



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 02:24 AM UTC

PDB ID : 5Y5S / pdb_00005y5s
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

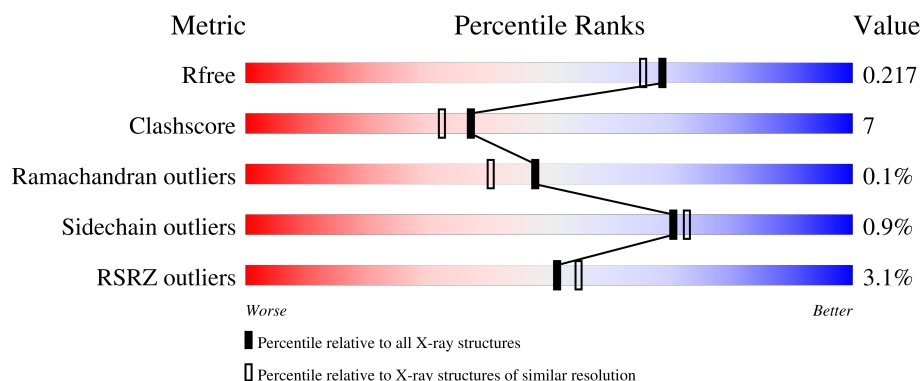
1 Overall quality at a glance

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.



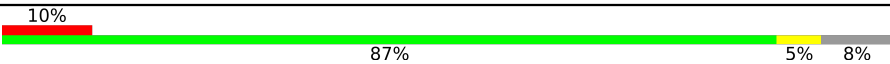
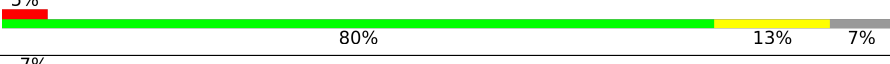
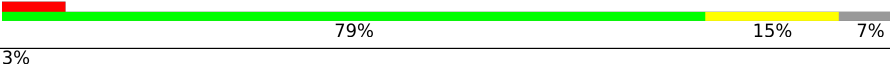
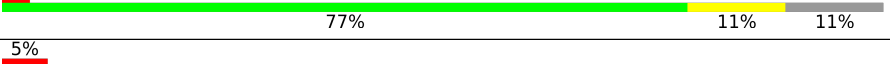
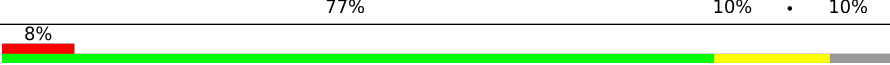
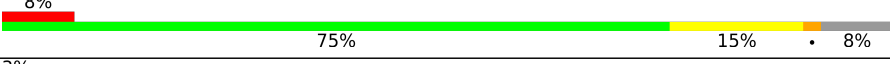
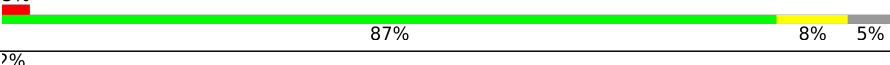
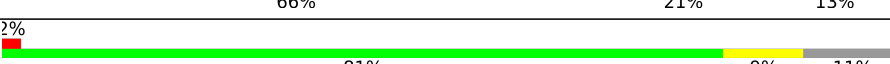
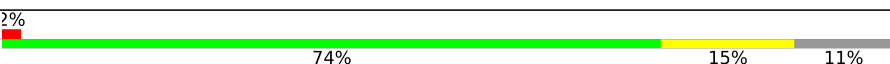
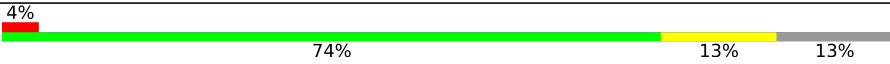
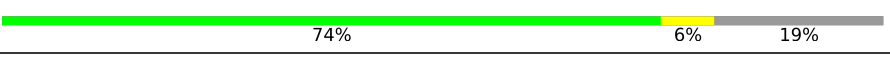
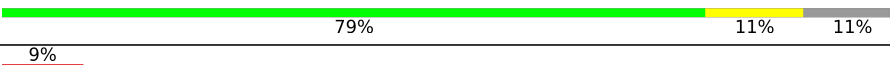
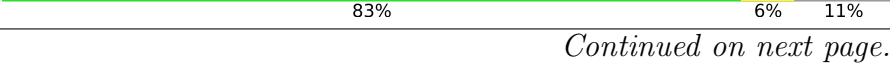
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
2	L	281	
3	M	325	
4	H	259	
5	1	61	

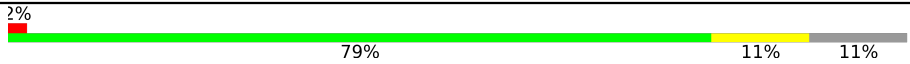
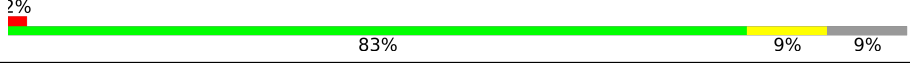
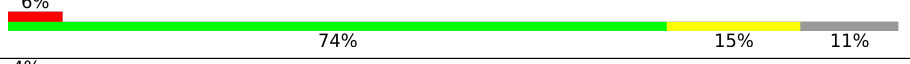
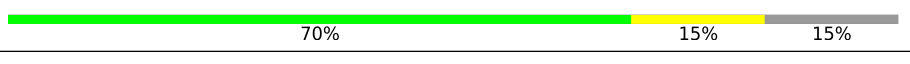
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	3	61	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	P	47	
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	105	-	X	-	-
20	PEF	3	104	-	X	-	-
20	PEF	5	104	-	X	-	-
20	PEF	I	104	-	X	-	-
20	PEF	M	408	-	X	-	-
20	PEF	M	410	-	X	-	-
20	PEF	U	105	-	X	-	-
20	PEF	U	106	-	X	-	-
20	PEF	W	104	-	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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

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

-
- The diagram shows the chemical structure of HEC (Hydroxyethylchlorin). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including hydroxyl groups (OH) and ethyl groups (CH₂CH₃). The structure is labeled with atom names: C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, C1AR, C2AR, C3AR, C4AR, C1AS, C2AS, C3AS, C4AS, C1AT, C2AT, C3AT, C4AT, C1AU, C2AU, C3AU, C4AU, C1AV, C2AV, C3AV, C4AV, C1AW, C2AW, C3AW, C4AW, C1AX, C2AX, C3AX, C4AX, C1AY, C2AY, C3AY, C4AY, C1AZ, C2AZ, C3AZ, C4AZ, C1BA, C2BA, C3BA, C4BA, C1BB, C2BB, C3BB, C4BB, C1BC, C2BC, C3BC, C4BC, C1BD, C2BD, C3BD, C4BD, C1BE, C2BE, C3BE, C4BE, C1BF, C2BF, C3BF, C4BF, C1BG, C2BG, C3BG, C4BG, C1BH, C2BH, C3BH, C4BH, C1BI, C2BI, C3BI, C4BI, C1BJ, C2BJ, C3BJ, C4BJ, C1BK, C2BK, C3BK, C4BK, C1BL, C2BL, C3BL, C4BL, C1BM, C2BM, C3BM, C4BM, C1BN, C2BN, C3BN, C4BN, C1BO, C2BO, C3BO, C4BO, C1BP, C2BP, C3BP, C4BP, C1BQ, C2BQ, C3BQ, C4BQ, C1BR, C2BR, C3BR, C4BR, C1BS, C2BS, C3BS, C4BS, C1BT, C2BT, C3BT, C4BT, C1BU, C2BU, C3BU, C4BU, C1BV, C2BV, C3BV, C4BV, C1BW, C2BW, C3BW, C4BW, C1BX, C2BX, C3BX, C4BX, C1BY, C2BY, C3BY, C4BY, C1BZ, C2BZ, C3BZ, C4BZ, C1CA, C2CA, C3CA, C4CA, C1CB, C2CB, C3CB, C4CB, C1CC, C2CC, C3CC, C4CC, C1CD, C2CD, C3CD, C4CD, C1CE, C2CE, C3CE, C4CE, C1CF, C2CF, C3CF, C4CF, C1CG, C2CG, C3CG, C4CG, C1CH, C2CH, C3CH, C4CH, C1CI, C2CI, C3CI, C4CI, C1CJ, C2CJ, C3CJ, C4CJ, C1CK, C2CK, C3CK, C4CK, C1CL, C2CL, C3CL, C4CL, C1CM, C2CM, C3CM, C4CM, C1CN, C2CN, C3CN, C4CN, C1CO, C2CO, C3CO, C4CO, C1CP, C2CP, C3CP, C4CP, C1CQ, C2CQ, C3CQ, C4CQ, C1CR, C2CR, C3CR, C4CR, C1CS, C2CS, C3CS, C4CS, C1CT, C2CT, C3CT, C4CT, C1CU, C2CU, C3CU, C4CU, C1CV, C2CV, C3CV, C4CV, C1CW, C2CW, C3CW, C4CW, C1CX, C2CX, C3CX, C4CX, C1CY, C2CY, C3CY, C4CY, C1CZ, C2CZ, C3CZ, C4CZ, C1DA, C2DA, C3DA, C4DA, C1DB, C2DB, C3DB, C4DB, C1DC, C2DC, C3DC, C4DC, C1DD, C2DD, C3DD, C4DD, C1DE, C2DE, C3DE, C4DE, C1DF, C2DF, C3DF, C4DF, C1DG, C2DG, C3DG, C4DG, C1DH, C2DH, C3DH, C4DH, C1DI, C2DI, C3DI, C4DI, C1DJ, C2DJ, C3DJ, C4DJ, C1DK, C2DK, C3DK, C4DK, C1DL, C2DL, C3DL, C4DL, C1DM, C2DM, C3DM, C4DM, C1DN, C2DN, C3DN, C4DN, C1DO, C2DO, C3DO, C4DO, C1DP, C2DP, C3DP, C4DP, C1DQ, C2DQ, C3DQ, C4DQ, C1DR, C2DR, C3DR, C4DR, C1DS, C2DS, C3DS, C4DS, C1DT, C2DT, C3DT, C4DT, C1DU, C2DU, C3DU, C4DU, C1DV, C2DV, C3DV, C4DV, C1DW, C2DW, C3DW, C4DW, C1DX, C2DX, C3DX, C4DX, C1DY, C2DY, C3DY, C4DY, C1DZ, C2DZ, C3DZ, C4DZ, C1EA, C2EA, C3EA, C4EA, C1EB, C2EB, C3EB, C4EB, C1EC, C2EC, C3EC, C4EC, C1ED, C2ED, C3ED, C4ED, C1EE, C2EE, C3EE, C4EE, C1EF, C2EF, C3EF, C4EF, C1EG, C2EG, C3EG, C4EG, C1EH, C2EH, C3EH, C4EH, C1EI, C2EI, C3EI, C4EI, C1EJ, C2EJ, C3EJ, C4EJ, C1EK, C2EK, C3EK, C4EK, C1EL, C2EL, C3EL, C4EL, C1EM, C2EM, C3EM, C4EM, C1EN, C2EN, C3EN, C4EN, C1EO, C2EO, C3EO, C4EO, C1EP, C2EP, C3EP, C4EP, C1EQ, C2EQ, C3EQ, C4EQ, C1ER, C2ER, C3ER, C4ER, C1ES, C2ES, C3ES, C4ES, C1ET, C2ET, C3ET, C4ET, C1EU, C2EU, C3EU, C4EU, C1EV, C2EV, C3EV, C4EV, C1EW, C2EW, C3EW, C4EW, C1EX, C2EX, C3EX, C4EX, C1EY, C2EY, C3EY, C4EY, C1EZ, C2EZ, C3EZ, C4EZ, C1FA, C2FA, C3FA, C4FA, C1FB, C2FB, C3FB, C4FB, C1FC, C2FC, C3FC, C4FC, C1FD, C2FD, C3FD, C4FD, C1FE, C2FE, C3FE, C4FE, C1FF, C2FF, C3FF, C4FF, C1FG, C2FG, C3FG, C4FG, C1FH, C2FH, C3FH, C4FH, C1FI, C2FI, C3FI, C4FI, C1FJ, C2FJ, C3FJ, C4FJ, C1FK, C2FK, C3FK, C4FK, C1FL, C2FL, C3FL, C4FL, C1FM, C2FM, C3FM, C4FM, C1FN, C2FN, C3FN, C4FN, C1FO, C2FO, C3FO, C4FO, C1FP, C2FP, C3FP, C4FP, C1FQ, C2FQ, C3FQ, C4FQ, C1FR, C2FR, C3FR, C4FR, C1FS, C2FS, C3FS, C4FS, C1FT, C2FT, C3FT, C4FT, C1FU, C2FU, C3FU, C4FU, C1FV, C2FV, C3FV, C4FV, C1FW, C2FW, C3FW, C4FW, C1FX, C2FX, C3FX, C4FX, C1FY, C2FY, C3FY, C4FY, C1FZ, C2FZ, C3FZ, C4FZ, C1GA, C2GA, C3GA, C4GA, C1GB, C2GB, C3GB, C4GB, C1GC, C2GC, C3GC, C4GC, C1GD, C2GD, C3GD, C4GD, C1GE, C2GE, C3GE, C4GE, C1GF, C2GF, C3GF, C4GF, C1GG, C2GG, C3GG, C4GG, C1GH, C2GH, C3GH, C4GH, C1GI, C2GI, C3GI, C4GI, C1GJ, C2GJ, C3GJ, C4GJ, C1GK, C2GK, C3GK, C4GK, C1GL, C2GL, C3GL, C4GL, C1GM, C2GM, C3GM, C4GM, C1GN, C2GN, C3GN, C4GN, C1GO, C2GO, C3GO, C4GO, C1GP, C2GP, C3GP, C4GP, C1GQ, C2GQ, C3GQ, C4GQ, C1GR, C2GR, C3GR, C4GR, C1GS, C2GS, C3GS, C4GS, C1GT, C2GT, C3GT, C4GT, C1GU, C2GU, C3GU, C4GU, C1GV, C2GV, C3GV, C4GV, C1GW, C2GW, C3GW, C4GW, C1GX, C2GX, C3GX, C4GX, C1GY, C2GY, C3GY, C4GY, C1GZ, C2GZ, C3GZ, C4GZ, C1HA, C2HA, C3HA, C4HA, C1HB, C2HB, C3HB, C4HB, C1HC, C2HC, C3HC, C4HC, C1HD, C2HD, C3HD, C4HD, C1HE, C2HE, C3HE, C4HE, C1HF, C2HF, C3HF, C4HF, C1HG, C2HG, C3HG, C4HG, C1HH, C2HH, C3HH, C4HH, C1HI, C2HI, C3HI, C4HI, C1HJ, C2HJ, C3HJ, C4HJ, C1HK, C2HK, C3HK, C4HK, C1HL, C2HL, C3HL, C4HL, C1HM, C2HM, C3HM, C4HM, C1HN, C2HN, C3HN, C4HN, C1HO, C2HO, C3HO, C4HO, C1HP, C2HP, C3HP, C4HP, C1HQ, C2HQ, C3HQ, C4HQ, C1HR, C2HR, C3HR, C4HR, C1HS, C2HS, C3HS, C4HS, C1HT, C2HT, C3HT, C4HT, C1HU, C2HU, C3HU, C4HU, C1HV, C2HV, C3HV, C4HV, C1HW, C2HW, C3HW, C4HW, C1HX, C2HX, C3HX, C4HX, C1HY, C2HY, C3HY, C4HY, C1HZ, C2HZ, C3HZ, C4HZ, C1IA, C2IA, C3IA, C4IA, C1IB, C2IB, C3IB, C4IB, C1IC, C2IC, C3IC, C4IC, C1ID, C2ID, C3ID, C4ID, C1IE, C2IE, C3IE, C4IE, C1IF, C2IF, C3IF, C4IF, C1IG, C2IG, C3IG, C4IG, C1IH, C2IH, C3IH, C4IH, C1II, C2II, C3II, C4

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



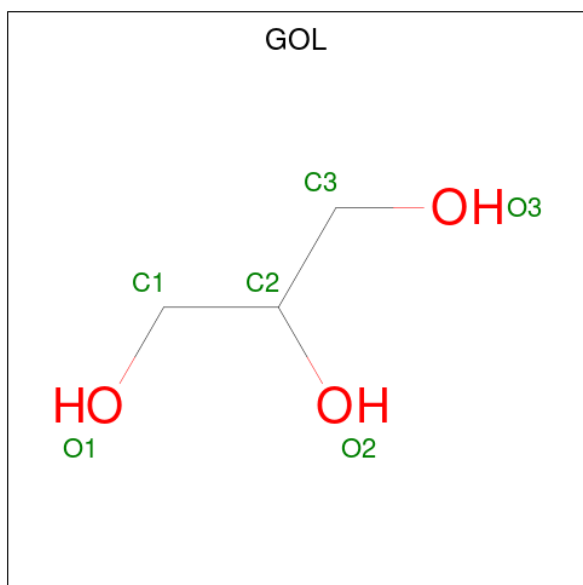
Continued from previous page...

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 (CCD ID: MG) (formula: Mg).

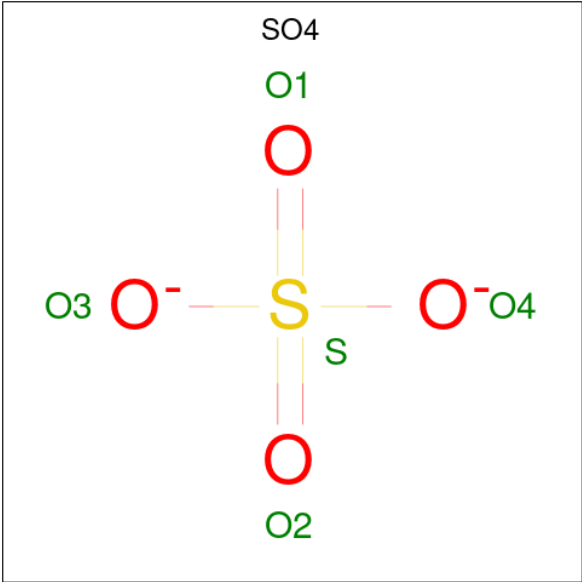
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg		
			1	1	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



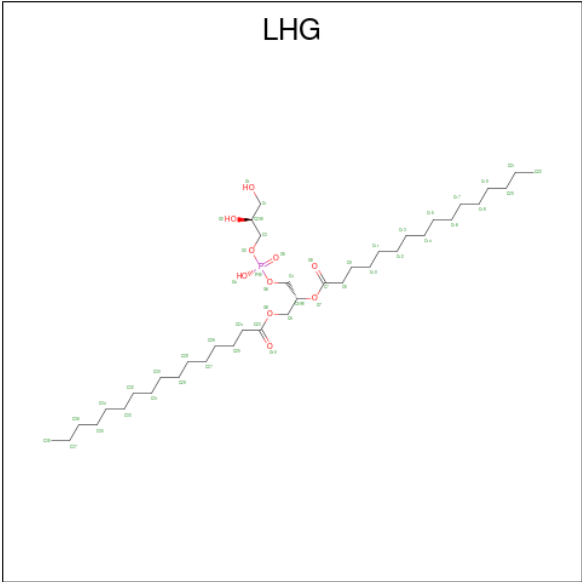
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O		
			6	3	3	0	0
9	H	1	Total	C	O		
			6	3	3	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



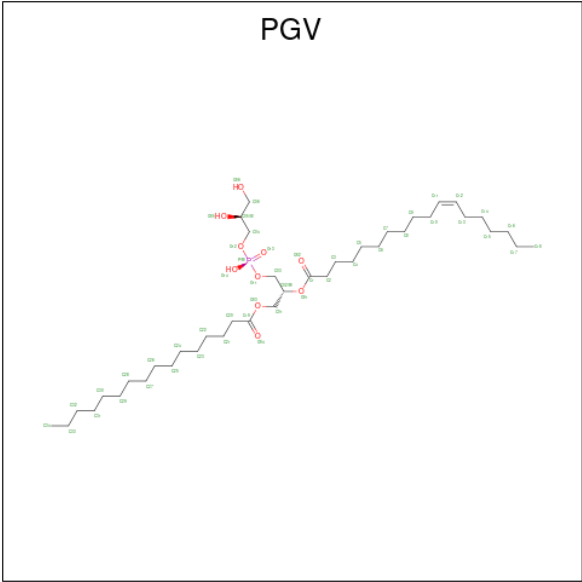
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	L	1	Total	O	S	0	0
			5	4	1		
10	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



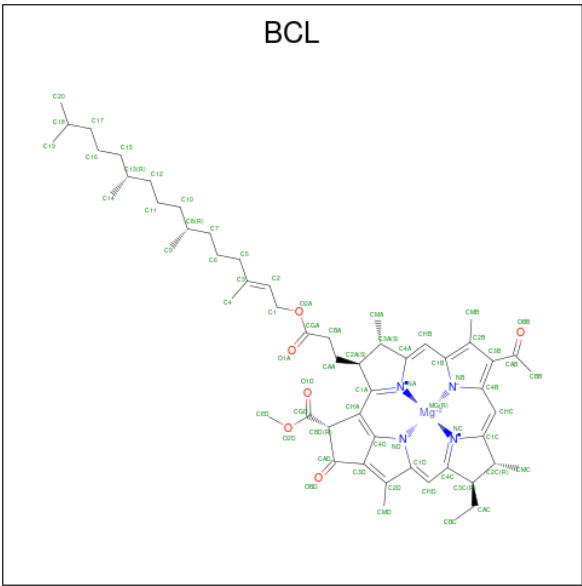
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			9	8	1		

- Molecule 12 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: 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 (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

Continued on next page...

Continued from previous page...

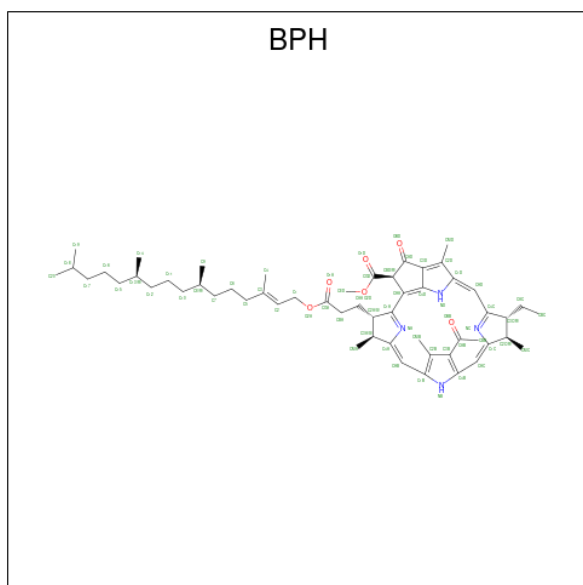
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

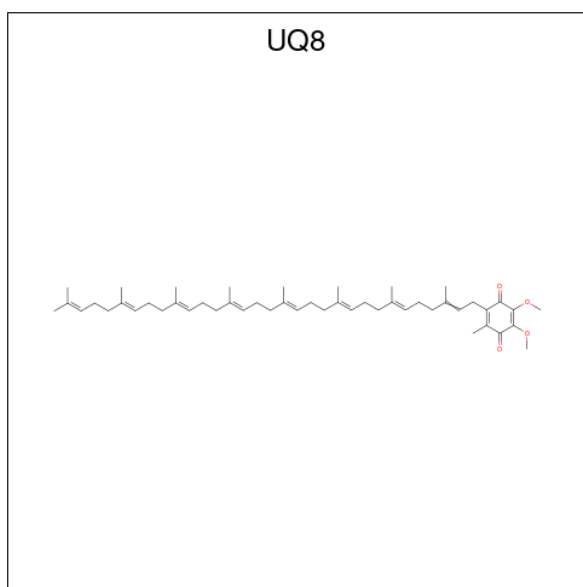
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 14 is BACTERIOPHEOPHYTIN A (CCD ID: 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 (CCD ID: 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 (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	1	Total	C	0	0
			12	12		
16	M	1	Total	C	0	0
			9	9		
16	B	1	Total	C	0	0
			12	12		
16	E	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	P	1	Total	C	0	0
			12	12		

Continued on next page...

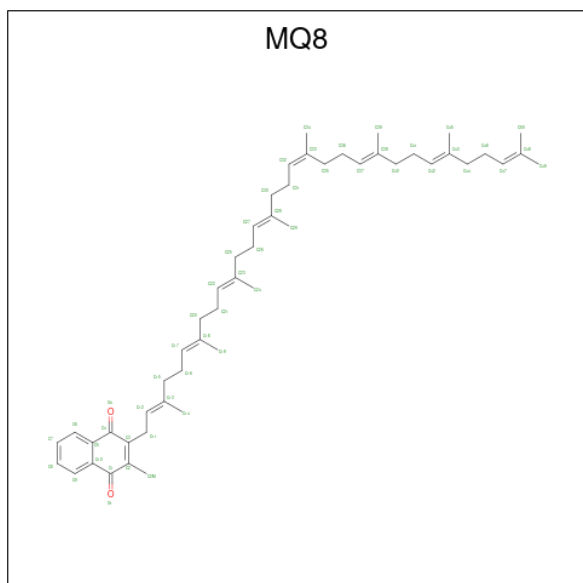
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	R	1	Total C 12 12	0	0
16	T	1	Total C 12 12	0	0
16	X	1	Total C 12 12	0	0
16	Z	1	Total C 12 12	0	0
16	2	1	Total C 12 12	0	0
16	4	1	Total C 12 12	0	0
16	6	1	Total C 12 12	0	0
16	8	1	Total C 12 12	0	0
16	0	1	Total C 12 12	0	0

- Molecule 17 is FE (III) ION (CCD ID: FE) (formula: Fe).

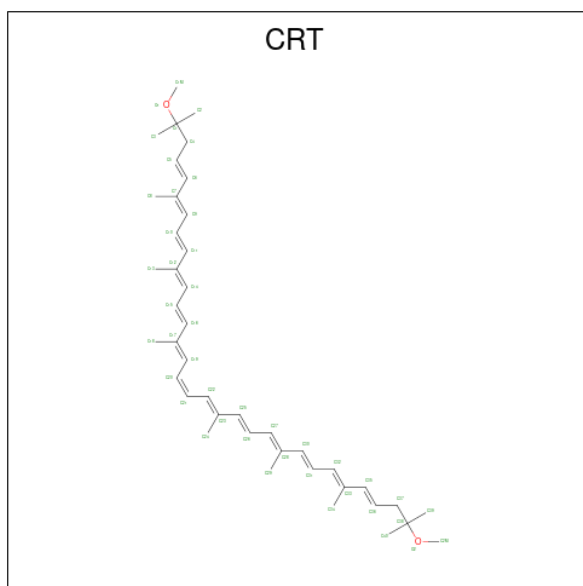
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	1	Total Fe 1 1	0	0

- Molecule 18 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



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

- Molecule 19 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



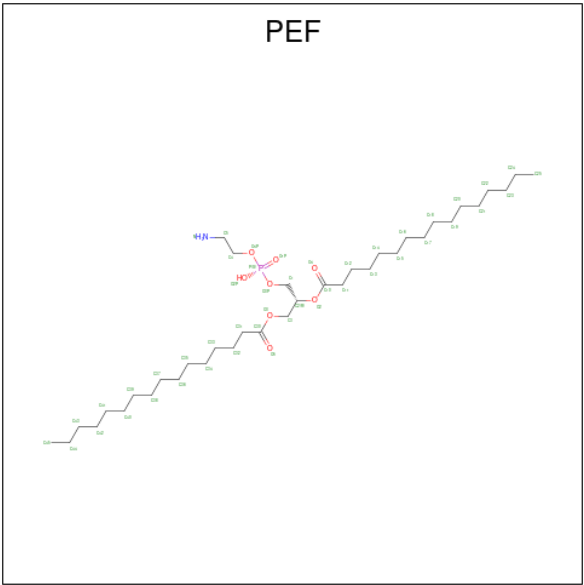
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	M	1	Total	C	O	0	0
			44	42	2		
19	A	1	Total	C	O	0	0
			44	42	2		
19	G	1	Total	C	O	0	0
			44	42	2		
19	J	1	Total	C	O	0	0
			44	42	2		
19	N	1	Total	C	O	0	0
			44	42	2		
19	O	1	Total	C	O	0	0
			44	42	2		
19	P	1	Total	C	O	0	0
			44	42	2		
19	Q	1	Total	C	O	0	0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

Continued on next page...

Continued from previous page...

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 (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



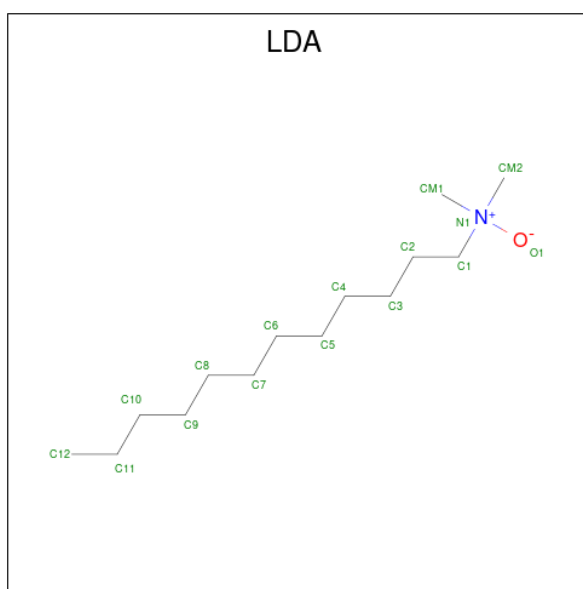
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

Continued on next page...

Continued from previous page...

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 (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



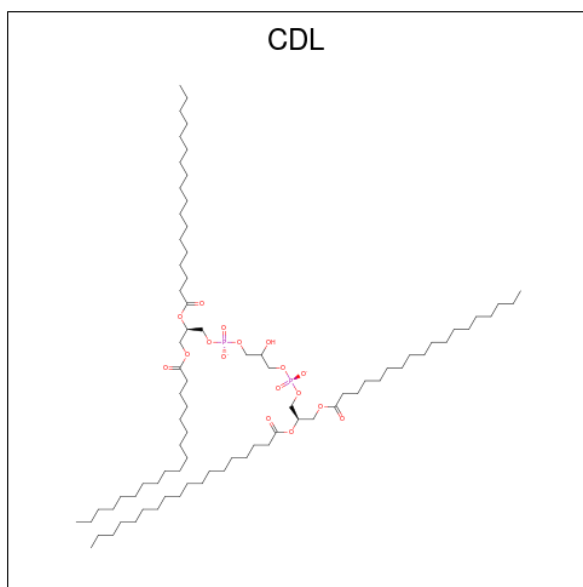
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	M	1	Total	C	N	O		
			14	12	1	1		
21	I	1	Total	C	N	O		
			16	14	1	1		
21	J	1	Total	C	N	O		
			16	14	1	1		

Continued on next page...

Continued from previous page...

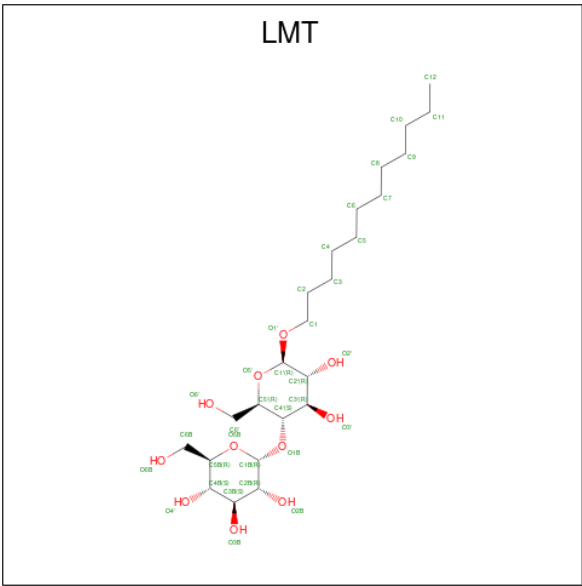
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	O	1	Total	C	N	O	0	0
			14	12	1	1		
21	V	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 22 is CARDIOLIPIN (CCD ID: 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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total	Ca	0	0
			1	1		
24	D	1	Total	Ca	0	0
			1	1		
24	F	1	Total	Ca	0	0
			1	1		
24	I	1	Total	Ca	0	0
			1	1		
24	K	1	Total	Ca	0	0
			1	1		
24	O	1	Total	Ca	0	0
			1	1		
24	Q	1	Total	Ca	0	0
			1	1		
24	S	1	Total	Ca	0	0
			1	1		
24	U	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	W	1	Total 1	Ca 1	0	0
24	Y	1	Total 1	Ca 1	0	0
24	1	1	Total 1	Ca 1	0	0
24	3	1	Total 1	Ca 1	0	0
24	5	1	Total 1	Ca 1	0	0
24	7	1	Total 1	Ca 1	0	0
24	9	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
25	J	4	Total 4	O 4	0	0

Continued on next page...

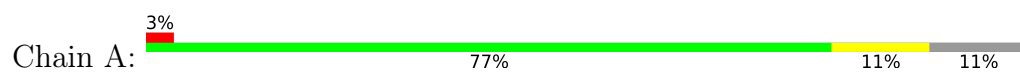
Continued from previous page...

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

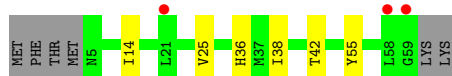
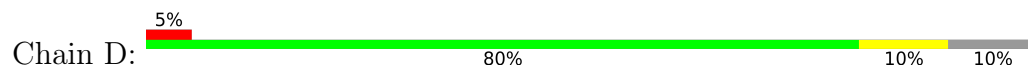
Continued on next page...

Continued from previous page...

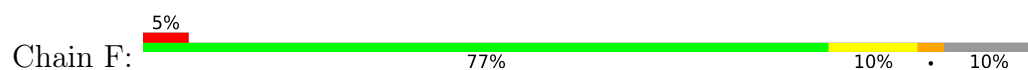
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	8	11	Total 11	O 11	0	0
25	9	13	Total 13	O 13	0	0
25	0	8	Total 8	O 8	0	0



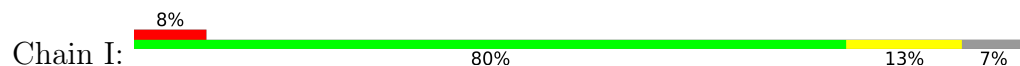
- Molecule 5: LH1 alpha polypeptide



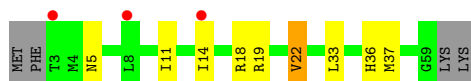
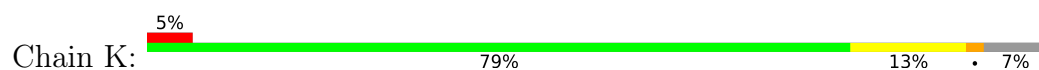
- Molecule 5: LH1 alpha polypeptide



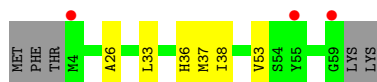
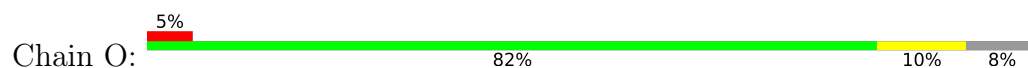
- Molecule 5: LH1 alpha polypeptide



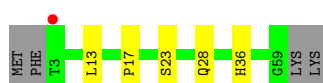
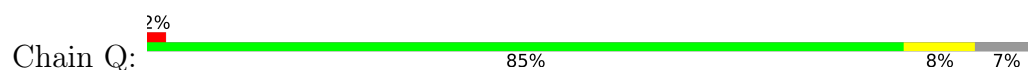
- Molecule 5: LH1 alpha polypeptide



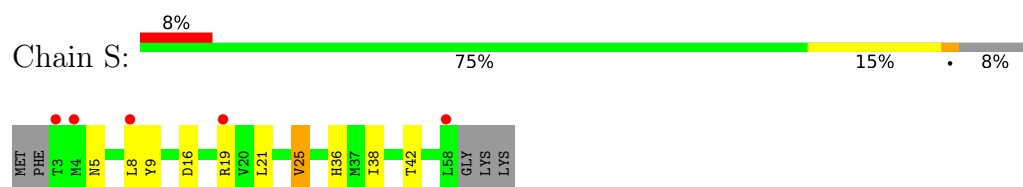
- Molecule 5: LH1 alpha polypeptide



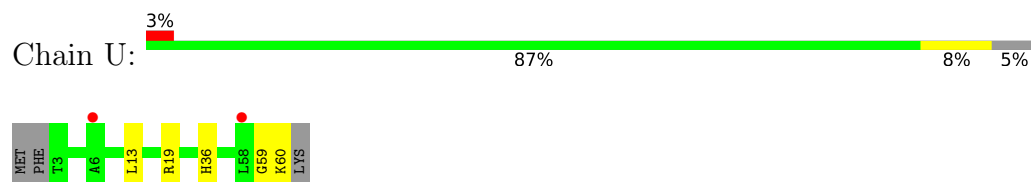
- Molecule 5: LH1 alpha polypeptide



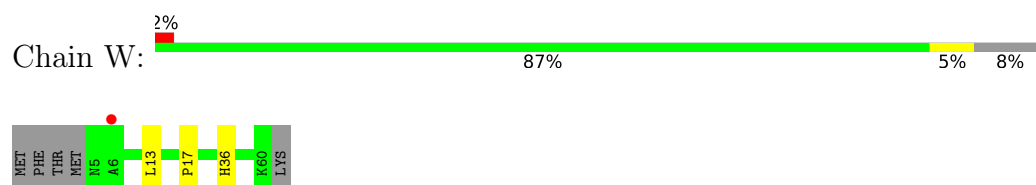
- Molecule 5: LH1 alpha polypeptide



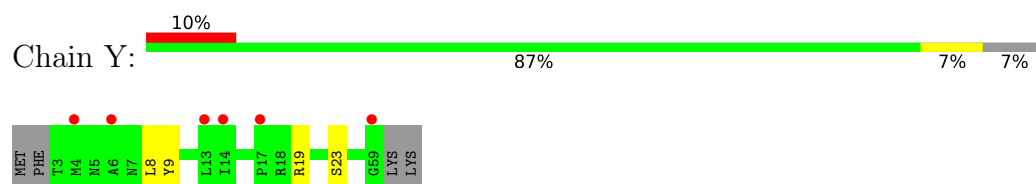
- Molecule 5: LH1 alpha polypeptide



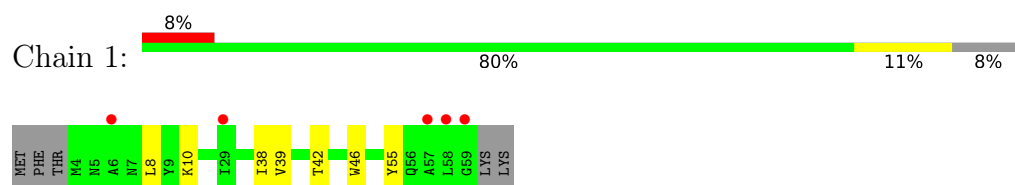
- Molecule 5: LH1 alpha polypeptide



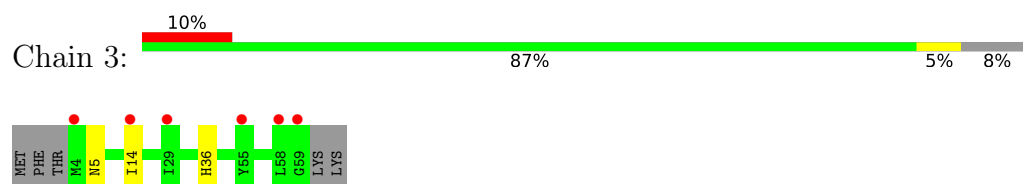
- Molecule 5: LH1 alpha polypeptide



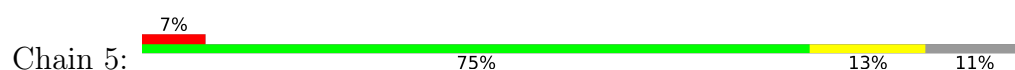
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

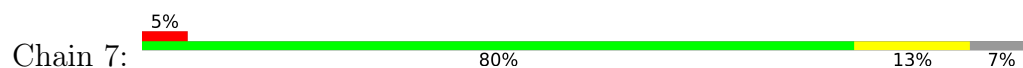


- Molecule 5: LH1 alpha polypeptide

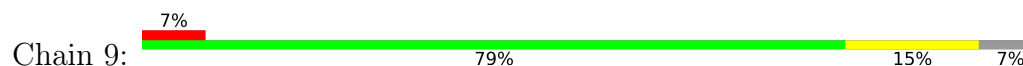




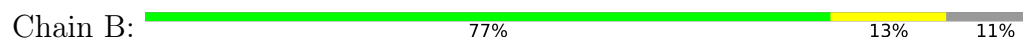
- Molecule 5: LH1 alpha polypeptide



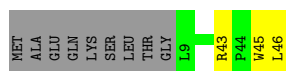
- Molecule 5: LH1 alpha polypeptide



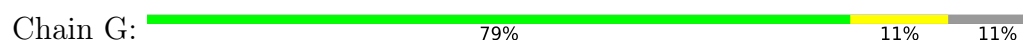
- Molecule 6: LH1 beta polypeptide



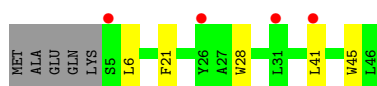
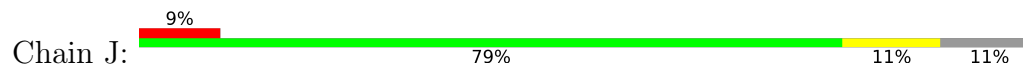
- Molecule 6: LH1 beta polypeptide



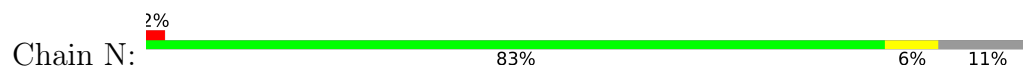
- Molecule 6: LH1 beta polypeptide

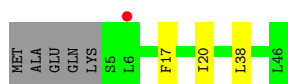


- Molecule 6: LH1 beta polypeptide

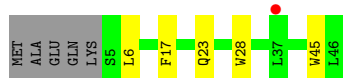
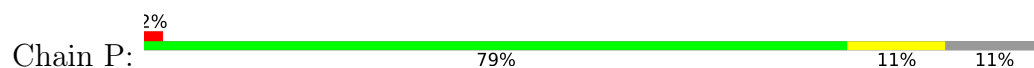


- Molecule 6: LH1 beta polypeptide

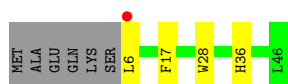
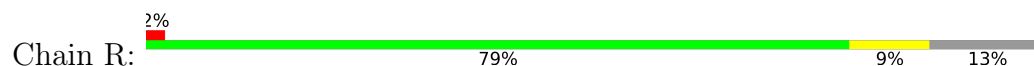




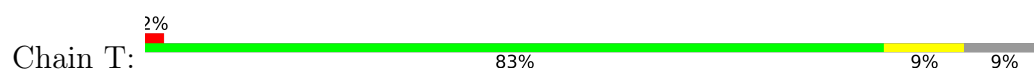
- Molecule 6: LH1 beta polypeptide



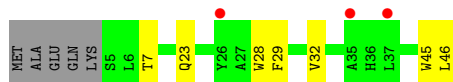
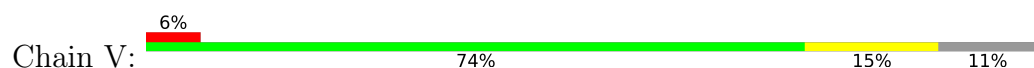
- Molecule 6: LH1 beta polypeptide



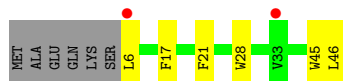
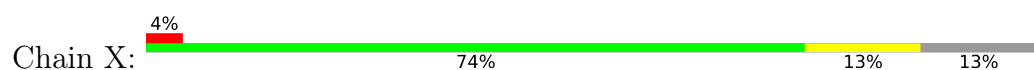
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



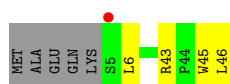
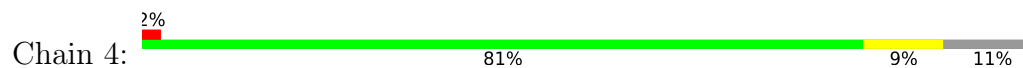
- Molecule 6: LH1 beta polypeptide



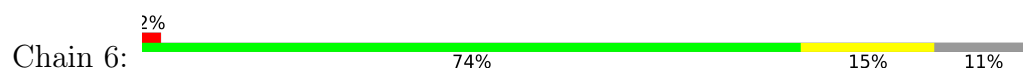
- Molecule 6: LH1 beta polypeptide



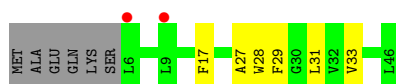
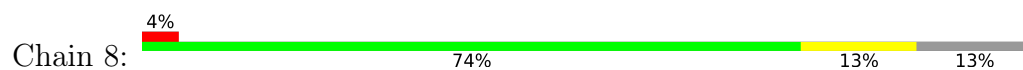
- Molecule 6: LH1 beta polypeptide



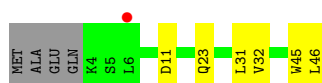
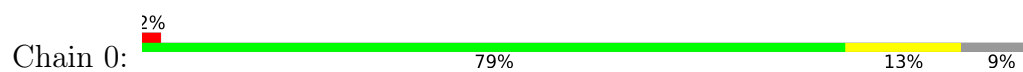
- Molecule 6: LH1 beta polypeptide



- 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 0.184 , 0.217	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 , 78.8	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	0.96	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

5.1 Standard geometry

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

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	0.36	0/2487	0.52	0/3396
2	L	0.46	0/2326	0.56	0/3177
3	M	0.44	0/2658	0.56	0/3637
4	H	0.39	0/2034	0.50	0/2773
5	1	0.62	0/459	0.44	0/628
5	3	0.21	0/467	0.39	0/638
5	5	0.23	0/443	0.43	0/607
5	7	0.28	0/466	0.46	0/638
5	9	0.24	0/466	0.47	0/638
5	A	0.24	0/443	0.44	0/607
5	D	0.21	0/457	0.39	0/626
5	F	0.36	0/457	0.44	0/626
5	I	0.19	0/472	0.34	0/646
5	K	0.22	0/466	0.38	0/638
5	O	0.27	0/467	0.43	0/638
5	Q	0.41	0/466	0.48	0/638
5	S	0.34	0/483	0.51	0/661
5	U	0.28	0/475	0.42	0/649
5	W	0.24	0/460	0.43	0/629
5	Y	0.20	0/466	0.38	0/638
6	0	0.21	0/373	0.34	0/506
6	2	0.15	0/358	0.33	0/487
6	4	0.17	0/364	0.32	0/495
6	6	0.22	0/364	0.34	0/495
6	8	0.23	0/358	0.37	0/487
6	B	0.17	0/364	0.27	0/495
6	E	0.14	0/339	0.26	0/461
6	G	0.11	0/364	0.27	0/495
6	J	0.12	0/364	0.25	0/495
6	N	0.15	0/364	0.28	0/495
6	P	0.23	0/364	0.33	0/495

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	R	0.27	0/358	0.39	0/487
6	T	0.29	0/373	0.37	0/506
6	V	0.20	0/364	0.34	0/495
6	X	0.21	0/358	0.31	0/487
6	Z	0.13	0/350	0.27	0/476
All	All	0.33	0/22697	0.46	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	11	0
2	L	2236	0	2201	21	0
3	M	2555	0	2530	24	0
4	H	1976	0	1977	21	0
5	1	450	0	475	6	0
5	3	455	0	484	4	0
5	5	434	0	460	7	0
5	7	457	0	482	9	0
5	9	457	0	482	8	0
5	A	434	0	460	6	0
5	D	445	0	471	8	0
5	F	445	0	471	8	0
5	I	460	0	487	11	0
5	K	457	0	482	7	0
5	O	455	0	484	4	0
5	Q	457	0	482	7	0
5	S	468	0	501	11	0
5	U	466	0	495	4	0
5	W	451	0	479	3	0
5	Y	457	0	480	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	0	360	0	352	5	0
6	2	345	0	334	19	0
6	4	351	0	339	3	0
6	6	351	0	339	7	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	2	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	10	0
13	3	132	0	144	8	0
13	5	132	0	144	12	0
13	7	127	0	131	7	0
13	9	66	0	72	4	0
13	A	132	0	144	7	0
13	D	132	0	144	6	0
13	F	132	0	144	5	0
13	I	132	0	144	8	0

Continued on next page...

Continued from previous page...

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	8	0
13	O	132	0	144	7	0
13	Q	132	0	144	11	0
13	S	132	0	144	10	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	6	0
14	L	65	0	74	5	0
14	M	65	0	74	7	0
15	7	33	0	39	10	0
15	L	104	0	128	10	0
15	M	18	0	15	4	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	M	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	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	44	0	60	3	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	2	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	1	1	0	0	0	0
24	3	1	0	0	0	0
24	5	1	0	0	0	0
24	7	1	0	0	0	0
24	9	1	0	0	0	0
24	A	1	0	0	0	0
24	D	1	0	0	0	0
24	F	1	0	0	0	0
24	I	1	0	0	0	0
24	K	1	0	0	0	0
24	O	1	0	0	0	0
24	Q	1	0	0	0	0
24	S	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	U	1	0	0	0	0
24	W	1	0	0	0	0
24	Y	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	3	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	0	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	385	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 385 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:104:CDL:OA4	1.88	1.20
6:2:9:LEU:HD21	6:2:14:ALA:N	1.54	1.19
22:S:104:CDL:C19	13:U:102:BCL:H51	1.83	1.08
5:S:19:ARG:NH1	22:S:104: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%)	21	13
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

Continued on next page...

Continued from previous page...

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%)	48	40

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%)	257 (99%)	3 (1%)	63	63
2	L	229/229 (100%)	227 (99%)	2 (1%)	70	73
3	M	258/261 (99%)	257 (100%)	1 (0%)	84	87
4	H	211/211 (100%)	210 (100%)	1 (0%)	81	84
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%)	50	47
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%)	49 (96%)	2 (4%)	28	21
5	I	53/56 (95%)	53 (100%)	0	100	100
5	K	52/56 (93%)	51 (98%)	1 (2%)	50	47
5	O	52/56 (93%)	51 (98%)	1 (2%)	50	47
5	Q	52/56 (93%)	52 (100%)	0	100	100
5	S	55/56 (98%)	53 (96%)	2 (4%)	31	23
5	U	53/56 (95%)	53 (100%)	0	100	100
5	W	51/56 (91%)	51 (100%)	0	100	100
5	Y	52/56 (93%)	51 (98%)	1 (2%)	50	47
6	0	36/39 (92%)	35 (97%)	1 (3%)	38	32
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

Continued on next page...

Continued from previous page...

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%)	33 (94%)	2 (6%)	18	11
6	N	35/39 (90%)	35 (100%)	0	100	100
6	P	35/39 (90%)	34 (97%)	1 (3%)	37	31
6	R	34/39 (87%)	34 (100%)	0	100	100
6	T	36/39 (92%)	35 (97%)	1 (3%)	38	32
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%)	2318 (99%)	20 (1%)	70	73

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	8	LEU
5	Y	8	LEU
6	O	31	LEU
5	9	53	VAL
4	H	237	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
5	I	7	ASN
5	K	7	ASN
5	1	7	ASN
5	Y	50	ASN
2	L	210	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 144 ligands modelled in this entry, 18 are monoatomic and 16 are unknown - 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
13	BCL	F	102	-	69,74,74	1.84	16 (23%)	79,115,115	2.17	24 (30%)
13	BCL	M	404	-	69,74,74	1.69	15 (21%)	79,115,115	1.94	18 (22%)
20	PEF	K	105	-	26,26,46	1.25	2 (7%)	29,31,51	1.47	4 (13%)
19	CRT	J	101	-	43,43,43	0.74	0	48,54,54	1.81	13 (27%)
9	GOL	H	301	-	5,5,5	0.91	0	5,5,5	1.02	0
15	UQ8	M	418	-	18,18,53	2.14	2 (11%)	24,25,67	1.50	5 (20%)
12	PGV	D	105	-	34,34,50	1.07	3 (8%)	37,40,56	1.22	5 (13%)
21	LDA	M	412	-	11,13,15	2.33	2 (18%)	12,15,17	0.48	0
13	BCL	3	103	-	69,74,74	1.83	15 (21%)	79,115,115	2.07	19 (24%)
12	PGV	M	415	-	36,36,50	1.08	2 (5%)	39,42,56	1.22	4 (10%)
20	PEF	U	105	-	4,4,46	2.62	2 (50%)	6,6,51	1.93	2 (33%)
20	PEF	U	106	-	4,4,46	2.74	2 (50%)	6,6,51	1.91	2 (33%)
21	LDA	I	105	-	13,15,15	2.18	2 (15%)	14,17,17	0.45	0
20	PEF	M	408	-	4,4,46	2.71	2 (50%)	6,6,51	1.89	2 (33%)
13	BCL	0	102	-	69,74,74	1.82	15 (21%)	79,115,115	2.13	22 (27%)
13	BCL	S	102	-	69,74,74	1.86	16 (23%)	79,115,115	2.18	23 (29%)
15	UQ8	L	309	-	18,18,53	2.14	2 (11%)	24,25,67	1.07	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEC	C	502	1	46,50,50	1.71	8 (17%)	58,82,82	1.61	12 (20%)
12	PGV	H	303	-	35,35,50	1.11	2 (5%)	38,41,56	1.29	4 (10%)
13	BCL	3	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.13	23 (29%)
22	CDL	Y	104	-	12,12,99	0.48	0	13,15,111	0.51	0
19	CRT	A	104	-	43,43,43	0.68	0	48,54,54	1.75	13 (27%)
10	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.13	0
18	MQ8	M	406	-	54,54,54	1.40	3 (5%)	67,69,69	1.48	15 (22%)
19	CRT	O	104	-	43,43,43	0.78	0	48,54,54	1.80	13 (27%)
20	PEF	3	104	-	4,4,46	2.71	2 (50%)	6,6,51	1.95	2 (33%)
22	CDL	S	104	-	61,61,99	1.11	5 (8%)	67,73,111	1.35	8 (11%)
13	BCL	O	103	-	69,74,74	1.78	14 (20%)	79,115,115	2.00	19 (24%)
15	UQ8	7	104	-	33,33,53	1.46	3 (9%)	42,43,67	2.12	16 (38%)
19	CRT	Z	101	-	43,43,43	0.65	0	48,54,54	2.00	14 (29%)
21	LDA	O	105	-	11,13,15	2.32	2 (18%)	12,15,17	0.47	0
19	CRT	6	101	-	43,43,43	0.72	0	48,54,54	1.77	11 (22%)
19	CRT	2	101	-	43,43,43	0.70	0	48,54,54	1.80	12 (25%)
20	PEF	W	104	-	4,4,46	2.73	2 (50%)	6,6,51	1.90	2 (33%)
12	PGV	M	414	-	45,45,50	1.06	2 (4%)	48,50,56	0.97	4 (8%)
19	CRT	Q	104	-	43,43,43	0.75	1 (2%)	48,54,54	1.83	8 (16%)
13	BCL	A	103	-	69,74,74	1.83	16 (23%)	79,115,115	2.08	20 (25%)
13	BCL	Z	102	-	69,74,74	1.80	15 (21%)	79,115,115	2.15	19 (24%)
21	LDA	V	102	-	13,15,15	2.15	2 (15%)	14,17,17	0.37	0
13	BCL	D	103	-	69,74,74	1.82	15 (21%)	79,115,115	2.13	18 (22%)
19	CRT	P	101	-	43,43,43	0.79	0	48,54,54	1.76	12 (25%)
13	BCL	5	103	-	69,74,74	1.79	16 (23%)	79,115,115	2.05	20 (25%)
22	CDL	Q	105	-	74,74,99	1.09	4 (5%)	80,86,111	1.15	8 (10%)
13	BCL	F	103	-	69,74,74	1.82	15 (21%)	79,115,115	2.10	19 (24%)
13	BCL	K	102	-	69,74,74	1.82	16 (23%)	79,115,115	2.19	23 (29%)
7	HEC	C	504	1	46,50,50	1.69	7 (15%)	58,82,82	1.70	11 (18%)
13	BCL	I	102	-	69,74,74	1.82	16 (23%)	79,115,115	2.20	22 (27%)
12	PGV	L	306	-	43,43,50	0.99	2 (4%)	46,49,56	1.14	3 (6%)
9	GOL	C	506	-	5,5,5	0.94	0	5,5,5	0.93	0
13	BCL	K	103	-	69,74,74	1.83	15 (21%)	79,115,115	2.14	19 (24%)
13	BCL	W	103	-	69,74,74	1.81	15 (21%)	79,115,115	2.04	18 (22%)
19	CRT	0	101	-	43,43,43	0.69	0	48,54,54	1.80	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CRT	M	407	-	43,43,43	0.87	0	48,54,54	1.77	11 (22%)
20	PEF	I	104	-	4,4,46	2.71	2 (50%)	6,6,51	1.88	2 (33%)
22	CDL	H	302	-	63,63,99	1.09	4 (6%)	69,75,111	1.35	9 (13%)
13	BCL	W	102	-	69,74,74	1.79	16 (23%)	79,115,115	2.35	24 (30%)
22	CDL	M	416	-	38,38,99	1.32	3 (7%)	43,49,111	1.20	3 (6%)
13	BCL	1	102	-	69,74,74	1.82	17 (24%)	79,115,115	2.21	23 (29%)
12	PGV	3	105	-	50,50,50	0.95	2 (4%)	53,56,56	0.93	3 (5%)
21	LDA	J	102	-	13,15,15	2.15	2 (15%)	14,17,17	0.44	0
10	SO4	M	413	-	4,4,4	0.24	0	6,6,6	0.11	0
11	LHG	C	508	-	7,8,48	0.34	0	6,7,54	0.43	0
13	BCL	U	103	-	69,74,74	1.85	15 (21%)	79,115,115	2.04	20 (25%)
19	CRT	1	104	-	43,43,43	0.70	0	48,54,54	1.71	11 (22%)
13	BCL	U	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.12	23 (29%)
23	LMT	F	104	-	36,36,36	0.49	0	47,47,47	1.46	9 (19%)
13	BCL	Q	102	-	69,74,74	1.78	15 (21%)	79,115,115	2.12	26 (32%)
10	SO4	L	304	-	4,4,4	0.23	0	6,6,6	0.06	0
22	CDL	H	304	-	78,78,99	1.04	4 (5%)	84,90,111	1.16	8 (9%)
13	BCL	I	103	-	69,74,74	1.82	16 (23%)	79,115,115	2.06	21 (26%)
13	BCL	7	103	-	69,74,74	1.77	16 (23%)	79,115,115	1.97	20 (25%)
13	BCL	M	402	-	69,74,74	1.80	16 (23%)	79,115,115	2.03	25 (31%)
12	PGV	A	105	-	32,32,50	1.18	2 (6%)	35,38,56	1.20	3 (8%)
13	BCL	7	102	-	64,69,74	1.85	16 (25%)	73,109,115	2.26	22 (30%)
22	CDL	D	104	-	39,39,99	1.45	4 (10%)	45,51,111	1.32	7 (15%)
13	BCL	5	102	-	69,74,74	1.75	16 (23%)	79,115,115	2.20	24 (30%)
13	BCL	O	102	-	69,74,74	1.78	16 (23%)	79,115,115	2.25	24 (30%)
13	BCL	D	102	-	69,74,74	1.80	16 (23%)	79,115,115	2.23	21 (26%)
13	BCL	Y	102	-	69,74,74	1.80	16 (23%)	79,115,115	2.28	25 (31%)
20	PEF	M	419	-	46,46,46	0.96	2 (4%)	49,51,51	1.08	3 (6%)
20	PEF	M	409	-	4,4,46	1.90	2 (50%)	6,6,51	1.22	1 (16%)
14	BPH	M	405	-	59,70,70	2.51	13 (22%)	59,101,101	2.31	22 (37%)
13	BCL	S	103	-	69,74,74	1.78	15 (21%)	79,115,115	2.04	20 (25%)
19	CRT	9	102	-	43,43,43	0.72	0	48,54,54	1.88	15 (31%)
20	PEF	5	104	-	4,4,46	2.72	2 (50%)	6,6,51	1.86	2 (33%)
20	PEF	M	410	-	4,4,46	2.74	2 (50%)	6,6,51	1.91	2 (33%)
19	CRT	V	101	-	43,43,43	0.71	0	48,54,54	1.86	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	K	104	-	85,85,99	1.00	4 (4%)	91,97,111	1.19	9 (9%)
22	CDL	Y	103	-	39,39,99	1.48	4 (10%)	45,51,111	1.22	4 (8%)
20	PEF	1	105	-	4,4,46	2.80	2 (50%)	6,6,51	1.88	2 (33%)
15	UQ8	L	303	-	33,33,53	1.67	2 (6%)	42,43,67	1.52	7 (16%)
19	CRT	U	104	-	43,43,43	0.71	0	48,54,54	1.95	14 (29%)
15	UQ8	L	308	-	53,53,53	1.23	2 (3%)	66,67,67	1.69	20 (30%)
14	BPH	L	302	-	59,70,70	2.46	14 (23%)	59,101,101	2.14	18 (30%)
20	PEF	M	411	-	4,4,46	2.46	1 (25%)	6,6,51	1.45	1 (16%)
13	BCL	L	301	-	69,74,74	1.74	14 (20%)	79,115,115	1.79	18 (22%)
7	HEC	C	501	1	46,50,50	1.68	9 (19%)	58,82,82	1.64	13 (22%)
7	HEC	C	503	1	46,50,50	1.68	10 (21%)	58,82,82	1.77	12 (20%)
12	PGV	1	106	-	30,30,50	1.21	2 (6%)	33,36,56	1.20	4 (12%)
13	BCL	9	104	-	69,74,74	1.78	15 (21%)	79,115,115	2.20	21 (26%)
23	LMT	M	420	-	36,36,36	0.47	1 (2%)	47,47,47	0.94	3 (6%)
12	PGV	C	509	-	20,20,50	1.45	3 (15%)	22,22,56	1.53	3 (13%)
19	CRT	G	101	-	43,43,43	0.69	0	48,54,54	1.83	13 (27%)
12	PGV	L	305	-	42,42,50	1.04	2 (4%)	45,48,56	1.27	3 (6%)
13	BCL	A	101	-	69,74,74	1.81	16 (23%)	79,115,115	2.16	24 (30%)
19	CRT	N	101	-	43,43,43	0.67	0	48,54,54	1.99	14 (29%)
13	BCL	Q	103	-	69,74,74	1.83	15 (21%)	79,115,115	2.04	19 (24%)
19	CRT	9	103	-	43,43,43	0.70	0	48,54,54	1.82	11 (22%)
13	BCL	1	103	-	69,74,74	1.82	15 (21%)	79,115,115	2.19	21 (26%)
13	BCL	M	403	-	69,74,74	1.78	14 (20%)	79,115,115	2.09	23 (29%)

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
13	BCL	F	102	-	-	13/41/137/137	-
13	BCL	M	404	-	-	4/41/137/137	-
20	PEF	K	105	-	-	3/30/30/50	-
19	CRT	J	101	-	-	1/51/51/51	-
9	GOL	H	301	-	-	0/4/4/4	-
15	UQ8	M	418	-	-	1/9/33/75	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGV	D	105	-	-	11/39/39/55	-
21	LDA	M	412	-	-	5/11/11/13	-
13	BCL	3	103	-	-	17/41/137/137	-
12	PGV	M	415	-	-	16/41/41/55	-
21	LDA	I	105	-	-	4/13/13/13	-
13	BCL	0	102	-	-	7/41/137/137	-
13	BCL	S	102	-	-	8/41/137/137	-
15	UQ8	L	309	-	-	1/9/33/75	0/1/1/1
7	HEC	C	502	1	-	8/14/54/54	-
12	PGV	H	303	-	-	16/40/40/55	-
13	BCL	3	102	-	-	18/41/137/137	-
22	CDL	Y	104	-	-	7/13/13/110	-
19	CRT	A	104	-	-	0/51/51/51	-
18	MQ8	M	406	-	-	2/47/67/67	0/2/2/2
19	CRT	O	104	-	-	4/51/51/51	-
22	CDL	S	104	-	-	28/71/71/110	-
13	BCL	O	103	-	-	16/41/137/137	-
15	UQ8	7	104	-	-	9/27/51/75	0/1/1/1
19	CRT	Z	101	-	-	0/51/51/51	-
21	LDA	O	105	-	-	8/11/11/13	-
19	CRT	6	101	-	-	0/51/51/51	-
19	CRT	2	101	-	-	2/51/51/51	-
12	PGV	M	414	-	-	16/47/47/55	-
19	CRT	Q	104	-	-	3/51/51/51	-
13	BCL	A	103	-	-	10/41/137/137	-
13	BCL	Z	102	-	-	15/41/137/137	-
21	LDA	V	102	-	-	5/13/13/13	-
13	BCL	D	103	-	-	7/41/137/137	-
19	CRT	P	101	-	-	0/51/51/51	-
13	BCL	5	103	-	-	13/41/137/137	-
22	CDL	Q	105	-	-	37/85/85/110	-
13	BCL	F	103	-	-	11/41/137/137	-
13	BCL	K	102	-	-	13/41/137/137	-
7	HEC	C	504	1	-	7/14/54/54	-
13	BCL	I	102	-	-	7/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGV	L	306	-	-	17/48/48/55	-
9	GOL	C	506	-	-	2/4/4/4	-
13	BCL	K	103	-	-	14/41/137/137	-
13	BCL	W	103	-	-	8/41/137/137	-
19	CRT	O	101	-	-	5/51/51/51	-
19	CRT	M	407	-	-	6/51/51/51	-
22	CDL	H	302	-	-	23/73/73/110	-
13	BCL	W	102	-	-	10/41/137/137	-
22	CDL	M	416	-	-	12/48/48/110	-
13	BCL	1	102	-	-	15/41/137/137	-
12	PGV	3	105	-	-	16/55/55/55	-
21	LDA	J	102	-	-	3/13/13/13	-
11	LHG	C	508	-	-	1/6/6/53	-
13	BCL	U	103	-	-	14/41/137/137	-
19	CRT	1	104	-	-	1/51/51/51	-
13	BCL	U	102	-	-	3/41/137/137	-
23	LMT	F	104	-	-	9/21/61/61	0/2/2/2
13	BCL	Q	102	-	-	15/41/137/137	-
22	CDL	H	304	-	-	20/89/89/110	-
13	BCL	I	103	-	-	10/41/137/137	-
13	BCL	7	103	-	-	13/41/137/137	-
13	BCL	M	402	-	-	3/41/137/137	-
12	PGV	A	105	-	-	13/37/37/55	-
13	BCL	7	102	-	-	6/35/131/137	-
22	CDL	D	104	-	-	17/50/50/110	-
13	BCL	5	102	-	-	11/41/137/137	-
13	BCL	O	102	-	-	5/41/137/137	-
13	BCL	D	102	-	-	10/41/137/137	-
13	BCL	Y	102	-	-	11/41/137/137	-
20	PEF	M	419	-	-	19/50/50/50	-
14	BPH	M	405	-	-	7/37/105/105	0/5/6/6
13	BCL	S	103	-	-	17/41/137/137	-
19	CRT	9	102	-	-	5/51/51/51	-
19	CRT	V	101	-	-	6/51/51/51	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	K	104	-	-	30/96/96/110	-
22	CDL	Y	103	-	-	24/50/50/110	-
15	UQ8	L	303	-	-	3/27/51/75	0/1/1/1
19	CRT	U	104	-	-	3/51/51/51	-
15	UQ8	L	308	-	-	10/51/75/75	0/1/1/1
14	BPH	L	302	-	-	6/37/105/105	0/5/6/6
13	BCL	L	301	-	-	1/41/137/137	-
7	HEC	C	501	1	-	6/14/54/54	-
7	HEC	C	503	1	-	4/14/54/54	-
12	PGV	1	106	-	-	8/35/35/55	-
13	BCL	9	104	-	-	16/41/137/137	-
23	LMT	M	420	-	-	6/21/61/61	0/2/2/2
12	PGV	C	509	-	-	4/21/21/55	-
19	CRT	G	101	-	-	2/51/51/51	-
12	PGV	L	305	-	-	13/47/47/55	-
13	BCL	A	101	-	-	14/41/137/137	-
19	CRT	N	101	-	-	0/51/51/51	-
13	BCL	Q	103	-	-	9/41/137/137	-
19	CRT	9	103	-	-	4/51/51/51	-
13	BCL	1	103	-	-	12/41/137/137	-
13	BCL	M	403	-	-	13/41/137/137	-

The worst 5 of 724 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	405	BPH	C1B-C2B	9.32	1.49	1.39
14	M	405	BPH	C1D-C2D	9.00	1.49	1.39
14	L	302	BPH	C1B-C2B	8.87	1.49	1.39
15	L	303	UQ8	C6-C1	8.19	1.49	1.35
15	M	418	UQ8	C6-C1	7.90	1.49	1.35

The worst 5 of 1261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	101	CRT	C37-C36-C35	-7.89	113.83	124.91
13	W	102	BCL	O2D-CGD-CBD	7.67	124.63	111.23
13	M	403	BCL	C4A-NA-C1A	-7.63	103.20	106.68
19	U	104	CRT	C37-C36-C35	-7.62	114.20	124.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	101	BCL	C4A-NA-C1A	-7.50	103.26	106.68

There are no chirality outliers.

