



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2023 – 08:32 PM EDT

PDB ID : 6W1V
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.09 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

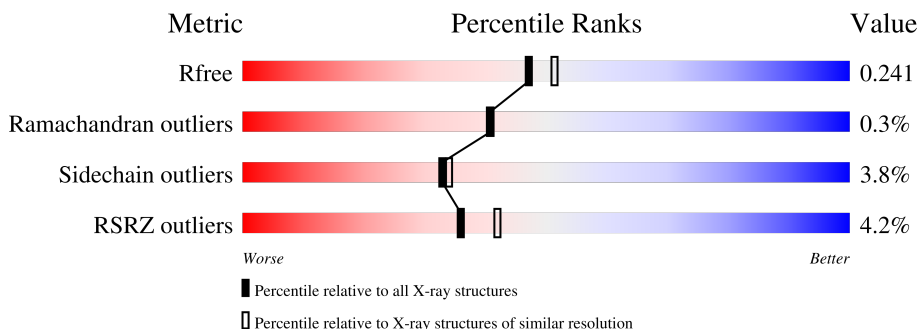
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

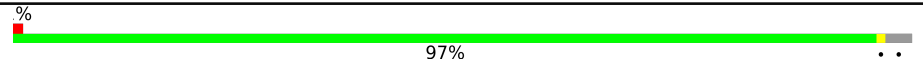
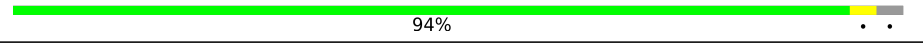
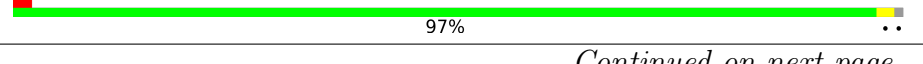
The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 94%
2	B	510	 97%

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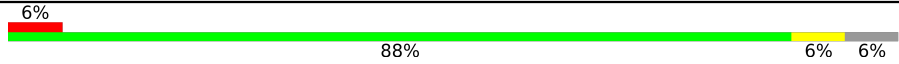
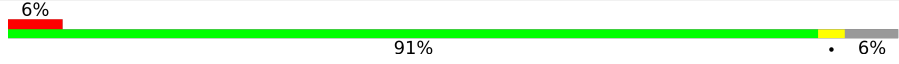
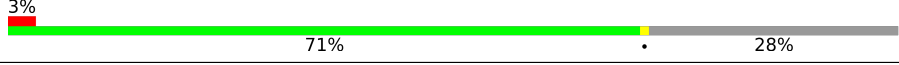



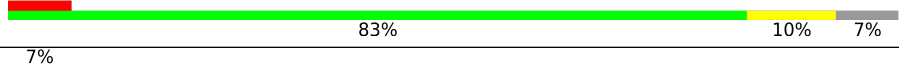
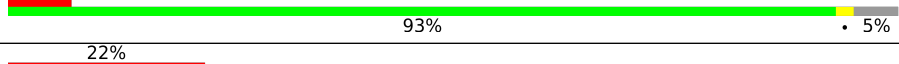



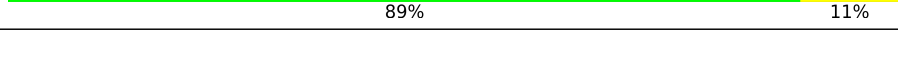
Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
2	b	510	 3% 96%
3	C	461	 % 94%
3	c	461	 2% 93% 5%
4	D	352	 96%
4	d	352	 95%
5	E	84	 2% 95%
5	e	84	 7% 93% 5%
6	F	45	 4% 76% 24%
6	f	45	 4% 73% 24%
7	H	66	 3% 91% 8%
7	h	66	 8% 89% 6% 5%
8	I	38	 5% 87% 8% 5%
8	i	38	 5% 89% 5% 5%
9	J	40	 10% 90% 10%
9	j	40	 10% 88% 10%
10	K	46	 2% 72% 9% 20%
10	k	46	 2% 76% 20%
11	L	37	 3% 100%
11	l	37	 5% 86% 11%
12	M	36	 86% 6% 8%
12	m	36	 78% 11% 11%
13	O	272	 4% 83% 6% 10%
13	o	272	 6% 85% 10%
14	R	41	 56% 78% 5% 17%
14	r	41	 66% 68% 7% 24%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	B	702	X	-	-	-
22	CLA	B	703	X	-	-	-
22	CLA	B	704	X	-	-	-
22	CLA	B	705	X	-	-	-
22	CLA	B	706	X	-	-	-
22	CLA	B	707	X	-	-	-
22	CLA	B	708	X	-	-	-
22	CLA	B	710	X	-	-	-
22	CLA	B	712	X	-	-	-
22	CLA	B	713	X	-	-	-
22	CLA	B	714	X	-	-	-
22	CLA	B	715	X	-	-	-
22	CLA	B	716	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	H	102	X	-	-	-
22	CLA	a	401	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	b	701	X	-	-	-
22	CLA	b	703	X	-	-	-
22	CLA	b	704	X	-	-	-
22	CLA	b	705	X	-	-	-
22	CLA	b	706	X	-	-	-
22	CLA	b	707	X	-	-	-
22	CLA	b	708	X	-	-	-
22	CLA	b	709	X	-	-	-
22	CLA	b	710	X	-	-	-
22	CLA	b	711	X	-	-	-
22	CLA	b	712	X	-	-	-
22	CLA	b	713	X	-	-	-
22	CLA	b	714	X	-	-	-
22	CLA	b	715	X	-	-	-
22	CLA	b	716	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 106211 atoms, of which 52744 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	6084	2030	2971	513	551	19	0	66	0
1	a	334	6072	2027	2962	513	551	19	0	66	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	442	6928	2302	3419	586	607	14	0	14	0
3	c	451	7073	2343	3490	602	624	14	0	14	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	5360	1809	2629	446	464	12	0	2	0
4	d	341	5372	1813	2635	446	466	12	0	3	0

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			490	162	250	42	36			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

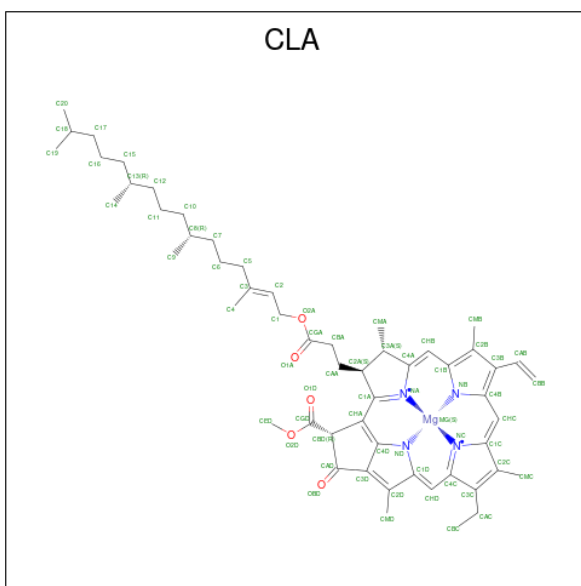
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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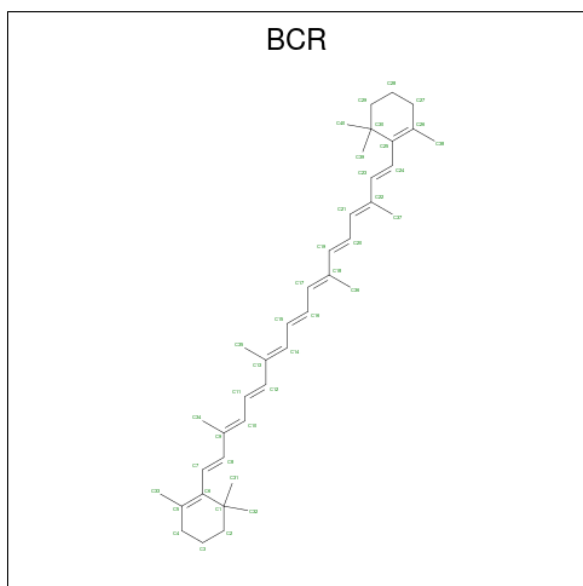
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	1	Total	C H	0	0
			96	40 56		
23	B	1	Total	C H	0	0
			96	40 56		
23	B	1	Total	C H	0	0
			96	40 56		
23	B	1	Total	C H	0	0
			96	40 56		
23	C	1	Total	C H	0	0
			96	40 56		

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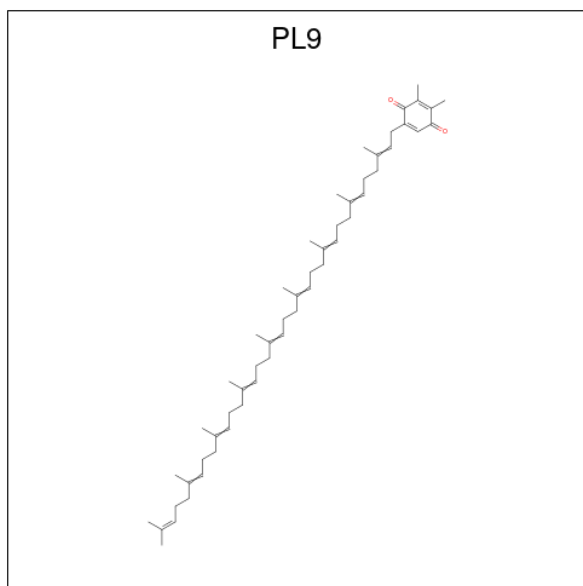
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total 96	C 40	H 56	0	0
23	D	1	Total 96	C 40	H 56	0	0
23	H	1	Total 96	C 40	H 56	0	0
23	K	1	Total 96	C 40	H 56	0	0
23	T	1	Total 96	C 40	H 56	0	0
23	Y	1	Total 96	C 40	H 56	0	0
23	a	1	Total 96	C 40	H 56	0	0
23	b	1	Total 96	C 40	H 56	0	0
23	b	1	Total 96	C 40	H 56	0	0
23	b	1	Total 96	C 40	H 56	0	0
23	c	1	Total 96	C 40	H 56	0	0
23	c	1	Total 96	C 40	H 56	0	0
23	d	1	Total 96	C 40	H 56	0	0
23	h	1	Total 96	C 40	H 56	0	0
23	k	1	Total 96	C 40	H 56	0	0
23	k	1	Total 96	C 40	H 56	0	0
23	t	1	Total 96	C 40	H 56	0	0

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

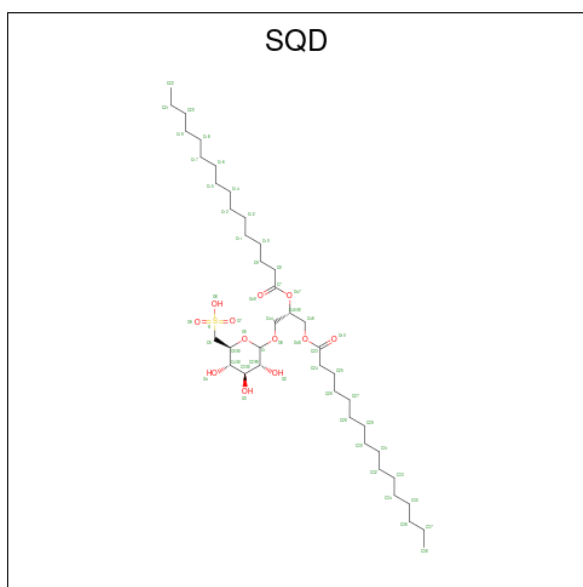
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total 2	Cl 2	0	0
24	a	2	Total 2	Cl 2	0	0

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



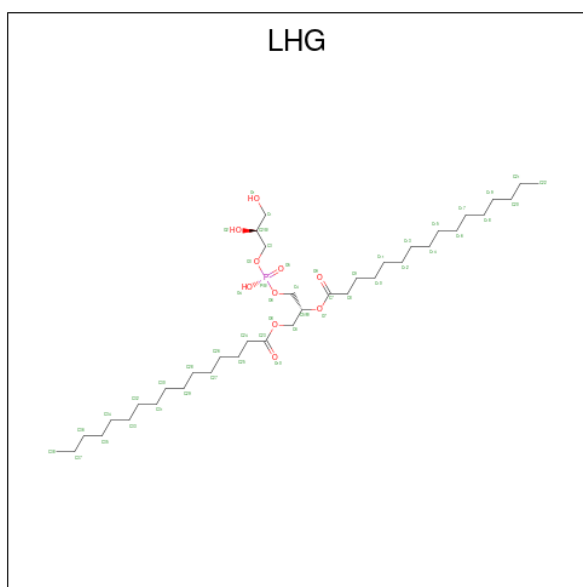
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
25	A	1	135	53	80	2	0	0
25	D	1	135	53	80	2	0	0
25	a	1	135	53	80	2	0	0
25	d	1	135	53	80	2	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



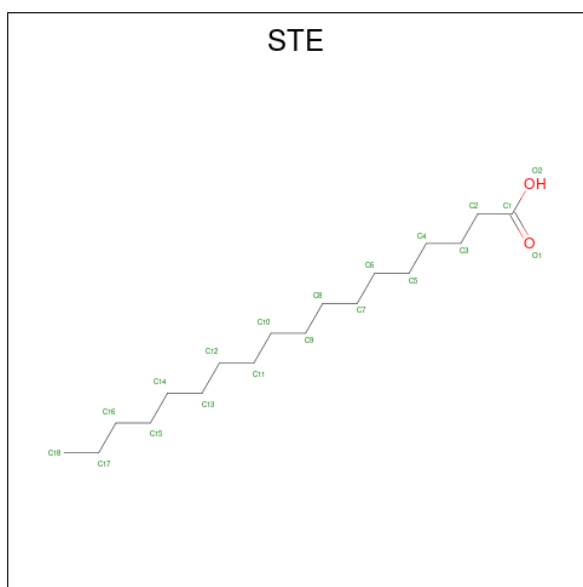
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
26	A	1	123	39	71	12	1	0	0
26	A	1	104	35	65	4		0	0
26	B	1	132	41	78	12	1	0	0
26	D	1	82	25	46	10	1	0	0
26	a	1	131	41	77	12	1	0	0
26	a	1	92	31	56	5		0	0
26	b	1	114	36	65	12	1	0	0
26	f	1	89	28	48	12	1	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 28 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H 47 16 31	0	0
28	A	1	Total C H 11 5 6	0	0
28	B	1	Total C H O 28 10 16 2	0	0
28	B	1	Total C H O 43 15 26 2	0	0
28	B	1	Total C H O 28 10 16 2	0	0
28	B	1	Total C H O 46 16 28 2	0	0
28	B	1	Total C H 47 16 31	0	0
28	C	1	Total C H O 28 10 16 2	0	0
28	C	1	Total C H 47 16 31	0	0
28	C	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H 17 7 10	0	0
28	H	1	Total C H 53 18 35	0	0
28	H	1	Total C H 20 8 12	0	0

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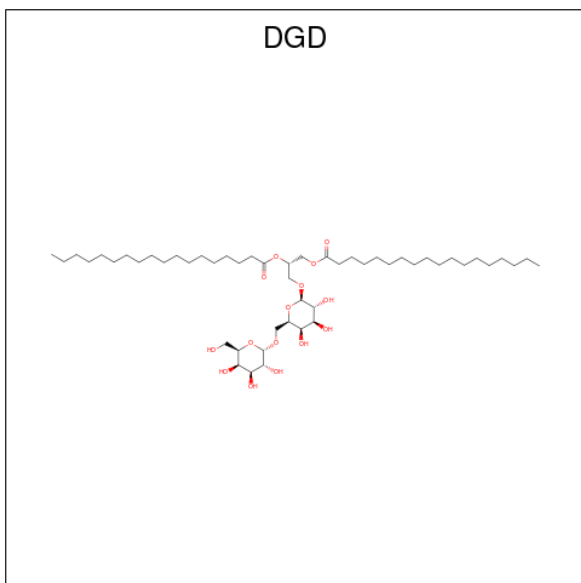
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	I	1	Total C H 41 15 26	0	0
28	J	1	Total C H O 28 10 16 2	0	0
28	M	1	Total C H O 37 13 22 2	0	0
28	M	1	Total C H 26 10 16	0	0
28	T	1	Total C H 44 15 29	0	0
28	X	1	Total C H O 55 18 35 2	0	0
28	Z	1	Total C H 20 8 12	0	0
28	a	1	Total C H 26 10 16	0	0
28	a	1	Total C H O 28 10 16 2	0	0
28	a	1	Total C H 41 15 26	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	b	1	Total C H O 40 14 24 2	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	b	1	Total C H 26 10 16	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	c	1	Total C H O 28 10 16 2	0	0
28	c	1	Total C H O 55 18 35 2	0	0
28	d	1	Total C H O 43 15 26 2	0	0
28	h	1	Total C H 41 14 27	0	0
28	j	1	Total C H O 28 10 16 2	0	0
28	l	1	Total C H 53 18 35	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	m	1	Total	C	H	O	0	0
			28	10	16	2		
28	t	1	Total	C	H	O	0	0
			34	12	20	2		
28	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



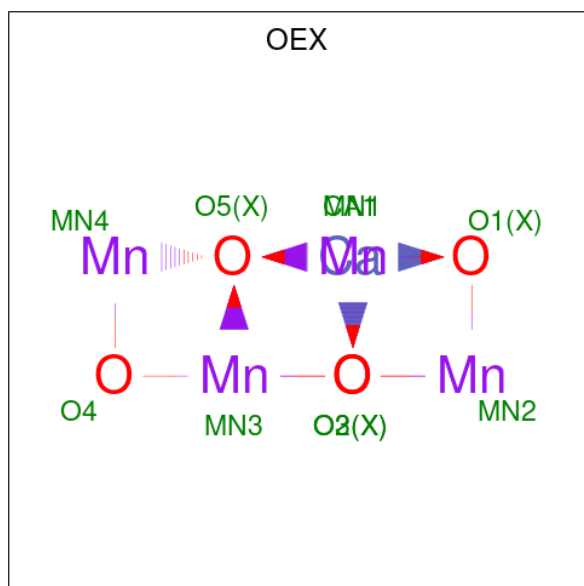
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			142	47	80	15		

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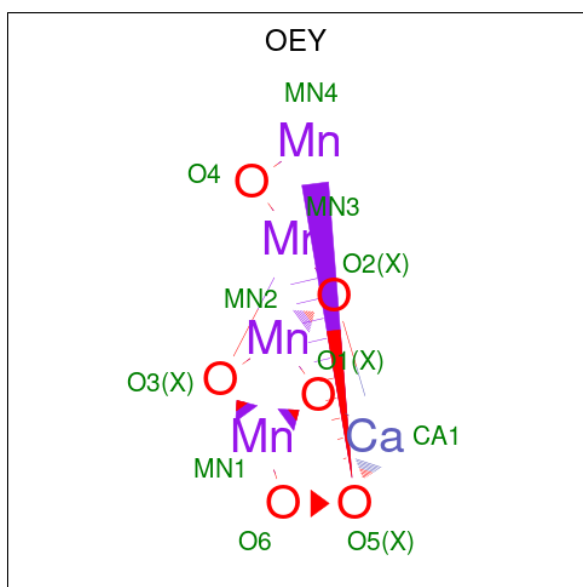
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
29	h	1	142	47	80	15	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



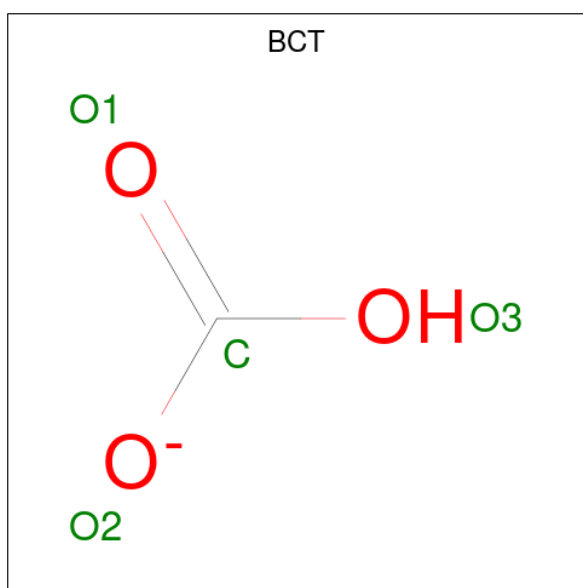
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
30	A	1	10	1	4	5	0	1
30	a	1	10	1	4	5	0	1

- Molecule 31 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



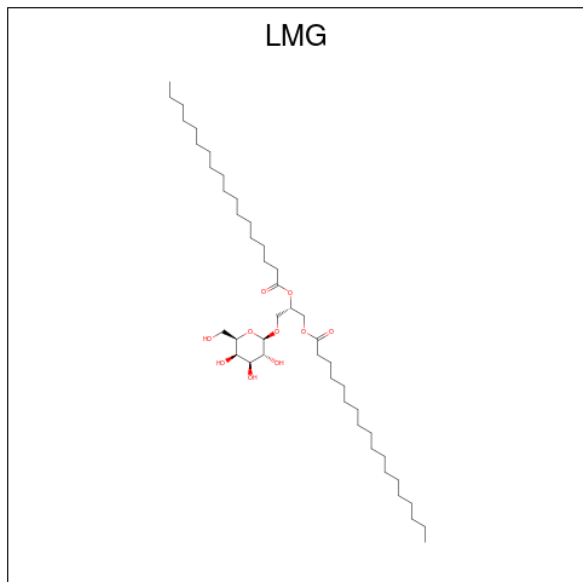
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
31	A	1	11	1	4	6	0	1
31	a	1	11	1	4	6	0	1

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



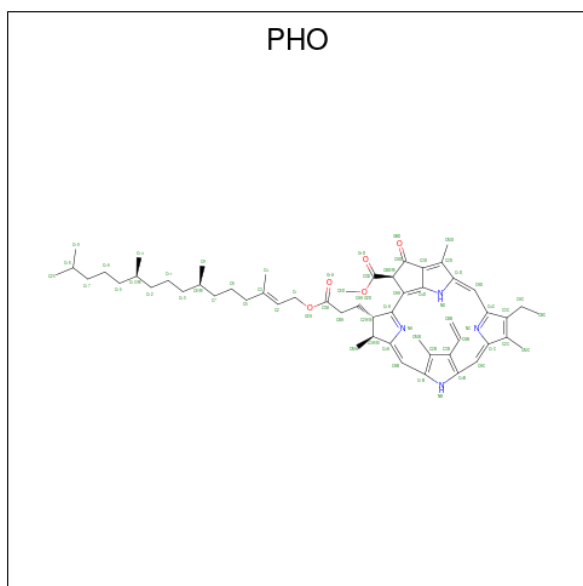
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
33	B	1	Total 68	C 24	H 40	O 4	0	0
33	C	1	Total 114	C 38	H 66	O 10	0	0
33	C	1	Total 114	C 38	H 66	O 10	0	0
33	D	1	Total 123	C 41	H 72	O 10	0	0
33	D	1	Total 77	C 27	H 45	O 5	0	0
33	M	1	Total 123	C 41	H 72	O 10	0	0
33	a	1	Total 141	C 45	H 86	O 10	0	0
33	b	1	Total 123	C 41	H 72	O 10	0	0
33	b	1	Total 141	C 45	H 86	O 10	0	0
33	c	1	Total 81	C 27	H 44	O 10	0	0
33	c	1	Total 117	C 38	H 69	O 10	0	0
33	c	1	Total 117	C 39	H 68	O 10	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	J	15	Total O 15 15	0	0
36	K	3	Total O 3 3	0	0
36	L	9	Total O 9 9	0	0
36	M	8	Total O 8 8	0	0
36	O	106	Total O 106 106	0	0
36	R	3	Total O 3 3	0	0
36	T	9	Total O 9 9	0	0
36	U	53	Total O 53 53	0	0
36	V	63	Total O 63 63	0	0
36	X	17	Total O 17 17	0	0
36	Y	3	Total O 3 3	0	0
36	a	130	Total O 130 130	0	8
36	b	193	Total O 193 193	0	0
36	c	169	Total O 169 169	0	0
36	d	106	Total O 106 106	0	0
36	e	23	Total O 23 23	0	0
36	f	4	Total O 4 4	0	0
36	h	22	Total O 22 22	0	0
36	i	17	Total O 17 17	0	0
36	j	7	Total O 7 7	0	0
36	k	4	Total O 4 4	0	0

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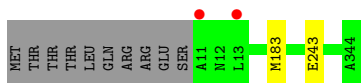
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	l	12	Total O 12 12	0	0
36	m	5	Total O 5 5	0	0
36	o	97	Total O 97 97	0	0
36	r	8	Total O 8 8	0	0
36	t	7	Total O 7 7	0	0
36	u	63	Total O 63 63	0	0
36	v	64	Total O 64 64	0	0
36	x	7	Total O 7 7	0	0
36	y	8	Total O 8 8	0	0
36	z	8	Total O 8 8	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1



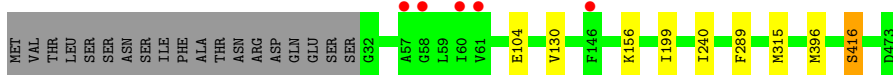
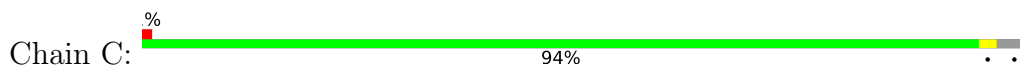
- Molecule 2: Photosystem II CP47 reaction center protein



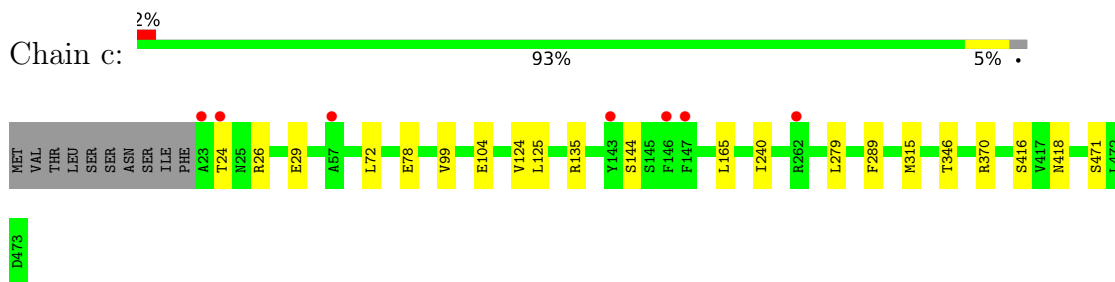
- Molecule 2: Photosystem II CP47 reaction center protein



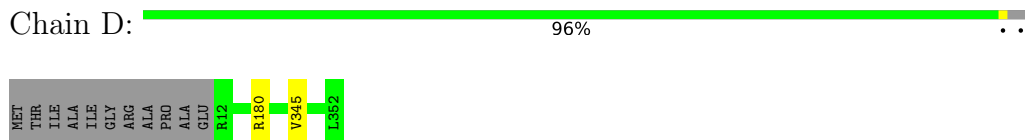
- Molecule 3: Photosystem II CP43 reaction center protein



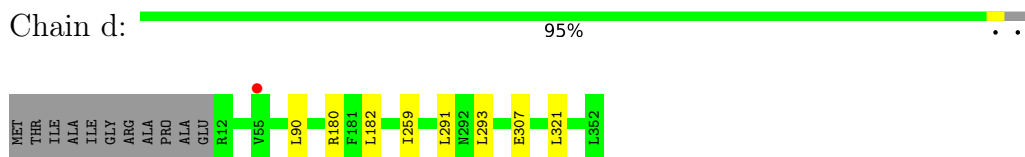
- Molecule 3: Photosystem II CP43 reaction center protein



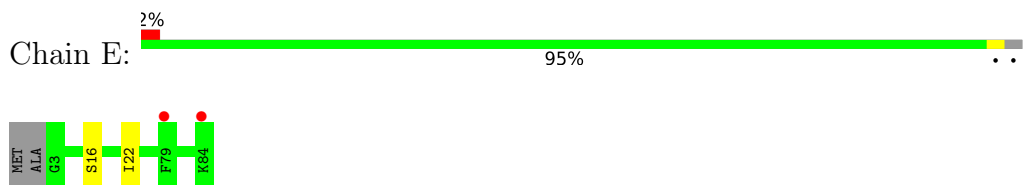
• Molecule 4: Photosystem II D2 protein



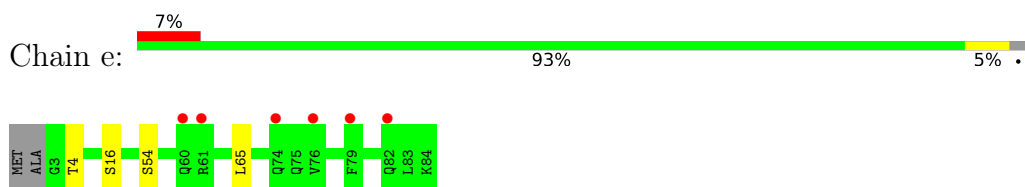
• Molecule 4: Photosystem II D2 protein



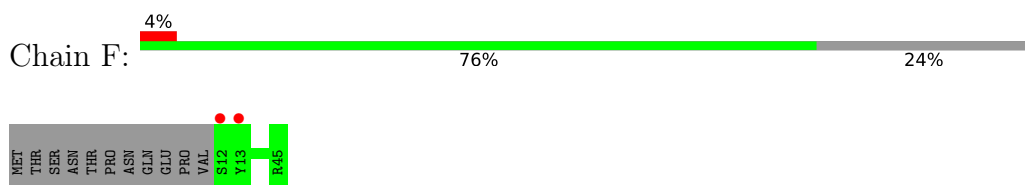
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

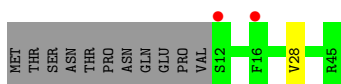


• Molecule 6: Cytochrome b559 subunit beta

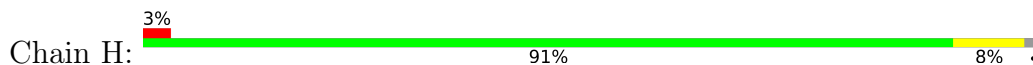


• Molecule 6: Cytochrome b559 subunit beta

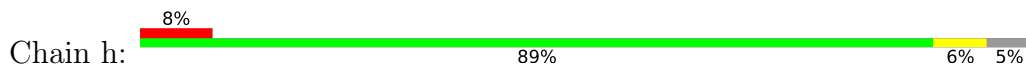




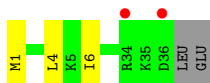
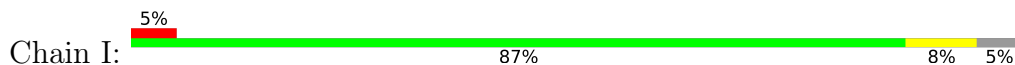
- Molecule 7: Photosystem II reaction center protein H



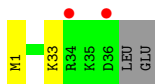
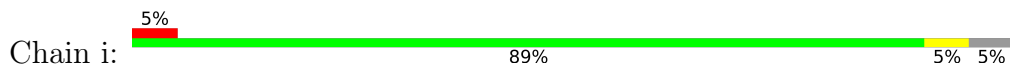
- Molecule 7: Photosystem II reaction center protein H



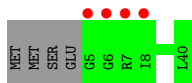
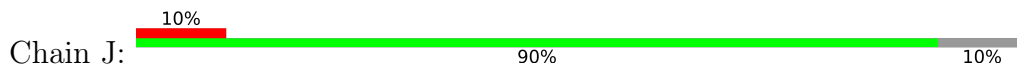
- Molecule 8: Photosystem II reaction center protein I



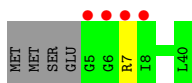
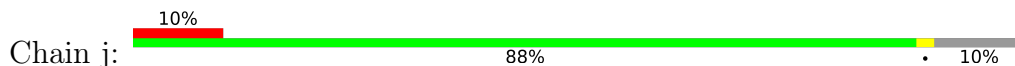
- Molecule 8: Photosystem II reaction center protein I



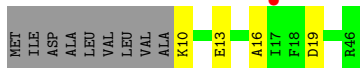
- Molecule 9: Photosystem II reaction center protein J



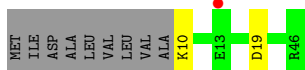
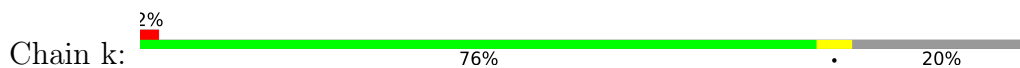
- Molecule 9: Photosystem II reaction center protein J



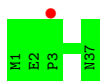
- Molecule 10: Photosystem II reaction center protein K



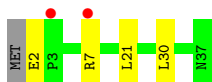
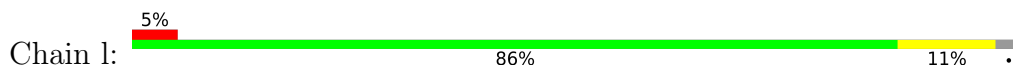
- Molecule 10: Photosystem II reaction center protein K



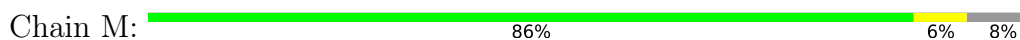
- Molecule 11: Photosystem II reaction center protein L



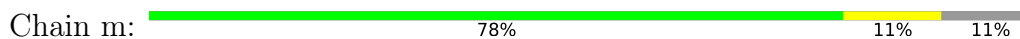
- Molecule 11: Photosystem II reaction center protein L



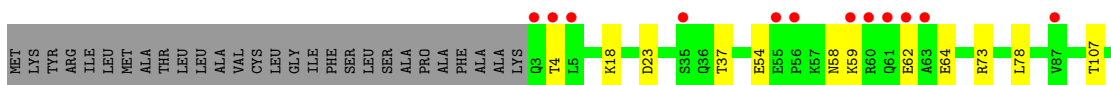
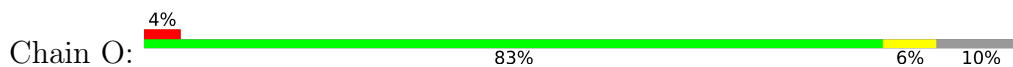
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

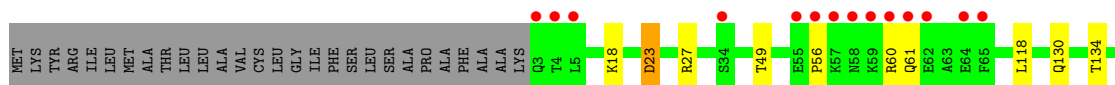
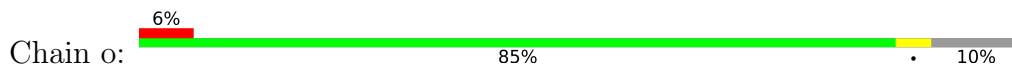


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

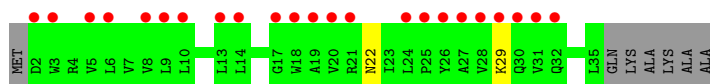
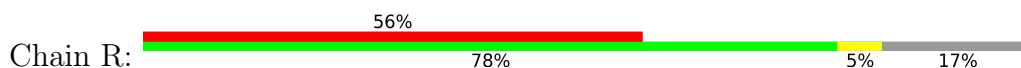




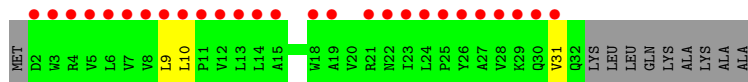
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



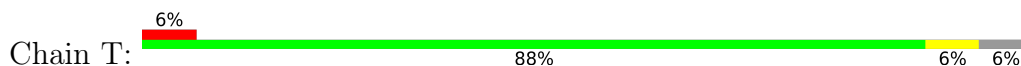
- Molecule 14: Photosystem II protein Y



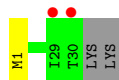
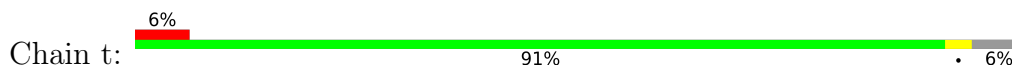
- Molecule 14: Photosystem II protein Y



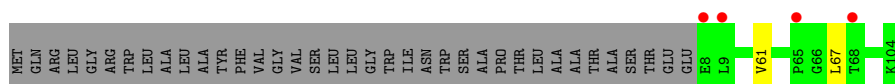
- Molecule 15: Photosystem II reaction center protein T

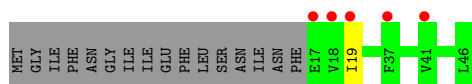


- Molecule 15: Photosystem II reaction center protein T

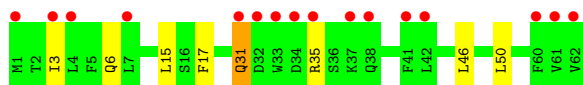
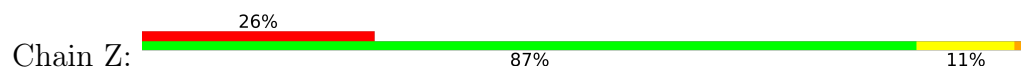


- Molecule 16: Photosystem II 12 kDa extrinsic protein

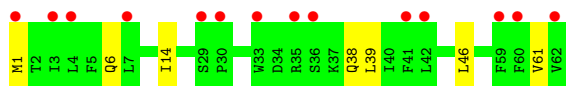
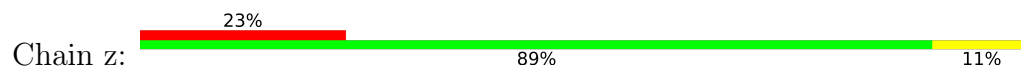




- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.65-2.09) 84.9 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.182 , 0.241 0.182 , 0.241	Depositor DCC
R_{free} test set	4165 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtrriage
Anisotropy	0.198	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	106211	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DGD, STE, OEY, LMG, FME, BCT, HEC, FE2, OEX, CLA, SQD, CL, PL9, BCR, LHG, PHO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/3227	0.68	2/4397 (0.0%)
1	a	0.62	0/3224	0.68	0/4393
2	B	0.64	0/4161	0.71	1/5669 (0.0%)
2	b	0.64	0/4118	0.68	0/5611
3	C	0.64	0/3647	0.67	1/4965 (0.0%)
3	c	0.60	0/3719	0.68	1/5061 (0.0%)
4	D	0.67	0/2825	0.70	0/3847
4	d	0.65	0/2834	0.71	0/3859
5	E	0.53	0/688	0.58	0/940
5	e	0.49	0/683	0.55	0/932
6	F	0.51	0/284	0.51	0/387
6	f	0.48	0/284	0.62	0/387
7	H	0.65	0/523	0.68	0/713
7	h	0.58	0/511	0.67	0/697
8	I	0.60	0/293	0.61	0/396
8	i	0.68	0/293	0.61	0/396
9	J	0.54	0/263	0.61	0/356
9	j	0.56	0/263	0.59	0/356
10	K	0.55	0/303	0.60	0/416
10	k	0.53	0/303	0.65	0/416
11	L	0.64	0/311	0.72	0/422
11	l	0.68	0/303	0.74	0/412
12	M	0.65	0/249	0.67	0/341
12	m	0.70	0/244	0.67	0/334
13	O	0.61	0/1904	0.73	1/2585 (0.0%)
13	o	0.61	0/1905	0.73	1/2583 (0.0%)
14	R	0.44	0/277	0.60	0/380
14	r	0.41	0/246	0.60	0/339
15	T	0.75	0/257	0.72	0/349
15	t	0.71	0/255	0.64	0/346
16	U	0.58	0/785	0.68	0/1064
16	u	0.62	0/785	0.74	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.60	0/1085	0.73	1/1473 (0.1%)
17	v	0.58	0/1085	0.67	0/1473
18	X	0.50	0/284	0.60	0/384
18	x	0.41	0/289	0.55	0/391
19	Y	0.43	0/197	0.56	0/264
19	y	0.38	0/219	0.55	0/294
20	Z	0.49	0/490	0.62	0/669
20	z	0.40	0/488	0.51	0/666
All	All	0.61	0/44104	0.68	8/60027 (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
17	V	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-7.20	104.76	120.60
2	B	15	ASP	CB-CG-OD2	-6.76	112.21	118.30
3	C	396	MET	CG-SD-CE	-5.43	91.51	100.20
1	A	183[A]	MET	CA-CB-CG	5.29	122.29	113.30
1	A	183[B]	MET	CA-CB-CG	5.29	122.29	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	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	397/344 (115%)	387 (98%)	10 (2%)	0	100	100
1	a	397/344 (115%)	387 (98%)	9 (2%)	1 (0%)	41	41
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	11 (2%)	1 (0%)	47	49
3	C	454/461 (98%)	440 (97%)	13 (3%)	1 (0%)	47	49
3	c	463/461 (100%)	447 (96%)	15 (3%)	1 (0%)	47	49
4	D	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	9	5
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%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	4	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	11 (4%)	4 (2%)	9	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	228 (94%)	12 (5%)	2 (1%)	19	15
14	R	32/41 (78%)	27 (84%)	5 (16%)	0	100	100
14	r	29/41 (71%)	27 (93%)	1 (3%)	1 (3%)	3	1
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	14	9
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	18
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	4
20	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	9	4
All	All	5396/5700 (95%)	5212 (97%)	166 (3%)	18 (0%)	41	41

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	59	LYS
17	V	64	PRO
14	r	31	VAL

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	324/280 (116%)	323 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	323/280 (115%)	311 (96%)	12 (4%)	34	35
2	B	408/407 (100%)	398 (98%)	10 (2%)	47	52
2	b	402/407 (99%)	387 (96%)	15 (4%)	34	35
3	C	356/362 (98%)	348 (98%)	8 (2%)	52	57
3	c	364/362 (101%)	345 (95%)	19 (5%)	23	21
4	D	277/283 (98%)	275 (99%)	2 (1%)	84	88
4	d	278/283 (98%)	270 (97%)	8 (3%)	42	46
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	30
5	e	71/73 (97%)	67 (94%)	4 (6%)	21	18
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	36
7	H	54/55 (98%)	50 (93%)	4 (7%)	13	10
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	10
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	15
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	43
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	30
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
10	k	30/37 (81%)	28 (93%)	2 (7%)	16	13
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	36
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	3
13	O	206/228 (90%)	194 (94%)	12 (6%)	20	17
13	o	207/228 (91%)	197 (95%)	10 (5%)	25	24
14	R	28/33 (85%)	26 (93%)	2 (7%)	14	11
14	r	23/33 (70%)	21 (91%)	2 (9%)	10	7
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	34
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	82 (98%)	2 (2%)	49	53
16	u	84/112 (75%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/138 (85%)	115 (98%)	2 (2%)	60	67
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	50
18	X	31/34 (91%)	27 (87%)	4 (13%)	4	2
18	x	31/34 (91%)	30 (97%)	1 (3%)	39	41
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2	1
19	y	22/37 (60%)	21 (96%)	1 (4%)	27	27
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
All	All	4458/4654 (96%)	4293 (96%)	165 (4%)	33	35

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	180	ARG
13	o	23	ASP
4	d	293	LEU
7	h	49	TYR
13	o	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
16	u	78	ASN
13	o	200	ASN
1	a	19	ASN
13	o	61	GLN
20	Z	31	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	1.11	1 (12%)	7,9,11	0.99	0
8	FME	I	1	8	8,9,10	1.01	1 (12%)	7,9,11	0.91	0
8	FME	i	1	8	8,9,10	1.09	1 (12%)	7,9,11	1.96	3 (42%)
12	FME	m	1	12	8,9,10	1.17	1 (12%)	7,9,11	1.47	2 (28%)
15	FME	T	1	15	8,9,10	1.17	1 (12%)	7,9,11	1.25	1 (14%)
15	FME	t	1	15	8,9,10	1.45	1 (12%)	7,9,11	0.60	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	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.92	1.42	1.46
12	m	1	FME	CA-N	-2.67	1.42	1.46
8	i	1	FME	CA-N	-2.37	1.43	1.46
15	T	1	FME	CB-CA	2.36	1.57	1.53
12	M	1	FME	CA-N	-2.29	1.43	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.44	117.53	122.82
8	i	1	FME	C-CA-N	2.52	114.27	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O1-CN-N	-2.25	119.35	125.27
12	m	1	FME	CA-N-CN	-2.22	119.40	122.82
12	m	1	FME	C-CA-N	-2.12	105.91	109.73

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

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 194 ligands modelled in this entry, 6 are monoatomic - leaving 188 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	503	-	65,73,73	1.53	11 (16%)	76,113,113	1.53	11 (14%)
33	LMG	D	408	-	51,51,55	1.00	4 (7%)	59,59,63	1.27	6 (10%)
34	PHO	a	405	-	51,69,69	1.04	3 (5%)	47,99,99	1.28	6 (12%)
22	CLA	B	713	-	65,73,73	1.52	10 (15%)	76,113,113	1.50	12 (15%)
22	CLA	H	102	36	65,73,73	1.99	11 (16%)	76,113,113	1.62	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	403	-	65,73,73	1.62	8 (12%)	76,113,113	1.60	13 (17%)
22	CLA	b	707	36	65,73,73	1.78	12 (18%)	76,113,113	1.37	11 (14%)
22	CLA	c	513	-	65,73,73	1.49	9 (13%)	76,113,113	1.45	10 (13%)
30	OEX	a	420[A]	3,36,1	0,15,15	-	-	-		
33	LMG	C	516	-	48,48,55	0.96	3 (6%)	56,56,63	1.36	6 (10%)
31	OEY	a	421[B]	3,36,1	0,16,16	-	-	-		
22	CLA	d	401	-	65,73,73	1.35	8 (12%)	76,113,113	1.41	9 (11%)
33	LMG	B	721	-	26,26,55	0.75	0	26,26,63	1.33	2 (7%)
22	CLA	B	704	-	65,73,73	1.48	6 (9%)	76,113,113	1.84	13 (17%)
28	STE	B	726	-	15,15,19	0.47	0	14,14,19	0.65	0
27	LHG	a	414	-	41,41,48	0.79	1 (2%)	44,47,54	1.23	3 (6%)
29	DGD	c	517	-	63,63,67	1.17	6 (9%)	77,77,81	1.35	10 (12%)
22	CLA	c	506	-	65,73,73	1.44	8 (12%)	76,113,113	1.37	10 (13%)
23	BCR	B	717	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	6 (10%)
22	CLA	b	712	-	65,73,73	1.41	9 (13%)	76,113,113	1.49	10 (13%)
23	BCR	a	407	-	41,41,41	1.10	4 (9%)	56,56,56	1.43	14 (25%)
27	LHG	D	410	-	48,48,48	0.91	3 (6%)	51,54,54	1.21	5 (9%)
23	BCR	d	403	-	41,41,41	1.04	2 (4%)	56,56,56	1.28	8 (14%)
27	LHG	L	101	-	48,48,48	0.83	2 (4%)	51,54,54	1.24	4 (7%)
32	BCT	A	417	21	2,3,3	1.05	0	2,3,3	3.83	2 (100%)
22	CLA	C	512	3	65,73,73	1.64	10 (15%)	76,113,113	1.34	8 (10%)
28	STE	B	701	-	11,11,19	0.97	0	11,11,19	1.05	1 (9%)
29	DGD	C	517	-	63,63,67	1.09	4 (6%)	77,77,81	1.31	11 (14%)
30	OEX	A	415[A]	3,36,1	0,15,15	-	-	-		
23	BCR	A	405	-	41,41,41	1.13	3 (7%)	56,56,56	1.40	8 (14%)
23	BCR	C	515	-	41,41,41	1.23	3 (7%)	56,56,56	1.36	8 (14%)
23	BCR	b	718	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	6 (10%)
28	STE	A	411	-	15,15,19	0.49	0	14,14,19	0.70	0
28	STE	h	703	-	13,13,19	0.41	0	12,12,19	0.72	0
23	BCR	Y	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.16	3 (5%)
28	STE	b	722	-	19,19,19	0.62	0	19,19,19	0.89	0
28	STE	B	720	-	16,16,19	0.63	0	16,16,19	1.36	2 (12%)
22	CLA	B	710	36	65,73,73	1.62	9 (13%)	76,113,113	1.49	9 (11%)
28	STE	Z	101	-	7,7,19	0.41	0	6,6,19	0.51	0
29	DGD	C	519	-	63,63,67	0.94	4 (6%)	77,77,81	1.43	13 (16%)
22	CLA	b	706	-	65,73,73	1.71	9 (13%)	76,113,113	1.64	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	c	516	-	41,41,41	1.20	3 (7%)	56,56,56	1.45	10 (17%)
22	CLA	b	703	-	65,73,73	1.58	10 (15%)	76,113,113	1.62	13 (17%)
22	CLA	A	402	-	65,73,73	1.41	8 (12%)	76,113,113	1.40	8 (10%)
22	CLA	a	404	36	65,73,73	1.63	7 (10%)	76,113,113	1.54	11 (14%)
22	CLA	B	702	-	65,73,73	1.65	7 (10%)	76,113,113	1.57	12 (15%)
22	CLA	c	504	-	65,73,73	1.52	10 (15%)	76,113,113	1.63	8 (10%)
22	CLA	B	705	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	12 (15%)
25	PL9	d	404	-	55,55,55	1.44	7 (12%)	68,69,69	1.78	15 (22%)
34	PHO	D	407	-	51,69,69	1.15	7 (13%)	47,99,99	1.47	8 (17%)
29	DGD	c	518	-	63,63,67	1.26	9 (14%)	77,77,81	1.43	11 (14%)
26	SQD	b	720	-	48,49,54	1.00	2 (4%)	57,60,65	2.16	14 (24%)
25	PL9	A	408	-	55,55,55	1.16	3 (5%)	68,69,69	1.59	17 (25%)
28	STE	E	101	-	11,11,19	0.93	0	11,11,19	0.85	0
22	CLA	C	508	36	65,73,73	1.47	7 (10%)	76,113,113	1.63	11 (14%)
28	STE	E	102	-	6,6,19	0.40	0	5,5,19	0.54	0
28	STE	I	101	-	14,14,19	0.61	0	13,13,19	0.35	0
27	LHG	d	407	-	38,38,48	0.88	3 (7%)	41,44,54	1.08	2 (4%)
28	STE	t	702	-	13,13,19	0.61	0	13,13,19	1.25	2 (15%)
22	CLA	b	705	-	65,73,73	1.60	8 (12%)	76,113,113	1.59	11 (14%)
23	BCR	t	701	-	41,41,41	1.08	3 (7%)	56,56,56	1.39	6 (10%)
28	STE	X	101	-	19,19,19	0.54	0	19,19,19	1.28	2 (10%)
22	CLA	c	508	36	65,73,73	1.47	7 (10%)	76,113,113	1.41	13 (17%)
28	STE	l	102	-	17,17,19	0.46	0	16,16,19	0.69	0
33	LMG	D	412	-	31,31,55	1.18	3 (9%)	33,33,63	1.08	2 (6%)
33	LMG	b	723	-	55,55,55	1.09	5 (9%)	63,63,63	1.46	10 (15%)
22	CLA	B	708	-	65,73,73	1.46	13 (20%)	76,113,113	1.77	14 (18%)
22	CLA	b	702	-	65,73,73	1.48	9 (13%)	76,113,113	1.63	13 (17%)
23	BCR	D	404	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	5 (8%)
27	LHG	d	406	-	48,48,48	0.76	1 (2%)	51,54,54	1.10	4 (7%)
29	DGD	A	413	-	67,67,67	1.21	9 (13%)	81,81,81	1.55	15 (18%)
28	STE	c	521	-	19,19,19	0.68	0	19,19,19	0.99	1 (5%)
31	OEY	A	416[B]	3,36,1	0,16,16	-	-	-	-	-
33	LMG	b	721	-	51,51,55	0.96	4 (7%)	59,59,63	1.44	7 (11%)
28	STE	C	523	-	11,11,19	0.83	0	11,11,19	1.03	1 (9%)
23	BCR	b	717	-	41,41,41	1.15	4 (9%)	56,56,56	1.51	12 (21%)
23	BCR	k	101	-	41,41,41	1.04	3 (7%)	56,56,56	1.09	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	714	-	65,73,73	1.62	8 (12%)	76,113,113	1.47	10 (13%)
28	STE	j	101	-	11,11,19	0.79	0	11,11,19	1.51	2 (18%)
33	LMG	c	523	-	49,49,55	1.00	2 (4%)	57,57,63	1.30	6 (10%)
22	CLA	B	709	-	65,73,73	1.48	11 (16%)	76,113,113	1.25	9 (11%)
25	PL9	a	411	-	55,55,55	0.87	1 (1%)	68,69,69	1.64	11 (16%)
22	CLA	a	401	36	65,73,73	1.64	7 (10%)	76,113,113	1.67	11 (14%)
27	LHG	a	412	-	48,48,48	0.85	1 (2%)	51,54,54	1.36	5 (9%)
23	BCR	b	719	-	41,41,41	1.07	2 (4%)	56,56,56	1.43	7 (12%)
29	DGD	c	519	-	63,63,67	1.29	9 (14%)	77,77,81	1.40	13 (16%)
23	BCR	B	719	-	41,41,41	1.09	1 (2%)	56,56,56	1.47	8 (14%)
22	CLA	b	709	-	65,73,73	1.66	8 (12%)	76,113,113	1.49	9 (11%)
22	CLA	c	514	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	10 (13%)
33	LMG	d	408	-	44,44,55	1.13	6 (13%)	52,52,63	1.45	8 (15%)
22	CLA	d	402	-	65,73,73	1.57	10 (15%)	76,113,113	1.31	9 (11%)
22	CLA	c	512	3	65,73,73	1.80	10 (15%)	76,113,113	1.60	7 (9%)
28	STE	d	409	-	16,16,19	0.72	0	16,16,19	1.33	2 (12%)
22	CLA	C	506	-	65,73,73	1.40	6 (9%)	76,113,113	1.35	9 (11%)
22	CLA	C	513	-	65,73,73	1.82	11 (16%)	76,113,113	1.52	13 (17%)
22	CLA	C	502	-	65,73,73	1.58	13 (20%)	76,113,113	1.44	10 (13%)
25	PL9	D	405	-	55,55,55	1.37	7 (12%)	68,69,69	1.80	14 (20%)
22	CLA	A	403	36	65,73,73	1.56	7 (10%)	76,113,113	1.39	10 (13%)
22	CLA	b	713	-	65,73,73	1.53	10 (15%)	76,113,113	1.68	13 (17%)
26	SQD	A	409	-	51,52,54	1.01	4 (7%)	60,63,65	2.08	17 (28%)
22	CLA	B	711	-	65,73,73	1.47	9 (13%)	76,113,113	1.45	10 (13%)
22	CLA	c	510	-	65,73,73	1.56	9 (13%)	76,113,113	1.80	11 (14%)
22	CLA	B	714	-	65,73,73	1.53	9 (13%)	76,113,113	1.21	8 (10%)
28	STE	C	522	-	15,15,19	0.45	0	14,14,19	0.81	0
29	DGD	H	103	-	63,63,67	1.34	9 (14%)	77,77,81	1.48	10 (12%)
23	BCR	C	501	-	41,41,41	1.04	2 (4%)	56,56,56	1.16	4 (7%)
22	CLA	b	708	-	65,73,73	1.59	10 (15%)	76,113,113	1.53	13 (17%)
22	CLA	b	704	-	65,73,73	1.54	7 (10%)	76,113,113	1.79	15 (19%)
34	PHO	d	405	-	51,69,69	1.14	5 (9%)	47,99,99	1.32	7 (14%)
26	SQD	D	409	-	35,36,54	0.98	4 (11%)	42,45,65	2.05	12 (28%)
23	BCR	K	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.45	10 (17%)
22	CLA	B	707	36	65,73,73	1.59	13 (20%)	76,113,113	1.54	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	701	36	65,73,73	1.66	10 (15%)	76,113,113	1.63	10 (13%)
22	CLA	D	403	-	65,73,73	1.42	11 (16%)	76,113,113	1.64	12 (15%)
27	LHG	D	411	-	46,46,48	1.21	5 (10%)	49,52,54	1.24	5 (10%)
22	CLA	D	401	-	65,73,73	1.59	12 (18%)	76,113,113	1.27	8 (10%)
34	PHO	D	406	-	51,69,69	1.07	6 (11%)	47,99,99	1.38	7 (14%)
22	CLA	c	507	-	65,73,73	1.46	12 (18%)	76,113,113	1.51	12 (15%)
28	STE	B	724	-	11,11,19	0.72	0	11,11,19	1.21	1 (9%)
22	CLA	B	715	-	65,73,73	1.93	10 (15%)	76,113,113	1.56	12 (15%)
35	HEC	E	103	5,6	32,50,50	2.19	3 (9%)	24,82,82	2.17	7 (29%)
22	CLA	b	710	36	65,73,73	1.50	11 (16%)	76,113,113	1.37	12 (15%)
33	LMG	C	520	-	48,48,55	1.00	3 (6%)	56,56,63	1.35	8 (14%)
29	DGD	C	518	-	63,63,67	1.35	6 (9%)	77,77,81	1.49	12 (15%)
23	BCR	k	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.19	5 (8%)
28	STE	H	105	-	7,7,19	0.42	0	6,6,19	0.59	0
28	STE	b	726	-	9,9,19	0.53	0	8,8,19	0.43	0
22	CLA	C	507	-	65,73,73	1.51	8 (12%)	76,113,113	1.38	10 (13%)
28	STE	b	727	-	19,19,19	0.50	0	19,19,19	1.21	2 (10%)
28	STE	B	725	-	17,17,19	0.74	0	17,17,19	0.85	0
28	STE	a	418	-	14,14,19	0.45	0	13,13,19	0.71	0
35	HEC	e	101	5,6	32,50,50	2.28	4 (12%)	24,82,82	2.28	5 (20%)
29	DGD	h	702	-	63,63,67	1.22	7 (11%)	77,77,81	1.58	17 (22%)
22	CLA	A	404	-	54,62,73	1.85	9 (16%)	62,99,113	1.76	14 (22%)
23	BCR	h	701	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	5 (8%)
28	STE	J	101	-	11,11,19	0.59	0	11,11,19	1.52	2 (18%)
28	STE	H	104	-	17,17,19	0.50	0	16,16,19	0.58	0
22	CLA	B	706	-	65,73,73	1.57	9 (13%)	76,113,113	1.60	12 (15%)
22	CLA	B	703	-	65,73,73	1.59	12 (18%)	76,113,113	1.32	9 (11%)
22	CLA	C	503	-	65,73,73	1.60	10 (15%)	76,113,113	1.34	8 (10%)
22	CLA	D	402	36	65,73,73	1.59	9 (13%)	76,113,113	1.25	7 (9%)
28	STE	M	103	-	9,9,19	0.47	0	8,8,19	0.64	0
32	BCT	a	410	21	2,3,3	1.34	0	2,3,3	3.23	2 (100%)
33	LMG	c	520	-	37,37,55	1.22	5 (13%)	45,45,63	1.29	4 (8%)
22	CLA	C	505	36	59,67,73	1.52	8 (13%)	68,105,113	1.32	9 (13%)
26	SQD	B	723	-	53,54,54	0.95	2 (3%)	62,65,65	1.70	11 (17%)
22	CLA	c	511	-	65,73,73	1.37	8 (12%)	76,113,113	1.59	12 (15%)
33	LMG	a	419	-	55,55,55	1.31	7 (12%)	63,63,63	1.33	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	M	102	-	14,14,19	0.69	0	14,14,19	1.09	0
28	STE	b	724	-	15,15,19	0.77	0	15,15,19	0.97	1 (6%)
27	LHG	B	722	-	48,48,48	1.05	3 (6%)	51,54,54	1.35	5 (9%)
22	CLA	C	510	-	65,73,73	1.57	12 (18%)	76,113,113	1.53	10 (13%)
33	LMG	c	522	-	48,48,55	1.21	4 (8%)	56,56,63	1.24	8 (14%)
22	CLA	c	505	36	60,68,73	1.66	9 (15%)	70,107,113	1.55	7 (10%)
22	CLA	a	406	-	65,73,73	1.64	10 (15%)	76,113,113	1.35	9 (11%)
26	SQD	a	413	-	53,54,54	0.99	7 (13%)	62,65,65	1.87	12 (19%)
26	SQD	f	101	-	40,41,54	1.13	5 (12%)	49,52,65	1.77	13 (26%)
27	LHG	A	410	-	48,48,48	0.79	2 (4%)	51,54,54	1.21	4 (7%)
35	HEC	V	201	17	32,50,50	2.04	3 (9%)	24,82,82	2.23	6 (25%)
22	CLA	c	509	-	64,72,73	1.48	8 (12%)	74,111,113	1.70	13 (17%)
22	CLA	C	511	-	65,73,73	1.56	8 (12%)	76,113,113	1.38	7 (9%)
22	CLA	c	502	-	65,73,73	1.46	9 (13%)	76,113,113	1.53	8 (10%)
23	BCR	B	718	-	41,41,41	1.11	3 (7%)	56,56,56	1.42	7 (12%)
22	CLA	b	711	-	65,73,73	1.48	7 (10%)	76,113,113	1.63	11 (14%)
22	CLA	C	509	-	65,73,73	1.70	8 (12%)	76,113,113	1.57	7 (9%)
22	CLA	C	504	-	65,73,73	1.94	8 (12%)	76,113,113	1.77	16 (21%)
28	STE	C	521	-	11,11,19	0.86	0	11,11,19	1.39	3 (27%)
22	CLA	B	712	-	65,73,73	1.31	4 (6%)	76,113,113	1.60	15 (19%)
28	STE	A	414	-	4,4,19	0.48	0	3,3,19	0.35	0
23	BCR	c	515	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	7 (12%)
28	STE	m	101	-	11,11,19	0.79	0	11,11,19	1.41	2 (18%)
28	STE	a	417	-	11,11,19	0.87	0	11,11,19	1.02	0
27	LHG	l	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.12	5 (9%)
26	SQD	A	412	-	38,38,54	1.05	3 (7%)	40,40,65	1.12	3 (7%)
28	STE	x	101	-	19,19,19	0.77	0	19,19,19	0.76	1 (5%)
35	HEC	v	201	17	32,50,50	2.22	5 (15%)	24,82,82	1.62	5 (20%)
22	CLA	B	716	-	60,68,73	1.55	10 (16%)	70,107,113	1.71	13 (18%)
26	SQD	a	415	-	35,35,54	1.10	2 (5%)	37,37,65	1.34	4 (10%)
28	STE	T	702	-	14,14,19	0.48	0	13,13,19	0.58	0
23	BCR	T	701	-	41,41,41	1.06	3 (7%)	56,56,56	1.32	7 (12%)
28	STE	b	725	-	19,19,19	0.76	0	19,19,19	0.99	1 (5%)
28	STE	c	501	-	11,11,19	0.76	0	11,11,19	1.10	1 (9%)
22	CLA	b	715	-	65,73,73	1.63	10 (15%)	76,113,113	1.48	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.28	6 (10%)
22	CLA	b	716	-	60,68,73	1.66	11 (18%)	70,107,113	1.60	9 (12%)
28	STE	a	416	-	9,9,19	0.57	0	8,8,19	0.31	0
33	LMG	M	101	-	51,51,55	1.00	3 (5%)	59,59,63	1.41	8 (13%)
22	CLA	C	514	-	65,73,73	1.59	8 (12%)	76,113,113	1.66	12 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	503	-	1/1/20/20	5/37/115/115	-
33	LMG	D	408	-	-	13/46/66/70	0/1/1/1
34	PHO	a	405	-	-	7/37/103/103	0/5/6/6
22	CLA	B	713	-	1/1/20/20	15/37/115/115	-
22	CLA	H	102	36	1/1/20/20	16/37/115/115	-
22	CLA	a	403	-	-	8/37/115/115	-
22	CLA	b	707	36	1/1/20/20	16/37/115/115	-
22	CLA	c	513	-	1/1/20/20	19/37/115/115	-
33	LMG	C	516	-	-	18/43/63/70	0/1/1/1
22	CLA	d	401	-	-	8/37/115/115	-
33	LMG	B	721	-	-	13/22/22/70	-
22	CLA	B	704	-	1/1/20/20	13/37/115/115	-
28	STE	B	726	-	-	5/13/13/17	-
27	LHG	a	414	-	-	20/46/46/53	-
29	DGD	c	517	-	-	22/51/91/95	0/2/2/2
22	CLA	c	506	-	1/1/20/20	12/37/115/115	-
23	BCR	B	717	-	-	8/29/63/63	0/2/2/2
22	CLA	b	712	-	1/1/20/20	6/37/115/115	-
23	BCR	a	407	-	-	3/29/63/63	0/2/2/2
27	LHG	D	410	-	-	18/53/53/53	-
23	BCR	d	403	-	-	10/29/63/63	0/2/2/2
27	LHG	L	101	-	-	20/53/53/53	-
22	CLA	C	512	3	1/1/20/20	6/37/115/115	-
28	STE	B	701	-	-	4/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	C	517	-	-	21/51/91/95	0/2/2/2
23	BCR	A	405	-	-	5/29/63/63	0/2/2/2
23	BCR	C	515	-	-	6/29/63/63	0/2/2/2
23	BCR	b	718	-	-	3/29/63/63	0/2/2/2
28	STE	A	411	-	-	7/13/13/17	-
28	STE	h	703	-	-	6/11/11/17	-
23	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
28	STE	b	722	-	-	10/17/17/17	-
28	STE	B	720	-	-	9/14/14/17	-
22	CLA	B	710	36	1/1/20/20	6/37/115/115	-
28	STE	Z	101	-	-	3/5/5/17	-
29	DGD	C	519	-	-	15/51/91/95	0/2/2/2
22	CLA	b	706	-	1/1/20/20	12/37/115/115	-
23	BCR	c	516	-	-	3/29/63/63	0/2/2/2
22	CLA	b	703	-	1/1/20/20	8/37/115/115	-
22	CLA	A	402	-	1/1/20/20	7/37/115/115	-
22	CLA	a	404	36	-	4/37/115/115	-
22	CLA	c	504	-	1/1/20/20	9/37/115/115	-
22	CLA	B	702	-	1/1/20/20	8/37/115/115	-
22	CLA	B	705	-	1/1/20/20	8/37/115/115	-
25	PL9	d	404	-	-	18/53/73/73	0/1/1/1
34	PHO	D	407	-	-	2/37/103/103	0/5/6/6
29	DGD	c	518	-	-	27/51/91/95	0/2/2/2
26	SQD	b	720	-	-	21/44/64/69	0/1/1/1
25	PL9	A	408	-	-	22/53/73/73	0/1/1/1
28	STE	E	101	-	-	5/9/9/17	-
22	CLA	C	508	36	1/1/20/20	9/37/115/115	-
28	STE	E	102	-	-	1/4/4/17	-
28	STE	I	101	-	-	4/12/12/17	-
27	LHG	d	407	-	-	11/43/43/53	-
28	STE	t	702	-	-	4/11/11/17	-
22	CLA	b	705	-	1/1/20/20	11/37/115/115	-
23	BCR	t	701	-	-	9/29/63/63	0/2/2/2
28	STE	X	101	-	-	9/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	508	36	1/1/20/20	1/37/115/115	-
28	STE	l	102	-	-	5/15/15/17	-
33	LMG	D	412	-	-	14/33/33/70	-
33	LMG	b	723	-	-	21/50/70/70	0/1/1/1
22	CLA	B	708	-	1/1/20/20	3/37/115/115	-
22	CLA	b	702	-	-	8/37/115/115	-
23	BCR	D	404	-	-	10/29/63/63	0/2/2/2
27	LHG	d	406	-	-	14/53/53/53	-
29	DGD	A	413	-	-	27/55/95/95	0/2/2/2
28	STE	c	521	-	-	7/17/17/17	-
33	LMG	b	721	-	-	14/46/66/70	0/1/1/1
28	STE	C	523	-	-	6/9/9/17	-
23	BCR	b	717	-	-	8/29/63/63	0/2/2/2
23	BCR	k	101	-	-	14/29/63/63	0/2/2/2
22	CLA	b	714	-	1/1/20/20	15/37/115/115	-
28	STE	j	101	-	-	2/9/9/17	-
33	LMG	c	523	-	-	20/44/64/70	0/1/1/1
22	CLA	B	709	-	-	4/37/115/115	-
25	PL9	a	411	-	-	20/53/73/73	0/1/1/1
22	CLA	a	401	36	1/1/20/20	6/37/115/115	-
27	LHG	a	412	-	-	25/53/53/53	-
23	BCR	b	719	-	-	5/29/63/63	0/2/2/2
29	DGD	c	519	-	-	18/51/91/95	0/2/2/2
23	BCR	B	719	-	-	1/29/63/63	0/2/2/2
22	CLA	b	709	-	1/1/20/20	12/37/115/115	-
22	CLA	c	514	-	1/1/20/20	9/37/115/115	-
33	LMG	d	408	-	-	12/39/59/70	0/1/1/1
22	CLA	d	402	-	-	7/37/115/115	-
22	CLA	c	512	3	1/1/20/20	12/37/115/115	-
28	STE	d	409	-	-	6/14/14/17	-
22	CLA	C	506	-	1/1/20/20	18/37/115/115	-
22	CLA	C	513	-	1/1/20/20	15/37/115/115	-
22	CLA	C	502	-	1/1/20/20	4/37/115/115	-
25	PL9	D	405	-	-	14/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	403	36	-	10/37/115/115	-
22	CLA	b	713	-	1/1/20/20	5/37/115/115	-
26	SQD	A	409	-	-	22/47/67/69	0/1/1/1
22	CLA	B	711	-	-	8/37/115/115	-
22	CLA	c	510	-	1/1/20/20	11/37/115/115	-
22	CLA	B	714	-	1/1/20/20	12/37/115/115	-
28	STE	C	522	-	-	3/13/13/17	-
29	DGD	H	103	-	-	18/51/91/95	0/2/2/2
23	BCR	C	501	-	-	12/29/63/63	0/2/2/2
22	CLA	b	708	-	1/1/20/20	9/37/115/115	-
22	CLA	b	704	-	1/1/20/20	10/37/115/115	-
34	PHO	d	405	-	-	6/37/103/103	0/5/6/6
26	SQD	D	409	-	-	6/28/48/69	0/1/1/1
23	BCR	K	101	-	-	8/29/63/63	0/2/2/2
22	CLA	B	707	36	1/1/20/20	7/37/115/115	-
22	CLA	b	701	36	1/1/20/20	9/37/115/115	-
22	CLA	D	403	-	-	8/37/115/115	-
27	LHG	D	411	-	-	21/51/51/53	-
22	CLA	D	401	-	1/1/20/20	5/37/115/115	-
34	PHO	D	406	-	-	6/37/103/103	0/5/6/6
22	CLA	c	507	-	1/1/20/20	15/37/115/115	-
28	STE	B	724	-	-	4/9/9/17	-
22	CLA	B	715	-	1/1/20/20	5/37/115/115	-
35	HEC	E	103	5,6	-	2/10/54/54	-
22	CLA	b	710	36	1/1/20/20	6/37/115/115	-
33	LMG	C	520	-	-	20/43/63/70	0/1/1/1
29	DGD	C	518	-	-	15/51/91/95	0/2/2/2
23	BCR	k	102	-	-	4/29/63/63	0/2/2/2
28	STE	H	105	-	-	3/5/5/17	-
28	STE	b	726	-	-	4/7/7/17	-
22	CLA	C	507	-	1/1/20/20	12/37/115/115	-
28	STE	b	727	-	-	9/17/17/17	-
28	STE	B	725	-	-	6/15/15/17	-
28	STE	a	418	-	-	4/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEC	e	101	5,6	-	2/10/54/54	-
29	DGD	h	702	-	-	14/51/91/95	0/2/2/2
22	CLA	A	404	-	1/1/17/20	4/24/102/115	-
23	BCR	h	701	-	-	9/29/63/63	0/2/2/2
28	STE	J	101	-	-	4/9/9/17	-
28	STE	H	104	-	-	6/15/15/17	-
22	CLA	B	706	-	1/1/20/20	6/37/115/115	-
22	CLA	B	703	-	1/1/20/20	12/37/115/115	-
22	CLA	D	402	36	1/1/20/20	9/37/115/115	-
22	CLA	C	503	-	-	10/37/115/115	-
28	STE	M	103	-	-	4/7/7/17	-
33	LMG	c	520	-	-	12/31/51/70	0/1/1/1
22	CLA	C	505	36	1/1/18/20	5/30/108/115	-
26	SQD	B	723	-	-	28/49/69/69	0/1/1/1
22	CLA	c	511	-	1/1/20/20	10/37/115/115	-
33	LMG	a	419	-	-	23/50/70/70	0/1/1/1
28	STE	M	102	-	-	5/12/12/17	-
28	STE	b	724	-	-	12/13/13/17	-
27	LHG	B	722	-	-	17/53/53/53	-
22	CLA	C	510	-	1/1/20/20	13/37/115/115	-
33	LMG	c	522	-	-	25/43/63/70	0/1/1/1
22	CLA	c	505	36	1/1/19/20	8/31/109/115	-
22	CLA	a	406	-	1/1/20/20	10/37/115/115	-
26	SQD	a	413	-	-	23/49/69/69	0/1/1/1
26	SQD	f	101	-	-	14/36/56/69	0/1/1/1
27	LHG	A	410	-	-	28/53/53/53	-
35	HEC	V	201	17	-	2/10/54/54	-
22	CLA	c	509	-	-	7/36/114/115	-
22	CLA	C	511	-	1/1/20/20	9/37/115/115	-
22	CLA	c	502	-	1/1/20/20	4/37/115/115	-
23	BCR	B	718	-	-	7/29/63/63	0/2/2/2
22	CLA	b	711	-	1/1/20/20	9/37/115/115	-
22	CLA	C	509	-	-	7/37/115/115	-
22	CLA	C	504	-	1/1/20/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	C	521	-	-	2/9/9/17	-
22	CLA	B	712	-	1/1/20/20	8/37/115/115	-
28	STE	A	414	-	-	1/2/2/17	-
23	BCR	c	515	-	-	11/29/63/63	0/2/2/2
28	STE	m	101	-	-	2/9/9/17	-
28	STE	a	417	-	-	4/9/9/17	-
27	LHG	l	101	-	-	23/53/53/53	-
26	SQD	A	412	-	-	14/39/39/69	-
28	STE	x	101	-	-	11/17/17/17	-
35	HEC	v	201	17	-	2/10/54/54	-
22	CLA	B	716	-	1/1/19/20	12/31/109/115	-
26	SQD	a	415	-	-	19/37/37/69	-
28	STE	T	702	-	-	8/12/12/17	-
23	BCR	T	701	-	-	4/29/63/63	0/2/2/2
28	STE	b	725	-	-	8/17/17/17	-
28	STE	c	501	-	-	4/9/9/17	-
22	CLA	b	715	-	1/1/20/20	10/37/115/115	-
23	BCR	H	101	-	-	5/29/63/63	0/2/2/2
22	CLA	b	716	-	1/1/19/20	12/31/109/115	-
28	STE	a	416	-	-	4/7/7/17	-
33	LMG	M	101	-	-	22/46/66/70	0/1/1/1
22	CLA	C	514	-	1/1/20/20	16/37/115/115	-

The worst 5 of 911 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	715	CLA	C4B-NB	9.40	1.43	1.35
22	b	714	CLA	C4B-NB	8.75	1.43	1.35
22	c	512	CLA	C4B-NB	8.49	1.42	1.35
22	B	702	CLA	C4B-NB	8.18	1.42	1.35
22	b	709	CLA	C4B-NB	8.06	1.42	1.35

The worst 5 of 1357 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	704	CLA	C4A-NA-C1A	9.79	111.11	106.71
22	c	510	CLA	C4A-NA-C1A	9.44	110.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	701	CLA	C4A-NA-C1A	9.42	110.94	106.71
22	c	512	CLA	C4A-NA-C1A	9.35	110.91	106.71
22	B	707	CLA	C4A-NA-C1A	9.06	110.78	106.71

5 of 58 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	404	CLA	ND
22	B	702	CLA	ND
22	B	703	CLA	ND
22	B	704	CLA	ND

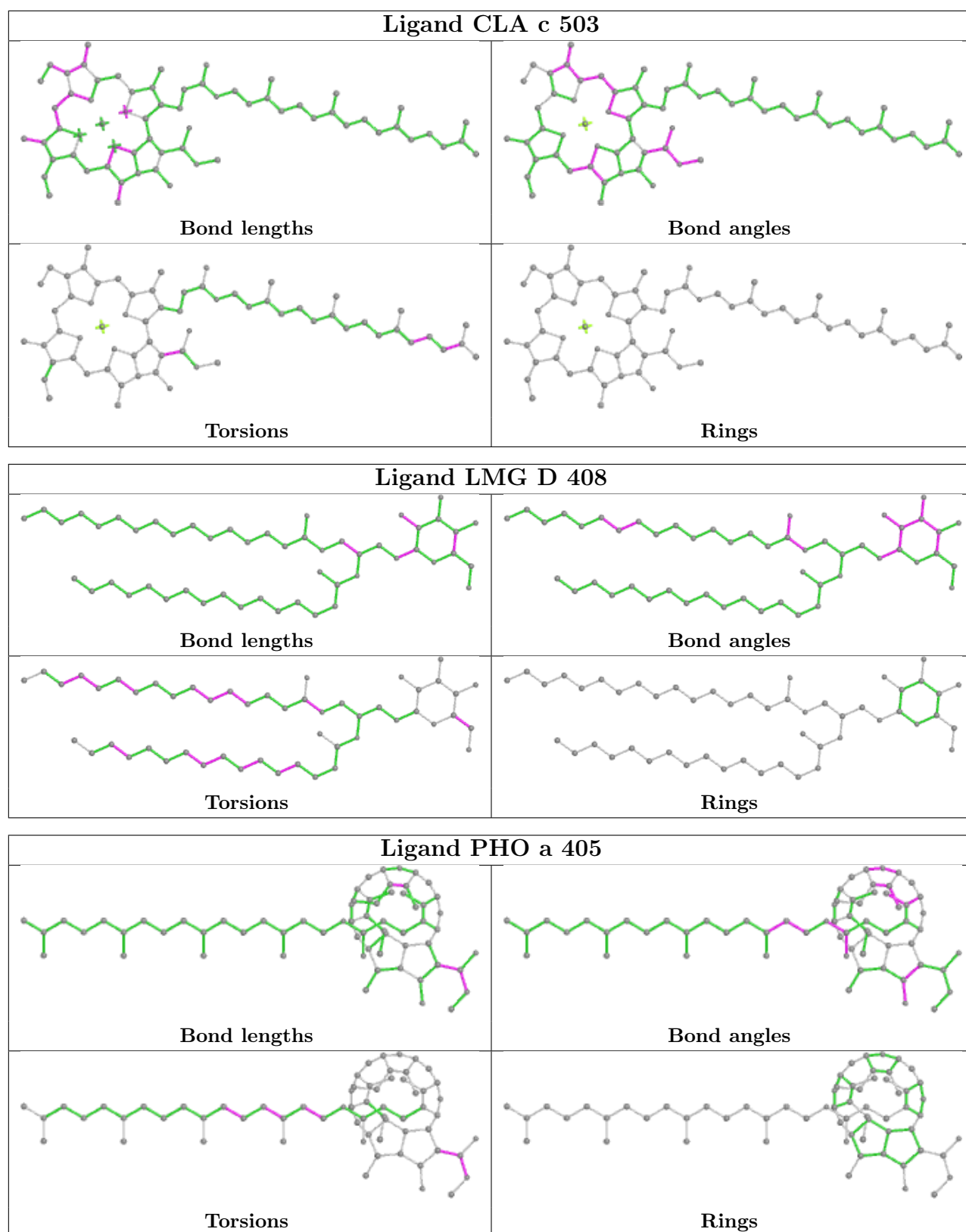
5 of 1844 torsion outliers are listed below:

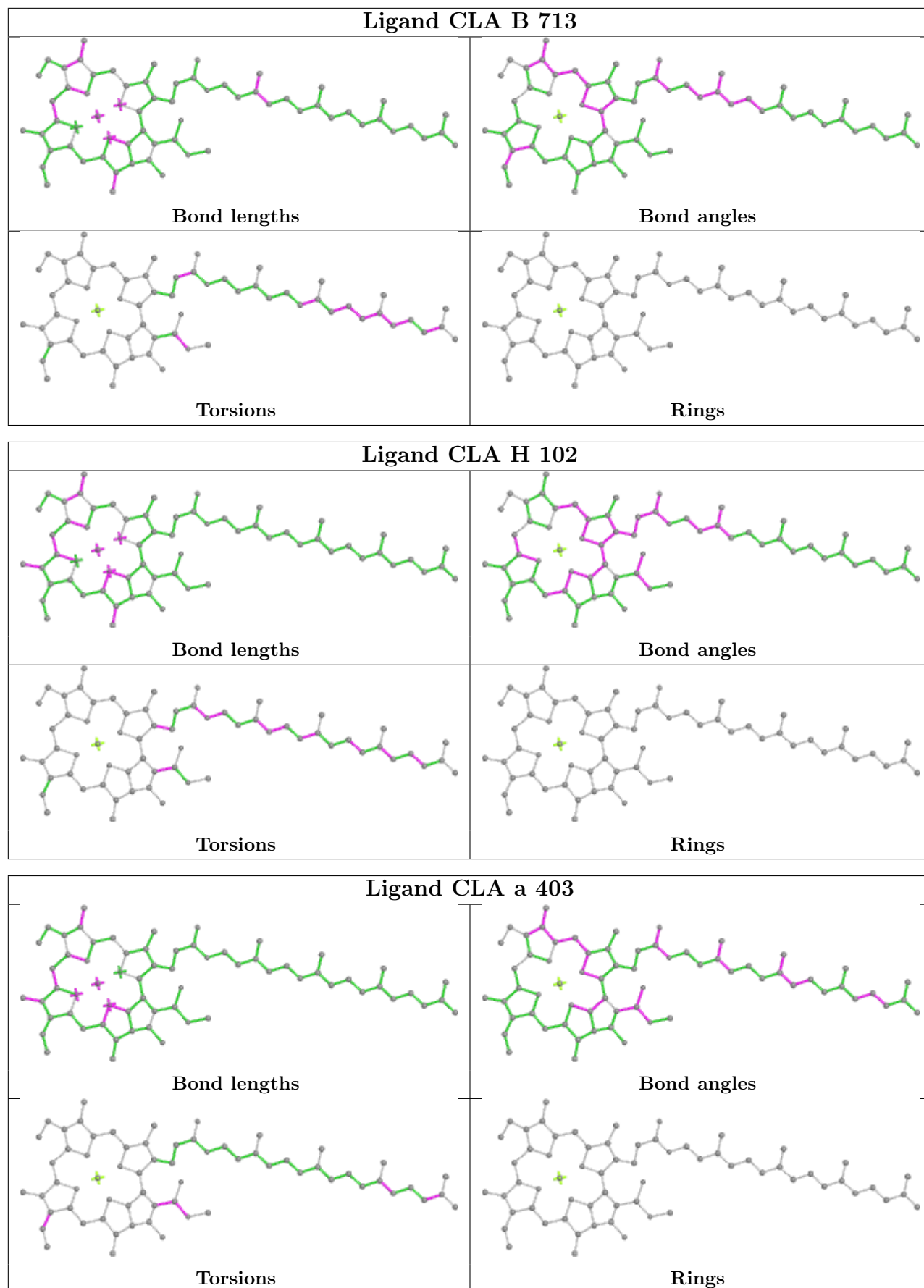
Mol	Chain	Res	Type	Atoms
22	B	705	CLA	C11-C12-C13-C14
22	B	706	CLA	CHA-CBD-CGD-O1D
22	B	714	CLA	CHA-CBD-CGD-O1D
22	B	714	CLA	CHA-CBD-CGD-O2D
22	B	714	CLA	CAD-CBD-CGD-O1D

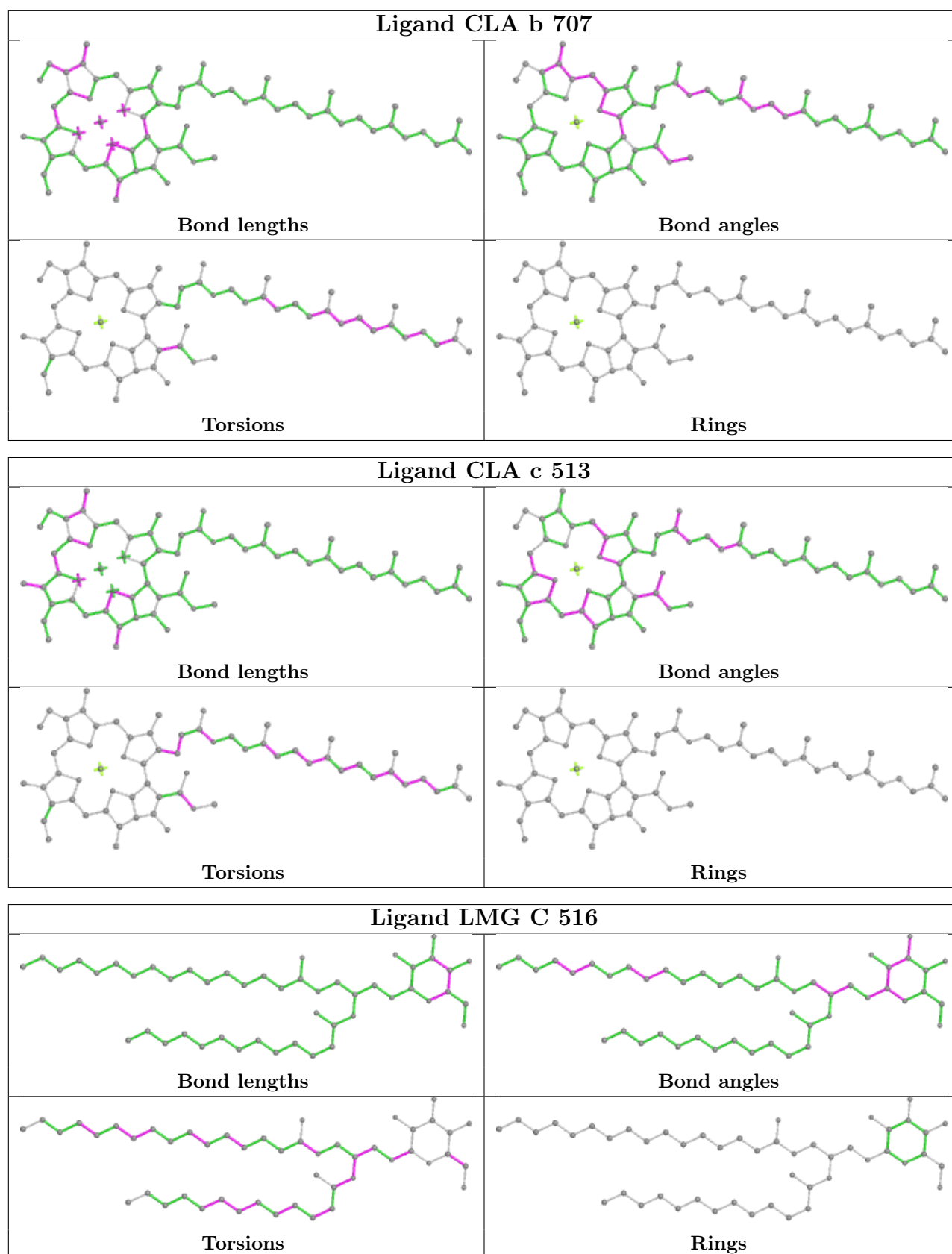
There are no ring outliers.

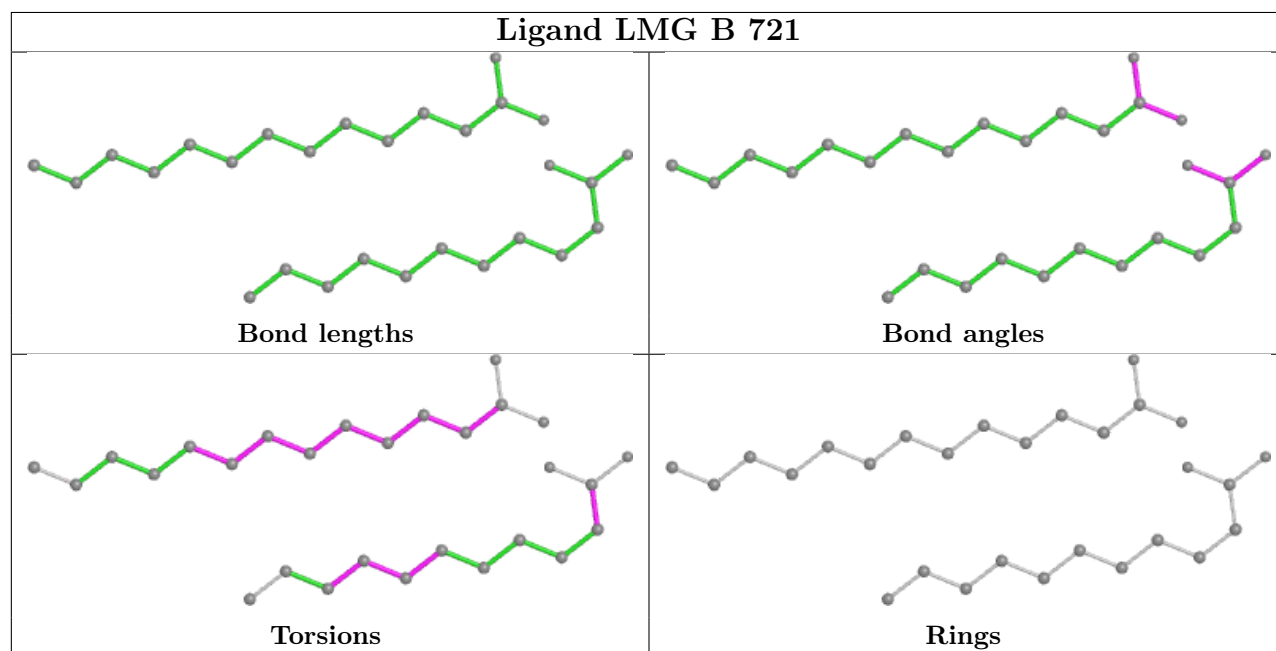
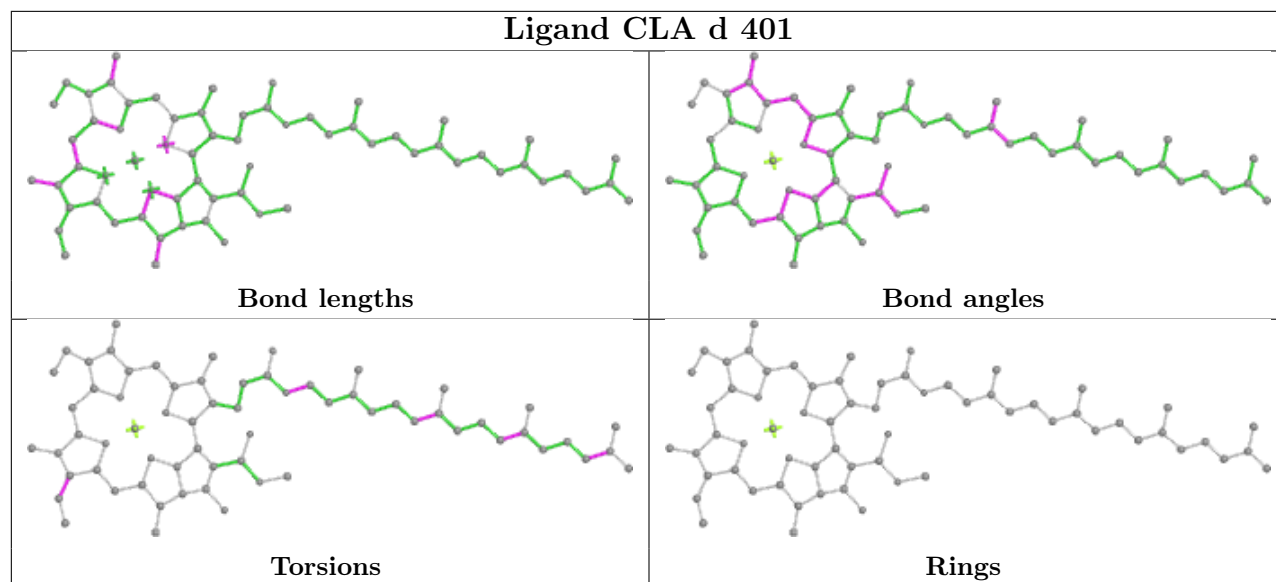
No monomer is involved in short contacts.

