



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2023 – 01:53 PM EDT

PDB ID : 8F4D
Title : RT XFEL structure of Photosystem II 50 microseconds after the third illumination at 2.15 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.15 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

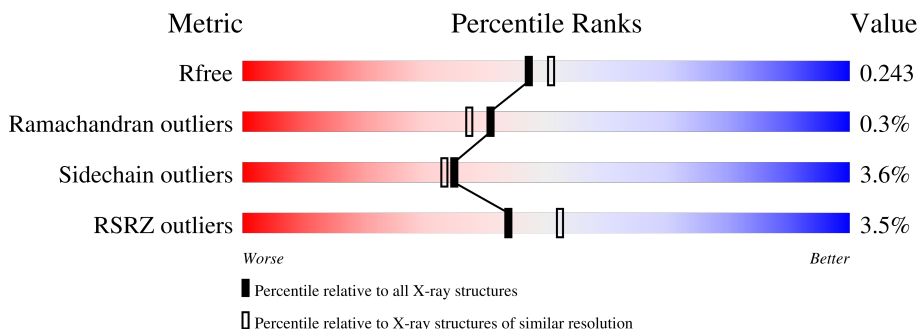
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	 96%
1	a	344	 94%

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buster-report : 1.1.7 (2018)
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
 Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35

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Mol	Chain	Length	Quality of chain
2	B	510	2% 97% ..
2	b	510	3% 97% ..
3	C	461	94% ..
3	c	461	3% 95% ..
4	D	352	95% ..
4	d	352	94% ..
5	E	84	7% 92% 6% .
5	e	84	5% 94% ..
6	F	45	2% 76% 24%
6	f	45	2% 69% 7% 24%
7	H	66	2% 95% ..
7	h	66	6% 88% 8% 5%
8	I	38	3% 87% 8% 5%
8	i	38	5% 92% 5%
9	J	40	8% 88% 10%
9	j	40	10% 85% 5% 10%
10	K	46	2% 74% 7% 20%
10	k	46	2% 76% 20%
11	L	37	100%
11	l	37	5% 86% 11% .
12	M	36	86% 6% 8%
12	m	36	86% 11%
13	O	272	6% 86% 10%
13	o	272	6% 87% 10%
14	T	32	3% 91% 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 52853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 3113	C 2030	N 513	O 551	S 19	0	64	0
1	a	334	Total 3110	C 2027	N 513	O 551	S 19	0	64	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	Total 4005	C 2631	N 666	O 695	S 13	0	4	0
2	b	505	Total 3978	C 2610	N 665	O 690	S 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	442	Total 3509	C 2302	N 586	O 607	S 14	0	11	0
3	c	451	Total 3583	C 2343	N 602	O 624	S 14	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	Total 2731	C 1809	N 446	O 464	S 12	0	2	0
4	d	341	Total 2737	C 1813	N 446	O 466	S 12	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	128	35	30	3			
17	y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O	S	0	0	0
			286	191	46	49				

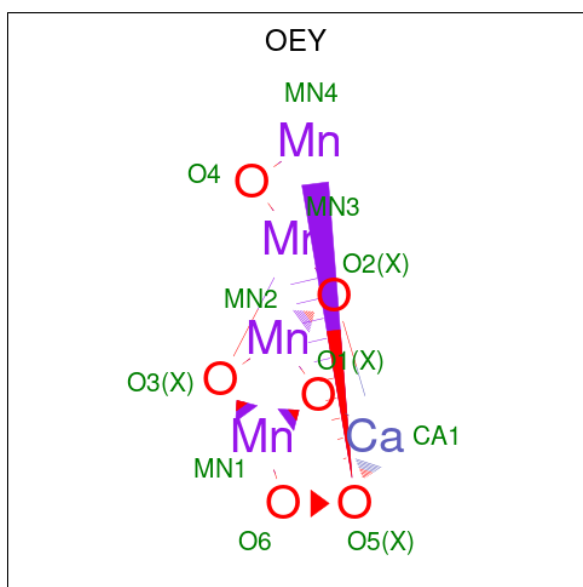
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

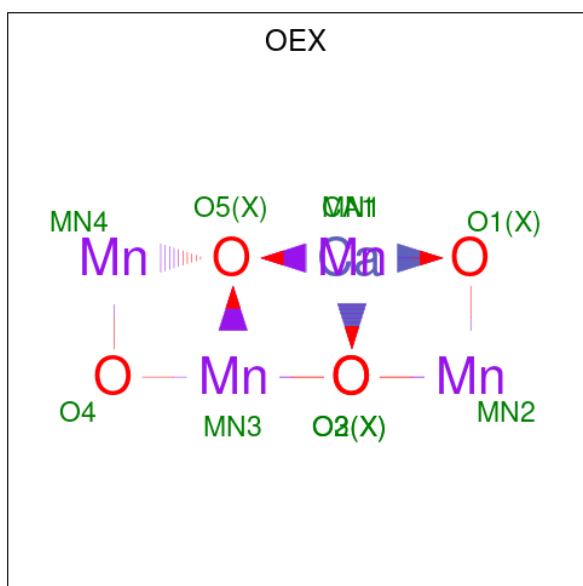
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O	S	0	0	0
			246	166	43	37				

- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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

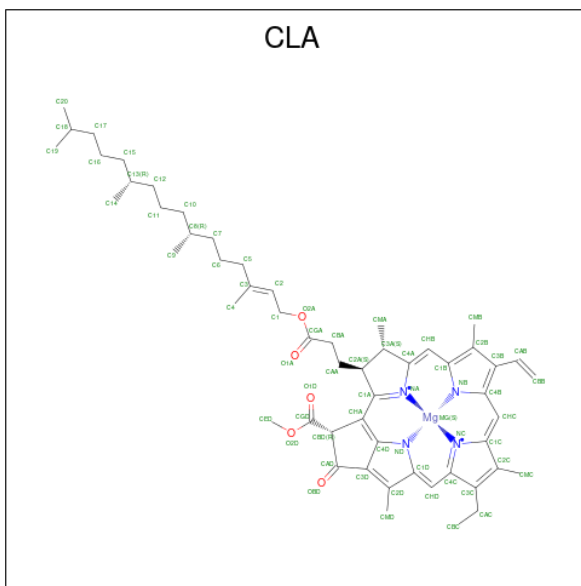
- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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

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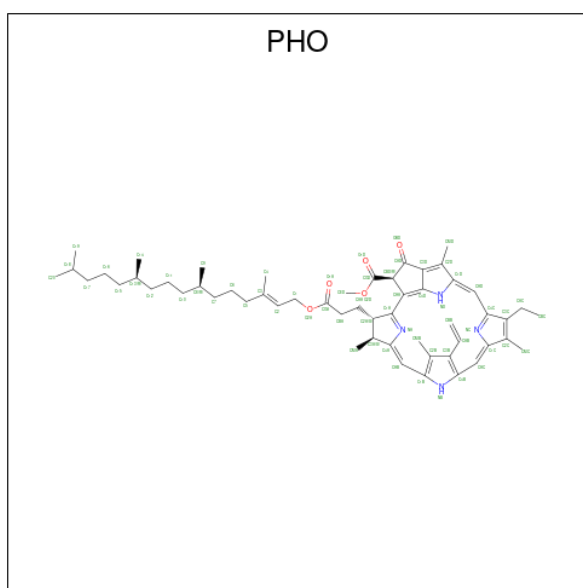
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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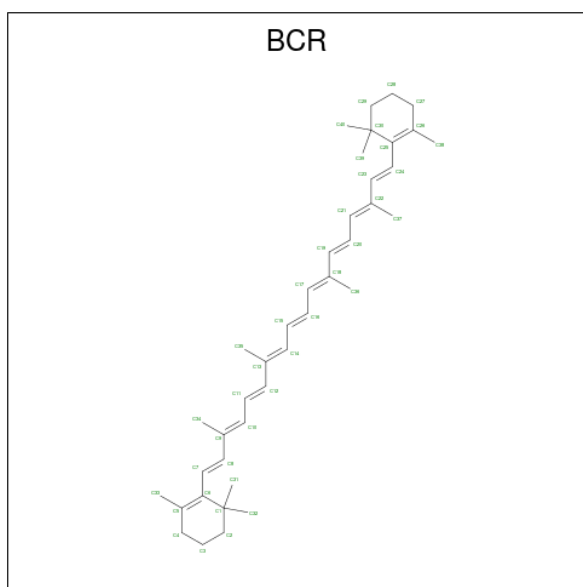
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



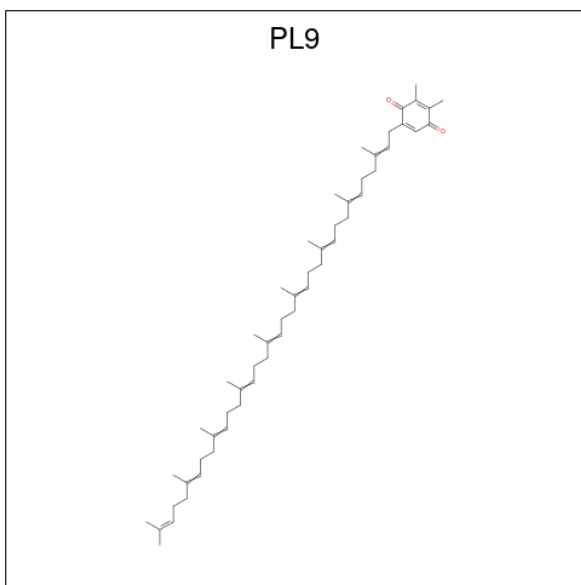
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



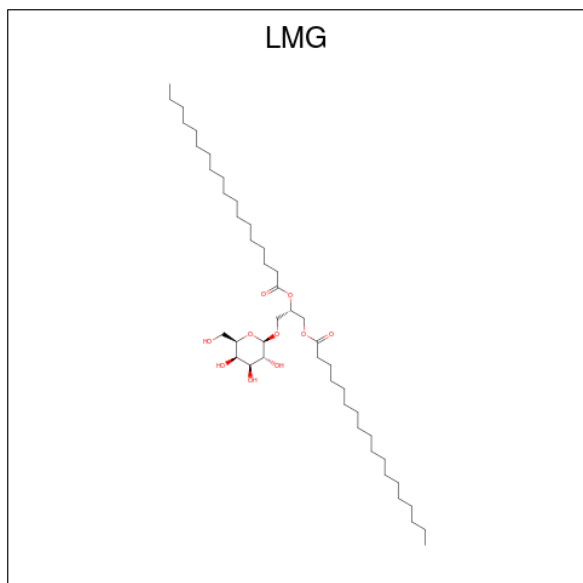
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



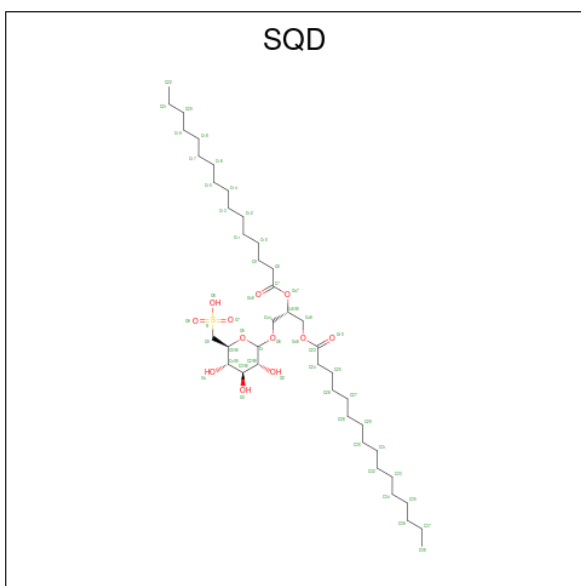
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C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

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

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



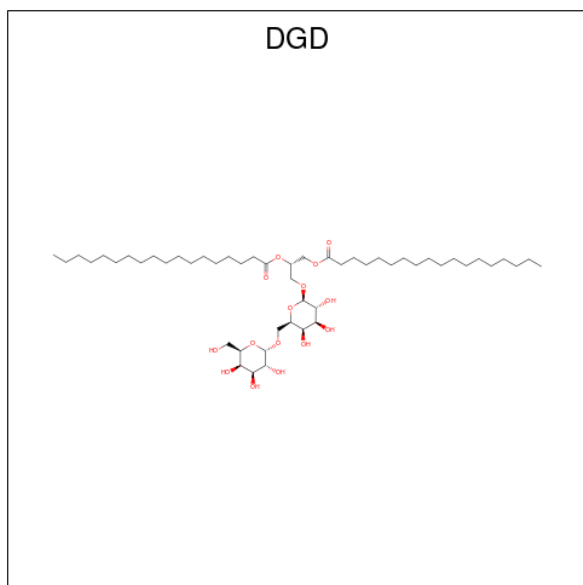
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	L	1	Total	C	O	S	0	0
			49	36	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	f	1	Total	C	O	S	0	0
		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

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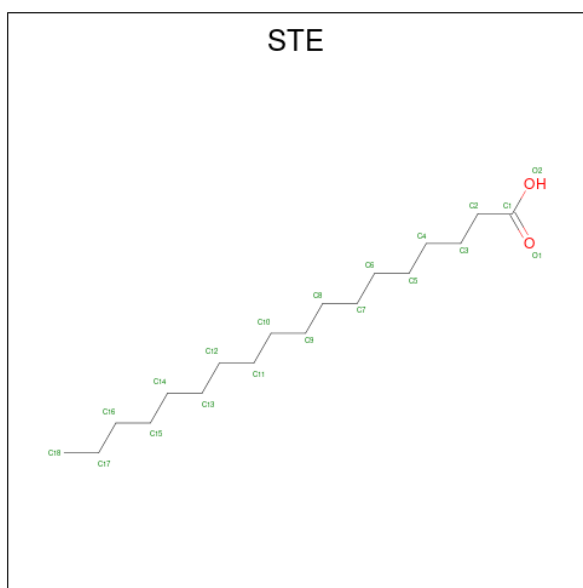
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
30	t	1	36	31	5	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



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

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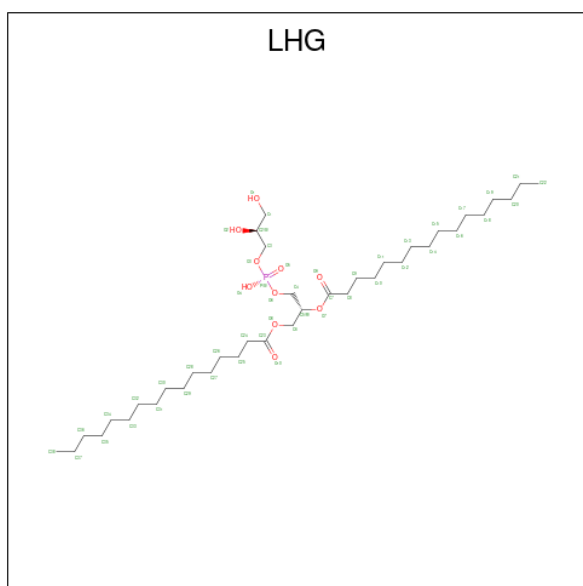
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 20 18 2	0	0
32	R	1	Total C O 12 10 2	0	0
32	a	1	Total C 10 10	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C 16 16	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 15 15	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	c	1	Total C O 12 10 2	0	0
32	d	1	Total C O 17 15 2	0	0
32	d	1	Total C O 20 18 2	0	0
32	j	1	Total C O 12 10 2	0	0
32	l	1	Total C 18 18	0	0
32	t	1	Total C O 14 12 2	0	0
32	t	1	Total C O 18 16 2	0	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



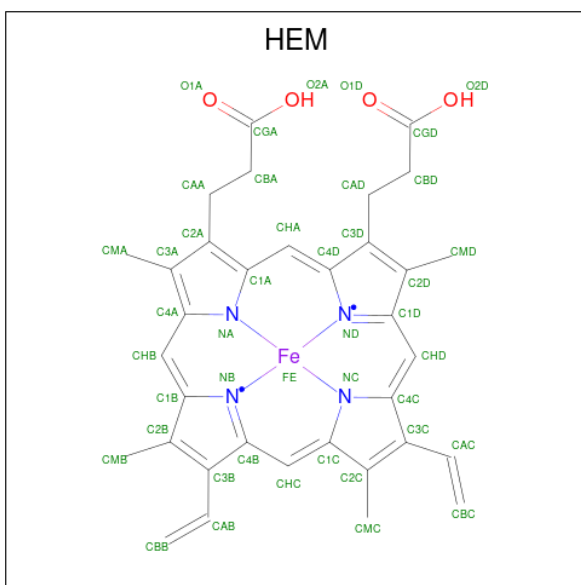
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	O	P	0	0
			49	38	10	1		

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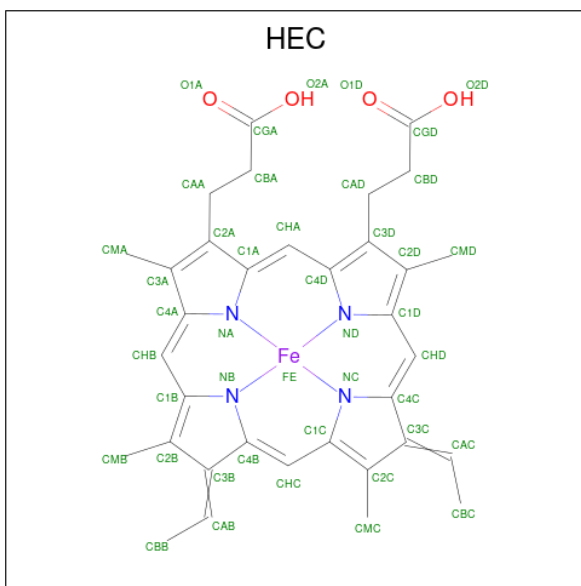
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	O	P	0	0
			47	36	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	L	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			39	28	10	1		
34	e	1	Total	C	O	P	0	0
			42	31	10	1		
34	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	120	Total	O	0	4
			124	124		
37	B	165	Total	O	0	0
			165	165		
37	C	112	Total	O	0	0
			112	112		
37	D	94	Total	O	0	0
			94	94		
37	E	22	Total	O	0	0
			22	22		
37	F	5	Total	O	0	0
			5	5		
37	H	24	Total	O	0	0
			24	24		
37	I	18	Total	O	0	0
			18	18		
37	J	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	K	2	Total O 2 2	0	0
37	L	8	Total O 8 8	0	0
37	M	7	Total O 7 7	0	0
37	O	66	Total O 66 66	0	0
37	T	6	Total O 6 6	0	0
37	U	30	Total O 30 30	0	0
37	V	45	Total O 45 45	0	0
37	Y	6	Total O 6 6	0	0
37	X	10	Total O 10 10	0	0
37	Z	5	Total O 5 5	0	0
37	R	9	Total O 9 9	0	0
37	a	103	Total O 107 107	0	4
37	b	132	Total O 132 132	0	0
37	c	128	Total O 128 128	0	0
37	d	77	Total O 77 77	0	0
37	e	14	Total O 14 14	0	0
37	f	2	Total O 2 2	0	0
37	h	20	Total O 20 20	0	0
37	i	10	Total O 10 10	0	0
37	j	7	Total O 7 7	0	0
37	k	5	Total O 5 5	0	0

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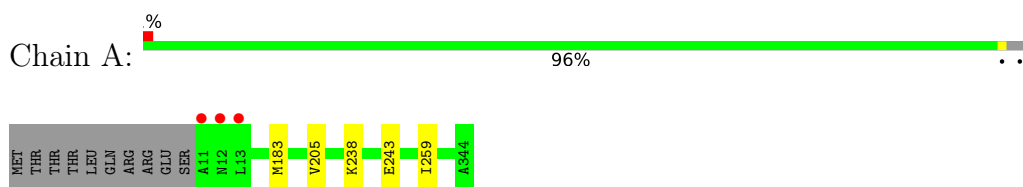
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	l	7	Total O 7 7	0	0
37	m	3	Total O 3 3	0	0
37	o	76	Total O 76 76	0	0
37	t	7	Total O 7 7	0	0
37	u	34	Total O 34 34	0	0
37	v	39	Total O 39 39	0	0
37	y	2	Total O 2 2	0	0
37	x	4	Total O 4 4	0	0
37	z	1	Total O 1 1	0	0
37	r	5	Total O 5 5	0	0

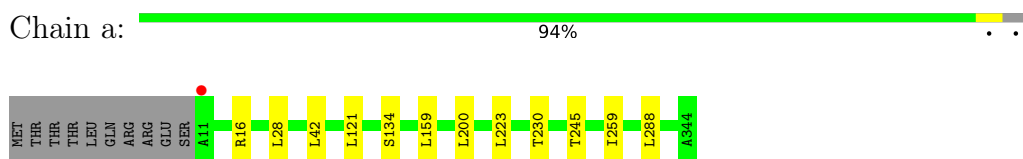
3 Residue-property plots [i](#)

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.

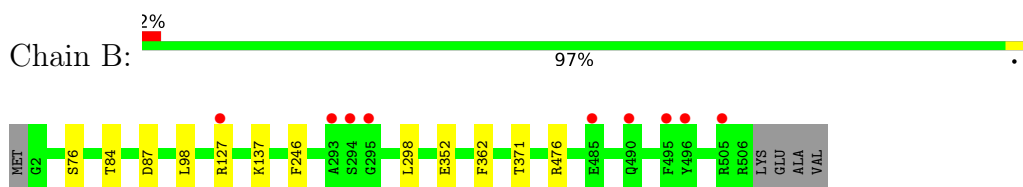
- Molecule 1: Photosystem II protein D1 1



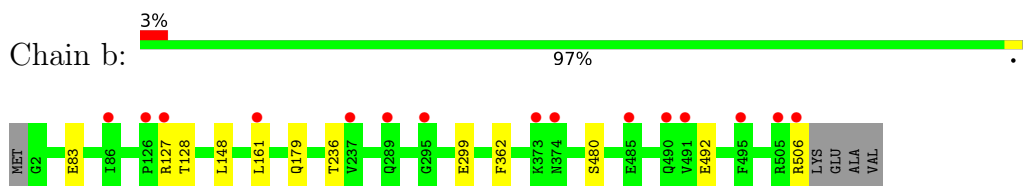
- Molecule 1: Photosystem II protein D1 1



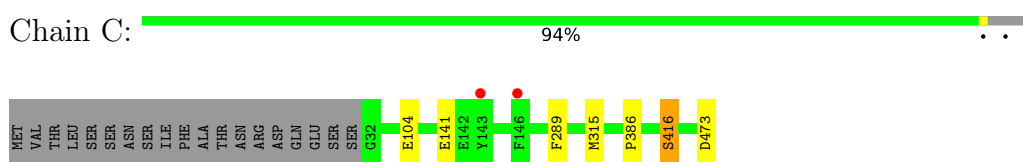
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



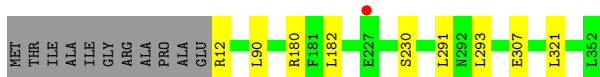
- Molecule 3: Photosystem II CP43 reaction center protein



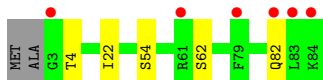
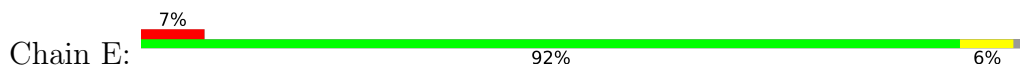
- Molecule 4: Photosystem II D2 protein



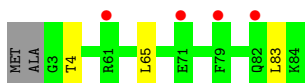
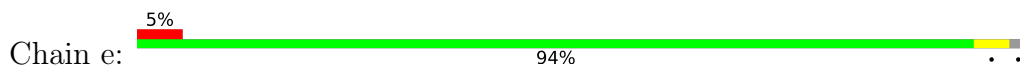
- Molecule 4: Photosystem II D2 protein



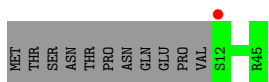
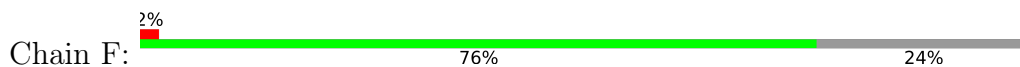
- Molecule 5: Cytochrome b559 subunit alpha



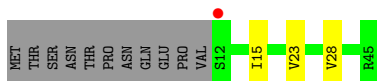
- Molecule 5: Cytochrome b559 subunit alpha



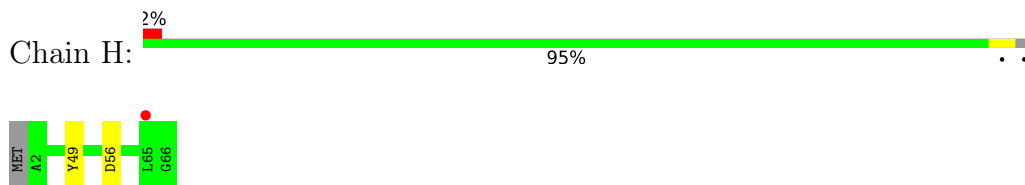
- Molecule 6: Cytochrome b559 subunit beta



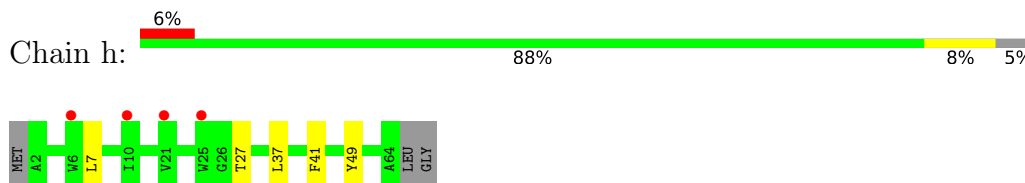
- Molecule 6: Cytochrome b559 subunit beta



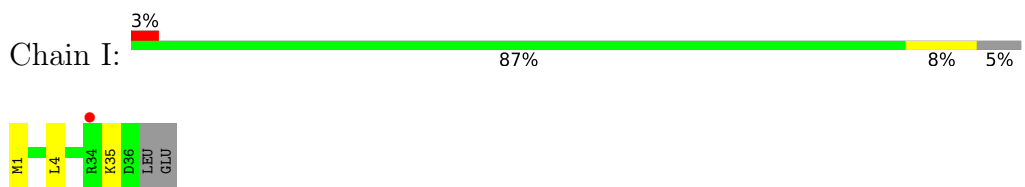
- Molecule 7: Photosystem II reaction center protein H



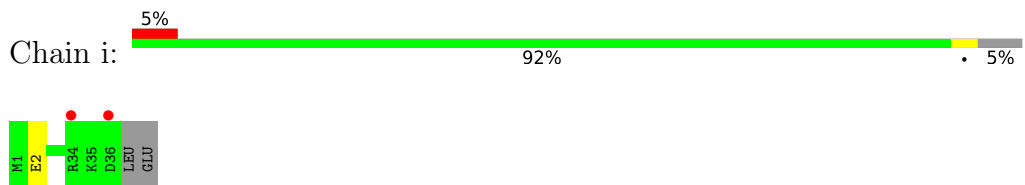
- Molecule 7: Photosystem II reaction center protein H



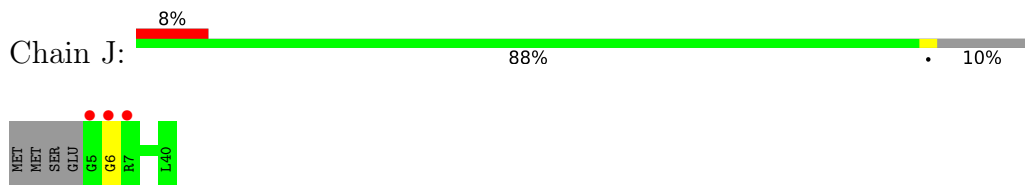
- Molecule 8: Photosystem II reaction center protein I



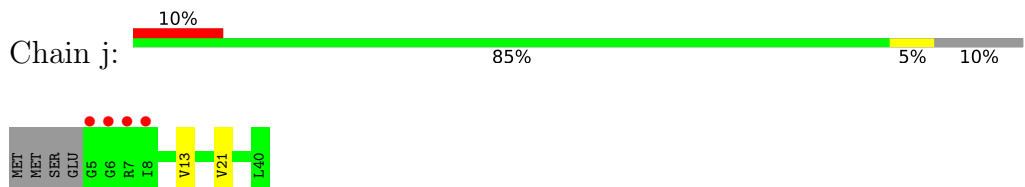
- Molecule 8: Photosystem II reaction center protein I



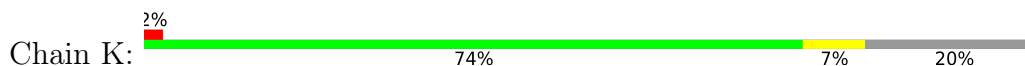
- Molecule 9: Photosystem II reaction center protein J

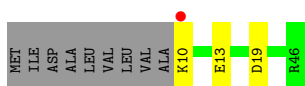


- Molecule 9: Photosystem II reaction center protein J

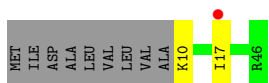
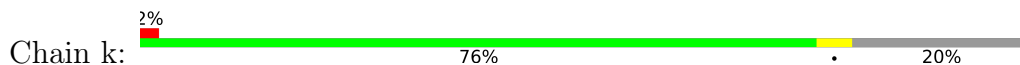


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

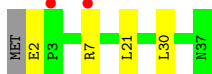
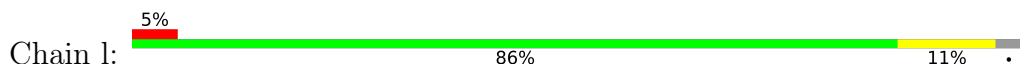


- Molecule 11: Photosystem II reaction center protein L

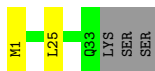
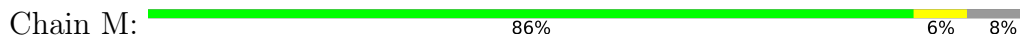


There are no outlier residues recorded for this chain.

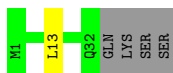
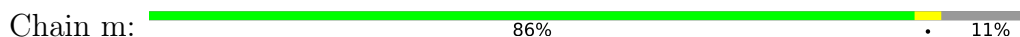
- Molecule 11: Photosystem II reaction center protein L



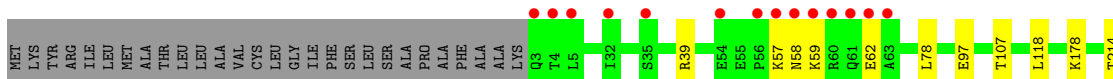
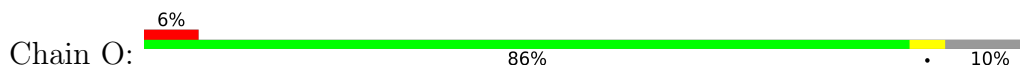
- Molecule 12: Photosystem II reaction center protein M



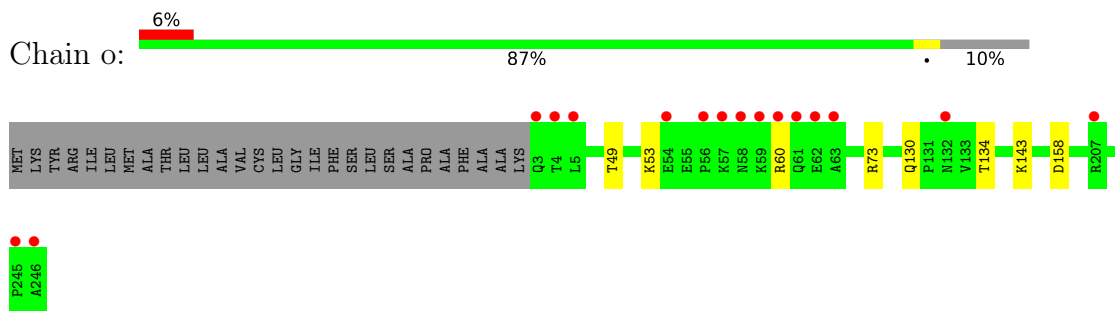
- Molecule 12: Photosystem II reaction center protein M



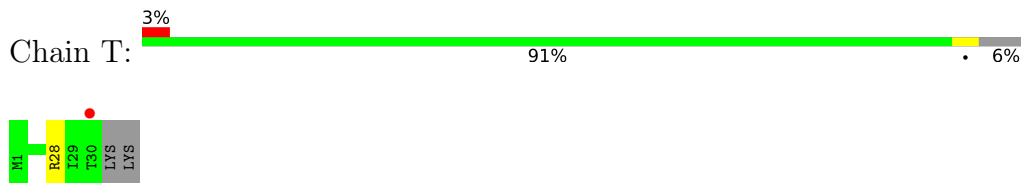
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



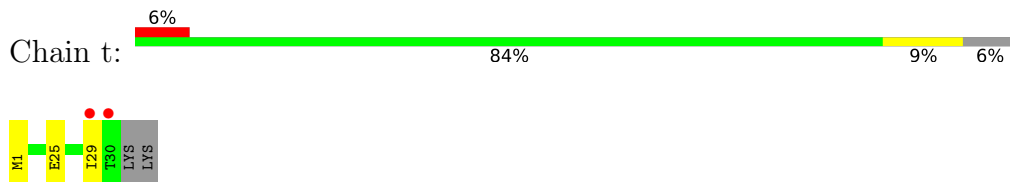
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



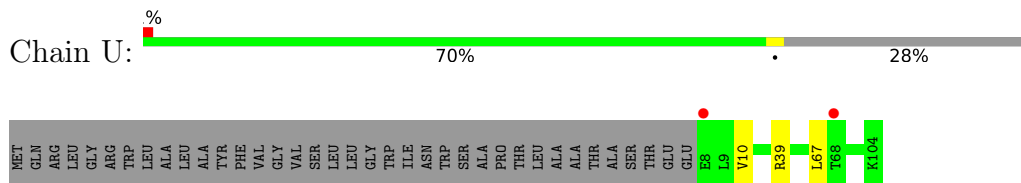
• Molecule 14: Photosystem II reaction center protein T



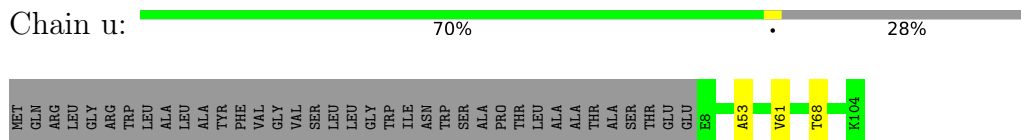
• Molecule 14: Photosystem II reaction center protein T



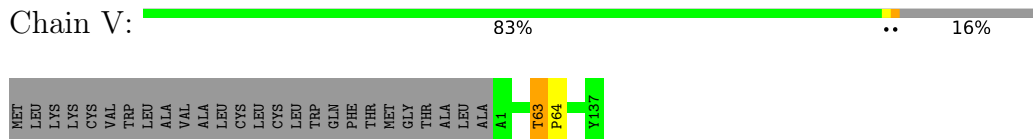
• Molecule 15: Photosystem II 12 kDa extrinsic protein



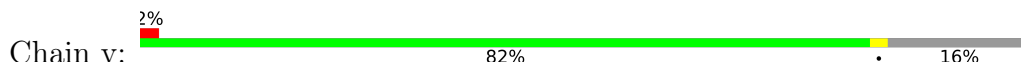
• Molecule 15: Photosystem II 12 kDa extrinsic protein

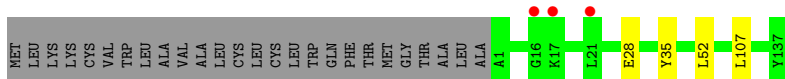


• Molecule 16: Cytochrome c-550

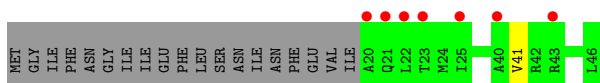


• Molecule 16: Cytochrome c-550

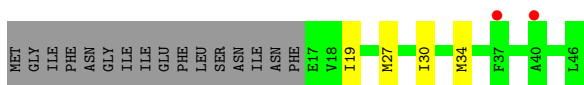




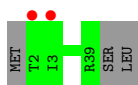
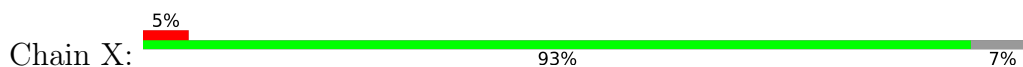
- Molecule 17: Photosystem II reaction center protein Ycf12



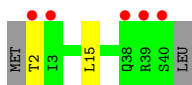
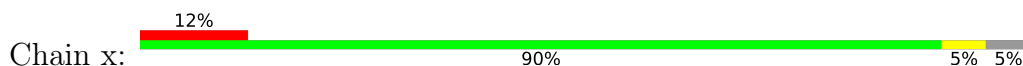
- Molecule 17: Photosystem II reaction center protein Ycf12



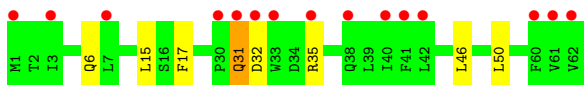
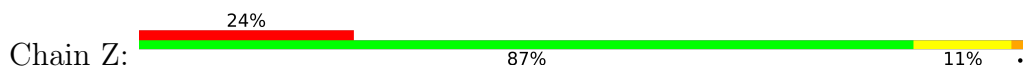
- Molecule 18: Photosystem II reaction center X protein



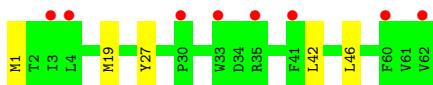
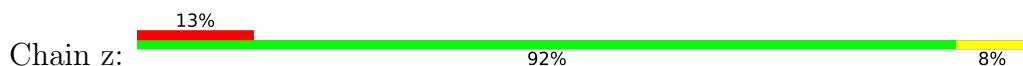
- Molecule 18: Photosystem II reaction center X protein



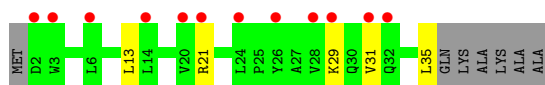
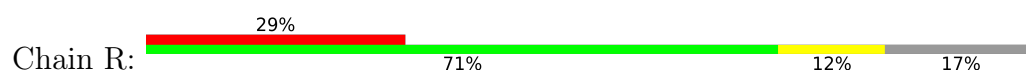
- Molecule 19: Photosystem II reaction center protein Z



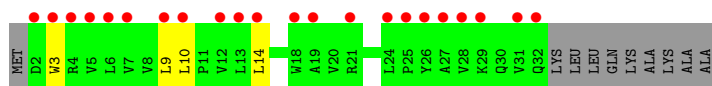
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.10Å 222.20Å 308.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.74 – 2.15 33.74 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.74-2.15) 85.1 (33.74-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.42 (at 2.16Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.243 0.188 , 0.243	Depositor DCC
R_{free} test set	3853 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtrriage
Anisotropy	0.171	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52853	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

5.1 Standard geometry

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

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	0.53	0/3212	0.64	2/4376 (0.0%)
1	a	0.52	0/3209	0.61	0/4372
2	B	0.43	0/4155	0.59	0/5661
2	b	0.40	0/4118	0.57	0/5611
3	C	0.43	0/3625	0.57	0/4935
3	c	0.40	0/3705	0.56	0/5042
4	D	0.43	0/2825	0.57	0/3847
4	d	0.42	0/2834	0.58	0/3859
5	E	0.37	0/688	0.53	0/940
5	e	0.34	0/683	0.53	0/932
6	F	0.36	0/284	0.51	0/387
6	f	0.33	0/284	0.52	0/387
7	H	0.41	0/523	0.60	0/713
7	h	0.40	0/511	0.60	0/697
8	I	0.43	0/293	0.59	0/396
8	i	0.44	0/293	0.58	0/396
9	J	0.41	0/263	0.58	0/356
9	j	0.34	0/263	0.52	0/356
10	K	0.39	0/303	0.54	0/416
10	k	0.37	0/303	0.53	0/416
11	L	0.41	0/311	0.58	0/422
11	l	0.39	0/303	0.59	0/412
12	M	0.37	0/249	0.53	0/341
12	m	0.44	0/244	0.57	0/334
13	O	0.38	0/1904	0.62	0/2585
13	o	0.39	0/1905	0.64	1/2583 (0.0%)
14	T	0.51	0/257	0.60	0/349
14	t	0.45	0/255	0.53	0/346
15	U	0.36	0/785	0.55	0/1064
15	u	0.38	0/785	0.62	0/1064
16	V	0.35	0/1085	0.61	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.36	0/1085	0.57	0/1473
17	Y	0.30	0/197	0.53	0/264
17	y	0.28	0/219	0.48	0/294
18	X	0.37	0/284	0.53	0/384
18	x	0.31	0/289	0.47	0/391
19	Z	0.33	0/490	0.48	0/669
19	z	0.31	0/488	0.43	0/666
20	R	0.34	0/277	0.57	0/380
20	r	0.31	0/252	0.51	0/347
All	All	0.42	0/44038	0.58	4/59936 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	V	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	63	THR	C-N-CD	-6.21	106.94	120.60
1	A	183[A]	MET	CA-CB-CG	6.10	123.67	113.30
1	A	183[B]	MET	CA-CB-CG	6.10	123.67	113.30
13	o	158	ASP	CB-CG-OD1	5.94	123.65	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/344 (115%)	389 (98%)	5 (1%)	1 (0%)	41	37
1	a	395/344 (115%)	388 (98%)	6 (2%)	1 (0%)	41	37
2	B	507/510 (99%)	502 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	495 (98%)	7 (1%)	1 (0%)	47	46
3	C	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	47	46
3	c	461/461 (100%)	447 (97%)	13 (3%)	1 (0%)	47	46
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	78 (96%)	2 (2%)	1 (1%)	13	7
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	30 (88%)	4 (12%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	4	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	9 (4%)	3 (1%)	13	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	34	29
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	14	8
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	15
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9	3
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5242 (97%)	130 (2%)	14 (0%)	41	37

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	O	62	GLU

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	322/280 (115%)	319 (99%)	3 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	321/280 (115%)	309 (96%)	12 (4%)	34	32
2	B	407/407 (100%)	395 (97%)	12 (3%)	42	42
2	b	402/407 (99%)	391 (97%)	11 (3%)	44	46
3	C	353/362 (98%)	346 (98%)	7 (2%)	55	59
3	c	362/362 (100%)	349 (96%)	13 (4%)	35	33
4	D	277/283 (98%)	272 (98%)	5 (2%)	59	63
4	d	278/283 (98%)	269 (97%)	9 (3%)	39	38
5	E	72/73 (99%)	67 (93%)	5 (7%)	15	10
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	28
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	32
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	4
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	13
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	39
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	6
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	28 (93%)	2 (7%)	16	11
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	33
12	m	28/32 (88%)	27 (96%)	1 (4%)	35	33
13	O	206/228 (90%)	198 (96%)	8 (4%)	32	30
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	42
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	31
14	t	25/28 (89%)	23 (92%)	2 (8%)	12	7
15	U	84/112 (75%)	81 (96%)	3 (4%)	35	33
15	u	84/112 (75%)	82 (98%)	2 (2%)	49	51
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	113 (97%)	4 (3%)	37	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	19/37 (51%)	18 (95%)	1 (5%)	22	19
17	y	22/37 (60%)	18 (82%)	4 (18%)	1	0
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	12
19	Z	52/52 (100%)	44 (85%)	8 (15%)	2	1
19	z	51/52 (98%)	46 (90%)	5 (10%)	8	4
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	0
20	r	25/33 (76%)	21 (84%)	4 (16%)	2	1
All	All	4450/4654 (96%)	4289 (96%)	161 (4%)	35	33

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	f	23	VAL
16	v	35	TYR
7	h	37	LEU
11	l	30	LEU
18	x	2	THR

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

Mol	Chain	Res	Type
19	Z	31	GLN
1	a	234	ASN
20	r	30	GLN
5	e	60	GLN
13	o	61	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	T	1	14	8,9,10	1.05	0	7,9,11	1.03	0
8	FME	I	1	8	8,9,10	1.02	0	7,9,11	1.41	1 (14%)
12	FME	m	1	12	8,9,10	1.00	0	7,9,11	0.75	0
14	FME	t	1	14	8,9,10	1.16	1 (12%)	7,9,11	0.88	0
8	FME	i	1	8	8,9,10	1.06	0	7,9,11	0.75	0
12	FME	M	1	12	8,9,10	1.00	1 (12%)	7,9,11	1.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.25	1.43	1.46
12	M	1	FME	CA-N	-2.04	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-3.18	117.93	122.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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
29	LMG	M	101	-	51,51,55	0.84	4 (7%)	59,59,63	1.38	7 (11%)
31	DGD	H	102	-	63,63,67	1.16	4 (6%)	77,77,81	1.43	11 (14%)
27	BCR	A	610	-	41,41,41	0.98	2 (4%)	56,56,56	1.27	6 (10%)
25	CLA	B	603	-	65,73,73	1.64	7 (10%)	76,113,113	1.47	9 (11%)
28	PL9	D	407	-	55,55,55	0.95	3 (5%)	68,69,69	1.54	16 (23%)
28	PL9	d	406	-	55,55,55	1.07	3 (5%)	68,69,69	1.71	17 (25%)
27	BCR	k	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.11	3 (5%)
36	HEC	v	201	16	32,50,50	2.14	3 (9%)	24,82,82	1.90	5 (20%)
25	CLA	b	605	-	65,73,73	1.47	5 (7%)	76,113,113	1.50	11 (14%)
25	CLA	b	608	-	65,73,73	1.56	7 (10%)	76,113,113	1.59	14 (18%)
25	CLA	B	613	-	65,73,73	1.50	8 (12%)	76,113,113	1.51	11 (14%)
29	LMG	B	621	-	26,26,55	0.76	2 (7%)	26,26,63	1.19	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PHO	d	402	-	51,69,69	1.00	3 (5%)	47,99,99	1.61	7 (14%)
31	DGD	a	614	-	43,43,67	0.72	2 (4%)	45,45,81	1.45	6 (13%)
25	CLA	B	612	-	65,73,73	1.46	8 (12%)	76,113,113	1.51	12 (15%)
34	LHG	D	410	-	48,48,48	0.77	1 (2%)	51,54,54	1.32	7 (13%)
25	CLA	C	502	-	65,73,73	1.64	9 (13%)	76,113,113	1.15	8 (10%)
25	CLA	A	609	-	54,62,73	1.59	6 (11%)	62,99,113	1.55	9 (14%)
31	DGD	c	517	-	63,63,67	1.01	6 (9%)	77,77,81	1.47	12 (15%)
25	CLA	c	508	-	64,72,73	1.59	7 (10%)	74,111,113	1.41	10 (13%)
32	STE	b	620	-	15,15,19	0.38	0	14,14,19	0.88	0
25	CLA	c	507	37	65,73,73	1.55	9 (13%)	76,113,113	1.36	8 (10%)
30	SQD	t	102	-	35,35,54	1.66	6 (17%)	37,37,65	1.48	4 (10%)
25	CLA	B	607	37	65,73,73	1.57	7 (10%)	76,113,113	1.53	7 (9%)
31	DGD	c	516	-	63,63,67	1.08	7 (11%)	77,77,81	1.40	10 (12%)
25	CLA	C	504	37	59,67,73	1.71	8 (13%)	68,105,113	1.41	10 (14%)
27	BCR	K	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	3 (5%)
29	LMG	C	519	-	48,48,55	0.86	2 (4%)	56,56,63	1.34	6 (10%)
27	BCR	d	405	-	41,41,41	1.04	2 (4%)	56,56,56	1.10	2 (3%)
25	CLA	B	606	-	65,73,73	1.58	8 (12%)	76,113,113	1.47	11 (14%)
25	CLA	b	610	37	65,73,73	1.47	6 (9%)	76,113,113	1.36	11 (14%)
25	CLA	a	612	37	65,73,73	1.65	8 (12%)	76,113,113	1.39	9 (11%)
25	CLA	d	404	-	65,73,73	1.55	7 (10%)	76,113,113	1.32	9 (11%)
25	CLA	b	616	-	60,68,73	1.44	7 (11%)	70,107,113	1.60	9 (12%)
25	CLA	C	507	37	65,73,73	1.52	7 (10%)	76,113,113	1.49	9 (11%)
32	STE	R	101	-	11,11,19	0.70	0	11,11,19	1.15	1 (9%)
32	STE	a	616	-	11,11,19	0.82	0	11,11,19	0.86	0
27	BCR	B	619	-	41,41,41	1.00	1 (2%)	56,56,56	1.34	7 (12%)
32	STE	L	103	-	11,11,19	0.64	0	11,11,19	1.37	1 (9%)
25	CLA	C	505	-	65,73,73	1.75	7 (10%)	76,113,113	1.40	10 (13%)
25	CLA	a	606	-	65,73,73	1.55	8 (12%)	76,113,113	1.39	8 (10%)
25	CLA	c	511	3	65,73,73	1.59	6 (9%)	76,113,113	1.42	6 (7%)
25	CLA	b	607	37	65,73,73	1.53	8 (12%)	76,113,113	1.40	8 (10%)
25	CLA	B	605	-	65,73,73	1.46	7 (10%)	76,113,113	1.29	7 (9%)
25	CLA	b	603	-	65,73,73	1.59	8 (12%)	76,113,113	1.57	12 (15%)
25	CLA	C	506	-	65,73,73	1.52	8 (12%)	76,113,113	1.41	7 (9%)
25	CLA	C	513	-	65,73,73	1.59	6 (9%)	76,113,113	1.39	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PL9	A	611	-	55,55,55	0.96	1 (1%)	68,69,69	1.49	11 (16%)
31	DGD	A	615	-	67,67,67	1.04	5 (7%)	81,81,81	1.41	15 (18%)
32	STE	j	101	-	11,11,19	0.78	0	11,11,19	1.16	0
27	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.28	7 (12%)
25	CLA	c	501	-	65,73,73	1.48	7 (10%)	76,113,113	1.51	7 (9%)
30	SQD	B	622	-	53,54,54	1.56	8 (15%)	62,65,65	1.80	11 (17%)
32	STE	B	623	-	11,11,19	0.75	0	11,11,19	1.13	0
27	BCR	D	406	-	41,41,41	1.13	3 (7%)	56,56,56	1.27	6 (10%)
25	CLA	b	613	-	65,73,73	1.71	10 (15%)	76,113,113	1.58	12 (15%)
35	HEM	F	101	5,6	41,50,50	1.48	4 (9%)	45,82,82	1.41	3 (6%)
25	CLA	c	509	-	65,73,73	1.38	5 (7%)	76,113,113	1.66	9 (11%)
25	CLA	B	602	-	65,73,73	1.64	8 (12%)	76,113,113	1.49	12 (15%)
31	DGD	c	518	-	63,63,67	0.92	3 (4%)	77,77,81	1.47	15 (19%)
32	STE	t	103	-	13,13,19	0.65	0	13,13,19	1.26	2 (15%)
25	CLA	b	612	-	65,73,73	1.55	7 (10%)	76,113,113	1.52	12 (15%)
26	PHO	A	608	-	51,69,69	1.02	4 (7%)	47,99,99	1.28	5 (10%)
29	LMG	d	410	-	21,21,55	0.59	0	20,20,63	1.15	0
32	STE	l	102	-	17,17,19	0.33	0	16,16,19	0.95	0
25	CLA	D	404	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)
29	LMG	D	408	-	51,51,55	0.78	1 (1%)	59,59,63	1.24	6 (10%)
32	STE	B	624	-	11,11,19	0.67	0	11,11,19	1.22	2 (18%)
25	CLA	a	609	-	65,73,73	1.48	8 (12%)	76,113,113	1.35	11 (14%)
25	CLA	b	606	-	65,73,73	1.64	6 (9%)	76,113,113	1.58	11 (14%)
27	BCR	k	102	-	41,41,41	1.05	4 (9%)	56,56,56	1.20	6 (10%)
32	STE	c	522	-	11,11,19	0.73	0	11,11,19	1.23	1 (9%)
32	STE	M	102	-	14,14,19	0.71	0	14,14,19	1.11	1 (7%)
32	STE	B	620	-	16,16,19	0.68	0	16,16,19	1.12	0
31	DGD	C	517	-	63,63,67	0.96	6 (9%)	77,77,81	1.42	11 (14%)
25	CLA	B	611	-	65,73,73	1.38	7 (10%)	76,113,113	1.57	9 (11%)
25	CLA	c	512	-	65,73,73	1.50	7 (10%)	76,113,113	1.43	10 (13%)
27	BCR	b	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.20	4 (7%)
32	STE	b	624	-	14,14,19	0.29	0	13,13,19	0.97	0
27	BCR	b	617	-	41,41,41	0.96	2 (4%)	56,56,56	1.24	5 (8%)
34	LHG	D	413	-	48,48,48	0.88	2 (4%)	51,54,54	1.37	6 (11%)
25	CLA	B	610	37	65,73,73	1.47	8 (12%)	76,113,113	1.49	12 (15%)
33	BCT	d	401	23	2,3,3	1.32	0	2,3,3	2.96	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	D	412	-	31,31,55	0.66	1 (3%)	33,33,63	1.19	2 (6%)
29	LMG	m	101	-	51,51,55	0.90	3 (5%)	59,59,63	1.47	9 (15%)
34	LHG	d	407	-	48,48,48	0.79	2 (4%)	51,54,54	1.33	7 (13%)
25	CLA	D	405	-	65,73,73	1.48	10 (15%)	76,113,113	1.44	9 (11%)
27	BCR	a	610	-	41,41,41	0.94	3 (7%)	56,56,56	1.25	5 (8%)
34	LHG	l	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.26	8 (15%)
29	LMG	c	519	-	37,37,55	1.03	4 (10%)	45,45,63	1.32	5 (11%)
25	CLA	B	604	-	65,73,73	1.54	8 (12%)	76,113,113	1.72	10 (13%)
25	CLA	b	609	-	65,73,73	1.53	8 (12%)	76,113,113	1.51	10 (13%)
25	CLA	c	504	37	60,68,73	1.58	6 (10%)	70,107,113	1.34	6 (8%)
25	CLA	b	602	-	65,73,73	1.58	9 (13%)	76,113,113	1.61	12 (15%)
25	CLA	C	511	3	65,73,73	1.66	6 (9%)	76,113,113	1.42	7 (9%)
25	CLA	c	506	-	65,73,73	1.57	8 (12%)	76,113,113	1.43	6 (7%)
25	CLA	c	502	-	65,73,73	1.50	9 (13%)	76,113,113	1.51	9 (11%)
32	STE	a	615	-	9,9,19	0.41	0	8,8,19	0.59	0
25	CLA	c	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.55	10 (13%)
27	BCR	K	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.38	9 (16%)
25	CLA	b	601	37	65,73,73	1.62	7 (10%)	76,113,113	1.45	8 (10%)
31	DGD	C	516	-	63,63,67	1.06	4 (6%)	77,77,81	1.36	10 (12%)
35	HEM	e	101	5,6	41,50,50	1.47	6 (14%)	45,82,82	1.68	12 (26%)
27	BCR	B	617	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	6 (10%)
32	STE	b	626	-	9,9,19	0.34	0	8,8,19	0.72	0
34	LHG	L	102	-	48,48,48	0.71	0	51,54,54	1.23	5 (9%)
32	STE	d	412	-	16,16,19	0.64	0	16,16,19	1.12	1 (6%)
22	OEX	a	602[A]	3,1,37	0,15,15	-	-	-	-	-
30	SQD	A	613	-	51,52,54	1.55	8 (15%)	60,63,65	2.05	13 (21%)
25	CLA	B	615	-	65,73,73	1.60	8 (12%)	76,113,113	1.31	8 (10%)
27	BCR	c	515	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
22	OEX	A	602[A]	3,1,37	0,15,15	-	-	-	-	-
26	PHO	a	608	-	51,69,69	0.97	2 (3%)	47,99,99	1.23	6 (12%)
32	STE	J	101	-	11,11,19	0.73	0	11,11,19	1.36	2 (18%)
25	CLA	C	510	-	65,73,73	1.47	8 (12%)	76,113,113	1.41	6 (7%)
29	LMG	c	521	-	48,48,55	0.97	4 (8%)	56,56,63	1.30	8 (14%)
32	STE	b	621	-	19,19,19	0.60	0	19,19,19	1.10	1 (5%)
27	BCR	t	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	611	-	65,73,73	1.51	7 (10%)	76,113,113	1.48	9 (11%)
32	STE	c	520	-	19,19,19	0.63	0	19,19,19	0.98	0
27	BCR	C	515	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	3 (5%)
32	STE	d	413	-	19,19,19	0.69	0	19,19,19	0.87	1 (5%)
21	OEY	a	601[B]	3,1,37	0,16,16	-	-	-	-	-
29	LMG	d	411	-	44,44,55	0.83	2 (4%)	52,52,63	1.33	7 (13%)
25	CLA	a	607	37	65,73,73	1.53	7 (10%)	76,113,113	1.43	12 (15%)
25	CLA	B	609	-	65,73,73	1.42	8 (12%)	76,113,113	1.35	10 (13%)
34	LHG	e	102	-	41,41,48	0.78	1 (2%)	44,47,54	1.30	6 (13%)
21	OEY	A	601[B]	3,1,37	0,16,16	-	-	-	-	-
30	SQD	L	101	-	48,49,54	1.62	10 (20%)	57,60,65	1.97	13 (22%)
32	STE	C	522	-	15,15,19	0.39	0	14,14,19	0.69	0
32	STE	b	625	-	19,19,19	0.59	0	19,19,19	1.02	1 (5%)
25	CLA	A	606	-	65,73,73	1.52	5 (7%)	76,113,113	1.45	6 (7%)
25	CLA	b	604	-	65,73,73	1.54	8 (12%)	76,113,113	1.64	11 (14%)
25	CLA	B	601	37	65,73,73	1.65	6 (9%)	76,113,113	1.38	12 (15%)
34	LHG	E	101	-	48,48,48	0.76	2 (4%)	51,54,54	1.21	6 (11%)
32	STE	X	101	-	19,19,19	0.64	0	19,19,19	1.07	0
26	PHO	D	402	-	51,69,69	1.04	5 (9%)	47,99,99	1.42	7 (14%)
30	SQD	A	614	-	38,38,54	1.74	5 (13%)	40,40,65	1.28	3 (7%)
25	CLA	C	512	-	65,73,73	1.70	8 (12%)	76,113,113	1.47	11 (14%)
28	PL9	a	611	-	55,55,55	0.74	1 (1%)	68,69,69	1.53	10 (14%)
32	STE	M	103	-	9,9,19	0.37	0	8,8,19	0.66	0
32	STE	t	104	-	17,17,19	0.56	0	17,17,19	1.21	1 (5%)
27	BCR	b	618	-	41,41,41	1.10	3 (7%)	56,56,56	1.26	6 (10%)
34	LHG	D	411	-	46,46,48	0.90	2 (4%)	49,52,54	1.24	4 (8%)
25	CLA	b	614	-	65,73,73	1.63	9 (13%)	76,113,113	1.36	11 (14%)
29	LMG	A	612	-	48,48,55	0.97	3 (6%)	56,56,63	1.31	8 (14%)
32	STE	b	623	-	15,15,19	0.78	0	15,15,19	0.89	0
34	LHG	d	408	-	48,48,48	0.62	0	51,54,54	1.32	7 (13%)
27	BCR	h	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.30	8 (14%)
29	LMG	c	523	-	49,49,55	0.83	1 (2%)	57,57,63	1.30	4 (7%)
30	SQD	D	409	-	35,36,54	1.52	5 (14%)	42,45,65	3.02	12 (28%)
30	SQD	a	613	-	53,54,54	1.52	7 (13%)	62,65,65	2.03	12 (19%)
25	CLA	A	607	37	65,73,73	1.49	9 (13%)	76,113,113	1.45	12 (15%)
27	BCR	C	514	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	C	521	-	11,11,19	0.72	0	11,11,19	1.18	1 (9%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.80	0
25	CLA	B	608	-	65,73,73	1.51	8 (12%)	76,113,113	1.45	9 (11%)
25	CLA	C	503	-	65,73,73	1.75	10 (15%)	76,113,113	1.46	8 (10%)
25	CLA	C	509	-	65,73,73	1.65	9 (13%)	76,113,113	1.52	9 (11%)
25	CLA	c	510	-	65,73,73	1.49	8 (12%)	76,113,113	1.54	10 (13%)
25	CLA	d	403	-	65,73,73	1.41	6 (9%)	76,113,113	1.30	8 (10%)
31	DGD	h	102	-	63,63,67	0.91	2 (3%)	77,77,81	1.50	14 (18%)
32	STE	B	625	-	15,15,19	0.35	0	14,14,19	0.83	0
27	BCR	T	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.20	5 (8%)
33	BCT	D	401	23	2,3,3	1.26	0	2,3,3	2.85	1 (50%)
25	CLA	D	403	37	65,73,73	1.50	6 (9%)	76,113,113	1.40	10 (13%)
25	CLA	C	508	-	65,73,73	1.54	7 (10%)	76,113,113	1.60	12 (15%)
25	CLA	b	615	-	65,73,73	1.53	7 (10%)	76,113,113	1.51	7 (9%)
27	BCR	H	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.23	4 (7%)
34	LHG	d	409	-	38,38,48	0.71	1 (2%)	41,44,54	1.14	3 (7%)
25	CLA	c	505	-	65,73,73	1.62	8 (12%)	76,113,113	1.40	10 (13%)
32	STE	I	101	-	14,14,19	0.38	0	13,13,19	0.66	0
25	CLA	c	513	-	65,73,73	1.57	8 (12%)	76,113,113	1.22	6 (7%)
29	LMG	b	622	-	55,55,55	0.81	1 (1%)	63,63,63	1.37	6 (9%)
27	BCR	c	514	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	8 (14%)
36	HEC	V	201	16	32,50,50	2.04	3 (9%)	24,82,82	1.94	7 (29%)
30	SQD	f	101	-	40,41,54	1.68	8 (20%)	49,52,65	1.84	12 (24%)
31	DGD	C	518	-	63,63,67	0.83	2 (3%)	77,77,81	1.45	11 (14%)
25	CLA	C	501	-	65,73,73	1.64	10 (15%)	76,113,113	1.51	11 (14%)
25	CLA	B	614	-	65,73,73	1.73	9 (13%)	76,113,113	1.24	9 (11%)
32	STE	C	520	-	11,11,19	0.66	0	11,11,19	1.54	1 (9%)
25	CLA	B	616	-	60,68,73	1.54	7 (11%)	70,107,113	1.44	8 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	M	101	-	-	20/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
27	BCR	A	610	-	-	6/29/63/63	0/2/2/2
25	CLA	B	603	-	1/1/15/20	10/37/115/115	-
28	PL9	D	407	-	-	16/53/73/73	0/1/1/1
28	PL9	d	406	-	-	16/53/73/73	0/1/1/1
27	BCR	k	101	-	-	9/29/63/63	0/2/2/2
36	HEC	v	201	16	-	2/10/54/54	-
25	CLA	b	605	-	1/1/15/20	10/37/115/115	-
25	CLA	b	608	-	1/1/15/20	7/37/115/115	-
25	CLA	B	613	-	1/1/15/20	16/37/115/115	-
29	LMG	B	621	-	-	14/22/22/70	-
26	PHO	d	402	-	-	5/37/103/103	0/5/6/6
31	DGD	a	614	-	-	26/45/45/95	-
25	CLA	B	612	-	1/1/15/20	13/37/115/115	-
34	LHG	D	410	-	-	18/53/53/53	-
25	CLA	C	502	-	1/1/15/20	10/37/115/115	-
25	CLA	A	609	-	1/1/12/20	6/24/102/115	-
31	DGD	c	517	-	-	19/51/91/95	0/2/2/2
25	CLA	c	508	-	-	8/36/114/115	-
32	STE	b	620	-	-	5/13/13/17	-
25	CLA	c	507	37	1/1/15/20	12/37/115/115	-
30	SQD	t	102	-	-	19/37/37/69	-
25	CLA	B	607	37	1/1/15/20	18/37/115/115	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
25	CLA	C	504	37	1/1/13/20	8/30/108/115	-
27	BCR	K	102	-	-	7/29/63/63	0/2/2/2
29	LMG	C	519	-	-	18/43/63/70	0/1/1/1
27	BCR	d	405	-	-	9/29/63/63	0/2/2/2
25	CLA	B	606	-	1/1/15/20	12/37/115/115	-
25	CLA	b	610	37	1/1/15/20	10/37/115/115	-
25	CLA	a	612	37	1/1/15/20	5/37/115/115	-
25	CLA	d	404	-	1/1/15/20	7/37/115/115	-
25	CLA	b	616	-	1/1/14/20	12/31/109/115	-
25	CLA	C	507	37	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	R	101	-	-	4/9/9/17	-
32	STE	a	616	-	-	4/9/9/17	-
27	BCR	B	619	-	-	9/29/63/63	0/2/2/2
32	STE	L	103	-	-	6/9/9/17	-
25	CLA	C	505	-	1/1/15/20	14/37/115/115	-
25	CLA	a	606	-	1/1/15/20	4/37/115/115	-
25	CLA	c	511	3	1/1/15/20	16/37/115/115	-
25	CLA	b	607	37	1/1/15/20	16/37/115/115	-
25	CLA	B	605	-	1/1/15/20	9/37/115/115	-
25	CLA	b	603	-	1/1/15/20	7/37/115/115	-
25	CLA	C	506	-	1/1/15/20	15/37/115/115	-
25	CLA	C	513	-	1/1/15/20	12/37/115/115	-
28	PL9	A	611	-	-	20/53/73/73	0/1/1/1
31	DGD	A	615	-	-	23/55/95/95	0/2/2/2
32	STE	j	101	-	-	5/9/9/17	-
27	BCR	B	618	-	-	8/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	4/37/115/115	-
30	SQD	B	622	-	-	24/49/69/69	0/1/1/1
32	STE	B	623	-	-	5/9/9/17	-
27	BCR	D	406	-	-	7/29/63/63	0/2/2/2
25	CLA	b	613	-	1/1/15/20	12/37/115/115	-
35	HEM	F	101	5,6	-	2/12/54/54	-
25	CLA	c	509	-	1/1/15/20	6/37/115/115	-
25	CLA	B	602	-	1/1/15/20	9/37/115/115	-
31	DGD	c	518	-	-	16/51/91/95	0/2/2/2
32	STE	t	103	-	-	3/11/11/17	-
25	CLA	b	612	-	1/1/15/20	11/37/115/115	-
26	PHO	A	608	-	-	11/37/103/103	0/5/6/6
29	LMG	d	410	-	-	13/17/17/70	-
32	STE	l	102	-	-	7/15/15/17	-
25	CLA	D	404	-	-	16/37/115/115	-
29	LMG	D	408	-	-	21/46/66/70	0/1/1/1
32	STE	B	624	-	-	4/9/9/17	-
25	CLA	a	609	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	606	-	1/1/15/20	7/37/115/115	-
27	BCR	k	102	-	-	7/29/63/63	0/2/2/2
32	STE	c	522	-	-	5/9/9/17	-
32	STE	M	102	-	-	8/12/12/17	-
32	STE	B	620	-	-	10/14/14/17	-
31	DGD	C	517	-	-	21/51/91/95	0/2/2/2
25	CLA	B	611	-	1/1/15/20	10/37/115/115	-
25	CLA	c	512	-	1/1/15/20	20/37/115/115	-
27	BCR	b	619	-	-	7/29/63/63	0/2/2/2
32	STE	b	624	-	-	9/12/12/17	-
27	BCR	b	617	-	-	8/29/63/63	0/2/2/2
34	LHG	D	413	-	-	22/53/53/53	-
25	CLA	B	610	37	1/1/15/20	5/37/115/115	-
29	LMG	D	412	-	-	19/33/33/70	-
29	LMG	m	101	-	-	20/46/66/70	0/1/1/1
34	LHG	d	407	-	-	18/53/53/53	-
25	CLA	D	405	-	1/1/15/20	8/37/115/115	-
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
34	LHG	l	101	-	-	22/53/53/53	-
29	LMG	c	519	-	-	10/31/51/70	0/1/1/1
25	CLA	B	604	-	1/1/15/20	17/37/115/115	-
25	CLA	b	609	-	1/1/15/20	9/37/115/115	-
25	CLA	c	504	37	1/1/14/20	7/31/109/115	-
25	CLA	b	602	-	1/1/15/20	8/37/115/115	-
25	CLA	C	511	3	1/1/15/20	6/37/115/115	-
25	CLA	c	506	-	1/1/15/20	15/37/115/115	-
25	CLA	c	502	-	-	7/37/115/115	-
32	STE	a	615	-	-	5/7/7/17	-
25	CLA	c	503	-	-	13/37/115/115	-
27	BCR	K	101	-	-	7/29/63/63	0/2/2/2
25	CLA	b	601	37	1/1/15/20	20/37/115/115	-
31	DGD	C	516	-	-	23/51/91/95	0/2/2/2
35	HEM	e	101	5,6	-	3/12/54/54	-
27	BCR	B	617	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	b	626	-	-	2/7/7/17	-
34	LHG	L	102	-	-	21/53/53/53	-
32	STE	d	412	-	-	7/14/14/17	-
30	SQD	A	613	-	-	19/47/67/69	0/1/1/1
25	CLA	B	615	-	1/1/15/20	8/37/115/115	-
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
26	PHO	a	608	-	-	4/37/103/103	0/5/6/6
32	STE	J	101	-	-	3/9/9/17	-
25	CLA	C	510	-	1/1/15/20	10/37/115/115	-
29	LMG	c	521	-	-	25/43/63/70	0/1/1/1
32	STE	b	621	-	-	10/17/17/17	-
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
25	CLA	b	611	-	1/1/15/20	10/37/115/115	-
32	STE	c	520	-	-	14/17/17/17	-
27	BCR	C	515	-	-	7/29/63/63	0/2/2/2
32	STE	d	413	-	-	11/17/17/17	-
29	LMG	d	411	-	-	10/39/59/70	0/1/1/1
25	CLA	a	607	37	1/1/15/20	16/37/115/115	-
25	CLA	B	609	-	-	7/37/115/115	-
34	LHG	e	102	-	-	23/46/46/53	-
30	SQD	L	101	-	-	23/44/64/69	0/1/1/1
32	STE	C	522	-	-	5/13/13/17	-
32	STE	b	625	-	-	11/17/17/17	-
25	CLA	A	606	-	1/1/15/20	3/37/115/115	-
25	CLA	b	604	-	1/1/15/20	9/37/115/115	-
25	CLA	B	601	37	1/1/15/20	21/37/115/115	-
34	LHG	E	101	-	-	29/53/53/53	-
32	STE	X	101	-	-	11/17/17/17	-
26	PHO	D	402	-	-	3/37/103/103	0/5/6/6
30	SQD	A	614	-	-	13/39/39/69	-
25	CLA	C	512	-	1/1/15/20	9/37/115/115	-
28	PL9	a	611	-	-	22/53/73/73	0/1/1/1
32	STE	M	103	-	-	3/7/7/17	-
32	STE	t	104	-	-	9/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	618	-	-	6/29/63/63	0/2/2/2
34	LHG	D	411	-	-	20/51/51/53	-
25	CLA	b	614	-	1/1/15/20	18/37/115/115	-
29	LMG	A	612	-	-	19/43/63/70	0/1/1/1
32	STE	b	623	-	-	8/13/13/17	-
34	LHG	d	408	-	-	23/53/53/53	-
27	BCR	h	101	-	-	4/29/63/63	0/2/2/2
29	LMG	c	523	-	-	27/44/64/70	0/1/1/1
30	SQD	D	409	-	-	14/28/48/69	0/1/1/1
30	SQD	a	613	-	-	24/49/69/69	0/1/1/1
25	CLA	A	607	37	-	7/37/115/115	-
27	BCR	C	514	-	-	8/29/63/63	0/2/2/2
32	STE	C	521	-	-	5/9/9/17	-
32	STE	H	103	-	-	10/15/15/17	-
25	CLA	B	608	-	1/1/15/20	5/37/115/115	-
25	CLA	C	503	-	1/1/15/20	12/37/115/115	-
25	CLA	C	509	-	1/1/15/20	12/37/115/115	-
25	CLA	c	510	-	1/1/15/20	13/37/115/115	-
25	CLA	d	403	-	1/1/15/20	9/37/115/115	-
31	DGD	h	102	-	-	14/51/91/95	0/2/2/2
32	STE	B	625	-	-	2/13/13/17	-
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
25	CLA	D	403	37	1/1/15/20	4/37/115/115	-
25	CLA	C	508	-	-	9/37/115/115	-
25	CLA	b	615	-	1/1/15/20	15/37/115/115	-
27	BCR	H	101	-	-	4/29/63/63	0/2/2/2
34	LHG	d	409	-	-	13/43/43/53	-
25	CLA	c	505	-	1/1/15/20	10/37/115/115	-
32	STE	I	101	-	-	5/12/12/17	-
25	CLA	c	513	-	1/1/15/20	12/37/115/115	-
29	LMG	b	622	-	-	24/50/70/70	0/1/1/1
27	BCR	c	514	-	-	8/29/63/63	0/2/2/2
36	HEC	V	201	16	-	2/10/54/54	-
30	SQD	f	101	-	-	15/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	C	518	-	-	14/51/91/95	0/2/2/2
25	CLA	C	501	-	1/1/15/20	8/37/115/115	-
25	CLA	B	614	-	1/1/15/20	19/37/115/115	-
32	STE	C	520	-	-	3/9/9/17	-
25	CLA	B	616	-	1/1/14/20	11/31/109/115	-

The worst 5 of 751 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	C4B-NB	8.56	1.42	1.35
25	c	504	CLA	C4B-NB	8.35	1.42	1.35
25	B	603	CLA	MG-NA	8.19	2.25	2.06
25	C	504	CLA	C4B-NB	8.19	1.42	1.35
25	B	601	CLA	C4B-NB	8.14	1.42	1.35

The worst 5 of 1231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	13.20	128.91	108.30
25	B	604	CLA	C4A-NA-C1A	9.31	110.89	106.71
25	c	509	CLA	C4A-NA-C1A	8.59	110.57	106.71
25	C	507	CLA	C4A-NA-C1A	7.99	110.30	106.71
25	b	615	CLA	C4A-NA-C1A	7.89	110.25	106.71

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	609	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND

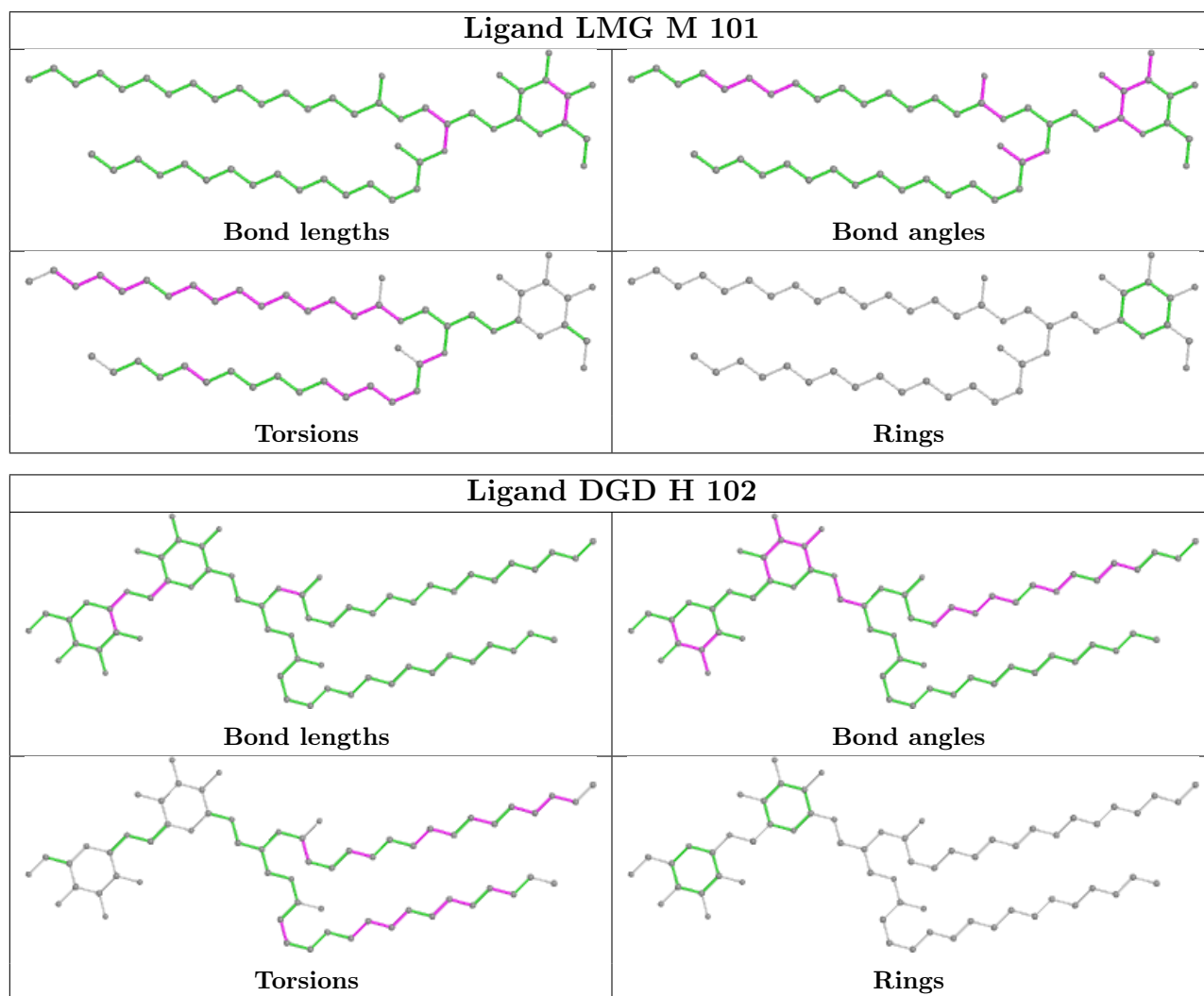
5 of 1988 torsion outliers are listed below:

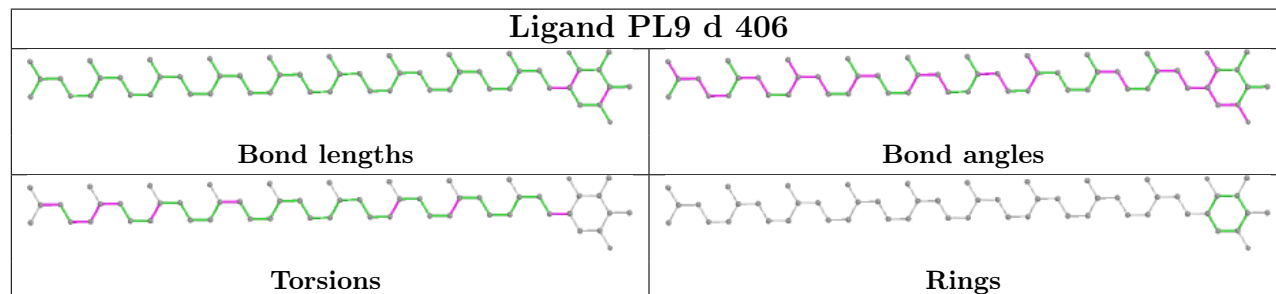
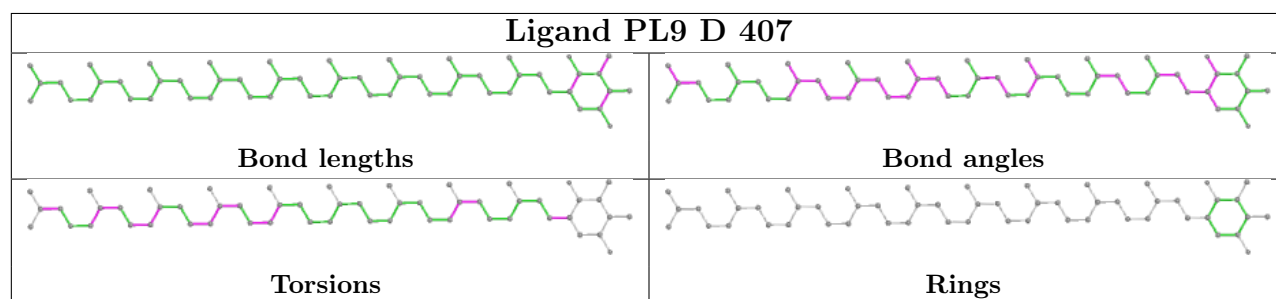
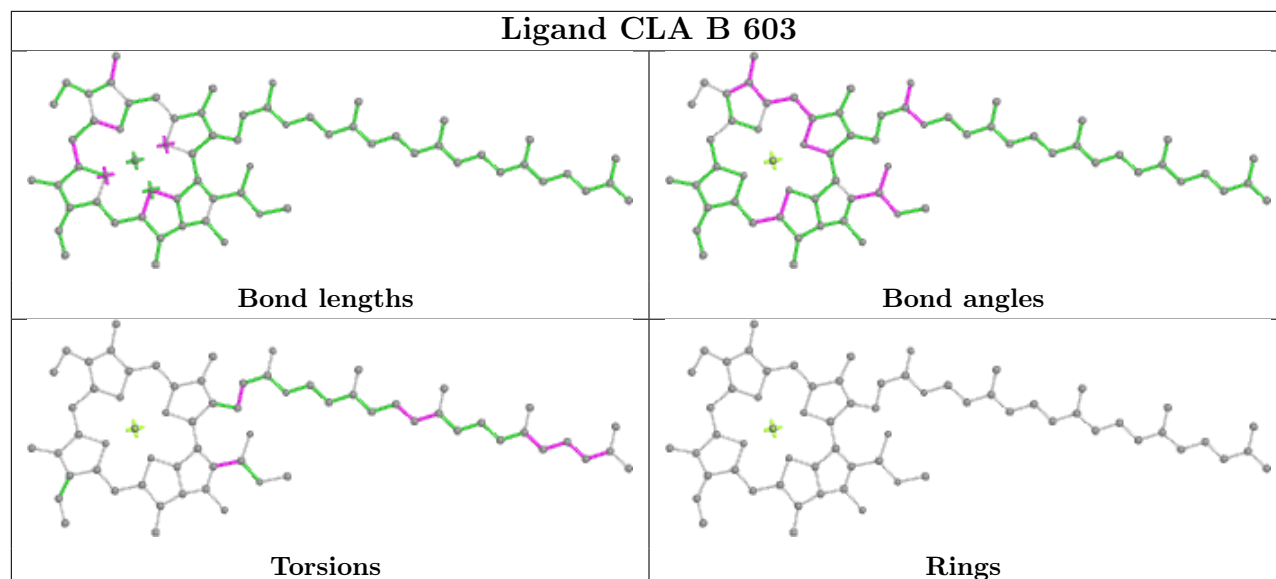
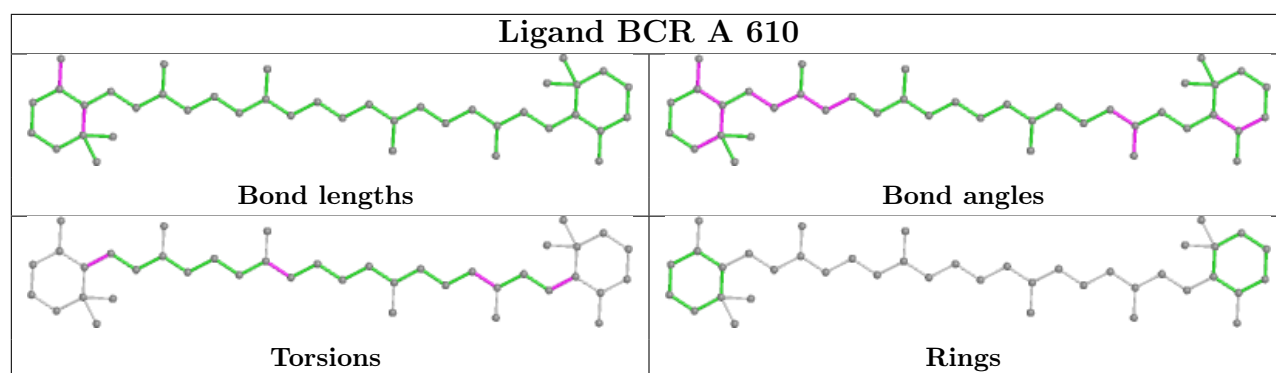
Mol	Chain	Res	Type	Atoms
25	A	607	CLA	CHA-CBD-CGD-O1D
25	A	607	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	C11-C12-C13-C14
25	B	604	CLA	C2-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6

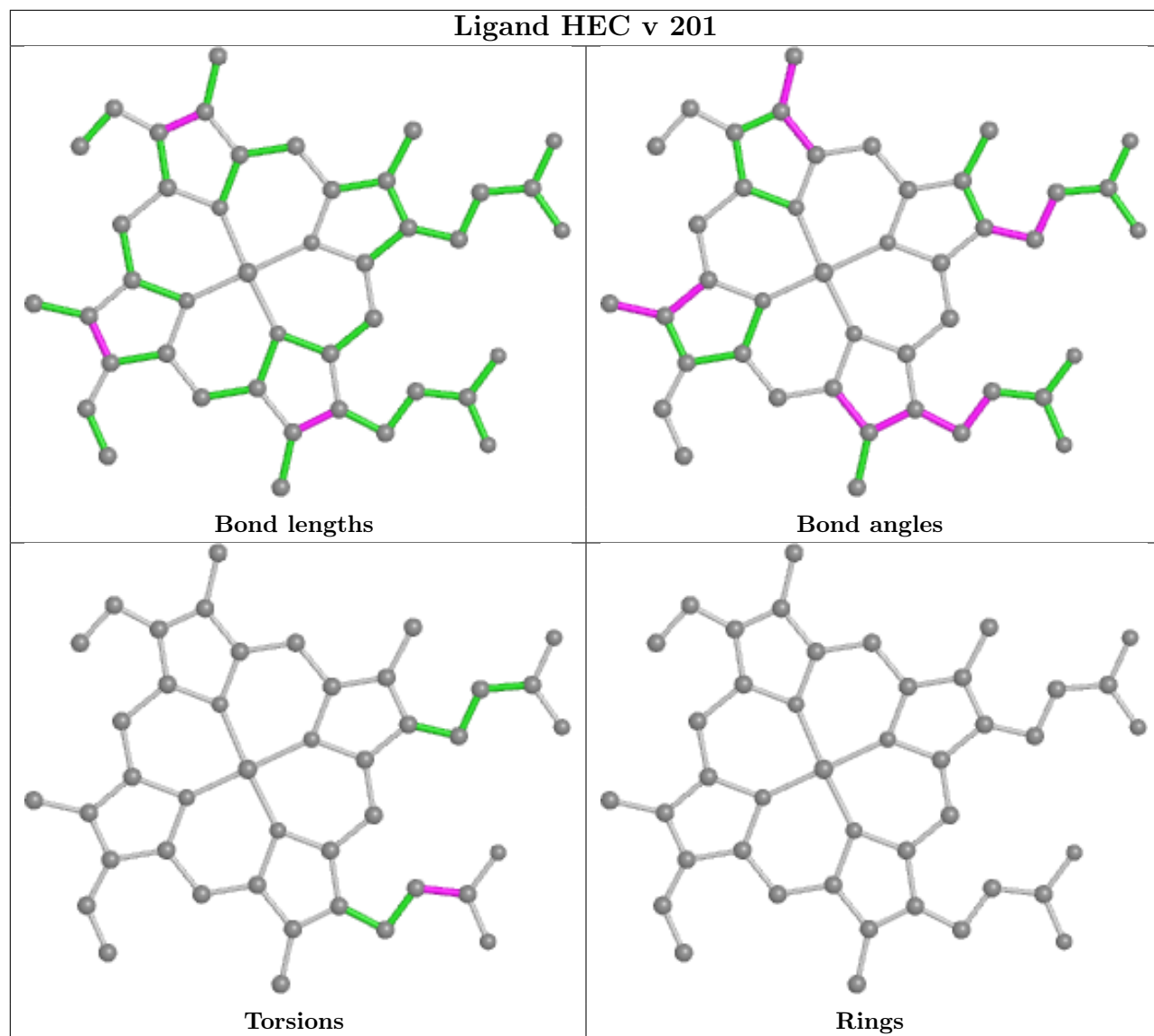
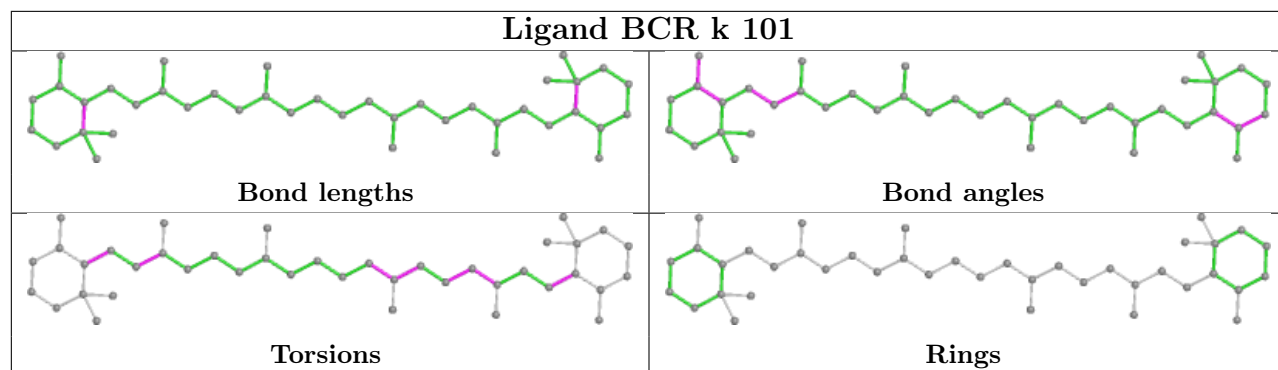
There are no ring outliers.

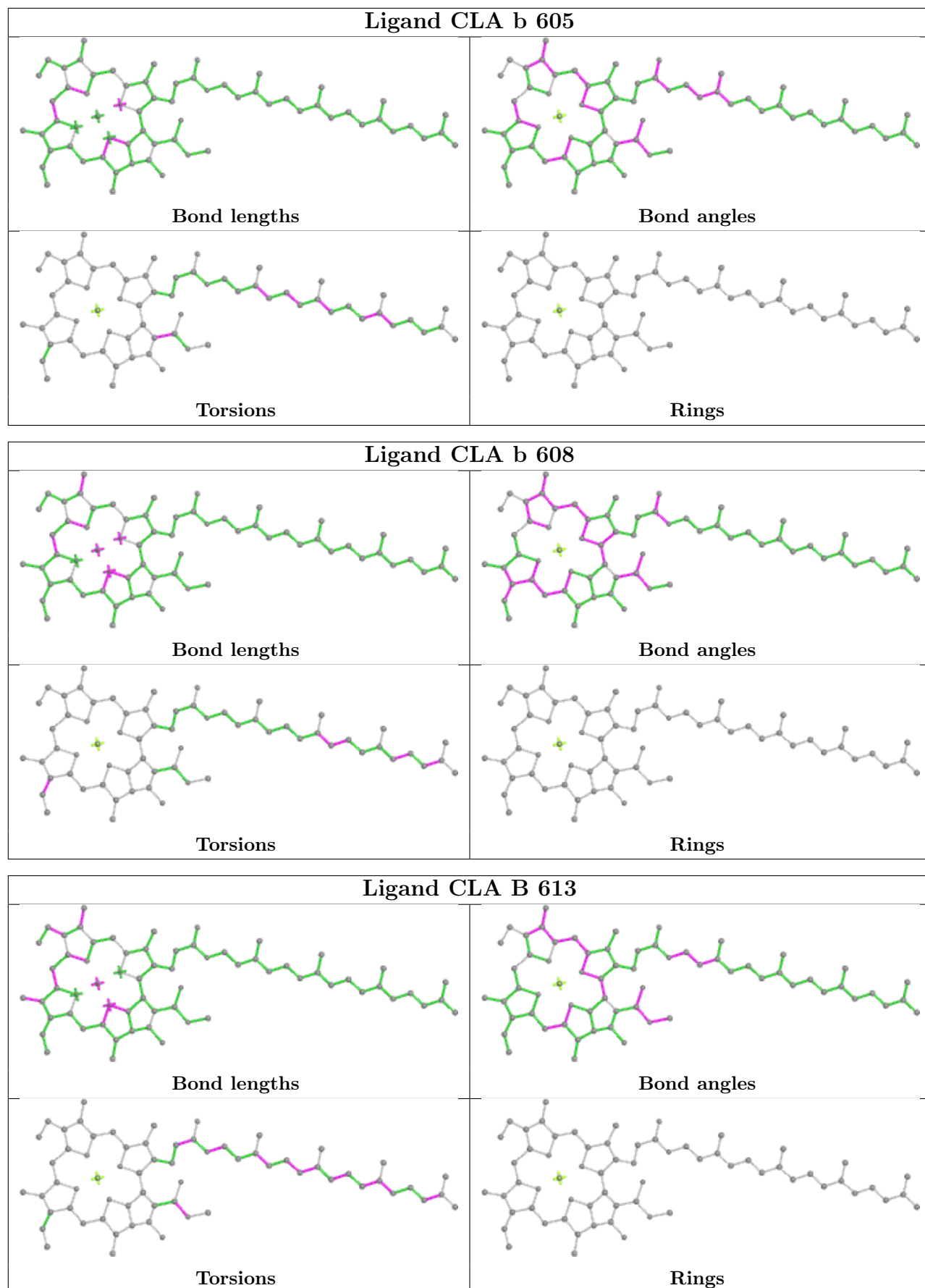
No monomer is involved in short contacts.

