



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 06:28 am GMT

PDB ID : 7O0W
EMDB ID : EMD-12681
Title : Cryo-EM structure of the RC-dLH complex (model_1b) from Gemmatimonas phototrophica at 2.47 Å
Authors : Qian, P.; Koblizek, M.
Deposited on : 2021-03-27
Resolution : 2.47 Å (reported)
Based on initial models : 6ET5, 1LGH, 5Y5S

This is a wwPDB EM 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/EMValidationReportHelp>
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:

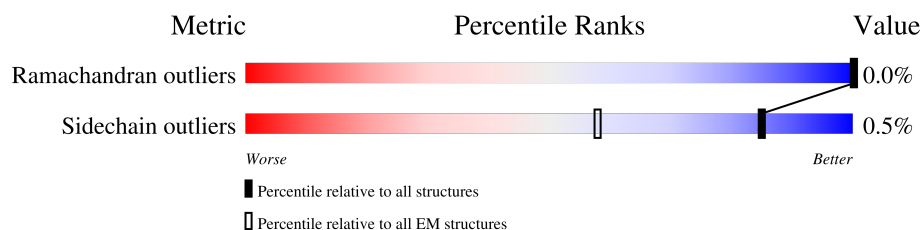
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY










The reported resolution of this entry is 2.47 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.














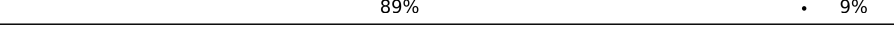







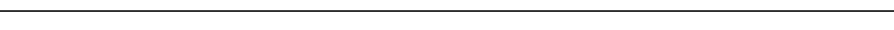

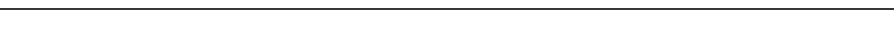
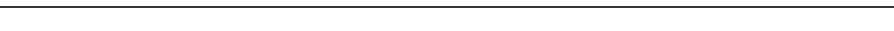


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	54	 89% • 9%
1	AB	54	 89% • 9%
1	AC	54	 89% 11%
1	AD	54	 87% • 11%
1	AE	54	 87% • 9%
1	AF	54	 91% 9%
1	AG	54	 91% 9%
1	AH	54	 87% • 9%
1	AI	54	 91% 9%


























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Mol	Chain	Length	Quality of chain
1	AJ	54	 89% 9%
1	AK	54	 91% 9%
1	AL	54	 89% 9%
1	AM	54	 91% 9%
1	AN	54	 89% 9%
1	AO	54	 89% 9%
1	AP	54	 89% 9%
1	AQ	54	 91% 9%
1	AR	54	 89% 9%
1	AS	54	 89% 9%
1	AT	54	 89% 9%
1	AU	54	 89% 9%
1	AV	54	 91% 9%
1	AW	54	 91% 9%
1	AX	54	 91% 9%
2	BA	44	 89% 11%
2	BB	44	 91% 9%
2	BC	44	 89% 11%
2	BD	44	 91% 9%
2	BE	44	 91% 9%
2	BF	44	 86% 11%
2	BG	44	 89% 11%
2	BH	44	 89% 11%
2	BI	44	 91% 9%
2	BJ	44	 89% 11%









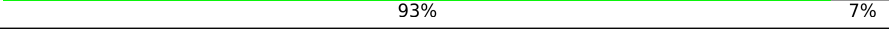
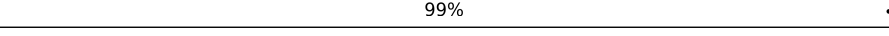
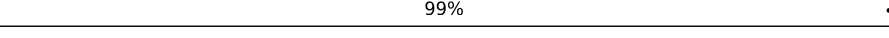
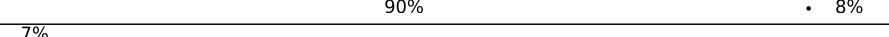

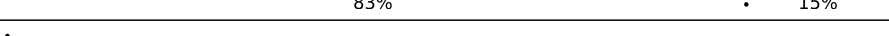


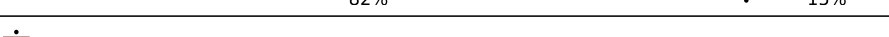

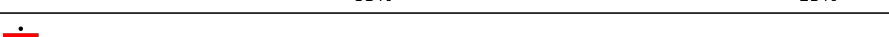






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Mol	Chain	Length	Quality of chain	
2	BK	44		
2	BL	44		
2	BM	44		
2	BN	44		
2	BO	44		
2	BP	44		
2	BQ	44		
2	BR	44		
2	BS	44		
2	BT	44		
2	BU	44		
2	BV	44		
2	BW	44		
2	BX	44		
2	ba	44		
2	bb	44		
2	bc	44		
2	bd	44		
2	be	44		
2	bf	44		
2	bg	44		
2	bh	44		
2	bi	44		
2	bj	44		
2	bk	44		



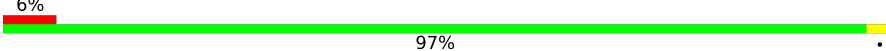
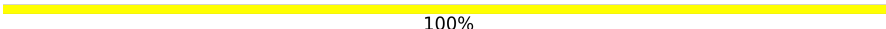
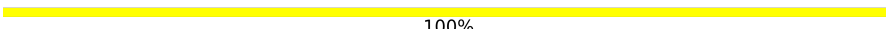
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Mol	Chain	Length	Quality of chain
2	bl	44	
2	bm	44	
2	bn	44	
2	bo	44	
2	bp	44	
3	C	354	
4	C1	202	
5	C2	125	
6	H1	67	
7	H2	181	
8	L	274	
9	M	367	
10	aa	71	
11	ab	71	
11	ac	71	
11	ad	71	
11	ae	71	
11	af	71	
11	ag	71	
11	ah	71	
11	ai	71	
11	aj	71	
11	ak	71	
11	al	71	
11	am	71	

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Mol	Chain	Length	Quality of chain
11	an	71	 80% 15%
11	ao	71	 6% 83% 15%
11	ap	71	 6% 97%
12	CG	2	 100%
12	MG	2	 100%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 56476 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 LHH-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AB	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AC	48	Total	C	N	O	S	0	0
			384	256	64	60	4		
1	AD	48	Total	C	N	O	S	0	0
			384	256	64	60	4		
1	AE	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AF	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AG	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AH	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AI	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AJ	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AK	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AL	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AM	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AN	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AO	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AP	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AQ	49	Total	C	N	O	S	0	0
			391	261	65	61	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AS	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AT	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AU	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AV	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AW	49	Total	C	N	O	S	0	0
			391	261	65	61	4		
1	AX	49	Total	C	N	O	S	0	0
			391	261	65	61	4		

- Molecule 2 is a protein called Light-harvesting protein B:885 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BB	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BC	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BD	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BE	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BF	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BG	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BH	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BI	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	BJ	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BK	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	BL	39	Total	C	N	O	S	0	0
			323	213	55	53	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BM	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BN	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BO	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BP	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BQ	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BR	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BS	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BT	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BU	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	BV	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BW	40	Total 327	C 215	N 56	O 54	S 2	0	0
2	BX	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	ba	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bb	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bc	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bd	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	be	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bf	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bg	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bh	39	Total 323	C 213	N 55	O 53	S 2	0	0
2	bi	39	Total 323	C 213	N 55	O 53	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	bj	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bk	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bl	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bm	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bn	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
2	bo	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
2	bp	39	Total	C	N	O	S	0	0
			323	213	55	53	2		

- Molecule 3 is a protein called MULTIHEME_CYTC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	299	Total	C	N	O	S	0	0
			2325	1464	419	423	19		

- Molecule 4 is a protein called RC-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C1	103	Total	C	N	O	S	0	0
			806	506	151	145	4		

- Molecule 5 is a protein called RC-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C2	101	Total	C	N	O	S	0	0
			779	491	150	135	3		

- Molecule 6 is a protein called PRCH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H1	62	Total	C	N	O	S	0	0
			522	343	89	88	2		

- Molecule 7 is a protein called RC-Hc.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H2	180	Total	C	N	O	S	0	0
			1404	894	239	267	4		

- Molecule 8 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	273	Total	C	N	O	S	0	0
			2165	1457	351	347	10		

- Molecule 9 is a protein called RC-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	336	Total	C	N	O	S	0	0
			2702	1795	443	454	10		

- Molecule 10 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aa	59	Total	C	N	O	S	0	0
			455	298	80	75	2		

- Molecule 11 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	ab	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ac	56	Total	C	N	O	S	0	0
			443	290	77	73	3		
11	ad	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ae	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	af	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ag	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ah	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ai	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	aj	60	Total	C	N	O	S	0	0
			465	304	81	77	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	ak	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
11	al	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	am	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	an	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ao	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ap	71	Total	C	N	O	S	0	0
			542	352	95	91	4		

- Molecule 12 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
12	CG	2	Total	C	O	0	0
			21	12	9		
12	MG	2	Total	C	O	0	0
			21	12	9		

- Molecule 13 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
13	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
13	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BH	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
13	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BO	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BP	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BR	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BS	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BT	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BU	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BV	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BW	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	BX	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	aa	1	Total 66	C 55	Mg 1	N 4	O 6	0

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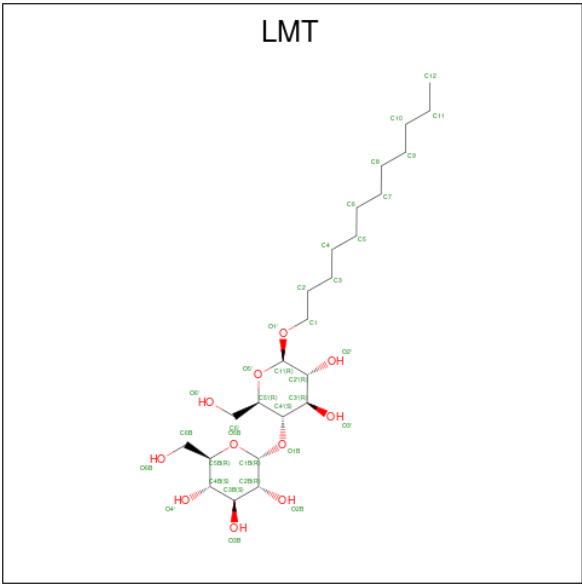
Mol	Chain	Residues	Atoms					AltConf
13	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ai	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	aj	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ak	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	al	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	am	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	an	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ao	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ap	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ba	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bb	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bc	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bd	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	be	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	bf	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
13	bg	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bh	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bi	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bj	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bk	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bl	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bm	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bn	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bo	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	bp	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 14 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
14	AA	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
14	AB	1	Total	C	O	0
			35	24	11	
14	AC	1	Total	C	O	0
			35	24	11	
14	AD	1	Total	C	O	0
			35	24	11	
14	AE	1	Total	C	O	0
			35	24	11	
14	AE	1	Total	C	O	0
			35	24	11	
14	AE	1	Total	C	O	0
			35	24	11	
14	AG	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			35	24	11	
14	AJ	1	Total	C	O	0
			35	24	11	
14	AJ	1	Total	C	O	0
			35	24	11	
14	AK	1	Total	C	O	0
			35	24	11	
14	AK	1	Total	C	O	0
			35	24	11	
14	AL	1	Total	C	O	0
			35	24	11	
14	AM	1	Total	C	O	0
			35	24	11	
14	AN	1	Total	C	O	0
			35	24	11	
14	AN	1	Total	C	O	0
			35	24	11	
14	AP	1	Total	C	O	0
			35	24	11	
14	AQ	1	Total	C	O	0
			35	24	11	
14	AS	1	Total	C	O	0
			35	24	11	
14	AT	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
14	AT	1	Total	C	O	0
			35	24	11	
14	AU	1	Total	C	O	0
			35	24	11	
14	AV	1	Total	C	O	0
			35	24	11	
14	AV	1	Total	C	O	0
			35	24	11	
14	AX	1	Total	C	O	0
			35	24	11	
14	BA	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BB	1	Total	C	O	0
			35	24	11	
14	BC	1	Total	C	O	0
			35	24	11	
14	BC	1	Total	C	O	0
			35	24	11	
14	BC	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BD	1	Total	C	O	0
			35	24	11	
14	BE	1	Total	C	O	0
			35	24	11	
14	BE	1	Total	C	O	0
			35	24	11	
14	BE	1	Total	C	O	0
			35	24	11	
14	BF	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
14	BF	1	Total	C	O	0
			35	24	11	
14	BG	1	Total	C	O	0
			35	24	11	
14	BG	1	Total	C	O	0
			35	24	11	
14	BG	1	Total	C	O	0
			35	24	11	
14	BH	1	Total	C	O	0
			35	24	11	
14	BH	1	Total	C	O	0
			35	24	11	
14	BH	1	Total	C	O	0
			35	24	11	
14	BI	1	Total	C	O	0
			35	24	11	
14	BI	1	Total	C	O	0
			35	24	11	
14	BI	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BJ	1	Total	C	O	0
			35	24	11	
14	BK	1	Total	C	O	0
			35	24	11	
14	BK	1	Total	C	O	0
			35	24	11	
14	BK	1	Total	C	O	0
			35	24	11	
14	BL	1	Total	C	O	0
			35	24	11	
14	BL	1	Total	C	O	0
			35	24	11	
14	BM	1	Total	C	O	0
			35	24	11	
14	BM	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
14	BM	1	Total	C	O	0
			35	24	11	
14	BN	1	Total	C	O	0
			35	24	11	
14	BN	1	Total	C	O	0
			35	24	11	
14	BN	1	Total	C	O	0
			35	24	11	
14	BO	1	Total	C	O	0
			35	24	11	
14	BO	1	Total	C	O	0
			35	24	11	
14	BO	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BP	1	Total	C	O	0
			35	24	11	
14	BQ	1	Total	C	O	0
			35	24	11	
14	BQ	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BR	1	Total	C	O	0
			35	24	11	
14	BS	1	Total	C	O	0
			35	24	11	
14	BS	1	Total	C	O	0
			35	24	11	
14	BS	1	Total	C	O	0
			35	24	11	
14	BT	1	Total	C	O	0
			35	24	11	

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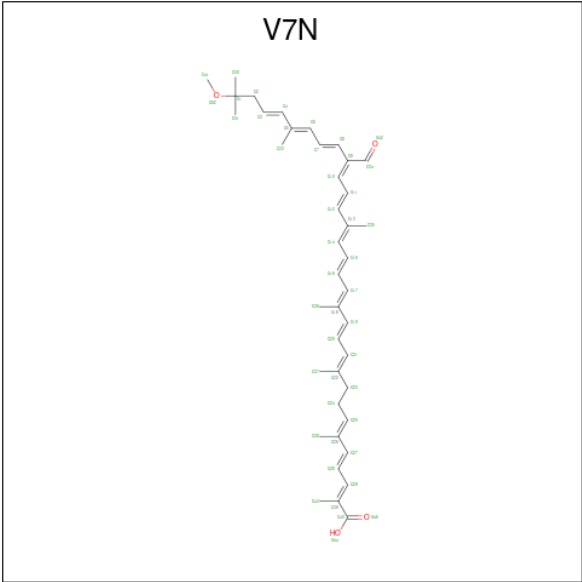
Mol	Chain	Residues	Atoms			AltConf
14	BT	1	Total	C	O	0
			35	24	11	
14	BT	1	Total	C	O	0
			35	24	11	
14	BU	1	Total	C	O	0
			35	24	11	
14	BU	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	C	1	Total	C	O	0
			35	24	11	
14	C2	1	Total	C	O	0
			35	24	11	
14	H2	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
14	L	1	Total	C	O	0
			35	24	11	
14	ac	1	Total	C	O	0
			35	24	11	
14	bc	1	Total	C	O	0
			35	24	11	
14	be	1	Total	C	O	0
			35	24	11	
14	be	1	Total	C	O	0
			35	24	11	
14	bf	1	Total	C	O	0
			35	24	11	
14	bg	1	Total	C	O	0
			35	24	11	
14	bh	1	Total	C	O	0
			35	24	11	
14	bi	1	Total	C	O	0
			35	24	11	
14	bj	1	Total	C	O	0
			35	24	11	
14	bk	1	Total	C	O	0
			35	24	11	
14	bl	1	Total	C	O	0
			35	24	11	
14	bm	1	Total	C	O	0
			35	24	11	
14	bn	1	Total	C	O	0
			35	24	11	
14	bo	1	Total	C	O	0
			35	24	11	
14	bp	1	Total	C	O	0
			35	24	11	
14	bp	1	Total	C	O	0
			35	24	11	

- Molecule 15 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-dotriaconta-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (three-letter code: V7N) (formula: C₄₁H₅₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
15	AA	1	Total	C	O	0
			45	41	4	
15	AD	1	Total	C	O	0
			45	41	4	
15	AM	1	Total	C	O	0
			45	41	4	
15	AS	1	Total	C	O	0
			45	41	4	
15	AW	1	Total	C	O	0
			45	41	4	
15	BA	1	Total	C	O	0
			45	41	4	
15	BD	1	Total	C	O	0
			45	41	4	
15	BE	1	Total	C	O	0
			45	41	4	
15	BF	1	Total	C	O	0
			45	41	4	
15	BG	1	Total	C	O	0
			45	41	4	
15	BH	1	Total	C	O	0
			45	41	4	
15	BI	1	Total	C	O	0
			45	41	4	
15	BJ	1	Total	C	O	0
			45	41	4	
15	BK	1	Total	C	O	0
			45	41	4	

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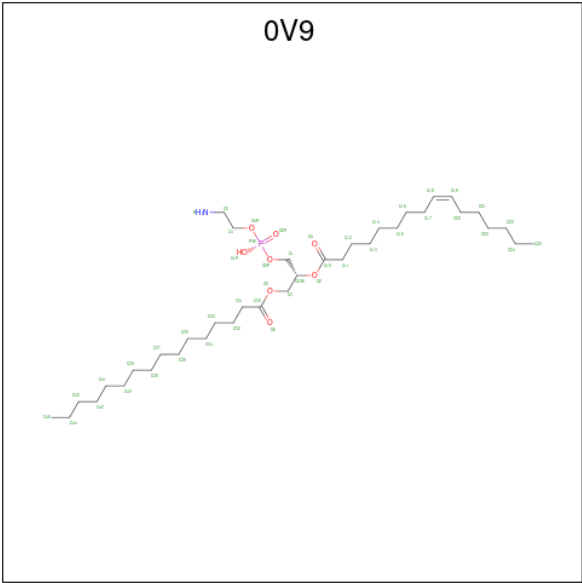
Mol	Chain	Residues	Atoms			AltConf
15	BM	1	Total	C	O	0
			45	41	4	
15	BN	1	Total	C	O	0
			45	41	4	
15	BO	1	Total	C	O	0
			45	41	4	
15	BP	1	Total	C	O	0
			45	41	4	
15	BQ	1	Total	C	O	0
			45	41	4	
15	BR	1	Total	C	O	0
			45	41	4	
15	BS	1	Total	C	O	0
			45	41	4	
15	BU	1	Total	C	O	0
			45	41	4	
15	BV	1	Total	C	O	0
			45	41	4	
15	BW	1	Total	C	O	0
			45	41	4	
15	ag	1	Total	C	O	0
			45	41	4	
15	ba	1	Total	C	O	0
			45	41	4	
15	bb	1	Total	C	O	0
			45	41	4	
15	bc	1	Total	C	O	0
			45	41	4	
15	bd	1	Total	C	O	0
			45	41	4	
15	be	1	Total	C	O	0
			45	41	4	
15	bg	1	Total	C	O	0
			45	41	4	
15	bh	1	Total	C	O	0
			45	41	4	
15	bi	1	Total	C	O	0
			45	41	4	
15	bj	1	Total	C	O	0
			45	41	4	
15	bk	1	Total	C	O	0
			45	41	4	

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Mol	Chain	Residues	Atoms			AltConf
15	bl	1	Total	C	O	0
			45	41	4	
15	bm	1	Total	C	O	0
			45	41	4	
15	bn	1	Total	C	O	0
			45	41	4	
15	bo	1	Total	C	O	0
			45	41	4	
15	bp	1	Total	C	O	0
			45	41	4	

- Molecule 16 is (19R,22S)-25-amino-22-hydroxy-22-oxido-16-oxo-17,21,23-trioxa-22lambda da 5 -phosphapentacosan-19-yl (9Z)-hexadec-9-enoate (three-letter code: 0V9) (formula: C₃₇H₇₂NO₈P) (labeled as "Ligand of Interest" by depositor).



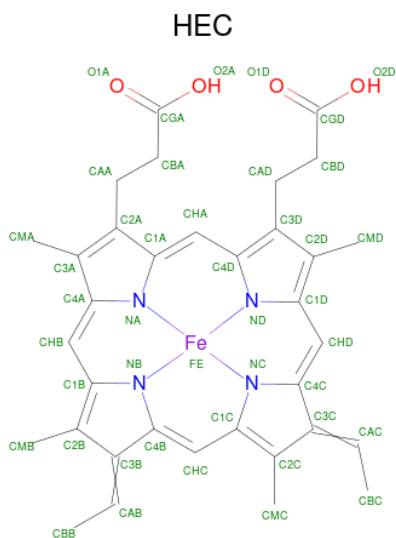
Mol	Chain	Residues	Atoms					AltConf
16	AQ	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	H1	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
16	ab	1	Total	C	N	O	P	0
			45	35	1	8	1	

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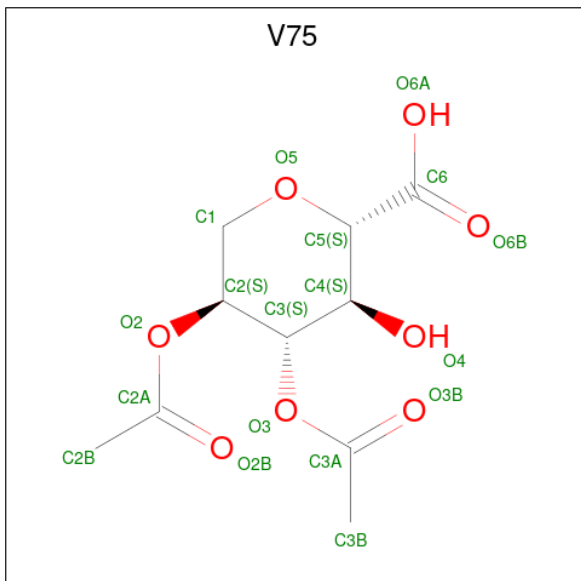
Mol	Chain	Residues	Atoms					AltConf
16	ad	1	Total 45	C 35	N 1	O 8	P 1	0
16	bb	1	Total 45	C 35	N 1	O 8	P 1	0
16	bd	1	Total 45	C 35	N 1	O 8	P 1	0
16	be	1	Total 45	C 35	N 1	O 8	P 1	0
16	bf	1	Total 45	C 35	N 1	O 8	P 1	0
16	bg	1	Total 45	C 35	N 1	O 8	P 1	0
16	bh	1	Total 45	C 35	N 1	O 8	P 1	0
16	bi	1	Total 45	C 35	N 1	O 8	P 1	0
16	bj	1	Total 45	C 35	N 1	O 8	P 1	0
16	bk	1	Total 45	C 35	N 1	O 8	P 1	0
16	bl	1	Total 45	C 35	N 1	O 8	P 1	0
16	bm	1	Total 45	C 35	N 1	O 8	P 1	0
16	bn	1	Total 45	C 35	N 1	O 8	P 1	0
16	bo	1	Total 45	C 35	N 1	O 8	P 1	0
16	bp	1	Total 45	C 35	N 1	O 8	P 1	0

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



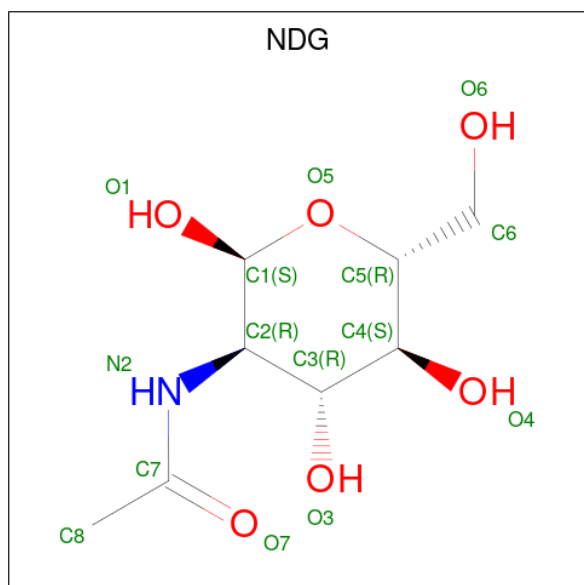
Mol	Chain	Residues	Atoms					AltConf
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
17	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 18 is (2 {S},3 {S},4 {S},5 {S})-4,5-diacetyloxy-3-oxidanyl-oxane-2-carboxylic acid (three-letter code: V75) (formula: C₁₀H₁₄O₈) (labeled as "Ligand of Interest" by depositor).



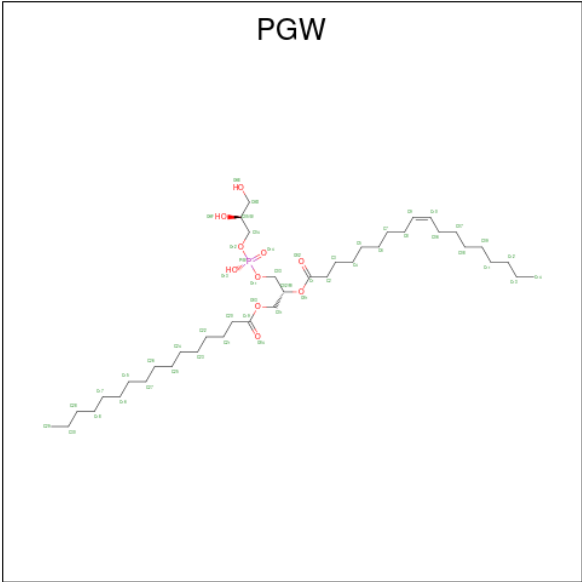
Mol	Chain	Residues	Atoms			AltConf
18	C	1	Total	C	O	0
			18	10	8	
18	M	1	Total	C	O	0
			18	10	8	

- Molecule 19 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



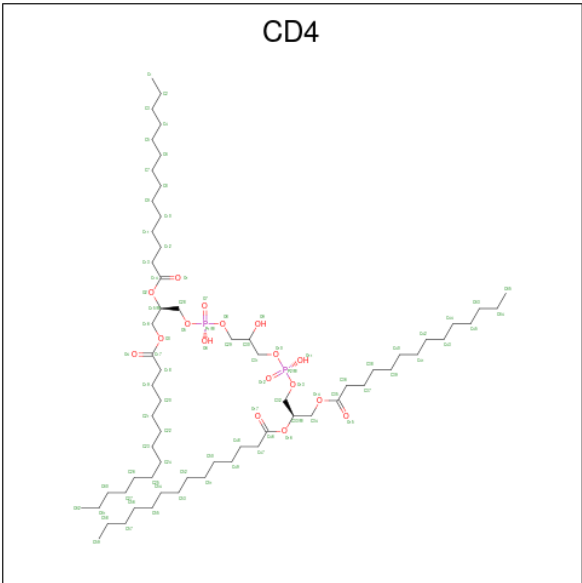
Mol	Chain	Residues	Atoms				AltConf
19	C	1	Total	C	N	O	0
			14	8	1	5	
19	C1	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 20 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	H1	1	51	40	10	1	0

- Molecule 21 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecano yloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (three-letter code: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).



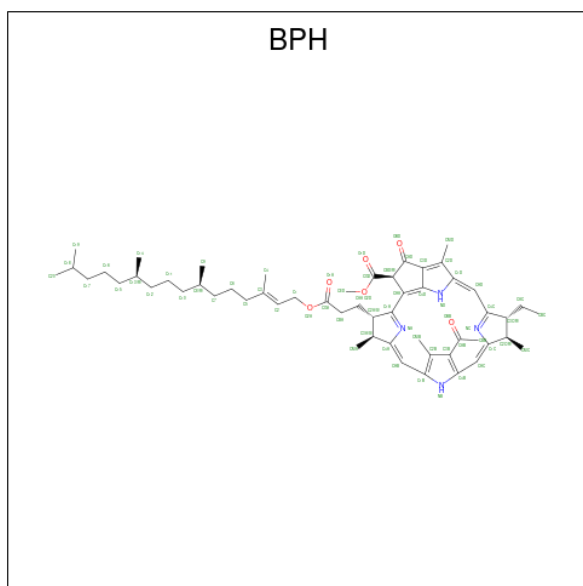
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	H1	1	84	65	17	2	0
21	M	1	84	65	17	2	0

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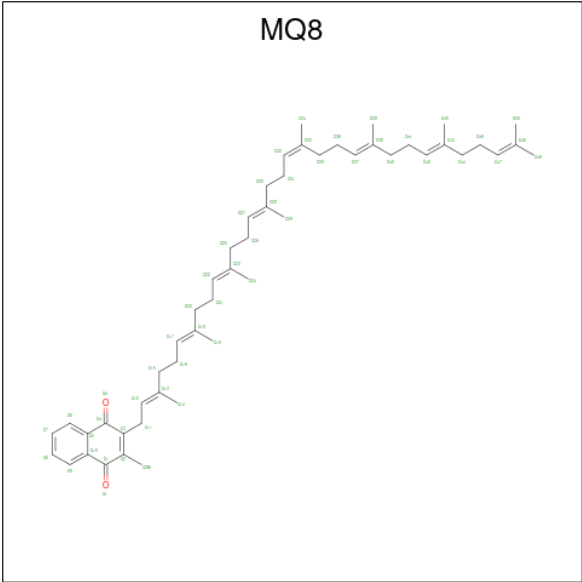
Mol	Chain	Residues	Atoms				AltConf
21	M	1	Total	C	O	P	0
			84	65	17	2	
21	ad	1	Total	C	O	P	0
			84	65	17	2	
21	af	1	Total	C	O	P	0
			84	65	17	2	
21	af	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 22 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).

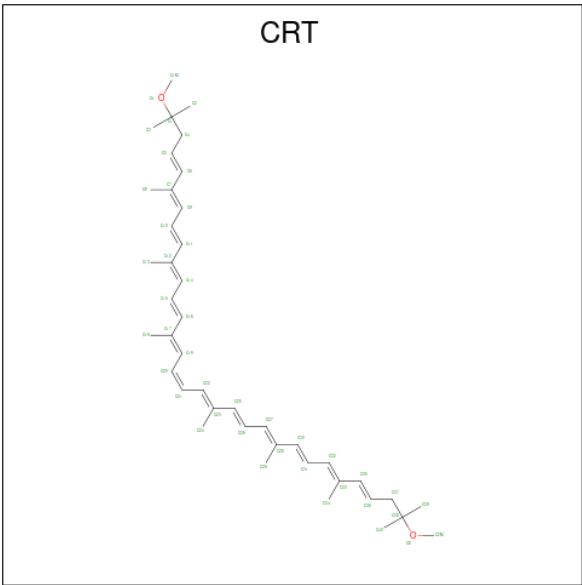


Mol	Chain	Residues	Atoms			AltConf
23	L	1	Total	C	O	0
			53	51	2	
23	M	1	Total	C	O	0
			53	51	2	
23	ao	1	Total	C	O	0
			53	51	2	

- Molecule 24 is FE (III) ION (three-letter code: FE) (formula: Fe).

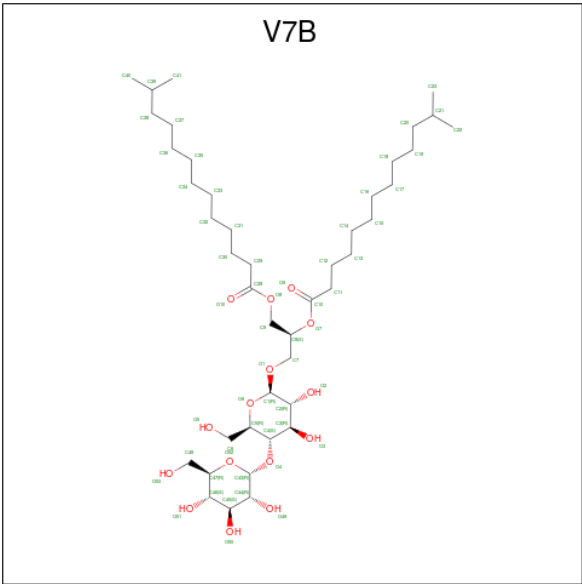
Mol	Chain	Residues	Atoms		AltConf
24	M	1	Total	Fe	0
			1	1	

- Molecule 25 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C₄₂H₆₀O₂).



Mol	Chain	Residues	Atoms			AltConf
25	M	1	Total	C	O	0
			44	42	2	

- Molecule 26 is [(2 {S})-3-[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-5-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]oxy-2-(12-methyltridecanoyloxy)propyl] 12-methyltridecanoate (three-letter code: V7B) (formula: C₄₃H₈₀O₁₅) (labeled as "Ligand of Interest" by depositor).



