



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:02 pm BST

PDB ID : 5Y5S
Title : Structure of photosynthetic LH1-RC super-complex at 1.9 angstrom resolution
Authors : Yu, L.-J.; Suga, M.; Wang-Otomo, Z.-Y.; Shen, J.-R.
Deposited on : 2017-08-09
Resolution : 1.90 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 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 : 2.11
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) : 2.11

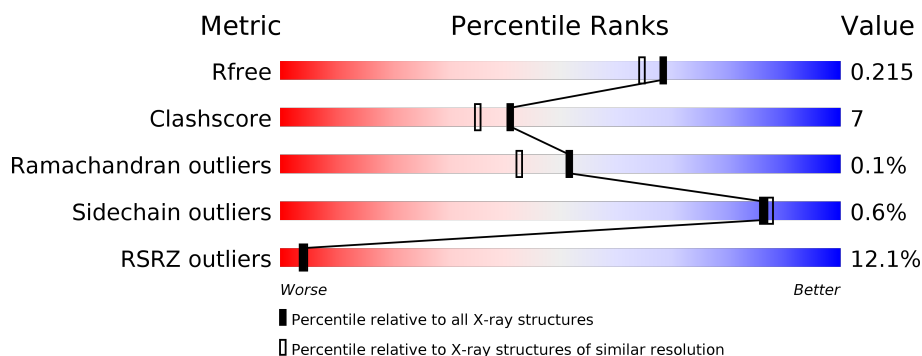
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	C	404	<div> <div>2%</div> <div>72% 5% 23%</div> </div>
2	L	281	<div> <div>7%</div> <div>92% 7%</div> </div>
3	M	325	<div> <div>3%</div> <div>90% 8% •</div> </div>
4	H	259	<div> <div>3%</div> <div>90% 8% •</div> </div>
5	1	61	<div> <div>18%</div> <div>79% 13% 8%</div> </div>
5	3	61	<div> <div>13%</div> <div>87% 5% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	
6	0	47	
6	2	47	
6	4	47	
6	6	47	
6	8	47	
6	B	47	
6	E	47	
6	G	47	
6	J	47	
6	N	47	
6	P	47	

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Mol	Chain	Length	Quality of chain
6	R	47	
6	T	47	
6	V	47	
6	X	47	
6	Z	47	

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
20	PEF	1	104	-	X	-	-
20	PEF	3	103	-	X	-	-
20	PEF	5	103	-	X	-	-
20	PEF	I	103	-	X	-	-
20	PEF	M	407	-	X	-	-
20	PEF	M	409	-	X	-	-
20	PEF	U	104	-	X	-	-
20	PEF	U	105	-	X	-	-
20	PEF	W	103	-	X	-	-

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 27981 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	311	Total	C	N	O	S	0	0	0
			2417	1524	424	453	16			

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	1	0
			2236	1505	359	361	11			

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	318	Total	C	N	O	S	0	2	0
			2555	1715	417	412	11			

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	255	Total	C	N	O	S	0	2	0
			1976	1272	337	361	6			

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	54	Total	C	N	O	S	0	0	0
			434	290	70	73	1			
5	D	55	Total	C	N	O	S	0	1	0
			445	296	72	76	1			
5	F	55	Total	C	N	O	S	0	1	0
			445	296	72	76	1			
5	I	57	Total	C	N	O	S	0	1	0
			460	305	74	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	O	56	Total	C	N	O	S	0	1	0
			455	303	73	76	3			
5	Q	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	S	56	Total	C	N	O	S	0	3	0
			468	312	74	79	3			
5	U	58	Total	C	N	O	S	0	0	0
			466	309	76	79	2			
5	W	56	Total	C	N	O	S	0	0	0
			451	300	74	76	1			
5	Y	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	1	56	Total	C	N	O	S	0	0	0
			450	299	73	76	2			
5	3	56	Total	C	N	O	S	0	1	0
			455	303	73	76	3			
5	5	54	Total	C	N	O	S	0	0	0
			434	290	70	73	1			
5	7	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	9	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	E	38	Total	C	N	O	S	0	0	0
			326	222	50	52	2			
6	G	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	J	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	N	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	P	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	R	41	Total	C	N	O	S	0	0	0
			345	234	53	56	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	43	Total 360	C 243	N 56	O 59	S 2	0	0	0
6	V	42	Total 351	C 237	N 54	O 58	S 2	0	0	0
6	X	41	Total 345	C 234	N 53	O 56	S 2	0	0	0
6	Z	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	2	41	Total 345	C 234	N 53	O 56	S 2	0	0	0
6	4	42	Total 351	C 237	N 54	O 58	S 2	0	0	0
6	6	42	Total 351	C 237	N 54	O 58	S 2	0	0	0
6	8	41	Total 345	C 234	N 53	O 56	S 2	0	0	0
6	0	43	Total 360	C 243	N 56	O 59	S 2	0	0	0

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- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and a central hydrogen atom (H). The atoms are labeled with their respective symbols and indices, such as O1A, O2A, O1D, O2D, CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, CMB, CAB, CBB, CMC, C2C, C3C, C4C, C1C, C1A, C2A, C3D, C4D, C1D, C2D, C3E, C4E, C1E, C2E, C3F, C4F, C1F, C2F, C3G, C4G, C1G, C2G, C3H, C4H, C1H, C2H, C3I, C4I, C1I, C2I, C3J, C4J, C1J, C2J, C3K, C4K, C1K, C2K, C3L, C4L, C1L, C2L, C3M, C4M, C1M, C2M, C3N, C4N, C1N, C2N, C3O, C4O, C1O, C2O, C3P, C4P, C1P, C2P, C3Q, C4Q, C1Q, C2Q, C3R, C4R, C1R, C2R, C3S, C4S, C1S, C2S, C3T, C4T, C1T, C2T, C3U, C4U, C1U, C2U, C3V, C4V, C1V, C2V, C3W, C4W, C1W, C2W, C3X, C4X, C1X, C2X, C3Y, C4Y, C1Y, C2Y, C3Z, C4Z, C1Z, C2Z, C3AA, C4AA, C1AA, C2AA, C3AB, C4AB, C1AB, C2AB, C3AC, C4AC, C1AC, C2AC, C3AD, C4AD, C1AD, C2AD, C3AE, C4AE, C1AE, C2AE, C3AF, C4AF, C1AF, C2AF, C3AG, C4AG, C1AG, C2AG, C3AH, C4AH, C1AH, C2AH, C3AI, C4AI, C1AI, C2AI, C3AJ, C4AJ, C1AJ, C2AJ, C3AK, C4AK, C1AK, C2AK, C3AL, C4AL, C1AL, C2AL, C3AM, C4AM, C1AM, C2AM, C3AN, C4AN, C1AN, C2AN, C3AO, C4AO, 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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



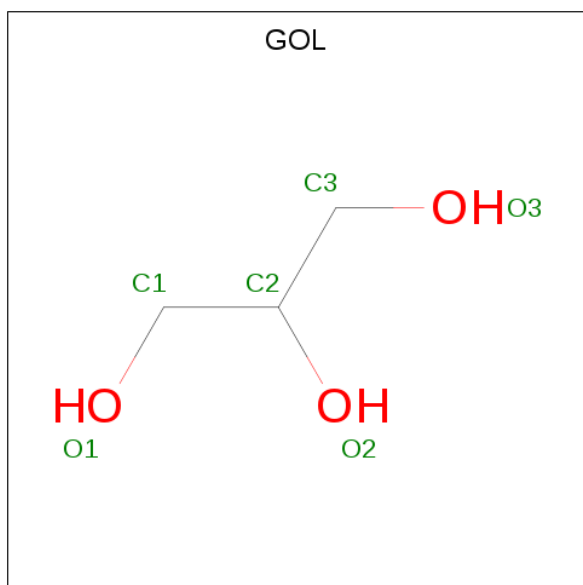
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

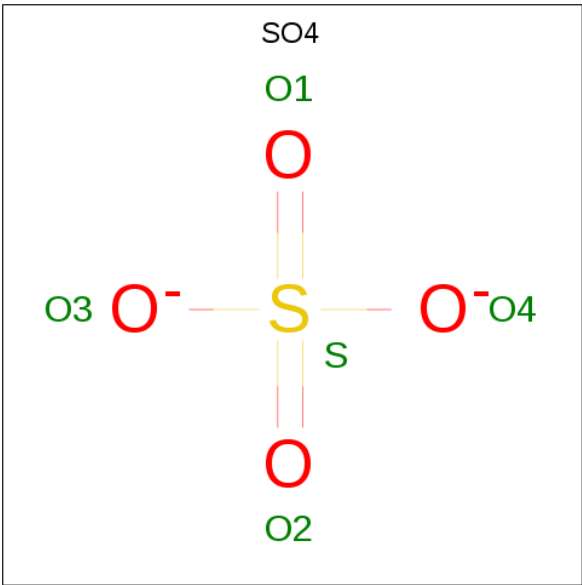
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg		
			1	1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



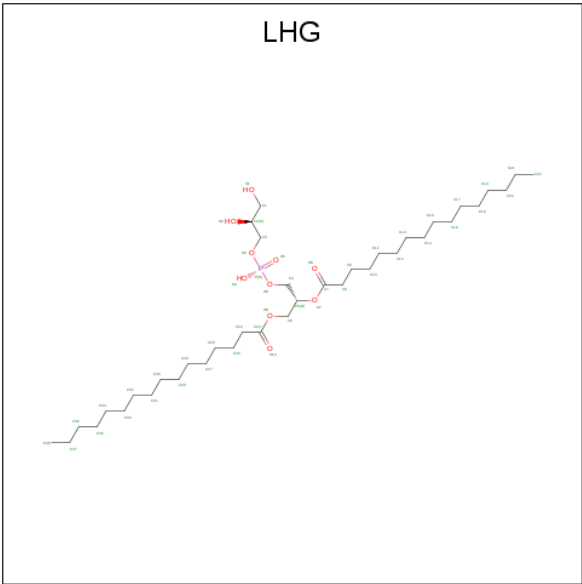
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O		
			6	3	3	0	0
9	H	1	Total	C	O		
			6	3	3	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



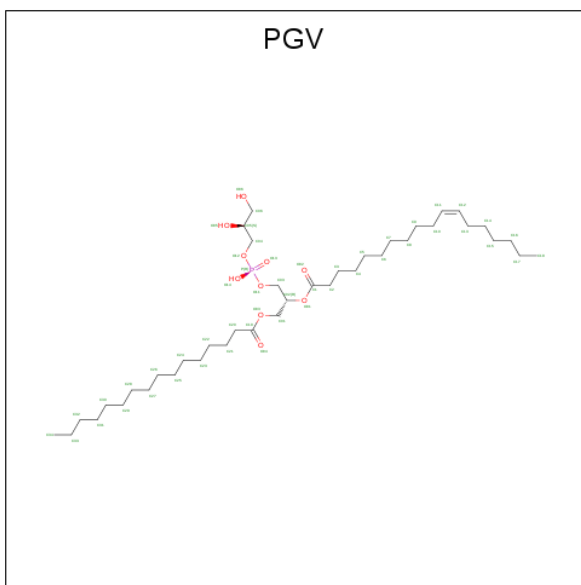
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	L	1	Total	O	S	0	0
			5	4	1		
10	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



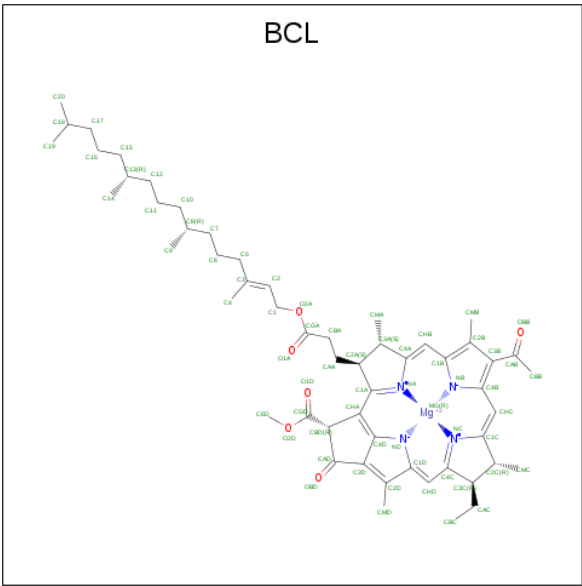
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			9	8	1		

- Molecule 12 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O		0	0
			21	17	4			
12	L	1	Total	C	O	P	0	0
			43	32	10	1		
12	L	1	Total	C	O	P	0	0
			44	33	10	1		
12	M	1	Total	C	O	P	0	0
			46	37	8	1		
12	M	1	Total	C	O	P	0	0
			37	26	10	1		
12	H	1	Total	C	O	P	0	0
			36	25	10	1		
12	A	1	Total	C	O	P	0	0
			33	22	10	1		
12	D	1	Total	C	O	P	0	0
			35	24	10	1		
12	1	1	Total	C	O	P	0	0
			31	20	10	1		
12	3	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 13 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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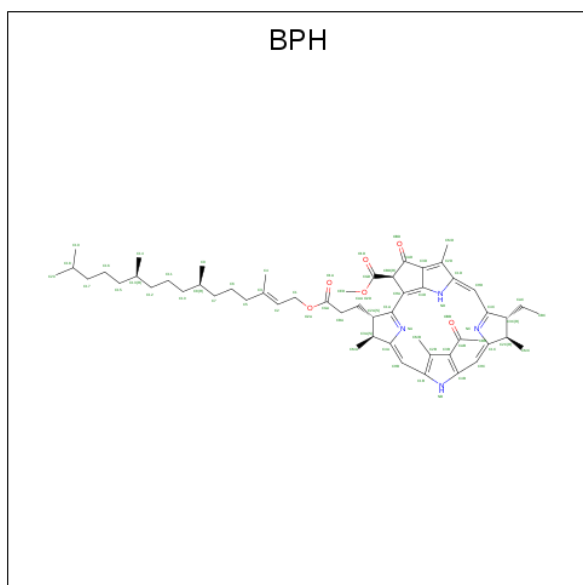
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	U	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	U	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	W	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	W	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	7	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
13	7	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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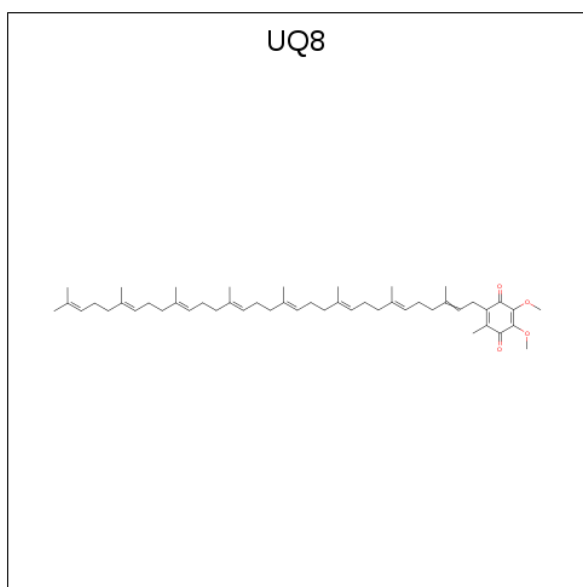
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 14 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	L	1	Total	C	N	O	0	0
			65	55	4	6		
14	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 15 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	L	1	Total	C	O	0	0
			33	29	4		
15	L	1	Total	C	O	0	0
			53	49	4		
15	L	1	Total	C	O	0	0
			18	14	4		
15	M	1	Total	C	O	0	0
			18	14	4		
15	7	1	Total	C	O	0	0
			33	29	4		

- Molecule 16 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	P	1	Total	C	0	0
			12	12		
16	G	1	Total	C	0	0
			12	12		
16	J	1	Total	C	0	0
			12	12		
16	E	1	Total	C	0	0
			12	12		
16	B	1	Total	C	0	0
			12	12		
16	6	1	Total	C	0	0
			12	12		
16	8	1	Total	C	0	0
			12	12		

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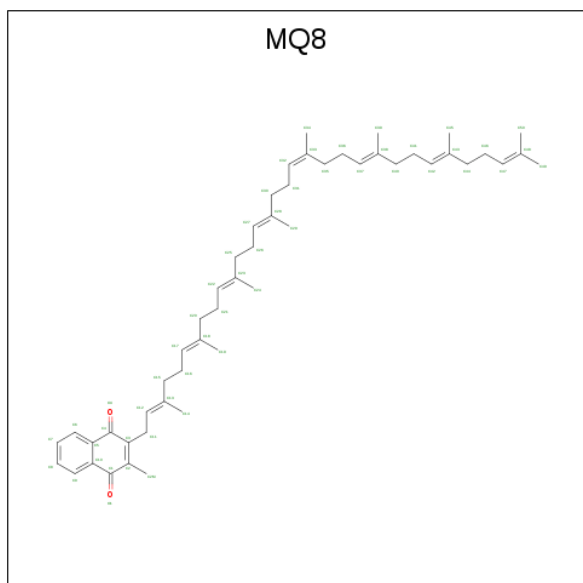
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	Z	1	Total C 12 12	0	0
16	T	1	Total C 12 12	0	0
16	O	1	Total C 12 12	0	0
16	X	1	Total C 12 12	0	0
16	4	1	Total C 12 12	0	0
16	R	1	Total C 12 12	0	0
16	L	1	Total C 12 12	0	0
16	2	1	Total C 12 12	0	0
16	M	1	Total C 9 9	0	0

- Molecule 17 is FE (III) ION (three-letter code: FE) (formula: Fe).

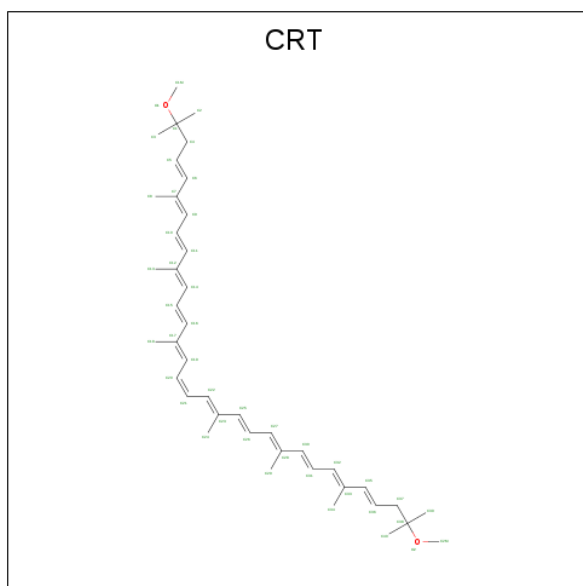
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	L	1	Total Fe 1 1	0	0

- Molecule 18 is MENAQUINONE 8 (three-letter code: MQ8) (formula: C₅₁H₇₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	M	1	Total	C	O	0	0
			53	51	2		

- Molecule 19 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C₄₂H₆₀O₂).



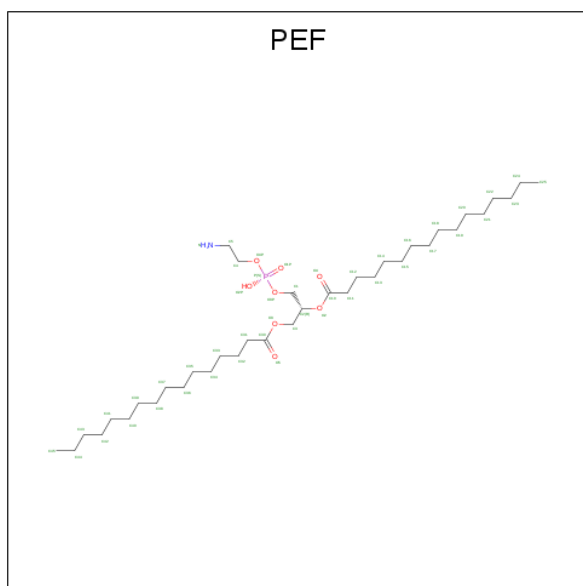
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	M	1	Total	C	O	0	0
			44	42	2		
19	A	1	Total	C	O	0	0
			44	42	2		
19	G	1	Total	C	O	0	0
			44	42	2		
19	J	1	Total	C	O	0	0
			44	42	2		
19	N	1	Total	C	O	0	0
			44	42	2		
19	O	1	Total	C	O	0	0
			44	42	2		
19	P	1	Total	C	O	0	0
			44	42	2		
19	Q	1	Total	C	O	0	0
			44	42	2		
19	U	1	Total	C	O	0	0
			44	42	2		
19	V	1	Total	C	O	0	0
			44	42	2		
19	Z	1	Total	C	O	0	0
			44	42	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	1	1	Total	C	O	0	0
			44	42	2		
19	2	1	Total	C	O	0	0
			44	42	2		
19	6	1	Total	C	O	0	0
			44	42	2		
19	9	1	Total	C	O	0	0
			44	42	2		
19	9	1	Total	C	O	0	0
			44	42	2		
19	0	1	Total	C	O	0	0
			44	42	2		

- Molecule 20 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



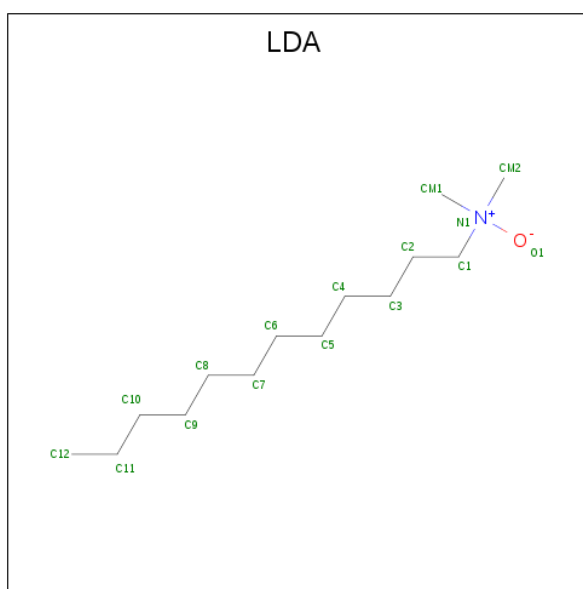
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	I	1	Total	O	P		0	0
			5	4	1			
20	K	1	Total	C	N	O	P	
			27	17	1	8	1	
20	U	1	Total	O	P			
			5	4	1			
20	U	1	Total	O	P			
			5	4	1			
20	W	1	Total	O	P			
			5	4	1			
20	1	1	Total	O	P			
			5	4	1			
20	3	1	Total	O	P			
			5	4	1			
20	5	1	Total	O	P			
			5	4	1			

- Molecule 21 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



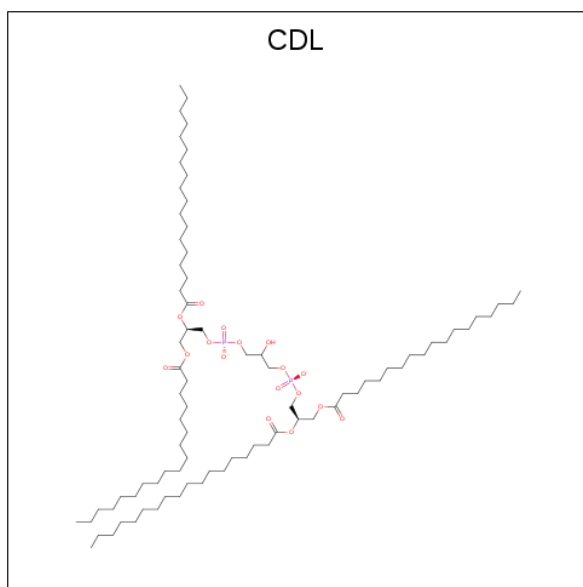
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	M	1	Total	C	N	O	0	0
			14	12	1	1		
21	I	1	Total	C	N	O	0	0
			16	14	1	1		
21	J	1	Total	C	N	O	0	0
			16	14	1	1		

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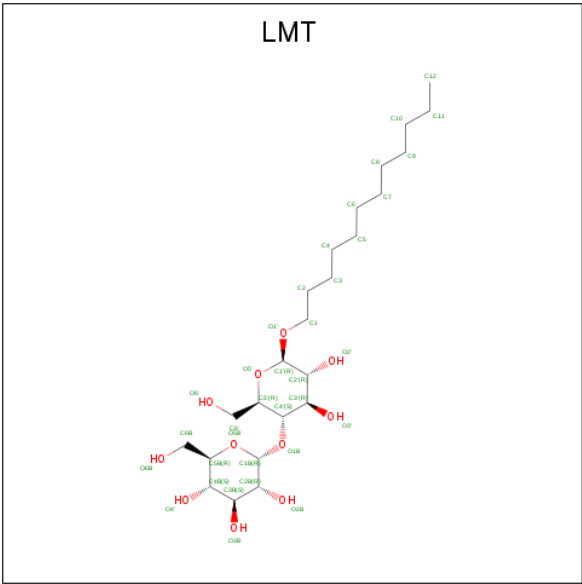
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	O	1	Total	C	N	O	0	0
			14	12	1	1		
21	V	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	M	1	Total	C	O	P	0	0
			39	21	16	2		
22	H	1	Total	C	O	P	0	0
			64	45	17	2		
22	H	1	Total	C	O	P	0	0
			79	60	17	2		
22	D	1	Total	C	O	P	0	0
			40	21	17	2		
22	K	1	Total	C	O	P	0	0
			86	67	17	2		
22	Q	1	Total	C	O	P	0	0
			75	56	17	2		
22	S	1	Total	C	O	P	0	0
			62	43	17	2		
22	Y	1	Total	C	O	P	0	0
			40	21	17	2		
22	Y	1	Total	C	O	P	0	0
			13	5	7	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	M	1	Total	C	O	0	0
			35	24	11		
23	F	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	Ca	0	0
			1	1		
24	G	1	Total	Ca	0	0
			1	1		
24	J	1	Total	Ca	0	0
			1	1		
24	E	1	Total	Ca	0	0
			1	1		
24	B	1	Total	Ca	0	0
			1	1		
24	V	1	Total	Ca	0	0
			1	1		
24	8	1	Total	Ca	0	0
			1	1		
24	Z	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total 1	Ca 1	0	0
24	T	1	Total 1	Ca 1	0	0
24	6	1	Total 1	Ca 1	0	0
24	N	1	Total 1	Ca 1	0	0
24	X	1	Total 1	Ca 1	0	0
24	4	1	Total 1	Ca 1	0	0
24	R	1	Total 1	Ca 1	0	0
24	2	1	Total 1	Ca 1	0	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	C	275	Total 277	O 277	0	2
25	L	108	Total 108	O 108	0	0
25	M	162	Total 162	O 162	0	0
25	H	158	Total 158	O 158	0	0
25	A	8	Total 8	O 8	0	0
25	B	5	Total 5	O 5	0	0
25	D	11	Total 11	O 11	0	0
25	E	5	Total 5	O 5	0	0
25	F	12	Total 12	O 12	0	0
25	G	2	Total 2	O 2	0	0
25	I	11	Total 11	O 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	J	4	Total 4	O 4	0	0
25	K	8	Total 8	O 8	0	0
25	N	3	Total 3	O 3	0	0
25	O	13	Total 13	O 13	0	0
25	P	7	Total 7	O 7	0	0
25	Q	18	Total 18	O 18	0	0
25	R	9	Total 9	O 9	0	0
25	S	12	Total 12	O 12	0	0
25	T	11	Total 11	O 11	0	0
25	U	15	Total 15	O 15	0	0
25	V	5	Total 5	O 5	0	0
25	W	11	Total 11	O 11	0	0
25	X	3	Total 3	O 3	0	0
25	Y	9	Total 9	O 9	0	0
25	Z	5	Total 5	O 5	0	0
25	1	3	Total 3	O 3	0	0
25	2	3	Total 3	O 3	0	0
25	3	6	Total 6	O 6	0	0
25	4	2	Total 2	O 2	0	0
25	5	10	Total 10	O 10	0	0
25	6	4	Total 4	O 4	0	0

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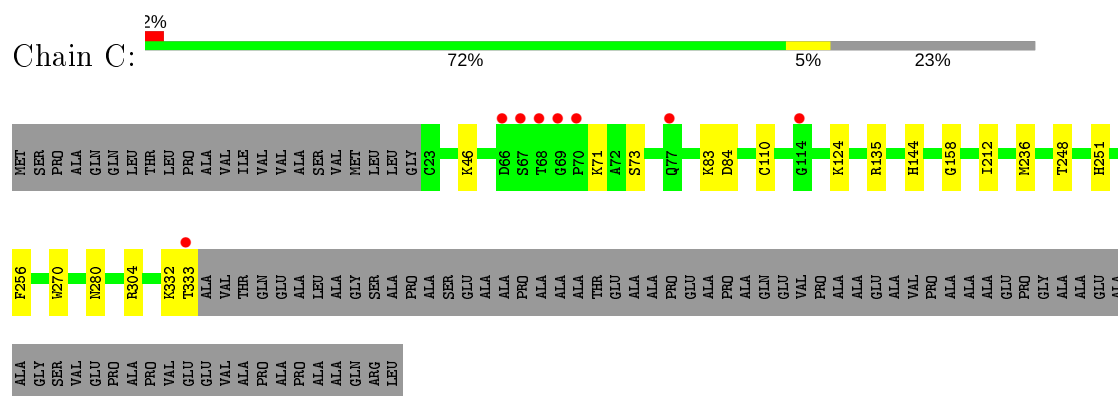
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	7	4	Total 4	O 4	0	0
25	8	11	Total 11	O 11	0	0
25	9	13	Total 13	O 13	0	0
25	0	8	Total 8	O 8	0	0

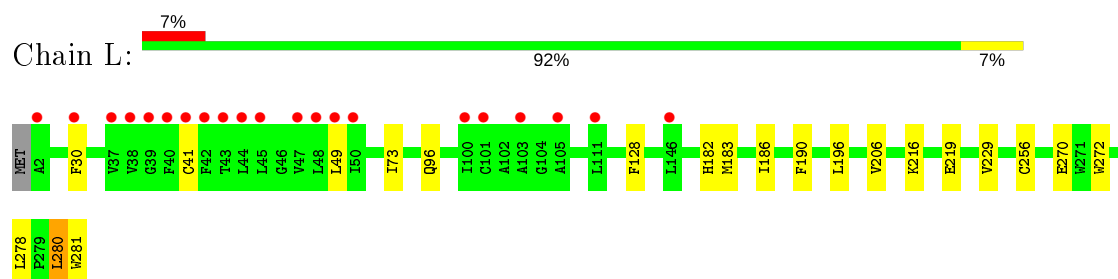
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

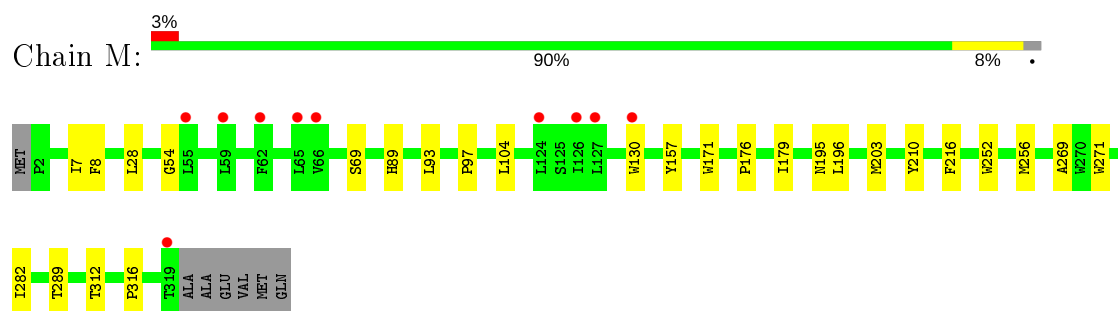
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



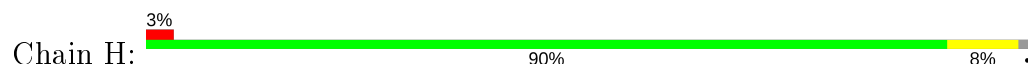
- Molecule 2: Photosynthetic reaction center L subunit



- Molecule 3: Photosynthetic reaction center M subunit

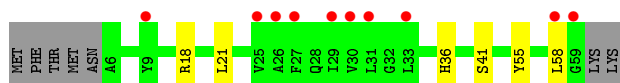
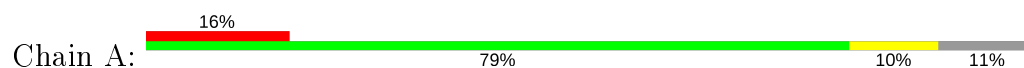


- Molecule 4: Photosynthetic reaction center H subunit

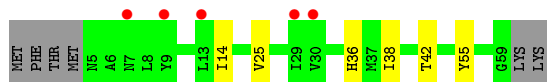
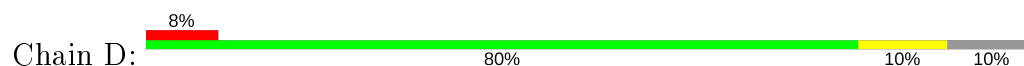




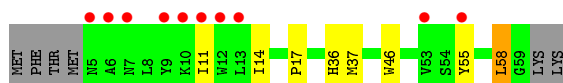
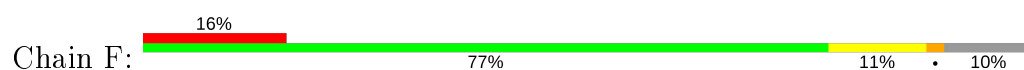
- Molecule 5: LH1 alpha polypeptide



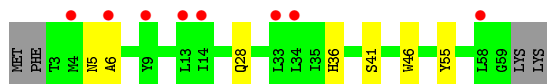
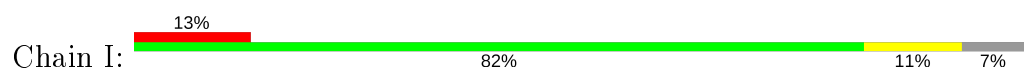
- Molecule 5: LH1 alpha polypeptide



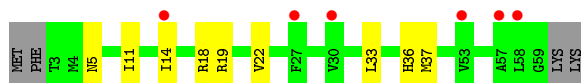
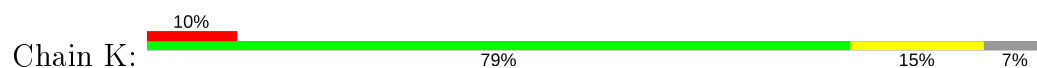
- Molecule 5: LH1 alpha polypeptide



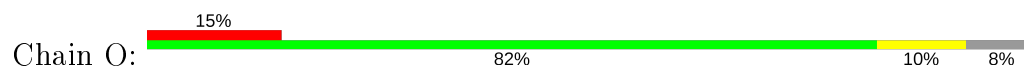
- Molecule 5: LH1 alpha polypeptide



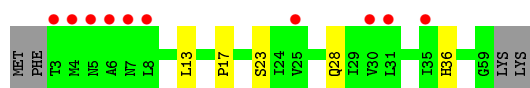
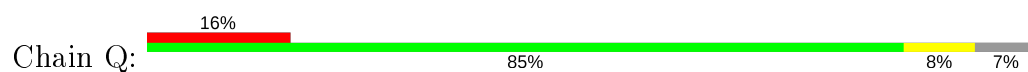
- Molecule 5: LH1 alpha polypeptide



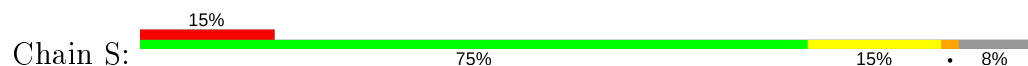
- Molecule 5: LH1 alpha polypeptide



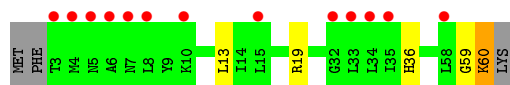
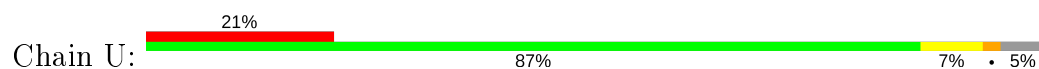
- Molecule 5: LH1 alpha polypeptide



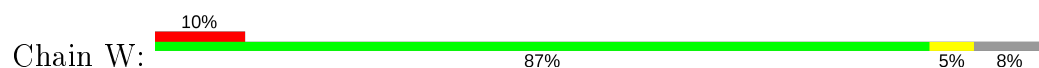
- Molecule 5: LH1 alpha polypeptide



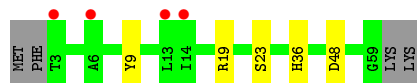
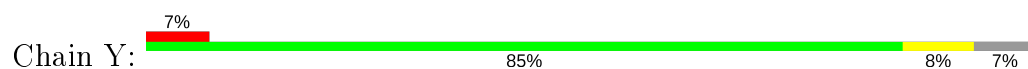
- Molecule 5: LH1 alpha polypeptide



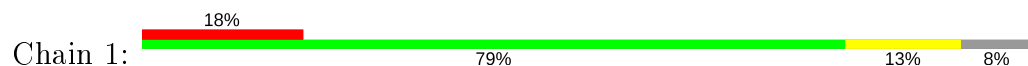
- Molecule 5: LH1 alpha polypeptide



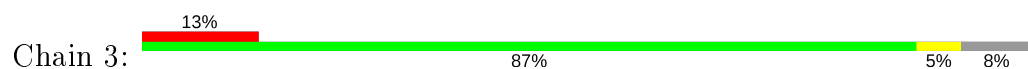
- Molecule 5: LH1 alpha polypeptide



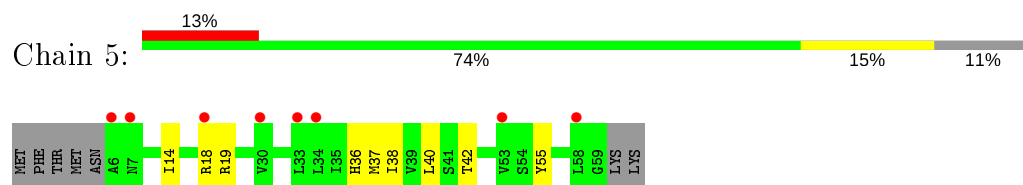
- Molecule 5: LH1 alpha polypeptide



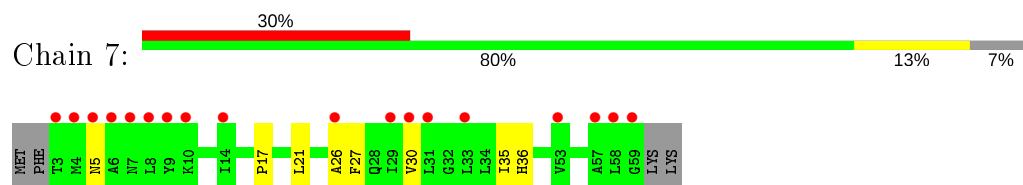
- Molecule 5: LH1 alpha polypeptide



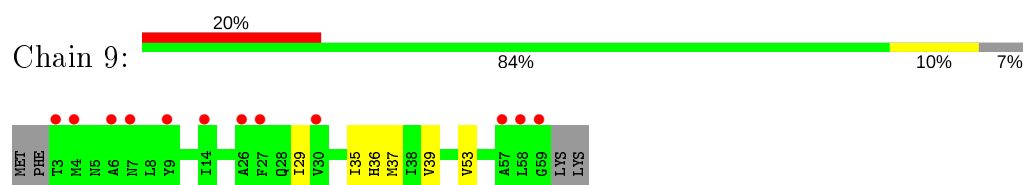
- Molecule 5: LH1 alpha polypeptide



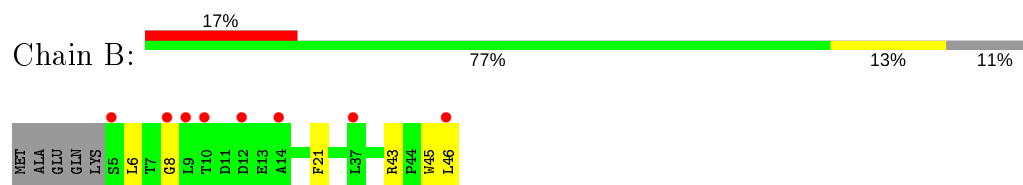
- Molecule 5: LH1 alpha polypeptide



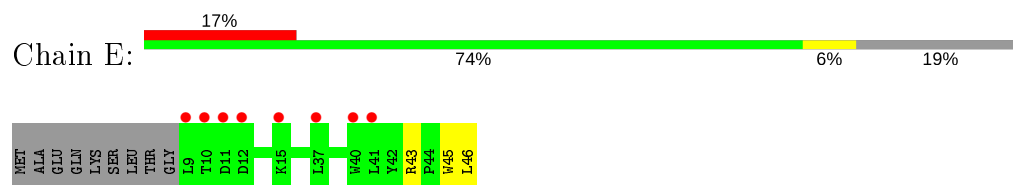
- Molecule 5: LH1 alpha polypeptide



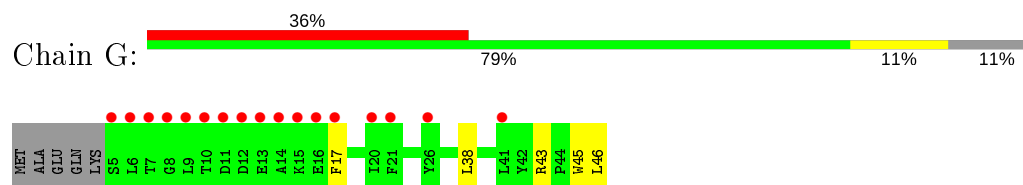
- Molecule 6: LH1 beta polypeptide



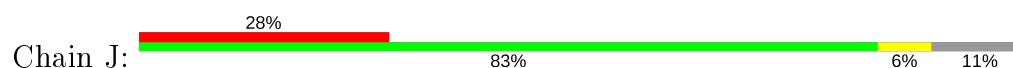
- Molecule 6: LH1 beta polypeptide

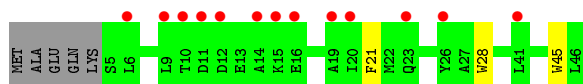


- Molecule 6: LH1 beta polypeptide

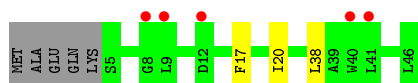
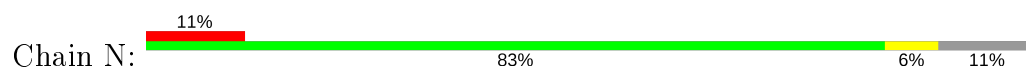


- Molecule 6: LH1 beta polypeptide

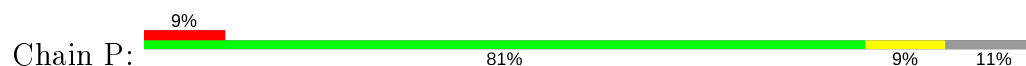




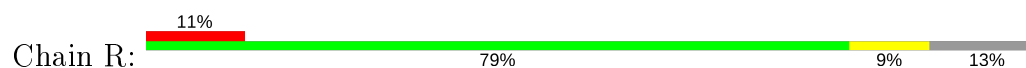
- Molecule 6: LH1 beta polypeptide



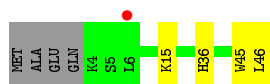
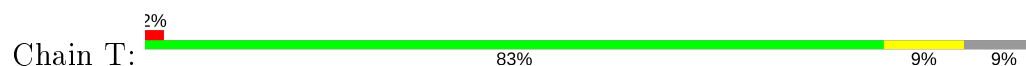
- Molecule 6: LH1 beta polypeptide



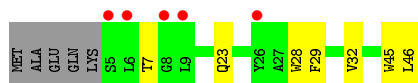
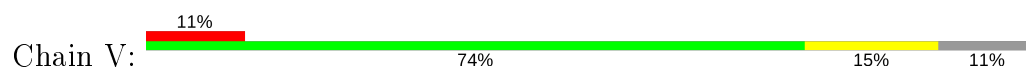
- Molecule 6: LH1 beta polypeptide



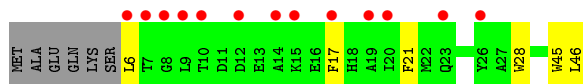
- Molecule 6: LH1 beta polypeptide



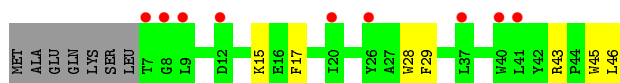
- Molecule 6: LH1 beta polypeptide



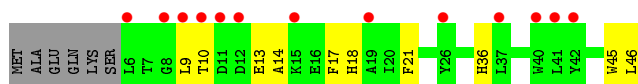
- Molecule 6: LH1 beta polypeptide



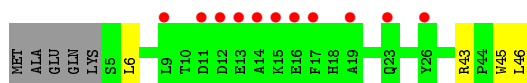
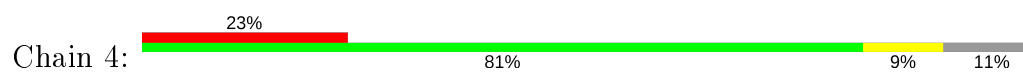
- Molecule 6: LH1 beta polypeptide



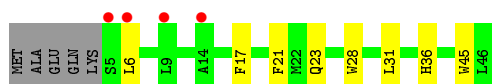
- Molecule 6: LH1 beta polypeptide



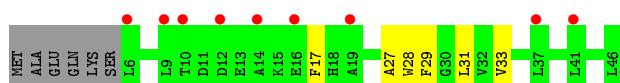
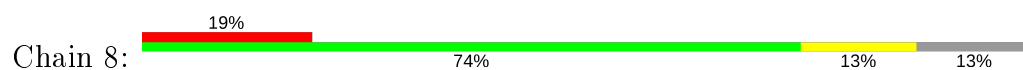
- Molecule 6: LH1 beta polypeptide



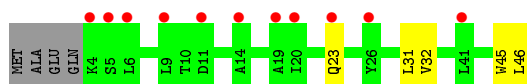
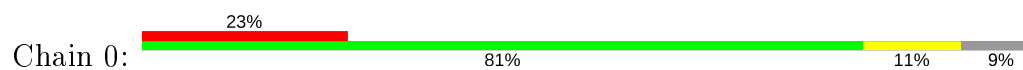
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.28Å 143.81Å 210.28Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	46.92 – 1.90 46.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.92-1.90) 91.8 (46.92-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.63 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.12rc0_2787	Depositor
R, R_{free}	0.181 , 0.215 0.181 , 0.215	Depositor DCC
R_{free} test set	16921 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l 0.019 for -k,-h,-l 0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27981	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LHG, LDA, CRT, GOL, CDL, BPH, CA, LMT, MG, PGV, UQ8, FE, HEC, MQ8, PEF, UNL, SO4

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	C	0.42	0/2487	0.55	0/3396
2	L	0.51	0/2326	0.55	0/3177
3	M	0.50	0/2658	0.56	0/3637
4	H	0.45	0/2034	0.57	0/2773
5	1	0.44	0/459	0.47	0/628
5	3	0.27	0/467	0.44	0/638
5	5	0.30	0/443	0.45	0/607
5	7	0.34	0/466	0.47	0/638
5	9	0.30	0/466	0.46	0/638
5	A	0.31	0/443	0.48	0/607
5	D	0.27	0/457	0.44	0/626
5	F	0.31	0/457	0.43	0/626
5	I	0.28	0/472	0.44	0/646
5	K	0.29	0/466	0.42	0/638
5	O	0.34	0/467	0.47	0/638
5	Q	0.44	0/466	0.53	0/638
5	S	0.41	0/483	0.51	0/661
5	U	0.34	0/475	0.49	0/649
5	W	0.30	0/460	0.46	0/629
5	Y	0.27	0/466	0.45	0/638
6	0	0.30	0/373	0.42	0/506
6	2	0.25	0/358	0.37	0/487
6	4	0.27	0/364	0.40	0/495
6	6	0.32	0/364	0.40	0/495
6	8	0.32	0/358	0.43	0/487
6	B	0.28	0/364	0.36	0/495
6	E	0.26	0/339	0.36	0/461
6	G	0.24	0/364	0.37	0/495
6	J	0.25	0/364	0.38	0/495
6	N	0.26	0/364	0.40	0/495
6	P	0.30	0/364	0.42	0/495

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	R	0.37	0/358	0.48	0/487
6	T	0.38	0/373	0.42	0/506
6	V	0.31	0/364	0.40	0/495
6	X	0.28	0/358	0.37	0/487
6	Z	0.25	0/350	0.40	0/476
All	All	0.39	0/22697	0.49	0/30985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2417	0	2328	12	0
2	L	2236	0	2201	18	0
3	M	2555	0	2530	23	0
4	H	1976	0	1977	20	0
5	1	450	0	475	7	0
5	3	455	0	484	3	0
5	5	434	0	460	8	0
5	7	457	0	482	9	0
5	9	457	0	482	6	0
5	A	434	0	460	6	0
5	D	445	0	471	7	0
5	F	445	0	471	8	0
5	I	460	0	487	10	0
5	K	457	0	482	7	0
5	O	455	0	484	4	0
5	Q	457	0	482	6	0
5	S	468	0	501	11	0
5	U	466	0	495	5	0
5	W	451	0	479	3	0
5	Y	457	0	480	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	0	360	0	352	4	0
6	2	345	0	334	19	0
6	4	351	0	339	3	0
6	6	351	0	339	8	0
6	8	345	0	334	4	0
6	B	351	0	339	7	0
6	E	326	0	313	2	0
6	G	351	0	339	6	0
6	J	351	0	339	3	0
6	N	351	0	339	4	0
6	P	351	0	339	4	0
6	R	345	0	334	4	0
6	T	360	0	352	3	0
6	V	351	0	339	8	0
6	X	345	0	334	5	0
6	Z	337	0	323	7	0
7	C	172	0	120	3	0
8	C	1	0	0	0	0
9	C	6	0	8	0	0
9	H	6	0	8	1	0
10	C	5	0	0	0	0
10	L	5	0	0	0	0
10	M	5	0	0	0	0
11	C	9	0	12	0	0
12	1	31	0	32	0	0
12	3	51	0	76	3	0
12	A	33	0	36	5	0
12	C	21	0	23	0	0
12	D	35	0	40	2	0
12	H	36	0	42	1	0
12	L	87	0	120	8	0
12	M	83	0	116	7	0
13	0	66	0	72	8	0
13	1	132	0	144	12	0
13	3	132	0	144	8	0
13	5	132	0	144	14	0
13	7	127	0	131	8	0
13	9	66	0	72	4	0
13	A	132	0	144	8	0
13	D	132	0	144	6	0
13	F	132	0	144	5	0
13	I	132	0	144	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	132	0	144	5	0
13	L	66	0	72	4	0
13	M	198	0	216	9	0
13	O	132	0	144	8	0
13	Q	132	0	144	10	0
13	S	132	0	144	11	0
13	U	132	0	144	12	0
13	W	132	0	144	7	0
13	Y	66	0	72	5	0
13	Z	66	0	72	7	0
14	L	65	0	74	6	0
14	M	65	0	74	6	0
15	7	33	0	39	8	0
15	L	104	0	128	10	0
15	M	18	0	15	3	0
16	0	12	0	0	0	0
16	2	12	0	0	0	0
16	4	12	0	0	0	0
16	6	12	0	0	0	0
16	8	12	0	0	0	0
16	B	12	0	0	0	0
16	E	12	0	0	0	0
16	G	12	0	0	0	0
16	J	12	0	0	0	0
16	L	12	0	0	0	0
16	M	9	0	0	0	0
16	P	12	0	0	0	0
16	R	12	0	0	0	0
16	T	12	0	0	0	0
16	X	12	0	0	0	0
16	Z	12	0	0	0	0
17	L	1	0	0	0	0
18	M	53	0	72	5	0
19	0	44	0	60	2	0
19	1	44	0	60	3	0
19	2	44	0	60	6	0
19	6	44	0	60	2	0
19	9	88	0	120	6	0
19	A	44	0	60	3	0
19	G	44	0	60	5	0
19	J	44	0	60	3	0
19	M	44	0	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	44	0	60	4	0
19	O	44	0	60	2	0
19	P	44	0	60	2	0
19	Q	44	0	60	2	0
19	U	44	0	60	2	0
19	V	44	0	60	1	0
19	Z	44	0	60	3	0
20	1	5	0	0	0	0
20	3	5	0	0	0	0
20	5	5	0	0	1	0
20	I	5	0	0	1	0
20	K	27	0	27	1	0
20	M	67	0	73	3	0
20	U	10	0	0	0	0
20	W	5	0	0	0	0
21	I	16	0	31	6	0
21	J	16	0	31	1	0
21	M	14	0	24	1	0
21	O	14	0	24	1	0
21	V	16	0	31	0	0
22	D	40	0	24	2	0
22	H	143	0	177	6	0
22	K	86	0	119	4	0
22	M	39	0	28	1	0
22	Q	75	0	94	3	0
22	S	62	0	68	10	0
22	Y	53	0	31	1	0
23	F	35	0	46	5	0
23	M	35	0	46	3	0
24	2	1	0	0	0	0
24	4	1	0	0	0	0
24	6	1	0	0	0	0
24	8	1	0	0	0	0
24	A	1	0	0	0	0
24	B	1	0	0	0	0
24	E	1	0	0	0	0
24	G	1	0	0	0	0
24	J	1	0	0	0	0
24	N	1	0	0	0	0
24	P	1	0	0	0	0
24	R	1	0	0	0	0
24	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	V	1	0	0	0	0
24	X	1	0	0	0	0
24	Z	1	0	0	0	0
25	0	8	0	0	0	0
25	1	3	0	0	0	0
25	2	3	0	0	0	0
25	3	6	0	0	0	0
25	4	2	0	0	0	0
25	5	10	0	0	0	0
25	6	4	0	0	0	0
25	7	4	0	0	0	0
25	8	11	0	0	0	0
25	9	13	0	0	0	0
25	A	8	0	0	0	0
25	B	5	0	0	0	0
25	C	277	0	0	1	0
25	D	11	0	0	0	0
25	E	5	0	0	0	0
25	F	12	0	0	0	0
25	G	2	0	0	0	0
25	H	158	0	0	1	1
25	I	11	0	0	0	0
25	J	4	0	0	0	0
25	K	8	0	0	0	0
25	L	108	0	0	1	0
25	M	162	0	0	2	0
25	N	3	0	0	0	0
25	O	13	0	0	0	0
25	P	7	0	0	0	0
25	Q	18	0	0	0	0
25	R	9	0	0	0	0
25	S	12	0	0	0	1
25	T	11	0	0	0	0
25	U	15	0	0	1	0
25	V	5	0	0	0	0
25	W	11	0	0	0	0
25	X	3	0	0	0	0
25	Y	9	0	0	0	0
25	Z	5	0	0	0	0
All	All	27981	0	27607	386	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 386 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:19:ARG:CZ	22:S:103:CDL:OA4	1.88	1.20
6:2:9:LEU:HD21	6:2:14:ALA:N	1.54	1.19
22:S:103:CDL:C19	13:U:101:BCL:H51	1.83	1.08
5:S:19:ARG:NH1	22:S:103:CDL:OA4	1.91	1.03
6:2:9:LEU:CD2	6:2:14:ALA:N	2.23	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:H:558:HOH:O	25:S:210:HOH:O[3_455]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

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	C	309/404 (76%)	295 (96%)	14 (4%)	0	100	100
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
3	M	318/325 (98%)	311 (98%)	5 (2%)	2 (1%)	25	15
4	H	255/259 (98%)	254 (100%)	1 (0%)	0	100	100
5	1	54/61 (88%)	54 (100%)	0	0	100	100
5	3	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	5	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
5	7	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	9	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	A	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
5	D	54/61 (88%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	54/61 (88%)	52 (96%)	2 (4%)	0	100	100
5	I	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
5	K	55/61 (90%)	55 (100%)	0	0	100	100
5	O	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	Q	55/61 (90%)	55 (100%)	0	0	100	100
5	S	57/61 (93%)	57 (100%)	0	0	100	100
5	U	56/61 (92%)	54 (96%)	2 (4%)	0	100	100
5	W	54/61 (88%)	54 (100%)	0	0	100	100
5	Y	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
6	0	41/47 (87%)	41 (100%)	0	0	100	100
6	2	39/47 (83%)	39 (100%)	0	0	100	100
6	4	40/47 (85%)	40 (100%)	0	0	100	100
6	6	40/47 (85%)	40 (100%)	0	0	100	100
6	8	39/47 (83%)	39 (100%)	0	0	100	100
6	B	40/47 (85%)	40 (100%)	0	0	100	100
6	E	36/47 (77%)	36 (100%)	0	0	100	100
6	G	40/47 (85%)	40 (100%)	0	0	100	100
6	J	40/47 (85%)	40 (100%)	0	0	100	100
6	N	40/47 (85%)	40 (100%)	0	0	100	100
6	P	40/47 (85%)	40 (100%)	0	0	100	100
6	R	39/47 (83%)	39 (100%)	0	0	100	100
6	T	41/47 (87%)	41 (100%)	0	0	100	100
6	V	40/47 (85%)	40 (100%)	0	0	100	100
6	X	39/47 (83%)	39 (100%)	0	0	100	100
6	Z	38/47 (81%)	38 (100%)	0	0	100	100
All	All	2667/2997 (89%)	2625 (98%)	40 (2%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	195	ASN
3	M	179	ILE

5.3.2 Protein sidechains ⓘ

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	C	260/317 (82%)	258 (99%)	2 (1%)	81	82
2	L	229/229 (100%)	226 (99%)	3 (1%)	69	68
3	M	258/261 (99%)	257 (100%)	1 (0%)	91	91
4	H	211/211 (100%)	210 (100%)	1 (0%)	88	89
5	1	51/56 (91%)	51 (100%)	0	100	100
5	3	52/56 (93%)	52 (100%)	0	100	100
5	5	49/56 (88%)	49 (100%)	0	100	100
5	7	52/56 (93%)	52 (100%)	0	100	100
5	9	52/56 (93%)	51 (98%)	1 (2%)	57	53
5	A	49/56 (88%)	49 (100%)	0	100	100
5	D	51/56 (91%)	51 (100%)	0	100	100
5	F	51/56 (91%)	50 (98%)	1 (2%)	55	51
5	I	53/56 (95%)	53 (100%)	0	100	100
5	K	52/56 (93%)	52 (100%)	0	100	100
5	O	52/56 (93%)	51 (98%)	1 (2%)	57	53
5	Q	52/56 (93%)	52 (100%)	0	100	100
5	S	55/56 (98%)	53 (96%)	2 (4%)	35	26
5	U	53/56 (95%)	52 (98%)	1 (2%)	57	53
5	W	51/56 (91%)	51 (100%)	0	100	100
5	Y	52/56 (93%)	51 (98%)	1 (2%)	57	53
6	0	36/39 (92%)	35 (97%)	1 (3%)	43	36
6	2	34/39 (87%)	34 (100%)	0	100	100
6	4	35/39 (90%)	35 (100%)	0	100	100
6	6	35/39 (90%)	35 (100%)	0	100	100
6	8	34/39 (87%)	34 (100%)	0	100	100
6	B	35/39 (90%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	E	32/39 (82%)	32 (100%)	0	100	100
6	G	35/39 (90%)	35 (100%)	0	100	100
6	J	35/39 (90%)	35 (100%)	0	100	100
6	N	35/39 (90%)	35 (100%)	0	100	100
6	P	35/39 (90%)	35 (100%)	0	100	100
6	R	34/39 (87%)	34 (100%)	0	100	100
6	T	36/39 (92%)	36 (100%)	0	100	100
6	V	35/39 (90%)	35 (100%)	0	100	100
6	X	34/39 (87%)	34 (100%)	0	100	100
6	Z	33/39 (85%)	33 (100%)	0	100	100
All	All	2338/2538 (92%)	2323 (99%)	15 (1%)	86	87

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	237	ASP
5	F	58	LEU
5	Y	48	ASP
3	M	216	PHE
5	U	60	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 144 ligands modelled in this entry, 16 are unknown and 18 are monoatomic - leaving 110 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	$\# Z > 2$
20	PEF	K	104	-	26,26,46	1.25	2 (7%)	29,31,51	1.45	4 (13%)
12	PGV	A	105	-	32,32,50	1.18	2 (6%)	35,38,56	1.18	3 (8%)
13	BCL	7	101	-	53,69,74	1.74	9 (16%)	63,109,115	2.36	20 (31%)
20	PEF	3	103	-	4,4,46	2.62	2 (50%)	6,6,51	1.88	2 (33%)
12	PGV	L	305	-	42,42,50	1.04	2 (4%)	45,48,56	1.26	3 (6%)
19	CRT	6	101	-	41,43,43	0.73	0	50,54,54	1.52	8 (16%)
22	CDL	Y	103	-	12,12,99	0.47	0	13,15,111	0.49	0
13	BCL	O	102	-	58,74,74	1.64	9 (15%)	69,115,115	2.15	18 (26%)
23	LMT	F	103	-	36,36,36	0.49	0	47,47,47	1.44	9 (19%)
15	UQ8	M	417	-	18,18,53	2.07	2 (11%)	22,25,67	1.44	4 (18%)
18	MQ8	M	405	-	54,54,54	1.38	3 (5%)	66,69,69	1.48	14 (21%)
12	PGV	L	306	-	43,43,50	0.99	2 (4%)	46,49,56	1.12	2 (4%)
13	BCL	S	101	-	58,74,74	1.78	9 (15%)	69,115,115	2.22	18 (26%)
11	LHG	C	508	1	8,8,48	0.39	0	7,7,54	0.47	0
10	SO4	C	507	-	4,4,4	0.13	0	6,6,6	0.10	0
22	CDL	H	304	-	78,78,99	1.04	4 (5%)	84,90,111	1.15	8 (9%)
12	PGV	1	105	-	30,30,50	1.21	2 (6%)	33,36,56	1.18	3 (9%)
21	LDA	O	104	-	10,13,15	2.28	1 (10%)	12,15,17	0.49	0
15	UQ8	7	103	-	33,33,53	1.41	2 (6%)	40,43,67	2.09	14 (35%)
19	CRT	G	101	-	41,43,43	0.73	0	50,54,54	1.49	11 (22%)
13	BCL	Z	102	-	58,74,74	1.71	9 (15%)	69,115,115	2.27	19 (27%)
10	SO4	M	412	-	4,4,4	0.14	0	6,6,6	0.09	0
22	CDL	H	302	-	63,63,99	1.08	4 (6%)	69,75,111	1.33	9 (13%)
13	BCL	0	102	-	58,74,74	1.70	8 (13%)	69,115,115	2.26	19 (27%)
20	PEF	W	103	-	4,4,46	2.64	2 (50%)	6,6,51	1.82	2 (33%)
12	PGV	3	104	-	50,50,50	0.94	2 (4%)	53,56,56	0.92	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CRT	Z	101	-	41,43,43	0.70	0	50,54,54	1.74	11 (22%)
13	BCL	W	101	-	58,74,74	1.68	9 (15%)	69,115,115	2.43	20 (28%)
19	CRT	V	101	-	41,43,43	0.74	0	50,54,54	1.56	9 (18%)
13	BCL	K	102	-	58,74,74	1.71	9 (15%)	69,115,115	2.31	19 (27%)
20	PEF	1	104	-	4,4,46	2.71	2 (50%)	6,6,51	1.81	2 (33%)
12	PGV	H	303	-	35,35,50	1.10	2 (5%)	38,41,56	1.27	4 (10%)
19	CRT	P	101	-	41,43,43	0.81	0	50,54,54	1.44	10 (20%)
9	GOL	C	506	-	5,5,5	0.89	0	5,5,5	0.87	0
13	BCL	Q	102	-	58,74,74	1.71	8 (13%)	69,115,115	2.27	19 (27%)
19	CRT	9	101	-	41,43,43	0.74	0	50,54,54	1.63	13 (26%)
12	PGV	M	414	-	36,36,50	1.07	2 (5%)	39,42,56	1.21	3 (7%)
19	CRT	N	101	-	41,43,43	0.70	0	50,54,54	1.56	13 (26%)
20	PEF	I	103	-	4,4,46	2.62	2 (50%)	6,6,51	1.81	2 (33%)
13	BCL	U	101	-	58,74,74	1.70	9 (15%)	69,115,115	2.27	23 (33%)
7	HEC	C	501	1	26,50,50	1.62	4 (15%)	18,82,82	1.66	3 (16%)
13	BCL	I	101	-	58,74,74	1.71	9 (15%)	69,115,115	2.25	18 (26%)
13	BCL	W	102	-	58,74,74	1.71	8 (13%)	69,115,115	2.24	17 (24%)
13	BCL	D	102	-	58,74,74	1.69	9 (15%)	69,115,115	2.25	19 (27%)
13	BCL	1	101	-	58,74,74	1.73	8 (13%)	69,115,115	2.23	18 (26%)
13	BCL	L	301	-	58,74,74	1.59	8 (13%)	69,115,115	1.93	18 (26%)
13	BCL	A	103	-	58,74,74	1.71	9 (15%)	69,115,115	2.20	17 (24%)
19	CRT	0	101	-	41,43,43	0.70	0	50,54,54	1.37	7 (14%)
13	BCL	5	102	-	58,74,74	1.69	8 (13%)	69,115,115	2.13	19 (27%)
7	HEC	C	504	1	26,50,50	1.59	4 (15%)	18,82,82	1.41	3 (16%)
20	PEF	U	104	-	4,4,46	2.53	2 (50%)	6,6,51	1.85	2 (33%)
13	BCL	F	102	-	58,74,74	1.73	8 (13%)	69,115,115	2.26	19 (27%)
12	PGV	C	509	-	20,20,50	1.44	3 (15%)	22,22,56	1.58	3 (13%)
19	CRT	U	103	-	41,43,43	0.74	0	50,54,54	1.52	12 (24%)
20	PEF	M	407	-	4,4,46	2.62	2 (50%)	6,6,51	1.82	2 (33%)
15	UQ8	L	309	-	18,18,53	2.07	2 (11%)	22,25,67	1.01	2 (9%)
13	BCL	M	401	-	58,74,74	1.66	9 (15%)	69,115,115	2.19	22 (31%)
21	LDA	I	104	-	12,15,15	1.95	1 (8%)	14,17,17	0.46	0
12	PGV	D	104	-	34,34,50	1.07	2 (5%)	37,40,56	1.20	5 (13%)
13	BCL	Q	101	-	58,74,74	1.65	9 (15%)	69,115,115	2.12	21 (30%)
19	CRT	2	101	-	41,43,43	0.71	0	50,54,54	1.46	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BPH	L	302	-	64,70,70	2.00	13 (20%)	76,101,101	1.86	20 (26%)
9	GOL	H	301	-	5,5,5	0.87	0	5,5,5	0.95	0
13	BCL	S	102	-	58,74,74	1.68	7 (12%)	69,115,115	2.22	20 (28%)
13	BCL	A	101	-	58,74,74	1.73	9 (15%)	69,115,115	2.28	21 (30%)
13	BCL	I	102	-	58,74,74	1.71	8 (13%)	69,115,115	2.19	21 (30%)
22	CDL	Q	104	-	74,74,99	1.09	4 (5%)	80,86,111	1.13	7 (8%)
14	BPH	M	404	-	64,70,70	1.96	12 (18%)	76,101,101	1.89	20 (26%)
19	CRT	J	101	-	41,43,43	0.75	0	50,54,54	1.56	12 (24%)
13	BCL	U	102	-	58,74,74	1.70	8 (13%)	69,115,115	2.22	20 (28%)
20	PEF	U	105	-	4,4,46	2.65	2 (50%)	6,6,51	1.84	2 (33%)
13	BCL	M	402	-	58,74,74	1.59	8 (13%)	69,115,115	2.17	21 (30%)
13	BCL	5	101	-	58,74,74	1.62	8 (13%)	69,115,115	2.24	19 (27%)
23	LMT	M	419	-	36,36,36	0.47	1 (2%)	47,47,47	0.93	3 (6%)
19	CRT	O	103	-	41,43,43	0.78	0	50,54,54	1.52	12 (24%)
19	CRT	M	406	-	41,43,43	0.88	0	50,54,54	1.35	9 (18%)
19	CRT	A	104	-	41,43,43	0.71	0	50,54,54	1.56	10 (20%)
13	BCL	Y	101	-	58,74,74	1.71	9 (15%)	69,115,115	2.33	20 (28%)
21	LDA	V	102	-	12,15,15	2.07	1 (8%)	14,17,17	0.38	0
22	CDL	M	415	-	38,38,99	1.32	3 (7%)	43,49,111	1.27	3 (6%)
7	HEC	C	502	1	26,50,50	1.53	4 (15%)	18,82,82	1.55	2 (11%)
20	PEF	5	103	-	4,4,46	2.63	2 (50%)	6,6,51	1.79	2 (33%)
22	CDL	D	103	-	39,39,99	1.45	4 (10%)	45,51,111	1.43	6 (13%)
21	LDA	M	411	-	10,13,15	2.26	1 (10%)	12,15,17	0.48	0
20	PEF	M	410	-	4,4,46	2.37	1 (25%)	6,6,51	1.39	1 (16%)
12	PGV	M	413	-	45,45,50	1.06	2 (4%)	49,50,56	0.97	4 (8%)
13	BCL	9	103	-	58,74,74	1.69	9 (15%)	69,115,115	2.32	16 (23%)
13	BCL	M	403	-	58,74,74	1.65	8 (13%)	69,115,115	2.13	18 (26%)
22	CDL	K	103	-	85,85,99	1.00	4 (4%)	91,97,111	1.17	9 (9%)
21	LDA	J	102	-	12,15,15	2.07	1 (8%)	14,17,17	0.45	0
13	BCL	D	101	-	58,74,74	1.69	9 (15%)	69,115,115	2.32	18 (26%)
22	CDL	S	103	-	61,61,99	1.10	4 (6%)	67,73,111	1.31	8 (11%)
13	BCL	3	102	-	58,74,74	1.75	8 (13%)	69,115,115	2.22	19 (27%)
13	BCL	1	102	-	58,74,74	1.72	8 (13%)	69,115,115	2.34	18 (26%)
7	HEC	C	503	1	26,50,50	1.53	4 (15%)	18,82,82	1.58	5 (27%)
13	BCL	3	101	-	58,74,74	1.69	9 (15%)	69,115,115	2.12	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CRT	Q	103	-	41,43,43	0.77	0	50,54,54	1.49	7 (14%)
15	UQ8	L	303	-	33,33,53	1.62	2 (6%)	40,43,67	1.57	7 (17%)
20	PEF	M	409	-	4,4,46	2.65	2 (50%)	6,6,51	1.84	2 (33%)
13	BCL	7	102	-	58,74,74	1.68	8 (13%)	69,115,115	2.03	18 (26%)
13	BCL	O	101	-	58,74,74	1.67	8 (13%)	69,115,115	2.40	20 (28%)
19	CRT	9	102	-	41,43,43	0.72	0	50,54,54	1.52	9 (18%)
20	PEF	M	408	-	4,4,46	1.84	2 (50%)	6,6,51	1.18	1 (16%)
20	PEF	M	418	-	46,46,46	0.96	2 (4%)	49,51,51	1.07	3 (6%)
19	CRT	1	103	-	41,43,43	0.72	0	50,54,54	1.48	8 (16%)
15	UQ8	L	308	-	53,53,53	1.19	2 (3%)	64,67,67	1.69	19 (29%)
13	BCL	F	101	-	58,74,74	1.73	10 (17%)	69,115,115	2.25	19 (27%)
13	BCL	K	101	-	58,74,74	1.72	10 (17%)	69,115,115	2.28	18 (26%)
10	SO4	L	304	-	4,4,4	0.13	0	6,6,6	0.05	0
22	CDL	Y	102	5	39,39,99	1.48	4 (10%)	45,51,111	1.33	4 (8%)

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
20	PEF	K	104	-	-	2/30/30/50	-
12	PGV	A	105	-	-	13/37/37/55	-
13	BCL	7	101	-	-	7/31/131/137	-
12	PGV	L	305	-	-	15/47/47/55	-
19	CRT	6	101	-	-	0/51/51/51	-
22	CDL	Y	103	-	-	7/13/13/110	-
13	BCL	O	102	-	-	16/37/137/137	-
23	LMT	F	103	-	-	9/21/61/61	0/2/2/2
15	UQ8	M	417	-	-	1/9/33/75	0/1/1/1
18	MQ8	M	405	-	-	2/47/67/67	0/2/2/2
12	PGV	L	306	-	-	17/48/48/55	-
13	BCL	S	101	-	-	10/37/137/137	-
11	LHG	C	508	1	-	1/5/6/53	-
22	CDL	H	304	-	-	22/89/89/110	-
12	PGV	1	105	-	-	10/35/35/55	-
21	LDA	O	104	-	-	8/11/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	UQ8	7	103	-	-	9/27/51/75	0/1/1/1
19	CRT	G	101	-	-	2/51/51/51	-
12	PGV	M	413	-	-	16/47/47/55	-
22	CDL	H	302	-	-	23/73/73/110	-
13	BCL	0	102	-	-	7/37/137/137	-
12	PGV	3	104	-	-	16/55/55/55	-
19	CRT	Z	101	-	-	0/51/51/51	-
13	BCL	W	101	-	-	10/37/137/137	-
19	CRT	V	101	-	-	6/51/51/51	-
13	BCL	K	102	-	-	14/37/137/137	-
12	PGV	H	303	-	-	16/40/40/55	-
19	CRT	P	101	-	-	1/51/51/51	-
13	BCL	3	101	-	-	18/37/137/137	-
13	BCL	Q	102	-	-	9/37/137/137	-
19	CRT	9	101	-	-	5/51/51/51	-
12	PGV	M	414	-	-	16/41/41/55	-
19	CRT	N	101	-	-	0/51/51/51	-
13	BCL	U	101	-	-	4/37/137/137	-
7	HEC	C	501	1	-	0/6/54/54	-
13	BCL	I	101	-	-	9/37/137/137	-
13	BCL	W	102	-	-	8/37/137/137	-
13	BCL	D	102	-	-	7/37/137/137	-
13	BCL	1	101	-	-	15/37/137/137	-
13	BCL	L	301	-	-	2/37/137/137	-
13	BCL	A	103	-	-	10/37/137/137	-
19	CRT	0	101	-	-	5/51/51/51	-
13	BCL	5	102	-	-	13/37/137/137	-
7	HEC	C	504	1	-	0/6/54/54	-
13	BCL	F	102	-	-	11/37/137/137	-
12	PGV	C	509	-	-	4/21/21/55	-
19	CRT	U	103	-	-	3/51/51/51	-
15	UQ8	L	309	-	-	1/9/33/75	0/1/1/1
13	BCL	M	401	-	-	4/37/137/137	-
21	LDA	I	104	-	-	4/13/13/13	-
12	PGV	D	104	-	-	11/39/39/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	Q	101	-	-	15/37/137/137	-
19	CRT	2	101	-	-	3/51/51/51	-
14	BPH	L	302	-	-	7/54/105/105	0/5/6/6
9	GOL	H	301	-	-	0/4/4/4	-
13	BCL	S	102	-	-	18/37/137/137	-
13	BCL	A	101	-	-	15/37/137/137	-
13	BCL	I	102	-	-	10/37/137/137	-
22	CDL	Q	104	-	-	36/85/85/110	-
14	BPH	M	404	-	-	10/54/105/105	0/5/6/6
19	CRT	J	101	-	-	1/51/51/51	-
13	BCL	U	102	-	-	15/37/137/137	-
13	BCL	M	402	-	-	15/37/137/137	-
13	BCL	5	101	-	-	11/37/137/137	-
23	LMT	M	419	-	-	6/21/61/61	0/2/2/2
19	CRT	O	103	-	-	4/51/51/51	-
19	CRT	M	406	-	-	5/51/51/51	-
19	CRT	A	104	-	-	0/51/51/51	-
13	BCL	Y	101	-	-	11/37/137/137	-
21	LDA	V	102	-	-	5/13/13/13	-
22	CDL	M	415	-	-	15/48/48/110	-
7	HEC	C	502	1	-	0/6/54/54	-
22	CDL	D	103	-	-	18/50/50/110	-
21	LDA	M	411	-	-	6/11/11/13	-
13	BCL	Z	102	-	-	15/37/137/137	-
13	BCL	9	103	-	-	16/37/137/137	-
13	BCL	M	403	-	-	6/37/137/137	-
22	CDL	K	103	-	-	32/96/96/110	-
21	LDA	J	102	-	-	3/13/13/13	-
13	BCL	D	101	-	-	13/37/137/137	-
22	CDL	S	103	-	-	29/71/71/110	-
13	BCL	3	102	-	-	18/37/137/137	-
13	BCL	1	102	-	-	14/37/137/137	-
7	HEC	C	503	1	-	0/6/54/54	-
9	GOL	C	506	-	-	2/4/4/4	-
19	CRT	Q	103	-	-	3/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	UQ8	L	303	-	-	3/27/51/75	0/1/1/1
13	BCL	7	102	-	-	13/37/137/137	-
13	BCL	O	101	-	-	5/37/137/137	-
19	CRT	9	102	-	-	4/51/51/51	-
20	PEF	M	418	-	-	19/50/50/50	-
19	CRT	1	103	-	-	1/51/51/51	-
15	UQ8	L	308	-	-	9/51/75/75	0/1/1/1
13	BCL	F	101	-	-	12/37/137/137	-
13	BCL	K	101	-	-	13/37/137/137	-
22	CDL	Y	102	5	-	25/50/50/110	-

The worst 5 of 445 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	303	UQ8	C6-C1	8.04	1.49	1.35
15	M	417	UQ8	C6-C1	7.75	1.49	1.35
15	L	309	UQ8	C6-C1	7.72	1.49	1.35
18	M	405	MQ8	C3-C2	7.48	1.48	1.35
21	O	104	LDA	O1-N1	-7.15	1.25	1.42

The worst 5 of 1094 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	102	BCL	C1D-CHD-C4C	-8.82	112.86	125.88
13	3	102	BCL	C1D-CHD-C4C	-8.24	113.71	125.88
13	M	402	BCL	C4A-NA-C1A	-7.80	103.20	106.71
13	A	101	BCL	C4A-NA-C1A	-7.67	103.26	106.71
13	K	102	BCL	C1D-CHD-C4C	-7.66	114.57	125.88

There are no chirality outliers.