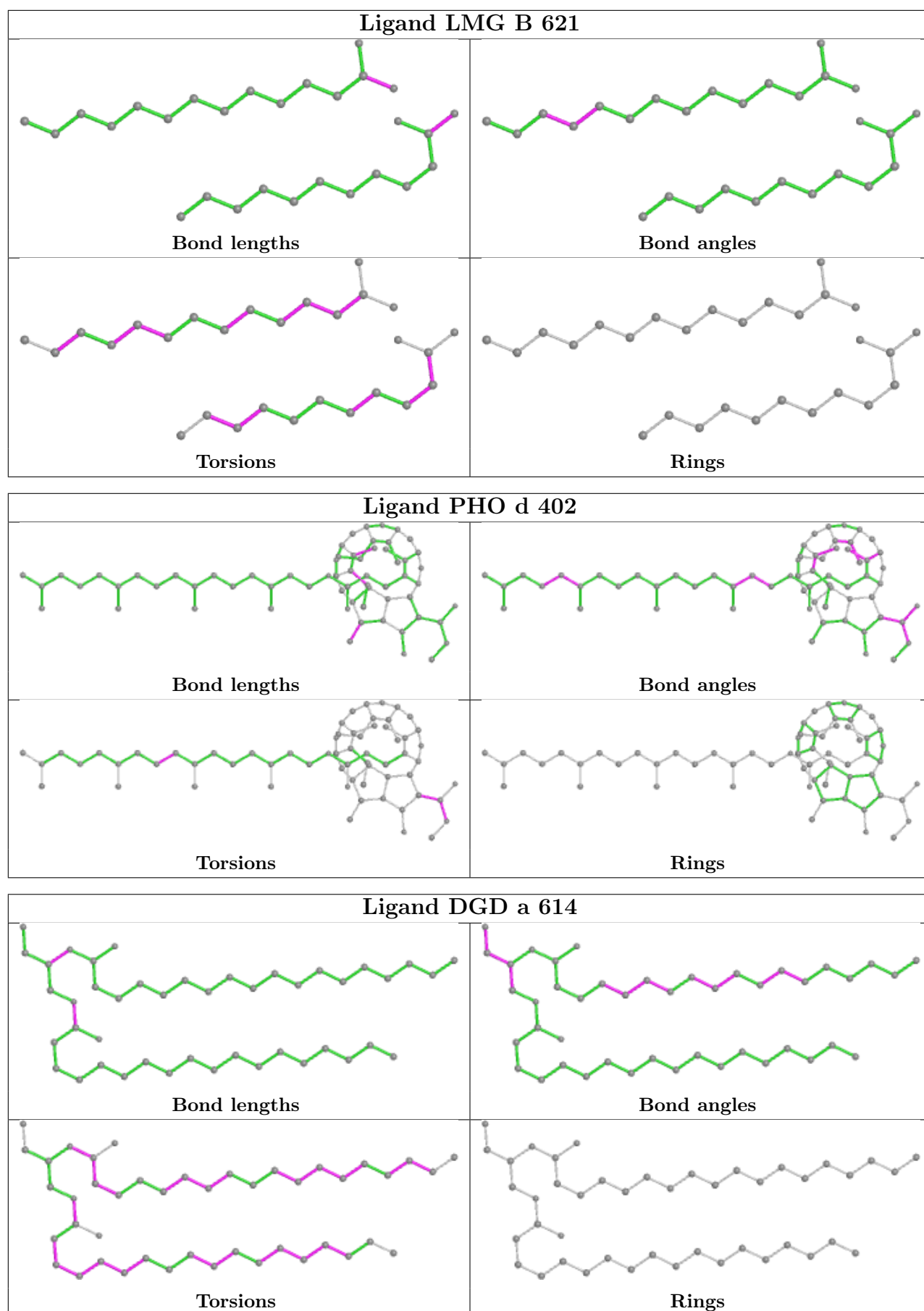
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

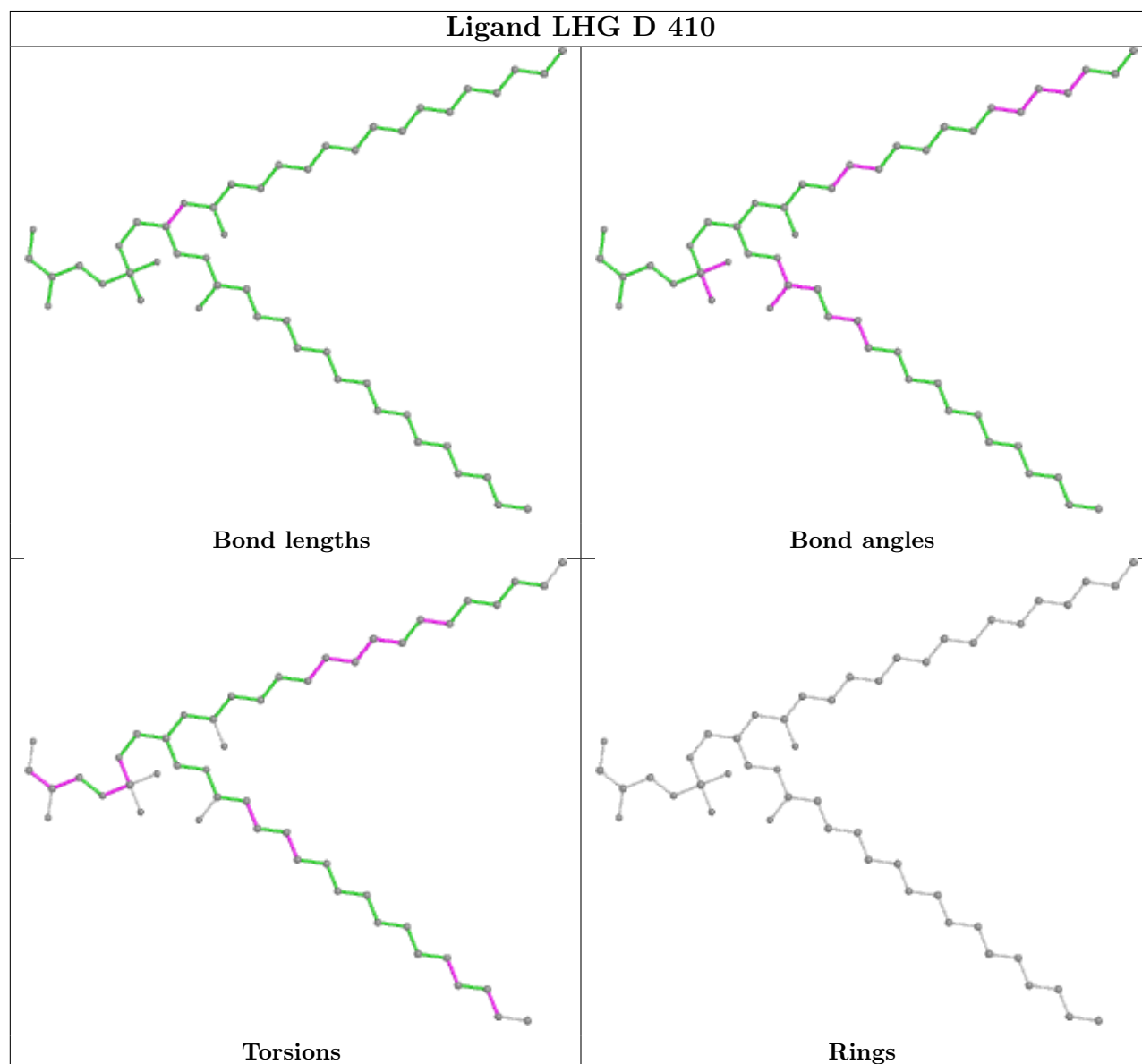
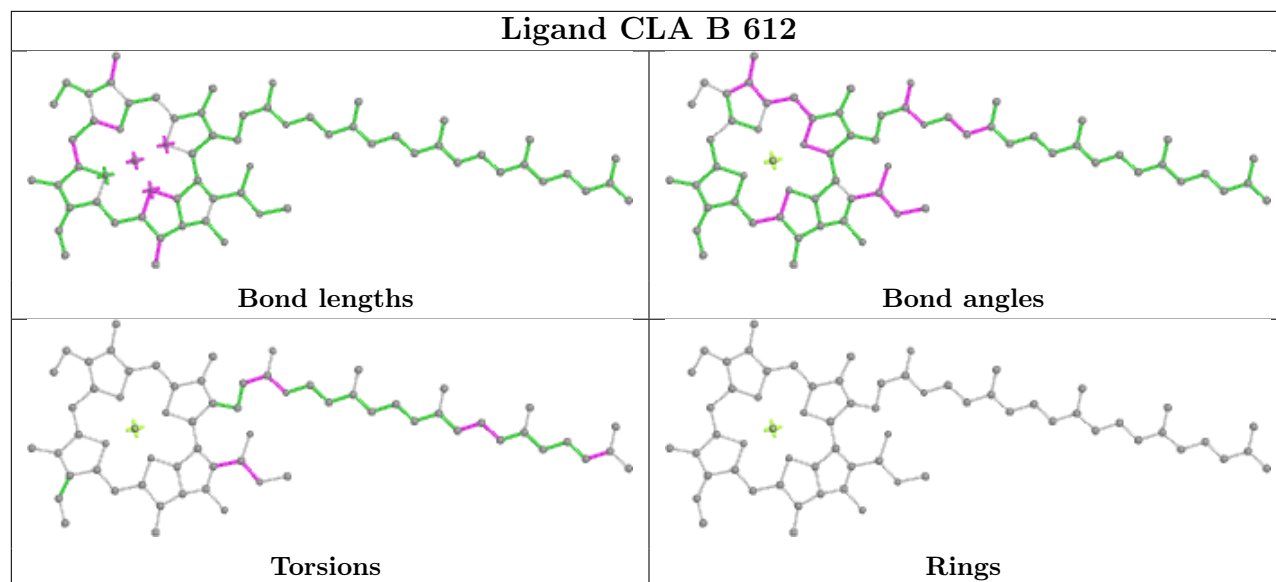


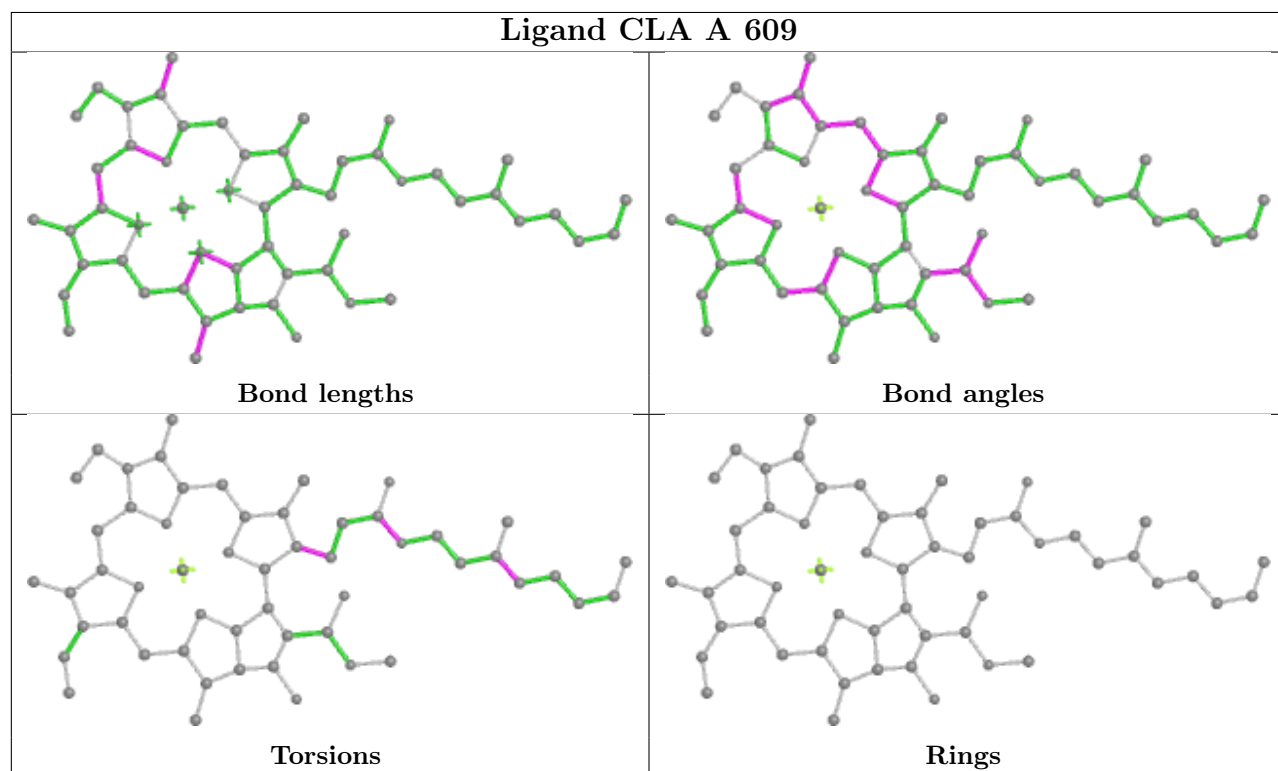
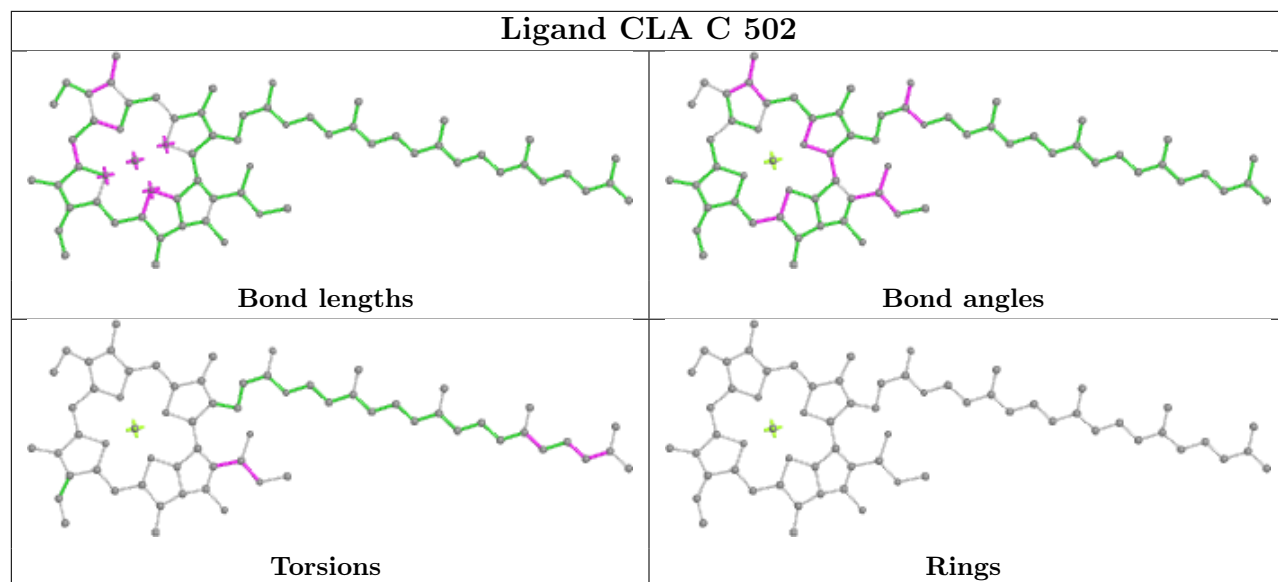


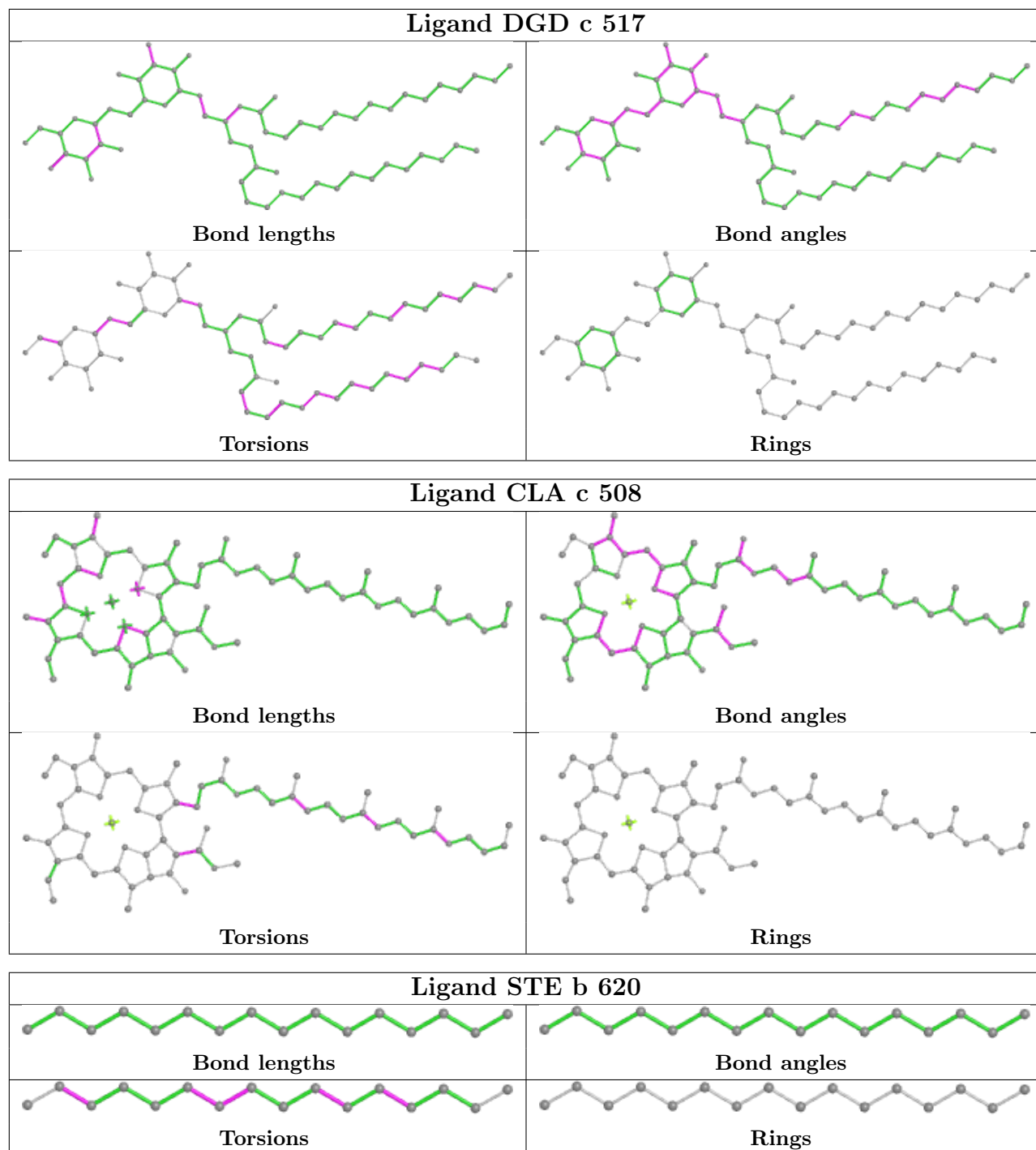


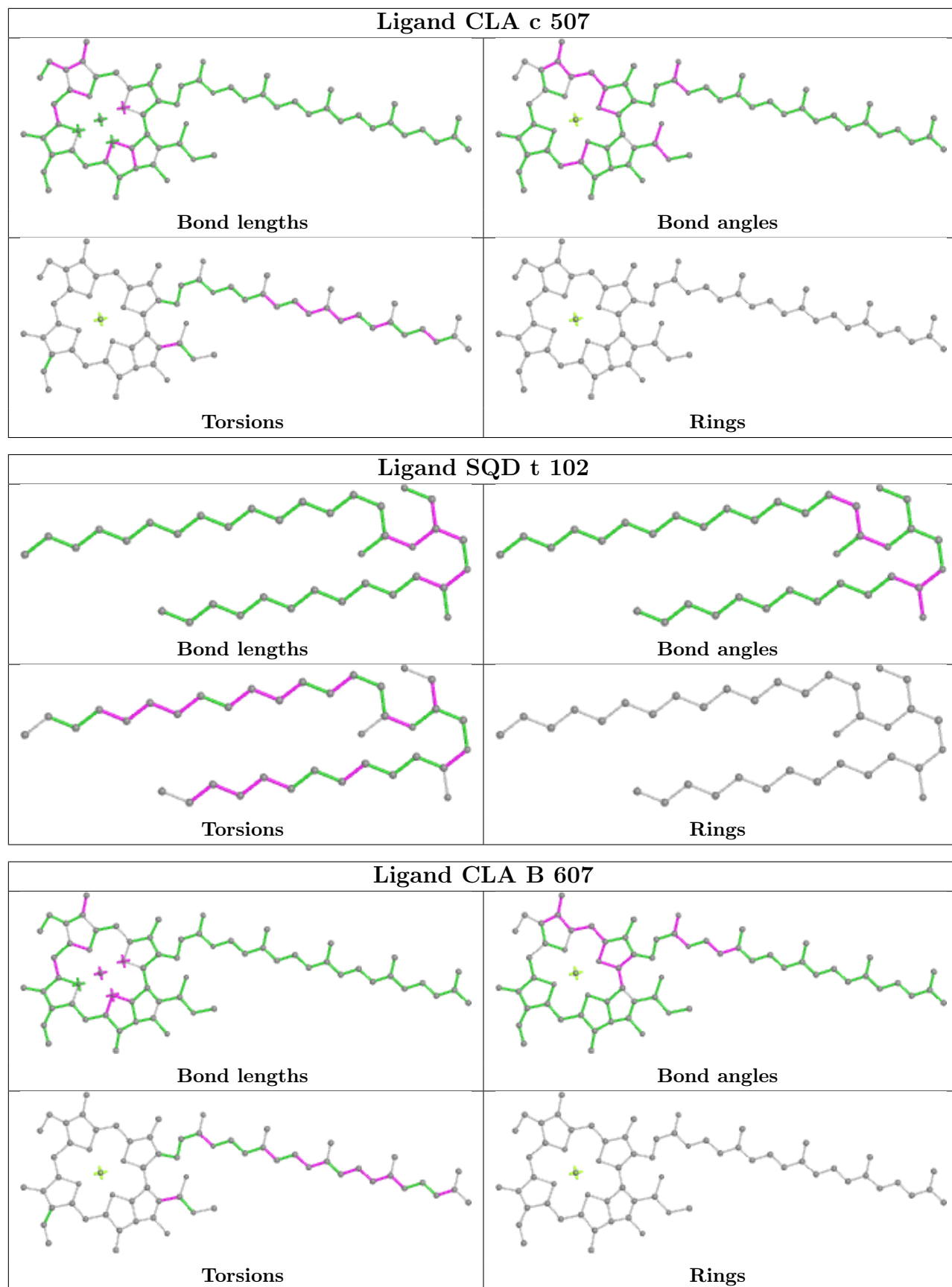


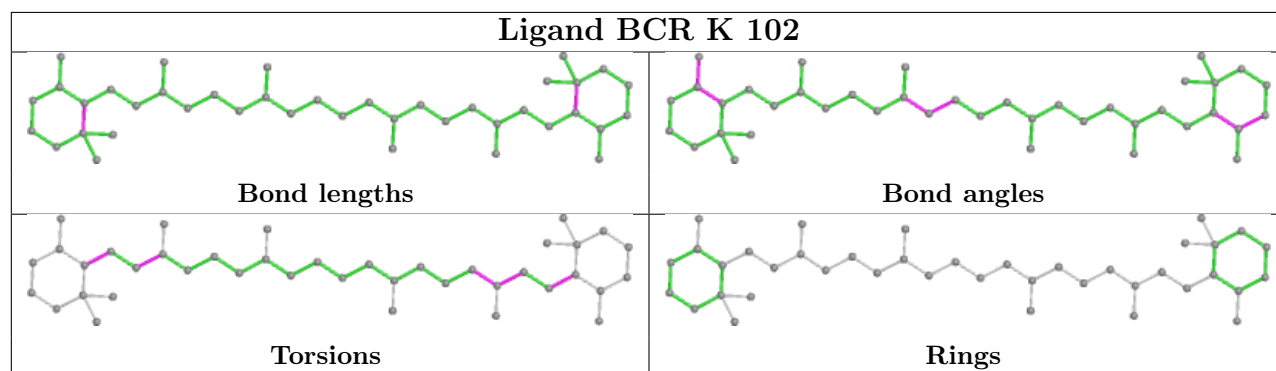
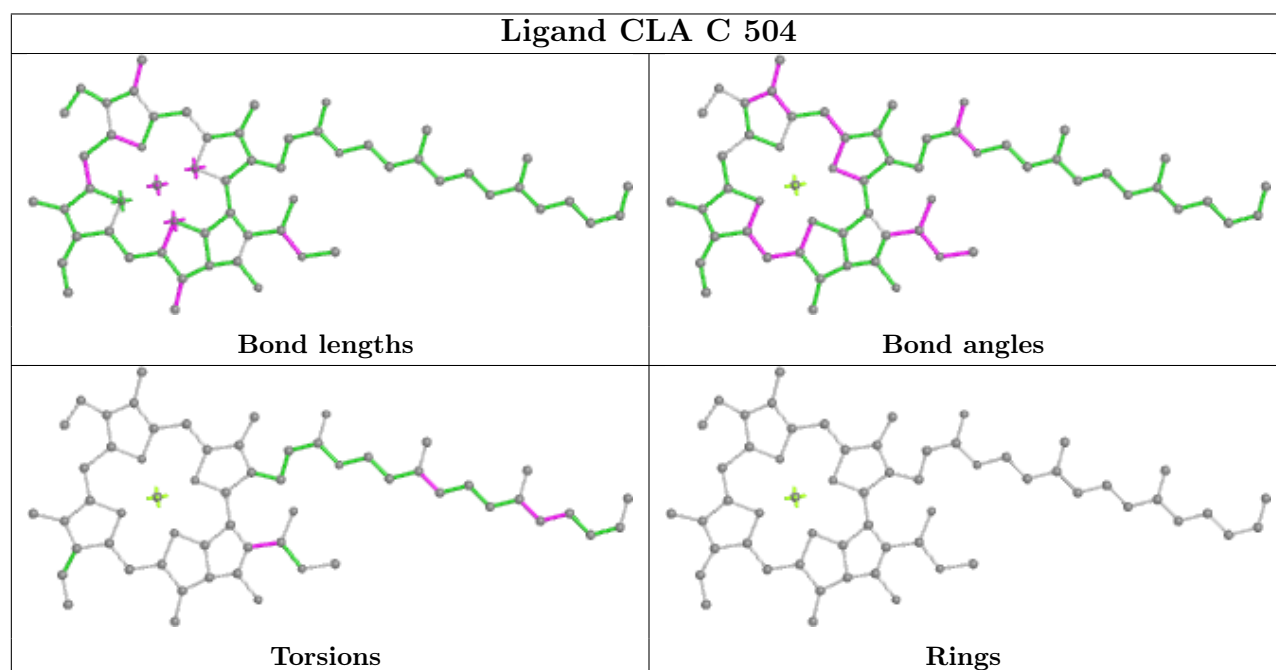
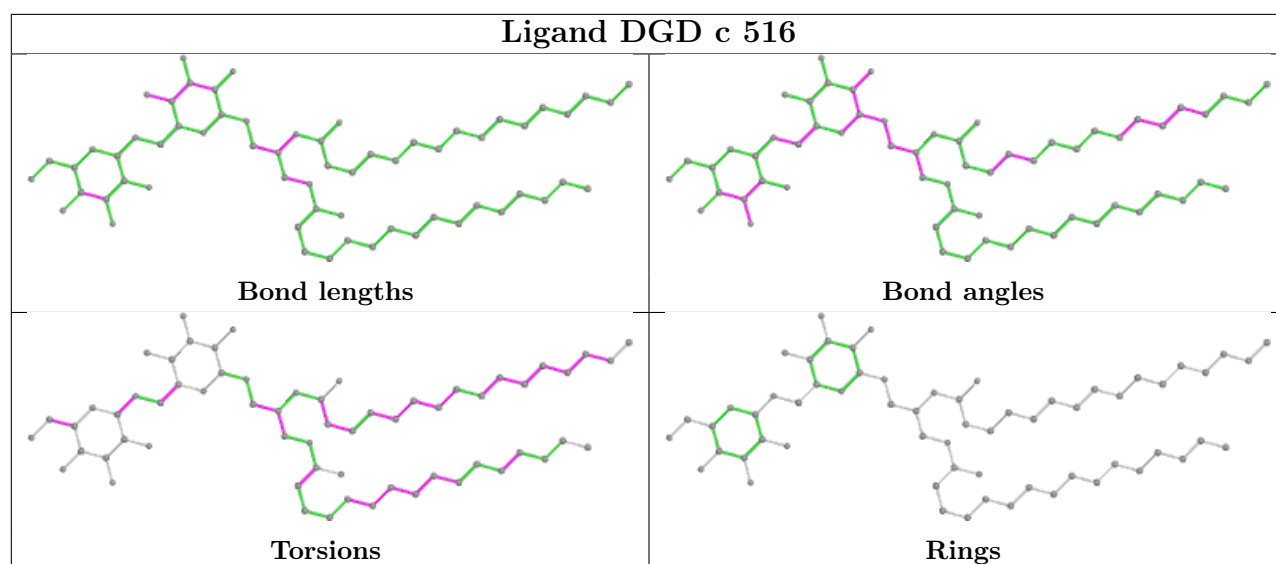


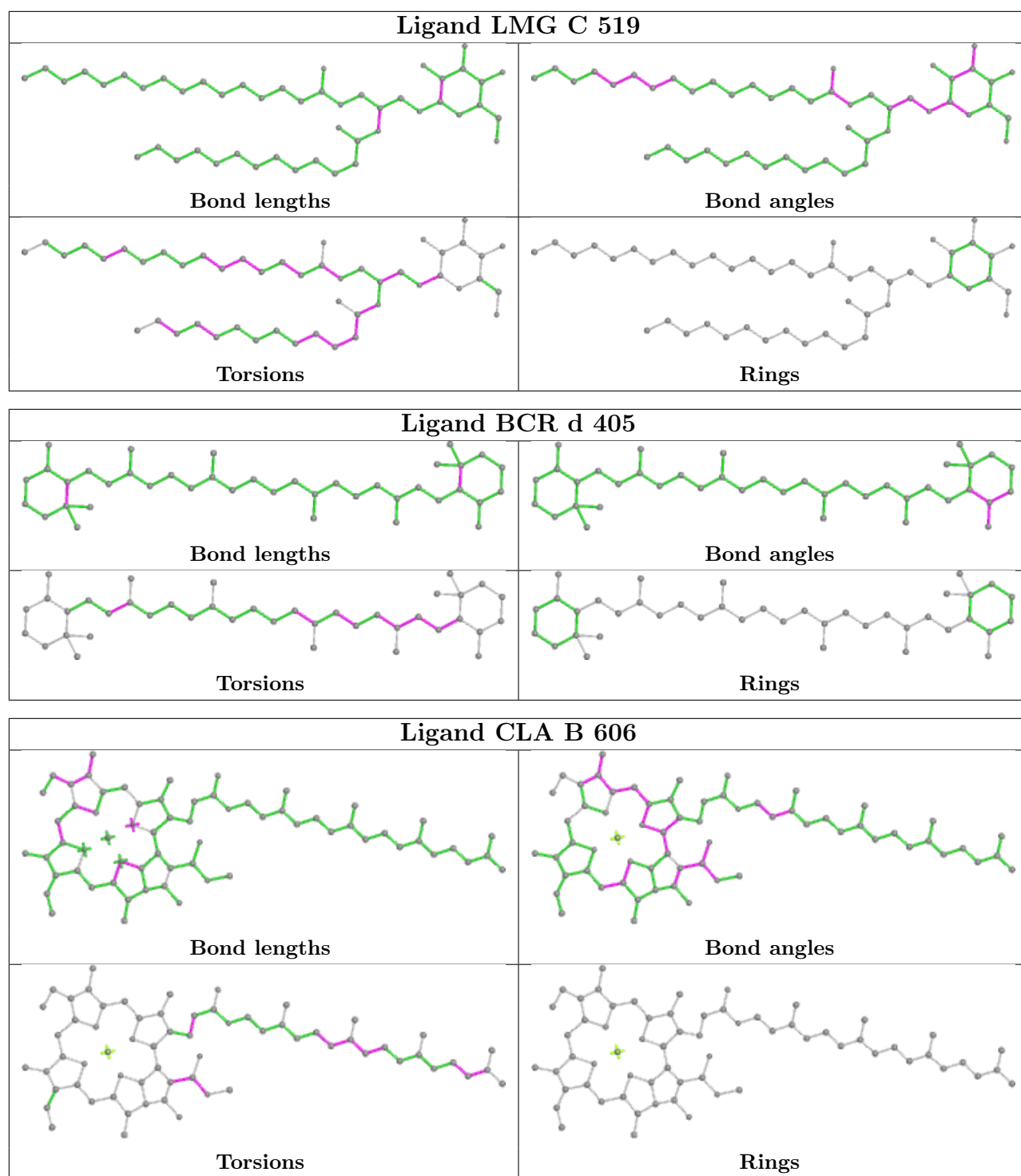


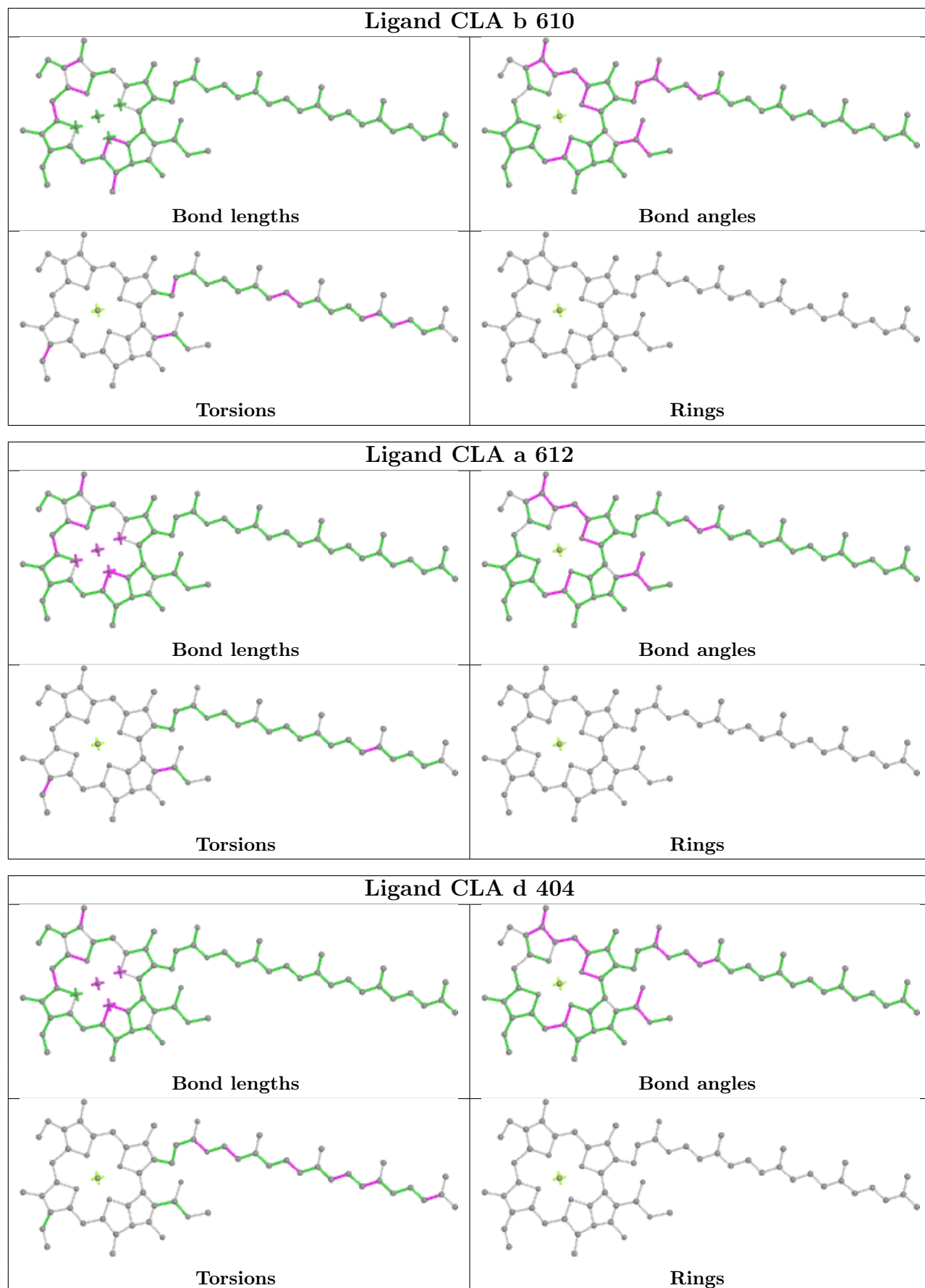


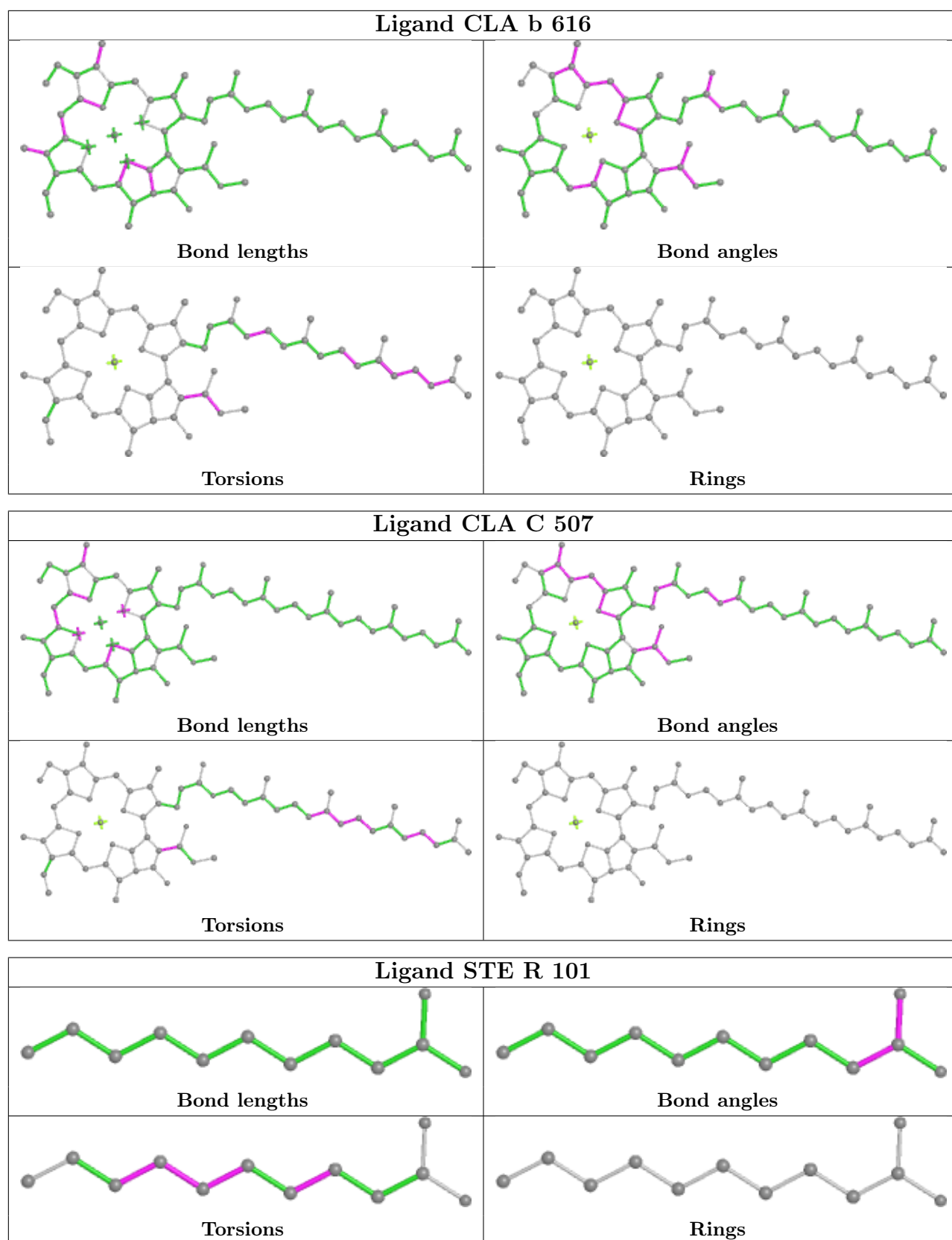


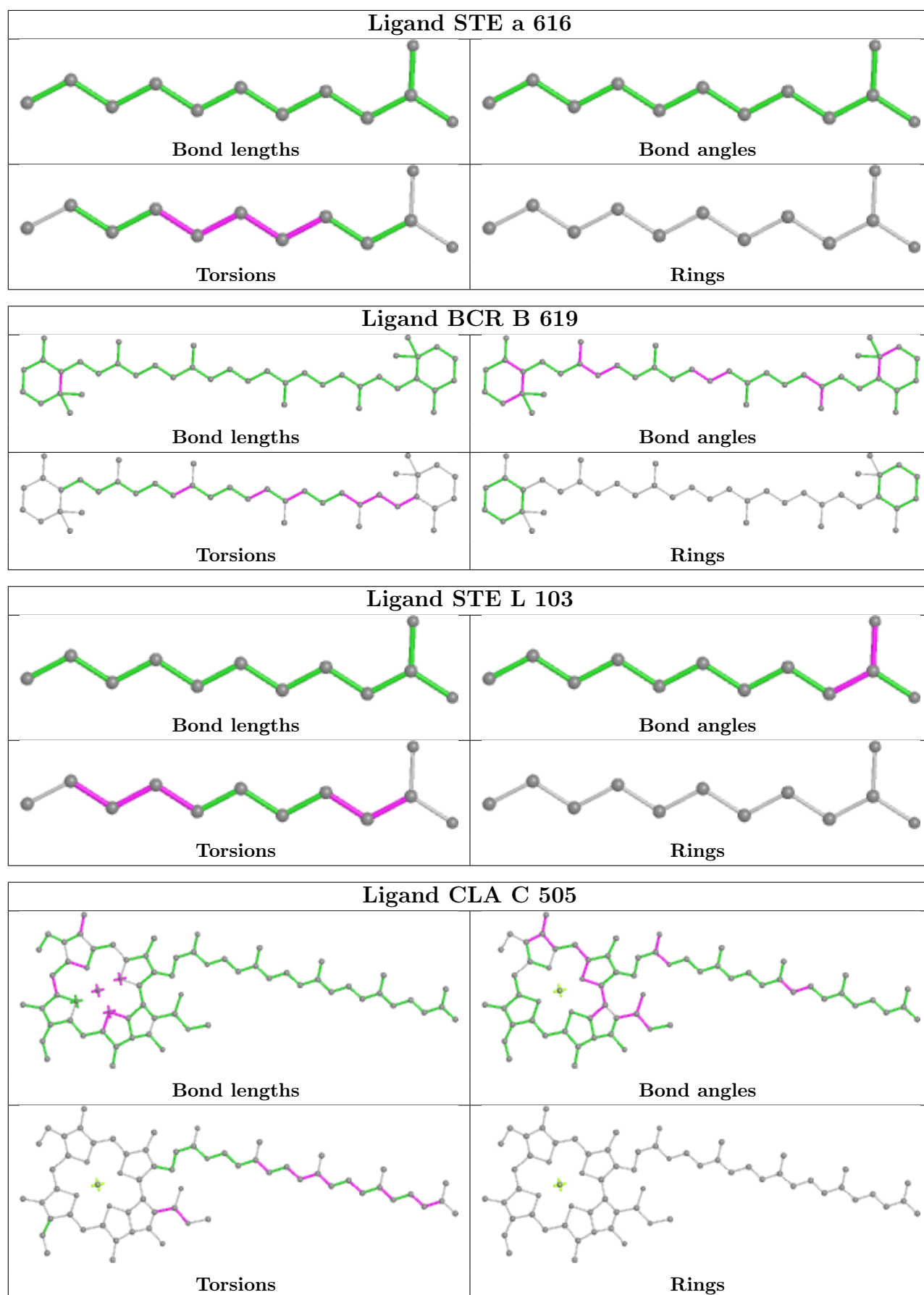


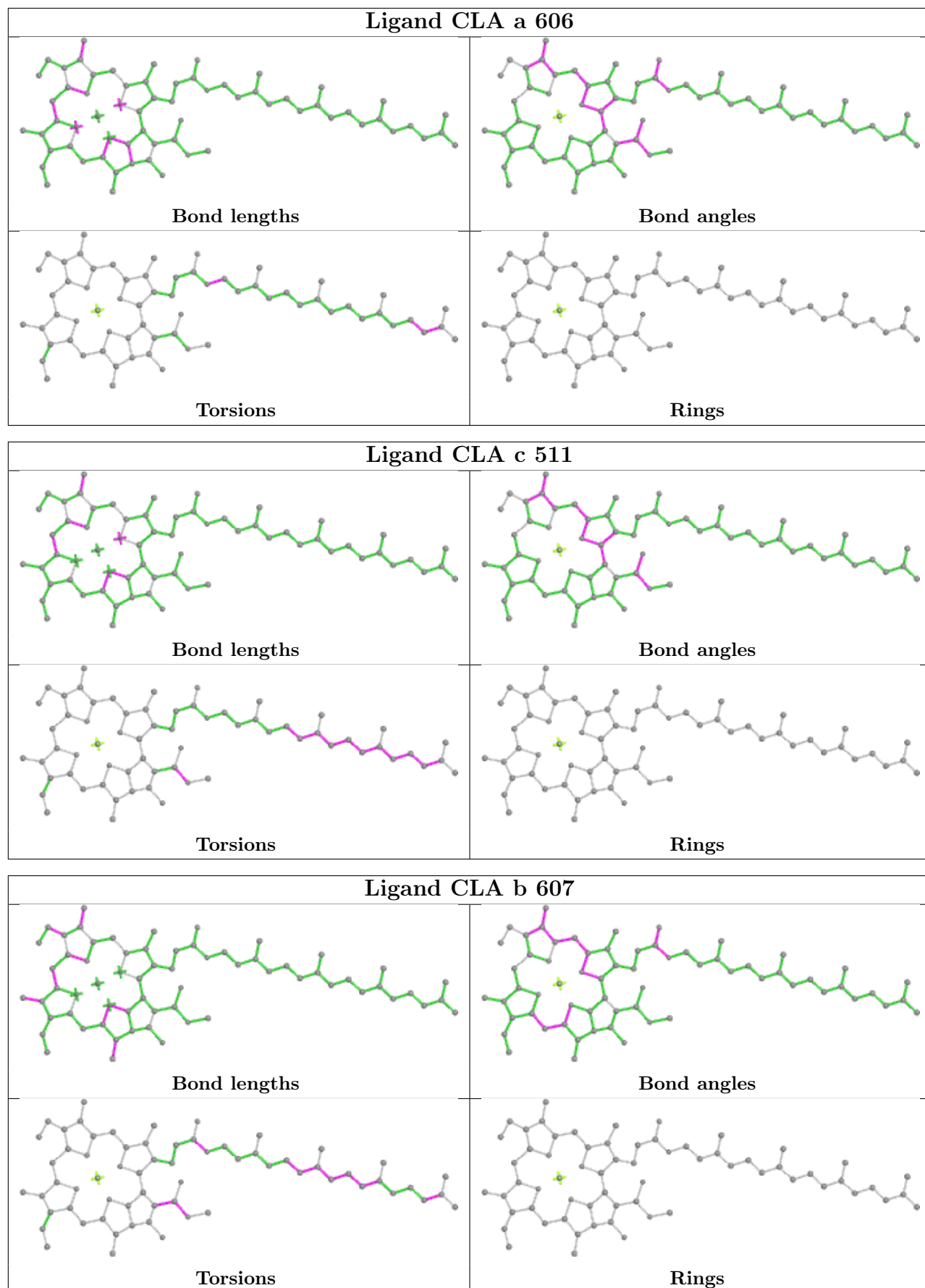


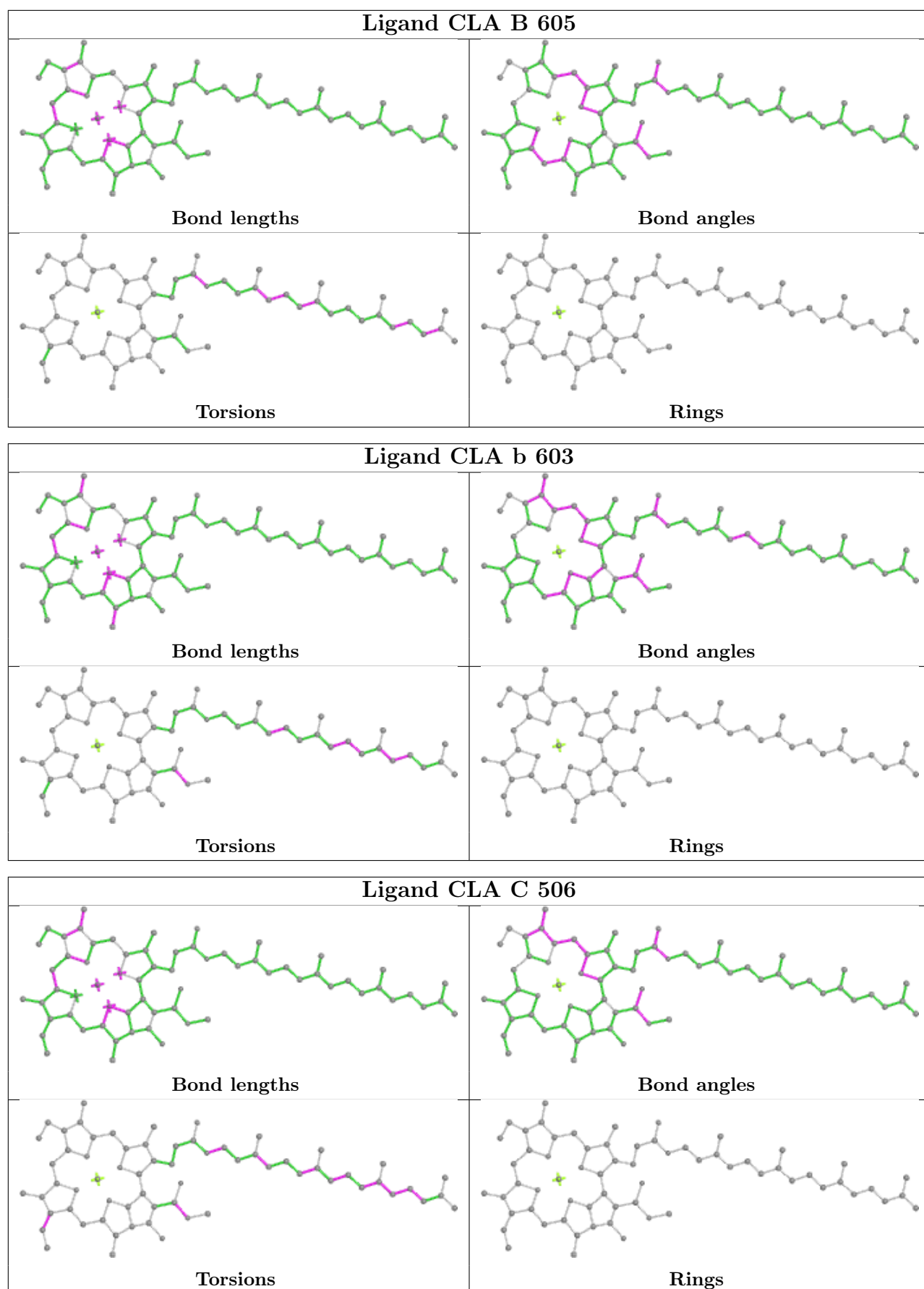


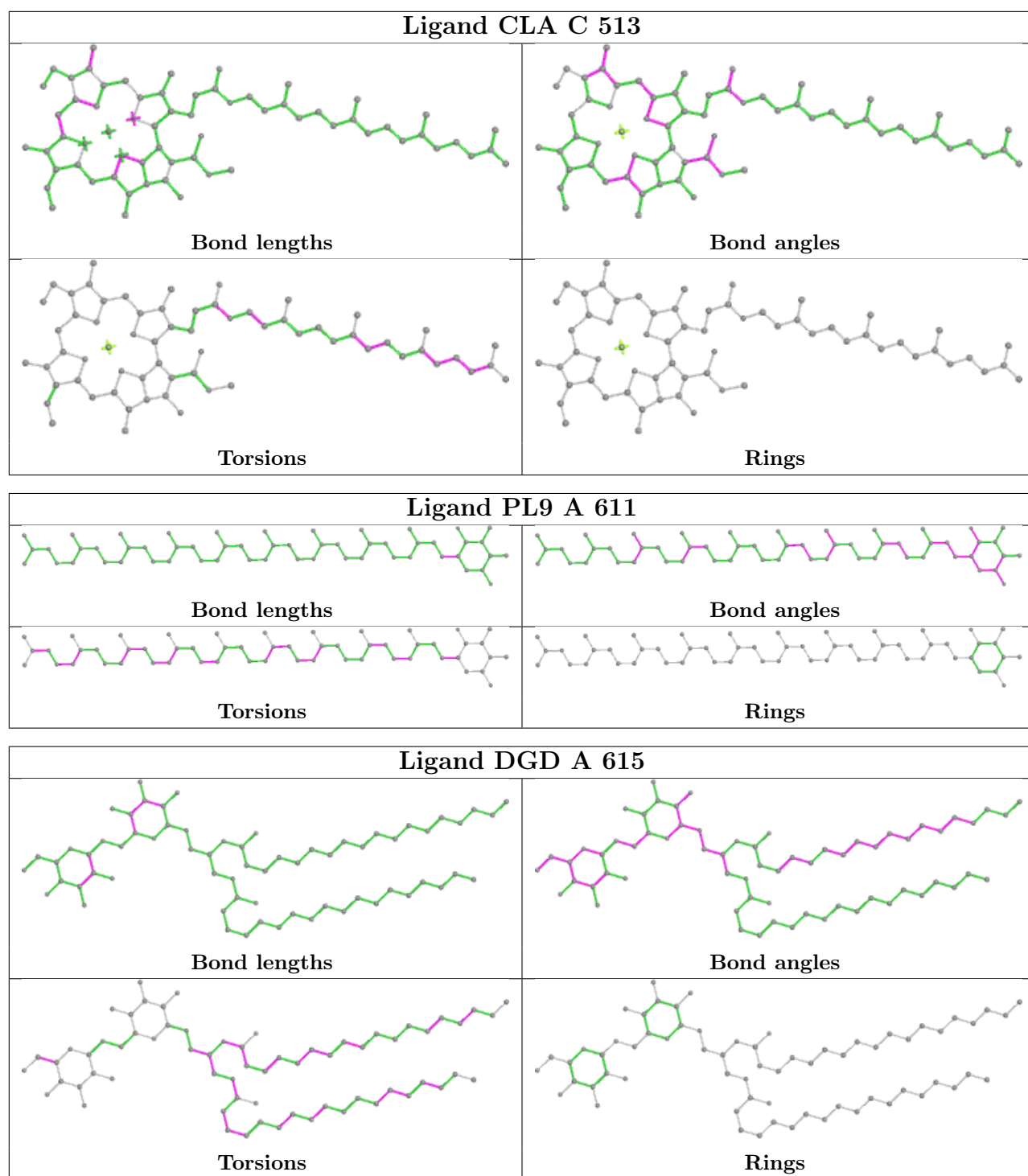


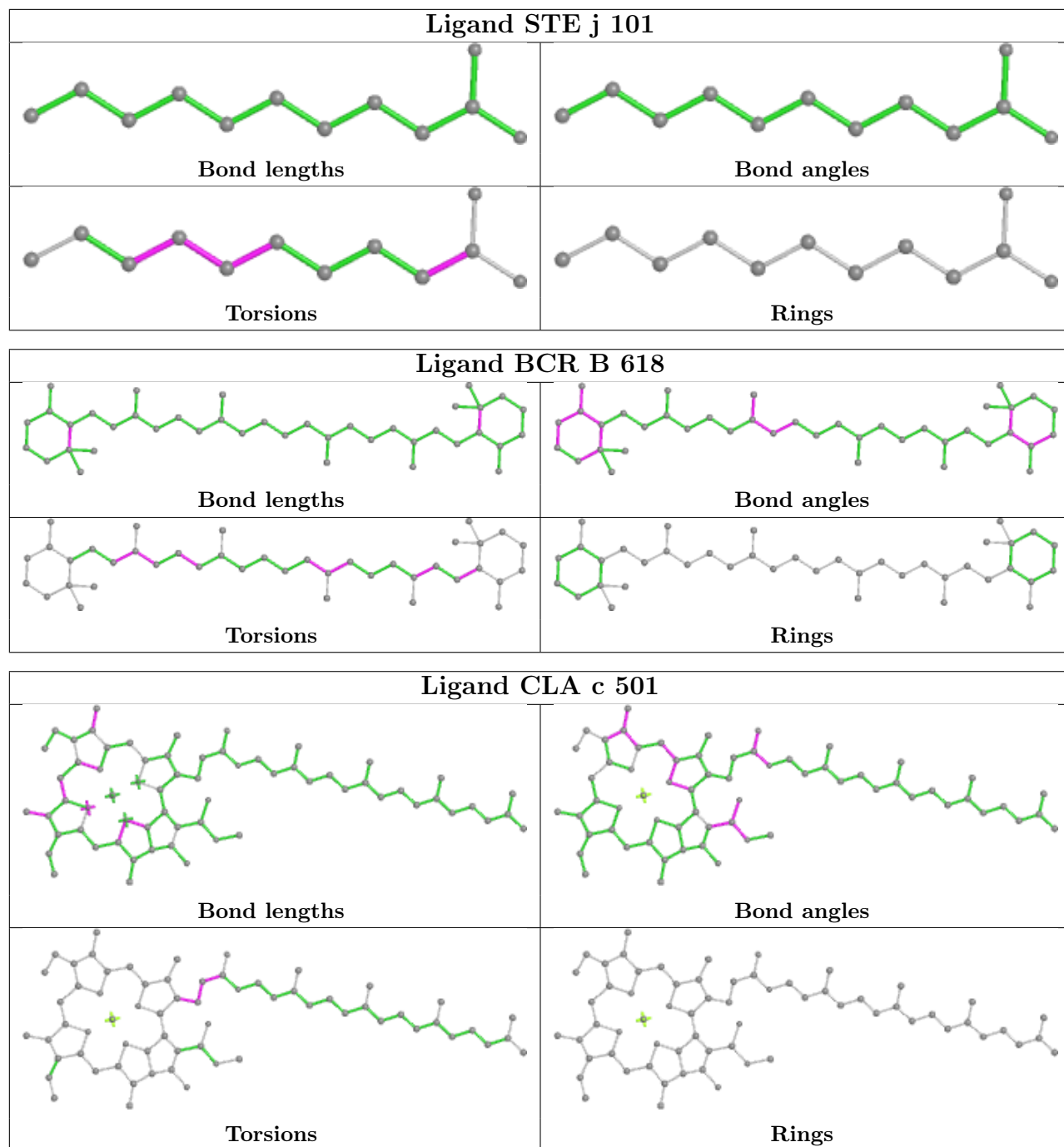


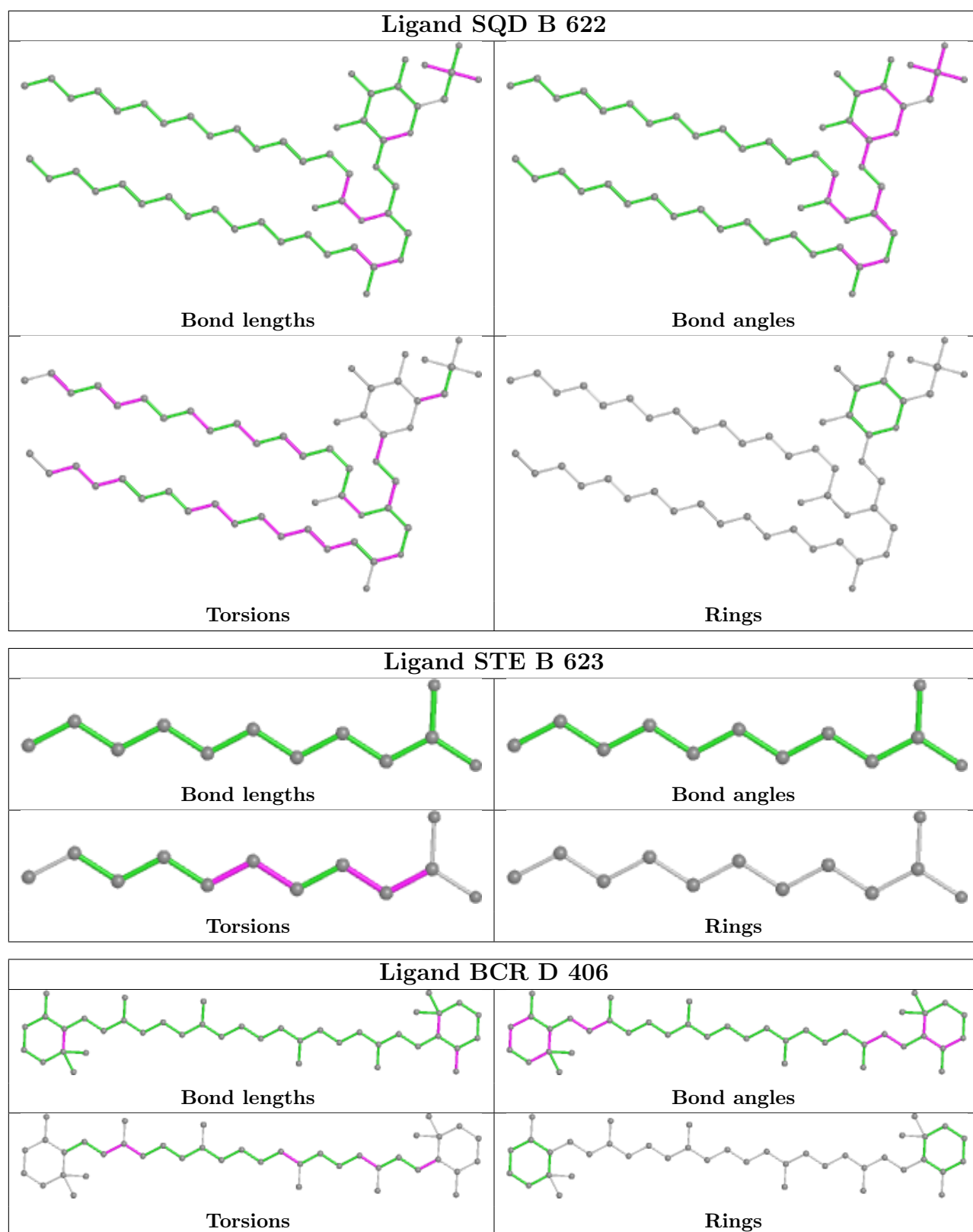


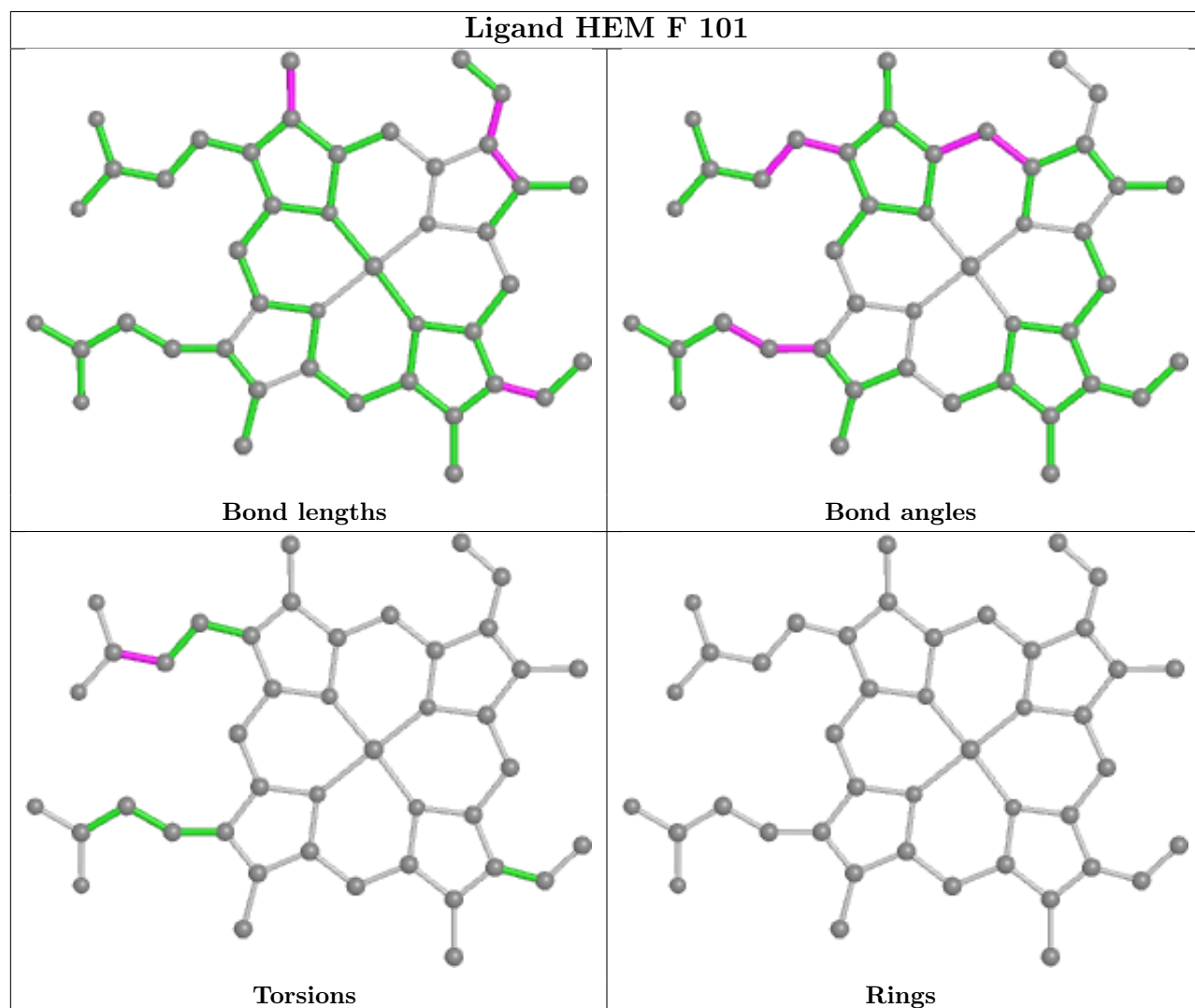
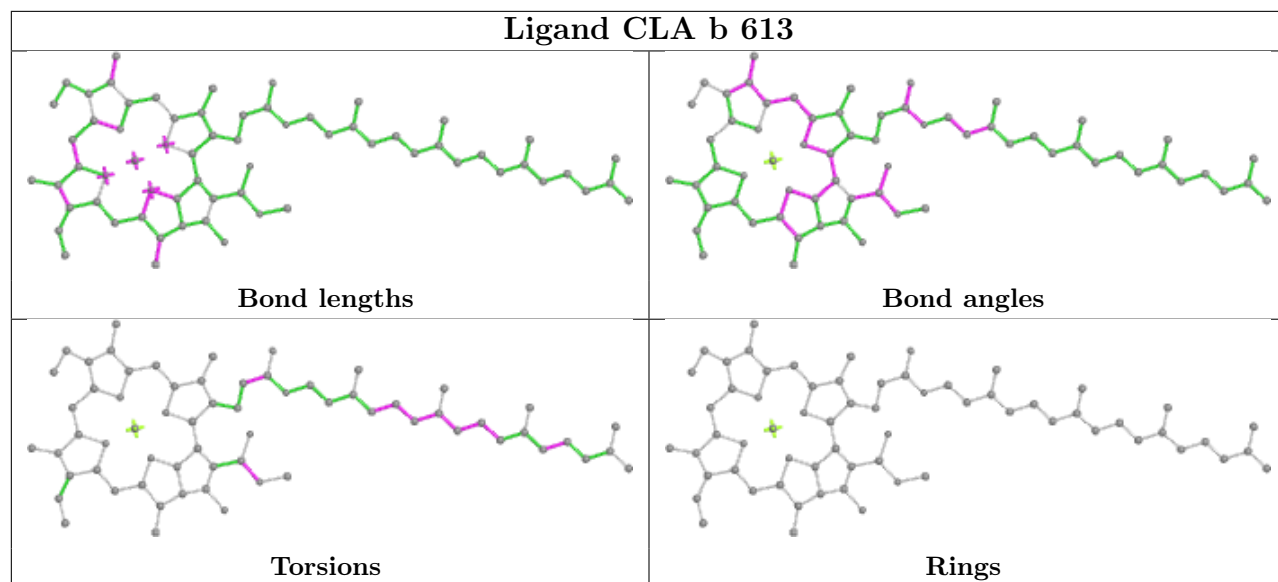


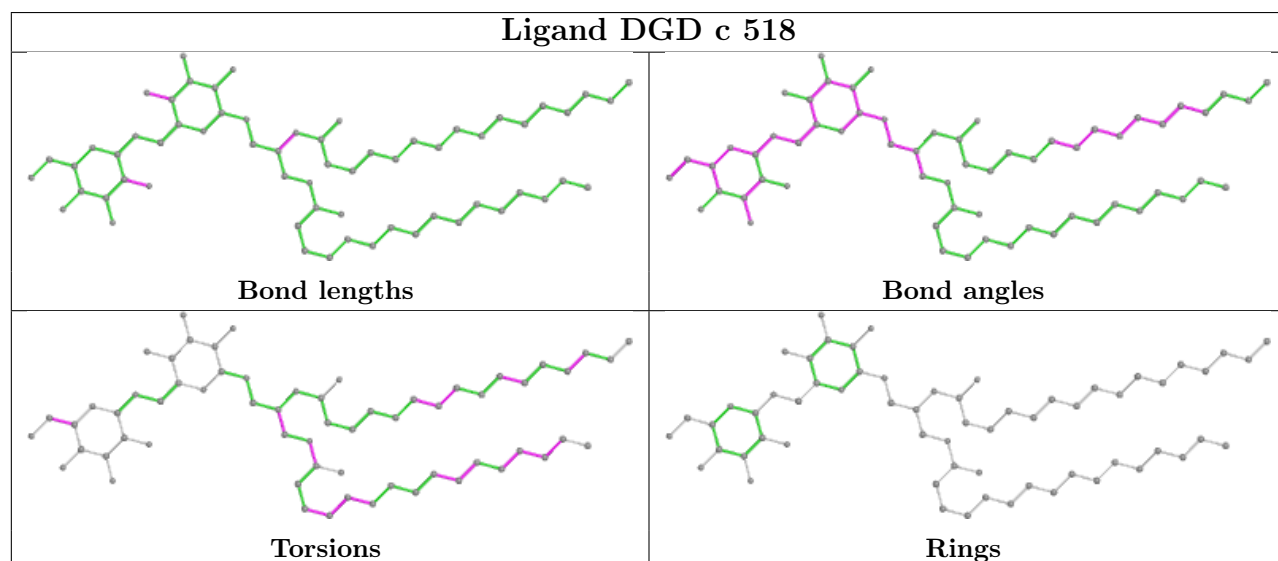
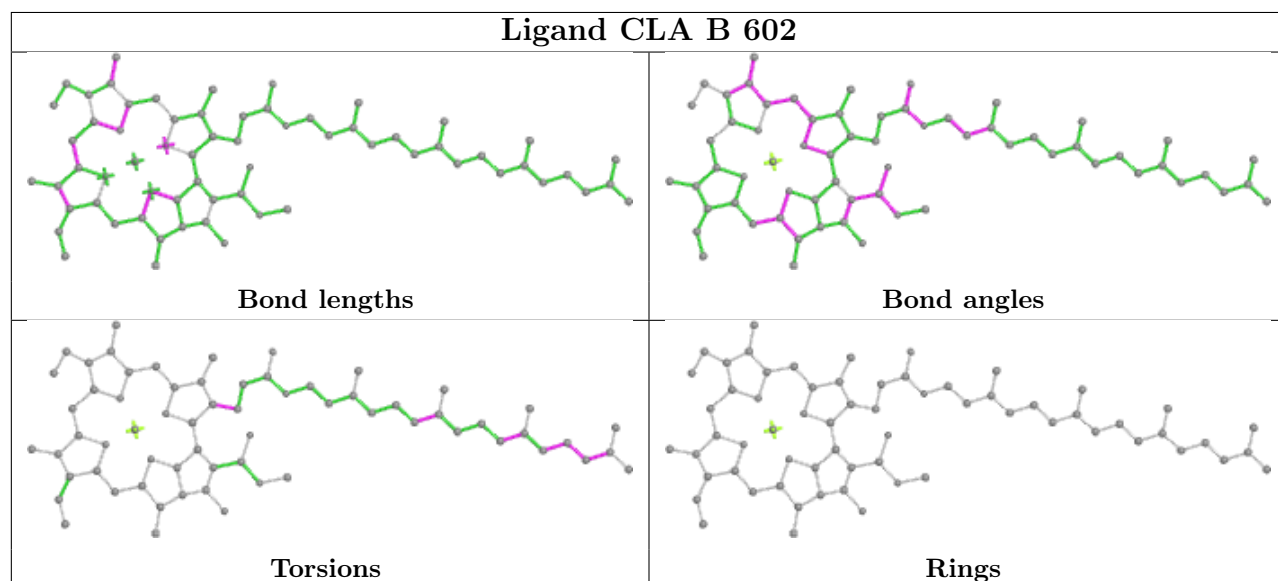
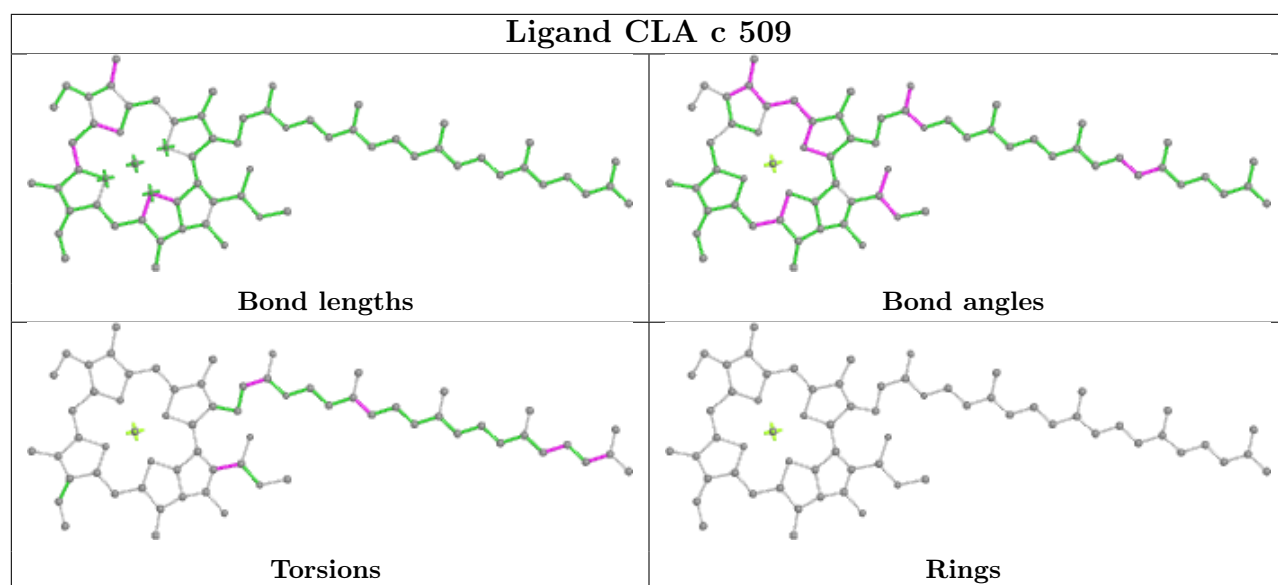


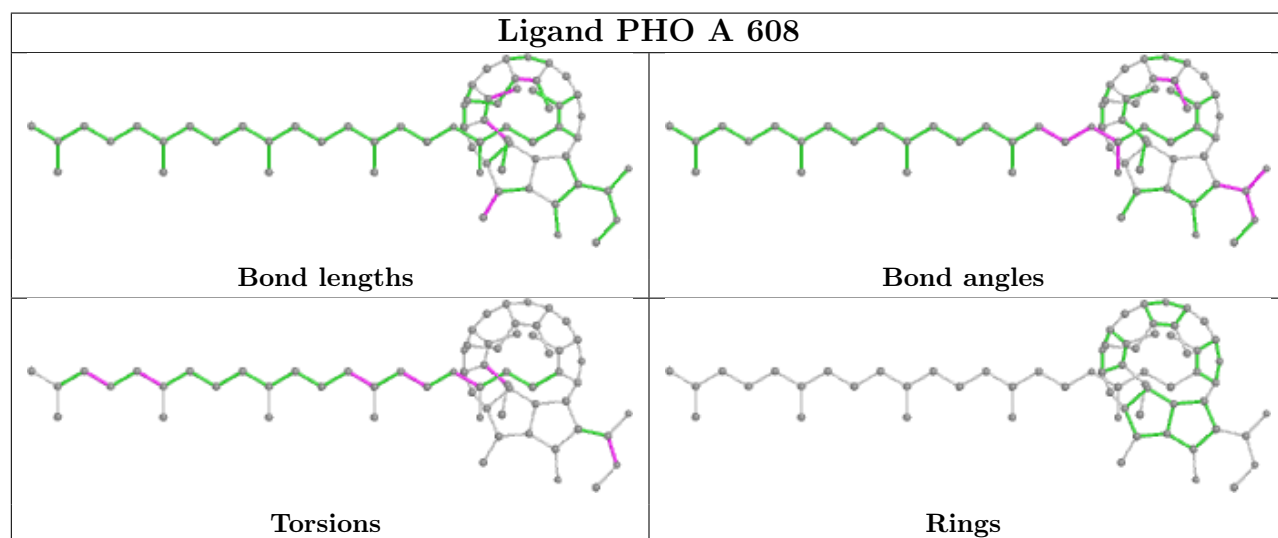
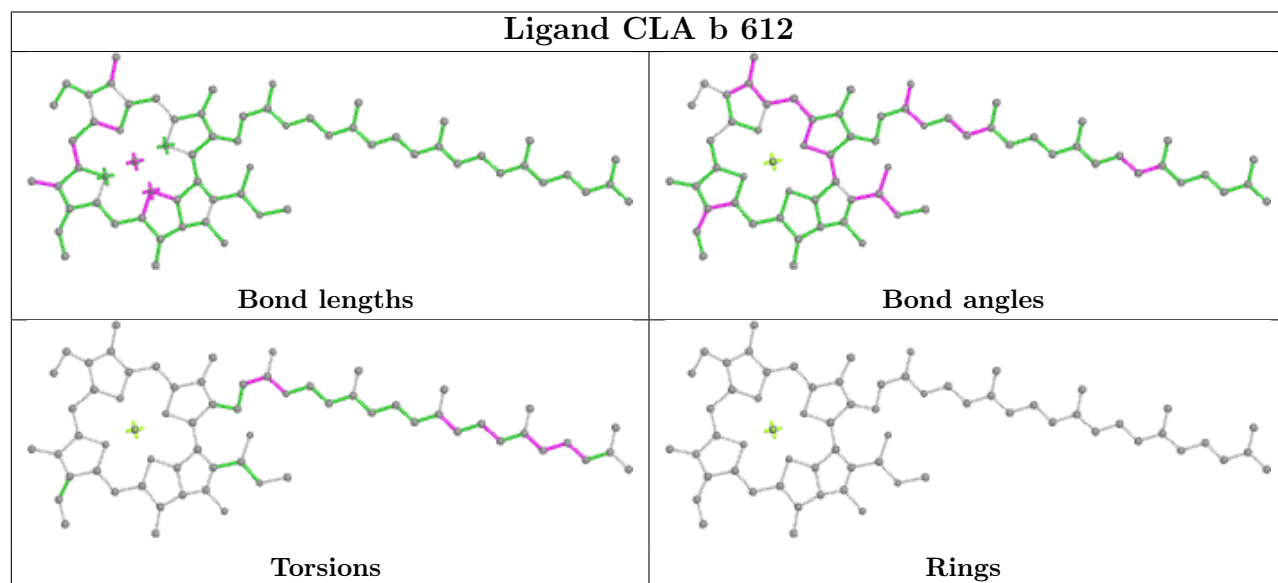
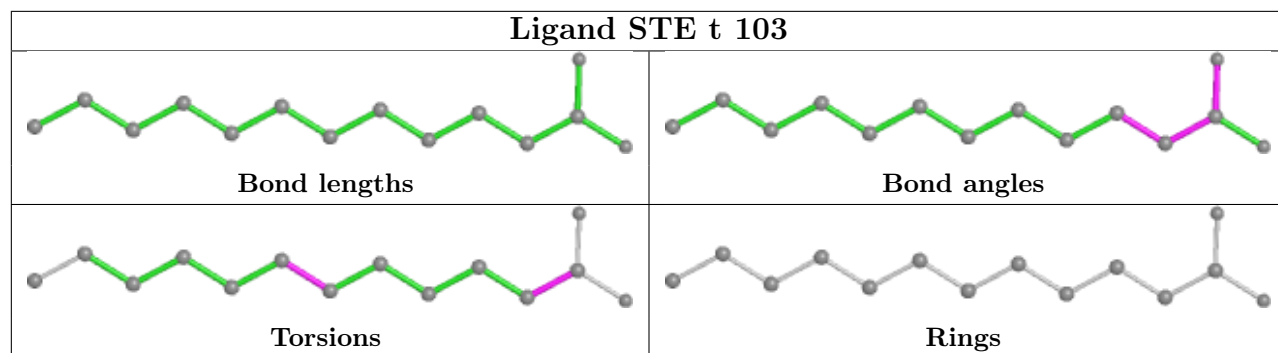


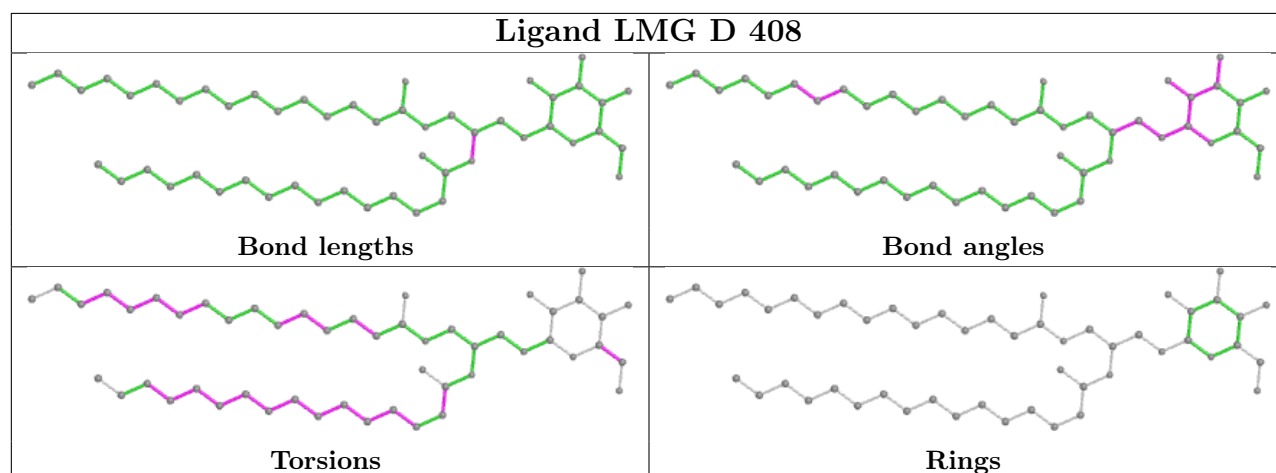
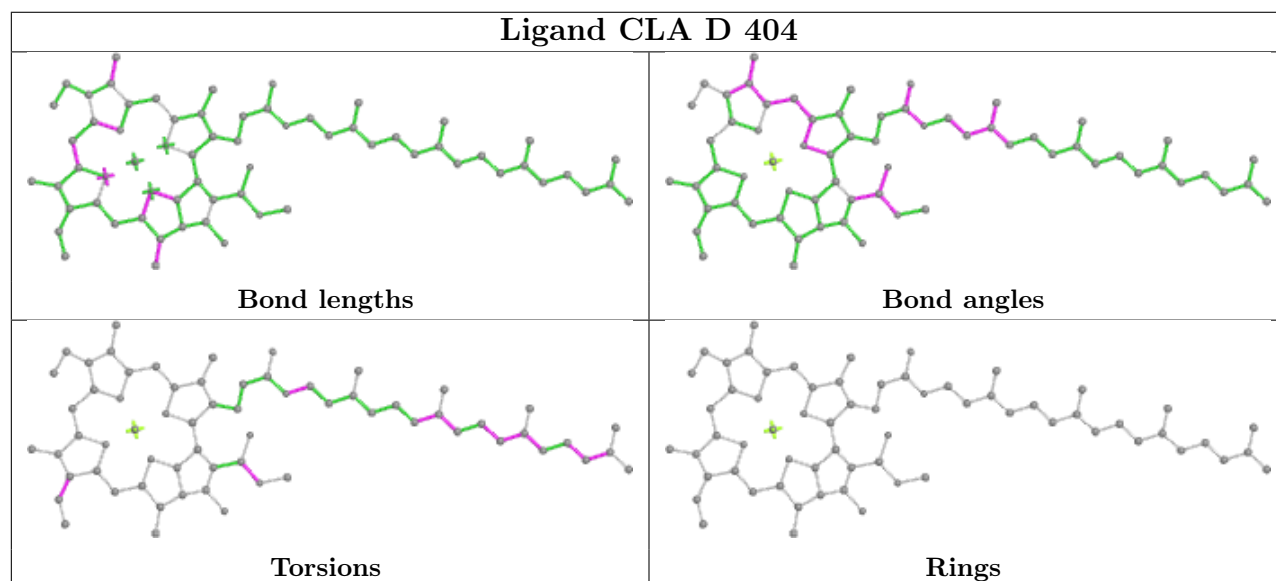
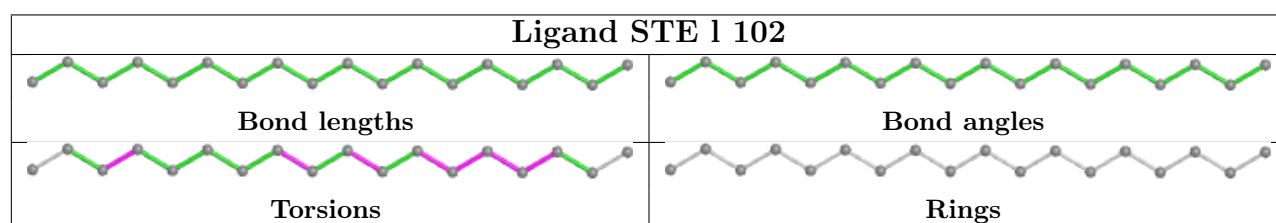
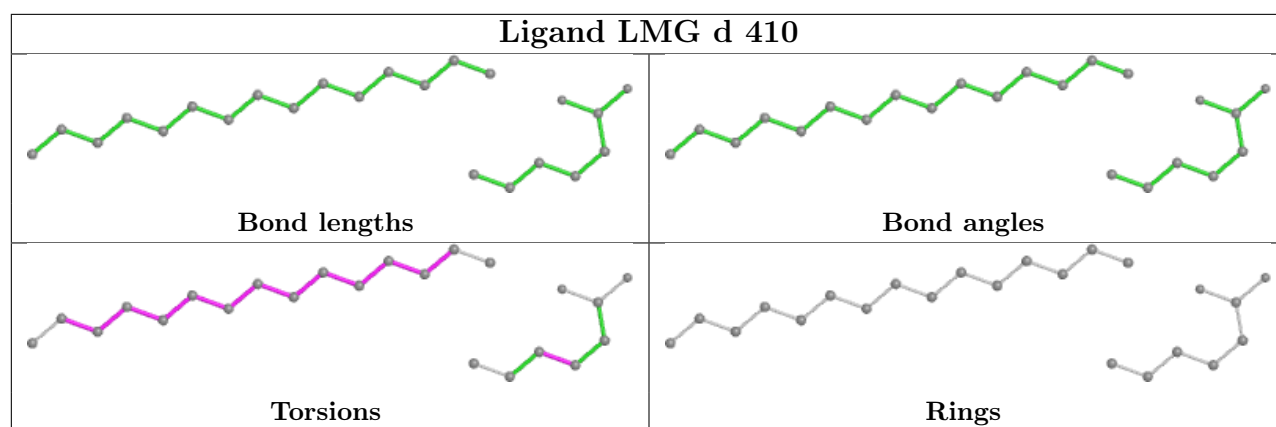