5 of 888 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	501	HEC	C2B-C3B-CAB-CBB
7	C	501	HEC	C4B-C3B-CAB-CBB
7	C	501	HEC	C2C-C3C-CAC-CBC
7	C	501	HEC	C4C-C3C-CAC-CBC
7	C	502	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

90 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	102	BCL	2	0
13	M	404	BCL	1	0
20	K	105	PEF	1	0
19	J	101	CRT	3	0
9	H	301	GOL	1	0
15	M	418	UQ8	4	0
12	D	105	PGV	2	0
21	M	412	LDA	1	0
13	3	103	BCL	4	0
12	M	415	PGV	3	0
21	I	105	LDA	6	0
13	0	102	BCL	8	0
13	S	102	BCL	4	0
15	L	309	UQ8	1	0
12	H	303	PGV	1	0
13	3	102	BCL	4	0
19	A	104	CRT	3	0
18	M	406	MQ8	5	0
19	O	104	CRT	2	0
22	S	104	CDL	10	0
13	O	103	BCL	4	0
15	7	104	UQ8	10	0
19	Z	101	CRT	2	0
21	O	105	LDA	1	0
19	6	101	CRT	2	0

Continued on next page...

Continued from previous page...

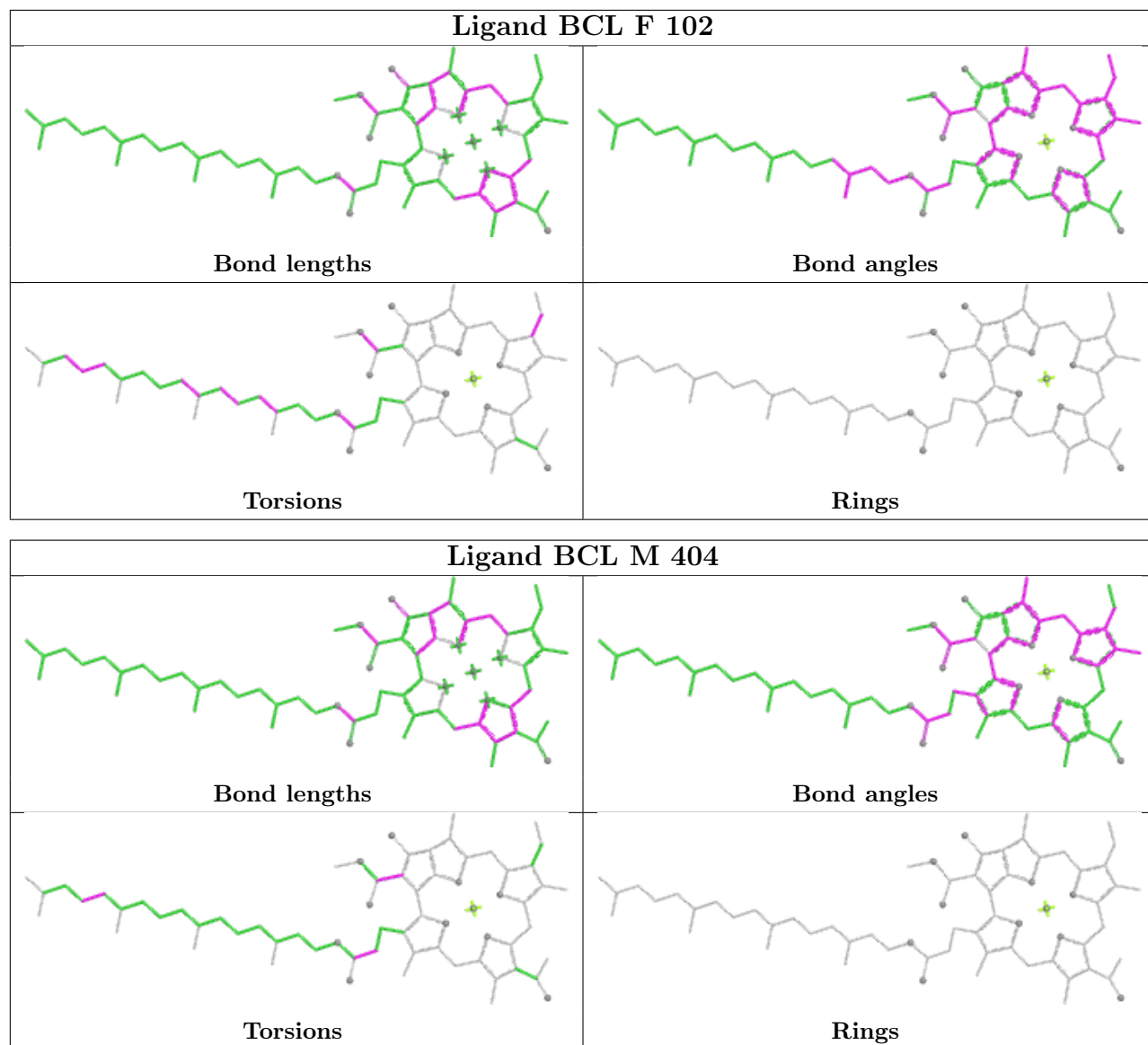
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	101	CRT	6	0
12	M	414	PGV	4	0
19	Q	104	CRT	2	0
13	A	103	BCL	3	0
13	Z	102	BCL	6	0
13	D	103	BCL	4	0
19	P	101	CRT	2	0
13	5	103	BCL	3	0
22	Q	105	CDL	3	0
13	F	103	BCL	3	0
13	K	102	BCL	2	0
7	C	504	HEC	2	0
13	I	102	BCL	4	0
12	L	306	PGV	4	0
13	K	103	BCL	3	0
13	W	103	BCL	2	0
19	0	101	CRT	2	0
19	M	407	CRT	5	0
20	I	104	PEF	1	0
22	H	302	CDL	3	0
13	W	102	BCL	5	0
22	M	416	CDL	1	0
13	1	102	BCL	4	0
12	3	105	PGV	3	0
21	J	102	LDA	1	0
13	U	103	BCL	4	0
19	1	104	CRT	3	0
13	U	102	BCL	8	0
23	F	104	LMT	5	0
13	Q	102	BCL	6	0
22	H	304	CDL	3	0
13	I	103	BCL	4	0
13	7	103	BCL	4	0
13	M	402	BCL	5	0
12	A	105	PGV	5	0
13	7	102	BCL	3	0
22	D	104	CDL	2	0
13	5	102	BCL	9	0
13	O	102	BCL	3	0
13	D	102	BCL	2	0
13	Y	102	BCL	5	0
20	M	419	PEF	3	0

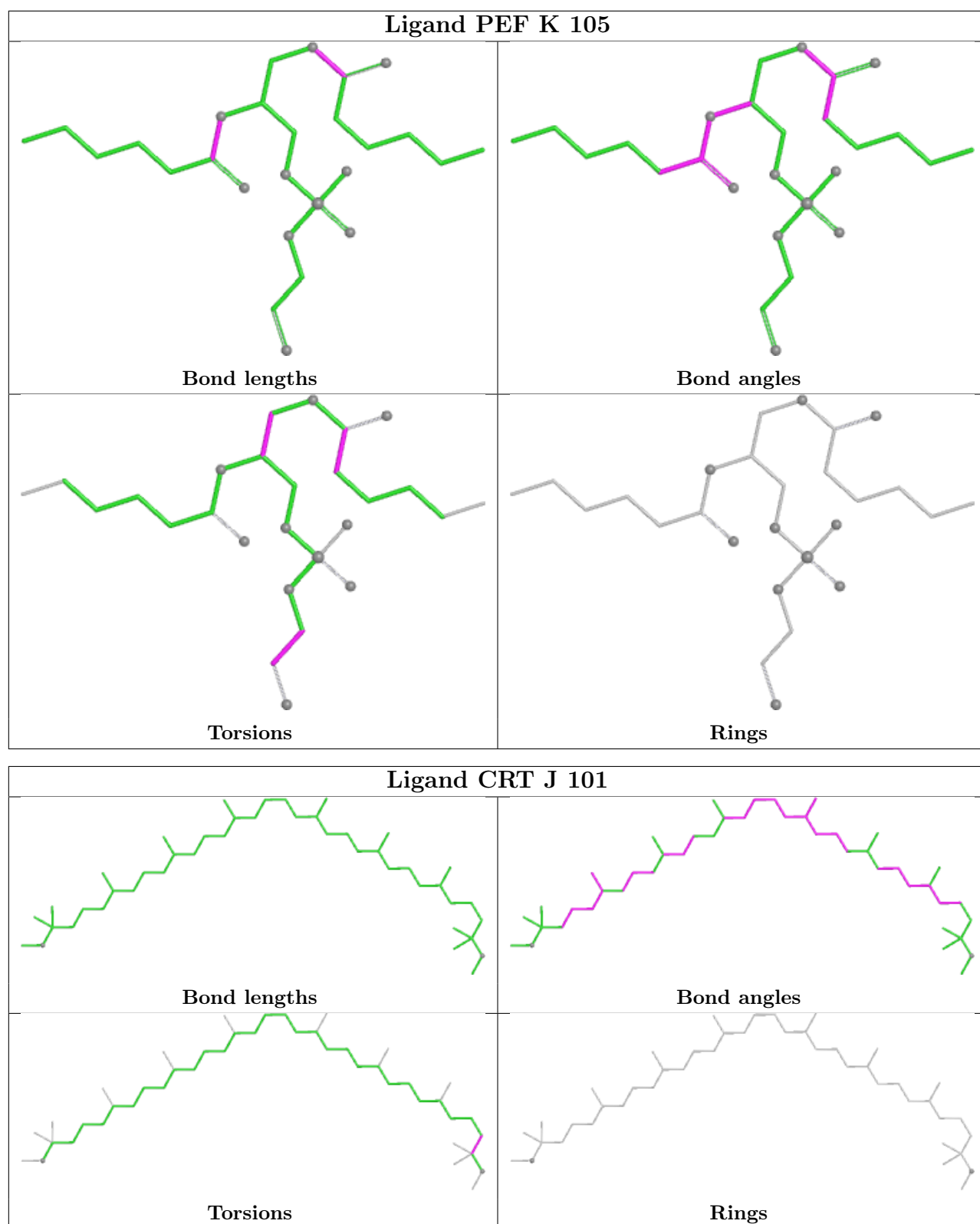
Continued on next page...

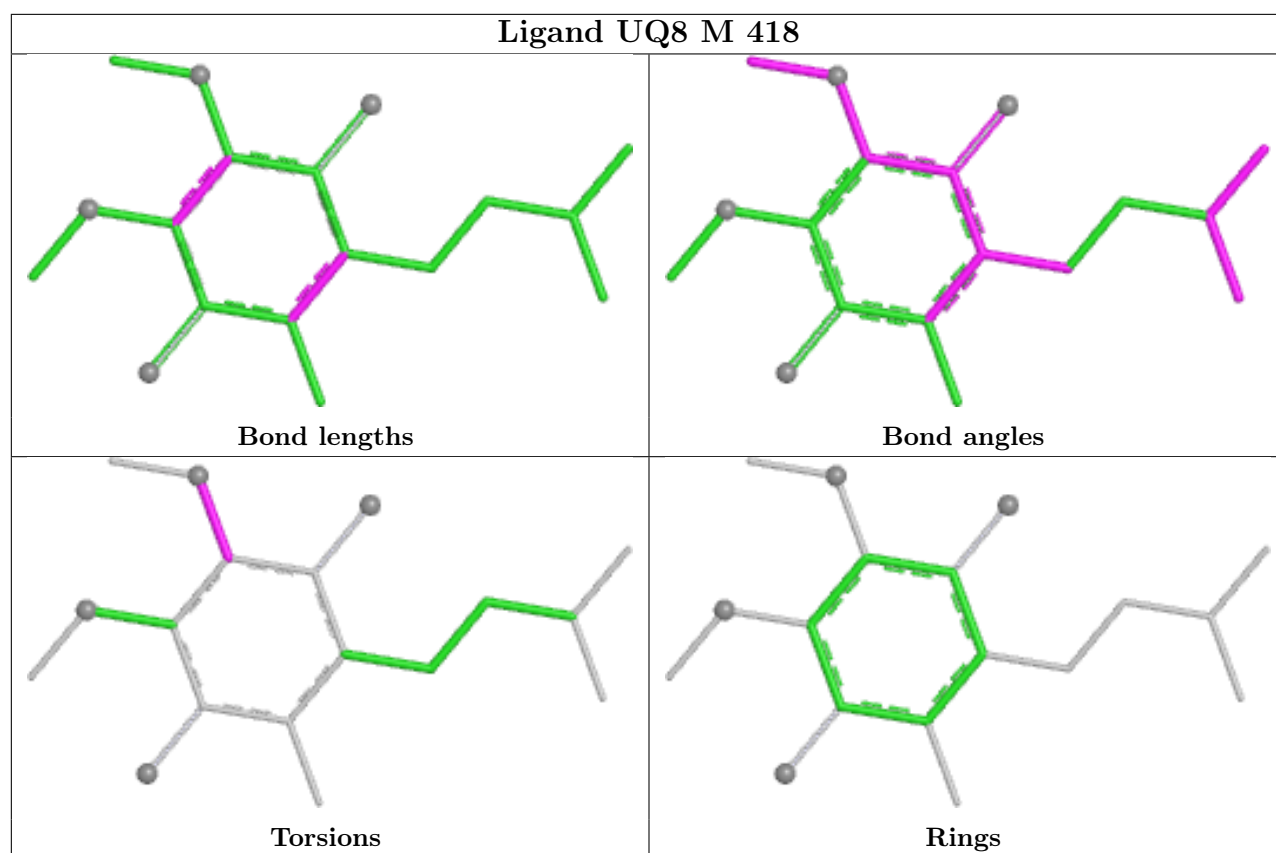
Continued from previous page...

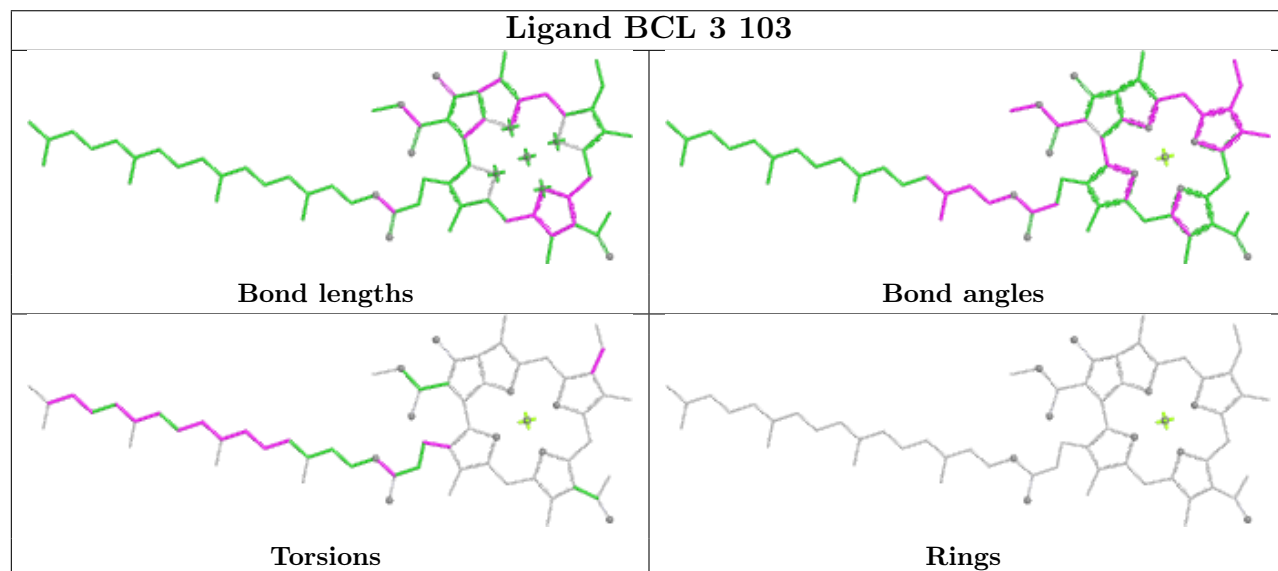
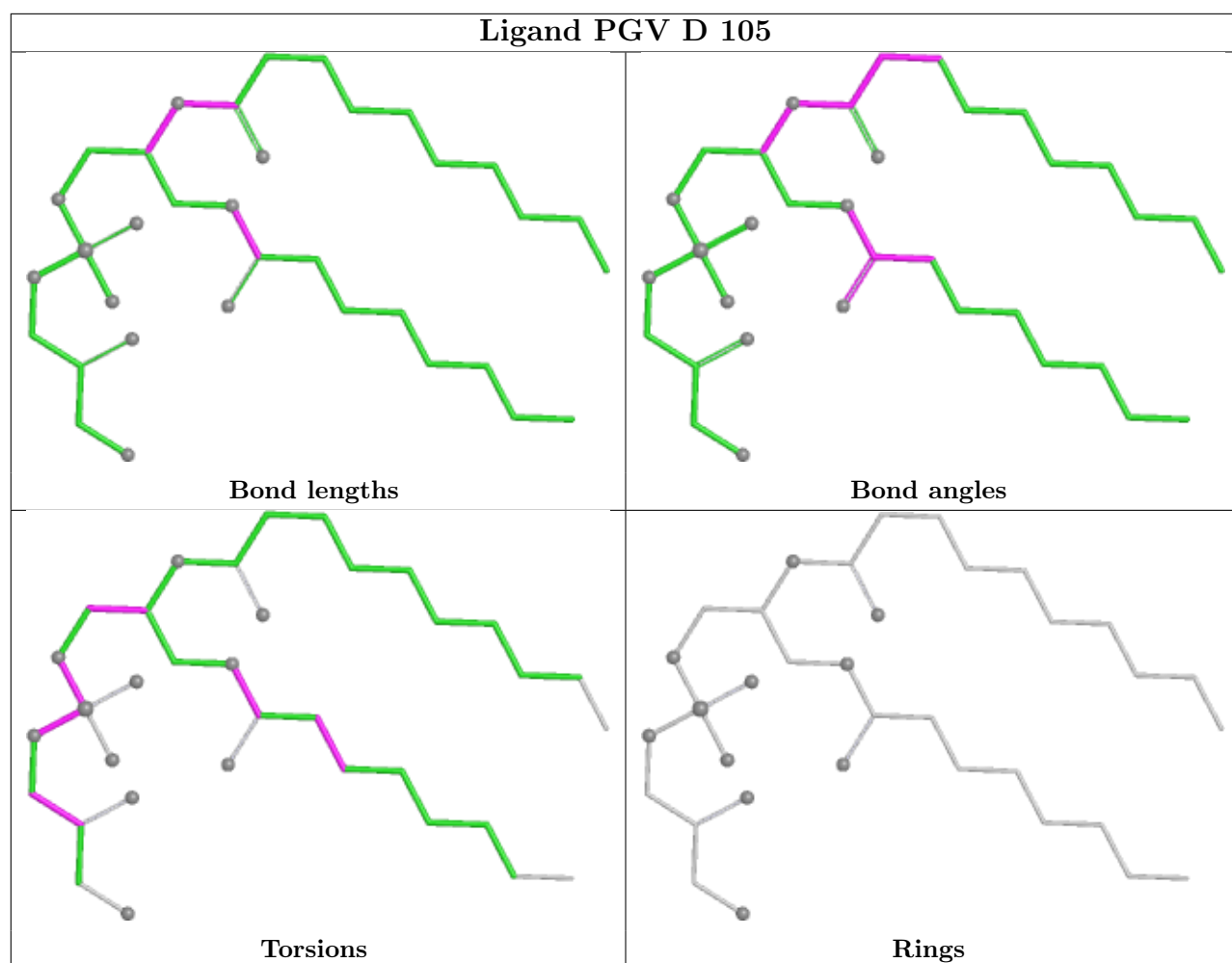
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	405	BPH	7	0
13	S	103	BCL	6	0
19	9	102	CRT	4	0
20	5	104	PEF	1	0
19	V	101	CRT	1	0
22	K	104	CDL	4	0
22	Y	103	CDL	1	0
15	L	303	UQ8	2	0
19	U	104	CRT	2	0
15	L	308	UQ8	7	0
14	L	302	BPH	5	0
13	L	301	BCL	4	0
7	C	503	HEC	1	0
13	9	104	BCL	4	0
23	M	420	LMT	3	0
19	G	101	CRT	5	0
12	L	305	PGV	4	0
13	A	101	BCL	4	0
19	N	101	CRT	3	0
13	Q	103	BCL	5	0
19	9	103	CRT	2	0
13	1	103	BCL	6	0
13	M	403	BCL	2	0

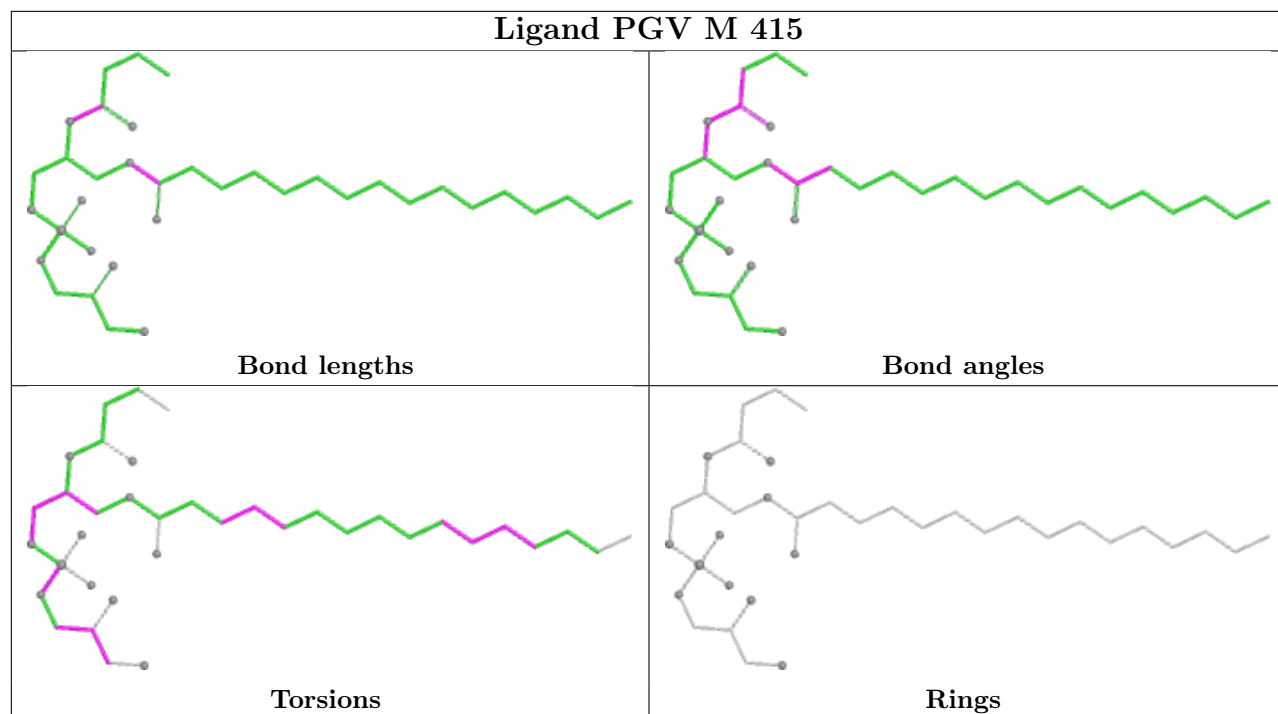
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

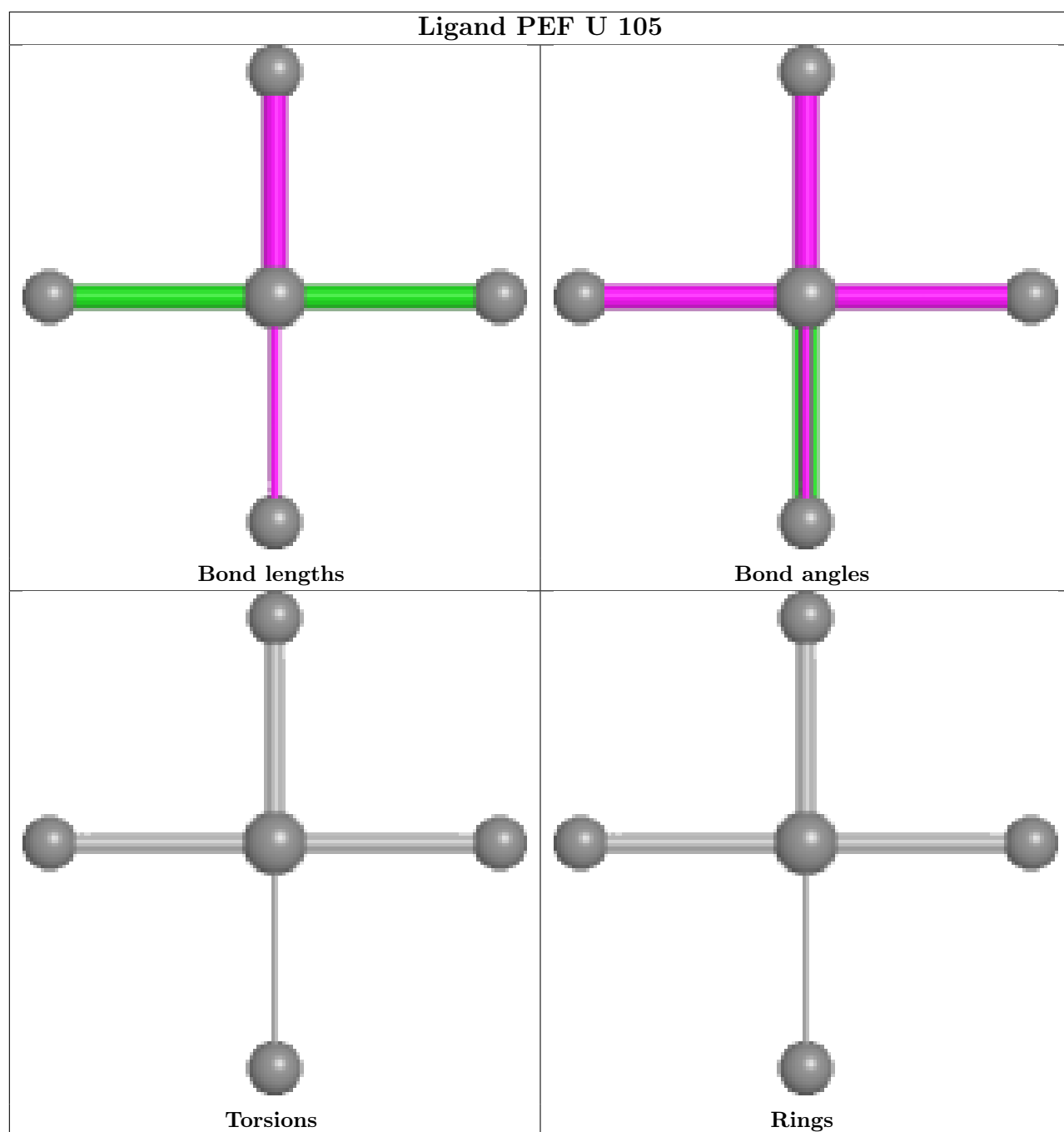


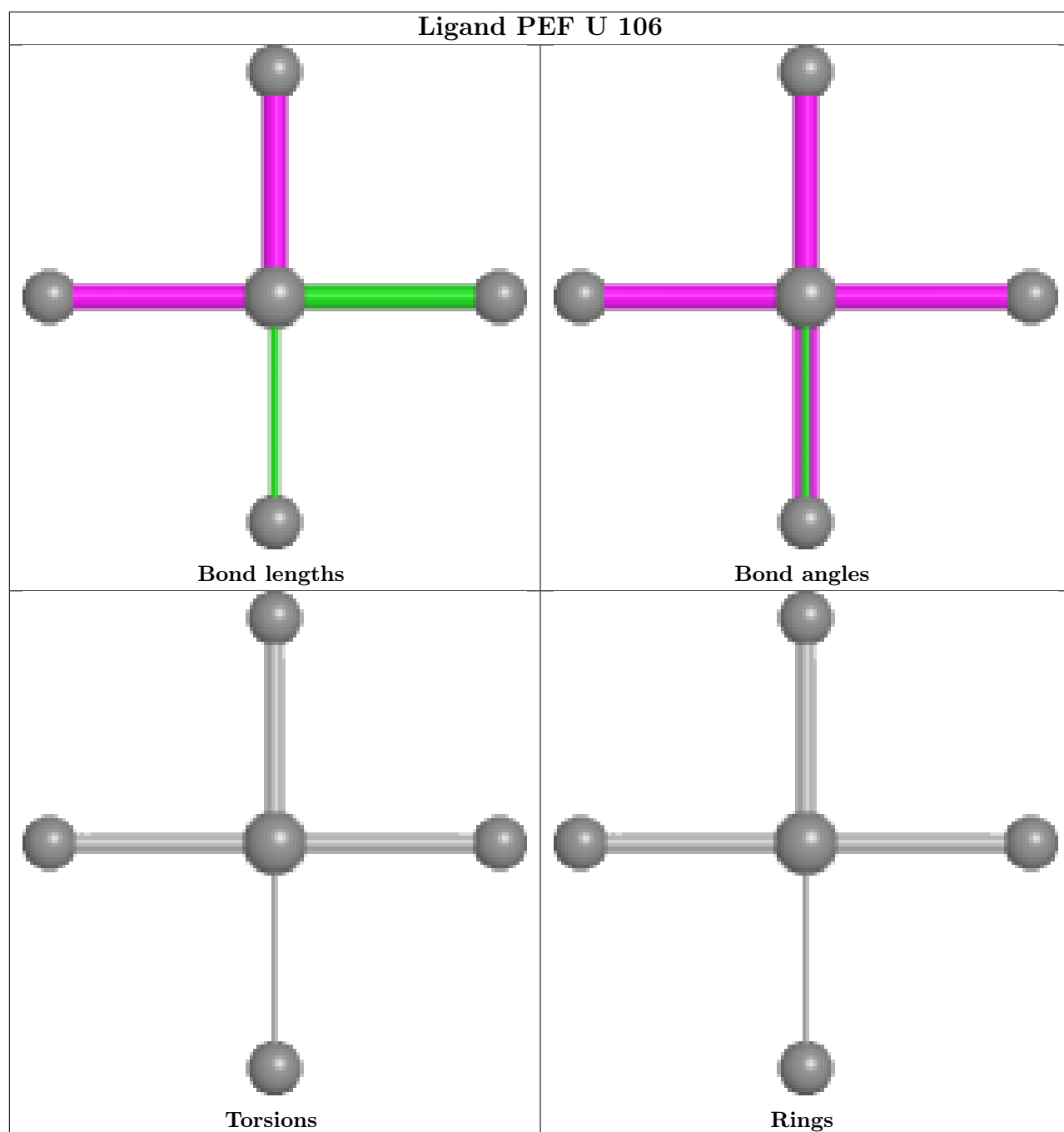


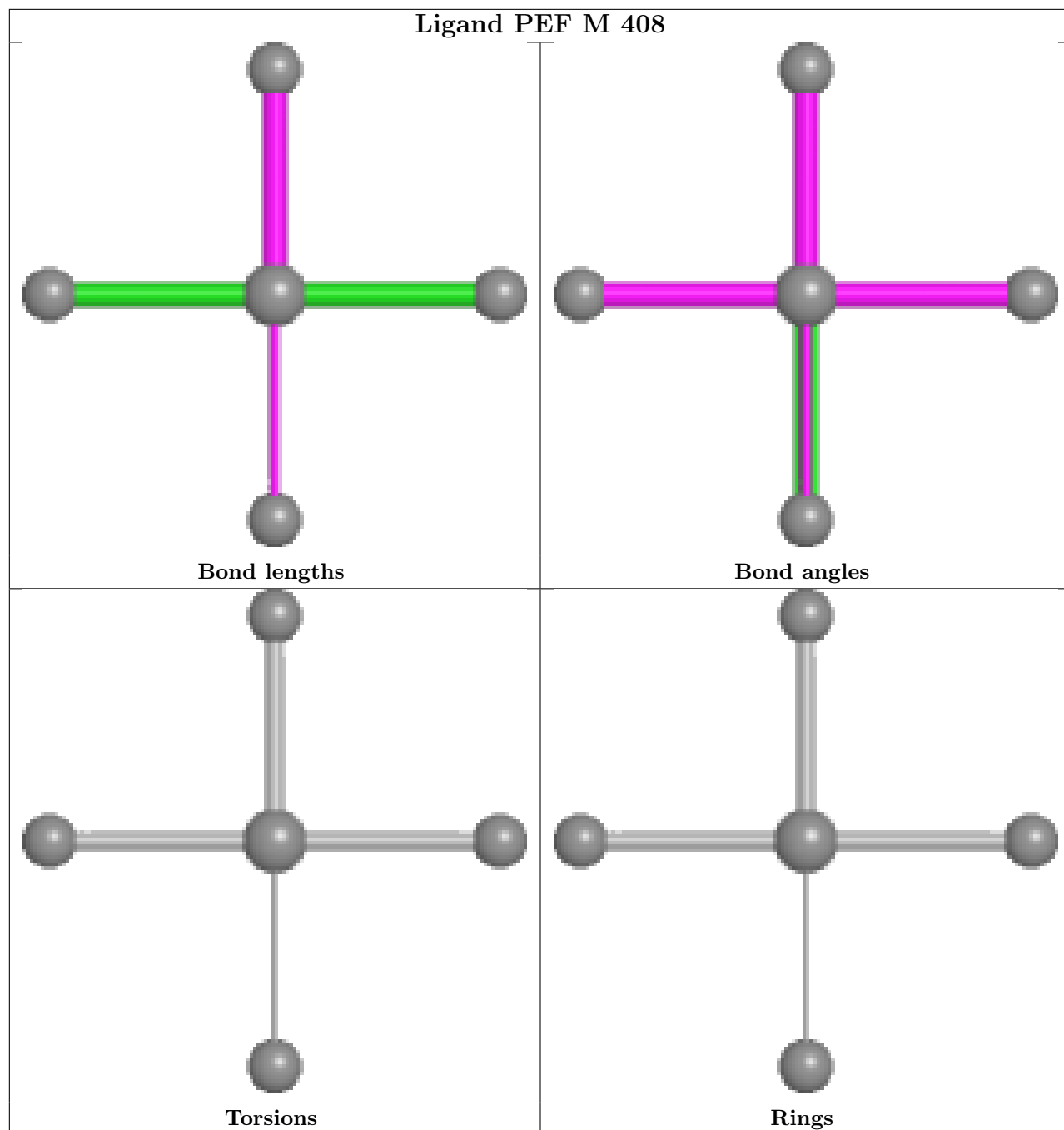


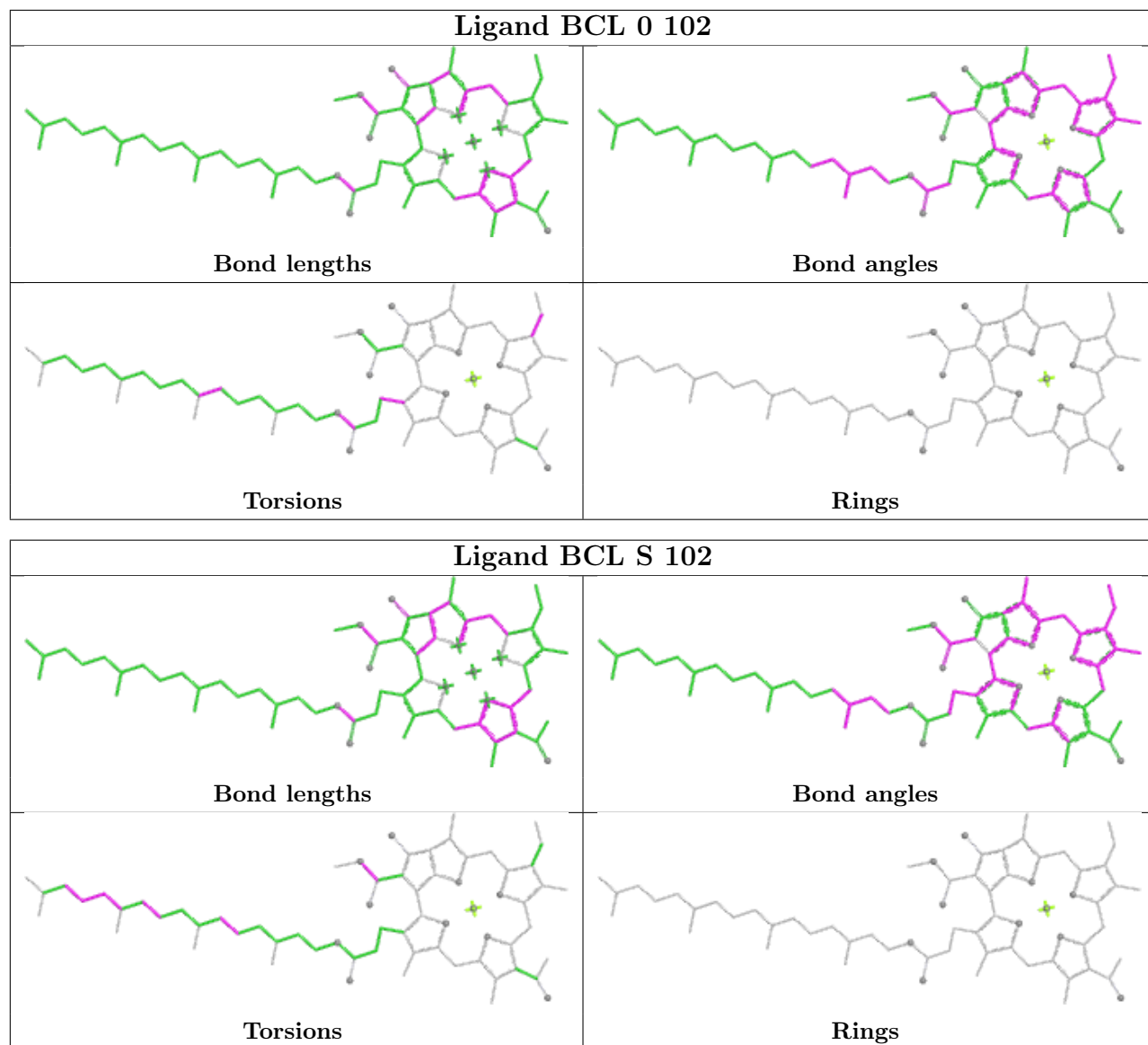


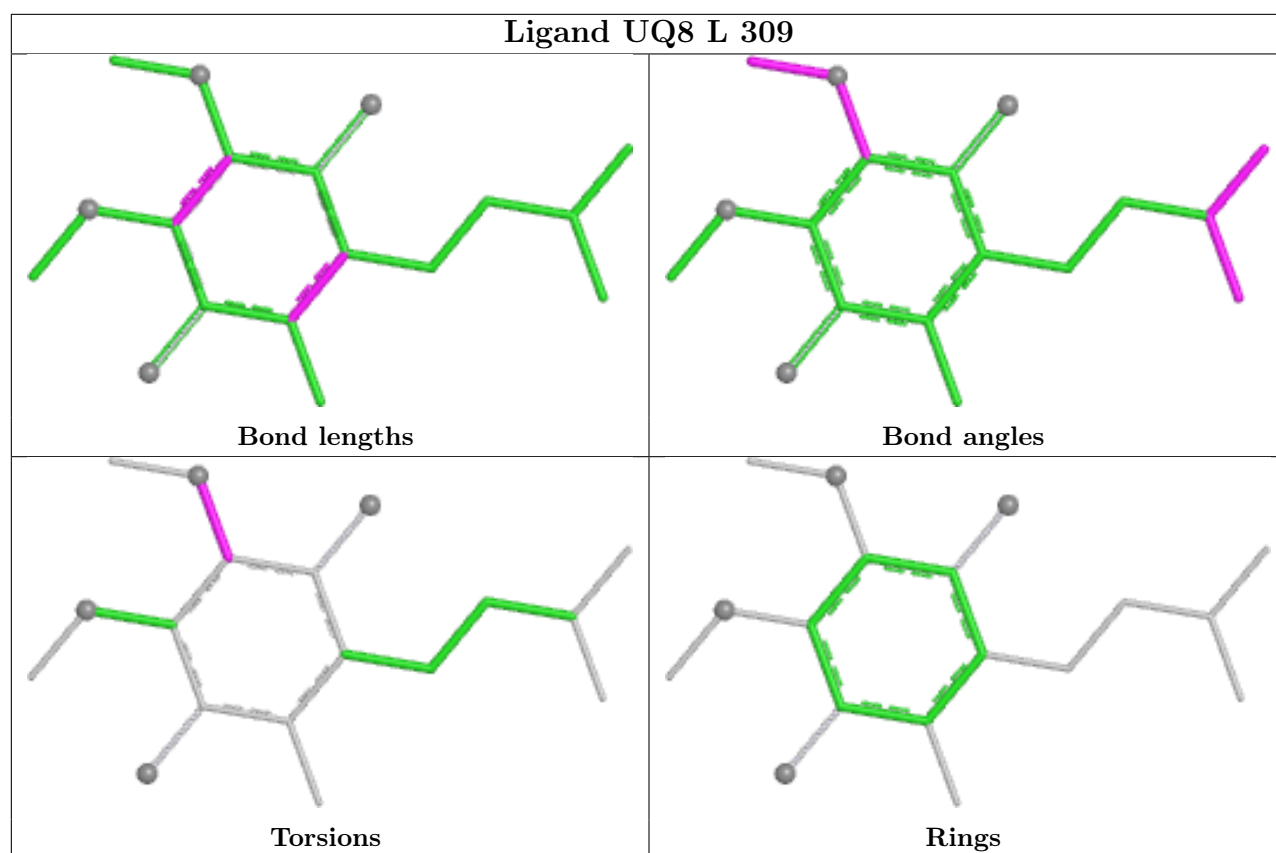




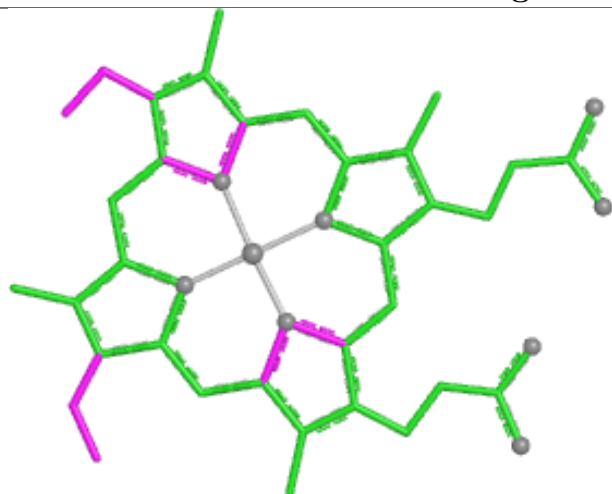




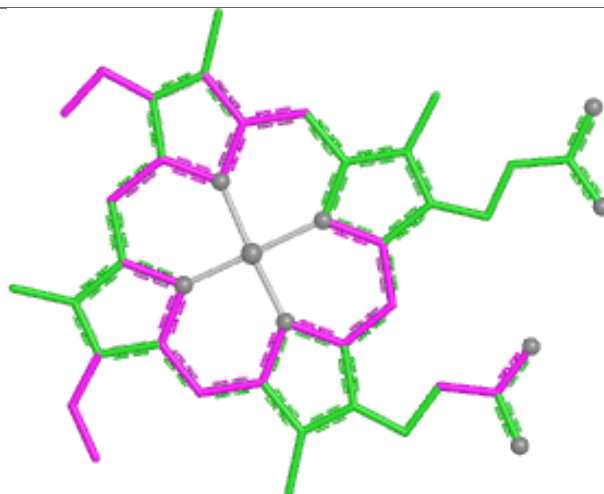




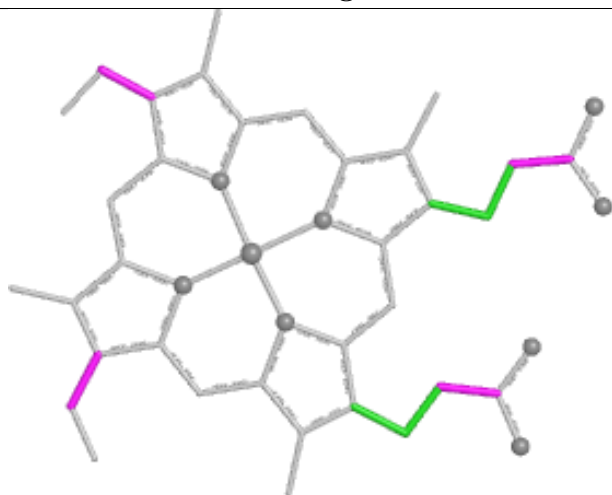
Ligand HEC C 502



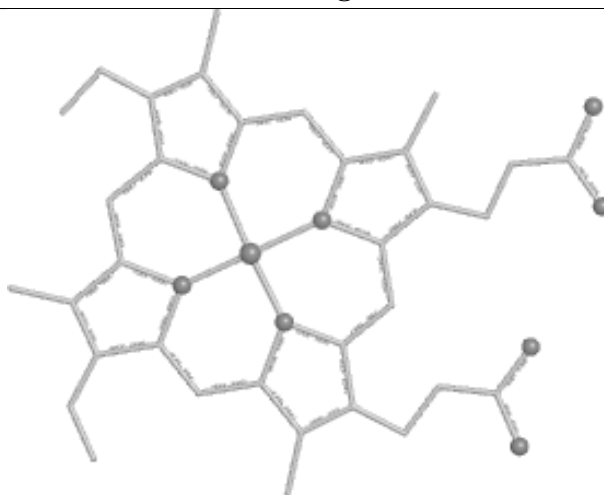
Bond lengths



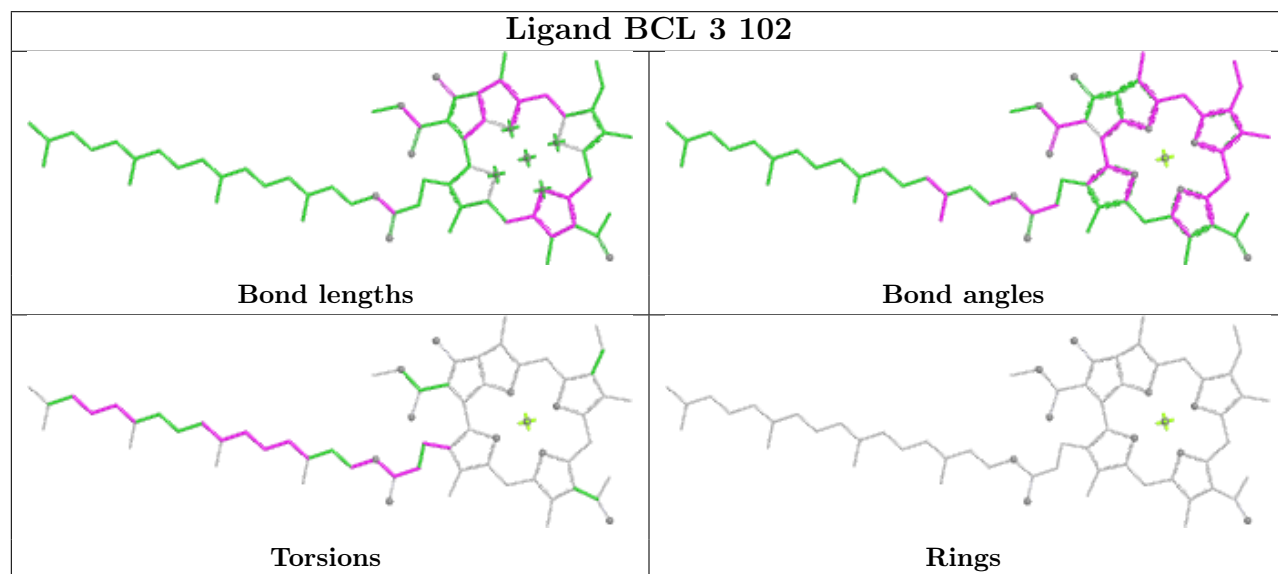
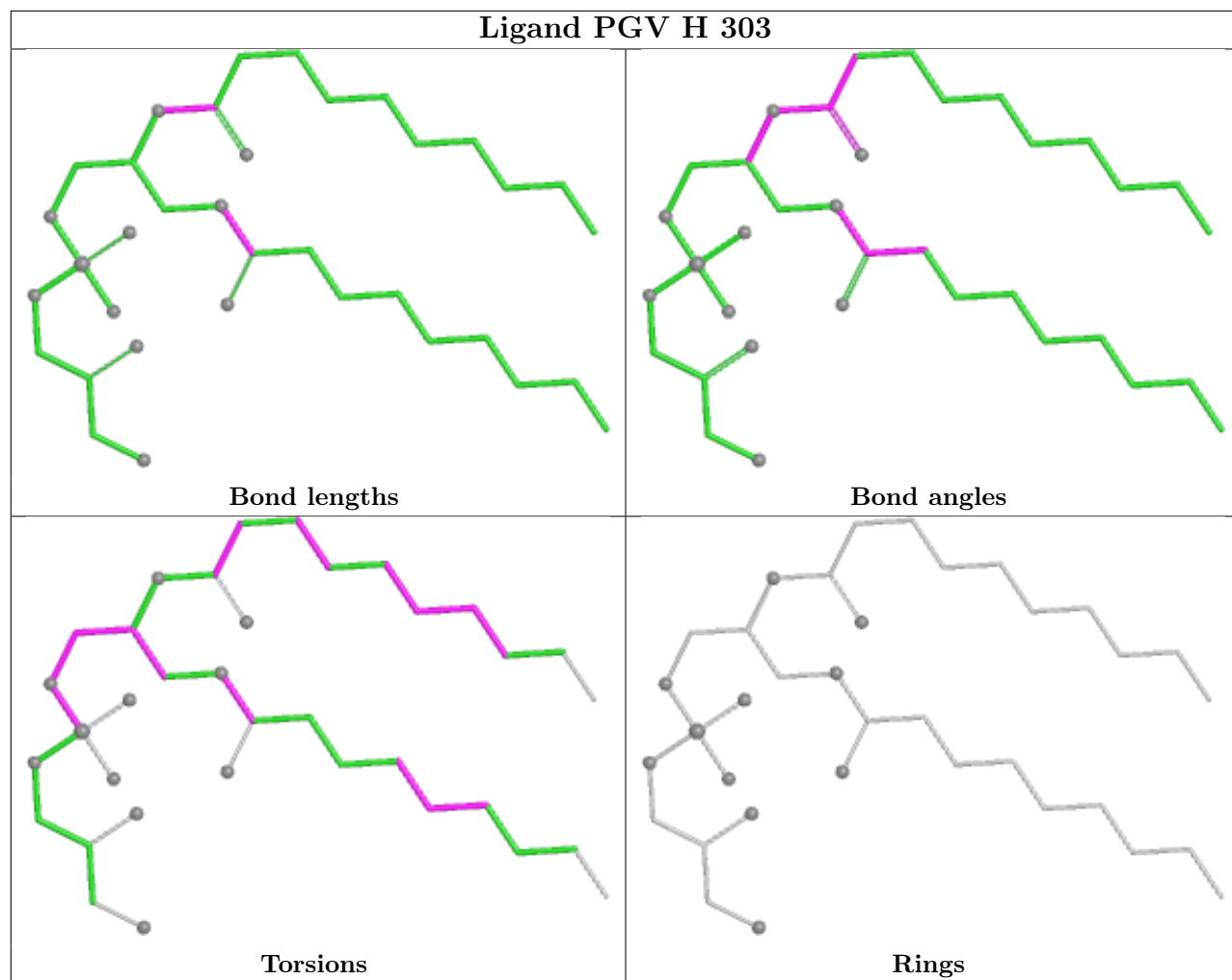
Bond angles

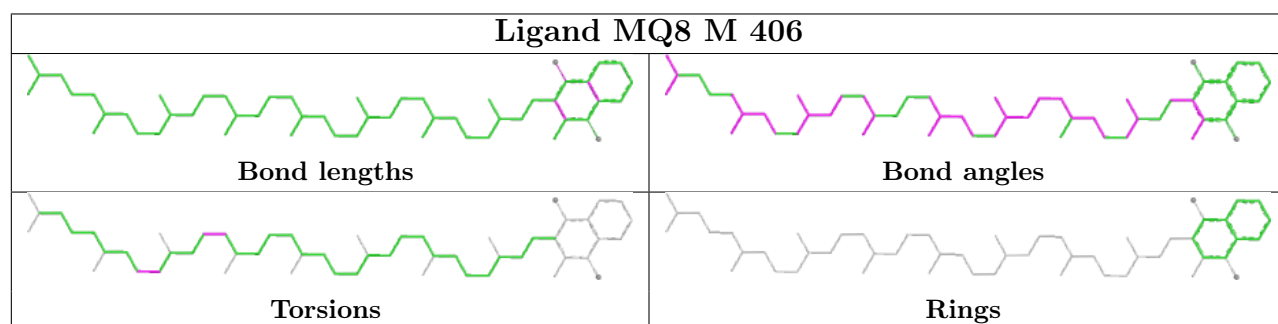
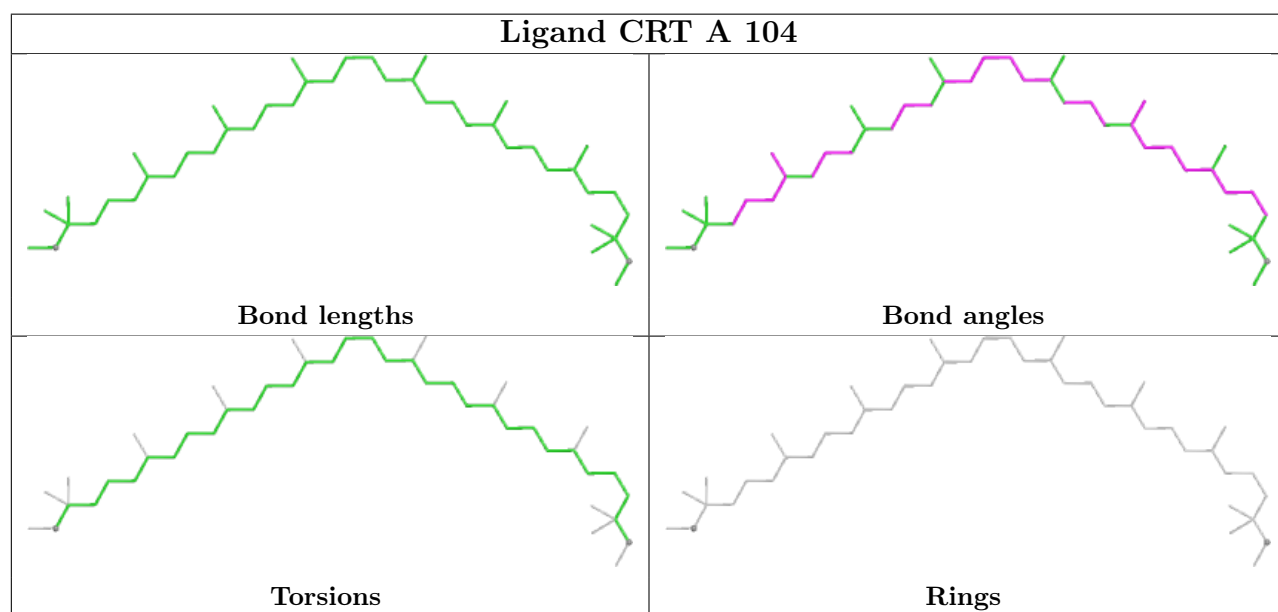
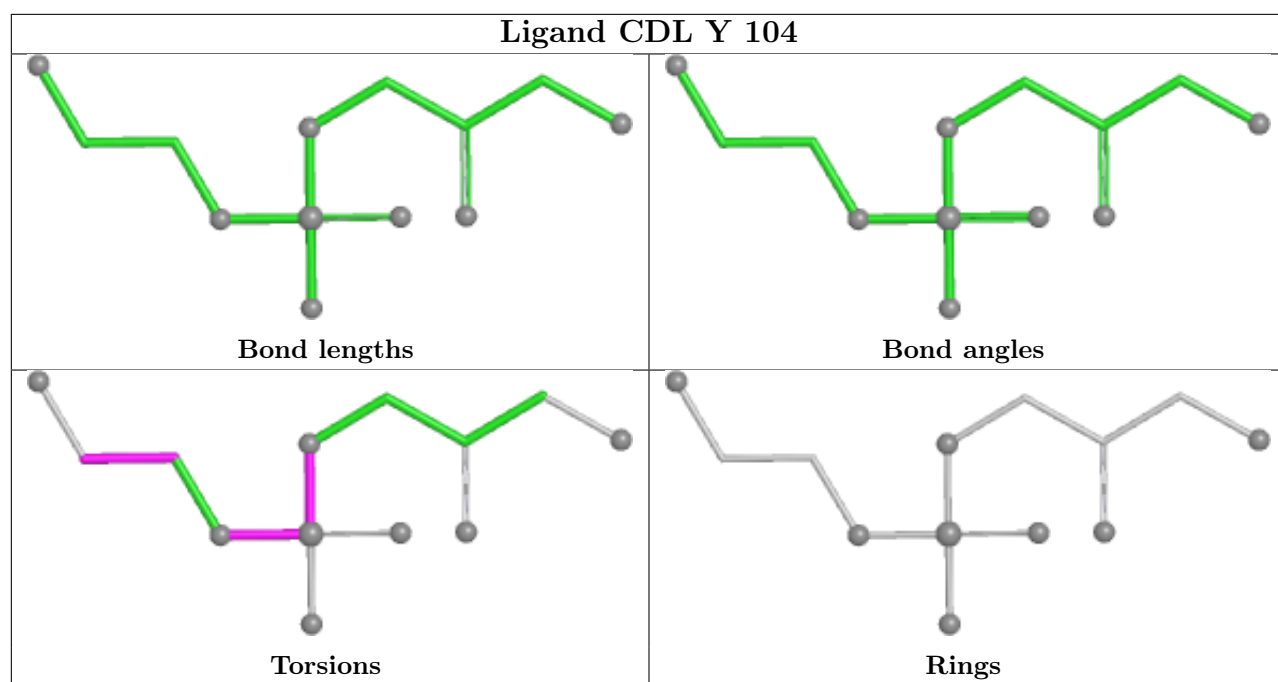


