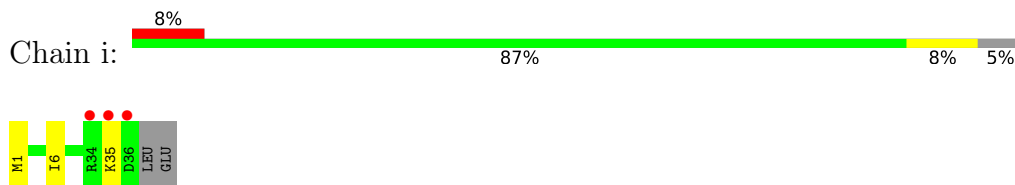
- Molecule 7: Photosystem II reaction center protein H



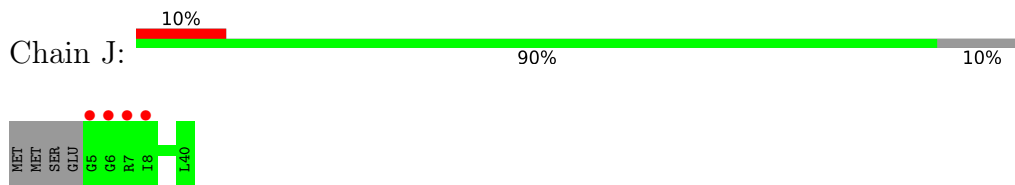
- Molecule 8: Photosystem II reaction center protein I



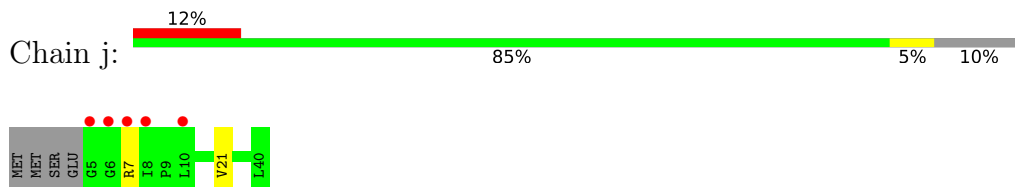
- Molecule 8: Photosystem II reaction center protein I



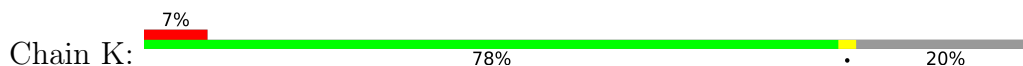
- Molecule 9: Photosystem II reaction center protein J

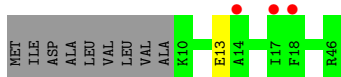


- Molecule 9: Photosystem II reaction center protein J

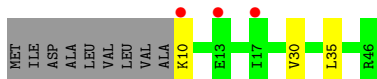
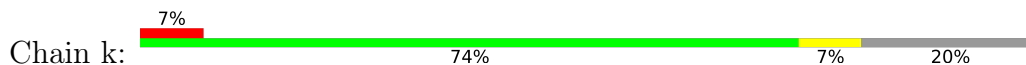


- Molecule 10: Photosystem II reaction center protein K





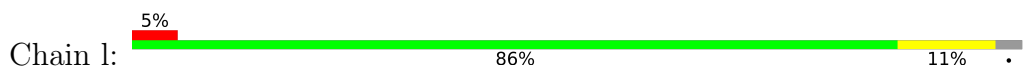
- Molecule 10: Photosystem II reaction center protein K



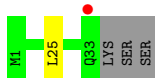
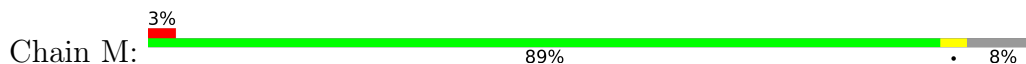
- Molecule 11: Photosystem II reaction center protein L



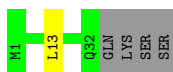
- Molecule 11: Photosystem II reaction center protein L



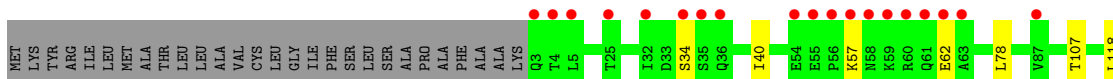
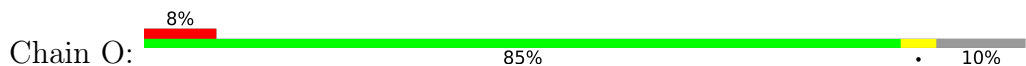
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

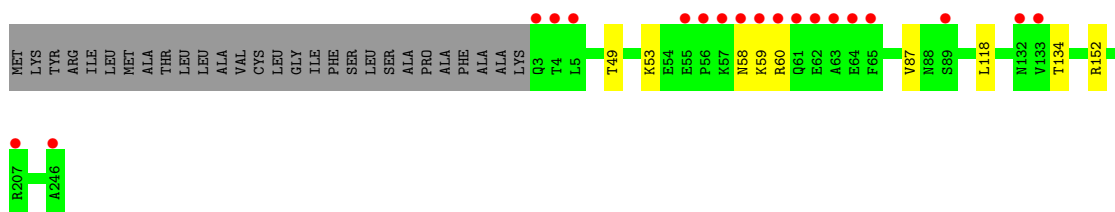
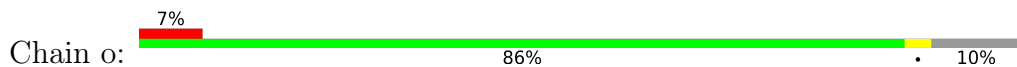


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

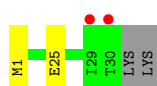
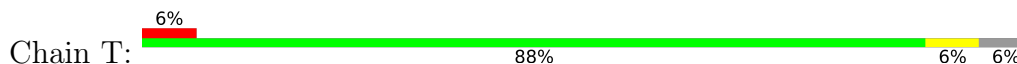




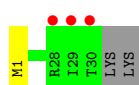
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



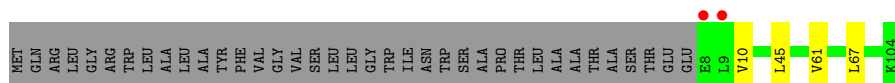
- Molecule 14: Photosystem II reaction center protein T



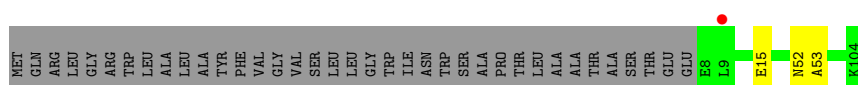
- Molecule 14: Photosystem II reaction center protein T



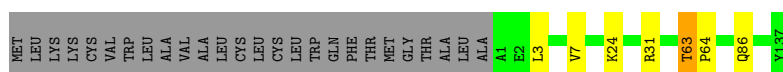
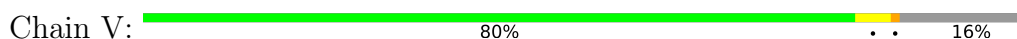
- Molecule 15: Photosystem II 12 kDa extrinsic protein



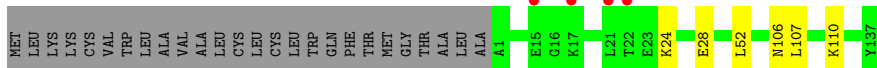
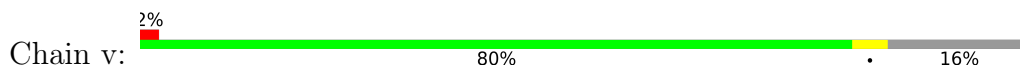
- Molecule 15: Photosystem II 12 kDa extrinsic protein



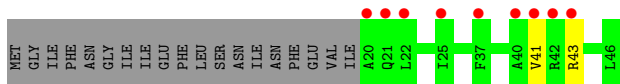
- Molecule 16: Cytochrome c-550



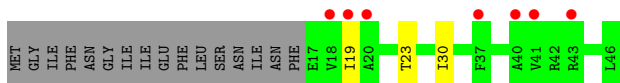
- Molecule 16: Cytochrome c-550



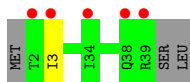
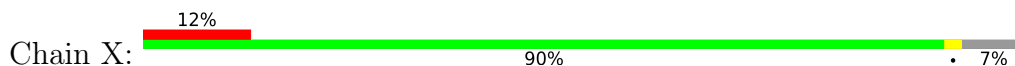
- Molecule 17: Photosystem II reaction center protein Ycf12



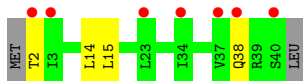
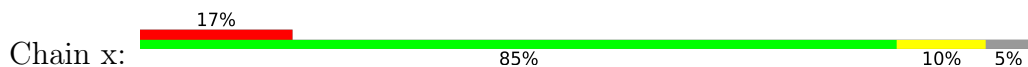
- Molecule 17: Photosystem II reaction center protein Ycf12



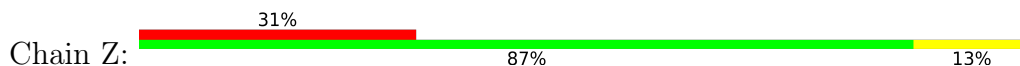
- Molecule 18: Photosystem II reaction center X protein



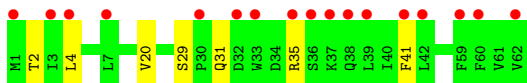
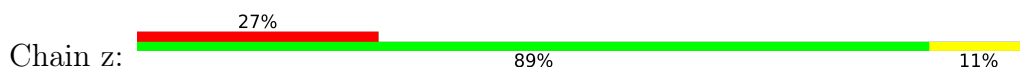
- Molecule 18: Photosystem II reaction center X protein



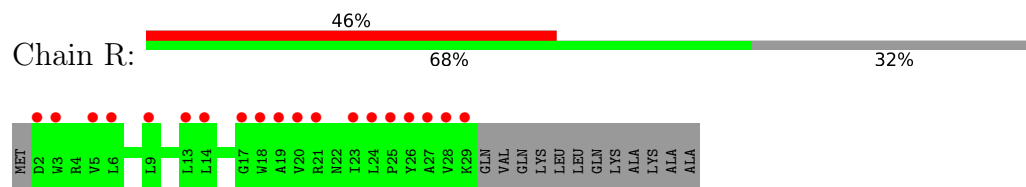
- Molecule 19: Photosystem II reaction center protein Z



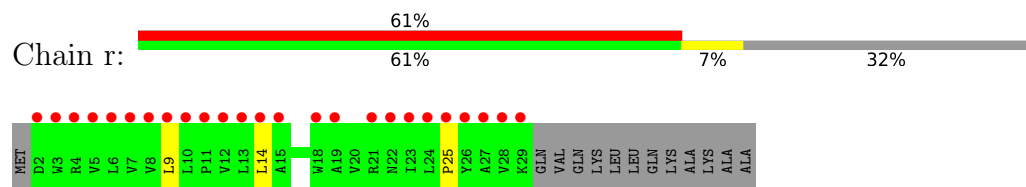
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.00Å 221.60Å 307.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.67 – 1.89 33.67 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.67-1.89) 89.2 (33.67-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.42 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.171 , 0.214 0.171 , 0.214	Depositor DCC
$R_{free}$ test set	5621 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	104284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.61	0/2707	0.67	0/3692
1	a	0.59	0/2704	0.68	1/3688 (0.0%)
2	B	0.59	0/4161	0.68	1/5669 (0.0%)
2	b	0.57	0/4127	0.68	2/5623 (0.0%)
3	C	0.57	0/3546	0.65	0/4828
3	c	0.53	0/3619	0.65	0/4926
4	D	0.63	0/2812	0.67	0/3832
4	d	0.57	0/2821	0.67	0/3844
5	E	0.62	0/688	0.63	0/940
5	e	0.54	0/683	0.63	0/932
6	F	0.64	0/284	0.64	0/387
6	f	0.59	0/284	0.63	0/387
7	H	0.72	0/523	0.74	0/713
7	h	0.60	0/511	0.72	0/697
8	I	0.72	0/293	0.74	0/396
8	i	0.73	0/293	0.76	0/396
9	J	0.55	0/263	0.63	0/356
9	j	0.65	0/263	0.65	0/356
10	K	0.55	0/303	0.72	0/416
10	k	0.54	0/303	0.62	0/416
11	L	0.73	0/311	0.72	0/422
11	l	0.67	0/303	0.72	0/412
12	M	0.67	0/249	0.64	0/341
12	m	0.73	0/244	0.72	0/334
13	O	0.66	0/1904	0.76	1/2585 (0.0%)
13	o	0.64	0/1905	0.77	0/2583
14	T	0.78	0/257	0.76	0/349
14	t	0.81	0/255	0.67	0/346
15	U	0.59	0/785	0.70	0/1064
15	u	0.67	0/785	0.78	0/1064
16	V	0.63	0/1085	0.73	1/1473 (0.1%)
16	v	0.61	0/1085	0.69	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.47	0/197	0.70	0/264
17	y	0.44	0/219	0.60	0/294
18	X	0.52	0/284	0.65	0/384
18	x	0.44	0/289	0.61	0/391
19	Z	0.49	0/490	0.61	0/669
19	z	0.50	0/488	0.61	0/666
20	R	0.41	0/227	0.61	0/313
20	r	0.38	0/227	0.61	0/313
All	All	0.60	0/42777	0.68	6/58234 (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
13	o	0	1
15	u	0	1
16	V	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	63	THR	C-N-CD	-7.32	104.49	120.60
2	b	267	LEU	CA-CB-CG	-6.88	99.47	115.30
2	B	15	ASP	CB-CG-OD2	-5.60	113.26	118.30
2	b	267	LEU	CB-CG-CD2	5.57	120.47	111.00
1	a	131	TRP	CA-CB-CG	-5.08	104.05	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide
13	o	152	ARG	Sidechain
15	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%)	328 (99%)	3 (1%)	1 (0%)	41	31
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	493 (98%)	10 (2%)	1 (0%)	47	38
3	C	442/461 (96%)	432 (98%)	9 (2%)	1 (0%)	47	38
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	47	38
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	10 (4%)	2 (1%)	19	9
13	o	242/272 (89%)	233 (96%)	7 (3%)	2 (1%)	19	9
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	14	5
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	12
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	0
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	9	2
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9	2
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	0	1 (4%)	3	0
All	All	5232/5700 (92%)	5089 (97%)	129 (2%)	14 (0%)	41	31

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	o	58	ASN
15	u	53	ALA

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

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	91	91
1	a	269/280 (96%)	257 (96%)	12 (4%)	27	18
2	B	408/407 (100%)	401 (98%)	7 (2%)	60	57
2	b	403/407 (99%)	391 (97%)	12 (3%)	41	33
3	C	346/362 (96%)	342 (99%)	4 (1%)	71	70
3	c	354/362 (98%)	343 (97%)	11 (3%)	40	32
4	D	276/283 (98%)	275 (100%)	1 (0%)	91	91
4	d	277/283 (98%)	269 (97%)	8 (3%)	42	35
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	11
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	20
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	25
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	3
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	3
8	i	32/34 (94%)	30 (94%)	2 (6%)	18	8
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	4
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	29
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	3
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	35
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	26
12	m	28/32 (88%)	27 (96%)	1 (4%)	35	26
13	O	206/228 (90%)	197 (96%)	9 (4%)	28	19
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	35
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	24
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	80 (95%)	4 (5%)	25	16
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/138 (85%)	112 (96%)	5 (4%)	29	19
16	v	117/138 (85%)	111 (95%)	6 (5%)	24	14
17	Y	19/37 (51%)	18 (95%)	1 (5%)	22	13
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	30
18	x	31/34 (91%)	27 (87%)	4 (13%)	4	1
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	20 (91%)	2 (9%)	9	3
All	All	4322/4654 (93%)	4178 (97%)	144 (3%)	38	29

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	m	13	LEU
20	r	14	LEU
13	o	87	VAL
17	y	23	THR
19	Z	34	ASP

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

Mol	Chain	Res	Type
7	h	59	ASN
16	v	106	ASN
13	o	61	GLN
18	x	33	GLN
13	O	88	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	m	1	12	8,9,10	1.01	0	7,9,11	0.81	0
14	FME	T	1	14	8,9,10	0.90	0	7,9,11	1.48	1 (14%)
14	FME	t	1	14	8,9,10	1.26	1 (12%)	7,9,11	0.96	0
8	FME	i	1	8	8,9,10	0.99	0	7,9,11	1.30	1 (14%)
8	FME	I	1	8	8,9,10	0.86	0	7,9,11	1.45	1 (14%)
12	FME	M	1	12	8,9,10	0.83	0	7,9,11	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.81	1.42	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.88	118.39	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.47	119.03	122.82
14	T	1	FME	O1-CN-N	-2.01	119.97	125.27

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

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 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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
25	BCR	b	617	-	41,41,41	1.24	2 (4%)	56,56,56	1.16	7 (12%)
27	STE	A	417	-	10,10,19	0.40	0	9,9,19	0.83	0
27	STE	C	526	-	15,15,19	0.56	0	14,14,19	0.46	0
23	CLA	B	602	-	65,73,73	1.71	8 (12%)	76,113,113	1.33	8 (10%)
35	HEC	v	201	16	32,50,50	2.22	4 (12%)	24,82,82	1.76	5 (20%)
26	PL9	a	410	-	55,55,55	0.95	4 (7%)	68,69,69	1.60	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	STE	l	103	-	17,17,19	0.36	0	16,16,19	0.70	0
30	DGD	A	414	-	67,67,67	1.32	10 (14%)	81,81,81	1.55	17 (20%)
23	CLA	a	405	-	65,73,73	1.47	9 (13%)	76,113,113	1.37	8 (10%)
23	CLA	b	612	-	65,73,73	1.48	8 (12%)	76,113,113	1.29	11 (14%)
27	STE	A	410	-	8,8,19	0.40	0	7,7,19	0.71	0
28	LMG	b	621	-	51,51,55	1.00	4 (7%)	59,59,63	1.46	9 (15%)
28	LMG	d	409	-	44,44,55	1.09	4 (9%)	52,52,63	1.33	7 (13%)
23	CLA	B	601	36	65,73,73	1.76	9 (13%)	76,113,113	1.61	7 (9%)
27	STE	E	104	-	19,19,19	0.80	1 (5%)	19,19,19	0.93	1 (5%)
23	CLA	c	509	-	65,73,73	1.42	9 (13%)	76,113,113	1.54	12 (15%)
27	STE	I	101	-	14,14,19	0.51	0	13,13,19	0.53	0
28	LMG	c	523	-	48,48,55	1.04	4 (8%)	56,56,63	1.31	8 (14%)
30	DGD	c	519	-	63,63,67	1.16	6 (9%)	77,77,81	1.45	11 (14%)
23	CLA	b	601	-	65,73,73	1.43	10 (15%)	76,113,113	1.67	12 (15%)
25	BCR	c	514	-	41,41,41	1.24	3 (7%)	56,56,56	1.28	6 (10%)
23	CLA	B	603	-	65,73,73	1.45	10 (15%)	76,113,113	1.64	14 (18%)
27	STE	B	621	-	16,16,19	0.70	0	16,16,19	0.97	0
27	STE	m	102	-	14,14,19	0.57	0	13,13,19	0.58	0
23	CLA	B	610	36	65,73,73	1.81	10 (15%)	76,113,113	1.46	9 (11%)
23	CLA	C	504	36	59,67,73	1.53	8 (13%)	68,105,113	1.36	10 (14%)
27	STE	D	414	-	8,8,19	0.38	0	7,7,19	0.99	0
23	CLA	b	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.31	9 (11%)
25	BCR	D	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.15	5 (8%)
27	STE	M	103	-	9,9,19	0.47	0	8,8,19	0.43	0
27	STE	J	101	-	11,11,19	0.60	0	11,11,19	1.47	2 (18%)
27	STE	E	103	-	11,11,19	0.46	0	10,10,19	0.62	0
29	SQD	A	413	-	53,54,54	1.64	10 (18%)	62,65,65	1.87	14 (22%)
27	STE	E	102	-	11,11,19	0.98	1 (9%)	11,11,19	0.94	0
23	CLA	B	606	-	65,73,73	1.76	11 (16%)	76,113,113	1.55	7 (9%)
25	BCR	k	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.12	3 (5%)
23	CLA	D	405	-	65,73,73	1.67	12 (18%)	76,113,113	1.31	9 (11%)
28	LMG	b	623	-	55,55,55	1.01	2 (3%)	63,63,63	1.51	10 (15%)
28	LMG	D	409	-	51,51,55	1.15	3 (5%)	59,59,63	1.34	5 (8%)
23	CLA	c	504	36	60,68,73	1.73	6 (10%)	70,107,113	1.41	10 (14%)
25	BCR	t	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.27	5 (8%)
29	SQD	f	102	-	40,41,54	1.70	10 (25%)	49,52,65	1.78	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	511	3	65,73,73	1.59	8 (12%)	76,113,113	1.42	7 (9%)
25	BCR	k	102	-	41,41,41	1.04	3 (7%)	56,56,56	1.13	3 (5%)
23	CLA	b	603	-	65,73,73	1.57	7 (10%)	76,113,113	1.50	10 (13%)
23	CLA	c	513	-	65,73,73	1.69	10 (15%)	76,113,113	1.23	7 (9%)
23	CLA	c	506	-	65,73,73	1.63	8 (12%)	76,113,113	1.35	10 (13%)
27	STE	x	102	-	19,19,19	0.87	1 (5%)	19,19,19	0.85	1 (5%)
27	STE	C	529	-	13,13,19	0.43	0	12,12,19	0.54	0
23	CLA	B	613	-	65,73,73	1.79	11 (16%)	76,113,113	1.16	8 (10%)
27	STE	C	527	-	7,7,19	0.60	0	6,6,19	0.40	0
25	BCR	b	616	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	7 (12%)
27	STE	b	622	-	19,19,19	0.77	1 (5%)	19,19,19	0.92	1 (5%)
24	PHO	A	406	-	51,69,69	1.03	4 (7%)	47,99,99	1.30	8 (17%)
23	CLA	B	609	-	65,73,73	1.43	8 (12%)	76,113,113	1.37	9 (11%)
23	CLA	b	606	36	65,73,73	1.28	8 (12%)	76,113,113	1.36	7 (9%)
25	BCR	C	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	5 (8%)
23	CLA	c	502	-	65,73,73	1.34	7 (10%)	76,113,113	1.45	10 (13%)
25	BCR	a	409	-	41,41,41	1.08	3 (7%)	56,56,56	1.15	5 (8%)
29	SQD	l	101	-	53,54,54	1.54	11 (20%)	62,65,65	2.03	8 (12%)
29	SQD	a	414	-	53,54,54	1.67	10 (18%)	62,65,65	1.77	9 (14%)
33	LHG	D	412	-	48,48,48	0.98	2 (4%)	51,54,54	1.32	6 (11%)
31	OEX	a	418	3,36,1	0,15,15	-	-	-	-	-
26	PL9	d	405	-	55,55,55	1.50	9 (16%)	68,69,69	1.59	13 (19%)
30	DGD	c	521	-	63,63,67	0.91	3 (4%)	77,77,81	1.48	11 (14%)
23	CLA	c	507	36	65,73,73	1.52	12 (18%)	76,113,113	1.36	11 (14%)
33	LHG	D	411	-	46,46,48	0.99	2 (4%)	49,52,54	1.27	4 (8%)
27	STE	b	626	-	9,9,19	0.39	0	8,8,19	0.70	0
32	BCT	D	401	21	2,3,3	1.14	0	2,3,3	3.92	2 (100%)
23	CLA	C	505	-	65,73,73	1.52	6 (9%)	76,113,113	1.29	6 (7%)
27	STE	B	623	-	14,14,19	0.52	0	13,13,19	0.74	0
29	SQD	F	102	-	35,36,54	1.64	6 (17%)	42,45,65	2.99	9 (21%)
27	STE	e	104	-	12,12,19	0.63	0	12,12,19	1.25	1 (8%)
23	CLA	C	513	-	65,73,73	1.59	12 (18%)	76,113,113	1.55	9 (11%)
23	CLA	b	615	-	60,68,73	1.51	9 (15%)	70,107,113	1.53	10 (14%)
27	STE	b	625	-	15,15,19	0.84	0	15,15,19	1.13	2 (13%)
27	STE	C	525	-	11,11,19	0.65	0	11,11,19	1.46	3 (27%)
27	STE	C	518	-	4,4,19	0.49	0	3,3,19	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	511	3	65,73,73	1.68	10 (15%)	76,113,113	1.31	10 (13%)
27	STE	b	624	-	19,19,19	0.65	0	19,19,19	1.13	0
23	CLA	C	503	-	65,73,73	1.60	8 (12%)	76,113,113	1.53	11 (14%)
33	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	1.13	6 (11%)
27	STE	I	102	-	16,16,19	0.84	0	16,16,19	0.89	1 (6%)
25	BCR	A	408	-	41,41,41	1.12	3 (7%)	56,56,56	1.37	7 (12%)
31	OEX	A	418	3,36,1	0,15,15	-	-	-	-	-
23	CLA	B	611	-	65,73,73	1.65	7 (10%)	76,113,113	1.62	10 (13%)
23	CLA	B	607	36	65,73,73	1.48	9 (13%)	76,113,113	1.51	6 (7%)
25	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.39	10 (17%)
26	PL9	A	409	-	55,55,55	1.29	3 (5%)	68,69,69	1.64	14 (20%)
24	PHO	D	402	-	51,69,69	1.01	4 (7%)	47,99,99	1.23	5 (10%)
27	STE	d	412	-	9,9,19	0.48	0	8,8,19	0.60	0
27	STE	e	101	-	8,8,19	0.54	0	7,7,19	0.61	0
23	CLA	B	615	-	65,73,73	1.61	10 (15%)	76,113,113	1.20	9 (11%)
27	STE	b	627	-	10,10,19	0.39	0	9,9,19	0.68	0
23	CLA	b	604	-	65,73,73	1.47	8 (12%)	76,113,113	1.53	15 (19%)
23	CLA	c	505	-	65,73,73	1.56	10 (15%)	76,113,113	1.17	6 (7%)
27	STE	t	103	-	17,17,19	0.66	0	17,17,19	1.05	1 (5%)
30	DGD	H	102	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	12 (15%)
24	PHO	a	407	-	51,69,69	1.09	5 (9%)	47,99,99	1.14	6 (12%)
23	CLA	b	614	-	65,73,73	1.56	10 (15%)	76,113,113	1.43	9 (11%)
23	CLA	b	613	-	65,73,73	1.64	9 (13%)	76,113,113	1.67	12 (15%)
30	DGD	C	523	-	63,63,67	0.93	3 (4%)	77,77,81	1.33	10 (12%)
26	PL9	D	407	-	55,55,55	1.66	7 (12%)	68,69,69	1.61	16 (23%)
23	CLA	c	508	-	64,72,73	1.59	8 (12%)	74,111,113	1.45	9 (12%)
23	CLA	C	510	-	65,73,73	1.46	10 (15%)	76,113,113	1.62	11 (14%)
25	BCR	H	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.27	7 (12%)
27	STE	i	101	-	11,11,19	0.84	0	11,11,19	1.03	0
30	DGD	C	521	-	63,63,67	1.22	8 (12%)	77,77,81	1.52	12 (15%)
23	CLA	A	407	-	54,62,73	1.99	8 (14%)	62,99,113	1.49	9 (14%)
23	CLA	d	403	-	65,73,73	1.69	11 (16%)	76,113,113	1.18	9 (11%)
27	STE	e	102	-	7,7,19	0.43	0	6,6,19	0.60	0
23	CLA	A	404	-	65,73,73	1.44	8 (12%)	76,113,113	1.25	7 (9%)
27	STE	T	102	-	15,15,19	0.50	0	14,14,19	0.55	0
27	STE	Z	101	-	16,16,19	0.49	0	15,15,19	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LMG	b	619	-	22,22,55	1.01	2 (9%)	23,23,63	1.06	1 (4%)
23	CLA	b	608	-	65,73,73	1.58	10 (15%)	76,113,113	1.57	10 (13%)
27	STE	H	103	-	17,17,19	0.55	0	16,16,19	0.66	0
27	STE	j	101	-	11,11,19	0.79	0	11,11,19	0.94	0
23	CLA	c	501	-	65,73,73	1.49	7 (10%)	76,113,113	1.60	11 (14%)
27	STE	i	102	-	5,5,19	0.47	0	4,4,19	0.40	0
23	CLA	b	610	-	65,73,73	1.23	5 (7%)	76,113,113	1.44	11 (14%)
23	CLA	A	405	36	65,73,73	1.39	7 (10%)	76,113,113	1.34	11 (14%)
28	LMG	C	517	-	35,35,55	1.39	3 (8%)	43,43,63	1.72	8 (18%)
30	DGD	C	522	-	63,63,67	1.48	10 (15%)	77,77,81	1.29	8 (10%)
23	CLA	d	402	-	65,73,73	1.62	9 (13%)	76,113,113	1.51	13 (17%)
27	STE	c	516	-	12,12,19	0.51	0	11,11,19	0.53	0
28	LMG	D	408	-	50,50,55	1.07	3 (6%)	58,58,63	1.27	4 (6%)
27	STE	j	102	-	15,15,19	0.54	0	14,14,19	0.55	0
28	LMG	M	101	-	51,51,55	1.05	4 (7%)	59,59,63	1.43	10 (16%)
23	CLA	B	612	-	65,73,73	1.55	5 (7%)	76,113,113	1.52	12 (15%)
23	CLA	B	616	-	60,68,73	1.52	7 (11%)	70,107,113	1.52	9 (12%)
33	LHG	d	408	-	38,38,48	0.97	2 (5%)	41,44,54	1.11	4 (9%)
25	BCR	C	515	-	41,41,41	1.27	3 (7%)	56,56,56	1.36	6 (10%)
29	SQD	a	412	-	53,54,54	1.43	8 (15%)	62,65,65	2.14	18 (29%)
23	CLA	B	608	-	65,73,73	1.23	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	C	502	-	65,73,73	1.62	8 (12%)	76,113,113	1.37	7 (9%)
27	STE	d	411	-	11,11,19	0.82	0	11,11,19	0.88	0
30	DGD	h	102	-	63,63,67	1.17	6 (9%)	77,77,81	1.45	13 (16%)
32	BCT	a	404	21	2,3,3	1.35	0	2,3,3	3.40	2 (100%)
23	CLA	B	604	-	65,73,73	1.45	10 (15%)	76,113,113	1.61	7 (9%)
23	CLA	c	510	-	65,73,73	1.58	8 (12%)	76,113,113	1.49	9 (11%)
35	HEC	V	201	16	32,50,50	2.28	4 (12%)	24,82,82	1.75	5 (20%)
28	LMG	C	524	-	48,48,55	1.02	4 (8%)	56,56,63	1.23	3 (5%)
29	SQD	b	620	-	48,49,54	1.57	9 (18%)	57,60,65	2.25	17 (29%)
33	LHG	L	101	-	48,48,48	0.94	1 (2%)	51,54,54	1.28	8 (15%)
23	CLA	b	611	-	65,73,73	1.63	10 (15%)	76,113,113	1.34	10 (13%)
25	BCR	d	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.10	2 (3%)
28	LMG	B	620	-	45,45,55	1.05	2 (4%)	53,53,63	1.37	4 (7%)
25	BCR	x	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.34	8 (14%)
25	BCR	T	101	-	41,41,41	1.28	6 (14%)	56,56,56	1.41	9 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	STE	A	416	-	16,16,19	0.63	0	15,15,19	0.28	0
27	STE	C	528	-	13,13,19	0.46	0	12,12,19	0.63	0
23	CLA	c	512	-	65,73,73	1.38	8 (12%)	76,113,113	1.58	13 (17%)
27	STE	C	519	-	6,6,19	0.45	0	5,5,19	0.79	0
27	STE	m	101	-	11,11,19	0.78	0	11,11,19	0.98	0
27	STE	C	516	-	13,13,19	0.76	0	13,13,19	0.88	0
23	CLA	D	403	36	65,73,73	1.66	11 (16%)	76,113,113	1.29	5 (6%)
23	CLA	C	506	-	65,73,73	1.60	6 (9%)	76,113,113	1.21	8 (10%)
23	CLA	B	605	-	65,73,73	1.32	8 (12%)	76,113,113	1.27	8 (10%)
28	LMG	c	524	-	49,49,55	1.02	4 (8%)	57,57,63	1.30	5 (8%)
33	LHG	l	102	-	48,48,48	0.82	2 (4%)	51,54,54	1.22	4 (7%)
23	CLA	C	507	36	65,73,73	1.23	7 (10%)	76,113,113	1.58	11 (14%)
23	CLA	a	408	-	65,73,73	1.62	9 (13%)	76,113,113	1.44	13 (17%)
25	BCR	C	520	-	41,41,41	1.13	4 (9%)	56,56,56	1.13	4 (7%)
28	LMG	a	415	-	55,55,55	1.45	8 (14%)	63,63,63	1.53	8 (12%)
34	HEM	f	101	5,6	41,50,50	1.50	6 (14%)	45,82,82	1.92	8 (17%)
33	LHG	E	101	-	48,48,48	1.08	4 (8%)	51,54,54	1.12	2 (3%)
23	CLA	a	406	36	65,73,73	1.57	8 (12%)	76,113,113	1.64	12 (15%)
27	STE	A	415	-	7,7,19	0.43	0	6,6,19	0.56	0
34	HEM	F	101	5,6	41,50,50	1.52	7 (17%)	45,82,82	1.72	11 (24%)
28	LMG	c	522	-	46,46,55	1.22	5 (10%)	54,54,63	1.27	8 (14%)
27	STE	B	622	-	11,11,19	0.88	0	11,11,19	0.96	0
25	BCR	b	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	7 (12%)
33	LHG	D	410	-	48,48,48	0.92	2 (4%)	51,54,54	1.14	5 (9%)
23	CLA	B	614	-	65,73,73	1.62	8 (12%)	76,113,113	1.33	11 (14%)
25	BCR	B	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.17	6 (10%)
27	STE	d	410	-	16,16,19	0.88	0	16,16,19	0.80	0
33	LHG	d	406	-	48,48,48	0.86	2 (4%)	51,54,54	1.35	8 (15%)
23	CLA	C	509	-	65,73,73	1.61	10 (15%)	76,113,113	1.49	10 (13%)
23	CLA	C	501	-	65,73,73	1.79	7 (10%)	76,113,113	1.39	6 (7%)
27	STE	D	413	-	19,19,19	0.69	0	19,19,19	1.29	2 (10%)
27	STE	a	416	-	9,9,19	0.68	0	8,8,19	0.39	0
23	CLA	b	602	-	65,73,73	1.46	10 (15%)	76,113,113	1.58	12 (15%)
27	STE	e	103	-	8,8,19	0.39	0	7,7,19	0.69	0
23	CLA	a	411	36	65,73,73	1.54	9 (13%)	76,113,113	1.38	9 (11%)
23	CLA	b	609	36	65,73,73	1.45	8 (12%)	76,113,113	1.57	12 (15%)
27	STE	M	102	-	14,14,19	0.73	0	14,14,19	0.98	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	STE	a	417	-	11,11,19	0.76	0	11,11,19	1.17	2 (18%)
23	CLA	b	605	-	65,73,73	1.87	10 (15%)	76,113,113	1.38	8 (10%)
23	CLA	c	503	-	65,73,73	1.43	10 (15%)	76,113,113	1.35	9 (11%)
27	STE	z	101	-	8,8,19	0.50	0	7,7,19	0.54	0
23	CLA	C	508	-	65,73,73	1.70	8 (12%)	76,113,113	1.52	11 (14%)
23	CLA	D	404	-	65,73,73	1.24	5 (7%)	76,113,113	1.24	12 (15%)
25	BCR	B	619	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	7 (12%)
28	LMG	A	411	-	48,48,55	1.03	2 (4%)	56,56,63	1.34	7 (12%)
23	CLA	C	512	-	65,73,73	1.53	11 (16%)	76,113,113	1.35	12 (15%)
30	DGD	c	520	-	63,63,67	1.33	10 (15%)	77,77,81	1.55	16 (20%)
25	BCR	K	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	6 (10%)
24	PHO	d	401	-	51,69,69	1.08	4 (7%)	47,99,99	1.21	8 (17%)
25	BCR	B	617	-	41,41,41	1.08	3 (7%)	56,56,56	1.33	10 (17%)
27	STE	c	517	-	17,17,19	0.56	0	16,16,19	0.56	0
33	LHG	a	413	-	41,41,48	1.50	7 (17%)	44,47,54	1.32	4 (9%)
28	LMG	c	518	-	29,29,55	1.11	2 (6%)	31,31,63	1.08	2 (6%)
29	SQD	A	412	-	51,52,54	1.54	9 (17%)	60,63,65	2.04	14 (23%)
23	CLA	h	101	36	65,73,73	1.62	10 (15%)	76,113,113	1.66	13 (17%)
27	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.05	2 (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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
27	STE	A	417	-	-	5/8/8/17	-
27	STE	C	526	-	-	4/13/13/17	-
23	CLA	B	602	-	1/1/20/20	7/37/115/115	-
35	HEC	v	201	16	-	2/10/54/54	-
26	PL9	a	410	-	-	24/53/73/73	0/1/1/1
27	STE	l	103	-	-	9/15/15/17	-
30	DGD	A	414	-	-	22/55/95/95	0/2/2/2
23	CLA	a	405	-	1/1/20/20	4/37/115/115	-
23	CLA	b	612	-	1/1/20/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	A	410	-	-	4/6/6/17	-
28	LMG	b	621	-	-	17/46/66/70	0/1/1/1
28	LMG	d	409	-	-	13/39/59/70	0/1/1/1
23	CLA	B	601	36	1/1/20/20	13/37/115/115	-
27	STE	E	104	-	-	13/17/17/17	-
23	CLA	c	509	-	1/1/20/20	11/37/115/115	-
27	STE	I	101	-	-	5/12/12/17	-
28	LMG	c	523	-	-	22/43/63/70	0/1/1/1
30	DGD	c	519	-	-	26/51/91/95	0/2/2/2
23	CLA	b	601	-	-	4/37/115/115	-
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/20/20	3/37/115/115	-
27	STE	B	621	-	-	7/14/14/17	-
27	STE	m	102	-	-	6/12/12/17	-
23	CLA	B	610	36	1/1/20/20	4/37/115/115	-
23	CLA	C	504	36	1/1/18/20	5/30/108/115	-
27	STE	D	414	-	-	5/6/6/17	-
23	CLA	b	607	-	-	1/37/115/115	-
25	BCR	D	406	-	-	4/29/63/63	0/2/2/2
27	STE	M	103	-	-	1/7/7/17	-
27	STE	J	101	-	-	3/9/9/17	-
27	STE	E	103	-	-	1/9/9/17	-
29	SQD	A	413	-	-	16/49/69/69	0/1/1/1
27	STE	E	102	-	-	5/9/9/17	-
23	CLA	B	606	-	1/1/20/20	9/37/115/115	-
25	BCR	k	101	-	-	11/29/63/63	0/2/2/2
23	CLA	D	405	-	-	13/37/115/115	-
28	LMG	b	623	-	-	28/50/70/70	0/1/1/1
28	LMG	D	409	-	-	16/46/66/70	0/1/1/1
23	CLA	c	504	36	1/1/19/20	5/31/109/115	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
29	SQD	f	102	-	-	13/36/56/69	0/1/1/1
23	CLA	c	511	3	1/1/20/20	8/37/115/115	-
25	BCR	k	102	-	-	2/29/63/63	0/2/2/2
23	CLA	b	603	-	1/1/20/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	-	1/1/20/20	18/37/115/115	-
23	CLA	c	506	-	1/1/20/20	15/37/115/115	-
27	STE	x	102	-	-	4/17/17/17	-
27	STE	C	529	-	-	6/11/11/17	-
23	CLA	B	613	-	1/1/20/20	11/37/115/115	-
27	STE	C	527	-	-	4/5/5/17	-
25	BCR	b	616	-	-	4/29/63/63	0/2/2/2
27	STE	b	622	-	-	8/17/17/17	-
24	PHO	A	406	-	-	1/37/103/103	0/5/6/6
23	CLA	B	609	-	-	4/37/115/115	-
23	CLA	b	606	36	1/1/20/20	12/37/115/115	-
25	BCR	C	514	-	-	8/29/63/63	0/2/2/2
23	CLA	c	502	-	-	5/37/115/115	-
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
29	SQD	l	101	-	-	23/49/69/69	0/1/1/1
29	SQD	a	414	-	-	20/49/69/69	0/1/1/1
33	LHG	D	412	-	-	14/53/53/53	-
26	PL9	d	405	-	-	9/53/73/73	0/1/1/1
30	DGD	c	521	-	-	18/51/91/95	0/2/2/2
23	CLA	c	507	36	1/1/20/20	7/37/115/115	-
33	LHG	D	411	-	-	13/51/51/53	-
27	STE	b	626	-	-	3/7/7/17	-
23	CLA	C	505	-	1/1/20/20	10/37/115/115	-
27	STE	B	623	-	-	7/12/12/17	-
29	SQD	F	102	-	-	12/28/48/69	0/1/1/1
27	STE	e	104	-	-	5/10/10/17	-
23	CLA	C	513	-	1/1/20/20	13/37/115/115	-
23	CLA	b	615	-	1/1/19/20	8/31/109/115	-
27	STE	b	625	-	-	6/13/13/17	-
27	STE	C	525	-	-	5/9/9/17	-
27	STE	C	518	-	-	1/2/2/17	-
23	CLA	C	511	3	-	4/37/115/115	-
27	STE	b	624	-	-	7/17/17/17	-
23	CLA	C	503	-	-	3/37/115/115	-
33	LHG	d	407	-	-	13/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	I	102	-	-	5/14/14/17	-
25	BCR	A	408	-	-	7/29/63/63	0/2/2/2
23	CLA	B	611	-	-	6/37/115/115	-
23	CLA	B	607	36	1/1/20/20	5/37/115/115	-
25	BCR	c	515	-	-	3/29/63/63	0/2/2/2
26	PL9	A	409	-	-	16/53/73/73	0/1/1/1
24	PHO	D	402	-	-	1/37/103/103	0/5/6/6
27	STE	d	412	-	-	3/7/7/17	-
27	STE	e	101	-	-	2/6/6/17	-
23	CLA	B	615	-	1/1/20/20	8/37/115/115	-
27	STE	b	627	-	-	6/8/8/17	-
23	CLA	b	604	-	1/1/20/20	5/37/115/115	-
23	CLA	c	505	-	1/1/20/20	9/37/115/115	-
27	STE	t	103	-	-	11/15/15/17	-
30	DGD	H	102	-	-	21/51/91/95	0/2/2/2
24	PHO	a	407	-	-	3/37/103/103	0/5/6/6
23	CLA	b	614	-	1/1/20/20	5/37/115/115	-
23	CLA	b	613	-	1/1/20/20	12/37/115/115	-
30	DGD	C	523	-	-	13/51/91/95	0/2/2/2
26	PL9	D	407	-	-	6/53/73/73	0/1/1/1
23	CLA	c	508	-	-	8/36/114/115	-
23	CLA	C	510	-	1/1/20/20	7/37/115/115	-
25	BCR	H	101	-	-	3/29/63/63	0/2/2/2
27	STE	i	101	-	-	6/9/9/17	-
30	DGD	C	521	-	-	20/51/91/95	0/2/2/2
23	CLA	A	407	-	1/1/17/20	2/24/102/115	-
23	CLA	d	403	-	-	7/37/115/115	-
27	STE	e	102	-	-	3/5/5/17	-
23	CLA	A	404	-	1/1/20/20	3/37/115/115	-
27	STE	T	102	-	-	8/13/13/17	-
27	STE	Z	101	-	-	9/14/14/17	-
28	LMG	b	619	-	-	9/21/21/70	-
23	CLA	b	608	-	1/1/20/20	4/37/115/115	-
27	STE	H	103	-	-	8/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	j	101	-	-	6/9/9/17	-
23	CLA	c	501	-	1/1/20/20	5/37/115/115	-
27	STE	i	102	-	-	3/3/3/17	-
23	CLA	b	610	-	1/1/20/20	4/37/115/115	-
23	CLA	A	405	36	-	2/37/115/115	-
28	LMG	C	517	-	-	17/30/50/70	0/1/1/1
30	DGD	C	522	-	-	17/51/91/95	0/2/2/2
23	CLA	d	402	-	1/1/20/20	8/37/115/115	-
27	STE	c	516	-	-	3/10/10/17	-
28	LMG	D	408	-	-	17/45/65/70	0/1/1/1
27	STE	j	102	-	-	6/13/13/17	-
28	LMG	M	101	-	-	21/46/66/70	0/1/1/1
23	CLA	B	612	-	1/1/20/20	11/37/115/115	-
23	CLA	B	616	-	1/1/19/20	6/31/109/115	-
33	LHG	d	408	-	-	12/43/43/53	-
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
29	SQD	a	412	-	-	20/49/69/69	0/1/1/1
23	CLA	B	608	-	-	1/37/115/115	-
23	CLA	C	502	-	-	6/37/115/115	-
27	STE	d	411	-	-	1/9/9/17	-
30	DGD	h	102	-	-	18/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/20/20	10/37/115/115	-
23	CLA	c	510	-	1/1/20/20	10/37/115/115	-
35	HEC	V	201	16	-	2/10/54/54	-
28	LMG	C	524	-	-	10/43/63/70	0/1/1/1
29	SQD	b	620	-	-	17/44/64/69	0/1/1/1
33	LHG	L	101	-	-	12/53/53/53	-
23	CLA	b	611	-	1/1/20/20	8/37/115/115	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
28	LMG	B	620	-	-	13/40/60/70	0/1/1/1
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
27	STE	A	416	-	-	9/14/14/17	-
27	STE	C	528	-	-	7/11/11/17	-
23	CLA	c	512	-	1/1/20/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	C	519	-	-	1/4/4/17	-
27	STE	m	101	-	-	4/9/9/17	-
27	STE	C	516	-	-	5/11/11/17	-
23	CLA	D	403	36	-	6/37/115/115	-
23	CLA	C	506	-	1/1/20/20	9/37/115/115	-
23	CLA	B	605	-	1/1/20/20	7/37/115/115	-
28	LMG	c	524	-	-	16/44/64/70	0/1/1/1
33	LHG	l	102	-	-	18/53/53/53	-
23	CLA	C	507	36	1/1/20/20	6/37/115/115	-
23	CLA	a	408	-	1/1/20/20	14/37/115/115	-
25	BCR	C	520	-	-	3/29/63/63	0/2/2/2
28	LMG	a	415	-	-	26/50/70/70	0/1/1/1
34	HEM	f	101	5,6	-	4/12/54/54	-
33	LHG	E	101	-	-	28/53/53/53	-
23	CLA	a	406	36	-	7/37/115/115	-
27	STE	A	415	-	-	4/5/5/17	-
34	HEM	F	101	5,6	-	2/12/54/54	-
28	LMG	c	522	-	-	17/41/61/70	0/1/1/1
27	STE	B	622	-	-	5/9/9/17	-
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
33	LHG	D	410	-	-	22/53/53/53	-
23	CLA	B	614	-	1/1/20/20	12/37/115/115	-
25	BCR	B	618	-	-	1/29/63/63	0/2/2/2
27	STE	d	410	-	-	5/14/14/17	-
33	LHG	d	406	-	-	18/53/53/53	-
23	CLA	C	509	-	1/1/20/20	11/37/115/115	-
23	CLA	C	501	-	1/1/20/20	4/37/115/115	-
27	STE	D	413	-	-	5/17/17/17	-
27	STE	a	416	-	-	4/7/7/17	-
23	CLA	b	602	-	1/1/20/20	13/37/115/115	-
27	STE	e	103	-	-	4/6/6/17	-
23	CLA	a	411	36	-	4/37/115/115	-
23	CLA	b	609	36	1/1/20/20	5/37/115/115	-
27	STE	M	102	-	-	9/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	a	417	-	-	4/9/9/17	-
23	CLA	b	605	-	1/1/20/20	7/37/115/115	-
23	CLA	c	503	-	-	9/37/115/115	-
27	STE	z	101	-	-	3/6/6/17	-
23	CLA	C	508	-	-	11/37/115/115	-
23	CLA	D	404	-	1/1/20/20	2/37/115/115	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2
28	LMG	A	411	-	-	16/43/63/70	0/1/1/1
23	CLA	C	512	-	1/1/20/20	13/37/115/115	-
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
25	BCR	K	101	-	-	7/29/63/63	0/2/2/2
24	PHO	d	401	-	-	1/37/103/103	0/5/6/6
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
27	STE	c	517	-	-	4/15/15/17	-
33	LHG	a	413	-	-	19/46/46/53	-
28	LMG	c	518	-	-	9/31/31/70	-
29	SQD	A	412	-	-	19/47/67/69	0/1/1/1
23	CLA	h	101	36	1/1/20/20	24/37/115/115	-
27	STE	t	102	-	-	4/11/11/17	-

The worst 5 of 949 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C4B-NB	9.02	1.43	1.35
23	C	501	CLA	C4B-NB	8.61	1.42	1.35
23	A	407	CLA	MG-ND	-8.47	1.89	2.05
23	B	613	CLA	MG-ND	-8.39	1.89	2.05
35	V	201	HEC	C3C-C2C	-8.38	1.32	1.40

The worst 5 of 1304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	102	SQD	O6-C1-C2	14.95	131.64	108.30
23	B	601	CLA	C4A-NA-C1A	10.21	111.30	106.71
29	l	101	SQD	O7-S-C6	9.75	118.53	106.94
23	B	604	CLA	C4A-NA-C1A	9.51	110.98	106.71
23	B	606	CLA	C4A-NA-C1A	9.23	110.86	106.71



5 of 52 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

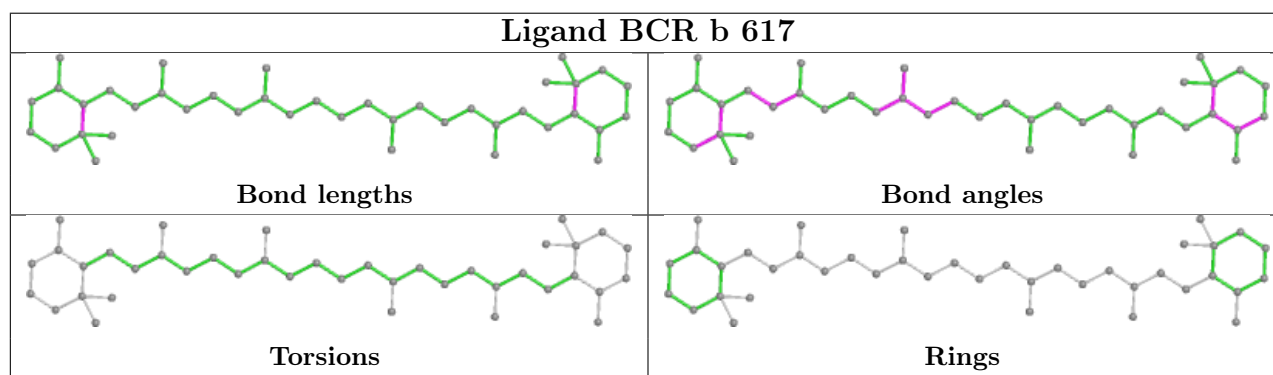
5 of 1732 torsion outliers are listed below:

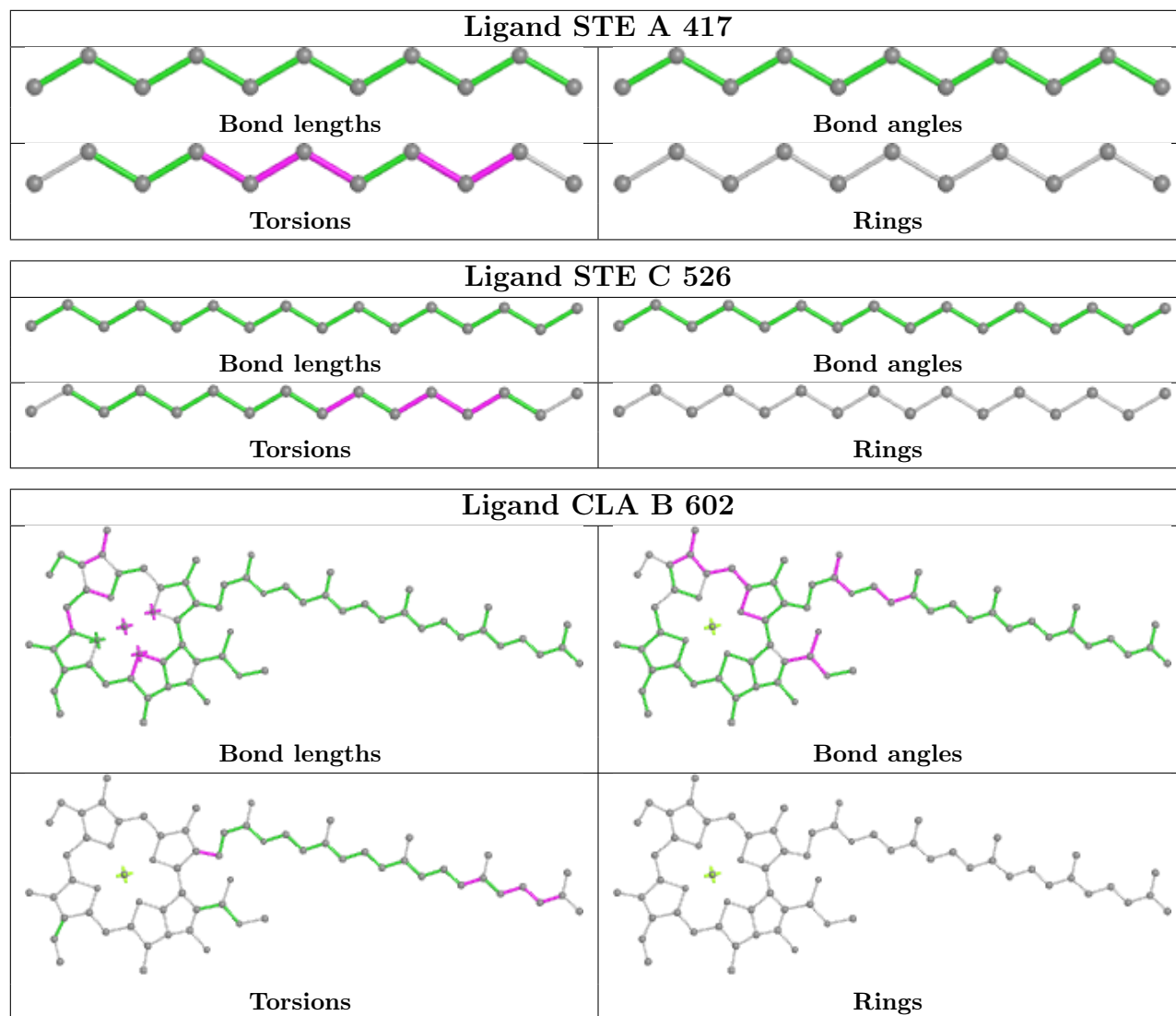
Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C4-C3-C5-C6
23	B	601	CLA	CBA-CGA-O2A-C1
23	B	601	CLA	O1A-CGA-O2A-C1
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D

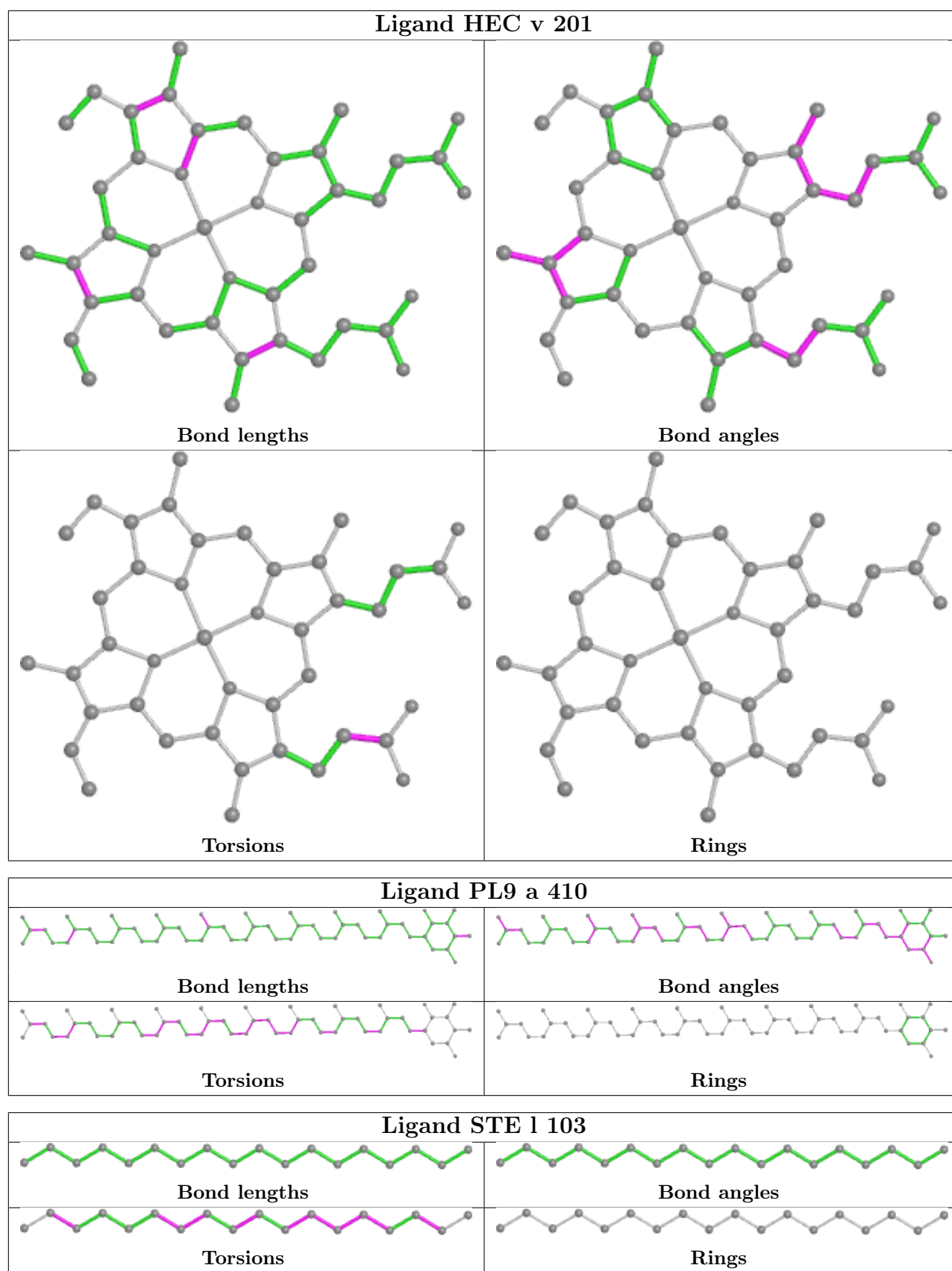
There are no ring outliers.

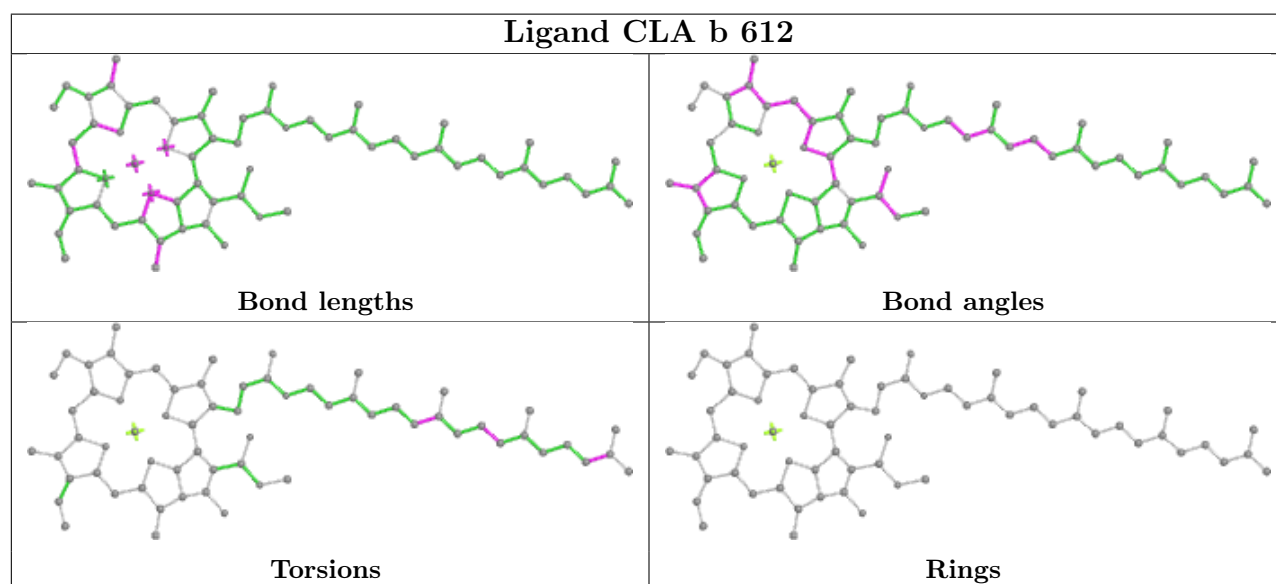
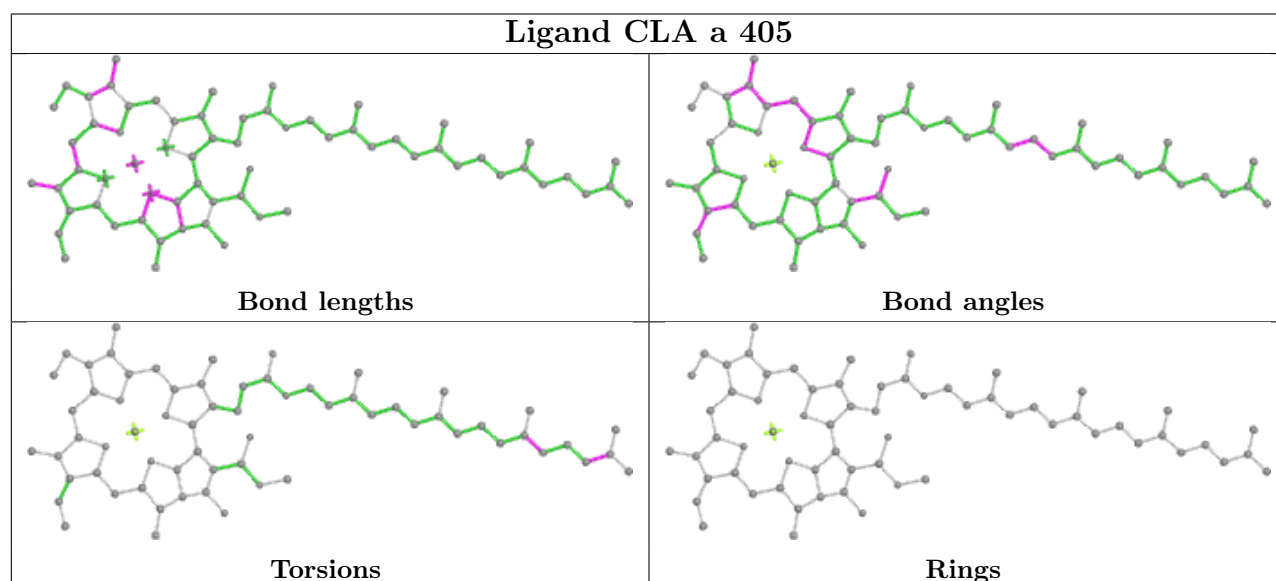
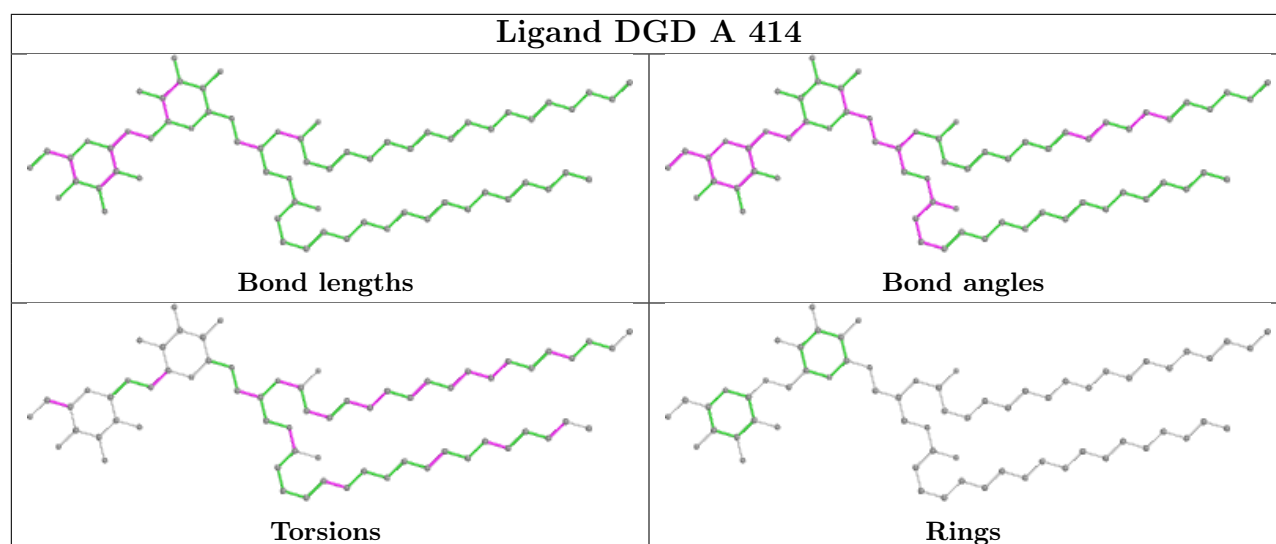
No monomer is involved in short contacts.

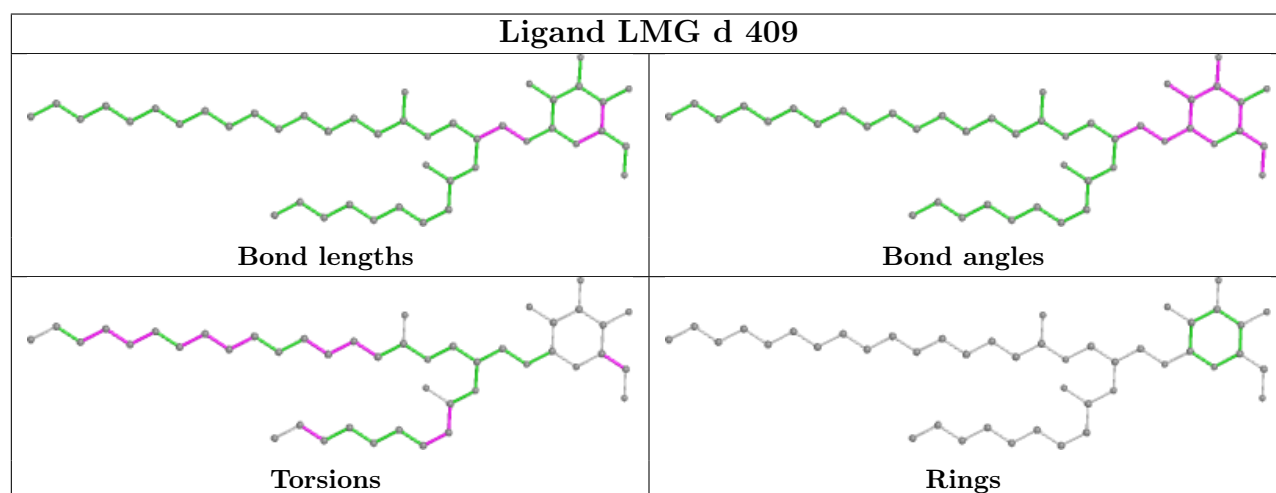
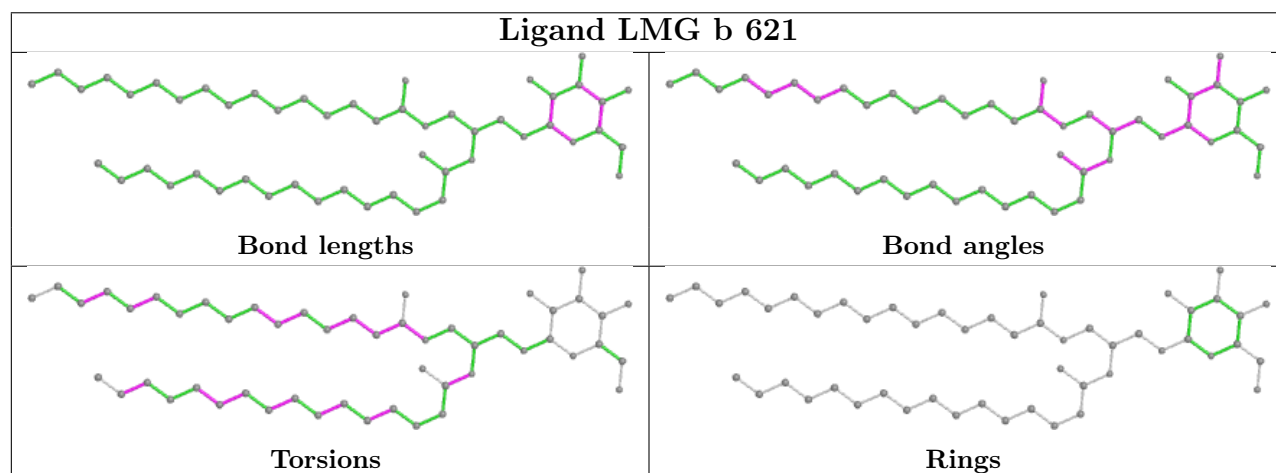
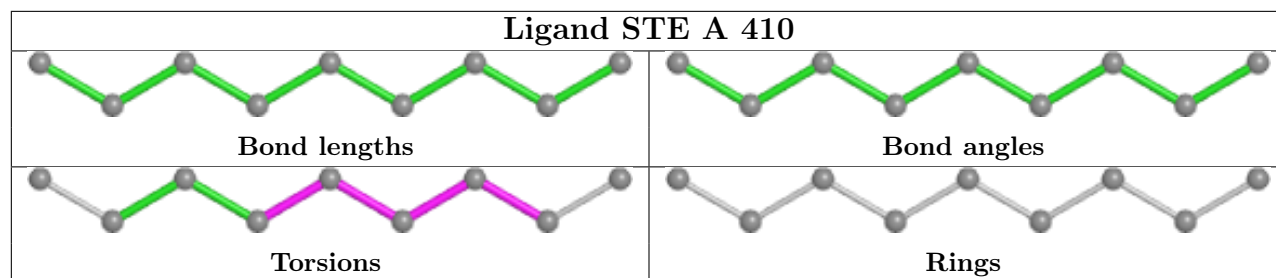
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

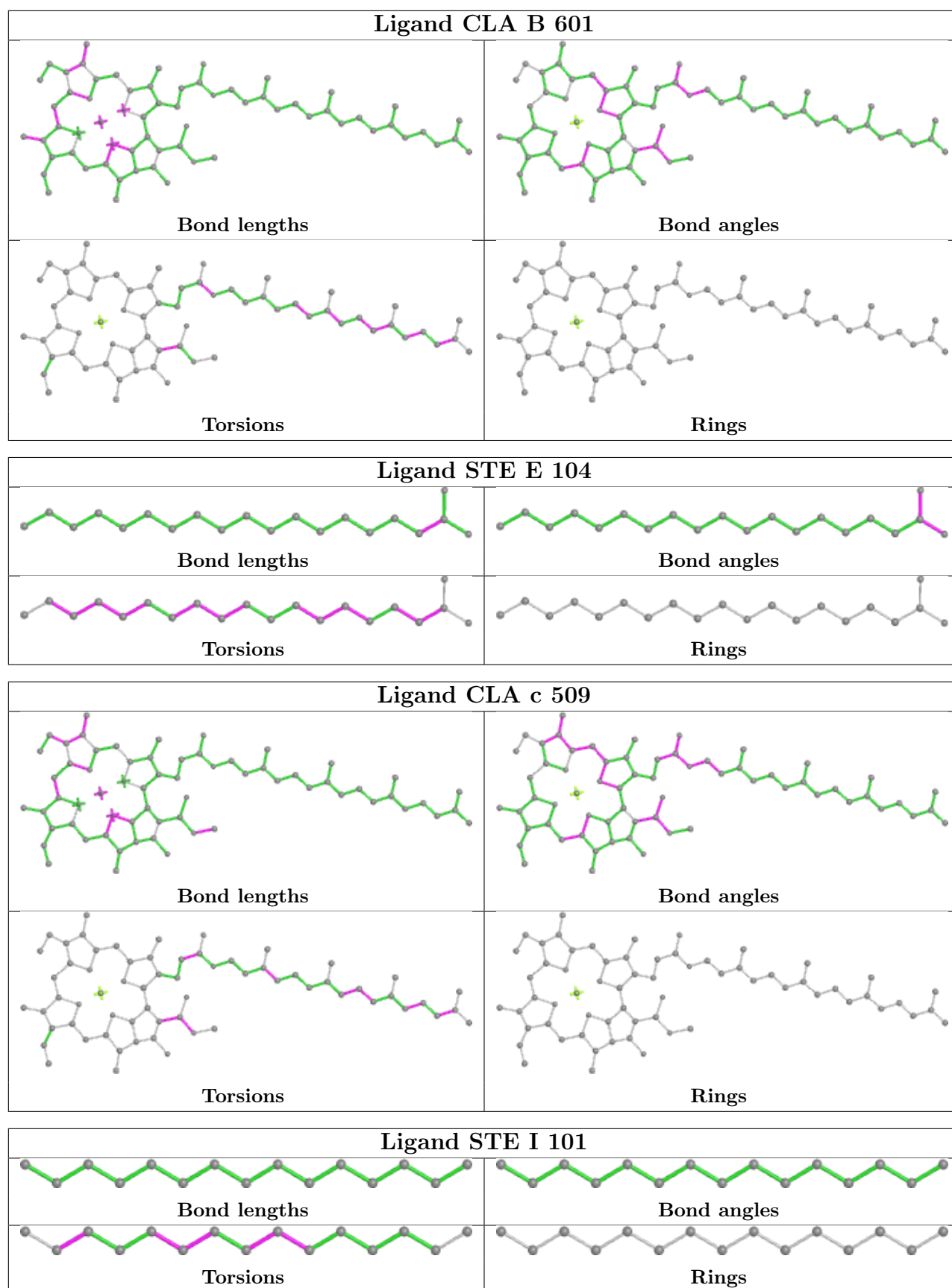


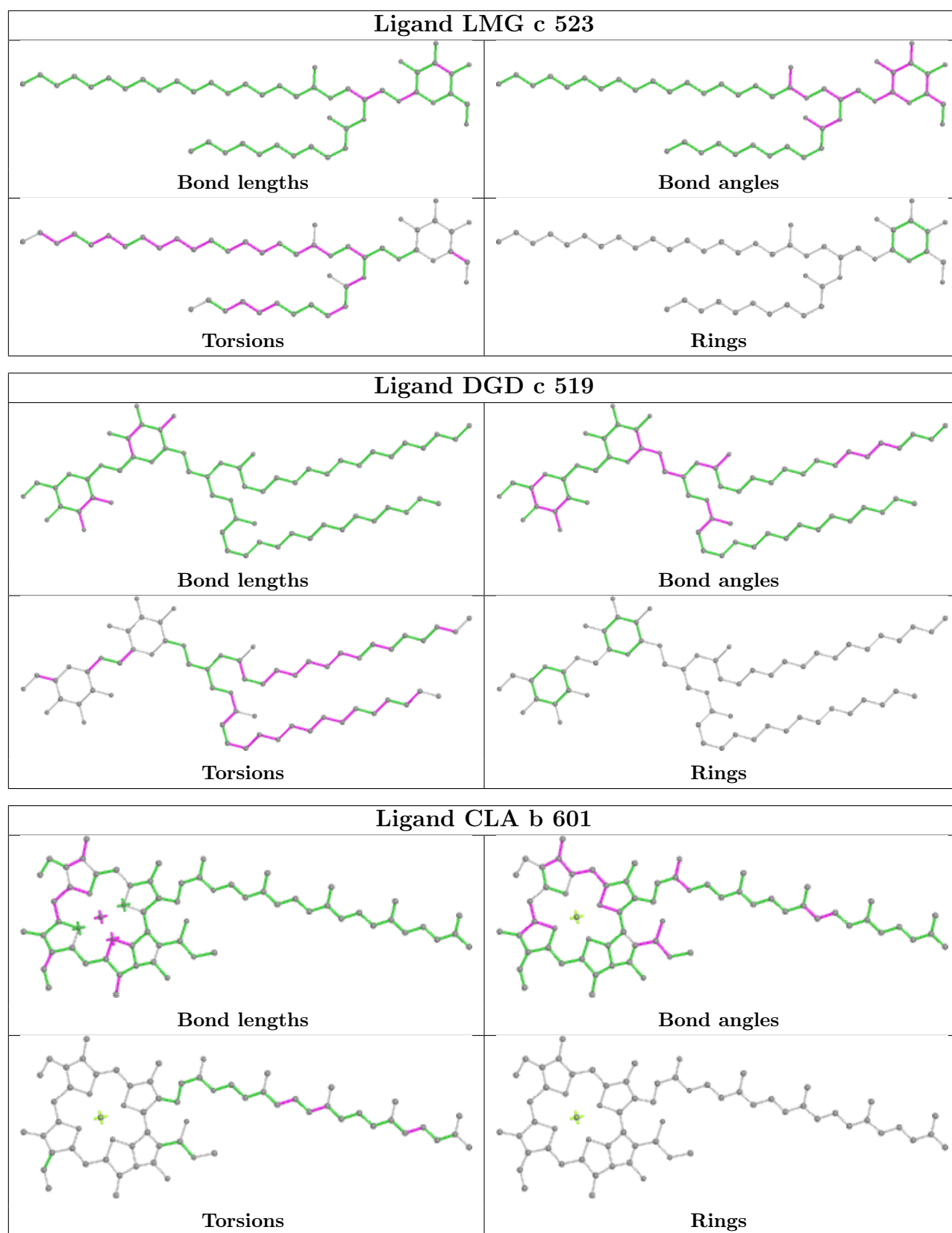


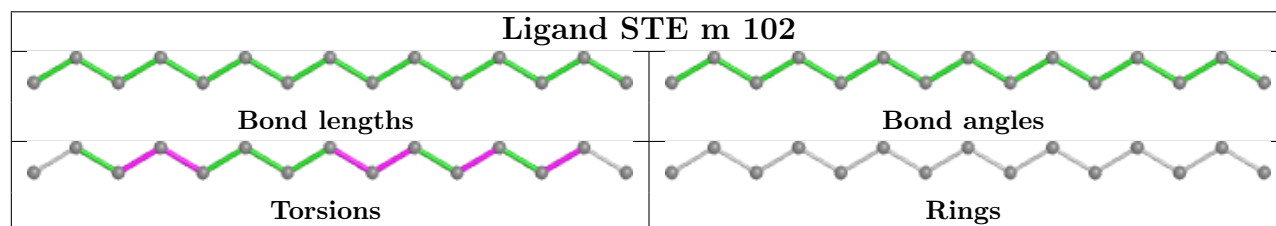
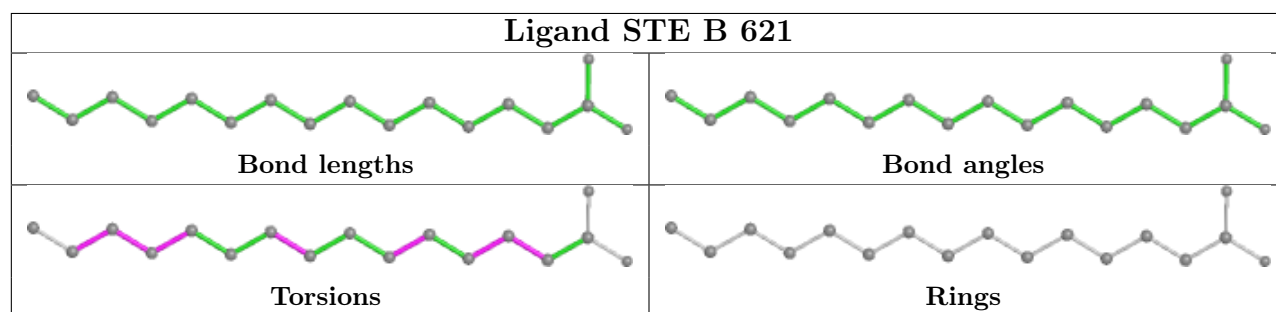
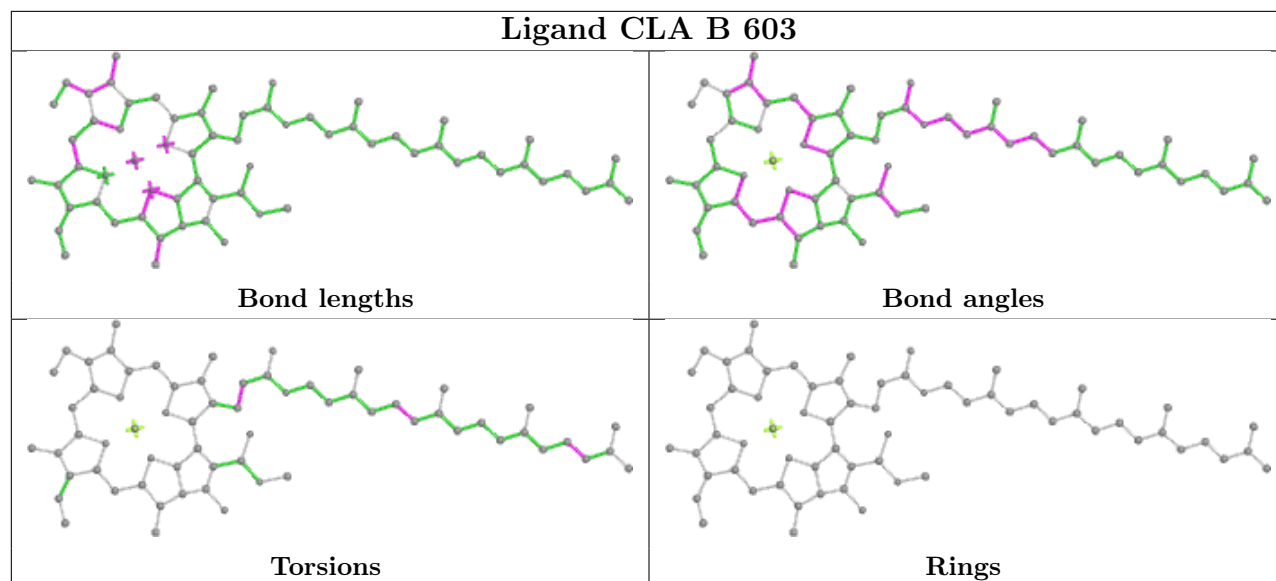
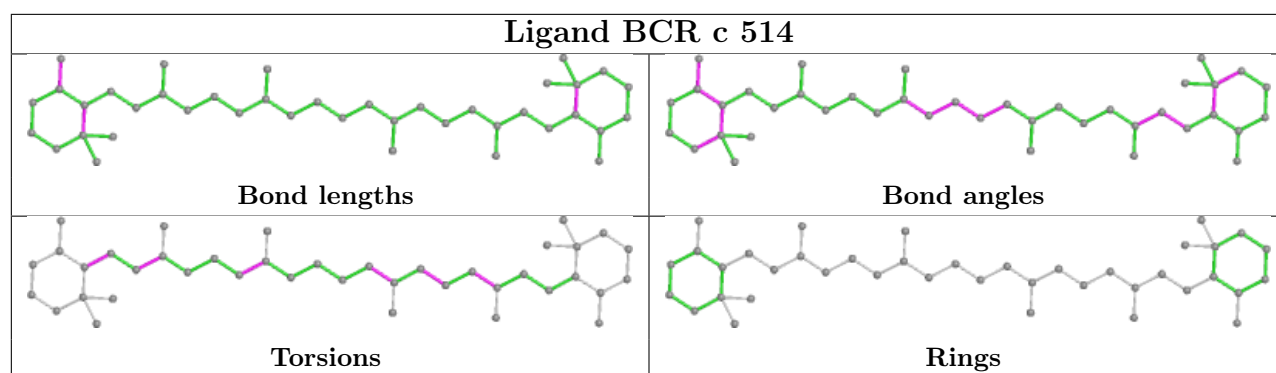




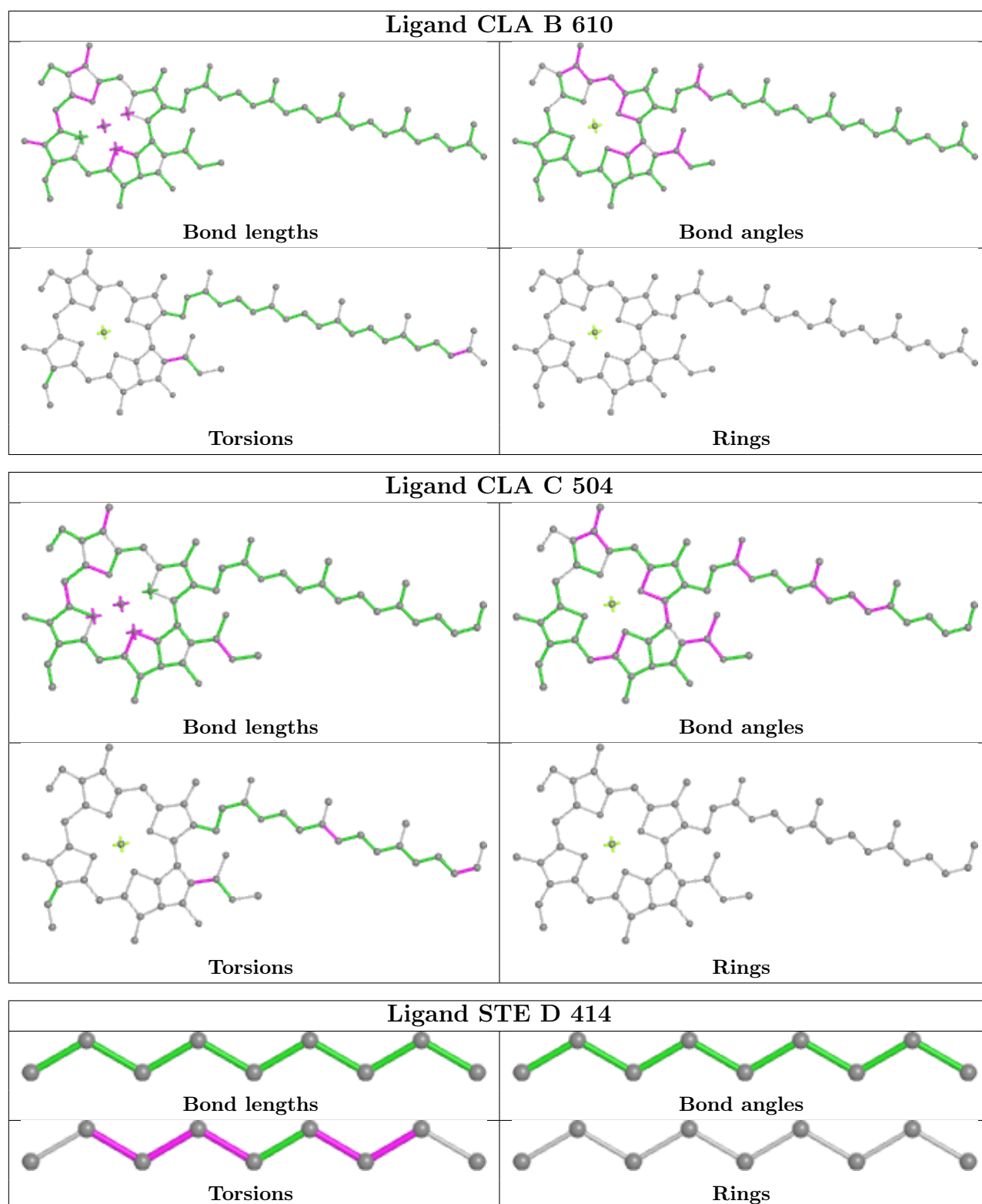


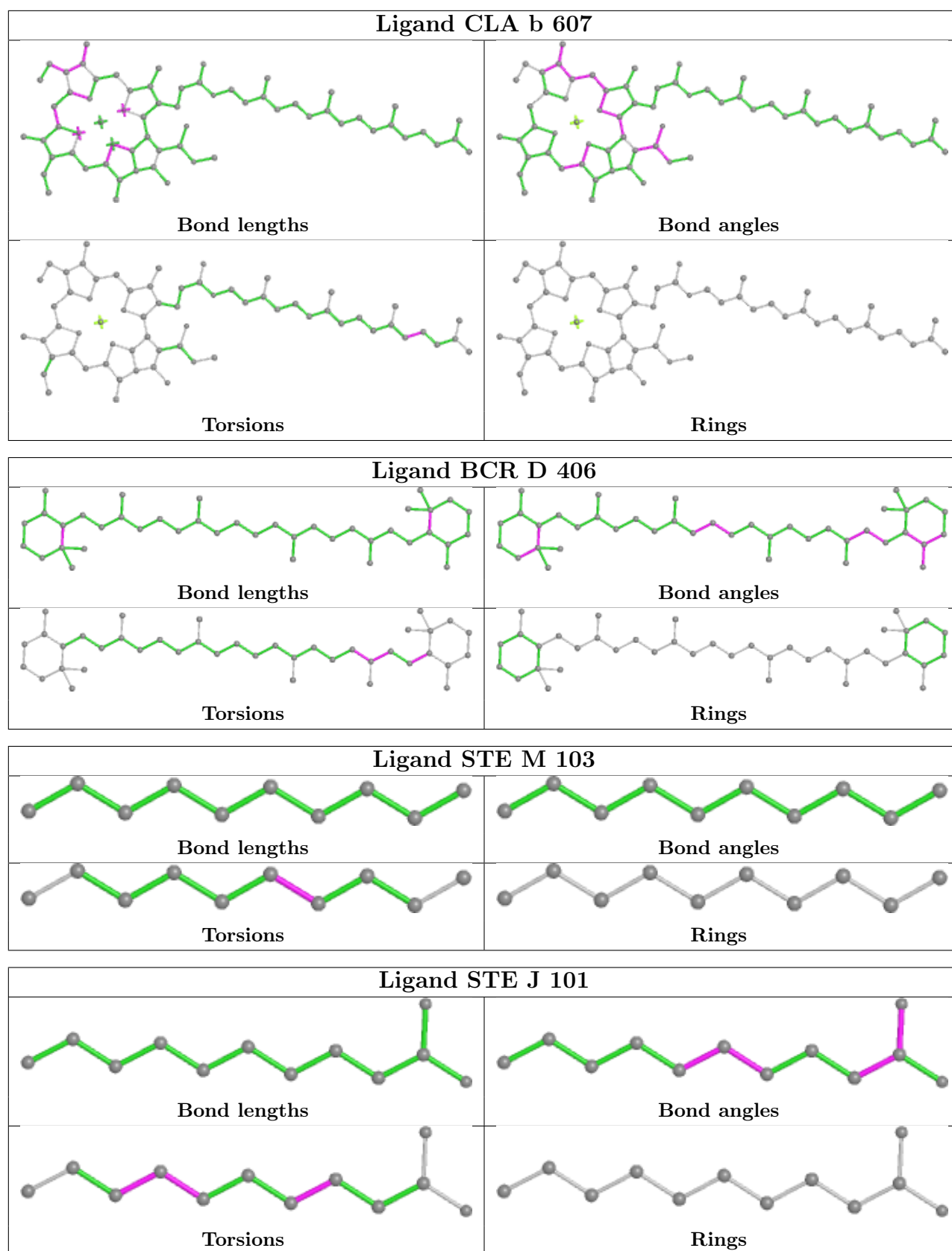


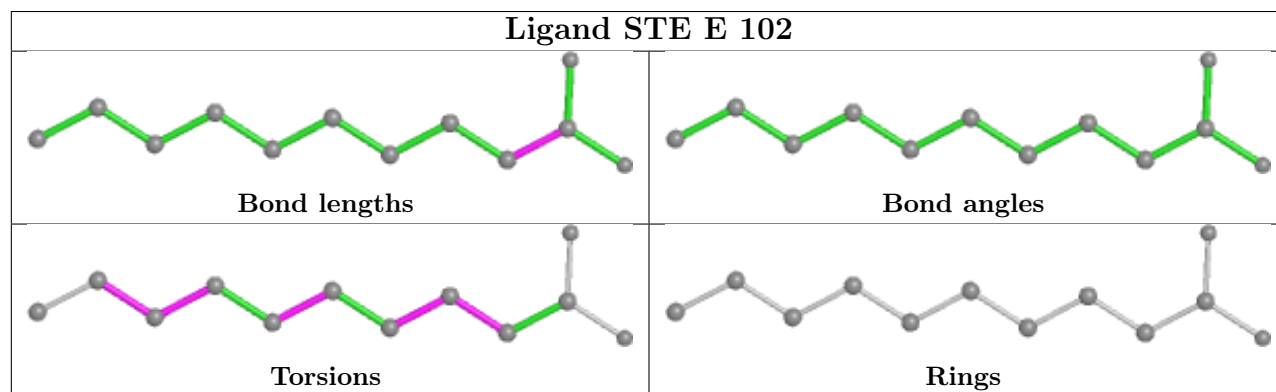
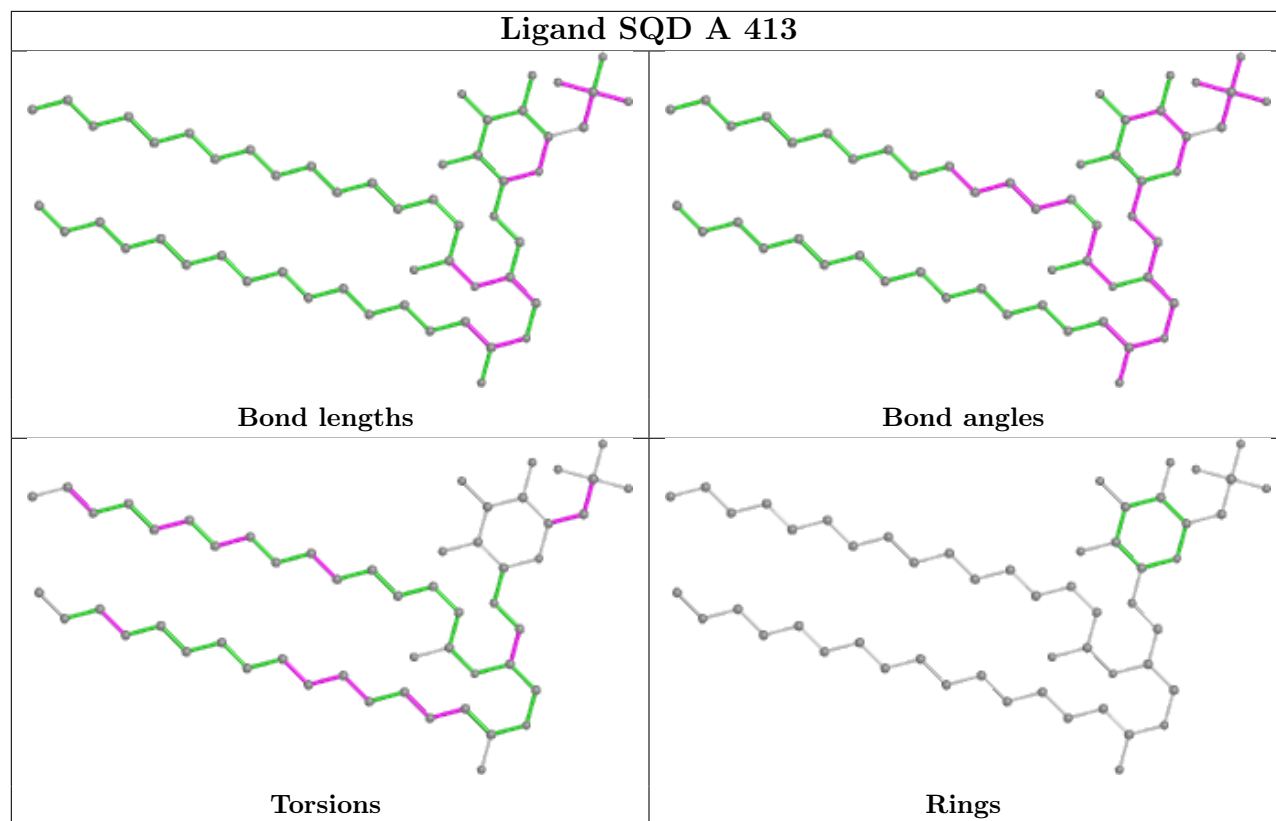
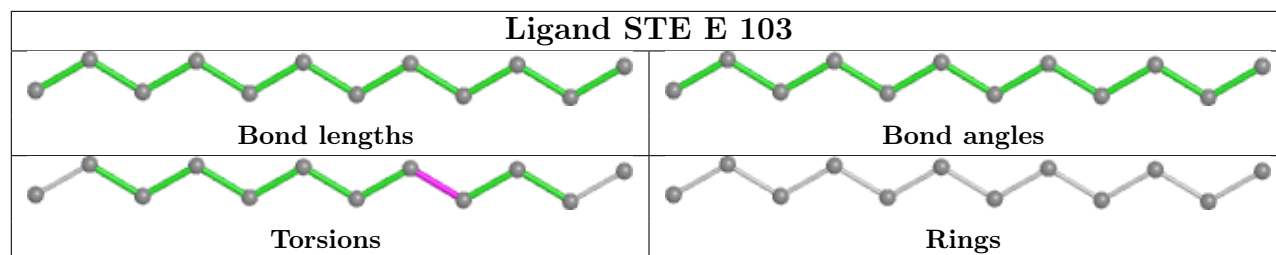