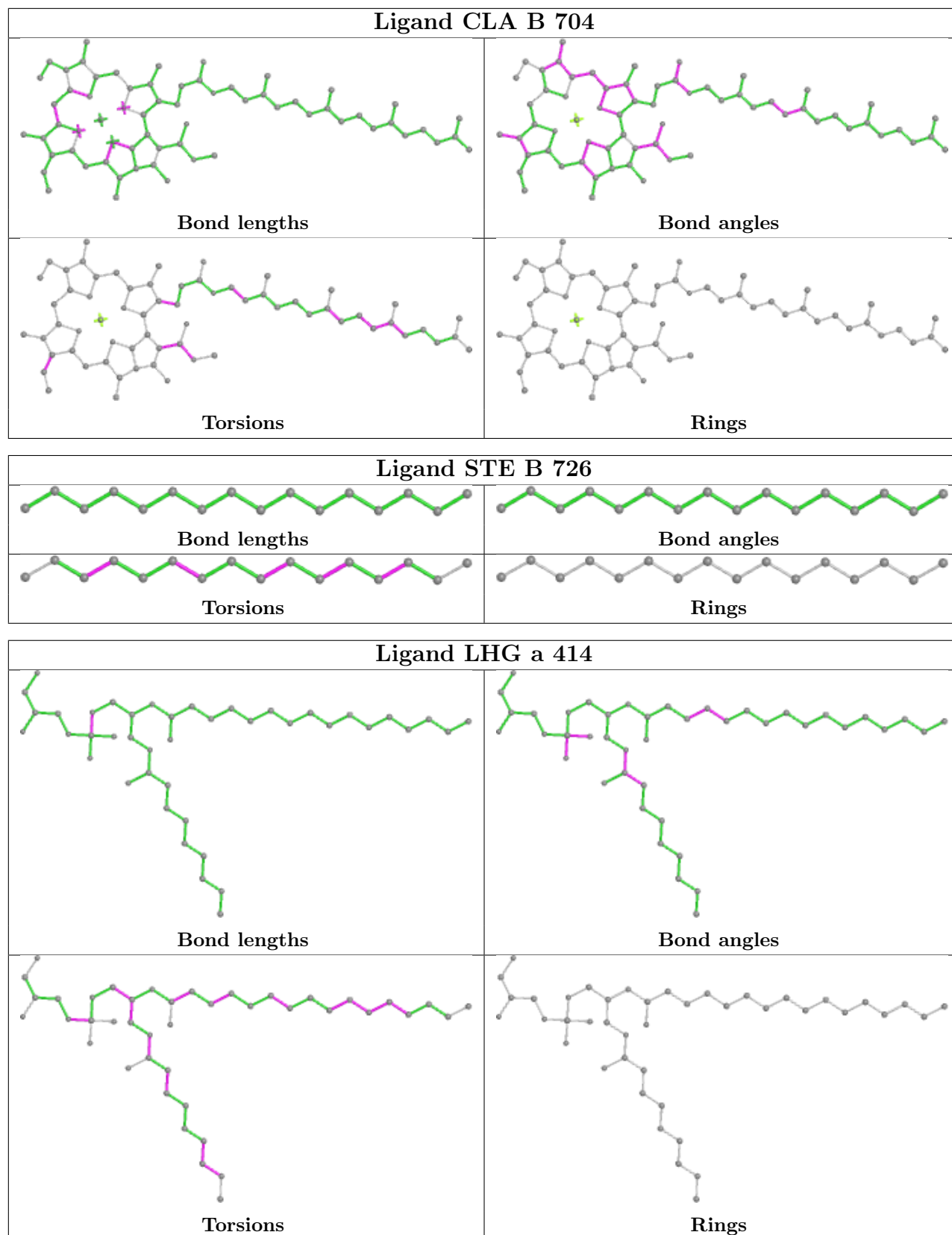
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

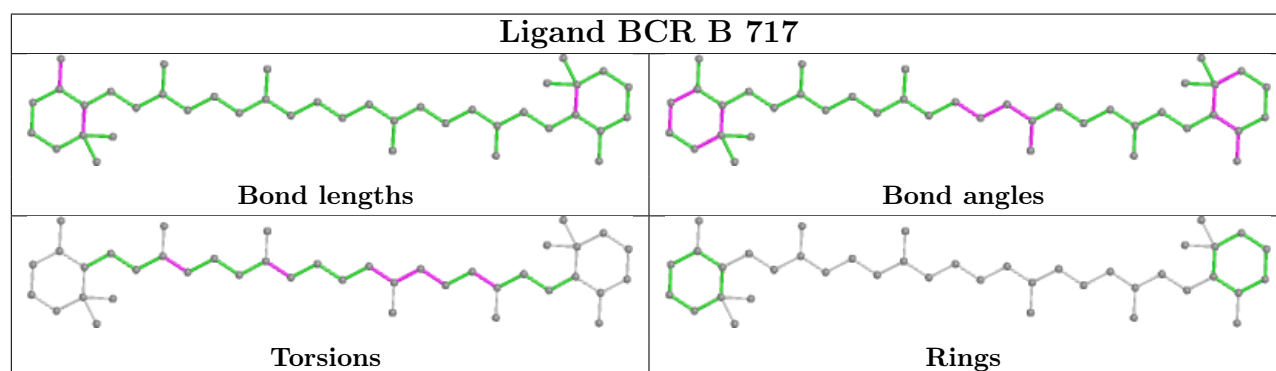
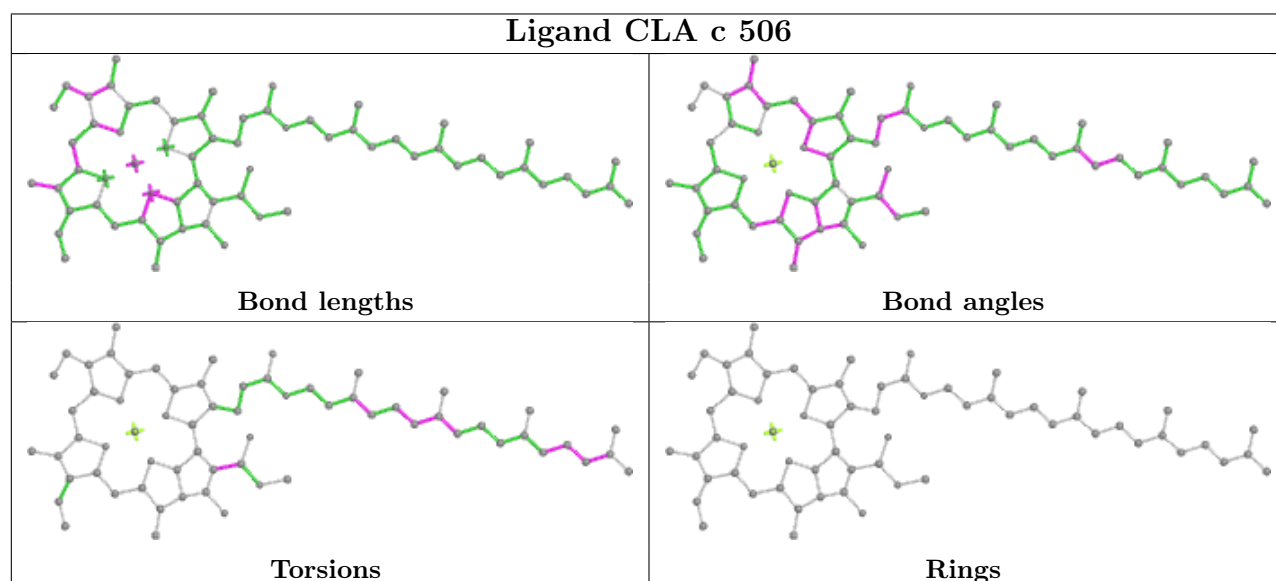
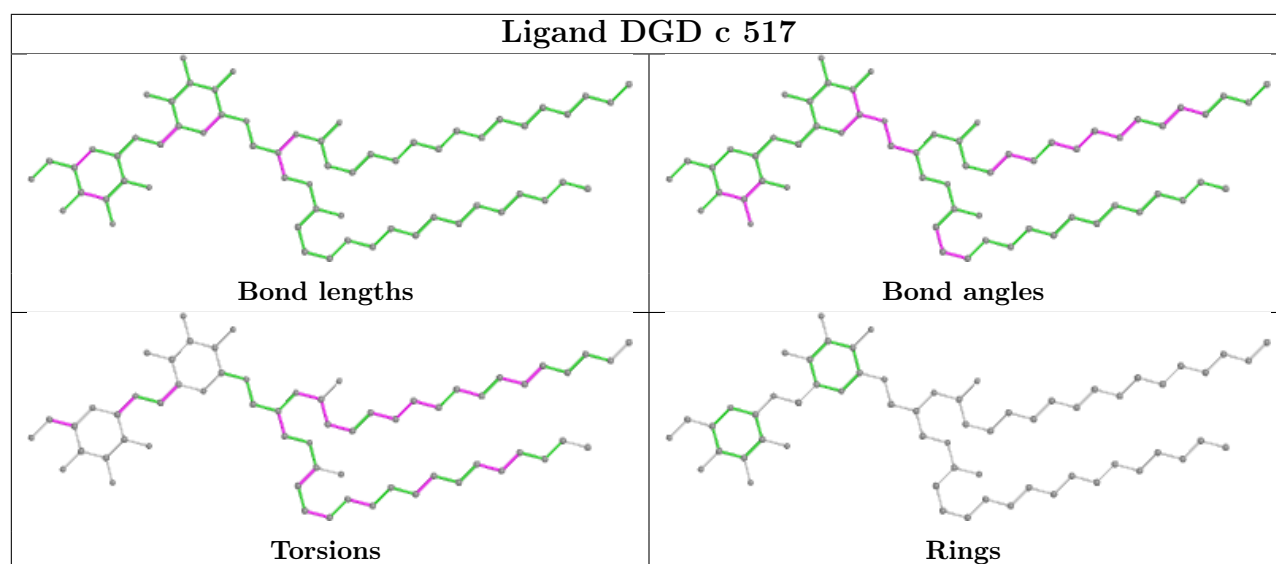


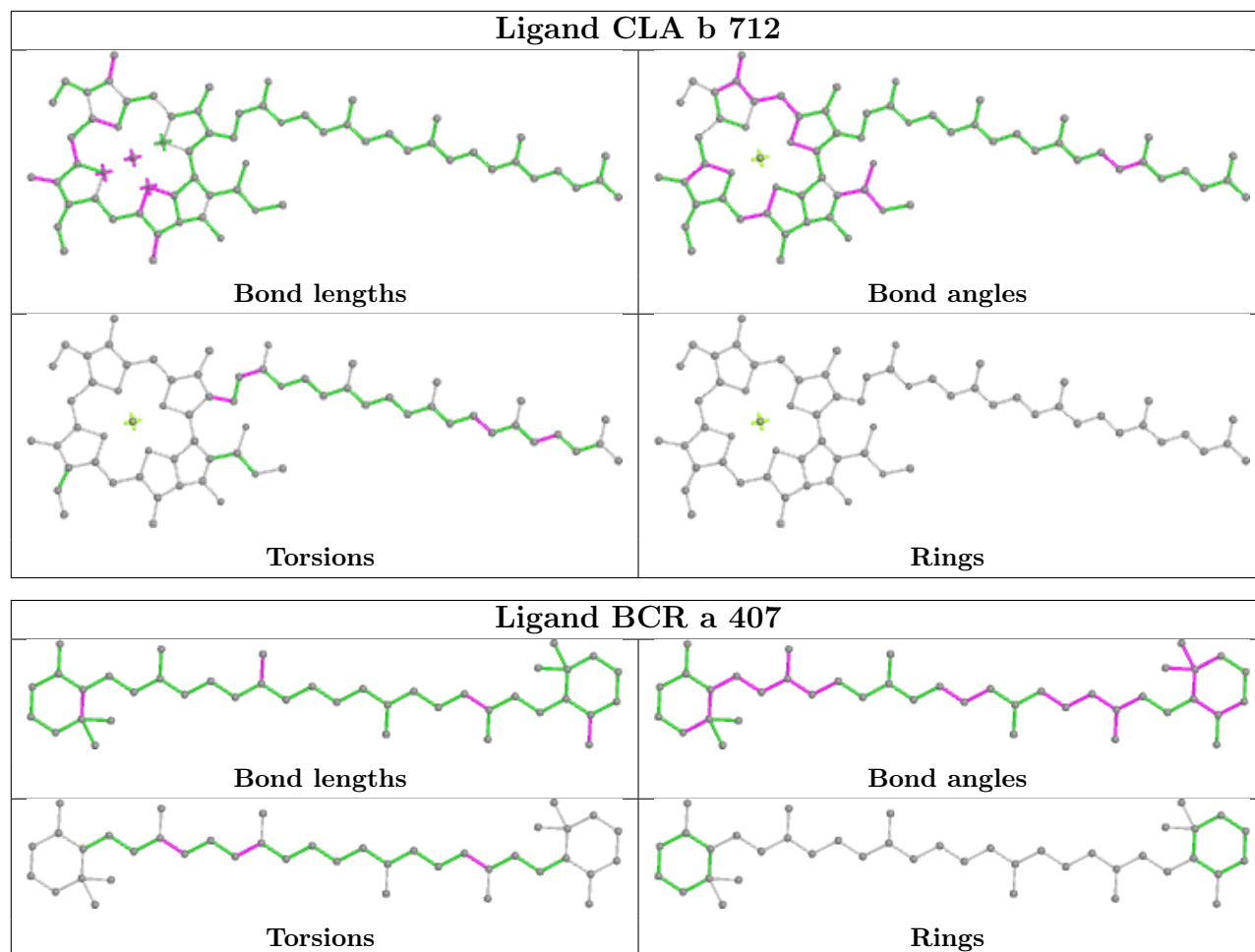


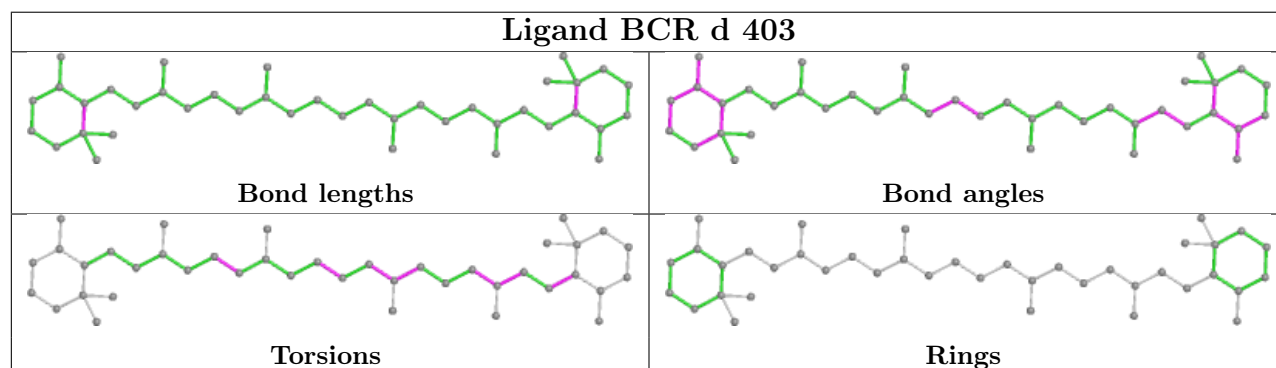
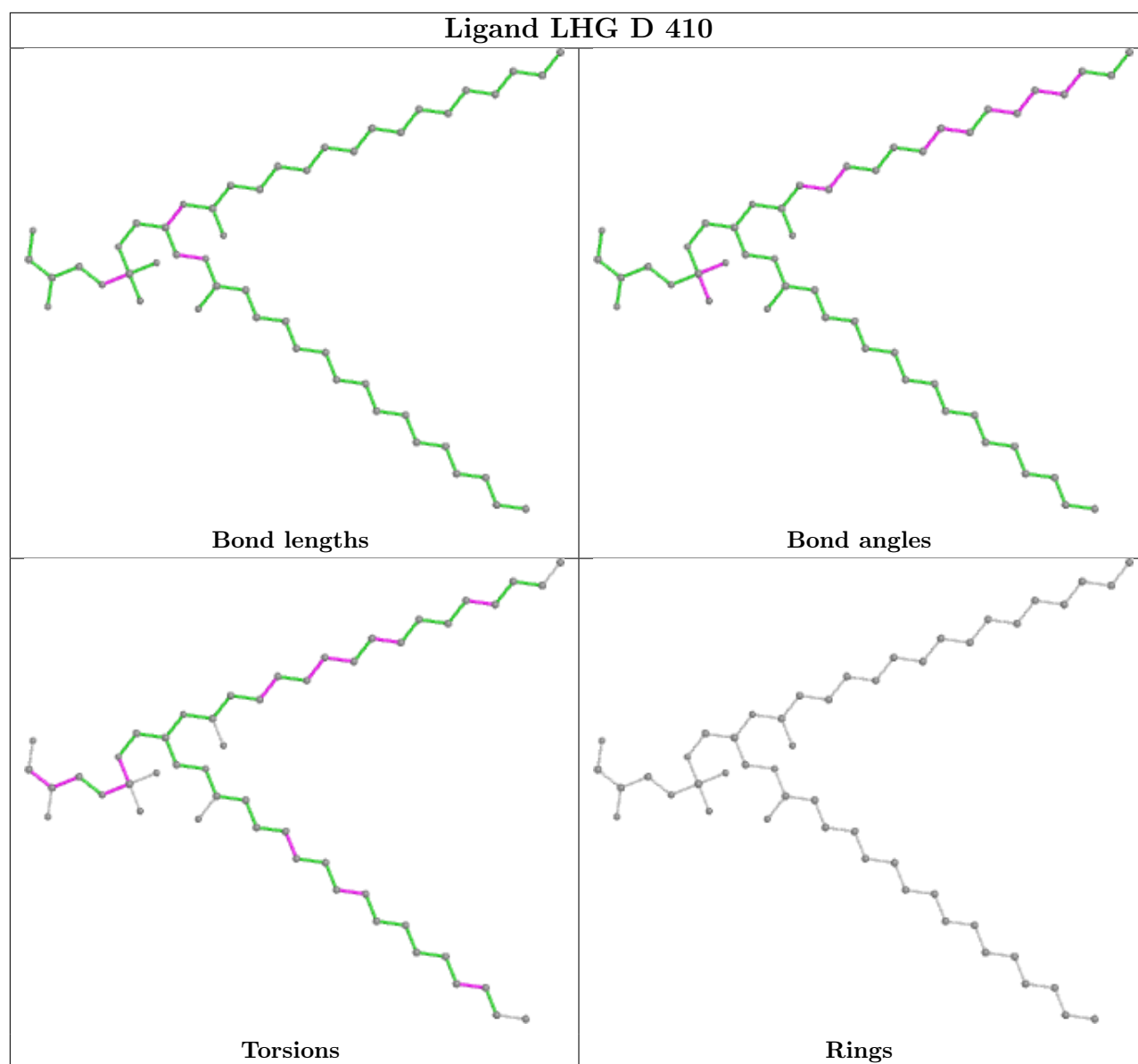


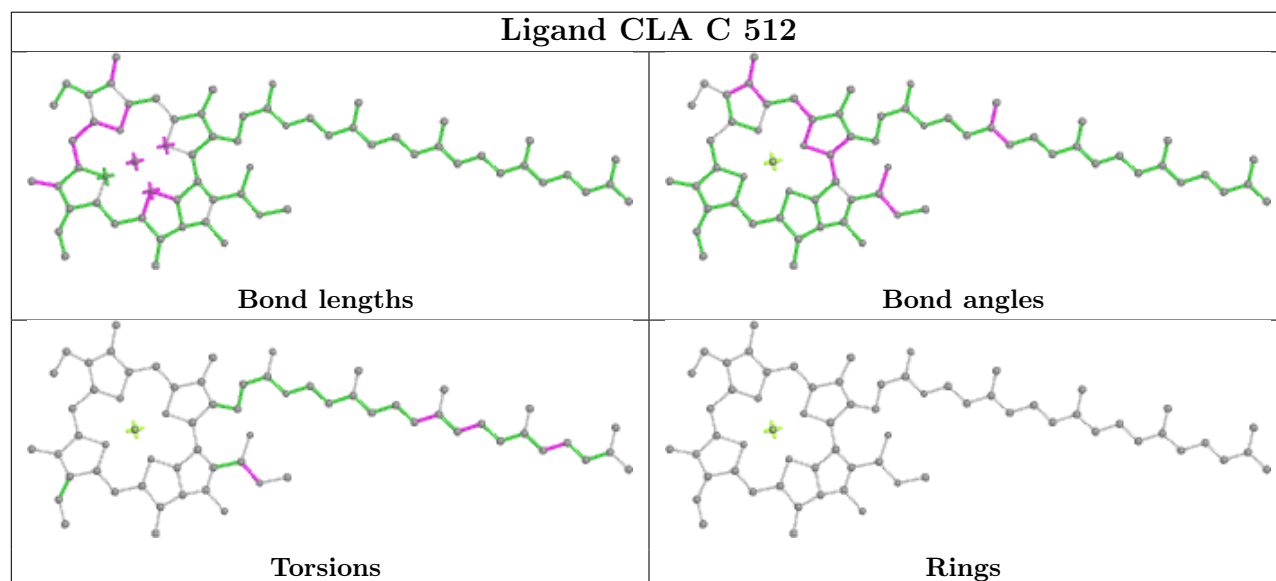
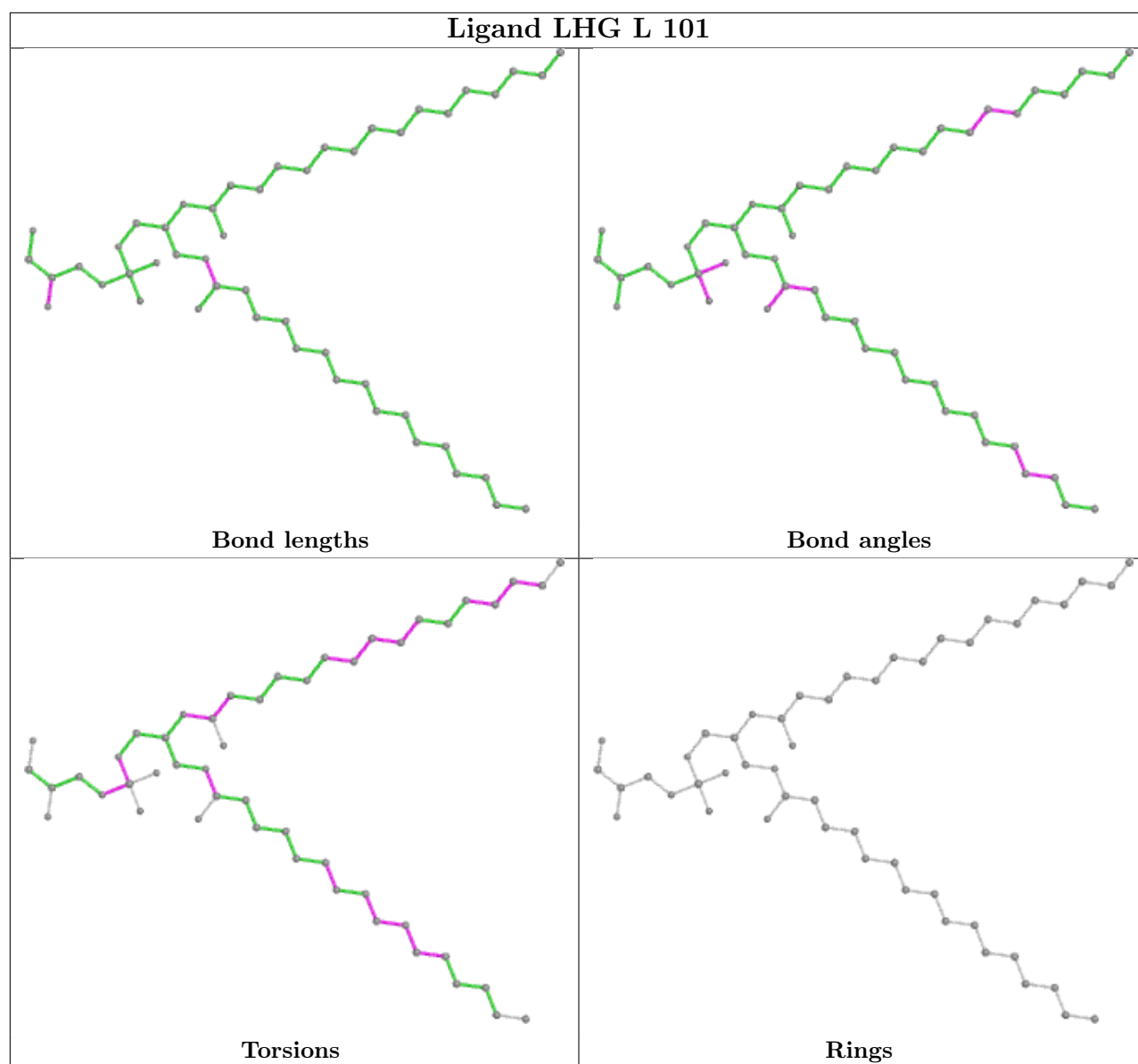


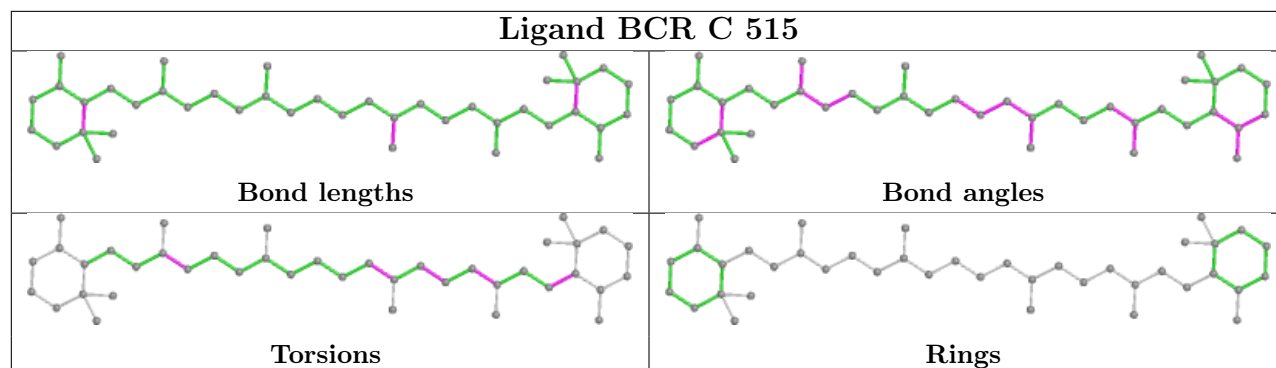
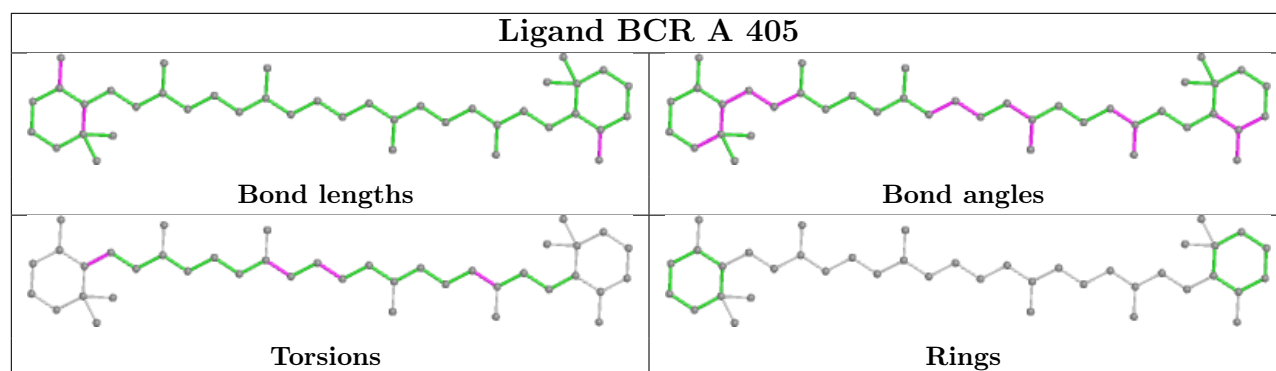
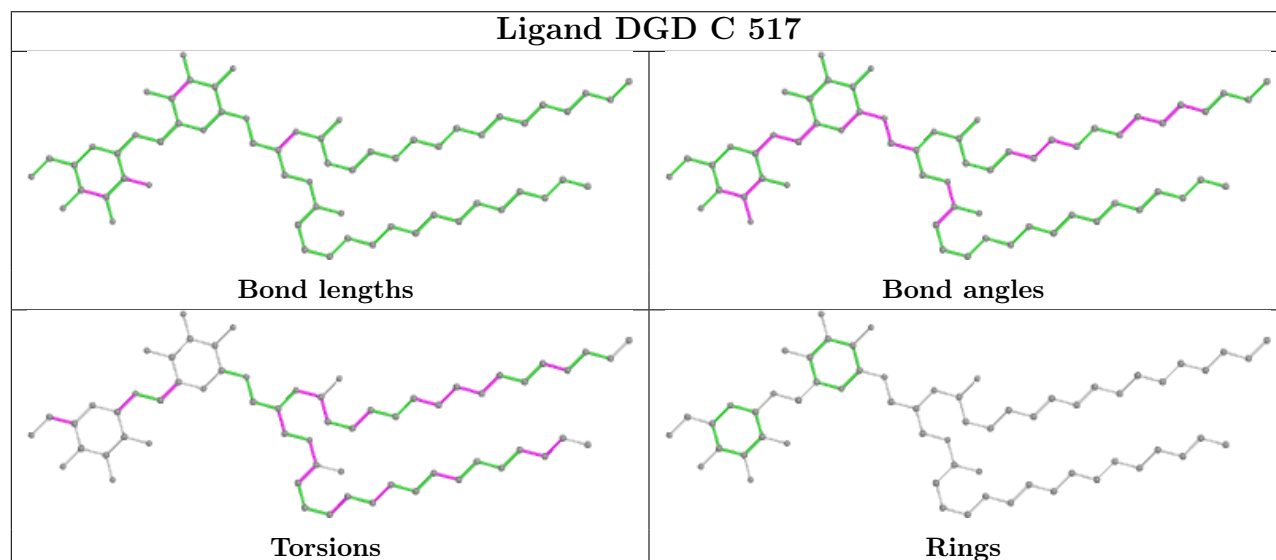
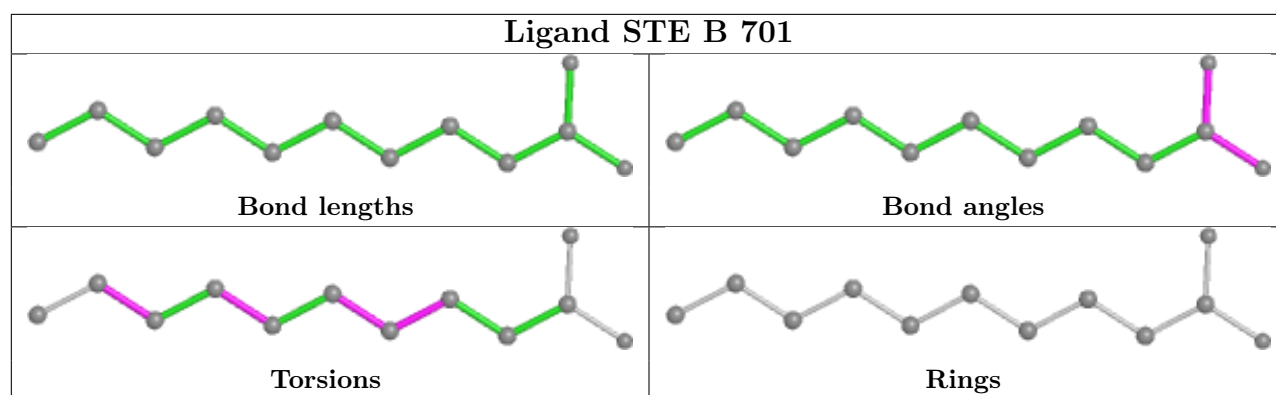


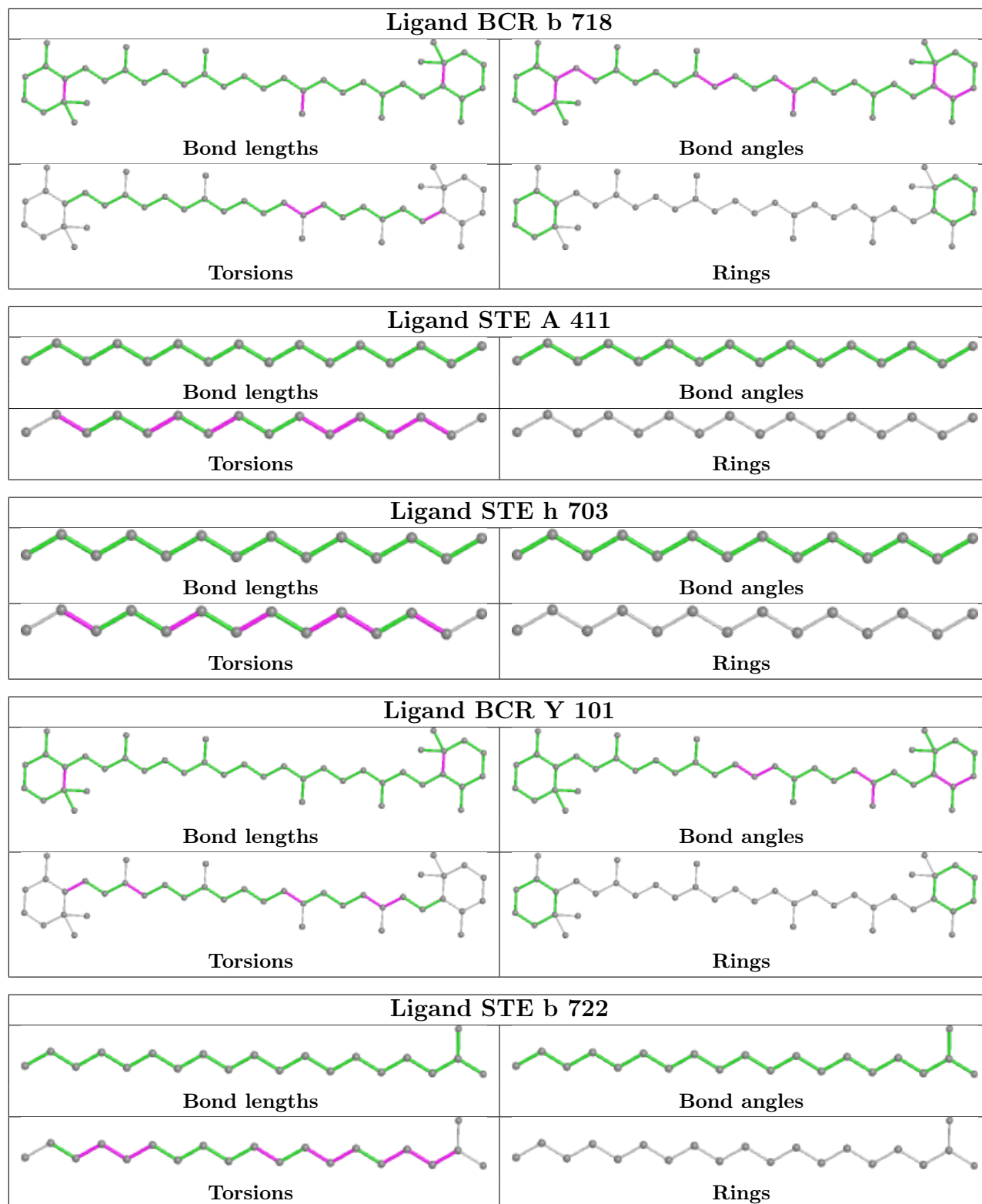


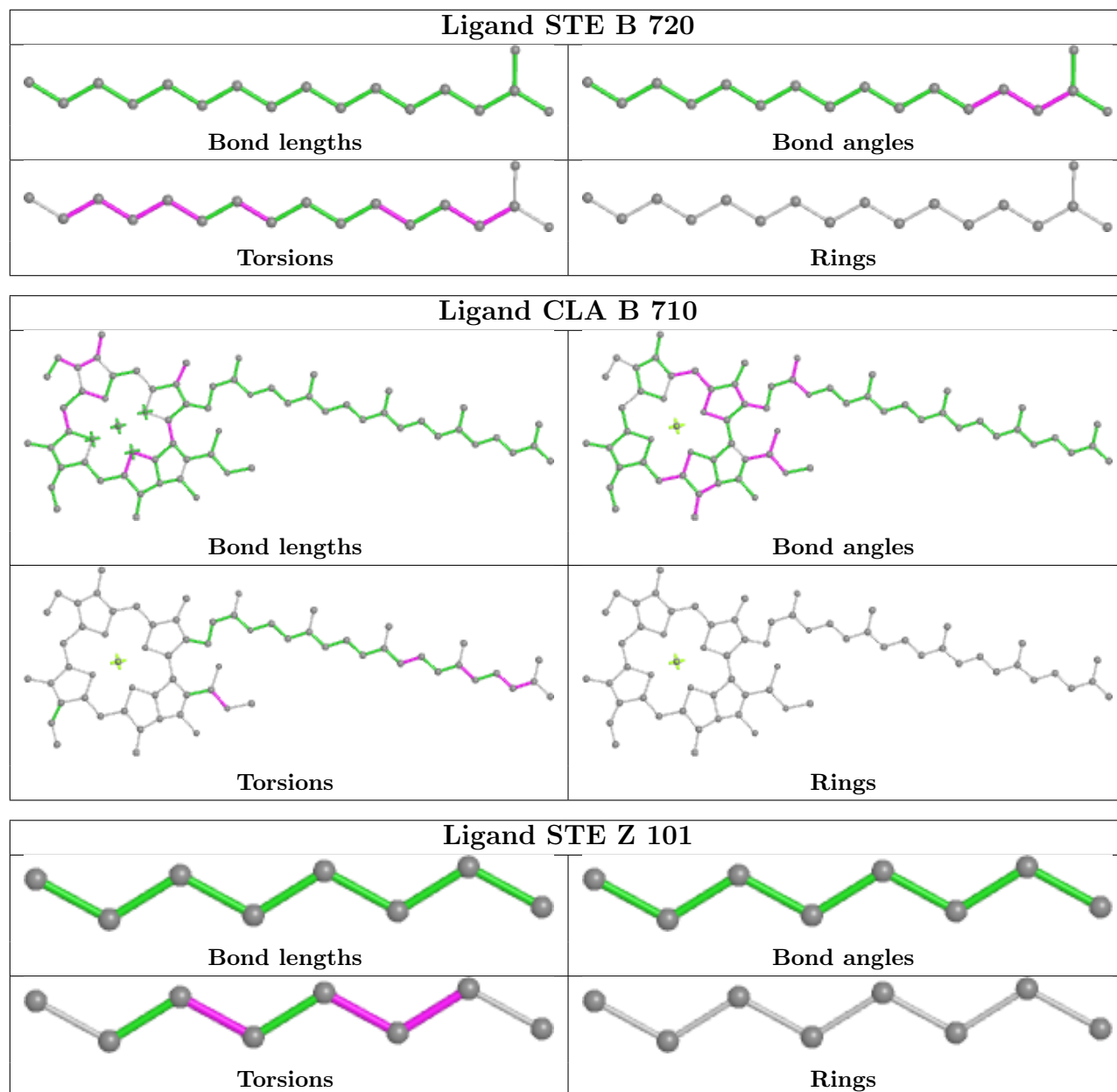


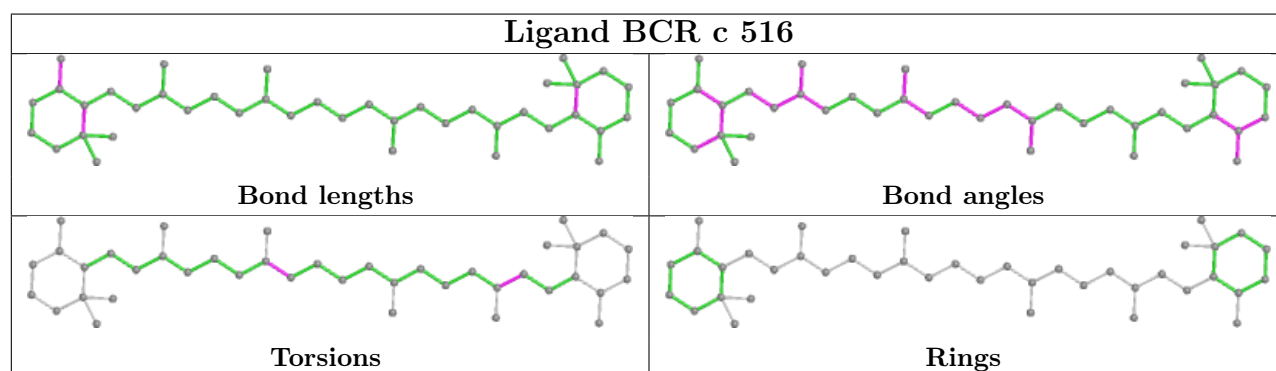
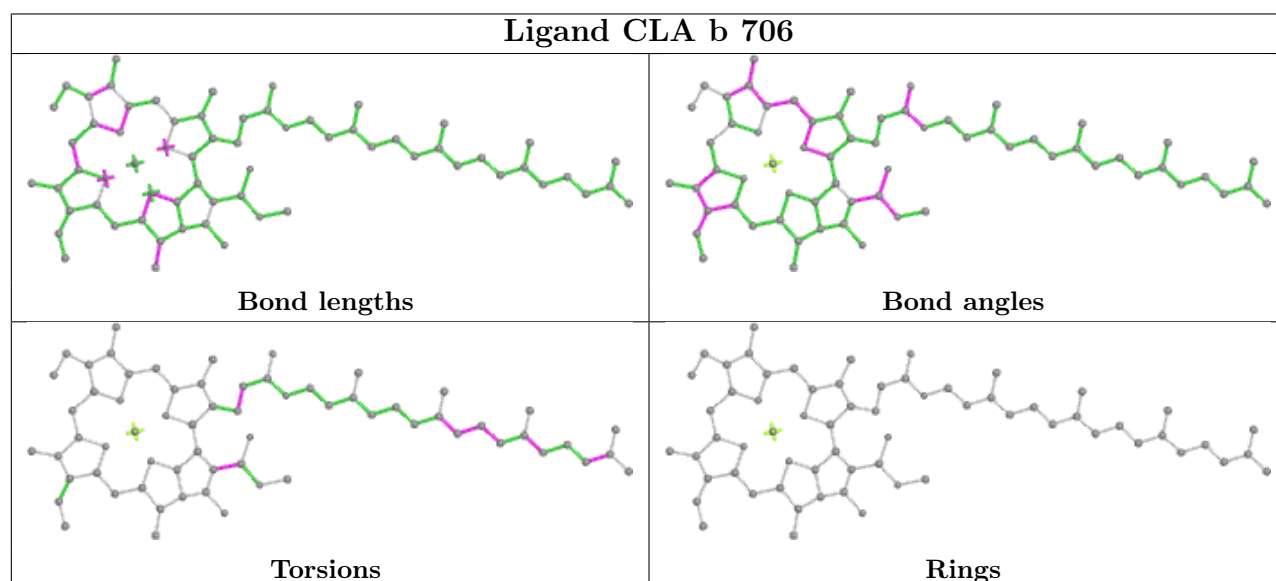
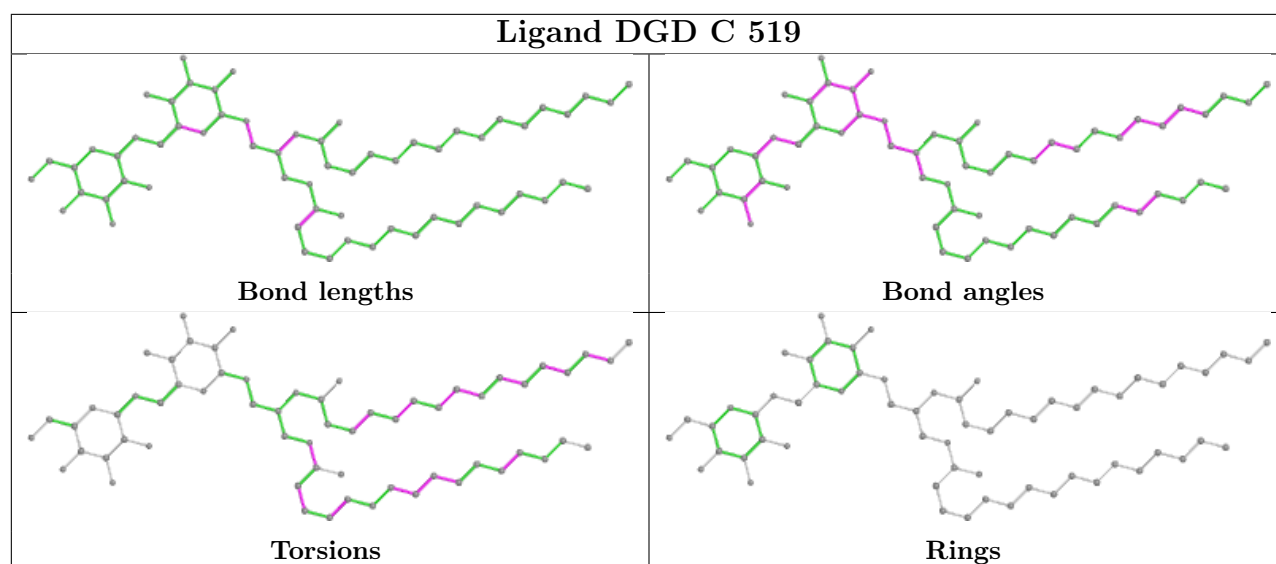


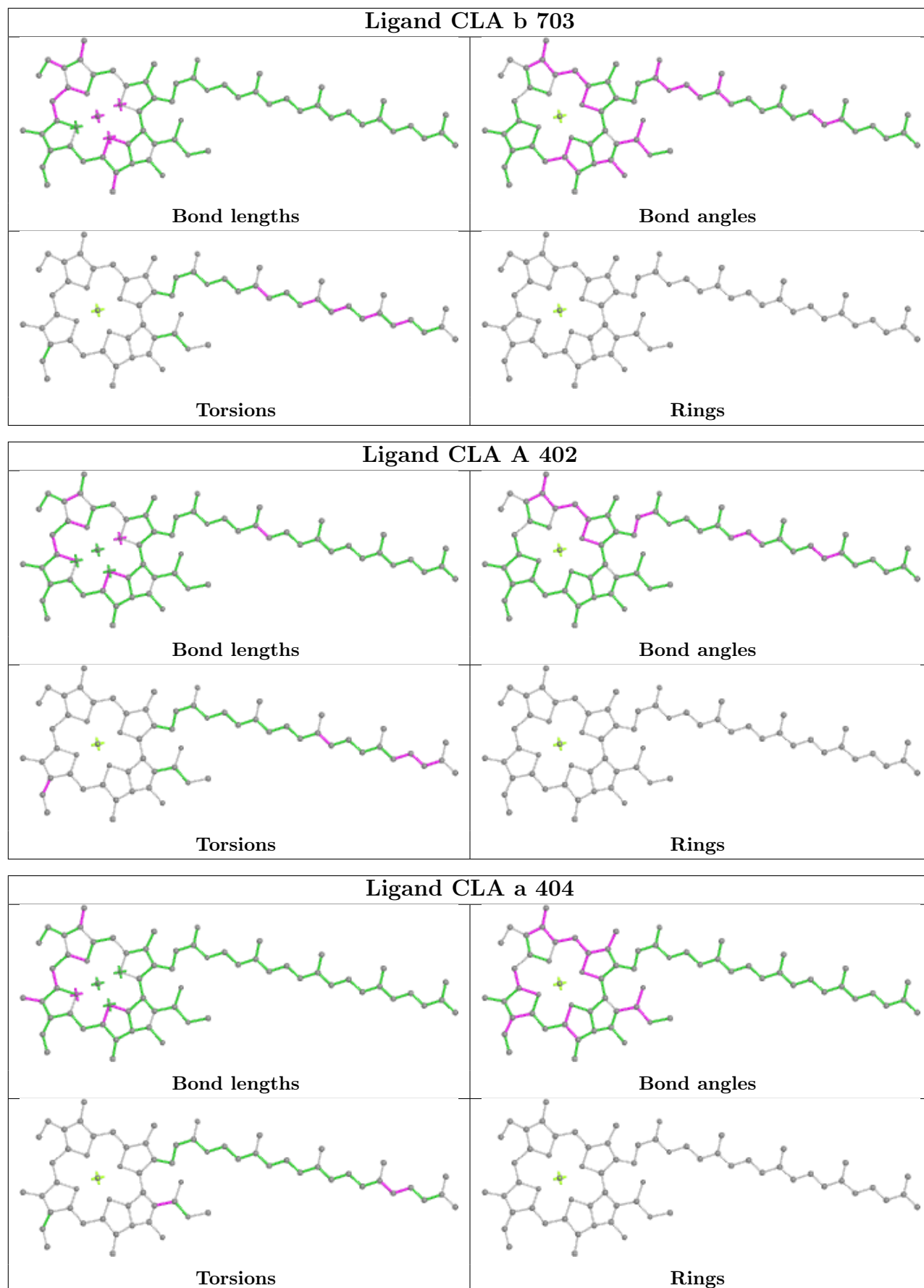


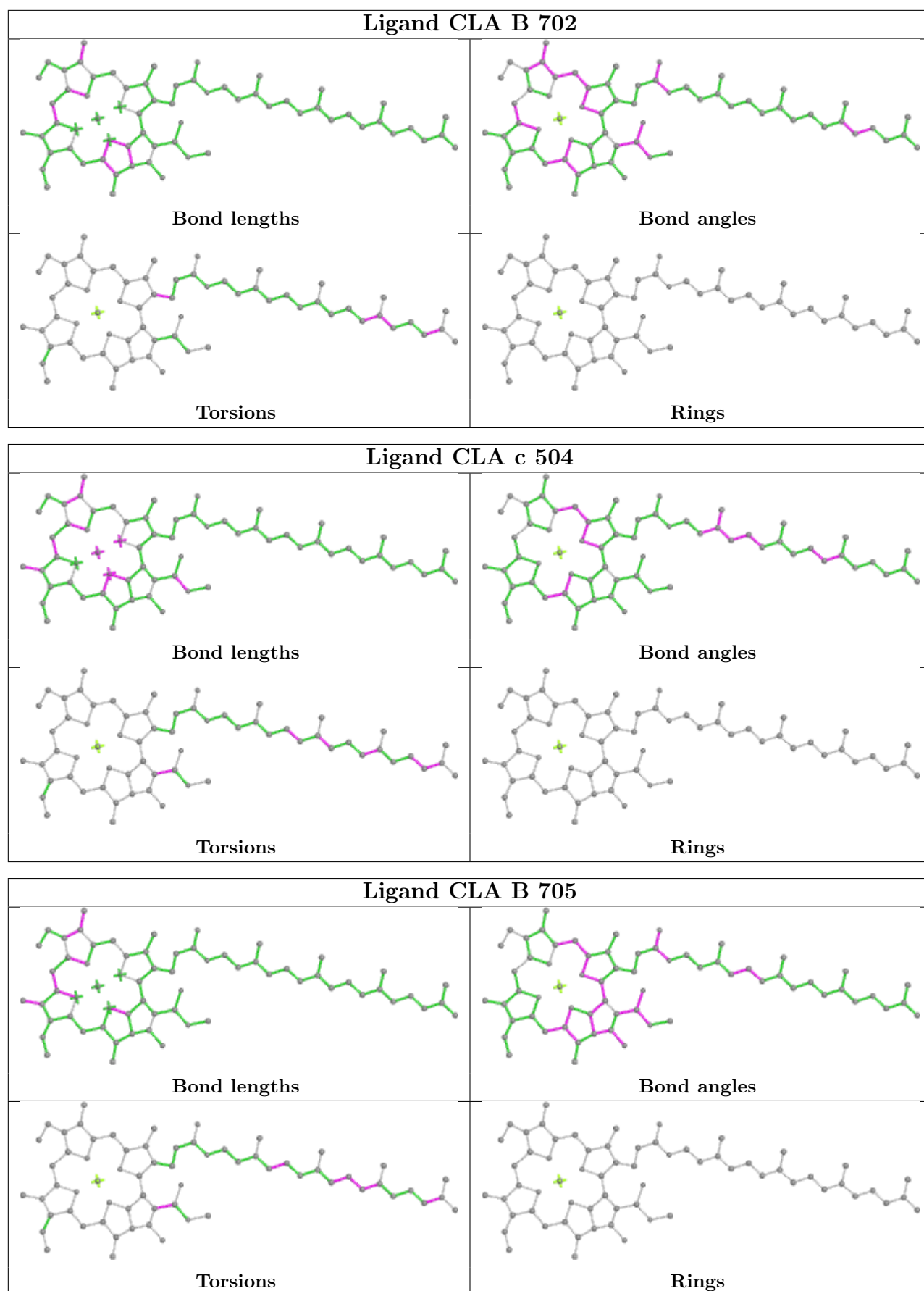


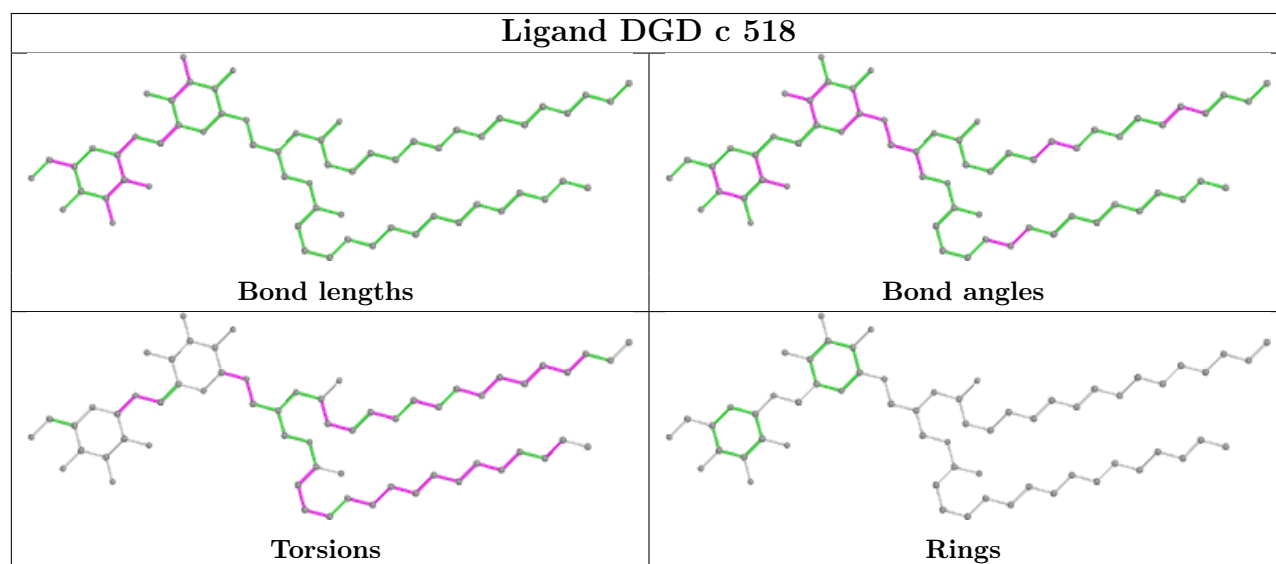
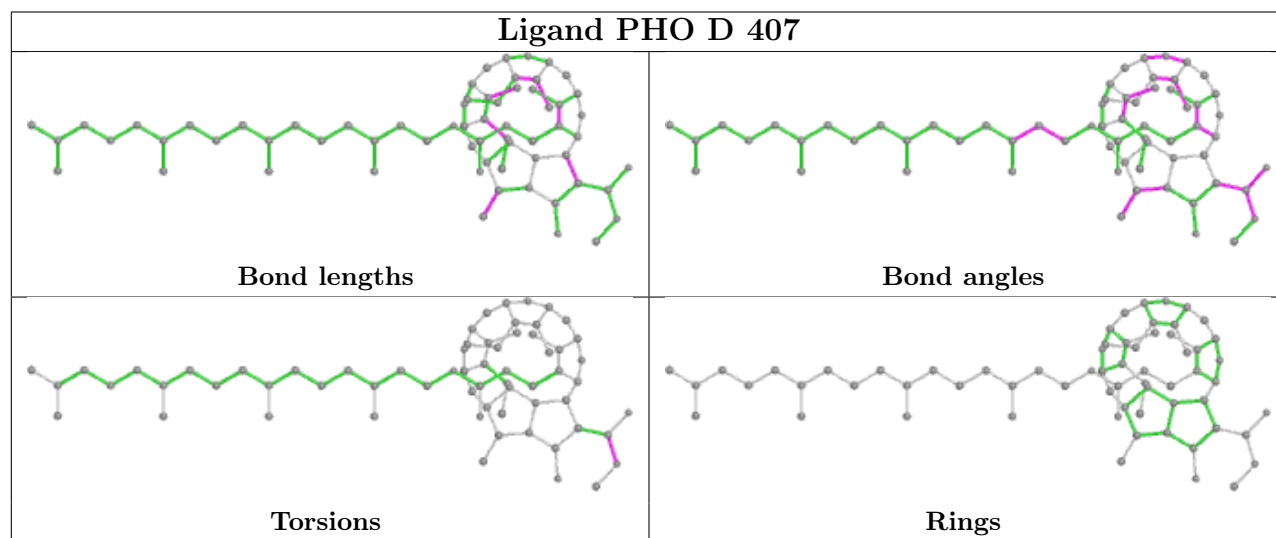
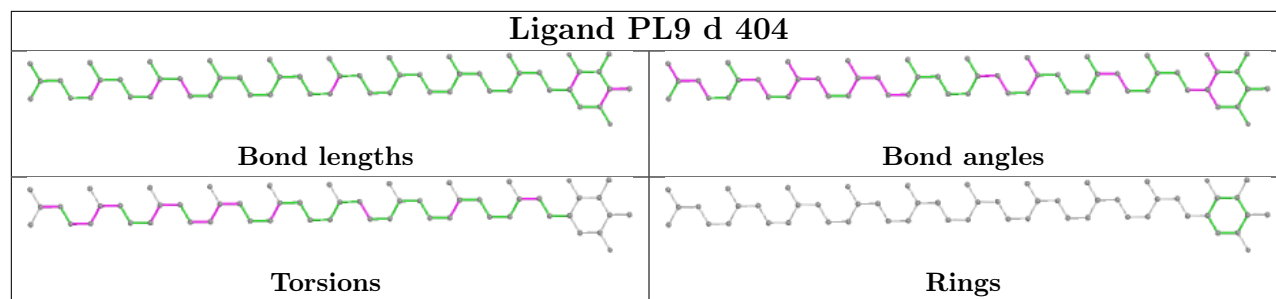


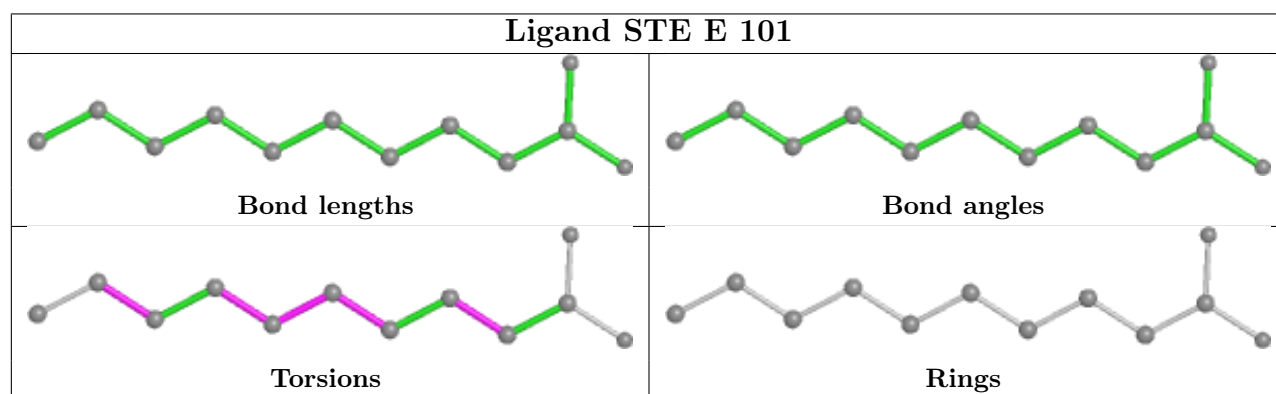
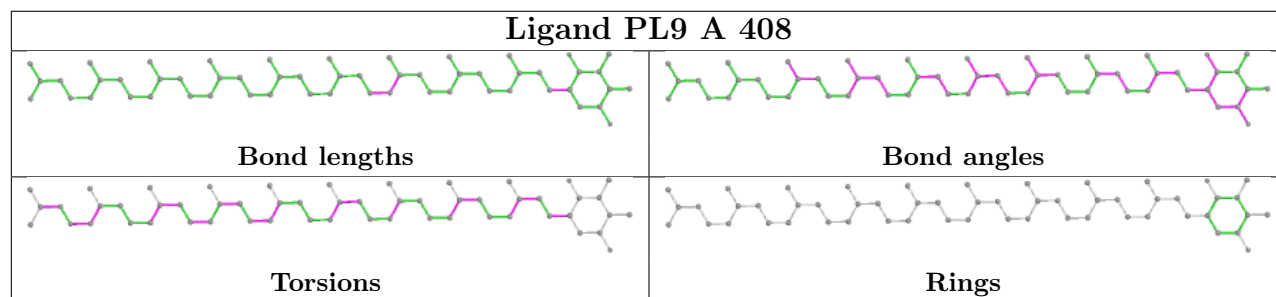
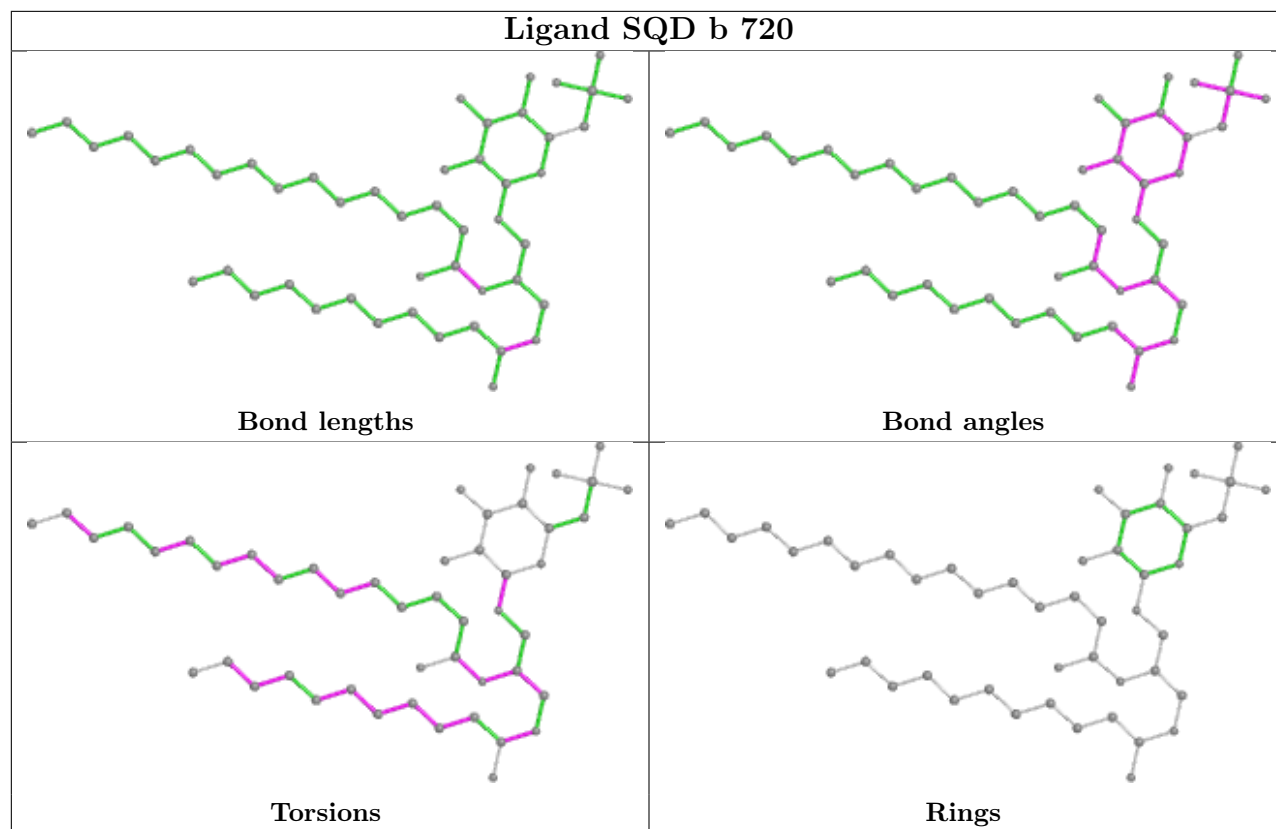


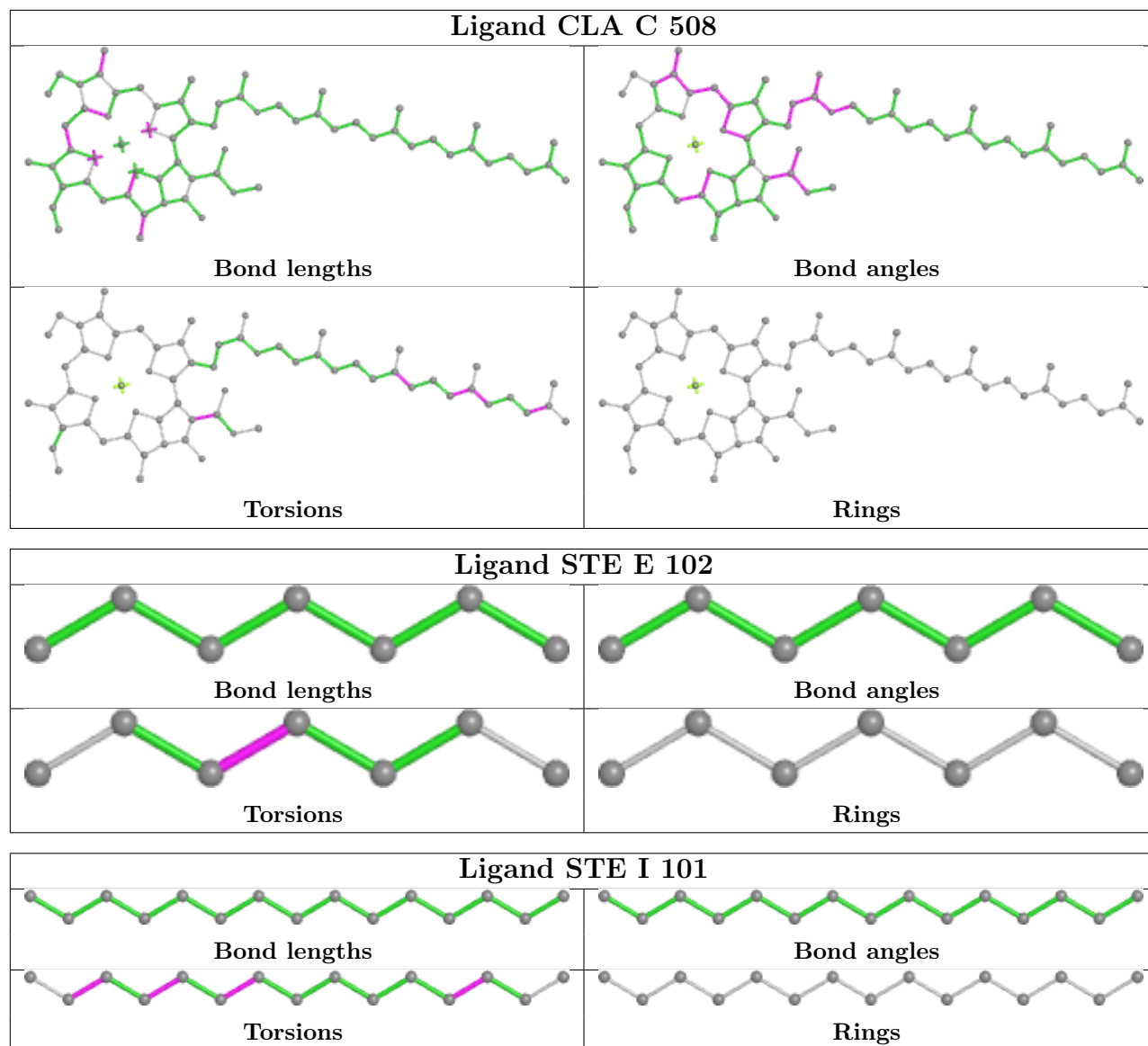


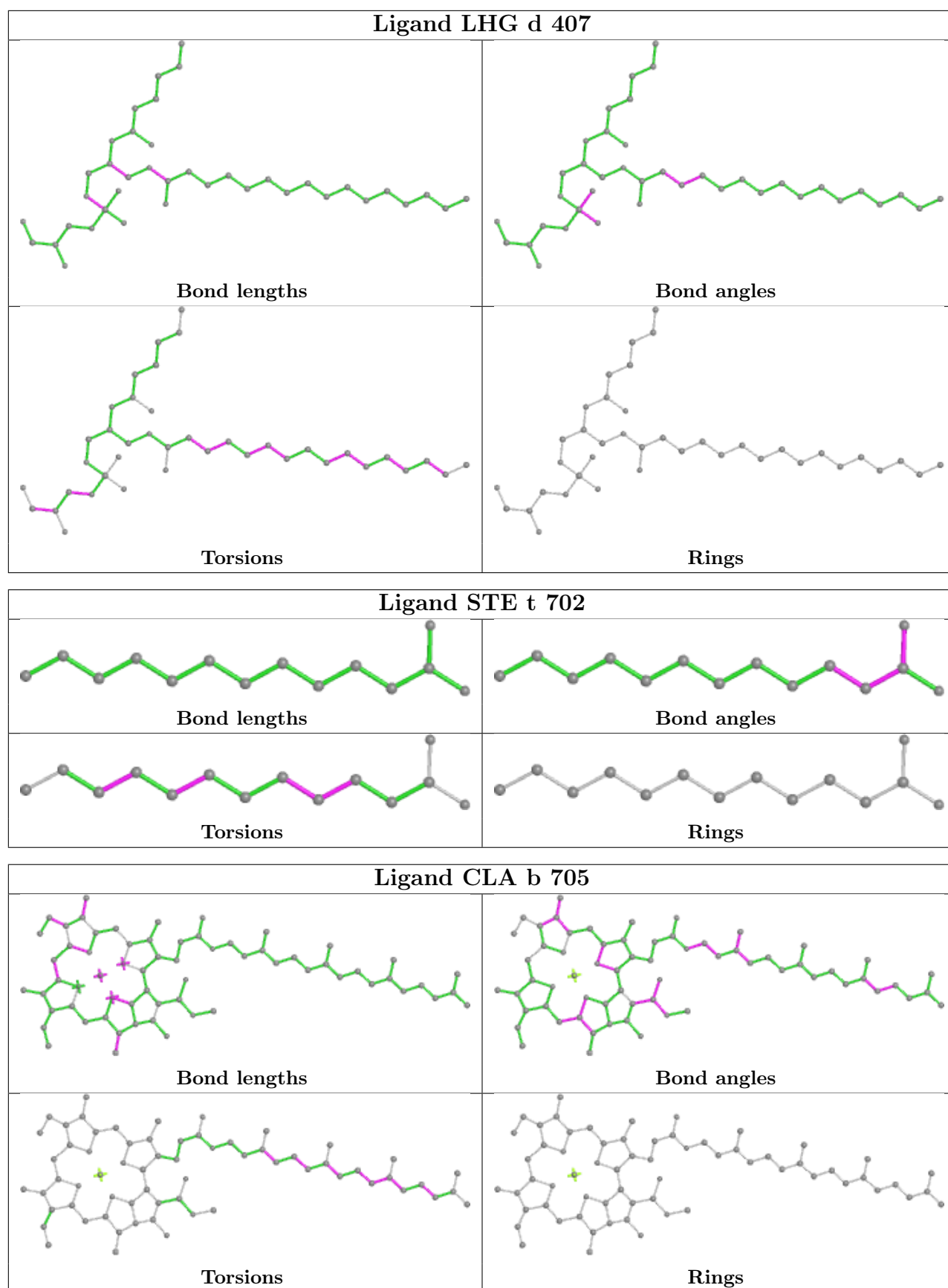


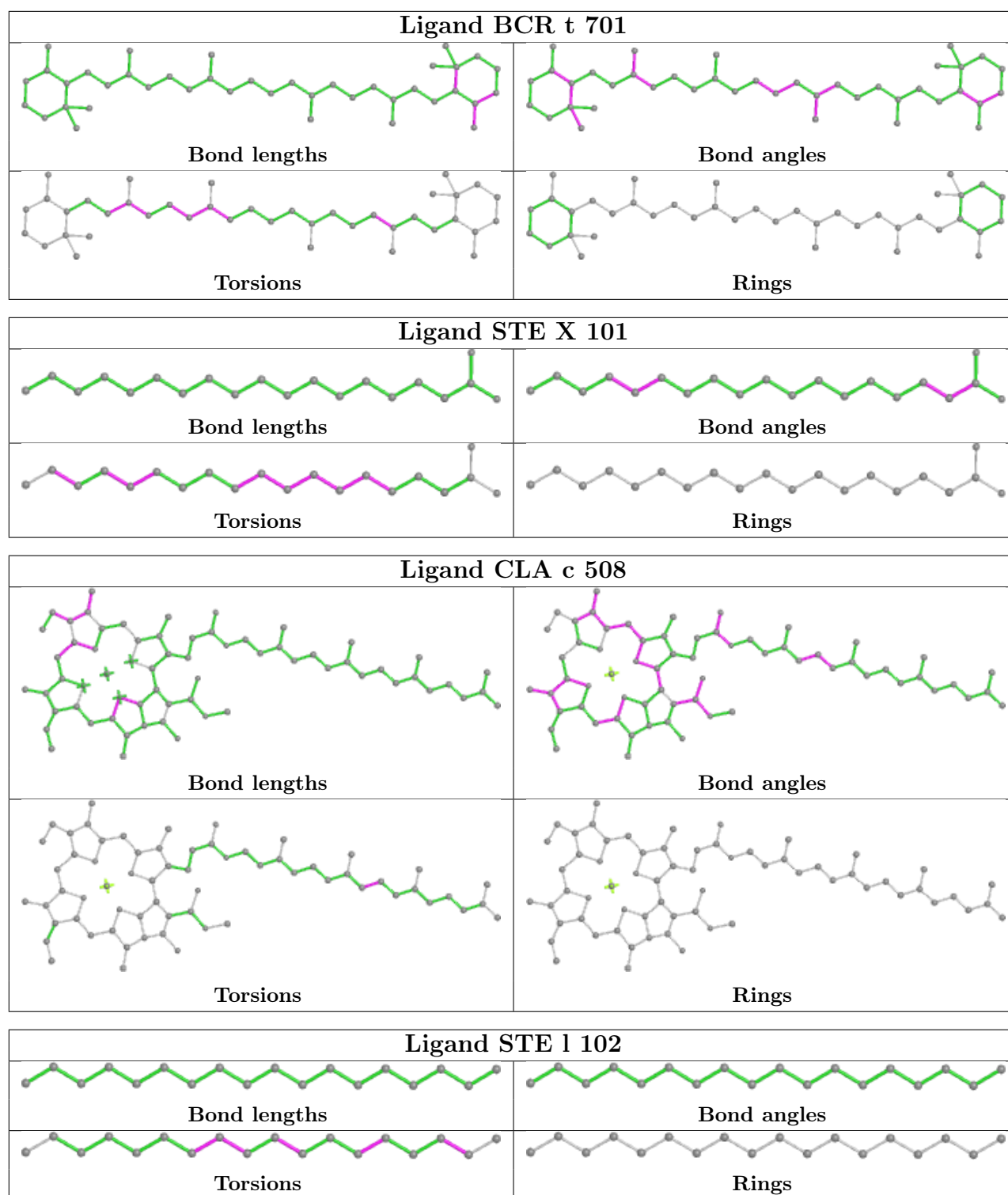


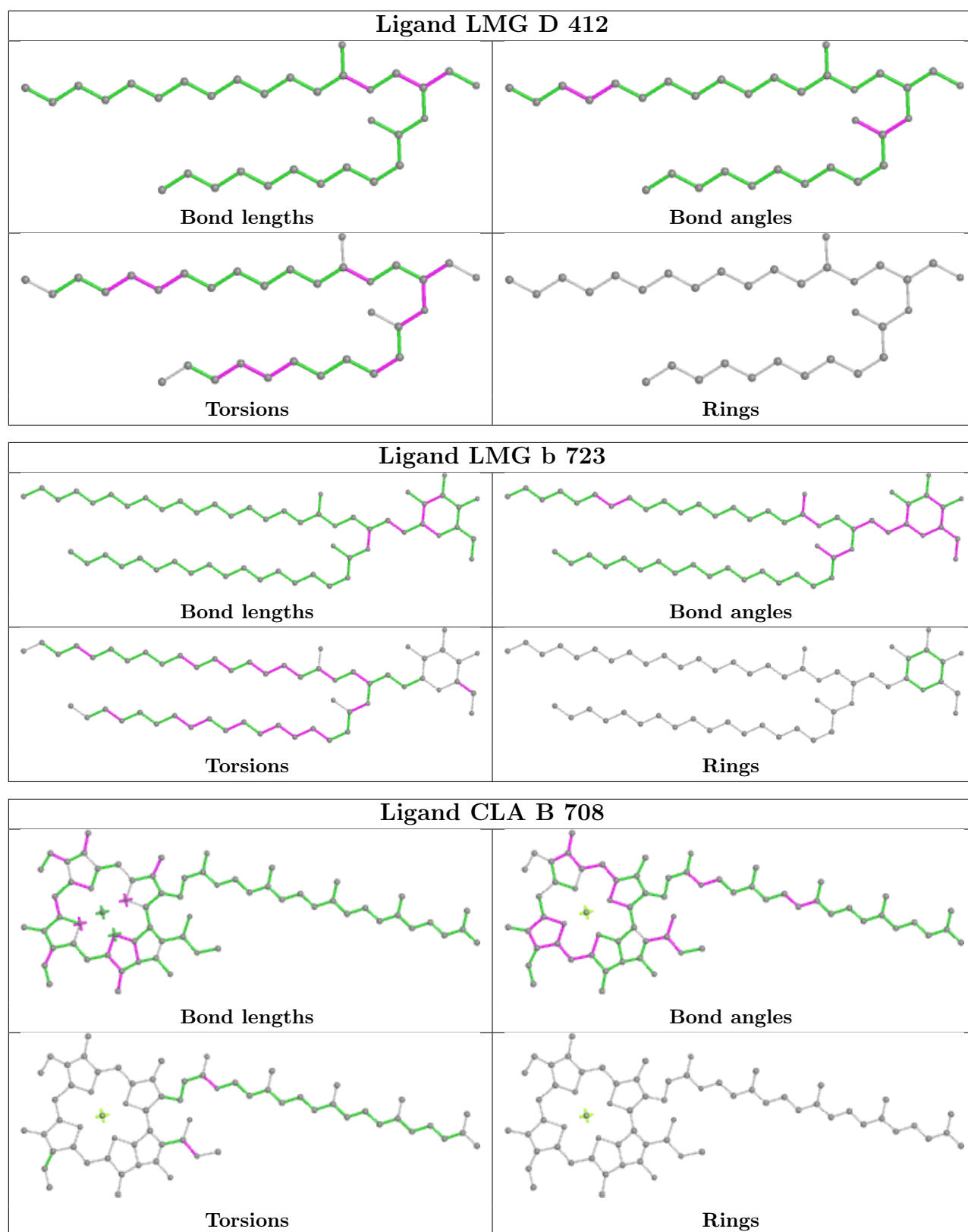


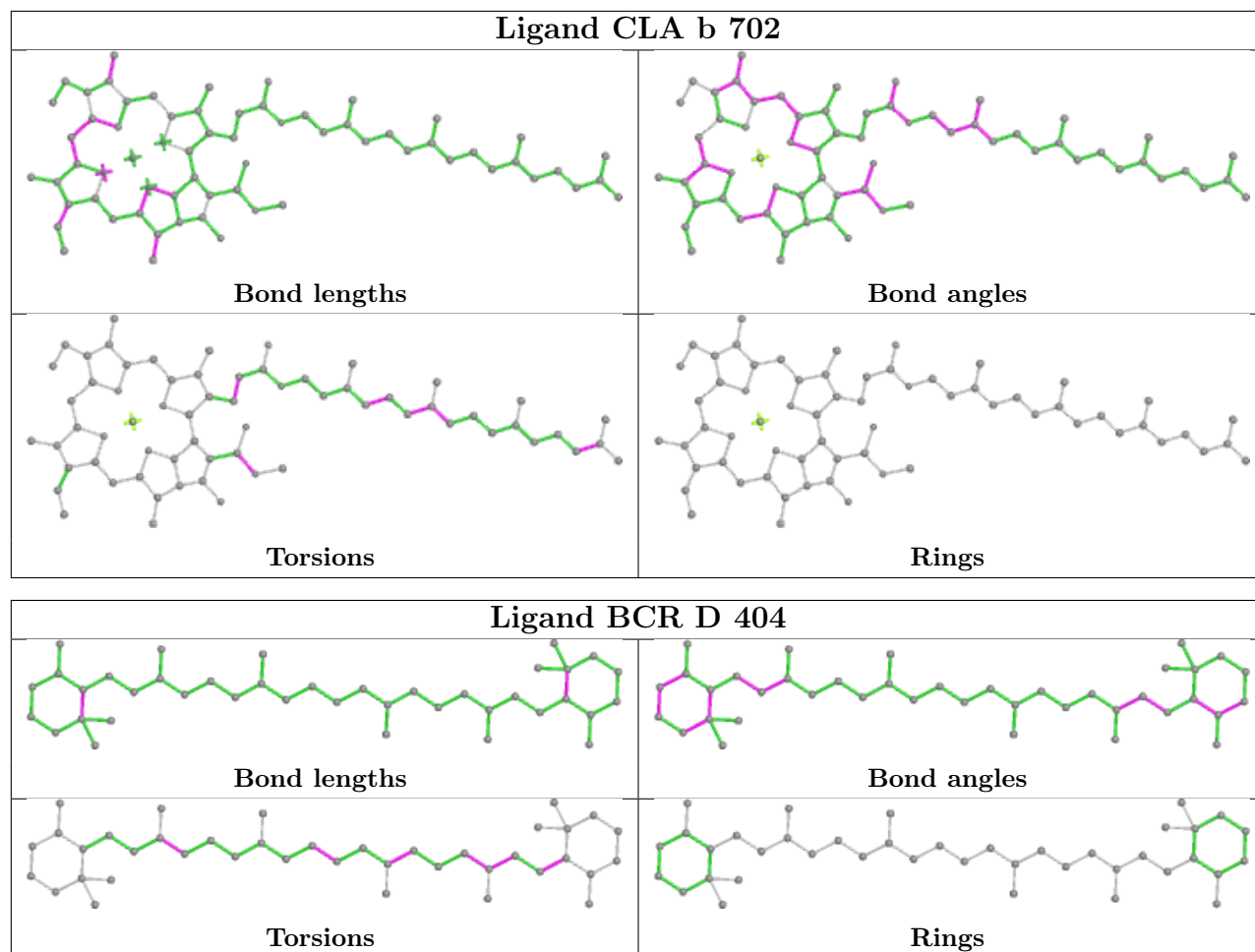


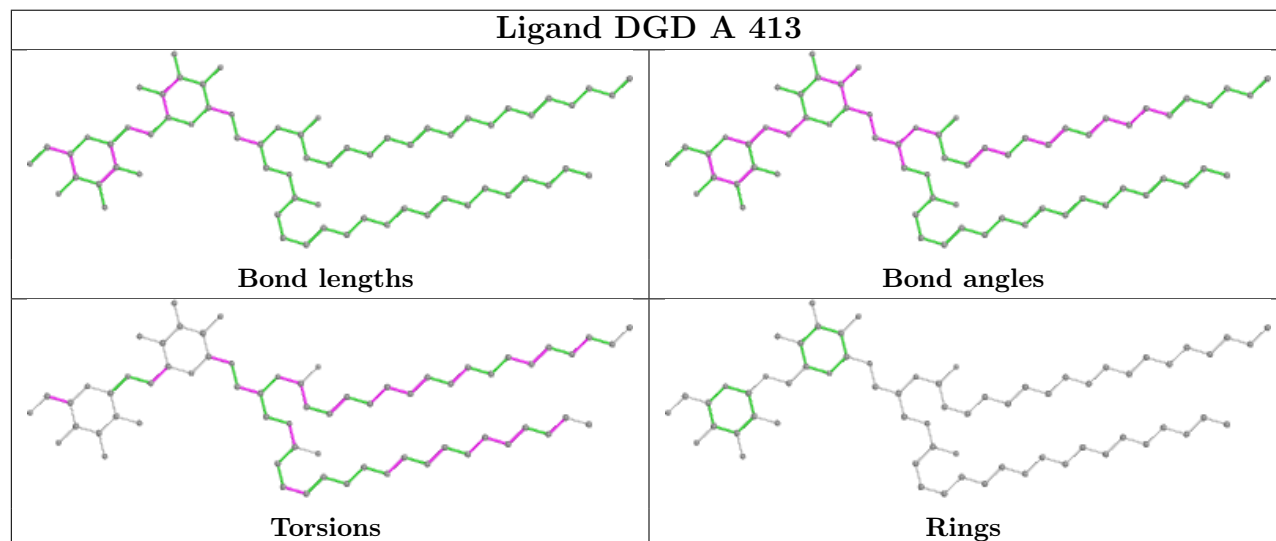
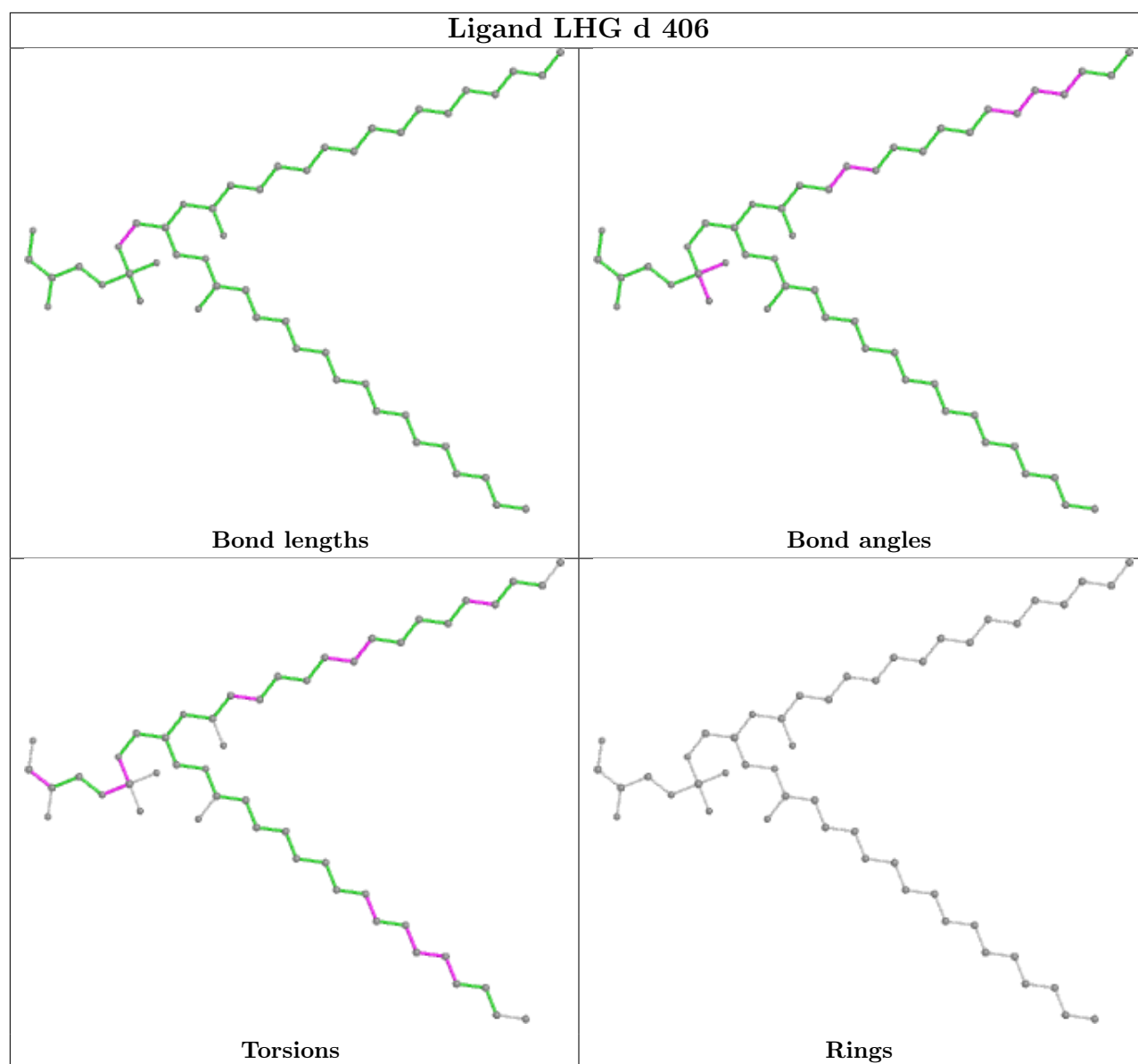


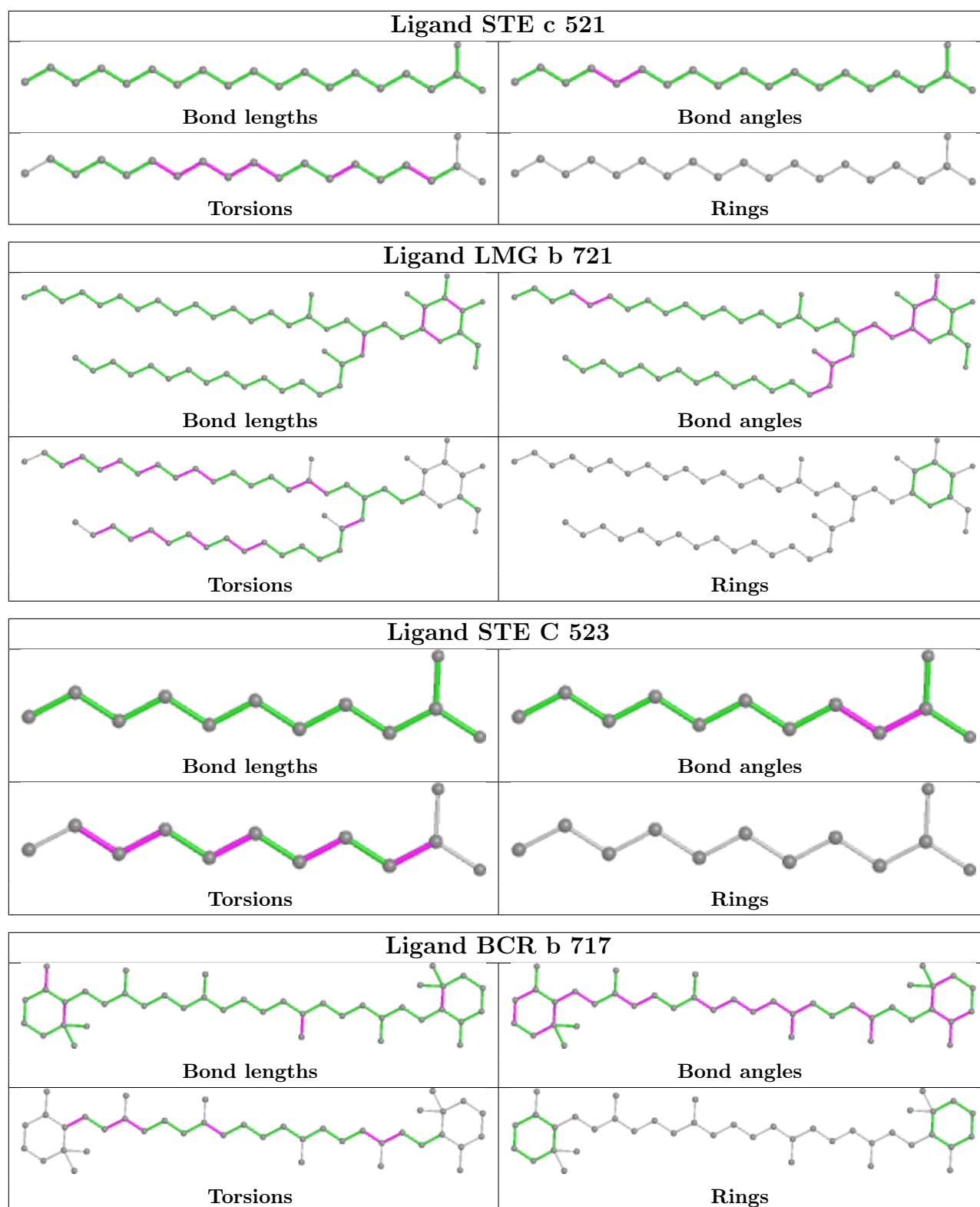


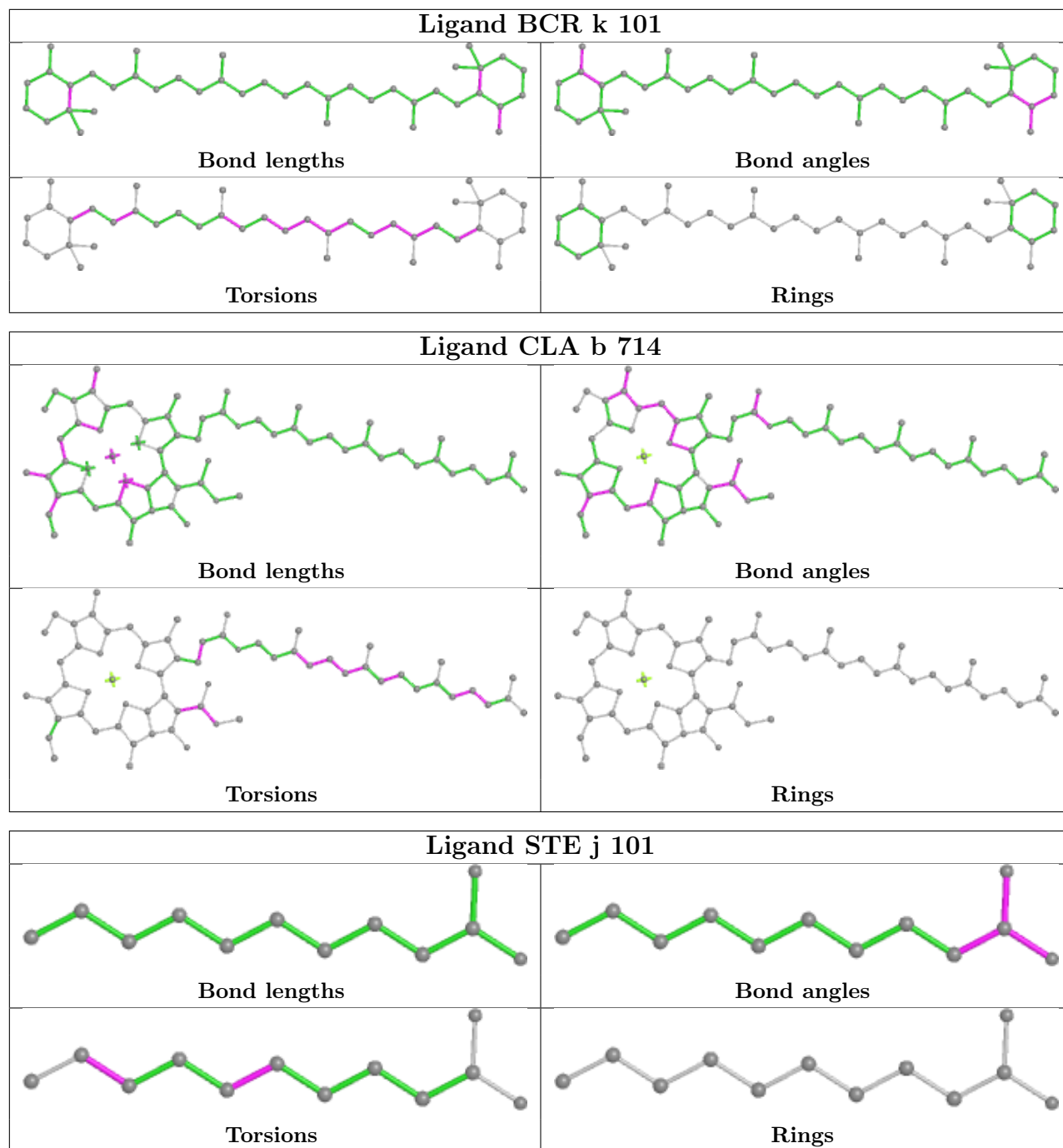


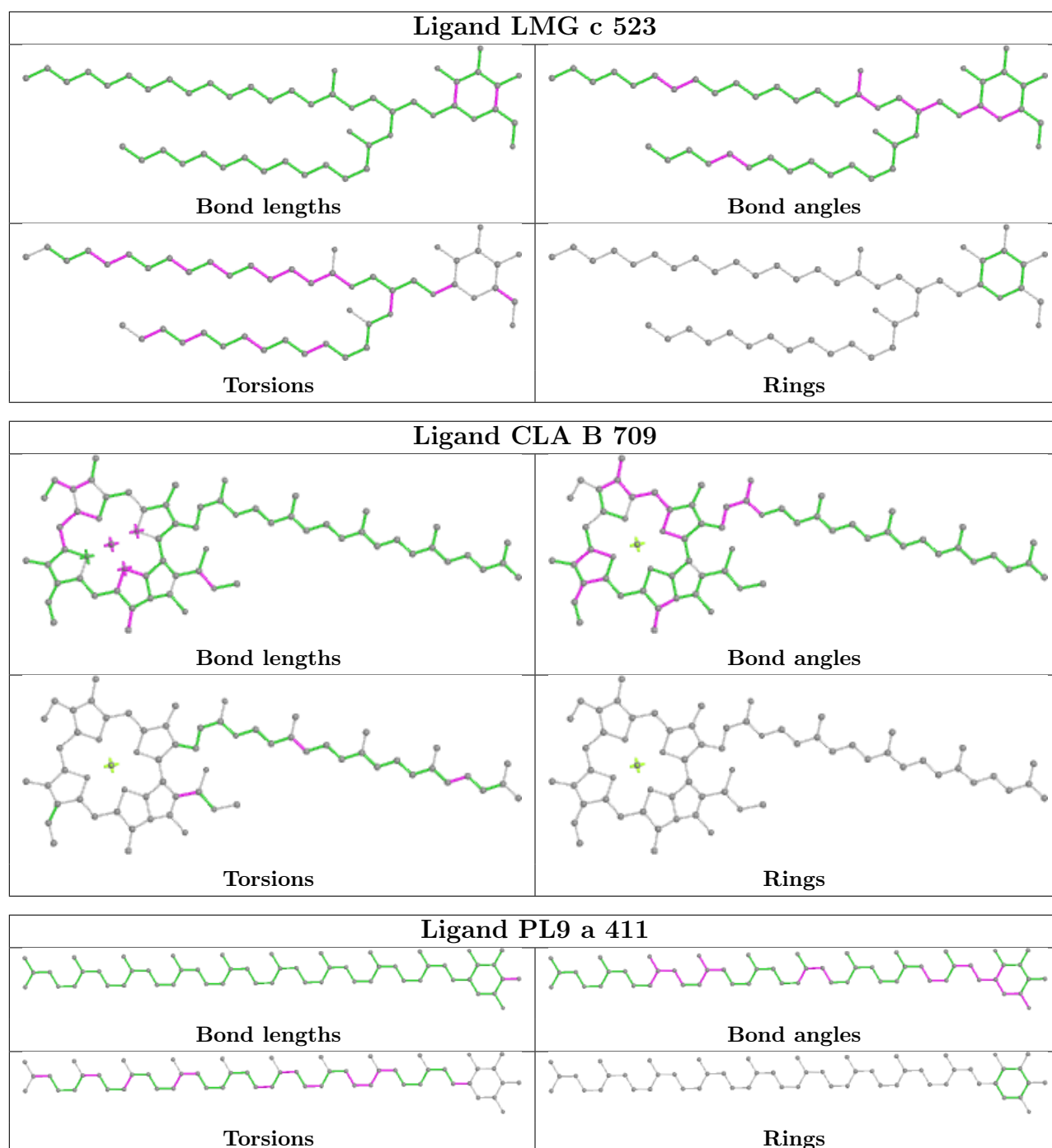


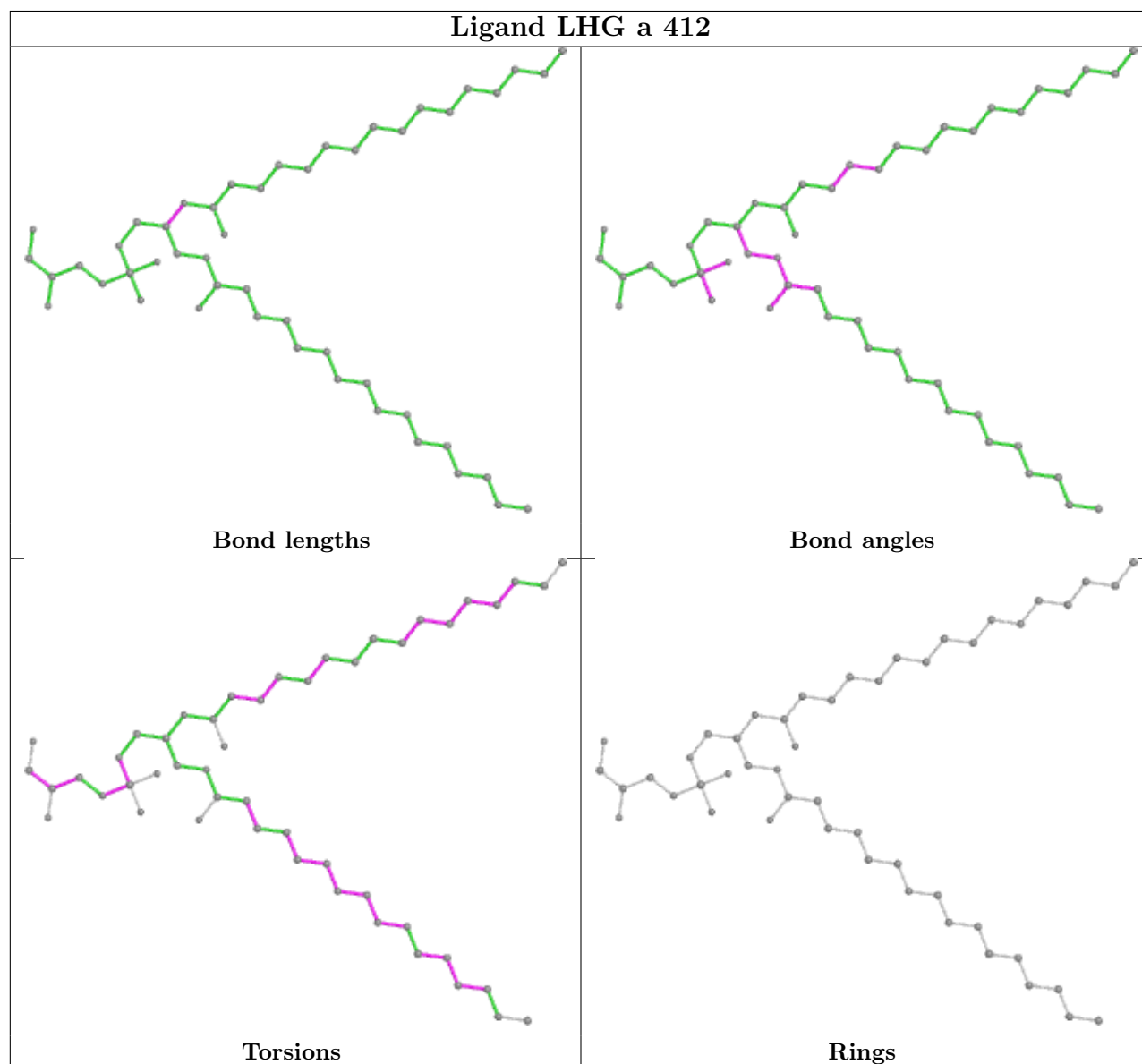
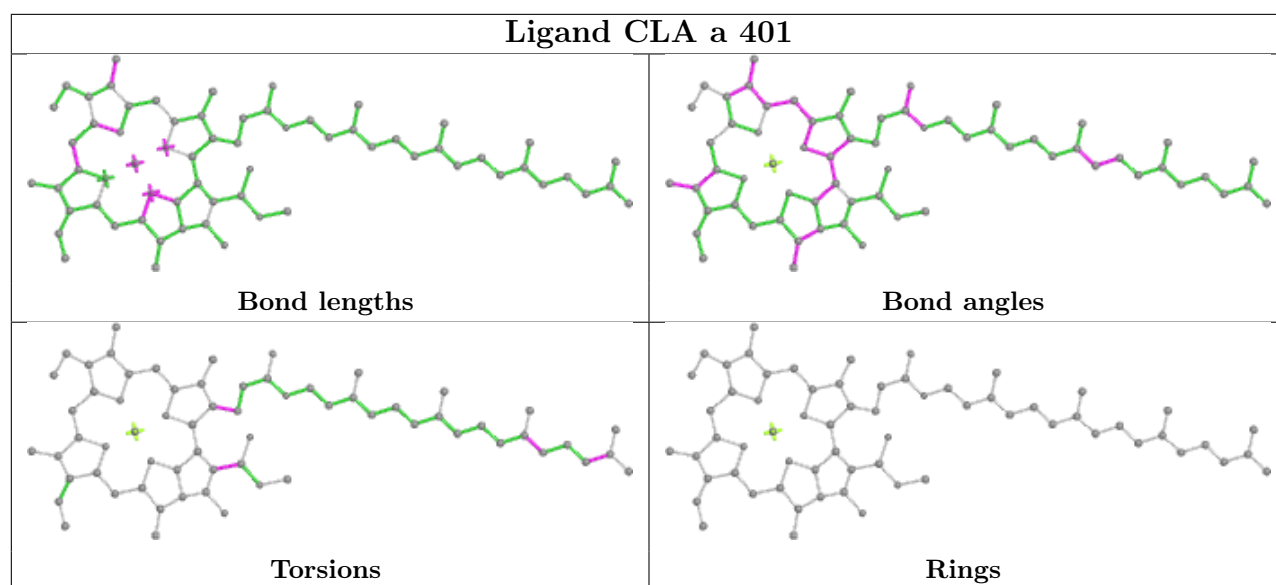