5 of 900 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	K	104	PEF	O4P-C4-C5-N
13	7	101	BCL	C2-C3-C5-C6
13	7	101	BCL	C4-C3-C5-C6
12	L	305	PGV	C04-O12-P-O13
22	Y	103	CDL	CB2-OB2-PB2-OB3

There are no ring outliers.

90 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	K	104	PEF	1	0
12	A	105	PGV	5	0
13	7	101	BCL	3	0
12	L	305	PGV	4	0
19	6	101	CRT	2	0
13	O	102	BCL	4	0
23	F	103	LMT	5	0
15	M	417	UQ8	3	0
18	M	405	MQ8	5	0
12	L	306	PGV	4	0
13	S	101	BCL	5	0
22	H	304	CDL	3	0
21	O	104	LDA	1	0
15	7	103	UQ8	8	0
19	G	101	CRT	5	0
13	Z	102	BCL	7	0
22	H	302	CDL	3	0
13	0	102	BCL	8	0
12	3	104	PGV	3	0
19	Z	101	CRT	3	0
13	W	101	BCL	5	0
19	V	101	CRT	1	0
13	K	102	BCL	3	0
12	H	303	PGV	1	0
19	P	101	CRT	2	0
13	Q	102	BCL	4	0
19	9	101	CRT	4	0
12	M	414	PGV	3	0
19	N	101	CRT	4	0
20	I	103	PEF	1	0
13	U	101	BCL	8	0
13	I	101	BCL	4	0
13	W	102	BCL	2	0
13	D	102	BCL	4	0
13	1	101	BCL	5	0
13	L	301	BCL	4	0
13	A	103	BCL	4	0
19	0	101	CRT	2	0
13	5	102	BCL	4	0
7	C	504	HEC	1	0
13	F	102	BCL	3	0
19	U	103	CRT	2	0

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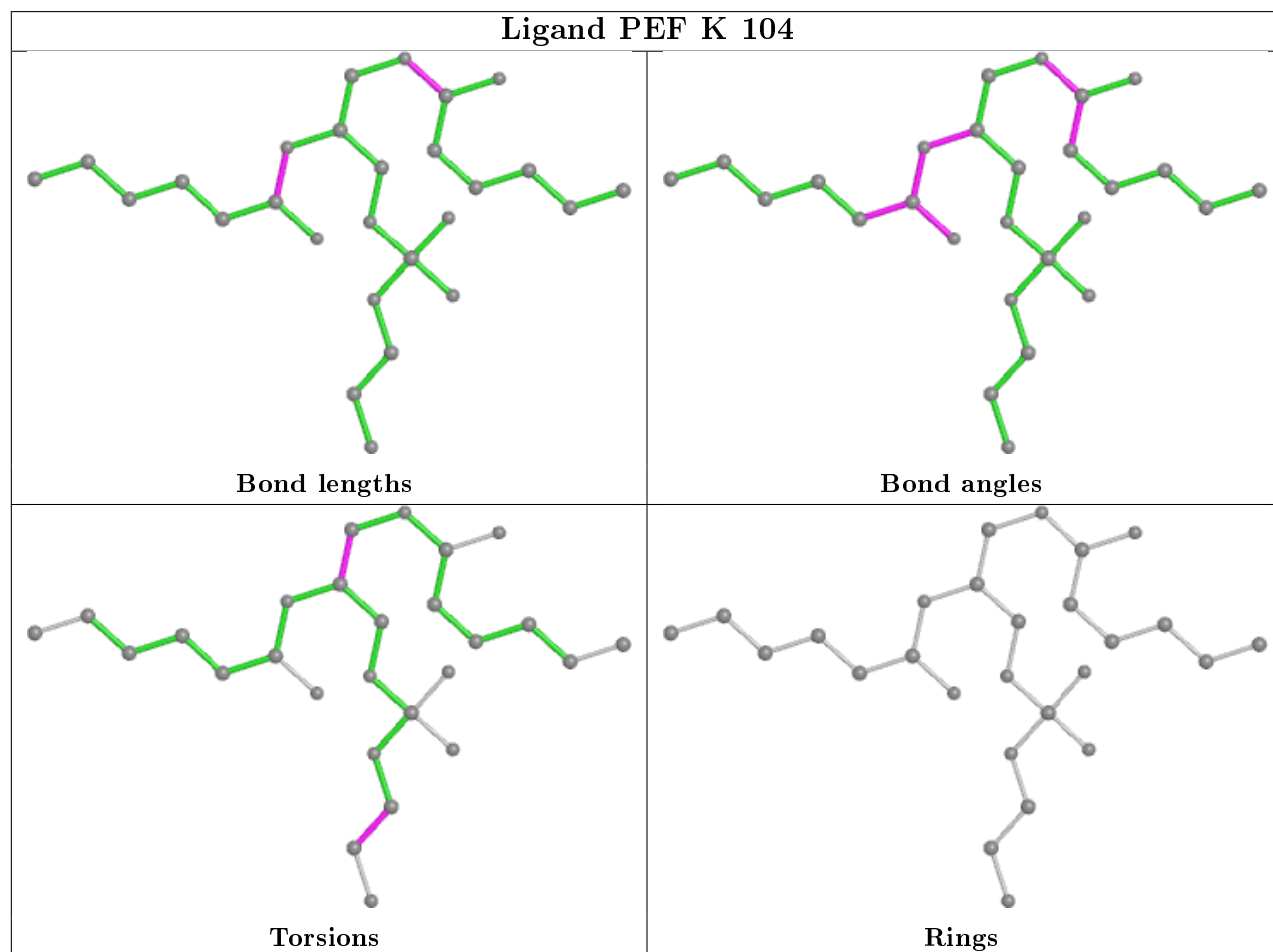
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L	309	UQ8	1	0
13	M	401	BCL	6	0
21	I	104	LDA	6	0
12	D	104	PGV	2	0
13	Q	101	BCL	6	0
19	2	101	CRT	6	0
14	L	302	BPH	6	0
9	H	301	GOL	1	0
13	S	102	BCL	6	0
13	A	101	BCL	4	0
13	I	102	BCL	4	0
22	Q	104	CDL	3	0
14	M	404	BPH	6	0
19	J	101	CRT	3	0
13	U	102	BCL	4	0
13	M	402	BCL	2	0
13	5	101	BCL	10	0
23	M	419	LMT	3	0
19	O	103	CRT	2	0
19	M	406	CRT	4	0
19	A	104	CRT	3	0
13	Y	101	BCL	5	0
22	M	415	CDL	1	0
20	5	103	PEF	1	0
22	D	103	CDL	2	0
21	M	411	LDA	1	0
12	M	413	PGV	4	0
13	9	103	BCL	4	0
13	M	403	BCL	1	0
22	K	103	CDL	4	0
21	J	102	LDA	1	0
13	D	101	BCL	2	0
22	S	103	CDL	10	0
13	3	102	BCL	4	0
13	1	102	BCL	7	0
7	C	503	HEC	2	0
13	3	101	BCL	4	0
19	Q	103	CRT	2	0
15	L	303	UQ8	2	0
13	7	102	BCL	5	0
13	O	101	BCL	4	0
19	9	102	CRT	2	0

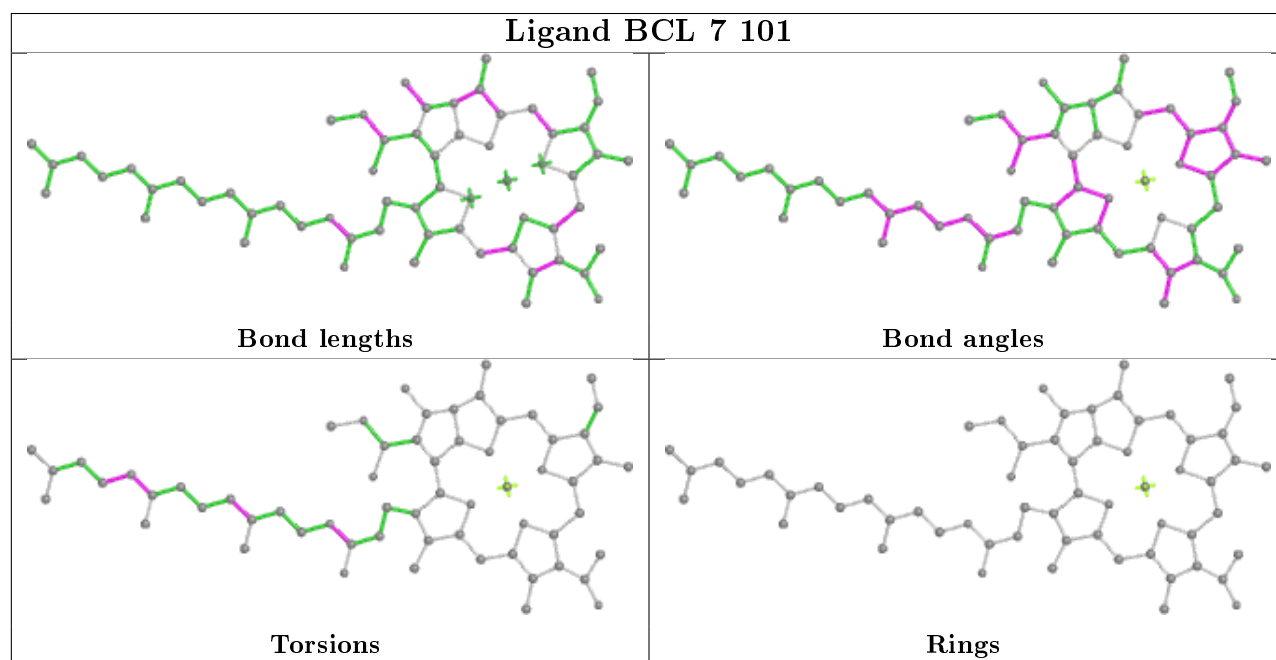
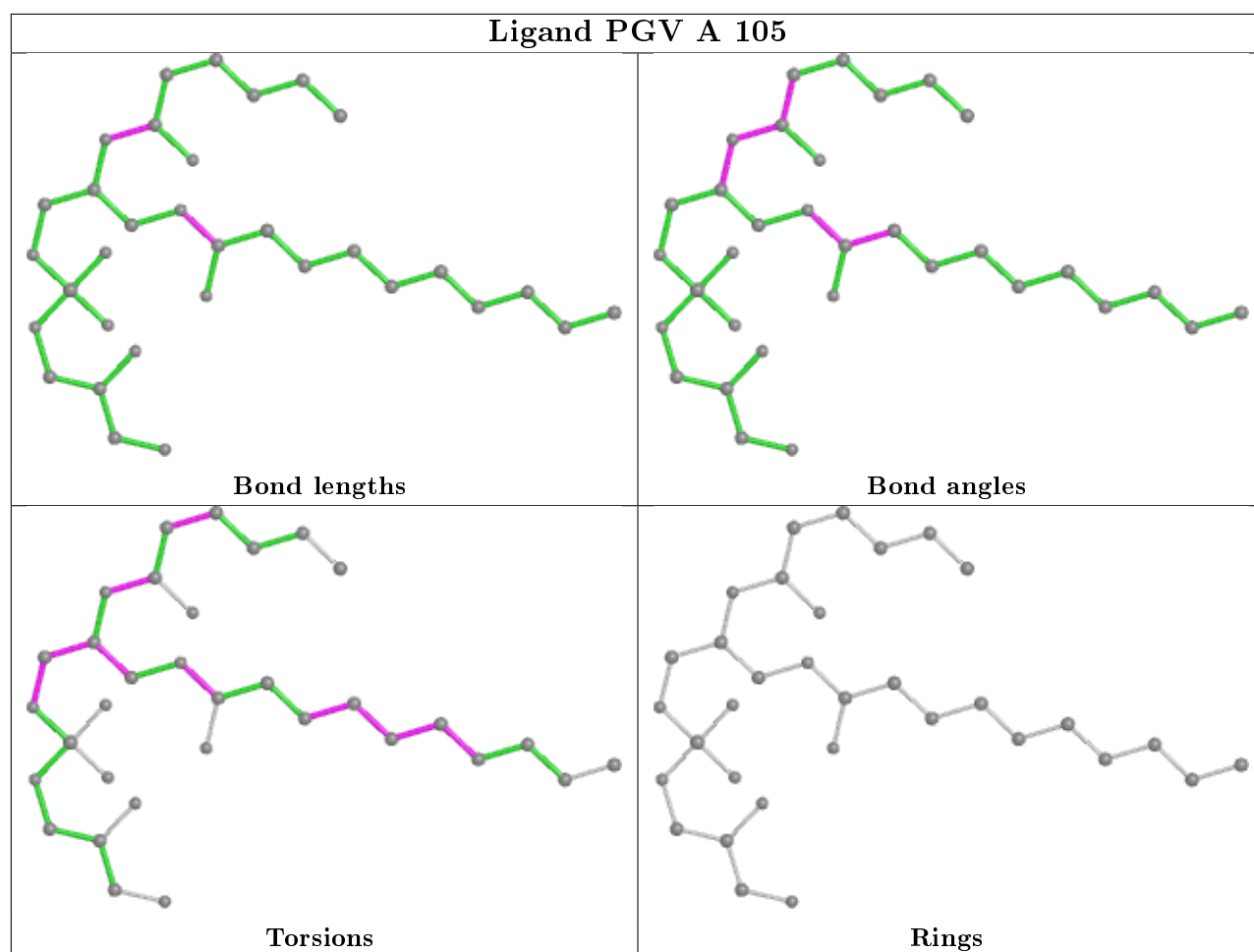
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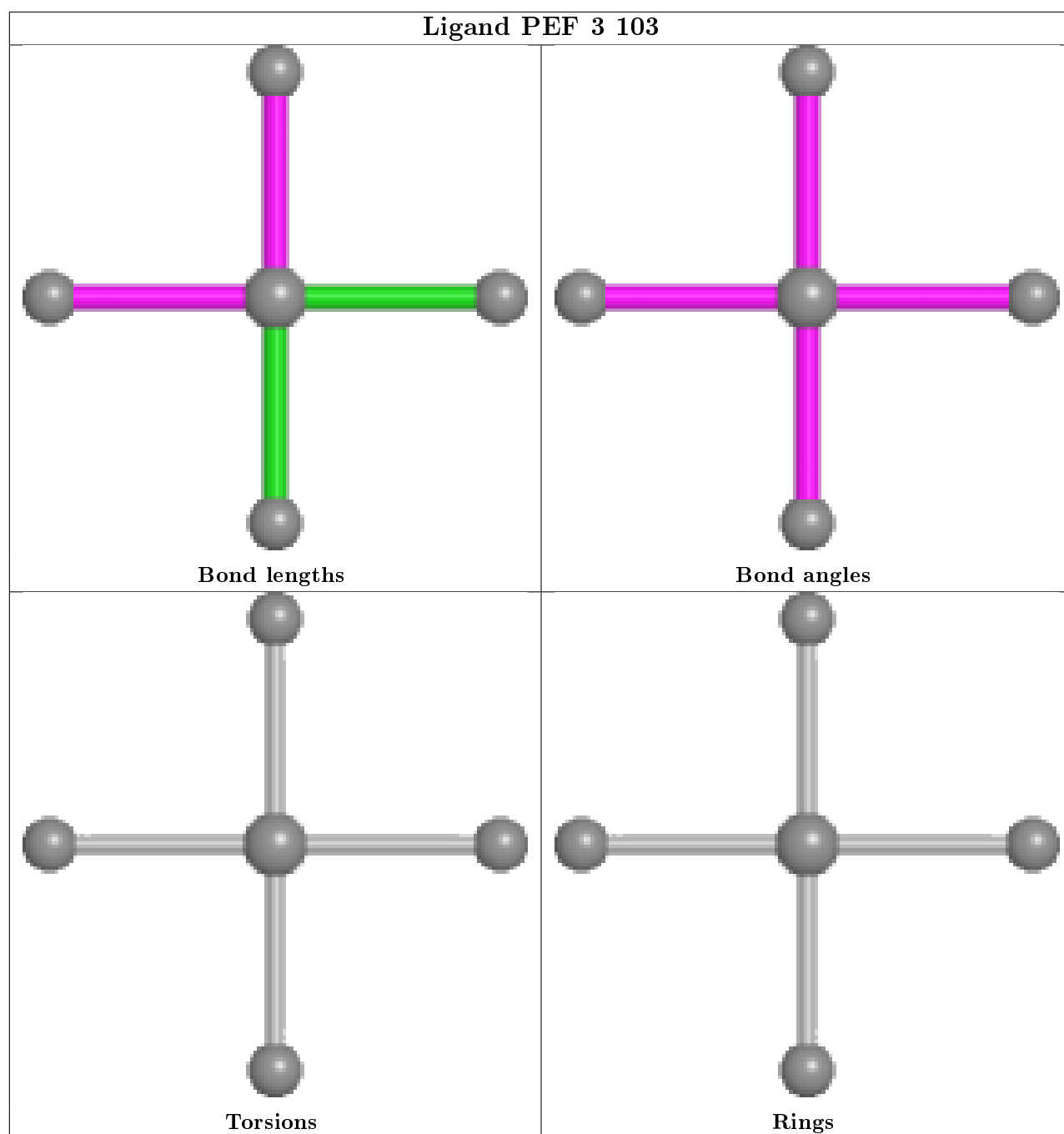
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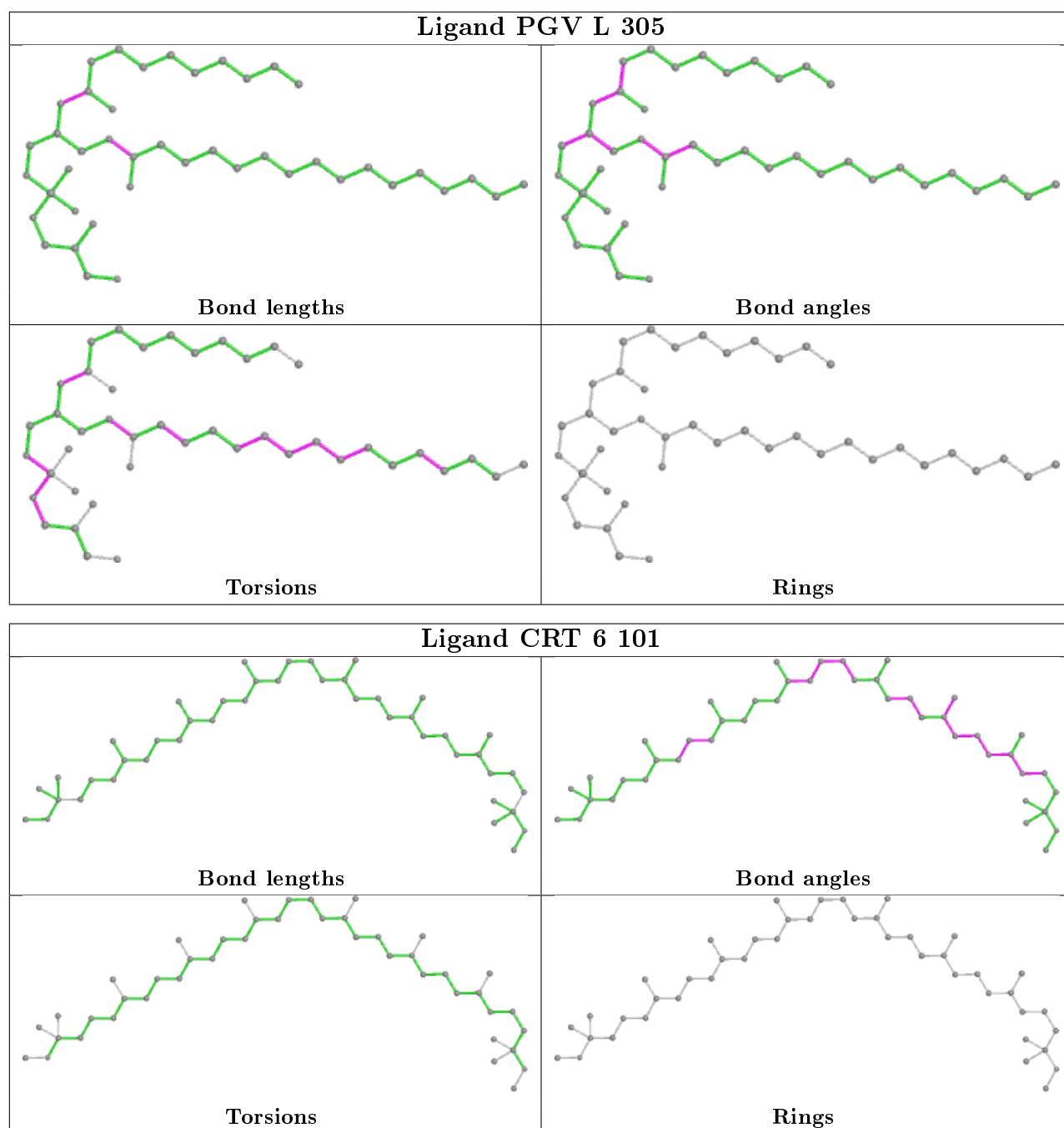
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	M	418	PEF	3	0
19	1	103	CRT	3	0
15	L	308	UQ8	7	0
13	F	101	BCL	2	0
13	K	101	BCL	2	0
22	Y	102	CDL	1	0

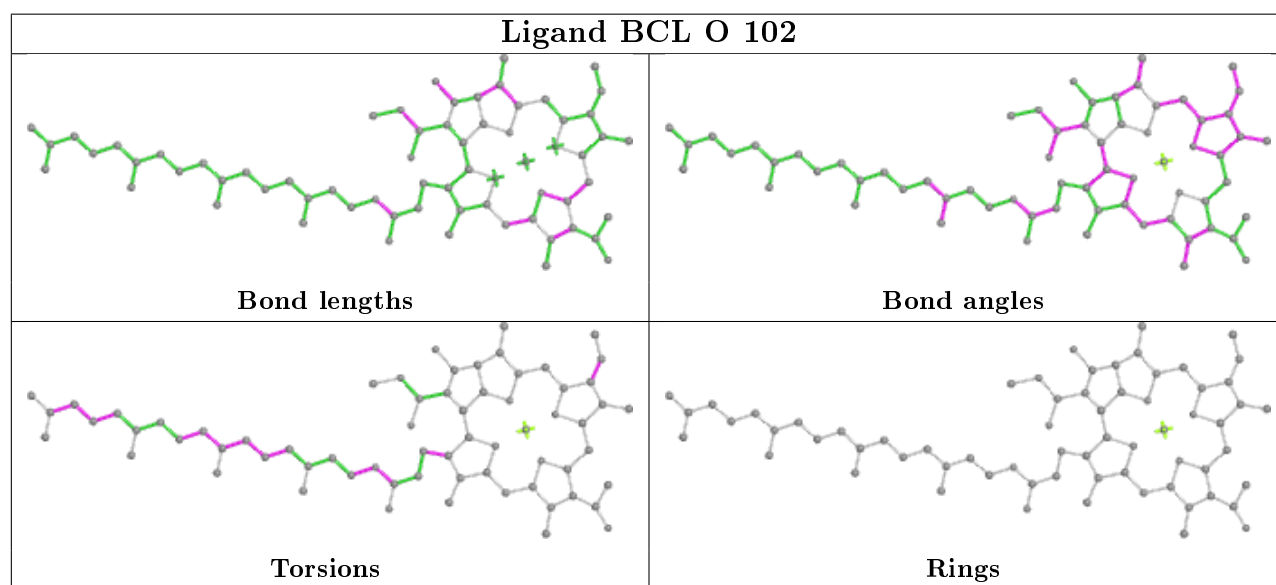
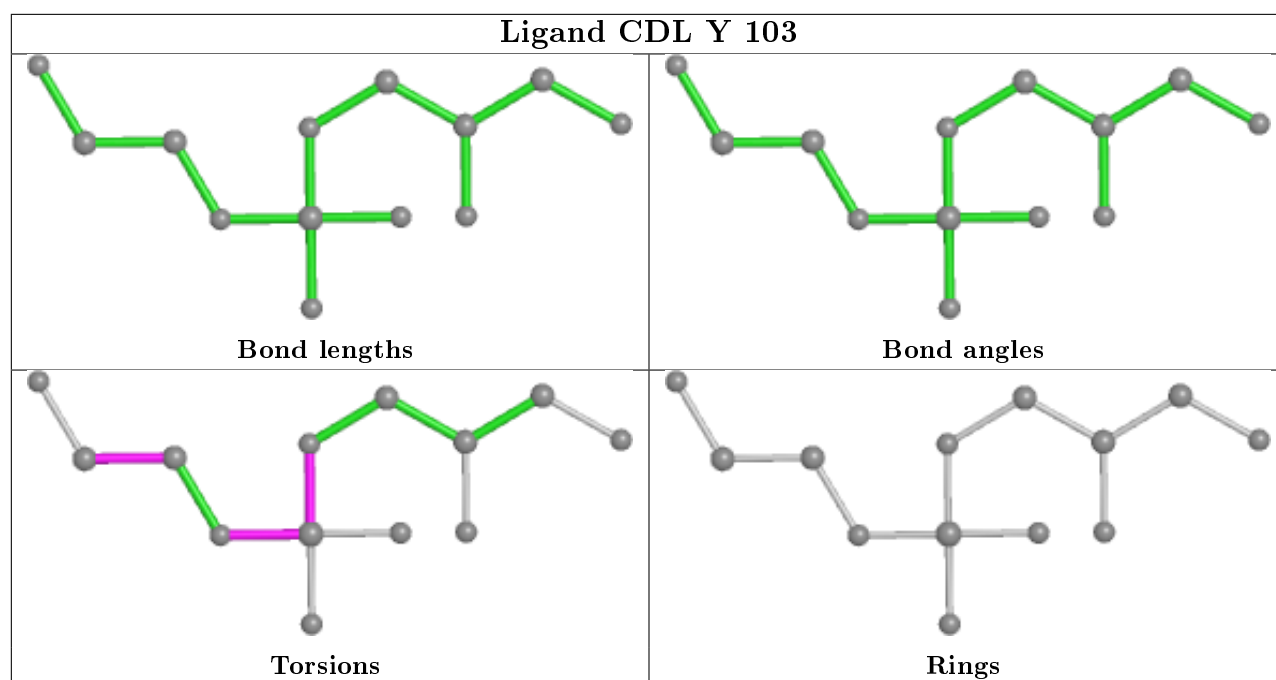
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

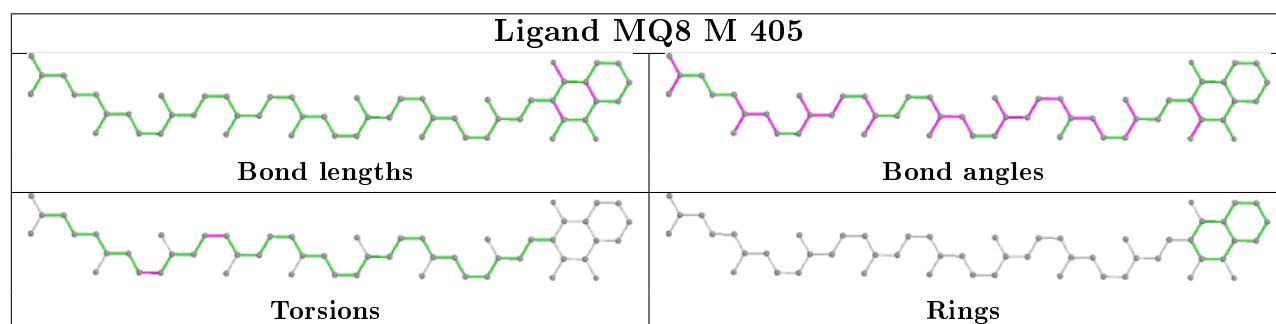
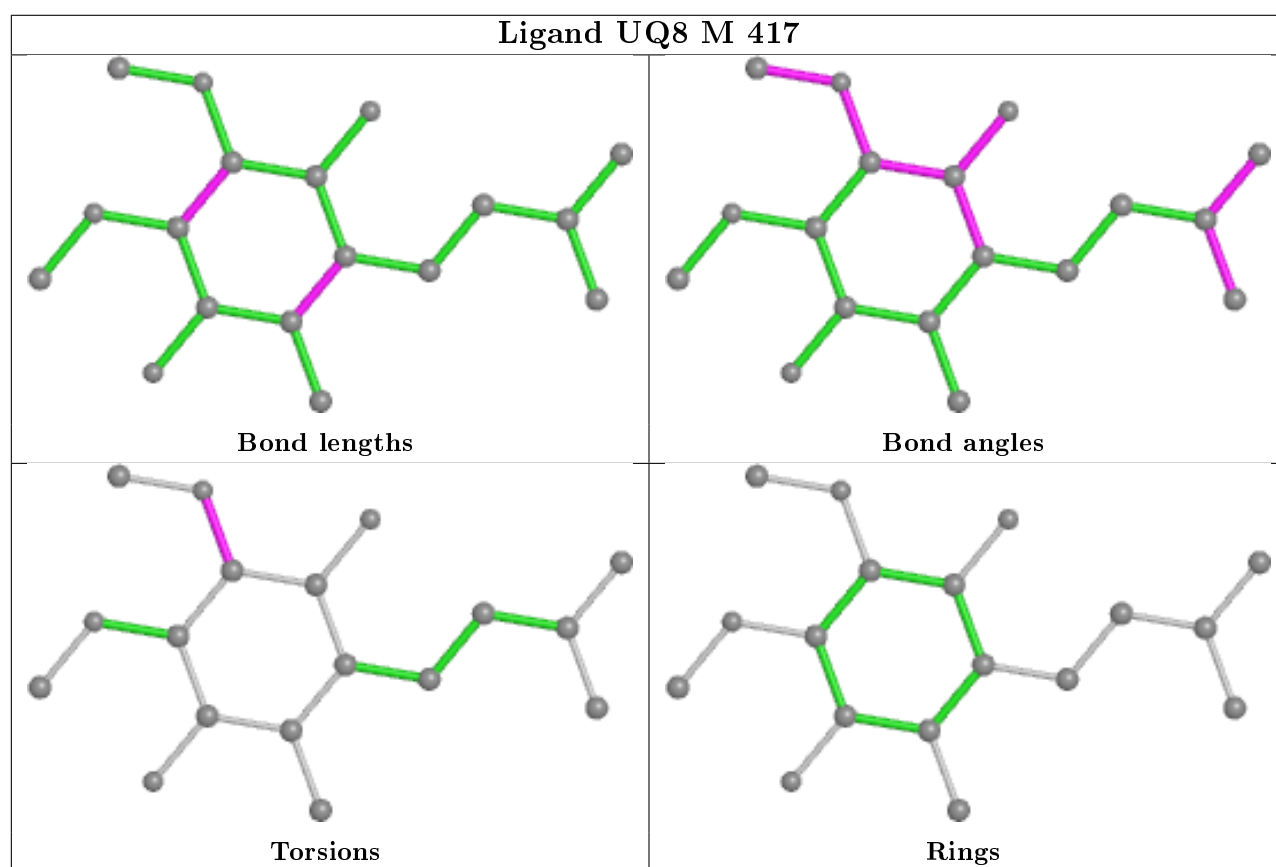
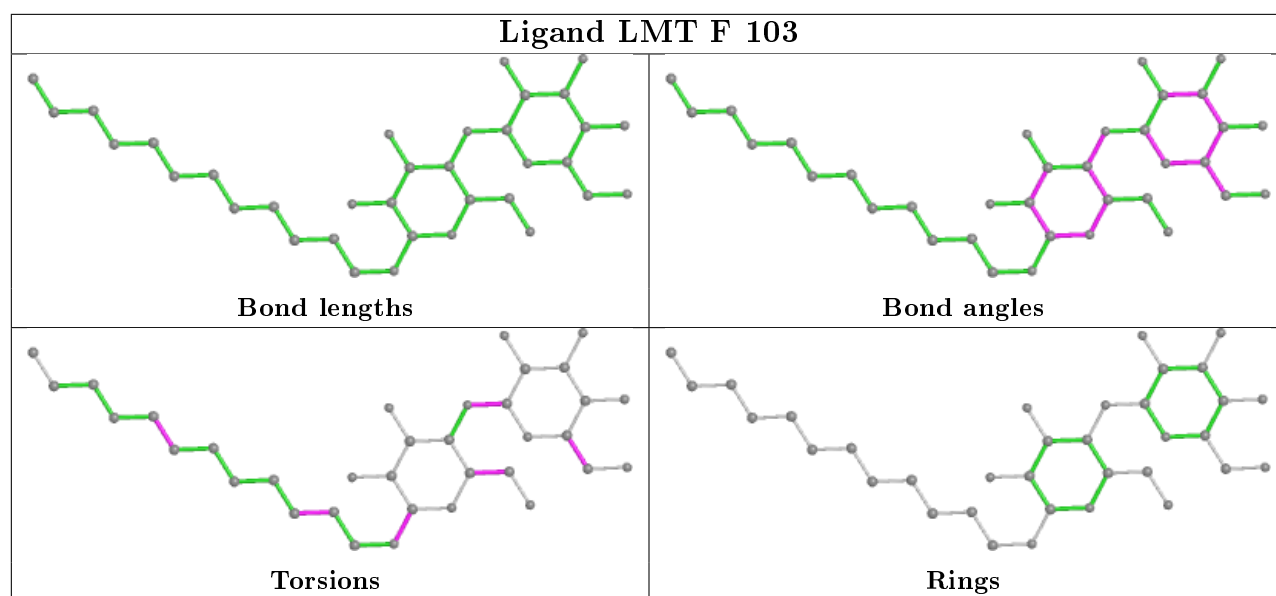


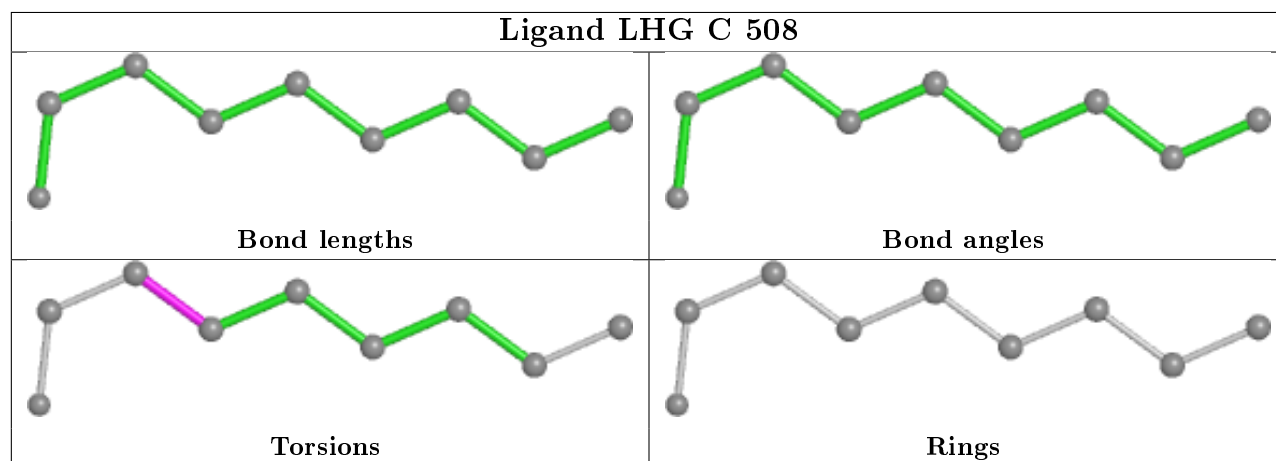
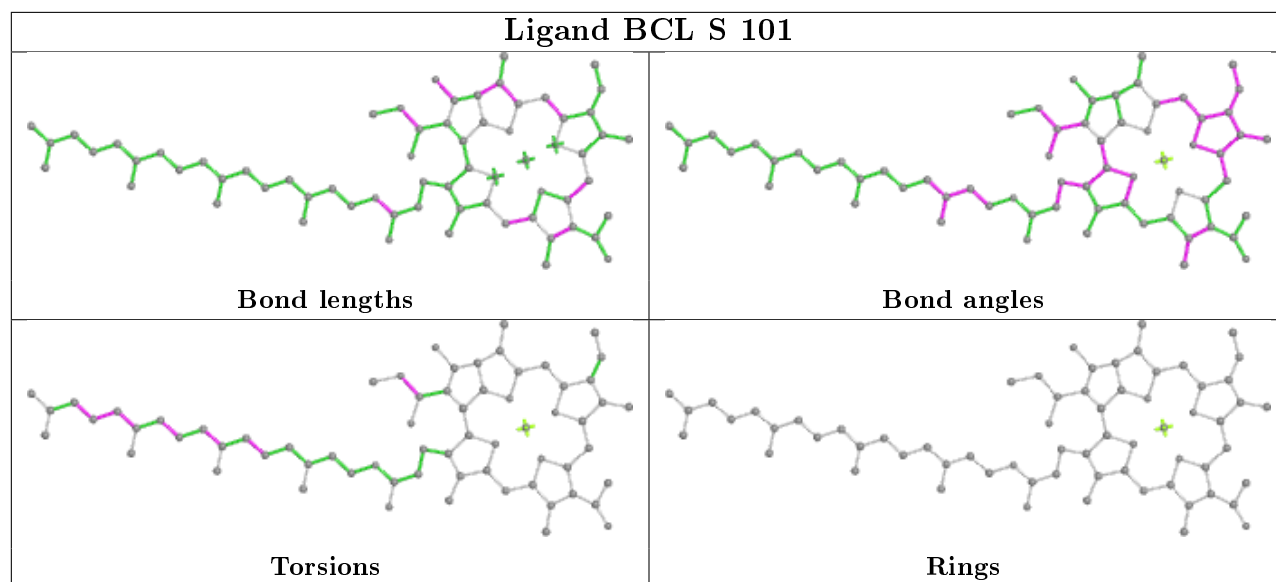
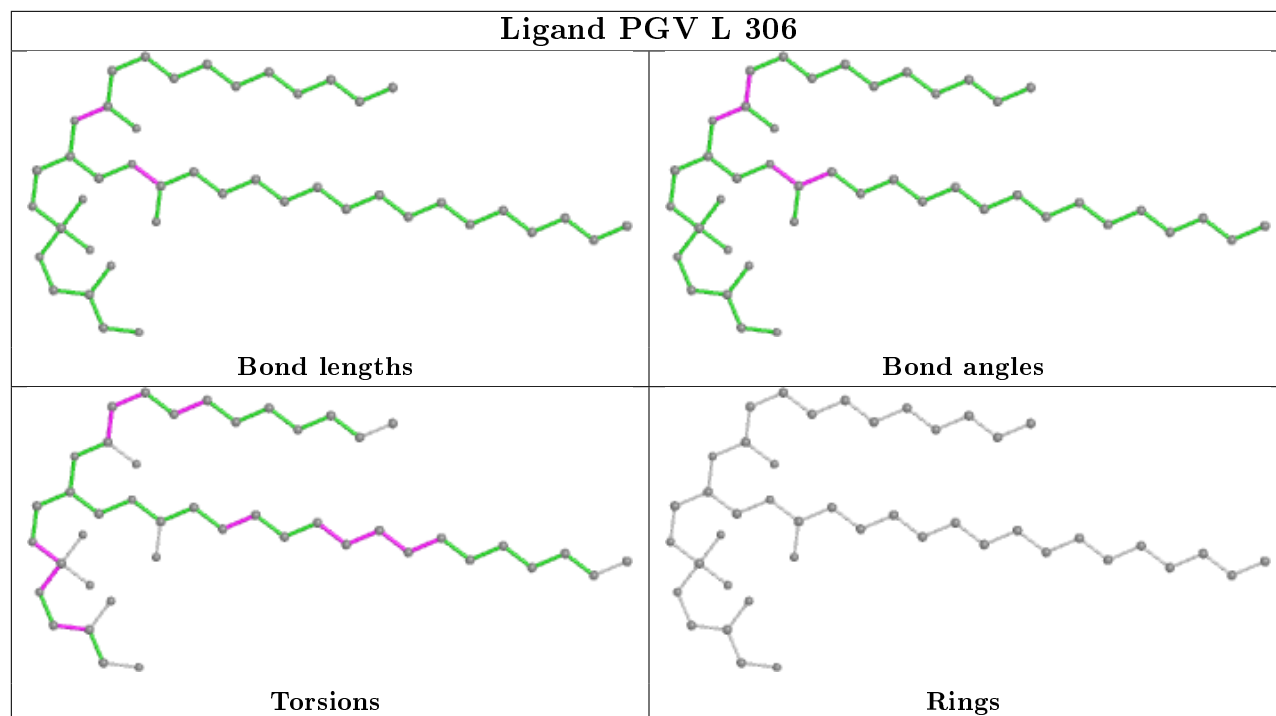


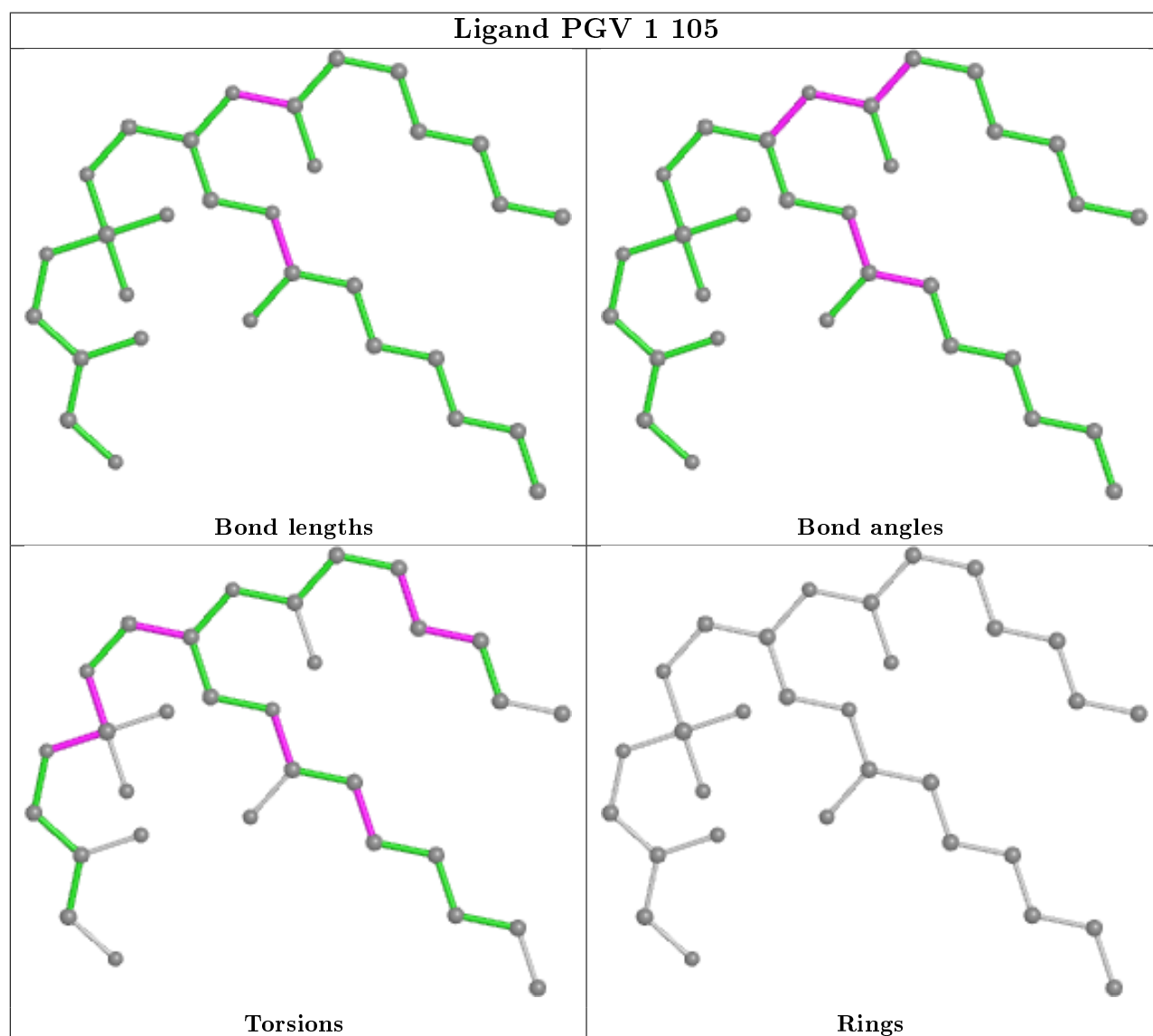
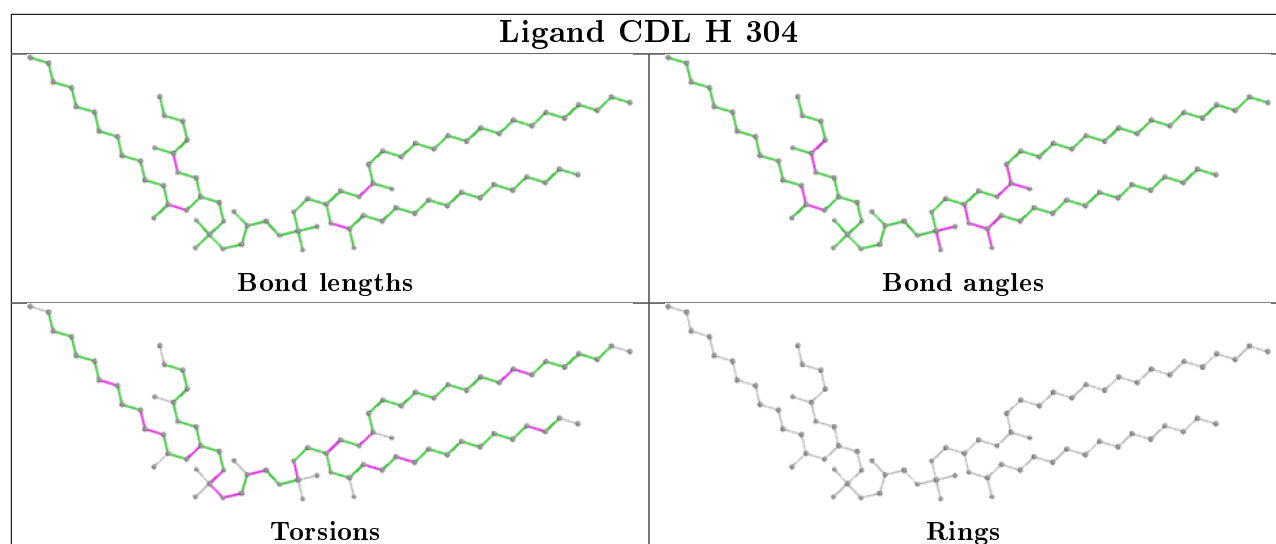


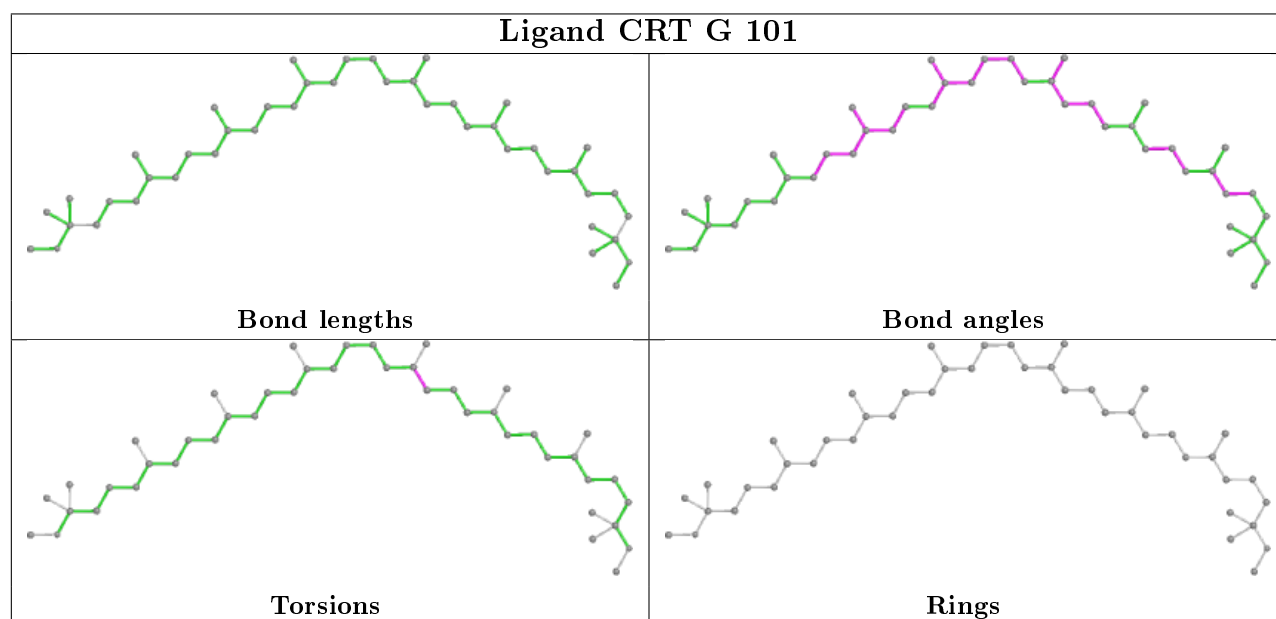
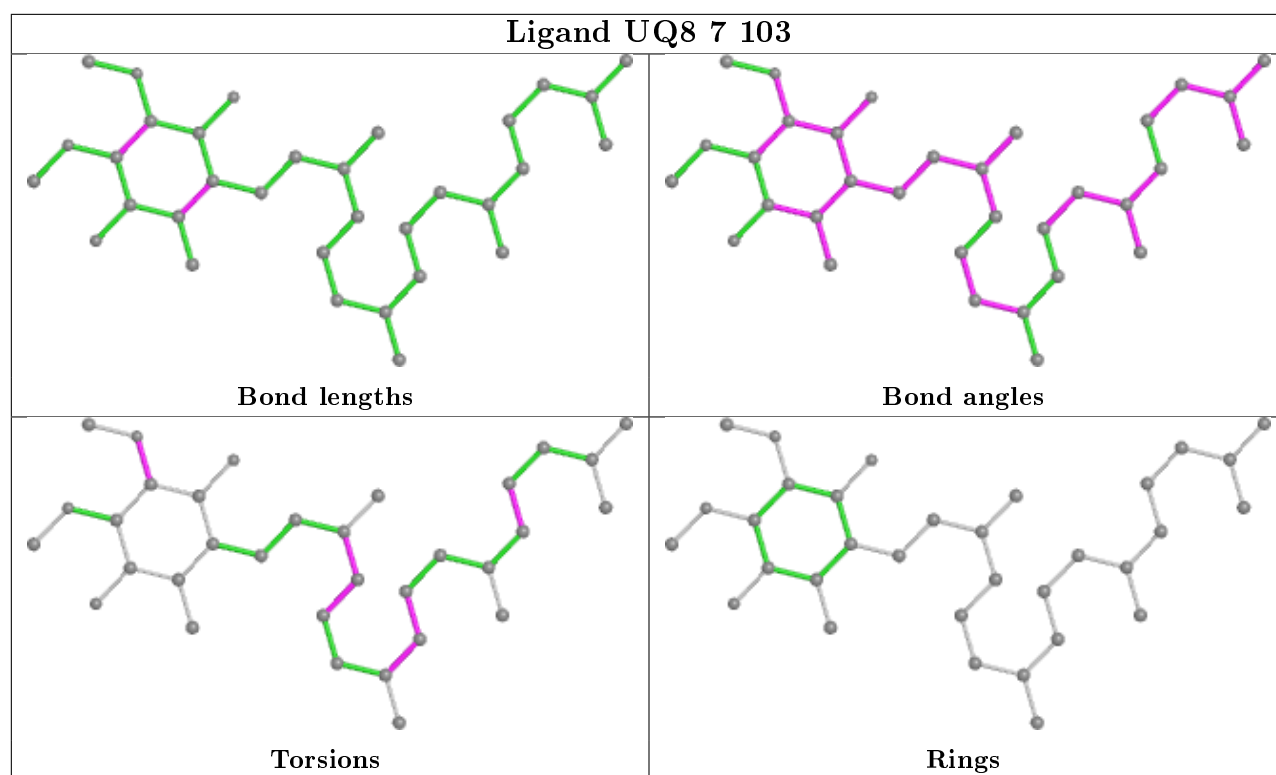


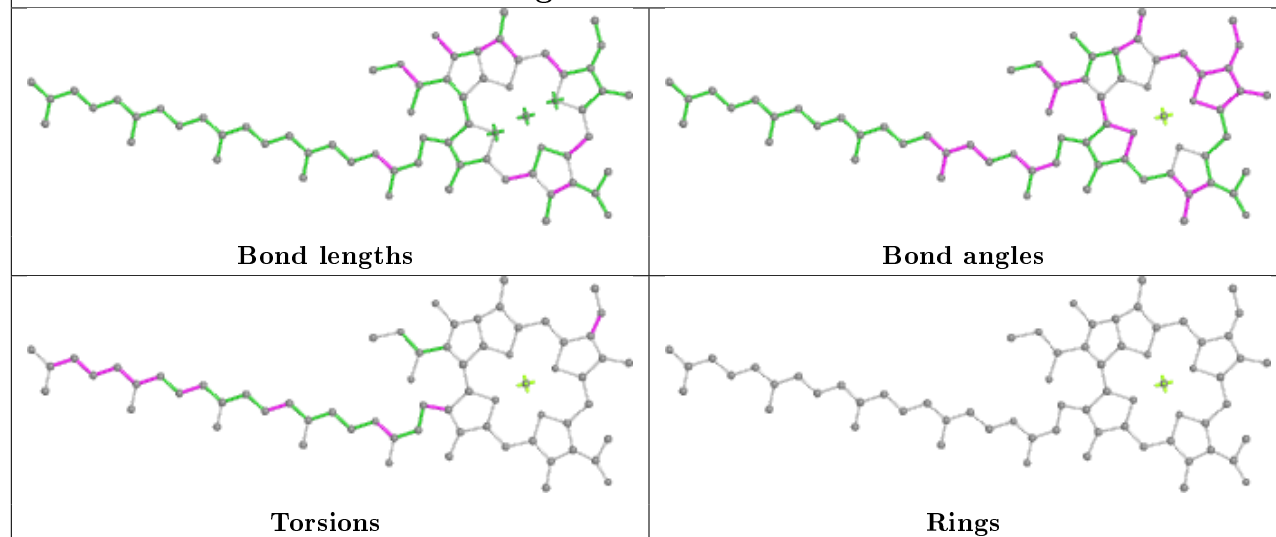
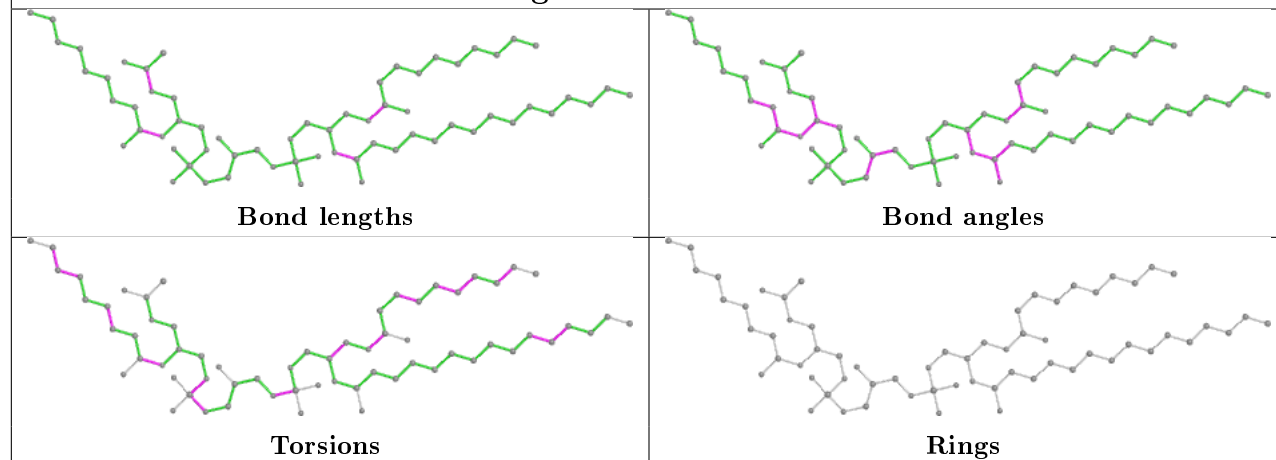
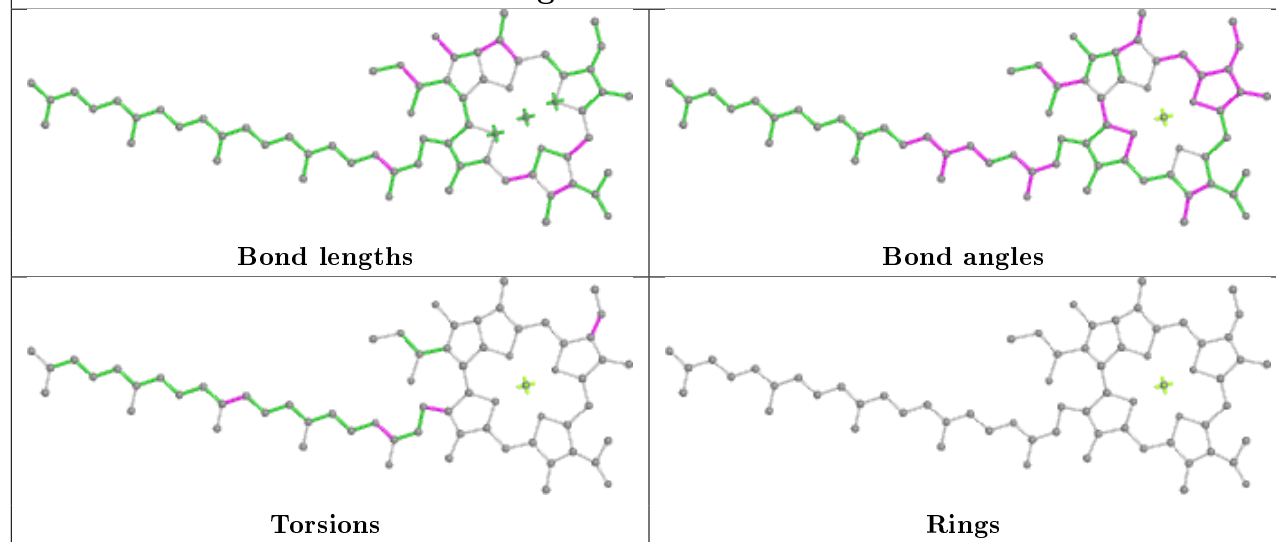