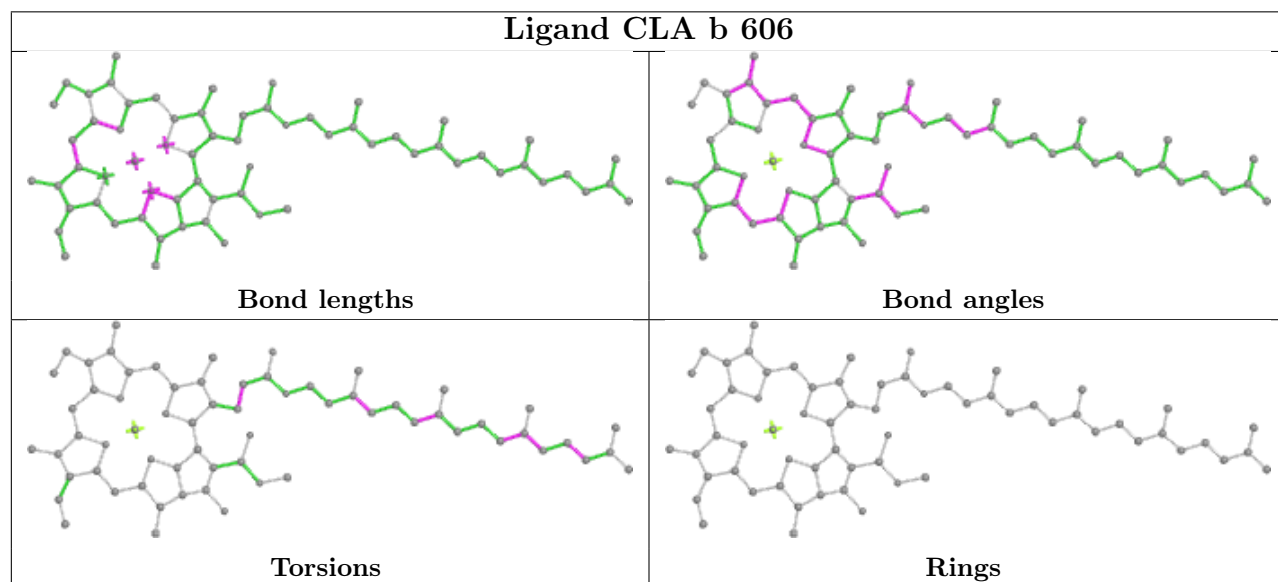
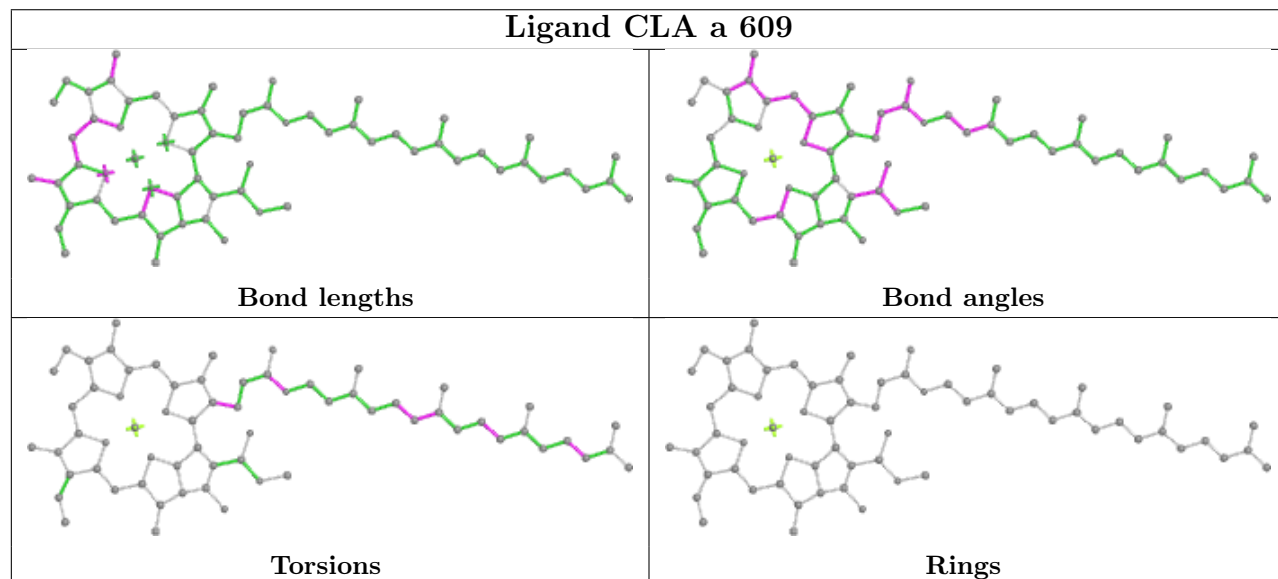
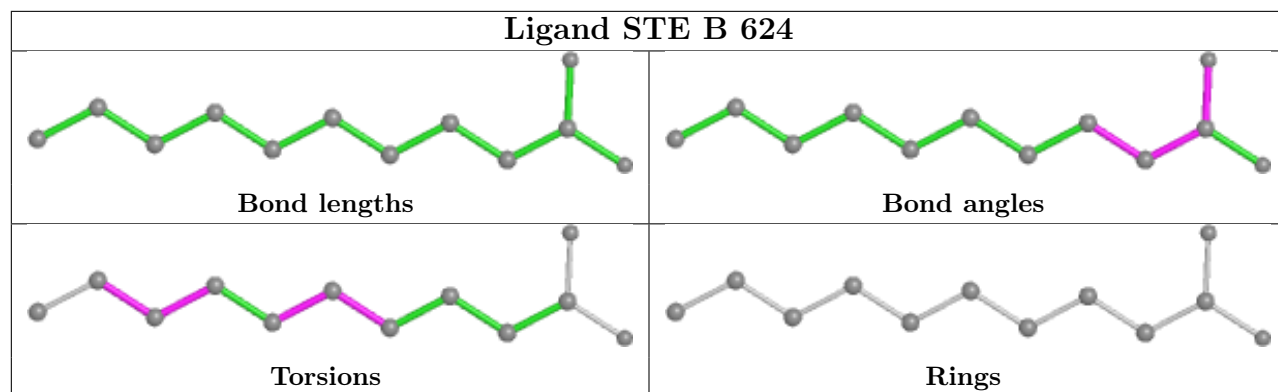


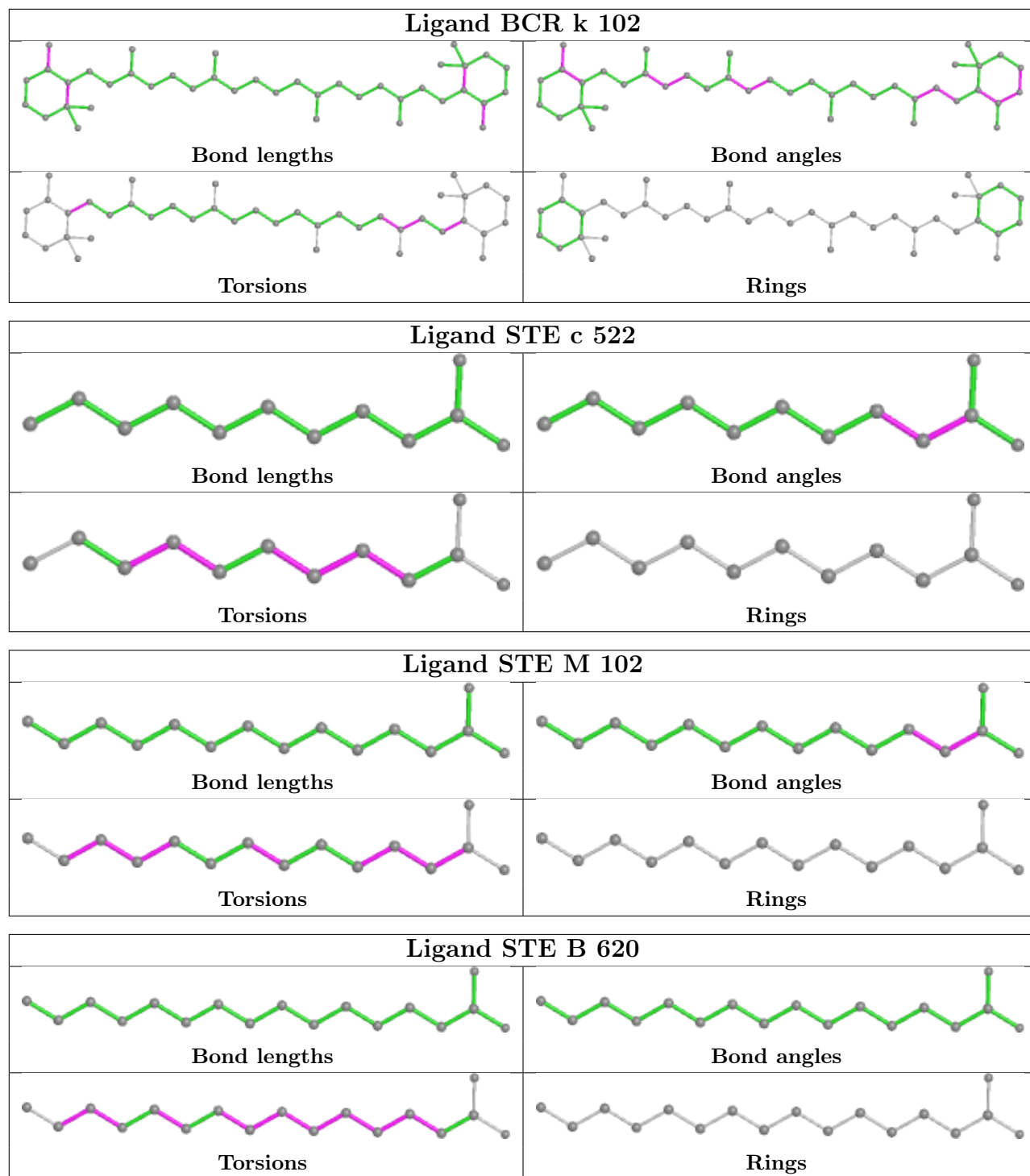


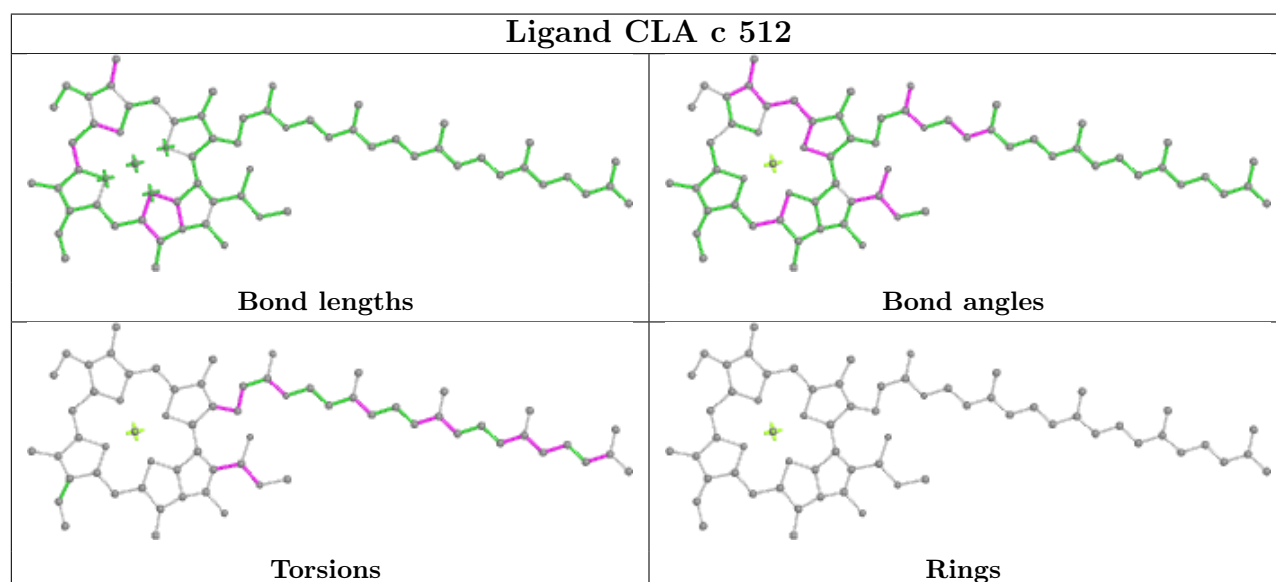
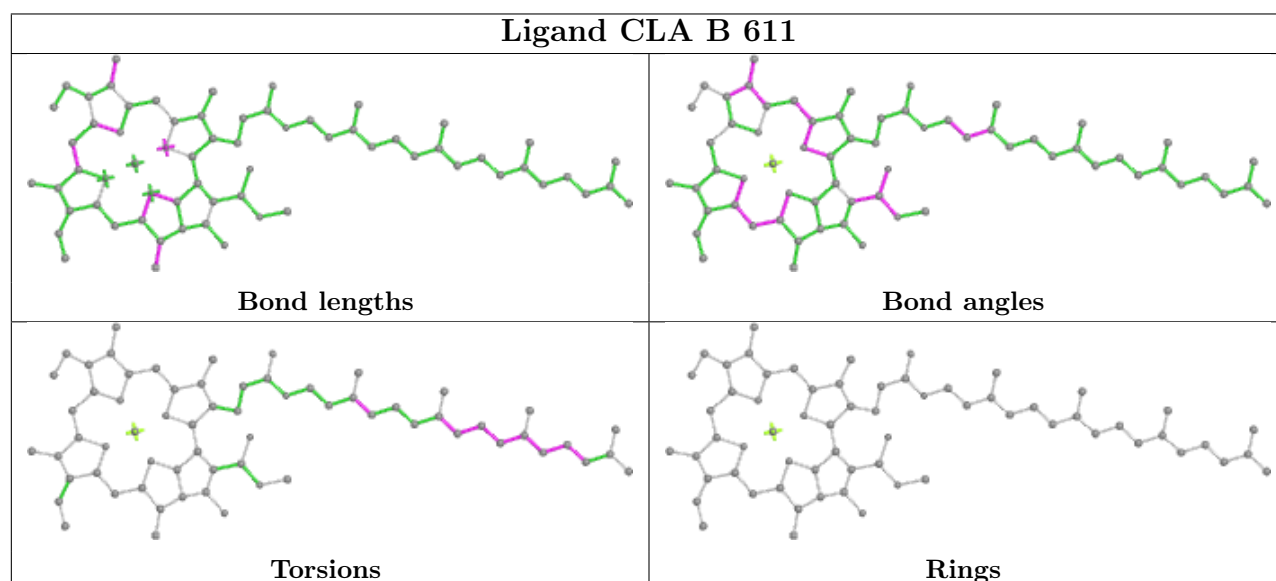
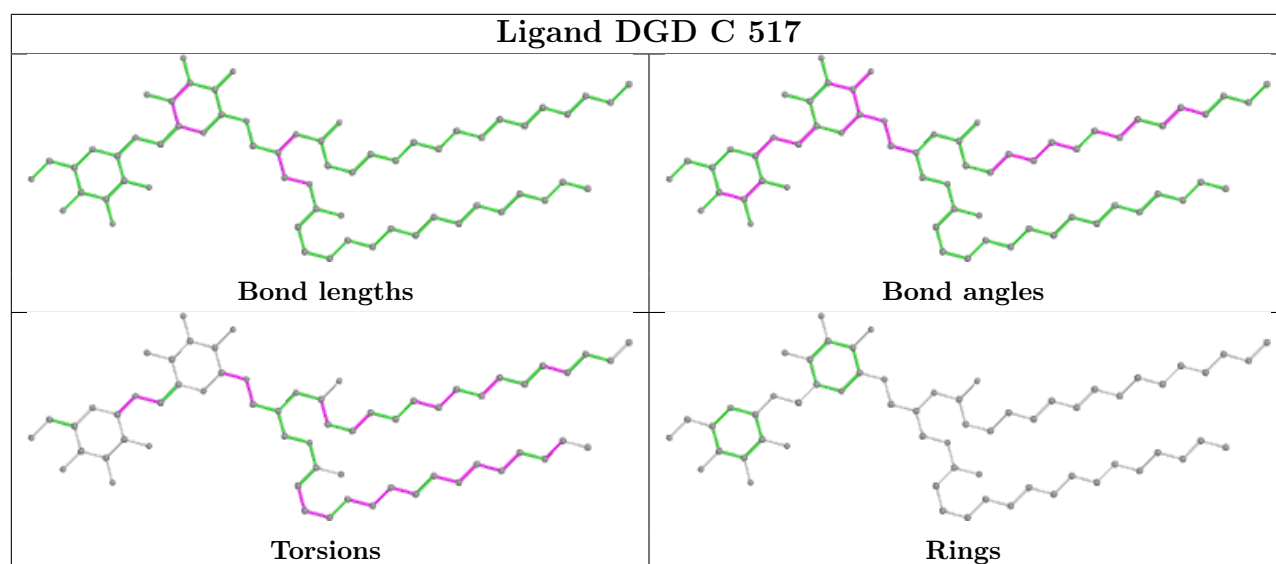


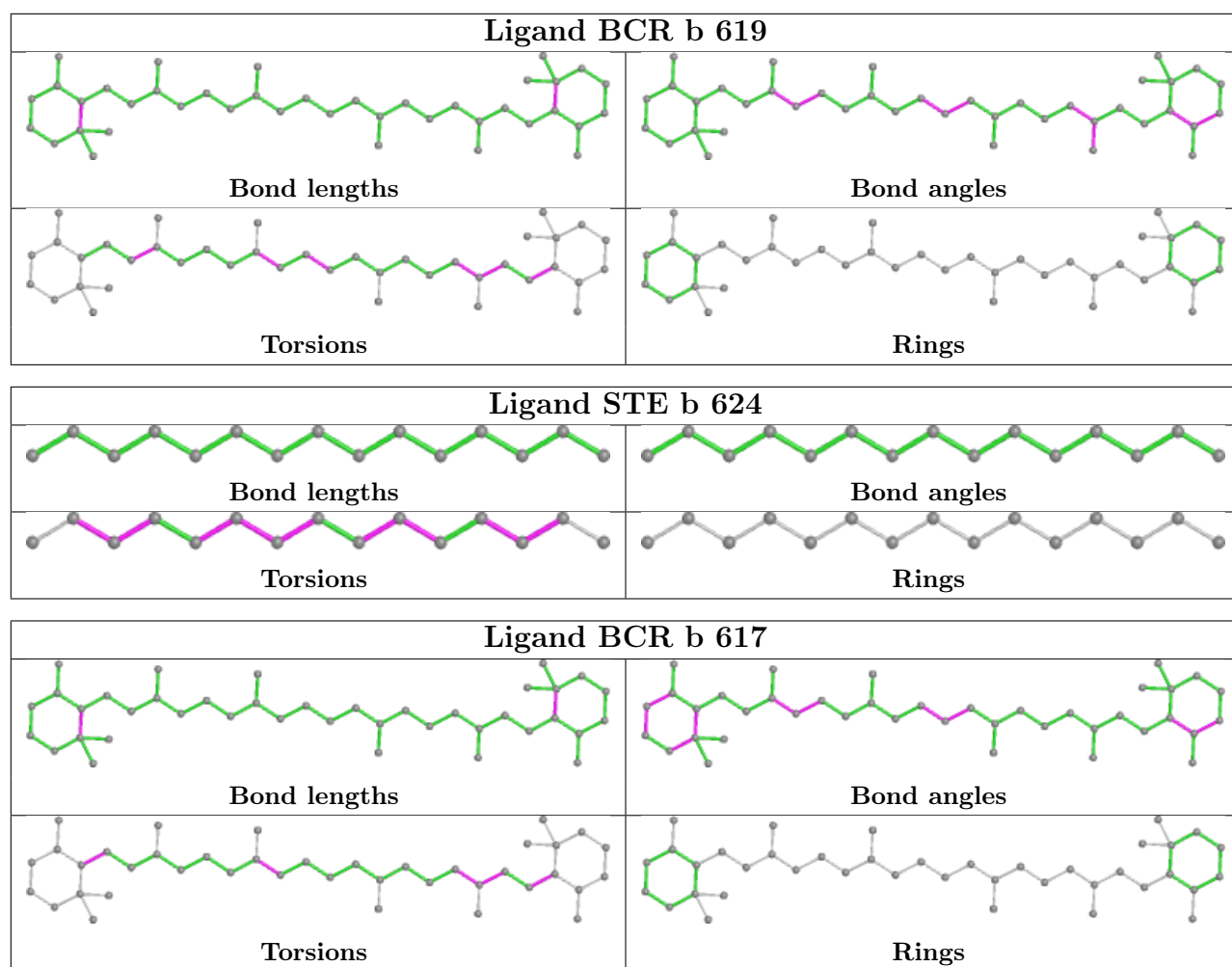


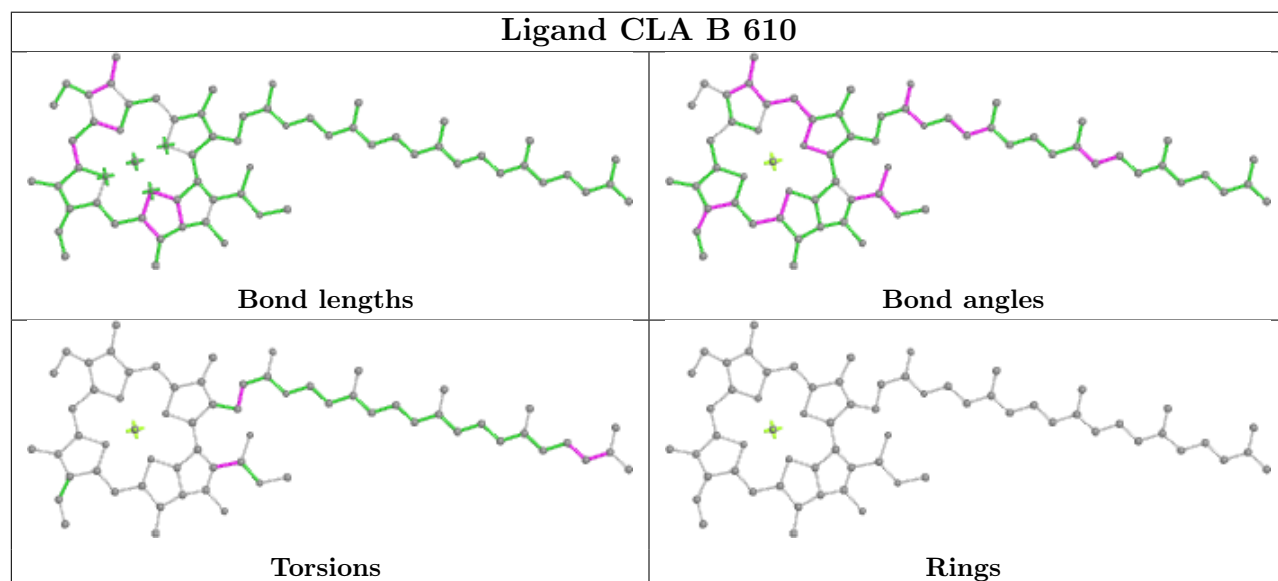
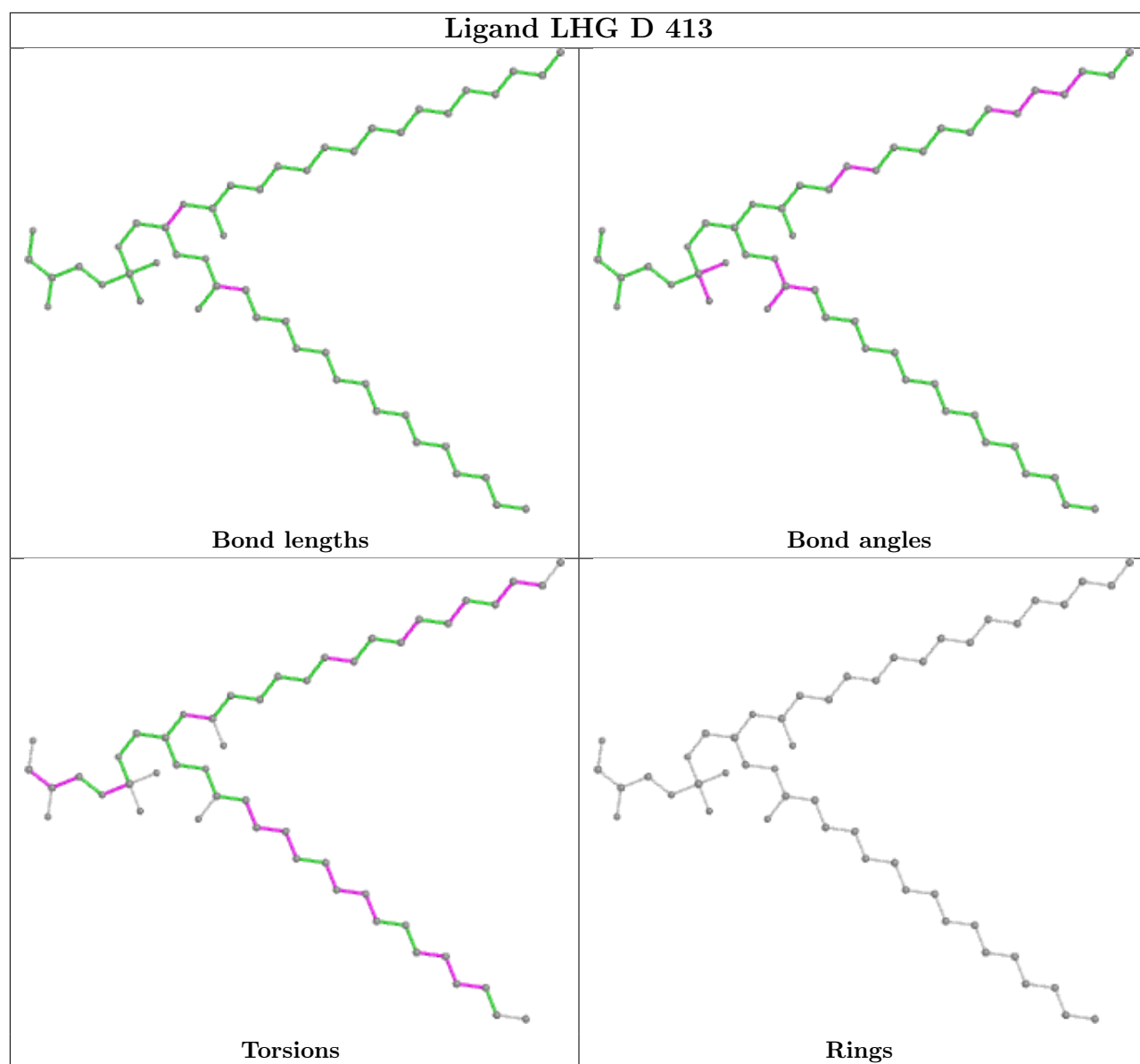


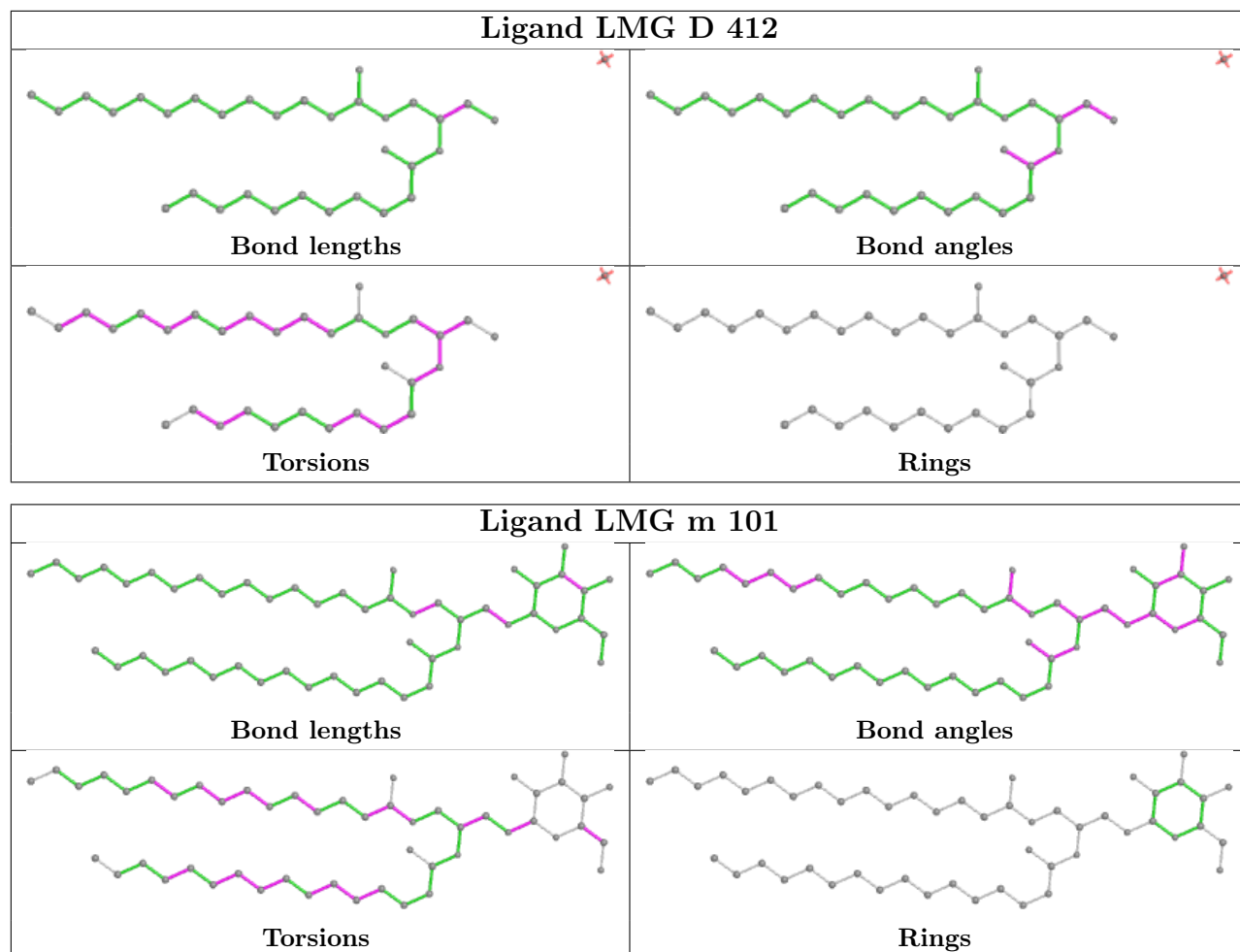


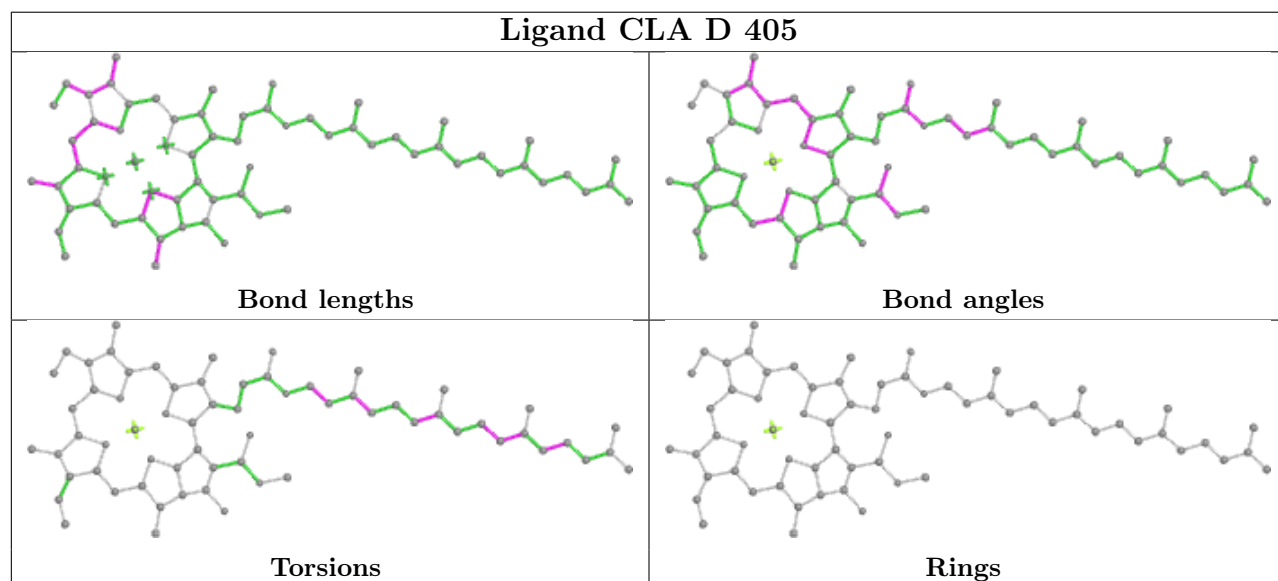
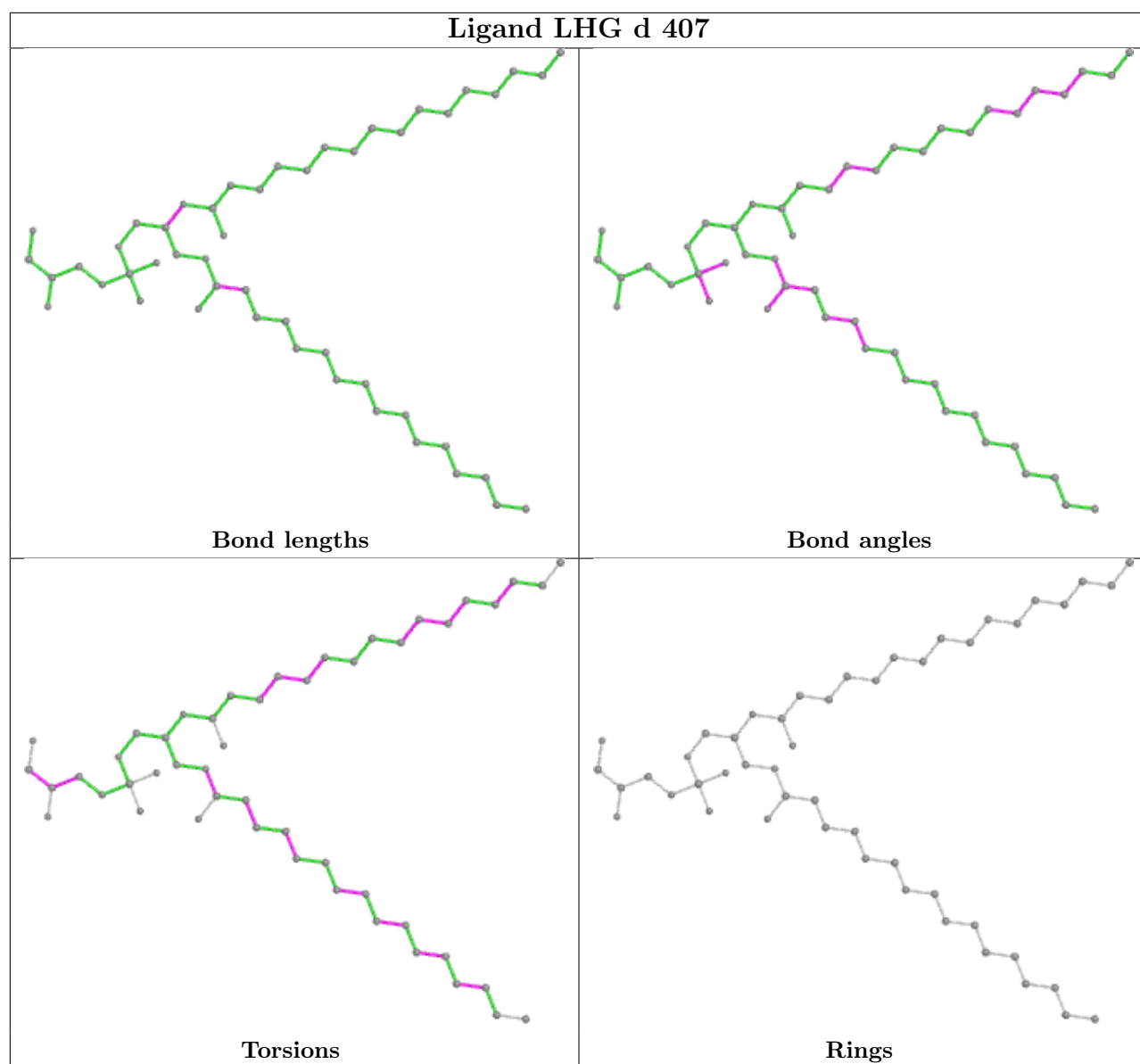


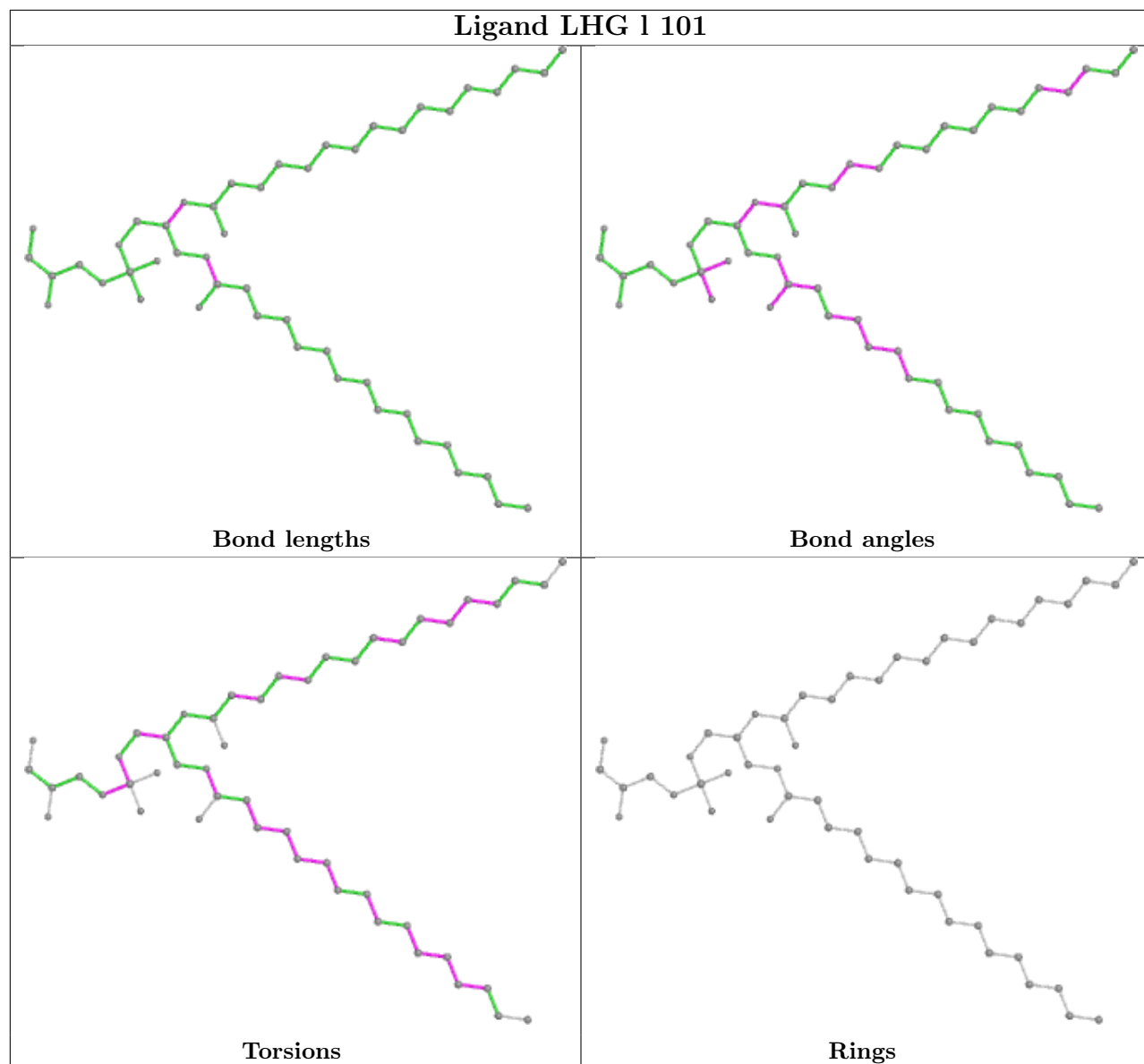
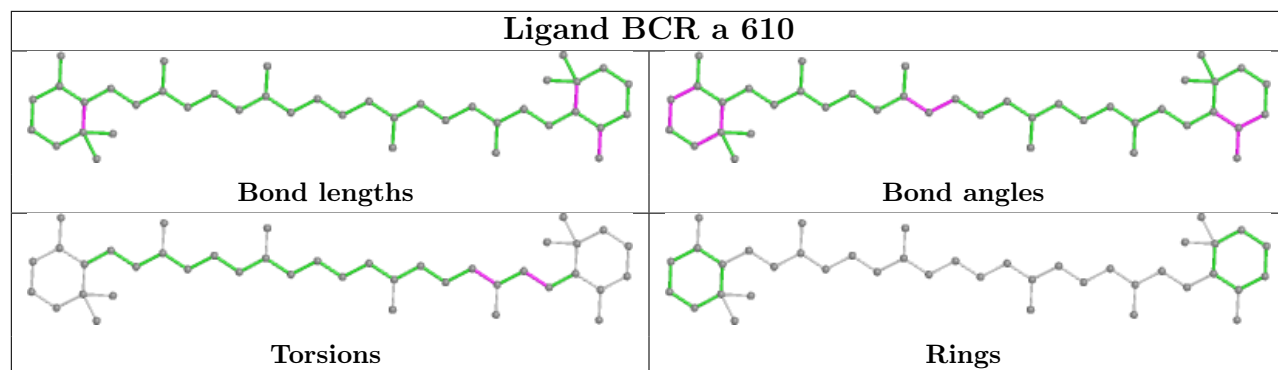


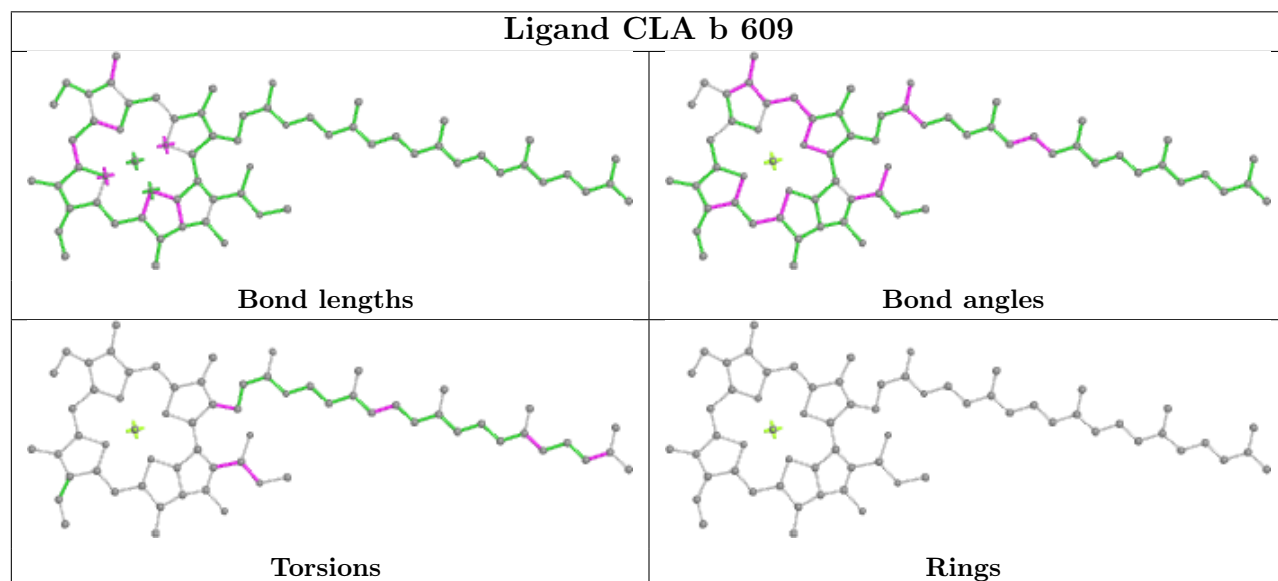
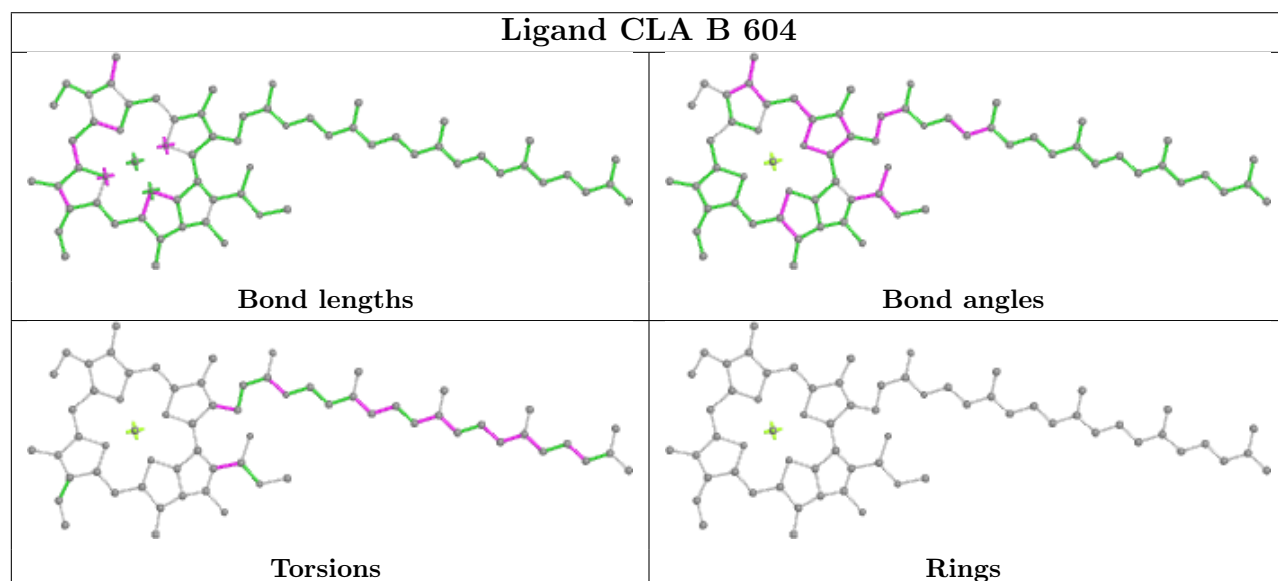
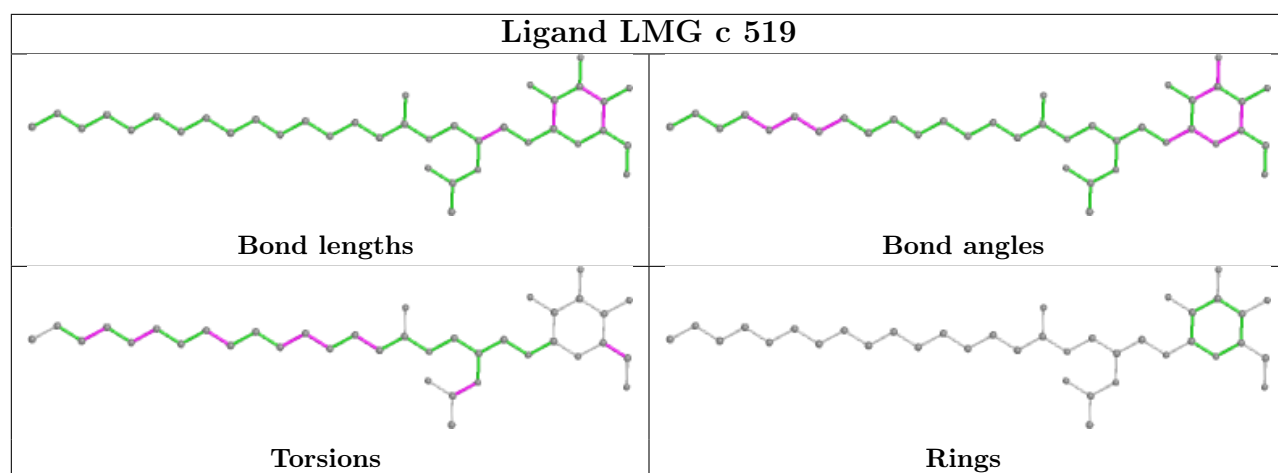


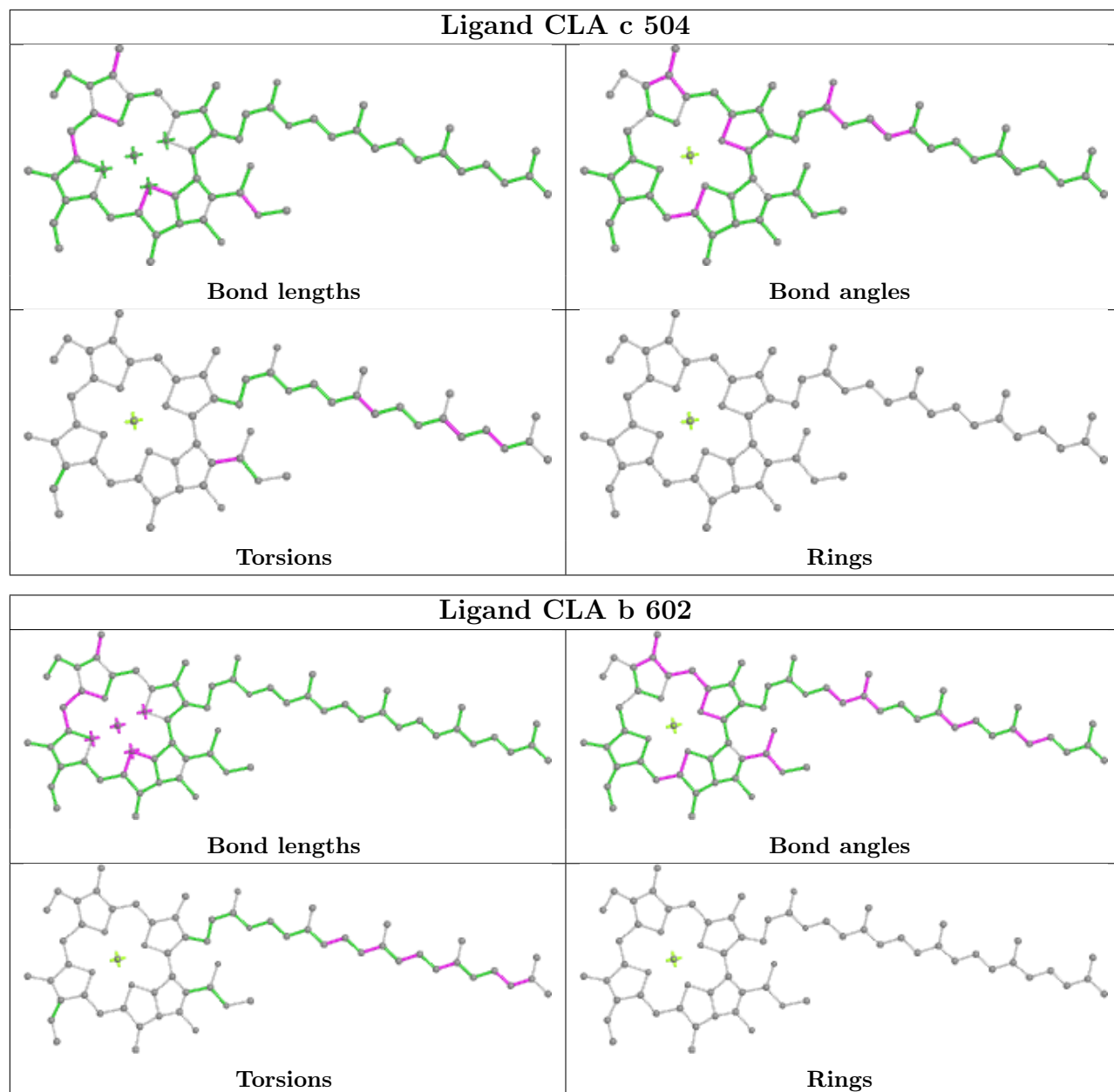


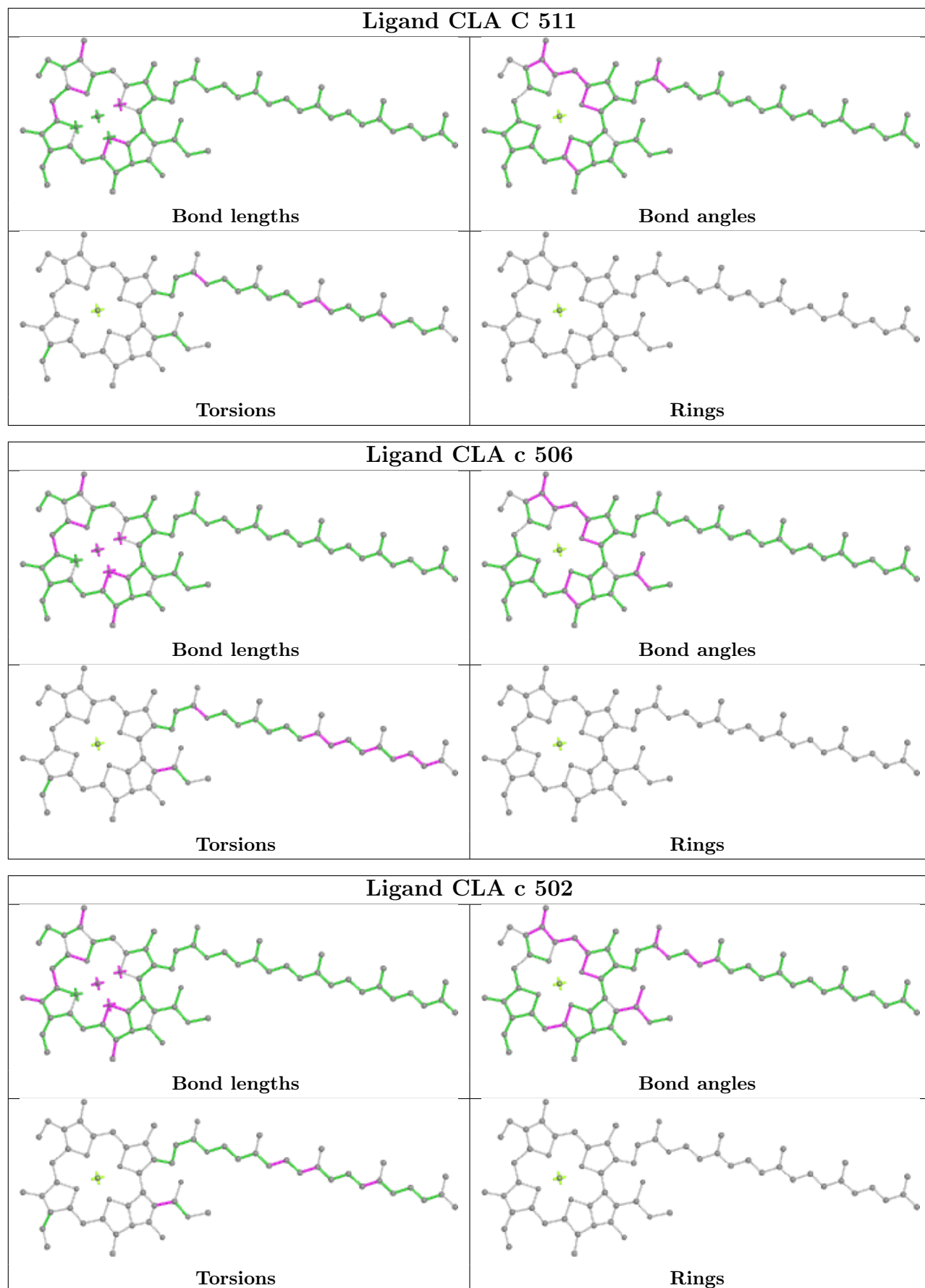


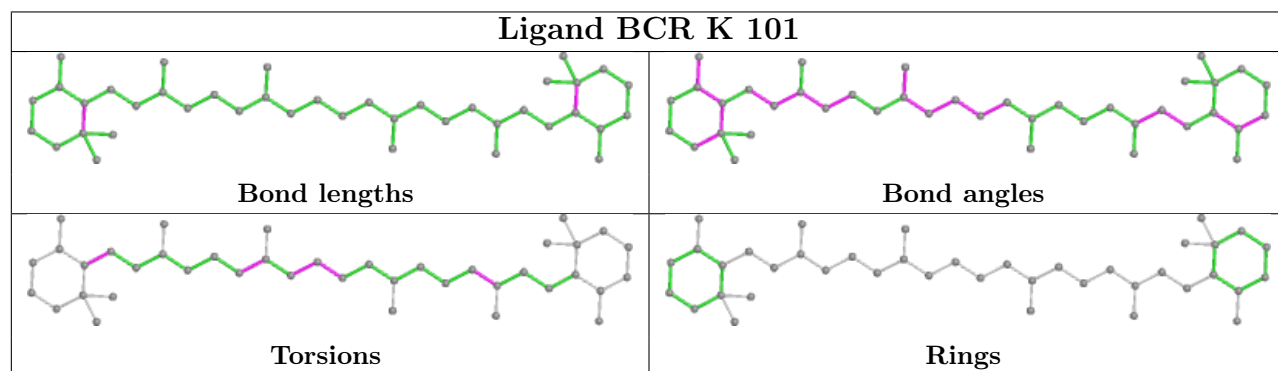
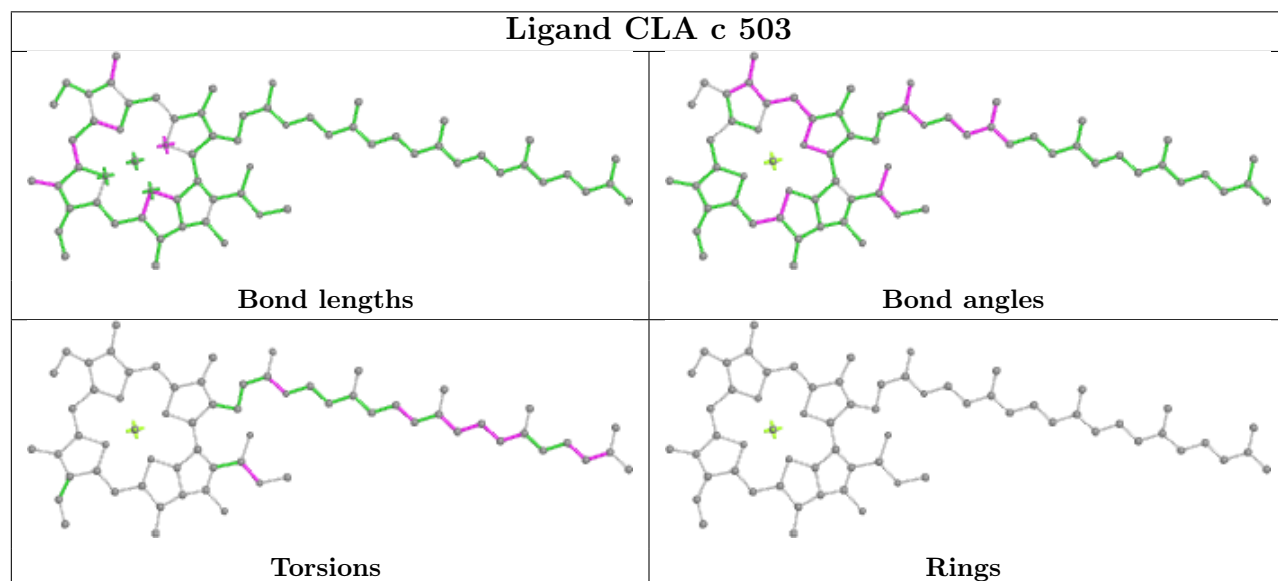
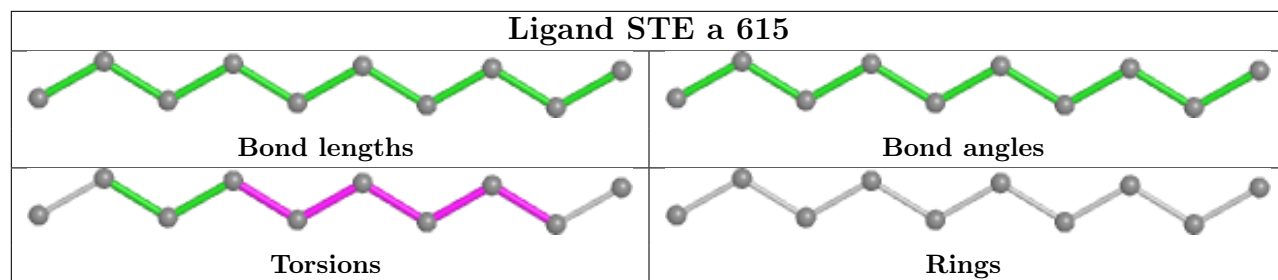


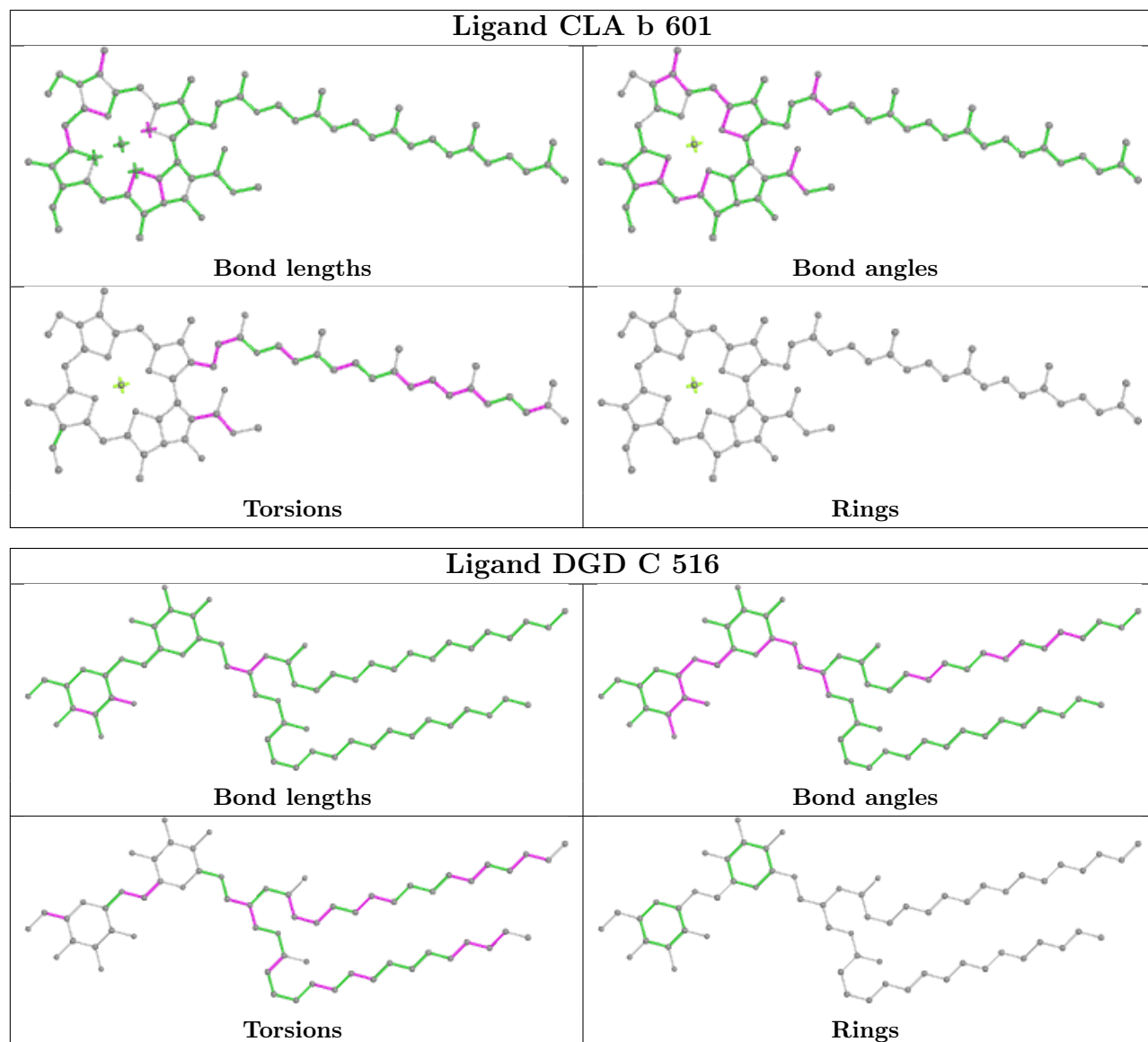


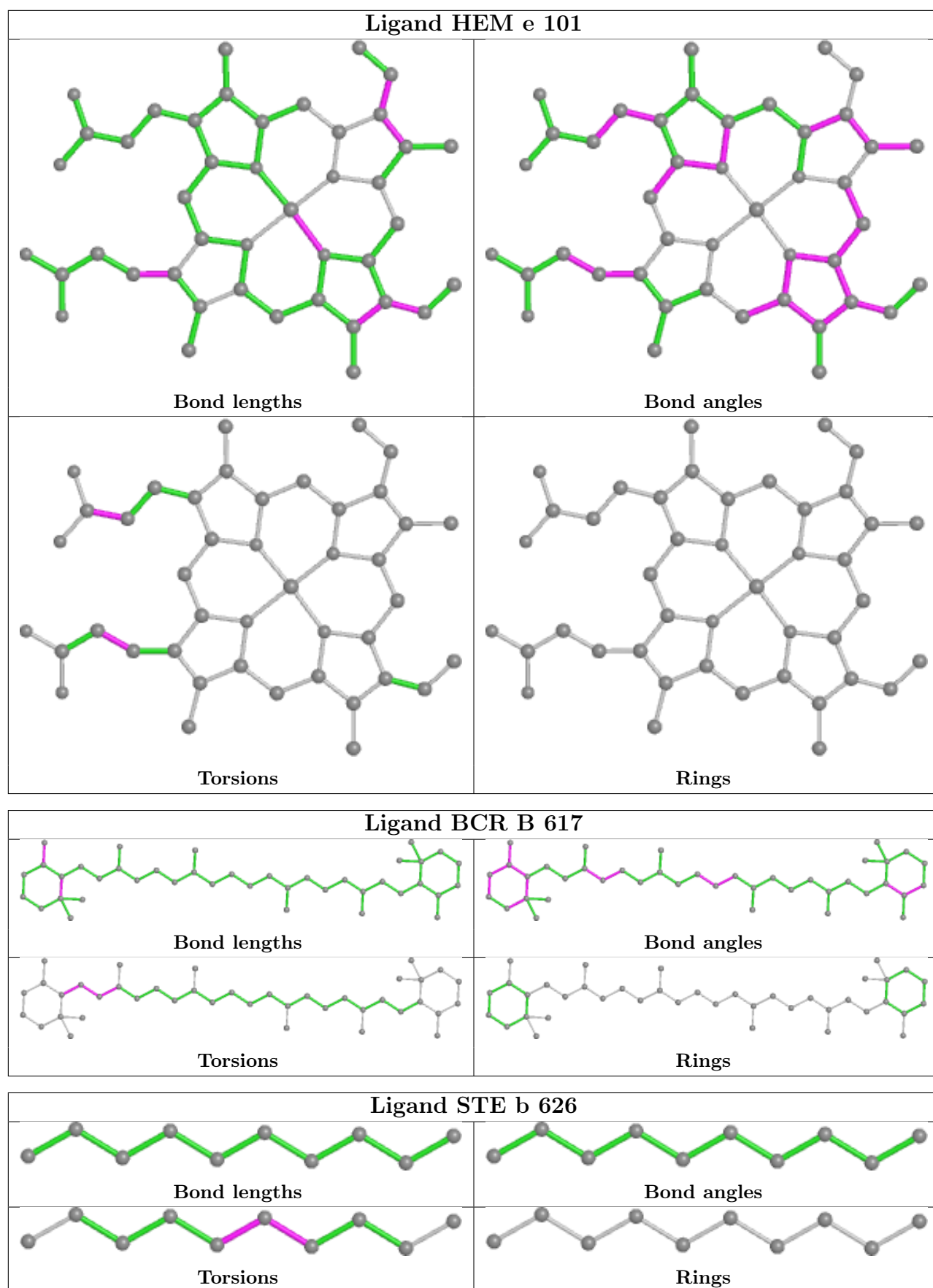


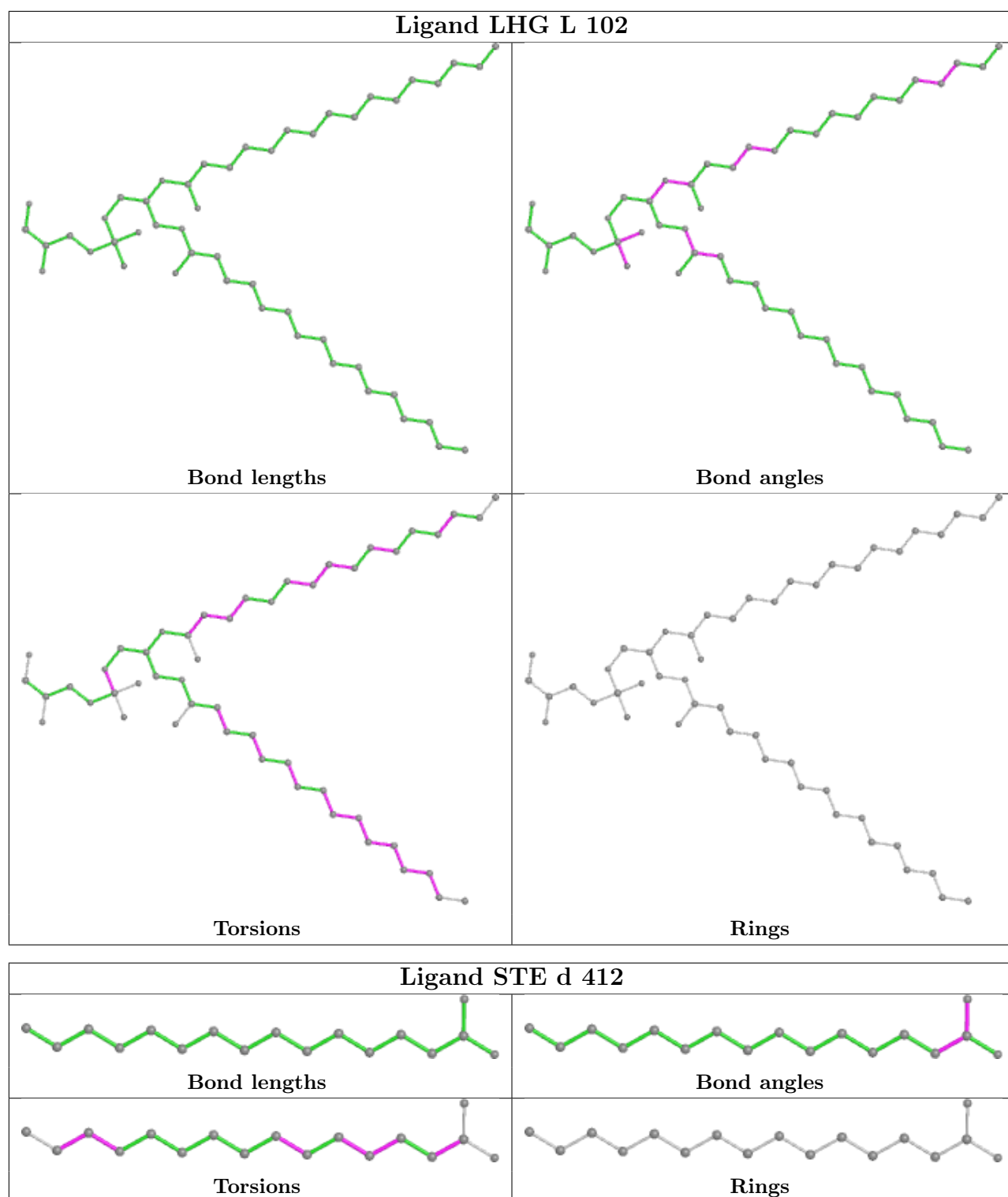


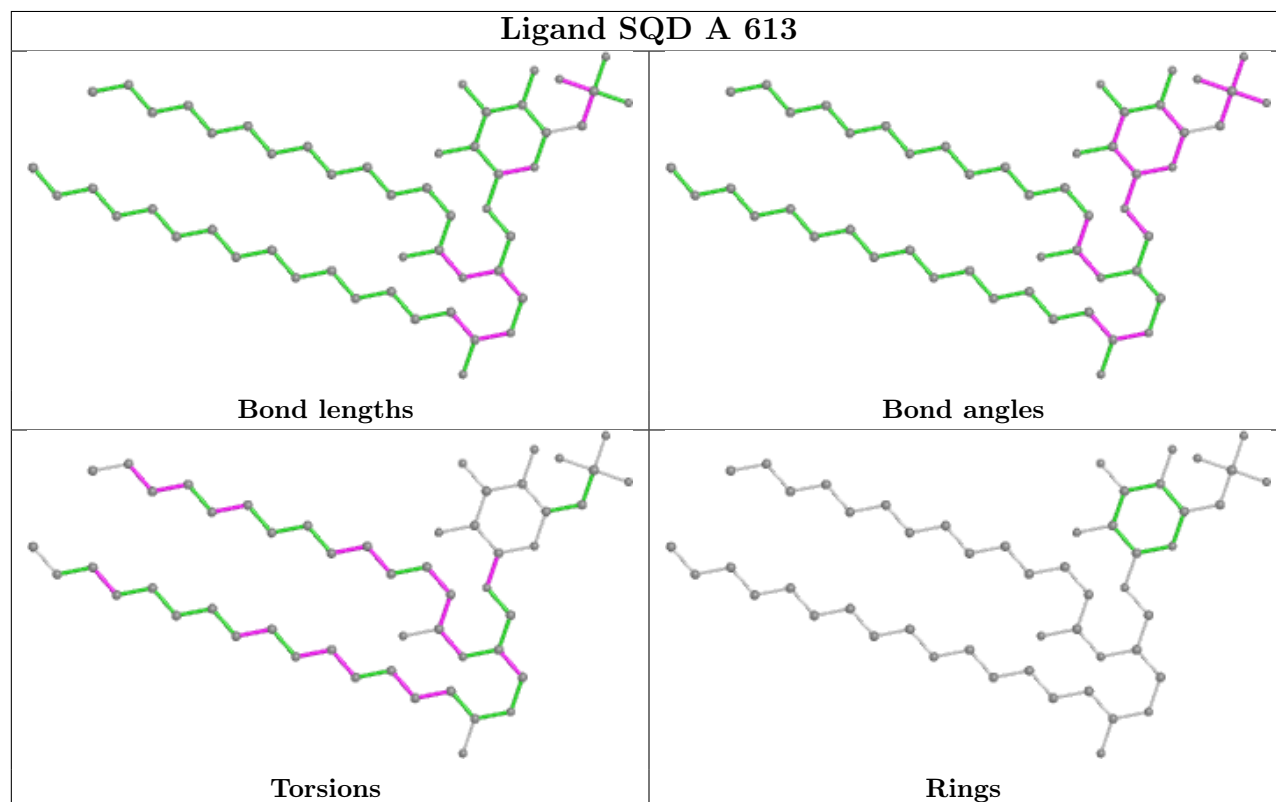
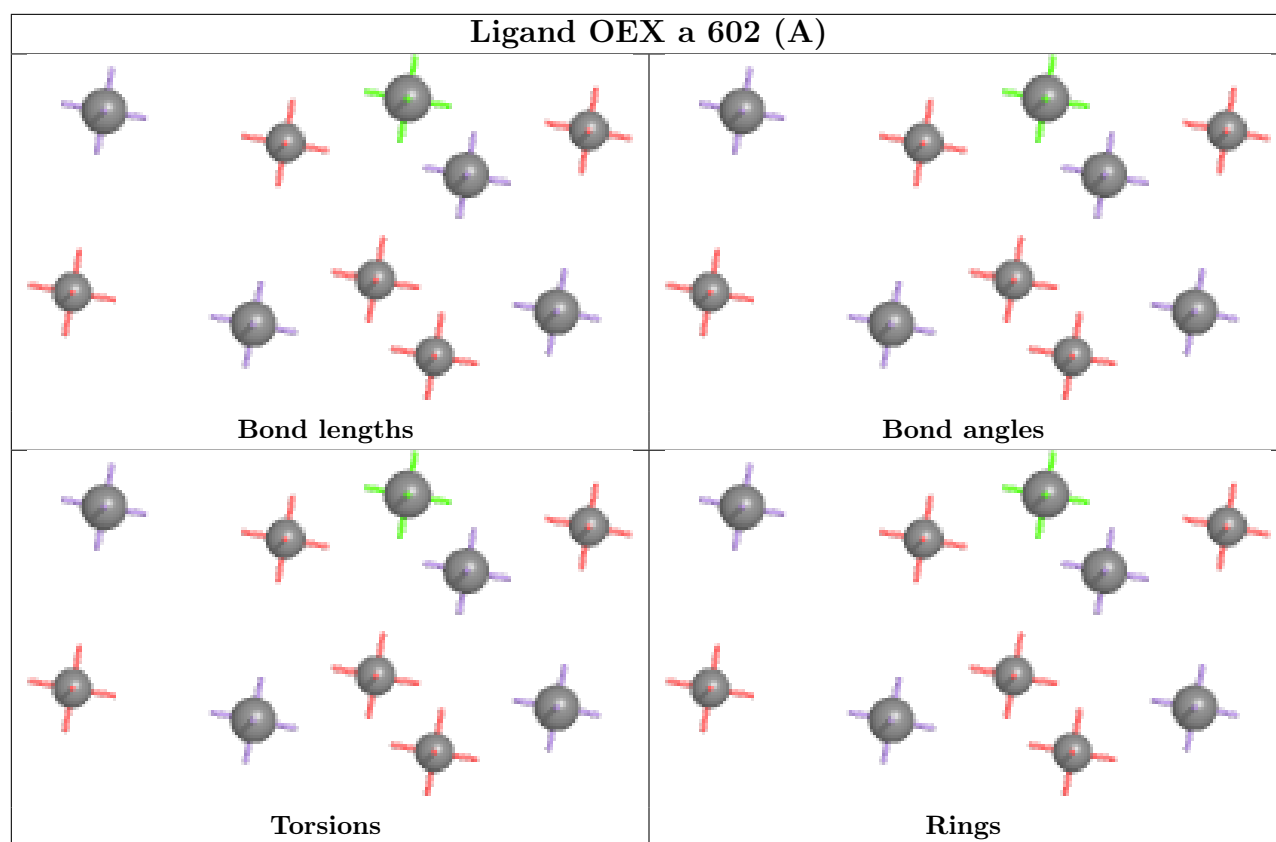


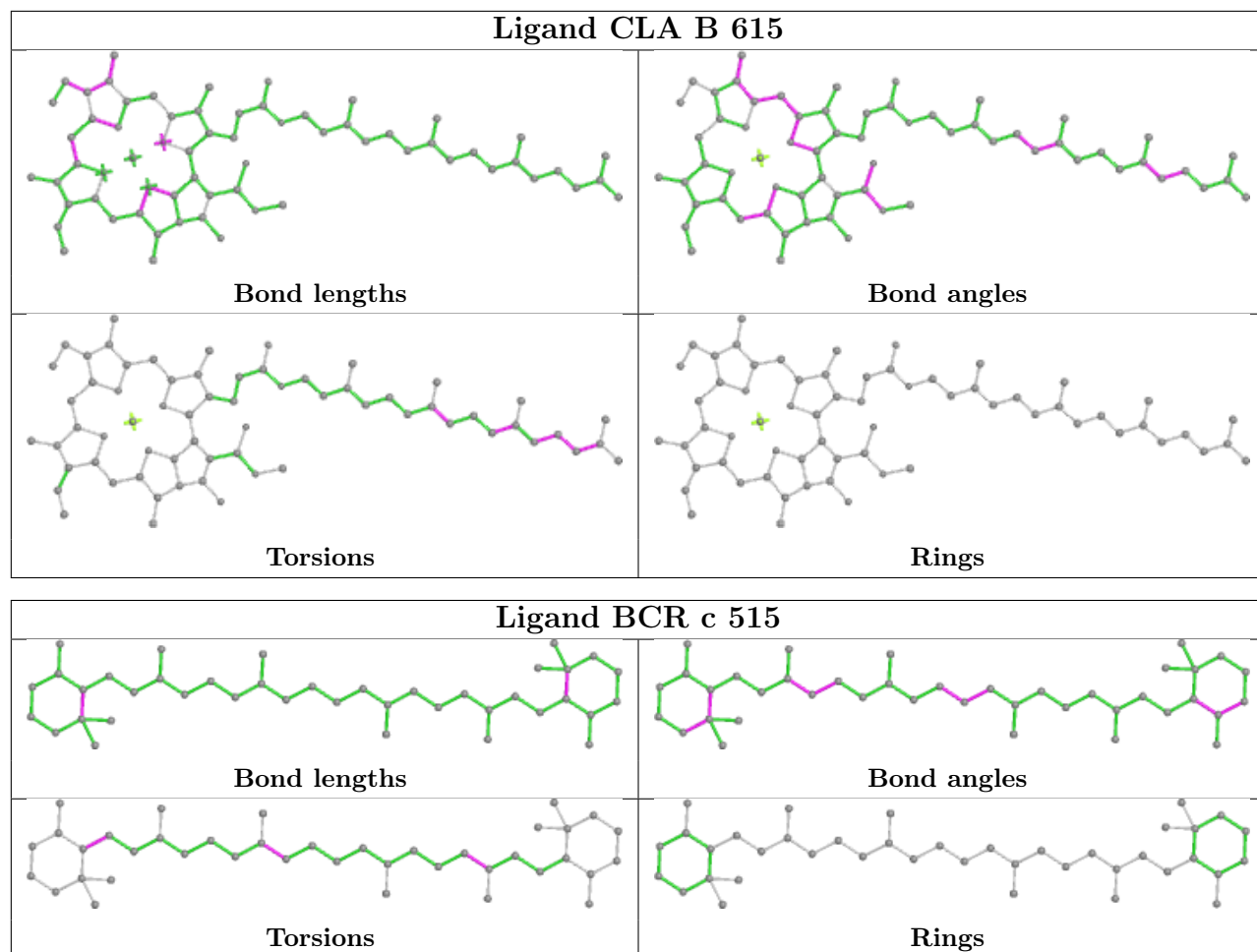


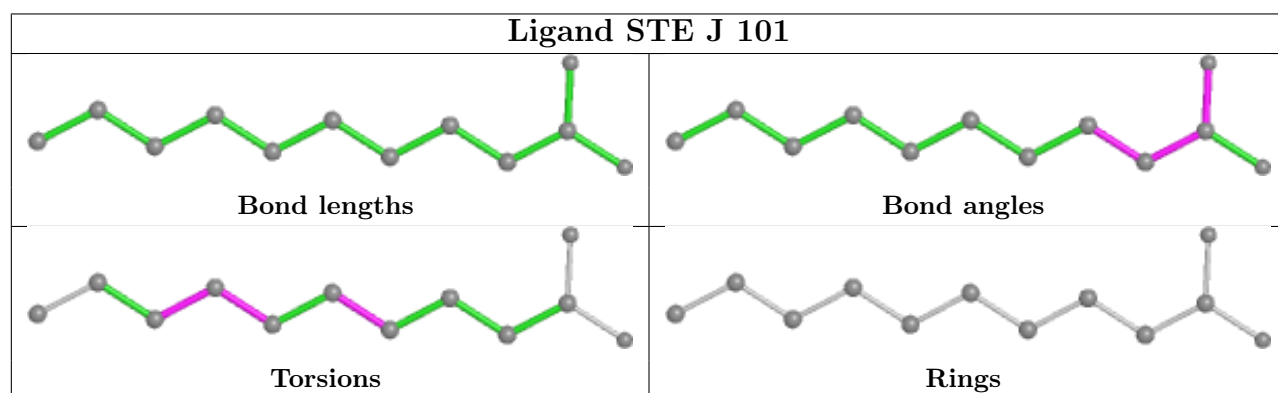
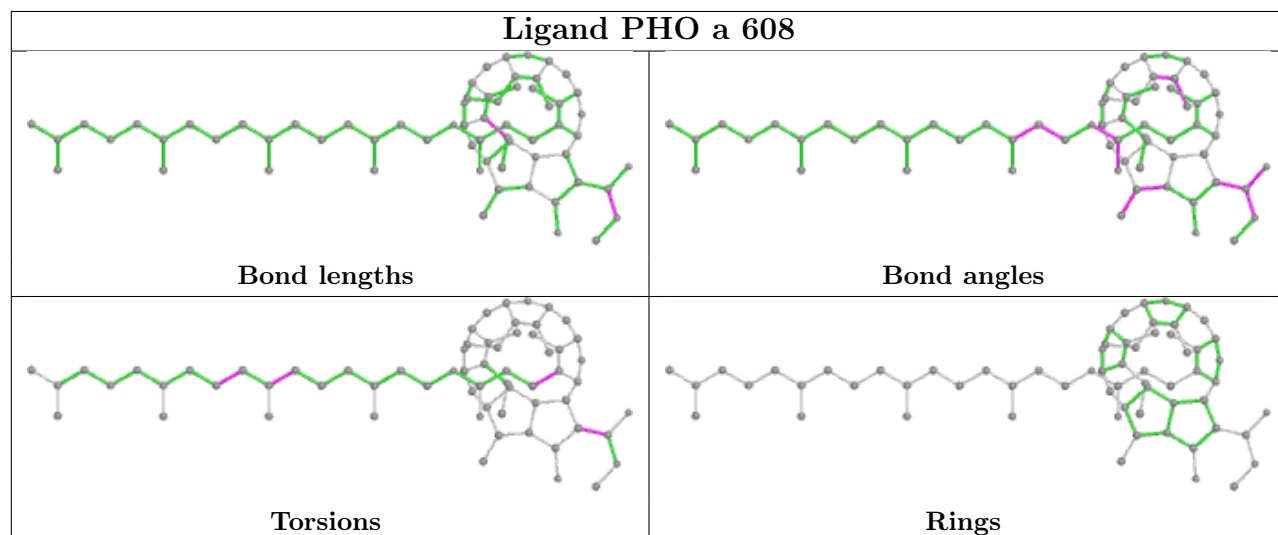
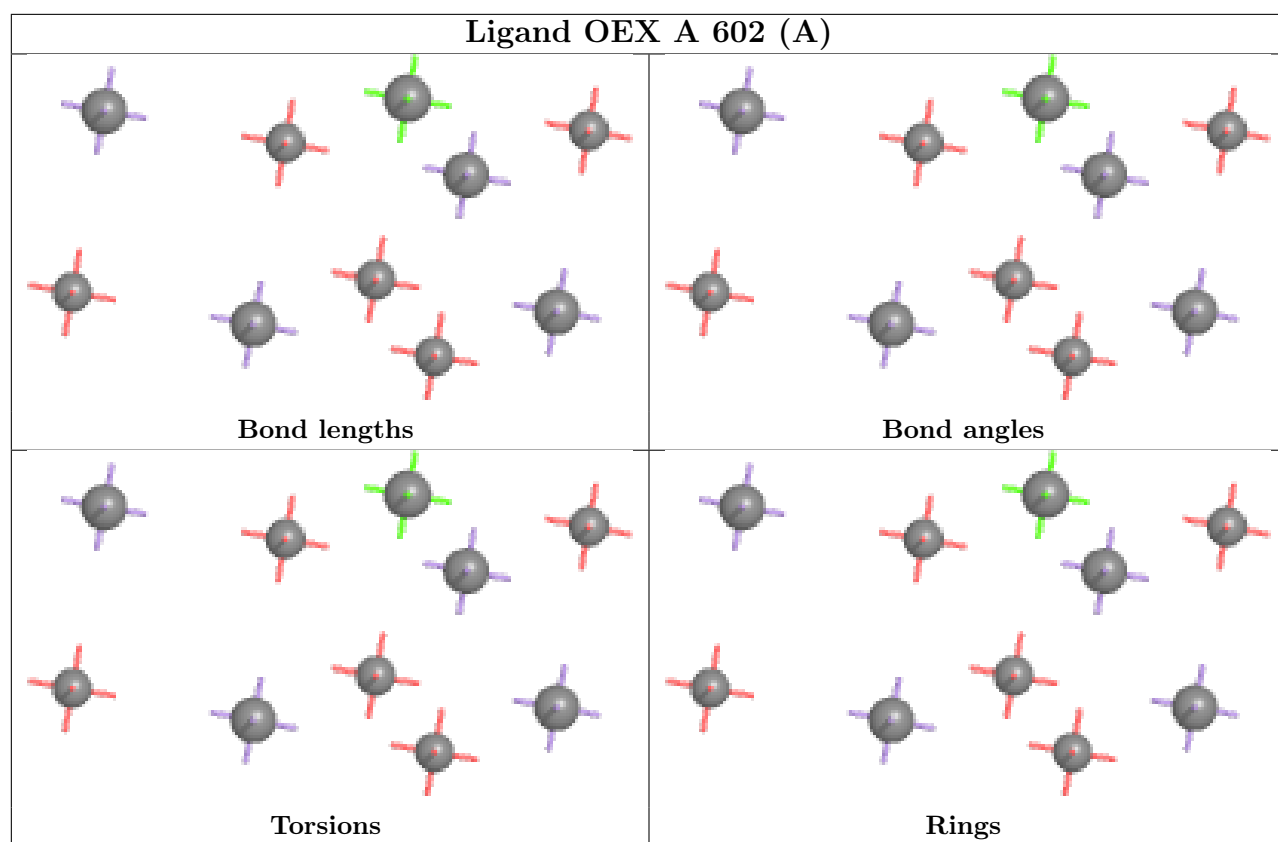


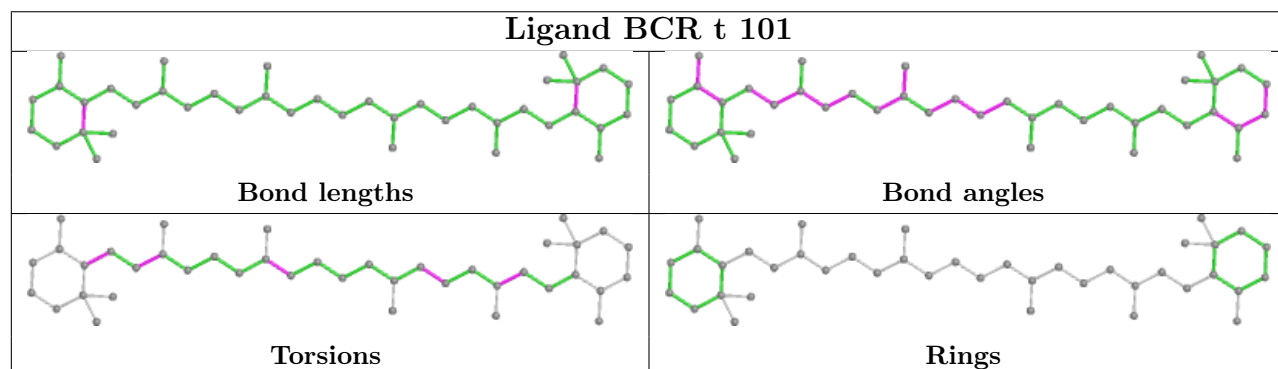
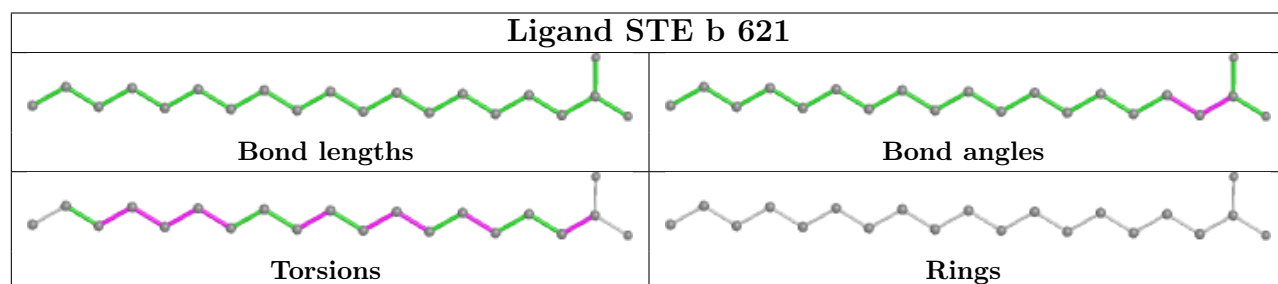
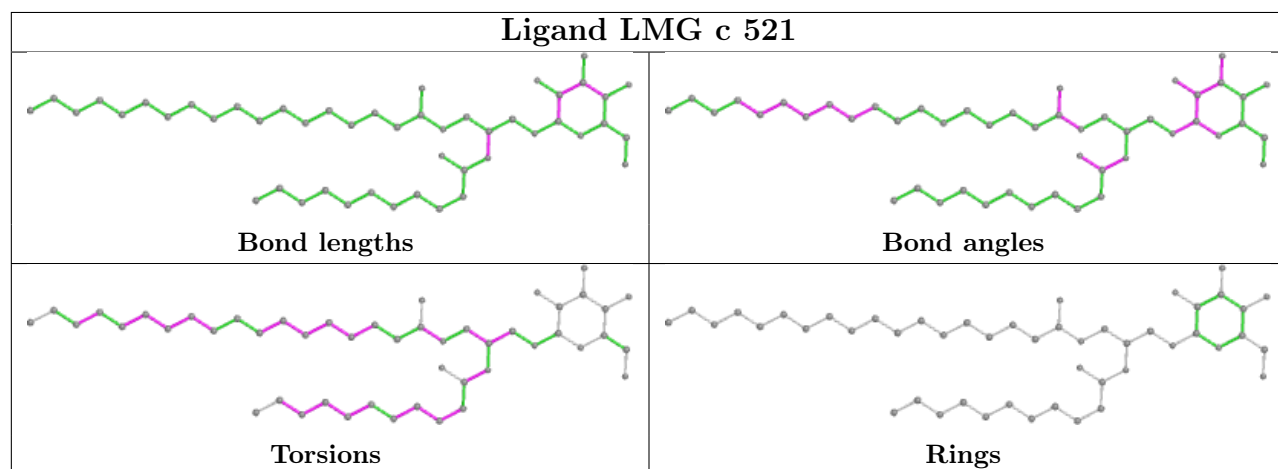
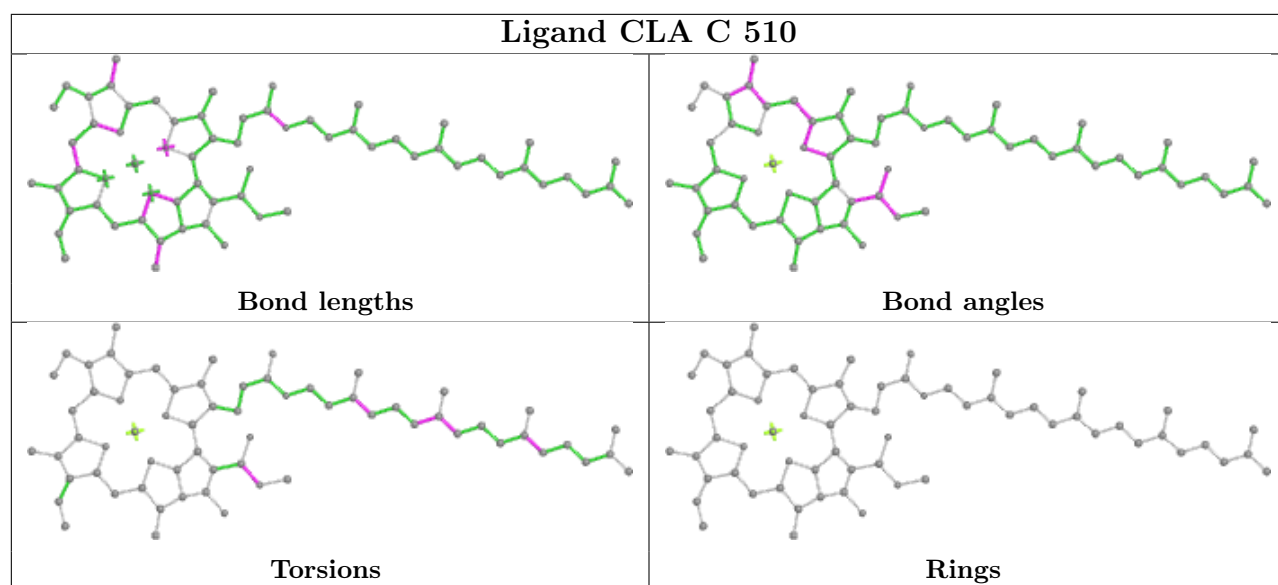