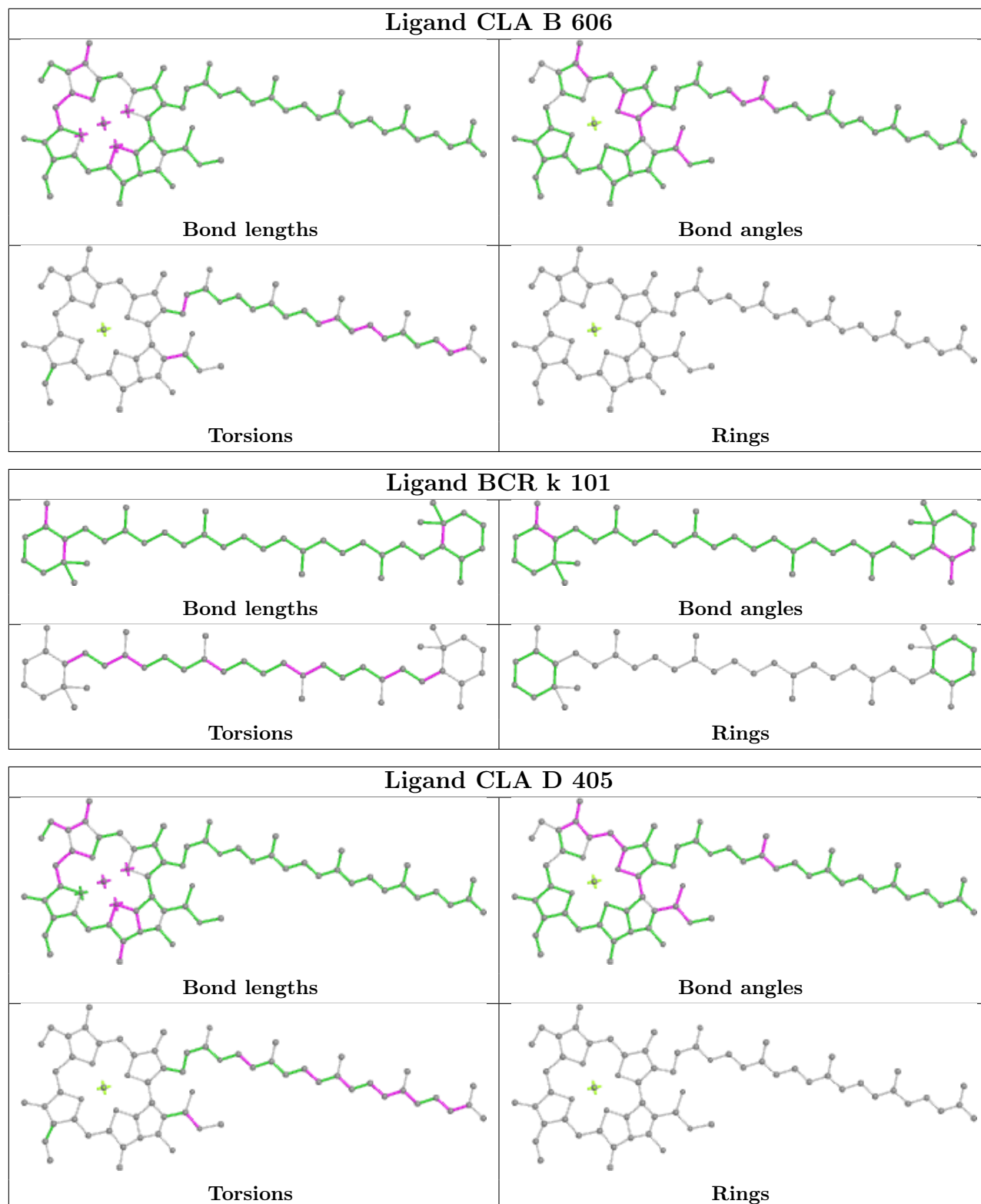


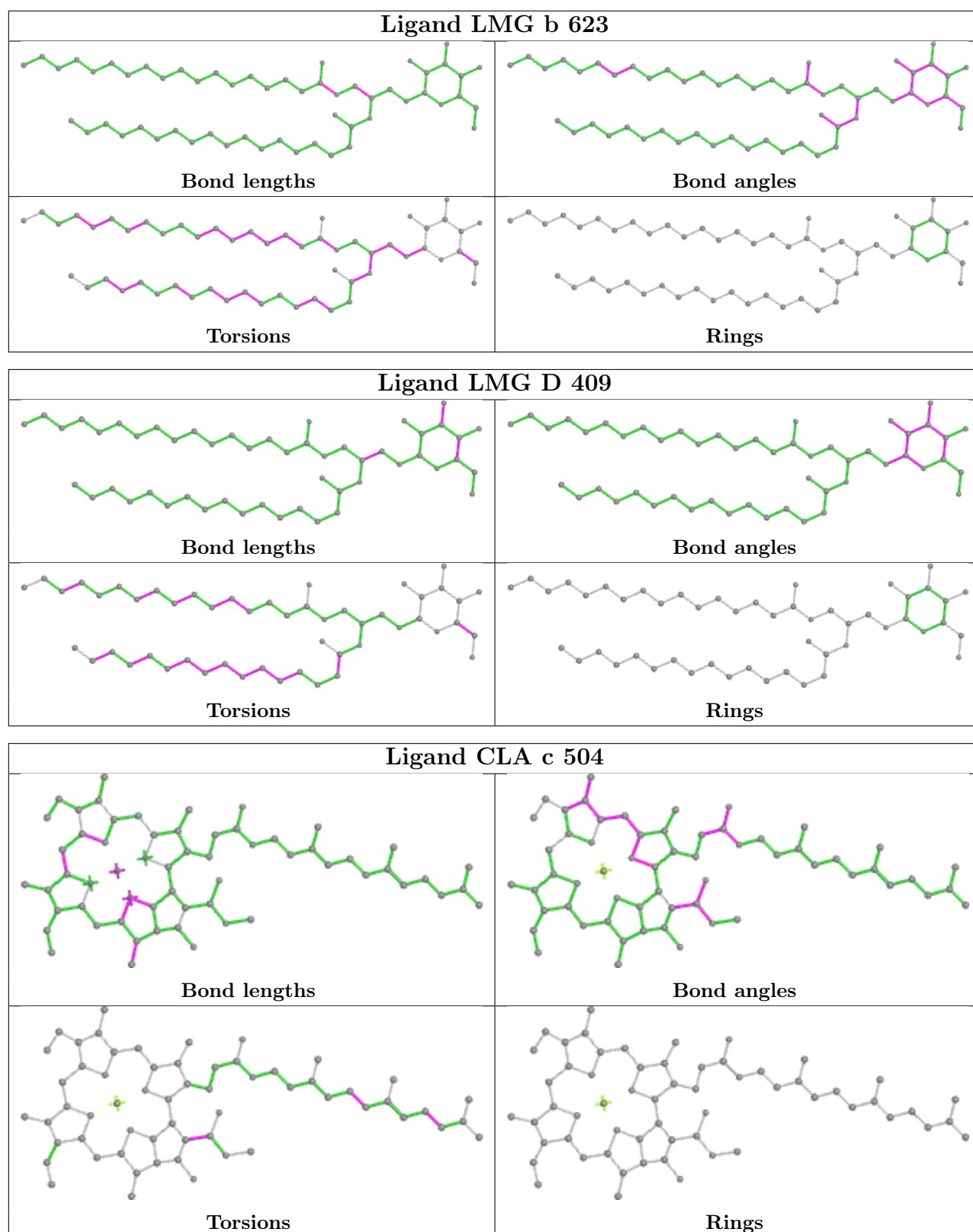


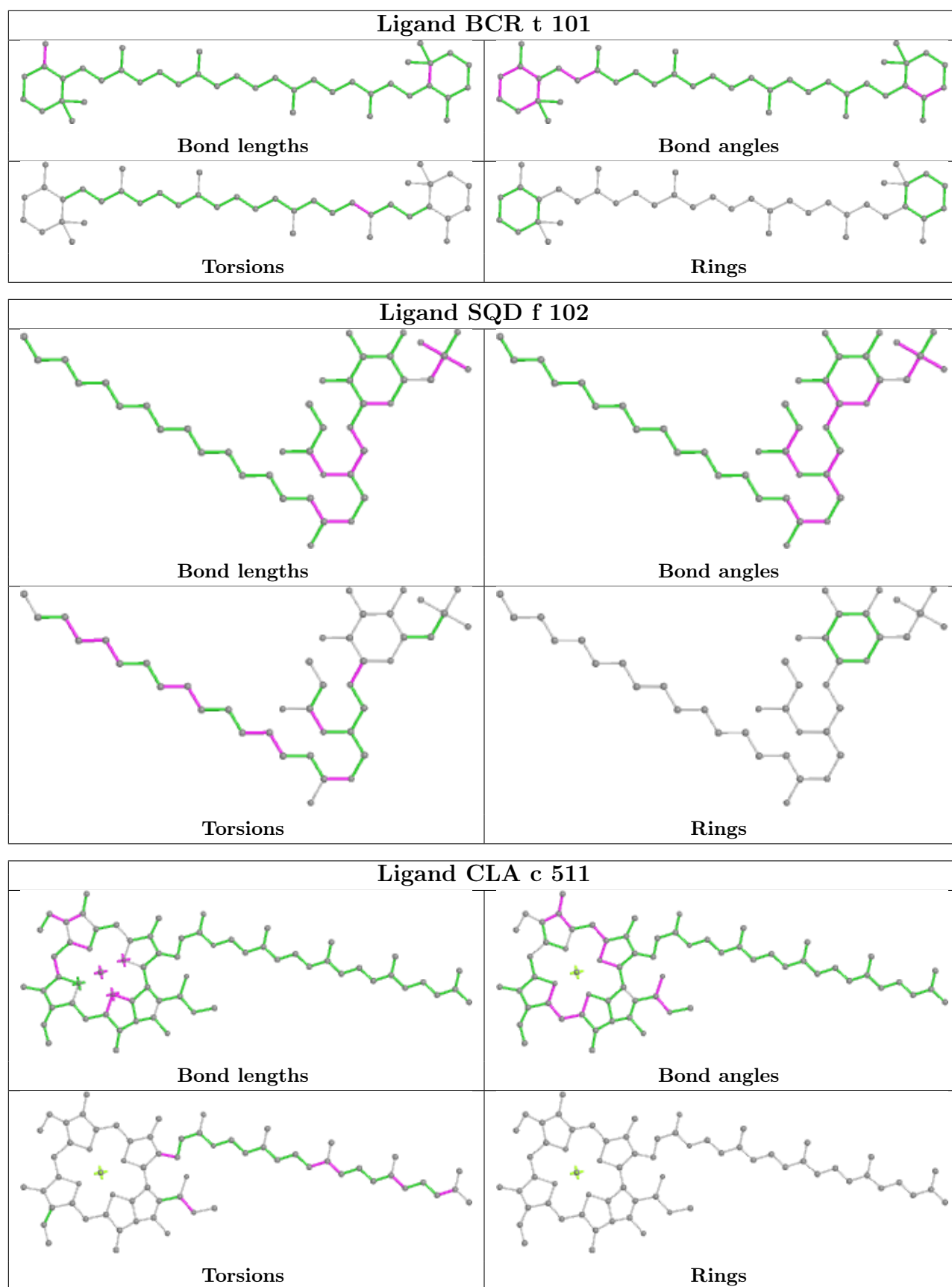


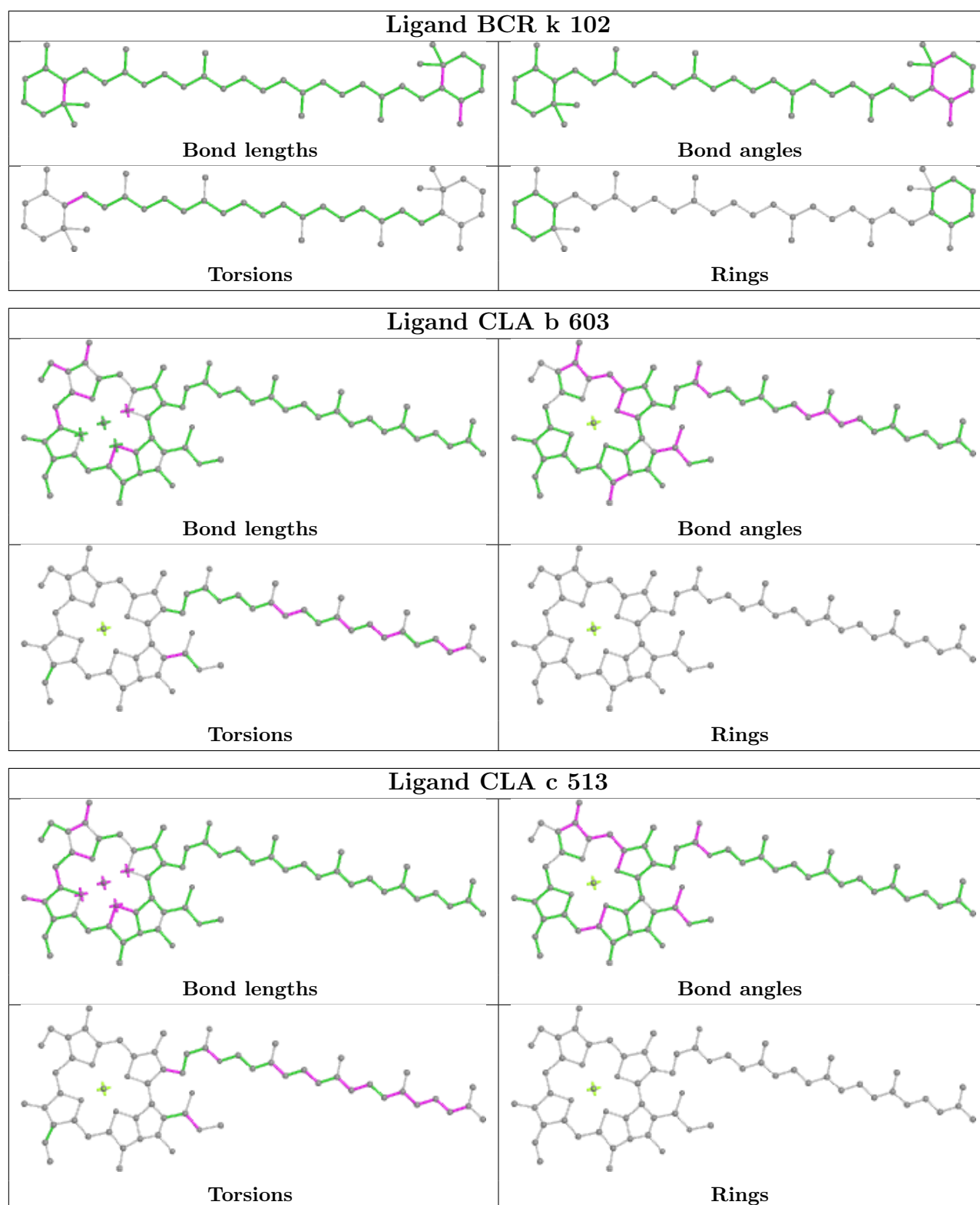


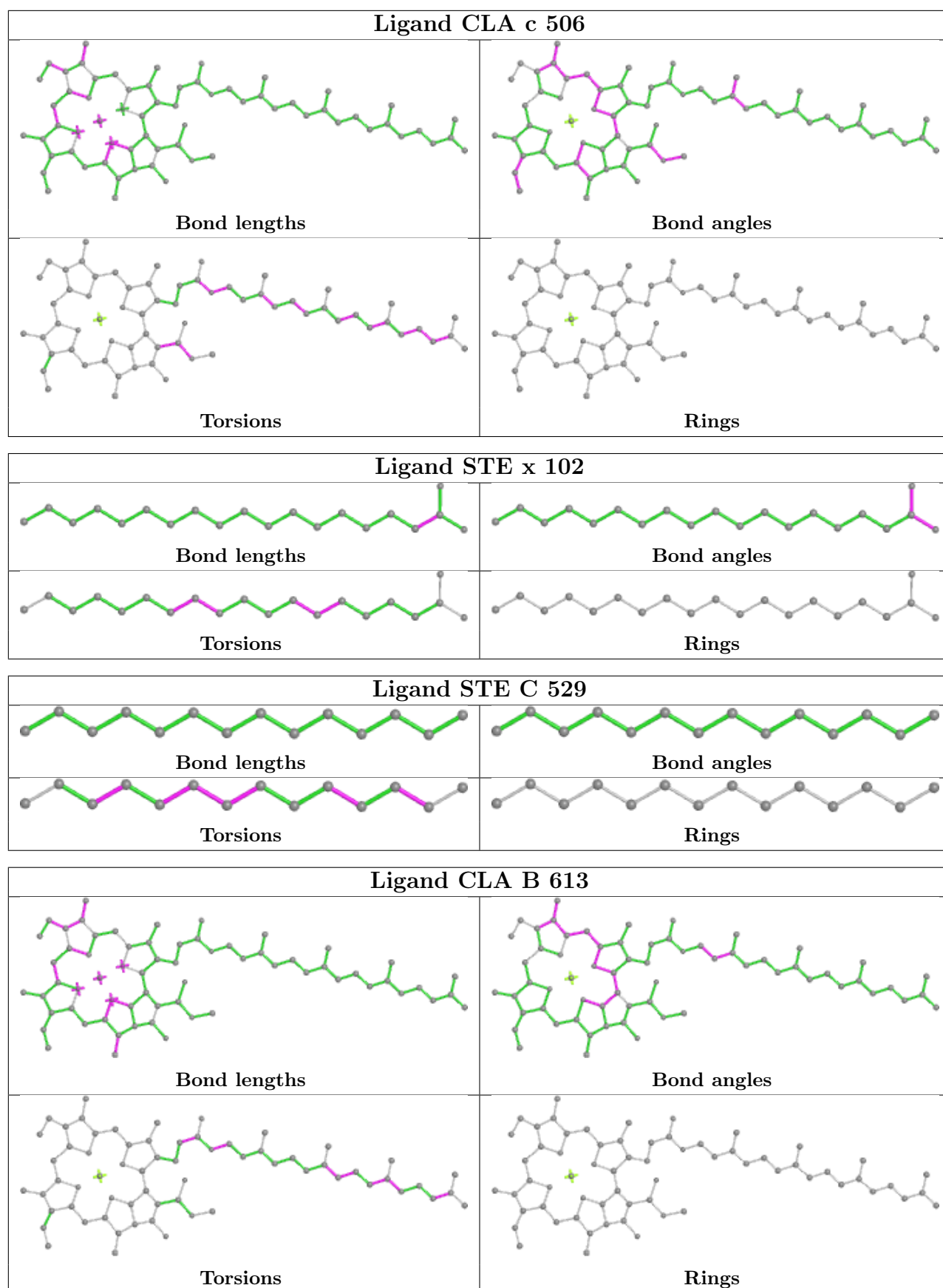




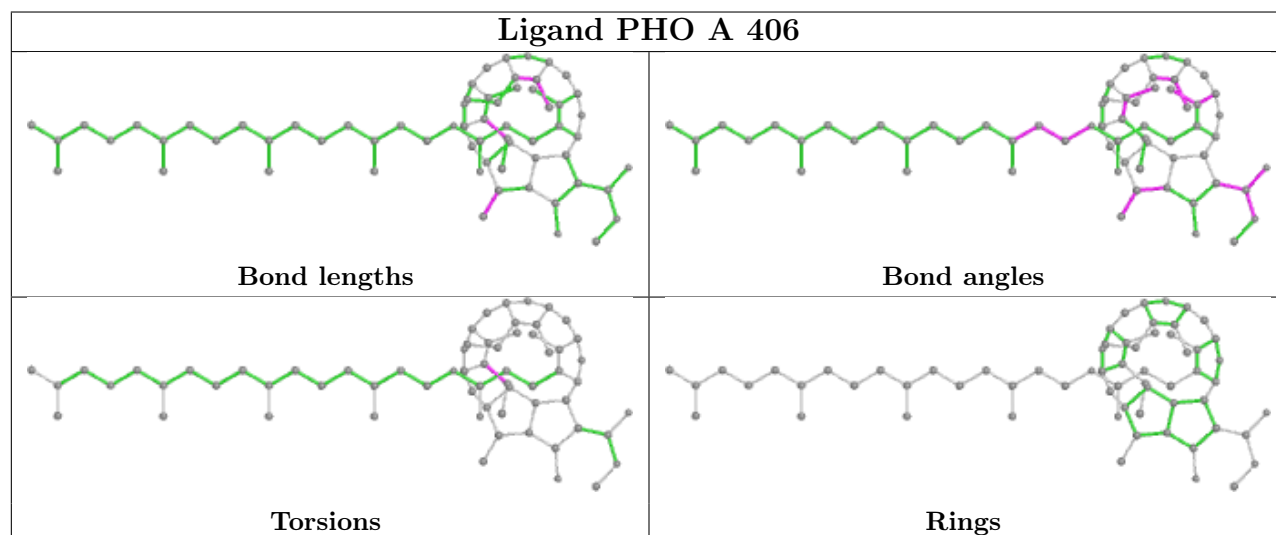
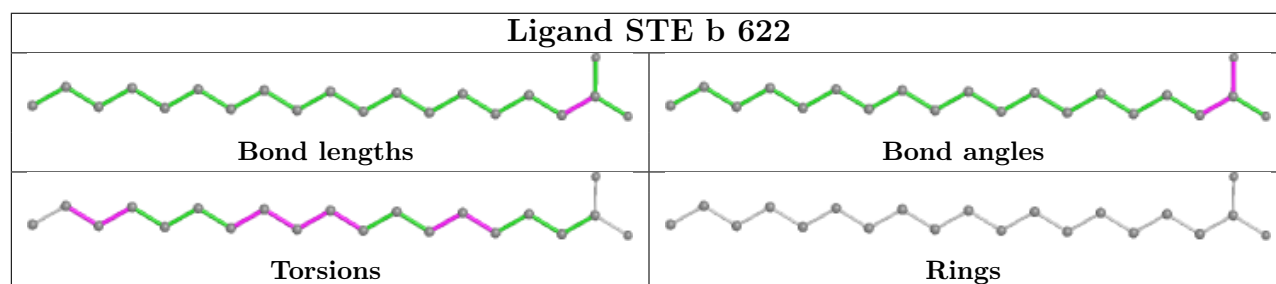
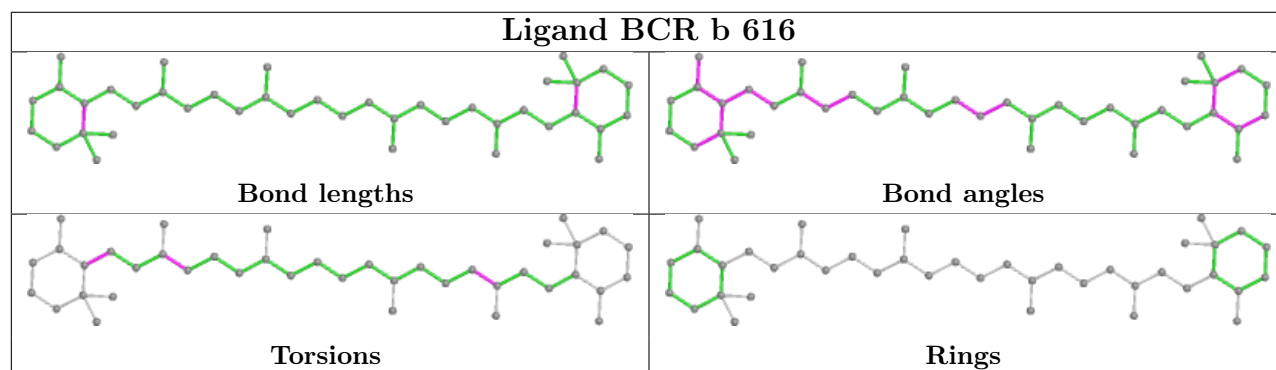
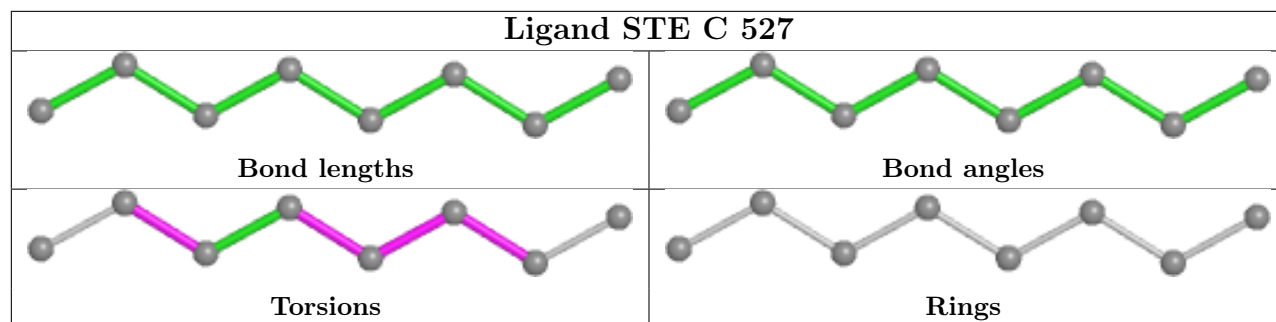


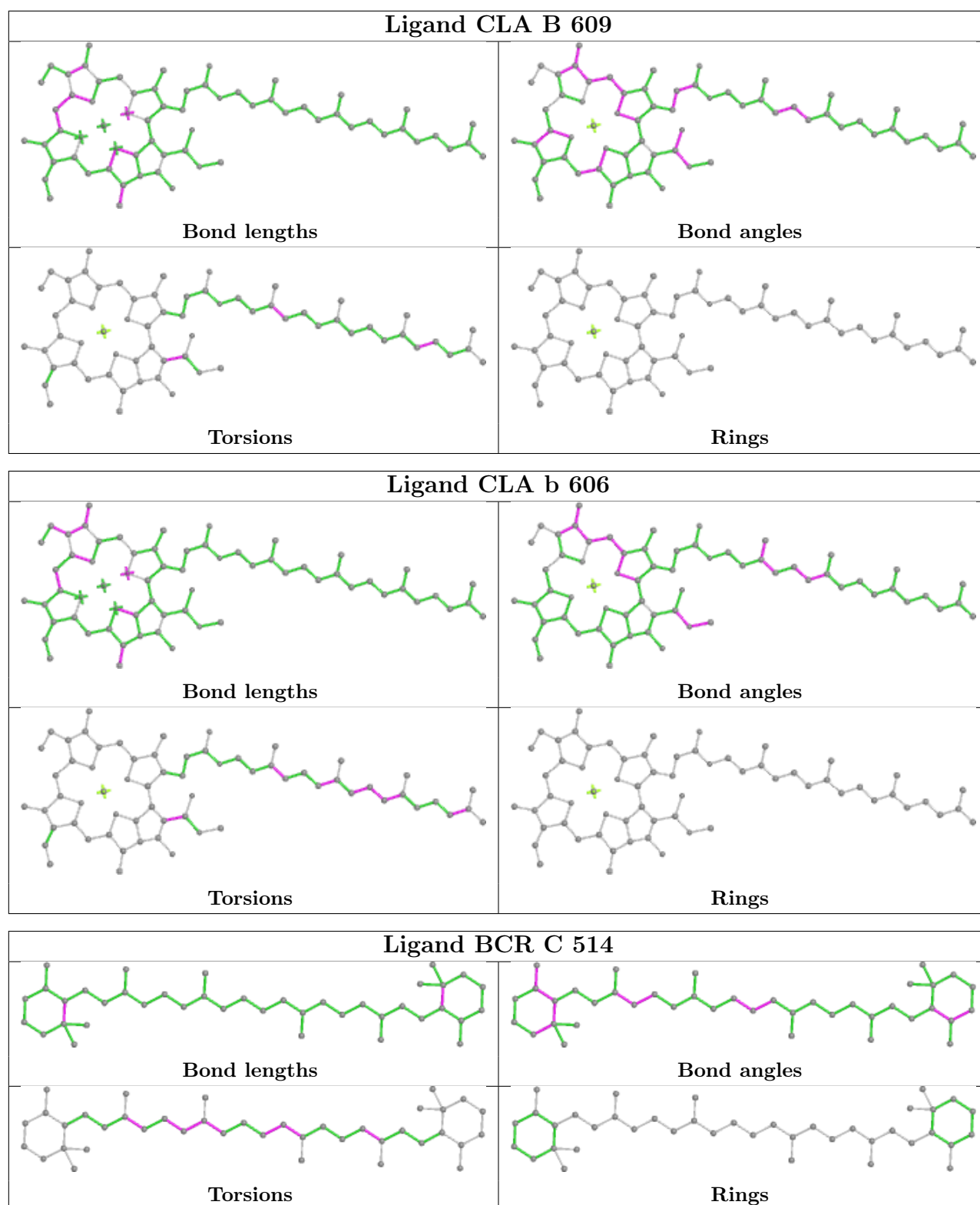


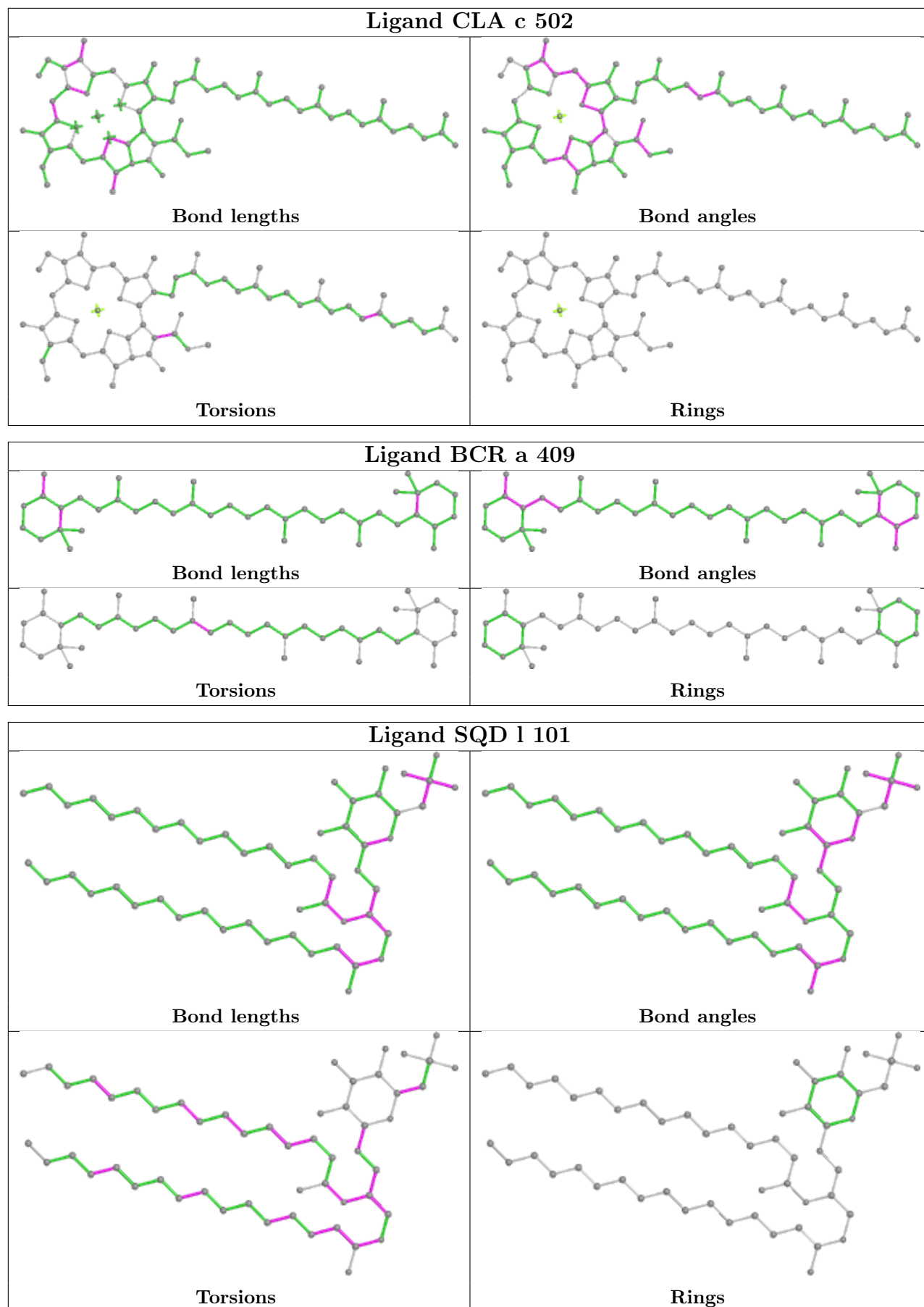


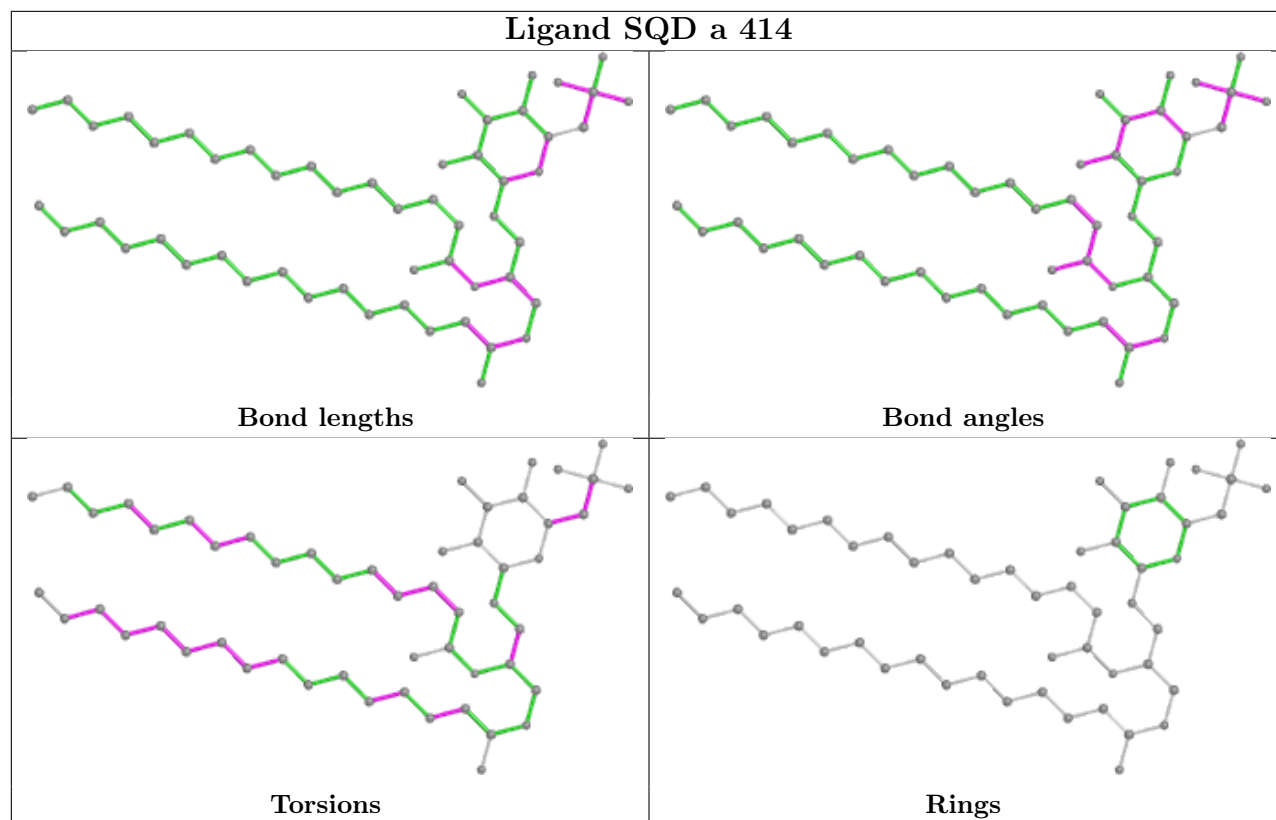


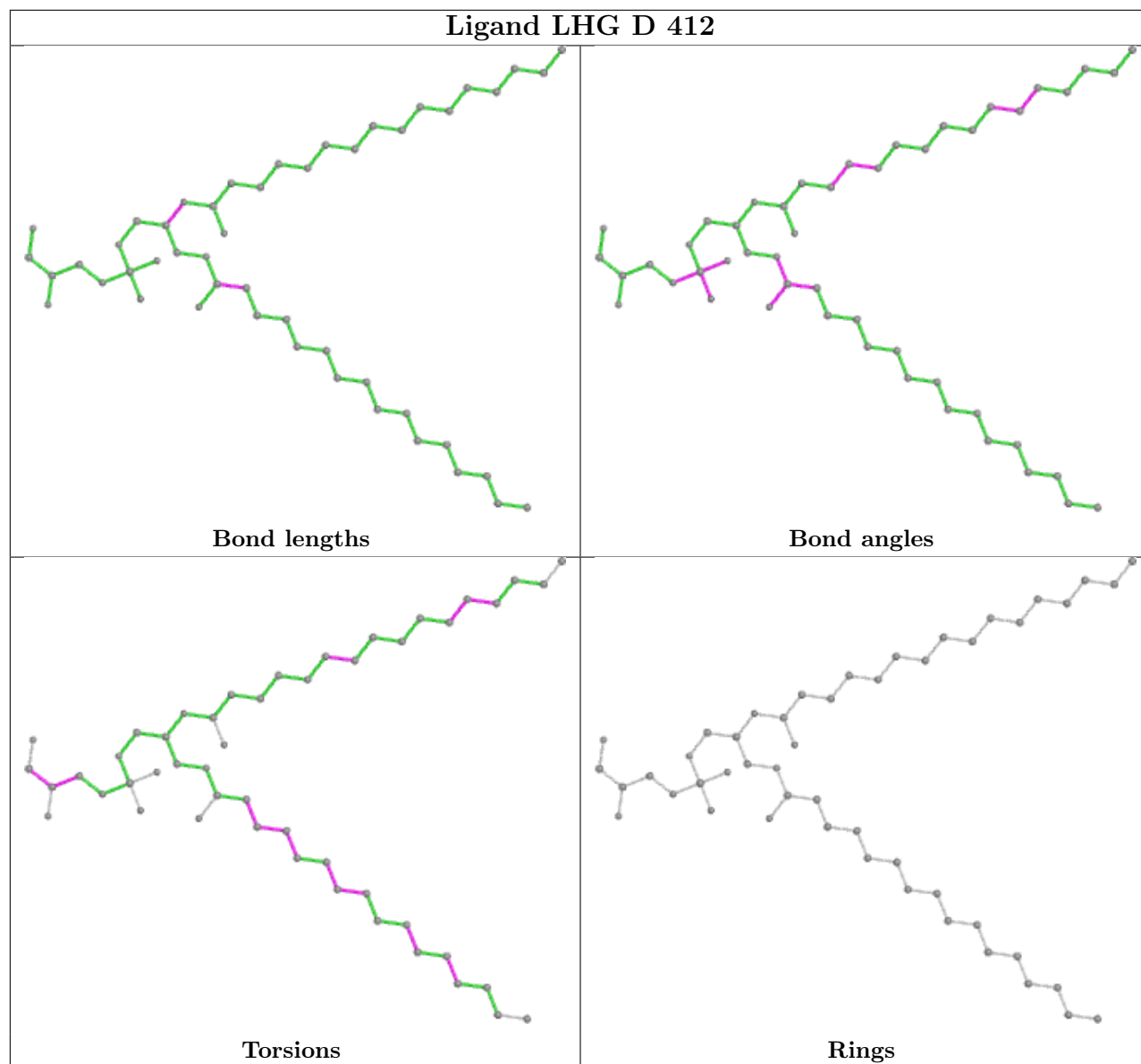


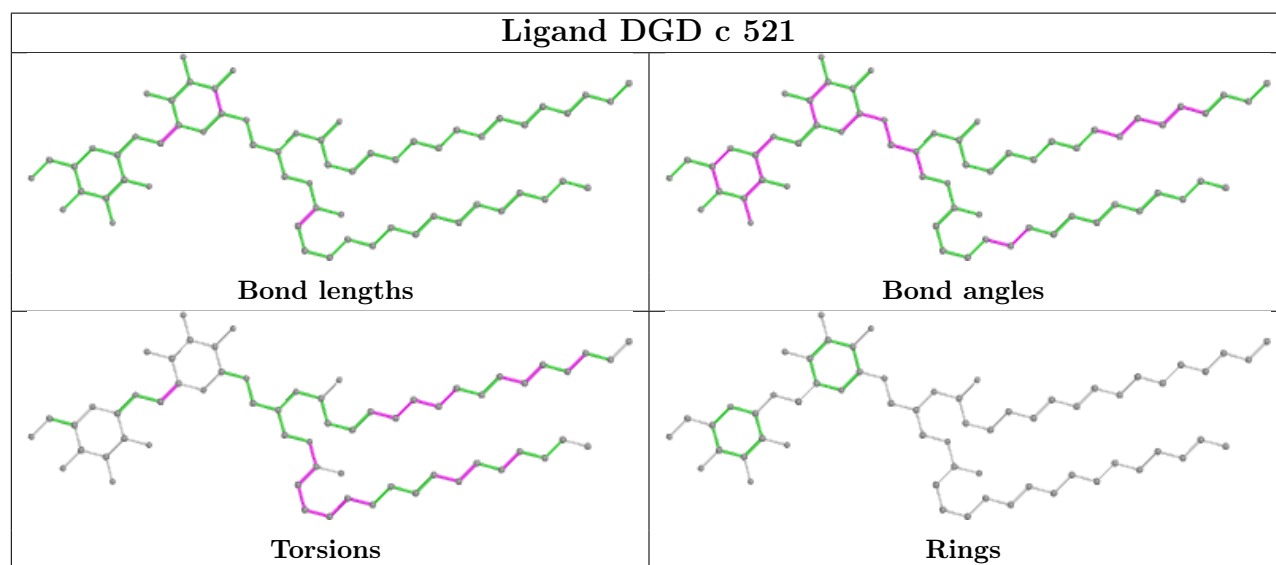
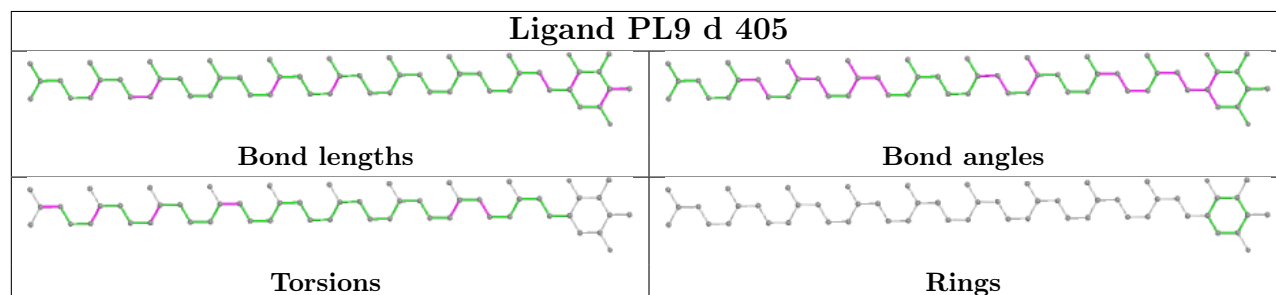
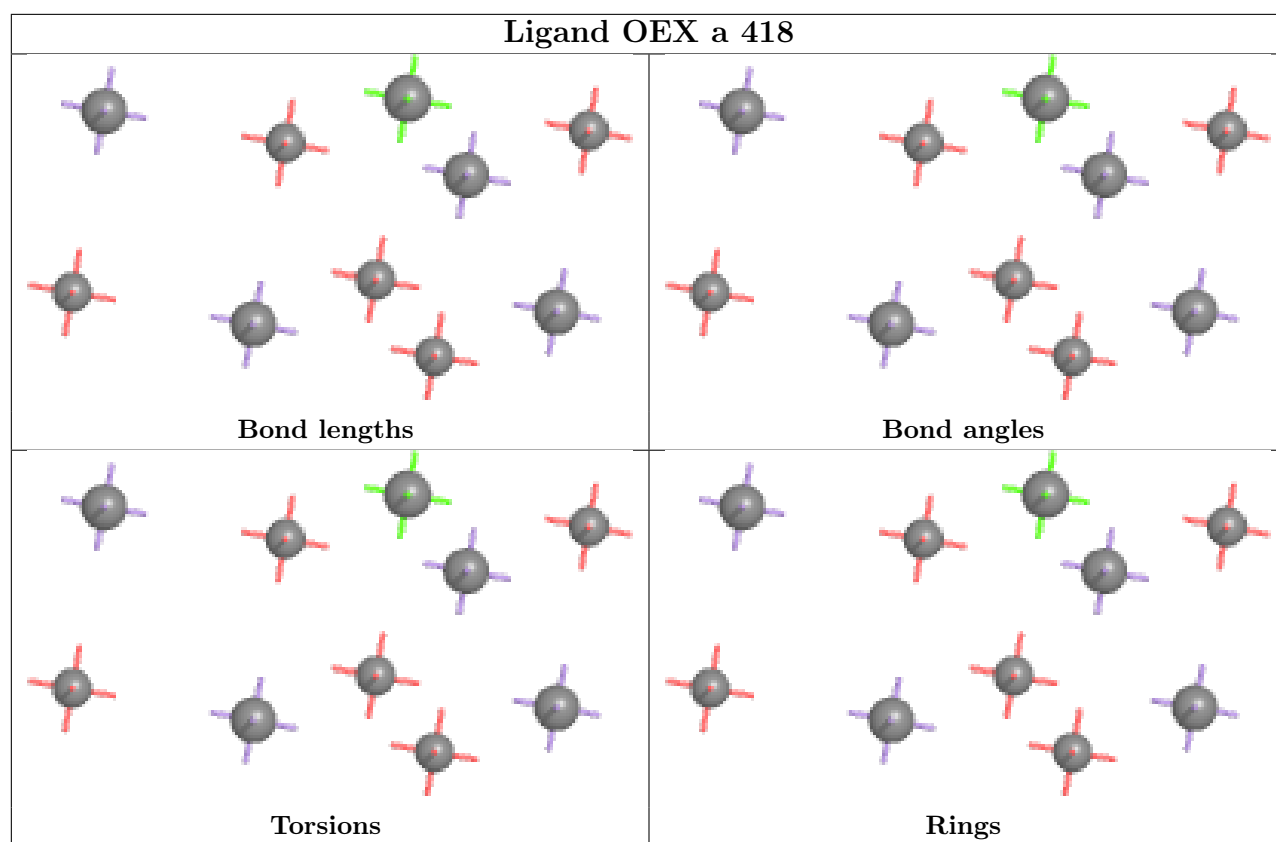


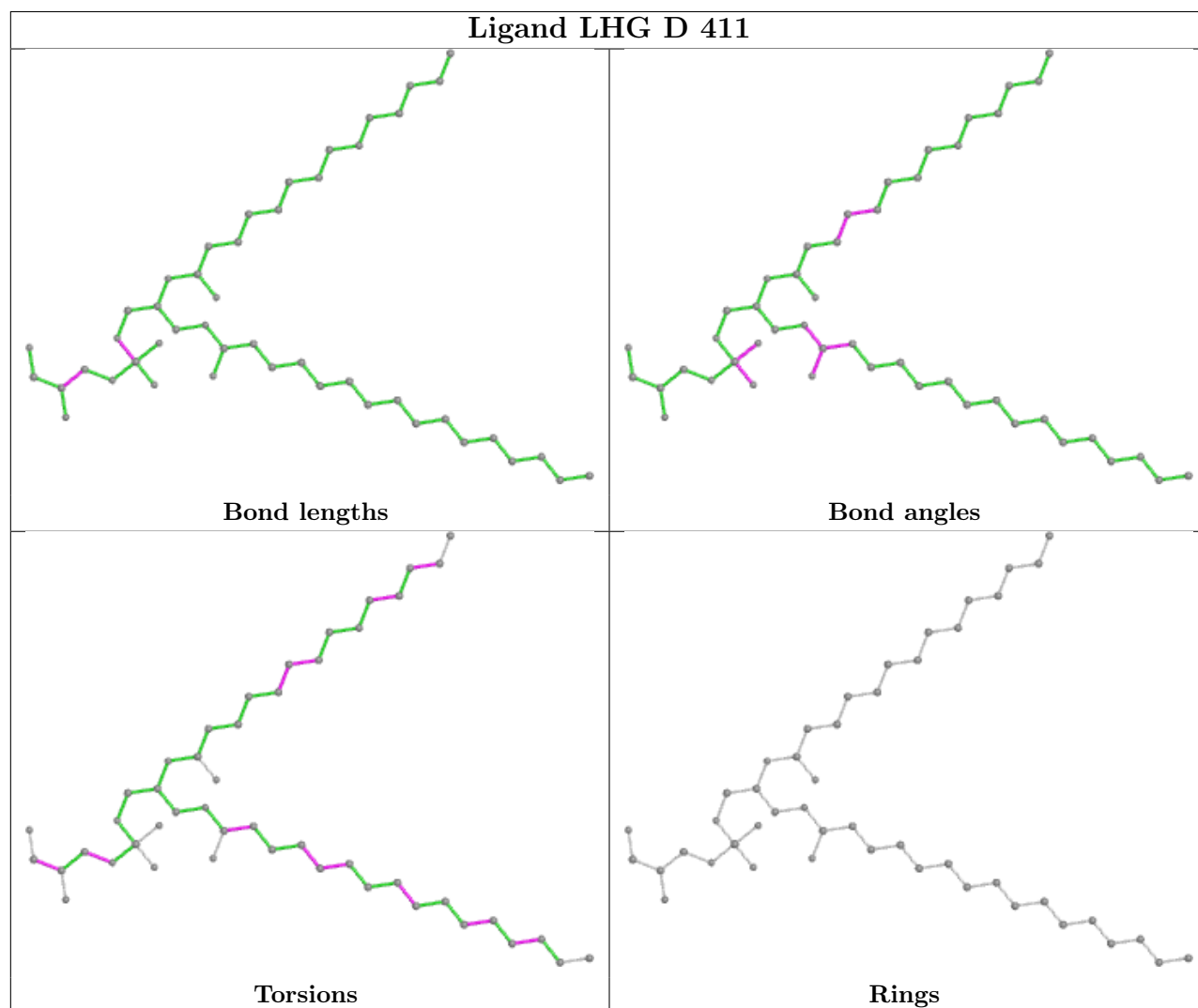
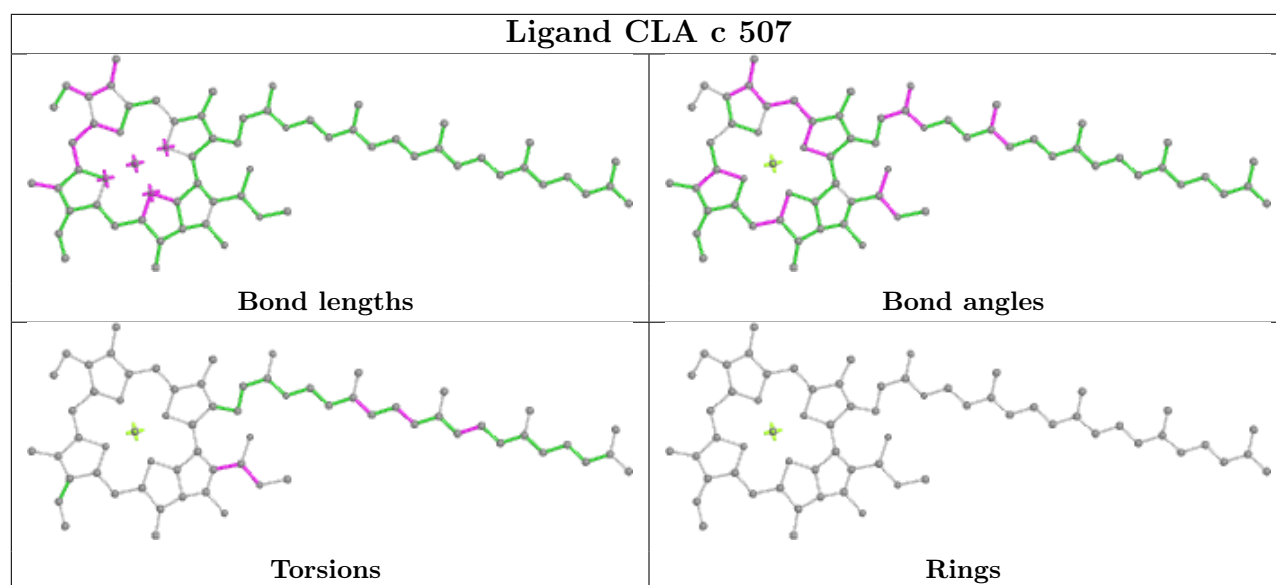


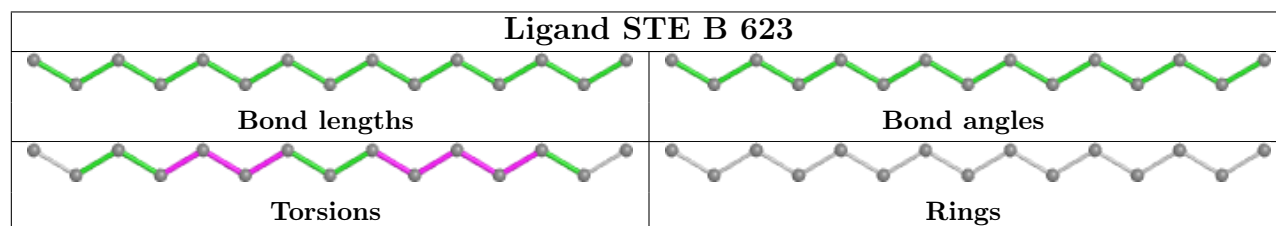
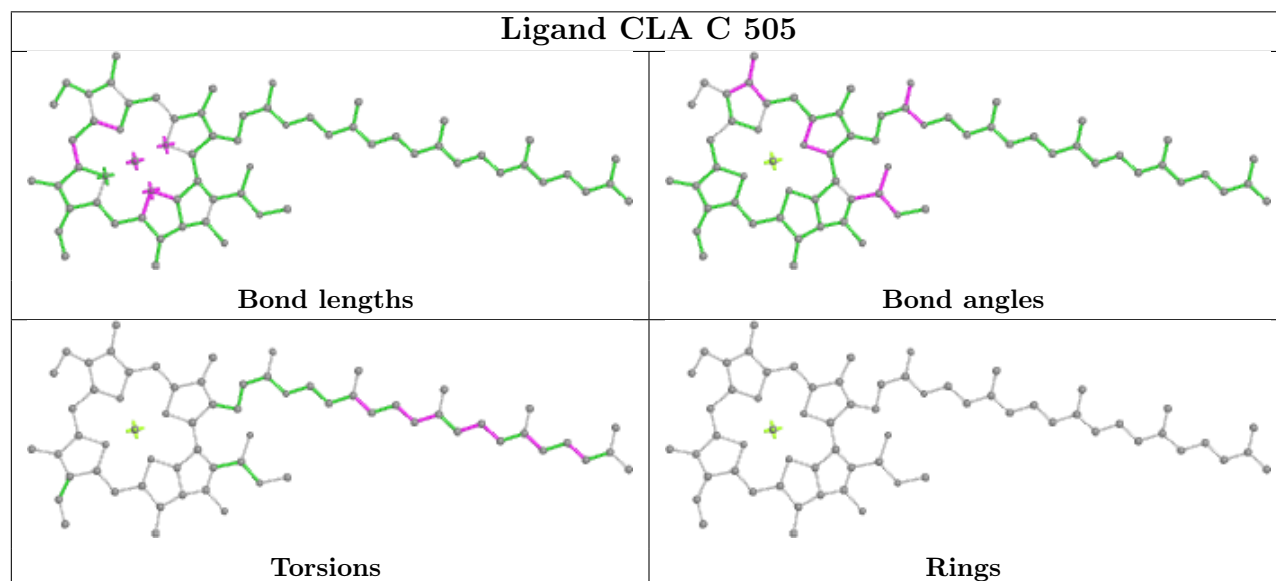
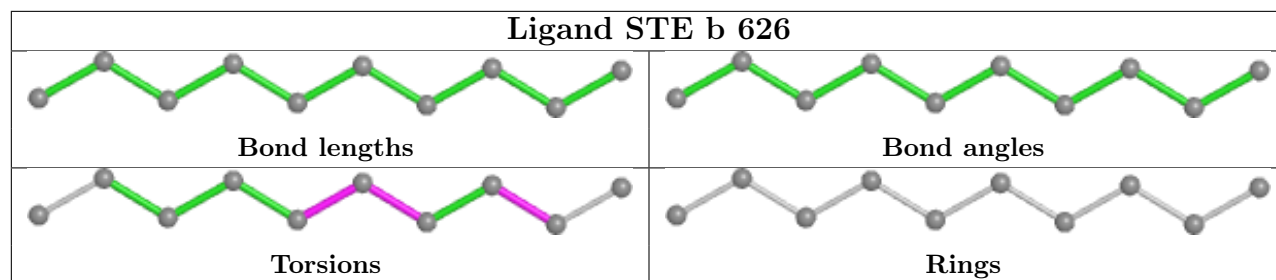




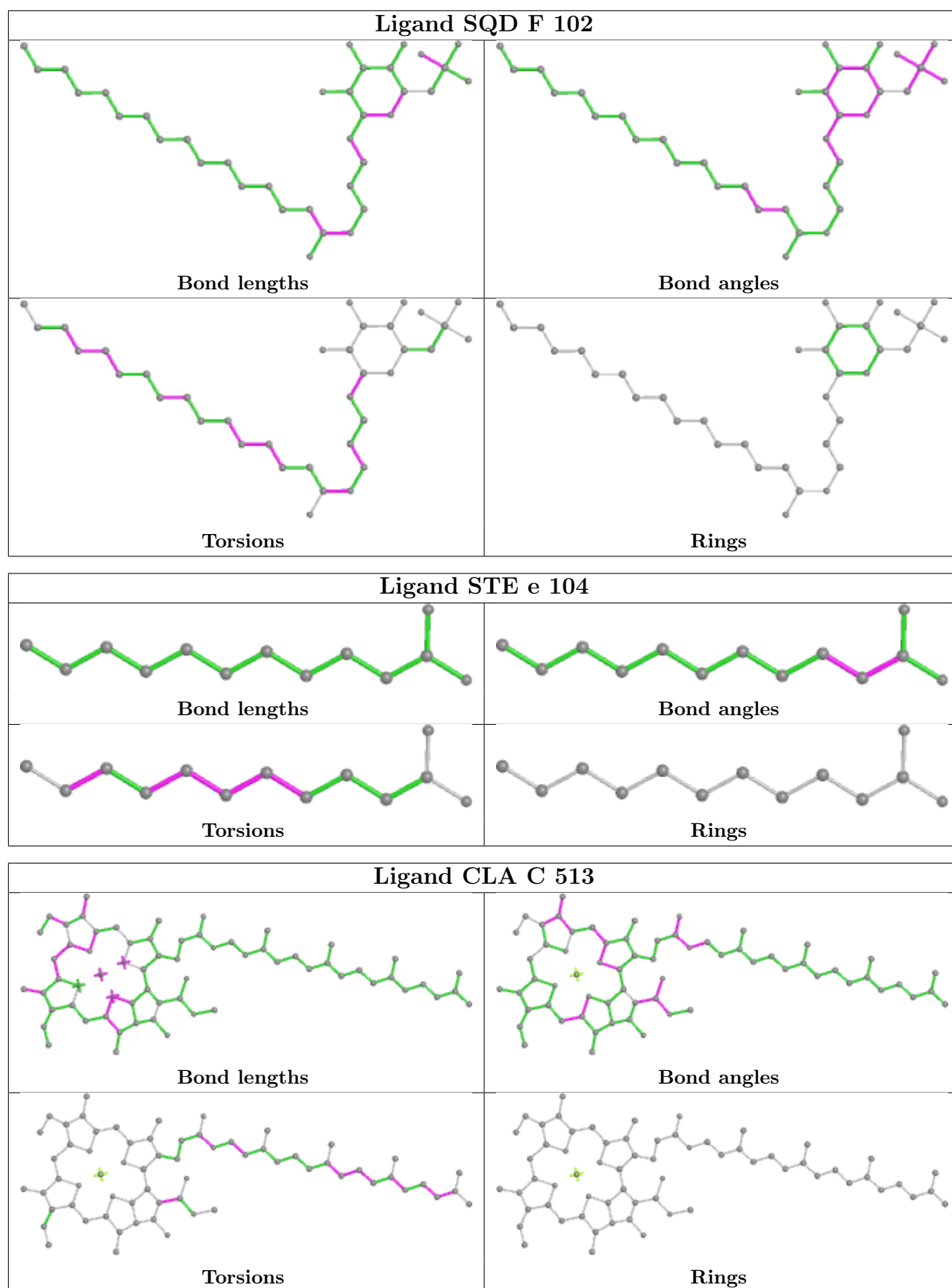


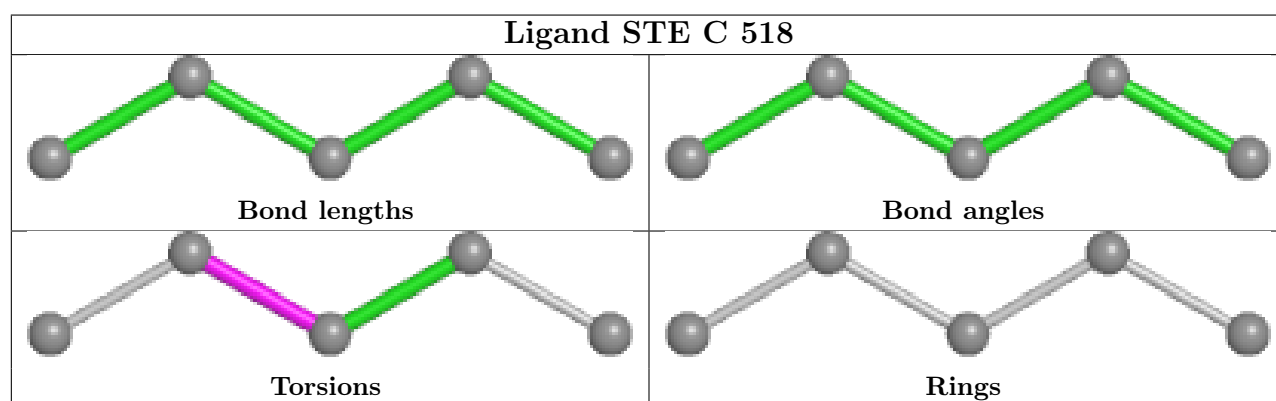
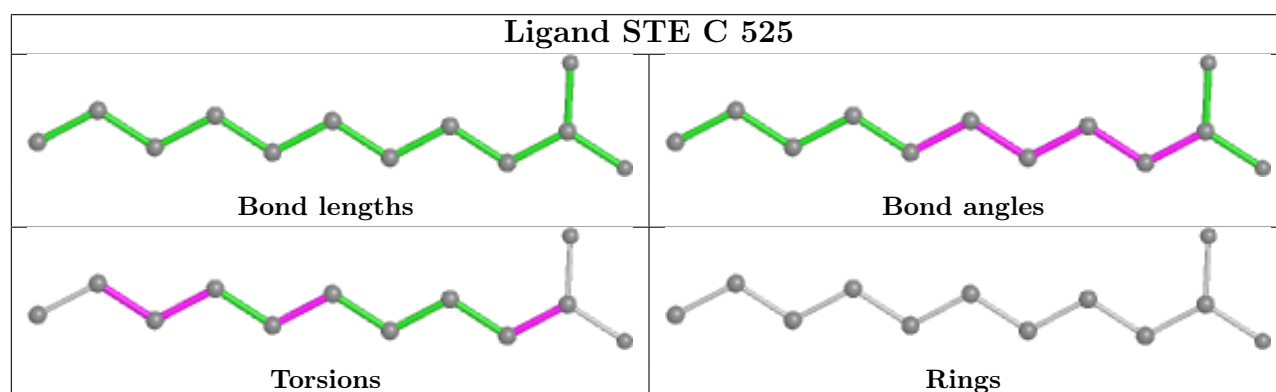
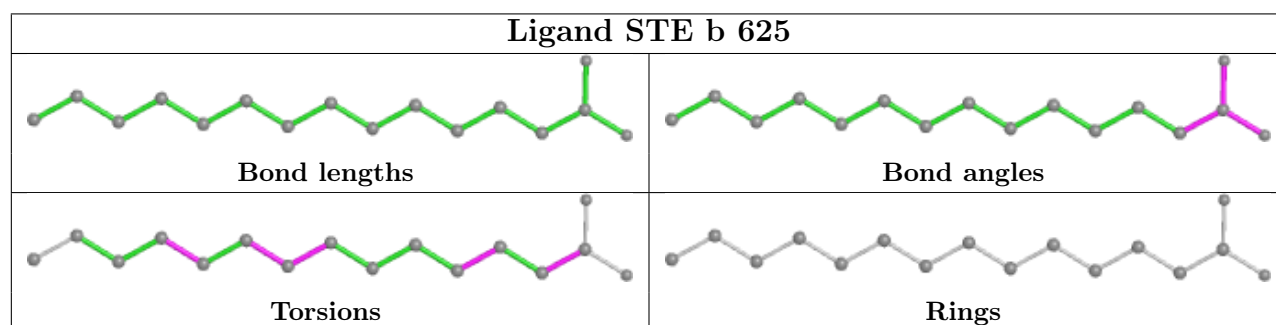
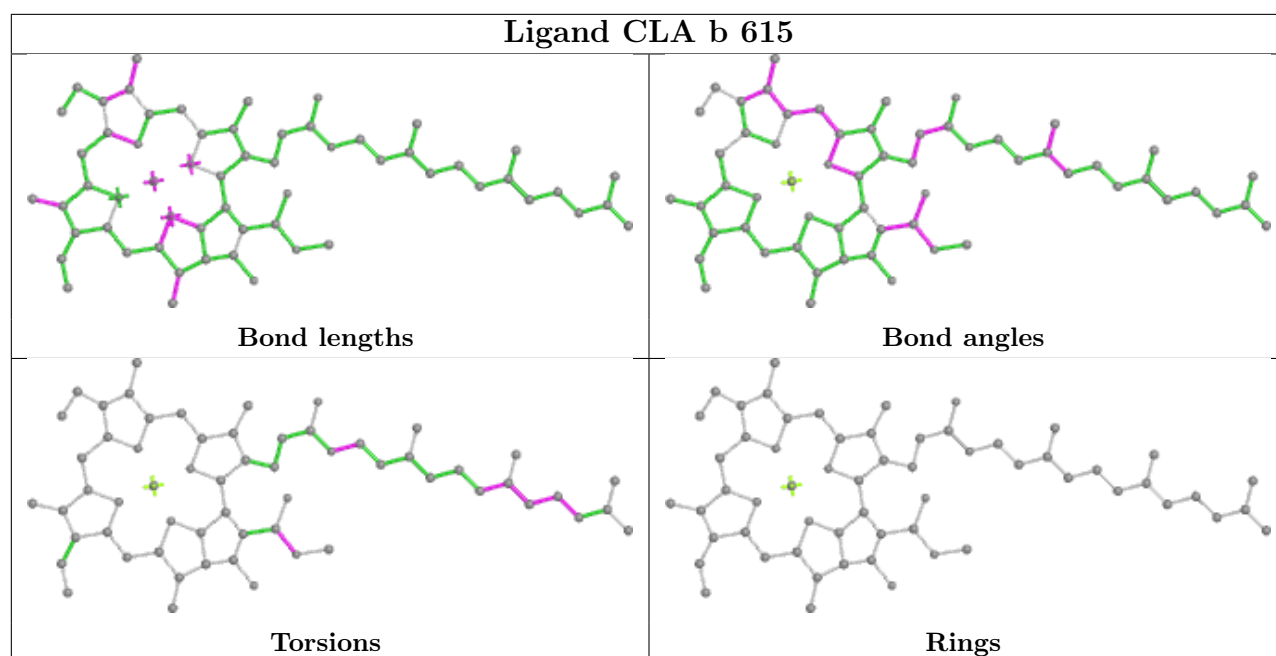


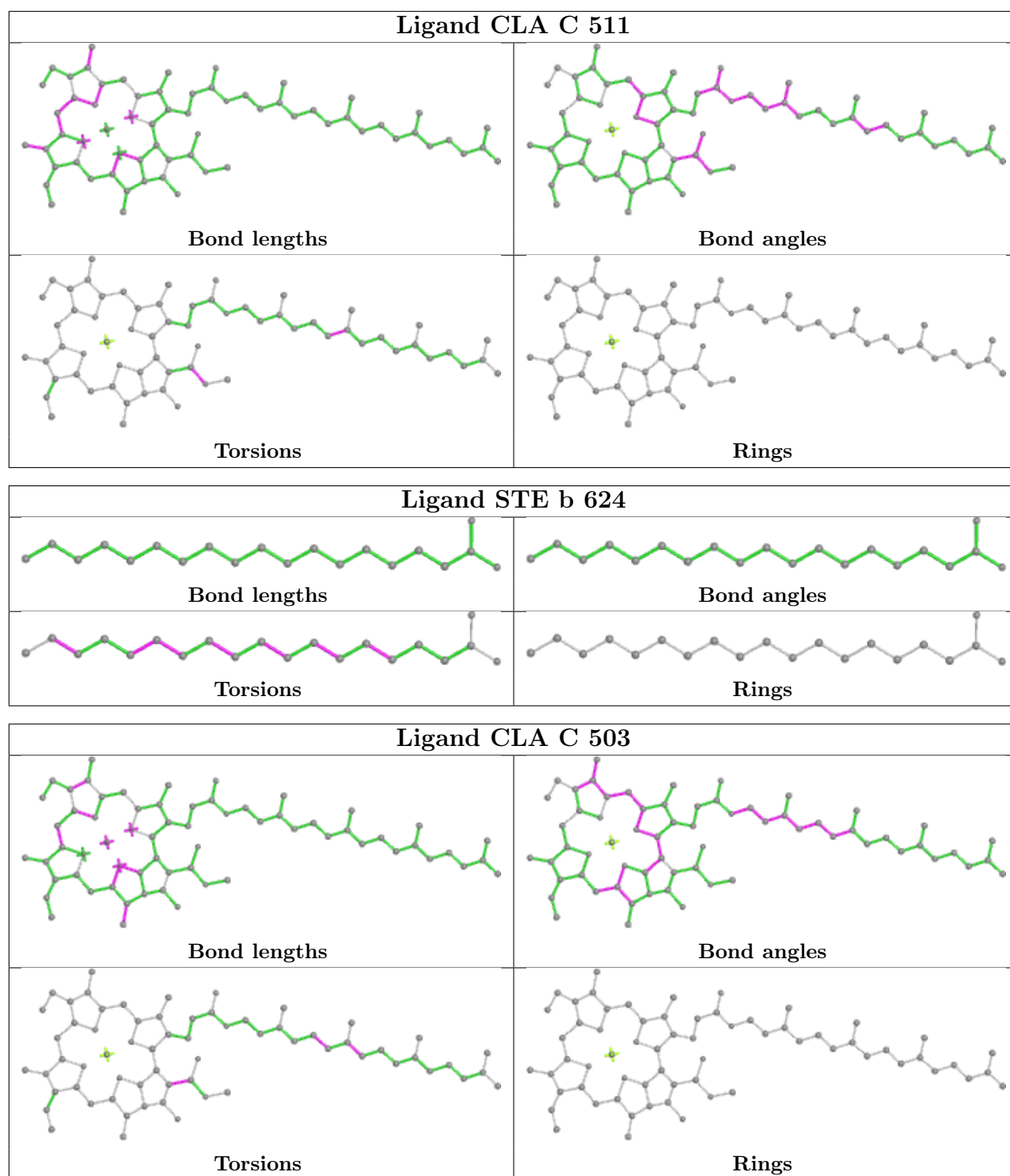


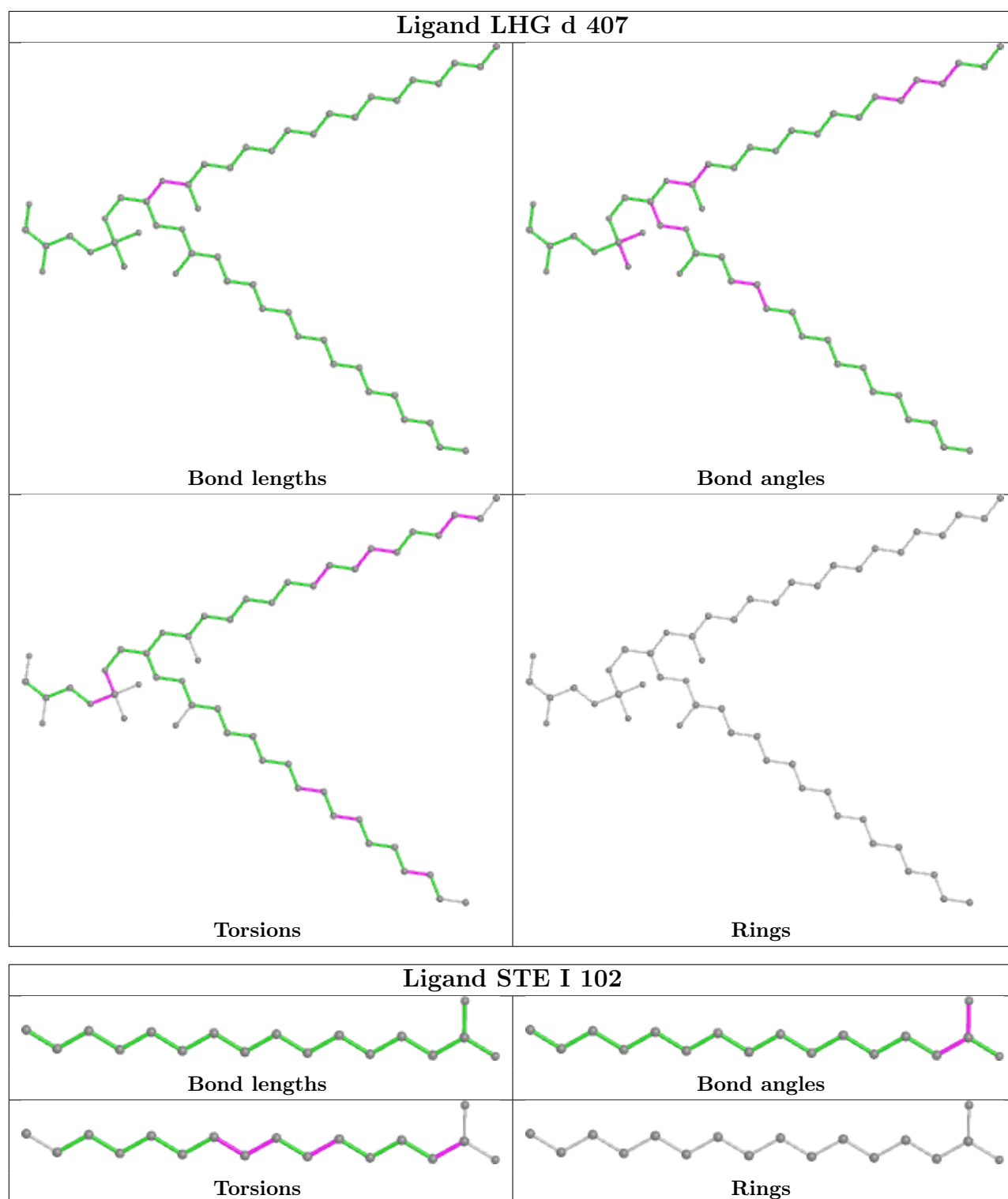


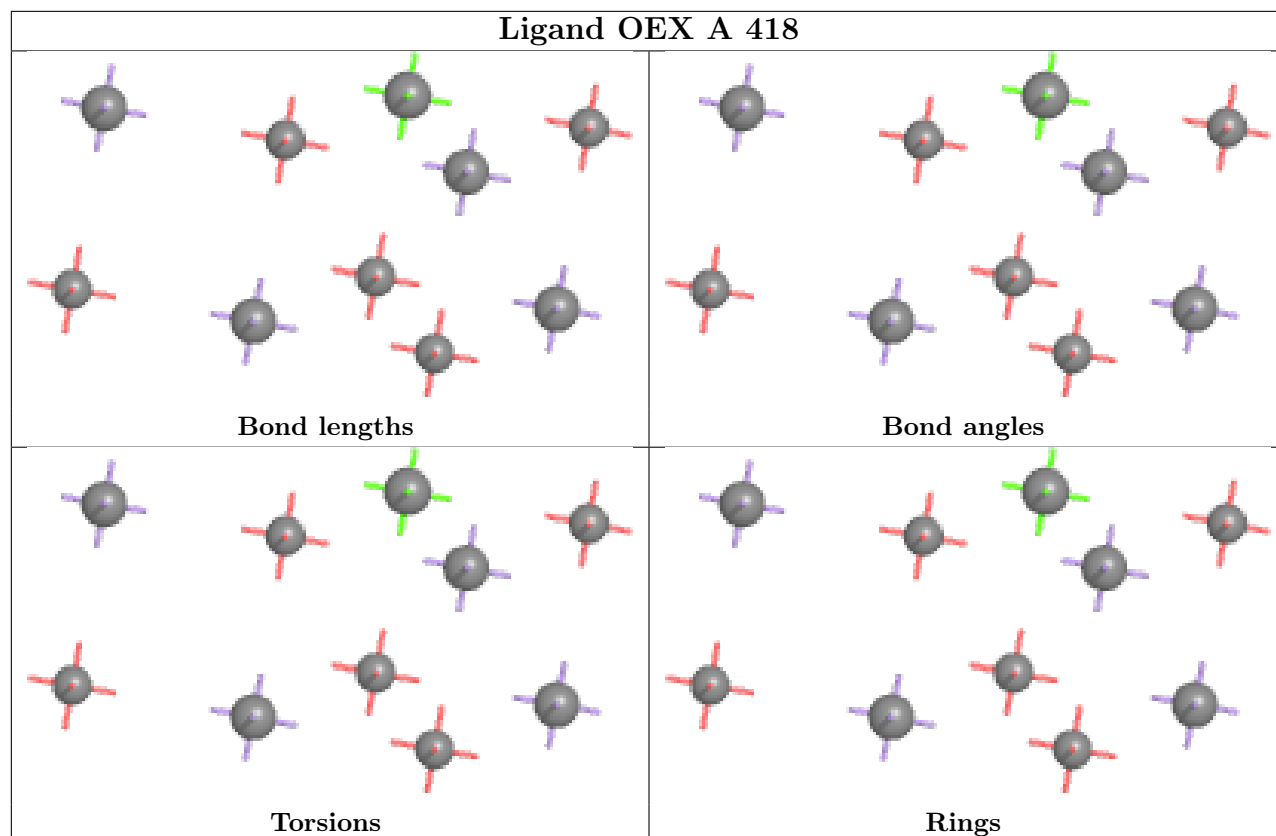
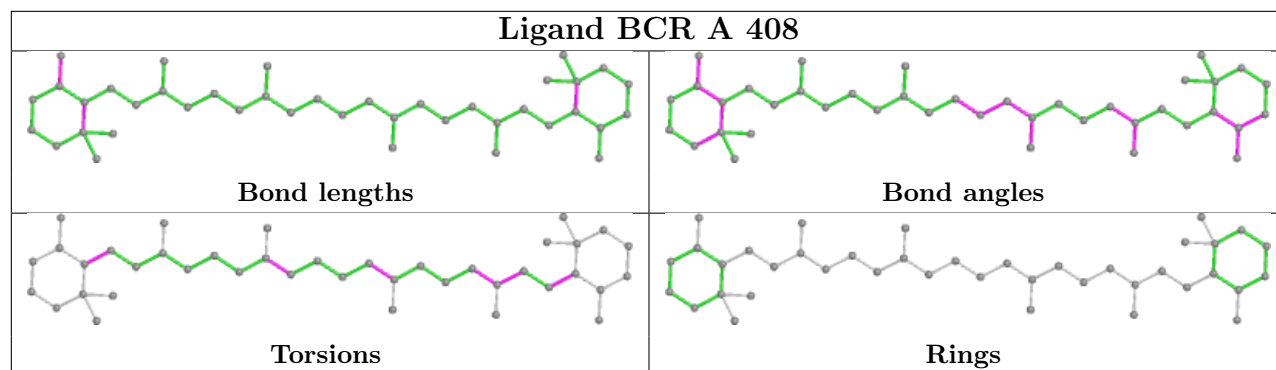


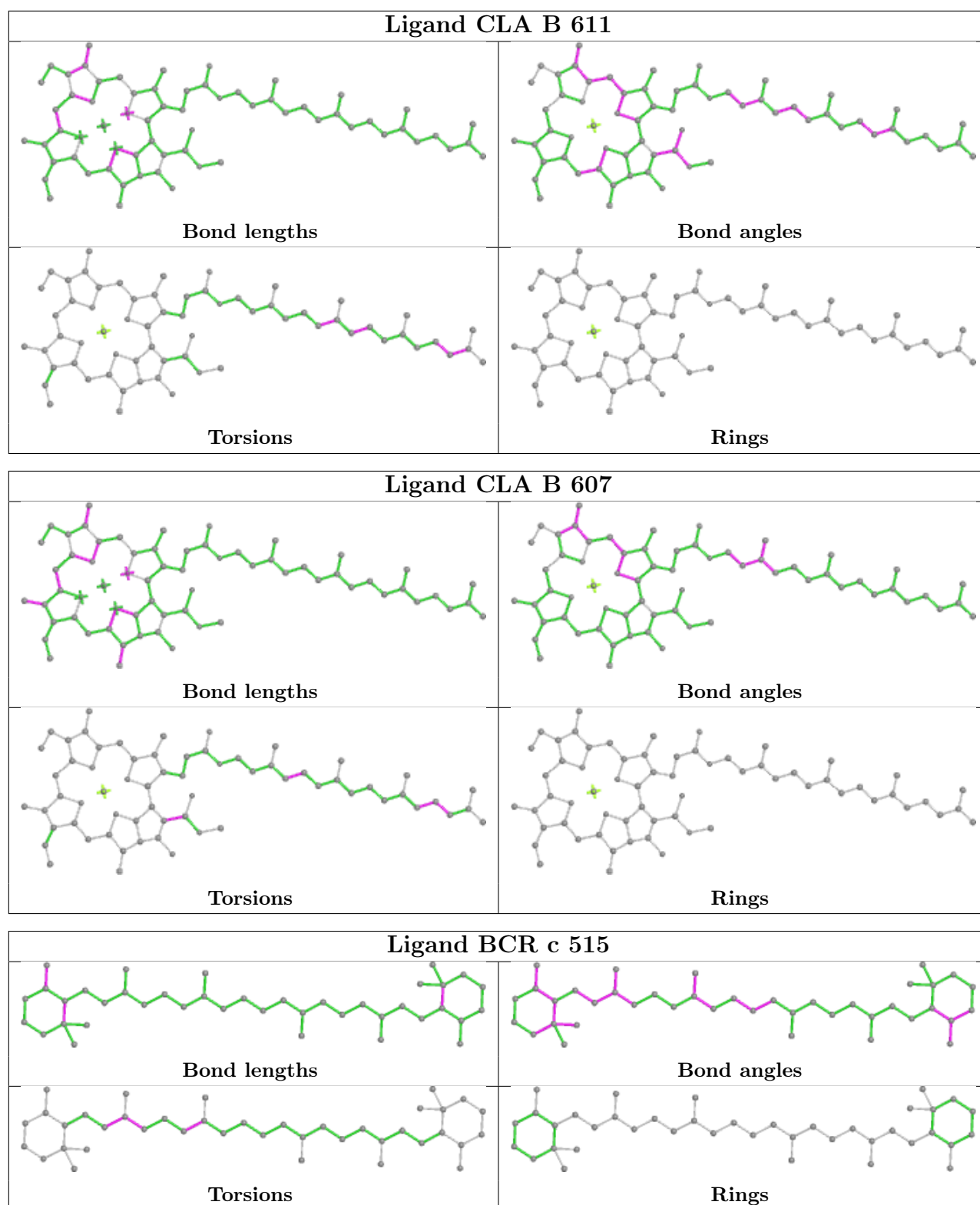


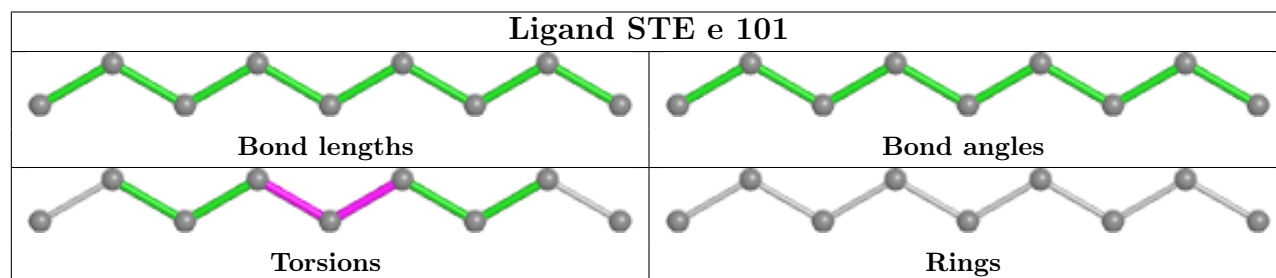
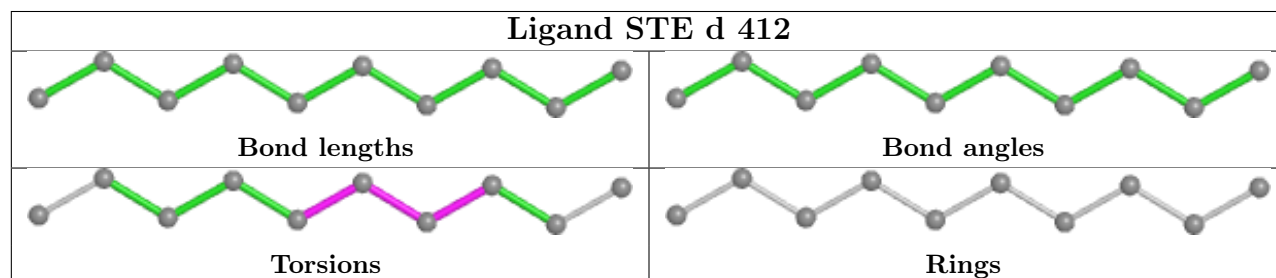
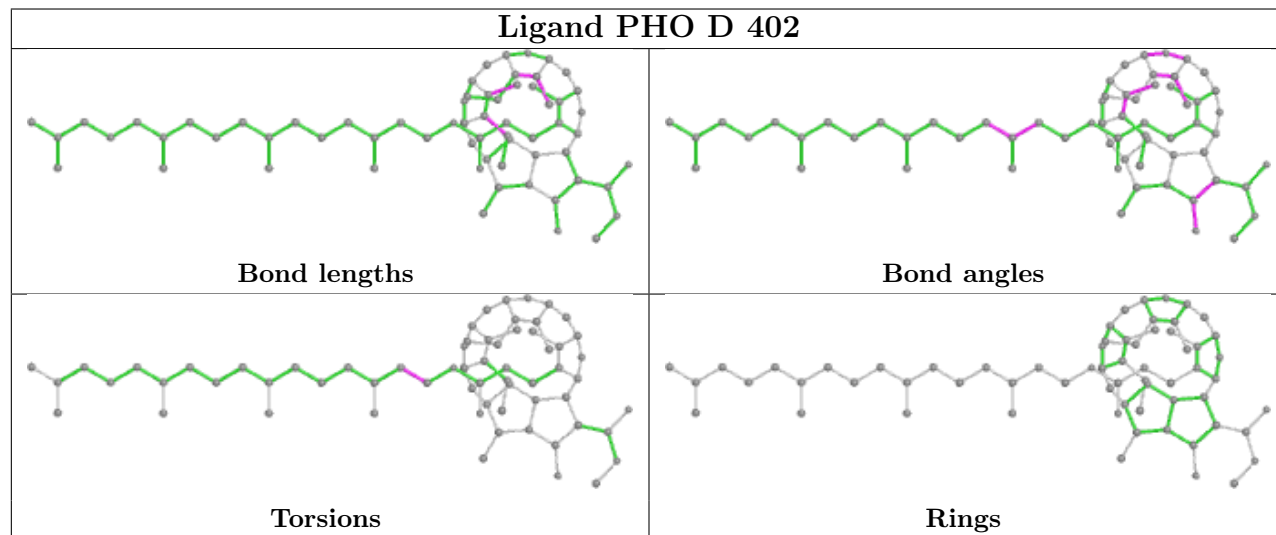
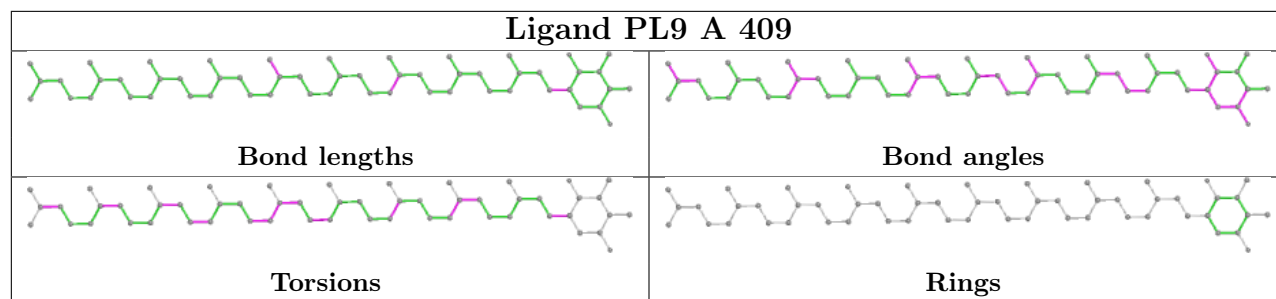


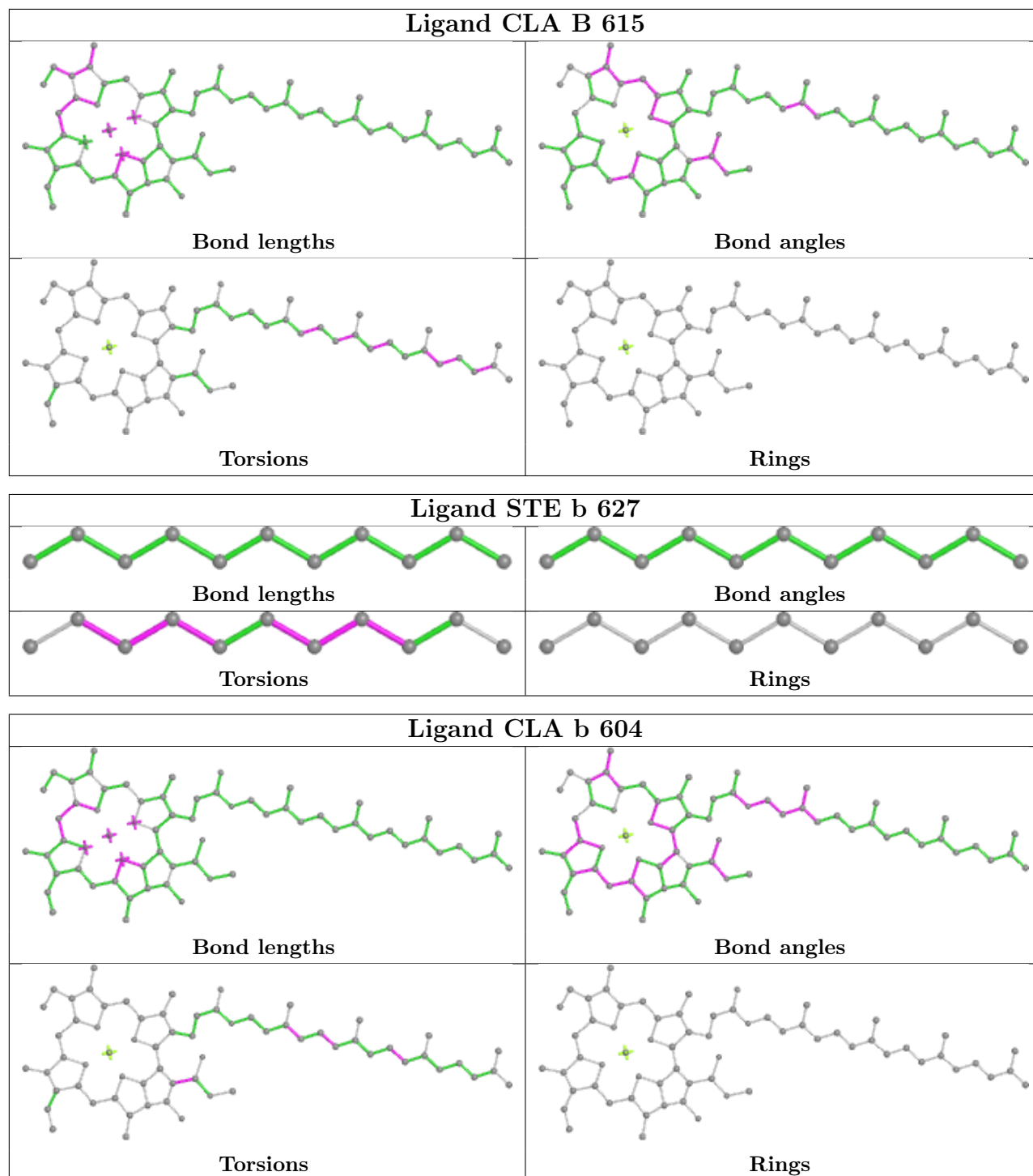




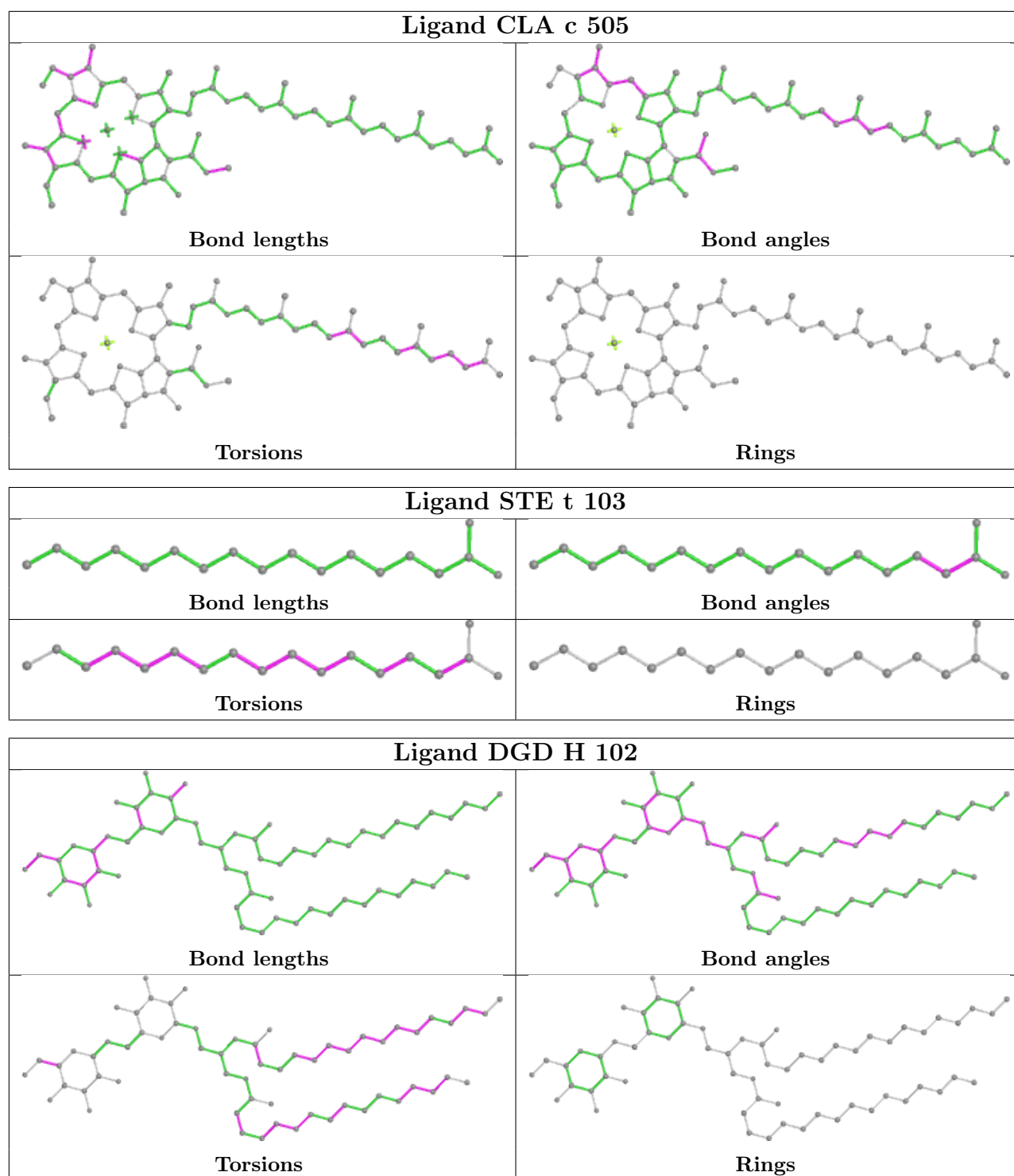


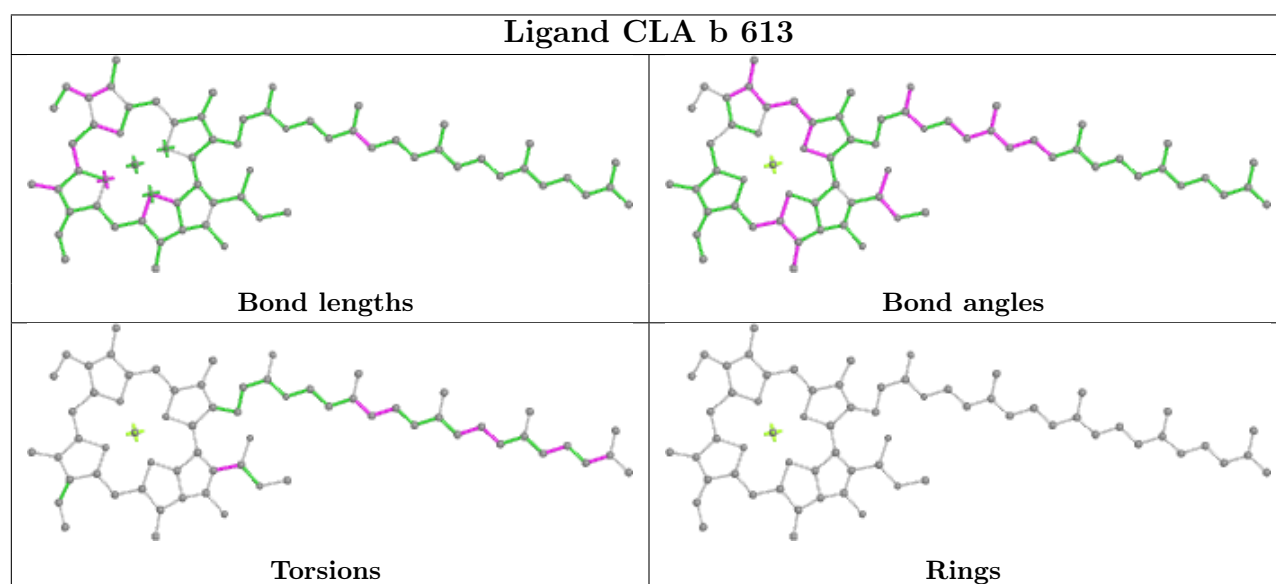
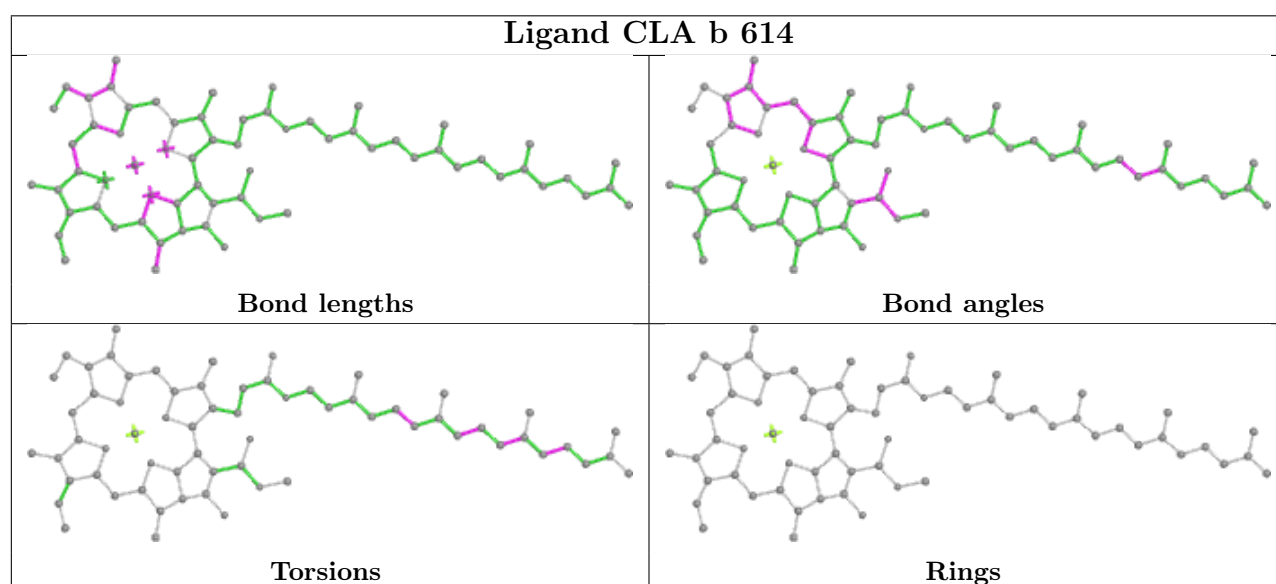
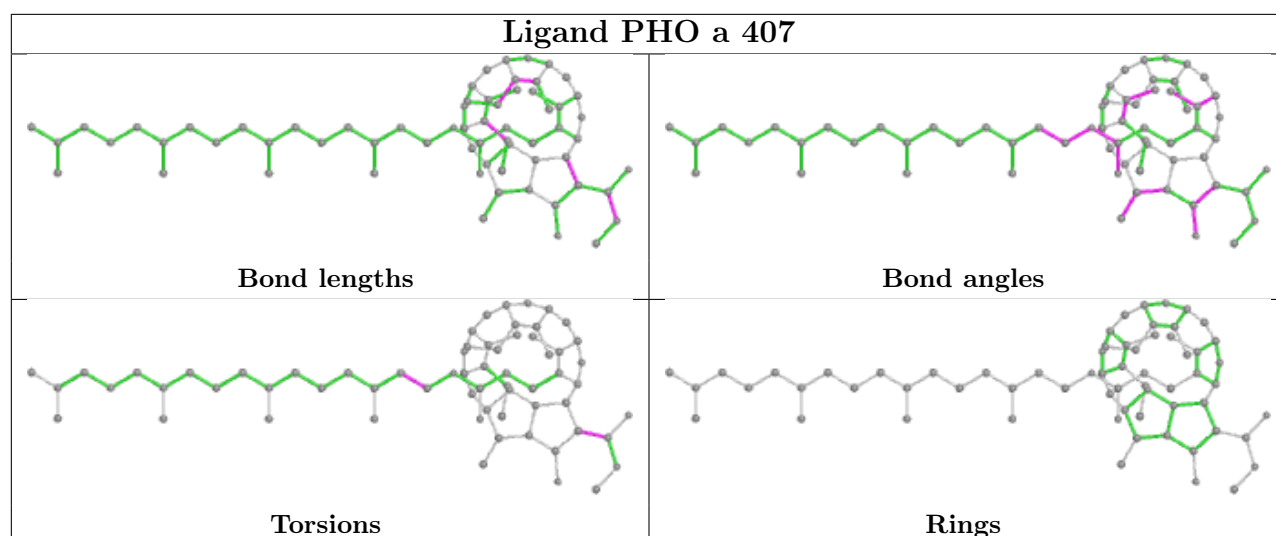