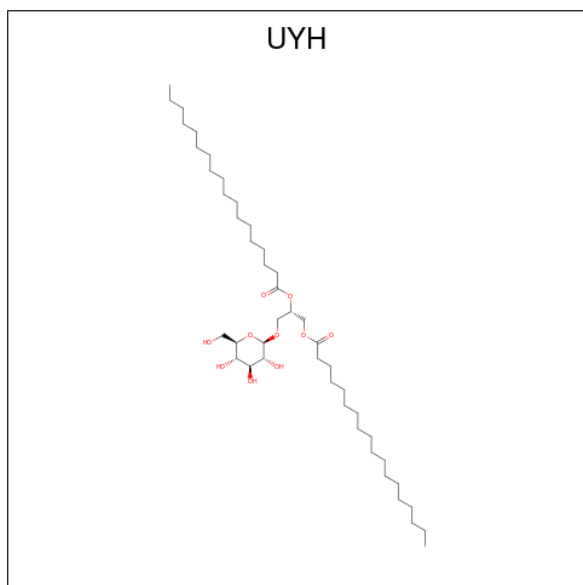
Mol	Chain	Residues	Atoms			AltConf
26	af	1	Total	C	O	0
			58	43	15	

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Mol	Chain	Residues	Atoms			AltConf
26	ag	1	Total	C	O	0
			58	43	15	

- Molecule 27 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-octadecanoyloxy-propyl] octadecanoate (three-letter code: UYH) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	ai	1	Total	C	O	0
			55	45	10	

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	AA	2	Total	O	0
			2	2	
28	AC	1	Total	O	0
			1	1	
28	AD	2	Total	O	0
			2	2	
28	AE	2	Total	O	0
			2	2	
28	AG	3	Total	O	0
			3	3	
28	AH	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
28	AI	1	Total O 1 1	0
28	AJ	5	Total O 5 5	0
28	AK	3	Total O 3 3	0
28	AL	2	Total O 2 2	0
28	AM	3	Total O 3 3	0
28	AN	2	Total O 2 2	0
28	AO	1	Total O 1 1	0
28	AP	3	Total O 3 3	0
28	AQ	5	Total O 5 5	0
28	AR	3	Total O 3 3	0
28	AS	4	Total O 4 4	0
28	AT	4	Total O 4 4	0
28	AV	2	Total O 2 2	0
28	AW	3	Total O 3 3	0
28	AX	1	Total O 1 1	0
28	BJ	1	Total O 1 1	0
28	C	67	Total O 67 67	0
28	C1	36	Total O 36 36	0
28	C2	1	Total O 1 1	0
28	H1	4	Total O 4 4	0
28	H2	27	Total O 27 27	0

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Mol	Chain	Residues	Atoms		AltConf
28	L	48	Total 48	O 48	0
28	M	63	Total 63	O 63	0
28	aa	4	Total 4	O 4	0
28	ab	2	Total 2	O 2	0
28	ac	1	Total 1	O 1	0
28	ad	7	Total 7	O 7	0
28	ae	9	Total 9	O 9	0
28	af	14	Total 14	O 14	0
28	ag	4	Total 4	O 4	0
28	ah	3	Total 3	O 3	0
28	ai	3	Total 3	O 3	0
28	aj	2	Total 2	O 2	0
28	ak	6	Total 6	O 6	0
28	al	6	Total 6	O 6	0
28	am	5	Total 5	O 5	0
28	an	7	Total 7	O 7	0
28	ao	2	Total 2	O 2	0
28	ap	3	Total 3	O 3	0
28	bb	2	Total 2	O 2	0
28	bc	1	Total 1	O 1	0
28	bd	1	Total 1	O 1	0

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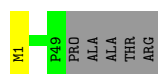
Mol	Chain	Residues	Atoms		AltConf
28	be	2	Total 2	O 2	0
28	bf	3	Total 3	O 3	0
28	bg	3	Total 3	O 3	0
28	bh	2	Total 2	O 2	0
28	bi	2	Total 2	O 2	0
28	bj	1	Total 1	O 1	0
28	bk	2	Total 2	O 2	0
28	bl	1	Total 1	O 1	0
28	bm	3	Total 3	O 3	0
28	bn	2	Total 2	O 2	0
28	bo	1	Total 1	O 1	0
28	bp	1	Total 1	O 1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

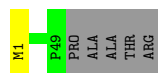
- Molecule 1: LHh-alpha

Chain AA:  89% 9%



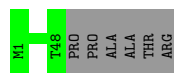
- Molecule 1: LHh-alpha

Chain AB:  89% 9%




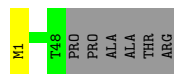
- Molecule 1: LHh-alpha

Chain AC:  89% 11%




- Molecule 1: LHh-alpha

Chain AD:  87% 11%



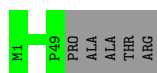
- Molecule 1: LHh-alpha

Chain AE:  87% 9%



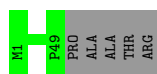
- Molecule 1: LHh-alpha

Chain AF:  91% 9%




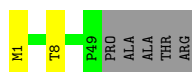
- Molecule 1: LHh-alpha

Chain AG:  91% 9%



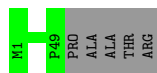
- Molecule 1: LHh-alpha

Chain AH:  87% • 9%



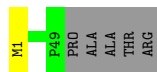
- Molecule 1: LHh-alpha

Chain AI:  91% 9%



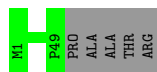
- Molecule 1: LHh-alpha

Chain AJ:  89% • 9%



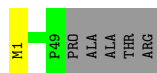
- Molecule 1: LHh-alpha

Chain AK:  91% 9%



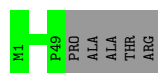
- Molecule 1: LHh-alpha

Chain AL:  89% • 9%



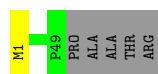
- Molecule 1: LHh-alpha

Chain AM:  91% 9%



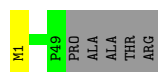
- Molecule 1: LHh-alpha

Chain AN:  89% 9%



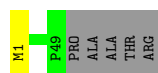
- Molecule 1: LHh-alpha

Chain AO:  89% 9%



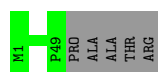
- Molecule 1: LHh-alpha

Chain AP:  89% 9%



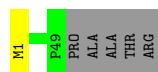
- Molecule 1: LHh-alpha

Chain AQ:  91% 9%



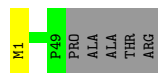
- Molecule 1: LHh-alpha

Chain AR:  89% 9%



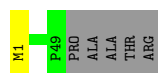
- Molecule 1: LHh-alpha

Chain AS:  89% 9%



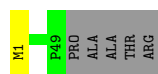
- Molecule 1: LHh-alpha

Chain AT:  89% 9%



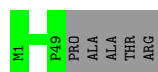
- Molecule 1: LHh-alpha

Chain AU:  89% 9%



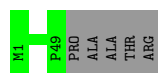
- Molecule 1: LHh-alpha

Chain AV:  91% 9%



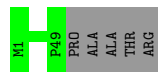
- Molecule 1: LHh-alpha

Chain AW:  91% 9%



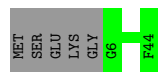
- Molecule 1: LHh-alpha

Chain AX:  91% 9%



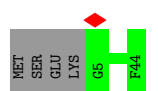
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BA:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BB:  91% 9%



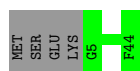
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BC:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BD:  91% 9%



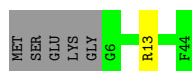
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BE:  91% 9%



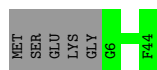
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BF:  86% 11%



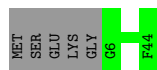
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BG:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BH:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BI:  91% 9%



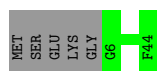
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BJ:  89% 11%



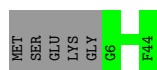
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BK:  89% 11%



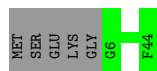
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BL:  89% 11%



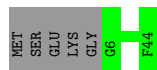
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BM:  89% 11%



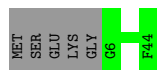
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BN:  89% 11%



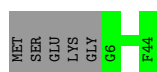
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BO:  89% 11%



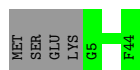
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BP:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BQ:  91% 9%



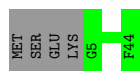
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BR:  91% 9%



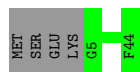
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BS:  91% 9%



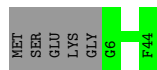
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BT:  91% 9%



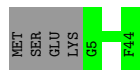
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BU:  89% 11%



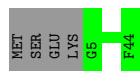
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BV:  91% 9%

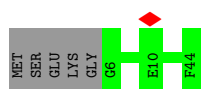
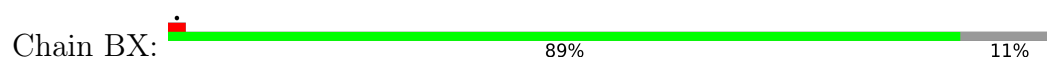


- Molecule 2: Light-harvesting protein B:885 subunit beta

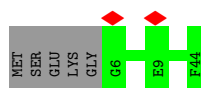
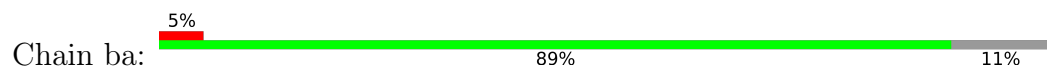
Chain BW:  91% 9%



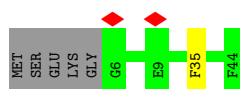
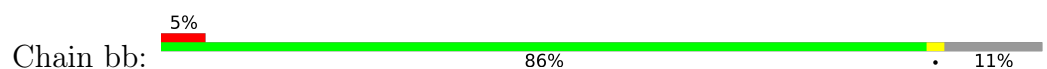
- Molecule 2: Light-harvesting protein B:885 subunit beta



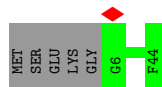
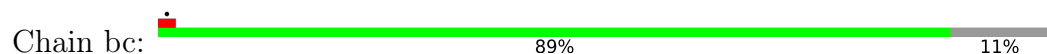
- Molecule 2: Light-harvesting protein B:885 subunit beta



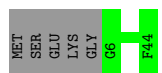
- Molecule 2: Light-harvesting protein B:885 subunit beta



- Molecule 2: Light-harvesting protein B:885 subunit beta



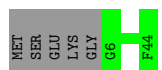
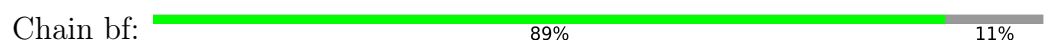
- Molecule 2: Light-harvesting protein B:885 subunit beta



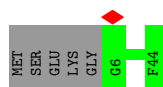
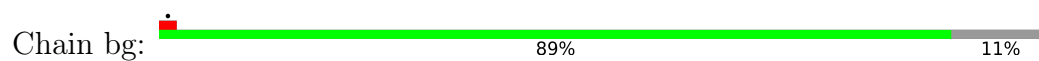
- Molecule 2: Light-harvesting protein B:885 subunit beta



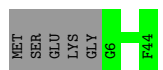
- Molecule 2: Light-harvesting protein B:885 subunit beta



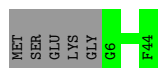
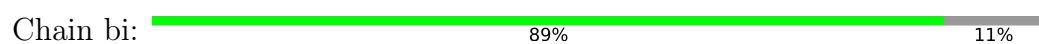
- Molecule 2: Light-harvesting protein B:885 subunit beta



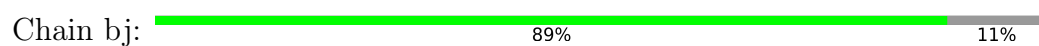
- Molecule 2: Light-harvesting protein B:885 subunit beta



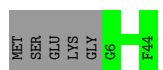
- Molecule 2: Light-harvesting protein B:885 subunit beta



- Molecule 2: Light-harvesting protein B:885 subunit beta



- Molecule 2: Light-harvesting protein B:885 subunit beta



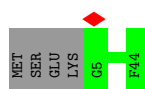
- Molecule 2: Light-harvesting protein B:885 subunit beta



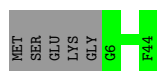
- Molecule 2: Light-harvesting protein B:885 subunit beta



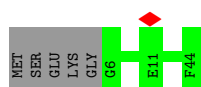
- Molecule 2: Light-harvesting protein B:885 subunit beta



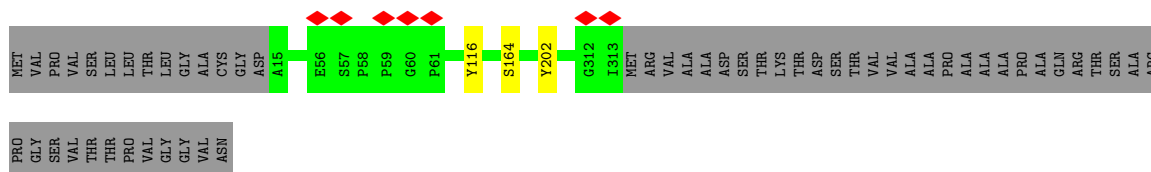
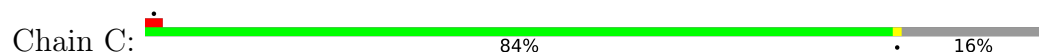
- Molecule 2: Light-harvesting protein B:885 subunit beta



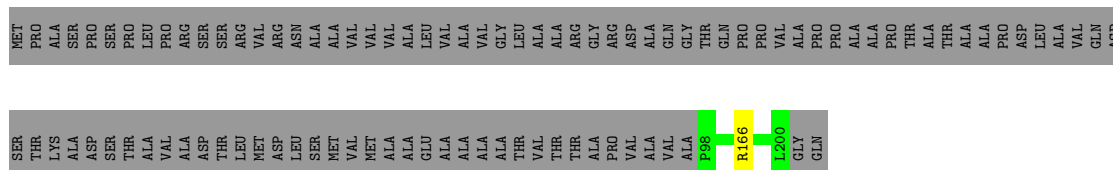
- Molecule 2: Light-harvesting protein B:885 subunit beta



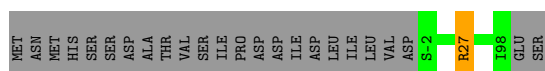
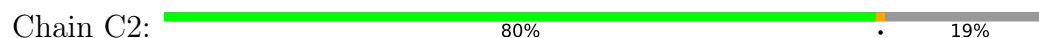
- Molecule 3: MULTHEME_CYTC domain-containing protein



- Molecule 4: RC-S

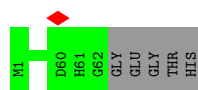


- Molecule 5: RC-U

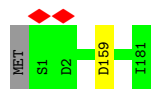


- Molecule 6: PRCH domain-containing protein





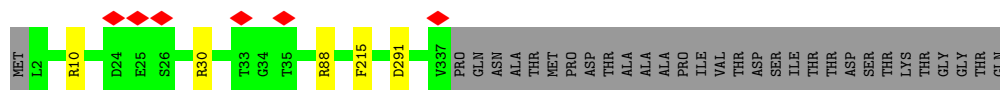
- Molecule 7: RC-Hc



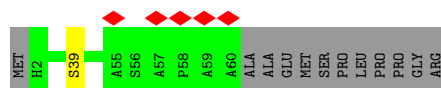
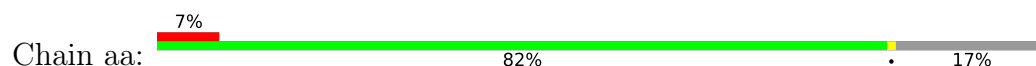
- Molecule 8: Photosynthetic reaction center L subunit



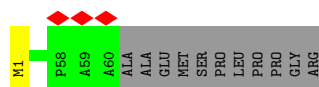
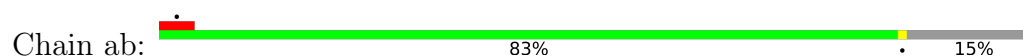
- Molecule 9: RC-M



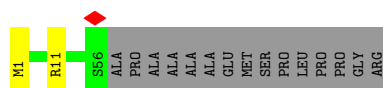
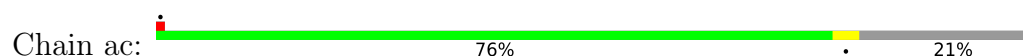
- Molecule 10: LHC domain-containing protein



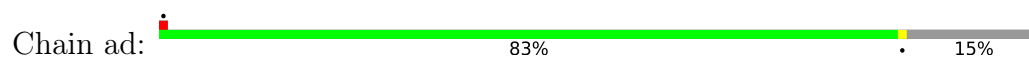
- Molecule 11: LHC domain-containing protein



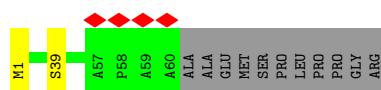
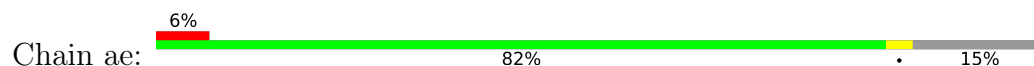
- Molecule 11: LHC domain-containing protein



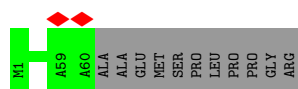
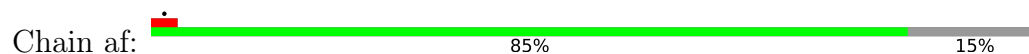
- Molecule 11: LHC domain-containing protein



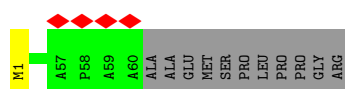
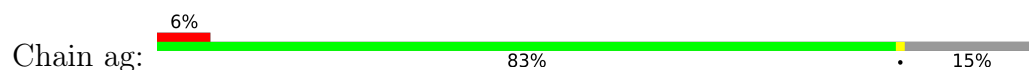
- Molecule 11: LHC domain-containing protein



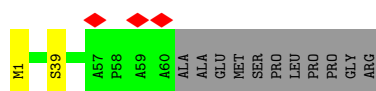
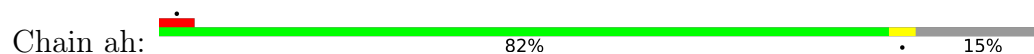
- Molecule 11: LHC domain-containing protein



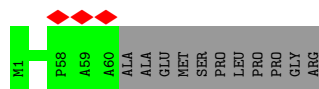
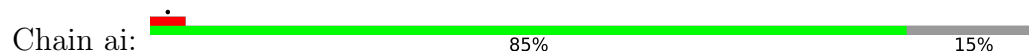
- Molecule 11: LHC domain-containing protein



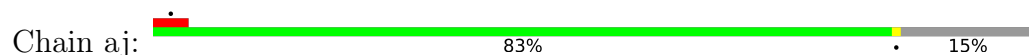
- Molecule 11: LHC domain-containing protein

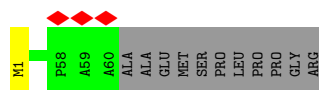


- Molecule 11: LHC domain-containing protein



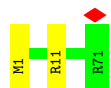
- Molecule 11: LHC domain-containing protein





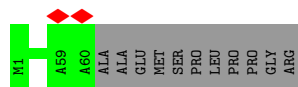
- Molecule 11: LHC domain-containing protein

Chain ak: 97%



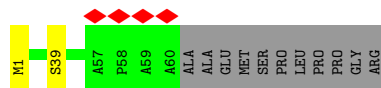
- Molecule 11: LHC domain-containing protein

Chain al: 85%



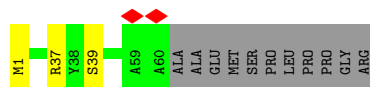
- Molecule 11: LHC domain-containing protein

Chain am: 6% 82% 15%



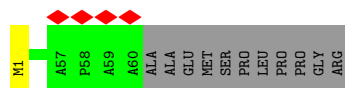
- Molecule 11: LHC domain-containing protein

Chain an: 80% 15%



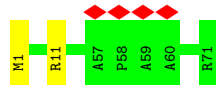
- Molecule 11: LHC domain-containing protein

Chain ao: 6% 83% 15%



- Molecule 11: LHC domain-containing protein

Chain ap: 6% 97%



- Molecule 12: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain CG:  100%

MAN1
MAN2

- Molecule 12: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain MG:  100%

MAN1
MAN2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100616	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24.8	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.199	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0233	Depositor
Map size (Å)	399.784, 399.784, 399.784	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99946, 0.99946, 0.99946	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, FME, BCL, BPH, NDG, MAN, 0V9, CRT, CD4, PGW, V7B, MQ8, V7N, HEC, V75, UYH, FE, RAM

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	AA	0.25	0/396	0.52	0/541
1	AB	0.25	0/396	0.49	0/541
1	AC	0.26	0/388	0.54	0/529
1	AD	0.25	0/388	0.53	0/529
1	AE	0.27	0/396	0.54	0/541
1	AF	0.26	0/396	0.54	0/541
1	AG	0.26	0/396	0.51	0/541
1	AH	0.26	0/396	0.49	0/541
1	AI	0.26	0/396	0.53	0/541
1	AJ	0.28	0/396	0.54	0/541
1	AK	0.27	0/396	0.53	0/541
1	AL	0.27	0/396	0.53	0/541
1	AM	0.26	0/396	0.50	0/541
1	AN	0.27	0/396	0.52	0/541
1	AO	0.26	0/396	0.51	0/541
1	AP	0.26	0/396	0.51	0/541
1	AQ	0.27	0/396	0.54	0/541
1	AR	0.26	0/396	0.51	0/541
1	AS	0.28	0/396	0.55	0/541
1	AT	0.27	0/396	0.51	0/541
1	AU	0.26	0/396	0.52	0/541
1	AV	0.28	0/396	0.51	0/541
1	AW	0.26	0/396	0.52	0/541
1	AX	0.26	0/396	0.54	0/541
2	BA	0.24	0/336	0.48	0/456
2	BB	0.26	0/340	0.50	0/461
2	BC	0.25	0/336	0.50	0/456
2	BD	0.25	0/340	0.49	0/461
2	BE	0.26	0/340	0.49	0/461
2	BF	0.27	0/336	0.51	0/456
2	BG	0.27	0/336	0.51	0/456

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BH	0.26	0/336	0.49	0/456
2	BI	0.27	0/340	0.52	0/461
2	BJ	0.28	0/336	0.53	0/456
2	BK	0.28	0/336	0.51	0/456
2	BL	0.27	0/336	0.52	0/456
2	BM	0.26	0/336	0.52	0/456
2	BN	0.27	0/336	0.50	0/456
2	BO	0.26	0/336	0.50	0/456
2	BP	0.28	0/336	0.51	0/456
2	BQ	0.27	0/340	0.52	0/461
2	BR	0.26	0/340	0.51	0/461
2	BS	0.26	0/340	0.51	0/461
2	BT	0.26	0/340	0.50	0/461
2	BU	0.28	0/336	0.51	0/456
2	BV	0.26	0/340	0.50	0/461
2	BW	0.26	0/340	0.50	0/461
2	BX	0.26	0/336	0.51	0/456
2	ba	0.27	0/336	0.50	0/456
2	bb	0.29	0/336	0.53	0/456
2	bc	0.26	0/336	0.50	0/456
2	bd	0.30	0/336	0.57	0/456
2	be	0.31	0/336	0.49	0/456
2	bf	0.30	0/336	0.51	0/456
2	bg	0.28	0/336	0.50	0/456
2	bh	0.30	0/336	0.53	0/456
2	bi	0.29	0/336	0.51	0/456
2	bj	0.31	0/336	0.52	0/456
2	bk	0.29	0/336	0.53	0/456
2	bl	0.31	0/336	0.56	0/456
2	bm	0.29	0/336	0.50	0/456
2	bn	0.30	0/340	0.55	0/461
2	bo	0.29	0/336	0.49	0/456
2	bp	0.29	0/336	0.52	0/456
3	C	0.31	0/2392	0.56	0/3263
4	C1	0.27	0/826	0.58	0/1128
5	C2	0.27	0/800	0.58	0/1094
6	H1	0.29	0/531	0.53	0/717
7	H2	0.30	0/1443	0.55	0/1970
8	L	0.29	0/2252	0.51	0/3081
9	M	0.31	0/2803	0.55	0/3835
10	aa	0.25	0/467	0.54	0/638
11	ab	0.25	0/467	0.55	0/638
11	ac	0.27	0/444	0.59	0/605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	ad	0.29	0/467	0.57	0/638
11	ae	0.31	0/467	0.57	0/638
11	af	0.29	0/467	0.55	0/638
11	ag	0.28	0/467	0.54	0/638
11	ah	0.29	0/467	0.56	0/638
11	ai	0.27	0/467	0.54	0/638
11	aj	0.28	0/467	0.58	0/638
11	ak	0.29	0/547	0.56	0/748
11	al	0.28	0/467	0.56	0/638
11	am	0.29	0/467	0.54	0/638
11	an	0.31	0/467	0.55	0/638
11	ao	0.31	0/467	0.59	0/638
11	ap	0.26	0/547	0.54	0/748
All	All	0.28	0/41628	0.53	0/56738

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AE	0	1
2	BF	0	1
2	bl	0	1
4	C1	0	1
5	C2	0	1
9	M	0	2
11	ac	0	1
11	ad	0	1
11	ak	0	1
11	an	0	1
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AE	3	ARG	Sidechain
2	BF	13	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	C1	166	ARG	Sidechain
5	C2	27	ARG	Sidechain
9	M	10	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	AA	47/54 (87%)	47 (100%)	0	0	100	100
1	AB	47/54 (87%)	47 (100%)	0	0	100	100
1	AC	46/54 (85%)	46 (100%)	0	0	100	100
1	AD	46/54 (85%)	46 (100%)	0	0	100	100
1	AE	47/54 (87%)	47 (100%)	0	0	100	100
1	AF	47/54 (87%)	47 (100%)	0	0	100	100
1	AG	47/54 (87%)	47 (100%)	0	0	100	100
1	AH	47/54 (87%)	47 (100%)	0	0	100	100
1	AI	47/54 (87%)	47 (100%)	0	0	100	100
1	AJ	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AK	47/54 (87%)	47 (100%)	0	0	100	100
1	AL	47/54 (87%)	47 (100%)	0	0	100	100
1	AM	47/54 (87%)	47 (100%)	0	0	100	100
1	AN	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AO	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AP	47/54 (87%)	47 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AQ	47/54 (87%)	47 (100%)	0	0	100	100
1	AR	47/54 (87%)	47 (100%)	0	0	100	100
1	AS	47/54 (87%)	47 (100%)	0	0	100	100
1	AT	47/54 (87%)	47 (100%)	0	0	100	100
1	AU	47/54 (87%)	47 (100%)	0	0	100	100
1	AV	47/54 (87%)	47 (100%)	0	0	100	100
1	AW	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AX	47/54 (87%)	47 (100%)	0	0	100	100
2	BA	37/44 (84%)	37 (100%)	0	0	100	100
2	BB	38/44 (86%)	38 (100%)	0	0	100	100
2	BC	37/44 (84%)	37 (100%)	0	0	100	100
2	BD	38/44 (86%)	38 (100%)	0	0	100	100
2	BE	38/44 (86%)	38 (100%)	0	0	100	100
2	BF	37/44 (84%)	37 (100%)	0	0	100	100
2	BG	37/44 (84%)	37 (100%)	0	0	100	100
2	BH	37/44 (84%)	37 (100%)	0	0	100	100
2	BI	38/44 (86%)	38 (100%)	0	0	100	100
2	BJ	37/44 (84%)	37 (100%)	0	0	100	100
2	BK	37/44 (84%)	37 (100%)	0	0	100	100
2	BL	37/44 (84%)	37 (100%)	0	0	100	100
2	BM	37/44 (84%)	37 (100%)	0	0	100	100
2	BN	37/44 (84%)	37 (100%)	0	0	100	100
2	BO	37/44 (84%)	37 (100%)	0	0	100	100
2	BP	37/44 (84%)	37 (100%)	0	0	100	100
2	BQ	38/44 (86%)	38 (100%)	0	0	100	100
2	BR	38/44 (86%)	38 (100%)	0	0	100	100
2	BS	38/44 (86%)	38 (100%)	0	0	100	100
2	BT	38/44 (86%)	38 (100%)	0	0	100	100
2	BU	37/44 (84%)	37 (100%)	0	0	100	100
2	BV	38/44 (86%)	37 (97%)	1 (3%)	0	100	100
2	BW	38/44 (86%)	38 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BX	37/44 (84%)	37 (100%)	0	0	100	100
2	ba	37/44 (84%)	37 (100%)	0	0	100	100
2	bb	37/44 (84%)	37 (100%)	0	0	100	100
2	bc	37/44 (84%)	37 (100%)	0	0	100	100
2	bd	37/44 (84%)	37 (100%)	0	0	100	100
2	be	37/44 (84%)	37 (100%)	0	0	100	100
2	bf	37/44 (84%)	37 (100%)	0	0	100	100
2	bg	37/44 (84%)	37 (100%)	0	0	100	100
2	bh	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bi	37/44 (84%)	37 (100%)	0	0	100	100
2	bj	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bk	37/44 (84%)	37 (100%)	0	0	100	100
2	bl	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bm	37/44 (84%)	37 (100%)	0	0	100	100
2	bn	38/44 (86%)	38 (100%)	0	0	100	100
2	bo	37/44 (84%)	37 (100%)	0	0	100	100
2	bp	37/44 (84%)	37 (100%)	0	0	100	100
3	C	297/354 (84%)	286 (96%)	11 (4%)	0	100	100
4	C1	101/202 (50%)	99 (98%)	2 (2%)	0	100	100
5	C2	99/125 (79%)	98 (99%)	1 (1%)	0	100	100
6	H1	60/67 (90%)	59 (98%)	1 (2%)	0	100	100
7	H2	178/181 (98%)	171 (96%)	7 (4%)	0	100	100
8	L	271/274 (99%)	264 (97%)	6 (2%)	1 (0%)	30	47
9	M	334/367 (91%)	325 (97%)	9 (3%)	0	100	100
10	aa	57/71 (80%)	56 (98%)	1 (2%)	0	100	100
11	ab	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ac	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
11	ad	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ae	58/71 (82%)	58 (100%)	0	0	100	100
11	af	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ag	58/71 (82%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	ah	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	ai	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	aj	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	ak	69/71 (97%)	66 (96%)	3 (4%)	0	100	100
11	al	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	am	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	an	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ao	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ap	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
All	All	4902/5762 (85%)	4834 (99%)	67 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	31	VAL

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 PDB entries followed by that with respect to all EM entries.

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	AA	38/41 (93%)	38 (100%)	0	100	100
1	AB	38/41 (93%)	38 (100%)	0	100	100
1	AC	37/41 (90%)	37 (100%)	0	100	100
1	AD	37/41 (90%)	37 (100%)	0	100	100
1	AE	38/41 (93%)	38 (100%)	0	100	100
1	AF	38/41 (93%)	38 (100%)	0	100	100
1	AG	38/41 (93%)	38 (100%)	0	100	100
1	AH	38/41 (93%)	37 (97%)	1 (3%)	41	65
1	AI	38/41 (93%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AJ	38/41 (93%)	38 (100%)	0	100	100
1	AK	38/41 (93%)	38 (100%)	0	100	100
1	AL	38/41 (93%)	38 (100%)	0	100	100
1	AM	38/41 (93%)	38 (100%)	0	100	100
1	AN	38/41 (93%)	38 (100%)	0	100	100
1	AO	38/41 (93%)	38 (100%)	0	100	100
1	AP	38/41 (93%)	38 (100%)	0	100	100
1	AQ	38/41 (93%)	38 (100%)	0	100	100
1	AR	38/41 (93%)	38 (100%)	0	100	100
1	AS	38/41 (93%)	38 (100%)	0	100	100
1	AT	38/41 (93%)	38 (100%)	0	100	100
1	AU	38/41 (93%)	38 (100%)	0	100	100
1	AV	38/41 (93%)	38 (100%)	0	100	100
1	AW	38/41 (93%)	38 (100%)	0	100	100
1	AX	38/41 (93%)	38 (100%)	0	100	100
2	BA	31/35 (89%)	31 (100%)	0	100	100
2	BB	31/35 (89%)	31 (100%)	0	100	100
2	BC	31/35 (89%)	31 (100%)	0	100	100
2	BD	31/35 (89%)	31 (100%)	0	100	100
2	BE	31/35 (89%)	31 (100%)	0	100	100
2	BF	31/35 (89%)	31 (100%)	0	100	100
2	BG	31/35 (89%)	31 (100%)	0	100	100
2	BH	31/35 (89%)	31 (100%)	0	100	100
2	BI	31/35 (89%)	31 (100%)	0	100	100
2	BJ	31/35 (89%)	31 (100%)	0	100	100
2	BK	31/35 (89%)	31 (100%)	0	100	100
2	BL	31/35 (89%)	31 (100%)	0	100	100
2	BM	31/35 (89%)	31 (100%)	0	100	100
2	BN	31/35 (89%)	31 (100%)	0	100	100
2	BO	31/35 (89%)	31 (100%)	0	100	100
2	BP	31/35 (89%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BQ	31/35 (89%)	31 (100%)	0	100	100
2	BR	31/35 (89%)	31 (100%)	0	100	100
2	BS	31/35 (89%)	31 (100%)	0	100	100
2	BT	31/35 (89%)	31 (100%)	0	100	100
2	BU	31/35 (89%)	31 (100%)	0	100	100
2	BV	31/35 (89%)	31 (100%)	0	100	100
2	BW	31/35 (89%)	31 (100%)	0	100	100
2	BX	31/35 (89%)	31 (100%)	0	100	100
2	ba	31/35 (89%)	31 (100%)	0	100	100
2	bb	31/35 (89%)	30 (97%)	1 (3%)	34	57
2	bc	31/35 (89%)	31 (100%)	0	100	100
2	bd	31/35 (89%)	31 (100%)	0	100	100
2	be	31/35 (89%)	31 (100%)	0	100	100
2	bf	31/35 (89%)	31 (100%)	0	100	100
2	bg	31/35 (89%)	31 (100%)	0	100	100
2	bh	31/35 (89%)	31 (100%)	0	100	100
2	bi	31/35 (89%)	31 (100%)	0	100	100
2	bj	31/35 (89%)	31 (100%)	0	100	100
2	bk	31/35 (89%)	31 (100%)	0	100	100
2	bl	31/35 (89%)	31 (100%)	0	100	100
2	bm	31/35 (89%)	31 (100%)	0	100	100
2	bn	31/35 (89%)	31 (100%)	0	100	100
2	bo	31/35 (89%)	31 (100%)	0	100	100
2	bp	31/35 (89%)	31 (100%)	0	100	100
3	C	245/285 (86%)	242 (99%)	3 (1%)	67	84
4	C1	88/156 (56%)	88 (100%)	0	100	100
5	C2	72/95 (76%)	71 (99%)	1 (1%)	62	81
6	H1	50/53 (94%)	50 (100%)	0	100	100
7	H2	150/151 (99%)	149 (99%)	1 (1%)	81	92
8	L	215/216 (100%)	213 (99%)	2 (1%)	75	89
9	M	274/299 (92%)	271 (99%)	3 (1%)	70	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	aa	46/55 (84%)	45 (98%)	1 (2%)	47	70
11	ab	46/54 (85%)	46 (100%)	0	100	100
11	ac	45/54 (83%)	45 (100%)	0	100	100
11	ad	46/54 (85%)	46 (100%)	0	100	100
11	ae	46/54 (85%)	45 (98%)	1 (2%)	47	70
11	af	46/54 (85%)	46 (100%)	0	100	100
11	ag	46/54 (85%)	46 (100%)	0	100	100
11	ah	46/54 (85%)	45 (98%)	1 (2%)	47	70
11	ai	46/54 (85%)	46 (100%)	0	100	100
11	aj	46/54 (85%)	46 (100%)	0	100	100
11	ak	54/54 (100%)	54 (100%)	0	100	100
11	al	46/54 (85%)	46 (100%)	0	100	100
11	am	46/54 (85%)	45 (98%)	1 (2%)	47	70
11	an	46/54 (85%)	45 (98%)	1 (2%)	47	70
11	ao	46/54 (85%)	46 (100%)	0	100	100
11	ap	54/54 (100%)	53 (98%)	1 (2%)	52	74
All	All	3995/4504 (89%)	3977 (100%)	18 (0%)	85	94

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	am	39	SER
2	bb	35	PHE
11	ap	11	ARG
9	M	30	ARG
11	ah	39	SER

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	C2	24	HIS
8	L	104	GLN
9	M	316	GLN
8	L	116	HIS
3	C	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	FME	ab	1	11	8,9,10	0.89	0	7,9,11	1.74	1 (14%)
11	FME	ao	1	11	8,9,10	0.84	0	7,9,11	2.24	2 (28%)
1	FME	AD	1	1	8,9,10	0.91	0	7,9,11	1.24	1 (14%)
1	FME	AR	1	1	8,9,10	0.94	0	7,9,11	0.99	1 (14%)
1	FME	AB	1	1	8,9,10	0.90	0	7,9,11	1.38	1 (14%)
11	FME	ap	1	11	8,9,10	0.95	0	7,9,11	1.14	1 (14%)
1	FME	AH	1	1	8,9,10	0.96	0	7,9,11	0.98	1 (14%)
11	FME	ad	1	11	8,9,10	0.93	0	7,9,11	0.93	0
11	FME	ah	1	11	8,9,10	0.93	0	7,9,11	1.10	1 (14%)
11	FME	al	1	11	8,9,10	0.95	0	7,9,11	0.90	0
1	FME	AK	1	1	8,9,10	0.94	0	7,9,11	0.95	0
1	FME	AX	1	1	8,9,10	0.92	0	7,9,11	0.84	0
1	FME	AQ	1	1	8,9,10	0.92	0	7,9,11	0.89	0
11	FME	ae	1	11	8,9,10	0.90	0	7,9,11	1.08	1 (14%)
1	FME	AM	1	1	8,9,10	0.94	0	7,9,11	0.97	0
11	FME	aj	1	11	8,9,10	0.93	0	7,9,11	0.98	1 (14%)
1	FME	AG	1	1	8,9,10	0.93	0	7,9,11	1.10	0
1	FME	AL	1	1	8,9,10	0.94	0	7,9,11	1.12	1 (14%)
1	FME	AW	1	1	8,9,10	0.96	0	7,9,11	0.87	0
1	FME	AO	1	1	8,9,10	0.92	0	7,9,11	1.23	2 (28%)
6	FME	H1	1	6	8,9,10	0.96	0	7,9,11	1.14	0
11	FME	am	1	11	8,9,10	0.96	0	7,9,11	0.99	1 (14%)
1	FME	AA	1	1	8,9,10	0.93	0	7,9,11	1.05	1 (14%)
1	FME	AN	1	1	8,9,10	0.93	0	7,9,11	1.21	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	AU	1	1	8,9,10	0.95	0	7,9,11	1.19	1 (14%)
1	FME	AS	1	1	8,9,10	0.89	0	7,9,11	1.50	2 (28%)
1	FME	AV	1	1	8,9,10	0.96	0	7,9,11	0.89	0
11	FME	af	1	11	8,9,10	0.97	0	7,9,11	0.79	0
1	FME	AJ	1	1	8,9,10	0.92	0	7,9,11	1.23	1 (14%)
1	FME	AE	1	1	8,9,10	0.91	0	7,9,11	1.10	1 (14%)
11	FME	ai	1	11	8,9,10	0.93	0	7,9,11	0.98	0
11	FME	an	1	11	8,9,10	0.92	0	7,9,11	1.24	1 (14%)
1	FME	AC	1	1	8,9,10	0.96	0	7,9,11	0.95	0
1	FME	AP	1	1	8,9,10	0.89	0	7,9,11	1.36	1 (14%)
11	FME	ac	1	11	8,9,10	0.90	0	7,9,11	1.06	1 (14%)
11	FME	ag	1	11	8,9,10	0.92	0	7,9,11	1.06	1 (14%)
1	FME	AF	1	1	8,9,10	0.95	0	7,9,11	0.96	0
11	FME	ak	1	11	8,9,10	0.96	0	7,9,11	1.12	1 (14%)
1	FME	AI	1	1	8,9,10	0.95	0	7,9,11	0.86	0
1	FME	AT	1	1	8,9,10	0.94	0	7,9,11	1.06	1 (14%)