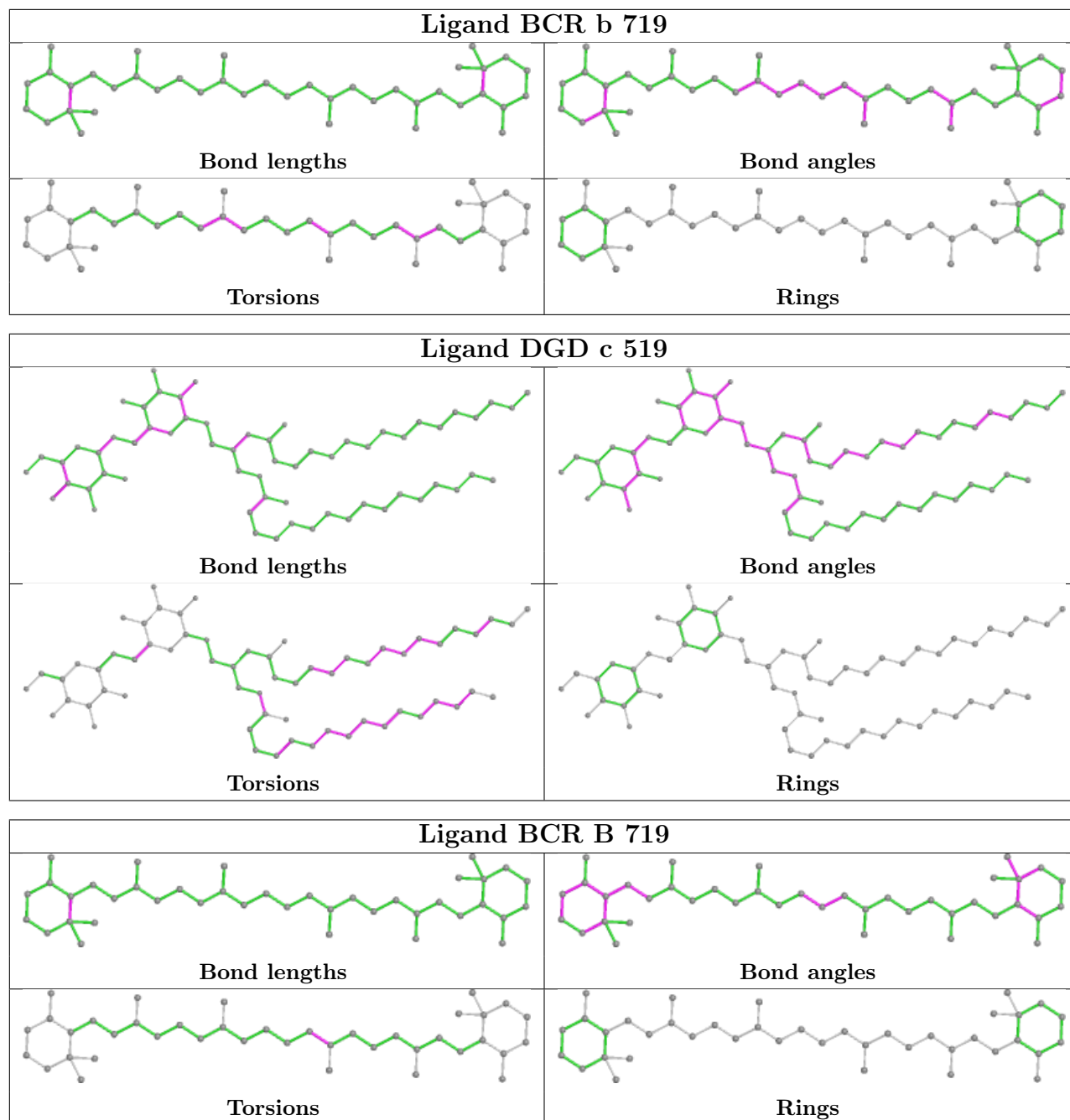


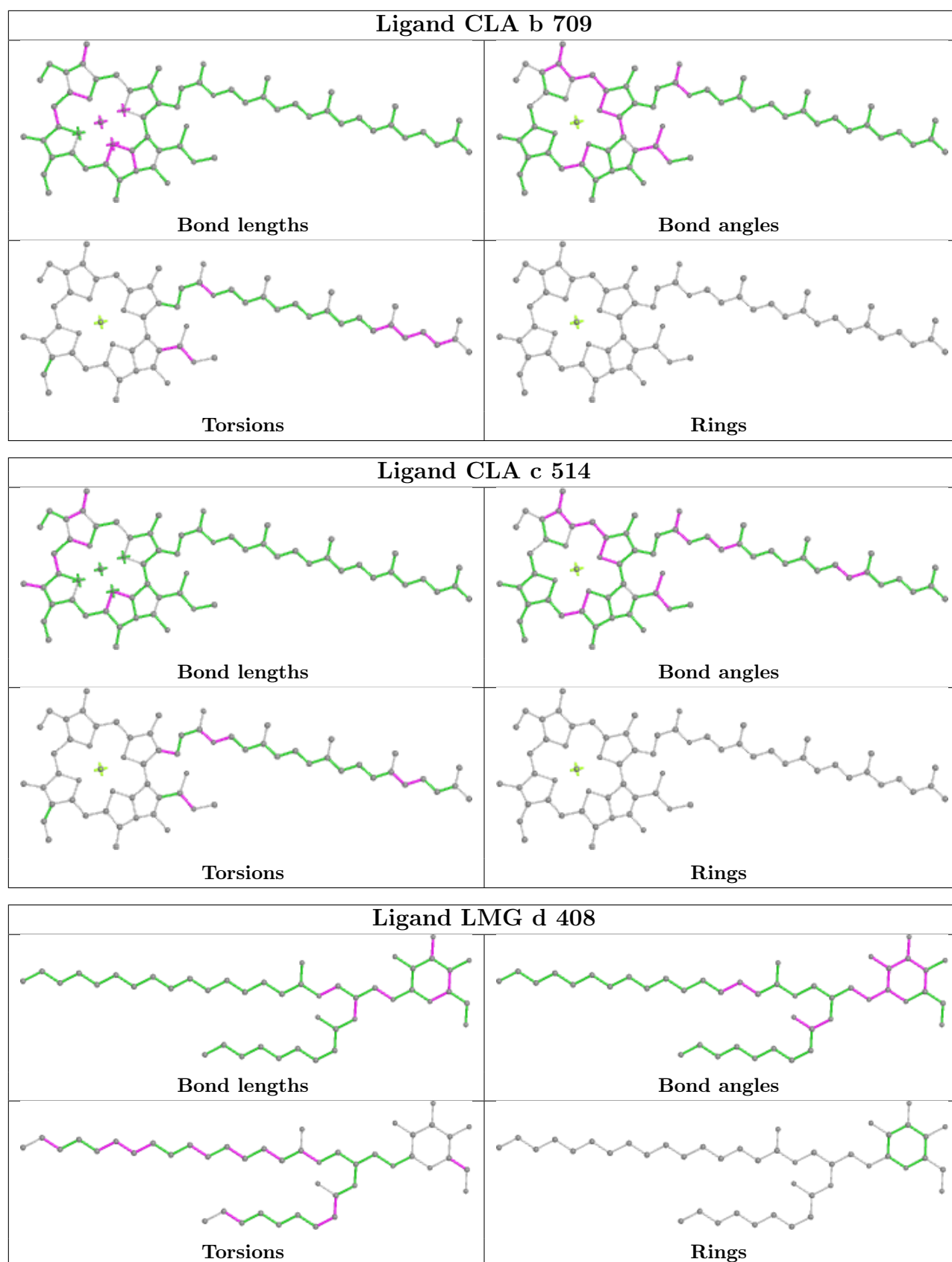


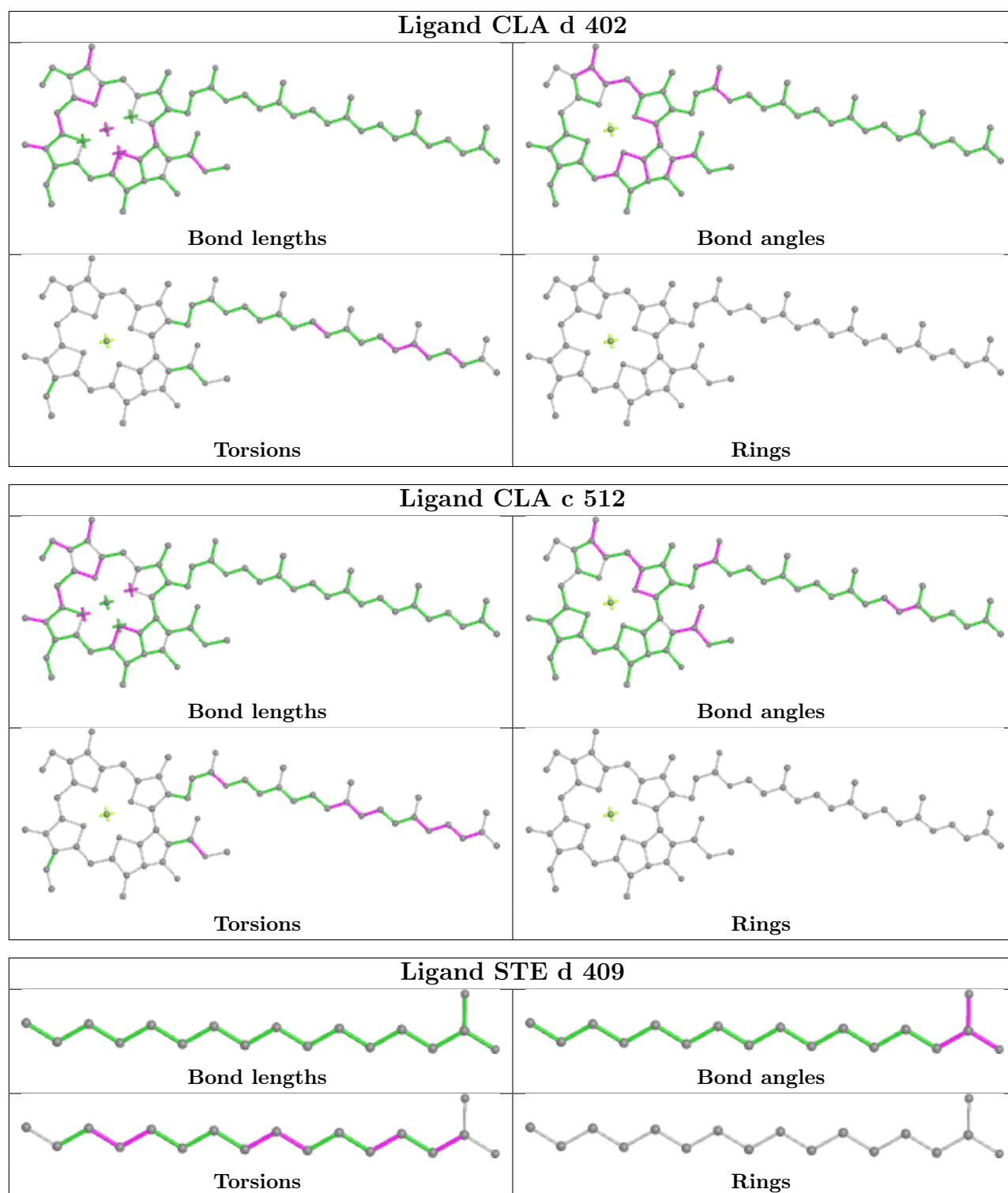


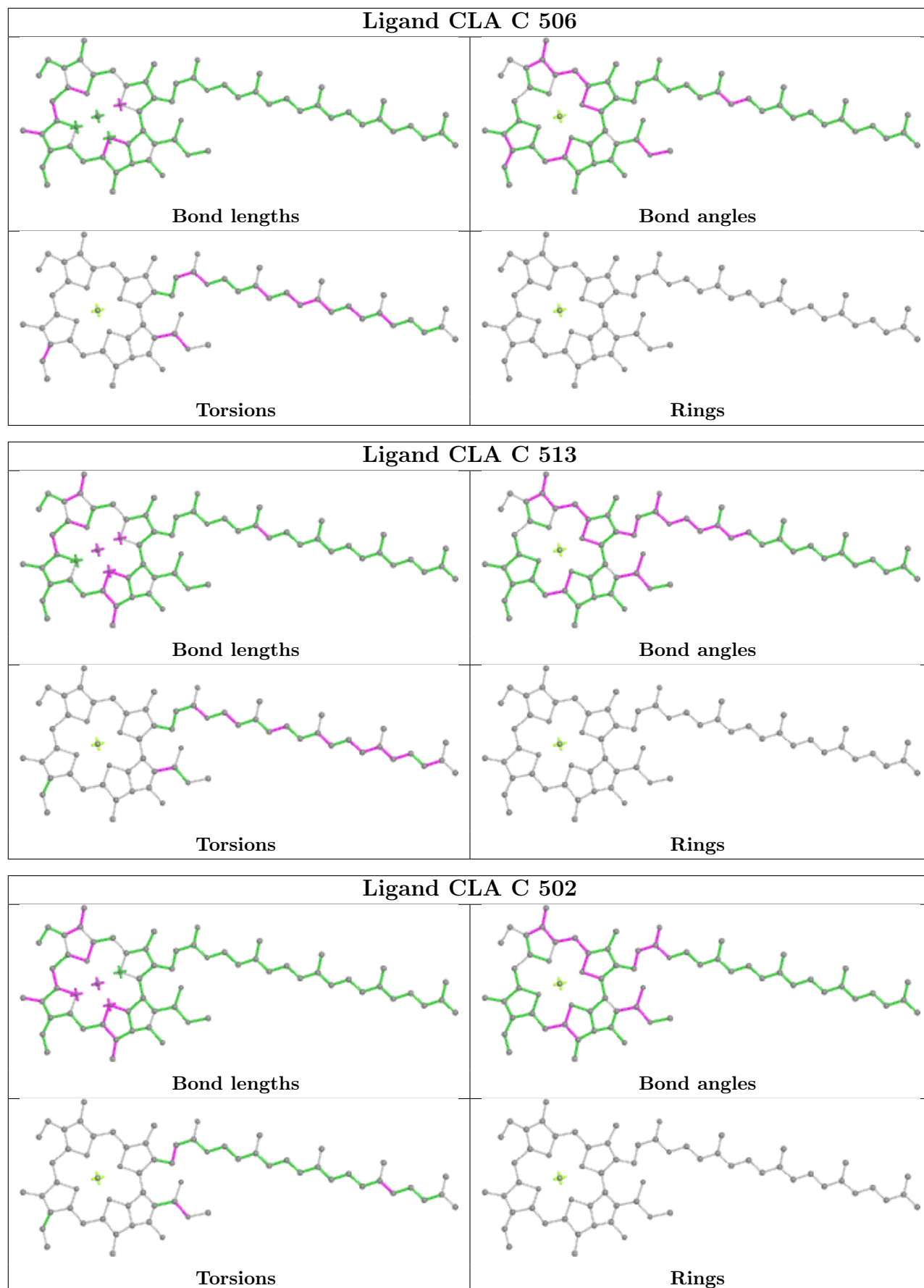


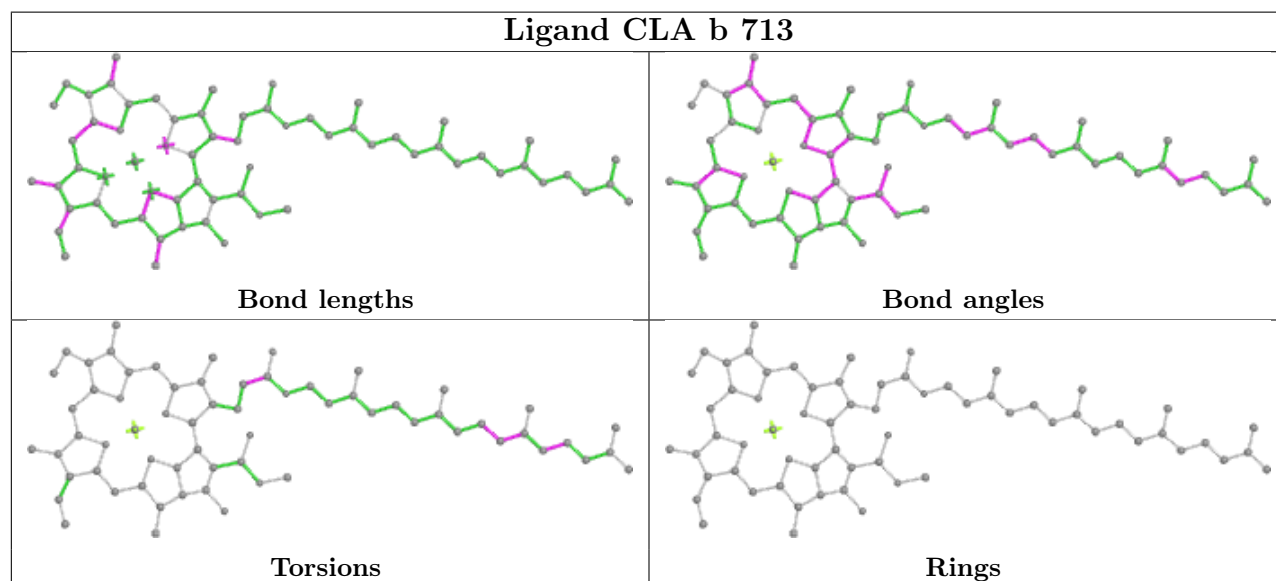
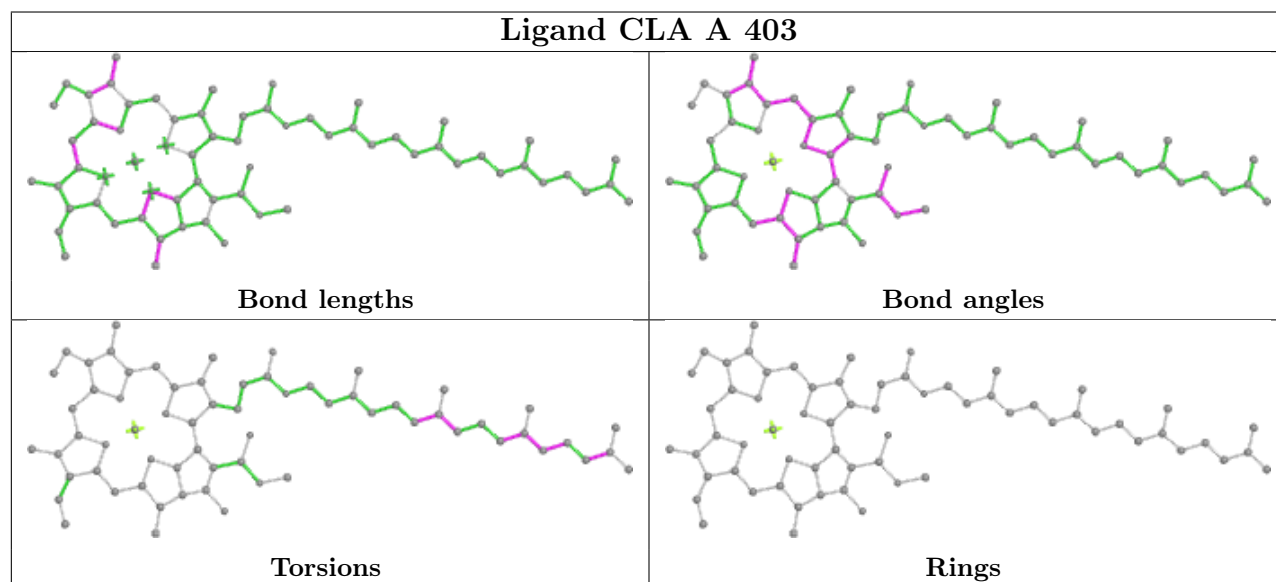
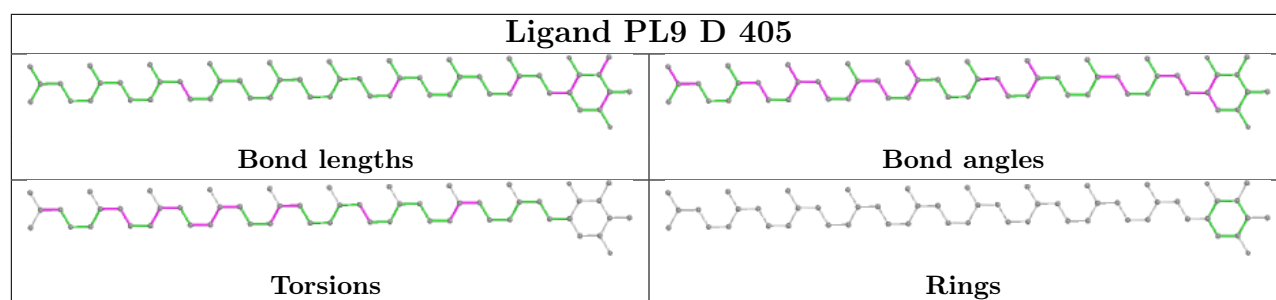


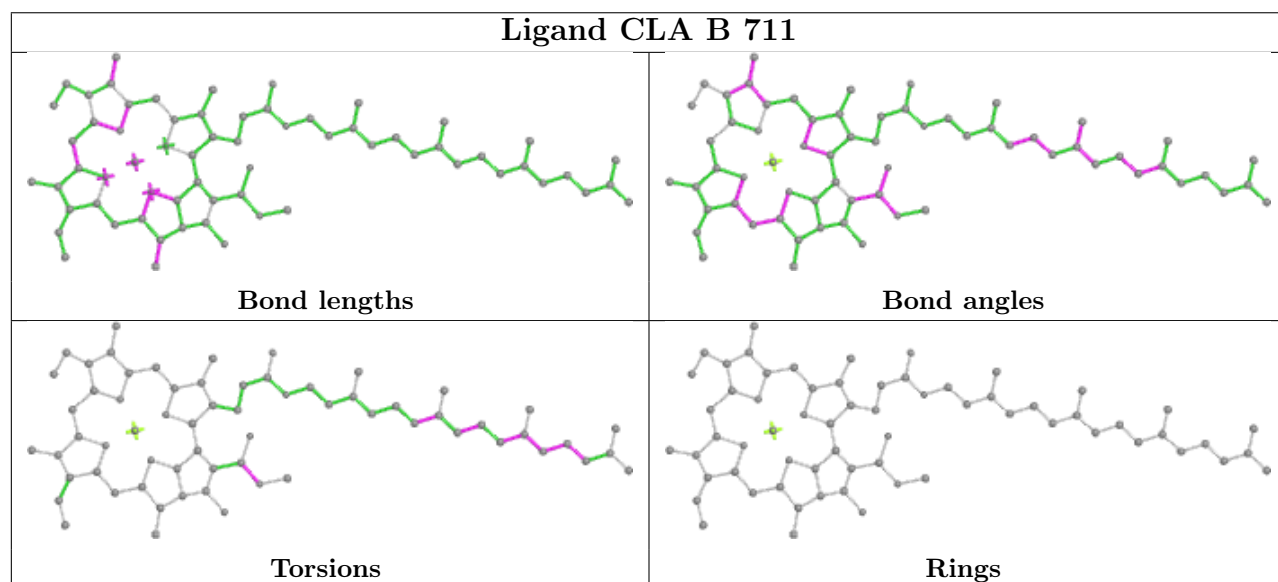
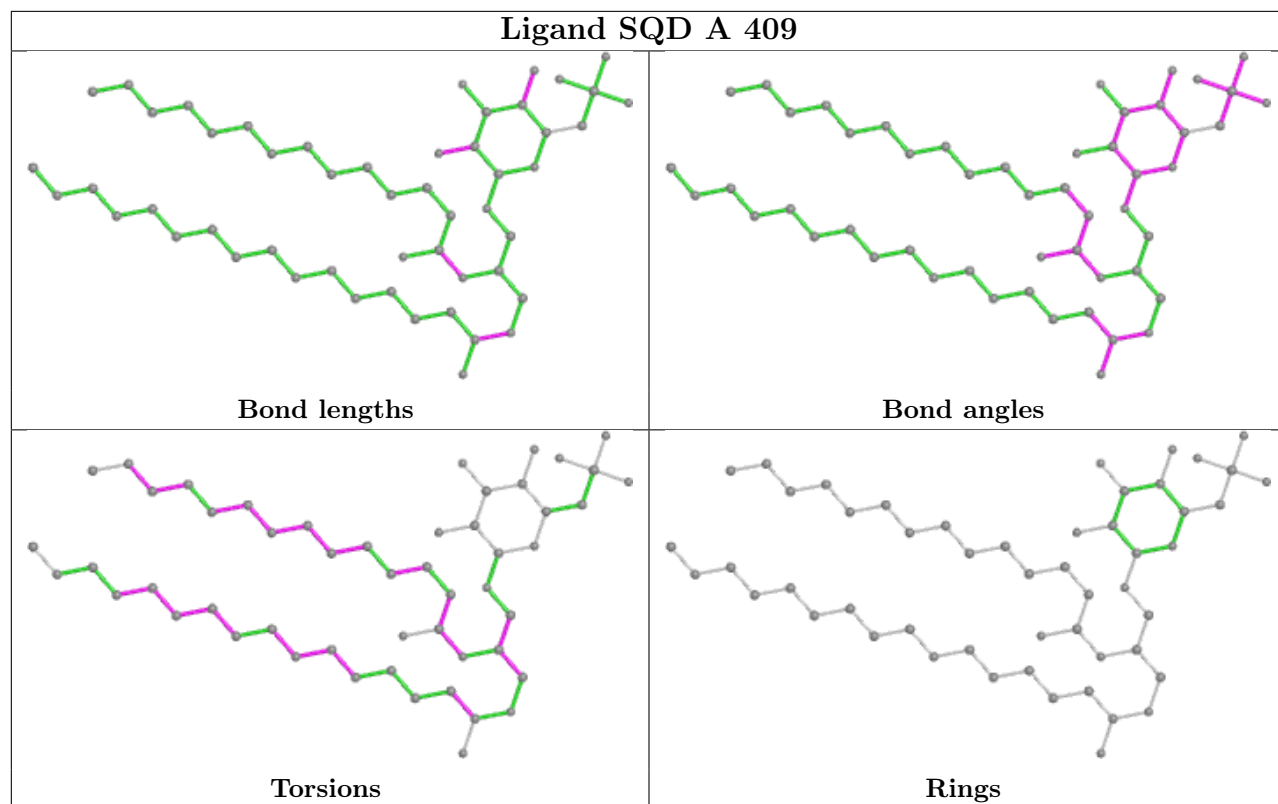


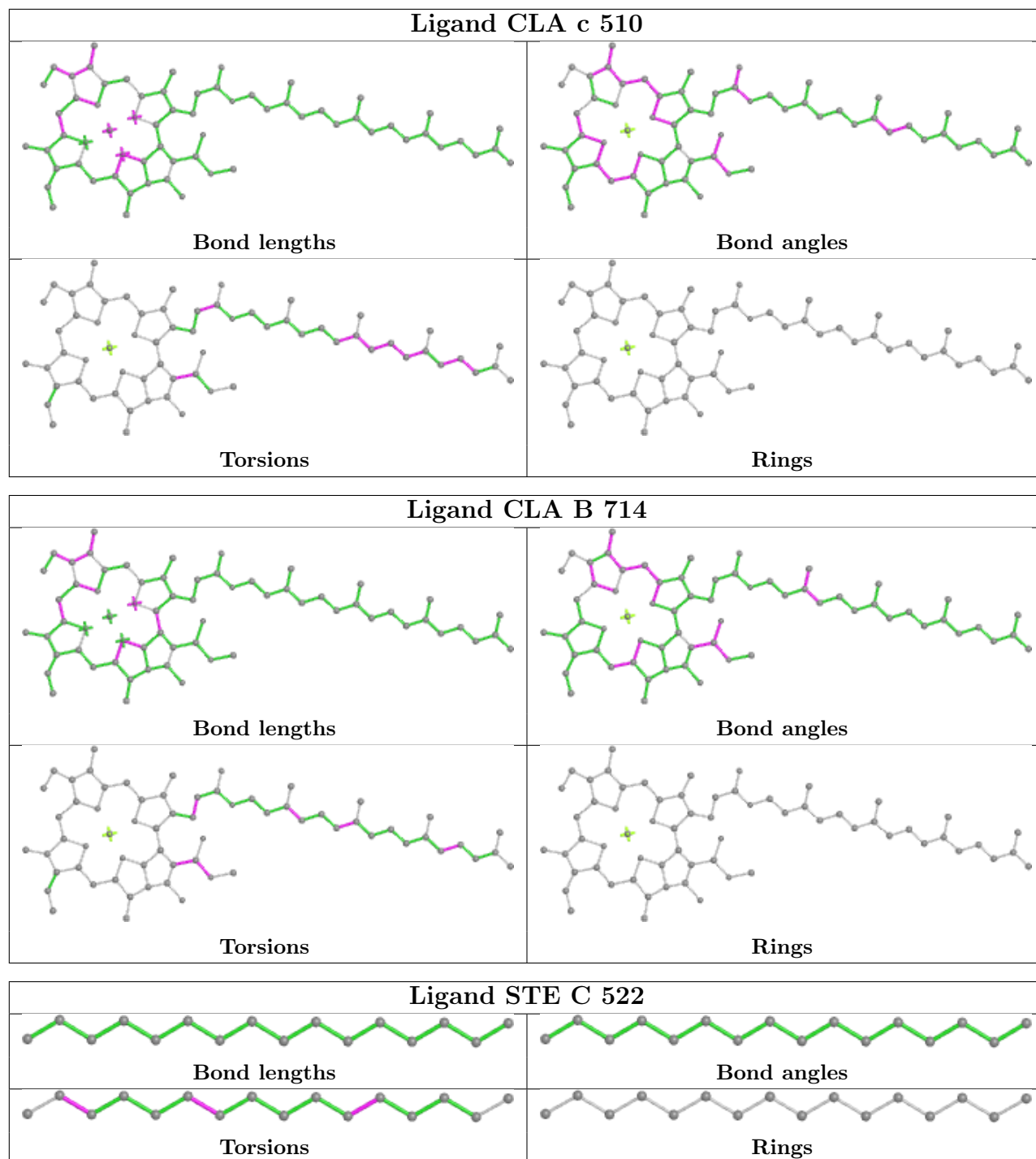


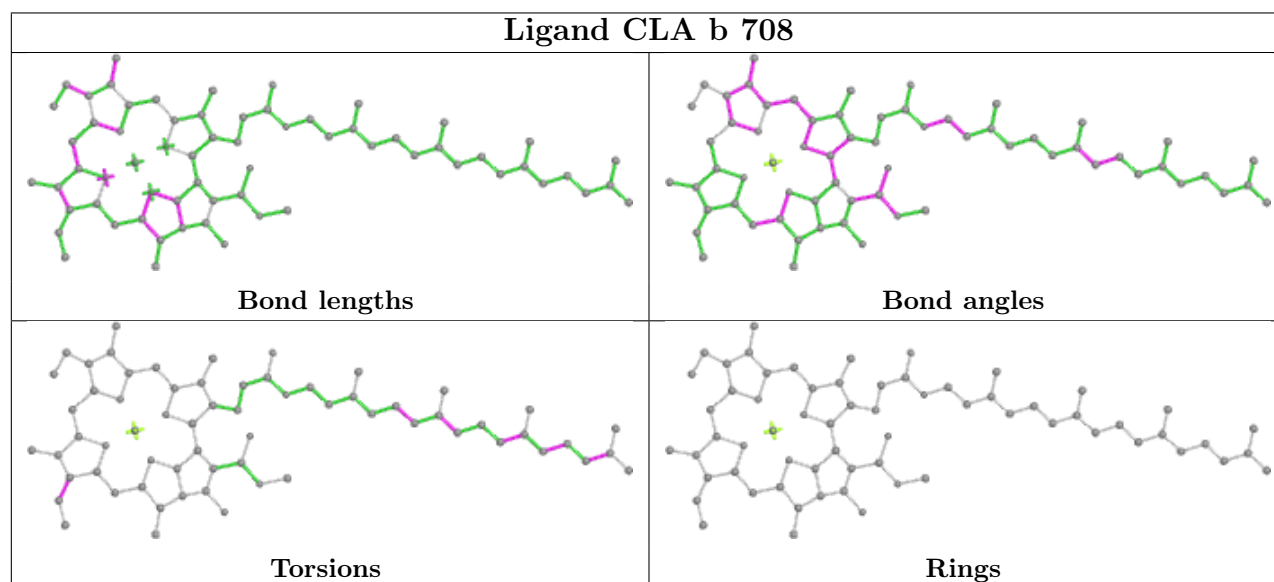
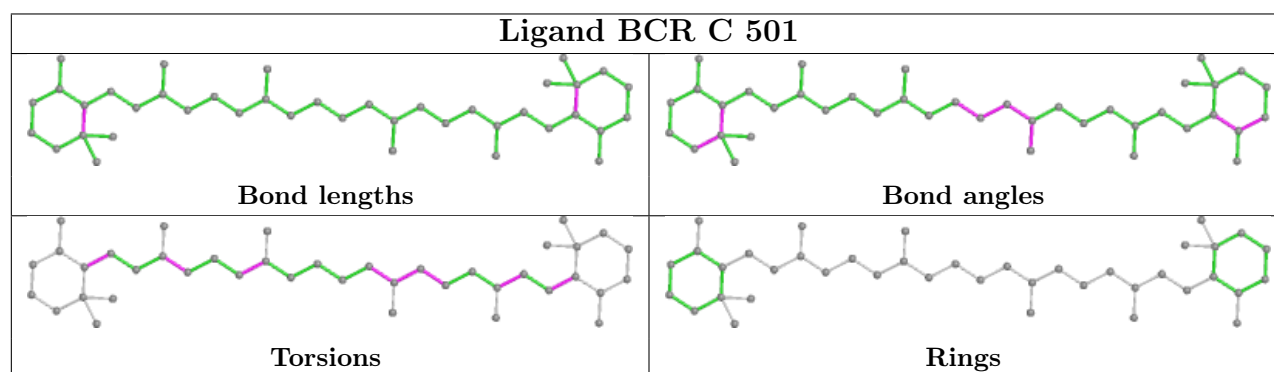
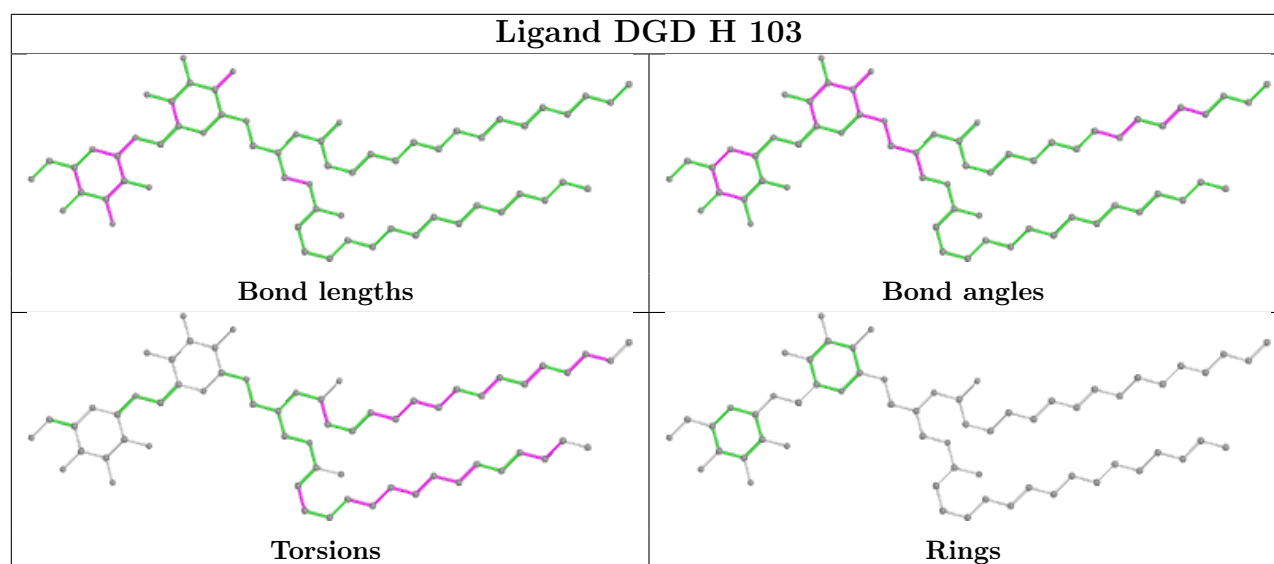


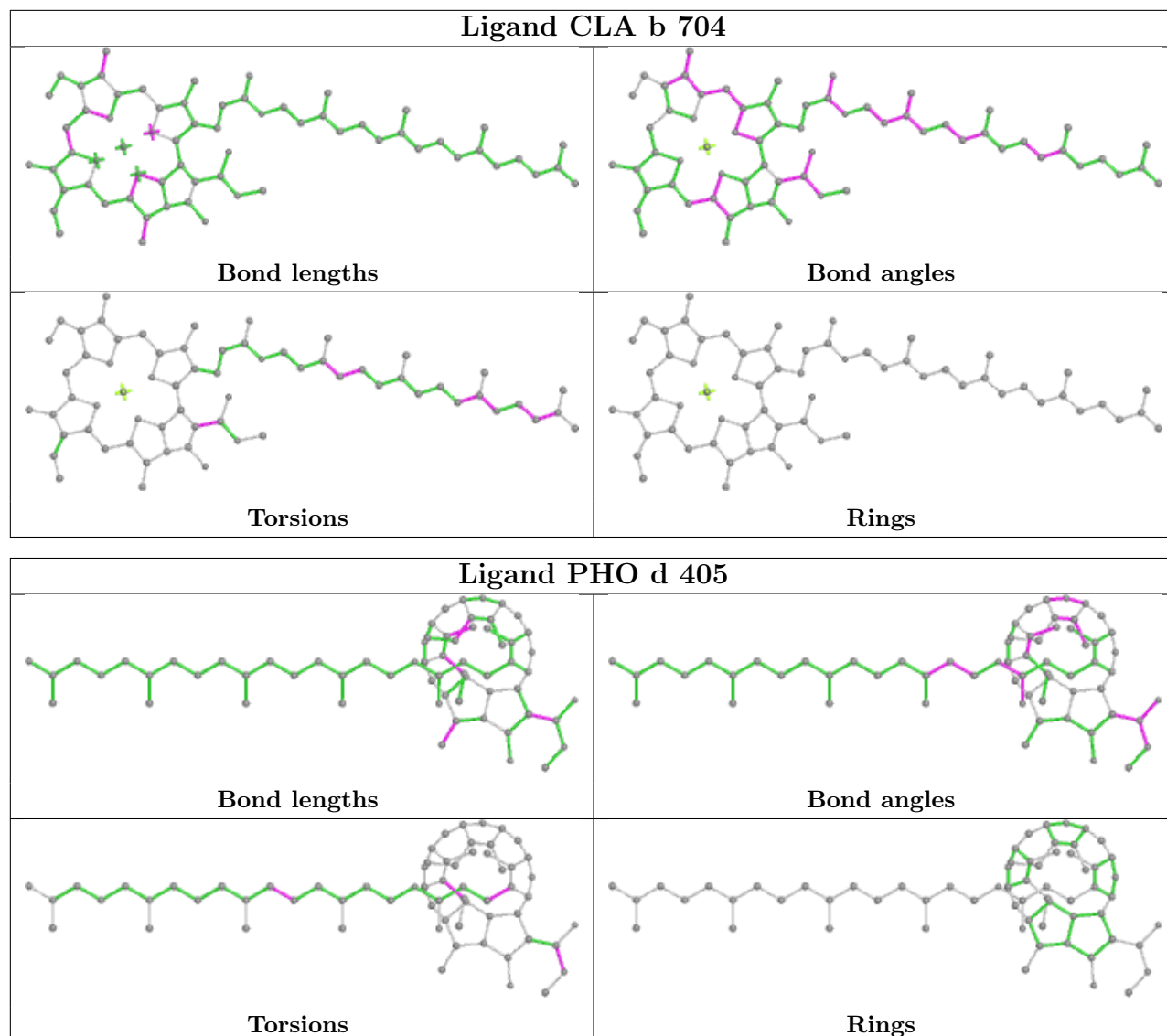


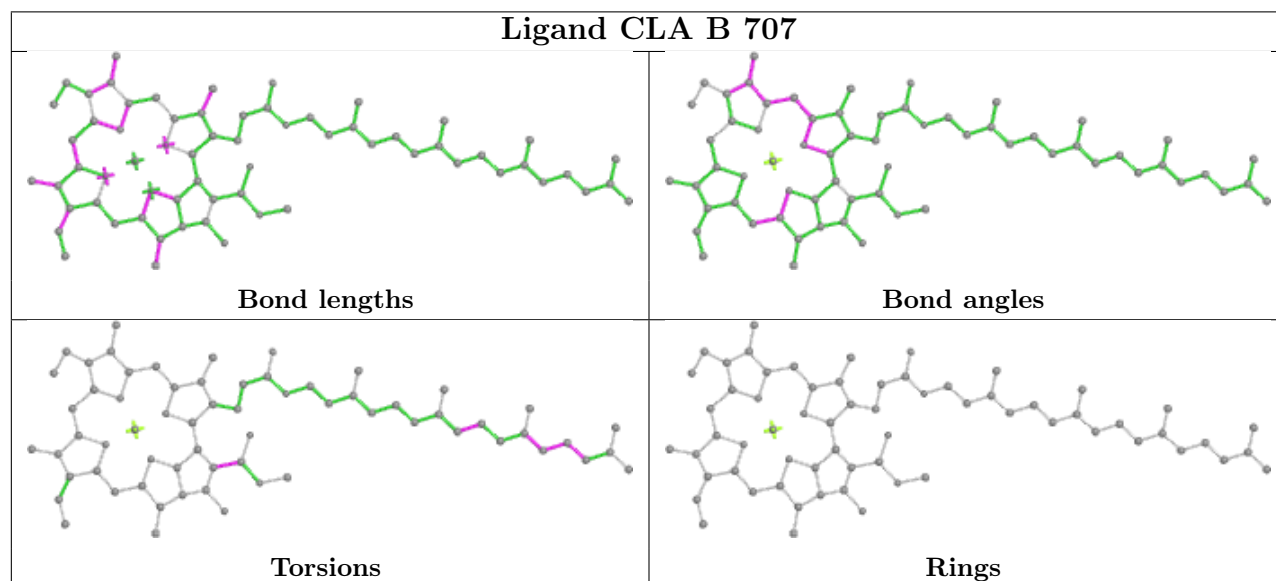
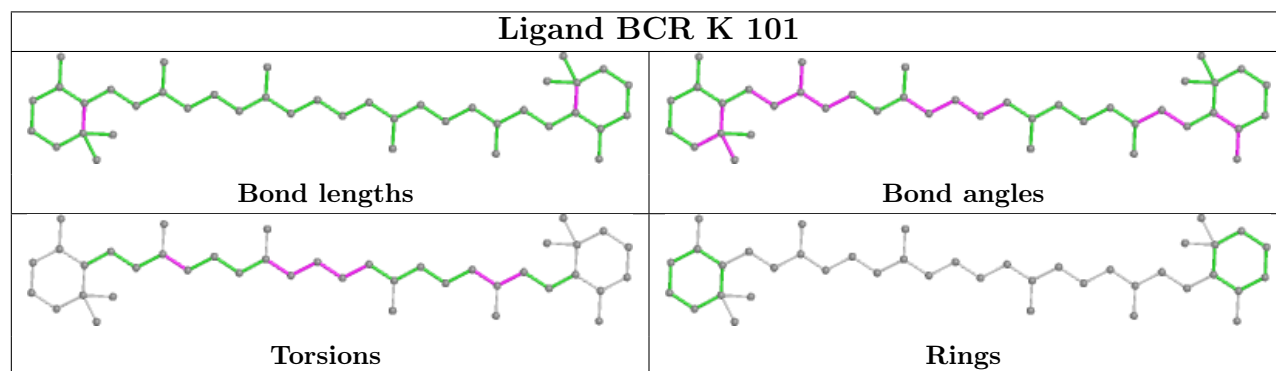
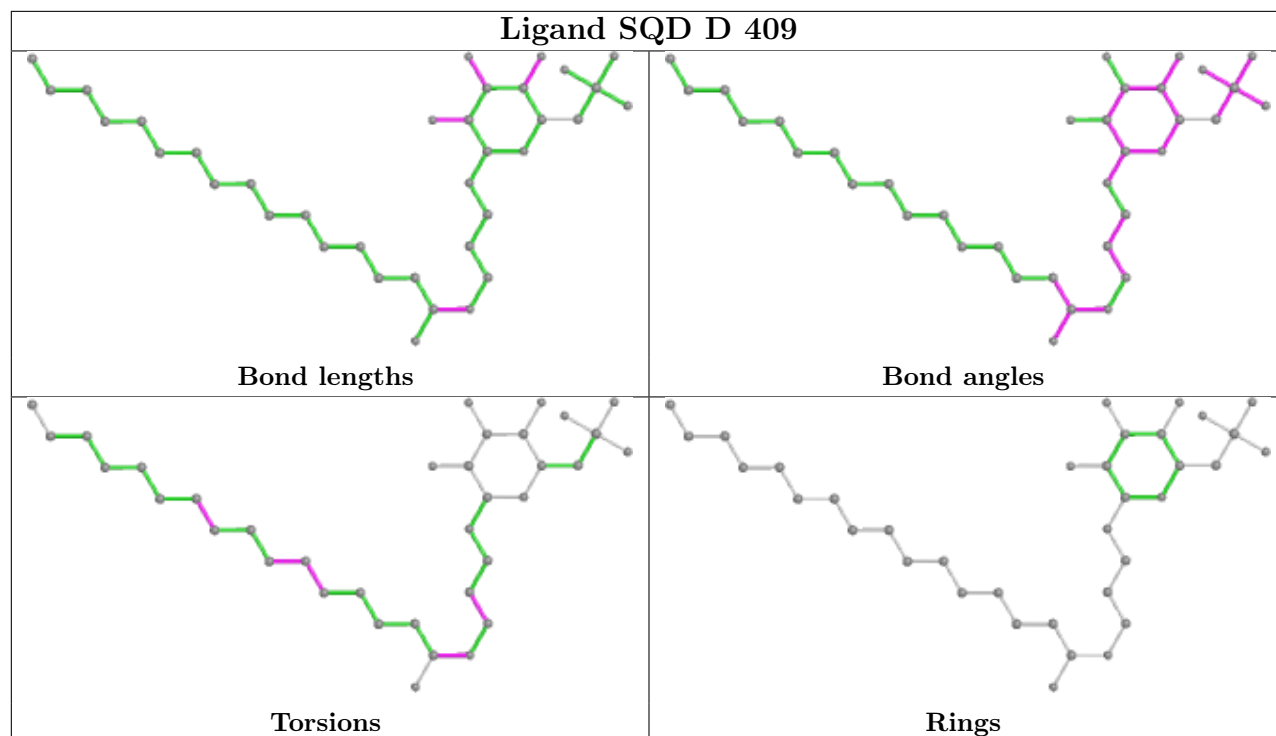


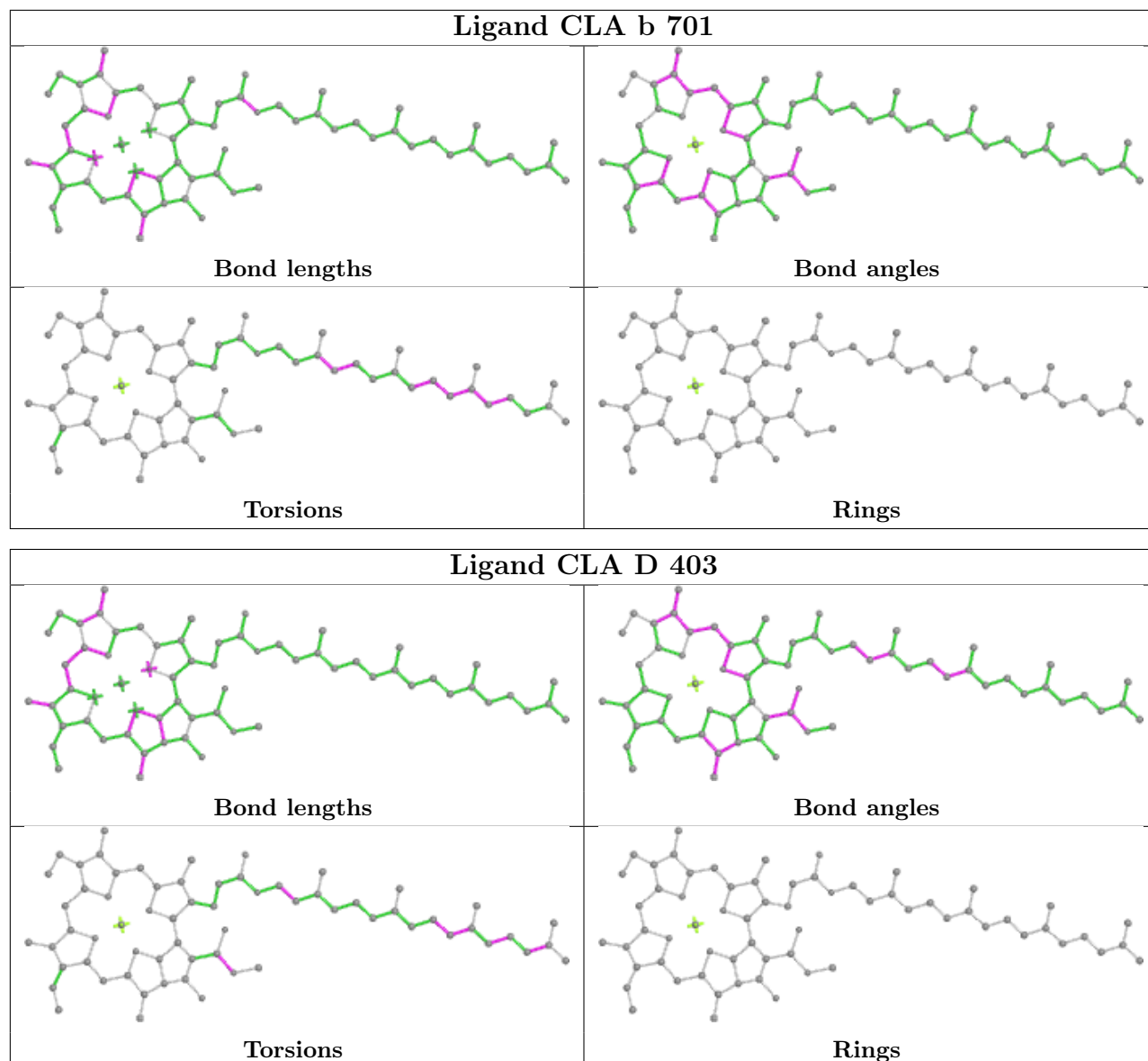


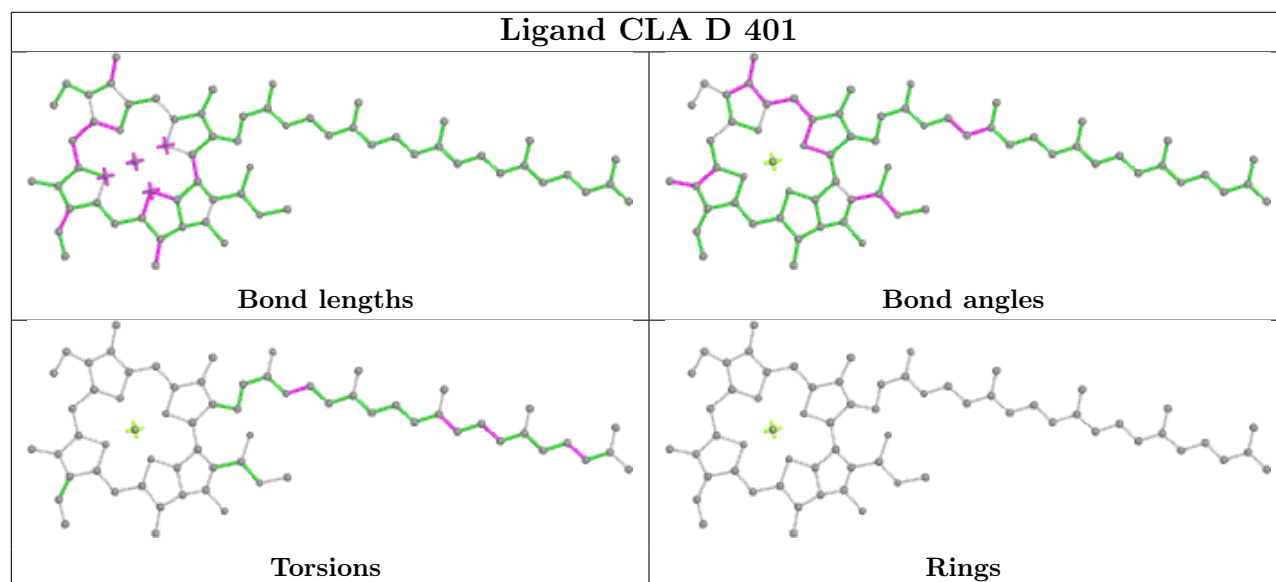
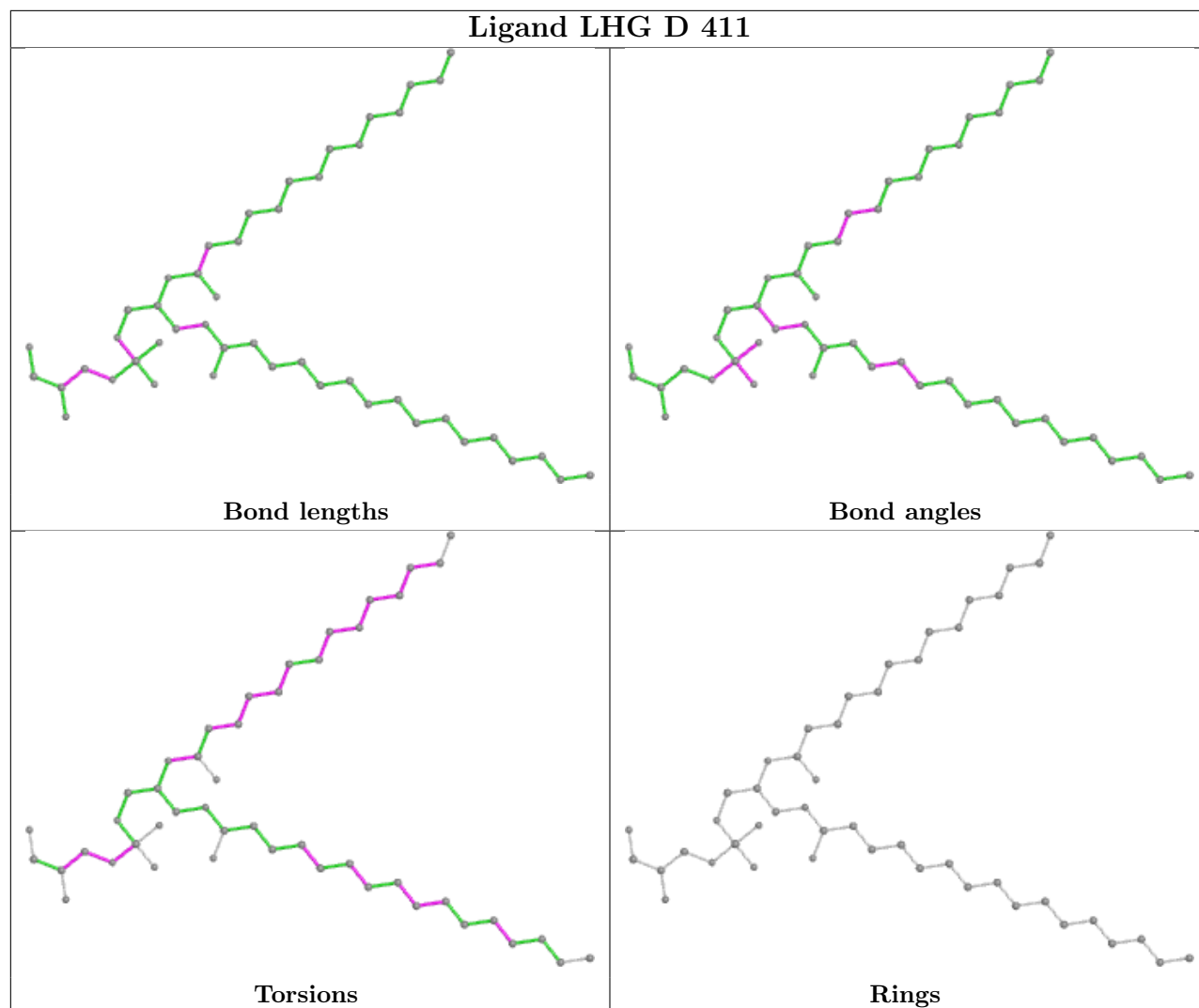


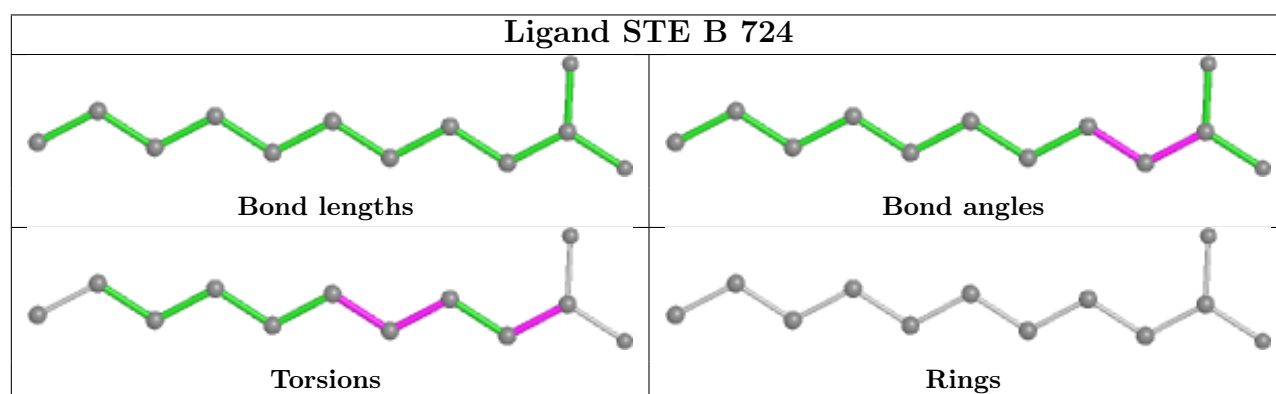
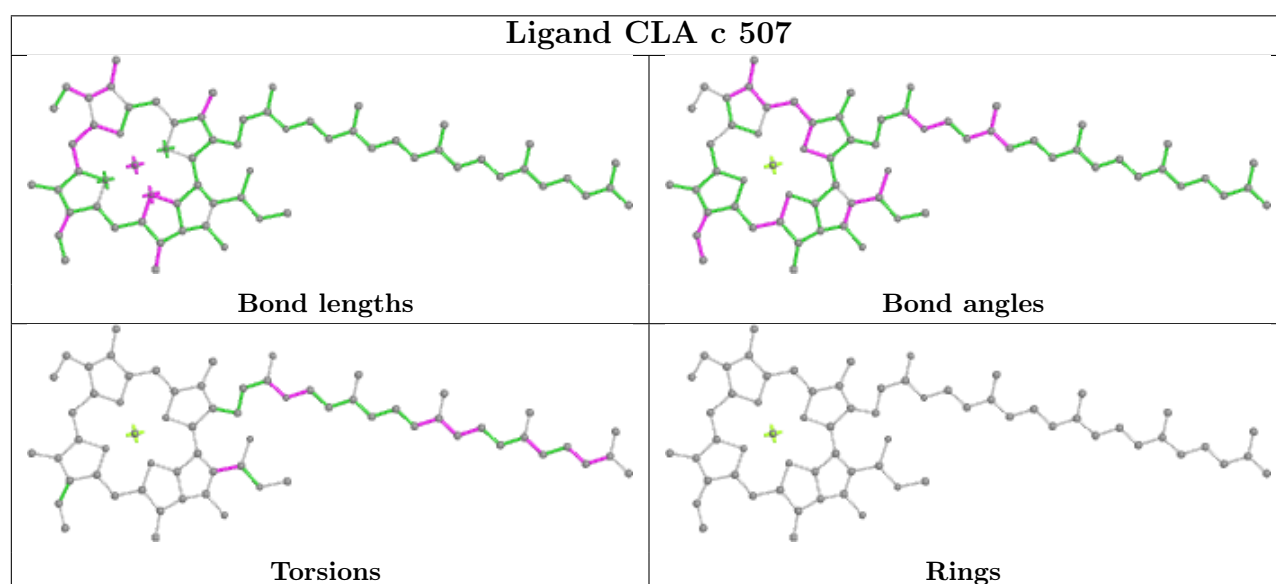
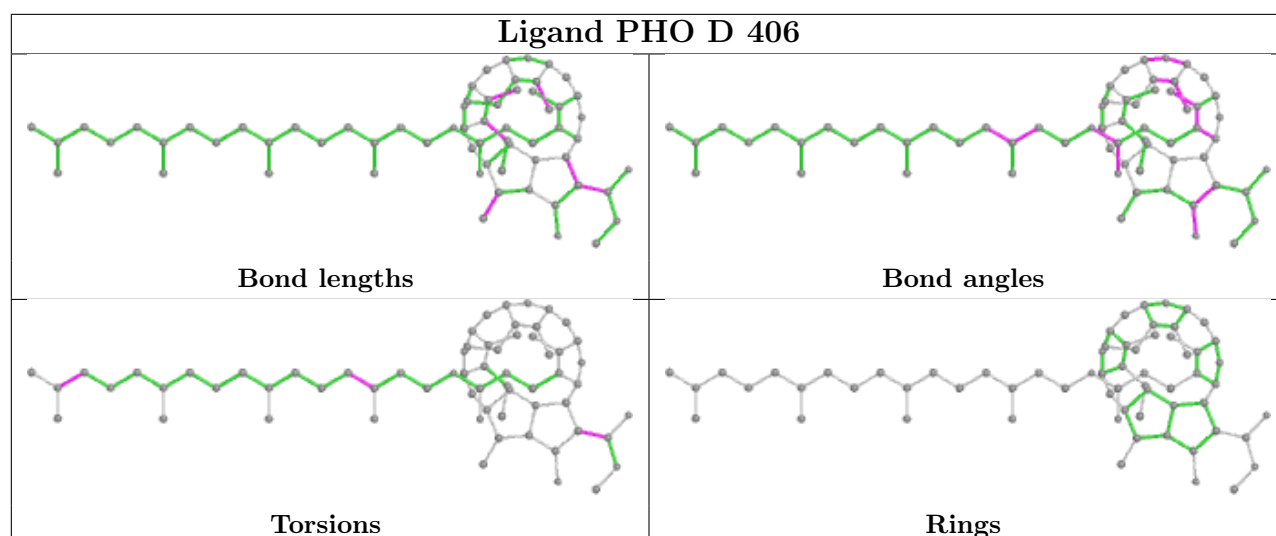


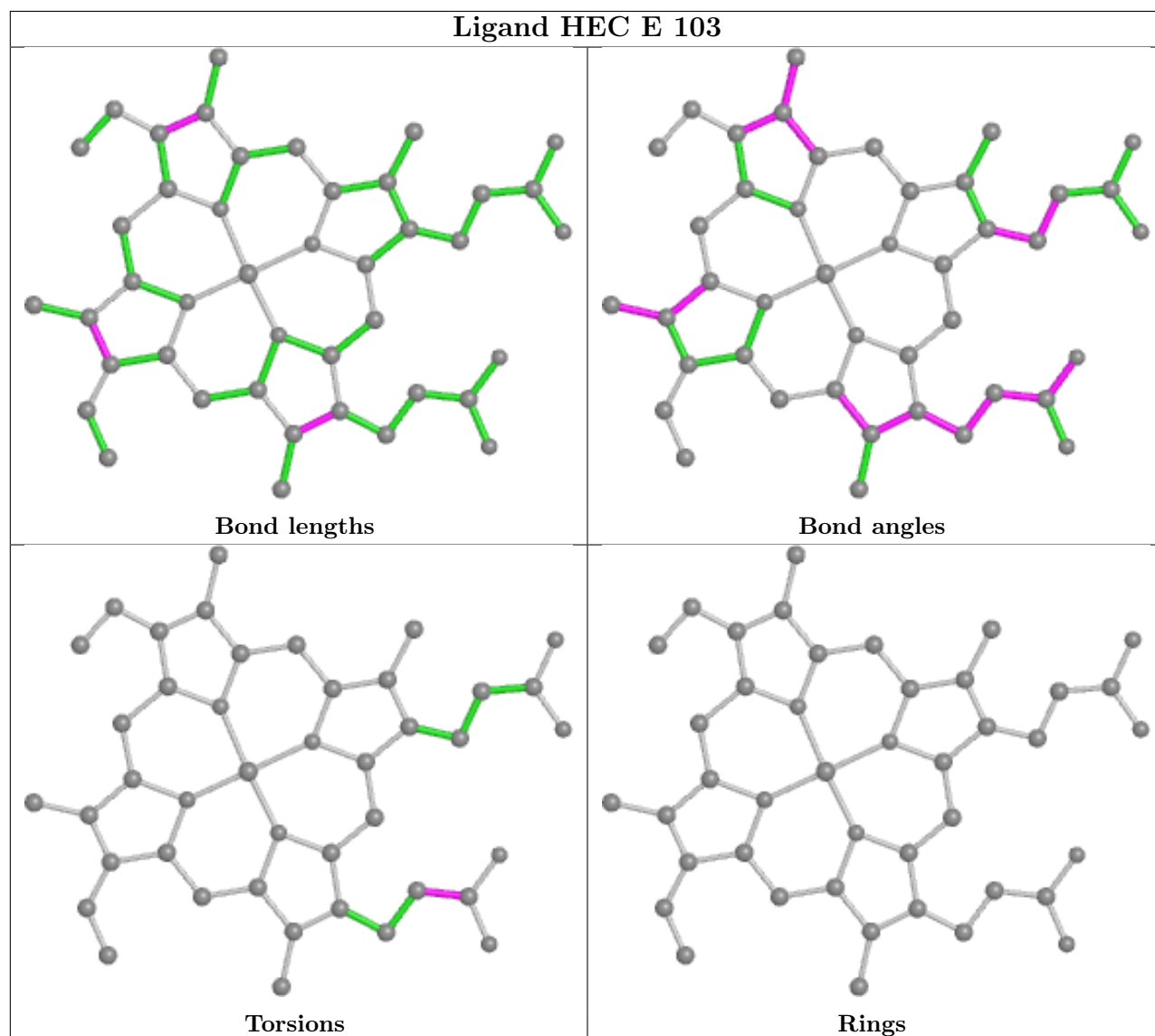
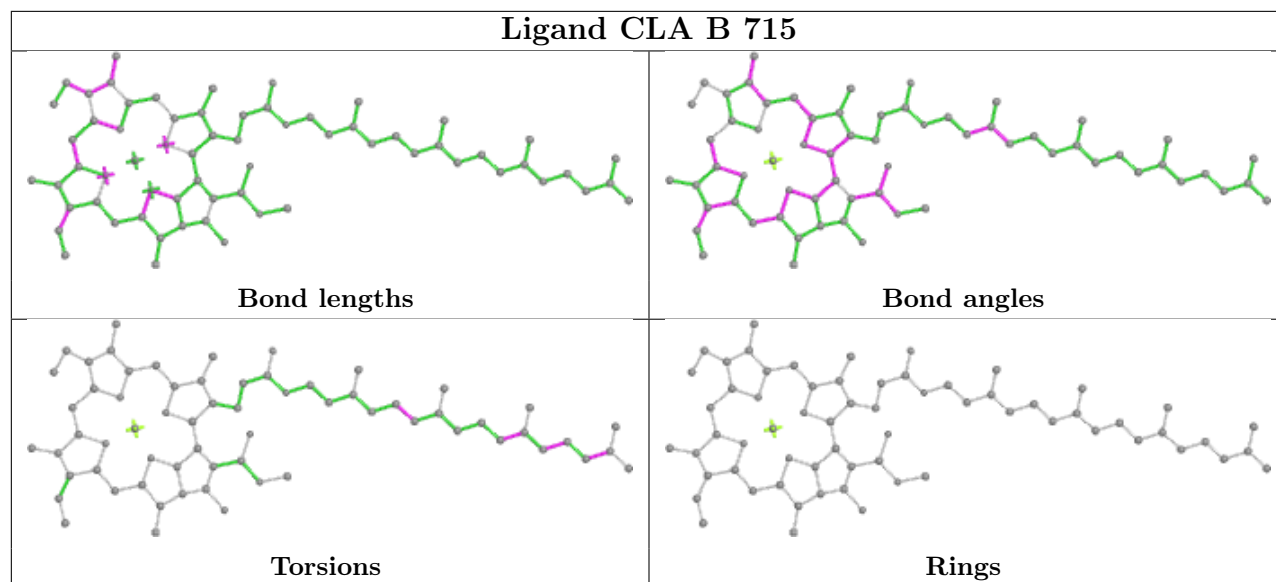


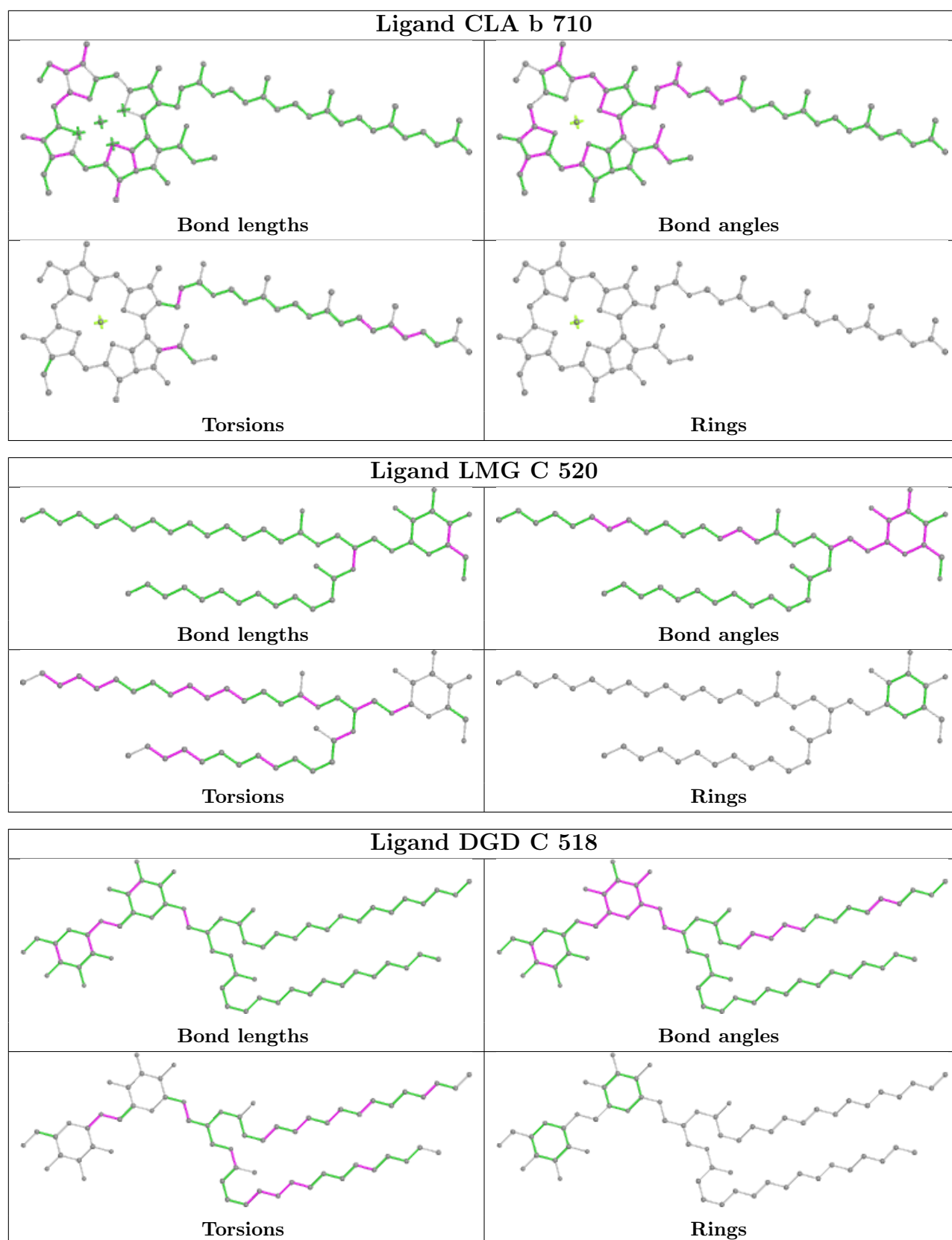


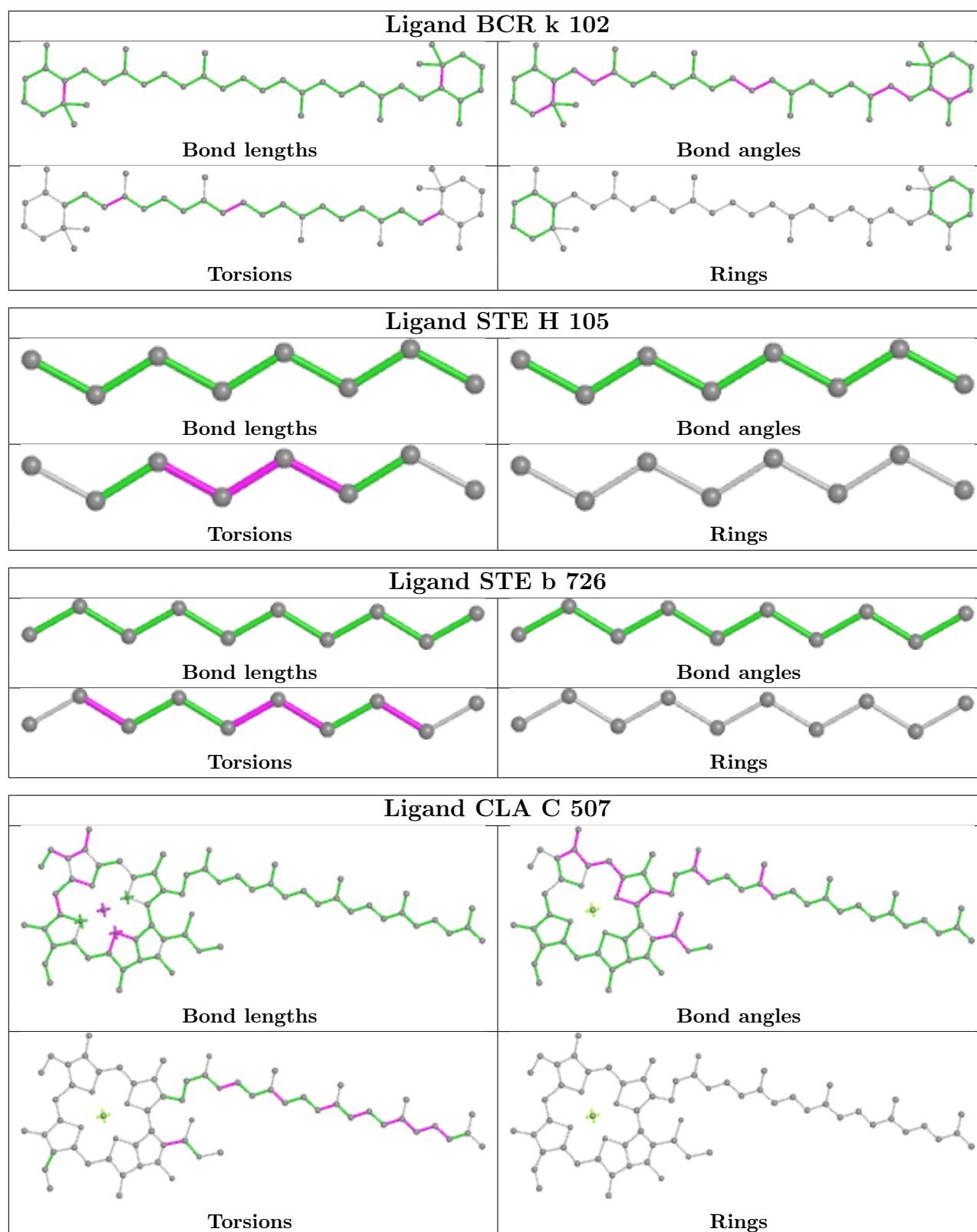


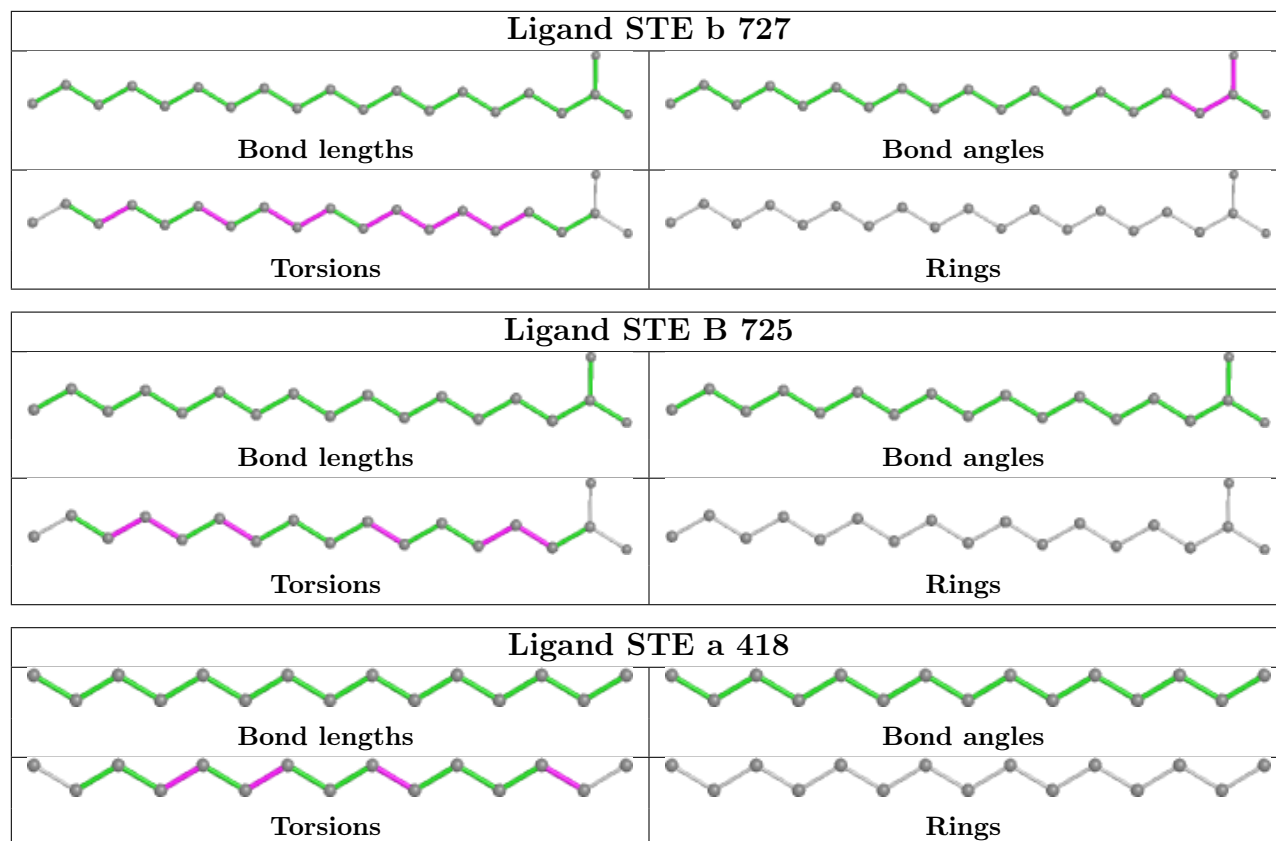


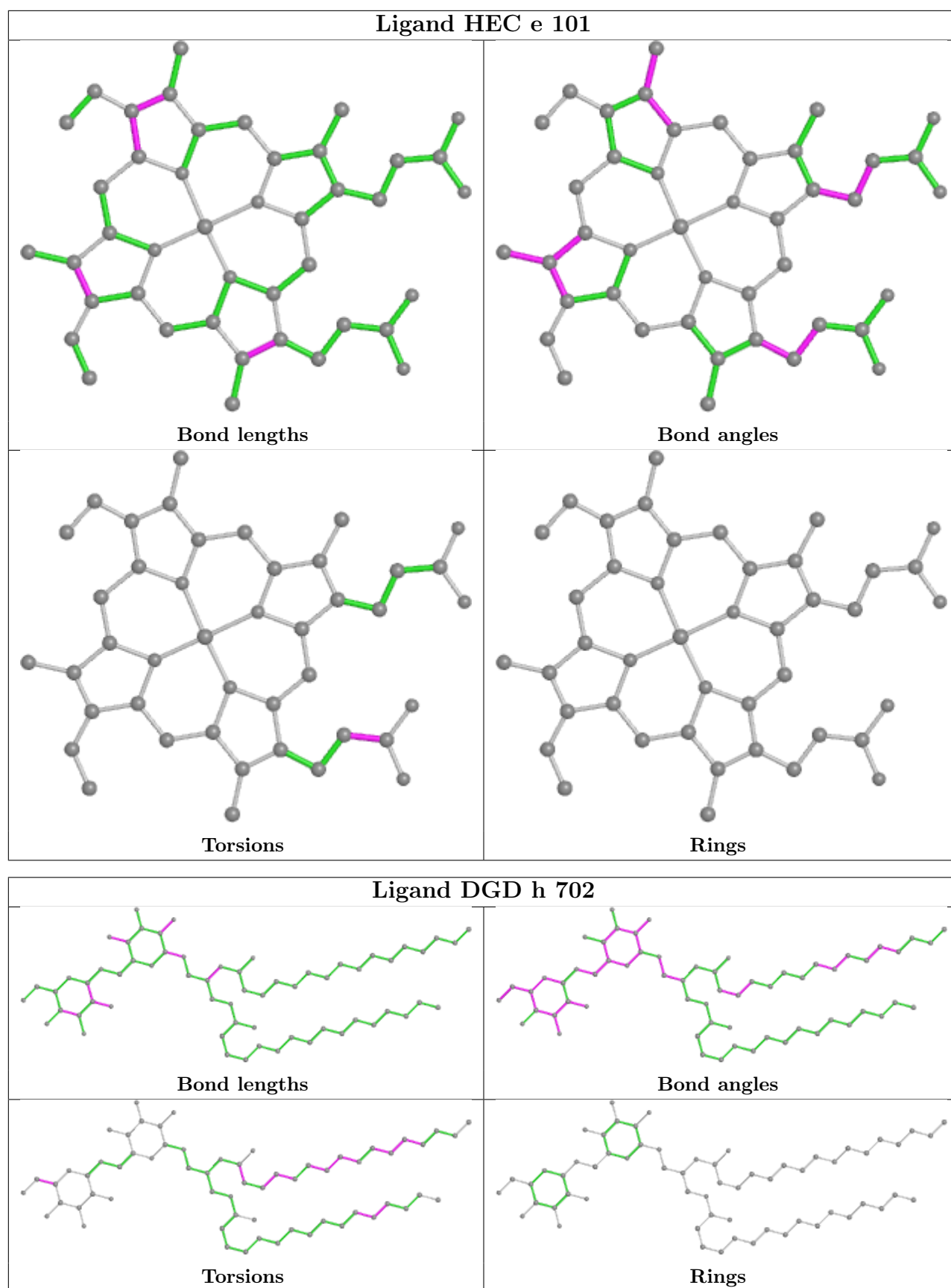


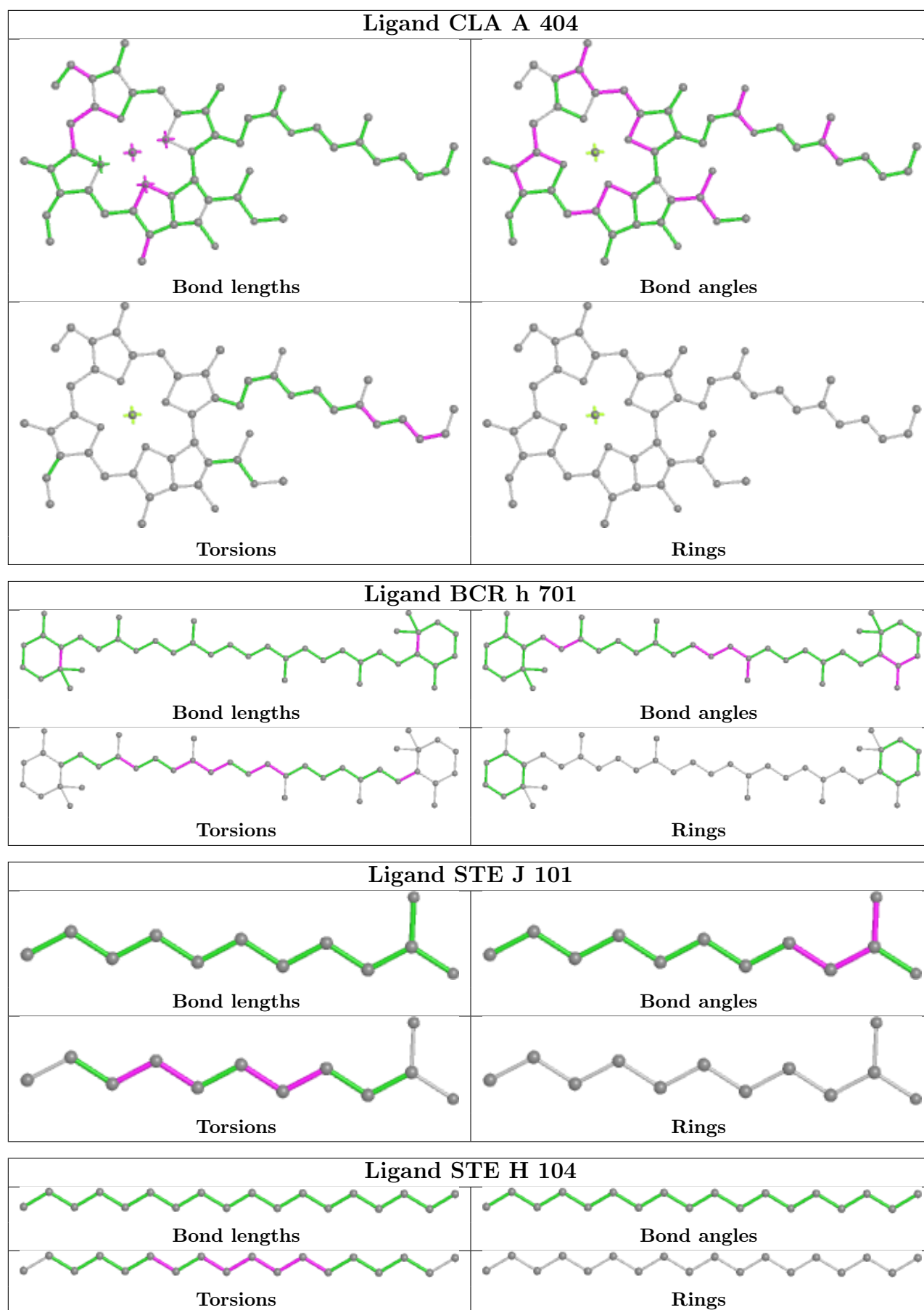


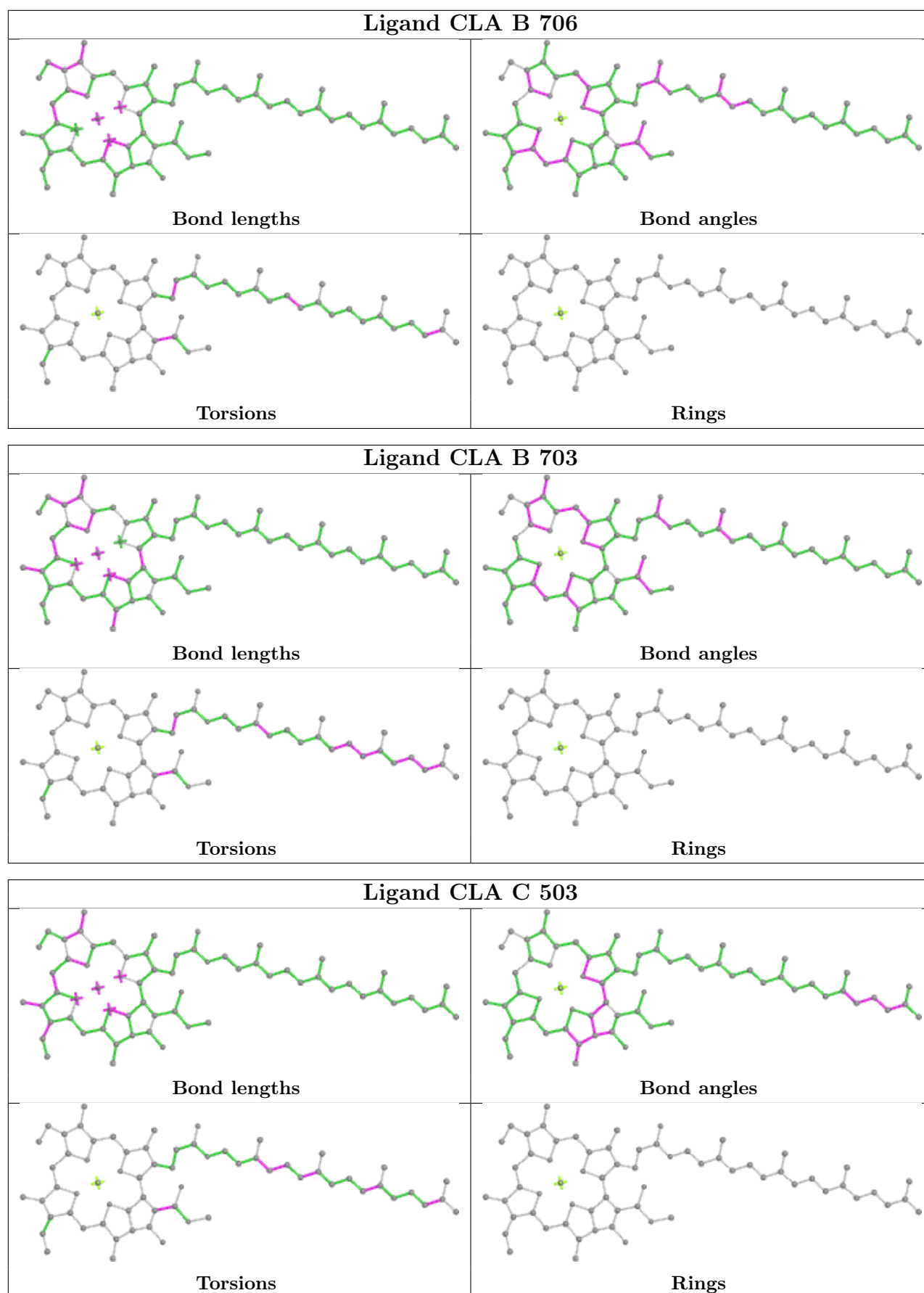


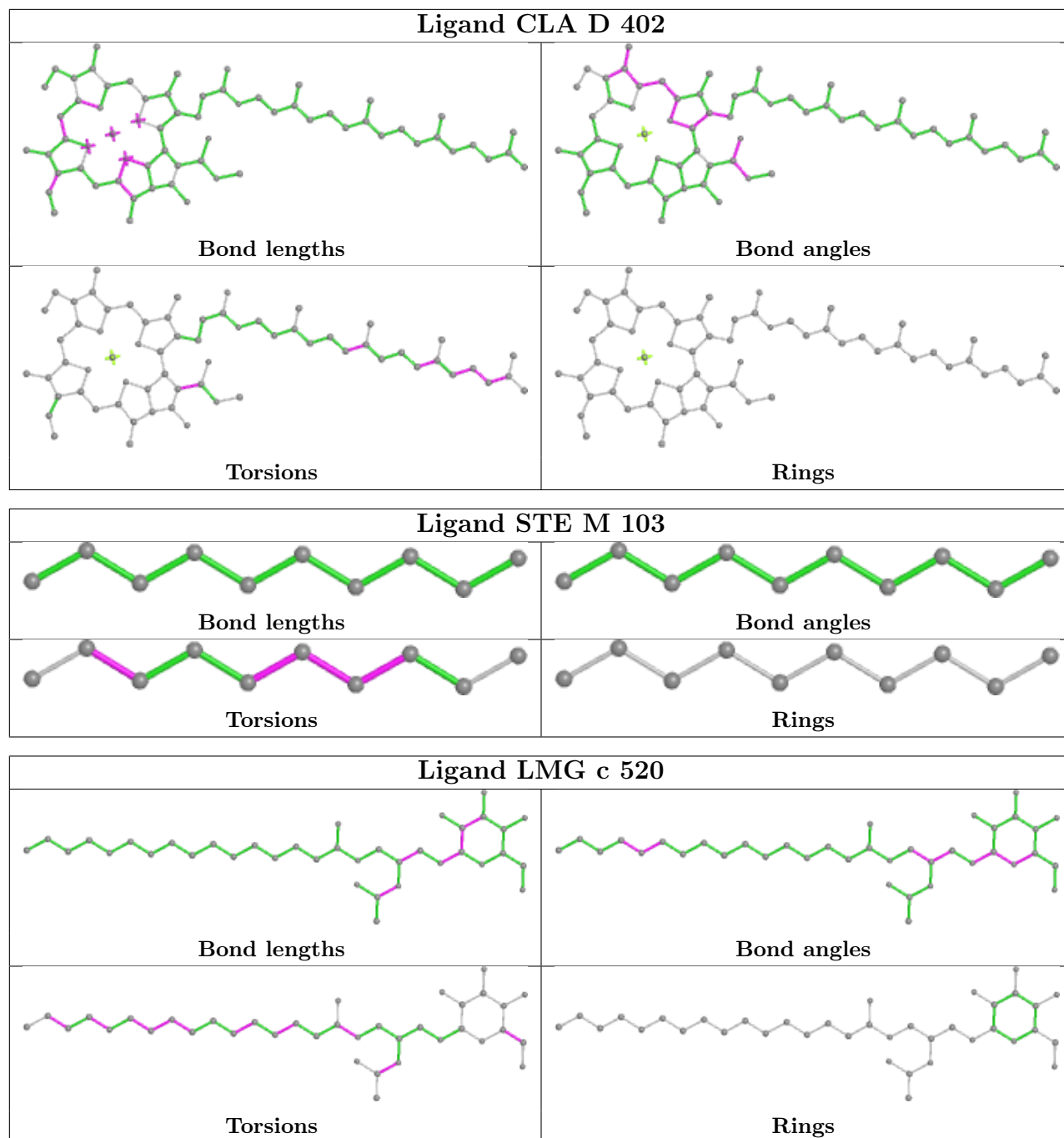


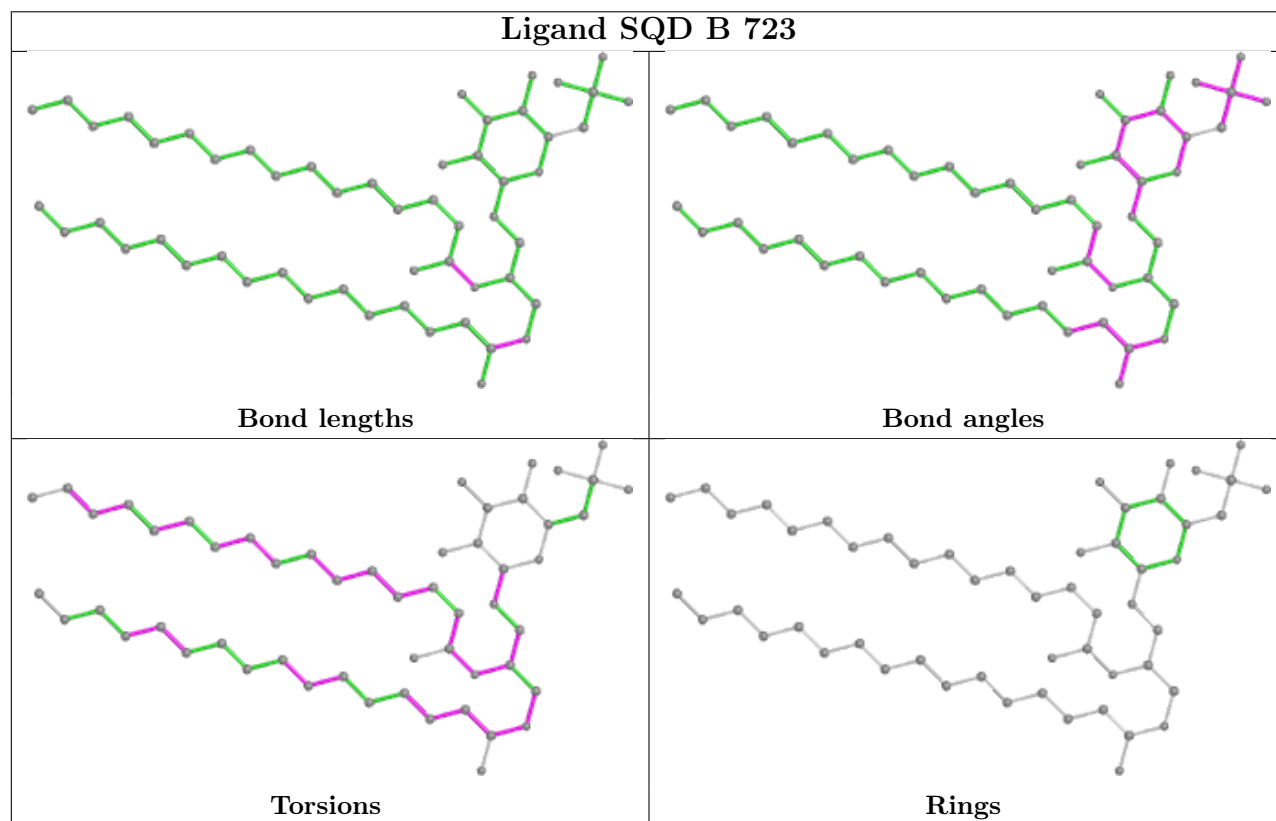
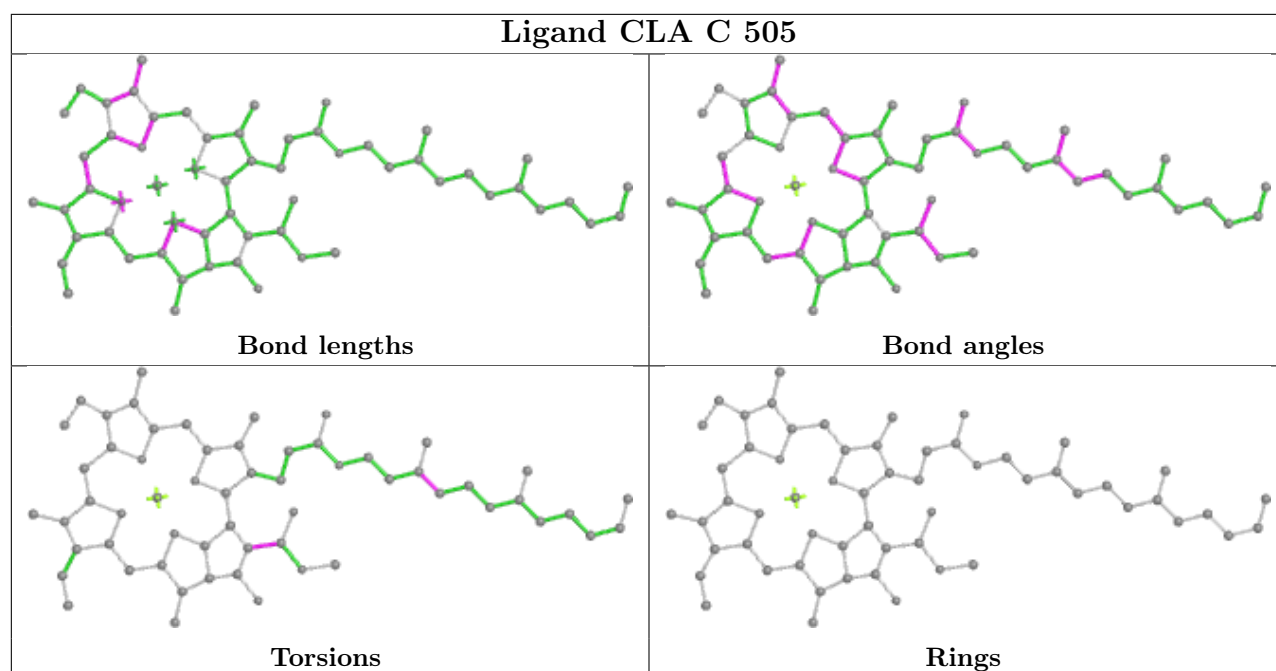