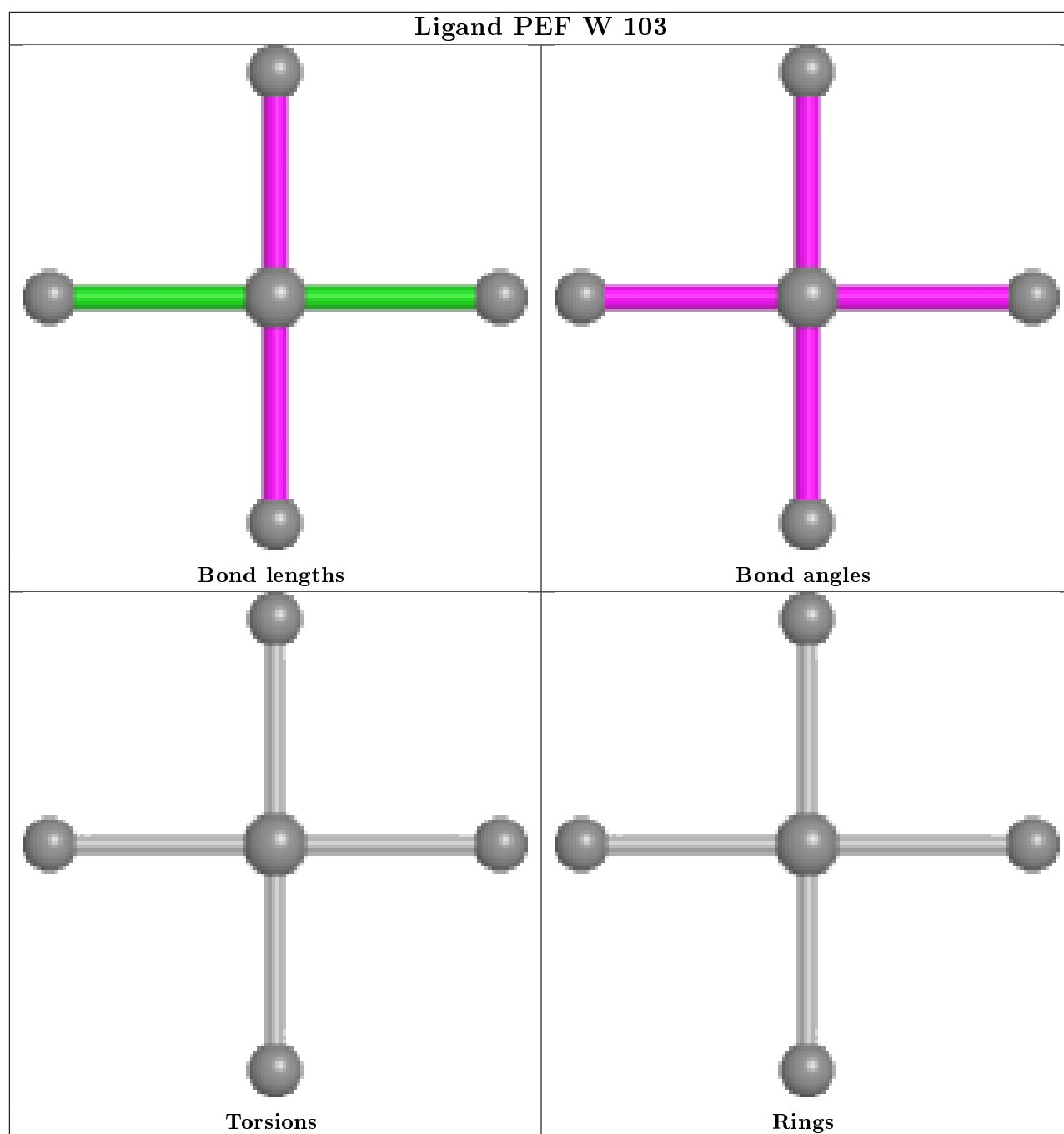




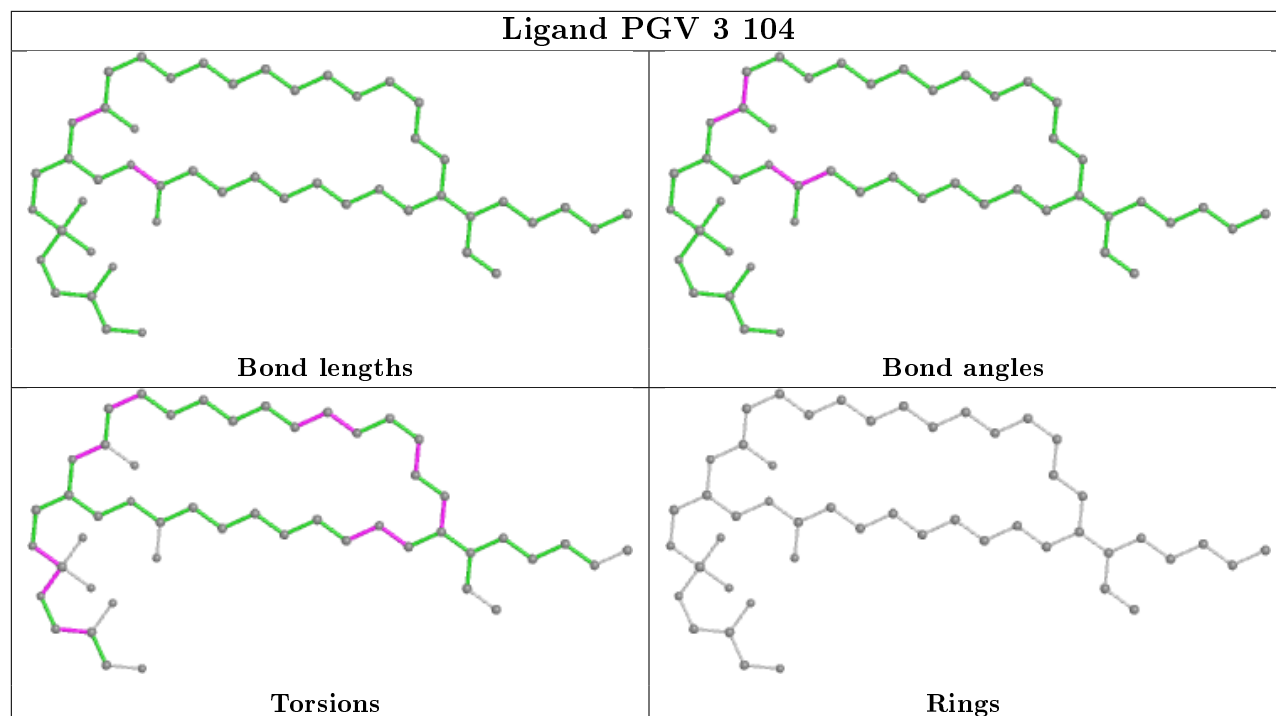




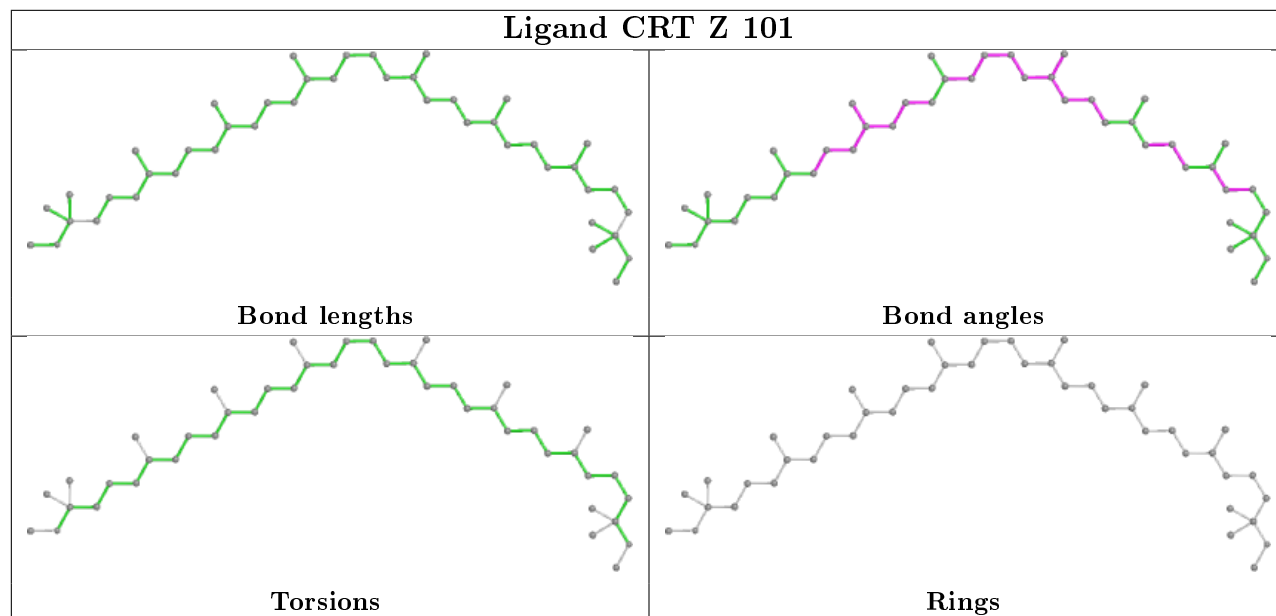
Ligand BCL Z 102**Ligand CDL H 302****Ligand BCL O 102**

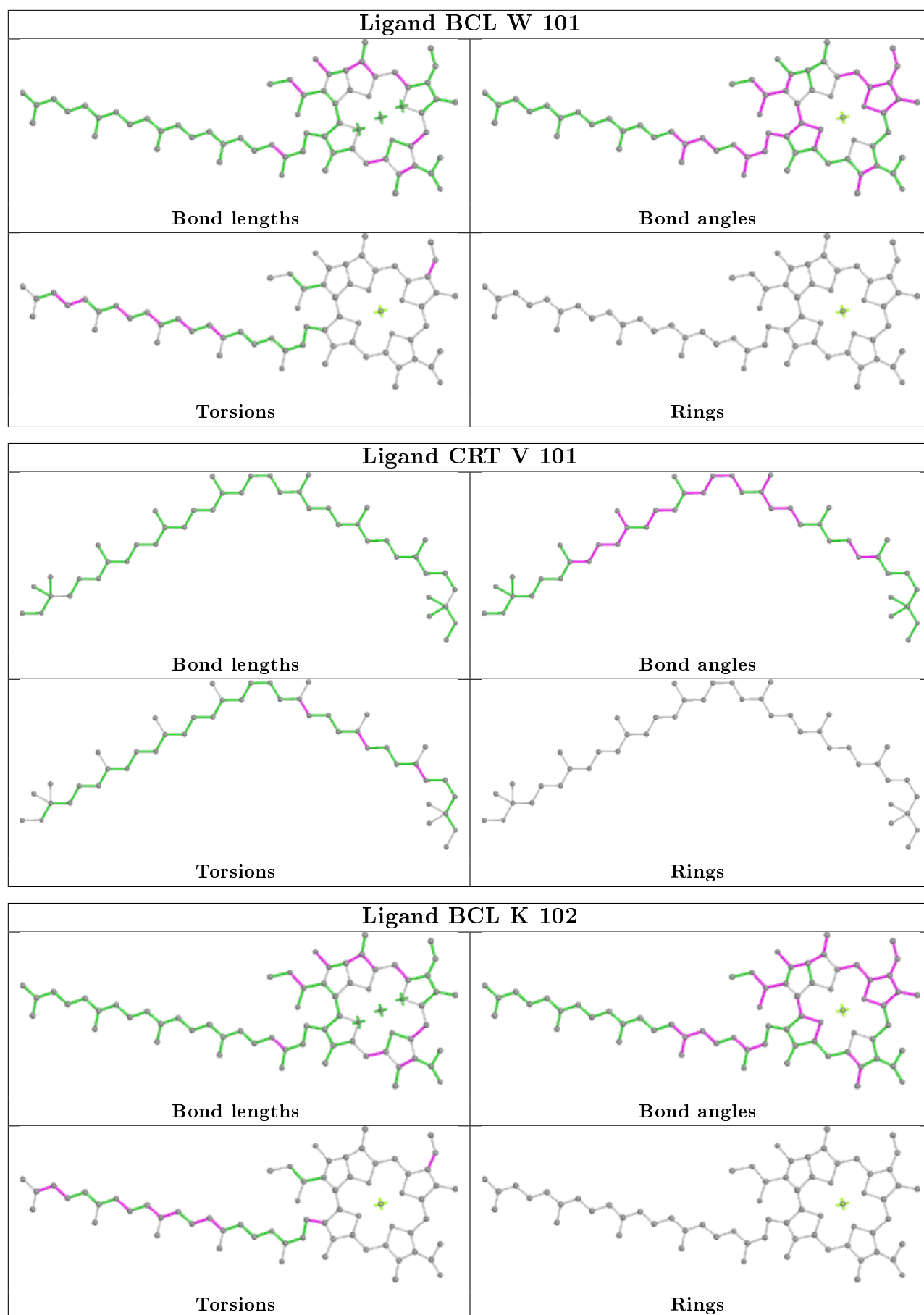


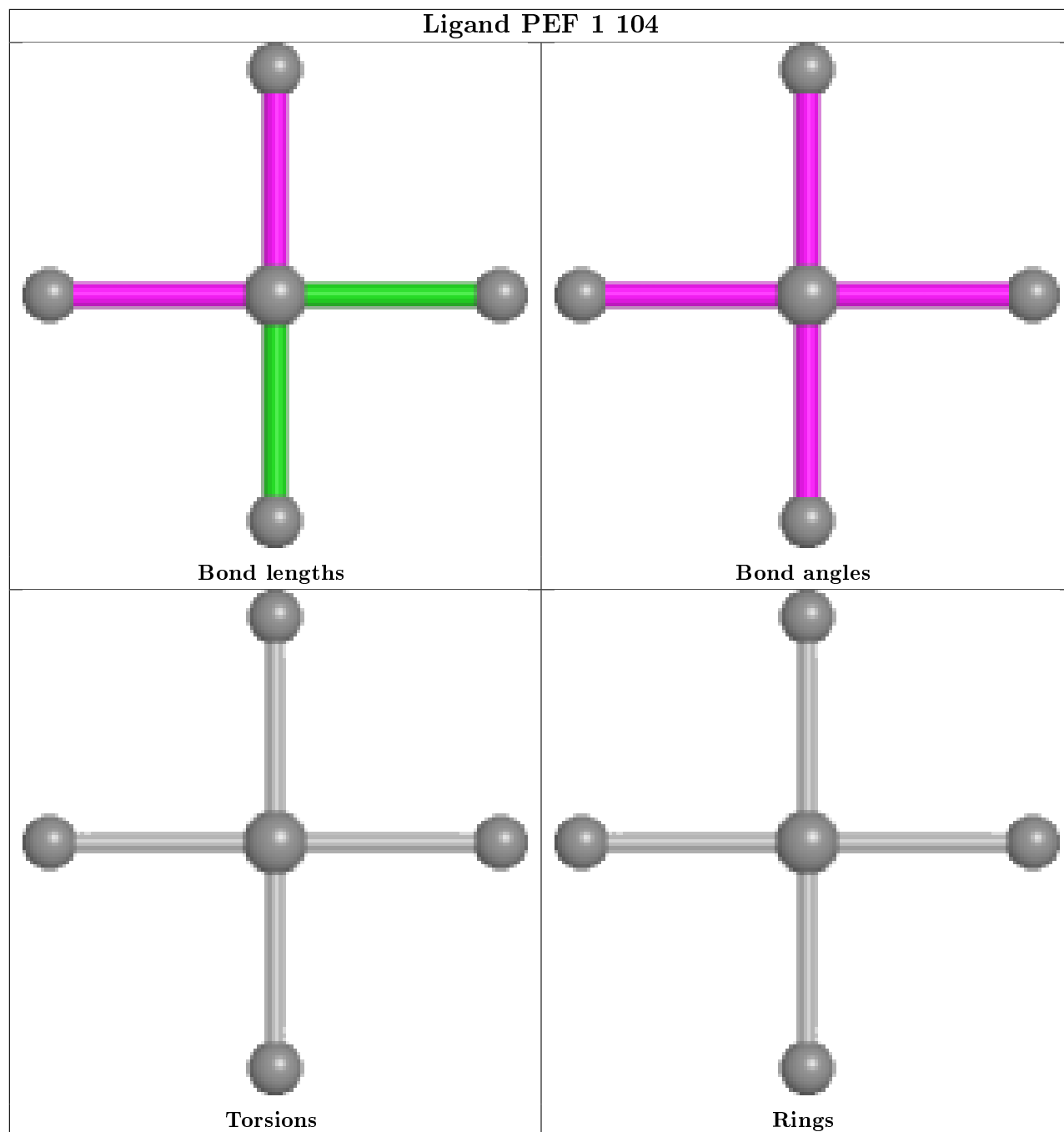
Ligand PGV 3 104

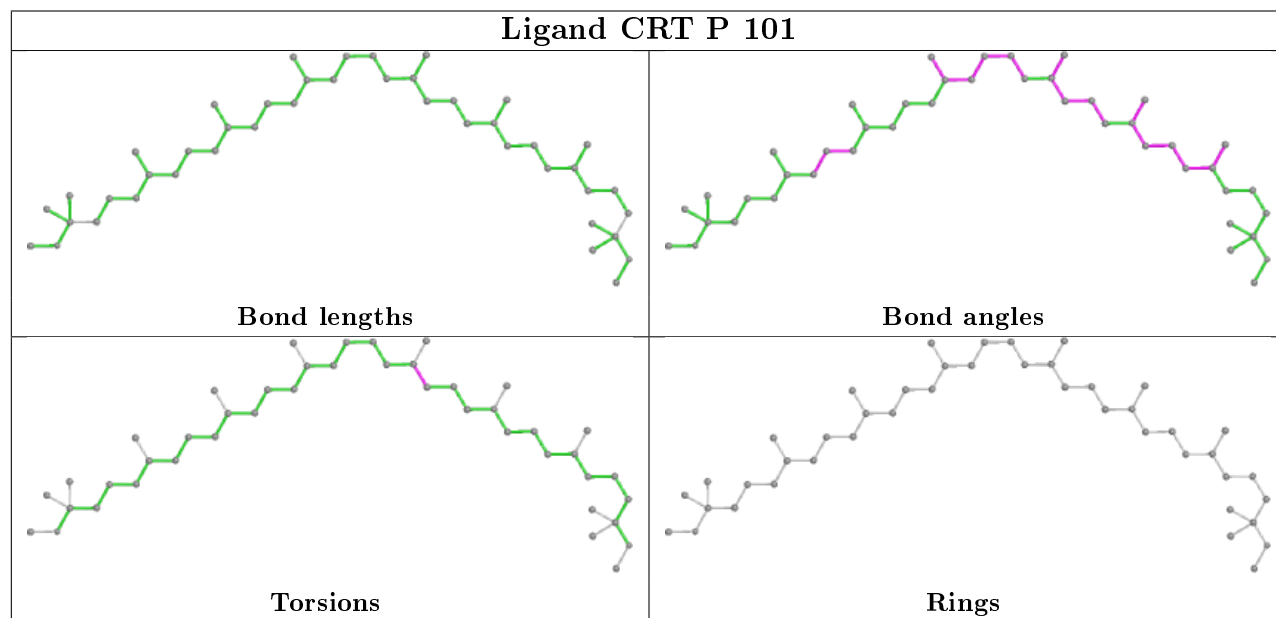
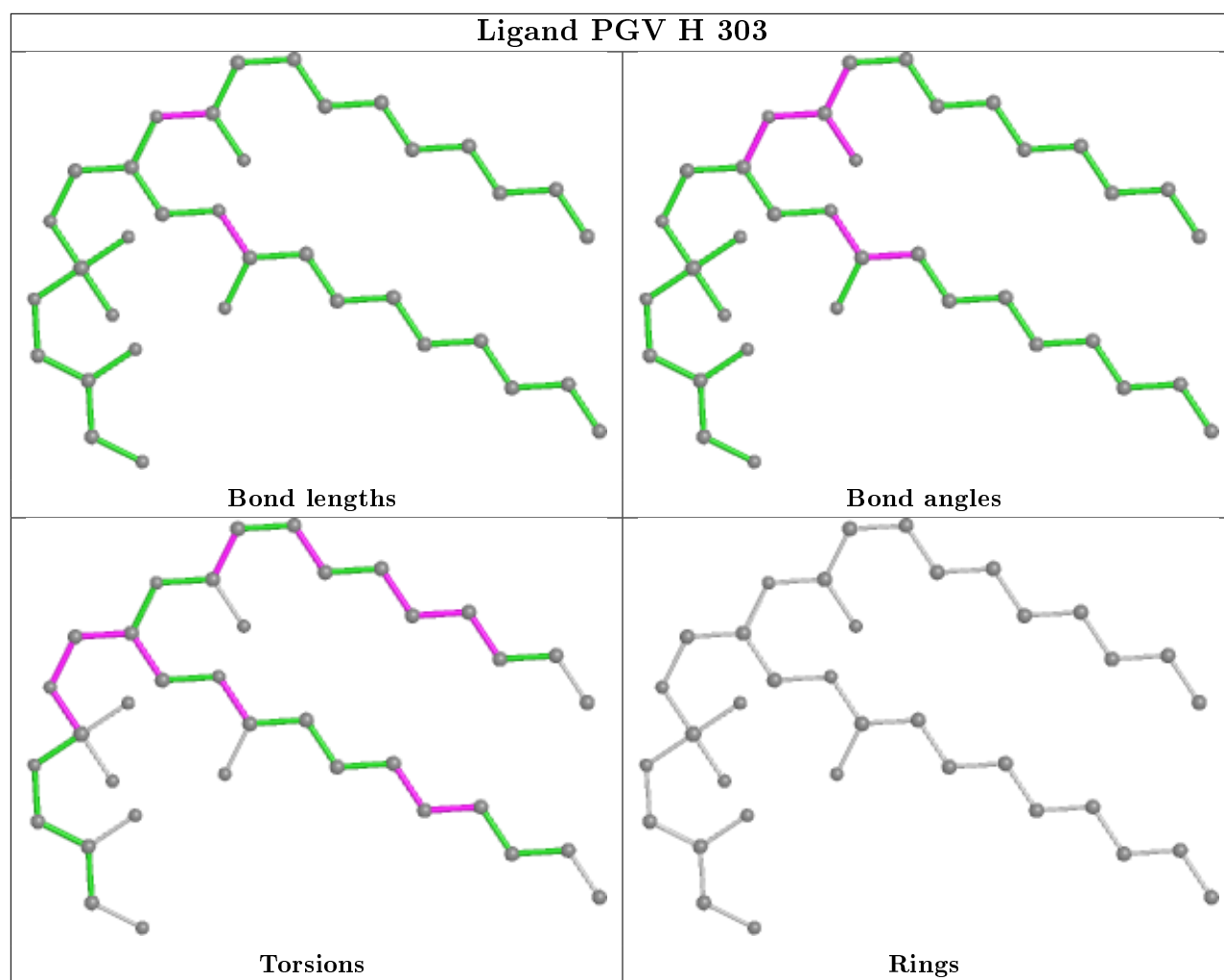


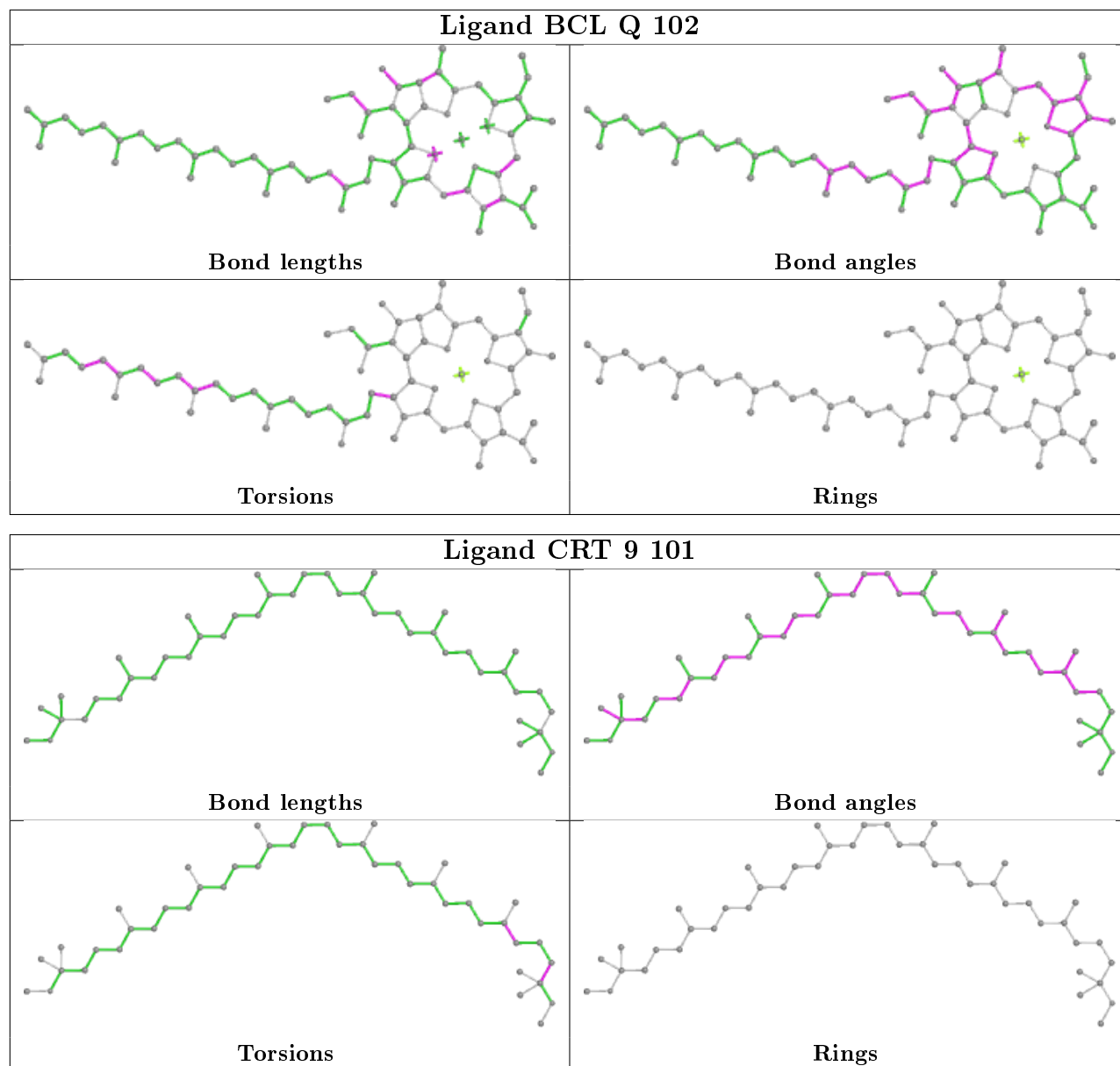
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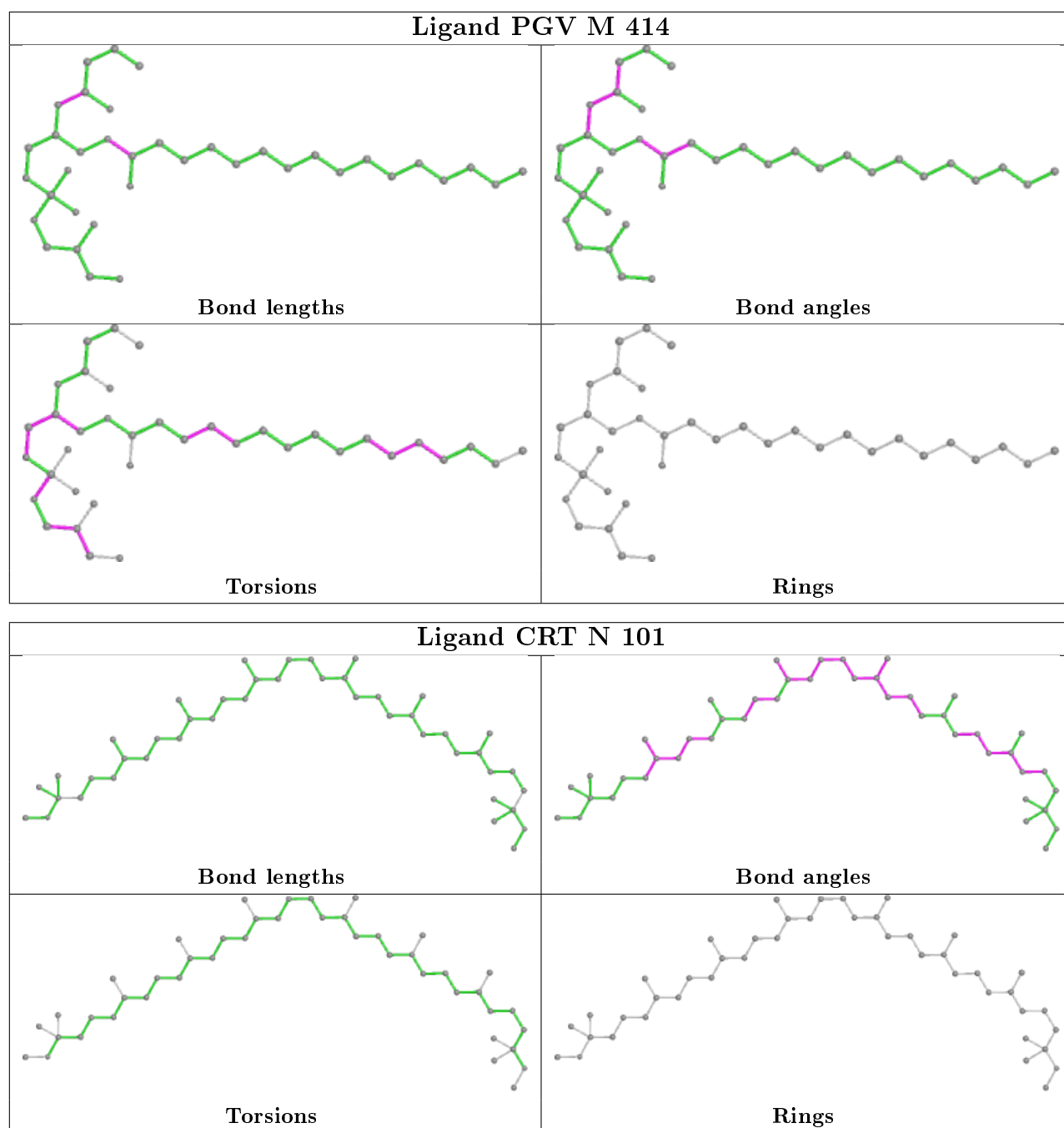


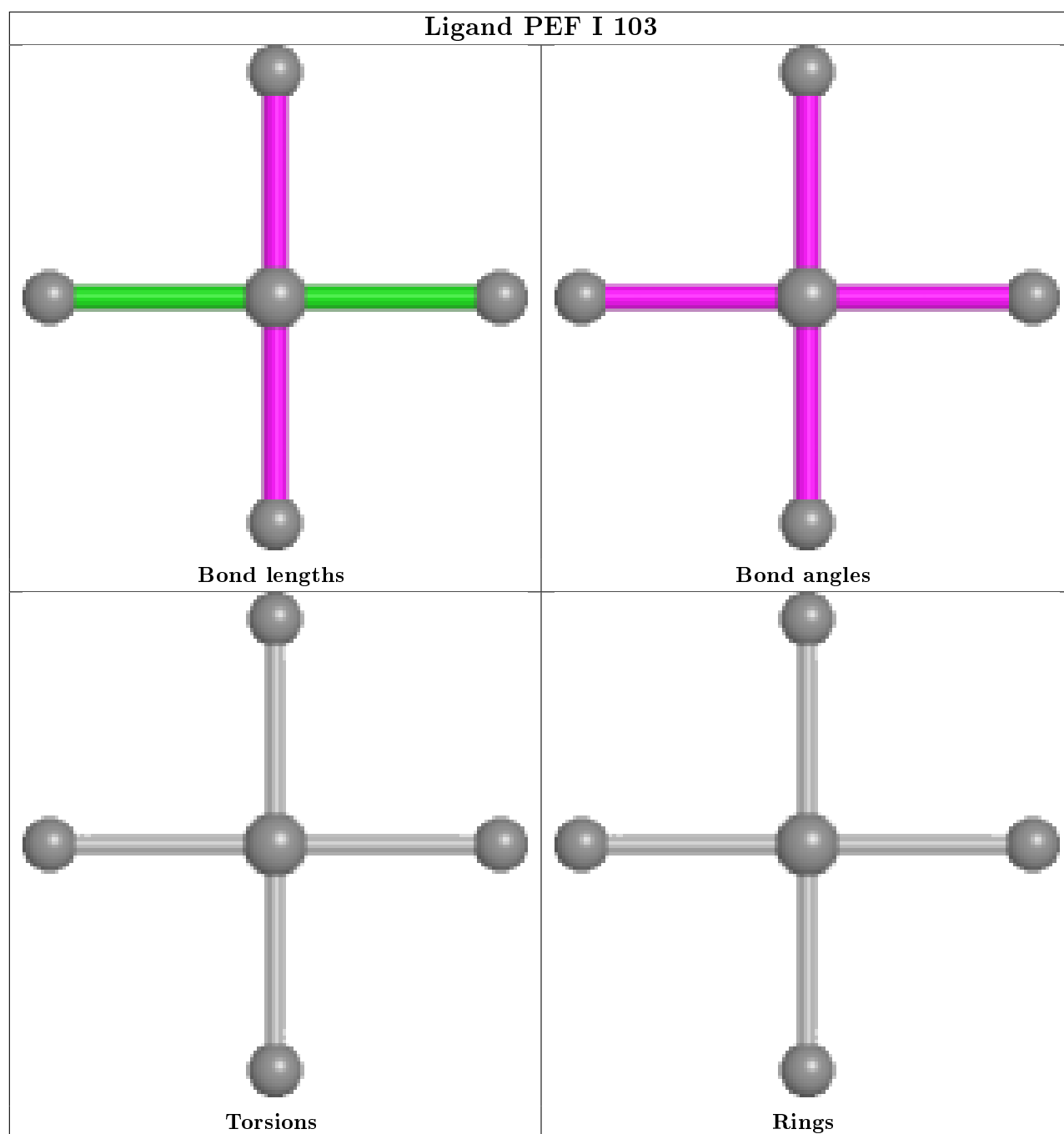


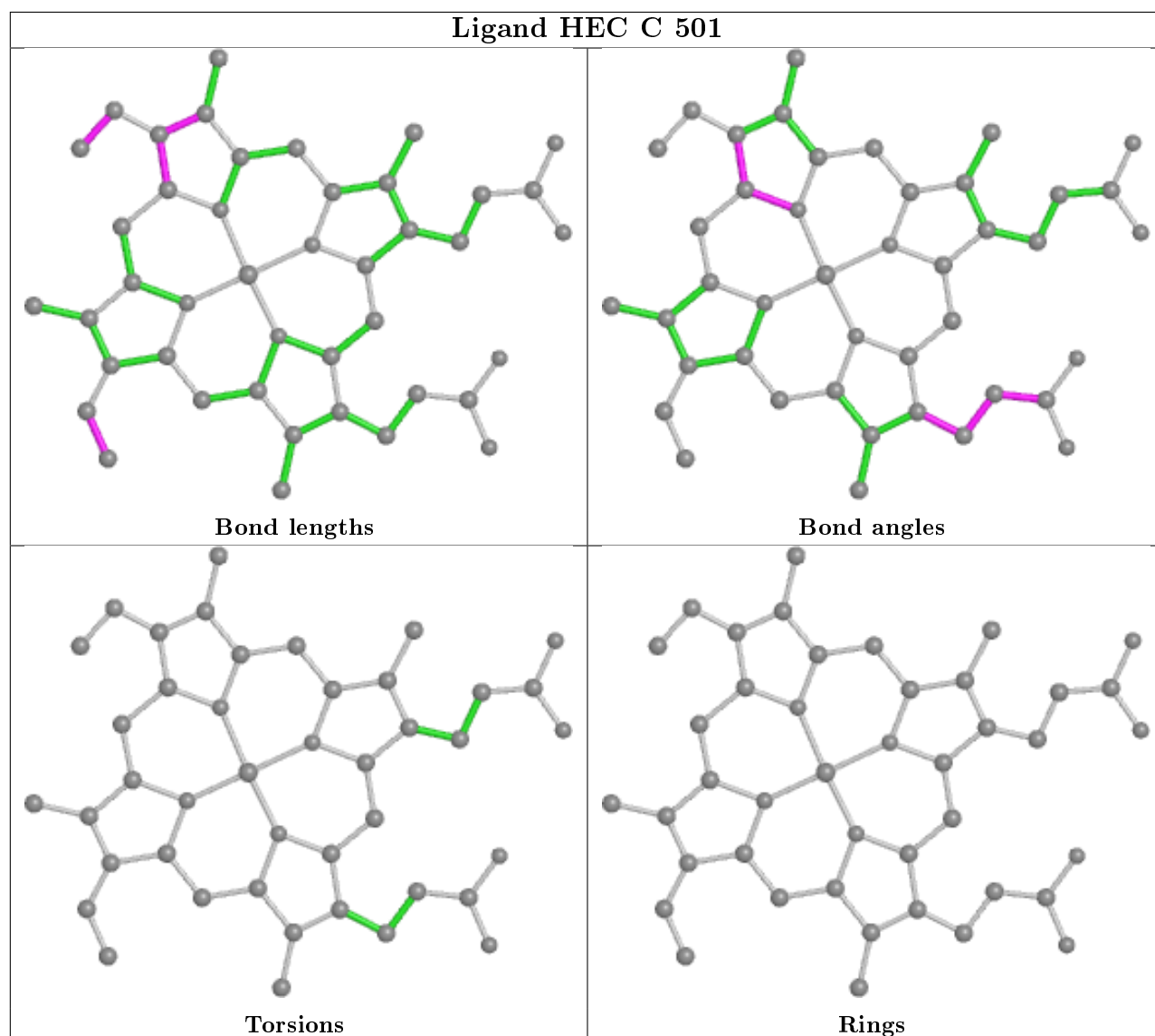
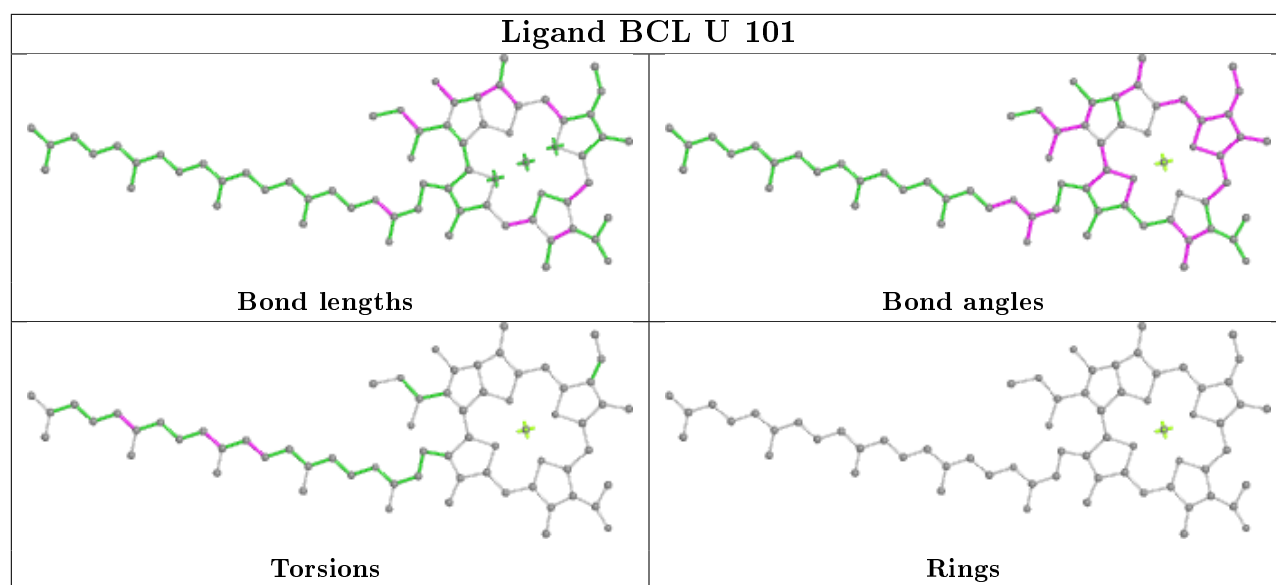


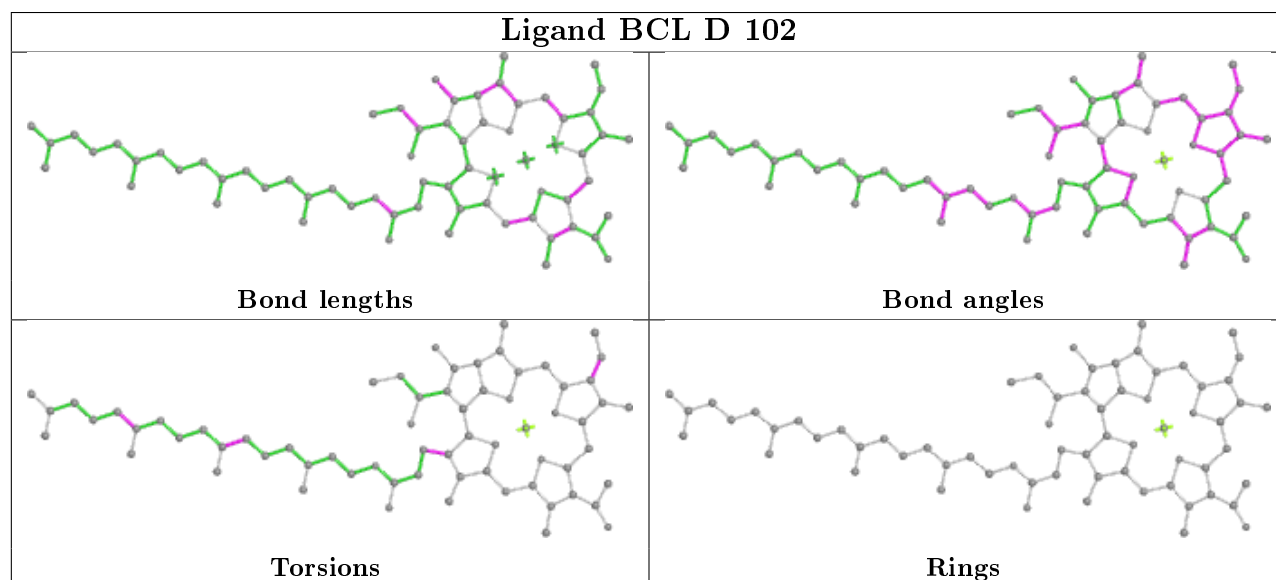
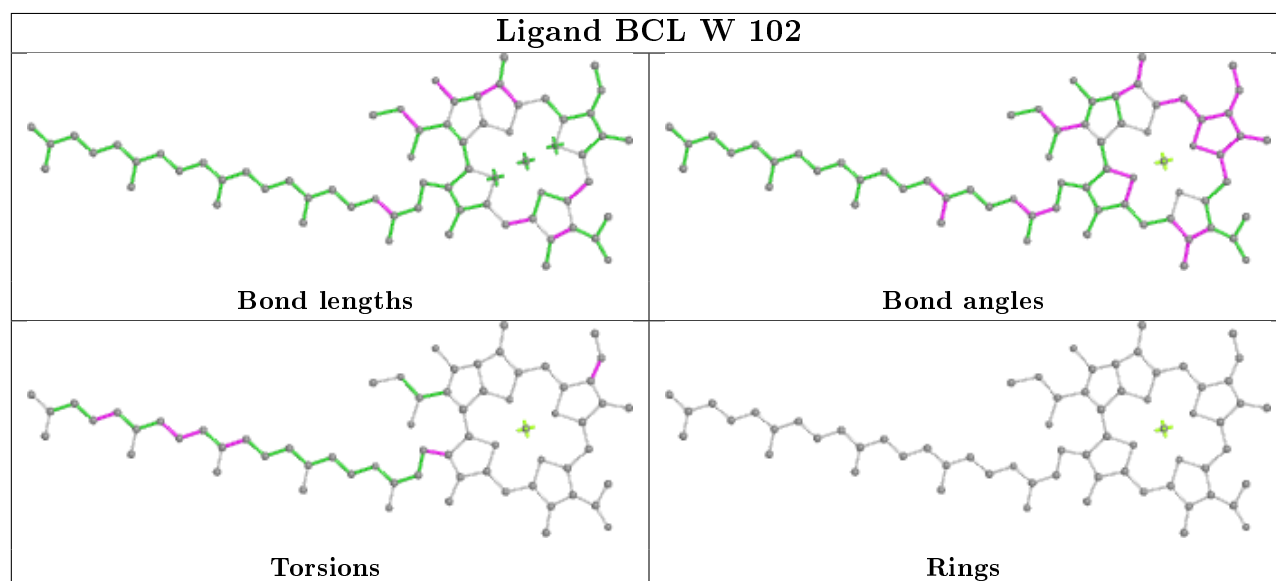
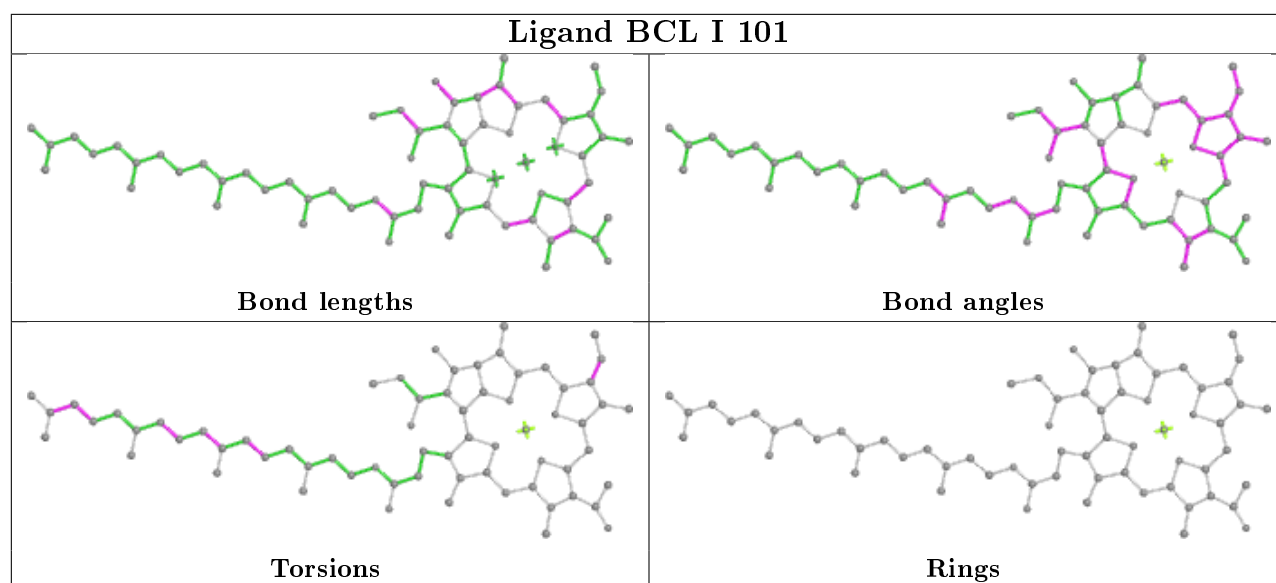


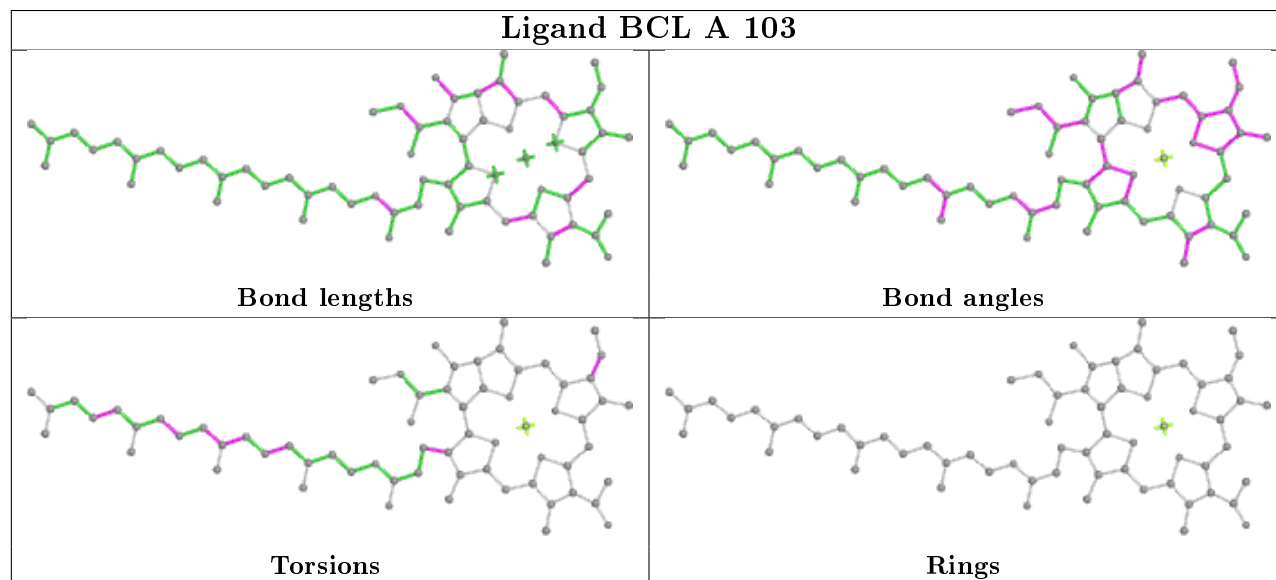
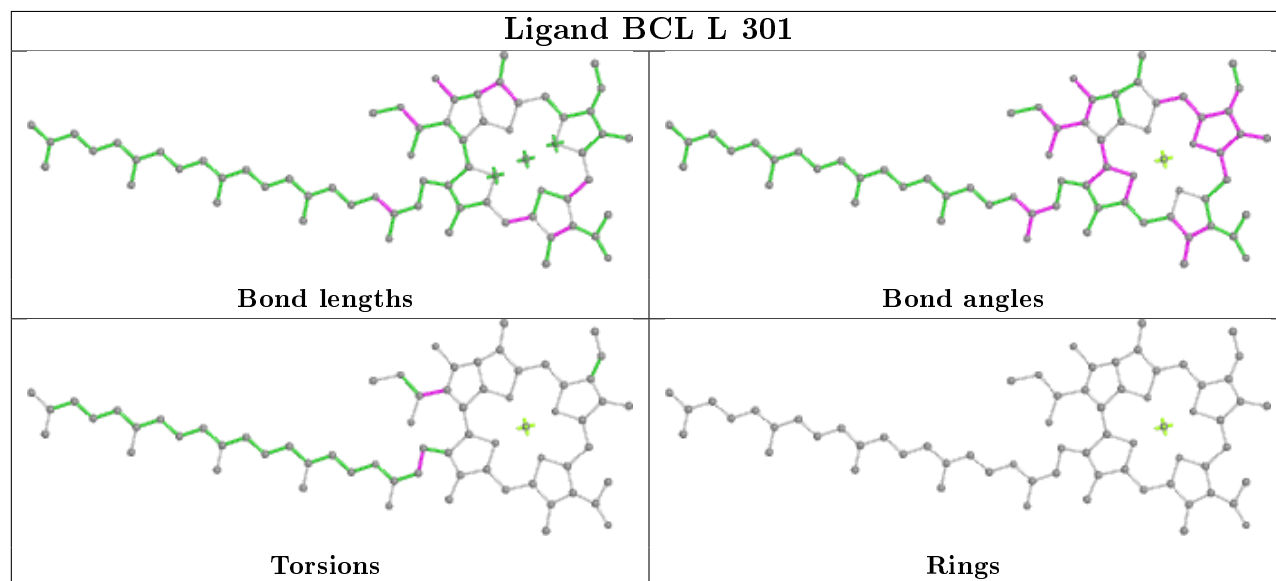
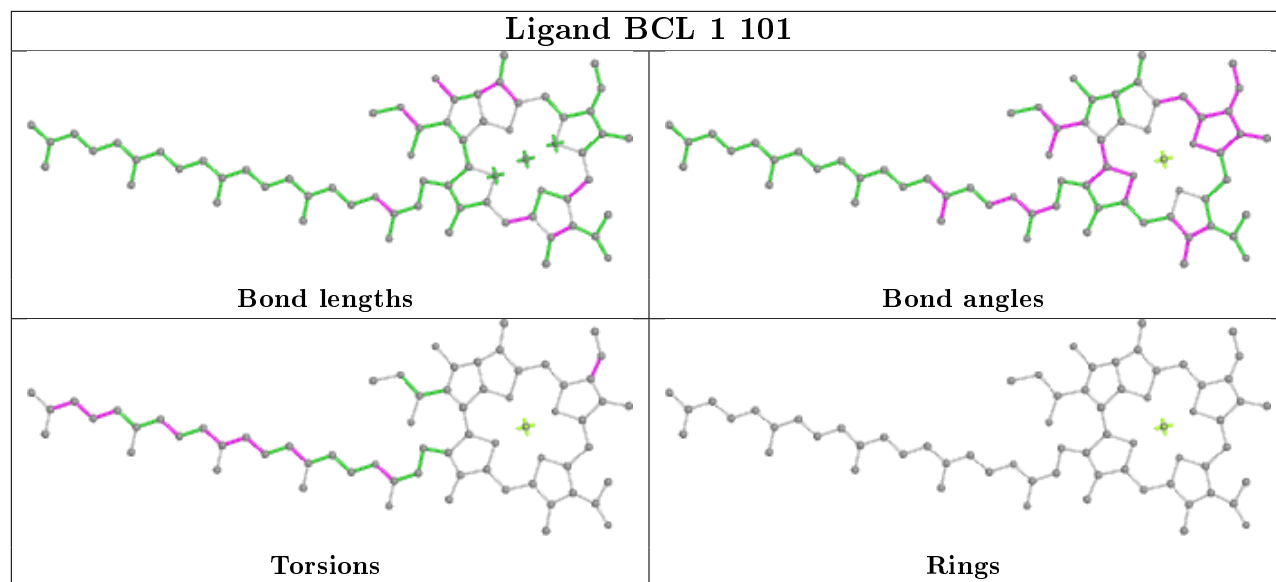


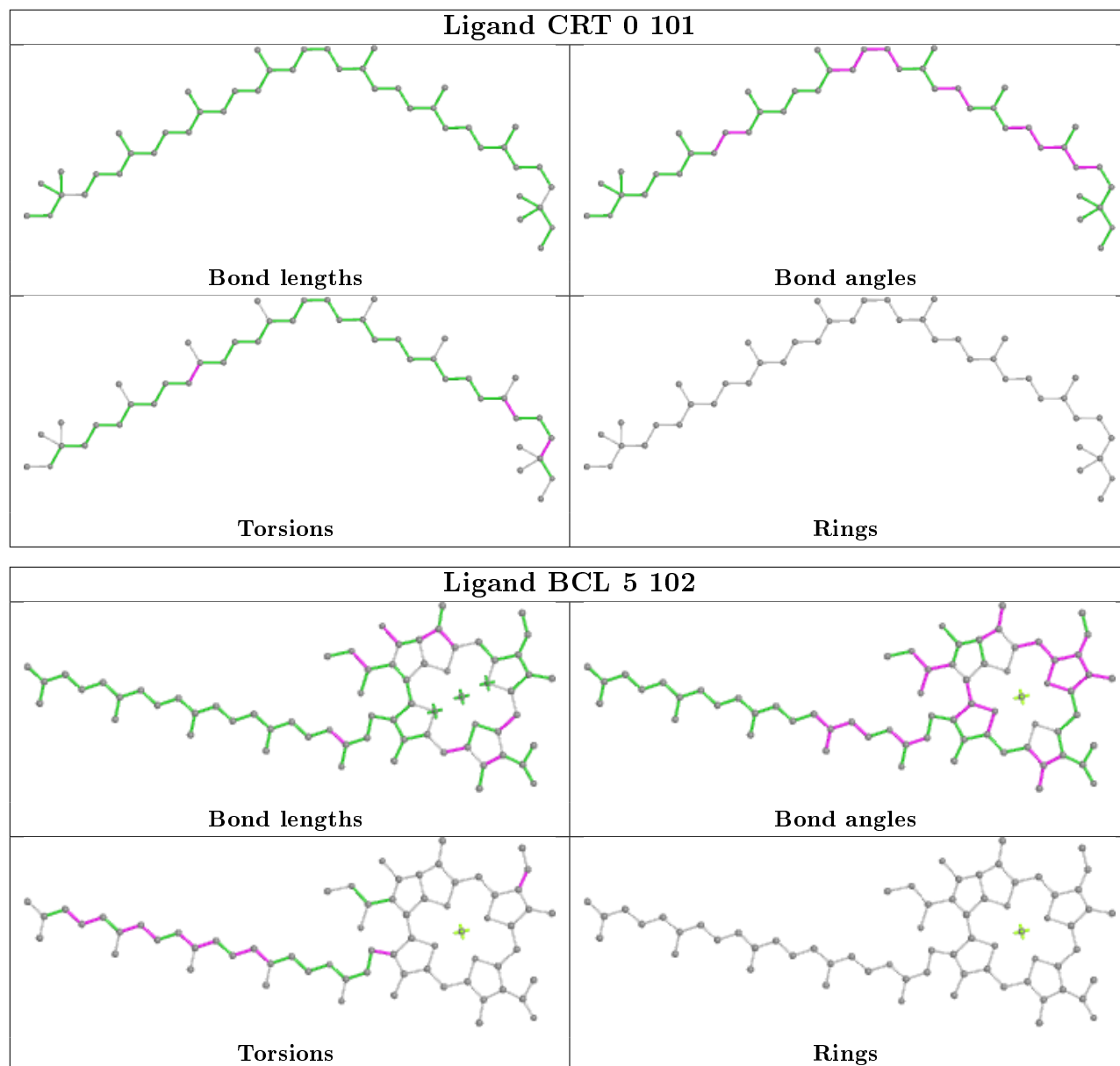


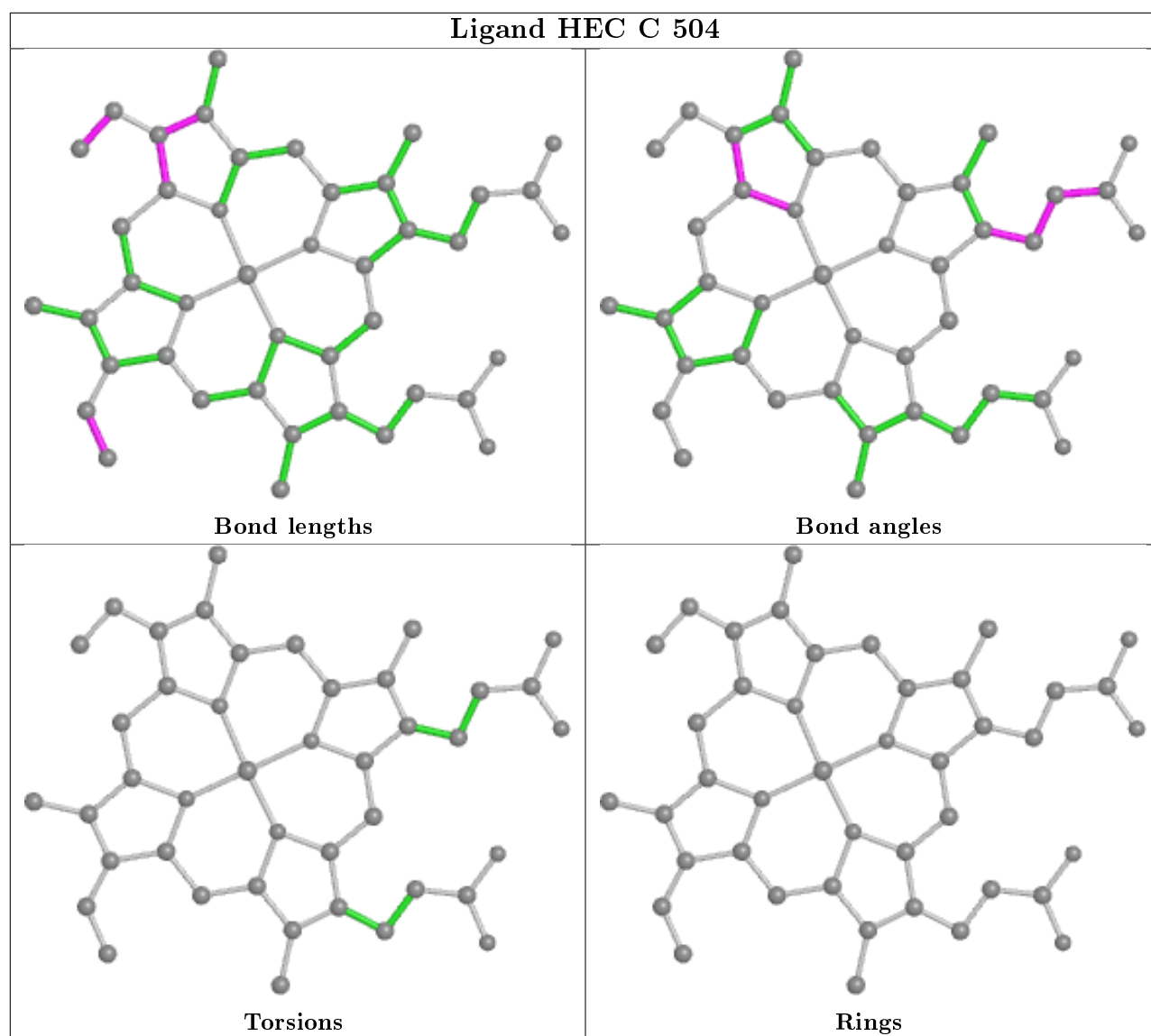


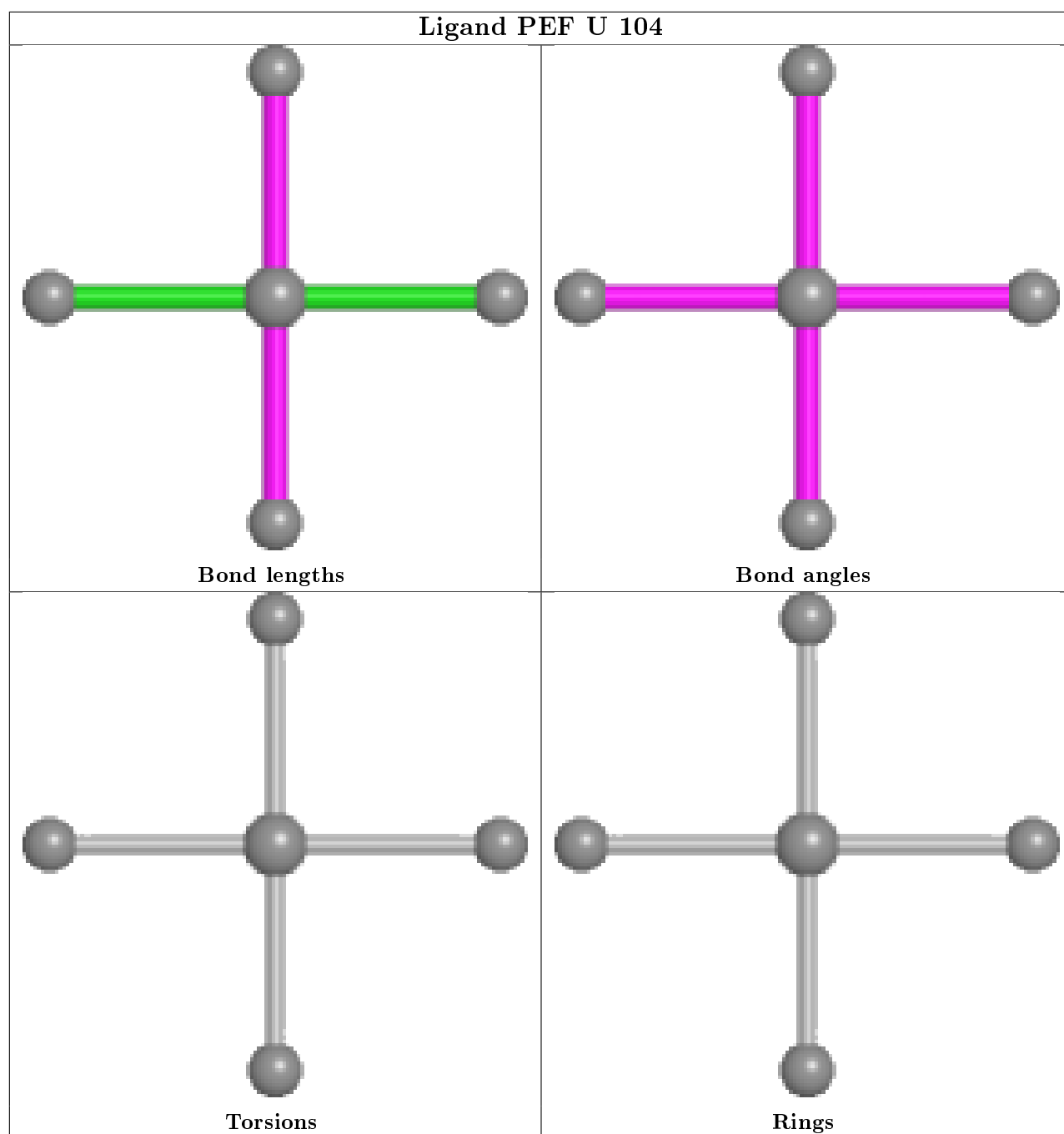


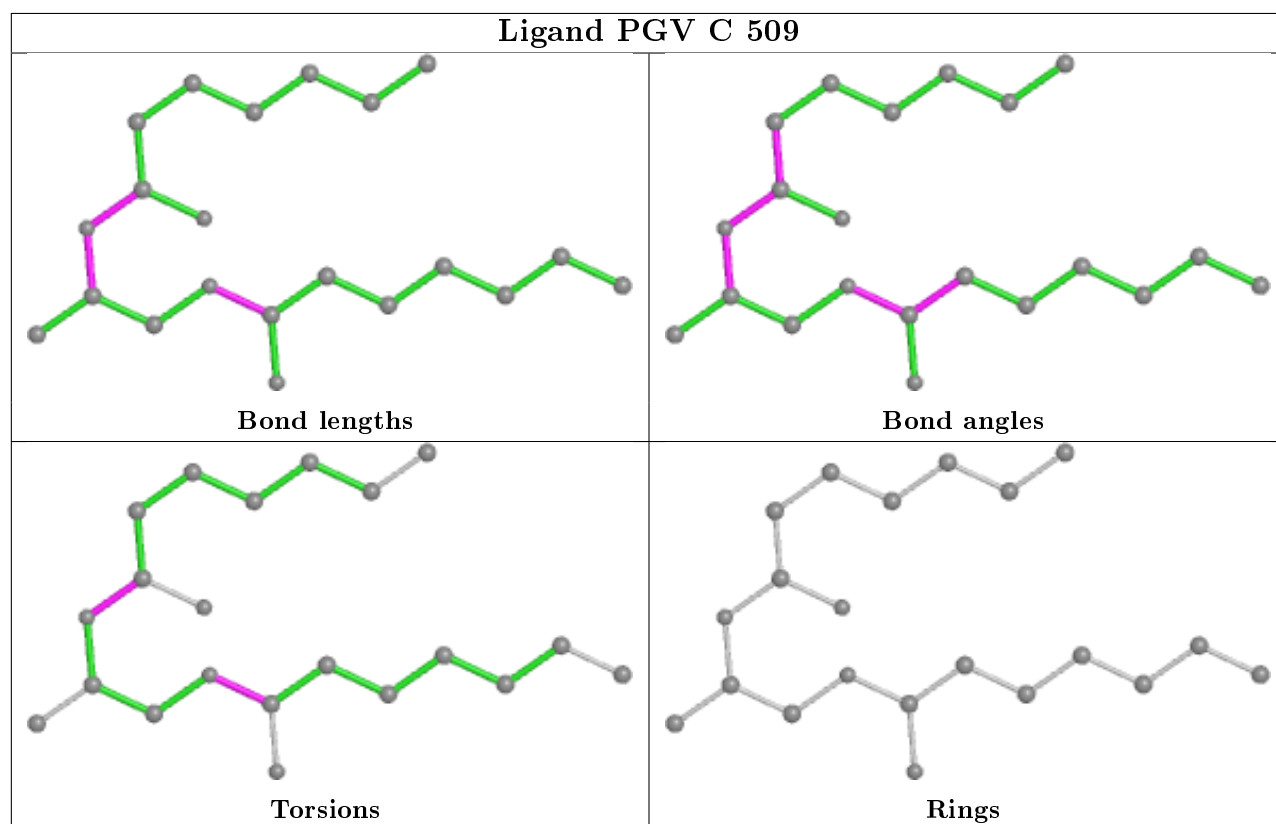
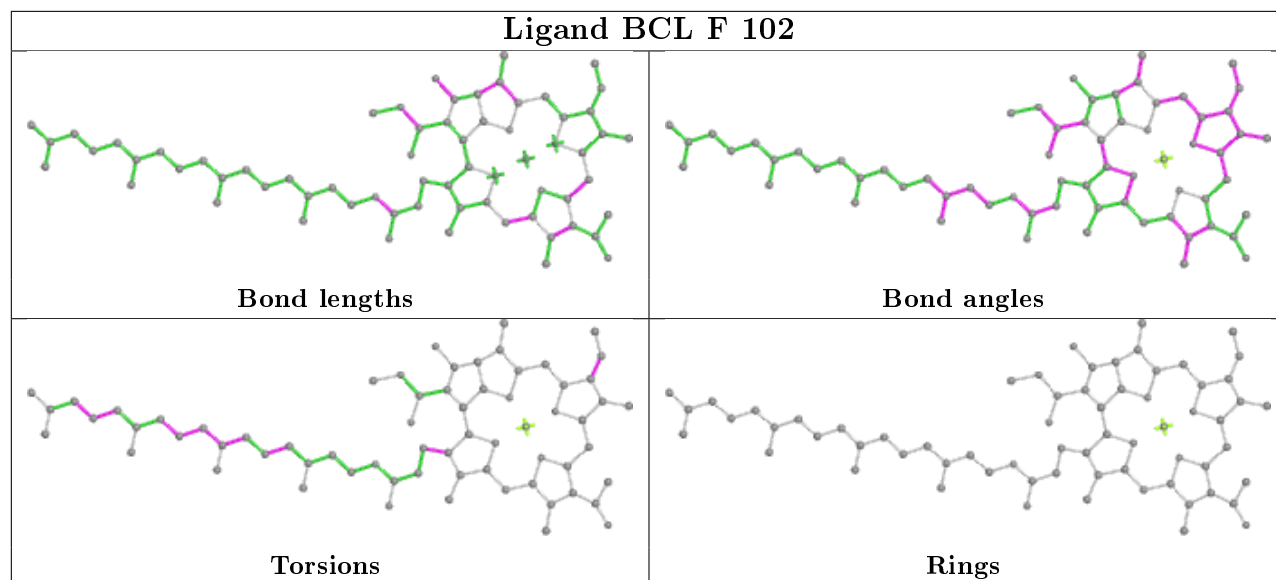