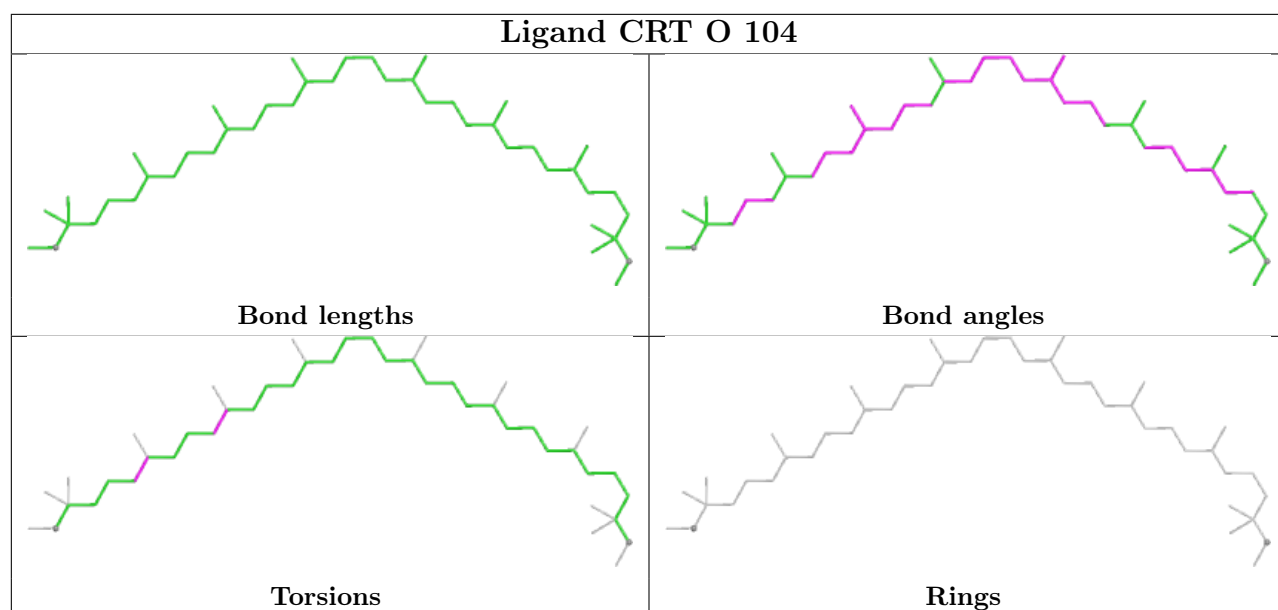
Torsions

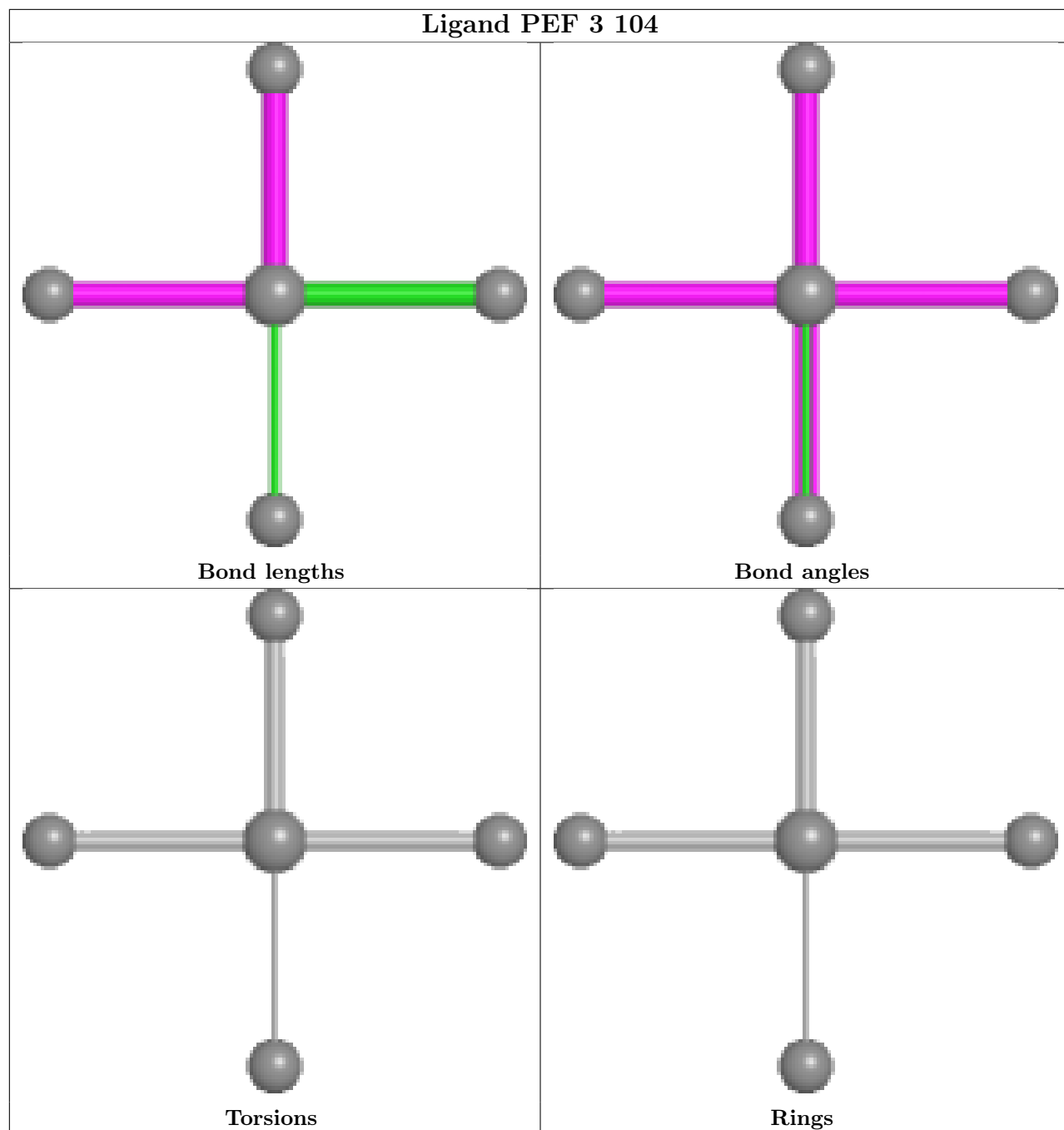


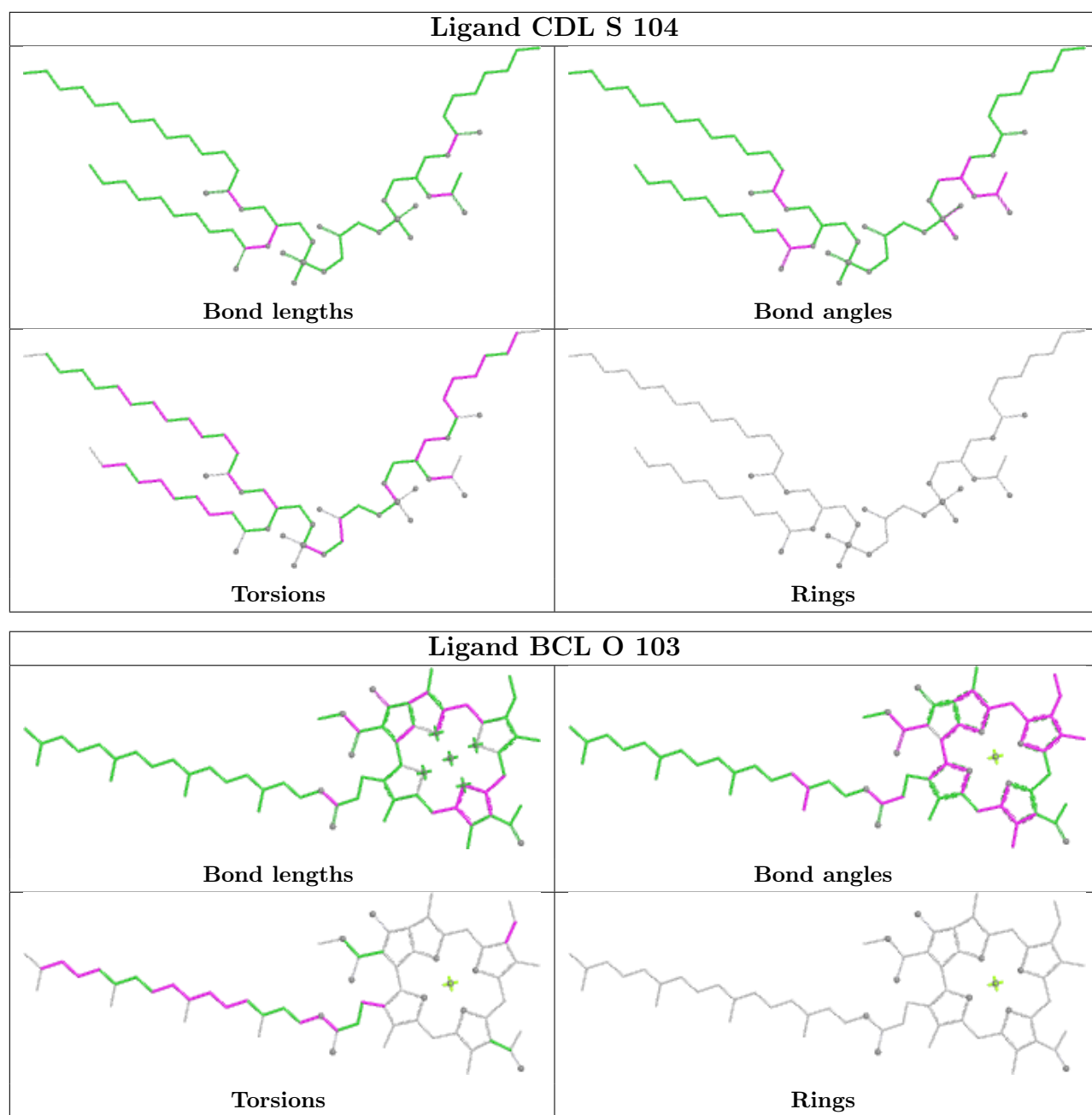
Rings

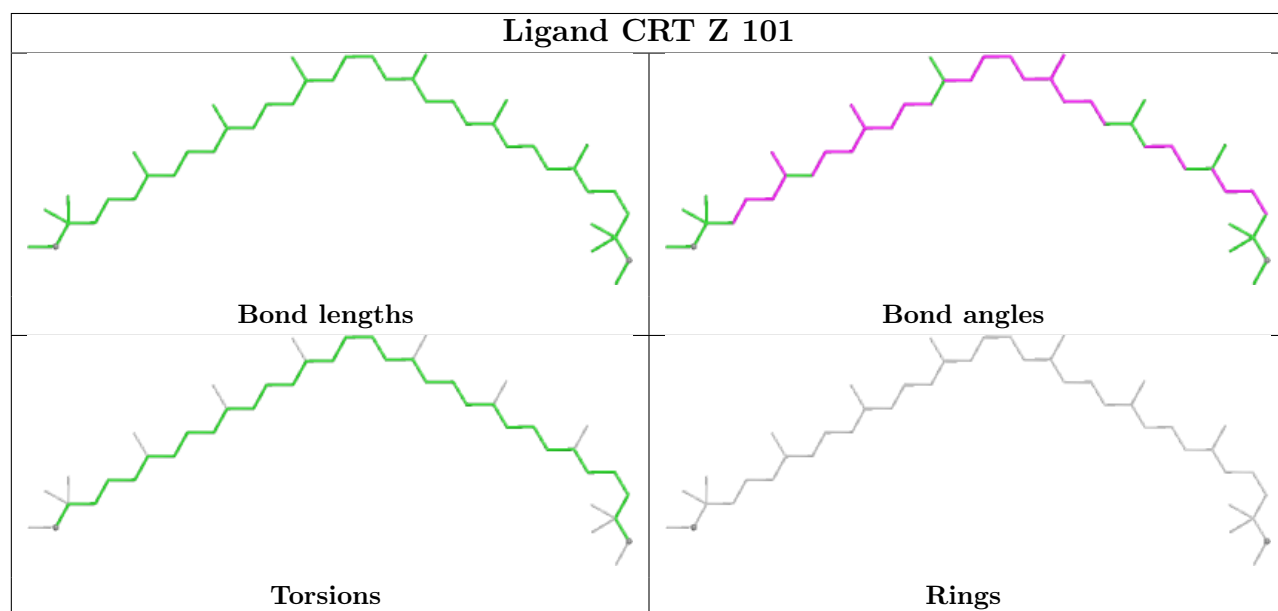
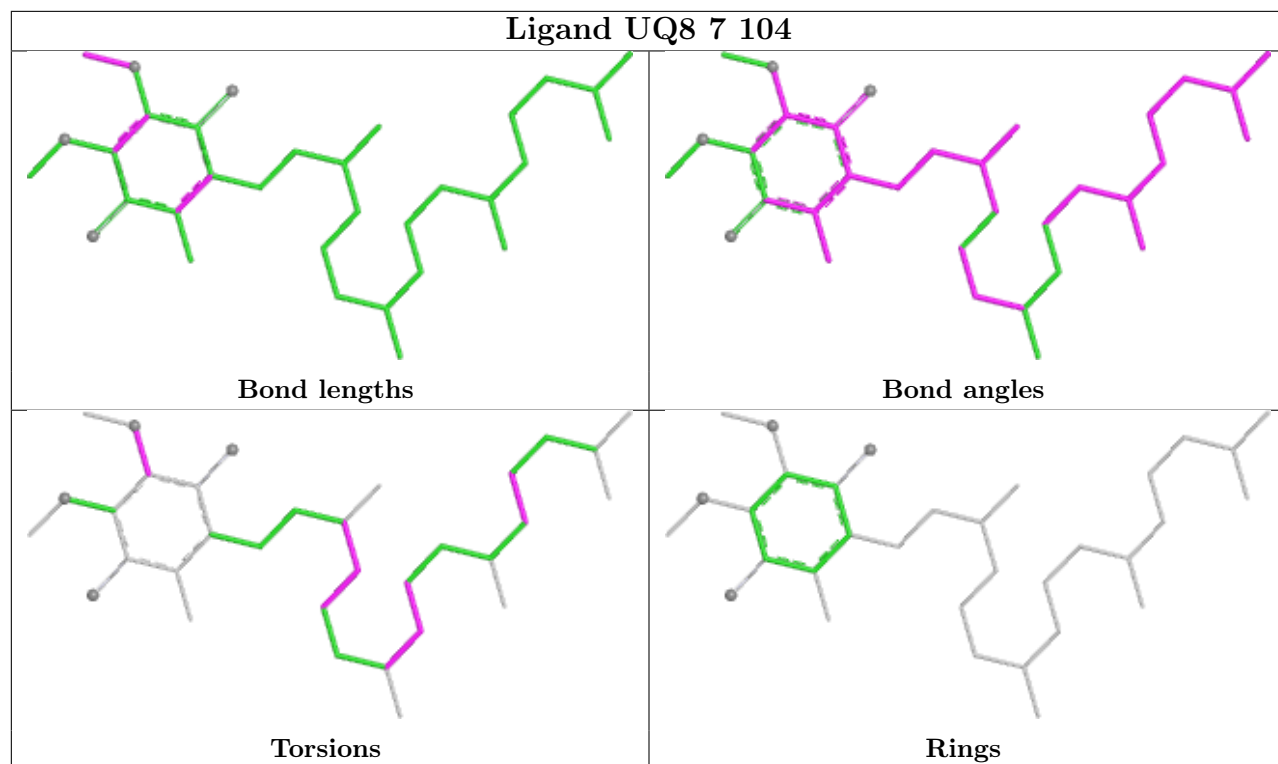


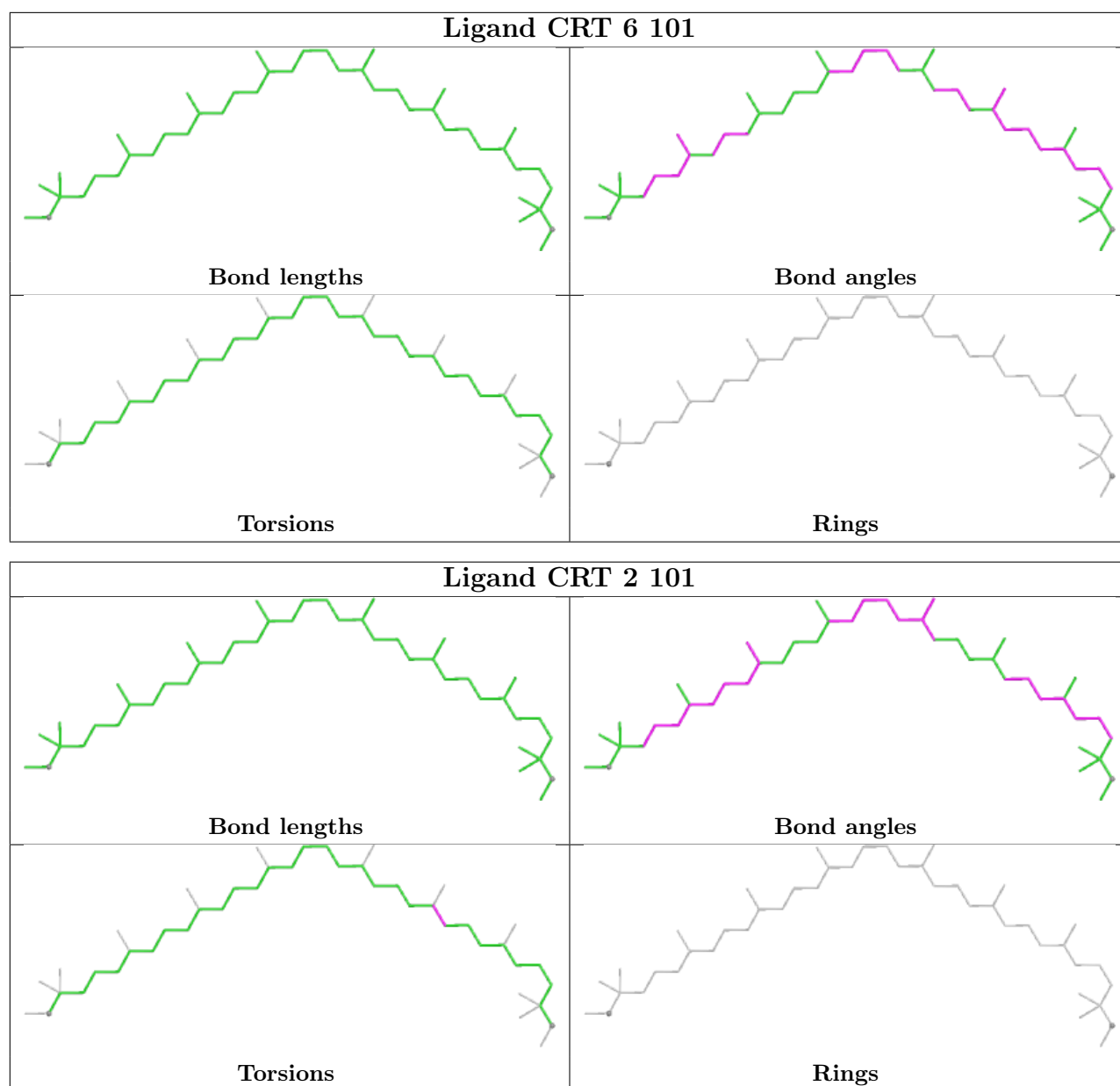


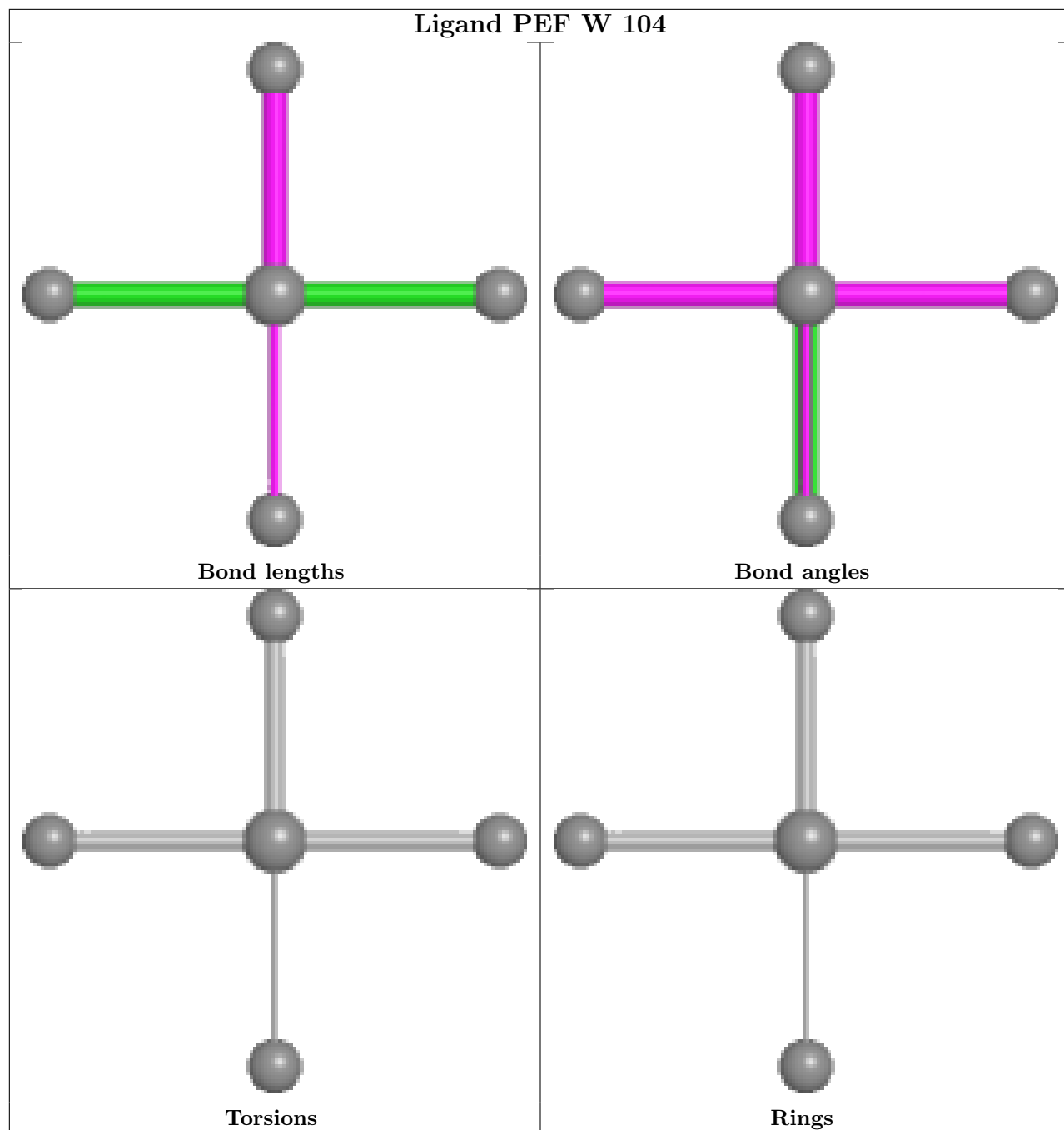


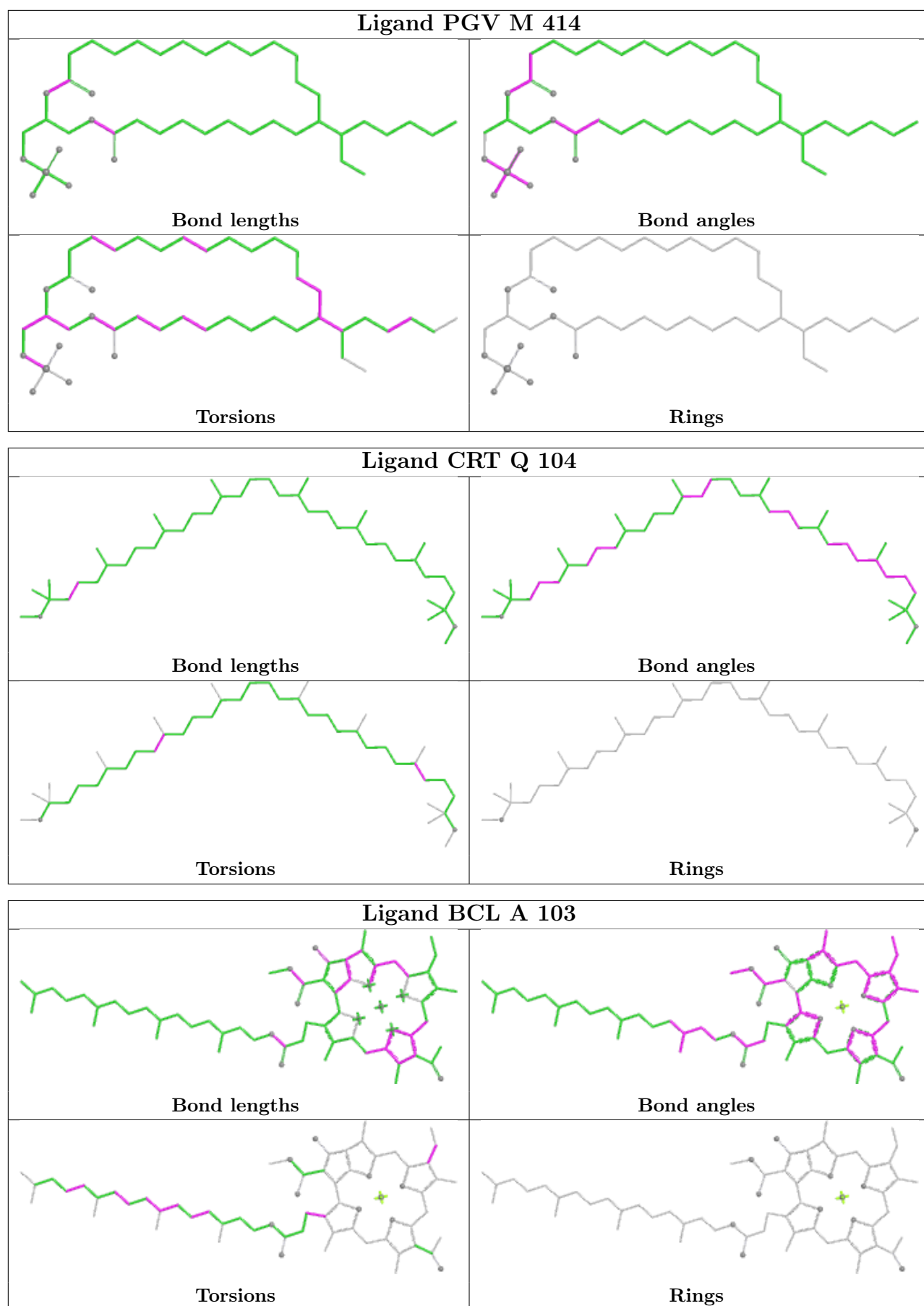


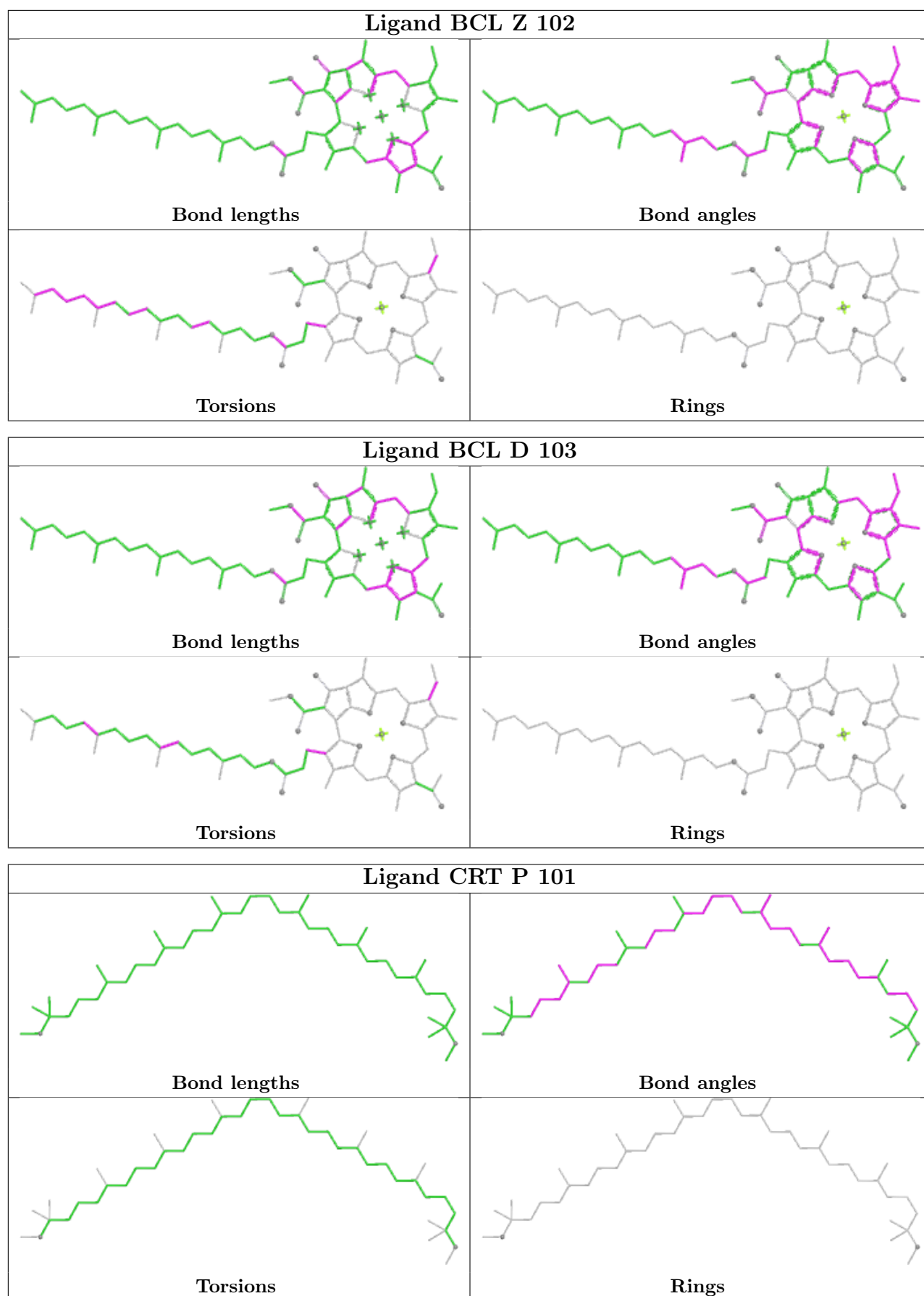


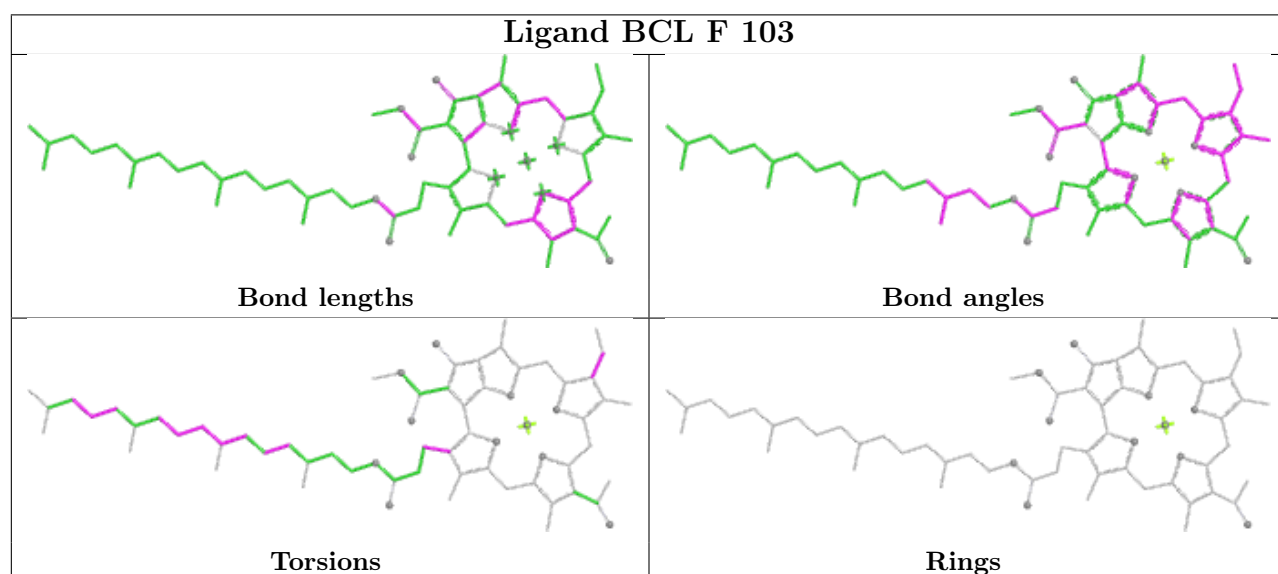
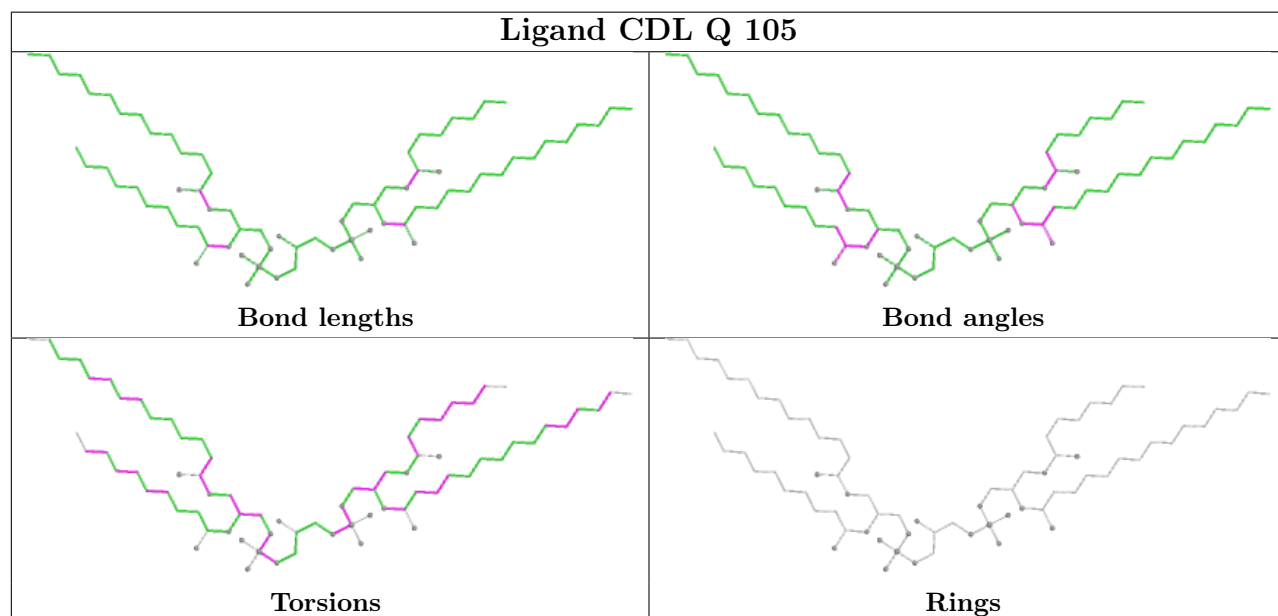
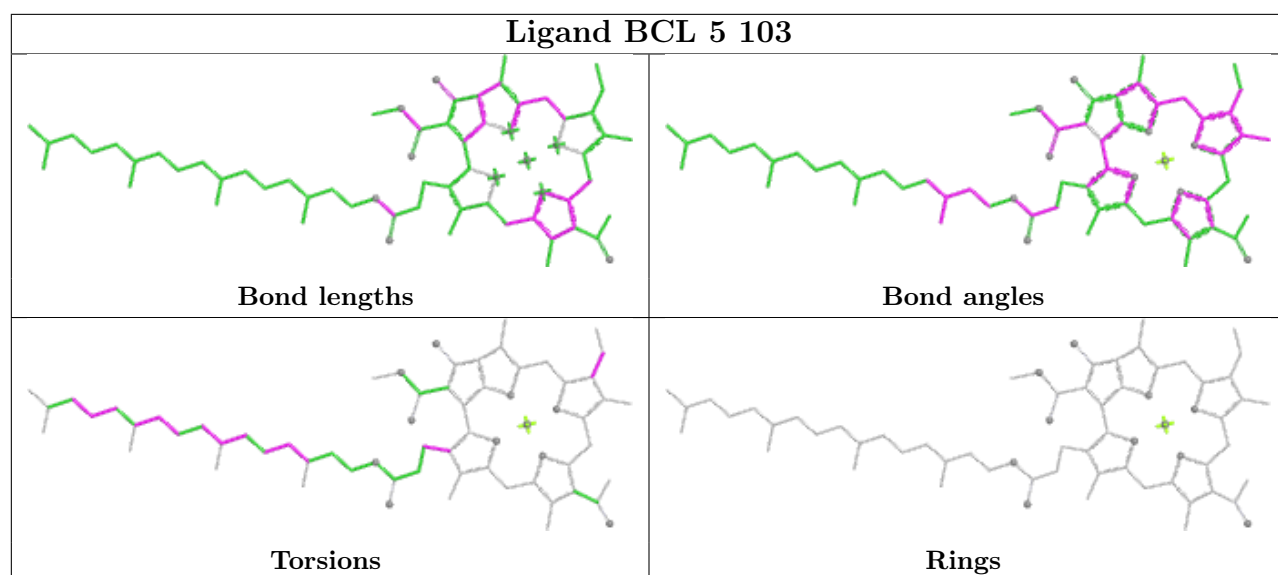


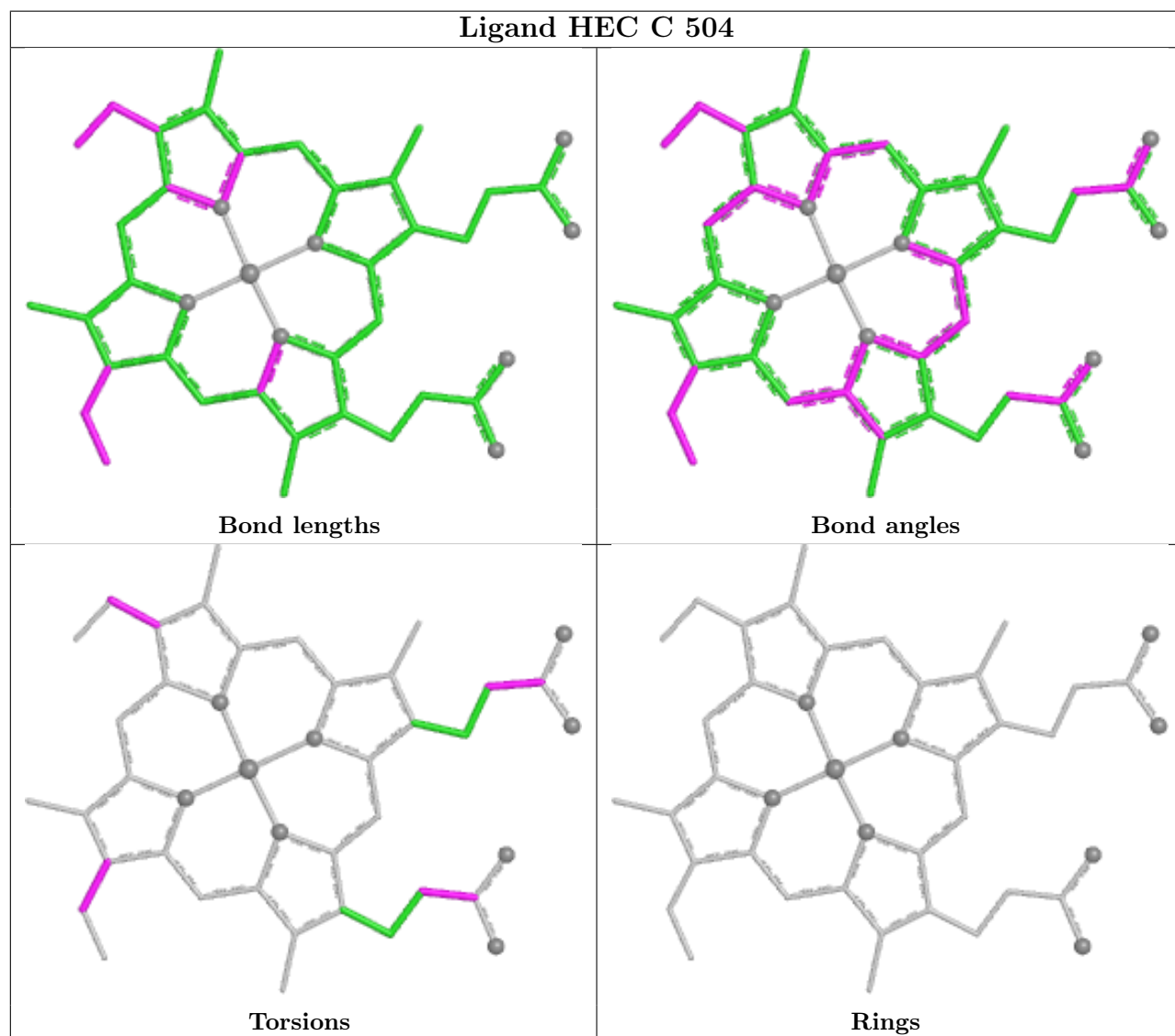
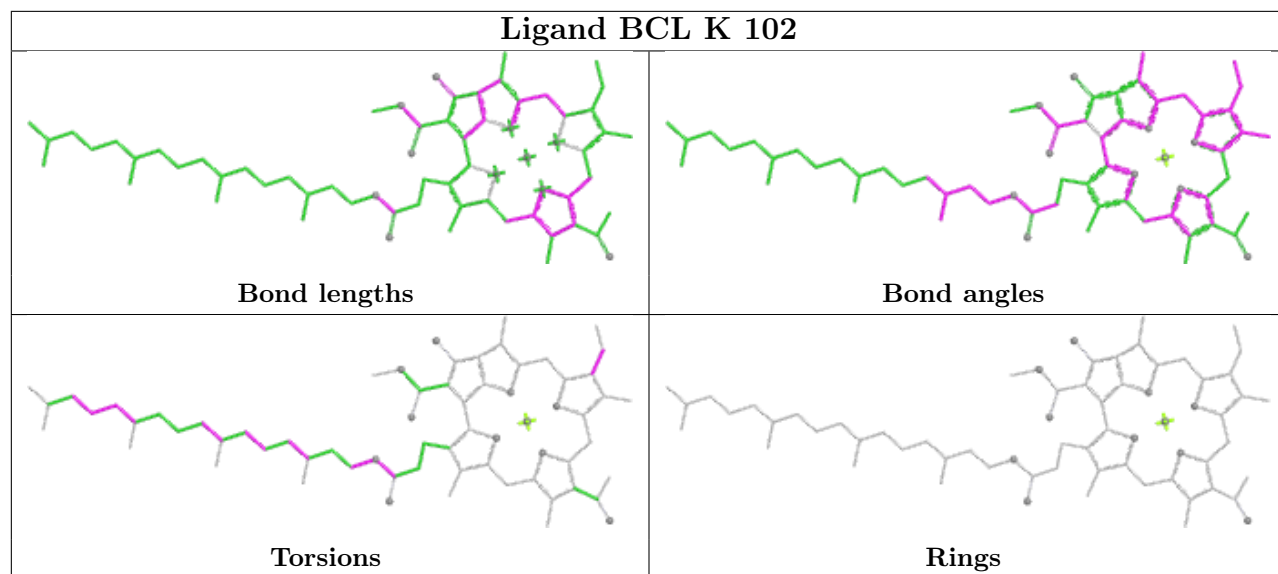


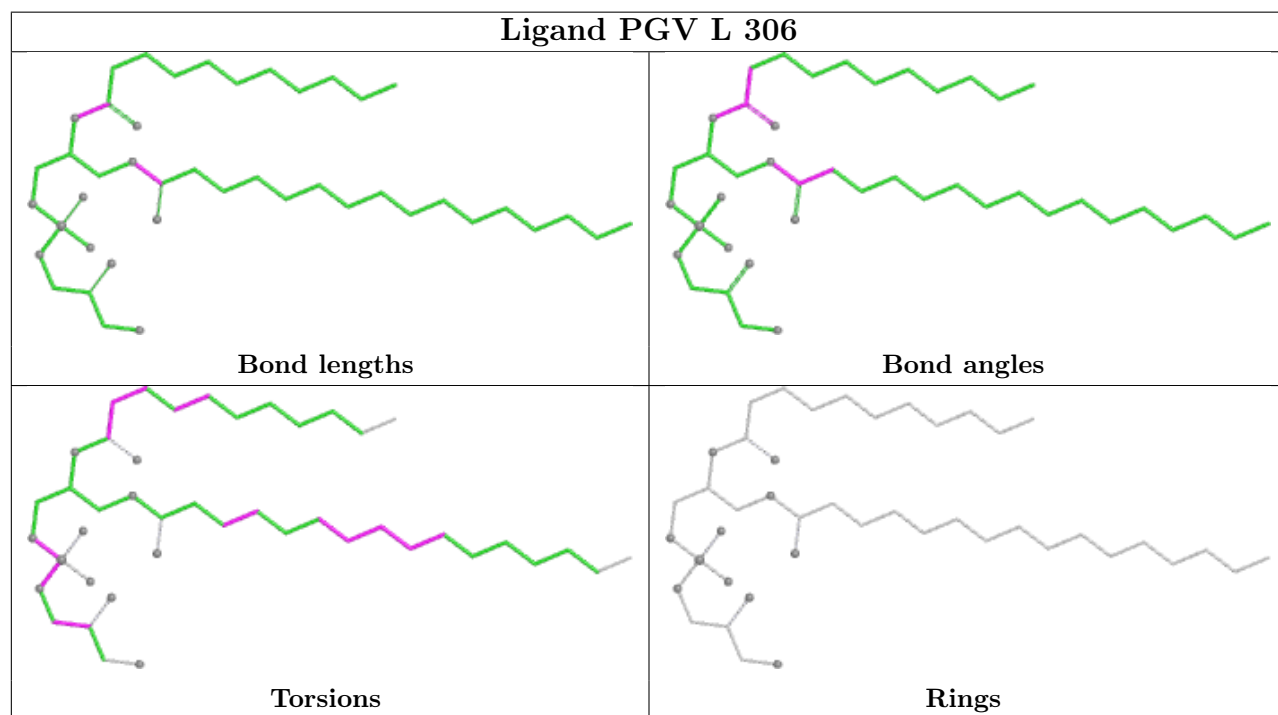
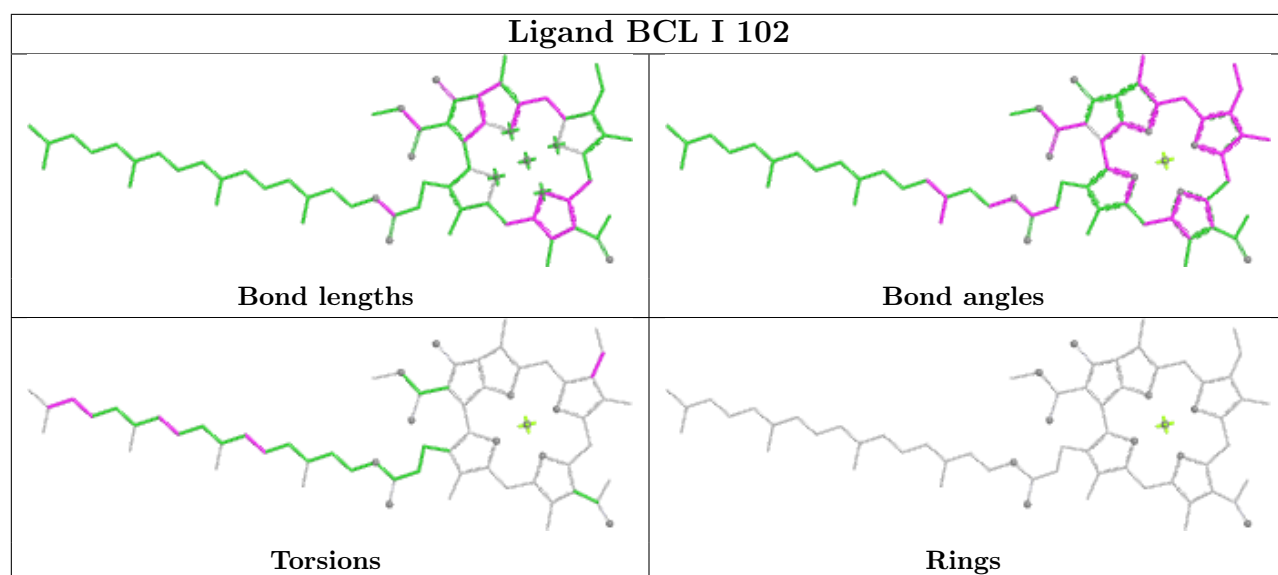


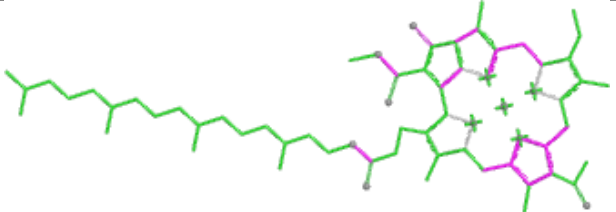
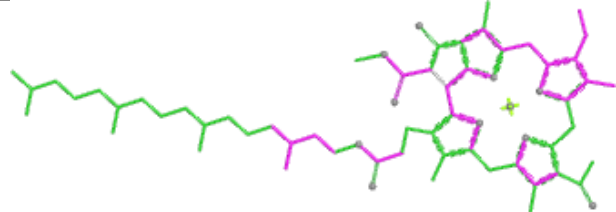
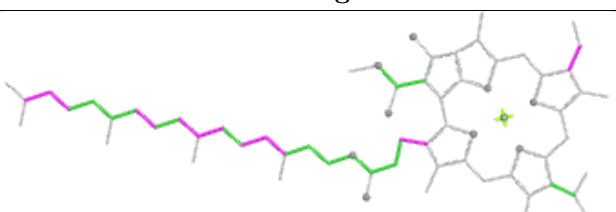
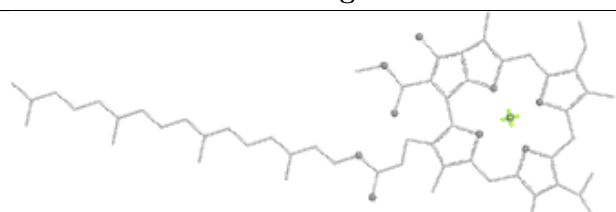


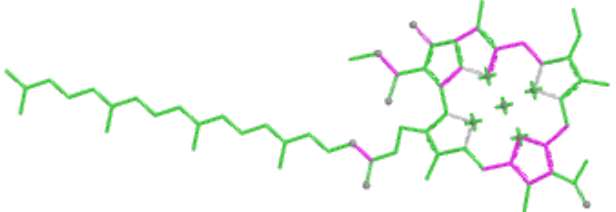
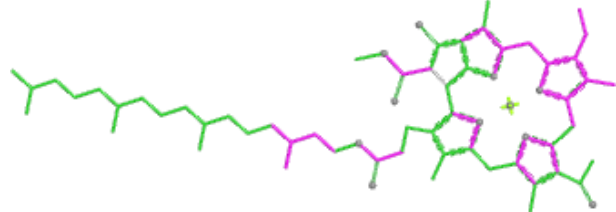
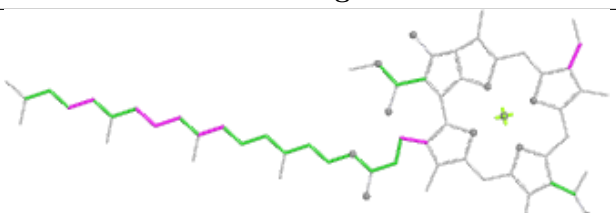
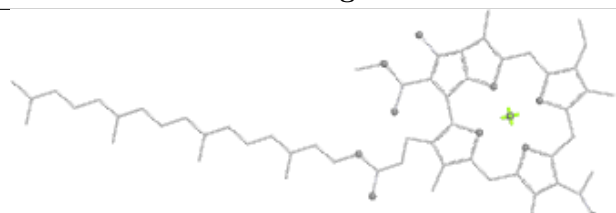


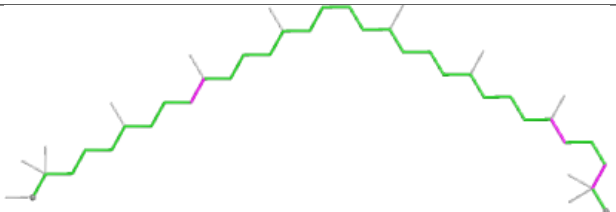
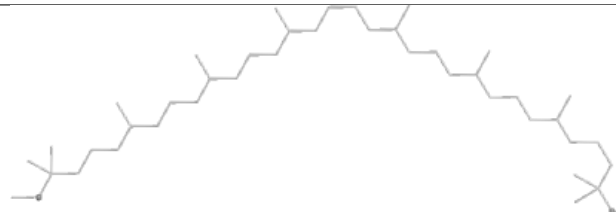


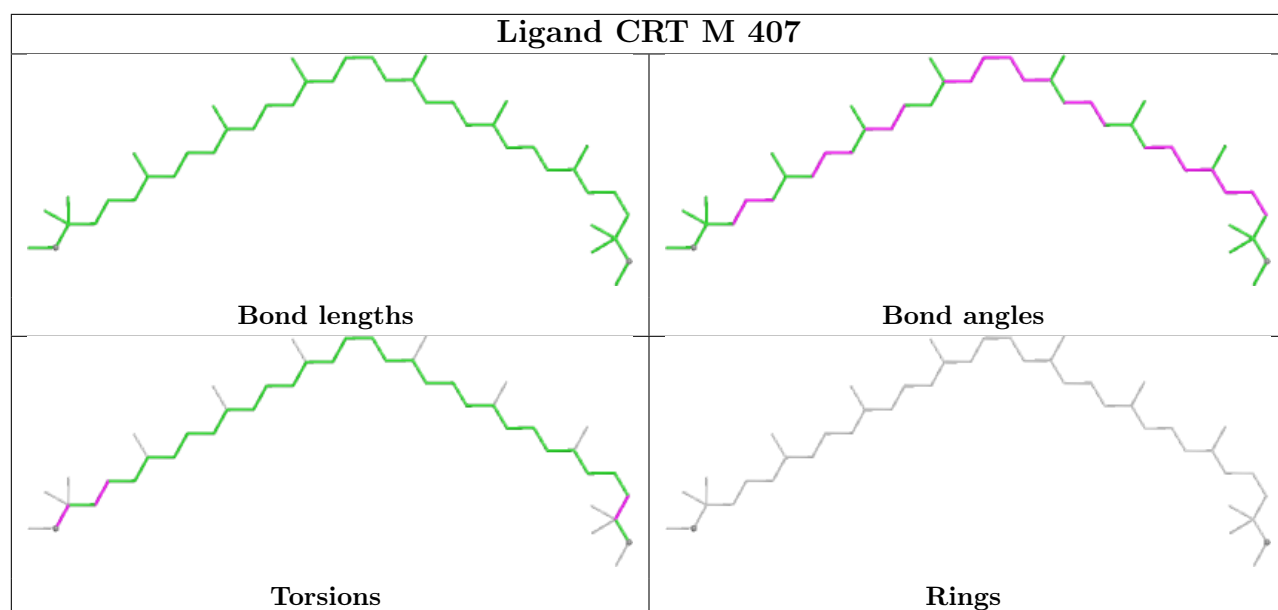


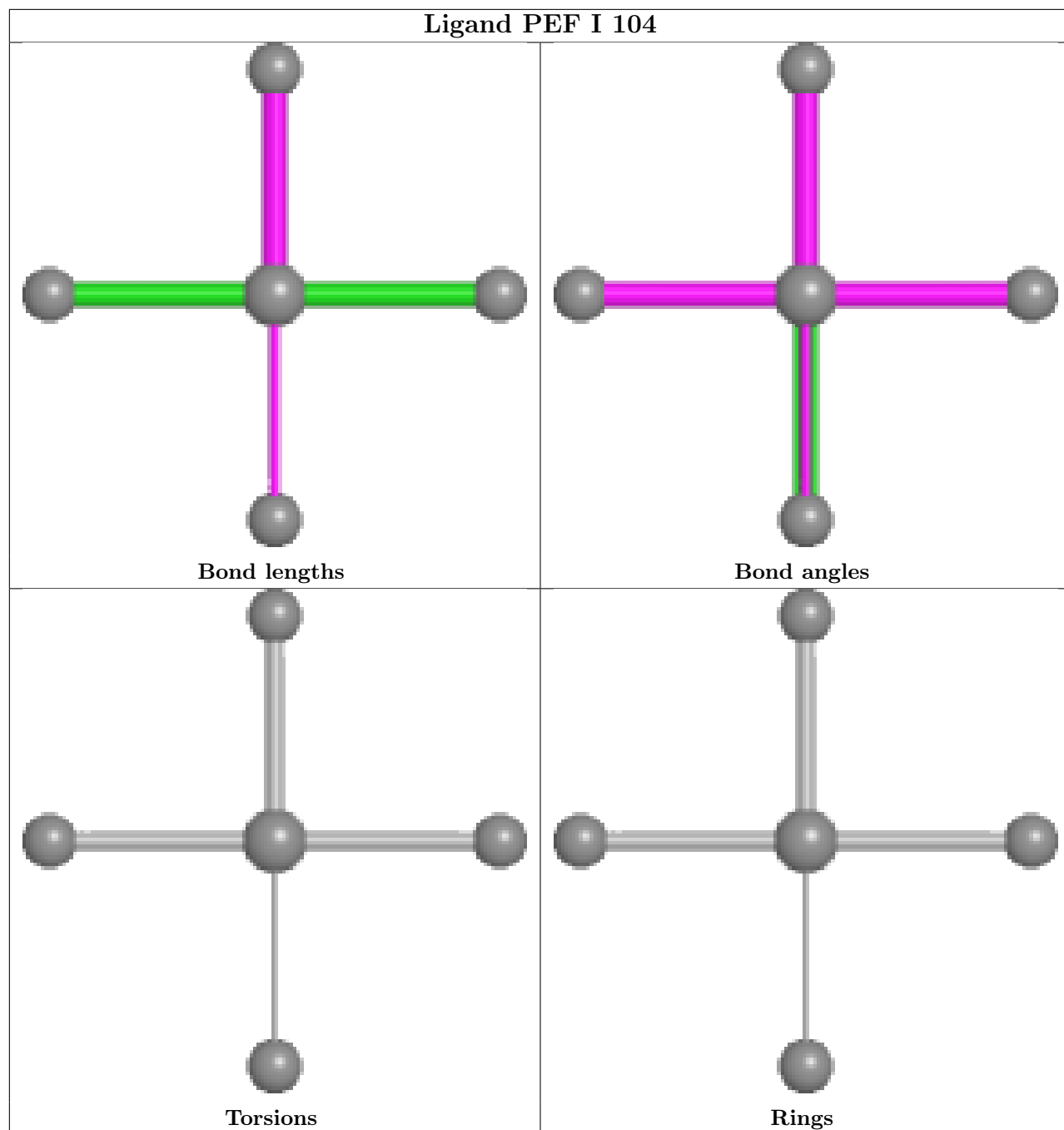


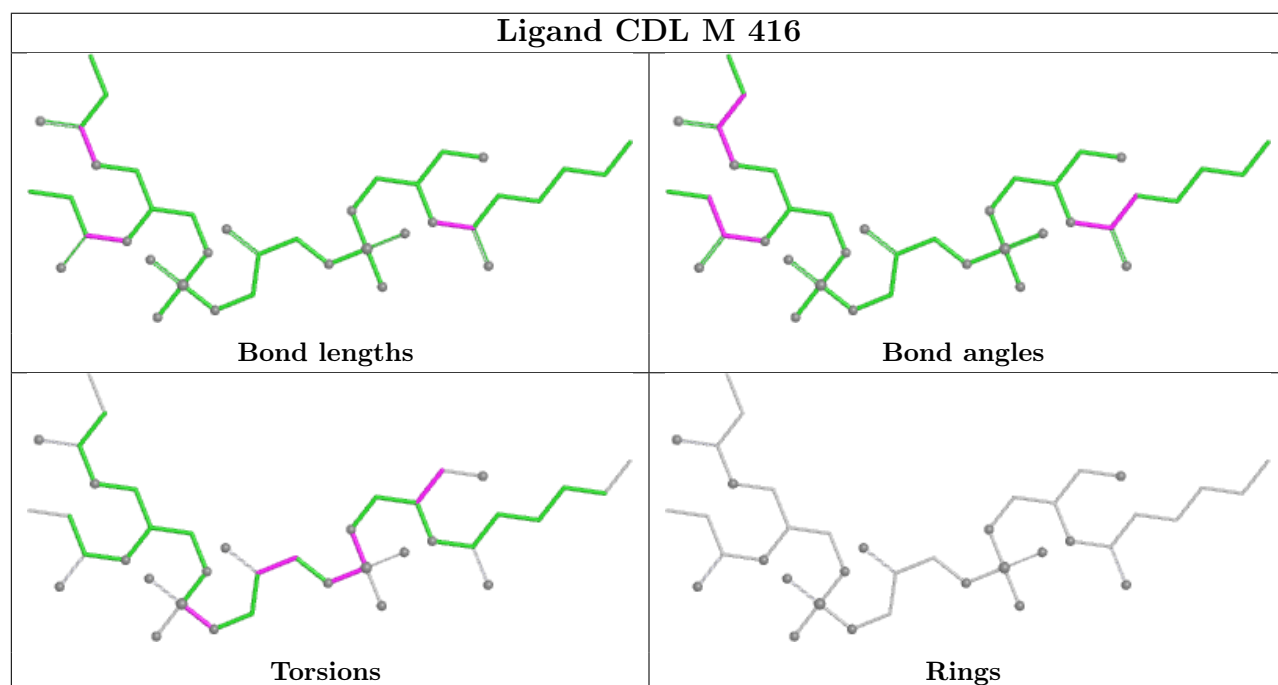
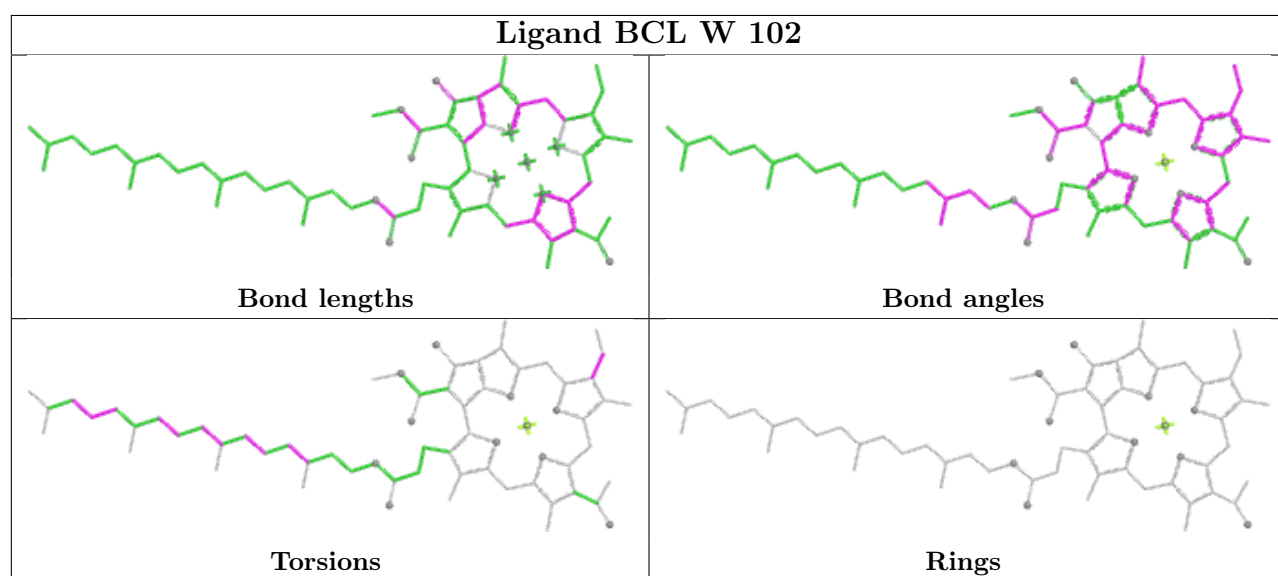
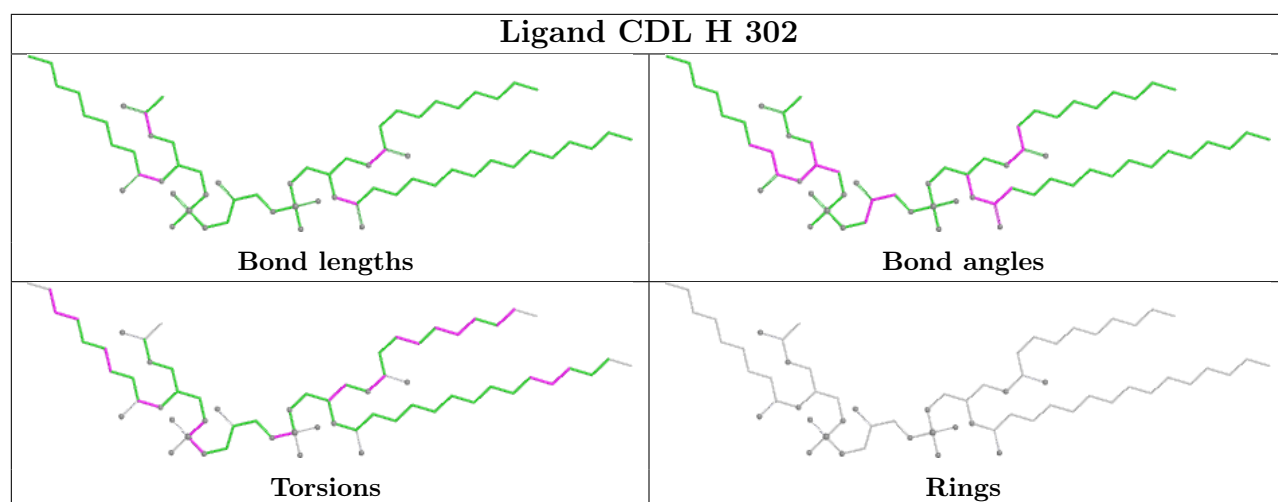
Ligand BCL K 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