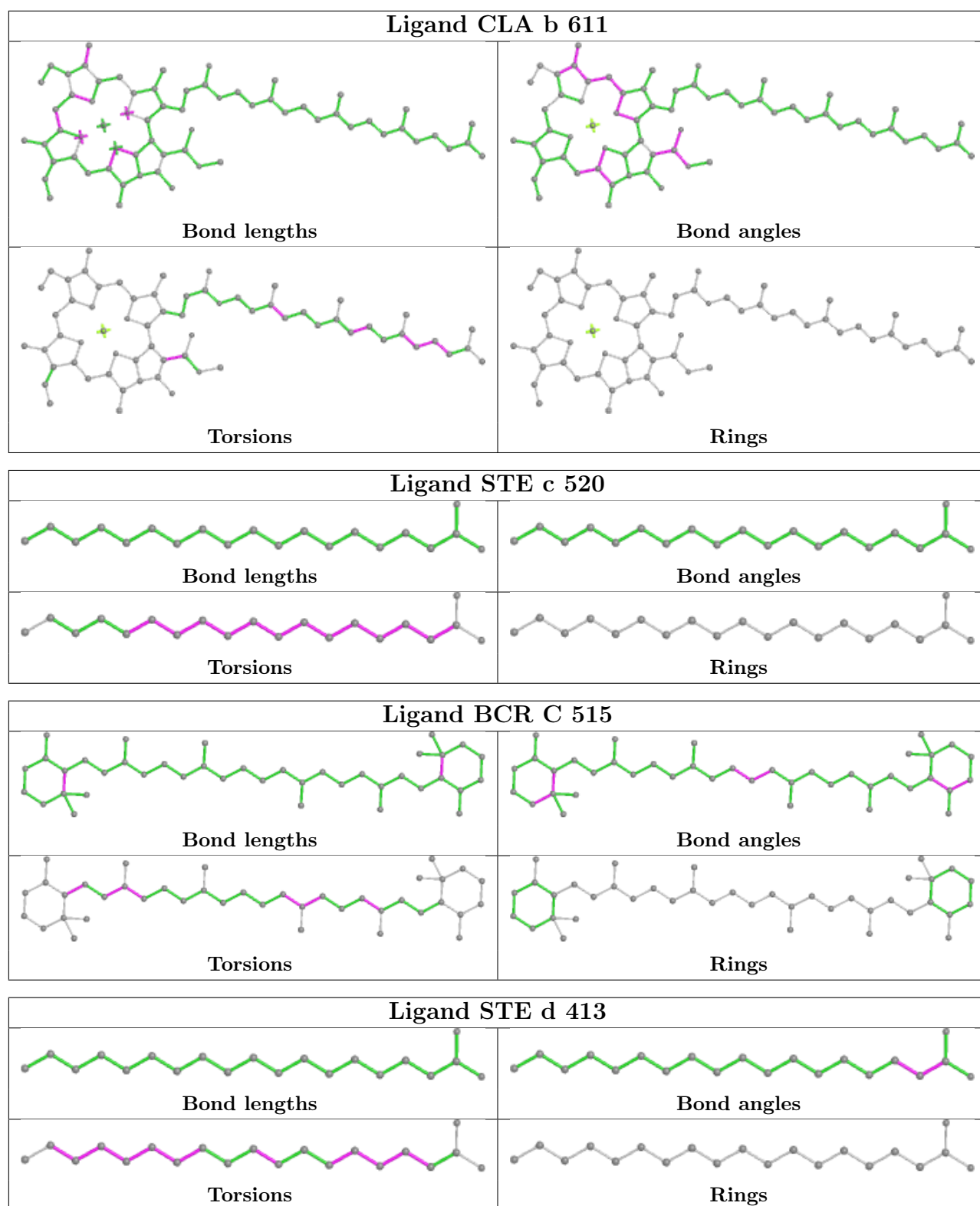


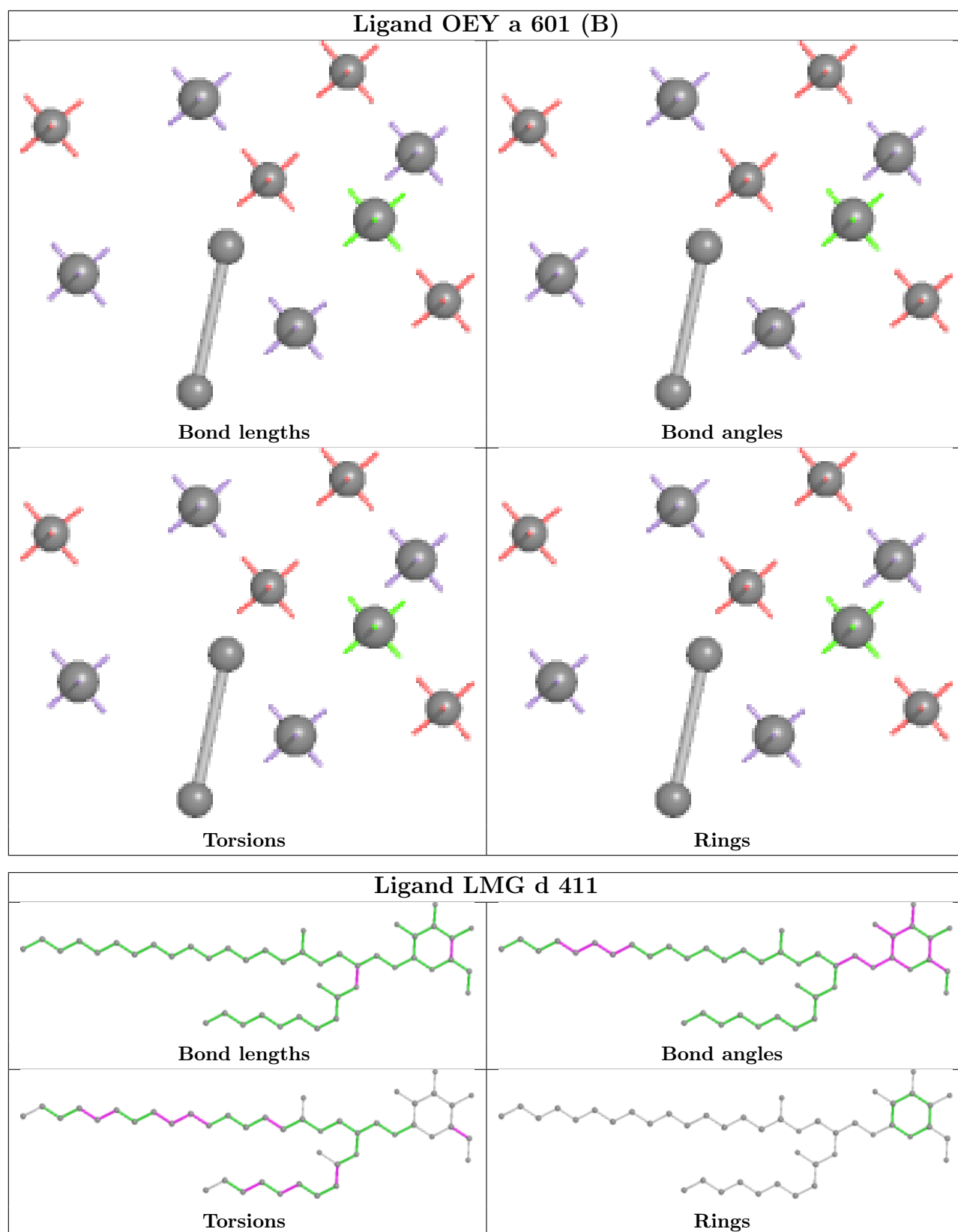


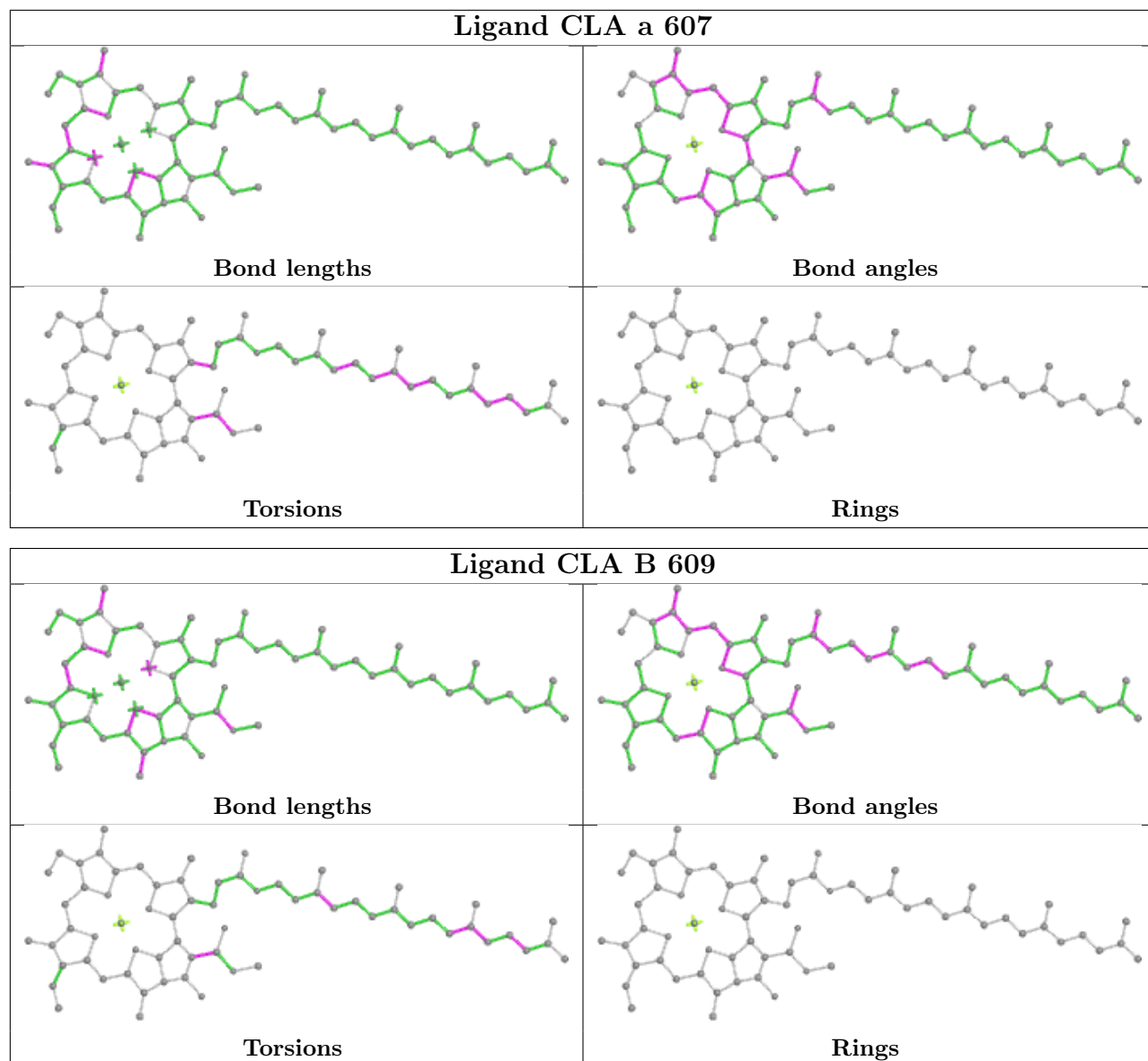


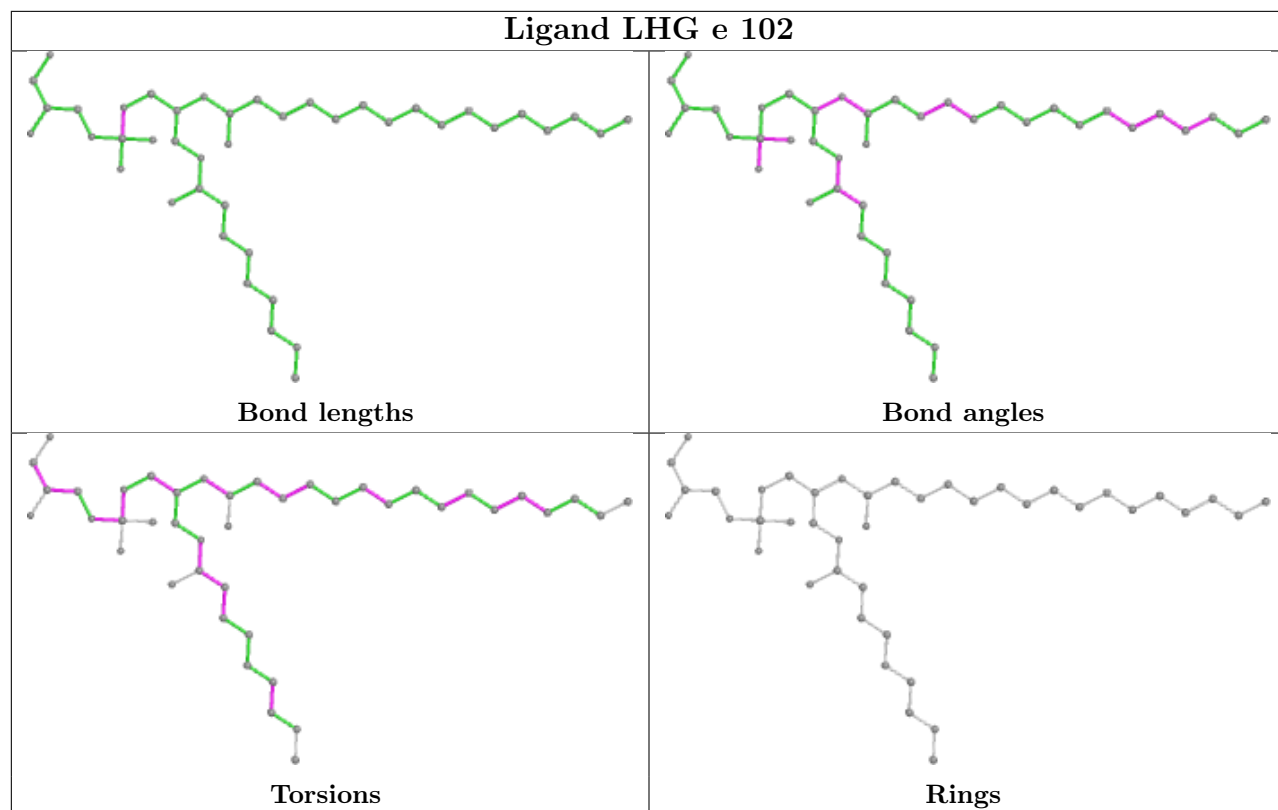


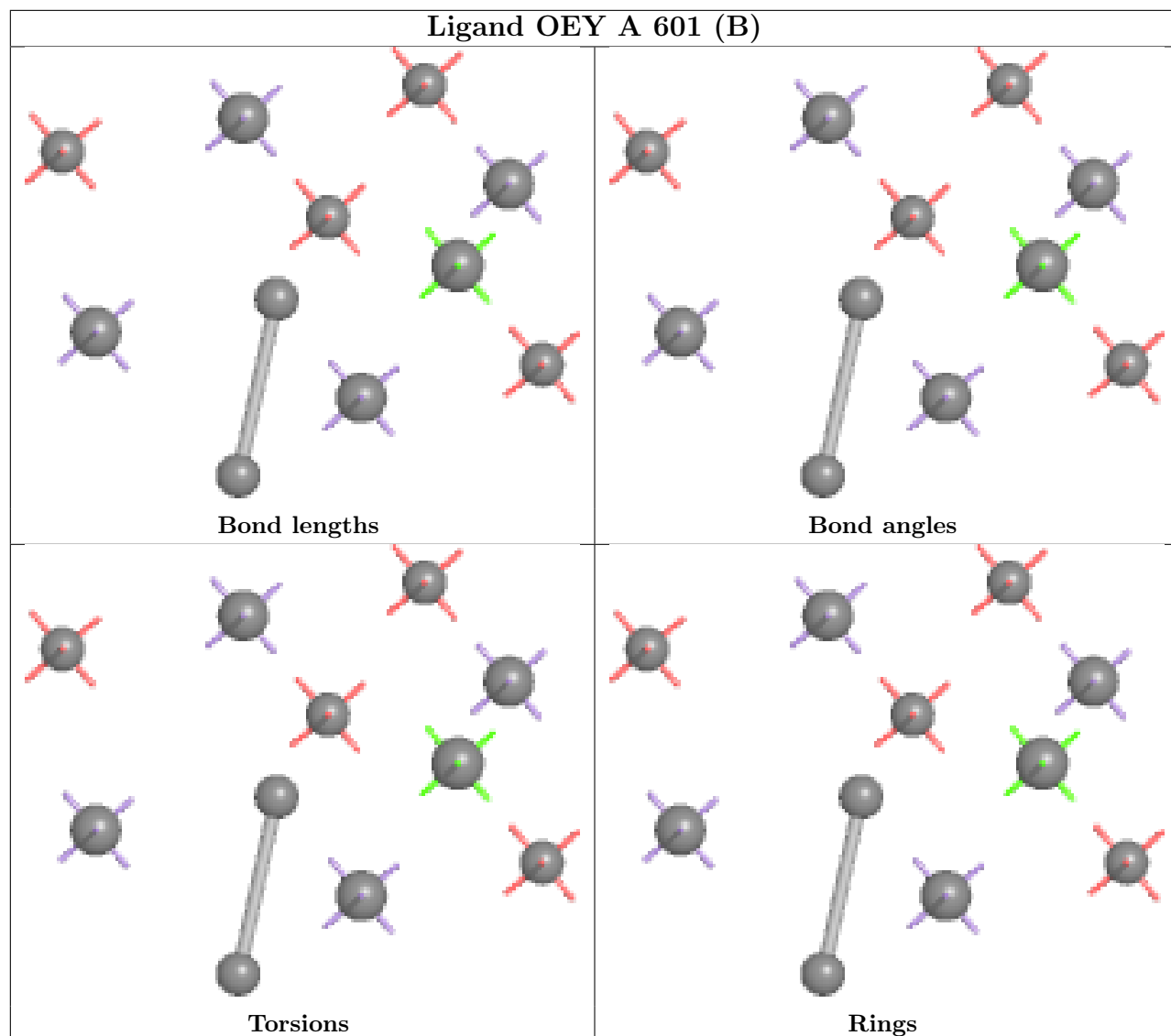


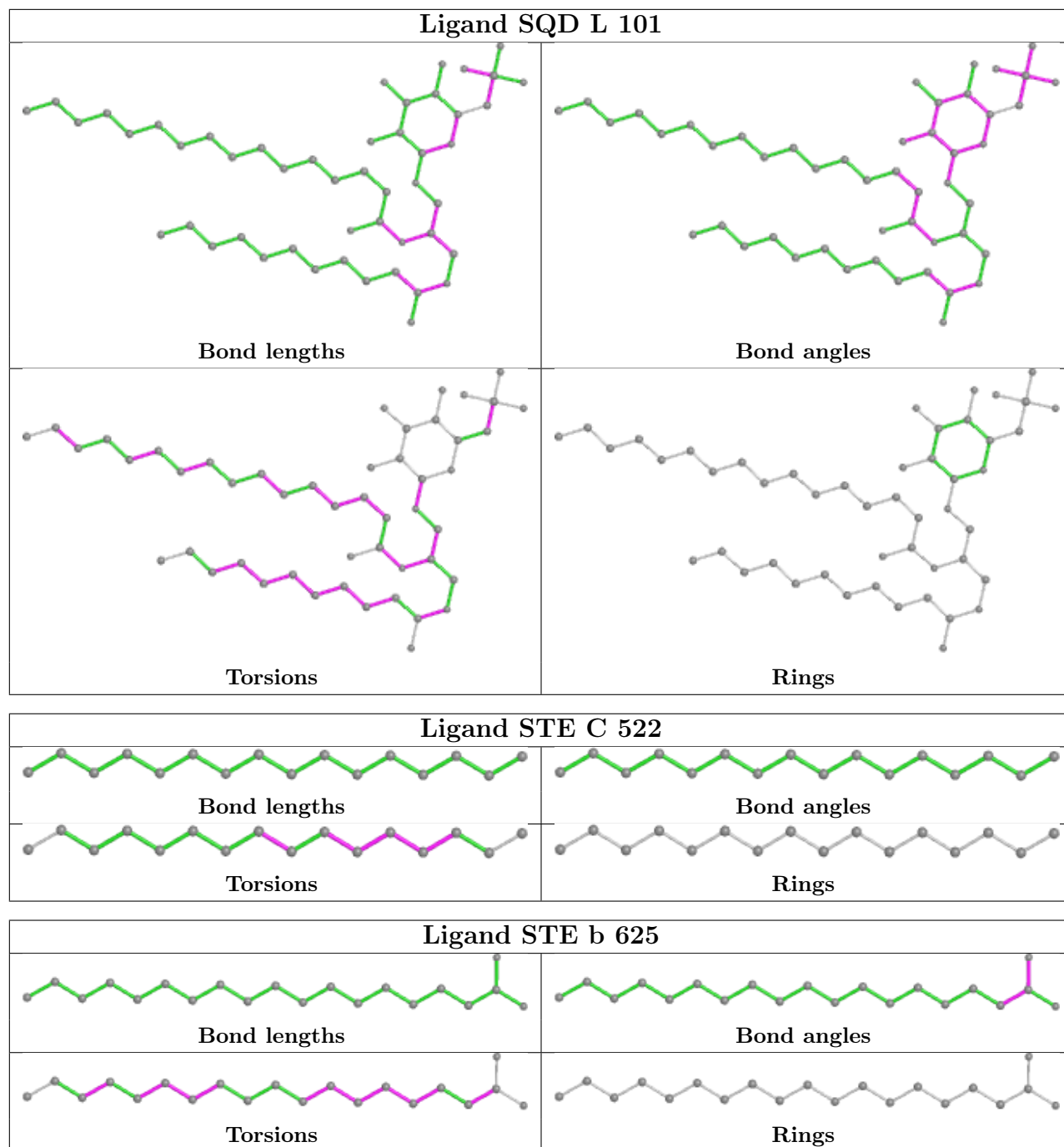


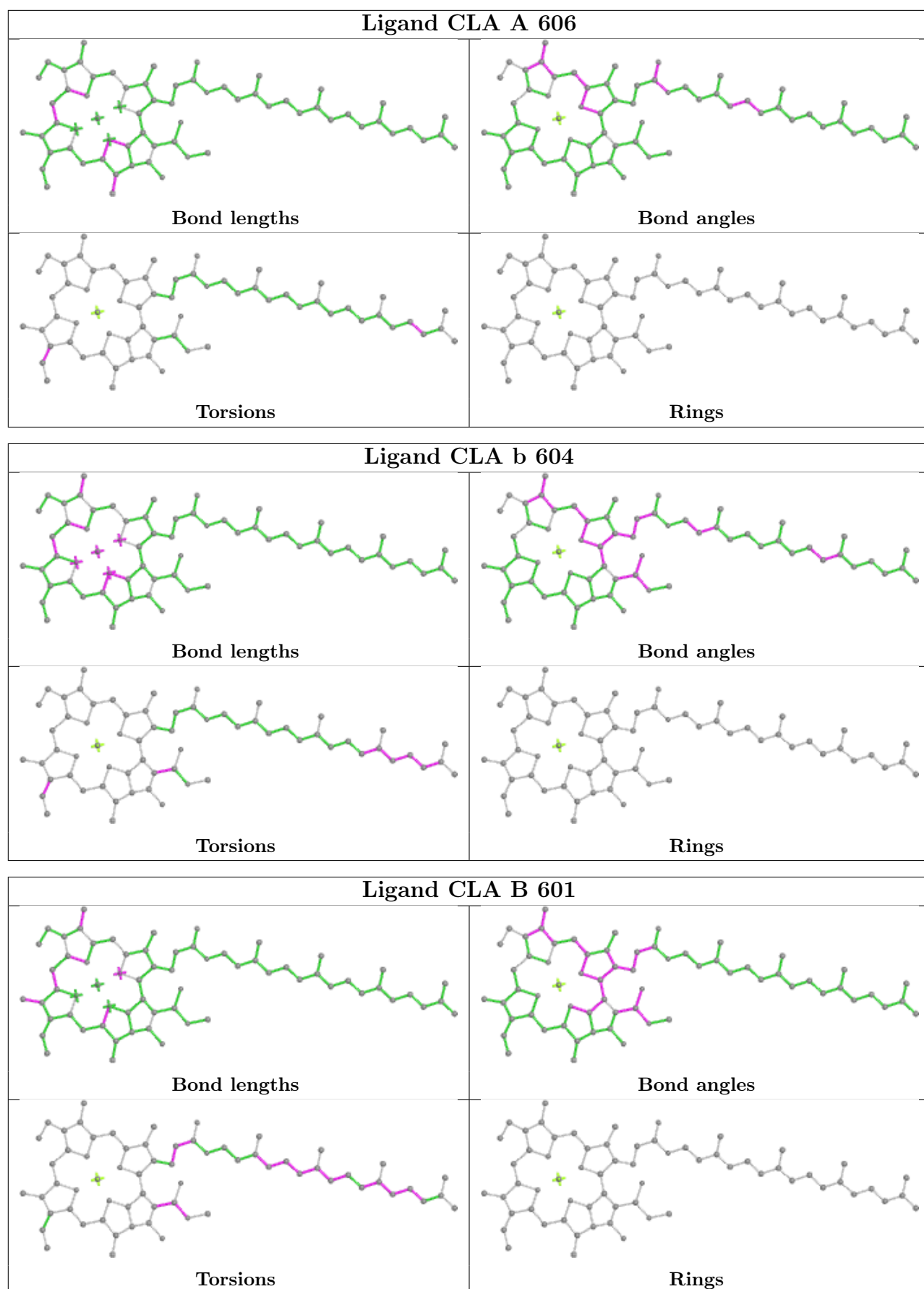


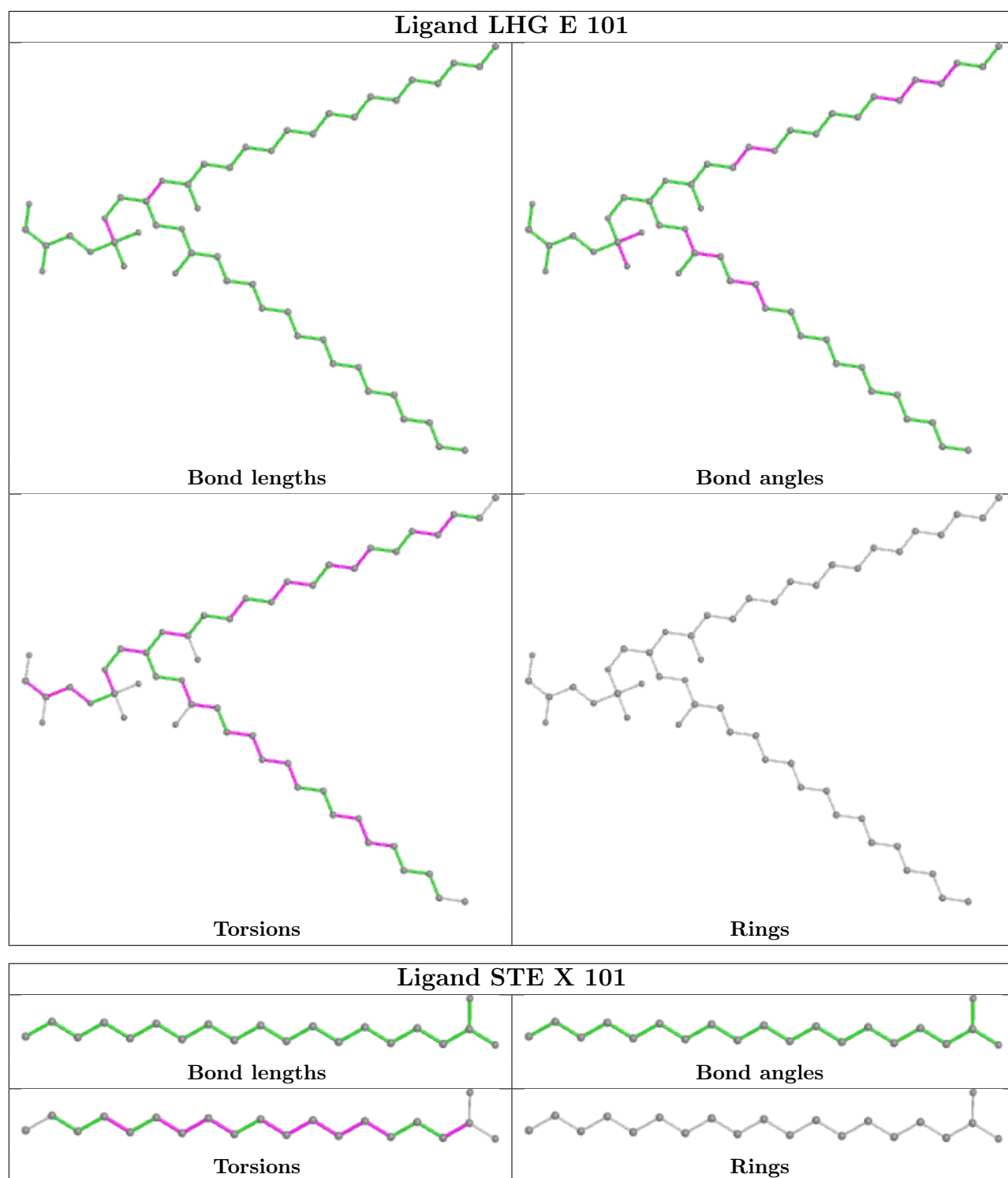


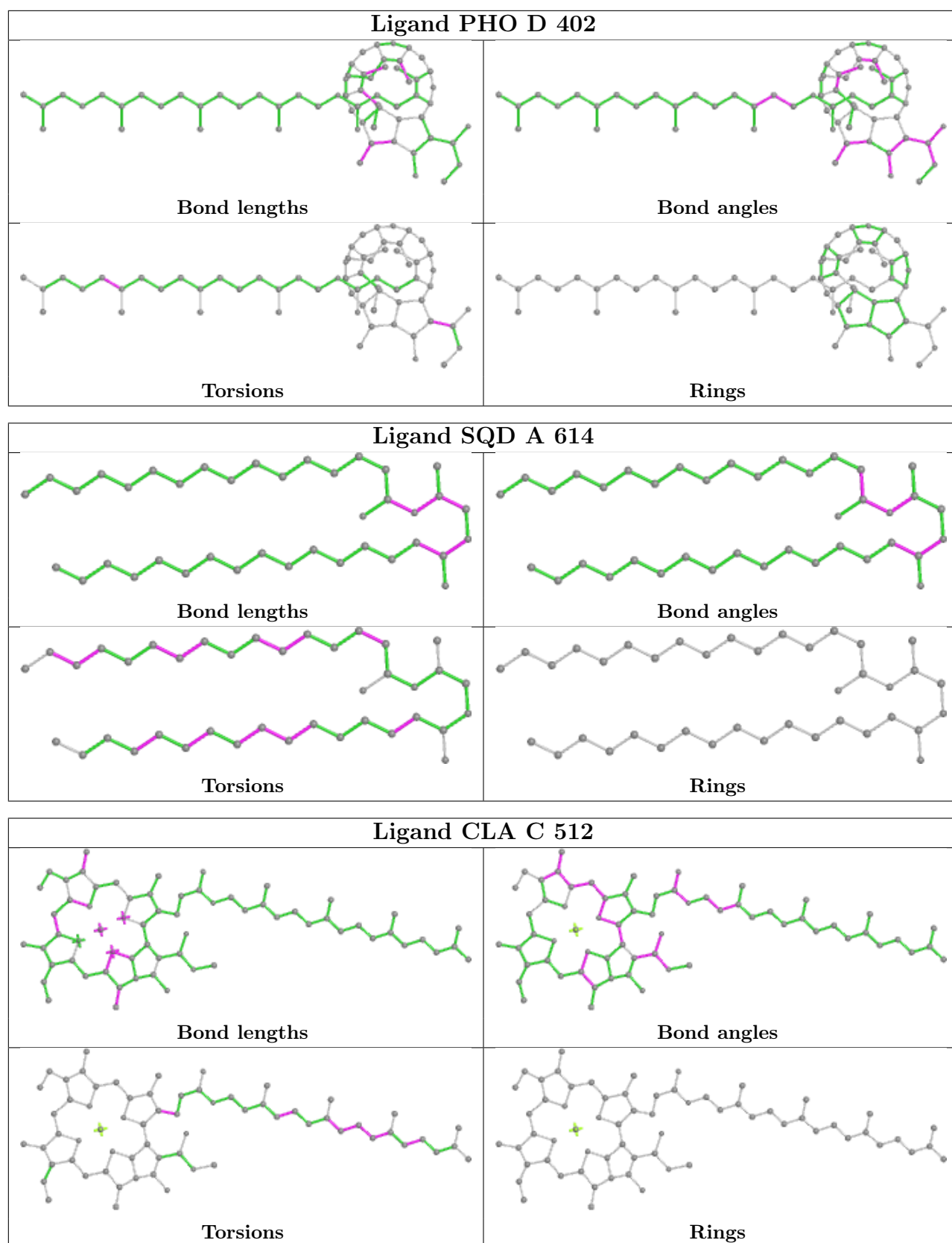


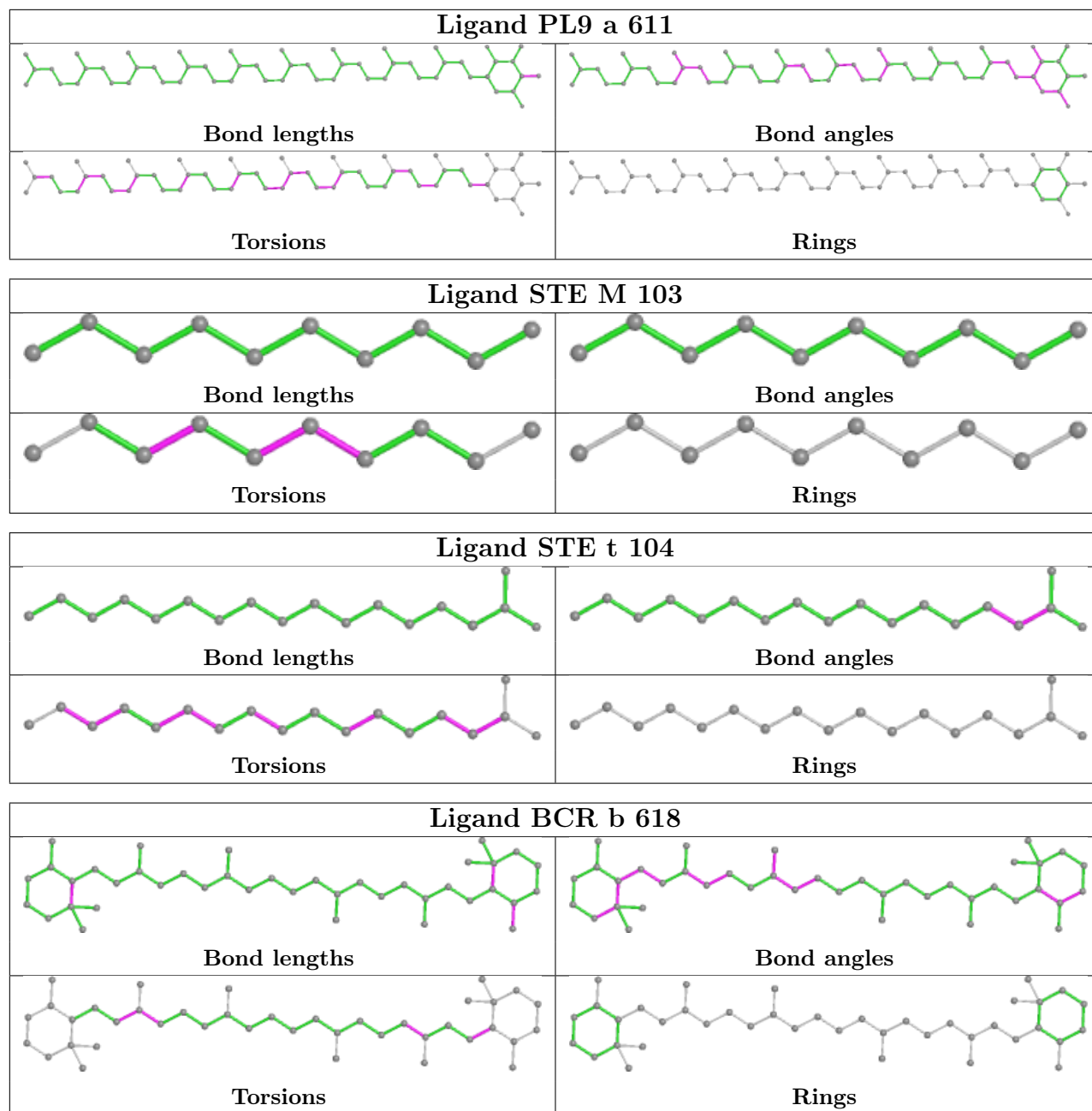


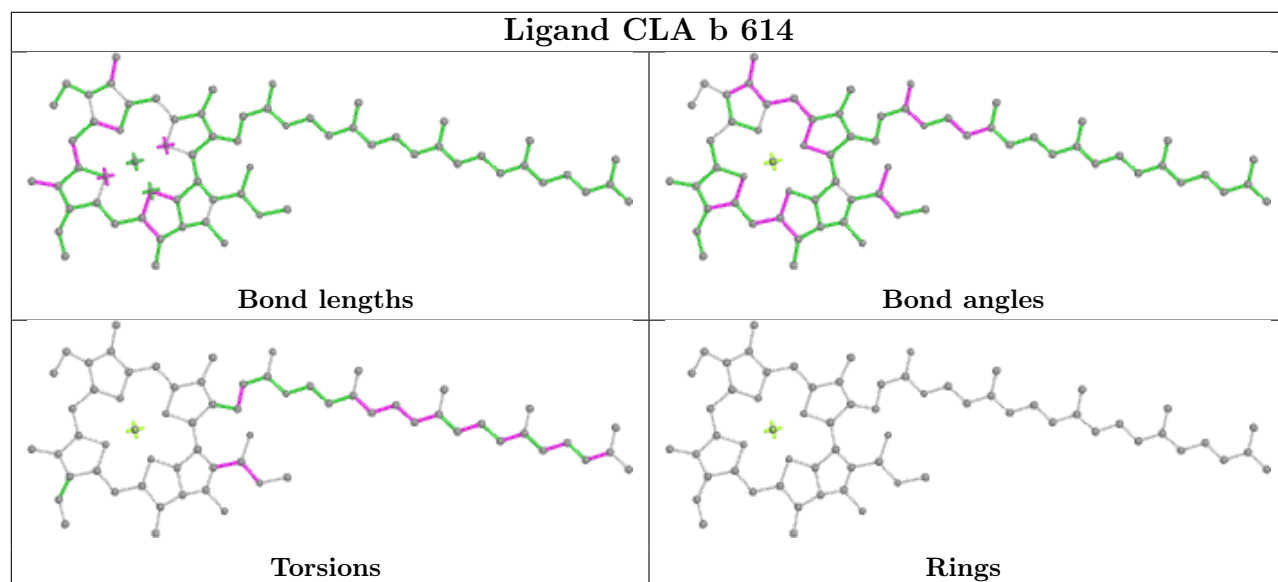
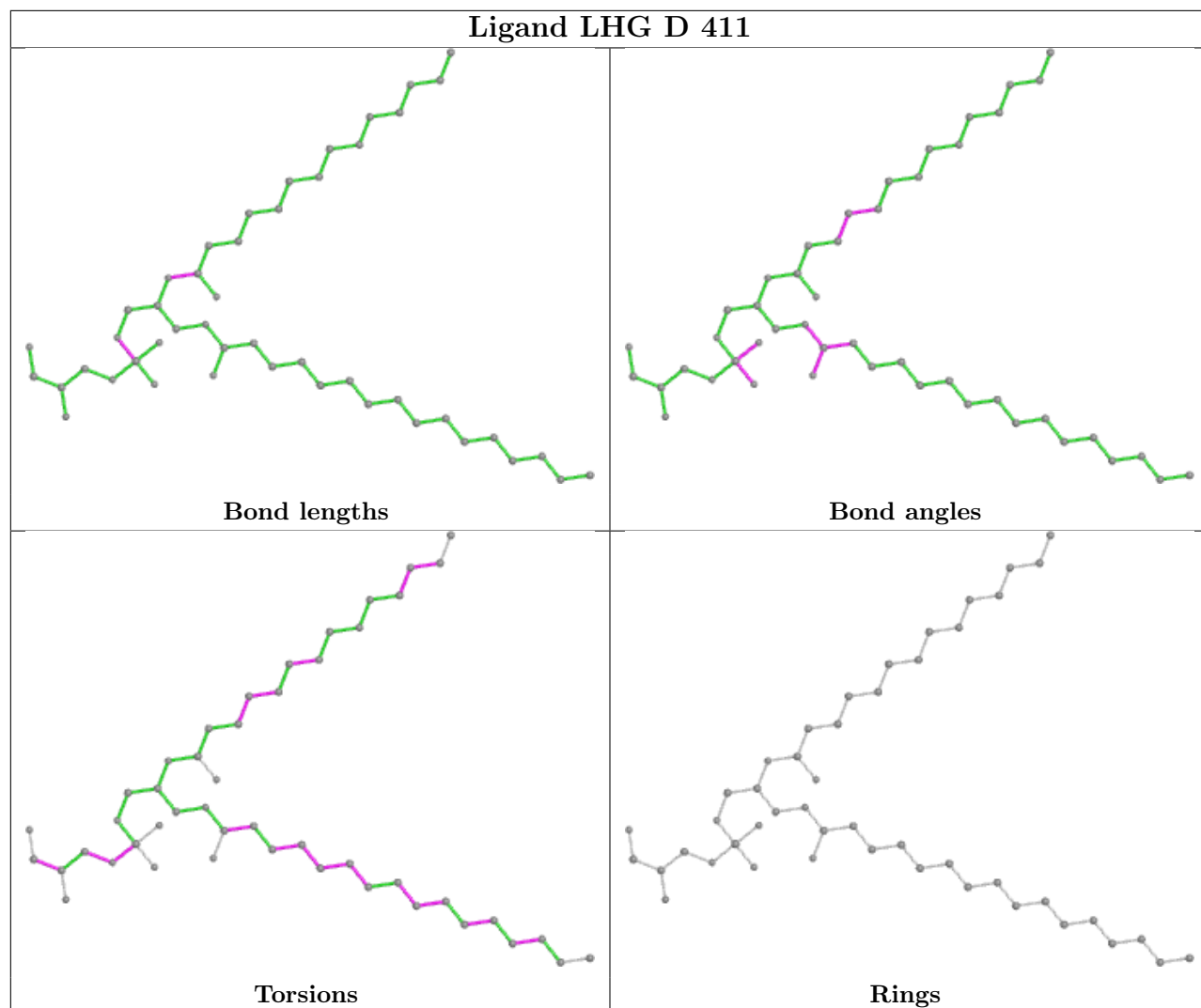


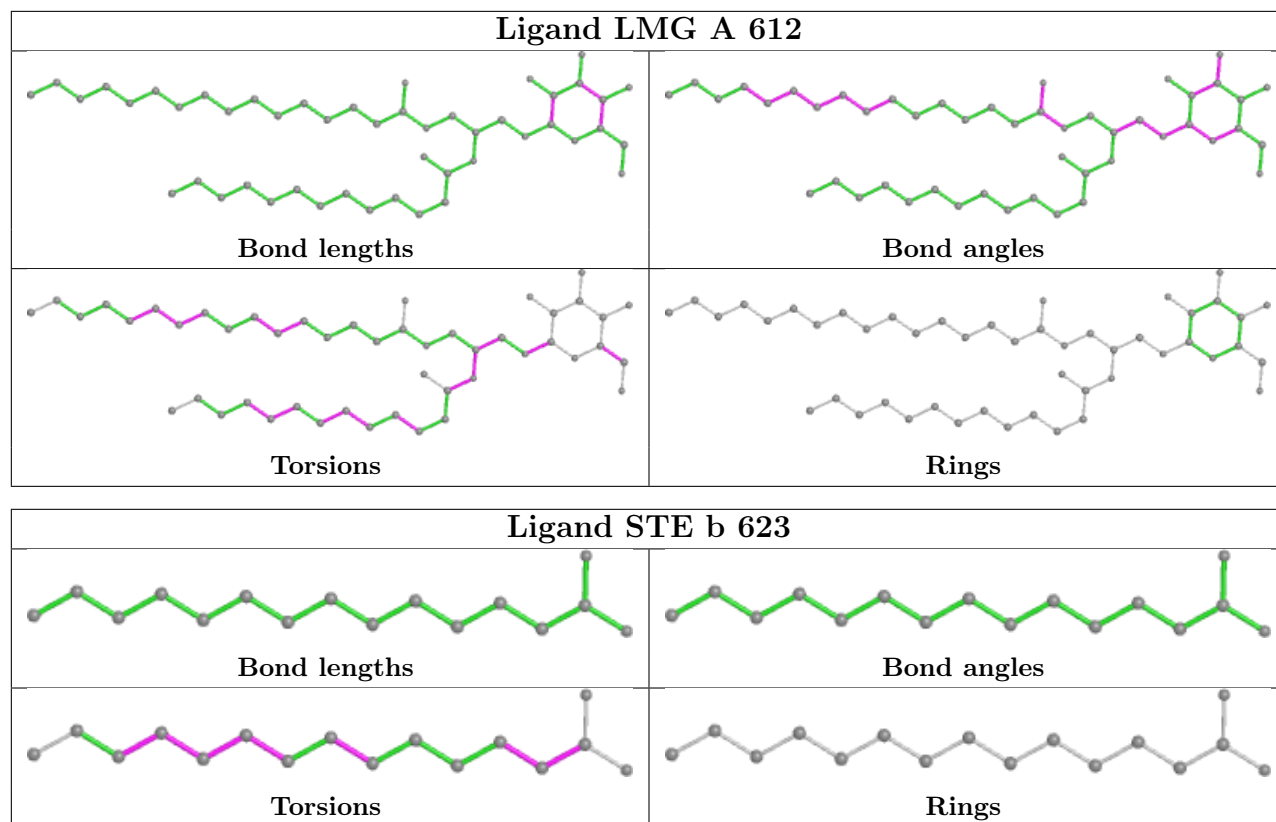


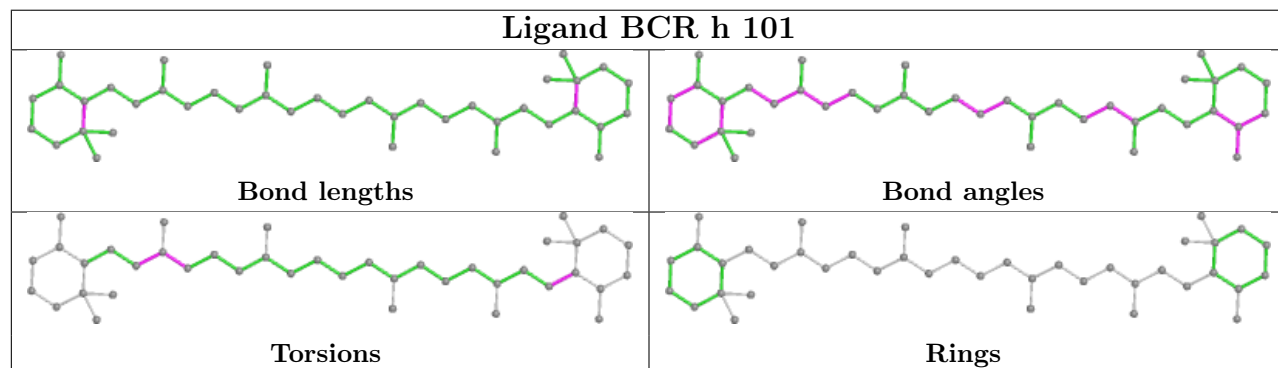
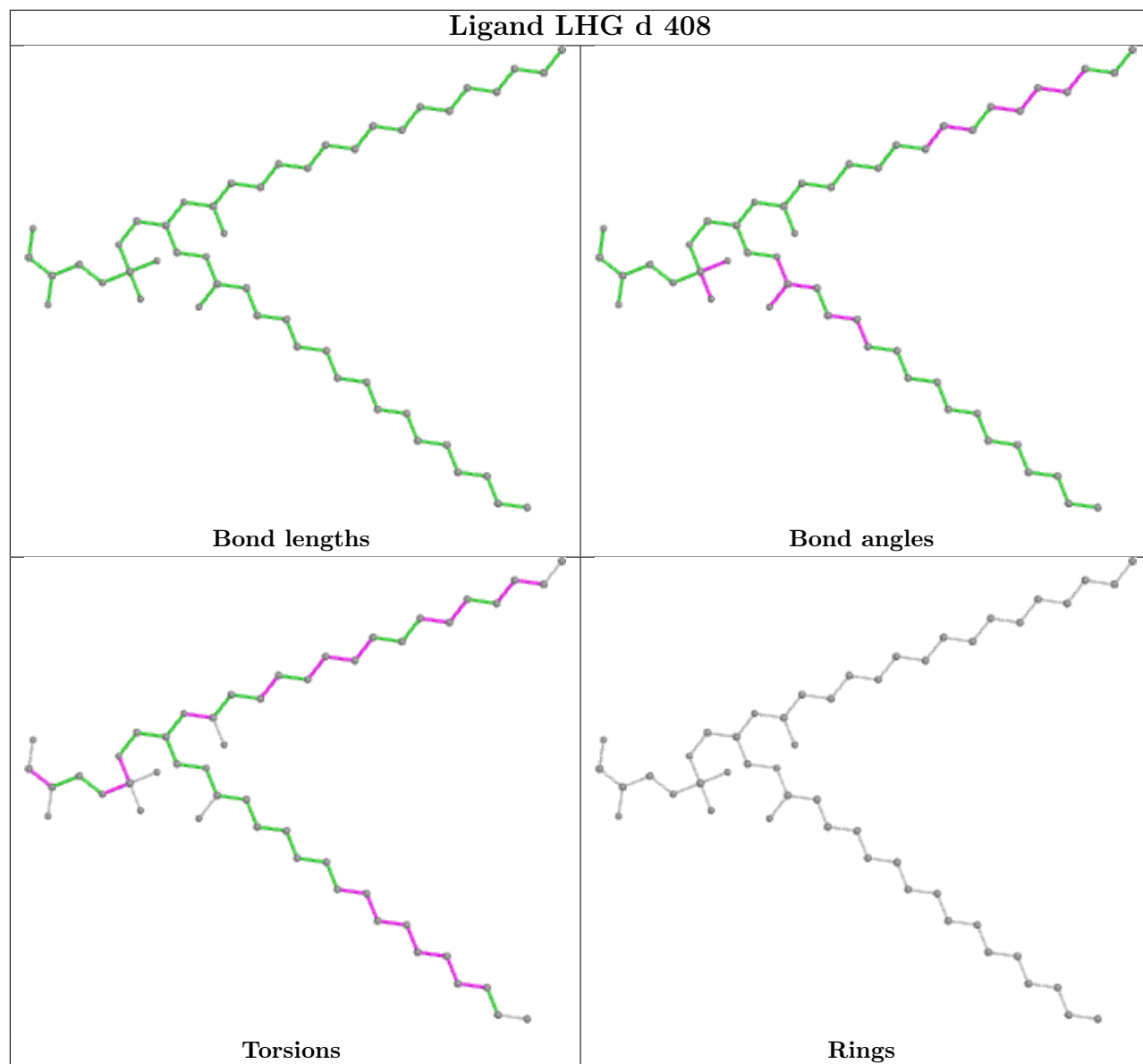


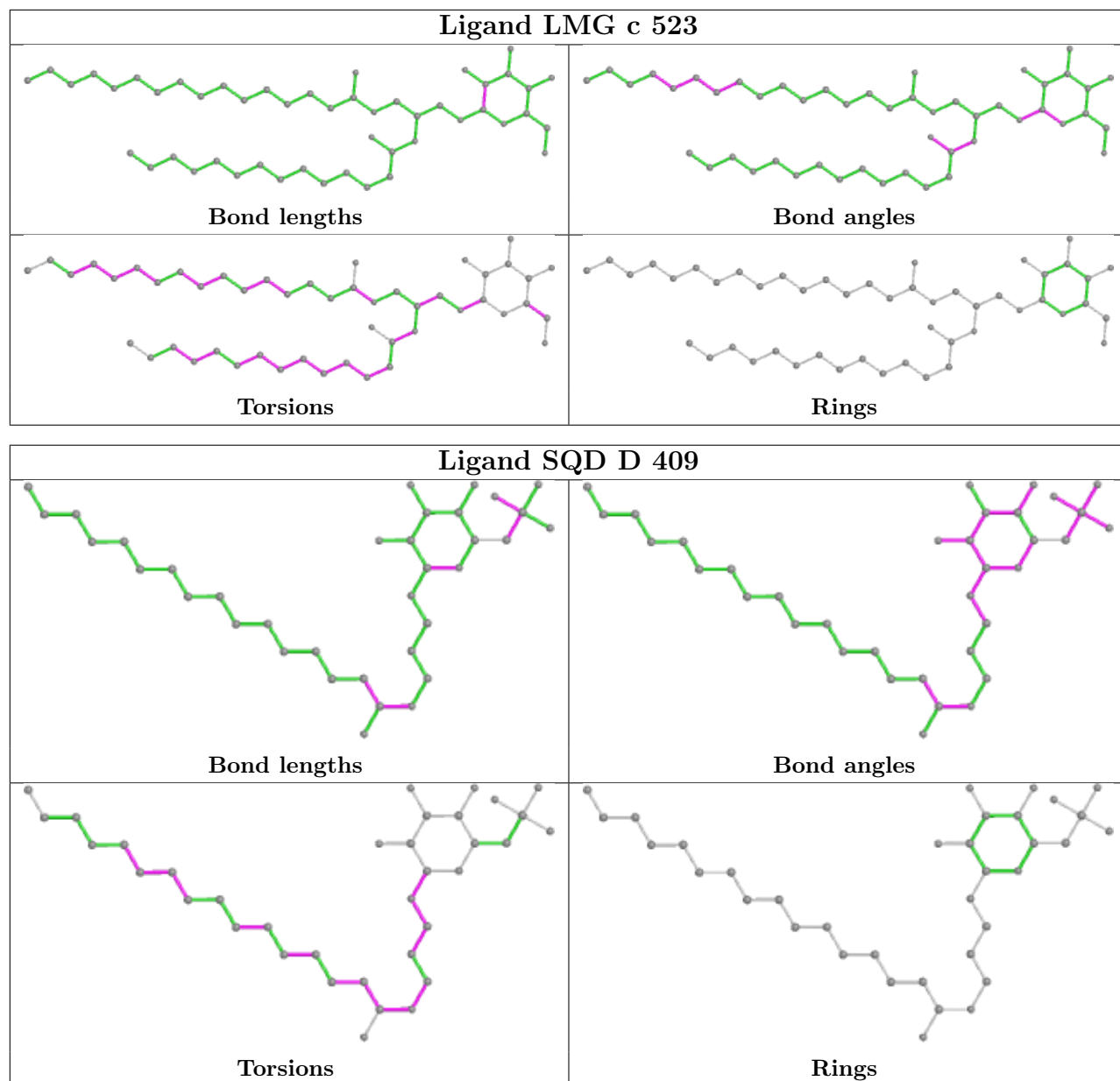


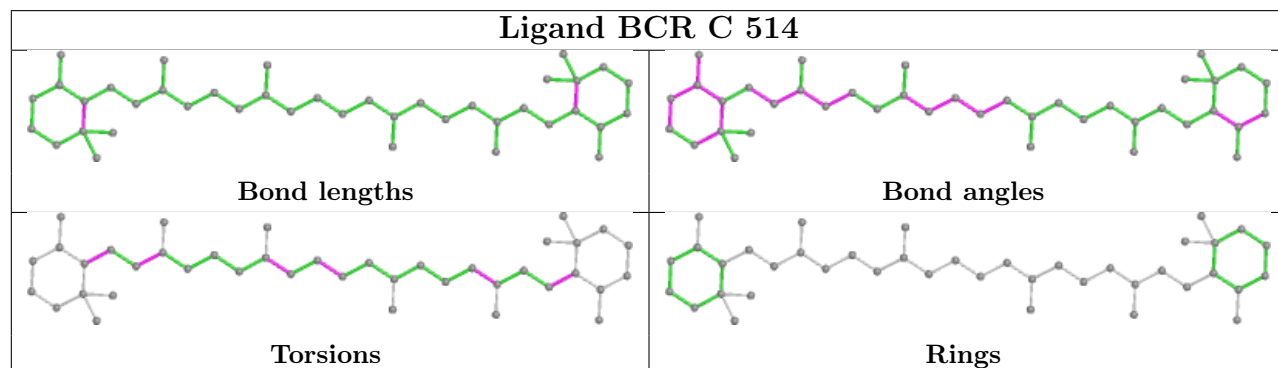
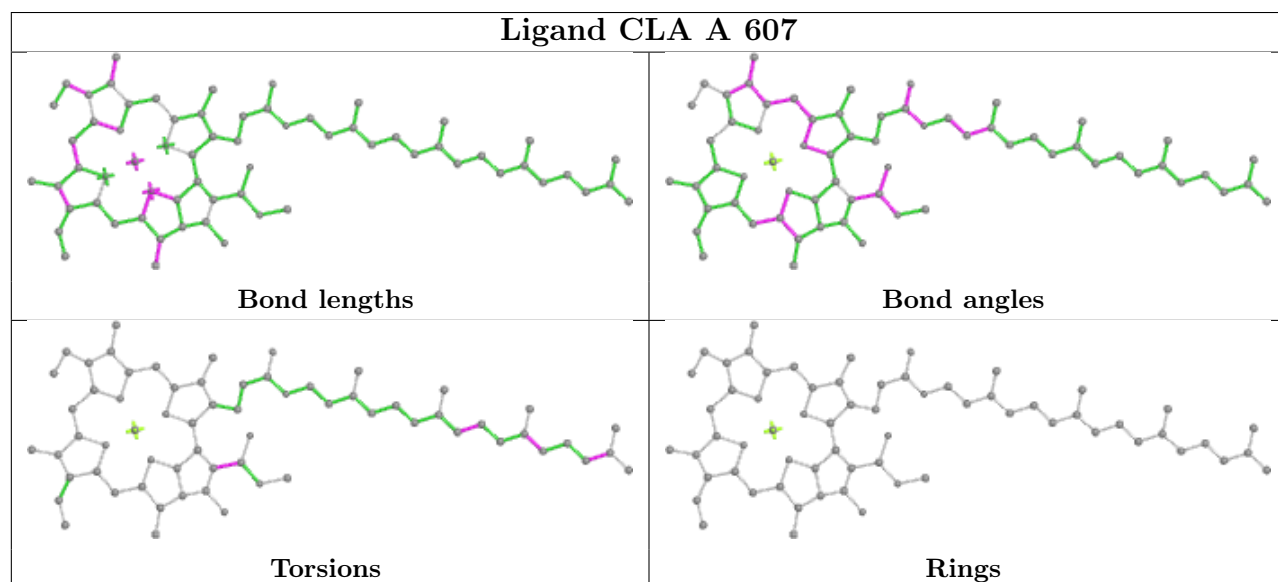
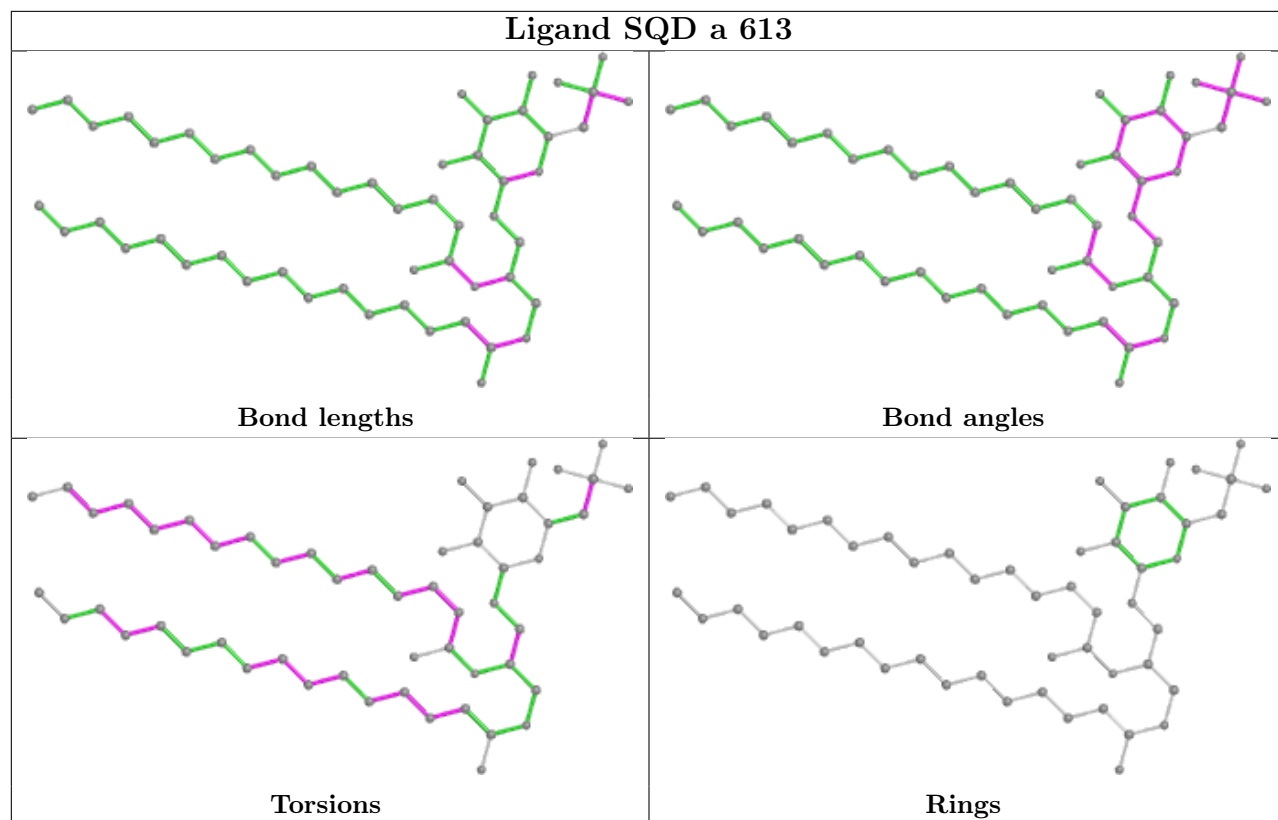


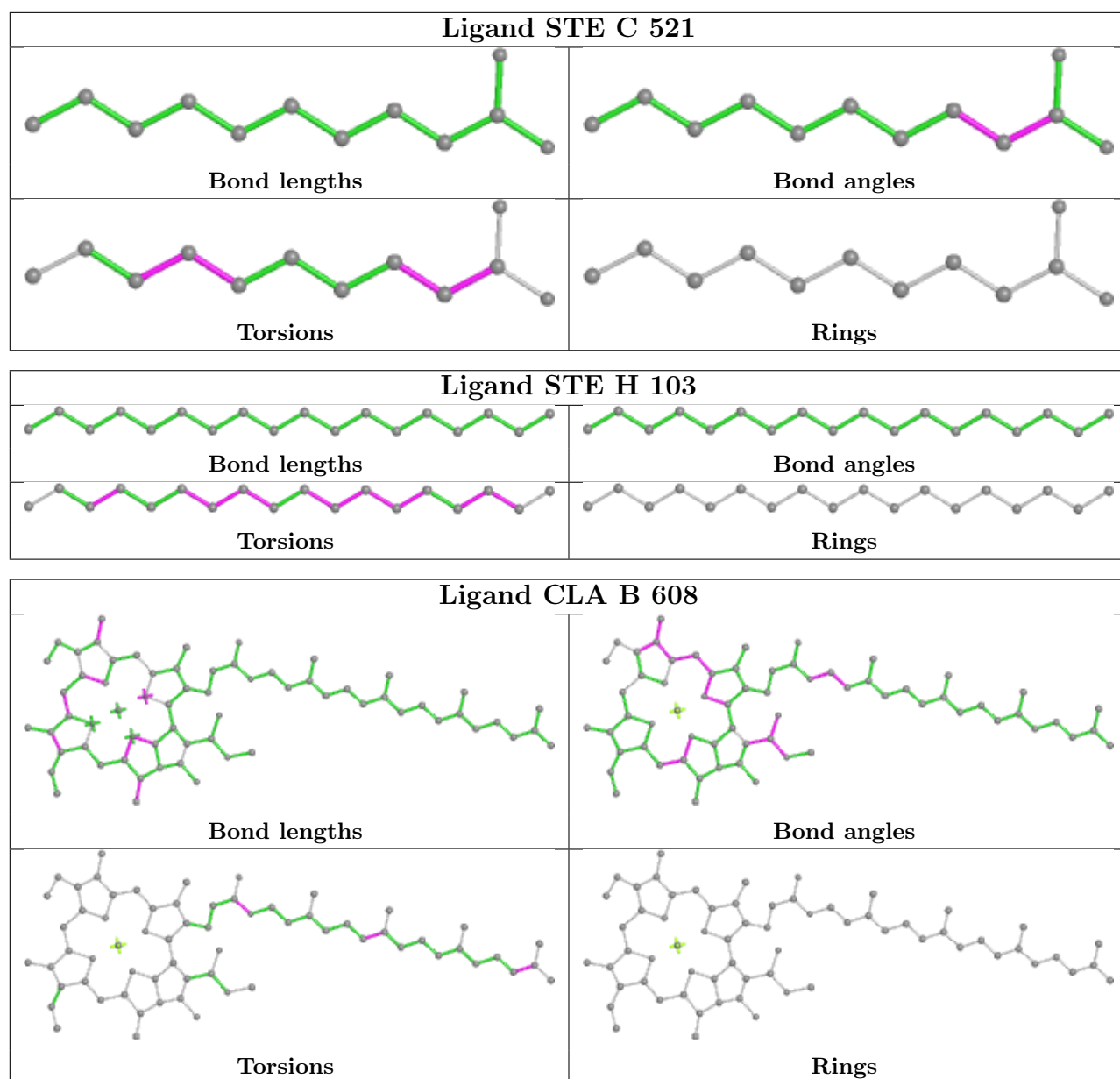


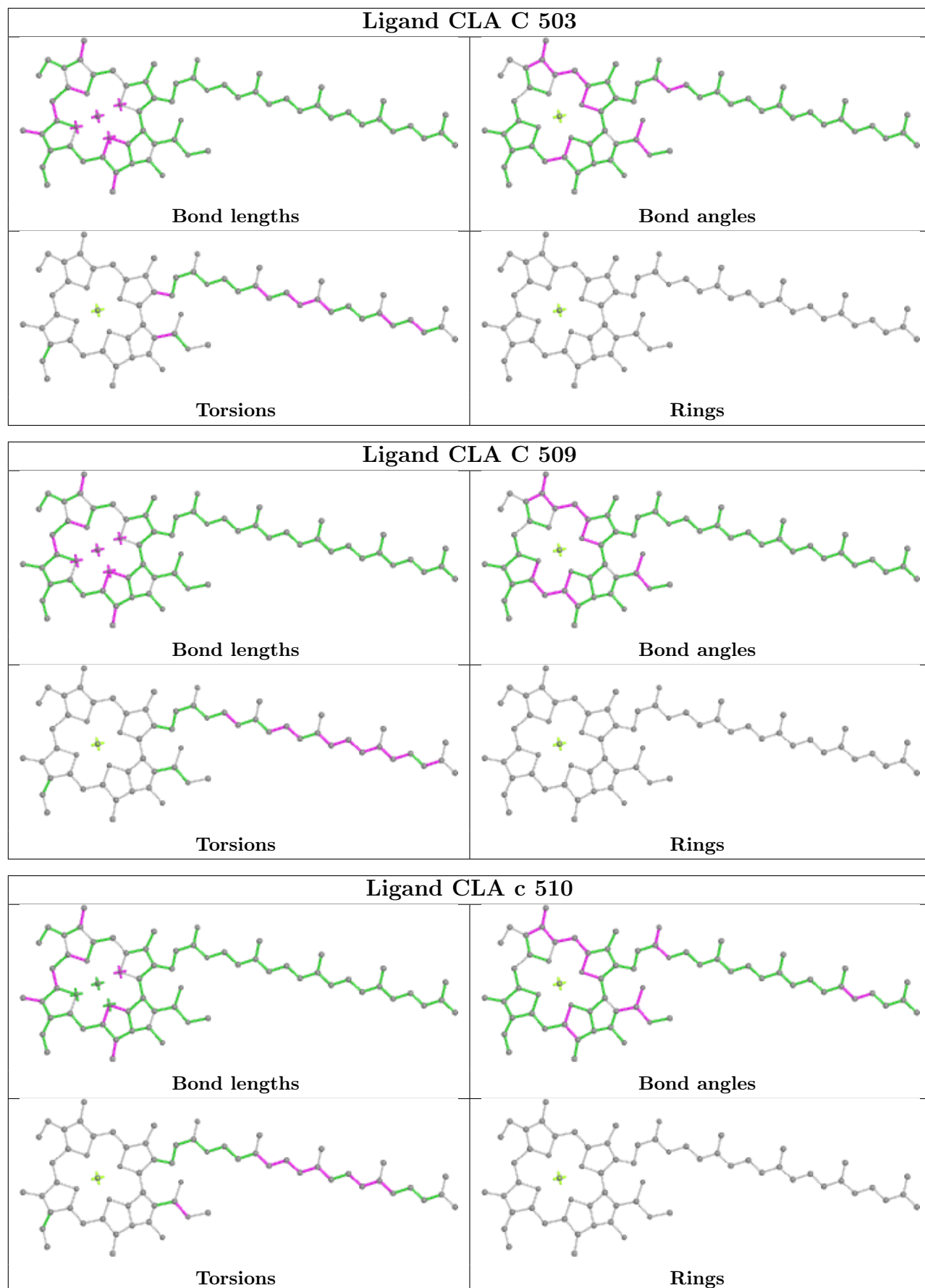


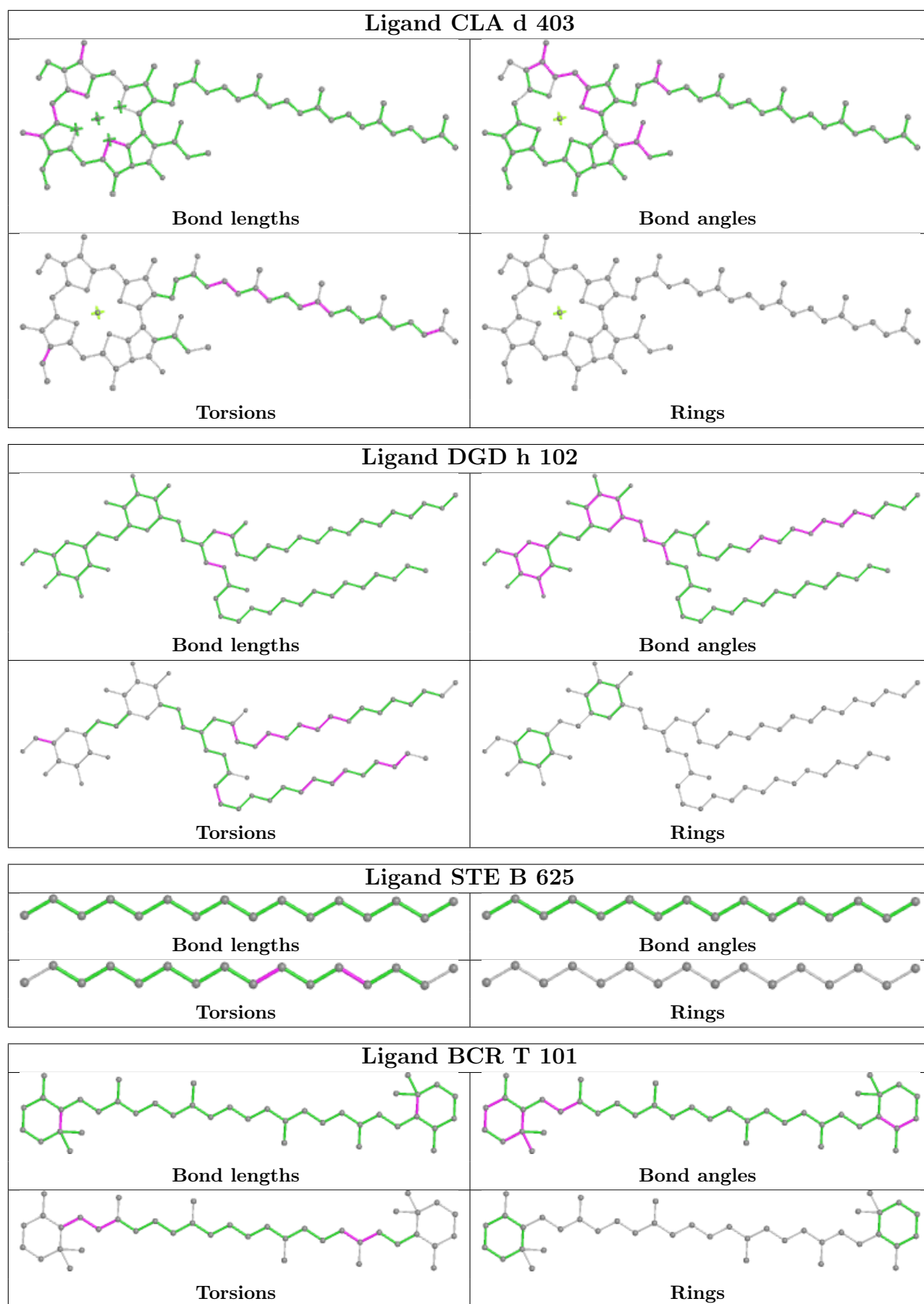


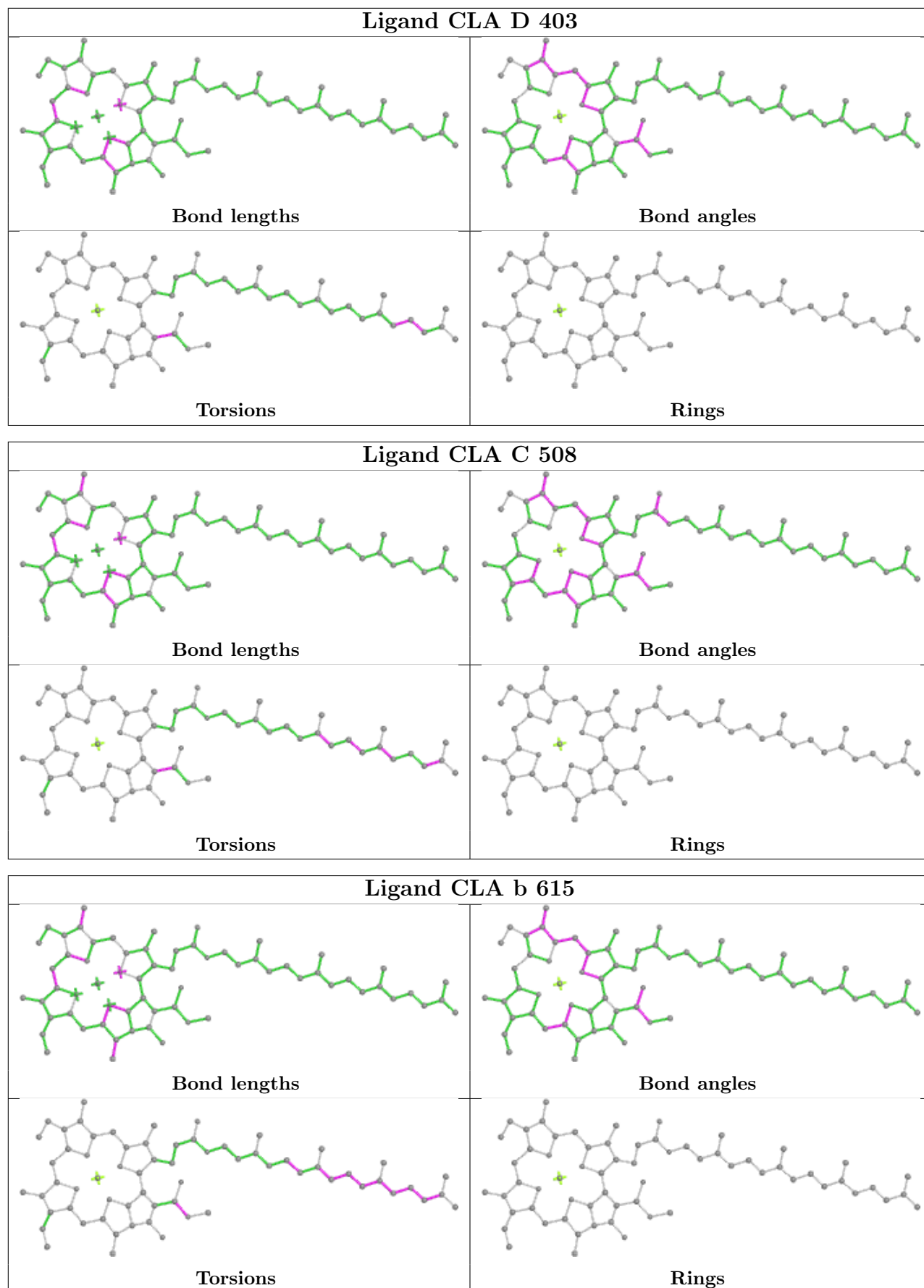


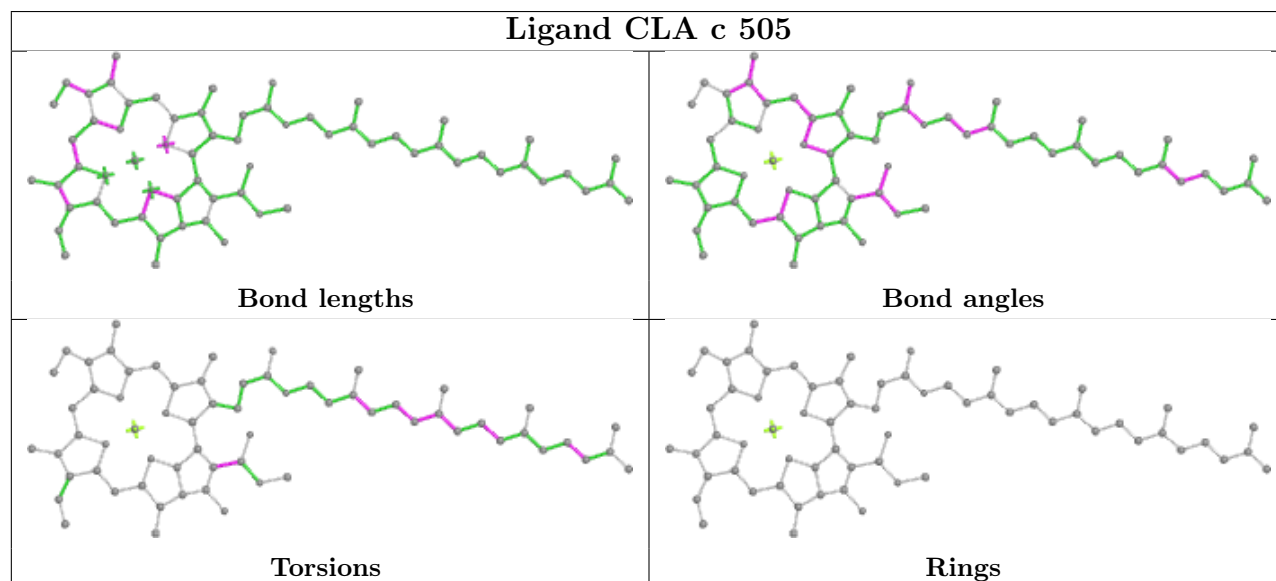
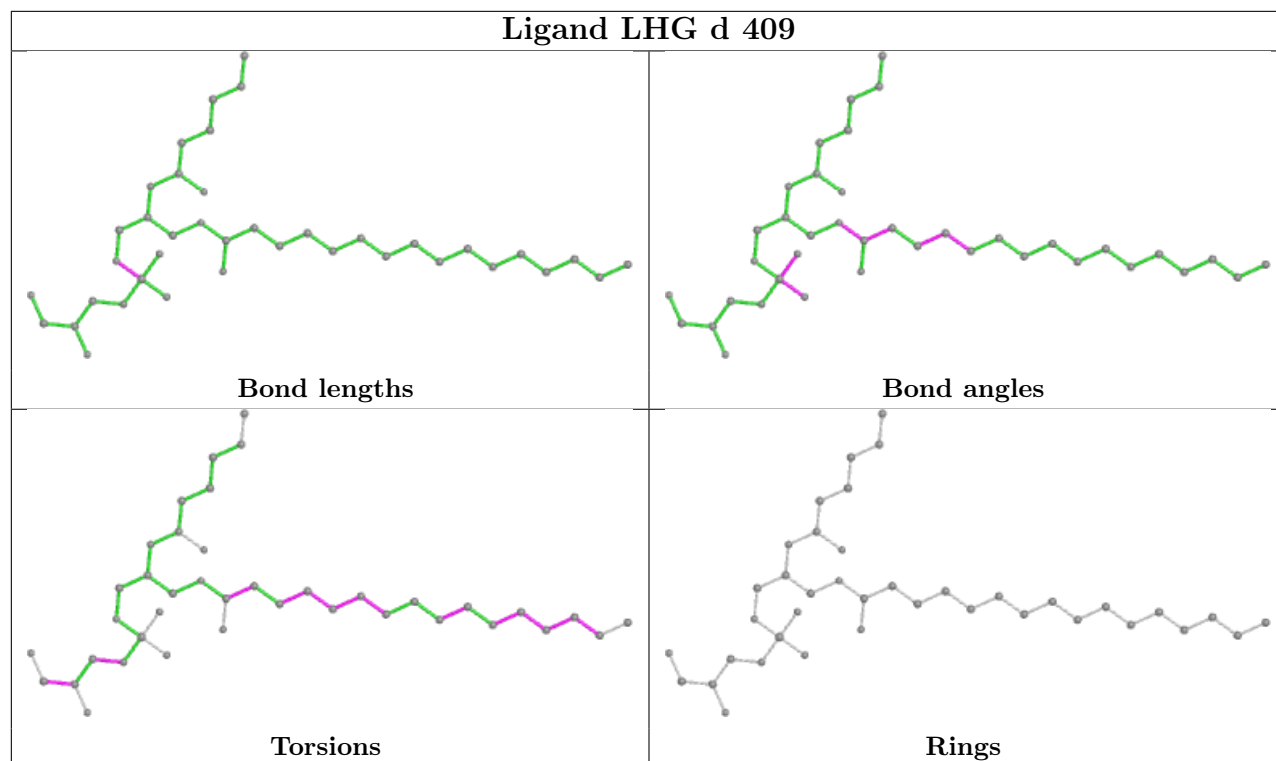
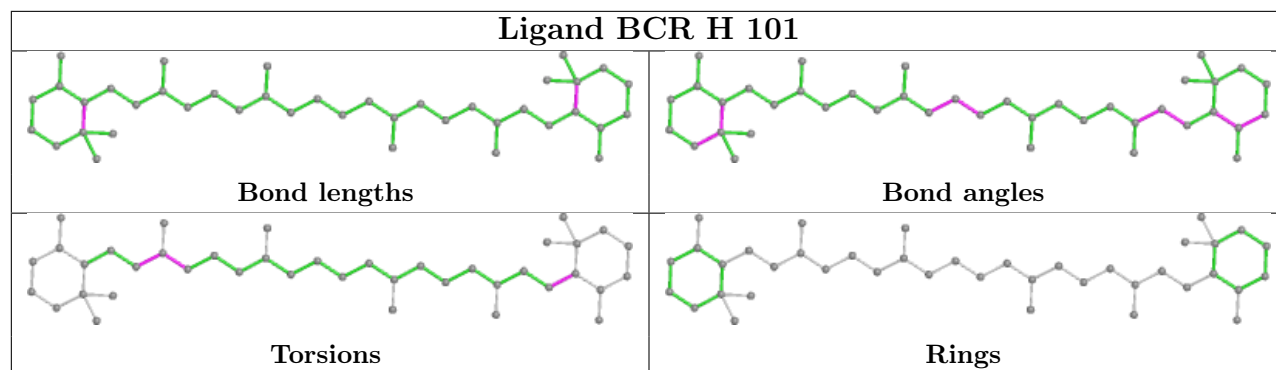


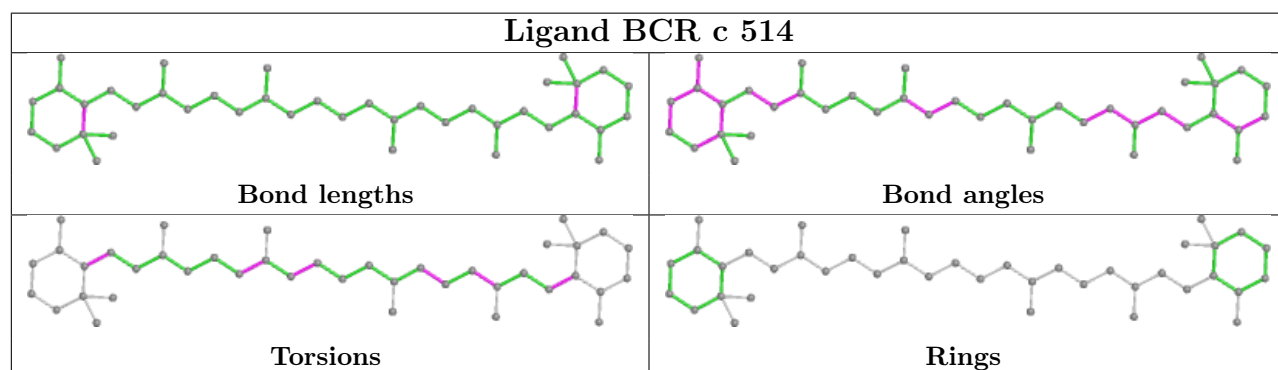
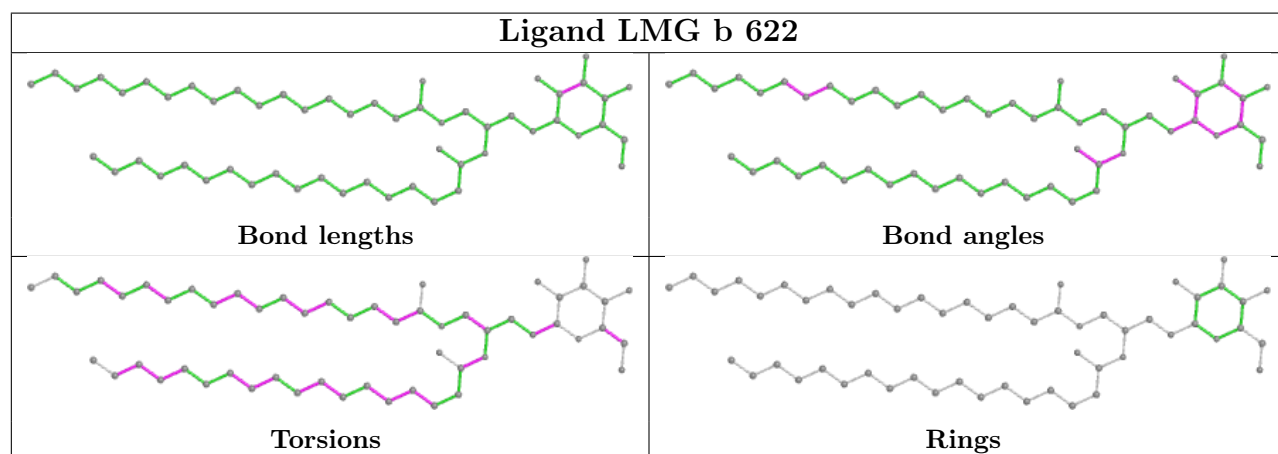
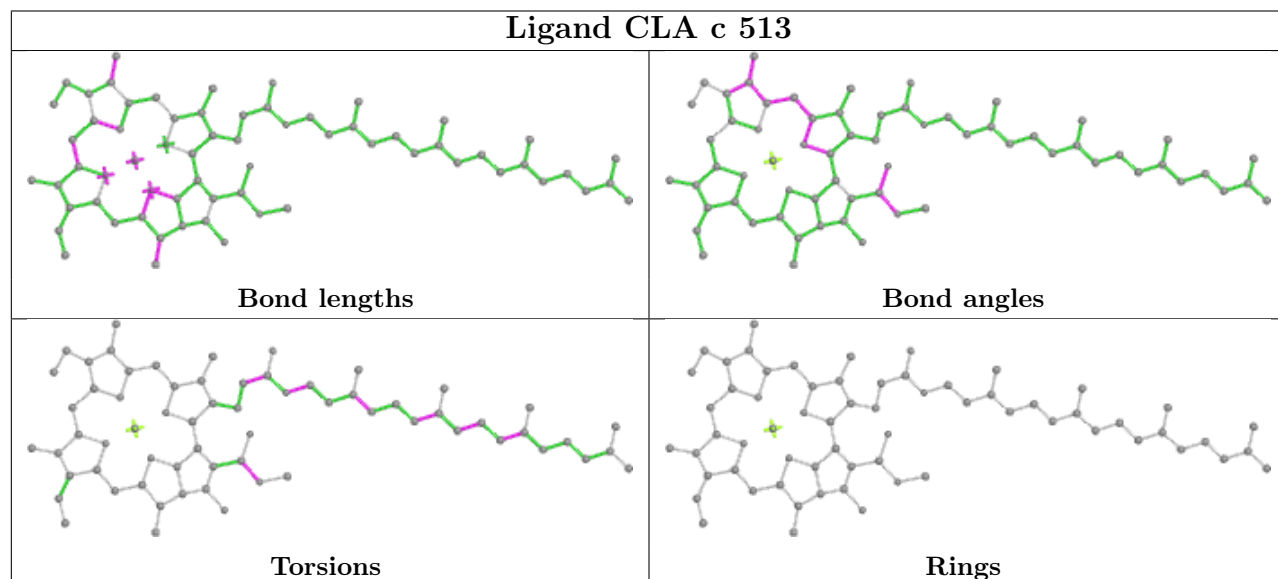
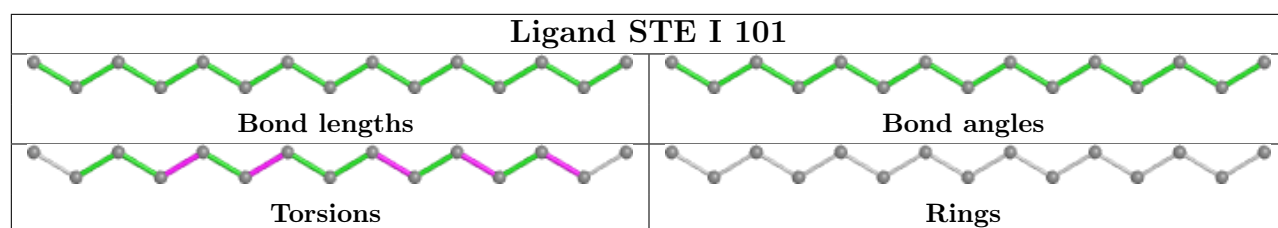