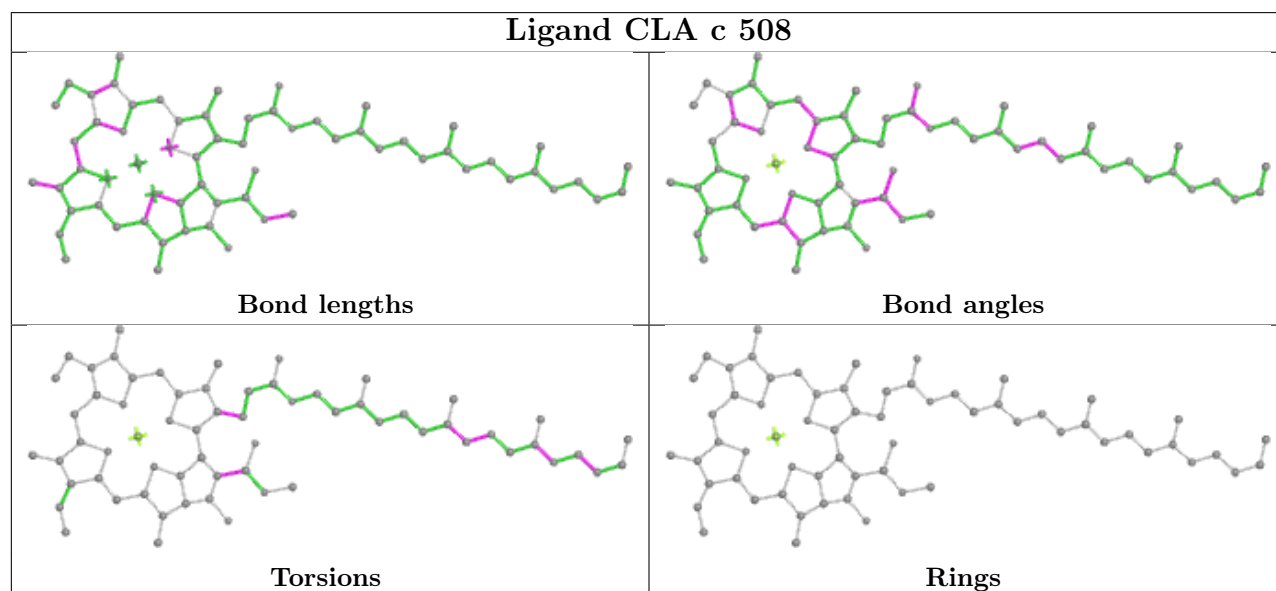
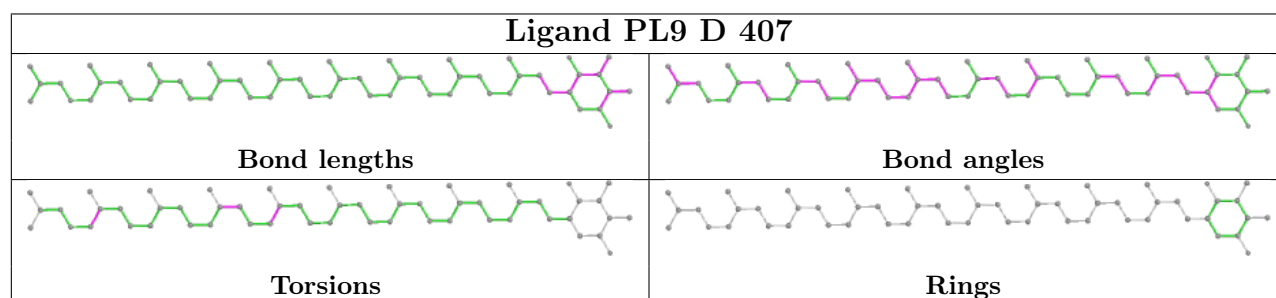
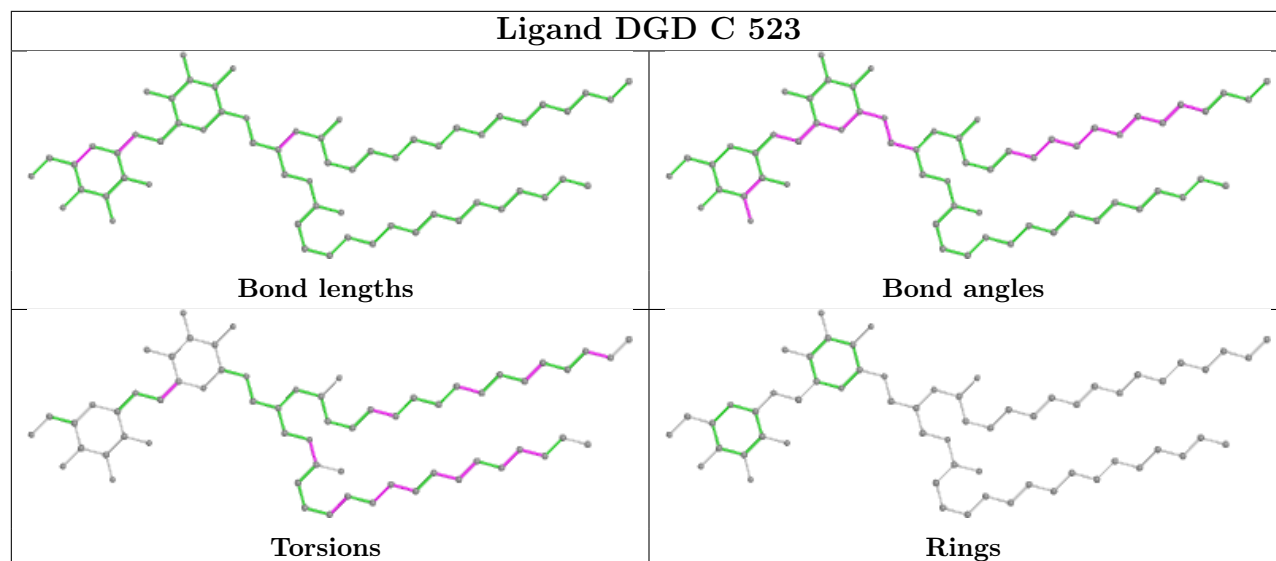


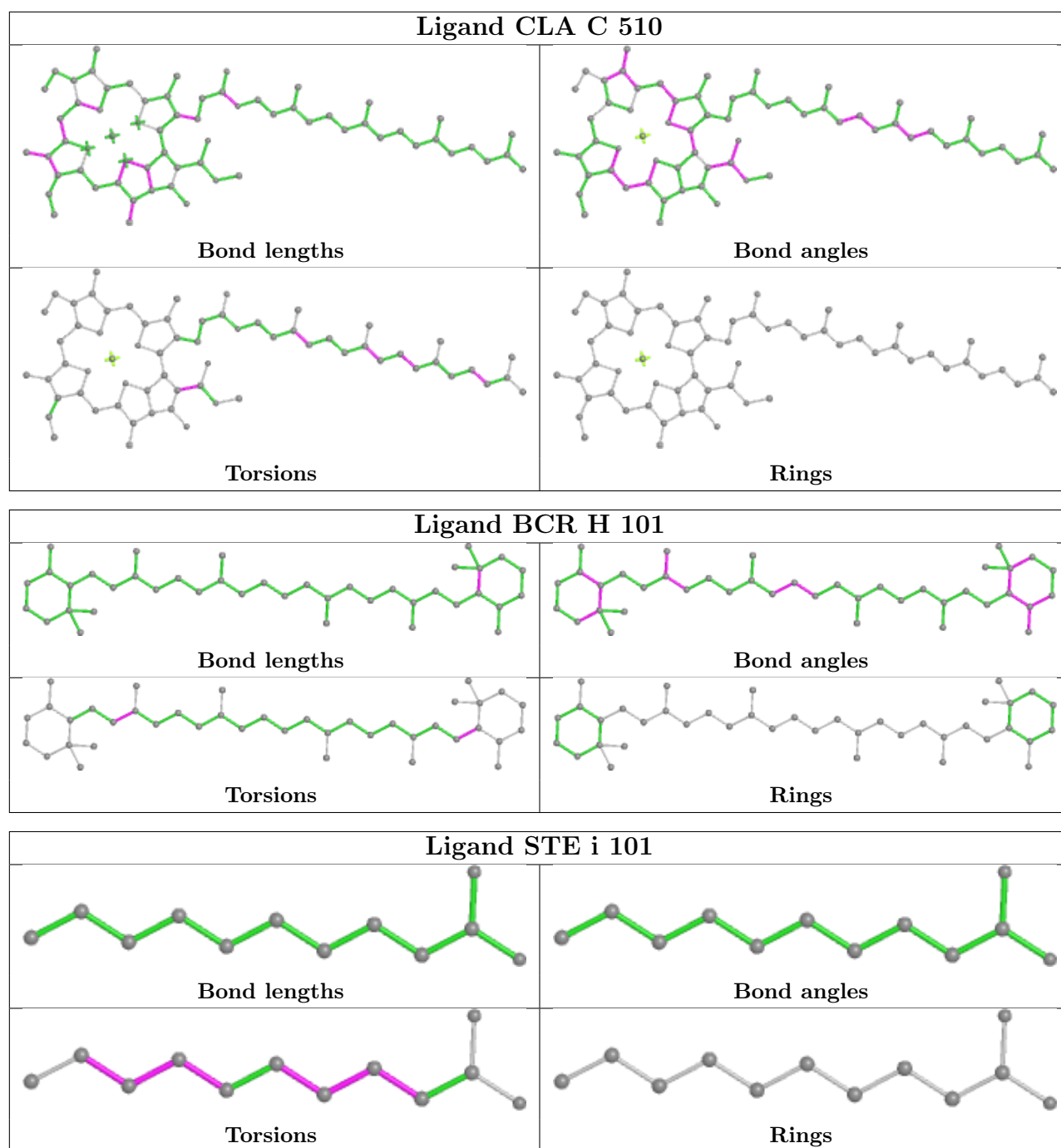


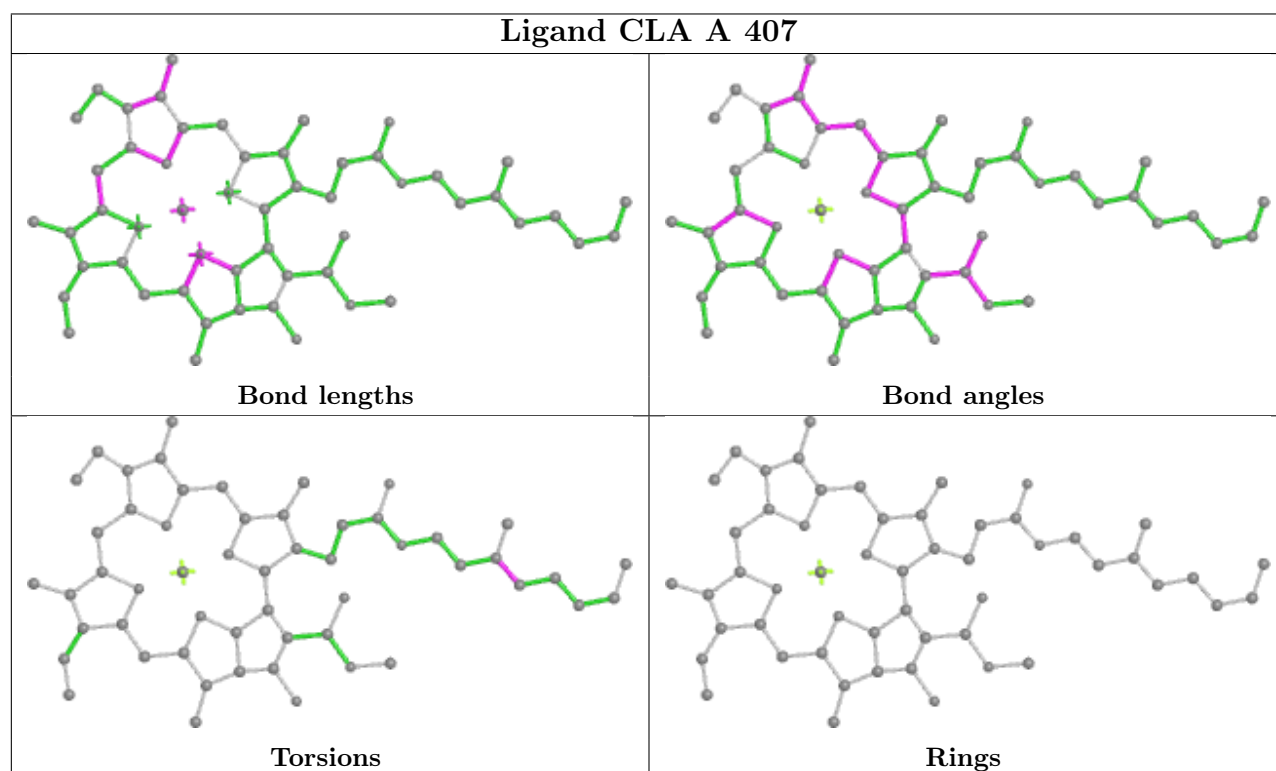
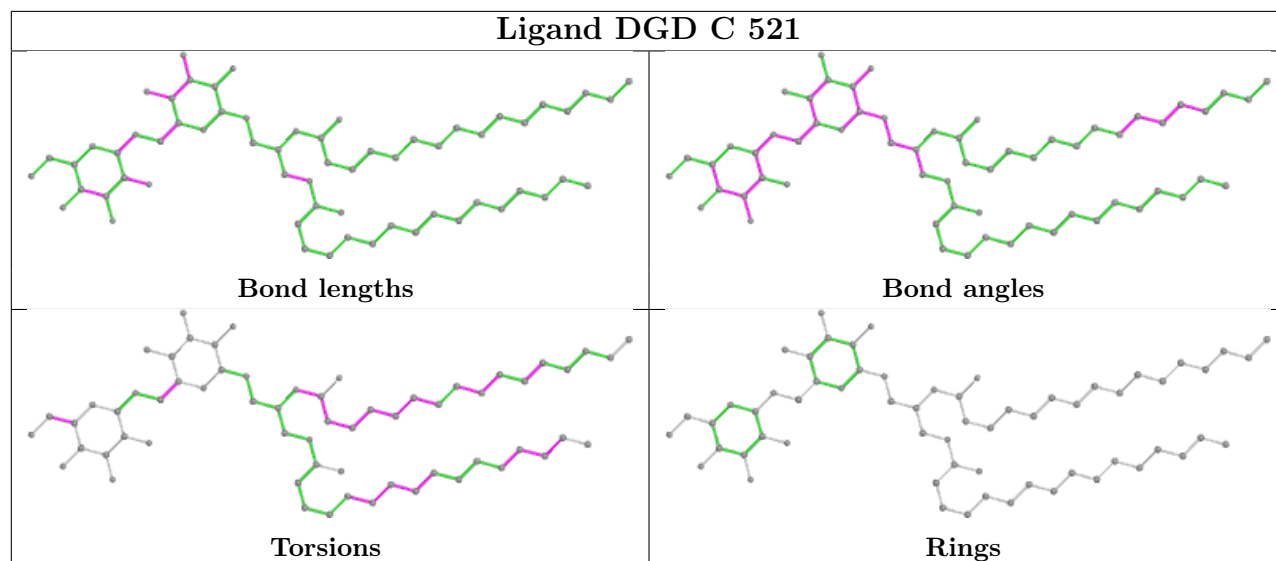


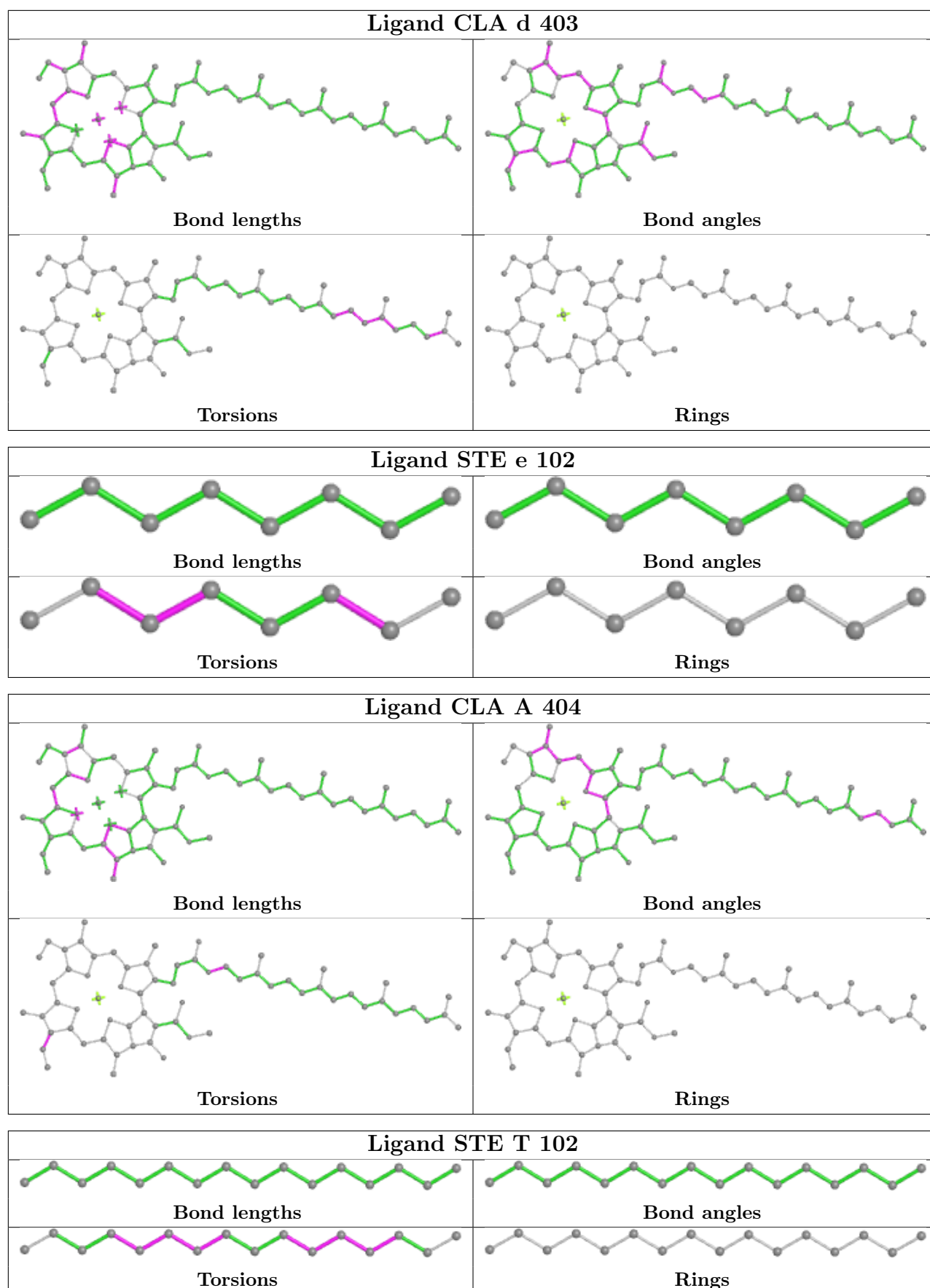


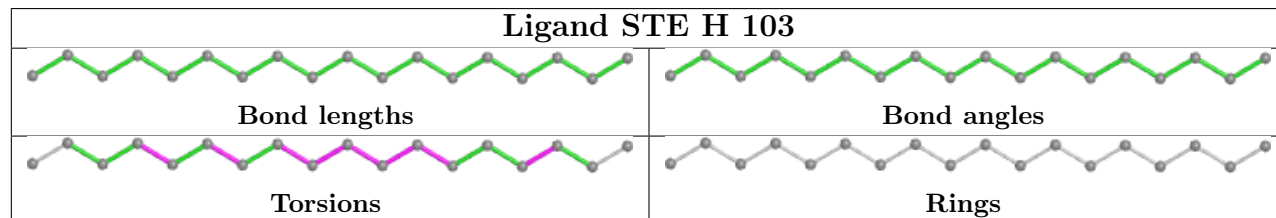
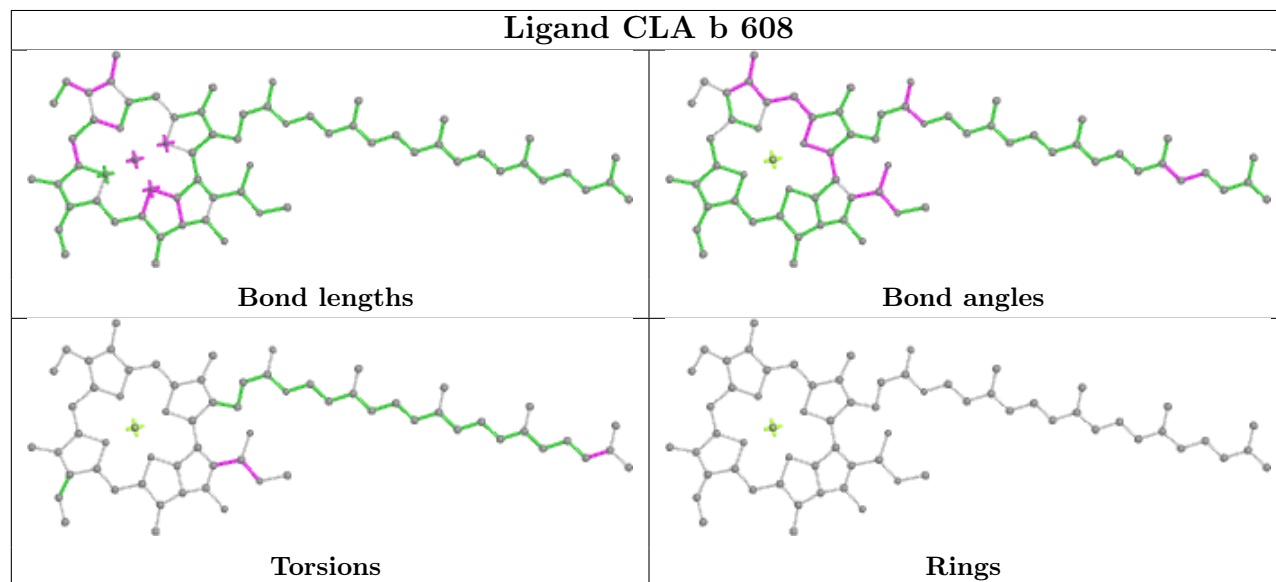
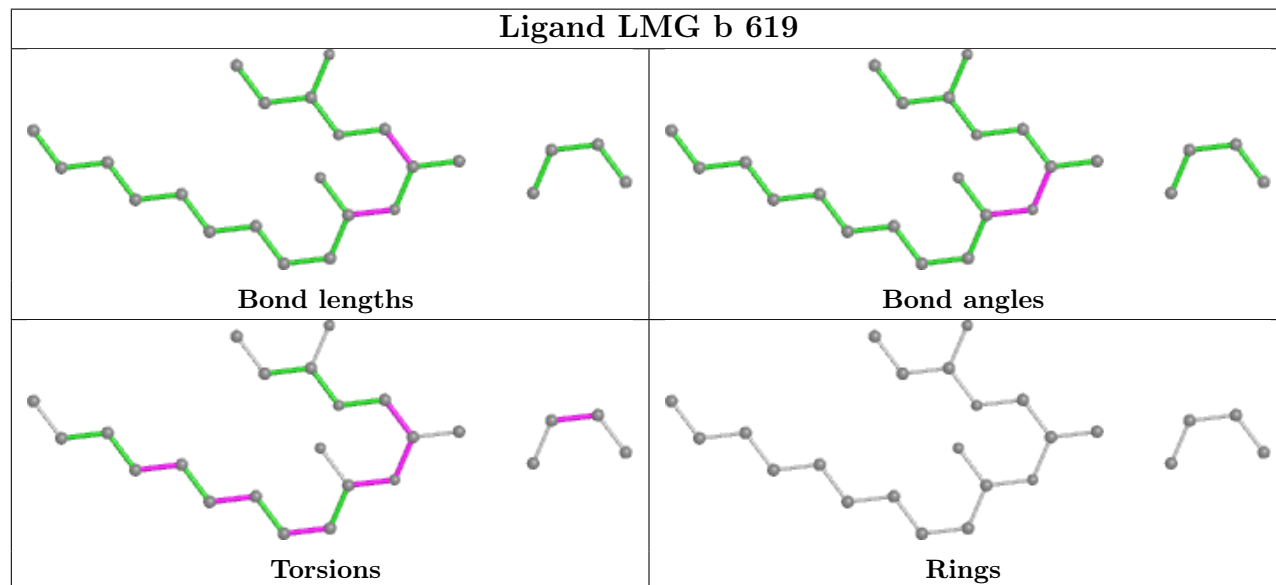
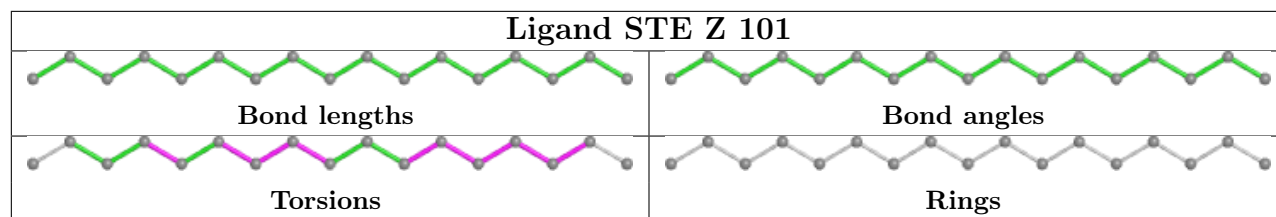


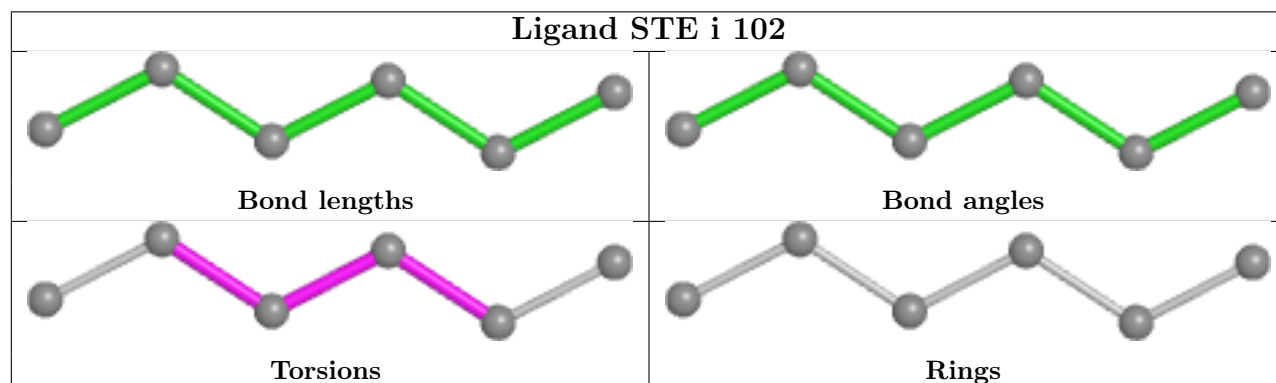
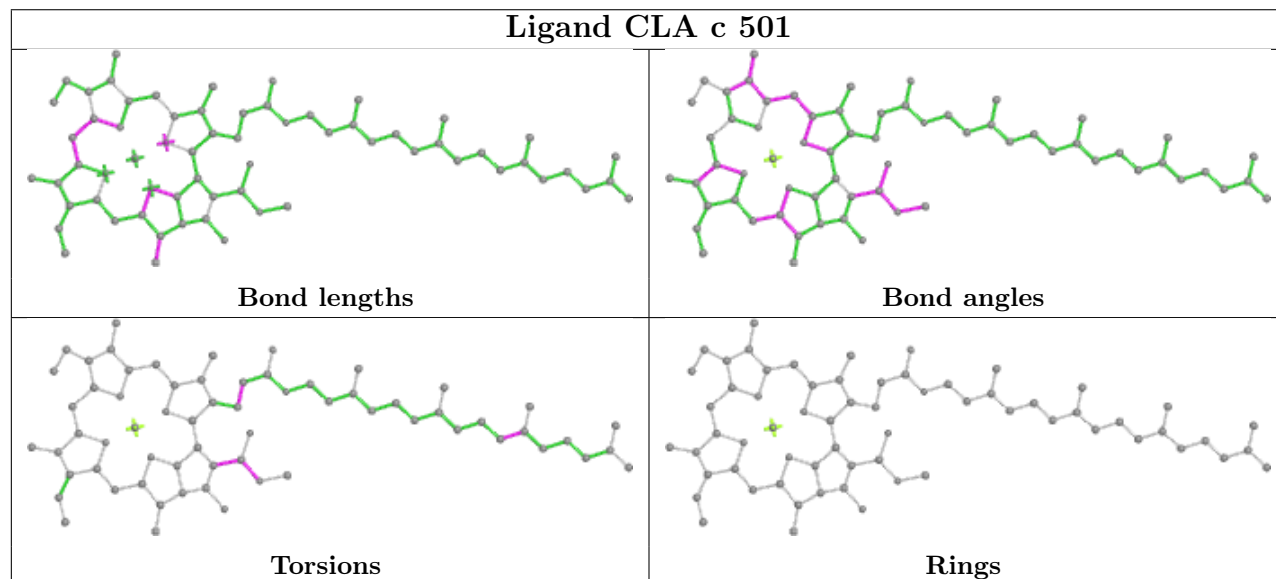
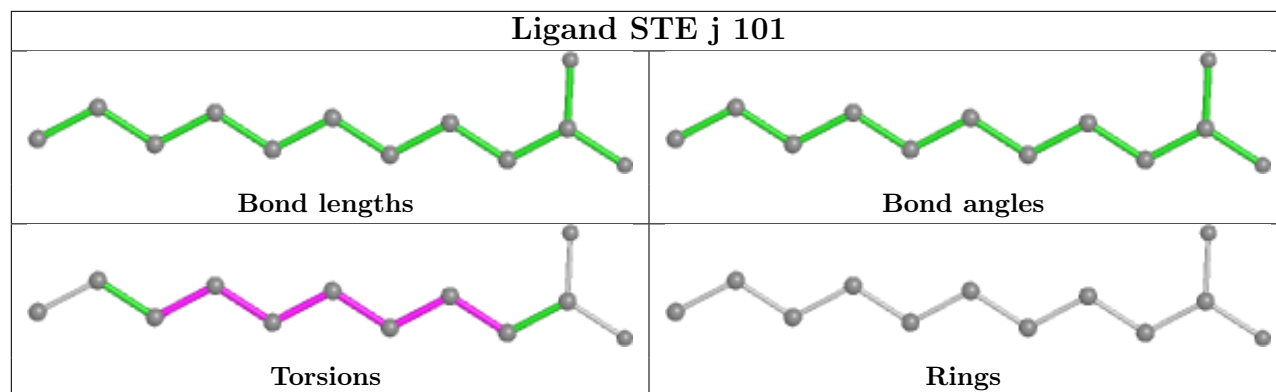




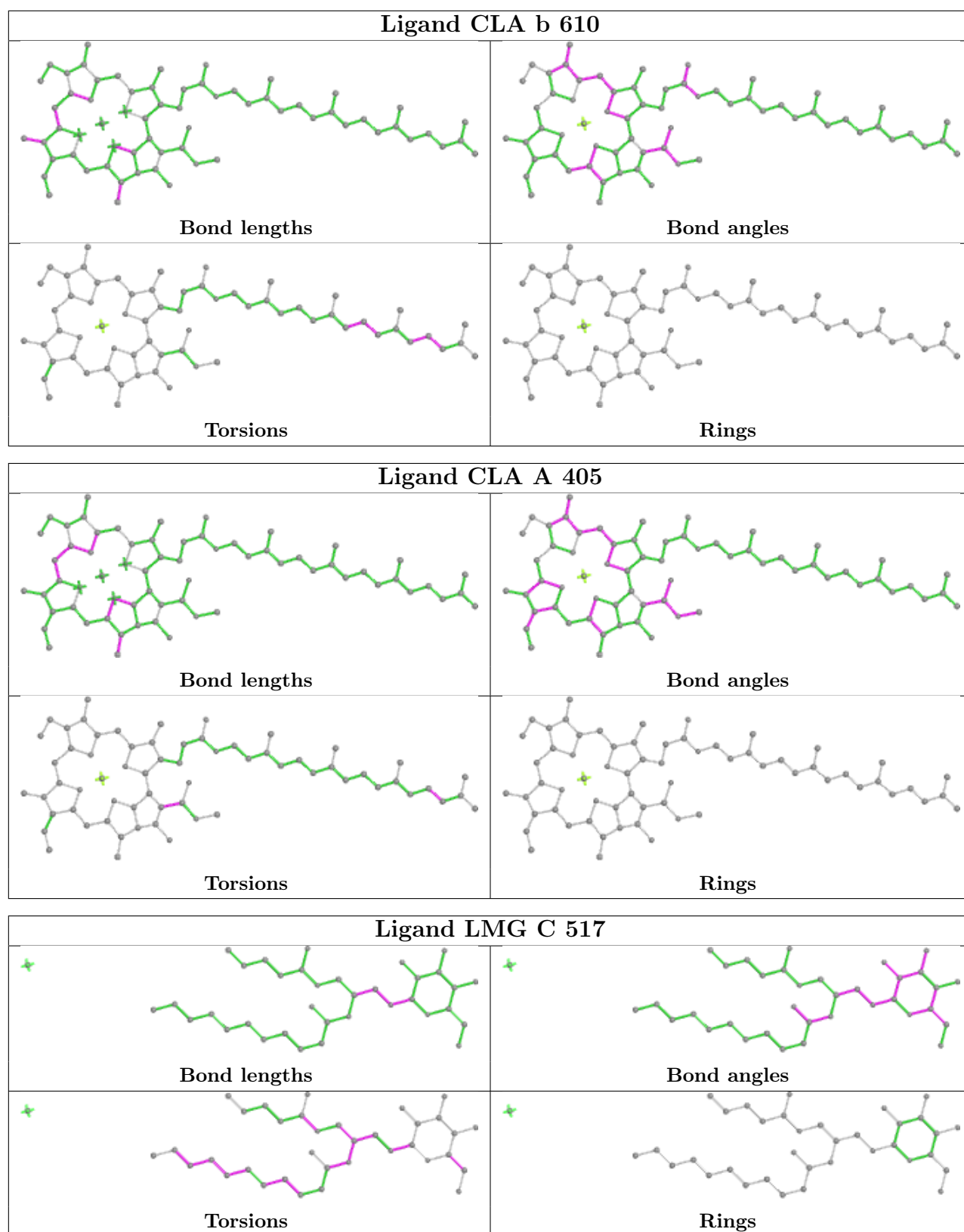


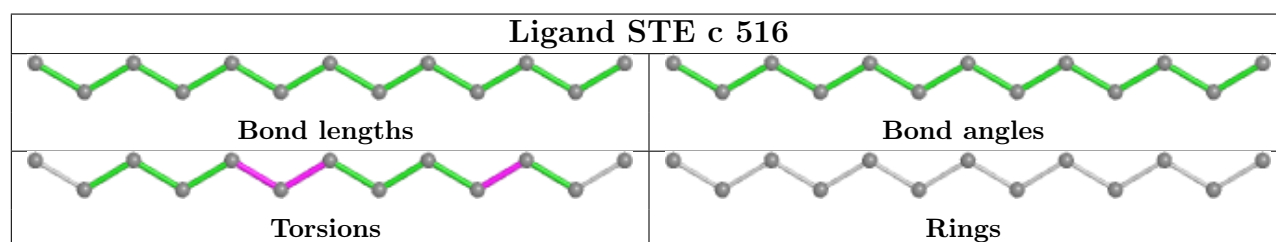
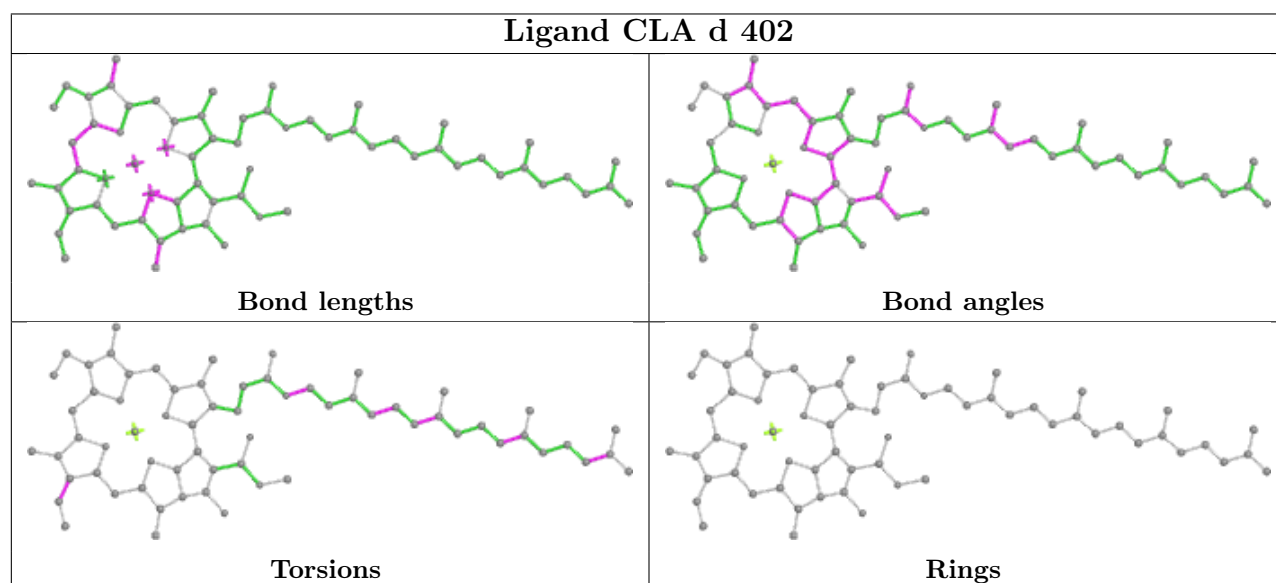
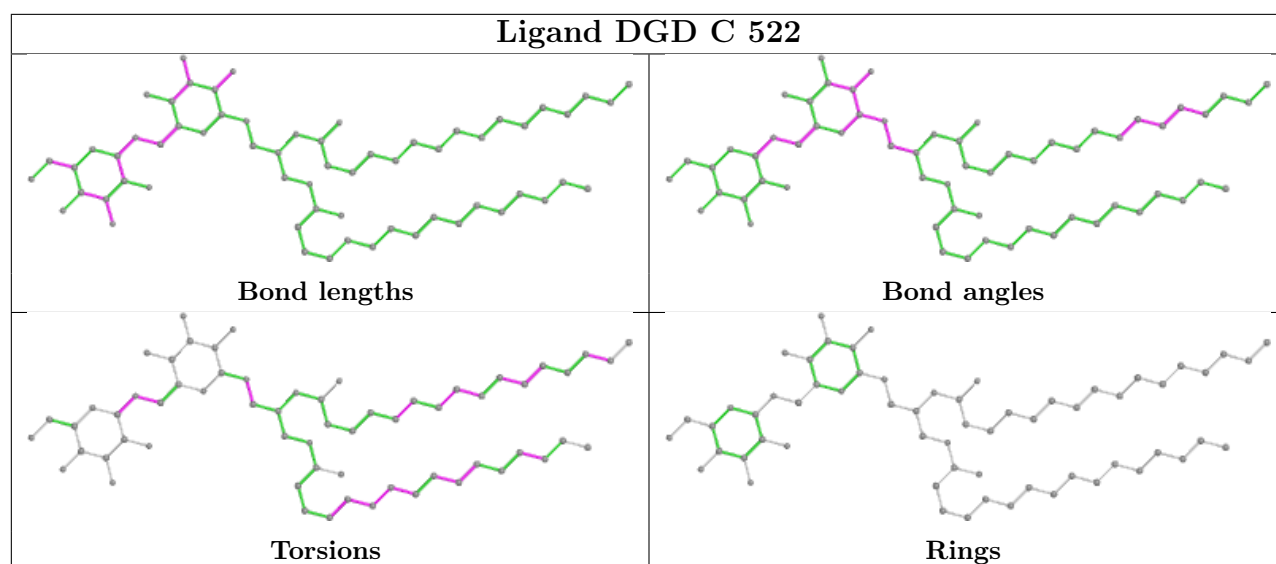


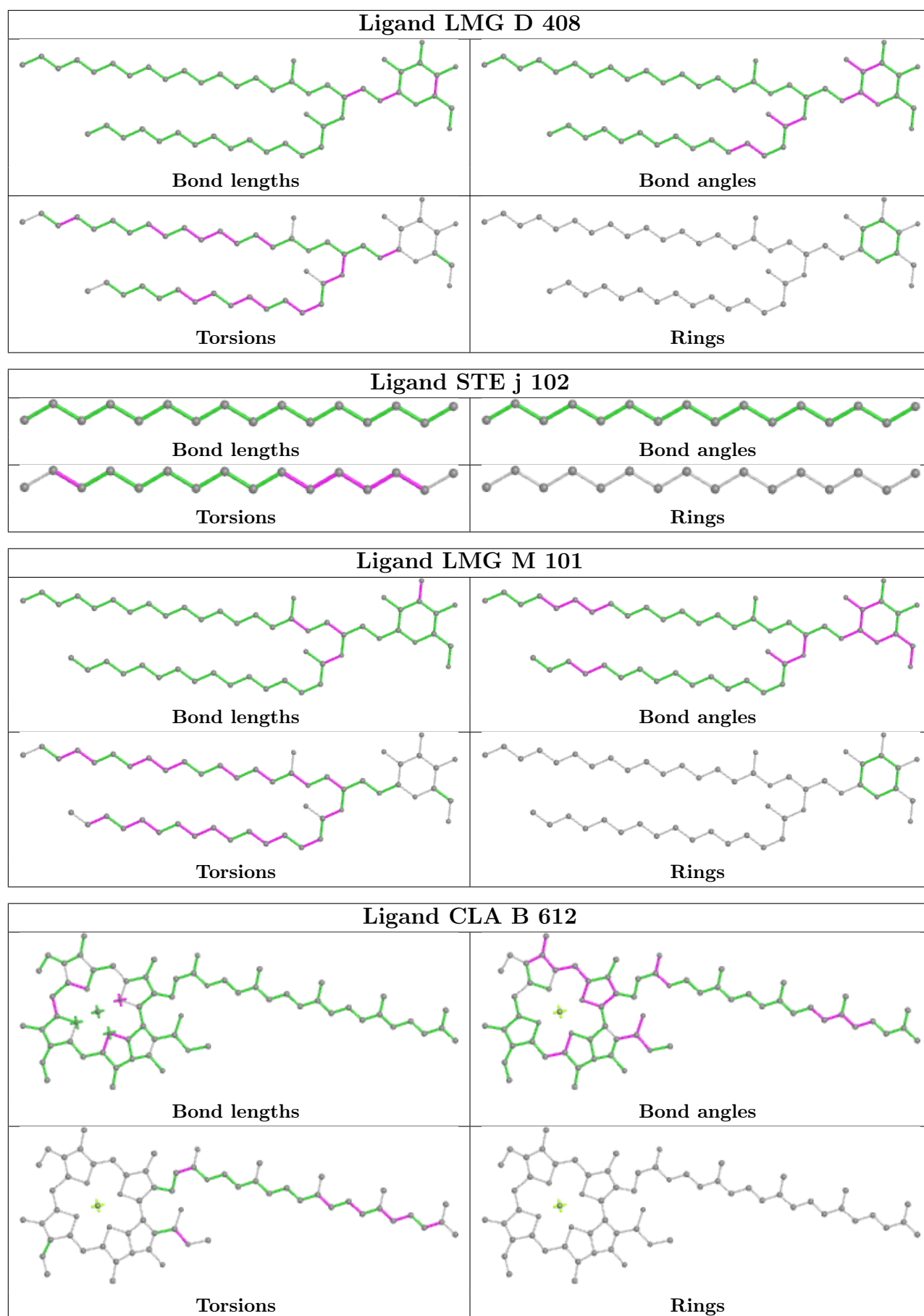


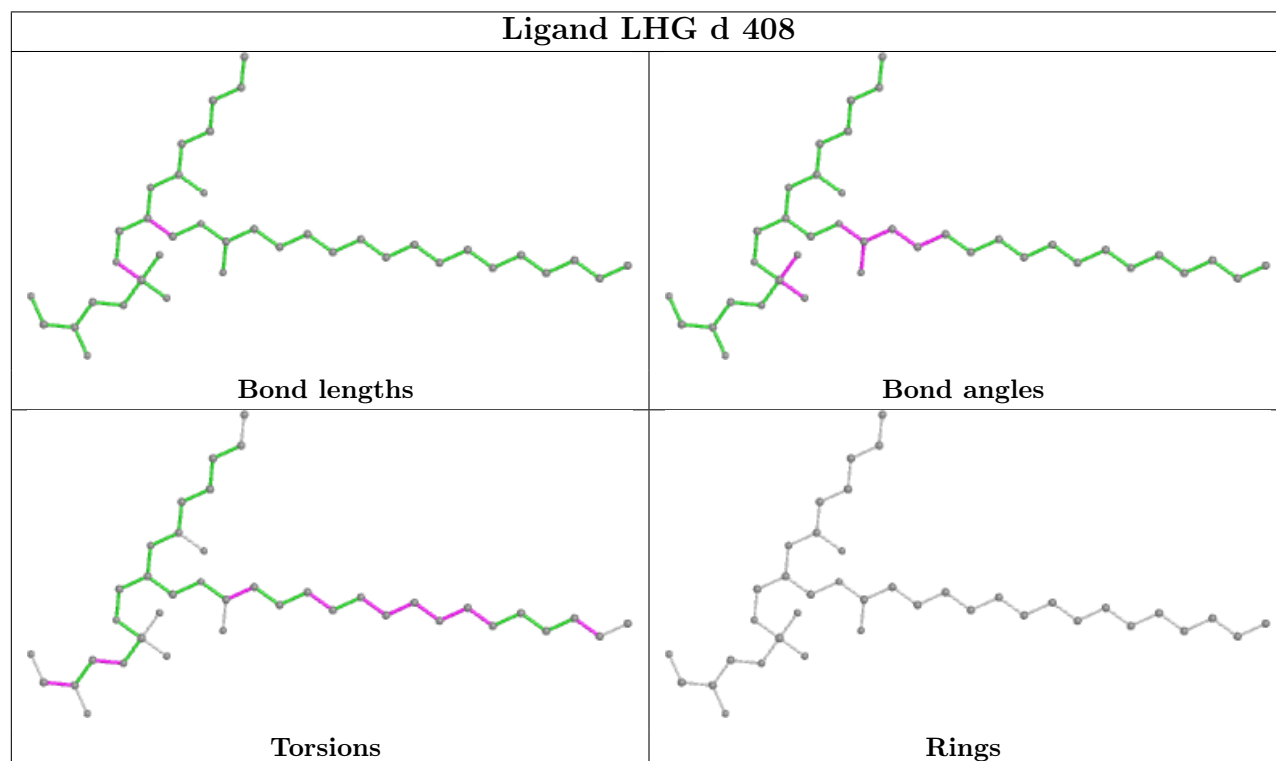
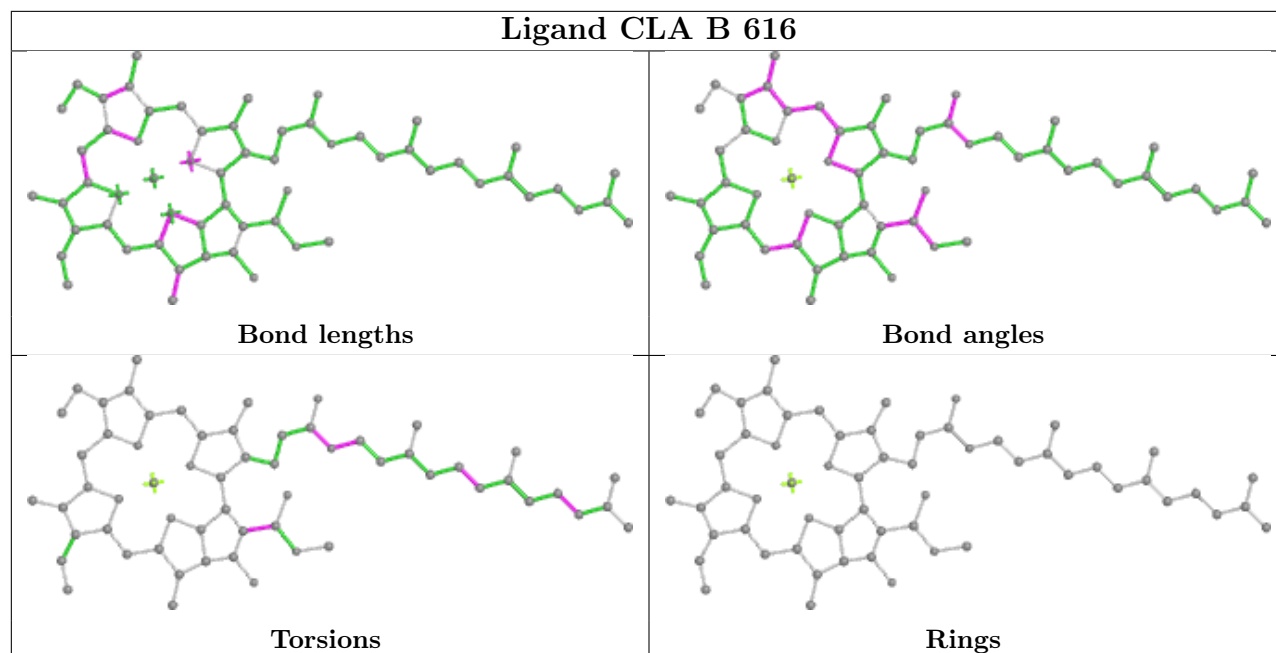


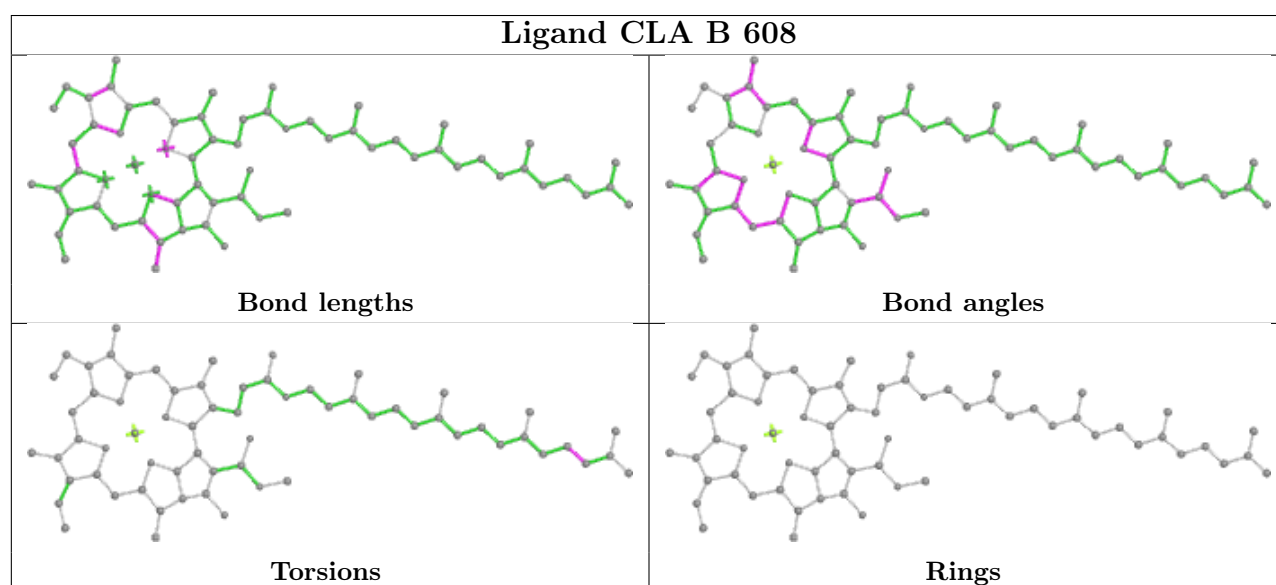
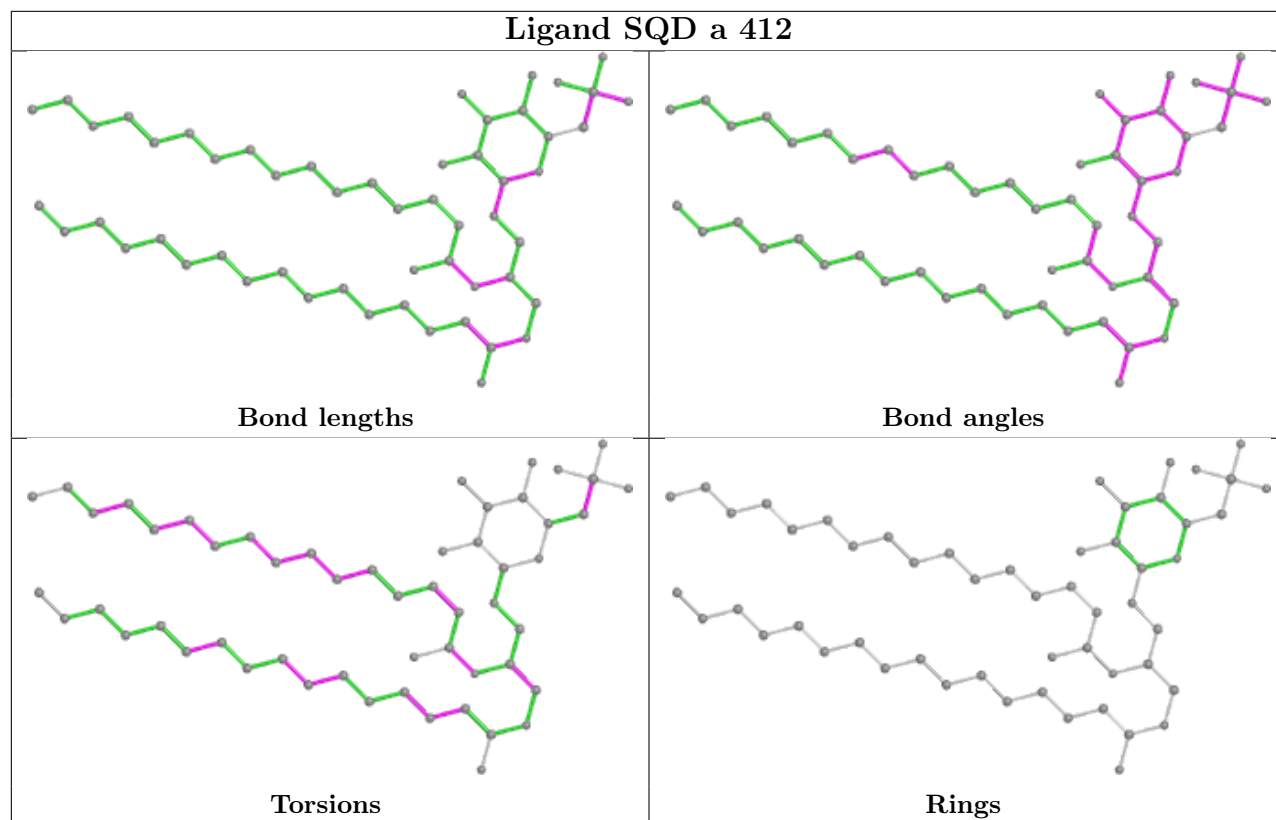
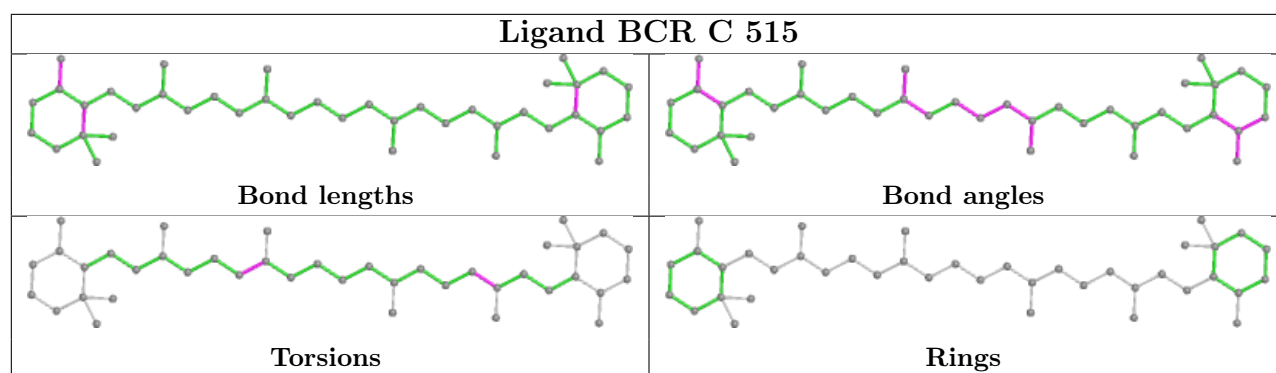


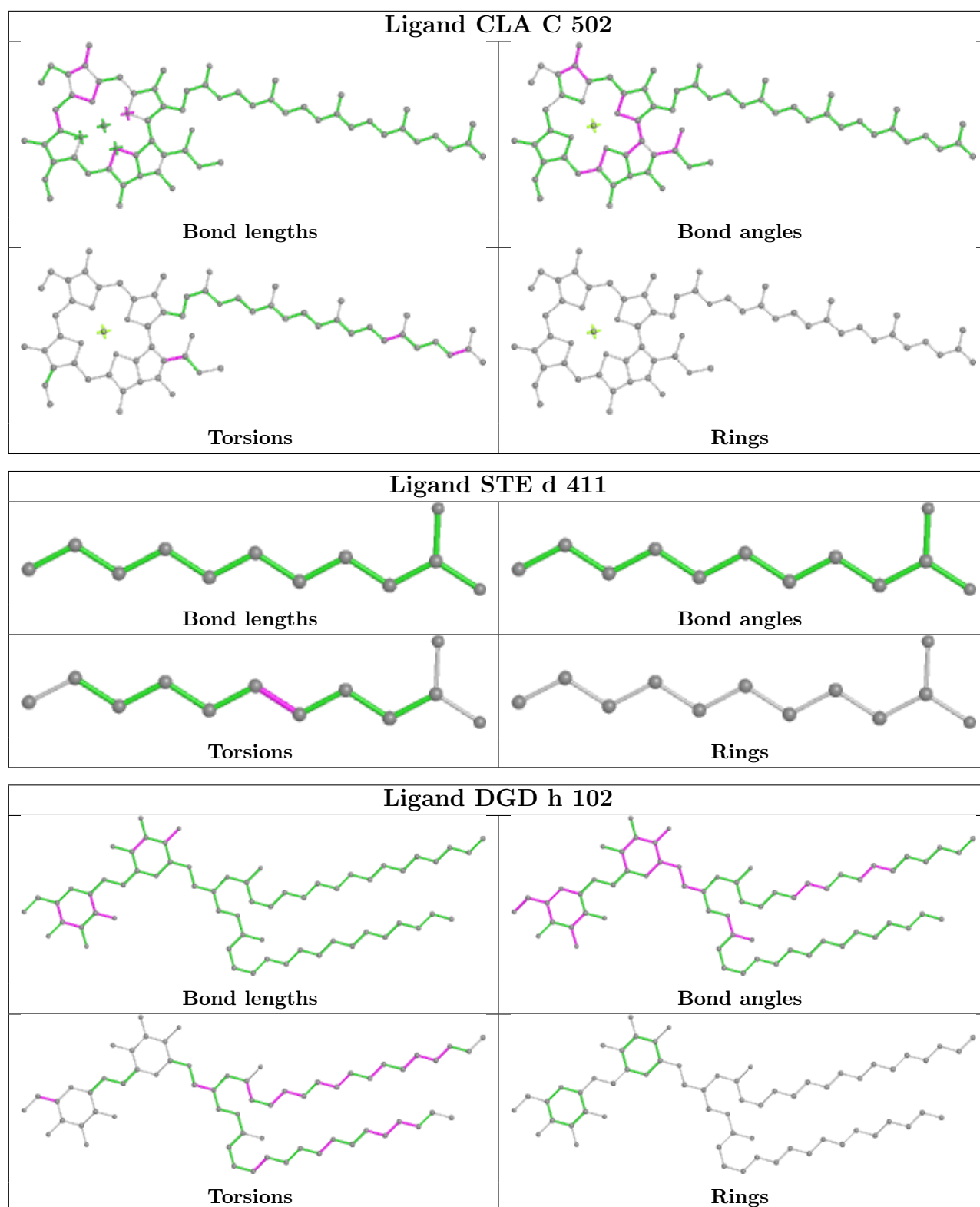


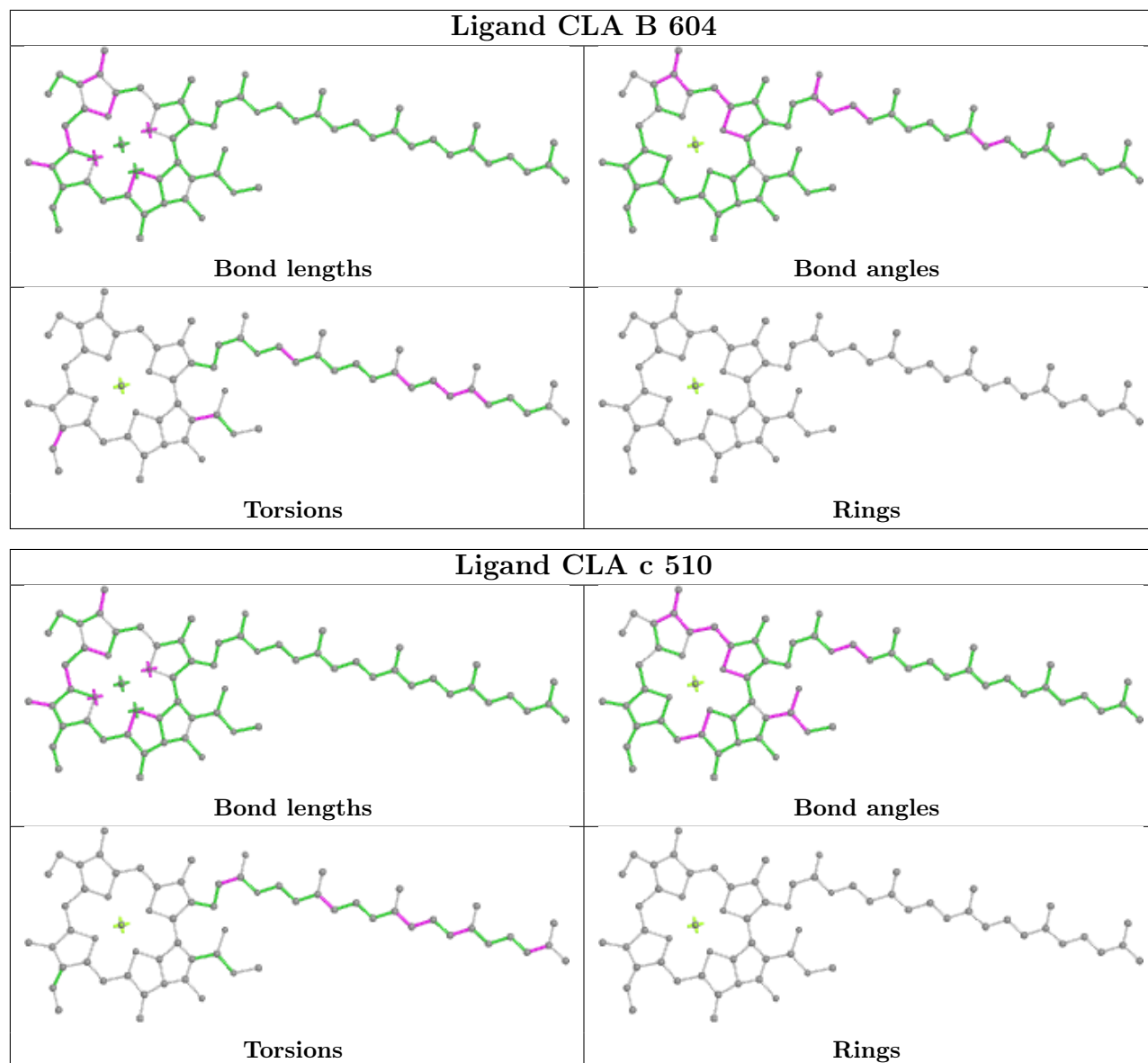


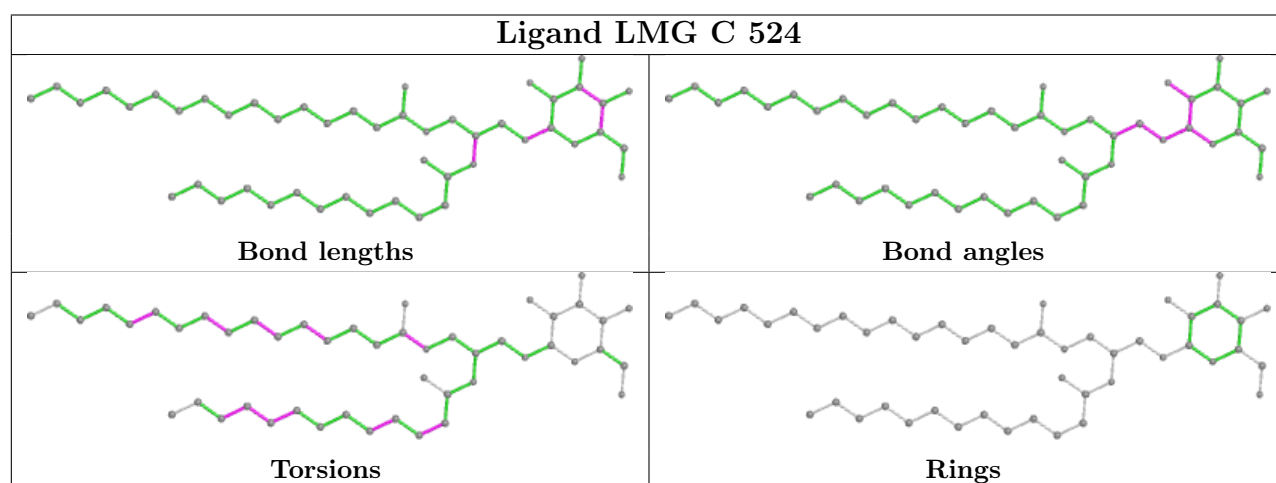
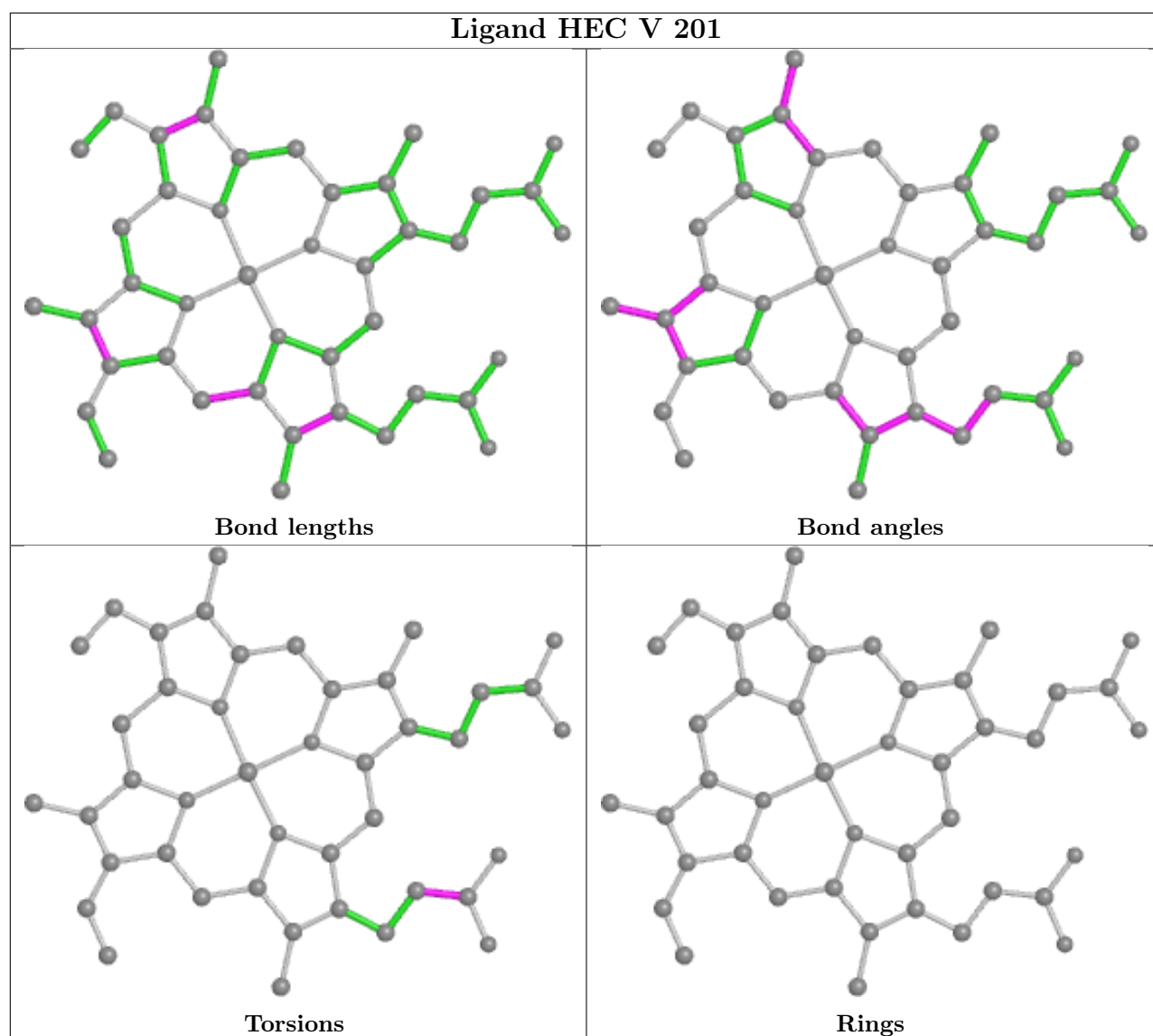




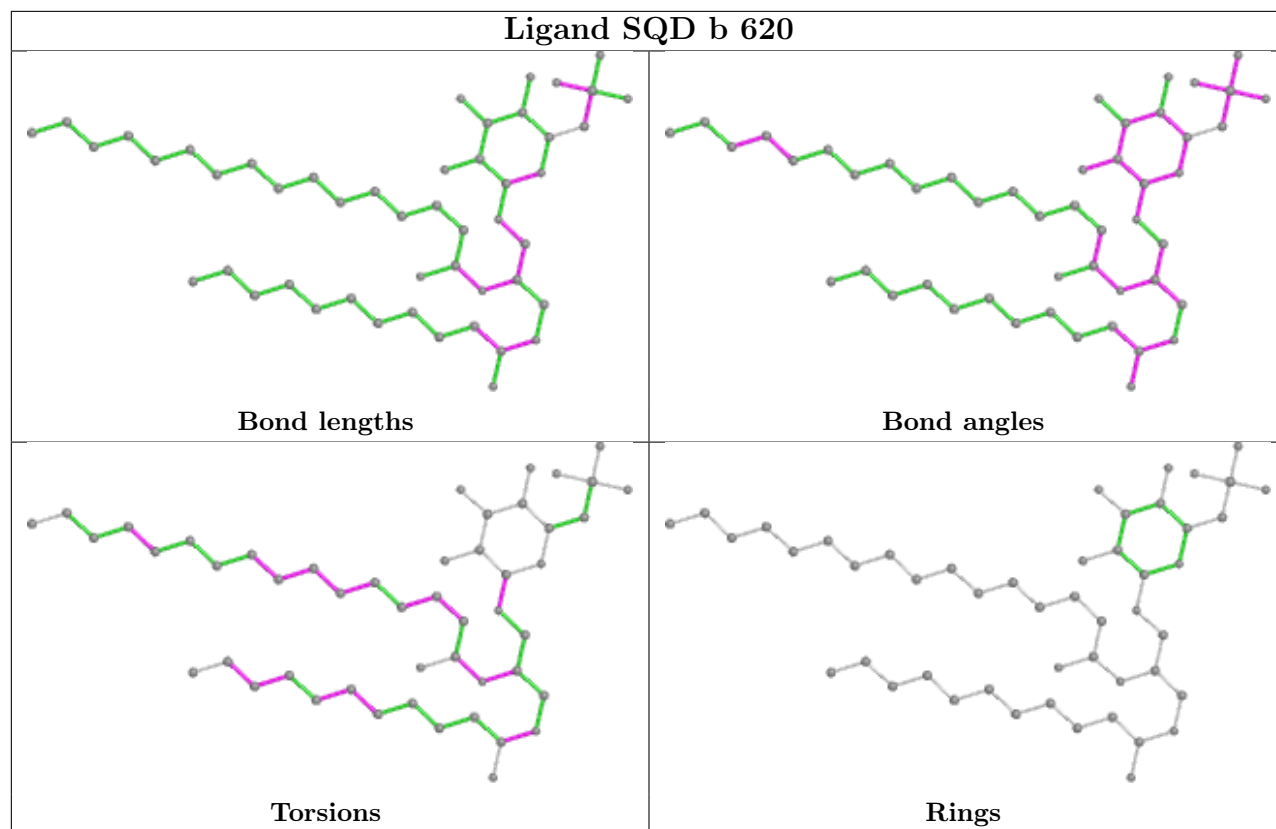


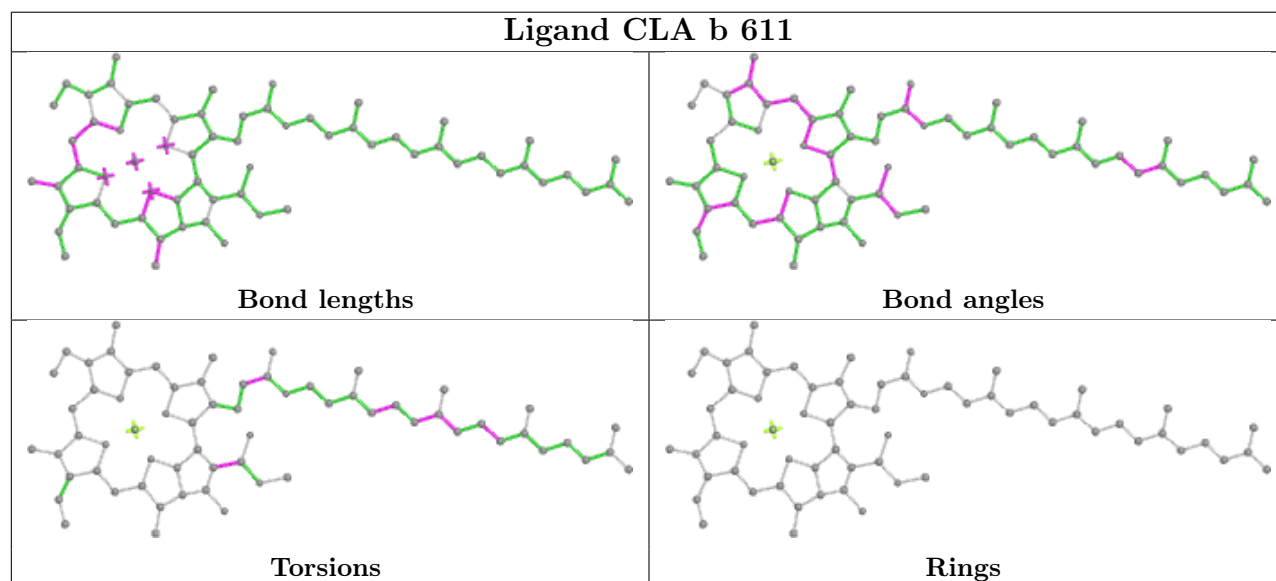
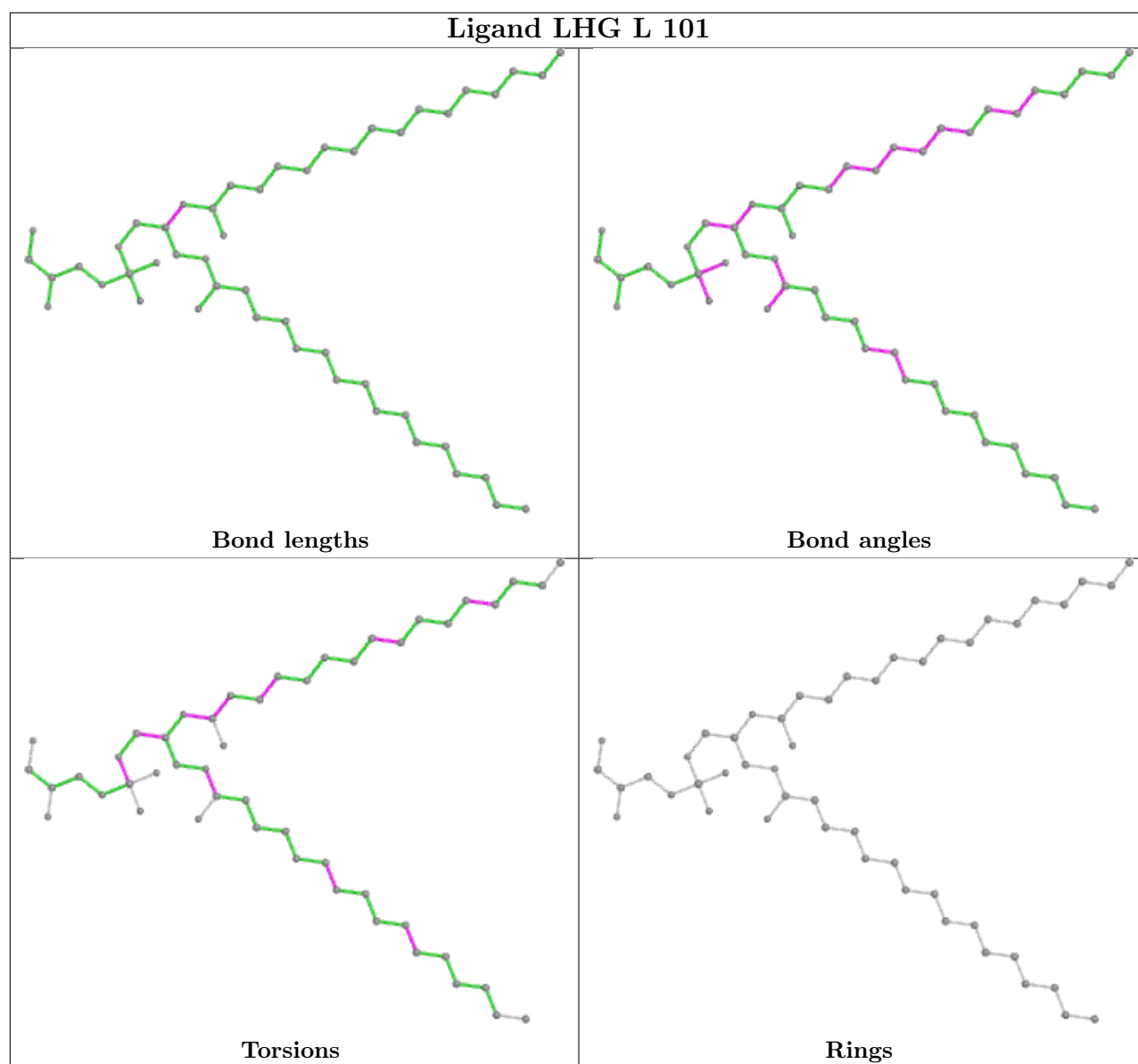


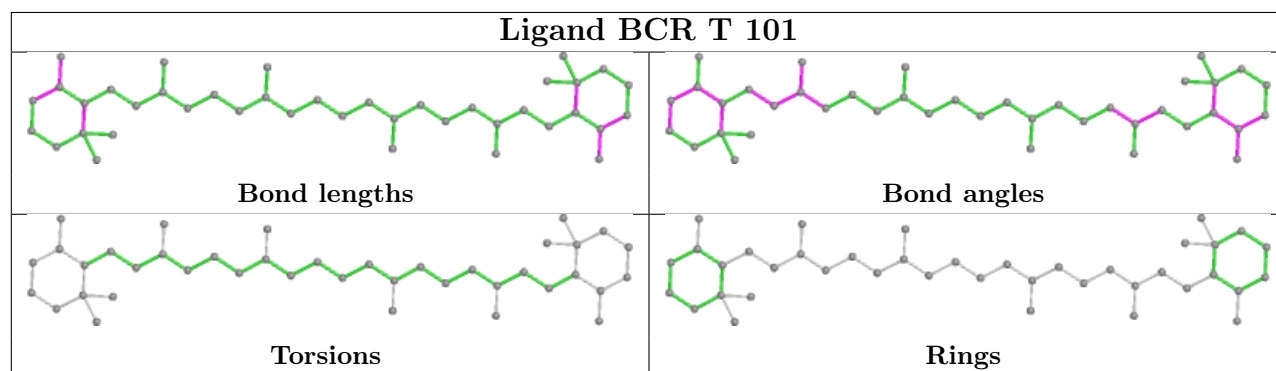
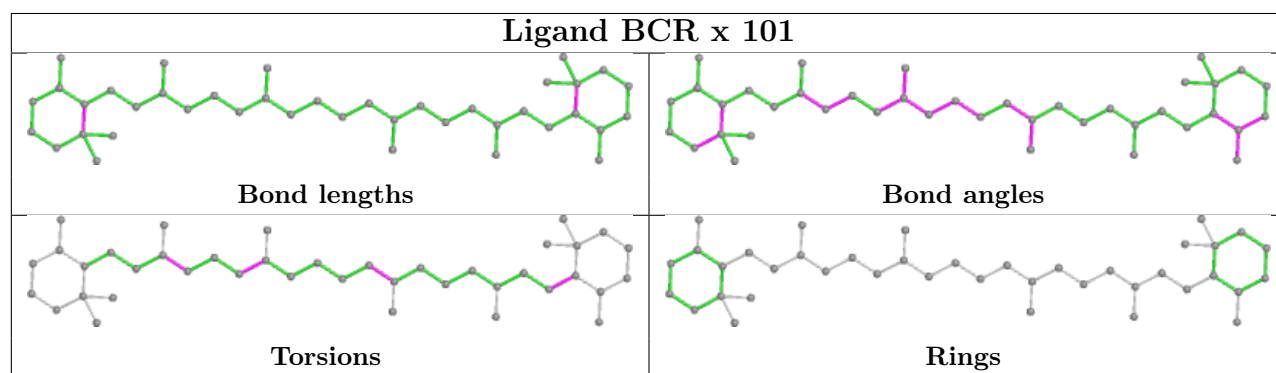
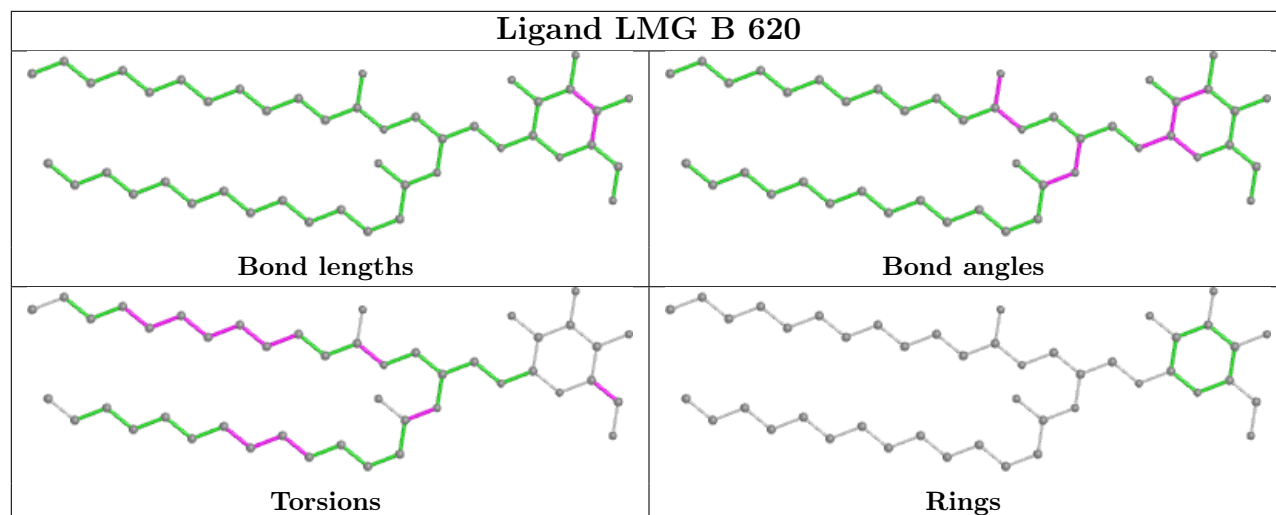
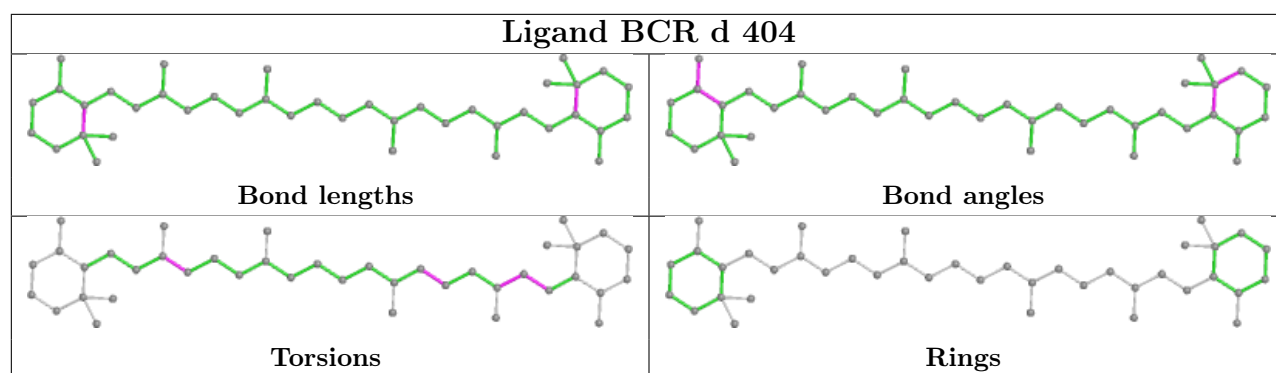


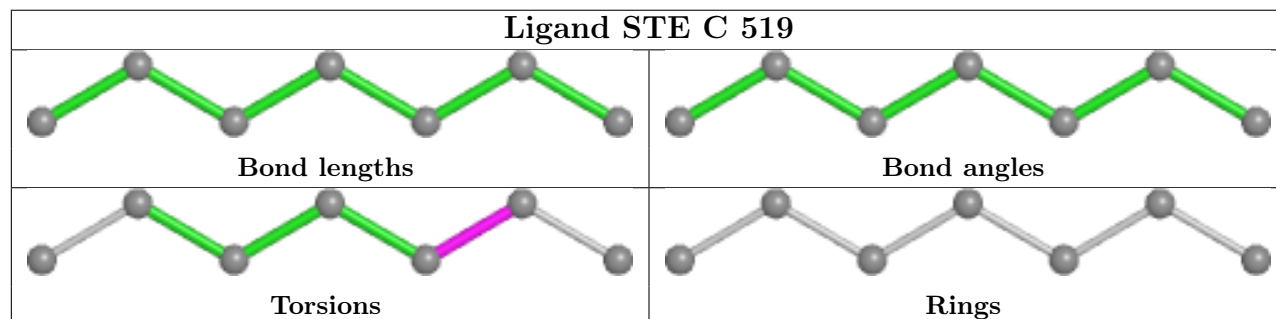
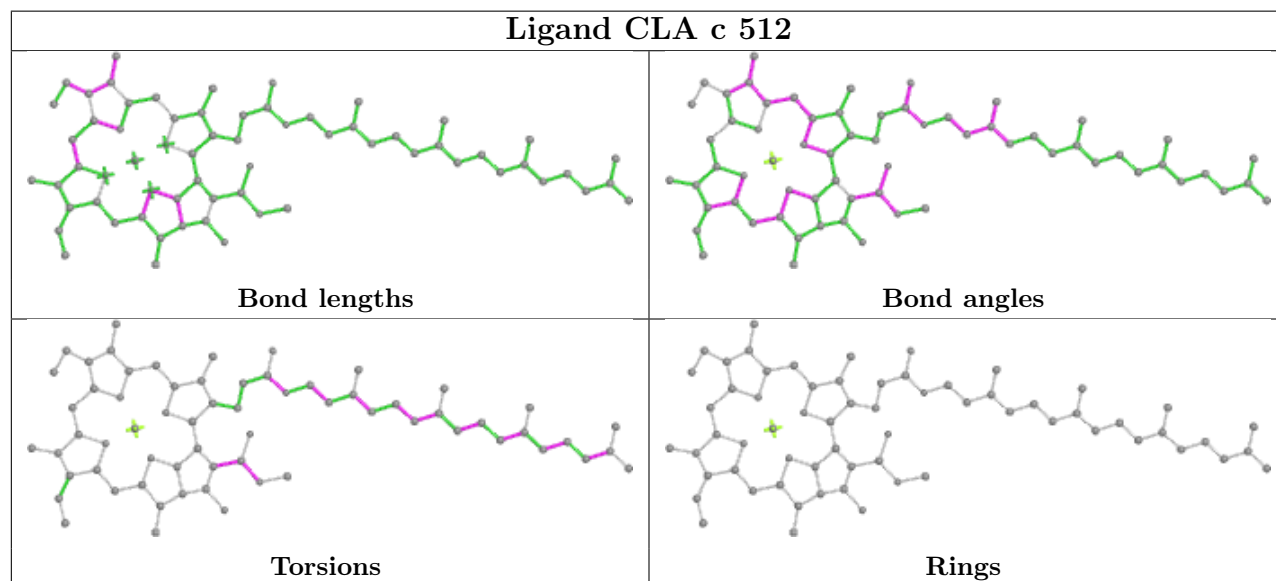
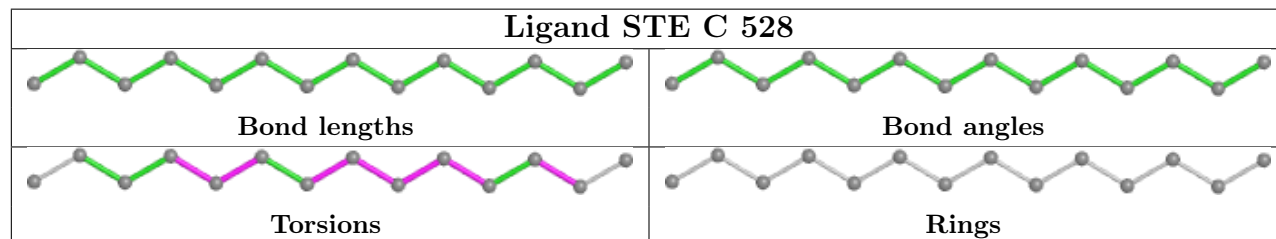
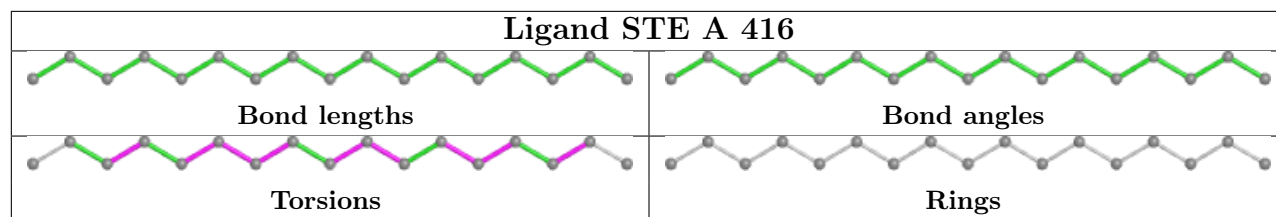


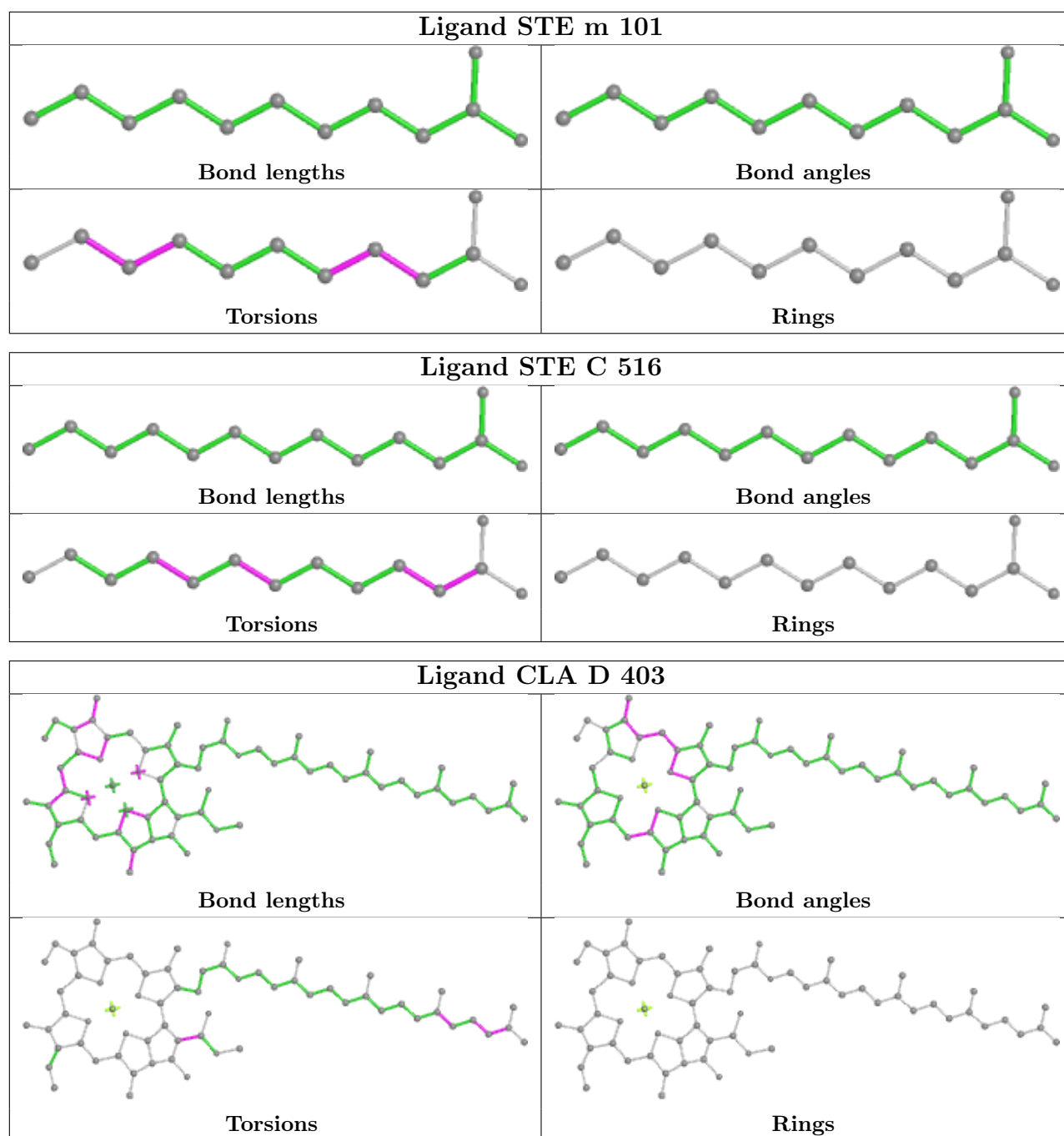


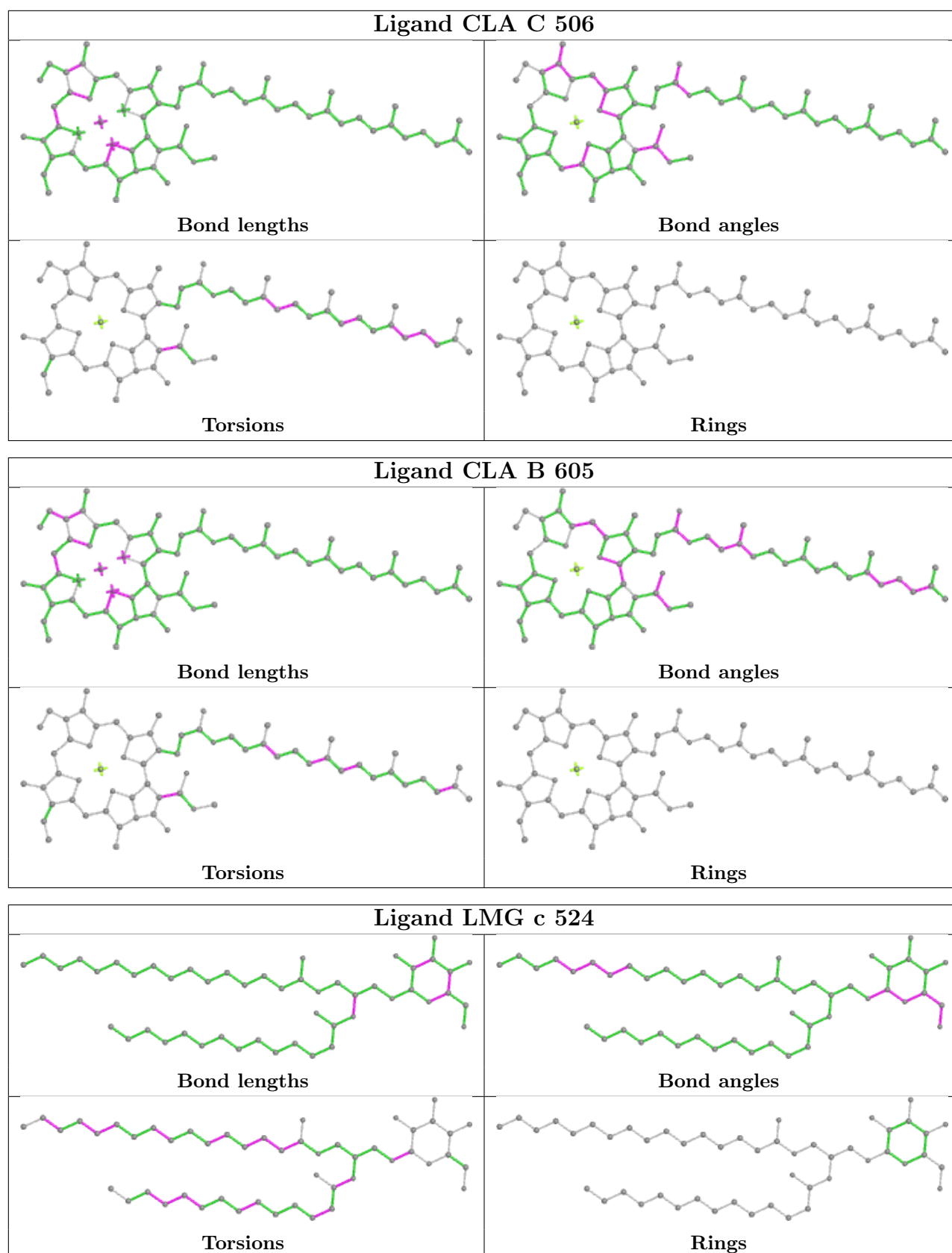


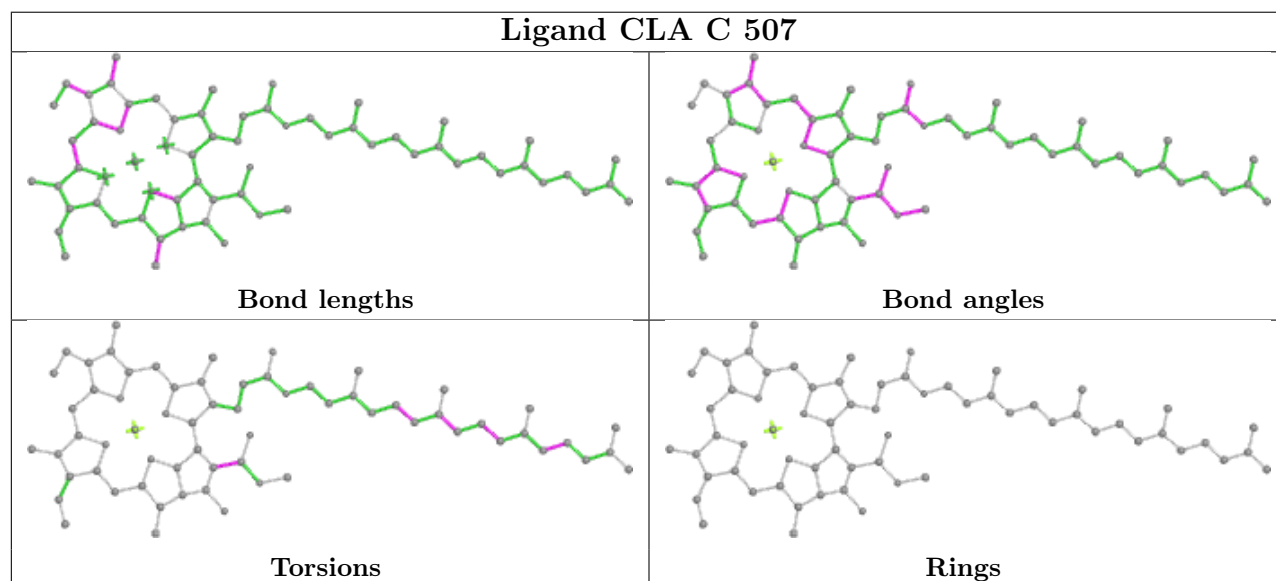
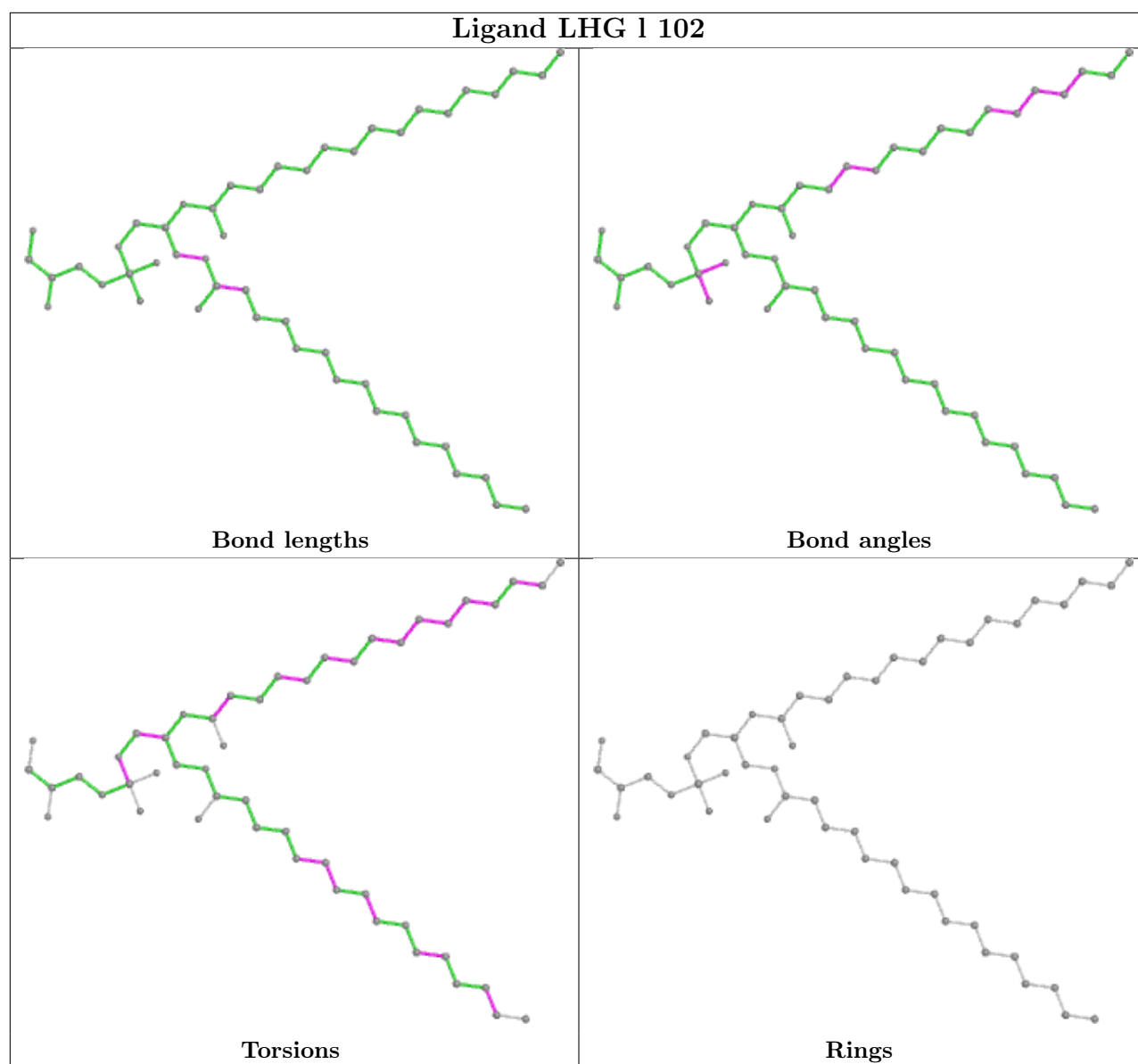