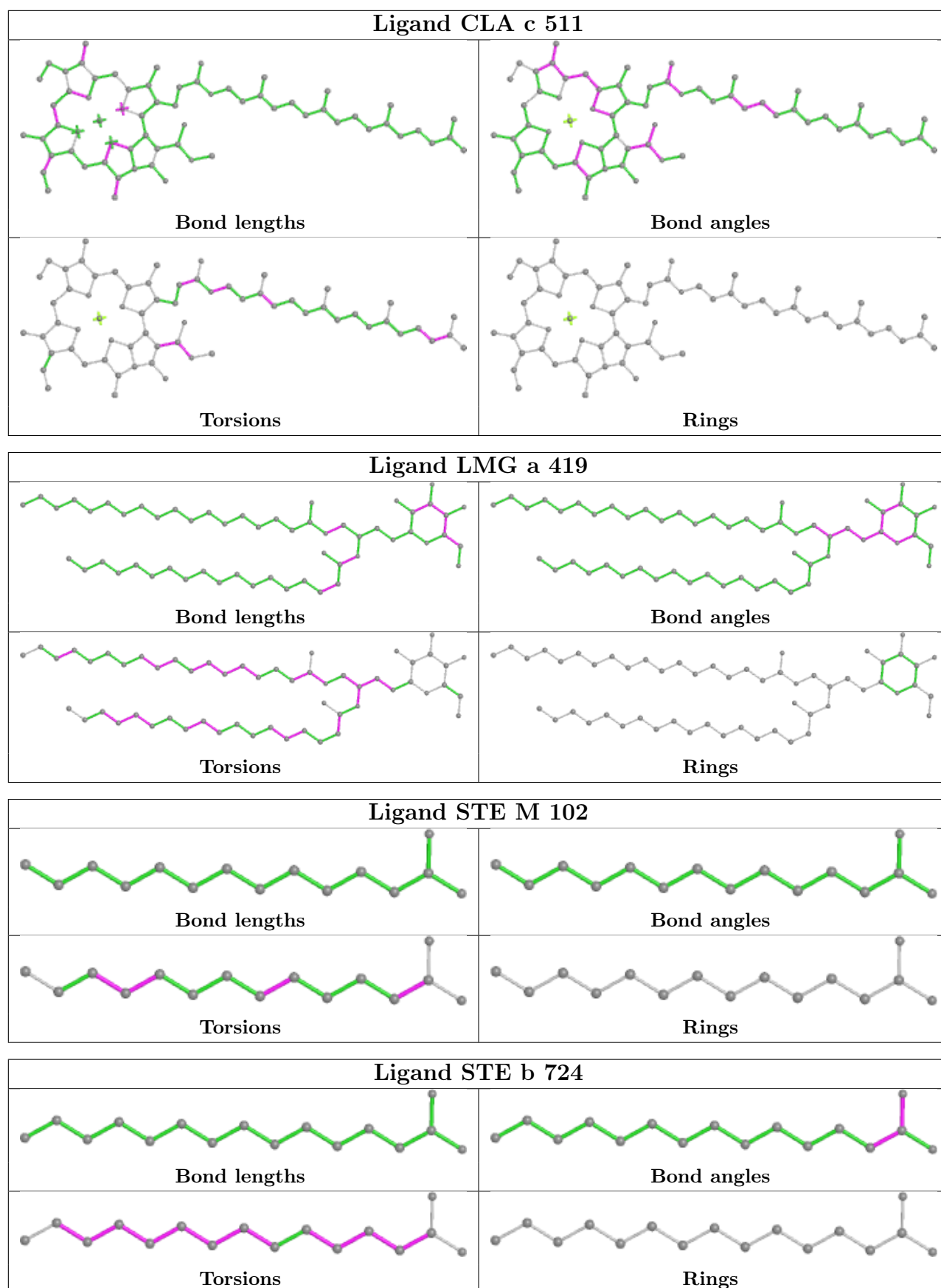


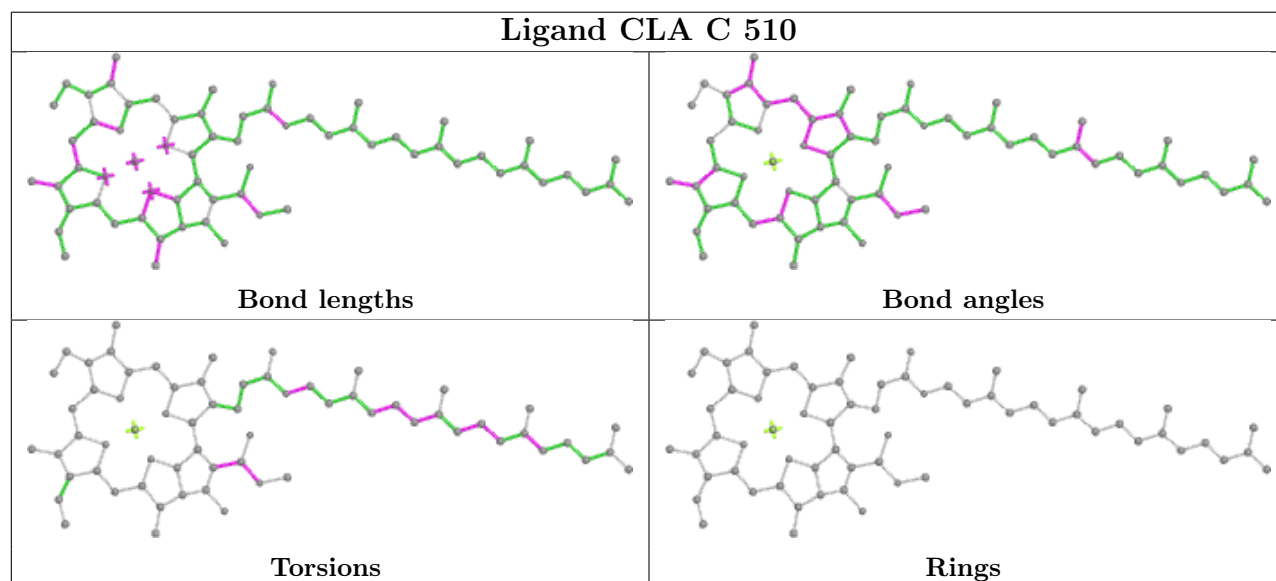
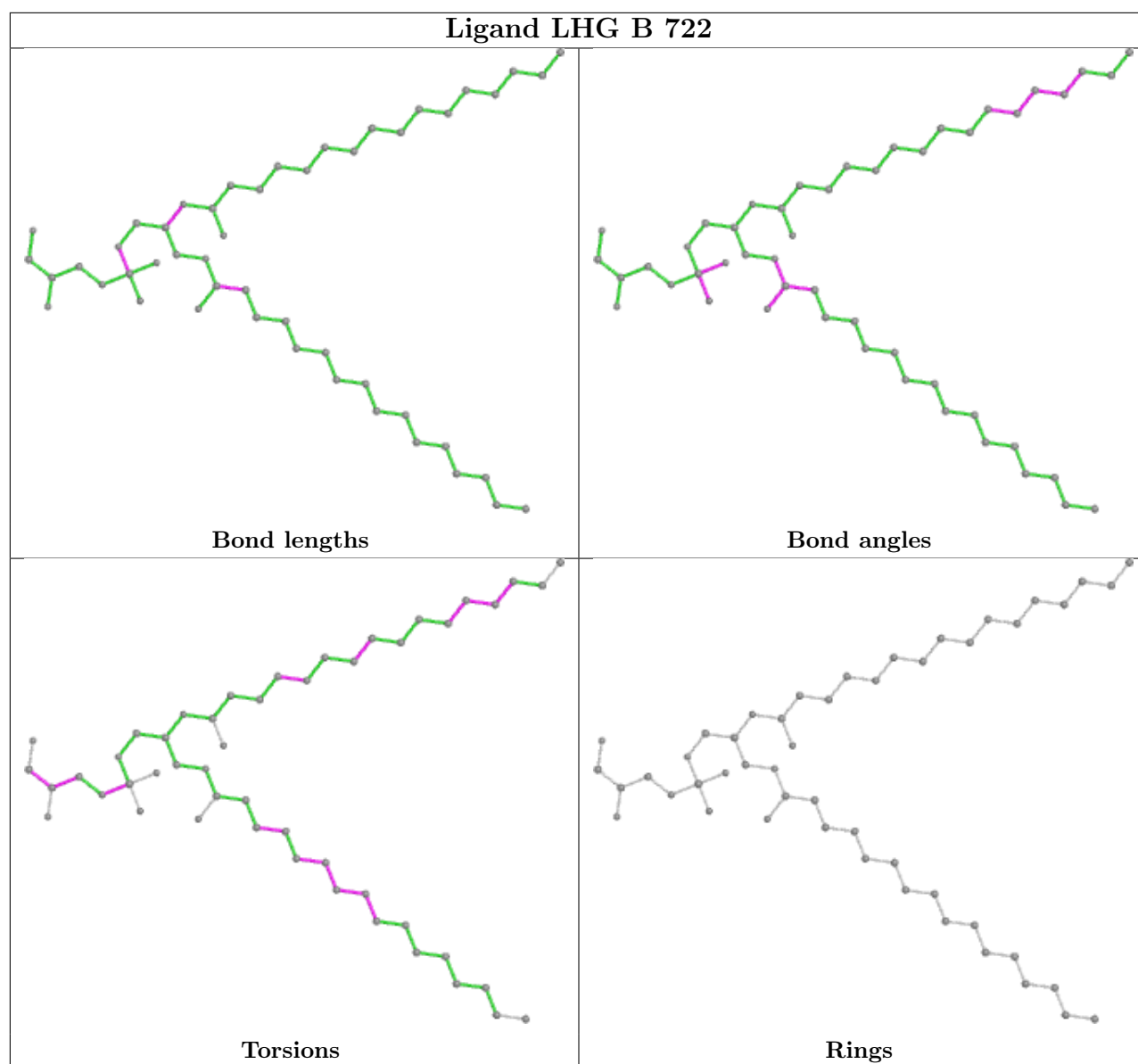


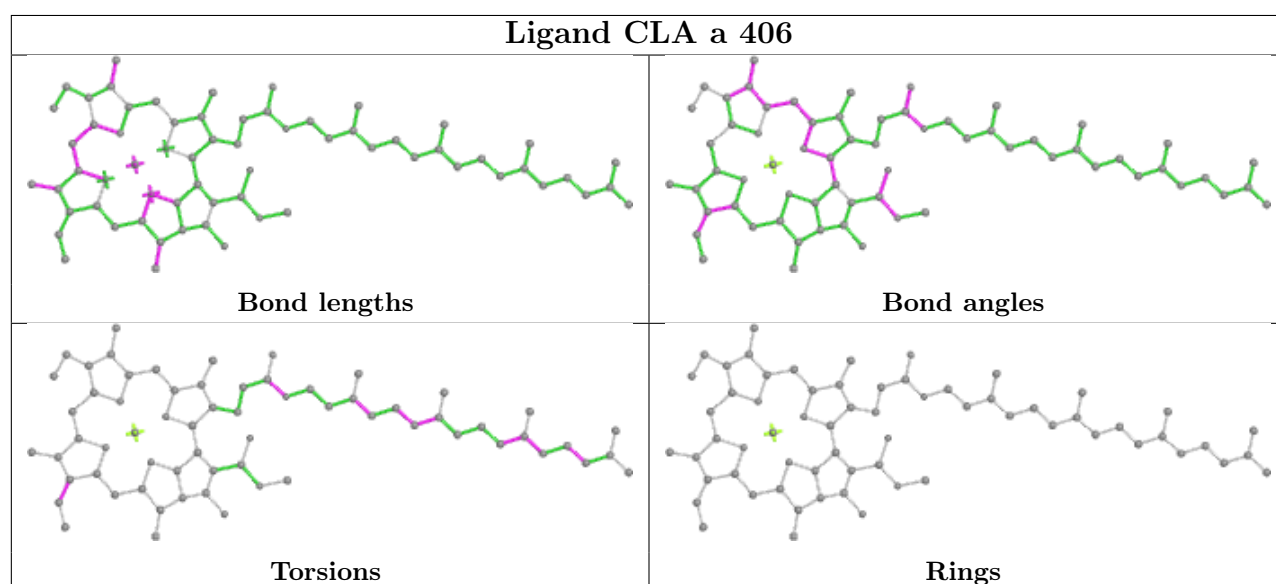
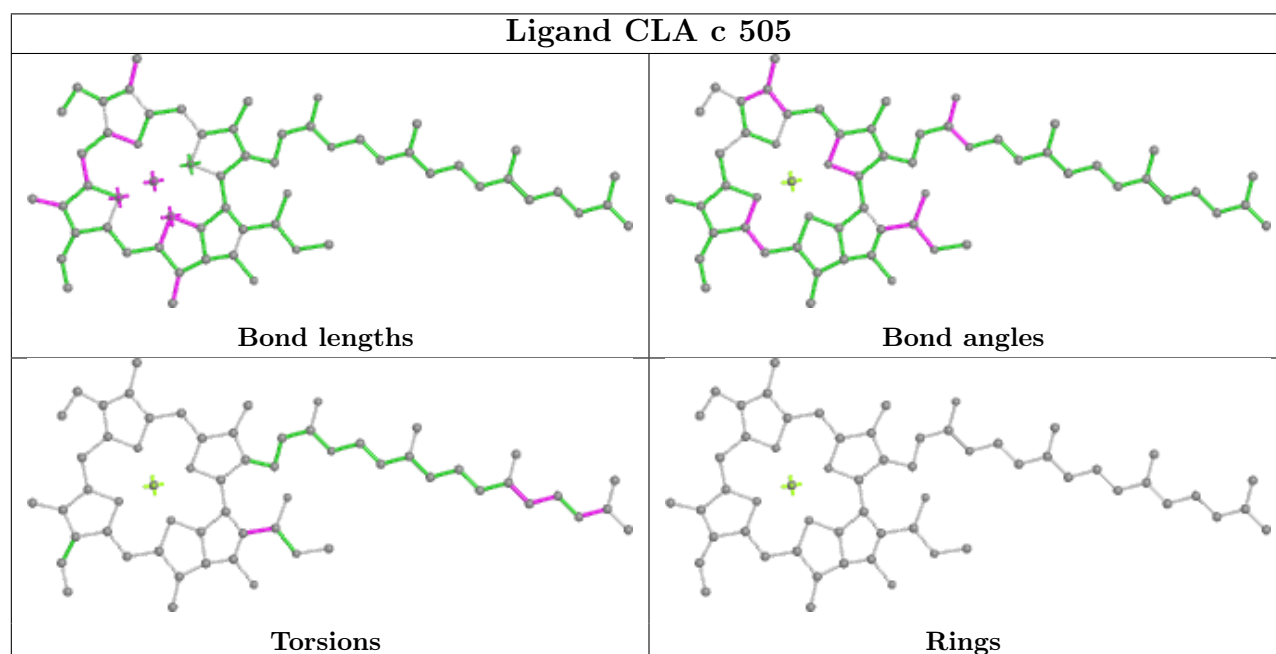
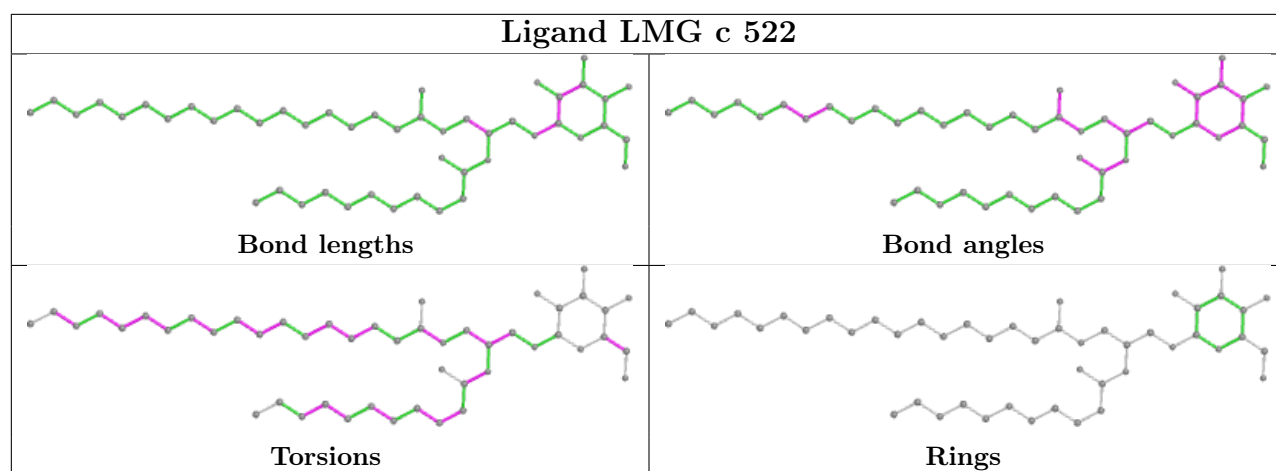


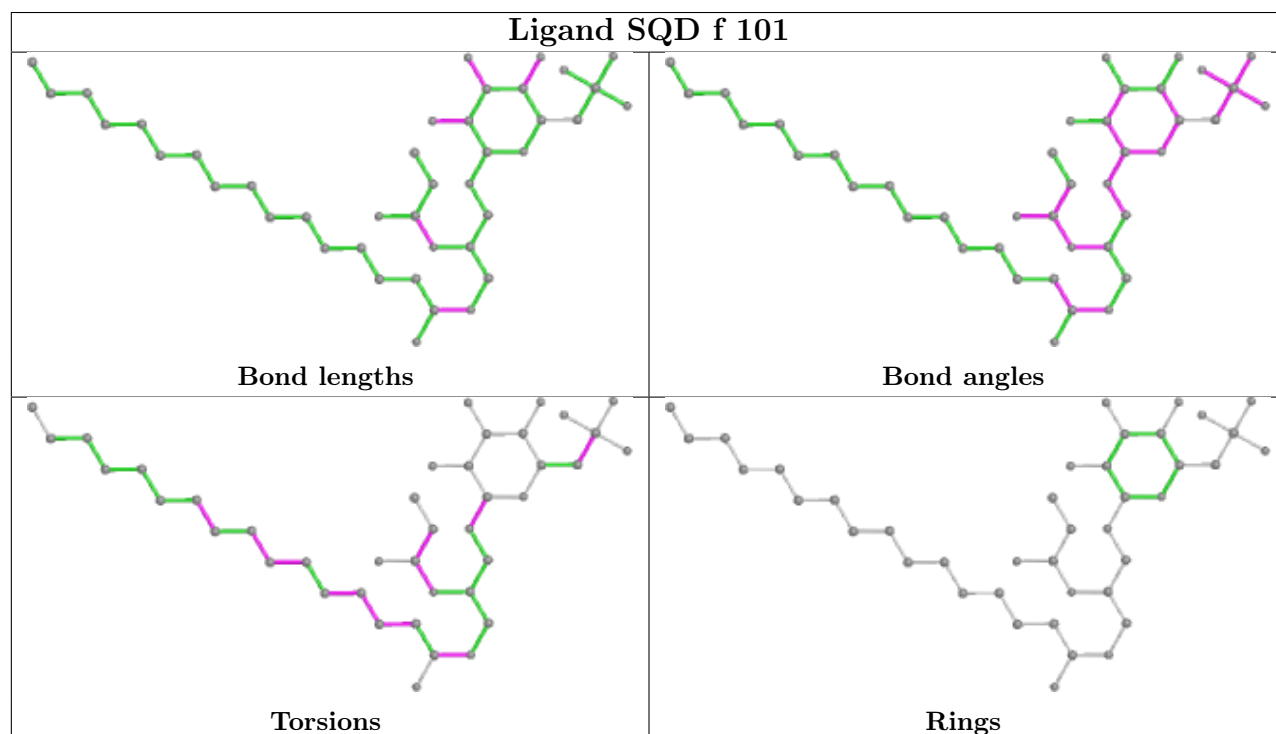
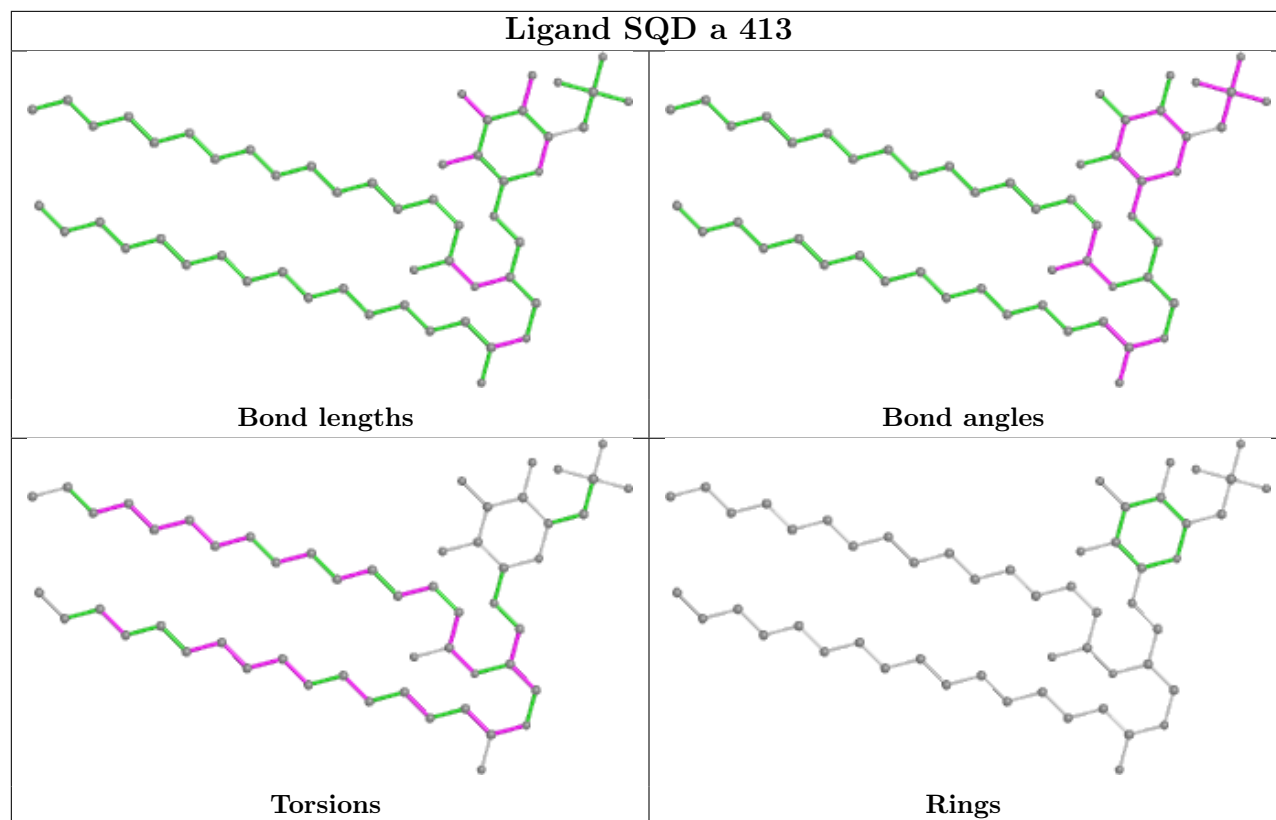


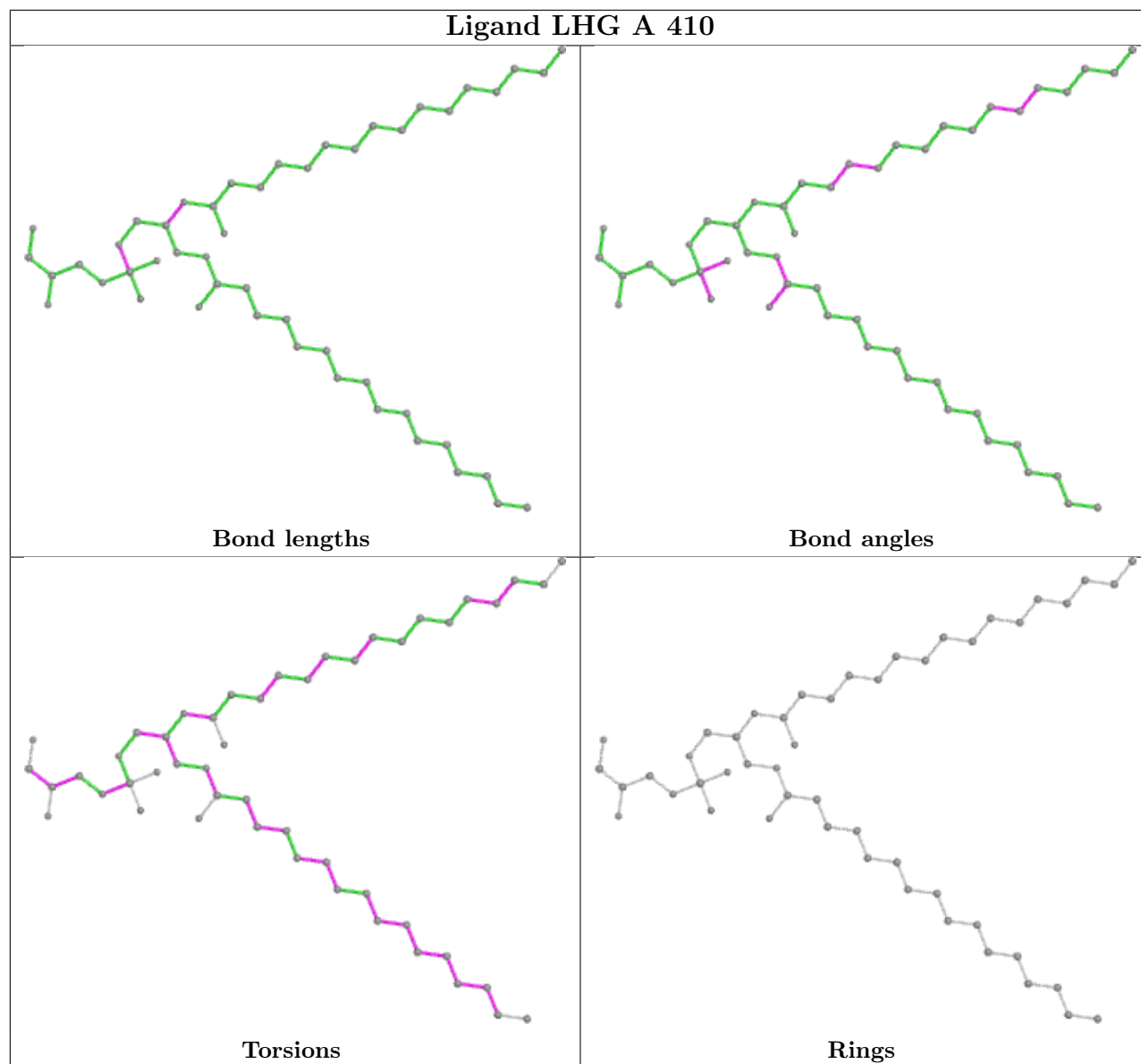


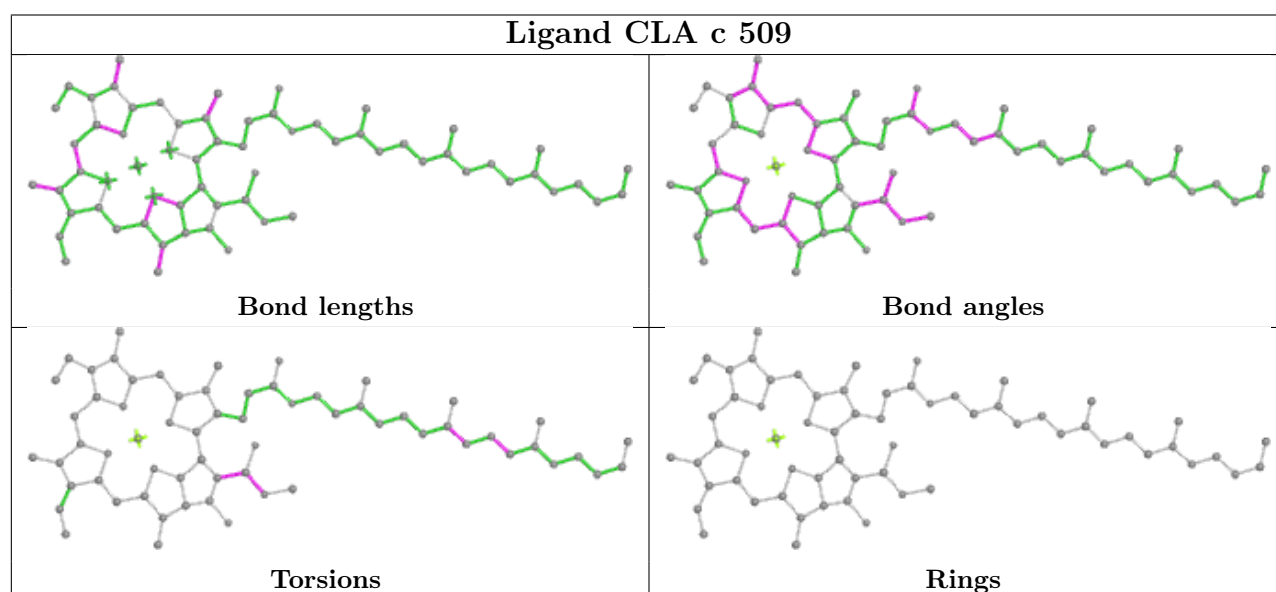
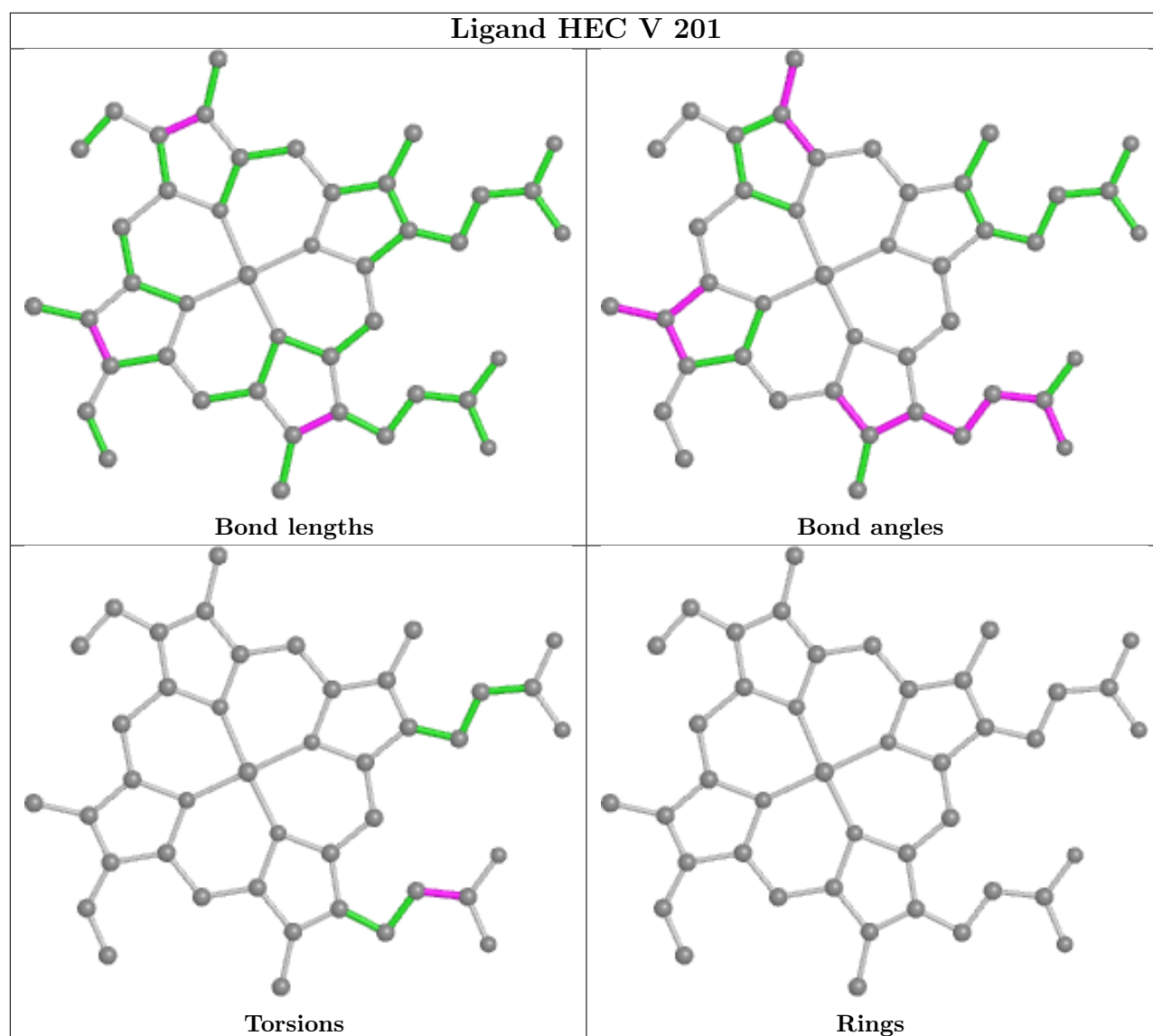


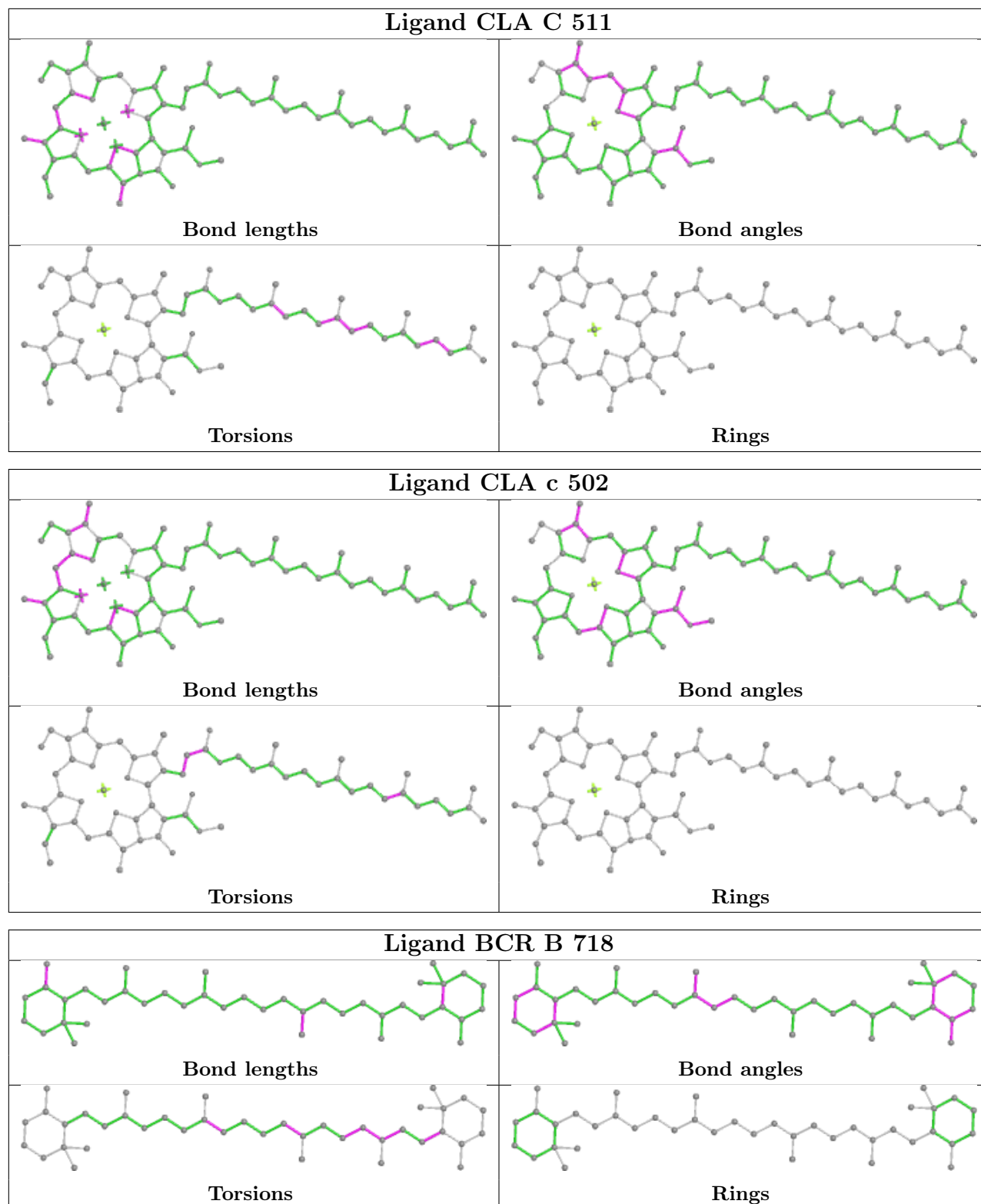


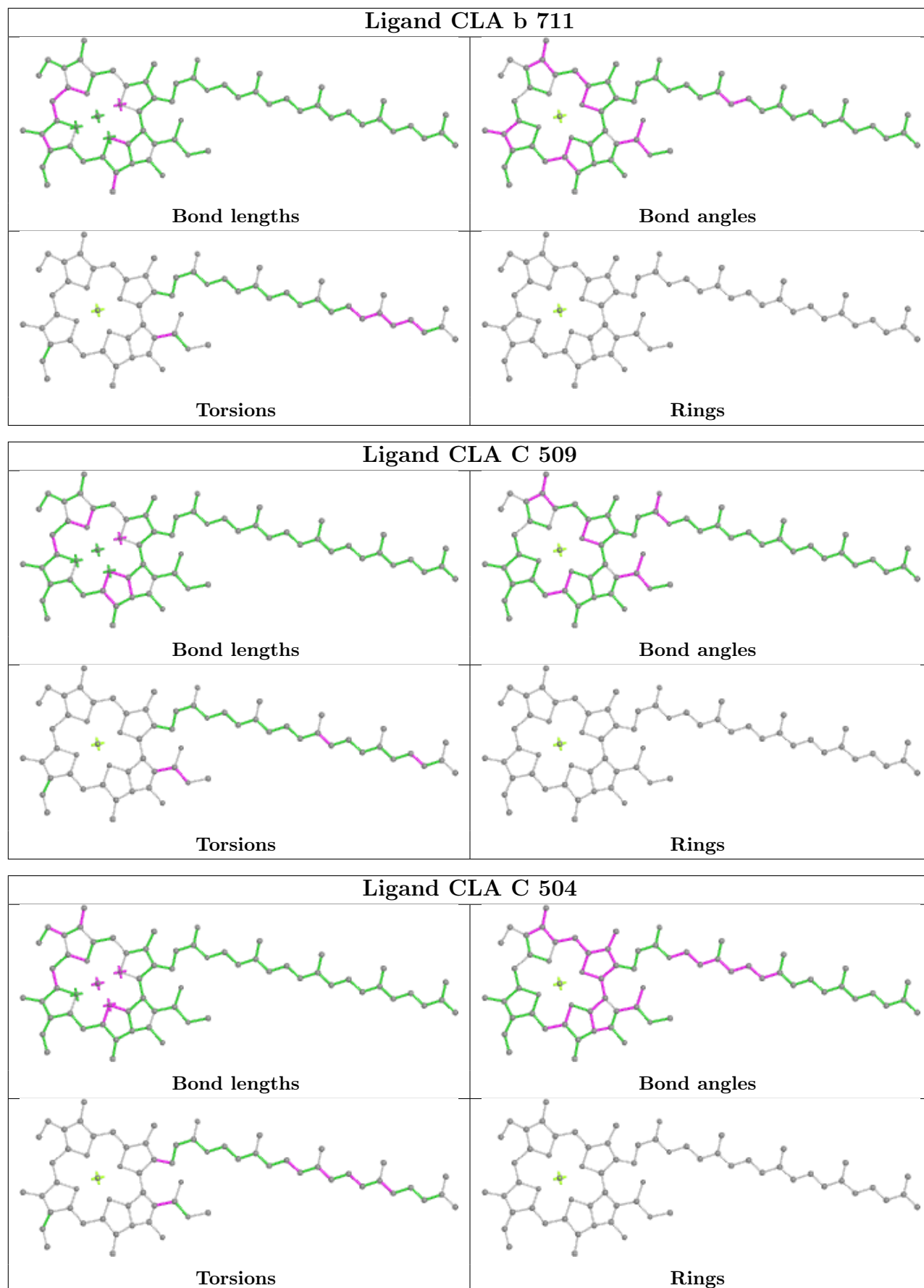


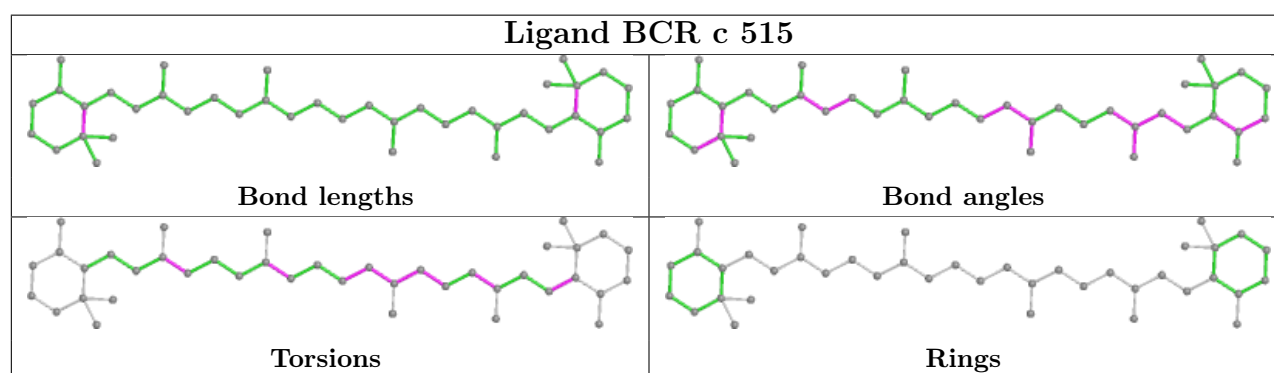
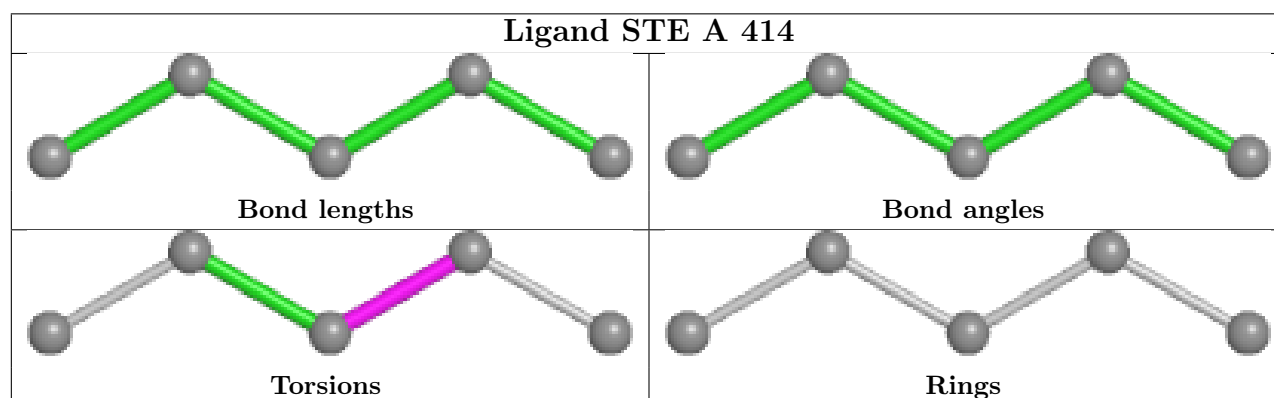
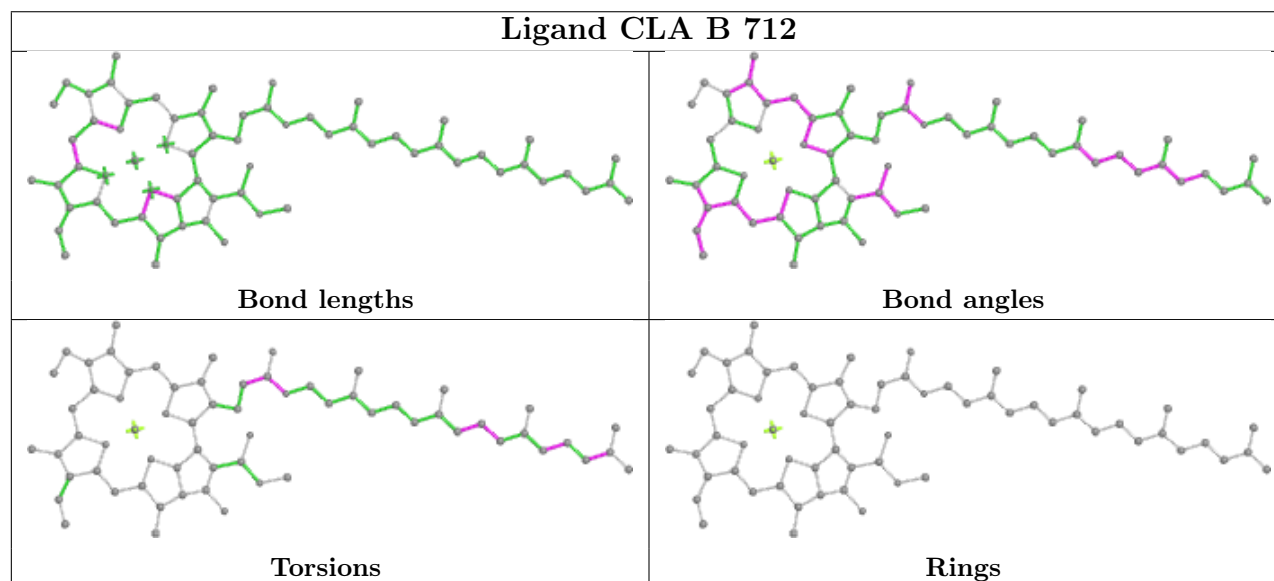
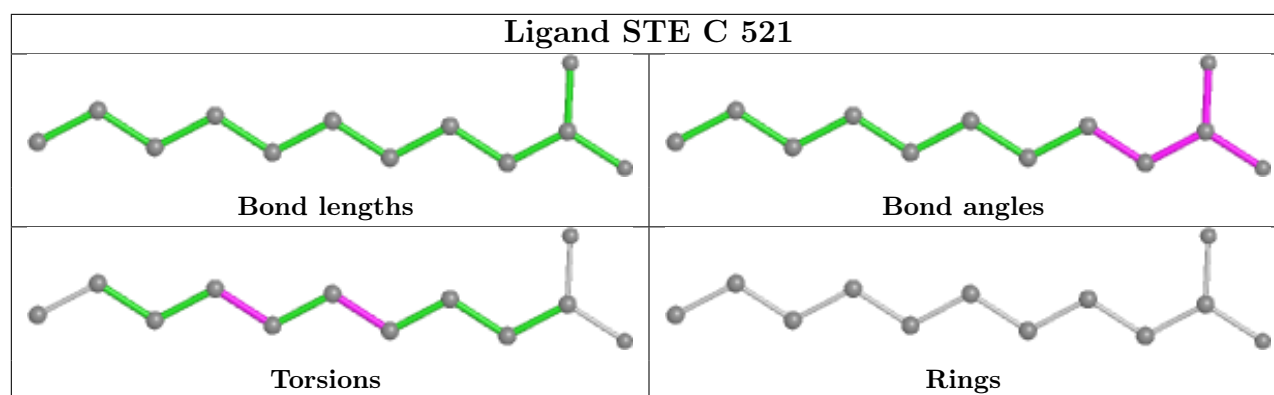


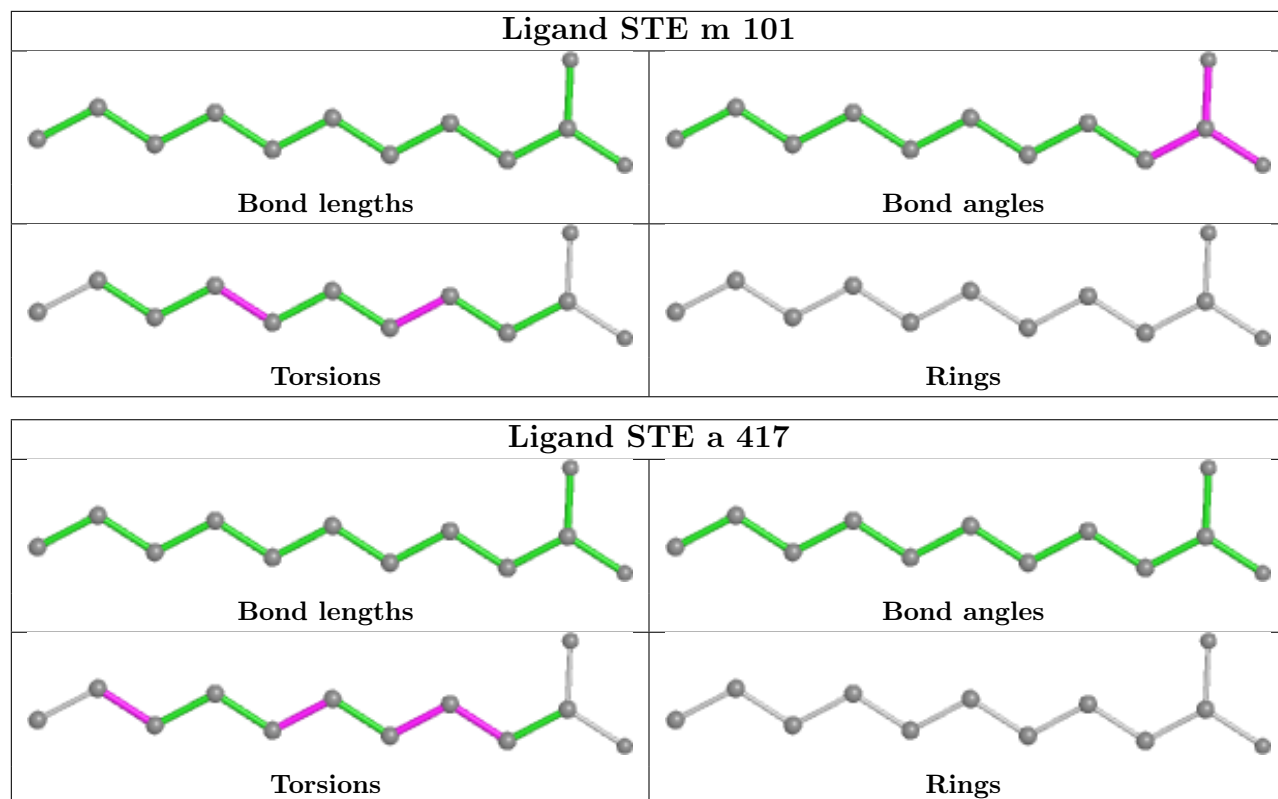


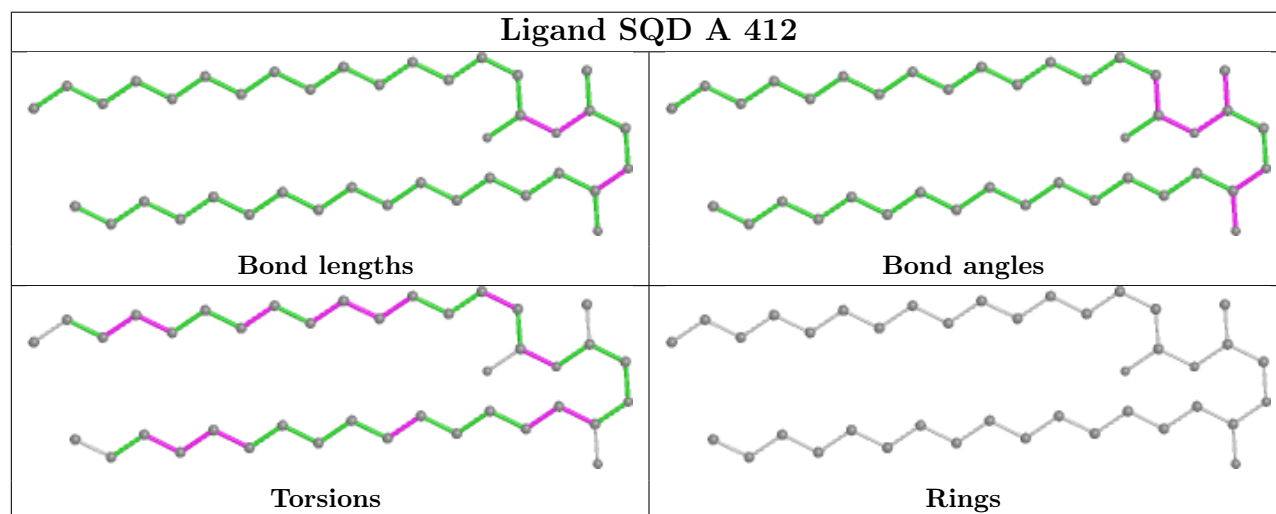
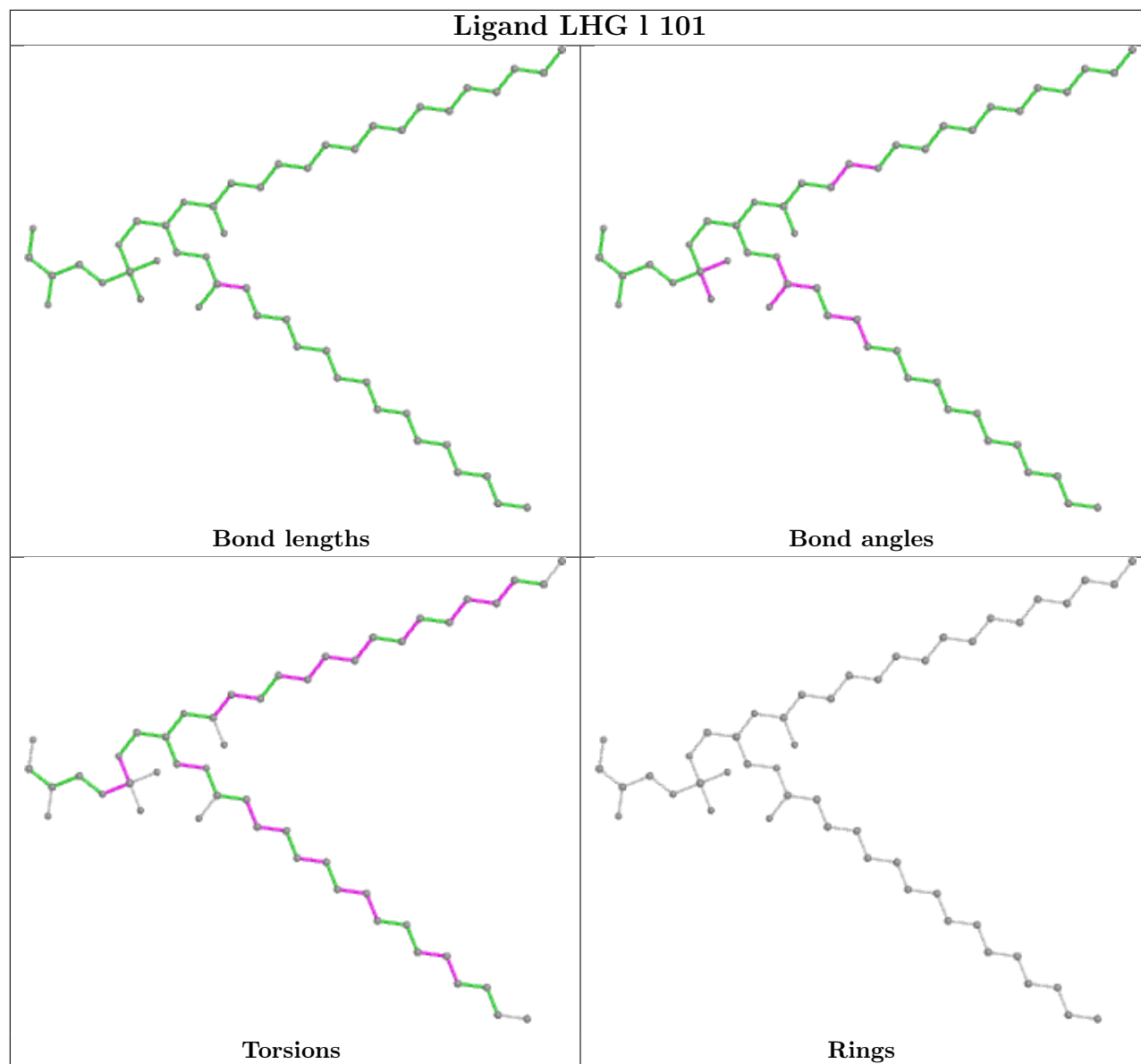


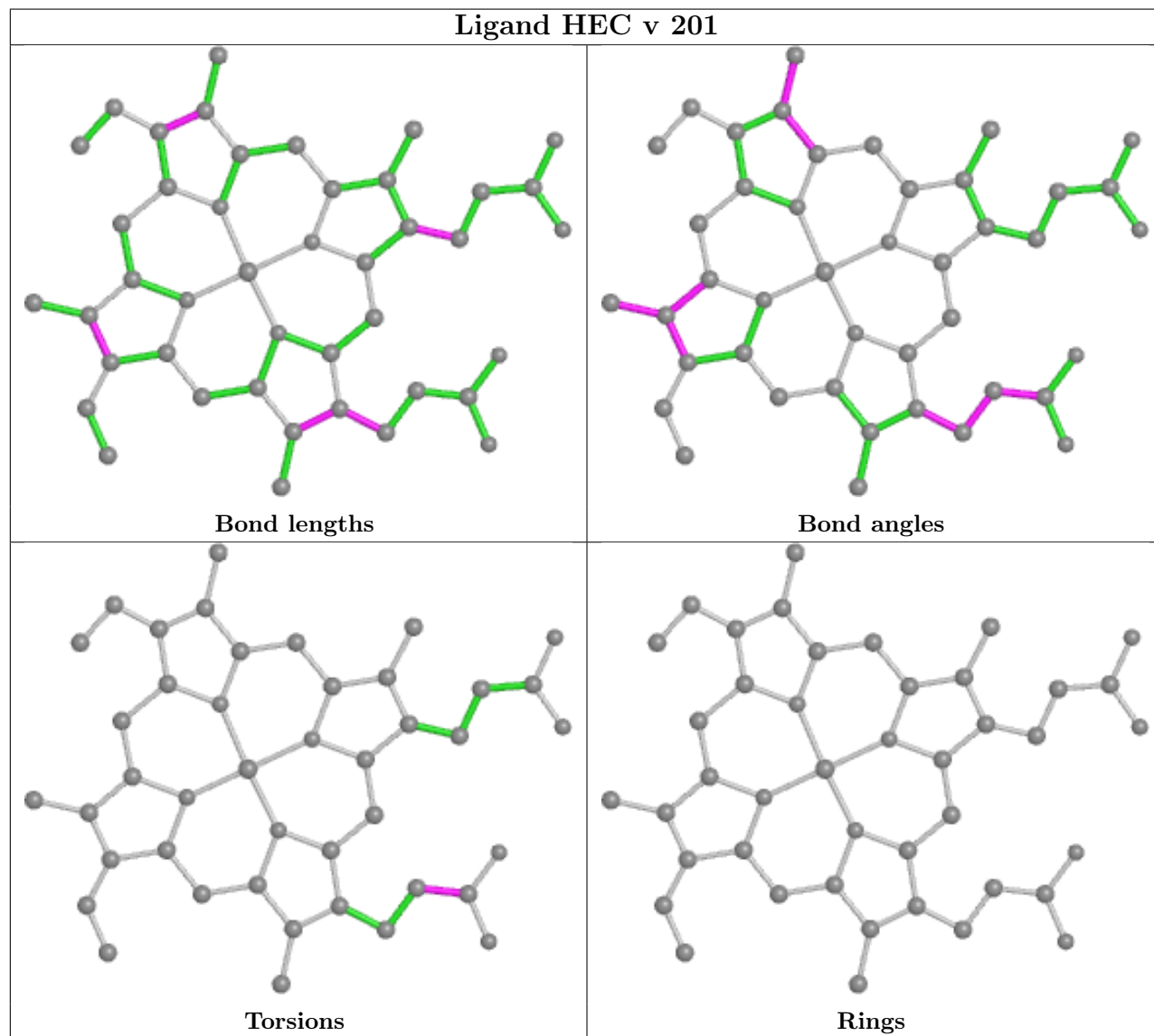
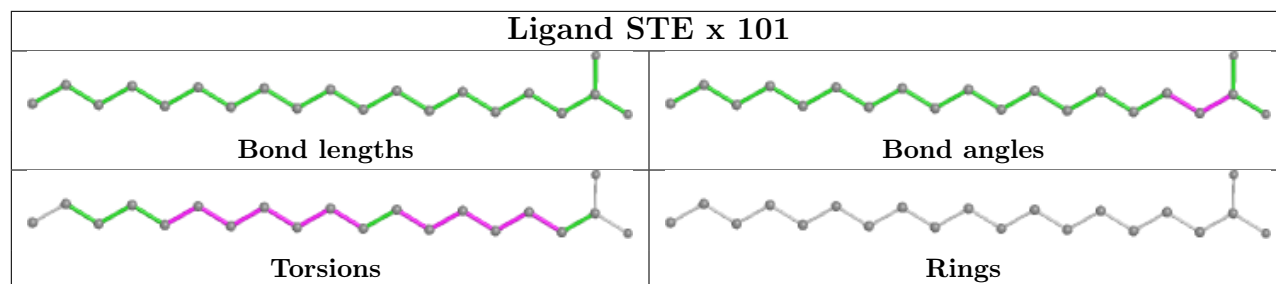


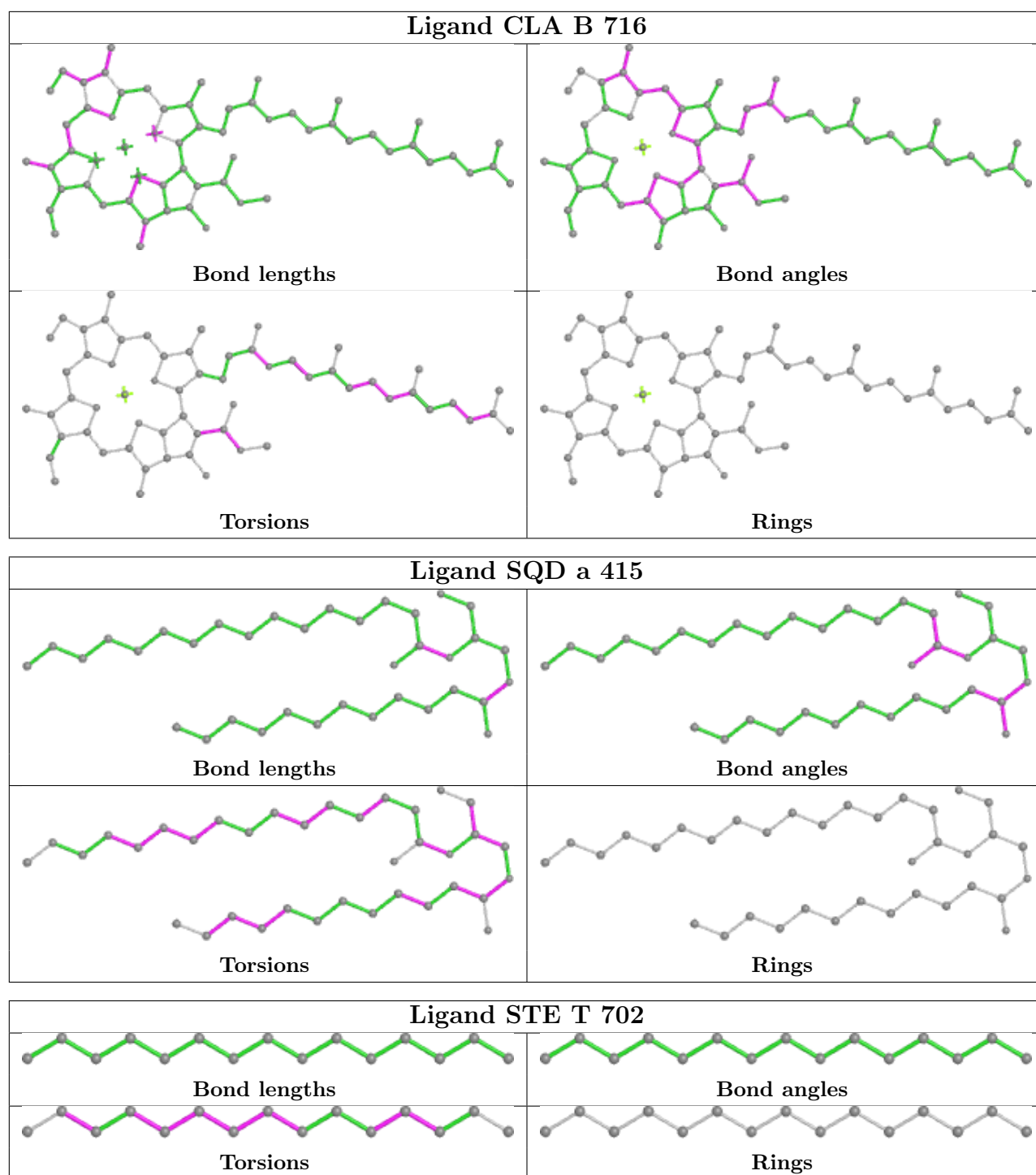


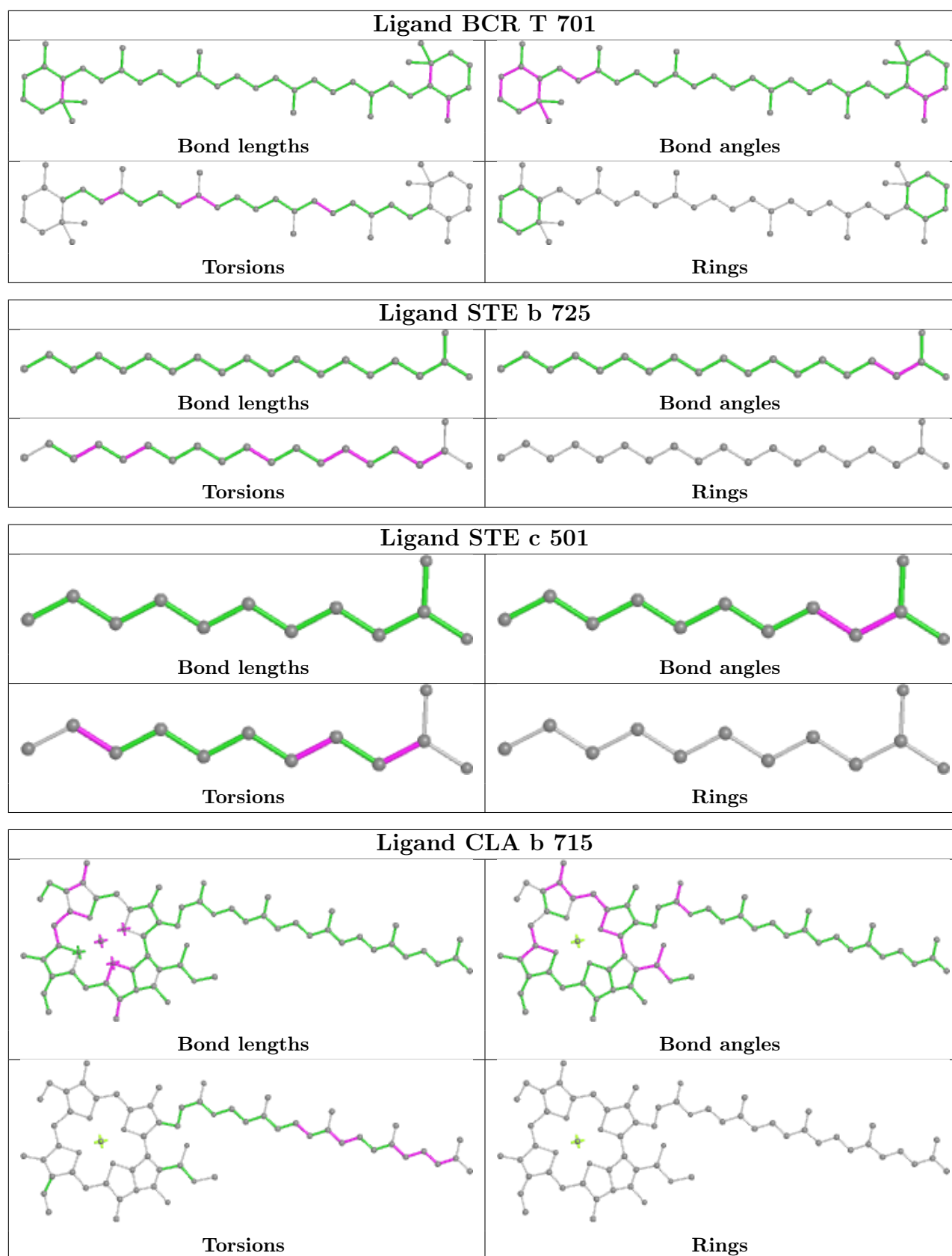


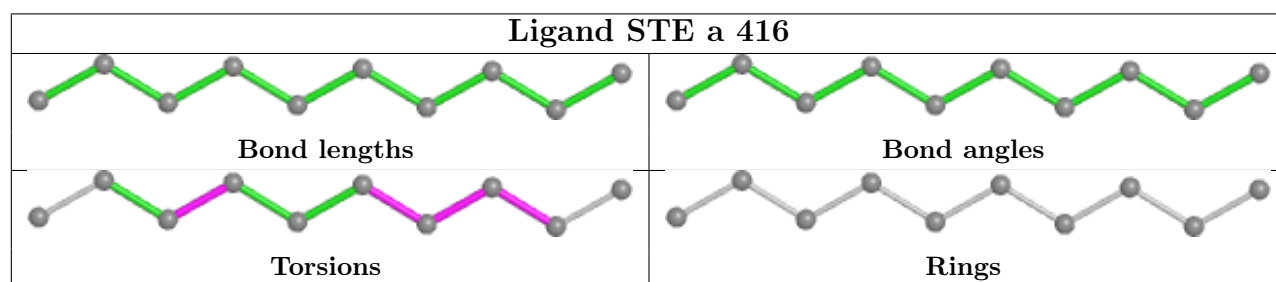
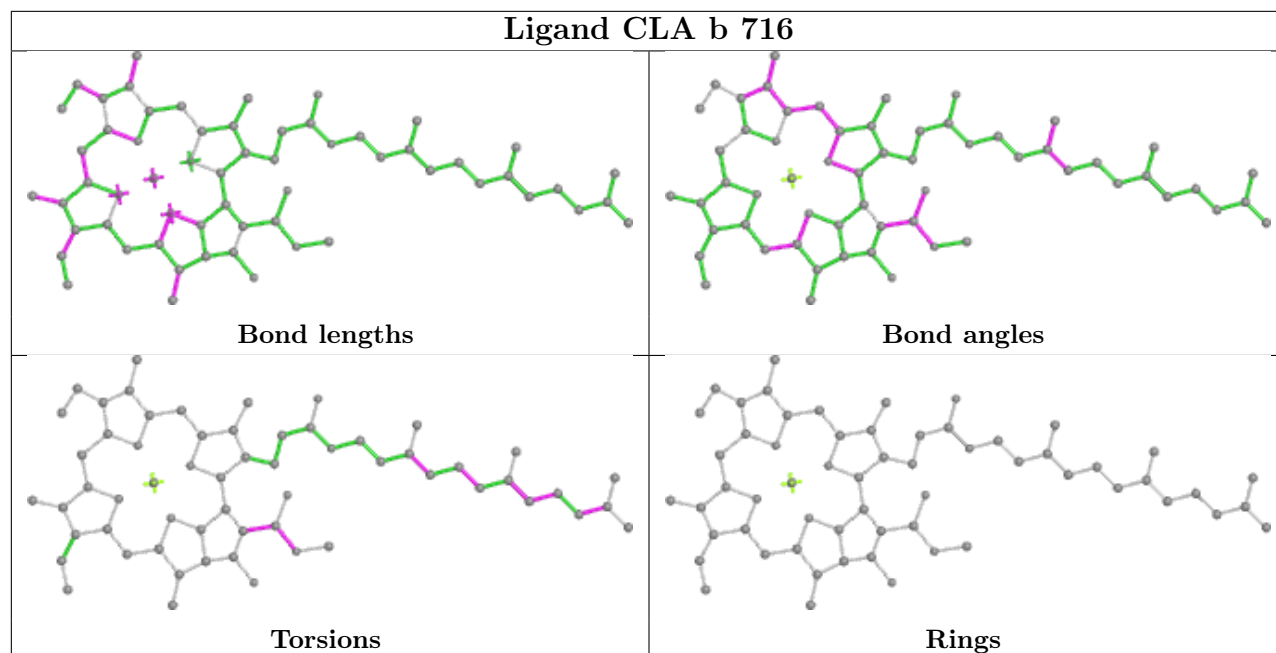
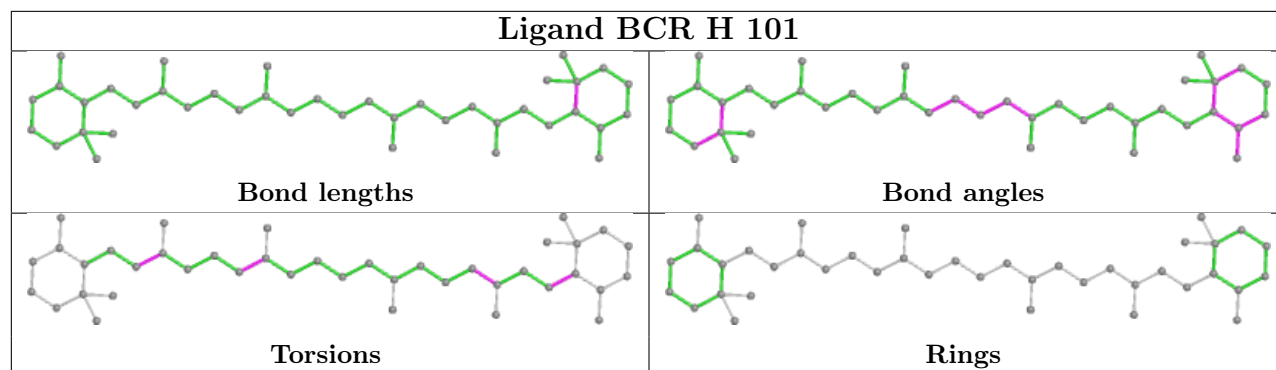


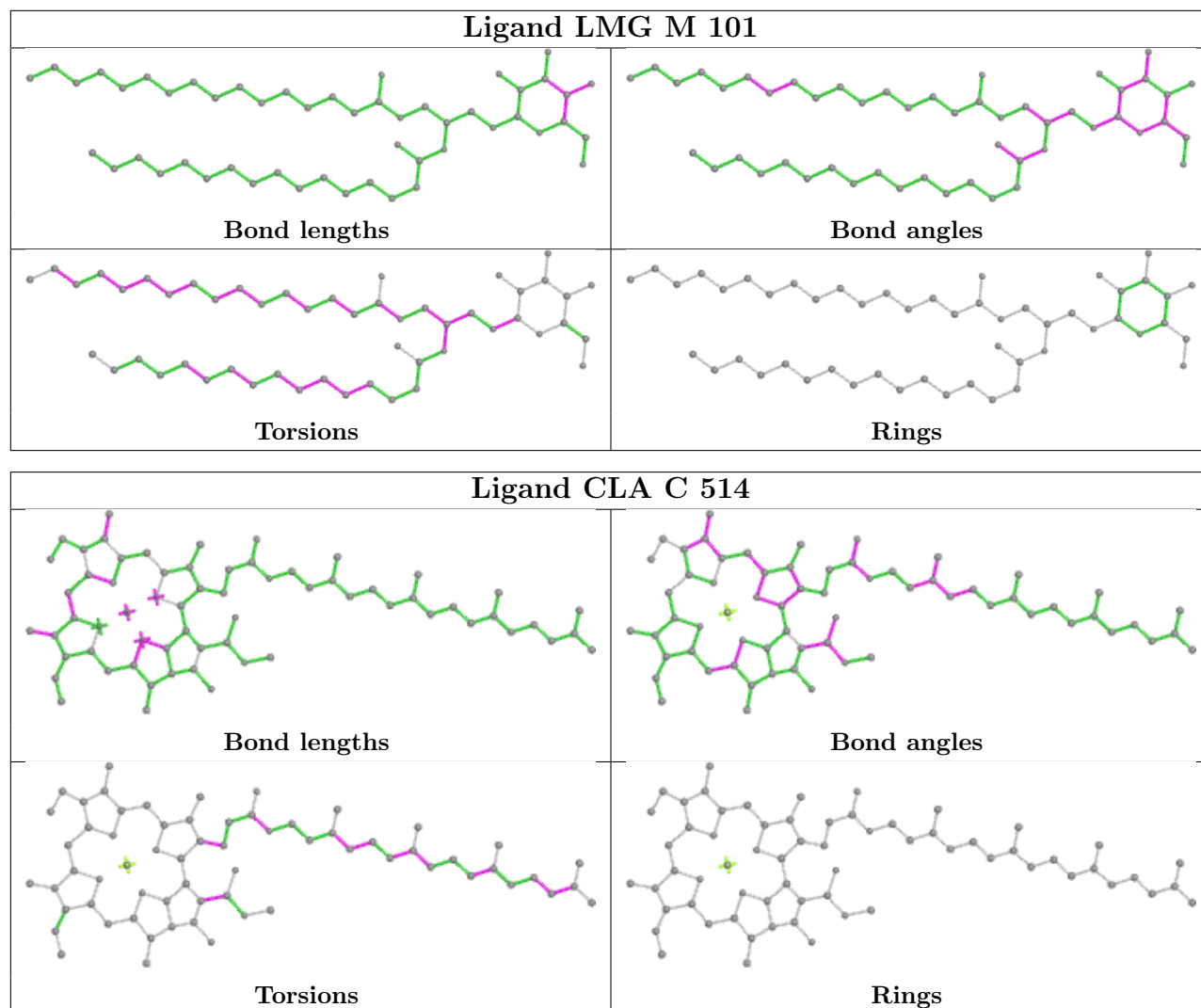












5.7 Other polymers [\(i\)](#)

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, 95th 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 ²)	Q<0.9
1	A	334/344 (97%)	-0.36	2 (0%) 89 91	22, 29, 50, 81	0
1	a	334/344 (97%)	-0.36	1 (0%) 94 94	22, 30, 58, 83	0
2	B	505/510 (99%)	-0.34	10 (1%) 65 69	23, 33, 60, 90	0
2	b	505/510 (99%)	-0.15	17 (3%) 45 51	23, 36, 72, 105	0
3	C	442/461 (95%)	-0.26	5 (1%) 80 84	24, 37, 54, 79	0
3	c	451/461 (97%)	-0.18	7 (1%) 72 75	25, 39, 62, 96	0
4	D	341/352 (96%)	-0.30	0 100 100	23, 30, 49, 78	0
4	d	341/352 (96%)	-0.28	1 (0%) 94 94	24, 34, 60, 74	0
5	E	82/84 (97%)	0.09	2 (2%) 59 64	35, 52, 68, 81	0
5	e	82/84 (97%)	0.20	6 (7%) 15 19	37, 57, 76, 81	0
6	F	34/45 (75%)	-0.31	2 (5%) 22 27	39, 44, 65, 85	0
6	f	34/45 (75%)	-0.14	2 (5%) 22 27	40, 48, 78, 91	0
7	H	65/66 (98%)	-0.04	2 (3%) 49 55	34, 41, 58, 67	0
7	h	63/66 (95%)	0.26	5 (7%) 12 16	40, 50, 61, 71	0
8	I	35/38 (92%)	-0.16	2 (5%) 23 29	31, 37, 72, 80	0
8	i	35/38 (92%)	-0.18	2 (5%) 23 29	32, 40, 70, 78	0
9	J	36/40 (90%)	-0.01	4 (11%) 5 7	31, 49, 78, 89	0
9	j	36/40 (90%)	0.17	4 (11%) 5 7	41, 50, 83, 93	0
10	K	37/46 (80%)	0.14	1 (2%) 54 60	42, 52, 69, 83	0
10	k	37/46 (80%)	0.13	1 (2%) 54 60	48, 55, 68, 81	0
11	L	37/37 (100%)	-0.36	1 (2%) 54 60	26, 31, 63, 71	0
11	l	36/37 (97%)	-0.27	2 (5%) 24 29	23, 29, 71, 86	0
12	M	32/36 (88%)	-0.05	0 100 100	27, 34, 60, 68	0
12	m	31/36 (86%)	-0.17	0 100 100	24, 34, 50, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.03	12 (4%) 29 35	25, 41, 79, 130	0
13	o	244/272 (89%)	-0.08	16 (6%) 18 23	25, 40, 77, 119	0
14	R	34/41 (82%)	2.52	23 (67%) 0 0	65, 78, 91, 104	0
14	r	31/41 (75%)	4.49	27 (87%) 0 0	81, 100, 114, 126	0
15	T	29/32 (90%)	-0.42	2 (6%) 16 21	26, 30, 61, 74	0
15	t	29/32 (90%)	-0.24	2 (6%) 16 21	28, 32, 78, 86	0
16	U	97/134 (72%)	-0.24	4 (4%) 37 43	31, 44, 69, 87	0
16	u	97/134 (72%)	-0.40	0 100 100	31, 39, 58, 77	0
17	V	137/163 (84%)	-0.48	0 100 100	30, 39, 55, 82	0
17	v	137/163 (84%)	-0.17	5 (3%) 42 49	30, 46, 68, 84	0
18	X	38/41 (92%)	-0.03	3 (7%) 12 16	41, 51, 73, 82	0
18	x	39/41 (95%)	0.39	3 (7%) 13 17	48, 58, 89, 103	0
19	Y	27/46 (58%)	1.44	10 (37%) 0 0	53, 74, 91, 93	0
19	y	30/46 (65%)	0.64	5 (16%) 1 2	60, 72, 85, 93	0
20	Z	62/62 (100%)	0.95	16 (25%) 0 0	54, 66, 108, 119	0
20	z	62/62 (100%)	0.95	14 (22%) 0 0	54, 71, 107, 114	0
All	All	5302/5700 (93%)	-0.13	221 (4%) 36 42	22, 38, 73, 130	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	28	VAL	8.0
14	r	25	PRO	7.4
13	o	58	ASN	7.2
20	Z	33	TRP	7.2
13	O	56	PRO	7.1