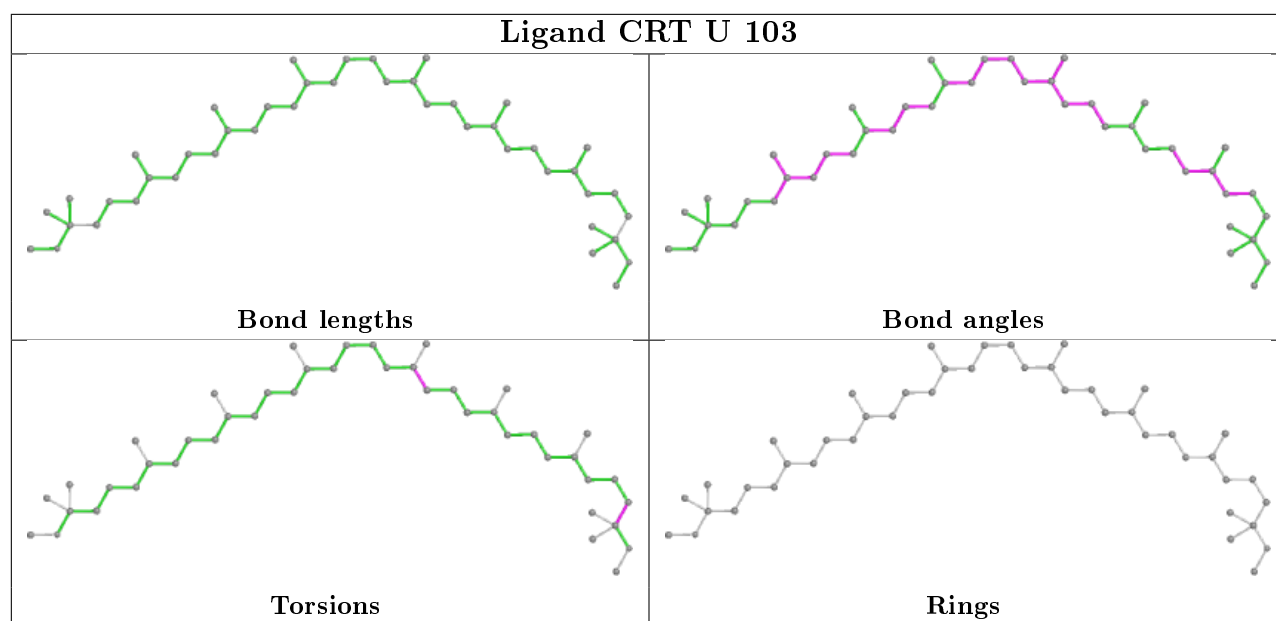


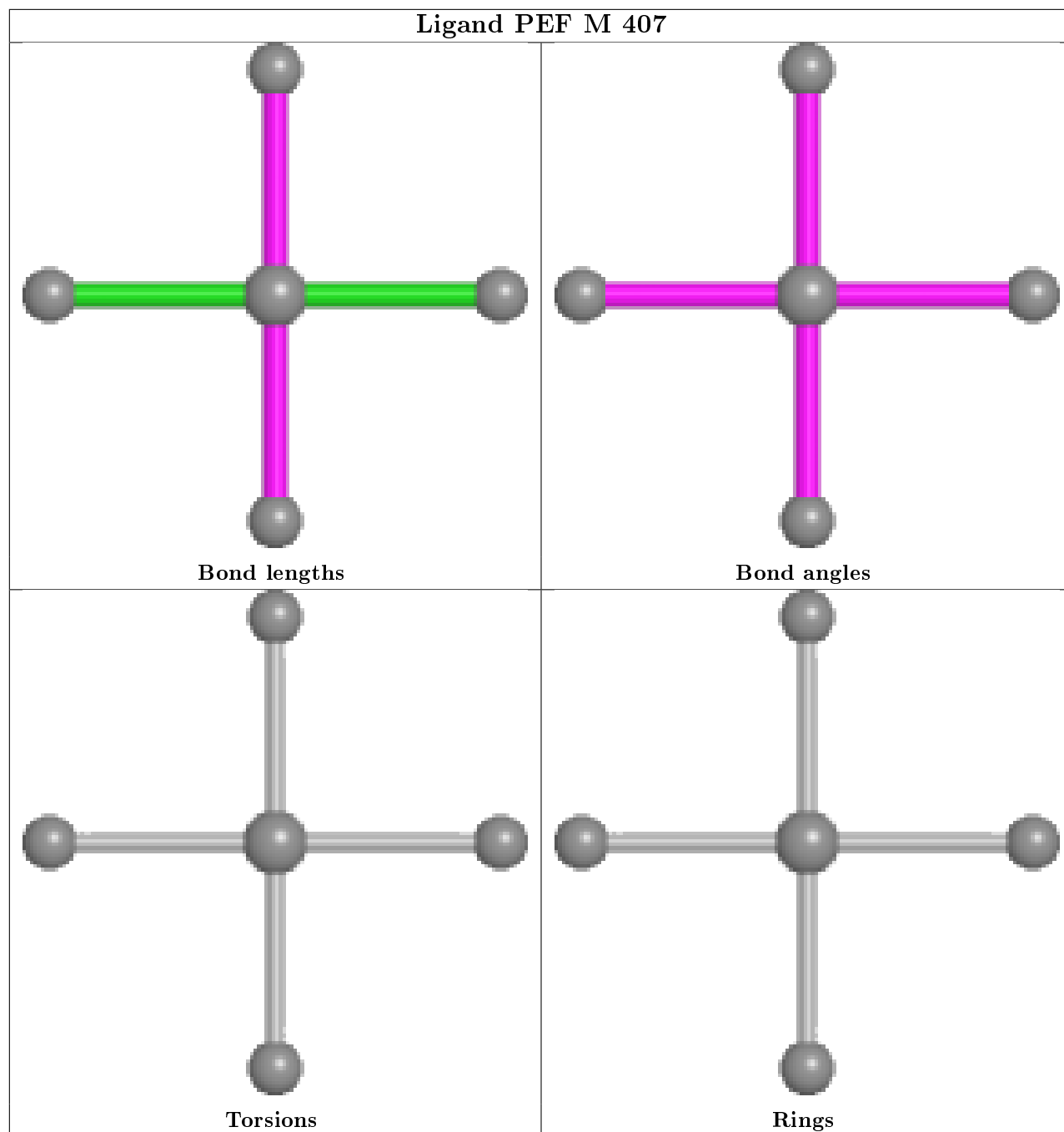


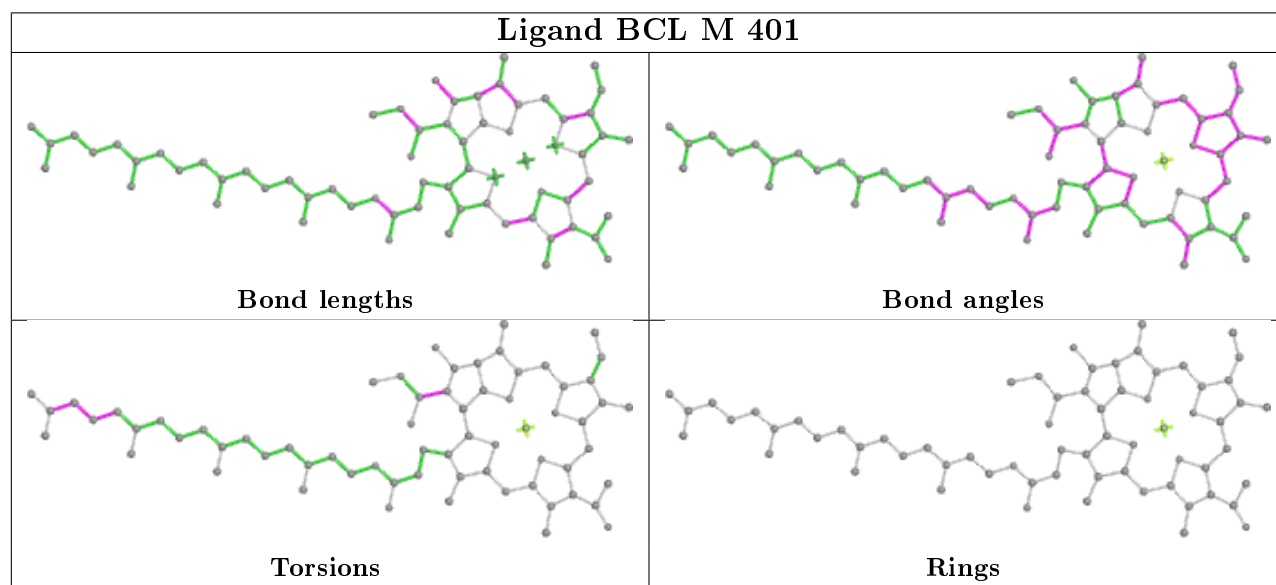
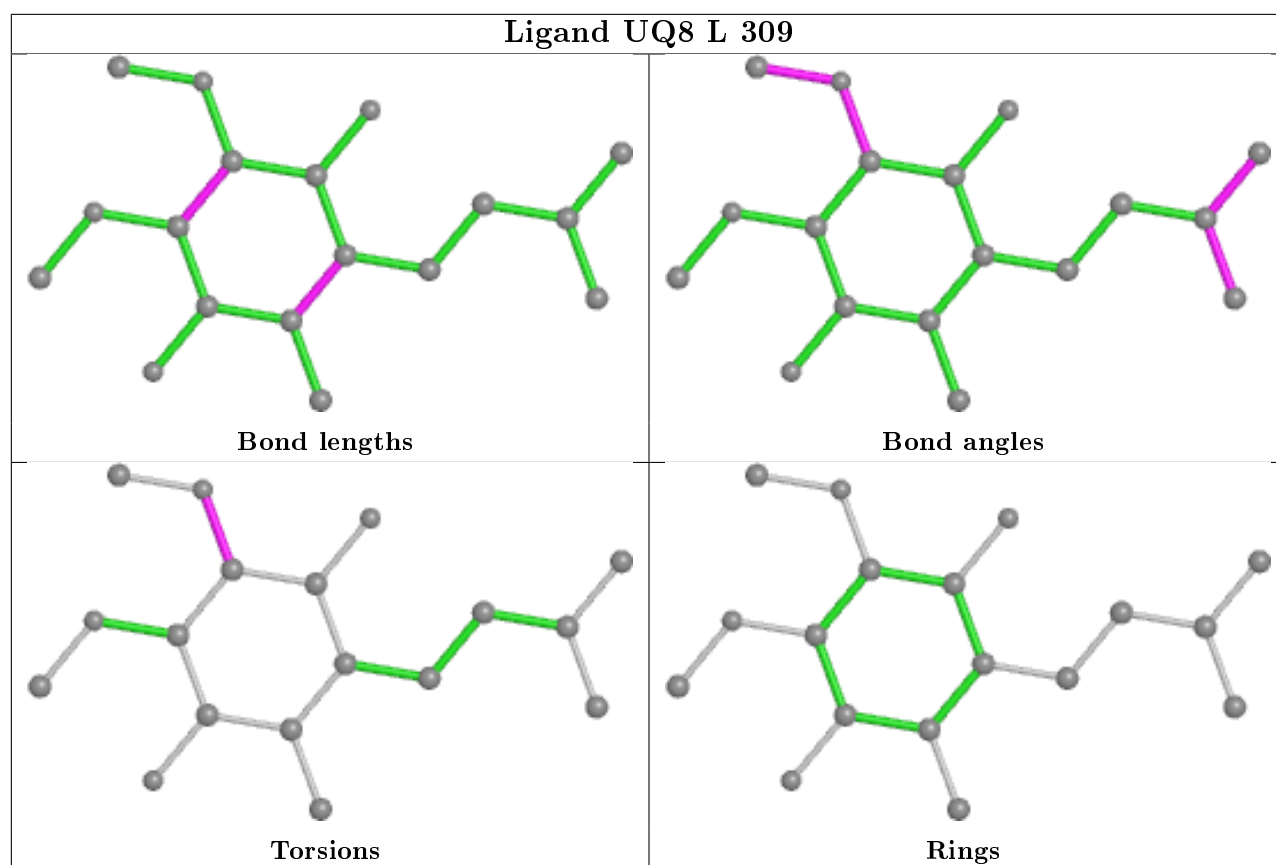


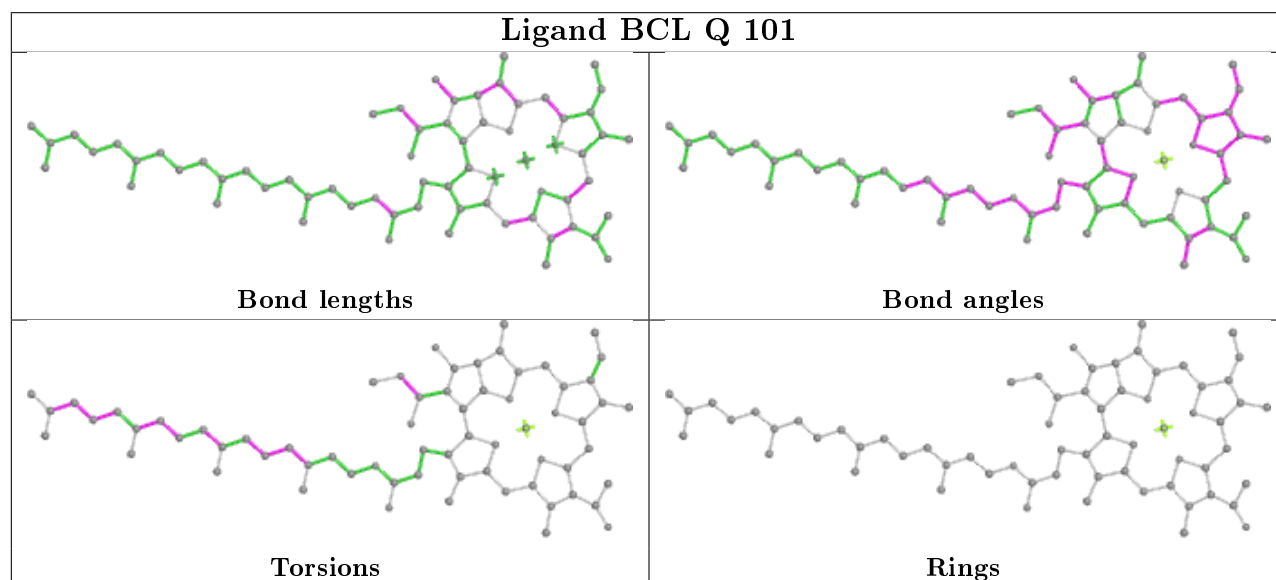
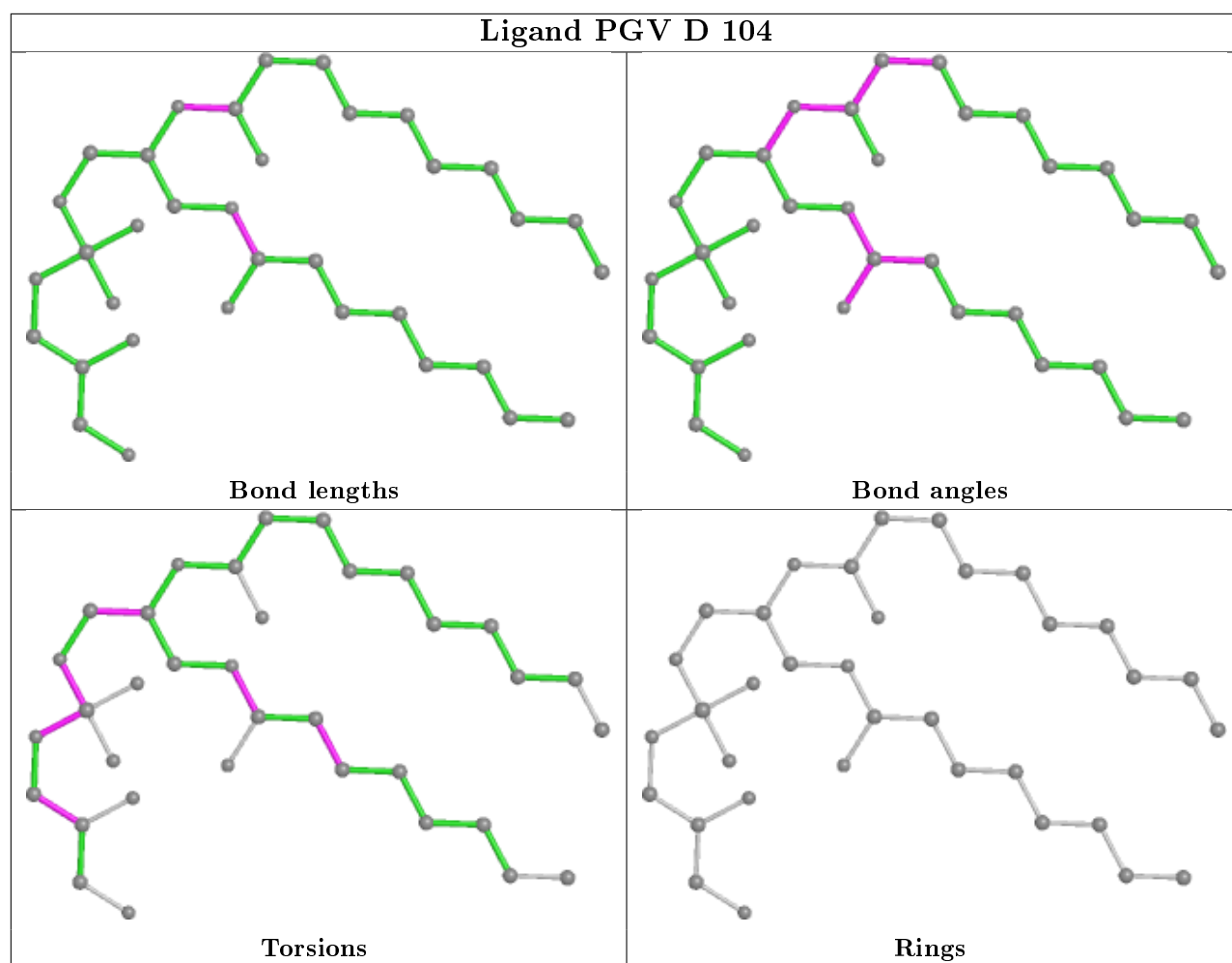


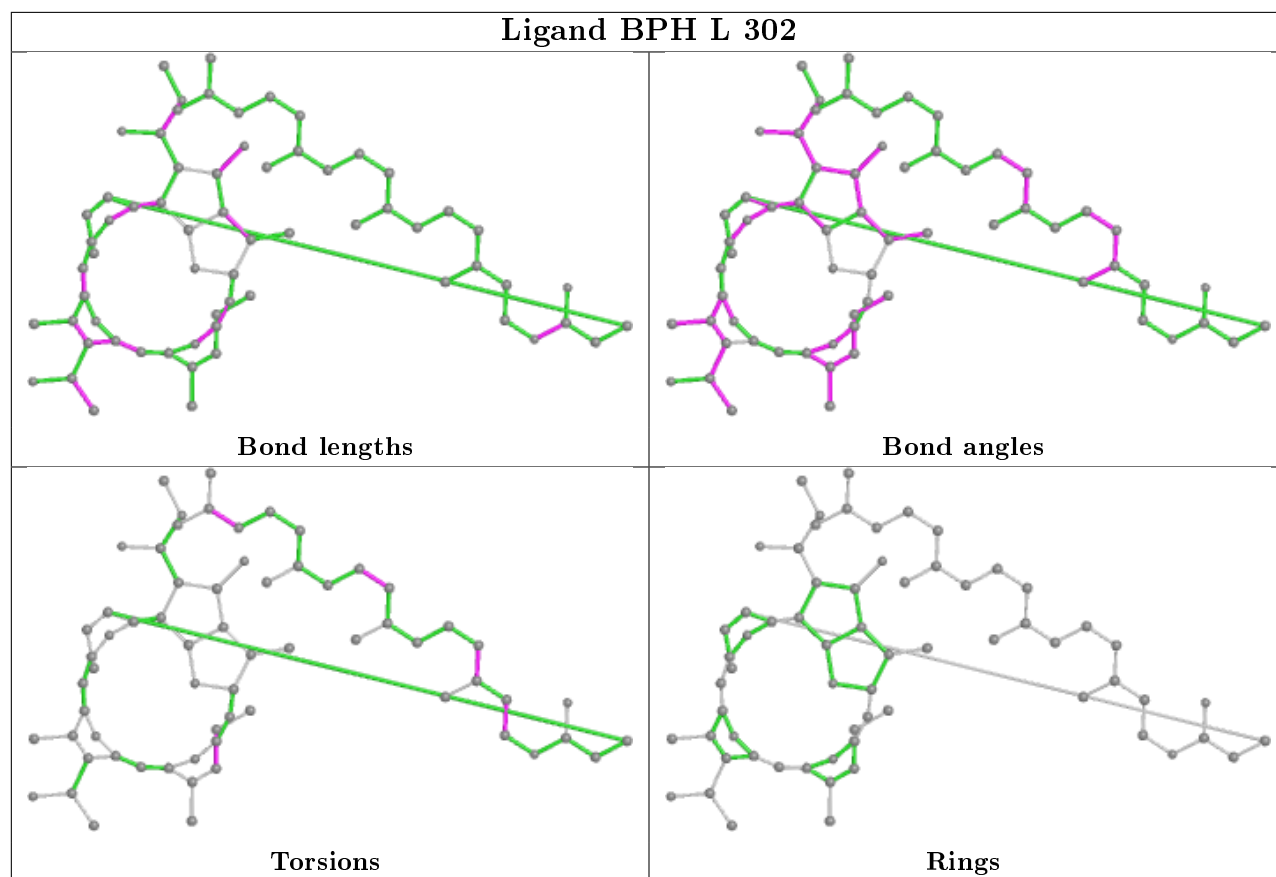
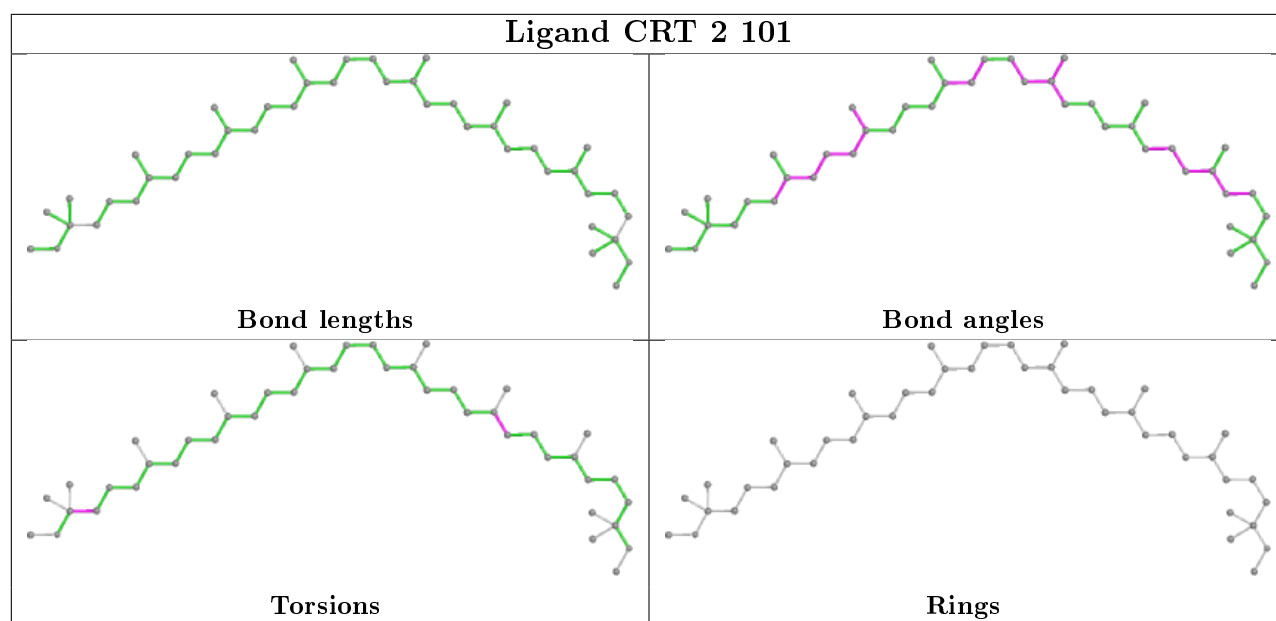


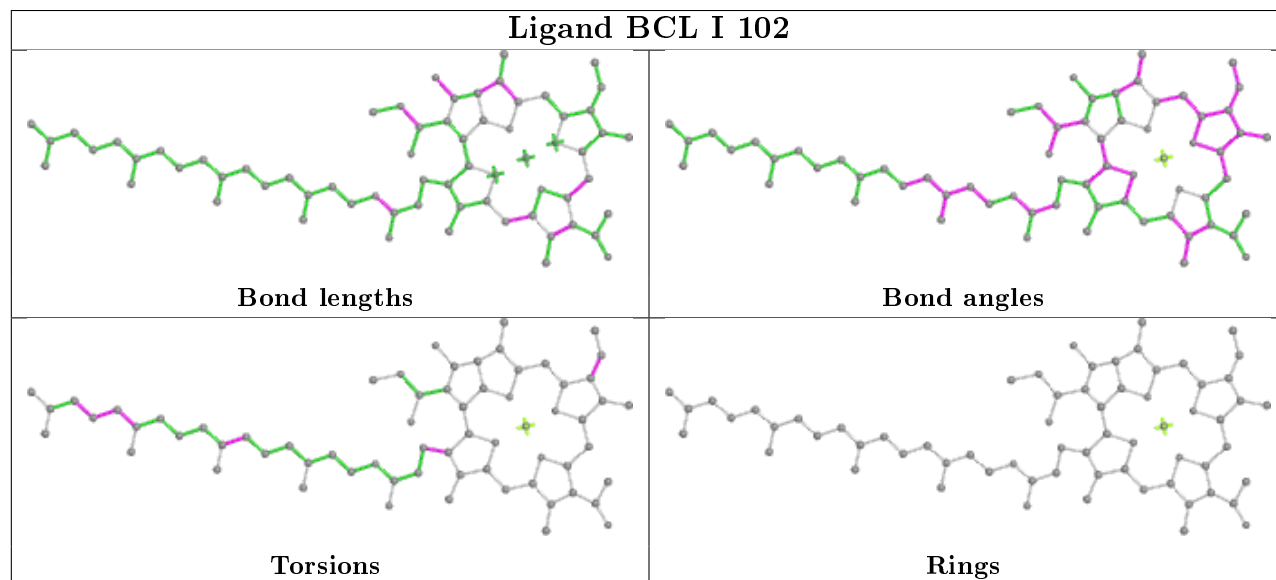
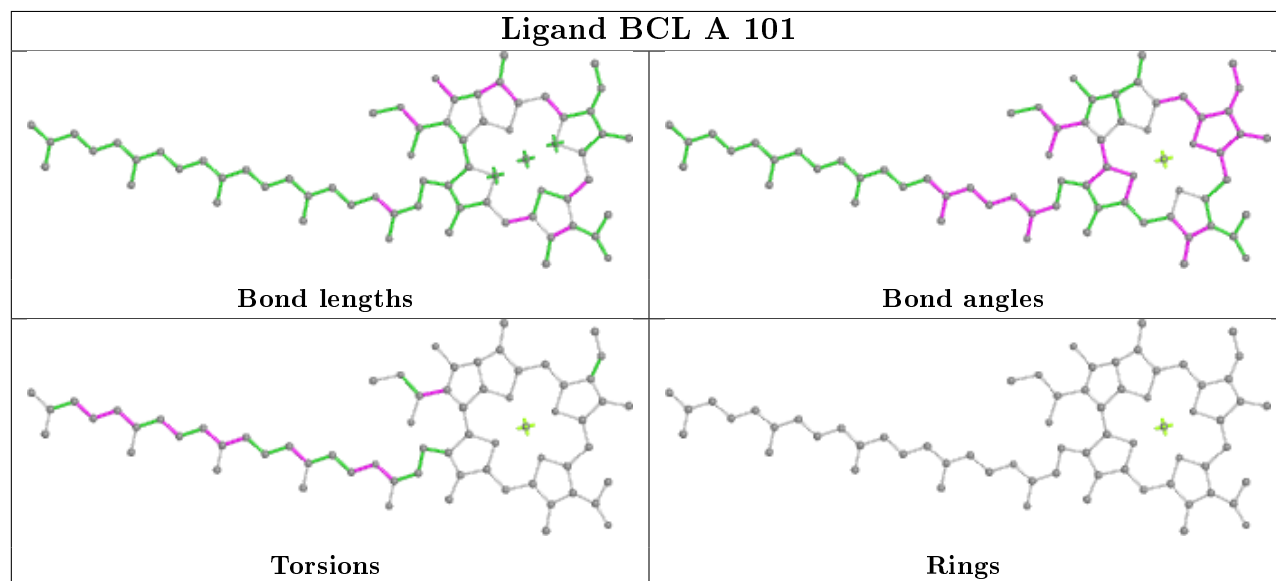
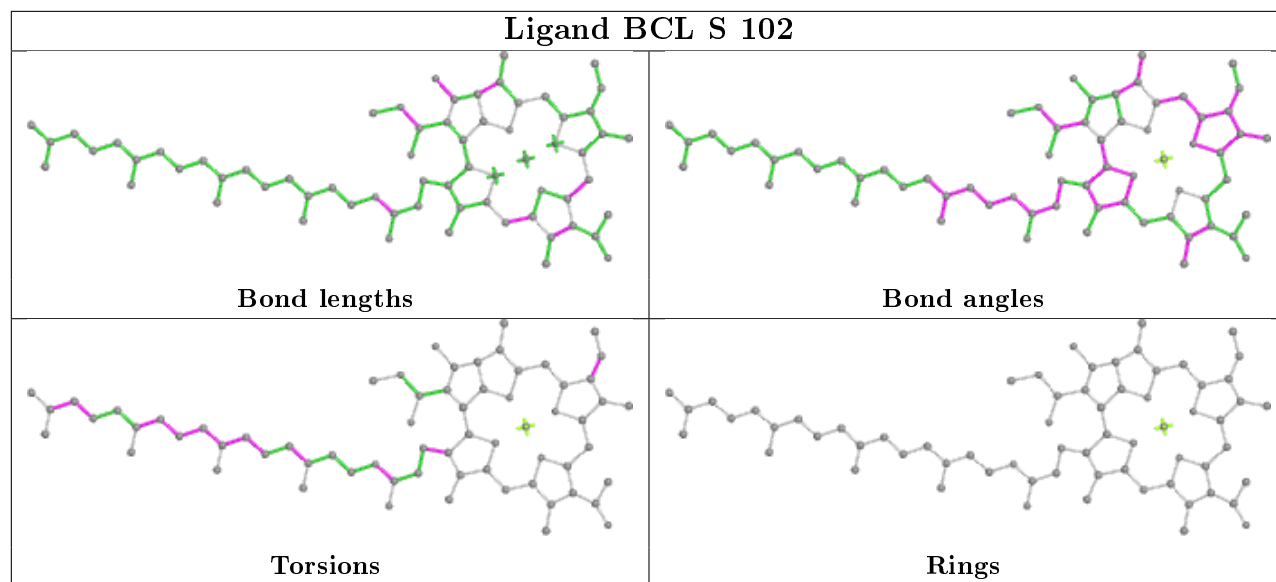


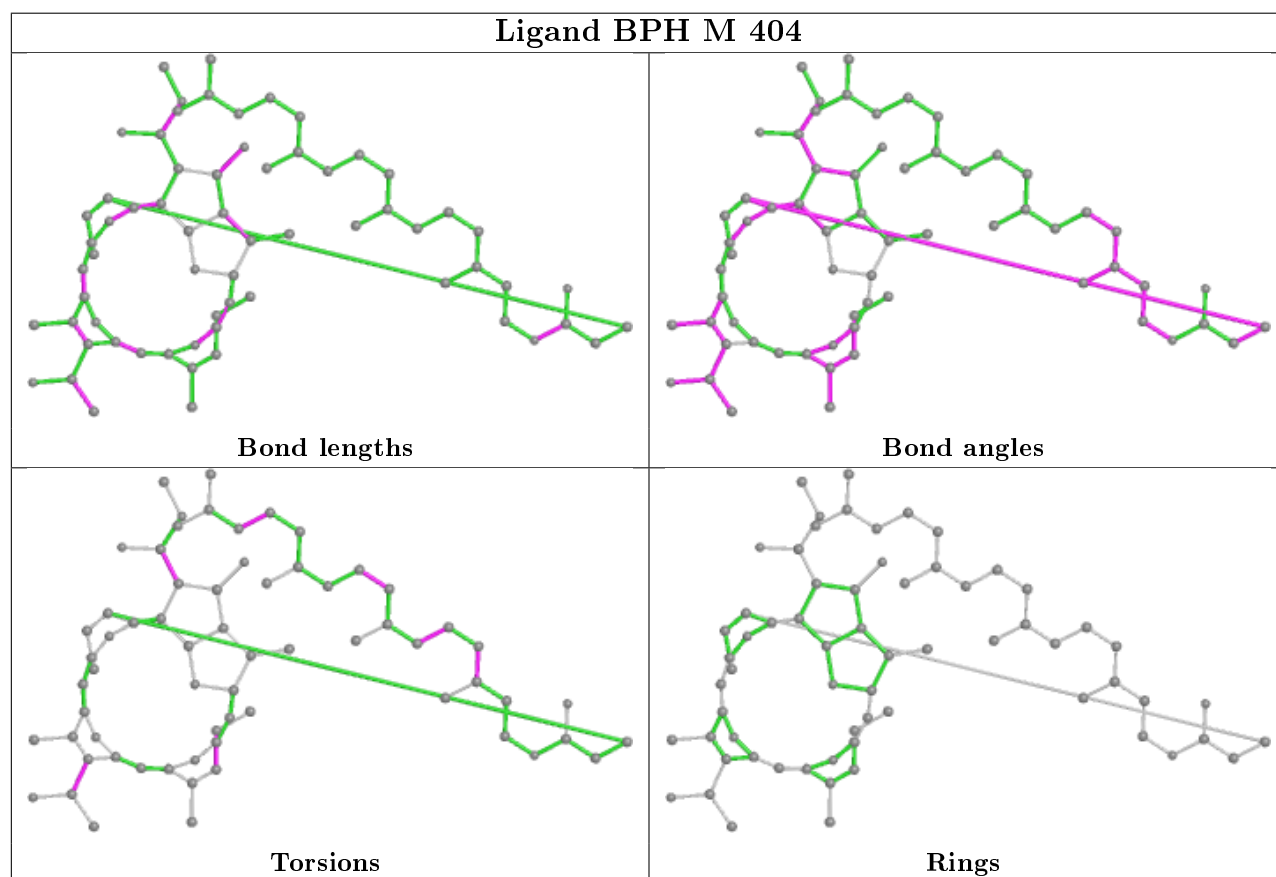
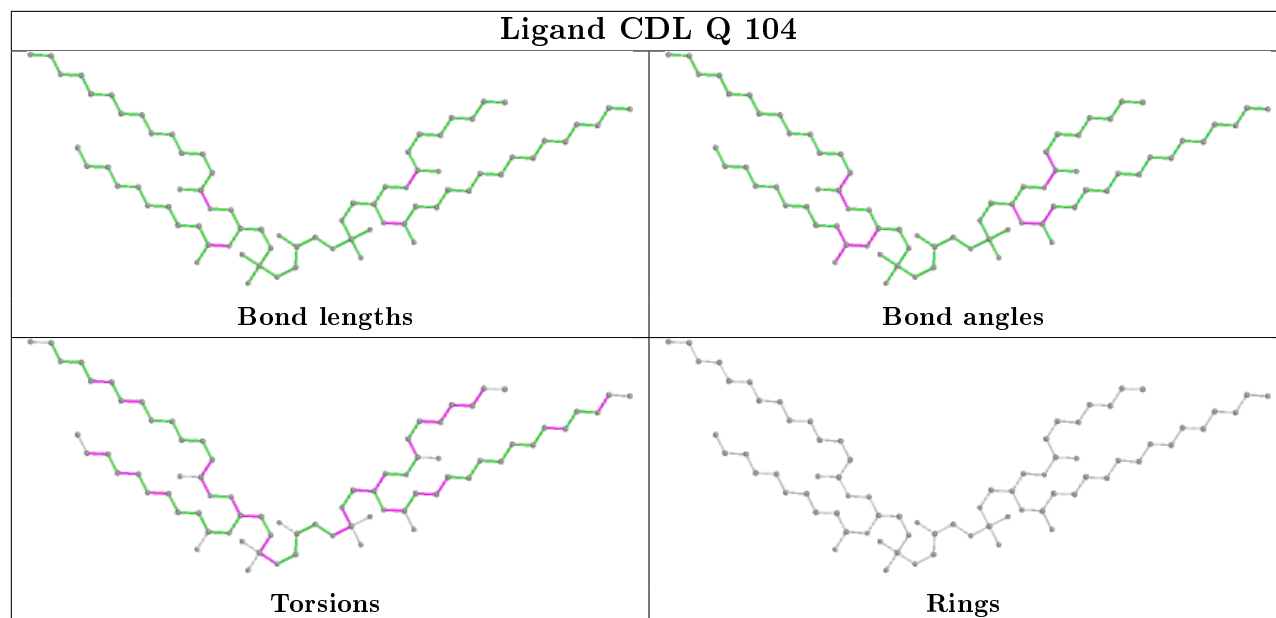


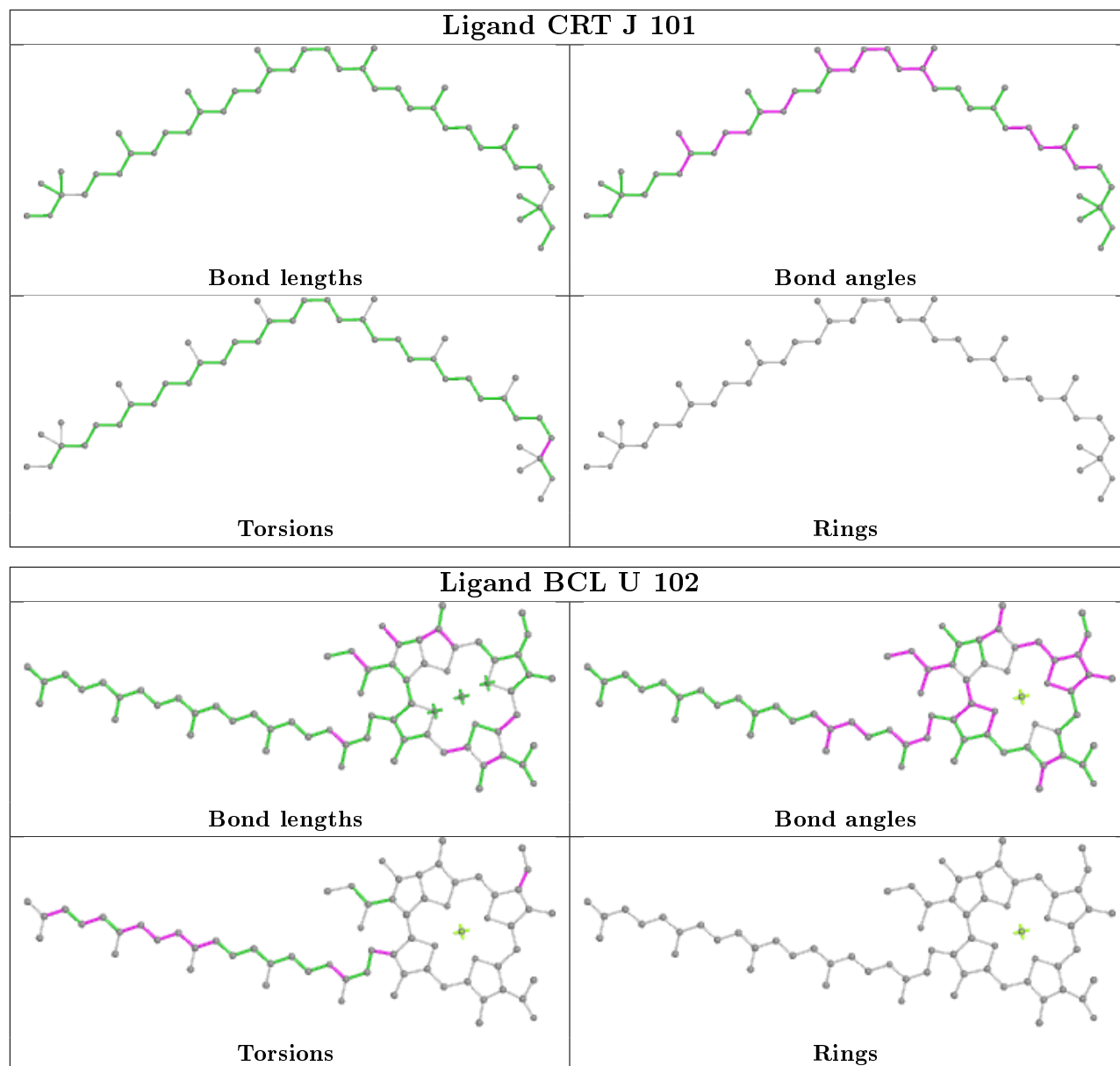


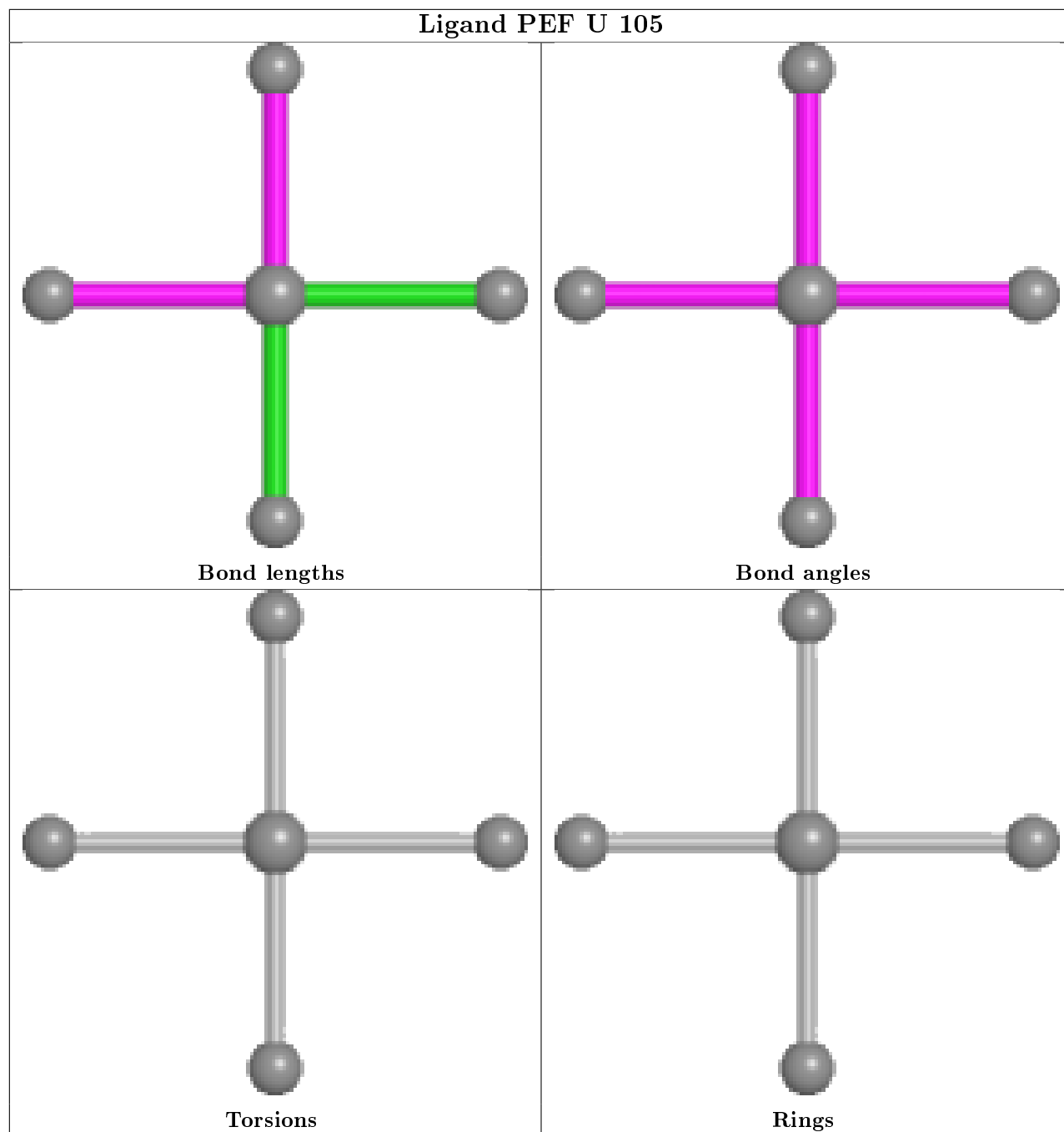


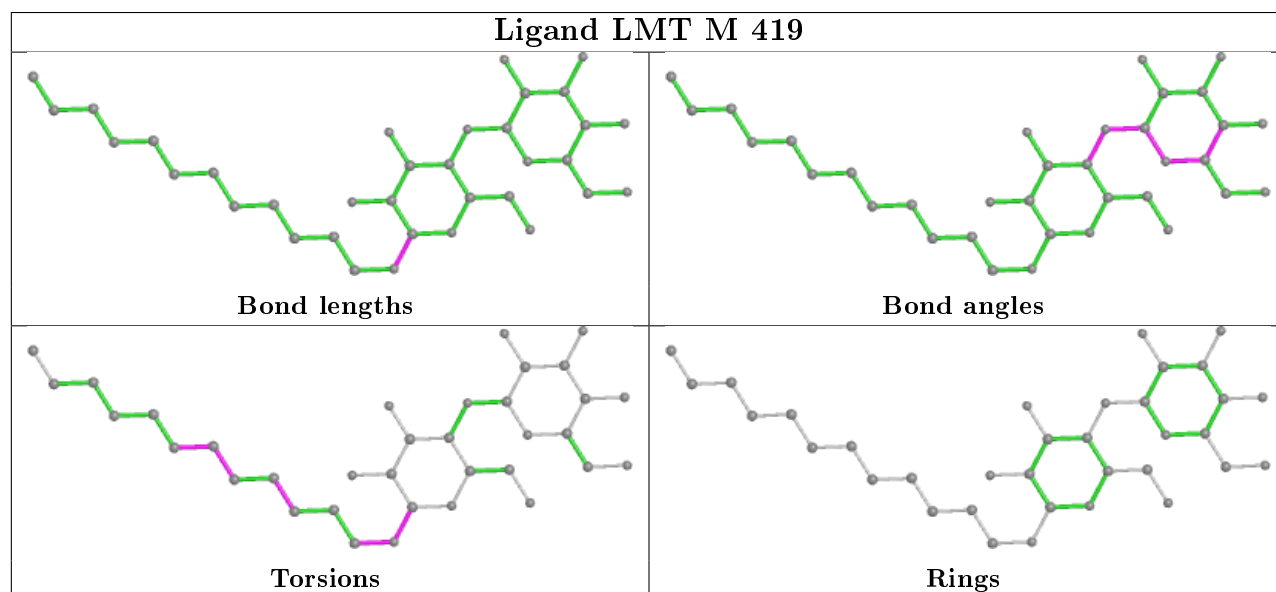
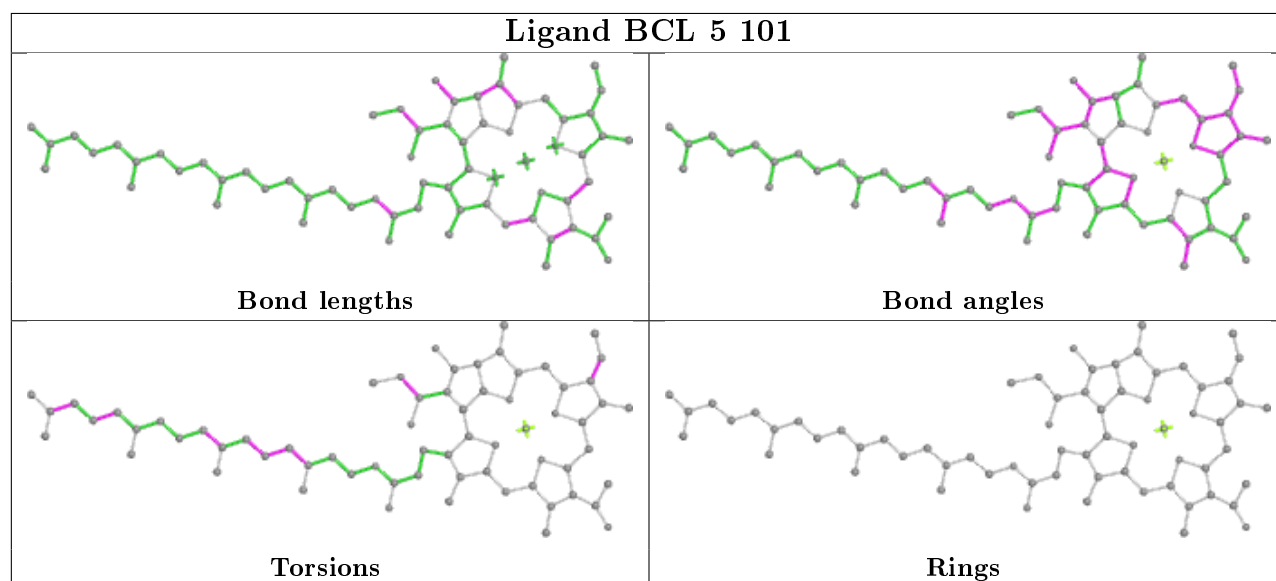
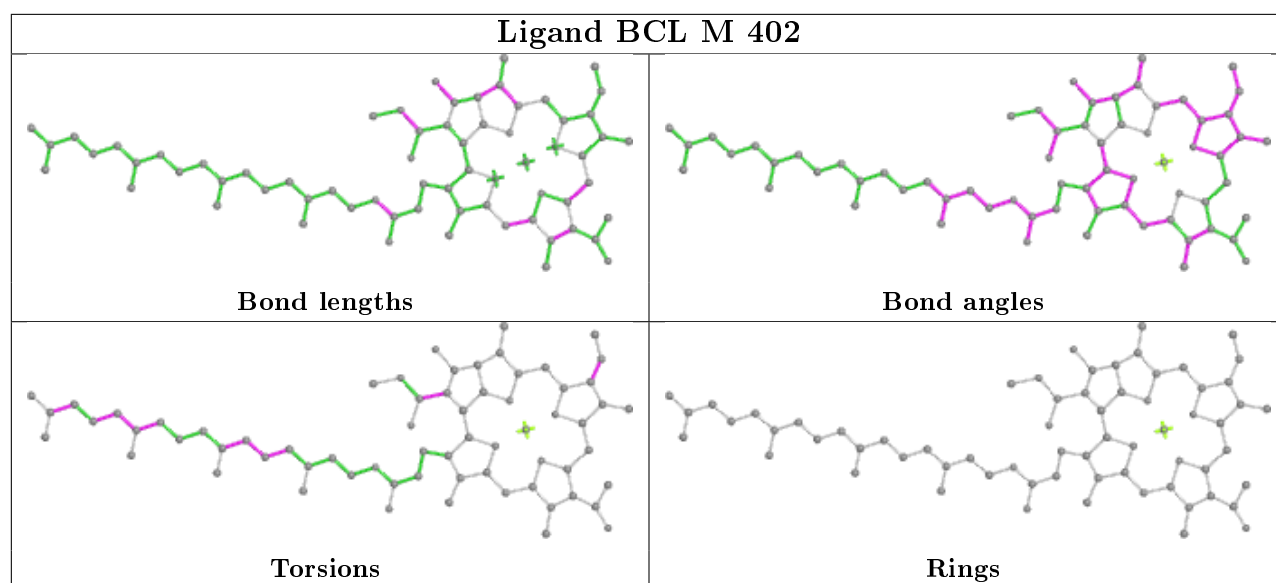