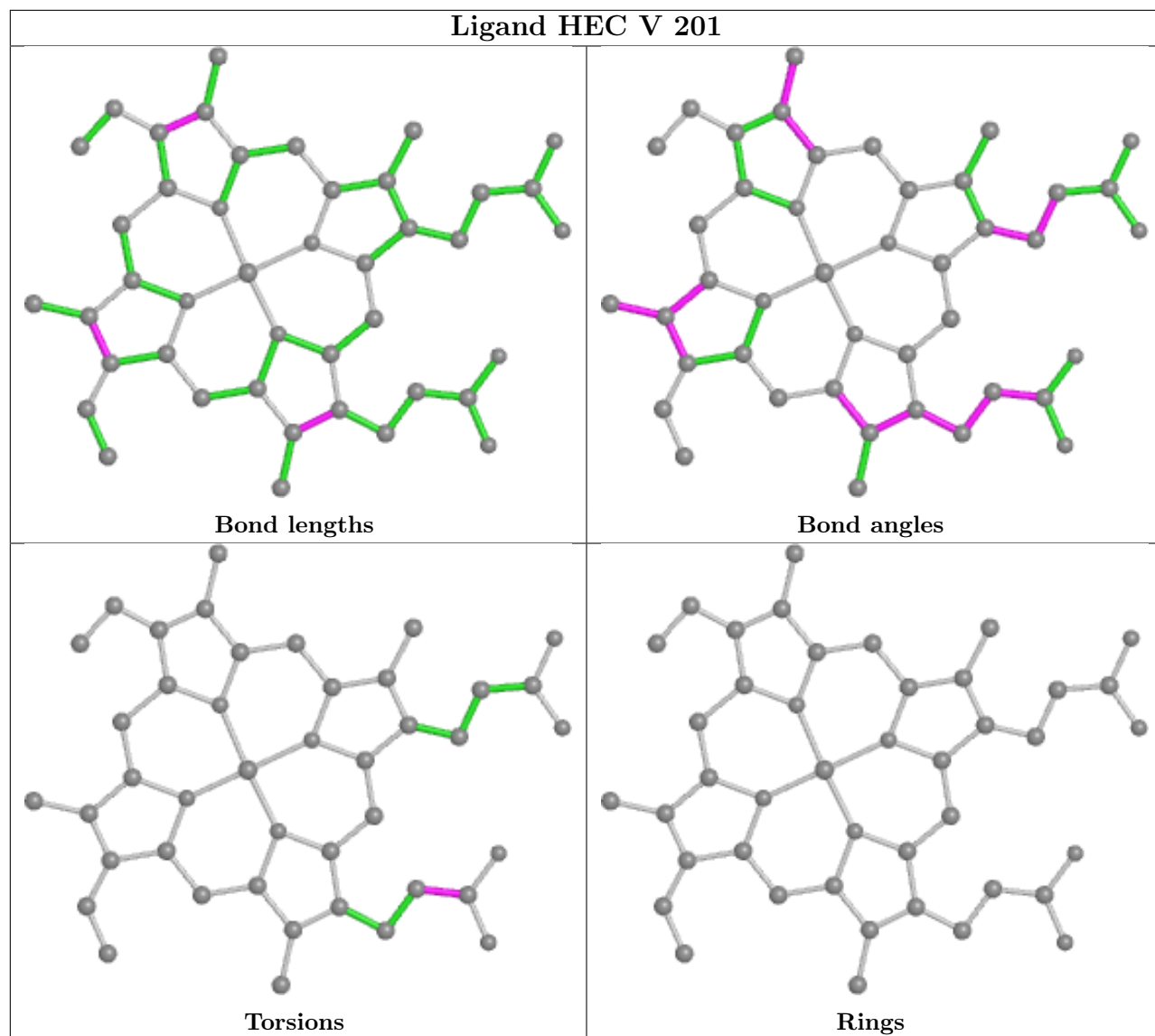


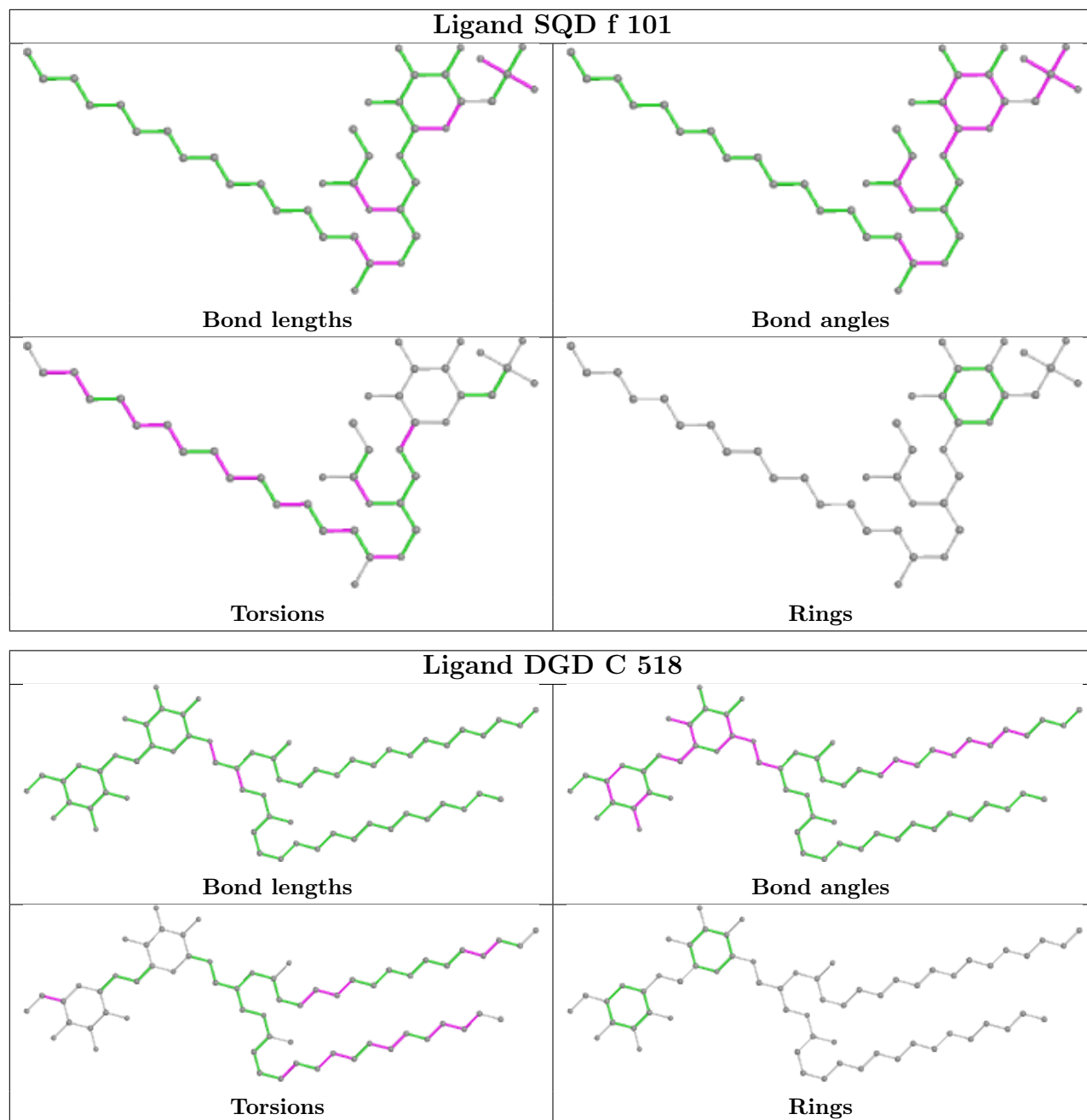


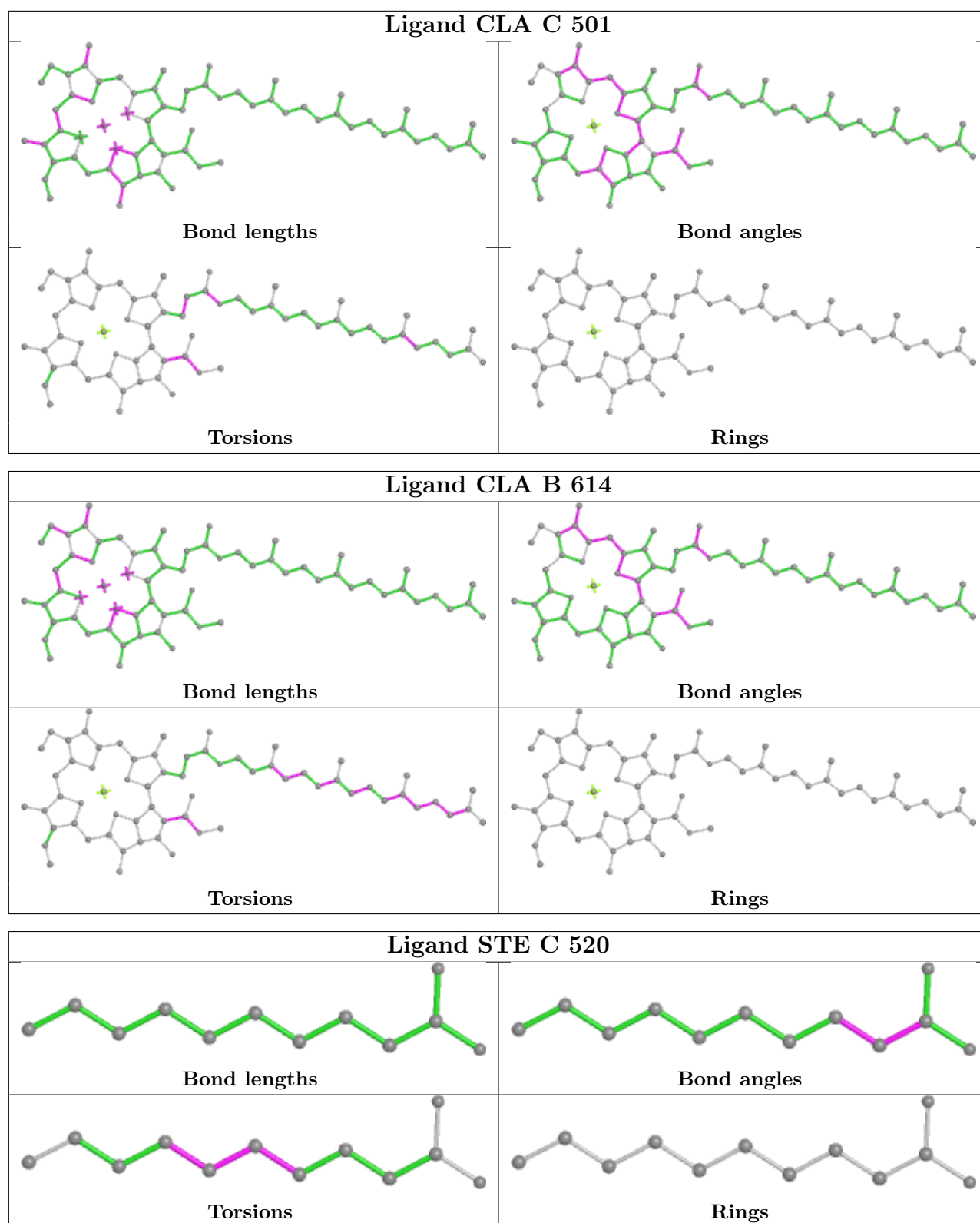


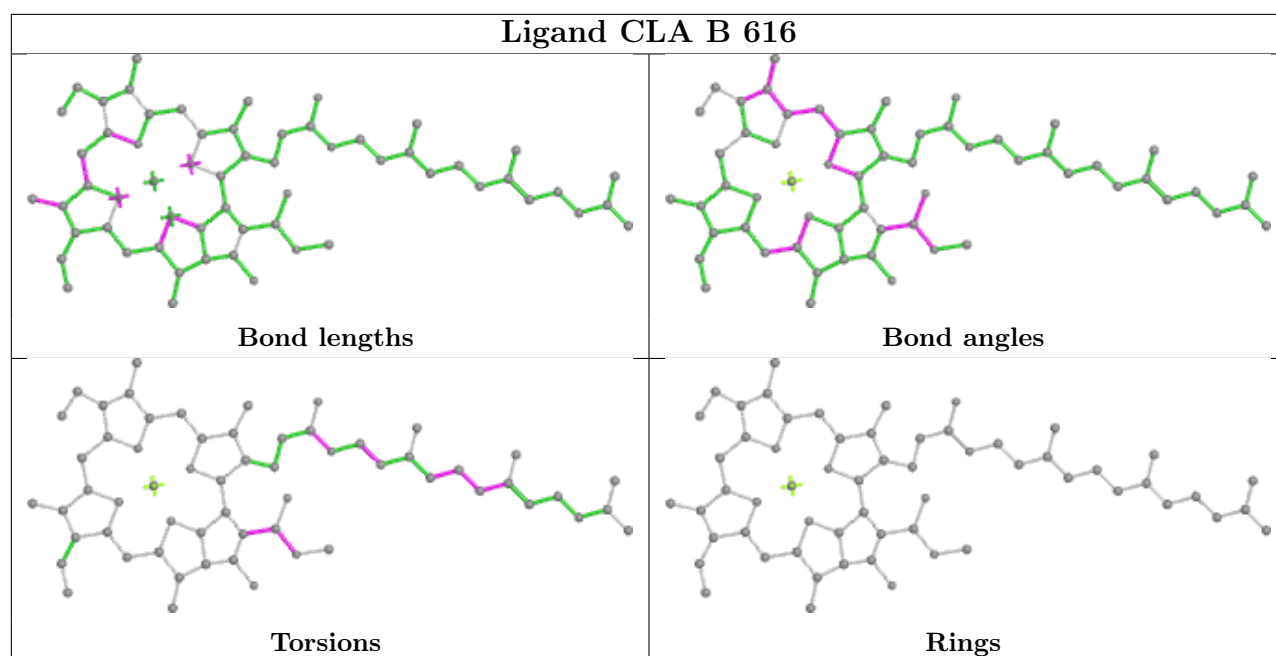












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.30	3 (0%) 84 88	24, 31, 50, 83	0
1	a	334/344 (97%)	-0.29	1 (0%) 94 95	26, 33, 59, 81	0
2	B	505/510 (99%)	-0.28	9 (1%) 68 75	26, 35, 63, 86	0
2	b	505/510 (99%)	-0.12	15 (2%) 50 59	28, 39, 70, 108	0
3	C	442/461 (95%)	-0.22	2 (0%) 91 93	28, 38, 54, 78	0
3	c	451/461 (97%)	-0.07	12 (2%) 54 63	29, 42, 63, 101	0
4	D	341/352 (96%)	-0.27	0 100 100	25, 33, 49, 81	0
4	d	341/352 (96%)	-0.24	1 (0%) 94 95	26, 37, 61, 83	0
5	E	82/84 (97%)	0.12	6 (7%) 15 21	35, 54, 70, 84	0
5	e	82/84 (97%)	0.34	4 (4%) 29 38	41, 60, 81, 90	0
6	F	34/45 (75%)	-0.37	1 (2%) 51 61	38, 46, 62, 86	0
6	f	34/45 (75%)	-0.26	1 (2%) 51 61	45, 53, 79, 90	0
7	H	65/66 (98%)	-0.05	1 (1%) 73 79	34, 42, 57, 74	0
7	h	63/66 (95%)	0.32	4 (6%) 20 27	43, 53, 64, 67	0
8	I	35/38 (92%)	-0.27	1 (2%) 51 61	34, 41, 66, 78	0
8	i	35/38 (92%)	-0.14	2 (5%) 23 32	35, 42, 70, 89	0
9	J	36/40 (90%)	0.06	3 (8%) 11 15	36, 50, 82, 91	0
9	j	36/40 (90%)	0.31	4 (11%) 5 7	40, 57, 91, 102	0
10	K	37/46 (80%)	0.20	1 (2%) 54 63	44, 52, 66, 72	0
10	k	37/46 (80%)	-0.06	1 (2%) 54 63	53, 57, 76, 83	0
11	L	37/37 (100%)	-0.28	0 100 100	27, 32, 61, 64	0
11	l	36/37 (97%)	-0.27	2 (5%) 24 33	28, 33, 72, 92	0
12	M	32/36 (88%)	-0.05	0 100 100	30, 35, 62, 72	0
12	m	31/36 (86%)	-0.17	0 100 100	30, 36, 57, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.07	15 (6%) 21 28	29, 45, 82, 141	0
13	o	244/272 (89%)	0.04	16 (6%) 18 24	30, 44, 79, 131	0
14	T	29/32 (90%)	-0.22	1 (3%) 45 53	29, 34, 60, 78	0
14	t	29/32 (90%)	-0.16	2 (6%) 16 23	31, 35, 70, 88	0
15	U	97/134 (72%)	-0.18	2 (2%) 63 71	34, 46, 71, 98	0
15	u	97/134 (72%)	-0.32	0 100 100	34, 43, 58, 83	0
16	V	137/163 (84%)	-0.39	0 100 100	32, 43, 56, 76	0
16	v	137/163 (84%)	-0.02	3 (2%) 62 69	37, 49, 71, 88	0
17	Y	27/46 (58%)	1.20	7 (25%) 0 0	52, 71, 95, 98	0
17	y	30/46 (65%)	0.55	2 (6%) 17 24	64, 77, 85, 100	0
18	X	38/41 (92%)	0.11	2 (5%) 26 35	44, 52, 68, 71	0
18	x	39/41 (95%)	0.25	5 (12%) 3 5	50, 61, 85, 100	0
19	Z	62/62 (100%)	0.83	15 (24%) 0 0	55, 69, 112, 127	0
19	z	62/62 (100%)	0.84	8 (12%) 3 5	63, 77, 115, 117	0
20	R	34/41 (82%)	1.54	12 (35%) 0 0	61, 70, 81, 89	0
20	r	31/41 (75%)	3.15	22 (70%) 0 0	72, 88, 113, 121	0
All	All	5302/5700 (93%)	-0.09	186 (3%) 44 52	24, 40, 75, 141	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.0
13	O	60	ARG	7.4
19	Z	33	TRP	7.0
13	o	3	GLN	6.7
18	X	2	THR	6.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
14	FME	t	1	10/11	0.91	0.11	35,42,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	FME	m	1	10/11	0.93	0.18	32,53,69,70	0
14	FME	T	1	10/11	0.94	0.12	36,44,53,66	0
8	FME	i	1	10/11	0.94	0.15	38,52,60,65	0
12	FME	M	1	10/11	0.95	0.19	41,53,66,68	0
8	FME	I	1	10/11	0.97	0.14	39,52,59,61	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
32	STE	H	103	18/20	0.70	0.28	56,63,72,72	0
32	STE	a	616	12/20	0.71	0.20	41,57,67,73	0
29	LMG	D	412	33/55	0.74	0.20	36,52,75,79	0
32	STE	c	522	12/20	0.77	0.22	58,68,79,85	0
29	LMG	d	410	23/55	0.78	0.27	51,61,75,75	0
32	STE	R	101	12/20	0.78	0.25	61,68,87,87	0
31	DGD	a	614	44/66	0.78	0.18	40,54,74,82	0
32	STE	B	625	16/20	0.78	0.26	46,60,71,71	0
32	STE	b	621	20/20	0.80	0.19	42,56,70,72	0
32	STE	b	623	16/20	0.80	0.20	50,60,78,82	0
32	STE	X	101	20/20	0.80	0.17	38,48,68,69	0
32	STE	I	101	15/20	0.81	0.16	43,53,69,73	0
32	STE	C	520	12/20	0.81	0.14	38,44,61,64	0
29	LMG	b	622	55/55	0.81	0.26	53,66,81,85	0
32	STE	b	625	20/20	0.81	0.18	49,58,70,73	0
32	STE	a	615	10/20	0.81	0.20	43,51,57,58	0
32	STE	C	522	16/20	0.82	0.15	44,49,57,59	0
28	PL9	a	611	55/55	0.82	0.23	45,63,78,82	0
29	LMG	c	521	48/55	0.82	0.25	41,68,89,92	0
32	STE	L	103	12/20	0.82	0.16	48,53,65,67	0
32	STE	l	102	18/20	0.82	0.16	32,44,65,68	0
28	PL9	A	611	55/55	0.83	0.25	43,59,72,76	0
32	STE	c	520	20/20	0.83	0.22	50,54,77,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	STE	B	620	17/20	0.83	0.16	39,49,62,64	0
32	STE	d	413	20/20	0.83	0.22	45,55,66,67	0
32	STE	M	103	10/20	0.83	0.18	30,45,53,58	0
32	STE	t	104	18/20	0.83	0.16	43,52,77,83	0
25	CLA	b	601	65/65	0.84	0.18	46,66,83,93	0
32	STE	b	620	16/20	0.84	0.20	38,49,62,63	0
27	BCR	H	101	40/40	0.84	0.16	33,44,52,55	0
30	SQD	t	102	36/54	0.84	0.17	34,53,67,70	0
31	DGD	A	615	66/66	0.84	0.18	47,59,68,71	0
34	LHG	E	101	49/49	0.84	0.21	46,74,91,94	0
27	BCR	h	101	40/40	0.86	0.14	40,52,63,66	0
29	LMG	c	519	37/55	0.86	0.17	47,62,72,74	0
29	LMG	B	621	28/55	0.86	0.16	37,49,60,61	0
29	LMG	c	523	49/55	0.86	0.16	36,50,78,82	0
29	LMG	C	519	48/55	0.86	0.18	44,62,77,82	0
27	BCR	K	102	40/40	0.86	0.15	40,50,58,62	0
32	STE	b	626	10/20	0.87	0.21	47,49,57,58	0
32	STE	B	624	12/20	0.87	0.35	51,55,65,71	0
32	STE	J	101	12/20	0.87	0.11	50,59,67,68	0
32	STE	d	412	17/20	0.87	0.15	44,54,69,70	0
25	CLA	c	513	65/65	0.87	0.19	48,62,83,88	0
29	LMG	A	612	48/55	0.87	0.15	43,54,65,71	0
30	SQD	B	622	54/54	0.87	0.17	38,58,78,81	0
30	SQD	L	101	49/54	0.87	0.16	37,53,76,83	0
34	LHG	e	102	42/49	0.87	0.26	62,79,89,95	0
27	BCR	D	406	40/40	0.88	0.16	32,43,69,72	0
29	LMG	m	101	51/55	0.88	0.13	33,47,64,67	0
30	SQD	A	614	39/54	0.88	0.17	39,53,69,74	0
32	STE	B	623	12/20	0.88	0.14	37,49,57,59	0
25	CLA	c	512	65/65	0.88	0.15	41,55,79,83	0
32	STE	t	103	14/20	0.88	0.12	39,46,53,62	0
32	STE	M	102	15/20	0.88	0.16	40,46,55,60	0
27	BCR	k	101	40/40	0.88	0.14	52,61,69,72	0
29	LMG	M	101	51/55	0.88	0.13	30,49,64,69	0
25	CLA	C	513	65/65	0.89	0.17	48,56,82,87	0
27	BCR	d	405	40/40	0.89	0.13	43,49,83,87	0
32	STE	j	101	12/20	0.89	0.13	51,59,64,67	0
32	STE	C	521	12/20	0.89	0.14	44,51,56,56	0
30	SQD	f	101	41/54	0.90	0.17	63,74,84,88	0
25	CLA	C	512	65/65	0.90	0.16	35,46,77,84	0
27	BCR	k	102	40/40	0.90	0.20	49,53,60,67	0
25	CLA	B	601	65/65	0.90	0.13	38,54,75,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	DGD	H	102	62/66	0.91	0.12	31,41,52,54	0
25	CLA	b	616	60/65	0.91	0.13	31,42,75,83	0
32	STE	b	624	15/20	0.91	0.14	45,52,70,74	0
31	DGD	C	517	62/66	0.92	0.13	35,46,84,99	0
27	BCR	B	618	40/40	0.92	0.13	28,38,49,52	0
27	BCR	C	514	40/40	0.92	0.12	31,39,45,54	0
25	CLA	C	502	65/65	0.92	0.13	31,38,46,54	0
25	CLA	c	502	65/65	0.92	0.13	33,40,48,57	0
27	BCR	K	101	40/40	0.92	0.13	37,54,60,63	0
25	CLA	c	508	64/65	0.92	0.14	35,43,81,94	0
27	BCR	b	619	40/40	0.92	0.12	33,47,61,63	0
29	LMG	D	408	51/55	0.92	0.15	34,46,66,70	0
27	BCR	c	514	40/40	0.92	0.13	48,57,63,67	0
25	CLA	a	609	65/65	0.92	0.12	23,30,69,73	0
25	CLA	B	606	65/65	0.92	0.12	27,37,57,68	0
29	LMG	d	411	44/55	0.93	0.12	43,52,72,79	0
25	CLA	c	506	65/65	0.93	0.12	40,46,72,75	0
27	BCR	b	618	40/40	0.93	0.11	25,36,47,48	0
25	CLA	C	511	65/65	0.93	0.11	31,46,58,60	0
30	SQD	D	409	36/54	0.93	0.15	45,62,74,79	0
25	CLA	C	501	65/65	0.93	0.13	27,35,44,46	0
30	SQD	a	613	54/54	0.93	0.15	38,55,77,82	0
25	CLA	b	614	65/65	0.93	0.14	30,38,66,71	0
25	CLA	b	615	65/65	0.93	0.12	28,38,50,54	0
25	CLA	B	616	60/65	0.93	0.14	28,36,71,73	0
25	CLA	D	405	65/65	0.93	0.13	27,33,90,96	0
31	DGD	C	518	62/66	0.93	0.12	33,43,68,70	0
27	BCR	t	101	40/40	0.93	0.10	27,38,45,48	0
25	CLA	c	503	65/65	0.93	0.14	36,44,48,54	0
31	DGD	c	517	62/66	0.93	0.12	42,48,78,81	0
25	CLA	c	504	60/65	0.93	0.10	29,43,64,72	0
31	DGD	h	102	62/66	0.94	0.11	32,44,53,56	0
25	CLA	C	508	65/65	0.94	0.11	32,38,86,92	0
25	CLA	c	505	65/65	0.94	0.14	32,38,54,55	0
28	PL9	D	407	55/55	0.94	0.11	23,31,40,43	0
25	CLA	C	510	65/65	0.94	0.12	31,42,51,67	0
25	CLA	c	507	65/65	0.94	0.12	34,41,51,56	0
25	CLA	A	609	54/65	0.94	0.10	25,30,57,59	0
25	CLA	c	510	65/65	0.94	0.14	36,45,51,58	0
25	CLA	c	511	65/65	0.94	0.12	41,55,63,66	0
25	CLA	B	609	65/65	0.94	0.13	27,38,47,55	0
25	CLA	B	614	65/65	0.94	0.16	25,33,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	d	404	65/65	0.94	0.12	33,41,71,83	0
27	BCR	B	617	40/40	0.94	0.11	26,39,45,49	0
25	CLA	B	615	65/65	0.94	0.11	28,36,53,59	0
27	BCR	B	619	40/40	0.94	0.10	31,40,53,54	0
25	CLA	A	607	65/65	0.94	0.13	23,33,70,78	0
27	BCR	C	515	40/40	0.94	0.15	35,47,57,62	0
25	CLA	B	602	65/65	0.94	0.14	30,37,48,56	0
25	CLA	b	602	65/65	0.94	0.13	30,40,52,56	0
25	CLA	b	604	65/65	0.94	0.12	26,33,58,73	0
25	CLA	b	606	65/65	0.94	0.11	30,38,62,71	0
27	BCR	T	101	40/40	0.94	0.09	31,40,46,50	0
27	BCR	b	617	40/40	0.94	0.12	35,43,49,51	0
25	CLA	b	609	65/65	0.94	0.13	30,42,55,66	0
25	CLA	b	613	65/65	0.94	0.15	25,31,66,71	0
25	CLA	B	604	65/65	0.94	0.12	24,31,59,63	0
31	DGD	C	516	62/66	0.94	0.12	26,34,66,70	0
27	BCR	c	515	40/40	0.94	0.11	33,45,54,56	0
25	CLA	C	503	65/65	0.94	0.14	34,42,46,51	0
25	CLA	C	505	65/65	0.94	0.15	23,36,60,62	0
25	CLA	C	506	65/65	0.94	0.12	32,43,72,77	0
31	DGD	c	516	62/66	0.94	0.11	30,41,60,64	0
25	CLA	C	507	65/65	0.94	0.12	29,37,49,56	0
34	LHG	d	407	49/49	0.94	0.14	33,46,62,63	0
31	DGD	c	518	62/66	0.94	0.13	34,46,69,77	0
28	PL9	d	406	55/55	0.95	0.12	23,34,38,42	0
25	CLA	a	612	65/65	0.95	0.10	24,31,38,46	0
25	CLA	C	509	65/65	0.95	0.15	32,39,52,56	0
25	CLA	B	603	65/65	0.95	0.14	23,31,46,51	0
25	CLA	b	603	65/65	0.95	0.12	26,32,58,66	0
25	CLA	C	504	59/65	0.95	0.11	31,38,68,74	0
24	CL	a	605	1/1	0.95	0.06	38,38,38,38	0
25	CLA	b	608	65/65	0.95	0.12	33,39,54,58	0
25	CLA	c	509	65/65	0.95	0.15	37,45,57,59	0
25	CLA	B	610	65/65	0.95	0.13	23,31,38,41	0
25	CLA	b	610	65/65	0.95	0.17	29,36,44,53	0
25	CLA	b	611	65/65	0.95	0.12	25,33,48,51	0
25	CLA	b	612	65/65	0.95	0.15	21,34,39,47	0
25	CLA	d	403	65/65	0.95	0.10	25,33,49,61	0
30	SQD	A	613	52/54	0.95	0.15	36,52,71,78	0
25	CLA	B	612	65/65	0.95	0.14	24,31,37,46	0
26	PHO	a	608	64/64	0.95	0.12	24,30,36,41	0
26	PHO	d	402	64/64	0.95	0.10	32,38,44,46	0

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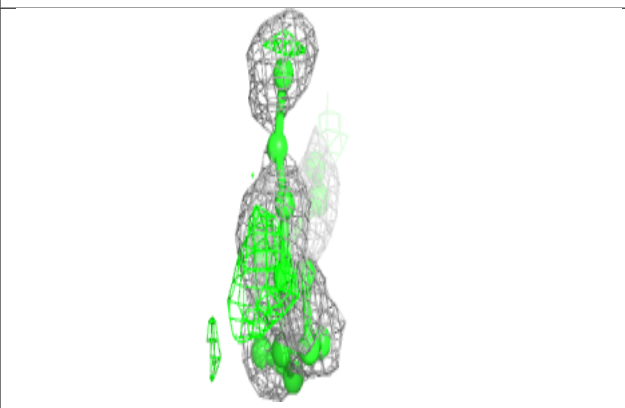
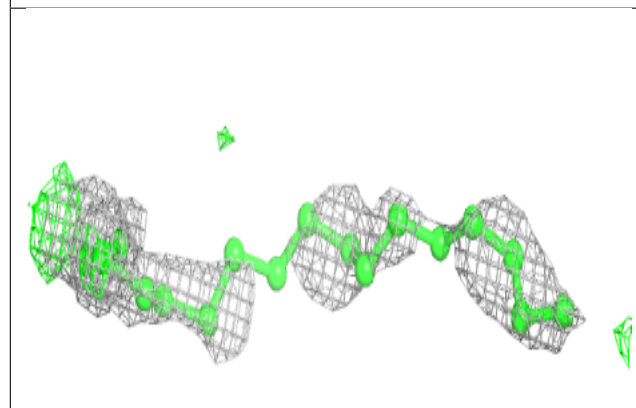
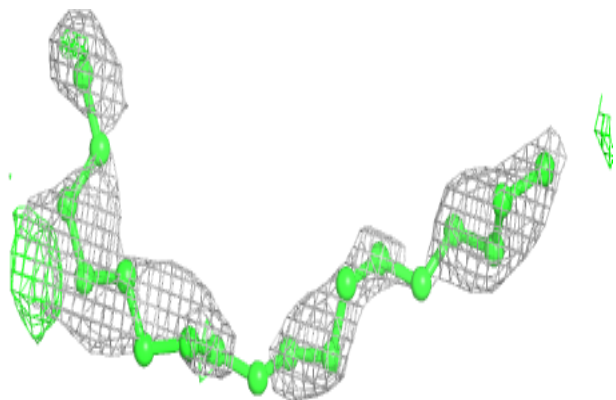
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	BCR	A	610	40/40	0.95	0.09	24,33,38,41	0
34	LHG	D	411	47/49	0.95	0.12	30,42,63,74	0
34	LHG	D	413	49/49	0.95	0.13	30,39,58,61	0
25	CLA	a	606	65/65	0.95	0.10	23,30,37,48	0
34	LHG	L	102	49/49	0.95	0.14	30,38,48,57	0
25	CLA	a	607	65/65	0.95	0.12	28,38,82,87	0
34	LHG	d	409	39/49	0.95	0.12	36,43,58,59	0
25	CLA	B	613	65/65	0.95	0.12	22,29,60,64	0
34	LHG	l	101	49/49	0.95	0.11	28,41,49,52	0
25	CLA	B	605	65/65	0.96	0.13	25,31,42,46	0
25	CLA	D	403	65/65	0.96	0.09	21,29,38,41	0
25	CLA	D	404	65/65	0.96	0.11	22,28,48,52	0
26	PHO	A	608	64/64	0.96	0.10	23,29,35,38	0
26	PHO	D	402	64/64	0.96	0.14	27,34,39,41	0
25	CLA	A	606	65/65	0.96	0.09	20,28,39,42	0
27	BCR	a	610	40/40	0.96	0.08	23,33,43,49	0
25	CLA	B	611	65/65	0.96	0.14	23,30,43,47	0
25	CLA	b	605	65/65	0.96	0.12	24,34,43,50	0
25	CLA	B	607	65/65	0.96	0.10	21,30,55,65	0
34	LHG	d	408	49/49	0.96	0.12	30,39,46,48	0
25	CLA	b	607	65/65	0.96	0.12	23,31,58,62	0
25	CLA	c	501	65/65	0.96	0.12	32,37,48,50	0
25	CLA	B	608	65/65	0.96	0.12	26,32,48,53	0
35	HEM	F	101	43/43	0.96	0.10	37,49,58,66	0
35	HEM	e	101	43/43	0.96	0.13	53,59,76,87	0
34	LHG	D	410	49/49	0.97	0.11	30,36,46,55	0
24	CL	a	604	1/1	0.97	0.04	38,38,38,38	0
24	CL	A	604	1/1	0.97	0.08	36,36,36,36	0
33	BCT	d	401	4/4	0.97	0.15	36,36,40,46	0
36	HEC	V	201	43/43	0.97	0.11	28,34,39,49	0
36	HEC	v	201	43/43	0.97	0.11	32,38,45,48	0
33	BCT	D	401	4/4	0.98	0.15	35,35,38,38	0
21	OEY	A	601[B]	11/11	0.98	0.12	29,32,34,34	11
22	OEX	A	602[A]	10/10	0.98	0.12	26,36,38,39	10
22	OEX	a	602[A]	10/10	0.98	0.10	29,35,38,43	10
23	FE2	A	603	1/1	0.99	0.06	34,34,34,34	0
23	FE2	a	603	1/1	0.99	0.04	36,36,36,36	0
21	OEY	a	601[B]	11/11	0.99	0.09	28,32,34,35	11
24	CL	A	605	1/1	0.99	0.03	36,36,36,36	0

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

orientation to approximate a three-dimensional view.

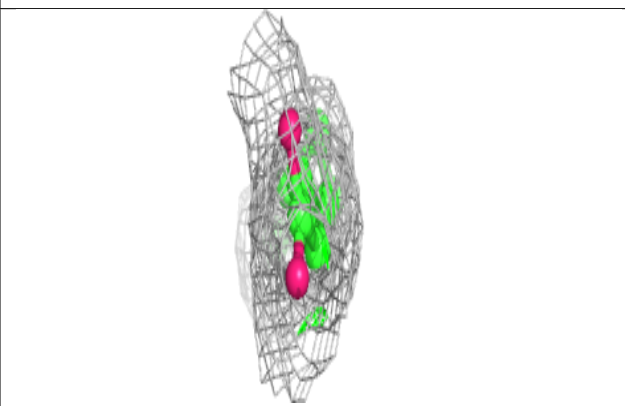
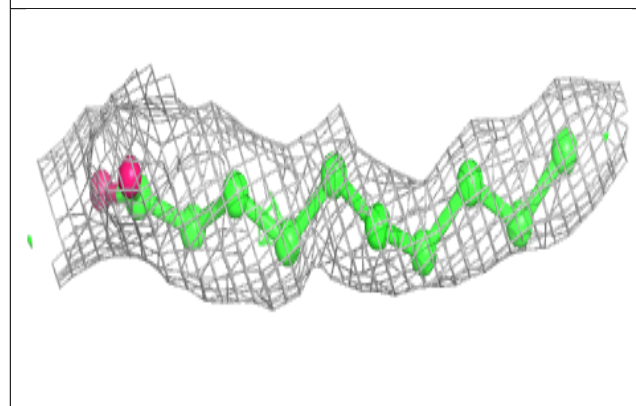
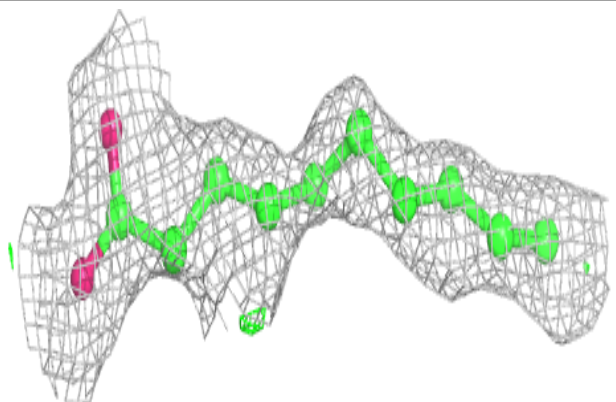
Electron density around STE H 103:

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



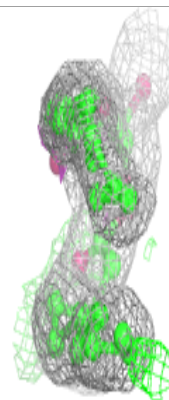
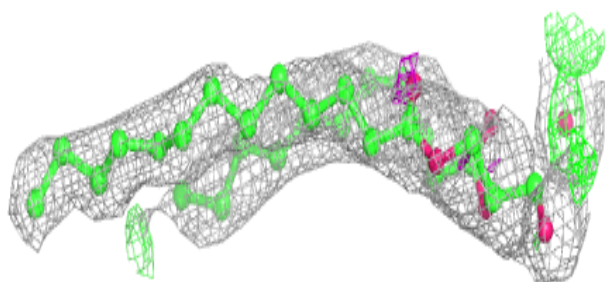
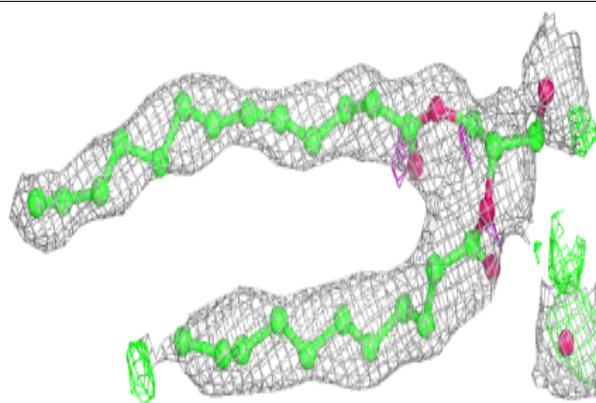
Electron density around STE a 616:

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

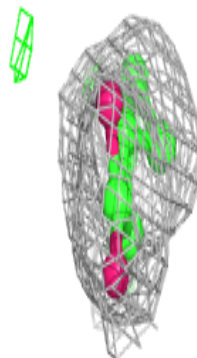
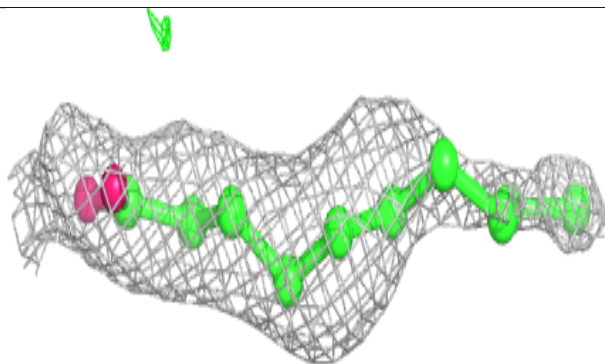
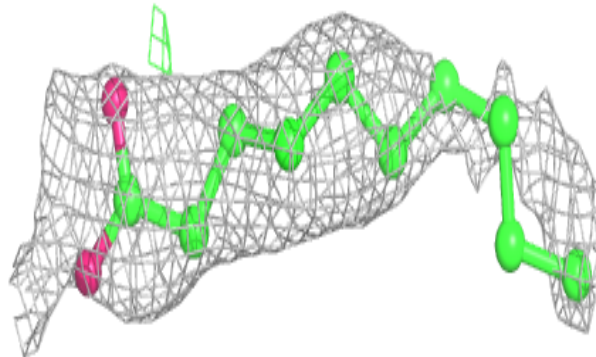


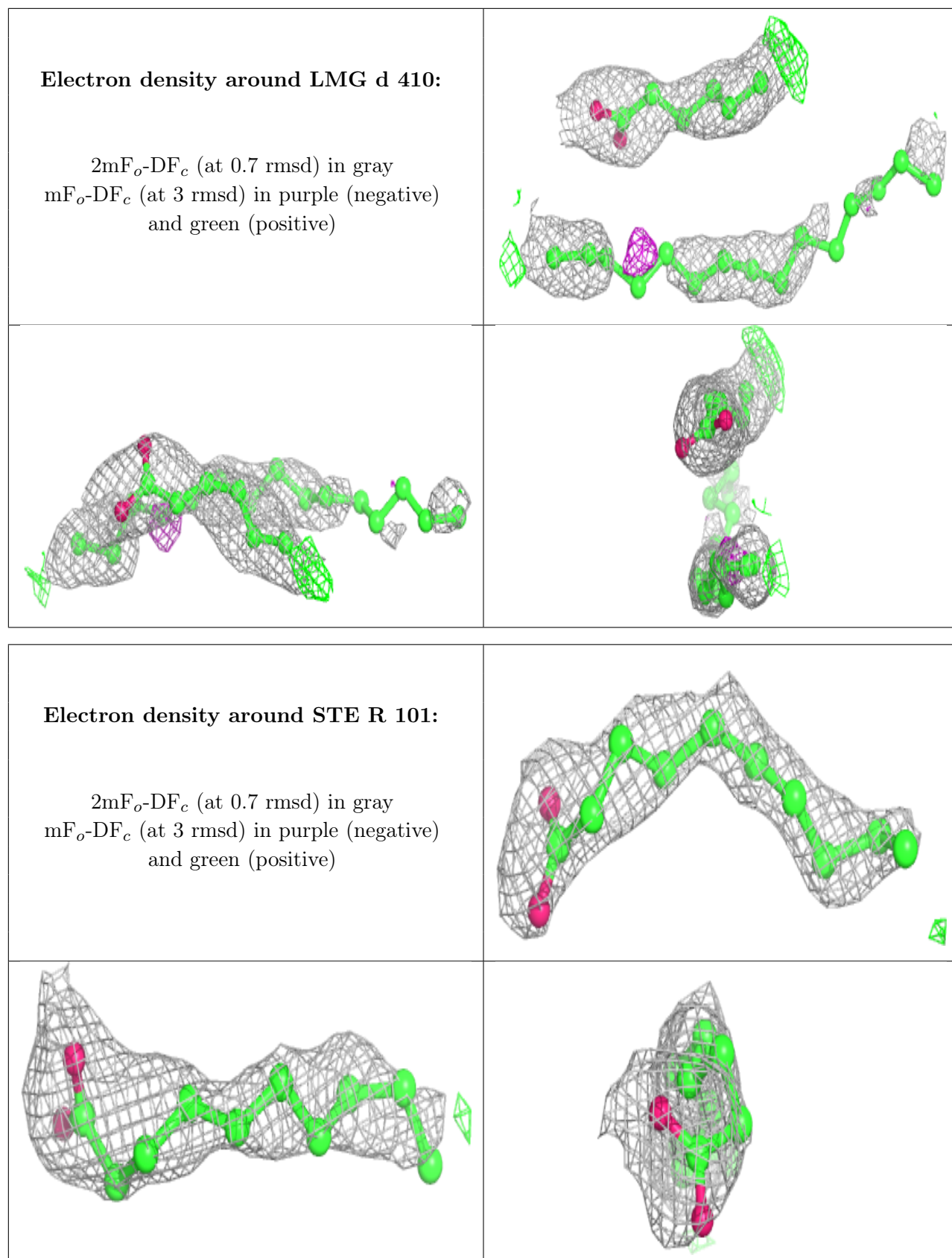
Electron density around LMG D 412:

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

**Electron density around STE c 522:**

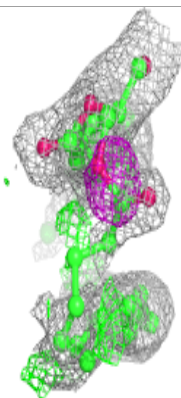
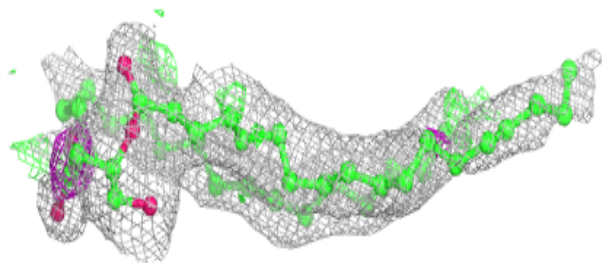
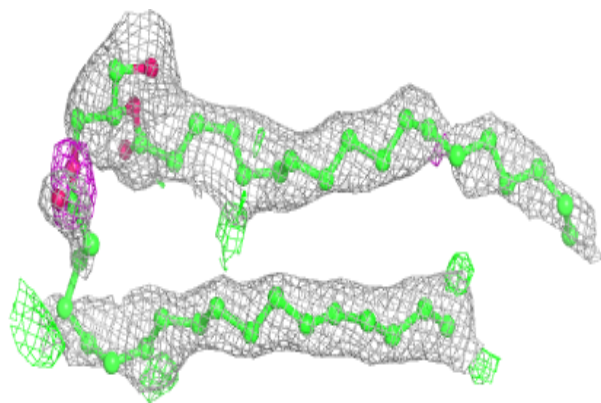
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



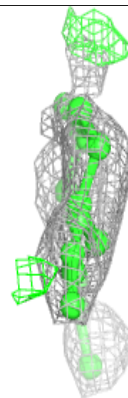
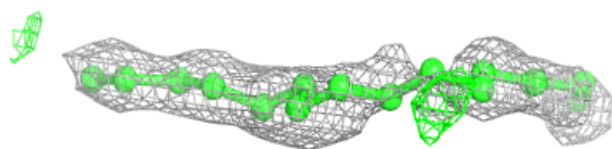
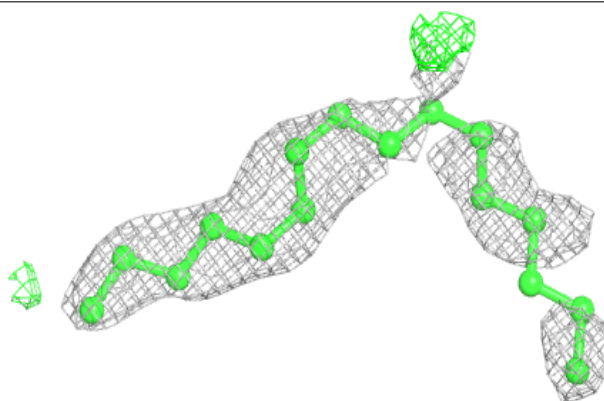


Electron density around DGD a 614:

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

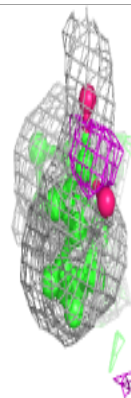
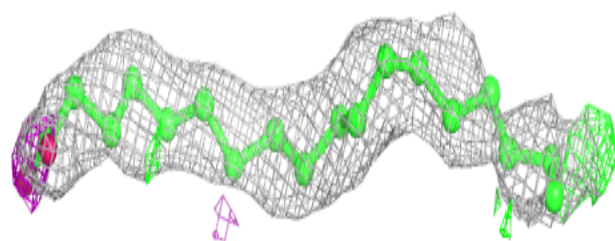
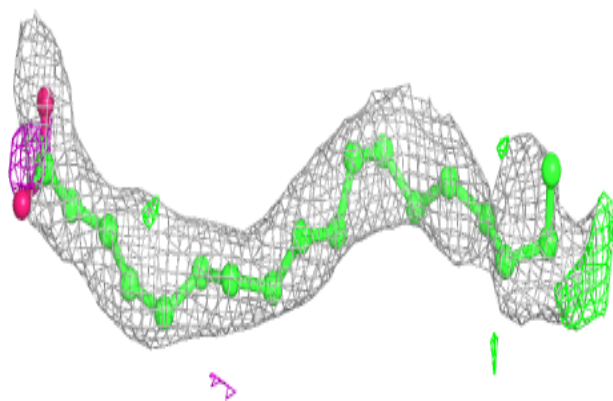
**Electron density around STE B 625:**

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

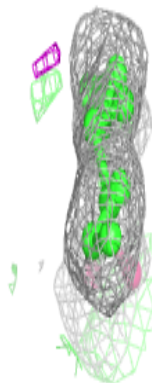
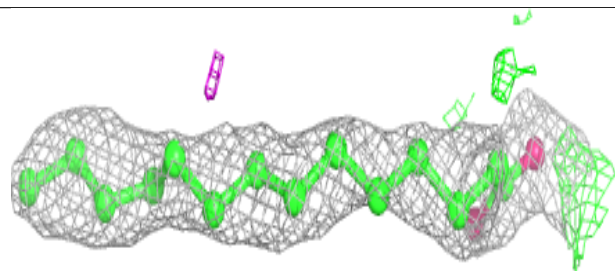
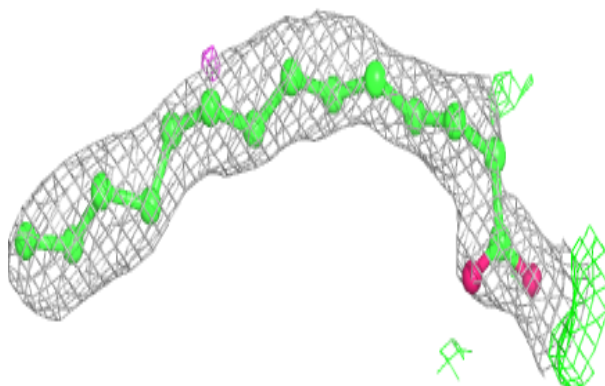


Electron density around STE b 621:

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

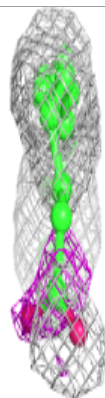
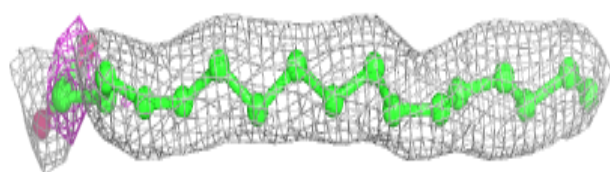
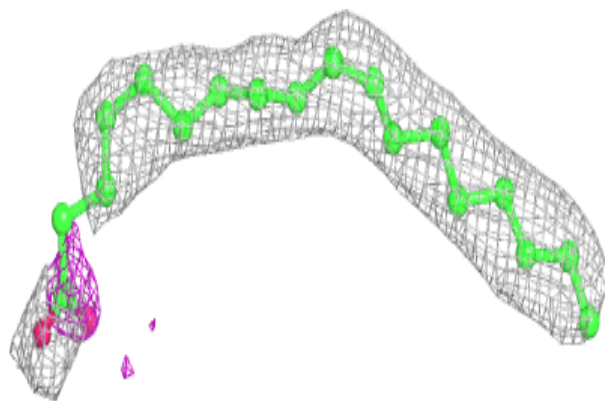
**Electron density around STE b 623:**

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

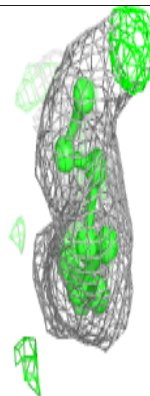
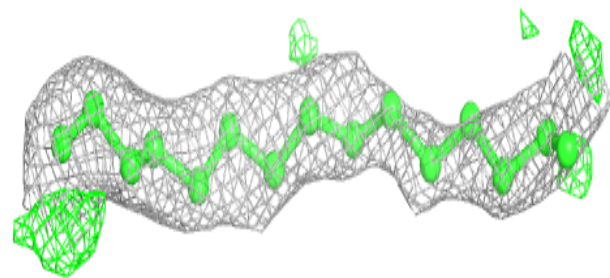
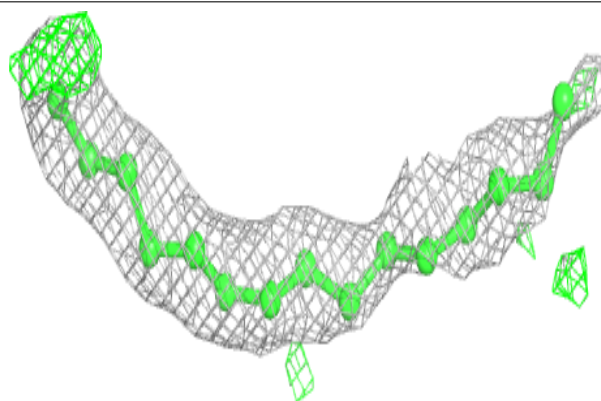


Electron density around STE X 101:

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

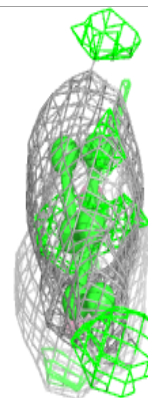
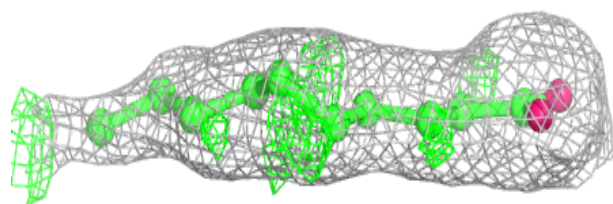
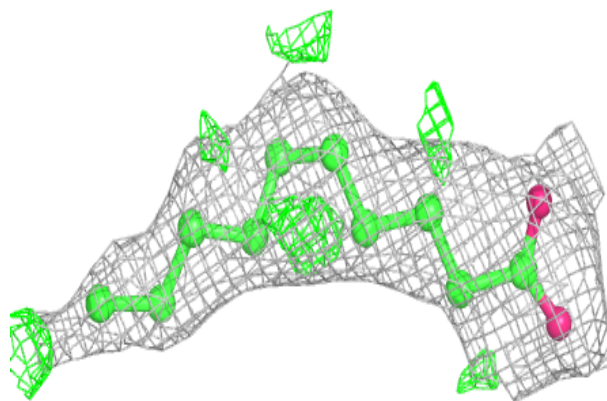
**Electron density around STE I 101:**

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

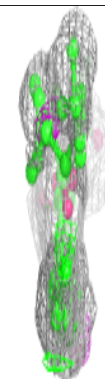
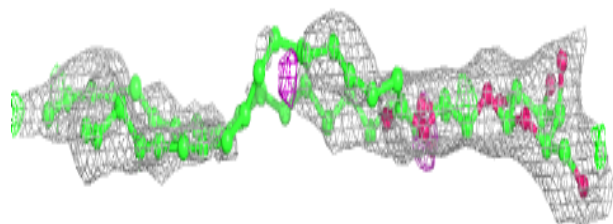
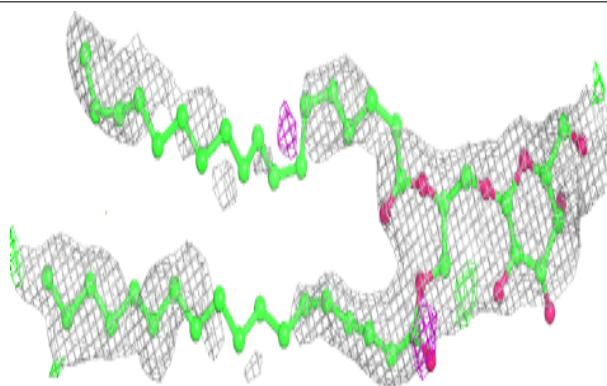


Electron density around STE C 520:

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

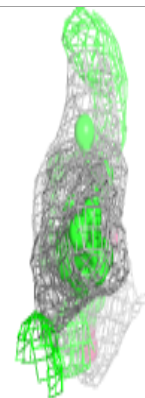
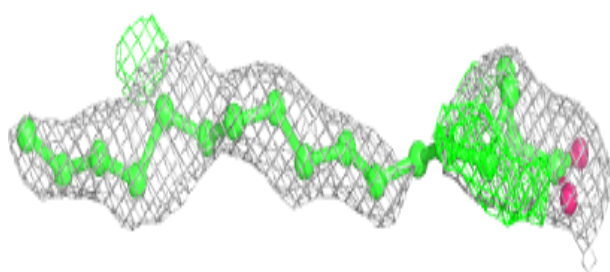
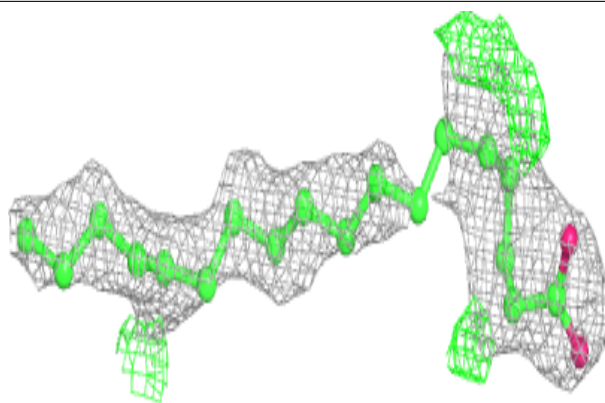
**Electron density around LMG b 622:**

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

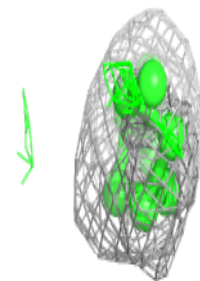
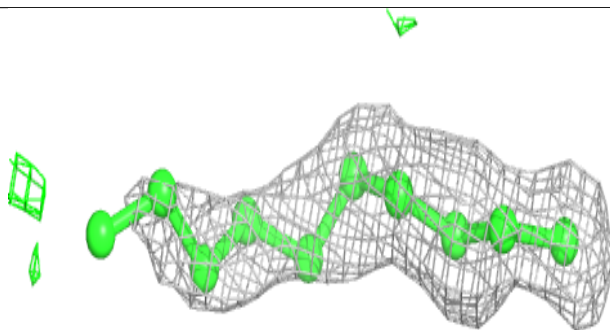
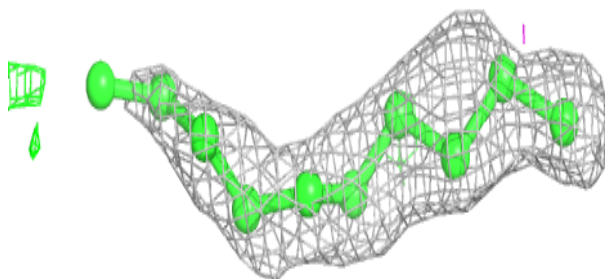


Electron density around STE b 625:

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

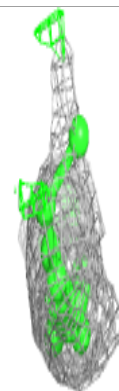
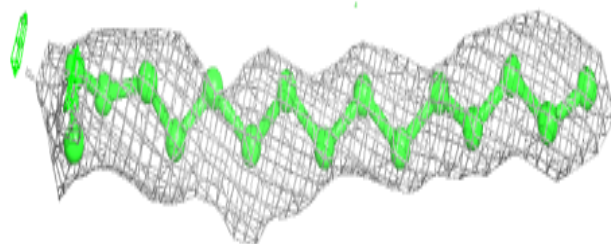
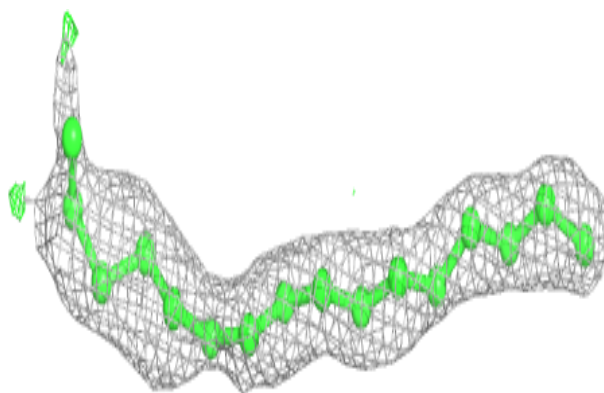
**Electron density around STE a 615:**

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

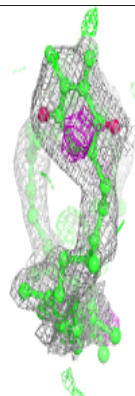
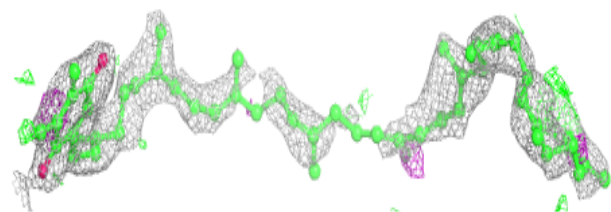
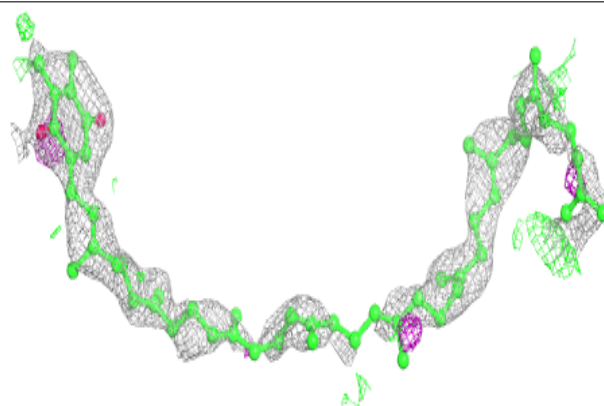


Electron density around STE C 522:

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

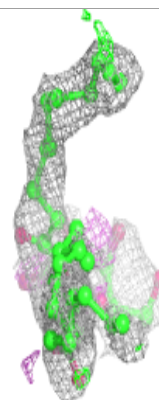
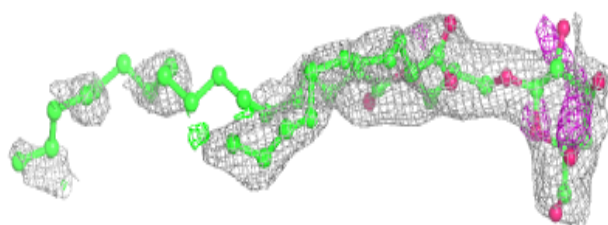
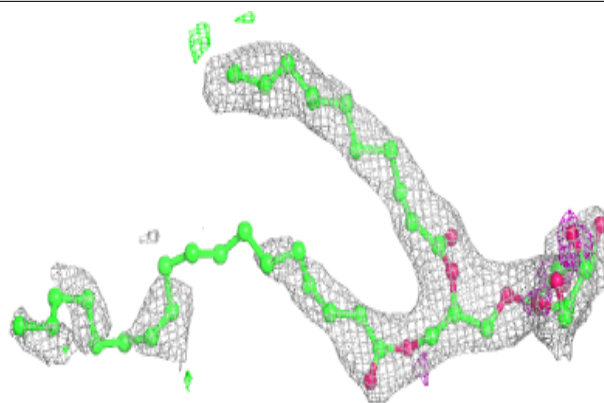
**Electron density around PL9 a 611:**

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

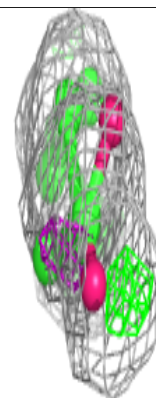
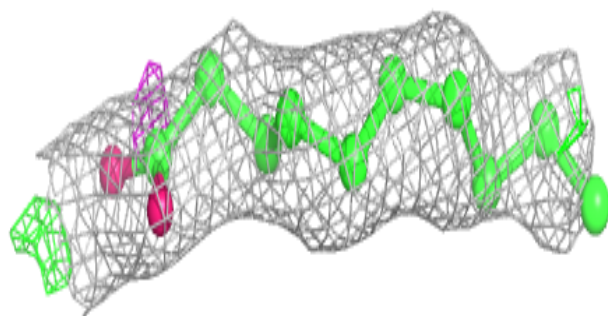
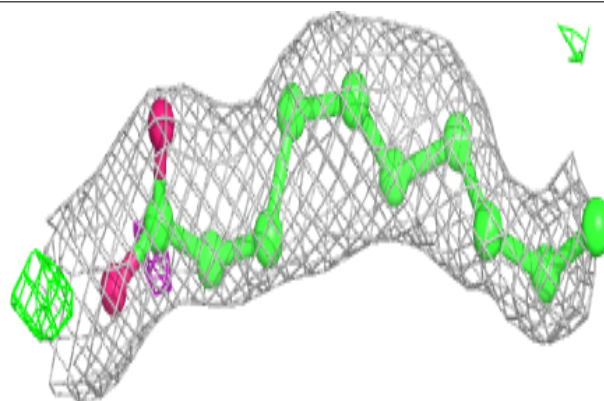


Electron density around LMG c 521:

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

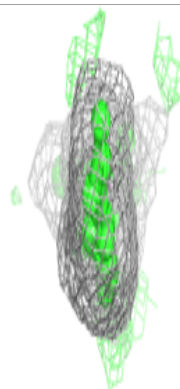
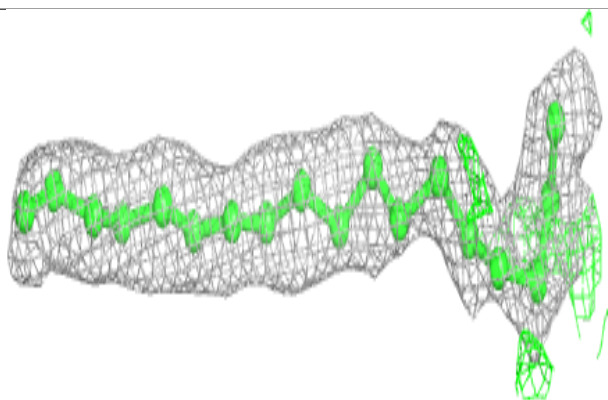
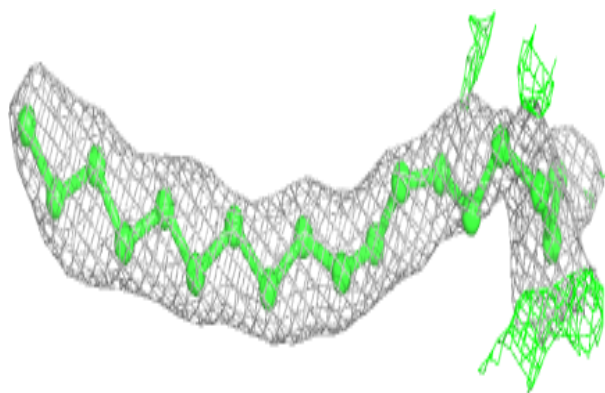
**Electron density around STE L 103:**

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

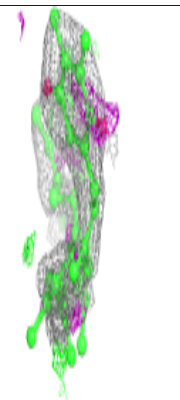
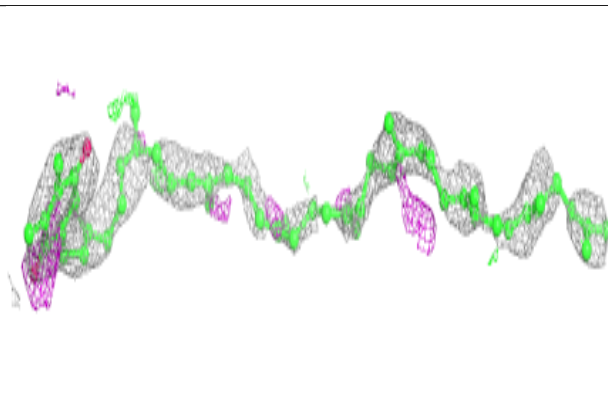
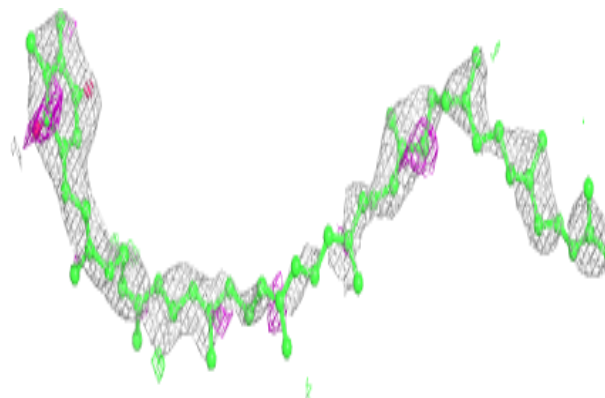


Electron density around STE 1 102:

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

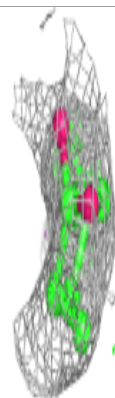
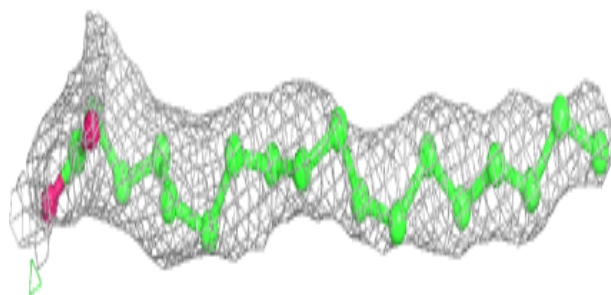
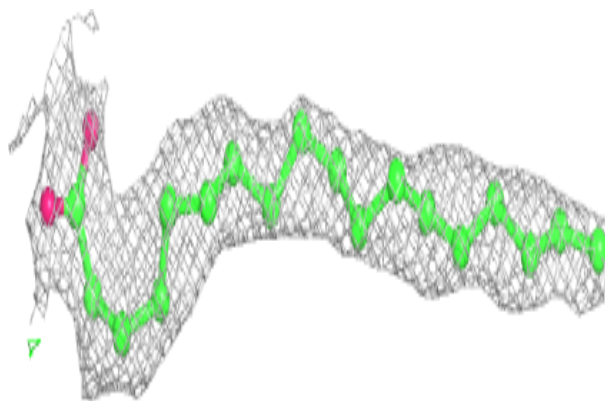
**Electron density around PL9 A 611:**

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

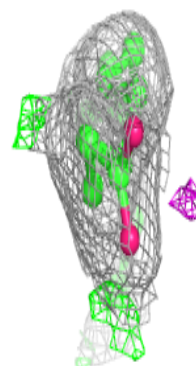
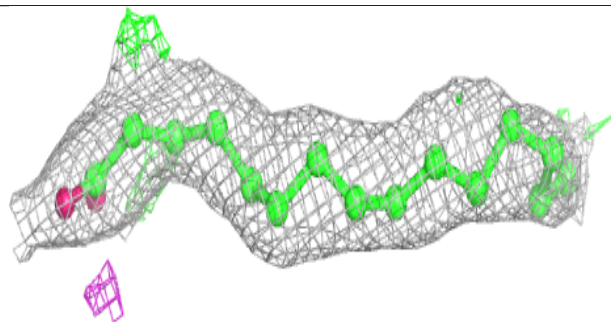
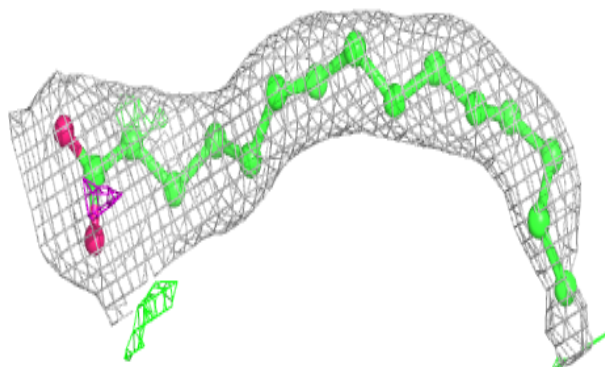


Electron density around STE c 520:

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

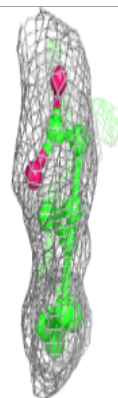
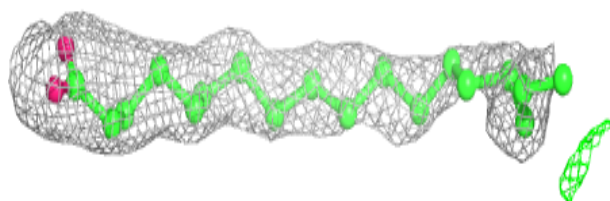
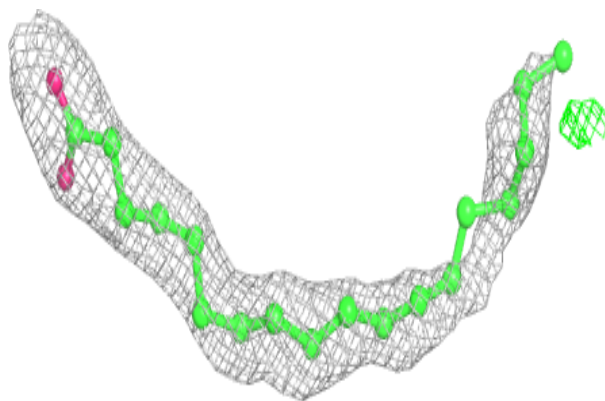
**Electron density around STE B 620:**

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

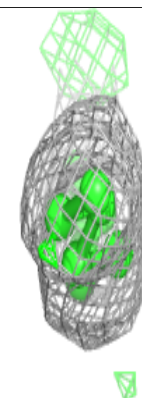
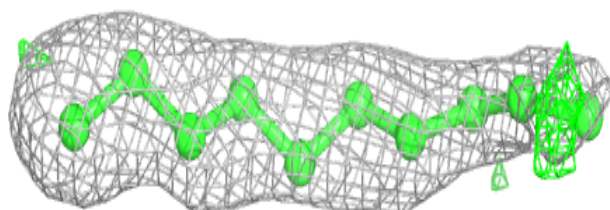
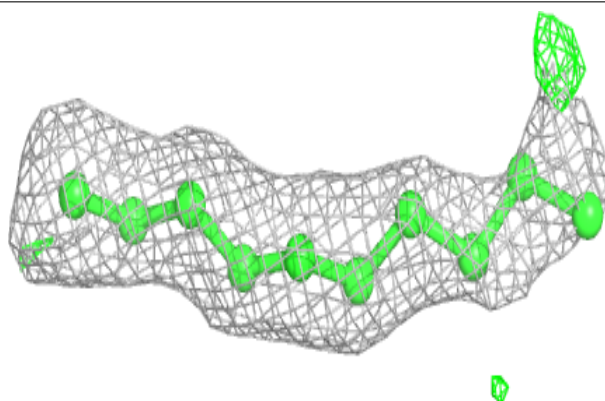


Electron density around STE d 413:

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

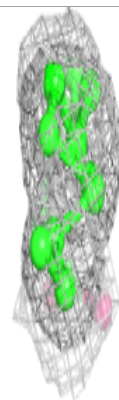
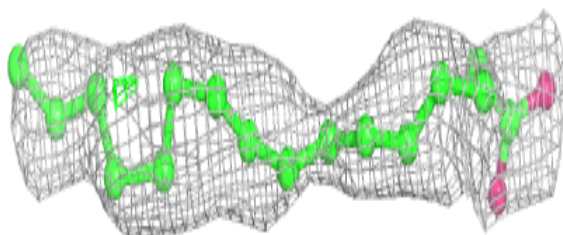
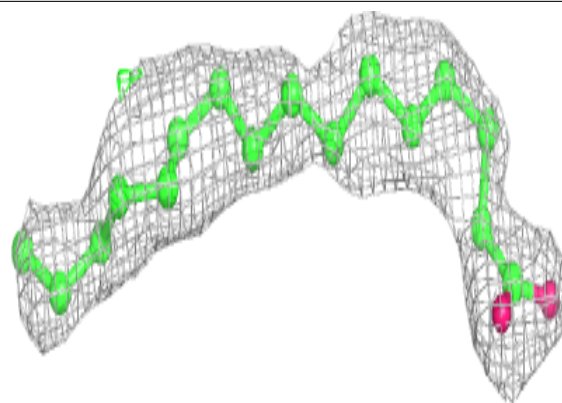
**Electron density around STE M 103:**

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

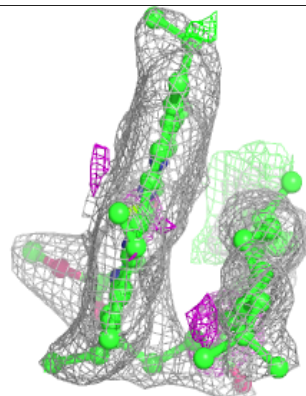
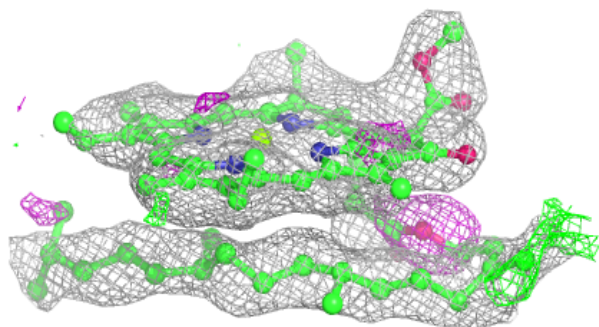
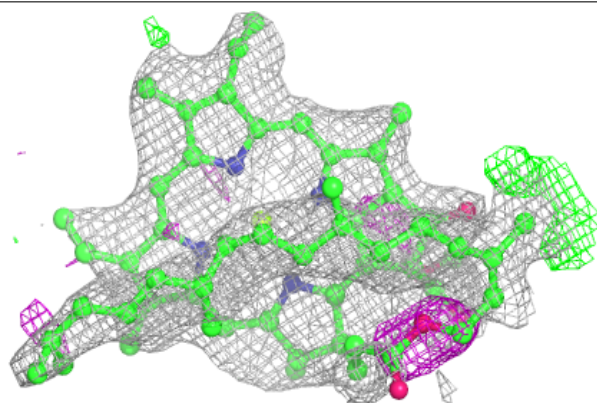


Electron density around STE t 104:

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

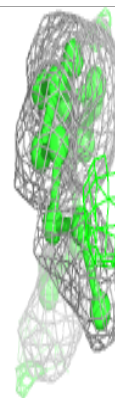
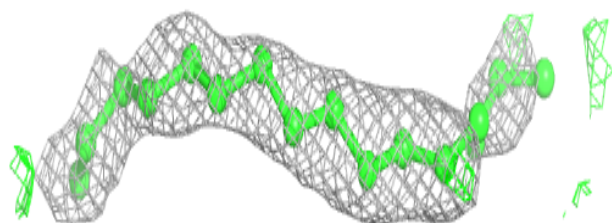
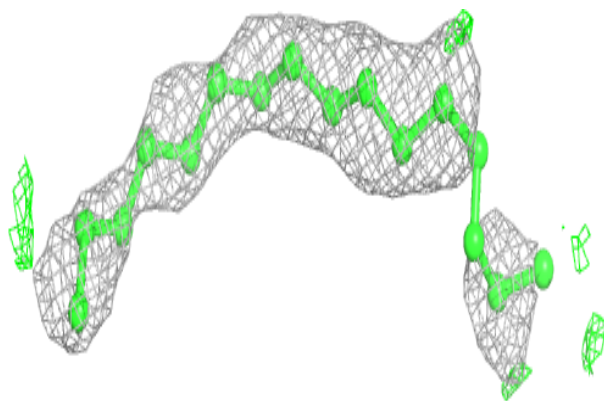
**Electron density around CLA b 601:**

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

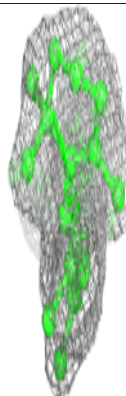
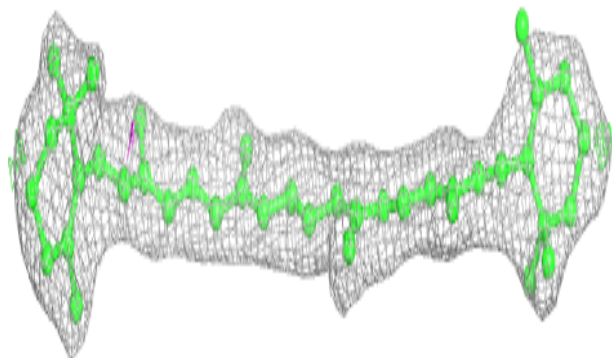
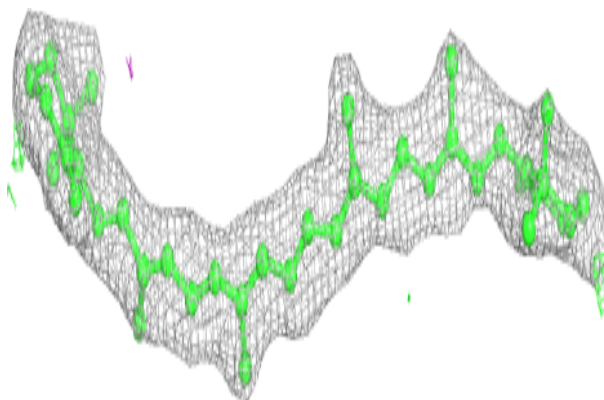


Electron density around STE b 620:

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

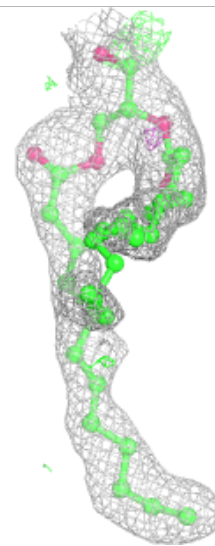
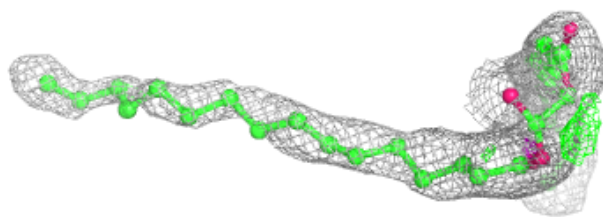
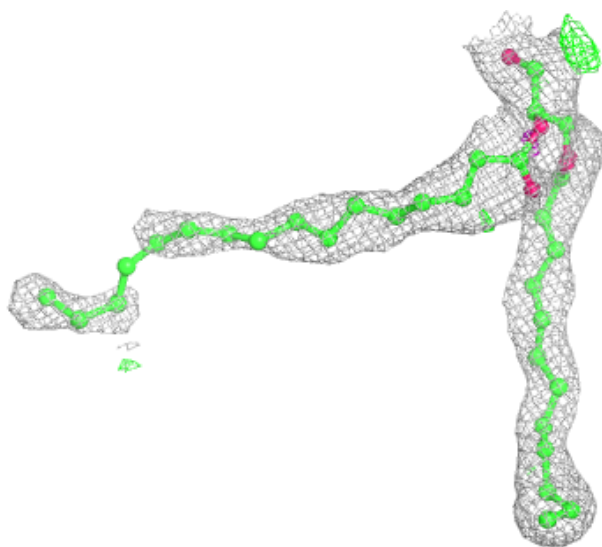
**Electron density around BCR H 101:**

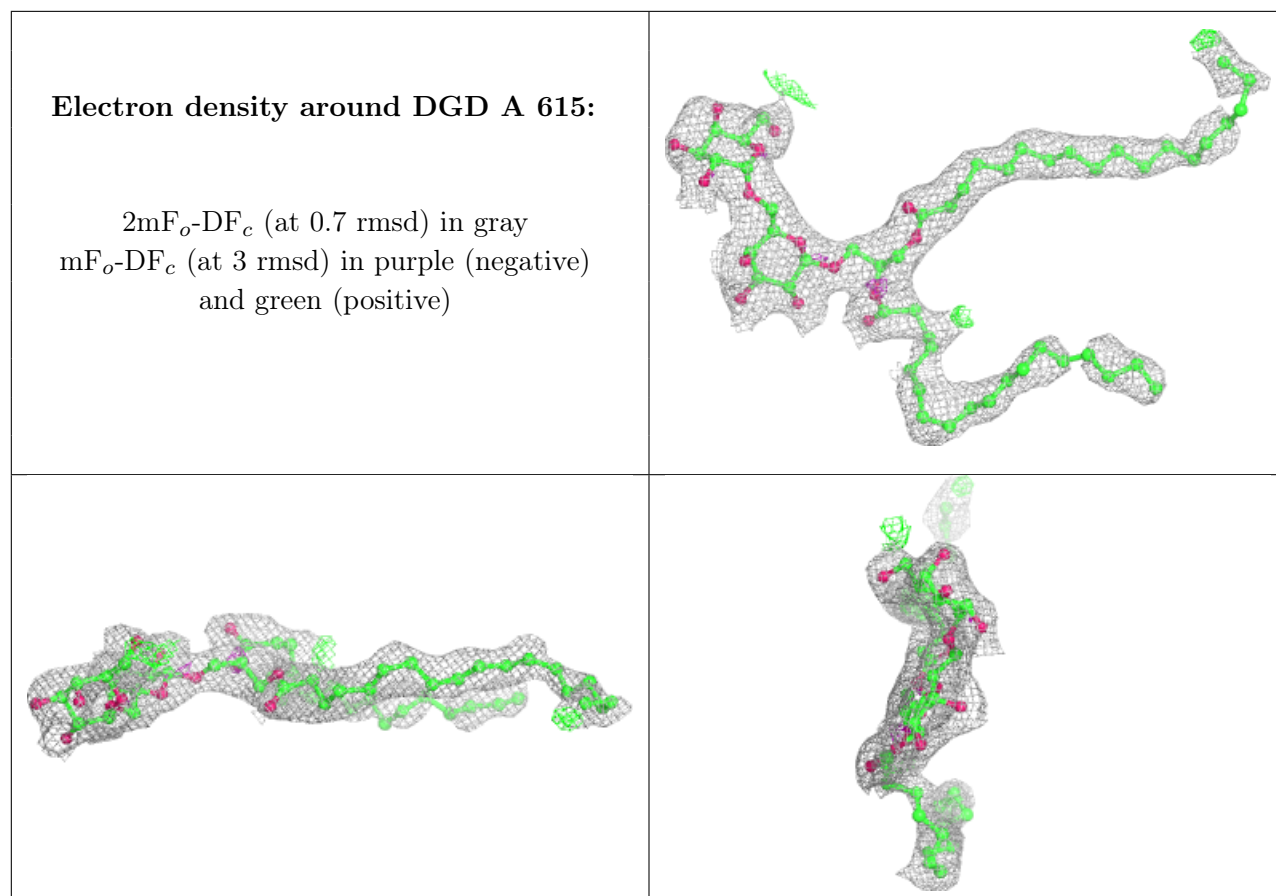
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD t 102:

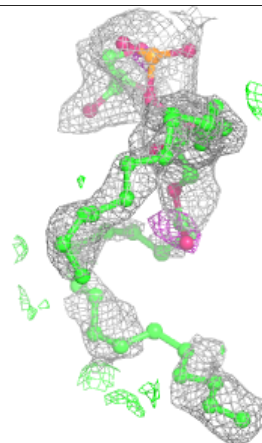
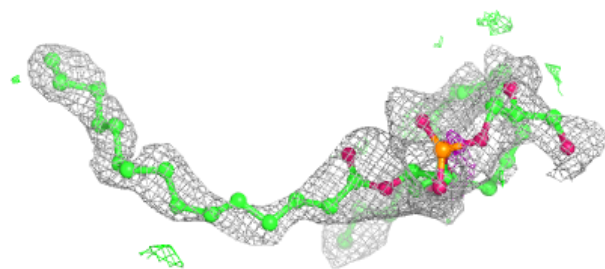
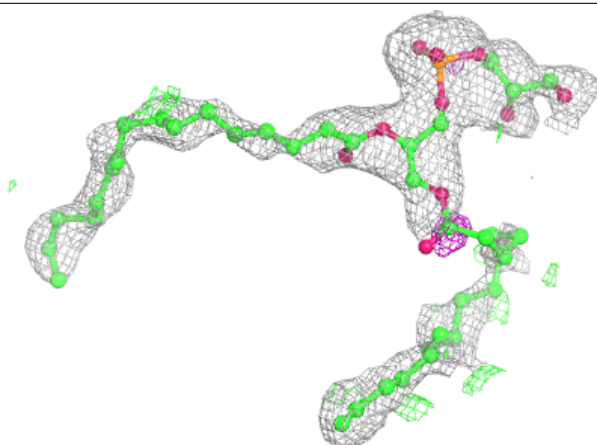
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



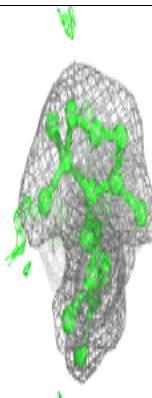
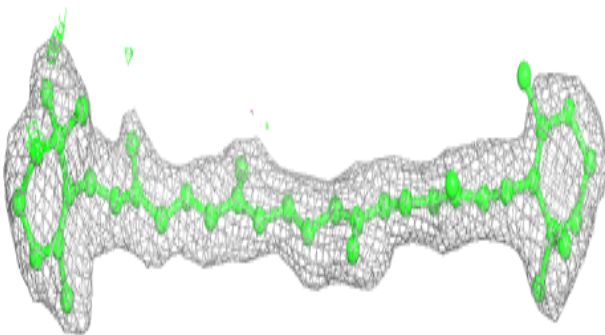
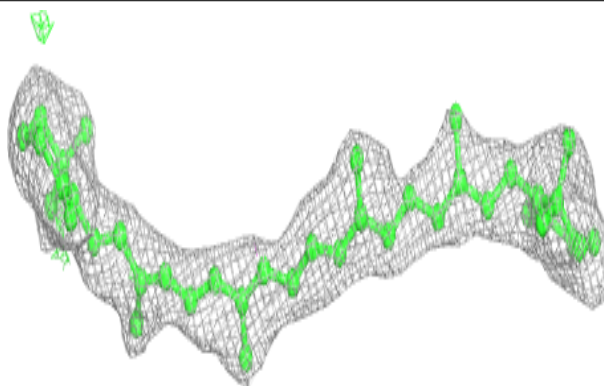


Electron density around LHG E 101:

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

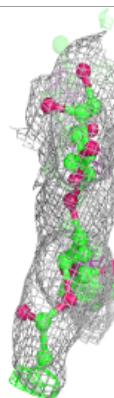
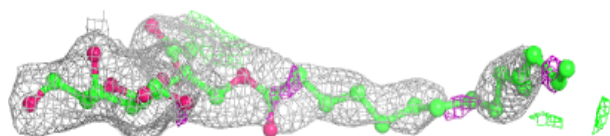
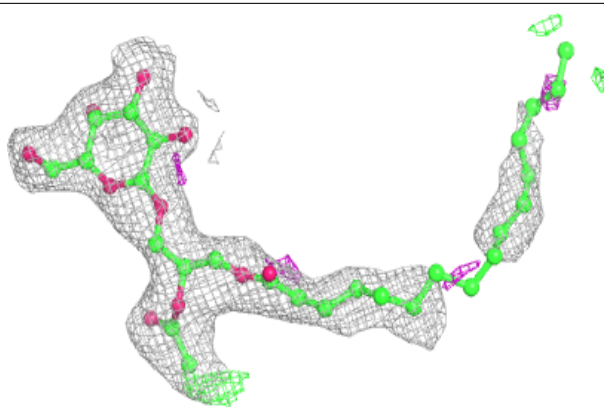
**Electron density around BCR h 101:**

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

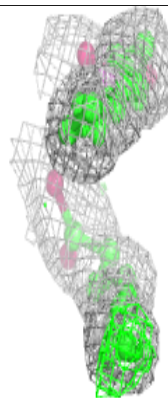
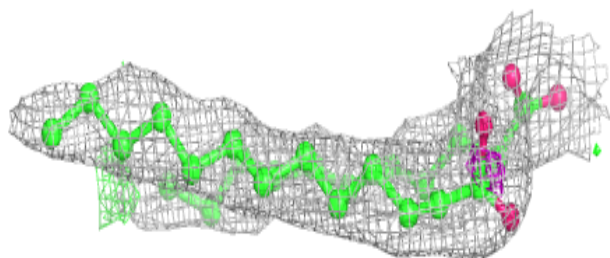
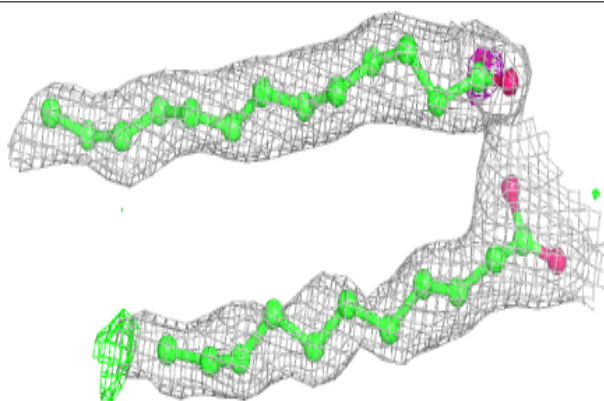


Electron density around LMG c 519:

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

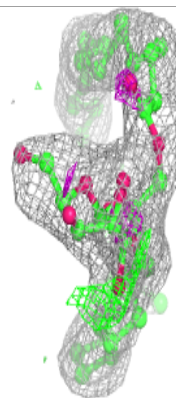
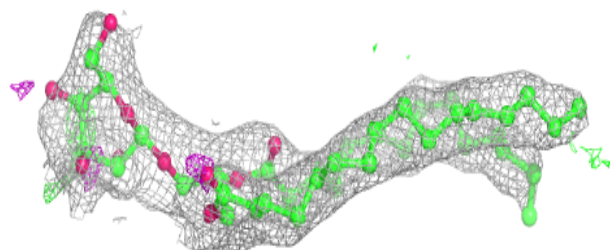
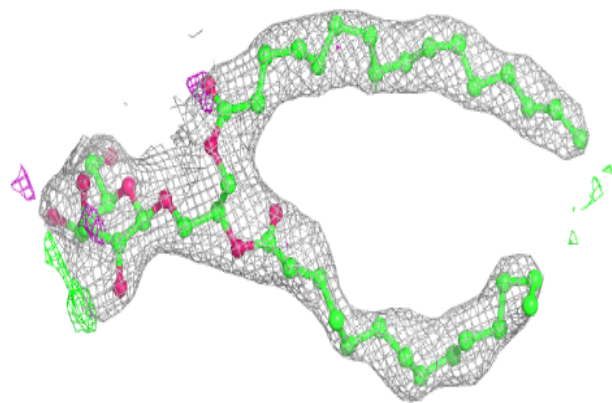
**Electron density around LMG B 621:**

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



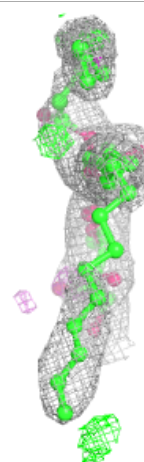
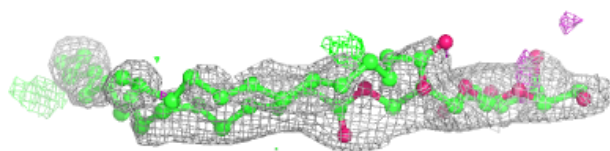
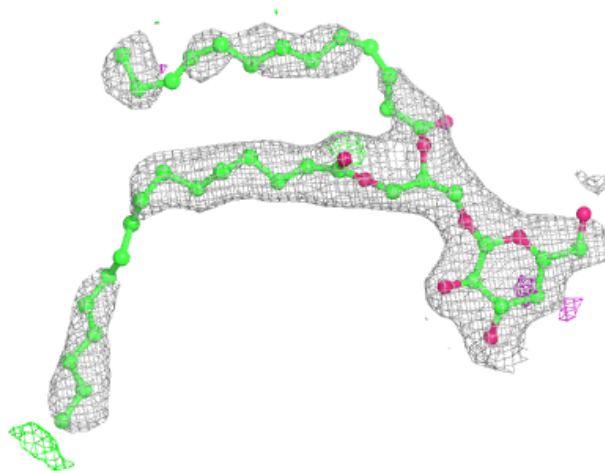
Electron density around LMG c 523:

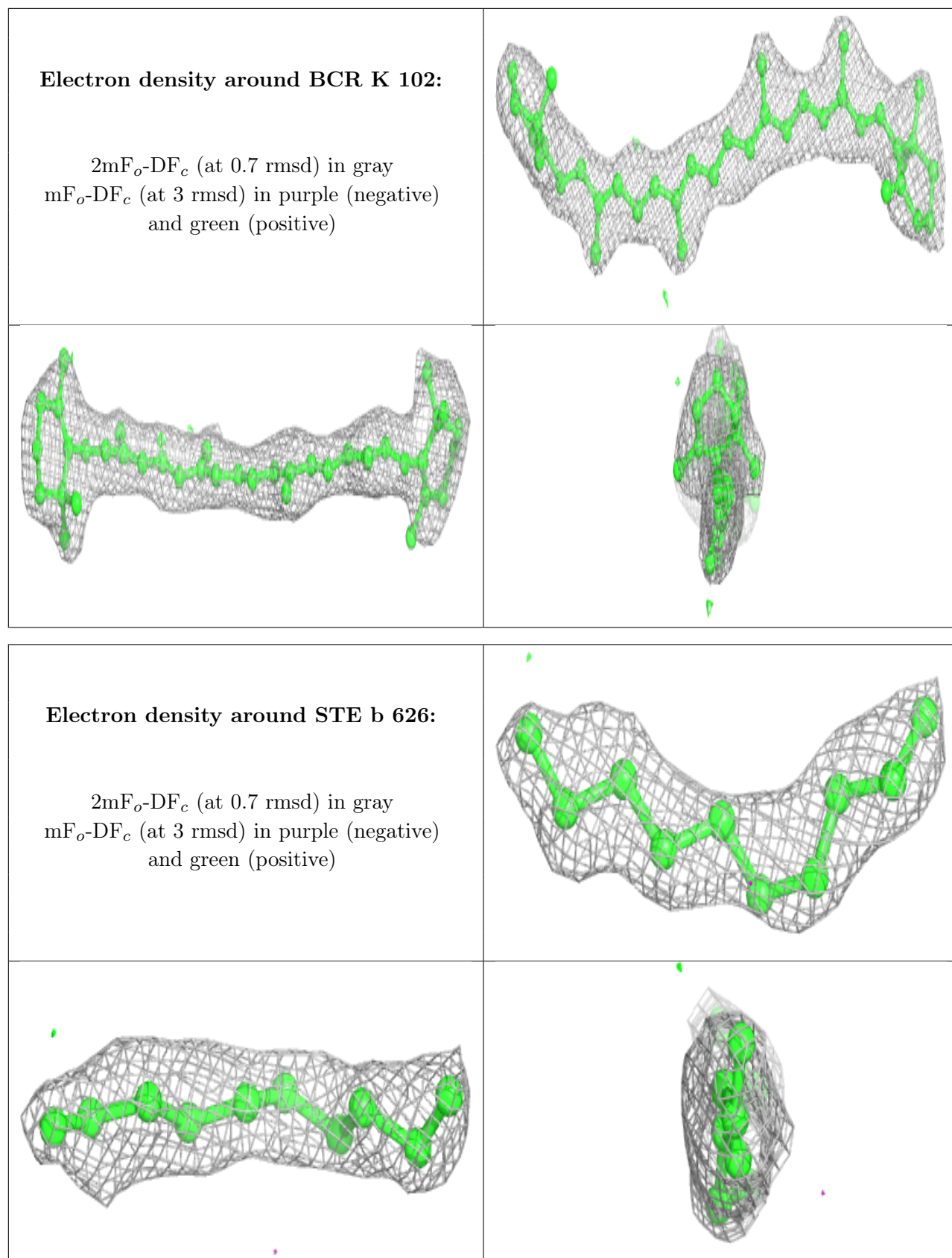
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMG C 519:

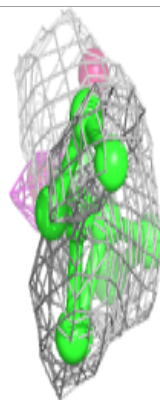
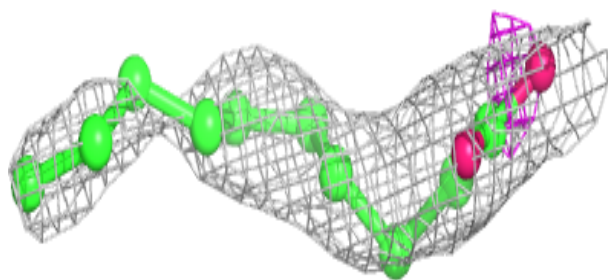
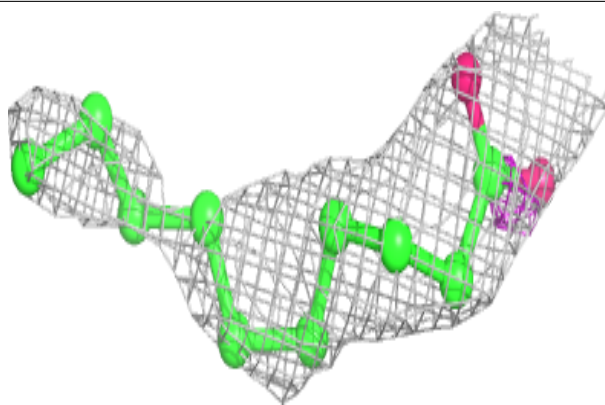
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



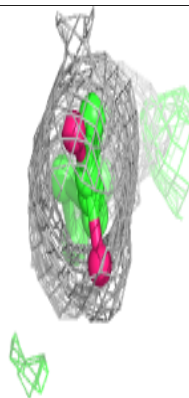
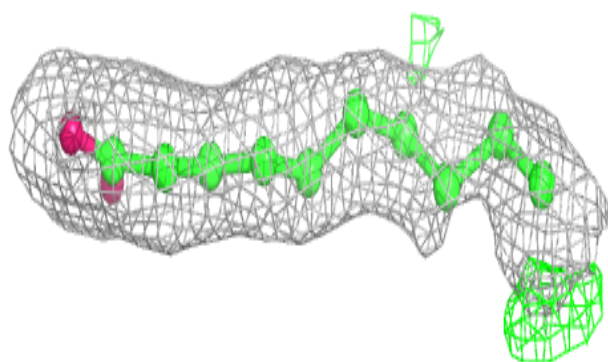
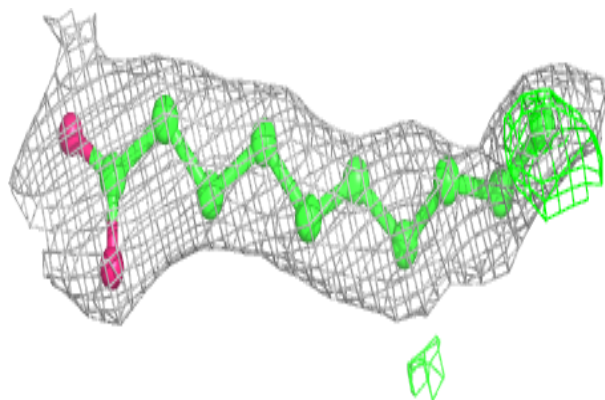


Electron density around STE B 624:

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

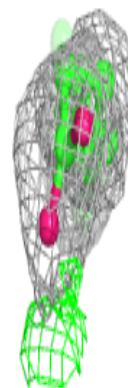
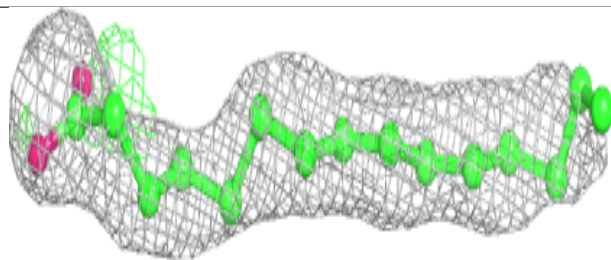
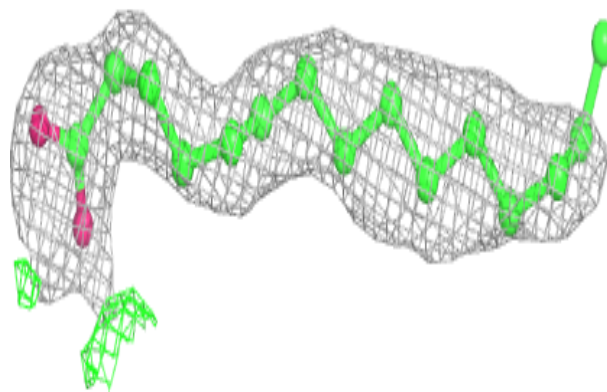
**Electron density around STE J 101:**

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

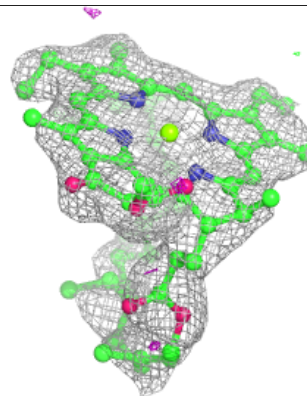
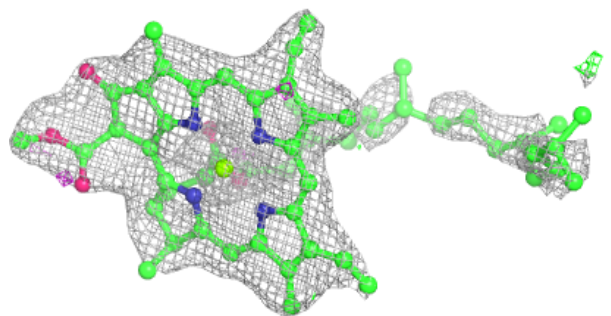
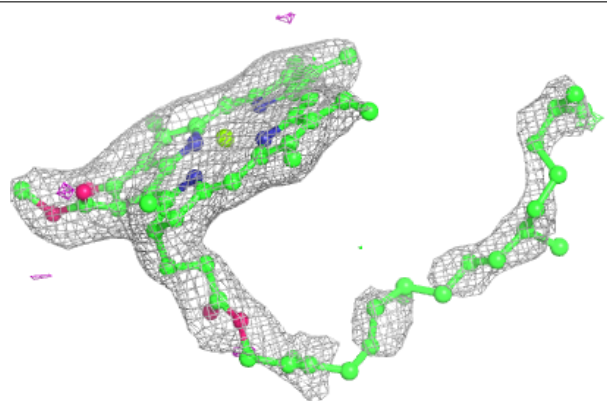


Electron density around STE d 412:

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

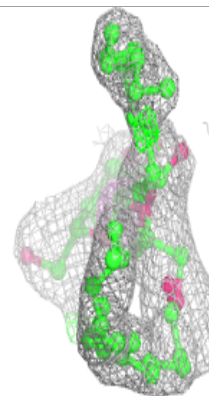
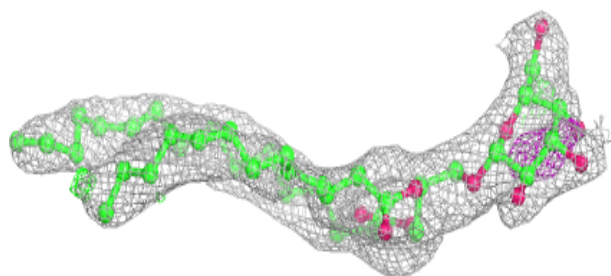
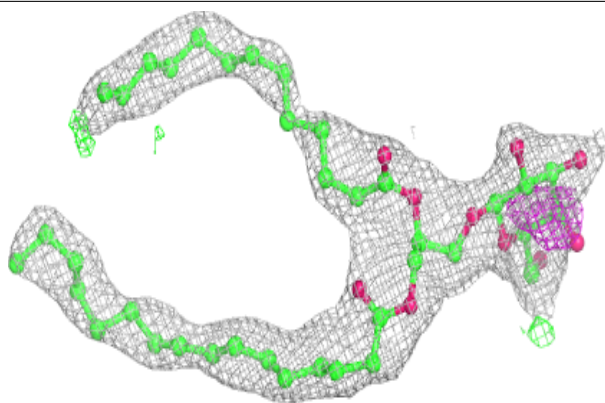
**Electron density around CLA c 513:**

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

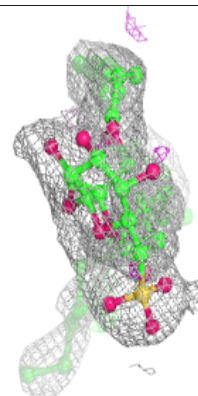
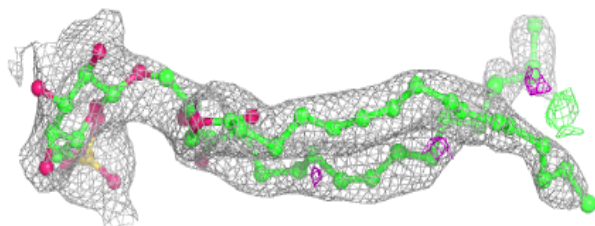
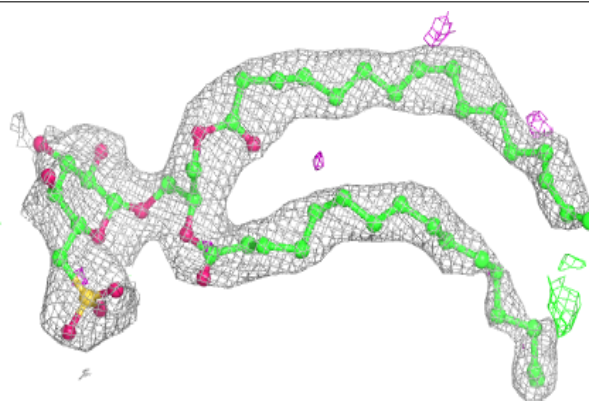


Electron density around LMG A 612:

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

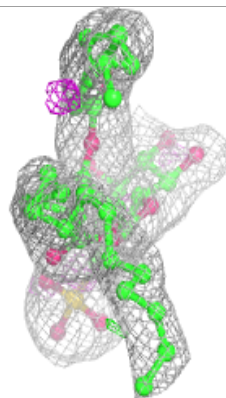
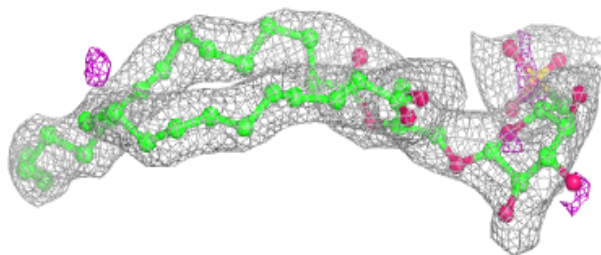
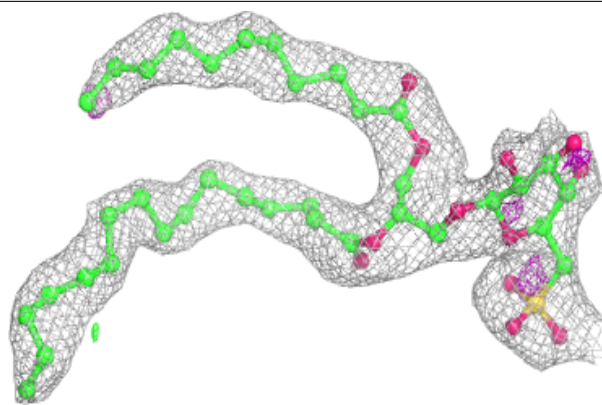
**Electron density around SQD B 622:**

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

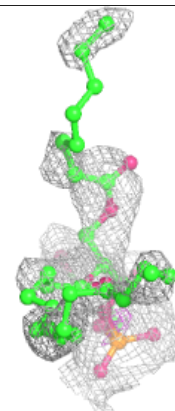
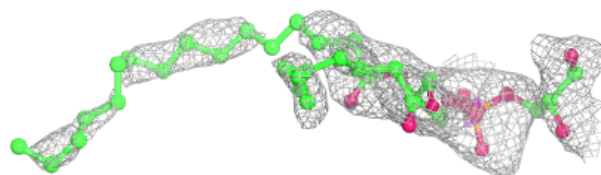
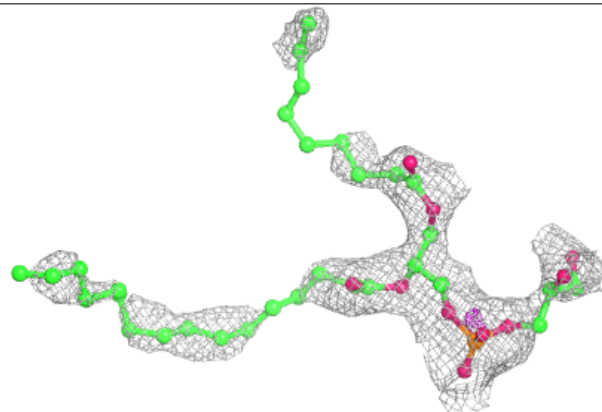


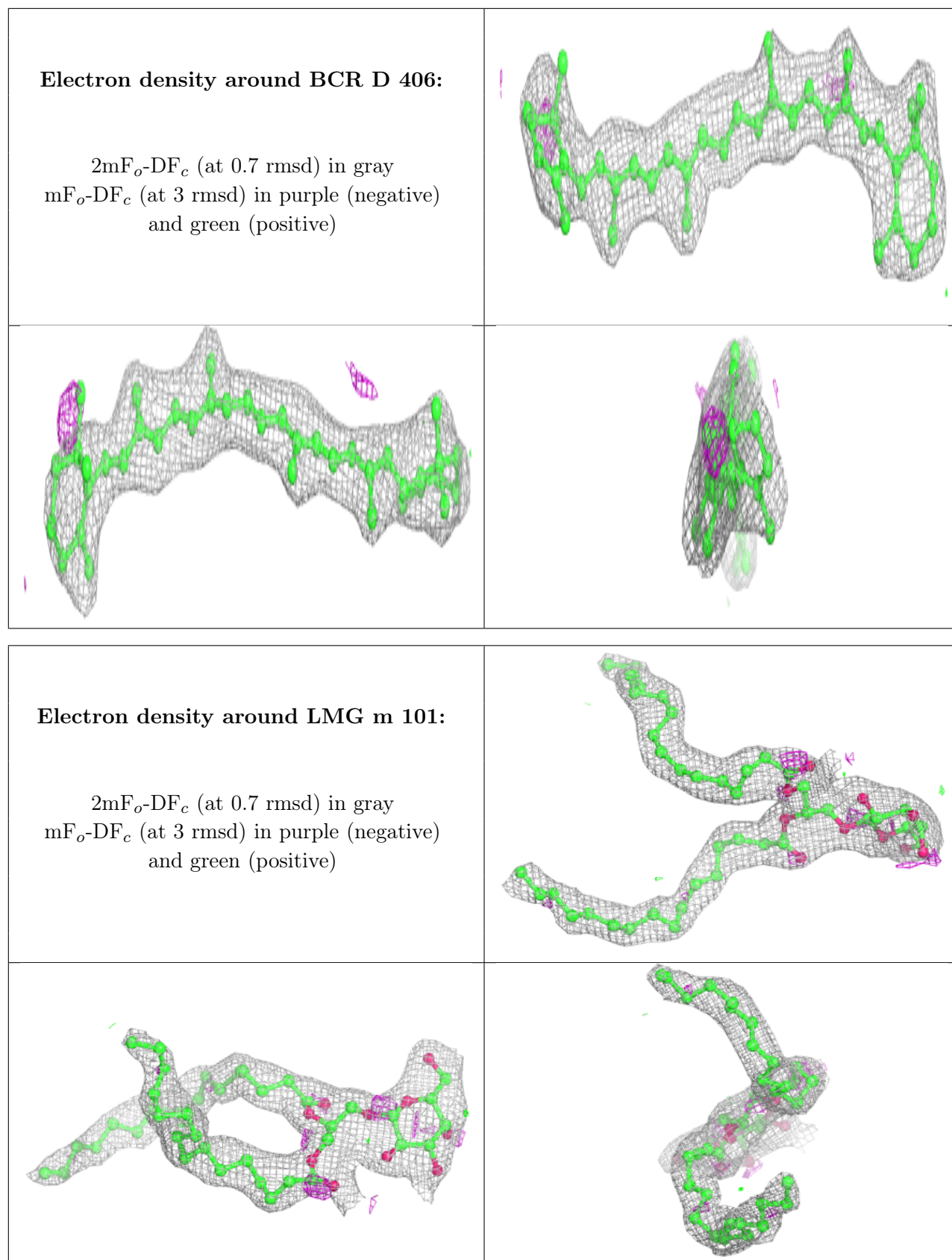
Electron density around SQD L 101:

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

**Electron density around LHG e 102:**

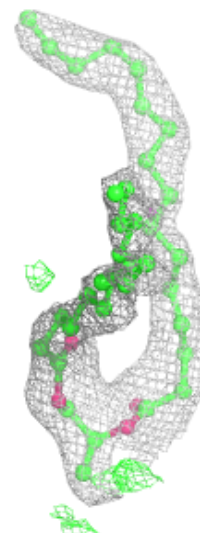
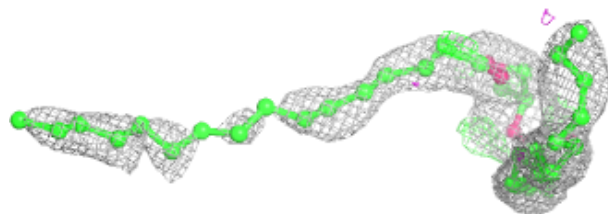
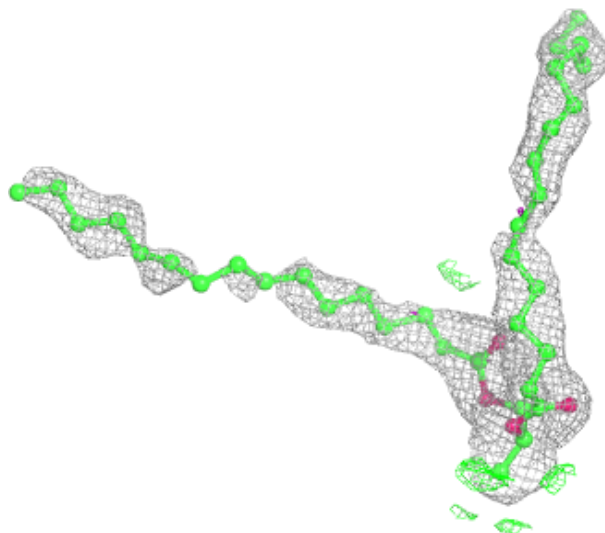
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





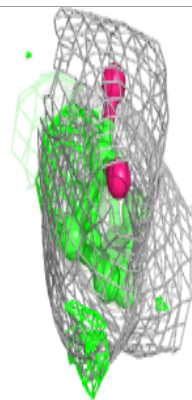
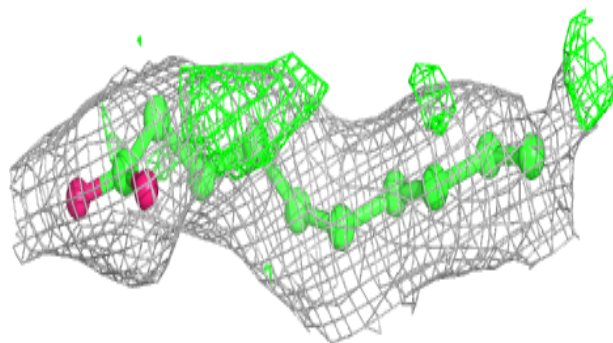
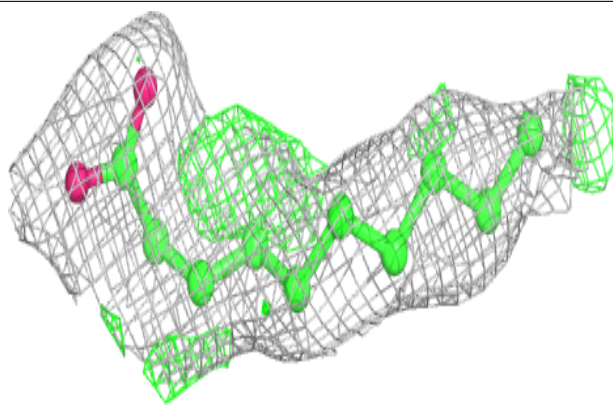
Electron density around SQD A 614:

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



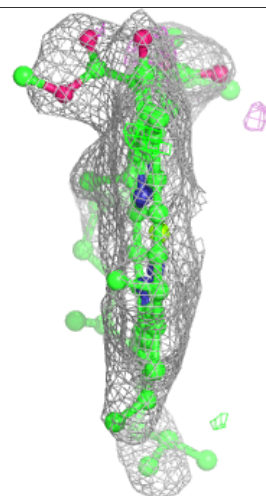
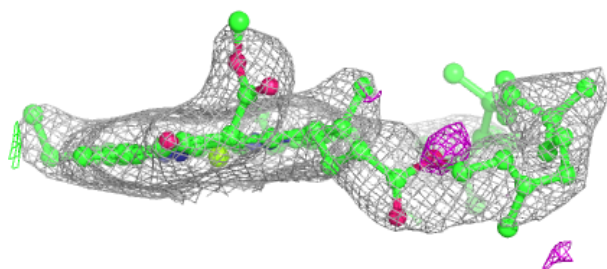
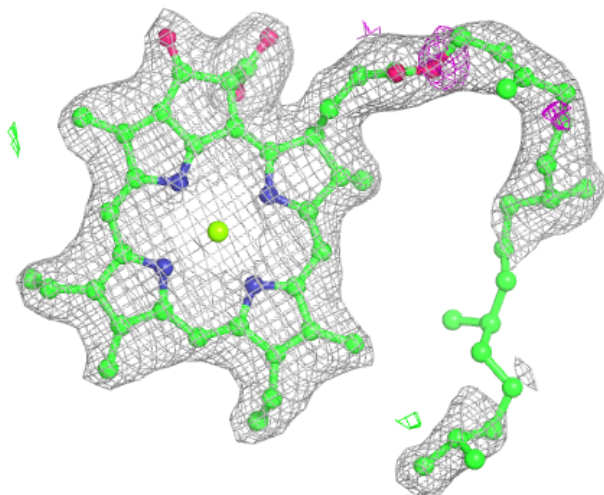
Electron density around STE B 623:

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



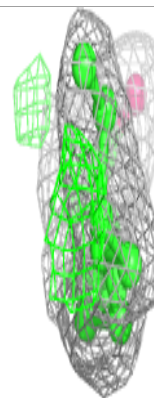
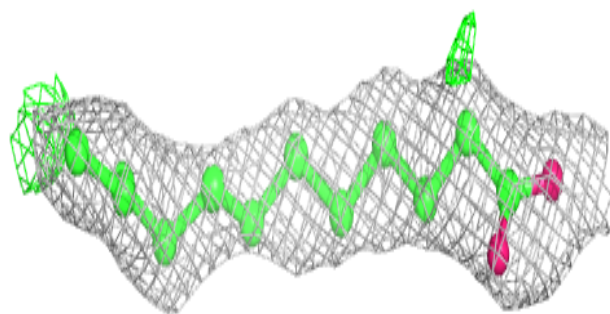
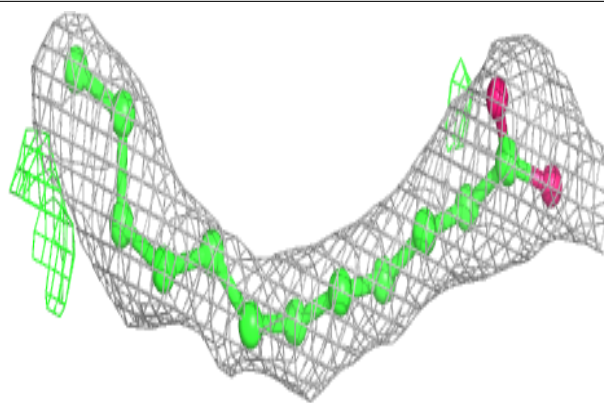
Electron density around CLA c 512:

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

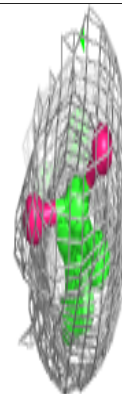
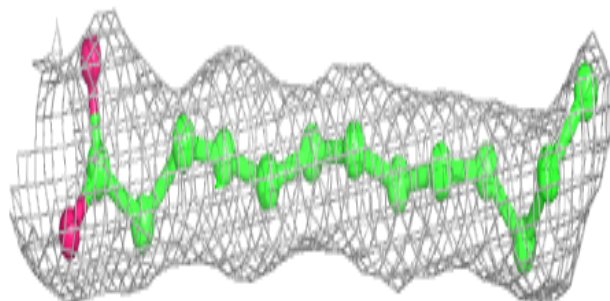
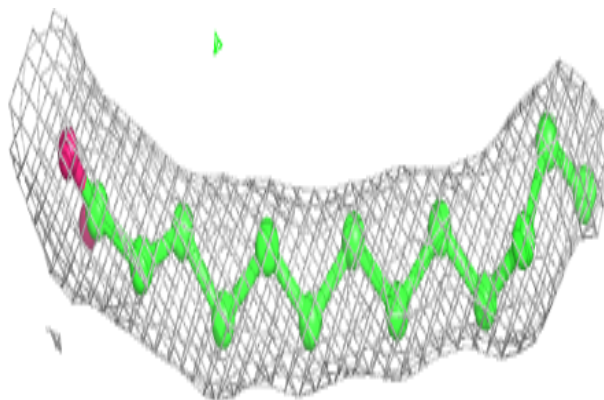


Electron density around STE t 103:

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

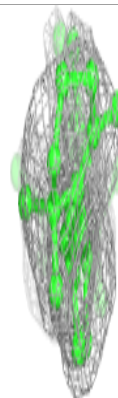
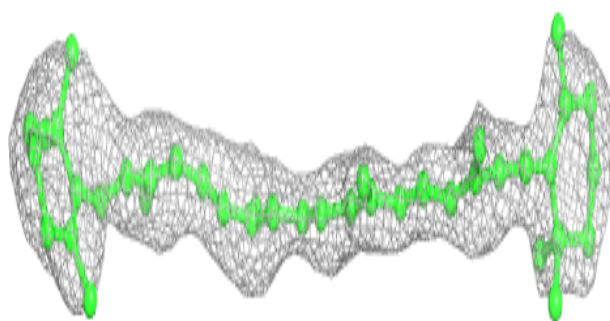
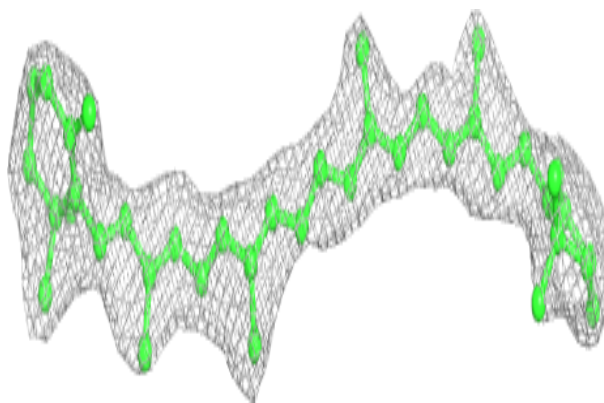
**Electron density around STE M 102:**

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

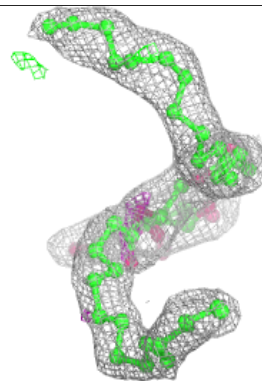
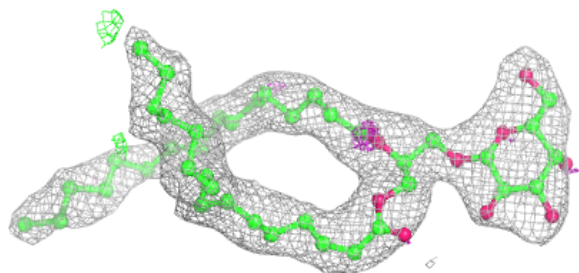
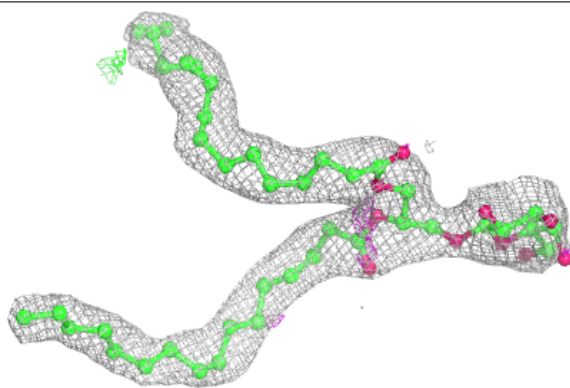


Electron density around BCR k 101:

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

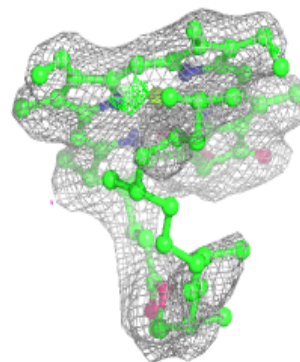
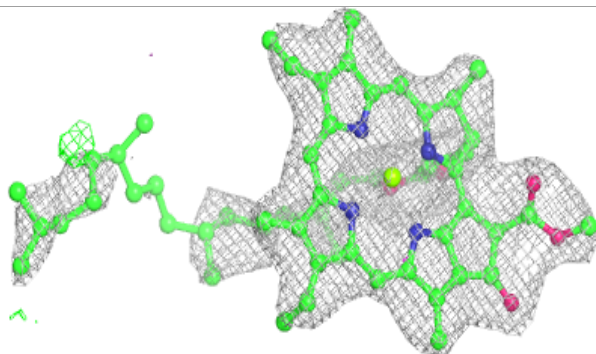
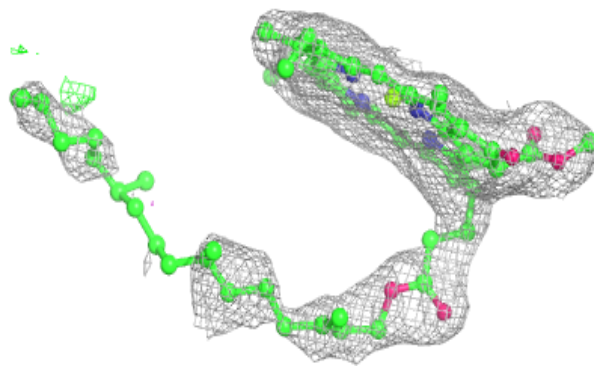
**Electron density around LMG M 101:**

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

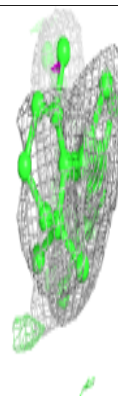
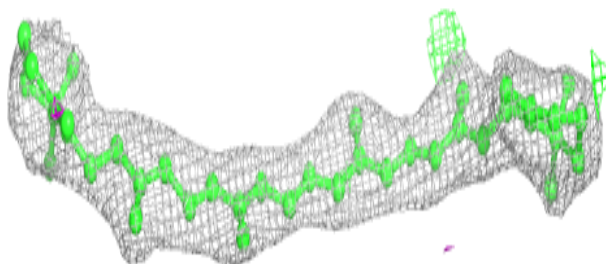
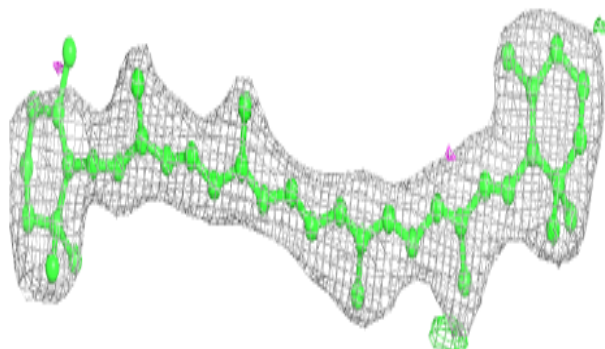


Electron density around CLA C 513:

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

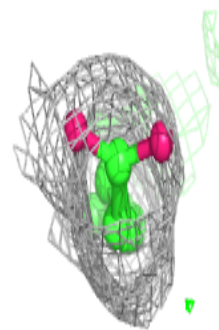
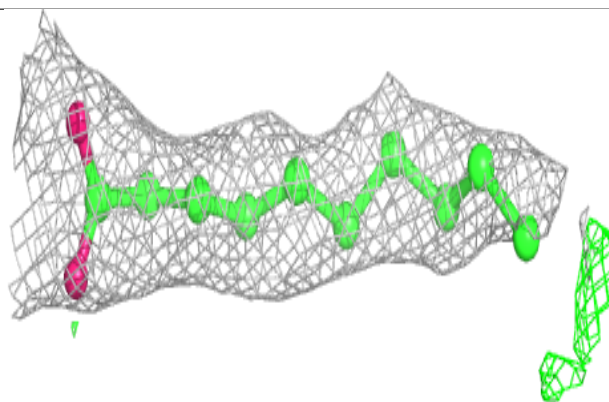
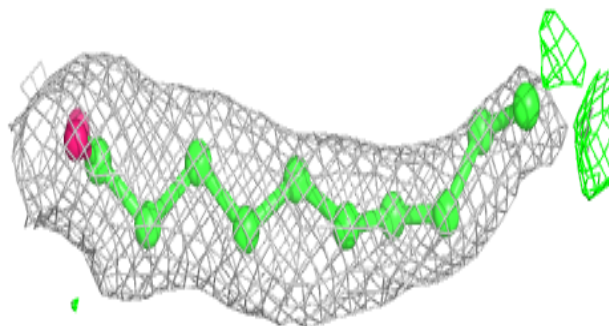
**Electron density around BCR d 405:**

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

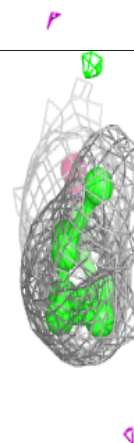
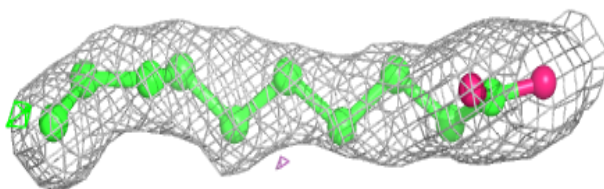
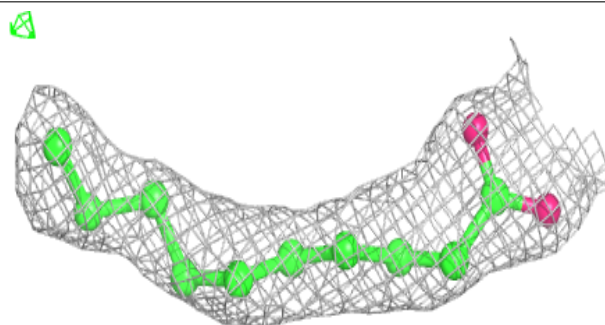


Electron density around STE j 101:

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

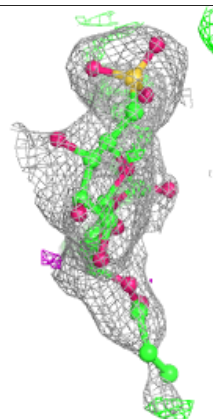
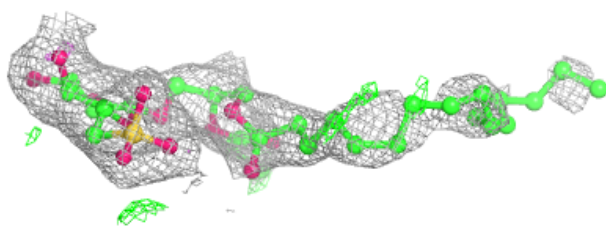
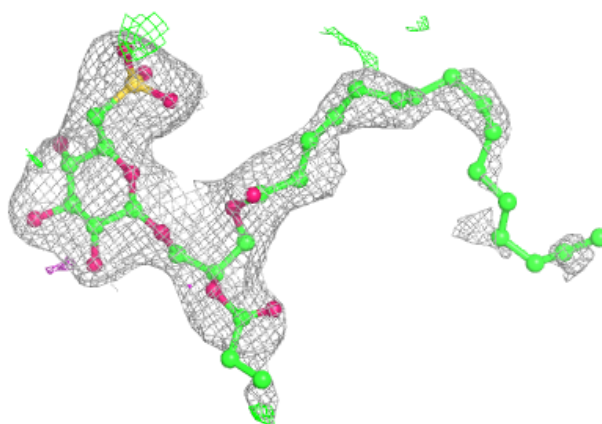
**Electron density around STE C 521:**

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



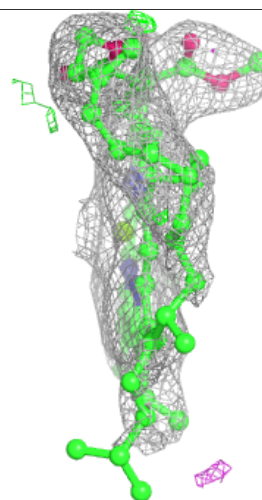
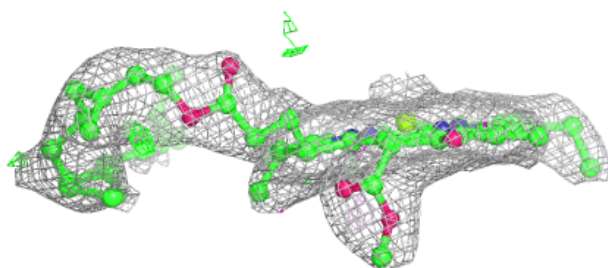
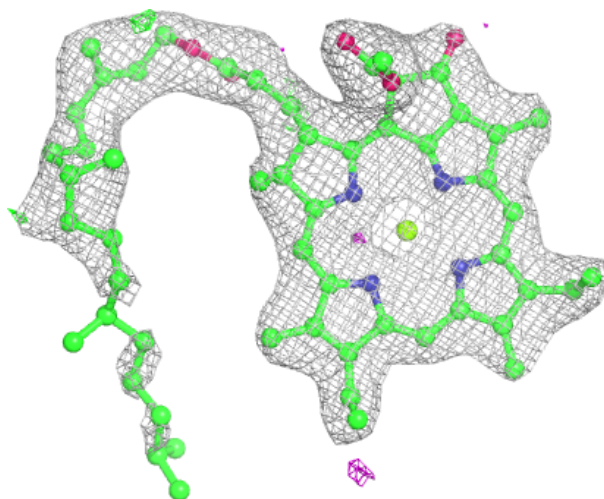
Electron density around SQD f 101:

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



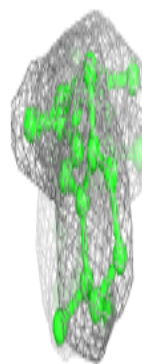
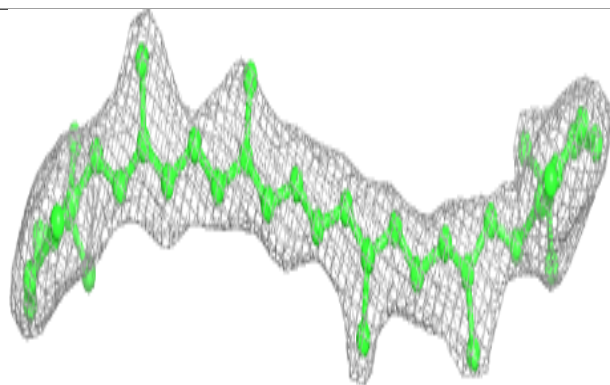
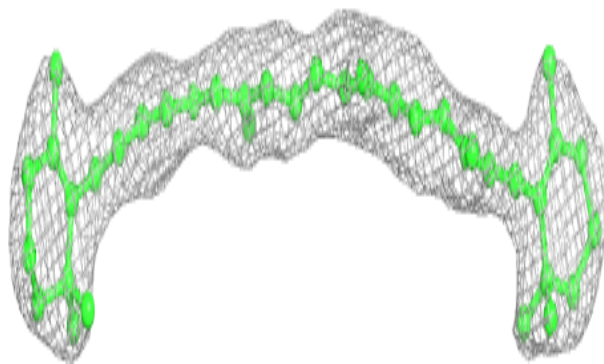
Electron density around CLA C 512:

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

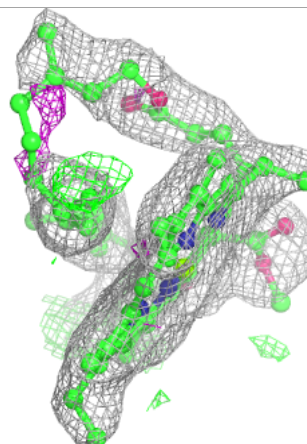
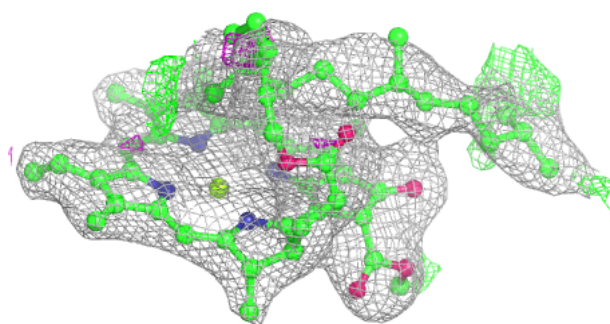
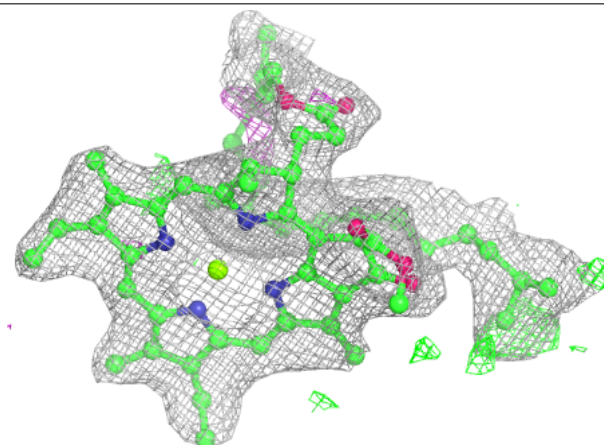


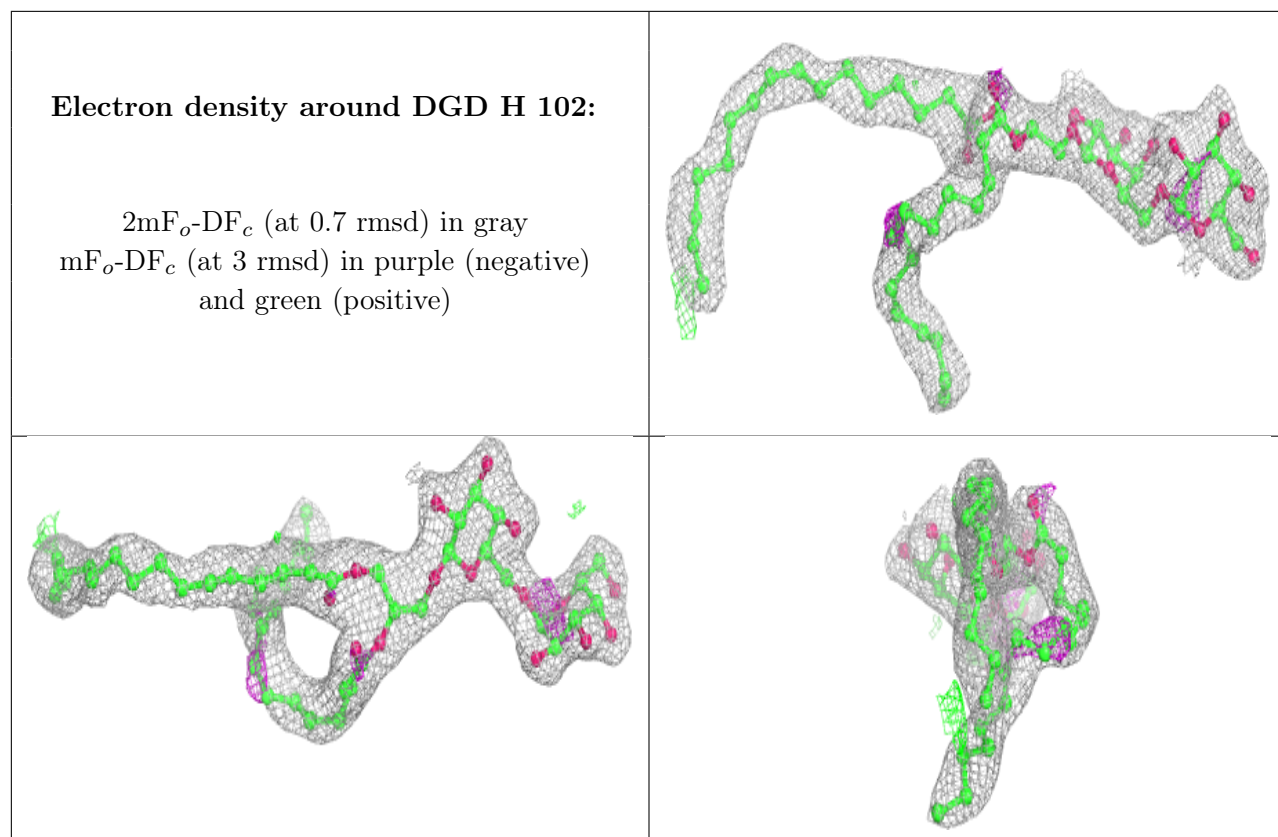
Electron density around BCR k 102:

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

**Electron density around CLA B 601:**

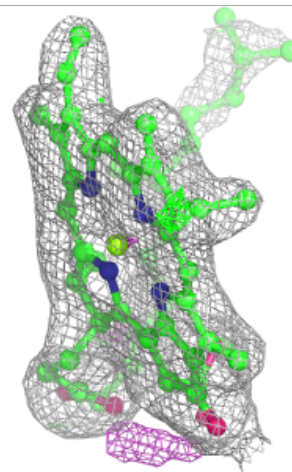
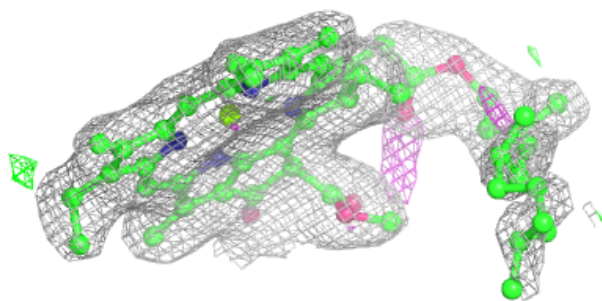
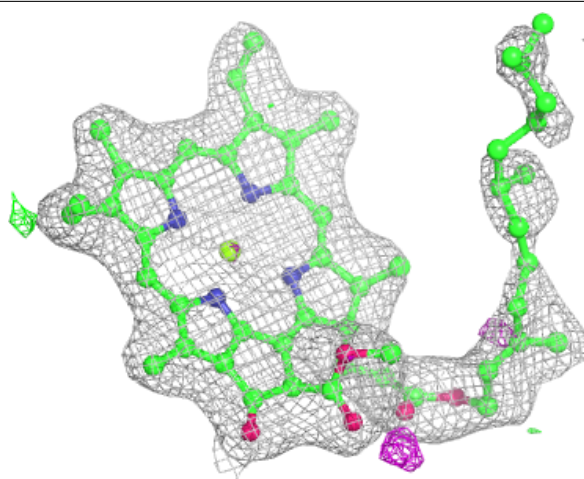
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





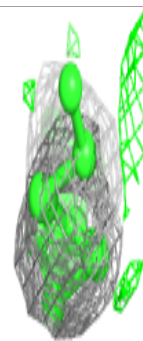
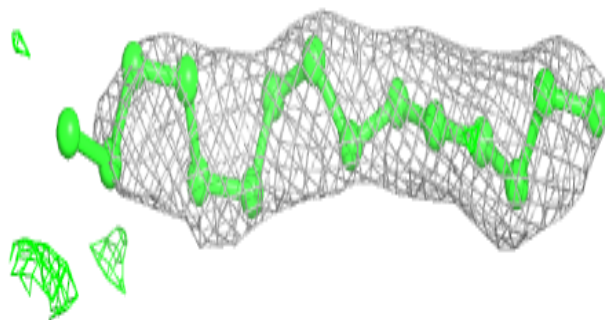
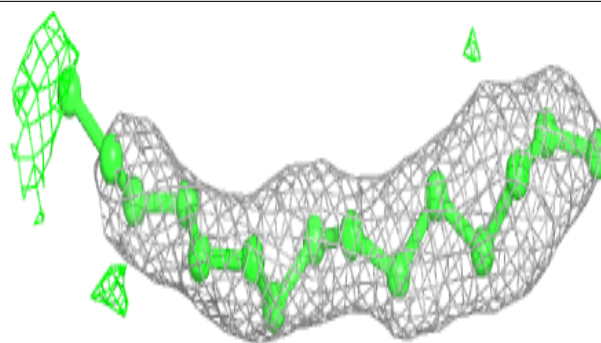
Electron density around CLA b 616:

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

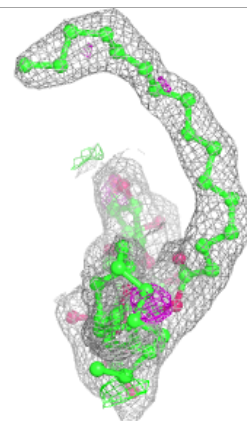
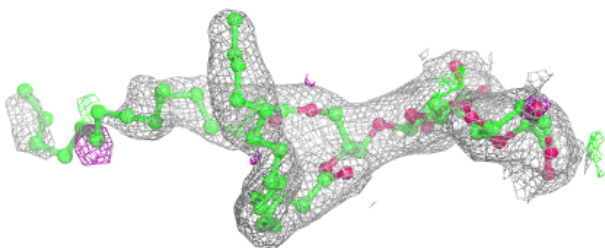
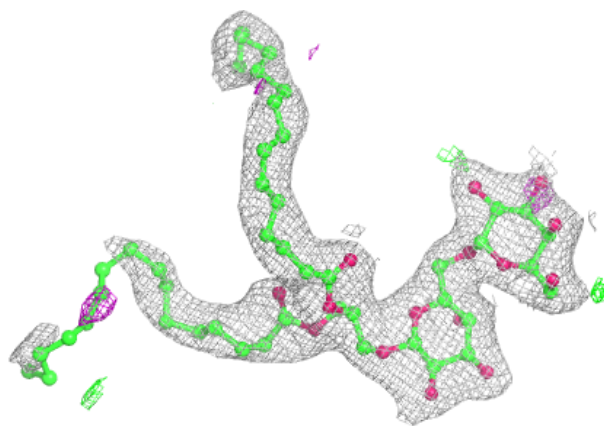


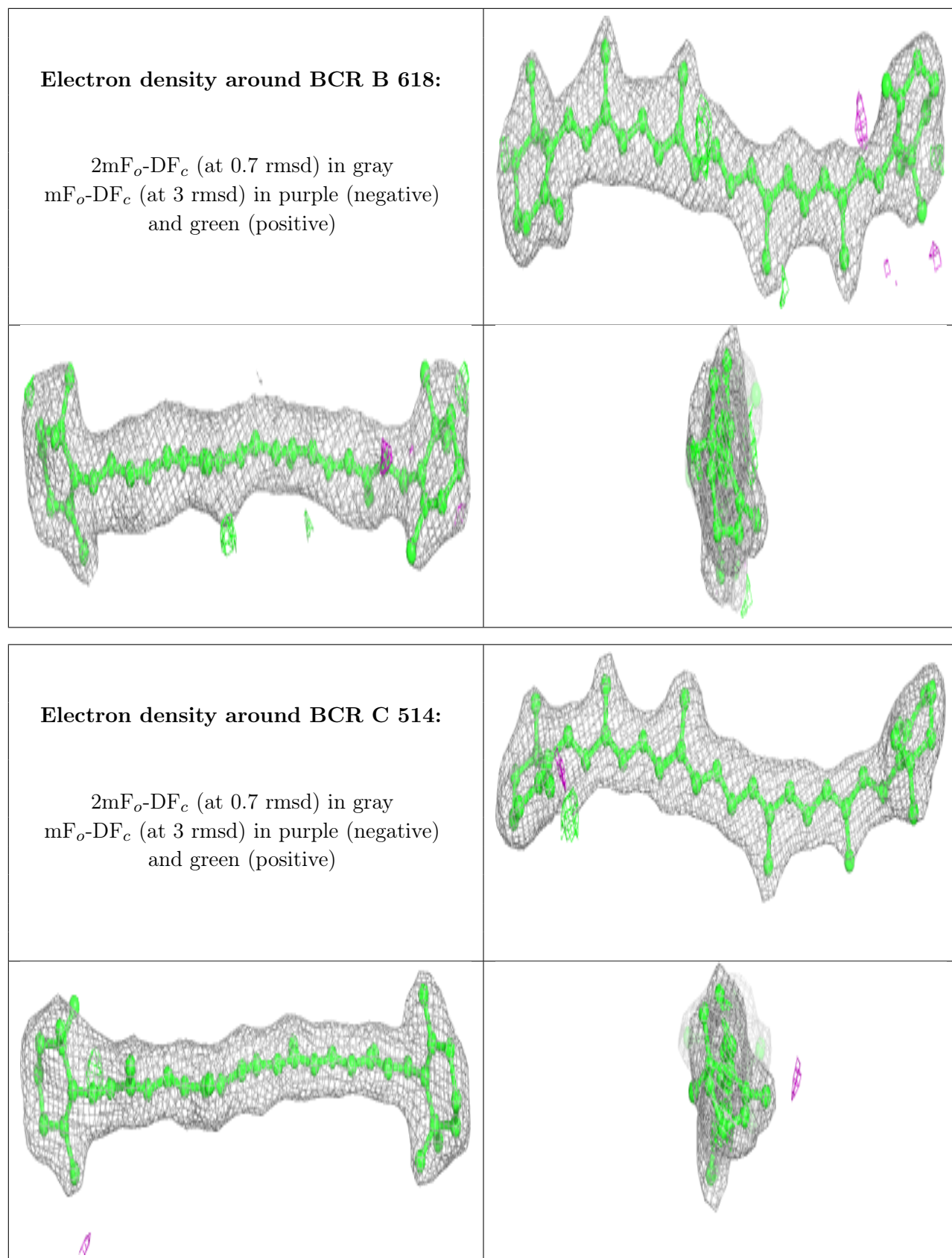
Electron density around STE b 624:

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

**Electron density around DGD C 517:**

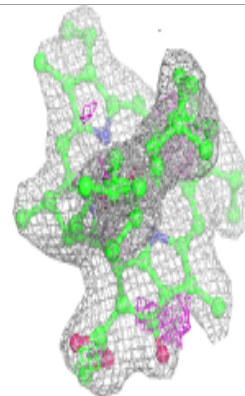
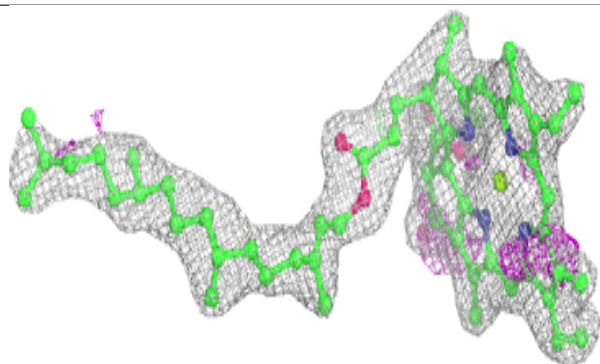
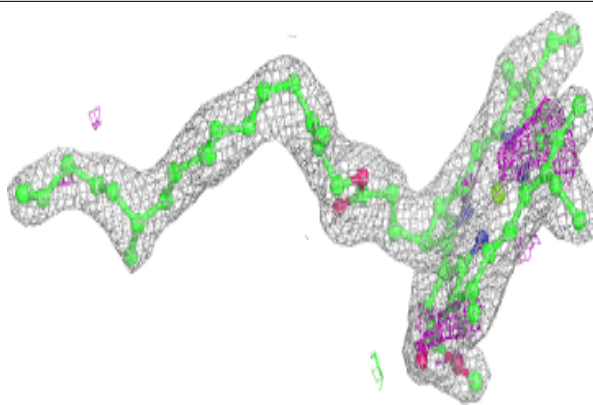
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



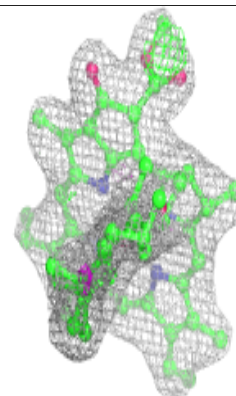
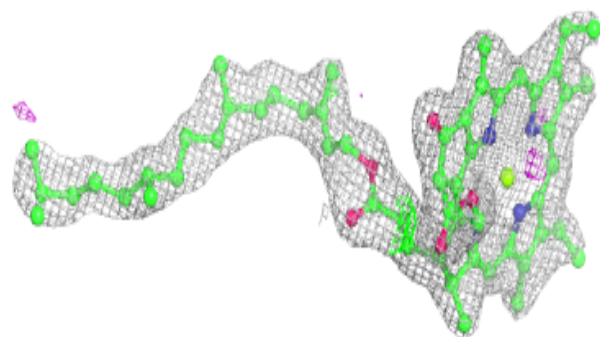
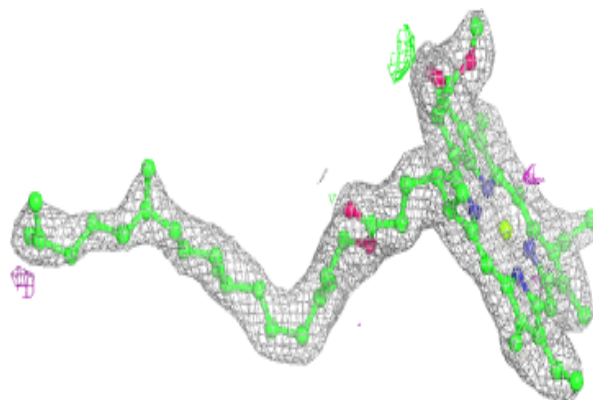


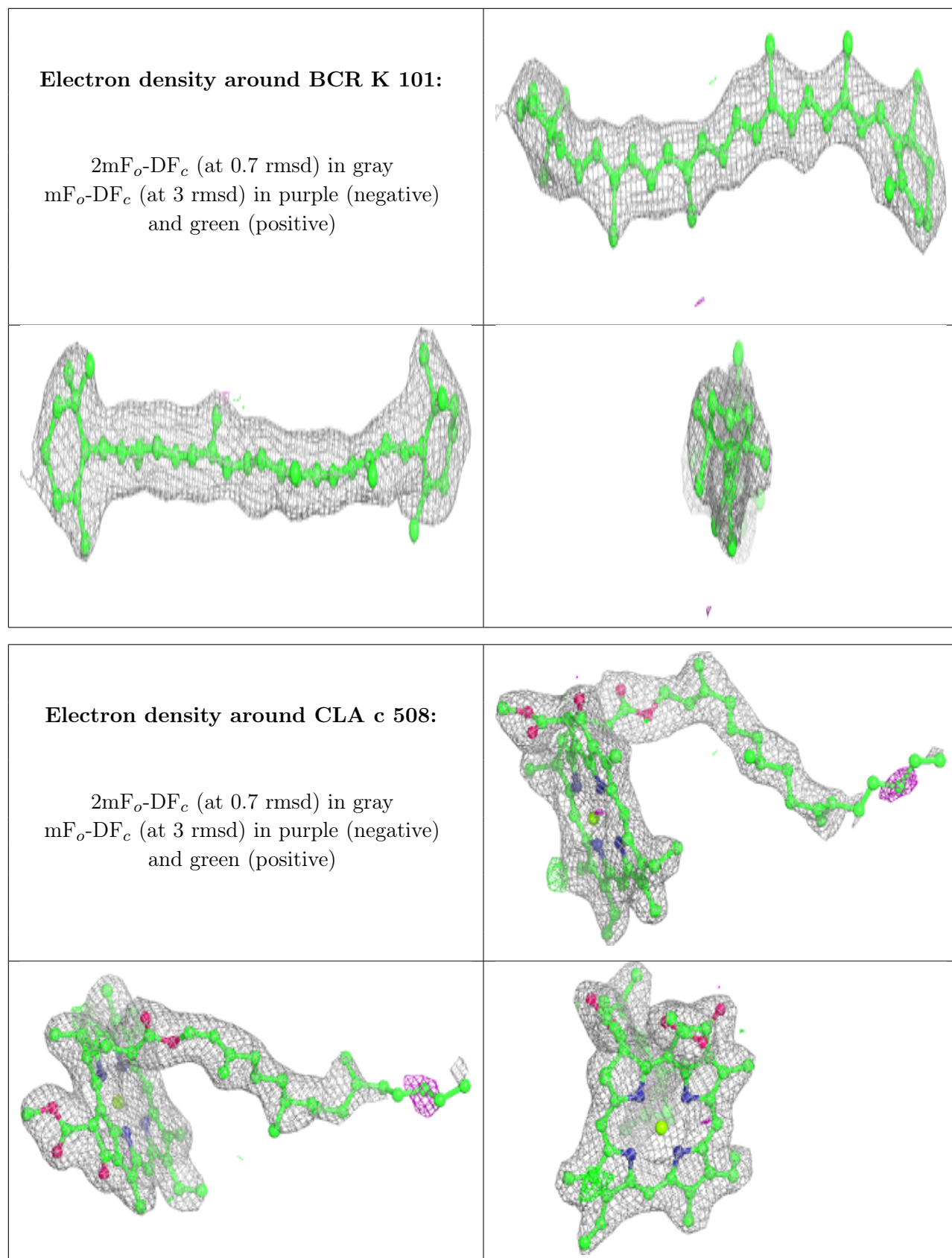
Electron density around CLA C 502:

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

**Electron density around CLA c 502:**

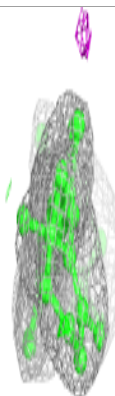
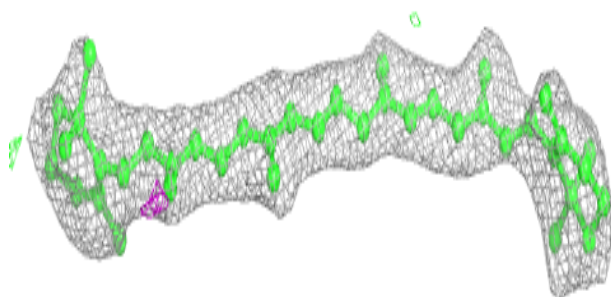
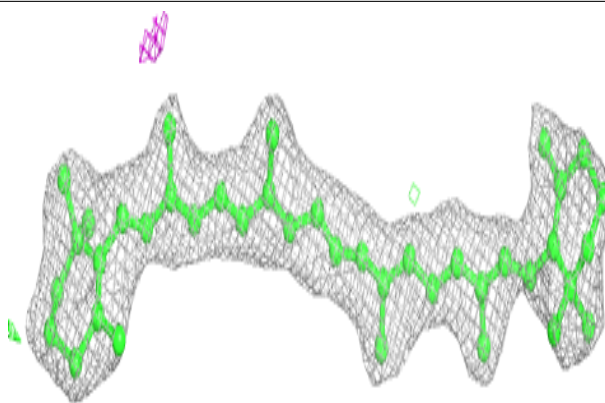
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



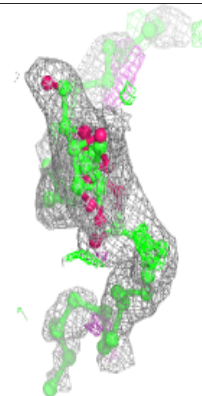
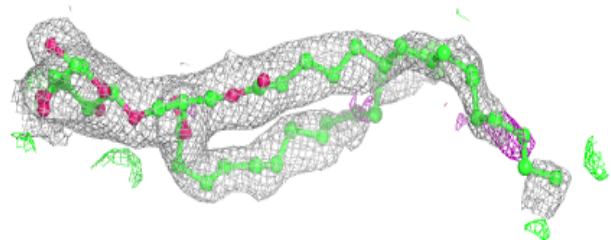
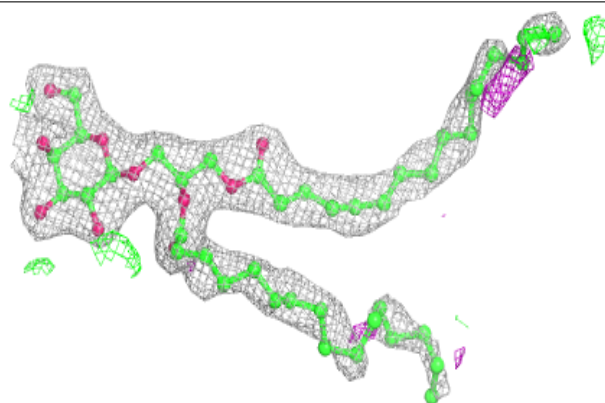


Electron density around BCR b 619:

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

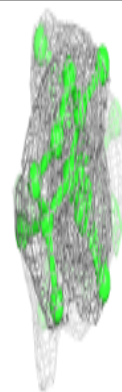
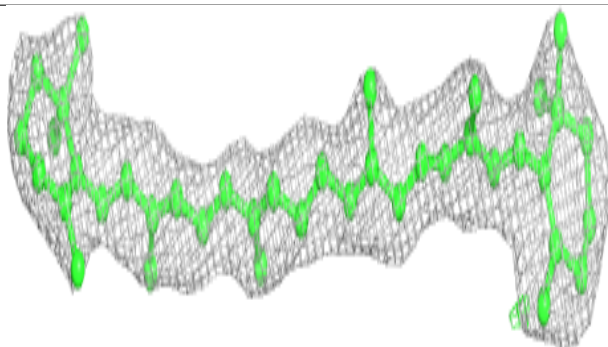
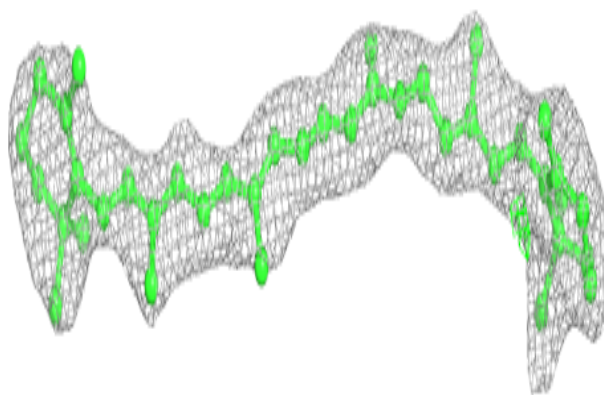
**Electron density around LMG D 408:**

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



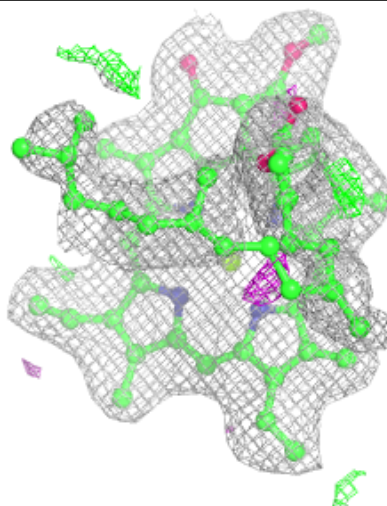
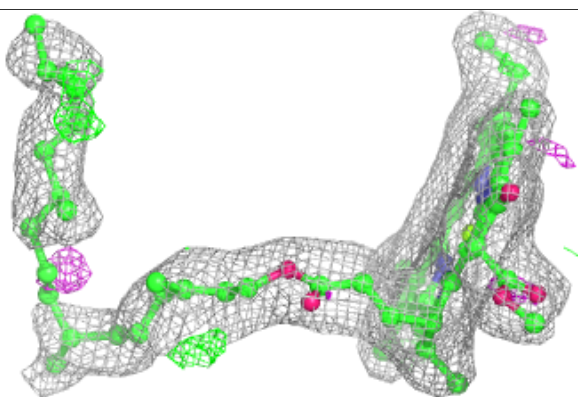
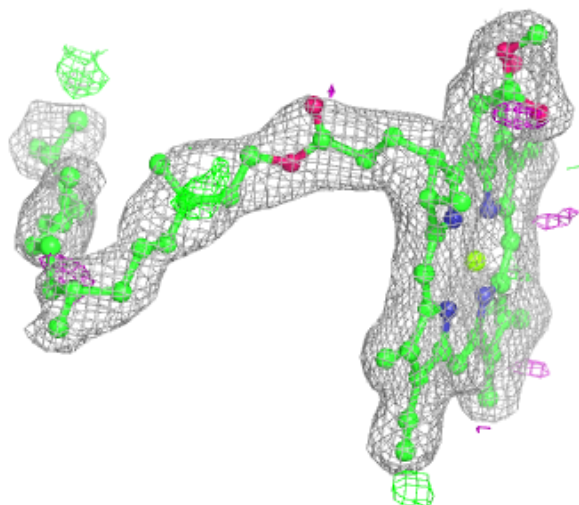
Electron density around BCR c 514:

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



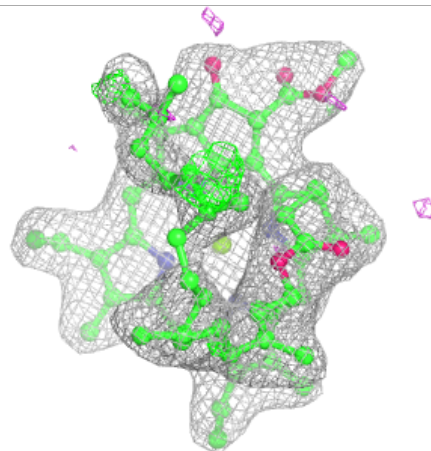
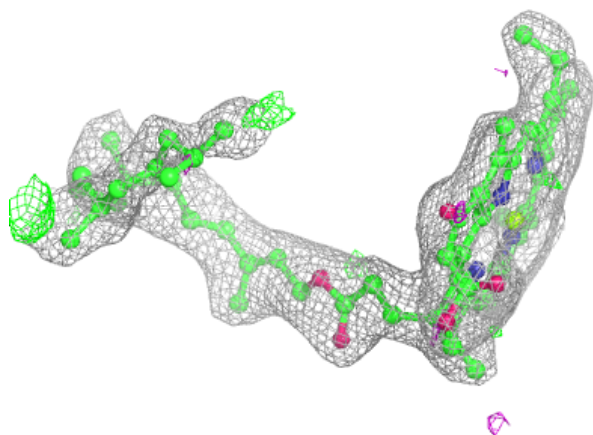
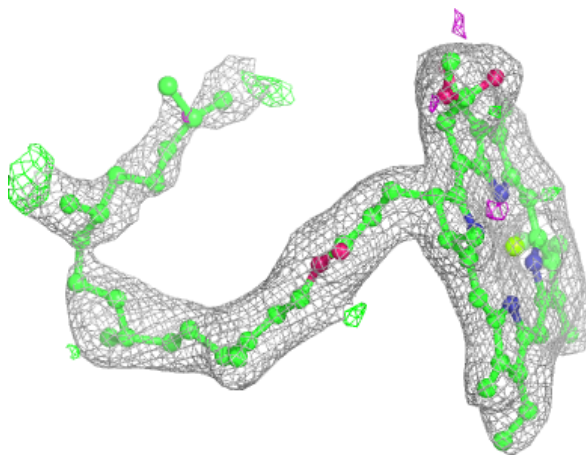
Electron density around CLA a 609:

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

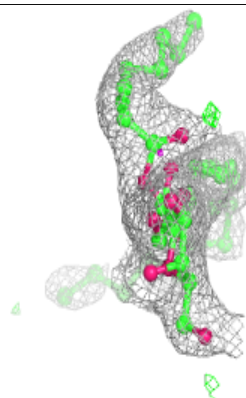
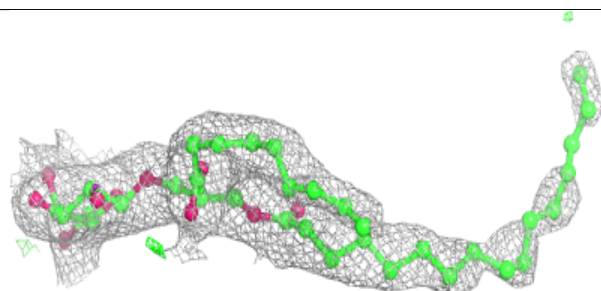
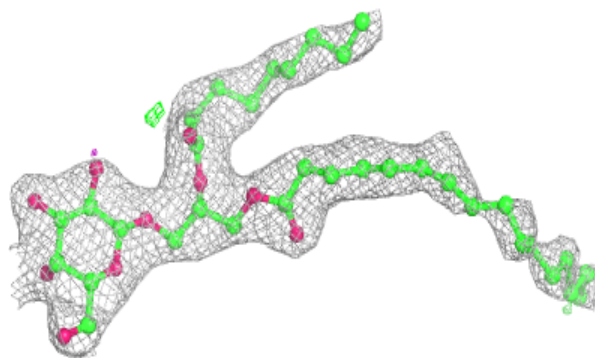


Electron density around CLA B 606:

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

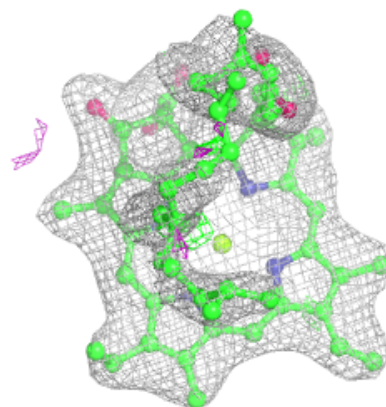
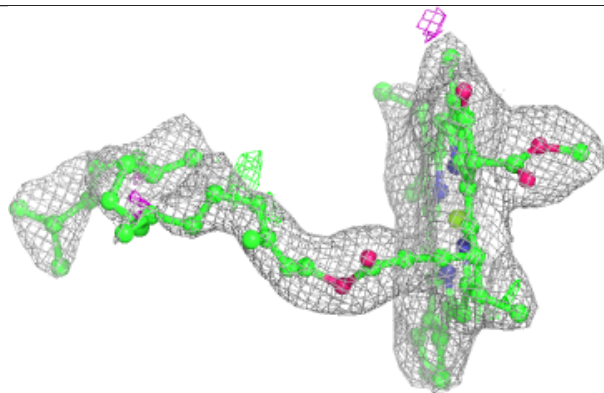
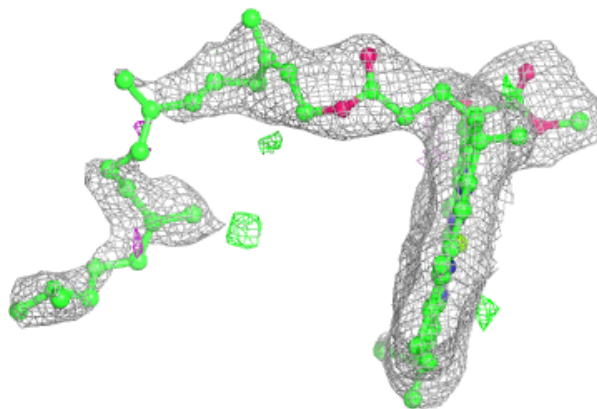
**Electron density around LMG d 411:**

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

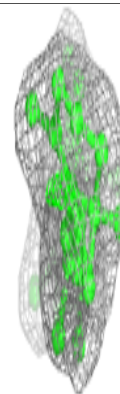
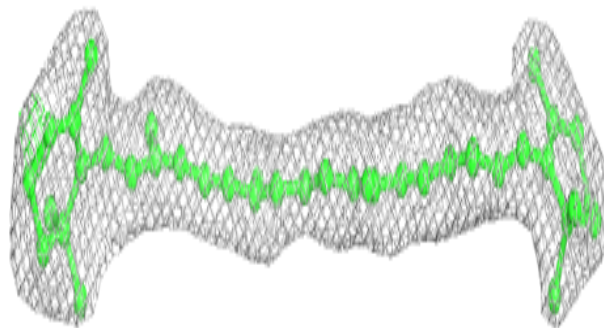
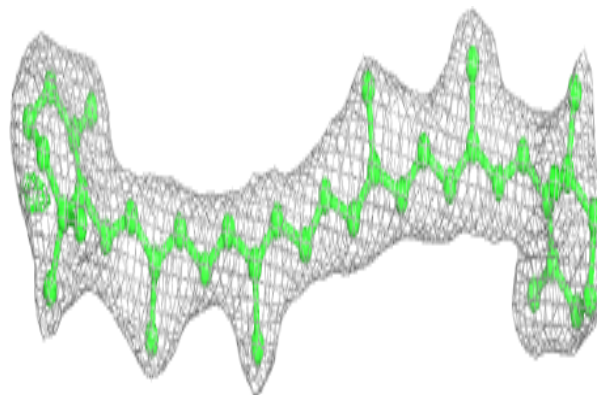


Electron density around CLA c 506:

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

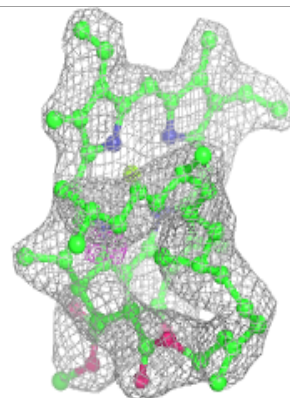
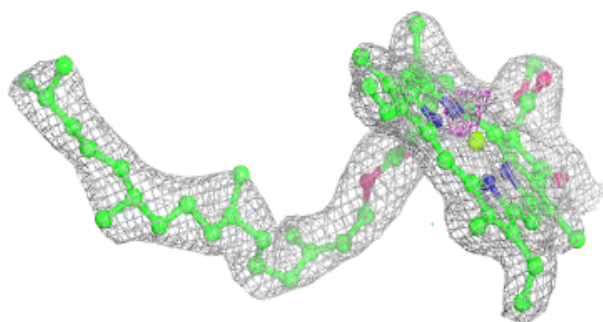
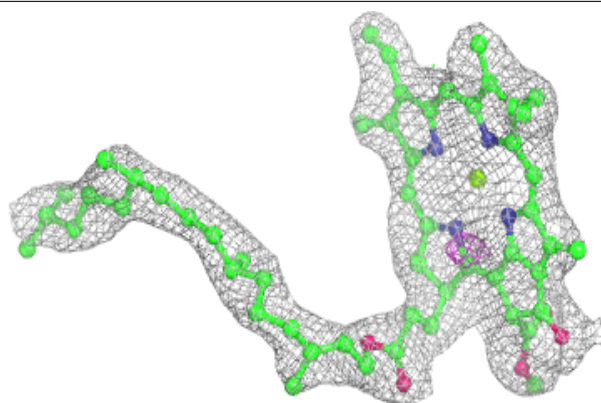
**Electron density around BCR b 618:**

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

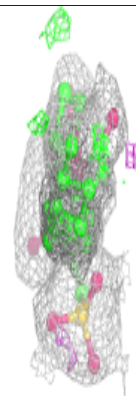
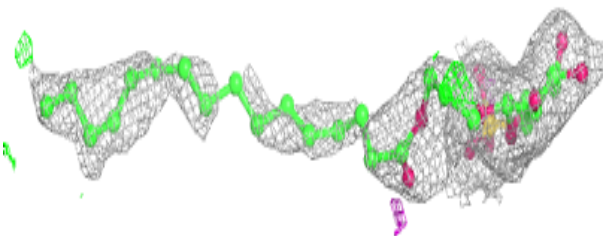
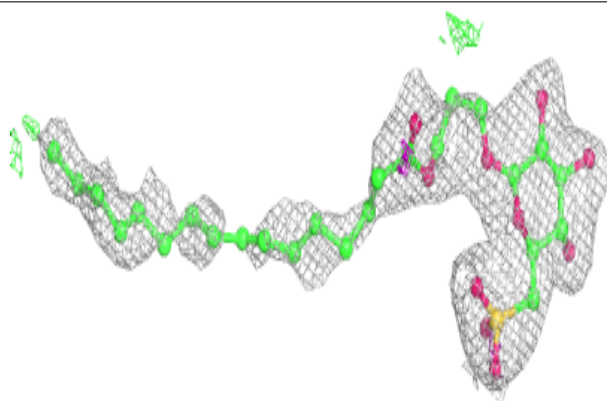


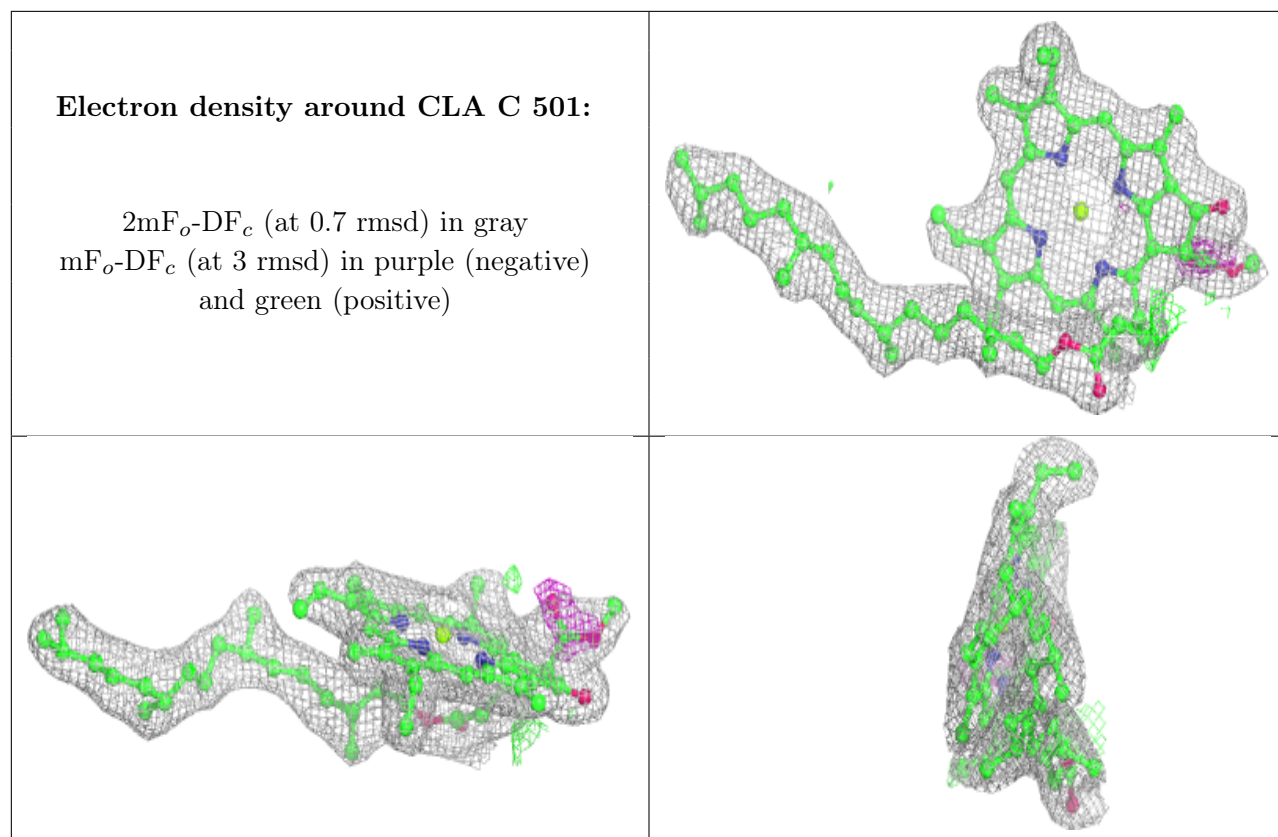
Electron density around CLA C 511:

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

**Electron density around SQD D 409:**

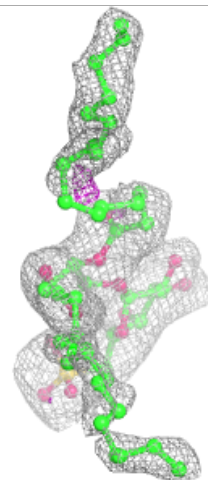
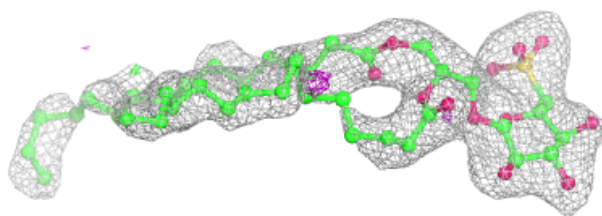
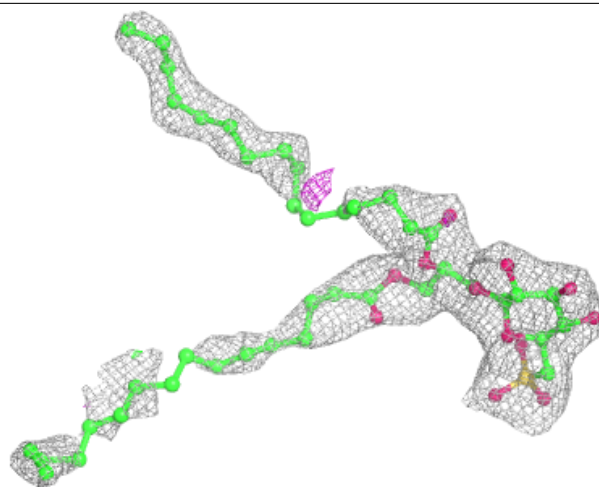
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





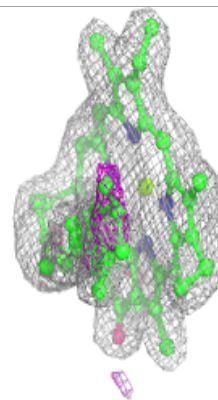
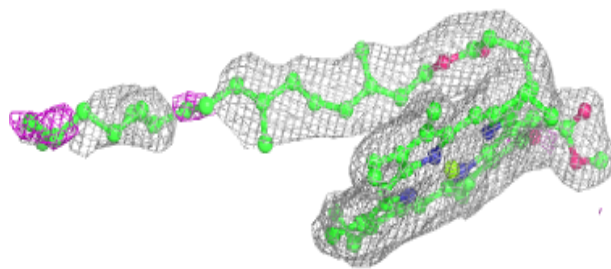
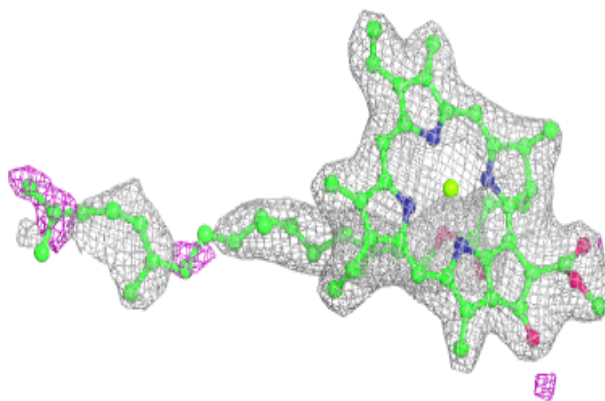
Electron density around SQD a 613:

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



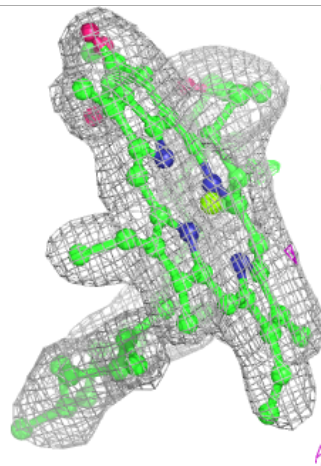
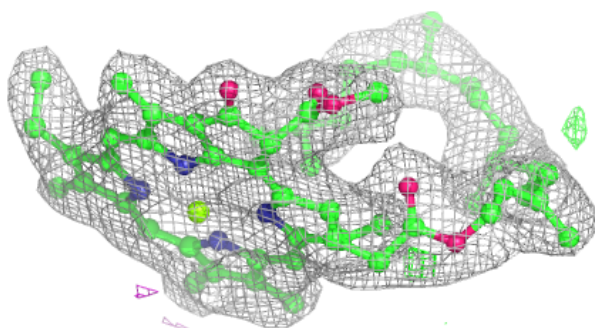
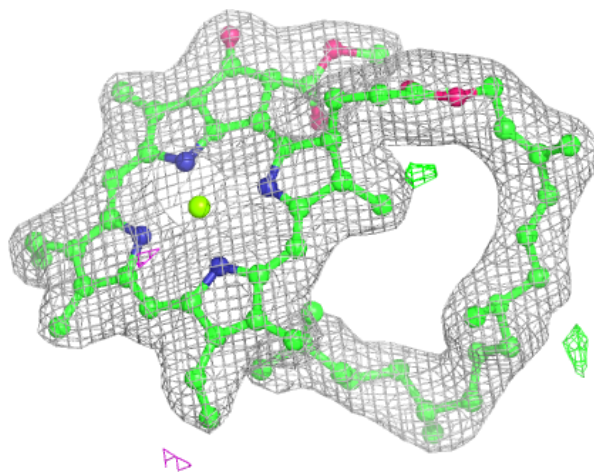
Electron density around CLA b 614:

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



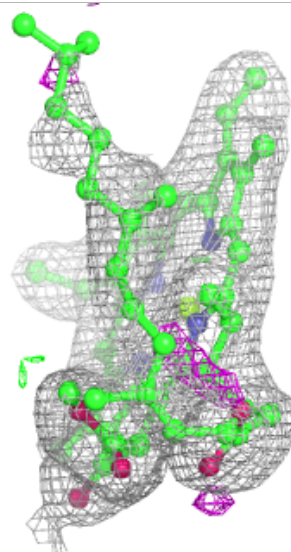
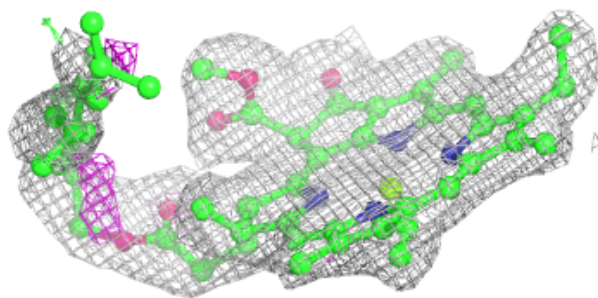
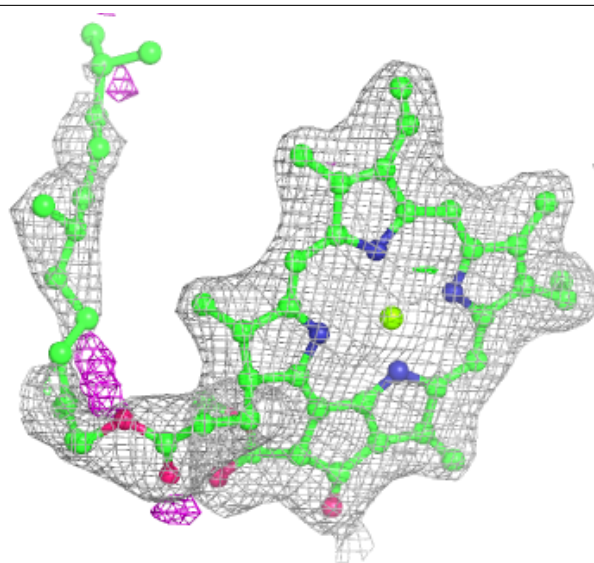
Electron density around CLA b 615:

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



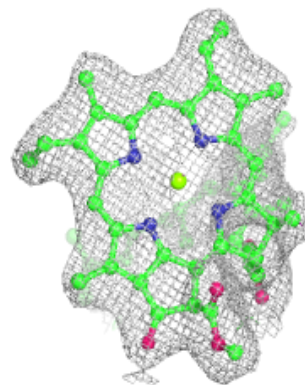
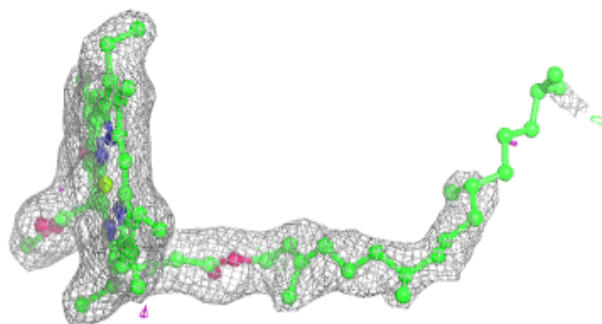
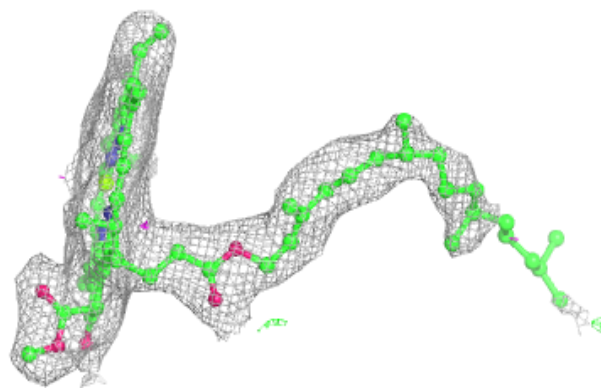
Electron density around CLA B 616:

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

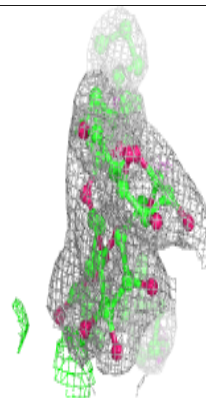
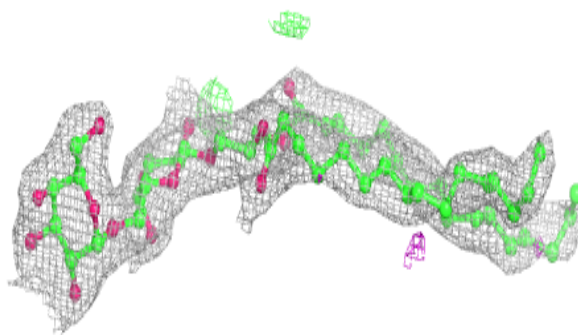
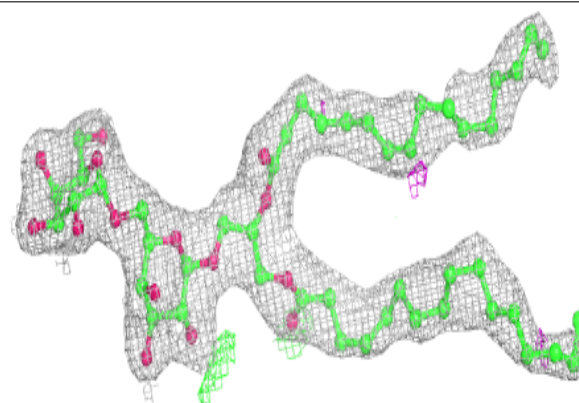


Electron density around CLA D 405:

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

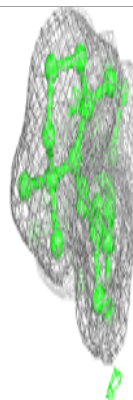
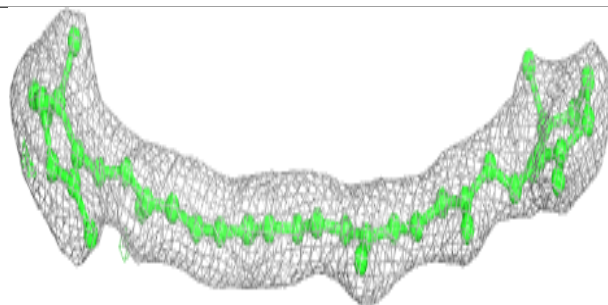
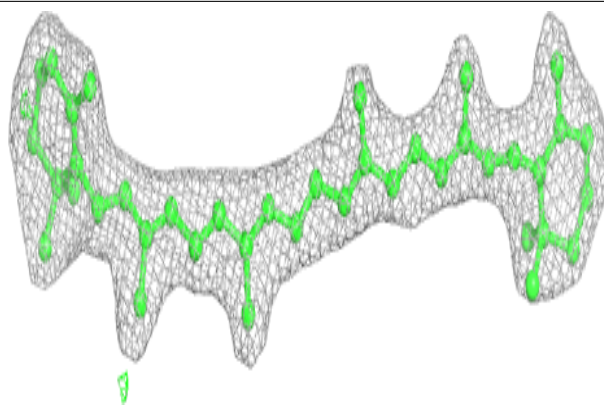
**Electron density around DGD C 518:**

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



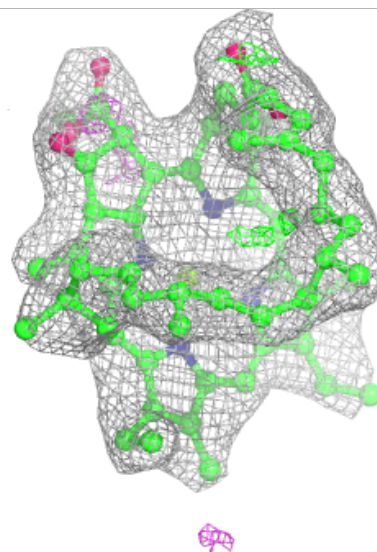
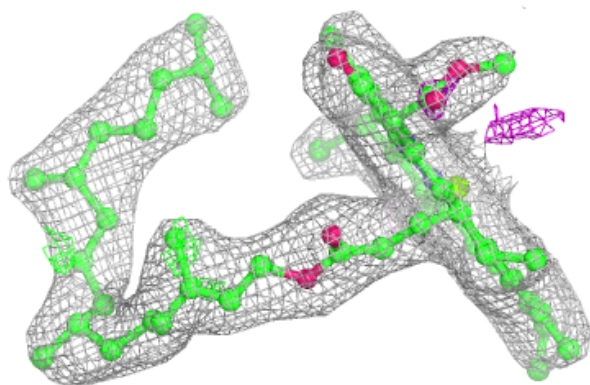
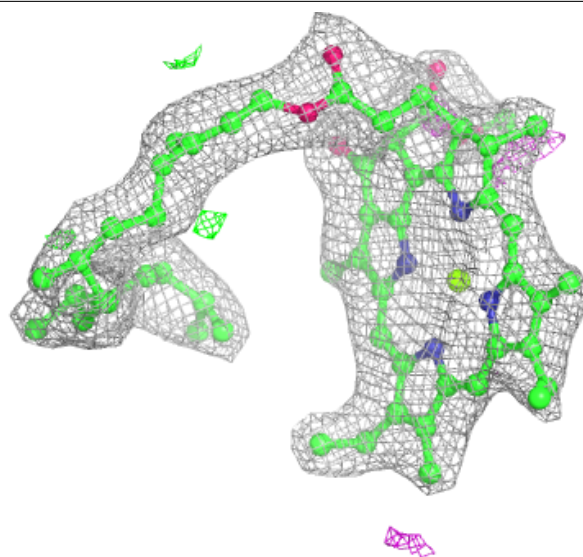
Electron density around BCR t 101:

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



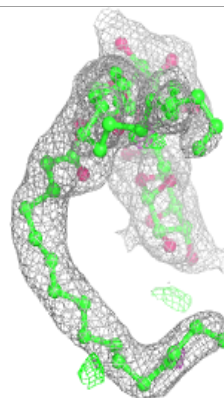
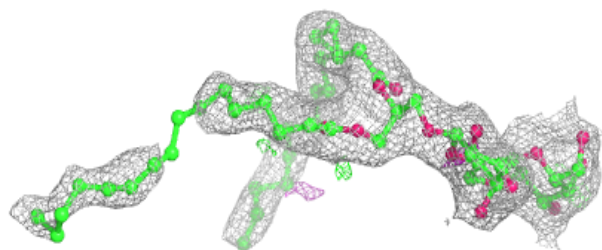
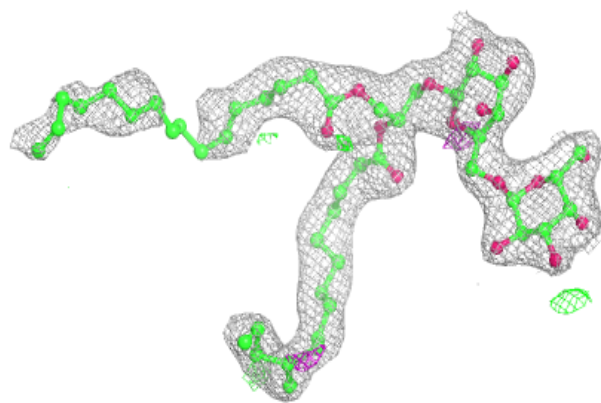
Electron density around CLA c 503:

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

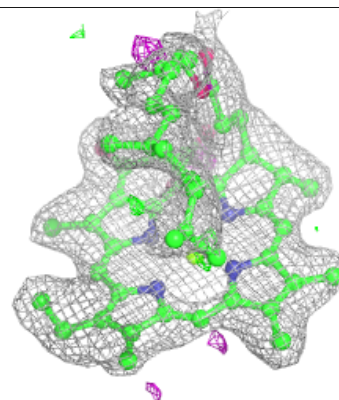
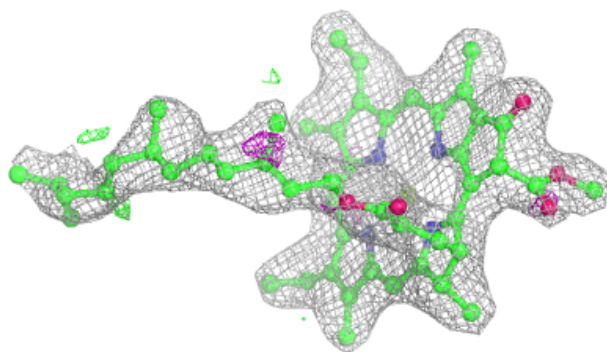
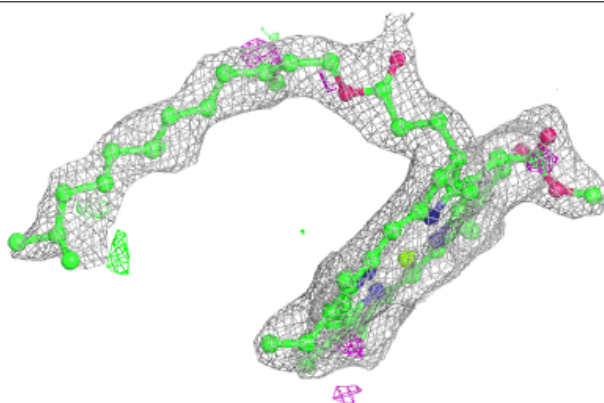


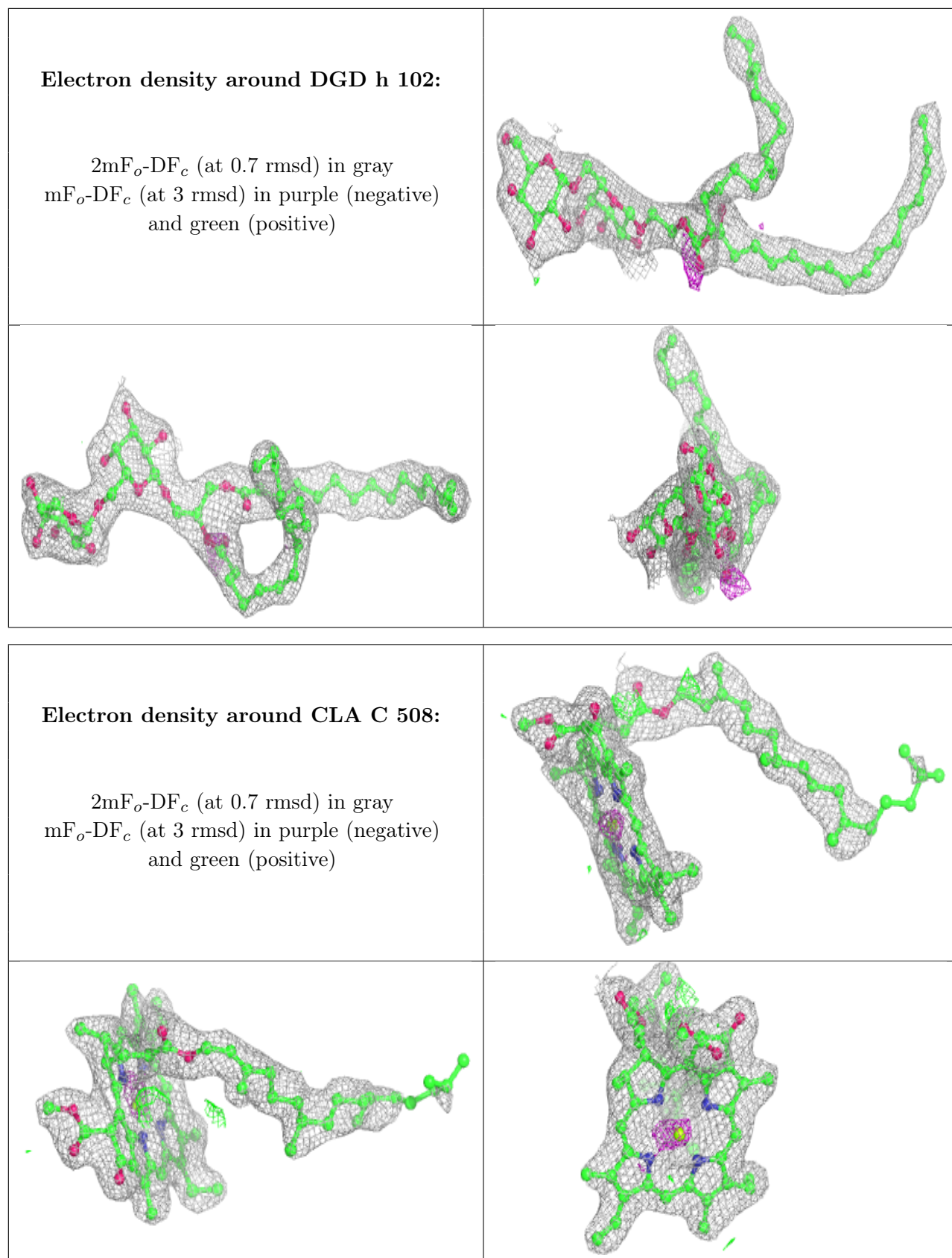
Electron density around DGD c 517:

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

**Electron density around CLA c 504:**

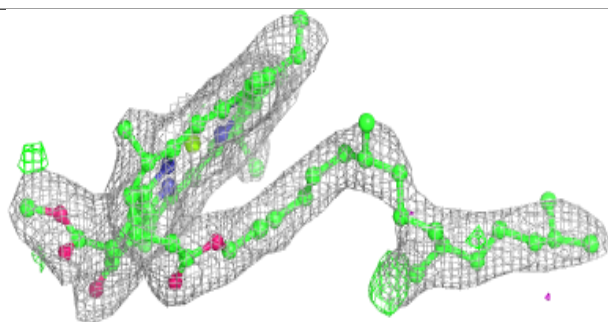
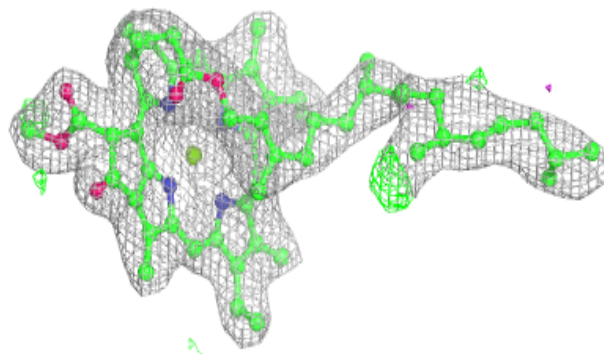
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



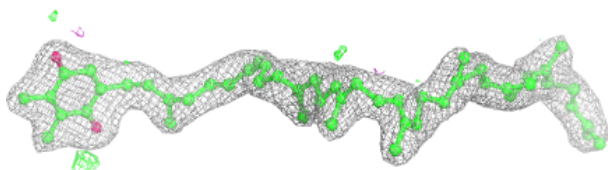
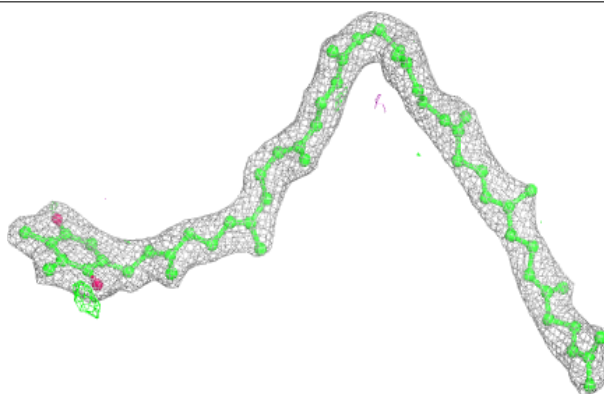


Electron density around CLA c 505:

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

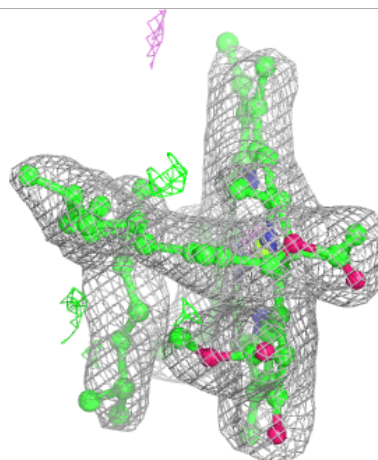
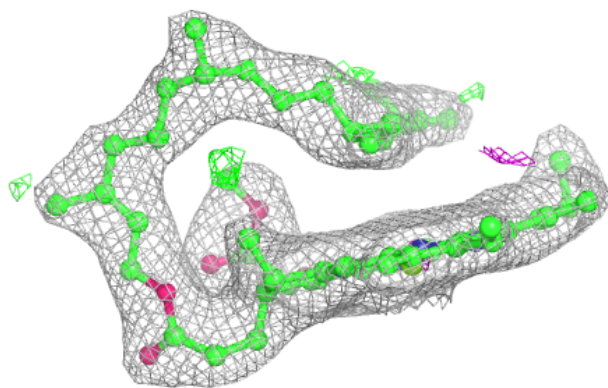
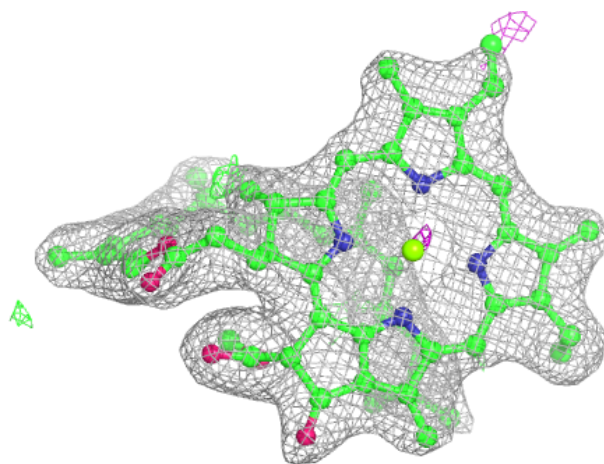
**Electron density around PL9 D 407:**

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



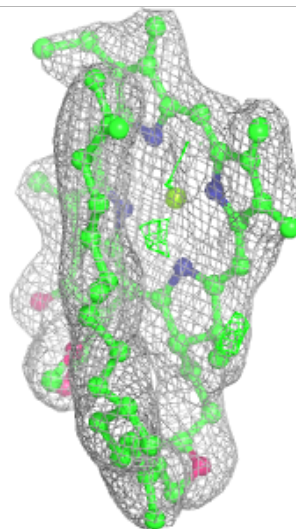
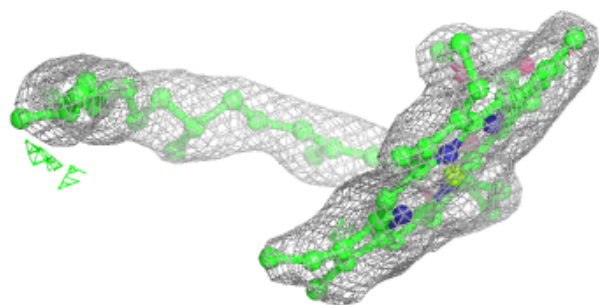
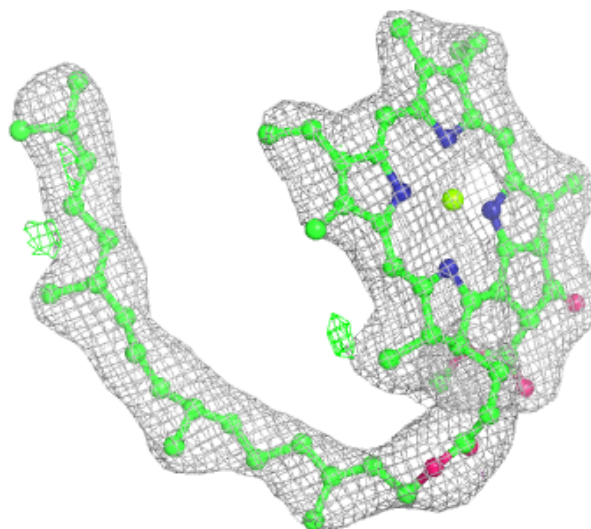
Electron density around CLA C 510:

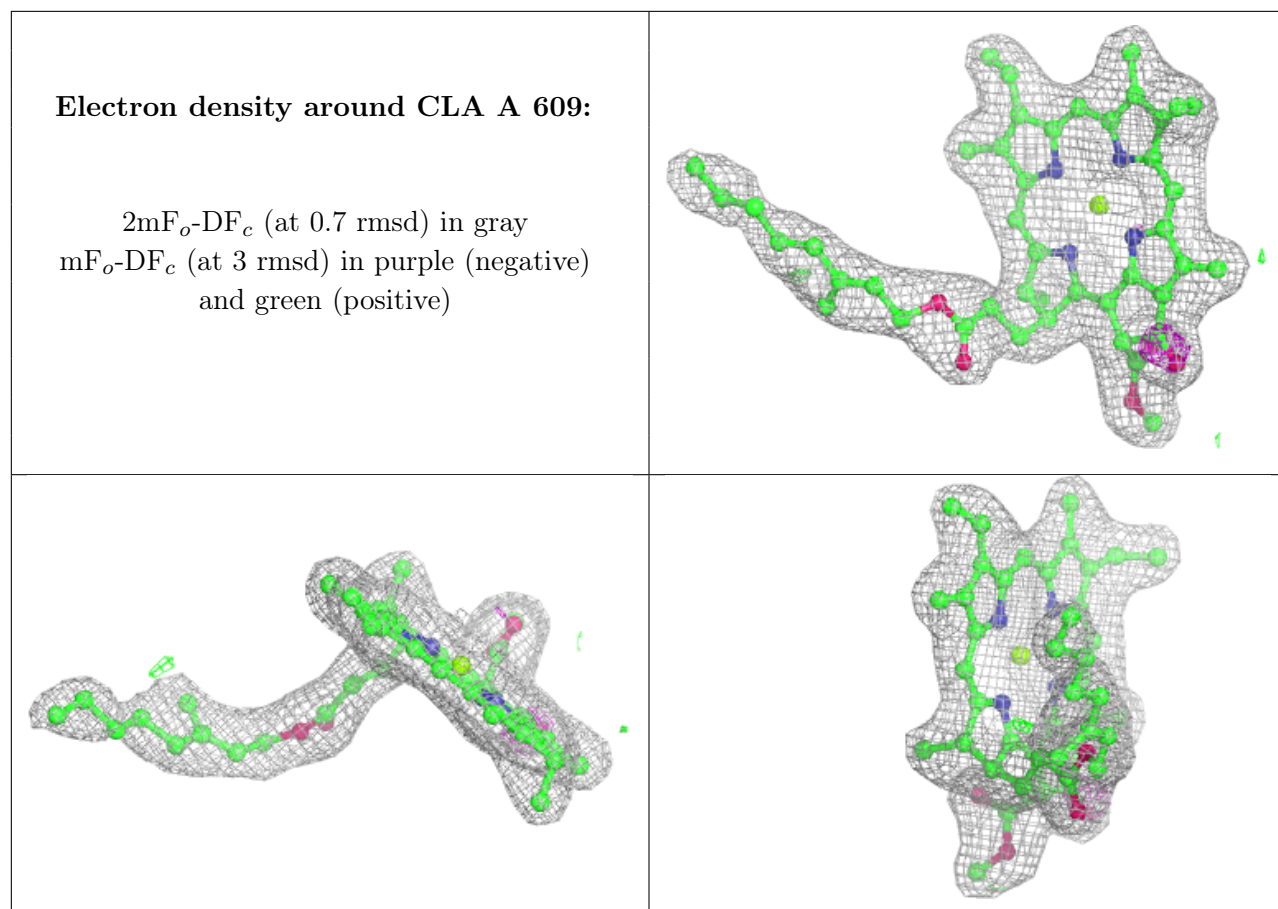
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 507:

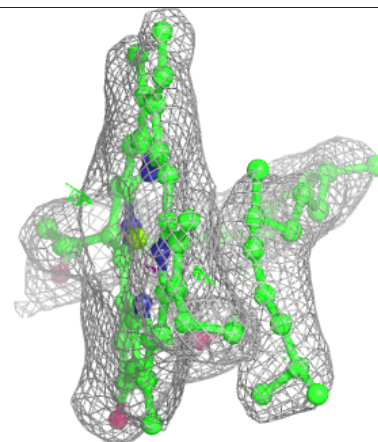
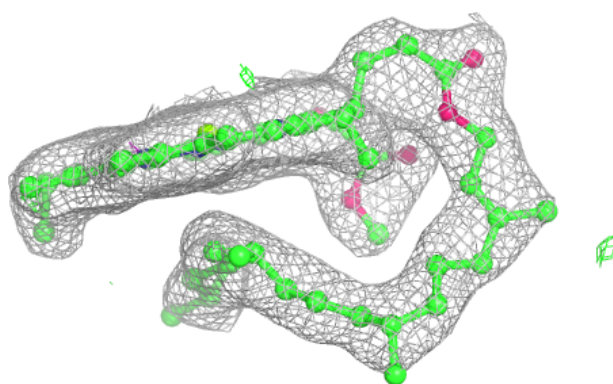
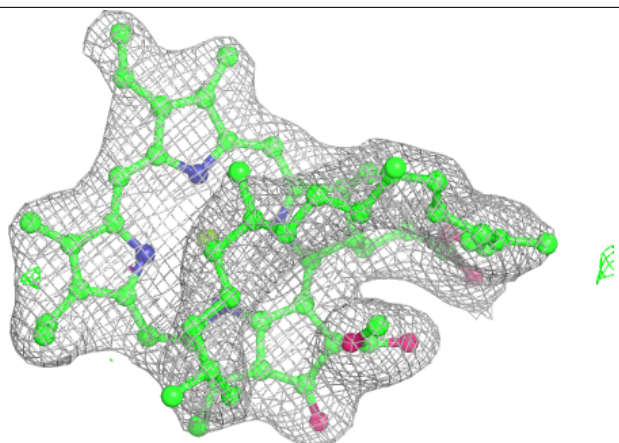
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



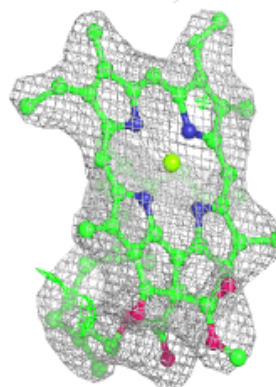
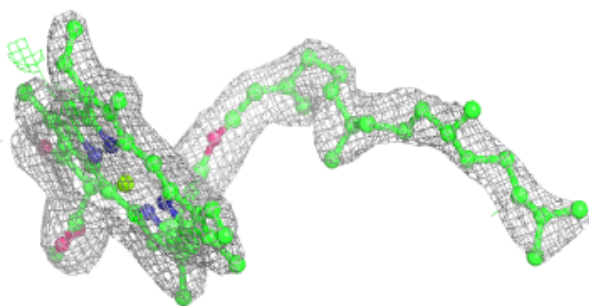
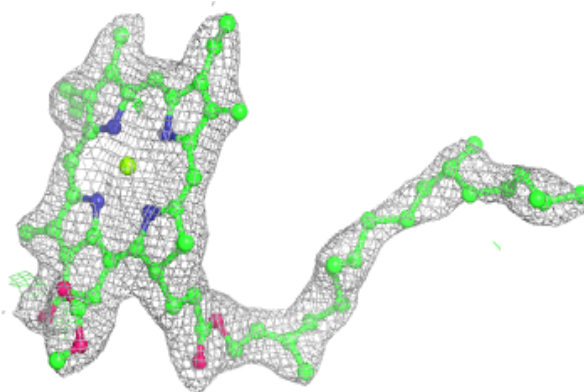


Electron density around CLA c 510:

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

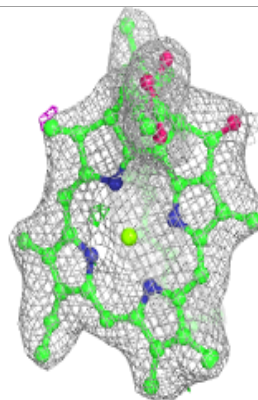
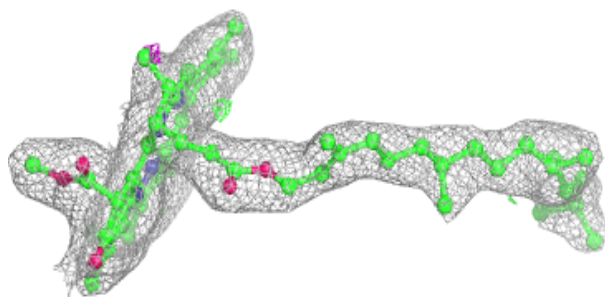
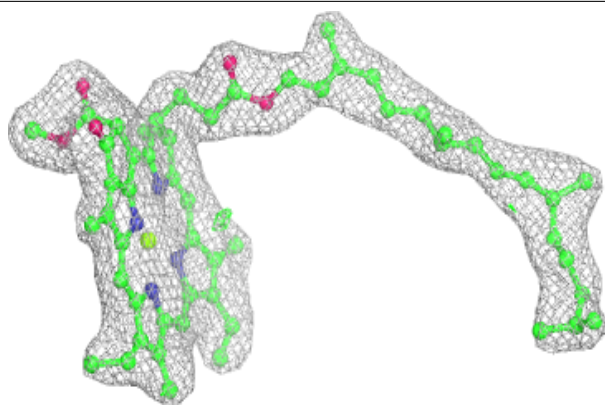
**Electron density around CLA c 511:**

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

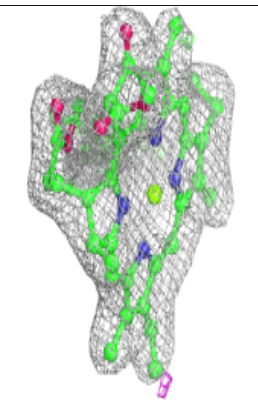
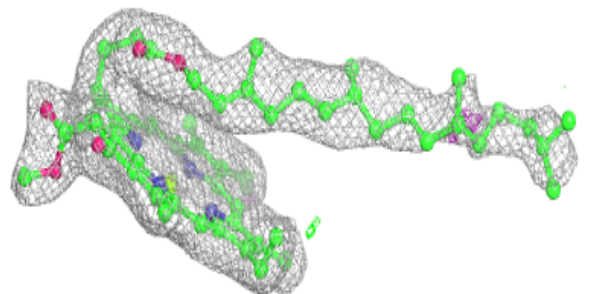
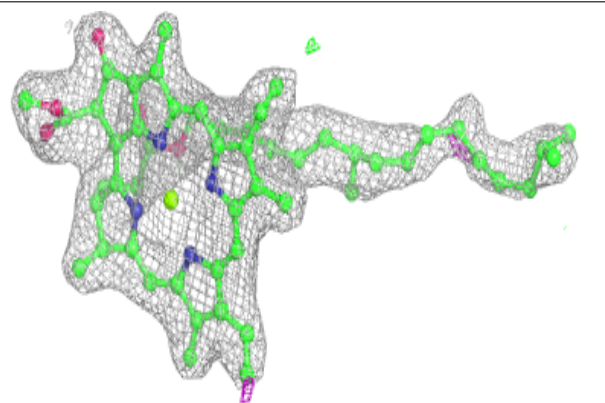


Electron density around CLA B 609:

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

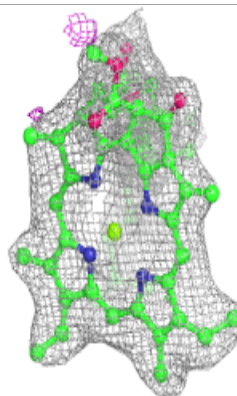
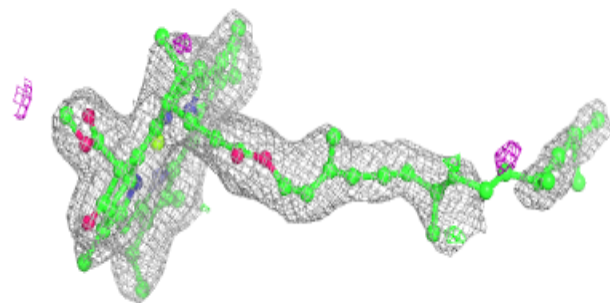
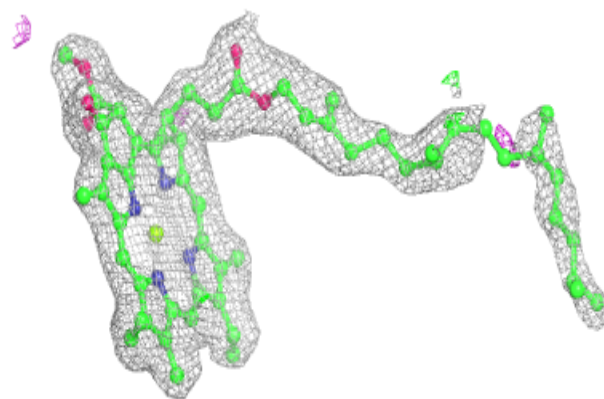
**Electron density around CLA B 614:**

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

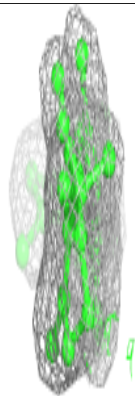
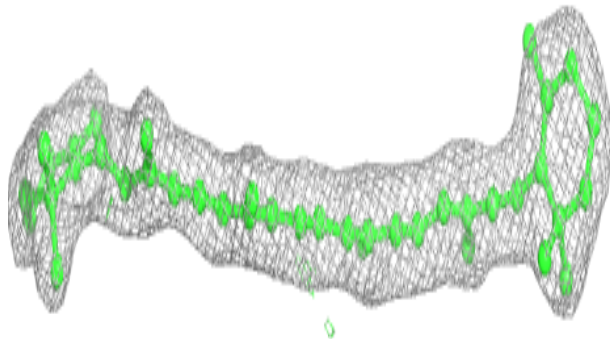
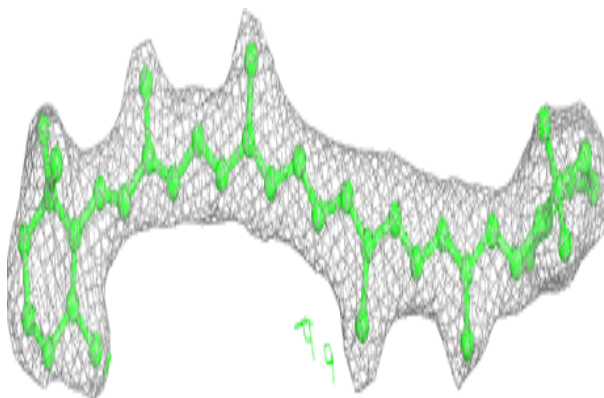


Electron density around CLA d 404:

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

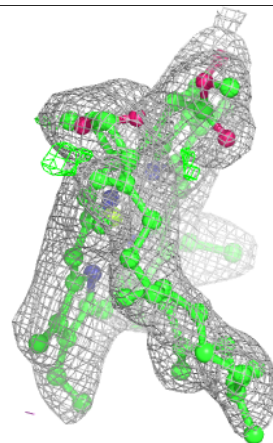
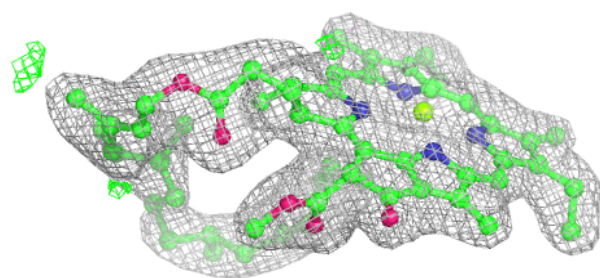
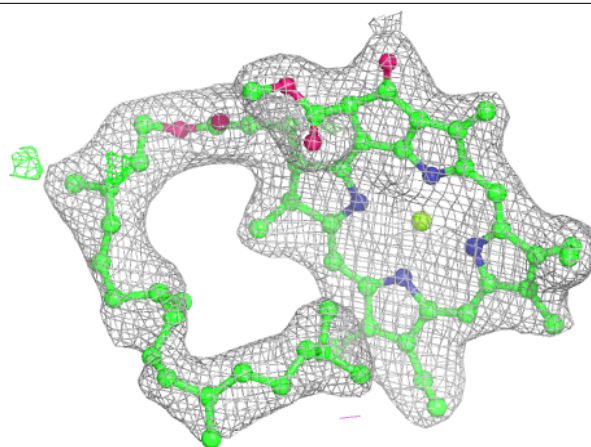
**Electron density around BCR B 617:**

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

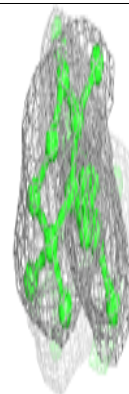
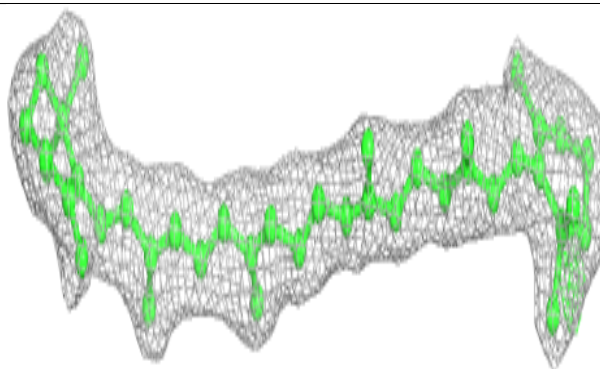
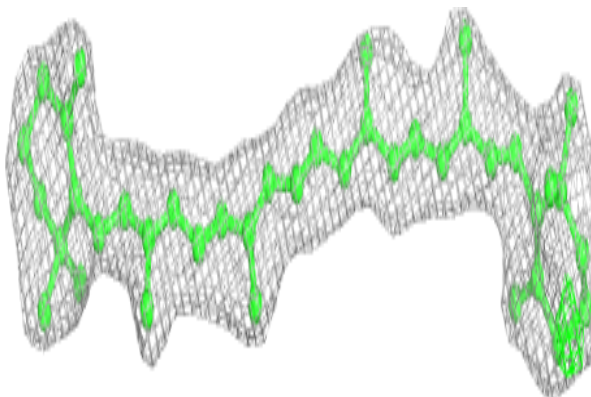


Electron density around CLA B 615:

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

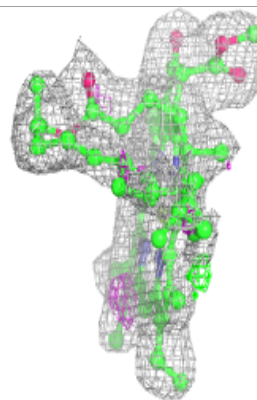
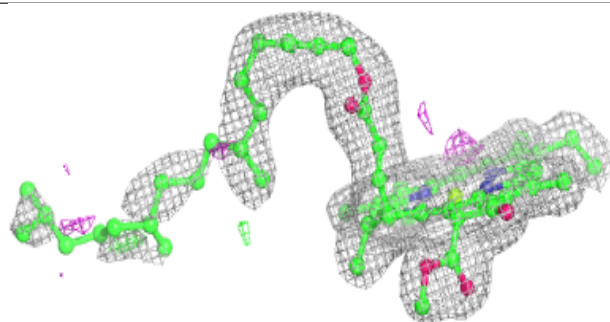
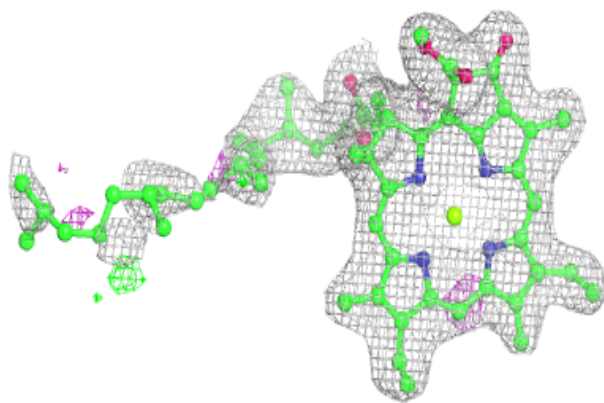
**Electron density around BCR B 619:**

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

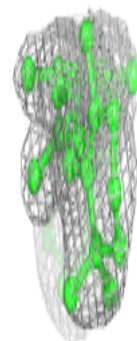
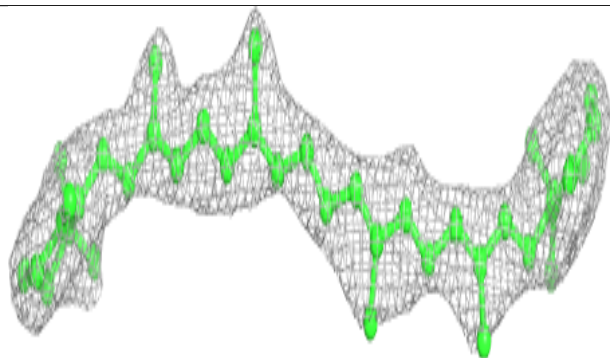
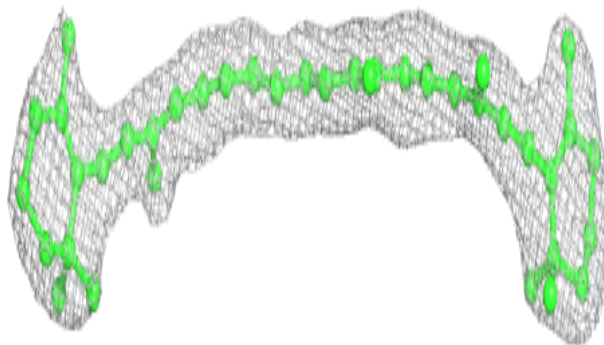


Electron density around CLA A 607:

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

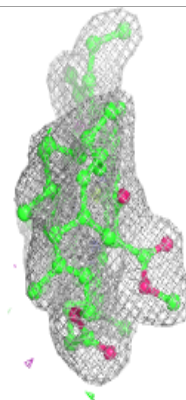
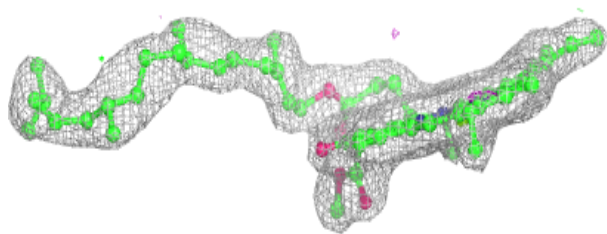
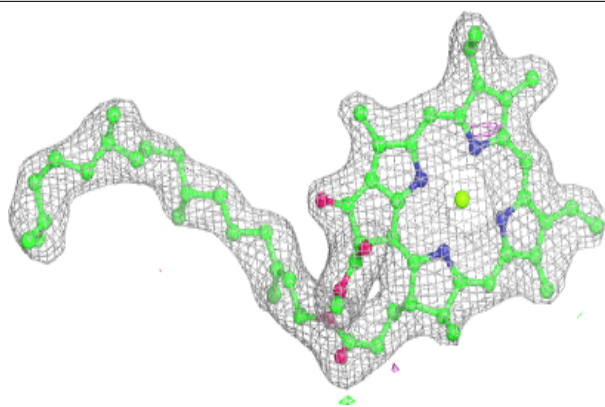
**Electron density around BCR C 515:**

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

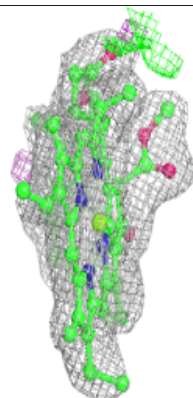
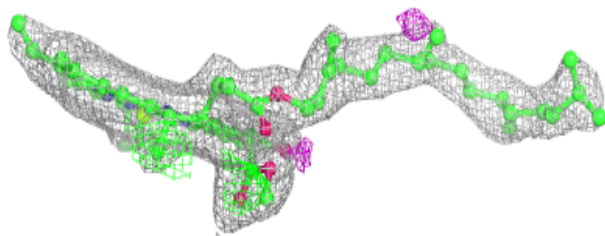
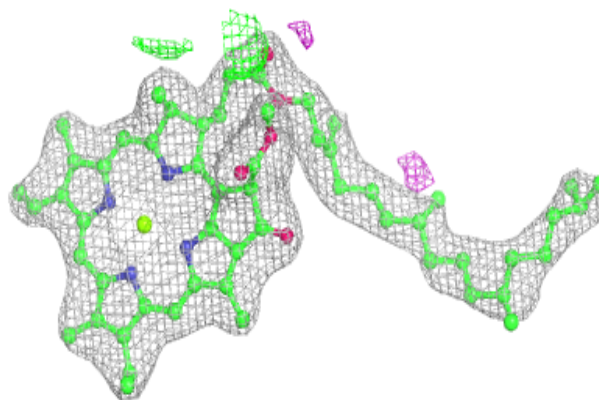


Electron density around CLA B 602:

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

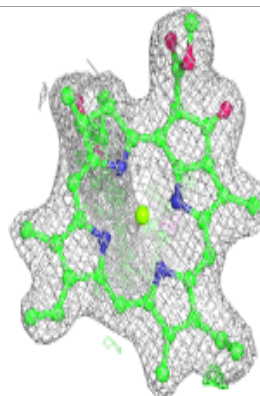
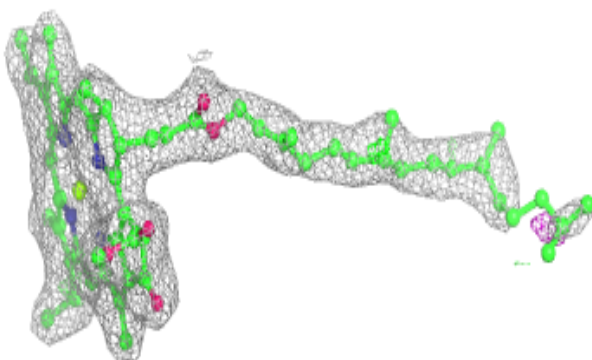
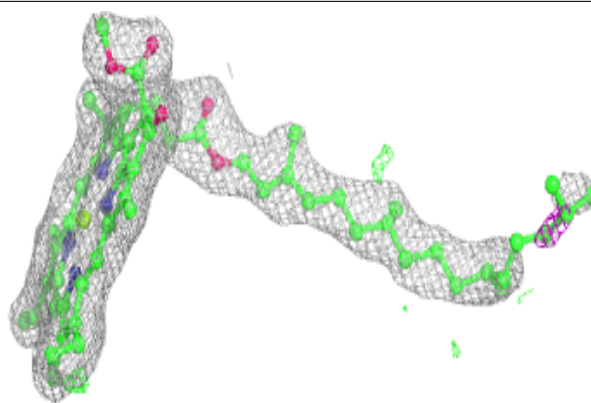
**Electron density around CLA b 602:**

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

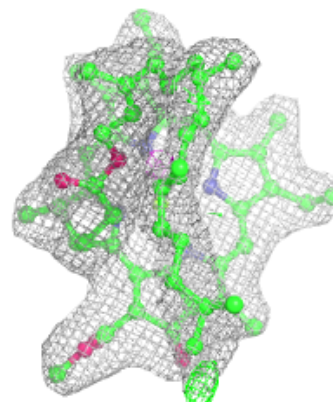
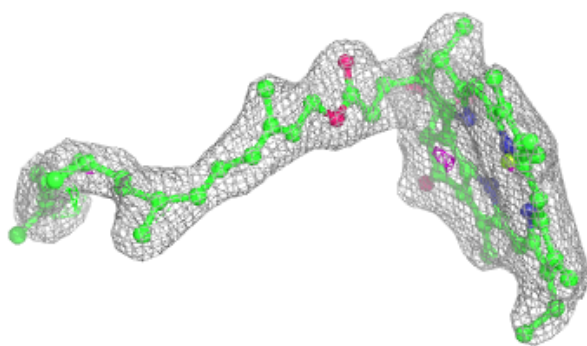
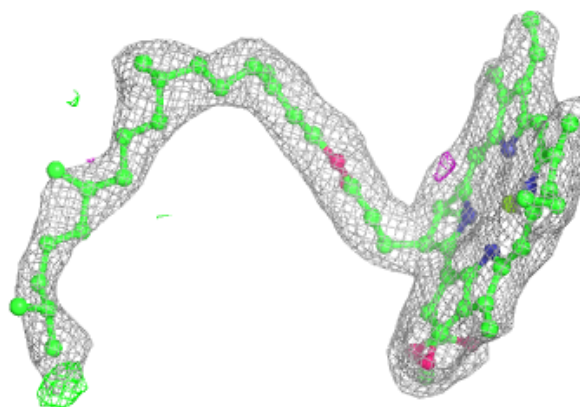


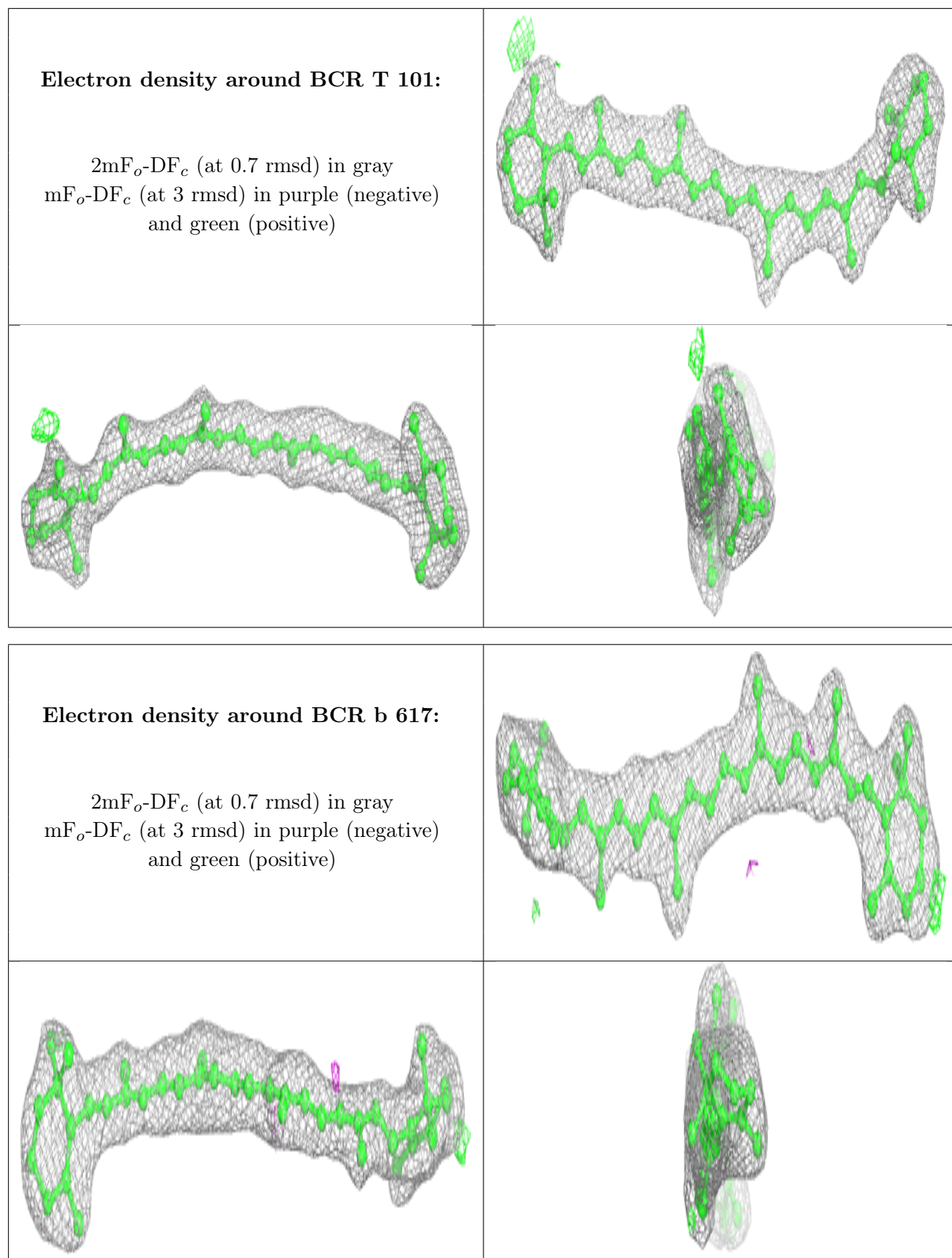
Electron density around CLA b 604:

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

**Electron density around CLA b 606:**

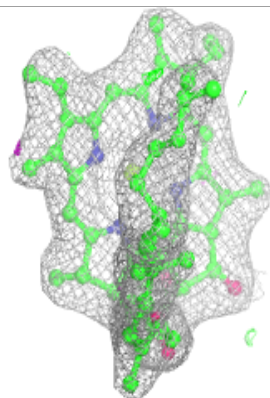
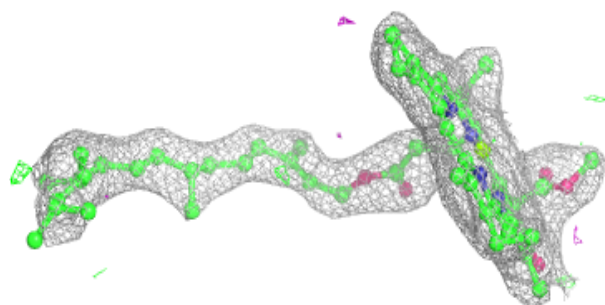
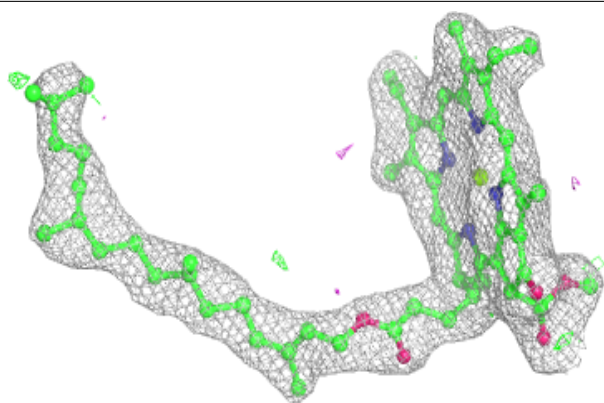
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





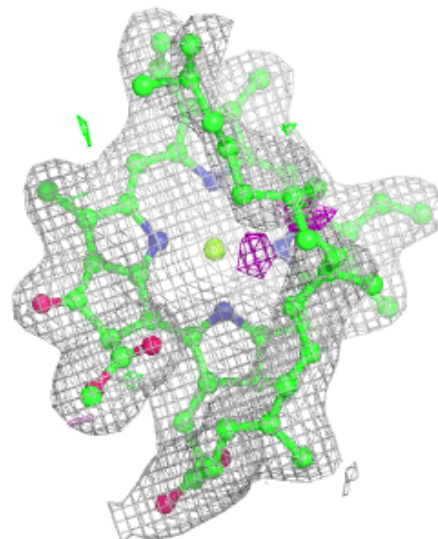
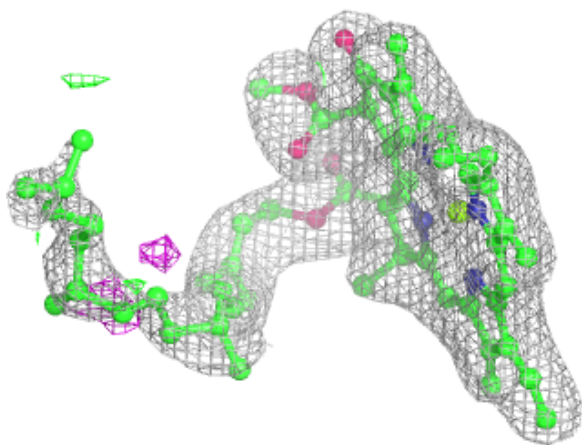
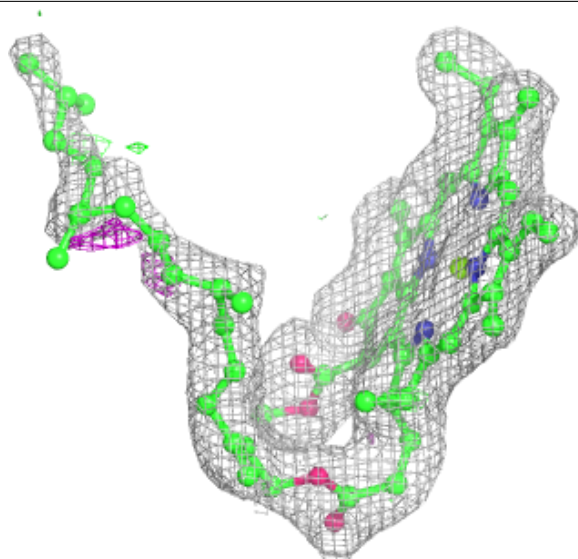
Electron density around CLA b 609:

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



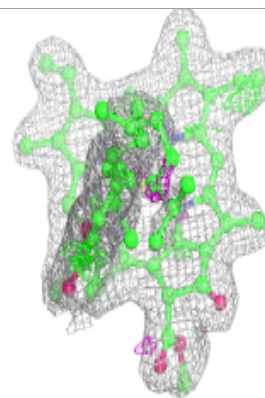
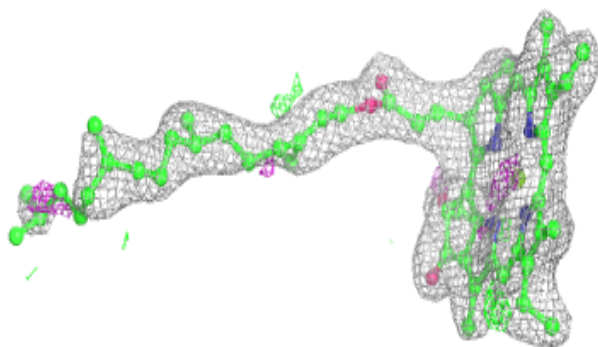
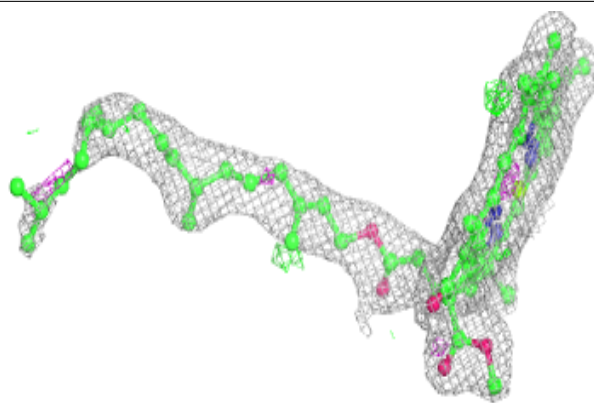
Electron density around CLA b 613:

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

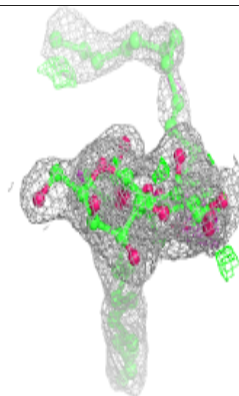
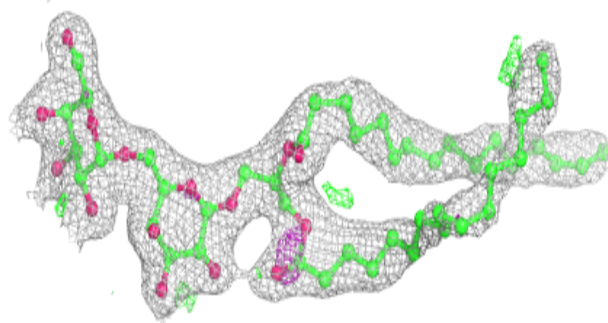
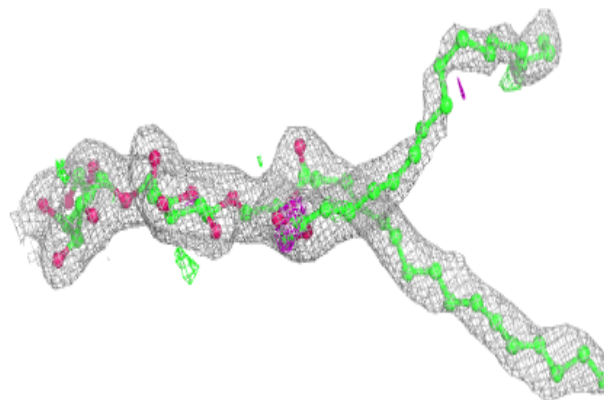


Electron density around CLA B 604:

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

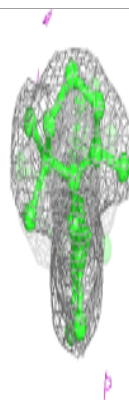
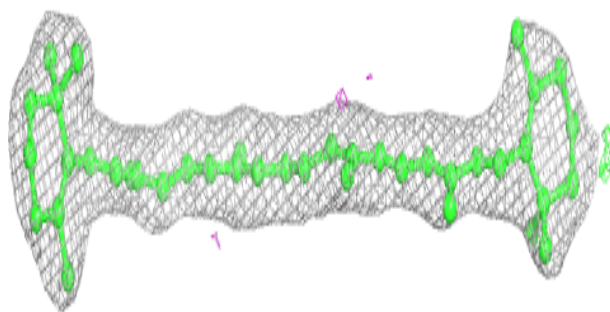
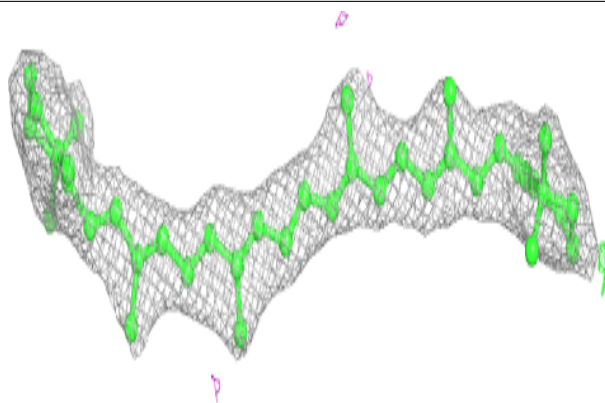
**Electron density around DGD C 516:**

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



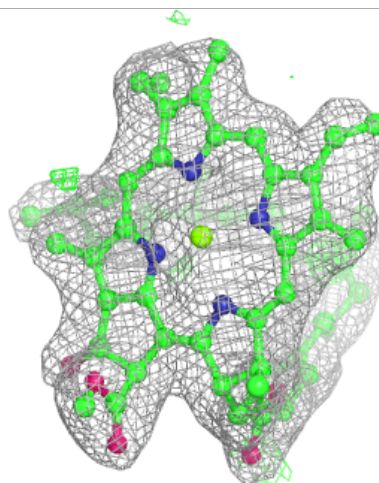
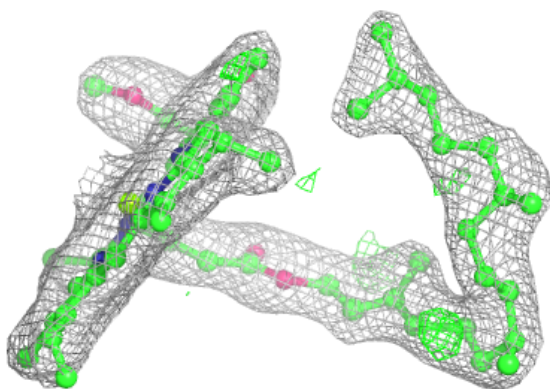
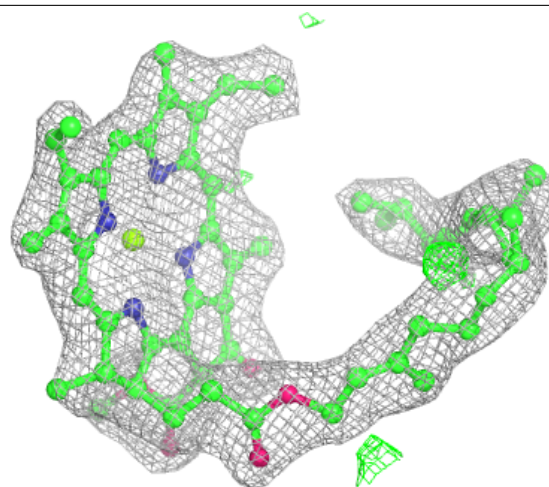
Electron density around BCR c 515:

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



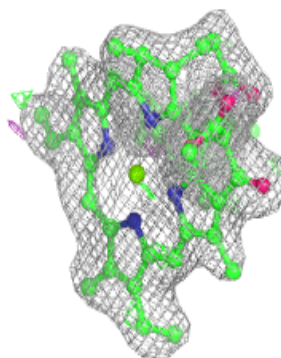
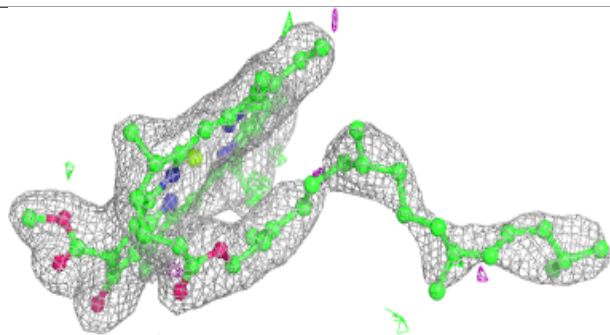
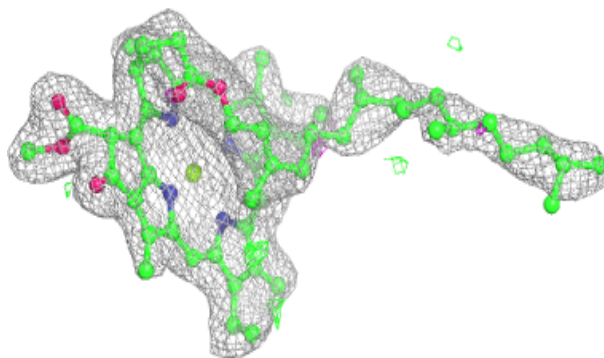
Electron density around CLA C 503:

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

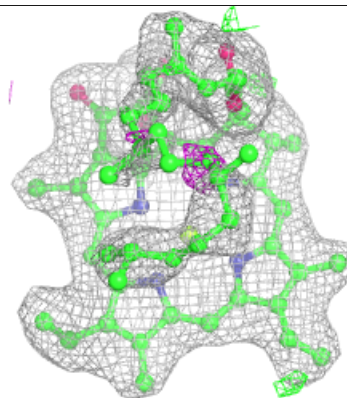
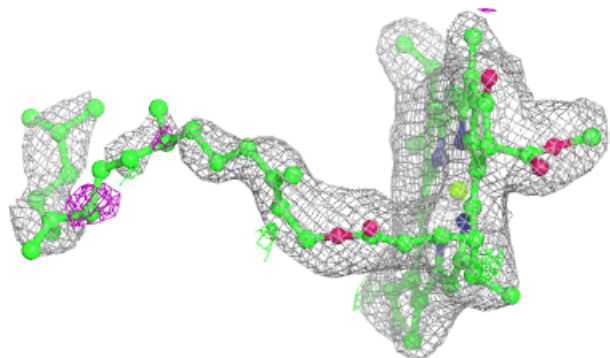
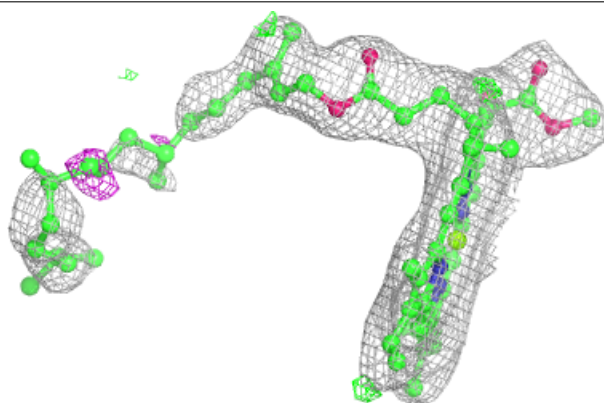


Electron density around CLA C 505:

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

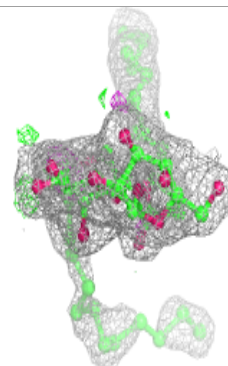
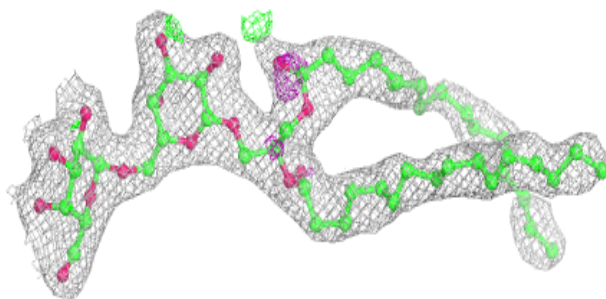
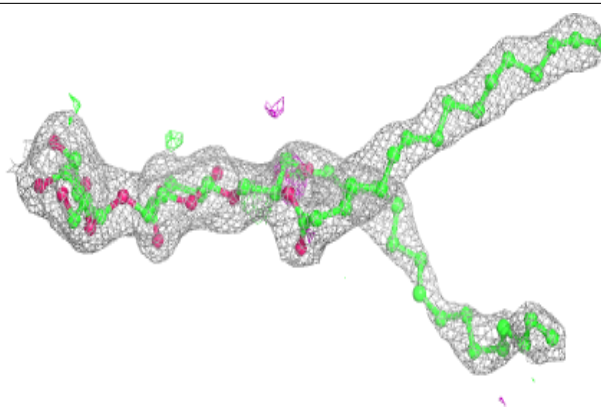
**Electron density around CLA C 506:**

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



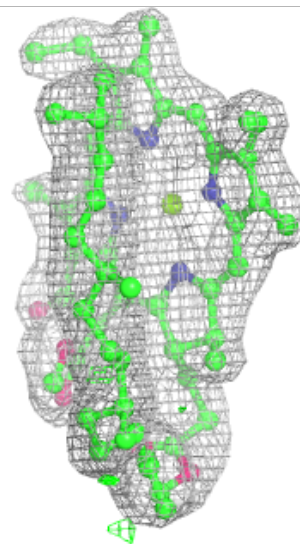
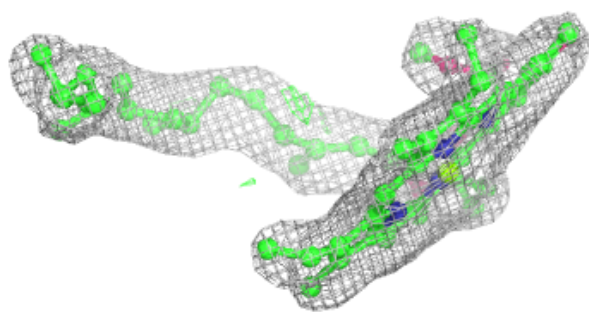
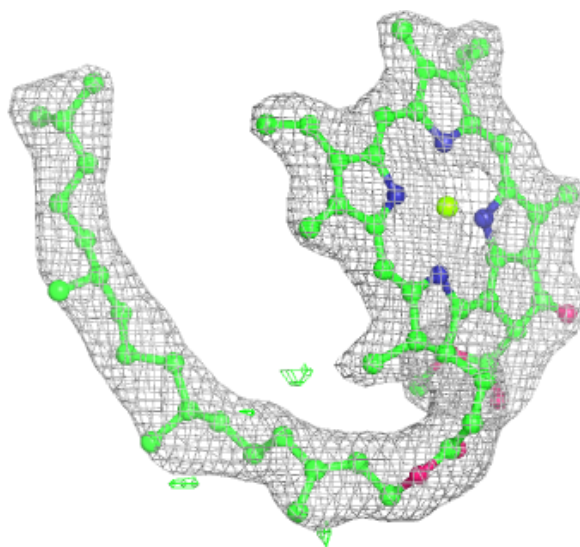
Electron density around DGD c 516:

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



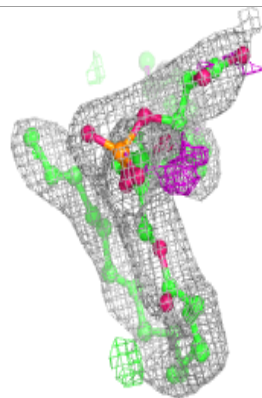
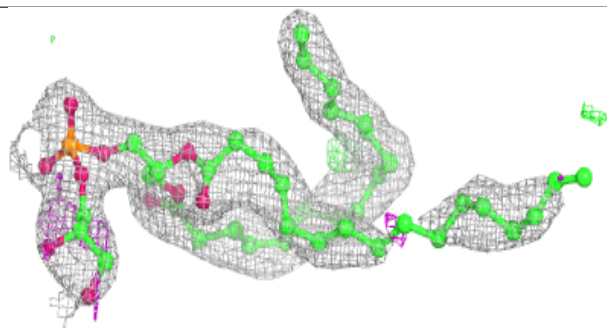
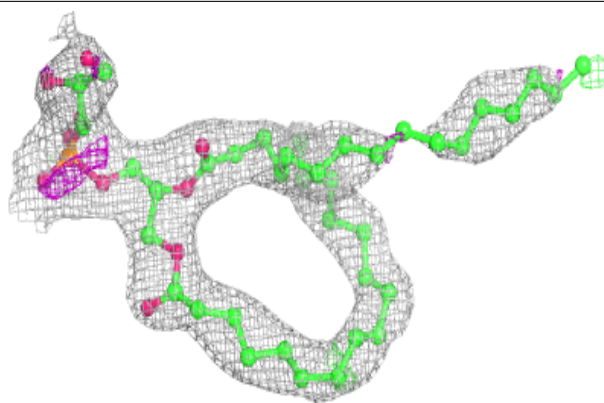
Electron density around CLA C 507:

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

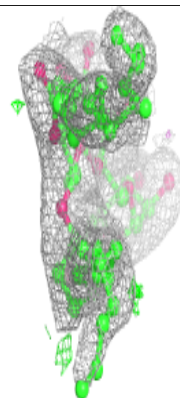
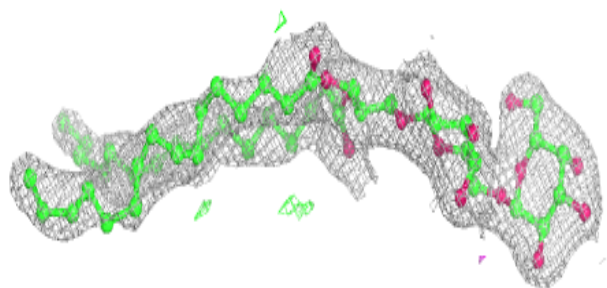
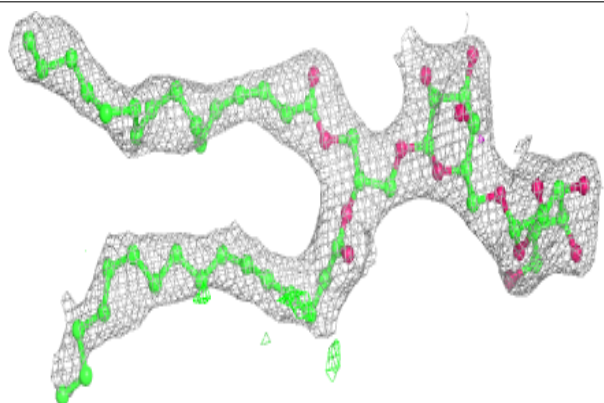


Electron density around LHG d 407:

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

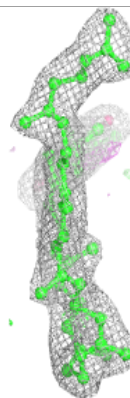
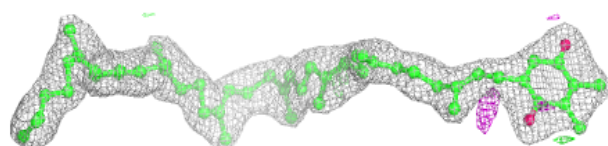
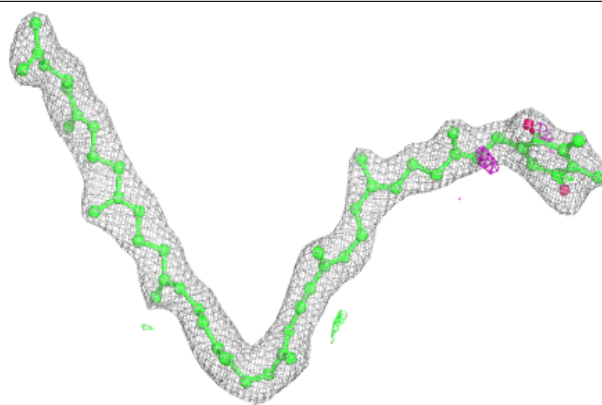
**Electron density around DGD c 518:**

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

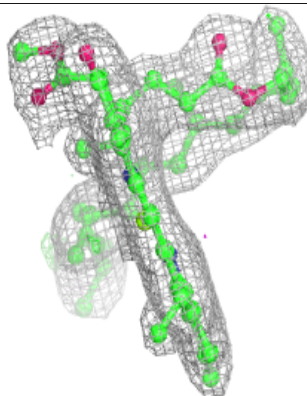
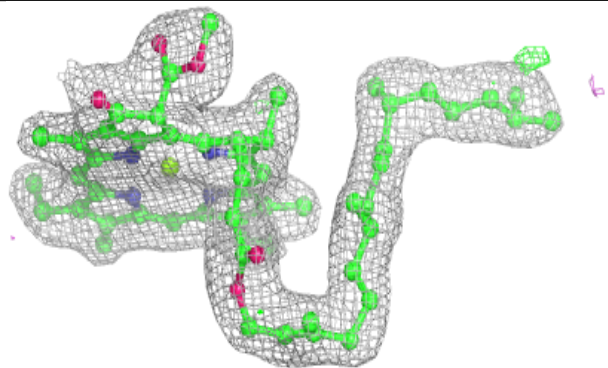
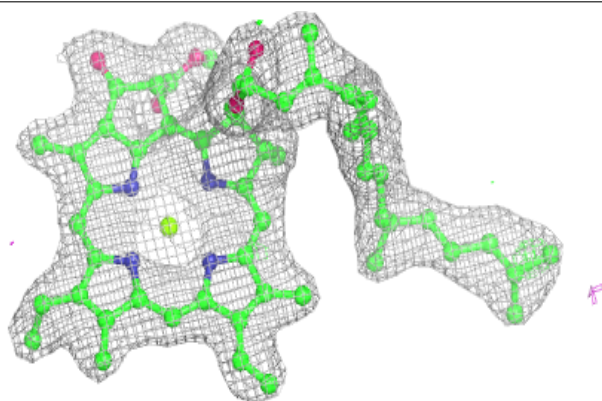


Electron density around PL9 d 406:

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

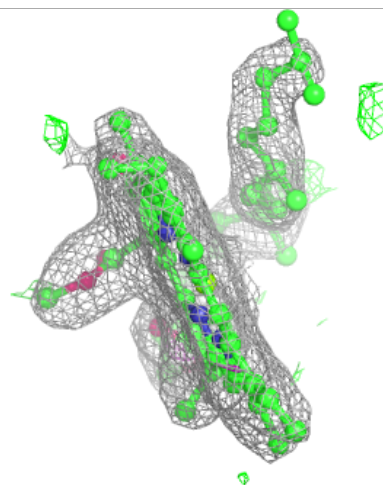
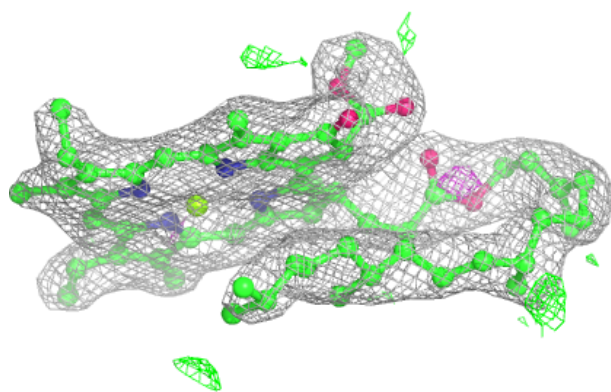
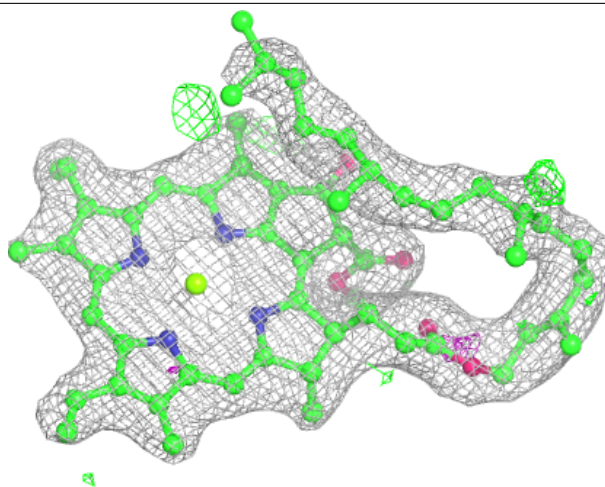
**Electron density around CLA a 612:**