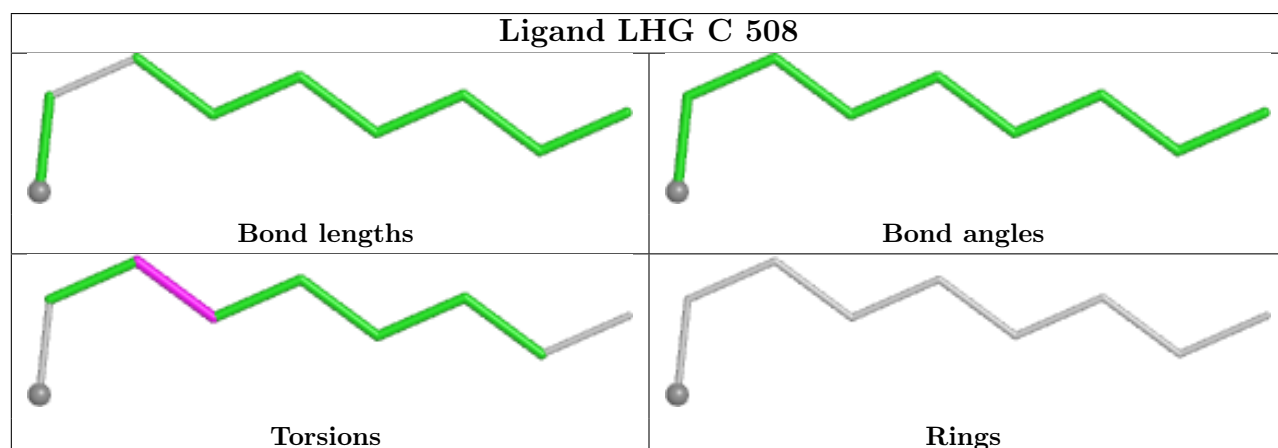
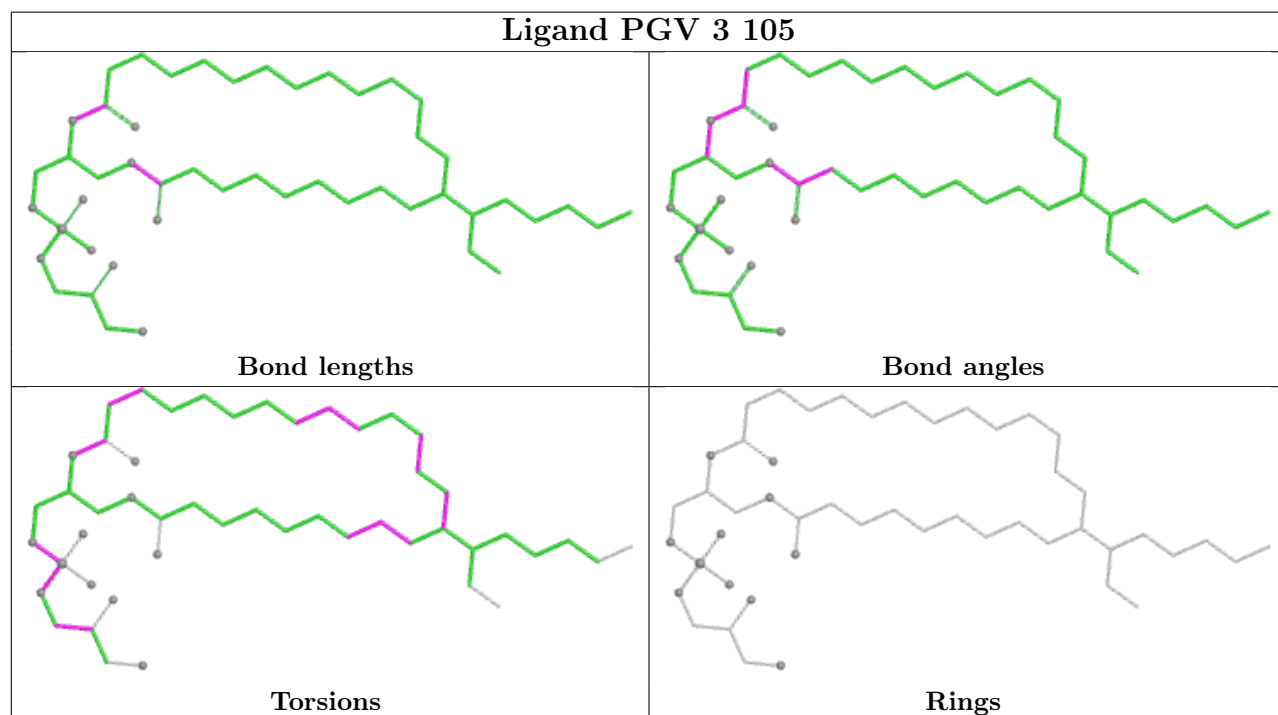
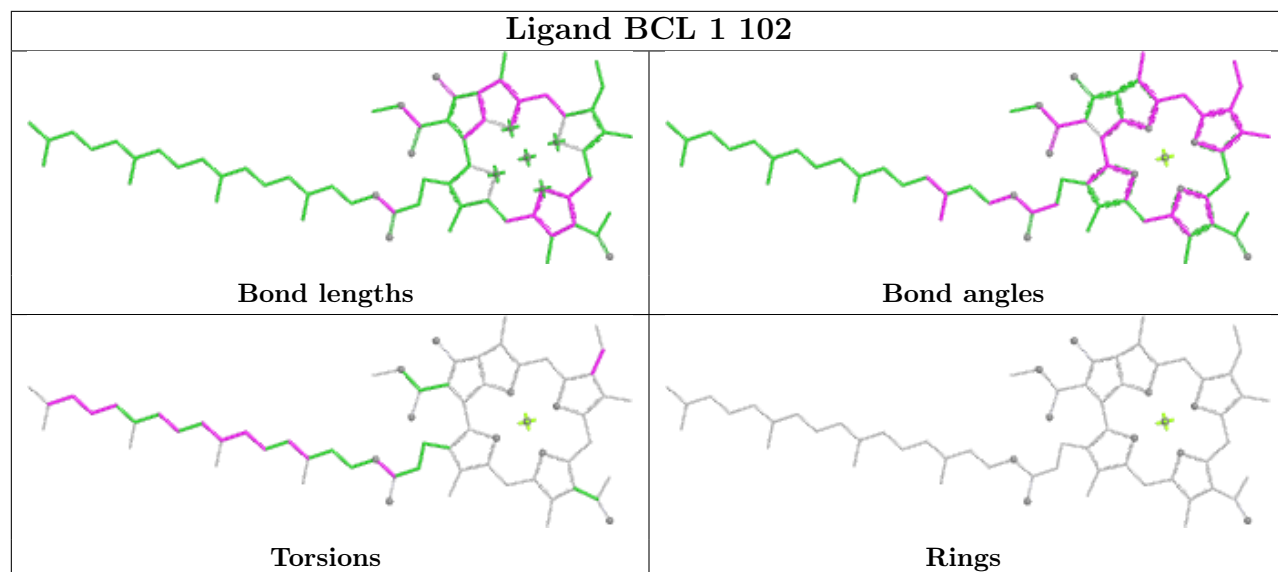
Ligand BCL W 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

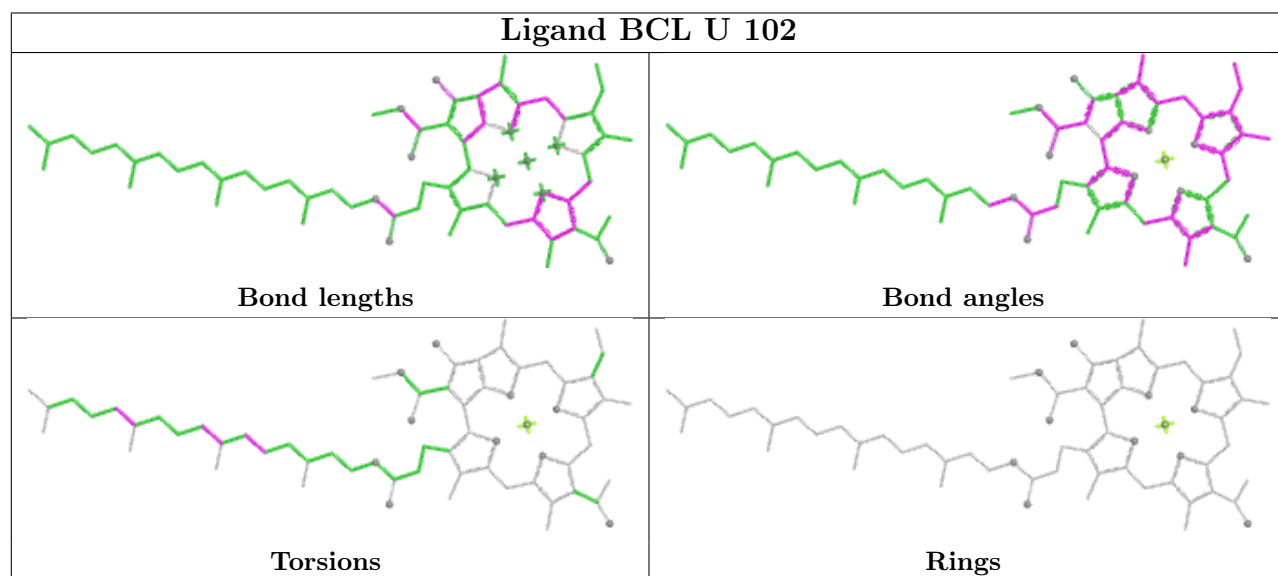
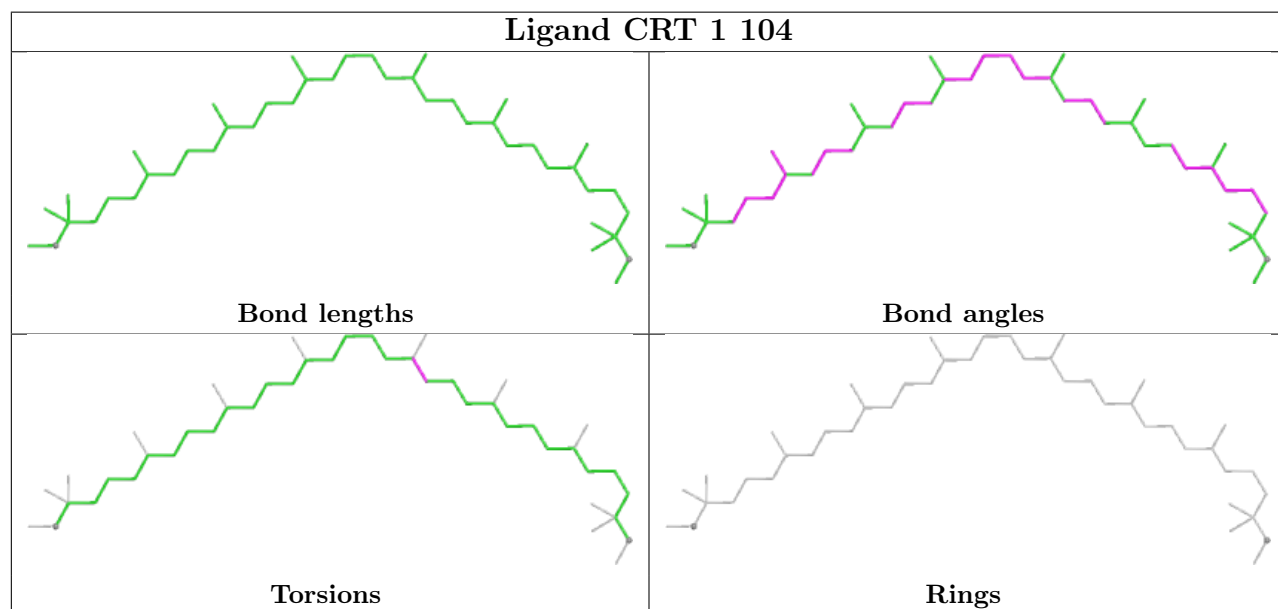
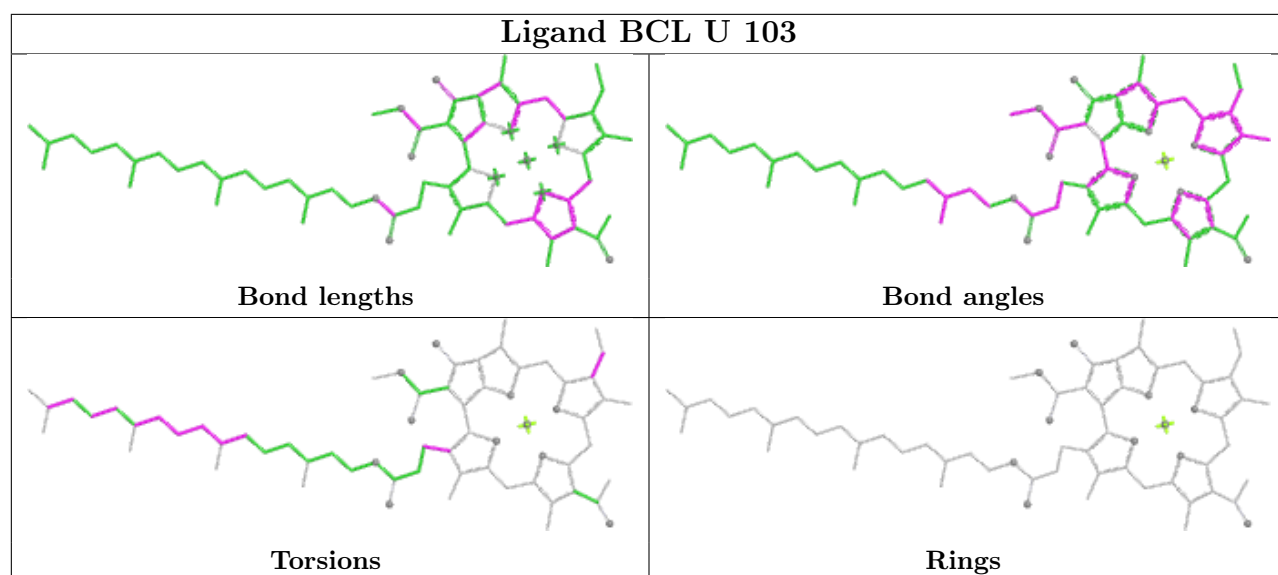
Ligand CRT 0 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

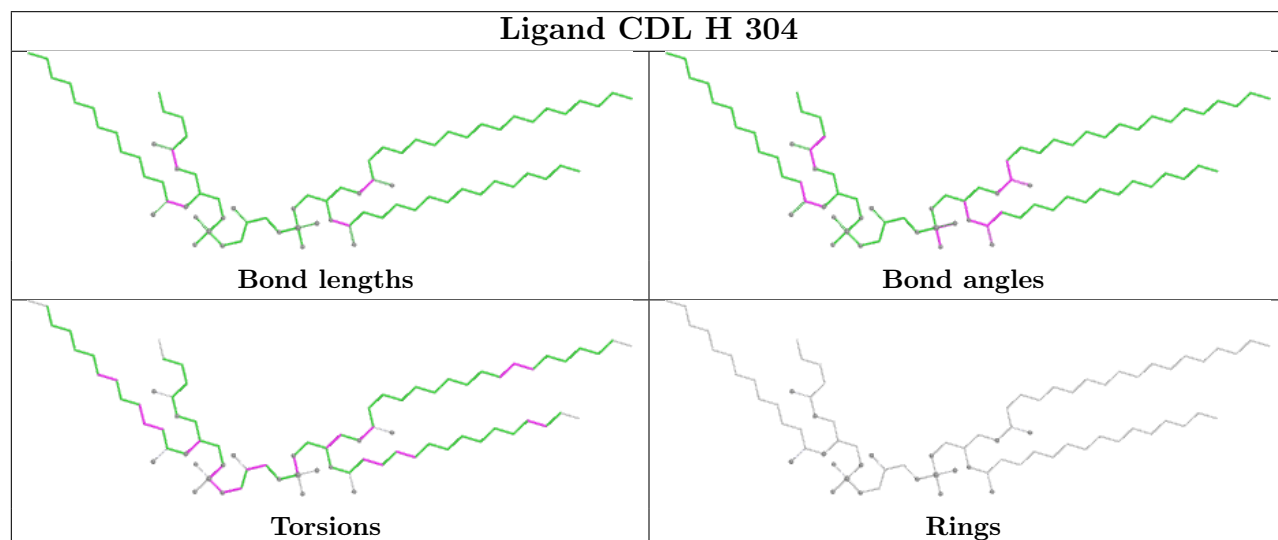
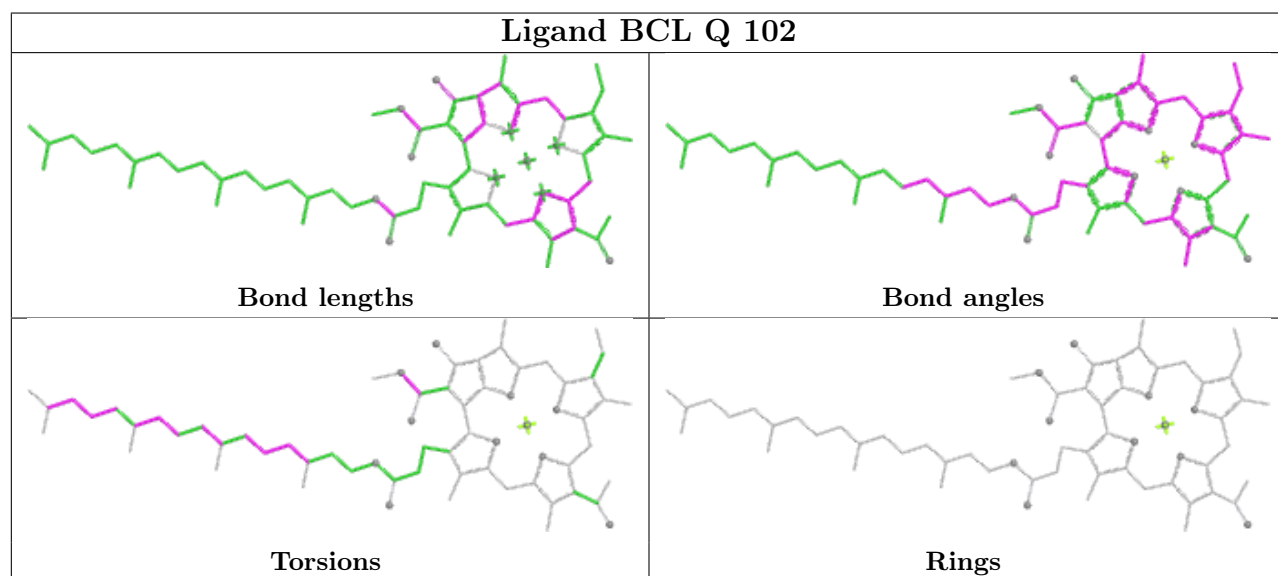
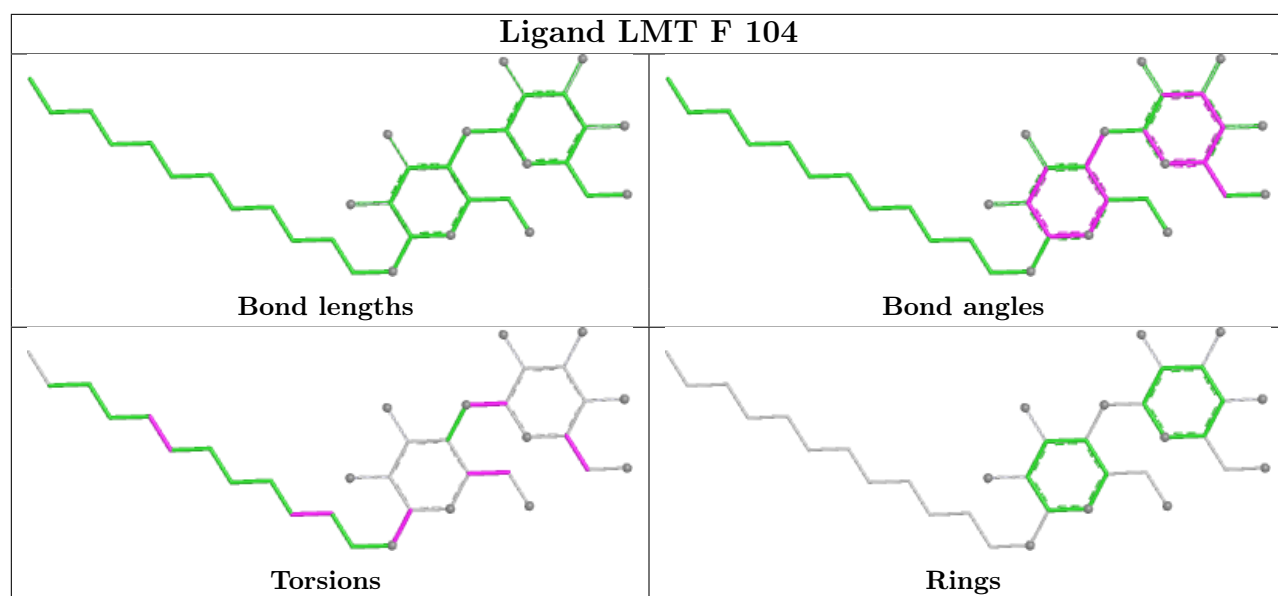


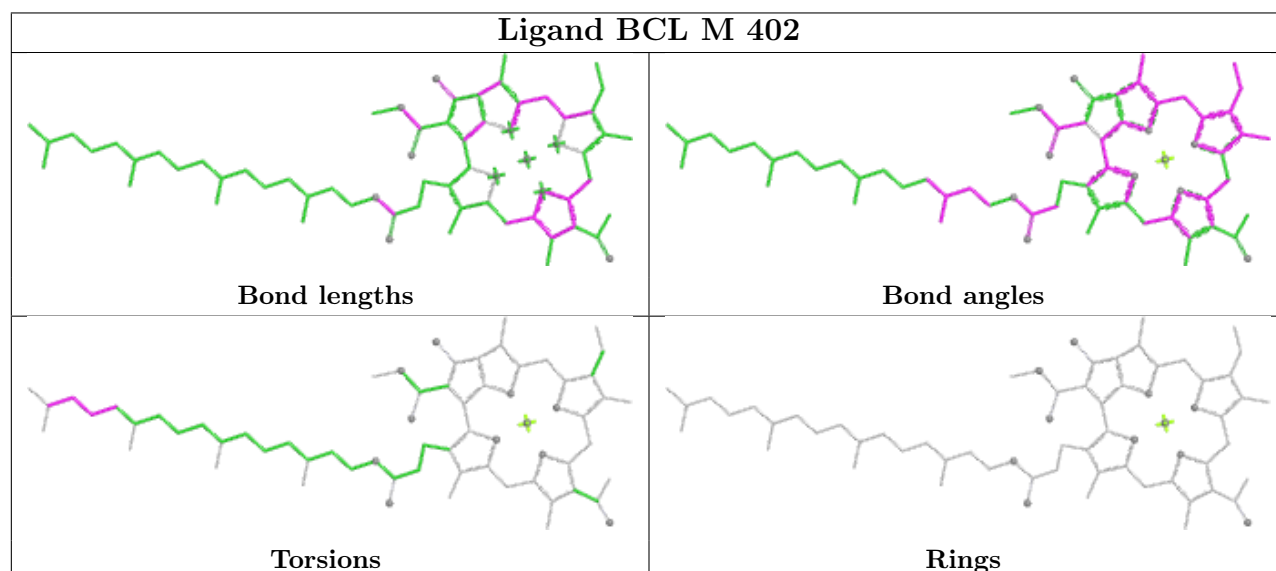
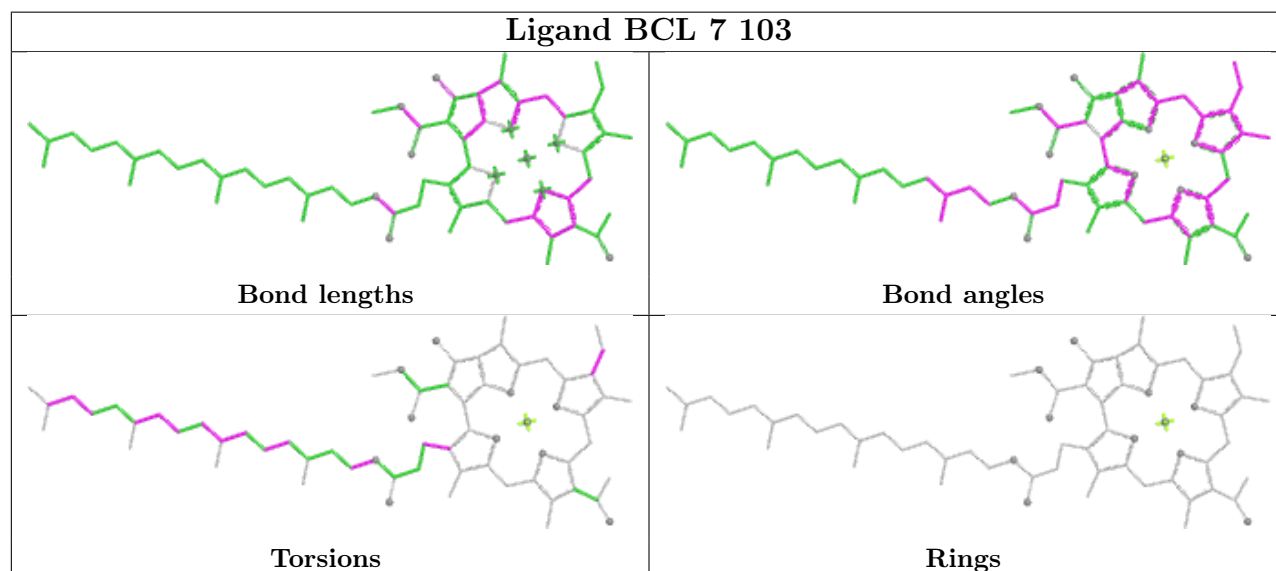
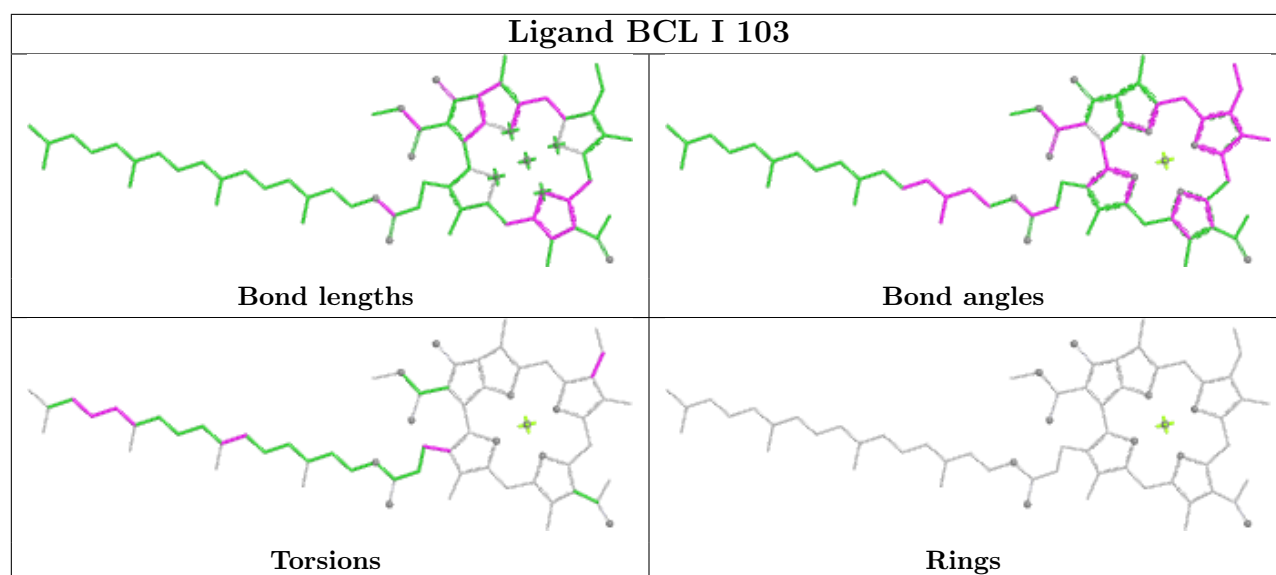


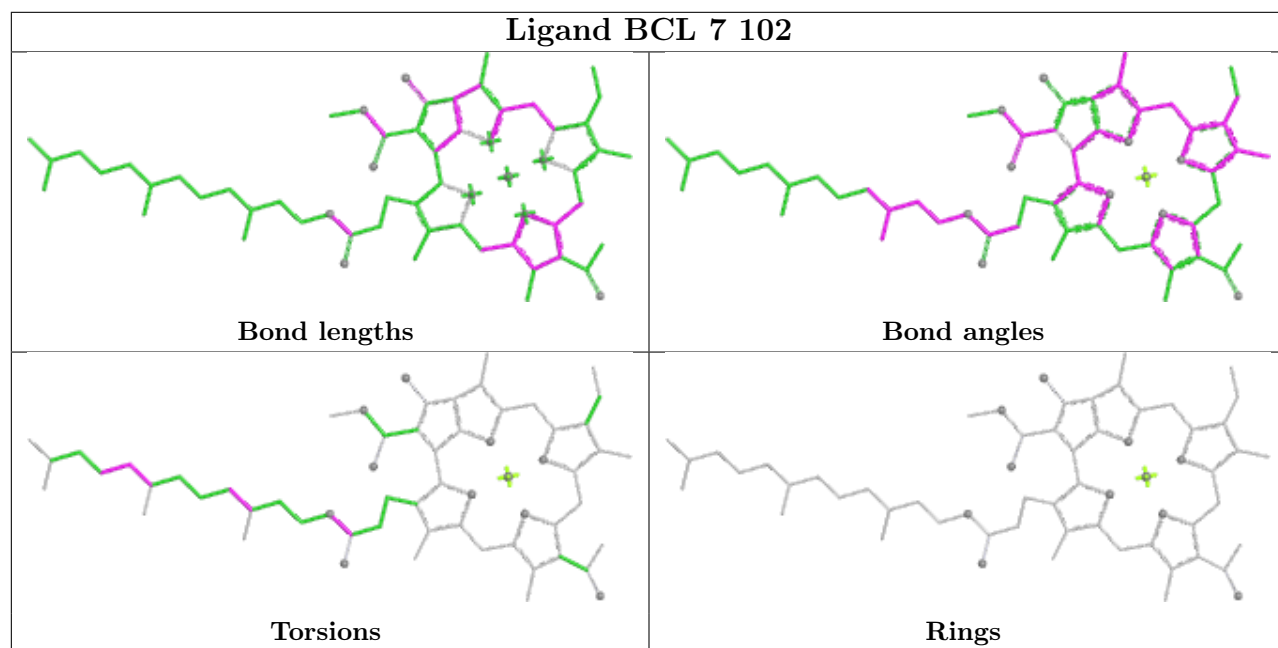
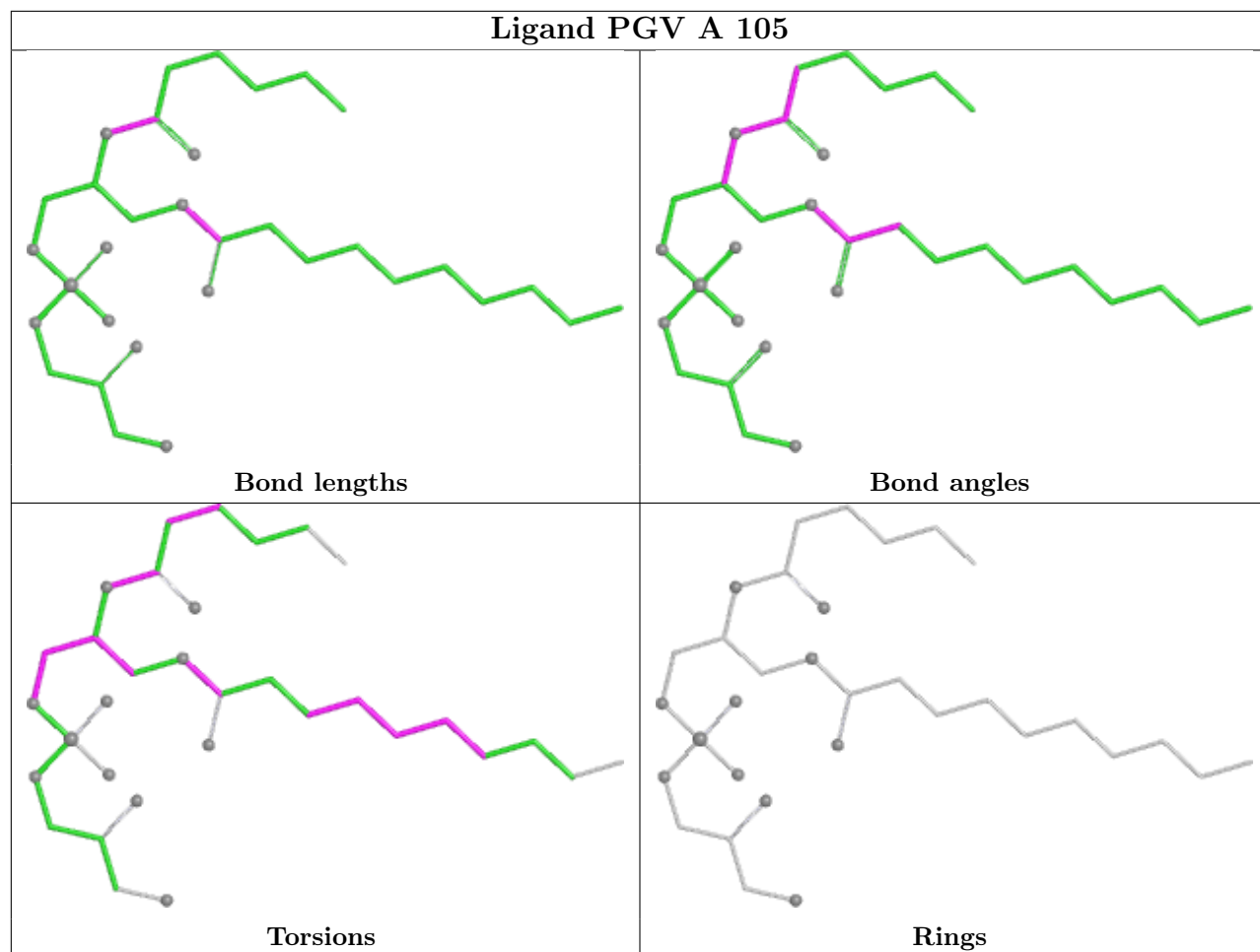


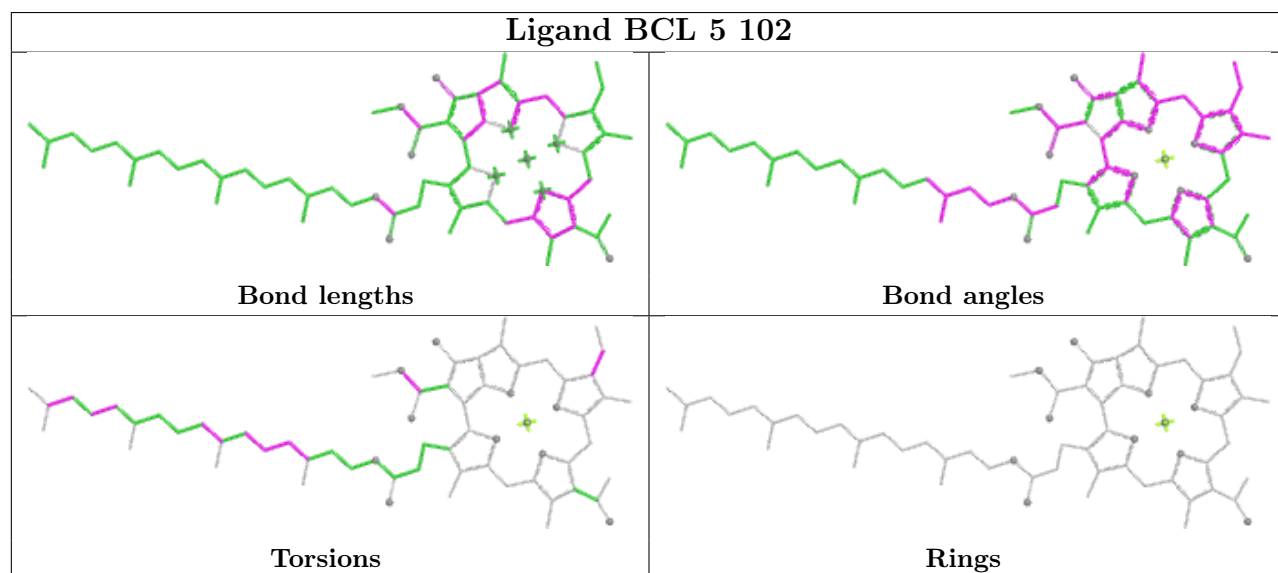
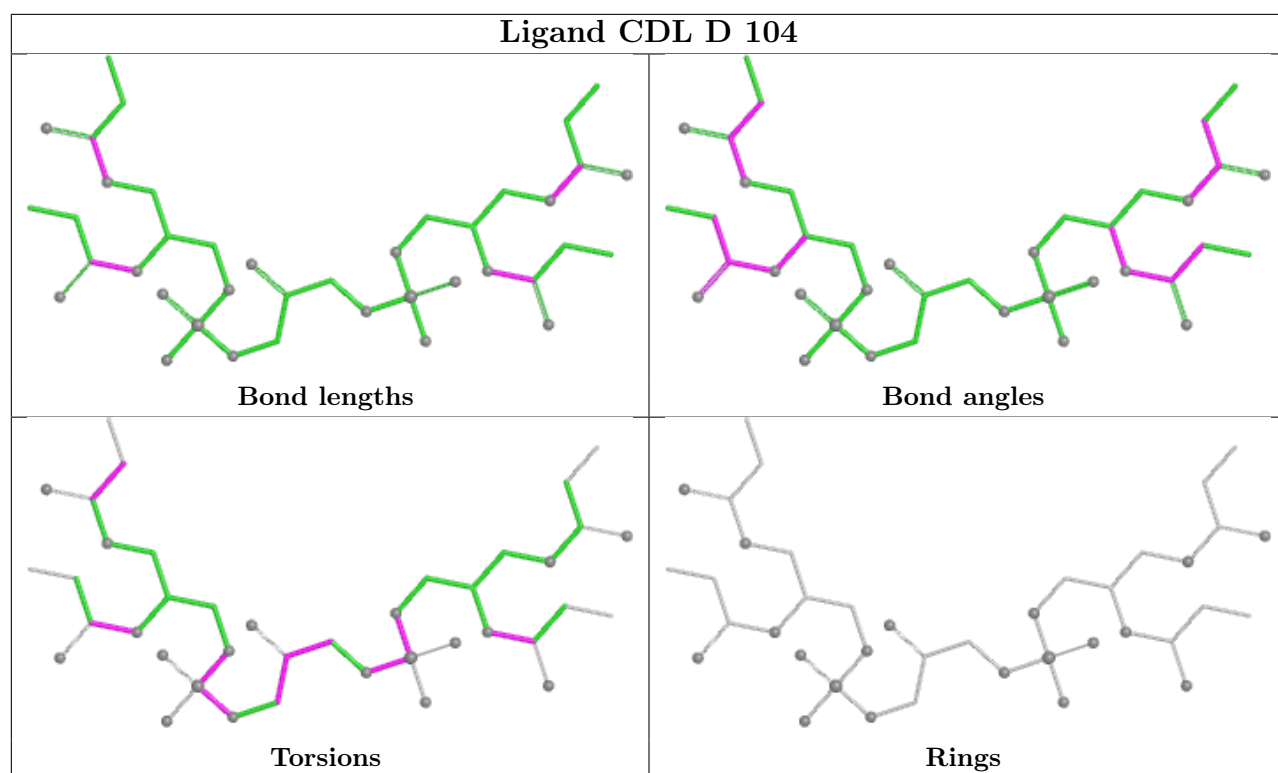


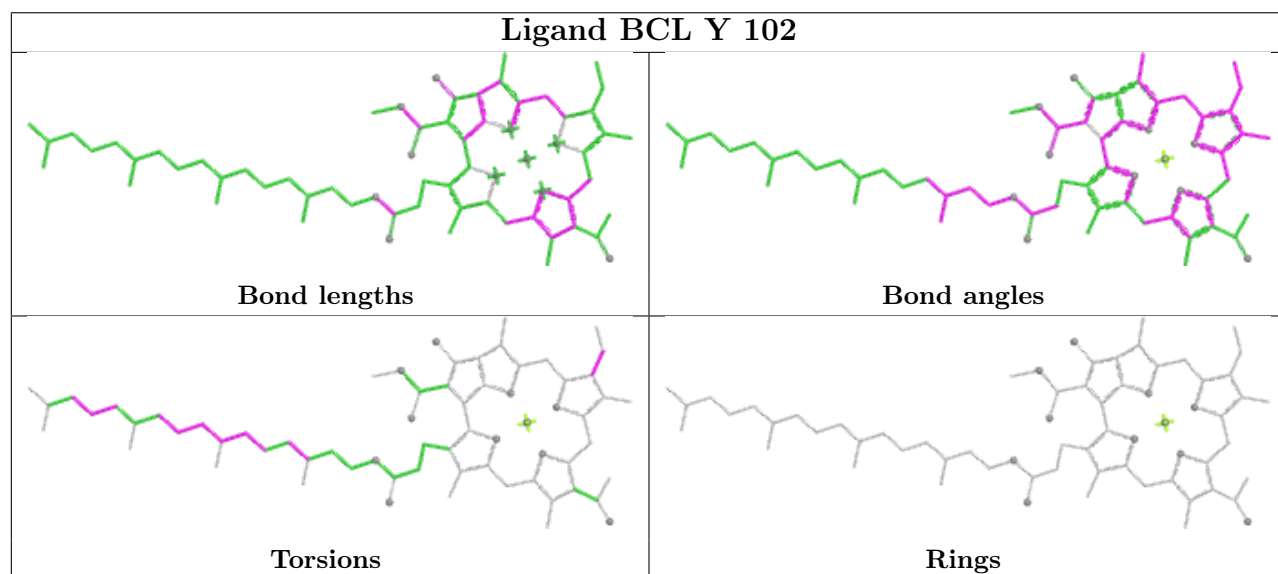
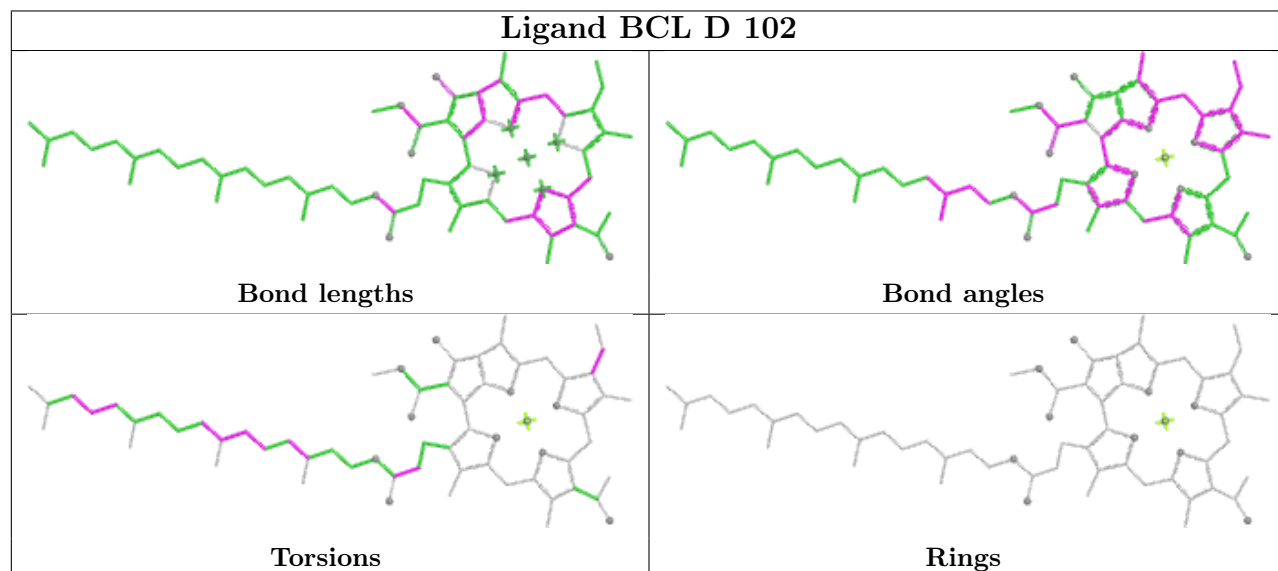
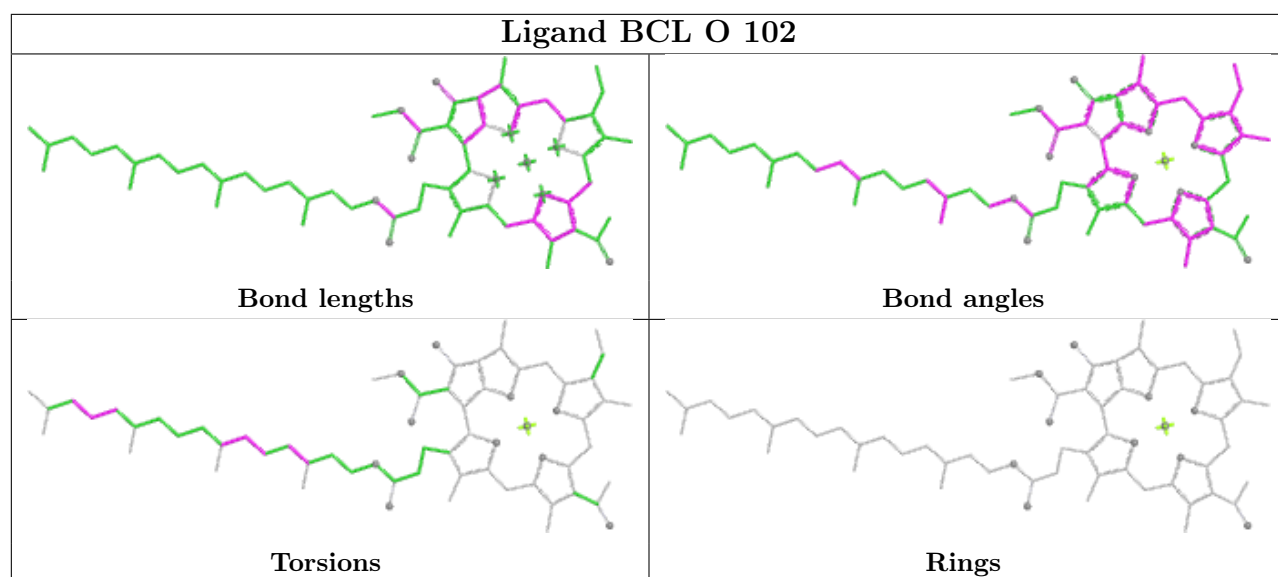


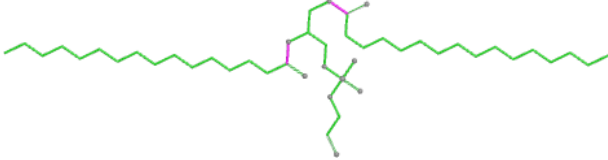
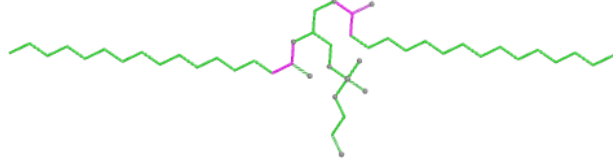
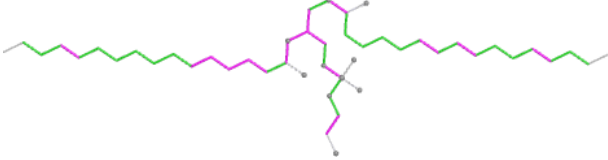
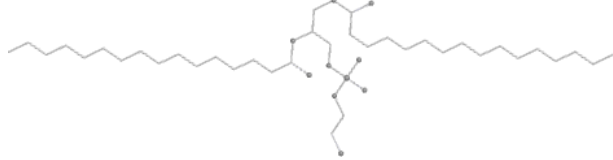


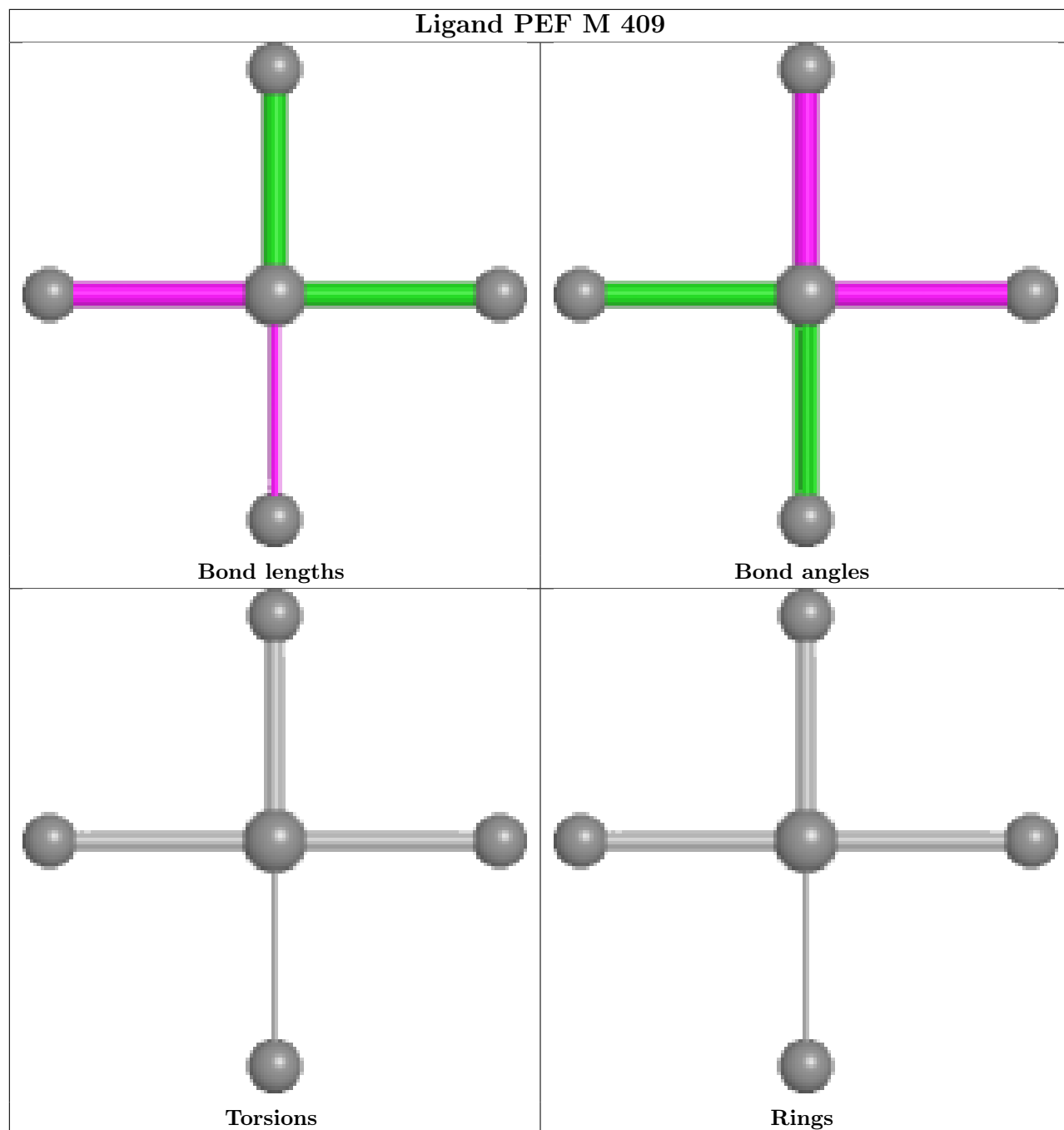


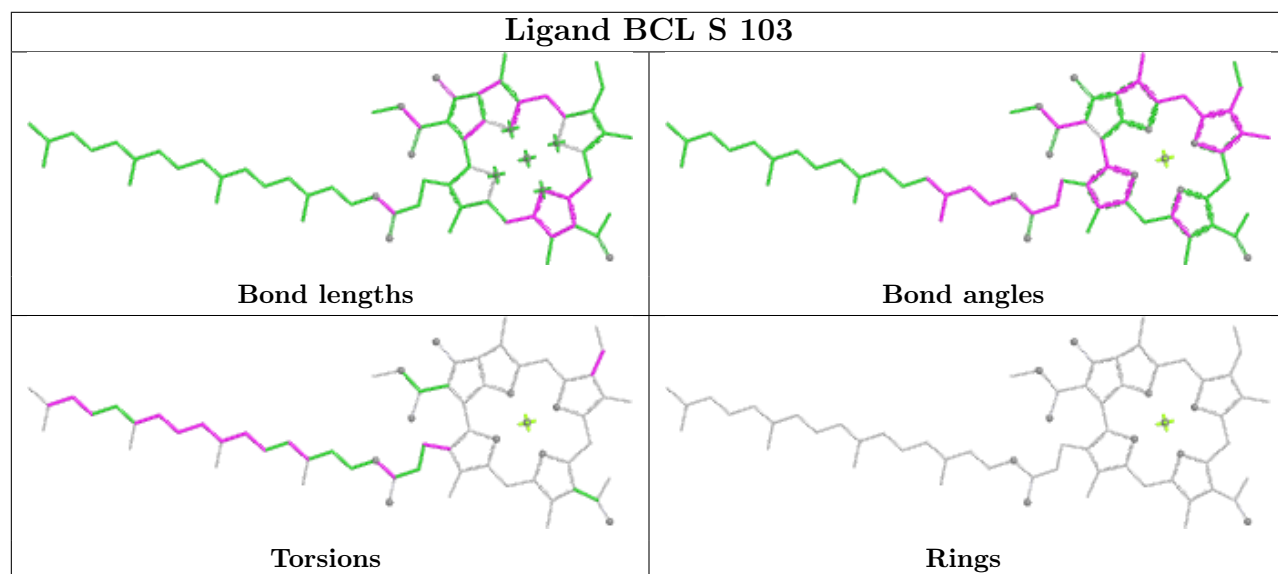
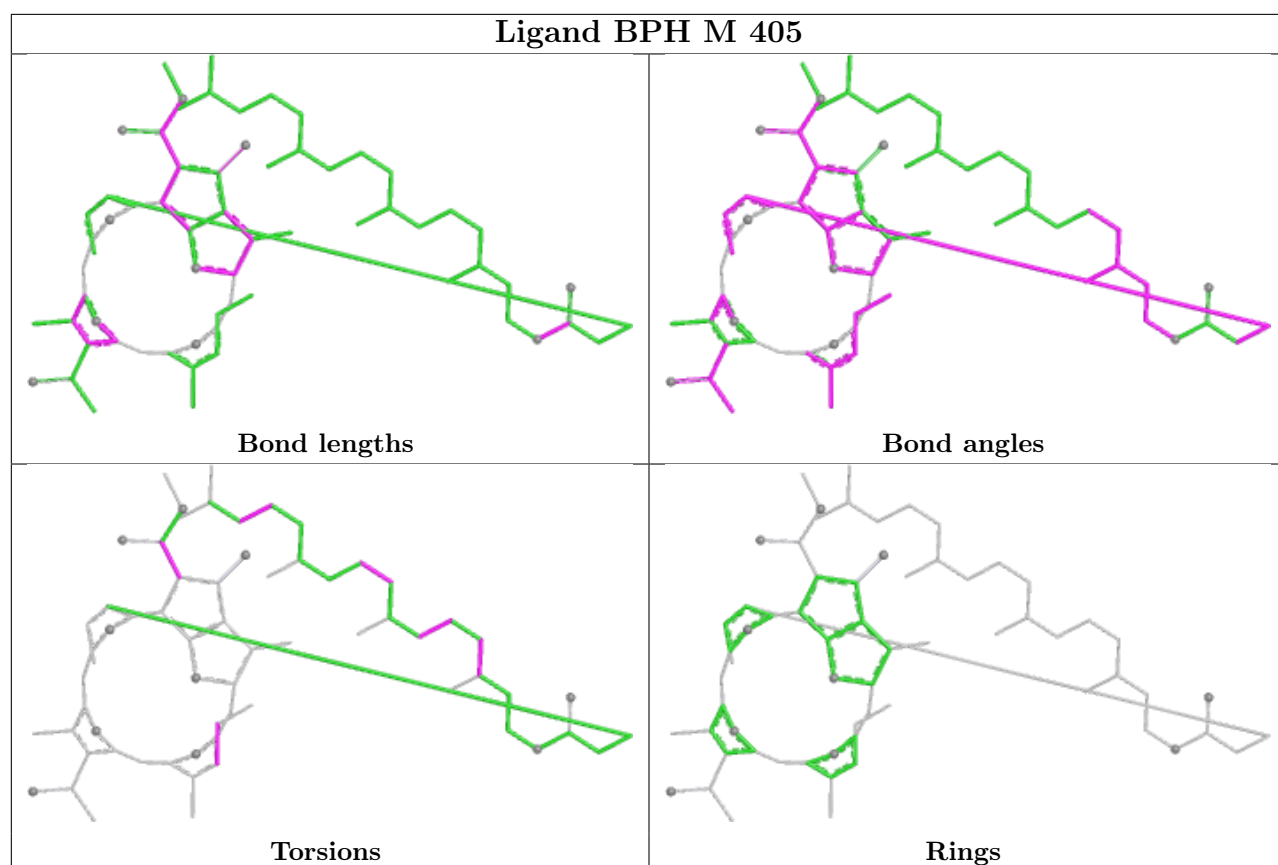