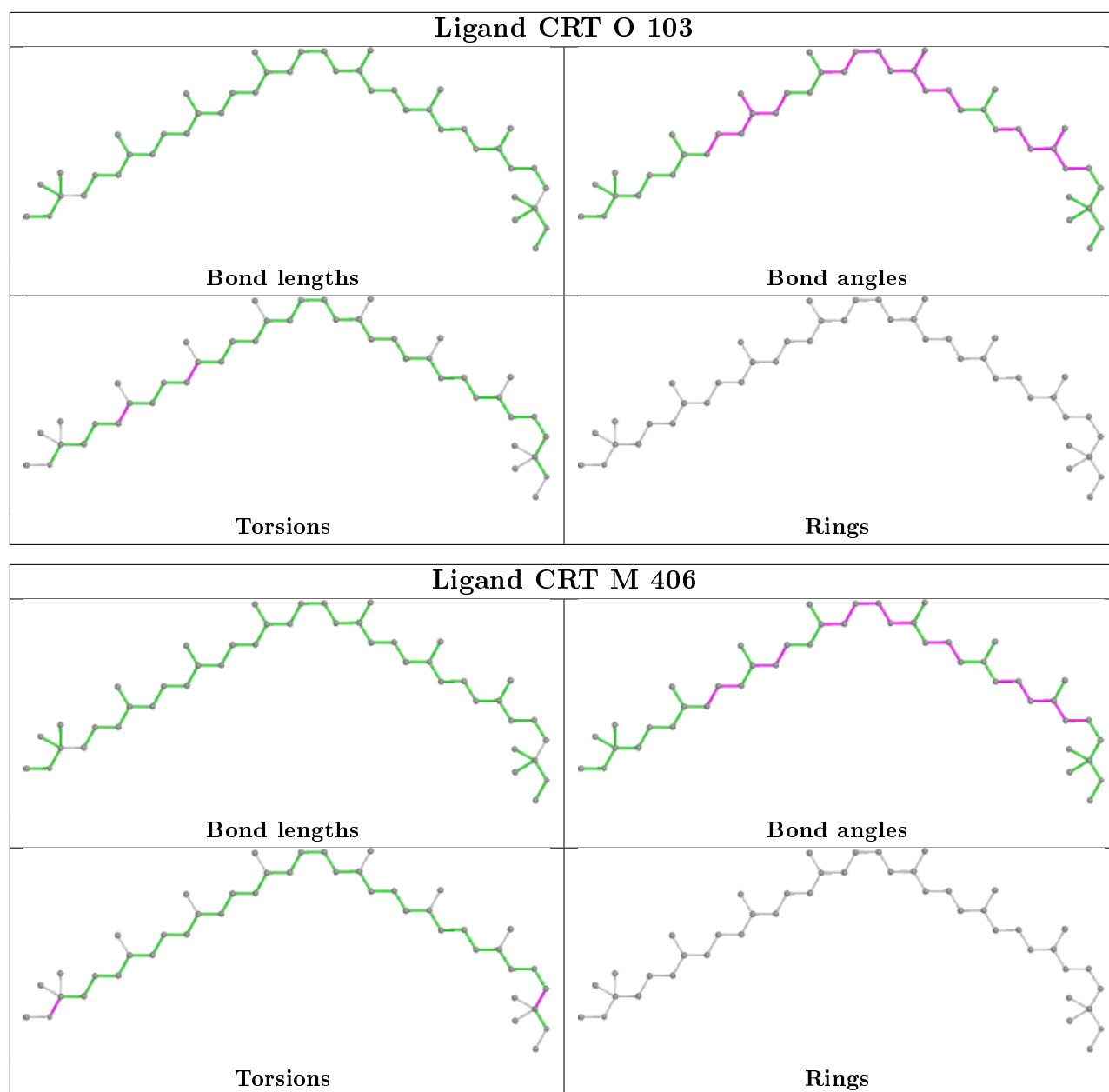


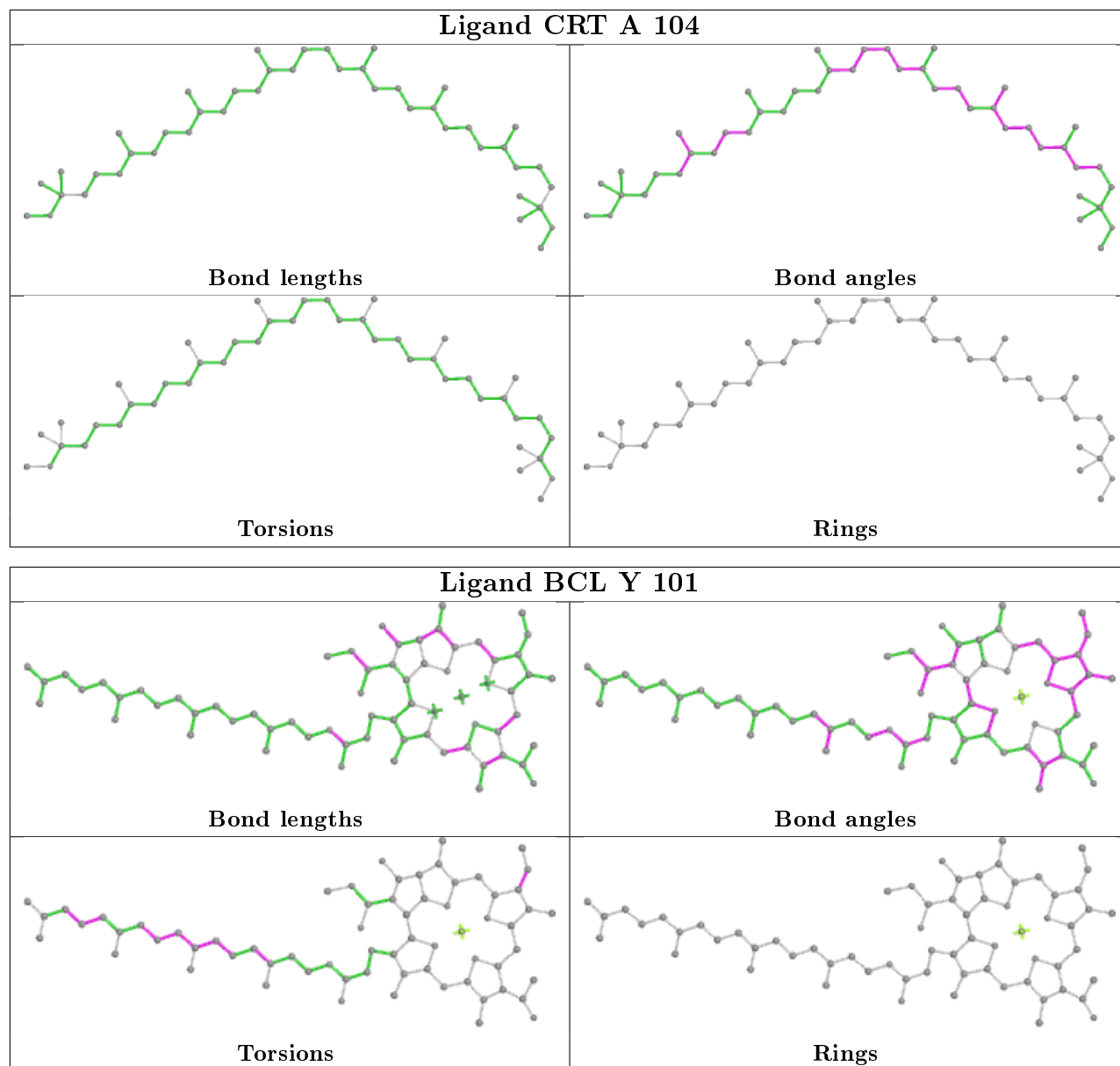


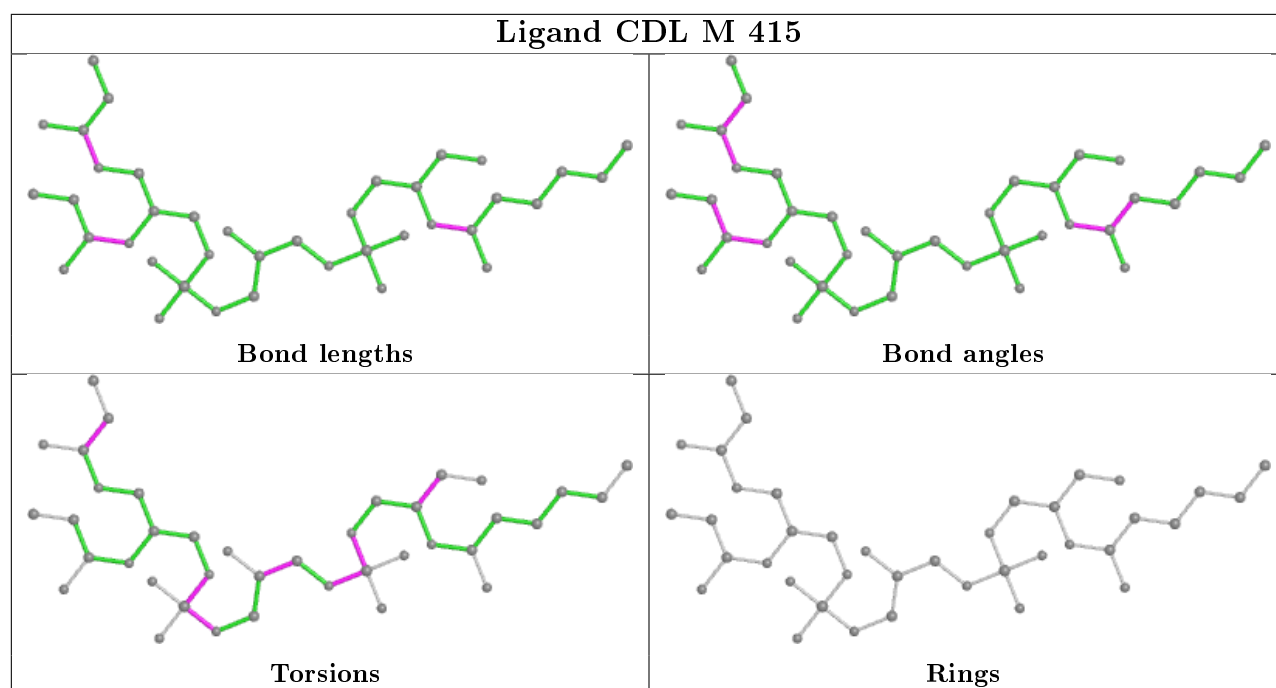


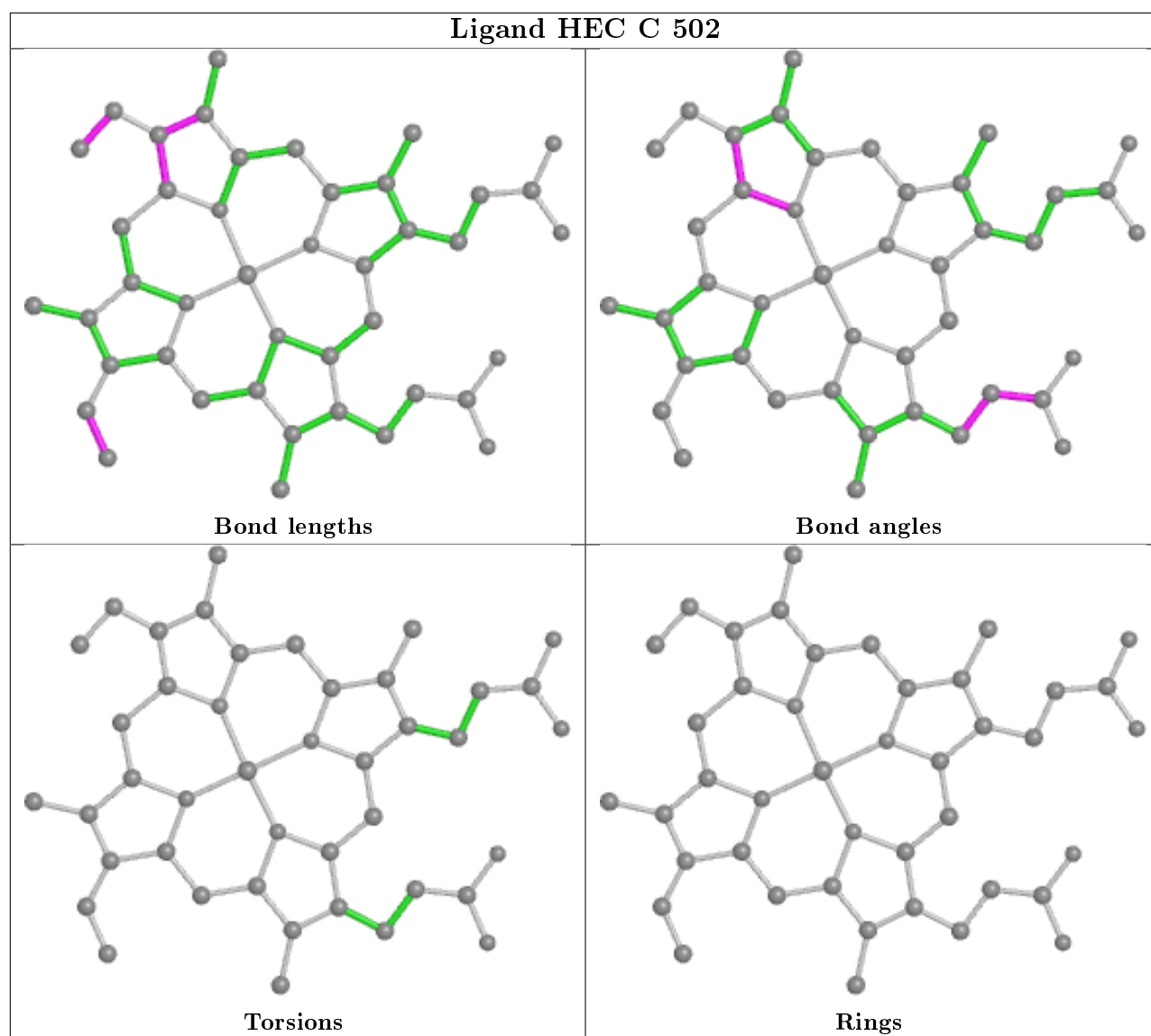


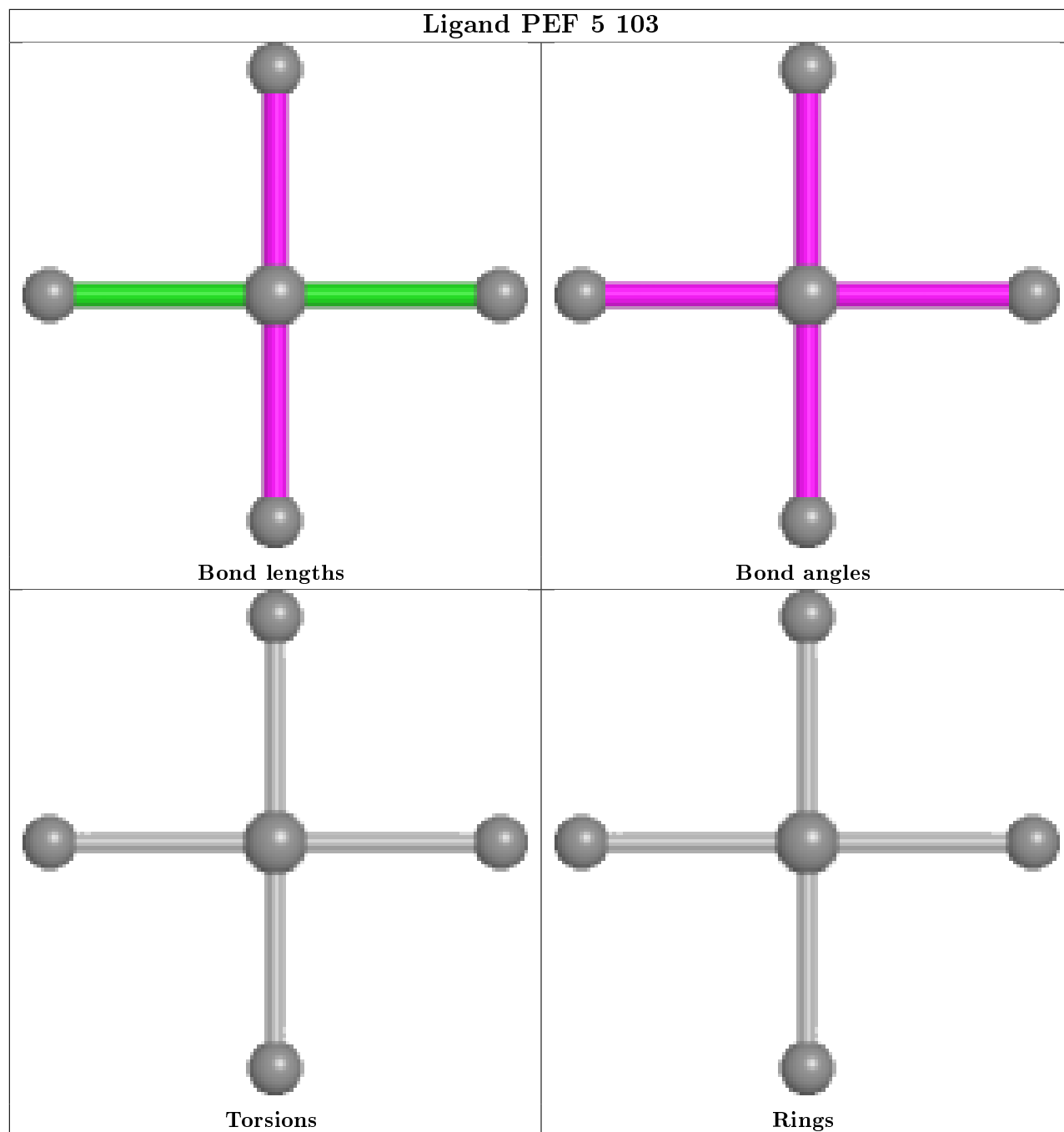


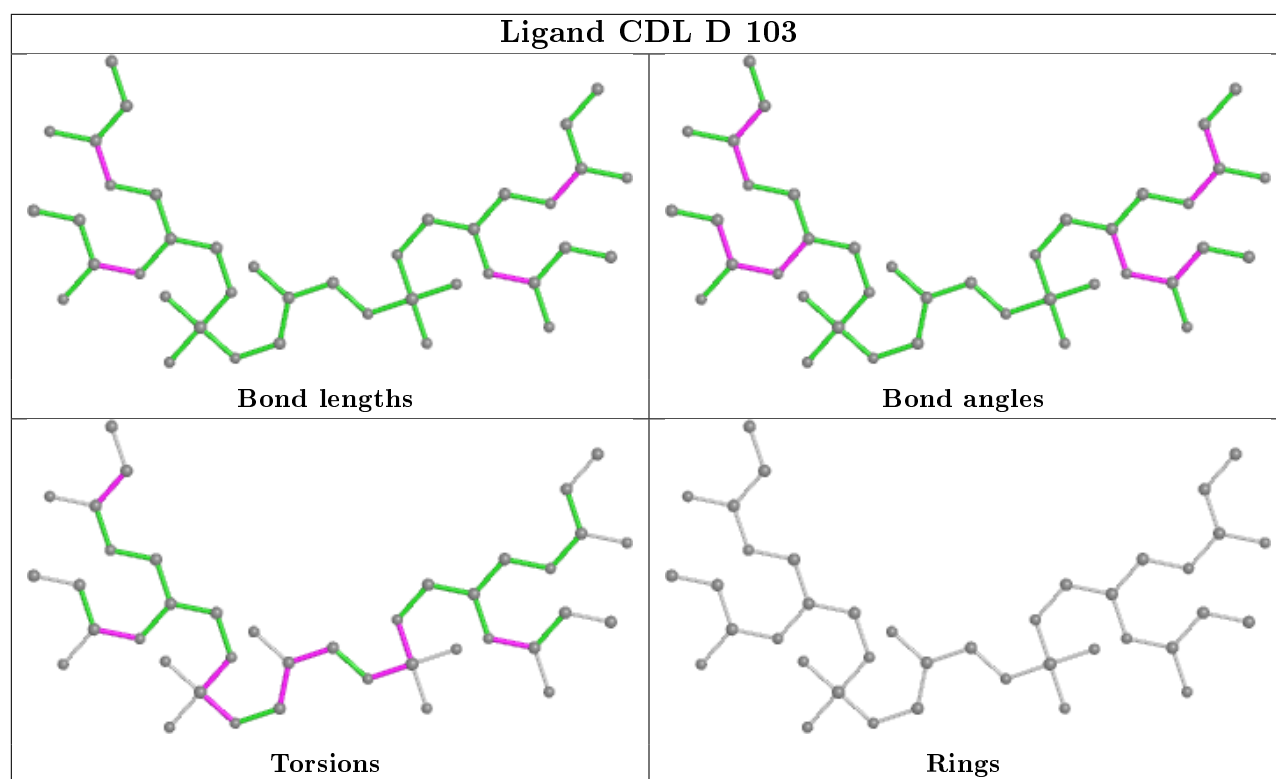


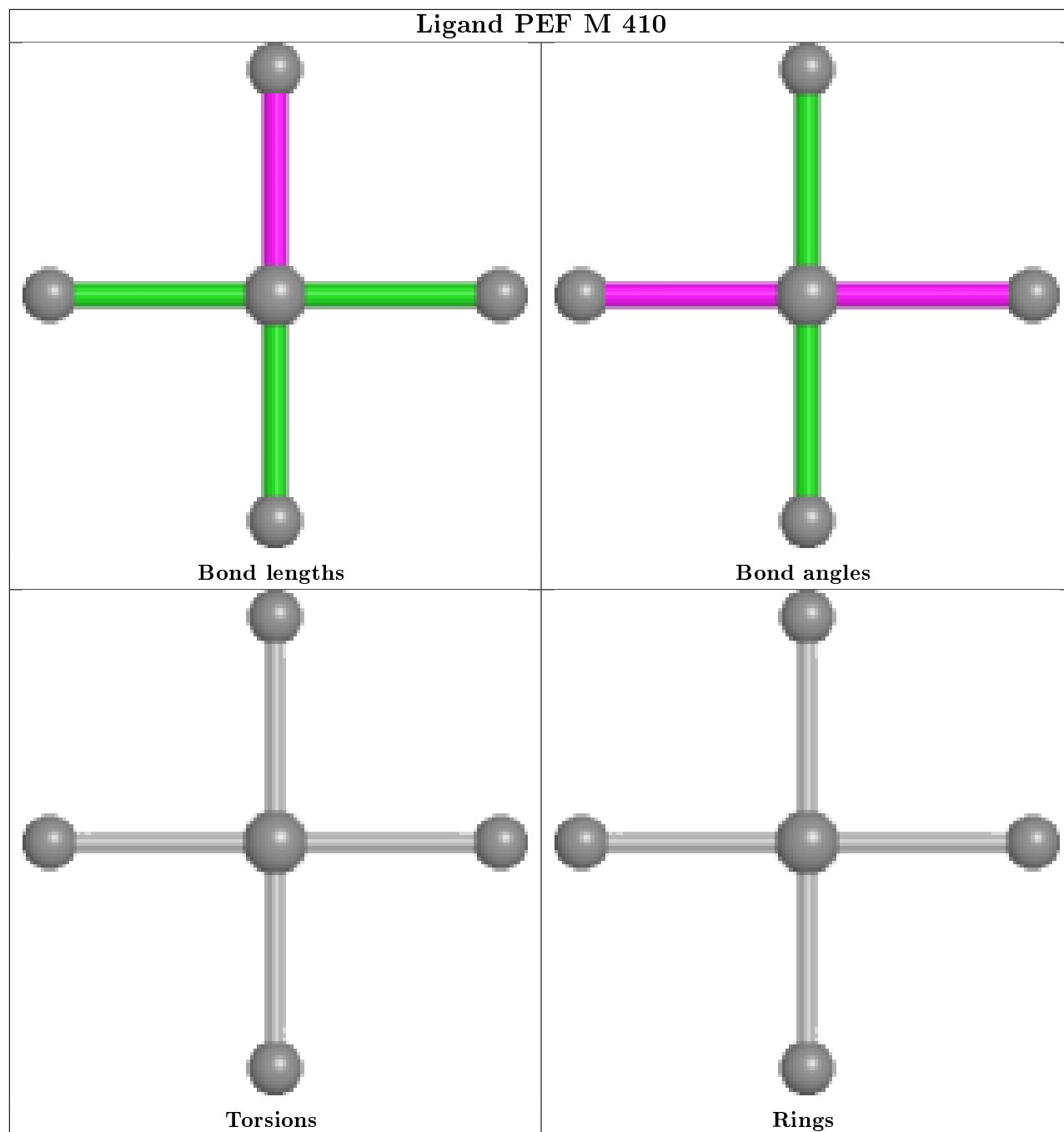


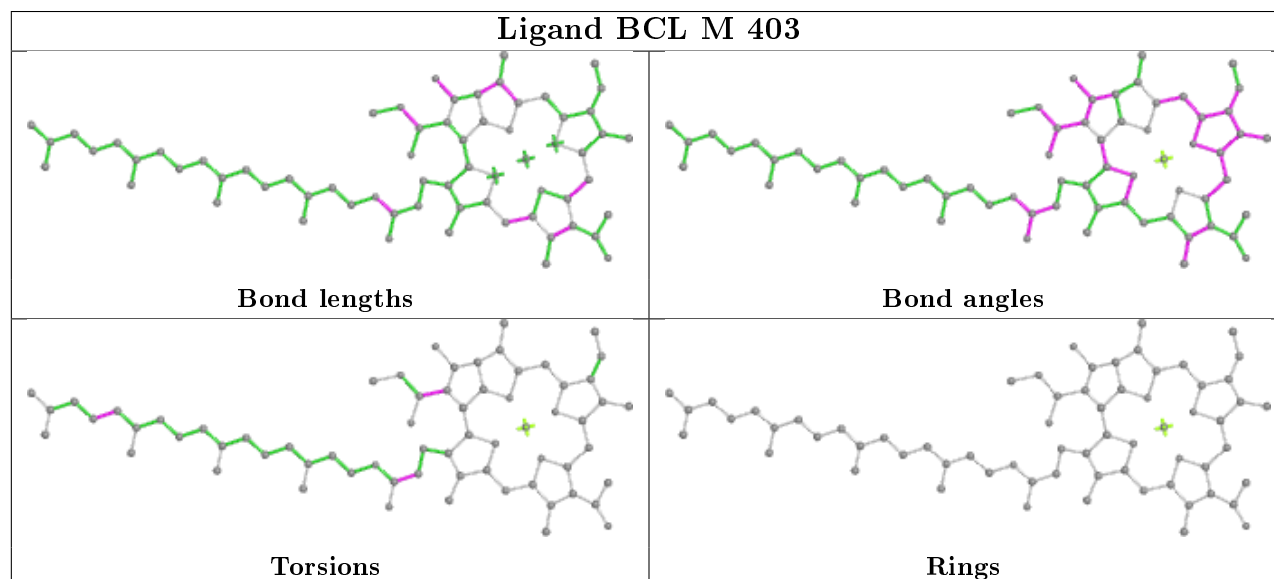
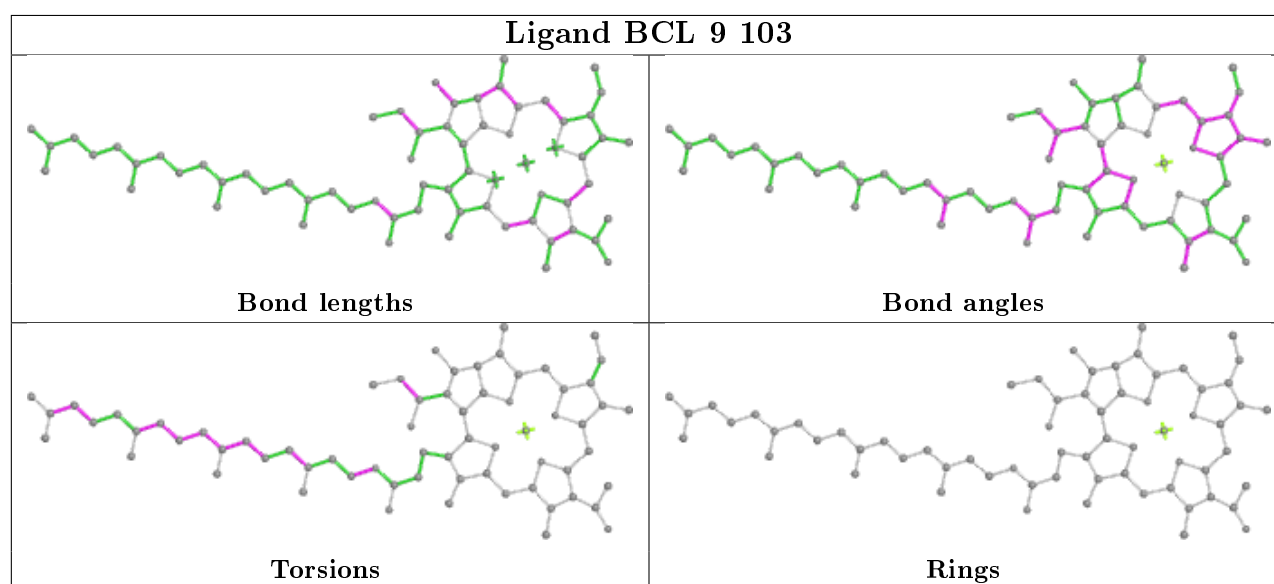
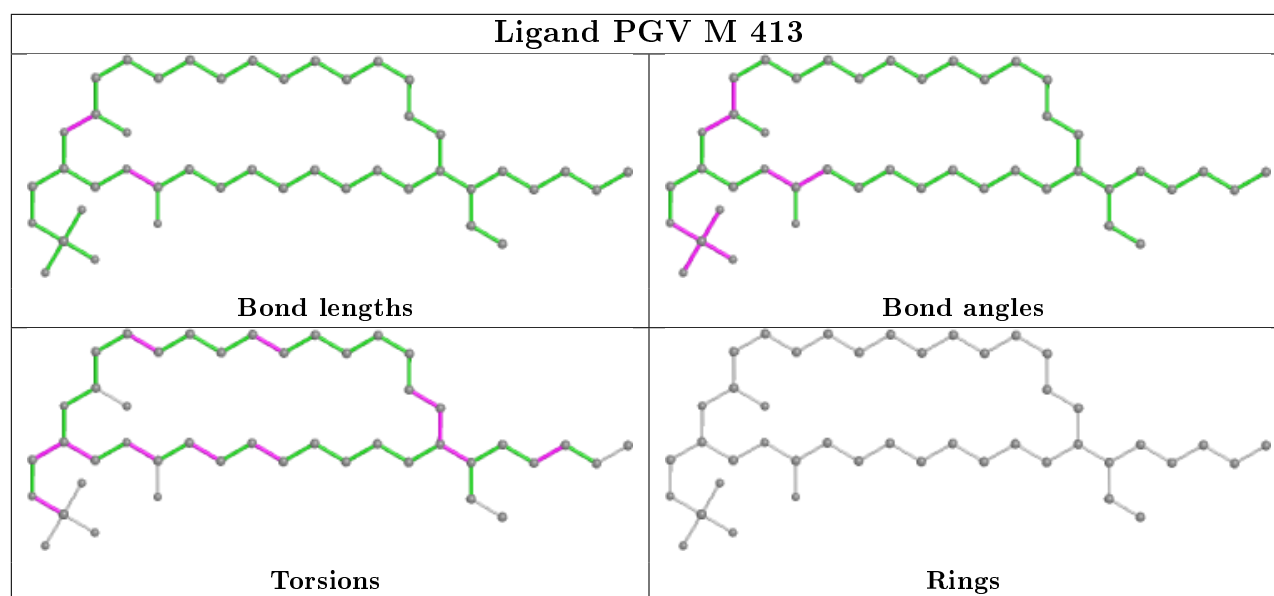


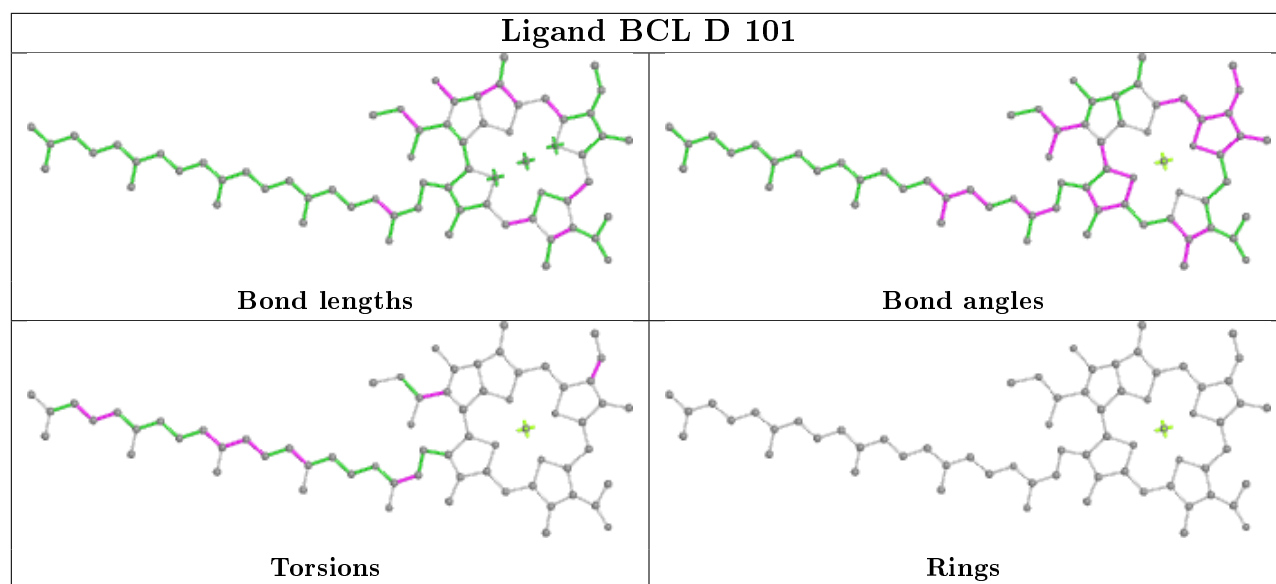
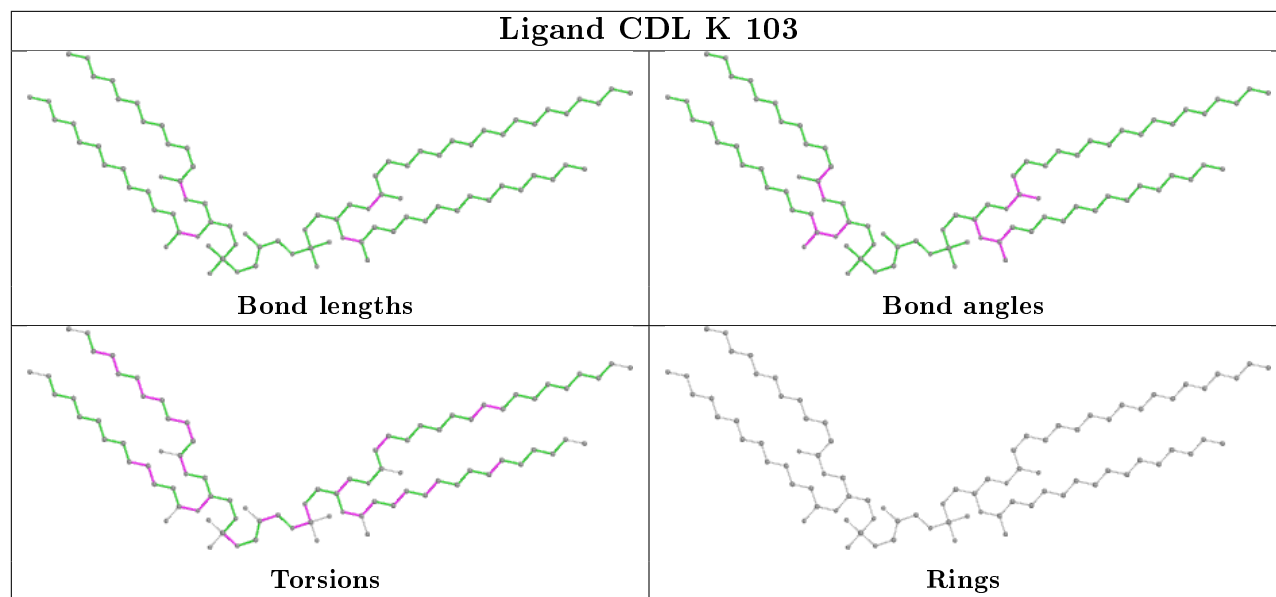


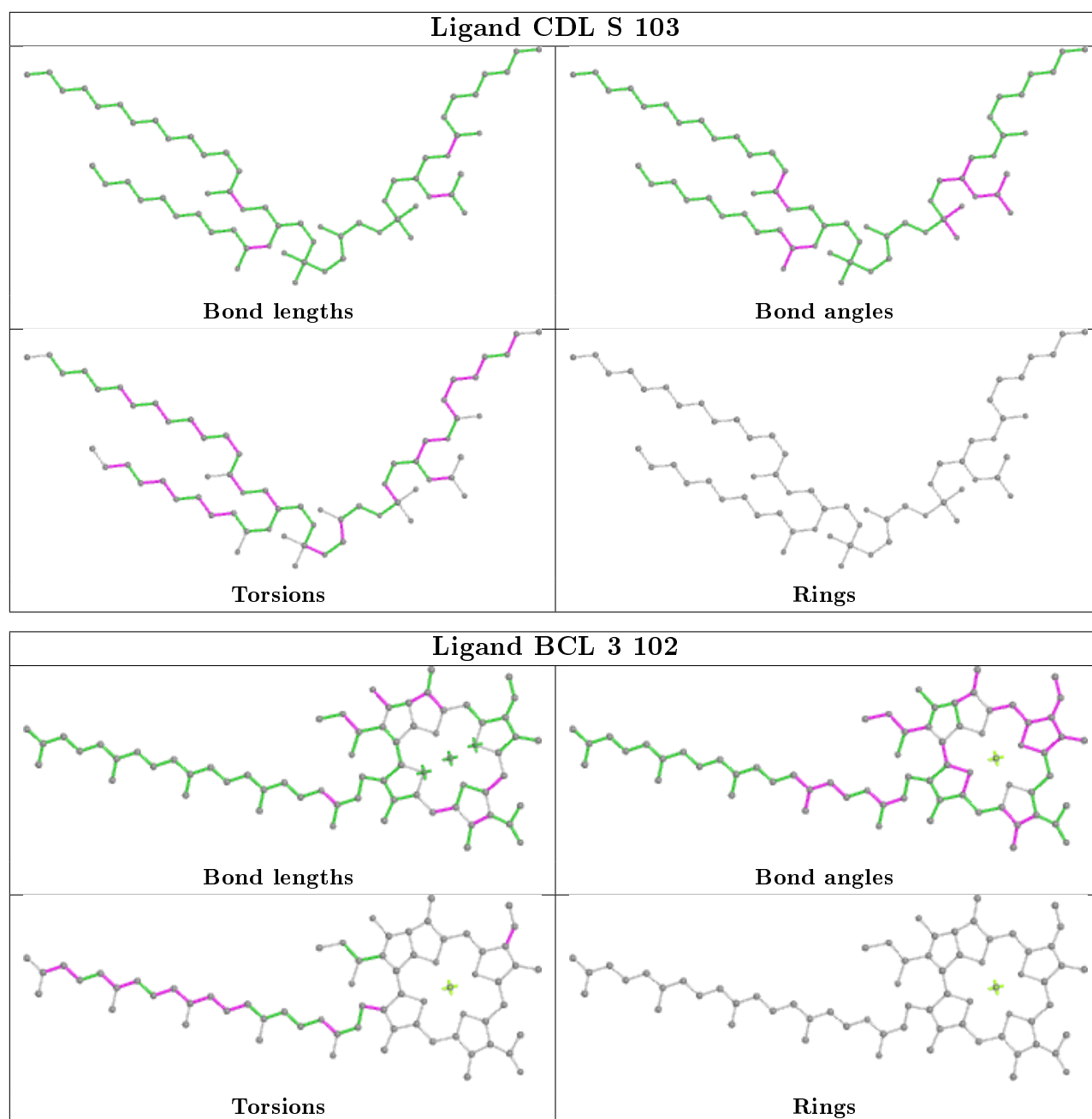


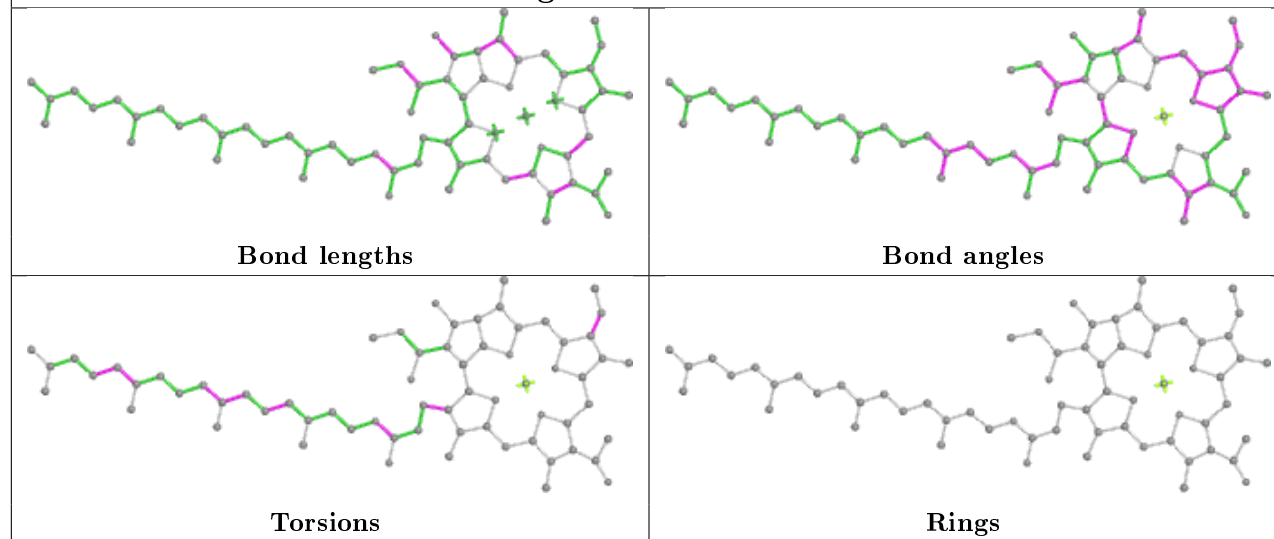
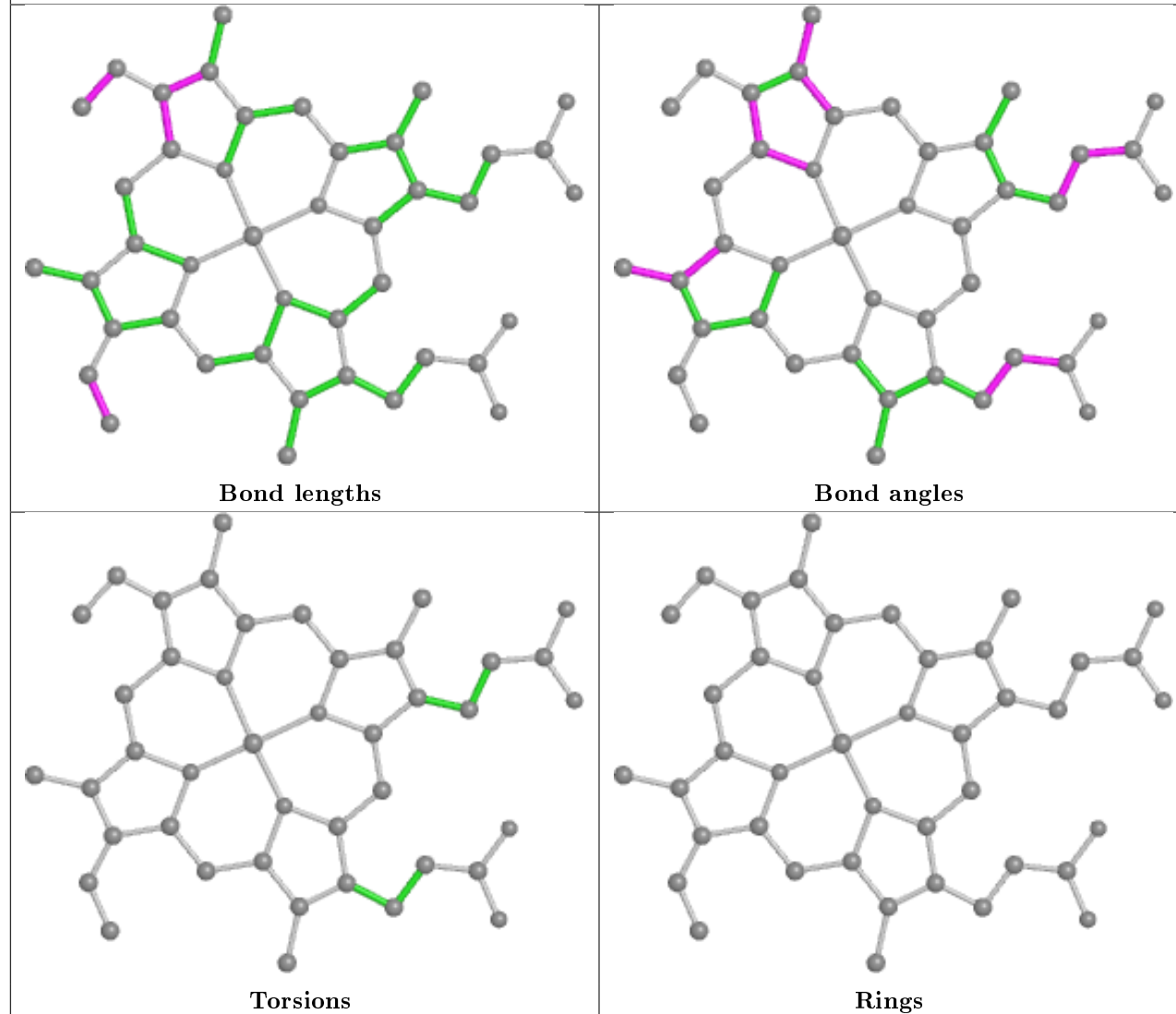


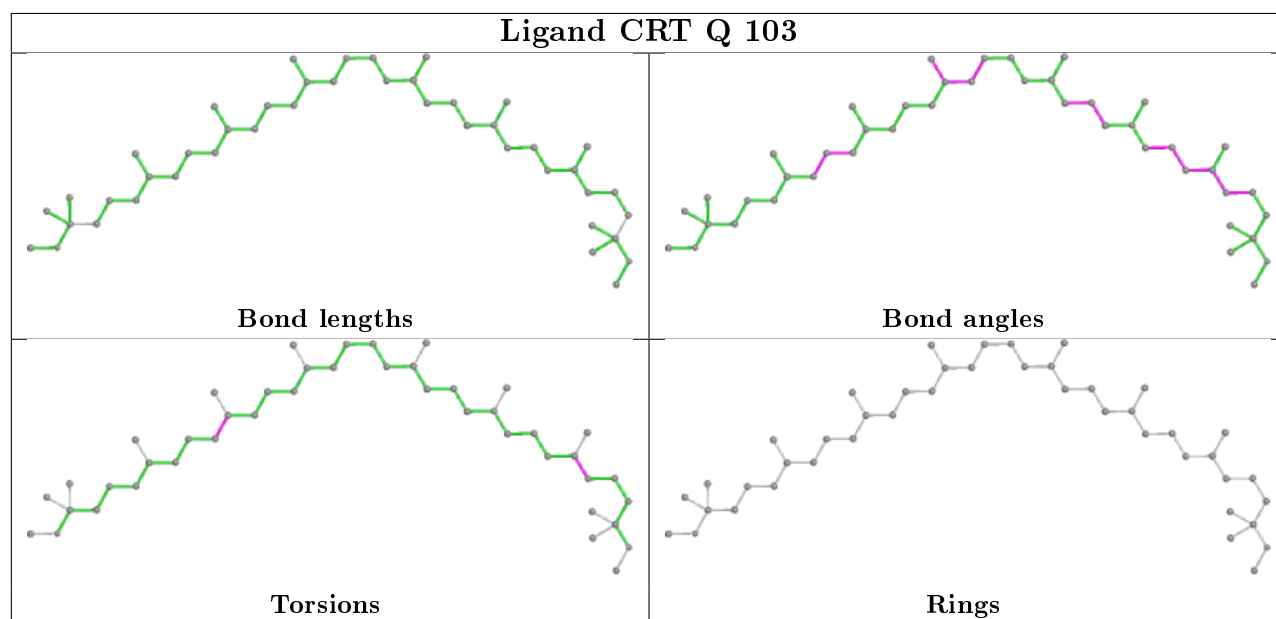
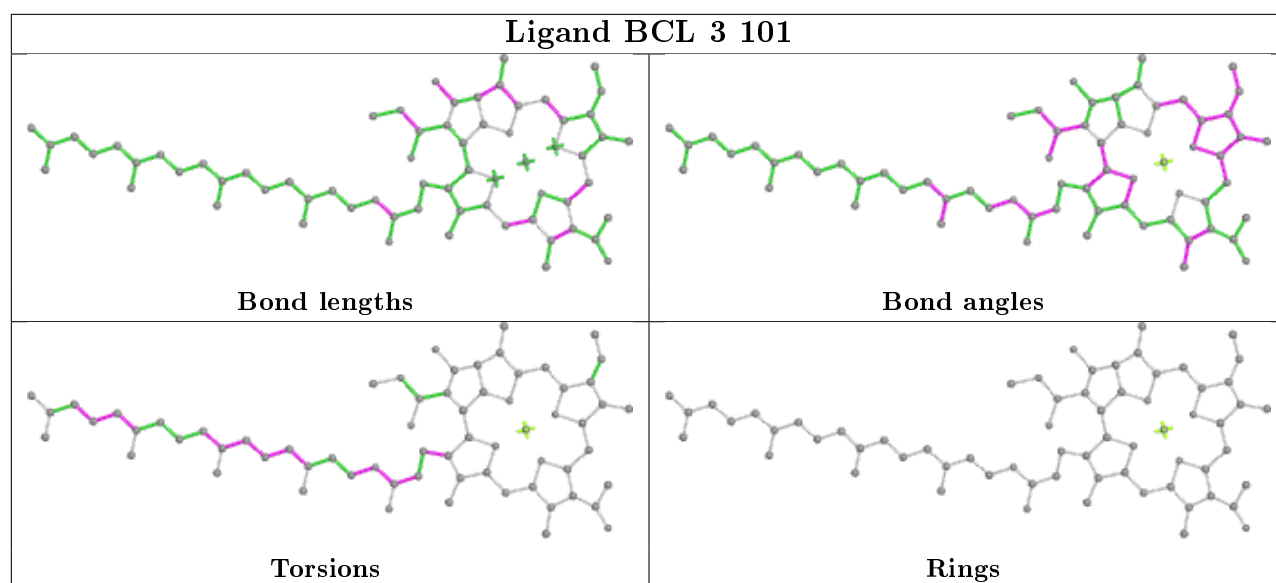


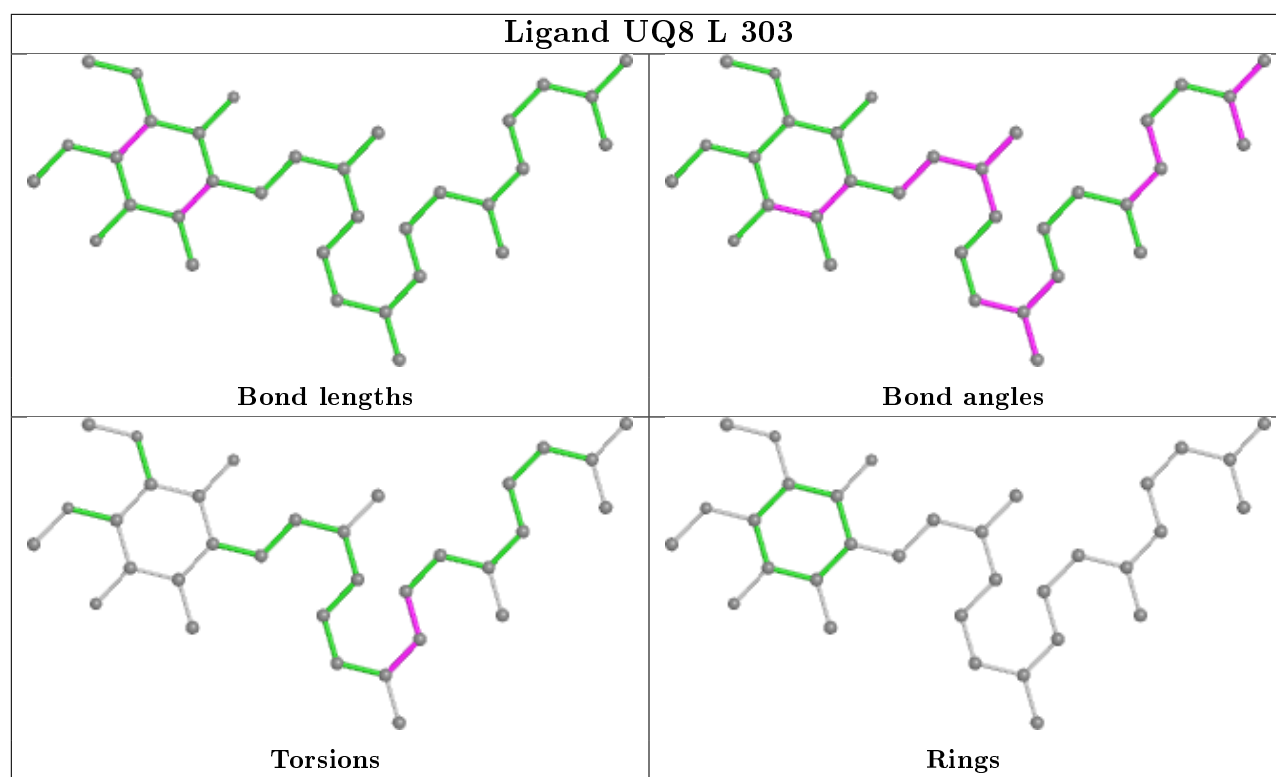


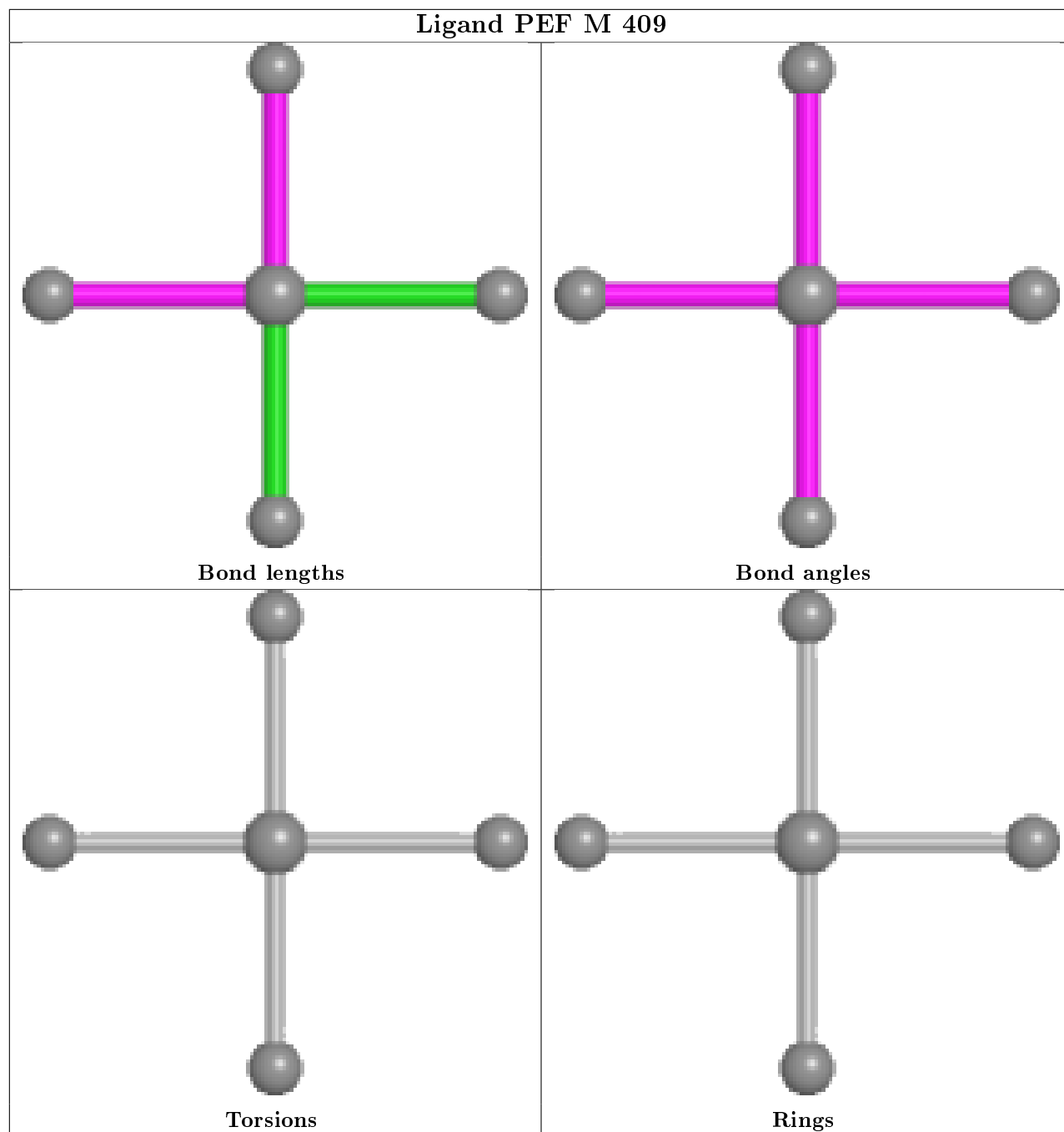


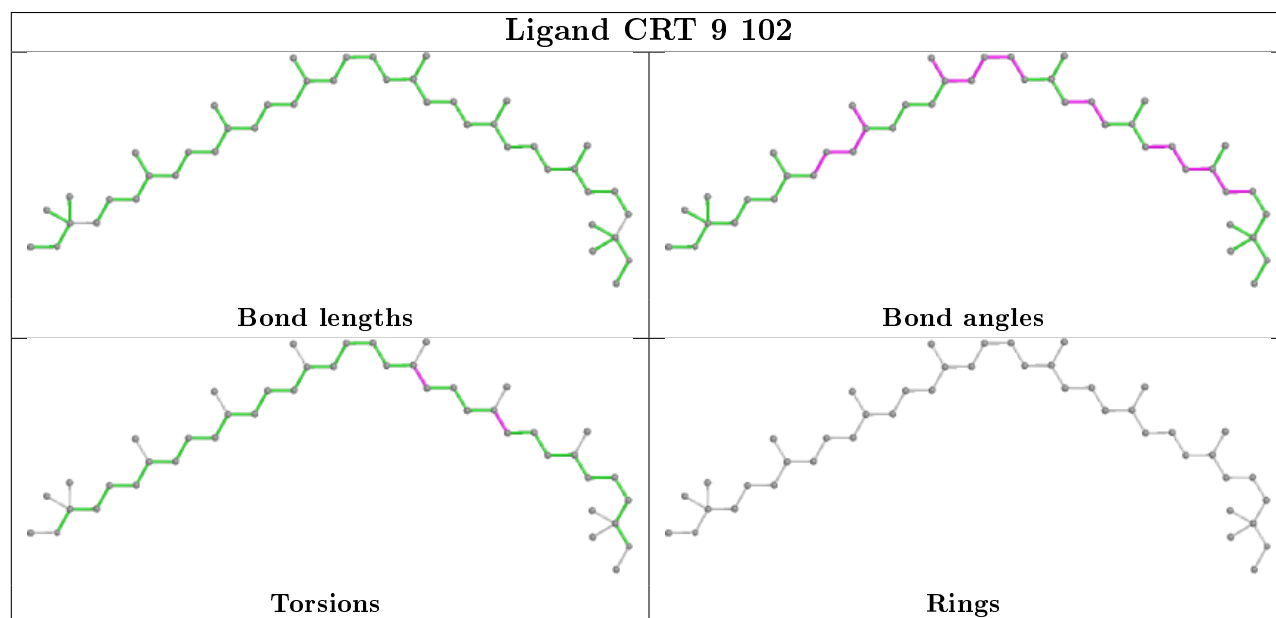
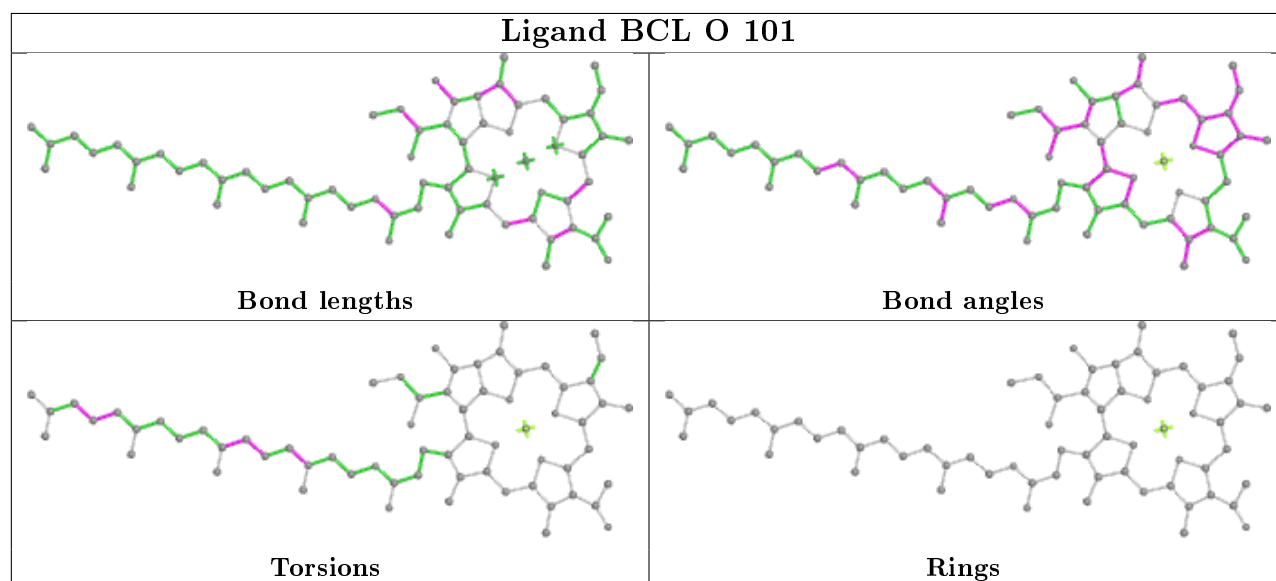
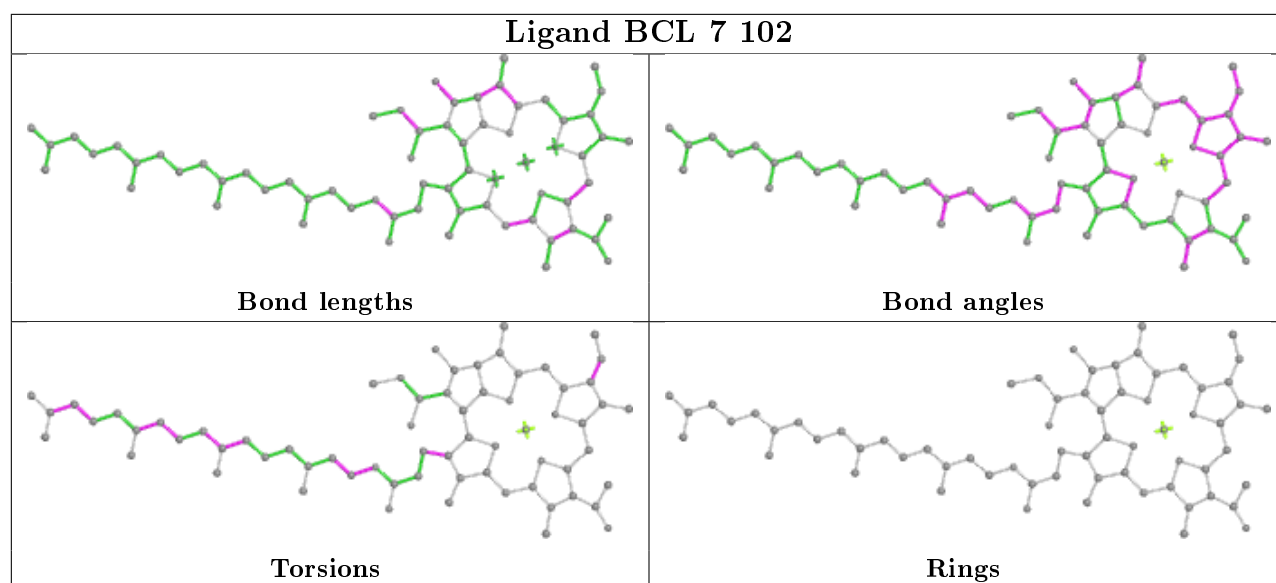


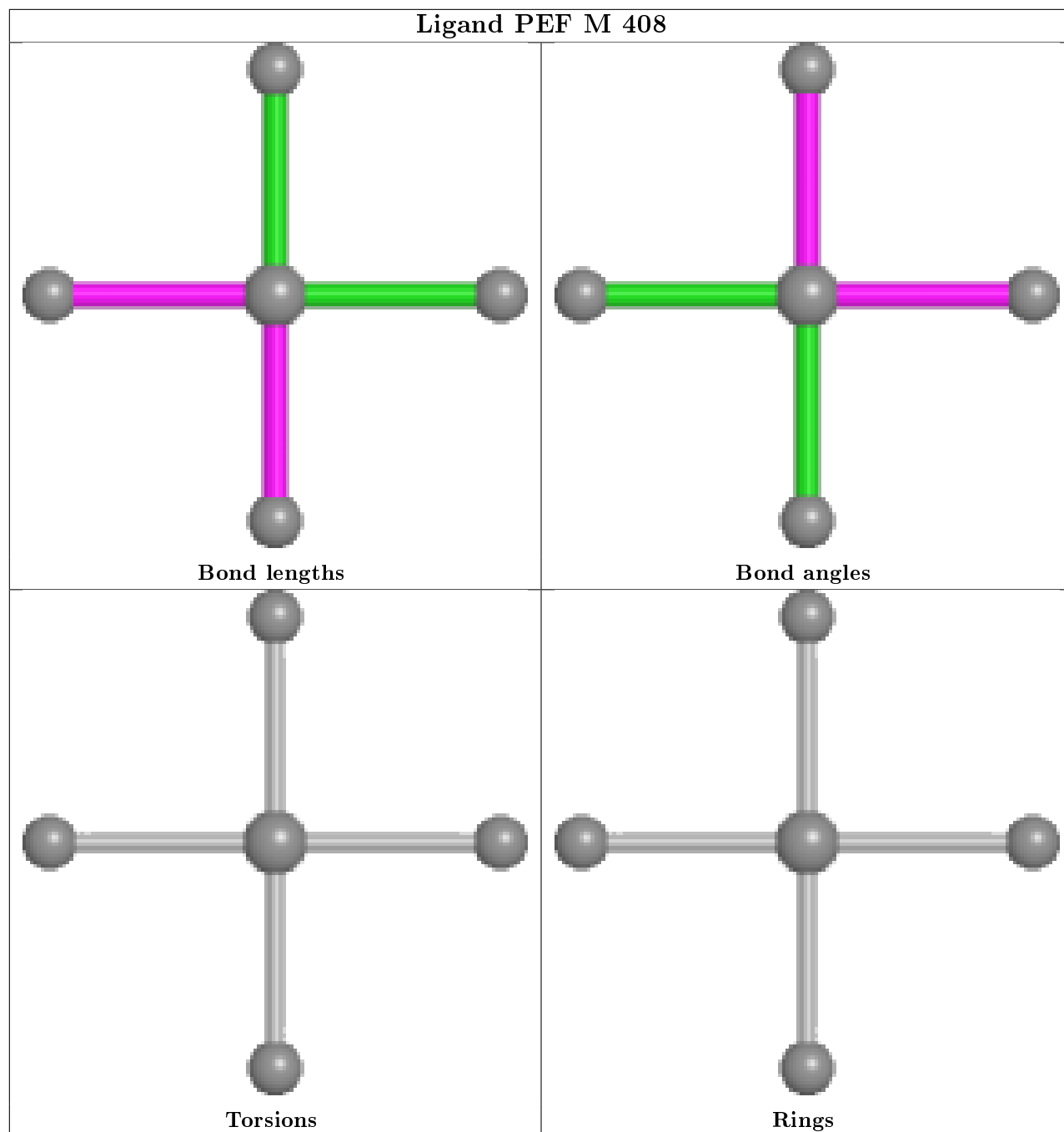
Ligand BCL 1 102**Ligand HEC C 503**

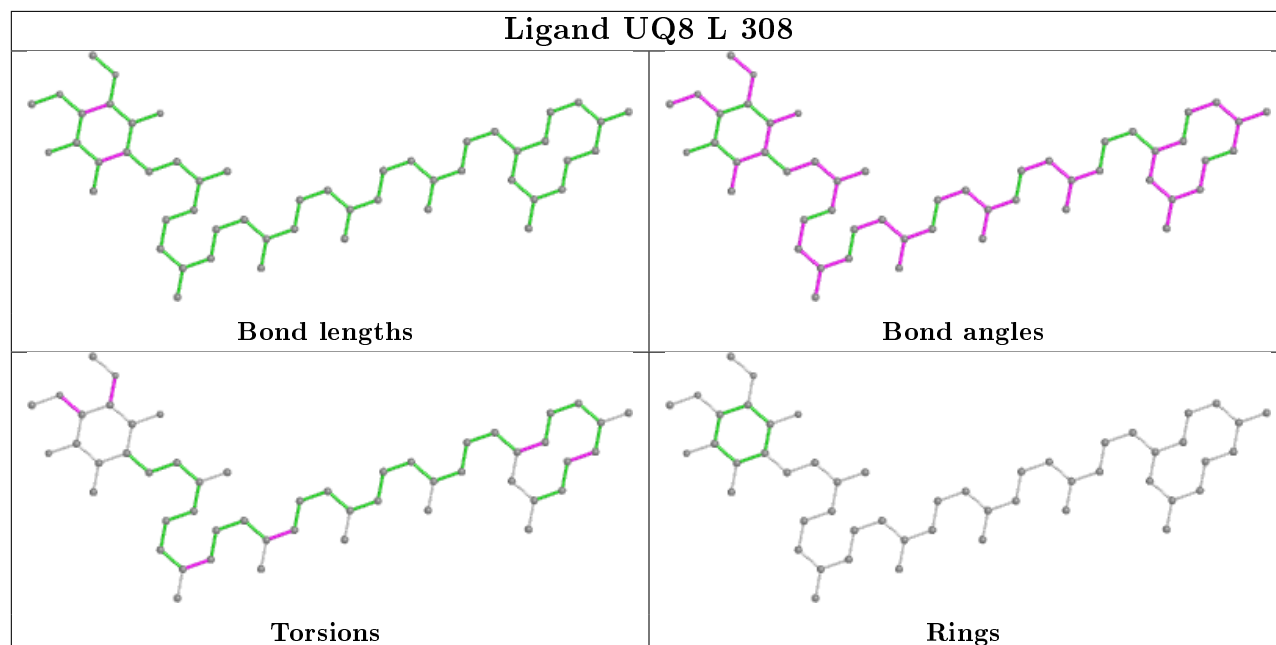
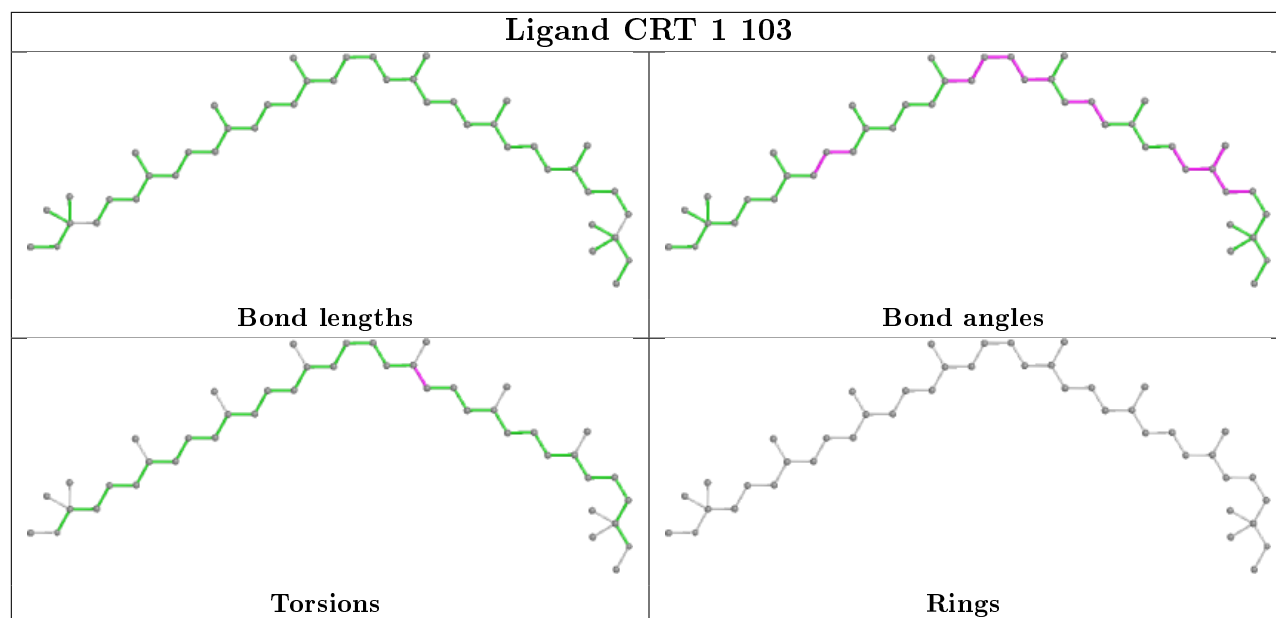
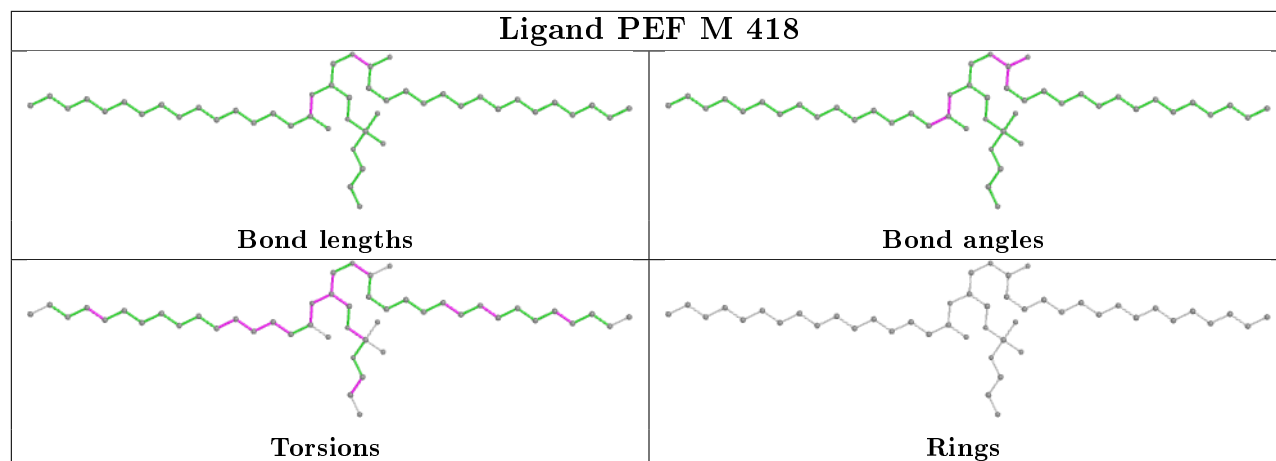


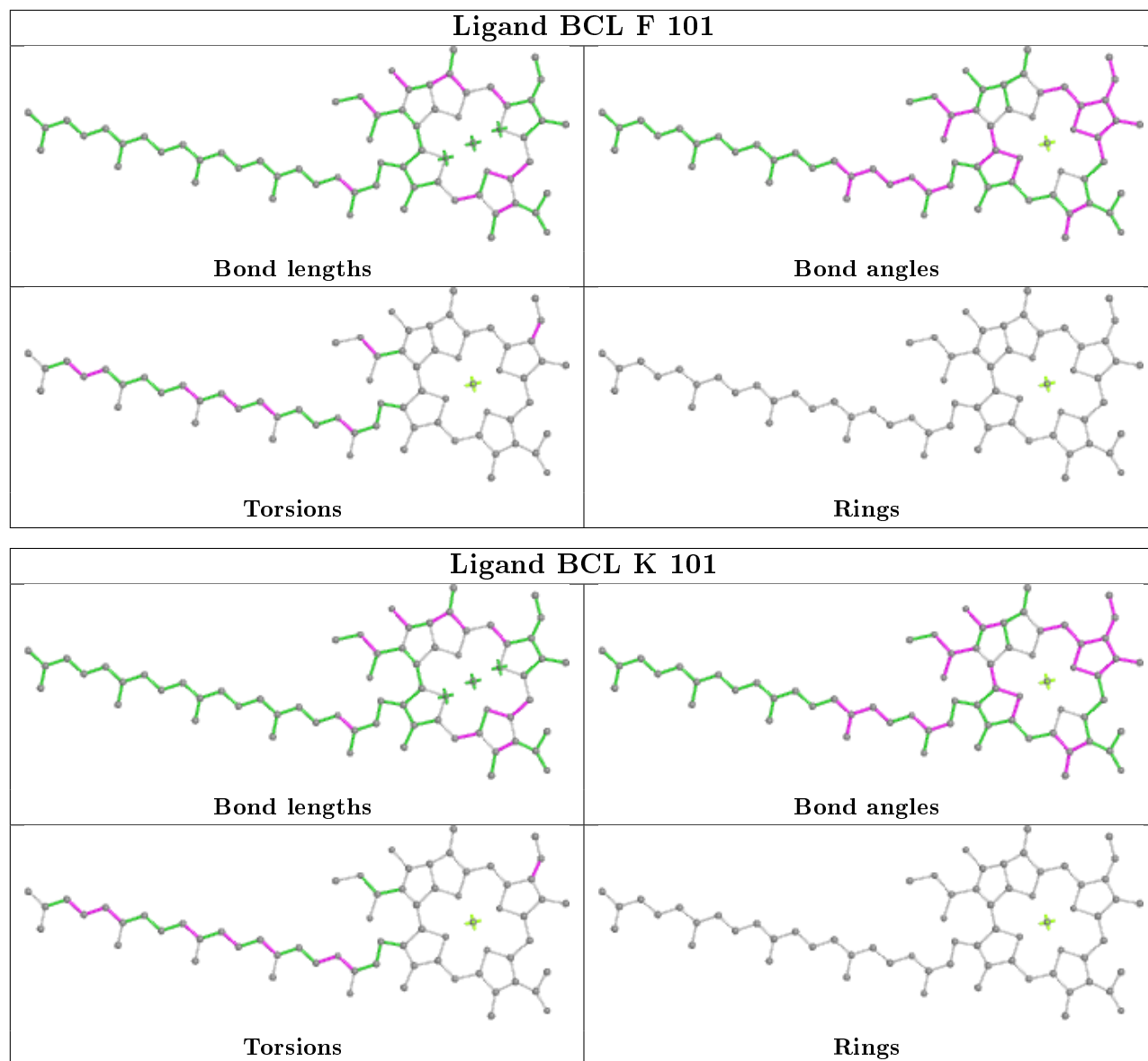


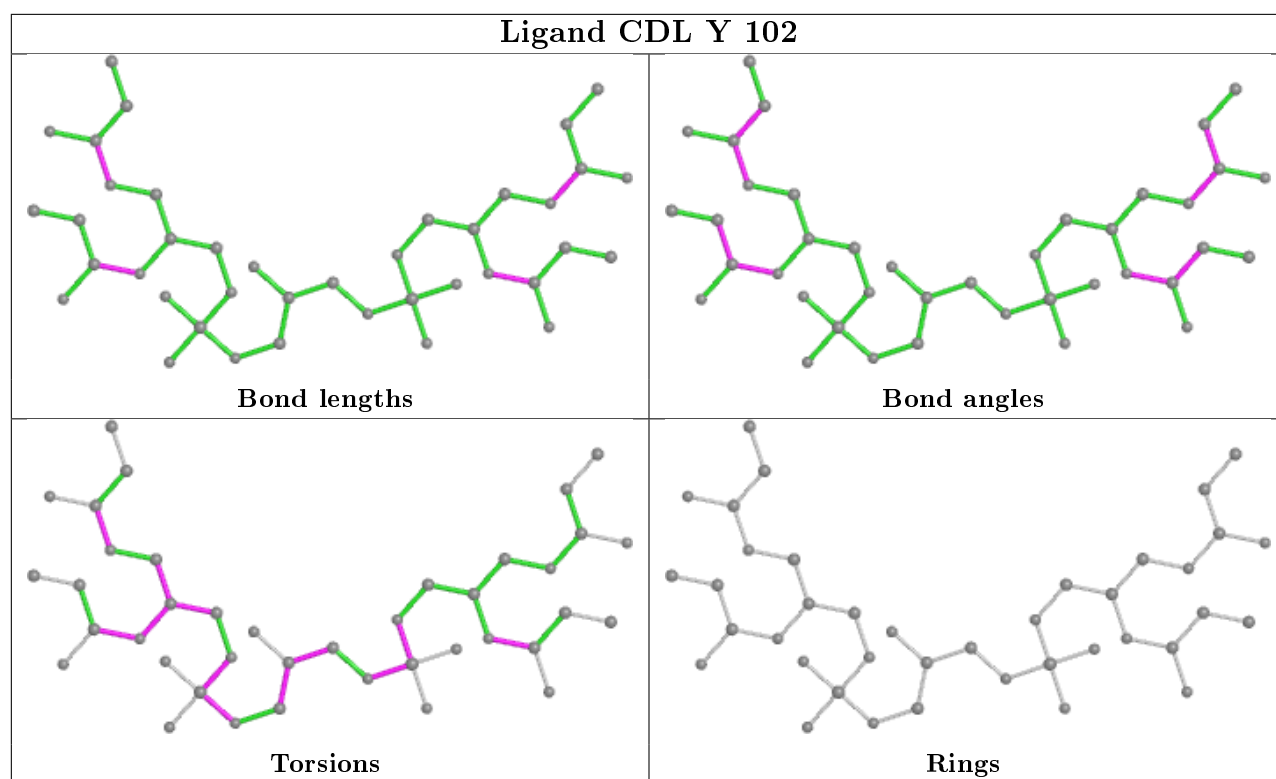












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	C	311/404 (76%)	-0.07	8 (2%) 56 58	32, 48, 81, 113	0
2	L	280/281 (99%)	0.28	21 (7%) 14 15	31, 44, 59, 100	0
3	M	318/325 (97%)	0.28	10 (3%) 49 51	30, 42, 54, 85	0
4	H	255/259 (98%)	0.07	9 (3%) 44 47	41, 58, 87, 130	0
5	1	56/61 (91%)	0.85	11 (19%) 1 1	58, 75, 118, 138	0
5	3	56/61 (91%)	0.84	8 (14%) 2 2	59, 77, 106, 145	0
5	5	54/61 (88%)	1.01	8 (14%) 2 2	54, 70, 95, 114	0
5	7	57/61 (93%)	1.83	18 (31%) 0 0	54, 65, 127, 139	0
5	9	57/61 (93%)	1.15	12 (21%) 1 0	51, 64, 122, 153	0
5	A	54/61 (88%)	0.76	10 (18%) 1 1	55, 67, 98, 117	0
5	D	55/61 (90%)	0.55	5 (9%) 9 10	55, 69, 101, 136	0
5	F	55/61 (90%)	0.81	10 (18%) 1 1	55, 70, 126, 136	0
5	I	57/61 (93%)	0.60	8 (14%) 2 2	54, 70, 120, 150	0
5	K	57/61 (93%)	0.76	6 (10%) 6 7	50, 64, 109, 131	0
5	O	56/61 (91%)	0.79	9 (16%) 1 2	45, 58, 97, 133	0
5	Q	57/61 (93%)	0.69	10 (17%) 1 1	37, 49, 87, 143	0
5	S	56/61 (91%)	1.00	9 (16%) 1 2	40, 53, 109, 147	0
5	U	58/61 (95%)	1.19	13 (22%) 0 0	43, 56, 117, 144	0
5	W	56/61 (91%)	0.47	6 (10%) 6 6	47, 60, 98, 120	0
5	Y	57/61 (93%)	0.37	4 (7%) 16 18	51, 67, 113, 145	0
6	0	43/47 (91%)	1.04	11 (25%) 0 0	64, 74, 91, 116	0
6	2	41/47 (87%)	1.35	13 (31%) 0 0	68, 84, 105, 109	0
6	4	42/47 (89%)	1.27	11 (26%) 0 0	65, 80, 98, 107	0
6	6	42/47 (89%)	0.68	4 (9%) 8 9	63, 73, 92, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	8	41/47 (87%)	0.94	9 (21%) 0 0	65, 74, 96, 119	0
6	B	42/47 (89%)	0.85	8 (19%) 1 1	68, 80, 97, 108	0
6	E	38/47 (80%)	1.11	8 (21%) 1 0	69, 84, 113, 118	0
6	G	42/47 (89%)	1.74	17 (40%) 0 0	66, 88, 125, 148	0
6	J	42/47 (89%)	1.49	13 (30%) 0 0	64, 82, 107, 112	0
6	N	42/47 (89%)	0.70	5 (11%) 4 5	57, 75, 95, 102	0
6	P	42/47 (89%)	0.26	4 (9%) 8 9	49, 63, 84, 88	0
6	R	41/47 (87%)	0.47	5 (12%) 4 4	46, 58, 80, 82	0
6	T	43/47 (91%)	0.16	1 (2%) 60 63	49, 61, 82, 97	0
6	V	42/47 (89%)	0.66	5 (11%) 4 5	53, 72, 101, 116	0
6	X	41/47 (87%)	1.28	13 (31%) 0 0	60, 78, 103, 108	0
6	Z	40/47 (85%)	0.88	9 (22%) 0 0	63, 80, 101, 107	0
All	All	2726/2997 (90%)	0.57	331 (12%) 4 4	30, 60, 101, 153	0