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



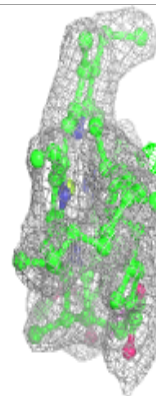
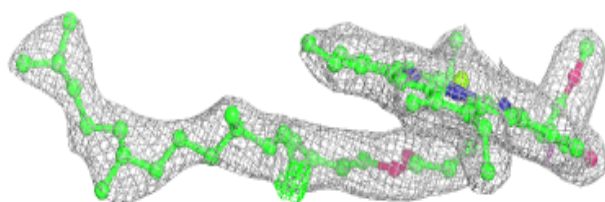
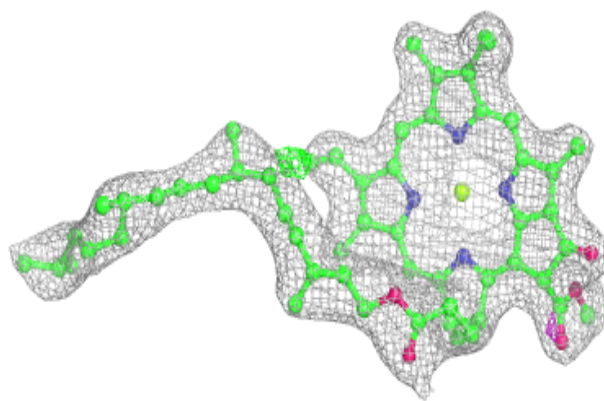
Electron density around CLA C 509:

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

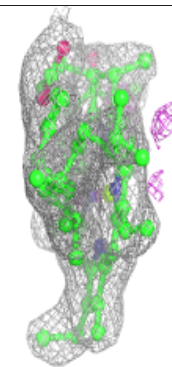
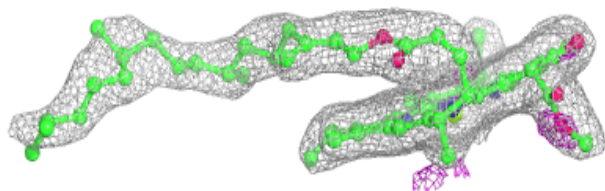
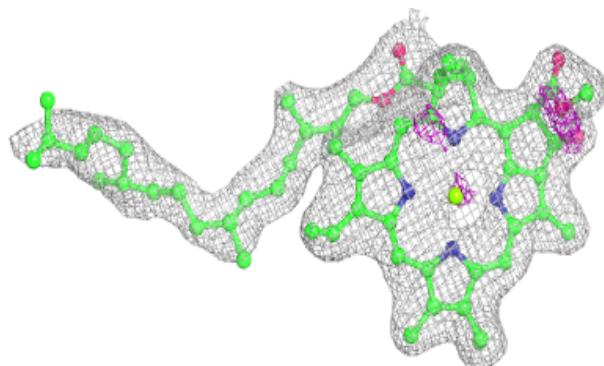


Electron density around CLA B 603:

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

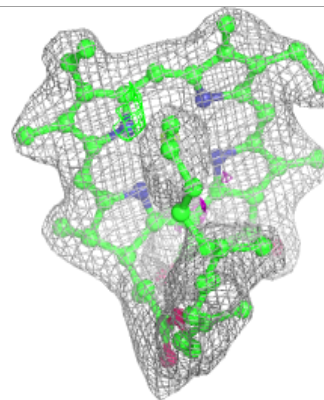
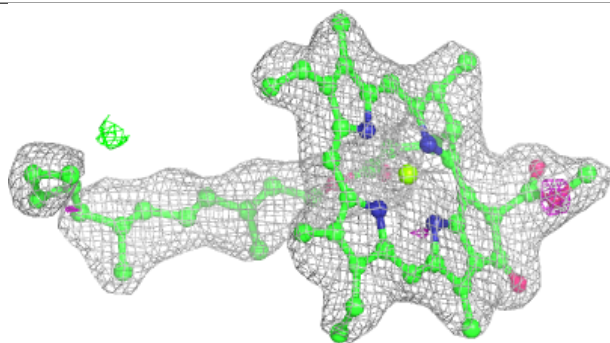
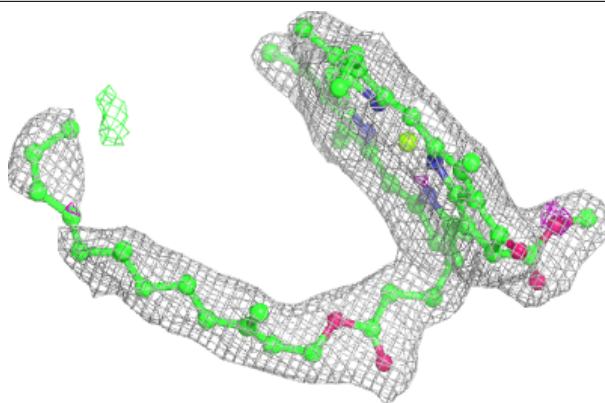
**Electron density around CLA b 603:**

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

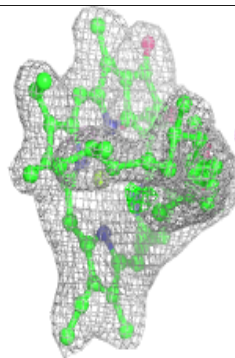
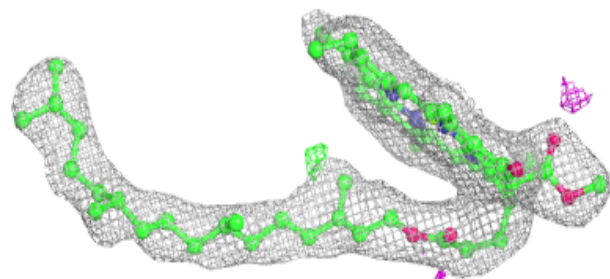
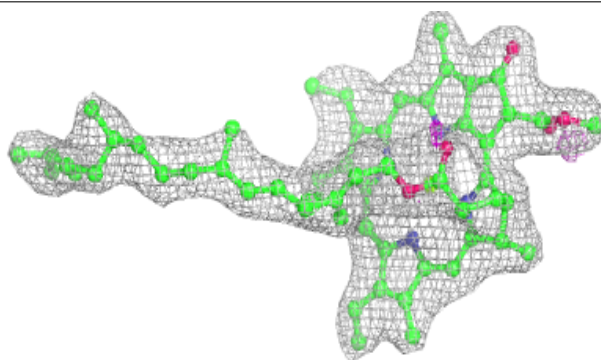


Electron density around CLA C 504:

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

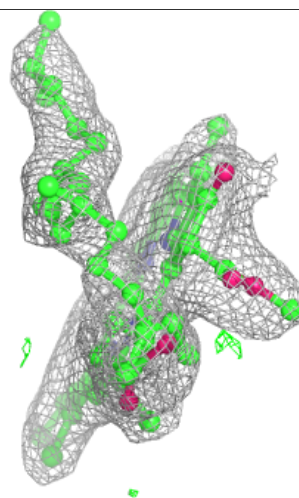
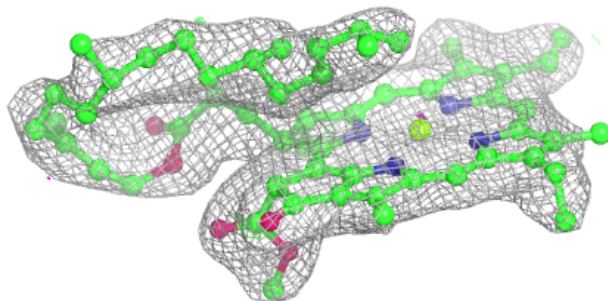
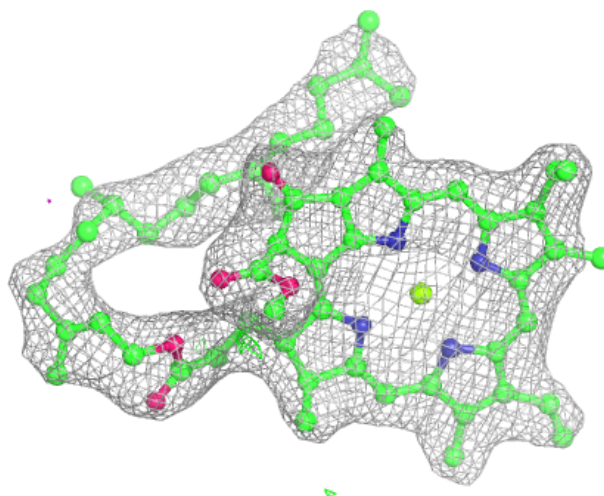
**Electron density around CLA b 608:**

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



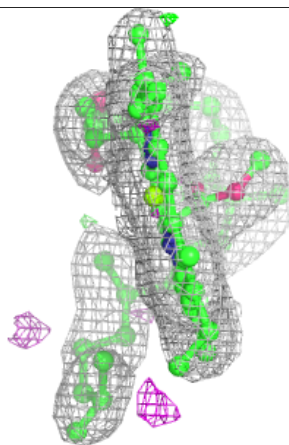
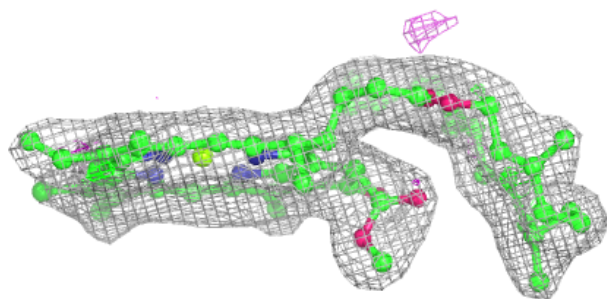
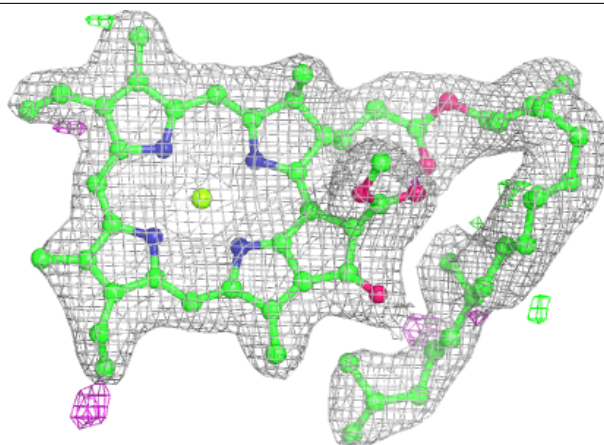
Electron density around CLA c 509:

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



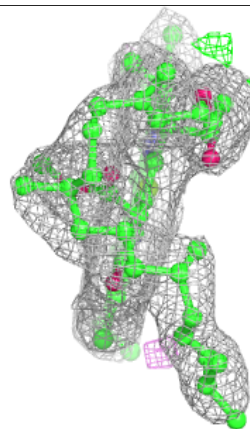
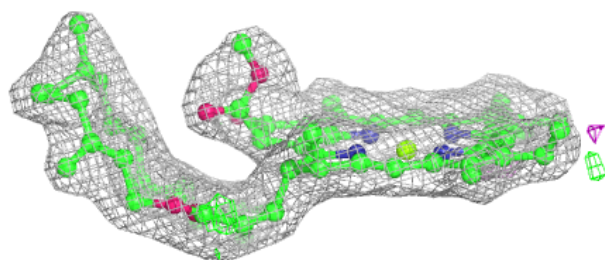
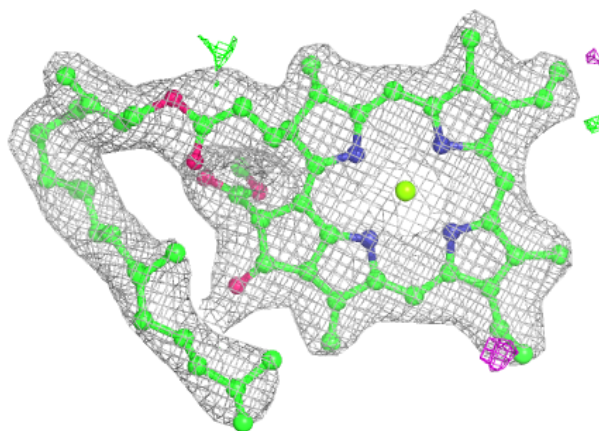
Electron density around CLA B 610:

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



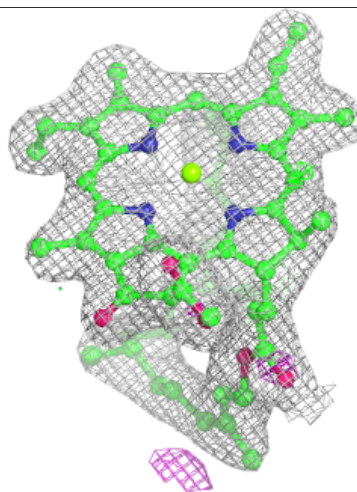
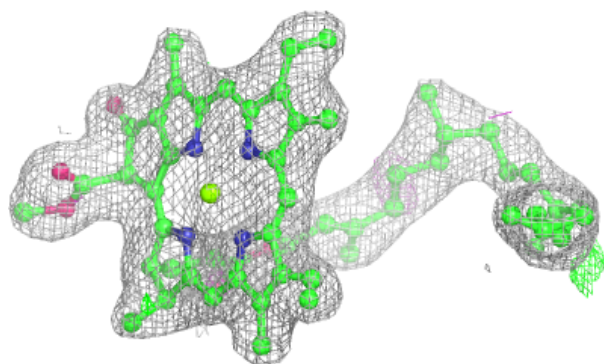
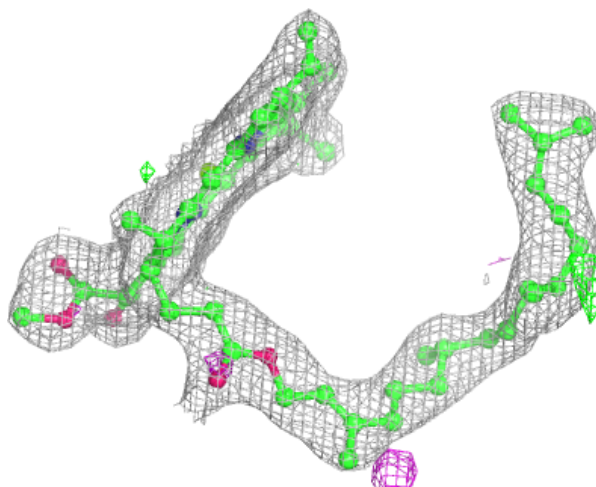
Electron density around CLA b 610:

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



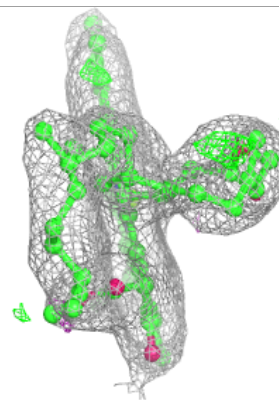
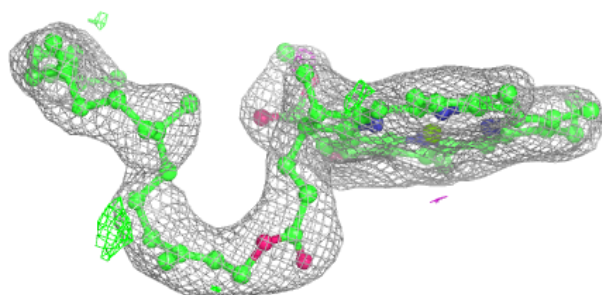
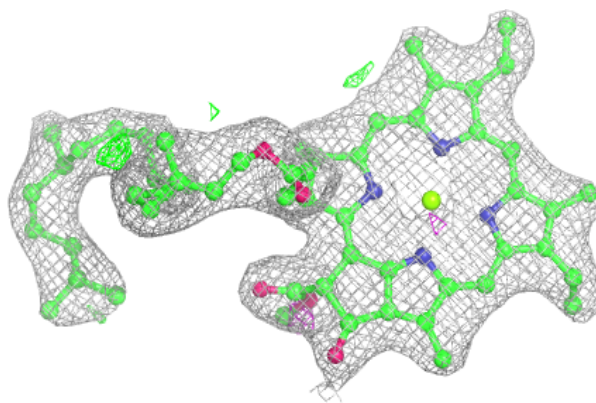
Electron density around CLA b 611:

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

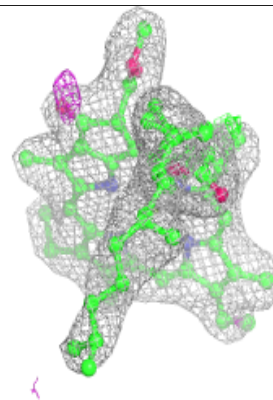
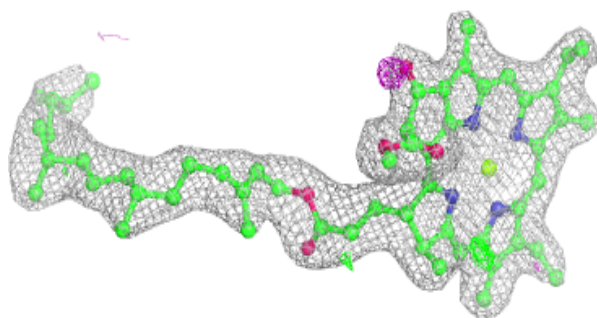
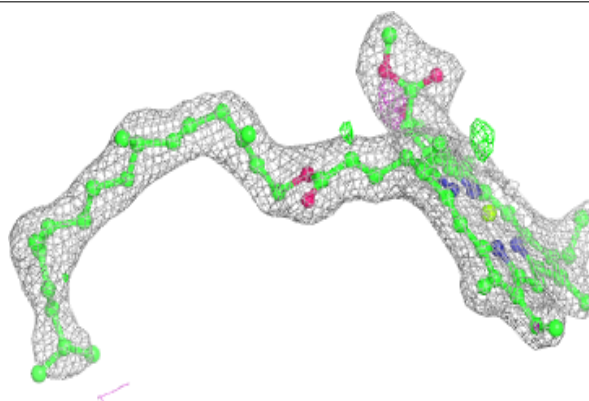


Electron density around CLA b 612:

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

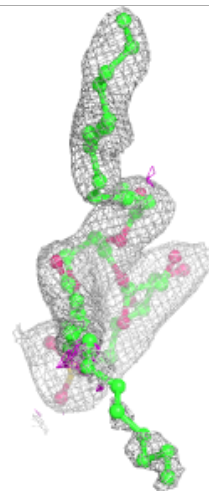
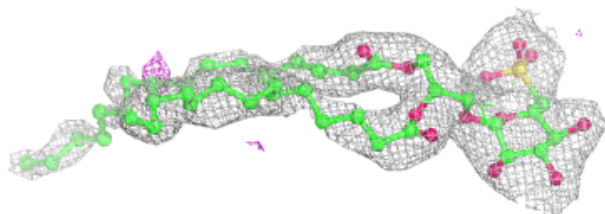
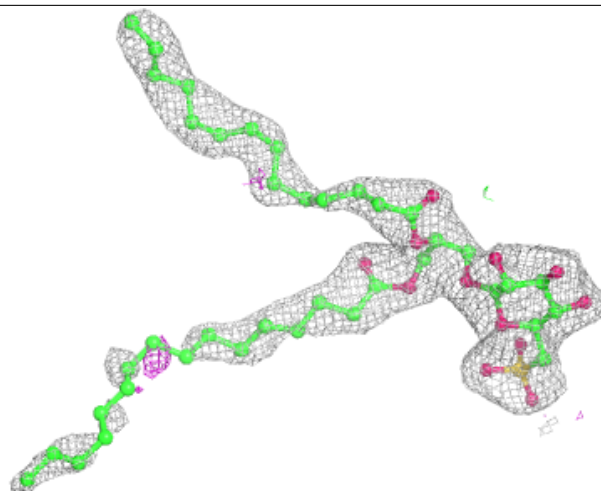
**Electron density around CLA d 403:**

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



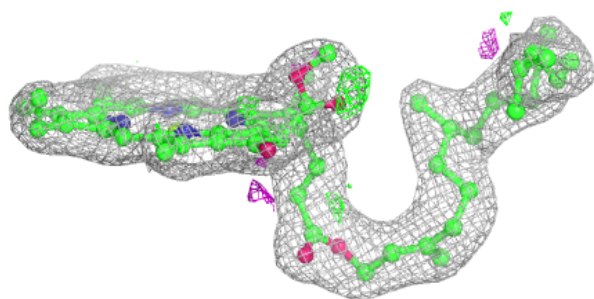
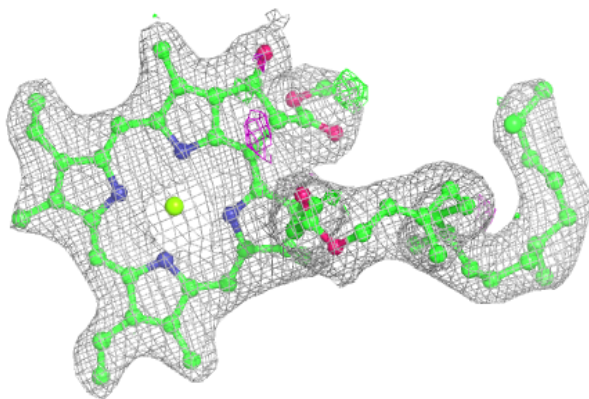
Electron density around SQD A 613:

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

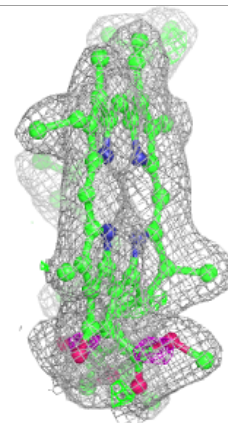
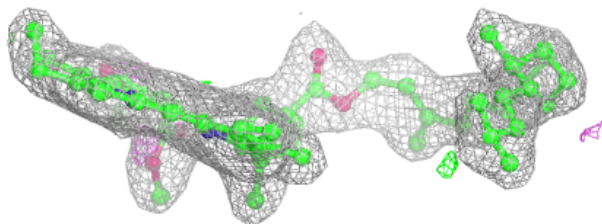
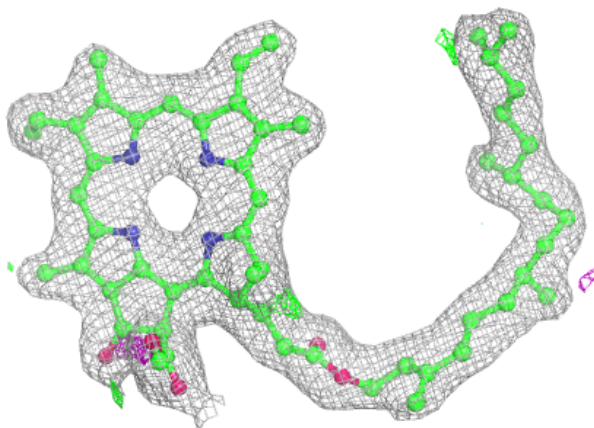


Electron density around CLA B 612:

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

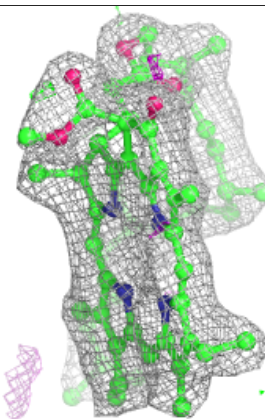
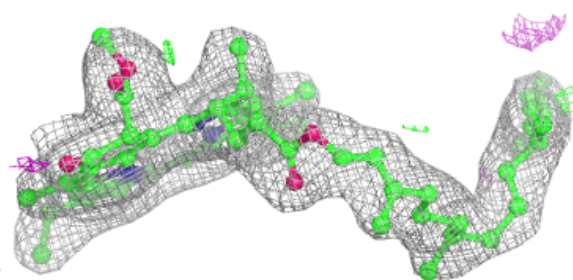
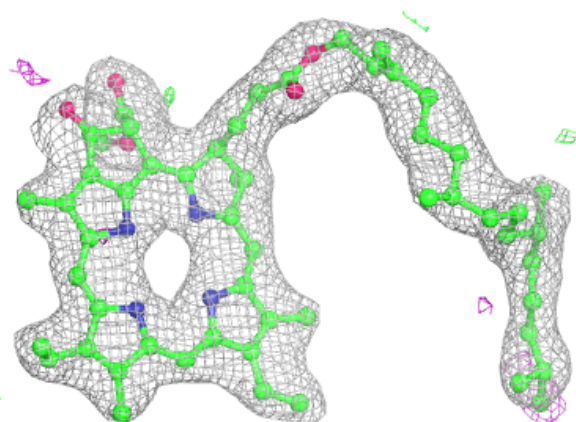
**Electron density around PHO a 608:**

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

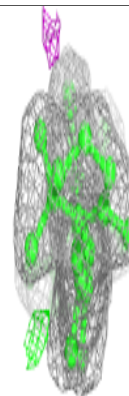
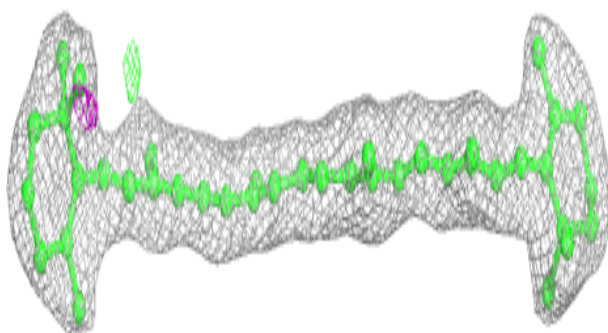
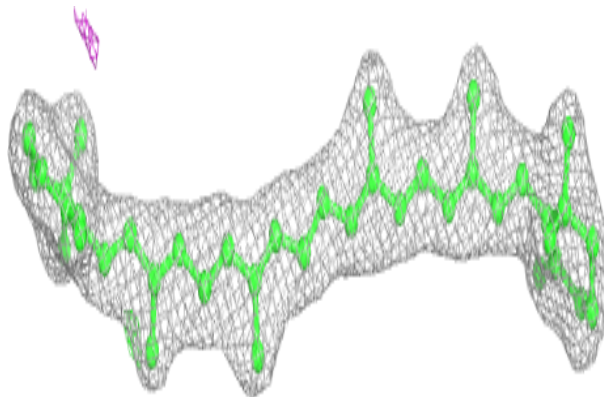


Electron density around PHO d 402:

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

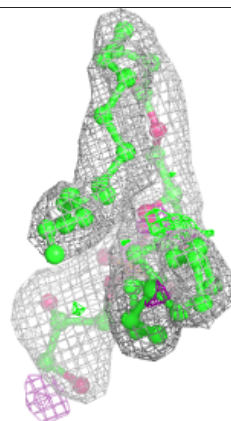
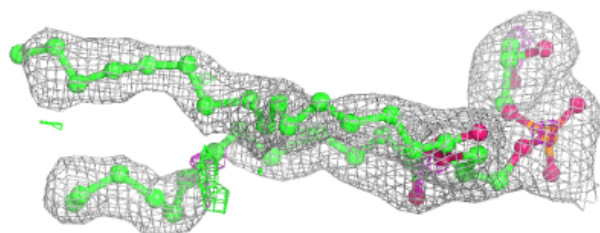
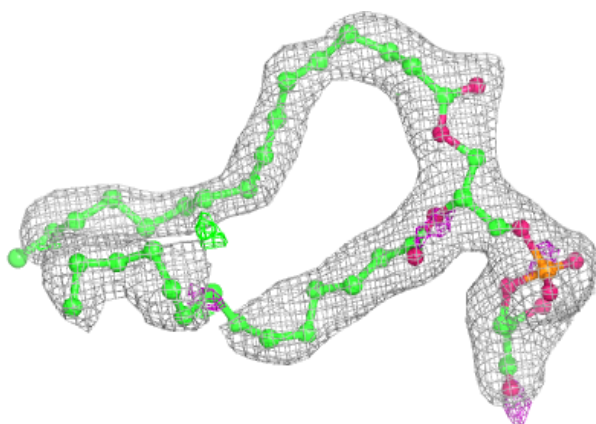
**Electron density around BCR A 610:**

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

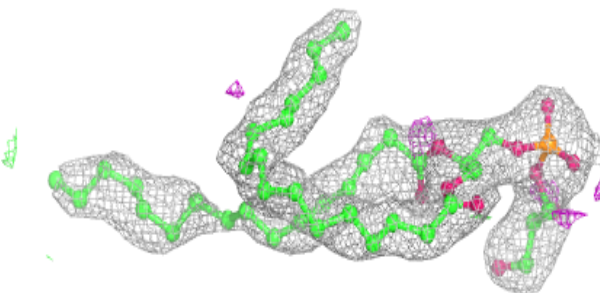
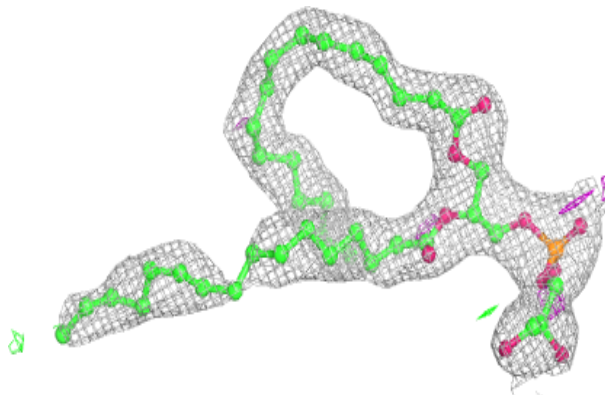


Electron density around LHG D 411:

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

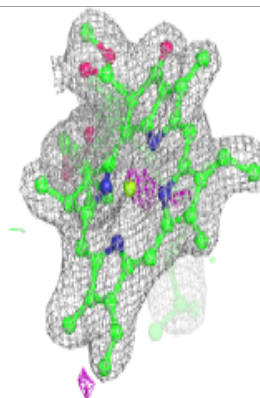
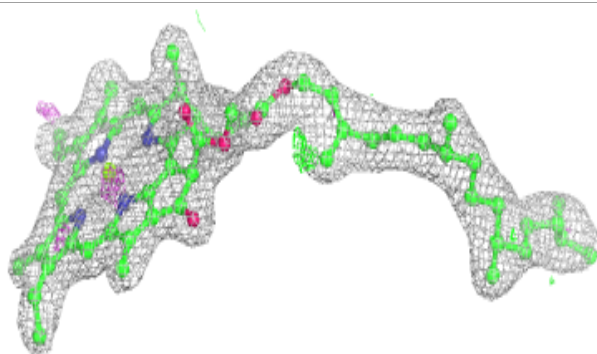
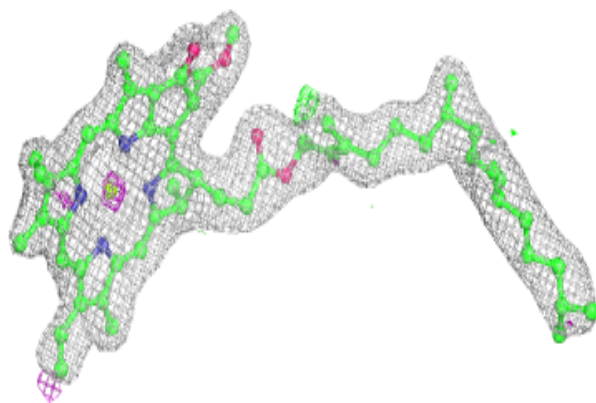
**Electron density around LHG D 413:**

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



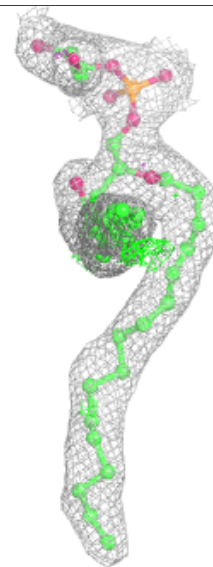
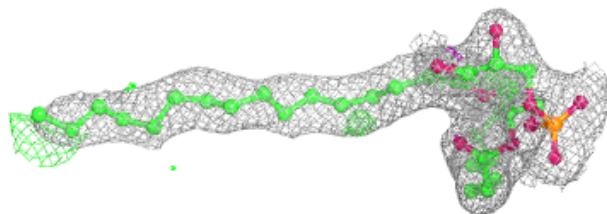
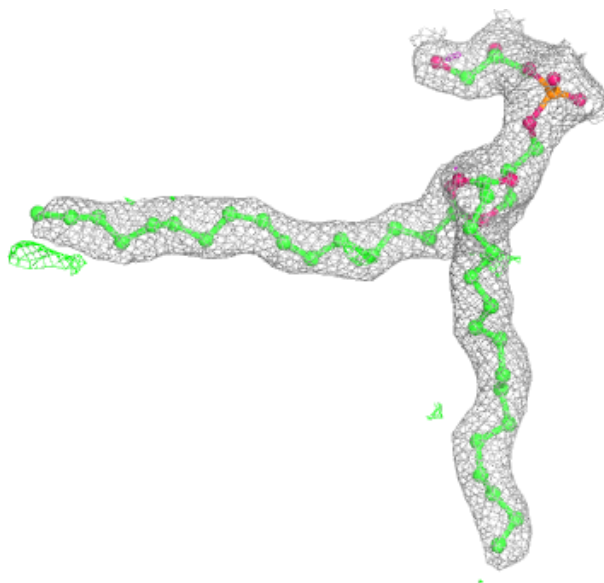
Electron density around CLA a 606:

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



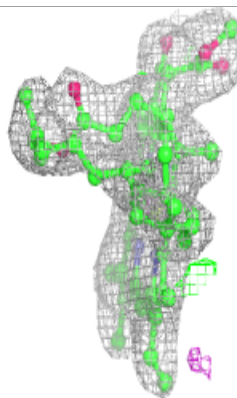
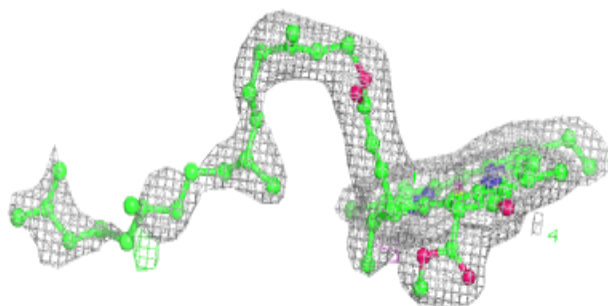
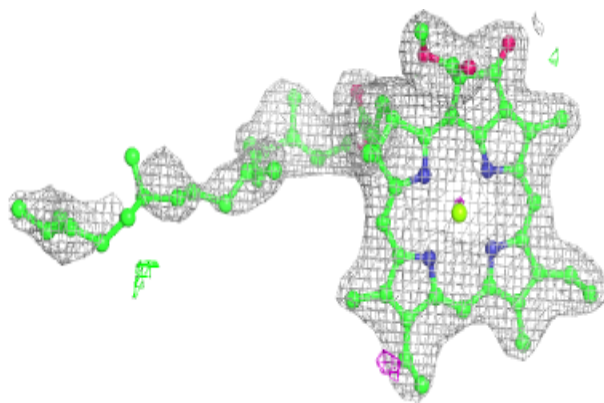
Electron density around LHG L 102:

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

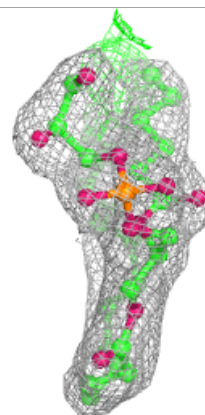
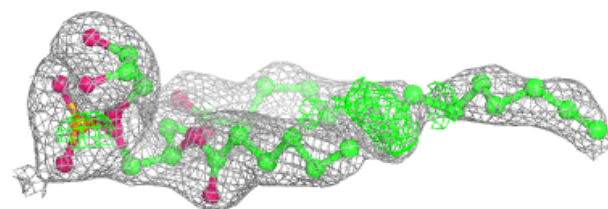
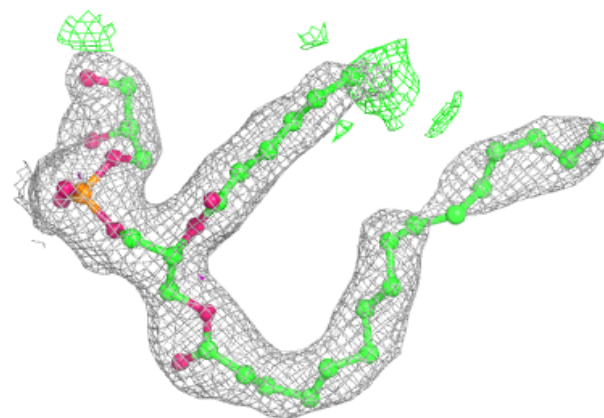


Electron density around CLA a 607:

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

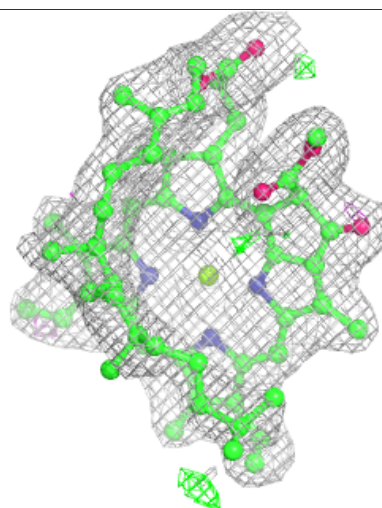
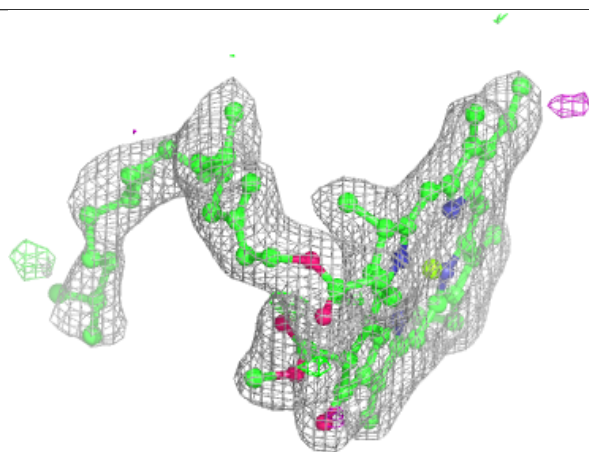
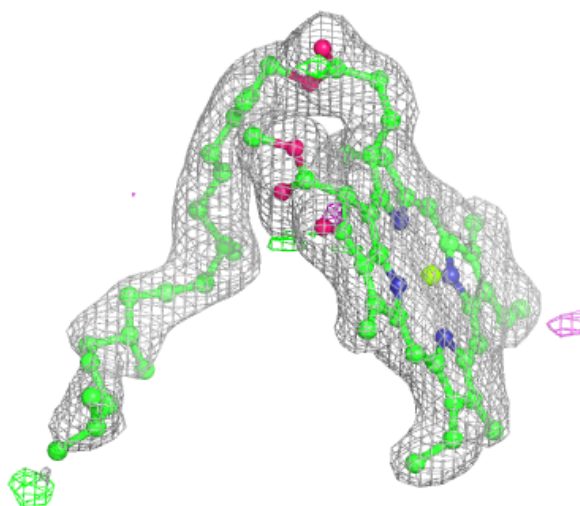
**Electron density around LHG d 409:**

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



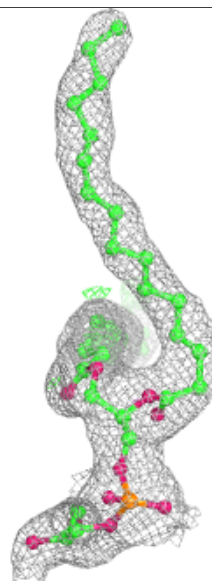
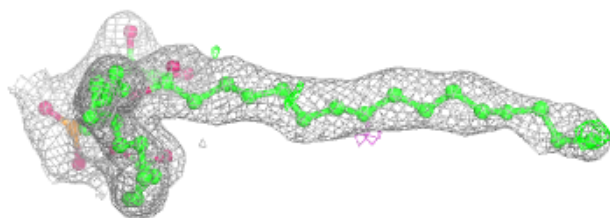
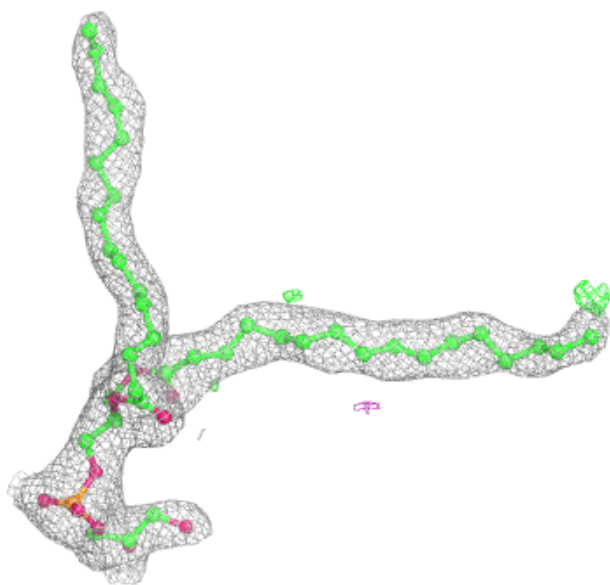
Electron density around CLA B 613:

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



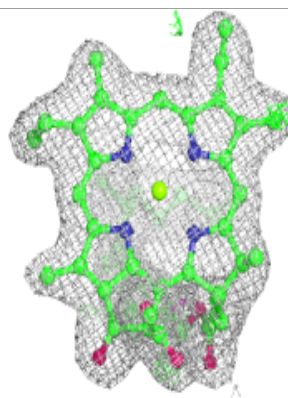
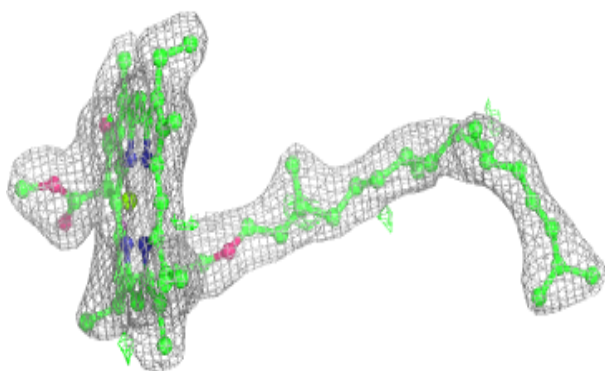
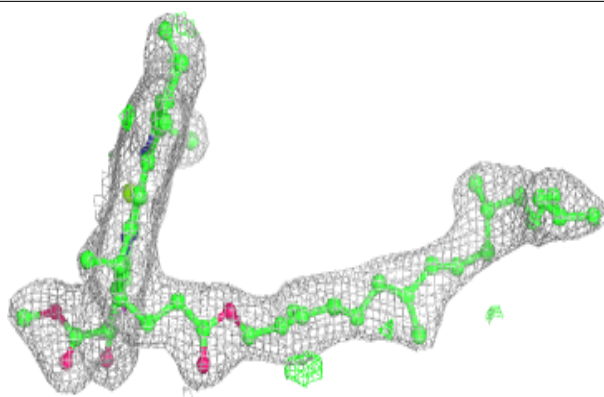
Electron density around LHG 1 101:

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

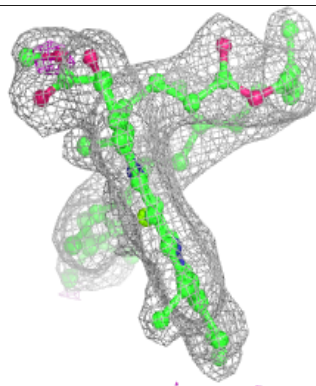
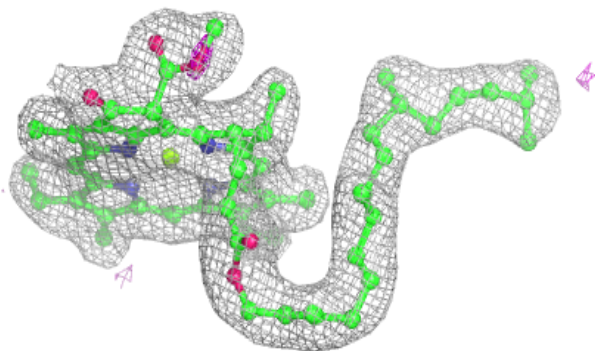
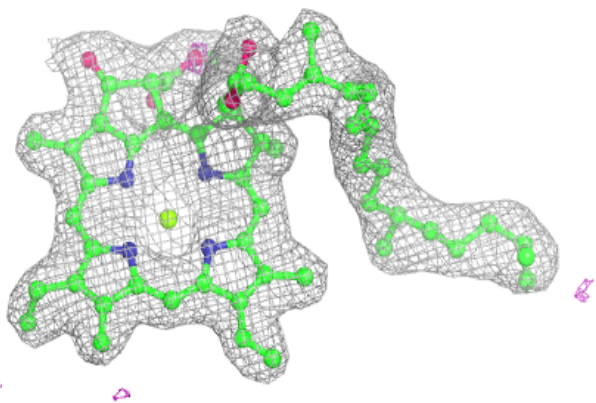


Electron density around CLA B 605:

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

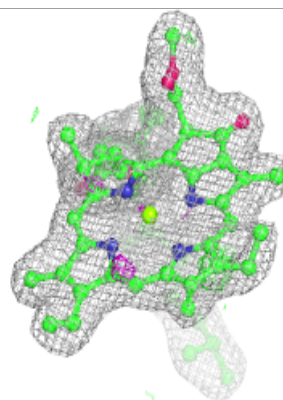
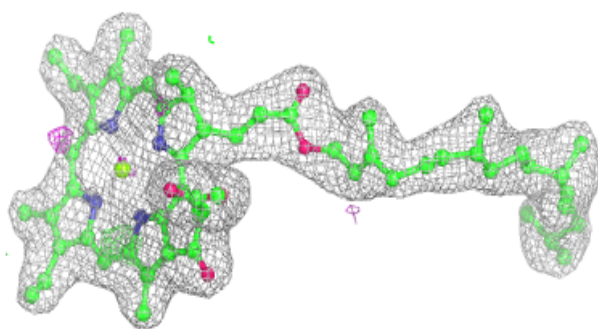
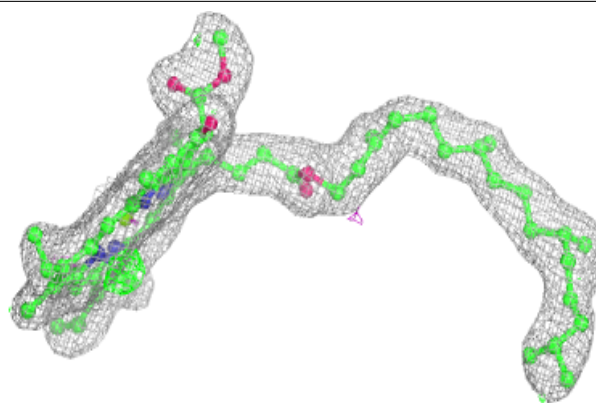
**Electron density around CLA D 403:**

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

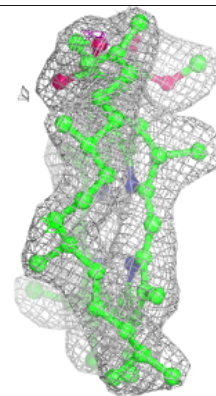
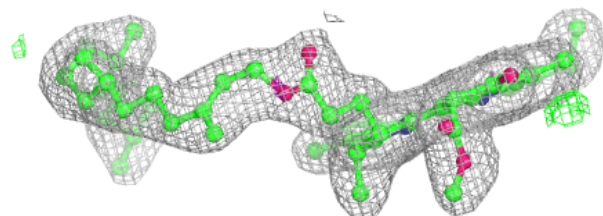
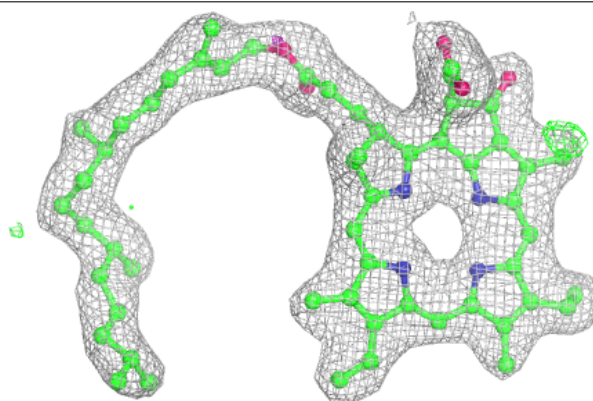


Electron density around CLA D 404:

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

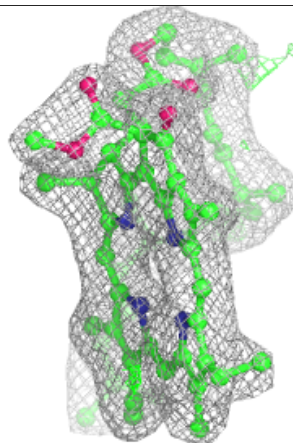
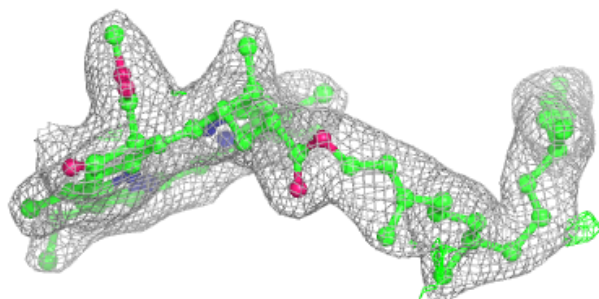
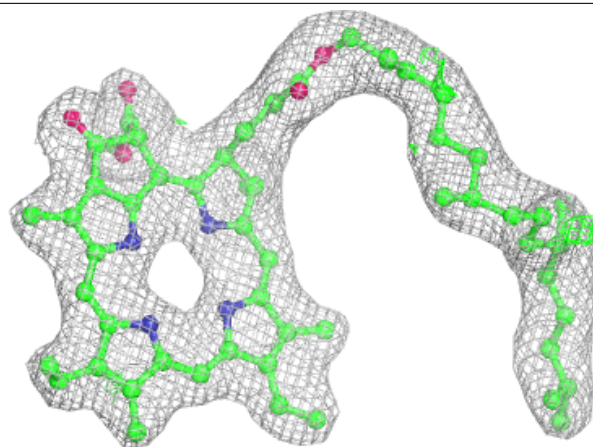
**Electron density around PHO A 608:**

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

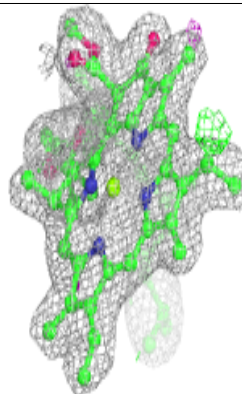
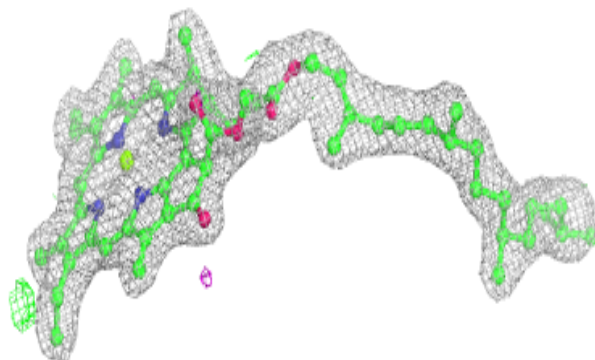
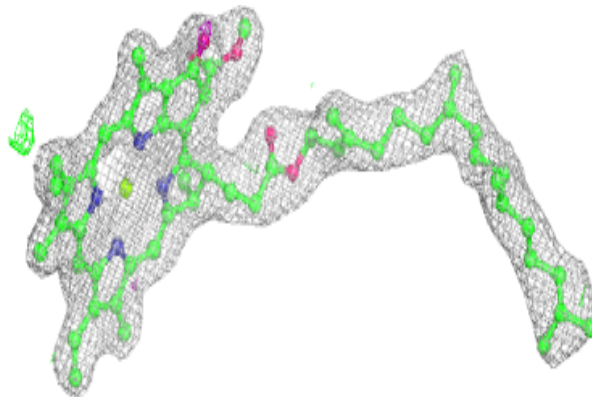


Electron density around PHO D 402:

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

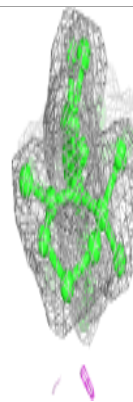
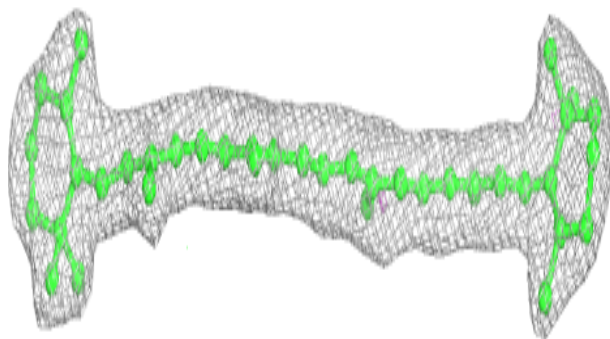
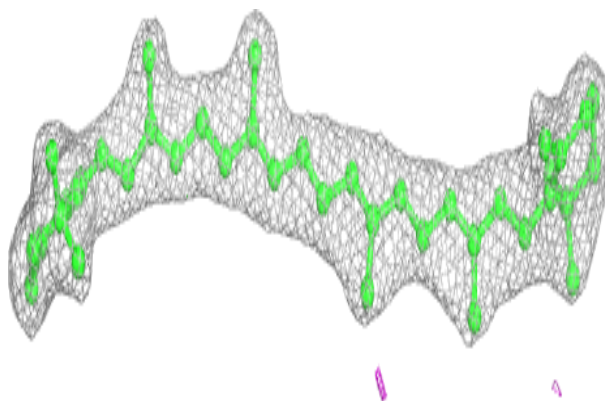
**Electron density around CLA A 606:**

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



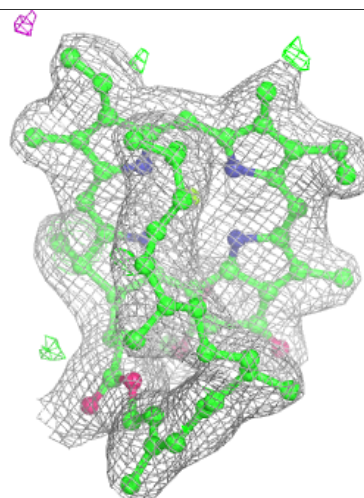
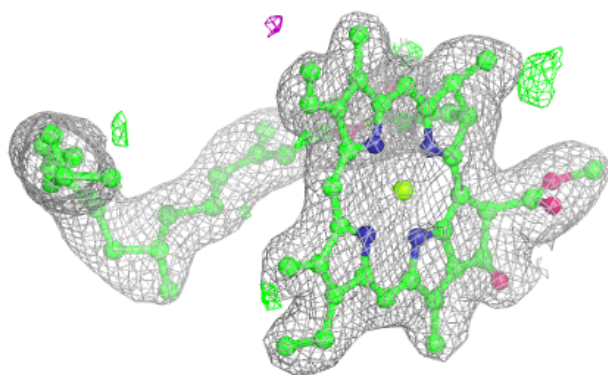
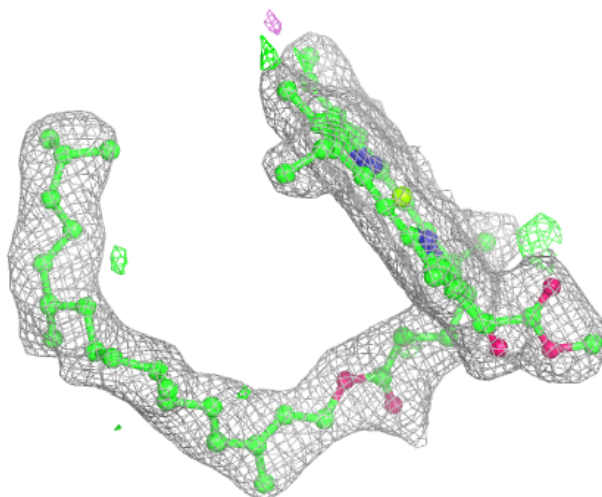
Electron density around BCR a 610:

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



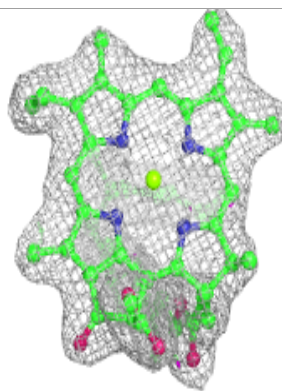
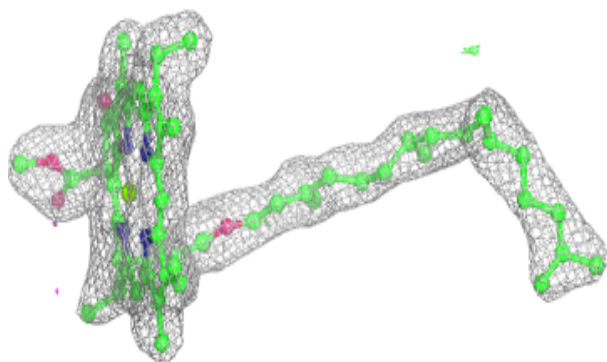
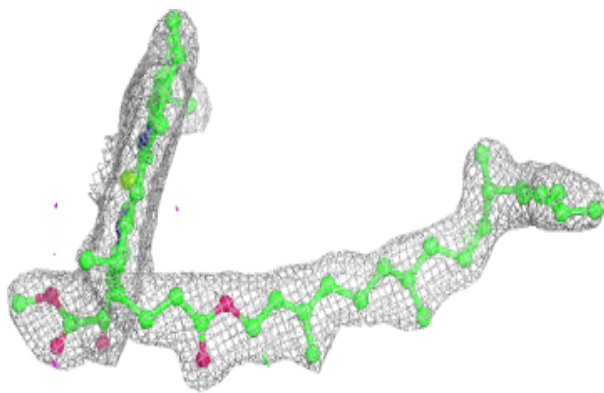
Electron density around CLA B 611:

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

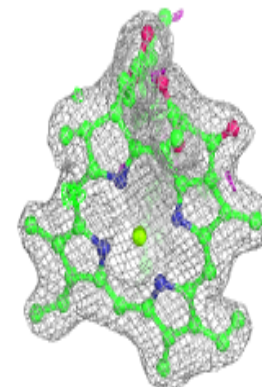
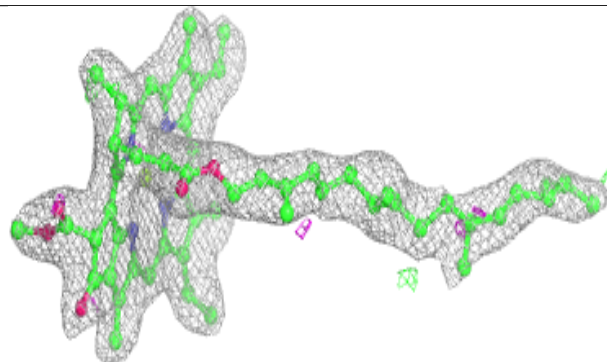
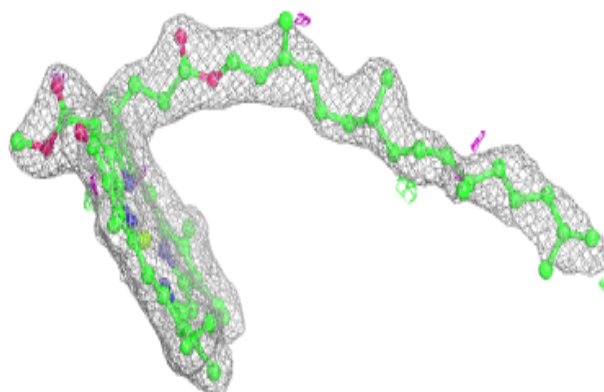


Electron density around CLA b 605:

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

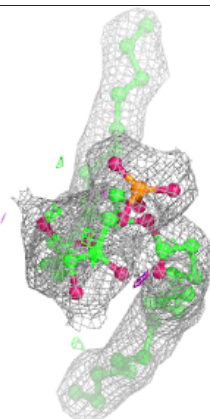
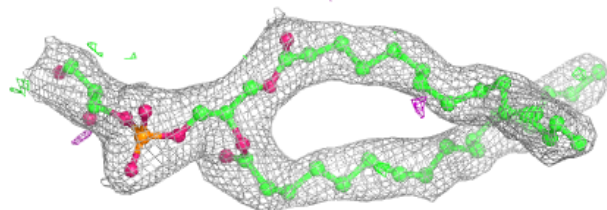
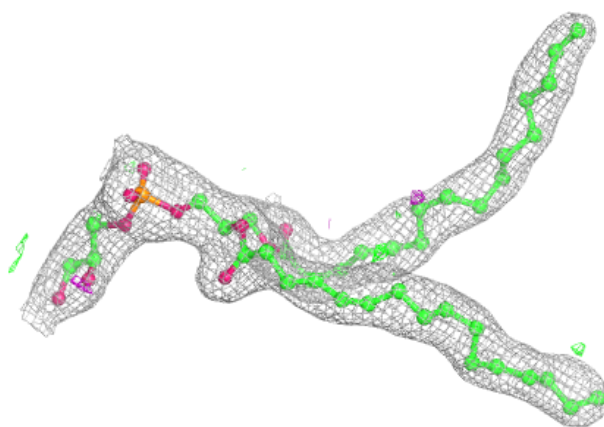
**Electron density around CLA B 607:**

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

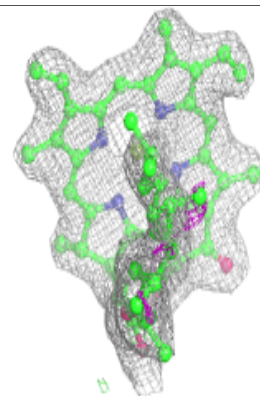
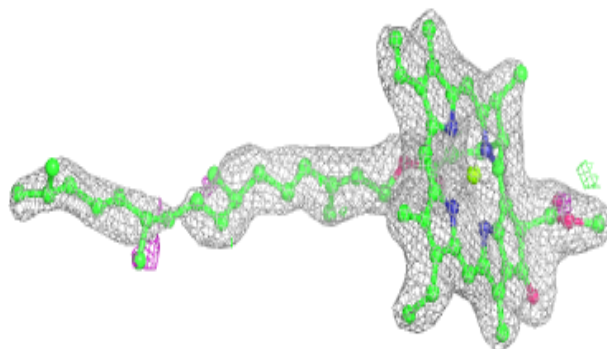
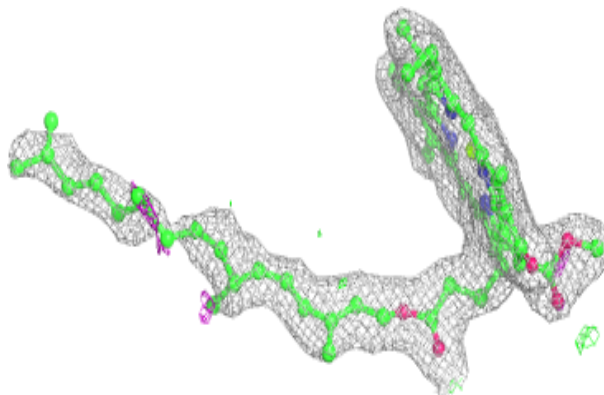


Electron density around LHG d 408:

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

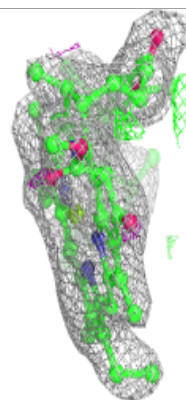
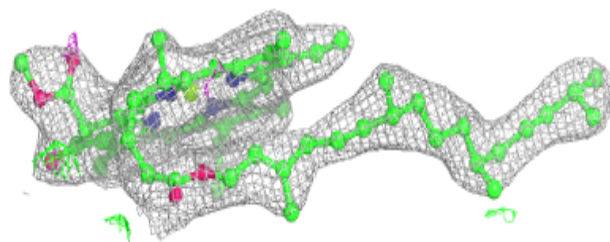
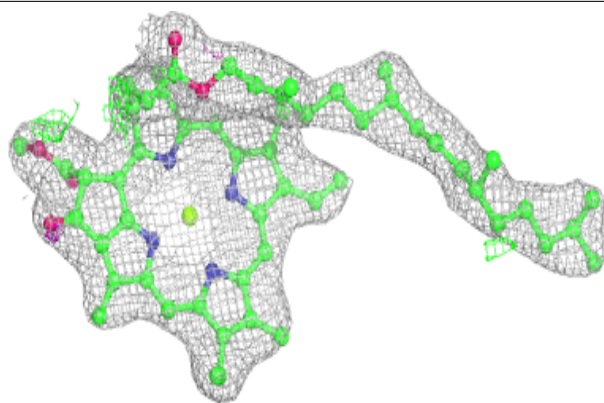
**Electron density around CLA b 607:**

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

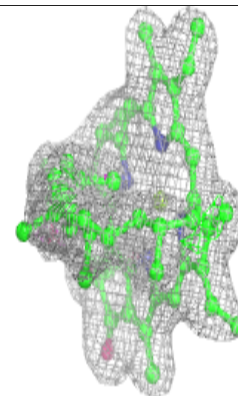
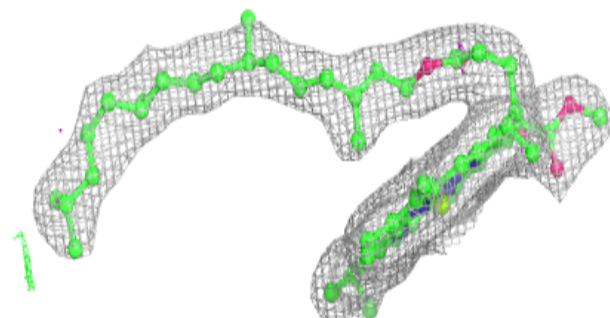
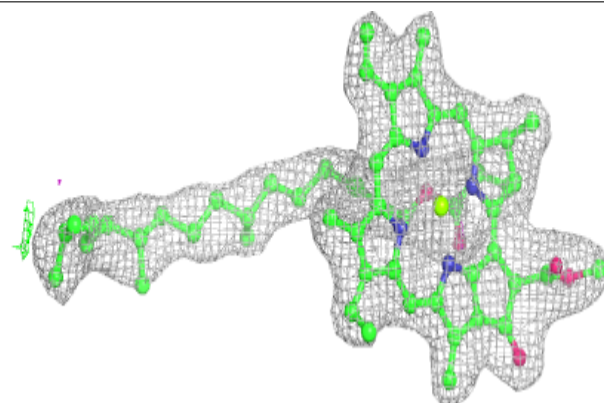


Electron density around CLA c 501:

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

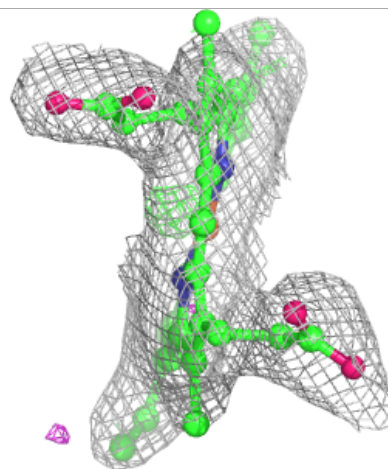
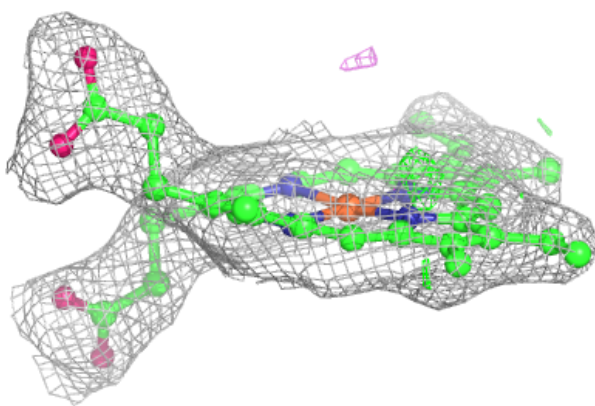
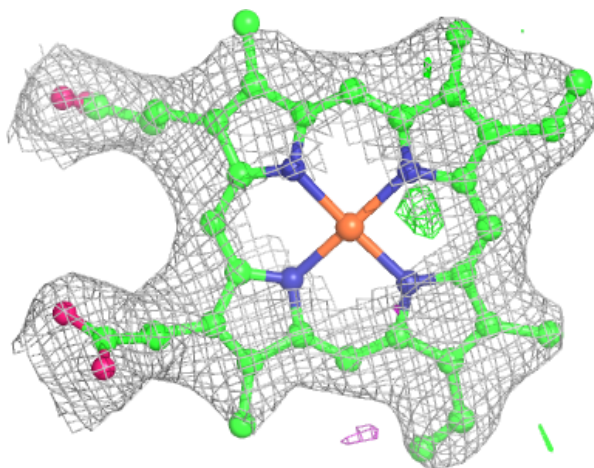
**Electron density around CLA B 608:**

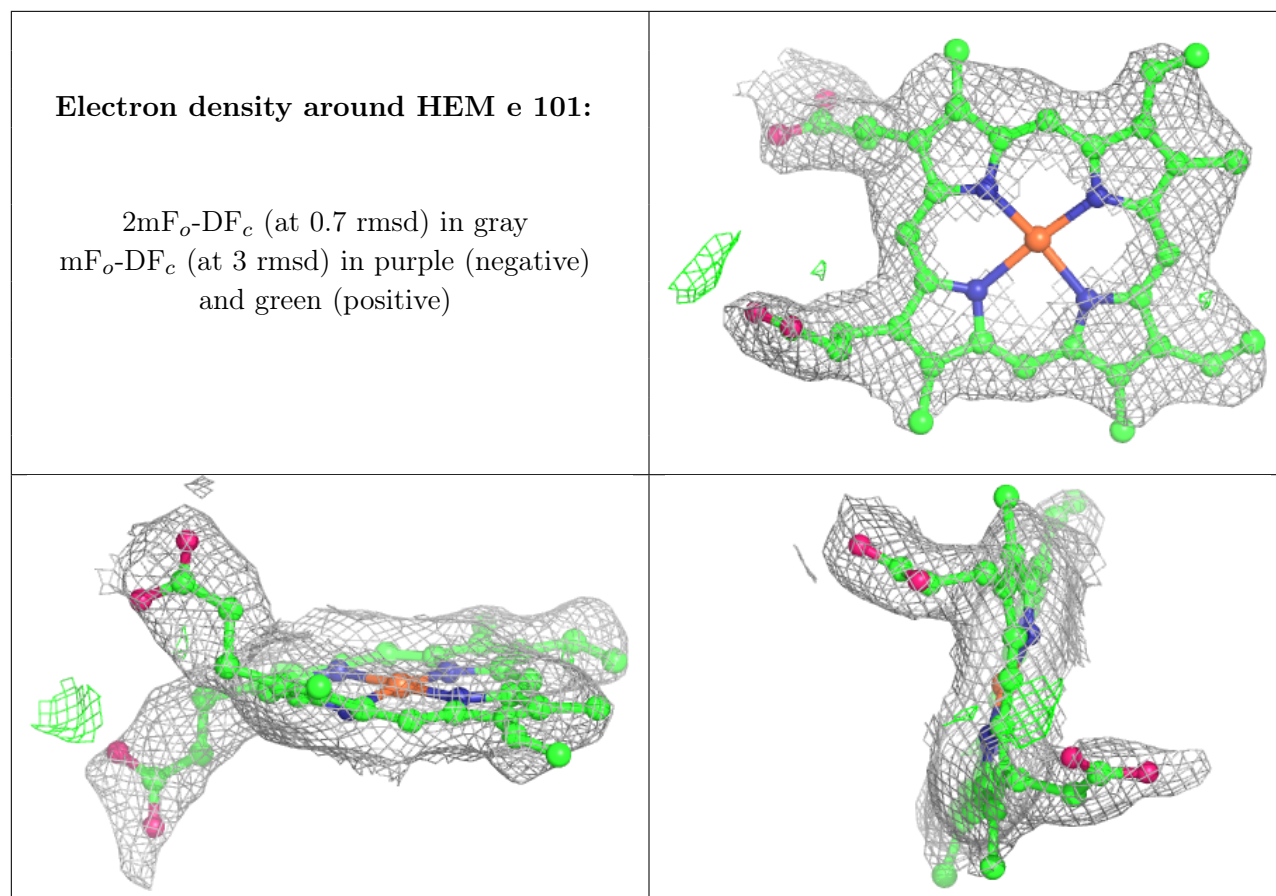
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

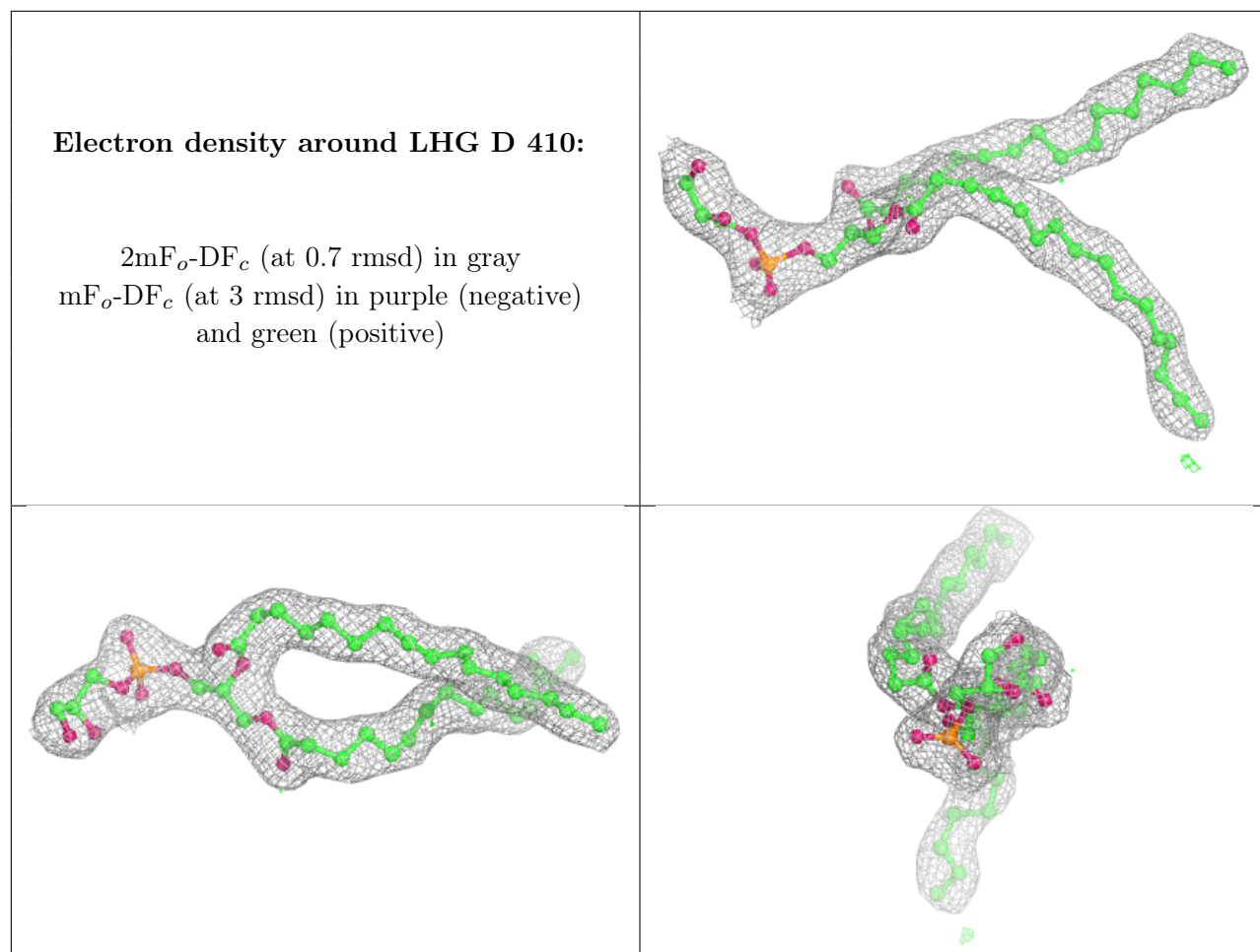


Electron density around HEM F 101:

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

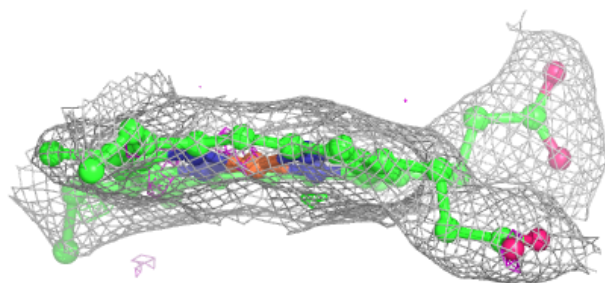
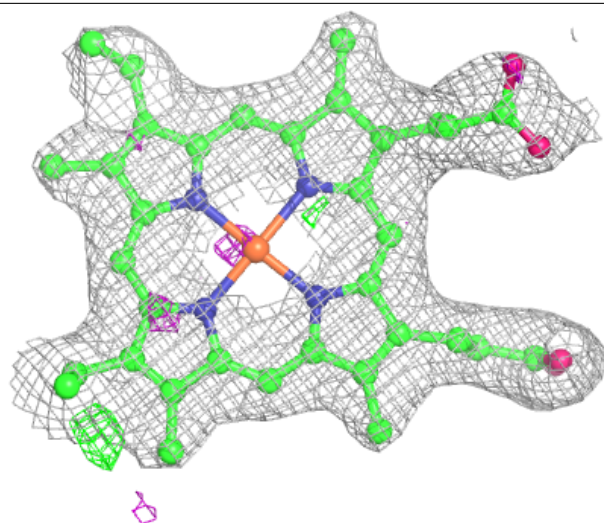






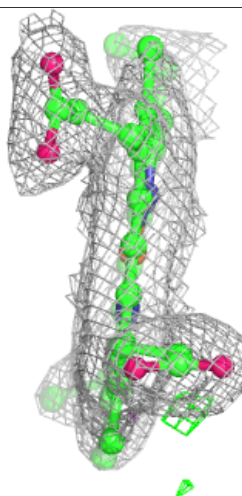
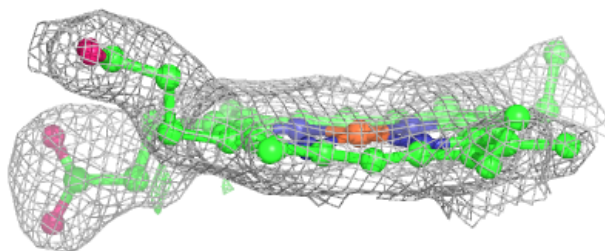
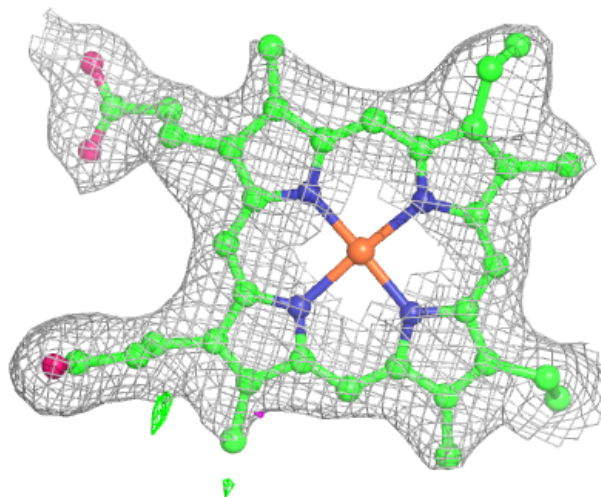
Electron density around HEC V 201:

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



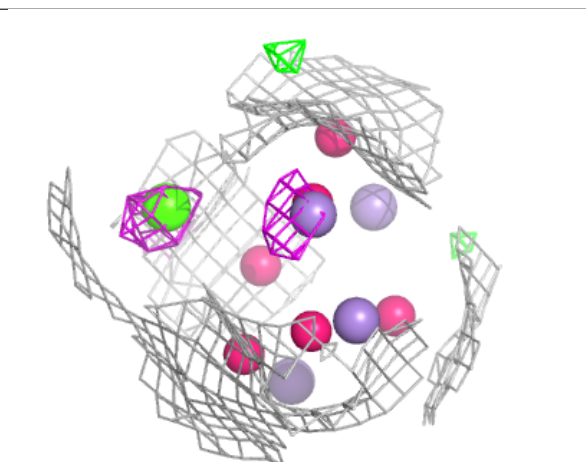
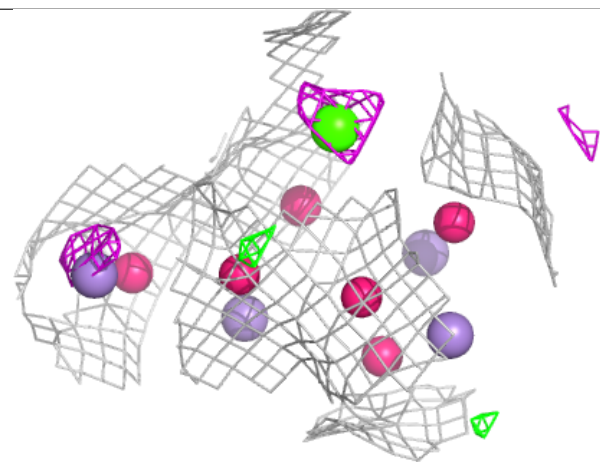
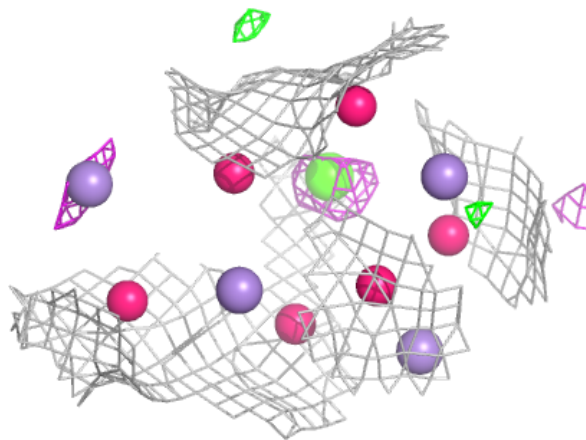
Electron density around HEC v 201:

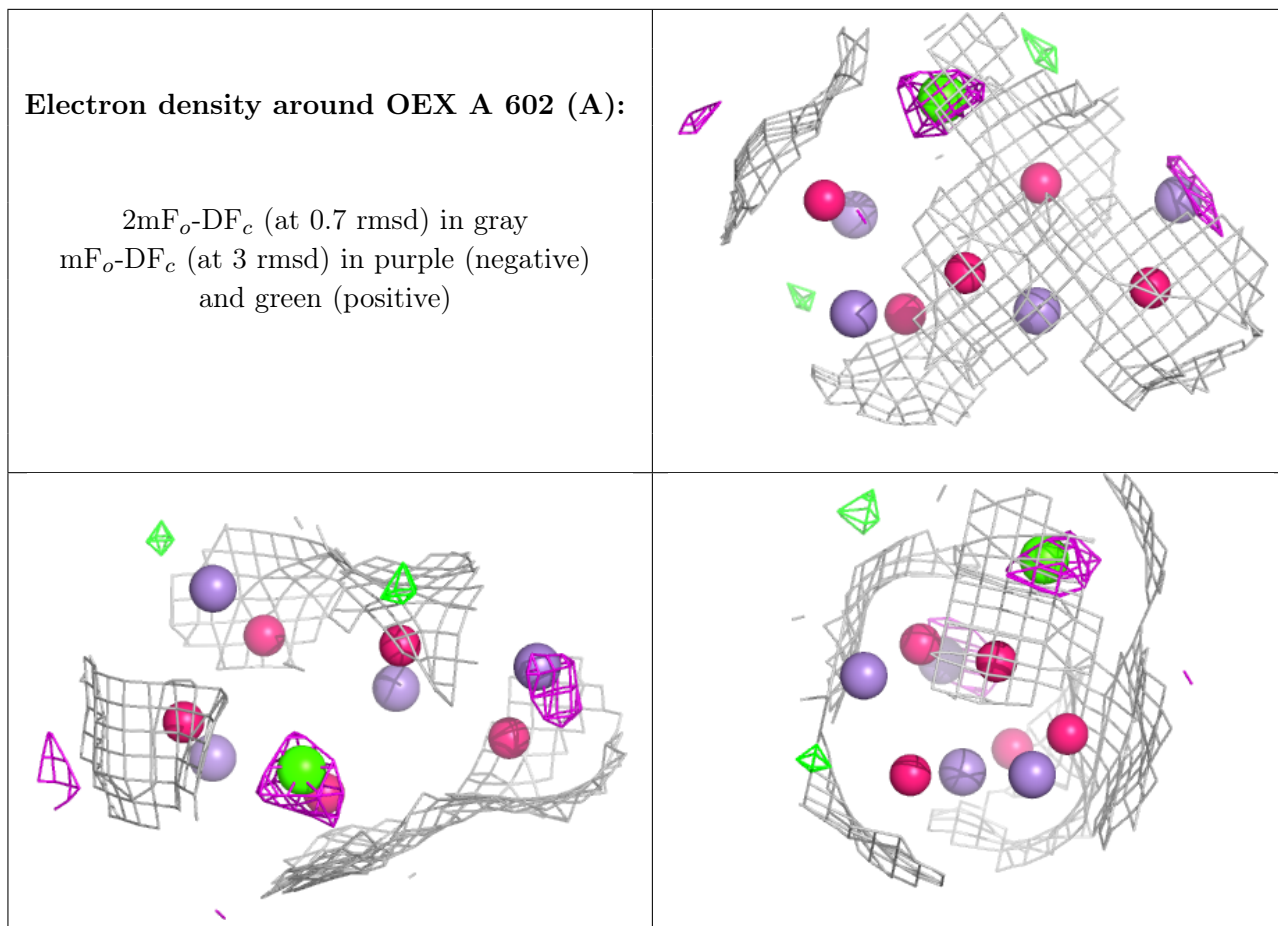
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEY A 601 (B):

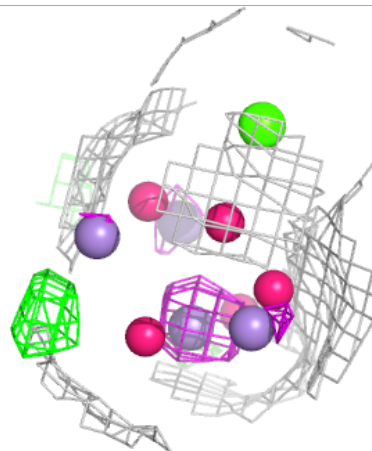
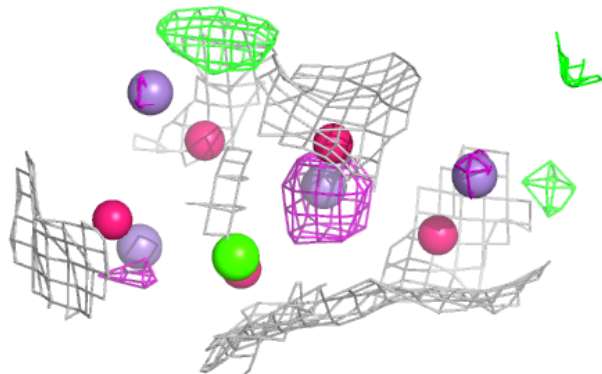
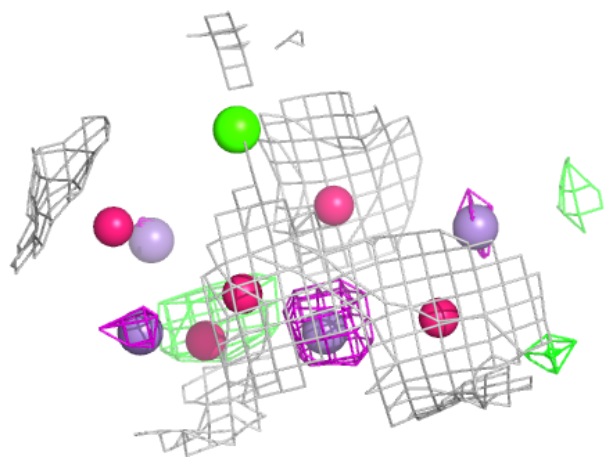
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

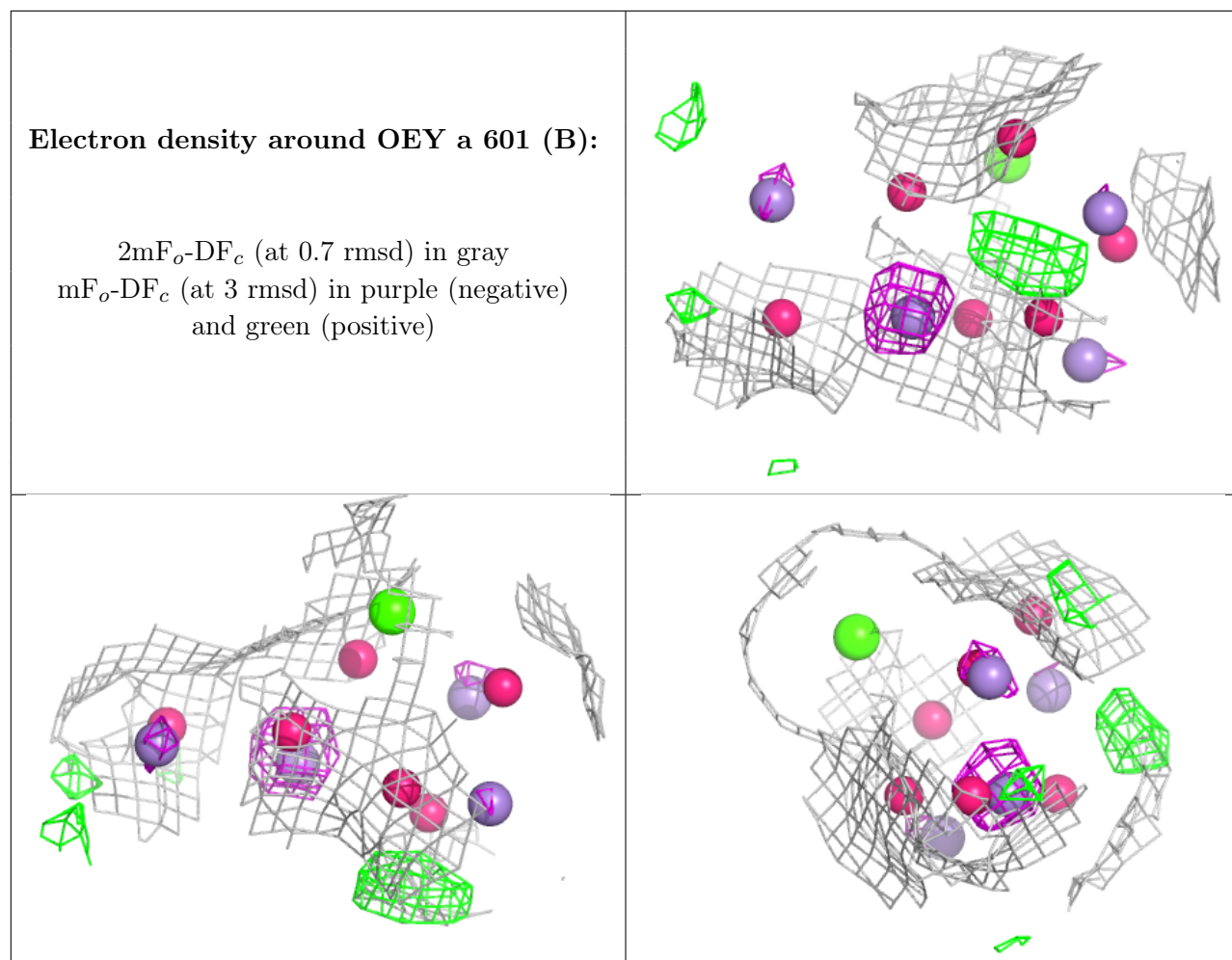




Electron density around OEX a 602 (A):

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





6.5 Other polymers [i](#)

There are no such residues in this entry.