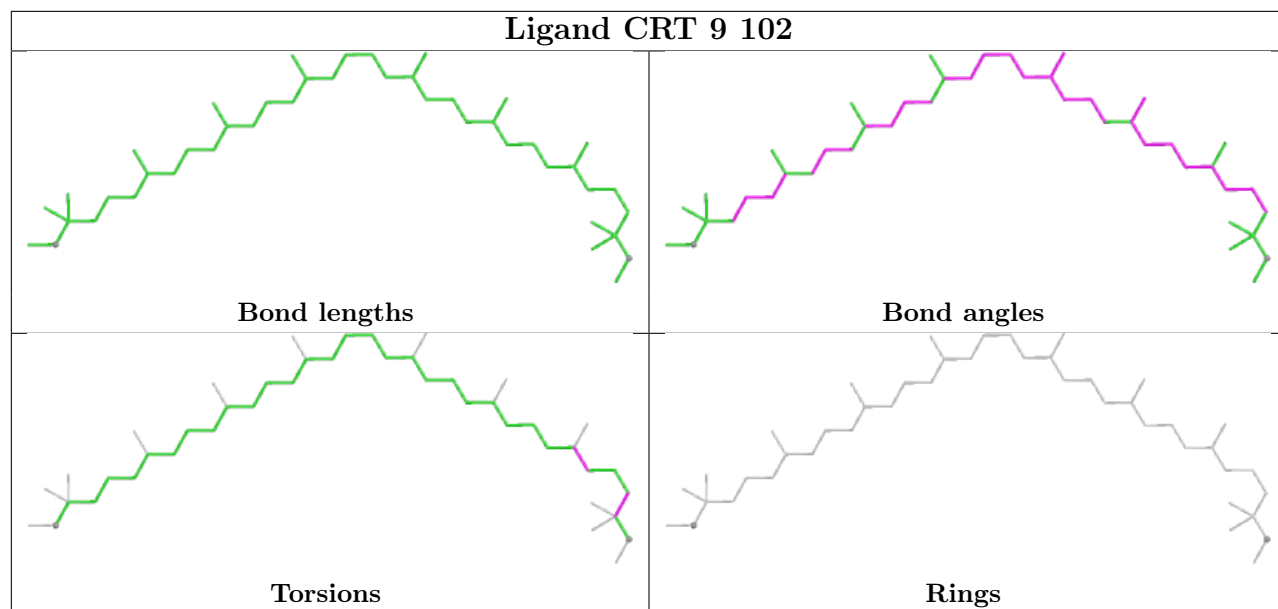


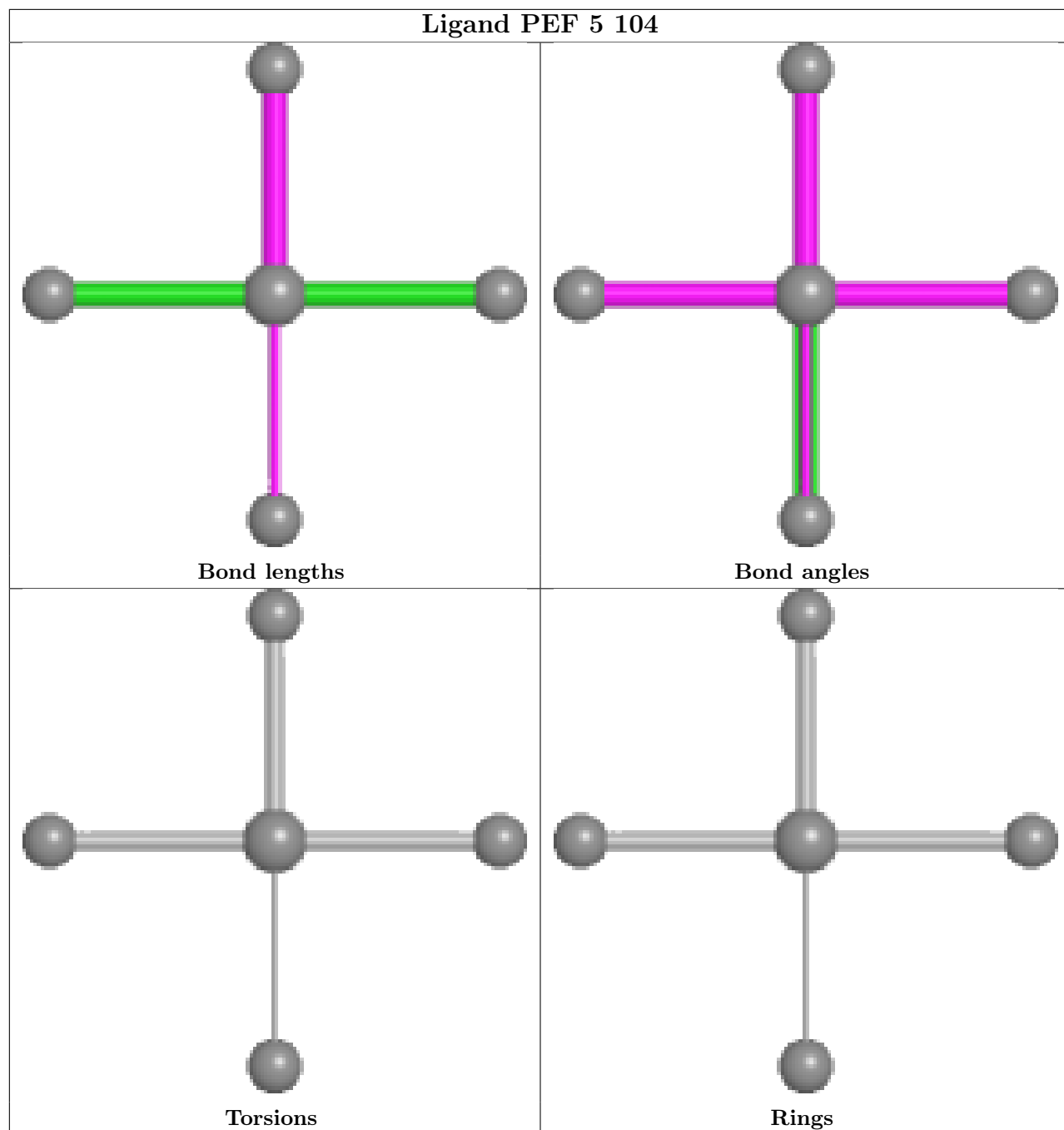


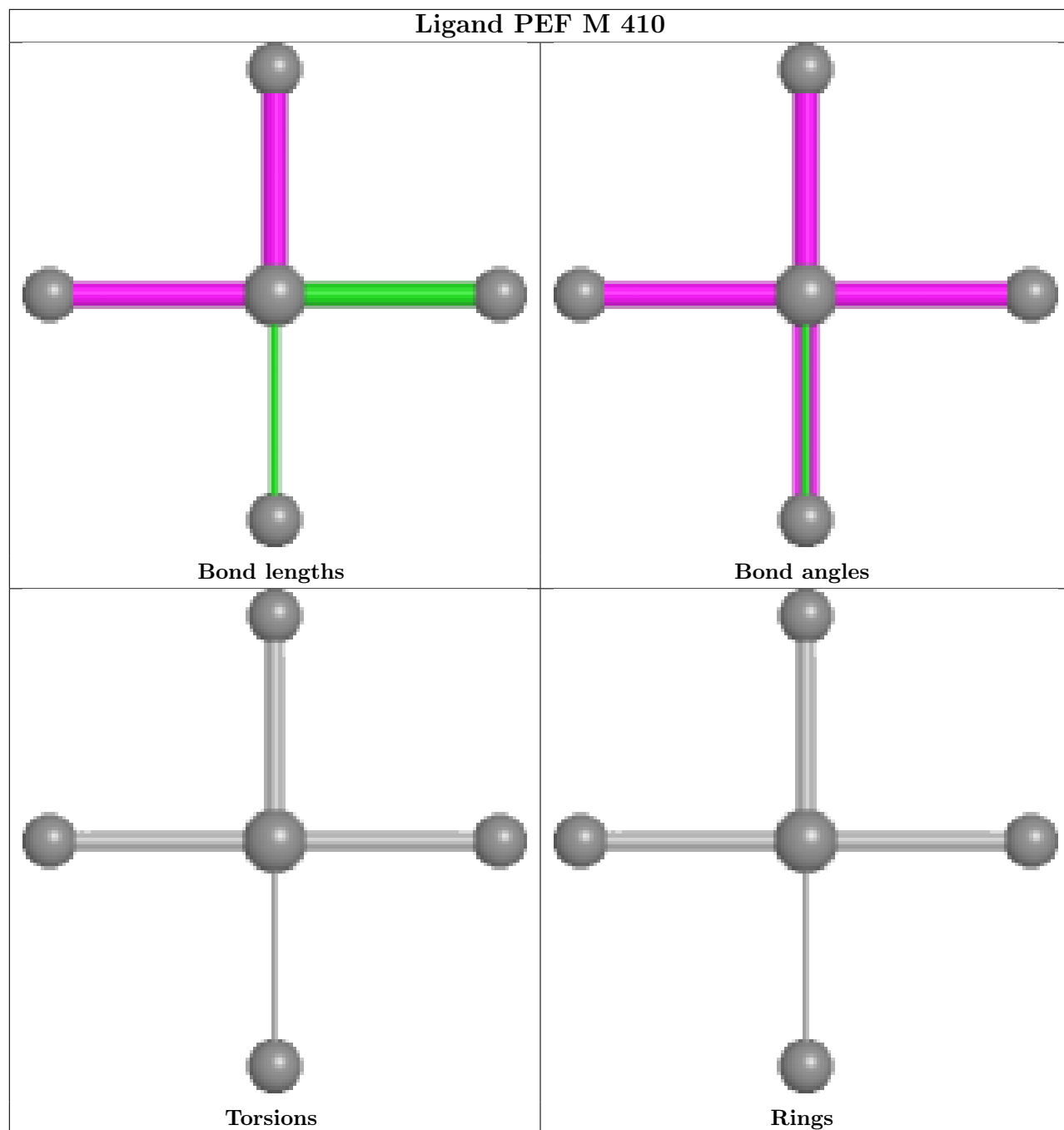
Ligand PEF M 419	
 Bond lengths	 Bond angles
 Torsions	 Rings

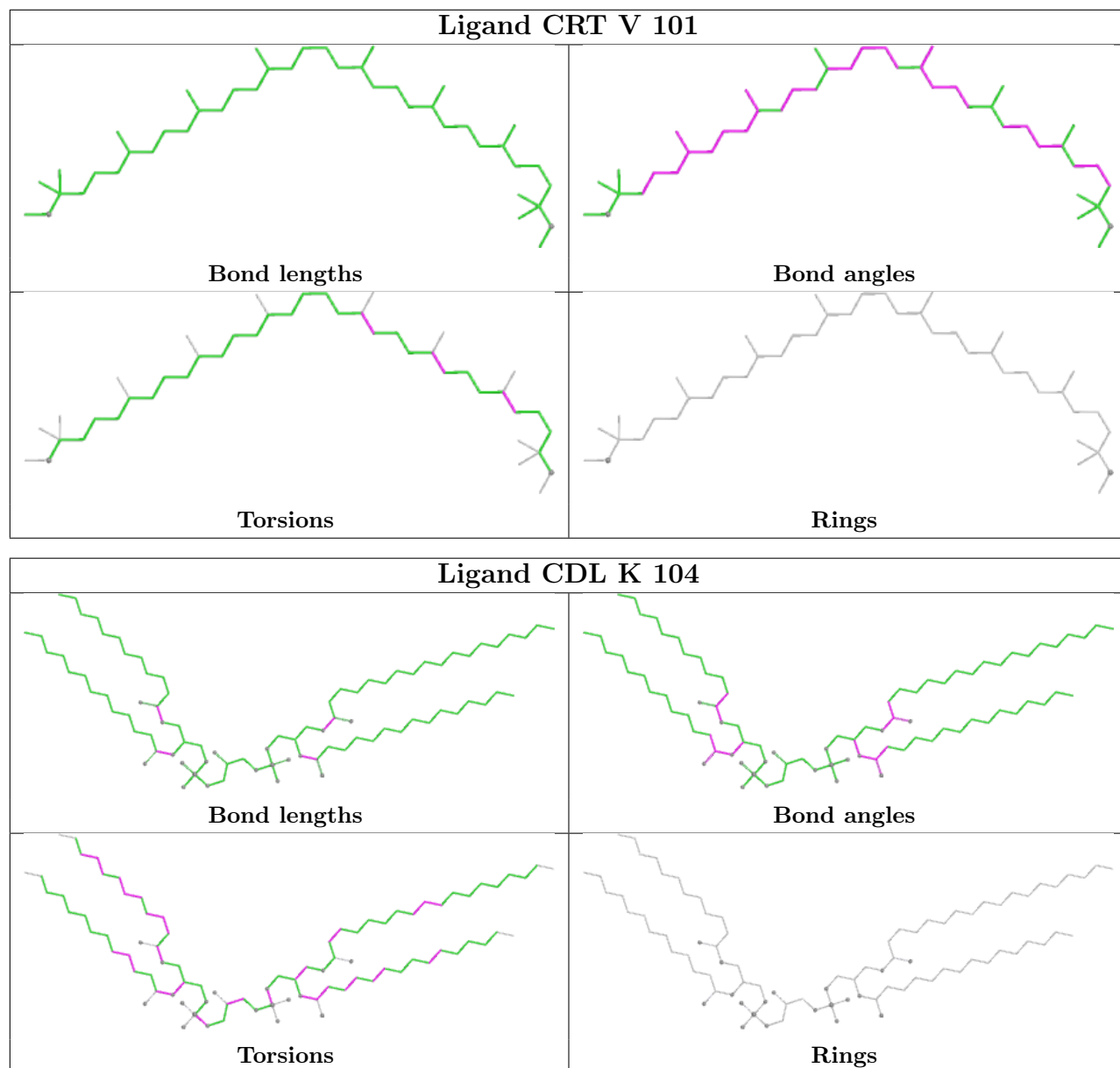


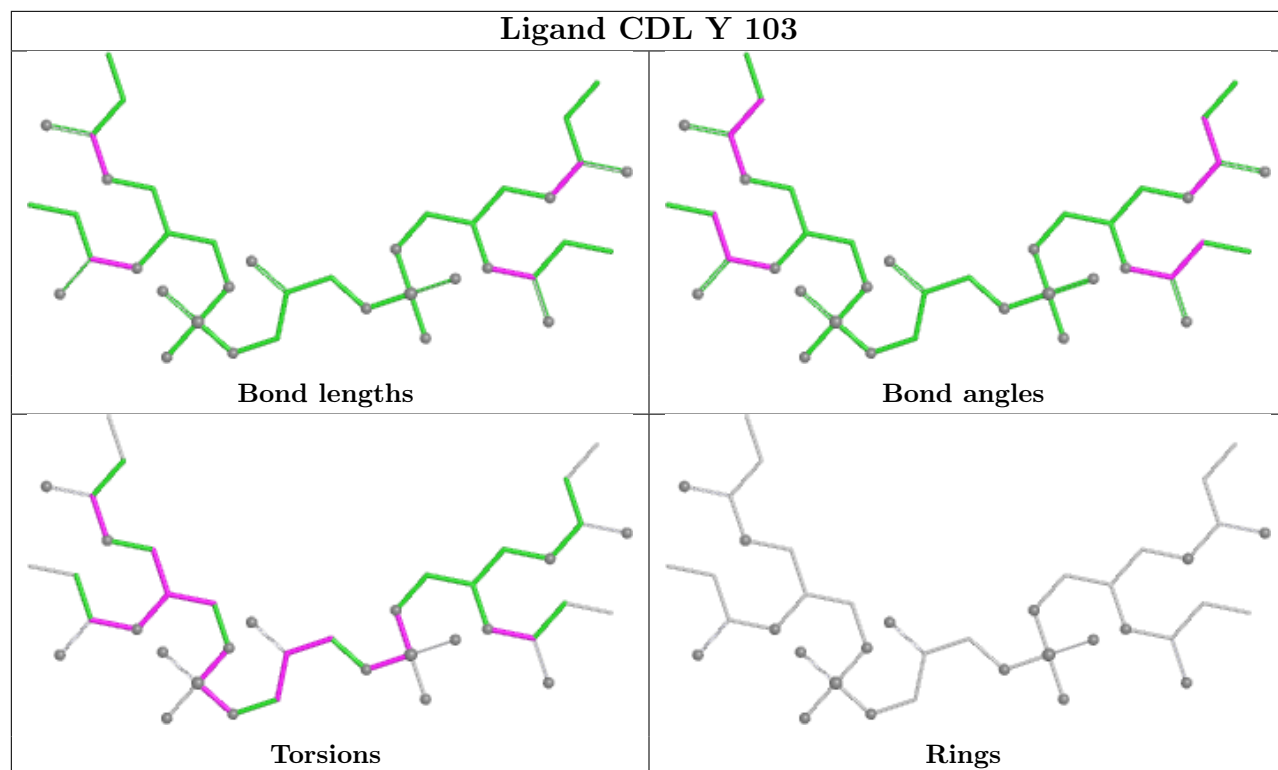


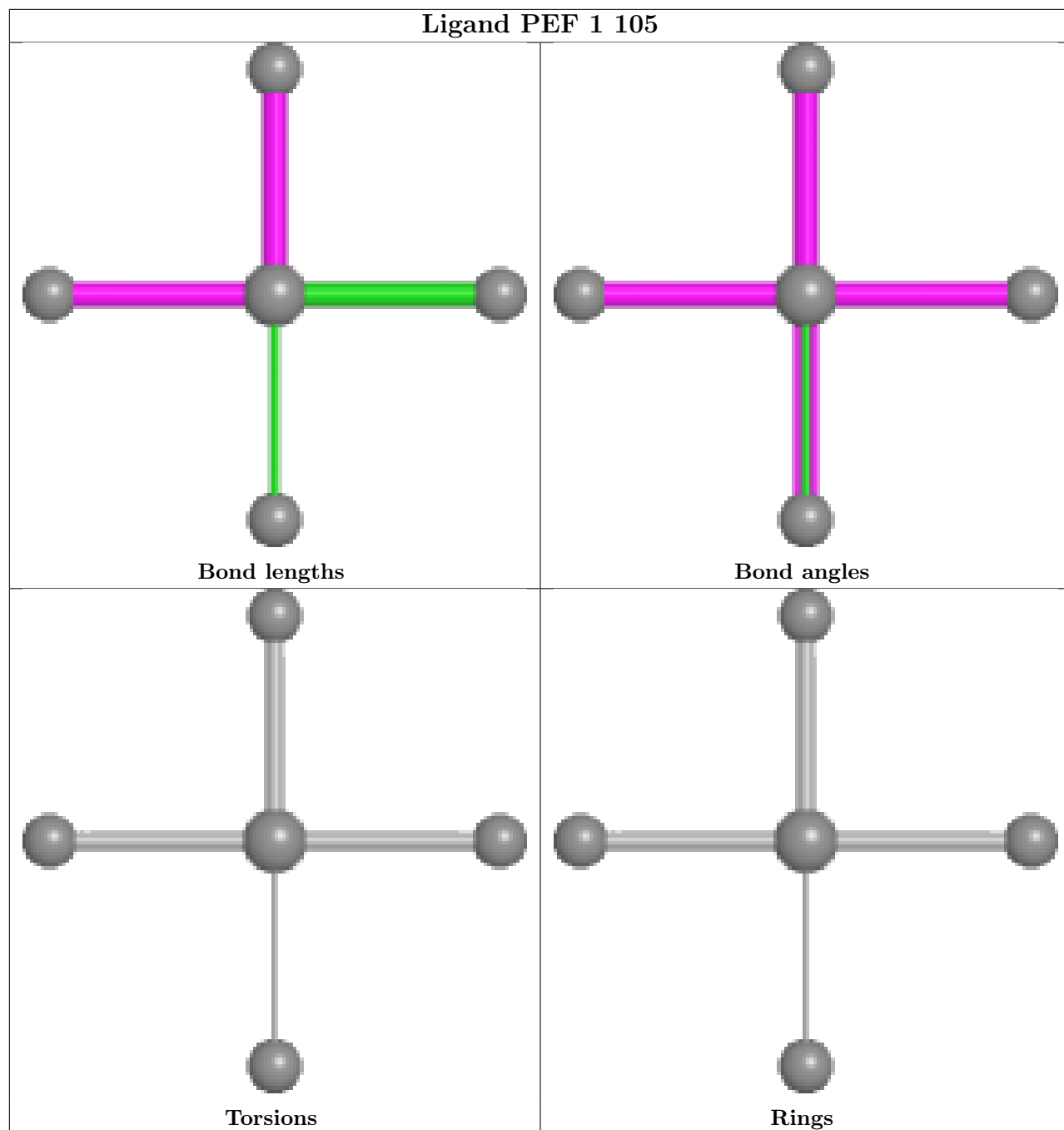


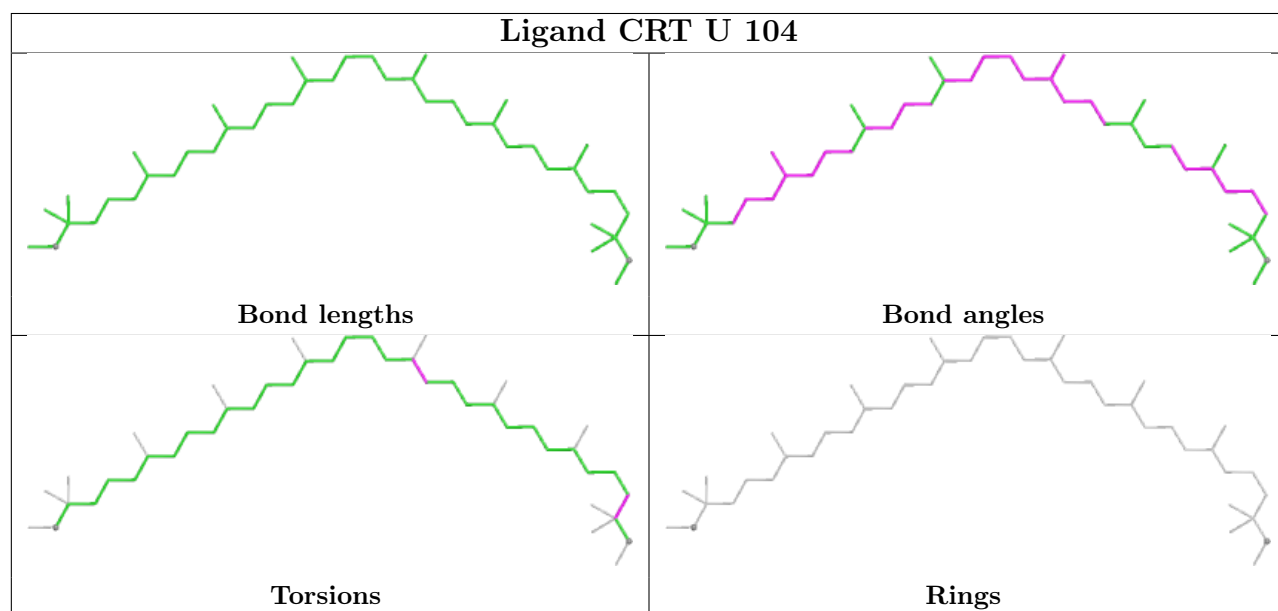
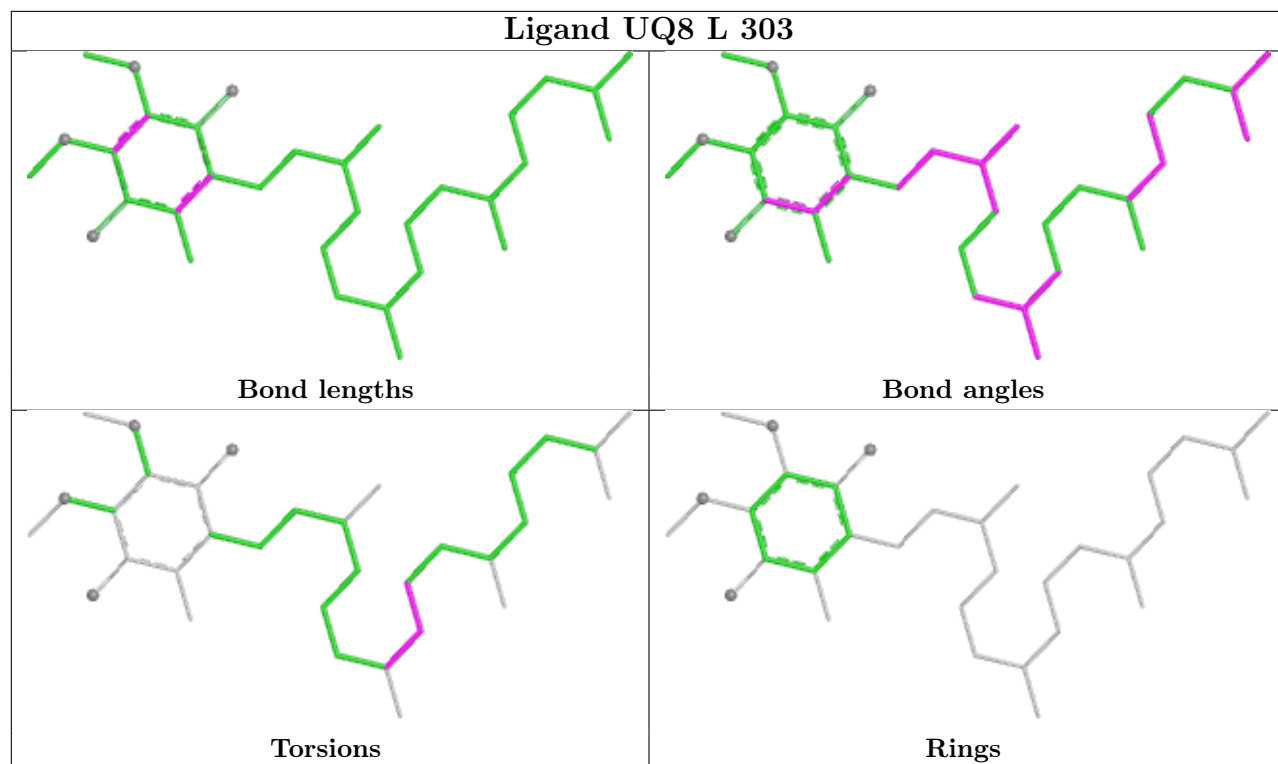




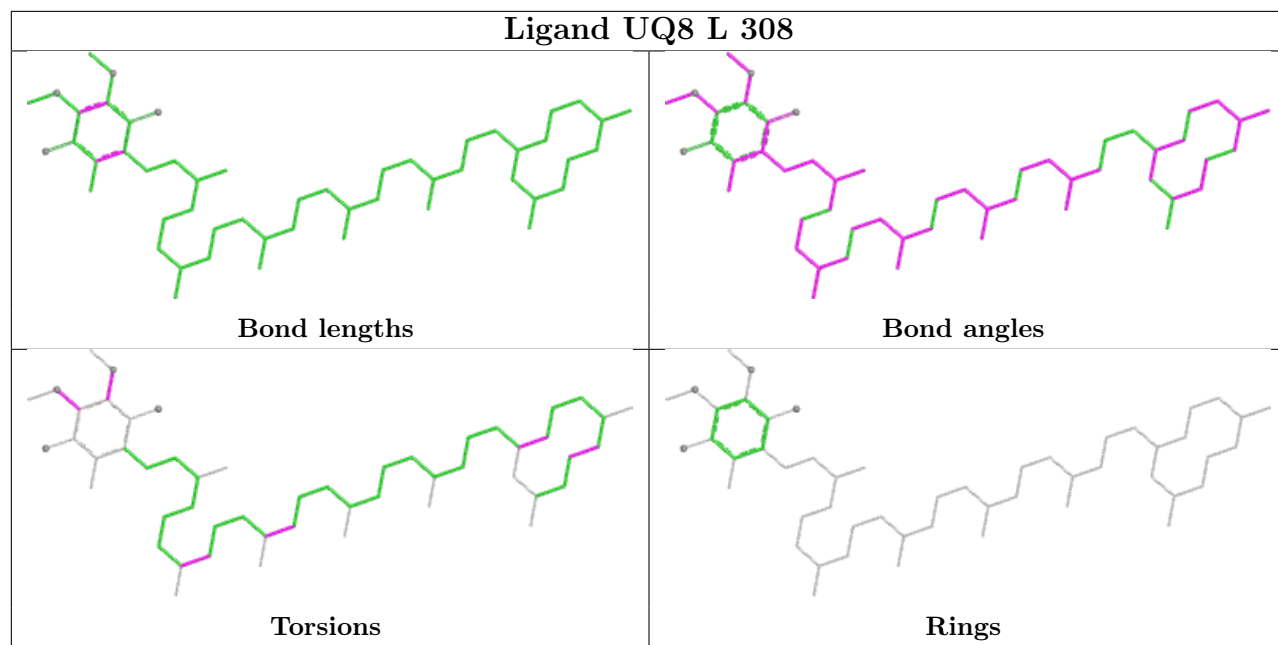




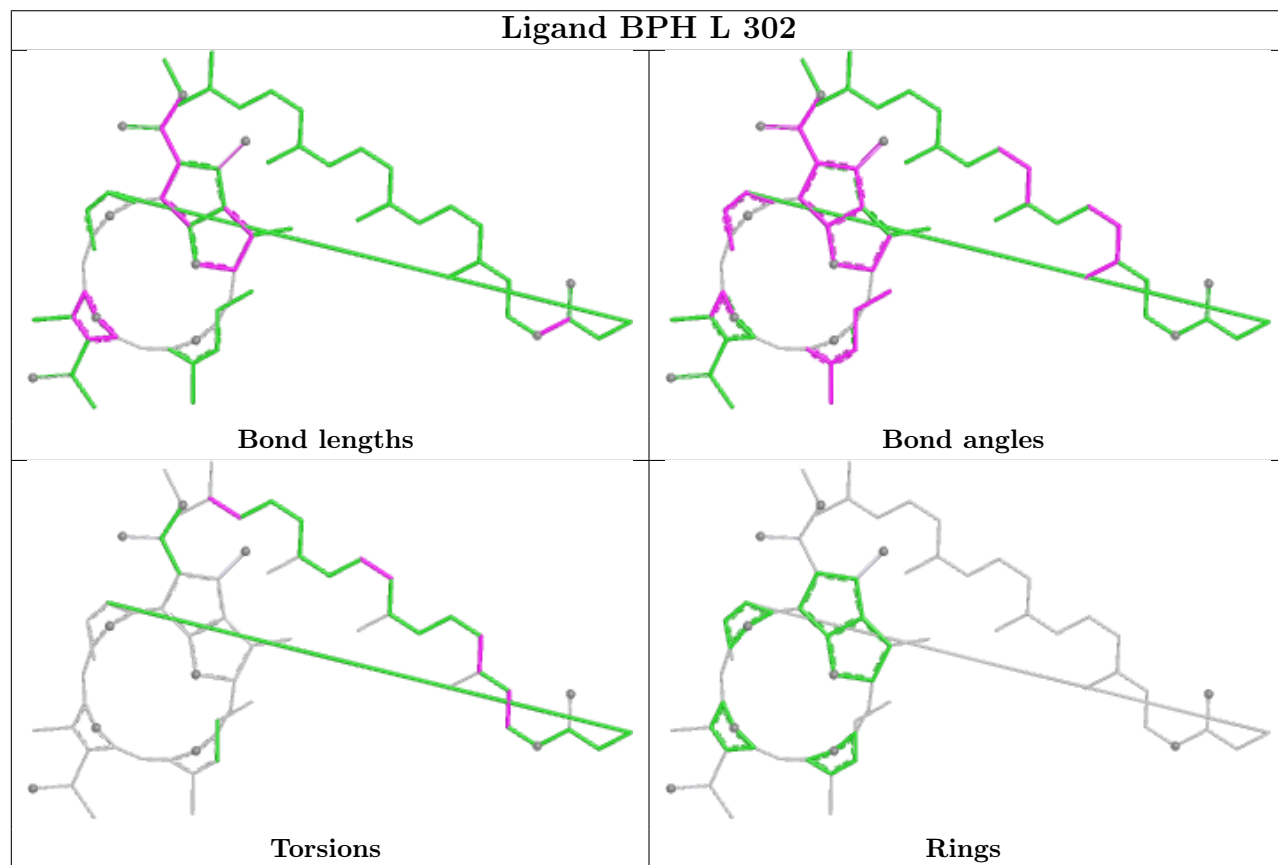


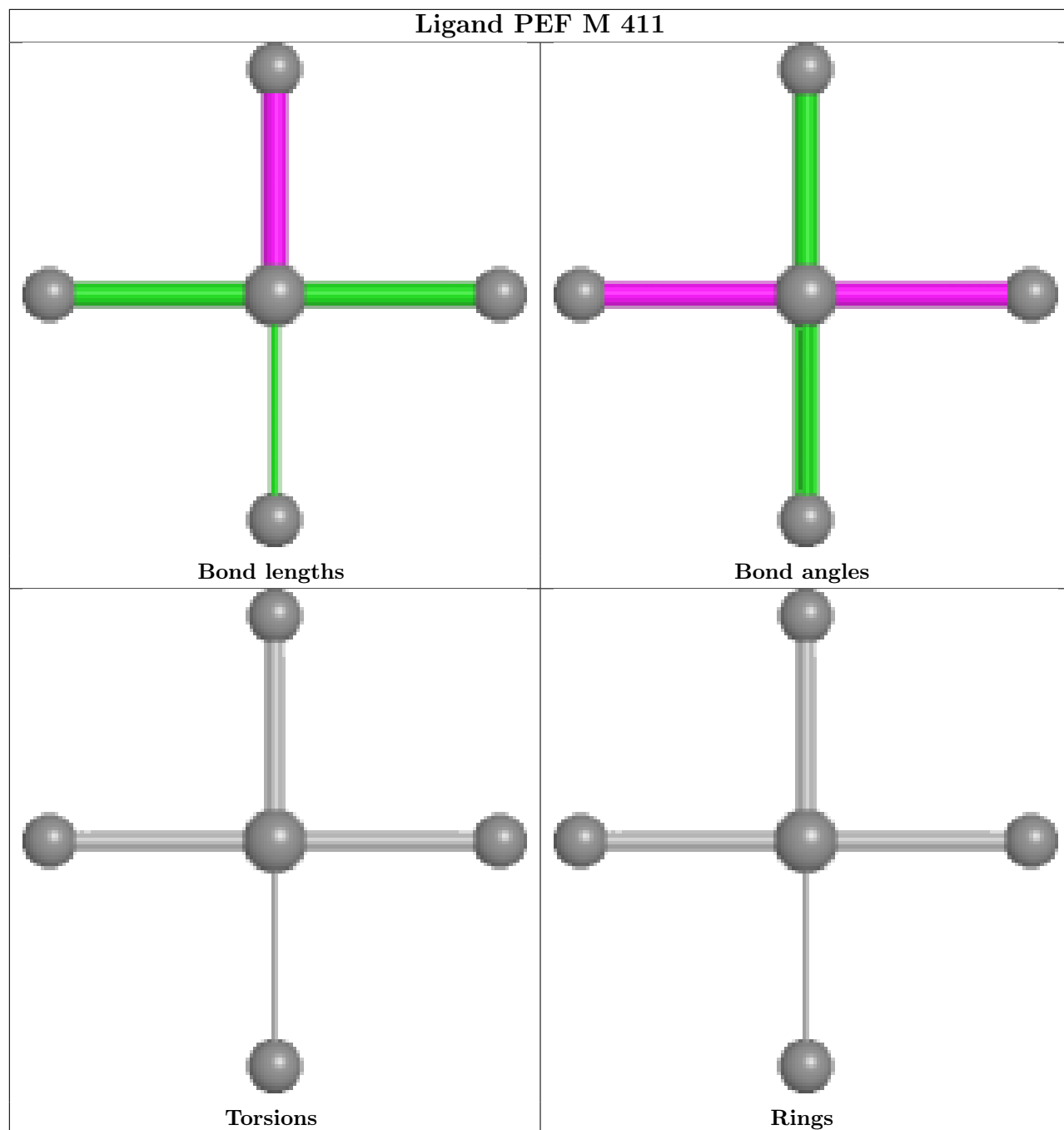


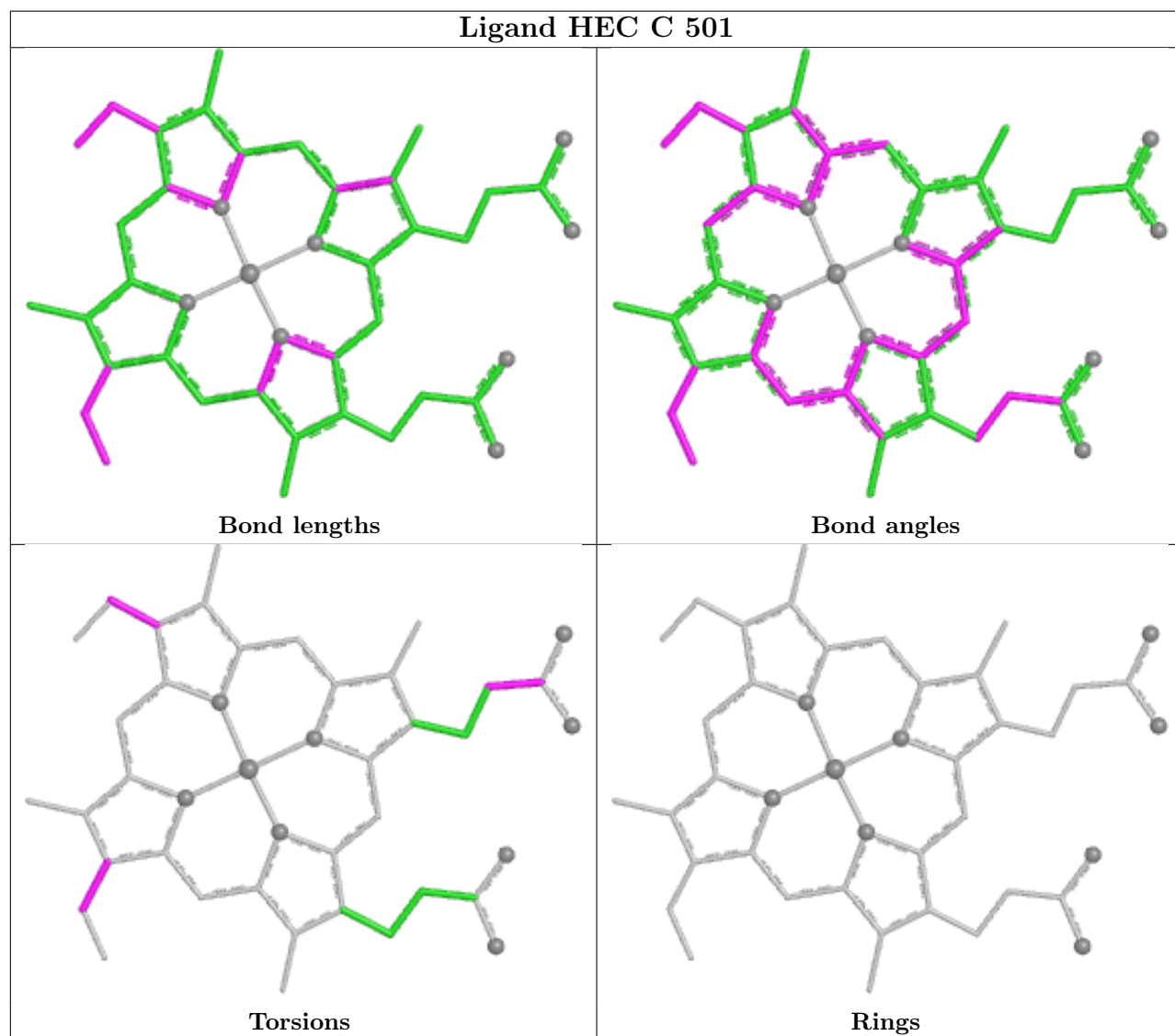
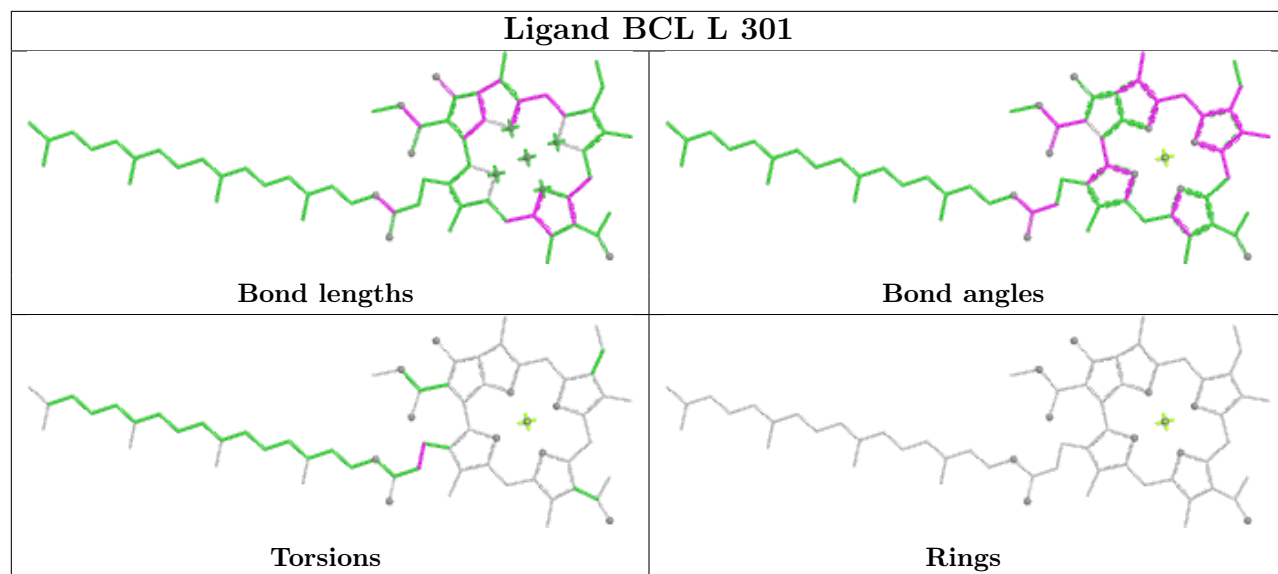
Ligand UQ8 L 308



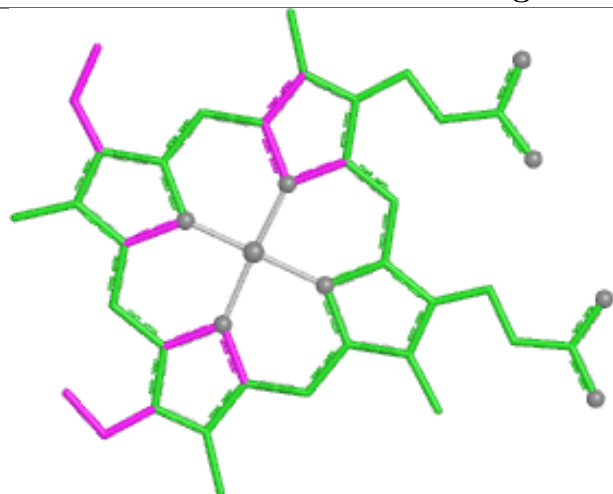
Ligand BPH L 302



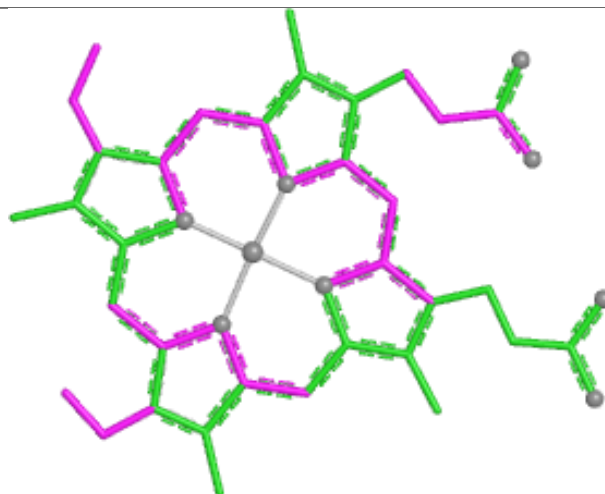




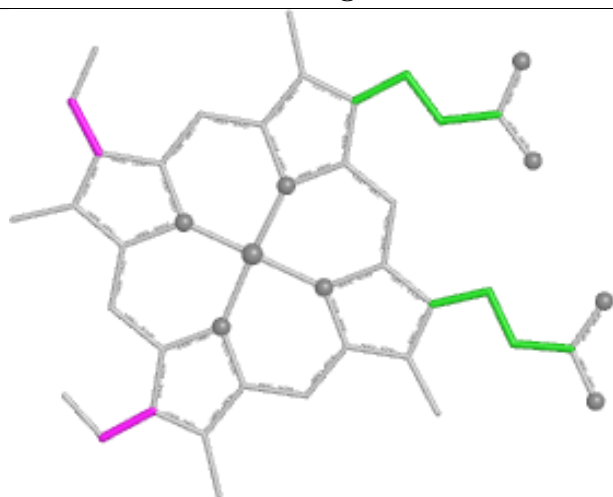
Ligand HEC C 503



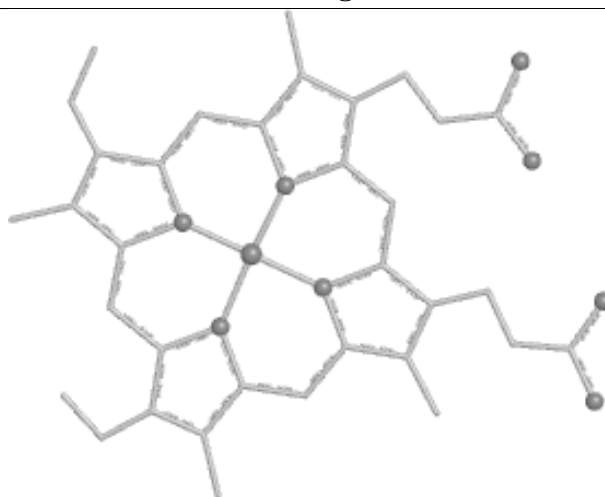
Bond lengths



Bond angles

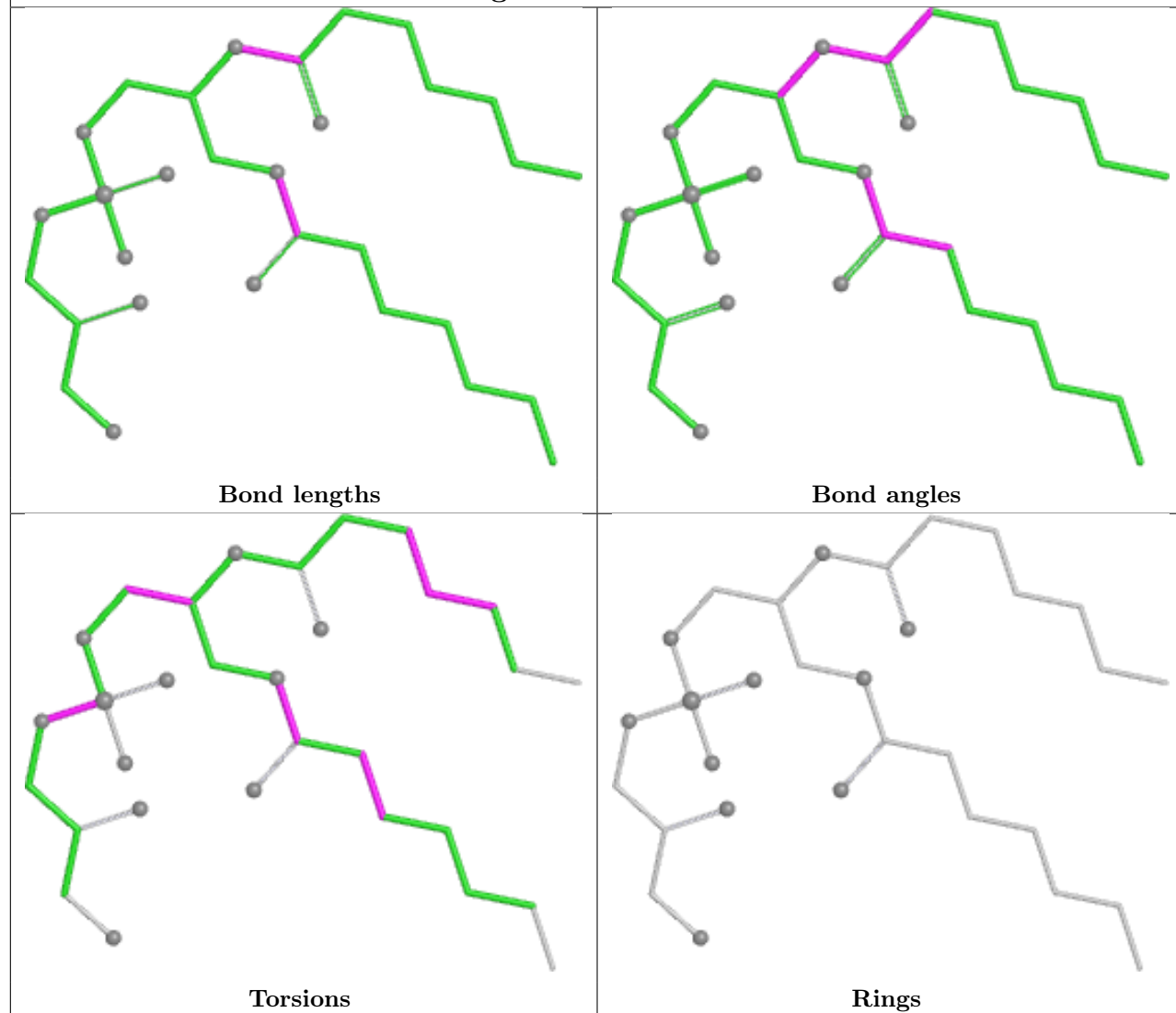


Torsions

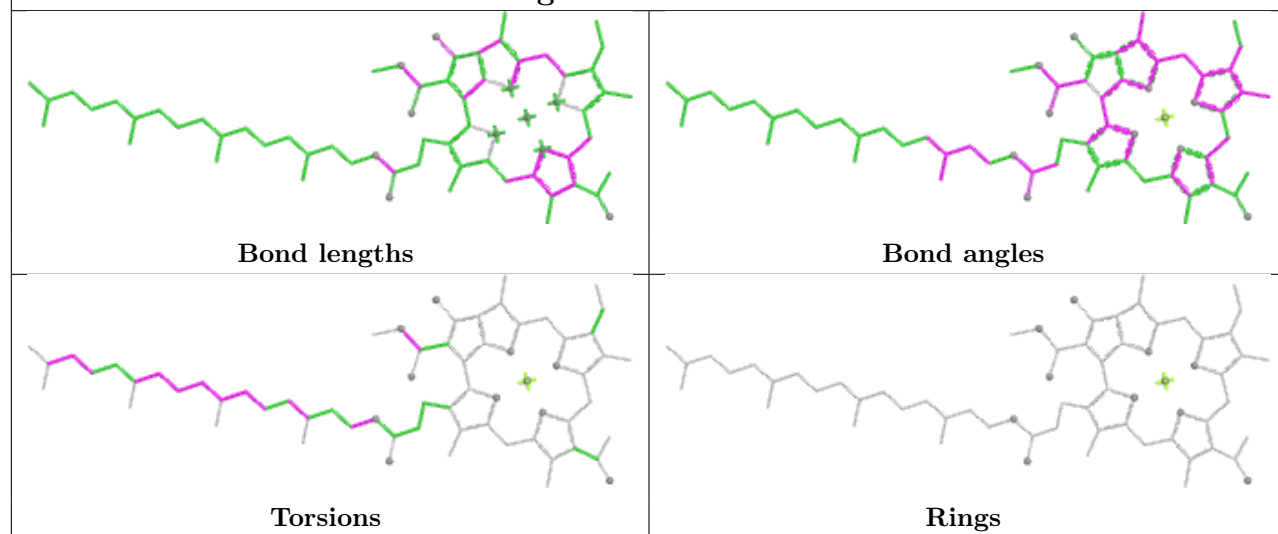


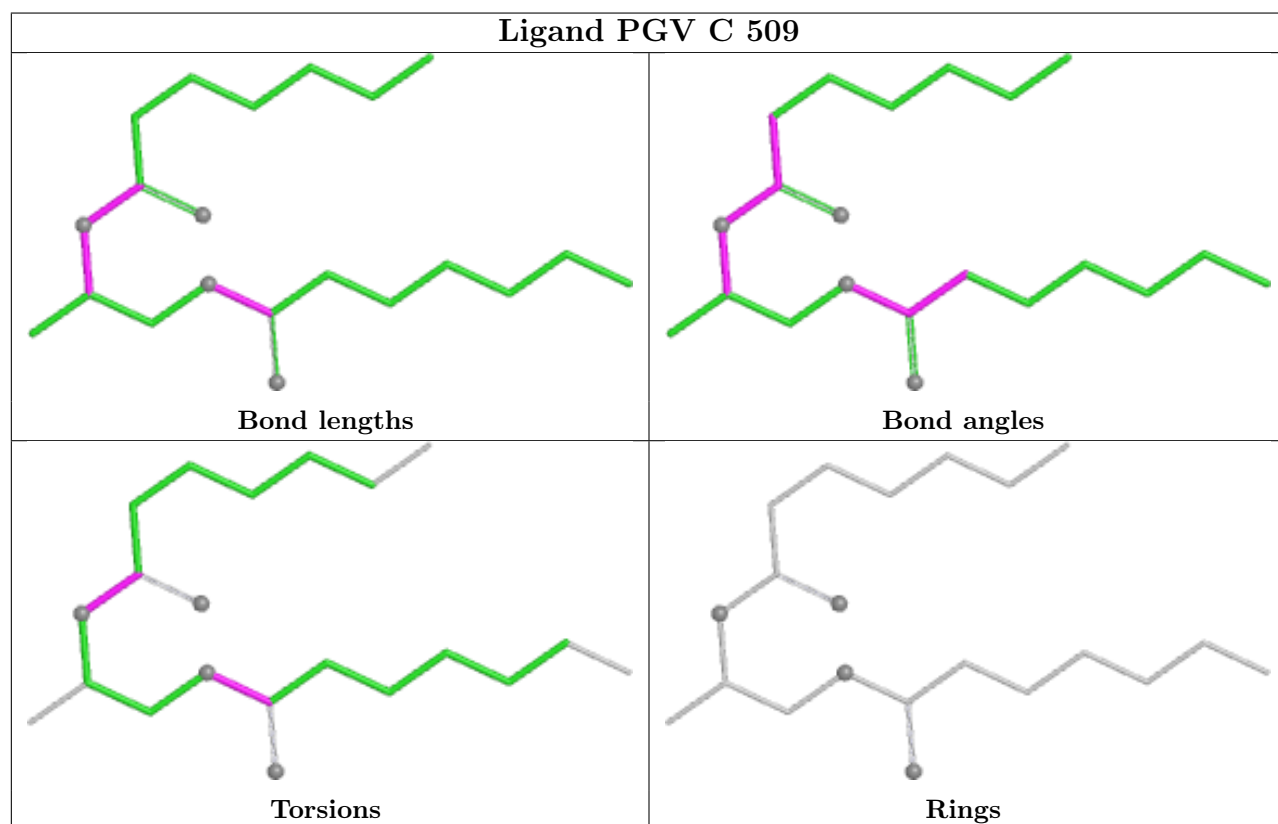
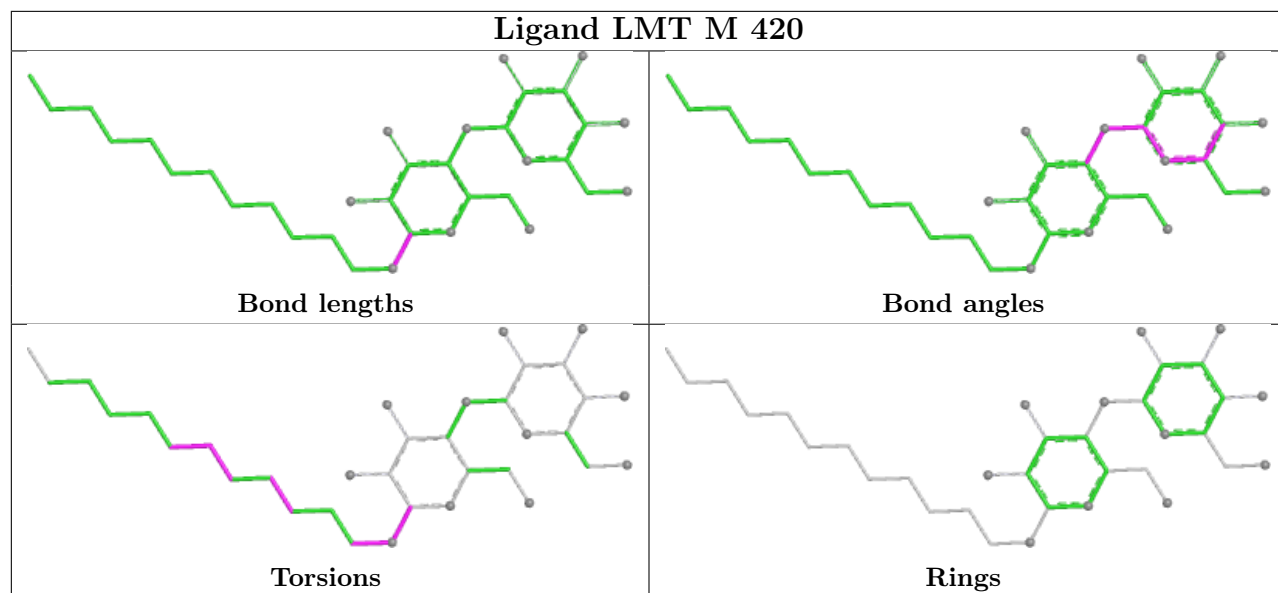
Rings

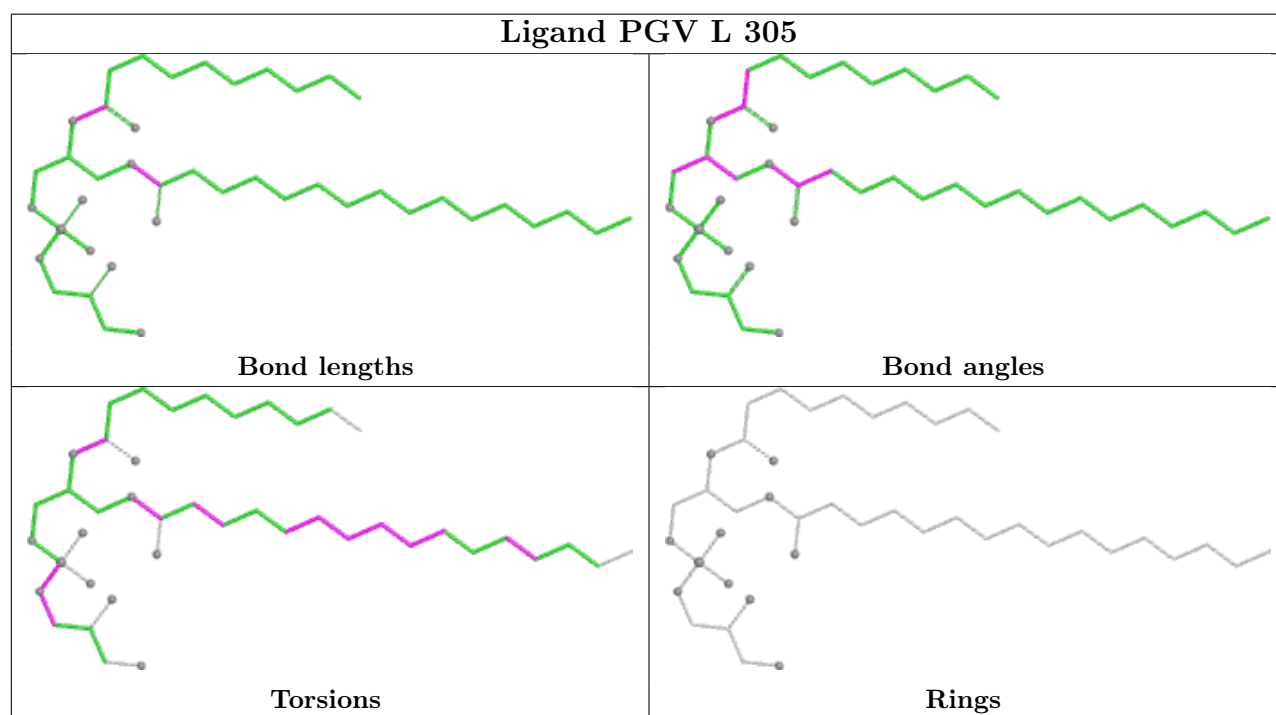
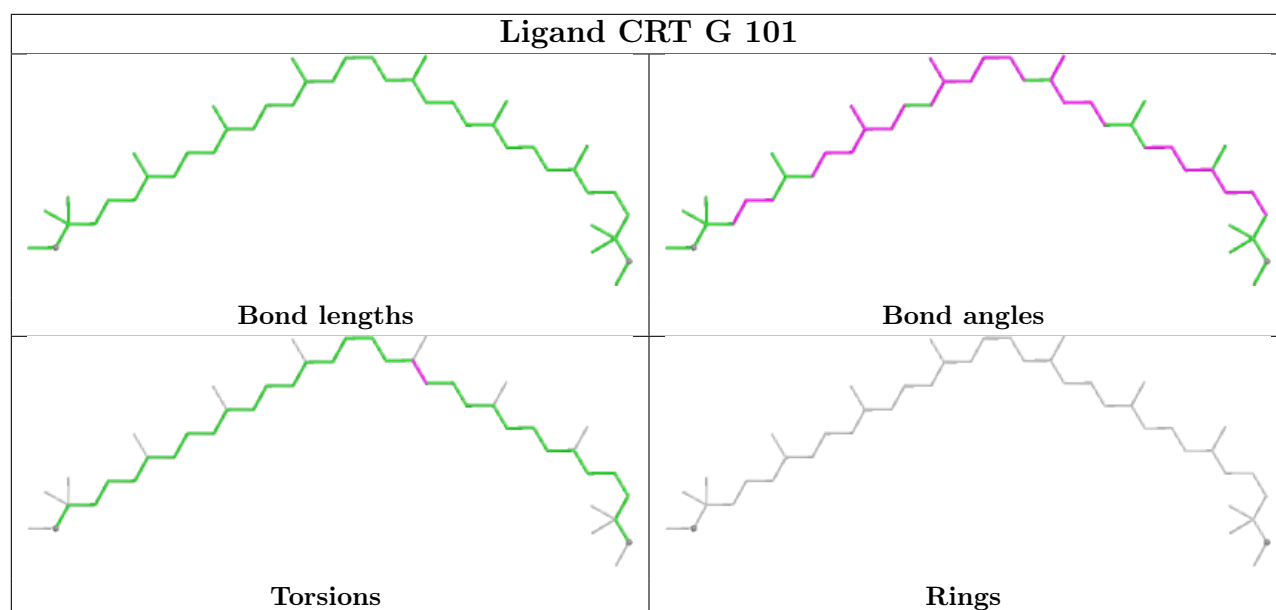
Ligand PGV 1 106

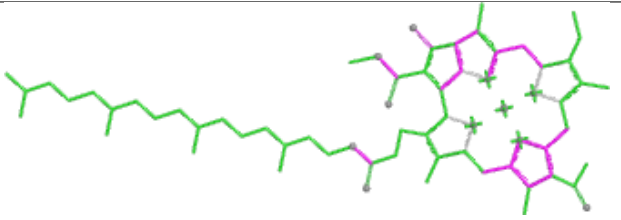
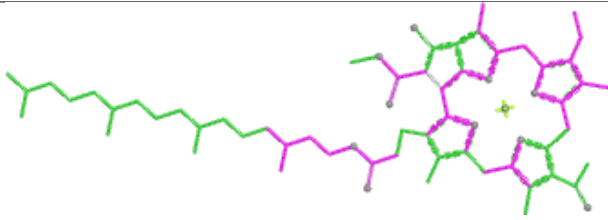
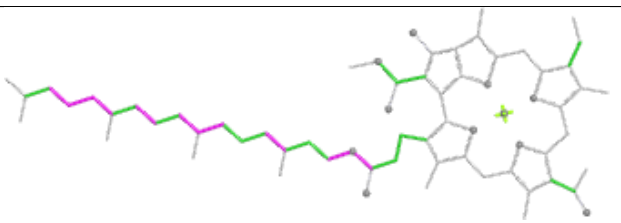
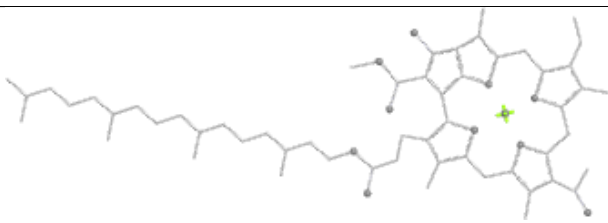
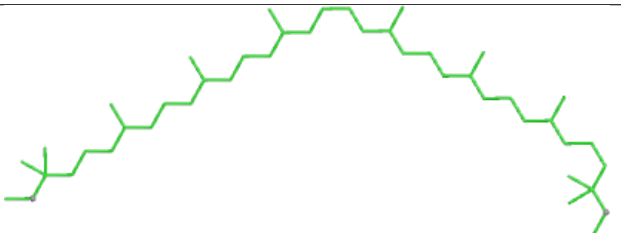
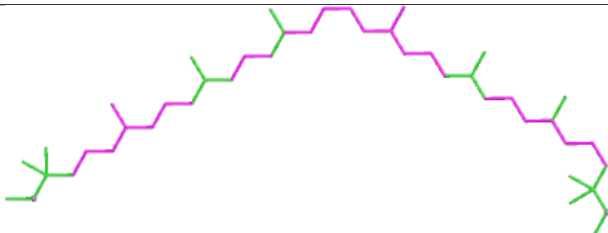
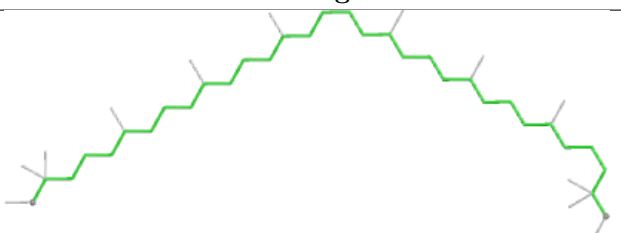
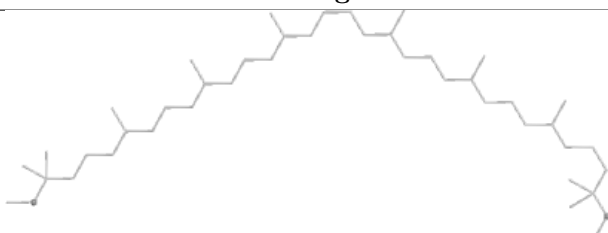
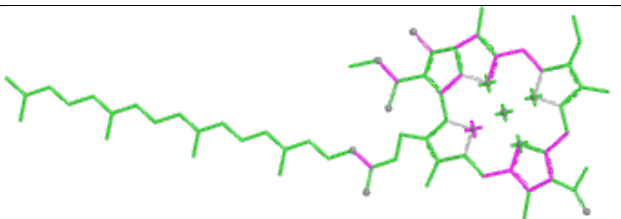
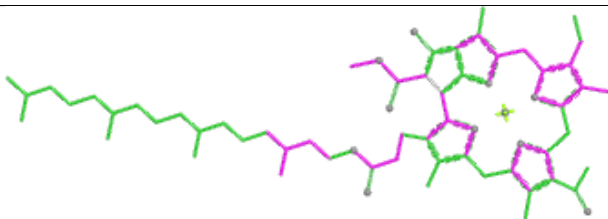
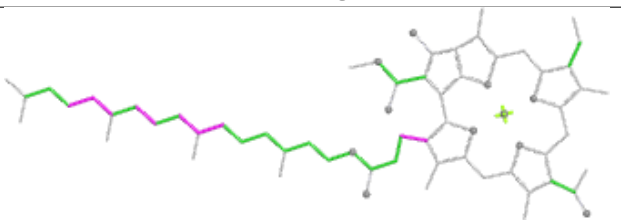
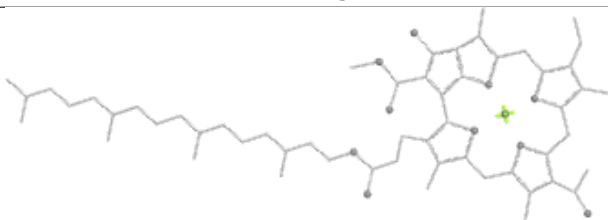