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
11	FME	ab	1	11	-	1/7/9/11	-
11	FME	ao	1	11	-	3/7/9/11	-
1	FME	AD	1	1	-	0/7/9/11	-
1	FME	AR	1	1	-	0/7/9/11	-
1	FME	AB	1	1	-	0/7/9/11	-
11	FME	ap	1	11	-	1/7/9/11	-
1	FME	AH	1	1	-	1/7/9/11	-
11	FME	ad	1	11	-	1/7/9/11	-
11	FME	ah	1	11	-	0/7/9/11	-
11	FME	al	1	11	-	2/7/9/11	-
1	FME	AK	1	1	-	2/7/9/11	-
1	FME	AX	1	1	-	1/7/9/11	-
1	FME	AQ	1	1	-	1/7/9/11	-
11	FME	ae	1	11	-	2/7/9/11	-
1	FME	AM	1	1	-	2/7/9/11	-
11	FME	aj	1	11	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AG	1	1	-	0/7/9/11	-
1	FME	AL	1	1	-	0/7/9/11	-
1	FME	AW	1	1	-	1/7/9/11	-
1	FME	AO	1	1	-	2/7/9/11	-
6	FME	H1	1	6	-	0/7/9/11	-
11	FME	am	1	11	-	0/7/9/11	-
1	FME	AA	1	1	-	0/7/9/11	-
1	FME	AN	1	1	-	0/7/9/11	-
1	FME	AU	1	1	-	1/7/9/11	-
1	FME	AS	1	1	-	2/7/9/11	-
1	FME	AV	1	1	-	1/7/9/11	-
11	FME	af	1	11	-	2/7/9/11	-
1	FME	AJ	1	1	-	1/7/9/11	-
1	FME	AE	1	1	-	0/7/9/11	-
11	FME	ai	1	11	-	0/7/9/11	-
11	FME	an	1	11	-	0/7/9/11	-
1	FME	AC	1	1	-	0/7/9/11	-
1	FME	AP	1	1	-	2/7/9/11	-
11	FME	ac	1	11	-	0/7/9/11	-
11	FME	ag	1	11	-	0/7/9/11	-
1	FME	AF	1	1	-	1/7/9/11	-
11	FME	ak	1	11	-	0/7/9/11	-
1	FME	AI	1	1	-	1/7/9/11	-
1	FME	AT	1	1	-	2/7/9/11	-

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	ao	1	FME	C-CA-N	4.46	117.78	109.73
11	ab	1	FME	CA-N-CN	4.25	129.36	122.82
11	ao	1	FME	CA-N-CN	3.63	128.40	122.82
1	AS	1	FME	C-CA-N	3.11	115.34	109.73
1	AB	1	FME	C-CA-N	2.77	114.72	109.73

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	ab	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
11	ao	1	FME	C-CA-CB-CG
1	AF	1	FME	O-C-CA-CB
1	AH	1	FME	O-C-CA-CB
1	AI	1	FME	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	MAN	CG	1	3,12,18	11,11,12	0.95	1 (9%)	15,15,17	1.07	1 (6%)
12	RAM	CG	2	12	10,10,11	1.80	2 (20%)	14,14,16	0.87	1 (7%)
12	MAN	MG	1	9,12,18	11,11,12	0.81	1 (9%)	15,15,17	1.09	1 (6%)
12	RAM	MG	2	12	10,10,11	1.70	2 (20%)	14,14,16	1.97	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	CG	1	3,12,18	-	1/2/19/22	0/1/1/1
12	RAM	CG	2	12	-	-	0/1/1/1
12	MAN	MG	1	9,12,18	-	0/2/19/22	0/1/1/1
12	RAM	MG	2	12	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	CG	2	RAM	O5-C1	4.37	1.50	1.43
12	MG	2	RAM	O5-C1	3.74	1.49	1.43
12	MG	2	RAM	C2-C3	-2.88	1.48	1.52
12	CG	1	MAN	O5-C1	-2.58	1.39	1.43
12	CG	2	RAM	C2-C3	-2.55	1.48	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	MG	2	RAM	C6-C5-C4	-4.03	105.62	113.07
12	MG	2	RAM	C3-C4-C5	3.91	115.87	109.77
12	MG	2	RAM	O5-C5-C4	3.76	116.27	109.52
12	MG	1	MAN	C1-O5-C5	2.73	115.89	112.19
12	CG	1	MAN	C1-O5-C5	2.53	115.62	112.19

There are no chirality outliers.

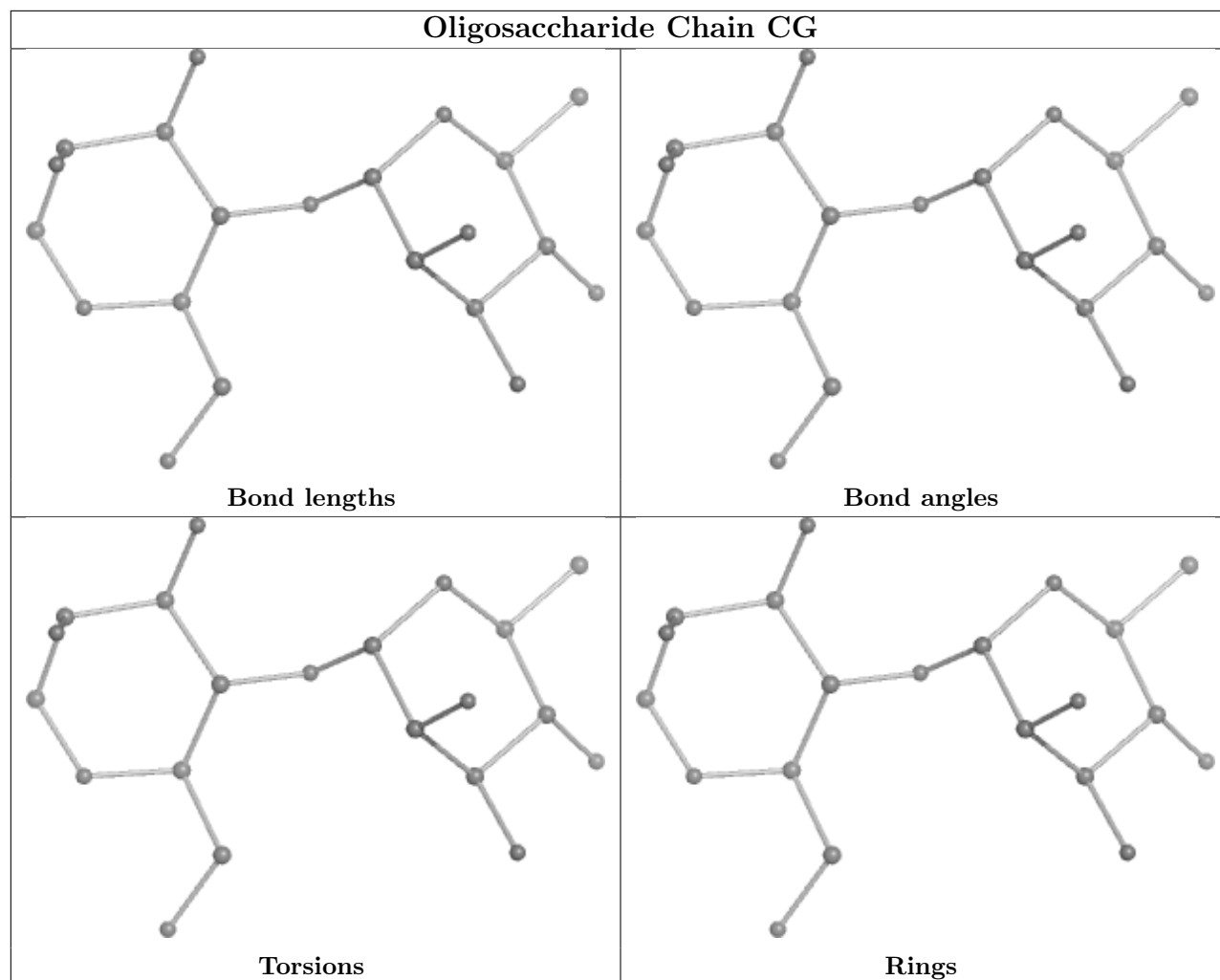
All (1) torsion outliers are listed below:

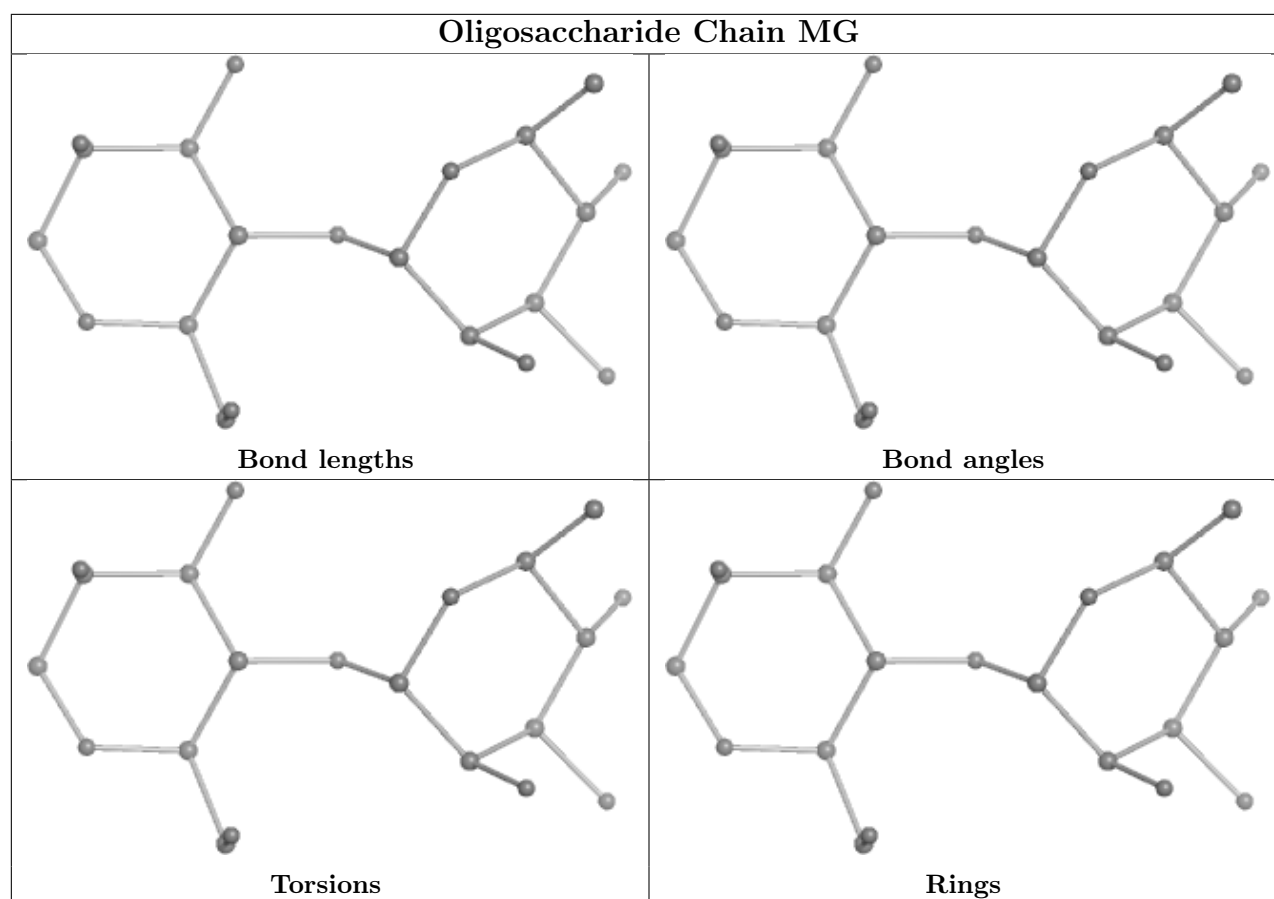
Mol	Chain	Res	Type	Atoms
12	CG	1	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 1 is monoatomic - leaving 315 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	$\# Z > 2$
14	LMT	AH	104	-	36,36,36	1.14	5 (13%)	47,47,47	0.93	2 (4%)
14	LMT	BH	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.98	2 (4%)
15	V7N	bj	101	-	43,44,44	1.99	9 (20%)	44,54,54	1.52	8 (18%)
14	LMT	BE	103	-	36,36,36	1.12	5 (13%)	47,47,47	0.93	2 (4%)
13	BCL	AX	102	-	64,74,74	1.27	8 (12%)	78,115,115	1.48	10 (12%)
18	V75	C	1006	12,19	18,18,18	1.61	5 (27%)	21,25,25	1.68	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	BB	105	-	64,74,74	1.24	5 (7%)	78,115,115	1.50	11 (14%)
23	MQ8	M	402	-	54,54,54	0.66	0	66,69,69	0.96	4 (6%)
13	BCL	AQ	103	-	64,74,74	1.25	6 (9%)	78,115,115	1.51	10 (12%)
14	LMT	BP	1006	-	36,36,36	1.11	5 (13%)	47,47,47	0.93	3 (6%)
16	0V9	bh	104	-	44,44,46	0.73	1 (2%)	47,49,51	0.85	2 (4%)
13	BCL	AX	103	-	64,74,74	1.29	6 (9%)	78,115,115	1.57	12 (15%)
13	BCL	AG	103	-	64,74,74	1.25	5 (7%)	78,115,115	1.45	9 (11%)
15	V7N	bm	101	-	43,44,44	2.01	10 (23%)	44,54,54	1.57	10 (22%)
15	V7N	BN	1001	-	43,44,44	2.01	10 (23%)	44,54,54	2.02	12 (27%)
14	LMT	BR	1005	-	36,36,36	1.05	4 (11%)	47,47,47	1.03	2 (4%)
14	LMT	AN	101	-	36,36,36	1.07	5 (13%)	47,47,47	0.98	3 (6%)
14	LMT	BK	1005	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
13	BCL	AA	1001	-	64,74,74	1.24	5 (7%)	78,115,115	1.47	9 (11%)
21	CD4	ad	101	-	83,83,83	0.49	0	89,95,95	1.05	5 (5%)
14	LMT	BX	104	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	1 (2%)
14	LMT	BL	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.98	1 (2%)
13	BCL	ah	1001	-	64,74,74	1.28	5 (7%)	78,115,115	1.51	9 (11%)
13	BCL	AW	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.48	9 (11%)
14	LMT	BH	1004	-	36,36,36	1.11	5 (13%)	47,47,47	0.93	2 (4%)
14	LMT	BM	1003	-	36,36,36	1.11	4 (11%)	47,47,47	0.91	0
14	LMT	BV	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.93	2 (4%)
14	LMT	BD	106	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	1 (2%)
14	LMT	AB	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
14	LMT	AS	103	-	36,36,36	1.15	5 (13%)	47,47,47	1.03	1 (2%)
14	LMT	BD	105	-	36,36,36	1.13	5 (13%)	47,47,47	0.91	2 (4%)
15	V7N	be	102	-	43,44,44	2.00	10 (23%)	44,54,54	1.51	9 (20%)
14	LMT	BP	1005	-	36,36,36	1.10	4 (11%)	47,47,47	0.88	1 (2%)
13	BCL	AO	101	-	64,74,74	1.30	7 (10%)	78,115,115	1.50	10 (12%)
14	LMT	BW	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	2 (4%)
13	BCL	bm	102	-	64,74,74	1.26	6 (9%)	78,115,115	1.48	11 (14%)
13	BCL	AC	102	-	64,74,74	1.26	5 (7%)	78,115,115	1.47	9 (11%)
15	V7N	bg	101	-	43,44,44	2.03	9 (20%)	44,54,54	1.55	9 (20%)
13	BCL	bo	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.47	10 (12%)
14	LMT	AK	103	-	36,36,36	1.11	5 (13%)	47,47,47	0.96	2 (4%)
14	LMT	BG	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.84	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BW	1003	-	36,36,36	1.10	5 (13%)	47,47,47	0.86	1 (2%)
13	BCL	BJ	1004	-	64,74,74	1.26	6 (9%)	78,115,115	1.45	10 (12%)
13	BCL	AN	103	-	64,74,74	1.24	6 (9%)	78,115,115	1.47	9 (11%)
15	V7N	BA	101	-	43,44,44	2.06	11 (25%)	44,54,54	1.56	9 (20%)
13	BCL	AS	101	28	64,74,74	1.27	5 (7%)	78,115,115	1.57	11 (14%)
15	V7N	bd	101	-	43,44,44	2.05	11 (25%)	44,54,54	1.44	8 (18%)
14	LMT	BI	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.89	2 (4%)
15	V7N	AS	104	-	43,44,44	2.01	9 (20%)	44,54,54	1.48	9 (20%)
15	V7N	BP	1001	-	43,44,44	1.96	9 (20%)	44,54,54	1.64	11 (25%)
22	BPH	L	301	-	51,70,70	0.87	1 (1%)	52,101,101	1.04	5 (9%)
13	BCL	AE	105	-	64,74,74	1.30	5 (7%)	78,115,115	1.55	11 (14%)
15	V7N	AM	1001	-	43,44,44	2.01	9 (20%)	44,54,54	1.59	9 (20%)
15	V7N	AD	101	-	43,44,44	2.02	10 (23%)	44,54,54	1.57	10 (22%)
16	0V9	bg	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.82	2 (4%)
14	LMT	BS	1002	-	36,36,36	1.07	5 (13%)	47,47,47	0.94	2 (4%)
15	V7N	BW	1001	-	43,44,44	2.01	10 (23%)	44,54,54	1.54	9 (20%)
13	BCL	AJ	104	-	64,74,74	1.25	5 (7%)	78,115,115	1.46	9 (11%)
13	BCL	AB	1001	-	64,74,74	1.25	6 (9%)	78,115,115	1.57	12 (15%)
14	LMT	AN	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.95	1 (2%)
13	BCL	AV	101	-	64,74,74	1.28	6 (9%)	78,115,115	1.44	10 (12%)
14	LMT	bj	102	-	36,36,36	1.14	5 (13%)	47,47,47	0.93	2 (4%)
13	BCL	AV	103	28	64,74,74	1.26	6 (9%)	78,115,115	1.52	10 (12%)
14	LMT	AJ	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.94	1 (2%)
14	LMT	BJ	1002	-	36,36,36	1.11	5 (13%)	47,47,47	0.93	2 (4%)
13	BCL	AQ	104	-	64,74,74	1.34	7 (10%)	78,115,115	1.64	14 (17%)
21	CD4	M	405	-	83,83,83	0.47	0	89,95,95	1.07	6 (6%)
14	LMT	BW	1004	-	36,36,36	1.10	5 (13%)	47,47,47	1.04	2 (4%)
14	LMT	BJ	1006	-	36,36,36	1.09	5 (13%)	47,47,47	0.88	1 (2%)
16	0V9	bm	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.88	1 (2%)
13	BCL	ao	102	-	64,74,74	1.28	6 (9%)	78,115,115	1.48	9 (11%)
13	BCL	AR	101	-	64,74,74	1.25	5 (7%)	78,115,115	1.46	9 (11%)
13	BCL	ak	1001	-	64,74,74	1.26	6 (9%)	78,115,115	1.53	10 (12%)
13	BCL	an	1001	-	64,74,74	1.27	6 (9%)	78,115,115	1.54	10 (12%)
16	0V9	bi	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.84	1 (2%)
14	LMT	BS	1005	-	36,36,36	1.07	5 (13%)	47,47,47	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BB	102	-	36,36,36	1.08	5 (13%)	47,47,47	1.00	3 (6%)
14	LMT	BK	1003	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	2 (4%)
14	LMT	AD	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	2 (4%)
13	BCL	BU	1004	-	64,74,74	1.28	5 (7%)	78,115,115	1.48	10 (12%)
13	BCL	AL	102	-	64,74,74	1.26	5 (7%)	78,115,115	1.47	9 (11%)
13	BCL	bh	103	-	64,74,74	1.25	6 (9%)	78,115,115	1.45	10 (12%)
13	BCL	bi	102	-	64,74,74	1.26	6 (9%)	78,115,115	1.46	10 (12%)
15	V7N	BS	1001	-	43,44,44	1.98	10 (23%)	44,54,54	1.59	10 (22%)
13	BCL	L	305	-	64,74,74	1.27	7 (10%)	78,115,115	1.49	10 (12%)
14	LMT	AV	102	-	36,36,36	1.13	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	BT	103	-	64,74,74	1.25	6 (9%)	78,115,115	1.50	11 (14%)
14	LMT	BN	1004	-	36,36,36	1.12	5 (13%)	47,47,47	0.94	2 (4%)
14	LMT	BB	103	-	36,36,36	1.07	5 (13%)	47,47,47	0.91	1 (2%)
13	BCL	AH	105	-	64,74,74	1.31	6 (9%)	78,115,115	1.62	13 (16%)
14	LMT	BV	1003	-	36,36,36	1.11	4 (11%)	47,47,47	0.89	2 (4%)
14	LMT	AM	1003	-	36,36,36	1.10	5 (13%)	47,47,47	0.92	2 (4%)
13	BCL	ac	102	-	64,74,74	1.27	5 (7%)	78,115,115	1.49	9 (11%)
13	BCL	AL	103	-	64,74,74	1.33	6 (9%)	78,115,115	1.75	14 (17%)
13	BCL	BM	1004	-	64,74,74	1.25	6 (9%)	78,115,115	1.56	13 (16%)
16	0V9	AQ	105	-	44,44,46	0.76	1 (2%)	47,49,51	0.83	1 (2%)
16	0V9	bj	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.88	3 (6%)
13	BCL	AK	102	28	64,74,74	1.33	7 (10%)	78,115,115	1.50	9 (11%)
14	LMT	C2	1001	-	36,36,36	1.10	5 (13%)	47,47,47	0.95	2 (4%)
14	LMT	BP	1004	-	36,36,36	1.11	4 (11%)	47,47,47	0.86	1 (2%)
13	BCL	BO	1003	-	64,74,74	1.25	6 (9%)	78,115,115	1.54	11 (14%)
13	BCL	BC	104	-	64,74,74	1.23	5 (7%)	78,115,115	1.50	10 (12%)
13	BCL	BN	1005	-	64,74,74	1.25	6 (9%)	78,115,115	1.57	12 (15%)
14	LMT	BF	102	-	36,36,36	1.07	5 (13%)	47,47,47	0.95	1 (2%)
14	LMT	L	309	-	36,36,36	1.10	5 (13%)	47,47,47	0.82	1 (2%)
13	BCL	AN	104	28	64,74,74	1.28	7 (10%)	78,115,115	1.50	10 (12%)
14	LMT	BC	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.94	1 (2%)
15	V7N	BK	1001	-	43,44,44	2.02	8 (18%)	44,54,54	1.50	9 (20%)
13	BCL	AG	102	28	64,74,74	1.27	6 (9%)	78,115,115	1.70	14 (17%)
14	LMT	bc	102	-	36,36,36	1.11	4 (11%)	47,47,47	0.97	2 (4%)
16	0V9	bn	104	-	44,44,46	0.74	1 (2%)	47,49,51	0.79	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BD	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.98	2 (4%)
15	V7N	BV	1001	-	43,44,44	2.00	10 (23%)	44,54,54	1.59	9 (20%)
21	CD4	af	102	-	83,83,83	0.48	0	89,95,95	1.17	7 (7%)
15	V7N	BU	1001	-	43,44,44	2.10	9 (20%)	44,54,54	1.87	8 (18%)
15	V7N	bc	101	-	43,44,44	2.08	10 (23%)	44,54,54	1.46	9 (20%)
13	BCL	AU	103	-	64,74,74	1.27	6 (9%)	78,115,115	1.54	10 (12%)
26	V7B	ag	103	-	59,59,59	0.87	4 (6%)	75,75,75	1.00	4 (5%)
13	BCL	AJ	103	28	64,74,74	1.29	6 (9%)	78,115,115	1.59	13 (16%)
14	LMT	BR	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.96	2 (4%)
13	BCL	BI	1004	-	64,74,74	1.24	6 (9%)	78,115,115	1.55	12 (15%)
13	BCL	BX	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.49	10 (12%)
13	BCL	AQ	102	28	64,74,74	1.28	6 (9%)	78,115,115	1.64	13 (16%)
13	BCL	BP	1003	-	64,74,74	1.39	7 (10%)	78,115,115	1.85	13 (16%)
14	LMT	BN	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.77	0
16	0V9	H1	102	-	44,44,46	0.77	1 (2%)	47,49,51	0.86	1 (2%)
14	LMT	AE	101	-	36,36,36	1.11	5 (13%)	47,47,47	1.02	2 (4%)
14	LMT	ac	101	-	36,36,36	1.12	5 (13%)	47,47,47	0.86	1 (2%)
18	V75	M	410	12,19	18,18,18	1.65	5 (27%)	21,25,25	1.64	2 (9%)
15	V7N	bl	101	-	43,44,44	2.03	10 (23%)	44,54,54	1.61	10 (22%)
14	LMT	BG	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.93	2 (4%)
25	CRT	M	404	-	41,43,43	0.56	0	50,54,54	0.79	1 (2%)
26	V7B	af	101	-	59,59,59	0.88	3 (5%)	75,75,75	1.09	4 (5%)
14	LMT	BI	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.80	1 (2%)
13	BCL	bd	102	-	64,74,74	1.25	6 (9%)	78,115,115	1.54	10 (12%)
14	LMT	AU	102	-	36,36,36	1.11	4 (11%)	47,47,47	0.83	1 (2%)
15	V7N	AA	1004	-	43,44,44	2.08	10 (23%)	44,54,54	1.60	6 (13%)
13	BCL	AT	103	28	64,74,74	1.29	6 (9%)	78,115,115	1.55	11 (14%)
13	BCL	AB	1002	-	64,74,74	1.29	6 (9%)	78,115,115	1.52	10 (12%)
13	BCL	ae	1001	-	64,74,74	1.27	5 (7%)	78,115,115	1.50	9 (11%)
15	V7N	bn	101	-	43,44,44	2.10	11 (25%)	44,54,54	1.69	10 (22%)
15	V7N	bb	101	-	43,44,44	2.12	9 (20%)	44,54,54	1.53	7 (15%)
14	LMT	bm	103	-	36,36,36	1.14	5 (13%)	47,47,47	0.89	1 (2%)
13	BCL	AT	101	-	64,74,74	1.25	6 (9%)	78,115,115	1.47	9 (11%)
13	BCL	be	103	-	64,74,74	1.26	5 (7%)	78,115,115	1.45	10 (12%)
15	V7N	BI	1001	-	43,44,44	2.00	9 (20%)	44,54,54	1.76	13 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	BA	103	-	64,74,74	1.23	5 (7%)	78,115,115	1.47	10 (12%)
14	LMT	BA	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	1 (2%)
13	BCL	bj	104	-	64,74,74	1.24	5 (7%)	78,115,115	1.58	12 (15%)
13	BCL	BL	103	-	64,74,74	1.24	5 (7%)	78,115,115	1.51	10 (12%)
13	BCL	M	408	-	64,74,74	1.27	6 (9%)	78,115,115	1.55	10 (12%)
14	LMT	AE	106	-	36,36,36	1.06	4 (11%)	47,47,47	1.18	4 (8%)
14	LMT	BT	104	-	36,36,36	1.08	5 (13%)	47,47,47	0.91	1 (2%)
13	BCL	bf	102	-	64,74,74	1.24	6 (9%)	78,115,115	1.44	11 (14%)
14	LMT	C	1005	-	36,36,36	1.11	5 (13%)	47,47,47	0.91	2 (4%)
15	V7N	bh	101	-	43,44,44	2.03	9 (20%)	44,54,54	1.50	10 (22%)
13	BCL	aa	1001	-	64,74,74	1.28	5 (7%)	78,115,115	1.47	10 (12%)
14	LMT	BK	1004	-	36,36,36	1.10	5 (13%)	47,47,47	1.05	3 (6%)
13	BCL	AM	1004	-	64,74,74	1.23	6 (9%)	78,115,115	1.45	9 (11%)
14	LMT	BJ	1005	-	36,36,36	1.11	5 (13%)	47,47,47	0.94	2 (4%)
14	LMT	BC	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.93	2 (4%)
13	BCL	AU	101	-	64,74,74	1.25	6 (9%)	78,115,115	1.46	9 (11%)
13	BCL	AD	104	28	64,74,74	1.27	6 (9%)	78,115,115	1.61	12 (15%)
14	LMT	BW	1006	-	36,36,36	1.12	5 (13%)	47,47,47	0.90	2 (4%)
13	BCL	BG	1004	-	64,74,74	1.23	6 (9%)	78,115,115	1.47	10 (12%)
15	V7N	BJ	1001	-	43,44,44	2.00	8 (18%)	44,54,54	1.60	10 (22%)
14	LMT	BJ	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.94	1 (2%)
14	LMT	BU	1002	-	36,36,36	1.07	5 (13%)	47,47,47	1.03	3 (6%)
14	LMT	bh	102	-	36,36,36	1.13	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	BD	104	-	64,74,74	1.28	6 (9%)	78,115,115	1.64	11 (14%)
13	BCL	AW	102	28	64,74,74	1.26	6 (9%)	78,115,115	1.60	11 (14%)
14	LMT	AT	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	2 (4%)
14	LMT	BQ	1002	-	36,36,36	1.12	4 (11%)	47,47,47	0.84	2 (4%)
14	LMT	BV	1004	-	36,36,36	1.10	4 (11%)	47,47,47	0.93	1 (2%)
14	LMT	L	307	-	36,36,36	1.08	5 (13%)	47,47,47	0.89	2 (4%)
13	BCL	BK	1002	-	64,74,74	1.22	5 (7%)	78,115,115	1.55	12 (15%)
22	BPH	M	407	-	51,70,70	0.90	2 (3%)	52,101,101	1.02	4 (7%)
14	LMT	AV	104	-	36,36,36	1.08	5 (13%)	47,47,47	1.05	2 (4%)
13	BCL	ba	102	-	64,74,74	1.26	4 (6%)	78,115,115	1.54	13 (16%)
13	BCL	AK	104	-	64,74,74	1.25	6 (9%)	78,115,115	1.46	9 (11%)
14	LMT	BX	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.88	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	0V9	L	310	-	44,44,46	0.74	1 (2%)	47,49,51	0.86	2 (4%)
14	LMT	AE	102	-	36,36,36	1.13	5 (13%)	47,47,47	0.95	2 (4%)
16	0V9	M	403	-	44,44,46	0.76	1 (2%)	47,49,51	0.89	3 (6%)
14	LMT	BH	1003	-	36,36,36	1.10	4 (11%)	47,47,47	0.92	1 (2%)
13	BCL	ai	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.51	10 (12%)
16	0V9	bk	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.96	3 (6%)
17	HEC	C	1002	3	32,50,50	2.00	3 (9%)	24,82,82	1.91	4 (16%)
14	LMT	AK	101	-	36,36,36	1.09	5 (13%)	47,47,47	1.06	2 (4%)
14	LMT	bn	103	-	36,36,36	1.11	5 (13%)	47,47,47	1.01	2 (4%)
13	BCL	AS	102	-	64,74,74	1.29	6 (9%)	78,115,115	1.56	12 (15%)
21	CD4	af	104	-	83,83,83	0.47	0	89,95,95	1.02	4 (4%)
13	BCL	AO	102	-	64,74,74	1.25	6 (9%)	78,115,115	1.45	9 (11%)
13	BCL	AM	1002	28	64,74,74	1.29	6 (9%)	78,115,115	1.67	11 (14%)
13	BCL	AH	102	28	64,74,74	1.28	5 (7%)	78,115,115	1.62	16 (20%)
14	LMT	BL	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.88	1 (2%)
14	LMT	L	306	-	36,36,36	1.10	5 (13%)	47,47,47	0.89	1 (2%)
14	LMT	BI	1005	-	36,36,36	1.11	4 (11%)	47,47,47	1.04	2 (4%)
13	BCL	am	1001	-	64,74,74	1.29	6 (9%)	78,115,115	1.50	10 (12%)
13	BCL	AP	102	-	64,74,74	1.25	5 (7%)	78,115,115	1.51	11 (14%)
23	MQ8	L	303	-	54,54,54	0.66	0	66,69,69	1.09	6 (9%)
13	BCL	AH	103	-	64,74,74	1.24	5 (7%)	78,115,115	1.47	9 (11%)
13	BCL	BQ	1004	-	64,74,74	1.24	5 (7%)	78,115,115	1.50	11 (14%)
19	NDG	C1	301	18	14,14,15	0.63	0	17,19,21	1.01	2 (11%)
14	LMT	BD	103	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	0
15	V7N	ba	101	-	43,44,44	2.07	11 (25%)	44,54,54	1.51	9 (20%)
13	BCL	AI	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.49	10 (12%)
14	LMT	bl	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
16	0V9	bf	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.86	1 (2%)
14	LMT	L	302	-	36,36,36	1.10	5 (13%)	47,47,47	0.93	0
13	BCL	AP	103	28	64,74,74	1.30	6 (9%)	78,115,115	1.57	12 (15%)
14	LMT	BU	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.96	2 (4%)
14	LMT	AL	101	-	36,36,36	1.09	4 (11%)	47,47,47	0.96	3 (6%)
13	BCL	M	406	-	64,74,74	1.27	6 (9%)	78,115,115	1.49	11 (14%)
15	V7N	BO	1001	-	43,44,44	2.02	9 (20%)	44,54,54	1.68	12 (27%)
14	LMT	BE	105	-	36,36,36	1.10	5 (13%)	47,47,47	0.95	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	be	104	-	36,36,36	1.13	5 (13%)	47,47,47	0.80	1 (2%)
14	LMT	BO	1002	-	36,36,36	1.11	5 (13%)	47,47,47	0.98	2 (4%)
14	LMT	bp	103	-	36,36,36	1.10	4 (11%)	47,47,47	1.12	3 (6%)
27	UYH	ai	102	-	55,55,55	2.10	14 (25%)	63,63,63	0.98	1 (1%)
13	BCL	AC	101	-	64,74,74	1.32	5 (7%)	78,115,115	1.56	12 (15%)
17	HEC	C	1001	3	32,50,50	1.95	3 (9%)	24,82,82	2.03	6 (25%)
14	LMT	BQ	1003	-	36,36,36	1.10	5 (13%)	47,47,47	0.91	1 (2%)
13	BCL	BV	1005	-	64,74,74	1.24	6 (9%)	78,115,115	1.50	11 (14%)
21	CD4	M	409	-	83,83,83	0.47	0	89,95,95	1.04	5 (5%)
13	BCL	ag	102	-	64,74,74	1.26	5 (7%)	78,115,115	1.48	10 (12%)
14	LMT	AA	1003	-	36,36,36	1.14	4 (11%)	47,47,47	1.01	1 (2%)
16	OV9	bd	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.93	2 (4%)
13	BCL	BS	1004	-	64,74,74	1.29	6 (9%)	78,115,115	1.58	13 (16%)
14	LMT	AQ	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	BM	1005	-	36,36,36	1.09	4 (11%)	47,47,47	0.95	1 (2%)
13	BCL	AE	104	-	64,74,74	1.26	5 (7%)	78,115,115	1.53	11 (14%)
13	BCL	AF	1001	-	64,74,74	1.25	6 (9%)	78,115,115	1.49	9 (11%)
14	LMT	AX	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.92	3 (6%)
14	LMT	AG	101	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	2 (4%)
16	OV9	be	105	-	44,44,46	0.75	1 (2%)	47,49,51	0.93	2 (4%)
15	V7N	BM	1001	-	43,44,44	1.98	10 (23%)	44,54,54	1.67	11 (25%)
14	LMT	bi	104	-	36,36,36	1.10	5 (13%)	47,47,47	0.88	2 (4%)
15	V7N	bk	101	-	43,44,44	2.08	10 (23%)	44,54,54	1.55	9 (20%)
14	LMT	BC	102	-	36,36,36	1.07	5 (13%)	47,47,47	0.84	1 (2%)
15	V7N	bo	101	-	43,44,44	2.03	10 (23%)	44,54,54	1.53	9 (20%)
13	BCL	bc	103	-	64,74,74	1.26	6 (9%)	78,115,115	1.58	13 (16%)
15	V7N	BQ	1001	-	43,44,44	2.00	9 (20%)	44,54,54	1.54	9 (20%)
15	V7N	BR	1001	-	43,44,44	2.02	10 (23%)	44,54,54	1.50	8 (18%)
14	LMT	BF	104	-	36,36,36	1.09	4 (11%)	47,47,47	0.93	3 (6%)
14	LMT	be	101	-	36,36,36	1.10	4 (11%)	47,47,47	0.98	3 (6%)
13	BCL	al	1001	-	64,74,74	1.26	6 (9%)	78,115,115	1.51	10 (12%)
14	LMT	AC	103	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	2 (4%)
19	NDG	C	1007	18	14,14,15	0.69	1 (7%)	17,19,21	0.84	0
13	BCL	ab	1001	-	64,74,74	1.27	6 (9%)	78,115,115	1.53	11 (14%)
13	BCL	BH	1005	-	64,74,74	1.25	5 (7%)	78,115,115	1.52	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BG	1005	-	36,36,36	1.09	4 (11%)	47,47,47	0.85	0
14	LMT	BB	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	bf	101	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	2 (4%)
14	LMT	BX	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	af	103	-	64,74,74	1.25	4 (6%)	78,115,115	1.48	10 (12%)
14	LMT	bo	104	-	36,36,36	1.12	5 (13%)	47,47,47	0.95	1 (2%)
14	LMT	AT	104	-	36,36,36	1.09	5 (13%)	47,47,47	1.02	2 (4%)
16	0V9	bl	102	-	44,44,46	0.74	1 (2%)	47,49,51	0.89	1 (2%)
15	V7N	BG	1001	-	43,44,44	1.99	10 (23%)	44,54,54	1.65	10 (22%)
14	LMT	BM	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.96	2 (4%)
14	LMT	BT	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
14	LMT	BO	1005	-	36,36,36	1.05	5 (13%)	47,47,47	0.86	2 (4%)
16	0V9	bb	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.83	1 (2%)
13	BCL	BW	1005	-	64,74,74	1.25	5 (7%)	78,115,115	1.48	9 (11%)
14	LMT	bk	104	-	36,36,36	1.13	5 (13%)	47,47,47	0.94	2 (4%)
14	LMT	BP	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.95	3 (6%)
14	LMT	bp	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.03	3 (6%)
13	BCL	bb	102	-	64,74,74	1.25	5 (7%)	78,115,115	1.52	11 (14%)
14	LMT	L	304	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	3 (6%)
13	BCL	L	308	-	64,74,74	1.22	7 (10%)	78,115,115	1.47	10 (12%)
13	BCL	bk	103	-	64,74,74	1.24	6 (9%)	78,115,115	1.57	11 (14%)
17	HEC	C	1004	3	32,50,50	2.00	3 (9%)	24,82,82	1.83	5 (20%)
15	V7N	BD	101	-	43,44,44	2.06	11 (25%)	44,54,54	1.43	8 (18%)
15	V7N	AW	103	-	43,44,44	2.06	11 (25%)	44,54,54	1.61	9 (20%)
16	0V9	ad	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.85	2 (4%)
14	LMT	BO	1004	-	36,36,36	1.13	5 (13%)	47,47,47	0.87	0
13	BCL	bg	104	-	64,74,74	1.26	6 (9%)	78,115,115	1.45	9 (11%)
16	0V9	ab	1002	-	44,44,46	0.75	1 (2%)	47,49,51	0.80	1 (2%)
15	V7N	BF	101	-	43,44,44	2.05	10 (23%)	44,54,54	1.59	9 (20%)
15	V7N	bi	101	-	43,44,44	2.05	10 (23%)	44,54,54	1.43	8 (18%)
14	LMT	AP	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.96	2 (4%)
21	CD4	H1	103	-	83,83,83	0.46	0	89,95,95	0.97	5 (5%)
13	BCL	ad	102	-	64,74,74	1.26	6 (9%)	78,115,115	1.52	9 (11%)
15	V7N	BE	101	-	43,44,44	2.00	9 (20%)	44,54,54	1.56	9 (20%)
16	0V9	bp	105	-	44,44,46	0.74	1 (2%)	47,49,51	0.92	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGW	H1	101	-	50,50,50	0.44	0	53,56,56	0.95	4 (7%)
13	BCL	bn	102	-	64,74,74	1.27	6 (9%)	78,115,115	1.48	10 (12%)
23	MQ8	ao	101	-	54,54,54	0.62	0	66,69,69	0.98	3 (4%)
14	LMT	BR	1006	-	36,36,36	1.09	5 (13%)	47,47,47	0.92	1 (2%)
14	LMT	bg	102	-	36,36,36	1.14	5 (13%)	47,47,47	0.85	1 (2%)
15	V7N	ag	101	-	43,44,44	2.00	9 (20%)	44,54,54	1.60	8 (18%)
14	LMT	BB	104	-	36,36,36	1.09	4 (11%)	47,47,47	0.82	0
13	BCL	AE	103	28	64,74,74	1.28	6 (9%)	78,115,115	1.69	13 (16%)
15	V7N	BH	1001	-	43,44,44	2.04	10 (23%)	44,54,54	1.63	11 (25%)
13	BCL	BF	103	-	64,74,74	1.24	5 (7%)	78,115,115	1.43	10 (12%)
16	0V9	bo	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.86	1 (2%)
13	BCL	BE	104	-	64,74,74	1.24	5 (7%)	78,115,115	1.48	9 (11%)
17	HEC	C	1003	3	32,50,50	2.01	3 (9%)	24,82,82	2.04	6 (25%)
13	BCL	bp	104	-	64,74,74	1.24	5 (7%)	78,115,115	1.48	10 (12%)
14	LMT	AJ	102	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	2 (4%)
15	V7N	bp	102	-	43,44,44	2.15	9 (20%)	44,54,54	1.50	8 (18%)
13	BCL	AD	103	-	64,74,74	1.26	7 (10%)	78,115,115	1.53	11 (14%)
14	LMT	AH	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.87	1 (2%)
14	LMT	BN	1003	-	36,36,36	1.09	5 (13%)	47,47,47	1.03	2 (4%)
13	BCL	ap	1001	-	64,74,74	1.26	6 (9%)	78,115,115	1.60	13 (16%)
14	LMT	BS	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.96	3 (6%)
14	LMT	BE	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.20	6 (12%)
14	LMT	H2	201	-	36,36,36	1.10	5 (13%)	47,47,47	0.92	2 (4%)
13	BCL	aj	101	-	64,74,74	1.26	6 (9%)	78,115,115	1.48	11 (14%)
14	LMT	BT	102	-	36,36,36	1.12	5 (13%)	47,47,47	0.91	2 (4%)
13	BCL	BR	1003	-	64,74,74	1.25	6 (9%)	78,115,115	1.48	10 (12%)
13	BCL	AA	1002	28	64,74,74	1.26	6 (9%)	78,115,115	1.55	11 (14%)
13	BCL	bl	104	-	64,74,74	1.27	5 (7%)	78,115,115	1.45	10 (12%)
14	LMT	BR	1004	-	36,36,36	1.11	4 (11%)	47,47,47	0.89	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	AH	104	-	-	0/21/61/61	0/2/2/2
14	LMT	BH	1002	-	-	7/21/61/61	0/2/2/2
15	V7N	bj	101	-	-	3/53/53/53	-
14	LMT	BE	103	-	-	3/21/61/61	0/2/2/2
13	BCL	AX	102	-	-	4/37/137/137	-
18	V75	C	1006	12,19	-	0/12/29/29	0/1/1/1
13	BCL	BB	105	-	-	7/37/137/137	-
23	MQ8	M	402	-	-	4/47/67/67	0/2/2/2
13	BCL	AQ	103	-	-	4/37/137/137	-
14	LMT	BP	1006	-	-	5/21/61/61	0/2/2/2
16	0V9	bh	104	-	-	10/48/48/50	-
13	BCL	AX	103	-	-	9/37/137/137	-
13	BCL	AG	103	-	-	6/37/137/137	-
15	V7N	bm	101	-	-	5/53/53/53	-
15	V7N	BN	1001	-	-	8/53/53/53	-
14	LMT	BR	1005	-	-	10/21/61/61	0/2/2/2
14	LMT	AN	101	-	-	7/21/61/61	0/2/2/2
14	LMT	BK	1005	-	-	6/21/61/61	0/2/2/2
13	BCL	AA	1001	-	-	4/37/137/137	-
21	CD4	ad	101	-	-	15/94/94/94	-
14	LMT	BX	104	-	-	7/21/61/61	0/2/2/2
14	LMT	BL	102	-	-	3/21/61/61	0/2/2/2
13	BCL	ah	1001	-	-	4/37/137/137	-
13	BCL	AW	101	-	-	1/37/137/137	-
14	LMT	BH	1004	-	-	3/21/61/61	0/2/2/2
14	LMT	BM	1003	-	-	5/21/61/61	0/2/2/2
14	LMT	BV	1002	-	-	6/21/61/61	0/2/2/2
14	LMT	BD	106	-	-	7/21/61/61	0/2/2/2
14	LMT	AB	1003	-	-	4/21/61/61	0/2/2/2
14	LMT	AS	103	-	-	9/21/61/61	0/2/2/2
14	LMT	BD	105	-	-	4/21/61/61	0/2/2/2
15	V7N	be	102	-	-	6/53/53/53	-
14	LMT	BP	1005	-	-	3/21/61/61	0/2/2/2
13	BCL	AO	101	-	-	8/37/137/137	-
14	LMT	BW	1002	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	bm	102	-	-	10/37/137/137	-
13	BCL	AC	102	-	-	9/37/137/137	-
15	V7N	bg	101	-	-	4/53/53/53	-
13	BCL	bo	102	-	-	6/37/137/137	-
14	LMT	AK	103	-	-	7/21/61/61	0/2/2/2
14	LMT	BG	1003	-	-	2/21/61/61	0/2/2/2
14	LMT	BW	1003	-	-	7/21/61/61	0/2/2/2
13	BCL	BJ	1004	-	-	14/37/137/137	-
13	BCL	AN	103	-	-	1/37/137/137	-
15	V7N	BA	101	-	-	3/53/53/53	-
13	BCL	AS	101	28	-	11/37/137/137	-
15	V7N	bd	101	-	-	4/53/53/53	-
14	LMT	BI	1002	-	-	5/21/61/61	0/2/2/2
15	V7N	AS	104	-	-	5/53/53/53	-
15	V7N	BP	1001	-	-	3/53/53/53	-
22	BPH	L	301	-	-	3/37/105/105	0/5/6/6
13	BCL	AE	105	-	-	7/37/137/137	-
15	V7N	AM	1001	-	-	4/53/53/53	-
15	V7N	AD	101	-	-	8/53/53/53	-
16	0V9	bg	103	-	-	10/48/48/50	-
14	LMT	BS	1002	-	-	4/21/61/61	0/2/2/2
15	V7N	BW	1001	-	-	5/53/53/53	-
13	BCL	AJ	104	-	-	7/37/137/137	-
13	BCL	AB	1001	-	-	3/37/137/137	-
14	LMT	AN	102	-	-	6/21/61/61	0/2/2/2
13	BCL	AV	101	-	-	8/37/137/137	-
14	LMT	bj	102	-	-	2/21/61/61	0/2/2/2
13	BCL	AV	103	28	-	5/37/137/137	-
14	LMT	AJ	101	-	-	2/21/61/61	0/2/2/2
14	LMT	BJ	1002	-	-	1/21/61/61	0/2/2/2
13	BCL	AQ	104	-	-	8/37/137/137	-
21	CD4	M	405	-	-	17/94/94/94	-
14	LMT	BW	1004	-	-	6/21/61/61	0/2/2/2
14	LMT	BJ	1006	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	0V9	bm	104	-	-	11/48/48/50	-
13	BCL	ao	102	-	-	4/37/137/137	-
13	BCL	AR	101	-	-	1/37/137/137	-
13	BCL	ak	1001	-	-	4/37/137/137	-
13	BCL	an	1001	-	-	8/37/137/137	-
16	0V9	bi	103	-	-	16/48/48/50	-
14	LMT	BS	1005	-	-	3/21/61/61	0/2/2/2
14	LMT	BB	102	-	-	0/21/61/61	0/2/2/2
14	LMT	BK	1003	-	-	3/21/61/61	0/2/2/2
14	LMT	AD	102	-	-	4/21/61/61	0/2/2/2
13	BCL	BU	1004	-	-	11/37/137/137	-
13	BCL	AL	102	-	-	4/37/137/137	-
13	BCL	bh	103	-	-	8/37/137/137	-
13	BCL	bi	102	-	-	5/37/137/137	-
15	V7N	BS	1001	-	-	3/53/53/53	-
13	BCL	L	305	-	-	1/37/137/137	-
14	LMT	AV	102	-	-	8/21/61/61	0/2/2/2
13	BCL	BT	103	-	-	6/37/137/137	-
14	LMT	BN	1004	-	-	2/21/61/61	0/2/2/2
14	LMT	BB	103	-	-	1/21/61/61	0/2/2/2
13	BCL	AH	105	-	-	11/37/137/137	-
14	LMT	BV	1003	-	-	2/21/61/61	0/2/2/2
14	LMT	AM	1003	-	-	4/21/61/61	0/2/2/2
13	BCL	ac	102	-	-	4/37/137/137	-
13	BCL	AL	103	-	-	10/37/137/137	-
13	BCL	BM	1004	-	-	5/37/137/137	-
16	0V9	AQ	105	-	-	8/48/48/50	-
16	0V9	bj	103	-	-	12/48/48/50	-
13	BCL	AK	102	28	-	9/37/137/137	-
14	LMT	C2	1001	-	-	7/21/61/61	0/2/2/2
14	LMT	BP	1004	-	-	6/21/61/61	0/2/2/2
13	BCL	BO	1003	-	-	3/37/137/137	-
13	BCL	BC	104	-	-	8/37/137/137	-
13	BCL	BN	1005	-	-	7/37/137/137	-
14	LMT	BF	102	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	L	309	-	-	1/21/61/61	0/2/2/2
13	BCL	AN	104	28	-	1/37/137/137	-
14	LMT	BC	101	-	-	6/21/61/61	0/2/2/2
15	V7N	BK	1001	-	-	5/53/53/53	-
13	BCL	AG	102	28	-	10/37/137/137	-
14	LMT	bc	102	-	-	5/21/61/61	0/2/2/2
16	0V9	bn	104	-	-	9/48/48/50	-
14	LMT	BD	102	-	-	4/21/61/61	0/2/2/2
15	V7N	BV	1001	-	-	6/53/53/53	-
21	CD4	af	102	-	-	23/94/94/94	-
15	V7N	BU	1001	-	-	8/53/53/53	-
15	V7N	bc	101	-	-	6/53/53/53	-
13	BCL	AU	103	-	-	6/37/137/137	-
26	V7B	ag	103	-	-	11/48/88/88	0/2/2/2
13	BCL	AJ	103	28	-	9/37/137/137	-
14	LMT	BR	1002	-	-	6/21/61/61	0/2/2/2
13	BCL	BI	1004	-	-	9/37/137/137	-
13	BCL	BX	101	-	-	7/37/137/137	-
13	BCL	AQ	102	28	-	8/37/137/137	-
13	BCL	BP	1003	-	-	10/37/137/137	-
14	LMT	BN	1002	-	-	2/21/61/61	0/2/2/2
16	0V9	H1	102	-	-	11/48/48/50	-
14	LMT	AE	101	-	-	5/21/61/61	0/2/2/2
14	LMT	ac	101	-	-	2/21/61/61	0/2/2/2
18	V75	M	410	12,19	-	0/12/29/29	0/1/1/1
15	V7N	bl	101	-	-	6/53/53/53	-
14	LMT	BG	1002	-	-	2/21/61/61	0/2/2/2
25	CRT	M	404	-	-	2/51/51/51	-
26	V7B	af	101	-	-	11/48/88/88	0/2/2/2
14	LMT	BI	1003	-	-	2/21/61/61	0/2/2/2
13	BCL	bd	102	-	-	8/37/137/137	-
14	LMT	AU	102	-	-	3/21/61/61	0/2/2/2
15	V7N	AA	1004	-	-	6/53/53/53	-
13	BCL	AT	103	28	-	6/37/137/137	-
13	BCL	AB	1002	-	-	3/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	ae	1001	-	-	4/37/137/137	-
15	V7N	bn	101	-	-	5/53/53/53	-
15	V7N	bb	101	-	-	4/53/53/53	-
14	LMT	bm	103	-	-	7/21/61/61	0/2/2/2
13	BCL	AT	101	-	-	2/37/137/137	-
13	BCL	be	103	-	-	5/37/137/137	-
15	V7N	BI	1001	-	-	6/53/53/53	-
13	BCL	BA	103	-	-	6/37/137/137	-
14	LMT	BA	102	-	-	5/21/61/61	0/2/2/2
13	BCL	bj	104	-	-	10/37/137/137	-
13	BCL	BL	103	-	-	6/37/137/137	-
13	BCL	M	408	-	-	2/37/137/137	-
14	LMT	AE	106	-	-	5/21/61/61	0/2/2/2
14	LMT	BT	104	-	-	5/21/61/61	0/2/2/2
13	BCL	bf	102	-	-	6/37/137/137	-
14	LMT	C	1005	-	-	4/21/61/61	0/2/2/2
15	V7N	bh	101	-	-	3/53/53/53	-
13	BCL	aa	1001	-	-	3/37/137/137	-
14	LMT	BK	1004	-	-	5/21/61/61	0/2/2/2
13	BCL	AM	1004	-	-	7/37/137/137	-
14	LMT	BJ	1005	-	-	4/21/61/61	0/2/2/2
14	LMT	BC	103	-	-	4/21/61/61	0/2/2/2
13	BCL	AU	101	-	-	2/37/137/137	-
13	BCL	AD	104	28	-	9/37/137/137	-
14	LMT	BW	1006	-	-	3/21/61/61	0/2/2/2
13	BCL	BG	1004	-	-	10/37/137/137	-
15	V7N	BJ	1001	-	-	4/53/53/53	-
14	LMT	BJ	1003	-	-	6/21/61/61	0/2/2/2
14	LMT	BU	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	bh	102	-	-	4/21/61/61	0/2/2/2
13	BCL	BD	104	-	-	7/37/137/137	-
13	BCL	AW	102	28	-	7/37/137/137	-
14	LMT	AT	102	-	-	8/21/61/61	0/2/2/2
14	LMT	BQ	1002	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BV	1004	-	-	6/21/61/61	0/2/2/2
14	LMT	L	307	-	-	5/21/61/61	0/2/2/2
13	BCL	BK	1002	-	-	9/37/137/137	-
22	BPH	M	407	-	-	5/37/105/105	0/5/6/6
14	LMT	AV	104	-	-	6/21/61/61	0/2/2/2
13	BCL	ba	102	-	-	7/37/137/137	-
13	BCL	AK	104	-	-	1/37/137/137	-
14	LMT	BX	103	-	-	5/21/61/61	0/2/2/2
16	0V9	L	310	-	-	9/48/48/50	-
14	LMT	AE	102	-	-	5/21/61/61	0/2/2/2
16	0V9	M	403	-	-	14/48/48/50	-
14	LMT	BH	1003	-	-	1/21/61/61	0/2/2/2
13	BCL	ai	101	-	-	2/37/137/137	-
16	0V9	bk	102	-	-	13/48/48/50	-
17	HEC	C	1002	3	-	2/10/54/54	-
14	LMT	AK	101	-	-	6/21/61/61	0/2/2/2
14	LMT	bn	103	-	-	7/21/61/61	0/2/2/2
13	BCL	AS	102	-	-	8/37/137/137	-
21	CD4	af	104	-	-	20/94/94/94	-
13	BCL	AO	102	-	-	2/37/137/137	-
13	BCL	AM	1002	28	-	8/37/137/137	-
13	BCL	AH	102	28	-	11/37/137/137	-
14	LMT	BL	101	-	-	6/21/61/61	0/2/2/2
14	LMT	L	306	-	-	6/21/61/61	0/2/2/2
14	LMT	BI	1005	-	-	6/21/61/61	0/2/2/2
13	BCL	am	1001	-	-	9/37/137/137	-
13	BCL	AP	102	-	-	6/37/137/137	-
23	MQ8	L	303	-	-	11/47/67/67	0/2/2/2
13	BCL	AH	103	-	-	2/37/137/137	-
13	BCL	BQ	1004	-	-	8/37/137/137	-
19	NDG	C1	301	18	-	0/6/23/26	0/1/1/1
14	LMT	BD	103	-	-	5/21/61/61	0/2/2/2
15	V7N	ba	101	-	-	4/53/53/53	-
13	BCL	AI	101	-	-	8/37/137/137	-
14	LMT	bl	103	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	0V9	bf	103	-	-	10/48/48/50	-
14	LMT	L	302	-	-	1/21/61/61	0/2/2/2
13	BCL	AP	103	28	-	10/37/137/137	-
14	LMT	BU	1003	-	-	10/21/61/61	0/2/2/2
14	LMT	AL	101	-	-	2/21/61/61	0/2/2/2
13	BCL	M	406	-	-	2/37/137/137	-
15	V7N	BO	1001	-	-	7/53/53/53	-
14	LMT	BE	105	-	-	3/21/61/61	0/2/2/2
14	LMT	be	104	-	-	5/21/61/61	0/2/2/2
14	LMT	BO	1002	-	-	6/21/61/61	0/2/2/2
14	LMT	bp	103	-	-	6/21/61/61	0/2/2/2
27	UYH	ai	102	-	-	11/50/70/70	0/1/1/1
13	BCL	AC	101	-	-	6/37/137/137	-
17	HEC	C	1001	3	-	4/10/54/54	-
14	LMT	BQ	1003	-	-	4/21/61/61	0/2/2/2
13	BCL	BV	1005	-	-	9/37/137/137	-
21	CD4	M	409	-	-	23/94/94/94	-
13	BCL	ag	102	-	-	5/37/137/137	-
14	LMT	AA	1003	-	-	7/21/61/61	0/2/2/2
16	0V9	bd	103	-	-	9/48/48/50	-
13	BCL	BS	1004	-	-	5/37/137/137	-
14	LMT	AQ	101	-	-	2/21/61/61	0/2/2/2
14	LMT	BM	1005	-	-	5/21/61/61	0/2/2/2
13	BCL	AE	104	-	-	2/37/137/137	-
13	BCL	AF	1001	-	-	8/37/137/137	-
14	LMT	AX	101	-	-	3/21/61/61	0/2/2/2
14	LMT	AG	101	-	-	8/21/61/61	0/2/2/2
16	0V9	be	105	-	-	17/48/48/50	-
15	V7N	BM	1001	-	-	6/53/53/53	-
14	LMT	bi	104	-	-	3/21/61/61	0/2/2/2
15	V7N	bk	101	-	-	5/53/53/53	-
14	LMT	BC	102	-	-	3/21/61/61	0/2/2/2
15	V7N	bo	101	-	-	7/53/53/53	-
13	BCL	bc	103	-	-	7/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	V7N	BQ	1001	-	-	4/53/53/53	-
15	V7N	BR	1001	-	-	7/53/53/53	-
14	LMT	BF	104	-	-	7/21/61/61	0/2/2/2
14	LMT	be	101	-	-	4/21/61/61	0/2/2/2
13	BCL	al	1001	-	-	3/37/137/137	-
14	LMT	AC	103	-	-	8/21/61/61	0/2/2/2
19	NDG	C	1007	18	-	0/6/23/26	0/1/1/1
13	BCL	ab	1001	-	-	4/37/137/137	-
13	BCL	BH	1005	-	-	10/37/137/137	-
14	LMT	BG	1005	-	-	3/21/61/61	0/2/2/2
14	LMT	BB	101	-	-	2/21/61/61	0/2/2/2
14	LMT	bf	101	-	-	6/21/61/61	0/2/2/2
14	LMT	BX	102	-	-	9/21/61/61	0/2/2/2
13	BCL	af	103	-	-	9/37/137/137	-
14	LMT	bo	104	-	-	4/21/61/61	0/2/2/2
14	LMT	AT	104	-	-	6/21/61/61	0/2/2/2
16	0V9	bl	102	-	-	11/48/48/50	-
15	V7N	BG	1001	-	-	4/53/53/53	-
14	LMT	BM	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	BT	101	-	-	6/21/61/61	0/2/2/2
14	LMT	BO	1005	-	-	4/21/61/61	0/2/2/2
16	0V9	bb	103	-	-	8/48/48/50	-
13	BCL	BW	1005	-	-	5/37/137/137	-
14	LMT	bk	104	-	-	5/21/61/61	0/2/2/2
14	LMT	BP	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	bp	101	-	-	4/21/61/61	0/2/2/2
13	BCL	bb	102	-	-	8/37/137/137	-
14	LMT	L	304	-	-	4/21/61/61	0/2/2/2
13	BCL	L	308	-	-	1/37/137/137	-
13	BCL	bk	103	-	-	7/37/137/137	-
17	HEC	C	1004	3	-	2/10/54/54	-
15	V7N	BD	101	-	-	4/53/53/53	-
15	V7N	AW	103	-	-	5/53/53/53	-
16	0V9	ad	103	-	-	12/48/48/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BO	1004	-	-	4/21/61/61	0/2/2/2
13	BCL	bg	104	-	-	8/37/137/137	-
16	0V9	ab	1002	-	-	13/48/48/50	-
15	V7N	BF	101	-	-	7/53/53/53	-
15	V7N	bi	101	-	-	5/53/53/53	-
14	LMT	AP	101	-	-	9/21/61/61	0/2/2/2
21	CD4	H1	103	-	-	18/94/94/94	-
13	BCL	ad	102	-	-	3/37/137/137	-
15	V7N	BE	101	-	-	4/53/53/53	-
16	0V9	bp	105	-	-	12/48/48/50	-
20	PGW	H1	101	-	-	13/55/55/55	-
13	BCL	bn	102	-	-	8/37/137/137	-
23	MQ8	ao	101	-	-	4/47/67/67	0/2/2/2
14	LMT	BR	1006	-	-	4/21/61/61	0/2/2/2
14	LMT	bg	102	-	-	5/21/61/61	0/2/2/2
15	V7N	ag	101	-	-	5/53/53/53	-
14	LMT	BB	104	-	-	4/21/61/61	0/2/2/2
13	BCL	AE	103	28	-	11/37/137/137	-
15	V7N	BH	1001	-	-	8/53/53/53	-
13	BCL	BF	103	-	-	9/37/137/137	-
16	0V9	bo	103	-	-	16/48/48/50	-
13	BCL	BE	104	-	-	8/37/137/137	-
17	HEC	C	1003	3	-	0/10/54/54	-
13	BCL	bp	104	-	-	11/37/137/137	-
14	LMT	AJ	102	-	-	9/21/61/61	0/2/2/2
15	V7N	bp	102	-	-	3/53/53/53	-
13	BCL	AD	103	-	-	6/37/137/137	-
14	LMT	AH	101	-	-	5/21/61/61	0/2/2/2
14	LMT	BN	1003	-	-	5/21/61/61	0/2/2/2
13	BCL	ap	1001	-	-	5/37/137/137	-
14	LMT	BS	1003	-	-	6/21/61/61	0/2/2/2
14	LMT	BE	102	-	-	4/21/61/61	0/2/2/2
14	LMT	H2	201	-	-	6/21/61/61	0/2/2/2
13	BCL	aj	101	-	-	7/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BT	102	-	-	2/21/61/61	0/2/2/2
13	BCL	BR	1003	-	-	9/37/137/137	-
13	BCL	AA	1002	28	-	8/37/137/137	-
13	BCL	bl	104	-	-	8/37/137/137	-
14	LMT	BR	1004	-	-	3/21/61/61	0/2/2/2

The worst 5 of 1657 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bc	101	V7N	C28-C27	7.13	1.53	1.34
15	BD	101	V7N	C28-C27	7.02	1.52	1.34
15	BF	101	V7N	C28-C27	6.98	1.52	1.34
15	bi	101	V7N	C28-C27	6.97	1.52	1.34
15	BU	1001	V7N	C28-C27	6.97	1.52	1.34

The worst 5 of 1857 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BP	1003	BCL	C1-O2A-CGA	8.67	139.18	116.44
15	BU	1001	V7N	C28-C27-C26	-7.29	105.93	126.42
15	AA	1004	V7N	C28-C27-C26	-6.84	107.20	126.42
13	AE	103	BCL	C1-O2A-CGA	6.04	132.28	116.44
13	AL	103	BCL	C1-O2A-CGA	6.01	132.22	116.44

There are no chirality outliers.

5 of 1906 torsion outliers are listed below:

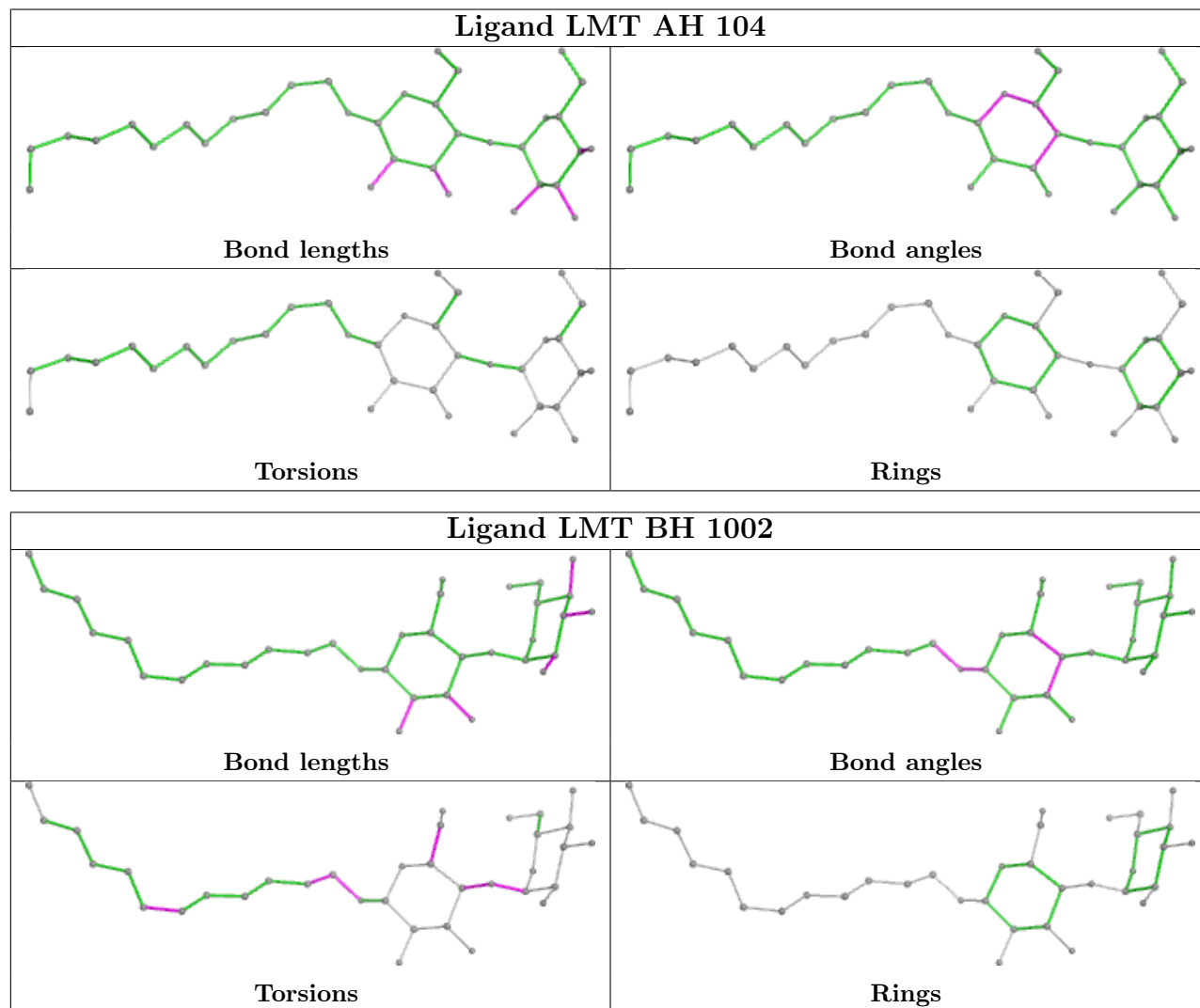
Mol	Chain	Res	Type	Atoms
13	AE	103	BCL	C3A-C2A-CAA-CBA
13	AE	105	BCL	C1A-C2A-CAA-CBA
13	AE	105	BCL	CHA-CBD-CGD-O1D
13	AE	105	BCL	CHA-CBD-CGD-O2D
13	AG	102	BCL	CHA-CBD-CGD-O1D

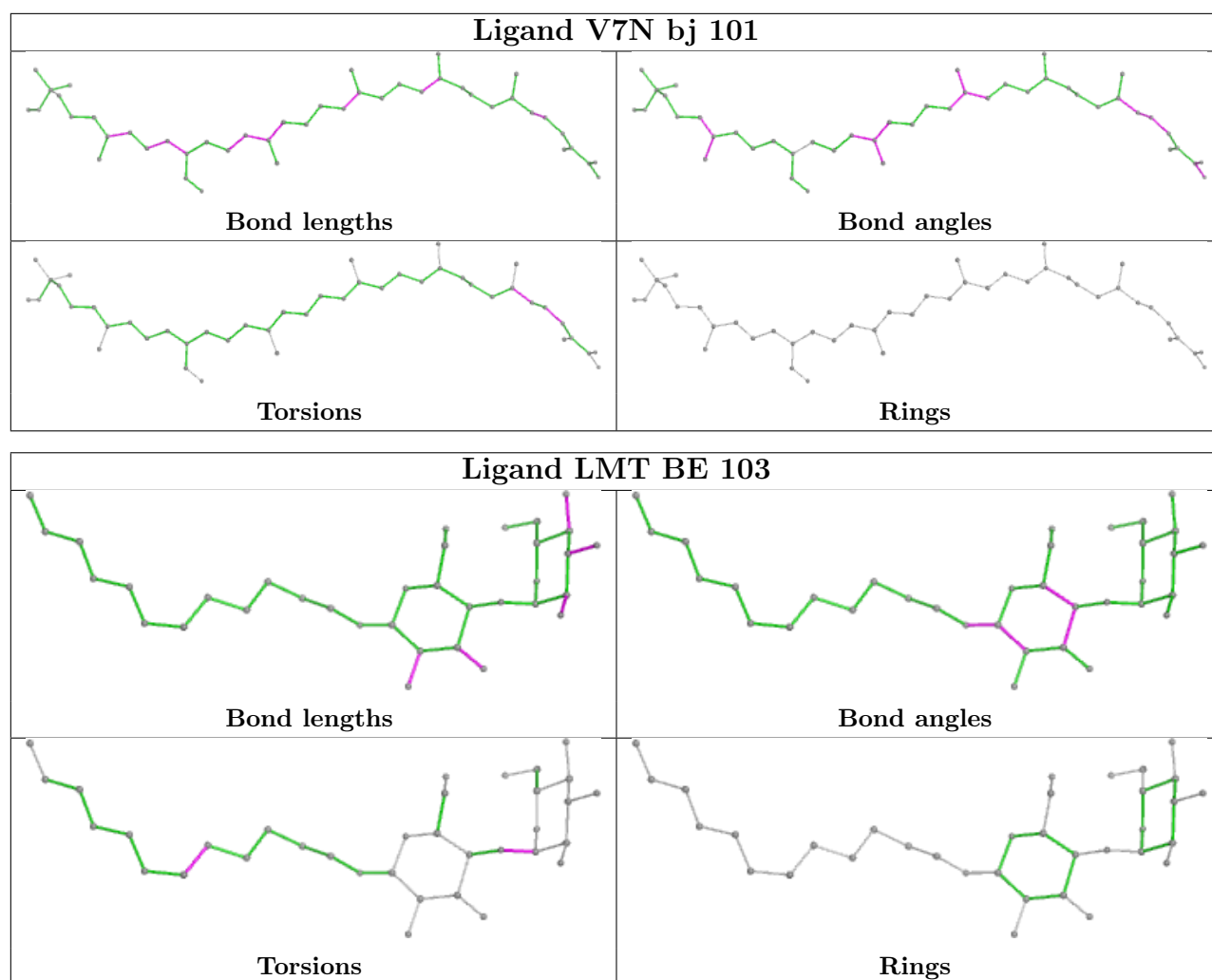
There are no ring outliers.