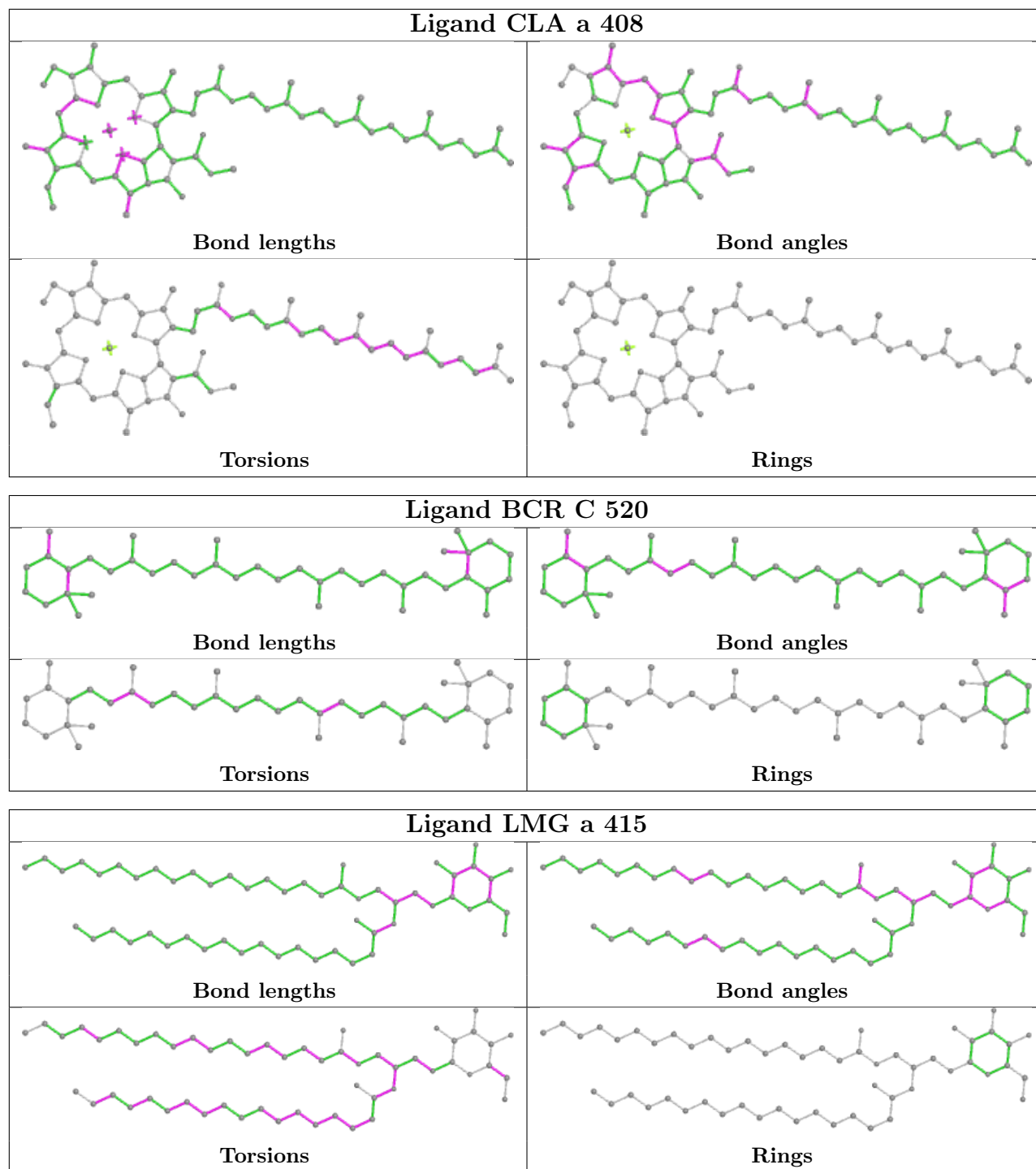




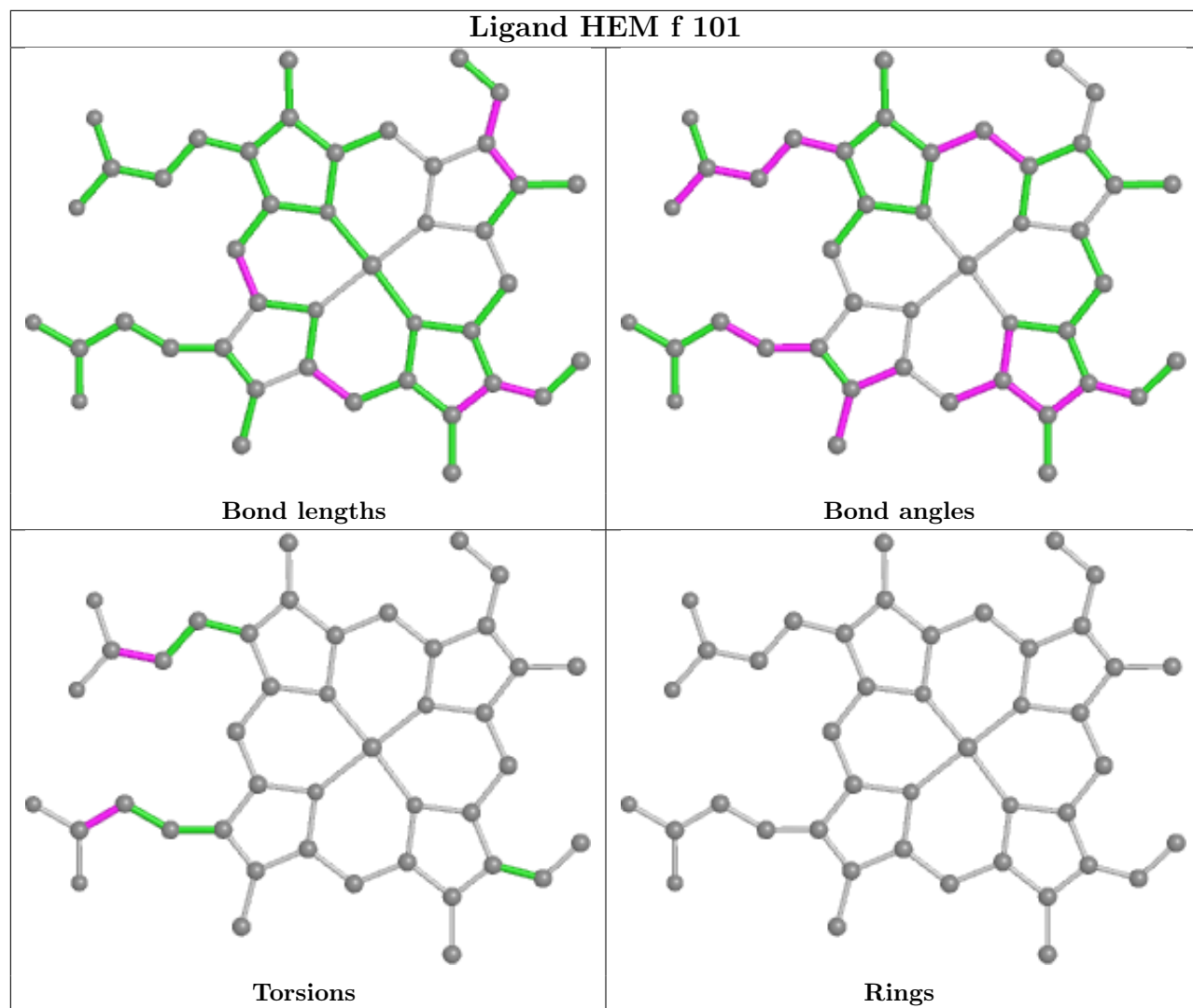


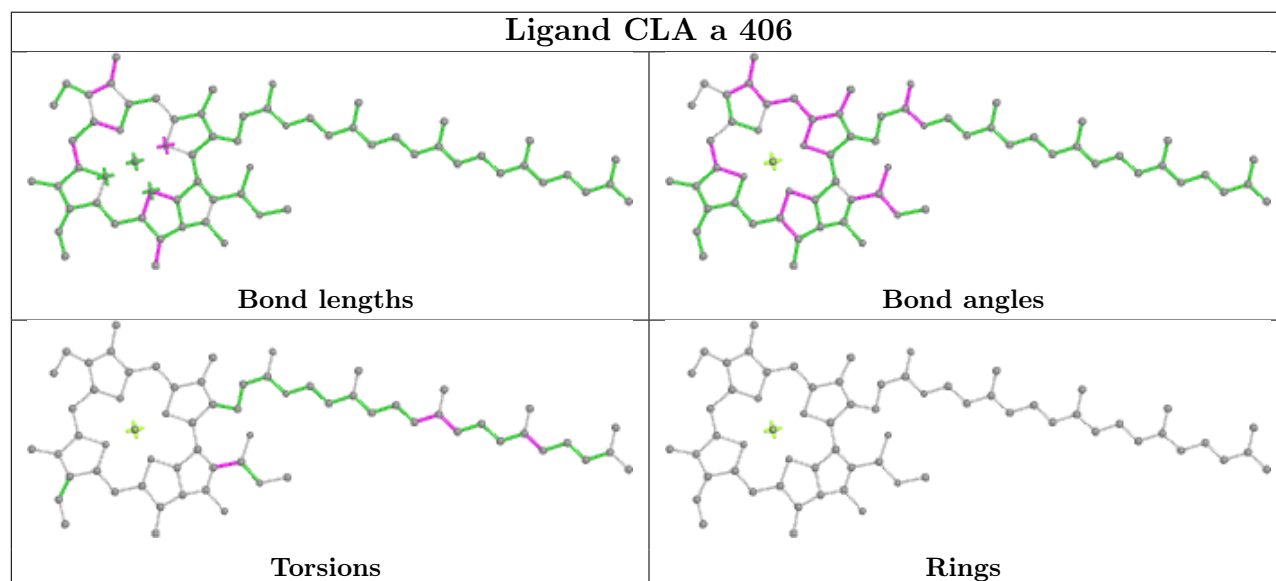
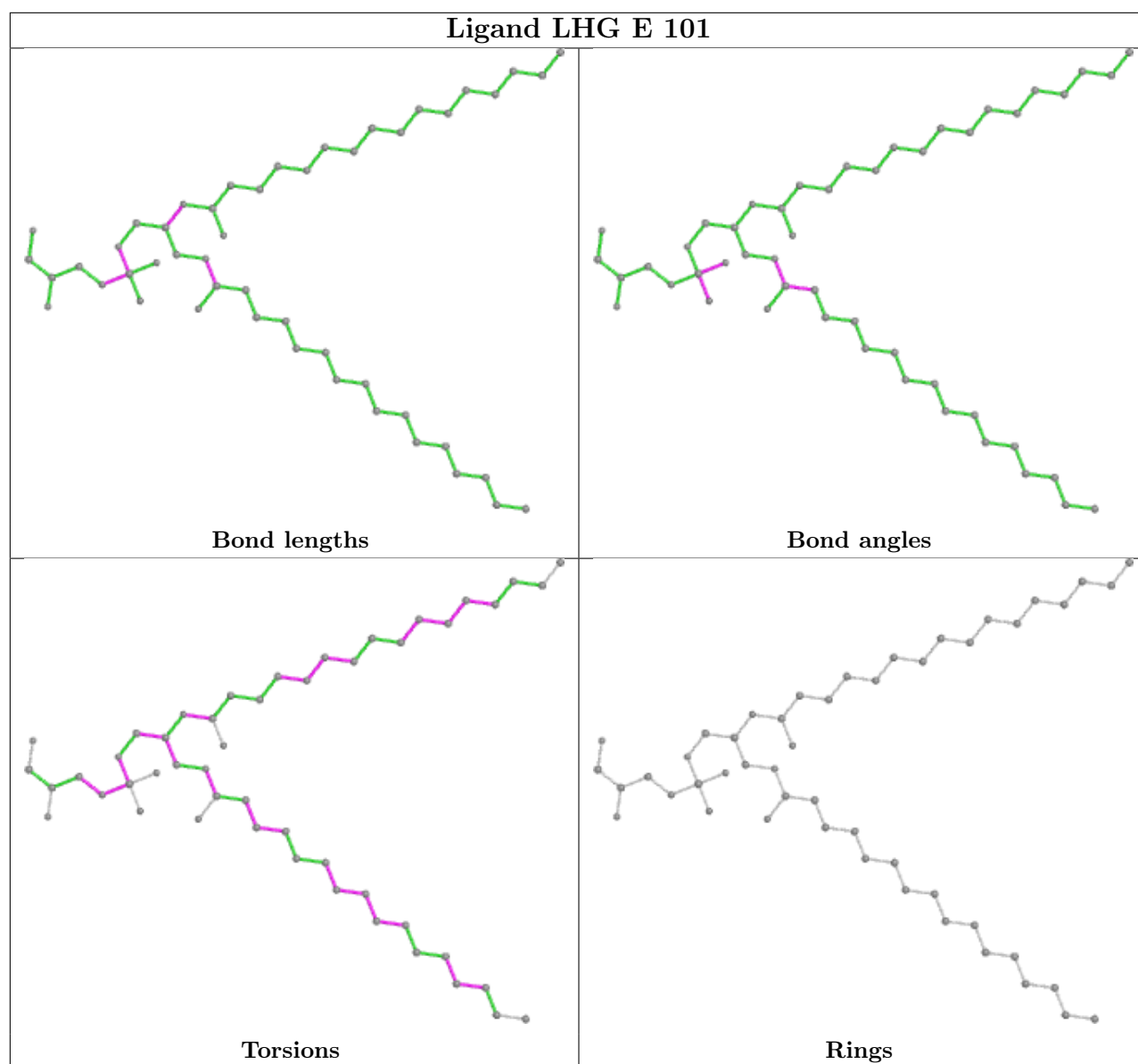


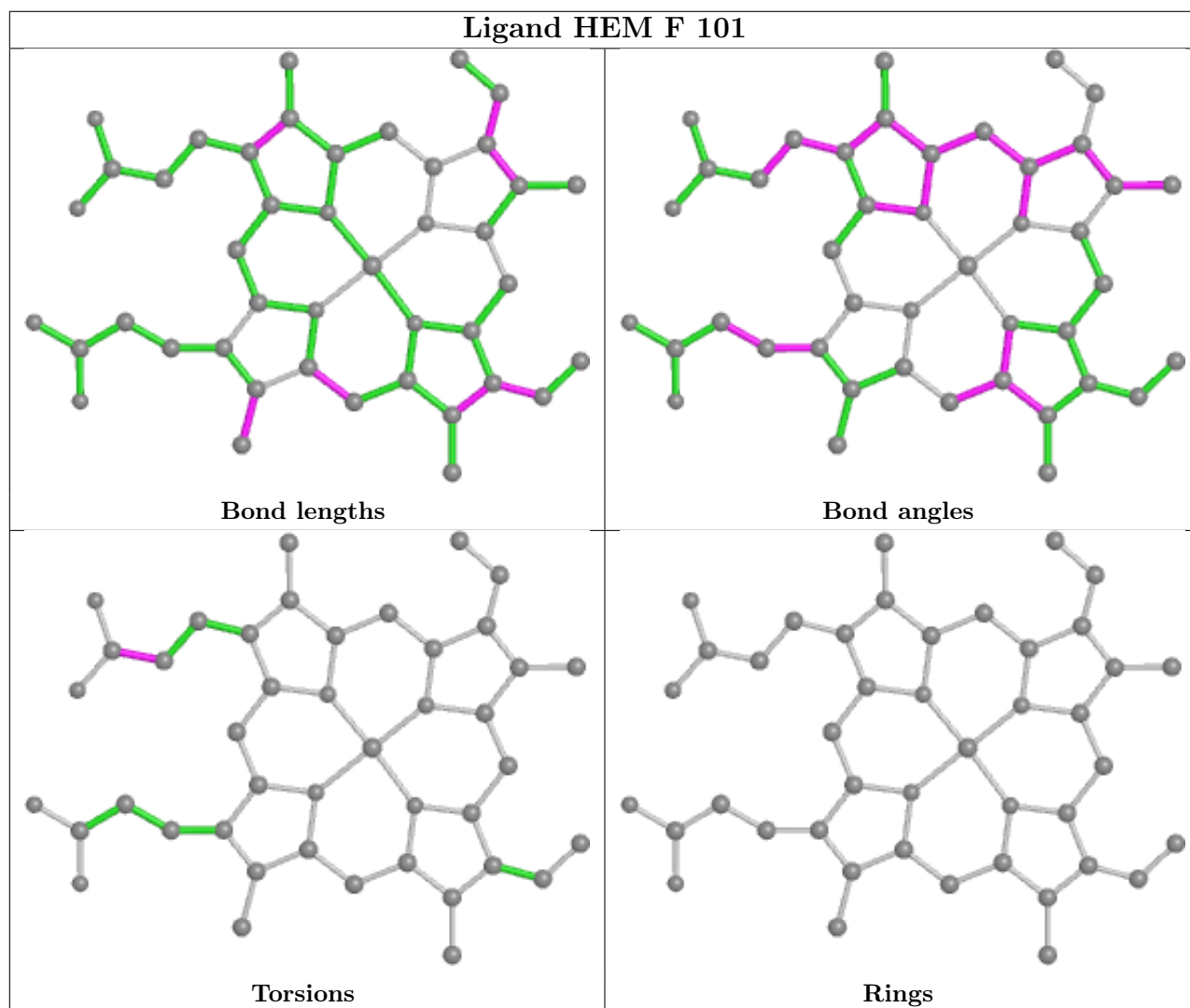
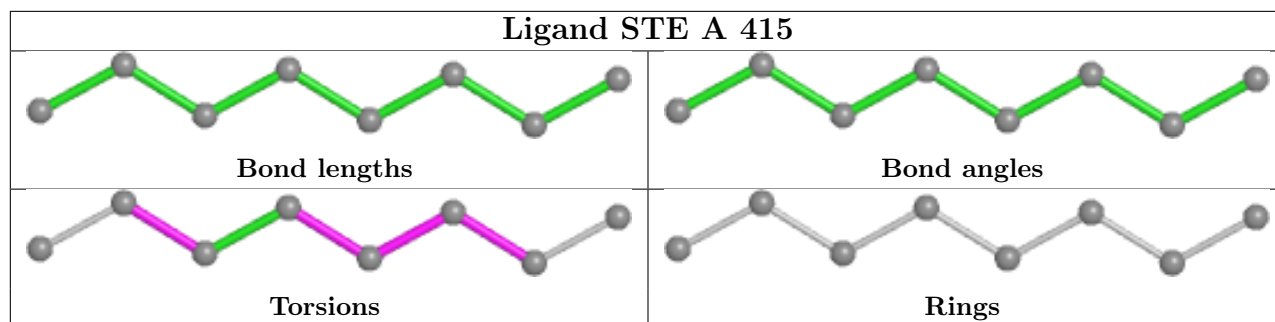


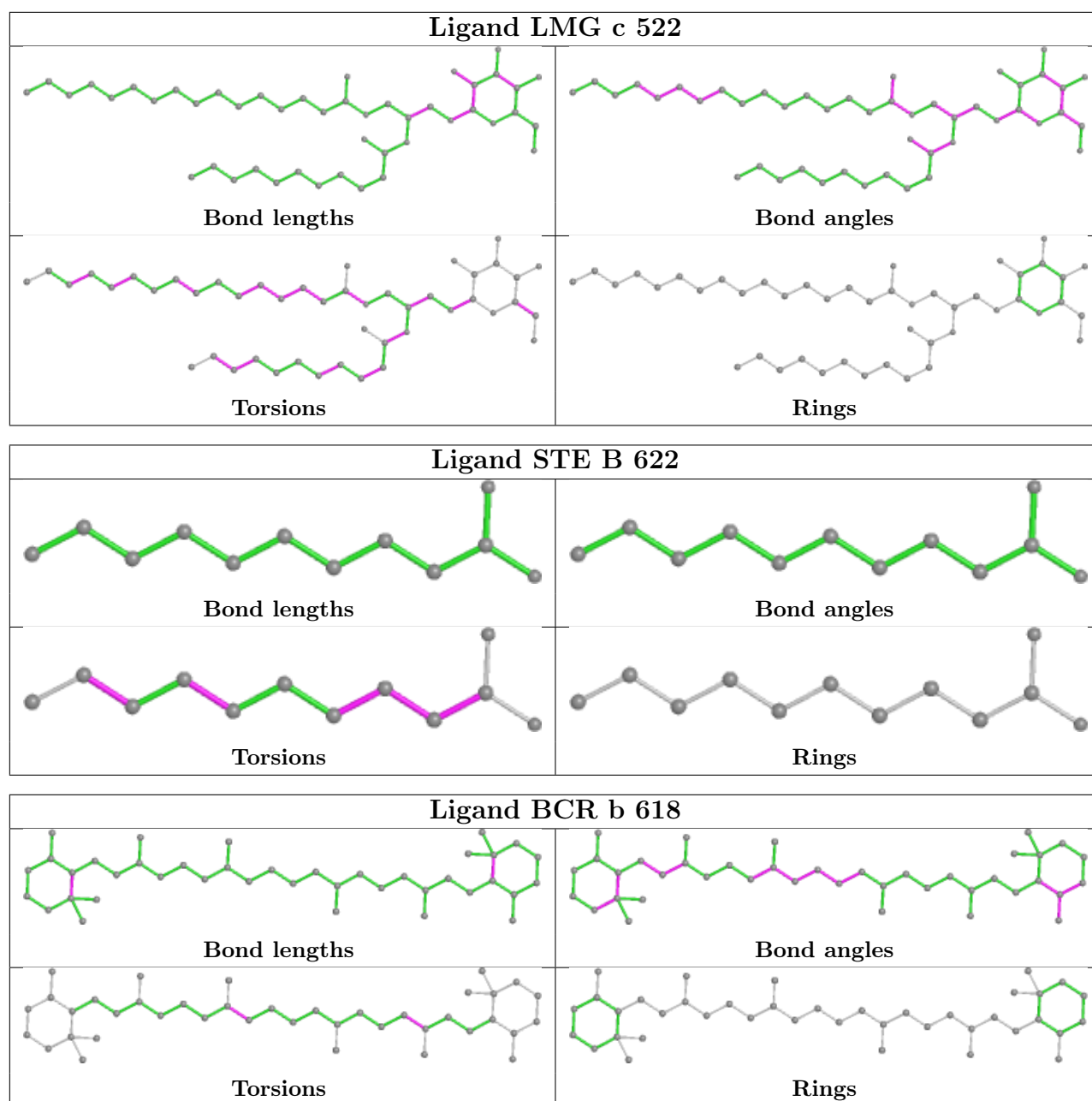


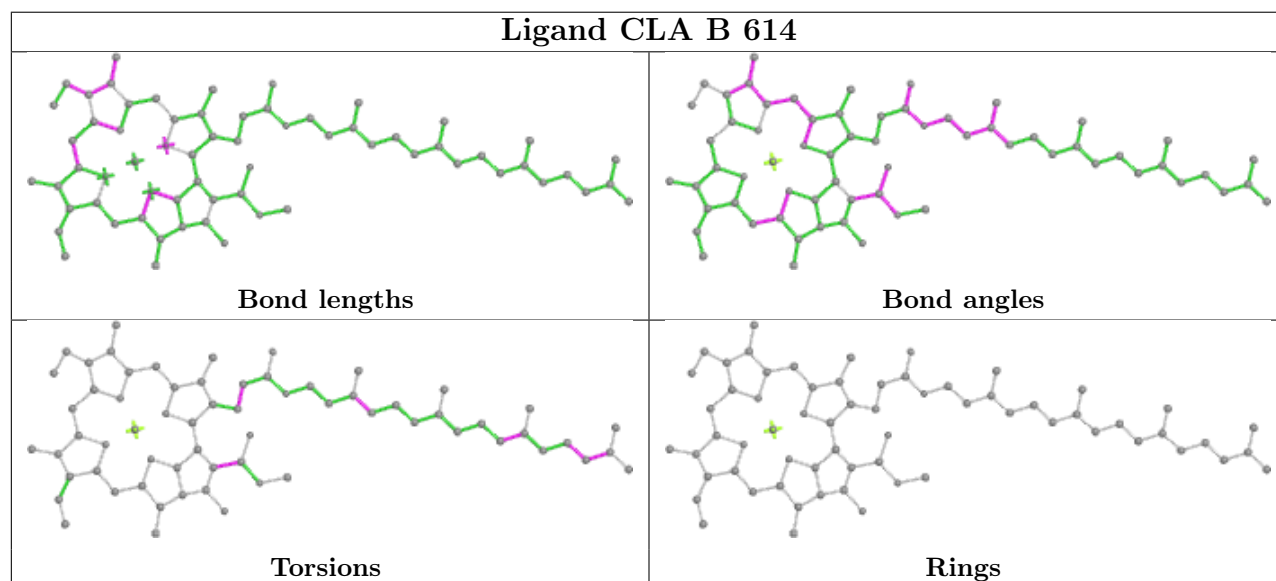
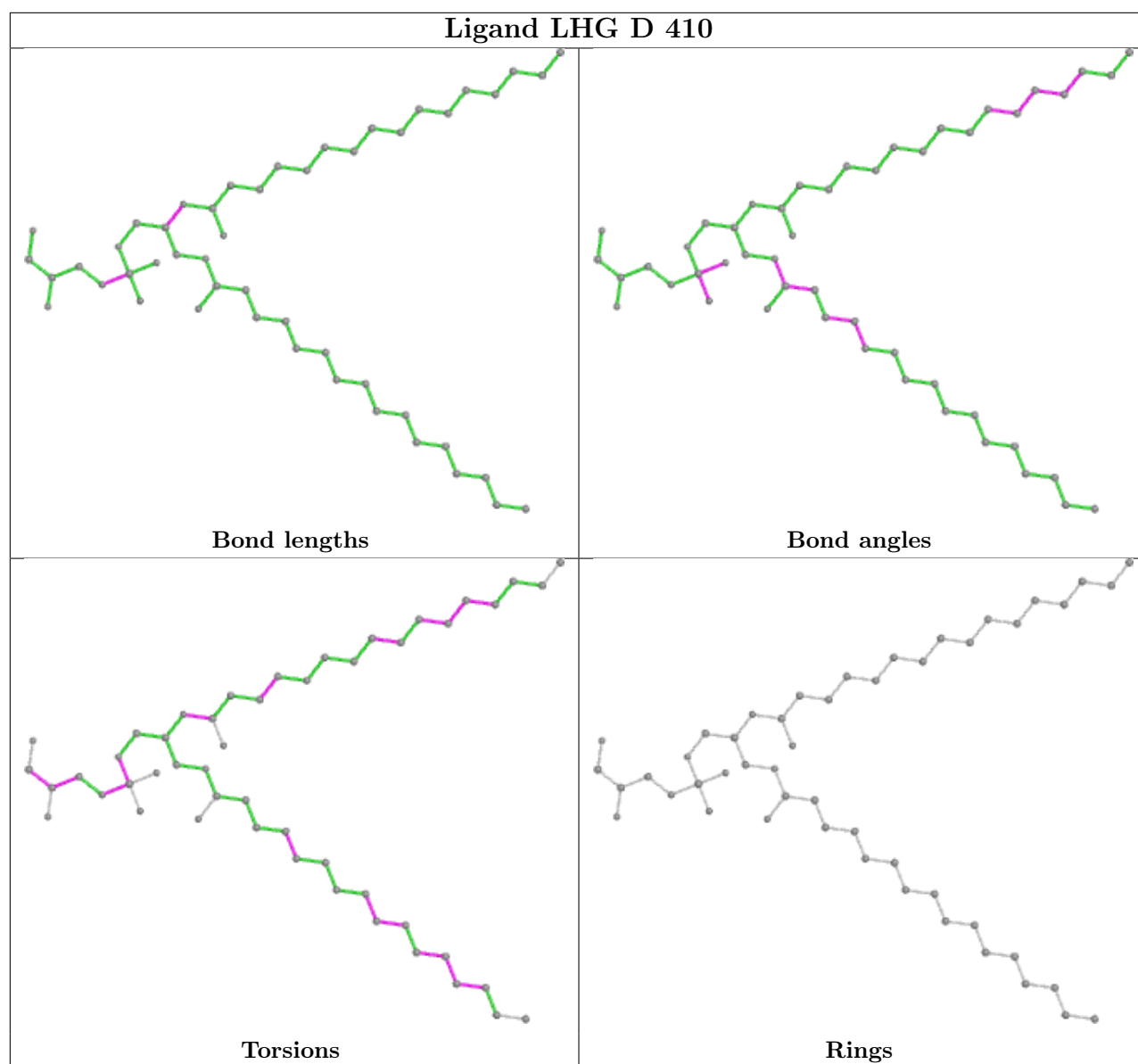


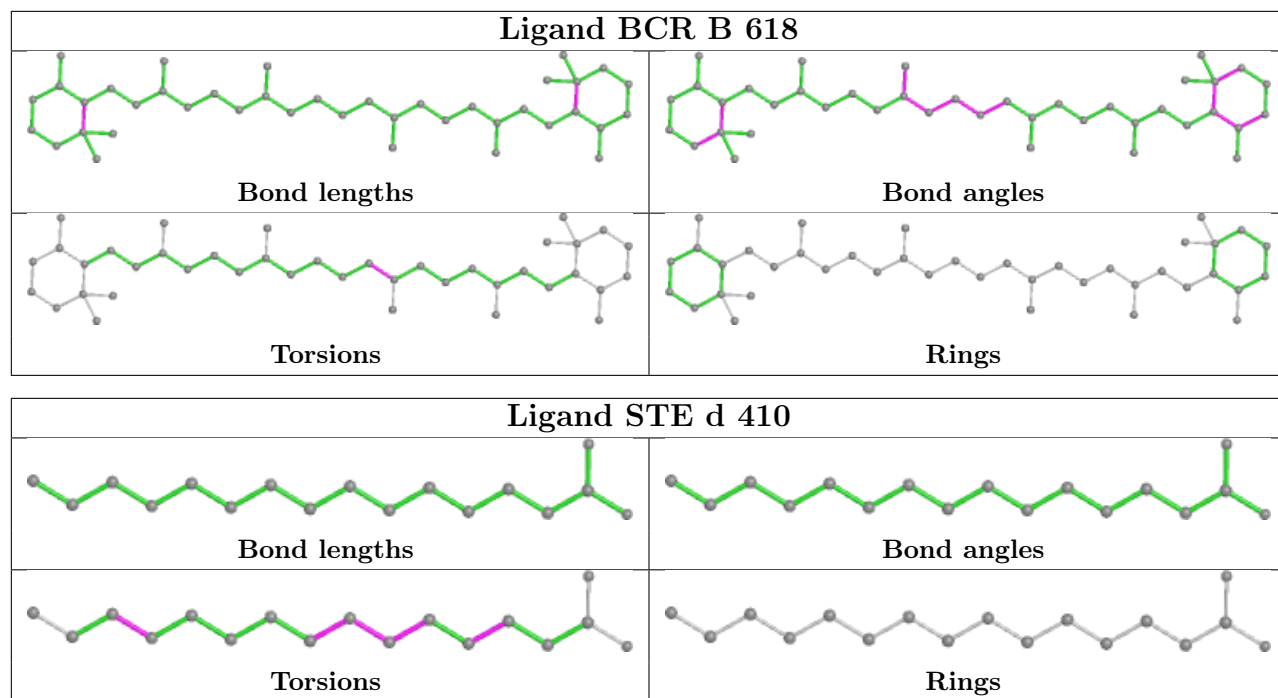


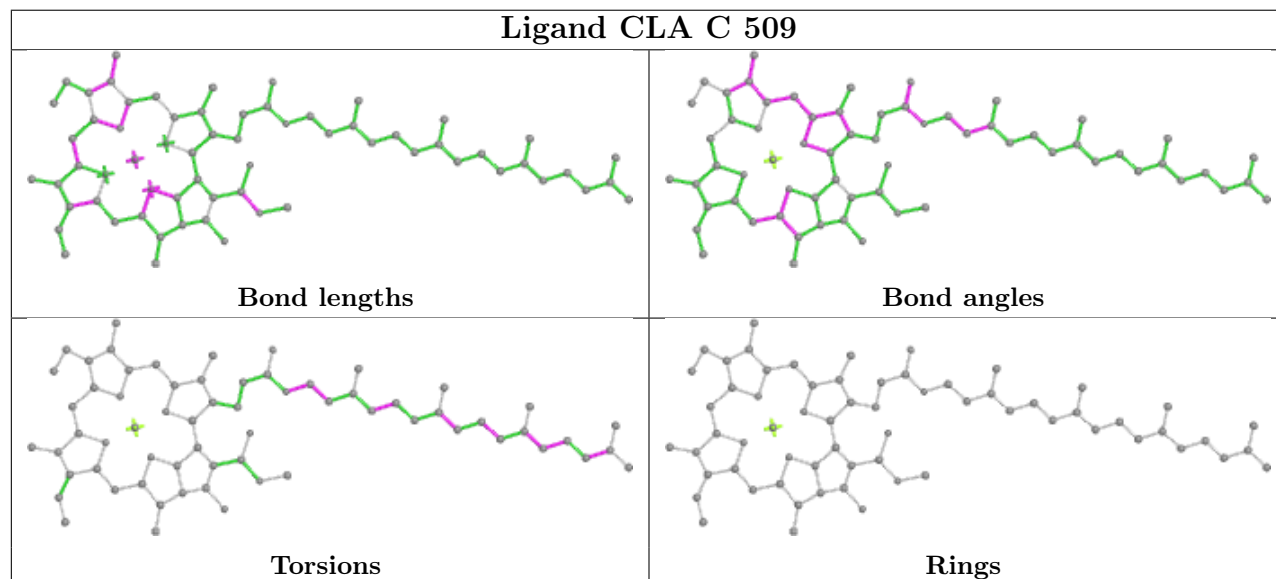
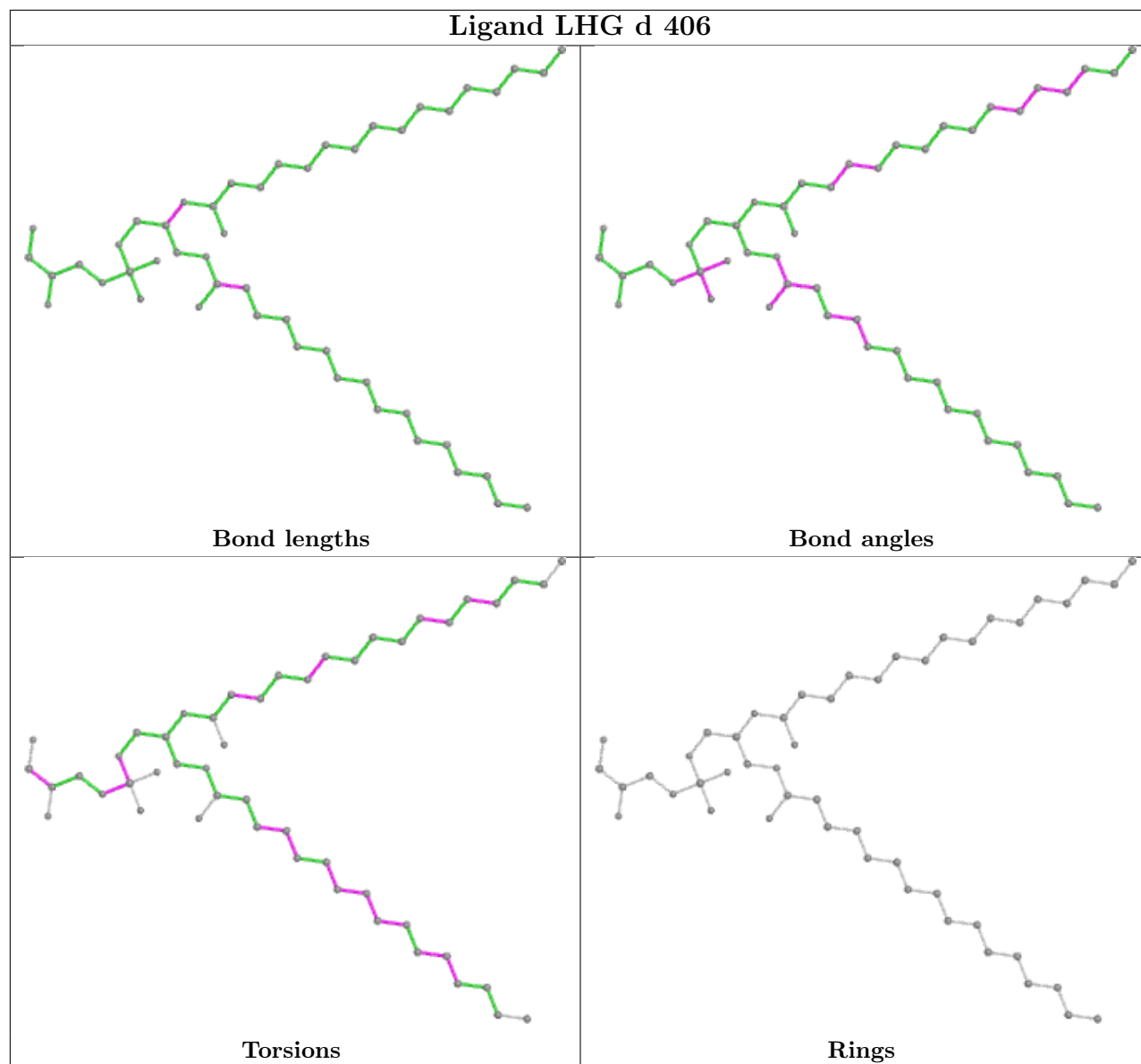


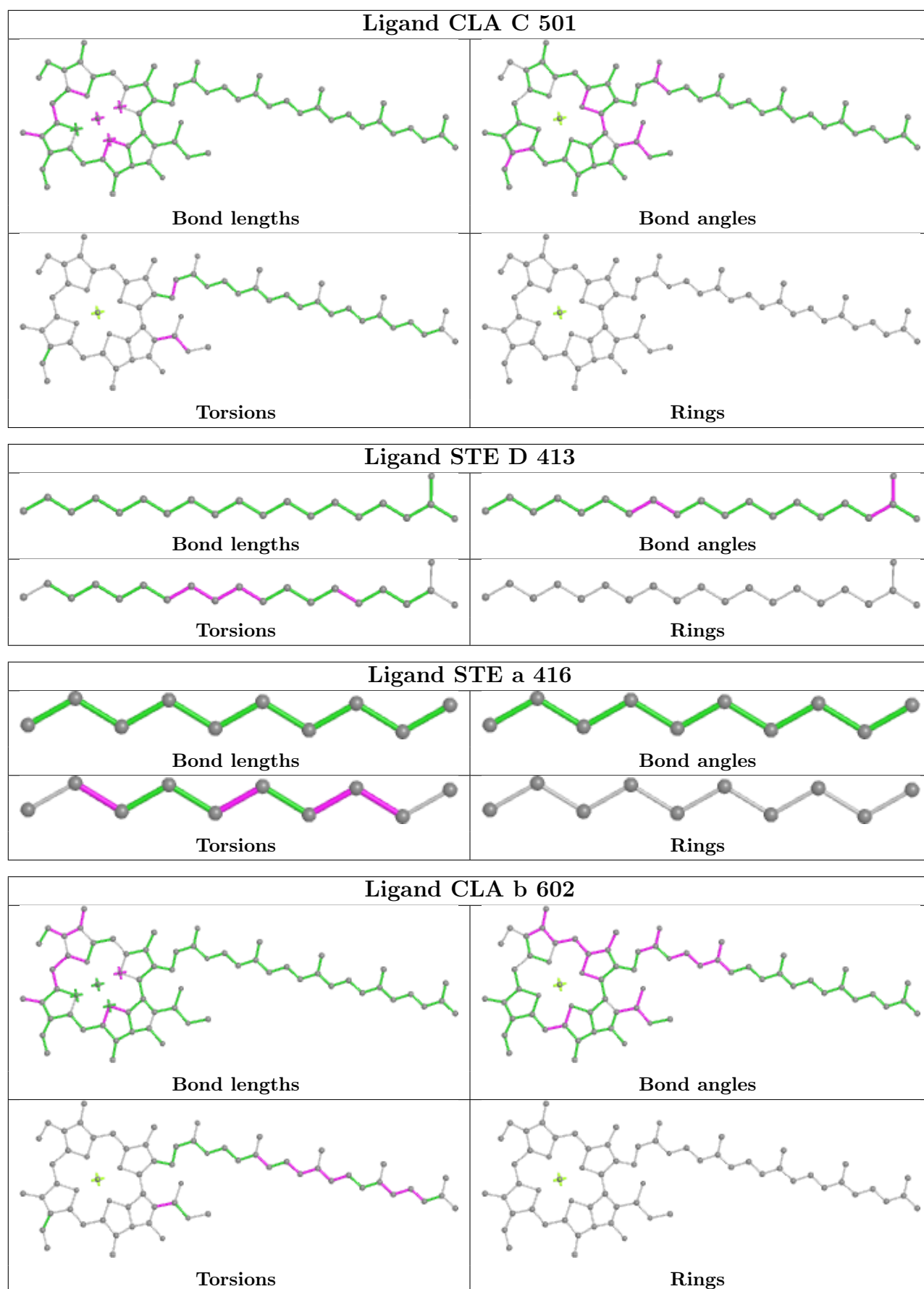




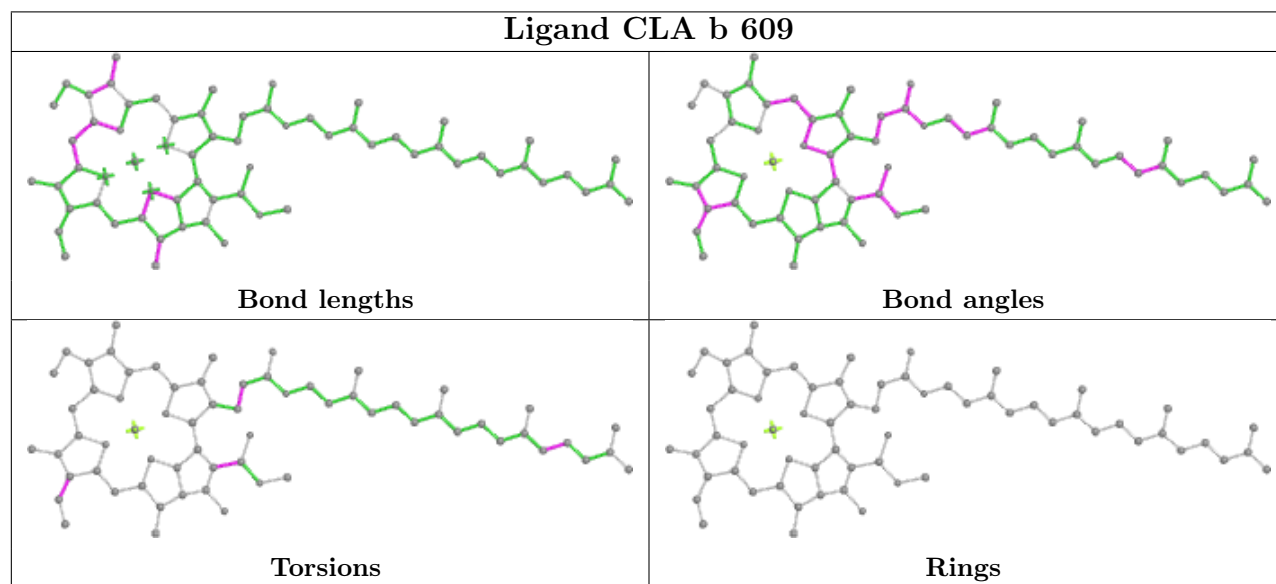
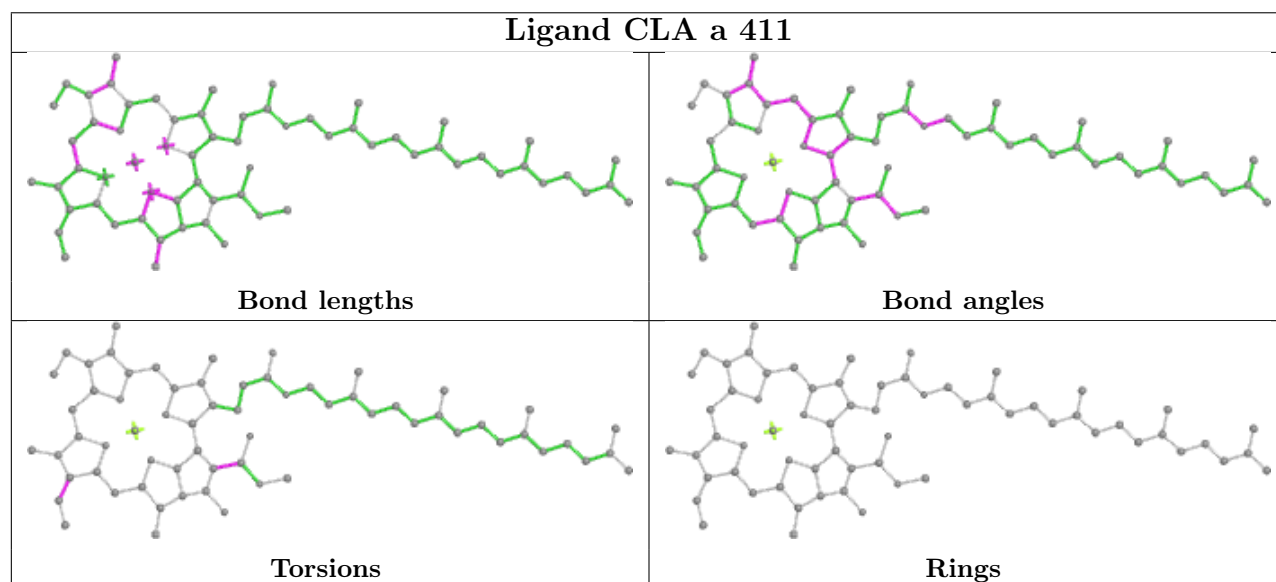
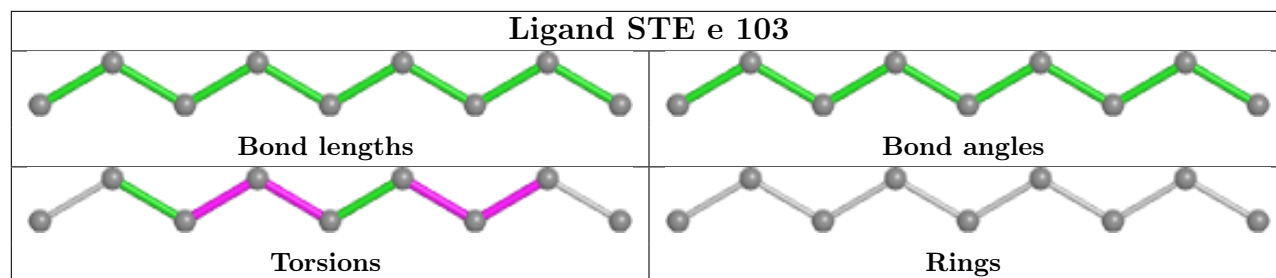


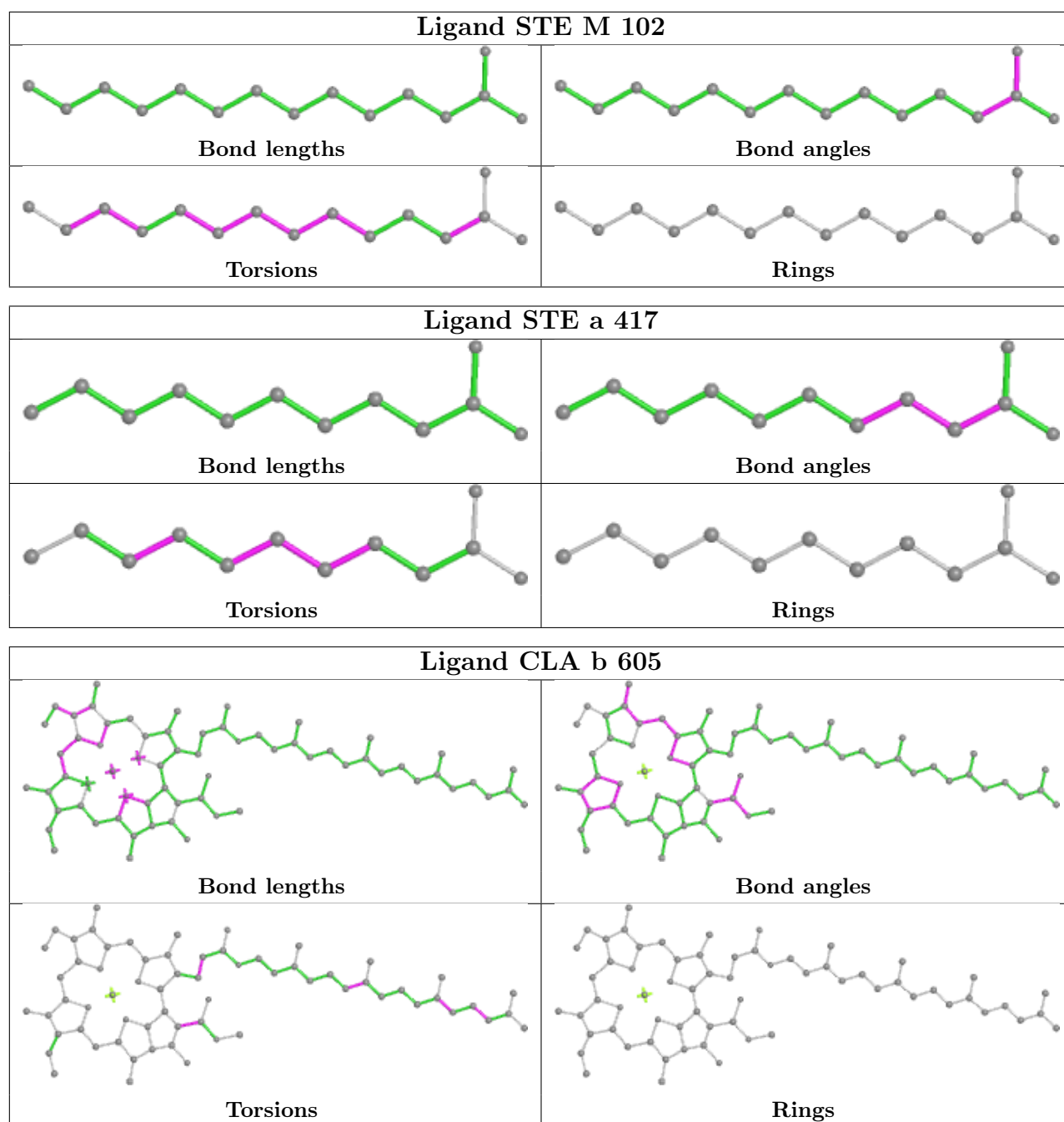


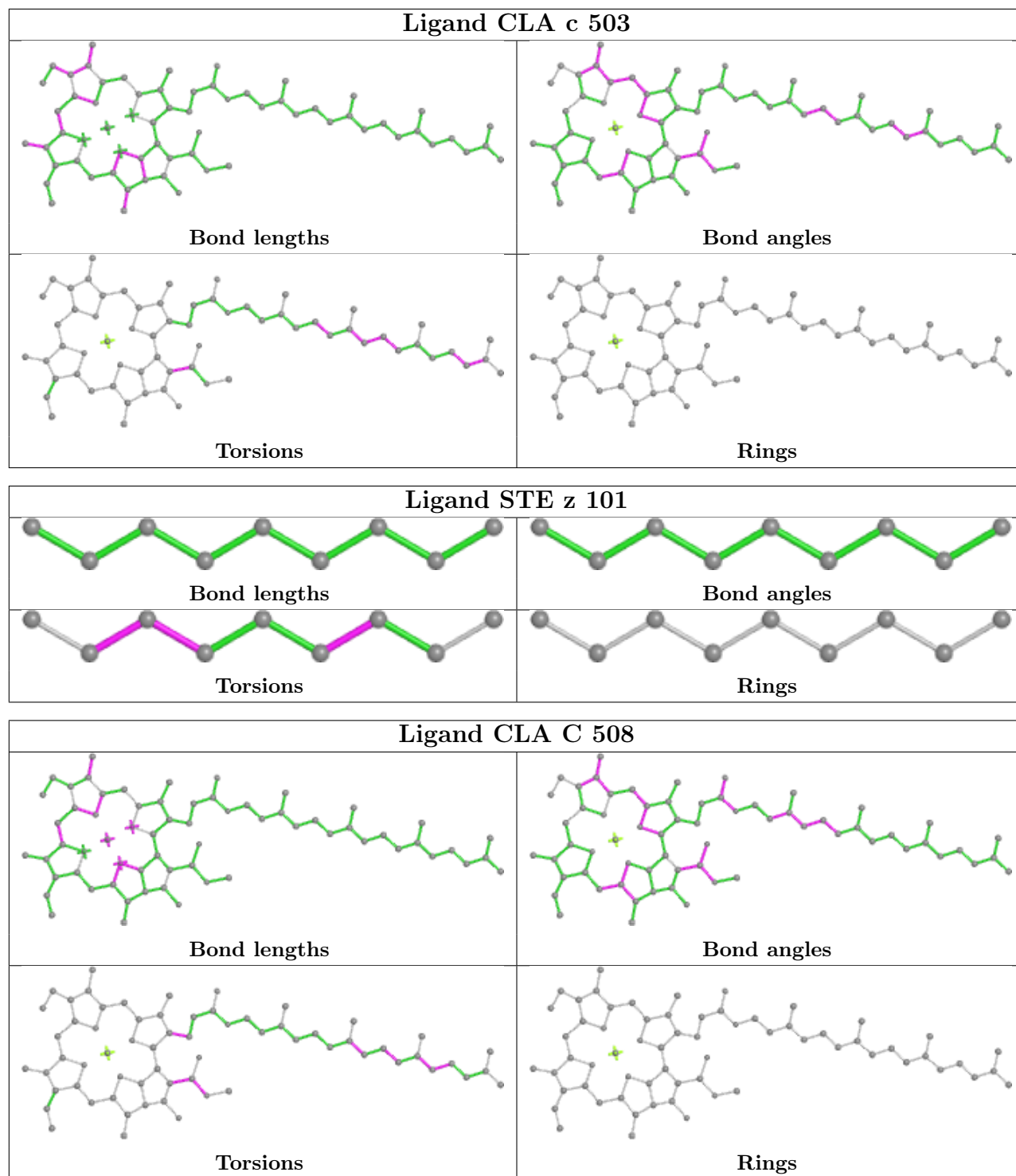


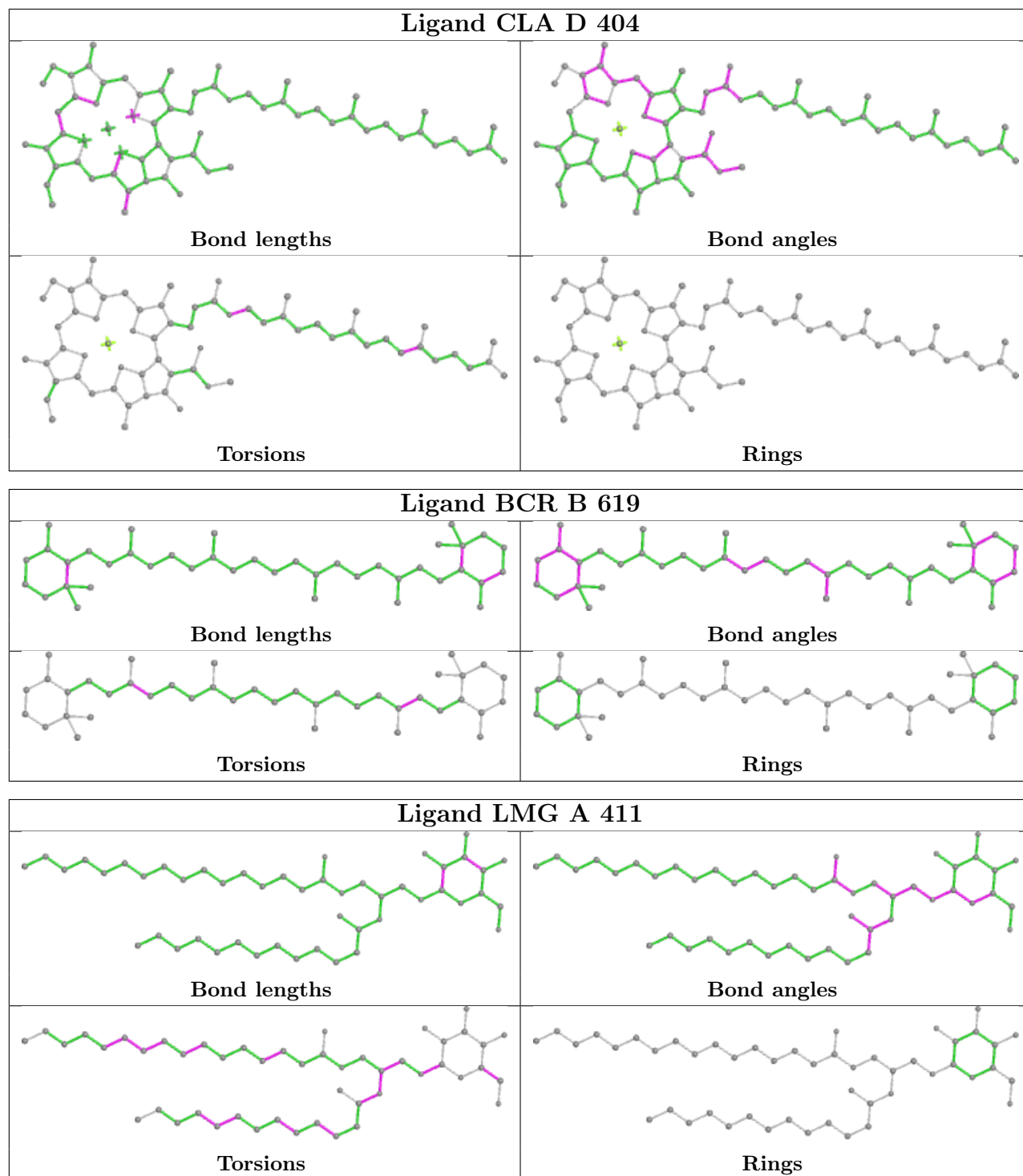


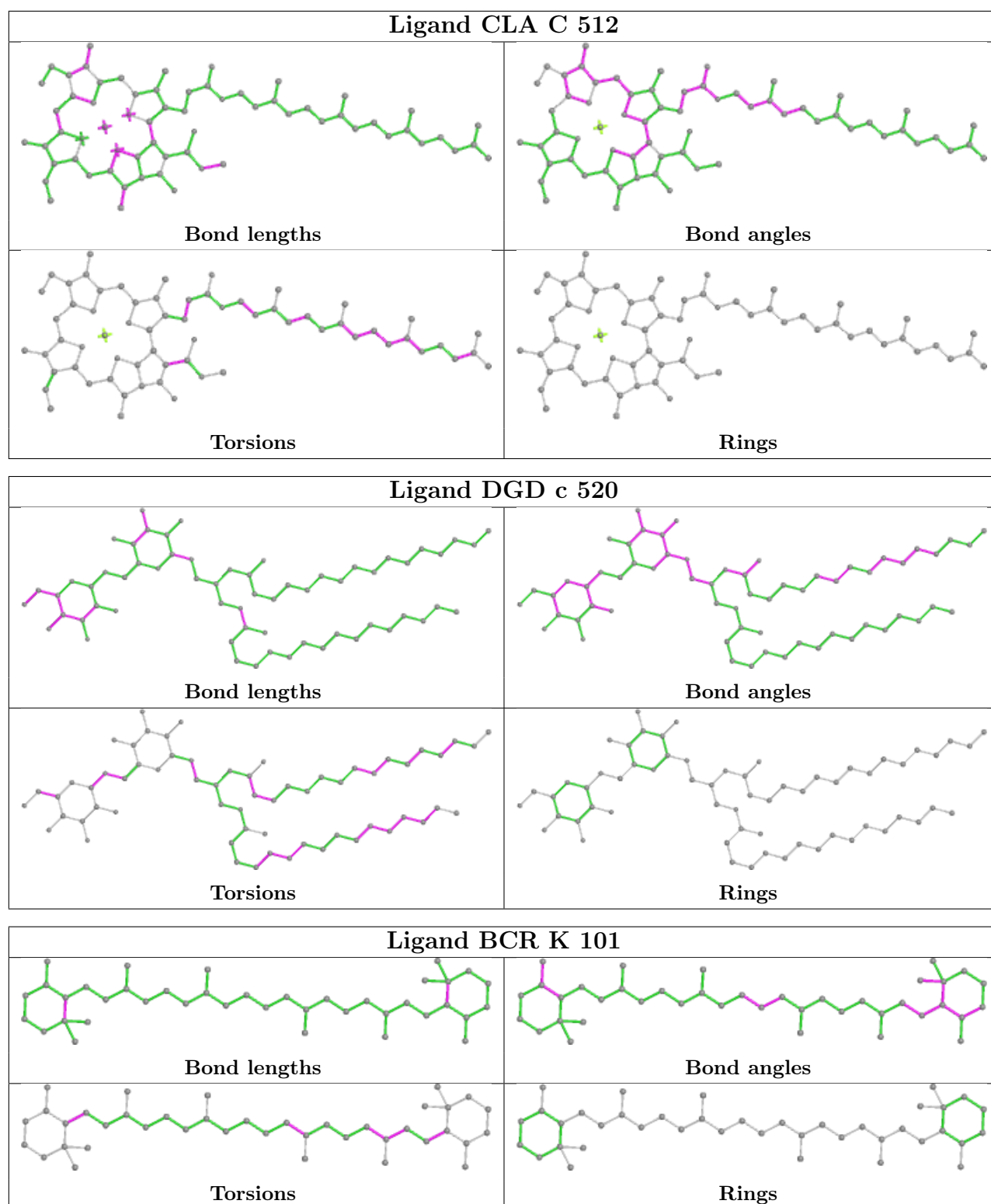


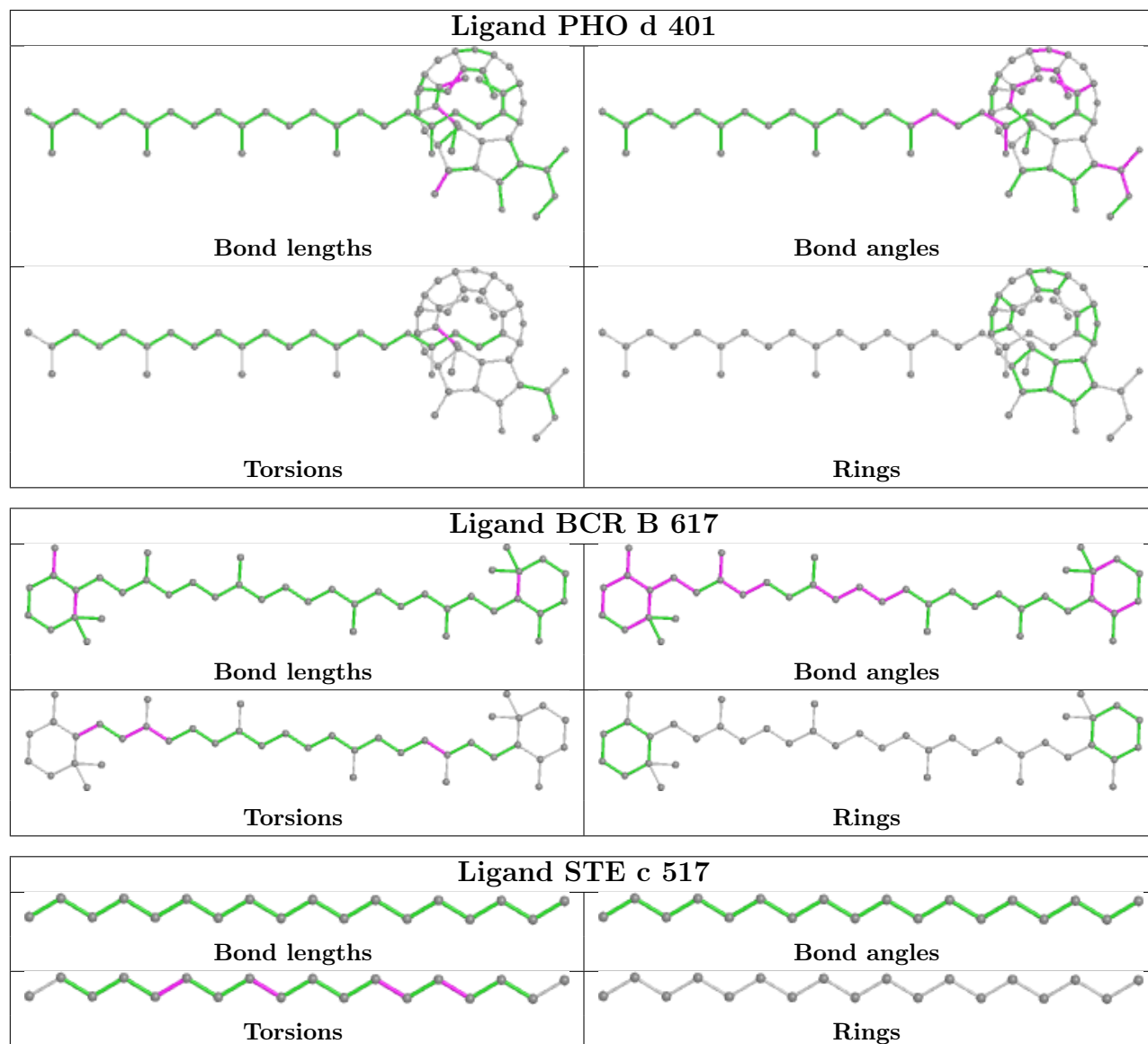


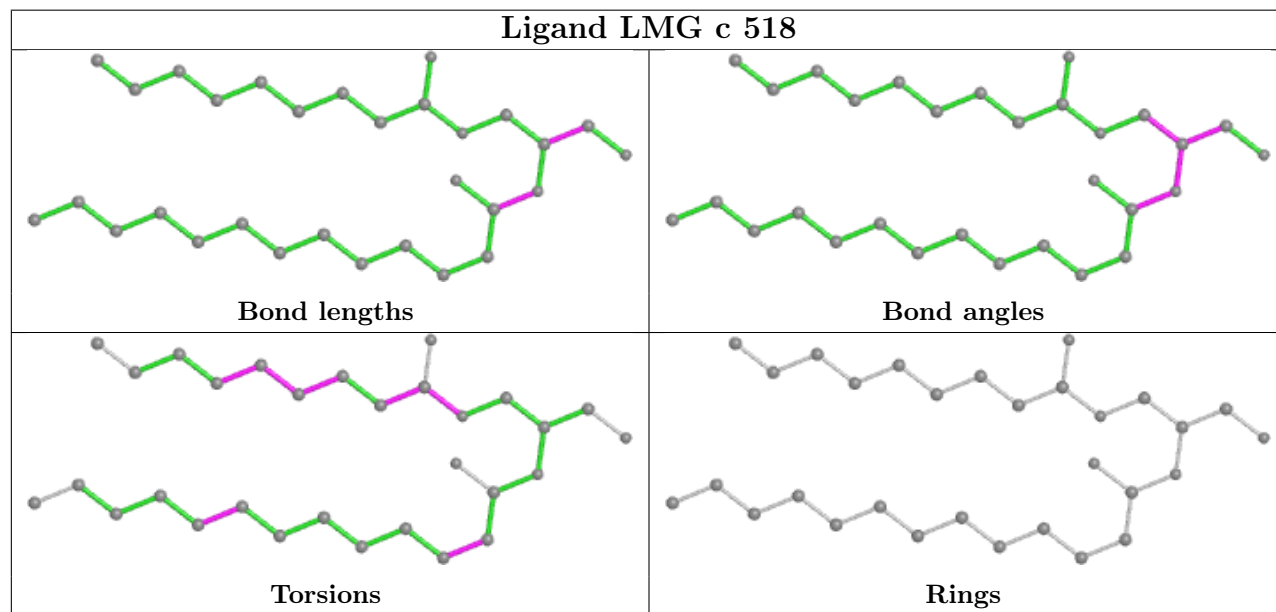
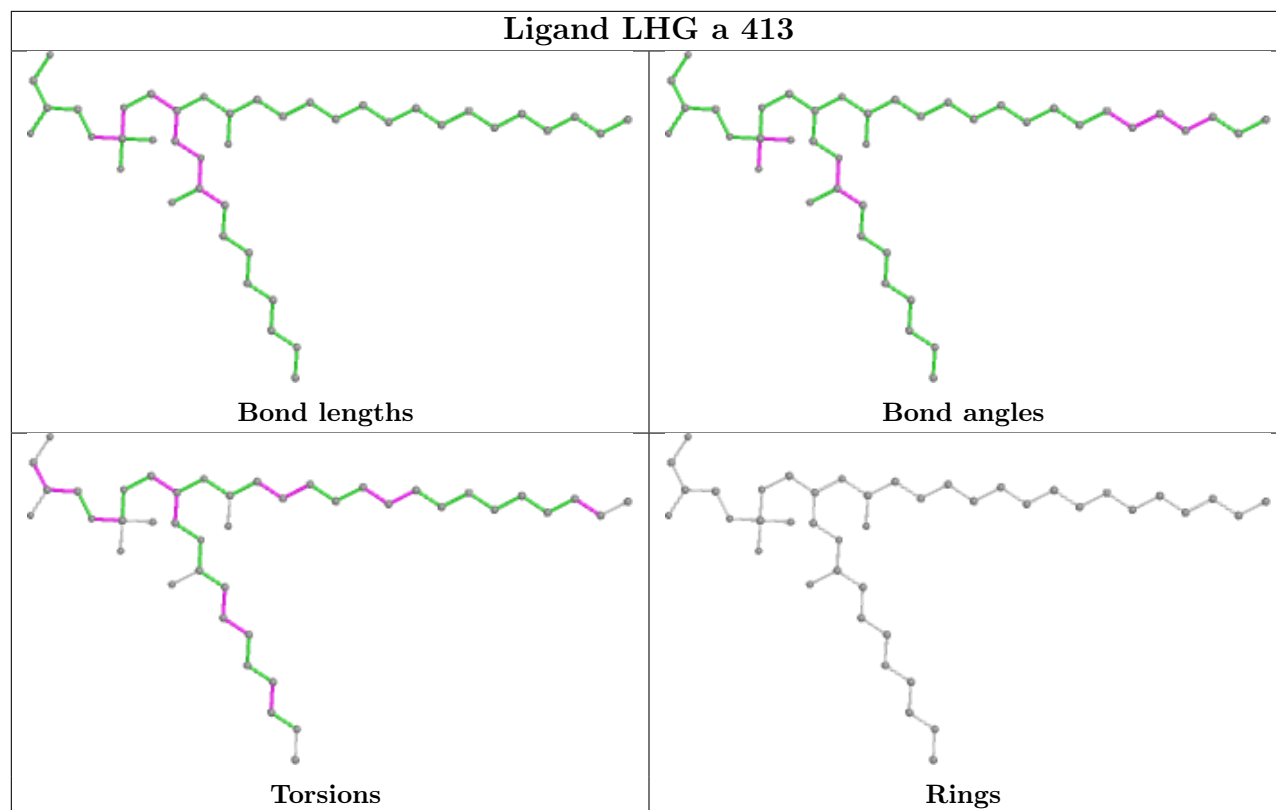


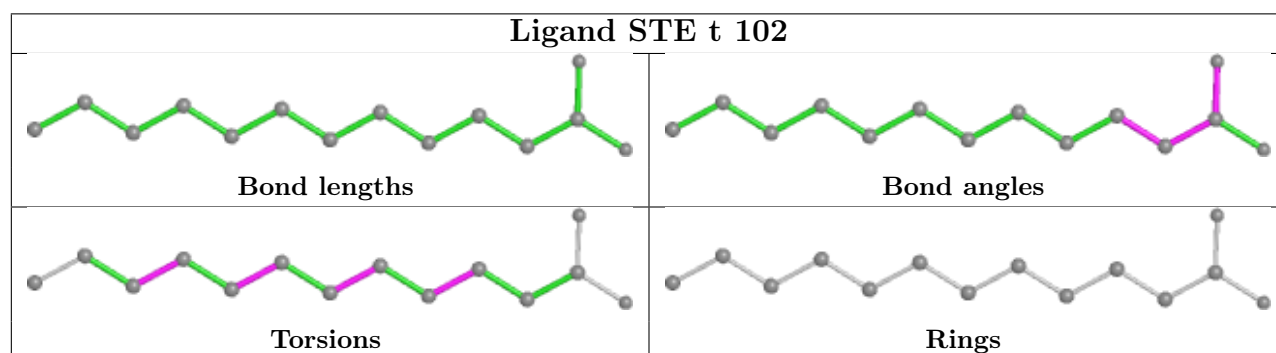
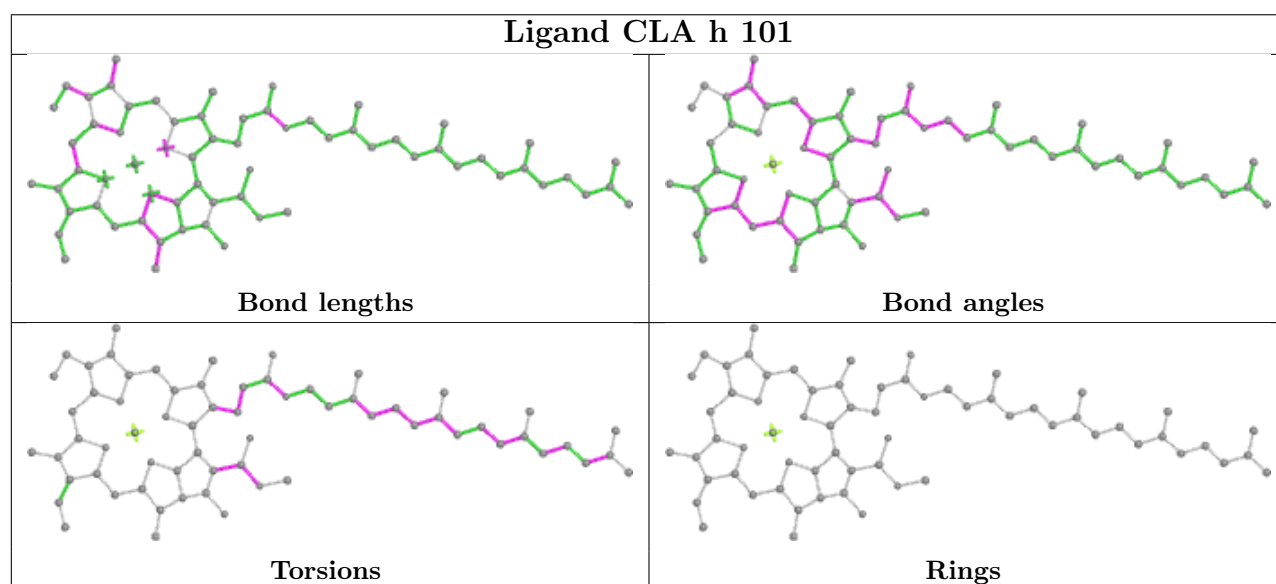
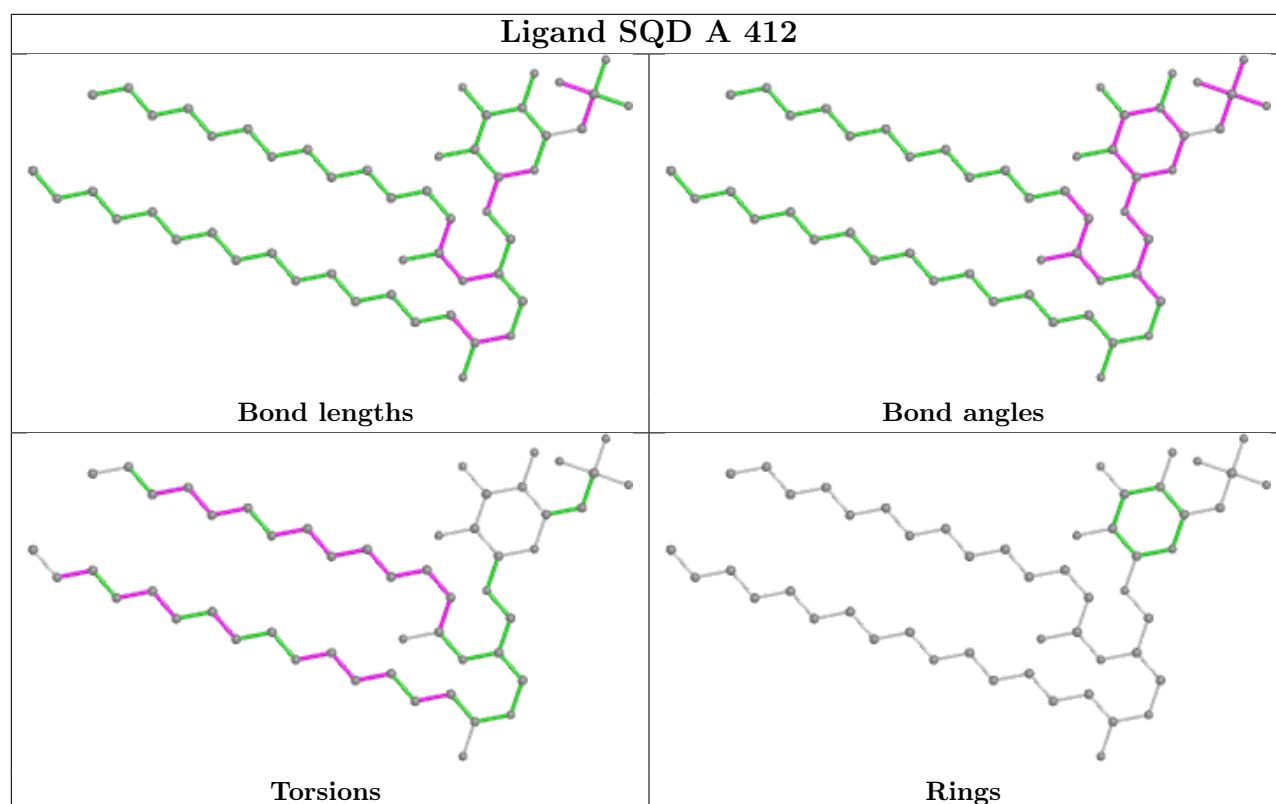














## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.13	3 (0%) 84 85	19, 25, 44, 77	0
1	a	334/344 (97%)	-0.17	4 (1%) 79 81	19, 27, 52, 79	0
2	B	505/510 (99%)	-0.12	9 (1%) 68 71	20, 29, 57, 88	0
2	b	505/510 (99%)	0.07	22 (4%) 34 37	23, 32, 67, 102	0
3	C	442/461 (95%)	-0.05	9 (2%) 65 68	21, 32, 48, 72	0
3	c	451/461 (97%)	0.03	10 (2%) 62 64	23, 35, 57, 92	0
4	D	341/352 (96%)	-0.09	1 (0%) 94 94	18, 26, 43, 76	0
4	d	341/352 (96%)	-0.09	0 100 100	21, 30, 53, 71	0
5	E	82/84 (97%)	0.37	7 (8%) 10 12	30, 45, 64, 75	0
5	e	82/84 (97%)	0.58	12 (14%) 2 2	34, 54, 73, 83	0
6	F	34/45 (75%)	-0.00	3 (8%) 10 11	32, 38, 59, 83	0
6	f	34/45 (75%)	0.11	2 (5%) 22 25	37, 45, 75, 94	0
7	H	65/66 (98%)	0.12	3 (4%) 32 35	27, 37, 56, 75	0
7	h	63/66 (95%)	0.45	5 (7%) 12 14	36, 45, 61, 70	0
8	I	35/38 (92%)	-0.03	2 (5%) 23 26	27, 34, 65, 77	0
8	i	35/38 (92%)	0.09	3 (8%) 10 12	28, 36, 72, 81	0
9	J	36/40 (90%)	0.22	4 (11%) 5 6	29, 45, 69, 87	0
9	j	36/40 (90%)	0.46	5 (13%) 2 3	34, 48, 82, 86	0
10	K	37/46 (80%)	0.38	3 (8%) 12 13	37, 45, 66, 72	0
10	k	37/46 (80%)	0.23	3 (8%) 12 13	43, 49, 61, 74	0
11	L	37/37 (100%)	-0.23	0 100 100	20, 25, 62, 70	0
11	l	36/37 (97%)	-0.13	2 (5%) 24 27	22, 26, 69, 77	0
12	M	32/36 (88%)	0.36	1 (3%) 49 51	24, 29, 56, 68	0
12	m	31/36 (86%)	-0.03	0 100 100	23, 30, 48, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	0.21	23 (9%) 8 9	22, 37, 79, 118	0
13	o	244/272 (89%)	0.13	19 (7%) 13 14	22, 36, 76, 118	0
14	T	29/32 (90%)	-0.26	2 (6%) 16 19	22, 26, 56, 72	0
14	t	29/32 (90%)	0.02	3 (10%) 6 7	24, 27, 77, 90	0
15	U	97/134 (72%)	-0.06	2 (2%) 63 66	27, 39, 63, 82	0
15	u	97/134 (72%)	-0.15	1 (1%) 82 84	25, 36, 52, 80	0
16	V	137/163 (84%)	-0.30	0 100 100	26, 35, 53, 75	0
16	v	137/163 (84%)	0.09	4 (2%) 51 54	29, 42, 62, 84	0
17	Y	27/46 (58%)	1.65	9 (33%) 0 0	49, 68, 85, 94	0
17	y	30/46 (65%)	0.91	7 (23%) 0 0	54, 67, 85, 87	0
18	X	38/41 (92%)	0.46	5 (13%) 3 3	34, 45, 72, 77	0
18	x	39/41 (95%)	0.79	7 (17%) 1 1	45, 53, 81, 91	0
19	Z	62/62 (100%)	1.30	19 (30%) 0 0	51, 63, 103, 113	0
19	z	62/62 (100%)	1.19	17 (27%) 0 0	53, 66, 98, 115	0
20	R	28/41 (68%)	2.69	19 (67%) 0 0	59, 67, 85, 90	0
20	r	28/41 (68%)	4.76	25 (89%) 0 0	73, 97, 104, 110	0
All	All	5293/5700 (92%)	0.09	275 (5%) 27 30	18, 33, 68, 118	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	r	10	LEU	10.3
13	o	58	ASN	9.3
19	z	33	TRP	8.8
20	r	28	VAL	8.7
20	r	6	LEU	8.7

## 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
14	FME	t	1	10/11	0.95	0.10	23,40,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	T	1	10/11	0.96	0.09	27,45,62,62	0
12	FME	M	1	10/11	0.96	0.12	39,50,77,85	0
8	FME	i	1	10/11	0.97	0.12	41,49,59,64	0
8	FME	I	1	10/11	0.97	0.14	37,48,62,65	0
12	FME	m	1	10/11	0.98	0.10	31,44,69,83	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
27	STE	i	102	6/20	0.46	0.34	66,89,108,108	0
27	STE	C	527	8/20	0.54	0.35	38,55,61,70	0
27	STE	d	412	10/20	0.59	0.29	43,55,70,73	0
27	STE	H	103	18/20	0.60	0.32	47,73,92,93	0
27	STE	Z	101	17/20	0.62	0.31	48,69,95,100	0
27	STE	i	101	12/20	0.62	0.51	58,75,94,95	0
27	STE	c	517	18/20	0.62	0.31	50,81,102,102	0
27	STE	E	102	12/20	0.65	0.37	50,74,88,91	0
27	STE	e	101	9/20	0.66	0.29	44,50,58,62	0
27	STE	j	102	16/20	0.67	0.27	42,60,69,70	0
28	LMG	c	518	30/55	0.69	0.28	37,70,100,110	0
28	LMG	D	408	50/55	0.71	0.22	35,67,111,123	0
27	STE	B	623	15/20	0.72	0.23	38,62,88,89	0
28	LMG	b	619	24/55	0.72	0.33	40,54,75,79	0
27	STE	E	103	12/20	0.72	0.27	49,57,79,82	0
27	STE	a	417	12/20	0.73	0.28	47,66,71,71	0
27	STE	I	102	17/20	0.74	0.42	56,72,86,87	0
27	STE	C	529	14/20	0.74	0.32	53,78,105,109	0
27	STE	A	417	11/20	0.74	0.26	45,56,73,77	0
27	STE	x	102	20/20	0.75	0.21	36,55,74,82	0
27	STE	C	528	14/20	0.76	0.47	43,61,87,92	0
27	STE	T	102	16/20	0.76	0.25	38,61,99,102	0
27	STE	d	411	12/20	0.77	0.23	46,73,99,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	STE	C	526	16/20	0.77	0.16	36,56,73,74	0
27	STE	D	414	9/20	0.77	0.15	39,45,58,58	0
27	STE	m	102	15/20	0.77	0.21	41,58,87,92	0
27	STE	e	102	8/20	0.78	0.27	48,58,60,67	0
27	STE	A	410	9/20	0.78	0.33	46,52,60,64	0
27	STE	z	101	9/20	0.78	0.20	49,64,75,76	0
27	STE	E	104	20/20	0.79	0.32	52,67,80,82	0
27	STE	C	518	5/20	0.79	0.26	47,56,67,67	0
27	STE	a	416	10/20	0.80	0.19	43,64,70,70	0
27	STE	b	626	10/20	0.80	0.26	46,58,66,69	0
33	LHG	E	101	49/49	0.80	0.25	43,80,110,116	0
33	LHG	a	413	42/49	0.80	0.26	61,86,110,123	0
28	LMG	a	415	55/55	0.81	0.17	37,64,89,93	0
27	STE	A	416	17/20	0.81	0.20	51,74,94,96	0
26	PL9	a	410	55/55	0.81	0.20	41,63,83,95	0
30	DGD	A	414	66/66	0.81	0.18	43,68,103,107	0
27	STE	e	104	13/20	0.81	0.30	61,66,79,81	0
27	STE	l	103	18/20	0.81	0.18	35,49,87,89	0
27	STE	B	622	12/20	0.82	0.35	49,66,81,85	0
28	LMG	C	517	36/55	0.82	0.17	36,65,90,102	0
26	PL9	A	409	55/55	0.82	0.26	37,66,87,103	0
29	SQD	a	414	54/54	0.83	0.17	36,53,87,104	0
27	STE	b	625	16/20	0.83	0.18	49,62,85,92	0
27	STE	C	516	14/20	0.84	0.28	54,70,89,93	0
27	STE	e	103	9/20	0.84	0.36	46,49,56,57	0
27	STE	d	410	17/20	0.84	0.13	35,56,72,74	0
28	LMG	c	523	48/55	0.84	0.21	46,78,112,122	0
23	CLA	h	101	65/65	0.84	0.20	39,64,95,103	0
28	LMG	B	620	45/55	0.84	0.18	38,60,103,130	0
27	STE	b	627	11/20	0.84	0.19	45,52,54,58	0
27	STE	c	516	13/20	0.84	0.29	47,75,84,88	0
27	STE	b	624	20/20	0.85	0.17	36,54,73,77	0
23	CLA	C	512	65/65	0.85	0.18	34,52,95,108	0
27	STE	C	519	7/20	0.85	0.22	45,47,51,52	0
29	SQD	A	413	54/54	0.85	0.19	39,60,97,100	0
28	LMG	b	623	55/55	0.86	0.28	48,77,98,104	0
25	BCR	x	101	40/40	0.86	0.14	34,51,70,71	0
25	BCR	K	101	40/40	0.86	0.13	33,51,69,76	0
27	STE	I	101	15/20	0.86	0.21	36,58,84,88	0
25	BCR	H	101	40/40	0.87	0.13	29,43,58,61	0
29	SQD	l	101	54/54	0.87	0.16	38,62,90,105	0
23	CLA	c	513	65/65	0.87	0.18	41,66,99,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	STE	b	622	20/20	0.87	0.18	38,59,75,77	0
25	BCR	k	101	40/40	0.87	0.14	40,56,69,72	0
27	STE	j	101	12/20	0.88	0.10	45,57,63,64	0
28	LMG	A	411	48/55	0.88	0.14	38,58,77,95	0
28	LMG	c	524	49/55	0.88	0.14	35,59,92,115	0
27	STE	C	525	12/20	0.88	0.12	37,50,60,60	0
27	STE	B	621	17/20	0.88	0.17	35,53,70,73	0
27	STE	m	101	12/20	0.88	0.14	44,57,75,75	0
23	CLA	C	513	65/65	0.88	0.19	38,62,92,99	0
27	STE	t	103	18/20	0.88	0.12	46,61,76,78	0
27	STE	J	101	12/20	0.88	0.13	48,62,68,73	0
28	LMG	C	524	48/55	0.89	0.16	35,69,87,101	0
23	CLA	c	512	65/65	0.90	0.14	37,56,96,103	0
27	STE	t	102	14/20	0.90	0.10	35,51,61,61	0
25	BCR	C	514	40/40	0.90	0.15	41,56,69,74	0
29	SQD	f	102	41/54	0.90	0.21	50,83,102,112	0
25	BCR	D	406	40/40	0.91	0.12	24,42,77,89	0
28	LMG	b	621	51/55	0.91	0.12	38,55,78,90	0
29	SQD	b	620	49/54	0.91	0.13	38,58,89,103	0
23	CLA	B	601	65/65	0.91	0.13	30,63,91,105	0
27	STE	A	415	8/20	0.92	0.16	41,49,54,55	0
25	BCR	d	404	40/40	0.92	0.12	32,48,86,93	0
23	CLA	a	408	65/65	0.92	0.14	18,34,79,90	0
28	LMG	c	522	46/55	0.92	0.16	40,67,84,89	0
25	BCR	k	102	40/40	0.92	0.16	35,49,64,69	0
23	CLA	b	614	65/65	0.92	0.14	24,38,61,64	0
23	CLA	c	502	65/65	0.92	0.14	26,39,59,63	0
27	STE	M	102	15/20	0.92	0.14	38,47,60,75	0
27	STE	M	103	10/20	0.92	0.14	32,47,57,65	0
27	STE	D	413	20/20	0.92	0.16	30,47,73,81	0
28	LMG	D	409	51/55	0.92	0.17	24,54,83,89	0
28	LMG	M	101	51/55	0.92	0.11	32,51,74,81	0
23	CLA	C	502	65/65	0.92	0.14	23,37,56,61	0
23	CLA	D	405	65/65	0.92	0.13	21,40,105,116	0
23	CLA	c	508	64/65	0.93	0.14	26,41,95,111	0
25	BCR	C	515	40/40	0.93	0.11	24,38,49,58	0
25	BCR	C	520	40/40	0.93	0.16	30,48,65,70	0
23	CLA	d	403	65/65	0.93	0.14	26,46,89,98	0
23	CLA	b	615	60/65	0.93	0.14	25,38,95,99	0
23	CLA	c	505	65/65	0.94	0.17	24,38,69,81	0
23	CLA	c	506	65/65	0.94	0.12	28,45,91,97	0
23	CLA	c	507	65/65	0.94	0.13	25,41,56,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	601	65/65	0.94	0.14	24,40,60,66	0
23	CLA	c	511	65/65	0.94	0.12	35,49,69,71	0
28	LMG	d	409	44/55	0.94	0.13	29,51,86,99	0
29	SQD	A	412	52/54	0.94	0.16	32,62,92,102	0
25	BCR	b	618	40/40	0.94	0.09	26,42,59,63	0
29	SQD	a	412	54/54	0.94	0.14	38,68,90,94	0
25	BCR	c	514	40/40	0.94	0.12	43,59,73,73	0
23	CLA	b	608	65/65	0.94	0.13	24,42,62,67	0
23	CLA	b	609	65/65	0.94	0.18	23,36,48,51	0
23	CLA	B	614	65/65	0.94	0.17	19,32,82,94	0
23	CLA	C	505	65/65	0.94	0.17	21,36,71,85	0
30	DGD	C	522	62/66	0.94	0.12	28,52,100,111	0
30	DGD	C	523	62/66	0.94	0.12	25,48,79,87	0
30	DGD	H	102	62/66	0.94	0.11	26,45,61,64	0
30	DGD	c	520	62/66	0.94	0.12	29,52,91,99	0
30	DGD	c	521	62/66	0.94	0.13	24,53,88,94	0
25	BCR	B	619	40/40	0.94	0.10	20,39,59,65	0
23	CLA	B	616	60/65	0.94	0.14	20,34,98,116	0
23	CLA	B	615	65/65	0.95	0.11	22,34,62,70	0
23	CLA	B	604	65/65	0.95	0.12	18,28,70,78	0
23	CLA	c	509	65/65	0.95	0.15	27,43,67,72	0
23	CLA	c	510	65/65	0.95	0.13	26,45,63,67	0
23	CLA	B	606	65/65	0.95	0.10	21,32,69,72	0
23	CLA	a	406	65/65	0.95	0.13	22,35,95,100	0
23	CLA	C	503	65/65	0.95	0.12	25,39,51,54	0
23	CLA	a	411	65/65	0.95	0.12	17,27,49,53	0
23	CLA	C	504	59/65	0.95	0.10	25,37,81,86	0
24	PHO	a	407	64/64	0.95	0.13	17,28,39,40	0
25	BCR	B	618	40/40	0.95	0.09	21,37,53,54	0
23	CLA	b	603	65/65	0.95	0.12	17,32,81,98	0
23	CLA	b	605	65/65	0.95	0.11	21,36,74,84	0
23	CLA	b	607	65/65	0.95	0.14	22,40,58,68	0
23	CLA	B	602	65/65	0.95	0.15	20,33,56,62	0
23	CLA	C	506	65/65	0.95	0.11	20,38,96,105	0
29	SQD	F	102	36/54	0.95	0.17	43,70,88,99	0
23	CLA	b	611	65/65	0.95	0.16	18,33,49,64	0
23	CLA	b	612	65/65	0.95	0.14	16,31,72,80	0
25	BCR	a	409	40/40	0.95	0.08	20,33,44,45	0
25	BCR	b	616	40/40	0.95	0.10	26,38,49,52	0
23	CLA	C	507	65/65	0.95	0.14	21,37,63,67	0
23	CLA	C	508	65/65	0.95	0.11	23,38,101,106	0
25	BCR	c	515	40/40	0.95	0.11	28,42,57,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	509	65/65	0.95	0.16	22,41,62,69	0
23	CLA	c	503	65/65	0.95	0.13	29,42,52,60	0
23	CLA	c	504	60/65	0.95	0.11	27,44,81,84	0
23	CLA	C	510	65/65	0.95	0.11	25,40,61,63	0
30	DGD	h	102	62/66	0.95	0.11	24,49,60,71	0
23	CLA	C	511	65/65	0.95	0.10	28,46,65,71	0
26	PL9	D	407	55/55	0.95	0.10	18,31,46,50	0
33	LHG	d	406	49/49	0.95	0.13	33,52,73,84	0
24	PHO	d	401	64/64	0.96	0.09	24,35,48,48	0
25	BCR	A	408	40/40	0.96	0.09	21,34,45,48	0
25	BCR	B	617	40/40	0.96	0.11	23,34,54,56	0
23	CLA	A	407	54/65	0.96	0.10	16,30,63,69	0
23	CLA	C	501	65/65	0.96	0.12	19,33,49,58	0
23	CLA	b	613	65/65	0.96	0.12	22,36,74,85	0
23	CLA	D	403	65/65	0.96	0.10	16,26,50,58	0
23	CLA	D	404	65/65	0.96	0.11	16,27,57,62	0
23	CLA	c	501	65/65	0.96	0.12	26,36,50,57	0
23	CLA	A	404	65/65	0.96	0.10	12,26,48,57	0
23	CLA	a	405	65/65	0.96	0.10	16,28,49,59	0
25	BCR	T	101	40/40	0.96	0.08	22,36,49,50	0
23	CLA	B	607	65/65	0.96	0.10	16,31,62,64	0
23	CLA	B	608	65/65	0.96	0.12	18,34,52,61	0
25	BCR	b	617	40/40	0.96	0.09	24,37,54,55	0
23	CLA	B	609	65/65	0.96	0.11	23,34,58,62	0
23	CLA	B	610	65/65	0.96	0.14	19,30,42,46	0
23	CLA	b	602	65/65	0.96	0.14	21,33,69,82	0
23	CLA	B	611	65/65	0.96	0.15	17,29,51,54	0
23	CLA	b	604	65/65	0.96	0.12	19,32,51,55	0
23	CLA	B	612	65/65	0.96	0.12	18,29,47,51	0
25	BCR	t	101	40/40	0.96	0.09	22,36,53,53	0
23	CLA	b	606	65/65	0.96	0.12	17,34,67,70	0
23	CLA	B	613	65/65	0.96	0.14	18,30,69,75	0
23	CLA	d	402	65/65	0.96	0.11	17,31,63,66	0
23	CLA	A	405	65/65	0.96	0.13	18,31,97,104	0
33	LHG	D	411	47/49	0.96	0.11	23,48,78,94	0
33	LHG	D	412	49/49	0.96	0.12	27,44,73,79	0
26	PL9	d	405	55/55	0.96	0.10	20,33,45,50	0
23	CLA	B	603	65/65	0.96	0.16	19,30,61,69	0
23	CLA	b	610	65/65	0.96	0.13	20,30,53,58	0
33	LHG	d	408	39/49	0.96	0.10	30,43,74,86	0
33	LHG	l	102	49/49	0.96	0.09	25,43,59,71	0
34	HEM	f	101	43/43	0.96	0.12	41,55,76,78	0

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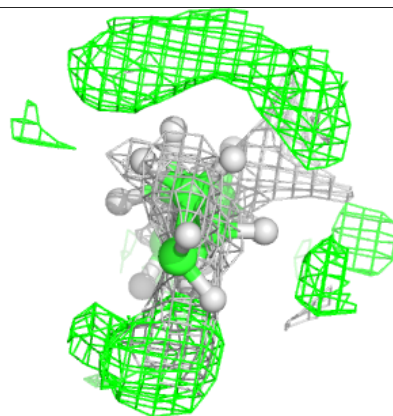
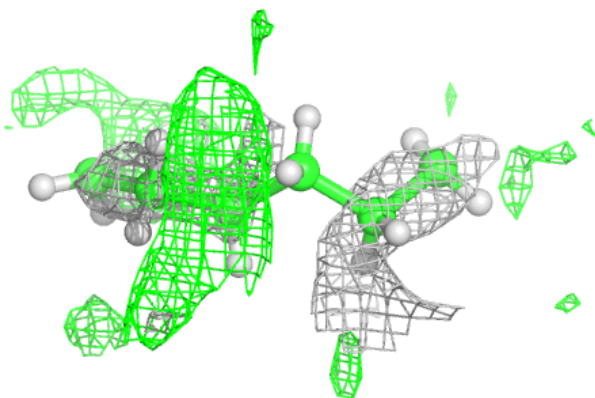
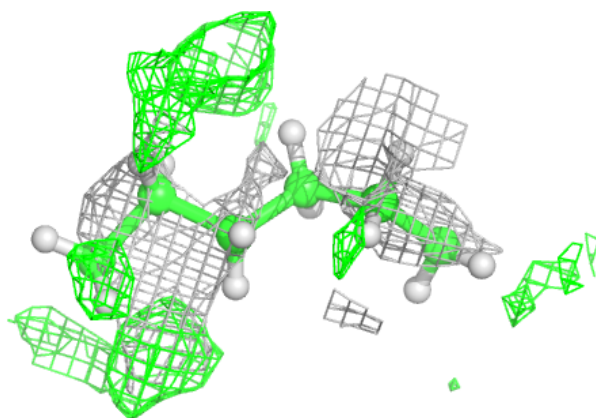
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	DGD	c	519	62/66	0.97	0.09	18,42,79,86	0
30	DGD	C	521	62/66	0.97	0.10	18,43,81,98	0
33	LHG	L	101	49/49	0.97	0.11	22,42,59,69	0
23	CLA	B	605	65/65	0.97	0.13	17,30,50,54	0
24	PHO	A	406	64/64	0.97	0.13	21,31,41,48	0
33	LHG	d	407	49/49	0.97	0.09	27,42,56,63	0
32	BCT	a	404	4/4	0.97	0.19	30,30,45,54	0
33	LHG	D	410	49/49	0.97	0.09	18,41,53,62	0
34	HEM	F	101	43/43	0.97	0.10	28,45,59,61	0
24	PHO	D	402	64/64	0.97	0.10	16,26,35,39	0
35	HEC	V	201	43/43	0.97	0.11	21,29,38,42	0
32	BCT	D	401	4/4	0.98	0.18	26,28,34,40	0
35	HEC	v	201	43/43	0.98	0.12	23,33,40,43	0
31	OEX	A	418	10/10	0.99	0.14	22,23,26,27	0
31	OEX	a	418	10/10	0.99	0.10	22,23,27,30	0
21	FE2	a	401	1/1	0.99	0.05	29,29,29,29	0
22	CL	A	402	1/1	1.00	0.08	25,25,25,25	0
22	CL	A	403	1/1	1.00	0.03	24,24,24,24	0
22	CL	a	402	1/1	1.00	0.03	25,25,25,25	0
22	CL	a	403	1/1	1.00	0.04	24,24,24,24	0
21	FE2	A	401	1/1	1.00	0.06	23,23,23,23	0