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, 95th 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 ²)	Q<0.9
8	FME	I	1	10/11	0.93	0.14	39,52,68,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	FME	t	1	10/11	0.93	0.10	29,46,71,71	0
12	FME	M	1	10/11	0.95	0.10	41,50,66,80	0
15	FME	T	1	10/11	0.96	0.10	27,47,63,64	0
12	FME	m	1	10/11	0.96	0.10	34,48,69,82	0
8	FME	i	1	10/11	0.97	0.18	38,48,60,62	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, 95th 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(\AA^2)	Q<0.9
28	STE	H	104	18/20	0.73	0.28	43,76,86,92	0
28	STE	B	726	16/20	0.76	0.36	43,64,79,86	0
28	STE	E	101	12/20	0.77	0.30	56,79,85,90	0
28	STE	C	522	16/20	0.78	0.17	38,53,66,67	0
28	STE	a	418	15/20	0.78	0.15	36,61,76,79	0
28	STE	b	725	20/20	0.78	0.18	45,63,80,83	0
33	LMG	c	522	48/55	0.78	0.24	35,77,108,113	0
28	STE	x	101	20/20	0.80	0.26	45,62,75,81	0
23	BCR	H	101	40/40	0.81	0.16	34,48,61,78	0
25	PL9	A	408	55/55	0.81	0.26	44,70,86,96	0
28	STE	c	501	12/20	0.81	0.21	55,68,85,93	0
28	STE	H	105	8/20	0.81	0.12	47,58,69,69	0
28	STE	I	101	15/20	0.81	0.17	40,55,81,86	0
28	STE	B	720	17/20	0.82	0.20	30,50,62,73	0
29	DGD	A	413	66/66	0.82	0.16	42,64,79,94	0
33	LMG	D	412	32/55	0.82	0.15	37,57,80,84	0
26	SQD	a	415	36/54	0.82	0.17	25,59,84,92	0
22	CLA	b	701	65/65	0.83	0.16	48,68,91,96	0
28	STE	b	726	10/20	0.83	0.28	43,56,67,75	0
25	PL9	a	411	55/55	0.83	0.22	42,69,93,98	0
22	CLA	C	513	65/65	0.83	0.18	35,56,93,98	0
28	STE	a	416	10/20	0.83	0.19	30,64,69,73	0
28	STE	a	417	12/20	0.83	0.26	51,64,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LHG	A	410	49/49	0.83	0.23	45,80,104,115	0
28	STE	l	102	18/20	0.84	0.15	37,50,81,85	0
27	LHG	a	414	42/49	0.84	0.25	45,87,109,127	0
23	BCR	h	701	40/40	0.84	0.15	37,56,75,86	0
28	STE	c	521	20/20	0.84	0.18	39,57,79,84	0
28	STE	h	703	14/20	0.84	0.21	43,66,89,90	0
28	STE	b	724	16/20	0.85	0.16	52,66,82,85	0
26	SQD	A	412	39/54	0.85	0.16	38,64,94,99	0
22	CLA	c	513	65/65	0.85	0.15	40,59,95,110	0
33	LMG	a	419	55/55	0.85	0.15	35,62,103,143	0
28	STE	b	727	20/20	0.85	0.15	43,67,93,95	0
22	CLA	c	514	65/65	0.86	0.18	43,71,109,112	0
23	BCR	k	101	40/40	0.86	0.13	36,63,79,87	0
28	STE	A	411	16/20	0.86	0.20	34,47,74,75	0
22	CLA	C	514	65/65	0.86	0.18	40,65,98,108	0
28	STE	b	722	20/20	0.86	0.22	35,54,74,77	0
28	STE	B	725	18/20	0.86	0.14	37,54,75,81	0
28	STE	X	101	20/20	0.87	0.18	33,49,69,79	0
33	LMG	b	723	55/55	0.87	0.26	45,73,94,109	0
28	STE	j	101	12/20	0.87	0.11	41,57,67,69	0
26	SQD	B	723	54/54	0.88	0.15	37,60,94,106	0
22	CLA	H	102	65/65	0.88	0.14	30,60,95,107	0
26	SQD	f	101	41/54	0.88	0.20	55,88,106,108	0
28	STE	B	701	12/20	0.88	0.35	46,61,86,87	0
28	STE	d	409	17/20	0.88	0.15	42,55,64,68	0
28	STE	M	102	15/20	0.88	0.14	34,51,65,75	0
28	STE	C	523	12/20	0.88	0.11	33,46,58,69	0
23	BCR	k	102	40/40	0.89	0.17	40,54,68,71	0
28	STE	T	702	15/20	0.89	0.16	39,54,81,81	0
33	LMG	C	516	48/55	0.89	0.15	38,59,78,100	0
33	LMG	C	520	48/55	0.89	0.14	43,70,88,94	0
23	BCR	d	403	40/40	0.89	0.13	36,54,93,108	0
28	STE	Z	101	8/20	0.89	0.15	39,57,68,68	0
23	BCR	D	404	40/40	0.89	0.13	26,42,91,98	0
33	LMG	c	520	37/55	0.89	0.15	44,70,84,92	0
23	BCR	Y	101	40/40	0.89	0.12	40,54,75,77	0
33	LMG	c	523	49/55	0.89	0.12	34,57,82,100	0
22	CLA	C	503	65/65	0.90	0.14	30,44,57,62	0
28	STE	E	102	7/20	0.90	0.20	49,62,76,76	0
22	CLA	b	715	65/65	0.90	0.14	27,42,60,65	0
22	CLA	d	402	65/65	0.90	0.15	28,49,81,95	0
28	STE	C	521	12/20	0.90	0.11	34,52,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	STE	J	101	12/20	0.90	0.10	48,67,71,71	0
22	CLA	c	503	65/65	0.90	0.15	27,45,68,75	0
22	CLA	c	509	64/65	0.90	0.14	31,47,87,108	0
28	STE	m	101	12/20	0.90	0.14	42,57,70,79	0
28	STE	t	702	14/20	0.90	0.11	34,53,65,67	0
26	SQD	b	720	49/54	0.91	0.12	37,59,91,109	0
33	LMG	D	408	51/55	0.91	0.17	34,55,84,90	0
22	CLA	b	716	60/65	0.91	0.14	29,46,92,95	0
33	LMG	M	101	51/55	0.91	0.12	30,48,73,79	0
22	CLA	c	511	65/65	0.91	0.16	34,49,63,75	0
23	BCR	c	515	40/40	0.91	0.17	45,61,76,80	0
22	CLA	D	403	65/65	0.91	0.13	24,42,107,122	0
33	LMG	B	721	28/55	0.91	0.13	33,50,62,68	0
28	STE	A	414	5/20	0.91	0.14	41,57,71,71	0
23	BCR	K	101	40/40	0.92	0.13	42,57,71,79	0
22	CLA	a	406	65/65	0.92	0.12	18,38,76,81	0
22	CLA	C	507	65/65	0.92	0.13	26,44,83,94	0
22	CLA	b	702	65/65	0.92	0.15	28,42,63,66	0
33	LMG	b	721	51/55	0.92	0.11	34,52,76,93	0
29	DGD	C	518	62/66	0.92	0.12	35,52,99,119	0
23	BCR	B	719	40/40	0.92	0.10	22,42,58,64	0
22	CLA	C	508	65/65	0.92	0.13	25,42,57,63	0
22	CLA	c	512	65/65	0.92	0.13	38,55,71,74	0
23	BCR	C	515	40/40	0.93	0.10	25,39,51,59	0
22	CLA	a	404	65/65	0.93	0.15	27,42,102,112	0
22	CLA	c	504	65/65	0.93	0.15	23,44,56,64	0
22	CLA	c	506	65/65	0.93	0.16	25,41,69,76	0
22	CLA	c	507	65/65	0.93	0.12	30,48,97,104	0
23	BCR	b	719	40/40	0.93	0.10	33,48,65,76	0
29	DGD	C	519	62/66	0.93	0.11	32,49,69,84	0
29	DGD	c	518	62/66	0.93	0.12	32,53,87,94	0
29	DGD	h	702	62/66	0.93	0.10	32,48,61,73	0
22	CLA	c	508	65/65	0.93	0.13	26,43,60,64	0
22	CLA	C	512	65/65	0.93	0.12	30,52,67,74	0
22	CLA	C	504	65/65	0.93	0.13	30,45,56,58	0
22	CLA	C	506	65/65	0.93	0.16	23,41,69,80	0
22	CLA	b	704	65/65	0.93	0.13	21,37,84,97	0
22	CLA	b	709	65/65	0.93	0.13	27,47,68,80	0
22	CLA	B	716	60/65	0.93	0.14	23,39,87,103	0
23	BCR	B	718	40/40	0.93	0.09	22,39,53,54	0
22	CLA	B	715	65/65	0.93	0.10	24,36,67,75	0
26	SQD	D	409	36/54	0.93	0.16	48,76,93,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	SQD	a	413	54/54	0.93	0.14	41,64,90,97	0
23	BCR	C	501	40/40	0.93	0.17	38,56,70,74	0
28	STE	M	103	10/20	0.94	0.10	34,47,51,58	0
23	BCR	c	516	40/40	0.94	0.12	30,43,58,70	0
22	CLA	b	714	65/65	0.94	0.13	22,40,73,86	0
22	CLA	B	702	65/65	0.94	0.14	25,36,56,64	0
22	CLA	B	706	65/65	0.94	0.10	24,37,81,90	0
29	DGD	H	103	62/66	0.94	0.10	28,46,60,64	0
23	BCR	B	717	40/40	0.94	0.12	24,41,58,62	0
28	STE	B	724	12/20	0.94	0.07	40,51,66,66	0
22	CLA	C	509	65/65	0.94	0.12	27,44,105,117	0
25	PL9	D	405	55/55	0.94	0.10	23,33,48,54	0
22	CLA	C	510	65/65	0.94	0.17	27,45,63,74	0
26	SQD	A	409	52/54	0.94	0.15	27,61,89,95	0
22	CLA	c	505	60/65	0.94	0.11	34,47,77,84	0
22	CLA	C	511	65/65	0.94	0.13	32,48,65,80	0
22	CLA	B	712	65/65	0.94	0.14	20,31,45,54	0
22	CLA	C	505	59/65	0.94	0.12	28,43,75,85	0
22	CLA	b	706	65/65	0.94	0.11	23,39,75,80	0
22	CLA	c	510	65/65	0.94	0.17	33,48,63,69	0
22	CLA	b	708	65/65	0.94	0.14	28,44,64,66	0
22	CLA	A	403	65/65	0.94	0.14	21,35,88,102	0
33	LMG	d	408	44/55	0.94	0.11	34,53,82,87	0
34	PHO	a	405	64/64	0.94	0.13	18,32,41,46	0
22	CLA	D	402	65/65	0.95	0.09	15,27,51,56	0
23	BCR	T	701	40/40	0.95	0.09	28,41,57,60	0
22	CLA	B	713	65/65	0.95	0.13	19,32,72,74	0
29	DGD	C	517	62/66	0.95	0.12	23,42,75,85	0
23	BCR	a	407	40/40	0.95	0.08	23,34,50,54	0
23	BCR	b	717	40/40	0.95	0.10	27,41,52,56	0
23	BCR	b	718	40/40	0.95	0.09	27,39,52,55	0
27	LHG	B	722	49/49	0.95	0.13	29,46,70,77	0
29	DGD	c	519	62/66	0.95	0.13	28,55,83,95	0
22	CLA	b	710	65/65	0.95	0.18	24,38,49,61	0
22	CLA	b	712	65/65	0.95	0.16	23,36,47,52	0
22	CLA	b	713	65/65	0.95	0.14	18,36,67,82	0
22	CLA	B	714	65/65	0.95	0.16	19,37,78,96	0
22	CLA	A	404	54/65	0.95	0.10	17,31,61,68	0
23	BCR	A	405	40/40	0.95	0.09	24,36,47,53	0
22	CLA	B	707	65/65	0.95	0.10	17,35,65,75	0
23	BCR	t	701	40/40	0.95	0.10	22,38,54,56	0
22	CLA	B	709	65/65	0.95	0.12	23,38,52,56	0

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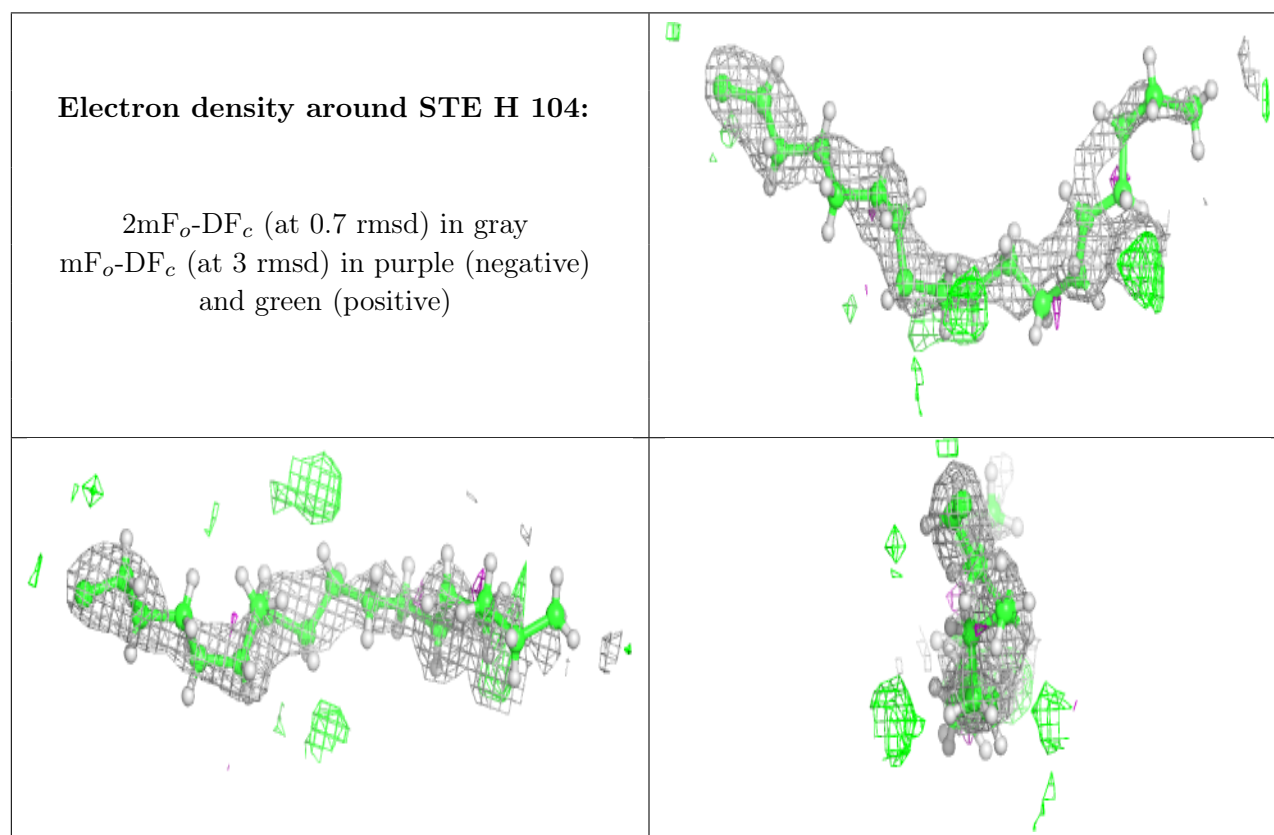
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CLA	B	710	65/65	0.95	0.13	17,33,45,48	0
22	CLA	B	711	65/65	0.95	0.14	18,30,50,56	0
25	PL9	d	404	55/55	0.95	0.10	21,34,43,47	0
22	CLA	b	705	65/65	0.95	0.12	19,35,49,61	0
22	CLA	B	704	65/65	0.95	0.11	20,32,76,78	0
34	PHO	D	406	64/64	0.95	0.10	16,28,37,42	0
22	CLA	b	707	65/65	0.95	0.13	19,36,68,75	0
29	DGD	c	517	62/66	0.96	0.10	24,42,78,87	0
22	CLA	c	502	65/65	0.96	0.12	27,41,52,56	0
22	CLA	a	403	65/65	0.96	0.10	19,31,42,58	0
22	CLA	d	401	65/65	0.96	0.11	20,36,54,62	0
32	BCT	a	410	4/4	0.96	0.18	30,32,44,53	0
22	CLA	B	705	65/65	0.96	0.13	15,31,45,52	0
27	LHG	D	411	47/49	0.96	0.11	24,49,85,96	0
27	LHG	L	101	49/49	0.96	0.10	31,41,55,65	0
27	LHG	a	412	49/49	0.96	0.13	30,48,76,83	0
22	CLA	B	703	65/65	0.96	0.14	20,33,57,65	0
27	LHG	d	406	49/49	0.96	0.10	26,45,56,62	0
27	LHG	d	407	39/49	0.96	0.10	33,49,68,71	0
27	LHG	l	101	49/49	0.96	0.11	31,44,53,61	0
22	CLA	D	401	65/65	0.96	0.11	14,29,57,68	0
22	CLA	b	711	65/65	0.96	0.13	22,34,59,64	0
22	CLA	A	402	65/65	0.96	0.09	15,29,44,57	0
22	CLA	b	703	65/65	0.96	0.13	24,37,68,78	0
22	CLA	B	708	65/65	0.96	0.11	19,36,54,59	0
22	CLA	C	502	65/65	0.96	0.11	22,36,50,61	0
34	PHO	D	407	64/64	0.96	0.13	23,32,44,51	0
22	CLA	a	401	65/65	0.96	0.11	21,32,41,47	0
34	PHO	d	405	64/64	0.96	0.10	28,39,48,63	0
35	HEC	E	103	43/43	0.96	0.12	34,51,70,74	0
35	HEC	e	101	43/43	0.96	0.12	42,59,80,88	0
35	HEC	V	201	43/43	0.97	0.12	17,33,43,50	0
27	LHG	D	410	49/49	0.97	0.09	21,40,54,65	0
35	HEC	v	201	43/43	0.97	0.12	26,37,51,52	0
24	CL	A	406	1/1	0.98	0.06	29,29,29,29	0
32	BCT	A	417	4/4	0.98	0.17	25,31,36,43	0
31	OEY	a	421[B]	11/11	0.99	0.10	19,25,29,33	11
24	CL	A	407	1/1	0.99	0.02	27,27,27,27	0
24	CL	a	408	1/1	0.99	0.03	28,28,28,28	0
24	CL	a	409	1/1	0.99	0.03	28,28,28,28	0
21	FE2	a	402	1/1	0.99	0.06	33,33,33,33	0
30	OEX	A	415[A]	10/10	0.99	0.12	32,35,38,40	10

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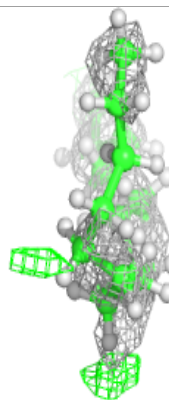
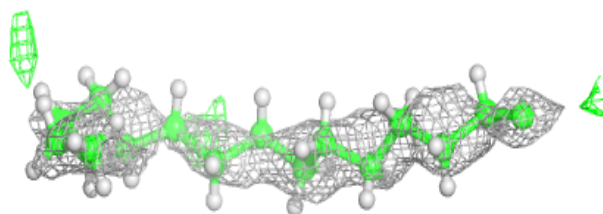
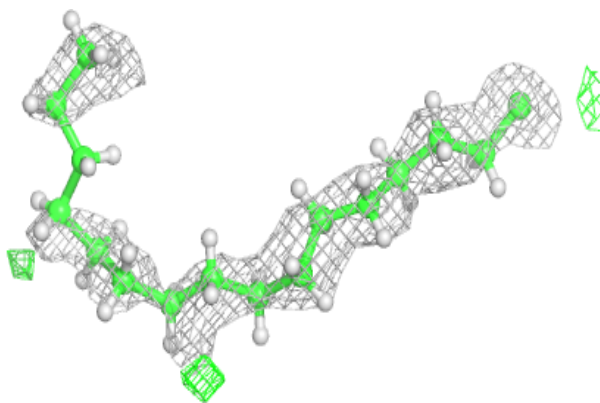
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	OEX	a	420[A]	10/10	0.99	0.10	29,35,39,39	10
31	OEY	A	416[B]	11/11	0.99	0.11	14,24,29,31	11
21	FE2	A	401	1/1	1.00	0.09	29,29,29,29	0

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

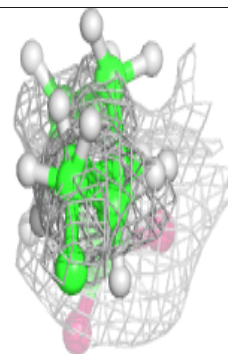
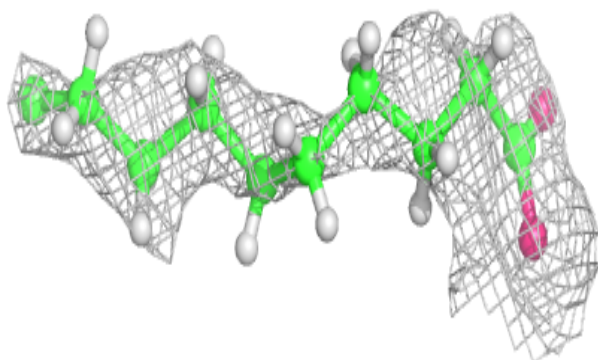
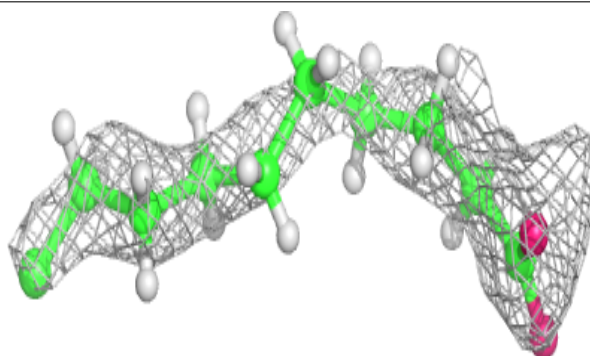


Electron density around STE B 726:

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

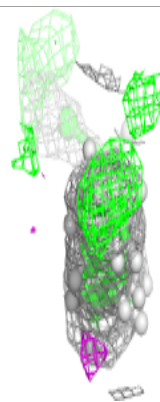
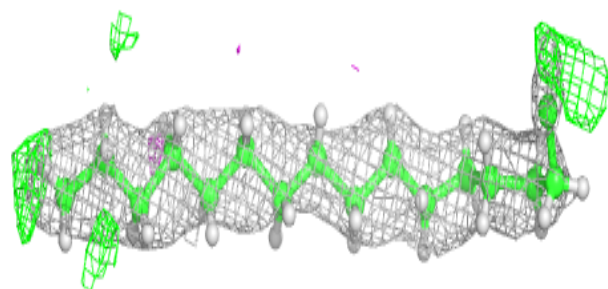
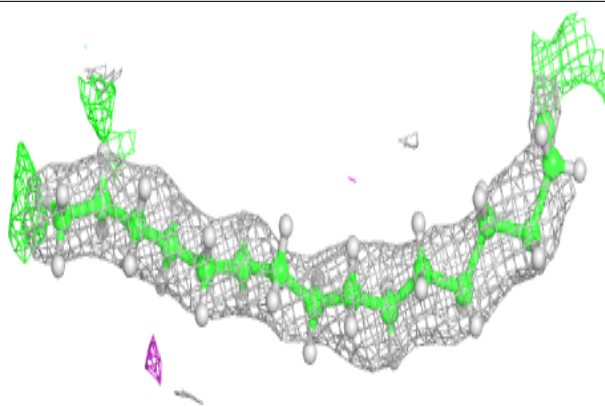
**Electron density around STE E 101:**

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

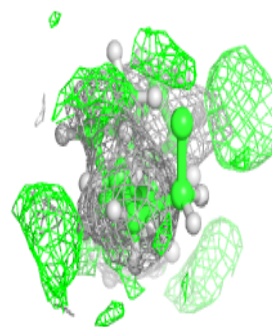
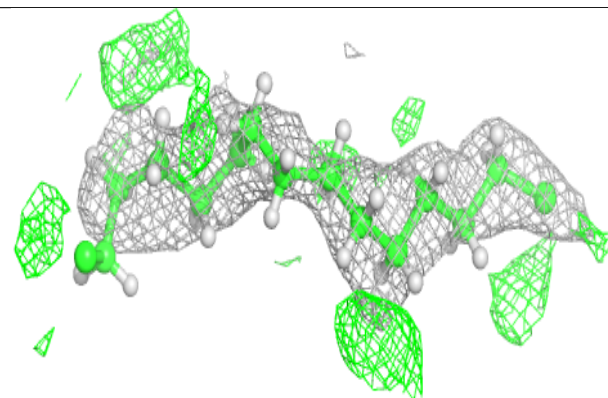
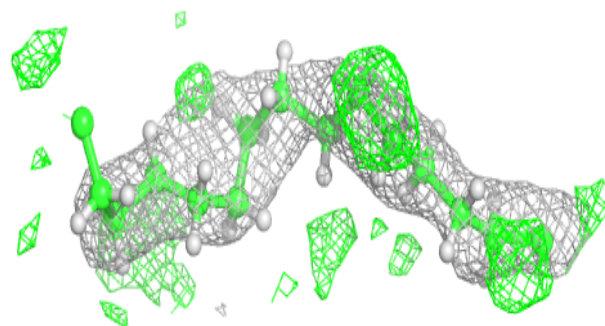


Electron density around STE C 522:

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

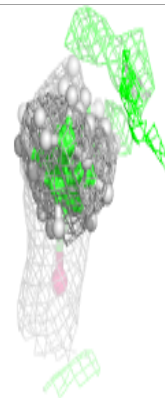
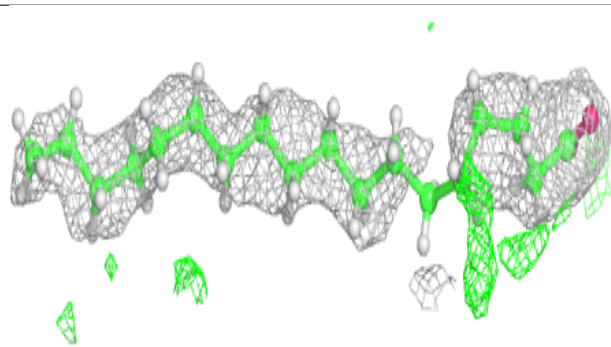
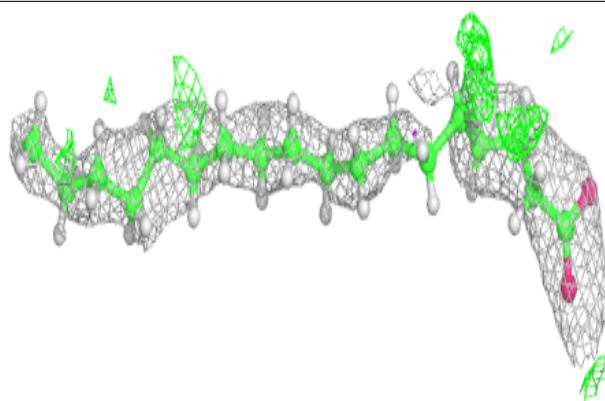
**Electron density around STE a 418:**

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

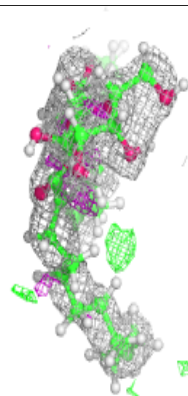
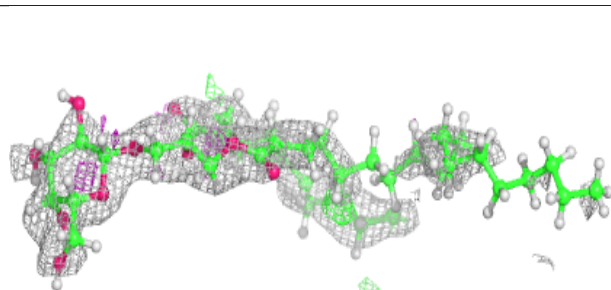
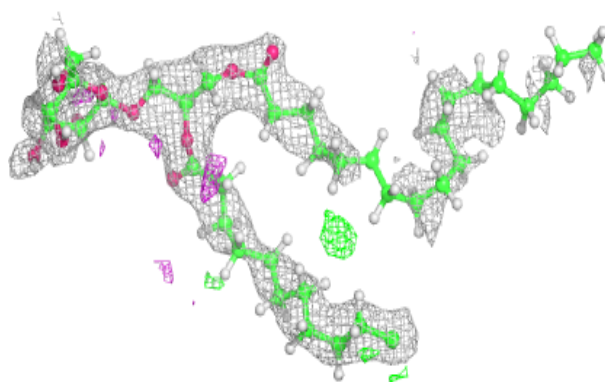


Electron density around STE b 725:

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

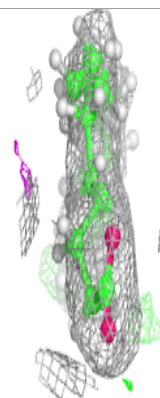
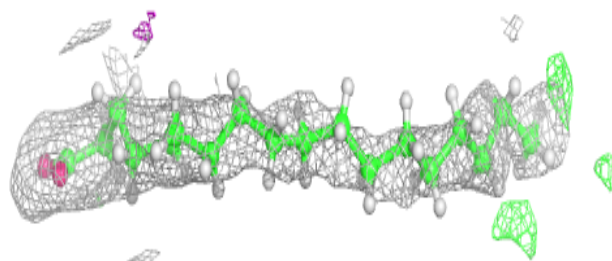
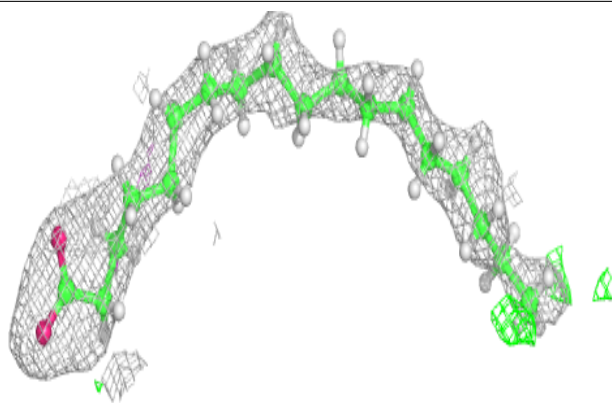
**Electron density around LMG c 522:**

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

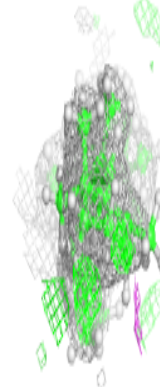
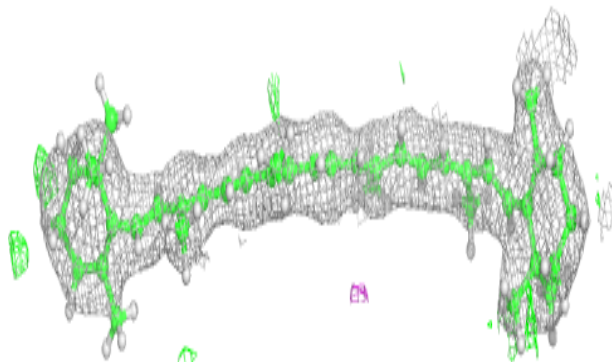
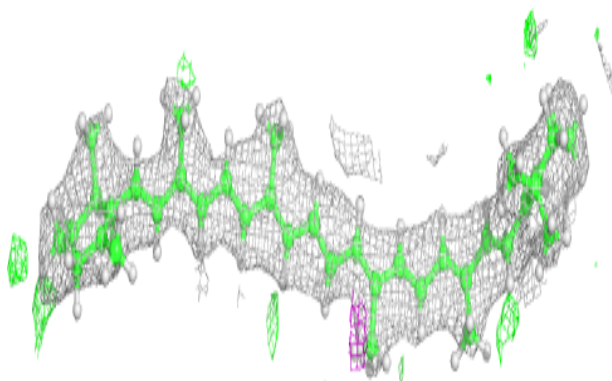


Electron density around STE x 101:

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

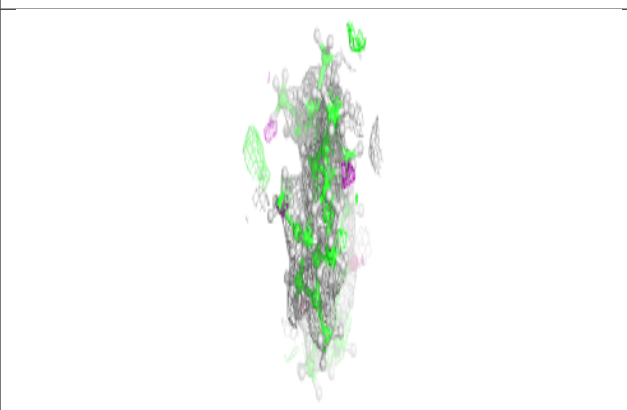
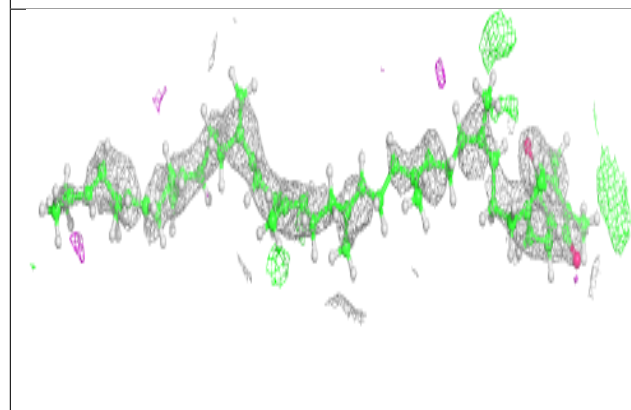
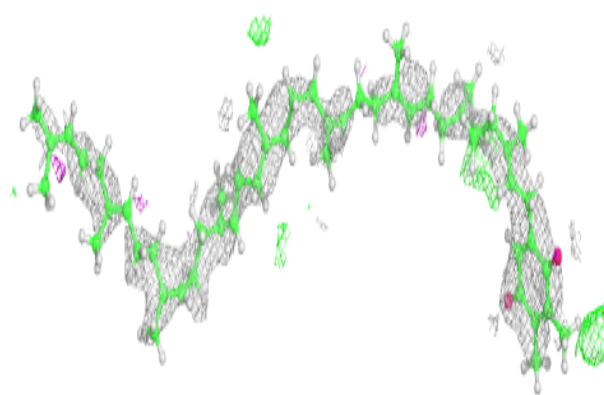
**Electron density around BCR H 101:**

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

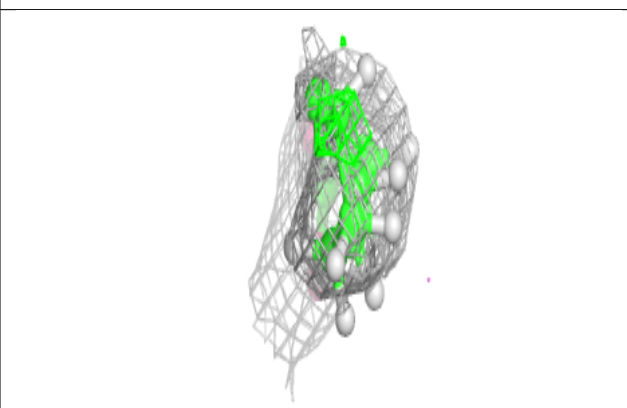
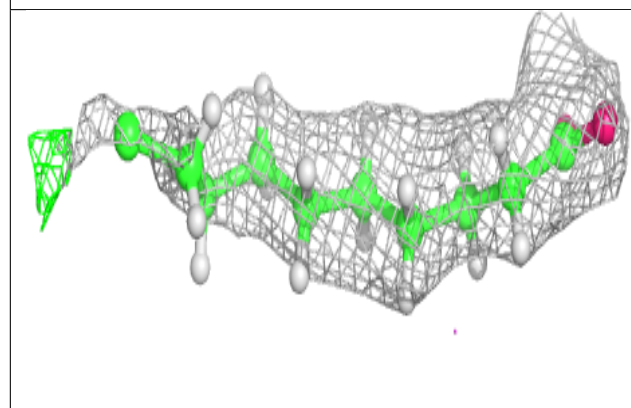
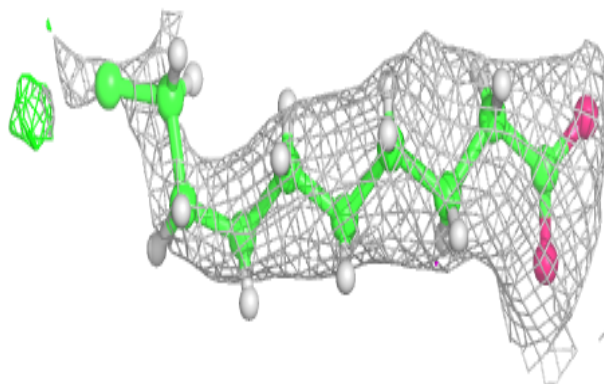


Electron density around PL9 A 408:

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

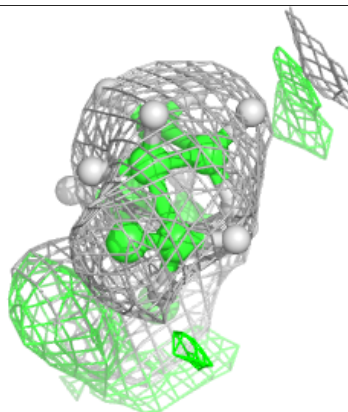
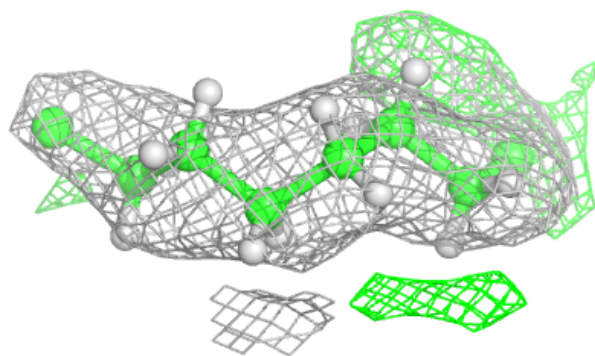
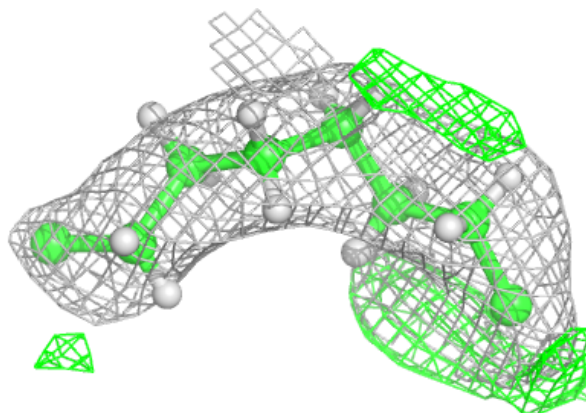
**Electron density around STE c 501:**

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

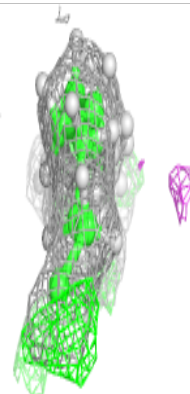
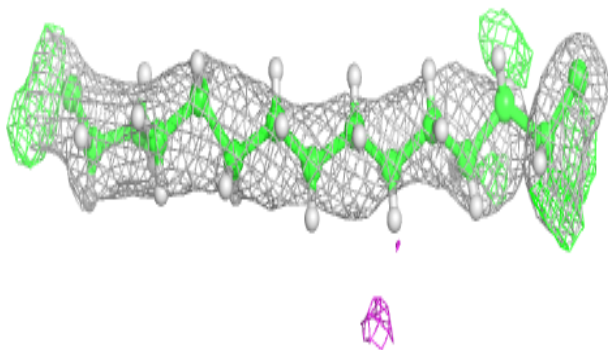
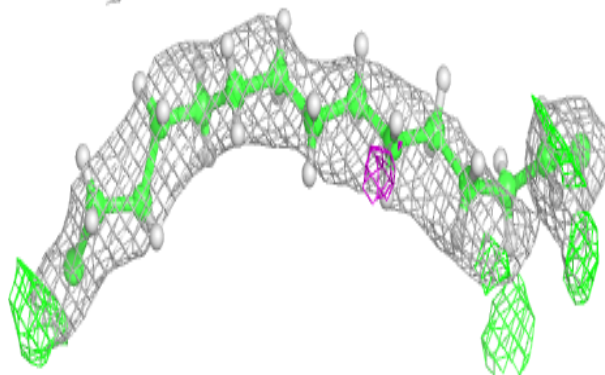


Electron density around STE H 105:

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

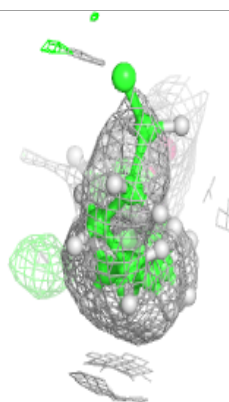
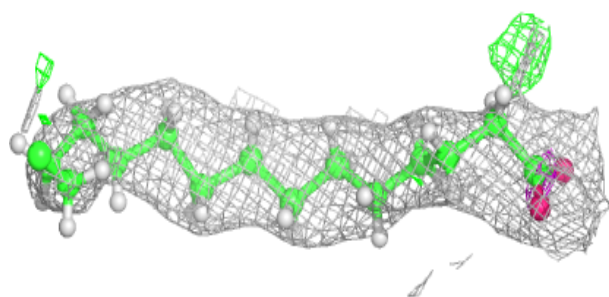
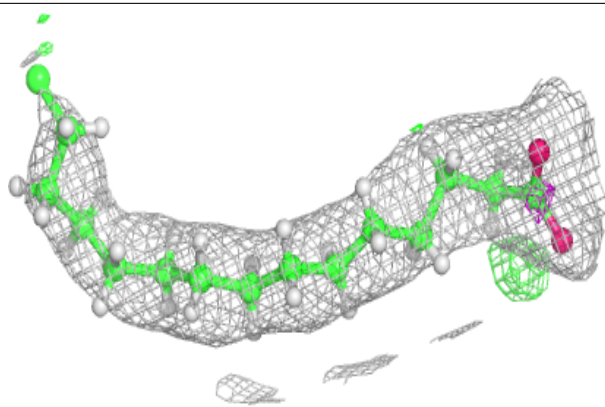
**Electron density around STE I 101:**

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

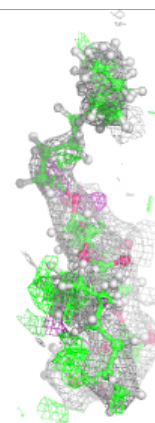
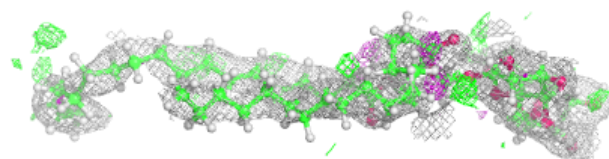
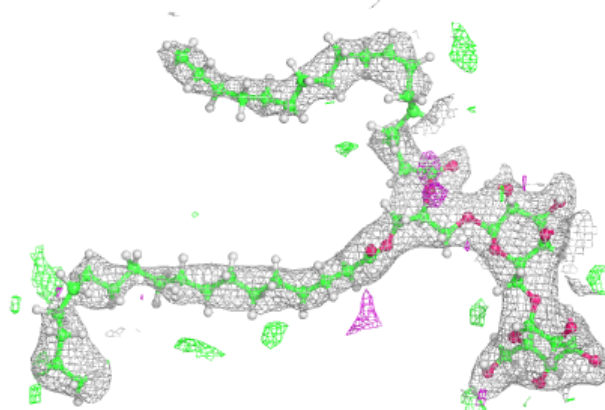


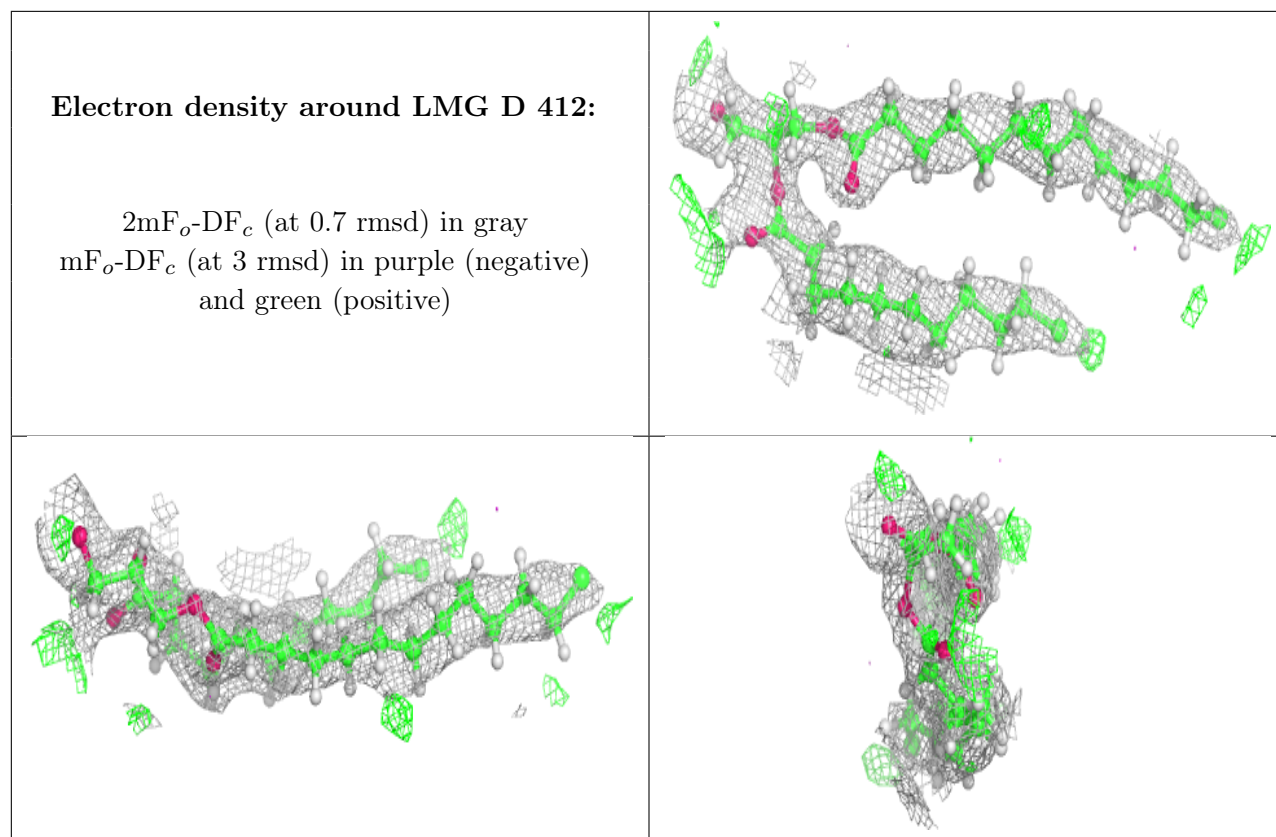
Electron density around STE B 720:

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

**Electron density around DGD A 413:**

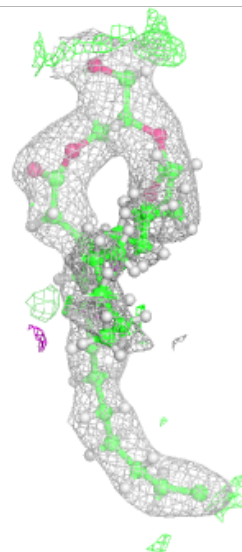
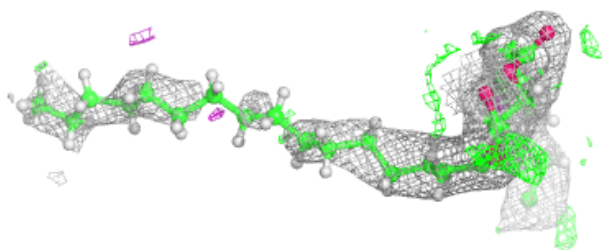
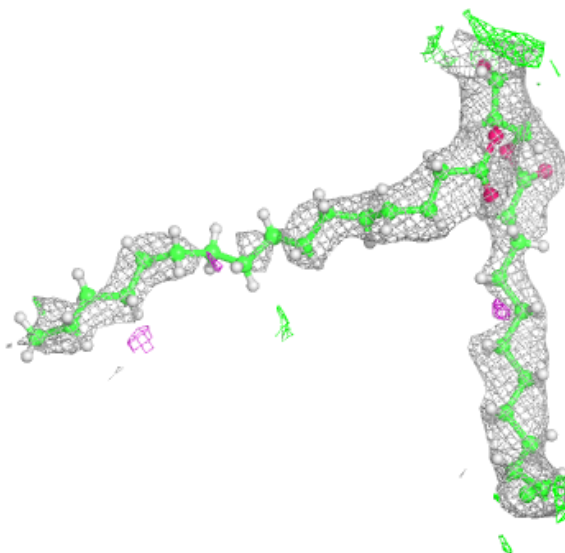
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





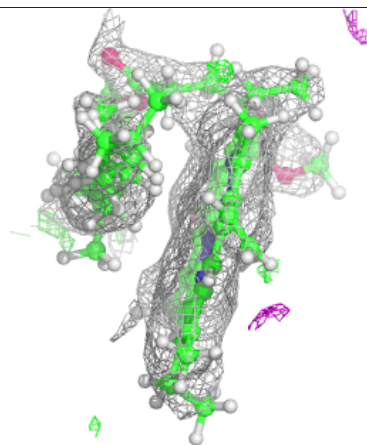
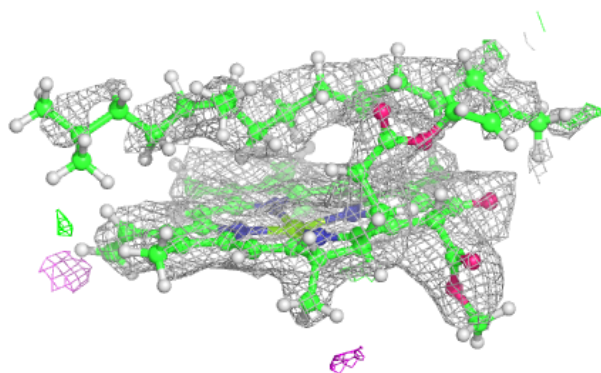
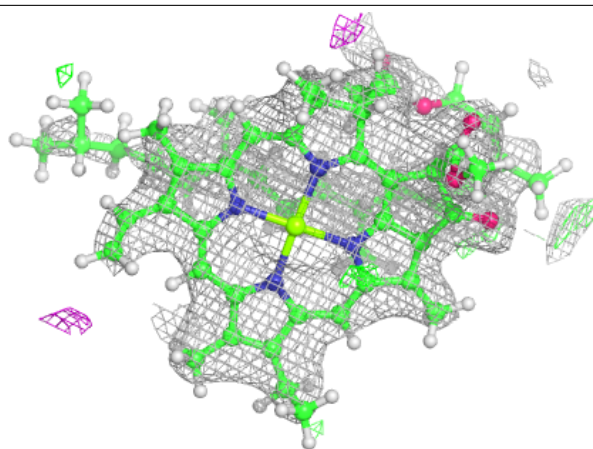
Electron density around SQD a 415:

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

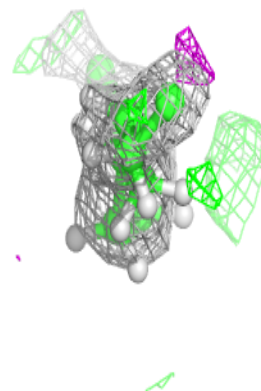
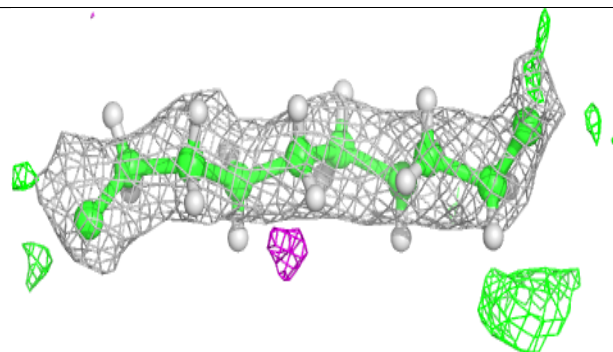
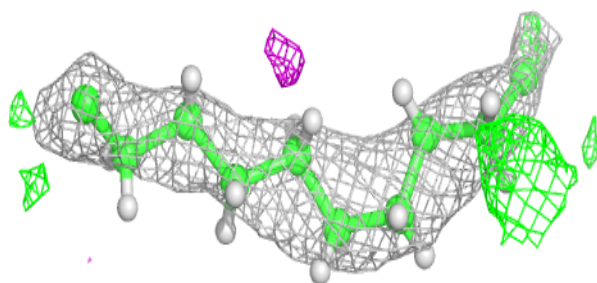


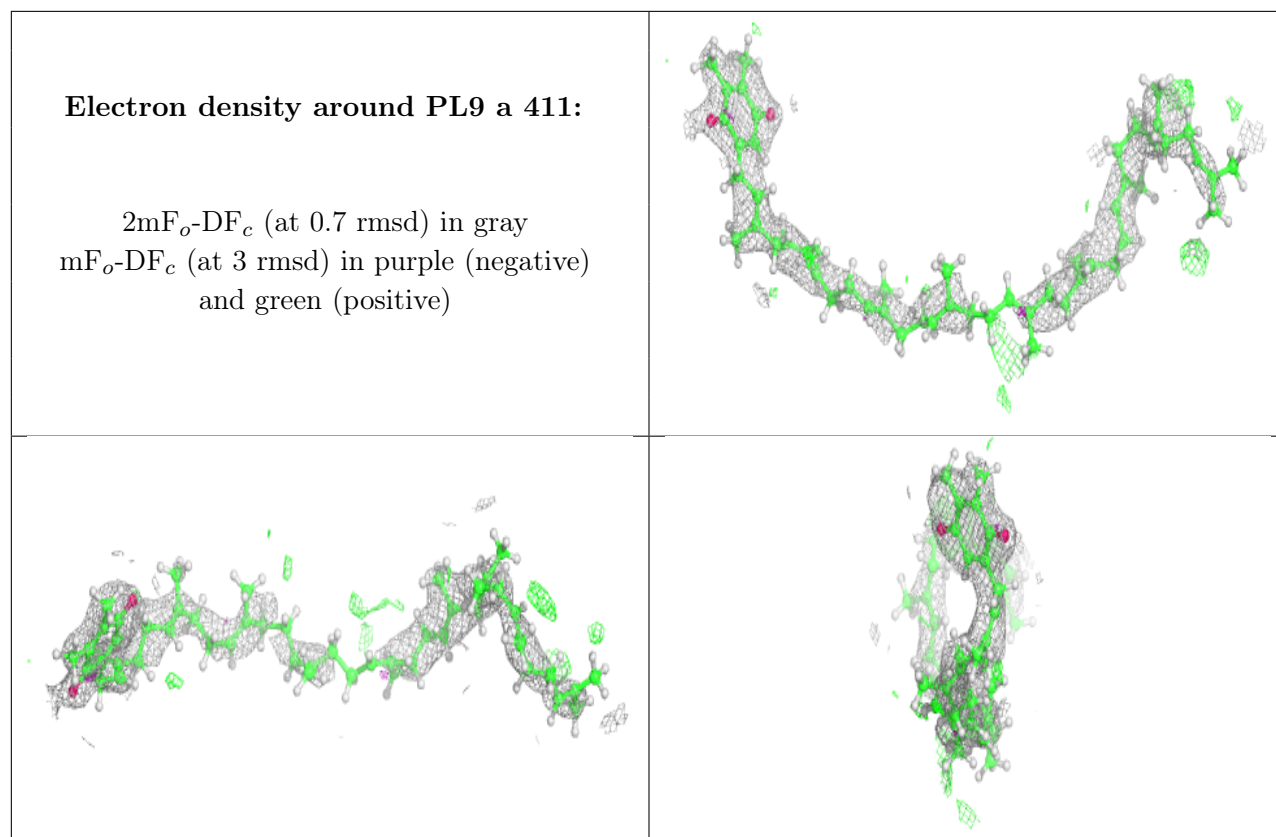
Electron density around CLA b 701:

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

**Electron density around STE b 726:**

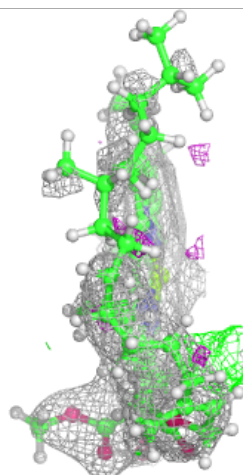
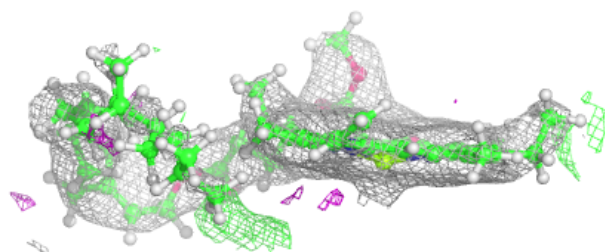
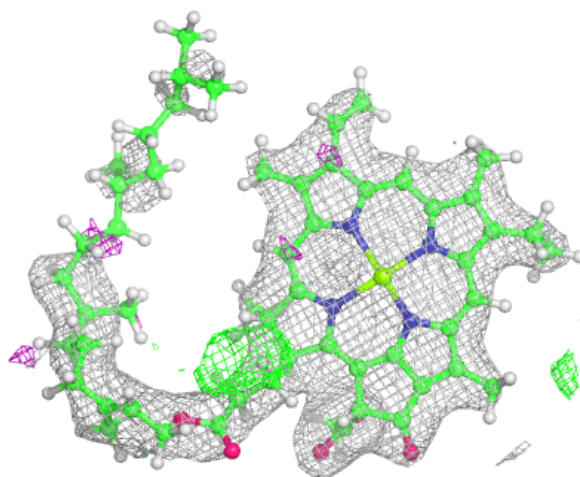
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





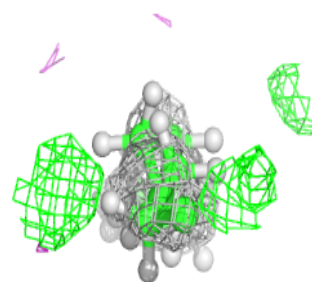
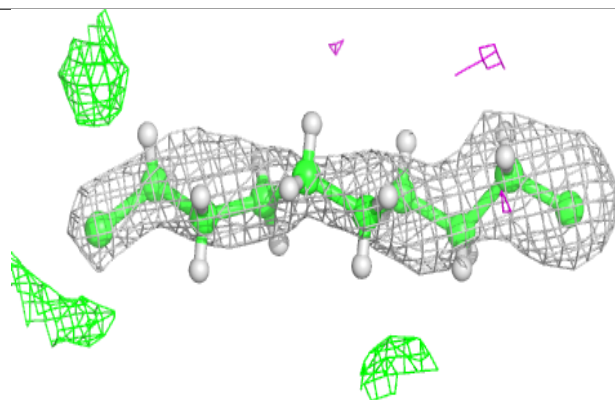
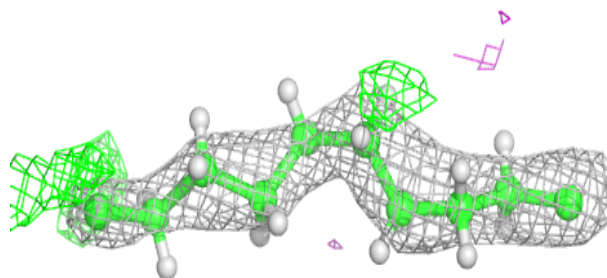
Electron density around CLA C 513:

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

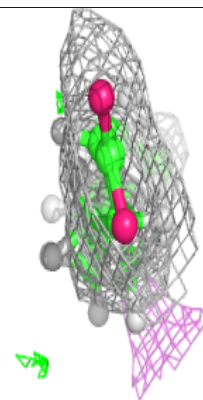
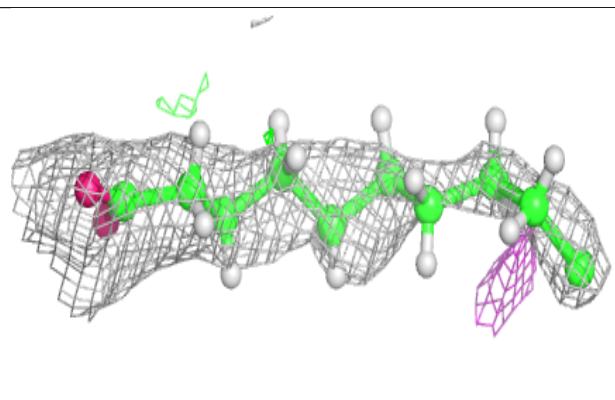
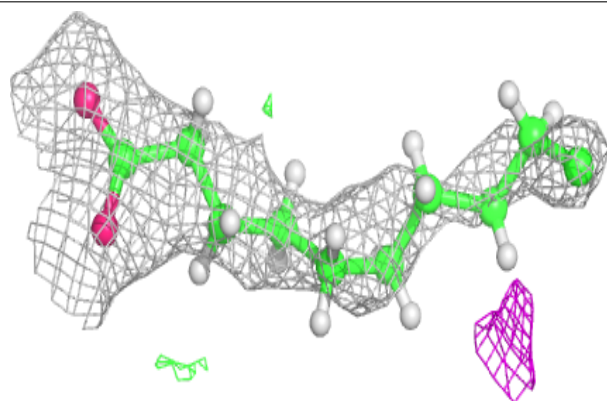


Electron density around STE a 416:

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

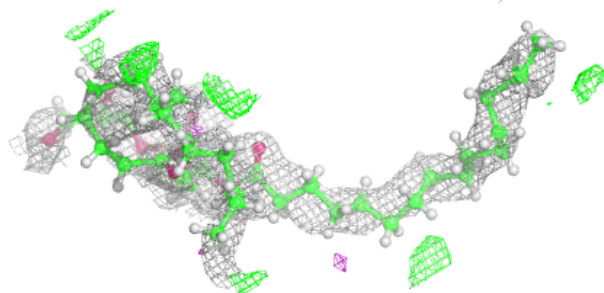
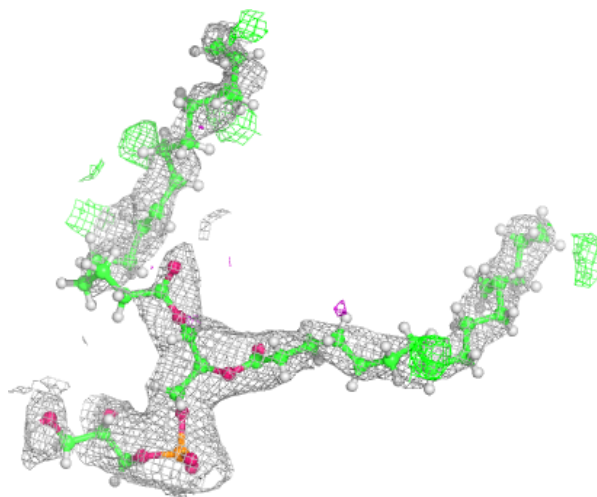
**Electron density around STE a 417:**

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



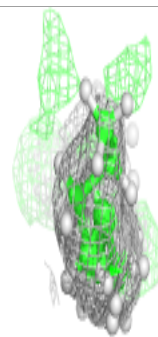
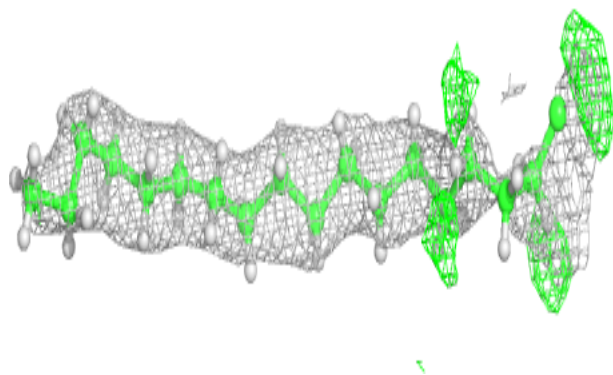
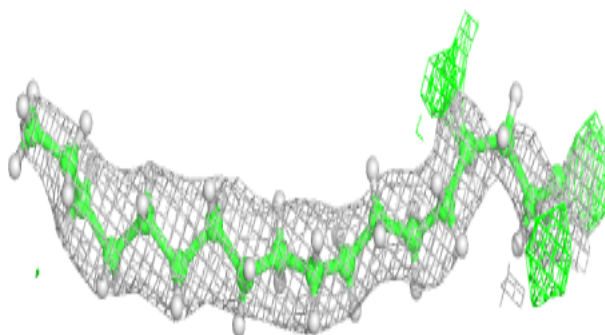
Electron density around LHG A 410:

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

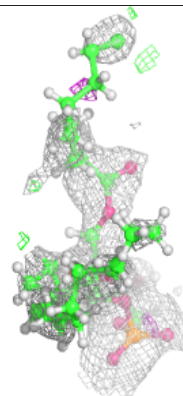
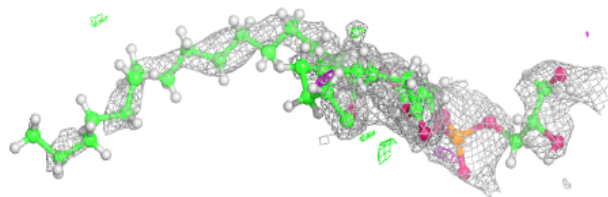
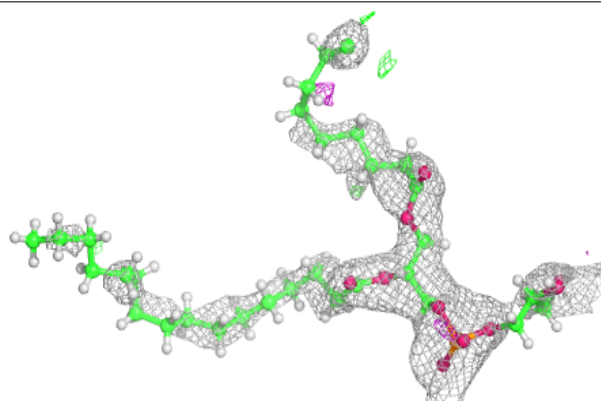


Electron density around STE 1 102:

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

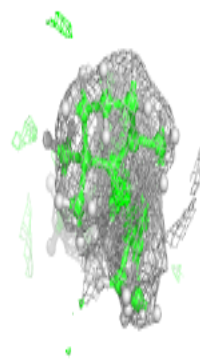
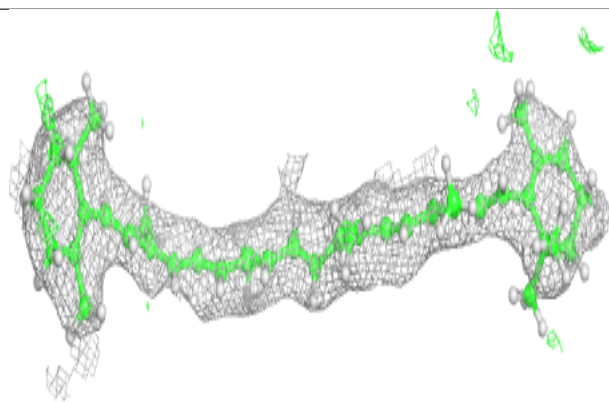
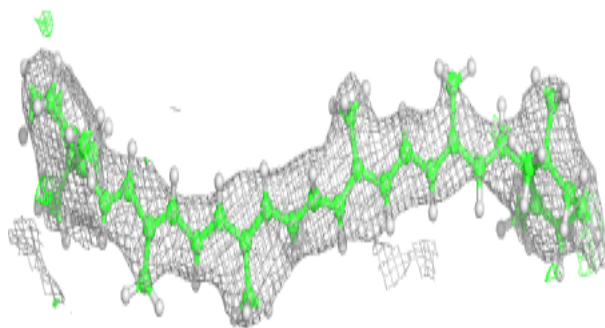
**Electron density around LHG a 414:**

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

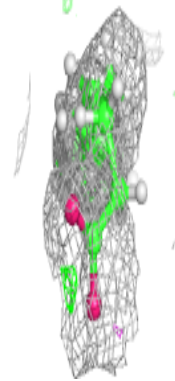
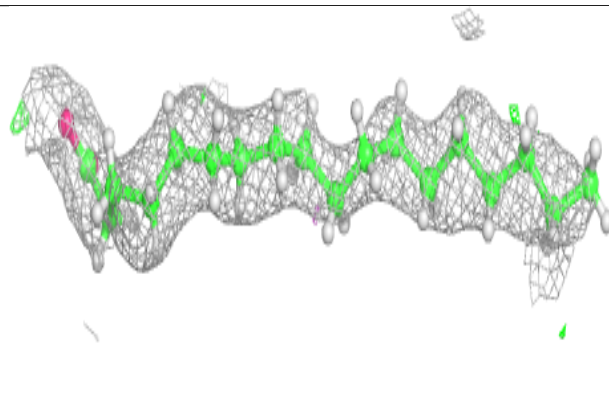
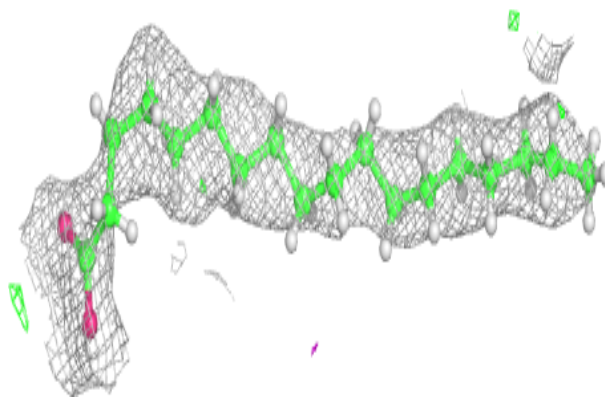


Electron density around BCR h 701:

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

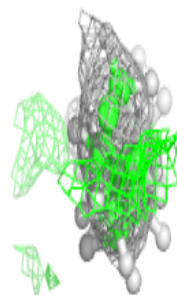
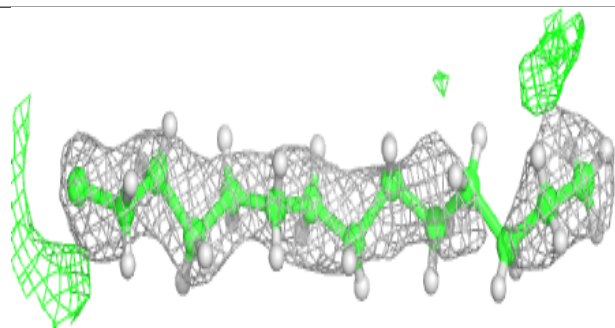
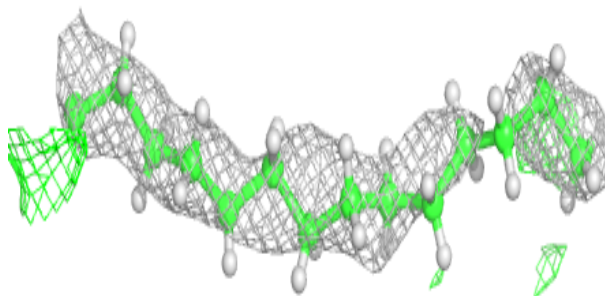
**Electron density around STE c 521:**

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

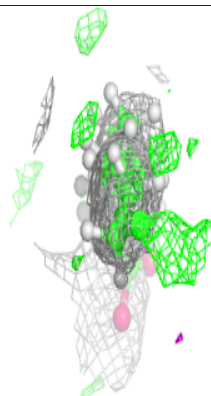
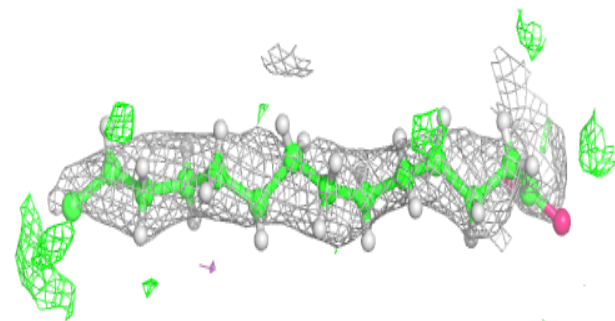
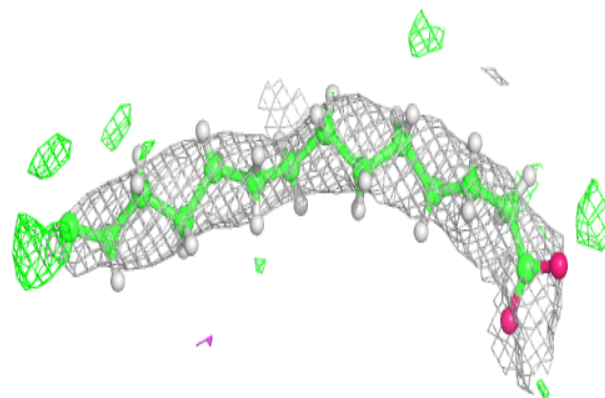


Electron density around STE h 703:

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

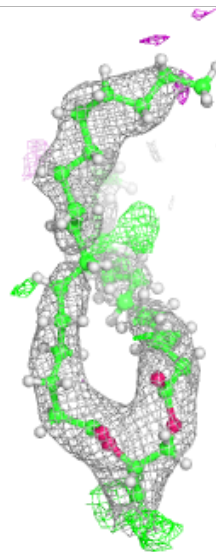
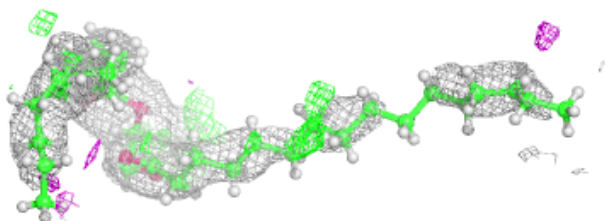
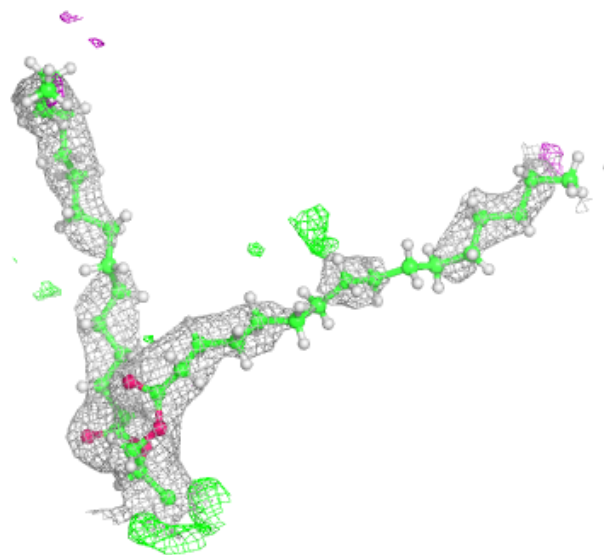
**Electron density around STE b 724:**

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



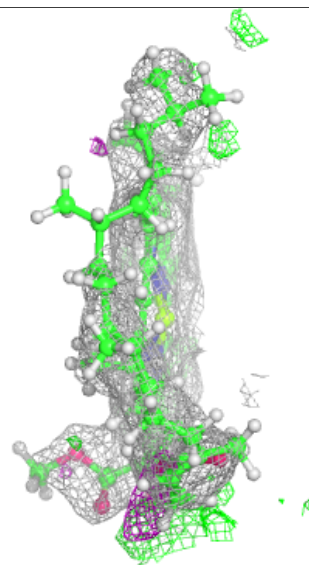
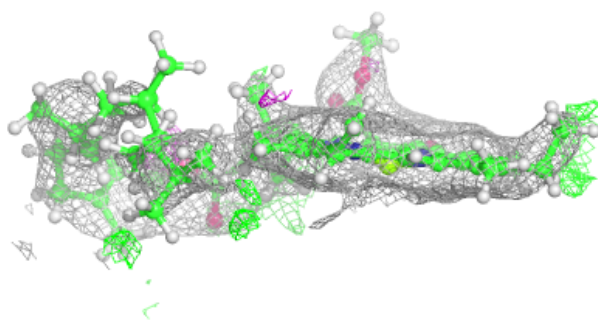
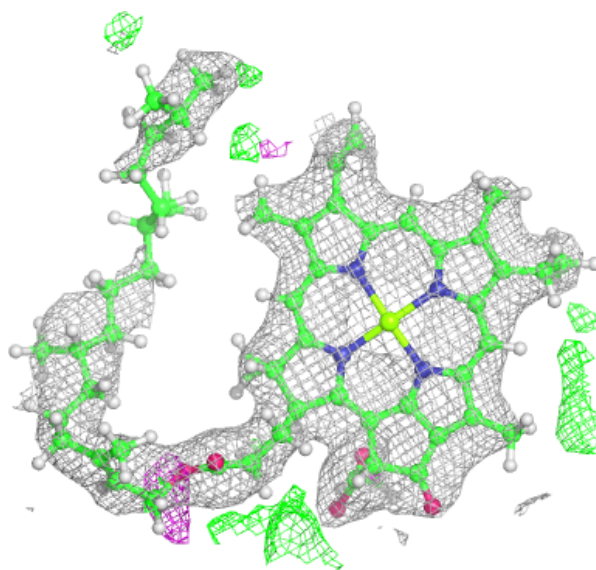
Electron density around SQD A 412:

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



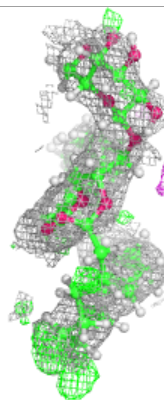
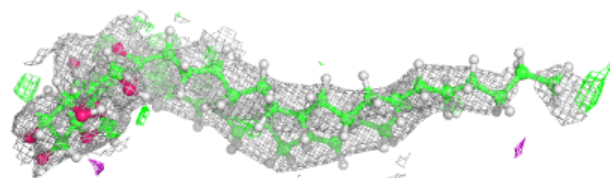
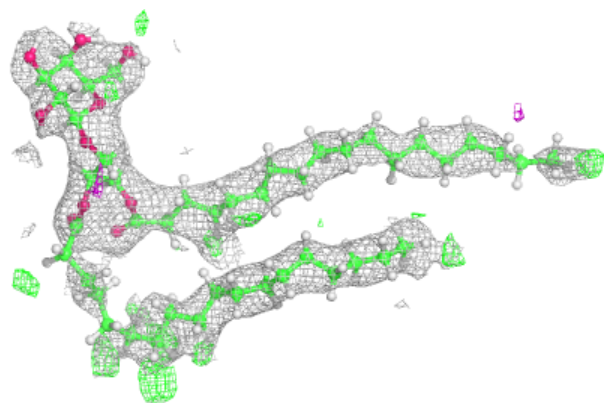
Electron density around CLA c 513:

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

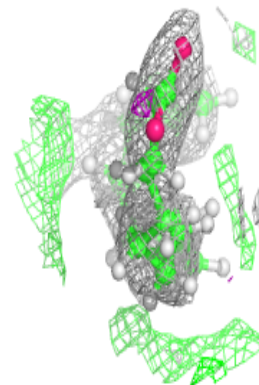
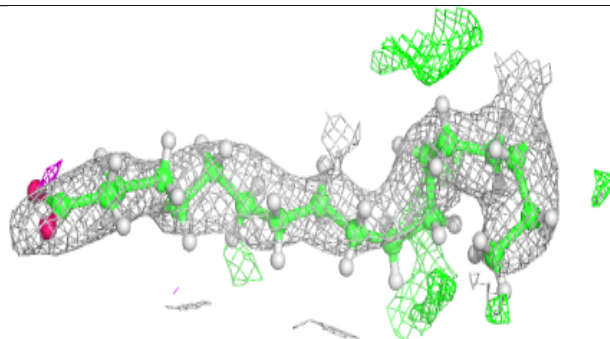
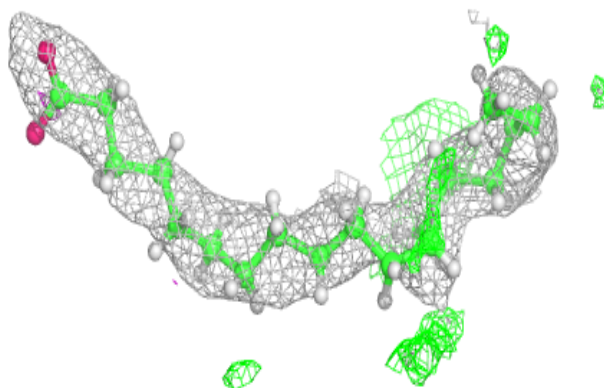


Electron density around LMG a 419:

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

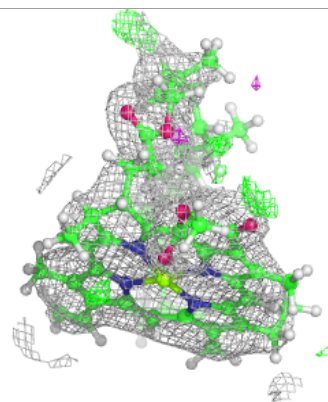
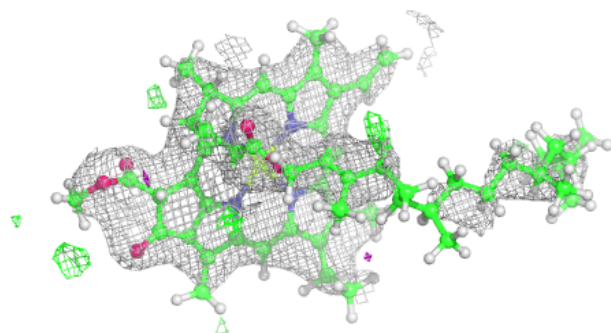
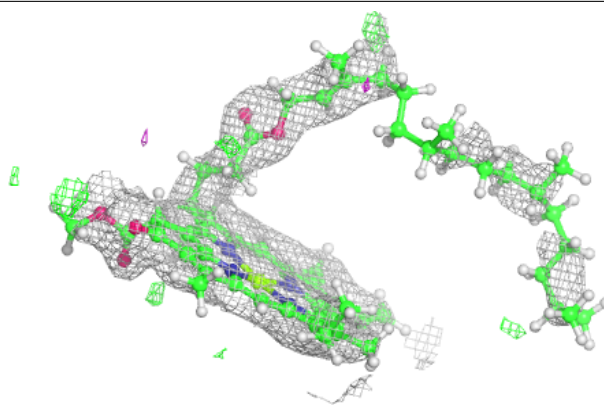
**Electron density around STE b 727:**

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

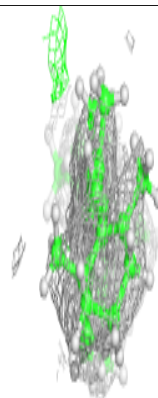
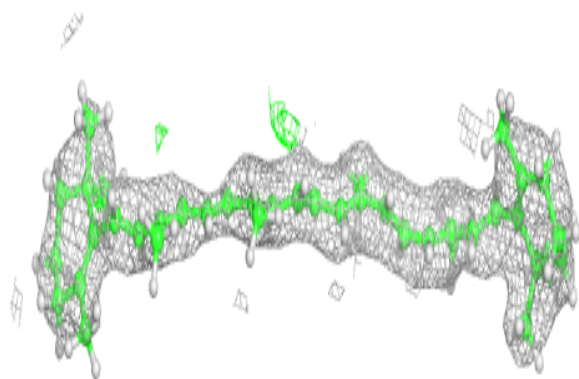
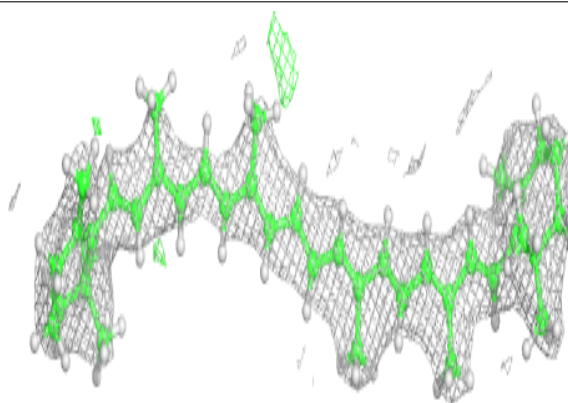


Electron density around CLA c 514:

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

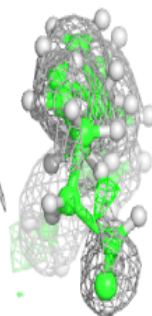
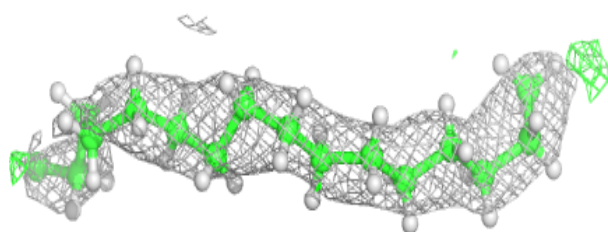
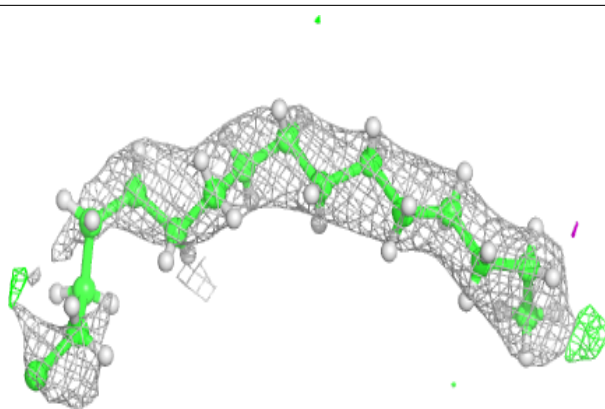
**Electron density around BCR k 101:**

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

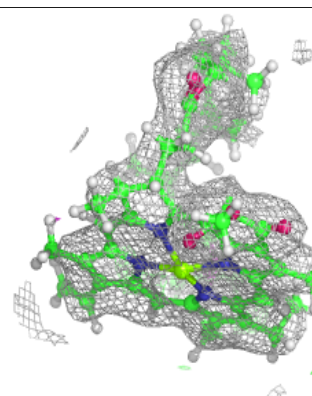
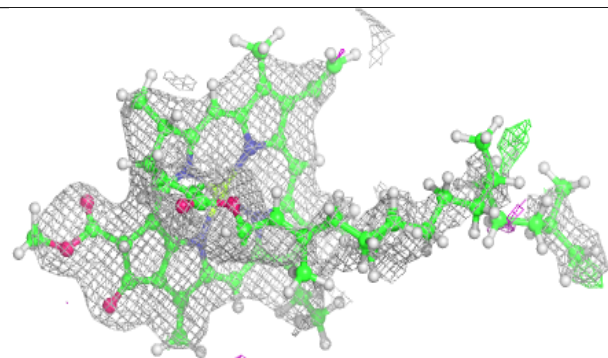
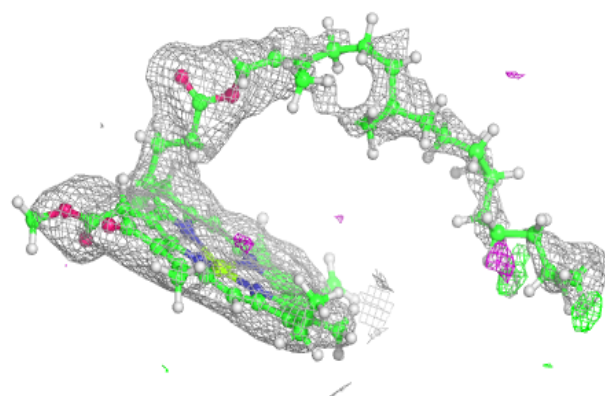


Electron density around STE A 411:

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

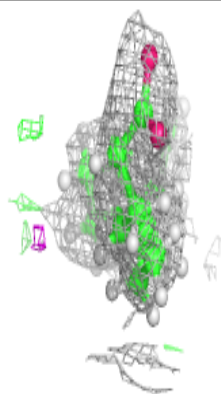
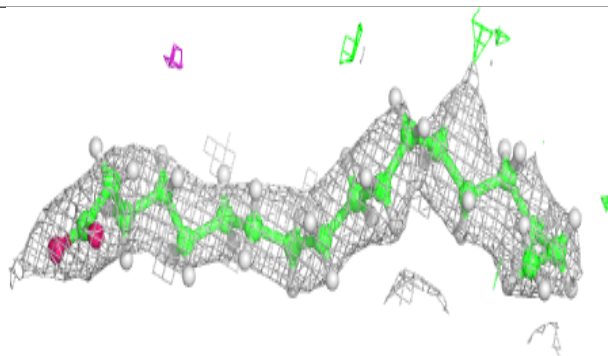
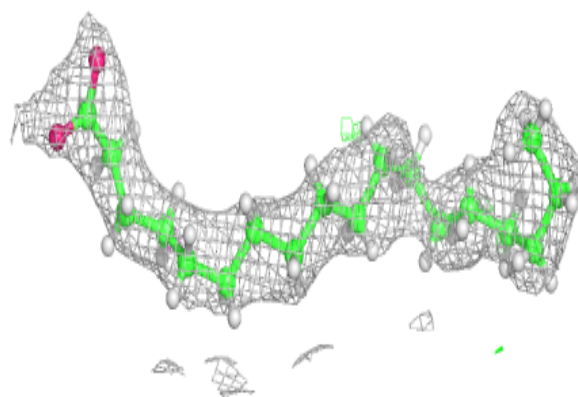
**Electron density around CLA C 514:**

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

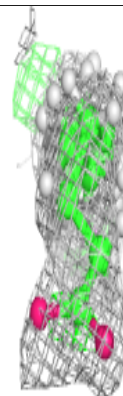
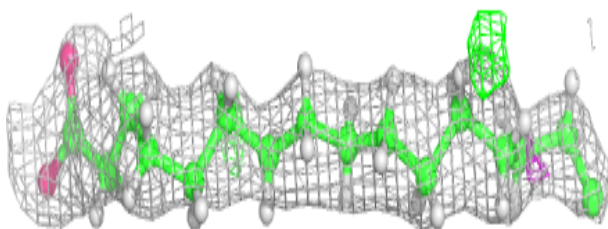
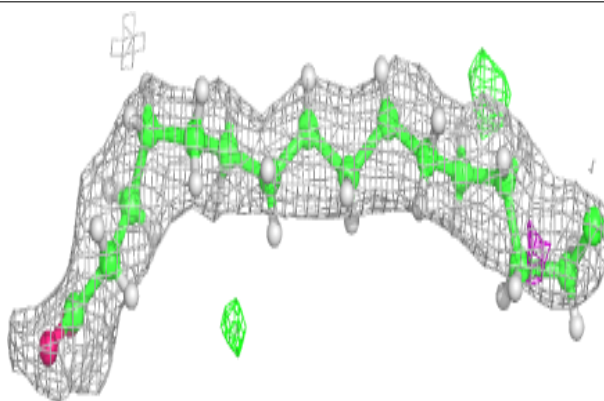


Electron density around STE b 722:

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

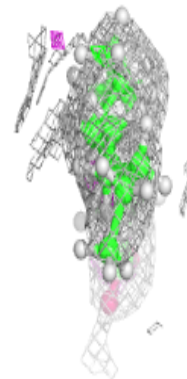
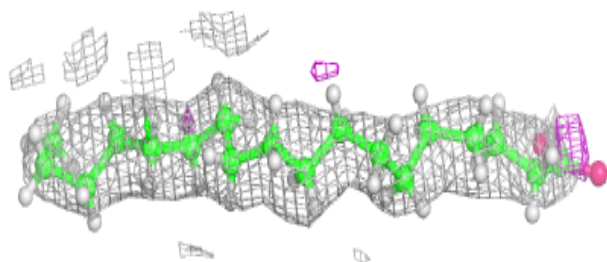
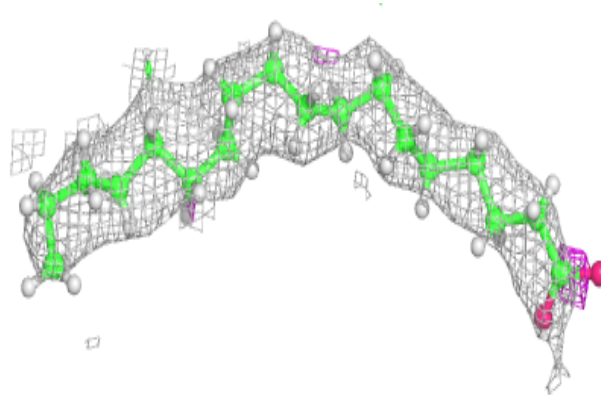
**Electron density around STE B 725:**

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

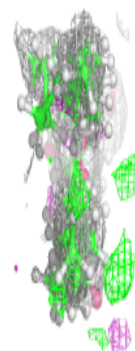
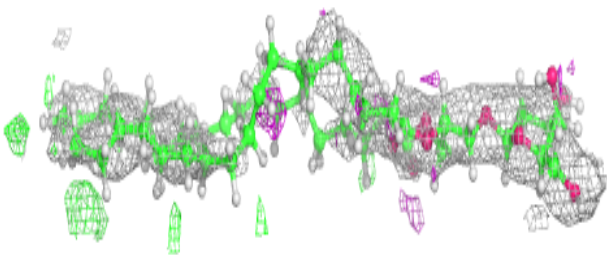
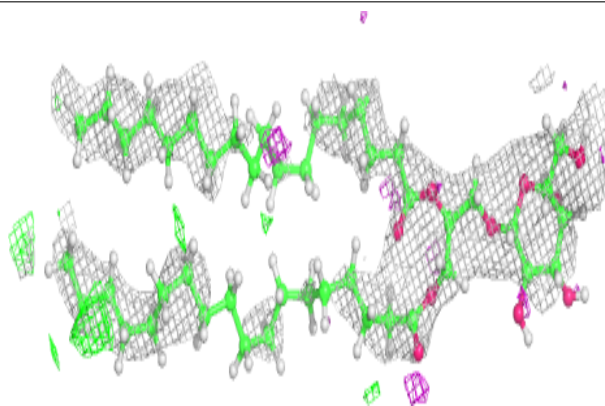


Electron density around STE X 101:

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

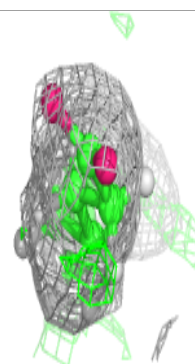
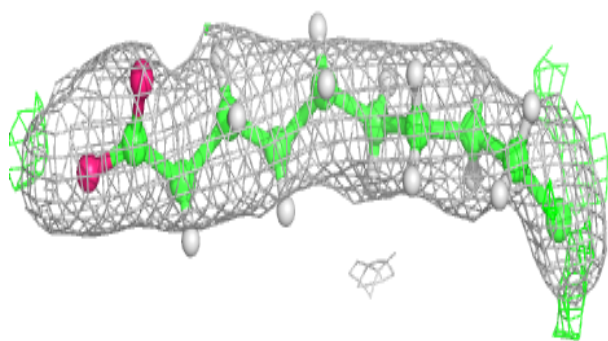
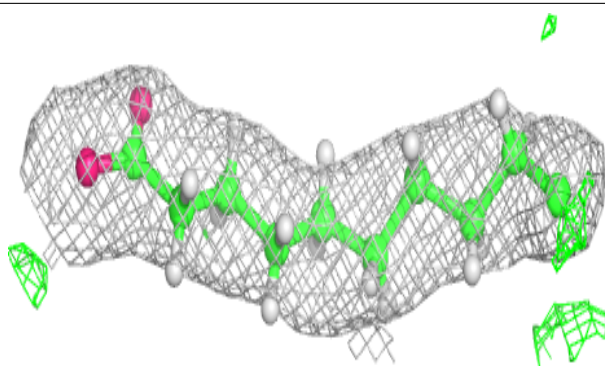
**Electron density around LMG b 723:**

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

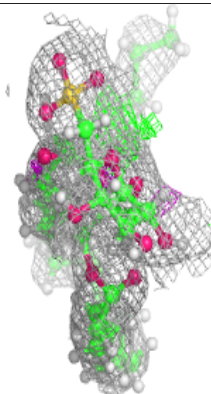
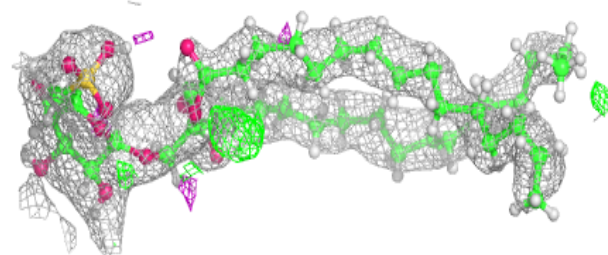
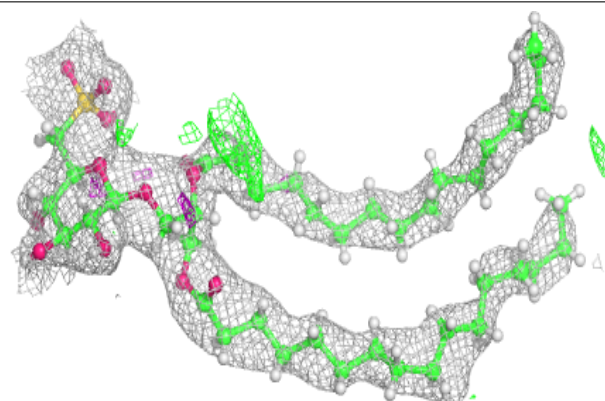


Electron density around STE j 101:

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

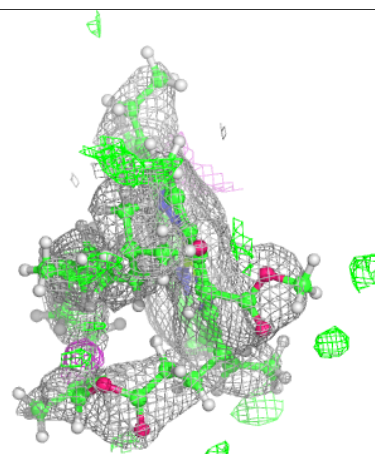
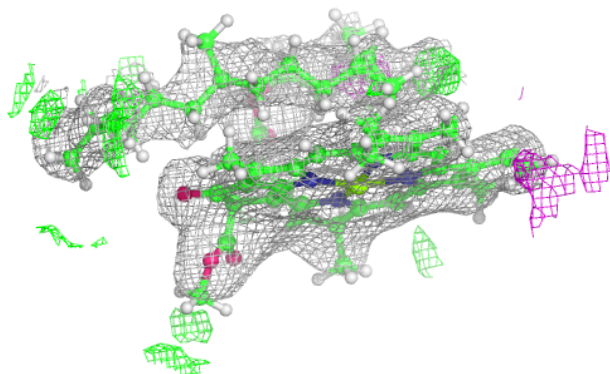
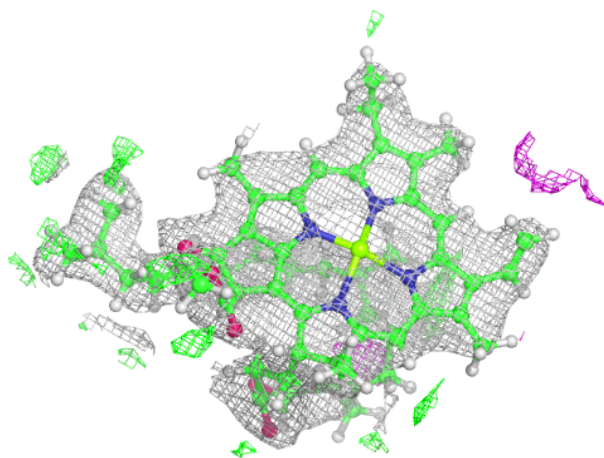
**Electron density around SQD B 723:**