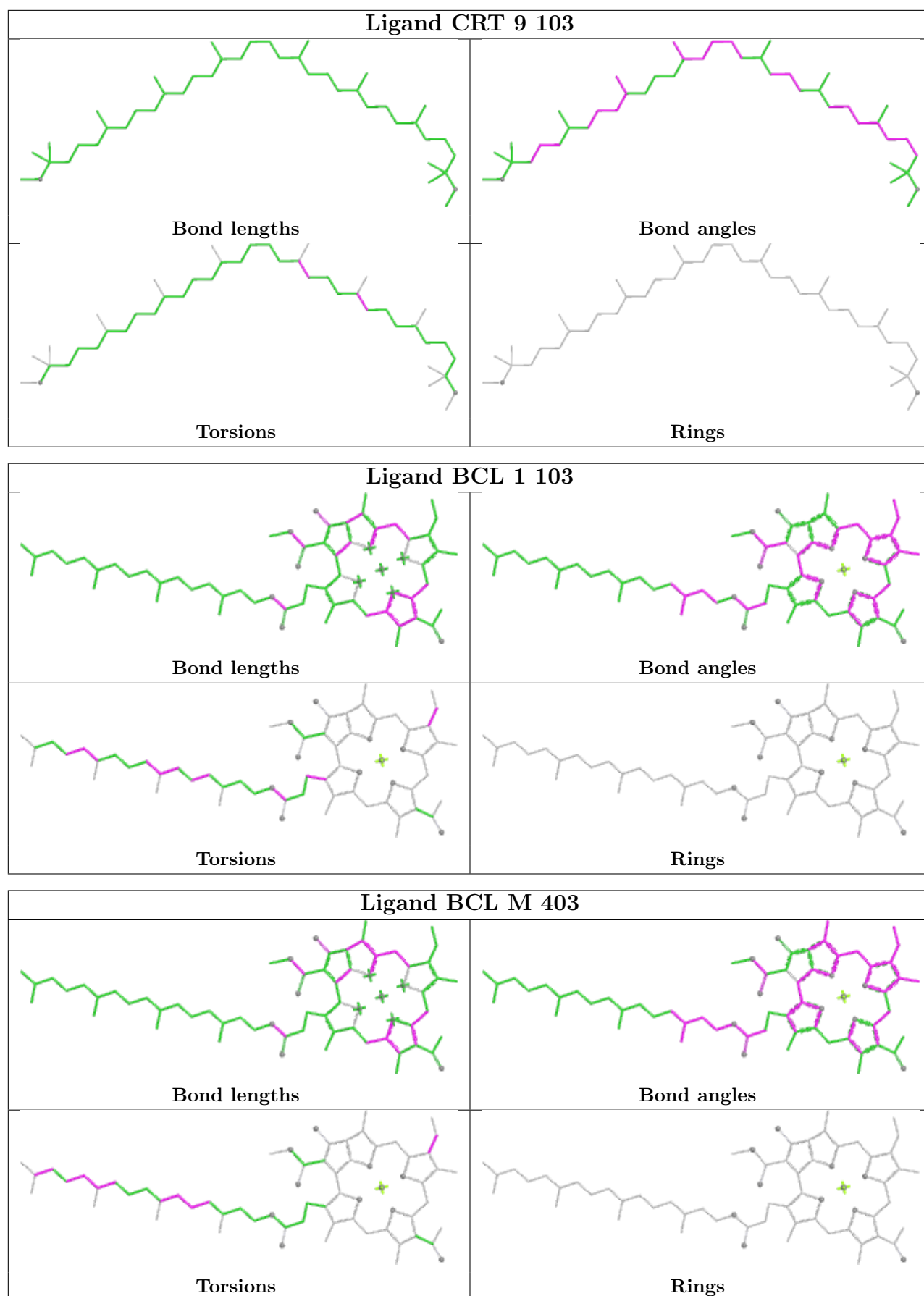
Ligand BCL 9 104







Ligand BCL A 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CRT N 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL Q 103	
 Bond lengths	 Bond angles
 Torsions	 Rings



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%)	0.04	1 (0%) 90 91	32, 48, 81, 113	0
2	L	280/281 (99%)	-0.12	2 (0%) 84 86	31, 44, 59, 100	1 (0%)
3	M	318/325 (97%)	-0.10	2 (0%) 85 87	20, 42, 54, 85	2 (0%)
4	H	255/259 (98%)	0.30	4 (1%) 70 74	29, 57, 87, 130	2 (0%)
5	1	56/61 (91%)	0.84	5 (8%) 15 16	58, 75, 118, 138	0
5	3	56/61 (91%)	0.92	6 (10%) 11 11	39, 77, 106, 145	1 (1%)
5	5	54/61 (88%)	0.73	4 (7%) 20 22	54, 70, 95, 114	0
5	7	57/61 (93%)	0.71	3 (5%) 32 34	54, 65, 127, 139	0
5	9	57/61 (93%)	0.68	4 (7%) 22 24	51, 64, 122, 153	0
5	A	54/61 (88%)	0.68	2 (3%) 45 48	55, 67, 98, 117	0
5	D	55/61 (90%)	0.64	3 (5%) 30 32	37, 69, 101, 136	1 (1%)
5	F	55/61 (90%)	0.63	3 (5%) 30 32	40, 70, 126, 136	1 (1%)
5	I	57/61 (93%)	0.72	5 (8%) 15 16	36, 70, 120, 150	1 (1%)
5	K	57/61 (93%)	0.56	3 (5%) 32 34	50, 64, 109, 131	0
5	O	56/61 (91%)	0.36	3 (5%) 31 33	30, 58, 97, 133	1 (1%)
5	Q	57/61 (93%)	0.27	1 (1%) 67 71	36, 49, 87, 143	0
5	S	56/61 (91%)	0.57	5 (8%) 15 16	20, 53, 109, 147	3 (5%)
5	U	58/61 (95%)	0.48	2 (3%) 48 51	43, 56, 117, 144	0
5	W	56/61 (91%)	0.50	1 (1%) 67 71	47, 60, 98, 120	0
5	Y	57/61 (93%)	0.73	6 (10%) 11 12	51, 67, 113, 145	0
6	0	43/47 (91%)	0.59	1 (2%) 61 65	64, 74, 91, 116	0
6	2	41/47 (87%)	0.75	1 (2%) 59 63	68, 84, 105, 109	0
6	4	42/47 (89%)	0.71	1 (2%) 59 63	65, 80, 98, 107	0
6	6	42/47 (89%)	0.81	1 (2%) 59 63	63, 73, 92, 121	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	8	41/47 (87%)	0.73	2 (4%) 35 37	65, 74, 96, 119	0
6	B	42/47 (89%)	0.63	0 100 100	68, 80, 97, 108	0
6	E	38/47 (80%)	0.45	0 100 100	69, 84, 113, 118	0
6	G	42/47 (89%)	0.53	0 100 100	66, 88, 125, 148	0
6	J	42/47 (89%)	0.74	4 (9%) 14 14	64, 82, 107, 112	0
6	N	42/47 (89%)	0.59	1 (2%) 59 63	57, 75, 95, 102	0
6	P	42/47 (89%)	0.22	1 (2%) 59 63	49, 63, 84, 88	0
6	R	41/47 (87%)	0.38	1 (2%) 59 63	46, 58, 80, 82	0
6	T	43/47 (91%)	0.48	1 (2%) 61 65	49, 61, 82, 97	0
6	V	42/47 (89%)	0.77	3 (7%) 22 23	53, 72, 101, 116	0
6	X	41/47 (87%)	0.53	2 (4%) 35 37	60, 78, 103, 108	0
6	Z	40/47 (85%)	0.48	0 100 100	63, 80, 101, 107	0
All	All	2726/2997 (90%)	0.36	84 (3%) 51 55	20, 60, 101, 153	13 (0%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	9	58	LEU	4.6
5	S	58	LEU	4.3
6	8	9	LEU	4.2
5	1	59	GLY	4.1
6	R	6	LEU	3.9

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 oligosaccharides 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
20	PEF	U	106	5/47	0.54	0.09	156,156,159,160	0
20	PEF	M	408	5/47	0.57	0.10	161,162,163,165	0
20	PEF	5	104	5/47	0.60	0.11	126,127,129,131	0
22	CDL	Y	103	40/100	0.66	0.17	114,129,148,149	0
20	PEF	W	104	5/47	0.71	0.08	146,148,148,149	0
22	CDL	D	104	40/100	0.74	0.19	116,142,163,164	0
22	CDL	S	104	62/100	0.77	0.16	73,116,153,162	0
20	PEF	U	105	5/47	0.77	0.16	113,115,116,118	0
10	SO4	M	413	5/5	0.78	0.12	125,126,126,130	0
15	UQ8	L	309	18/53	0.80	0.24	102,114,125,132	0
21	LDA	M	412	14/16	0.81	0.20	65,82,109,113	0
20	PEF	1	105	5/47	0.81	0.10	119,119,121,121	0
20	PEF	3	104	5/47	0.81	0.10	136,137,138,142	0
10	SO4	C	507	5/5	0.81	0.12	113,114,117,120	0
16	UNL	4	101	12/-	0.82	0.22	72,88,103,105	0
12	PGV	C	509	21/51	0.82	0.22	81,101,108,113	0
16	UNL	J	103	12/-	0.82	0.20	74,79,93,94	0
16	UNL	P	102	12/-	0.82	0.23	67,74,82,82	0
12	PGV	3	105	51/51	0.83	0.20	76,101,155,158	0
20	PEF	M	410	5/47	0.83	0.10	94,98,100,102	0
16	UNL	8	101	12/-	0.83	0.20	64,74,96,96	0
21	LDA	O	105	14/16	0.84	0.23	61,75,110,112	0
16	UNL	T	101	12/-	0.84	0.19	45,68,81,82	0
22	CDL	Q	105	75/100	0.84	0.17	62,97,142,143	0
20	PEF	I	104	5/47	0.84	0.09	99,107,109,112	0
12	PGV	L	306	44/51	0.84	0.17	53,75,98,108	0
21	LDA	V	102	16/16	0.85	0.17	60,77,119,122	0
16	UNL	R	101	12/-	0.85	0.19	57,68,75,77	0
15	UQ8	L	308	53/53	0.85	0.20	60,90,99,104	0
16	UNL	X	101	12/-	0.85	0.20	68,76,82,85	0
15	UQ8	M	418	18/53	0.85	0.17	61,74,96,102	0
9	GOL	C	506	6/6	0.86	0.14	63,68,72,75	0
16	UNL	0	103	12/-	0.86	0.20	77,84,87,87	0
21	LDA	J	102	16/16	0.86	0.17	74,90,112,114	0
22	CDL	Y	104	13/100	0.86	0.14	107,120,124,128	0
23	LMT	M	420	35/35	0.86	0.15	64,99,112,121	0
12	PGV	M	415	37/51	0.87	0.13	60,83,116,121	0
20	PEF	M	409	5/47	0.87	0.10	56,67,83,95	0
12	PGV	1	106	31/51	0.87	0.17	83,102,125,129	0
10	SO4	L	304	5/5	0.87	0.11	136,137,138,138	0
15	UQ8	7	104	33/53	0.87	0.17	60,74,94,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	UNL	B	101	12/-	0.88	0.16	69,80,88,91	0
12	PGV	M	414	46/51	0.88	0.15	52,74,89,94	0
12	PGV	A	105	33/51	0.88	0.17	60,93,108,109	0
22	CDL	H	302	64/100	0.88	0.15	75,89,107,113	0
16	UNL	L	307	12/-	0.88	0.21	79,88,96,96	0
23	LMT	F	104	35/35	0.88	0.13	61,78,92,92	0
20	PEF	K	105	27/47	0.89	0.16	63,85,92,97	0
22	CDL	K	104	86/100	0.89	0.15	56,92,114,120	0
16	UNL	E	101	12/-	0.89	0.20	78,93,101,102	0
16	UNL	G	102	12/-	0.89	0.19	77,85,93,93	0
16	UNL	Z	103	12/-	0.90	0.17	68,80,92,95	0
16	UNL	M	417	9/-	0.91	0.15	58,64,73,75	0
16	UNL	2	102	12/-	0.91	0.17	71,80,90,92	0
22	CDL	M	416	39/100	0.91	0.13	46,80,113,119	0
12	PGV	L	305	43/51	0.91	0.14	45,76,104,109	0
9	GOL	H	301	6/6	0.91	0.13	58,78,82,84	0
20	PEF	M	419	47/47	0.91	0.14	58,75,93,97	0
19	CRT	J	101	44/44	0.92	0.14	59,74,97,100	0
19	CRT	1	104	44/44	0.92	0.13	58,78,96,99	0
19	CRT	2	101	44/44	0.92	0.14	67,78,94,99	0
13	BCL	1	103	66/66	0.92	0.13	49,70,97,104	0
16	UNL	6	102	12/-	0.92	0.17	76,81,91,93	0
13	BCL	3	102	66/66	0.92	0.13	61,75,105,110	0
12	PGV	D	105	35/51	0.92	0.12	55,72,100,113	0
22	CDL	H	304	79/100	0.92	0.14	44,73,107,111	0
12	PGV	H	303	36/51	0.93	0.13	47,59,82,89	0
13	BCL	1	102	66/66	0.93	0.12	59,67,107,113	0
19	CRT	9	102	44/44	0.93	0.12	53,68,100,105	0
18	MQ8	M	406	53/53	0.93	0.14	36,53,116,123	0
13	BCL	3	103	66/66	0.93	0.12	53,69,93,96	0
19	CRT	N	101	44/44	0.93	0.12	50,67,86,94	0
13	BCL	5	102	66/66	0.94	0.12	55,69,109,111	0
19	CRT	U	104	44/44	0.94	0.11	48,72,91,96	0
19	CRT	Z	101	44/44	0.94	0.13	58,72,99,100	0
13	BCL	7	102	61/66	0.94	0.11	53,64,96,103	0
13	BCL	7	103	66/66	0.94	0.11	53,63,95,102	0
19	CRT	6	101	44/44	0.94	0.11	48,69,84,87	0
11	LHG	C	508	9/49	0.94	0.12	52,61,67,69	0
19	CRT	M	407	44/44	0.94	0.10	31,39,82,90	0
19	CRT	A	104	44/44	0.94	0.13	62,74,97,101	0
21	LDA	I	105	16/16	0.94	0.14	36,70,75,77	0
19	CRT	G	101	44/44	0.94	0.12	61,80,114,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	BCL	O	103	66/66	0.94	0.11	41,51,89,96	0
13	BCL	5	103	66/66	0.95	0.10	50,62,90,98	0
13	BCL	K	102	66/66	0.95	0.11	50,63,102,105	0
13	BCL	A	101	66/66	0.95	0.10	54,69,113,118	0
13	BCL	9	104	66/66	0.95	0.10	54,63,103,106	0
13	BCL	0	102	66/66	0.95	0.10	54,65,97,108	0
15	UQ8	L	303	33/53	0.95	0.11	36,45,77,85	0
19	CRT	9	103	44/44	0.95	0.11	51,67,94,105	0
19	CRT	0	101	44/44	0.95	0.10	51,68,88,95	0
13	BCL	S	103	66/66	0.95	0.10	40,48,90,96	0
13	BCL	W	102	66/66	0.95	0.12	48,59,114,118	0
13	BCL	W	103	66/66	0.95	0.10	49,60,94,97	0
13	BCL	Y	102	66/66	0.95	0.11	49,60,110,113	0
13	BCL	Z	102	66/66	0.95	0.11	52,64,98,103	0
13	BCL	A	103	66/66	0.95	0.11	58,70,104,109	0
13	BCL	D	102	66/66	0.95	0.11	55,70,117,121	0
13	BCL	F	102	66/66	0.95	0.10	57,69,114,117	0
13	BCL	F	103	66/66	0.95	0.11	55,70,107,113	0
13	BCL	I	102	66/66	0.95	0.10	61,68,100,104	0
13	BCL	D	103	66/66	0.96	0.10	57,69,91,92	0
13	BCL	K	103	66/66	0.96	0.09	47,58,98,102	0
13	BCL	M	403	66/66	0.96	0.09	26,35,84,90	0
19	CRT	O	104	44/44	0.96	0.09	37,51,75,82	0
20	PEF	M	411	5/47	0.96	0.07	40,45,52,54	0
19	CRT	P	101	44/44	0.96	0.09	38,55,77,80	0
19	CRT	Q	104	44/44	0.96	0.09	42,55,73,76	0
13	BCL	Q	102	66/66	0.96	0.10	40,48,94,99	0
19	CRT	V	101	44/44	0.96	0.09	41,62,85,87	0
13	BCL	Q	103	66/66	0.96	0.09	39,47,84,93	0
14	BPH	L	302	65/65	0.96	0.08	29,40,54,59	0
13	BCL	S	102	66/66	0.96	0.09	38,49,96,110	0
13	BCL	I	103	66/66	0.96	0.09	51,65,93,95	0
13	BCL	U	102	66/66	0.96	0.09	42,53,101,104	0
13	BCL	U	103	66/66	0.96	0.10	44,55,92,101	0
13	BCL	M	404	66/66	0.97	0.06	27,34,45,54	0
13	BCL	O	102	66/66	0.97	0.09	44,54,102,112	0
13	BCL	L	301	66/66	0.97	0.07	27,34,43,70	0
14	BPH	M	405	65/65	0.97	0.08	29,38,111,115	0
13	BCL	M	402	66/66	0.98	0.06	30,39,54,62	0
7	HEC	C	502	43/43	0.98	0.06	39,46,52,55	0
7	HEC	C	503	43/43	0.98	0.06	29,35,42,46	0
7	HEC	C	504	43/43	0.98	0.06	34,40,47,54	0

Continued on next page...

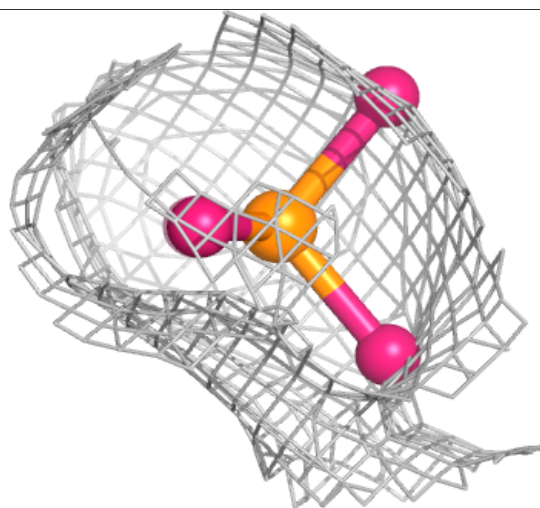
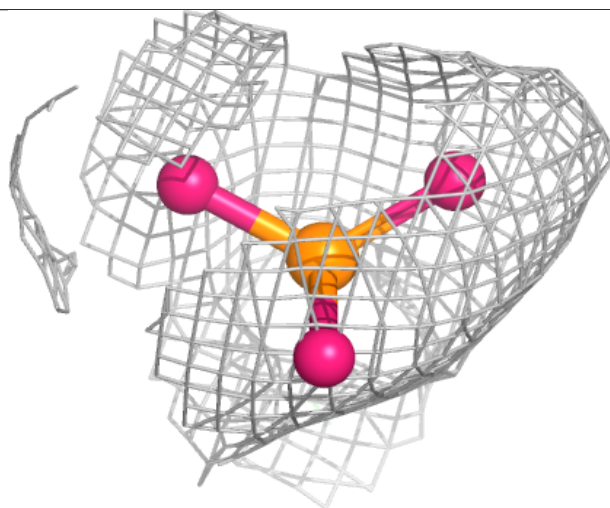
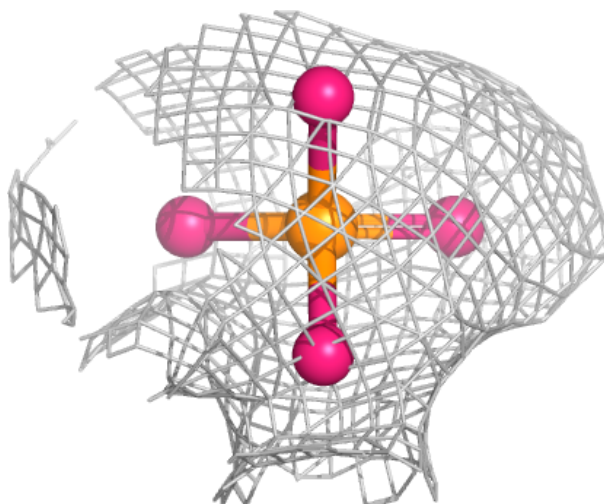
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	HEC	C	501	43/43	0.98	0.07	52,60,67,75	0
8	MG	C	505	1/1	0.99	0.02	36,36,36,36	0
24	CA	A	102	1/1	0.99	0.03	64,64,64,64	0
24	CA	Y	101	1/1	0.99	0.03	60,60,60,60	0
24	CA	1	101	1/1	0.99	0.03	60,60,60,60	0
24	CA	3	101	1/1	0.99	0.05	68,68,68,68	0
24	CA	5	101	1/1	0.99	0.03	68,68,68,68	0
24	CA	9	101	1/1	0.99	0.03	67,67,67,67	0
24	CA	O	101	1/1	1.00	0.02	56,56,56,56	0
24	CA	Q	101	1/1	1.00	0.02	47,47,47,47	0
24	CA	S	101	1/1	1.00	0.02	44,44,44,44	0
24	CA	U	101	1/1	1.00	0.02	48,48,48,48	0
24	CA	W	101	1/1	1.00	0.02	52,52,52,52	0
17	FE	M	401	1/1	1.00	0.02	39,39,39,39	0
24	CA	D	101	1/1	1.00	0.02	64,64,64,64	0
24	CA	F	101	1/1	1.00	0.02	65,65,65,65	0
24	CA	I	101	1/1	1.00	0.02	64,64,64,64	0
24	CA	7	101	1/1	1.00	0.02	67,67,67,67	0
24	CA	K	101	1/1	1.00	0.02	63,63,63,63	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.

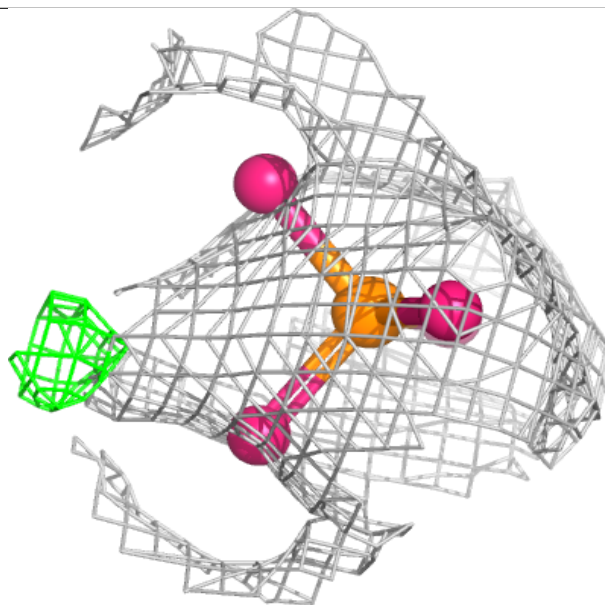
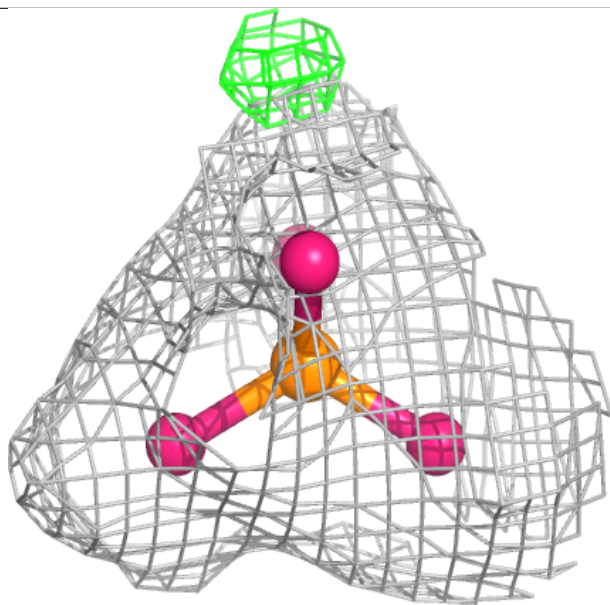
Electron density around PEF U 106:

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



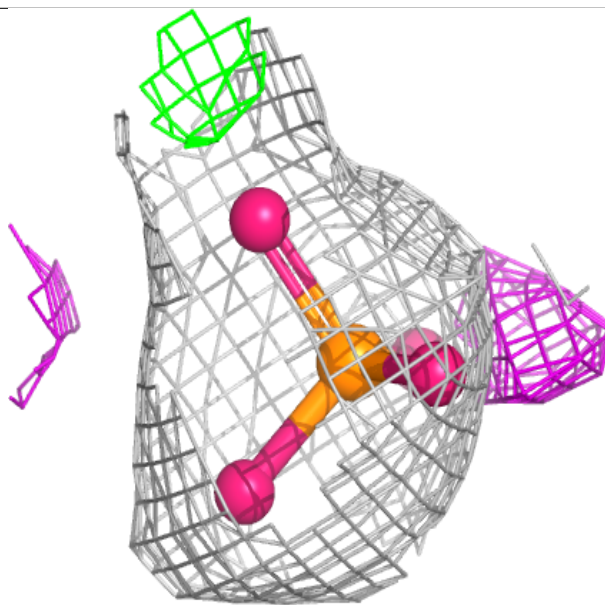
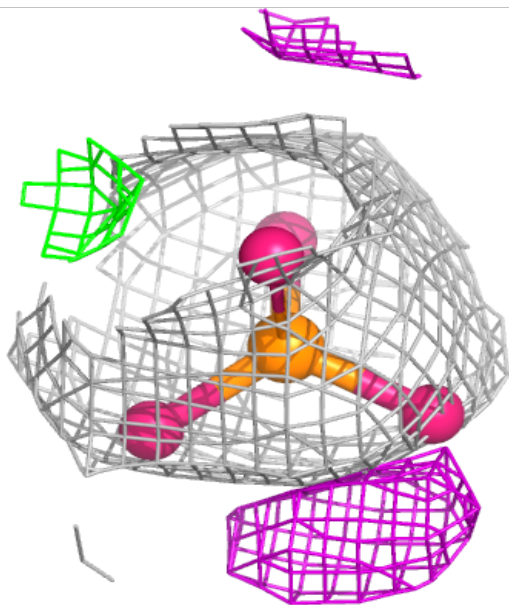
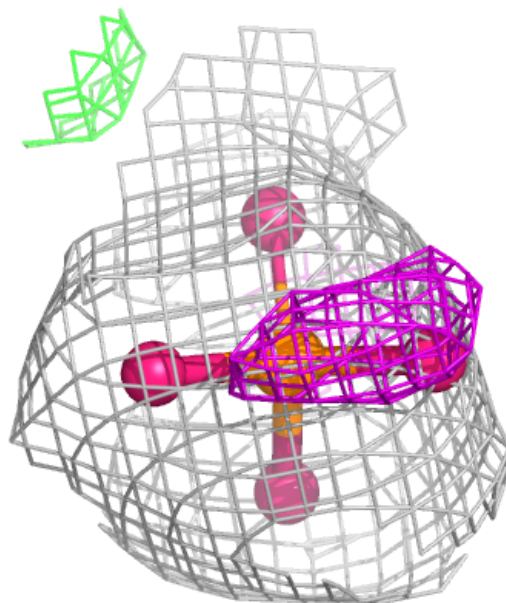
Electron density around PEF M 408:

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



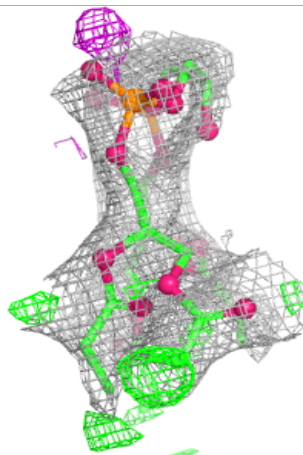
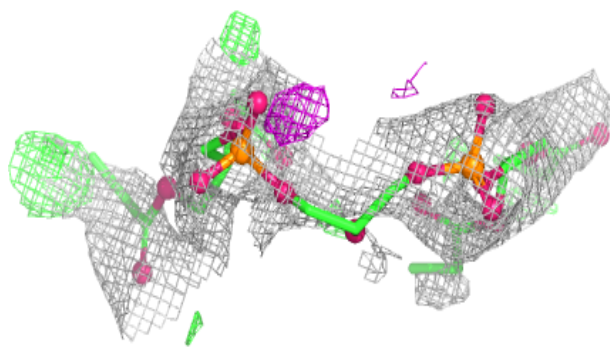
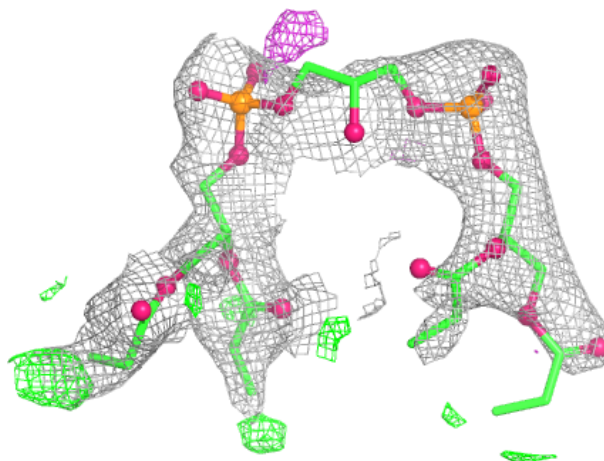
Electron density around PEF 5 104:

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



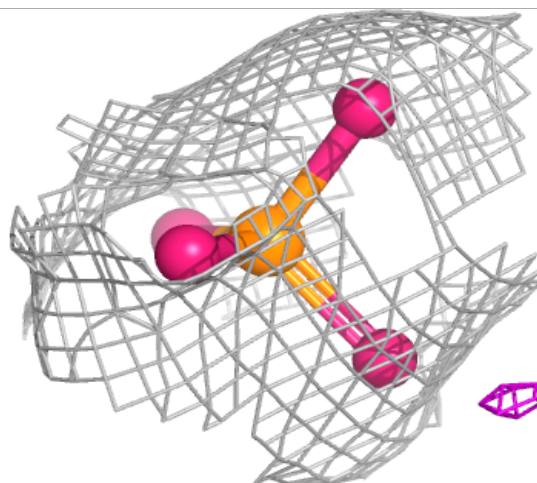
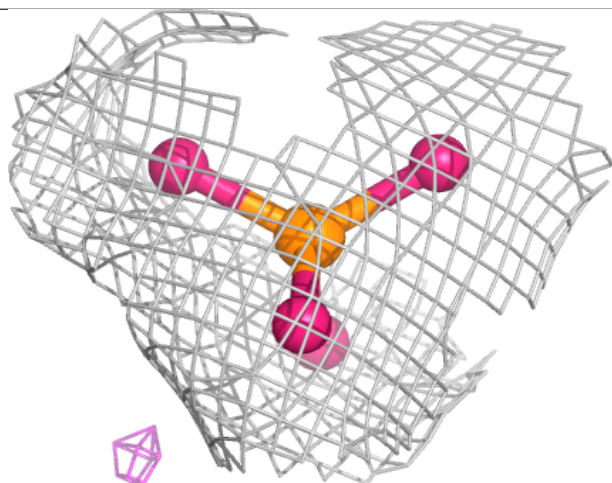
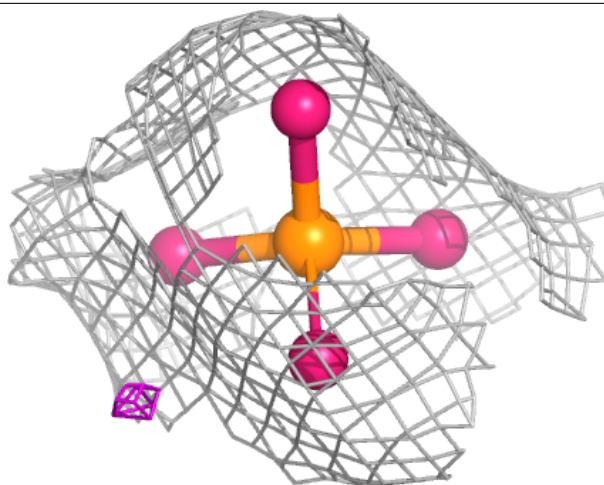
Electron density around CDL Y 103:

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



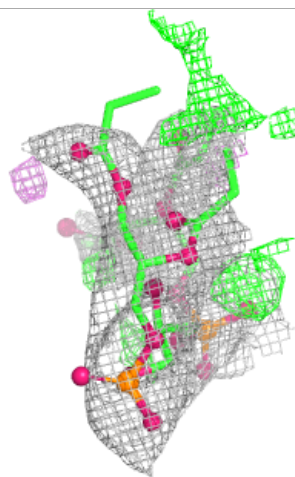
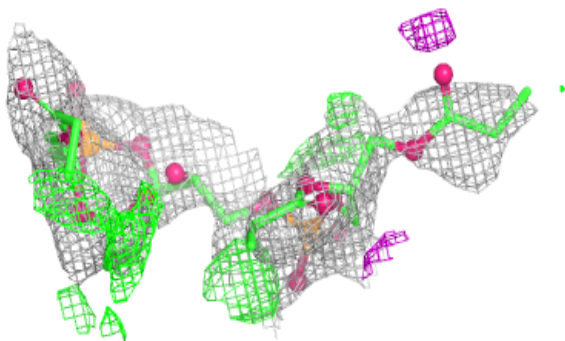
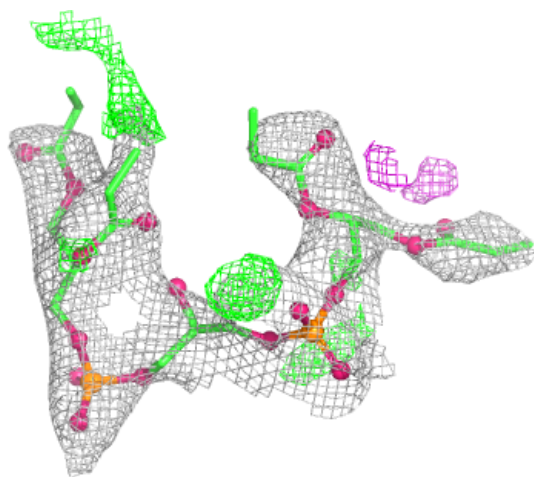
Electron density around PEF W 104:

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



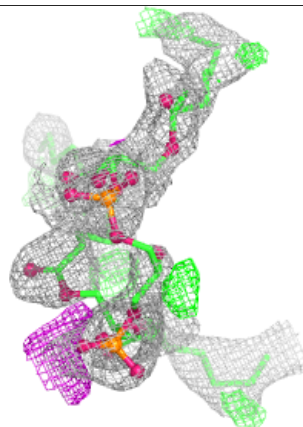
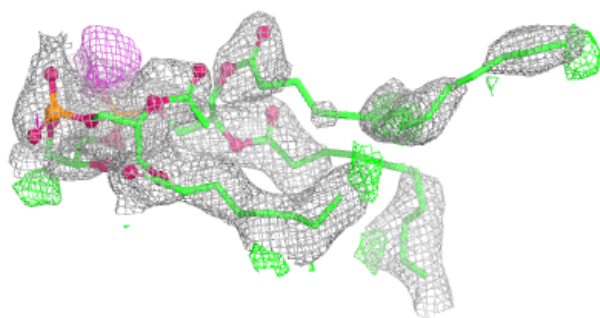
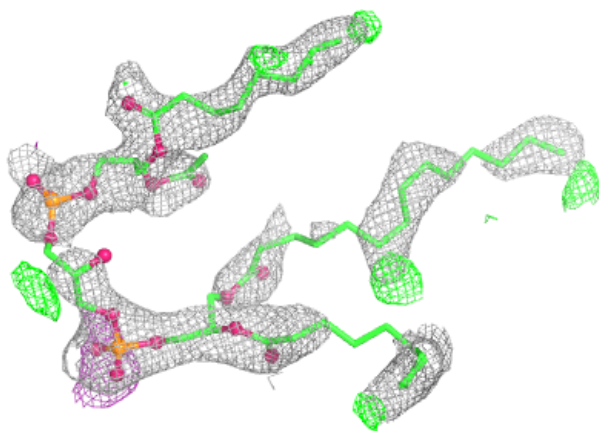
Electron density around CDL D 104:

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



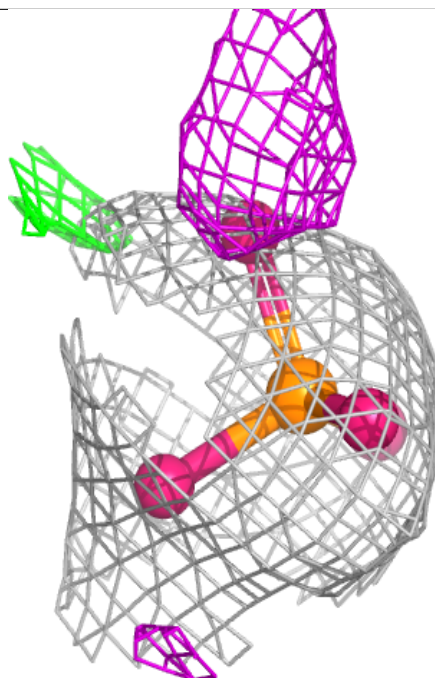
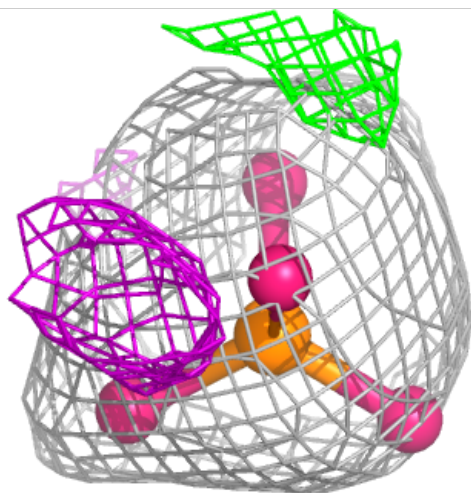
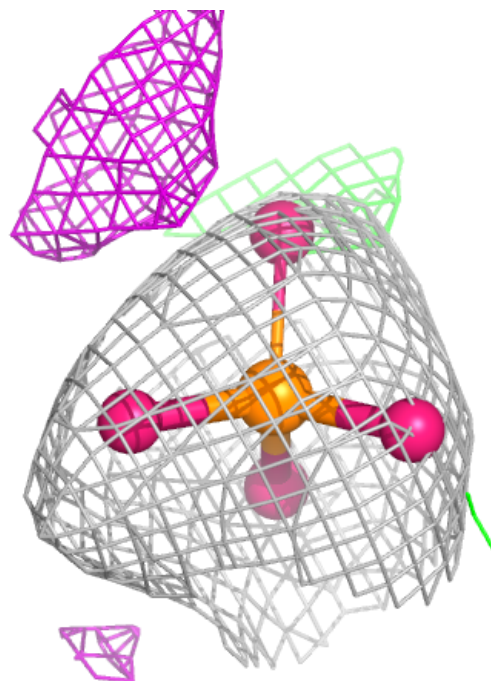
Electron density around CDL S 104:

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



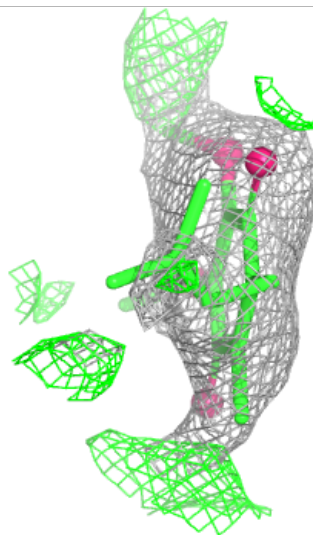
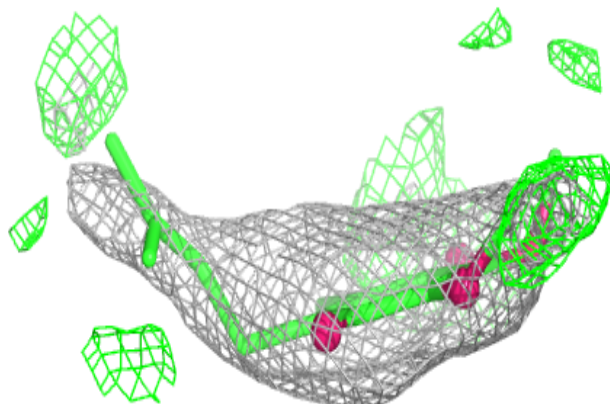
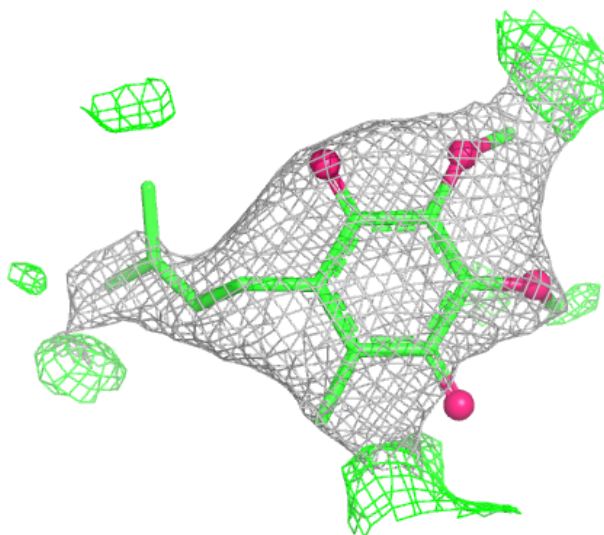
Electron density around PEF U 105:

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



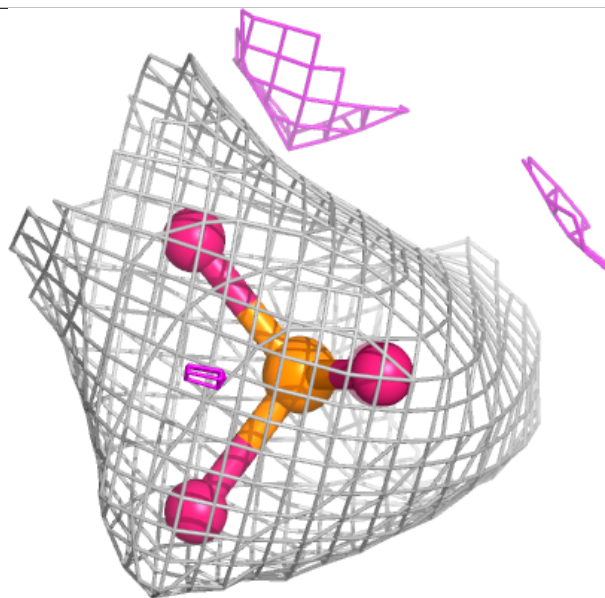
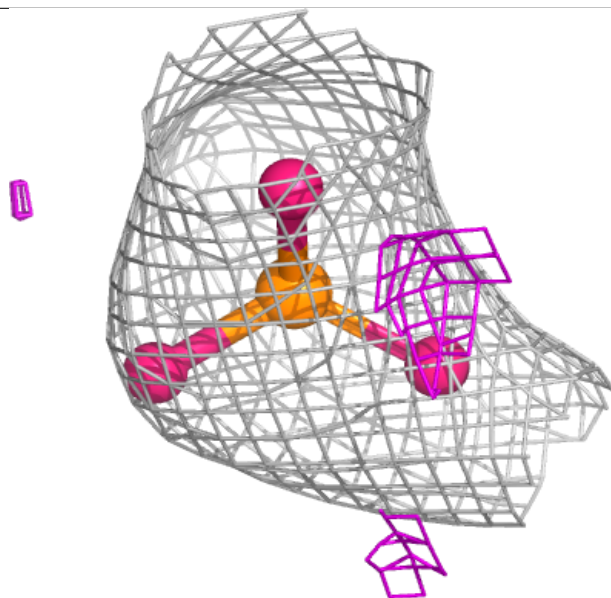
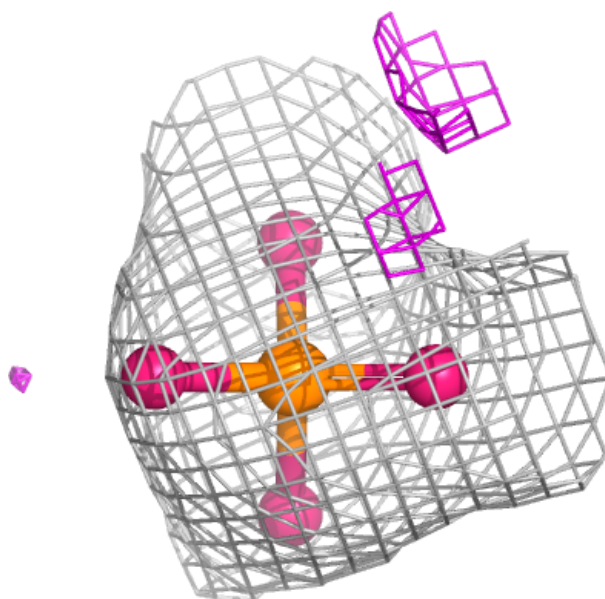
Electron density around UQ8 L 309:

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



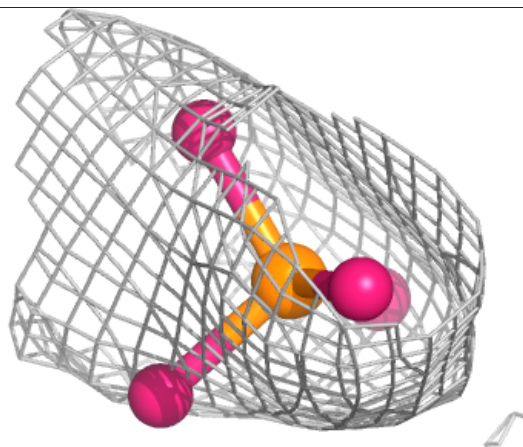
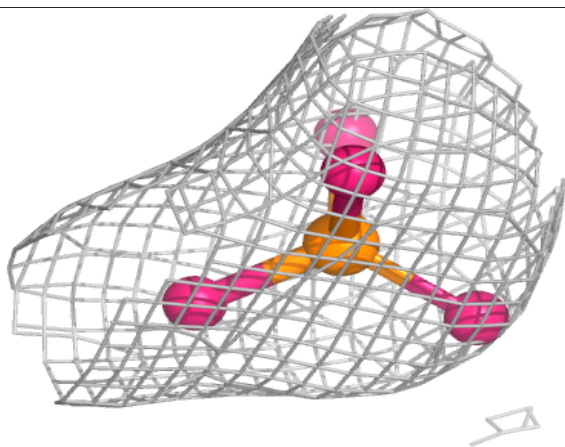
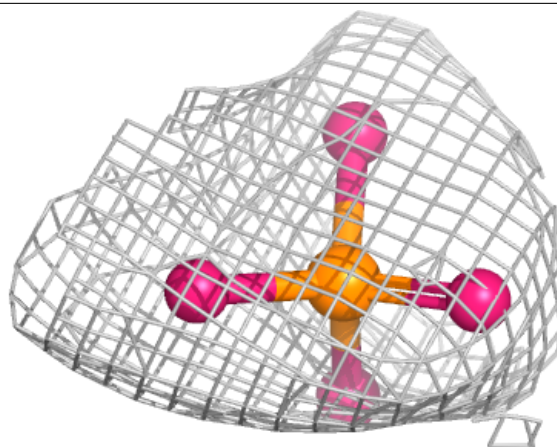
Electron density around PEF 1 105:

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



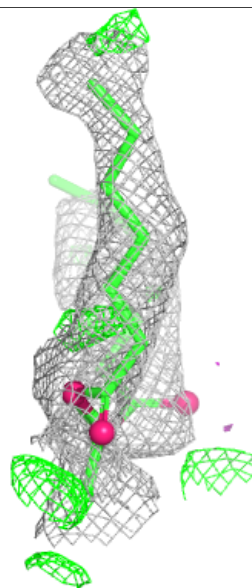
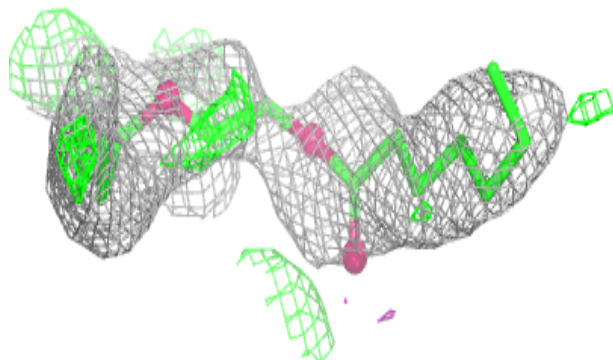
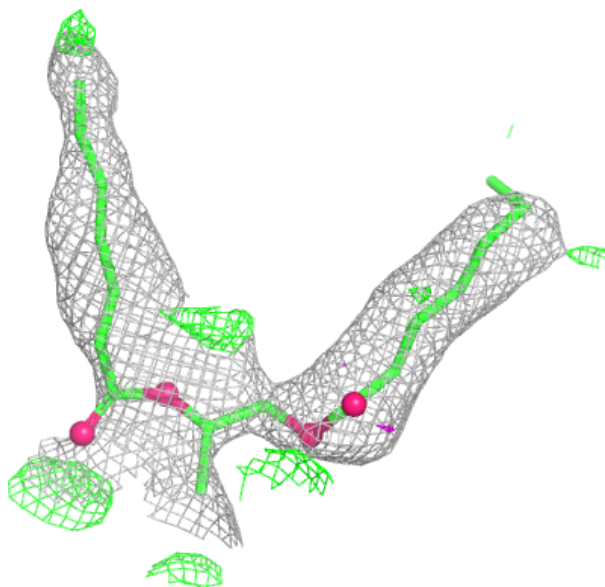
Electron density around PEF 3 104:

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



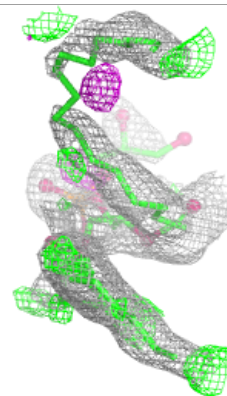
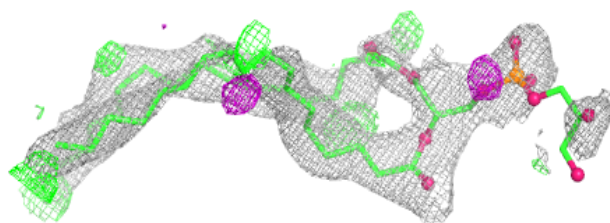
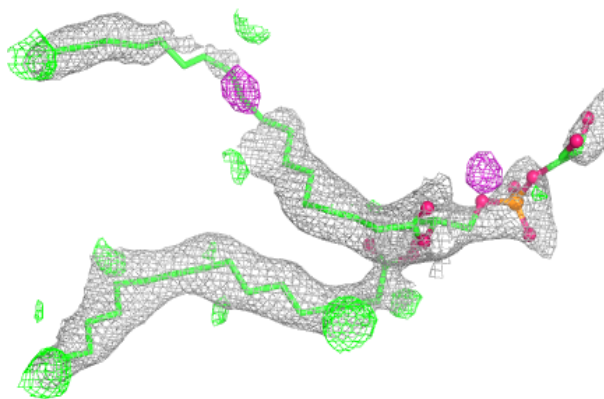
Electron density around PGV C 509:

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



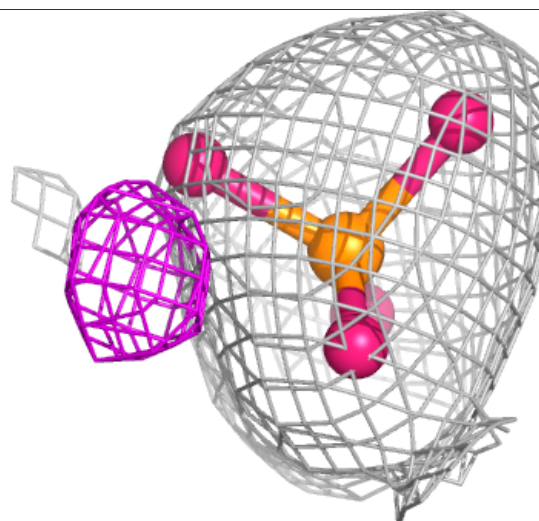
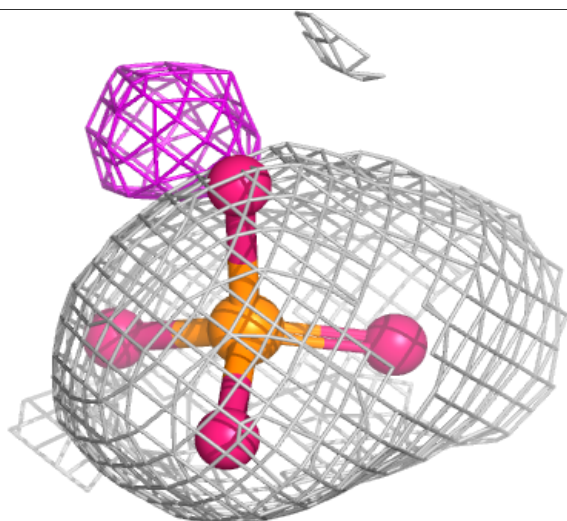
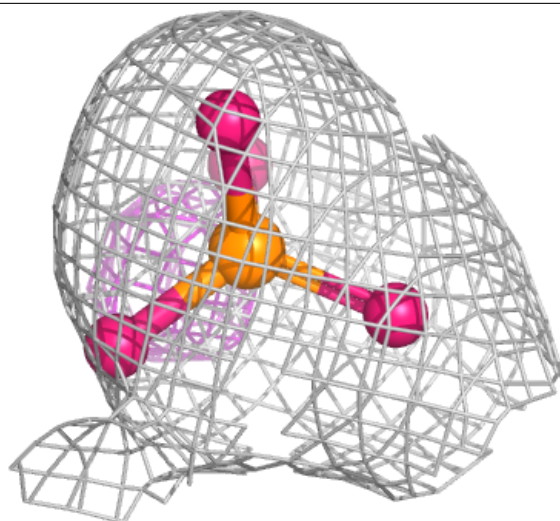
Electron density around PGV 3 105:

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



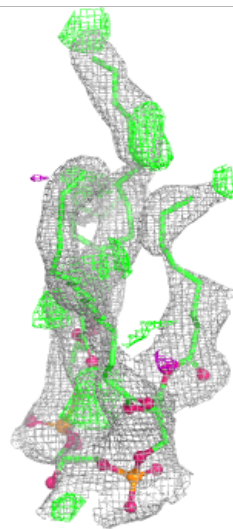
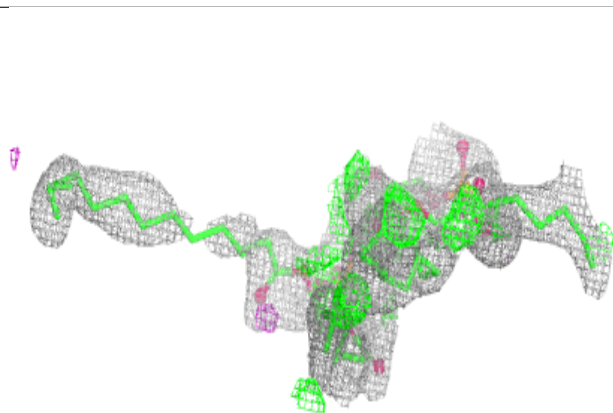
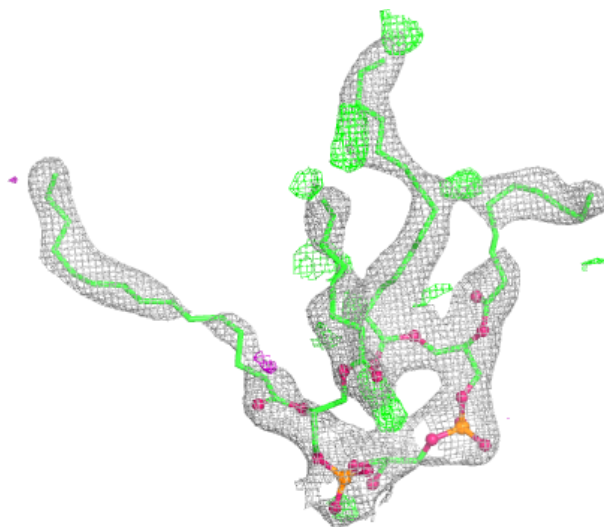
Electron density around PEF M 410:

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



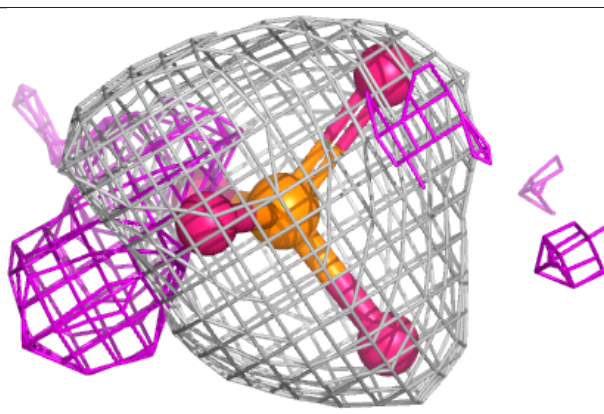
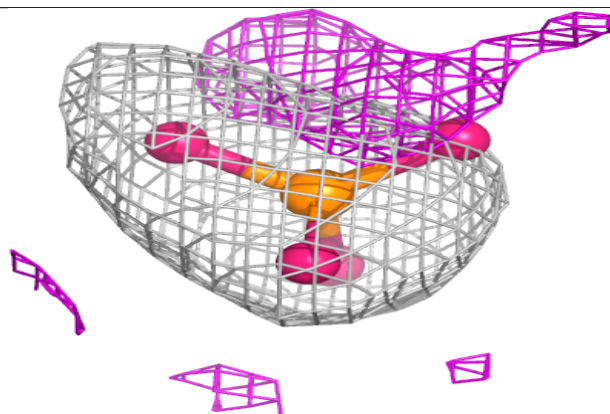
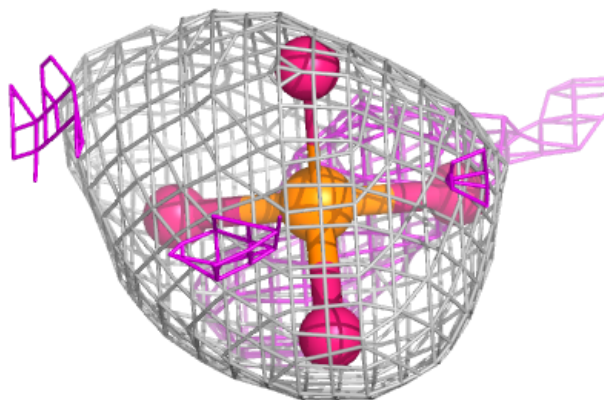
Electron density around CDL Q 105:

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

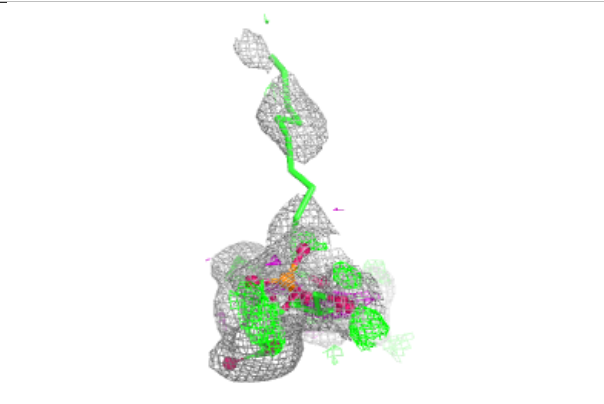
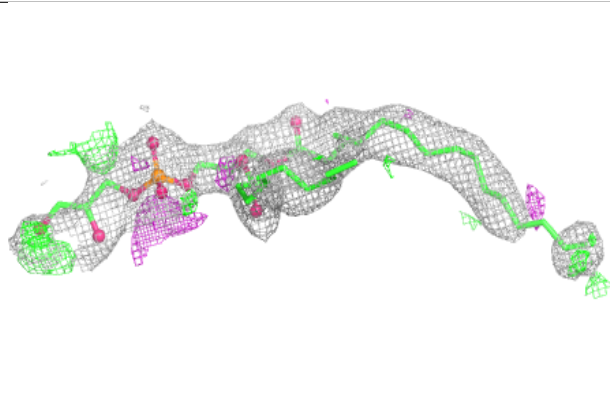
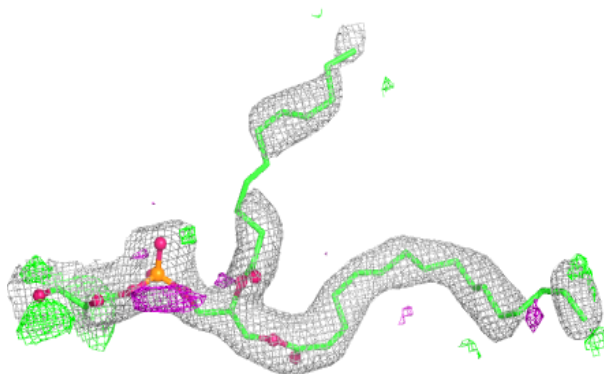


Electron density around PEF I 104:

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

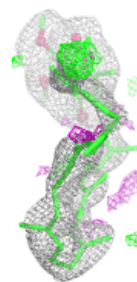
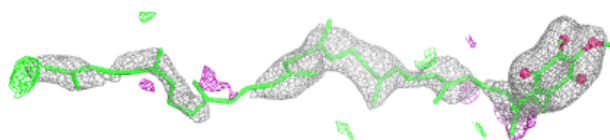
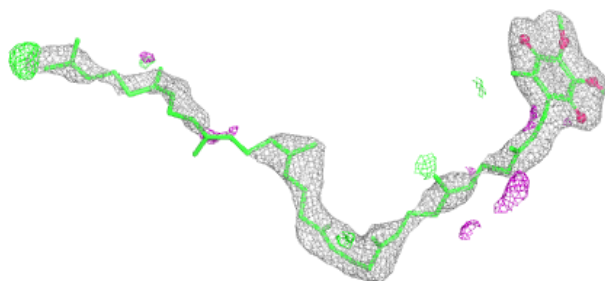
**Electron density around PGV L 306:**

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

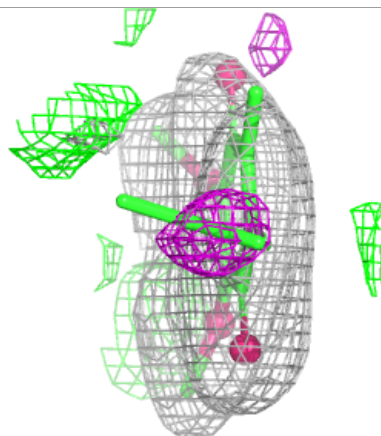
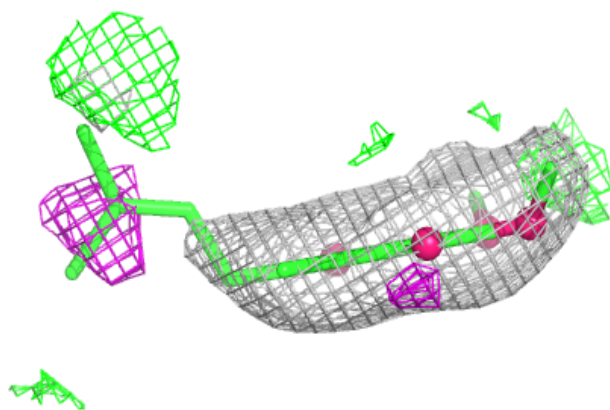
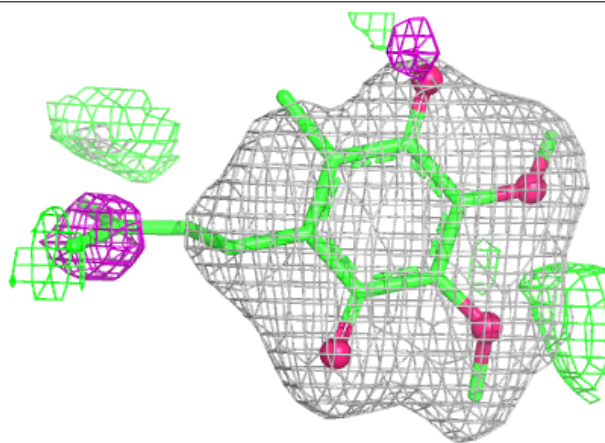