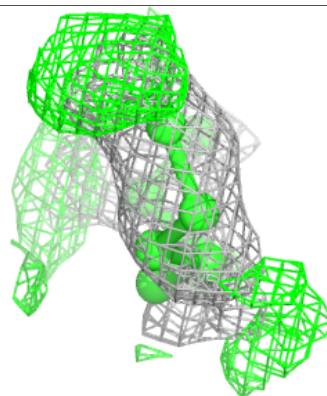
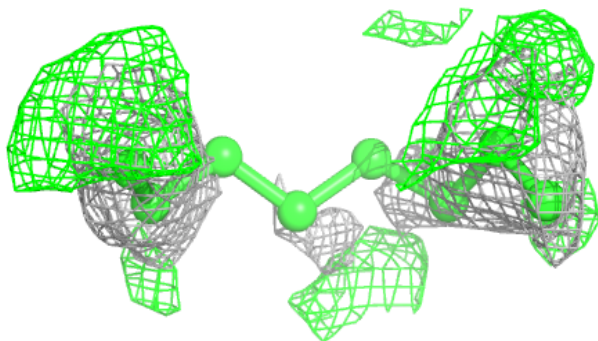
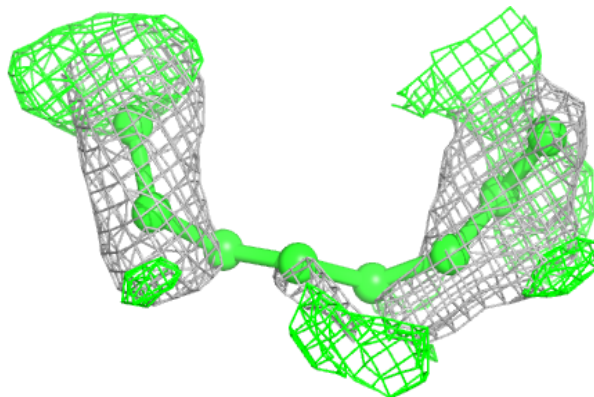
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around STE 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)

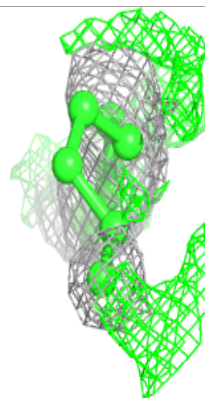
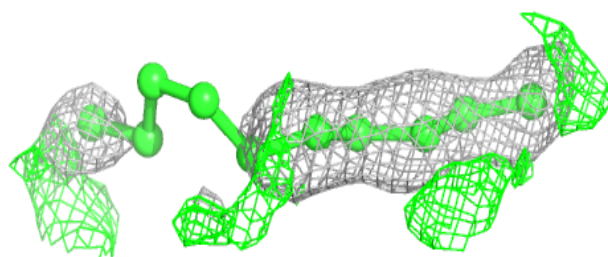
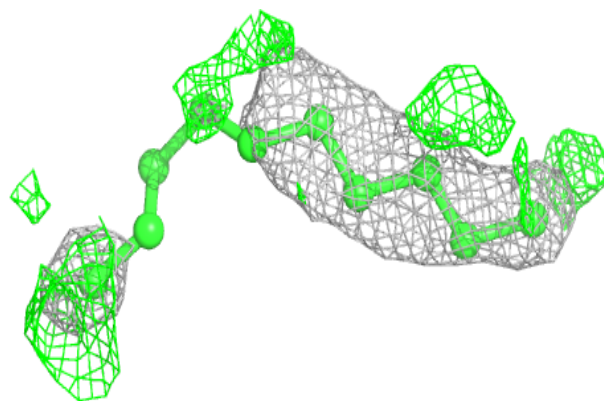
**Electron density around STE C 527:**

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

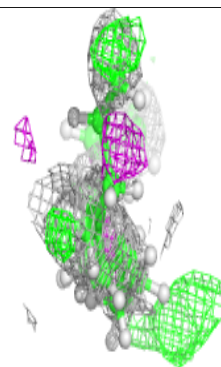
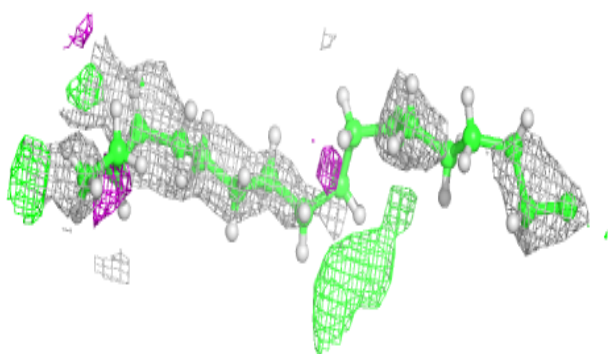
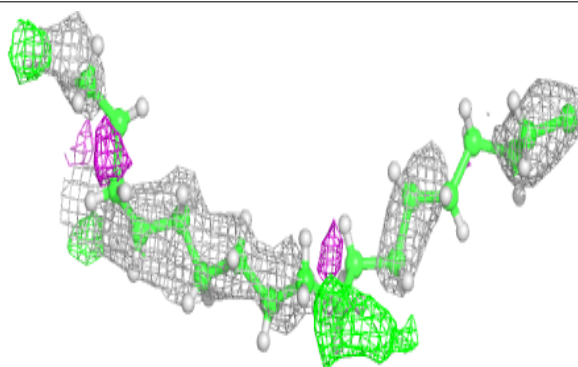


**Electron density around STE d 412:**

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

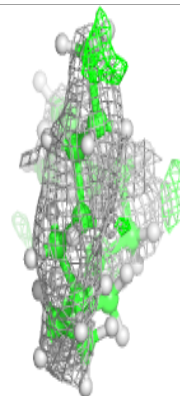
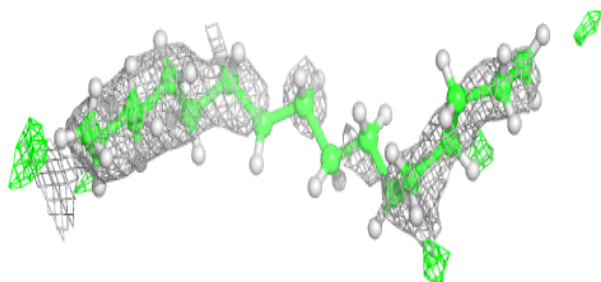
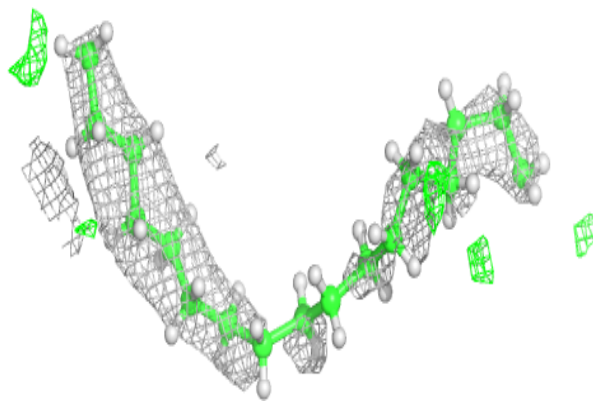
**Electron density around STE H 103:**

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



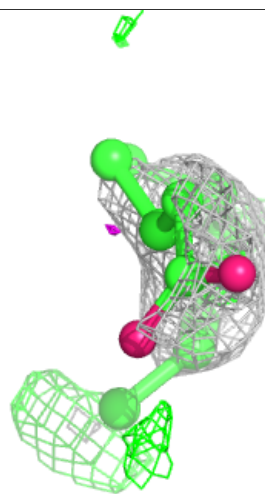
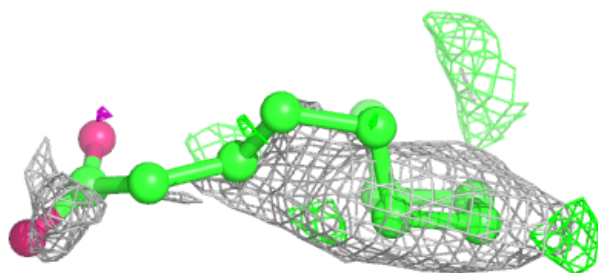
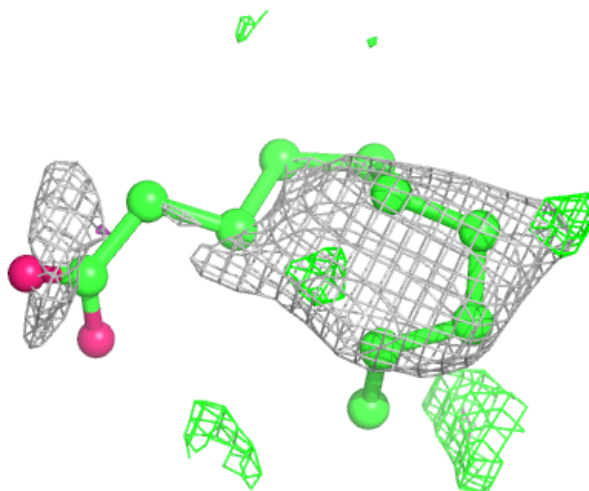
**Electron density around STE Z 101:**

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



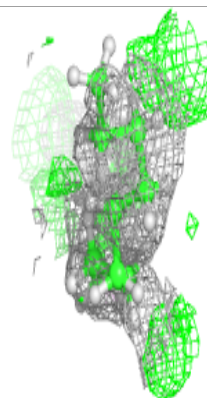
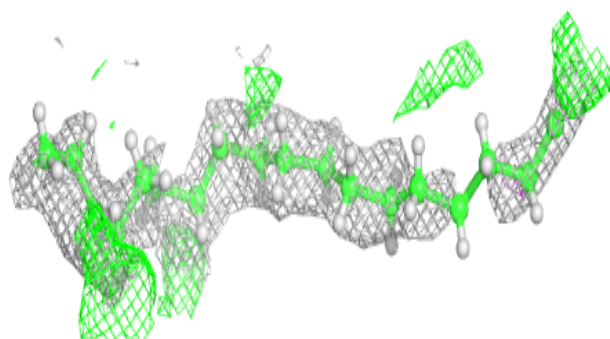
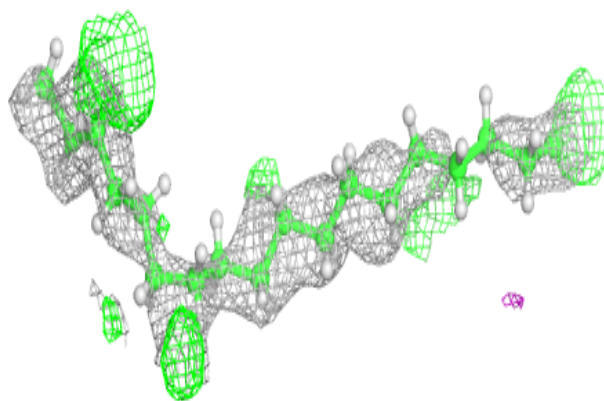
**Electron density around STE i 101:**

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

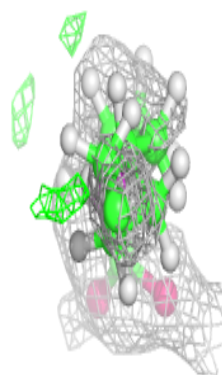
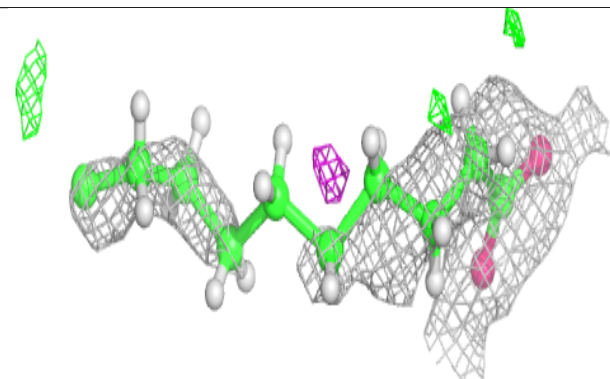
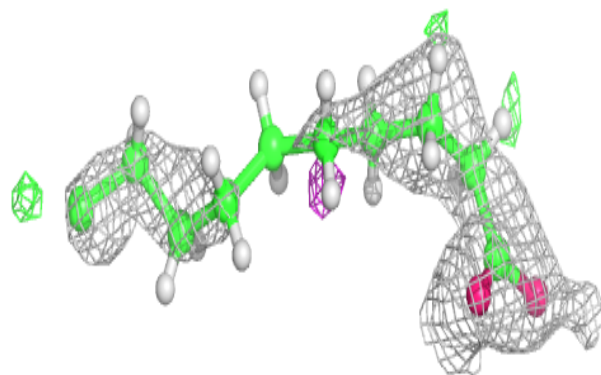


**Electron density around STE c 517:**

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

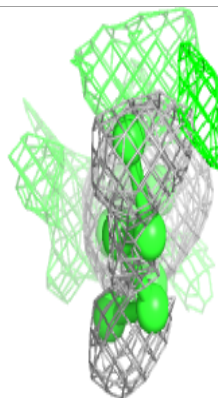
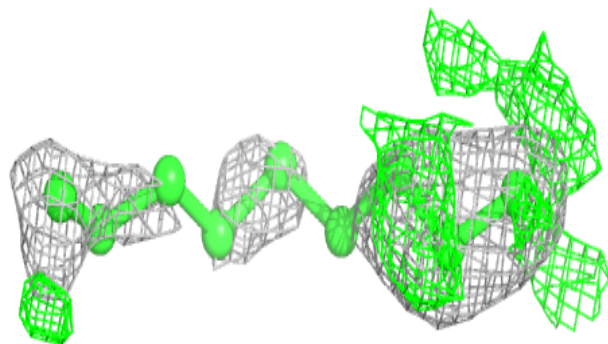
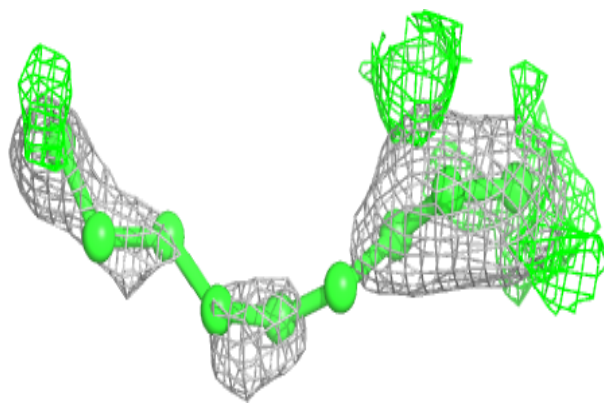
**Electron density around STE E 102:**

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

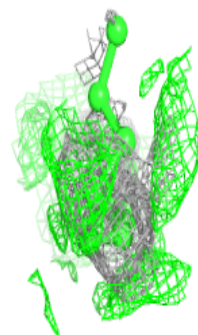
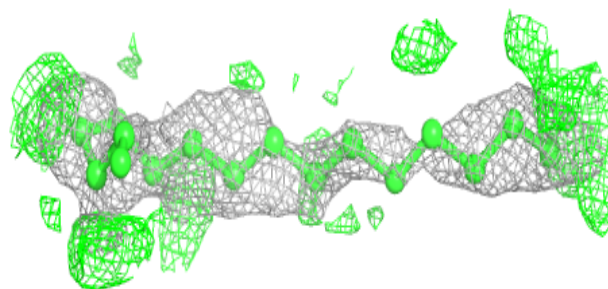
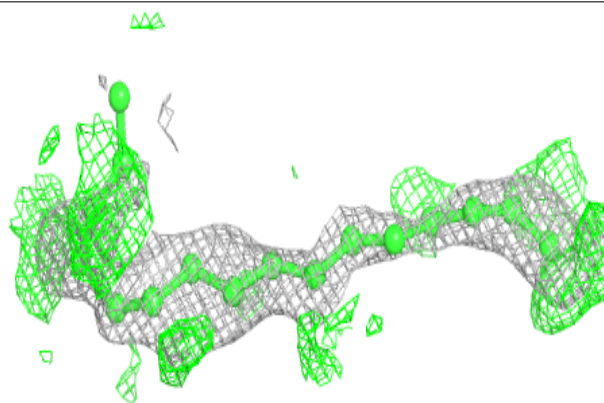


**Electron density around STE e 101:**

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

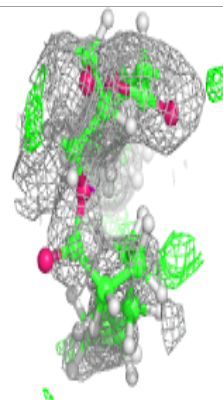
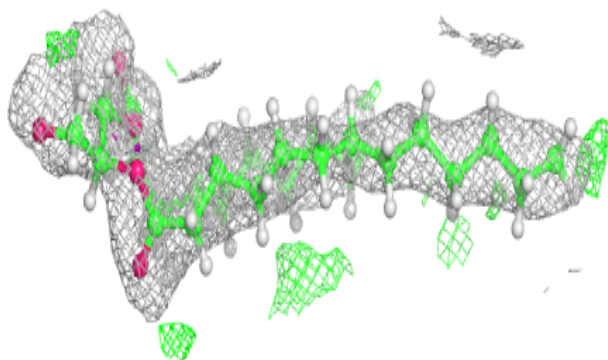
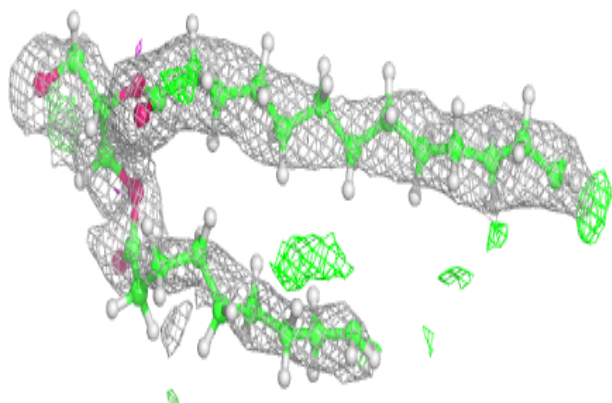
**Electron density around STE j 102:**

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

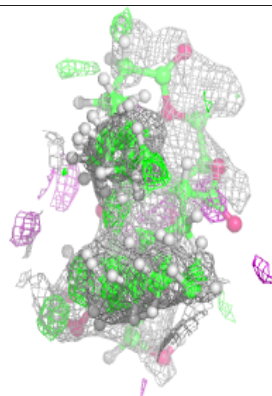
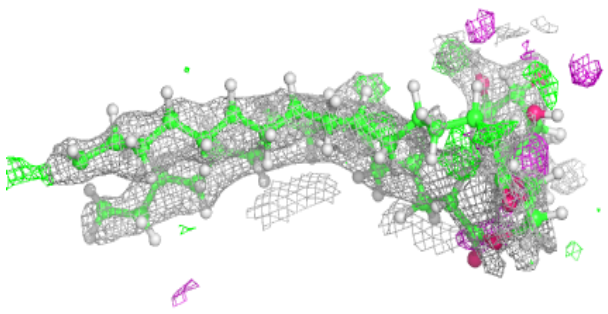
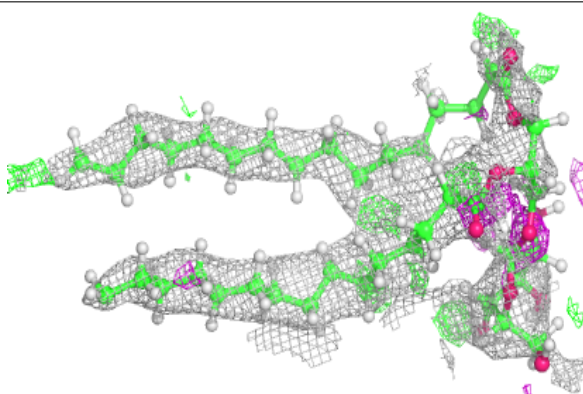


**Electron density around LMG c 518:**

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

**Electron density around LMG D 408:**

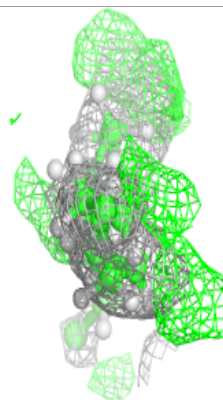
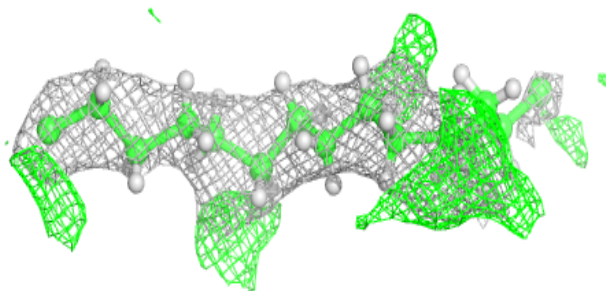
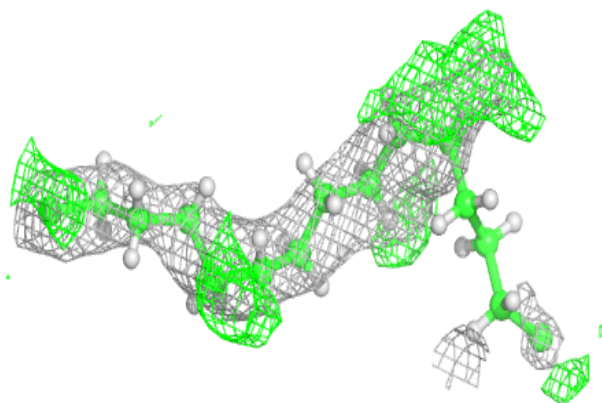
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



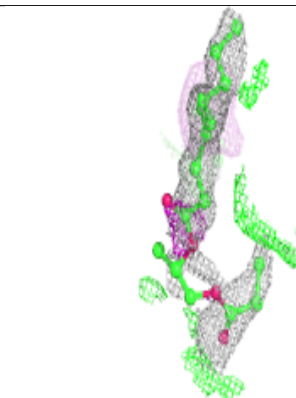
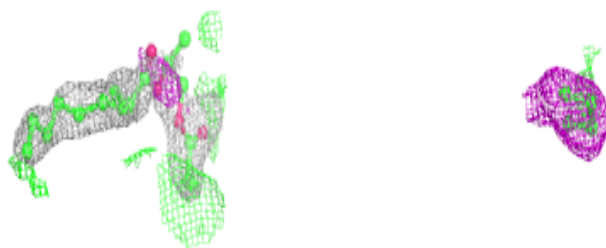
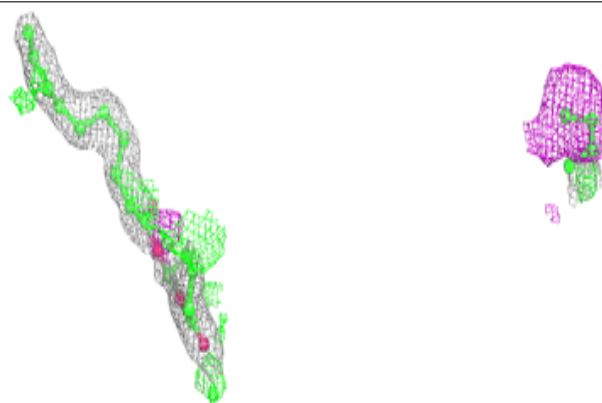


**Electron density around STE B 623:**

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

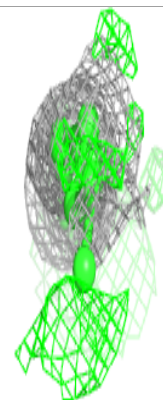
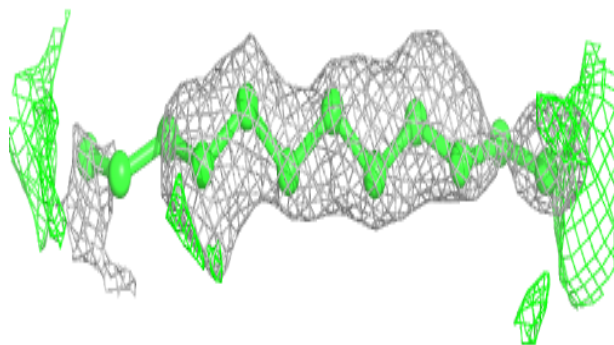
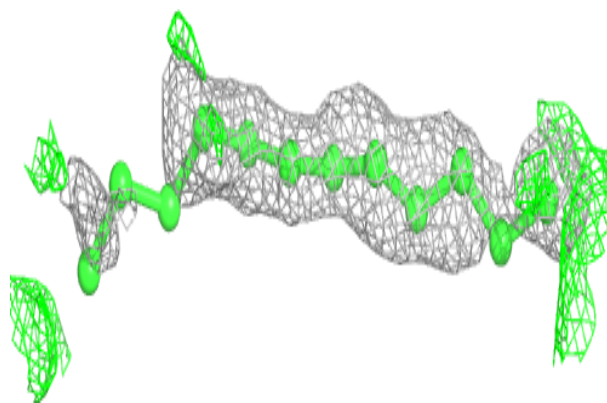
**Electron density around LMG b 619:**

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

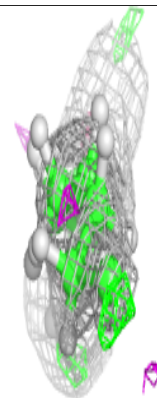
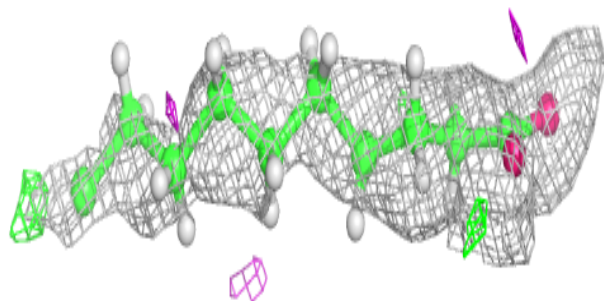
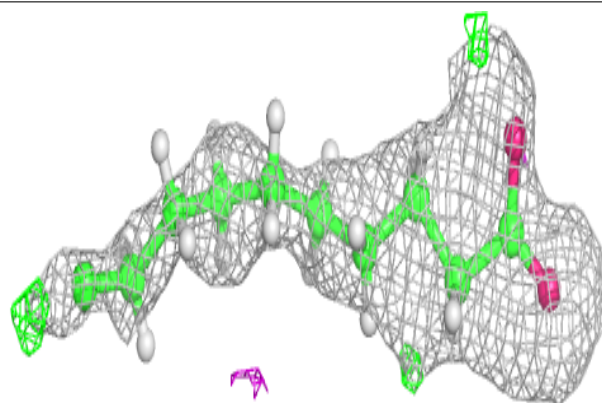


**Electron density around STE E 103:**

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

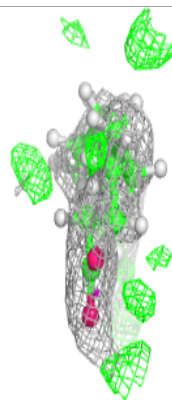
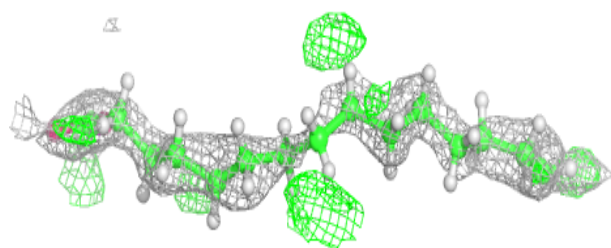
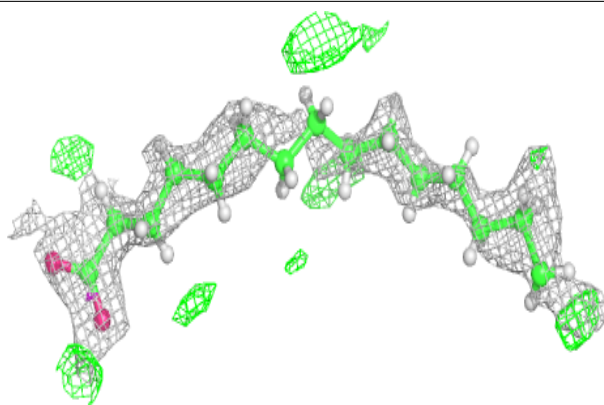
**Electron density around STE a 417:**

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

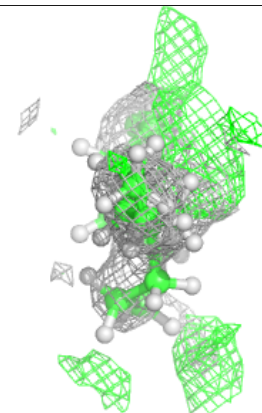
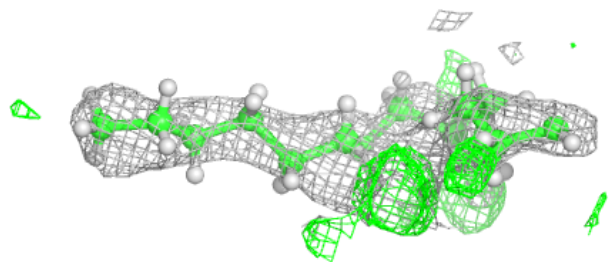
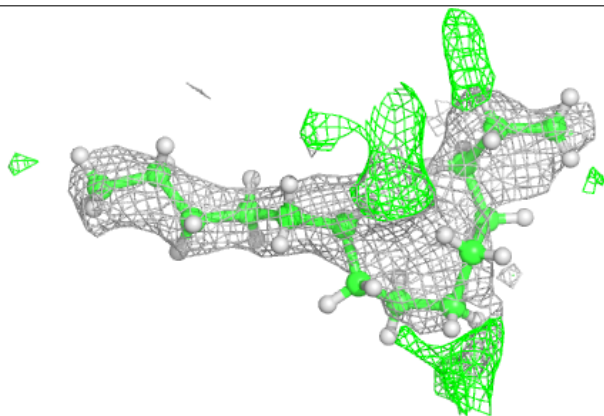


**Electron density around STE I 102:**

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

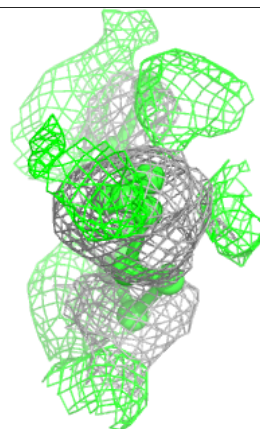
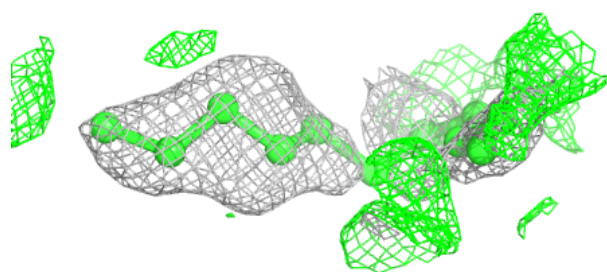
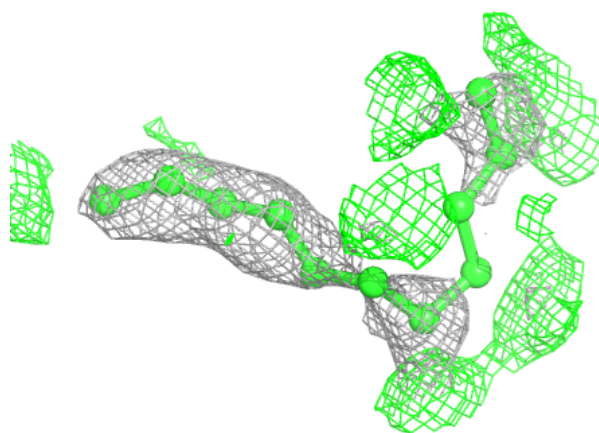
**Electron density around STE C 529:**

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

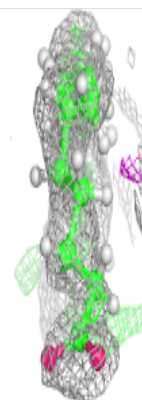
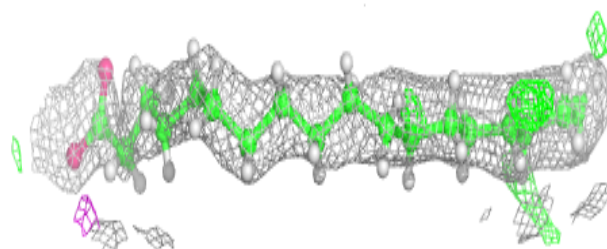
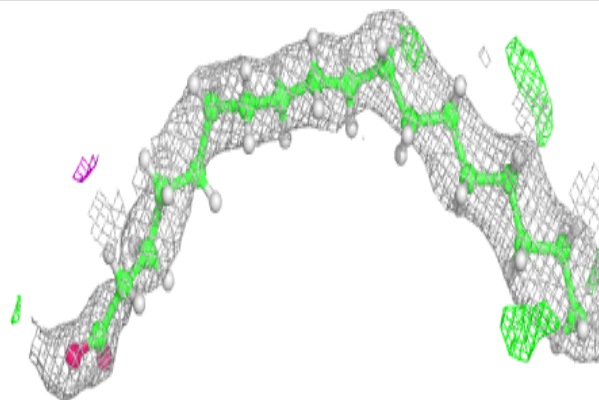


**Electron density around STE A 417:**

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

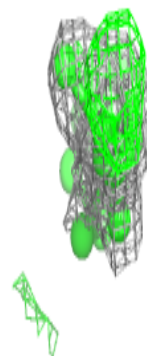
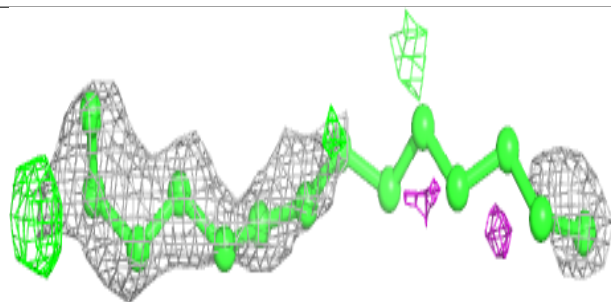
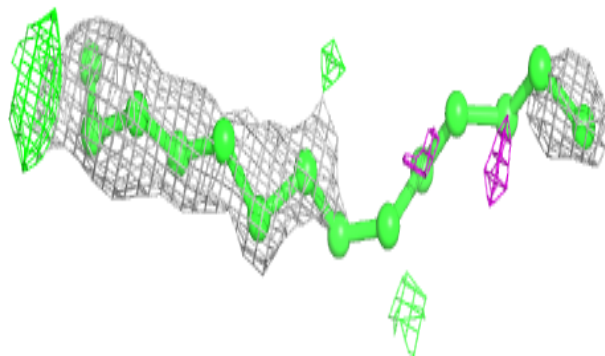
**Electron density around STE x 102:**

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

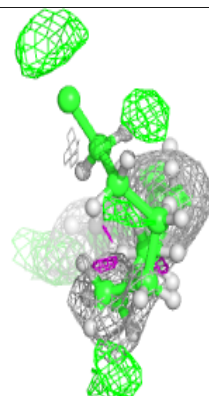
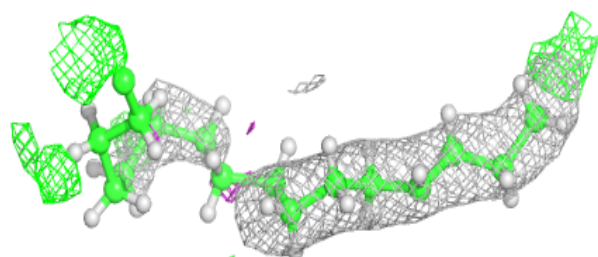
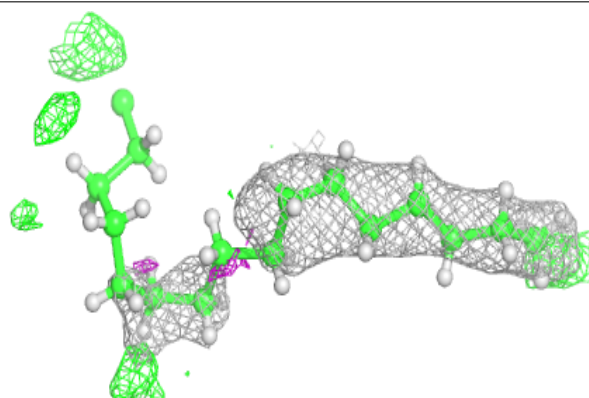


**Electron density around STE C 528:**

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

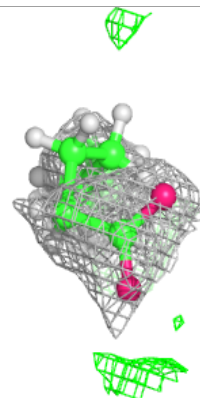
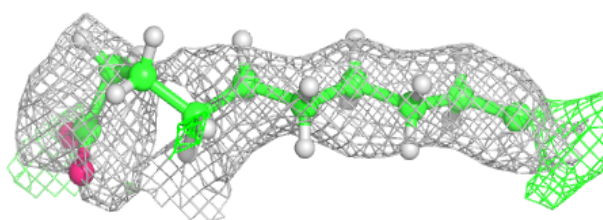
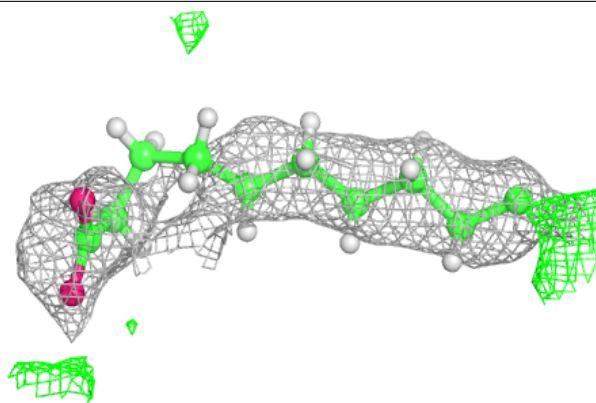
**Electron density around STE T 102:**

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

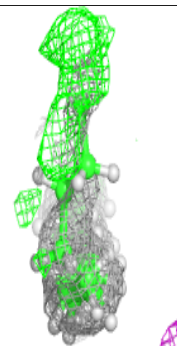
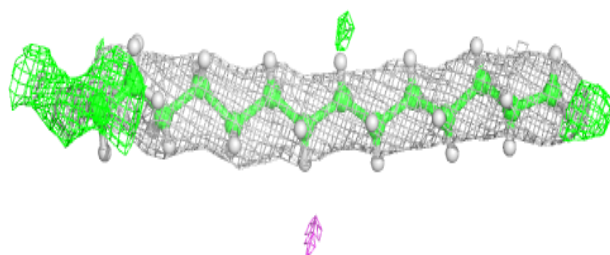
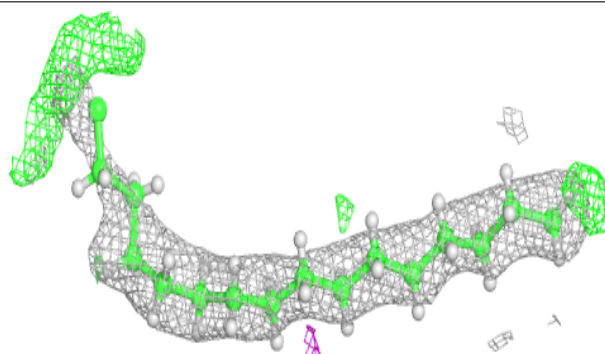


**Electron density around STE d 411:**

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

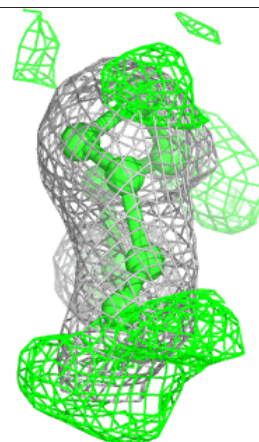
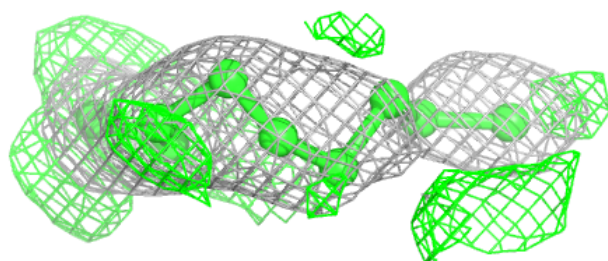
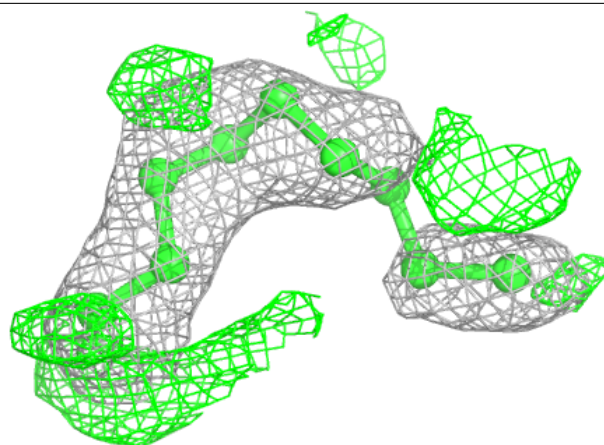
**Electron density around STE C 526:**

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

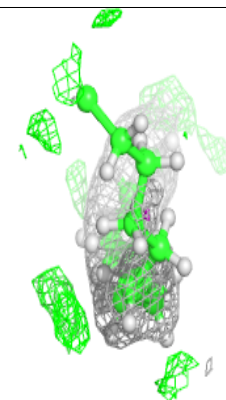
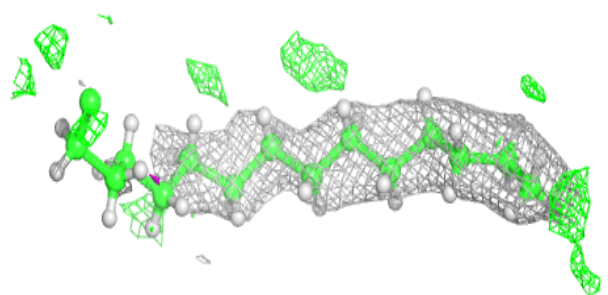
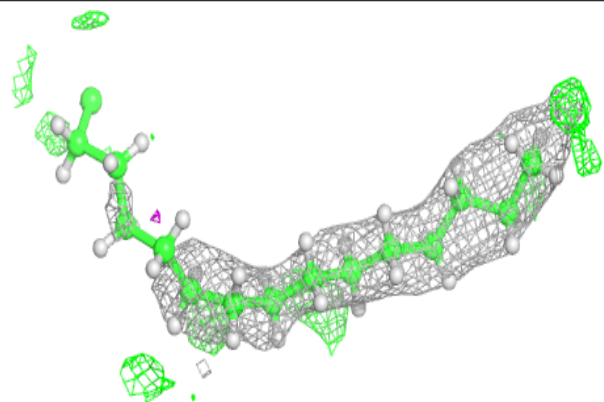


**Electron density around STE D 414:**

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

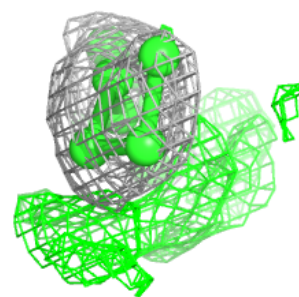
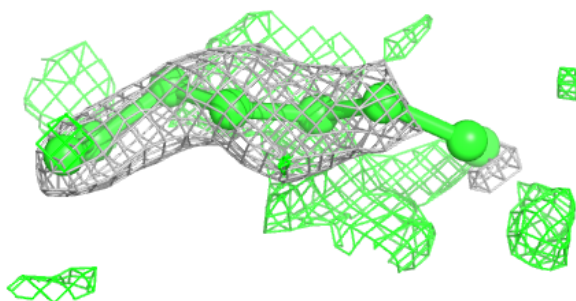
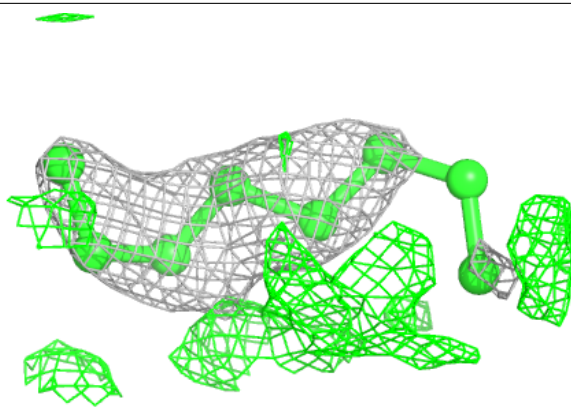
**Electron density around STE m 102:**

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

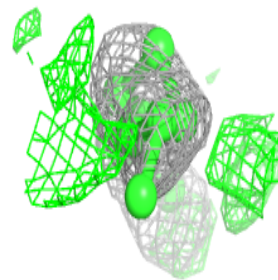
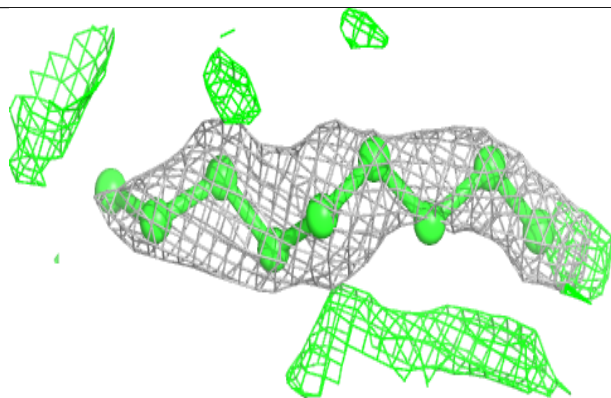
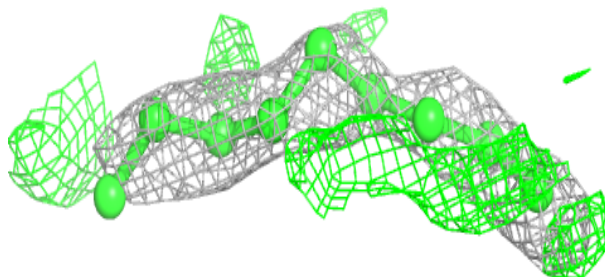


**Electron density around STE e 102:**

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

**Electron density around STE A 410:**

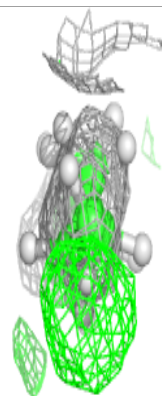
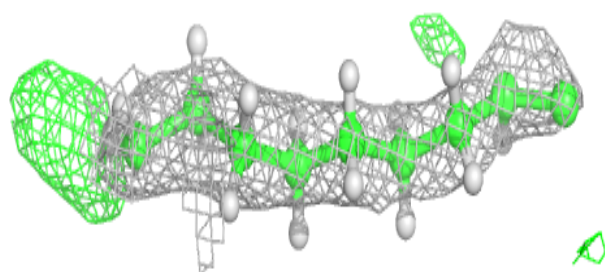
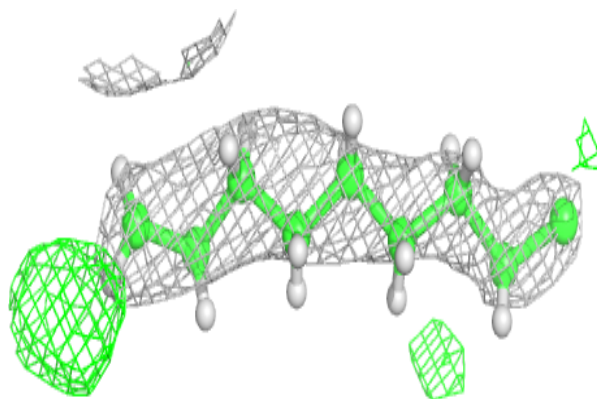
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



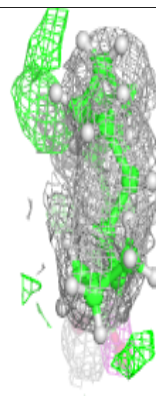
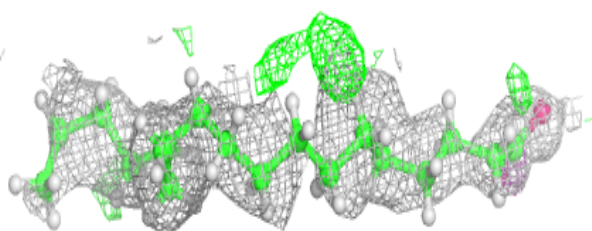
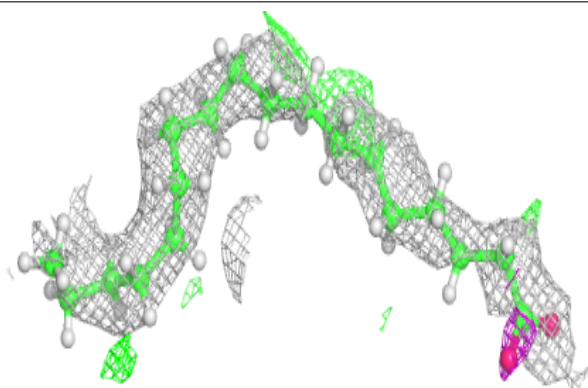


**Electron density around STE z 101:**

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

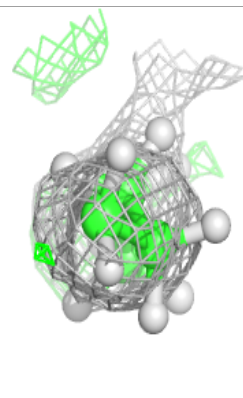
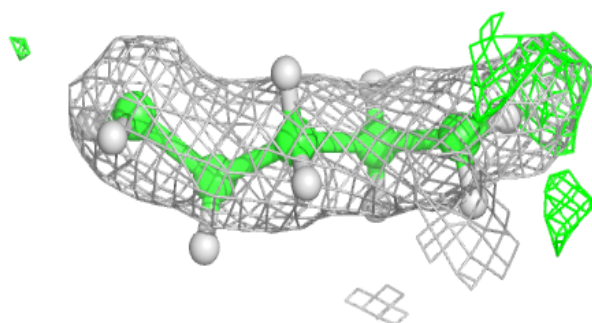
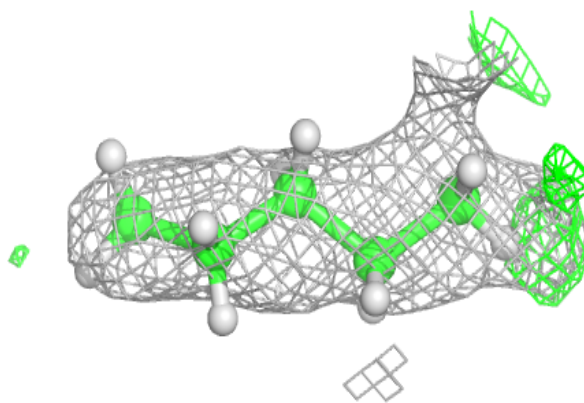
**Electron density around STE E 104:**

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

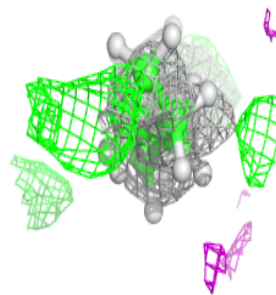
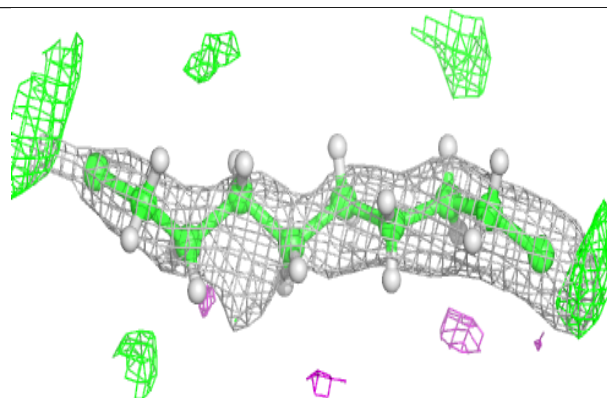
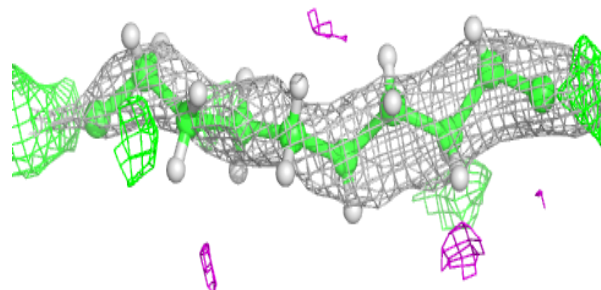


**Electron density around STE C 518:**

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

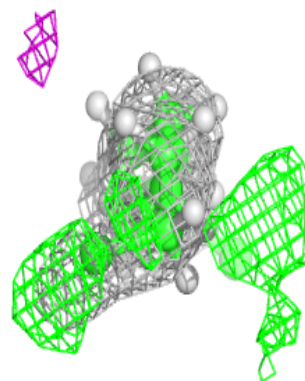
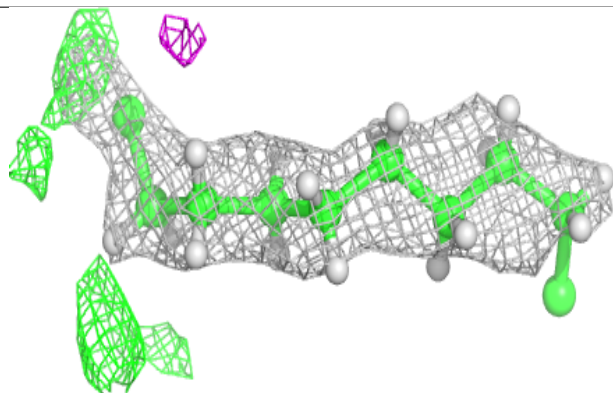
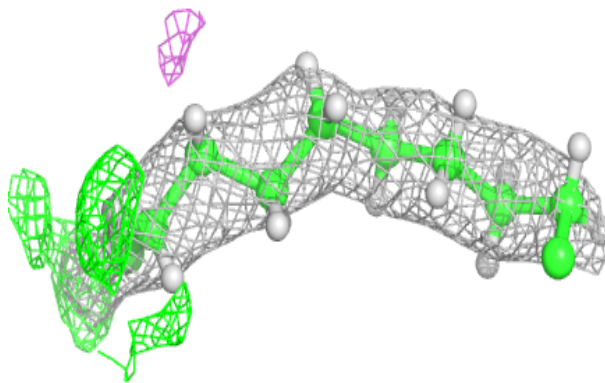
**Electron density around STE a 416:**

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

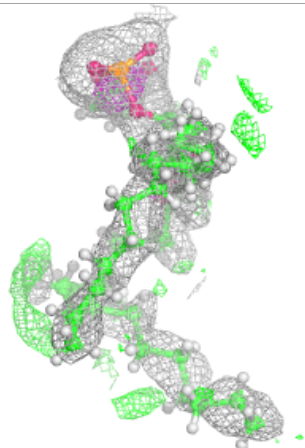
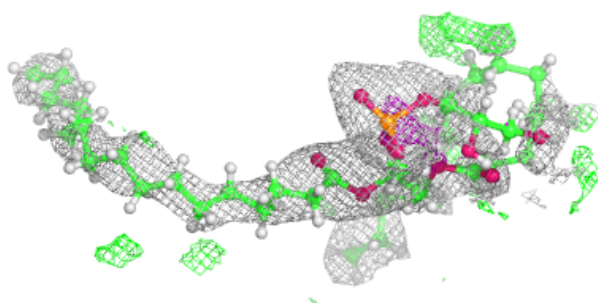
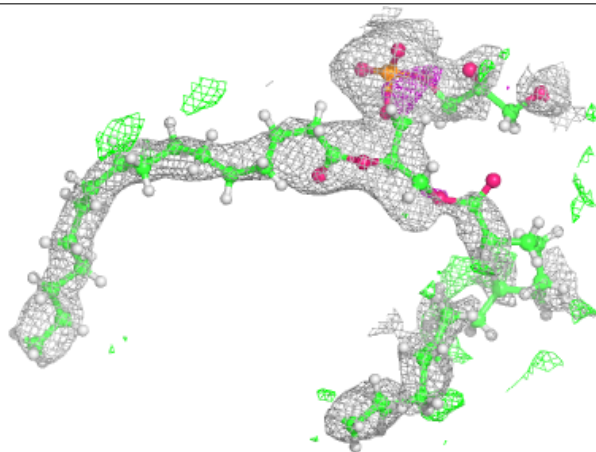


**Electron density around STE b 626:**

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

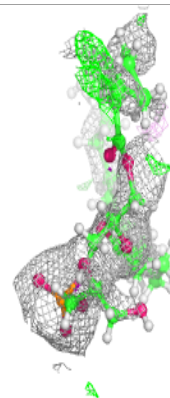
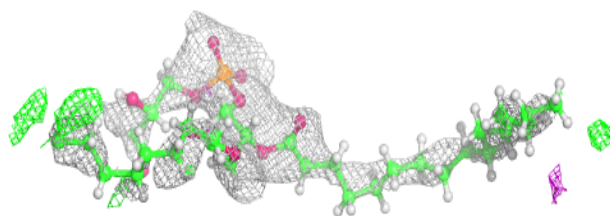
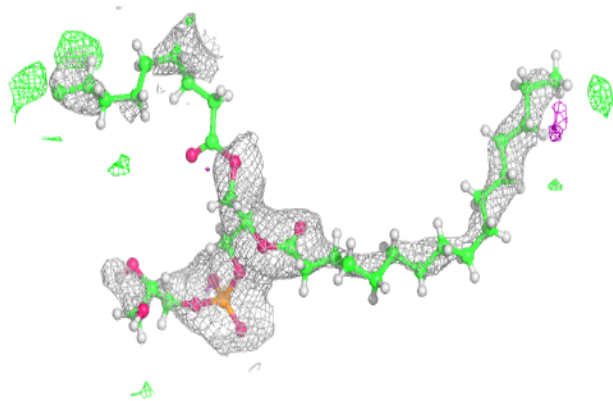
**Electron density around LHG E 101:**

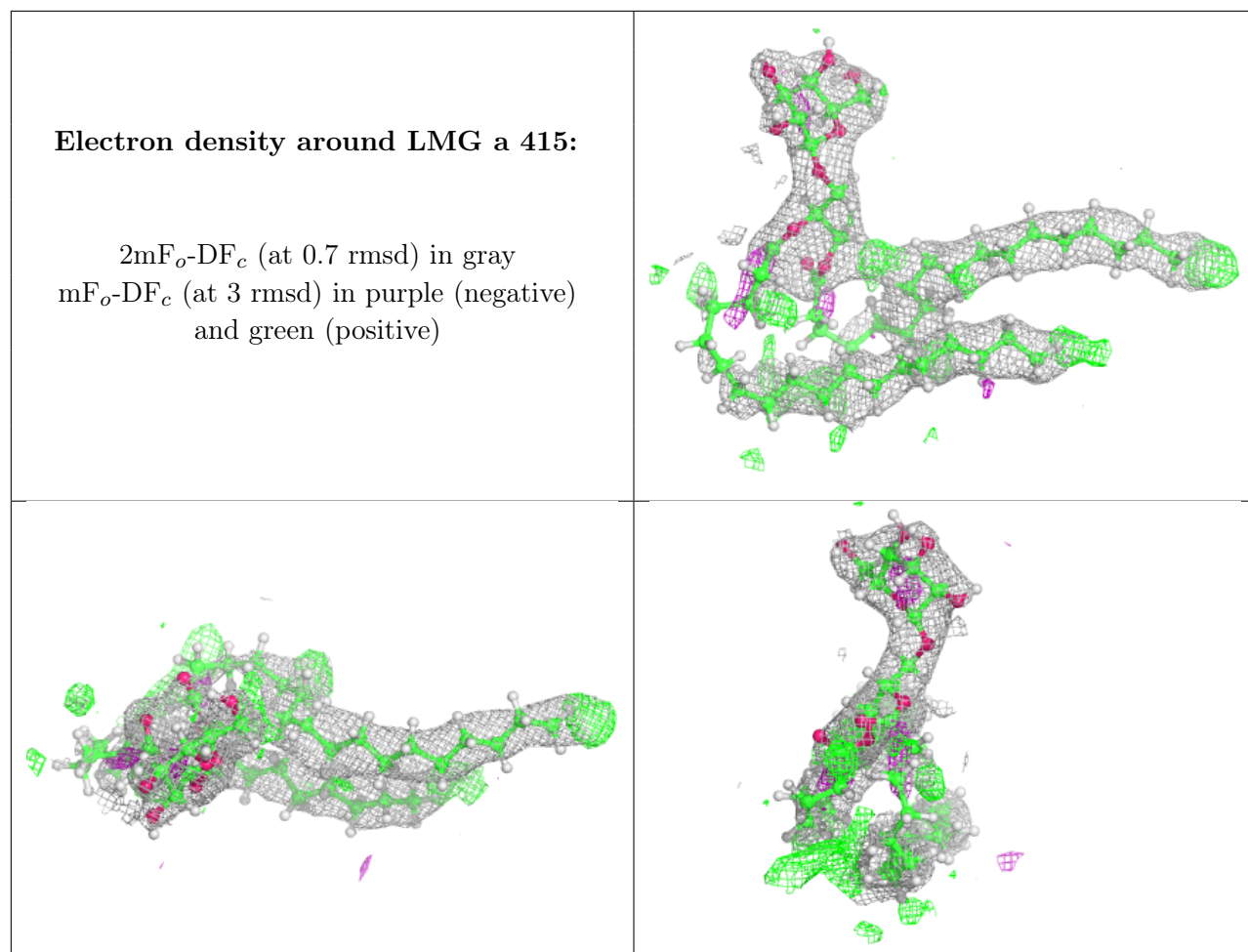
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG a 413:**

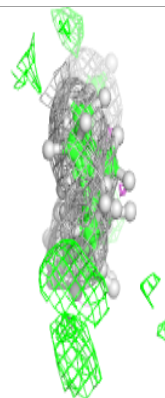
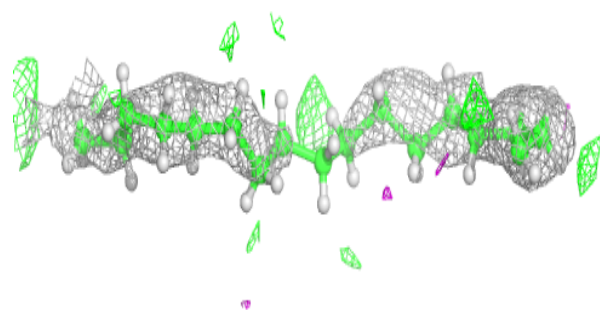
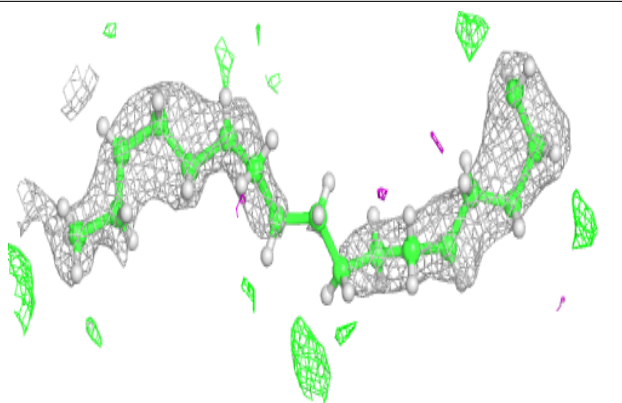
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



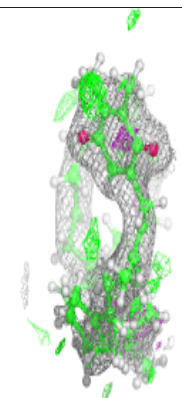
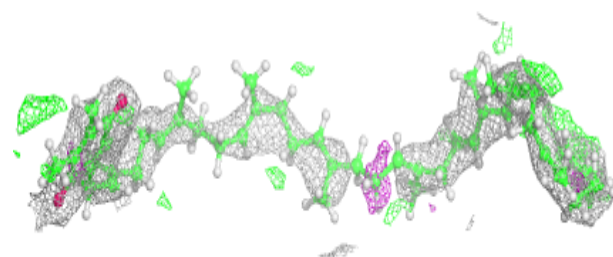
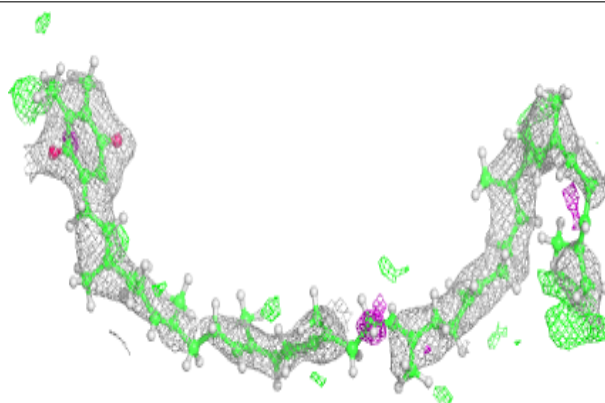


**Electron density around STE A 416:**

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

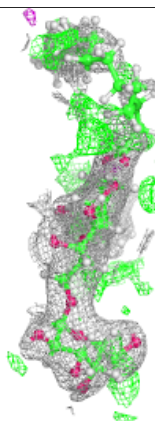
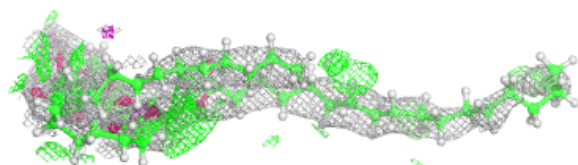
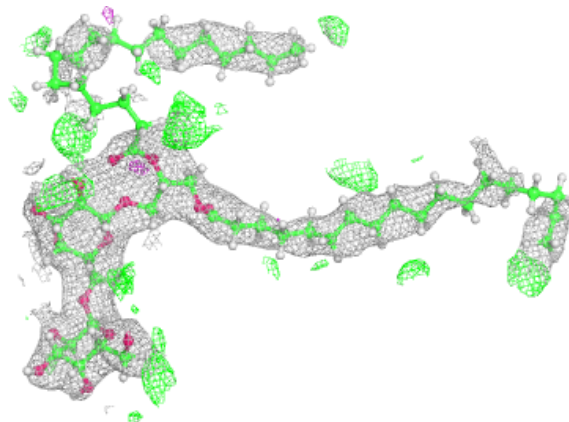
**Electron density around PL9 a 410:**

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

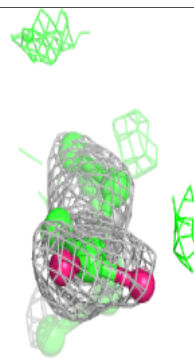
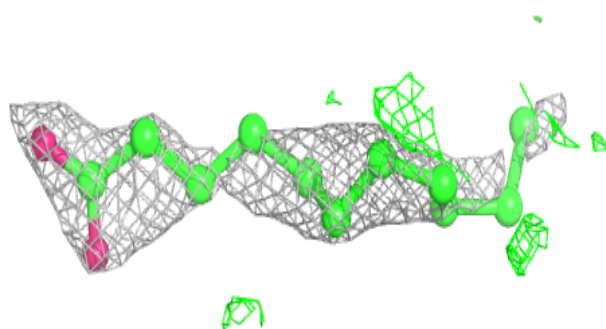
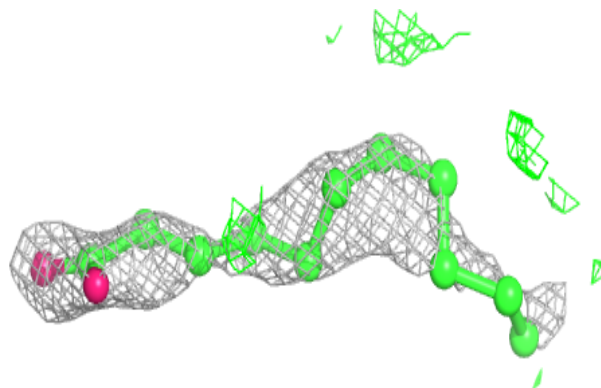


**Electron density around DGD A 414:**

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

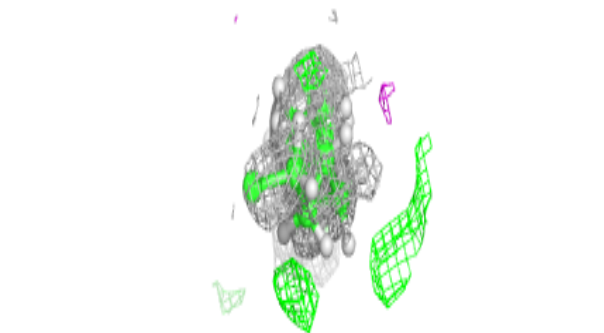
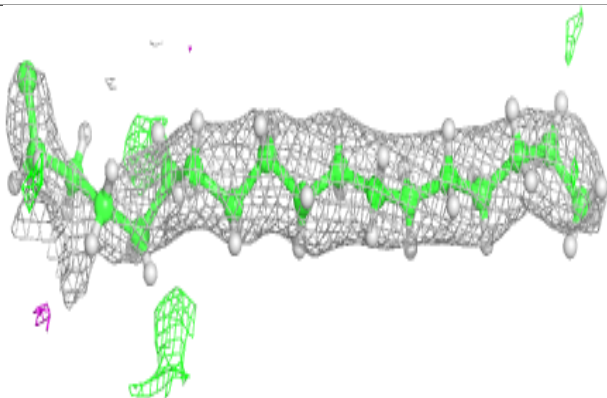
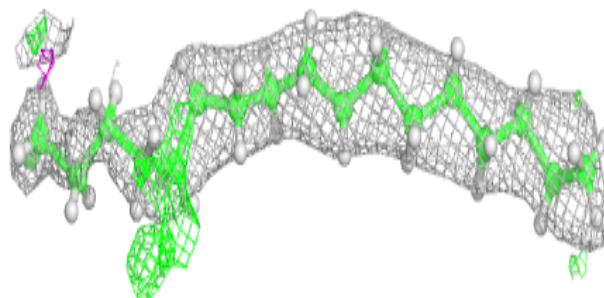
**Electron density around STE e 104:**

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

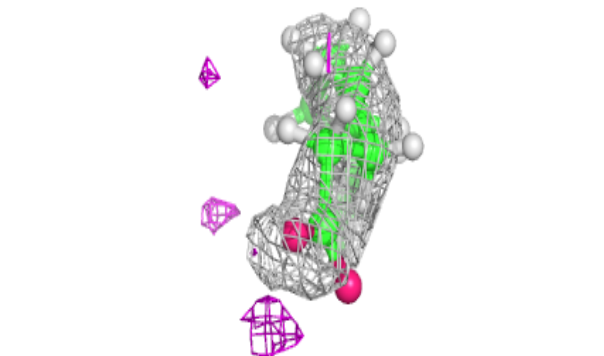
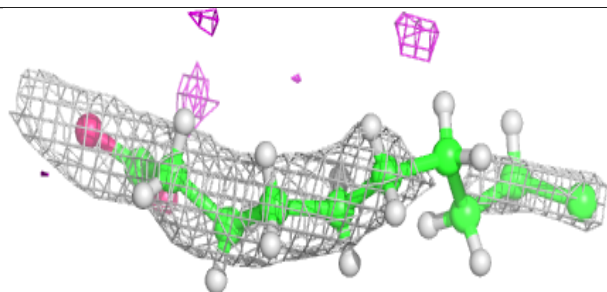
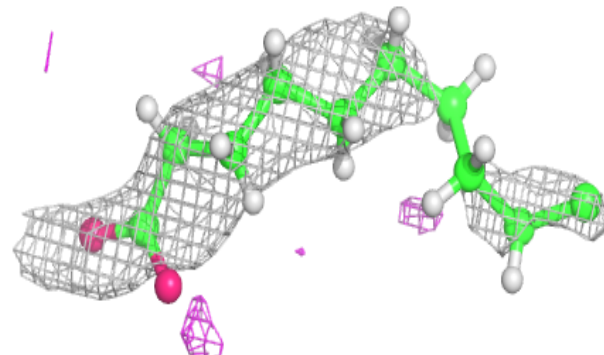


**Electron density around STE I 103:**

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

**Electron density around STE B 622:**

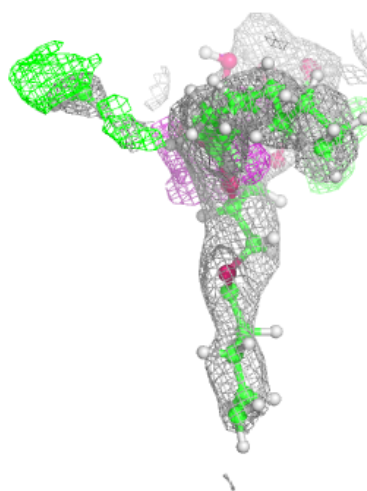
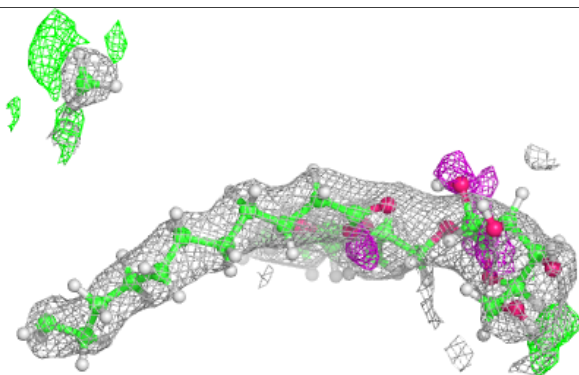
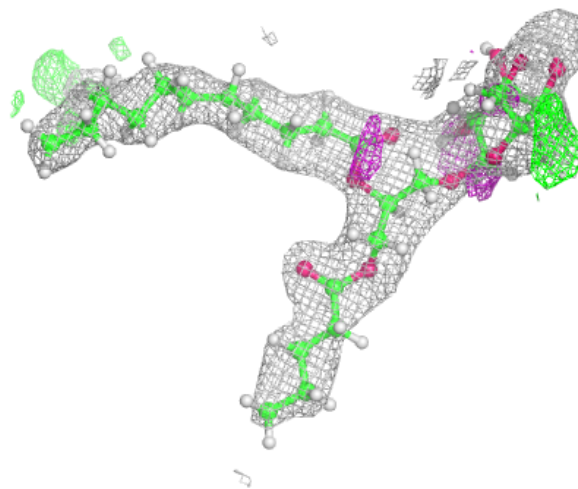
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





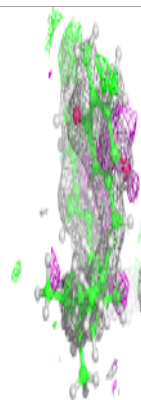
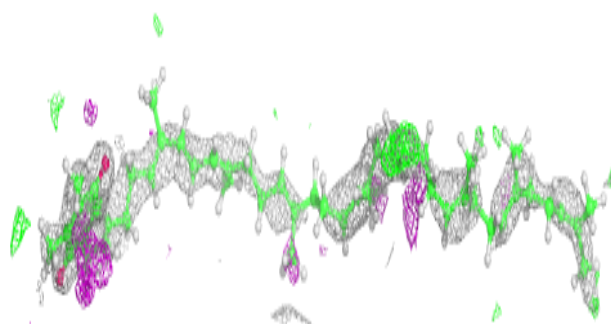
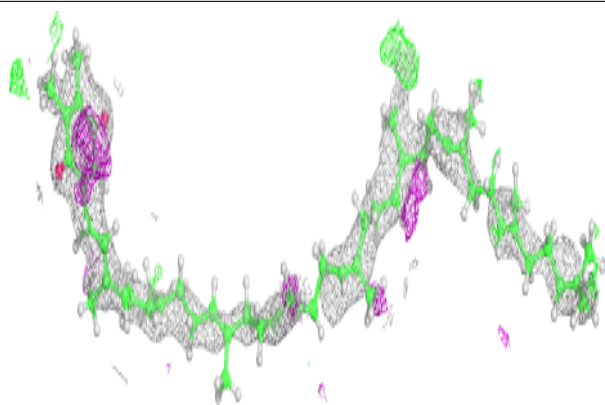
**Electron density around LMG C 517:**

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

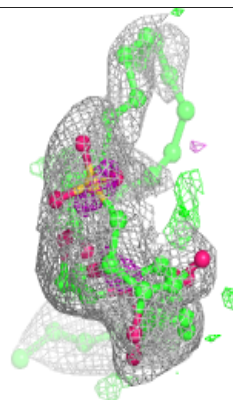
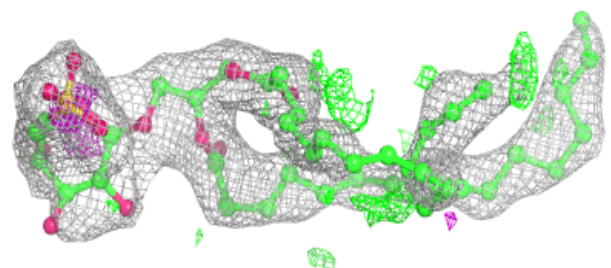
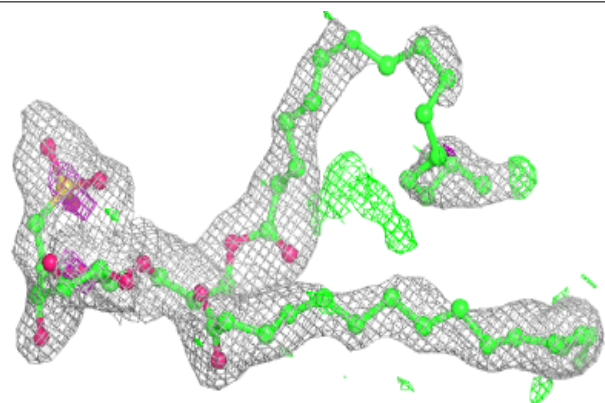


**Electron density around PL9 A 409:**

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

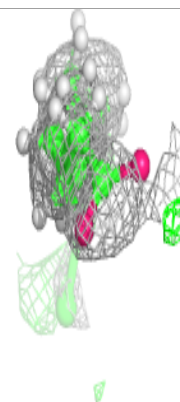
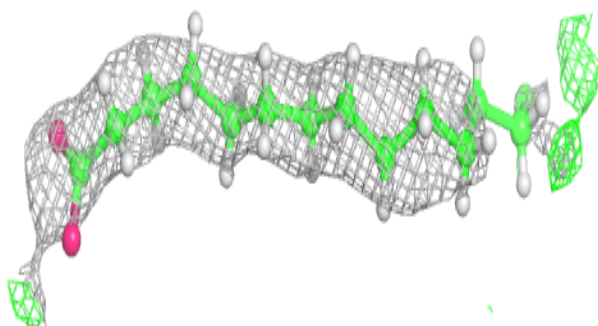
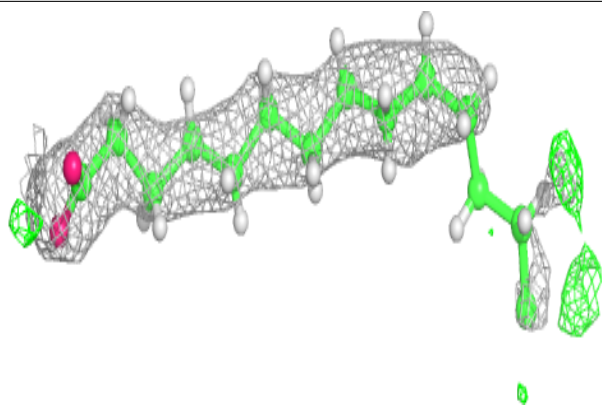
**Electron density around SQD a 414:**

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

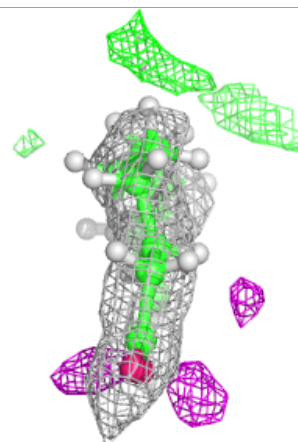
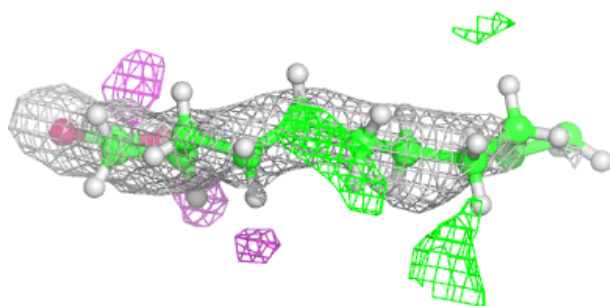
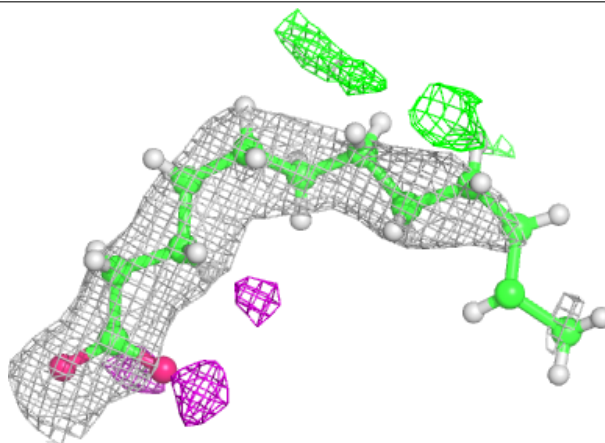


**Electron density around STE b 625:**

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

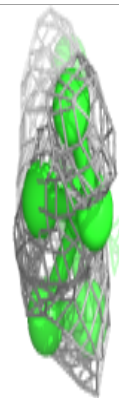
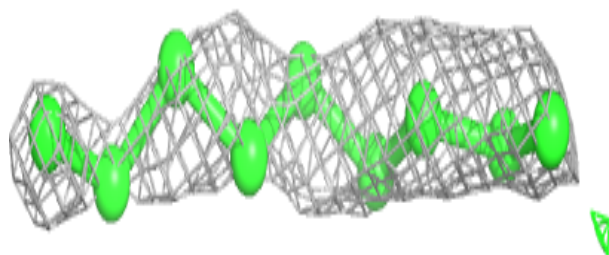
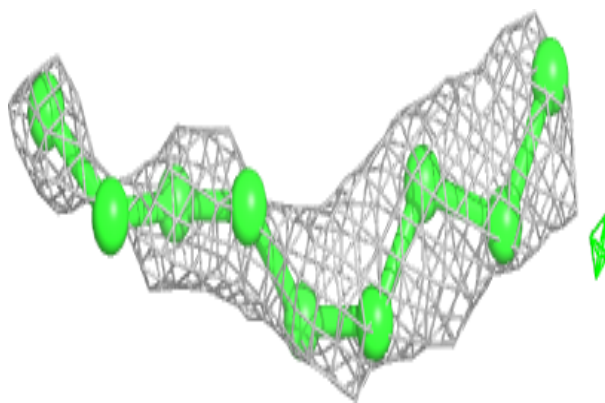
**Electron density around STE C 516:**

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

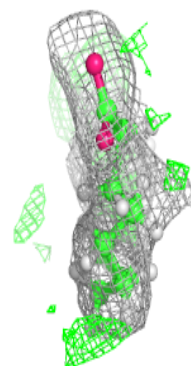
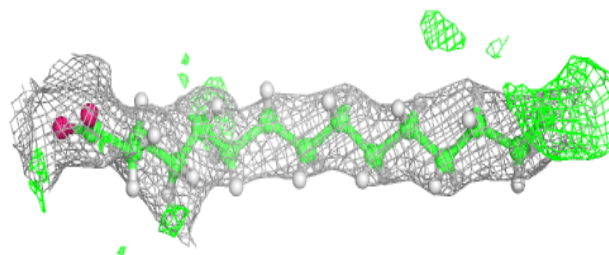
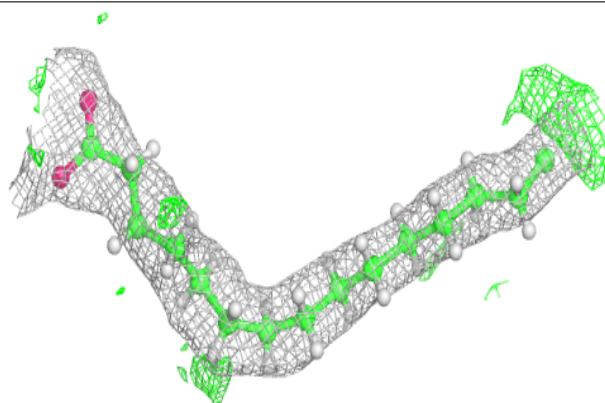


**Electron density around STE e 103:**

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

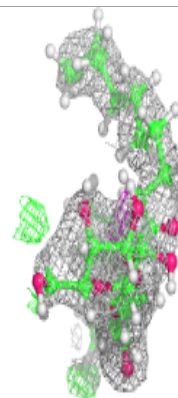
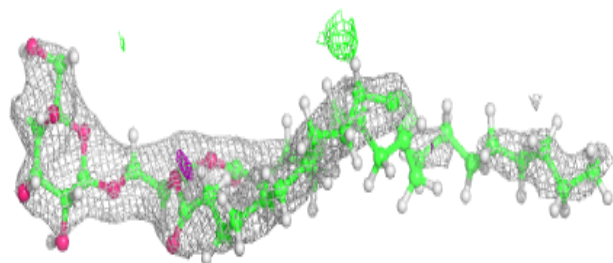
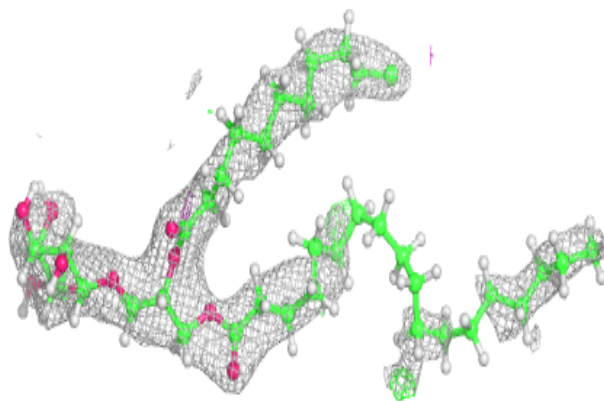
**Electron density around STE d 410:**

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

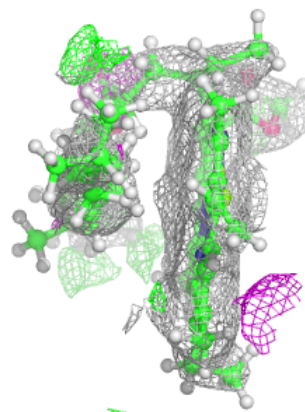
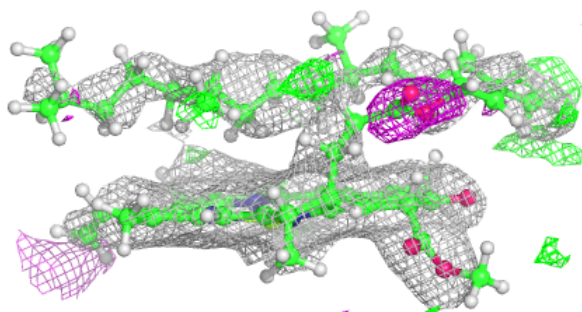
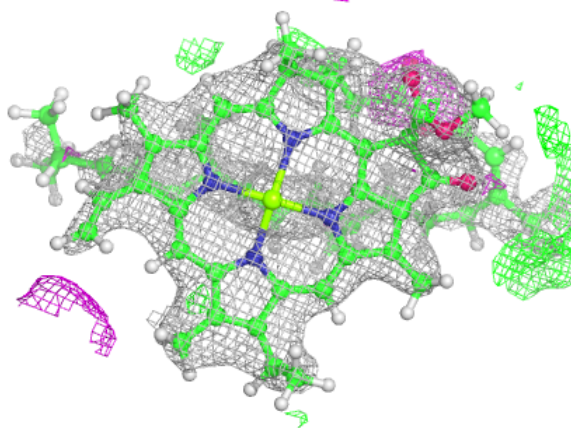


**Electron density around LMG c 523:**

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

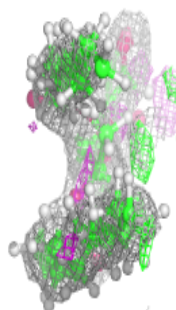
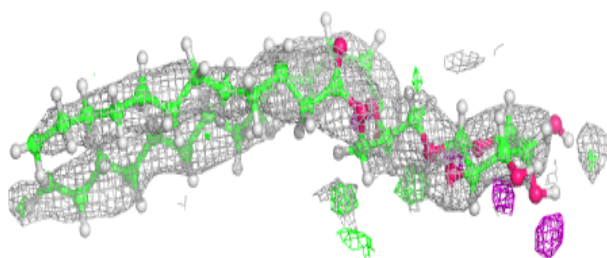
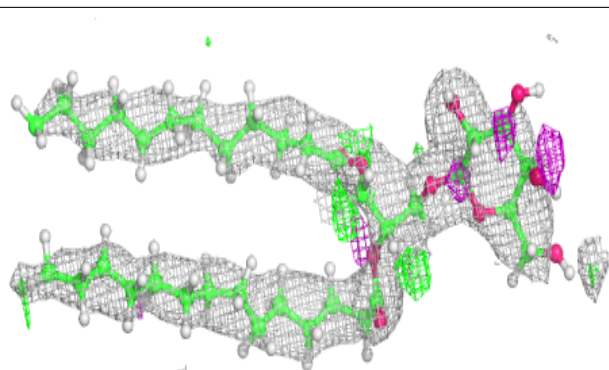
**Electron density around CLA h 101:**

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

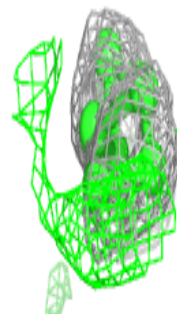
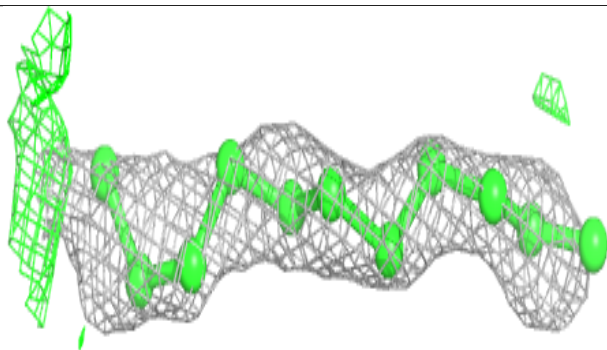
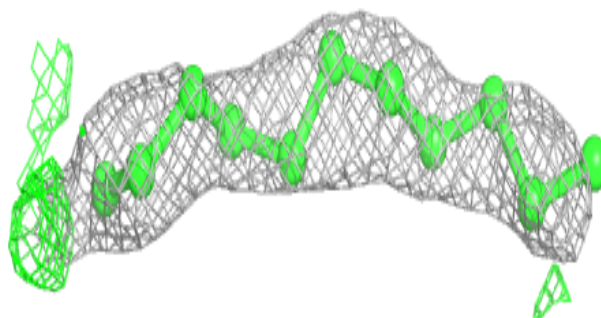


**Electron density around LMG B 620:**

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

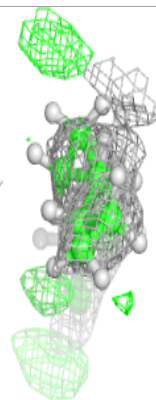
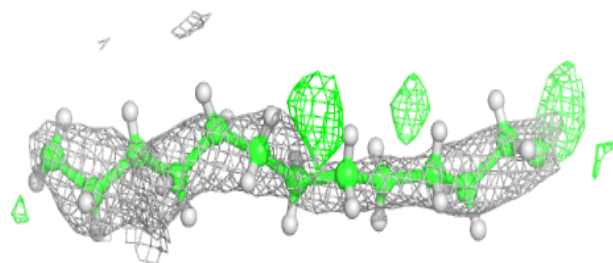
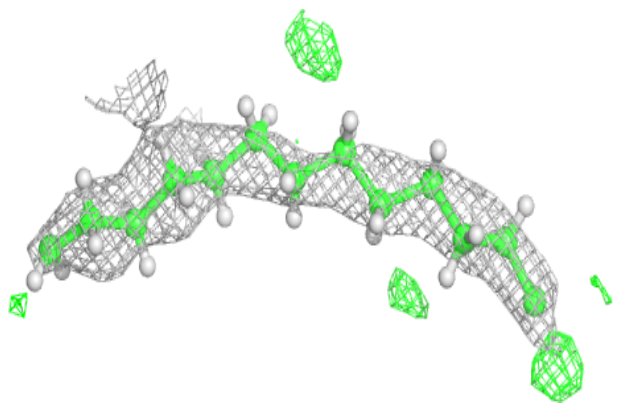
**Electron density around STE b 627:**

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

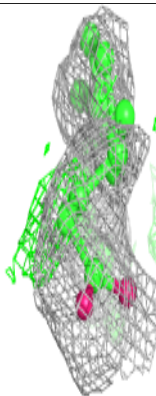
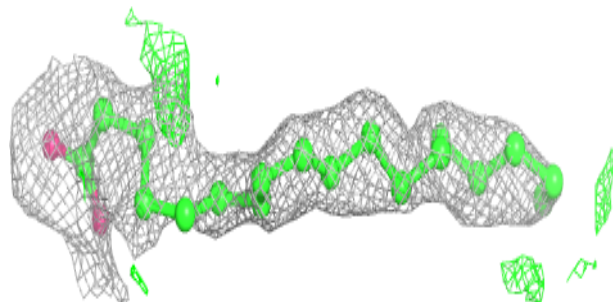
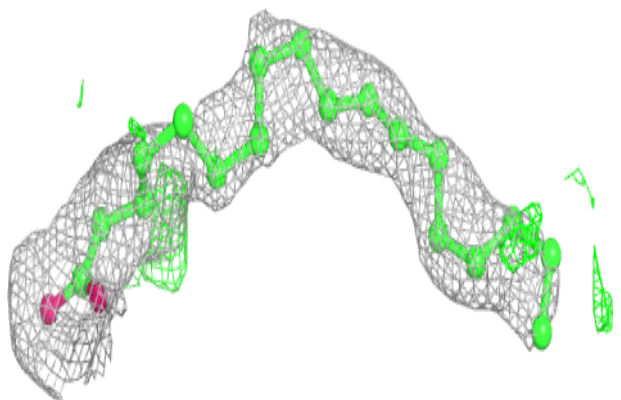


**Electron density around STE c 516:**

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

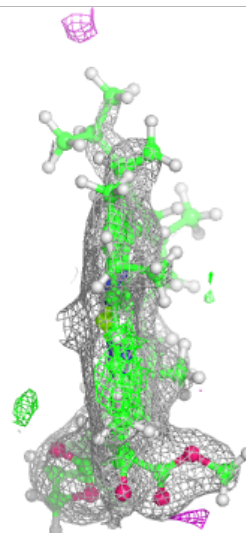
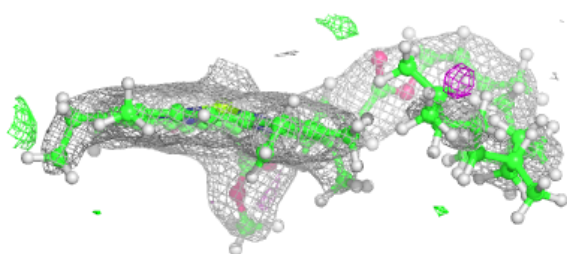
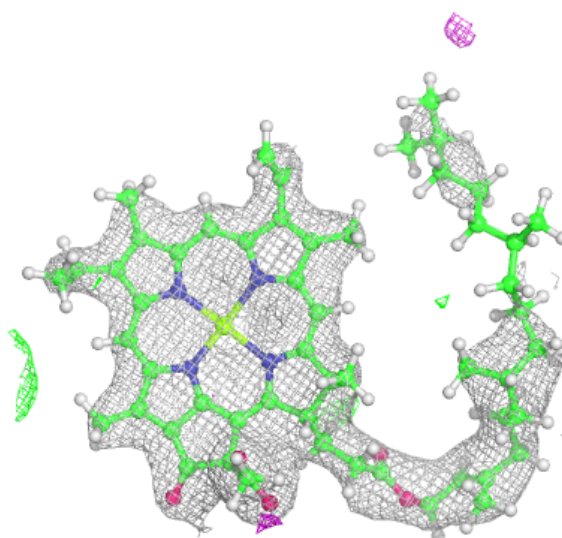
**Electron density around STE b 624:**

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



**Electron density around CLA C 512:**

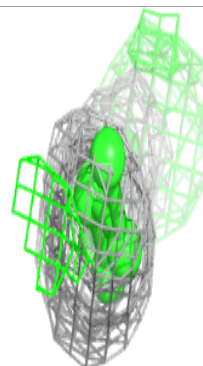
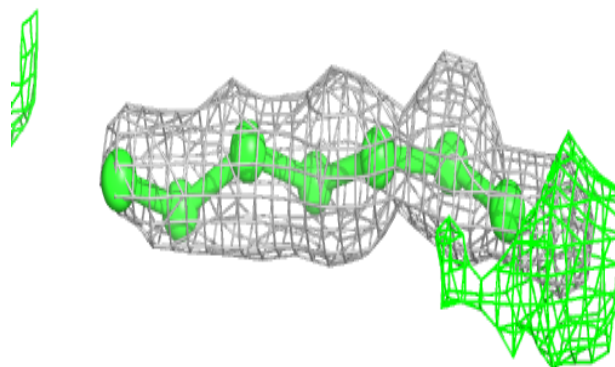
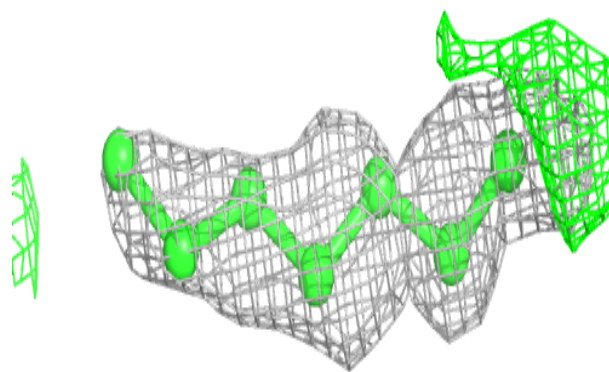
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



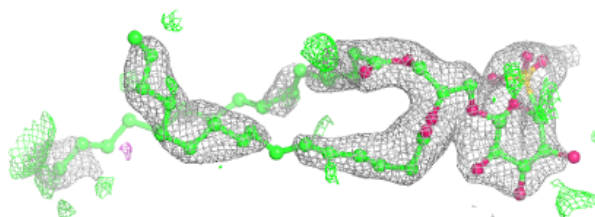
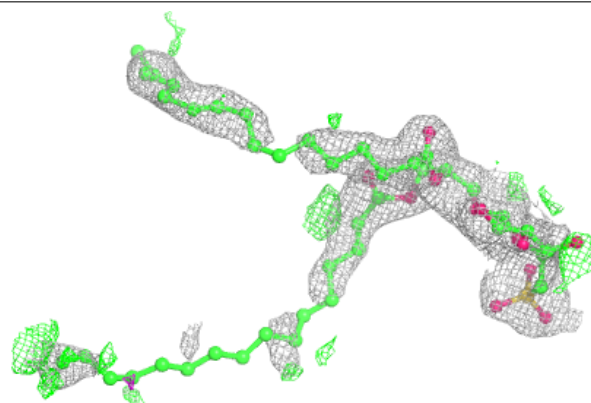