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



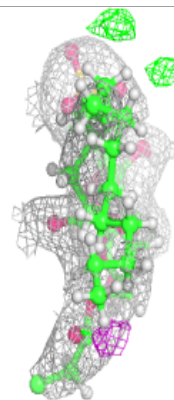
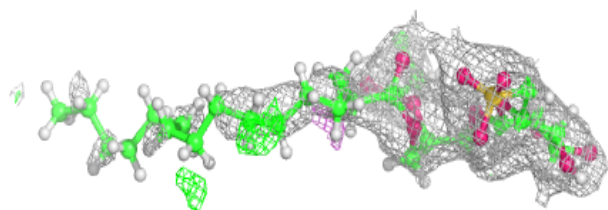
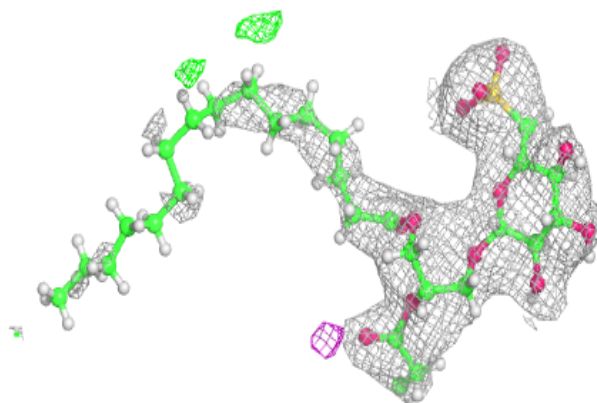
Electron density around CLA H 102:

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

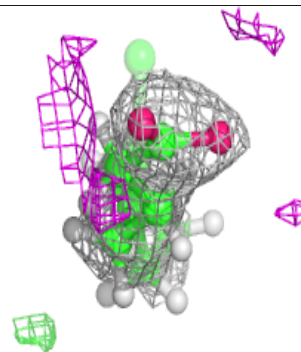
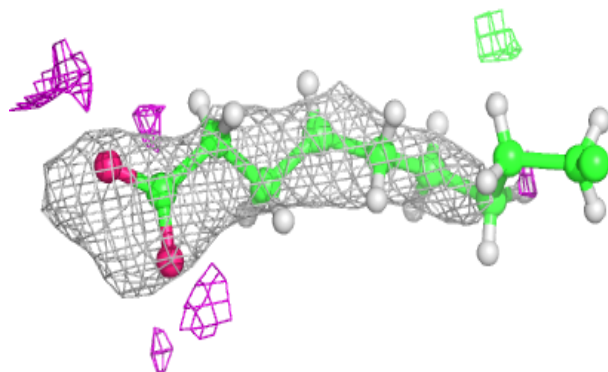
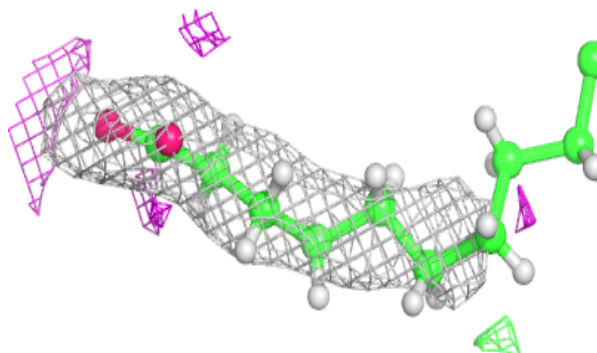


Electron density around SQD f 101:

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

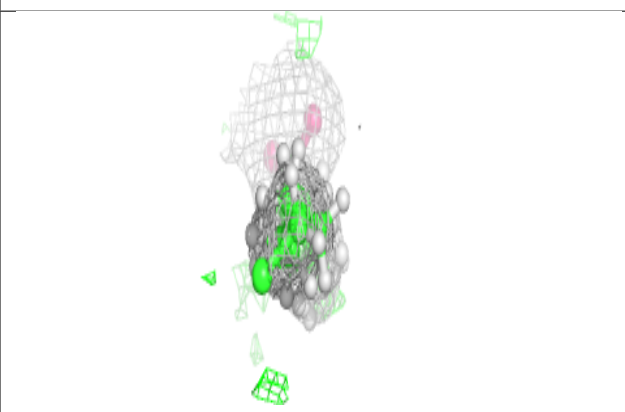
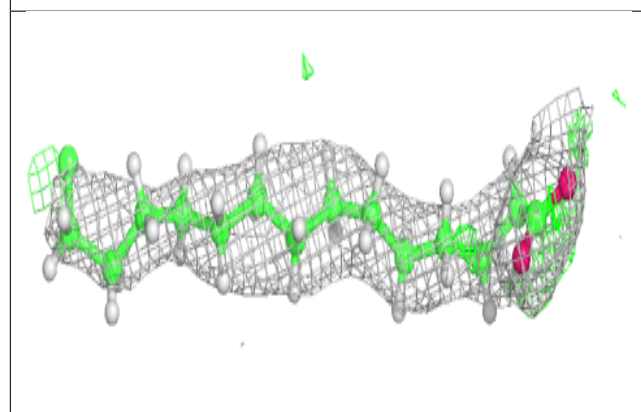
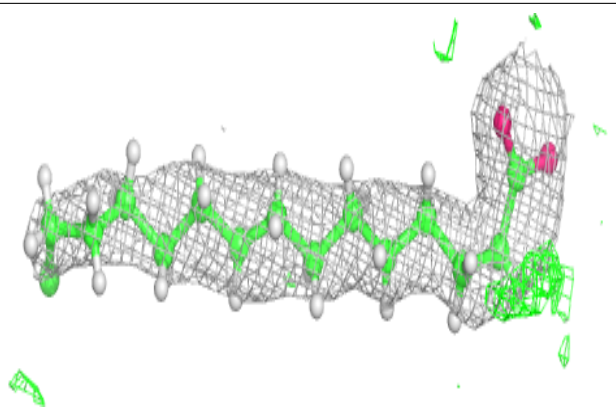
**Electron density around STE B 701:**

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

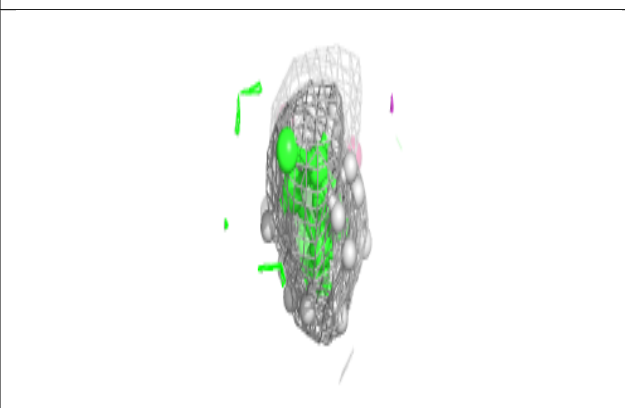
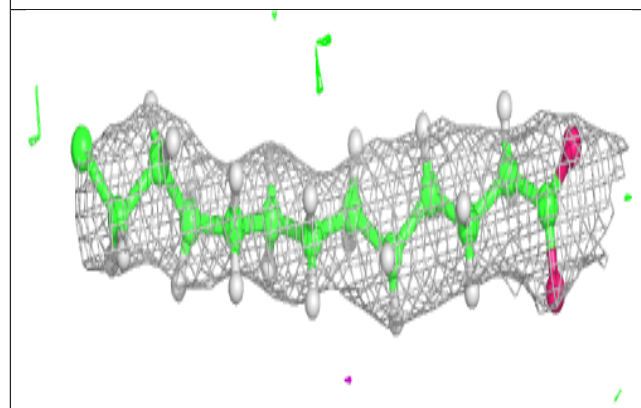
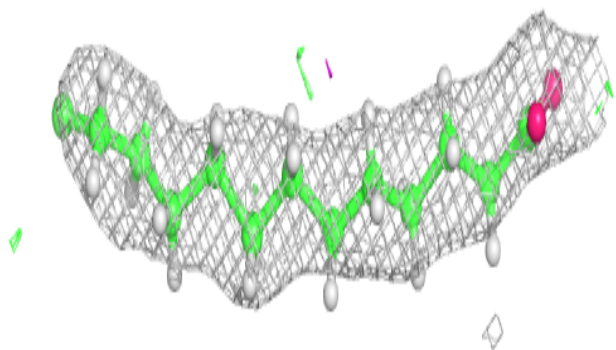


Electron density around STE d 409:

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

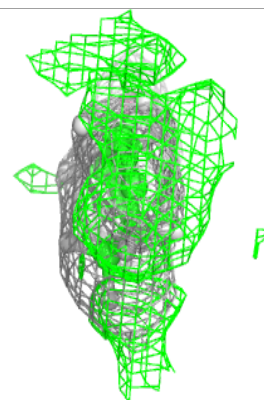
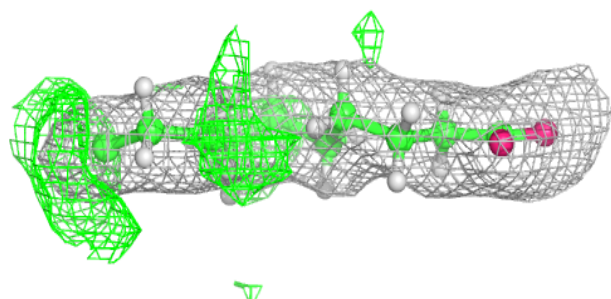
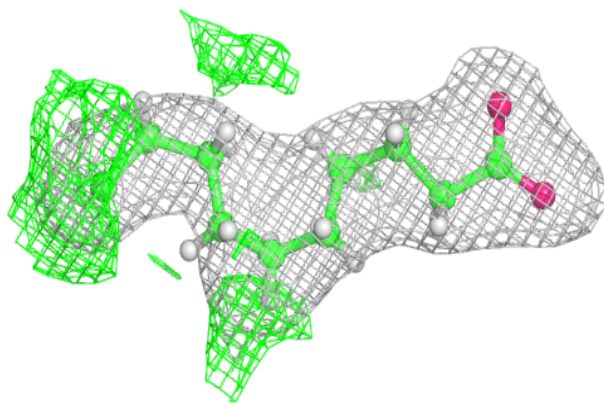
**Electron density around STE M 102:**

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

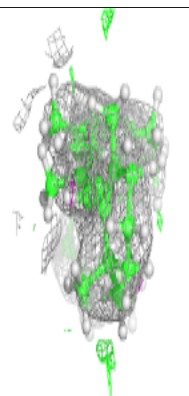
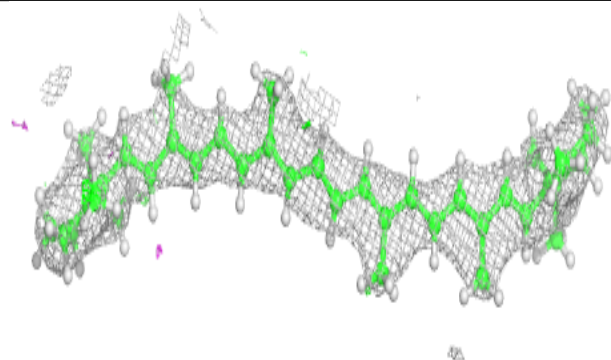
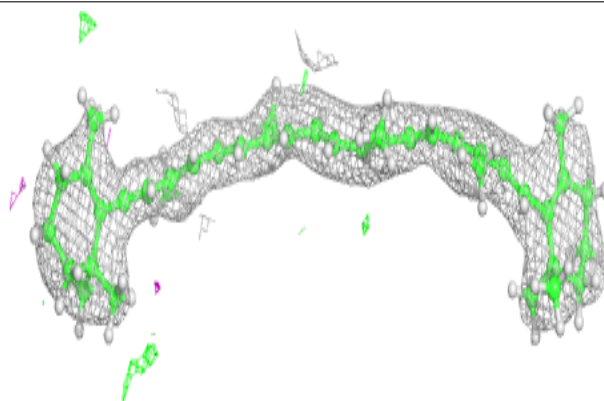


Electron density around STE C 523:

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

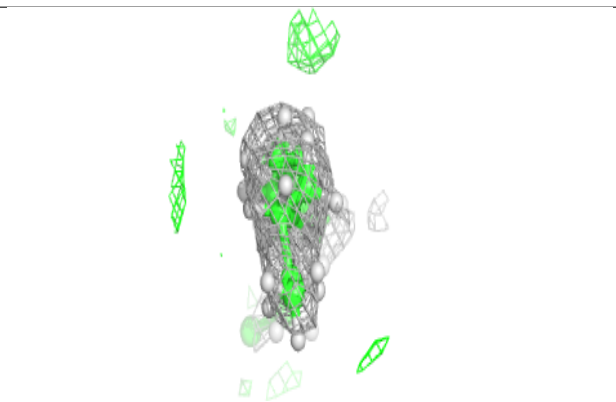
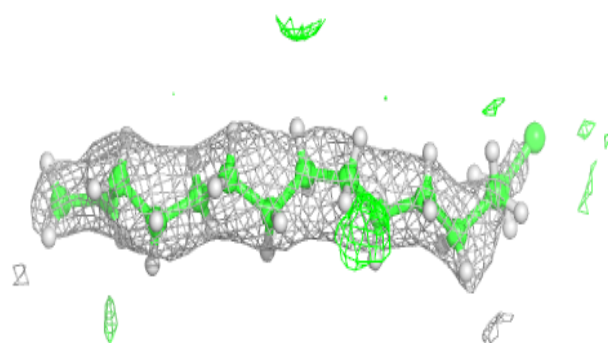
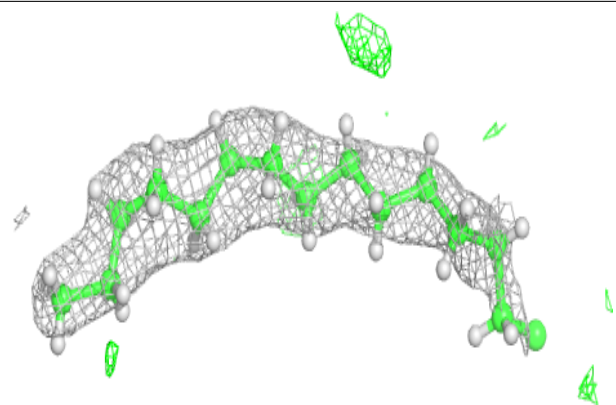
**Electron density around BCR k 102:**

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

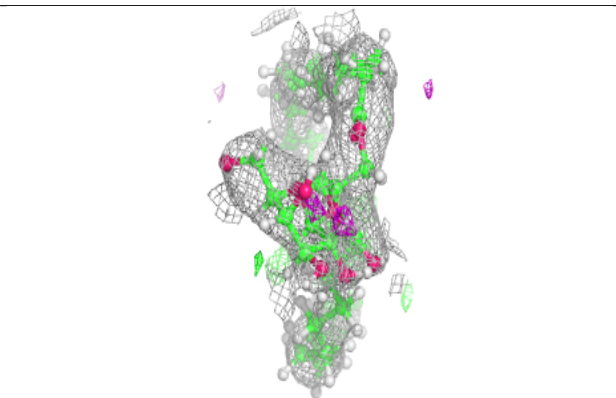
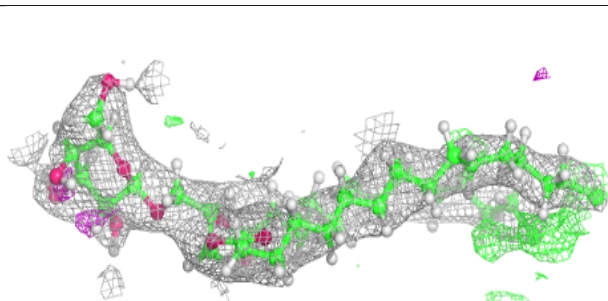
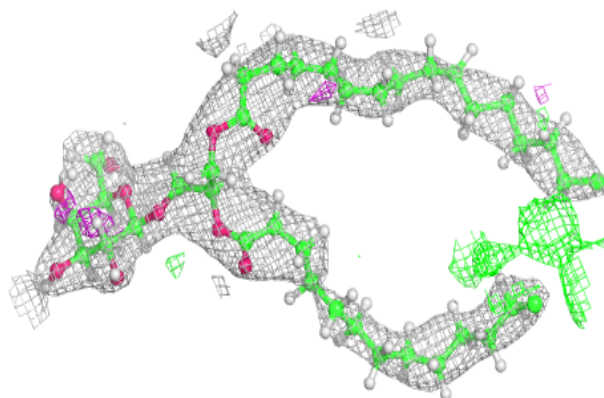


Electron density around STE T 702:

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

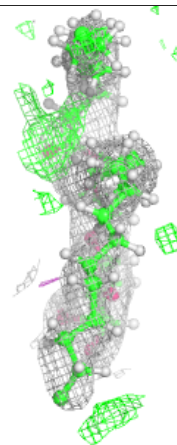
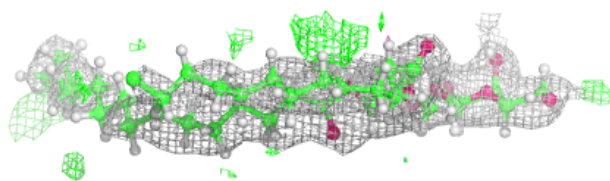
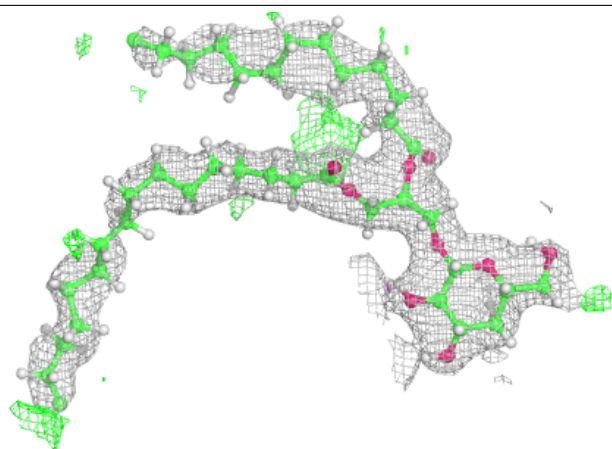
**Electron density around LMG C 516:**

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

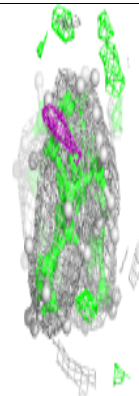
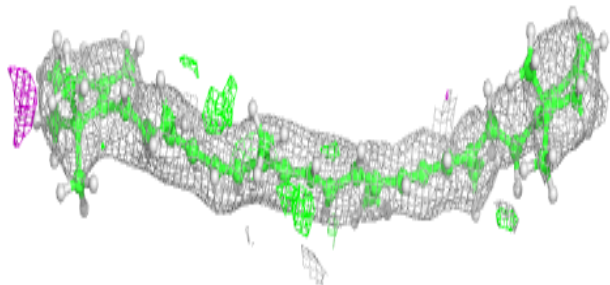
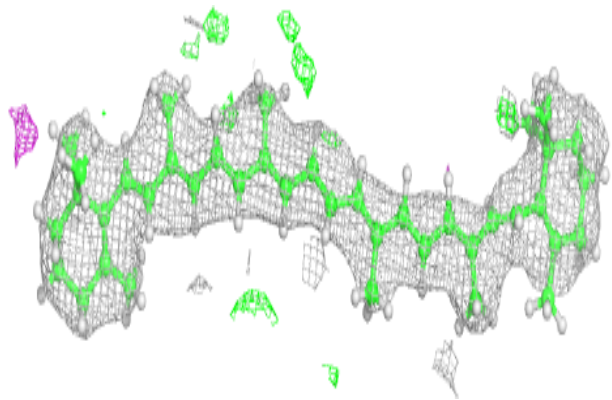


Electron density around LMG C 520:

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

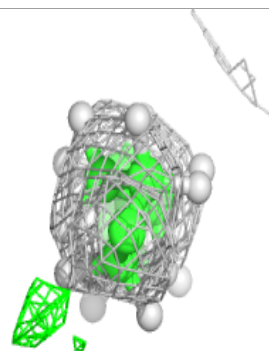
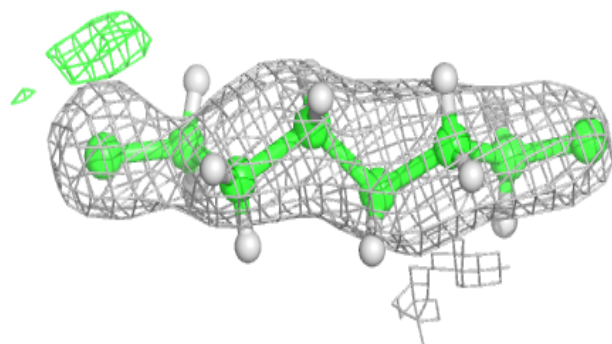
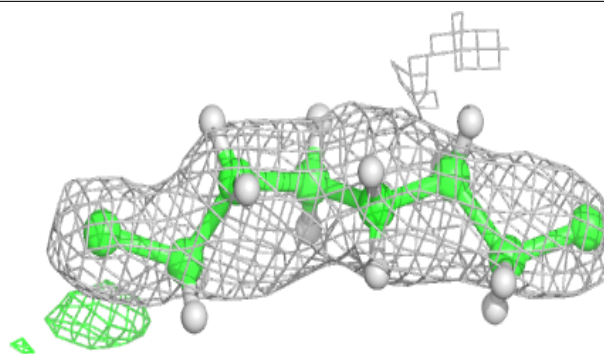
**Electron density around BCR d 403:**

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

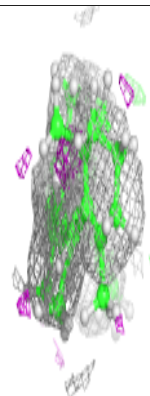
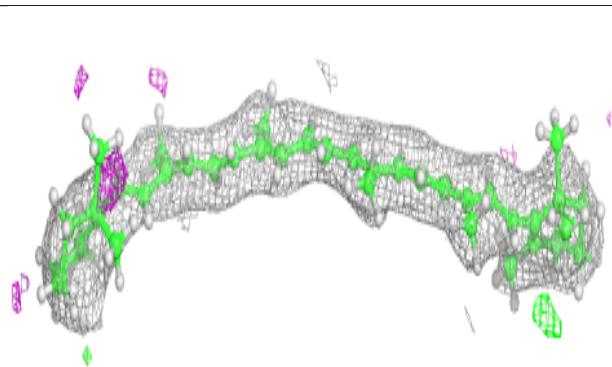
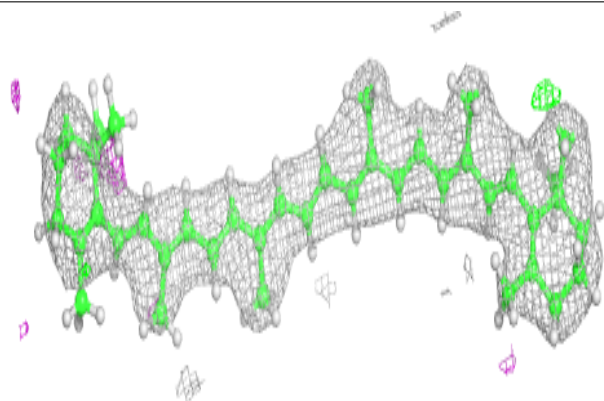


Electron density around STE Z 101:

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

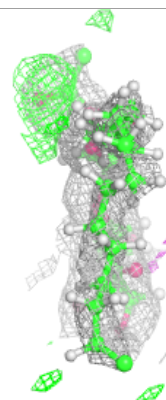
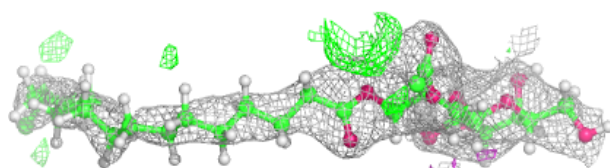
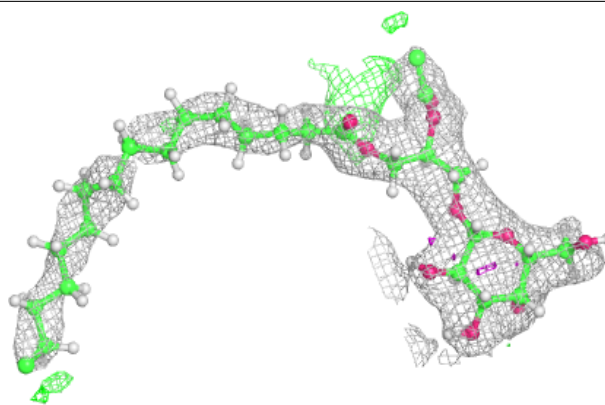
**Electron density around BCR D 404:**

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

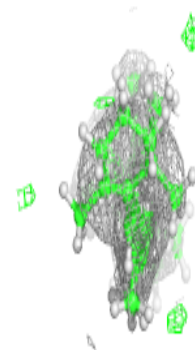
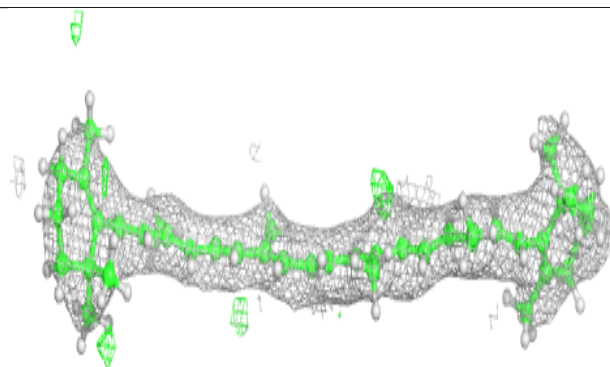
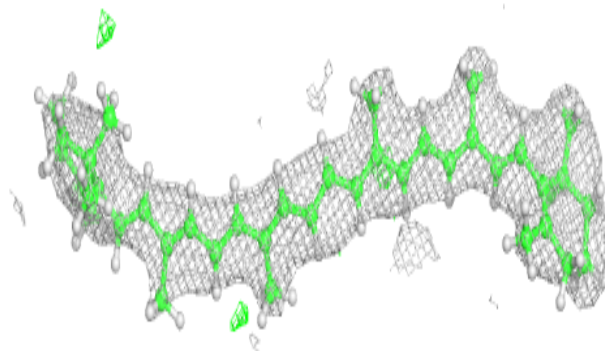


Electron density around LMG c 520:

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

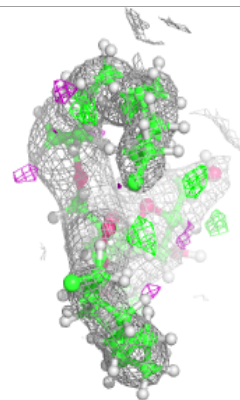
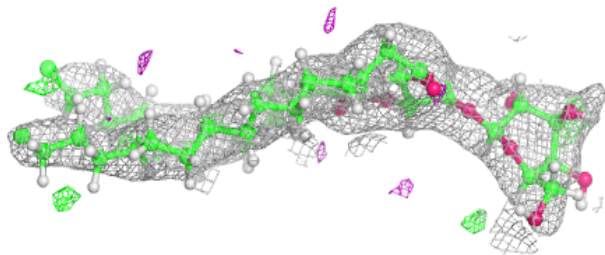
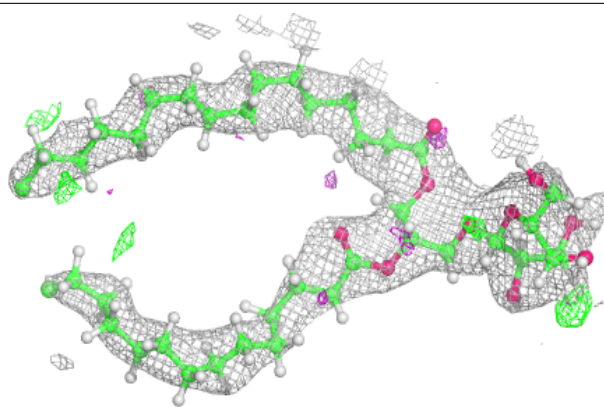
**Electron density around BCR Y 101:**

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

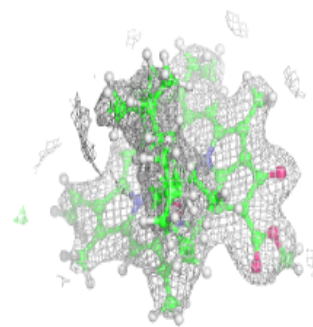
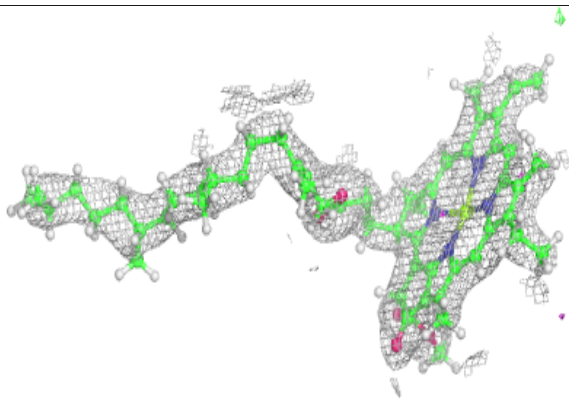
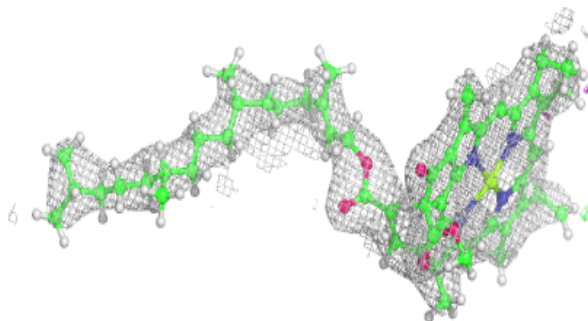


Electron density around LMG c 523:

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

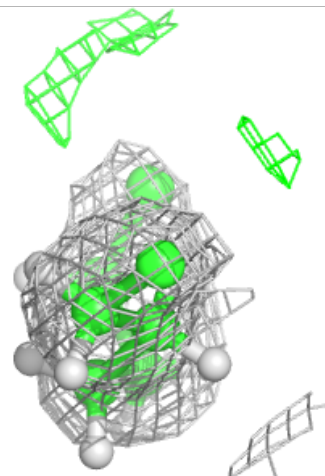
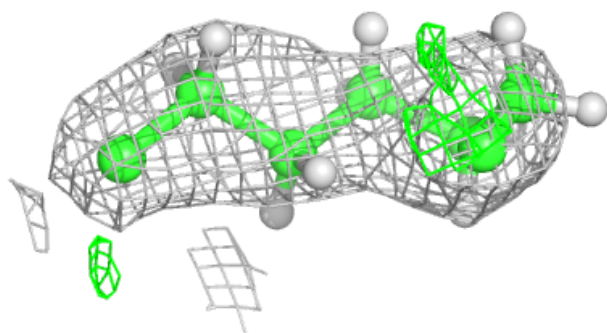
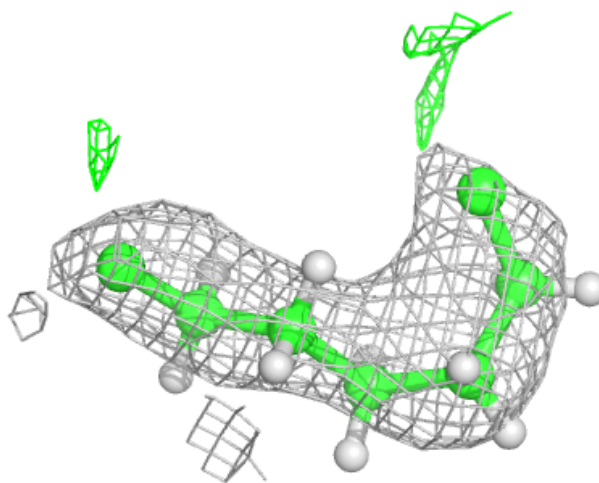
**Electron density around CLA C 503:**

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



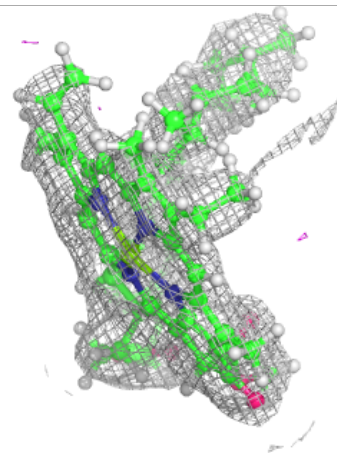
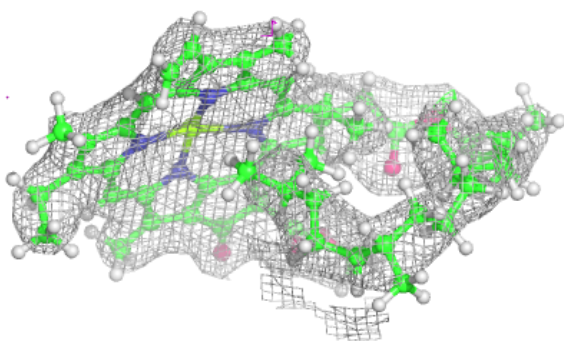
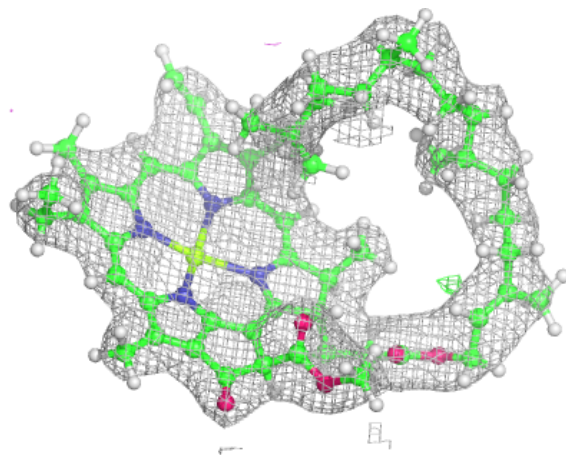
Electron density around STE E 102:

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



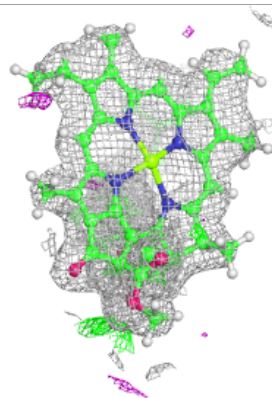
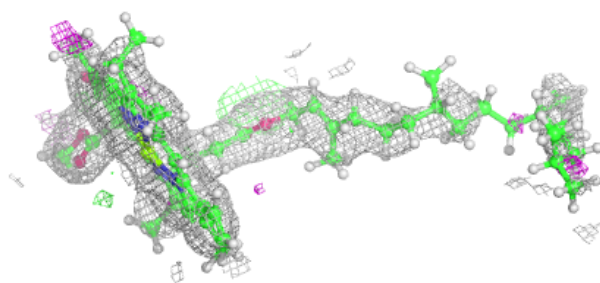
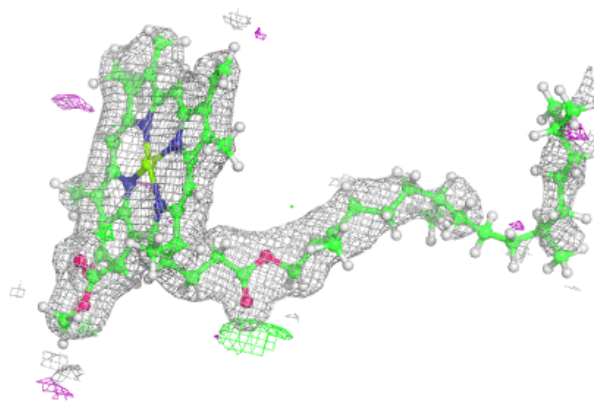
Electron density around CLA b 715:

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

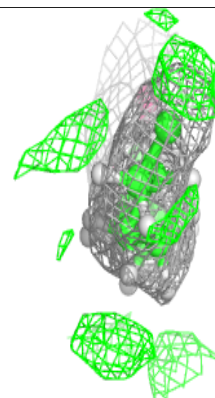
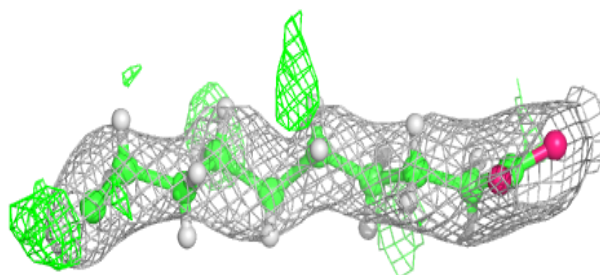
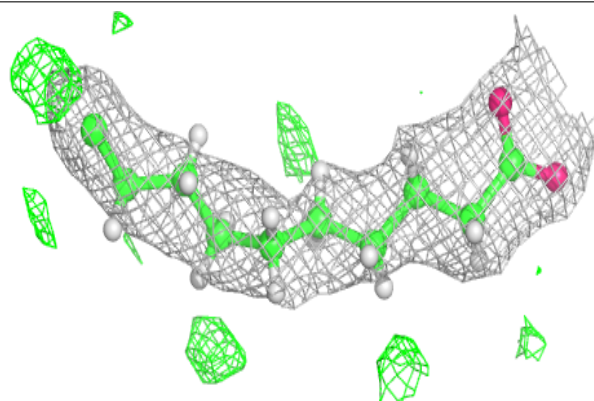


Electron density around CLA d 402:

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

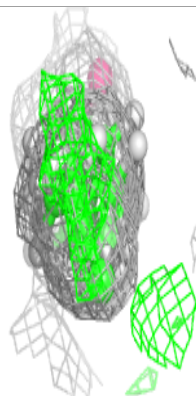
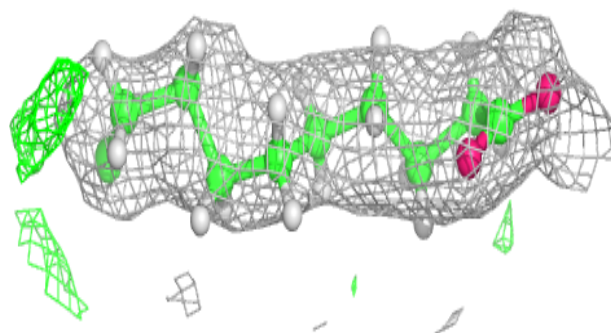
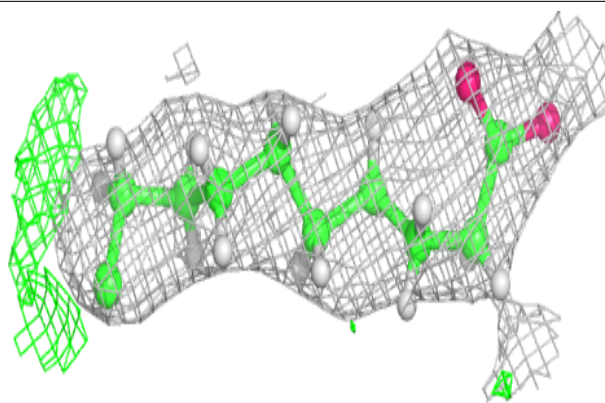
**Electron density around STE C 521:**

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

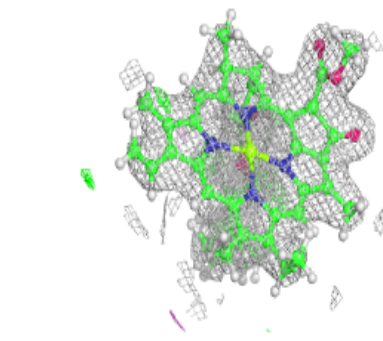
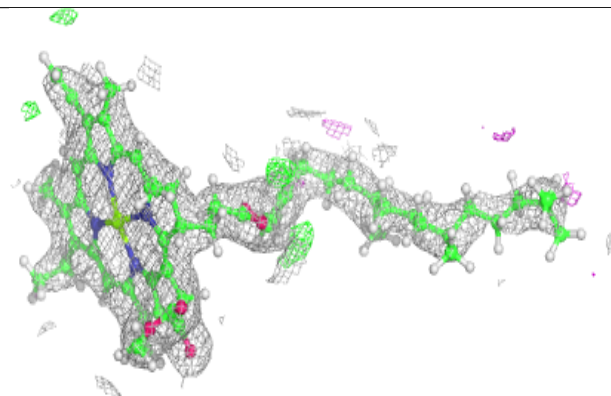
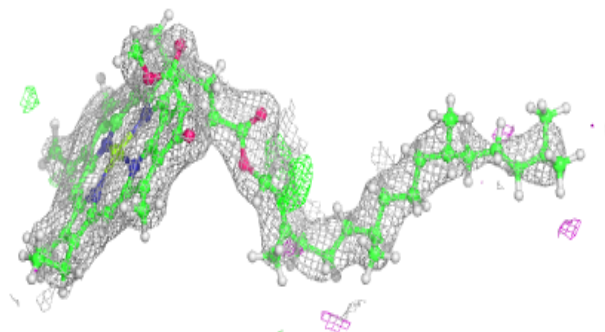


Electron density around STE J 101:

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

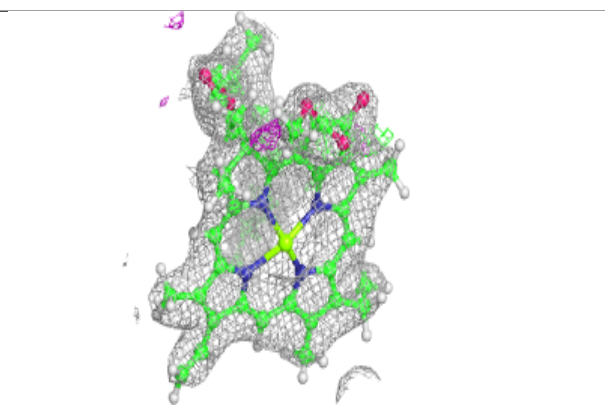
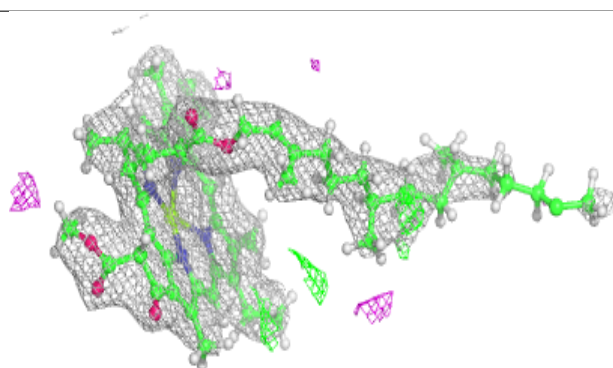
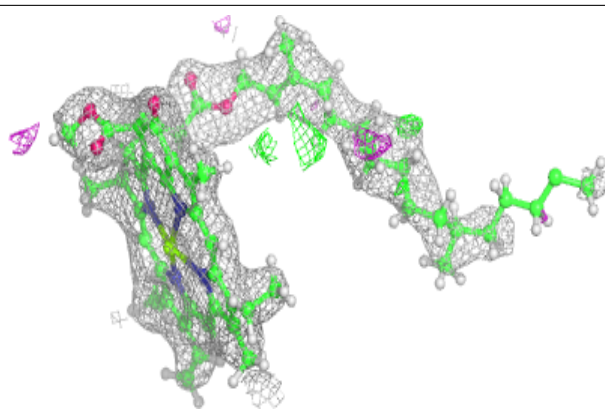
**Electron density around CLA c 503:**

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

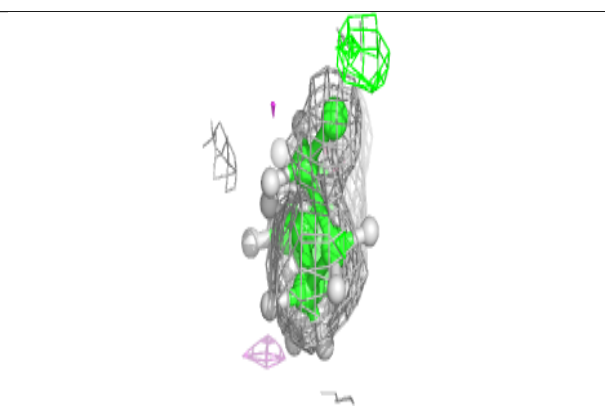
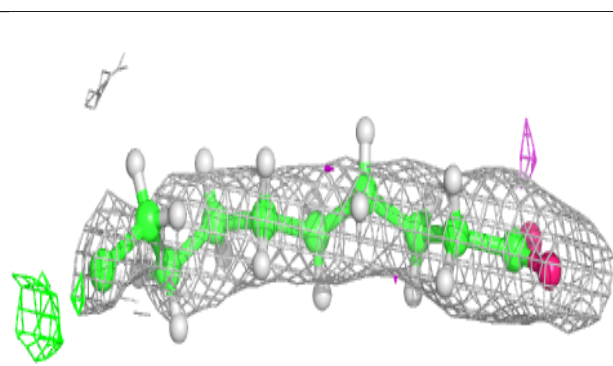
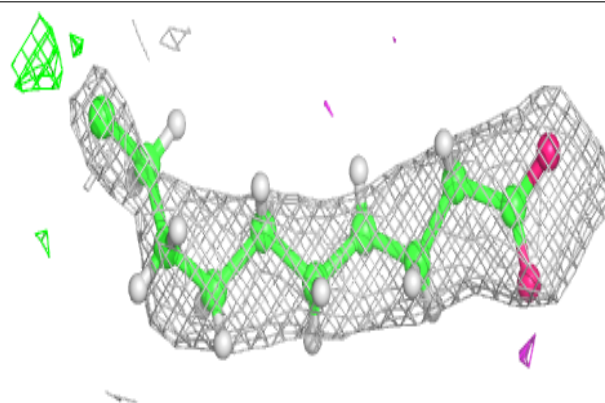


Electron density around CLA c 509:

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

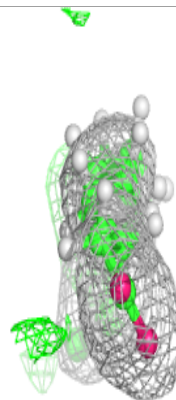
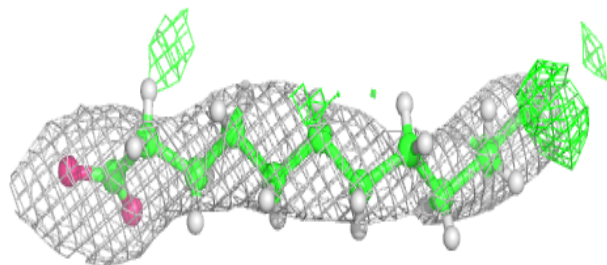
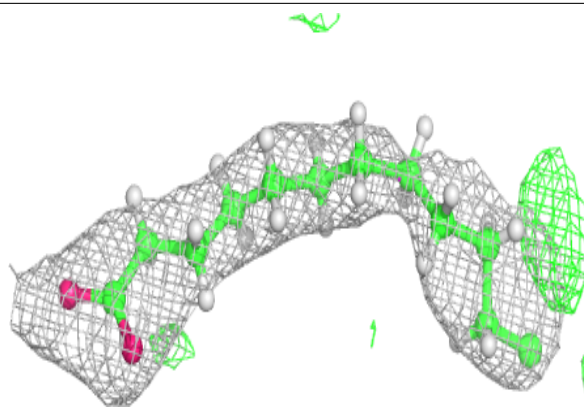
**Electron density around STE m 101:**

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

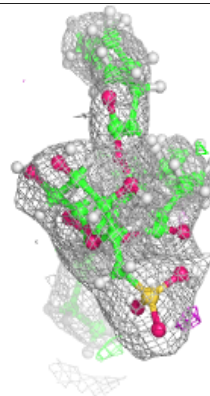
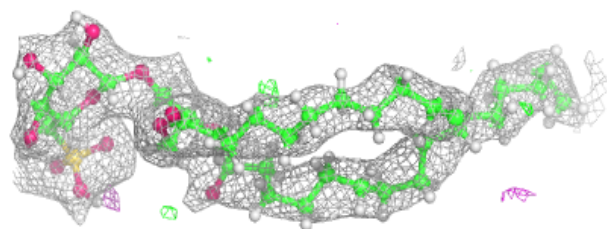
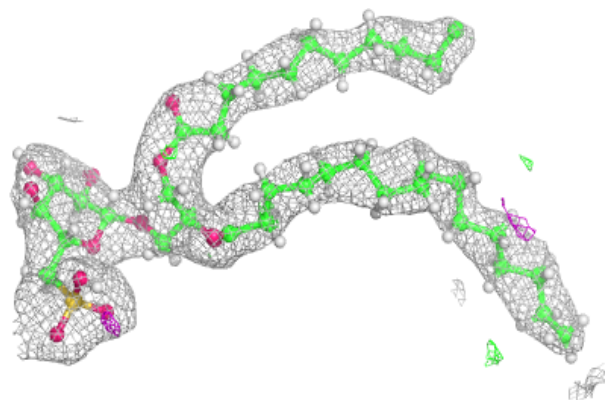


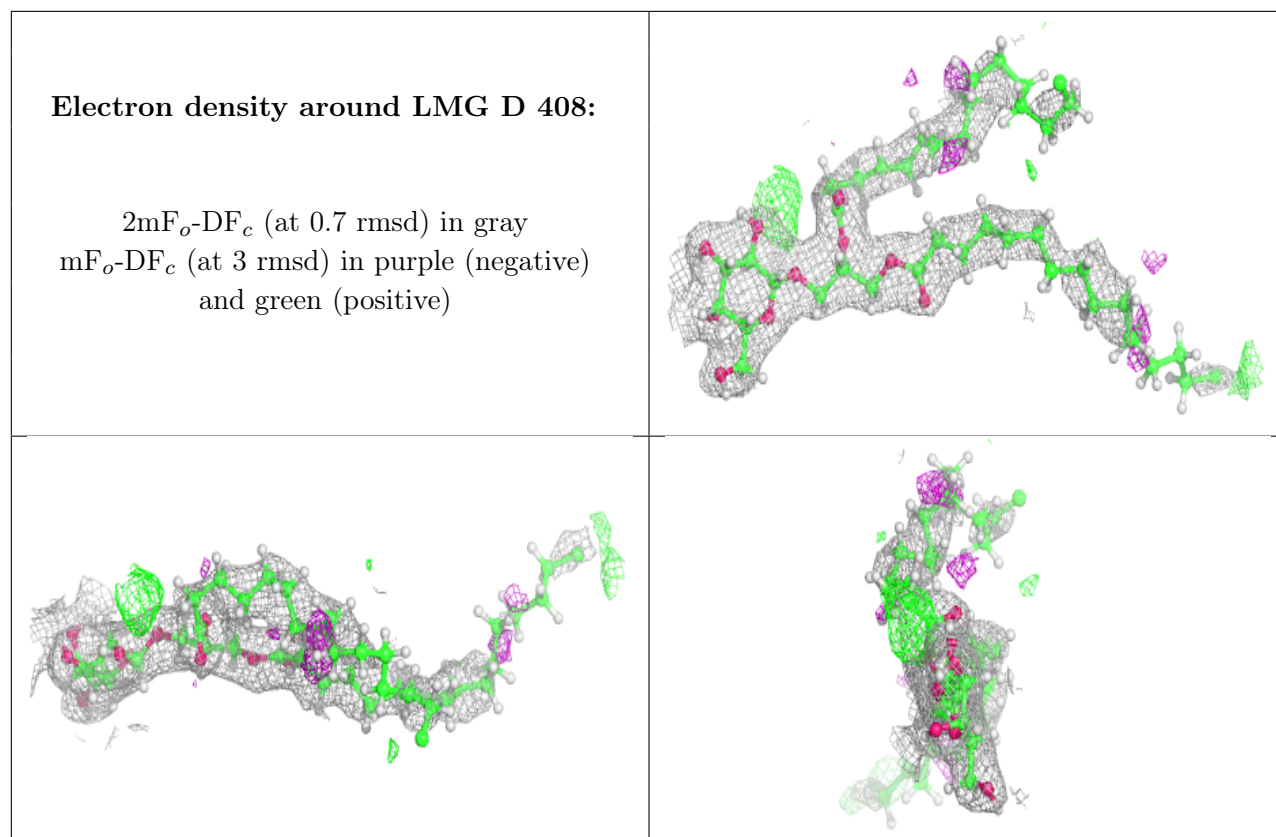
Electron density around STE t 702:

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

**Electron density around SQD b 720:**

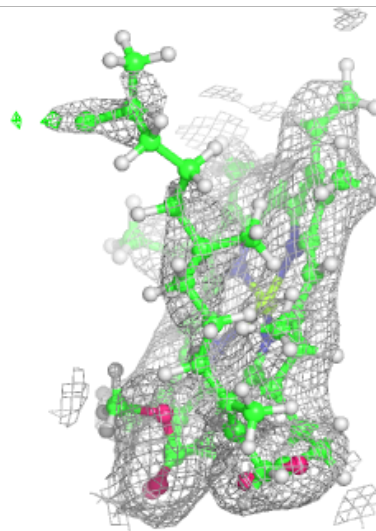
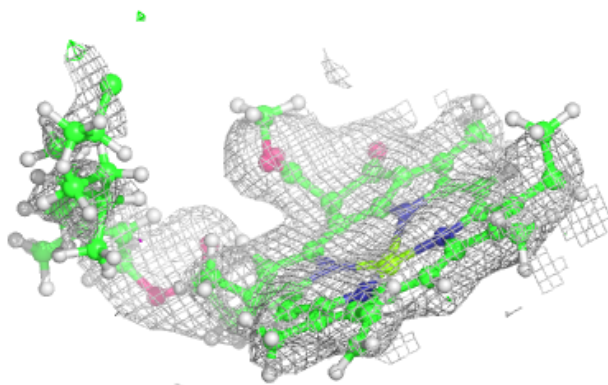
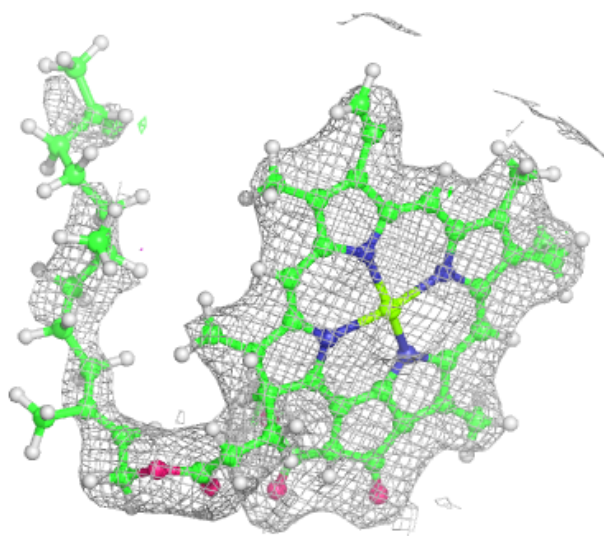
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





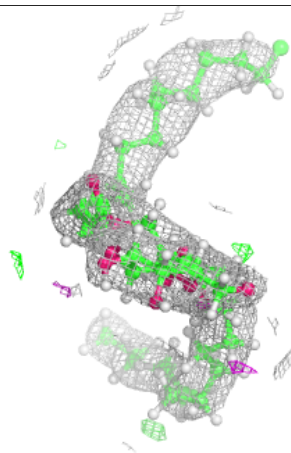
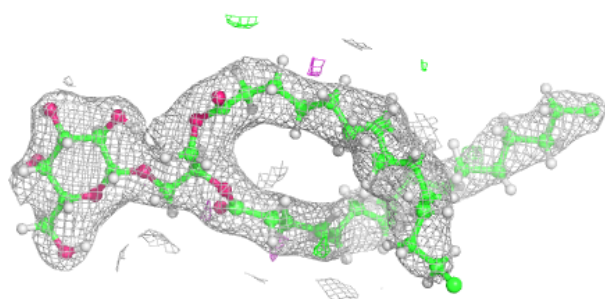
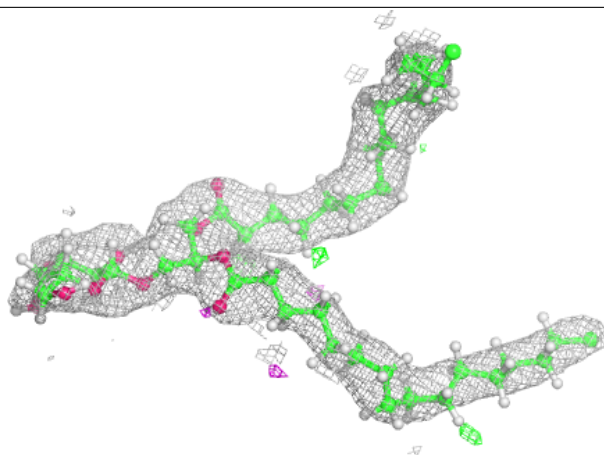
Electron density around CLA b 716:

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



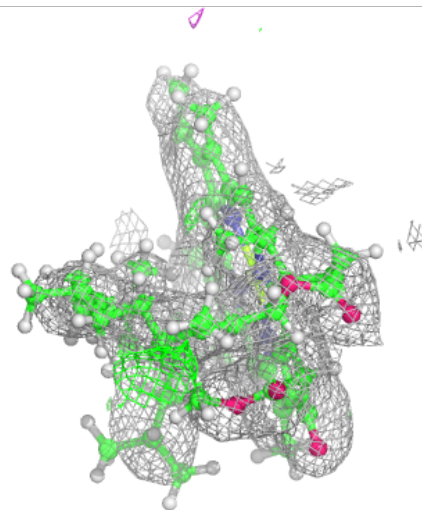
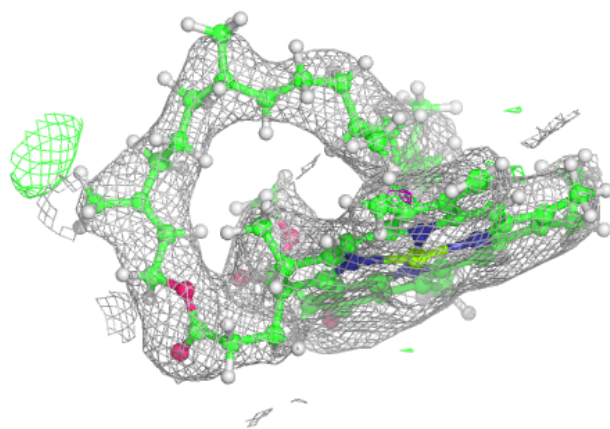
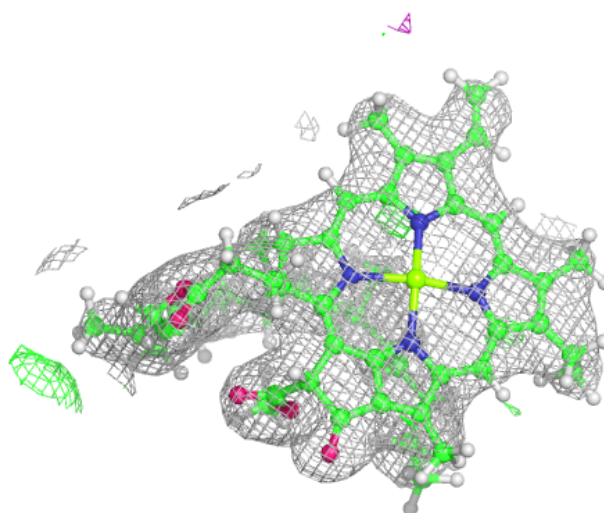
Electron density around LMG M 101:

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



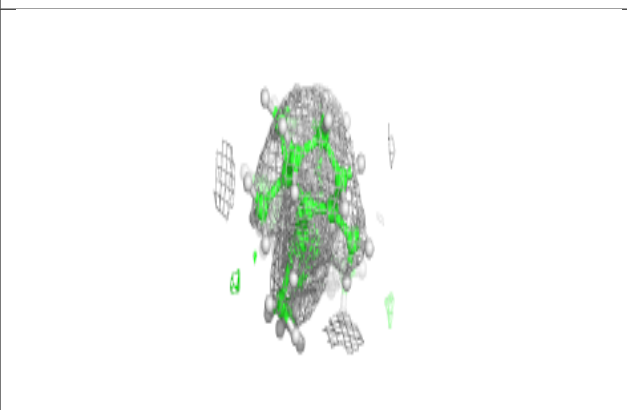
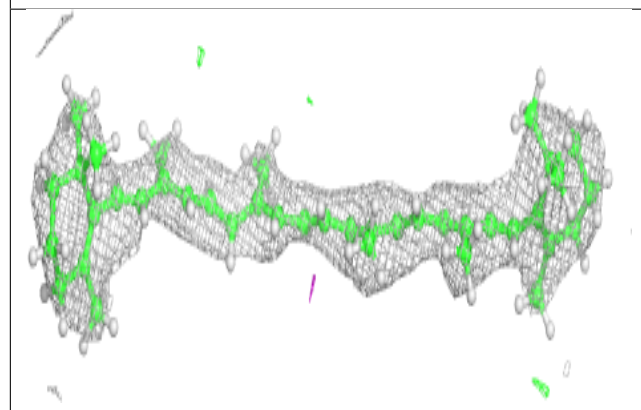
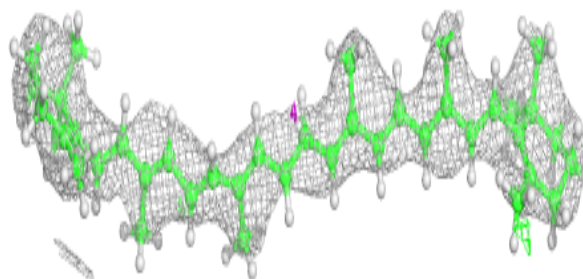
Electron density around CLA c 511:

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

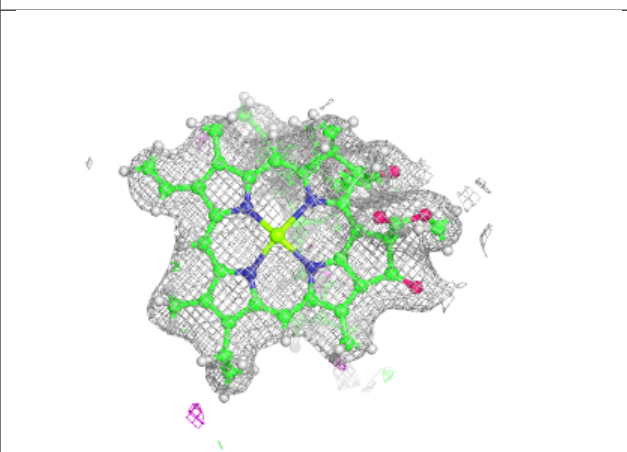
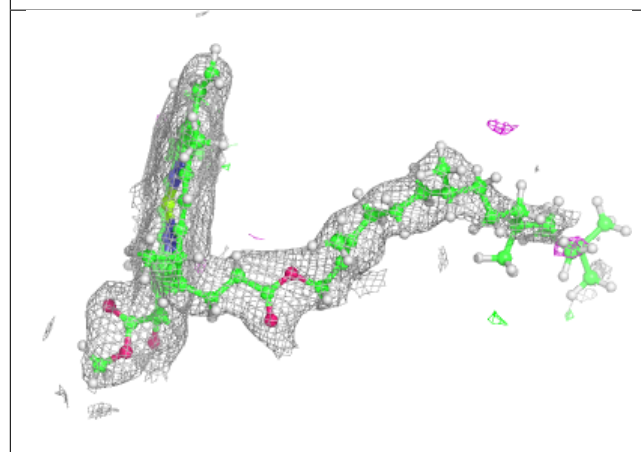
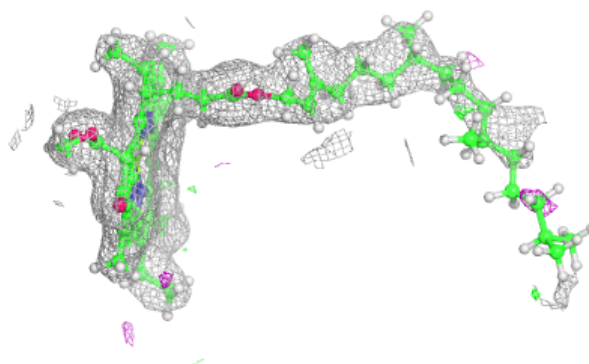


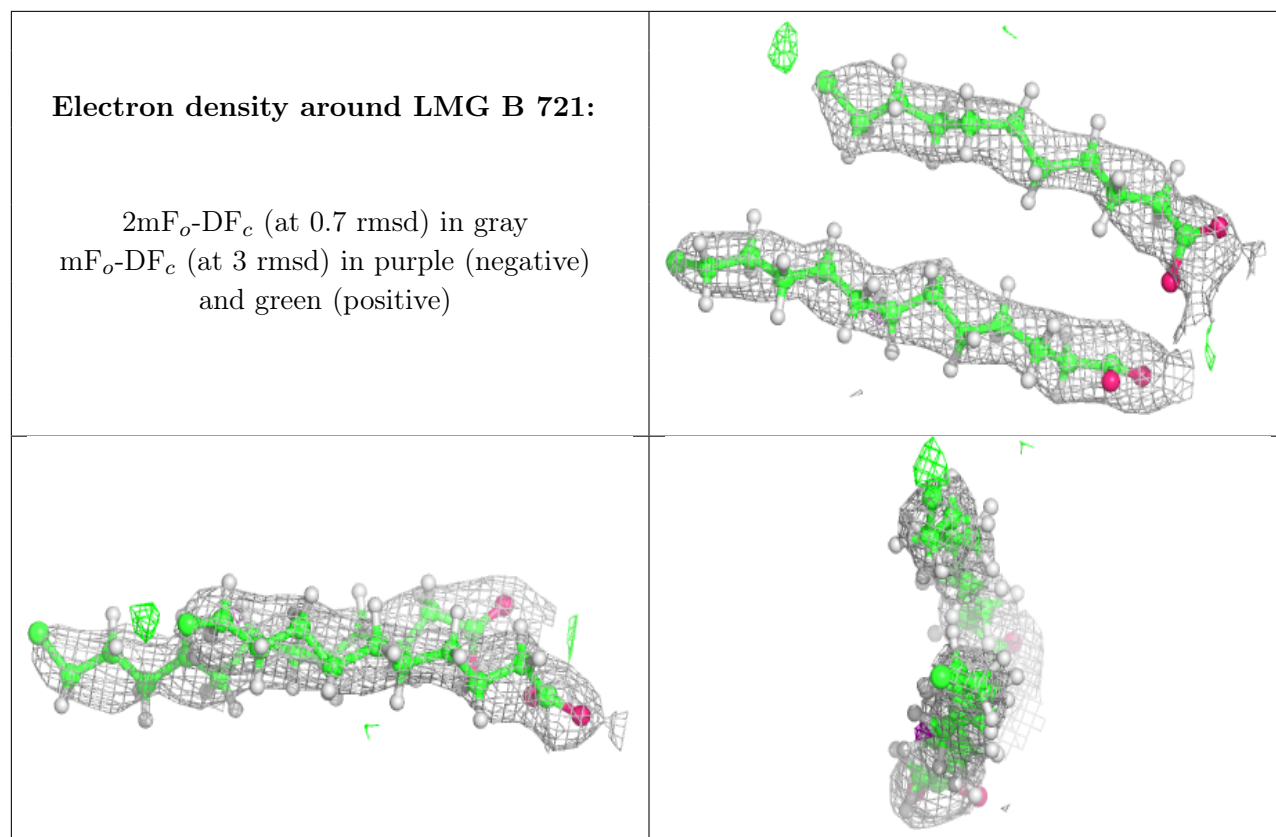
Electron density around BCR c 515:

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

**Electron density around CLA D 403:**

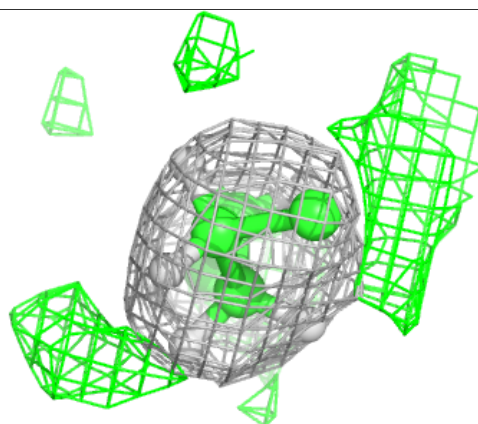
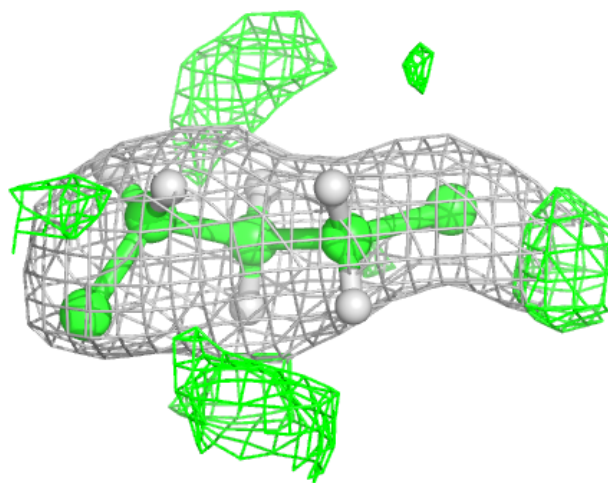
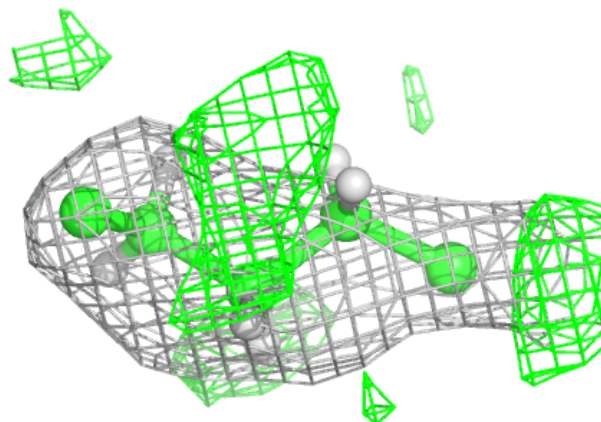
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

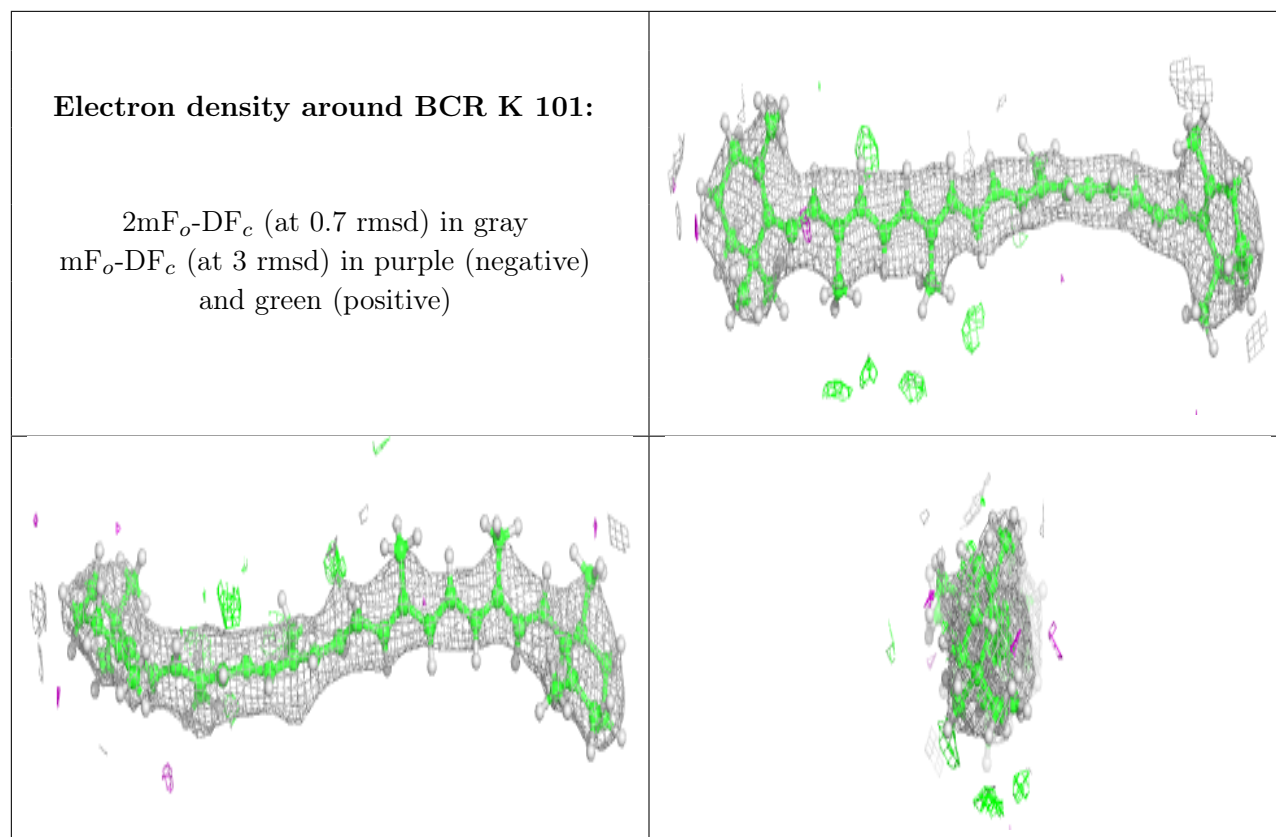




Electron density around STE A 414:

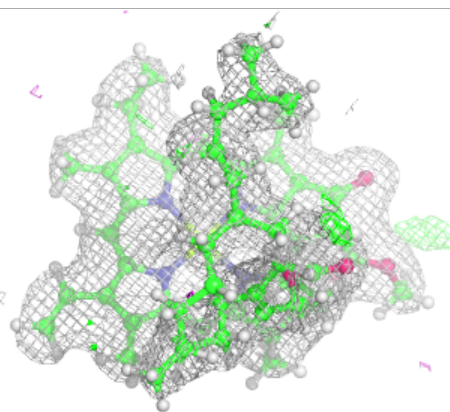
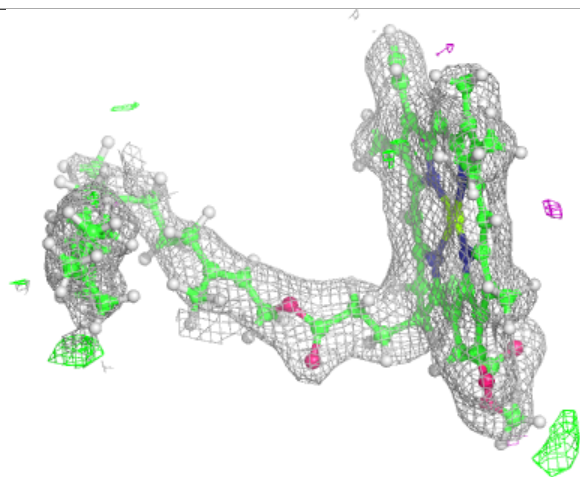
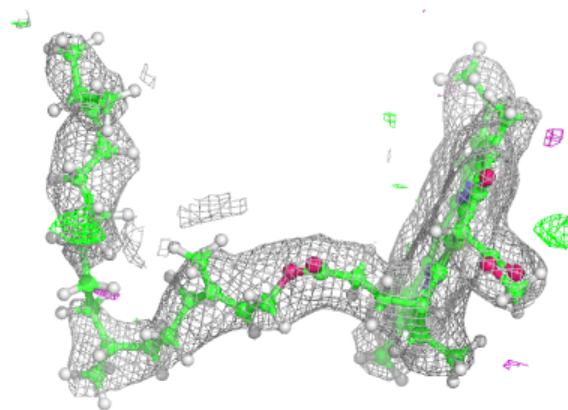
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





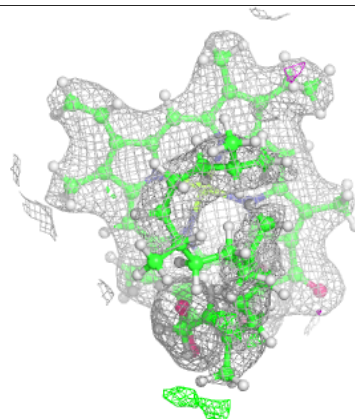
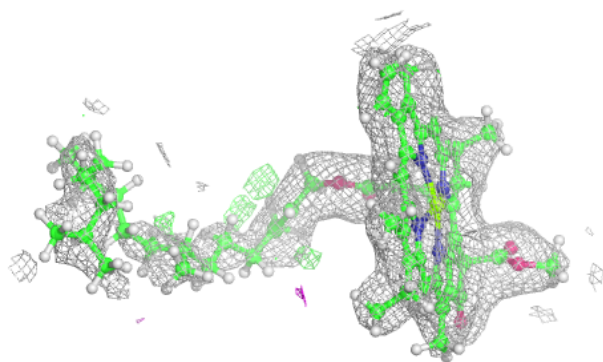
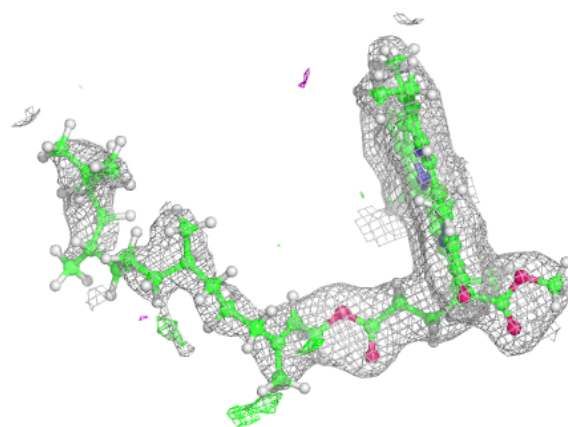
Electron density around CLA a 406:

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

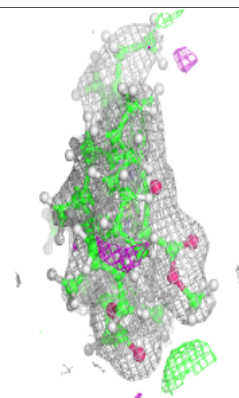
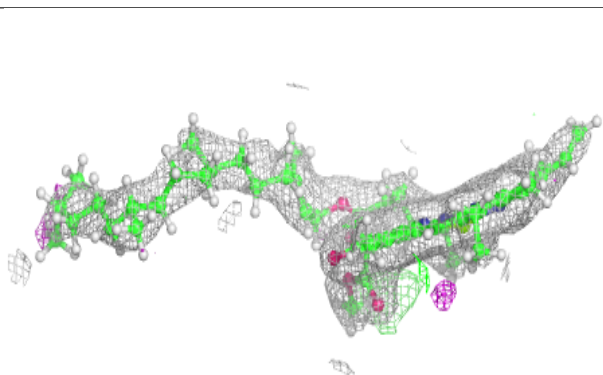
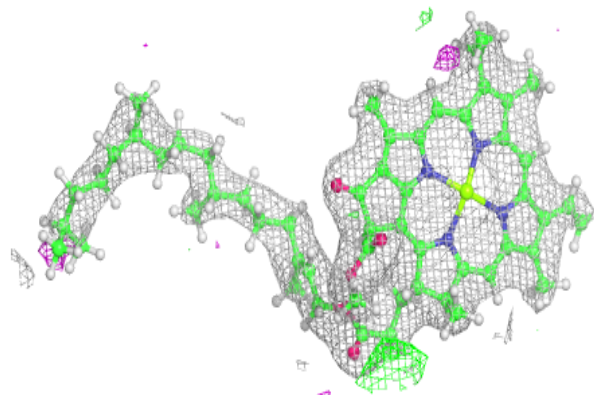


Electron density around CLA C 507:

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

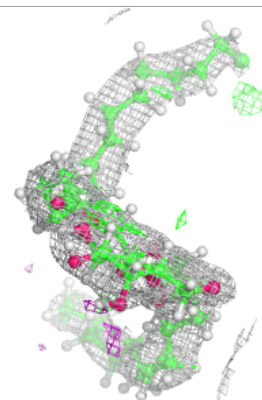
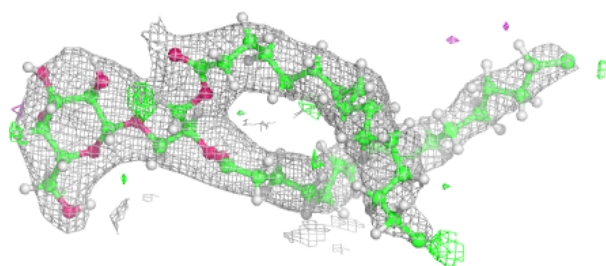
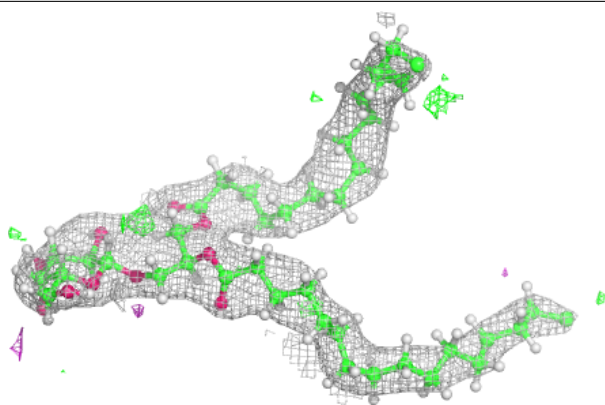
**Electron density around CLA b 702:**

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

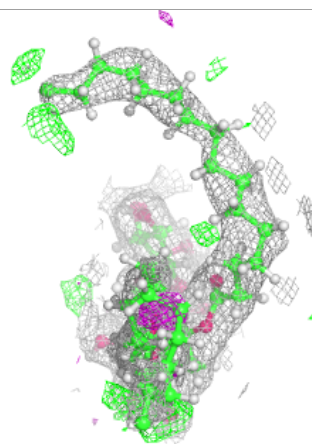
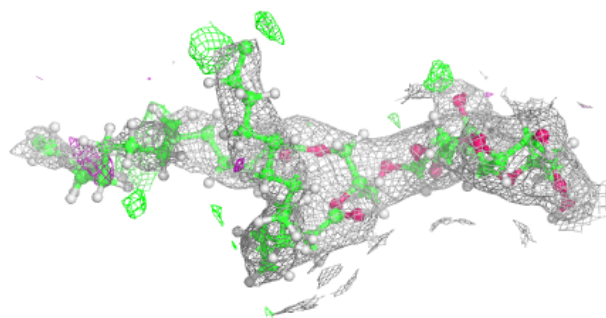
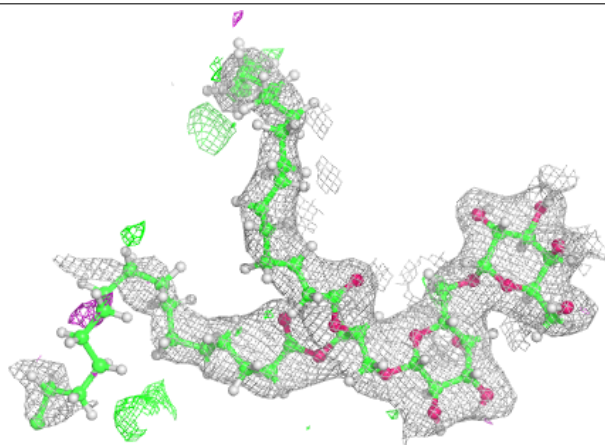


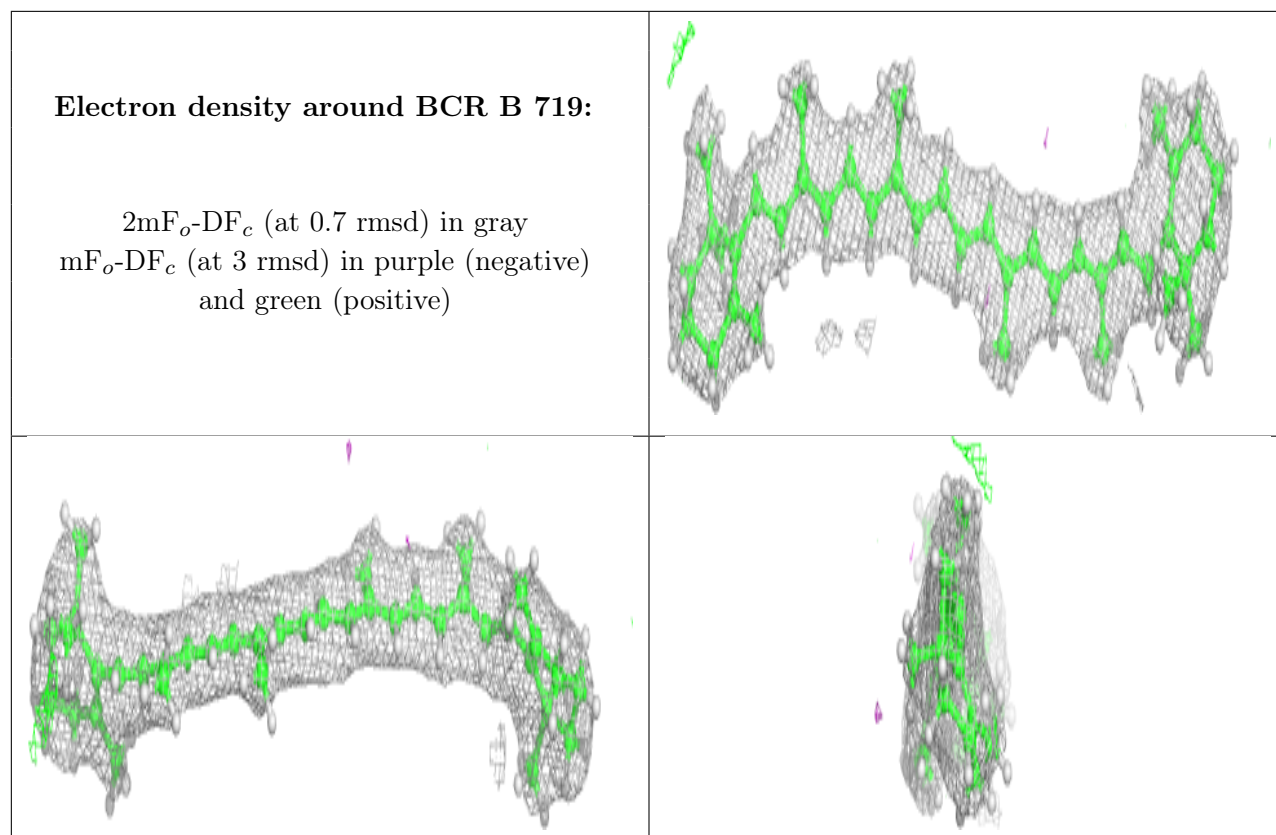
Electron density around LMG b 721:

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

**Electron density around DGD C 518:**

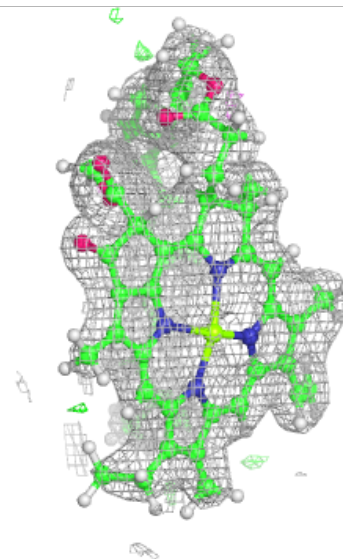
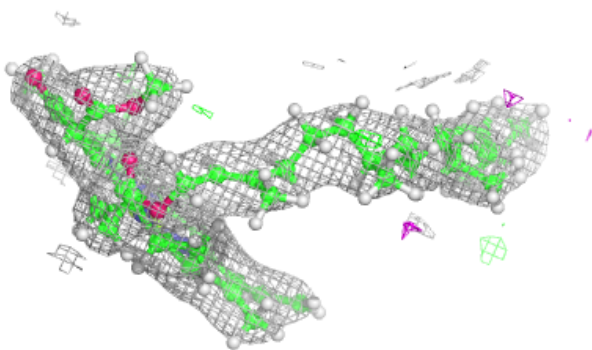
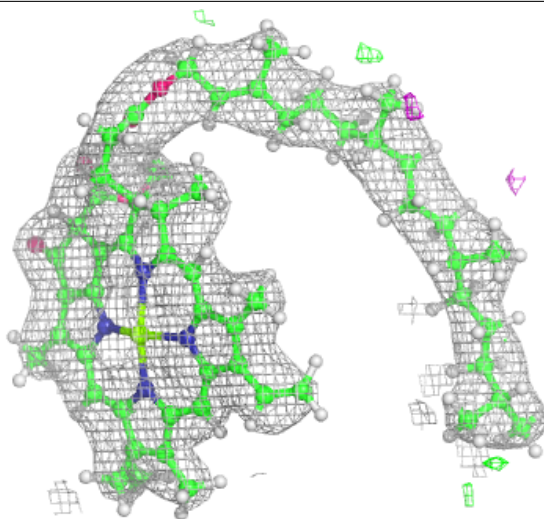
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





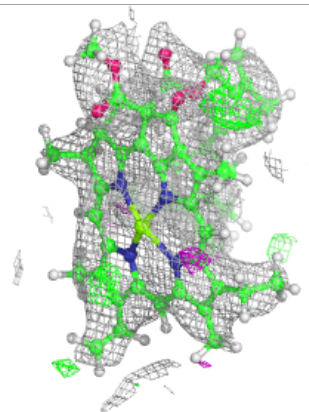
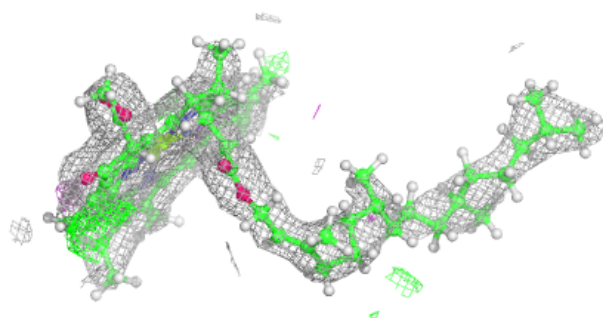
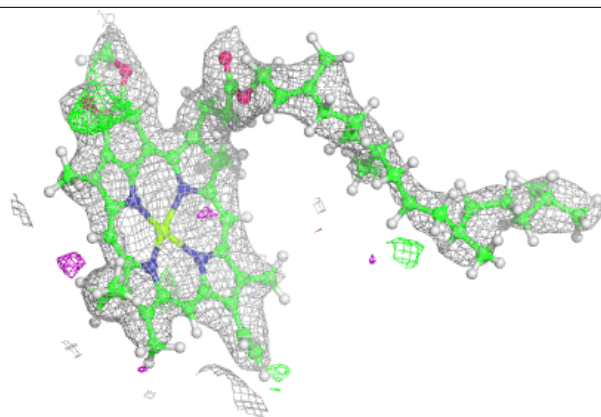
Electron density around CLA C 508:

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

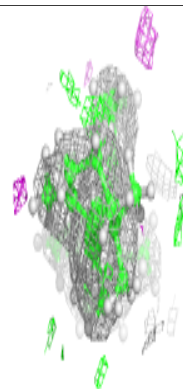
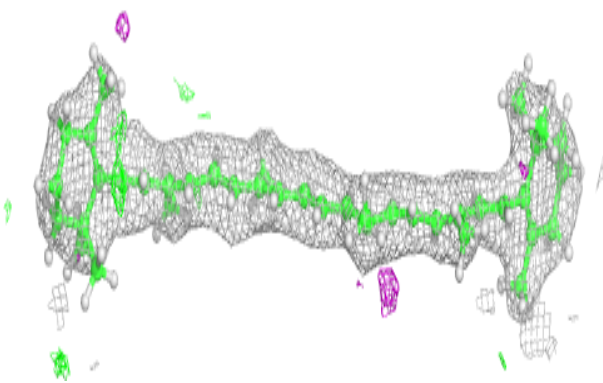
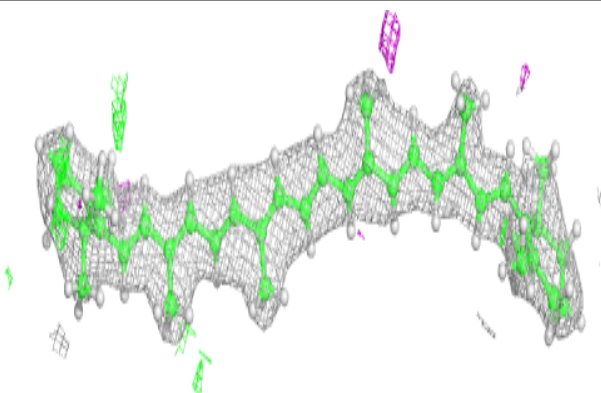


Electron density around CLA c 512:

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

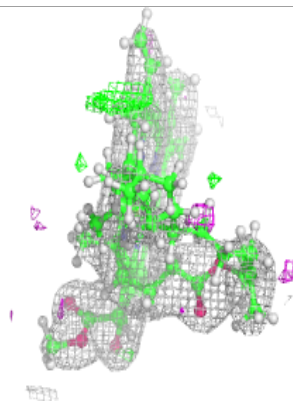
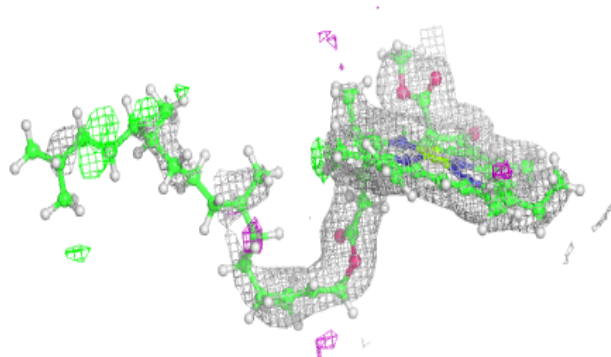
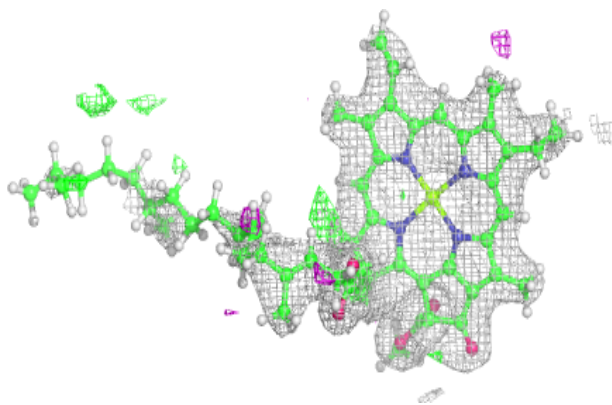
**Electron density around BCR C 515:**