The worst 5 of 331 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	3	58	LEU	11.3
5	U	6	ALA	9.6
5	7	58	LEU	9.5
5	9	58	LEU	7.6
5	7	8	LEU	7.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
12	PGV	3	104	51/51	0.48	0.39	76,101,155,158	0
16	UNL	P	102	12/-	0.62	0.23	67,74,82,82	0
21	LDA	M	411	14/16	0.64	0.30	65,82,109,113	0
20	PEF	M	407	5/47	0.64	0.15	161,162,163,165	0
20	PEF	3	103	5/47	0.67	0.18	136,137,138,142	0
16	UNL	J	103	12/-	0.68	0.20	74,79,93,94	0
12	PGV	C	509	21/51	0.69	0.27	81,101,108,113	0
22	CDL	Y	102	40/100	0.69	0.25	114,129,148,149	0
19	CRT	1	103	44/44	0.70	0.21	58,78,96,99	0
21	LDA	O	104	14/16	0.71	0.31	61,75,110,112	0
20	PEF	U	105	5/47	0.72	0.15	156,156,159,160	0
22	CDL	S	103	62/100	0.73	0.23	73,116,153,162	0
23	LMT	M	419	35/35	0.73	0.23	64,99,112,121	0
22	CDL	Q	104	75/100	0.73	0.25	62,97,142,143	0
16	UNL	0	103	12/-	0.73	0.19	77,84,87,87	0
19	CRT	J	101	44/44	0.74	0.23	59,74,97,100	0
21	LDA	J	102	16/16	0.74	0.19	74,90,112,114	0
22	CDL	D	103	40/100	0.75	0.24	116,142,163,164	0
16	UNL	E	101	12/-	0.75	0.28	78,93,101,102	0
16	UNL	B	101	12/-	0.77	0.16	69,80,88,91	0
16	UNL	R	101	12/-	0.77	0.20	57,68,75,77	0
16	UNL	G	102	12/-	0.77	0.16	77,85,93,93	0
16	UNL	2	102	12/-	0.77	0.22	71,80,90,92	0
9	GOL	C	506	6/6	0.78	0.19	63,68,72,75	0
16	UNL	8	101	12/-	0.80	0.17	64,74,96,96	0
12	PGV	L	305	43/51	0.80	0.23	45,76,104,109	0
16	UNL	T	101	12/-	0.80	0.22	45,68,81,82	0
19	CRT	G	101	44/44	0.80	0.20	61,80,114,123	0
20	PEF	M	409	5/47	0.81	0.25	94,98,100,102	0
16	UNL	Z	103	12/-	0.81	0.17	68,80,92,95	0
21	LDA	V	102	16/16	0.81	0.20	60,77,119,122	0
16	UNL	X	101	12/-	0.81	0.14	68,76,82,85	0
12	PGV	1	105	31/51	0.82	0.18	83,102,125,129	0
19	CRT	U	103	44/44	0.82	0.18	48,72,91,96	0
16	UNL	6	102	12/-	0.82	0.23	76,81,91,93	0
15	UQ8	L	309	18/53	0.82	0.26	102,114,125,132	0
9	GOL	H	301	6/6	0.82	0.16	58,78,82,84	0
16	UNL	4	101	12/-	0.82	0.20	72,88,103,105	0
15	UQ8	L	308	53/53	0.82	0.31	60,90,99,104	0
20	PEF	5	103	5/47	0.82	0.15	126,127,129,131	0
19	CRT	9	101	44/44	0.82	0.19	53,68,100,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	PGV	L	306	44/51	0.83	0.22	53,75,98,108	0
10	SO4	M	412	5/5	0.83	0.14	125,126,126,130	0
15	UQ8	7	103	33/53	0.83	0.30	60,74,94,100	0
19	CRT	0	101	44/44	0.83	0.18	51,68,88,95	0
22	CDL	Y	103	13/100	0.84	0.17	107,120,124,128	0
20	PEF	K	104	27/47	0.84	0.28	63,85,92,97	0
22	CDL	K	103	86/100	0.84	0.31	56,92,114,120	0
23	LMT	F	103	35/35	0.84	0.18	61,78,92,92	0
20	PEF	1	104	5/47	0.84	0.15	119,119,121,121	0
19	CRT	2	101	44/44	0.85	0.18	67,78,94,99	0
20	PEF	U	104	5/47	0.85	0.18	113,115,116,118	0
16	UNL	M	416	9/-	0.86	0.44	58,64,73,75	0
19	CRT	6	101	44/44	0.86	0.17	48,69,84,87	0
10	SO4	L	304	5/5	0.86	0.26	136,137,138,138	0
19	CRT	A	104	44/44	0.87	0.18	62,74,97,101	0
22	CDL	H	302	64/100	0.87	0.29	75,89,107,113	0
20	PEF	W	103	5/47	0.87	0.11	146,148,148,149	0
12	PGV	D	104	35/51	0.88	0.19	55,72,100,113	0
12	PGV	M	414	37/51	0.88	0.17	60,83,116,121	0
12	PGV	M	413	46/51	0.89	0.16	52,74,89,94	0
12	PGV	A	105	33/51	0.89	0.22	60,93,108,109	0
16	UNL	L	307	12/-	0.89	0.21	79,88,96,96	0
19	CRT	9	102	44/44	0.90	0.17	51,67,94,105	0
20	PEF	M	408	5/47	0.90	0.09	56,67,83,95	0
19	CRT	Z	101	44/44	0.90	0.17	58,72,99,100	0
15	UQ8	M	417	18/53	0.90	0.27	61,74,96,102	0
19	CRT	V	101	44/44	0.90	0.15	41,62,85,87	0
19	CRT	O	103	44/44	0.90	0.16	37,51,75,82	0
10	SO4	C	507	5/5	0.90	0.15	113,114,117,120	0
19	CRT	N	101	44/44	0.90	0.14	50,67,86,94	0
19	CRT	Q	103	44/44	0.91	0.14	42,55,73,76	0
20	PEF	M	418	47/47	0.91	0.24	58,75,93,97	0
20	PEF	I	103	5/47	0.92	0.12	99,107,109,112	0
21	LDA	I	104	16/16	0.92	0.27	36,70,75,77	0
22	CDL	H	304	79/100	0.92	0.31	44,73,107,111	0
19	CRT	P	101	44/44	0.92	0.15	38,55,77,80	0
13	BCL	3	101	66/66	0.93	0.15	61,75,105,110	0
13	BCL	7	101	61/66	0.93	0.12	53,64,96,103	0
11	LHG	C	508	9/49	0.93	0.14	52,61,67,69	0
12	PGV	H	303	36/51	0.93	0.20	47,59,82,89	0
18	MQ8	M	405	53/53	0.93	0.24	36,53,116,123	0
13	BCL	1	102	66/66	0.93	0.14	49,70,97,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	BCL	L	301	66/66	0.94	0.11	27,34,43,70	0
13	BCL	Z	102	66/66	0.94	0.14	52,64,98,103	0
13	BCL	5	101	66/66	0.94	0.14	55,69,109,111	0
13	BCL	3	102	66/66	0.94	0.12	53,69,93,96	0
13	BCL	5	102	66/66	0.94	0.16	50,62,90,98	0
8	MG	C	505	1/1	0.94	0.11	36,36,36,36	0
14	BPH	L	302	65/65	0.94	0.17	29,40,54,59	0
13	BCL	9	103	66/66	0.94	0.13	54,63,103,106	0
13	BCL	7	102	66/66	0.94	0.14	53,63,95,102	0
13	BCL	K	102	66/66	0.95	0.14	47,58,98,102	0
13	BCL	F	102	66/66	0.95	0.14	55,70,107,113	0
15	UQ8	L	303	33/53	0.95	0.14	36,45,77,85	0
22	CDL	M	415	39/100	0.95	0.13	46,80,113,119	0
13	BCL	A	103	66/66	0.95	0.14	58,70,104,109	0
13	BCL	1	101	66/66	0.95	0.11	59,67,107,113	0
19	CRT	M	406	44/44	0.95	0.15	31,39,82,90	0
13	BCL	0	102	66/66	0.96	0.12	54,65,97,108	0
13	BCL	M	401	66/66	0.96	0.13	30,39,54,62	0
13	BCL	O	102	66/66	0.96	0.14	41,51,89,96	0
13	BCL	U	102	66/66	0.96	0.14	44,55,92,101	0
13	BCL	W	101	66/66	0.96	0.14	48,59,114,118	0
13	BCL	M	402	66/66	0.96	0.12	26,35,84,90	0
13	BCL	Q	101	66/66	0.96	0.13	40,48,94,99	0
13	BCL	Q	102	66/66	0.96	0.13	39,47,84,93	0
13	BCL	I	101	66/66	0.96	0.13	61,68,100,104	0
13	BCL	W	102	66/66	0.96	0.12	49,60,94,97	0
13	BCL	A	101	66/66	0.96	0.12	54,69,113,118	0
13	BCL	F	101	66/66	0.96	0.13	57,69,114,117	0
13	BCL	K	101	66/66	0.96	0.14	50,63,102,105	0
13	BCL	Y	101	66/66	0.96	0.12	49,60,110,113	0
13	BCL	D	101	66/66	0.96	0.12	55,70,117,121	0
13	BCL	I	102	66/66	0.96	0.13	51,65,93,95	0
13	BCL	D	102	66/66	0.96	0.12	57,69,91,92	0
13	BCL	O	101	66/66	0.97	0.12	44,54,102,112	0
14	BPH	M	404	65/65	0.97	0.13	29,38,111,115	0
13	BCL	S	102	66/66	0.97	0.12	40,48,90,96	0
13	BCL	U	101	66/66	0.97	0.12	42,53,101,104	0
13	BCL	M	403	66/66	0.97	0.11	27,34,45,54	0
13	BCL	S	101	66/66	0.97	0.13	38,49,96,110	0
7	HEC	C	504	43/43	0.98	0.09	34,40,47,54	0
7	HEC	C	502	43/43	0.98	0.09	39,46,52,55	0
20	PEF	M	410	5/47	0.98	0.11	40,45,52,54	0

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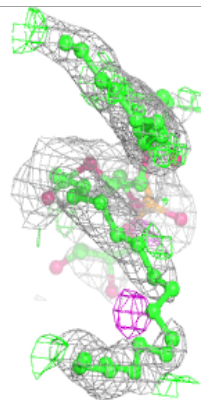
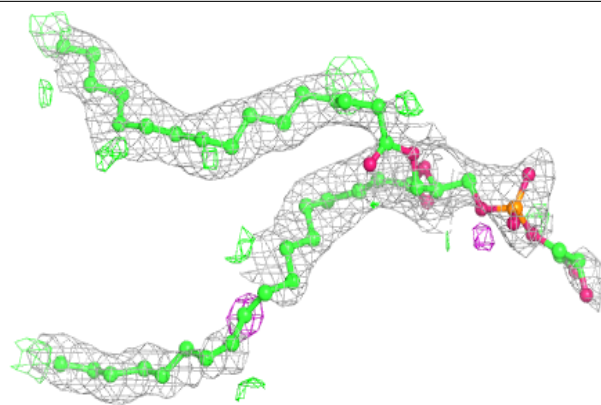
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	HEC	C	503	43/43	0.98	0.09	29,35,42,46	0
24	CA	2	103	1/1	0.98	0.03	68,68,68,68	0
7	HEC	C	501	43/43	0.98	0.10	52,60,67,75	0
24	CA	4	102	1/1	0.98	0.07	68,68,68,68	0
24	CA	J	104	1/1	0.99	0.06	63,63,63,63	0
24	CA	6	103	1/1	0.99	0.04	67,67,67,67	0
24	CA	A	102	1/1	0.99	0.09	64,64,64,64	0
24	CA	N	102	1/1	0.99	0.07	56,56,56,56	0
24	CA	G	103	1/1	0.99	0.08	64,64,64,64	0
24	CA	X	102	1/1	0.99	0.05	60,60,60,60	0
24	CA	8	102	1/1	0.99	0.06	67,67,67,67	0
24	CA	V	103	1/1	0.99	0.09	52,52,52,52	0
24	CA	E	102	1/1	0.99	0.04	65,65,65,65	0
24	CA	Z	104	1/1	0.99	0.03	60,60,60,60	0
24	CA	B	102	1/1	0.99	0.04	64,64,64,64	0
24	CA	T	102	1/1	1.00	0.07	48,48,48,48	0
24	CA	R	102	1/1	1.00	0.10	44,44,44,44	0
17	FE	L	310	1/1	1.00	0.10	39,39,39,39	0
24	CA	P	103	1/1	1.00	0.11	47,47,47,47	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.

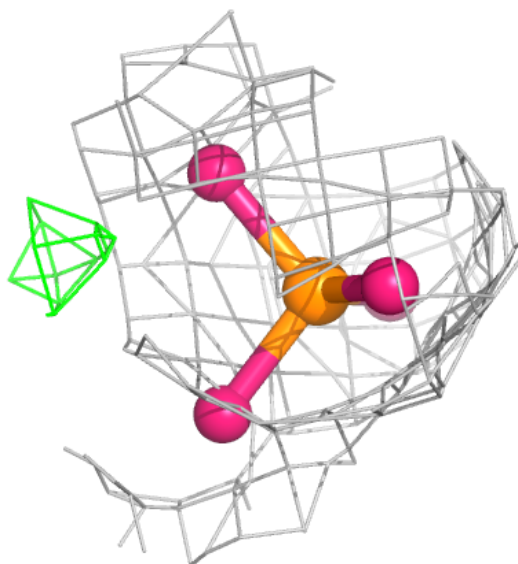
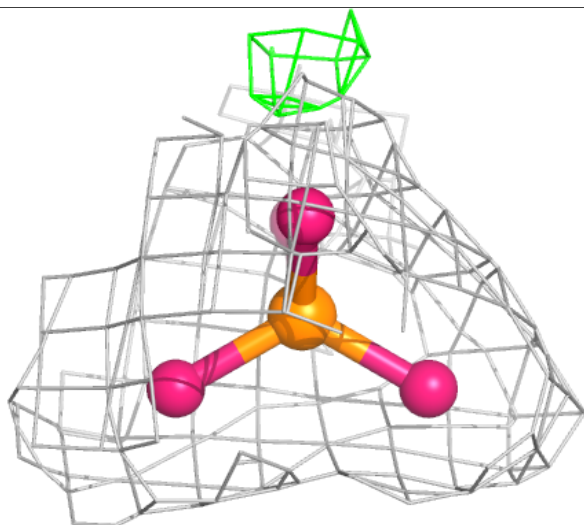
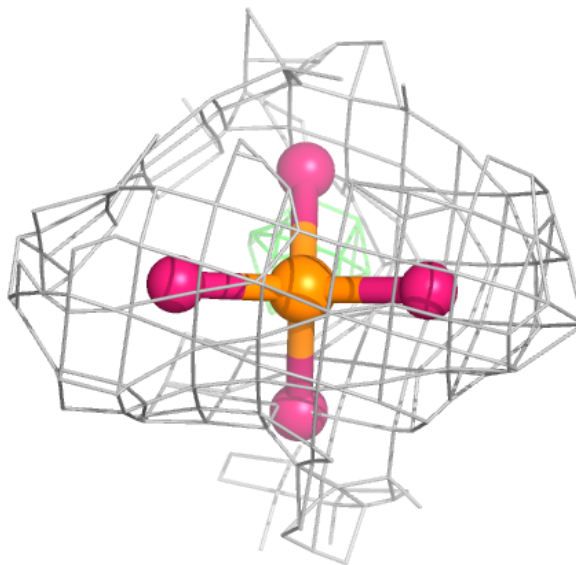
Electron density around PGV 3 104:

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



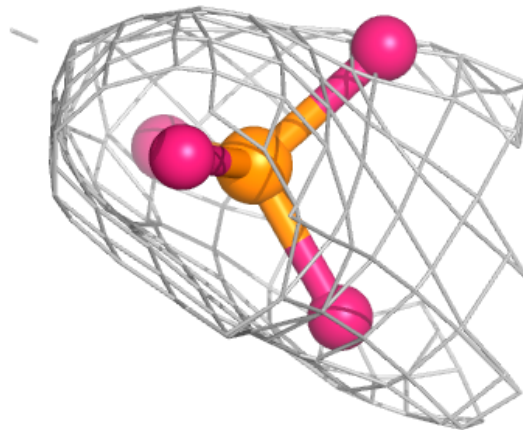
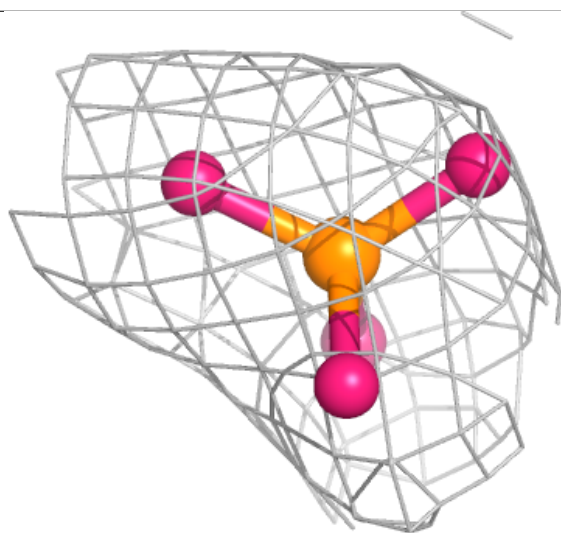
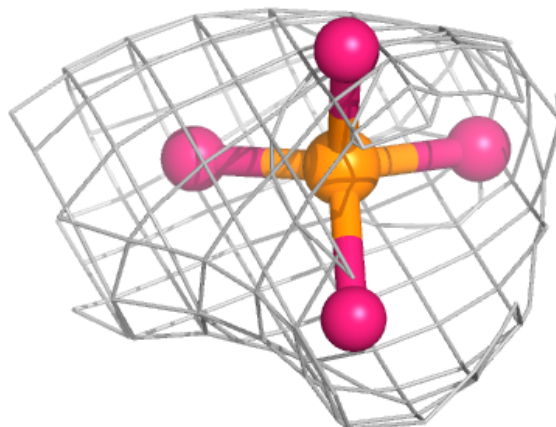
Electron density around PEF M 407:

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



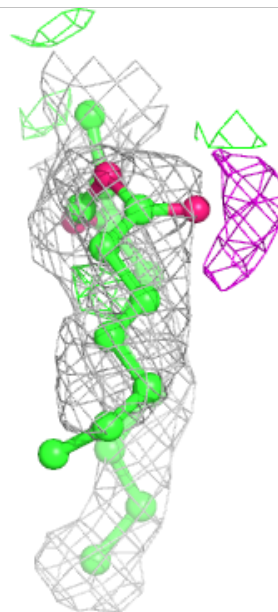
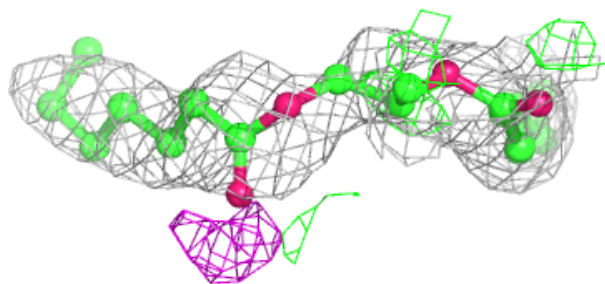
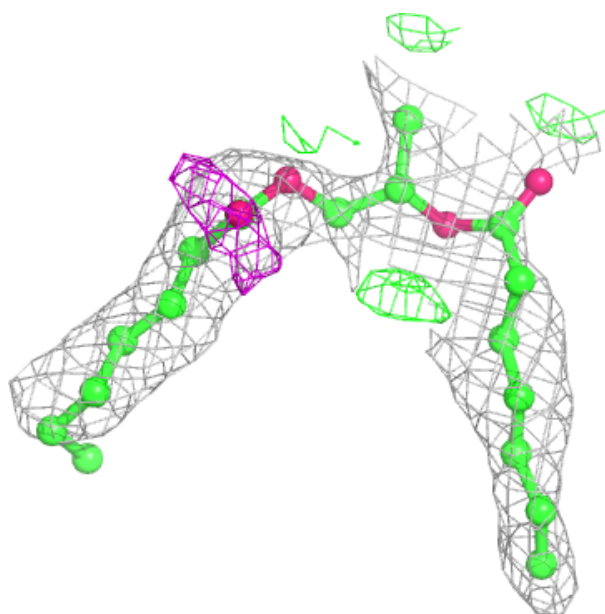
Electron density around PEF 3 103:

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



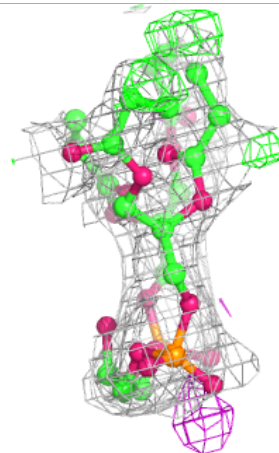
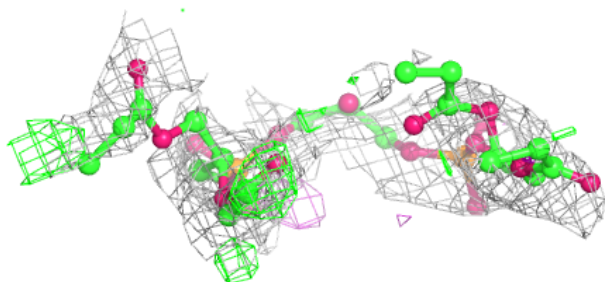
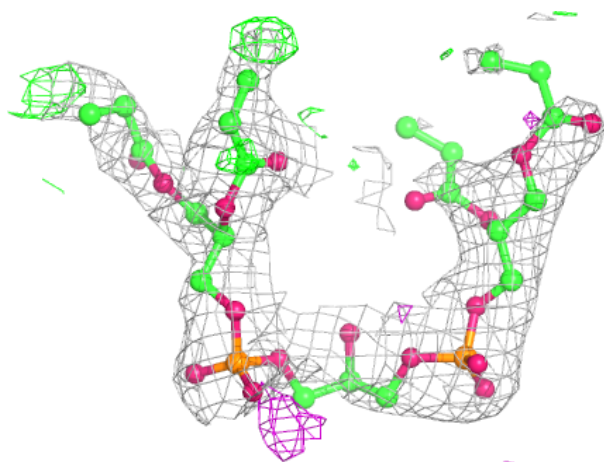
Electron density around PGV C 509:

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



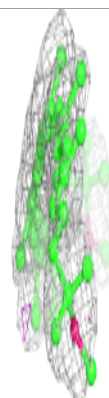
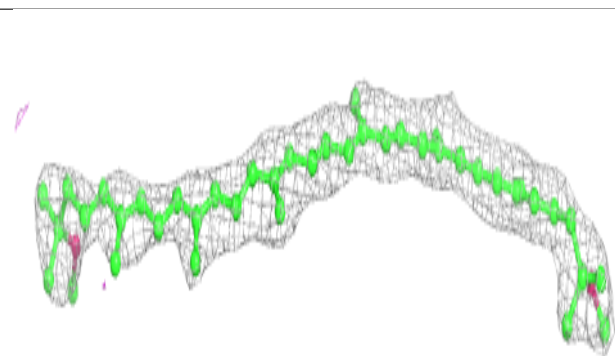
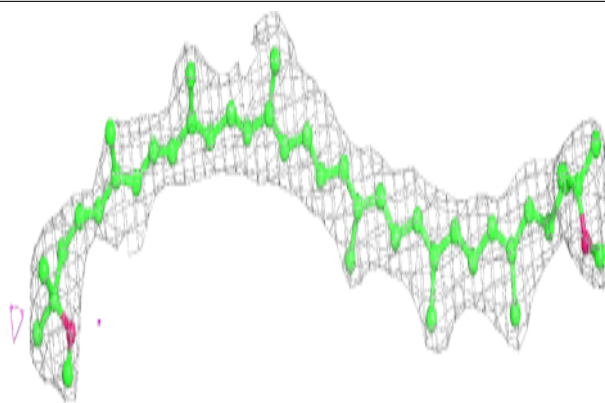
Electron density around CDL Y 102:

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



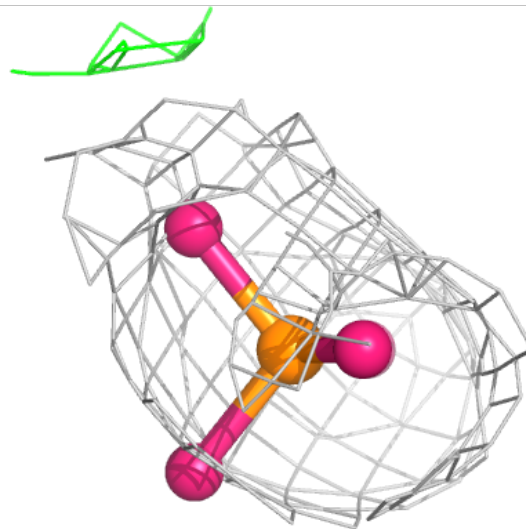
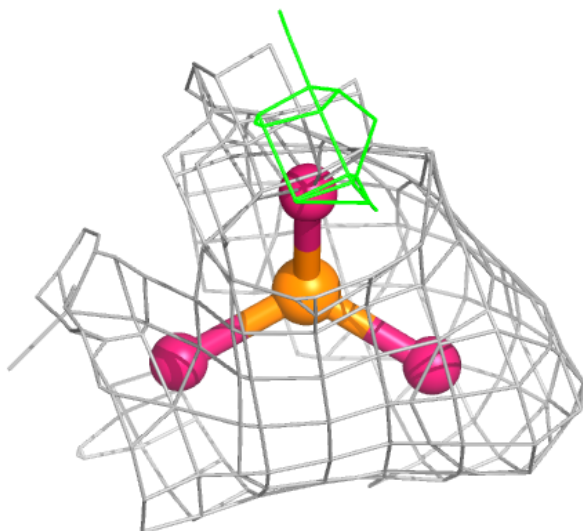
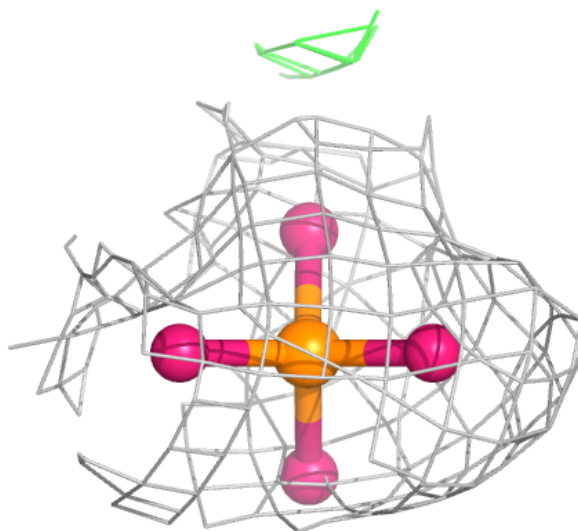
Electron density around CRT 1 103:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



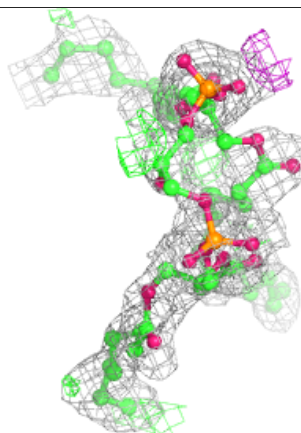
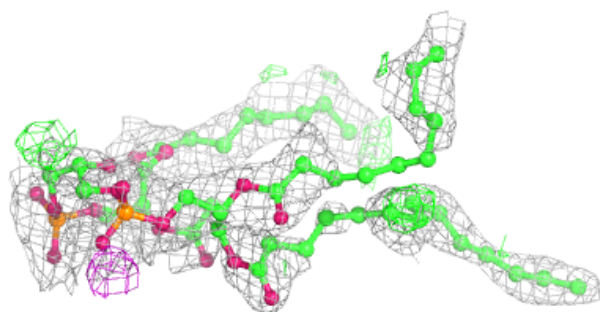
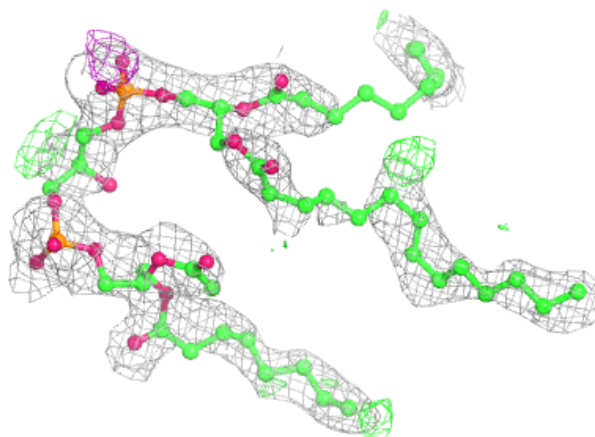
Electron density around PEF U 105:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

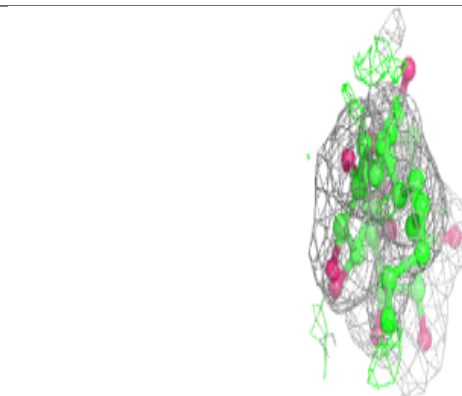
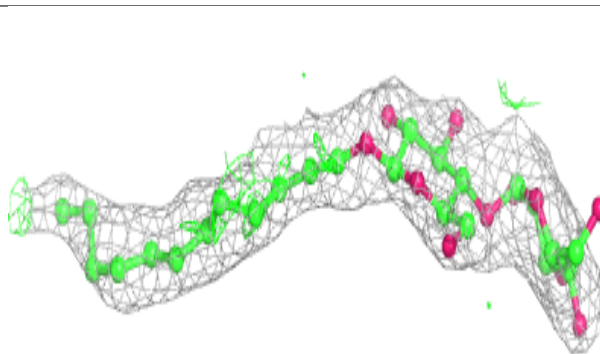
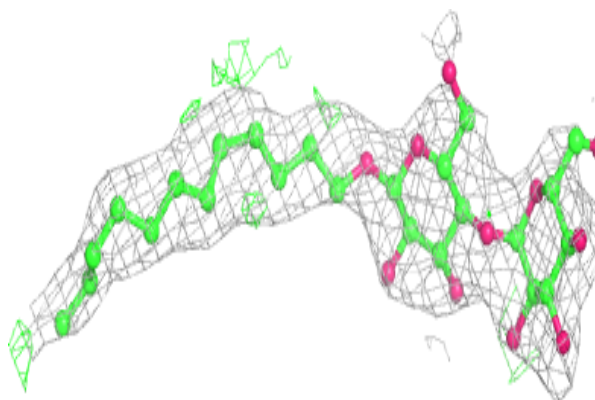


Electron density around CDL S 103:

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

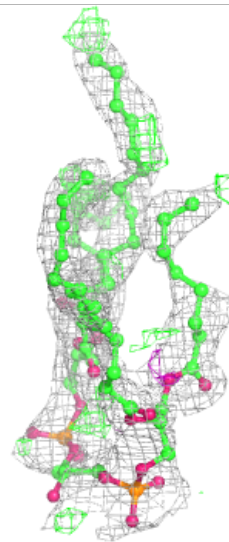
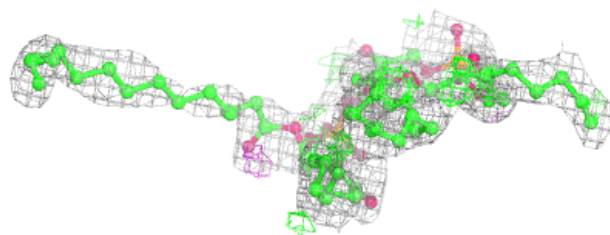
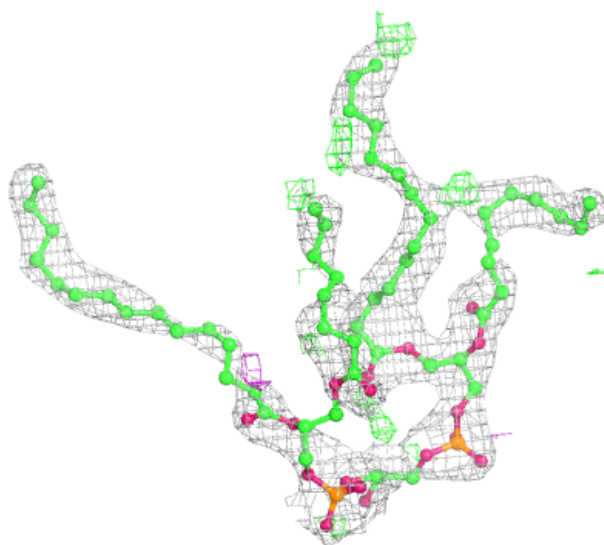
**Electron density around LMT M 419:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



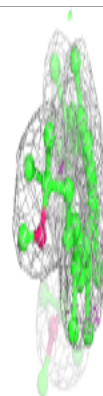
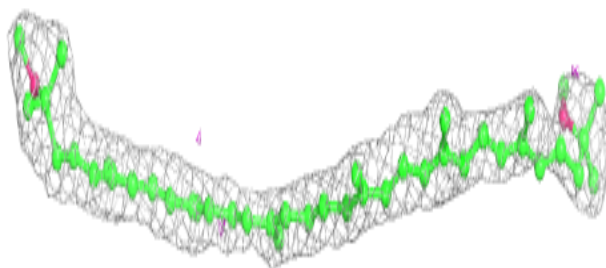
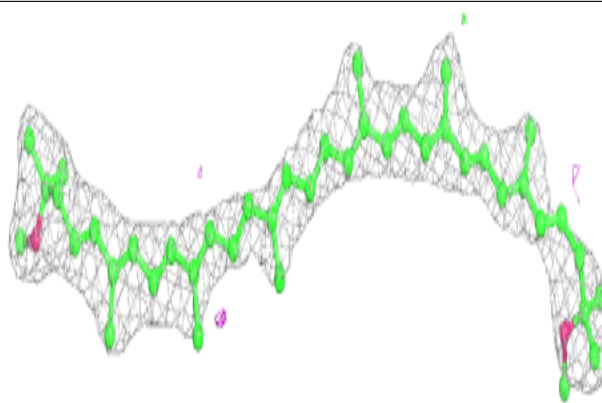
Electron density around CDL Q 104:

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



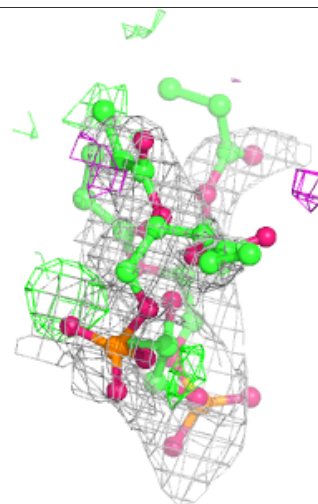
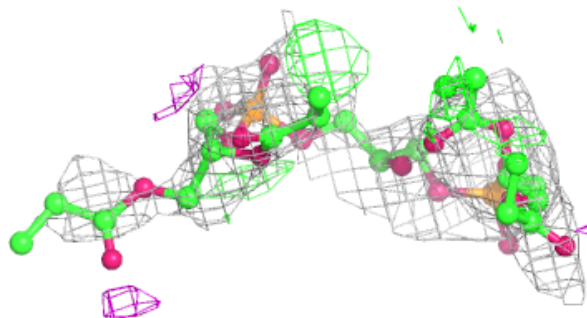
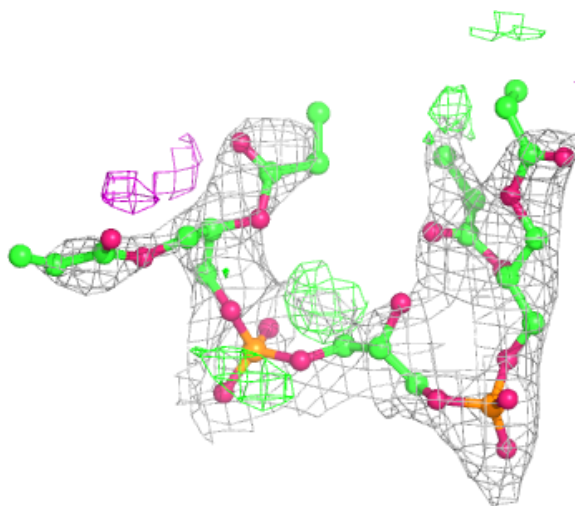
Electron density around CRT J 101:

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



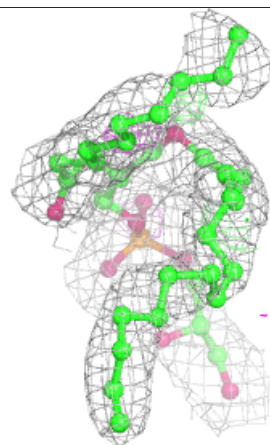
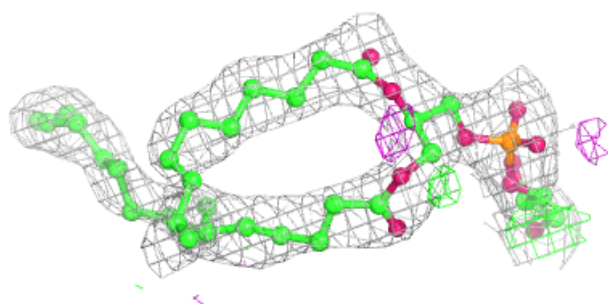
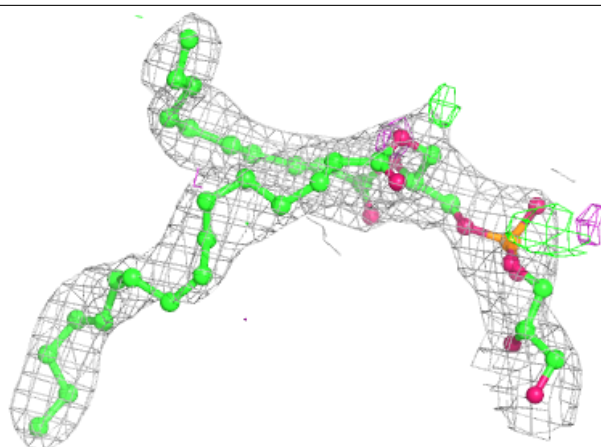
Electron density around CDL D 103:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

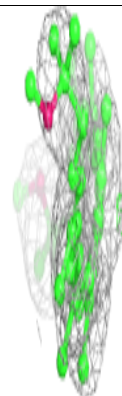
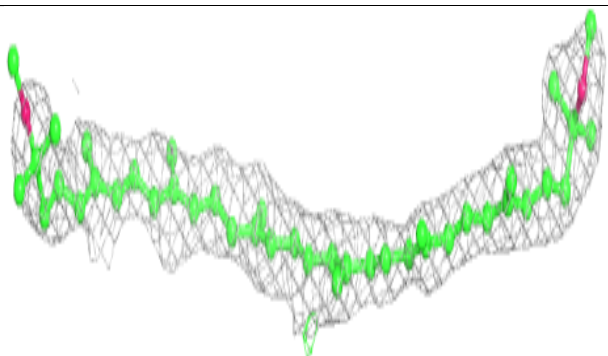
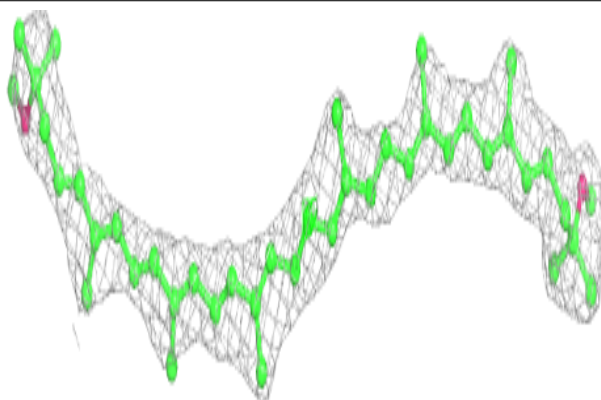


Electron density around PGV L 305:

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

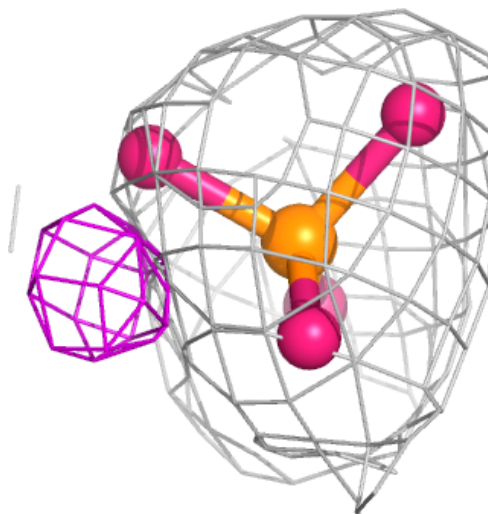
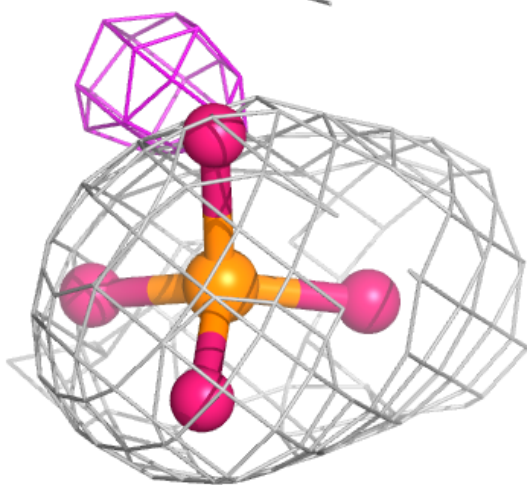
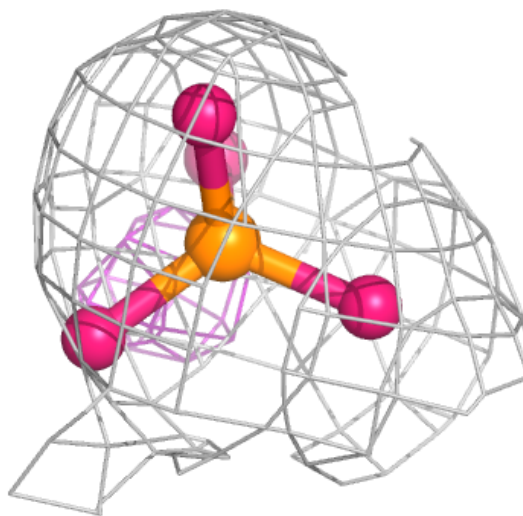
**Electron density around CRT G 101:**

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



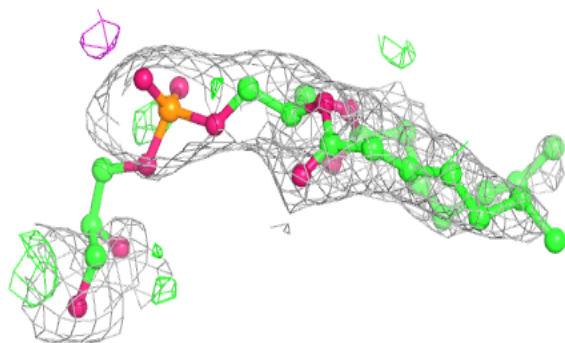
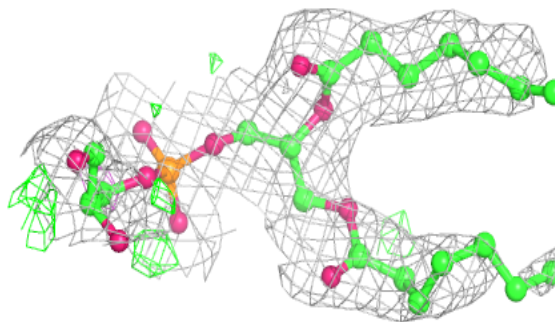
Electron density around PEF M 409:

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

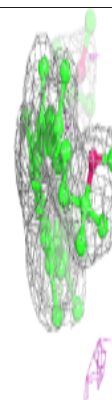
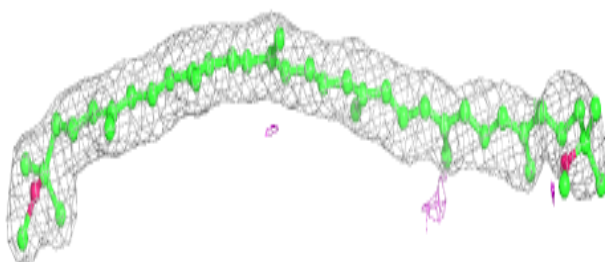
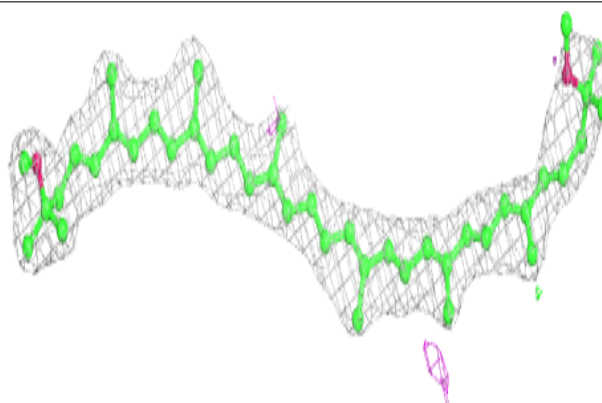


Electron density around PGV 1 105:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

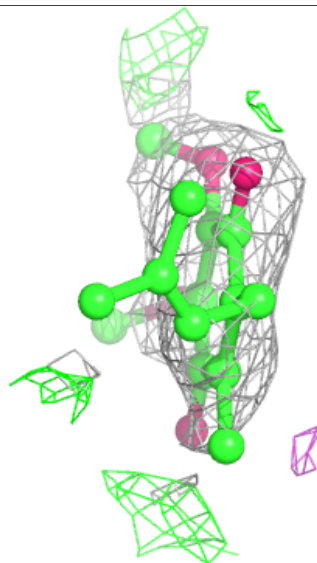
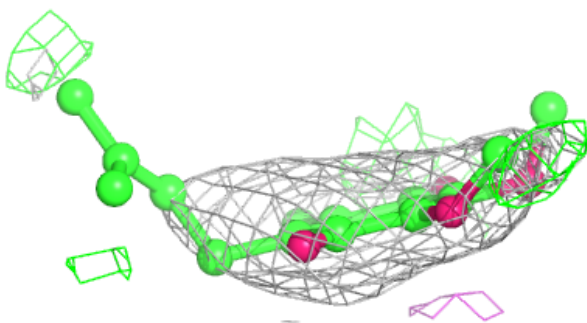
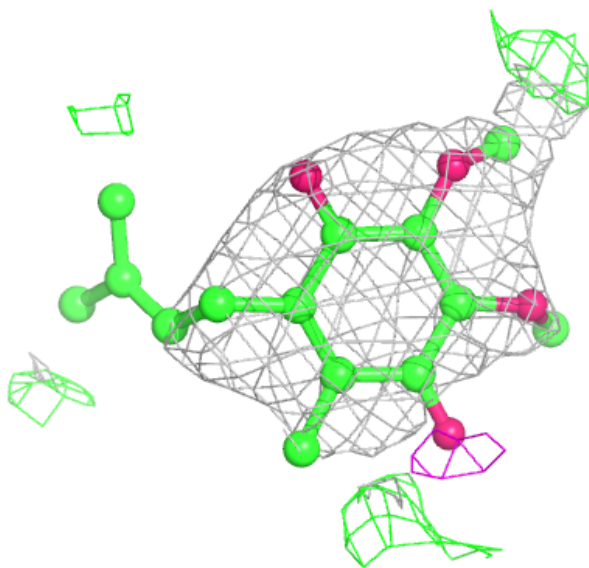
**Electron density around CRT U 103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



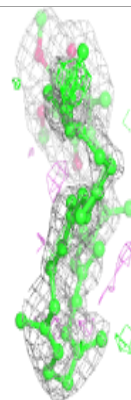
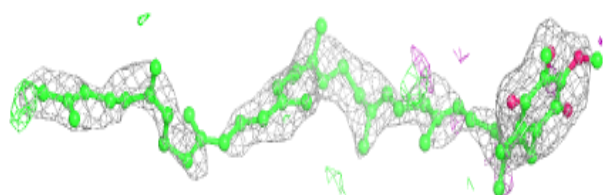
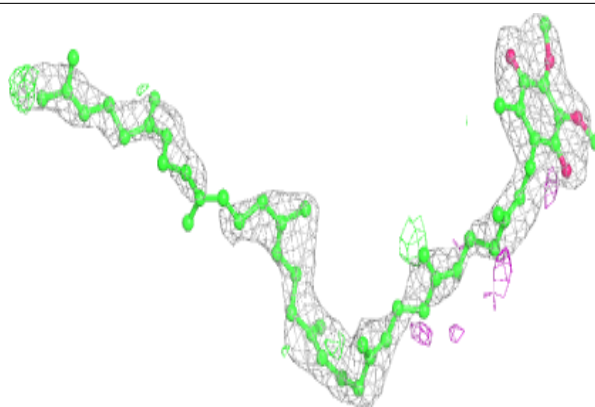
Electron density around UQ8 L 309:

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



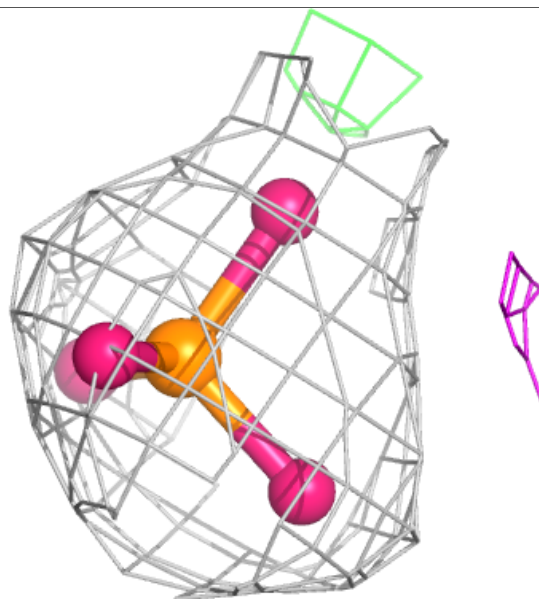
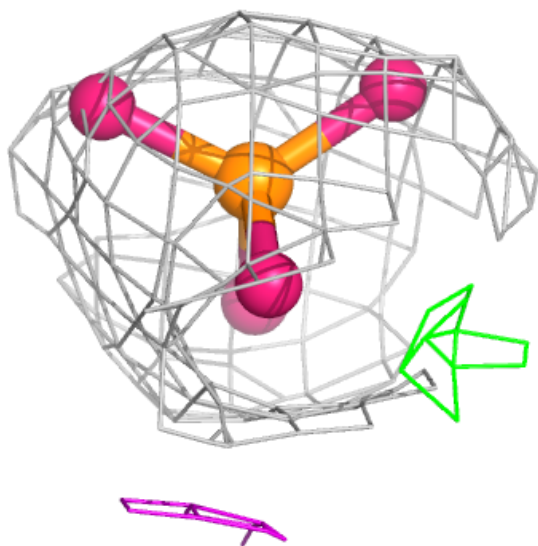
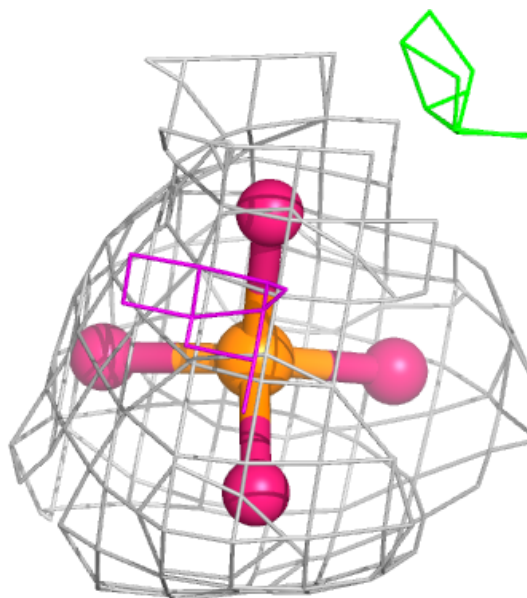
Electron density around UQ8 L 308:

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



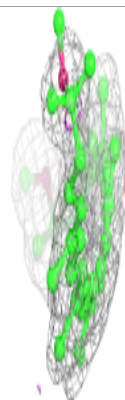
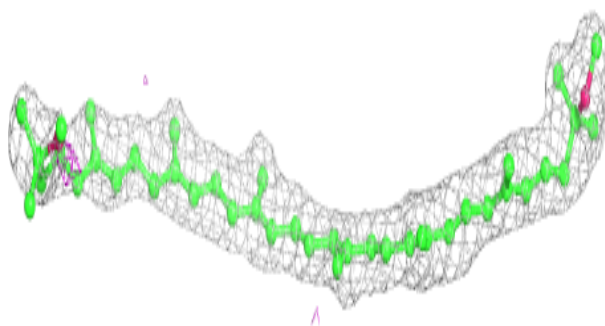
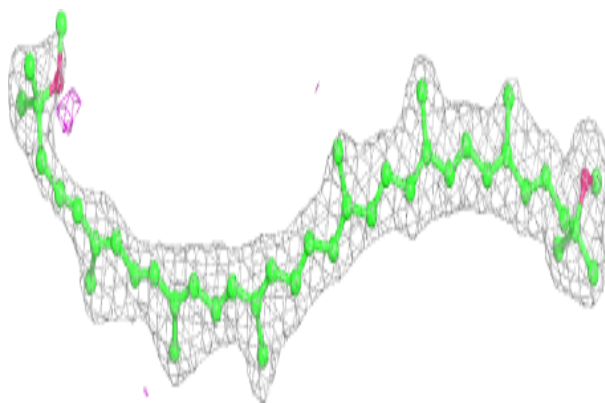
Electron density around PEF 5 103:

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

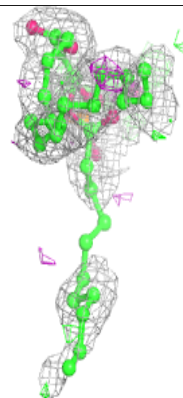
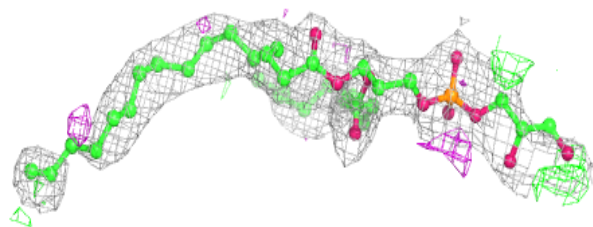
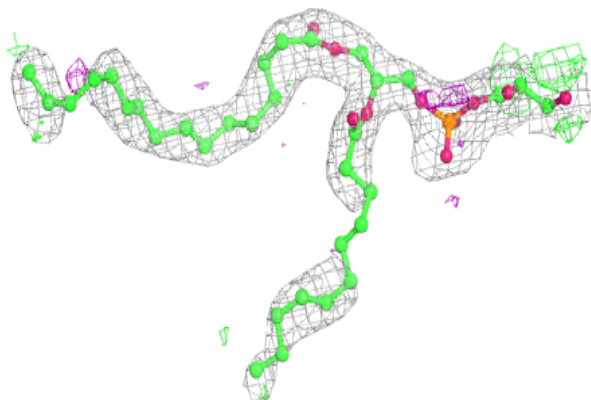


Electron density around CRT 9 101:

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

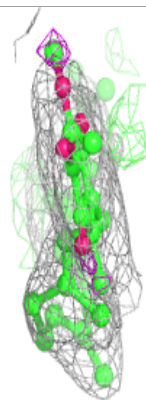
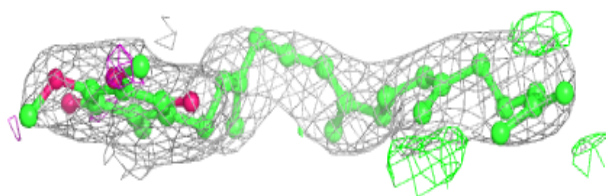
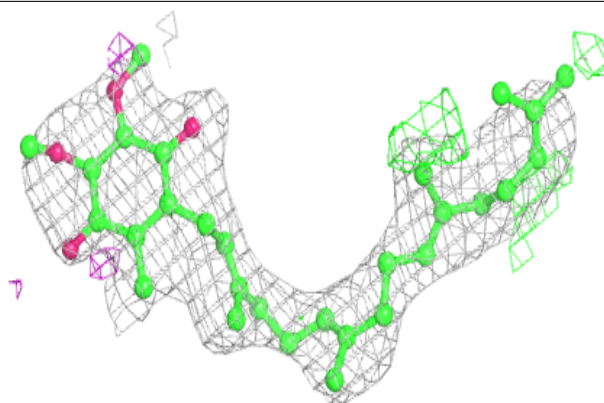
**Electron density around PGV L 306:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

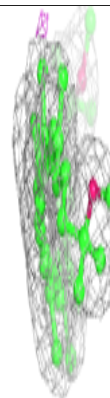
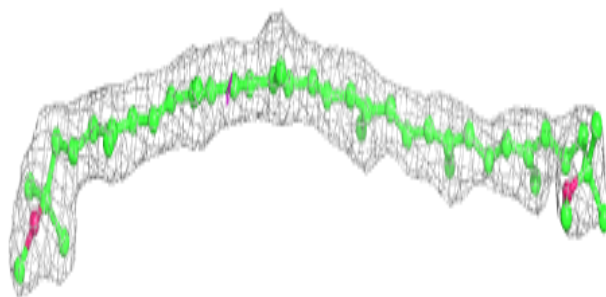
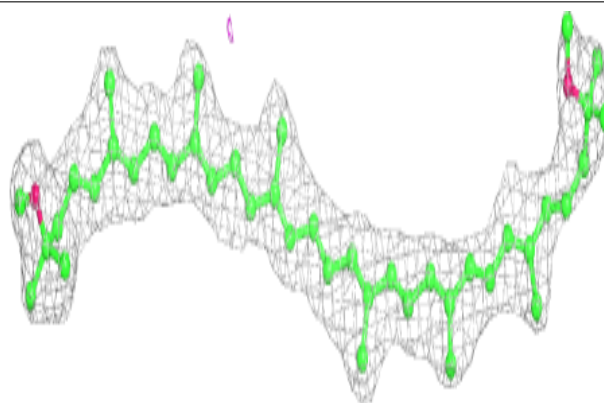


Electron density around UQ8 7 103:

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

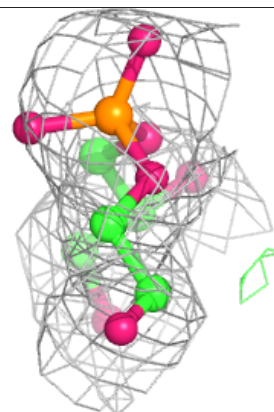
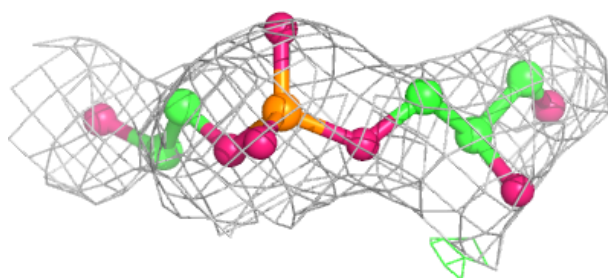
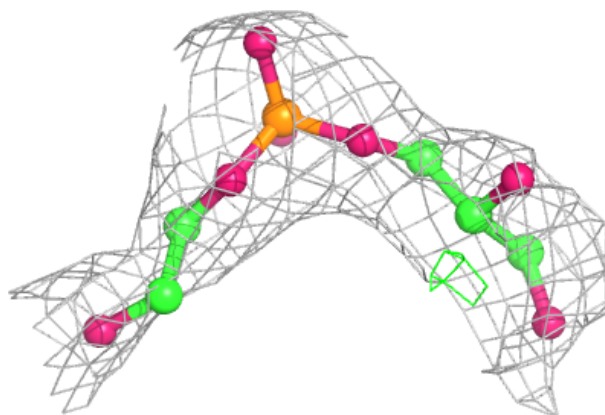
**Electron density around CRT 0 101:**

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

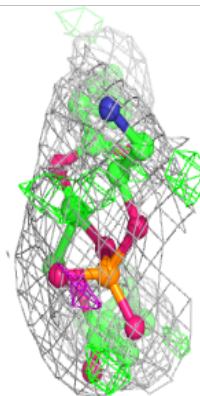
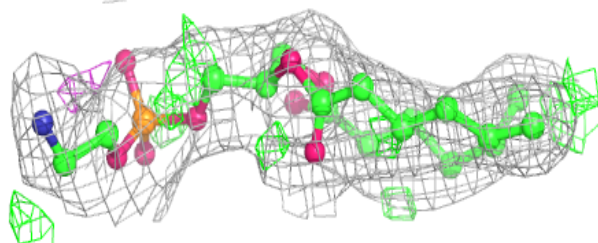
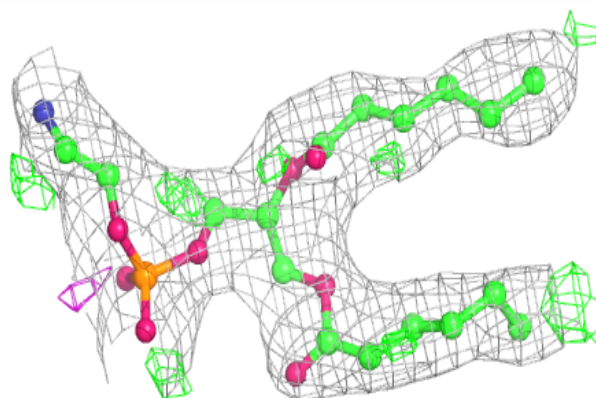


Electron density around CDL Y 103:

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

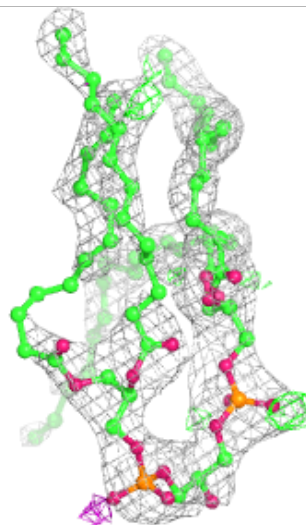
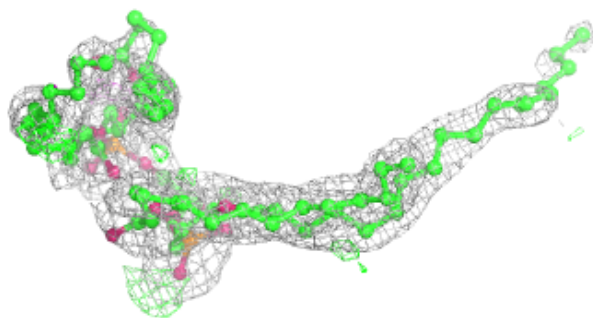
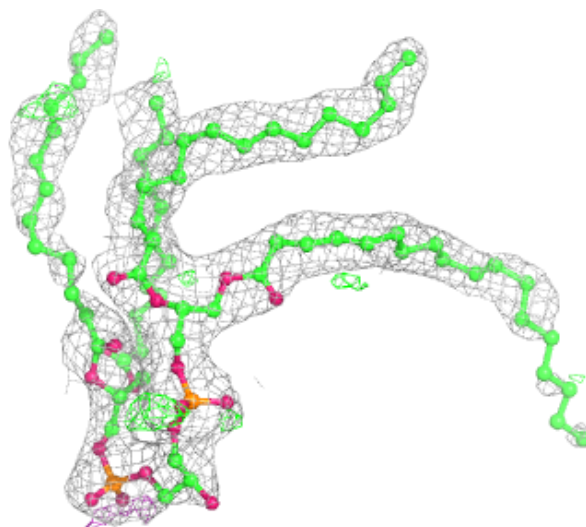
**Electron density around PEF K 104:**