Electron density around UQ8 L 308:

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

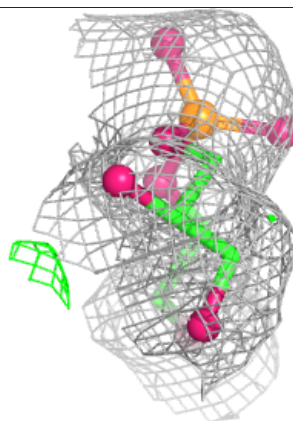
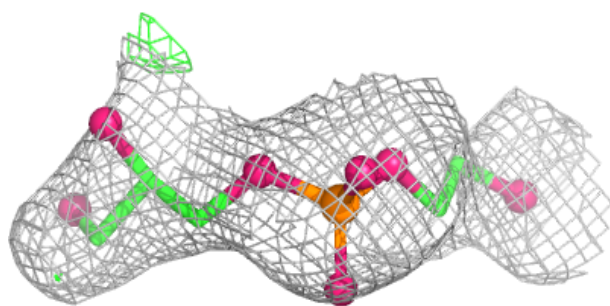
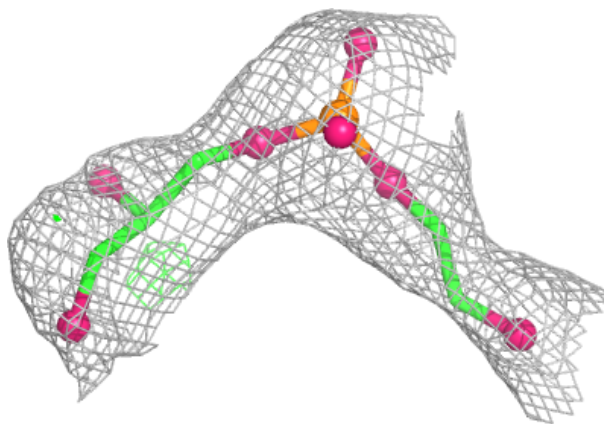
**Electron density around UQ8 M 418:**

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

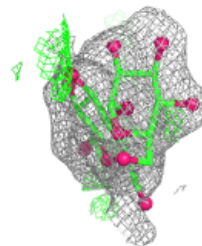
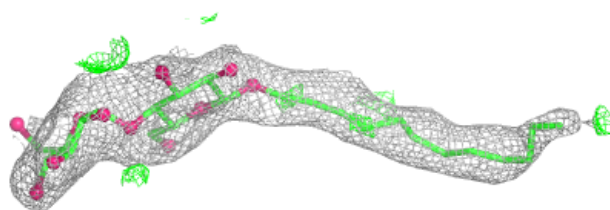
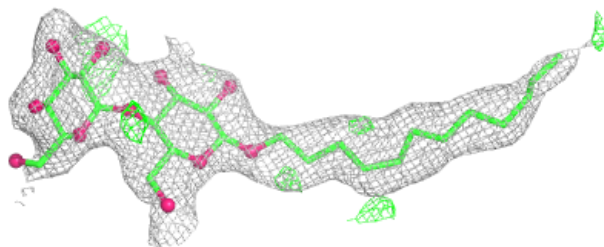


Electron density around CDL Y 104:

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

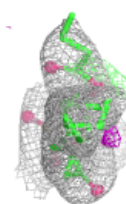
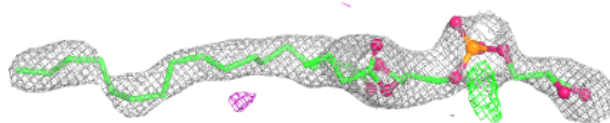
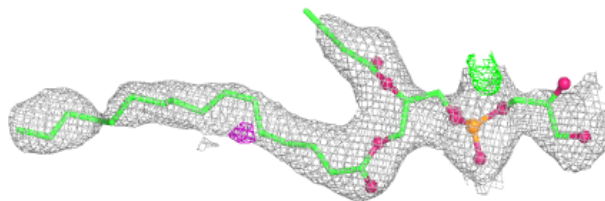
**Electron density around LMT M 420:**

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



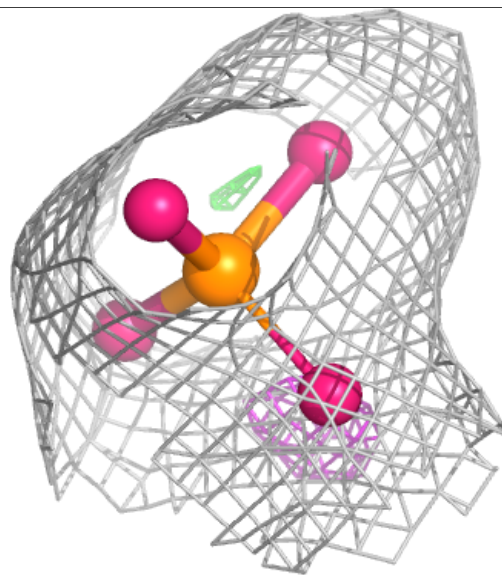
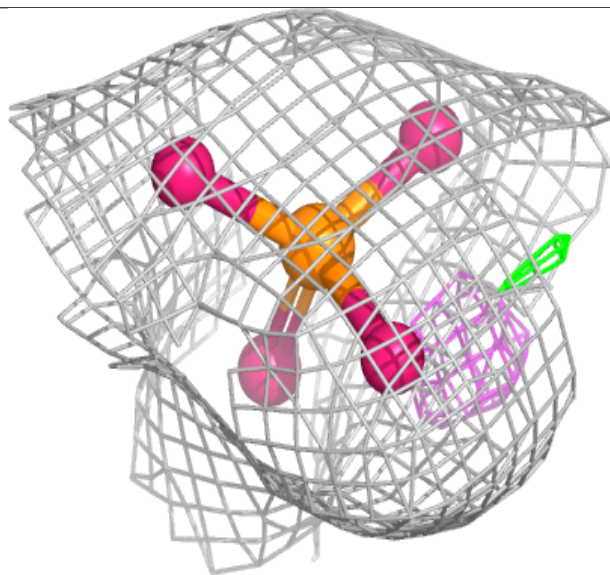
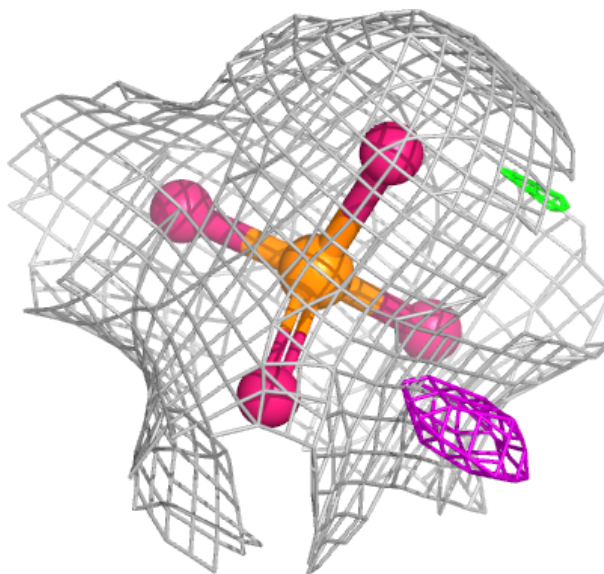
Electron density around PGV M 415:

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



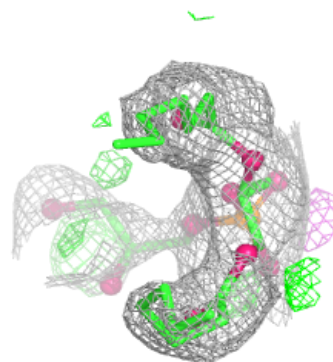
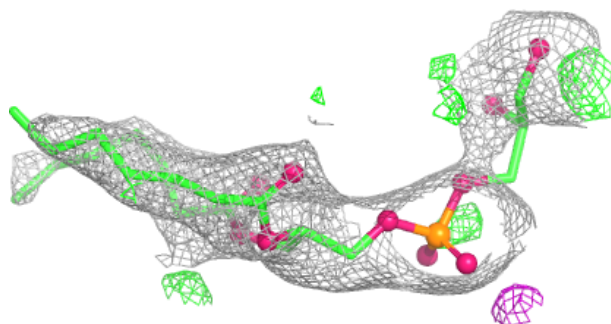
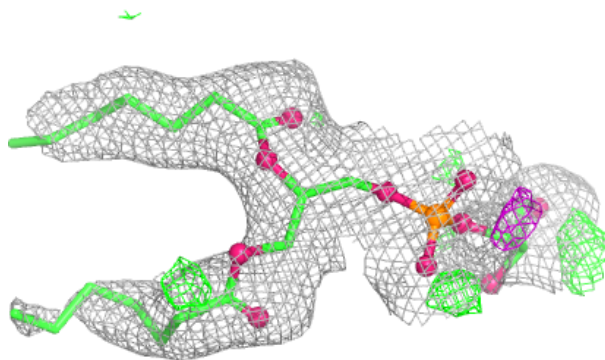
Electron density around PEF M 409:

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

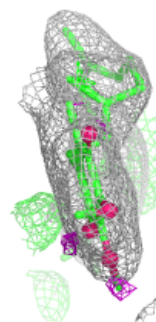
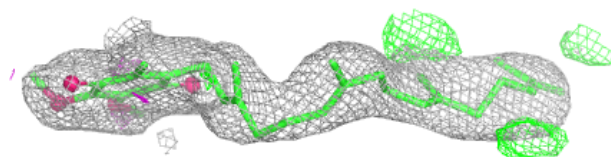
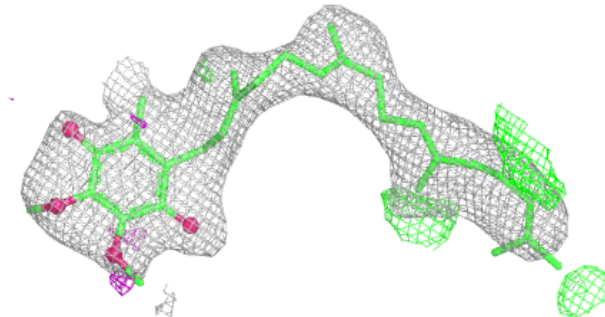


Electron density around PGV 1 106:

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

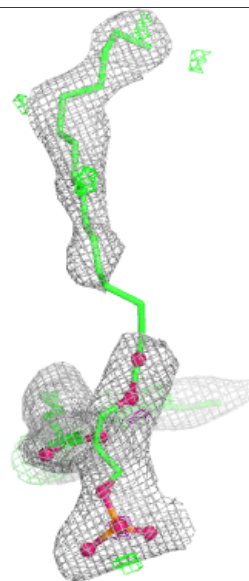
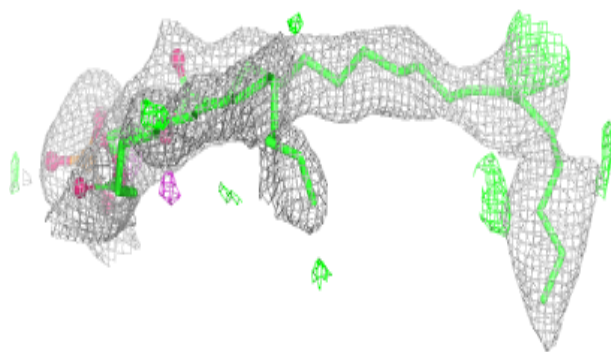
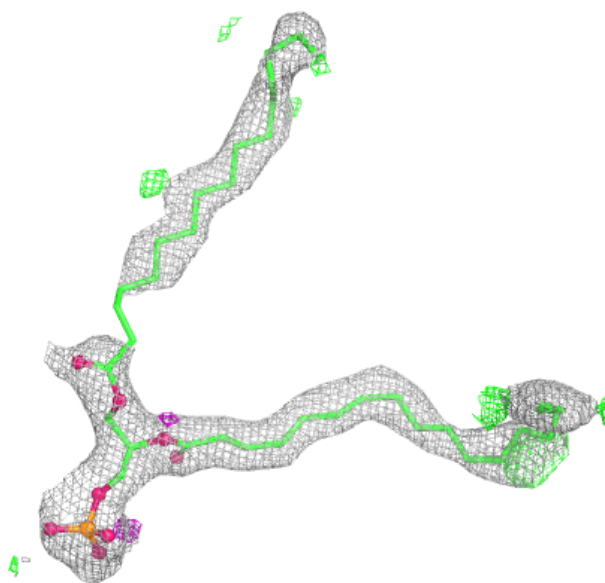
**Electron density around UQ8 7 104:**

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



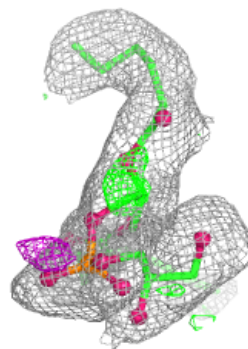
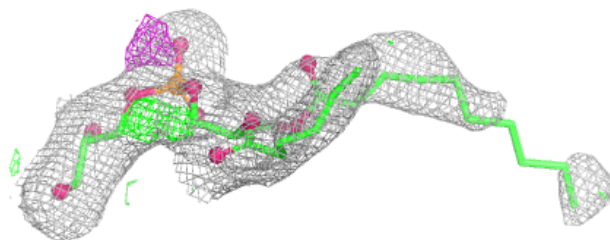
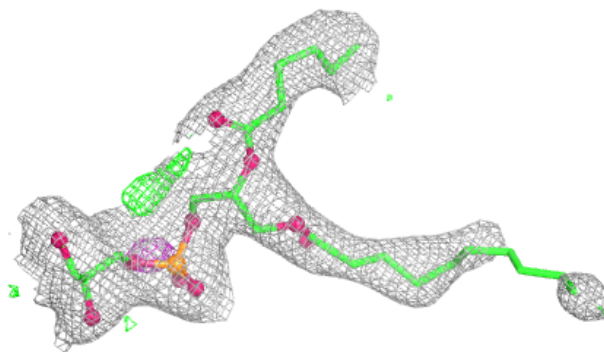
Electron density around PGV M 414:

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



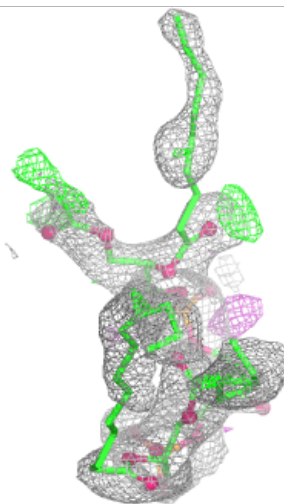
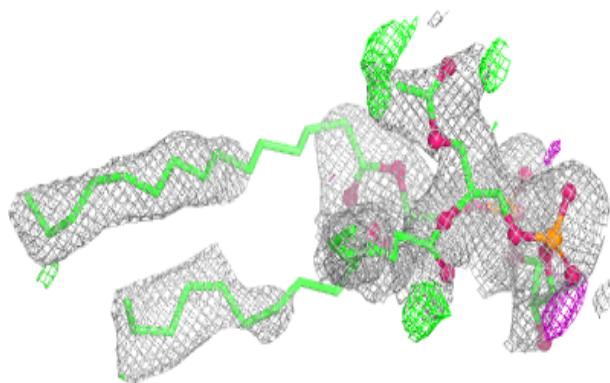
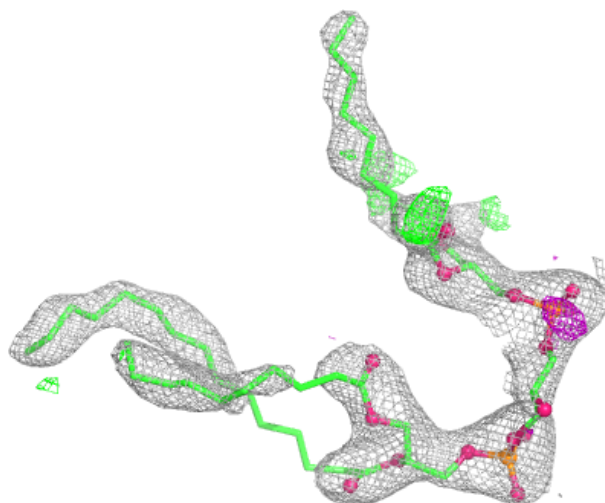
Electron density around PGV A 105:

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



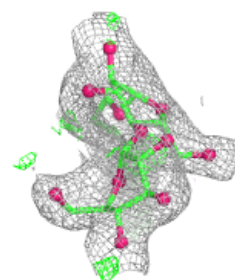
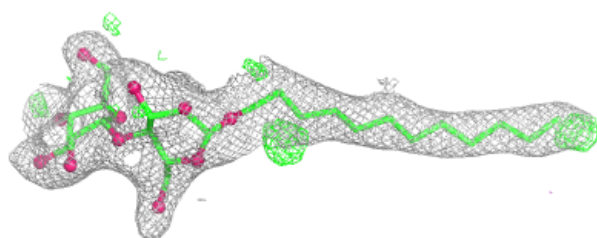
Electron density around CDL H 302:

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

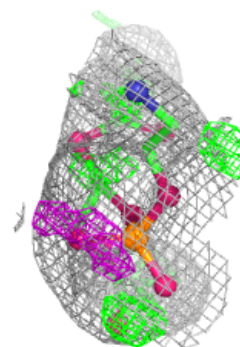
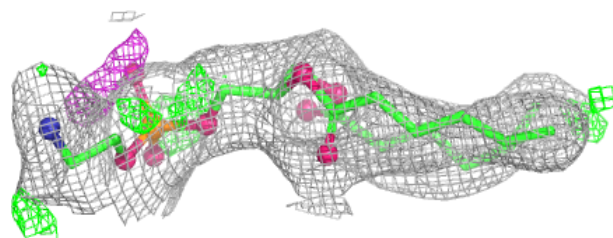
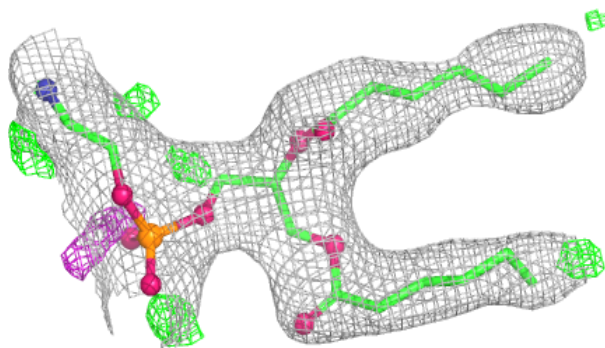


Electron density around LMT F 104:

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

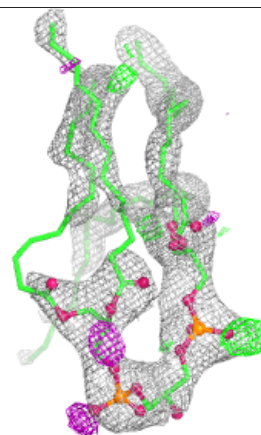
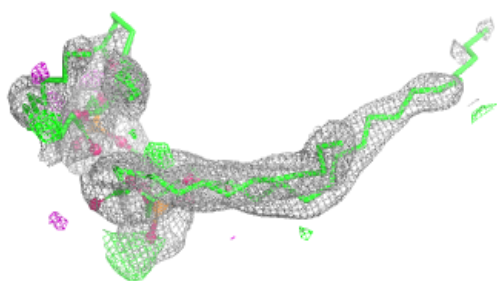
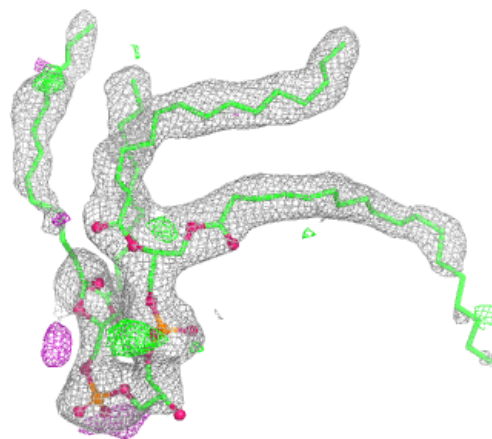
**Electron density around PEF K 105:**

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



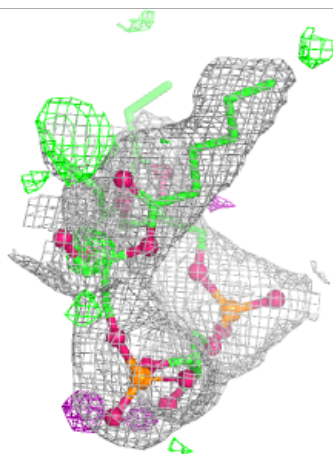
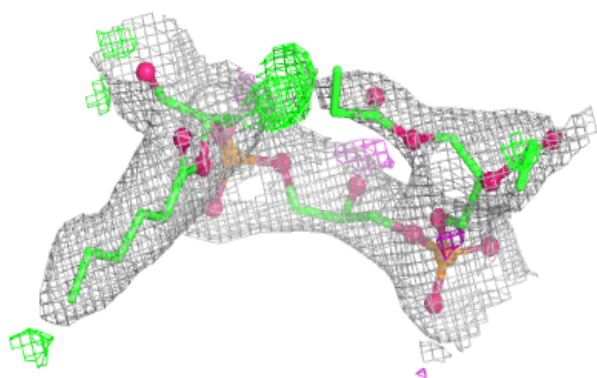
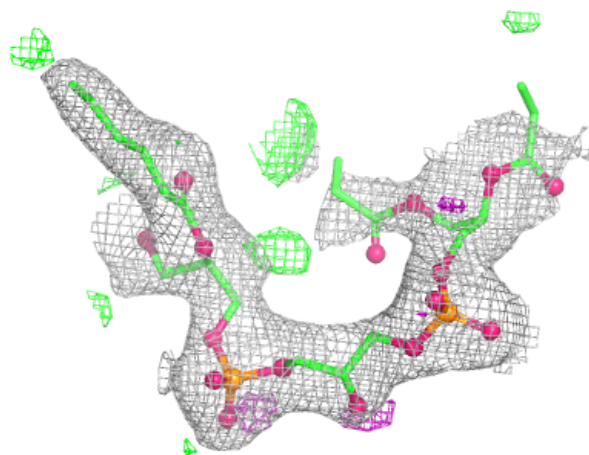
Electron density around CDL K 104:

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



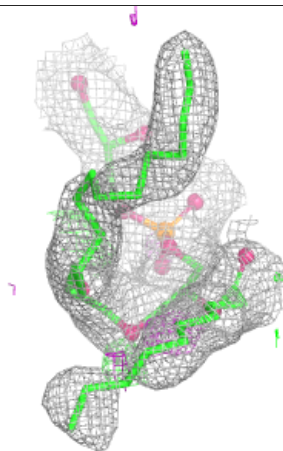
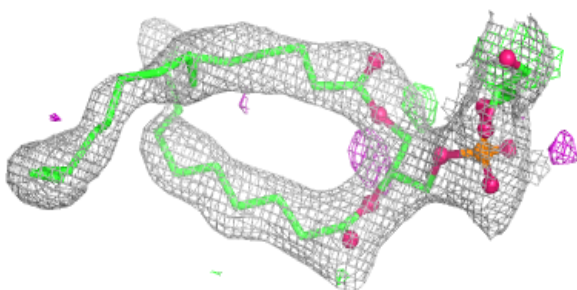
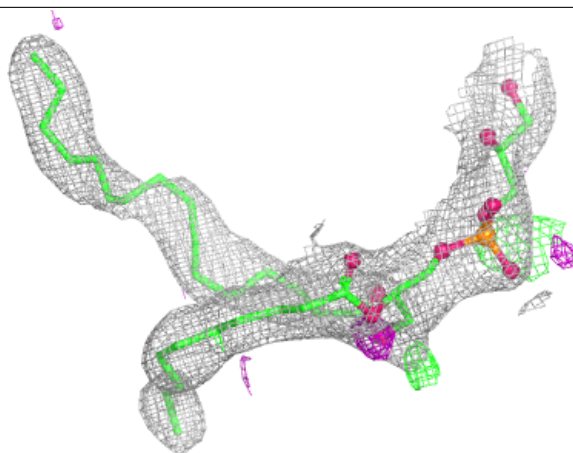
Electron density around CDL M 416:

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

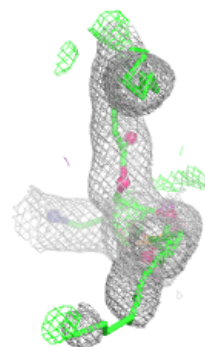
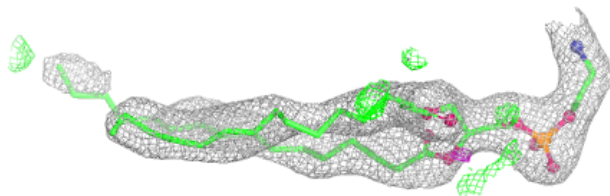
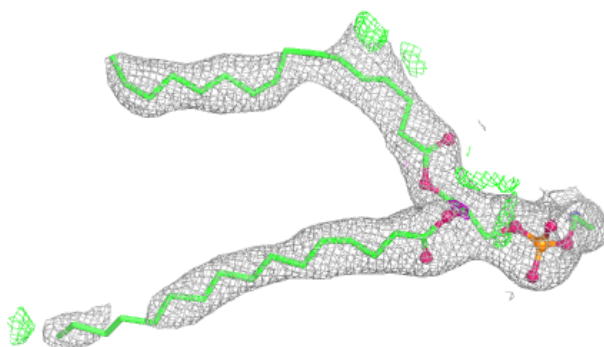


Electron density around PGV L 305:

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

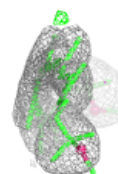
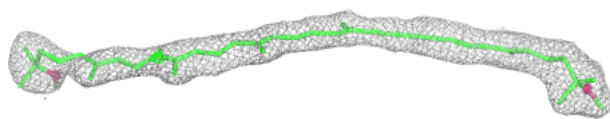
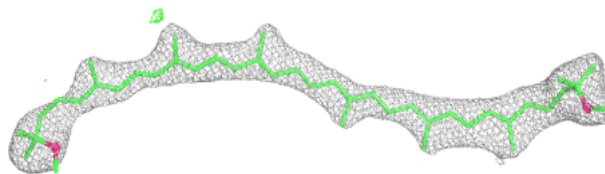
**Electron density around PEF M 419:**

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

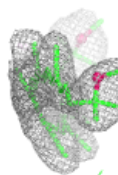
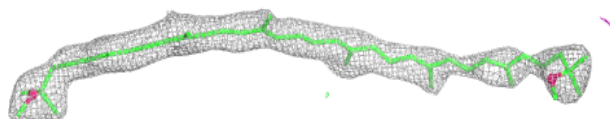
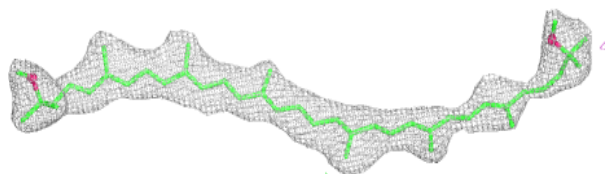


Electron density around CRT J 101:

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

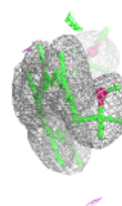
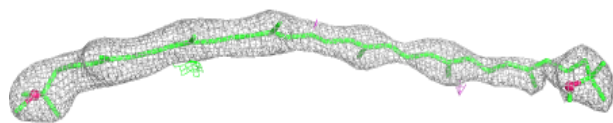
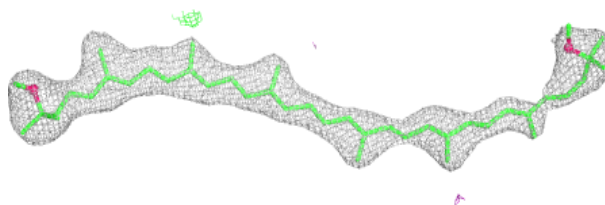
**Electron density around CRT 1 104:**

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



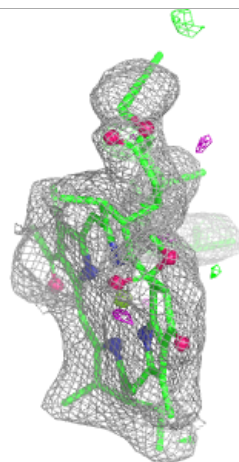
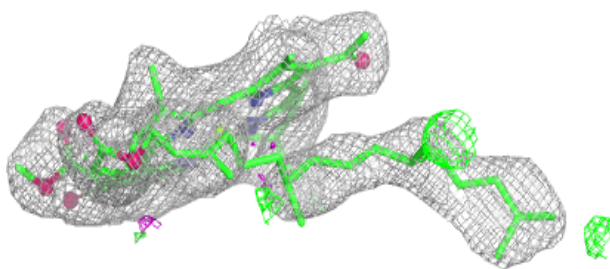
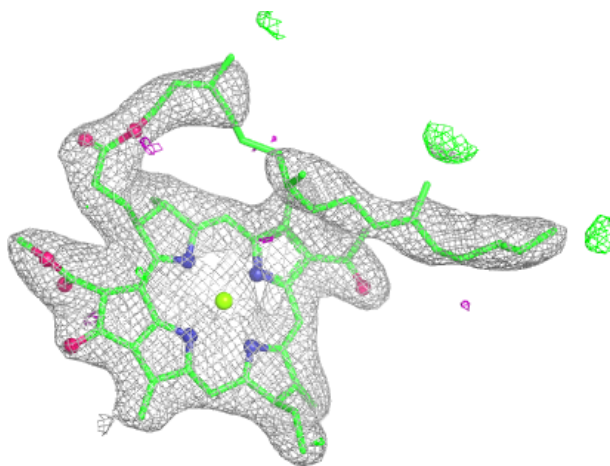
Electron density around CRT 2 101:

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



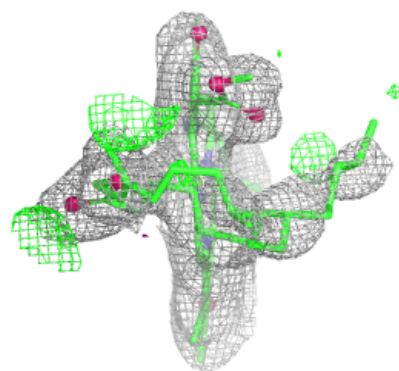
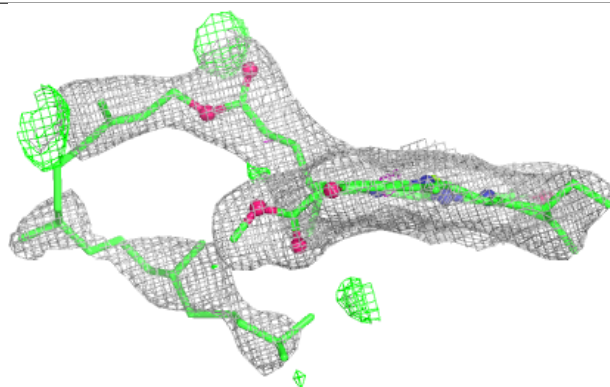
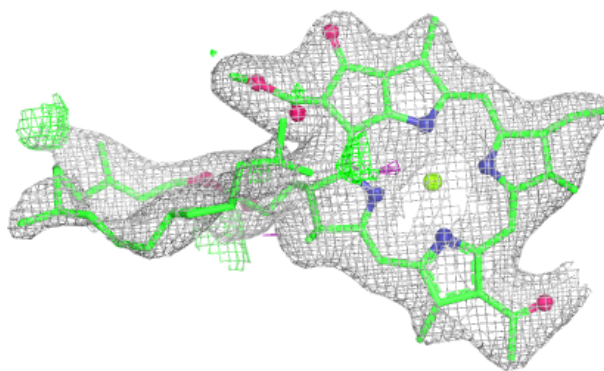
Electron density around BCL 1 103:

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

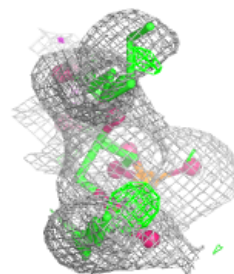
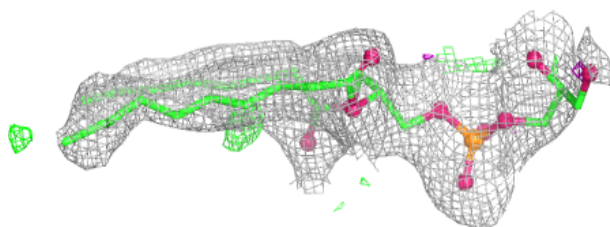
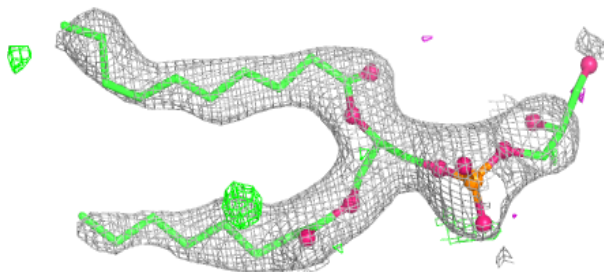


Electron density around BCL 3 102:

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

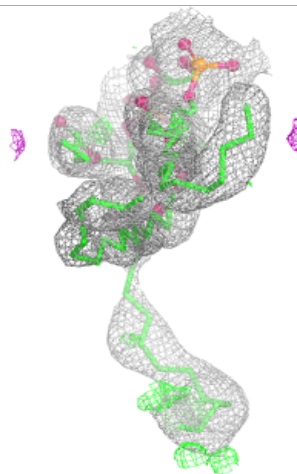
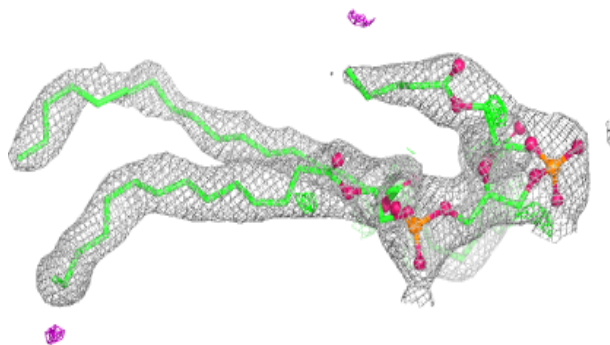
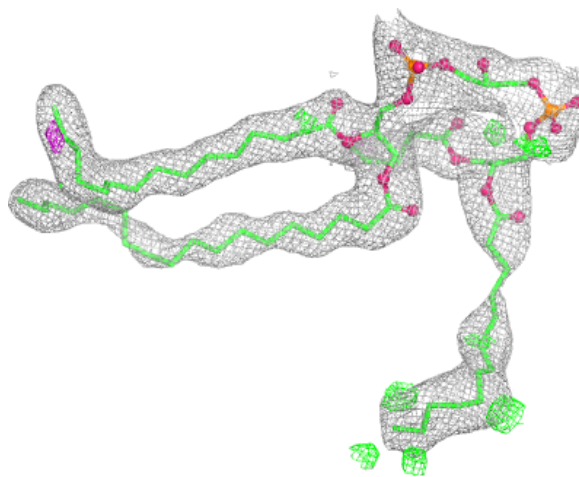
**Electron density around PGV D 105:**

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



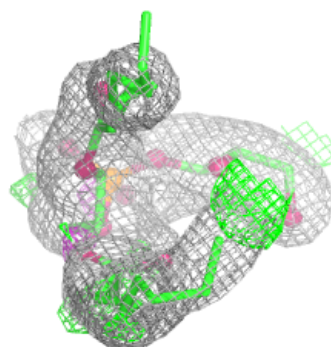
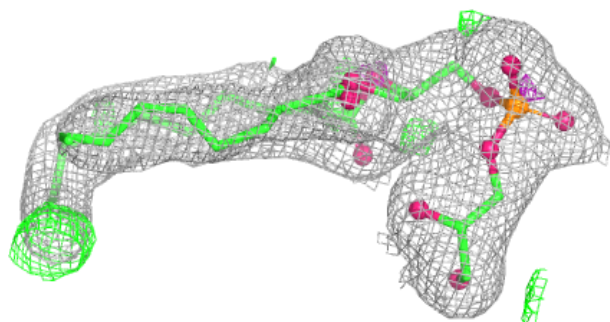
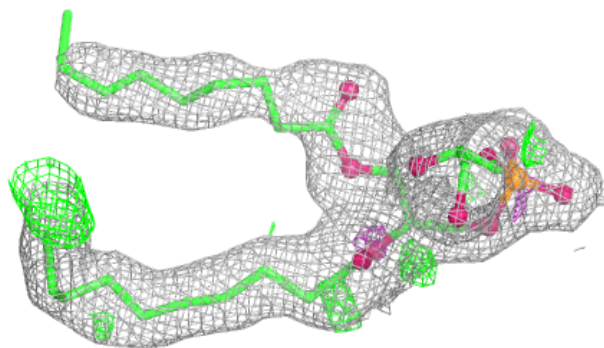
Electron density around CDL H 304:

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

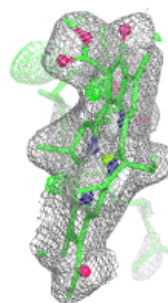
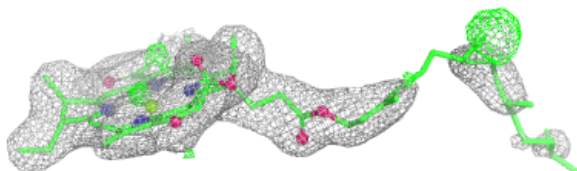


Electron density around PGV H 303:

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

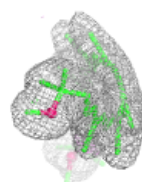
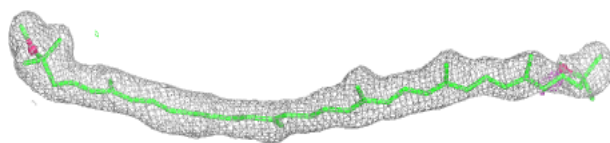
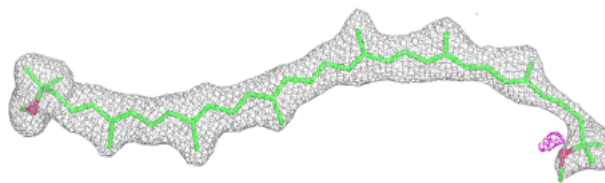
**Electron density around BCL 1 102:**

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

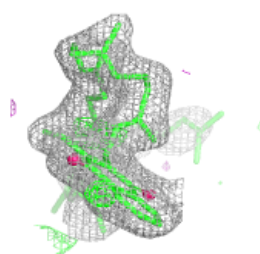
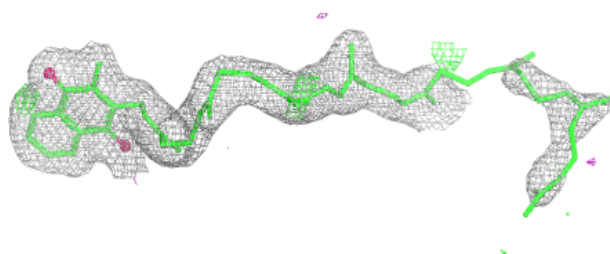
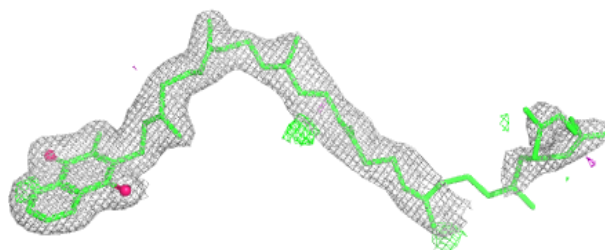


Electron density around CRT 9 102:

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

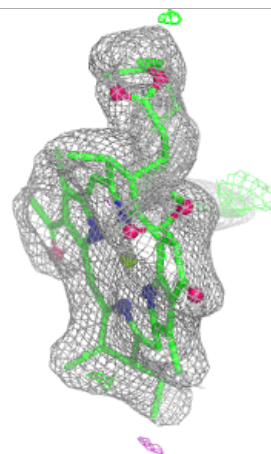
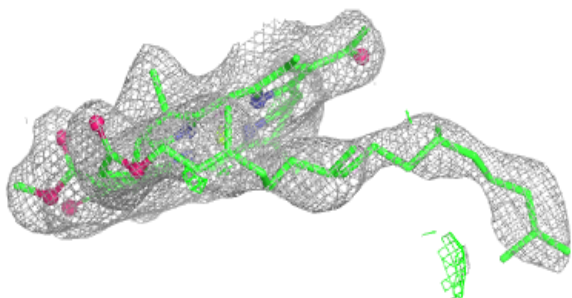
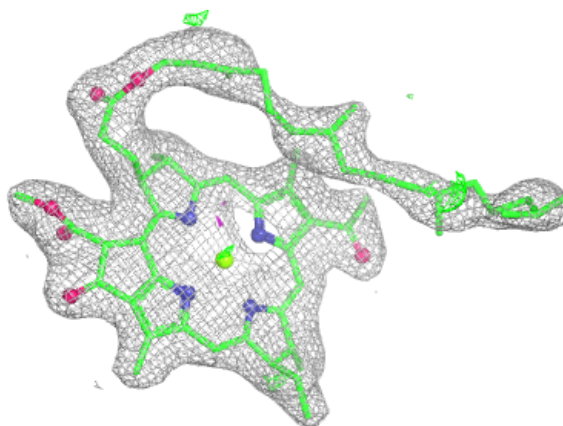
**Electron density around MQ8 M 406:**

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



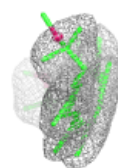
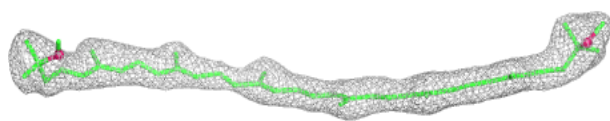
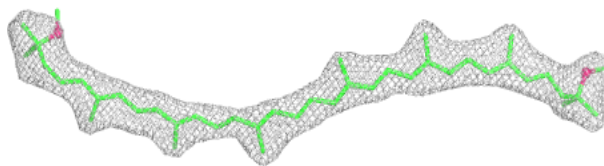
Electron density around BCL 3 103:

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

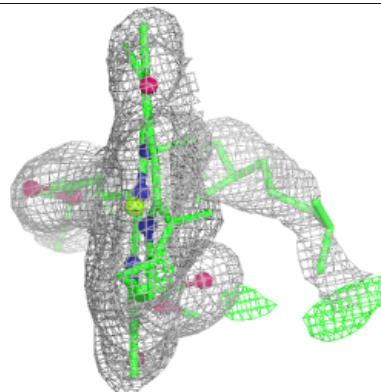
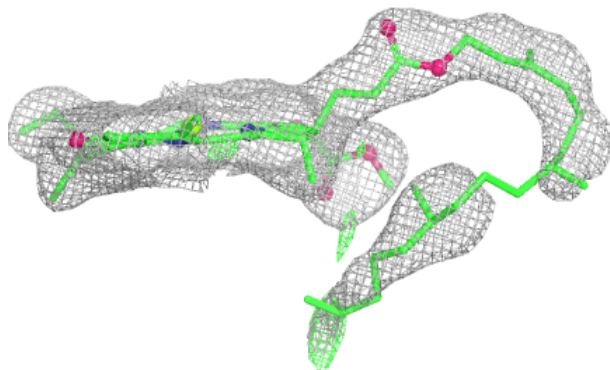
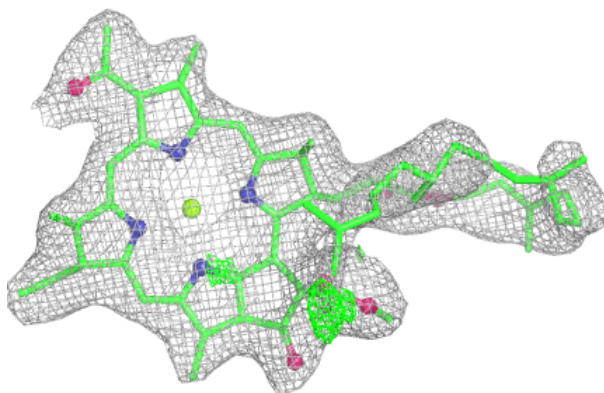


Electron density around CRT N 101:

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

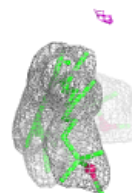
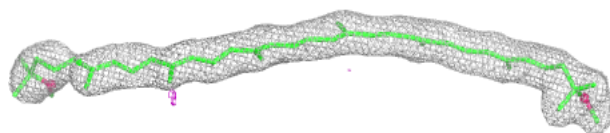
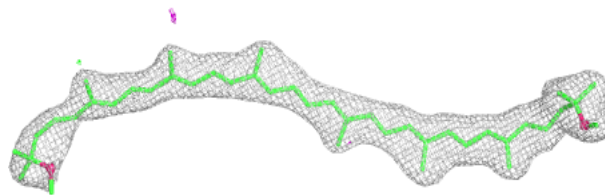
**Electron density around BCL 5 102:**

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

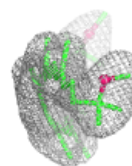
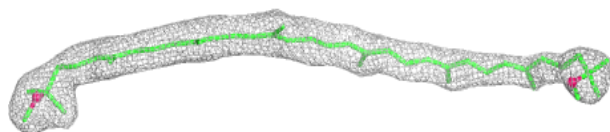
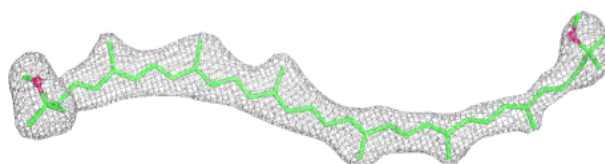


Electron density around CRT U 104:

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

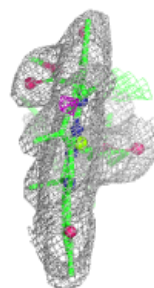
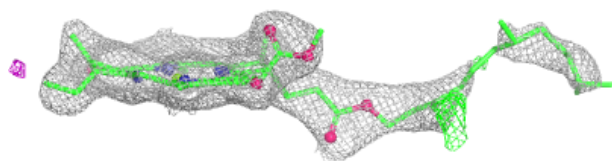
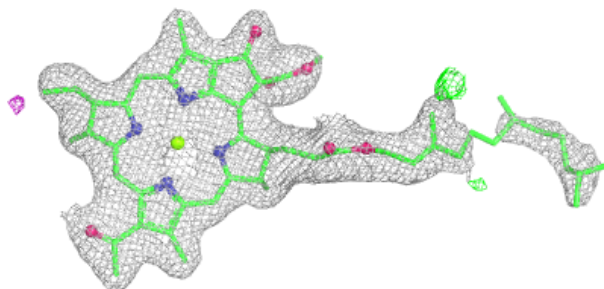
**Electron density around CRT Z 101:**

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



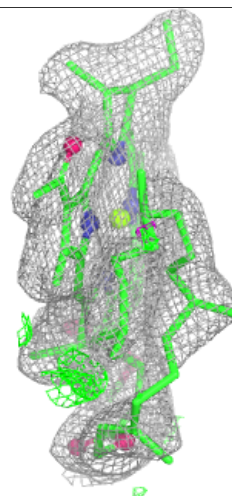
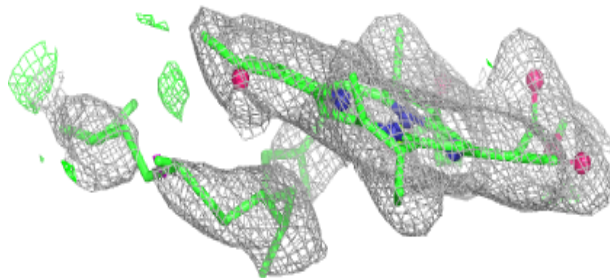
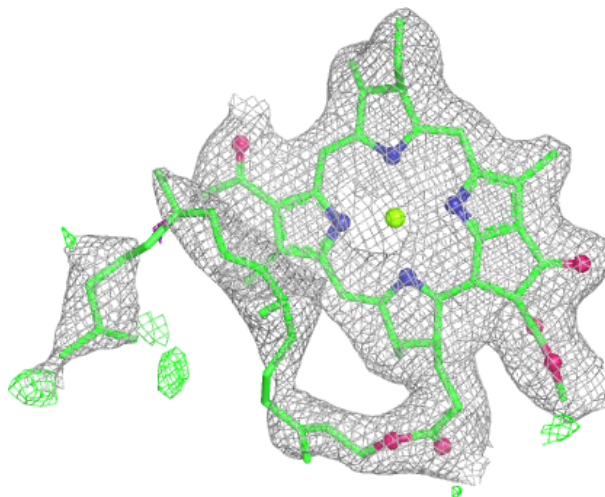
Electron density around BCL 7 102:

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



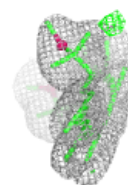
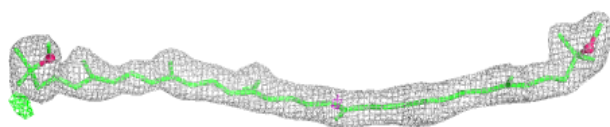
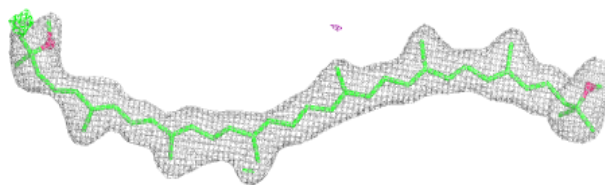
Electron density around BCL 7 103:

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

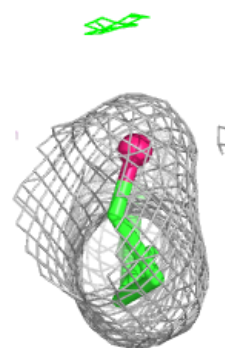
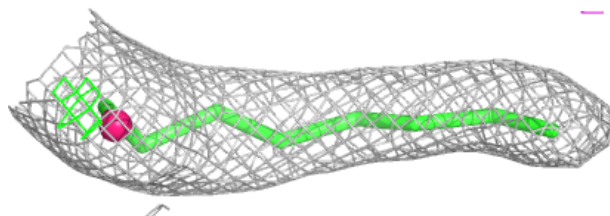
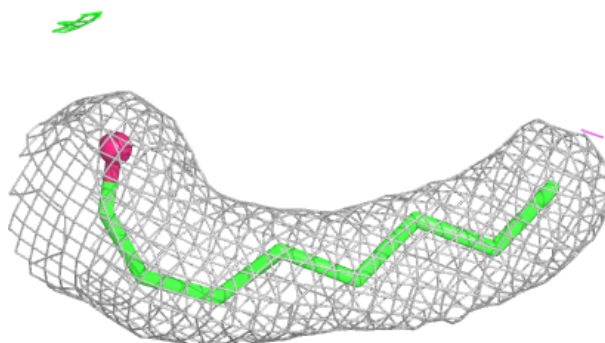


Electron density around CRT 6 101:

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

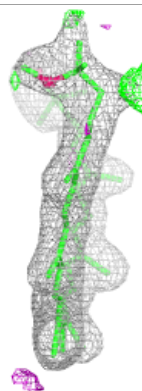
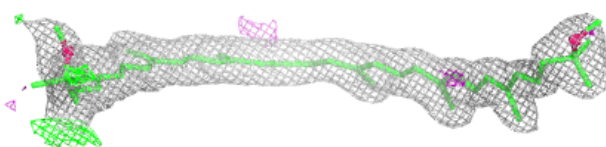
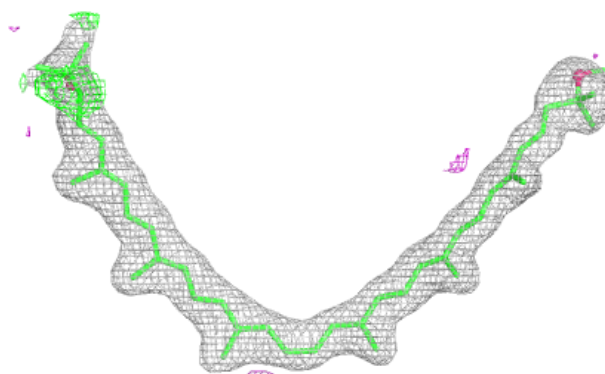
**Electron density around LHG C 508:**

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

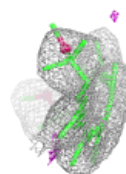
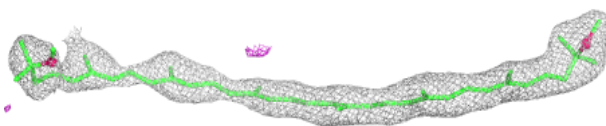
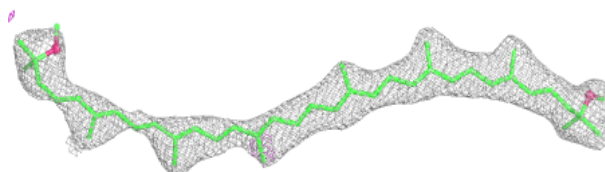


Electron density around CRT M 407:

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

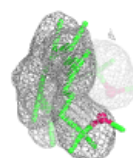
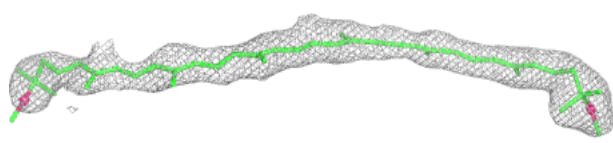
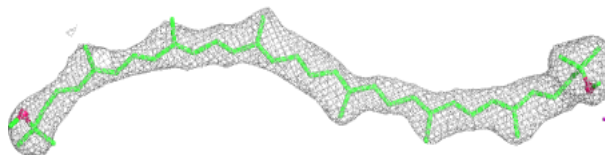
**Electron density around CRT A 104:**

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

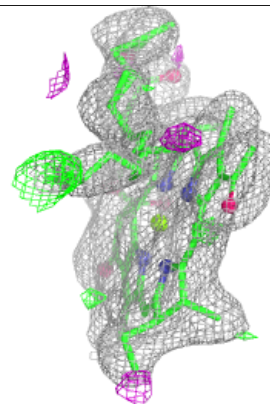
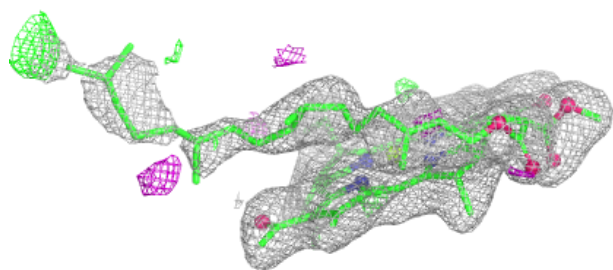
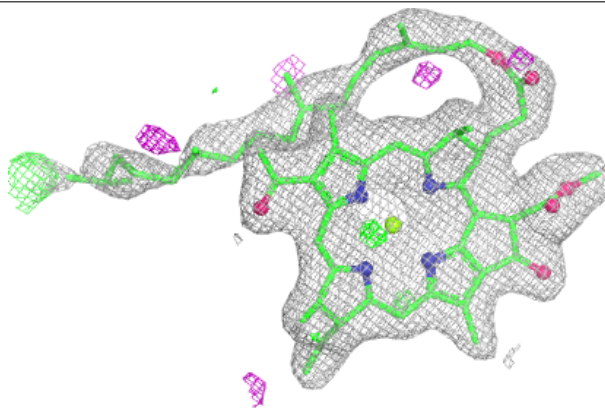


Electron density around CRT G 101:

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

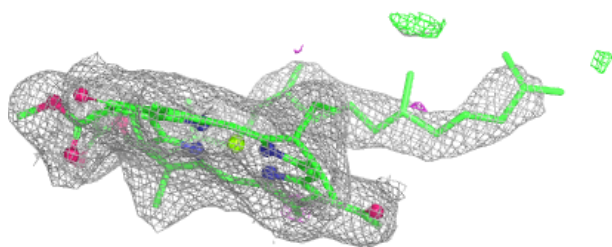
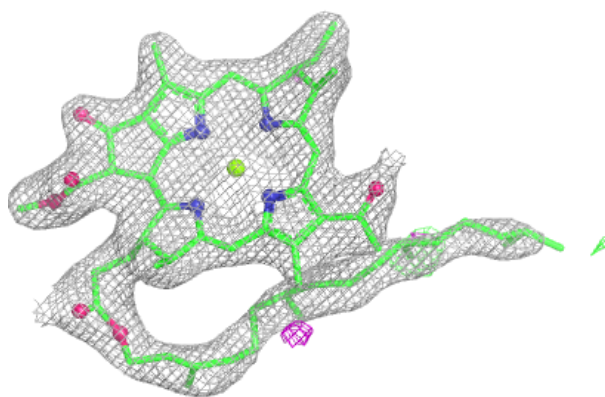
**Electron density around BCL O 103:**

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

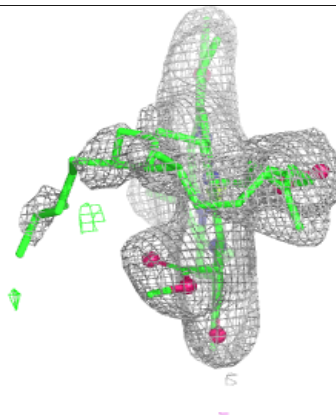
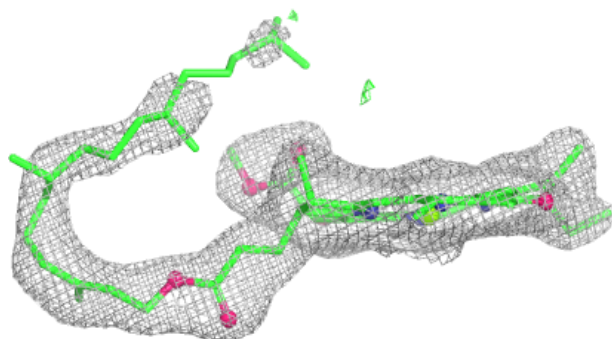
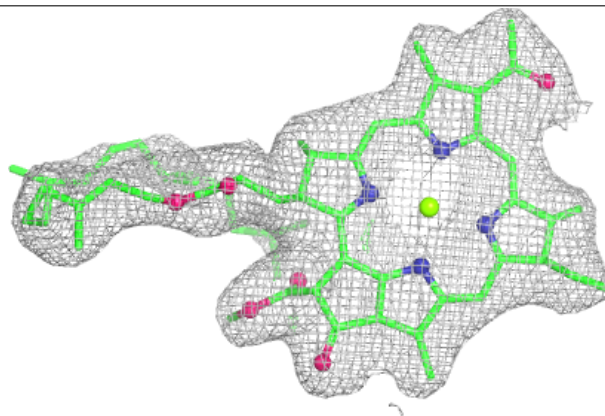


Electron density around BCL 5 103:

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

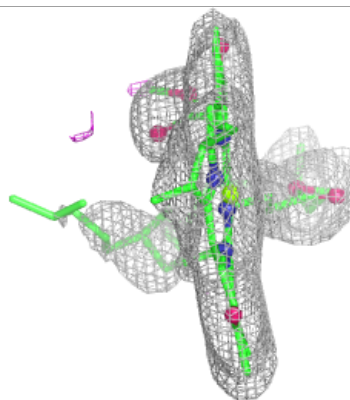
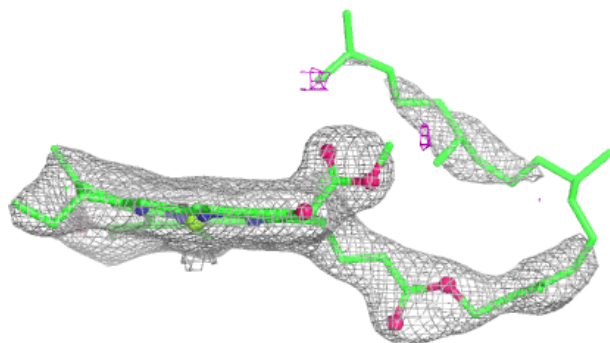
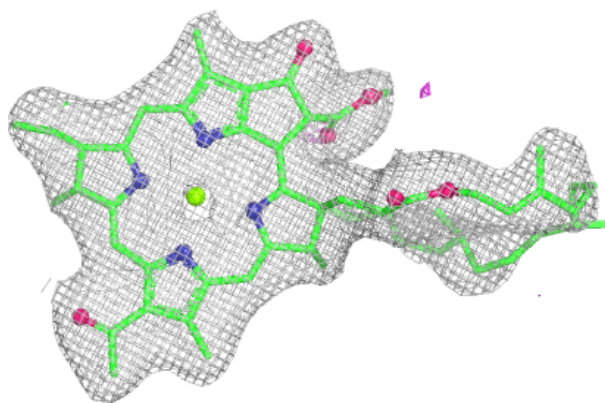
**Electron density around BCL K 102:**

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

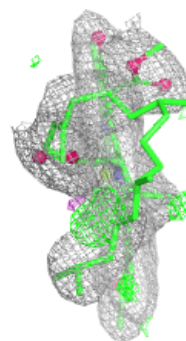
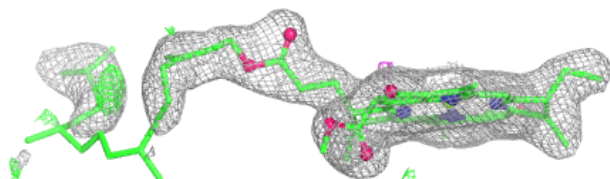
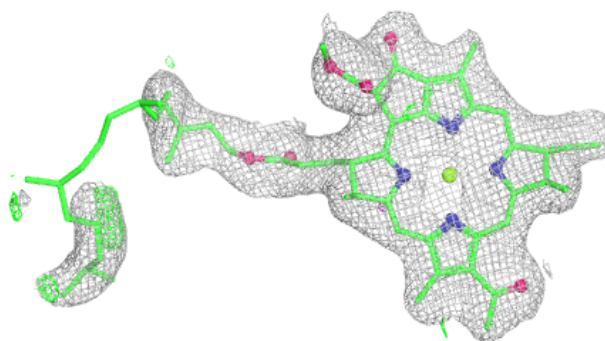


Electron density around BCL A 101:

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

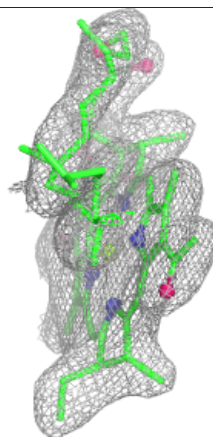
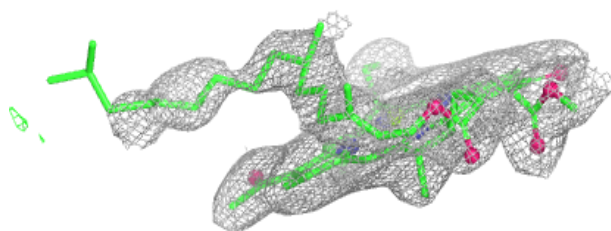
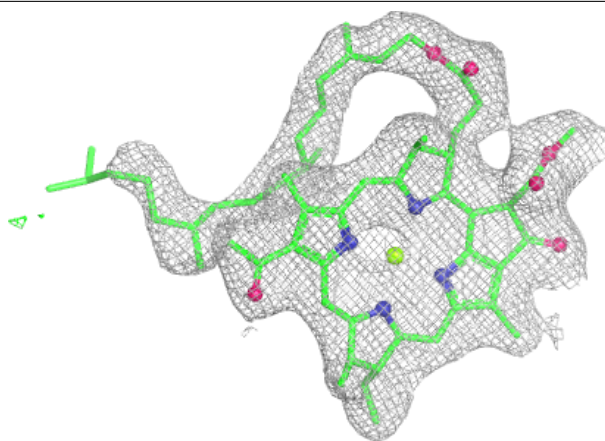
**Electron density around BCL 9 104:**