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



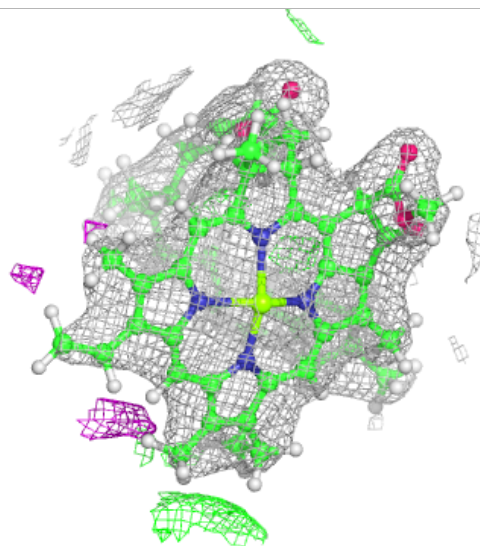
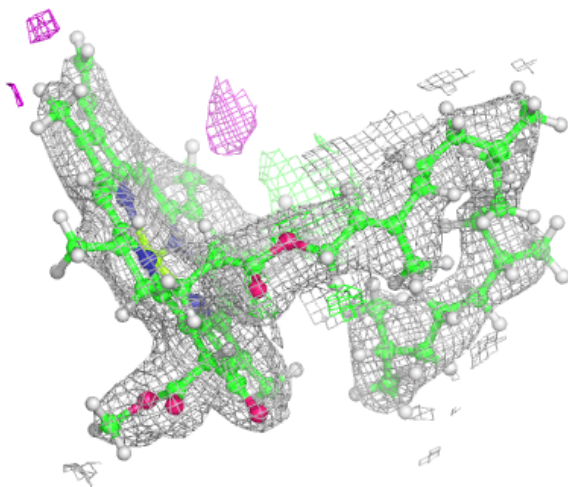
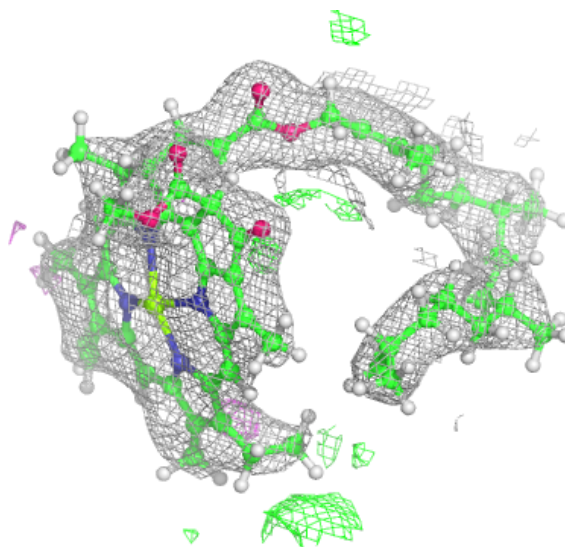
Electron density around CLA a 404:

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



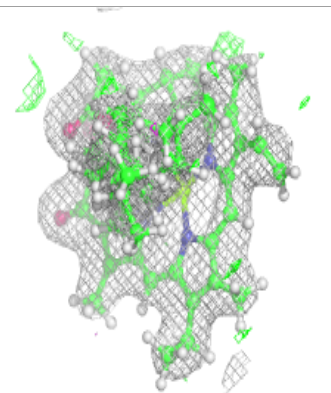
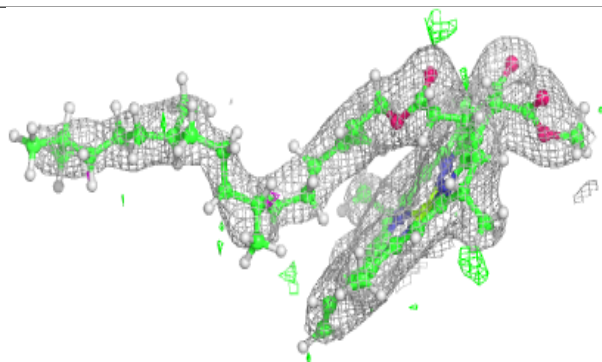
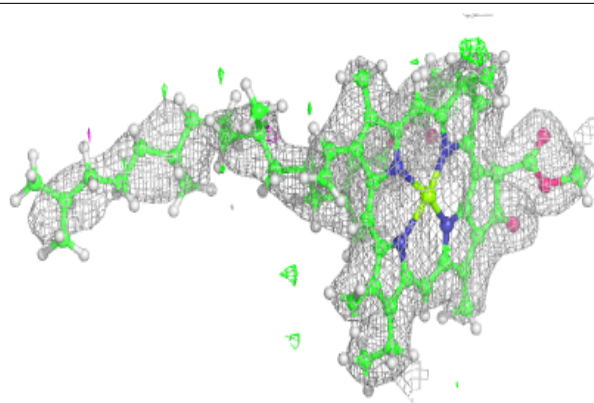
Electron density around CLA c 504:

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

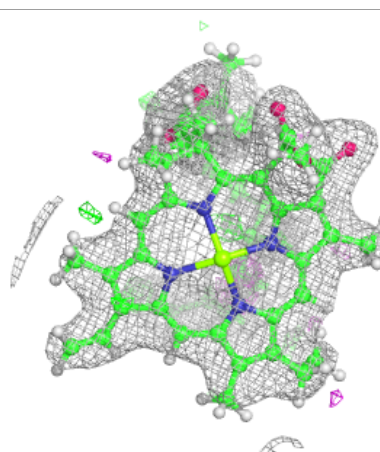
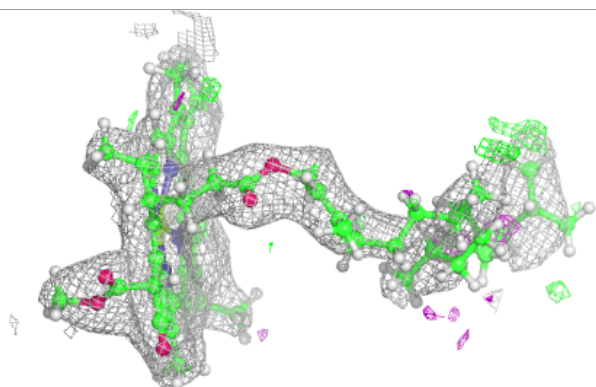
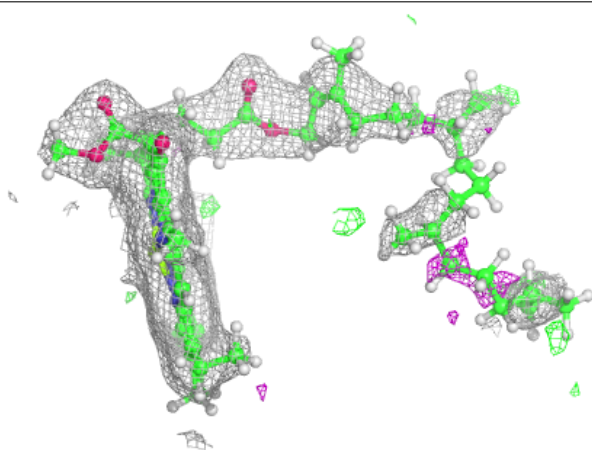


Electron density around CLA c 506:

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

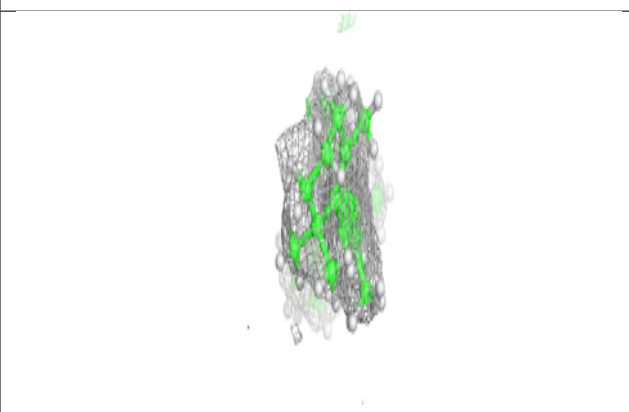
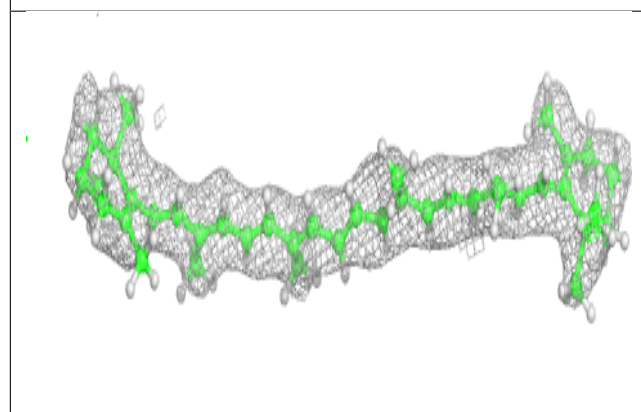
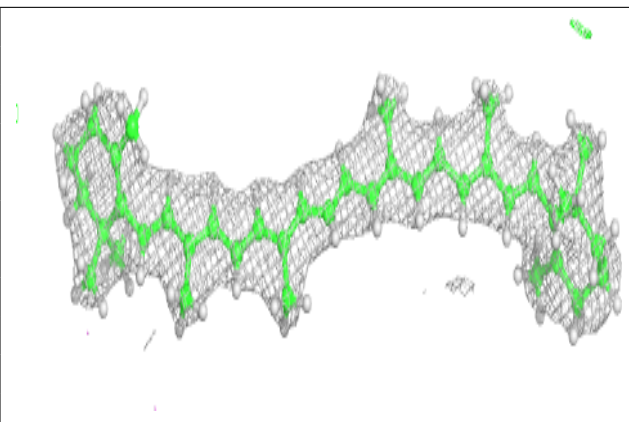
**Electron density around CLA c 507:**

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

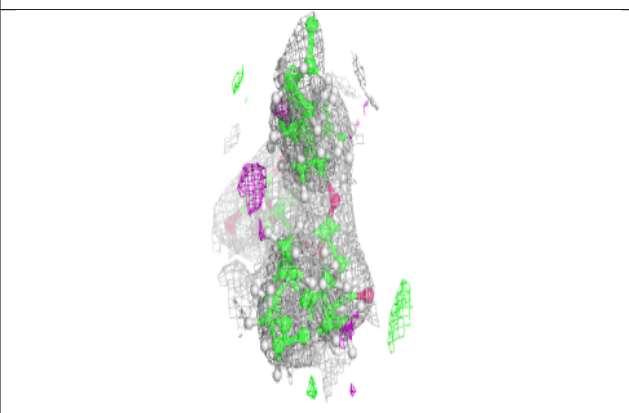
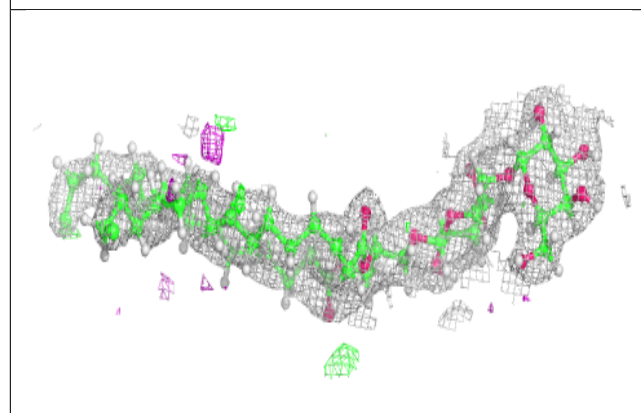
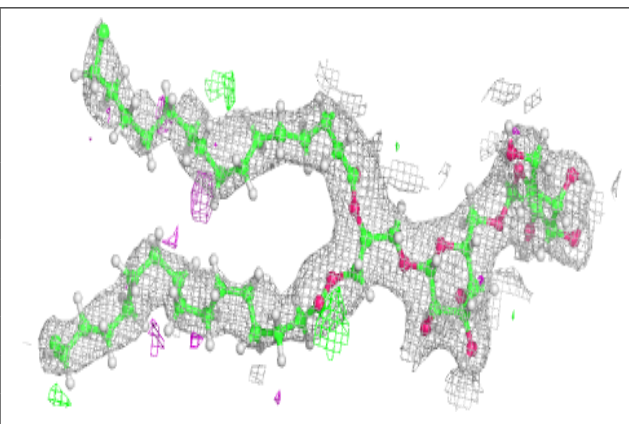


Electron density around BCR b 719:

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

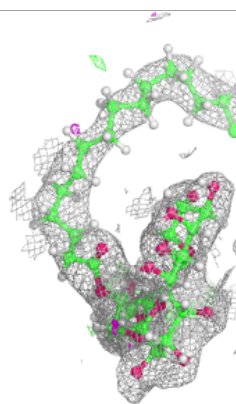
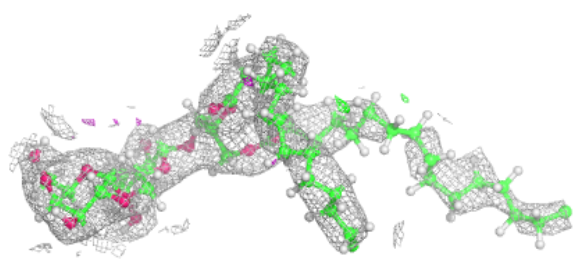
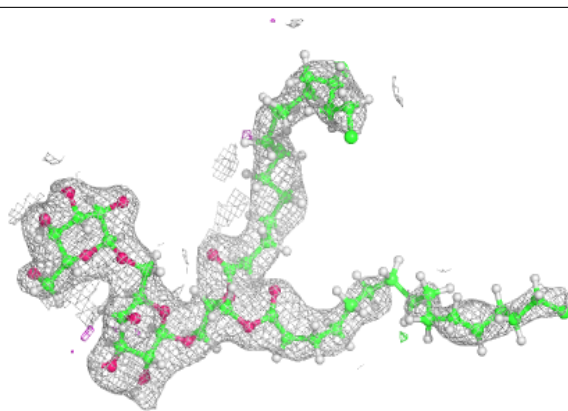
**Electron density around DGD C 519:**

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

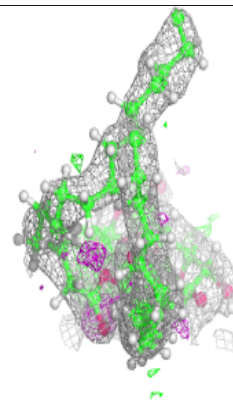
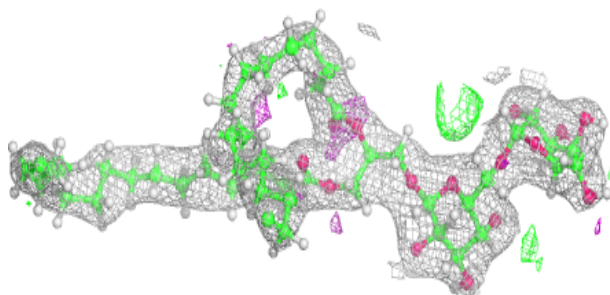
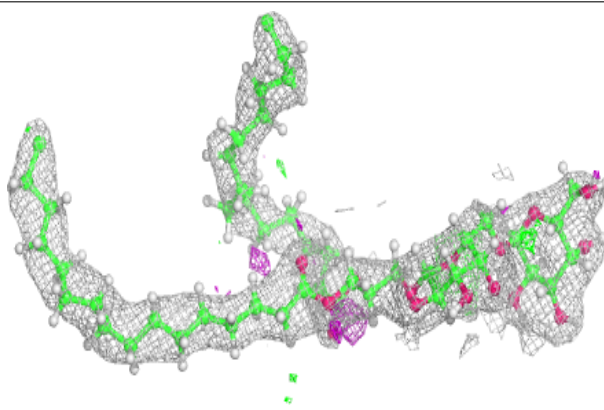


Electron density around DGD c 518:

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

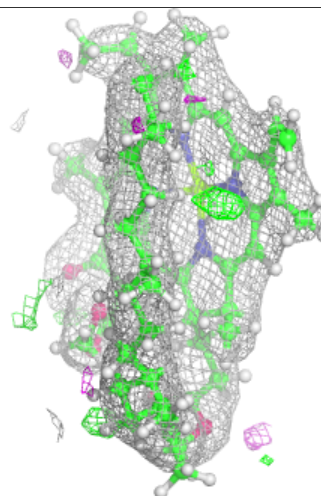
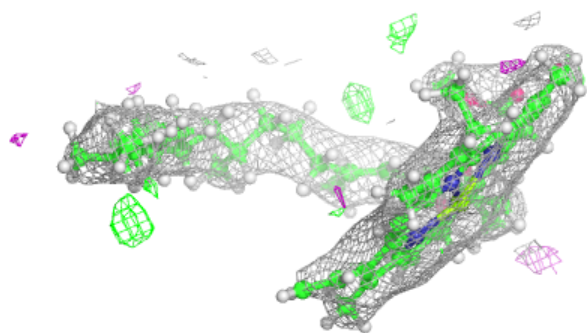
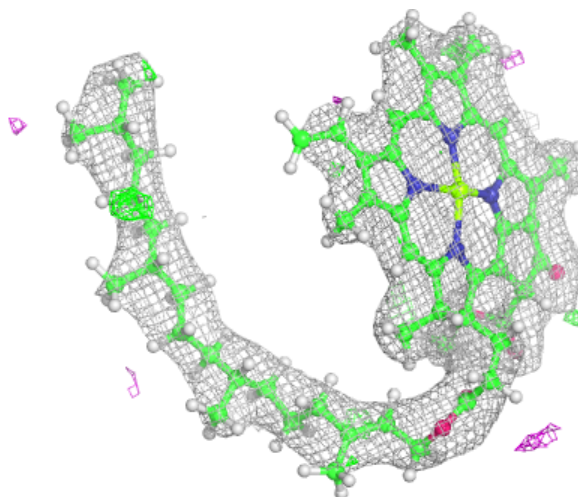
**Electron density around DGD h 702:**

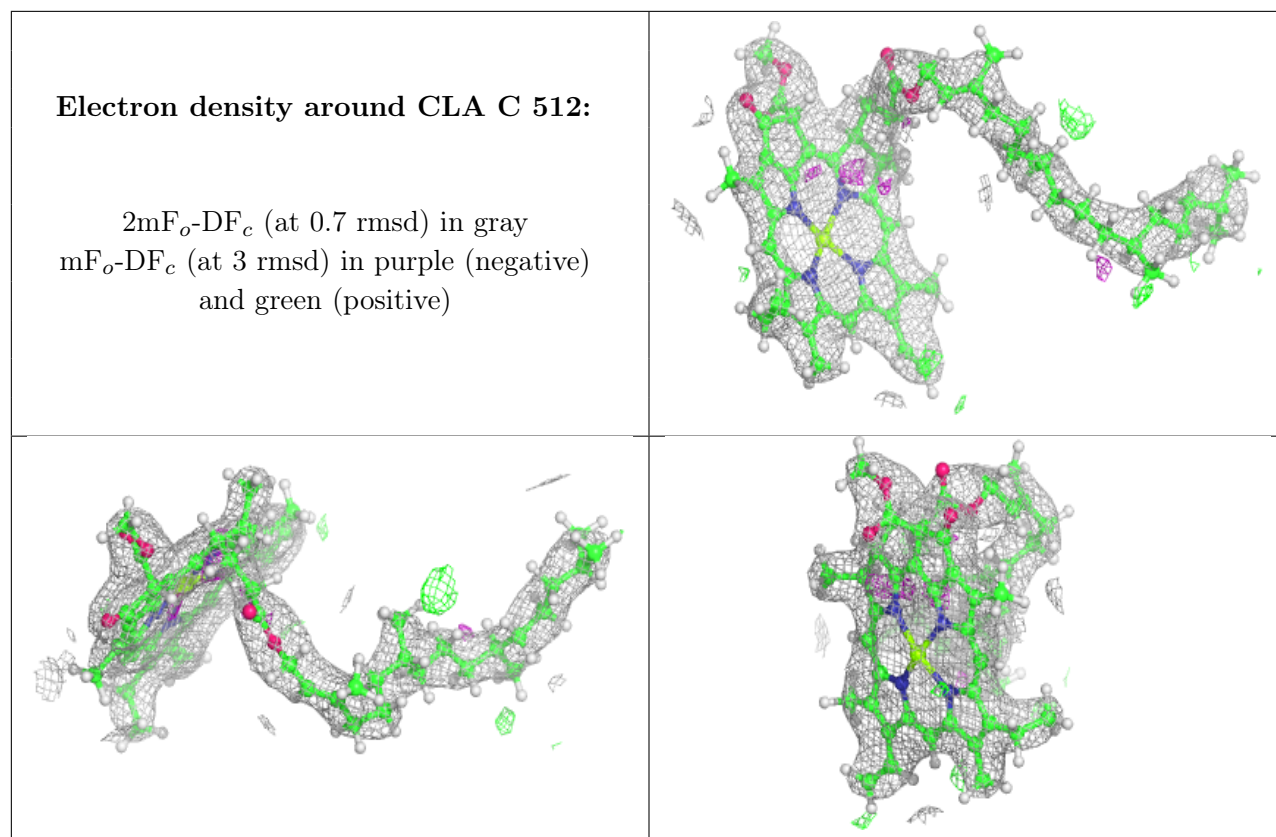
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 508:

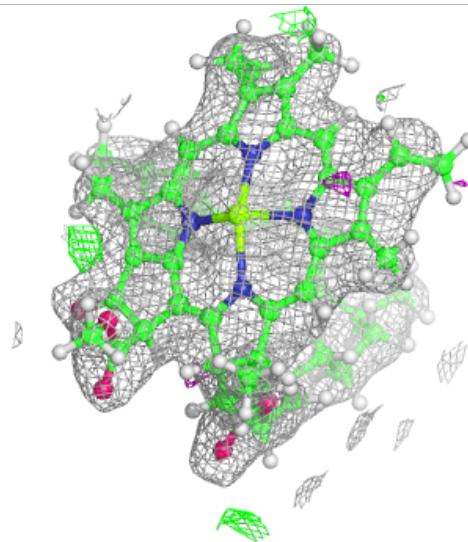
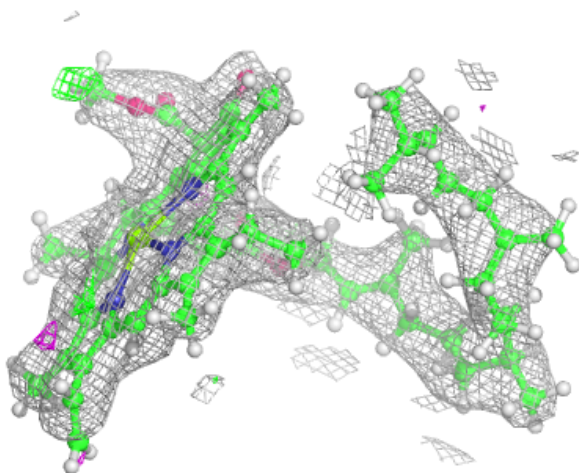
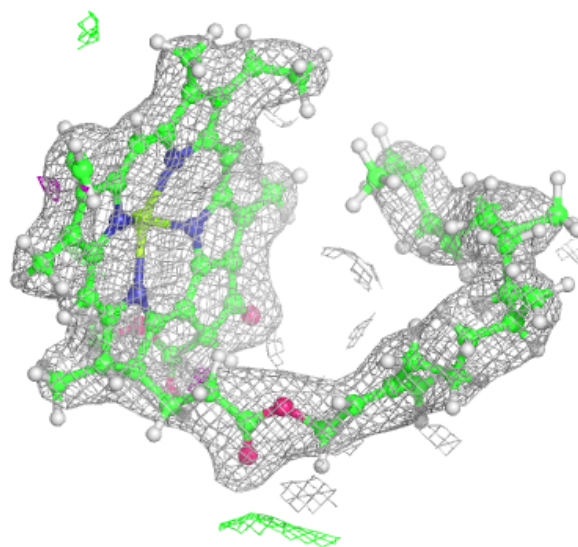
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





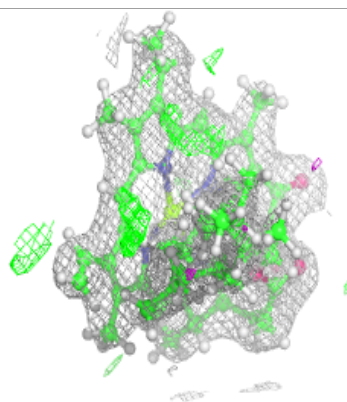
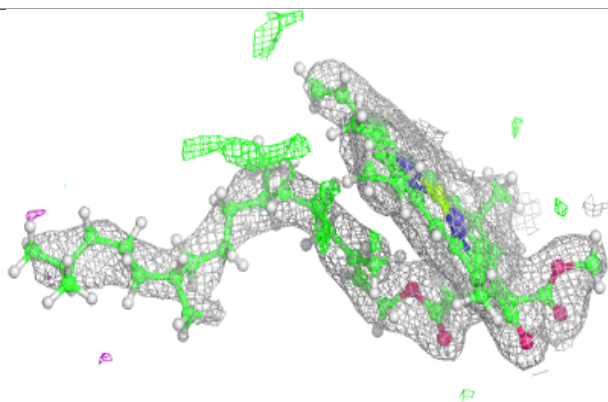
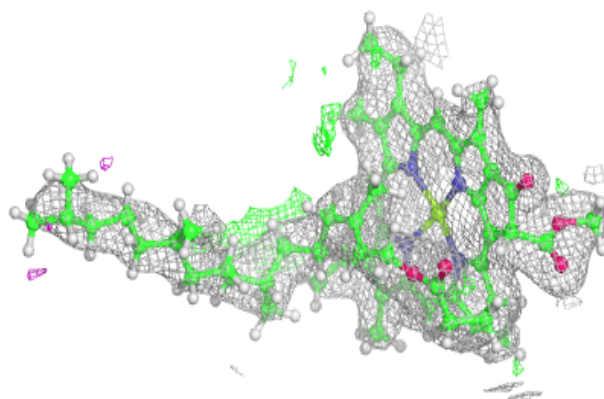
Electron density around CLA C 504:

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

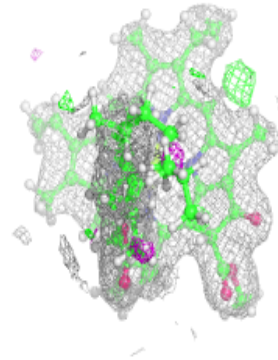
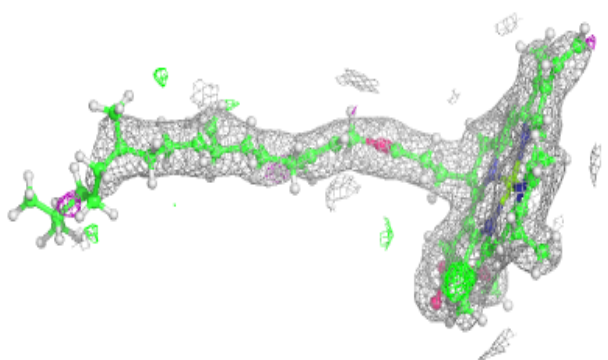
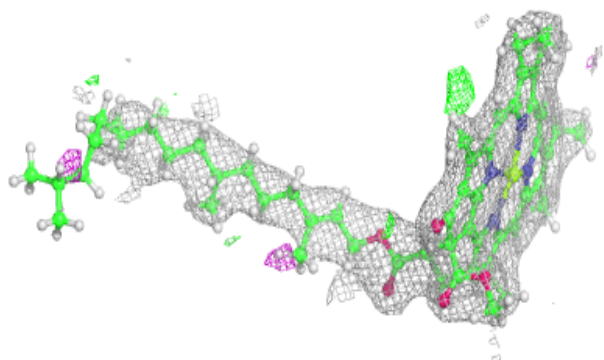


Electron density around CLA C 506:

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

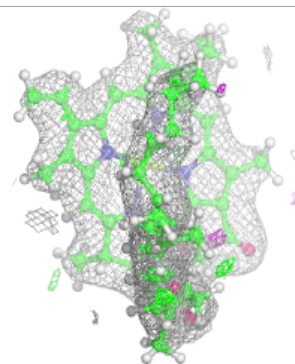
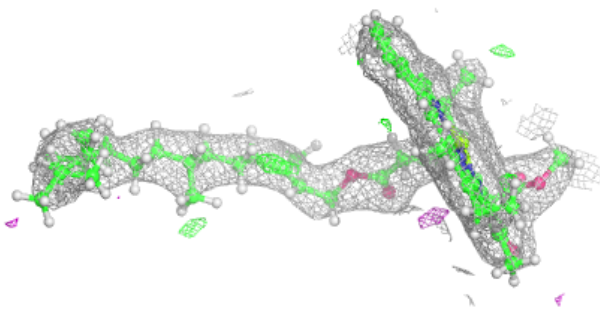
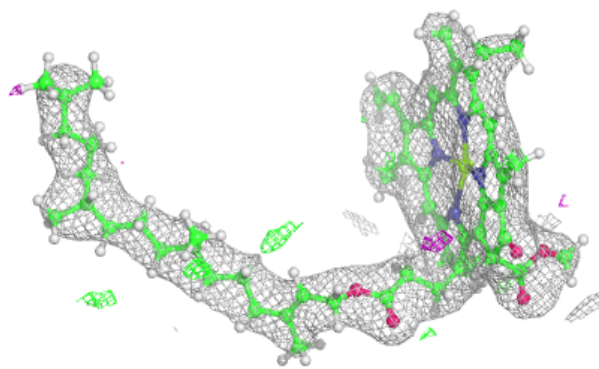
**Electron density around CLA b 704:**

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



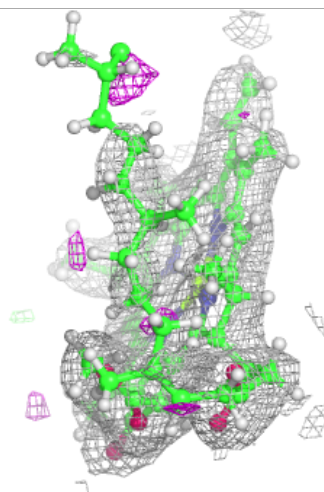
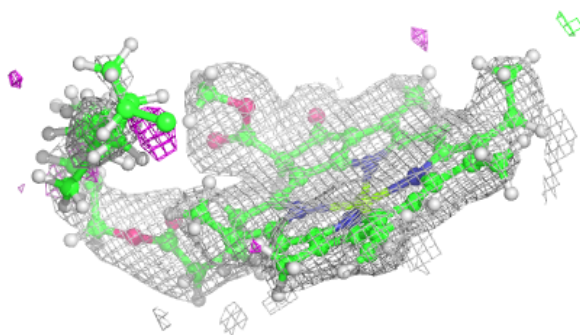
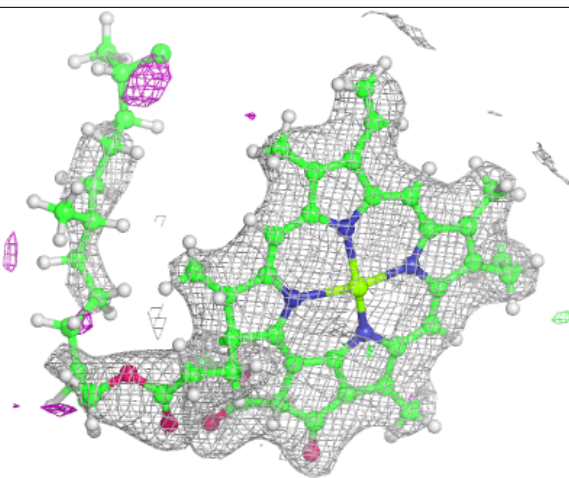
Electron density around CLA b 709:

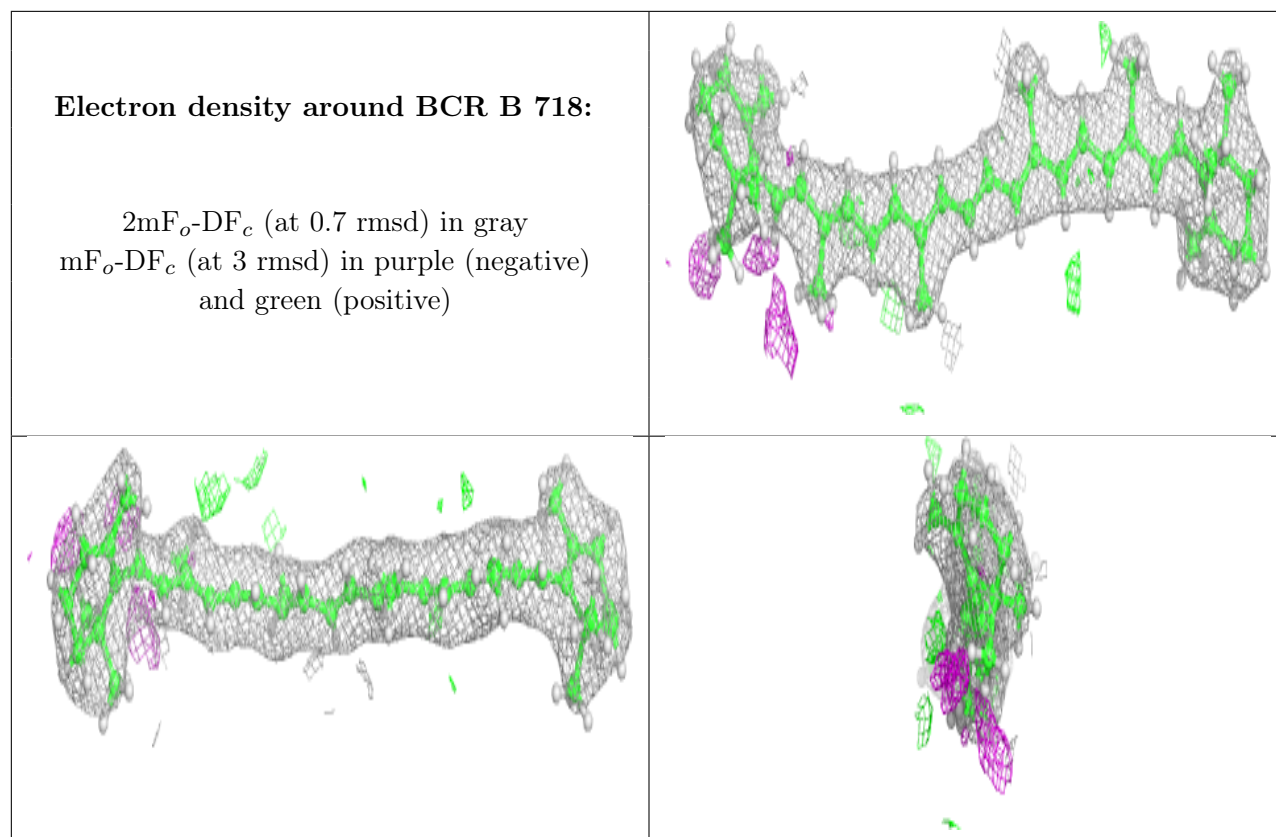
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 716:

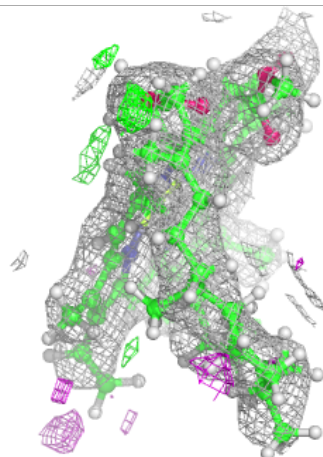
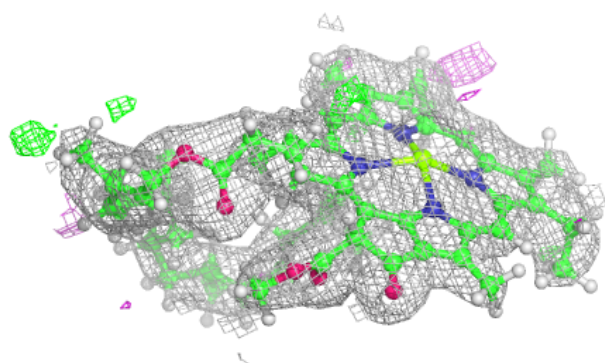
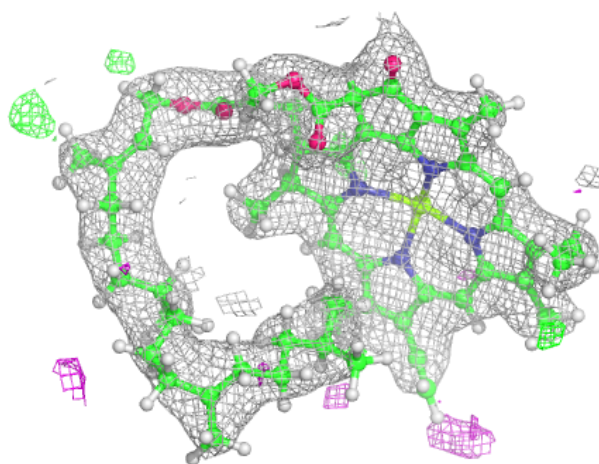
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

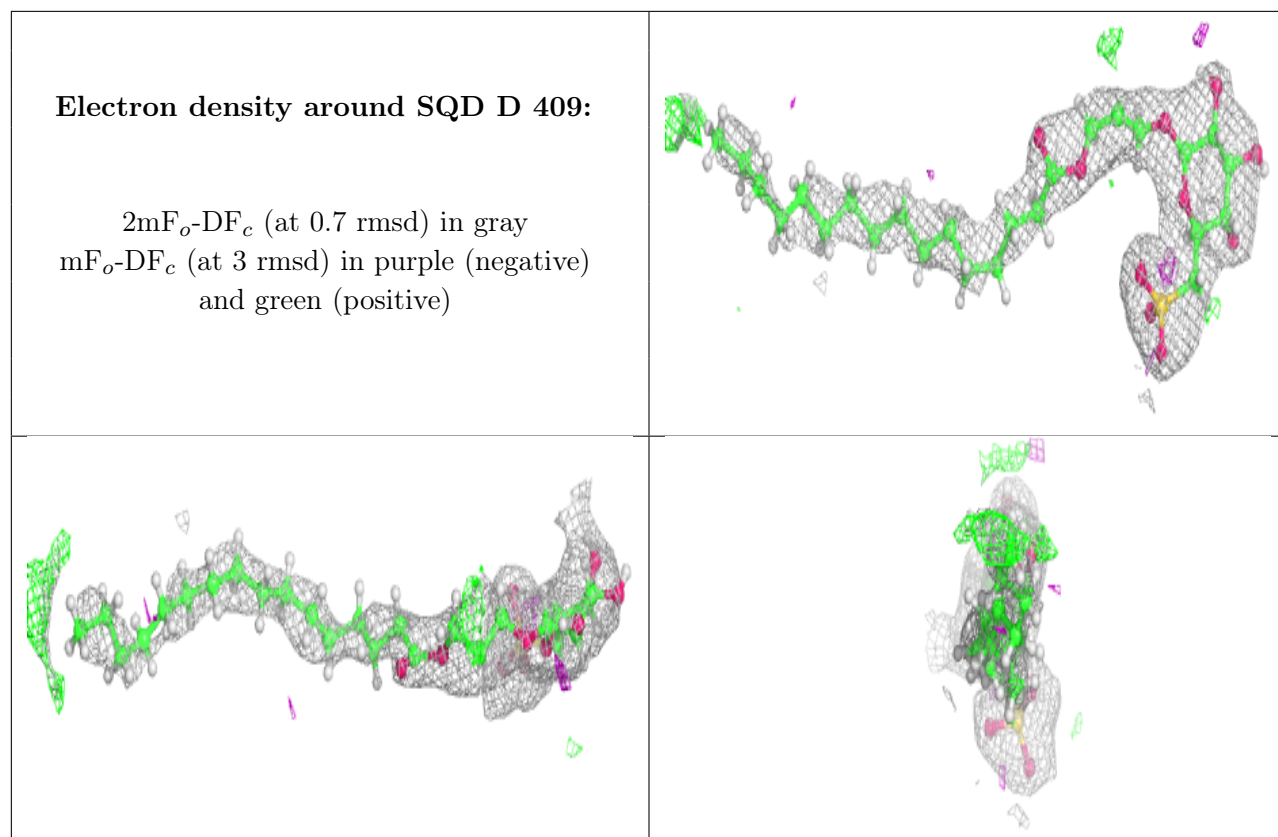




Electron density around CLA B 715:

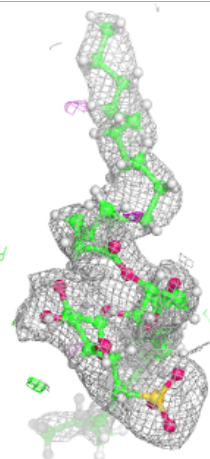
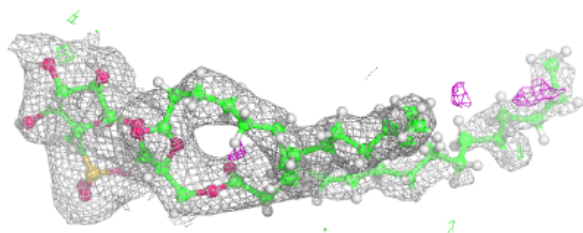
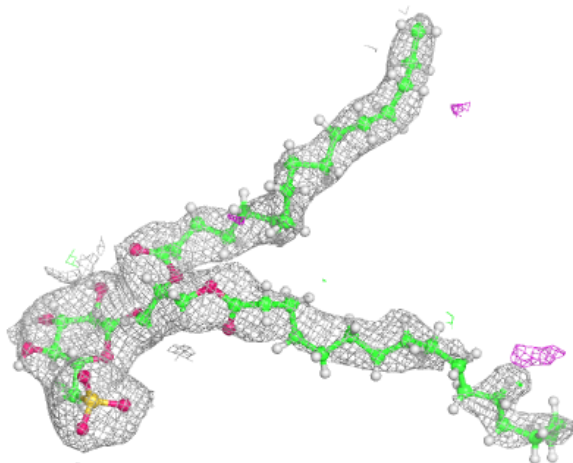
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

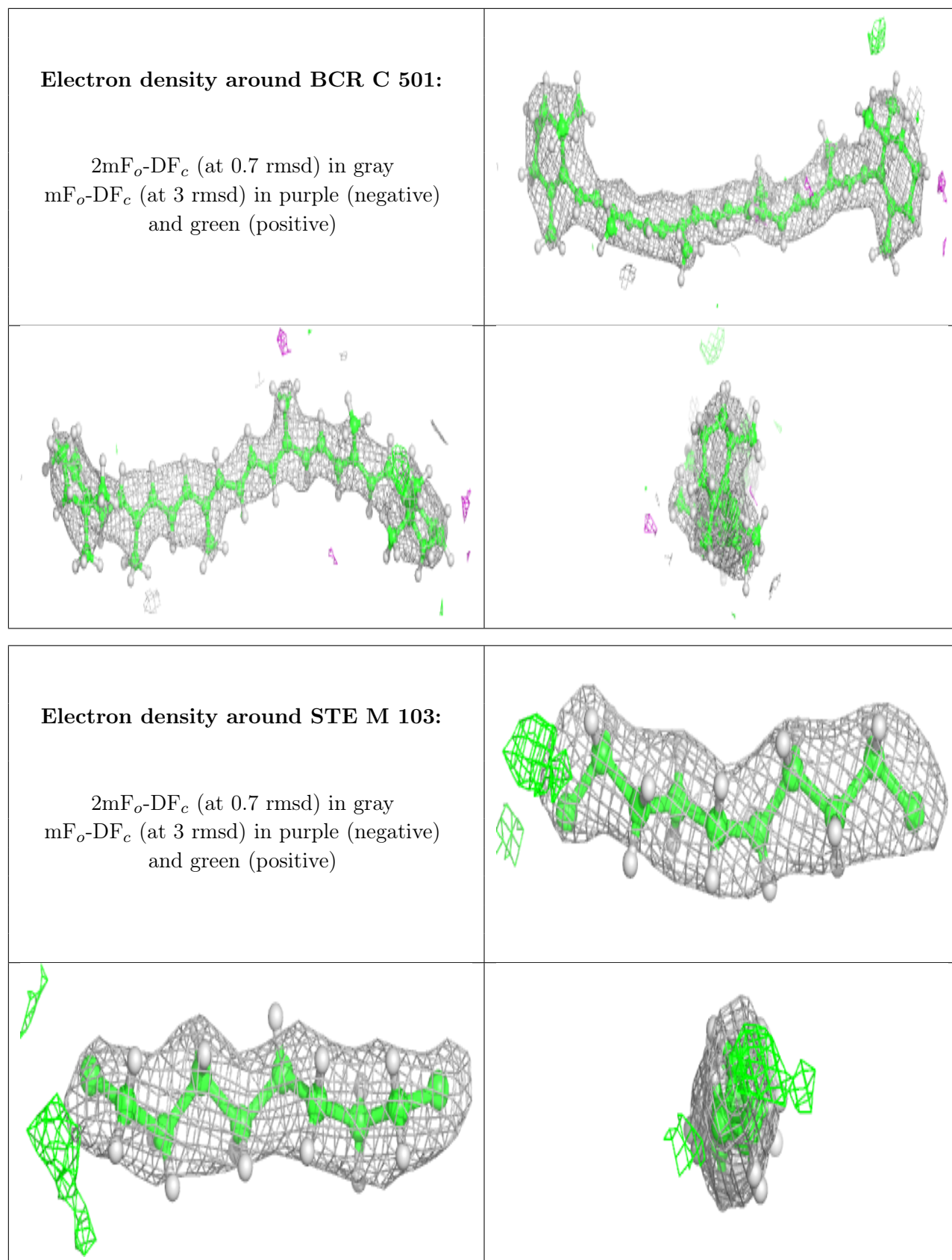




Electron density around SQD a 413:

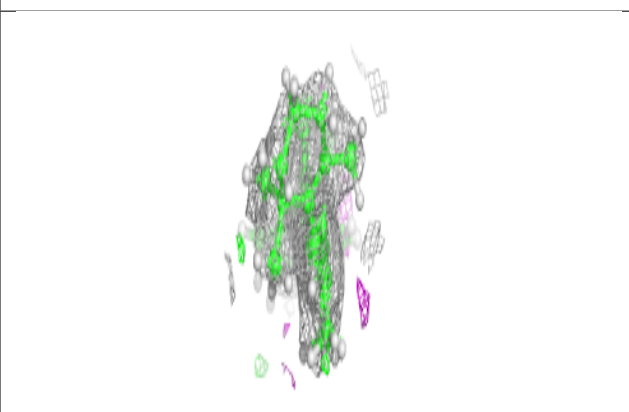
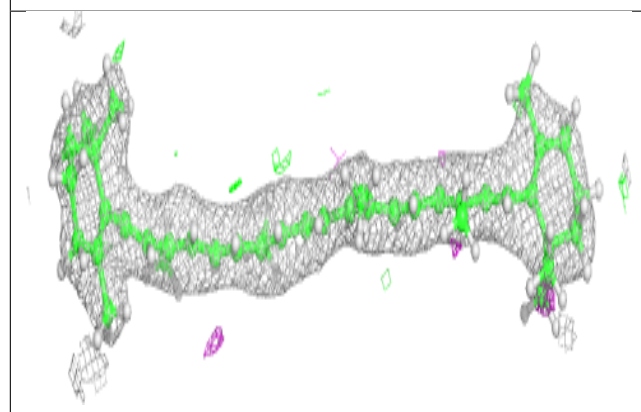
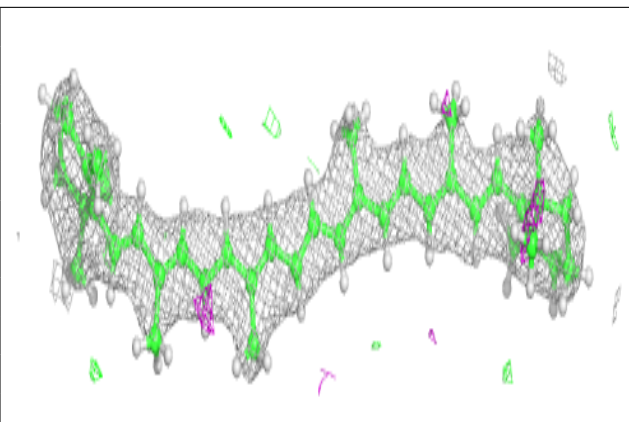
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



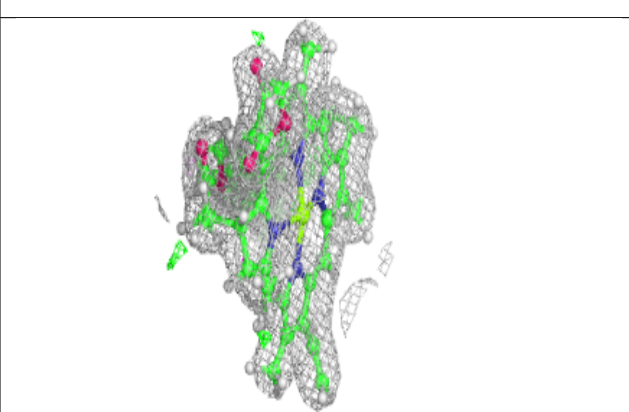
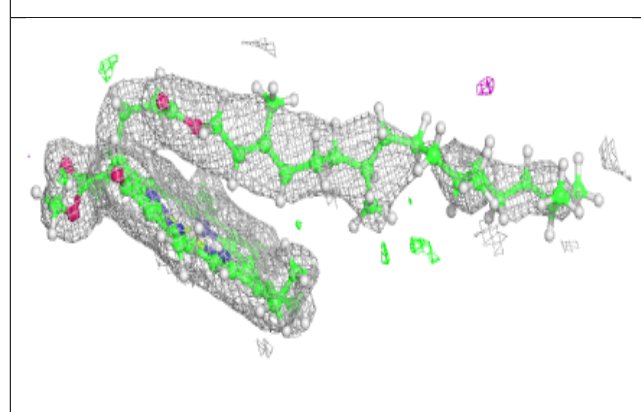
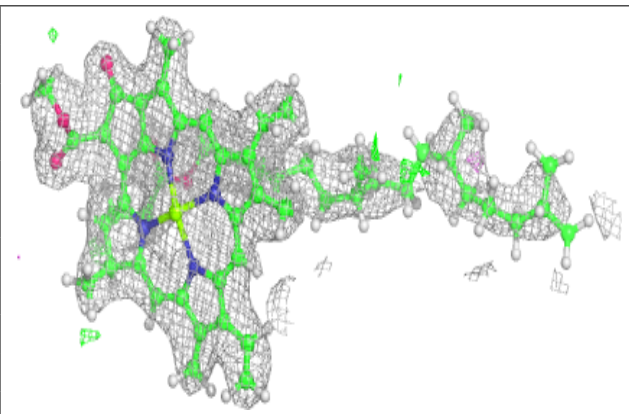


Electron density around BCR c 516:

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

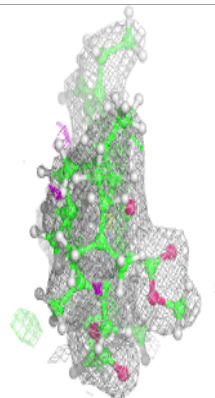
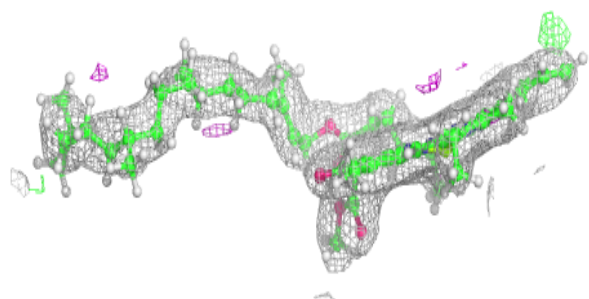
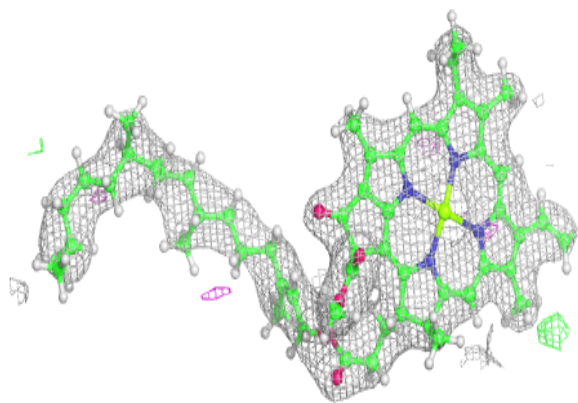
**Electron density around CLA b 714:**

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



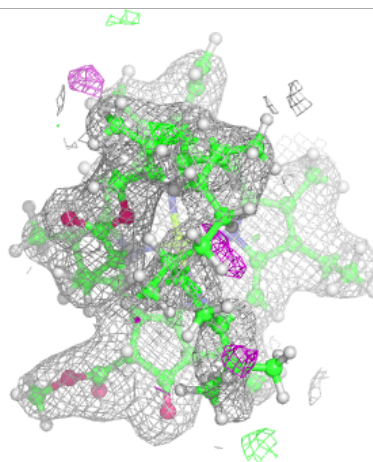
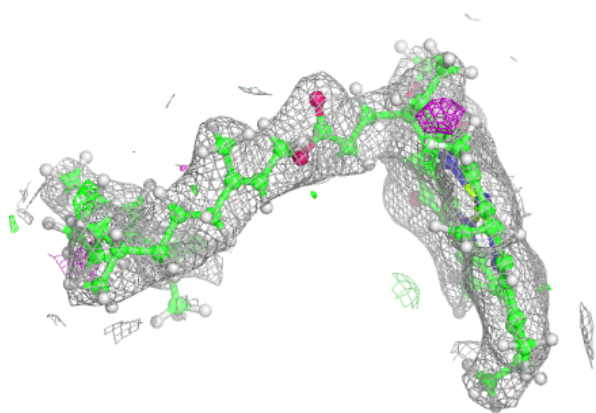
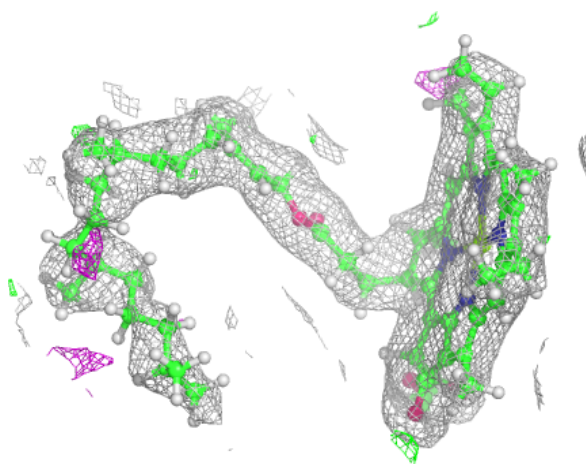
Electron density around CLA B 702:

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



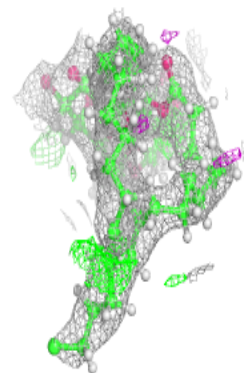
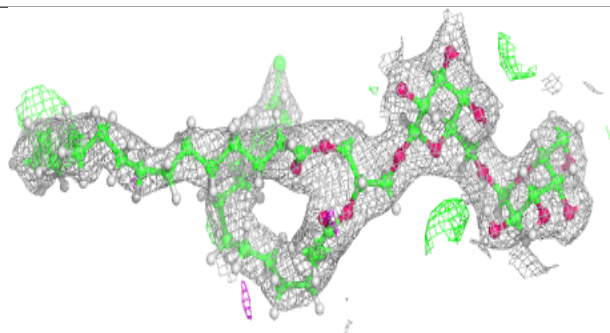
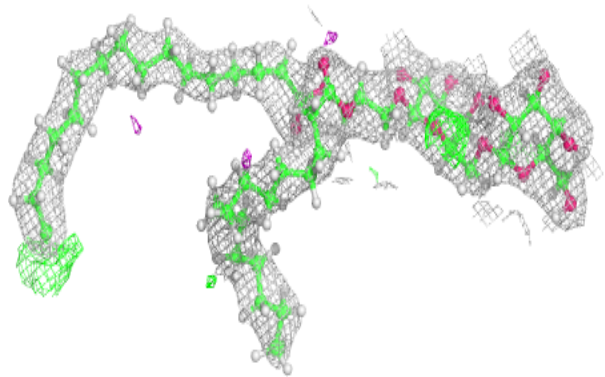
Electron density around CLA B 706:

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

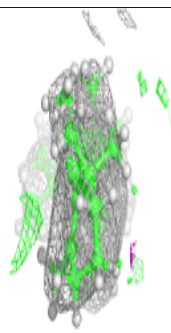
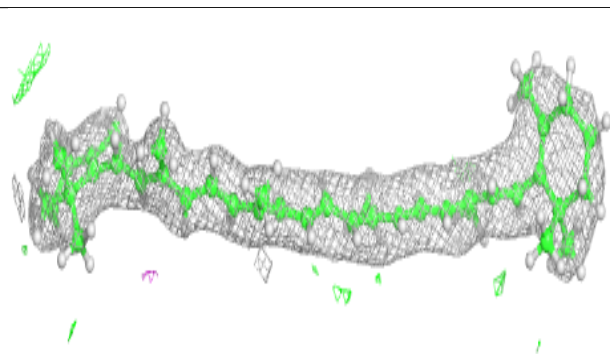
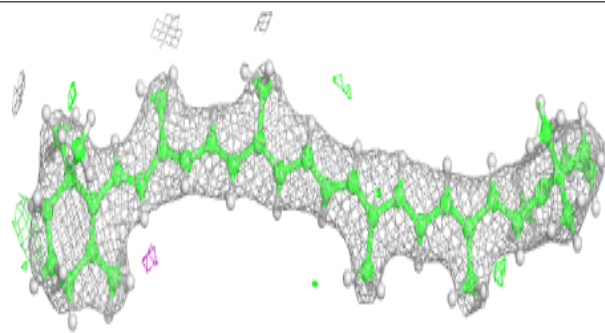


Electron density around DGD H 103:

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

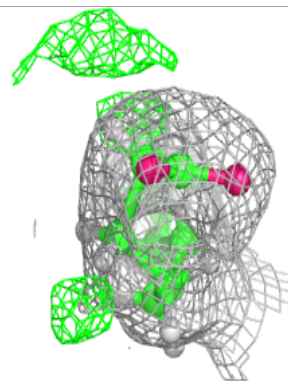
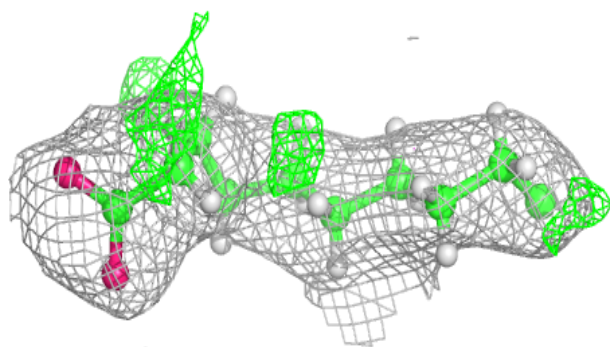
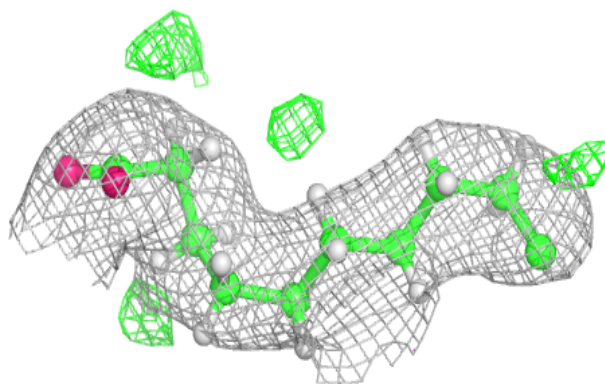
**Electron density around BCR B 717:**

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

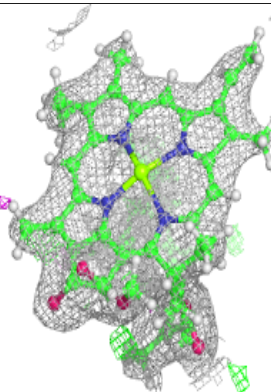
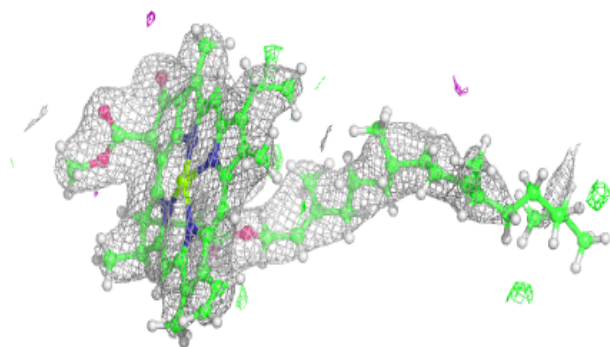
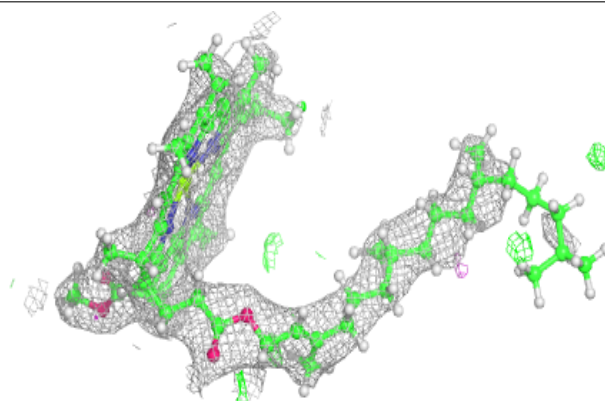


Electron density around STE B 724:

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

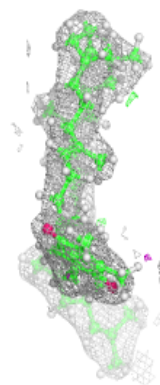
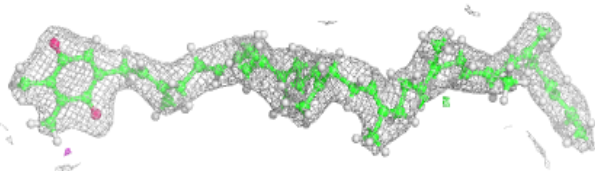
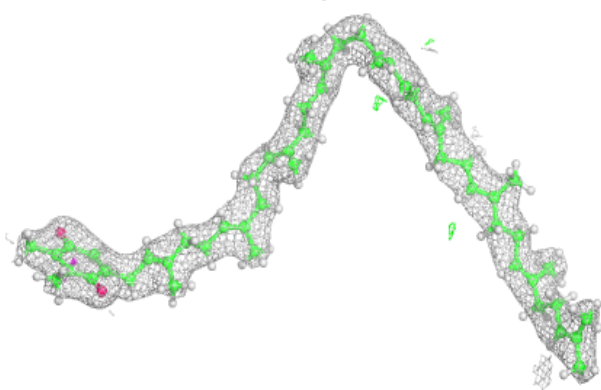
**Electron density around CLA C 509:**

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



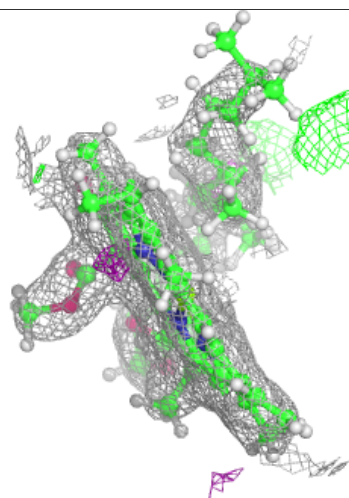
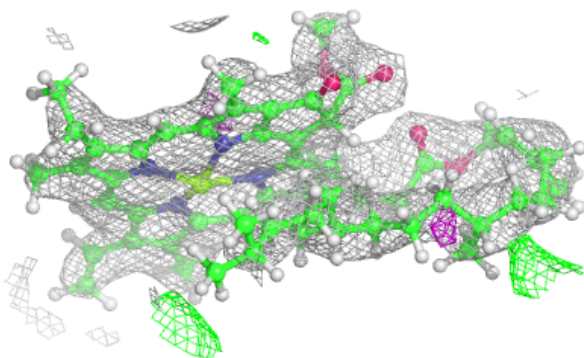
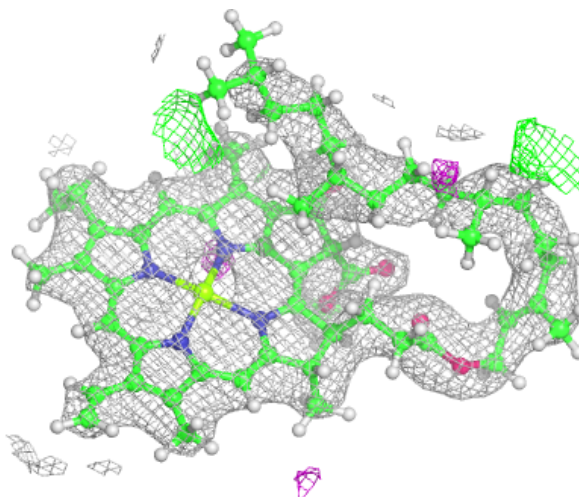
Electron density around PL9 D 405:

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



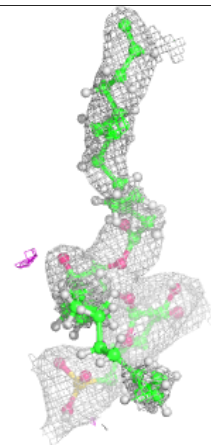
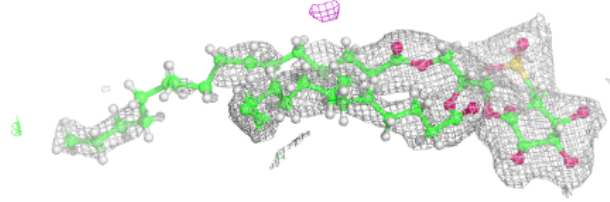
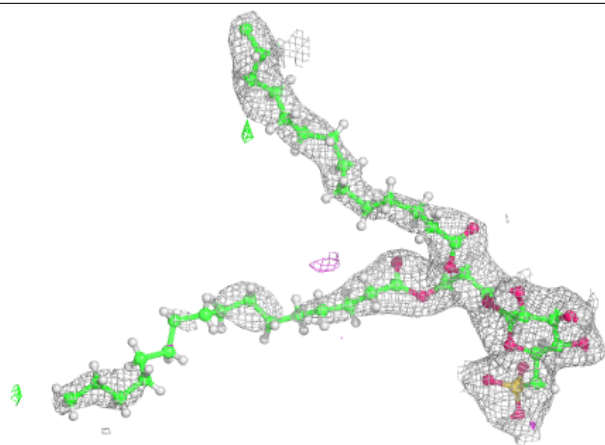
Electron density around CLA C 510:

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

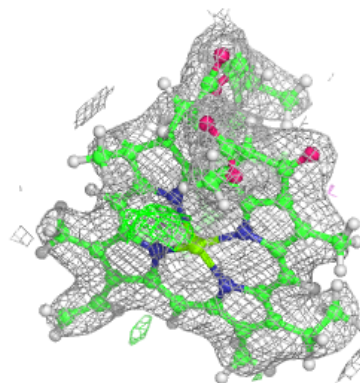
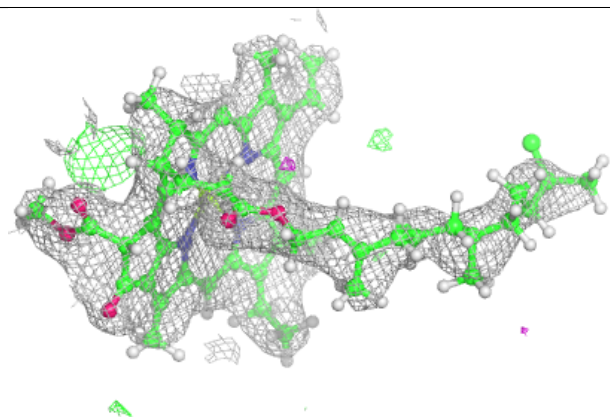
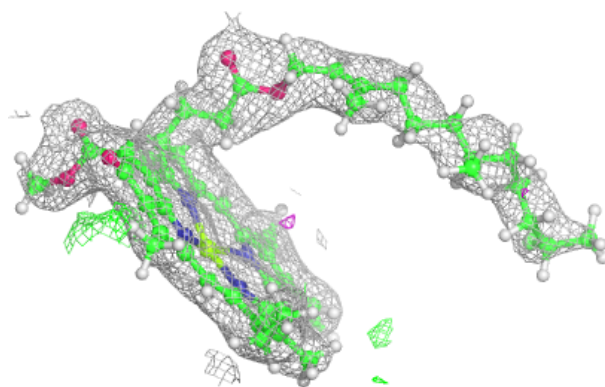


Electron density around SQD A 409:

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

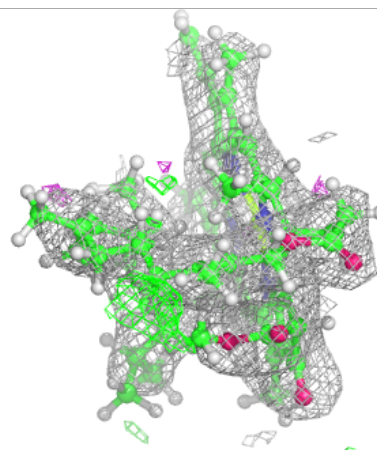
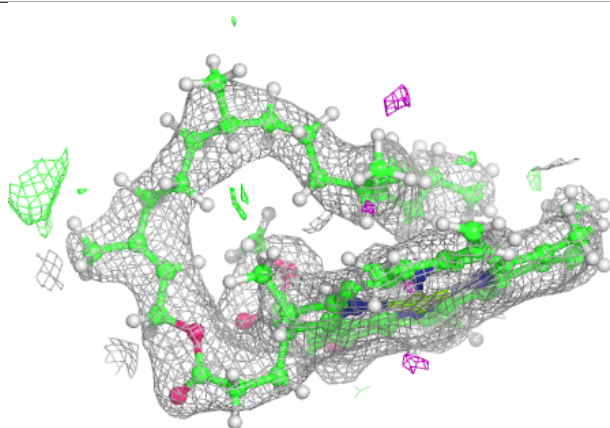
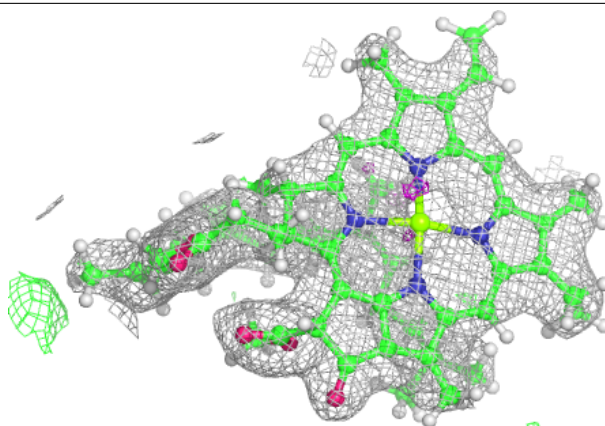
**Electron density around CLA c 505:**

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



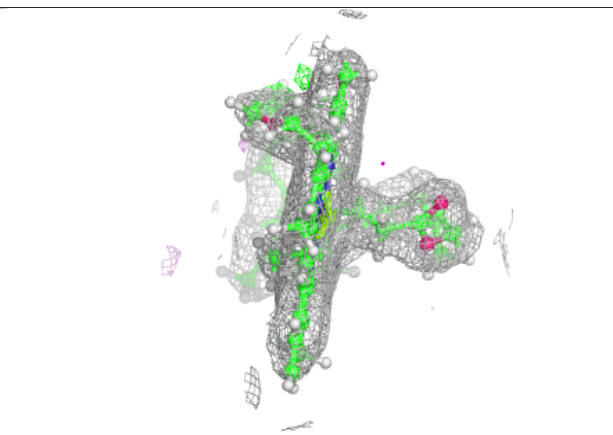
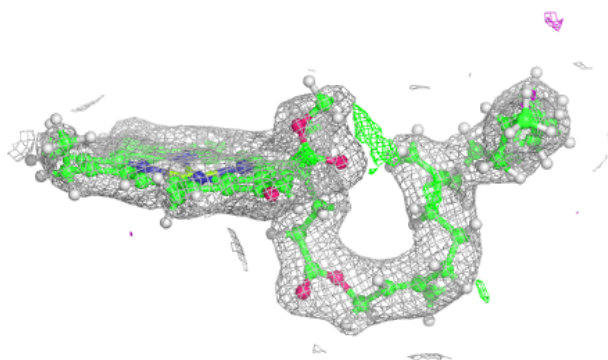
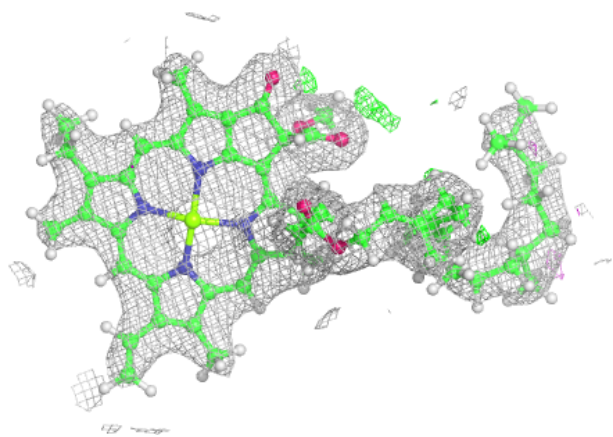
Electron density around CLA C 511:

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

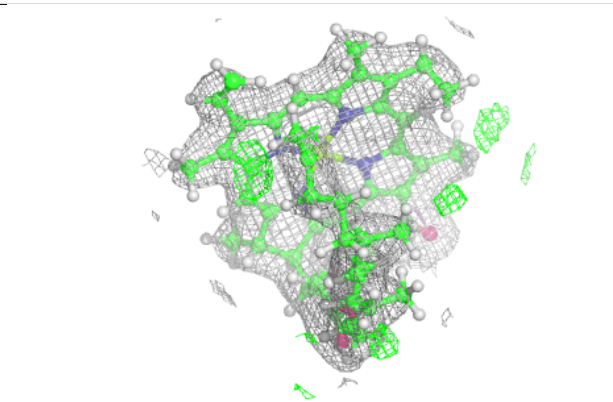
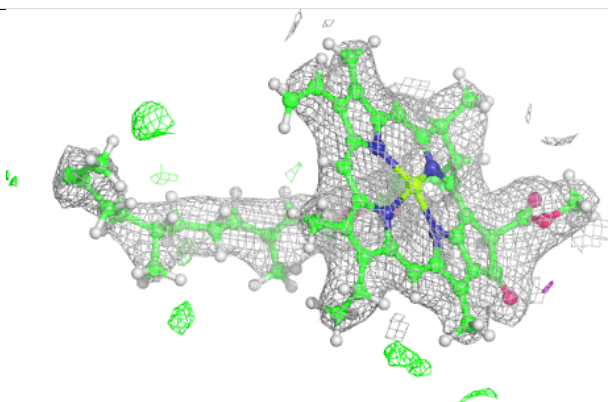
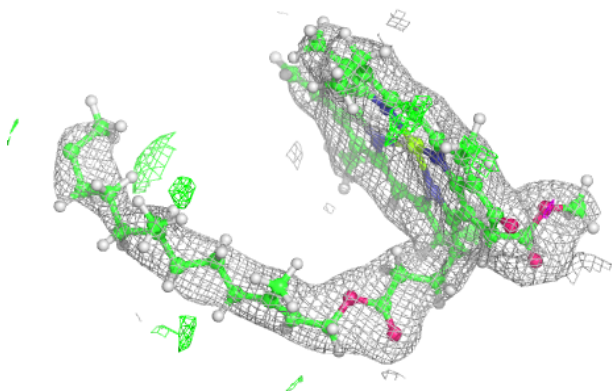


Electron density around CLA B 712:

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

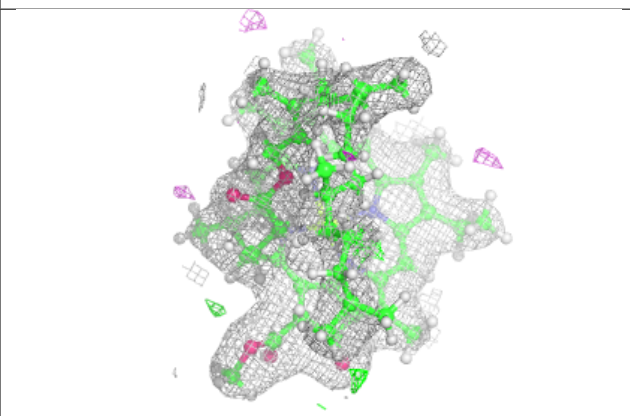
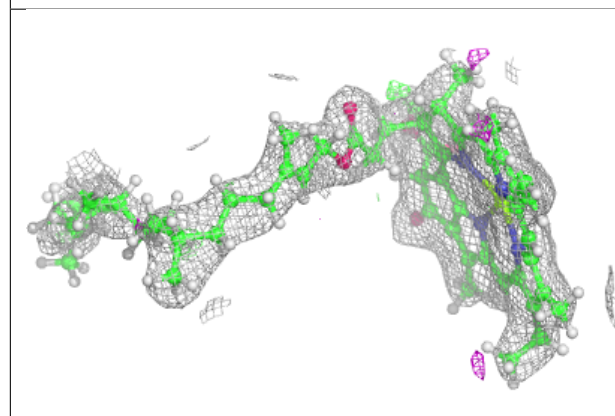
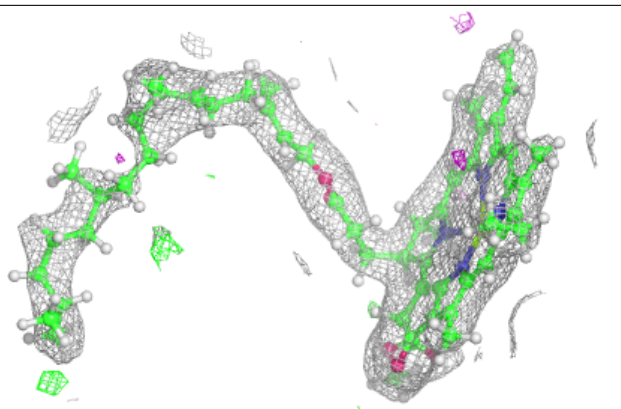
**Electron density around CLA C 505:**

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



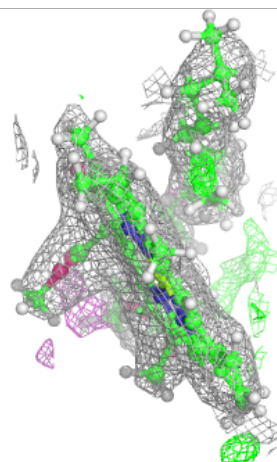
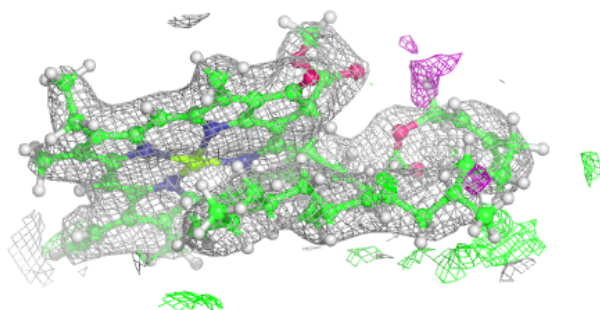
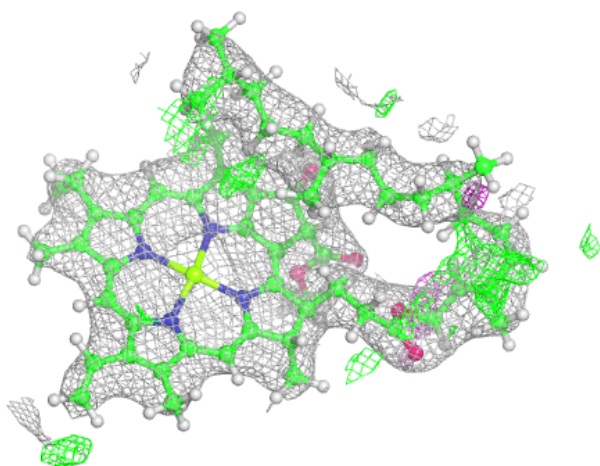
Electron density around CLA b 706:

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



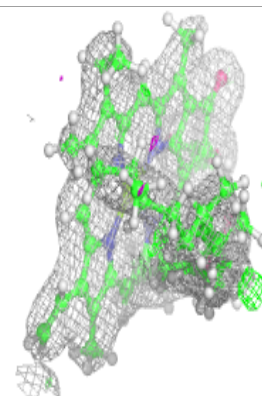
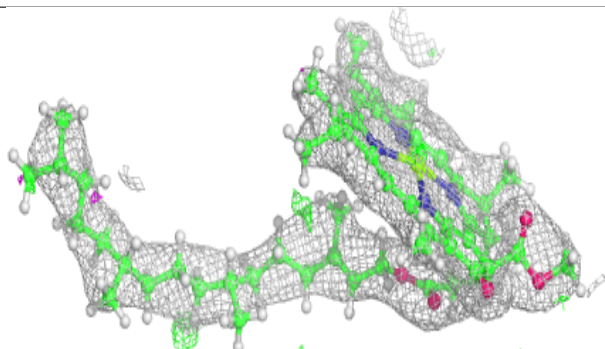
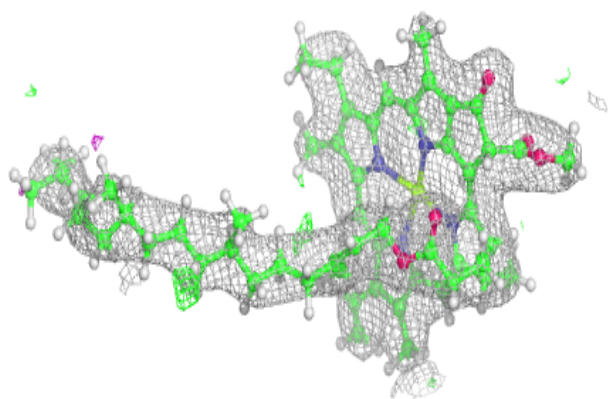
Electron density around CLA c 510:

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

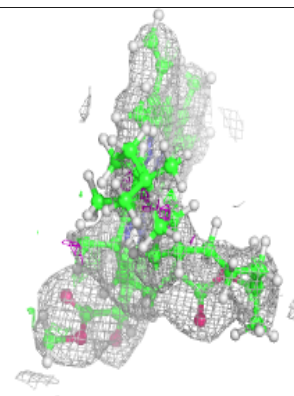
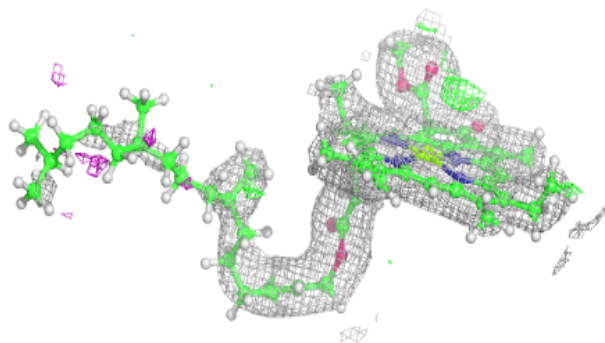
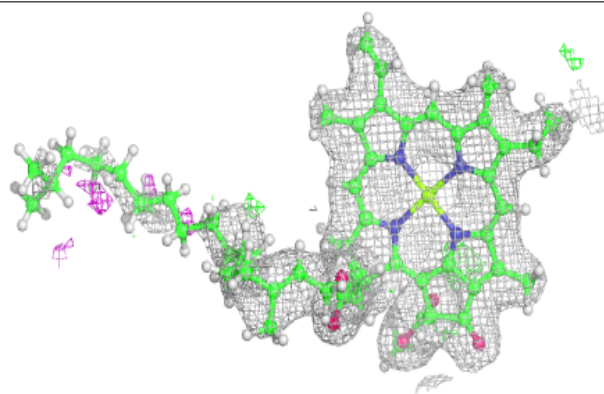


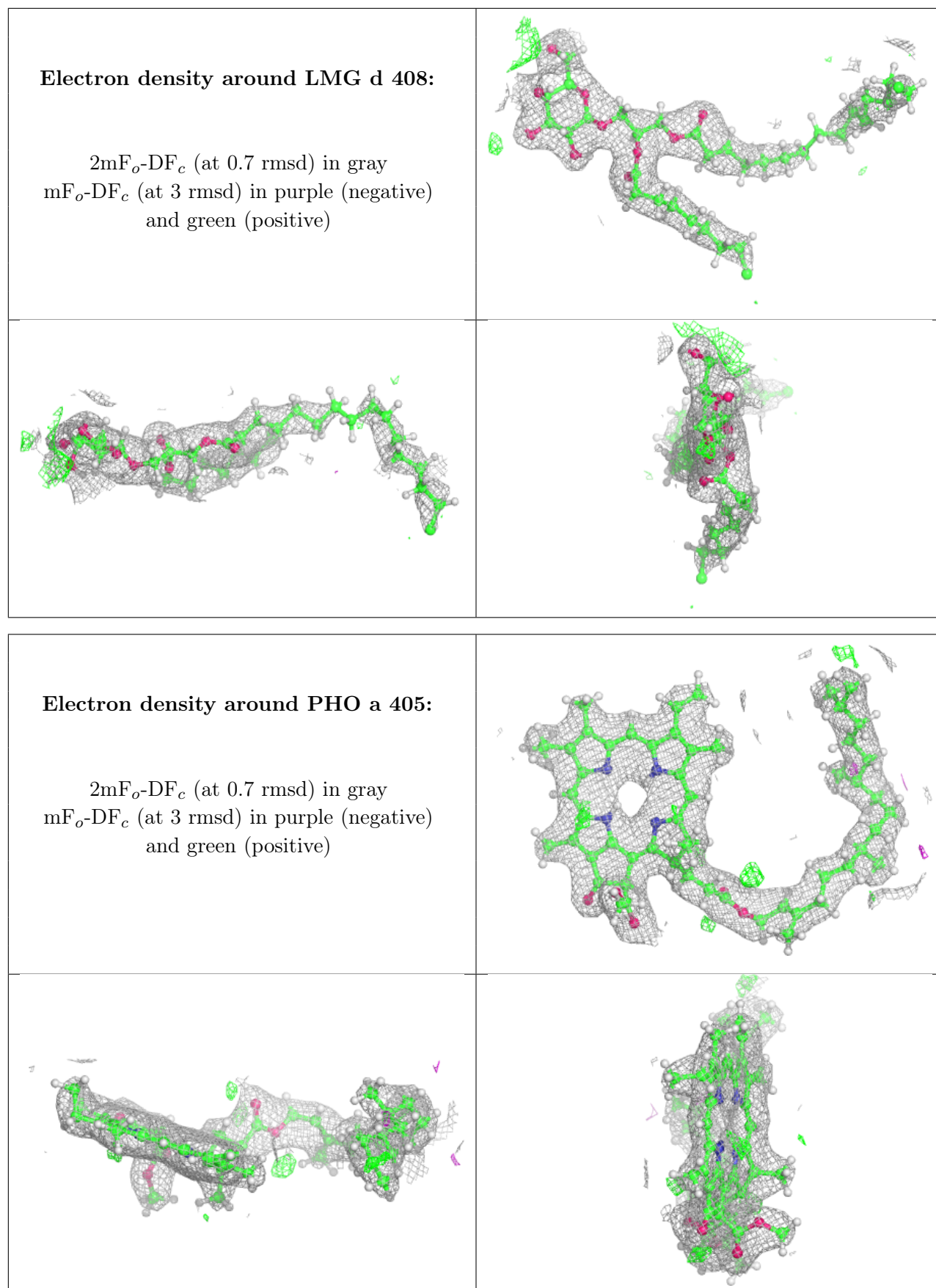
Electron density around CLA b 708:

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

**Electron density around CLA A 403:**

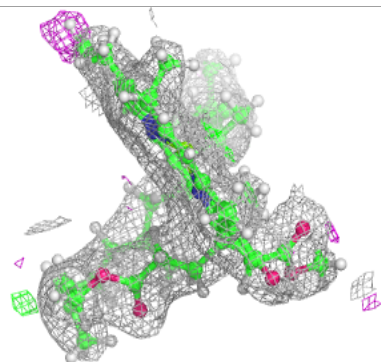
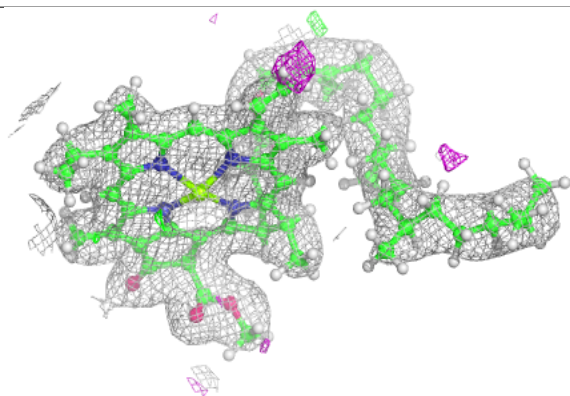
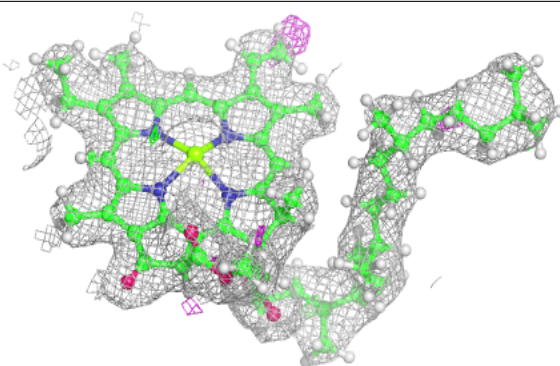
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



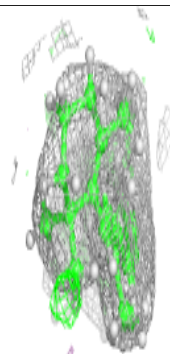
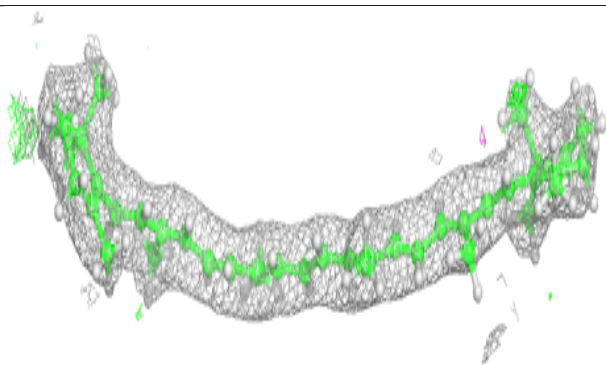
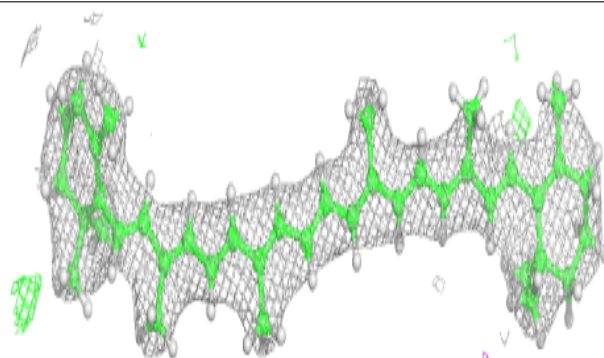


Electron density around CLA D 402:

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

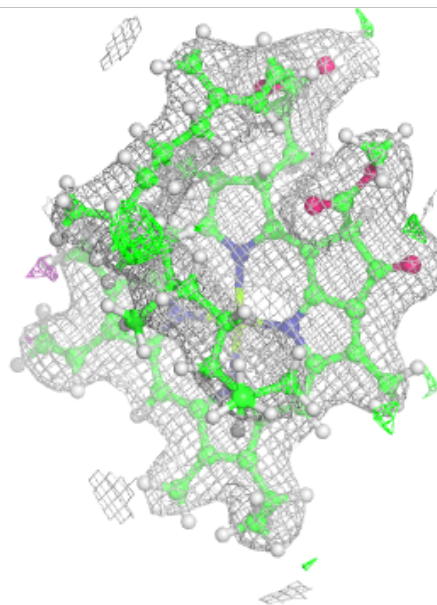
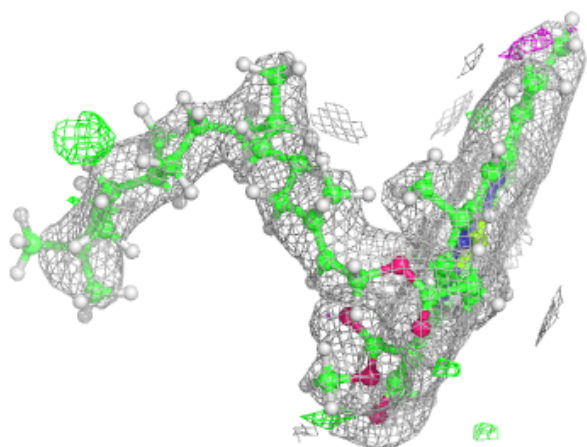
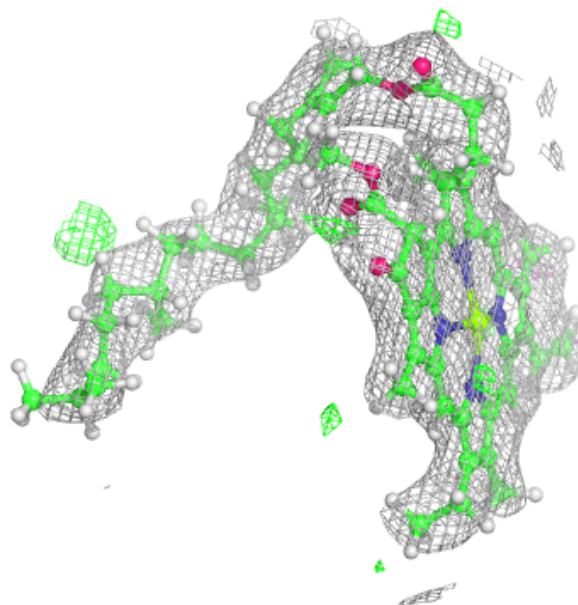
**Electron density around BCR T 701:**

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



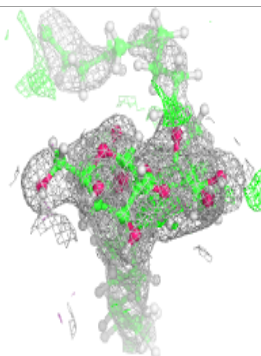
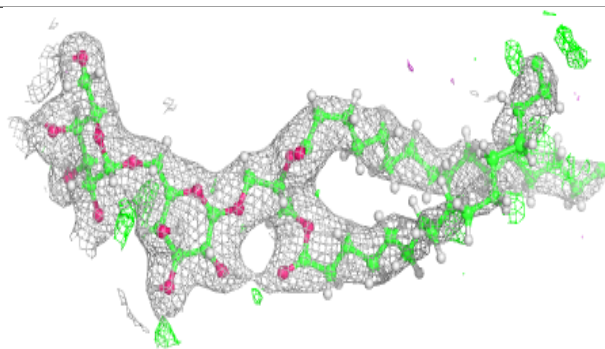
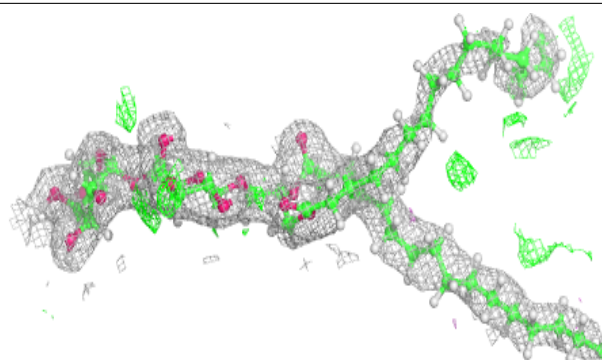
Electron density around CLA B 713:

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

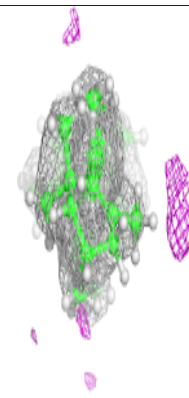
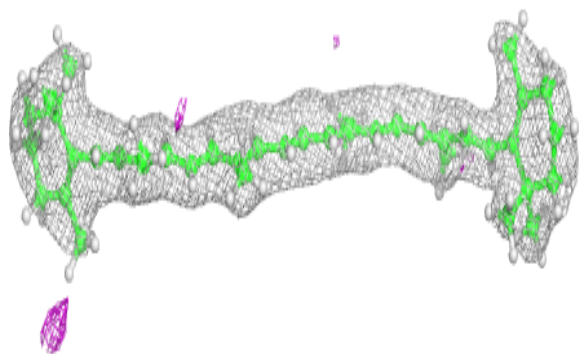
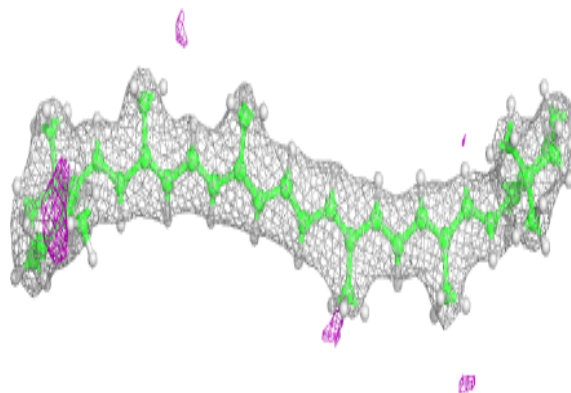