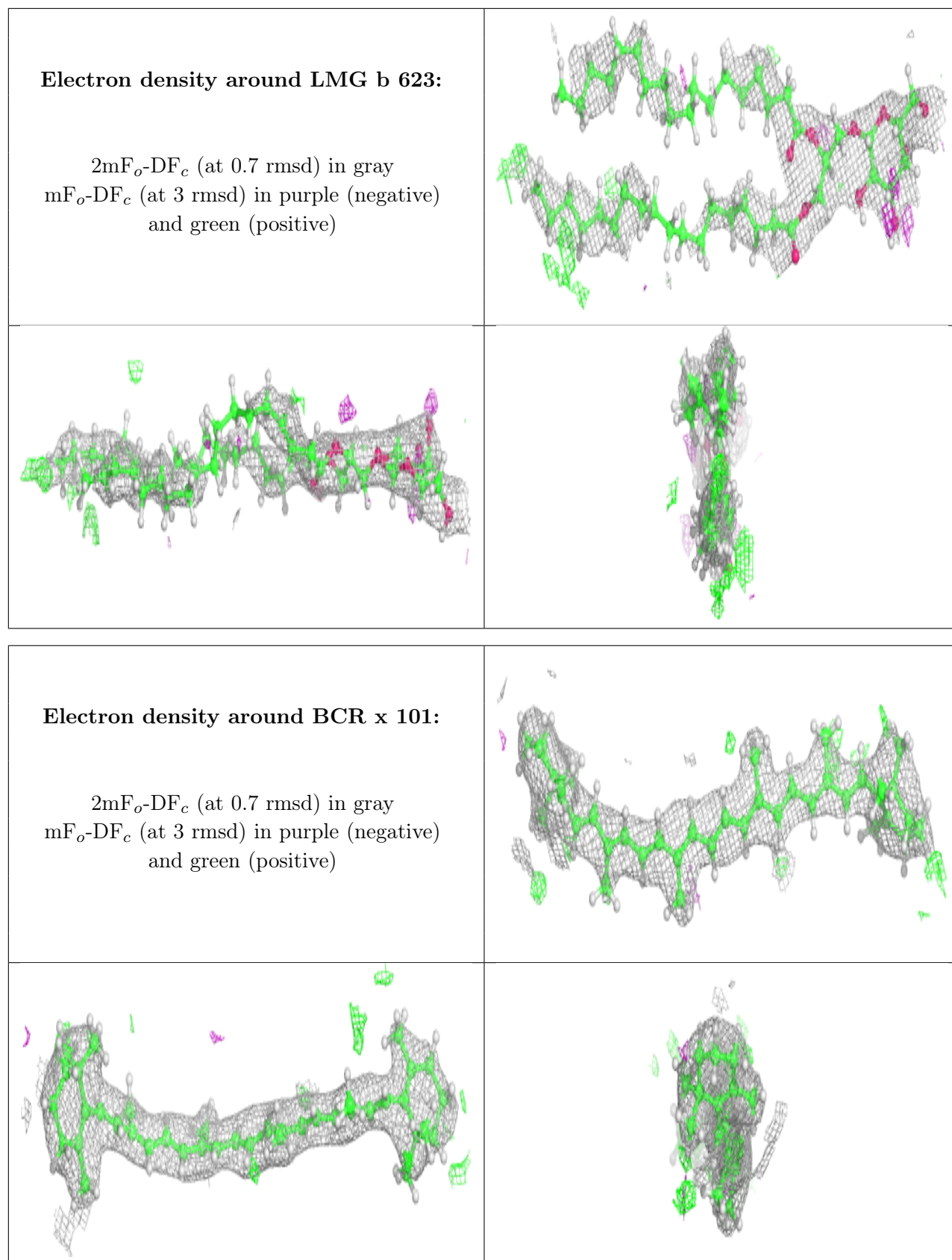
**Electron density around STE C 519:**

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

**Electron density around SQD A 413:**

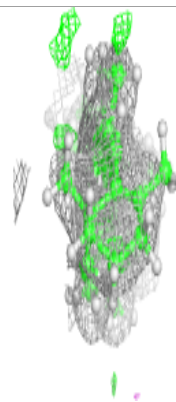
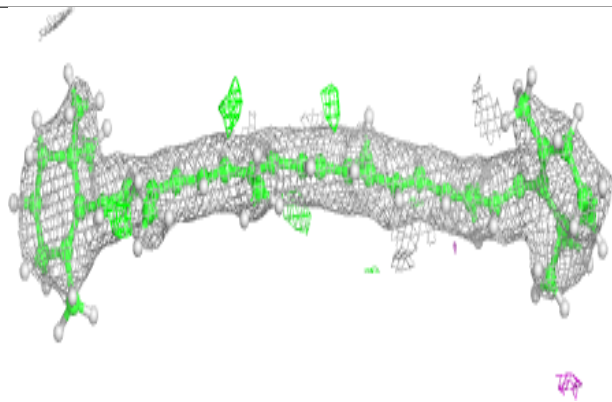
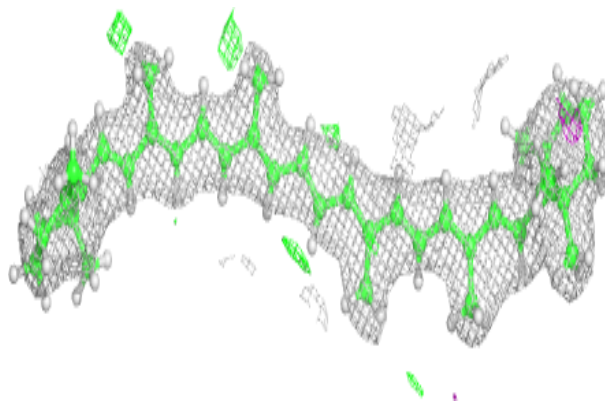
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



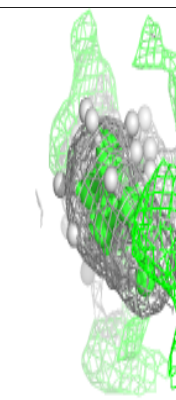
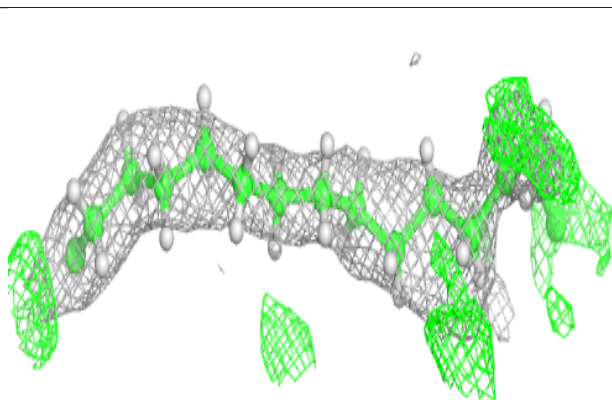
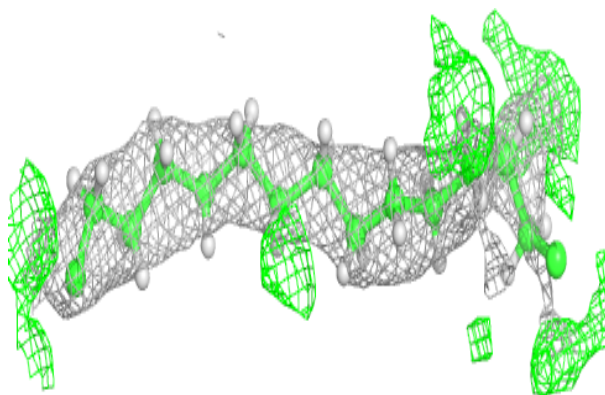


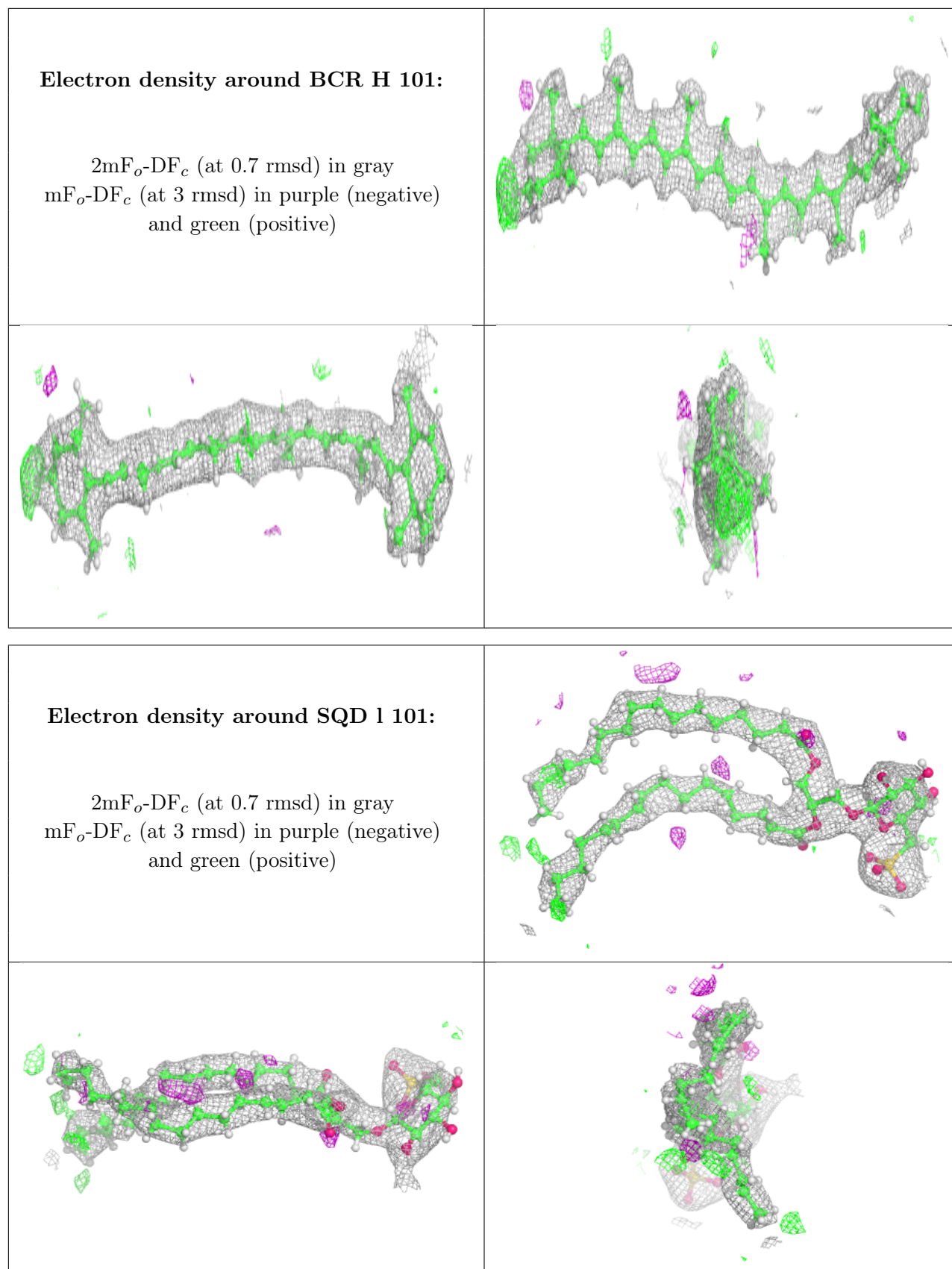
**Electron density around BCR K 101:**

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

**Electron density around STE I 101:**

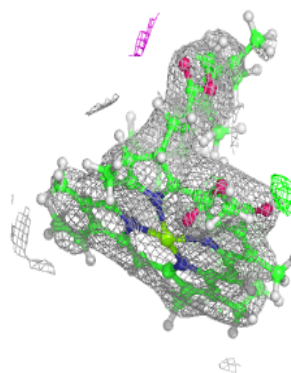
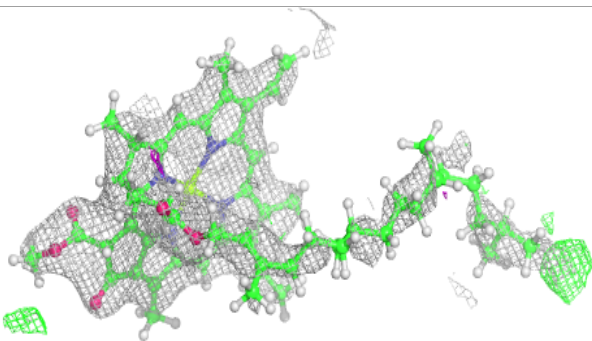
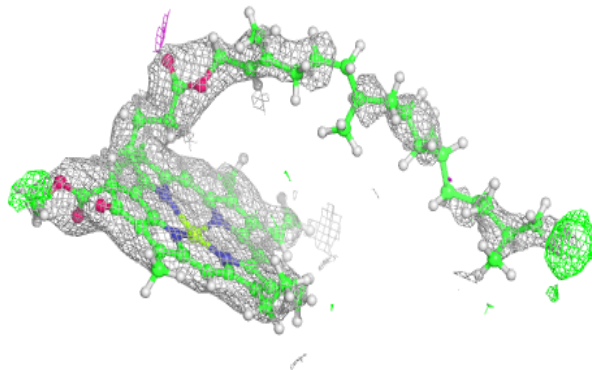
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



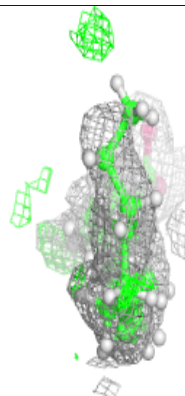
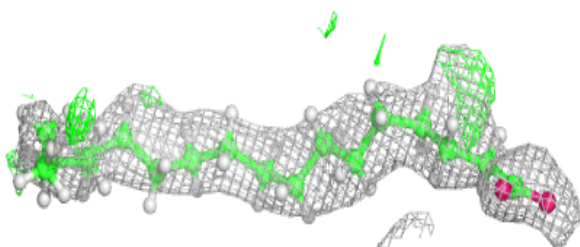
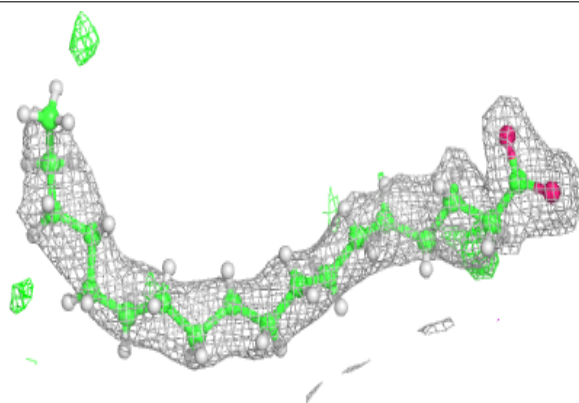


**Electron density around CLA c 513:**

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

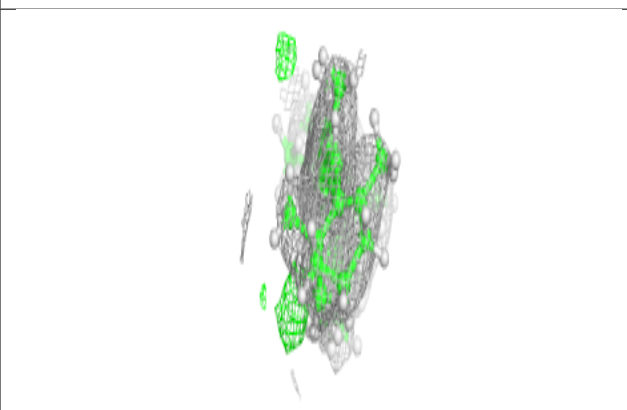
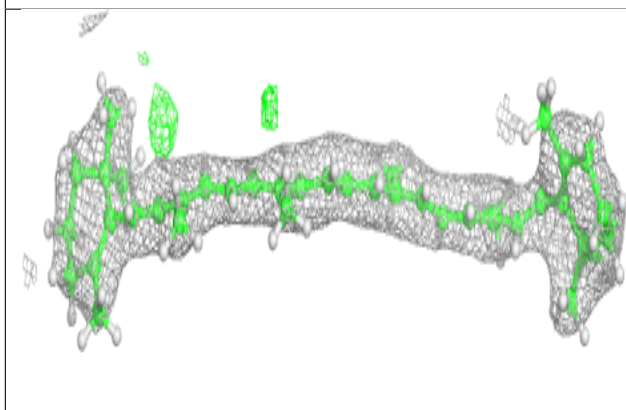
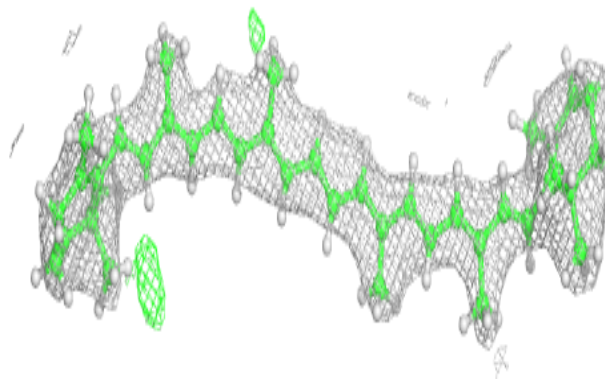
**Electron density around STE b 622:**

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

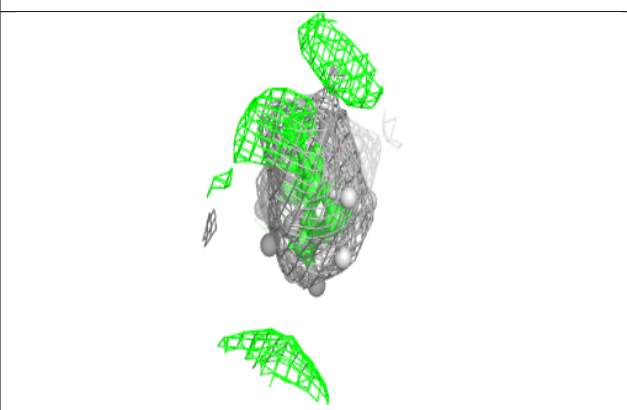
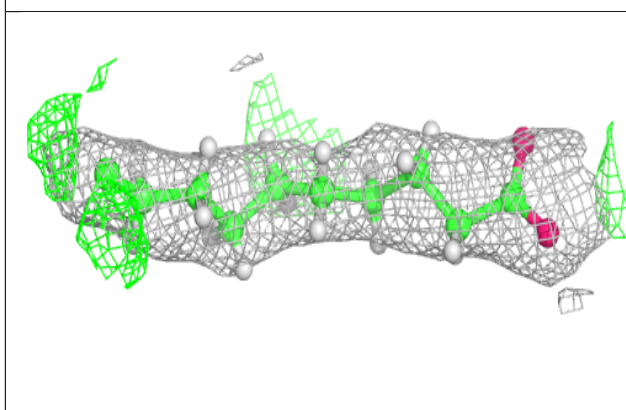
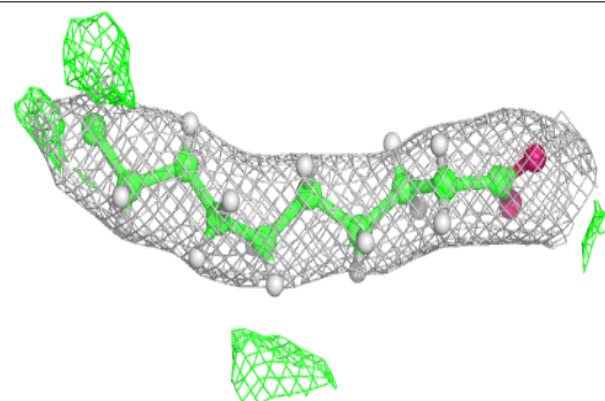


**Electron density around BCR k 101:**

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

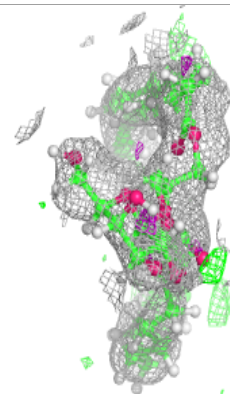
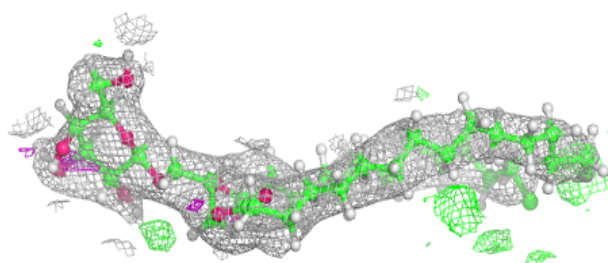
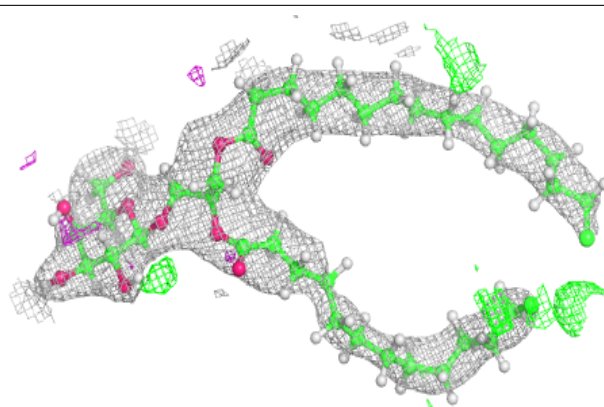
**Electron density around STE j 101:**

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

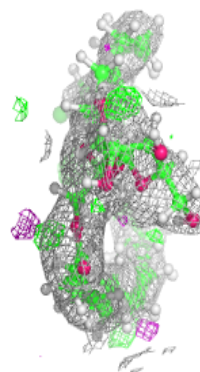
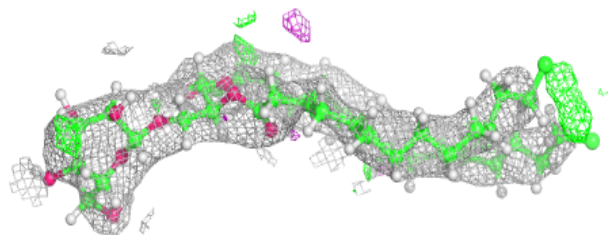
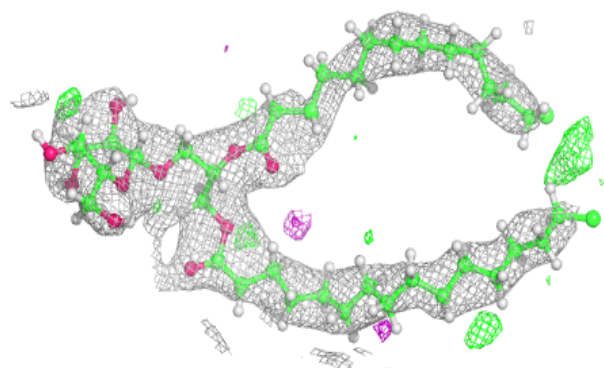


**Electron density around LMG A 411:**

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

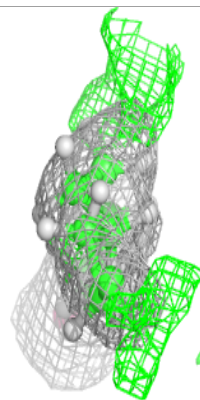
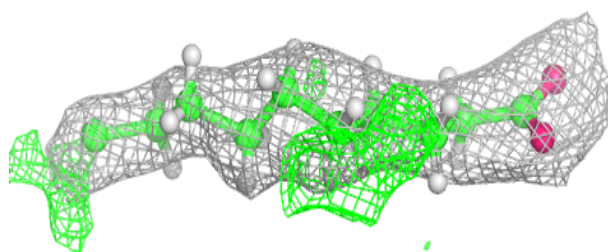
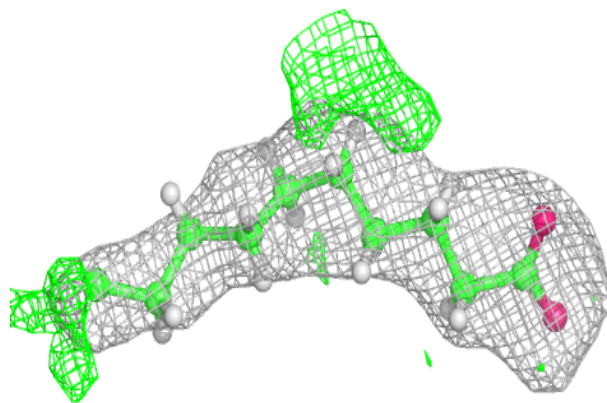
**Electron density around LMG c 524:**

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

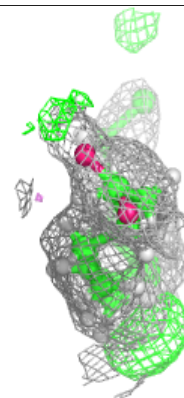
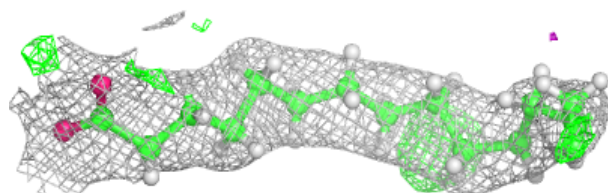
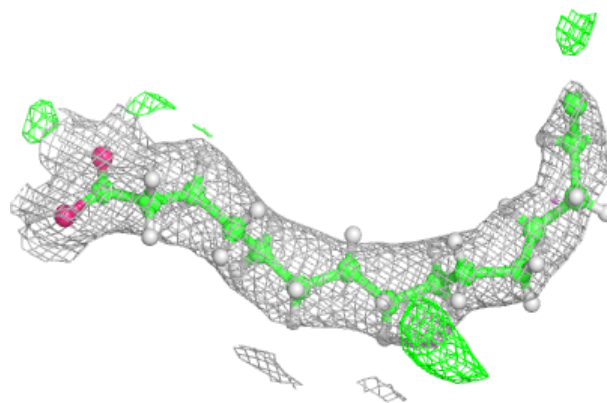


**Electron density around STE C 525:**

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

**Electron density around STE B 621:**

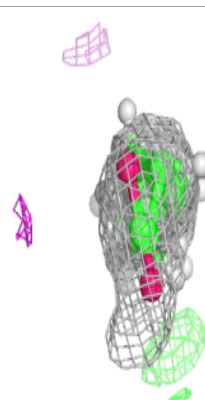
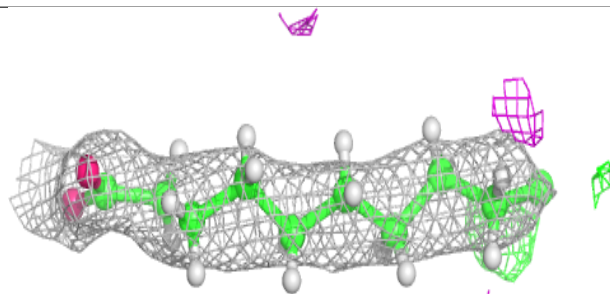
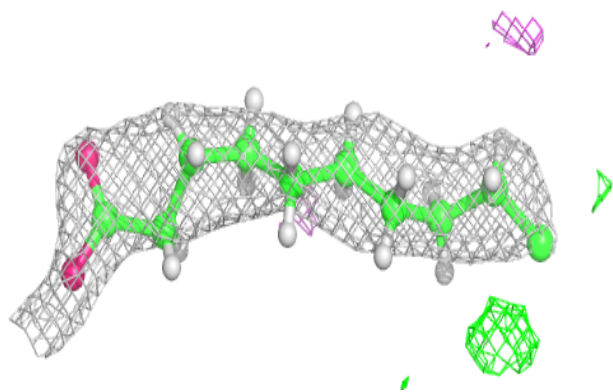
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



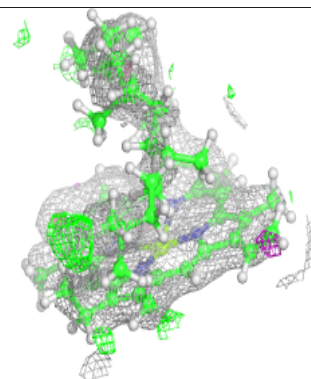
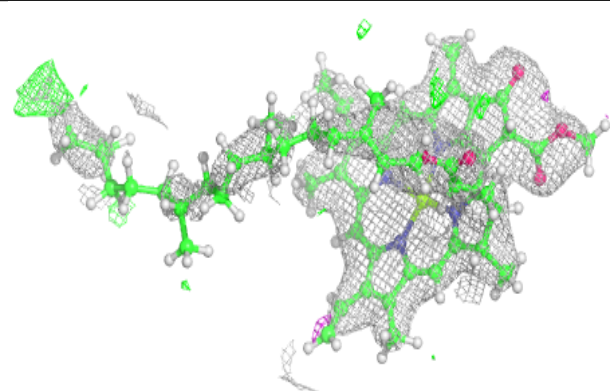
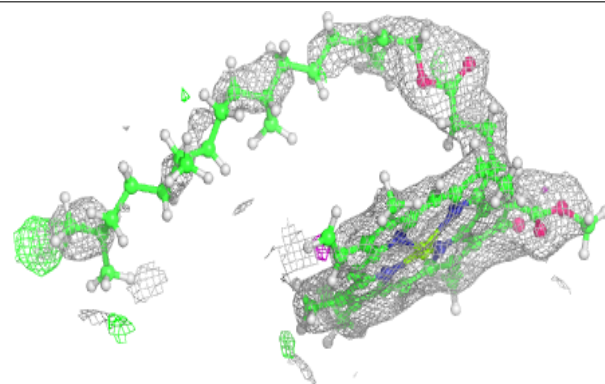


**Electron density around STE m 101:**

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

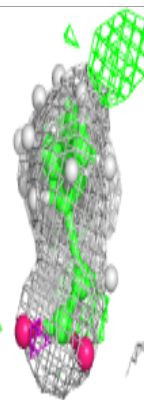
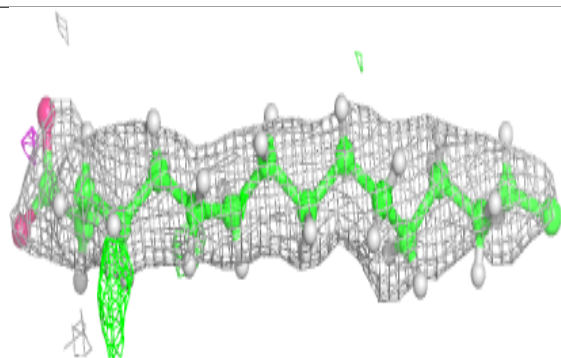
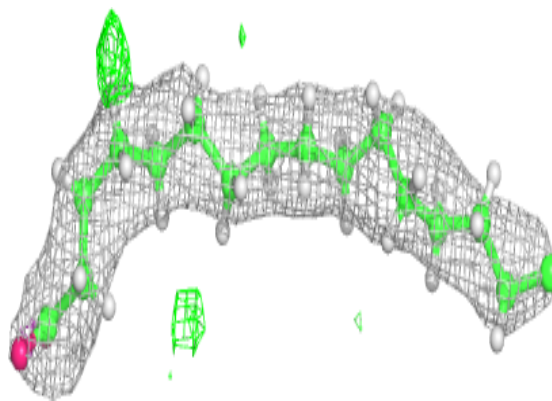
**Electron density around CLA C 513:**

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

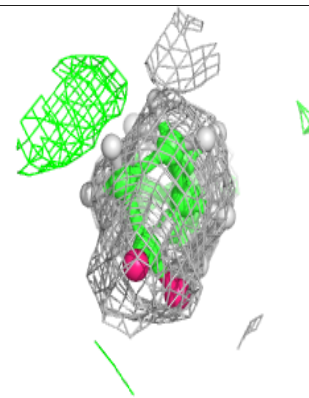
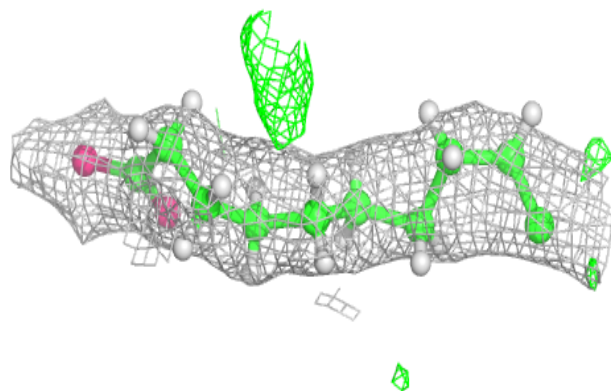
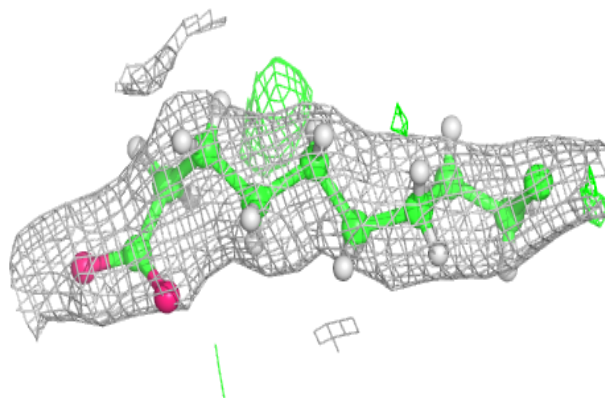


**Electron density around STE t 103:**

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

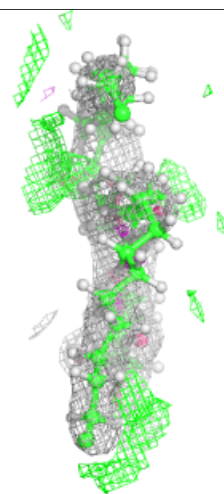
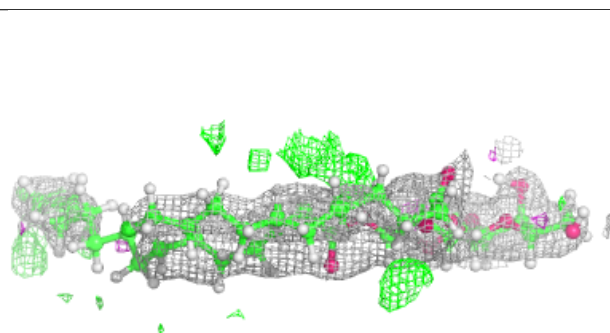
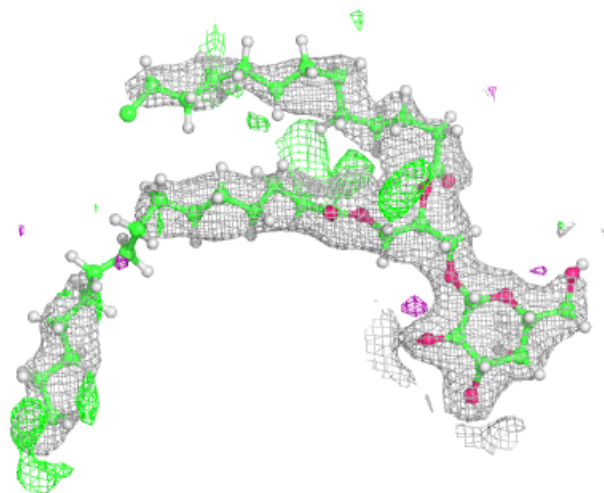
**Electron density around STE J 101:**

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



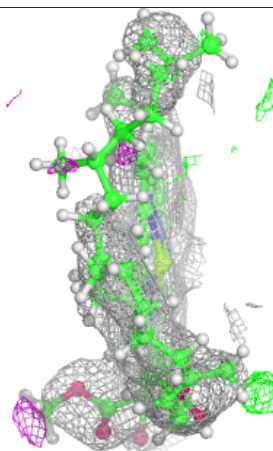
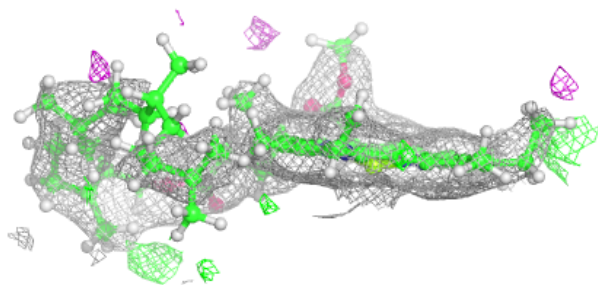
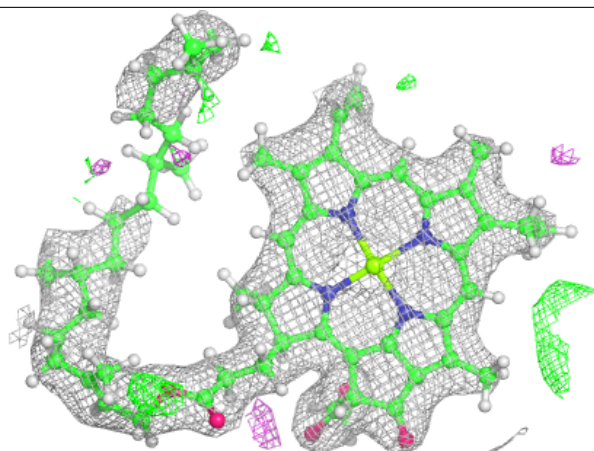
**Electron density around LMG C 524:**

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

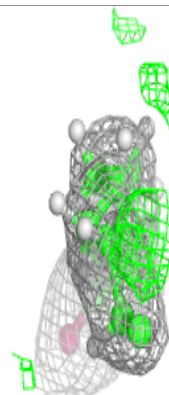
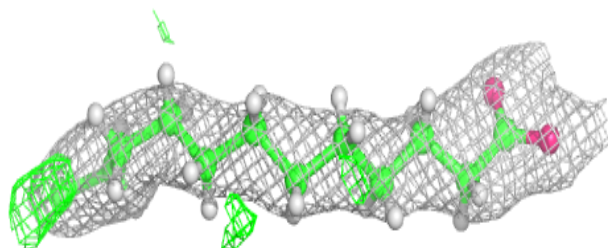
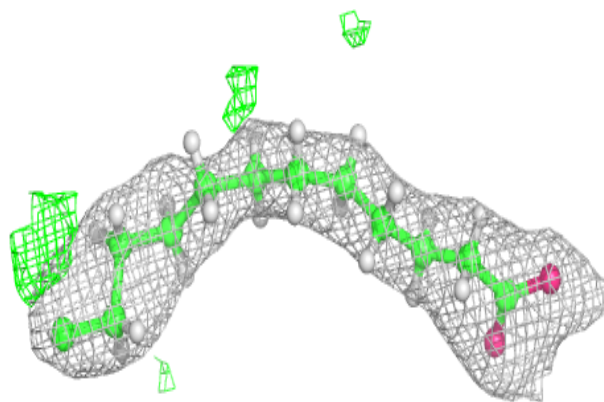


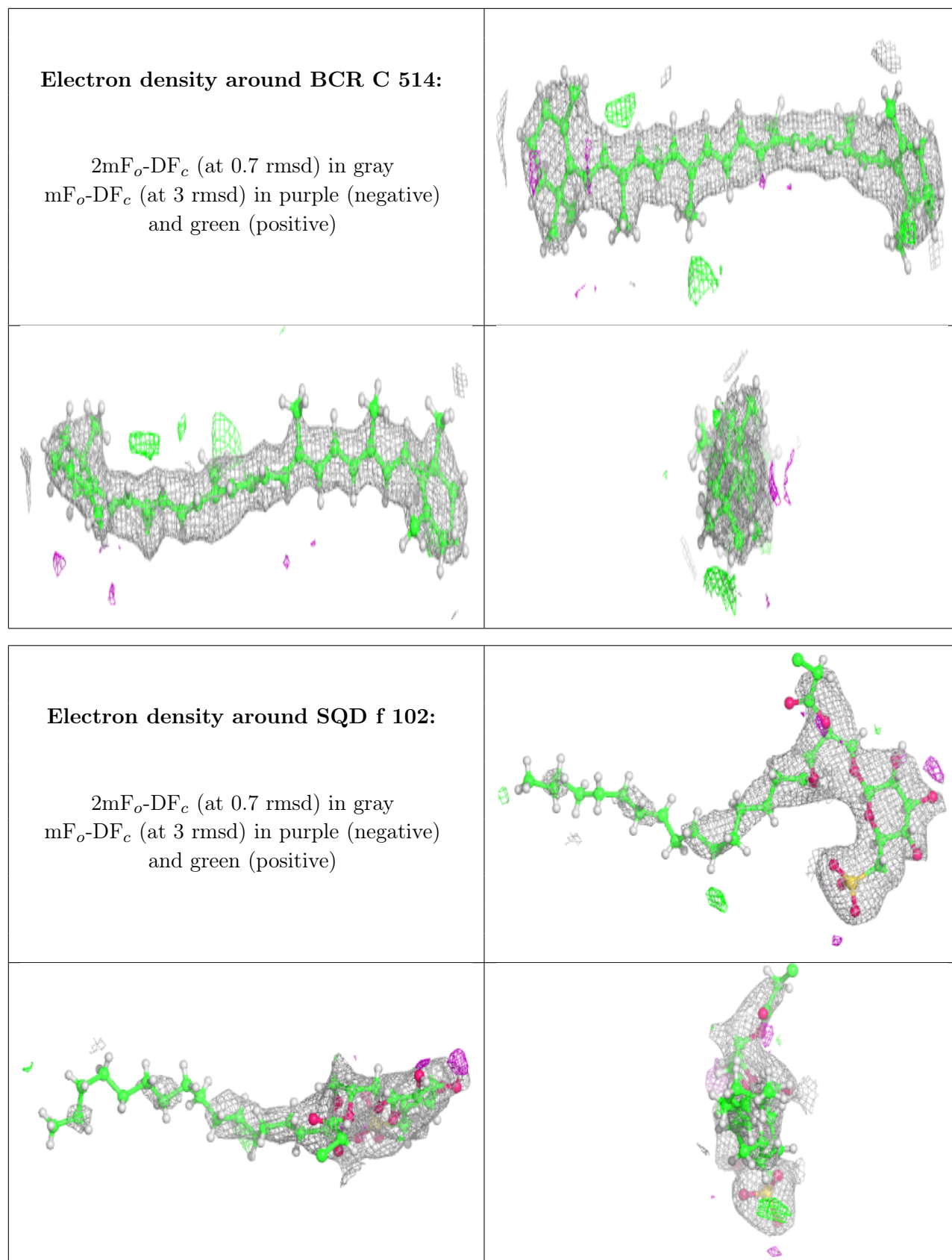
**Electron density around CLA c 512:**

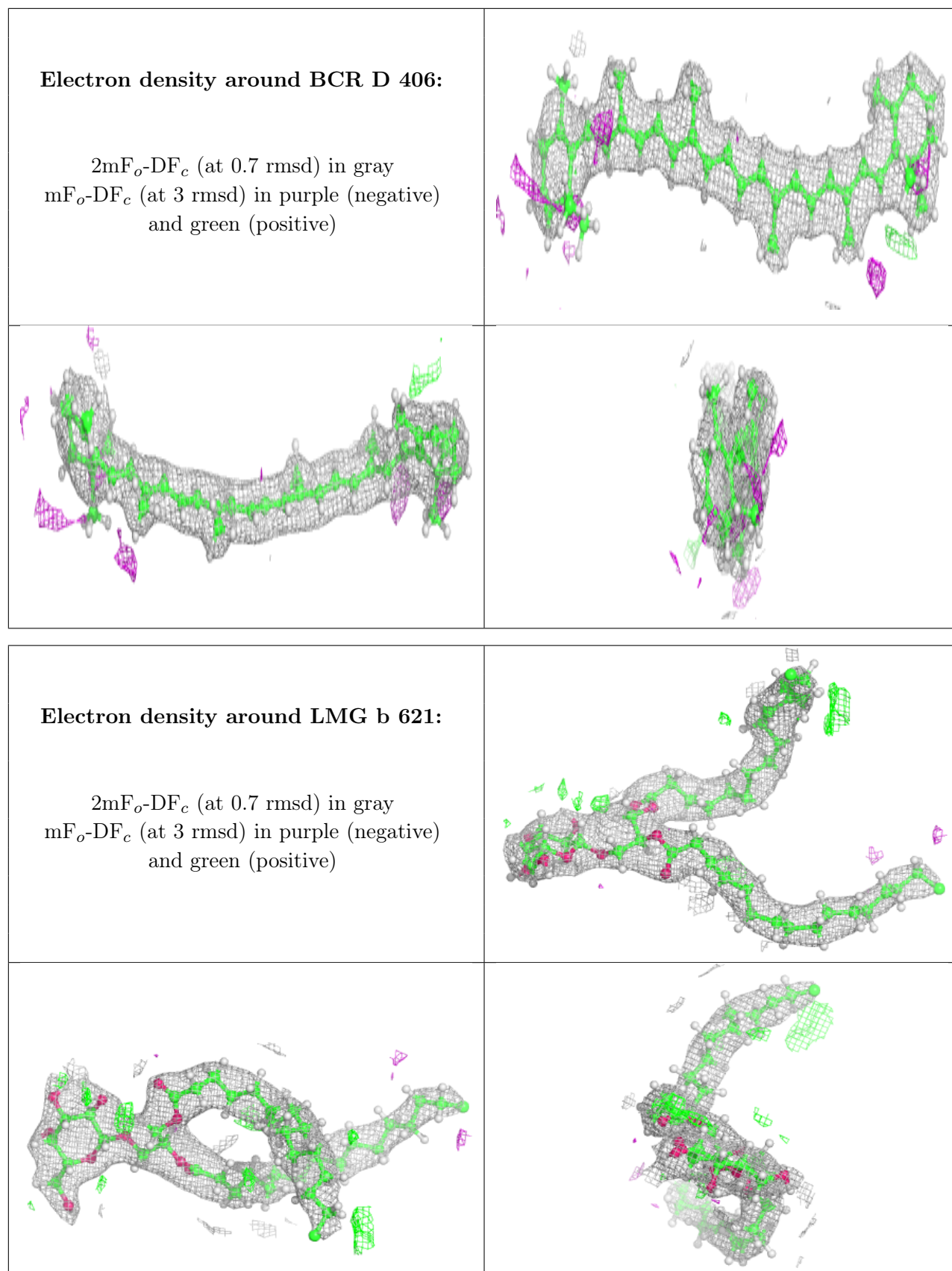
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around STE t 102:**

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

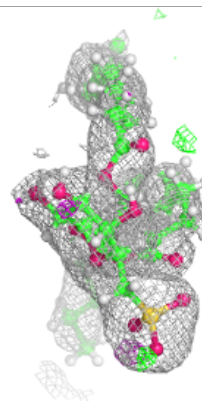
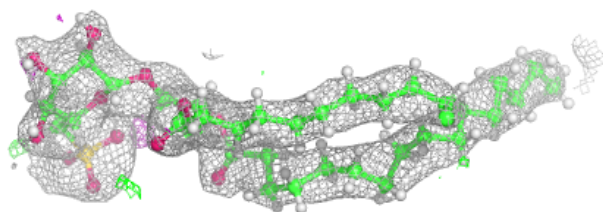
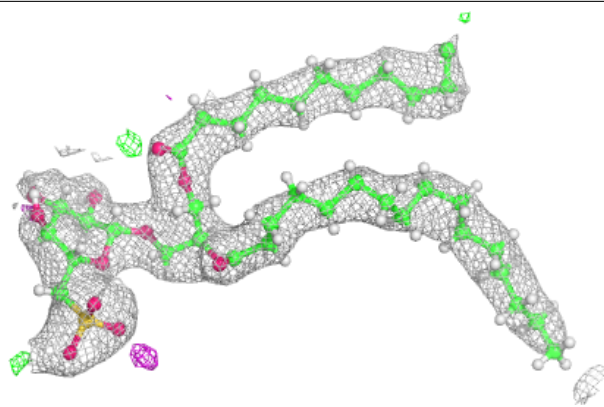






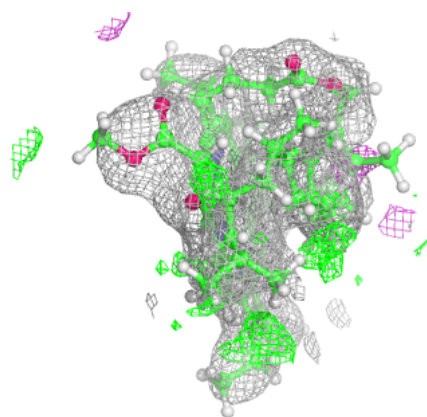
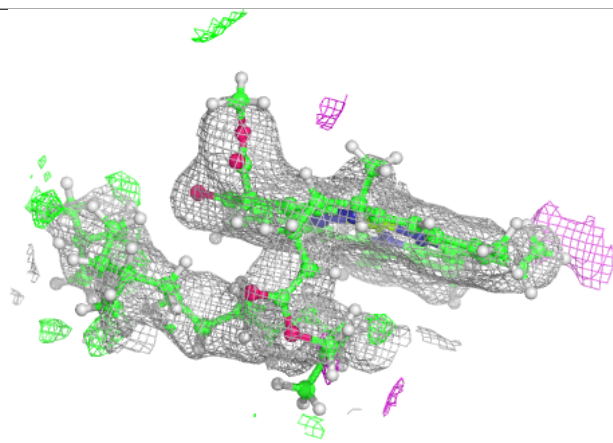
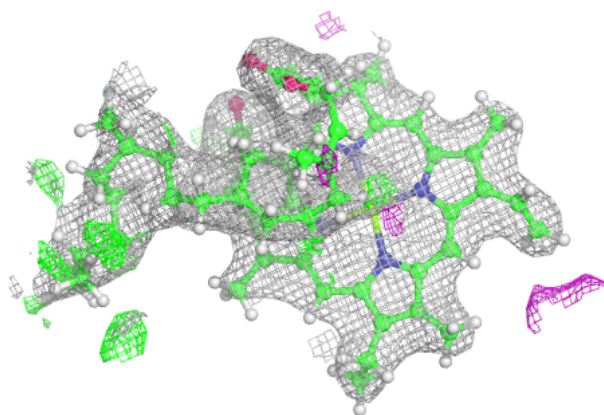
**Electron density around SQD b 620:**

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



**Electron density around CLA B 601:**

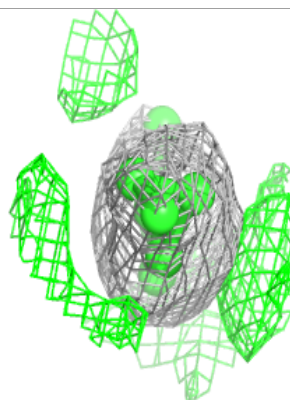
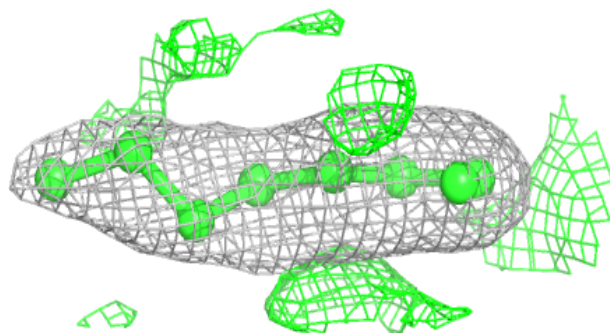
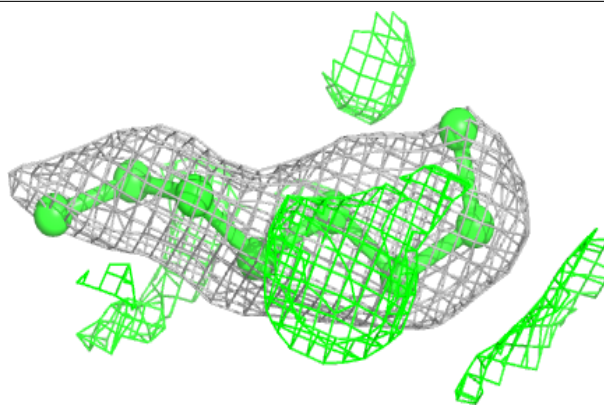
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



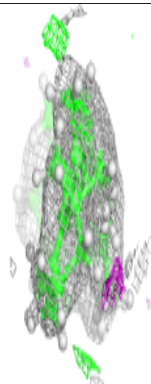
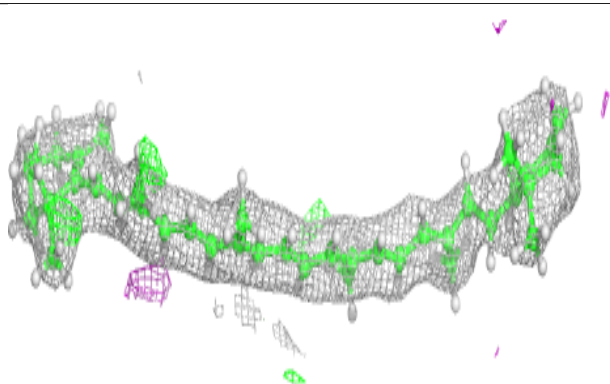
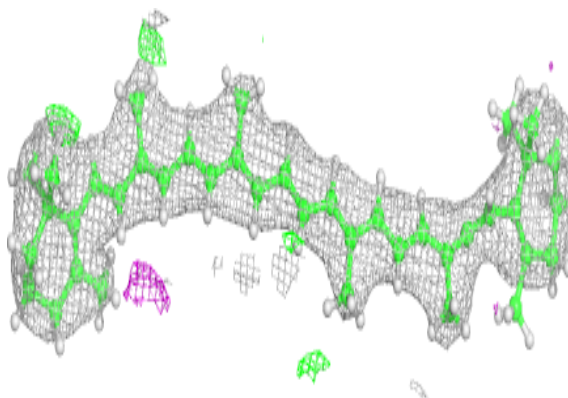


**Electron density around STE A 415:**

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

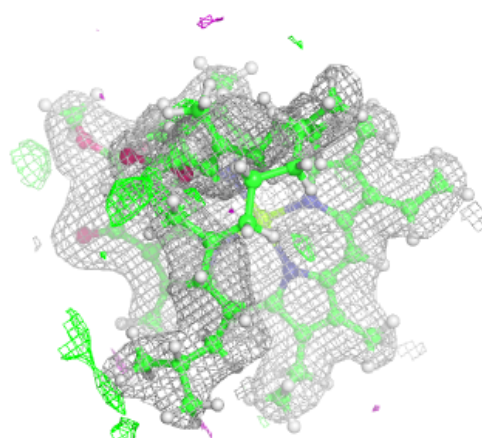
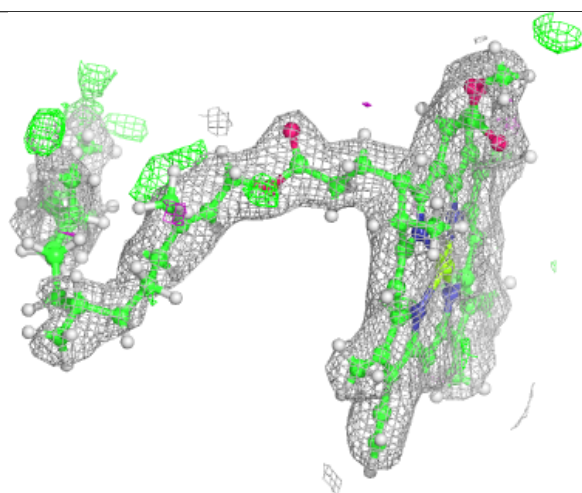
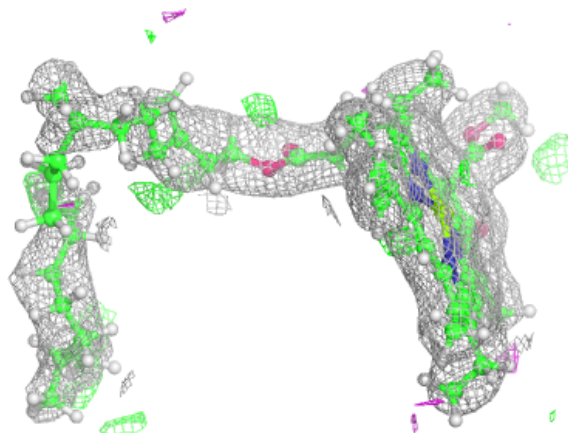
**Electron density around BCR d 404:**

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



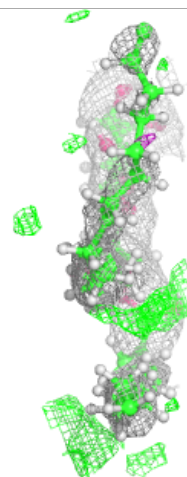
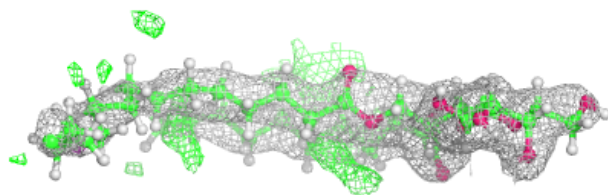
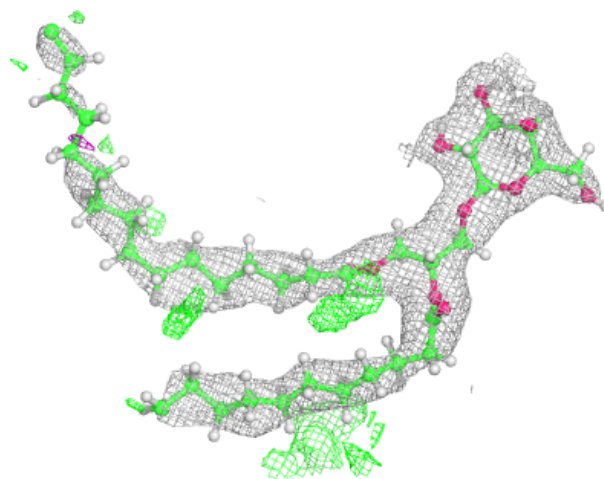
**Electron density around CLA a 408:**

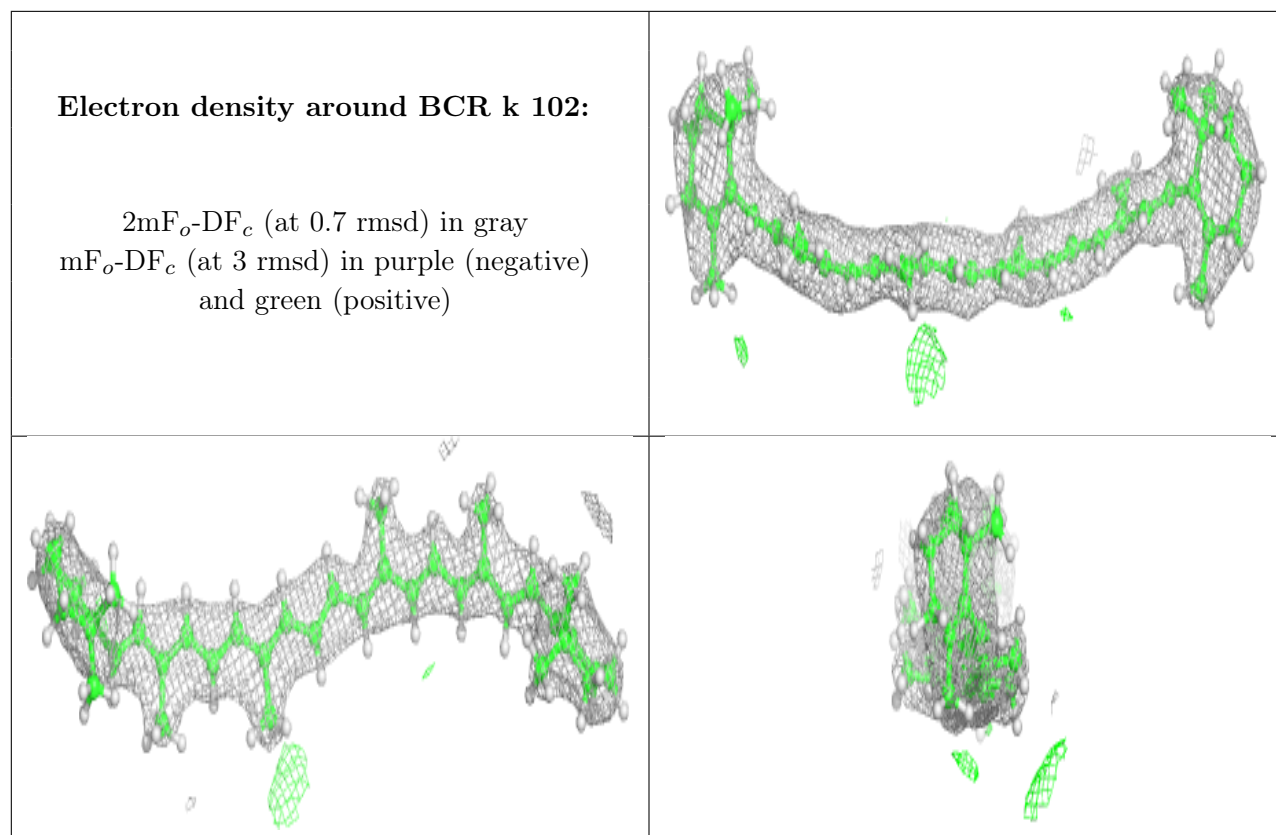
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMG c 522:**

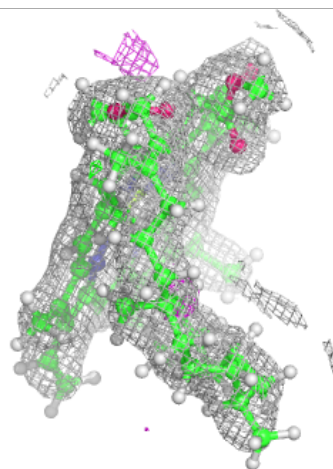
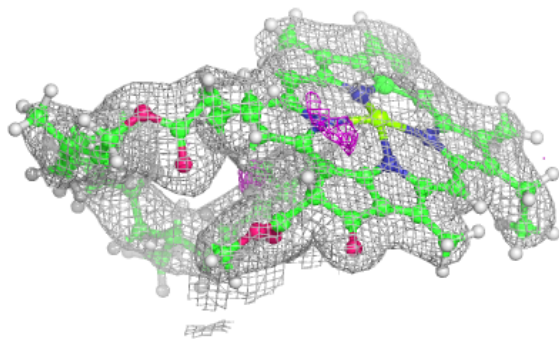
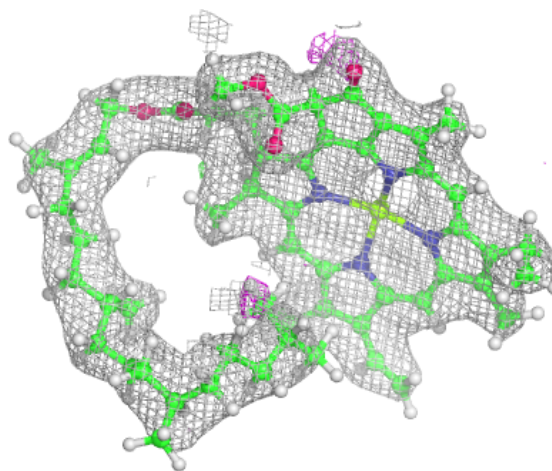
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





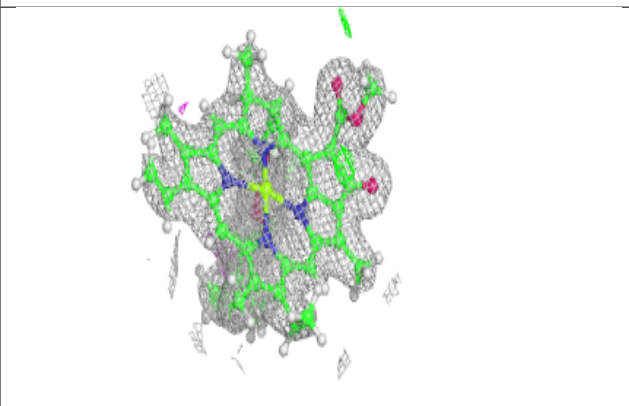
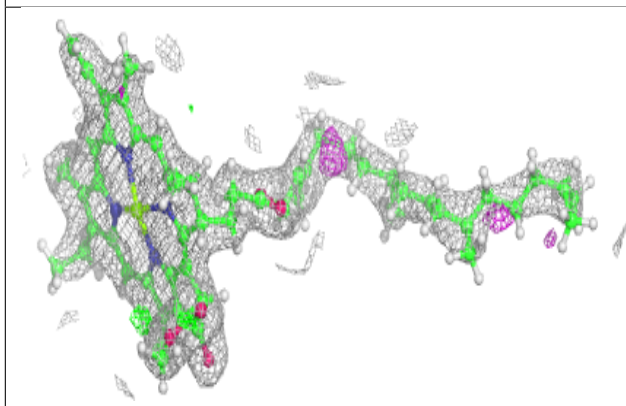
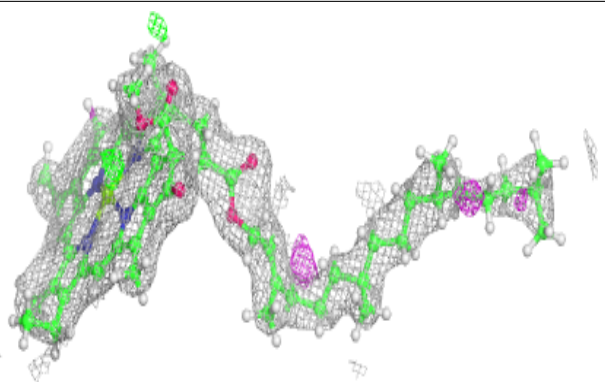
**Electron density around CLA b 614:**

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

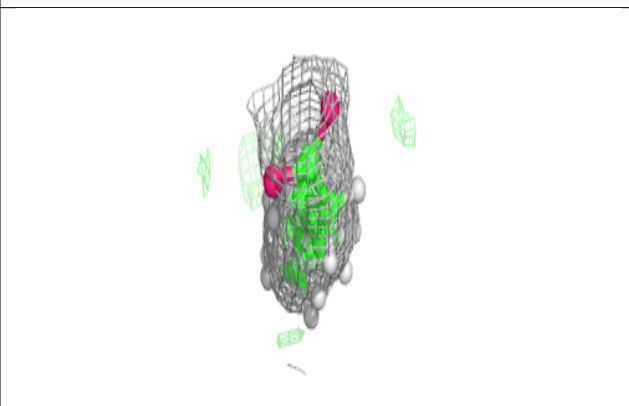
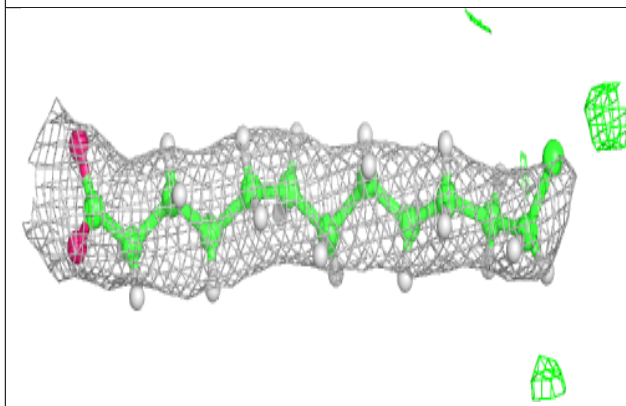
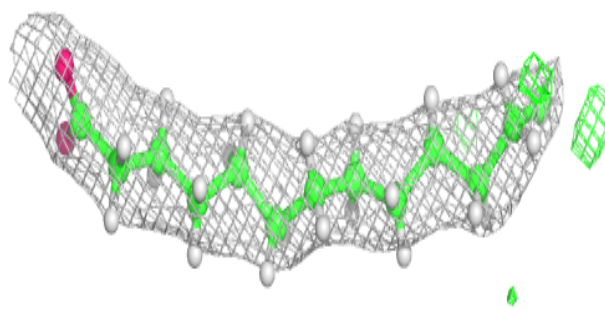


**Electron density around CLA c 502:**

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

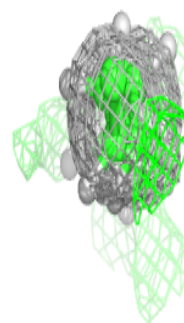
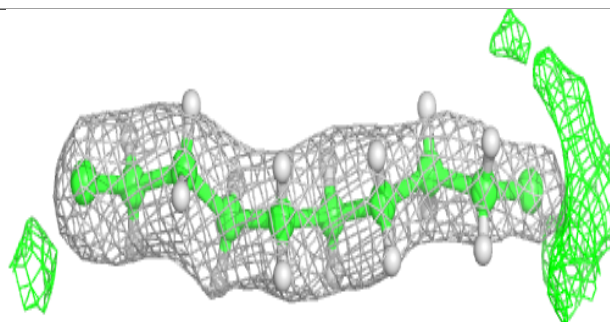
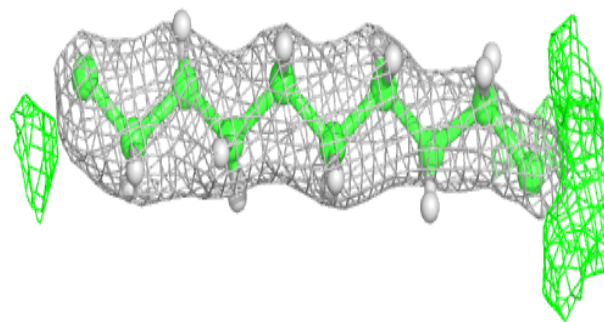
**Electron density around STE M 102:**

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

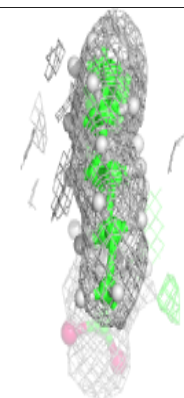
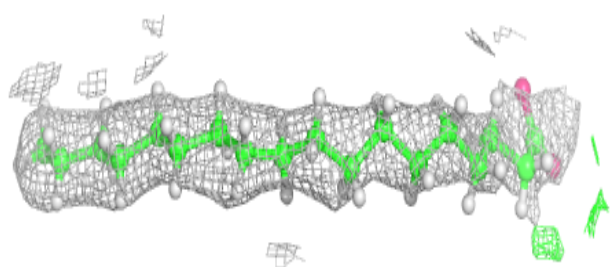
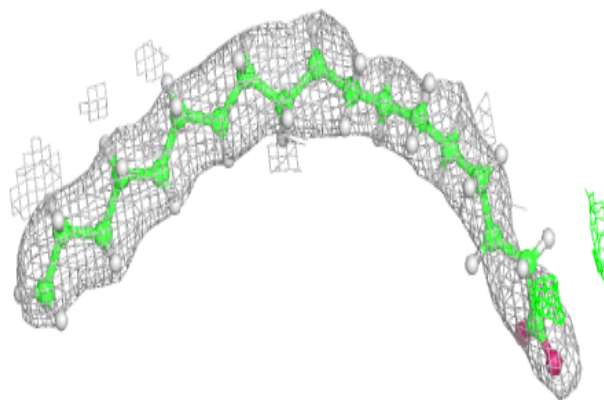


**Electron density around STE M 103:**

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

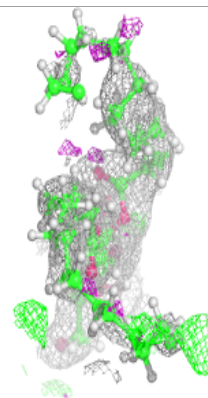
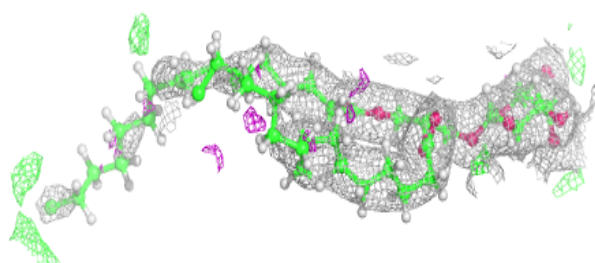
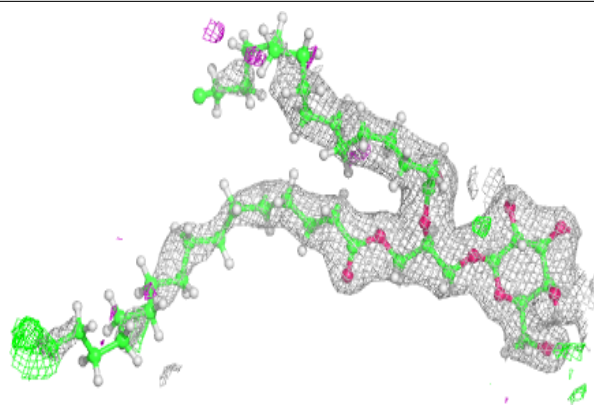
**Electron density around STE D 413:**

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

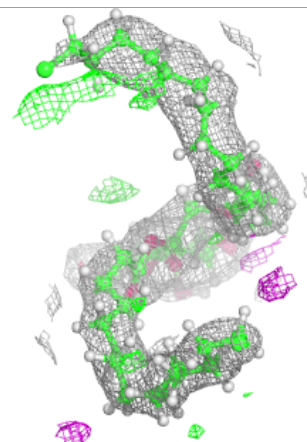
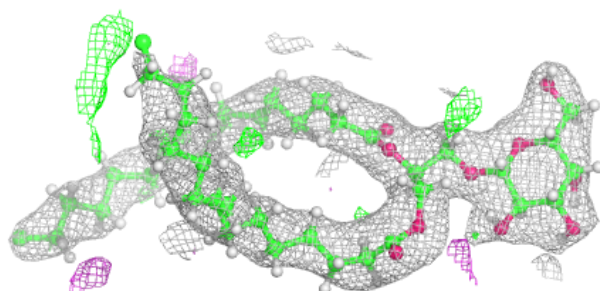
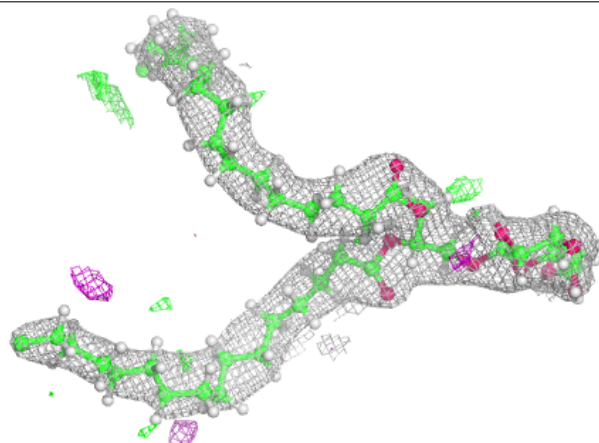


**Electron density around LMG D 409:**

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

**Electron density around LMG M 101:**

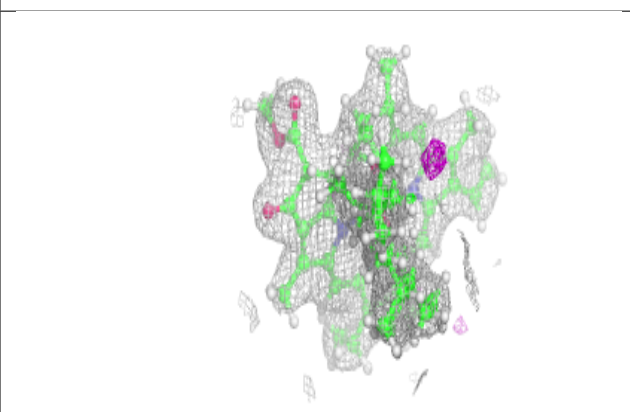
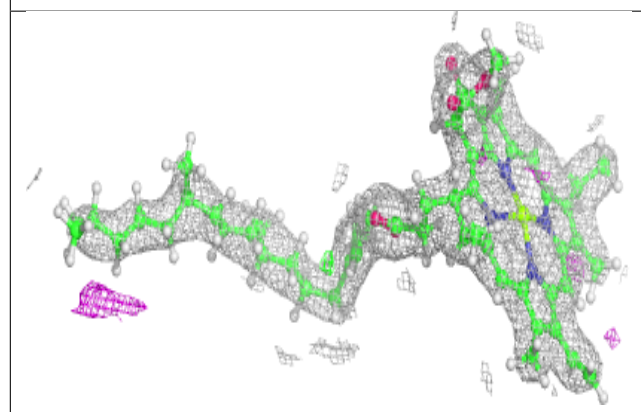
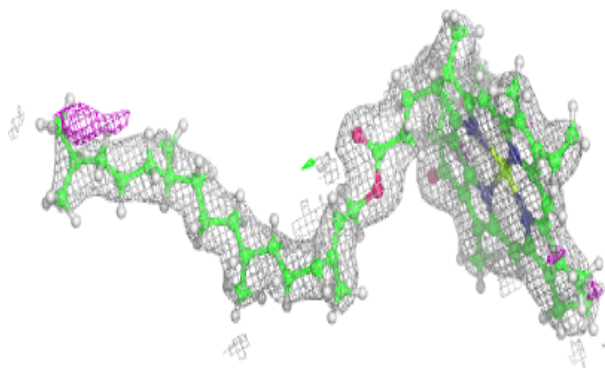
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



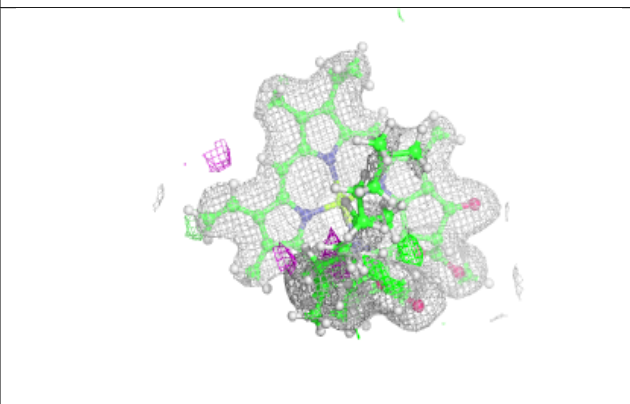
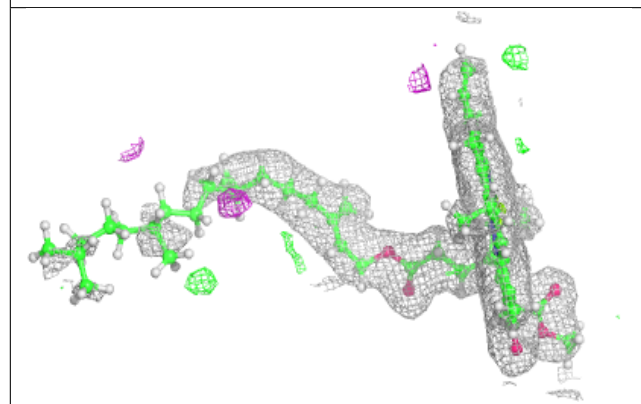
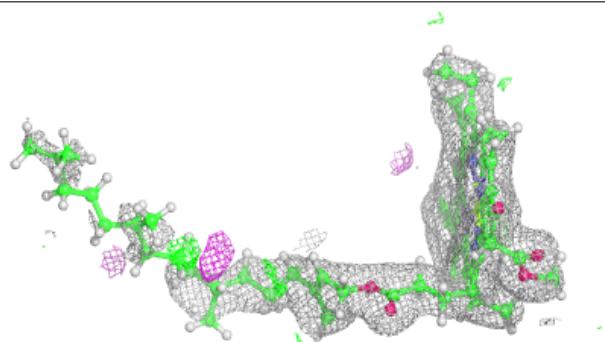


**Electron density around CLA C 502:**

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

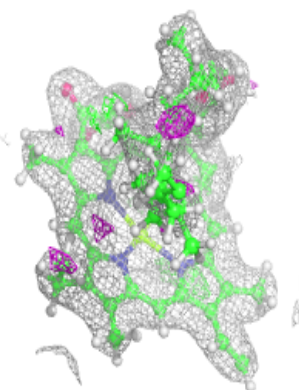
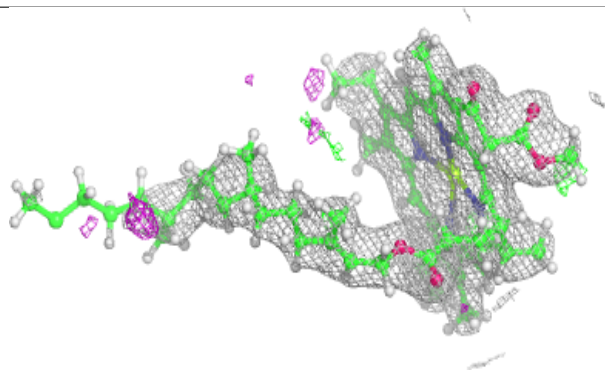
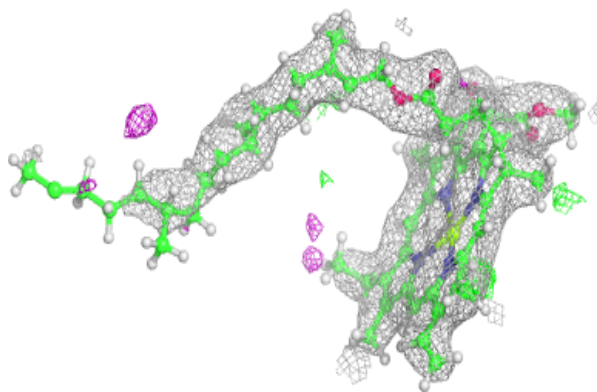
**Electron density around CLA D 405:**

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

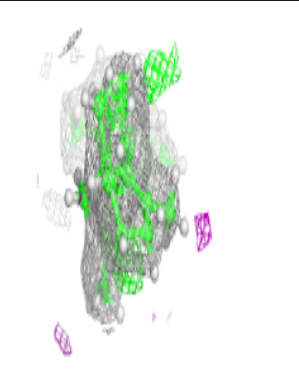
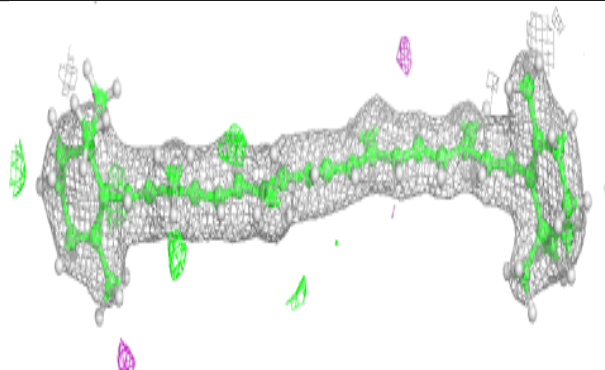
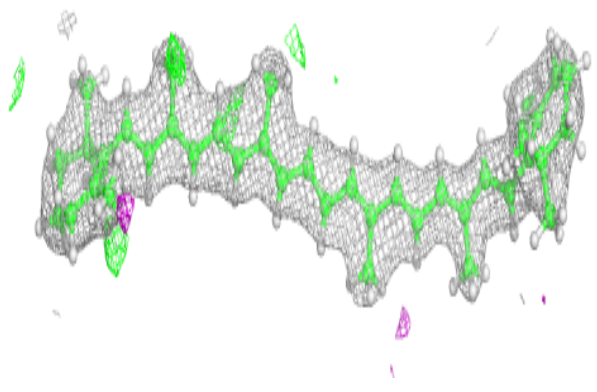


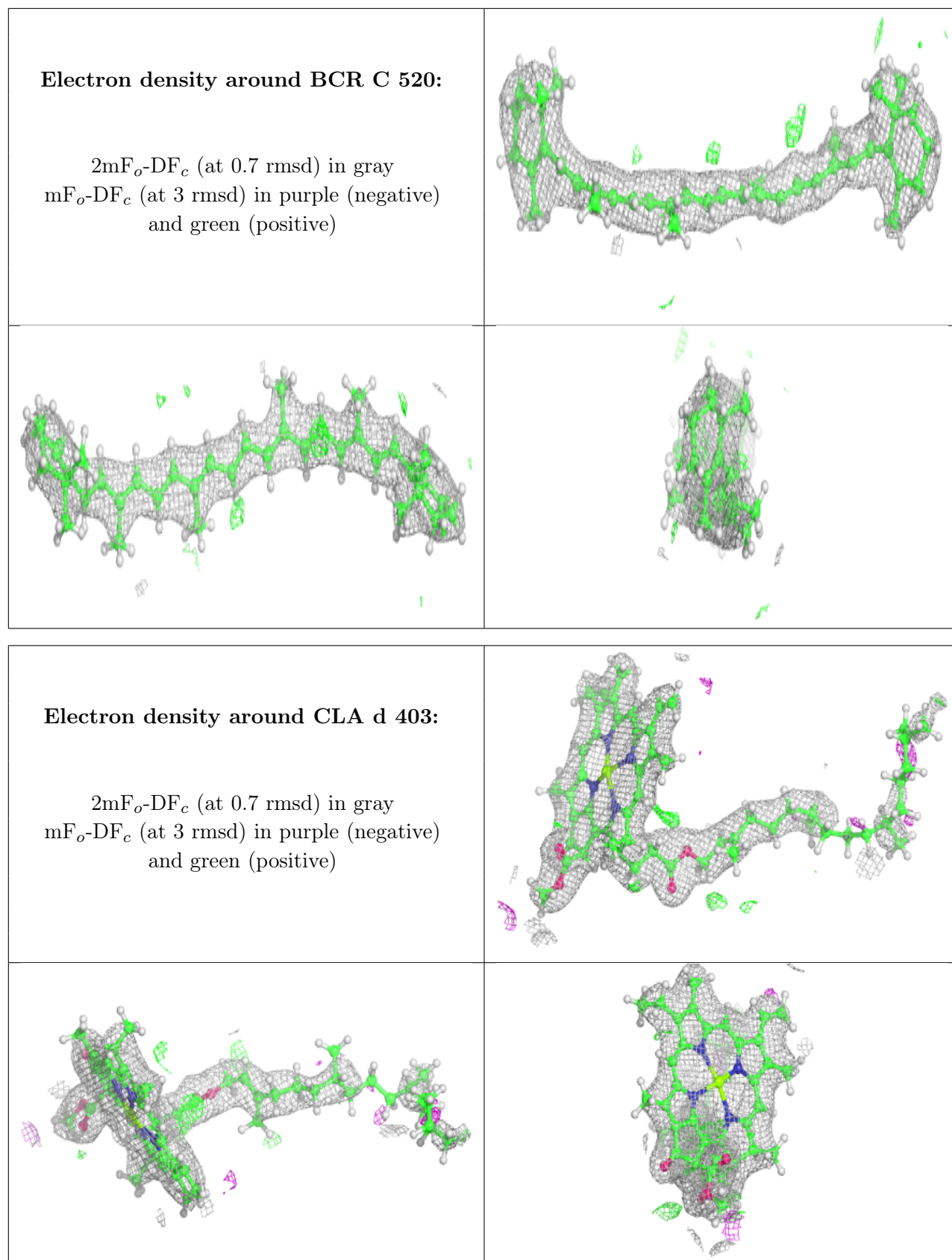
**Electron density around CLA c 508:**

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

**Electron density around BCR C 515:**

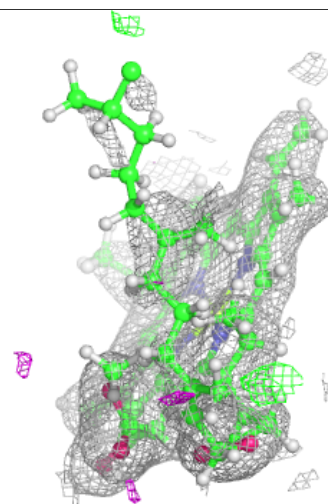
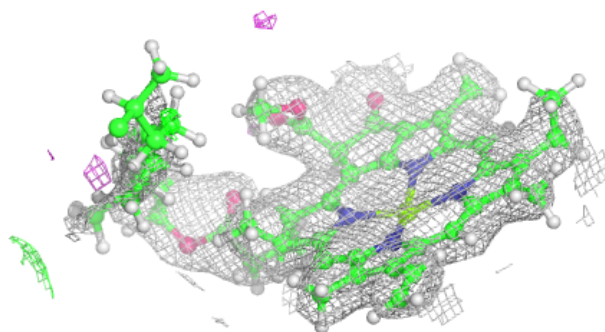
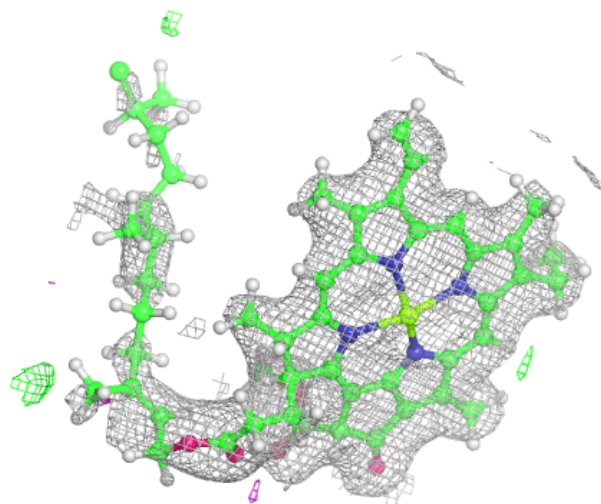
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





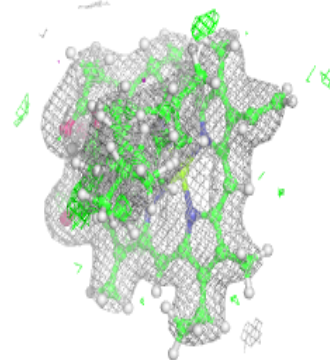
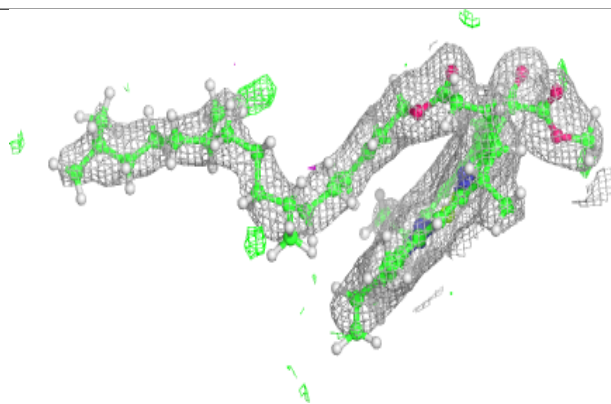
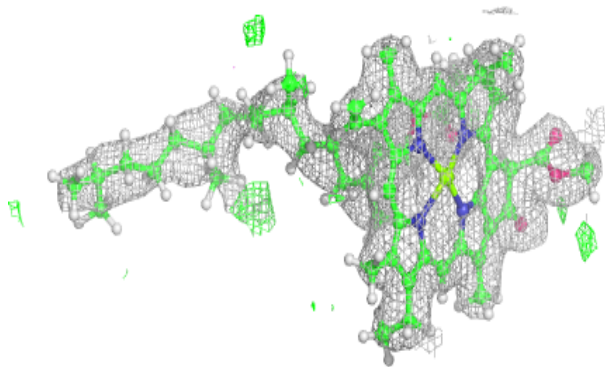
**Electron density around CLA b 615:**

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

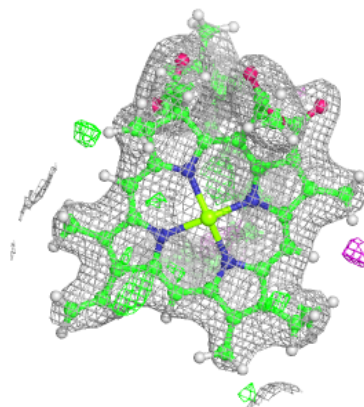
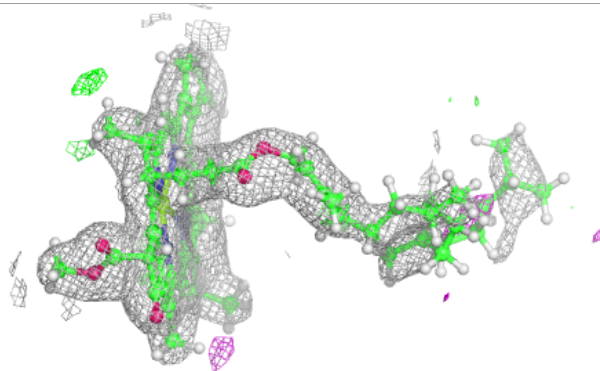
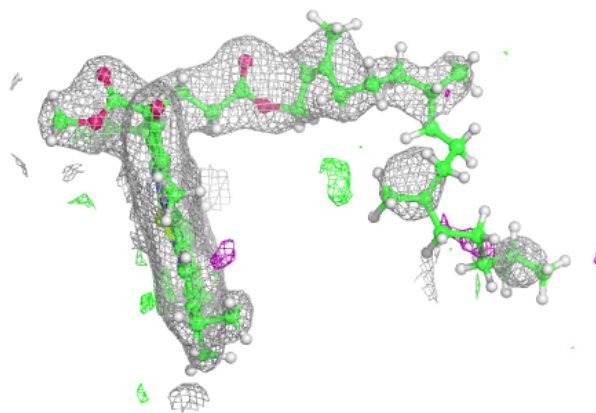


**Electron density around CLA c 505:**

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

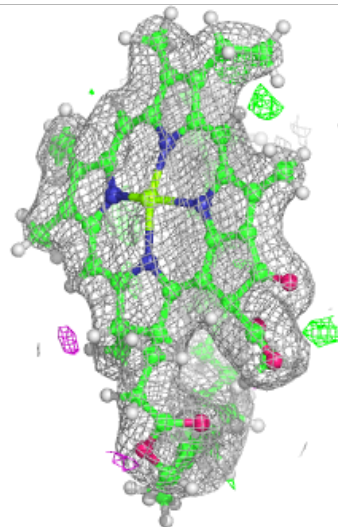
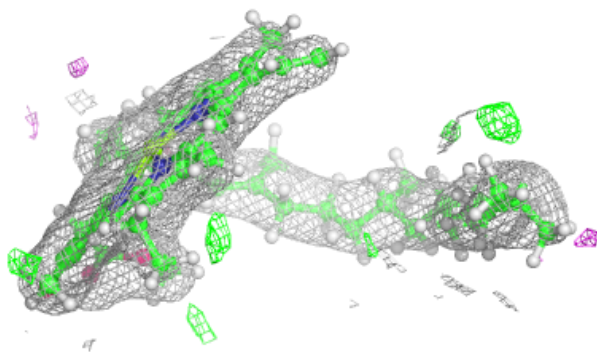
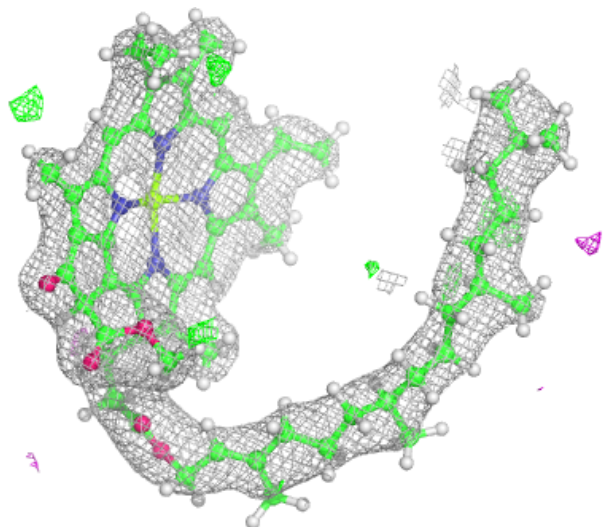
**Electron density around CLA c 506:**

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



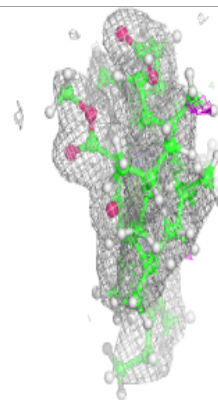
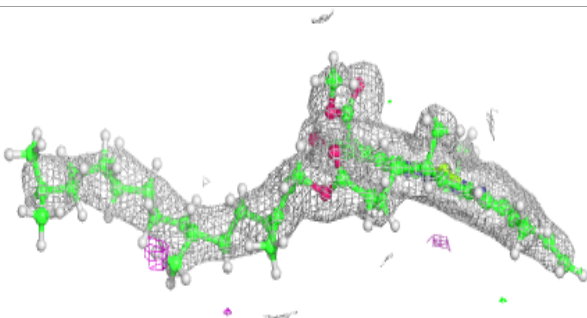
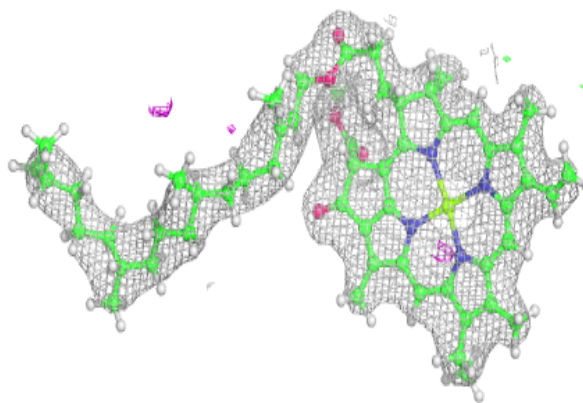
**Electron density around CLA c 507:**

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

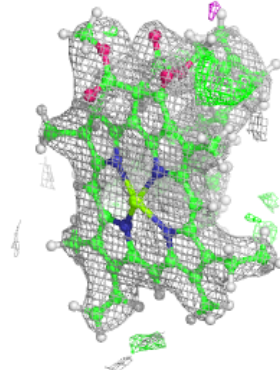
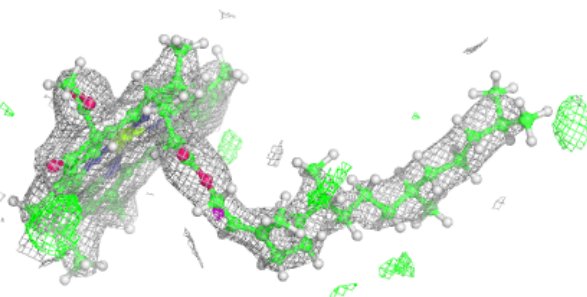
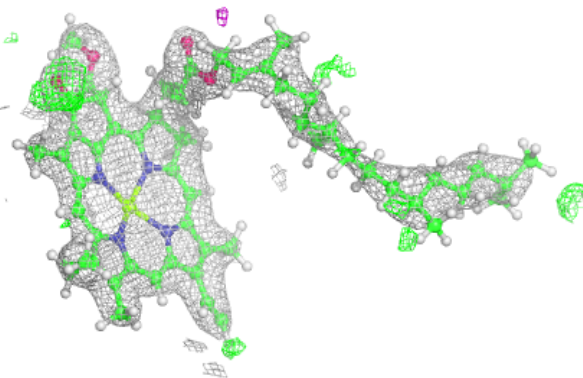