No monomer is involved in short contacts.

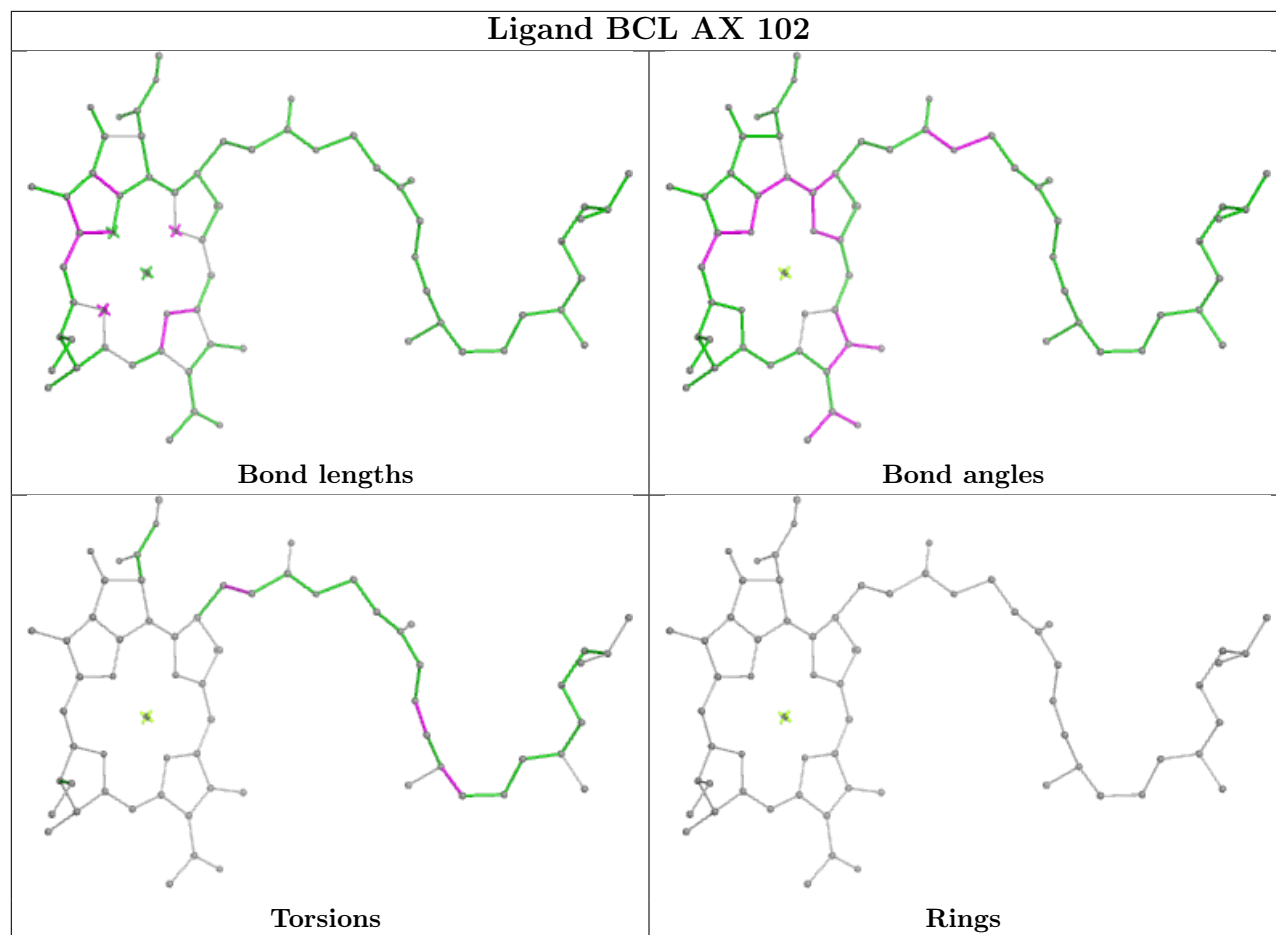
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

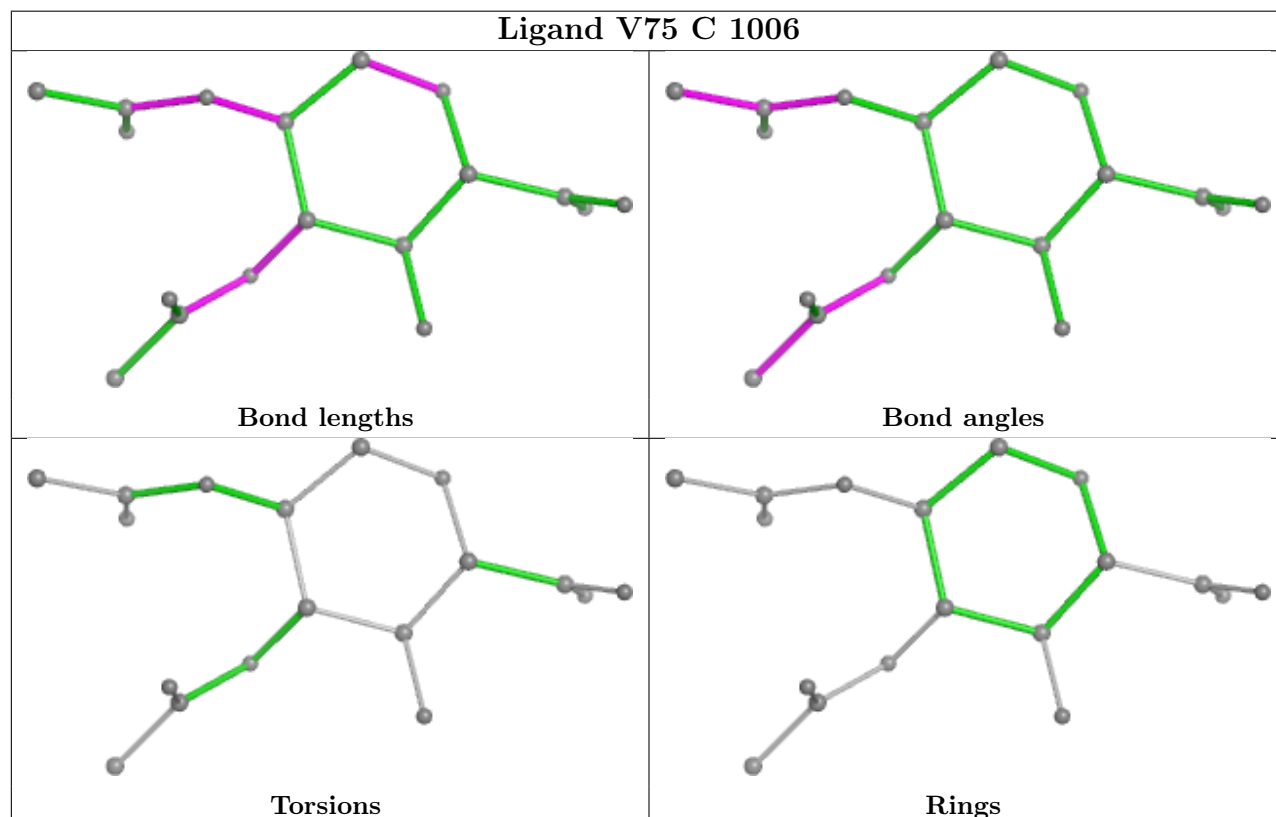


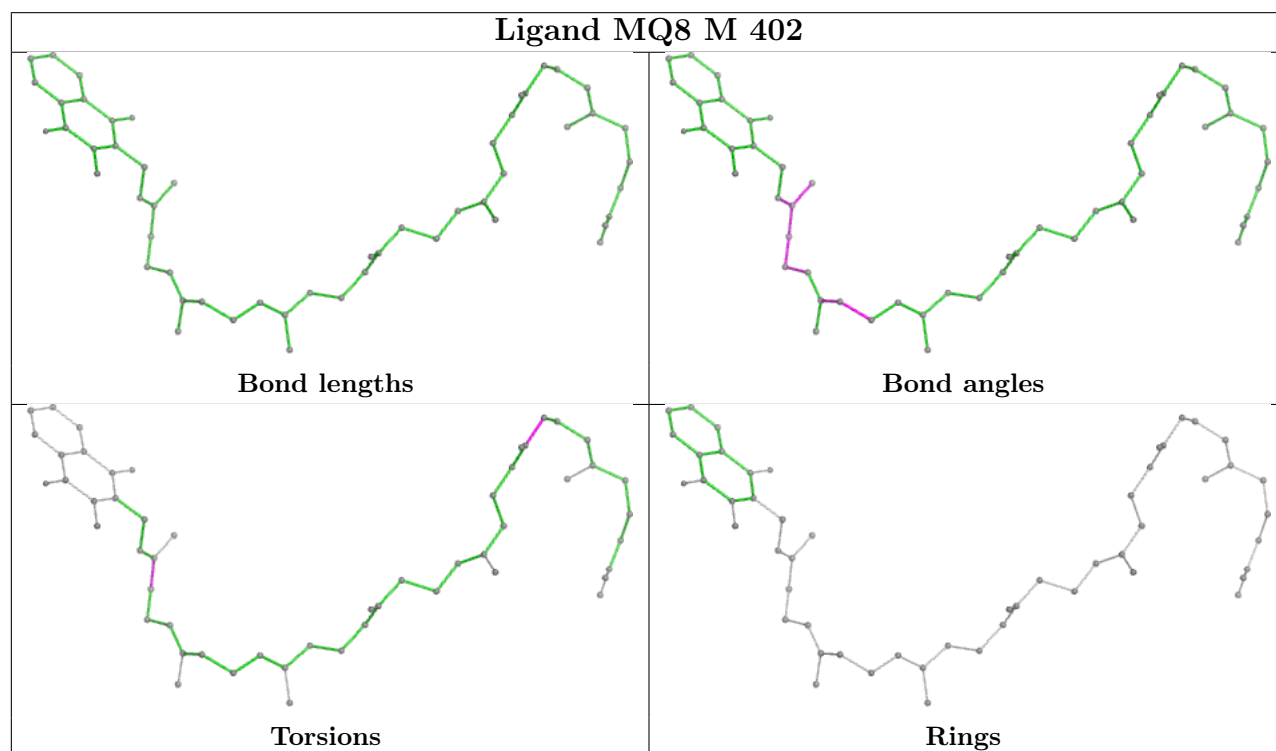
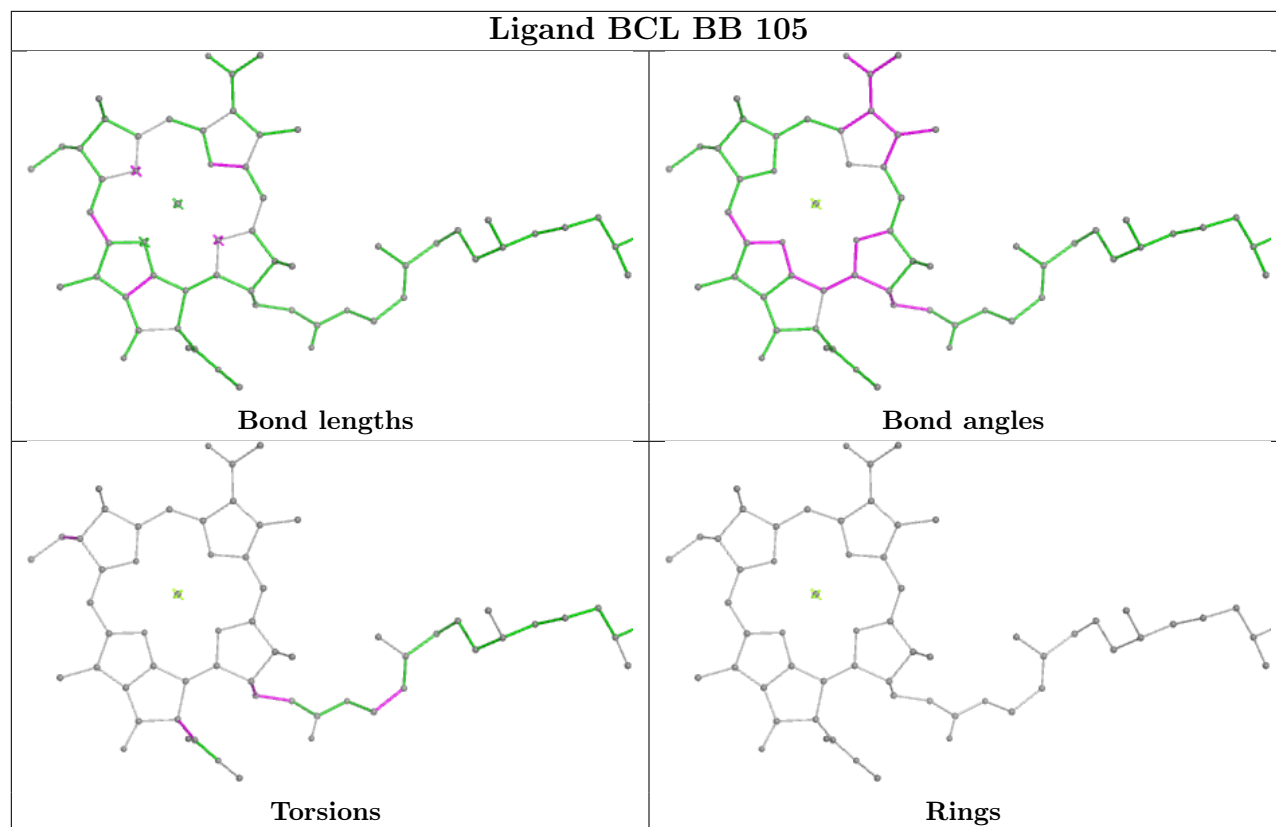


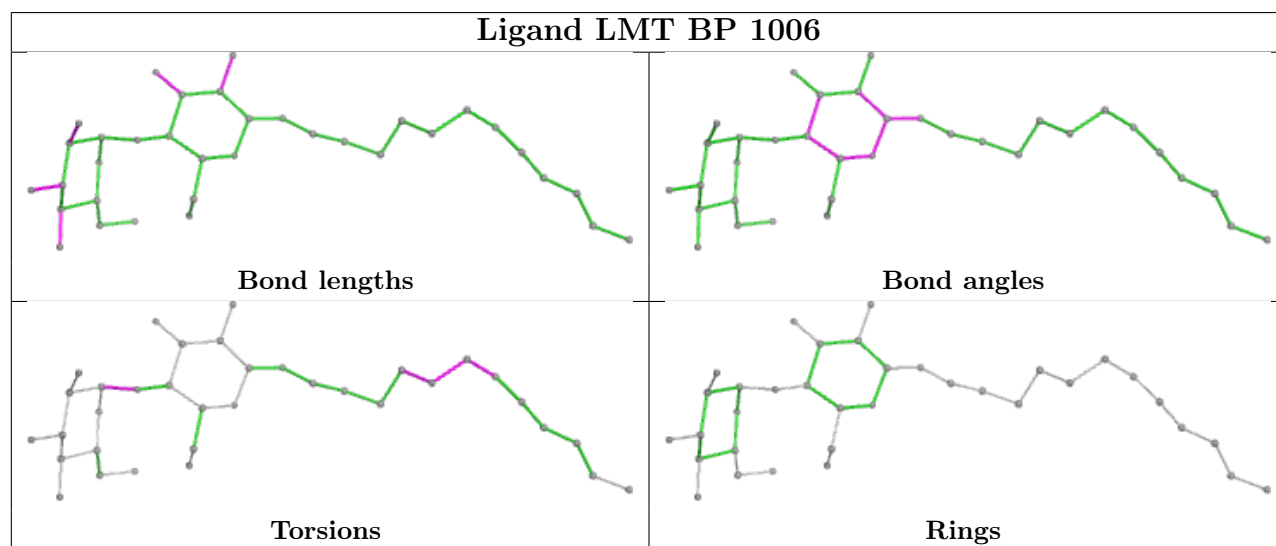
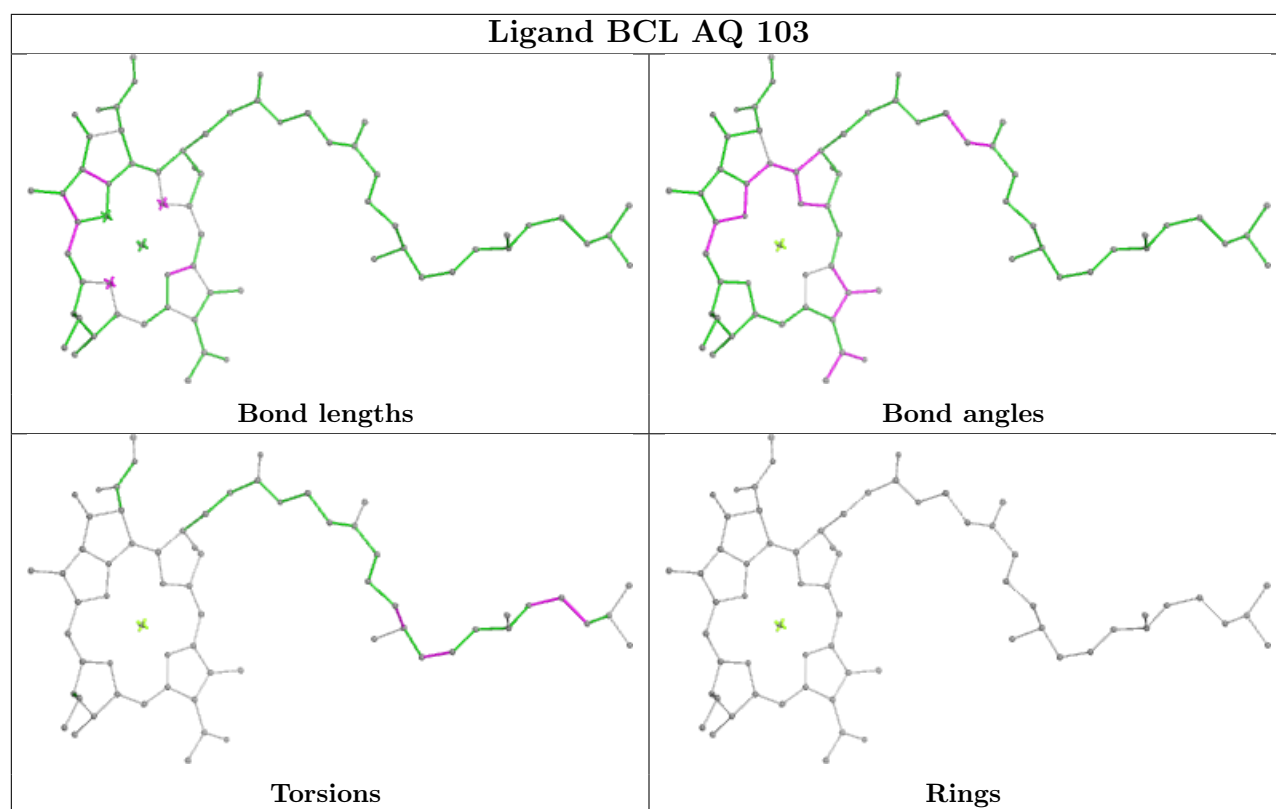
Ligand BCL AX 102

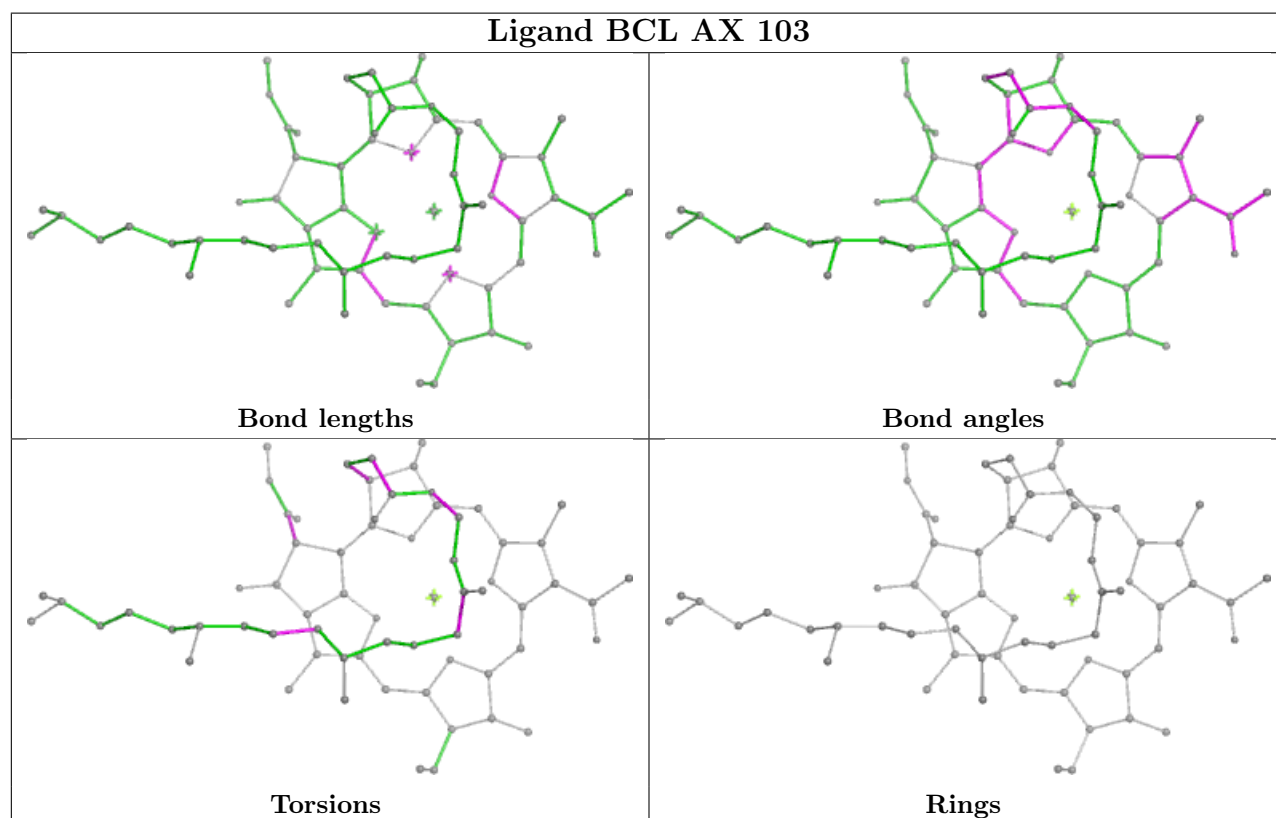
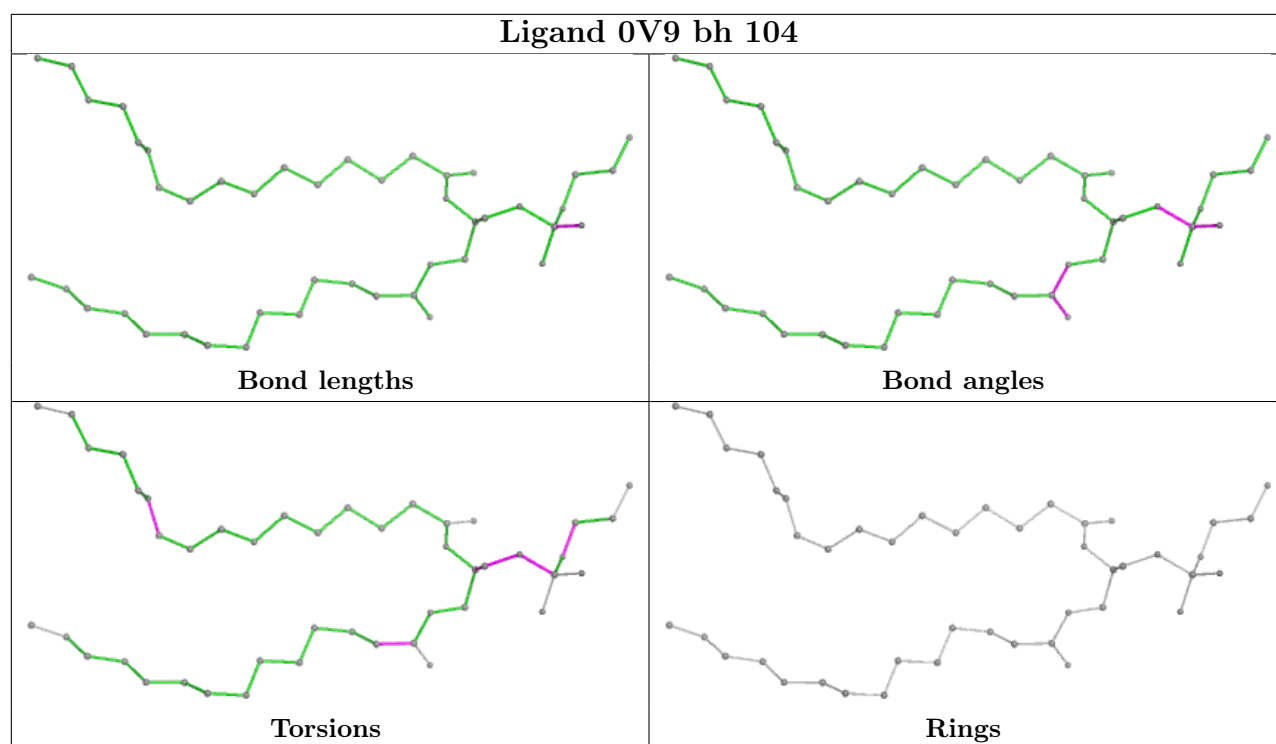


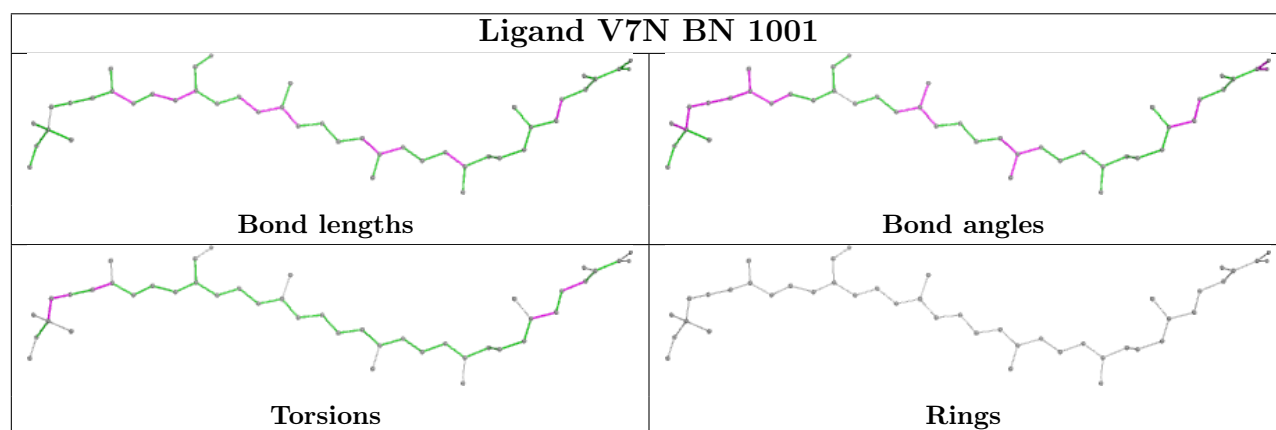
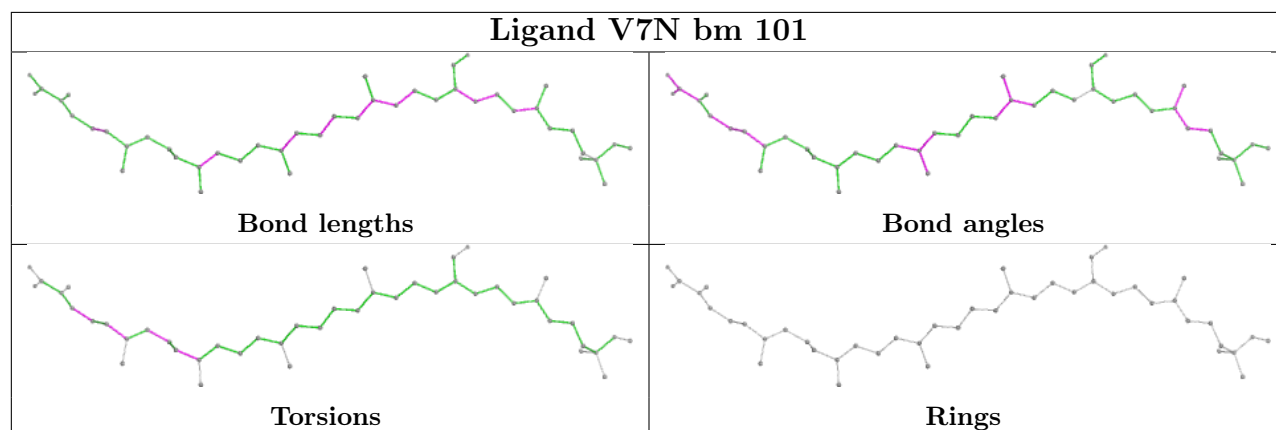
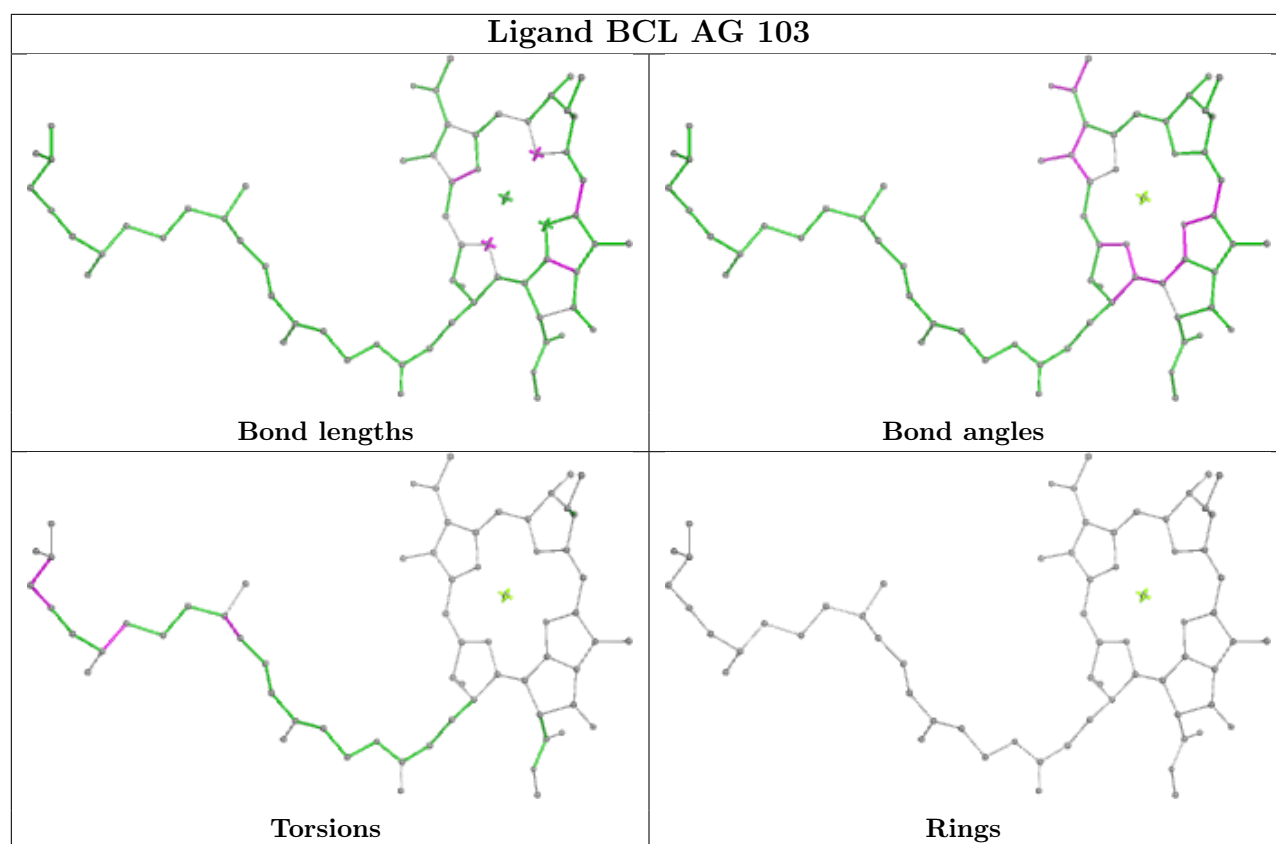
Ligand V75 C 1006