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

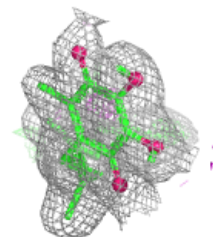
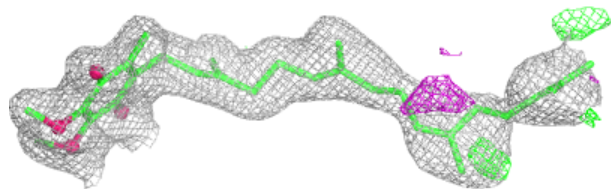
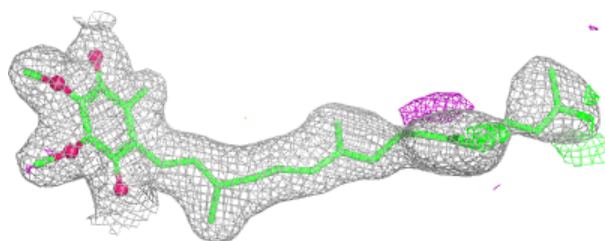


Electron density around BCL 0 102:

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

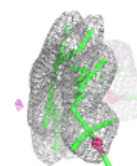
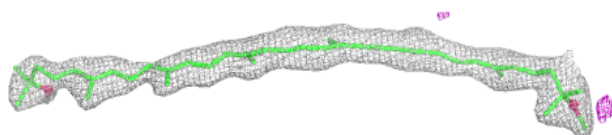
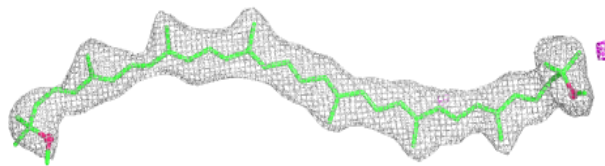
**Electron density around UQ8 L 303:**

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

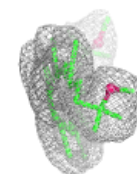
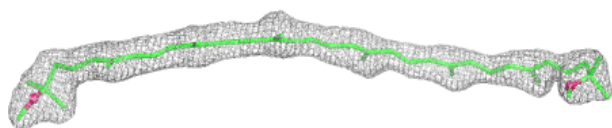
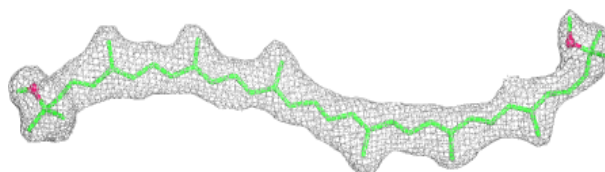


Electron density around CRT 9 103:

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

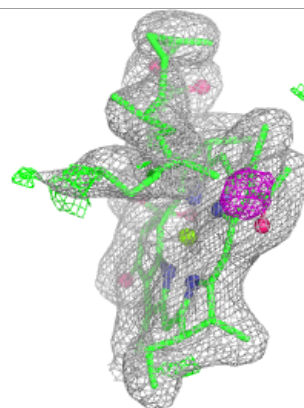
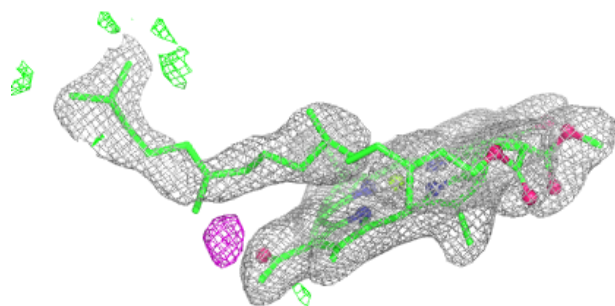
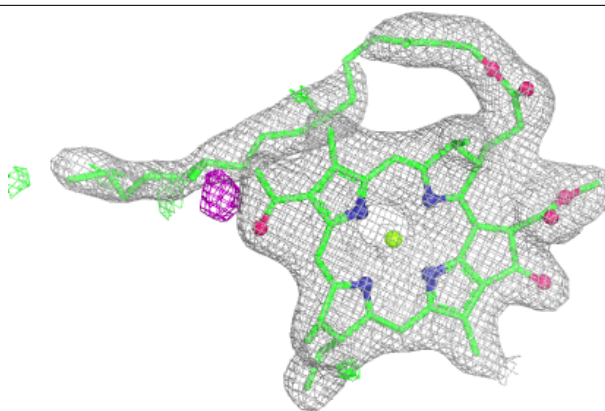
**Electron density around CRT 0 101:**

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

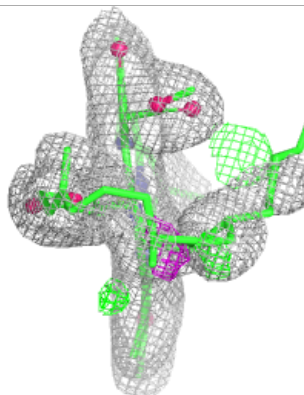
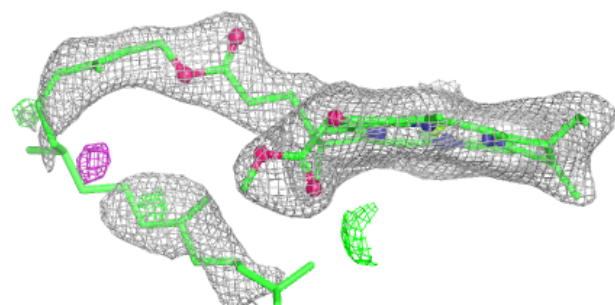
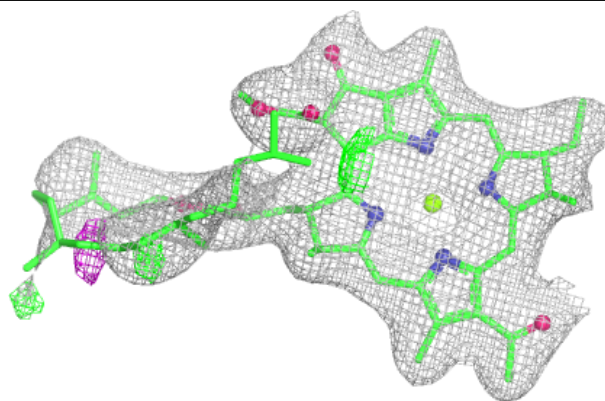


Electron density around BCL S 103:

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

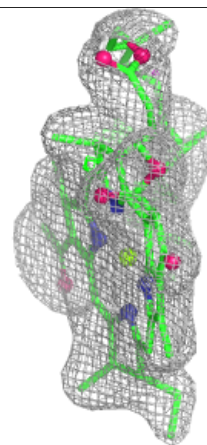
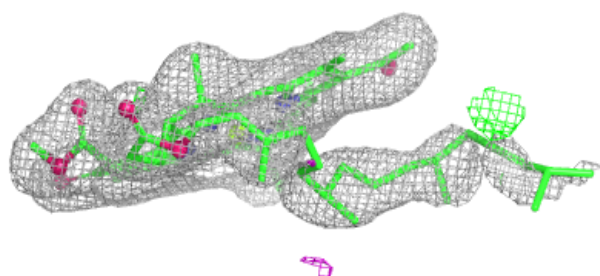
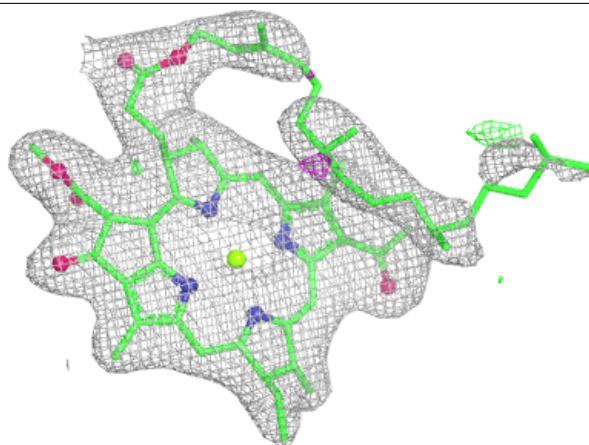
**Electron density around BCL W 102:**

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

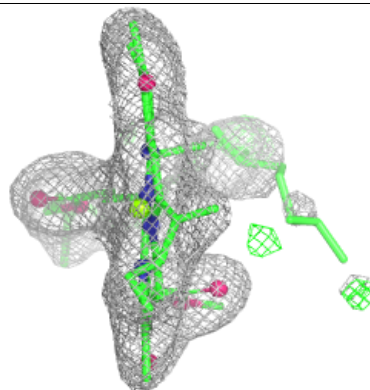
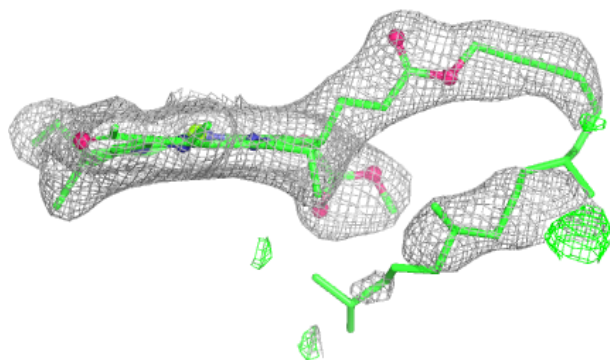
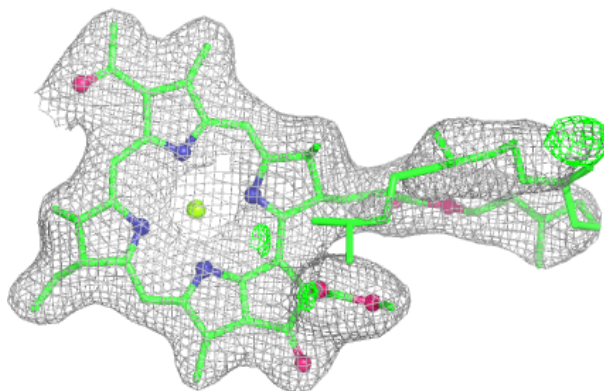


Electron density around BCL W 103:

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

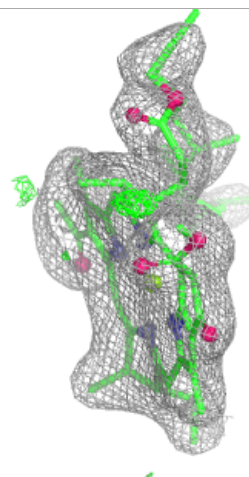
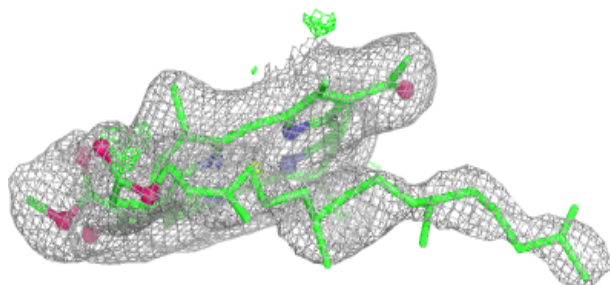
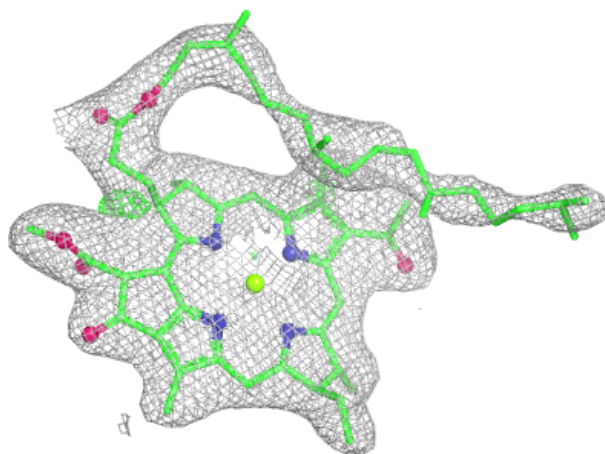
**Electron density around BCL Y 102:**

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



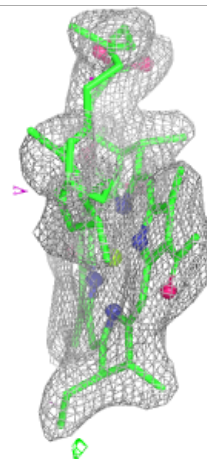
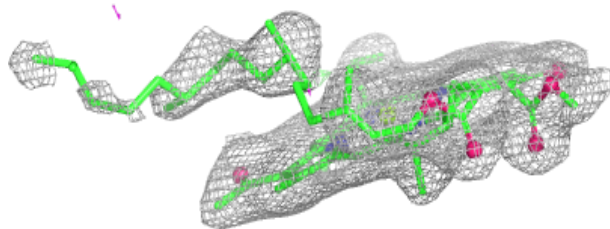
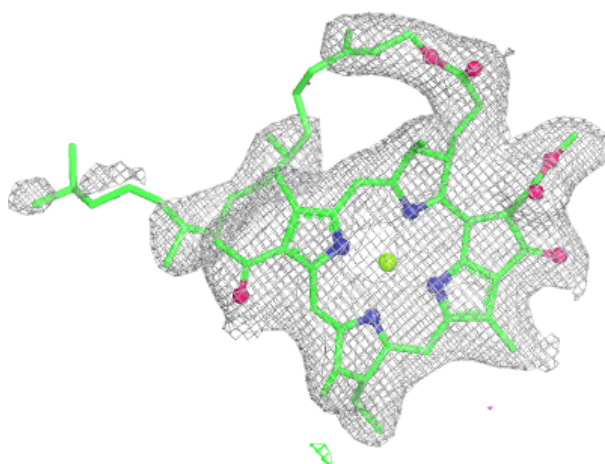
Electron density around BCL Z 102:

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



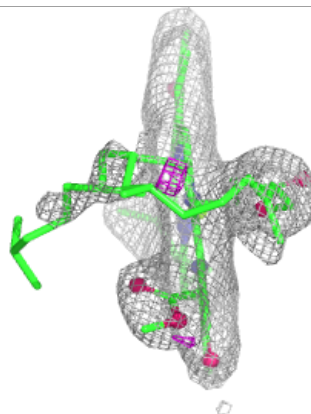
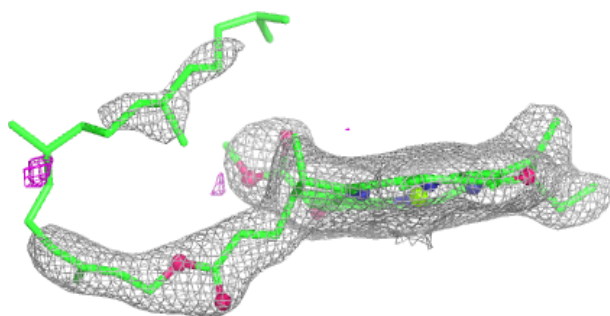
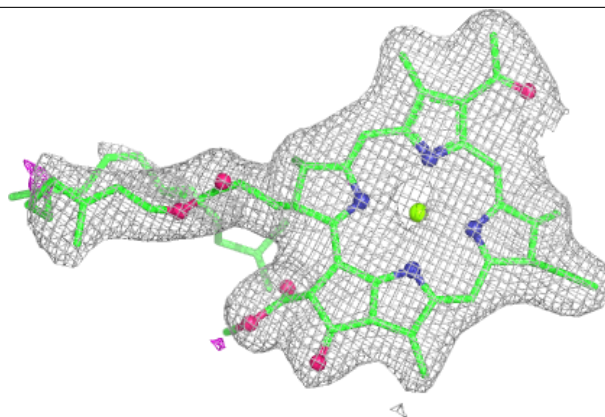
Electron density around BCL A 103:

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

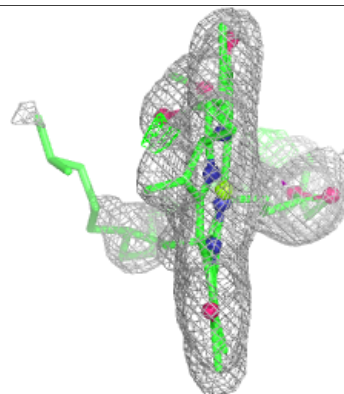
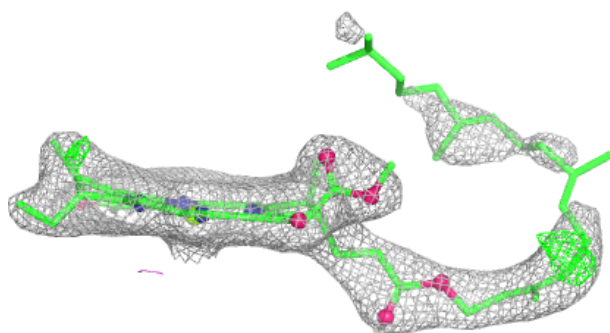
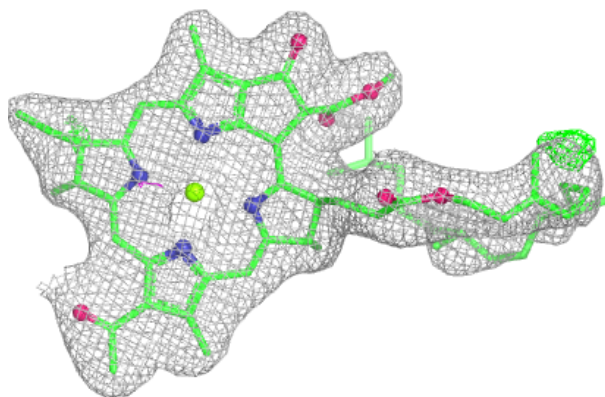


Electron density around BCL D 102:

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

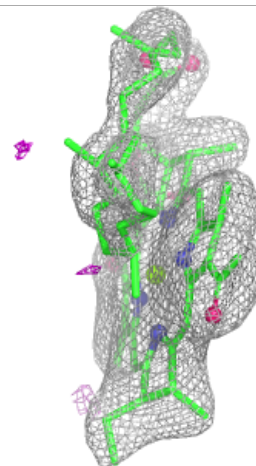
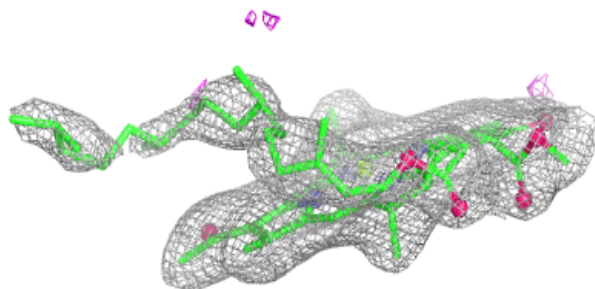
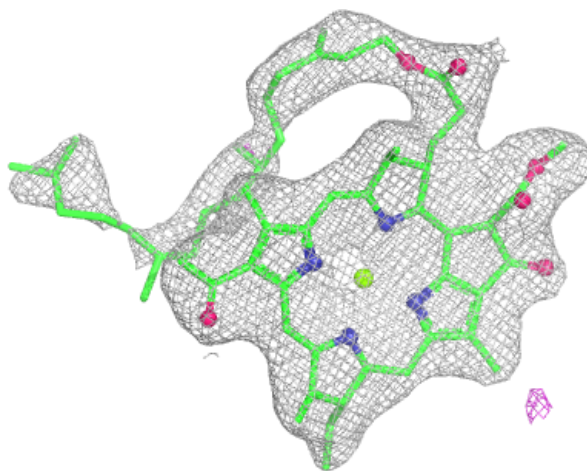
**Electron density around BCL F 102:**

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



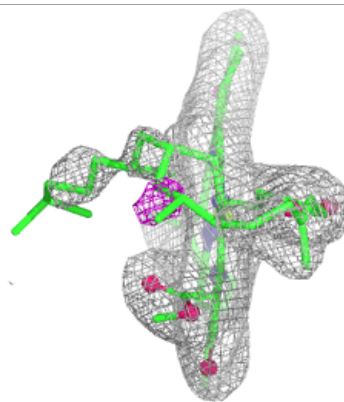
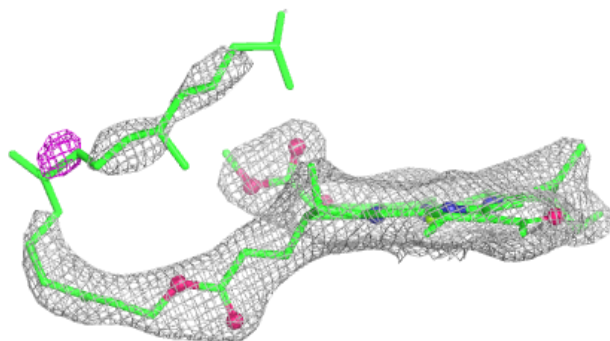
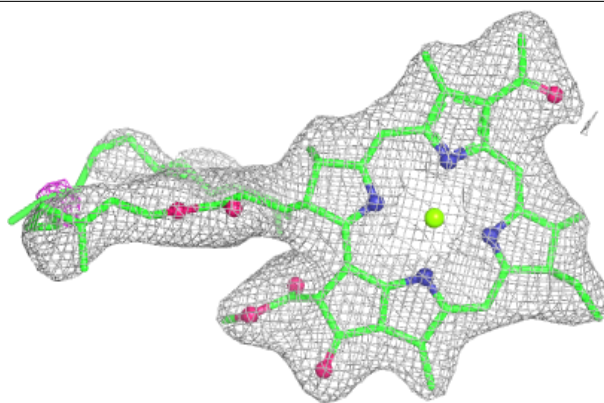
Electron density around BCL F 103:

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



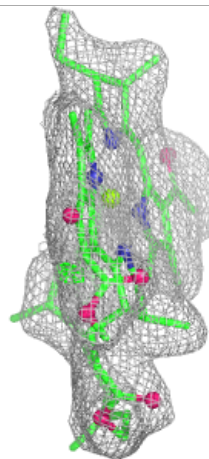
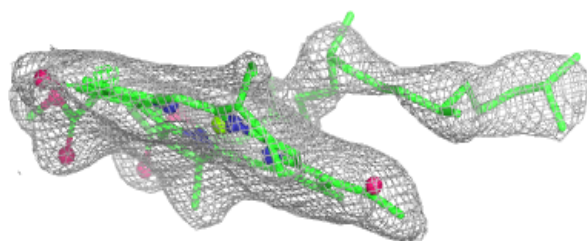
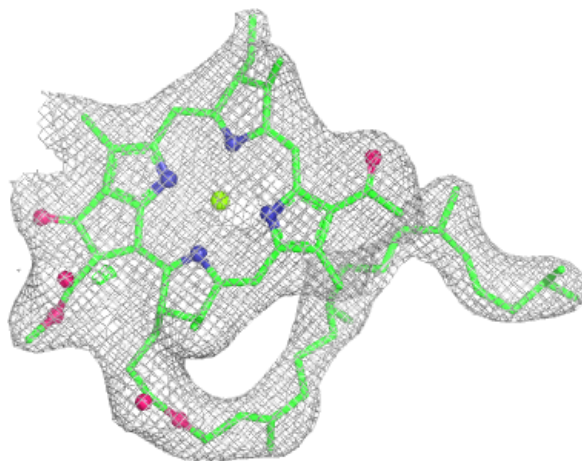
Electron density around BCL I 102:

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



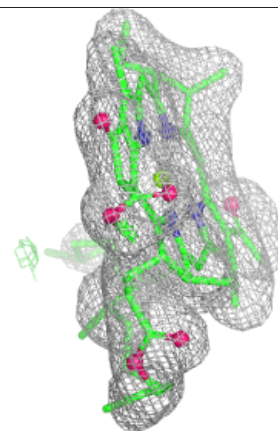
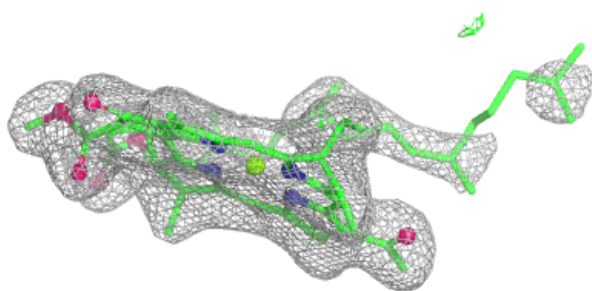
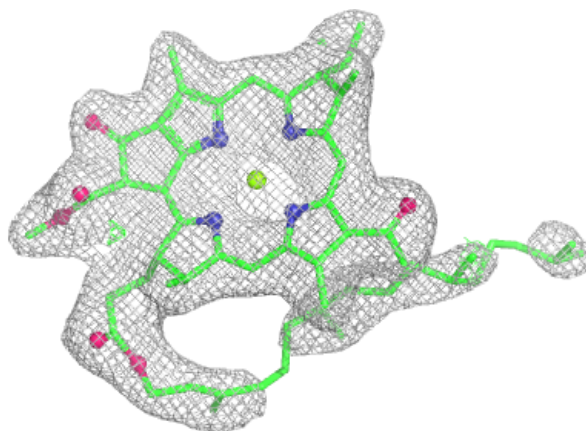
Electron density around BCL D 103:

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



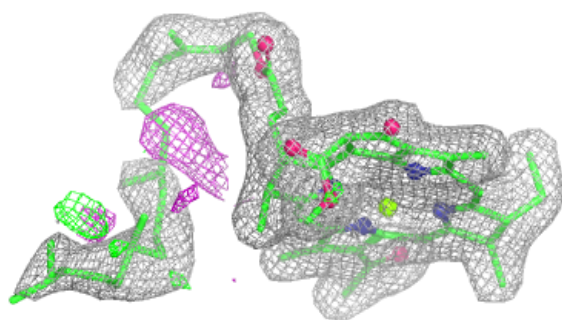
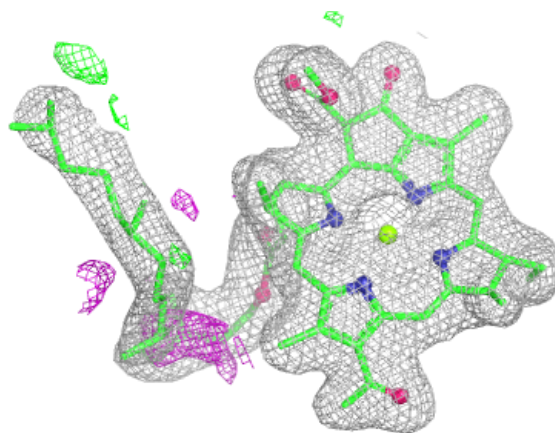
Electron density around BCL K 103:

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

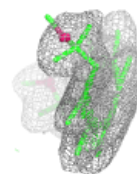
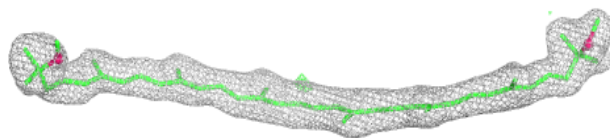
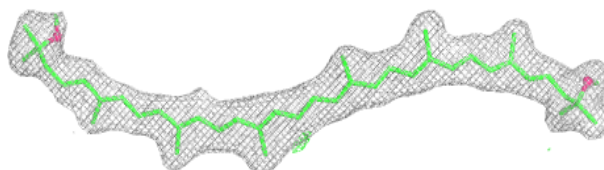


Electron density around BCL M 403:

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

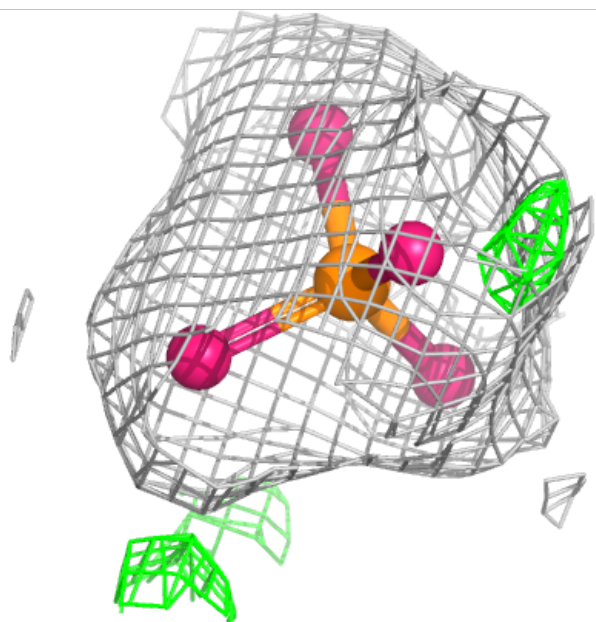
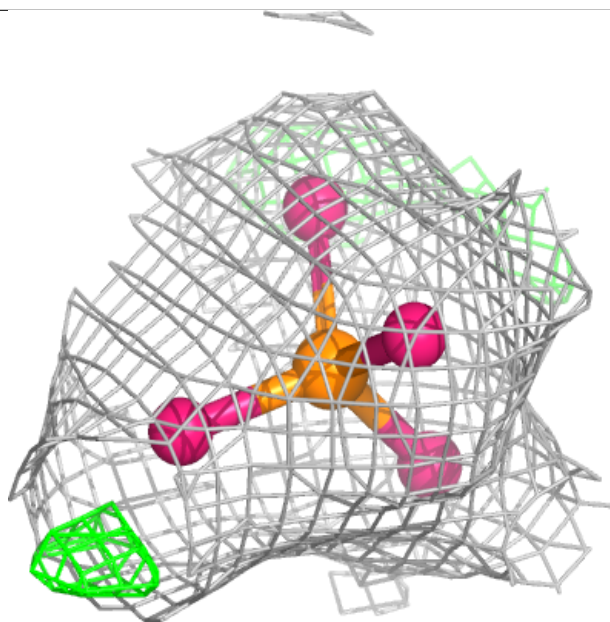
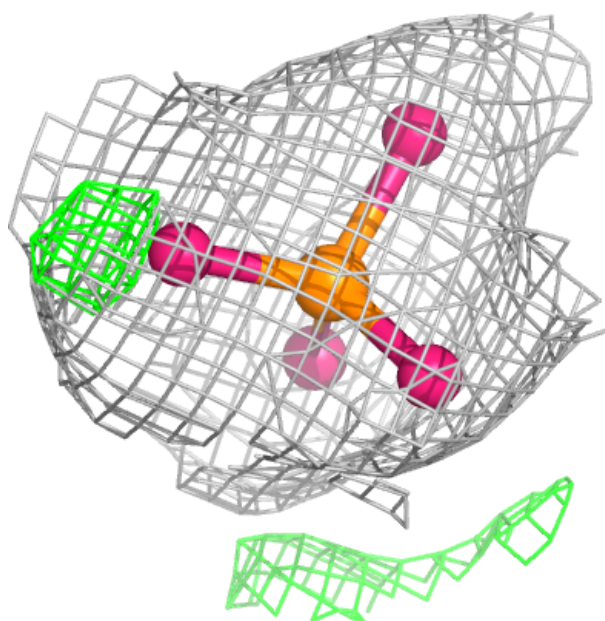
**Electron density around CRT O 104:**

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



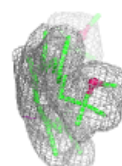
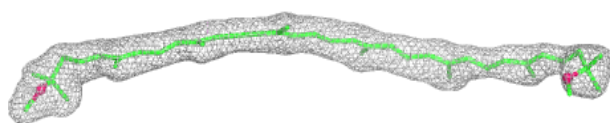
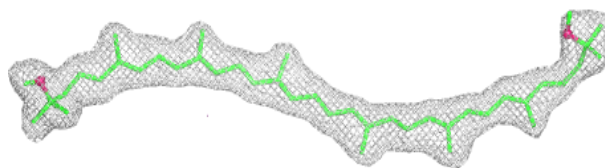
Electron density around PEF M 411:

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

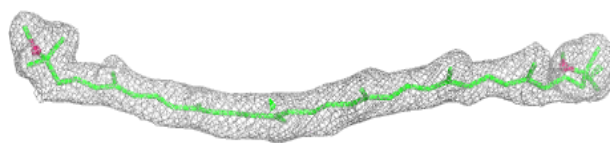
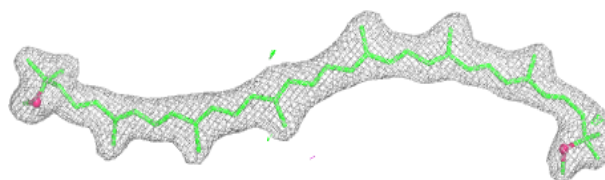


Electron density around CRT P 101:

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

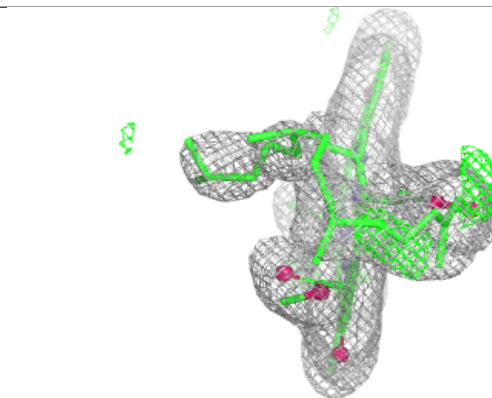
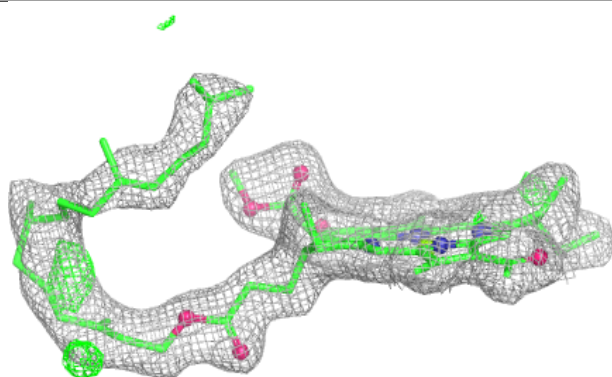
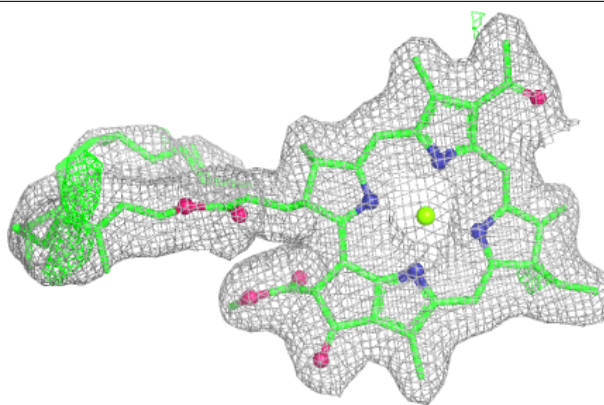
**Electron density around CRT Q 104:**

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

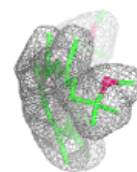
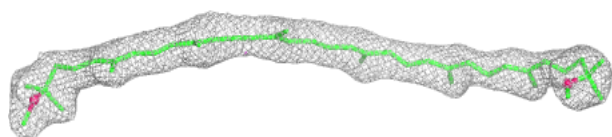
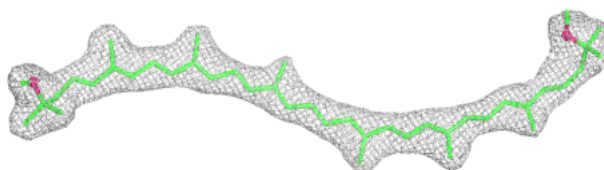


Electron density around BCL Q 102:

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

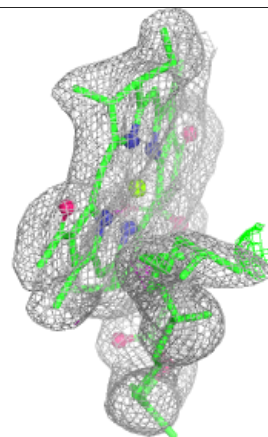
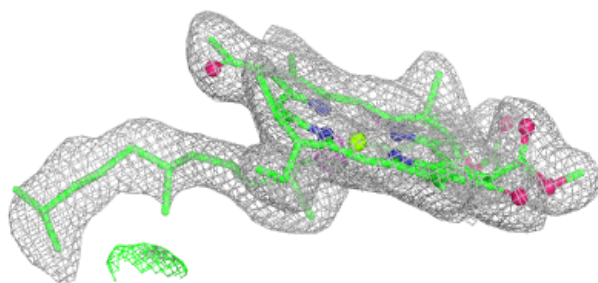
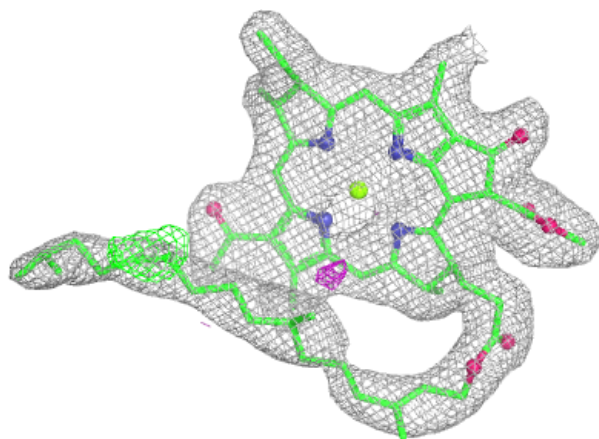
**Electron density around CRT V 101:**

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



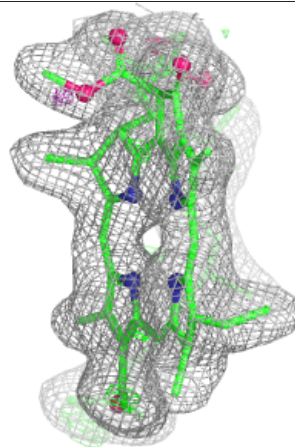
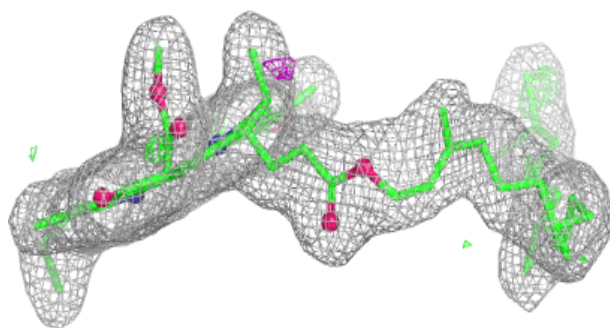
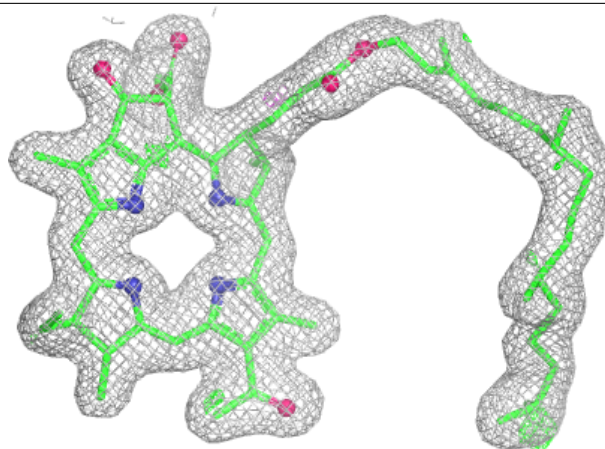
Electron density around BCL Q 103:

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

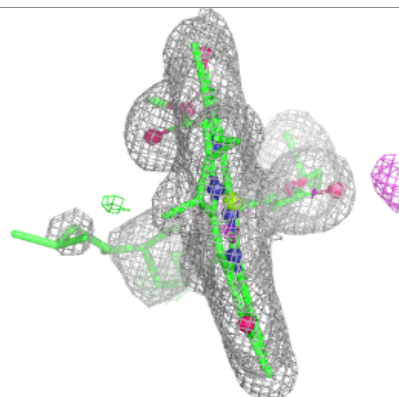
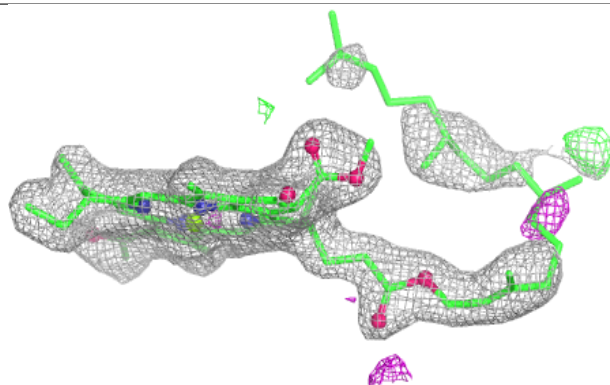
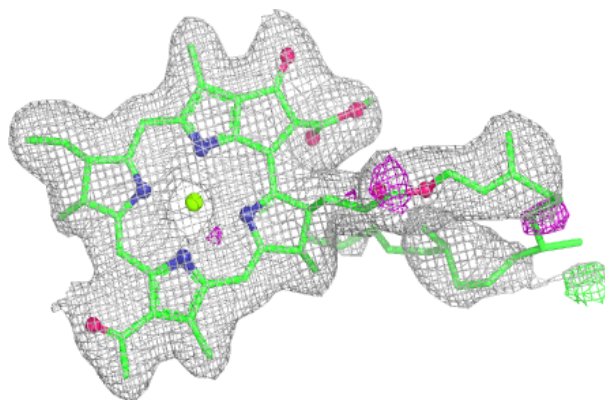


Electron density around BPH L 302:

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

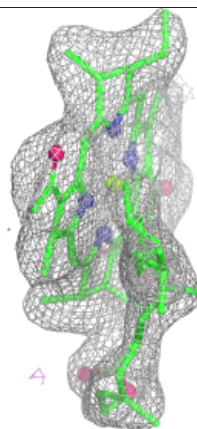
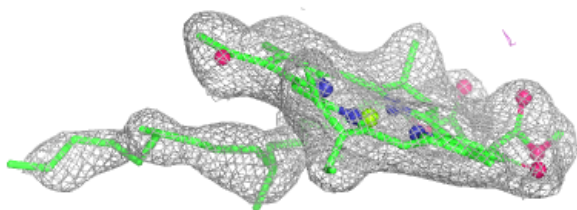
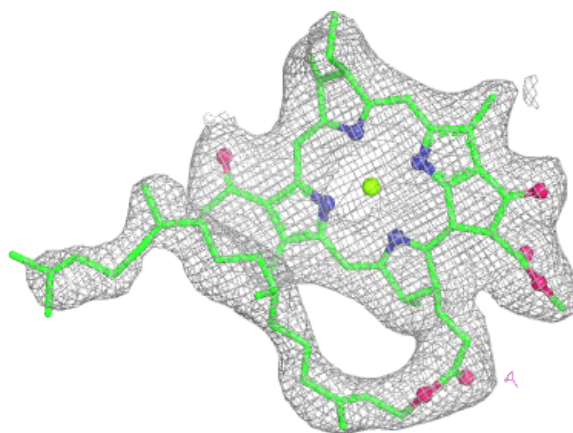
**Electron density around BCL S 102:**

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

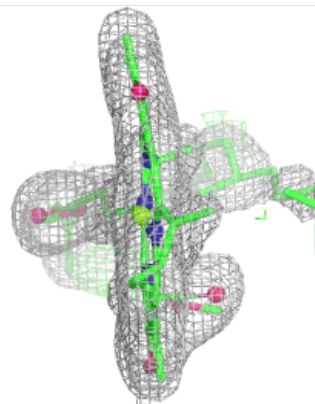
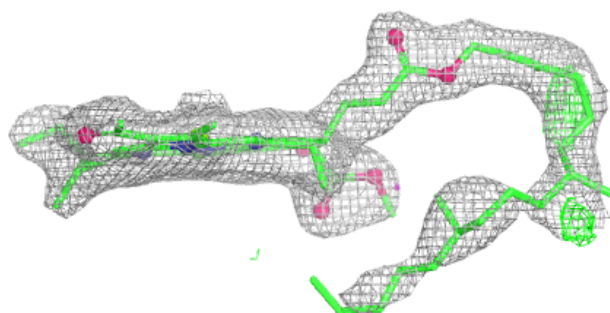
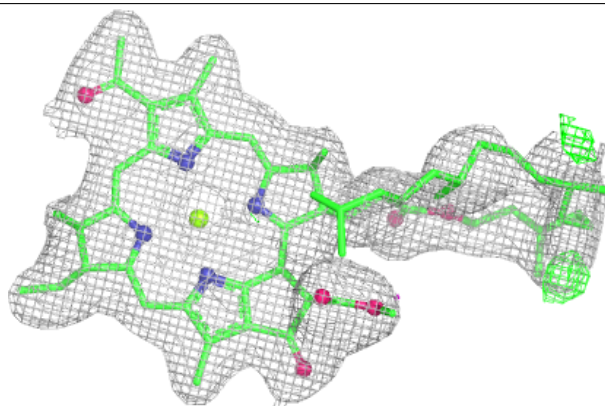


Electron density around BCL I 103:

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

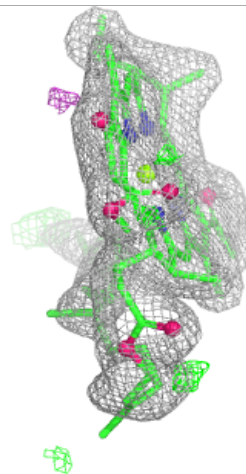
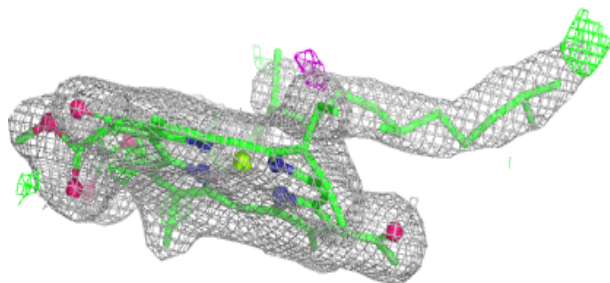
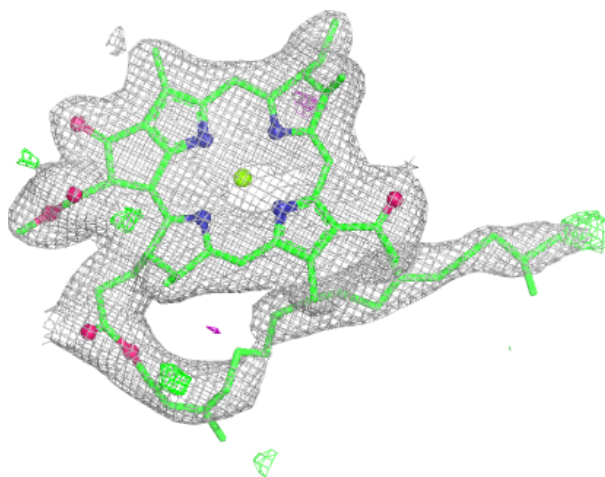
**Electron density around BCL U 102:**

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



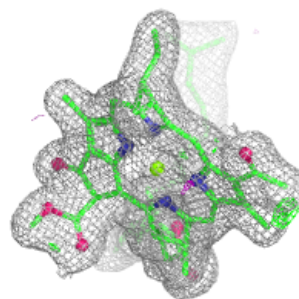
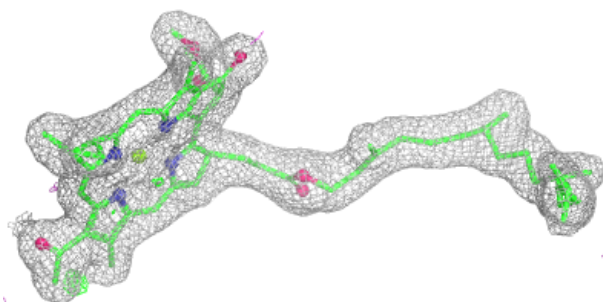
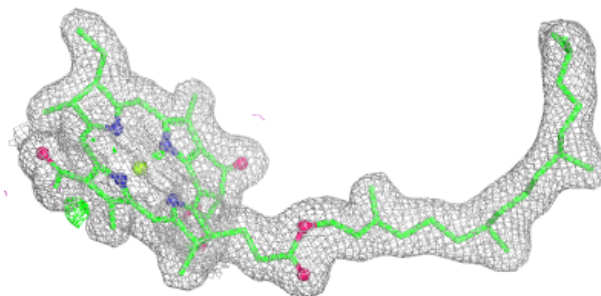
Electron density around BCL U 103:

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

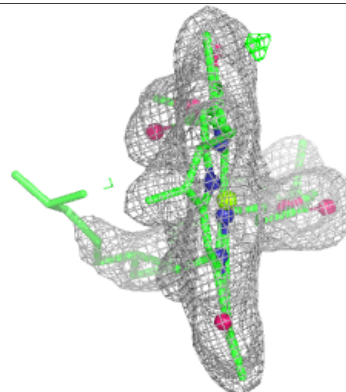
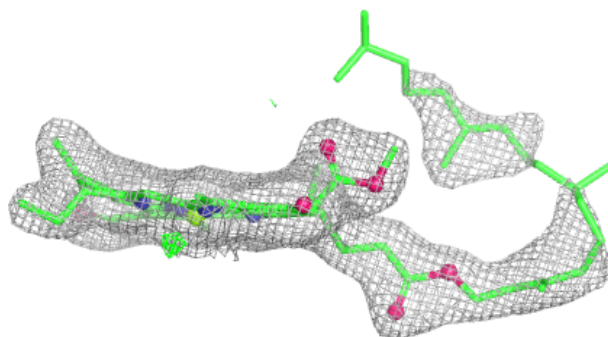
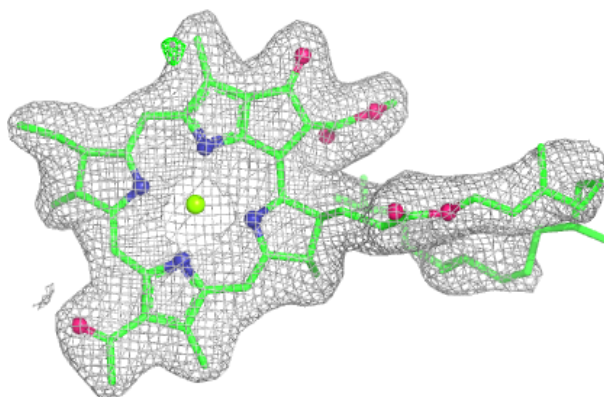


Electron density around BCL M 404:

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

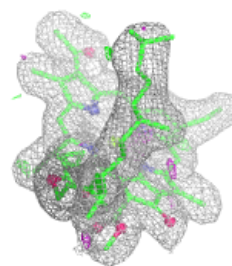
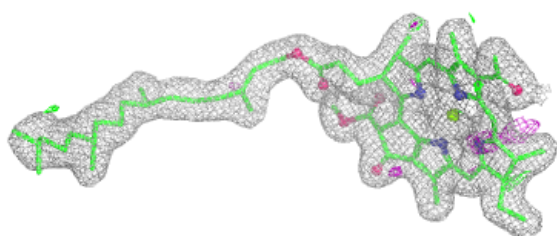
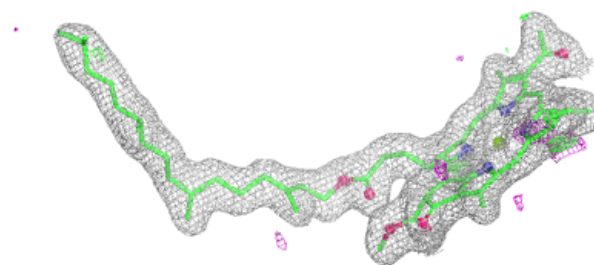
**Electron density around BCL O 102:**

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

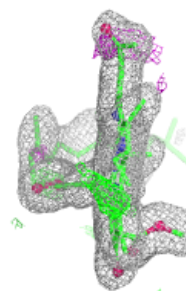
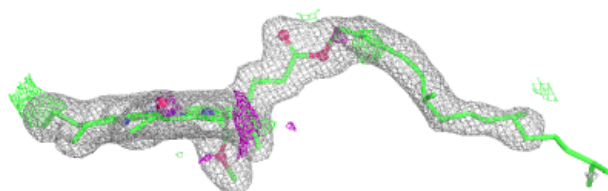
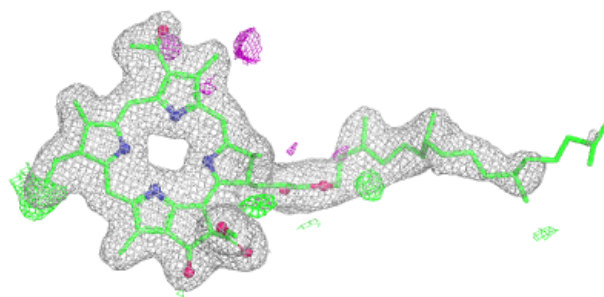


Electron density around BCL L 301:

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

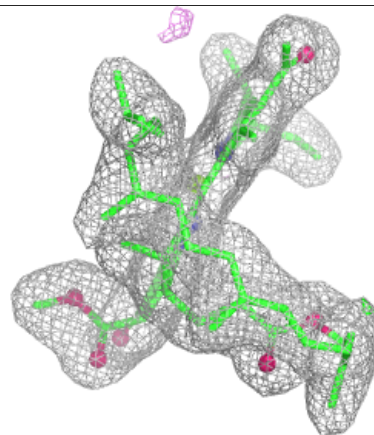
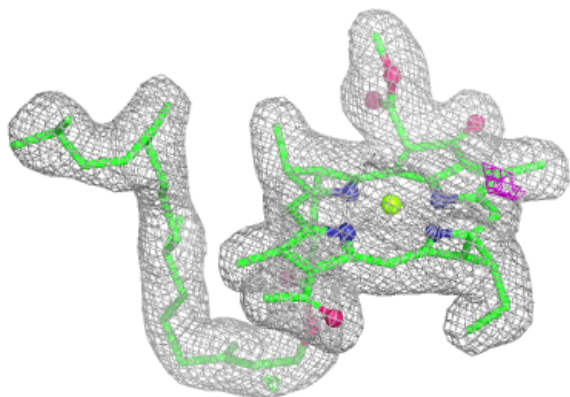
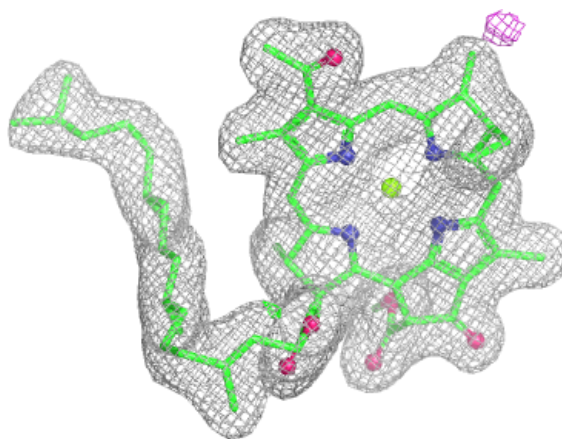
**Electron density around BPH M 405:**

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



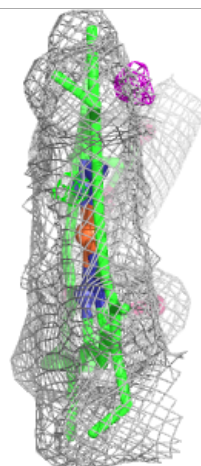
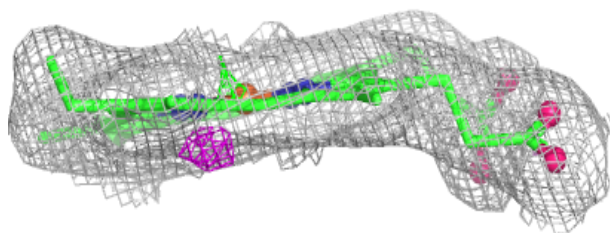
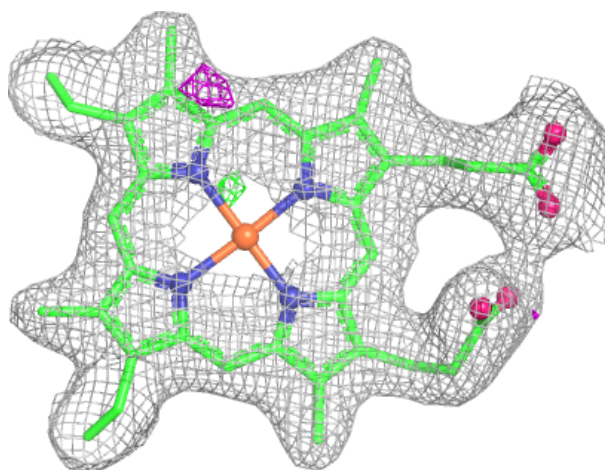
Electron density around BCL M 402:

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



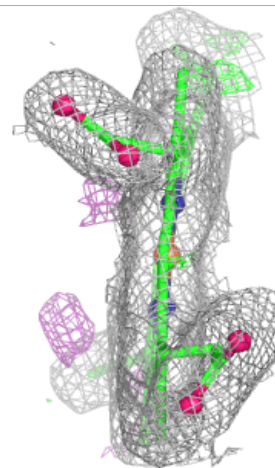
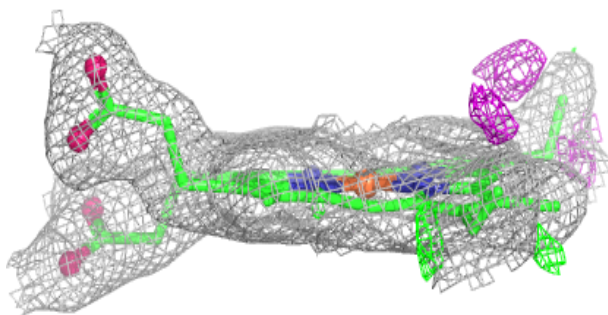
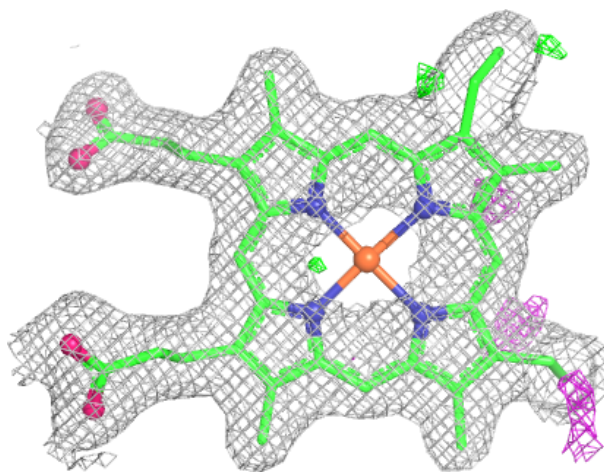
Electron density around HEC C 502:

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



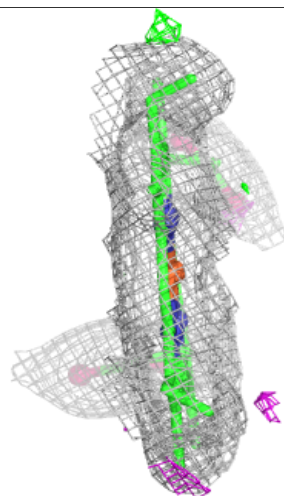
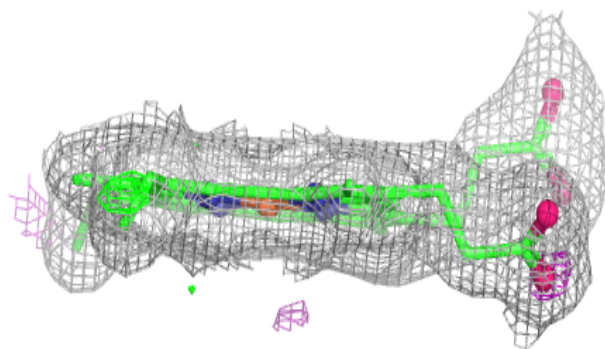
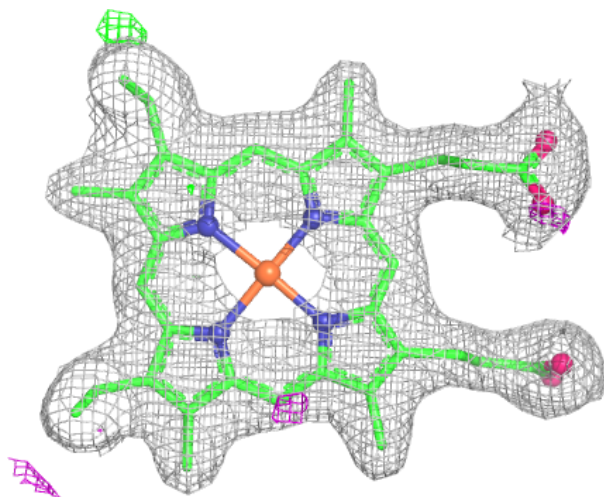
Electron density around HEC C 503:

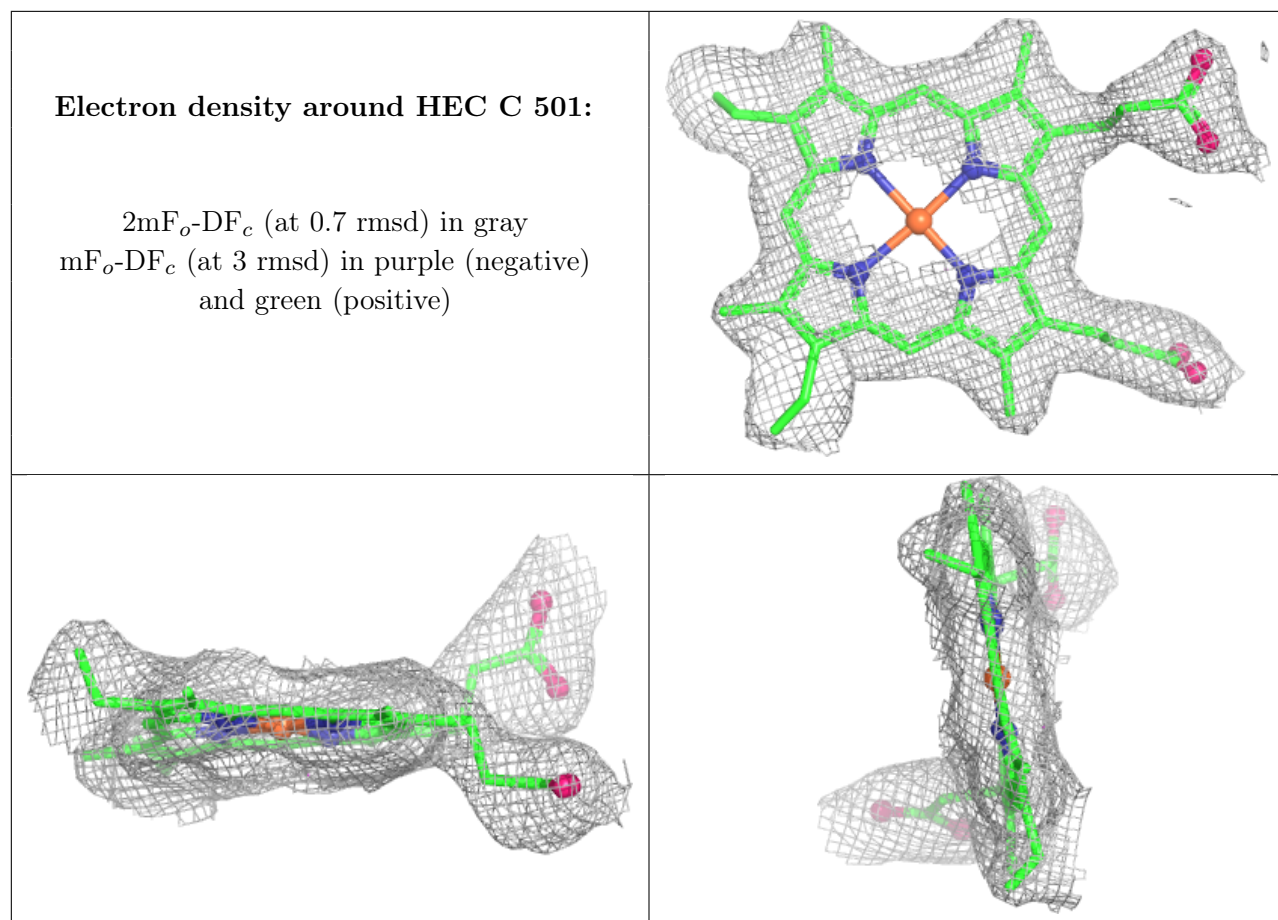
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.