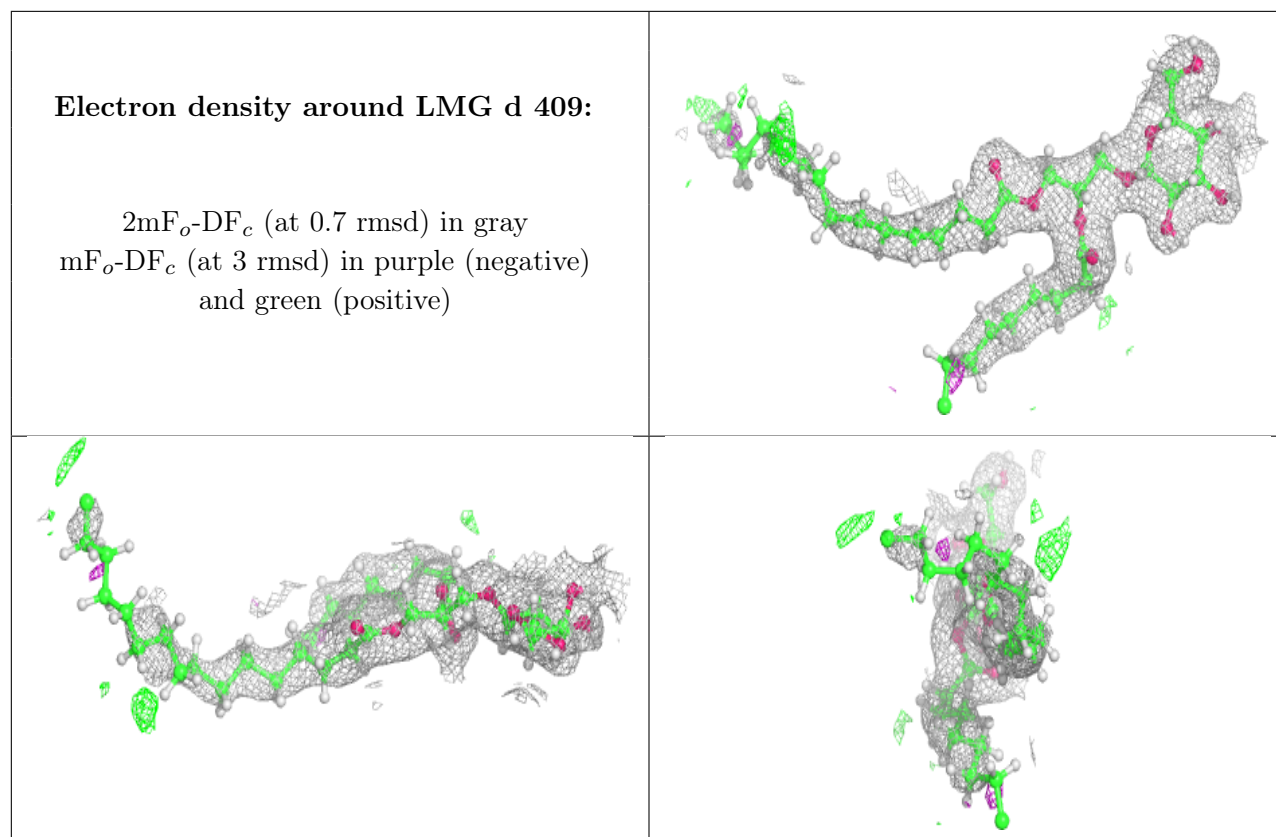
**Electron density around CLA b 601:**

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

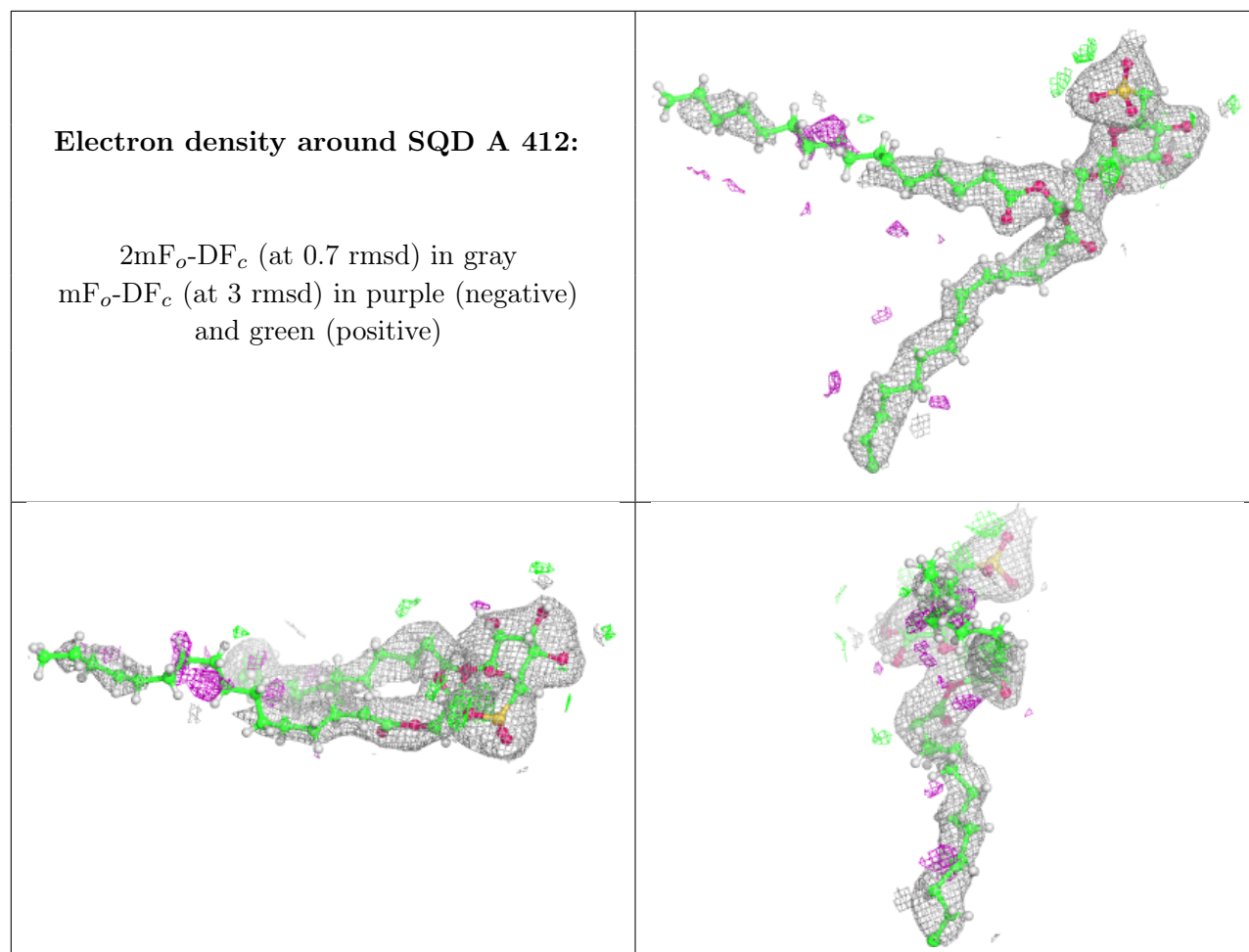
**Electron density around CLA c 511:**

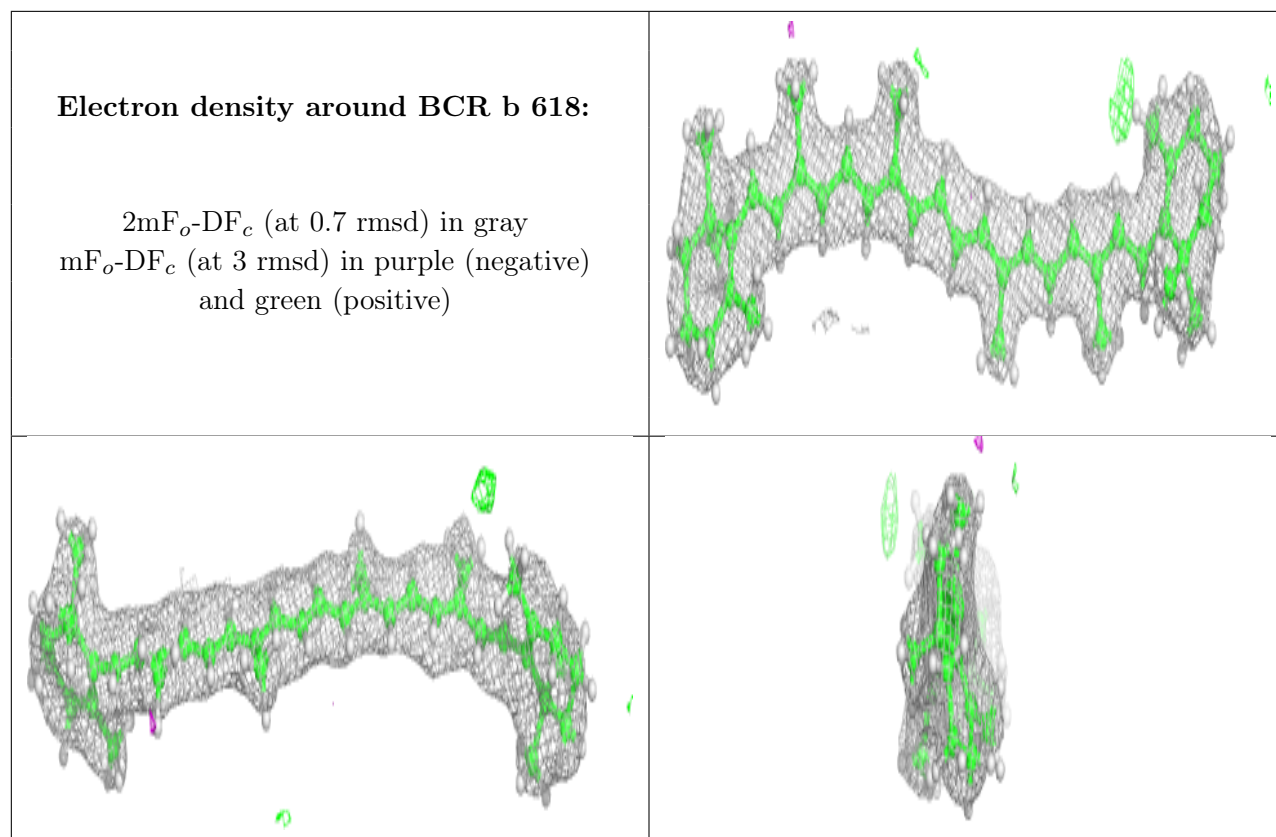
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





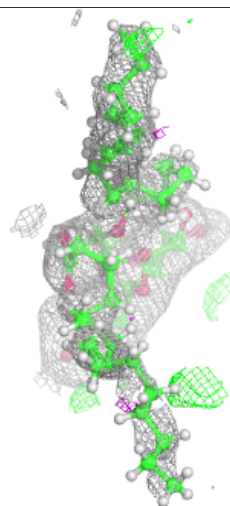
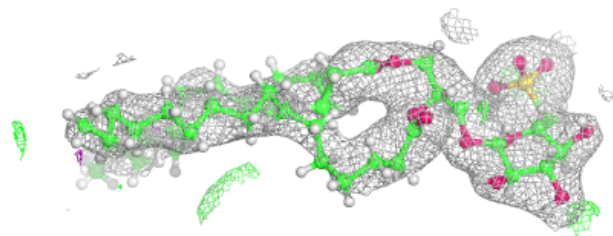
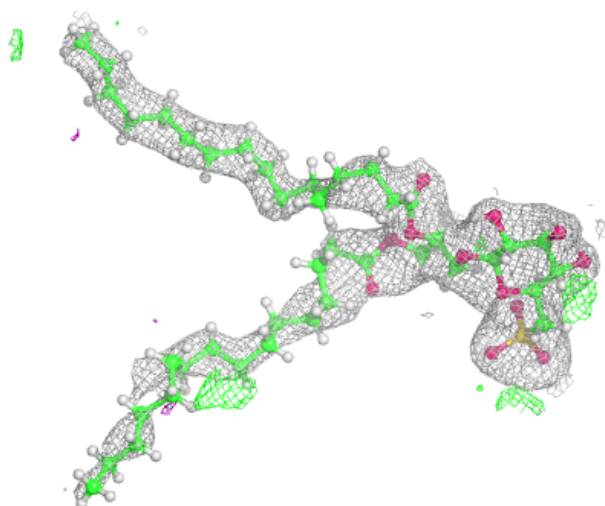






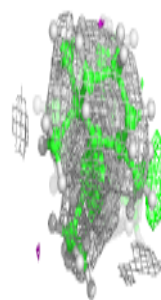
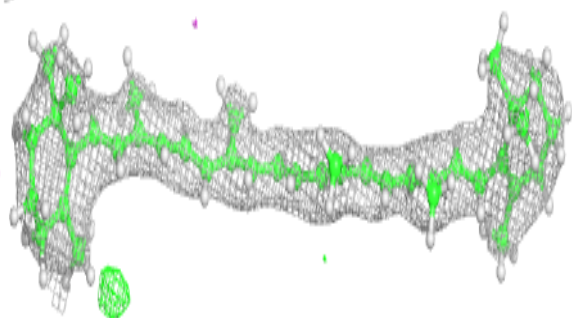
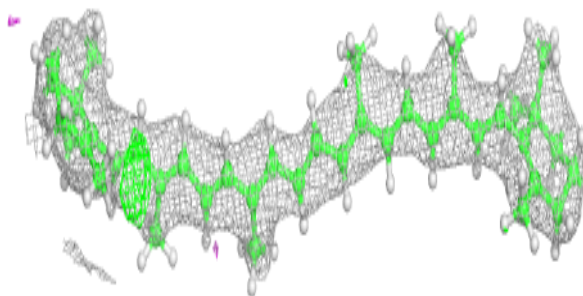
**Electron density around SQD a 412:**

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

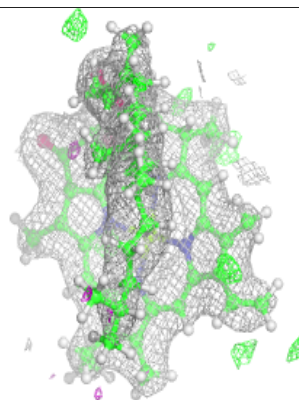
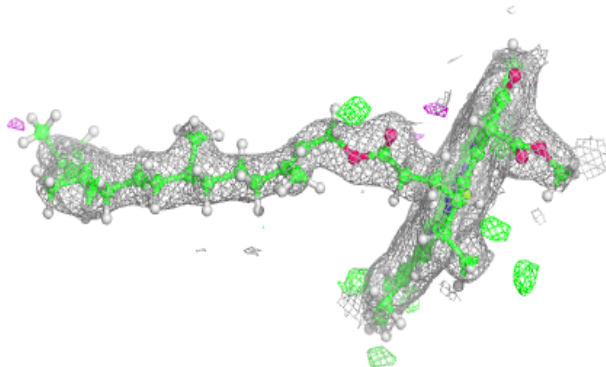
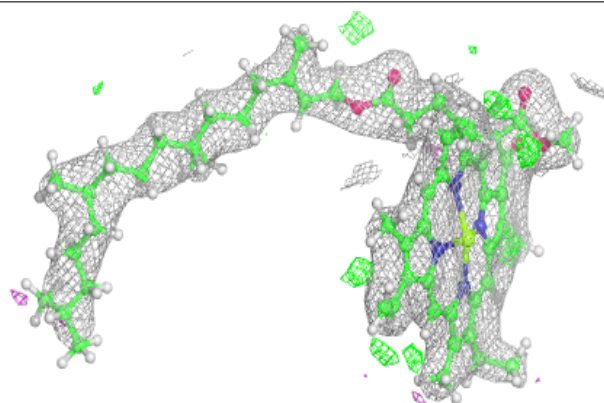


**Electron density around BCR c 514:**

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

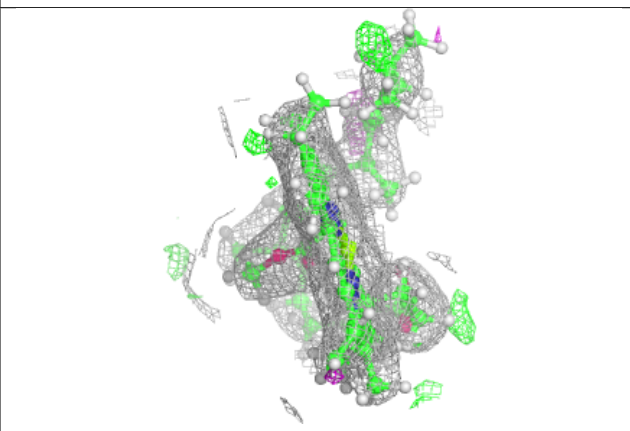
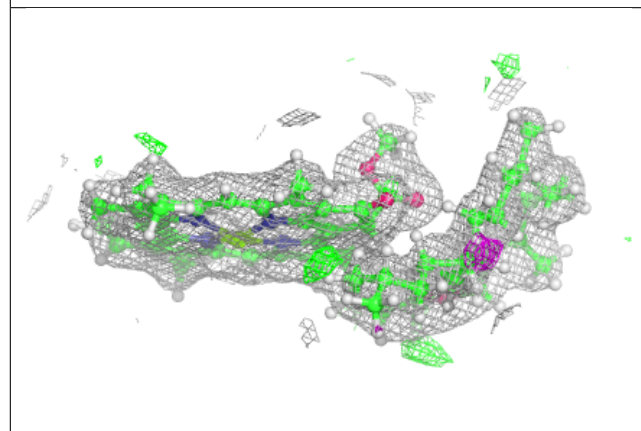
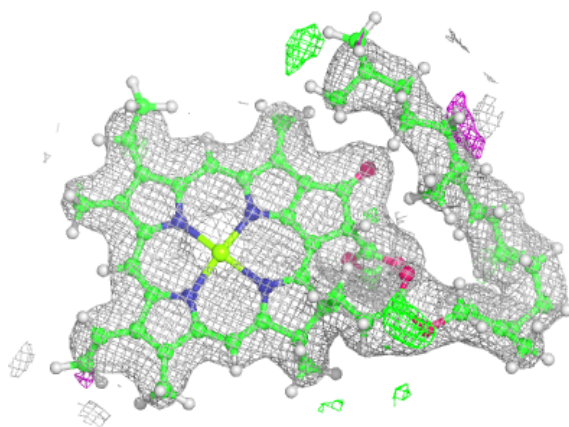
**Electron density around CLA b 608:**

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

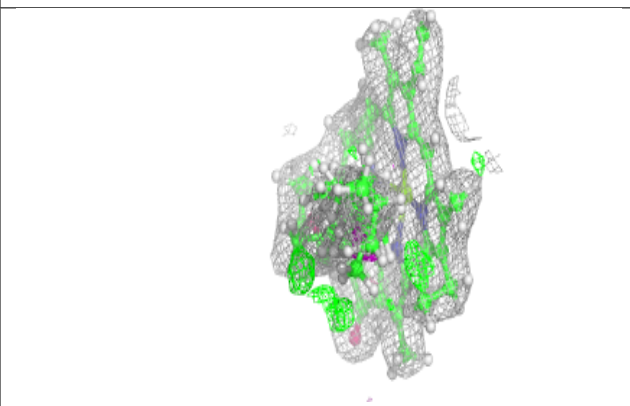
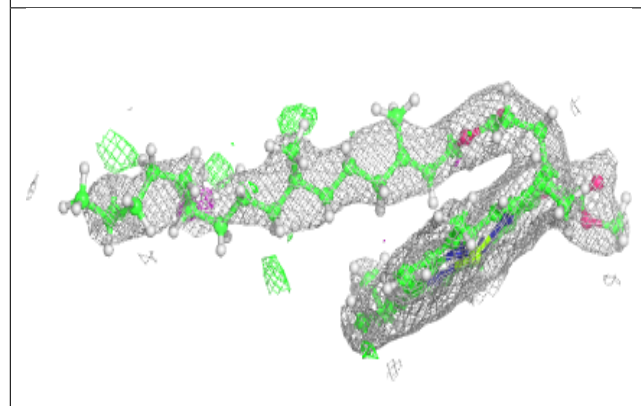
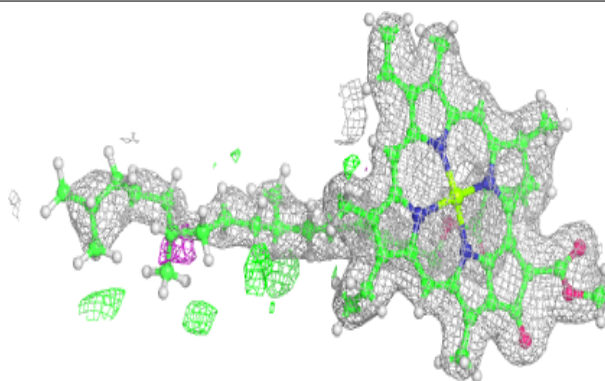


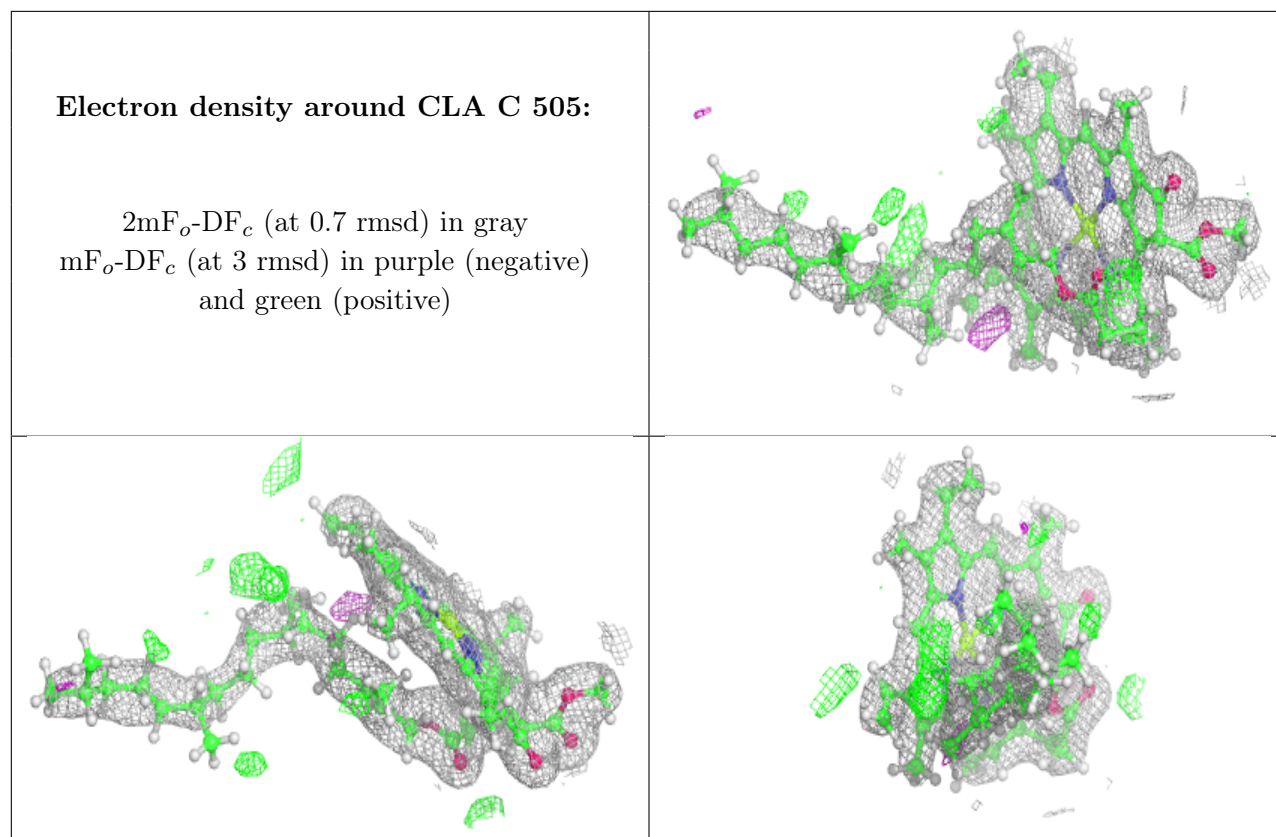
**Electron density around CLA b 609:**

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

**Electron density around CLA B 614:**

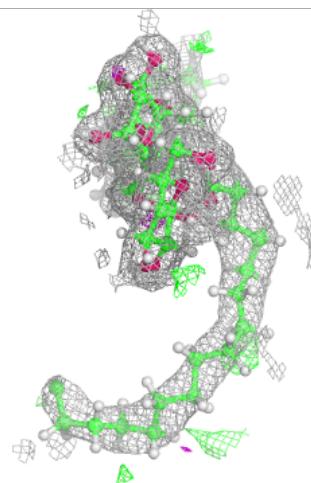
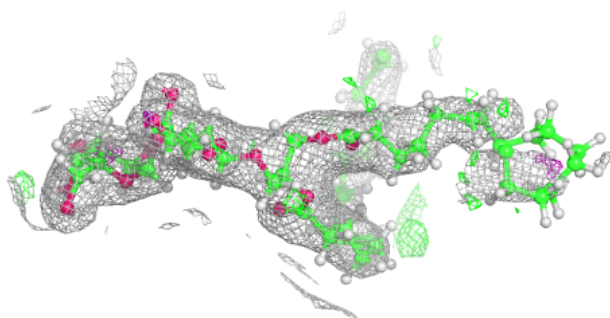
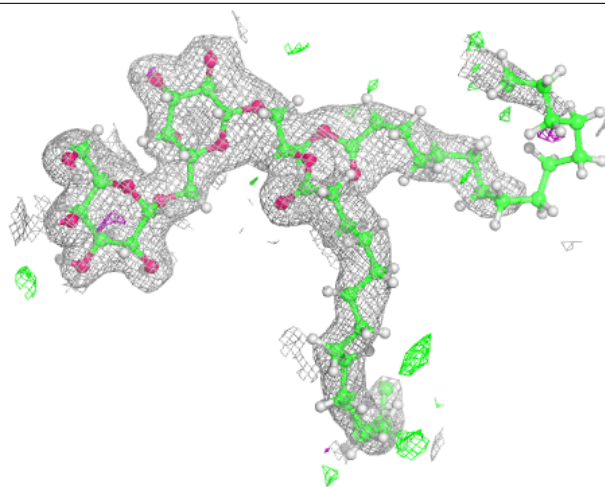
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





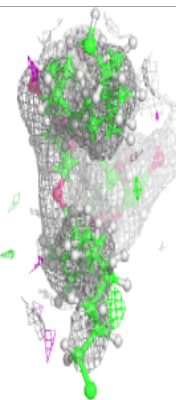
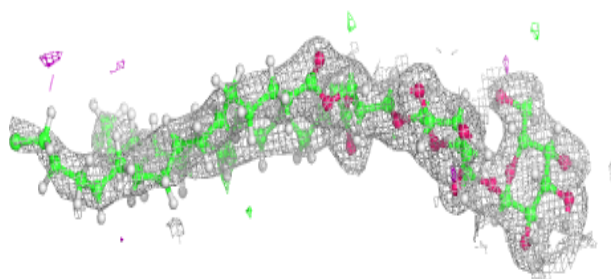
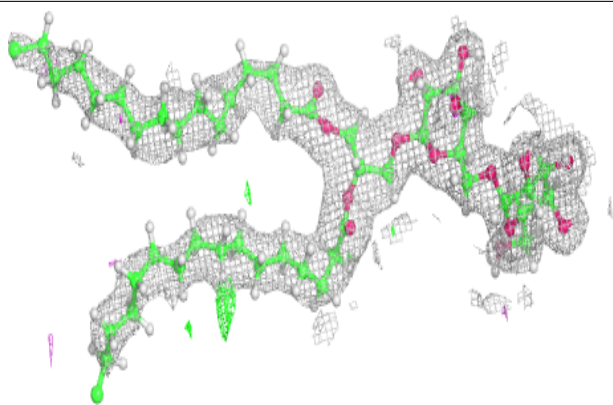
**Electron density around DGD C 522:**

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

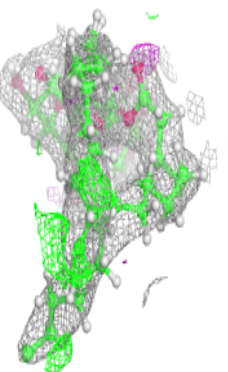
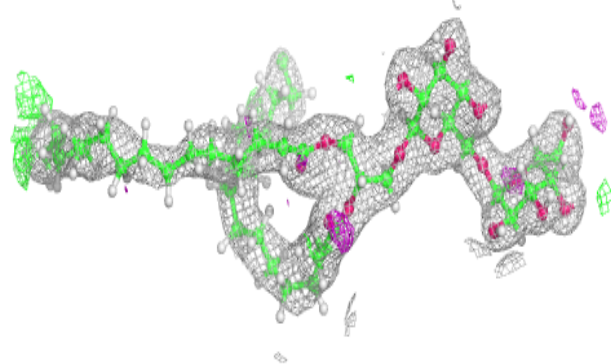
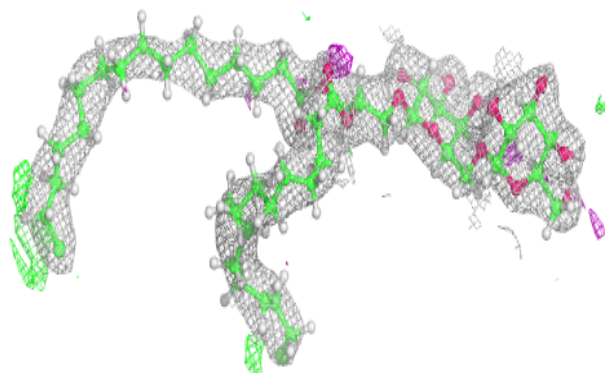


**Electron density around DGD C 523:**

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

**Electron density around DGD H 102:**

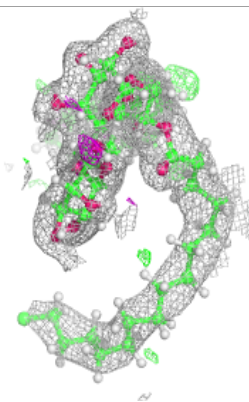
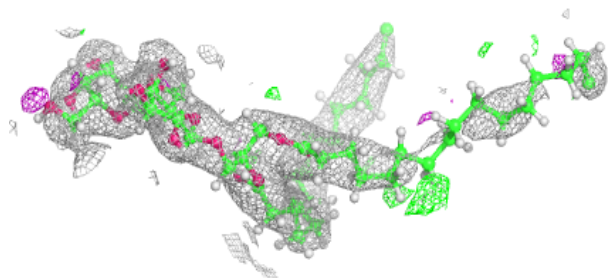
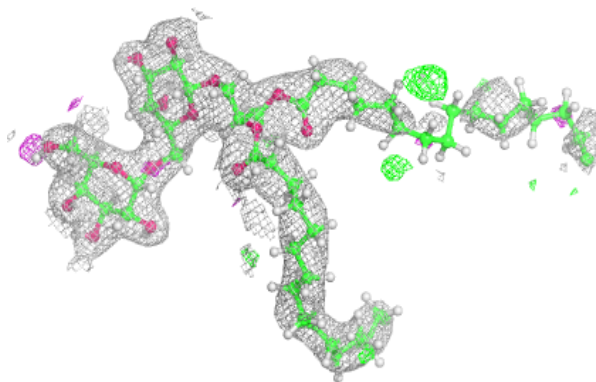
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



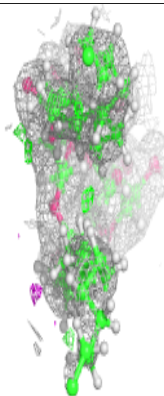
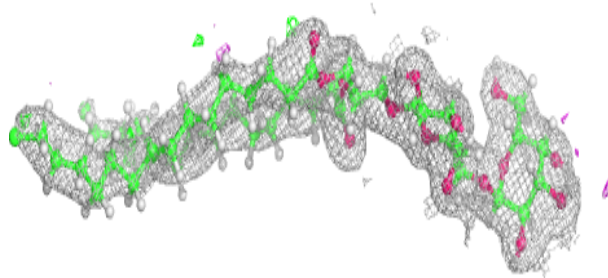
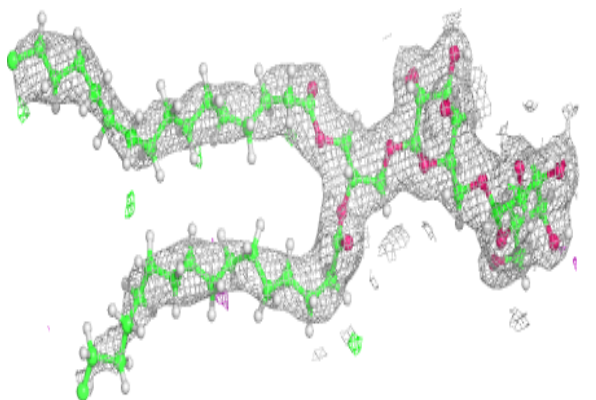


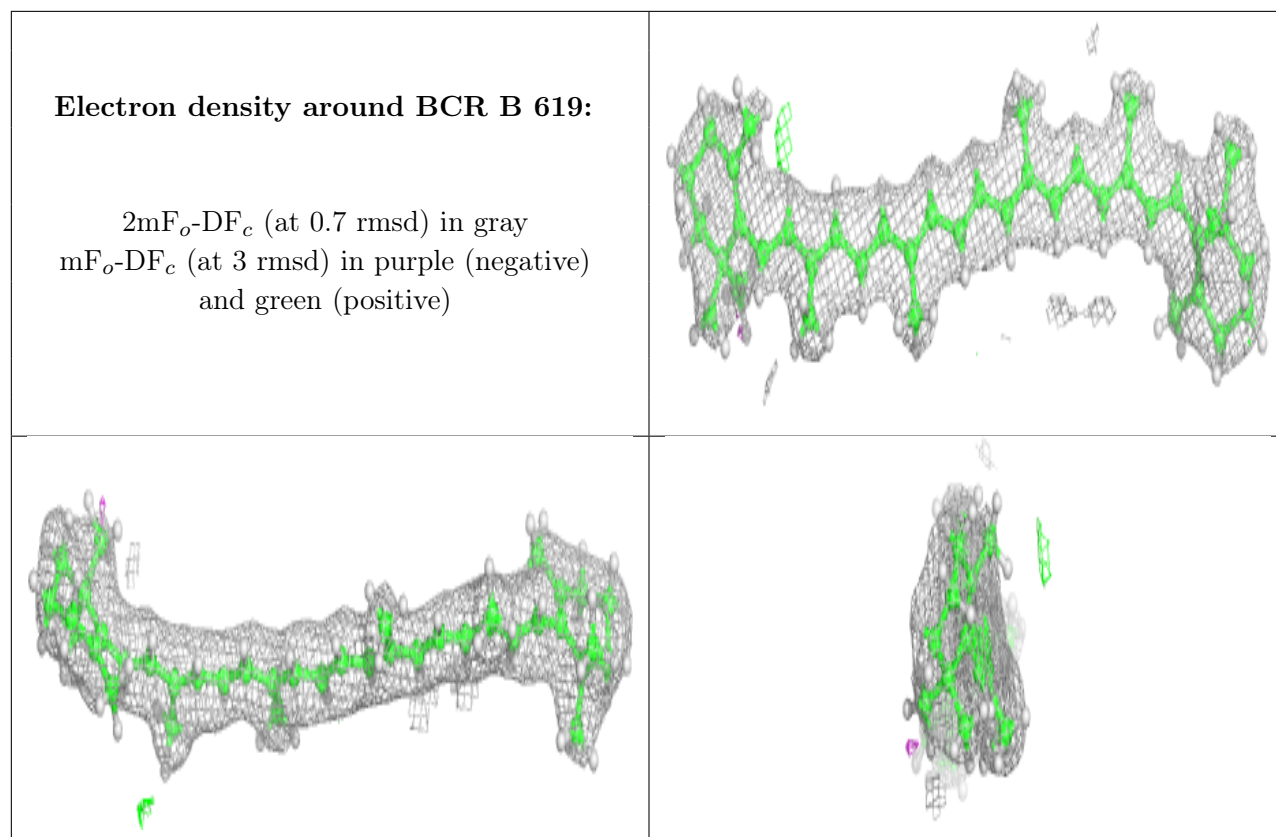
**Electron density around DGD c 520:**

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

**Electron density around DGD c 521:**

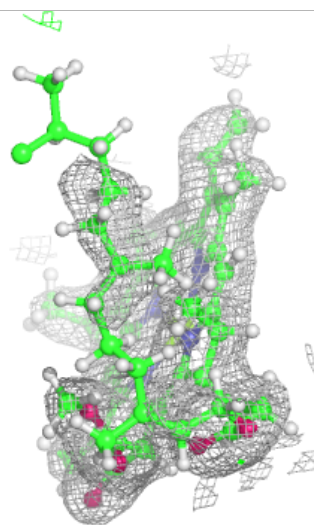
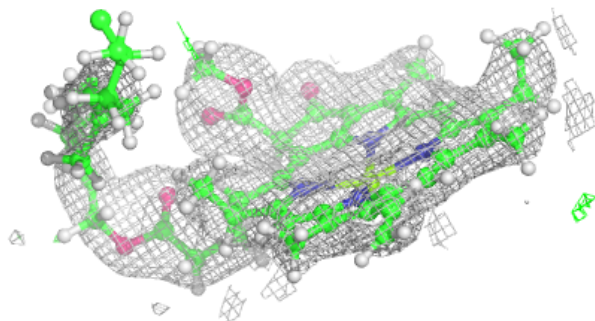
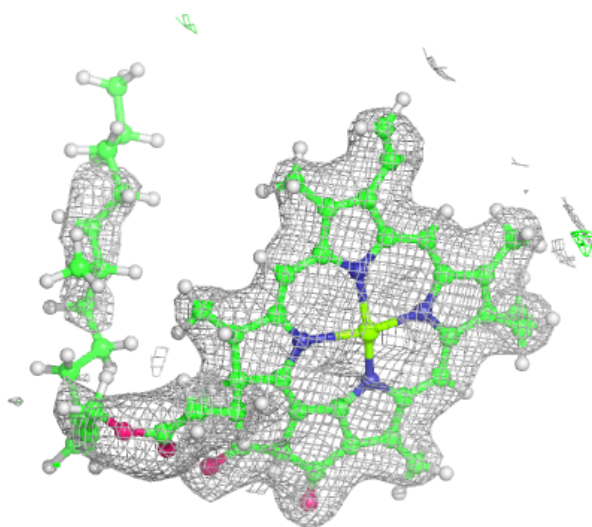
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





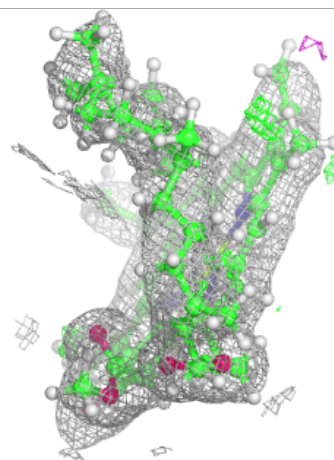
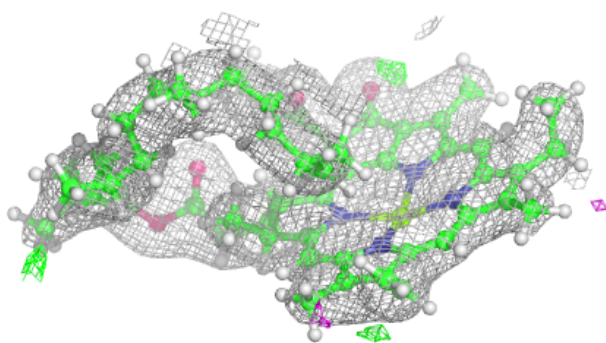
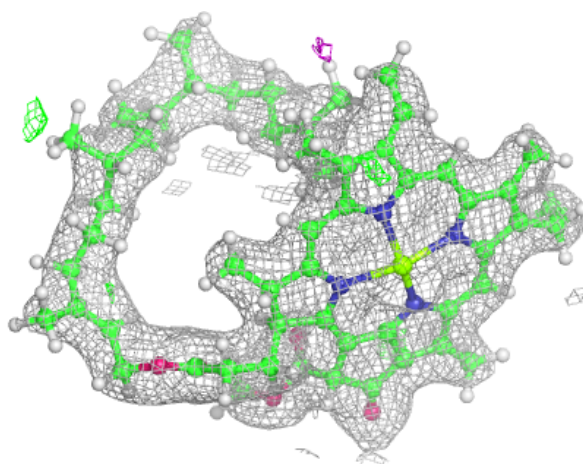
**Electron density around CLA B 616:**

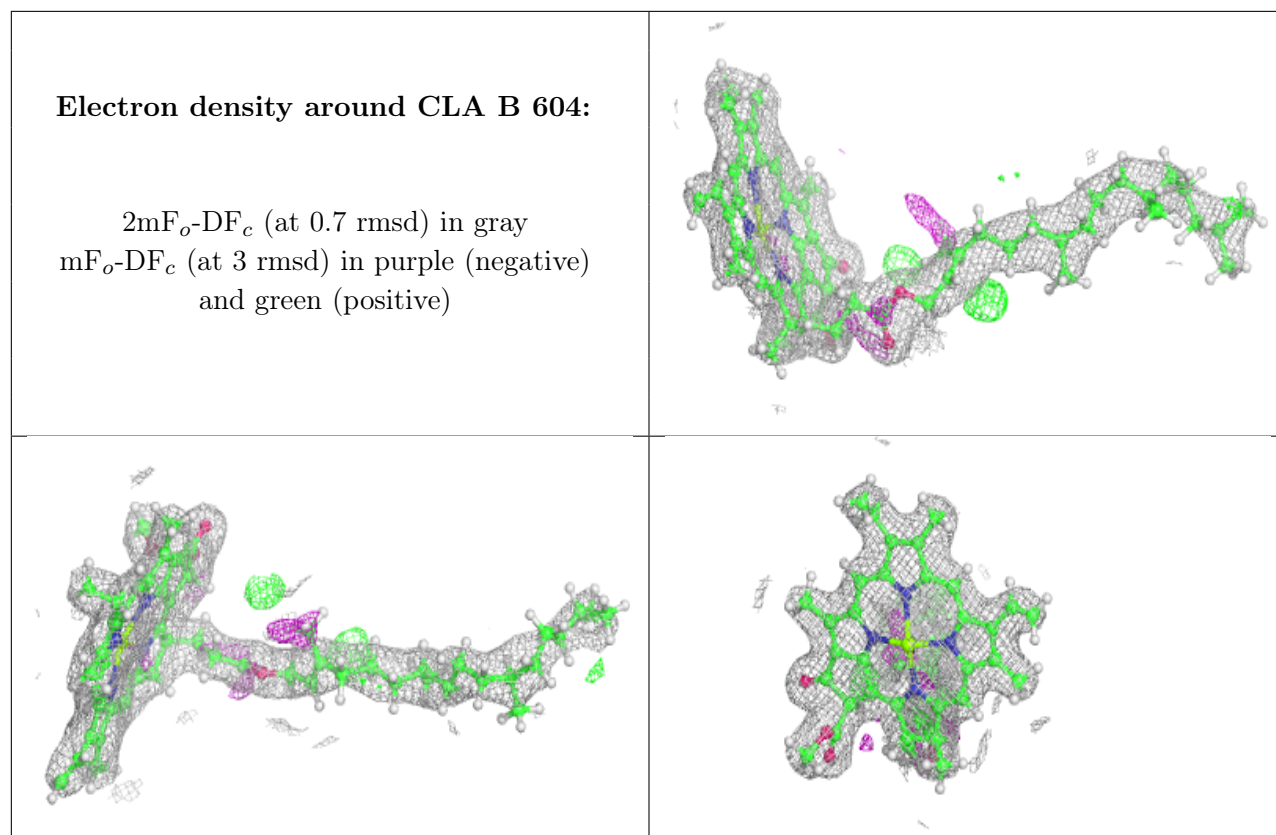
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 615:**

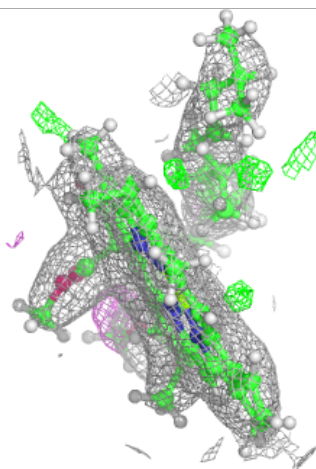
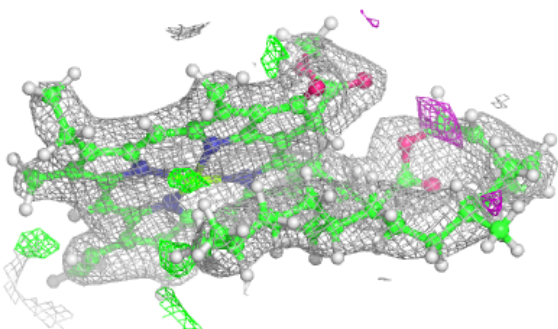
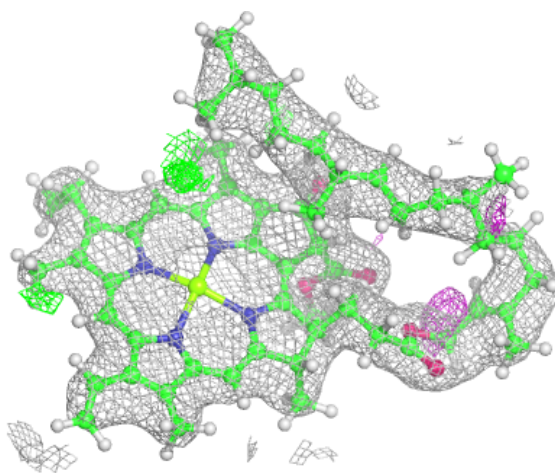
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





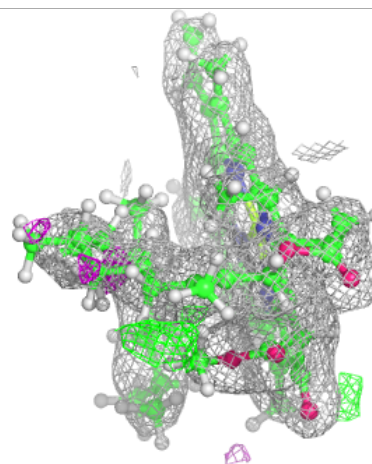
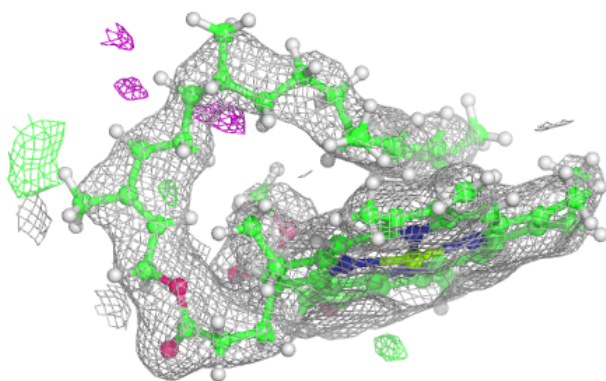
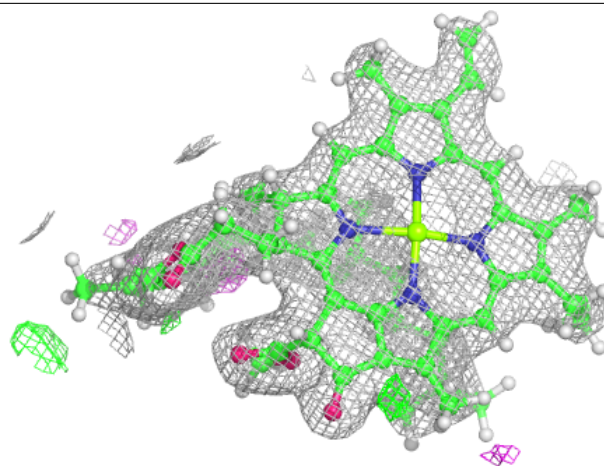
**Electron density around CLA c 509:**

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



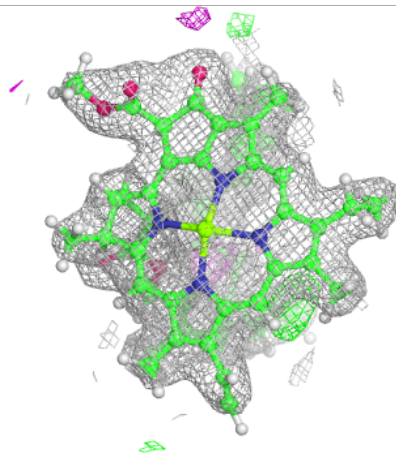
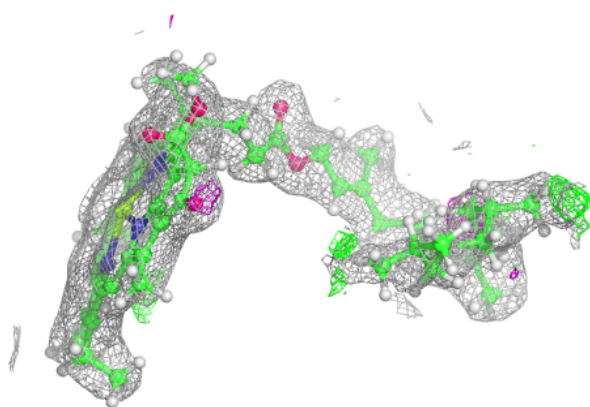
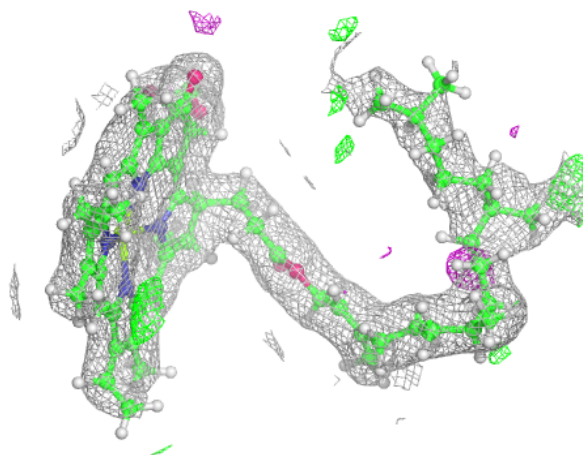
**Electron density around CLA c 510:**

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



**Electron density around CLA B 606:**

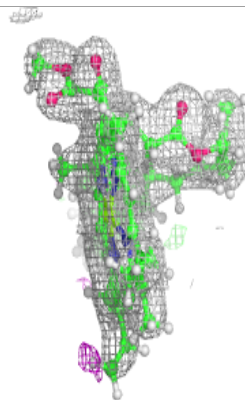
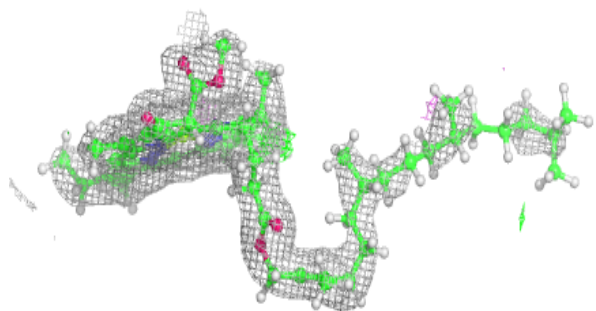
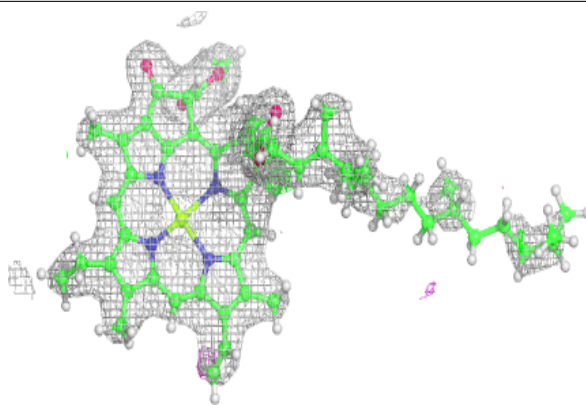
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





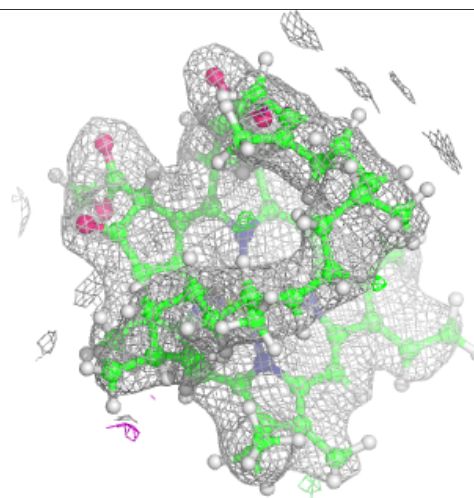
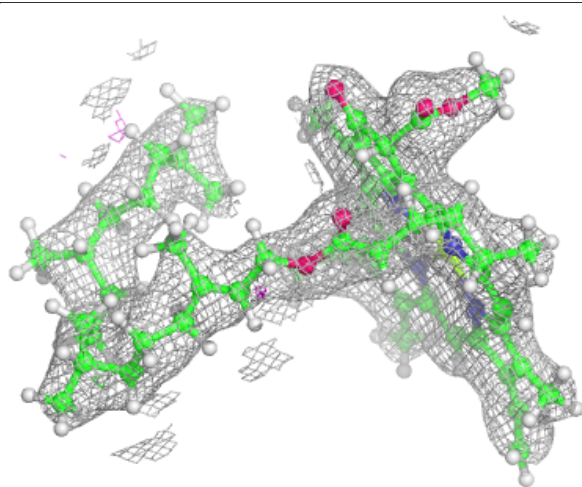
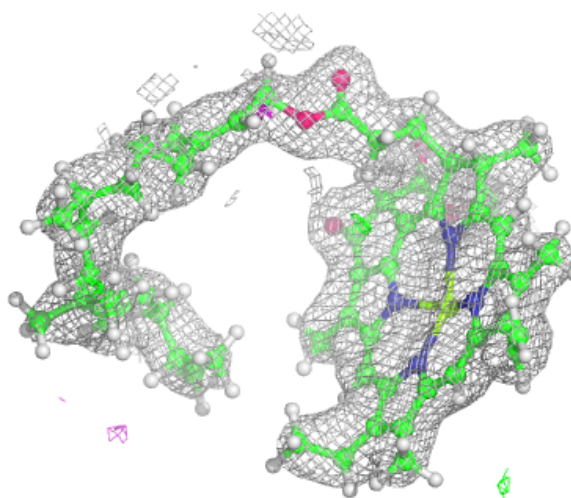
**Electron density around CLA a 406:**

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



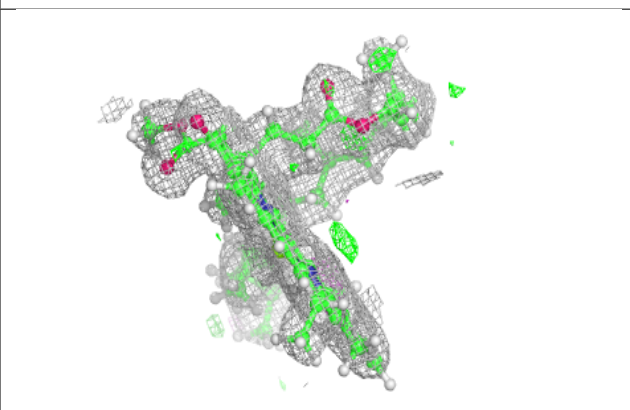
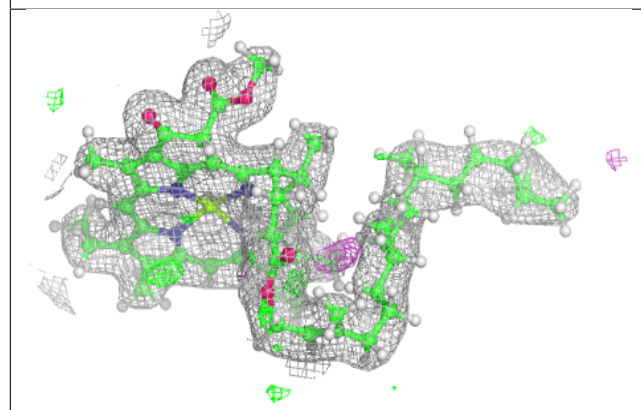
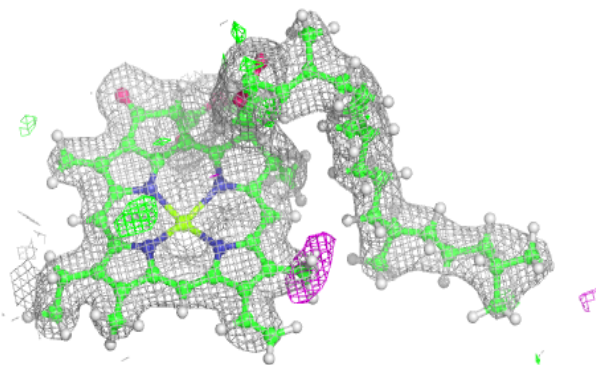
**Electron density around CLA C 503:**

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

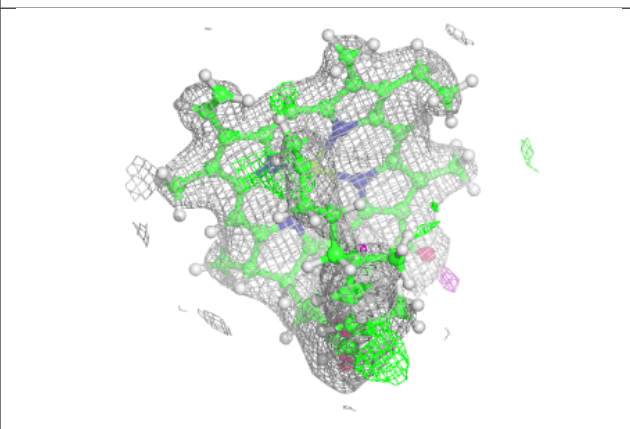
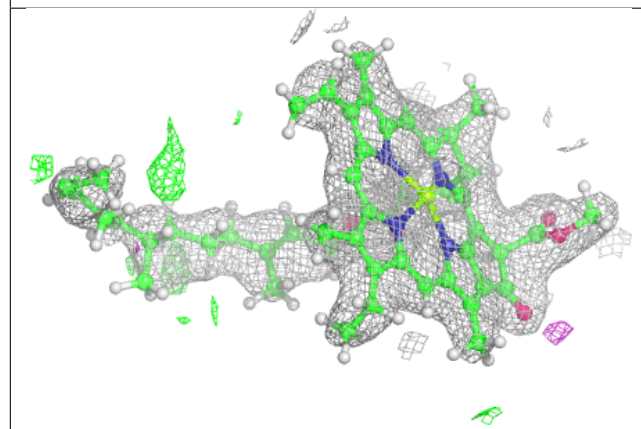
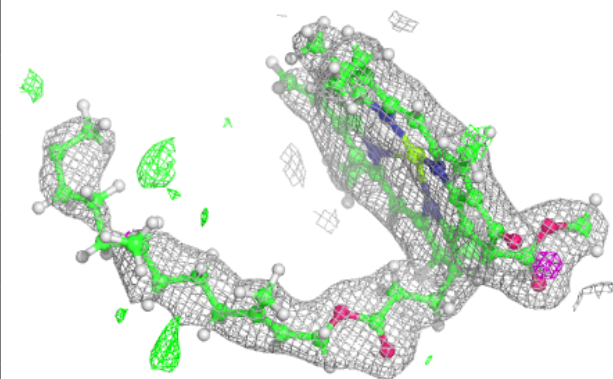


**Electron density around CLA a 411:**

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

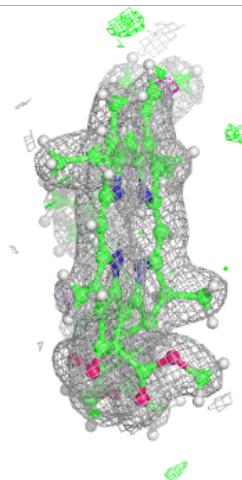
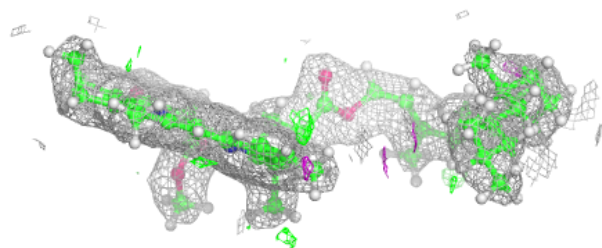
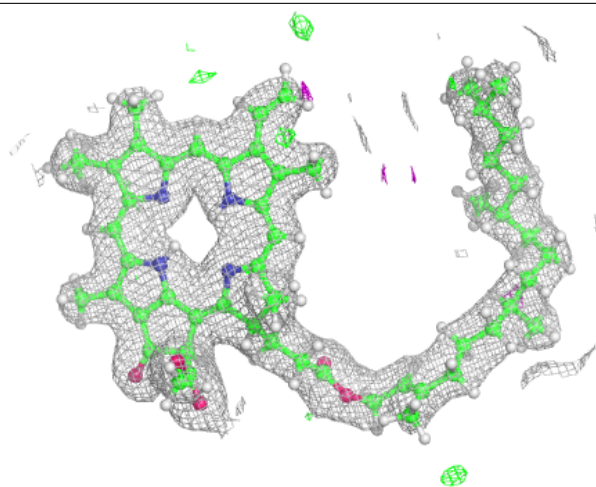
**Electron density around CLA C 504:**

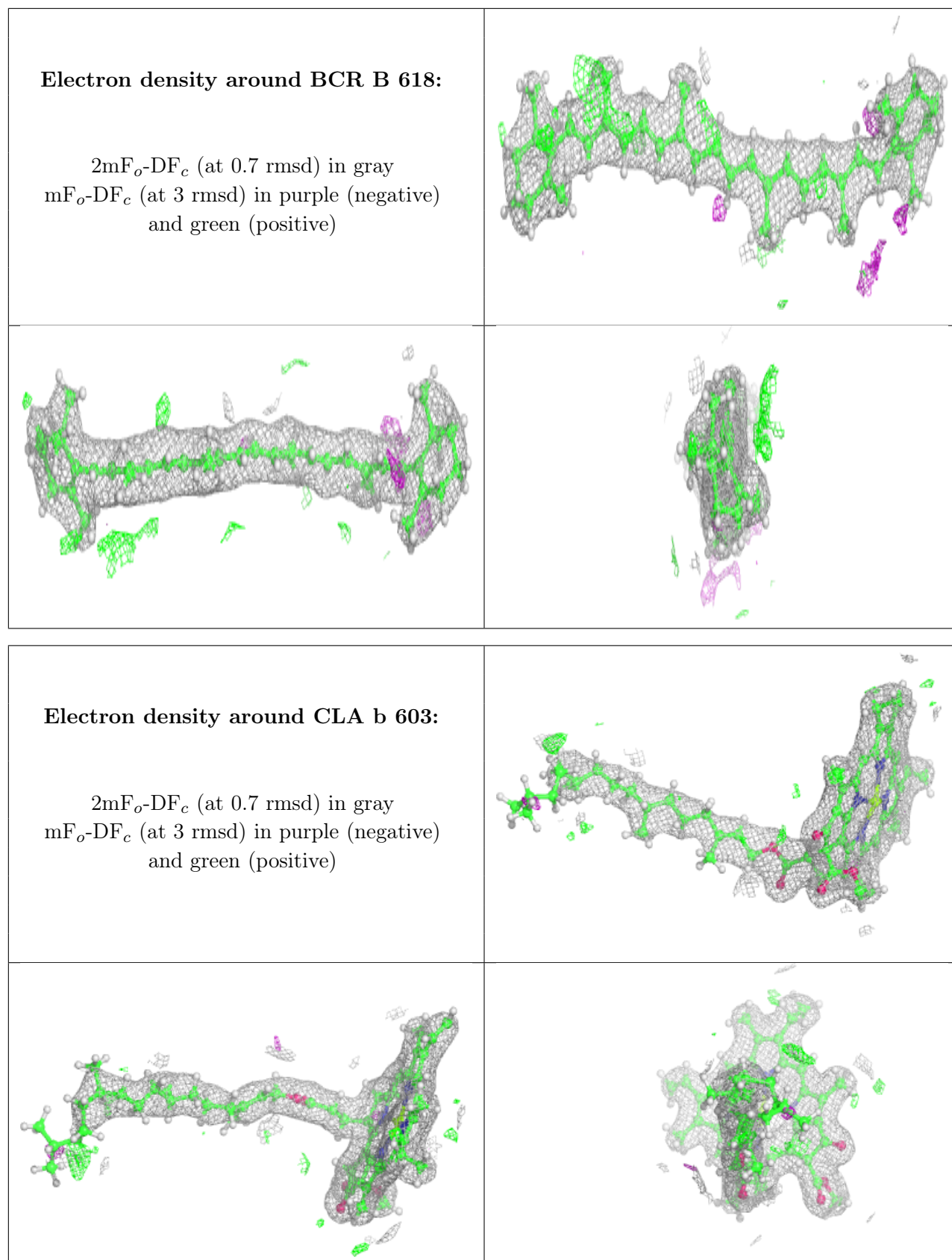
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO a 407:**

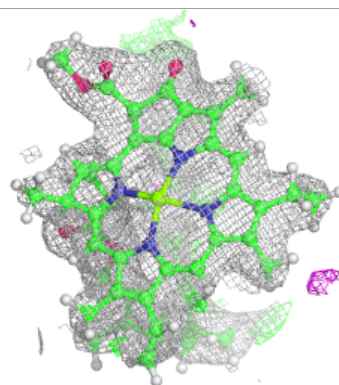
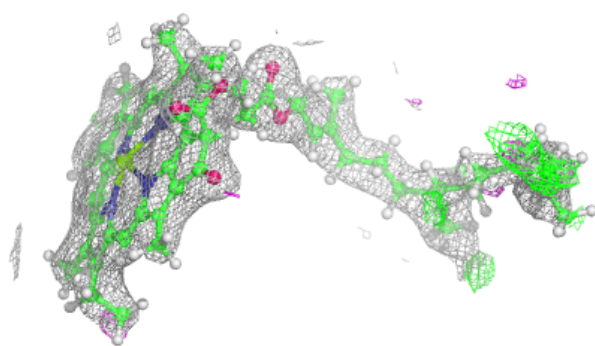
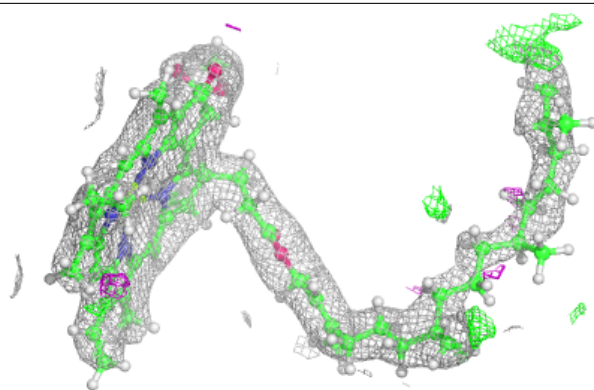
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



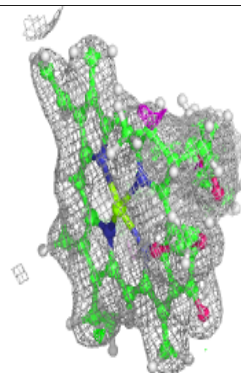
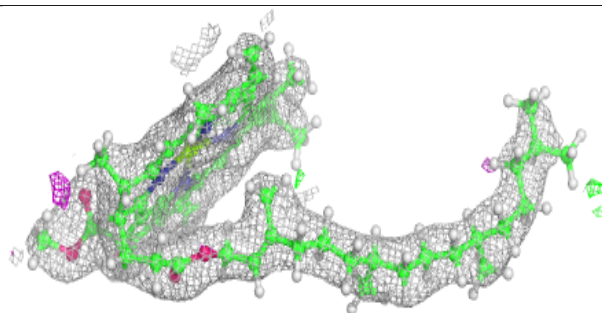
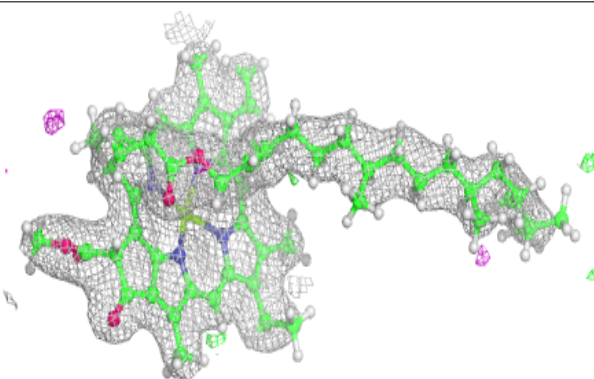


**Electron density around CLA b 605:**

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

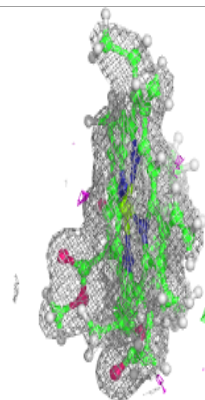
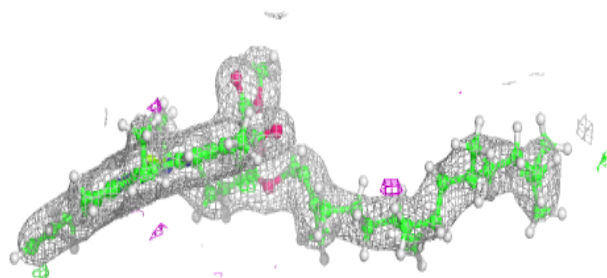
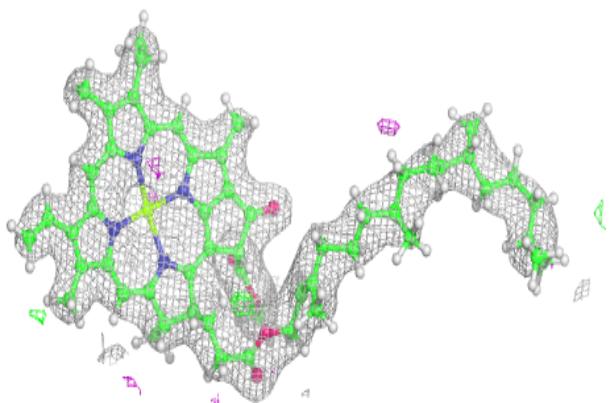
**Electron density around CLA b 607:**

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

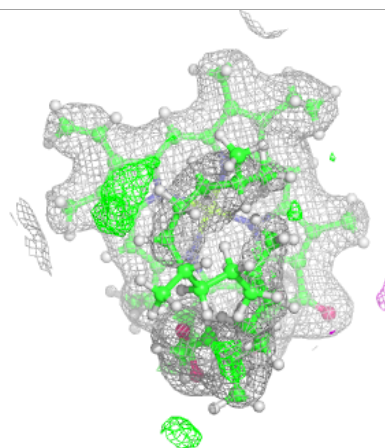
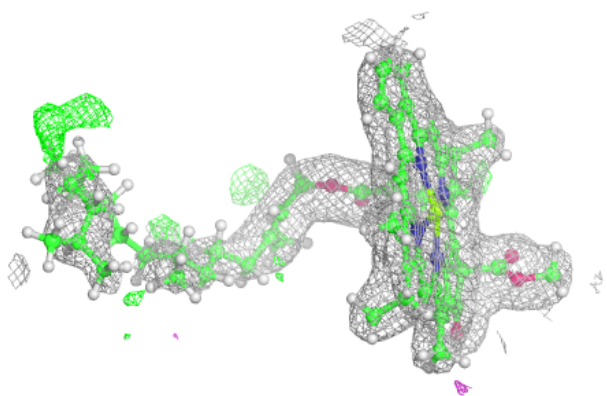
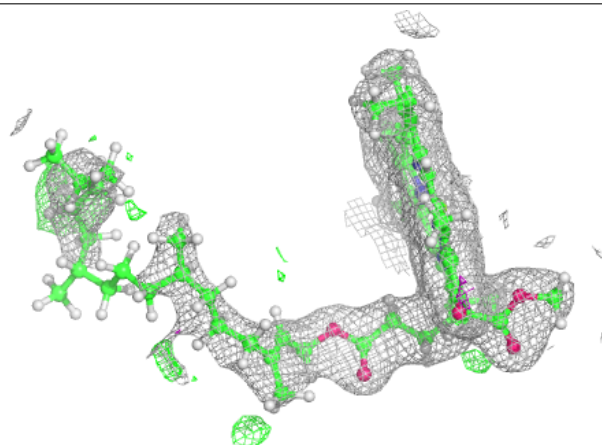


**Electron density around CLA B 602:**

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

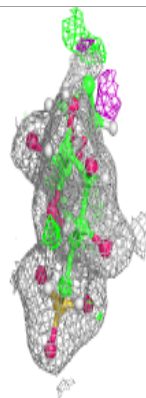
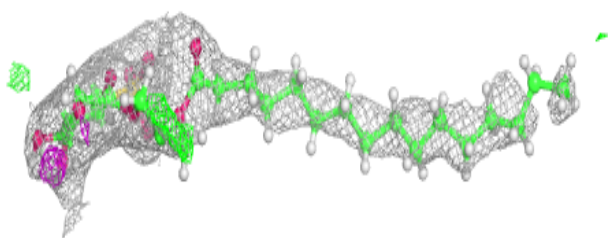
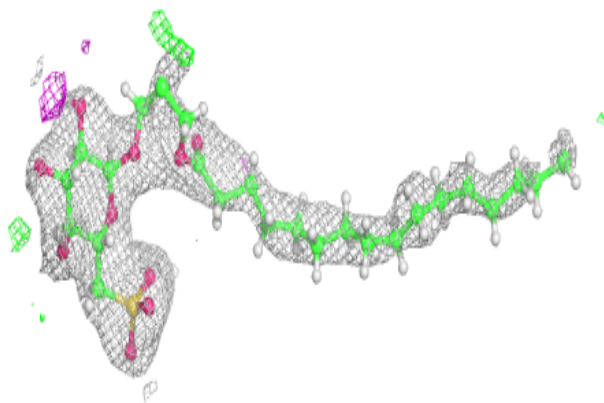
**Electron density around CLA C 506:**

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

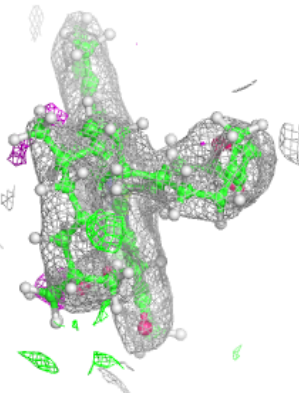
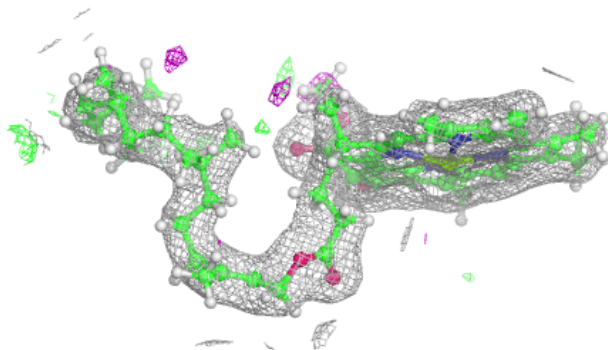
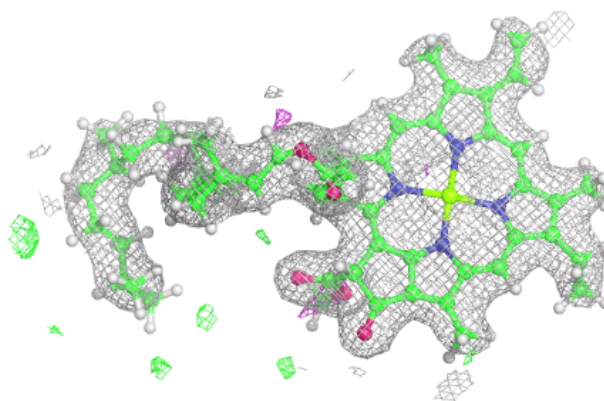


**Electron density around SQD F 102:**

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

**Electron density around CLA b 611:**

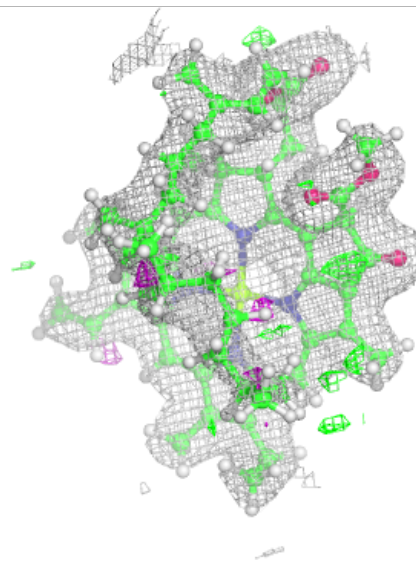
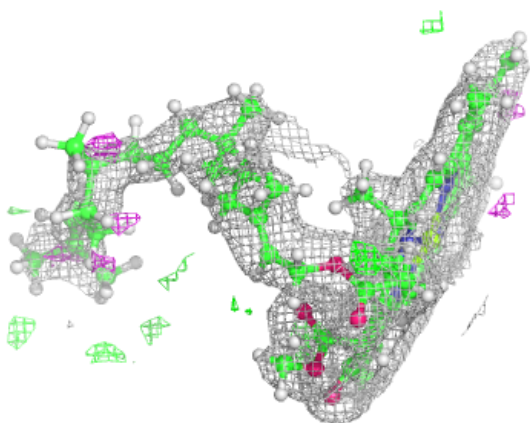
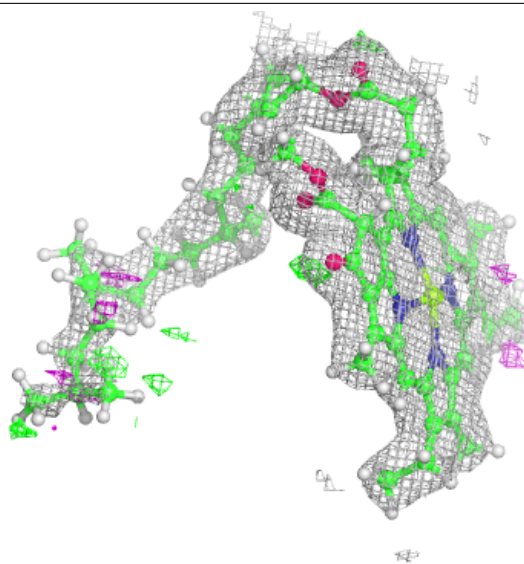
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





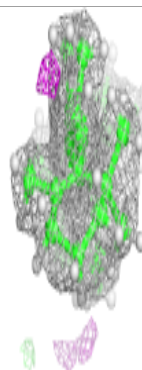
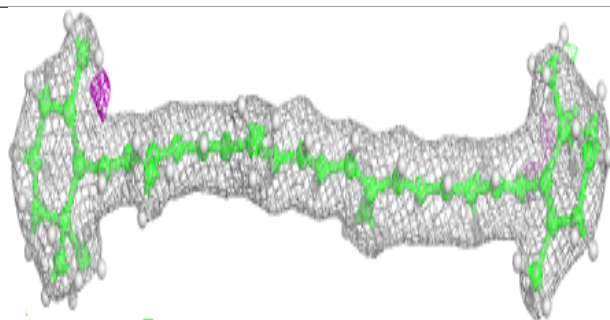
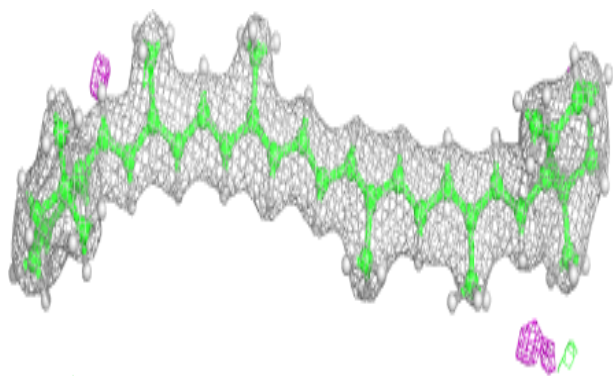
**Electron density around CLA b 612:**

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

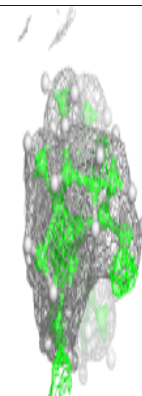
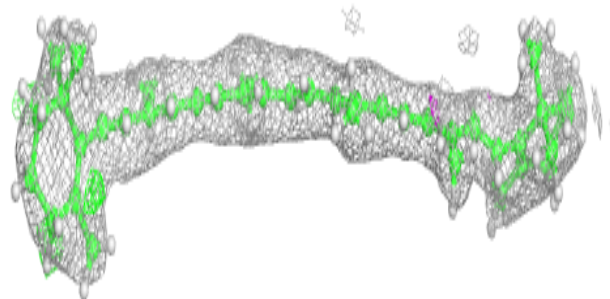
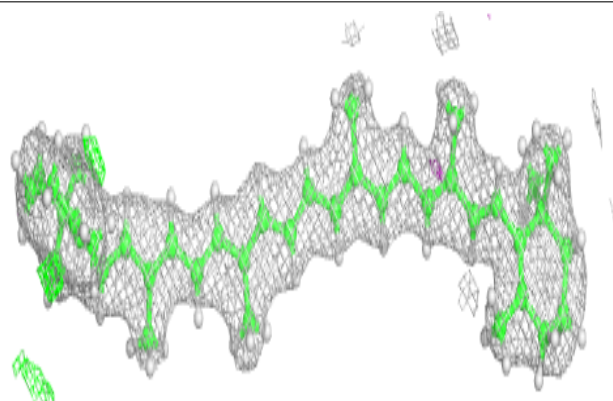


**Electron density around BCR a 409:**

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

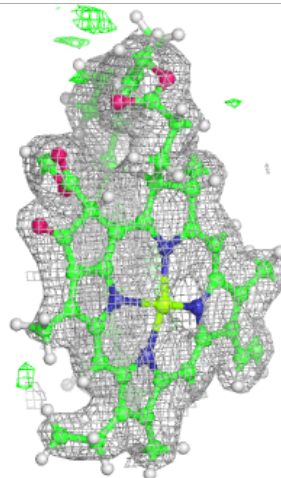
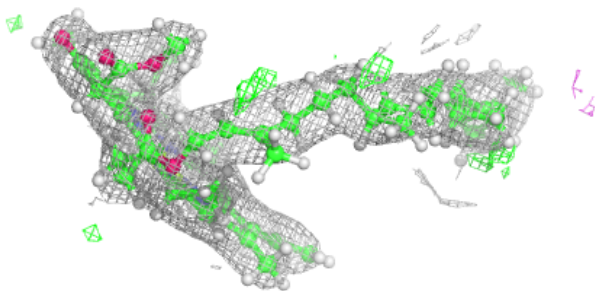
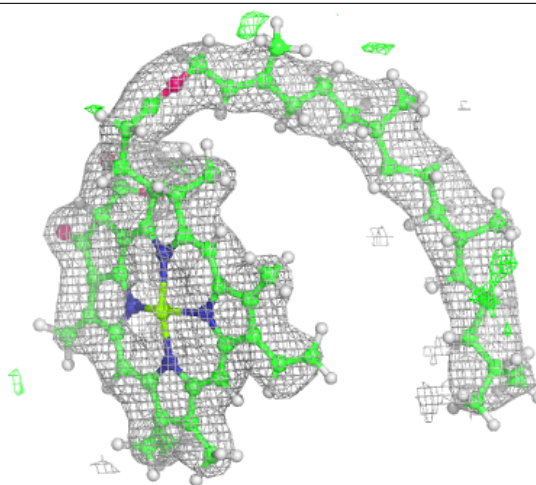
**Electron density around BCR b 616:**

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



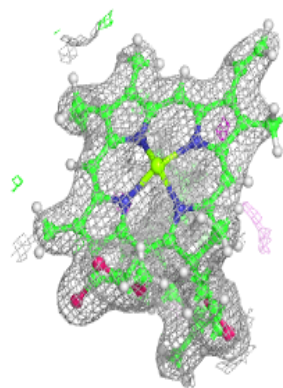
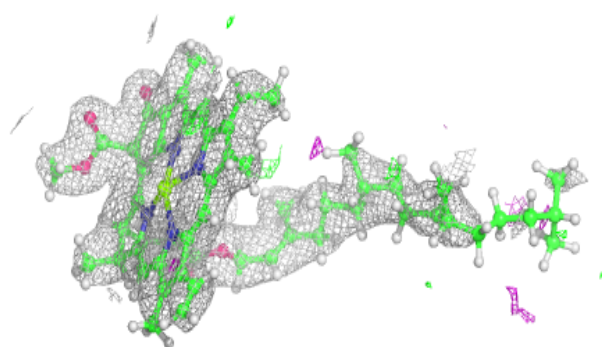
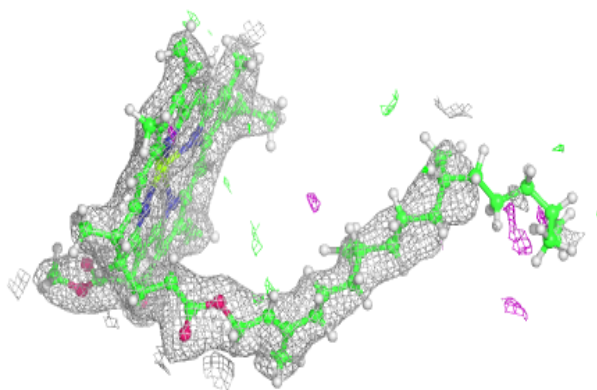
**Electron density around CLA C 507:**

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

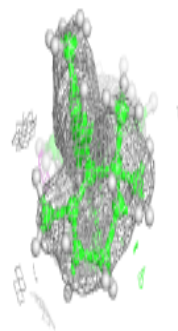
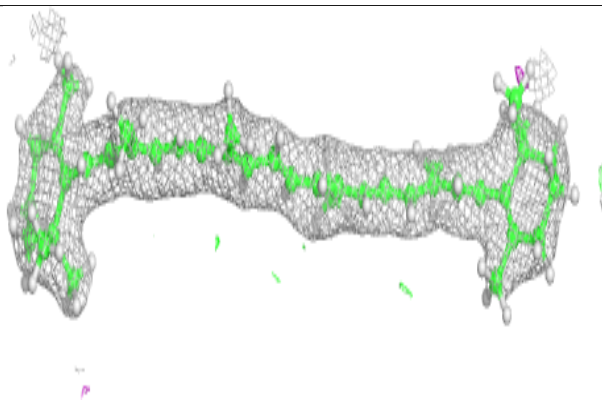
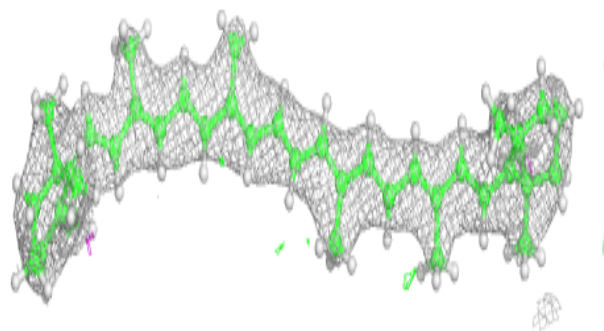


**Electron density around CLA C 508:**

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

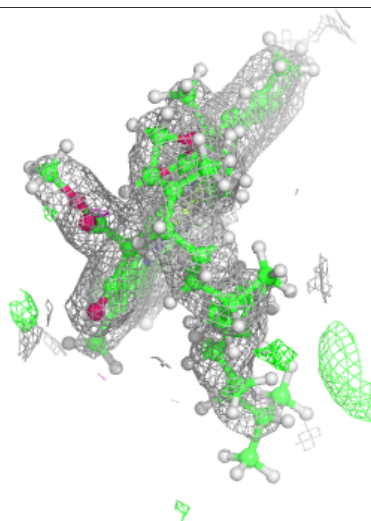
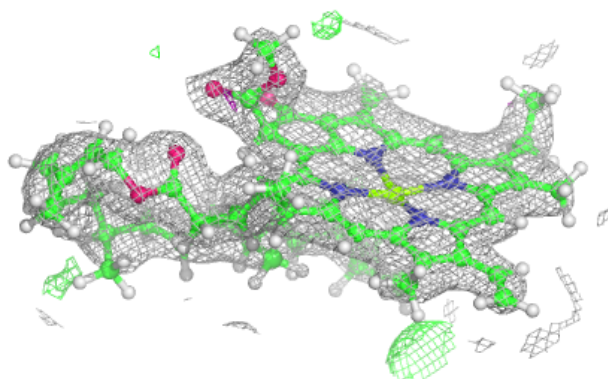
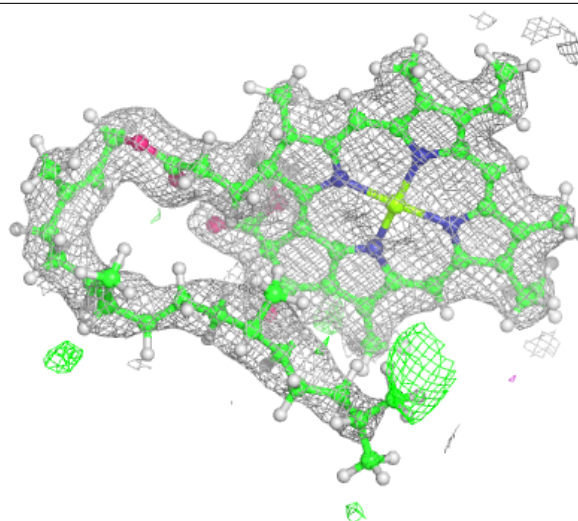
**Electron density around BCR c 515:**

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



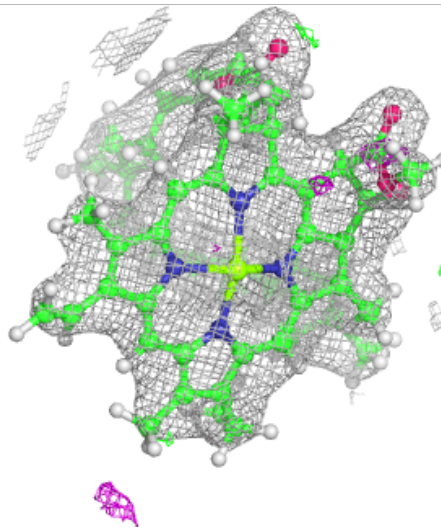
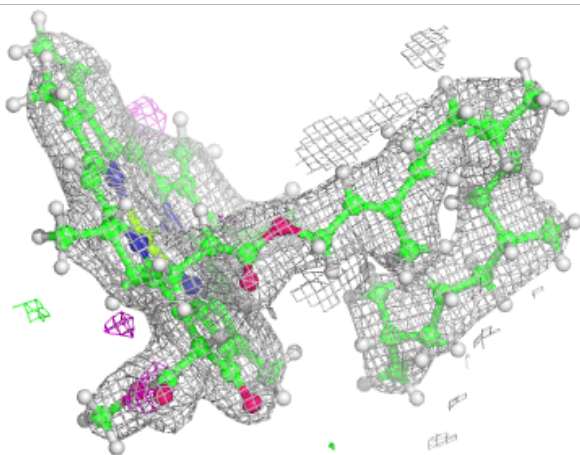
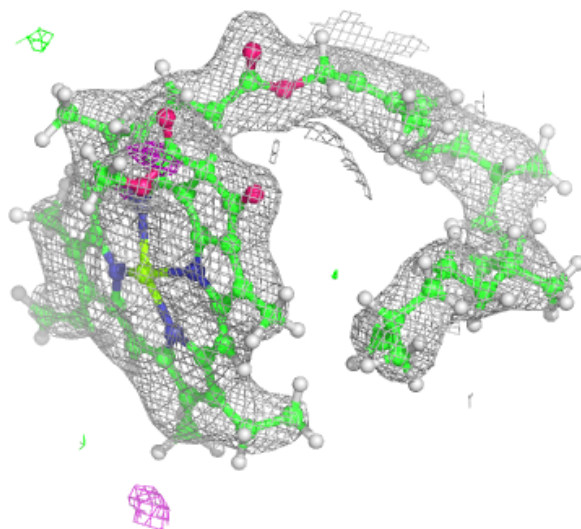
**Electron density around CLA C 509:**

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



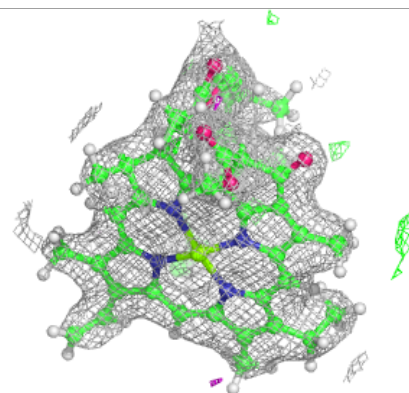
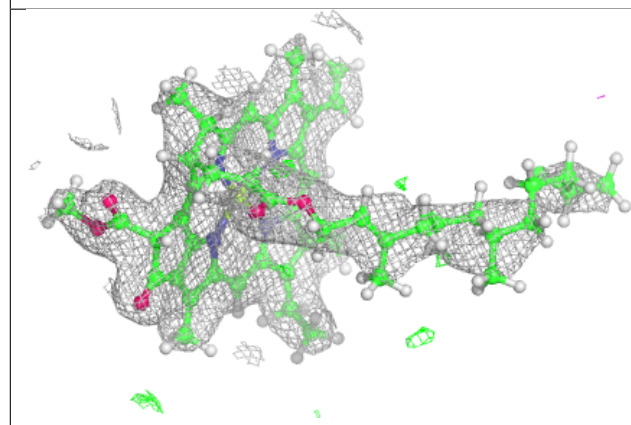
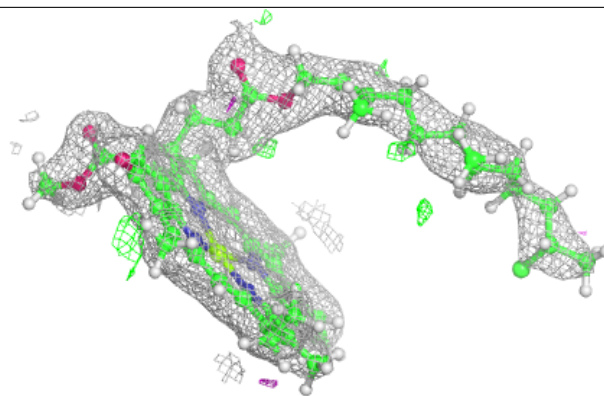
**Electron density around CLA c 503:**

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



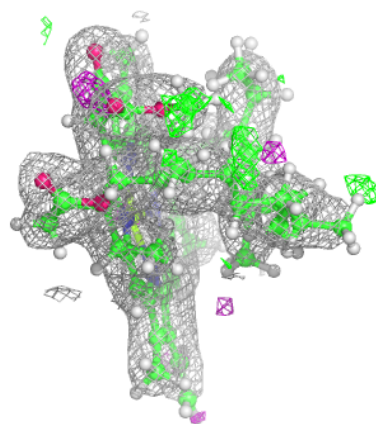
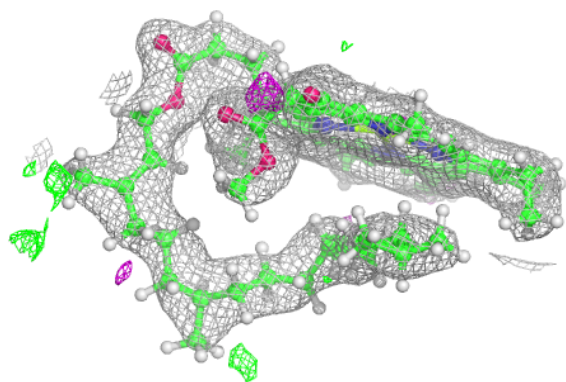
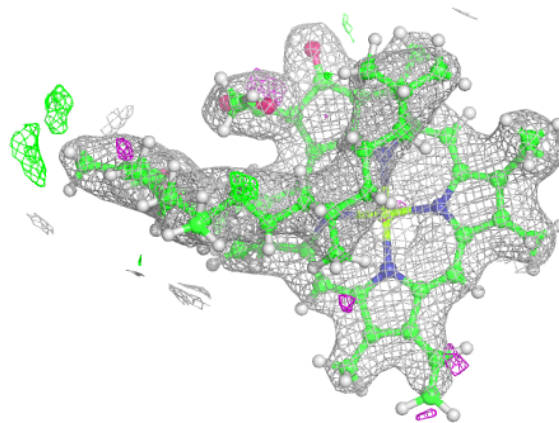
**Electron density around CLA c 504:**

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

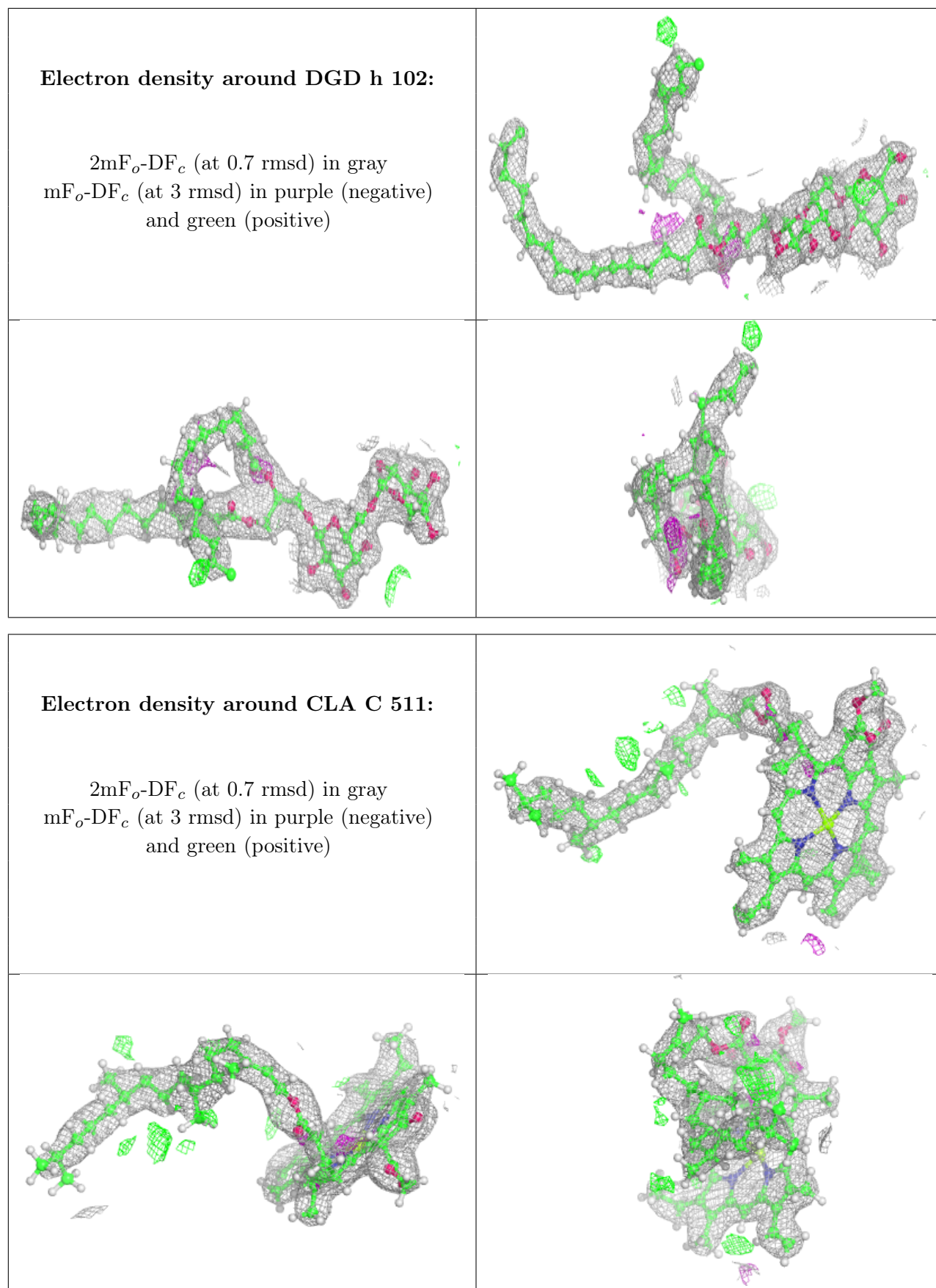


**Electron density around CLA C 510:**

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

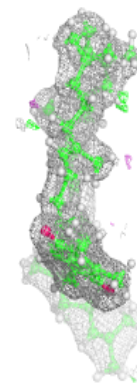
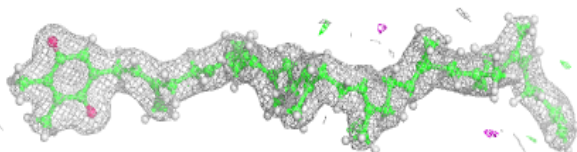
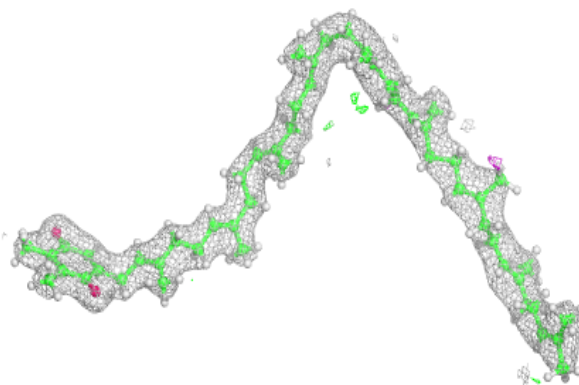




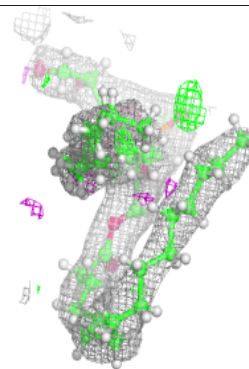
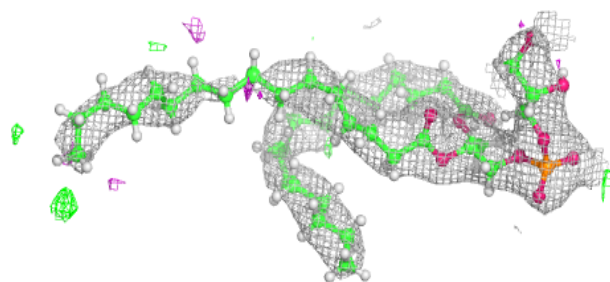
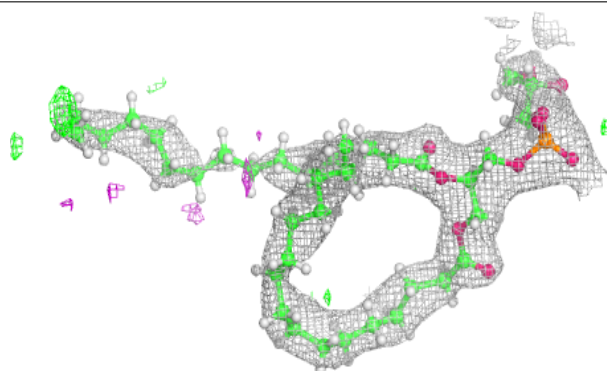