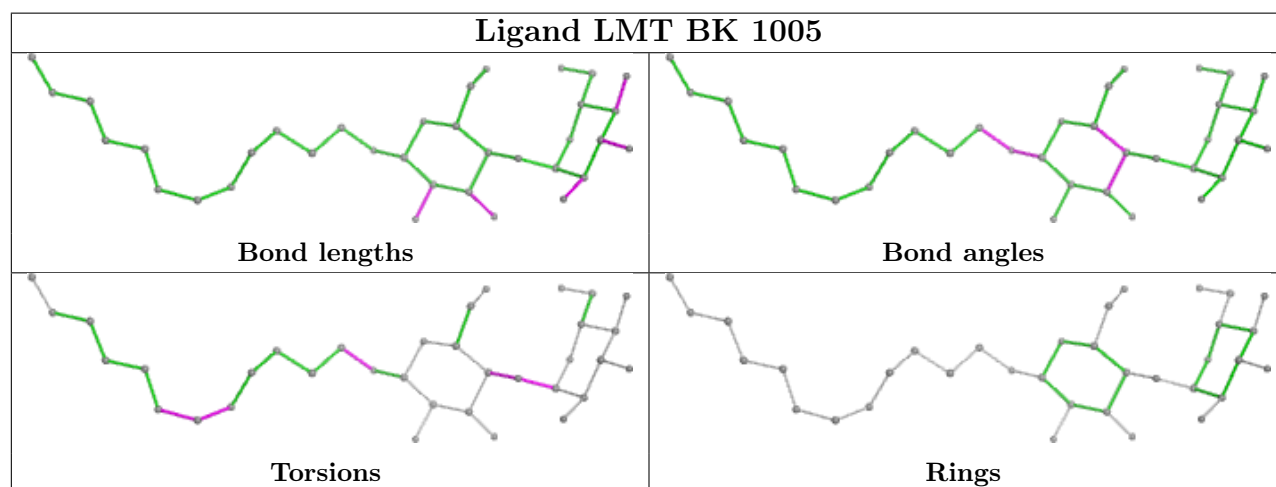
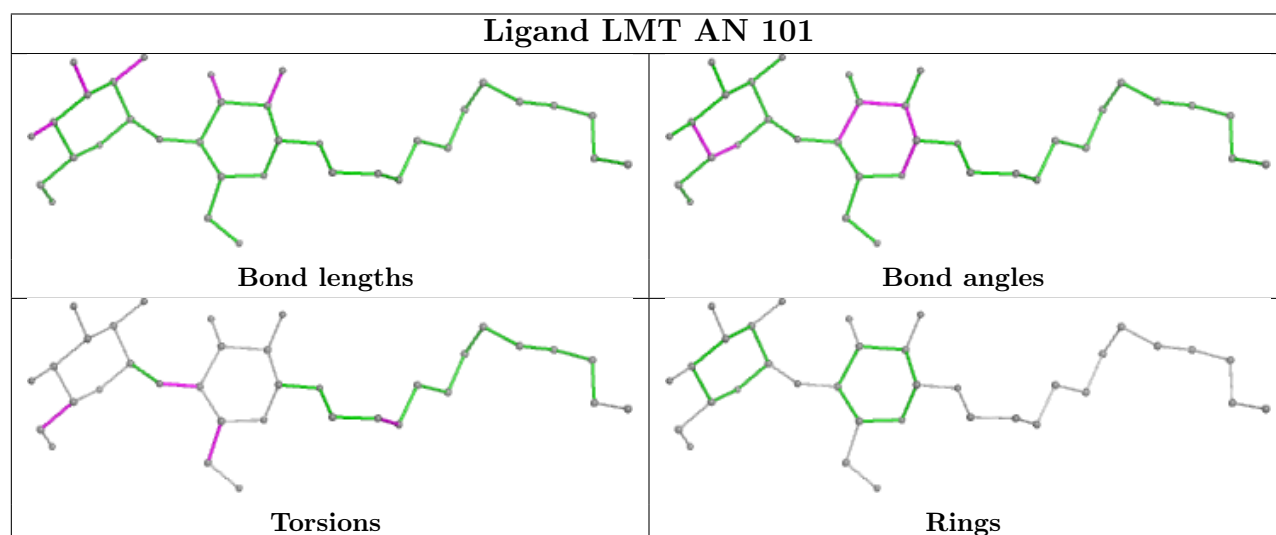
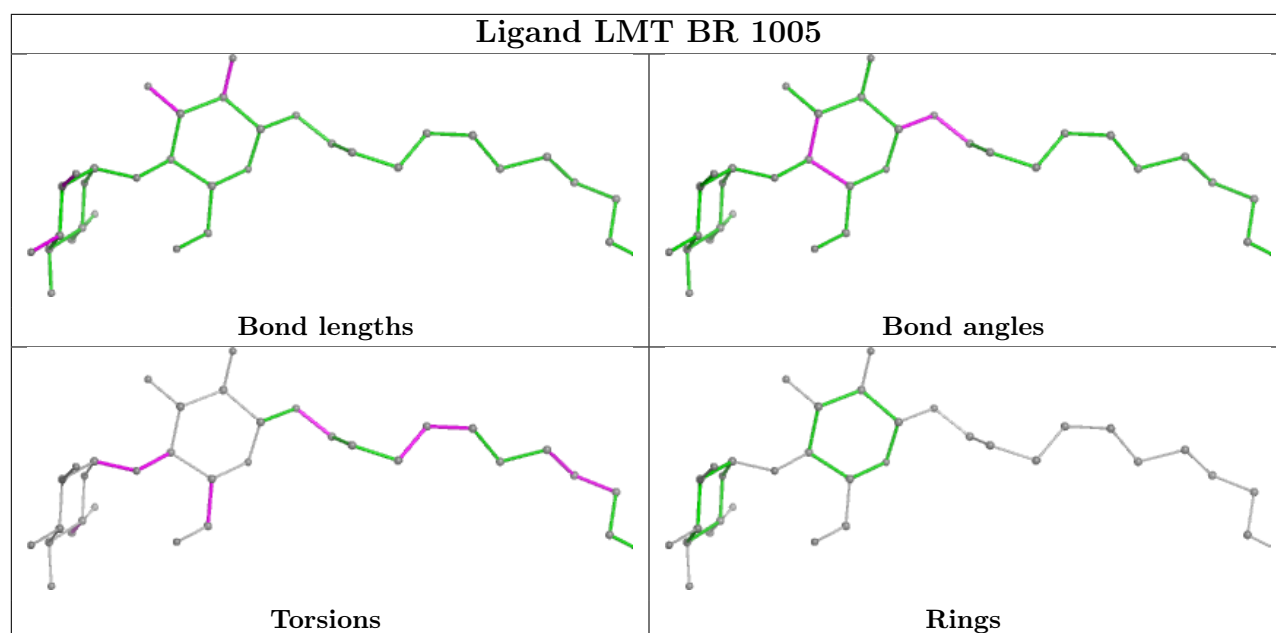


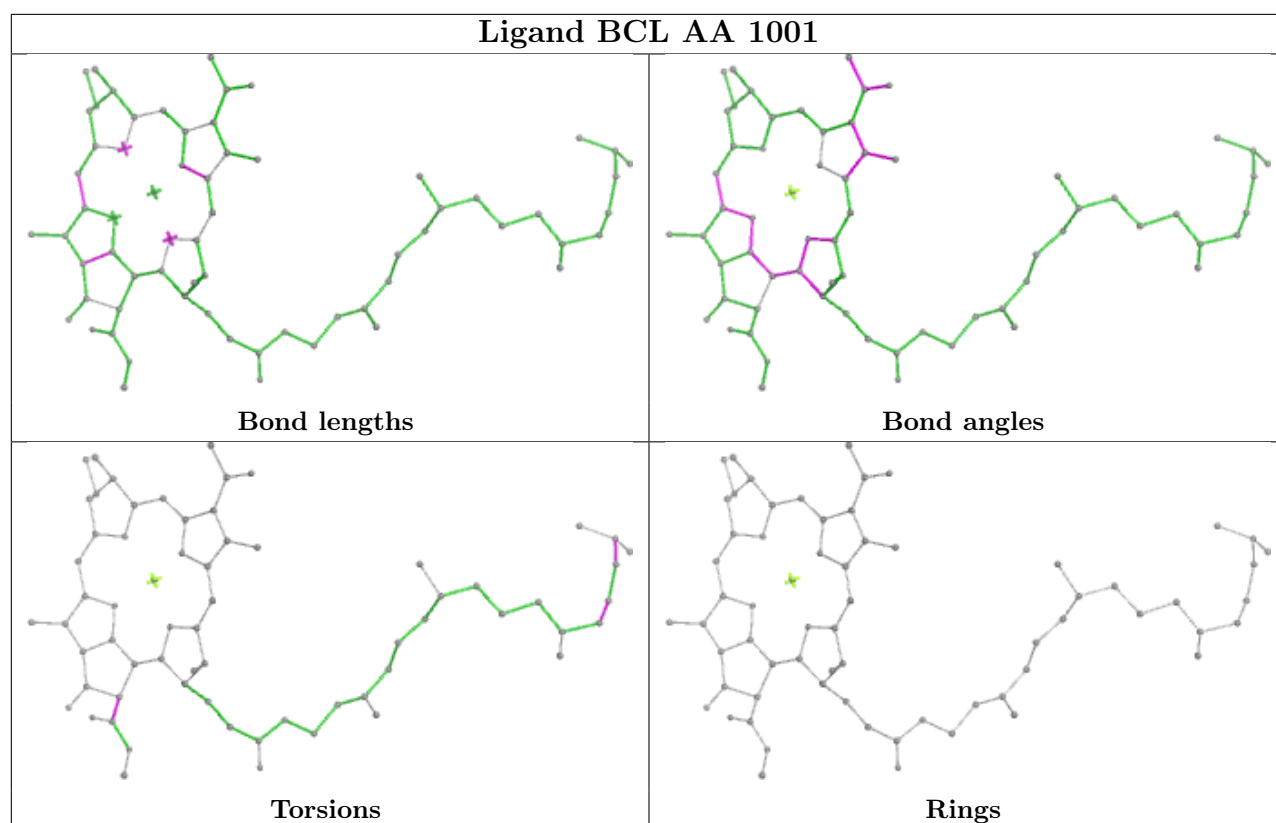


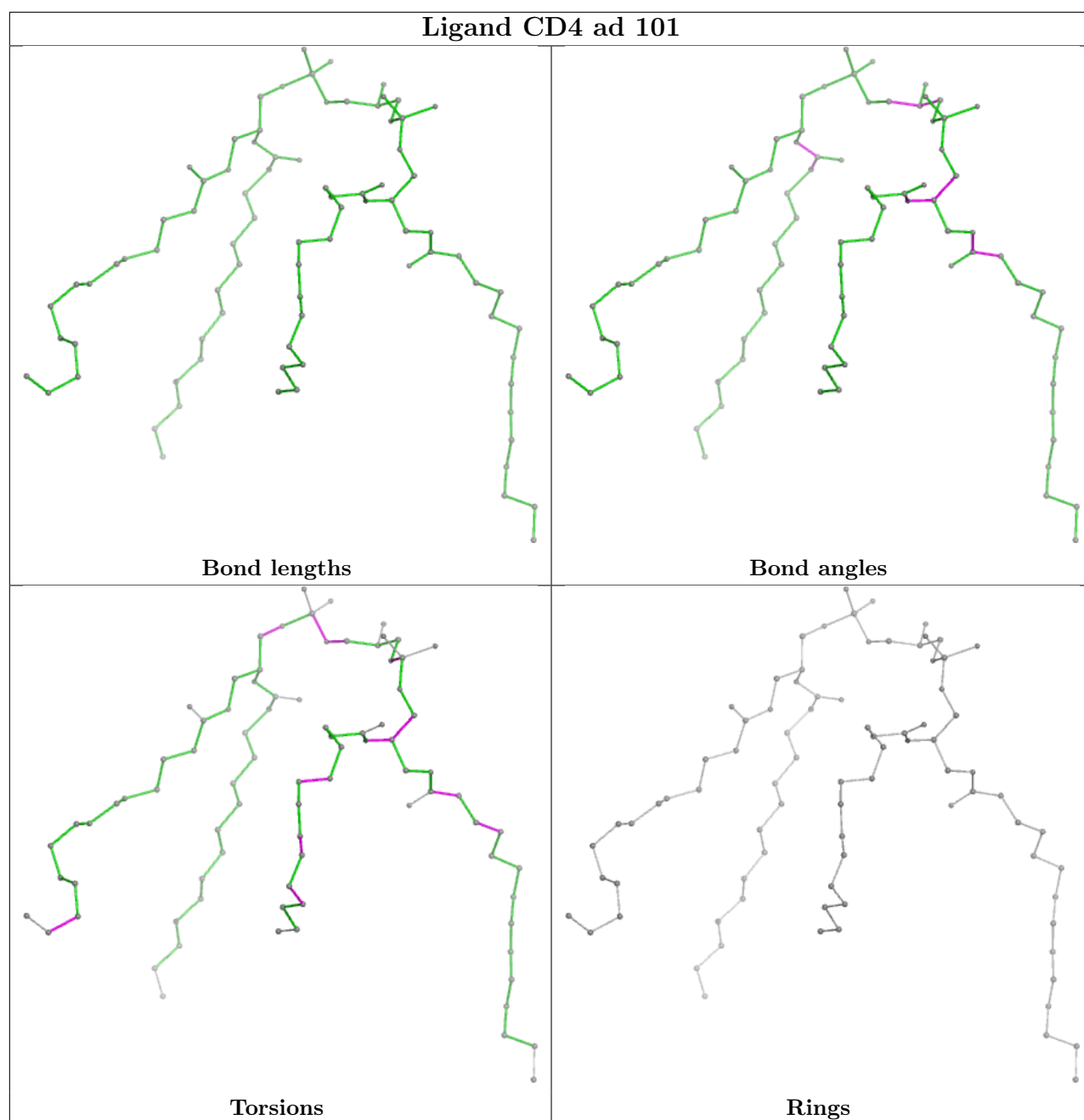


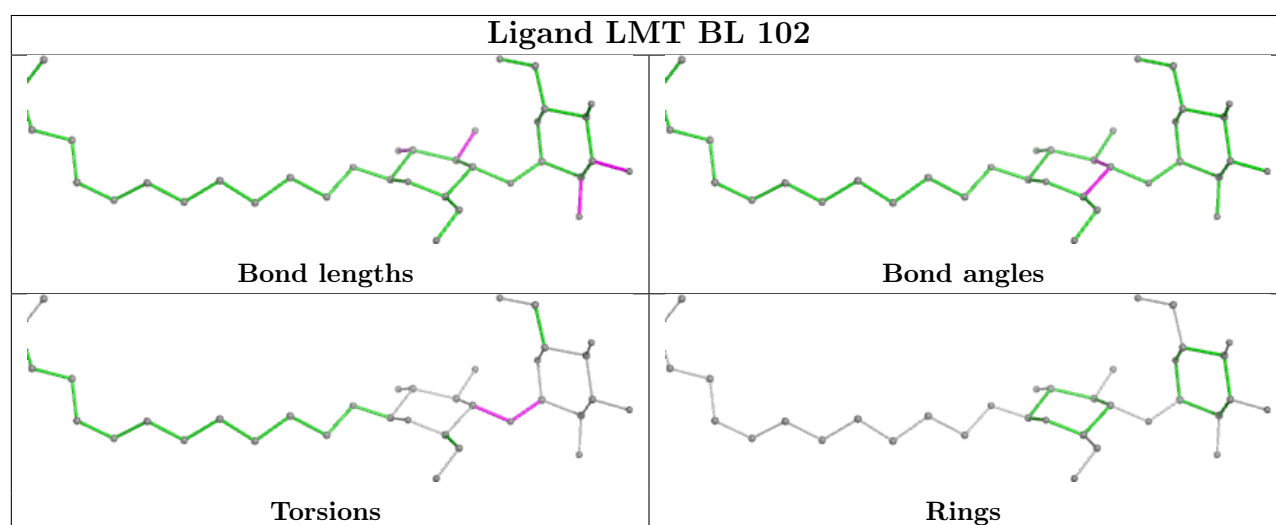
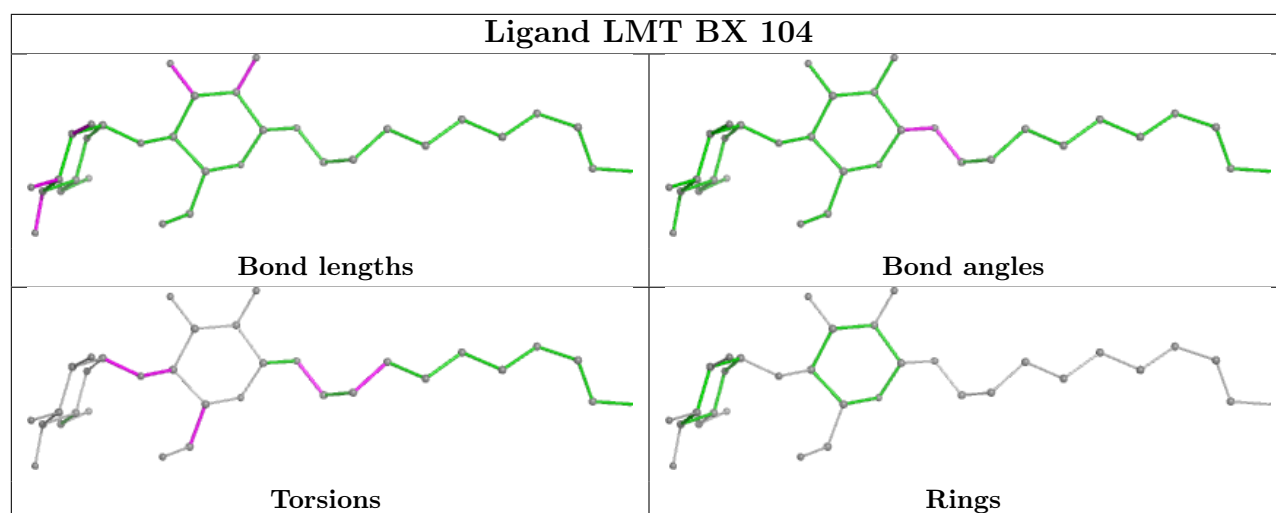




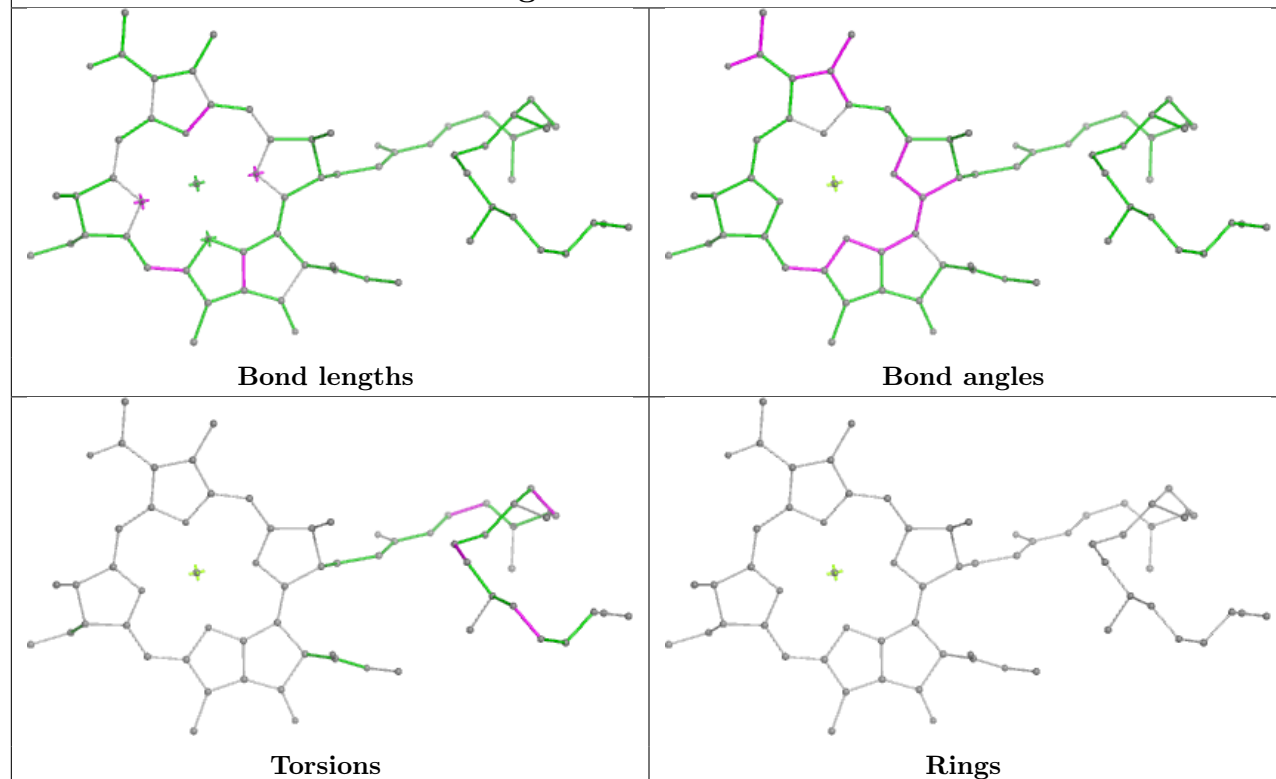




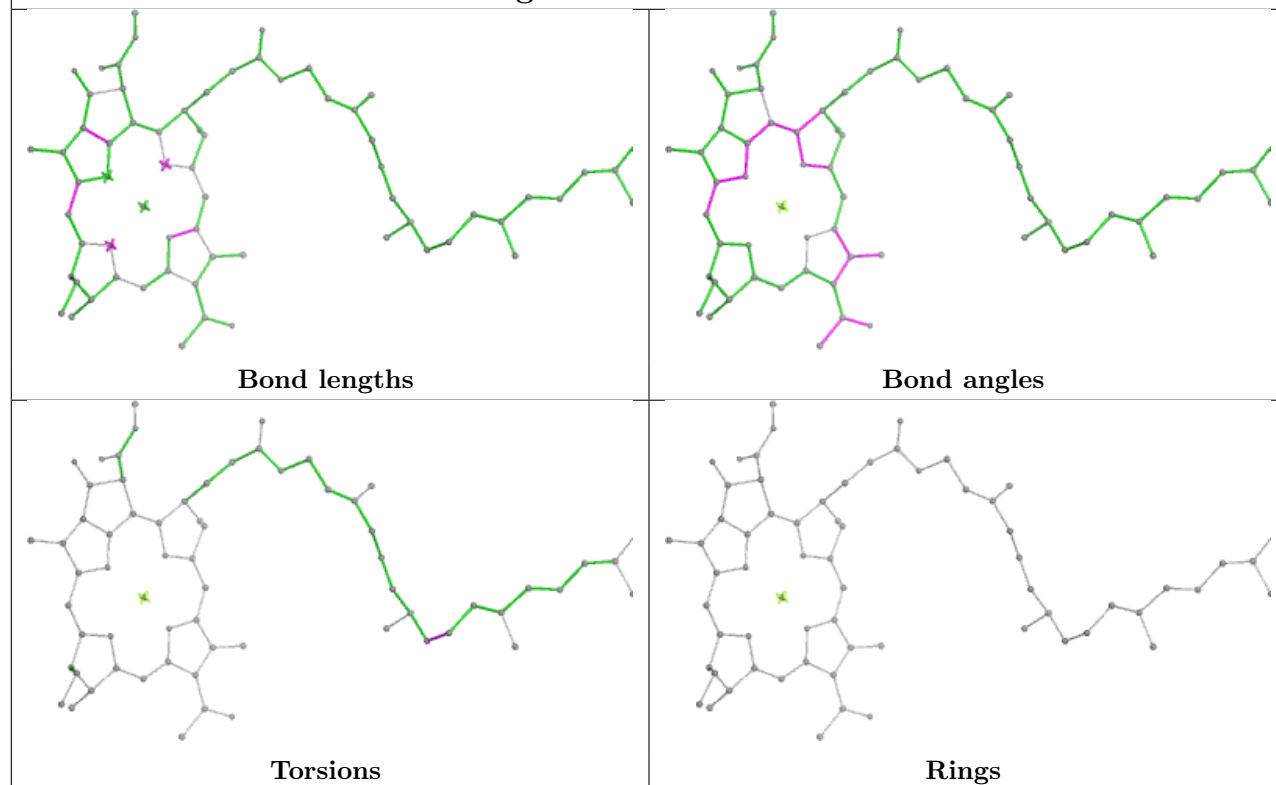


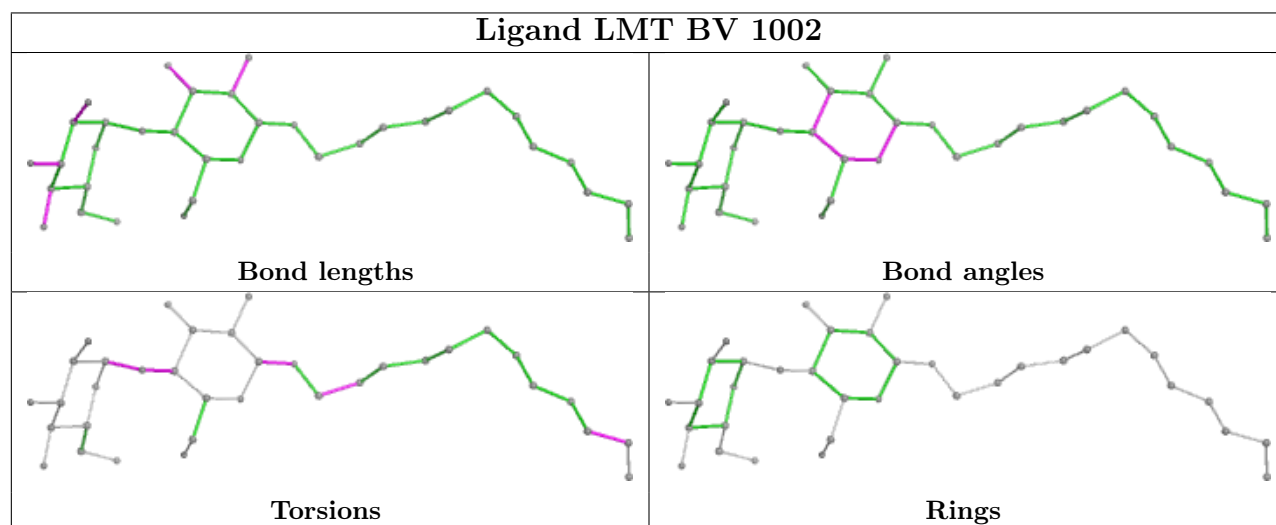
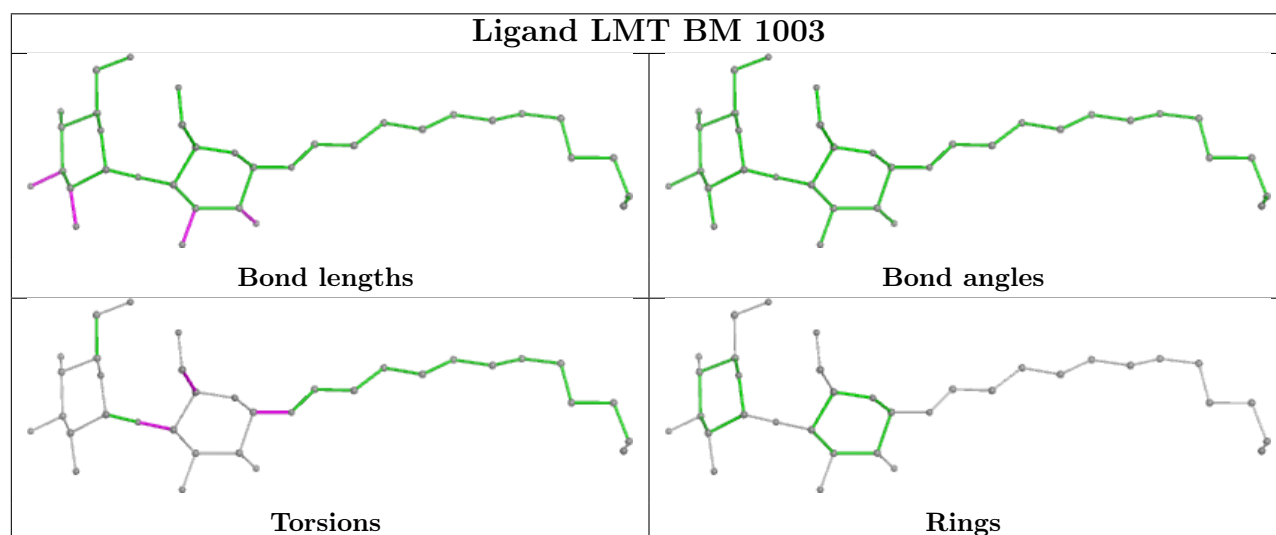
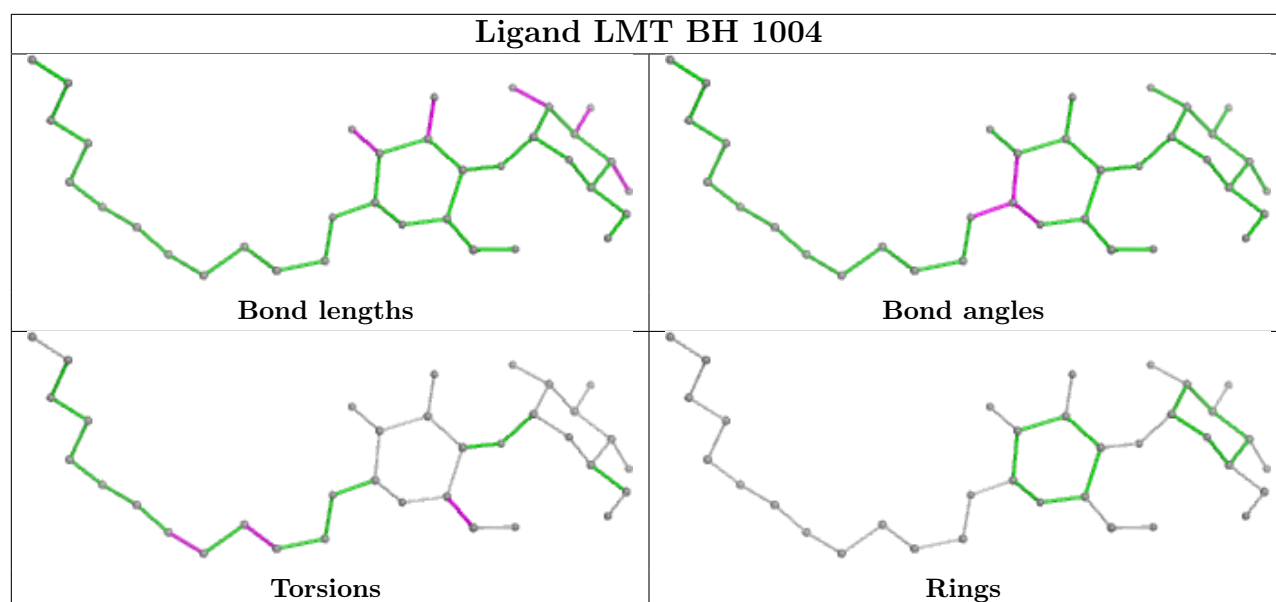