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



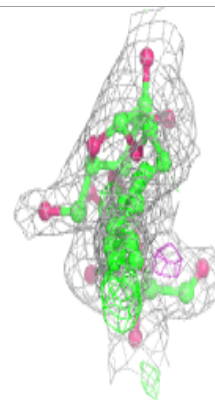
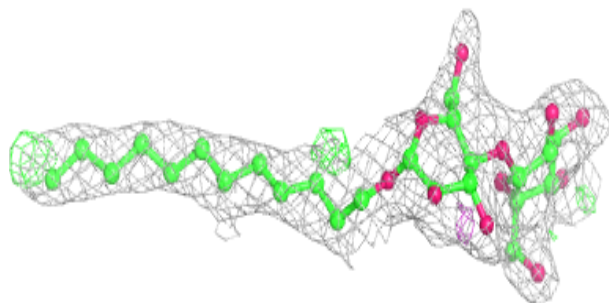
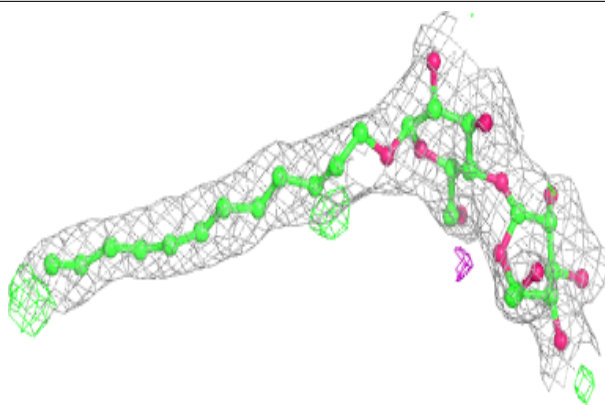
Electron density around CDL K 103:

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



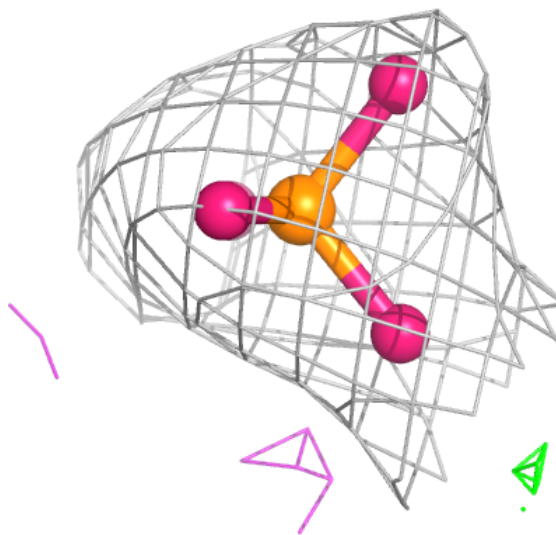
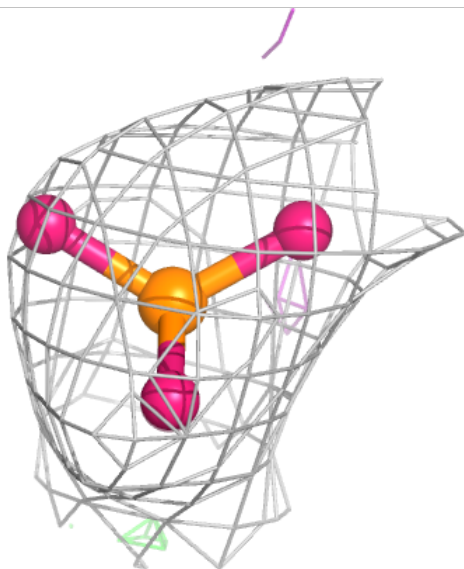
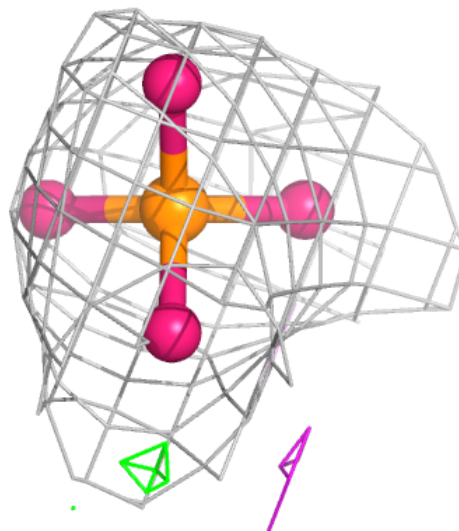
Electron density around LMT F 103:

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



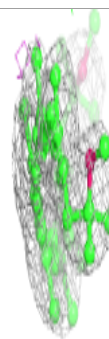
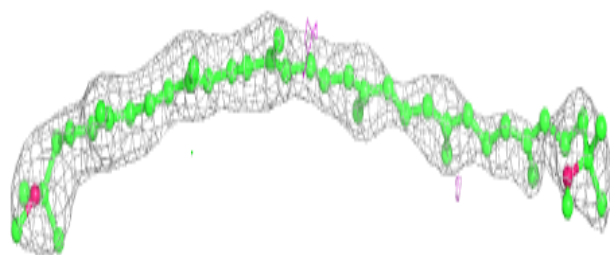
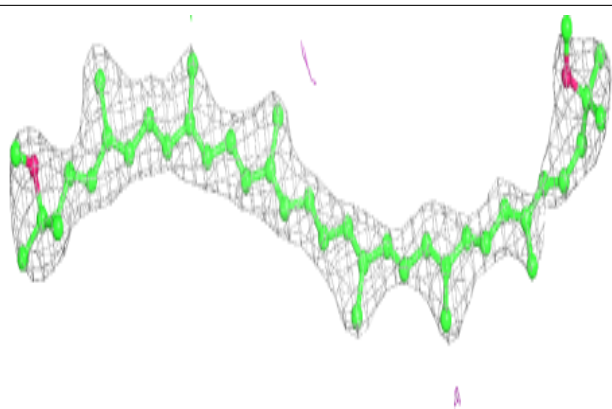
Electron density around PEF 1 104:

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



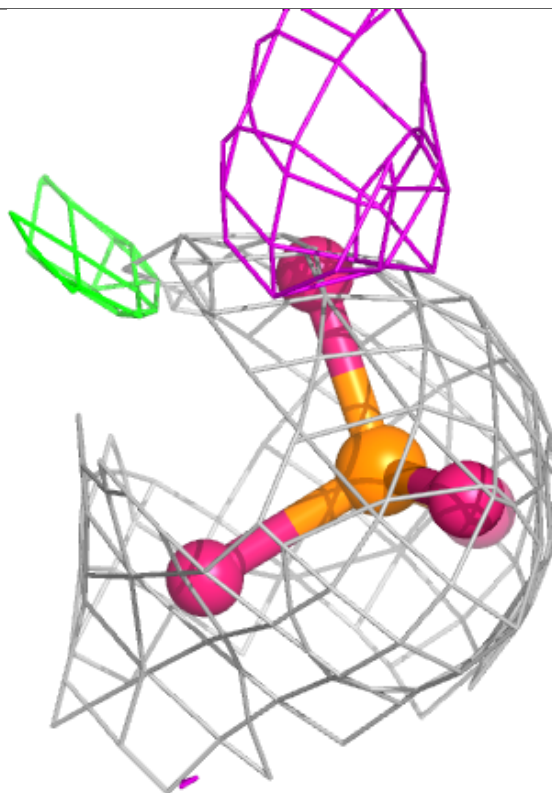
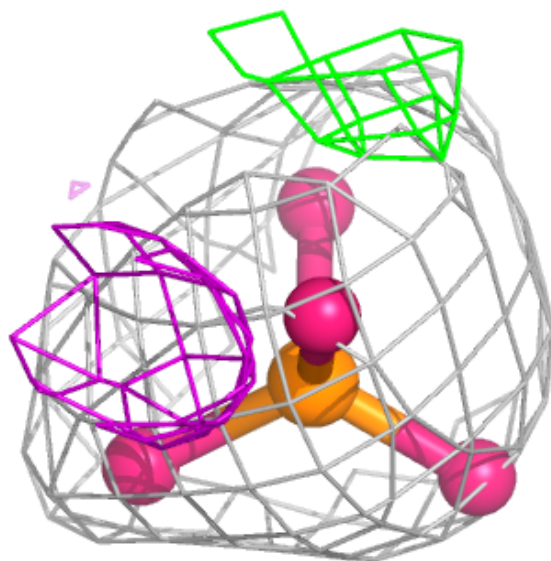
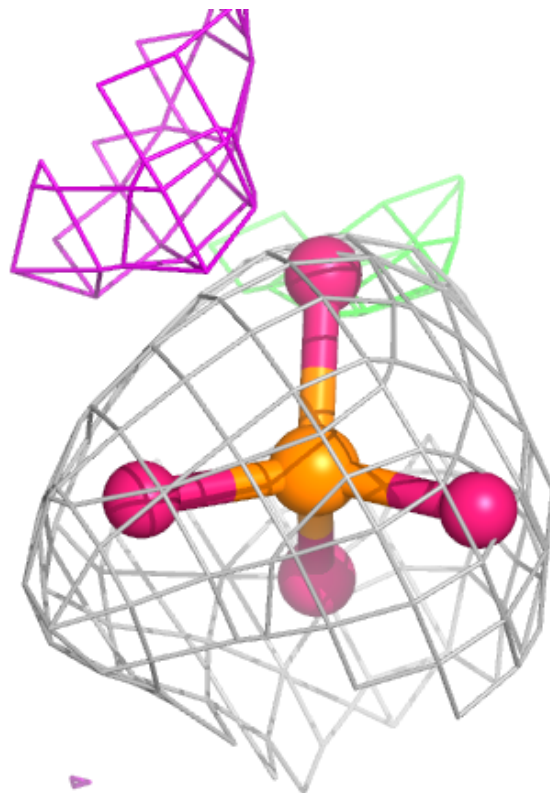
Electron density around CRT 2 101:

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



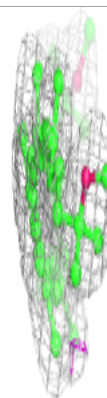
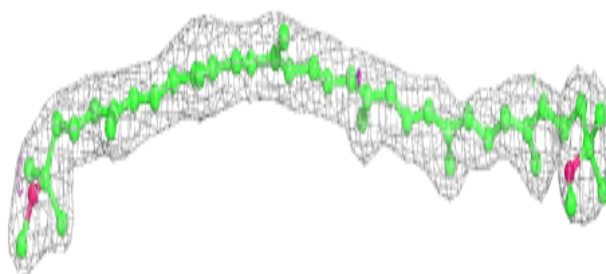
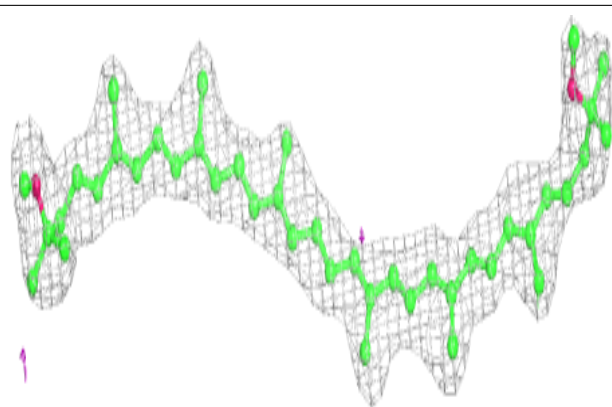
Electron density around PEF U 104:

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

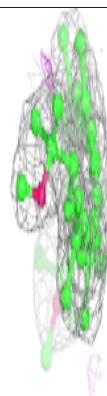
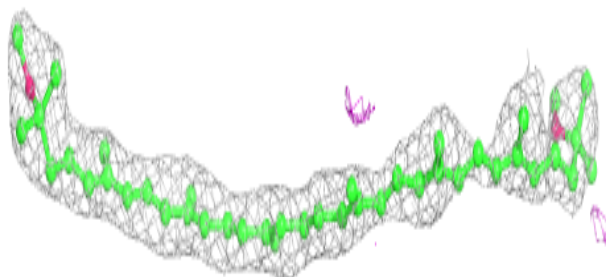
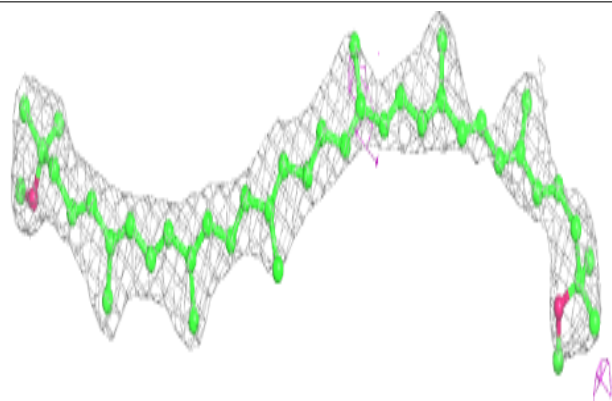


Electron density around CRT 6 101:

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

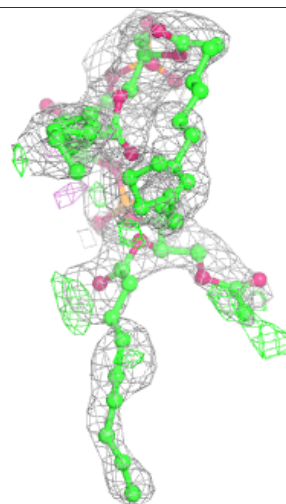
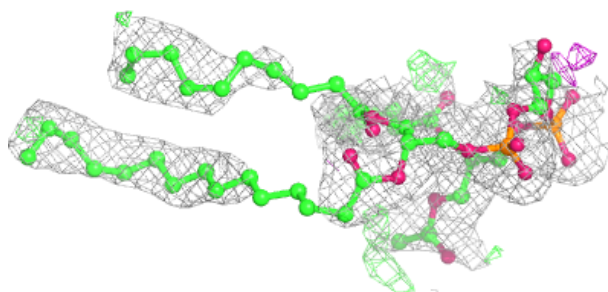
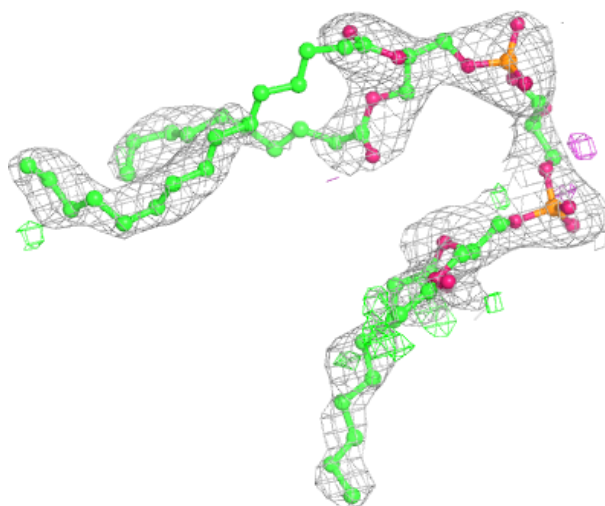
**Electron density around CRT A 104:**

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



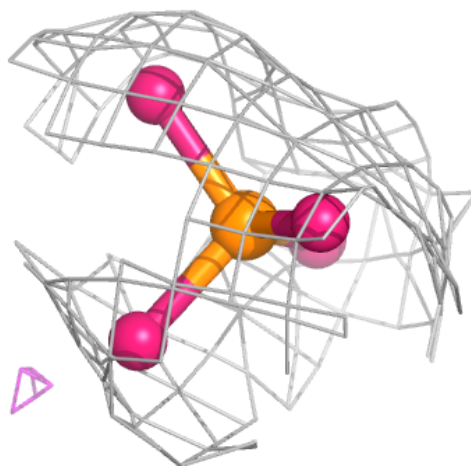
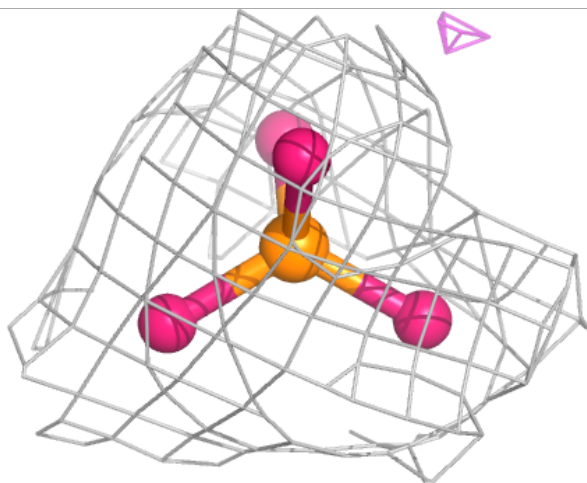
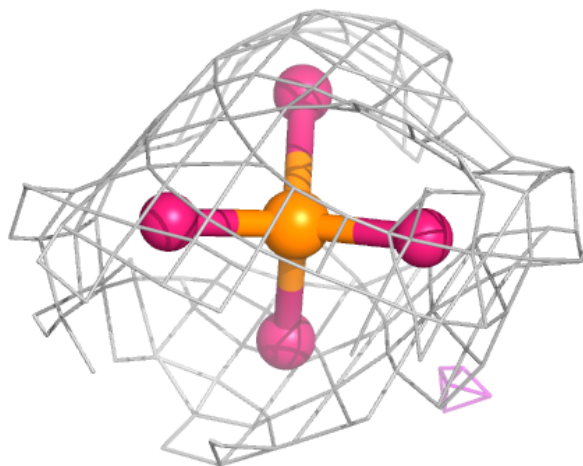
Electron density around CDL H 302:

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



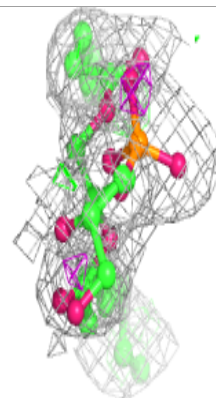
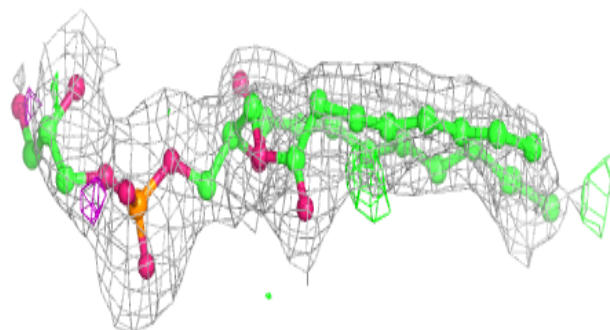
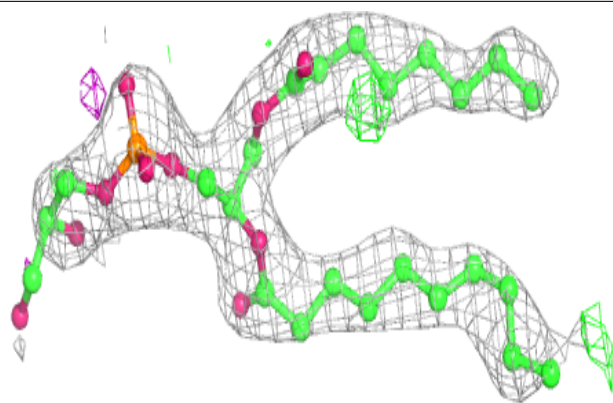
Electron density around PEF W 103:

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

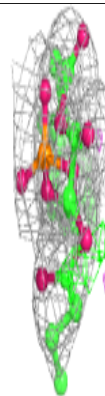
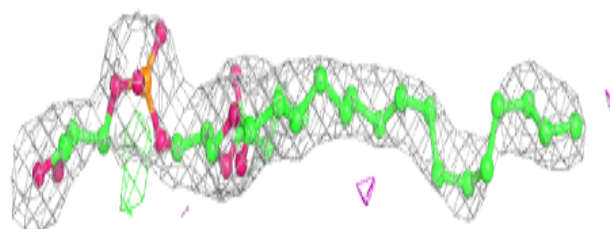
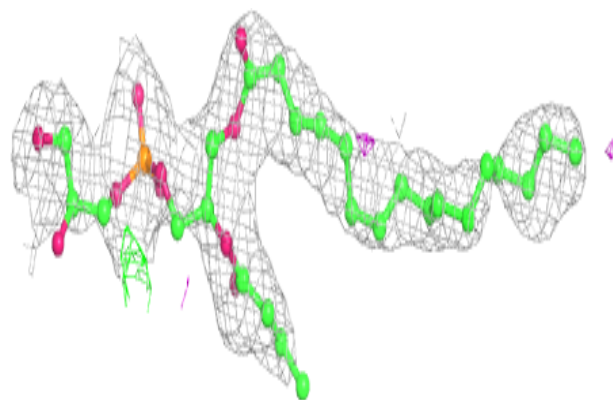


Electron density around PGV D 104:

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

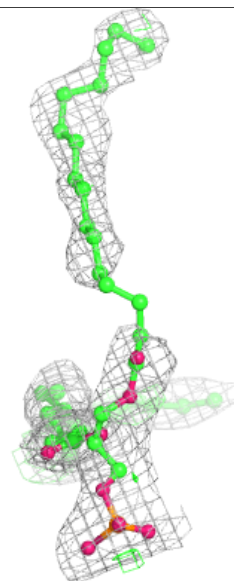
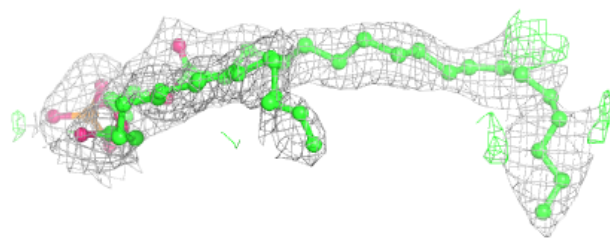
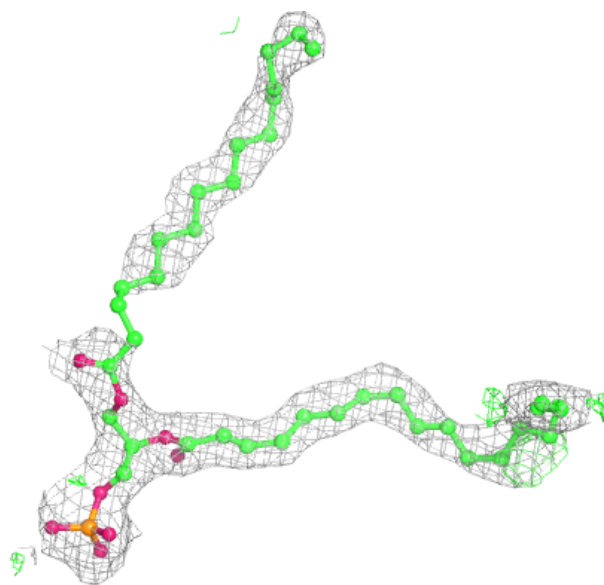
**Electron density around PGV M 414:**

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



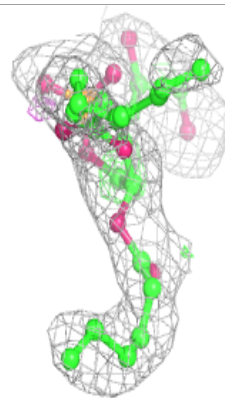
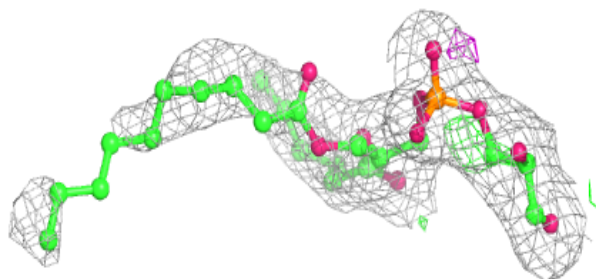
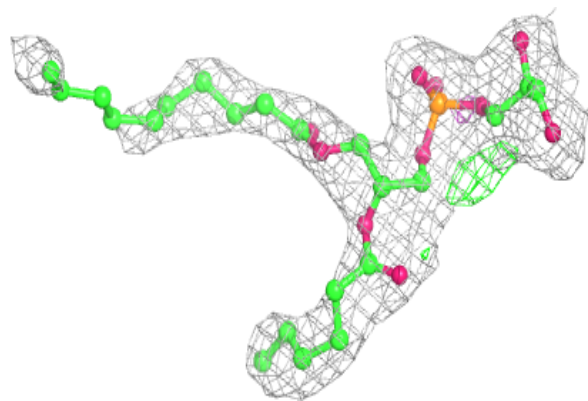
Electron density around PGV M 413:

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

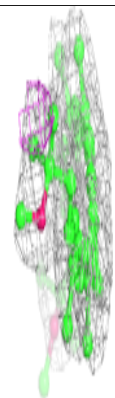
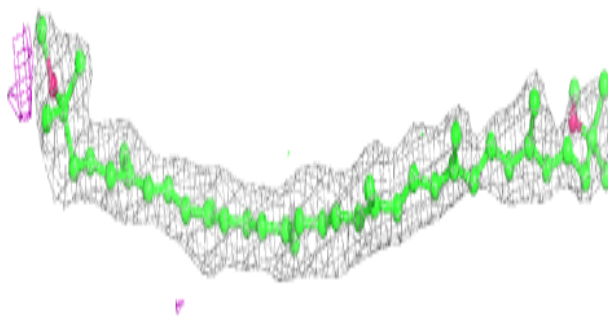
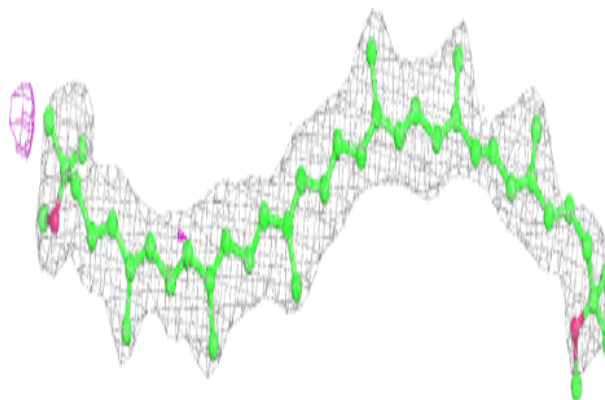


Electron density around PGV A 105:

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

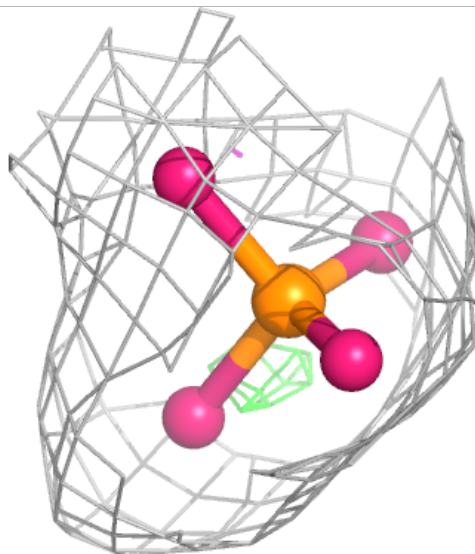
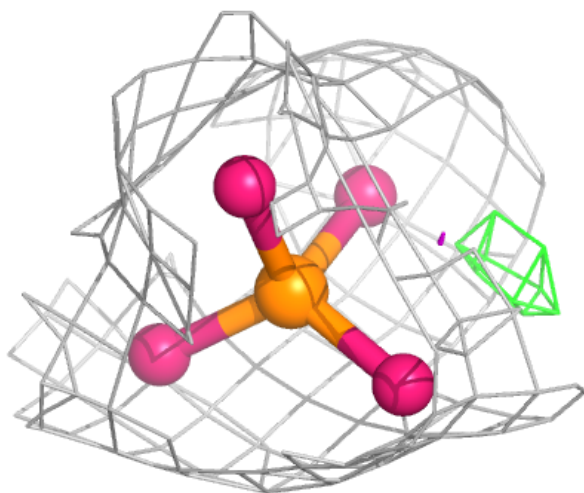
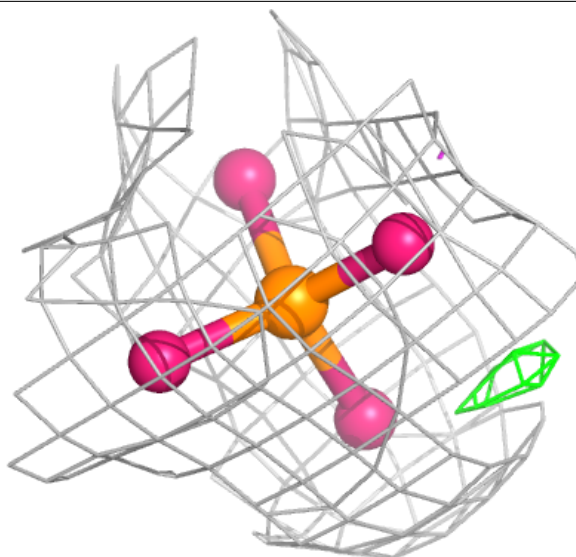
**Electron density around CRT 9 102:**

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



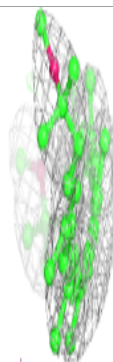
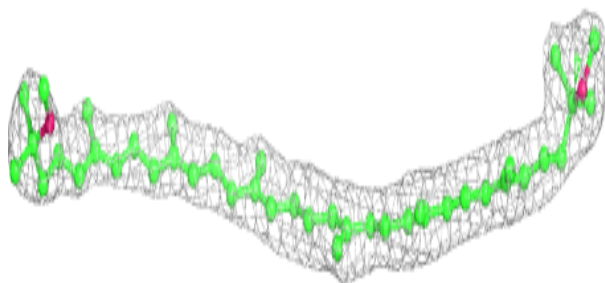
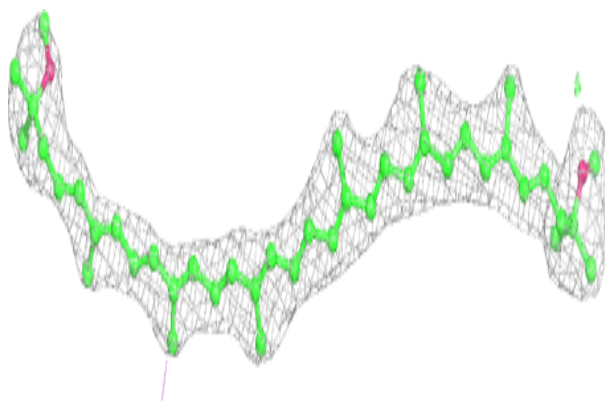
Electron density around PEF M 408:

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

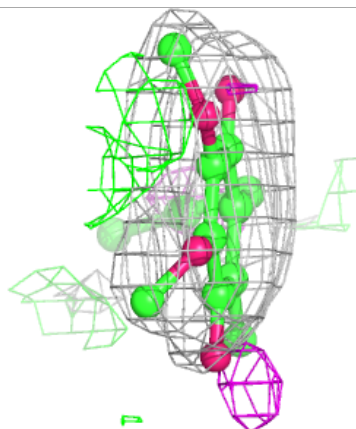
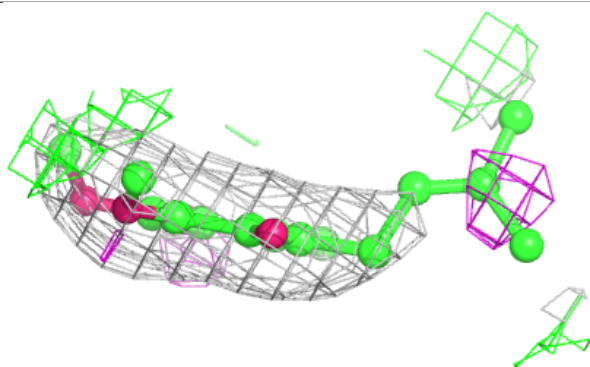
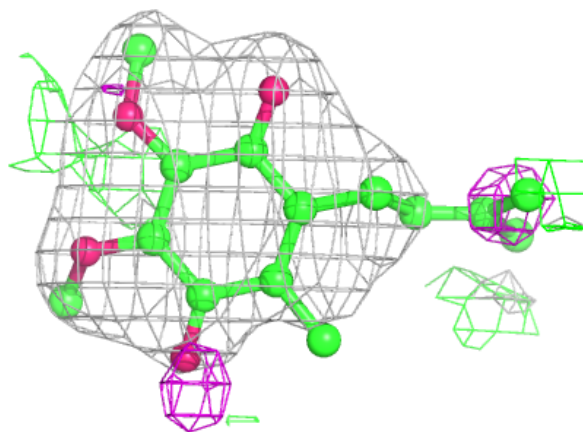


Electron density around CRT Z 101:

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

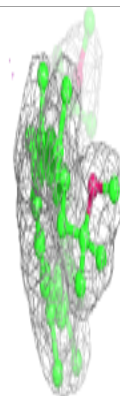
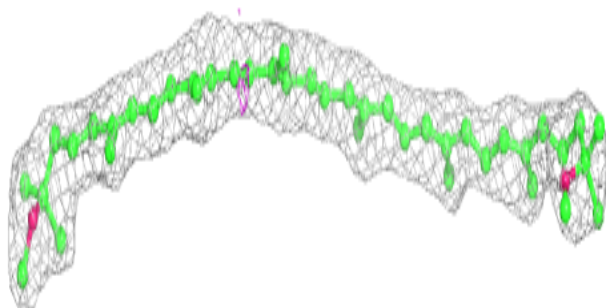
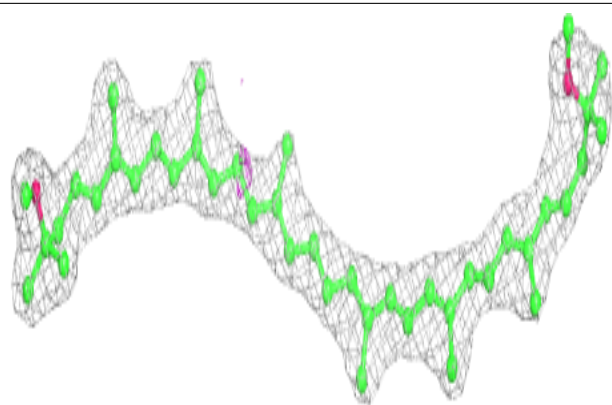
**Electron density around UQ8 M 417:**

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

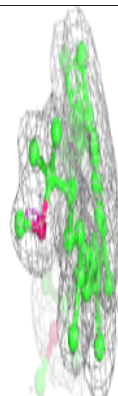
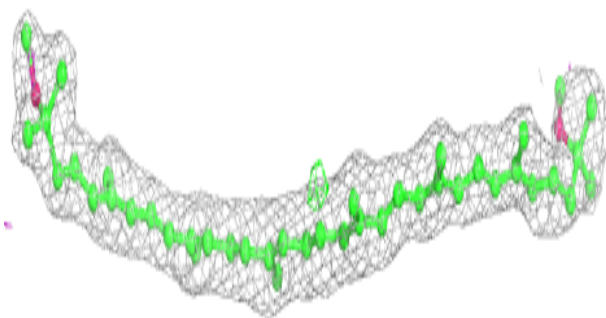
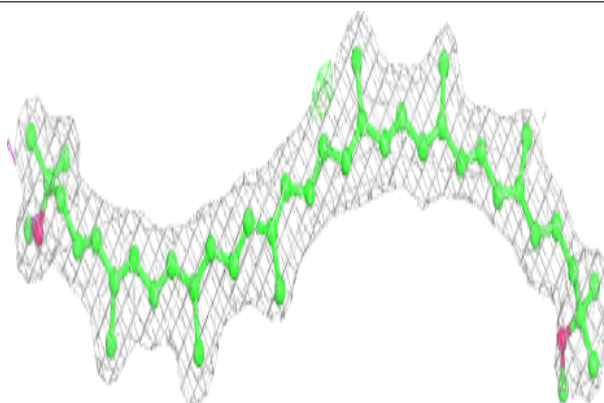


Electron density around CRT V 101:

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

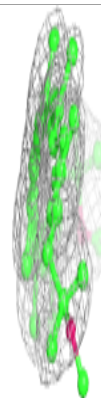
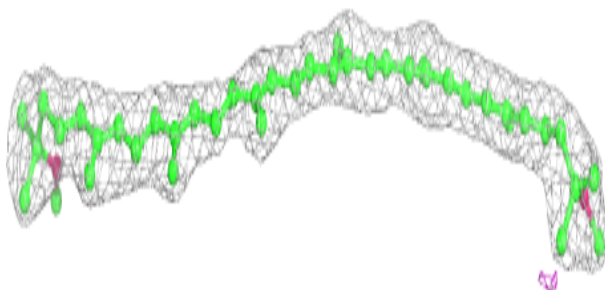
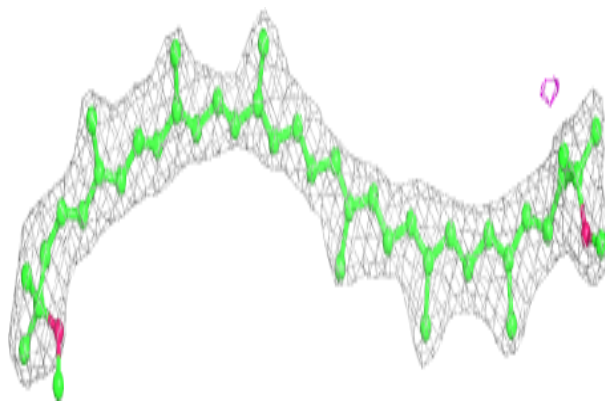
**Electron density around CRT O 103:**

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

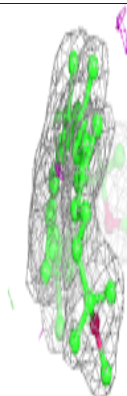
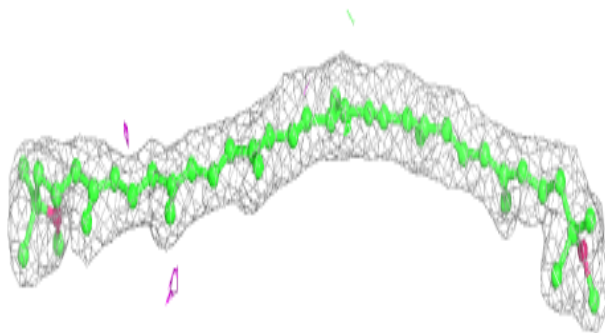
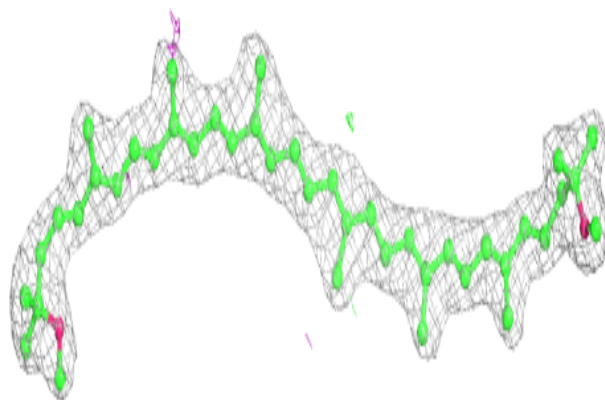


Electron density around CRT N 101:

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

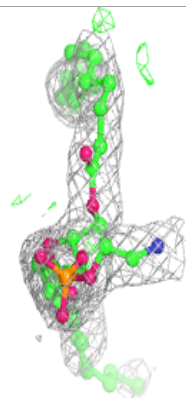
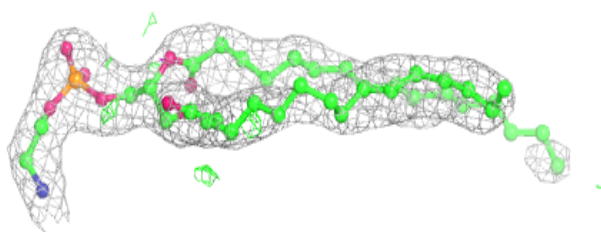
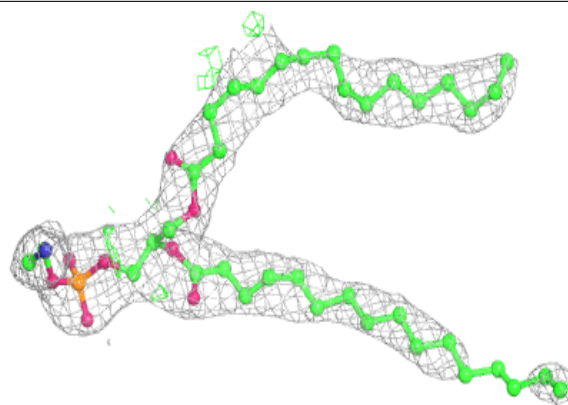
**Electron density around CRT Q 103:**

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



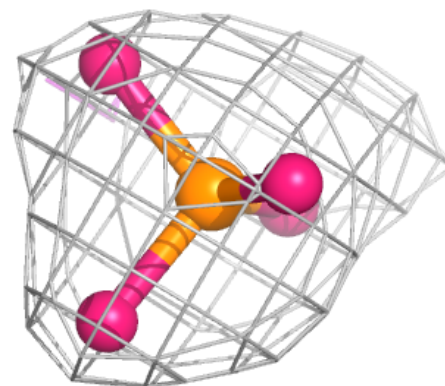
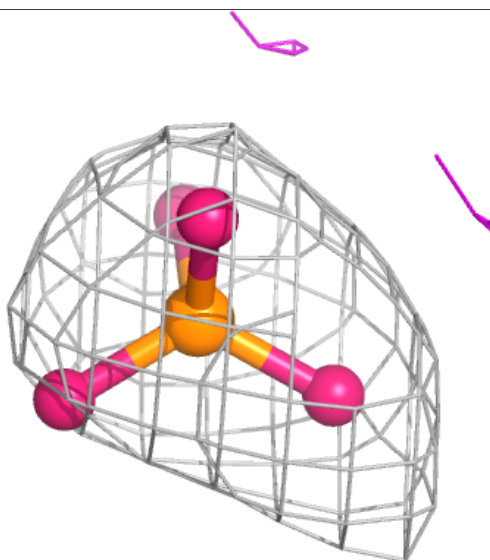
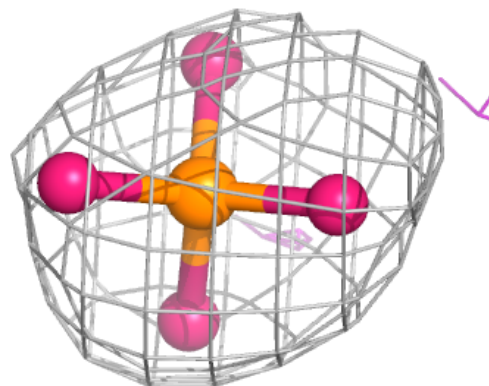
Electron density around PEF M 418:

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



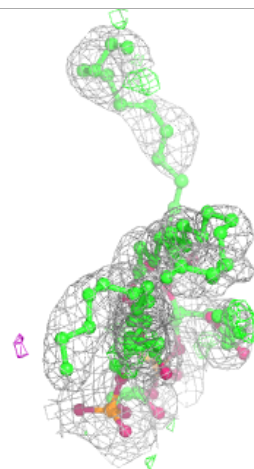
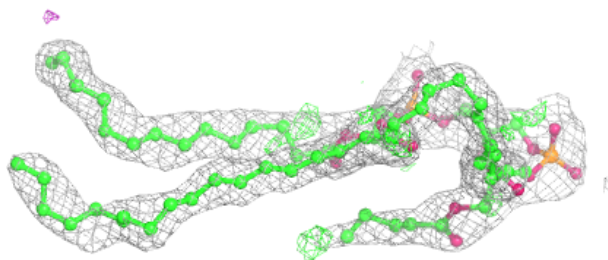
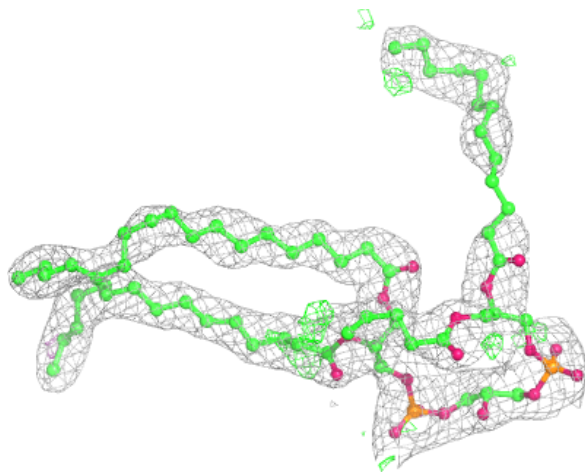
Electron density around PEF I 103:

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



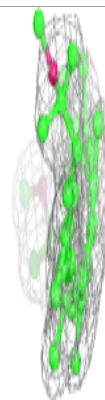
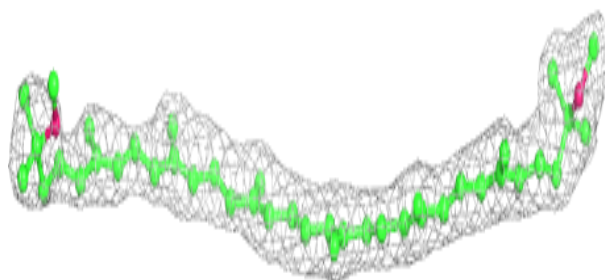
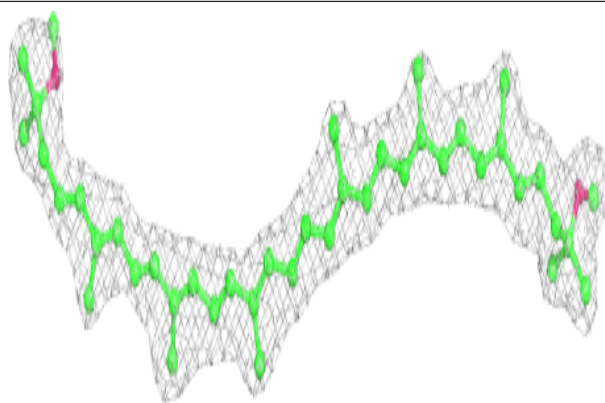
Electron density around CDL H 304:

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

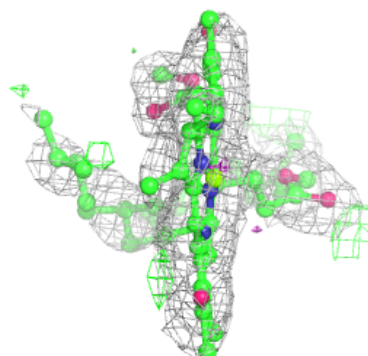
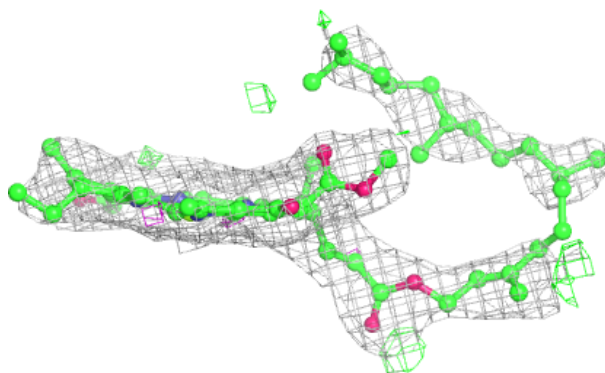
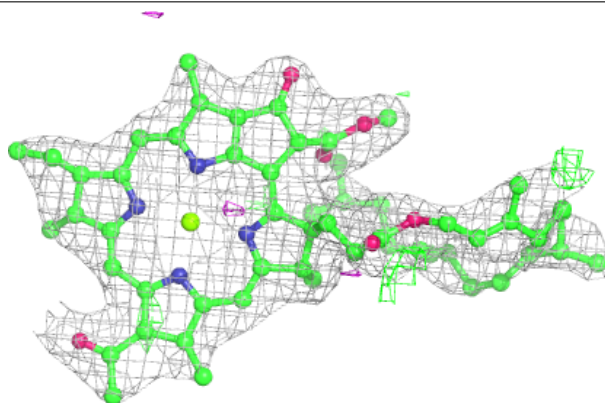


Electron density around CRT P 101:

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

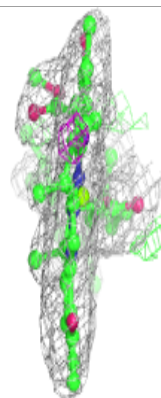
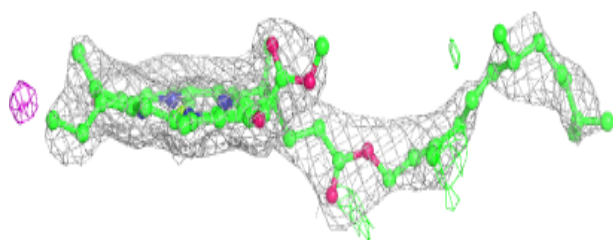
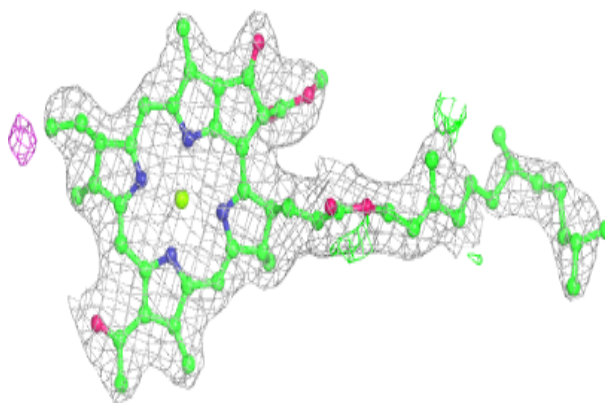
**Electron density around BCL 3 101:**

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

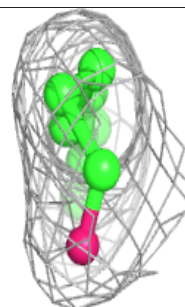
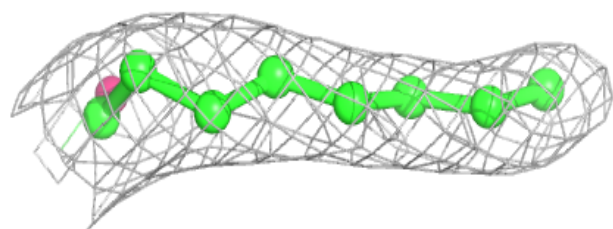
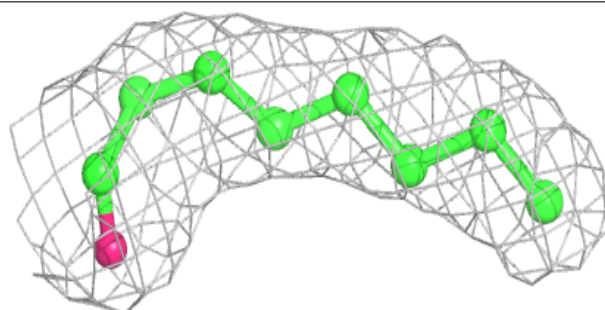


Electron density around BCL 7 101:

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

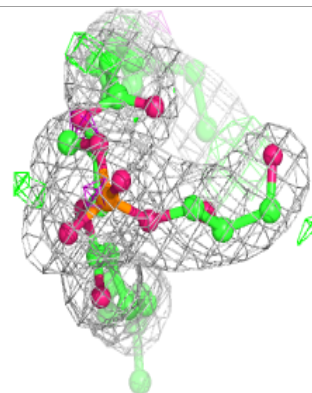
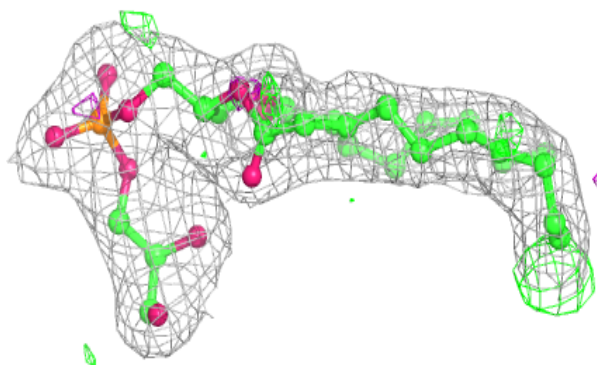
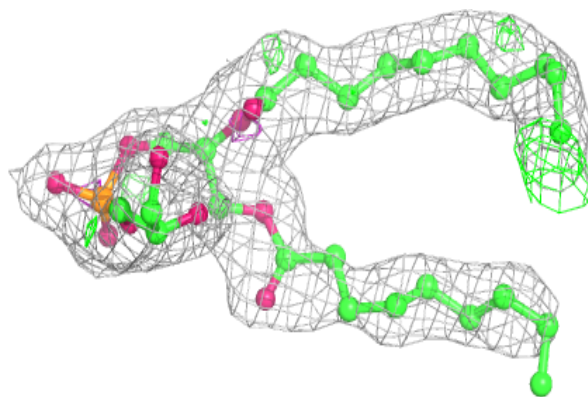
**Electron density around LHG C 508:**

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

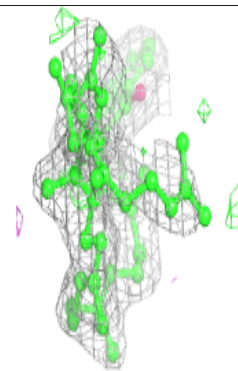
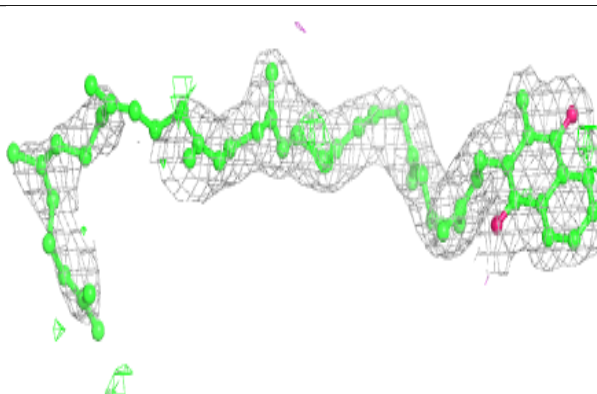
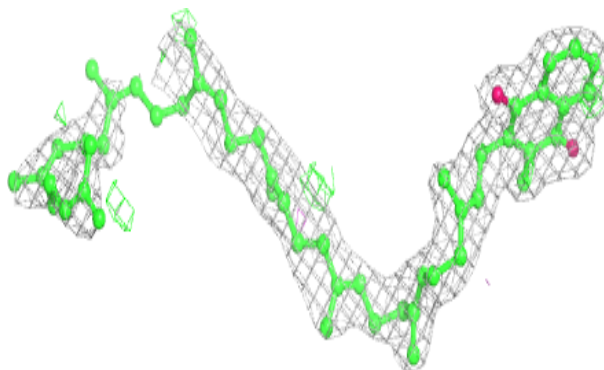


Electron density around PGV H 303:

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

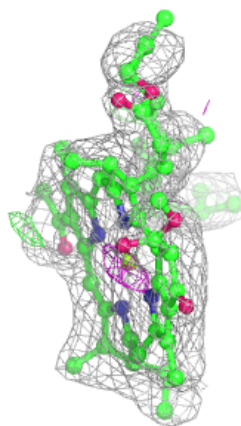
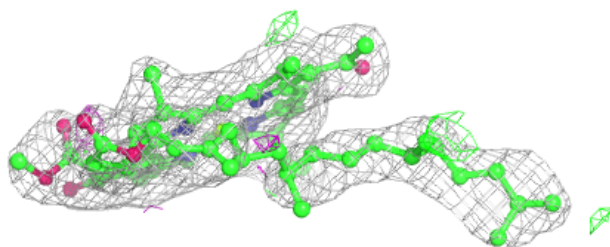
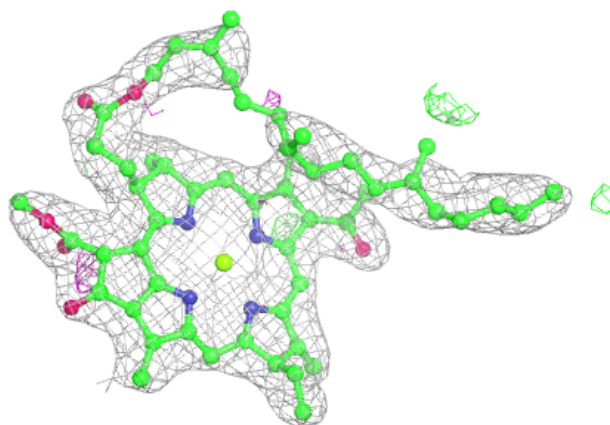
**Electron density around MQ8 M 405:**

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

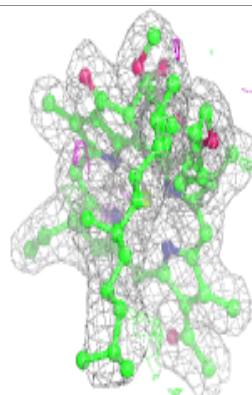
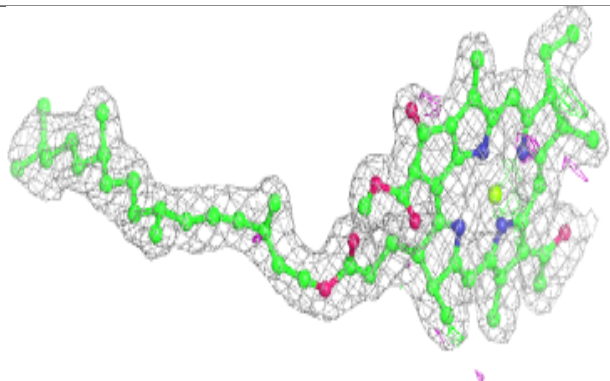
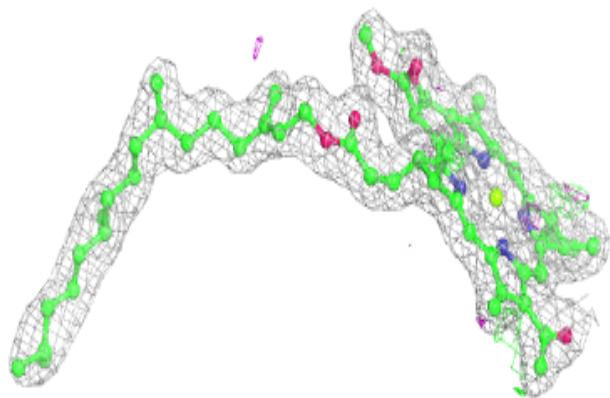


Electron density around BCL 1 102:

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

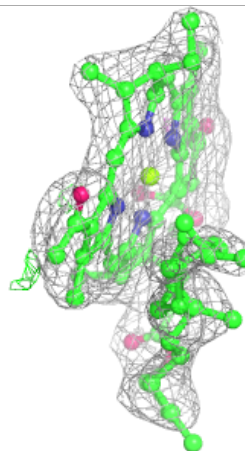
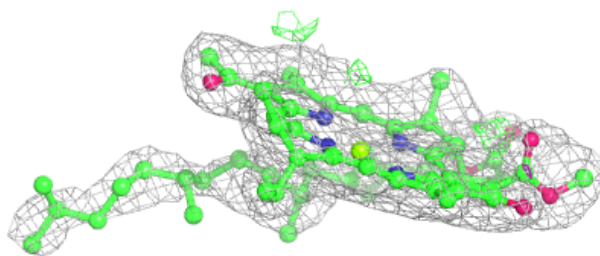
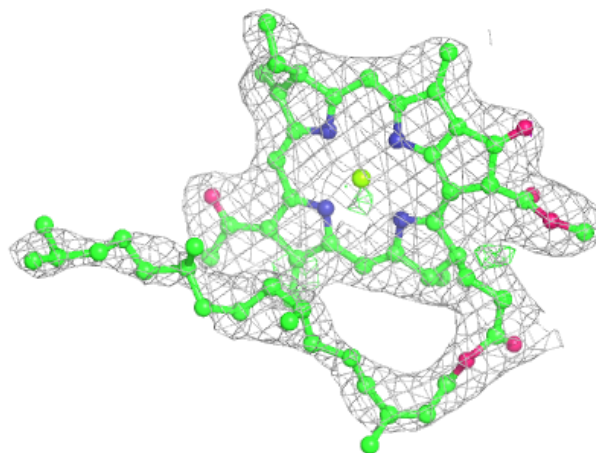
**Electron density around BCL L 301:**

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



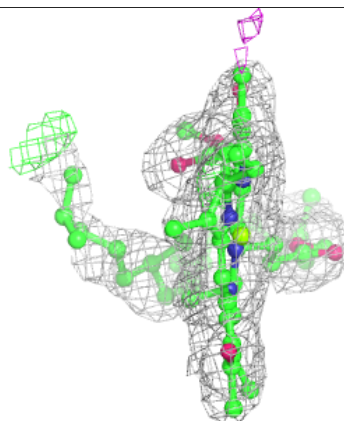
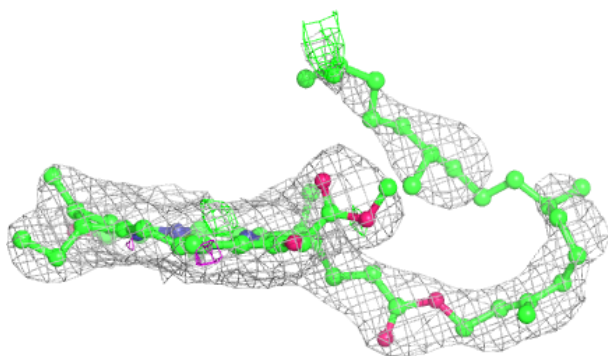
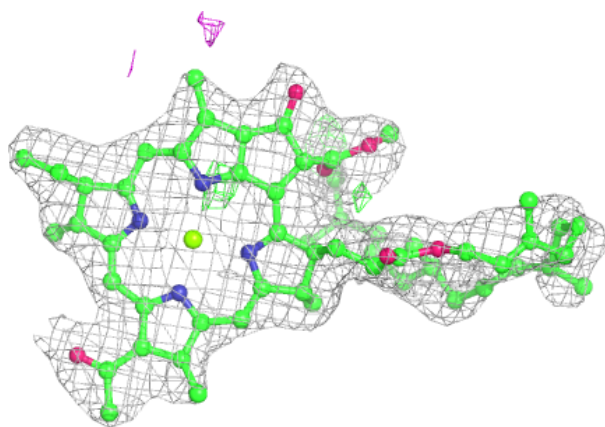
Electron density around BCL Z 102:

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



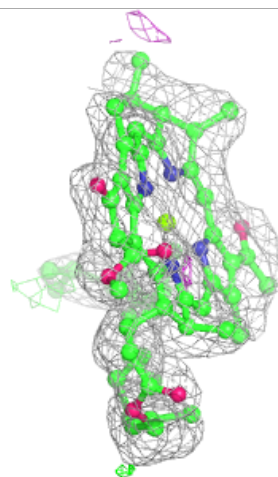
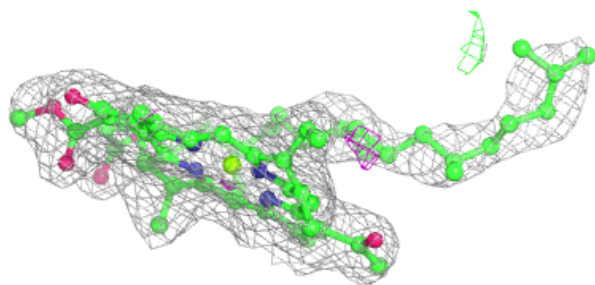
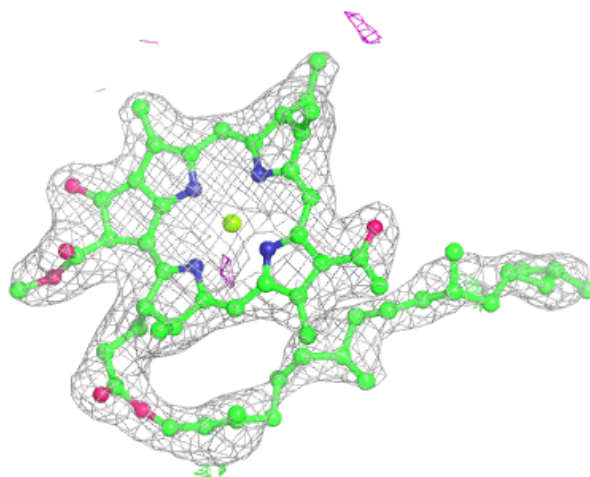
Electron density around BCL 5 101:

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



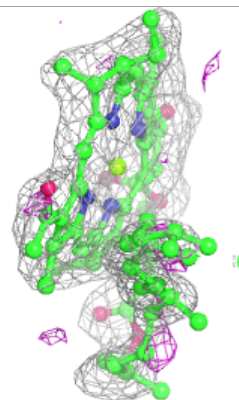
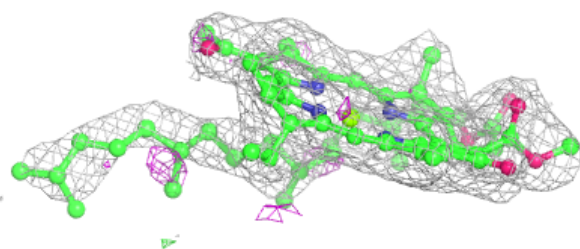
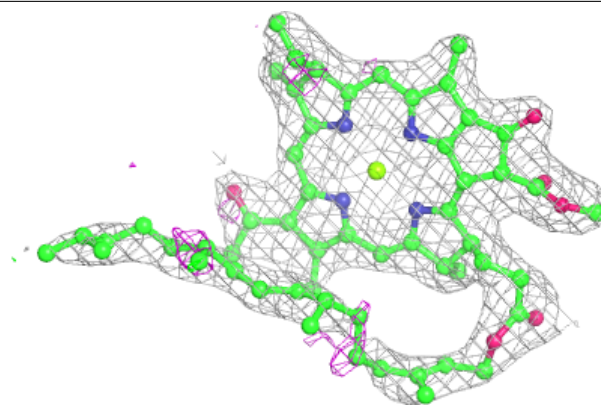
Electron density around BCL 3 102:

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

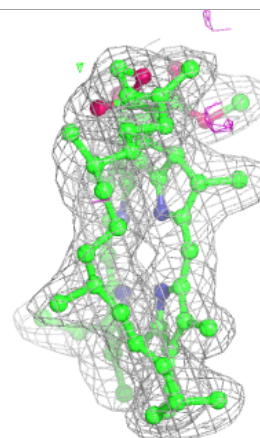
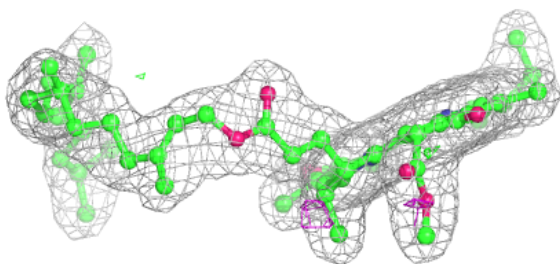
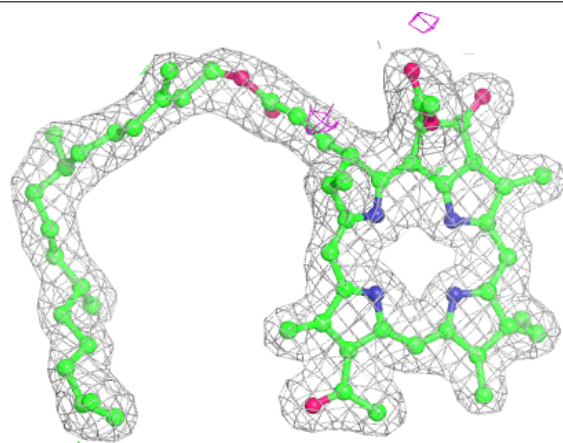


Electron density around BCL 5 102:

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

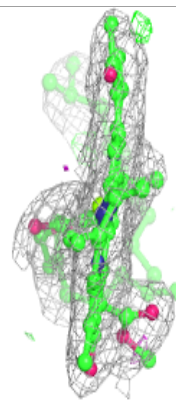
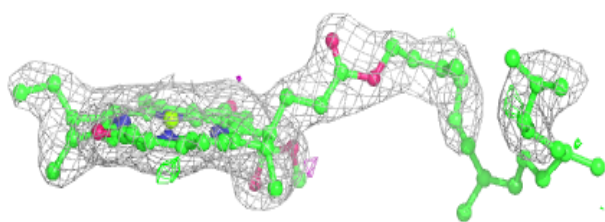
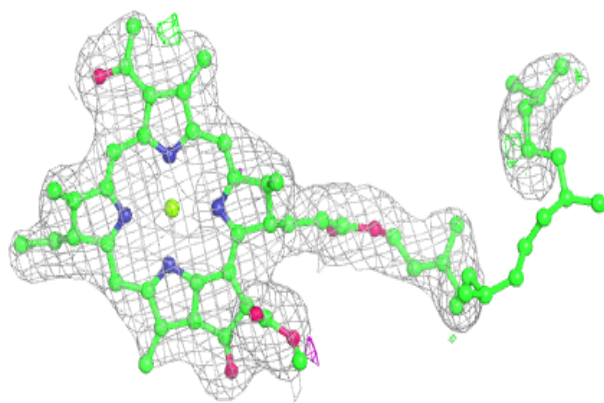
**Electron density around BPH L 302:**

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



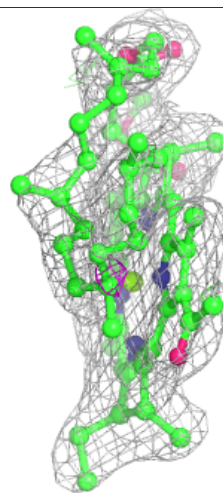
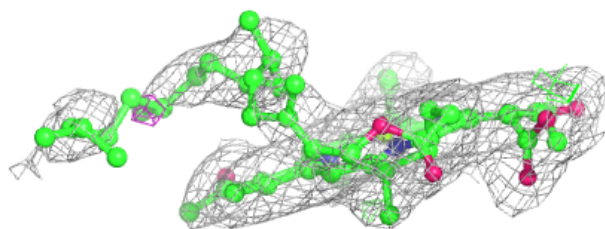
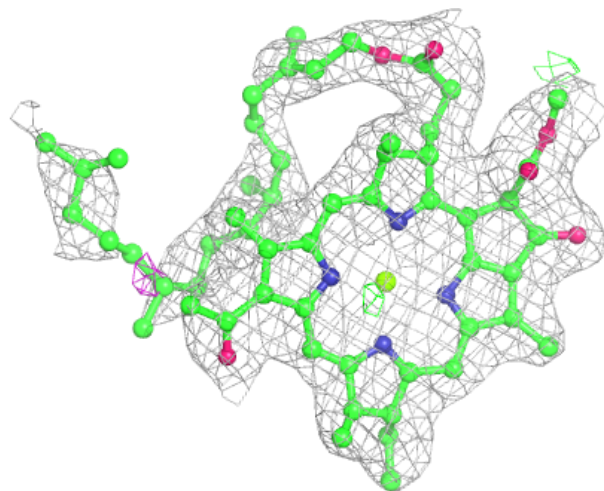
Electron density around BCL 9 103:

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



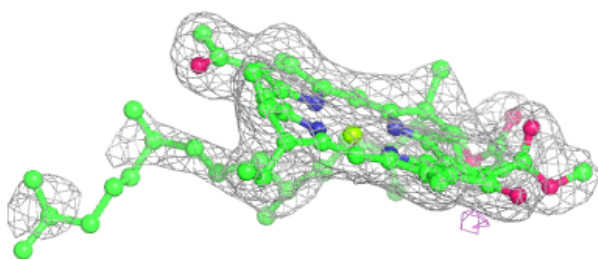
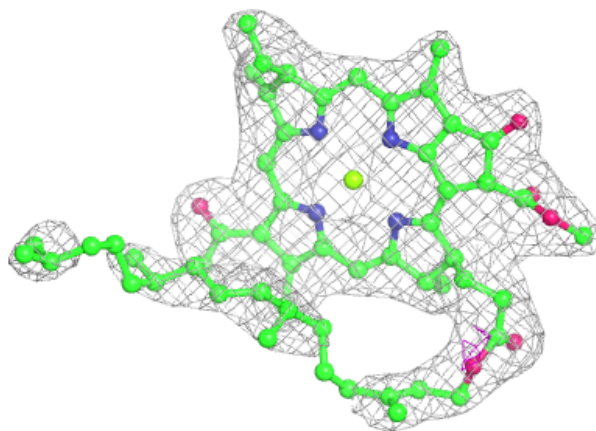
Electron density around BCL 7 102:

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



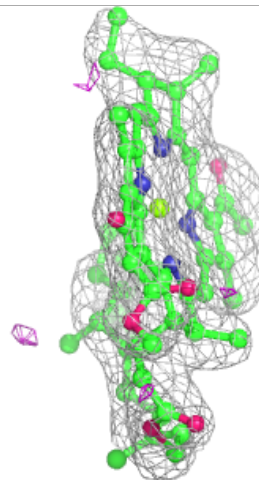
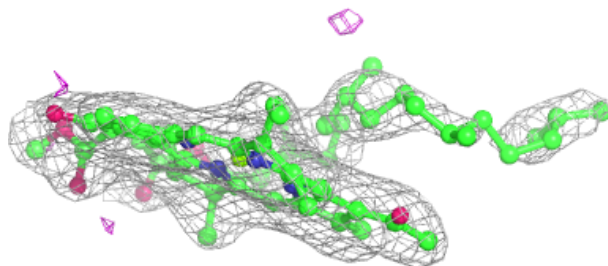
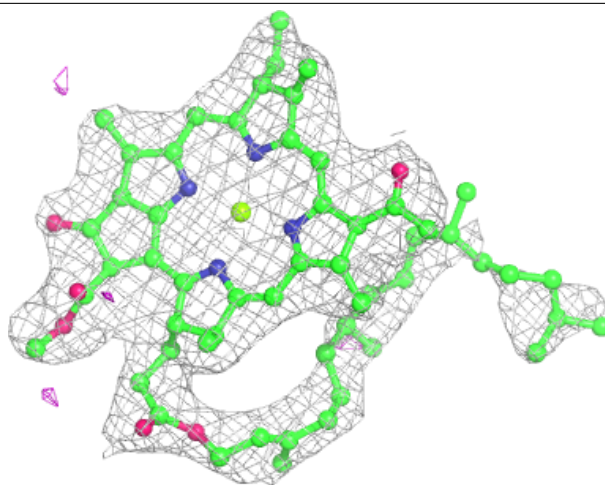
Electron density around BCL K 102:

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



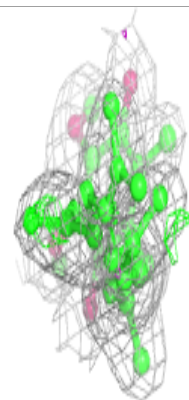
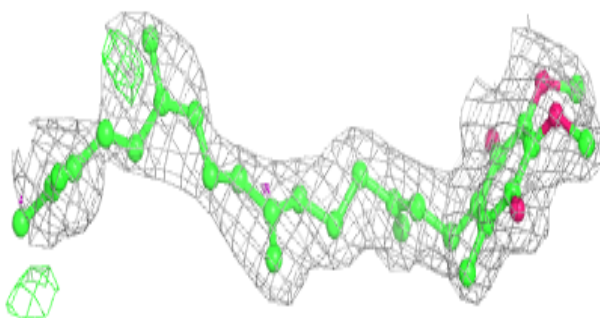
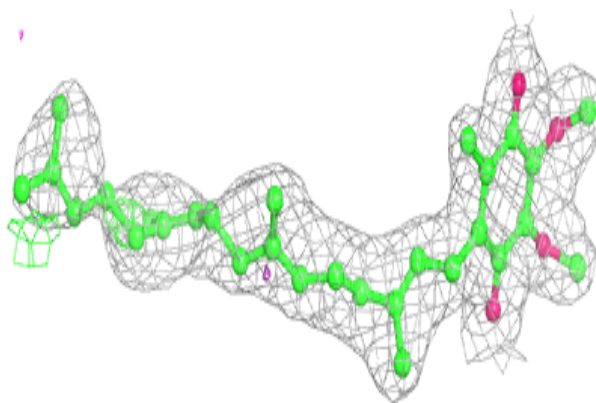
Electron density around BCL F 102:

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

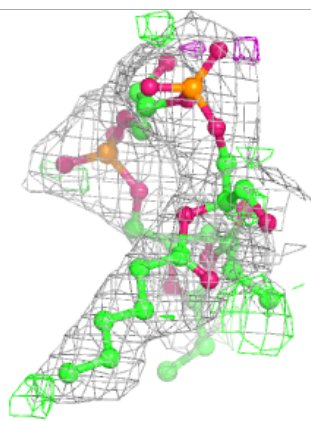
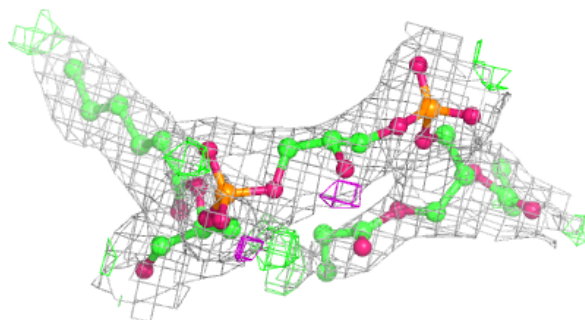
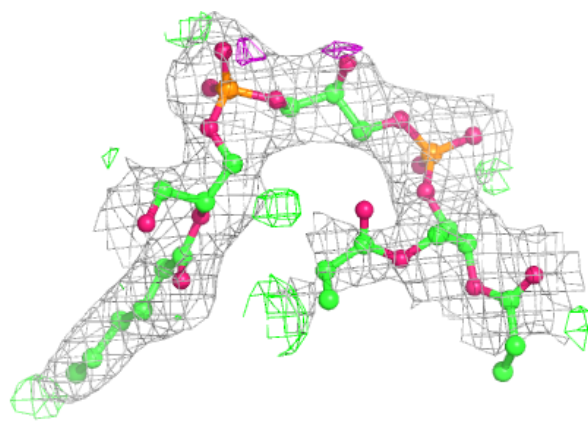


Electron density around UQ8 L 303:

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

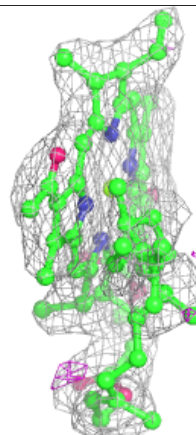
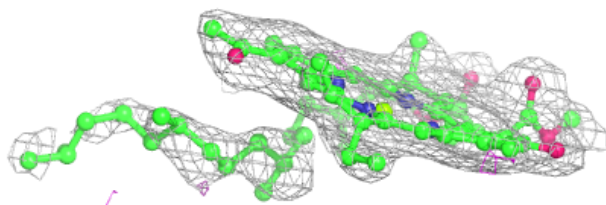
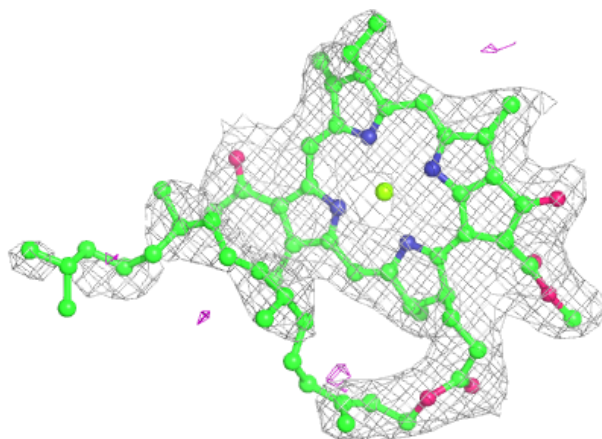
**Electron density around CDL M 415:**

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

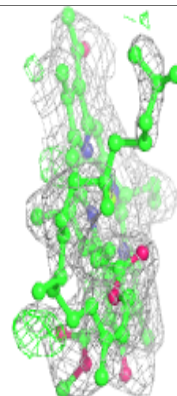
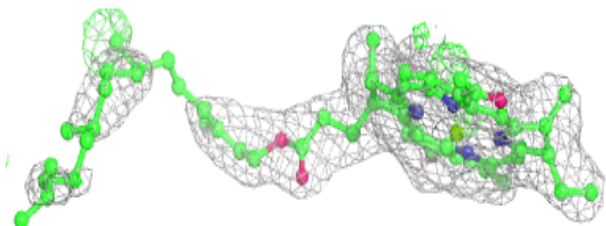
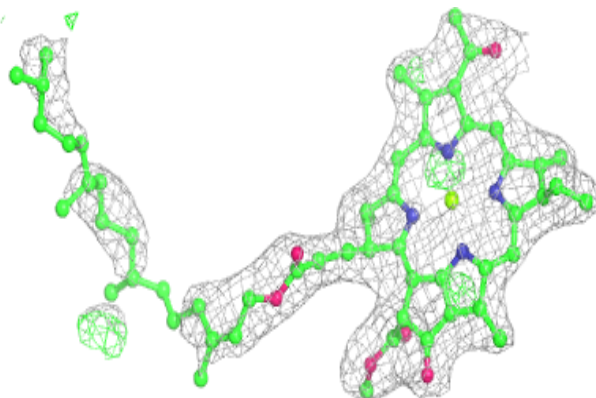


Electron density around BCL A 103:

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

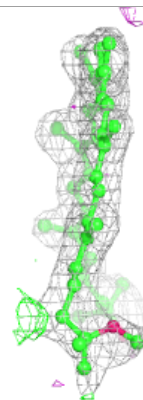
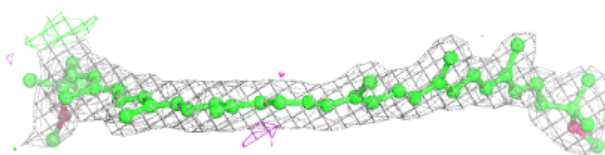
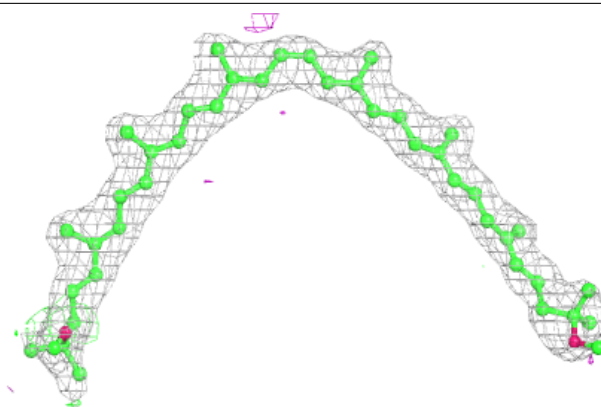
**Electron density around BCL 1 101:**

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



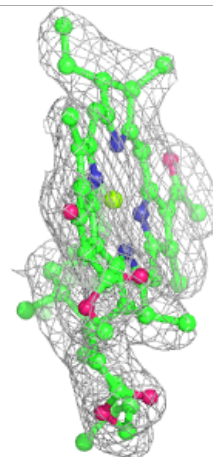
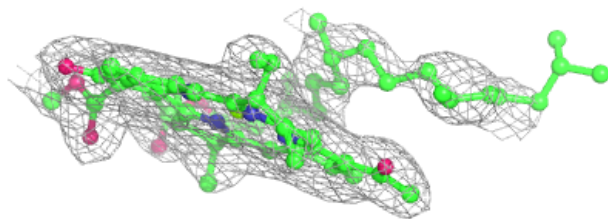
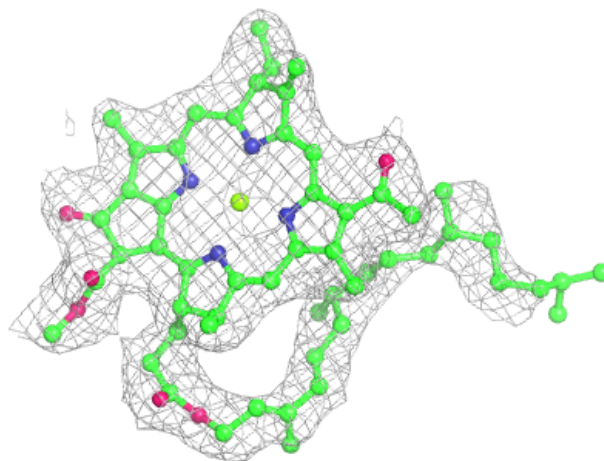
Electron density around CRT M 406:

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



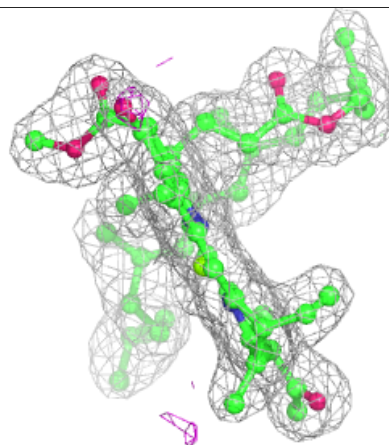
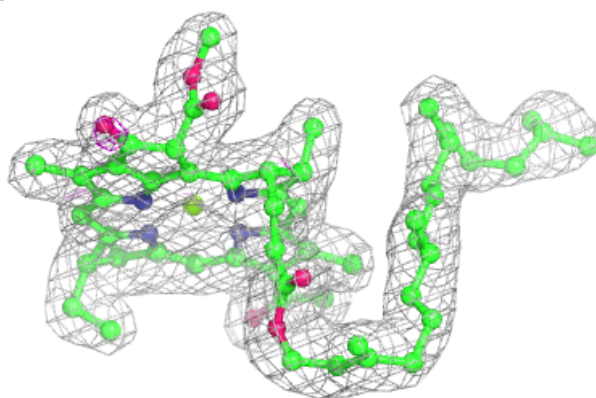
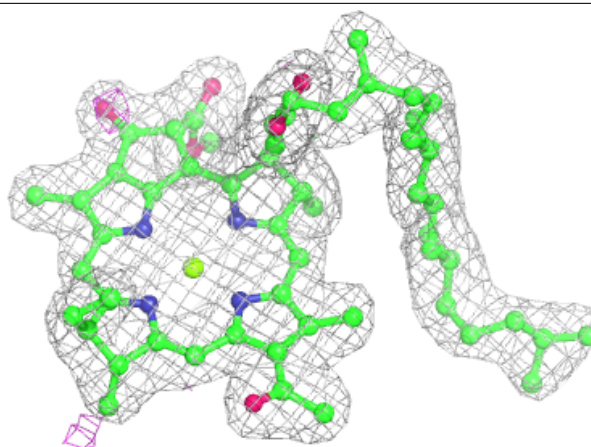
Electron density around BCL 0 102:

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



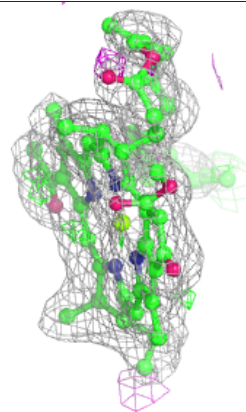
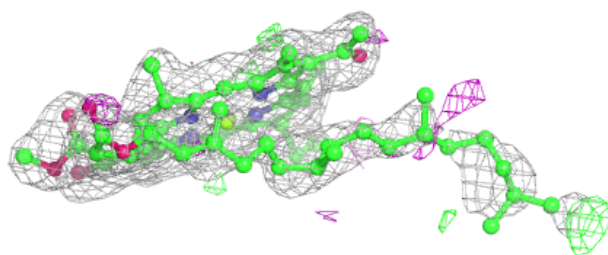
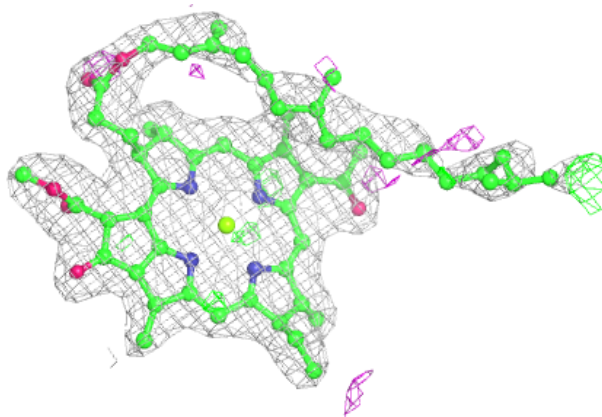
Electron density around BCL M 401:

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



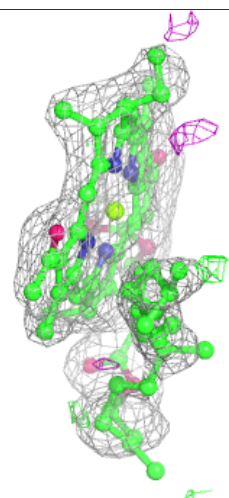
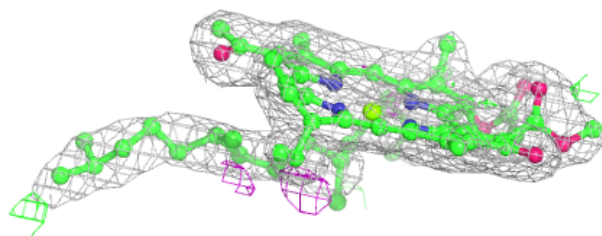
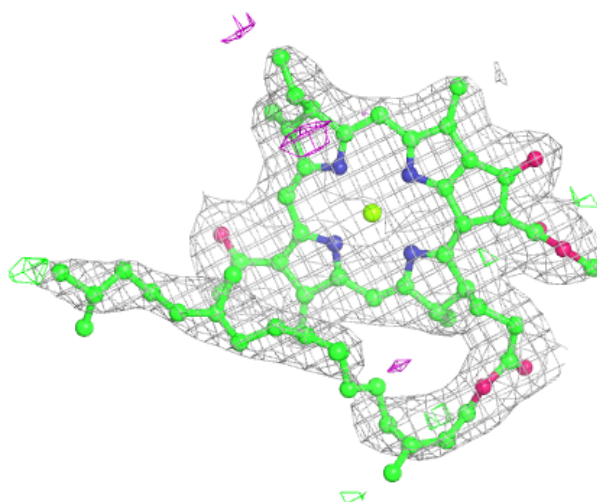
Electron density around BCL O 102:

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



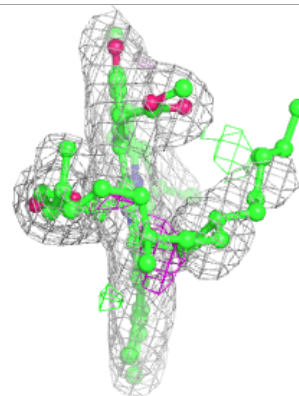
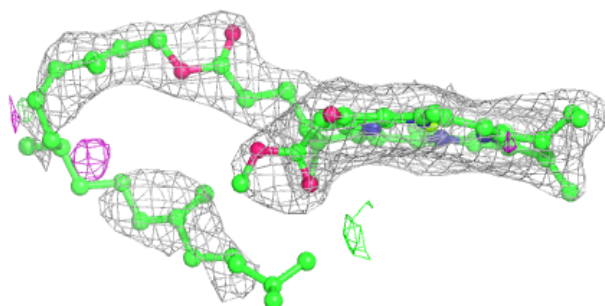
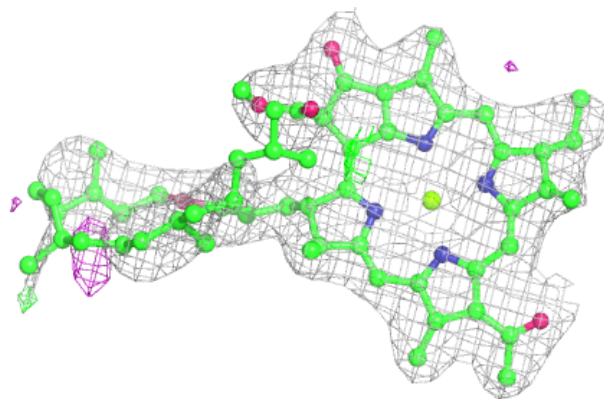
Electron density around BCL U 102:

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



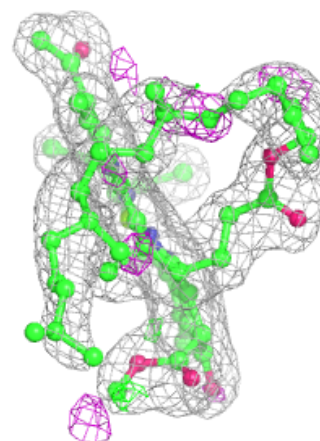
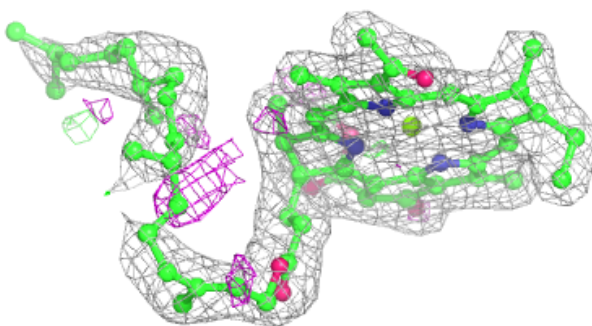
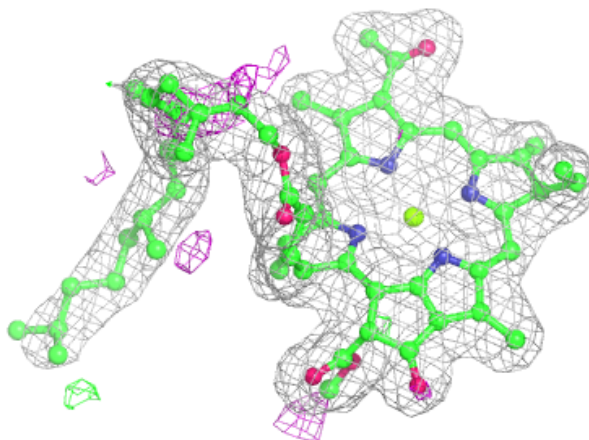
Electron density around BCL W 101:

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



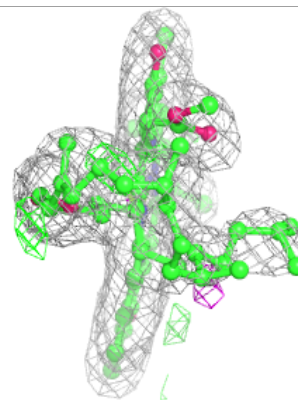
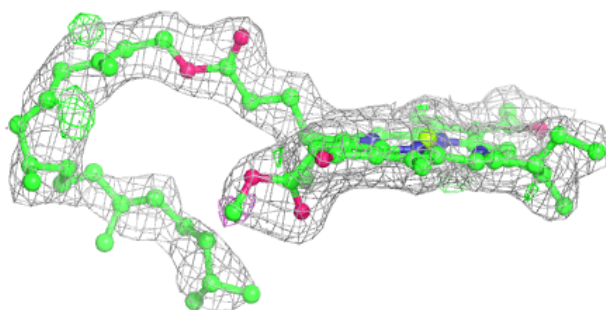
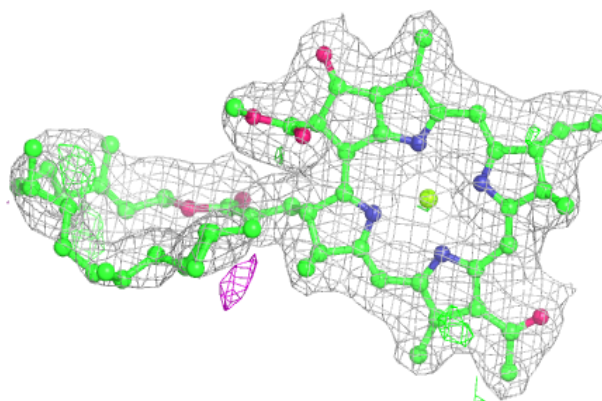
Electron density around BCL M 402:

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

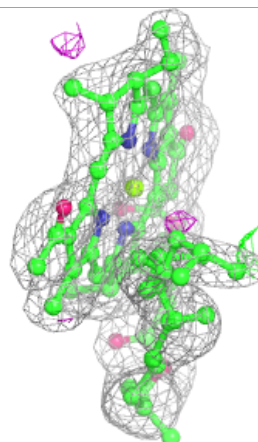
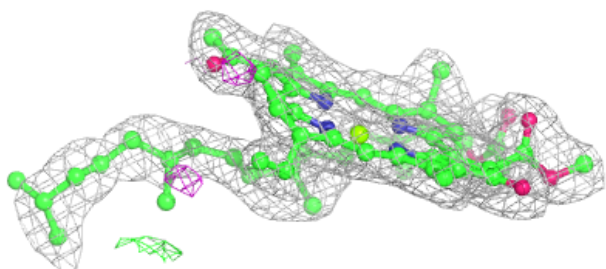
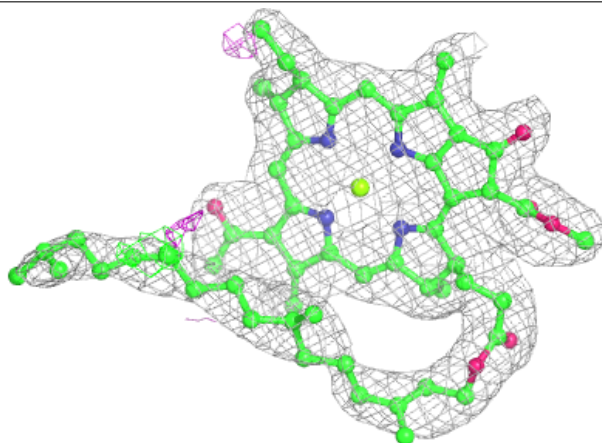


Electron density around BCL Q 101:

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

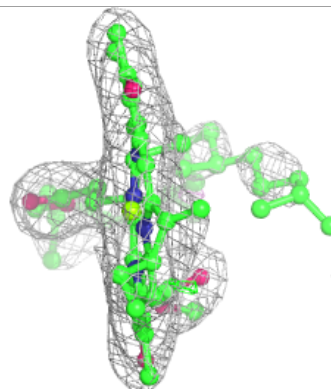
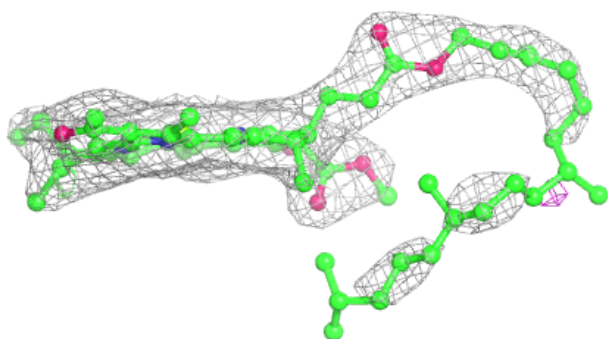
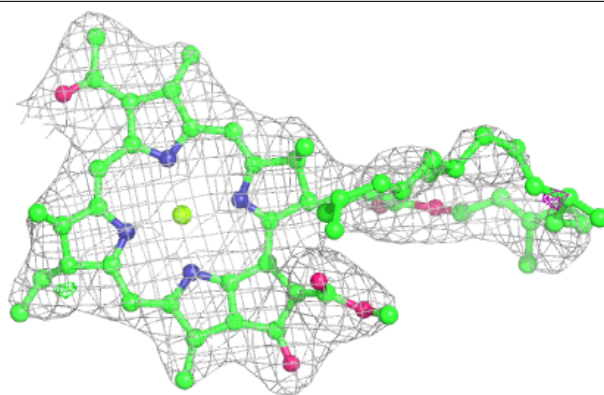
**Electron density around BCL Q 102:**

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

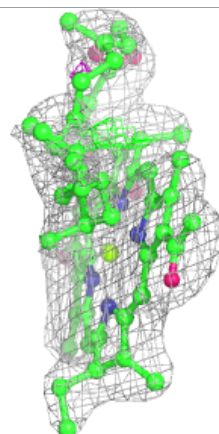
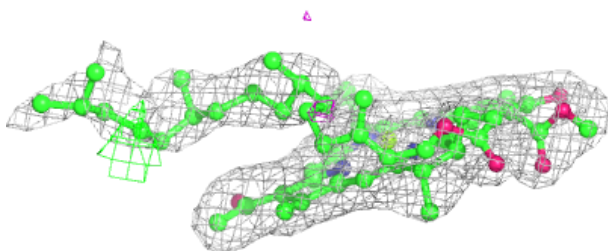
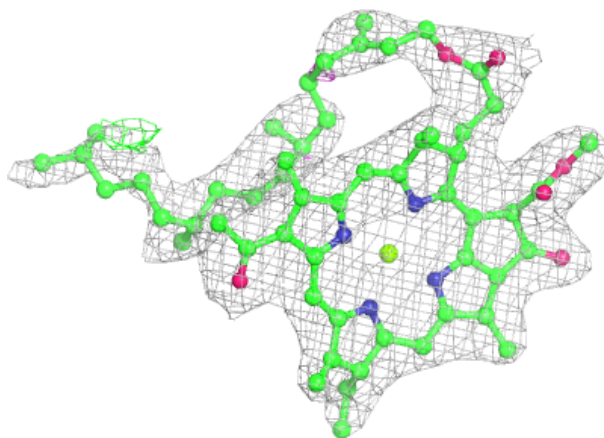


Electron density around BCL I 101:

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

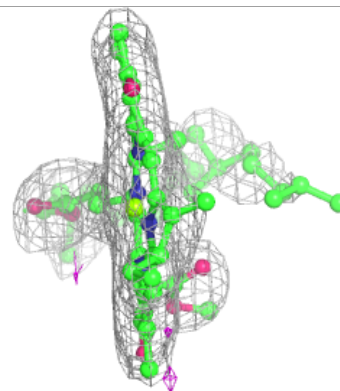
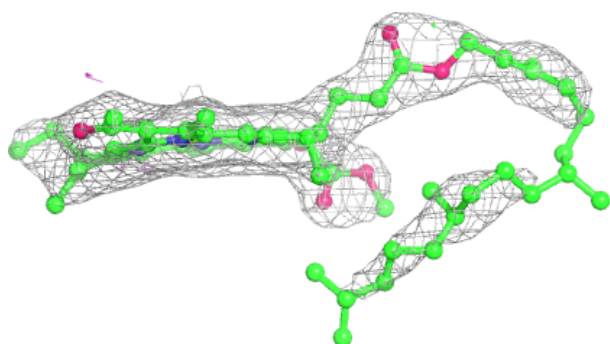
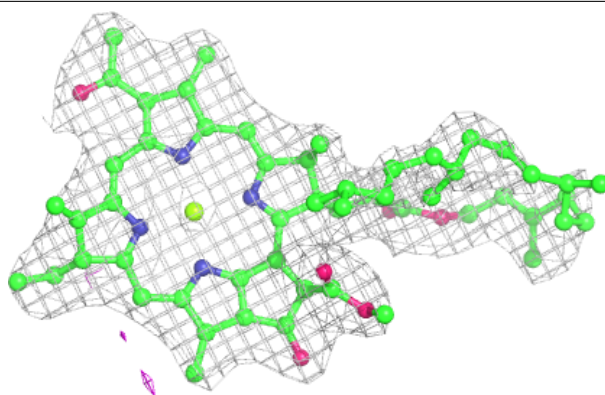
**Electron density around BCL W 102:**

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

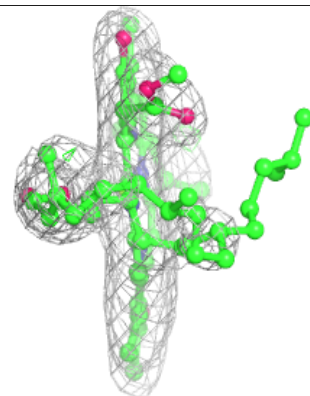
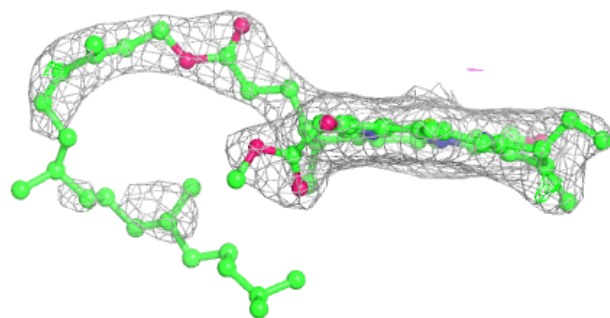
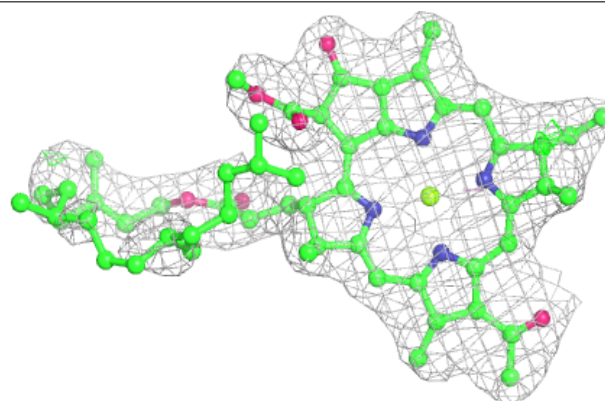


Electron density around BCL A 101:

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

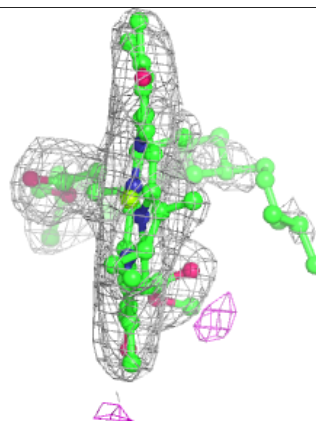
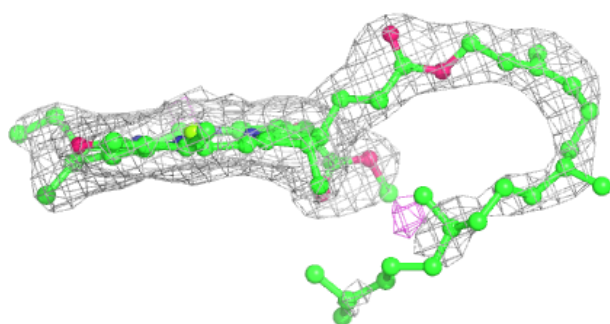
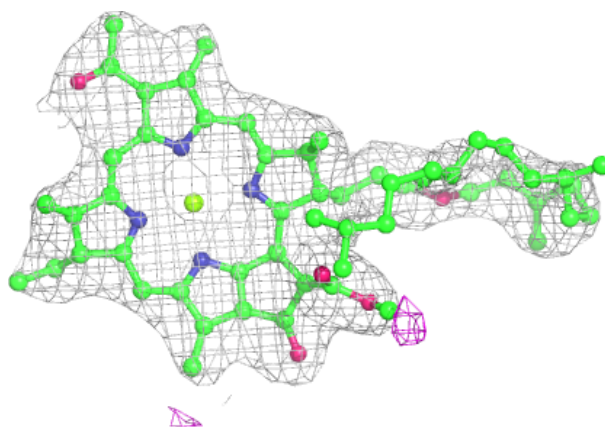
**Electron density around BCL F 101:**

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

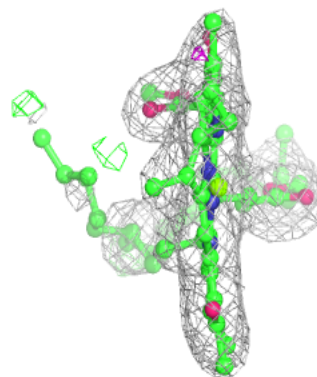
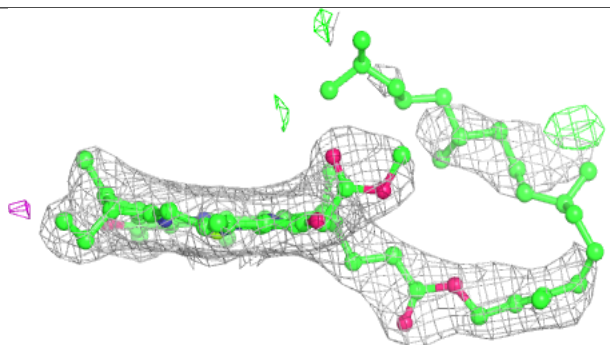
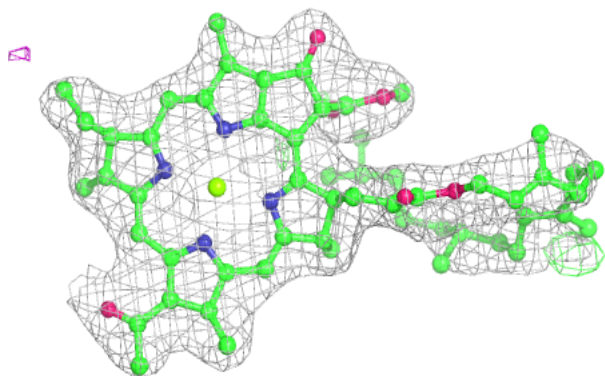


Electron density around BCL K 101:

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

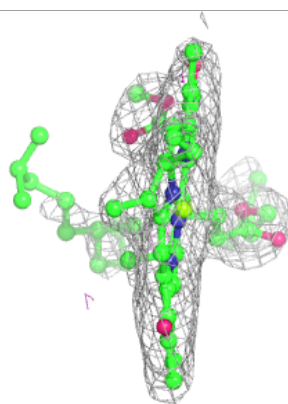
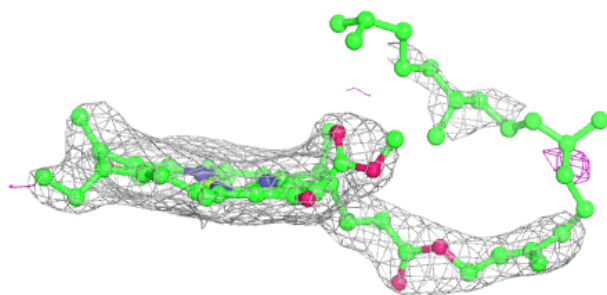
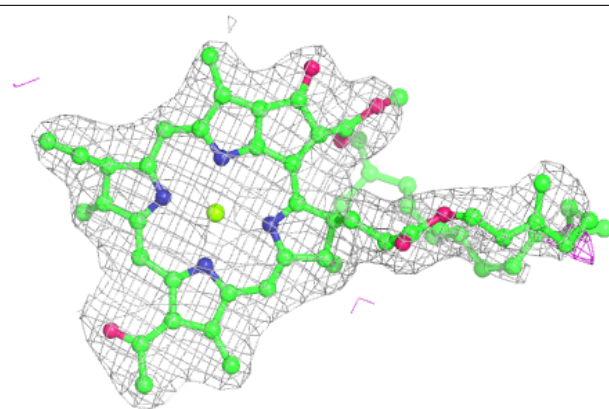
**Electron density around BCL Y 101:**

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

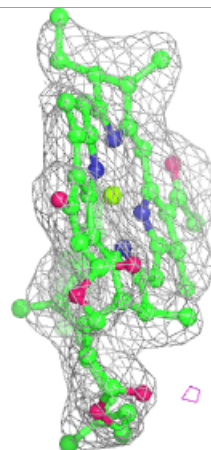
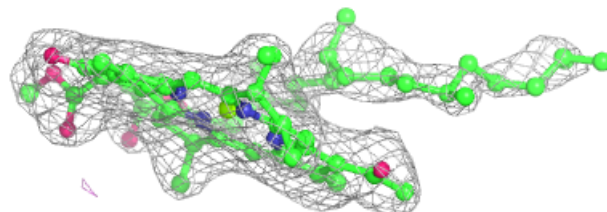
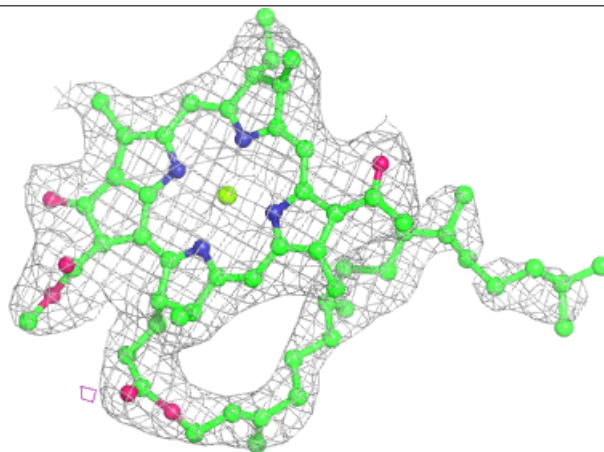


Electron density around BCL D 101:

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

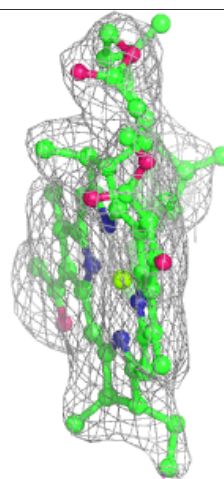
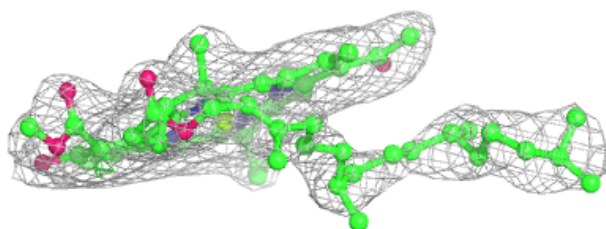
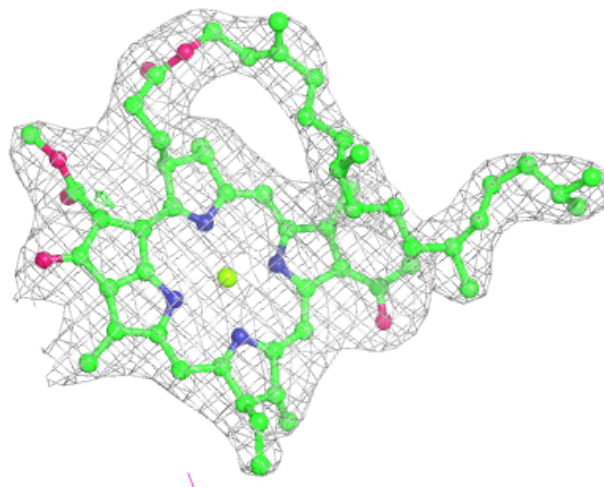
**Electron density around BCL I 102:**

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



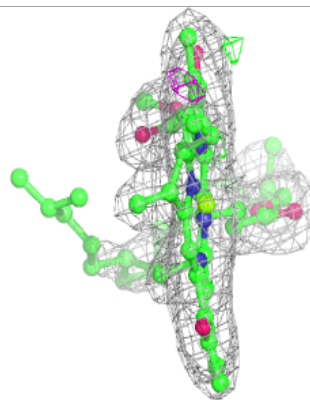
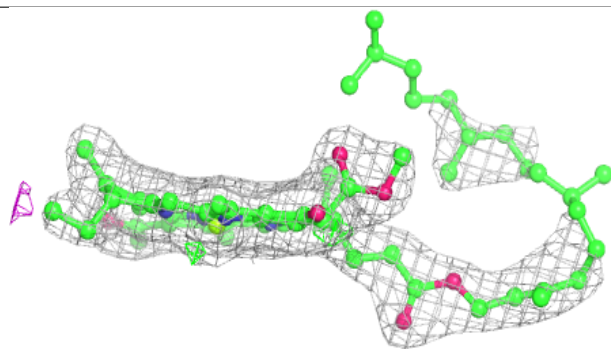
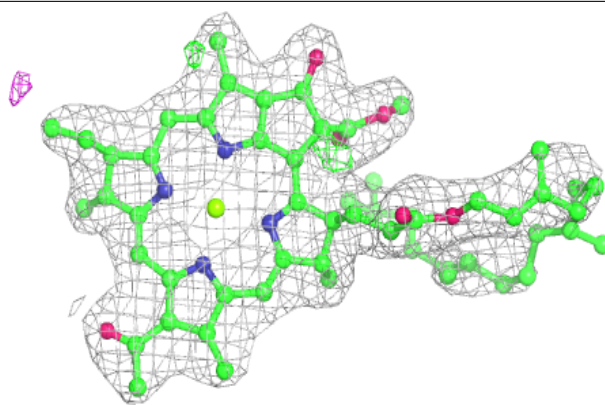
Electron density around BCL D 102:

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

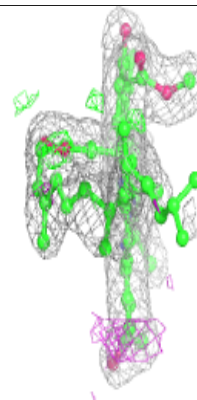
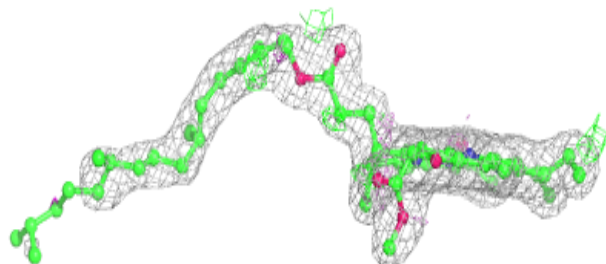
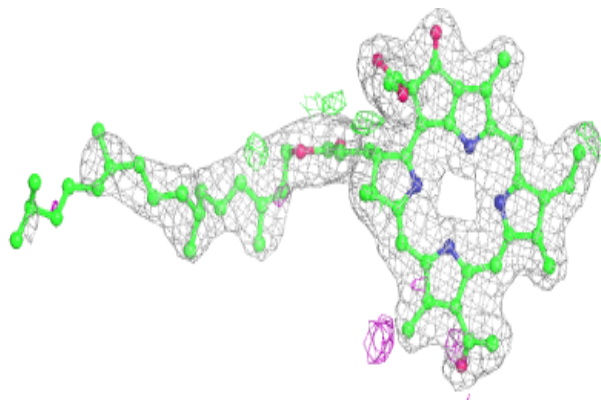


Electron density around BCL O 101:

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

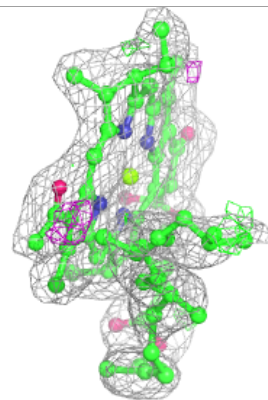
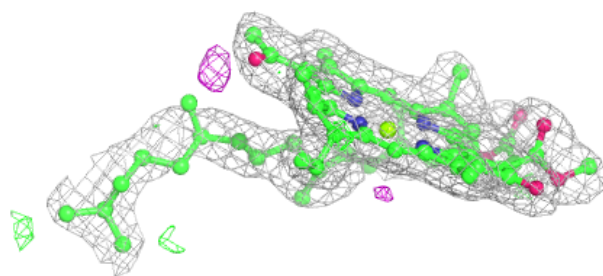
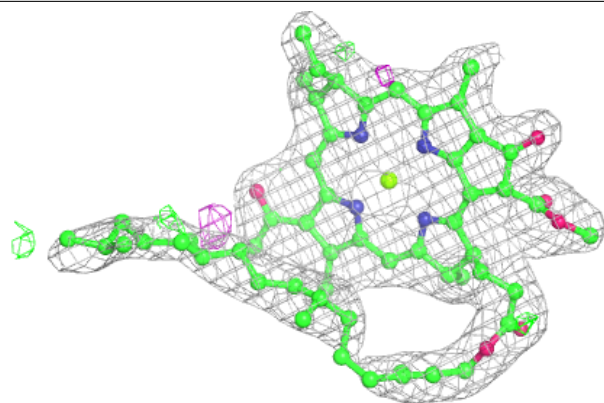
**Electron density around BPH M 404:**

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

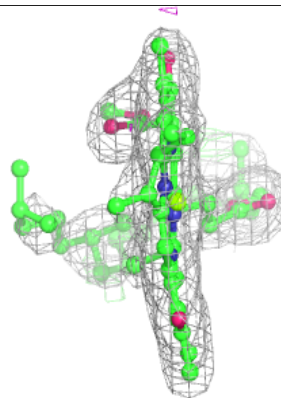
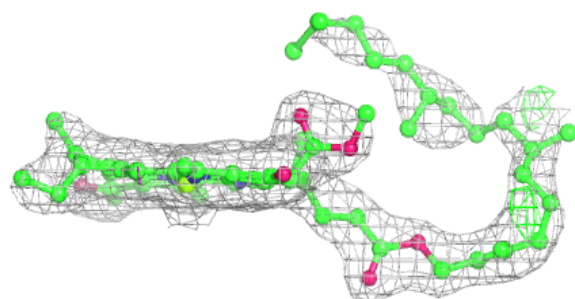
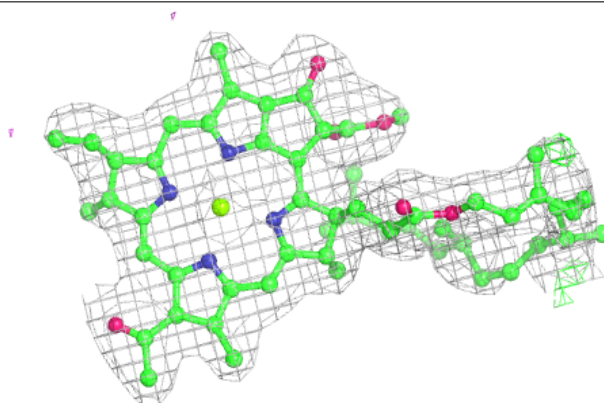


Electron density around BCL S 102:

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

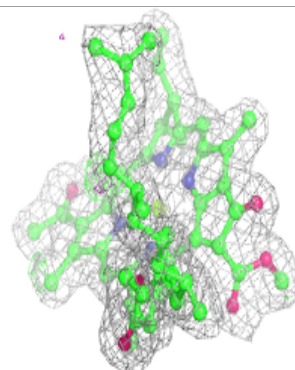
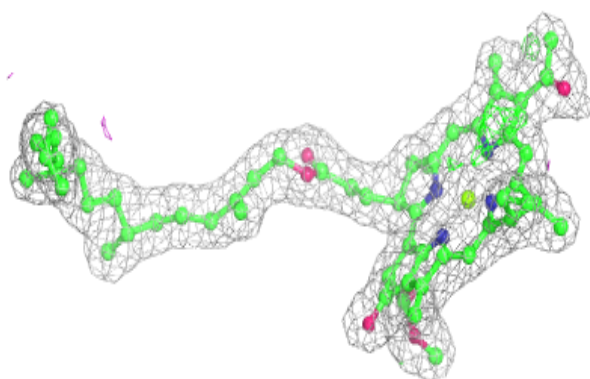
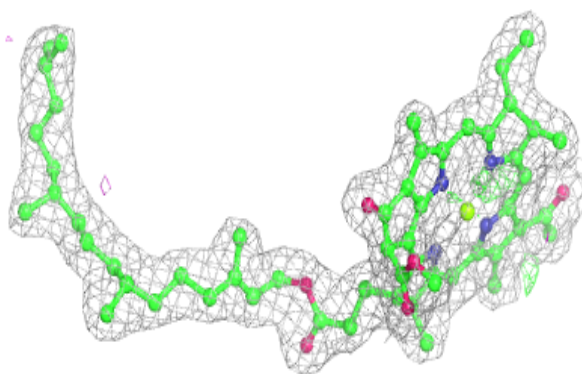
**Electron density around BCL U 101:**

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

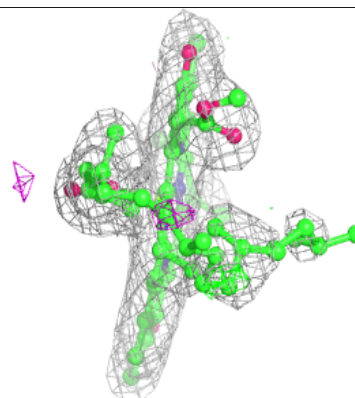
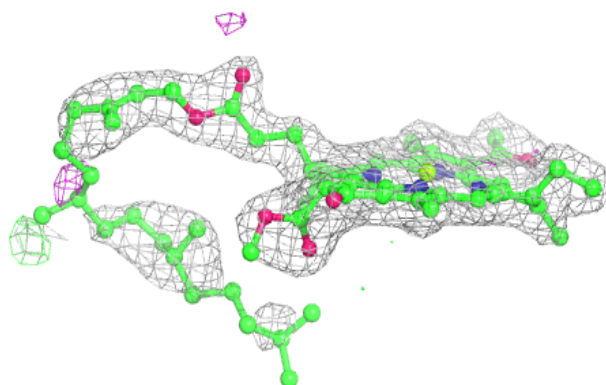
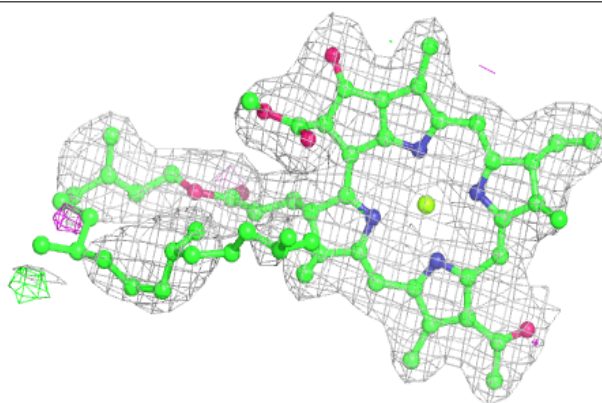


Electron density around BCL M 403:

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

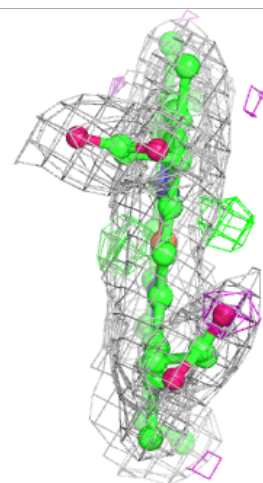
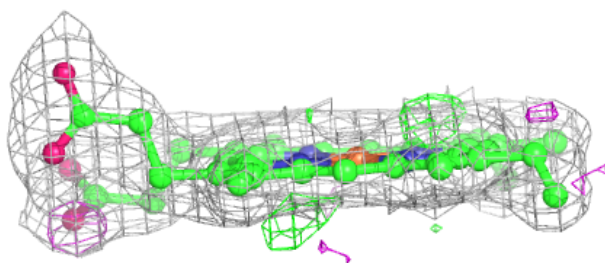
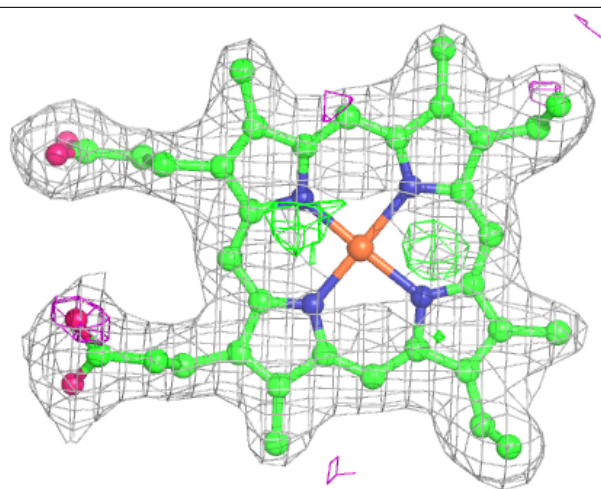
**Electron density around BCL S 101:**

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



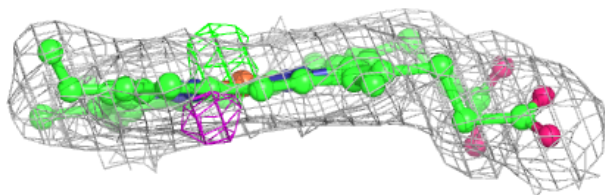
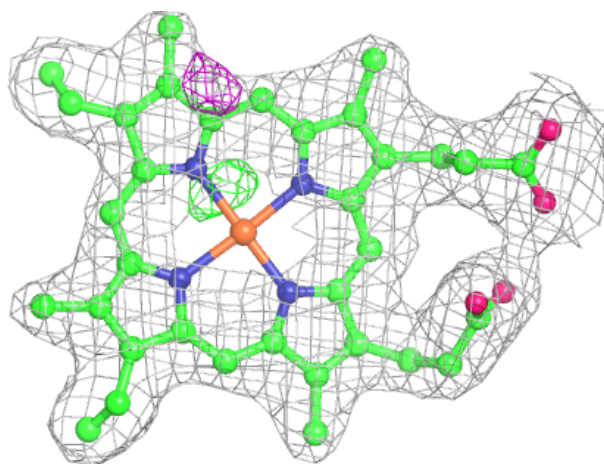
Electron density around HEC C 504:

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



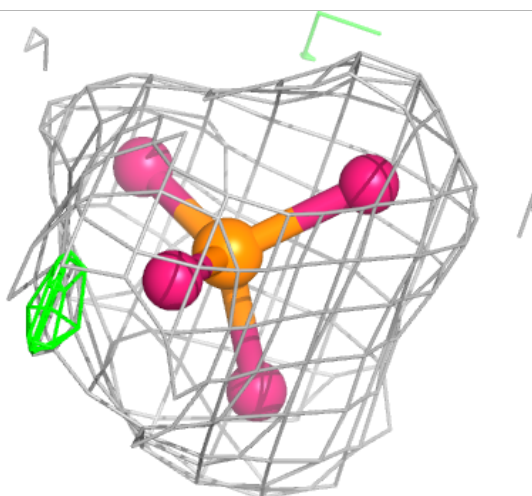
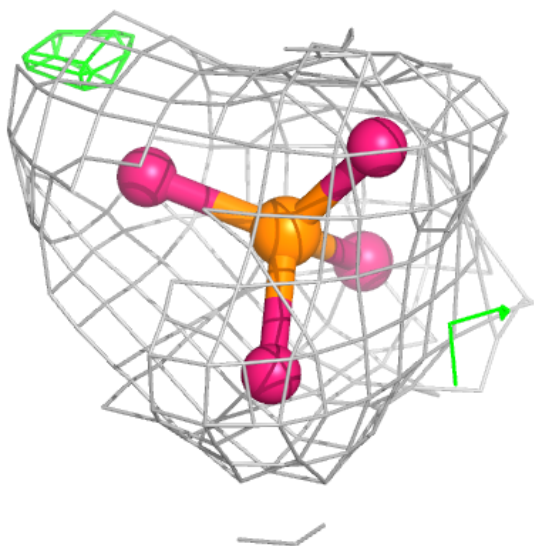
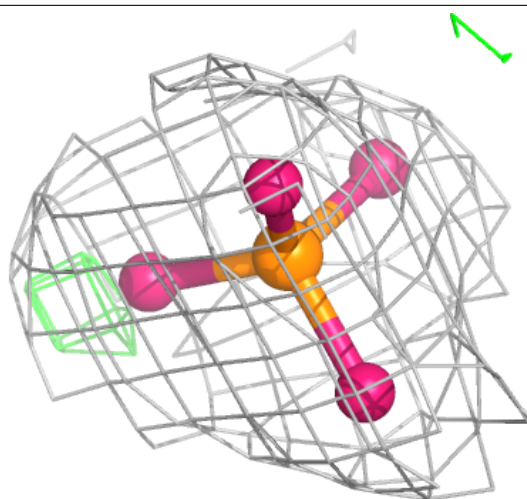
Electron density around HEC C 502:

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



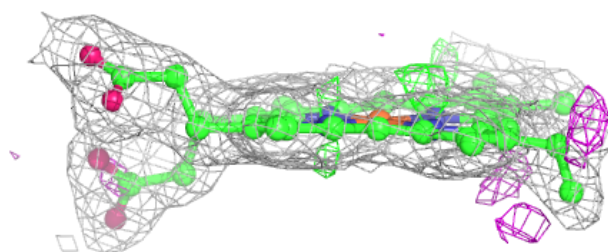
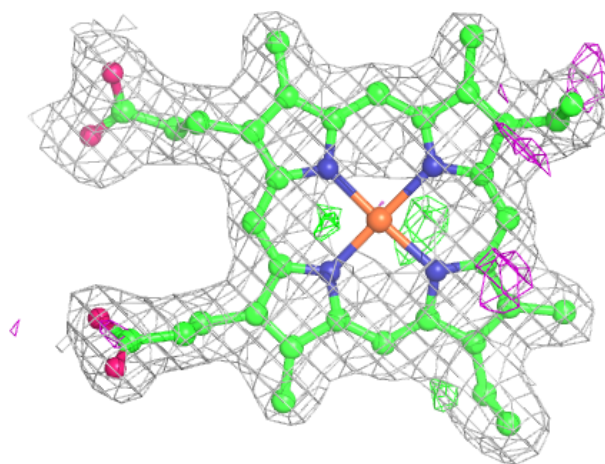
Electron density around PEF M 410:

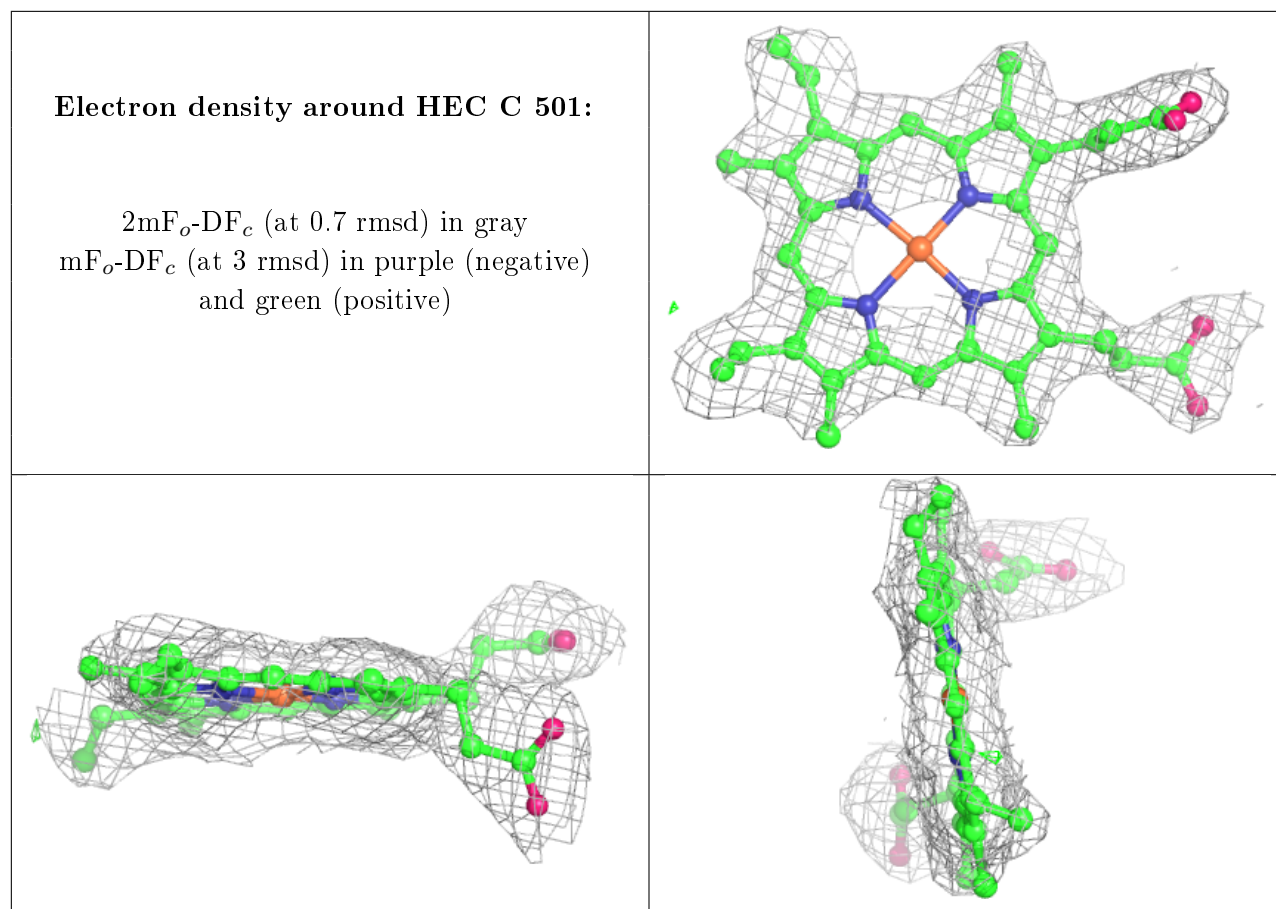
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.