**Electron density around PL9 D 407:**

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

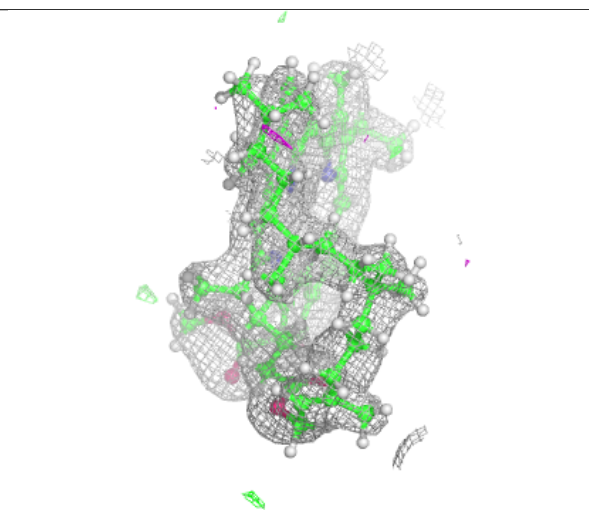
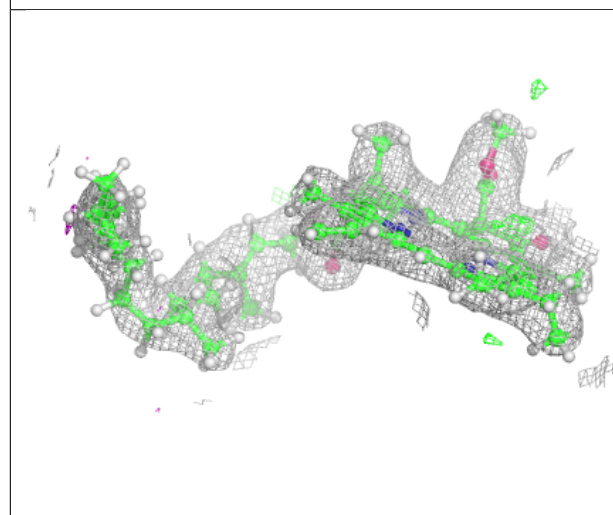
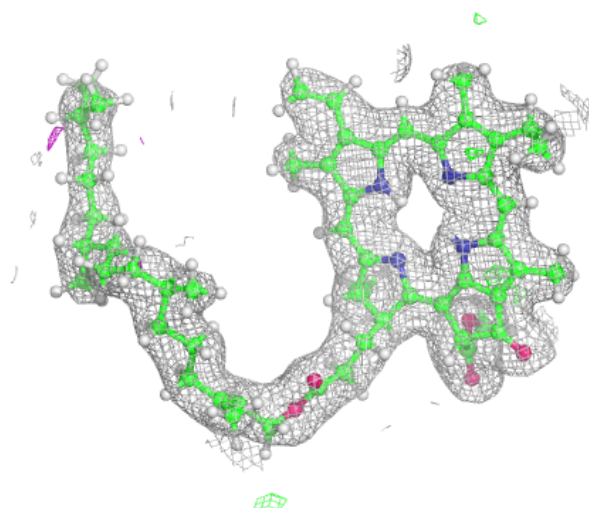
**Electron density around LHG d 406:**

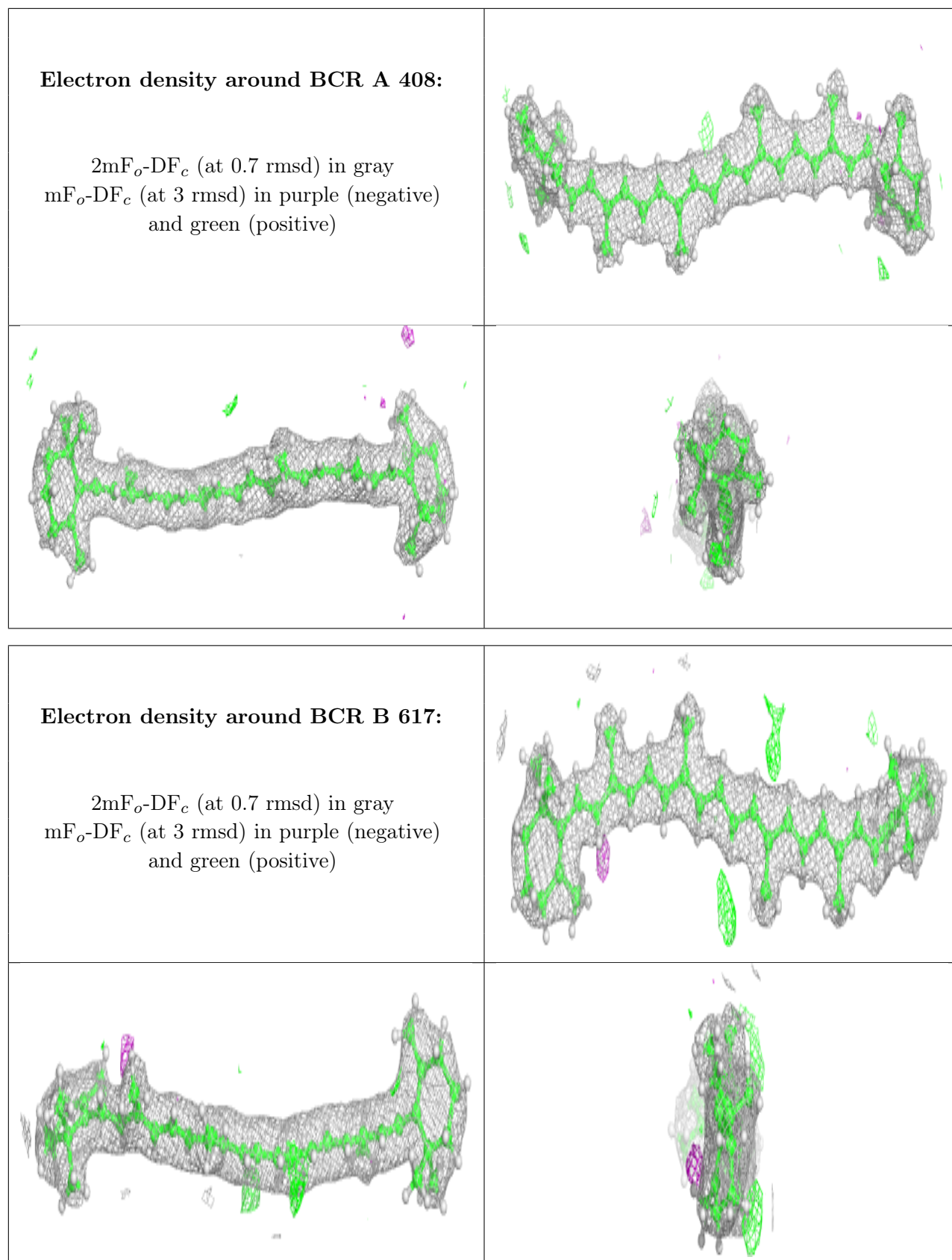
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO d 401:**

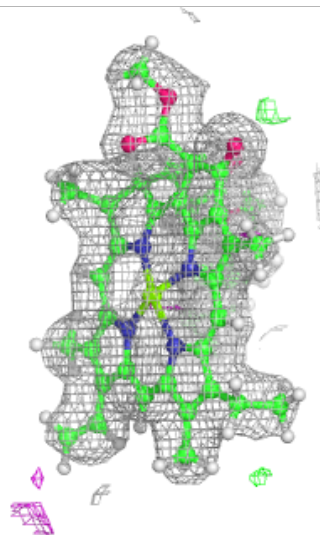
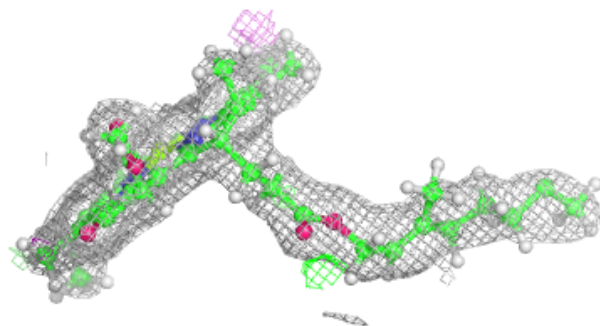
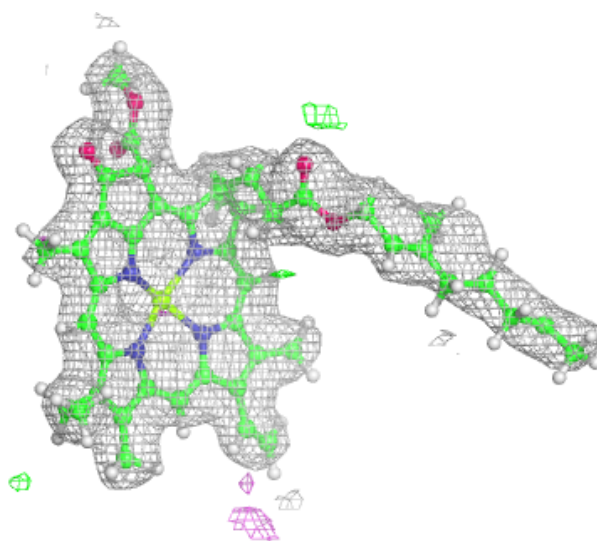
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





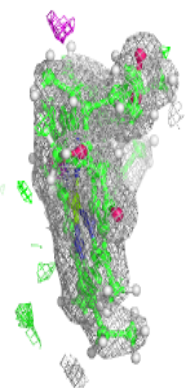
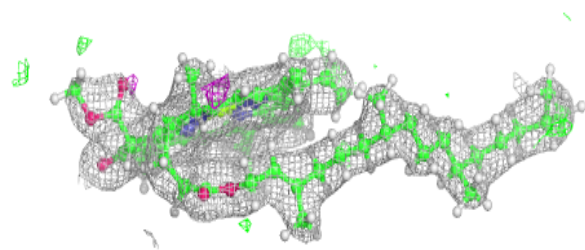
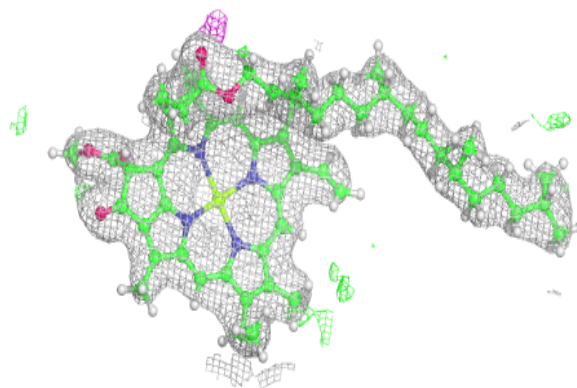
**Electron density around CLA A 407:**

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

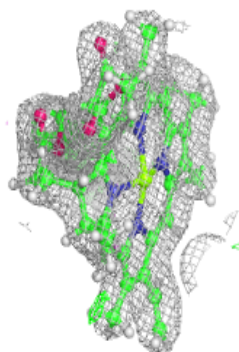
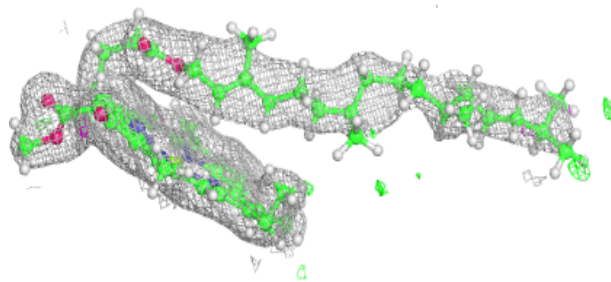
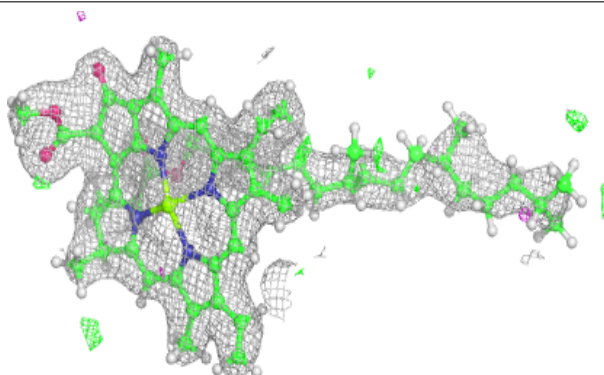


**Electron density around CLA C 501:**

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

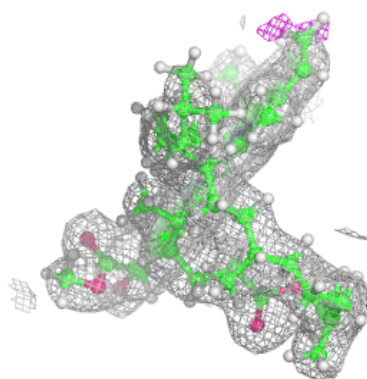
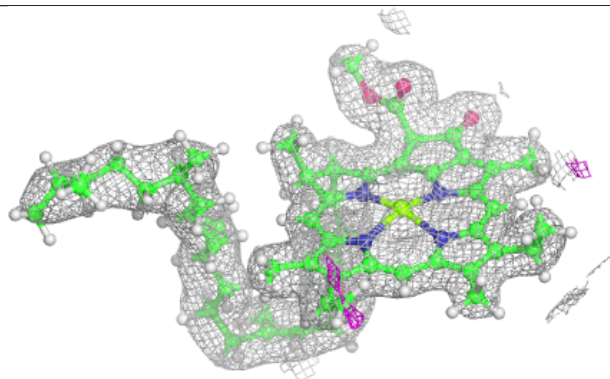
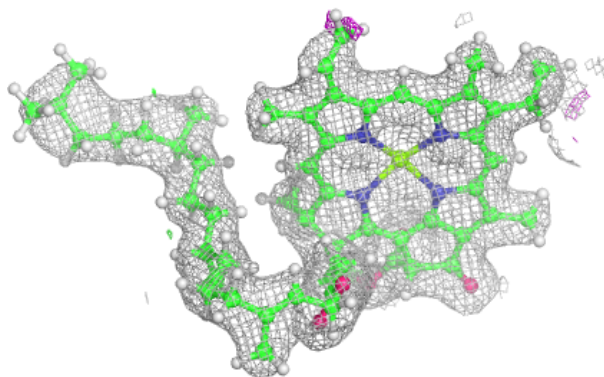
**Electron density around CLA b 613:**

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

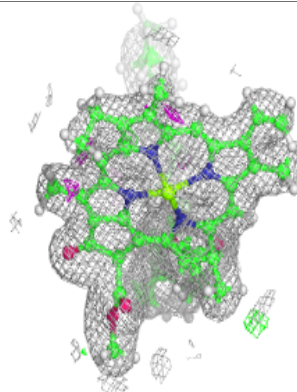
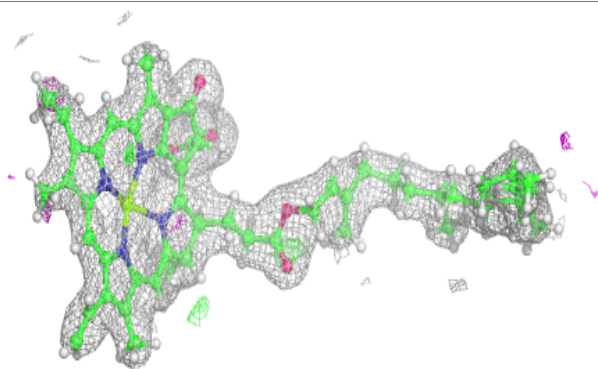
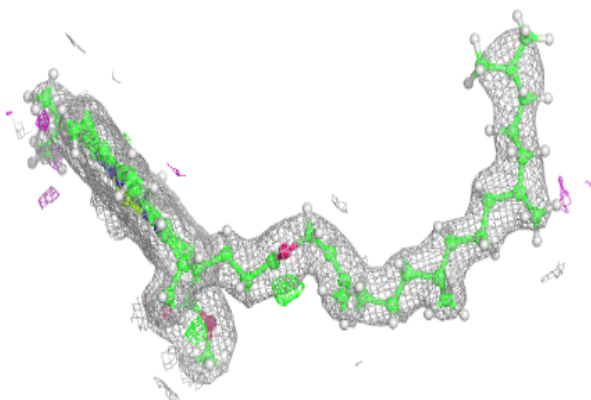


**Electron density around CLA D 403:**

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

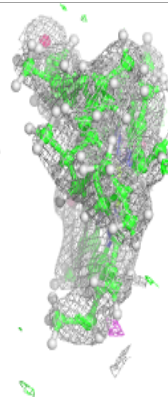
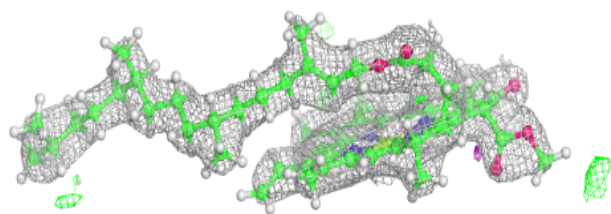
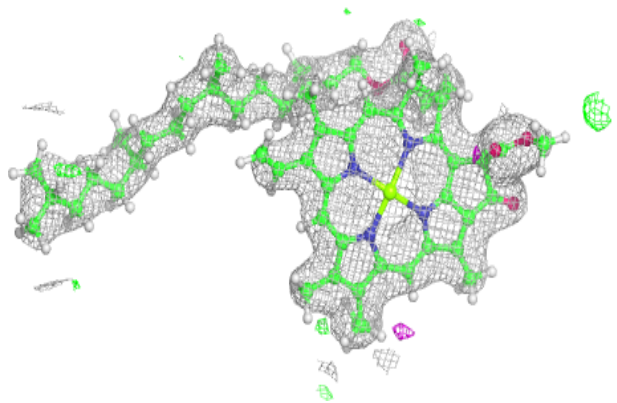
**Electron density around CLA D 404:**

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

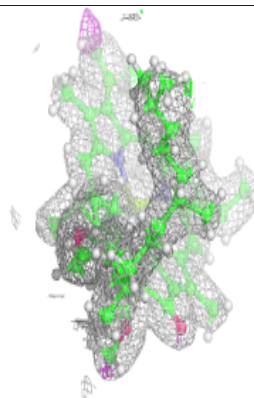
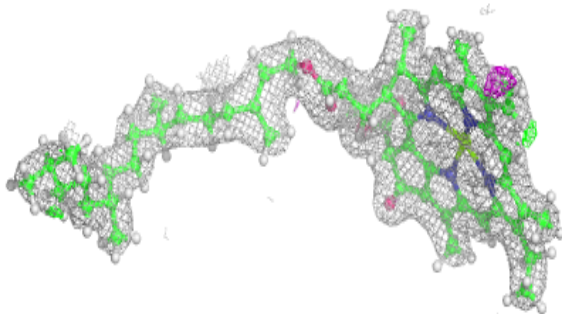
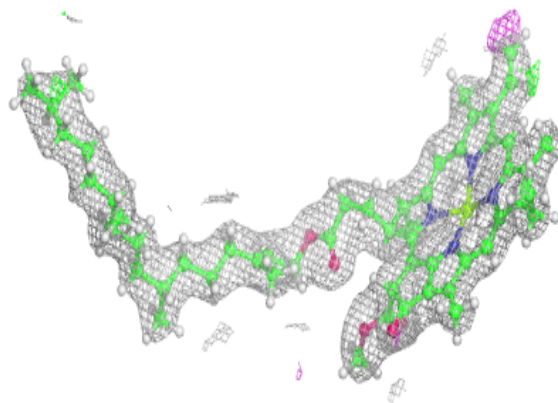


**Electron density around CLA c 501:**

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

**Electron density around CLA A 404:**

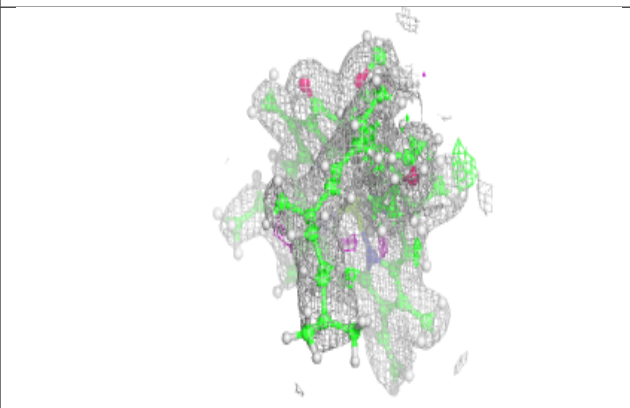
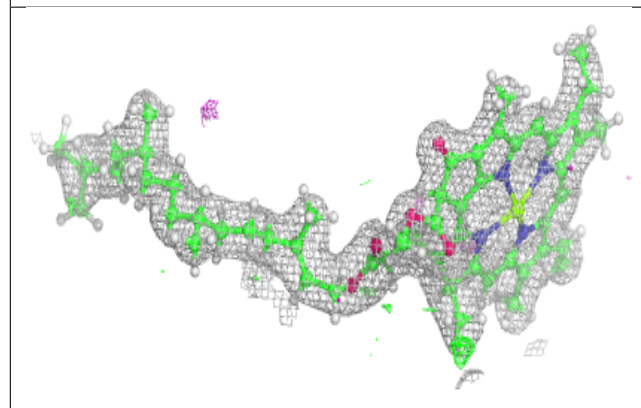
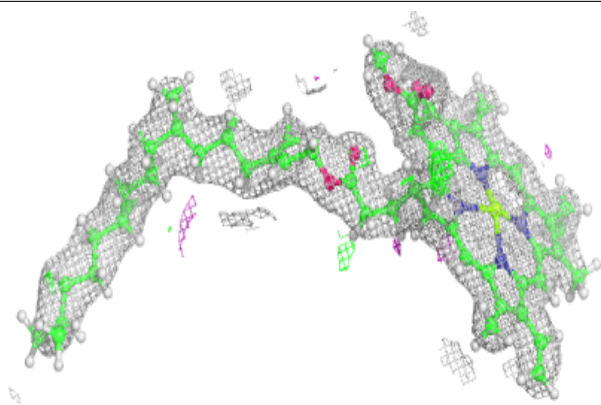
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



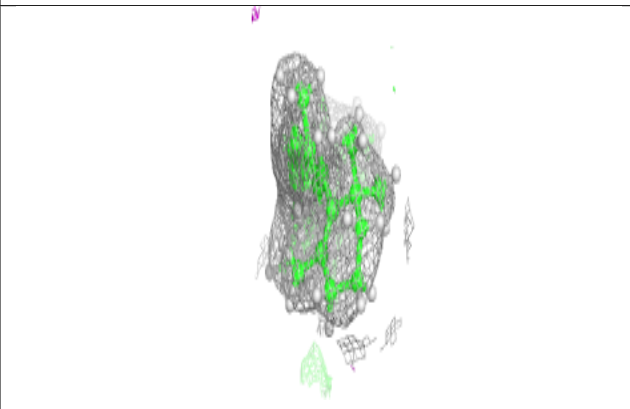
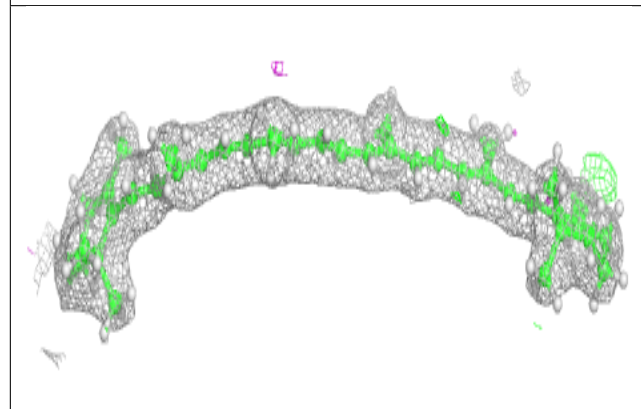
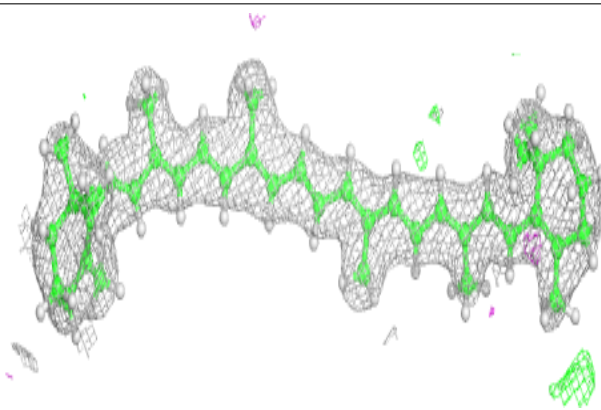


**Electron density around CLA a 405:**

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

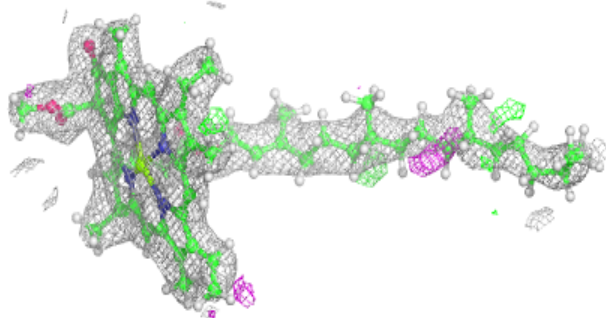
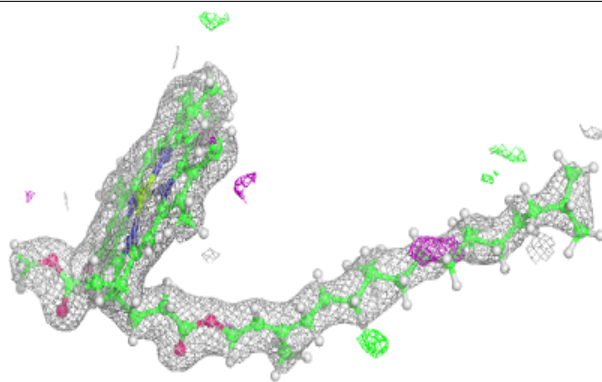
**Electron density around BCR T 101:**

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

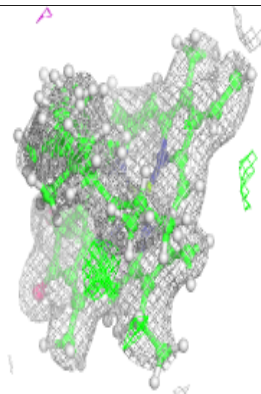
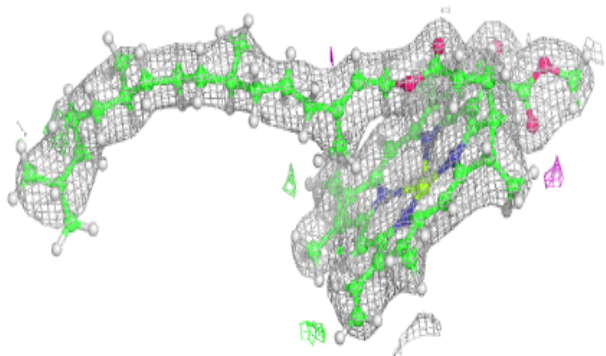
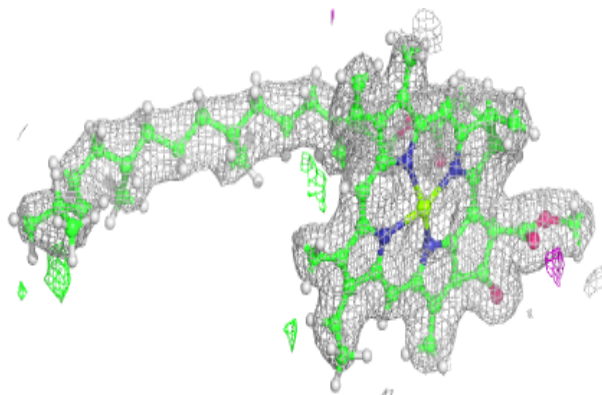


**Electron density around CLA B 607:**

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

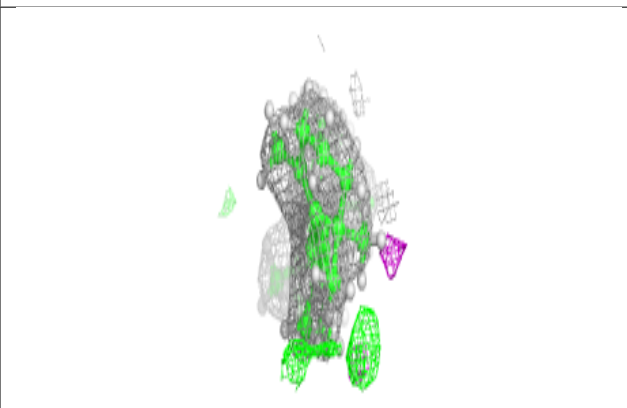
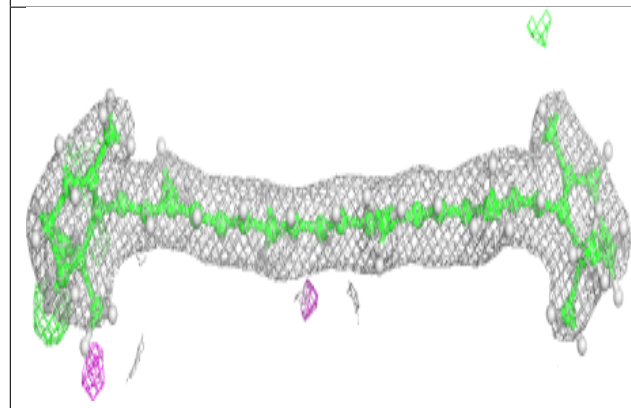
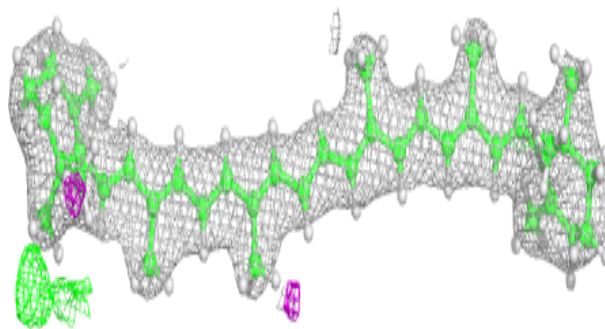
**Electron density around CLA B 608:**

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

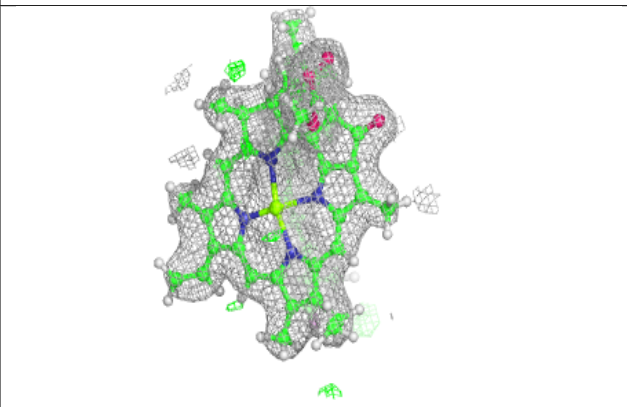
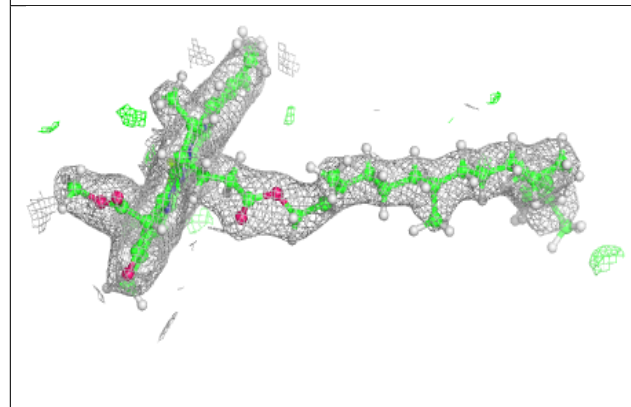
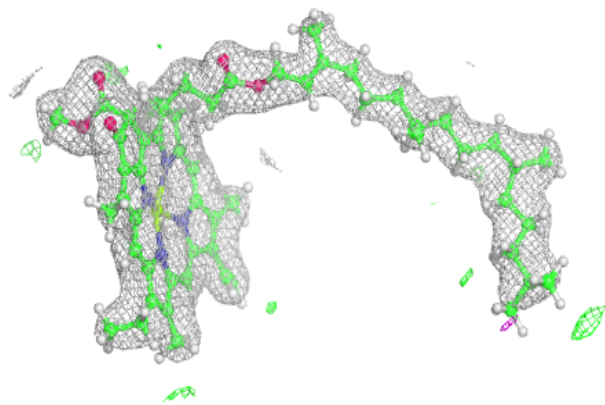


**Electron density around BCR b 617:**

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

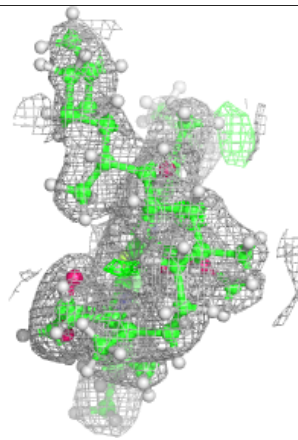
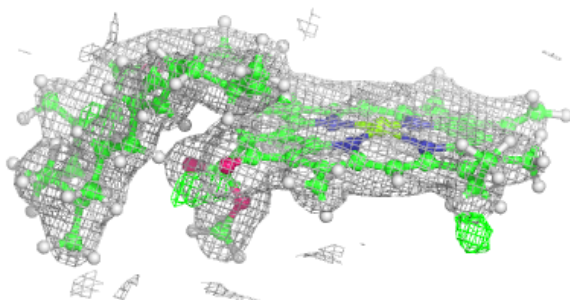
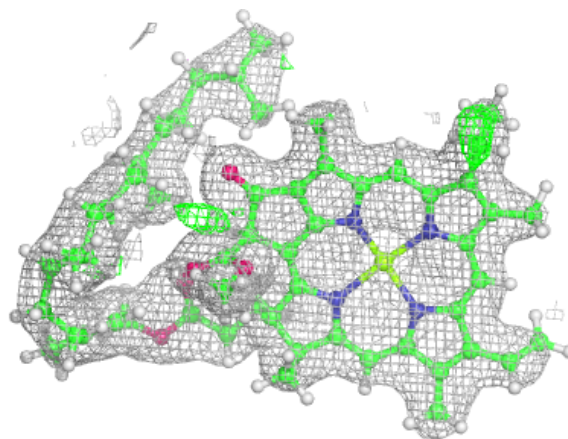
**Electron density around CLA B 609:**

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

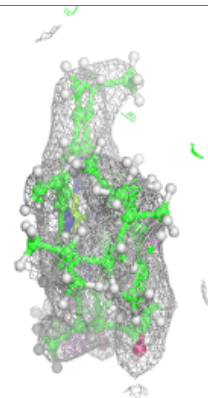
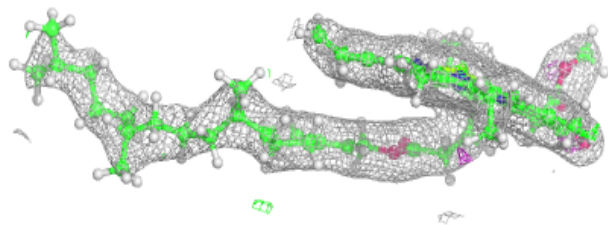
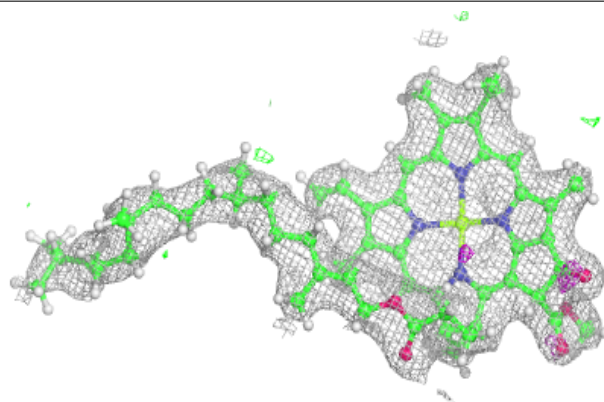


**Electron density around CLA B 610:**

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

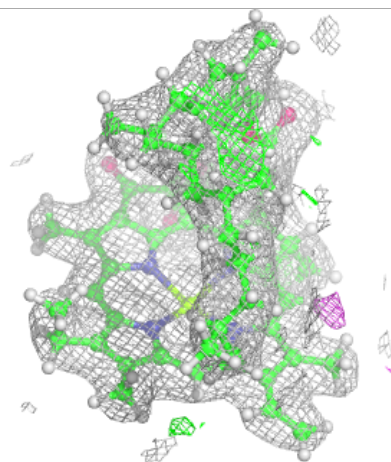
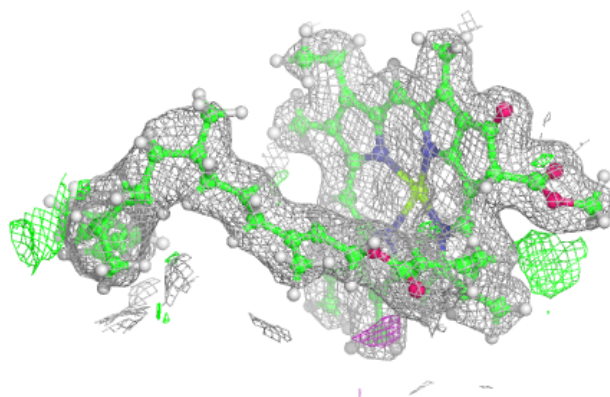
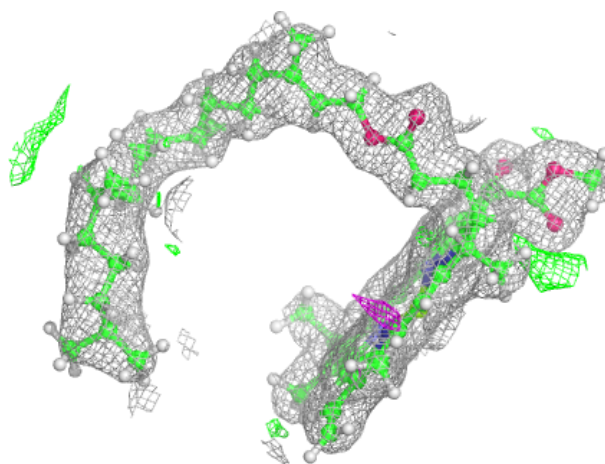
**Electron density around CLA b 602:**

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



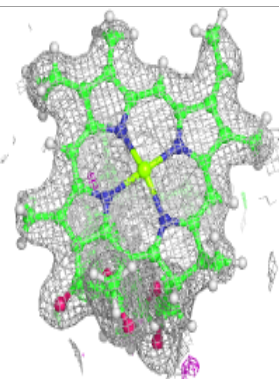
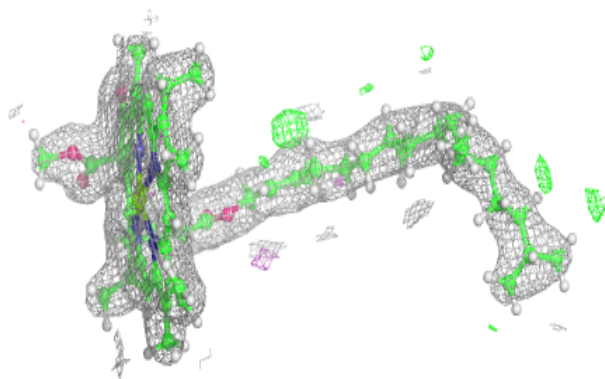
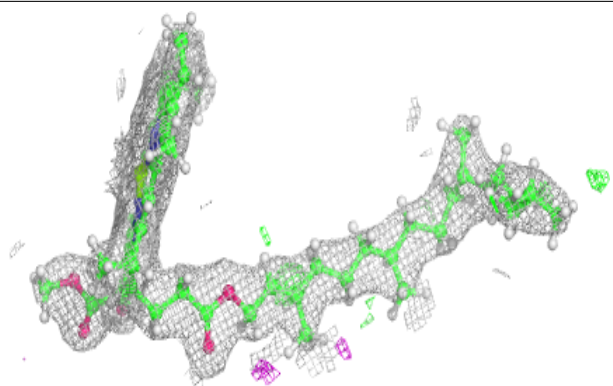
**Electron density around CLA B 611:**

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

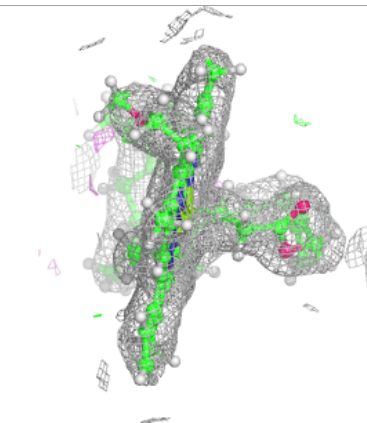
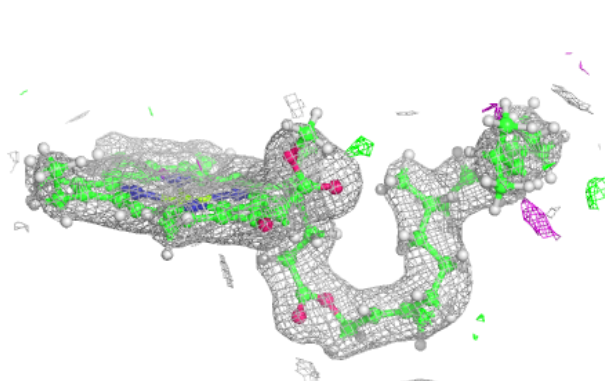
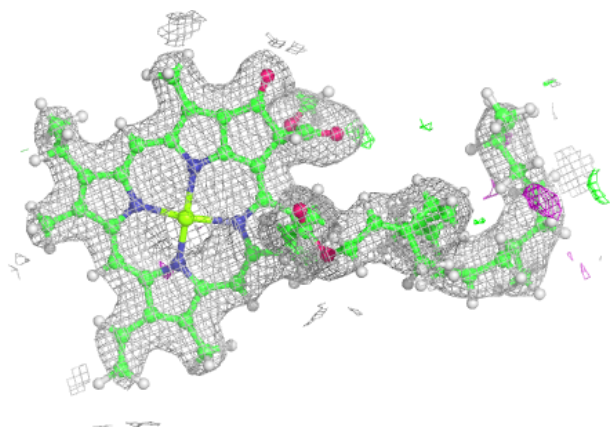


**Electron density around CLA b 604:**

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

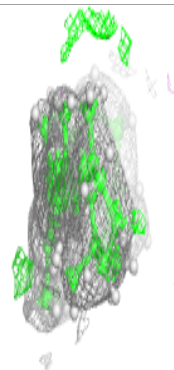
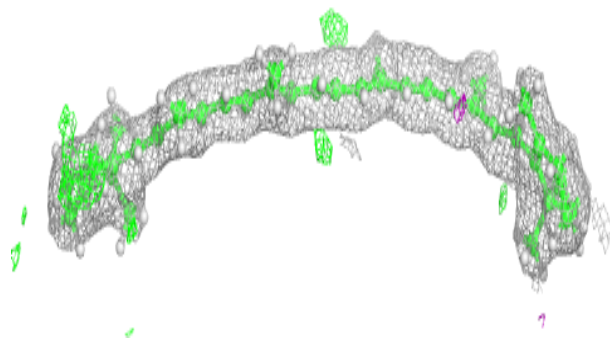
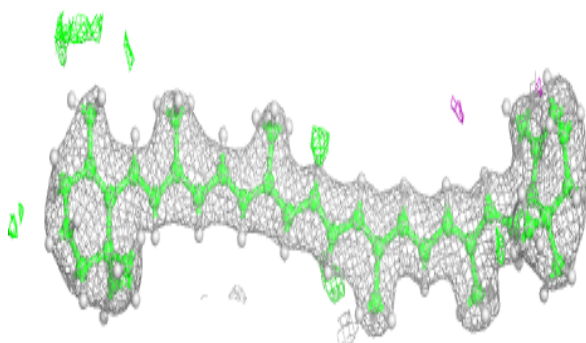
**Electron density around CLA B 612:**

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

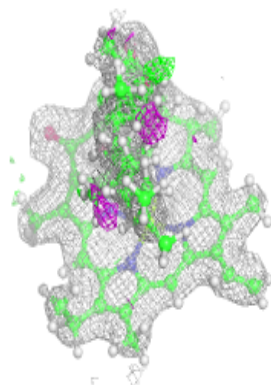
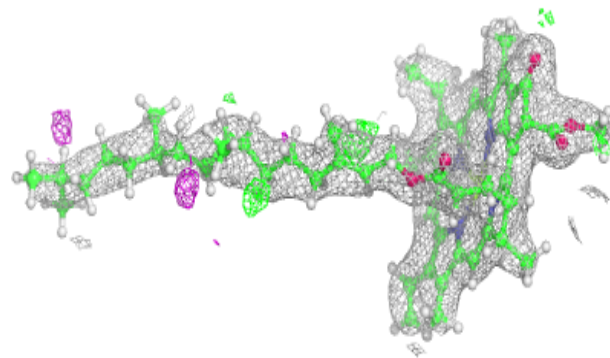
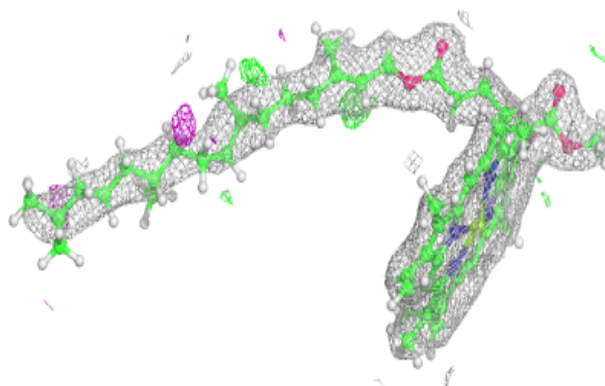


**Electron density around BCR t 101:**

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

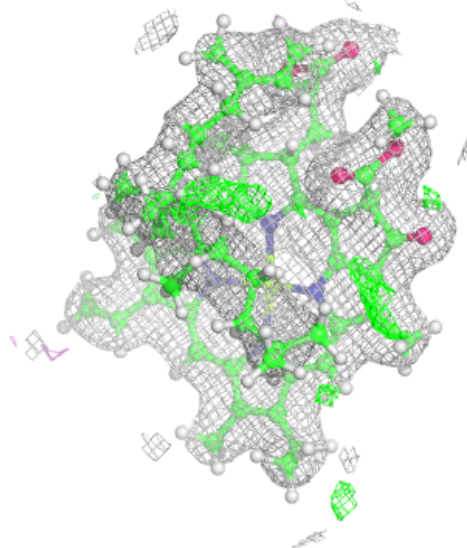
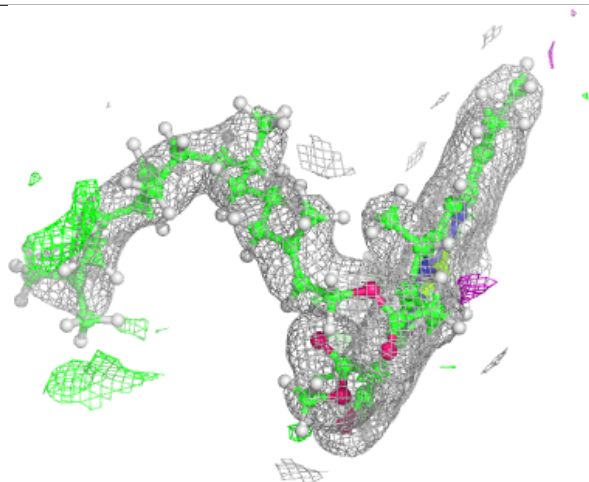
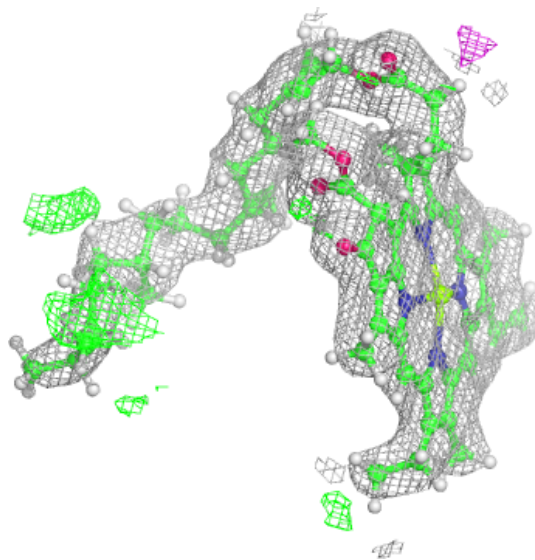
**Electron density around CLA b 606:**

$2mF_o-DF_c$  (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:**

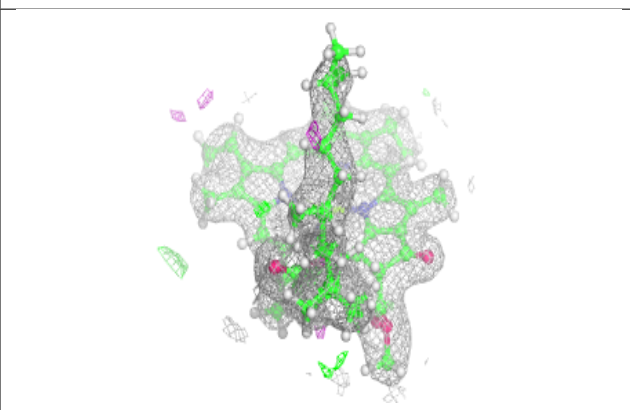
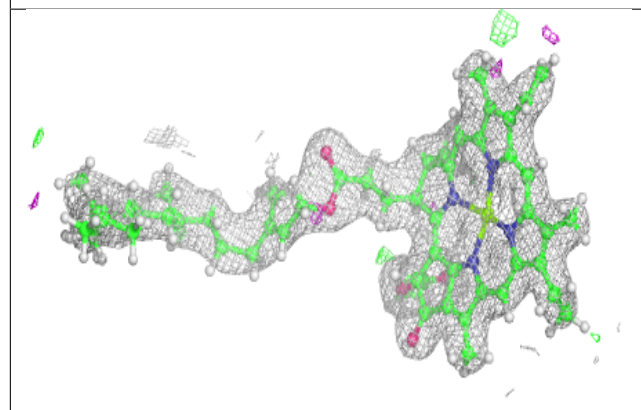
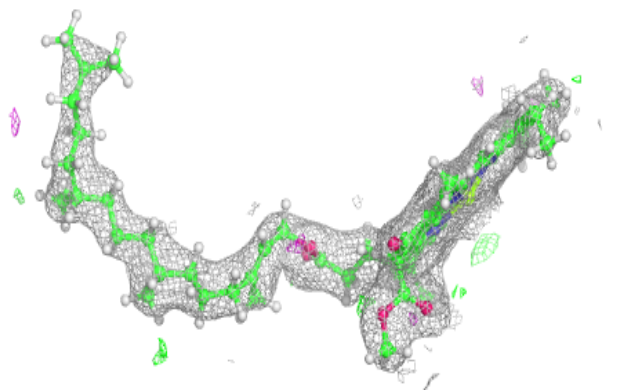
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



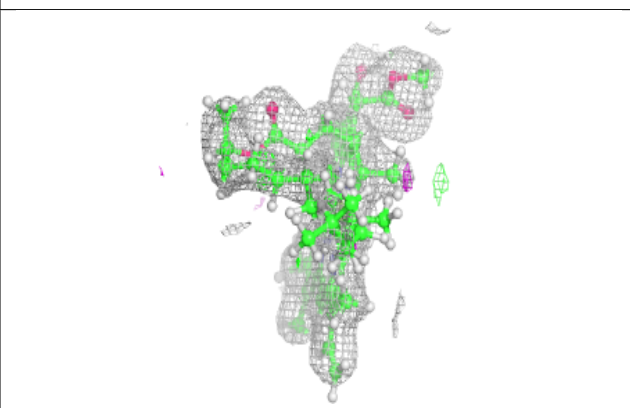
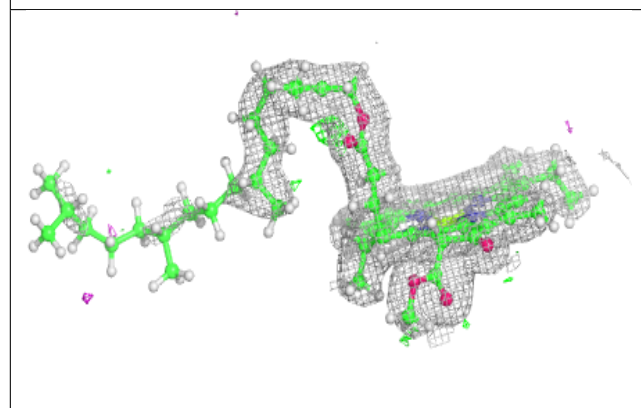
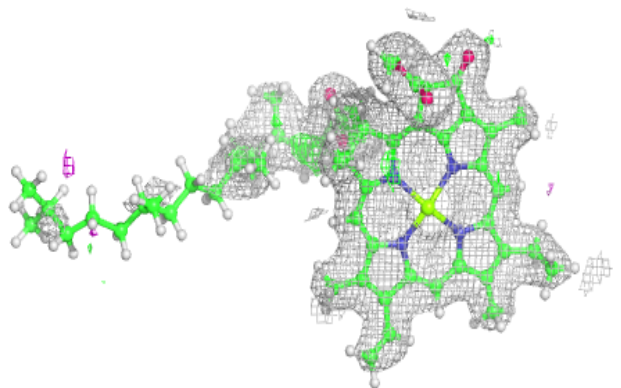


**Electron density around CLA d 402:**

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

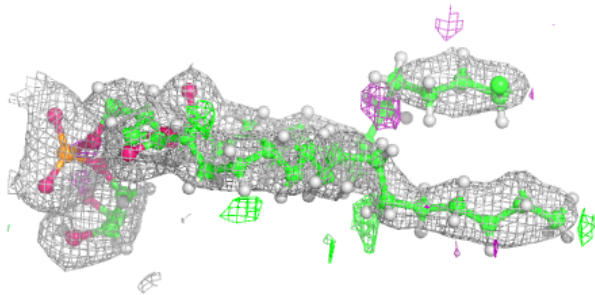
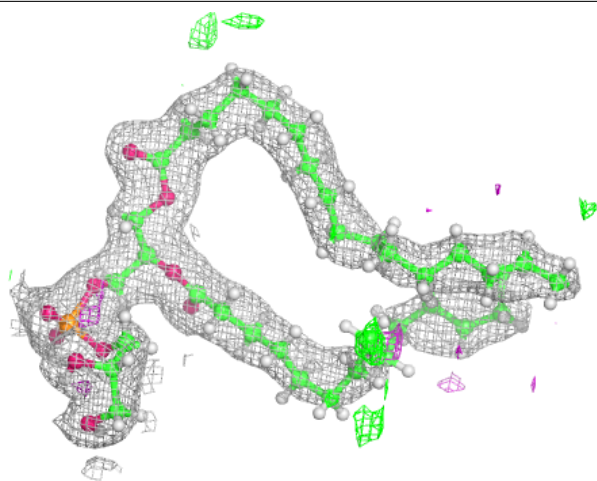
**Electron density around CLA A 405:**

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



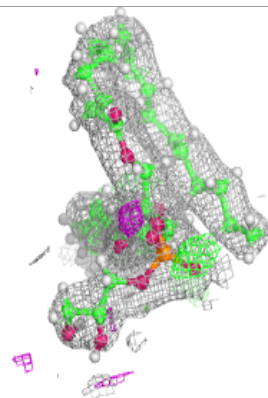
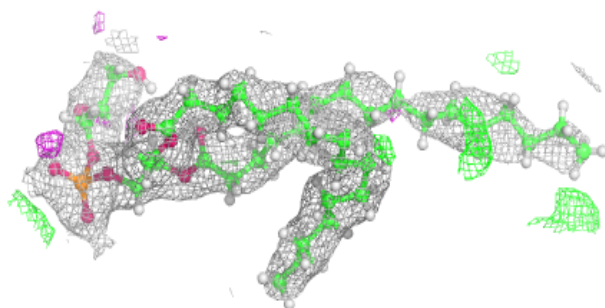
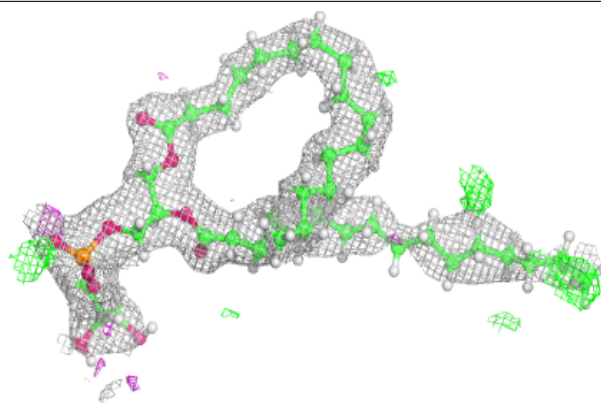
**Electron density around LHG D 411:**

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

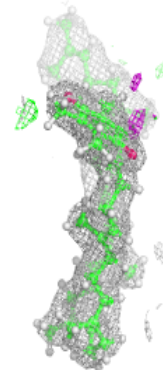
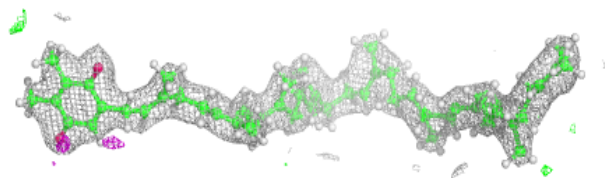
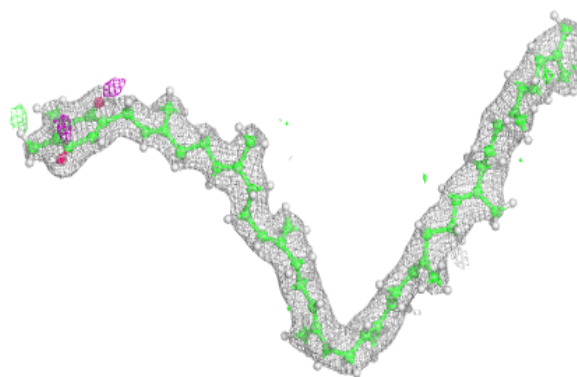


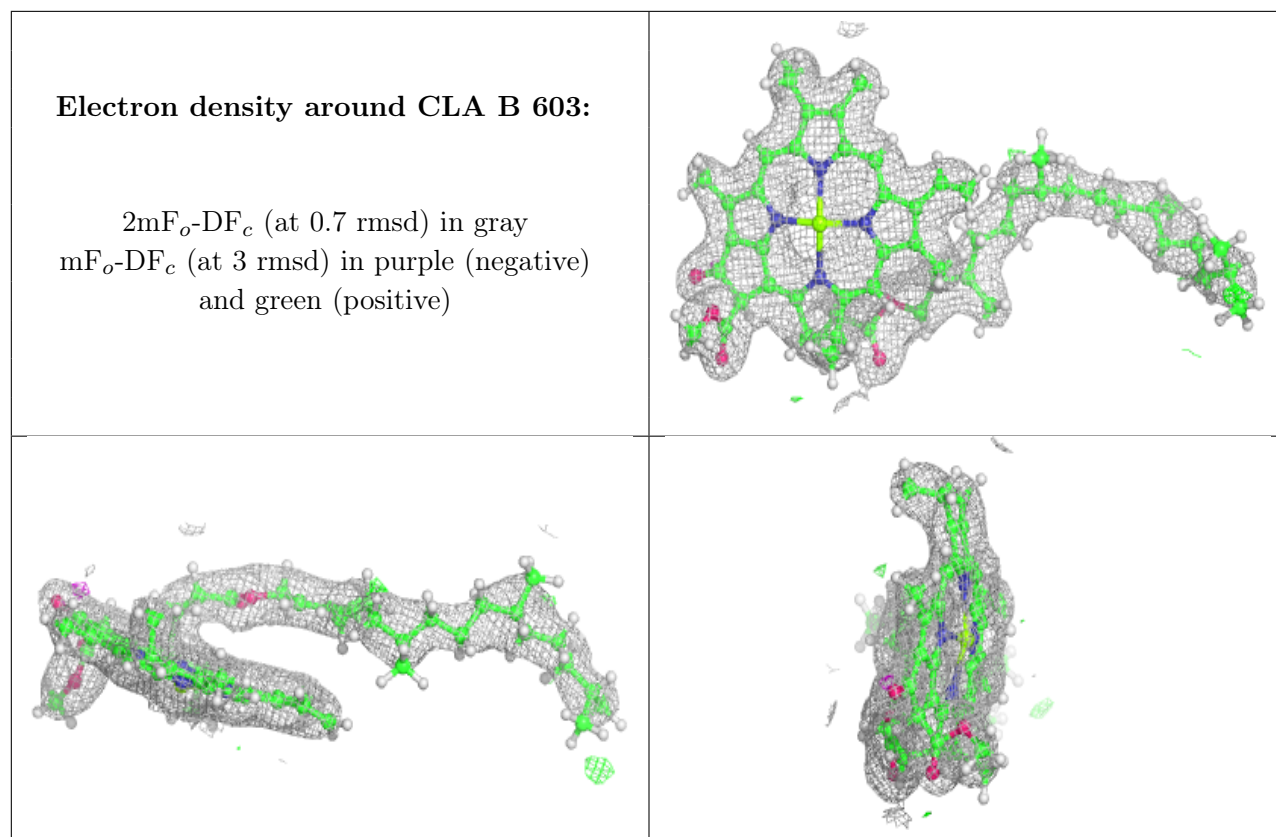
**Electron density around LHG D 412:**

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

**Electron density around PL9 d 405:**

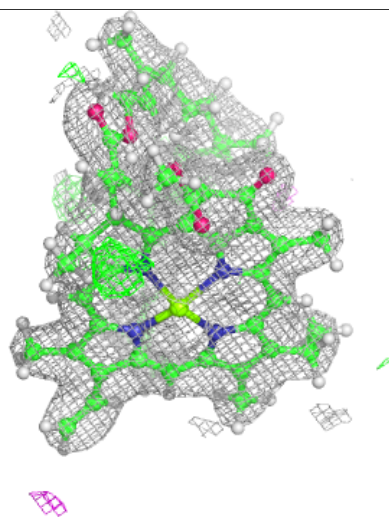
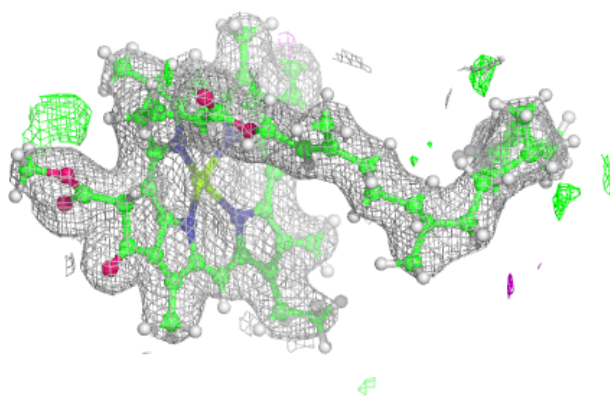
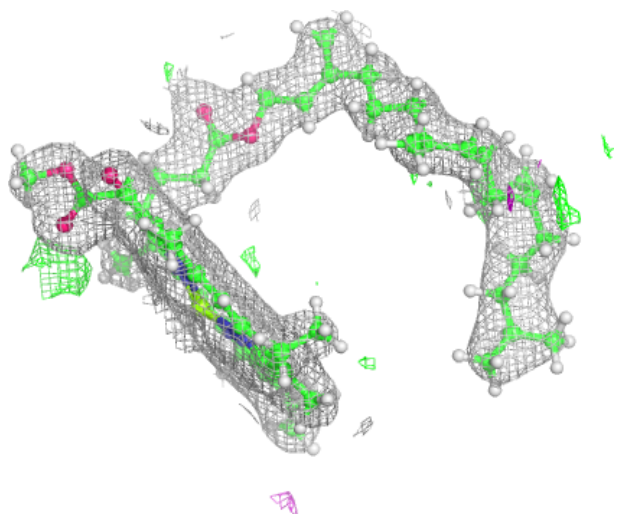
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





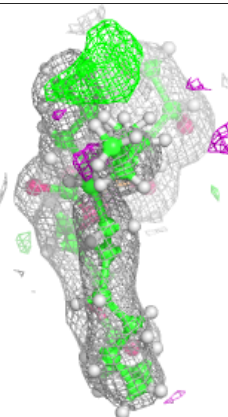
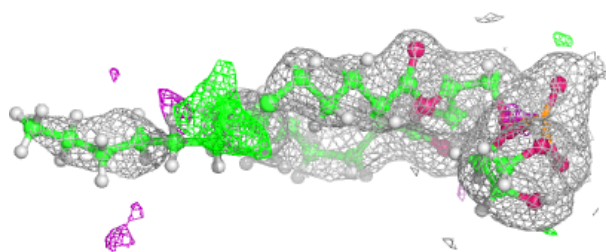
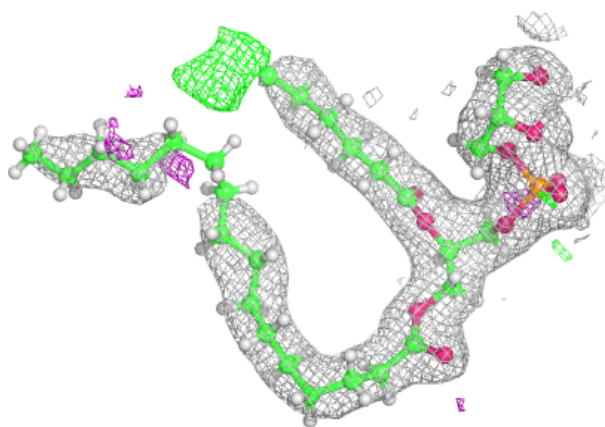
**Electron density around CLA b 610:**

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



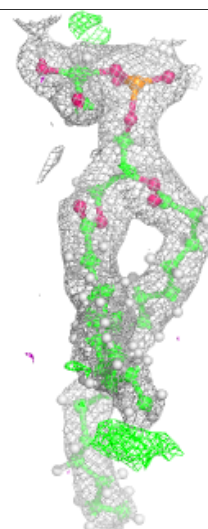
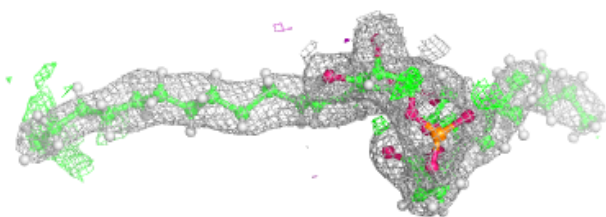
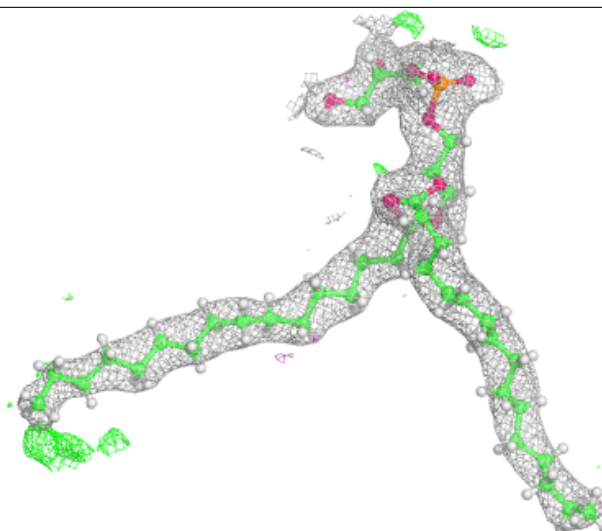
**Electron density around LHG d 408:**

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



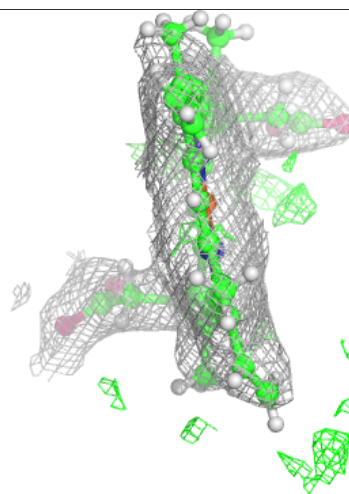
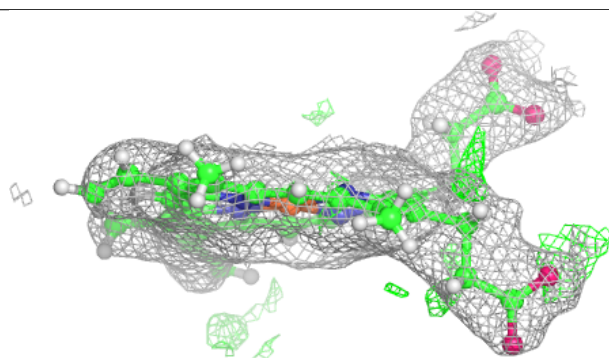
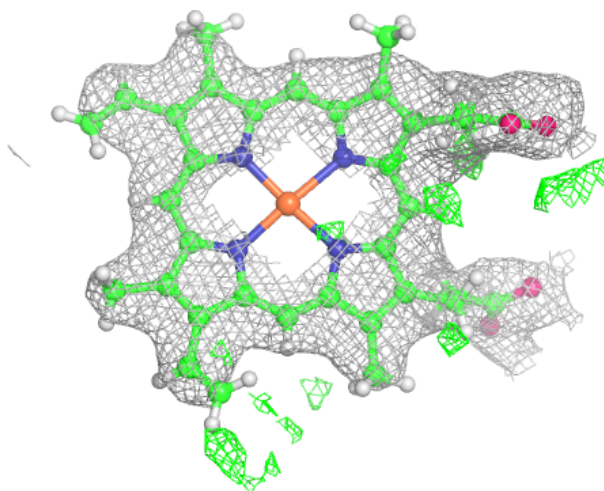
**Electron density around LHG 1 102:**

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



**Electron density around HEM f 101:**

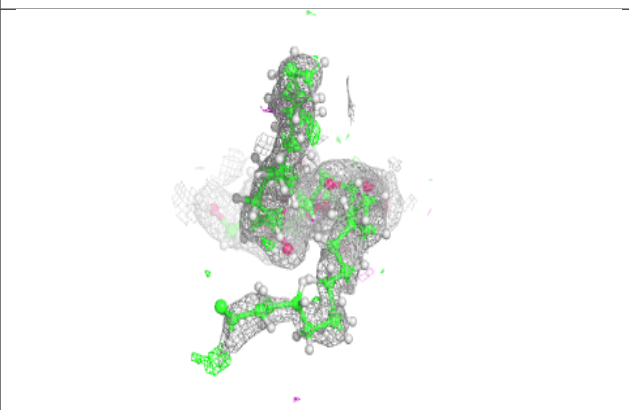
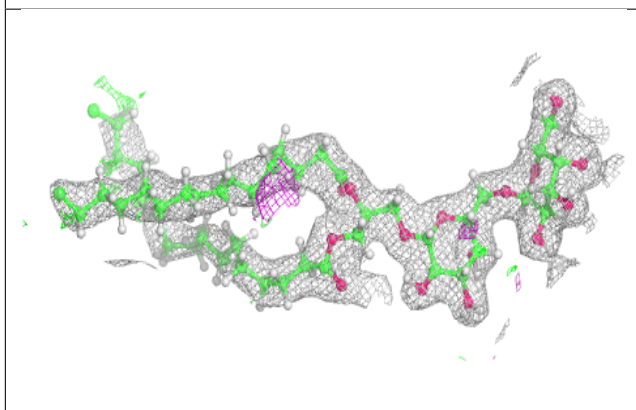
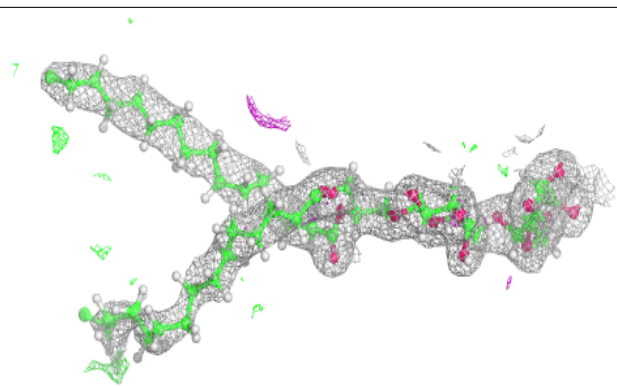
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



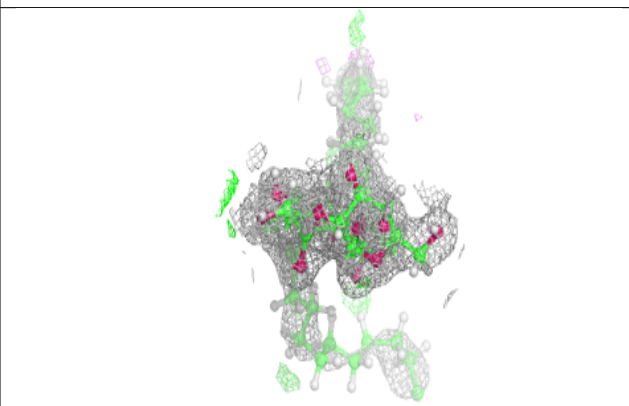
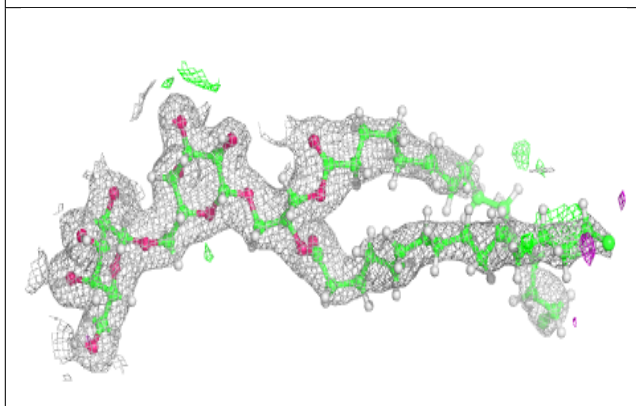
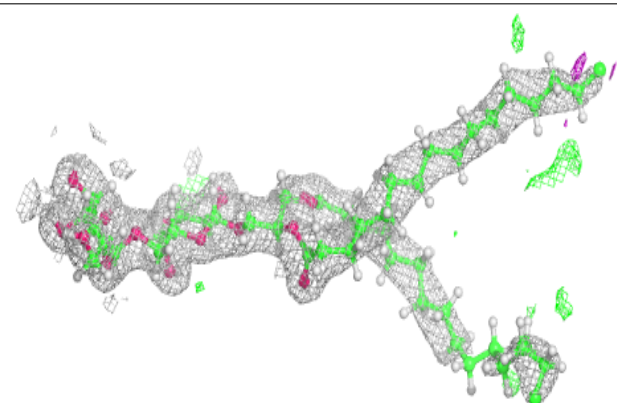


**Electron density around DGD c 519:**

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

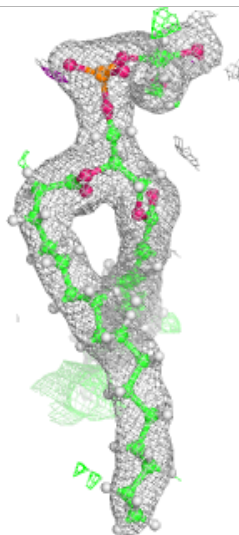
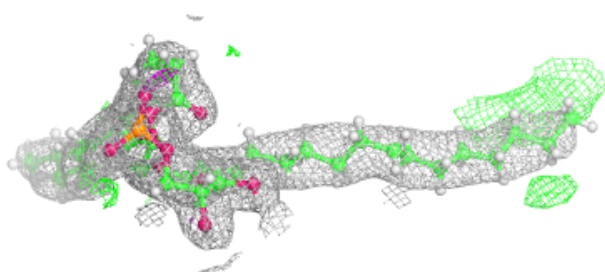
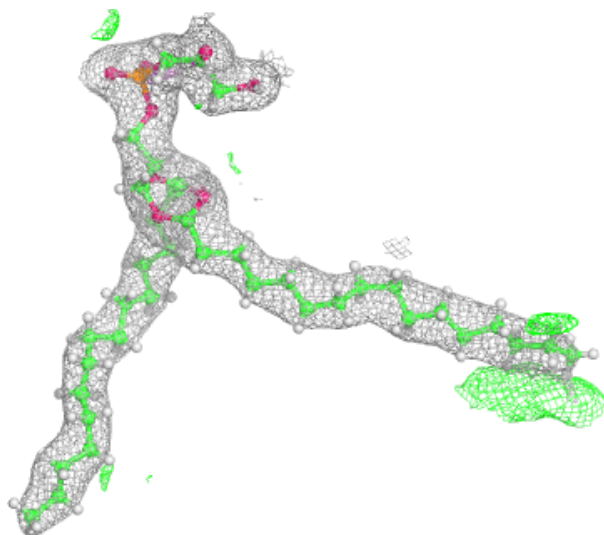
**Electron density around DGD C 521:**

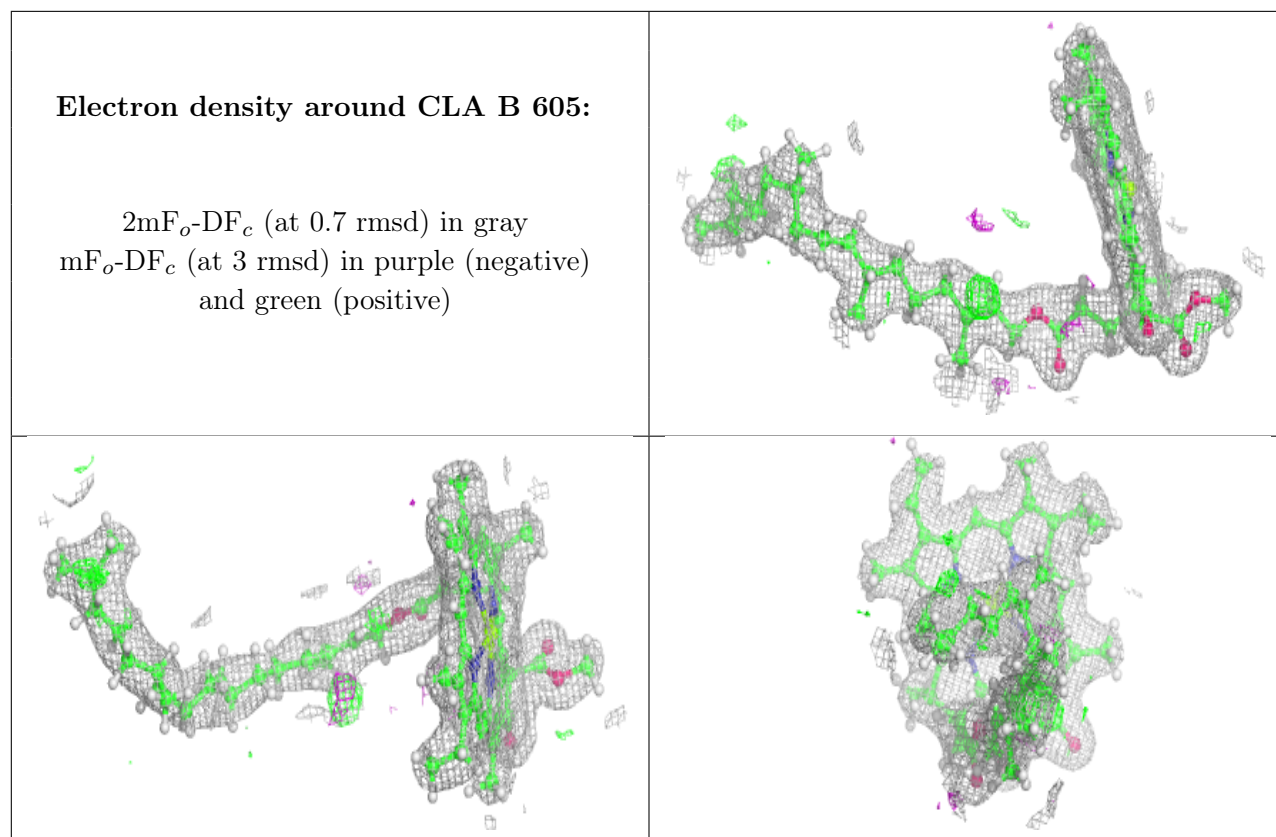
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG L 101:**

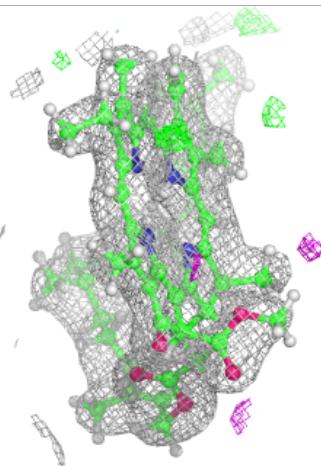
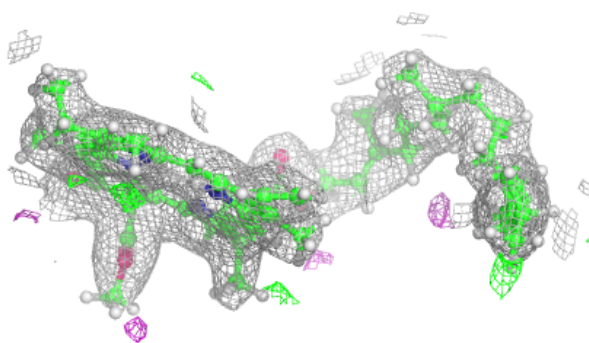
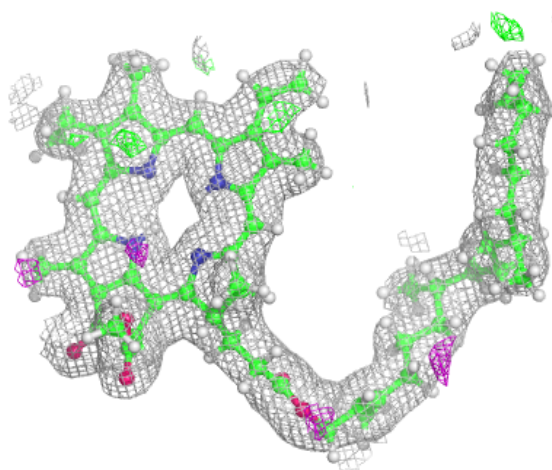
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





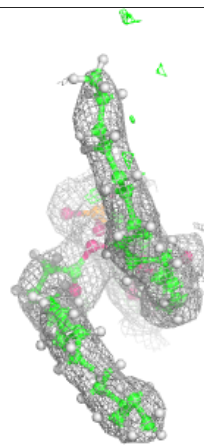
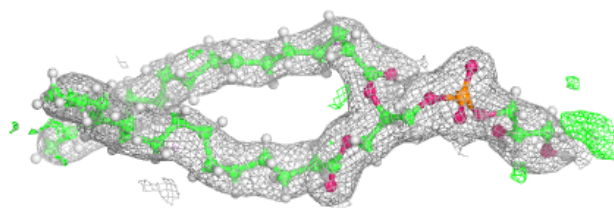
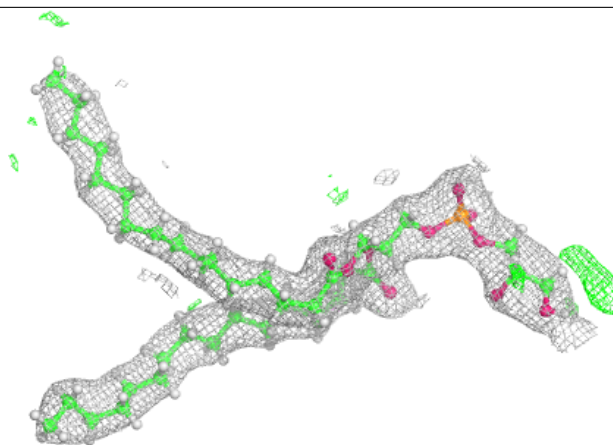
**Electron density around PHO A 406:**

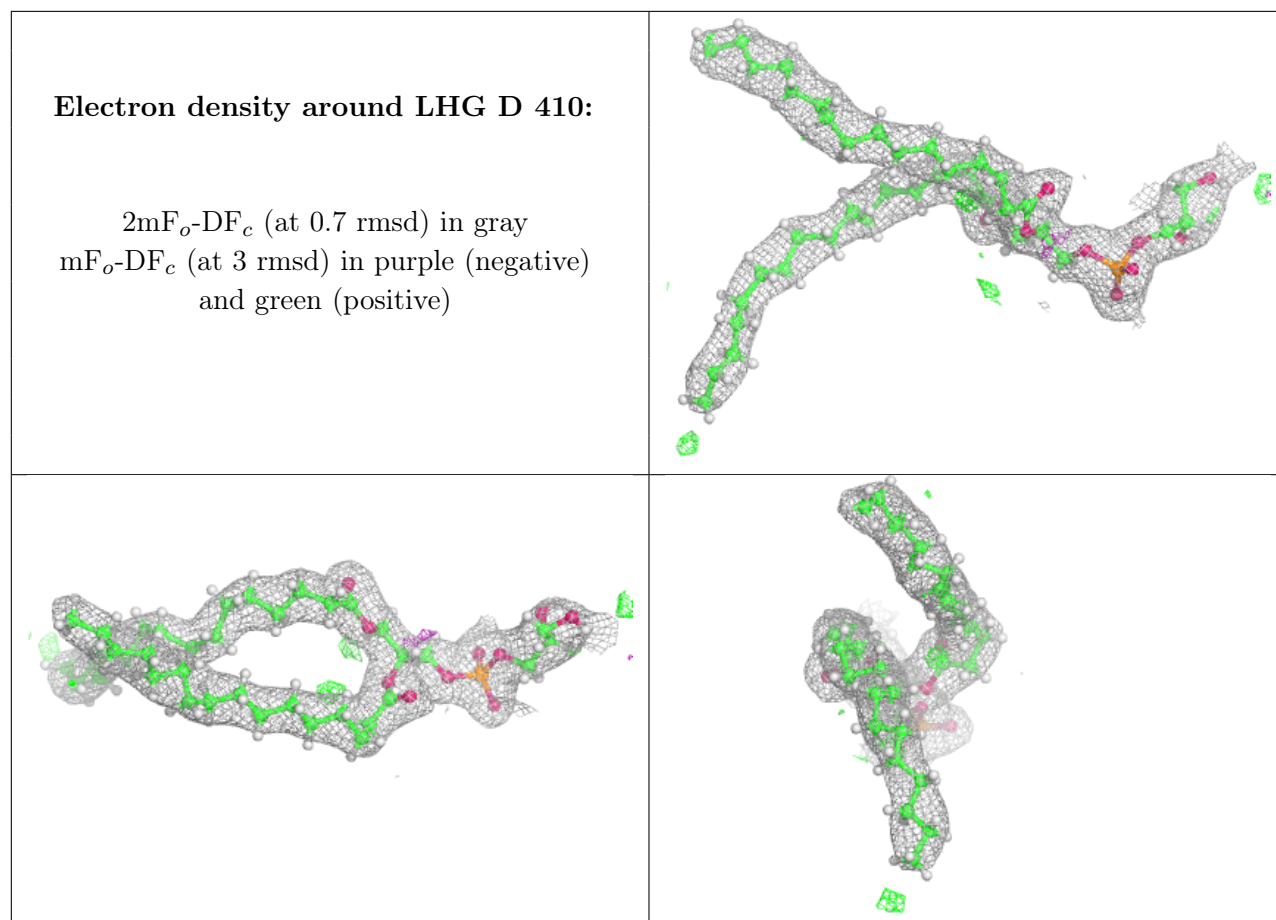
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG d 407:**

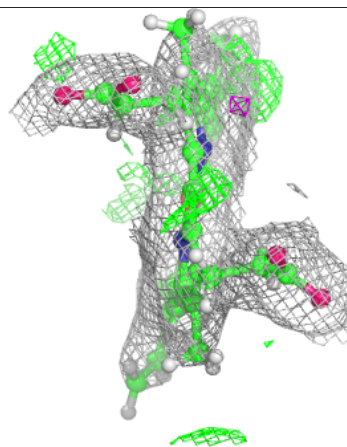
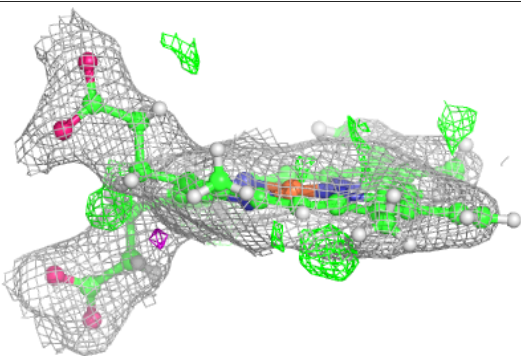
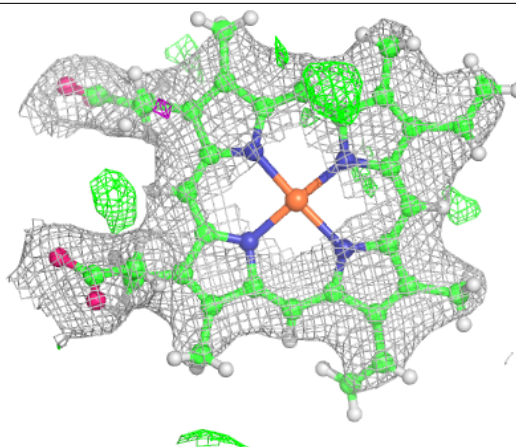
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





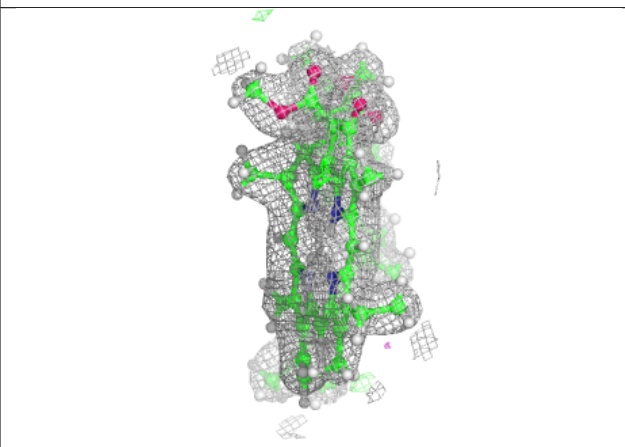
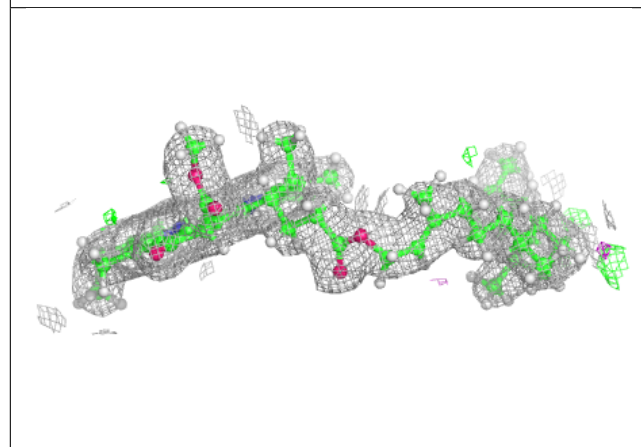
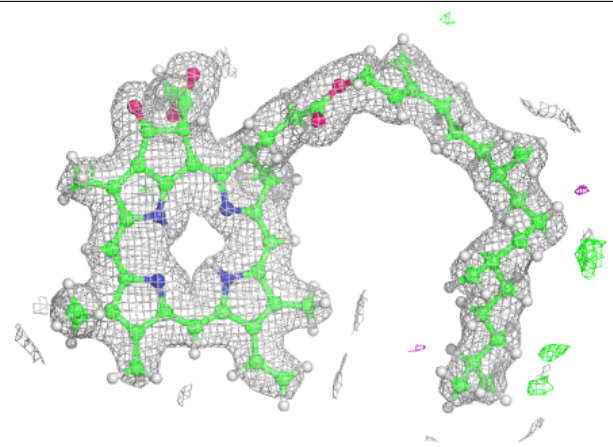
**Electron density around HEM F 101:**

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



**Electron density around PHO D 402:**

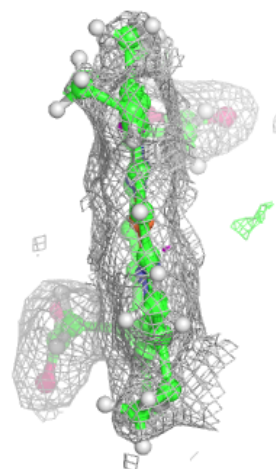
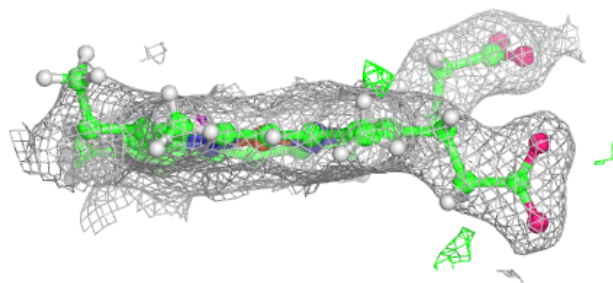
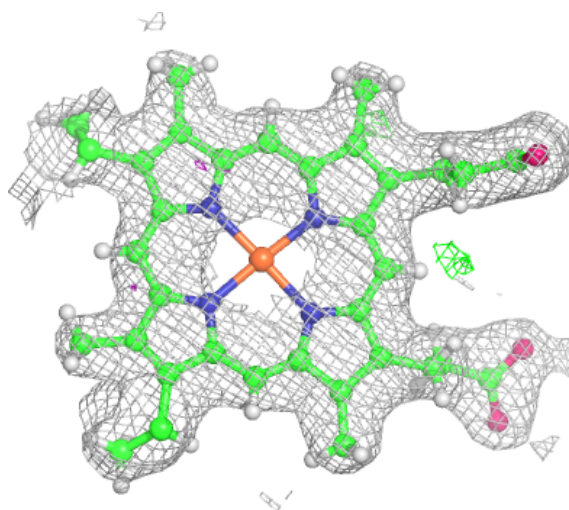
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





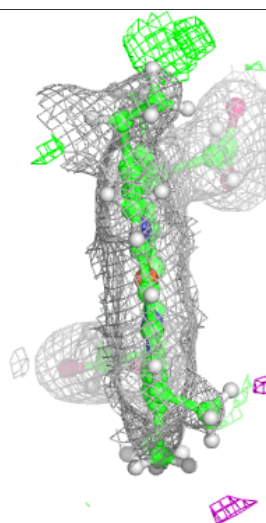
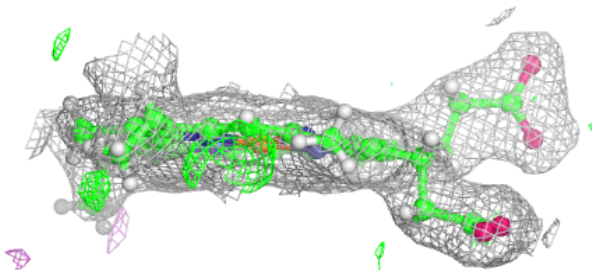
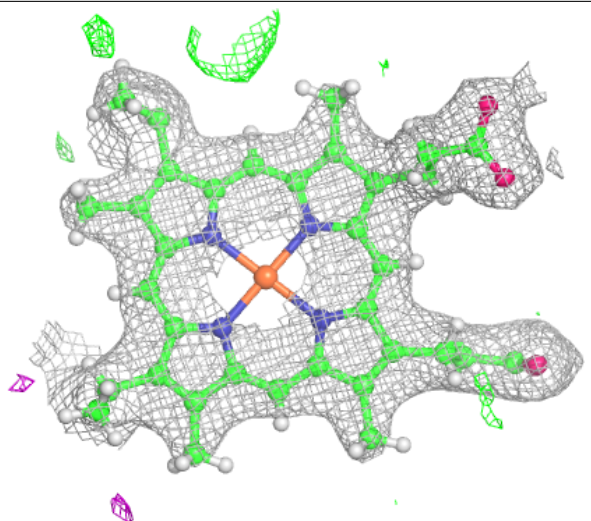
**Electron density around HEC V 201:**

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



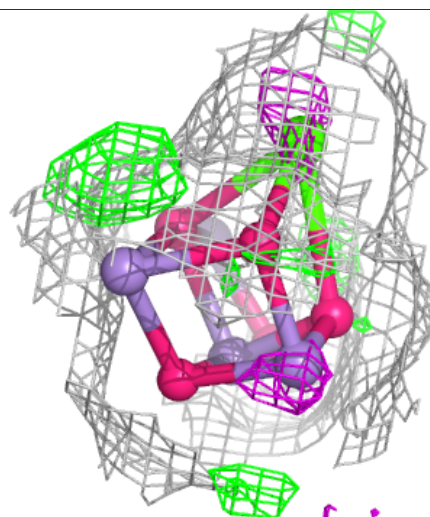
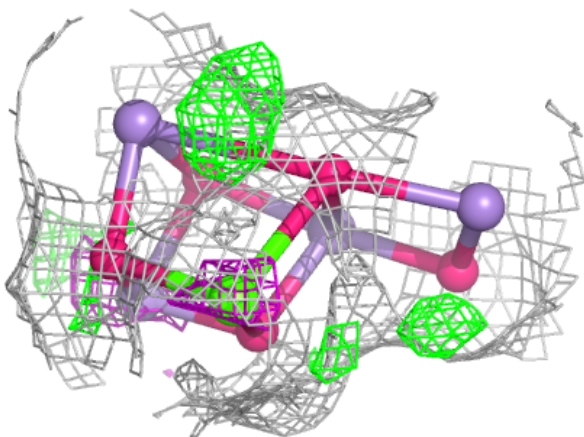
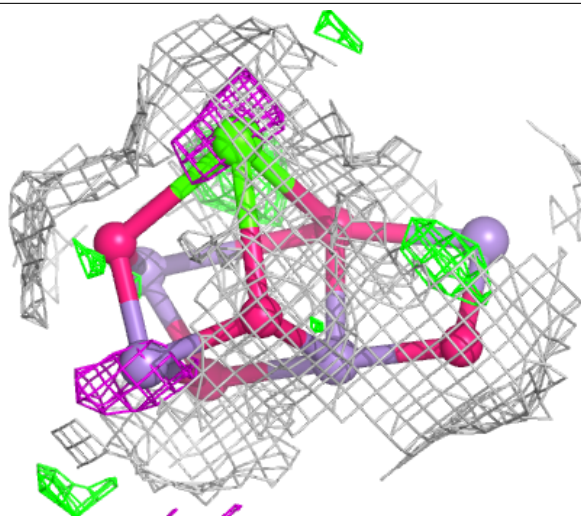
**Electron density around HEC v 201:**

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



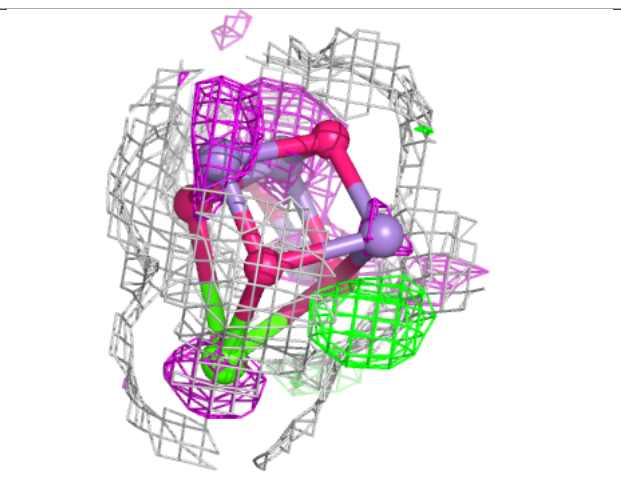
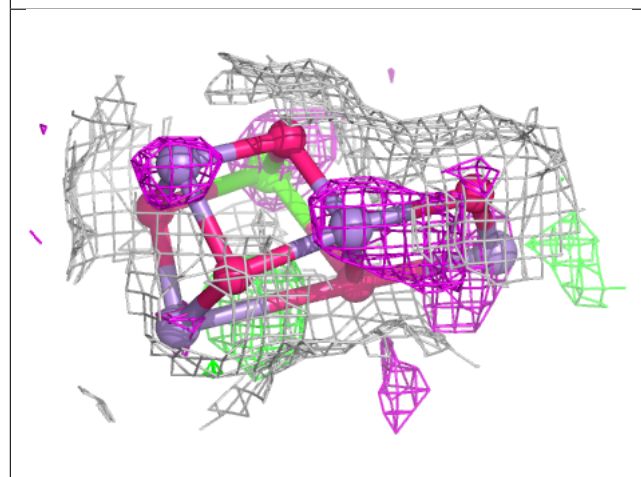
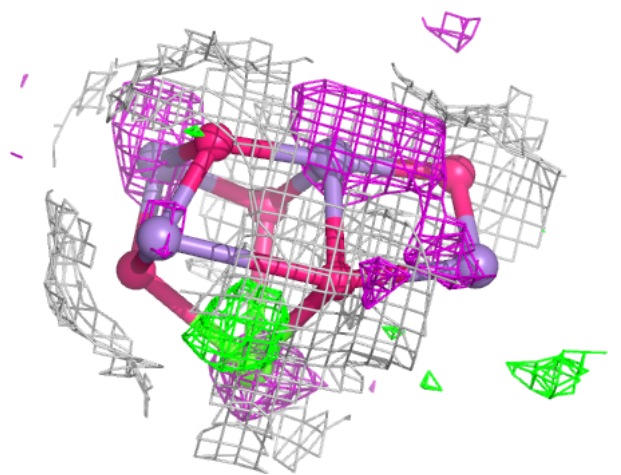
**Electron density around OEX A 418:**

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



**Electron density around OEX a 418:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.