Ligand BCL ah 1001

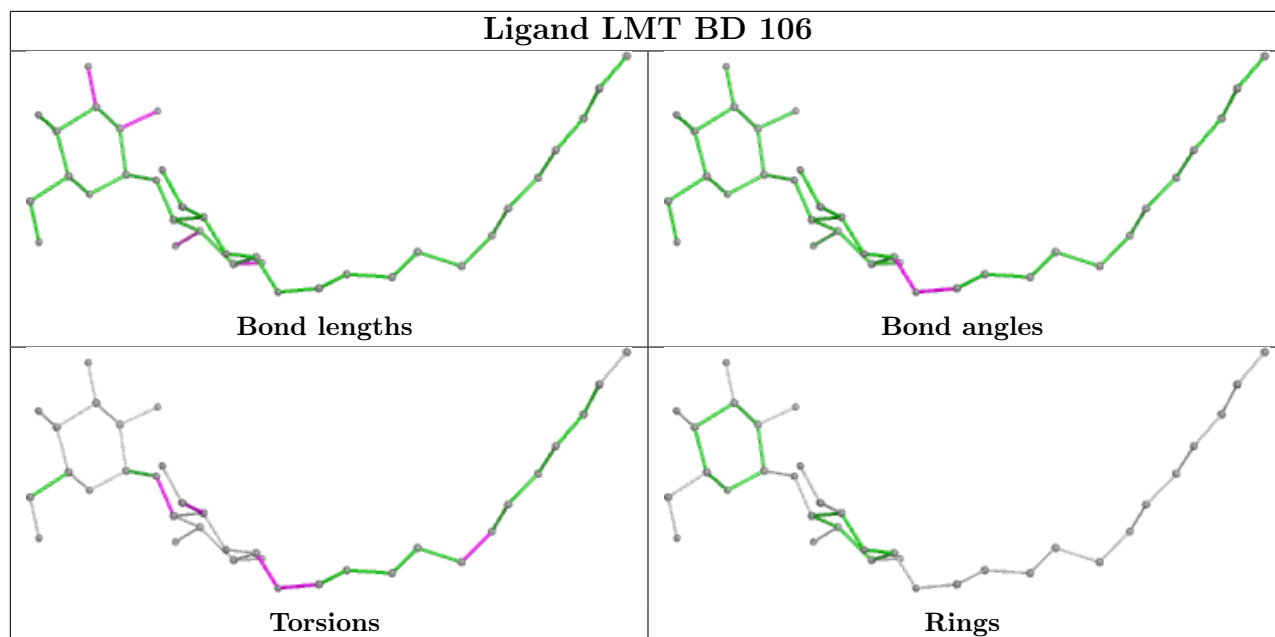


Ligand BCL AW 101

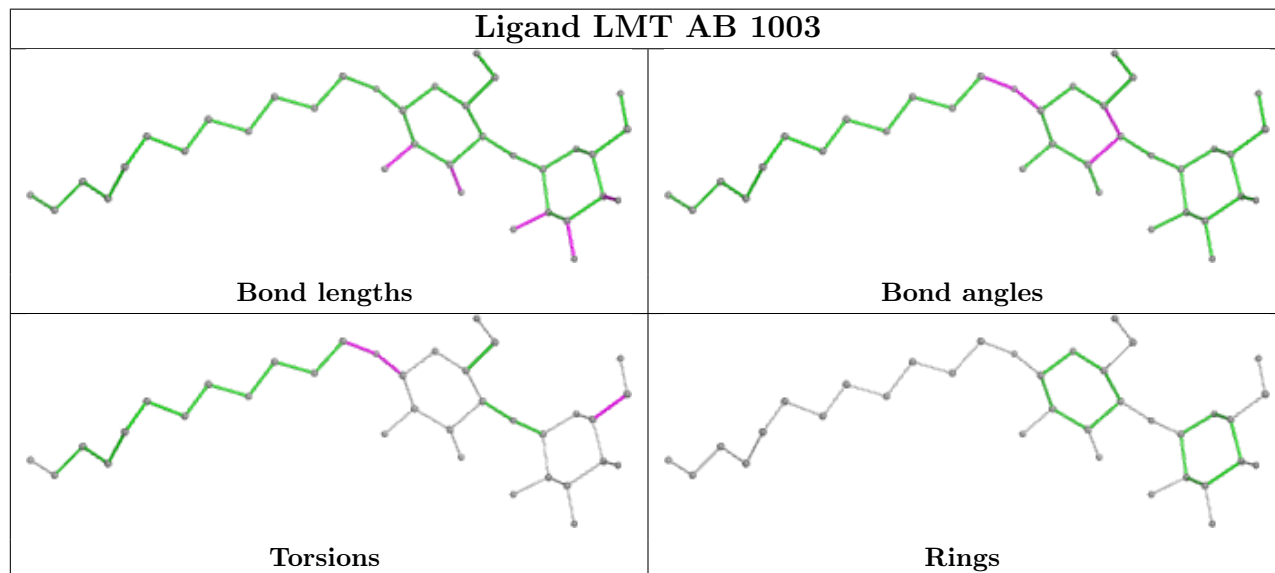




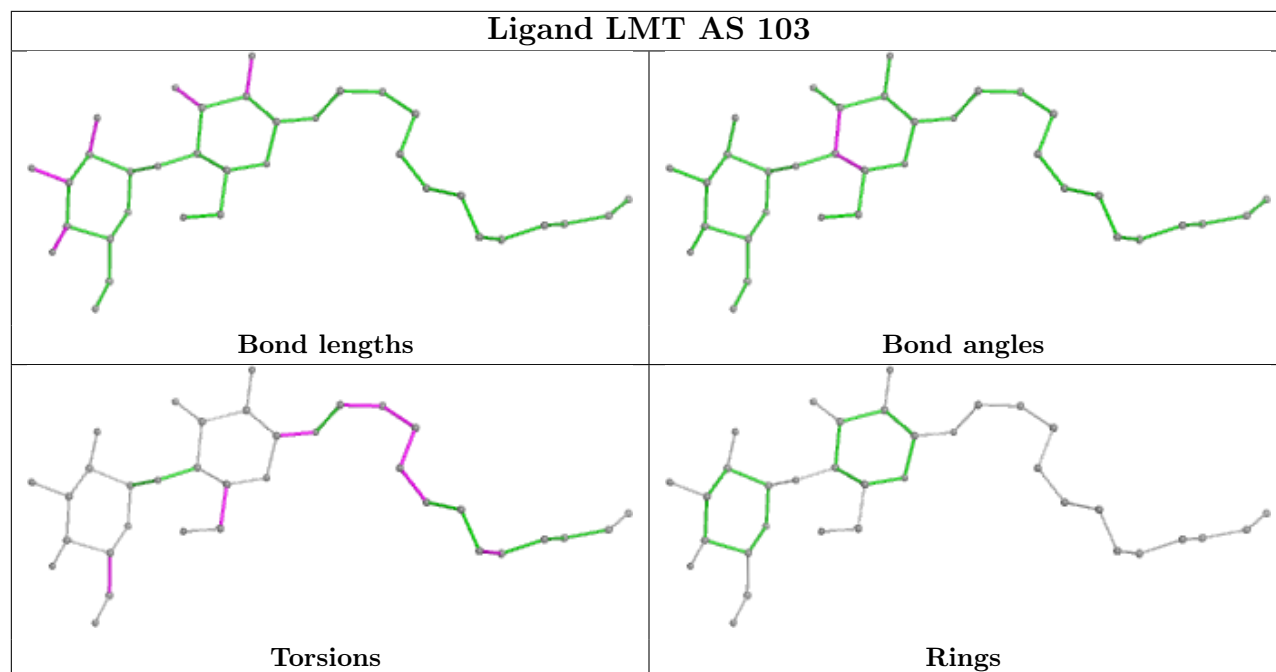
Ligand LMT BD 106



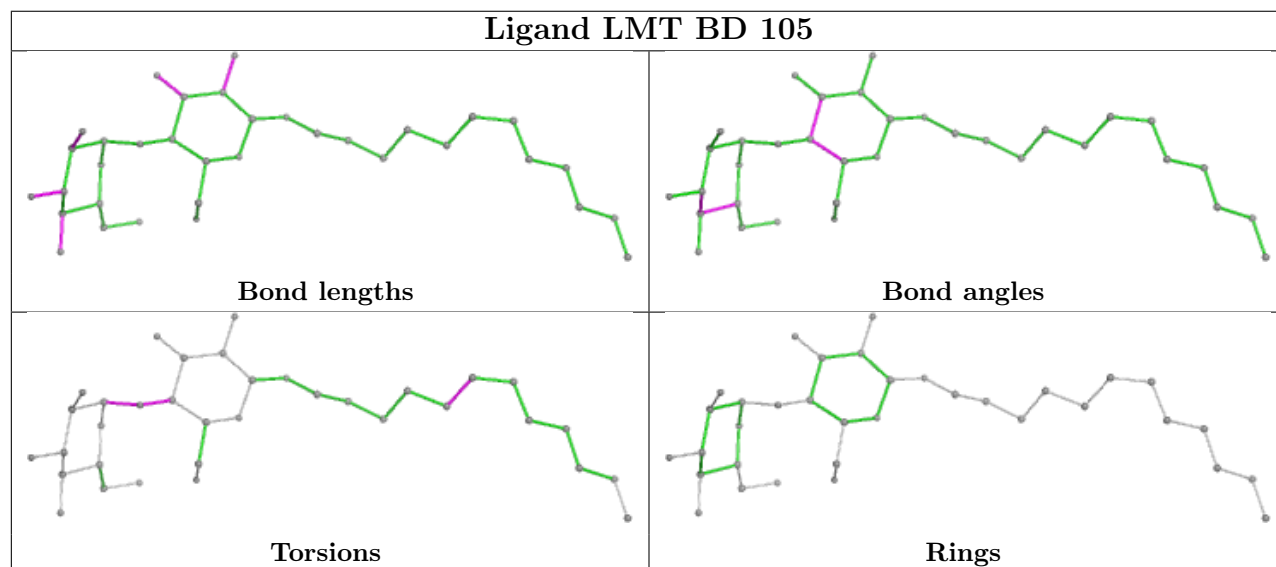
Ligand LMT AB 1003



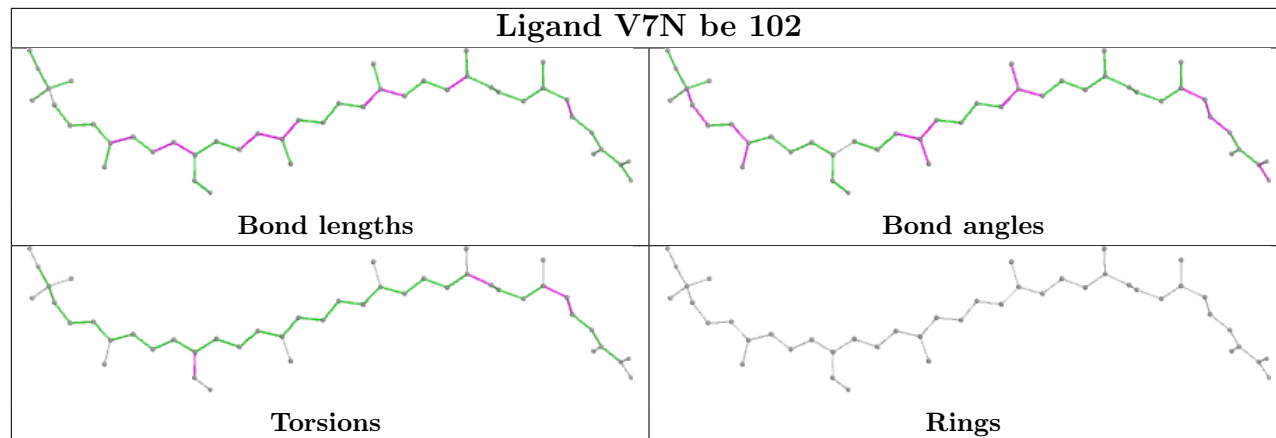
Ligand LMT AS 103

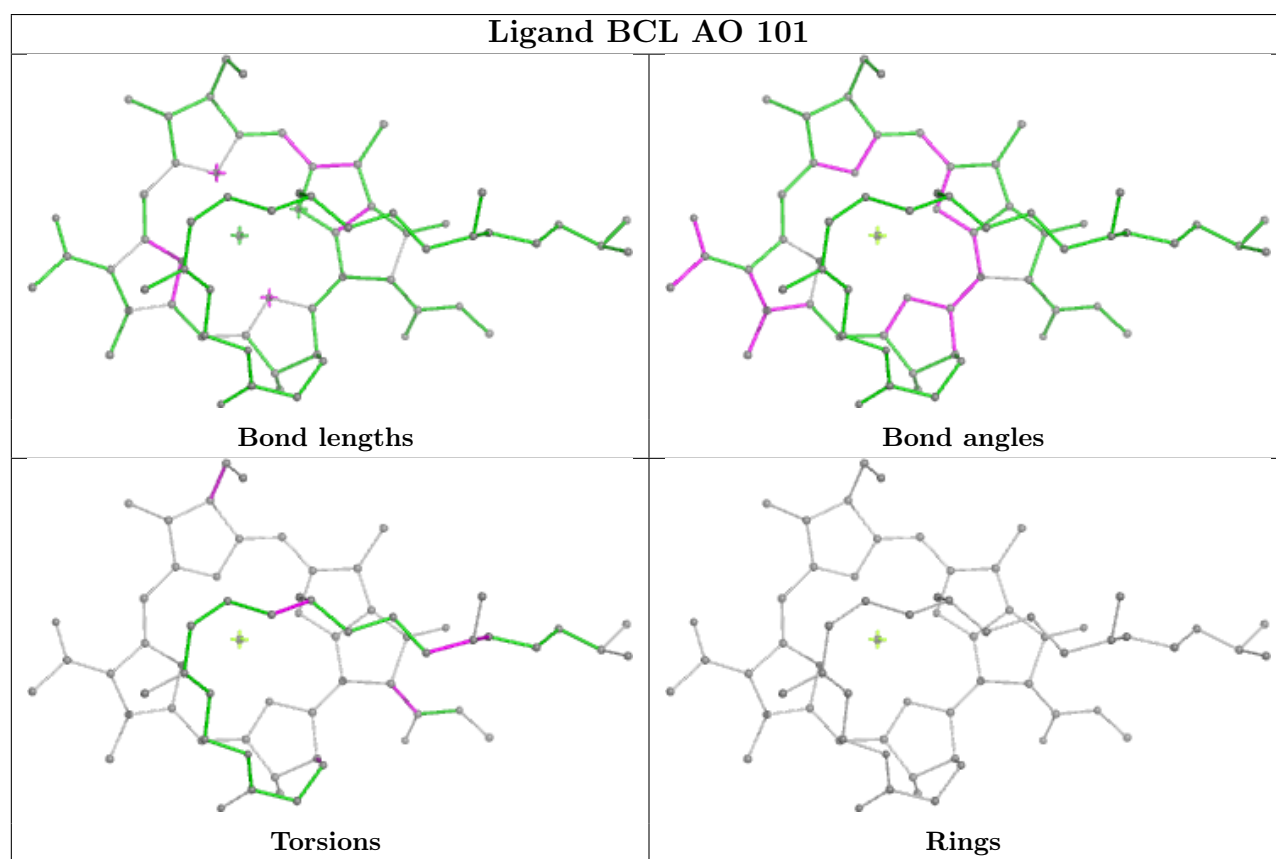
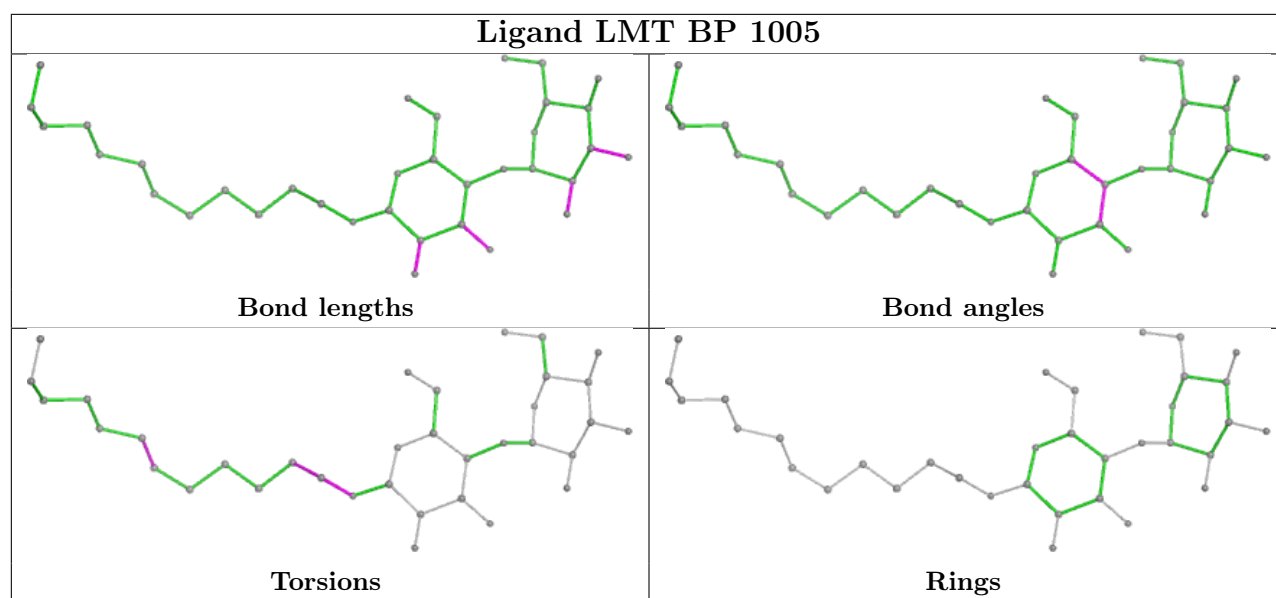


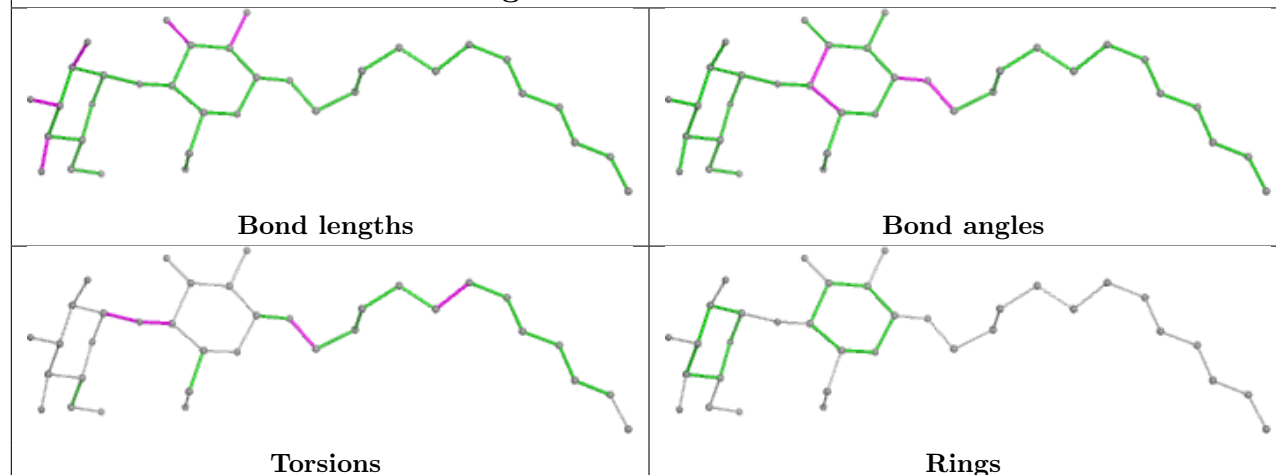
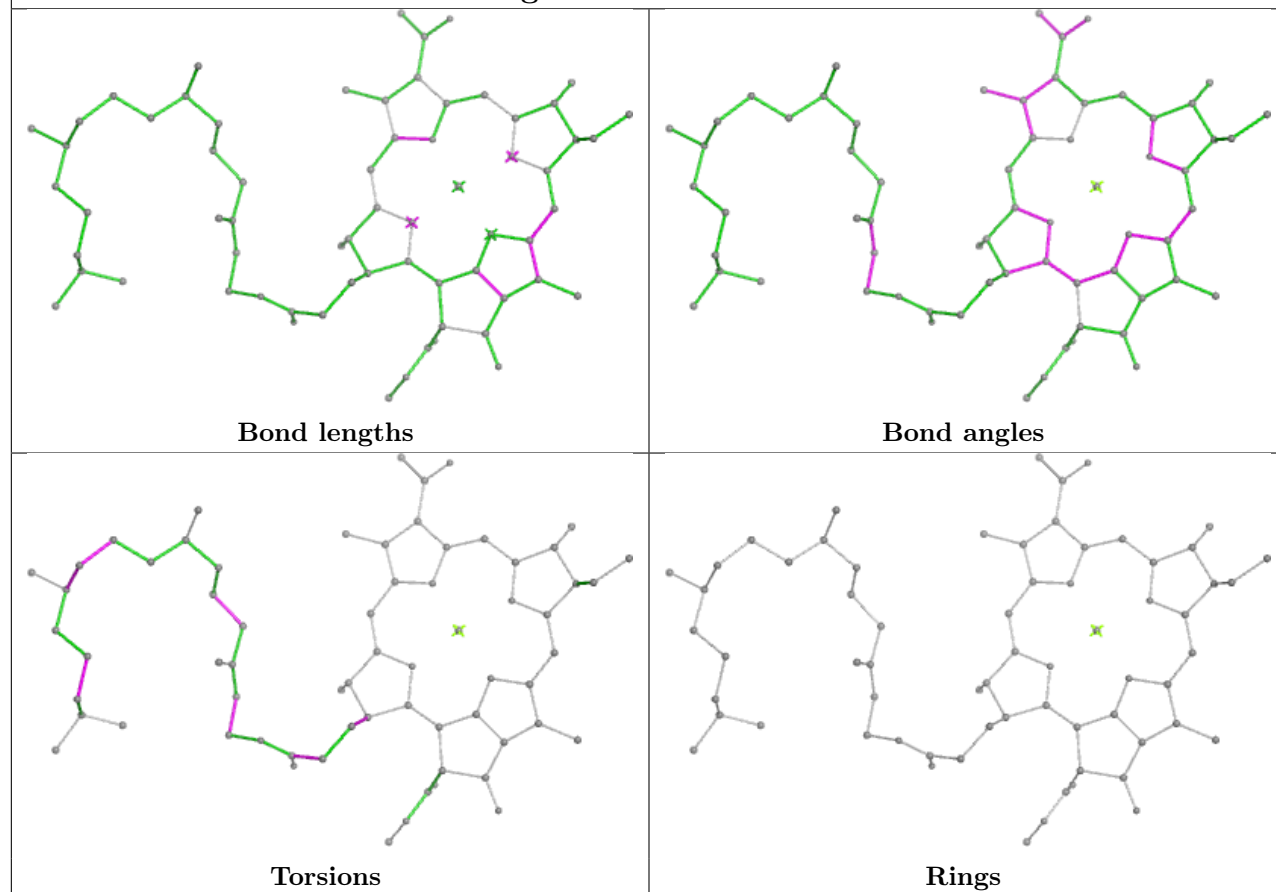
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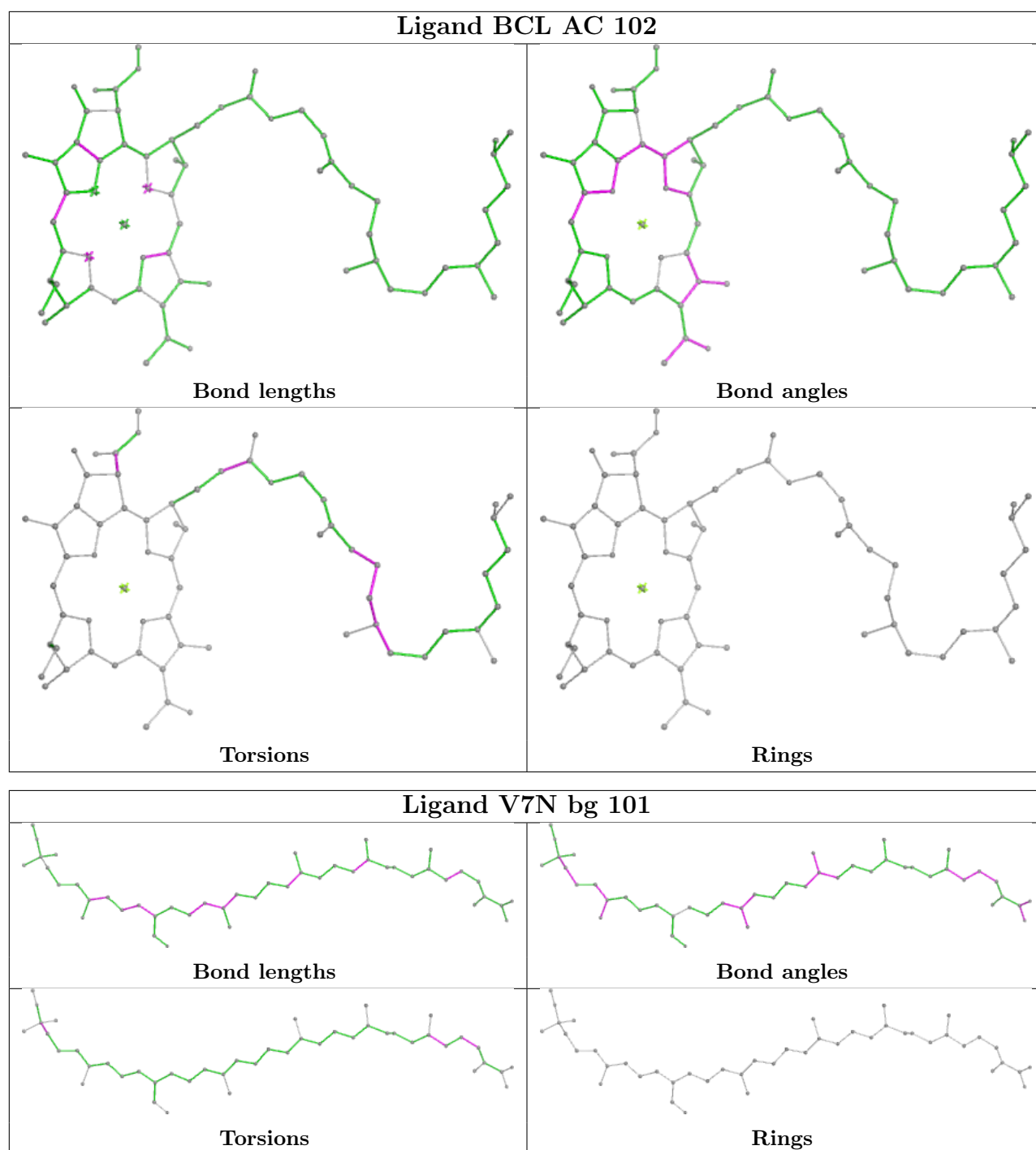


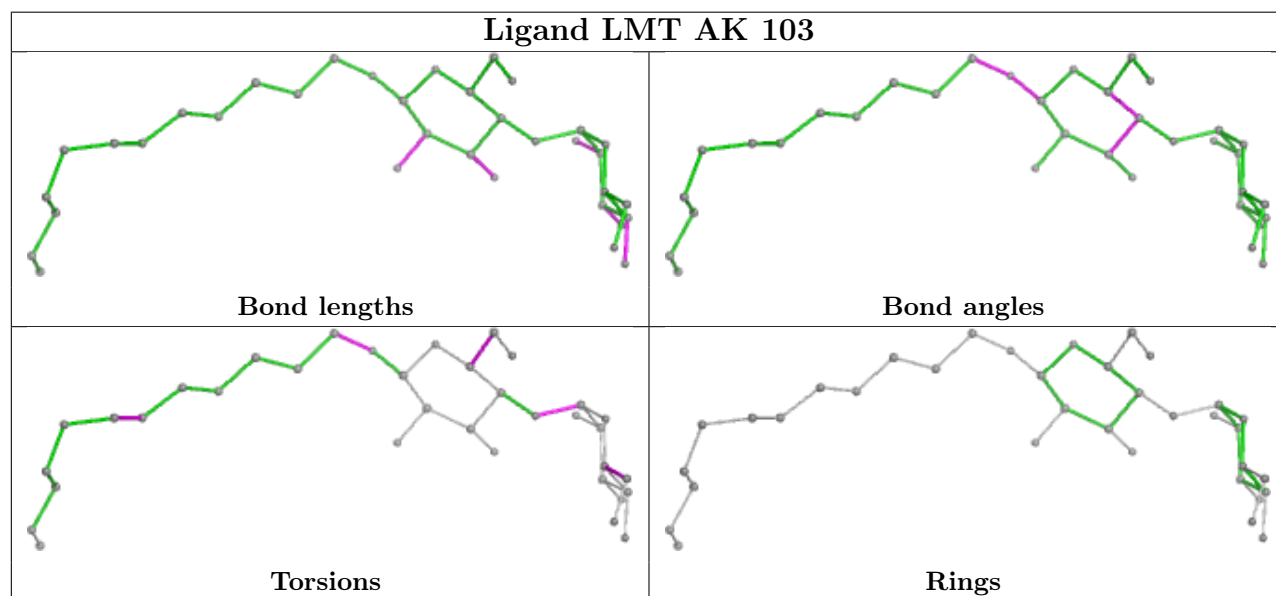
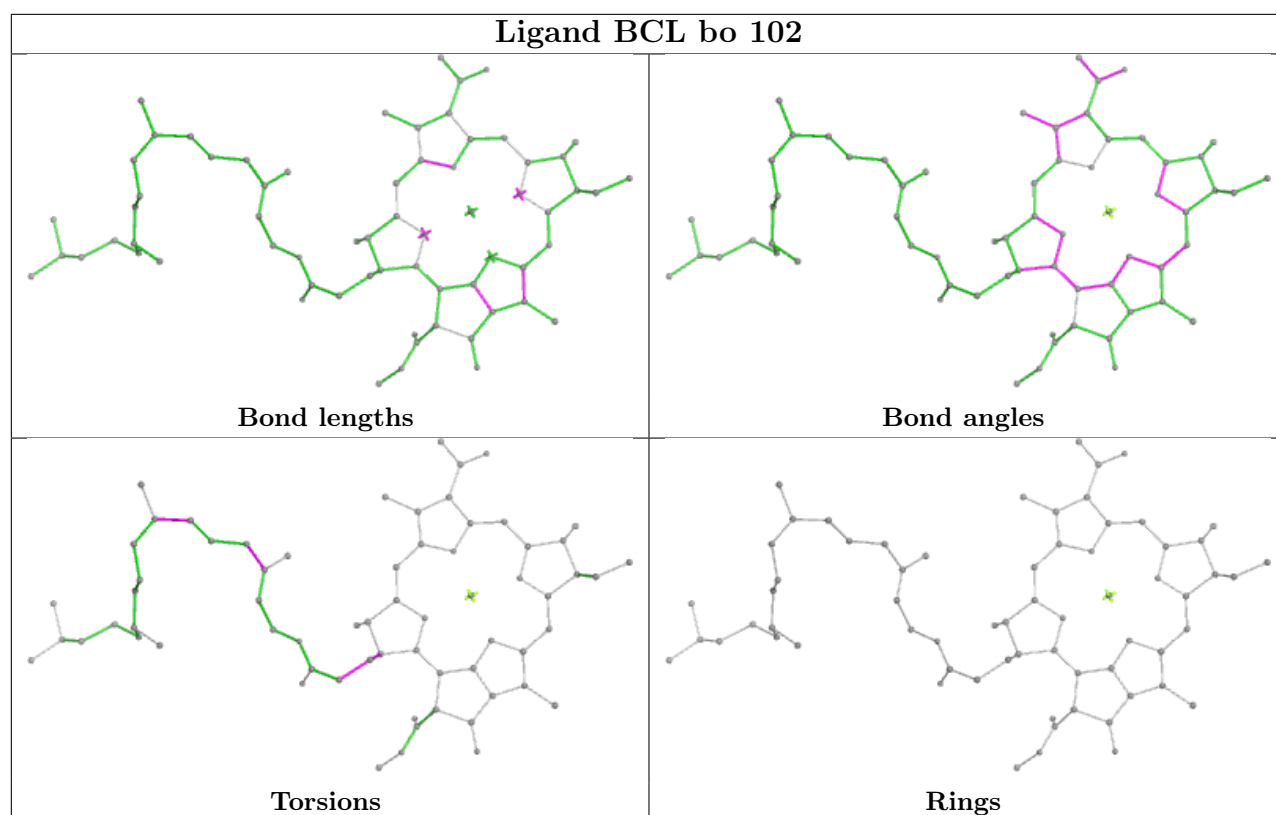
Ligand V7N be 102

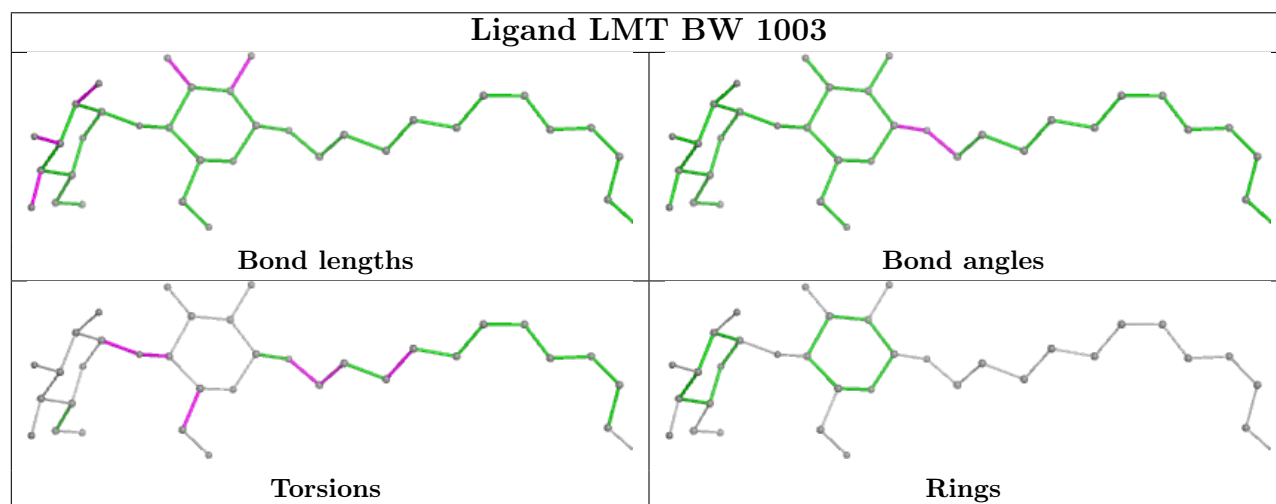
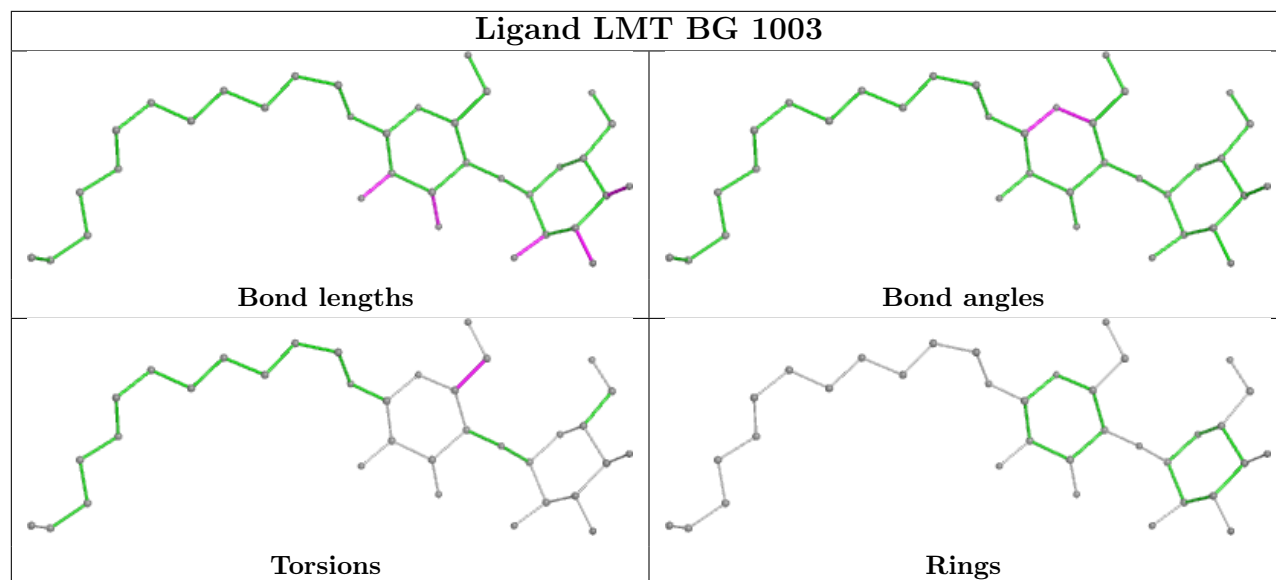