Electron density around DGD C 517:

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

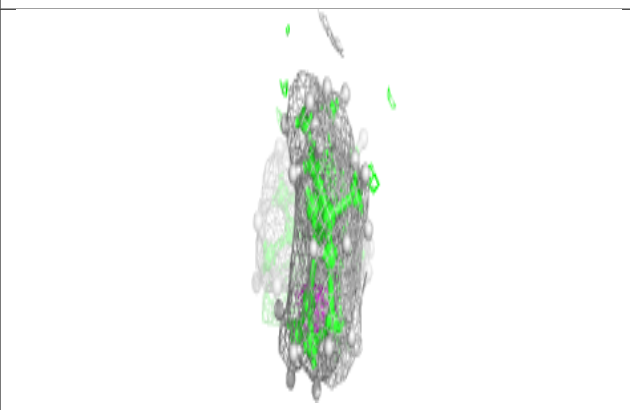
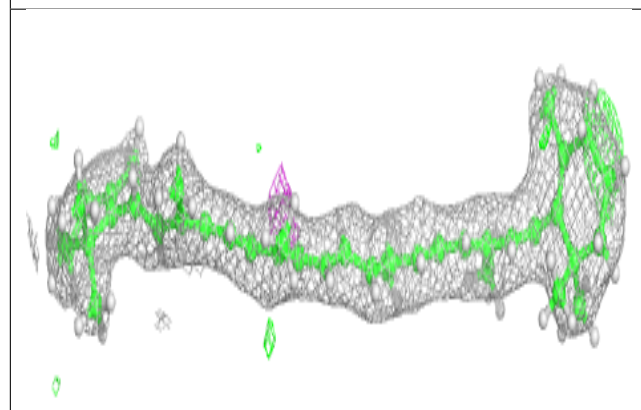
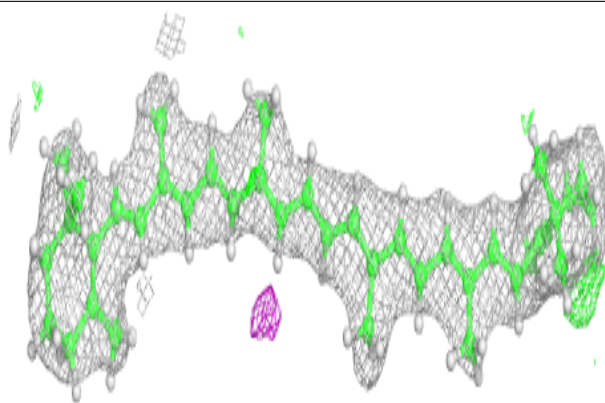
**Electron density around BCR a 407:**

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

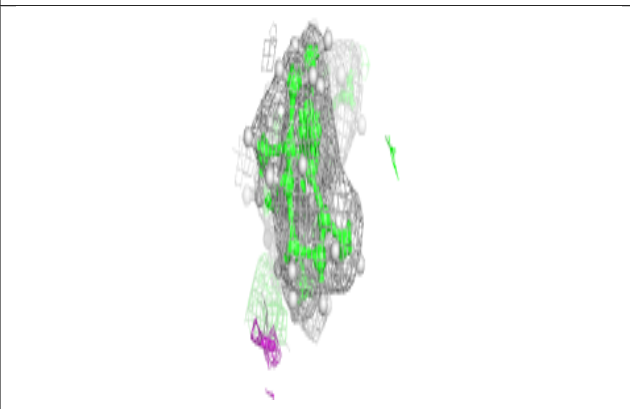
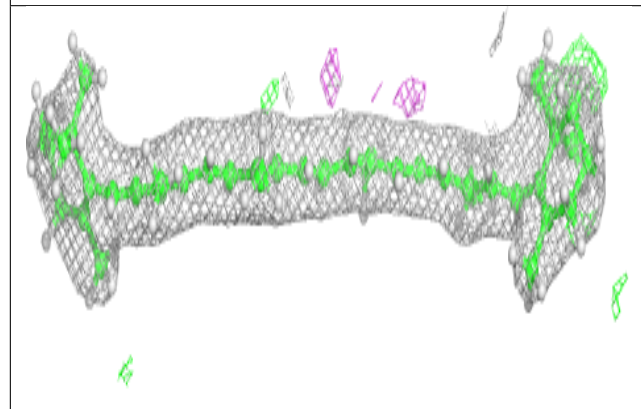
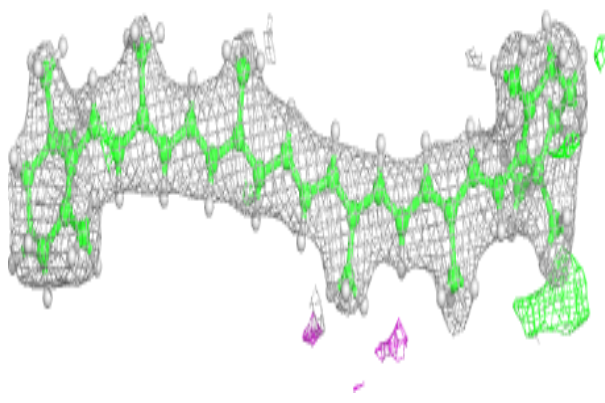


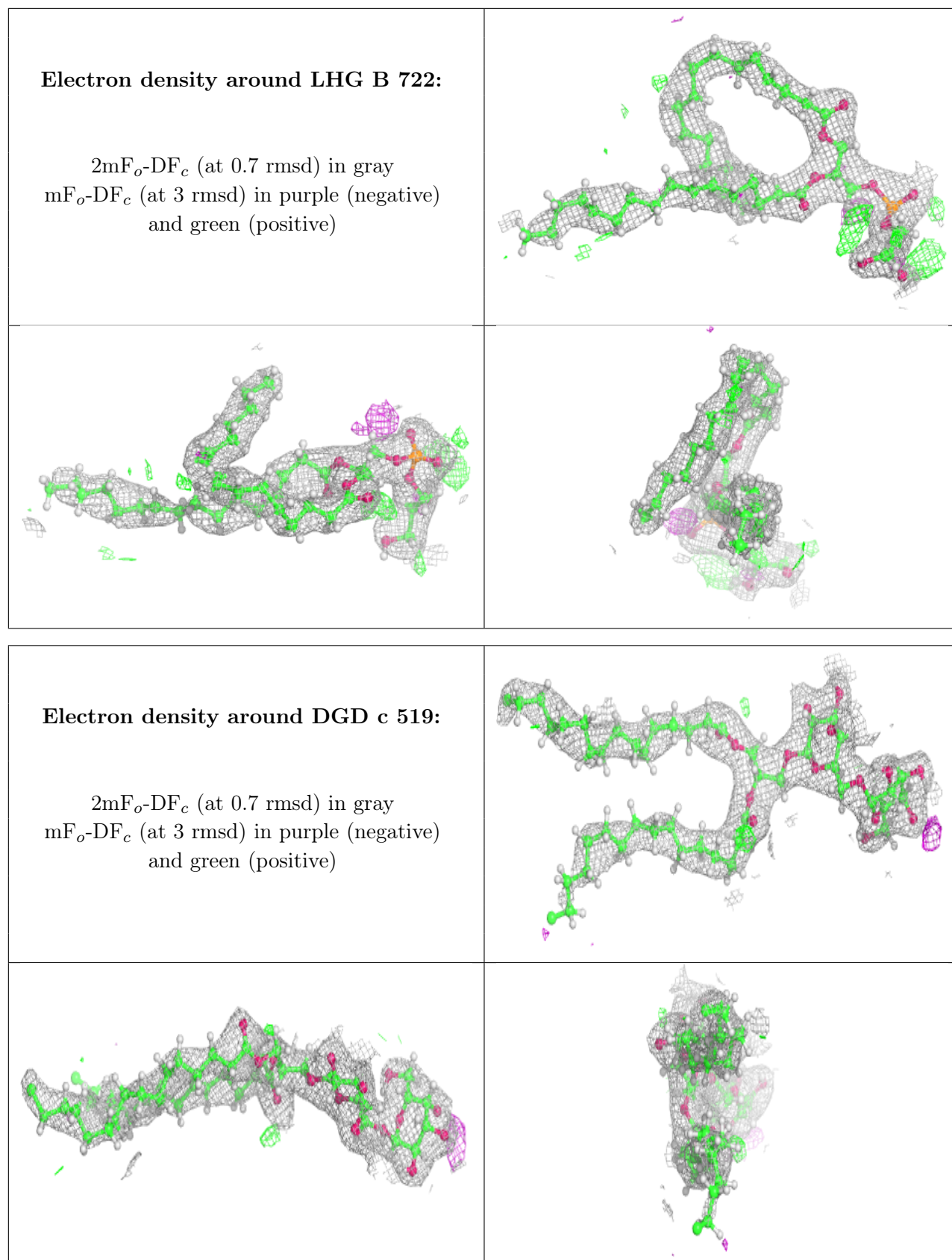
Electron density around BCR b 717:

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

**Electron density around BCR b 718:**

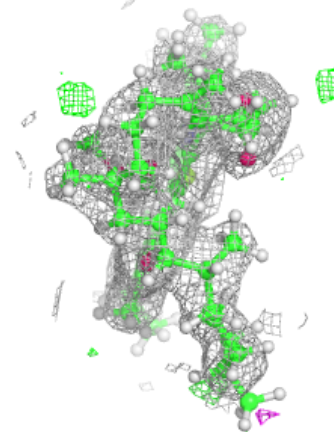
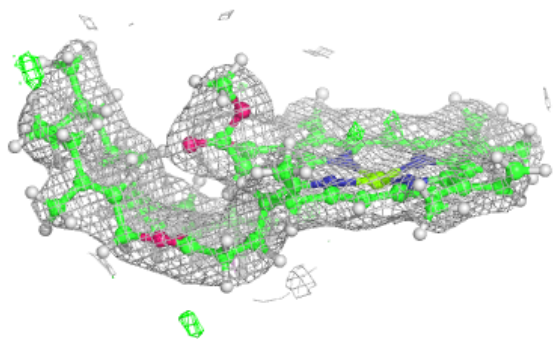
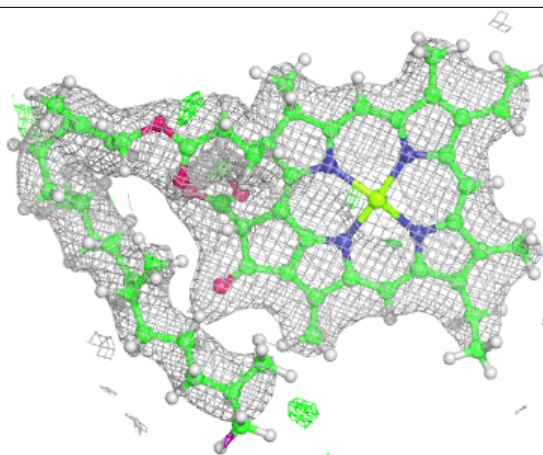
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



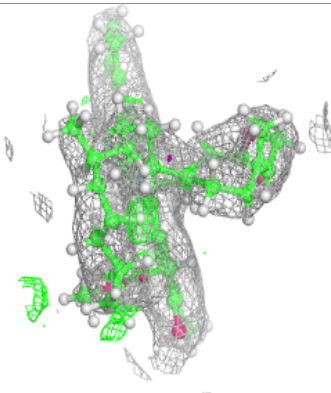
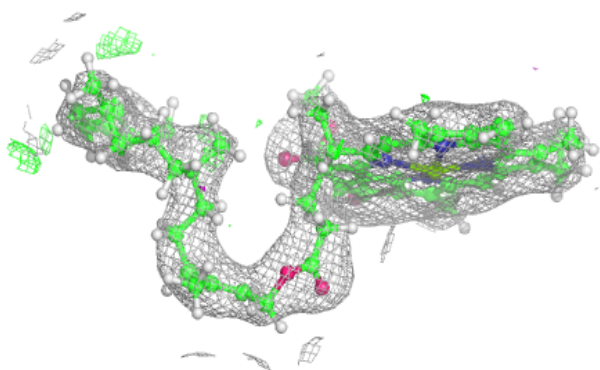
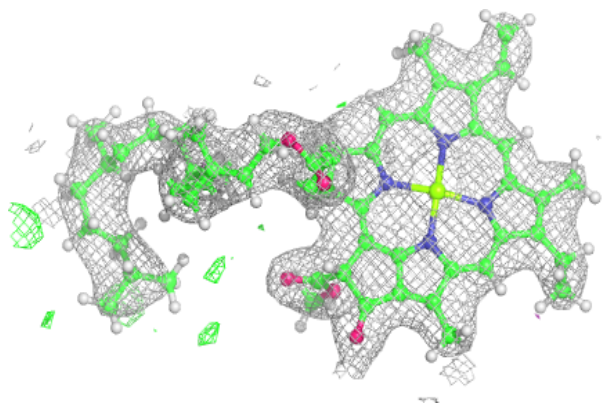


Electron density around CLA b 710:

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

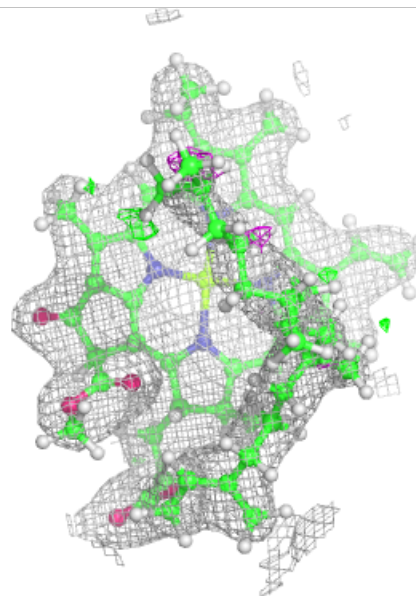
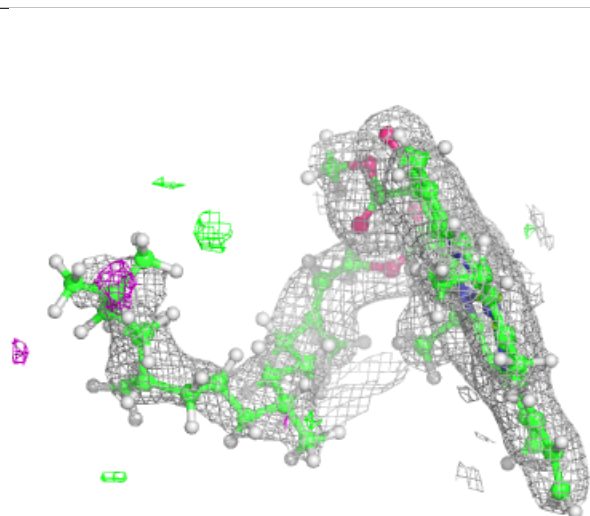
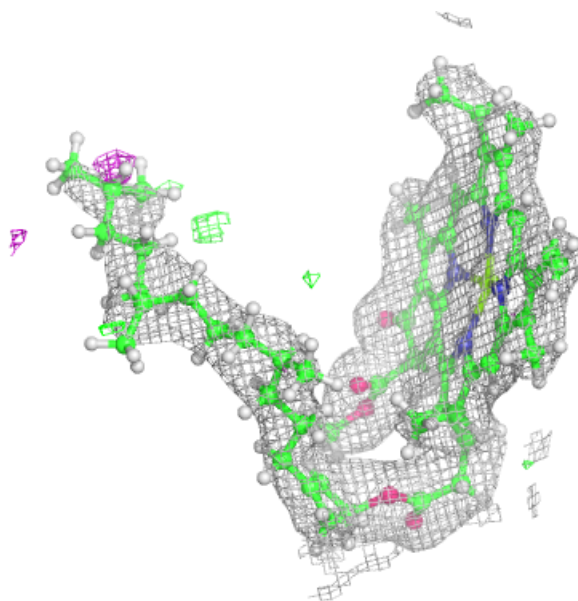
**Electron density around CLA b 712:**

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



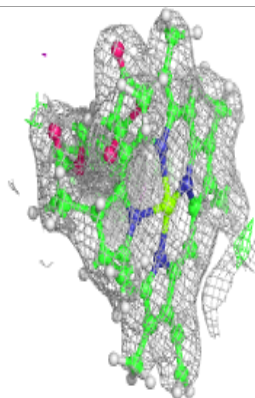
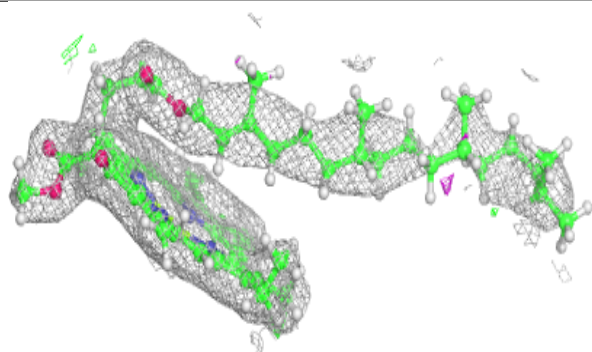
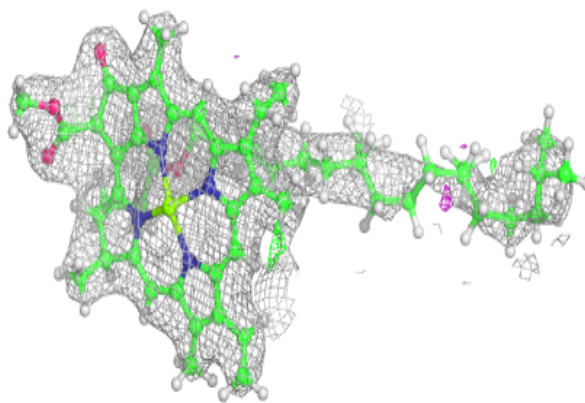
Electron density around CLA b 713:

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



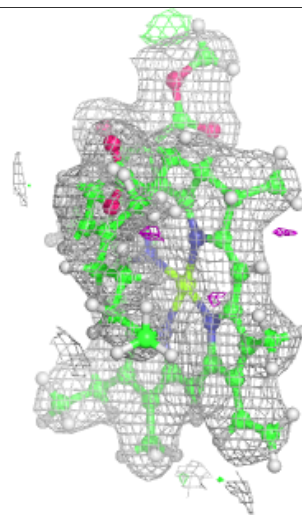
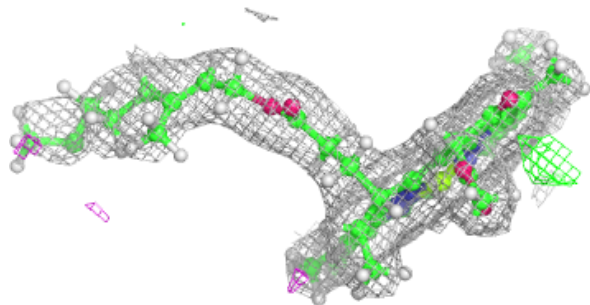
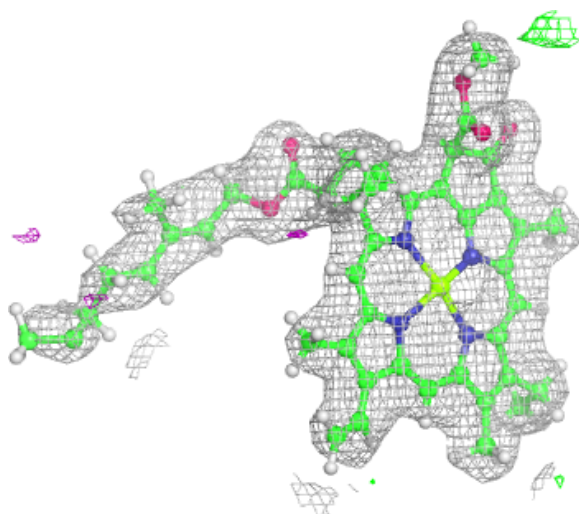
Electron density around CLA B 714:

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



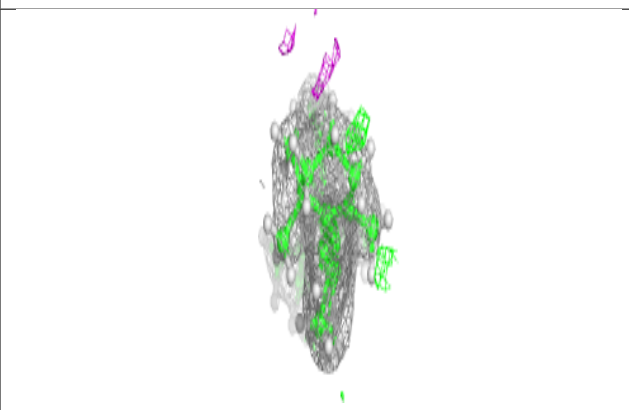
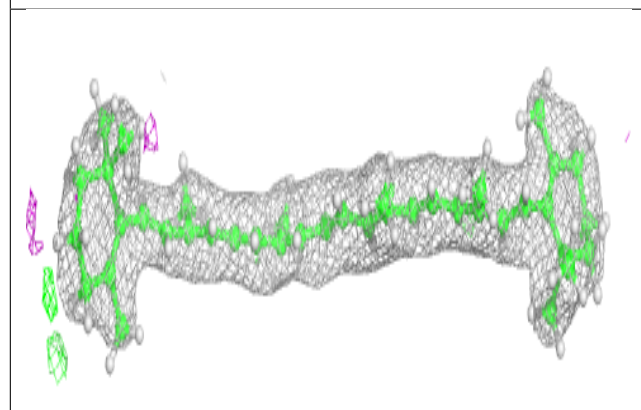
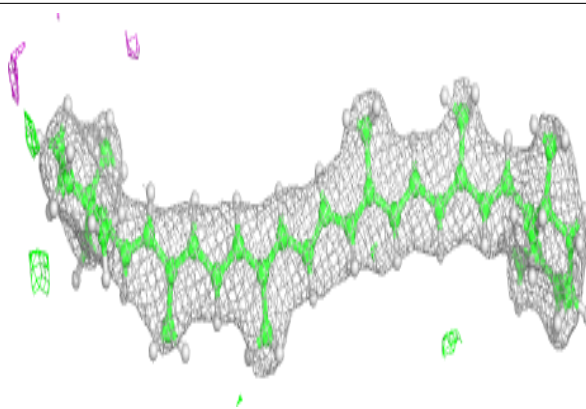
Electron density around CLA A 404:

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

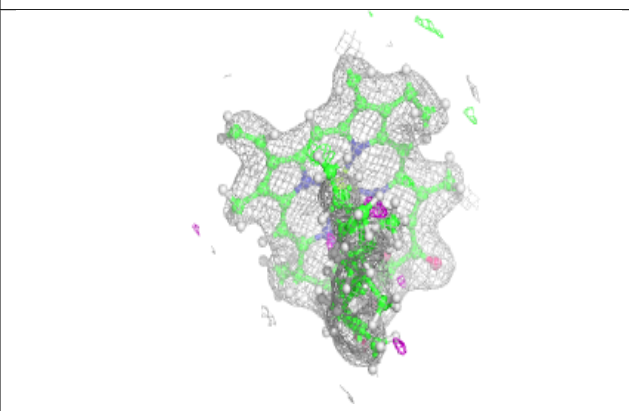
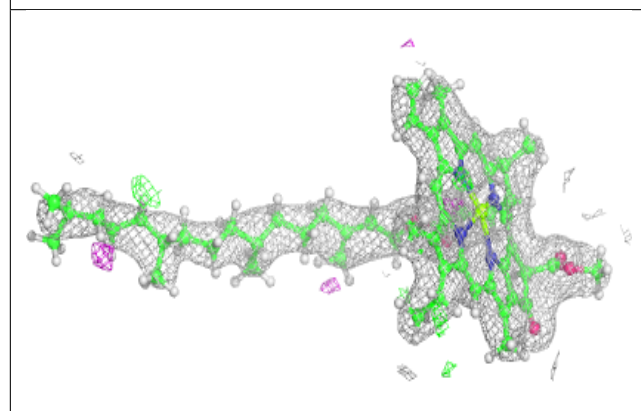
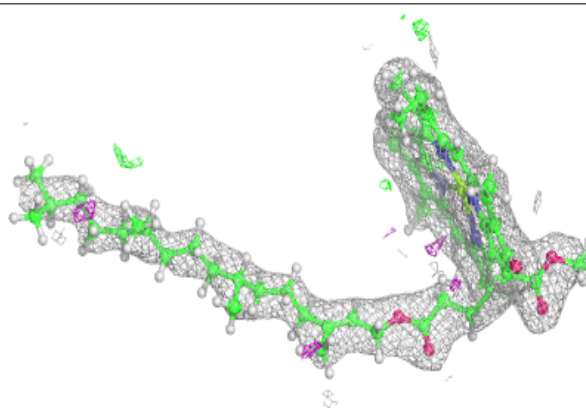


Electron density around BCR A 405:

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

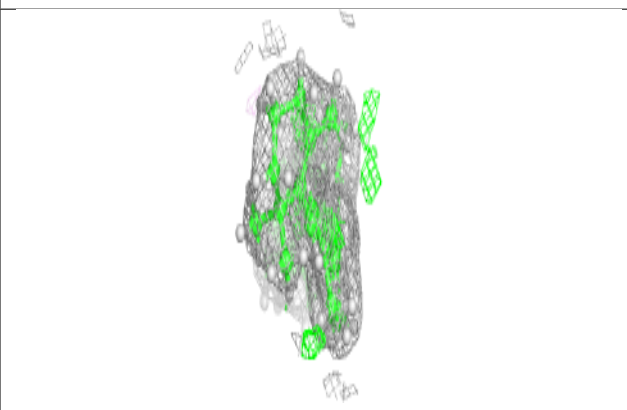
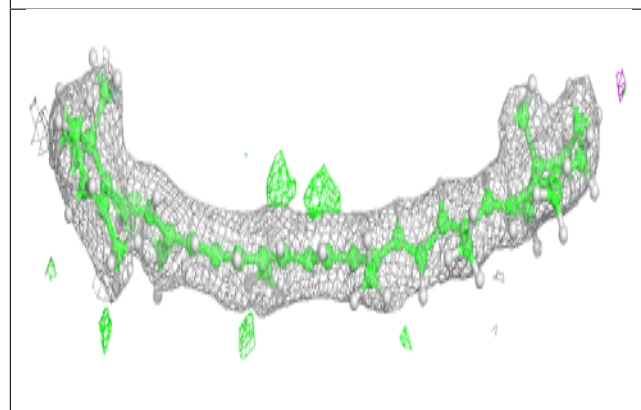
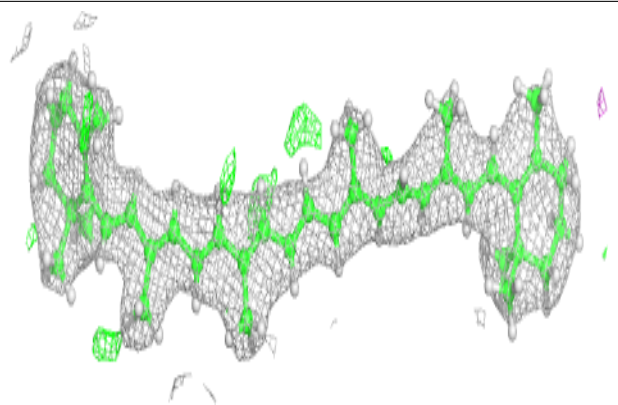
**Electron density around CLA B 707:**

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

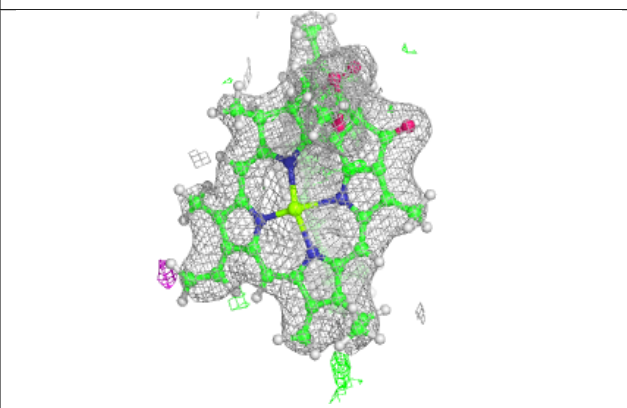
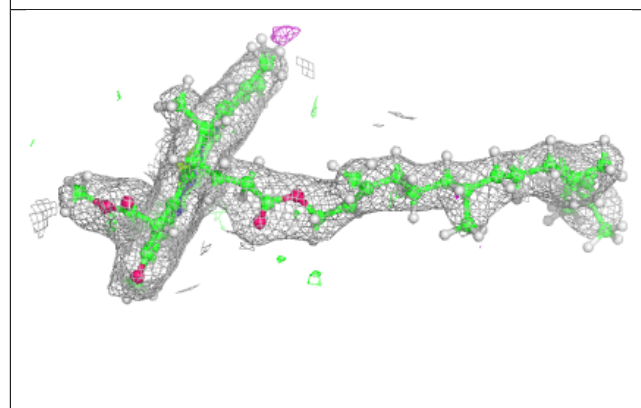
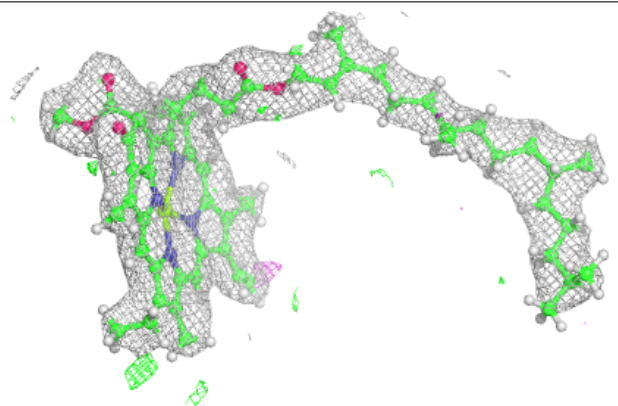


Electron density around BCR t 701:

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

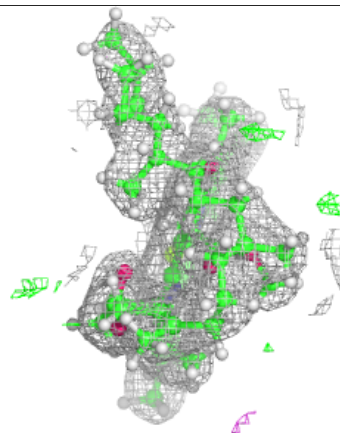
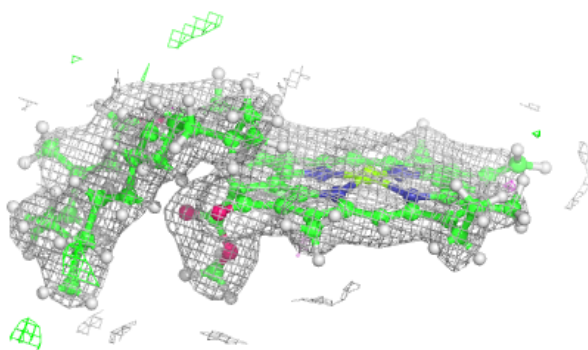
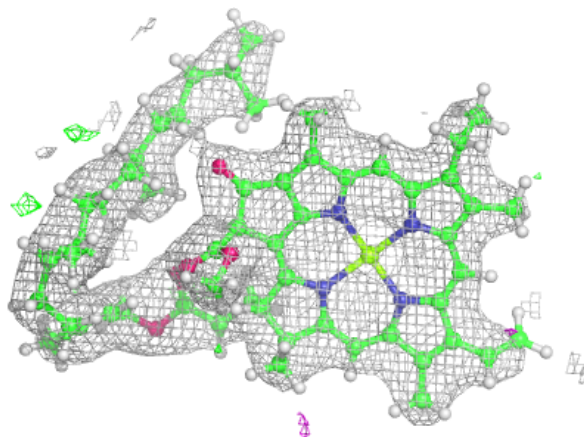
**Electron density around CLA B 709:**

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



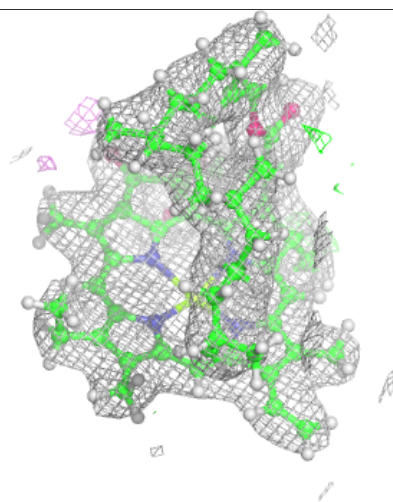
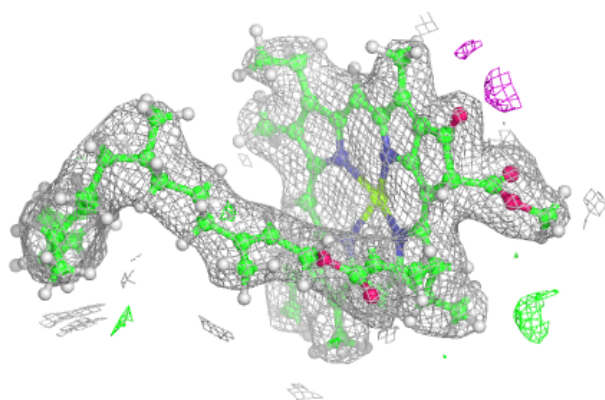
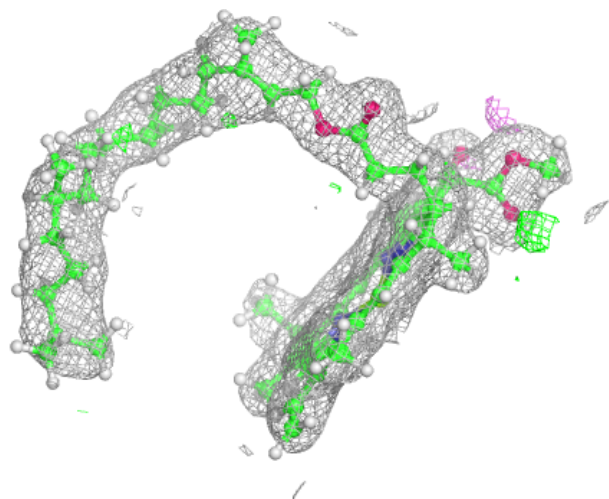
Electron density around CLA B 710:

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



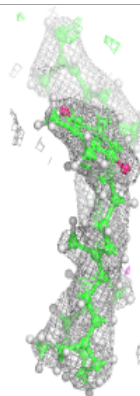
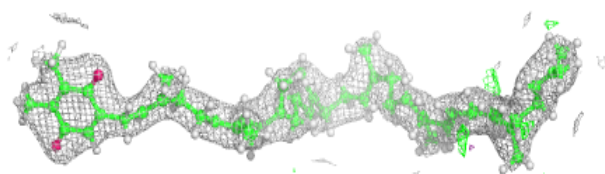
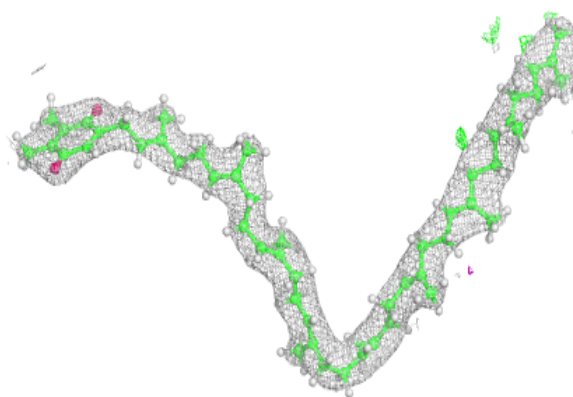
Electron density around CLA B 711:

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

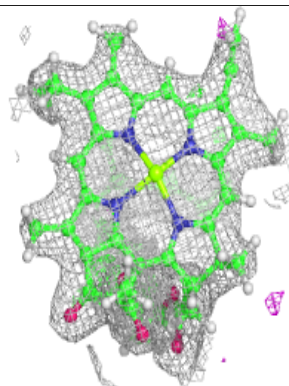
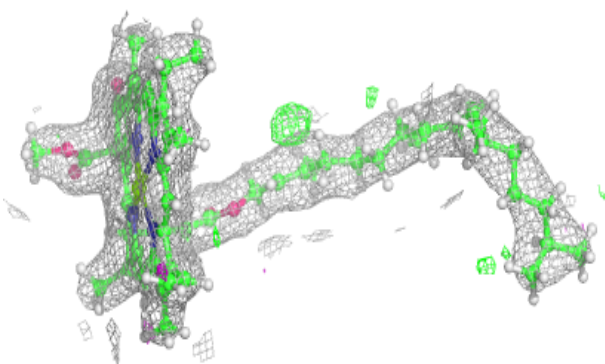
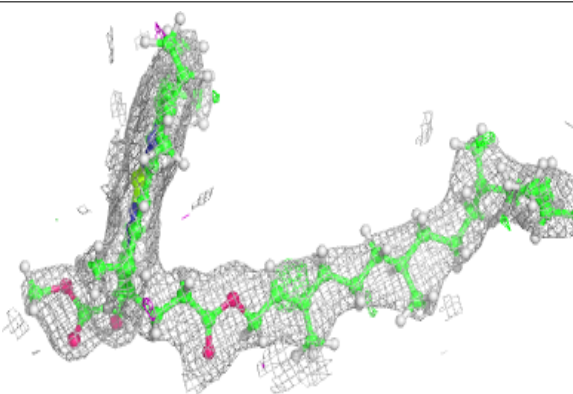


Electron density around PL9 d 404:

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

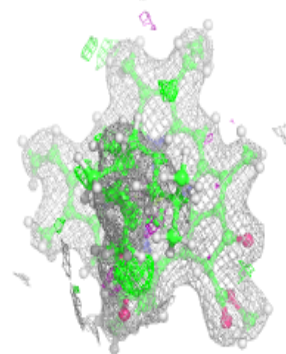
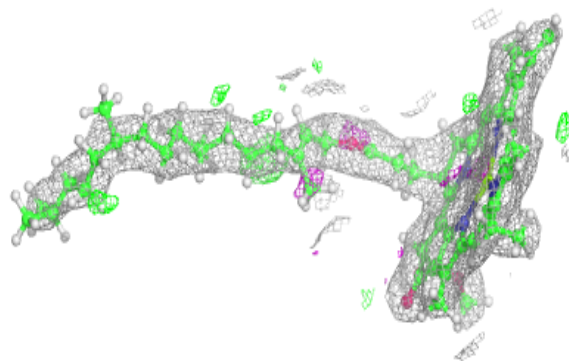
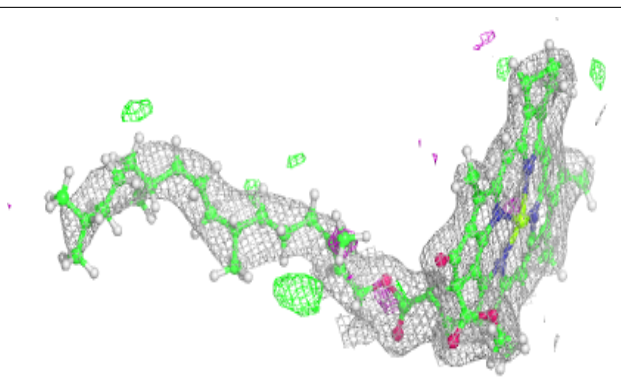
**Electron density around CLA b 705:**

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

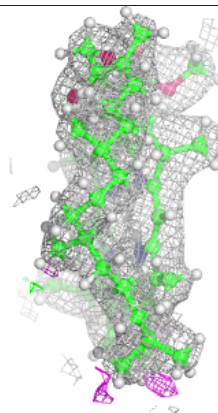
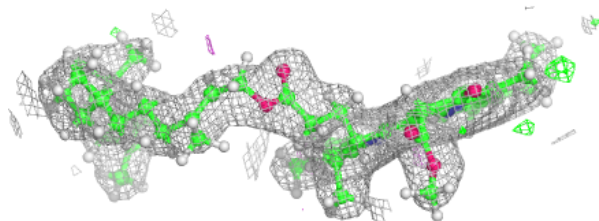
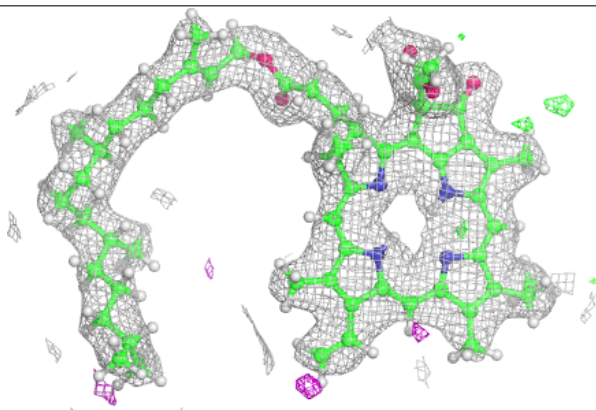


Electron density around CLA B 704:

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

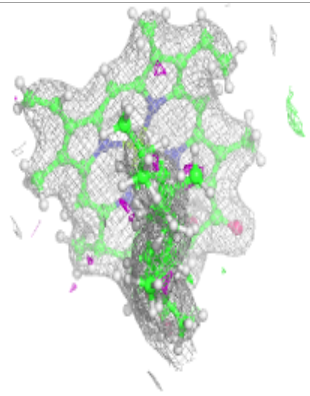
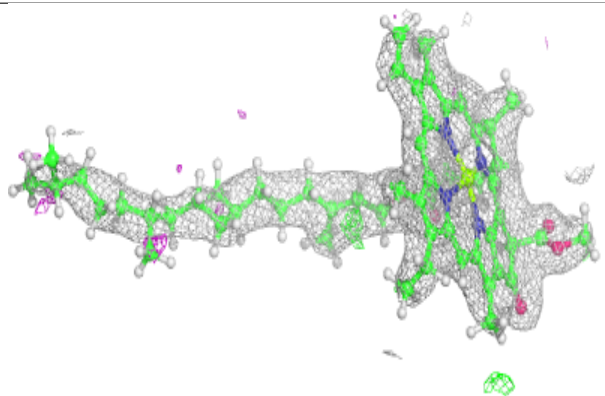
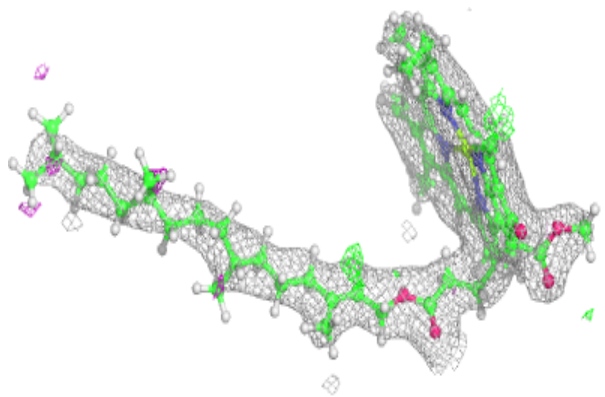
**Electron density around PHO D 406:**

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

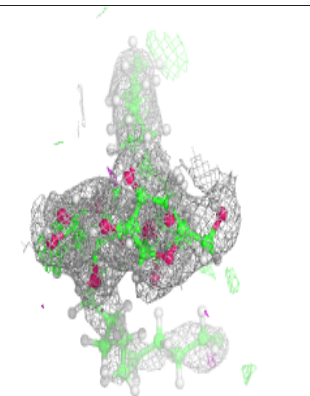
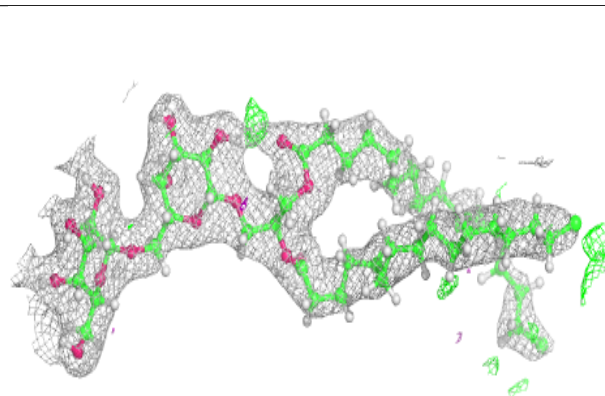
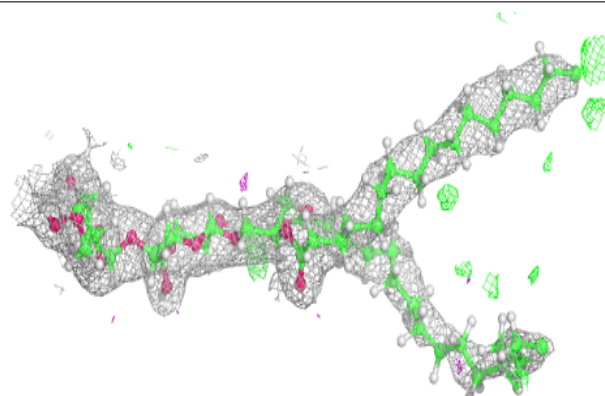


Electron density around CLA b 707:

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

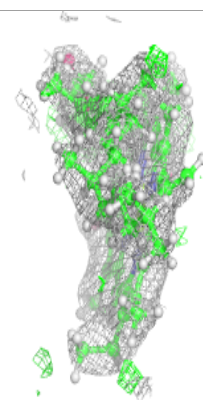
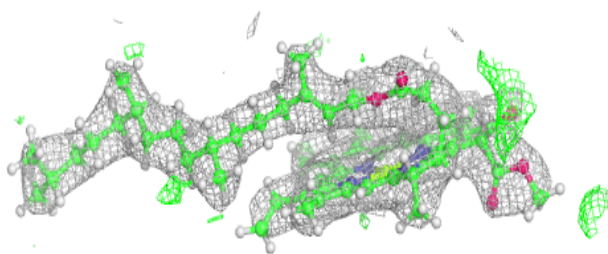
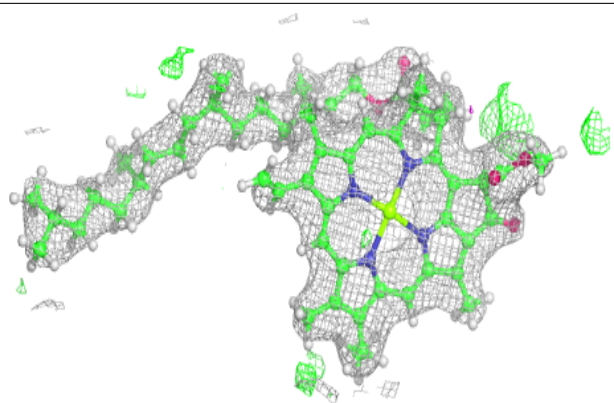
**Electron density around DGD c 517:**

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

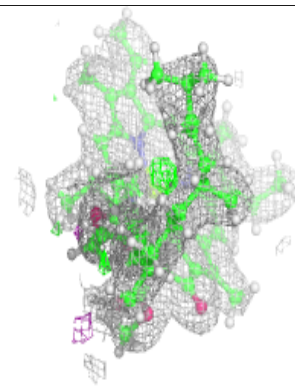
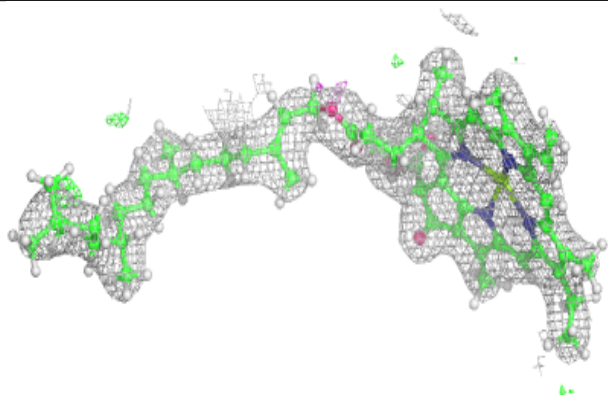
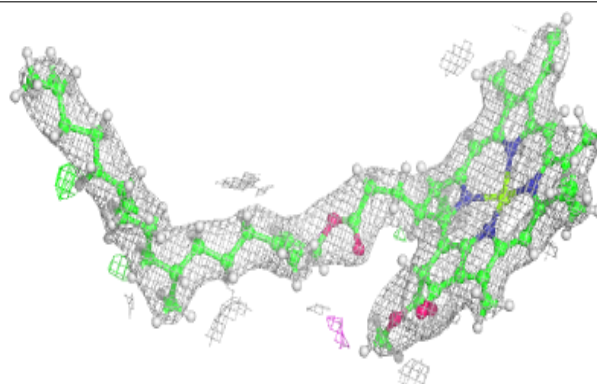


Electron density around CLA c 502:

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

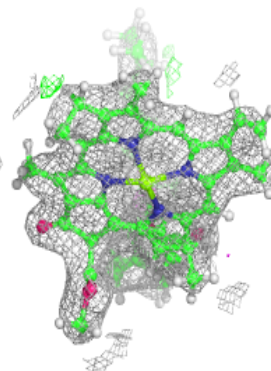
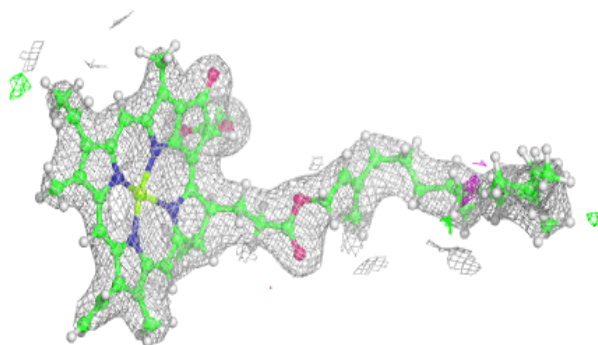
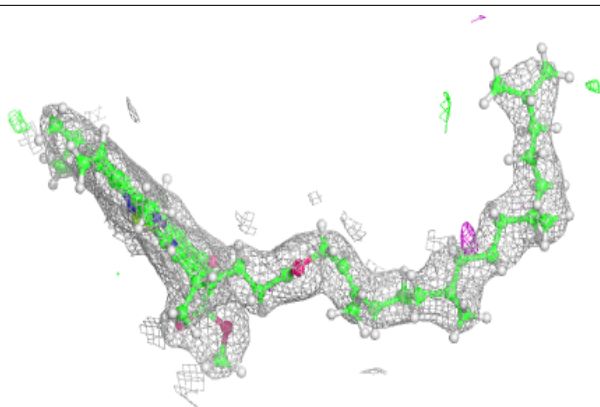
**Electron density around CLA a 403:**

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

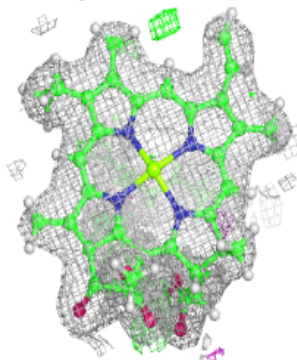
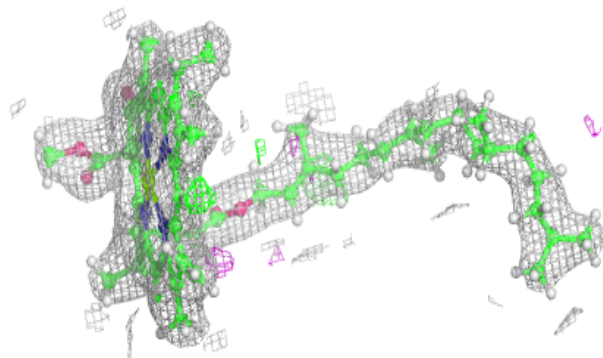
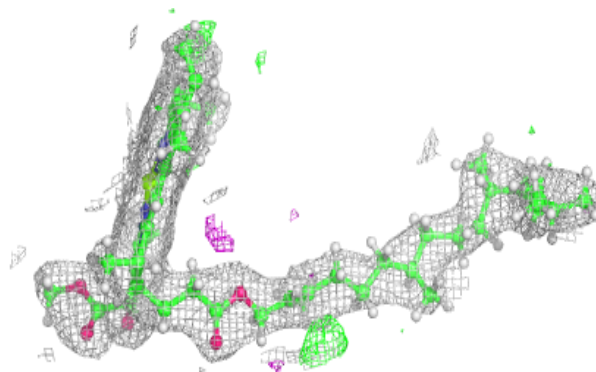


Electron density around CLA d 401:

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

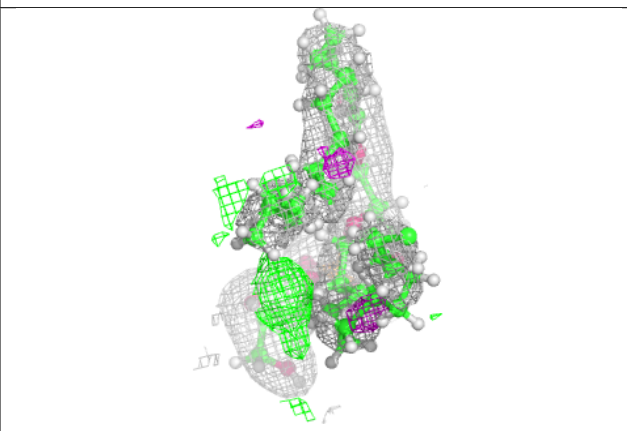
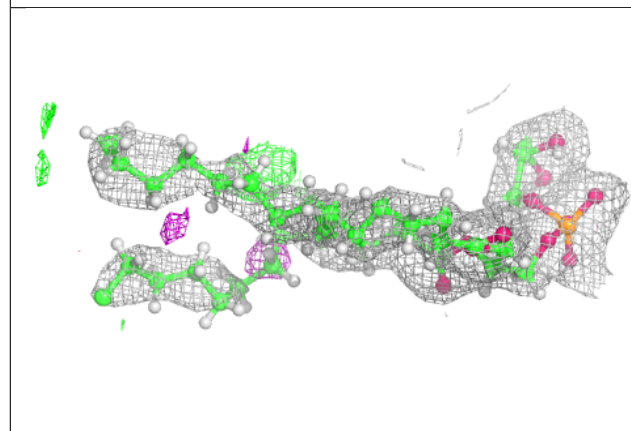
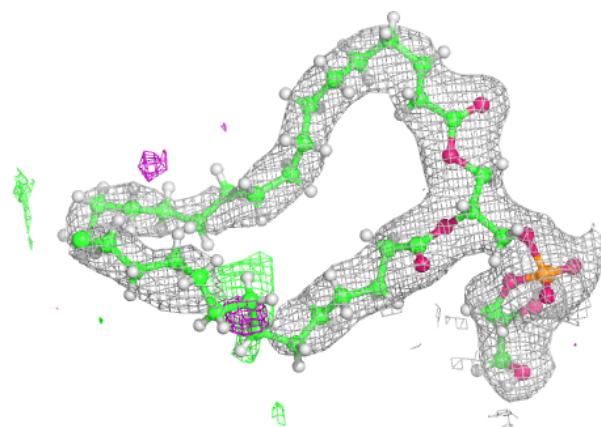
**Electron density around CLA B 705:**

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



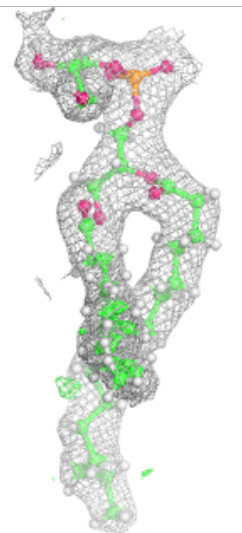
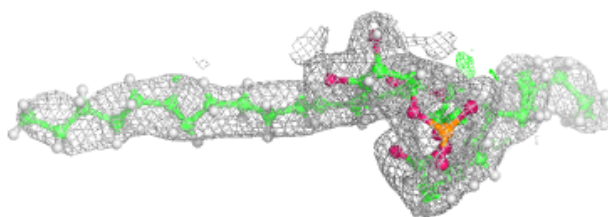
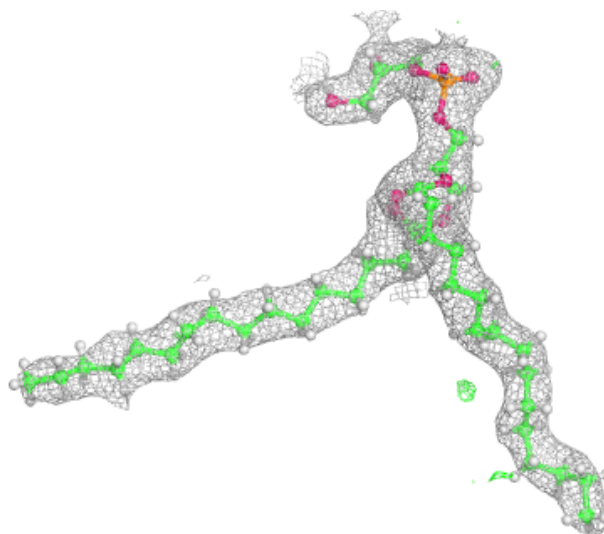
Electron density around LHG D 411:

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



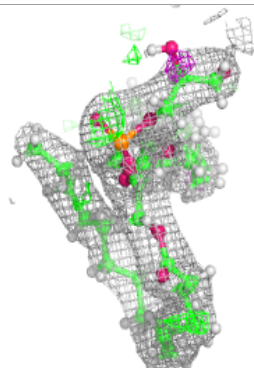
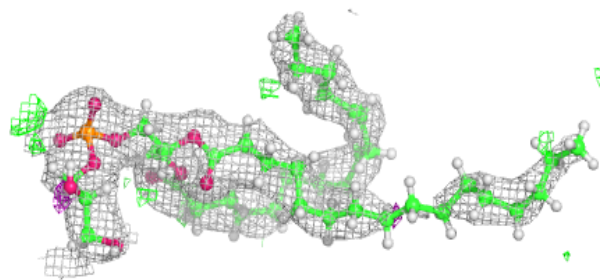
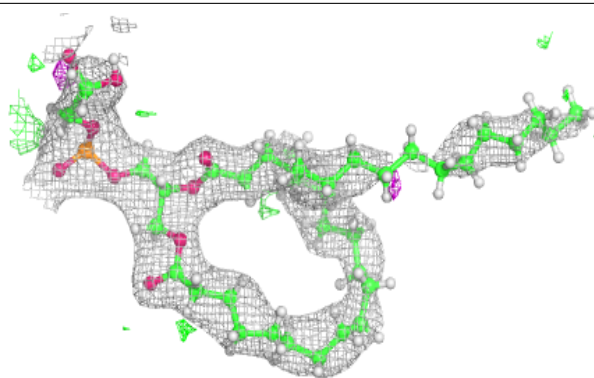
Electron density around LHG L 101:

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

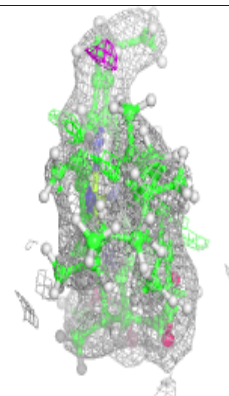
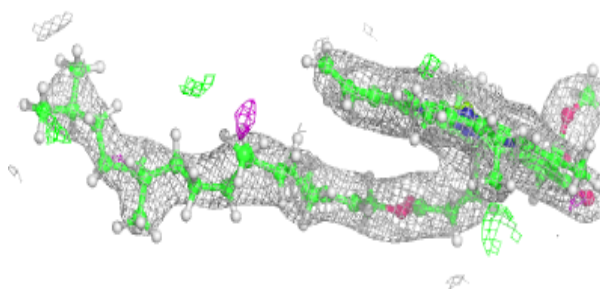
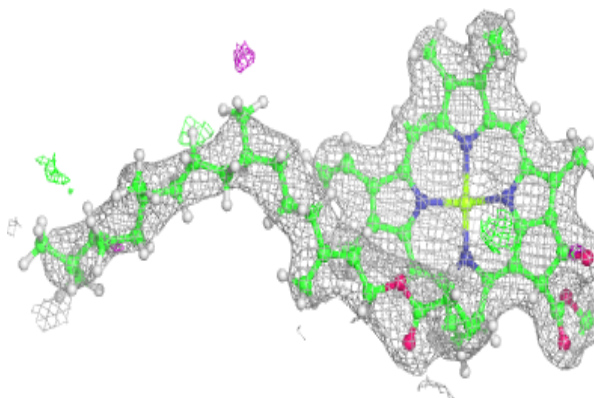


Electron density around LHG a 412:

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

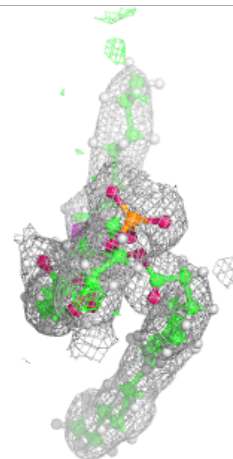
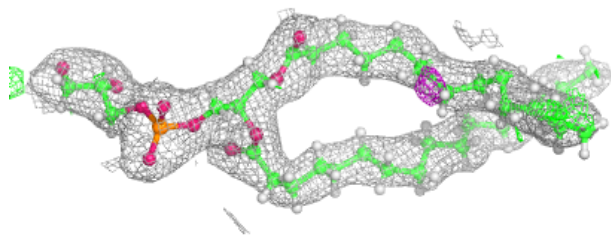
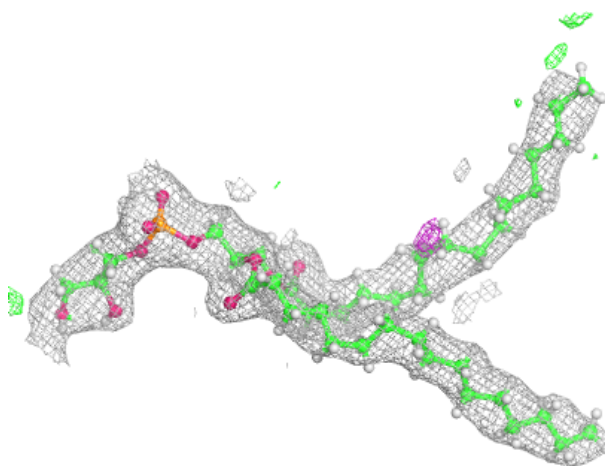
**Electron density around CLA B 703:**

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



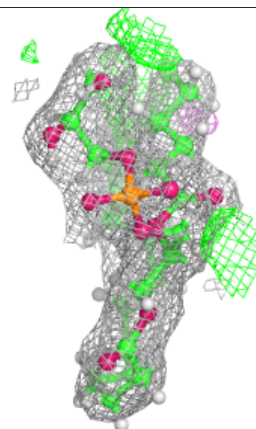
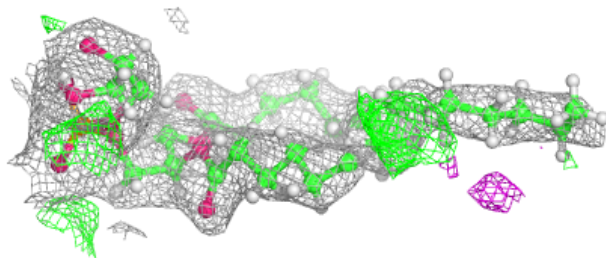
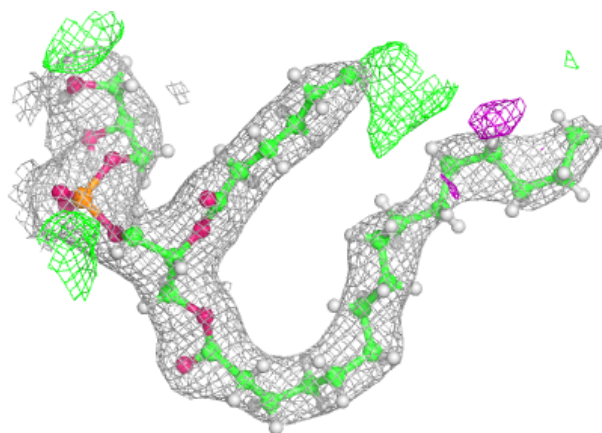
Electron density around LHG d 406:

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



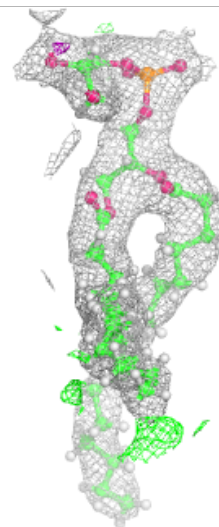
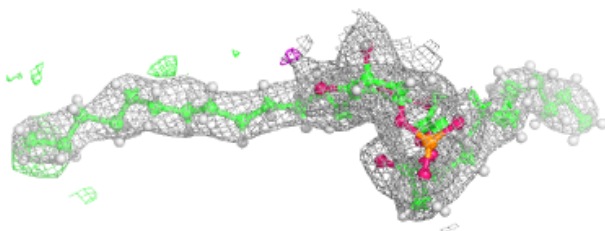
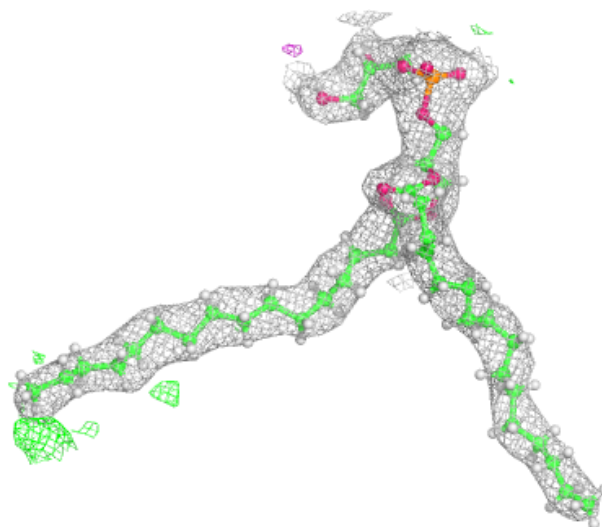
Electron density around LHG d 407:

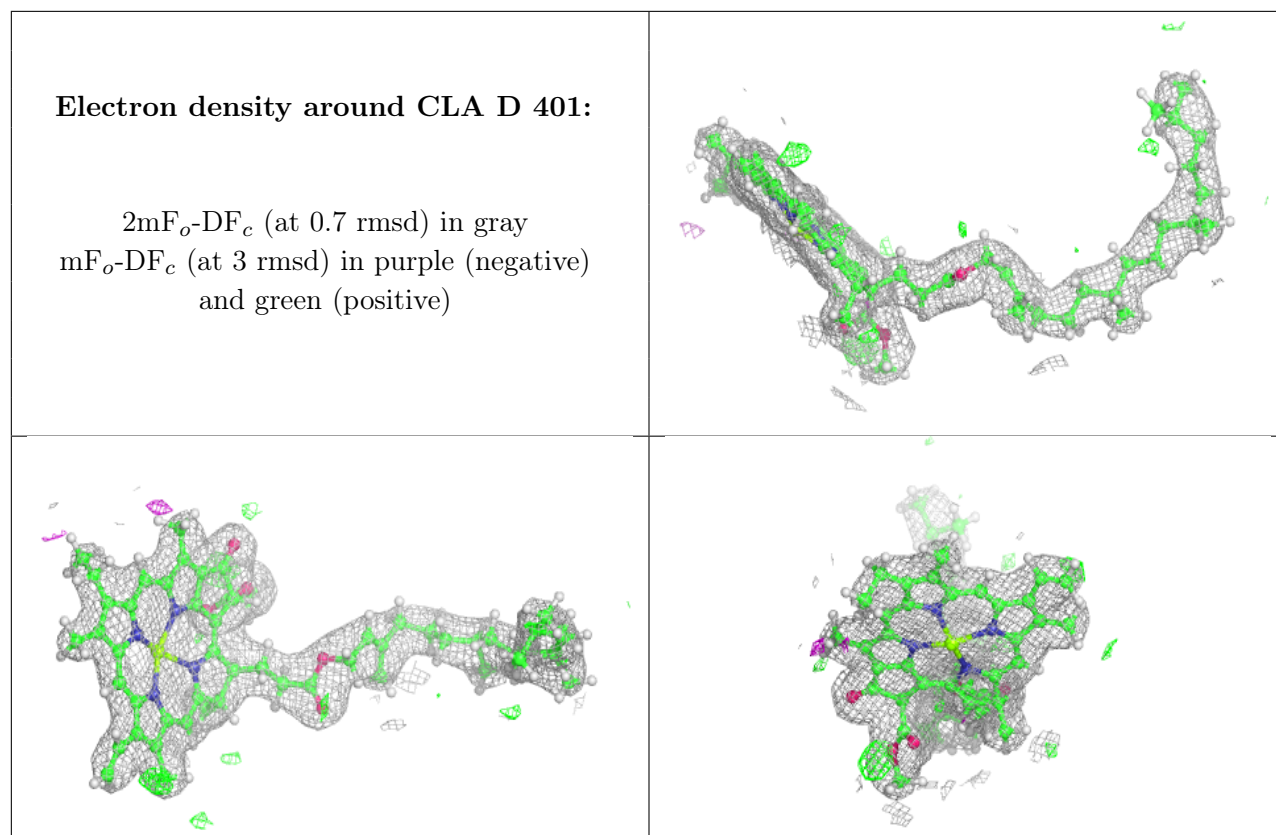
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG 1 101:

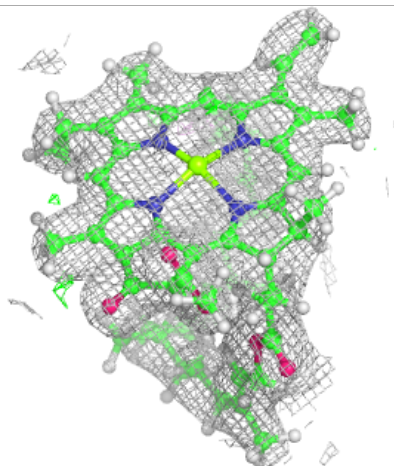
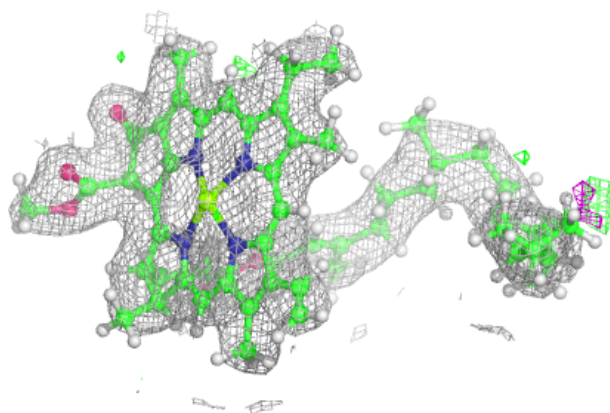
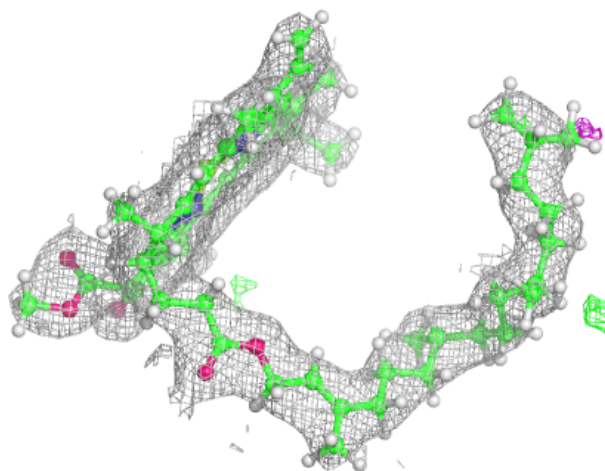
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





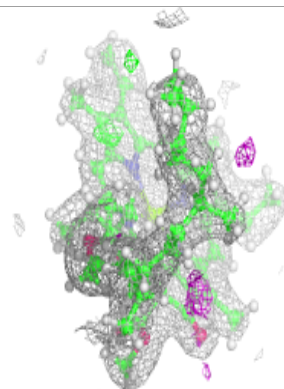
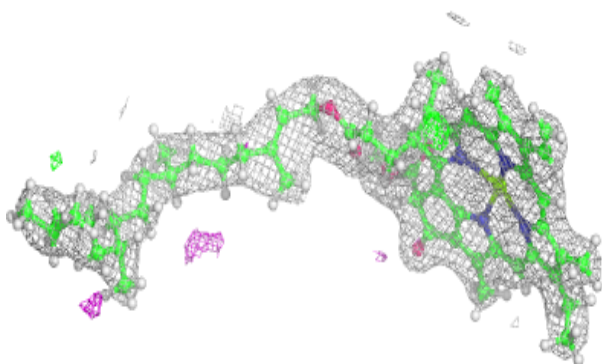
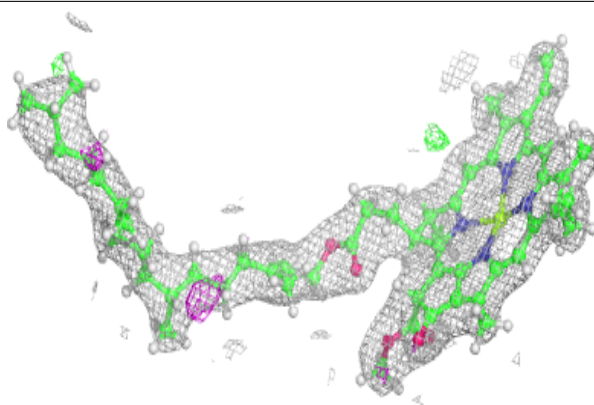
Electron density around CLA b 711:

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

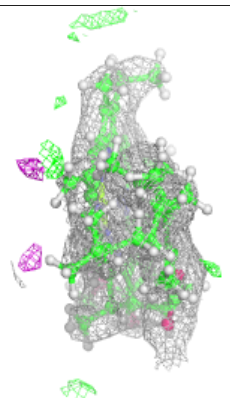
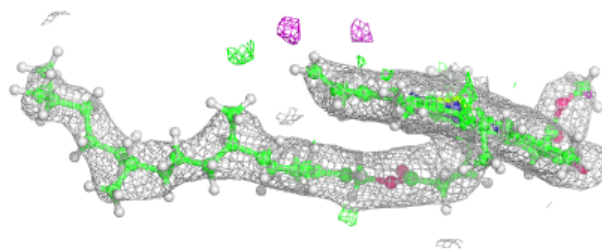
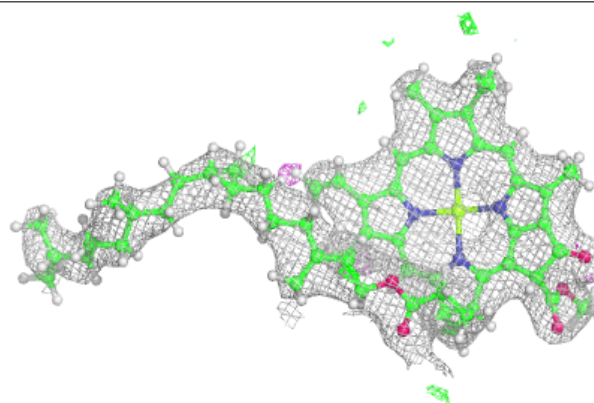


Electron density around CLA A 402:

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

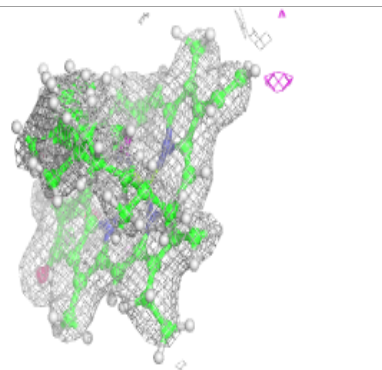
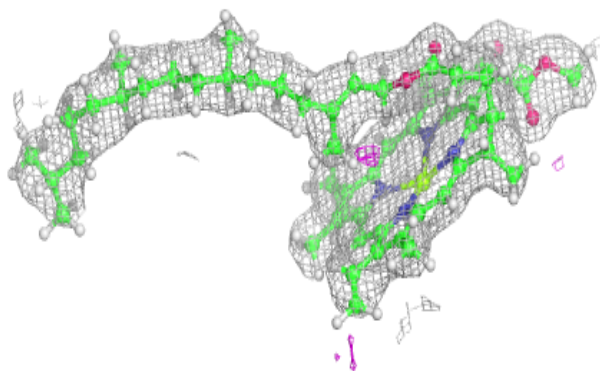
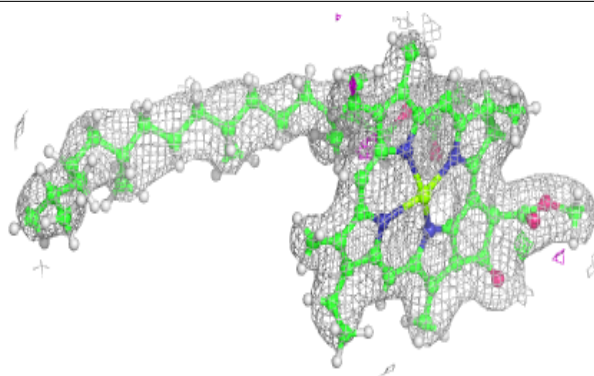
**Electron density around CLA b 703:**

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

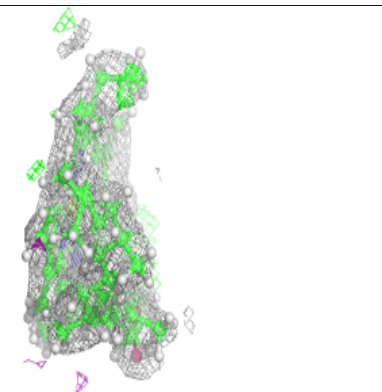
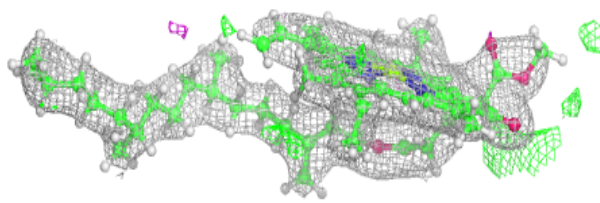
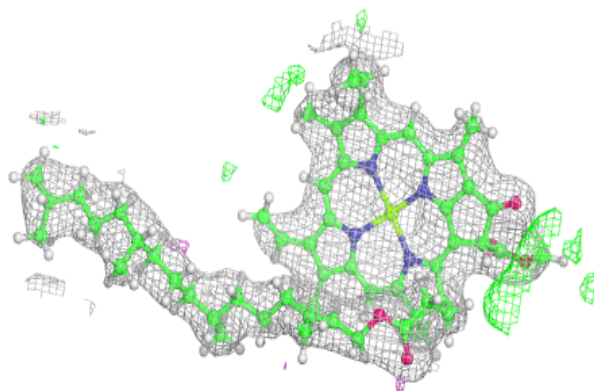


Electron density around CLA B 708:

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

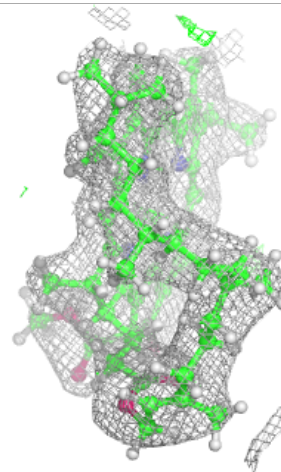
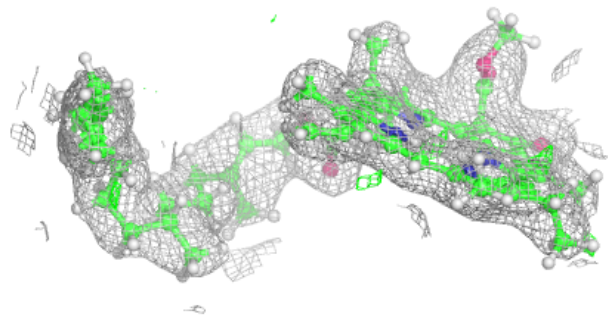
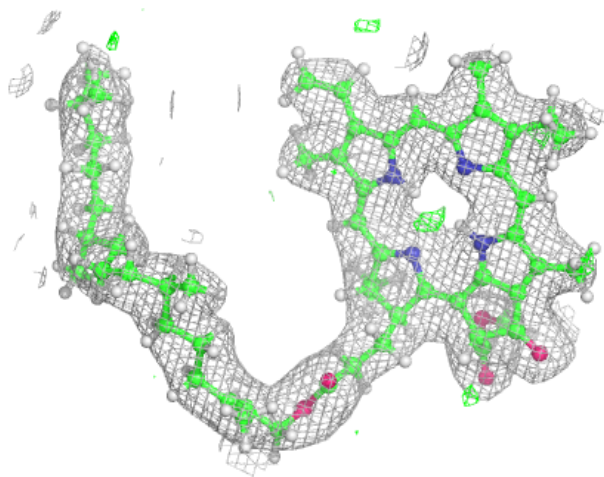
**Electron density around CLA C 502:**

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



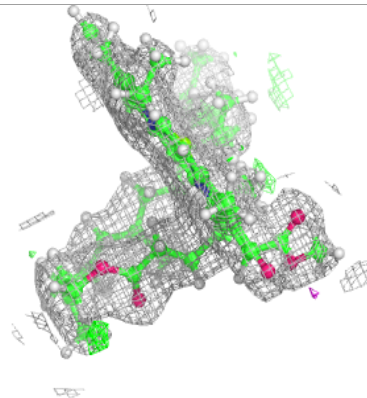
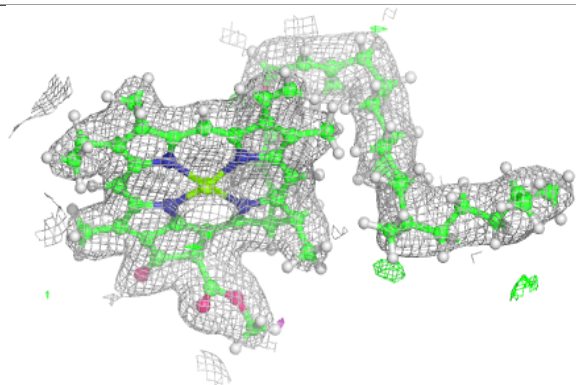
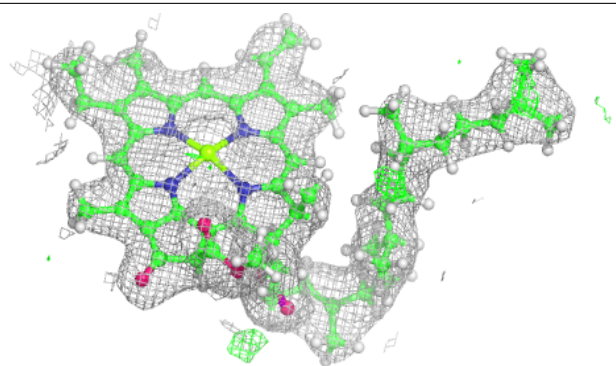
Electron density around PHO D 407:

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



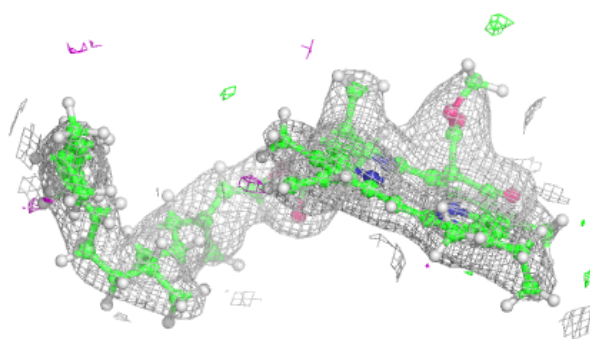
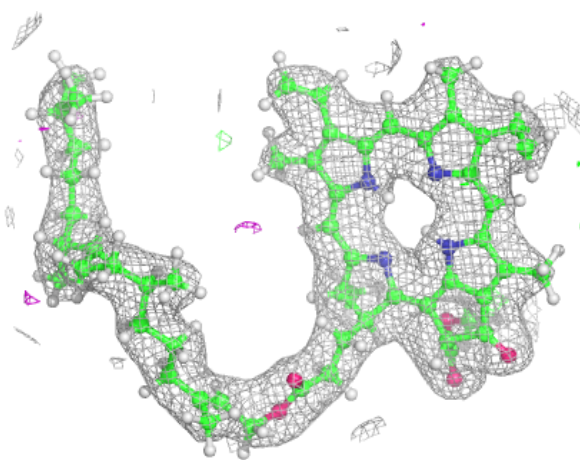
Electron density around CLA a 401:

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



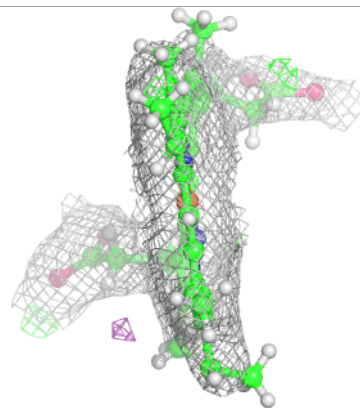
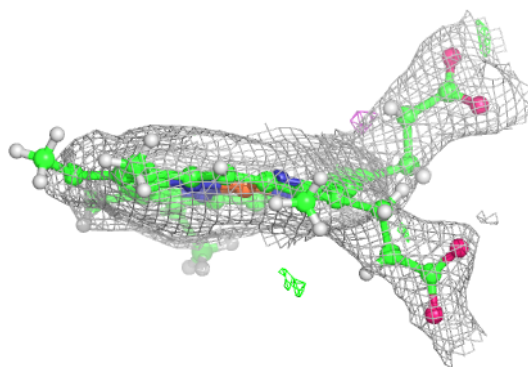
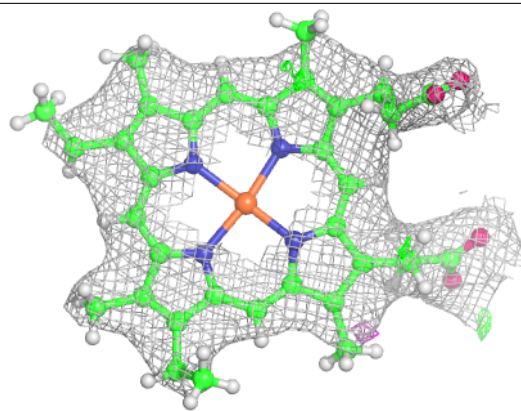
Electron density around PHO d 405:

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

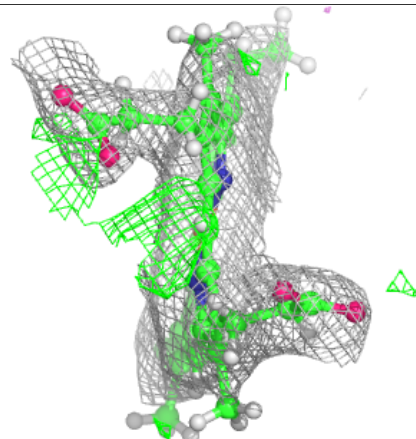
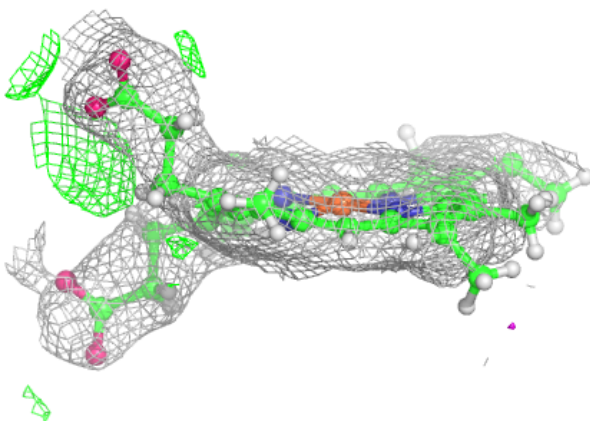
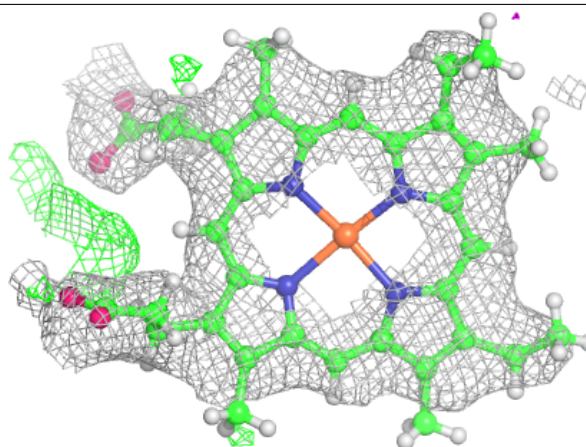


Electron density around HEC E 103:

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

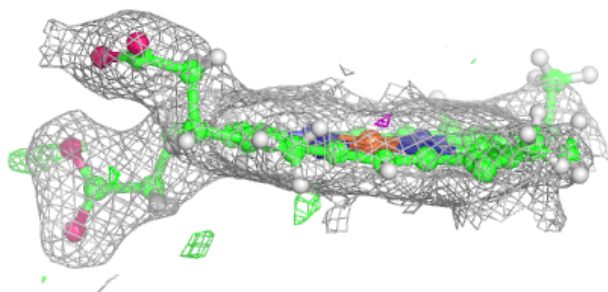
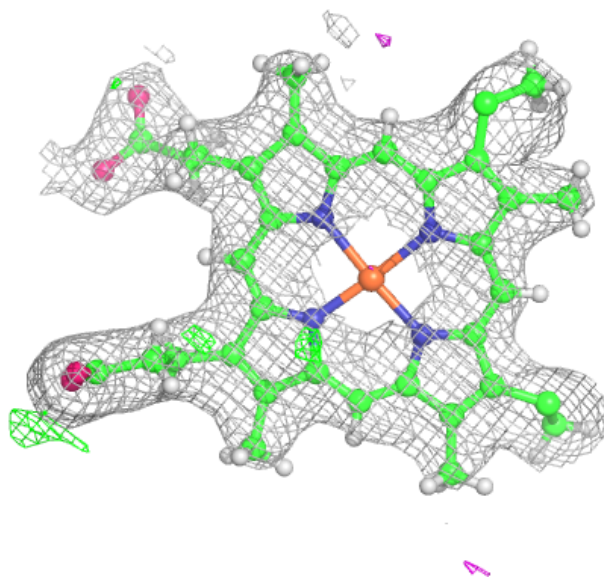
**Electron density around HEC e 101:**

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



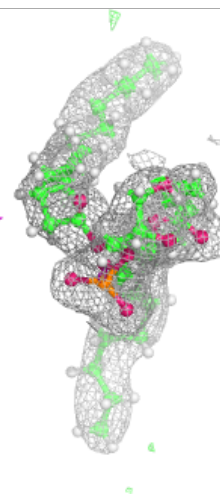
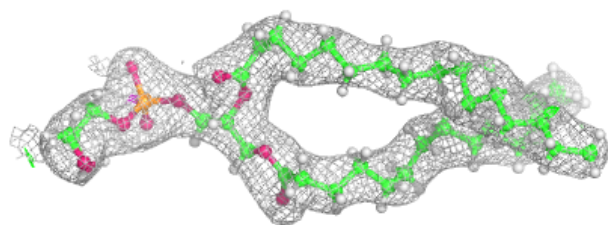
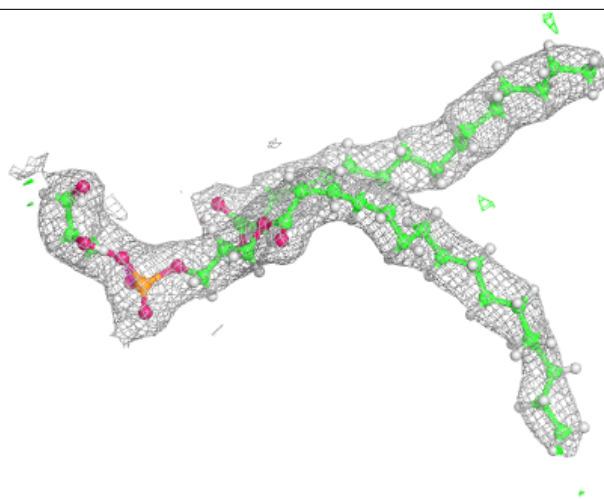
Electron density around HEC V 201:

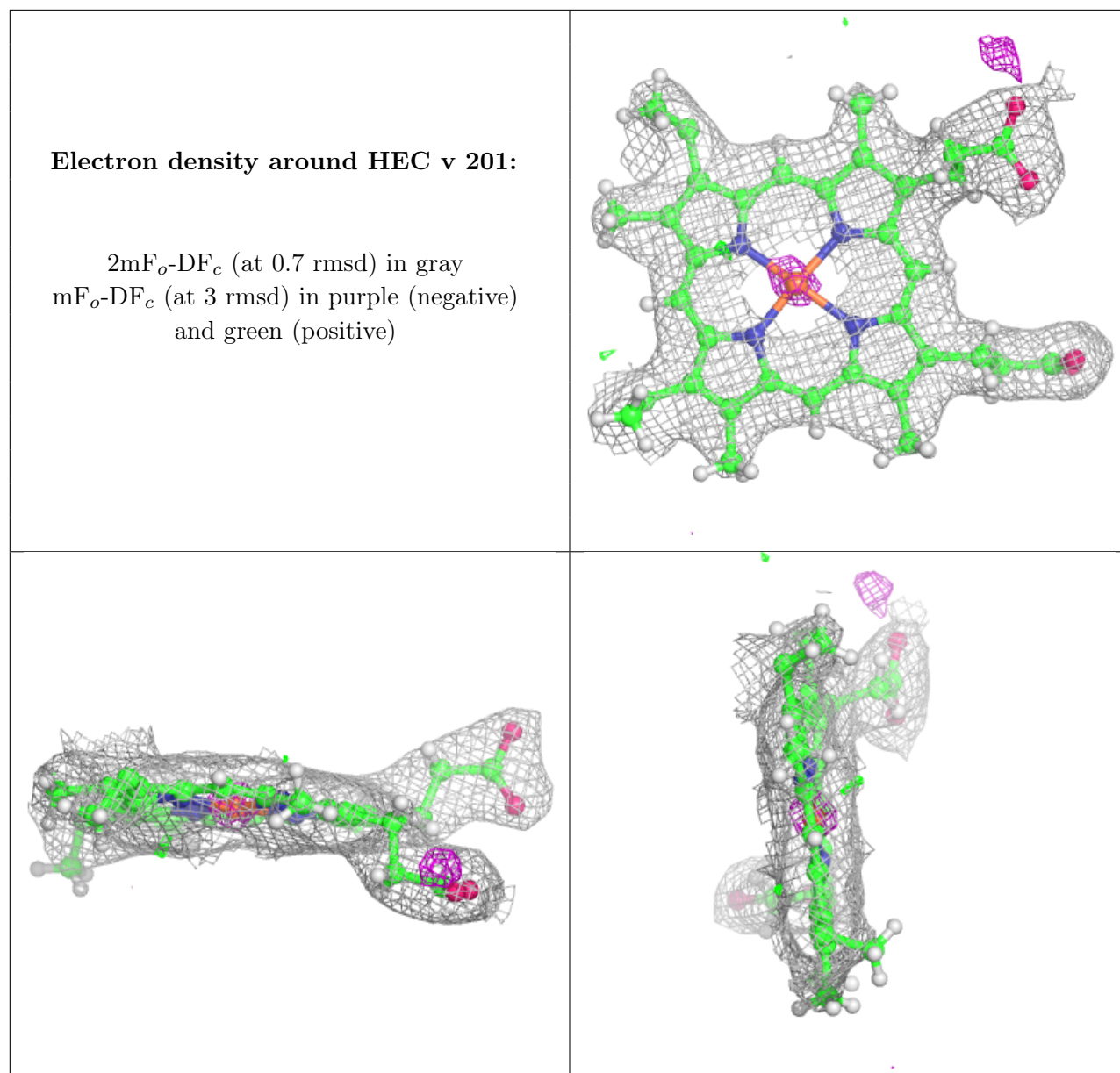
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG D 410:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.