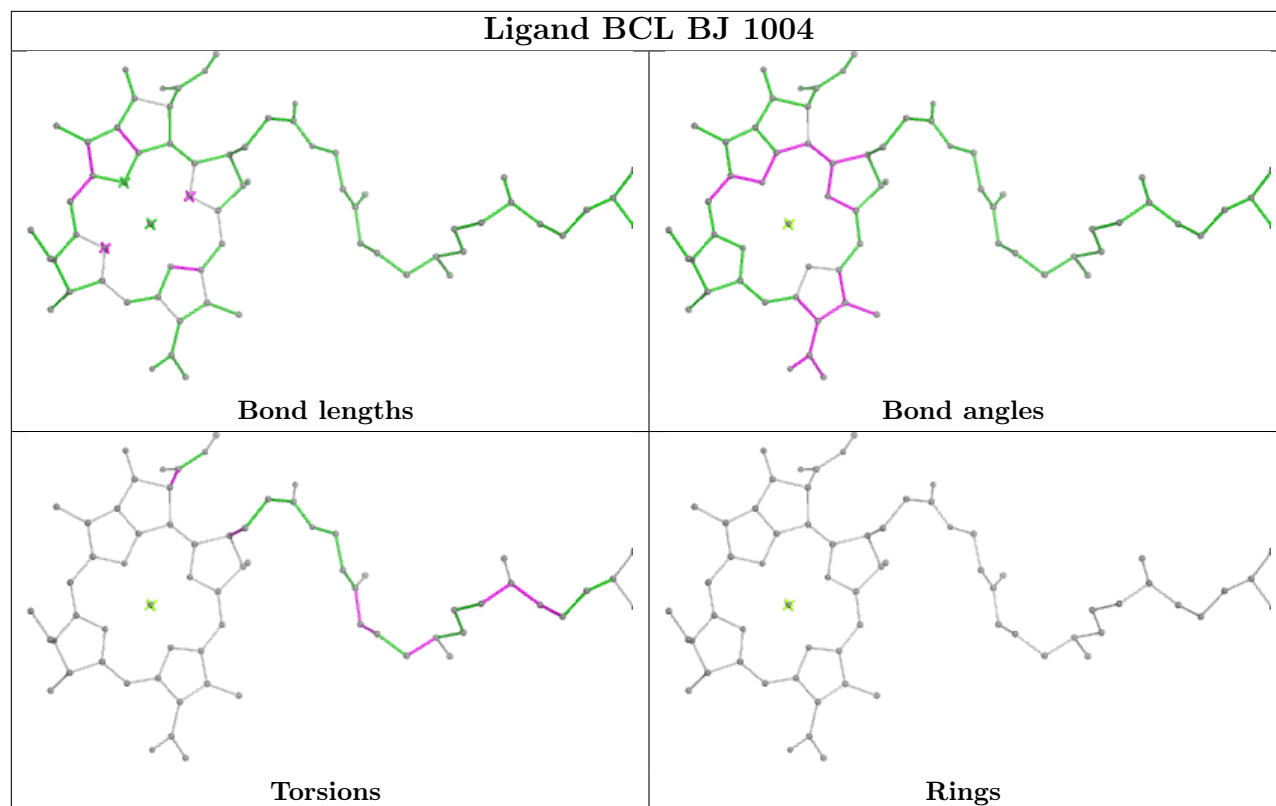
Ligand LMT BW 1002**Ligand BCL bm 102**



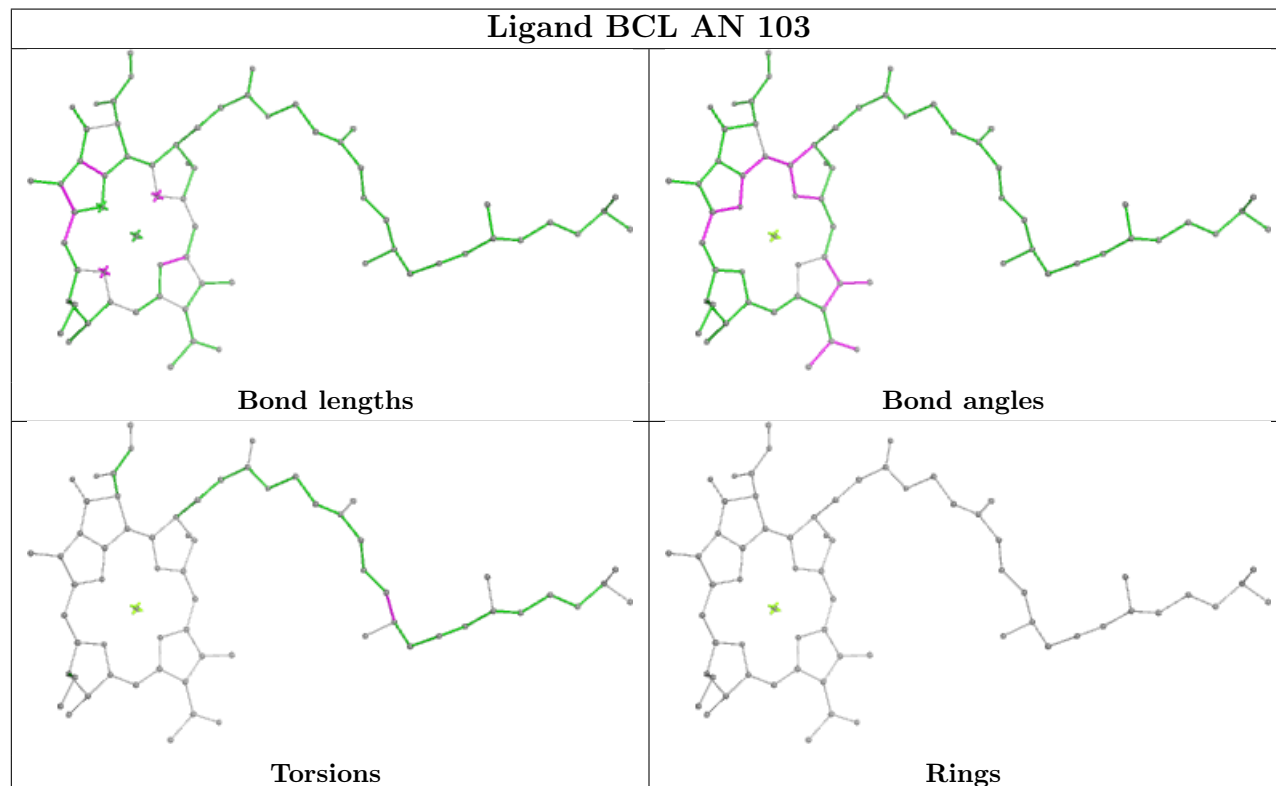


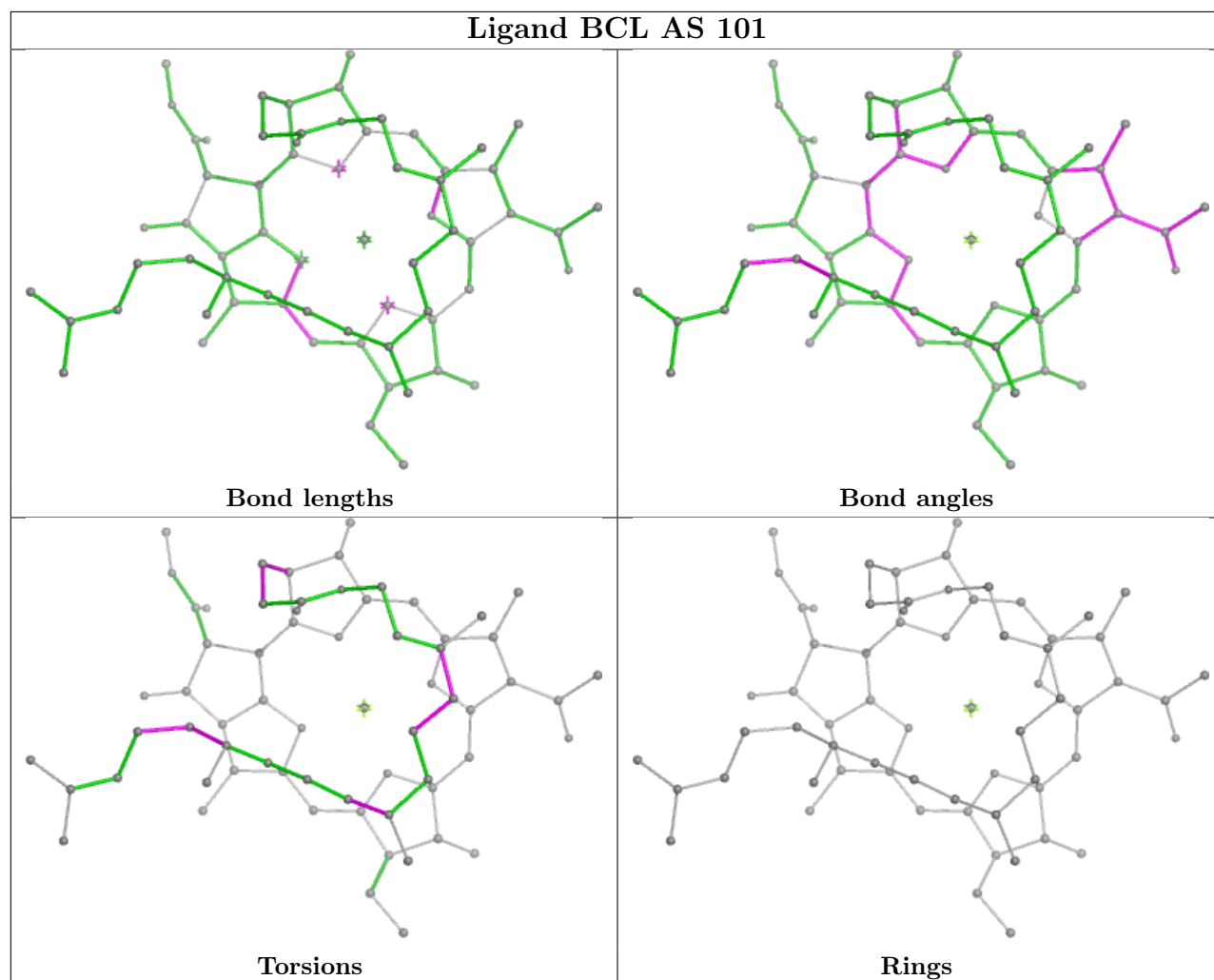
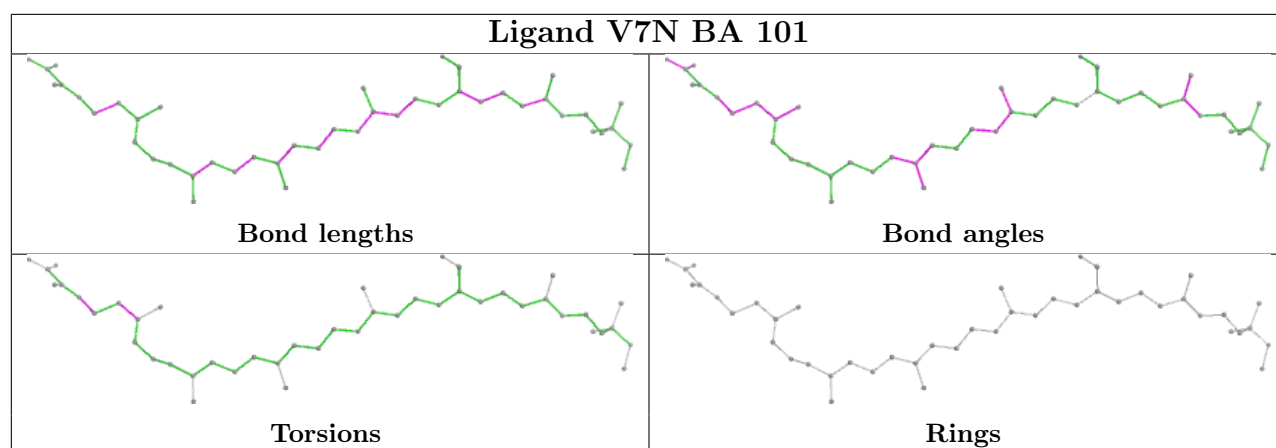


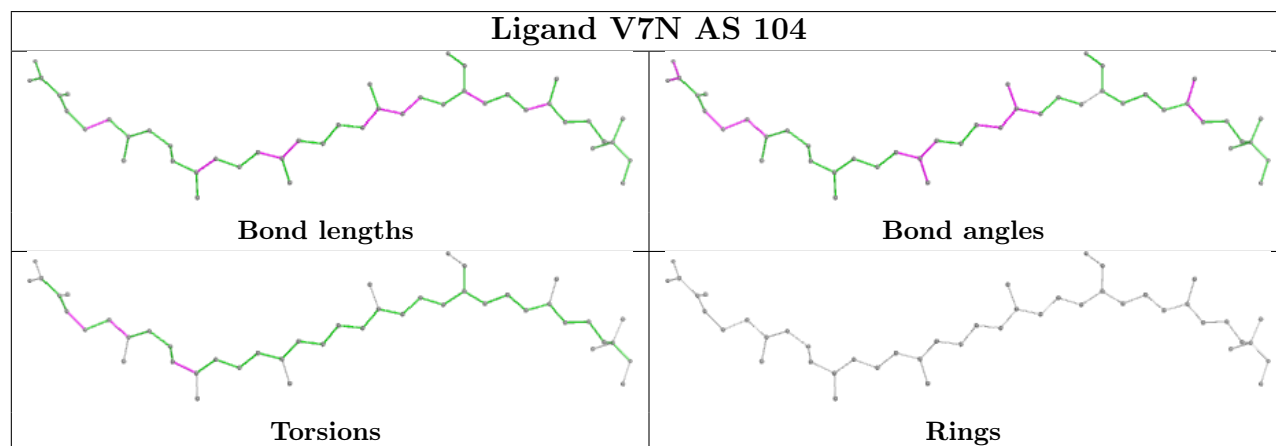
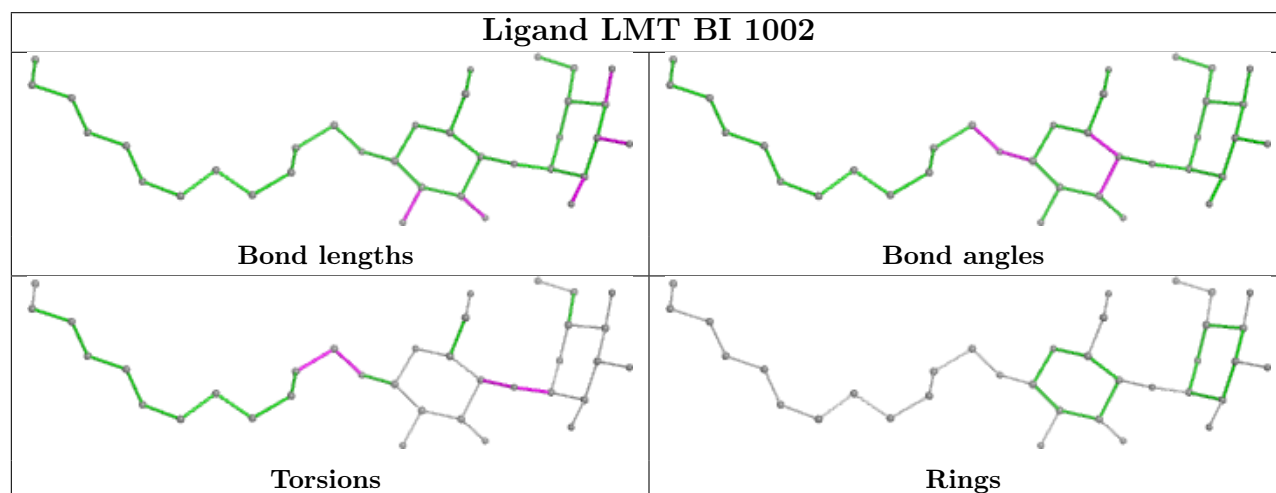
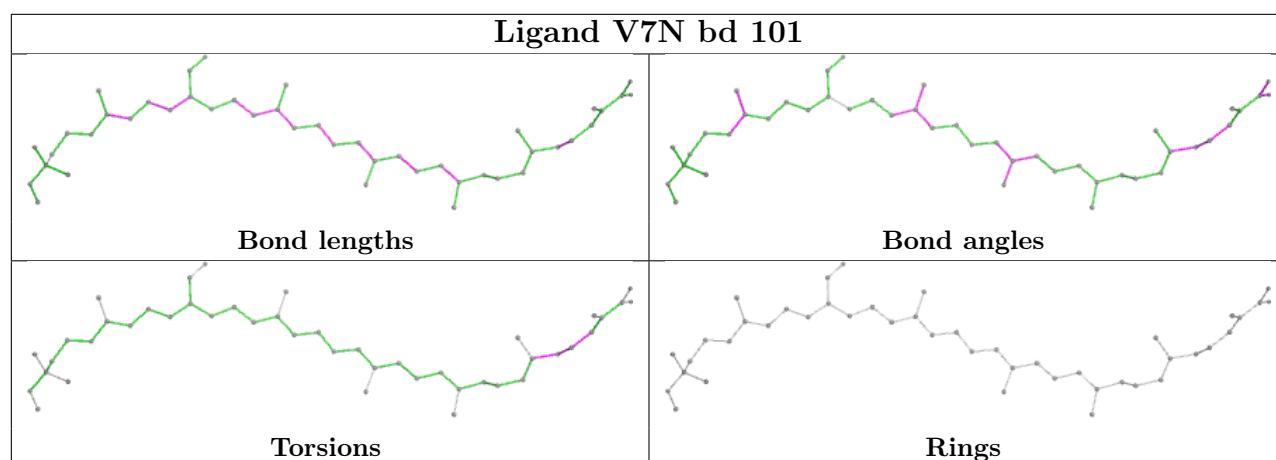
Ligand BCL BJ 1004

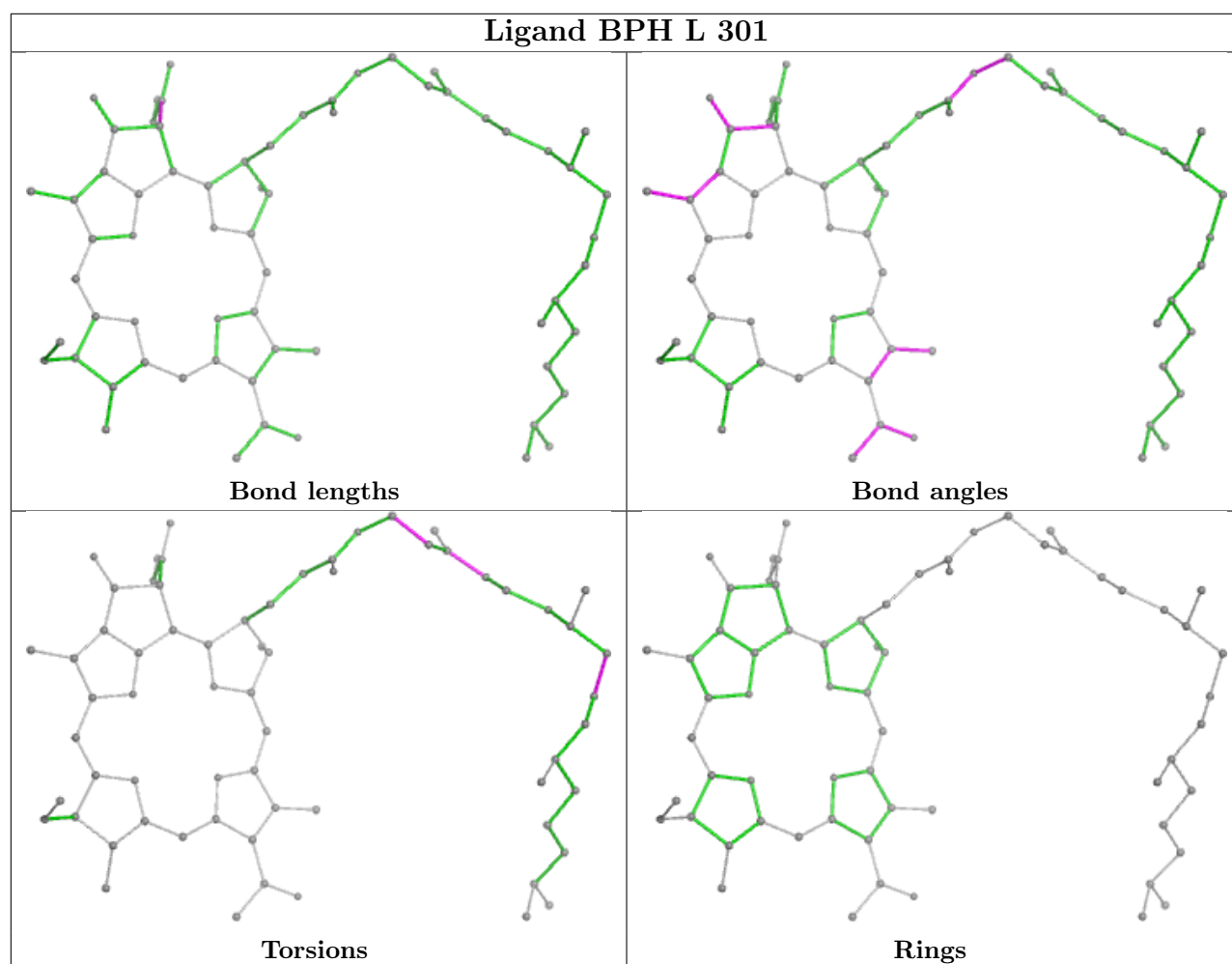
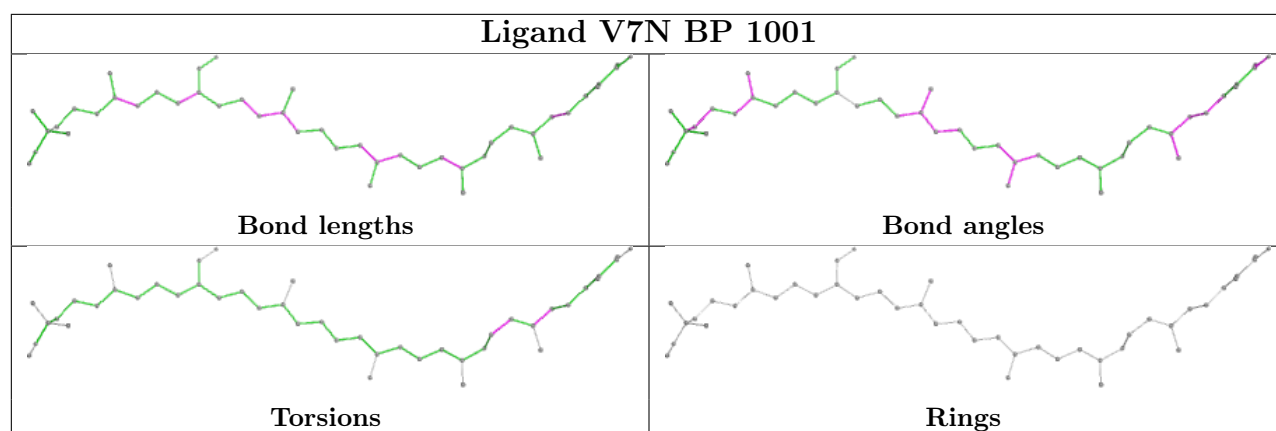


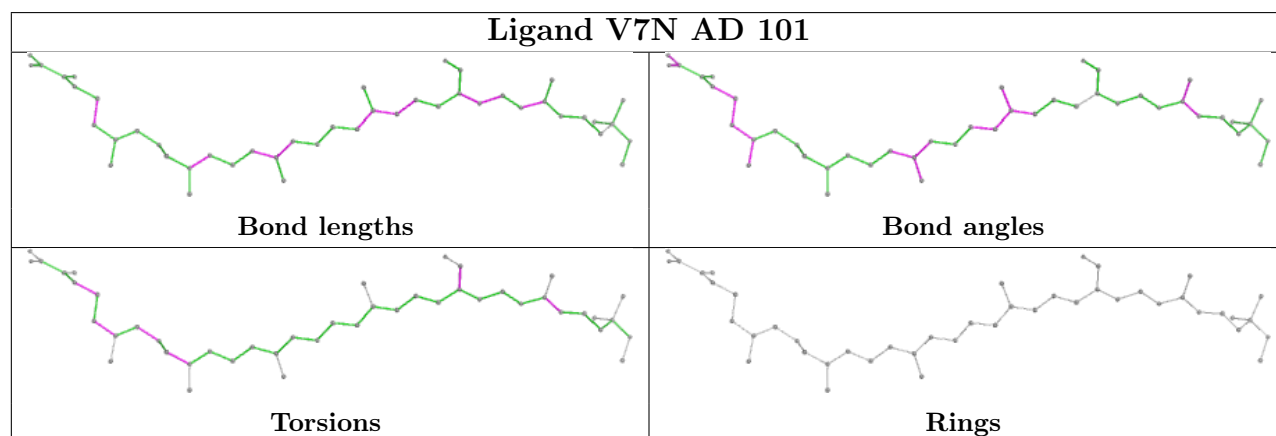
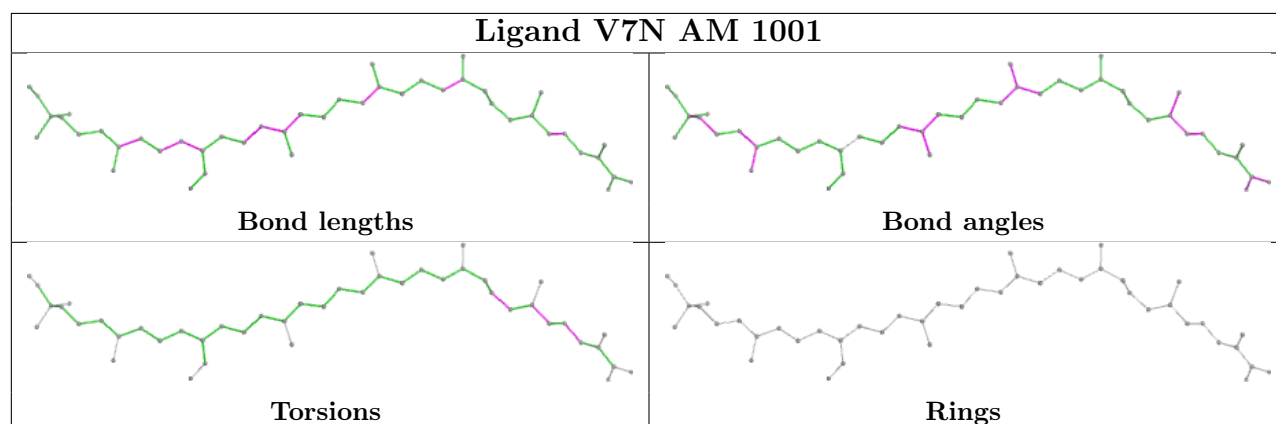
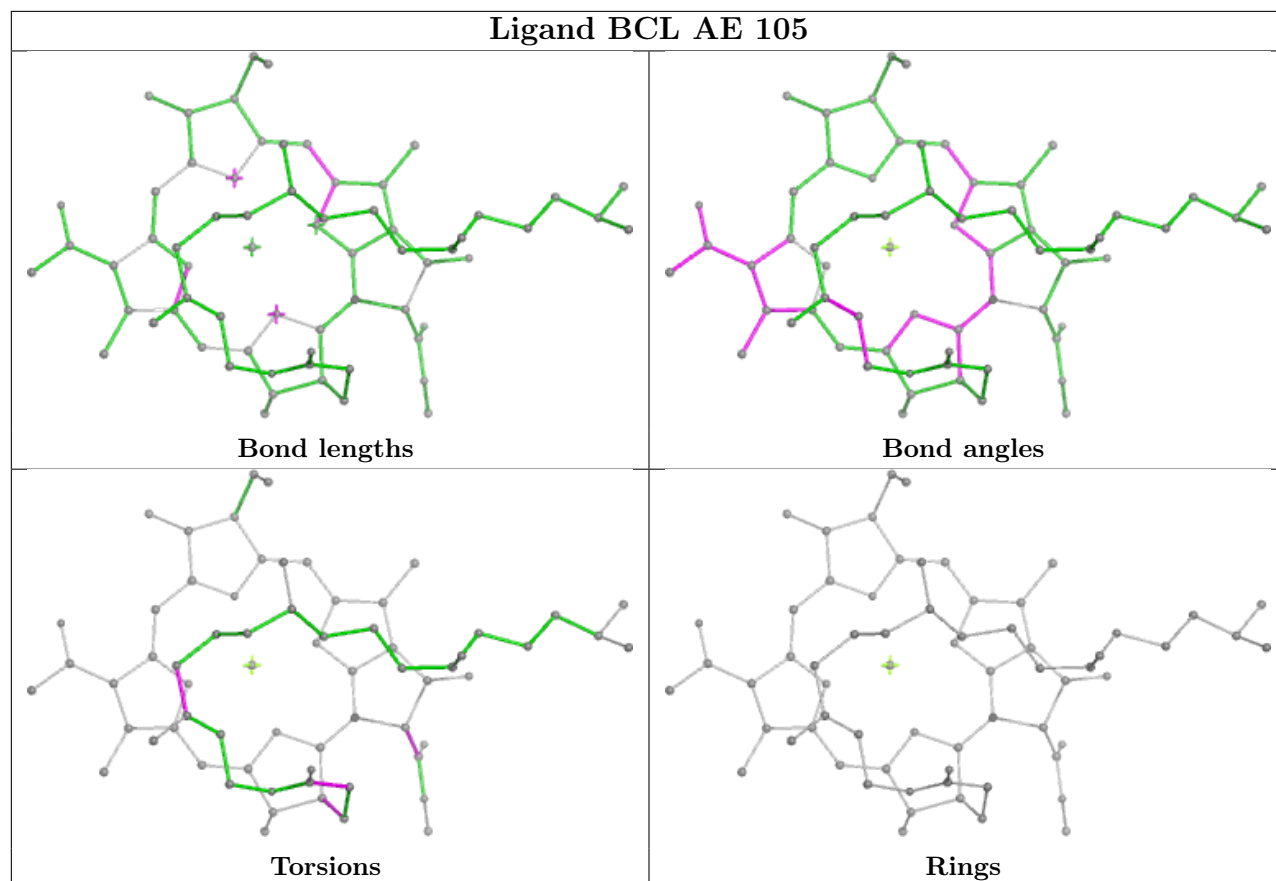
Ligand BCL AN 103

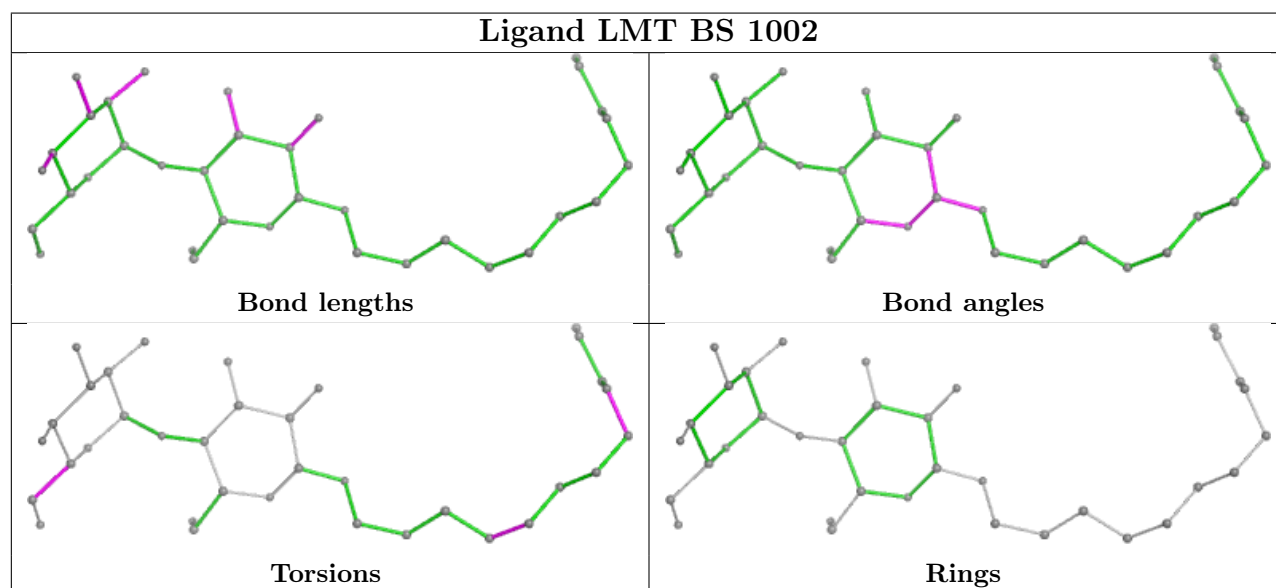
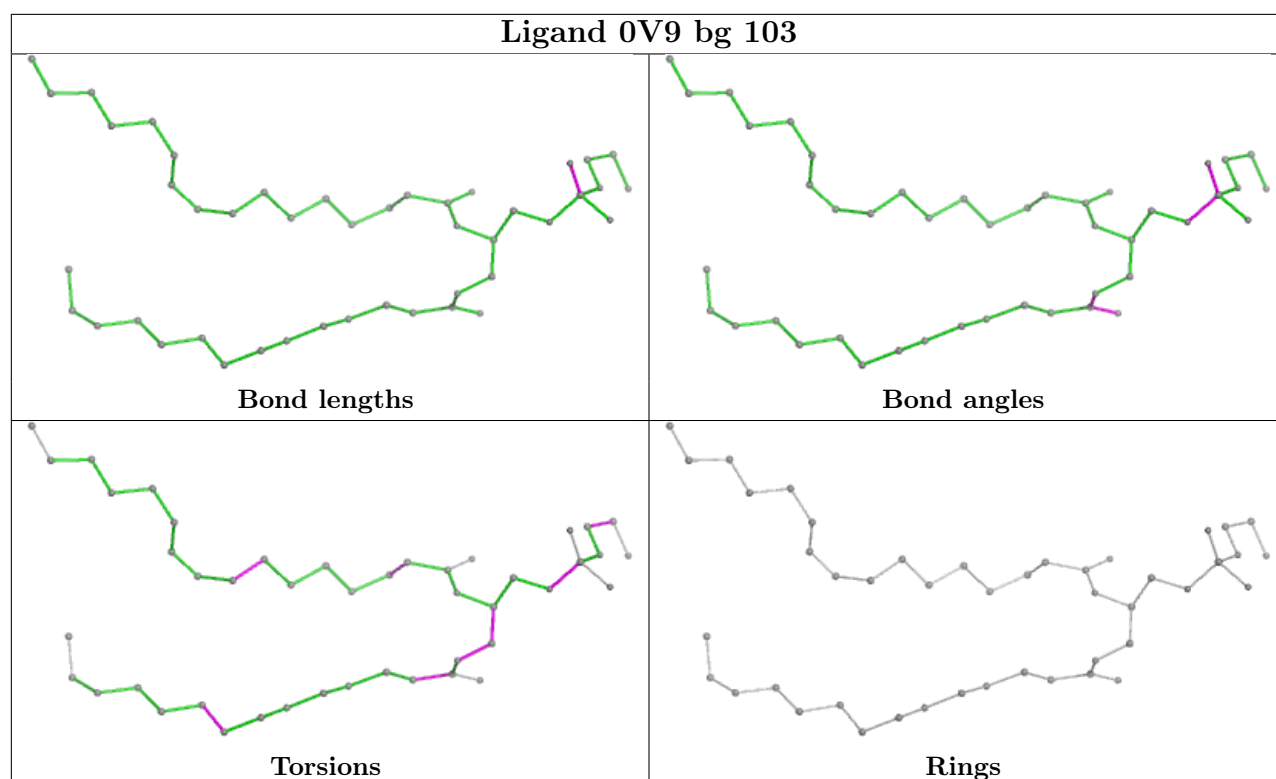


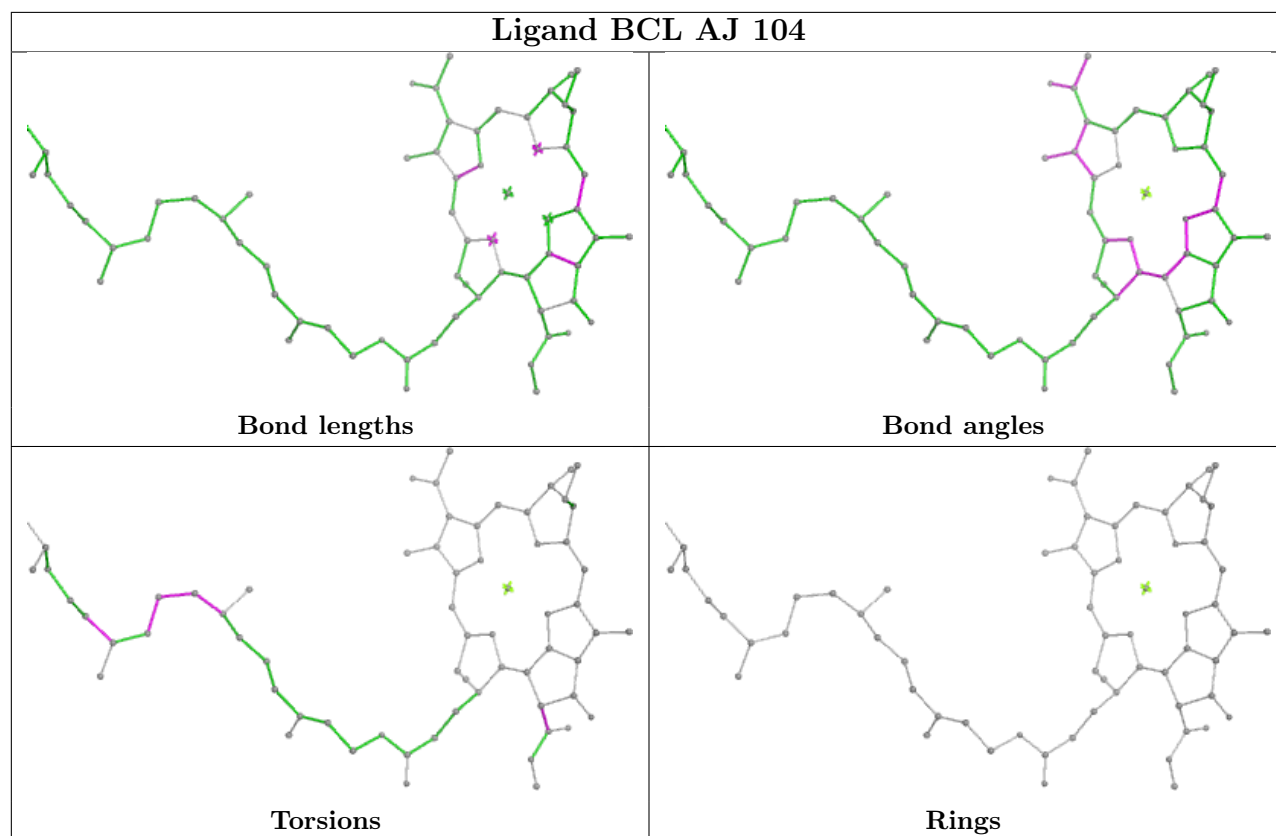
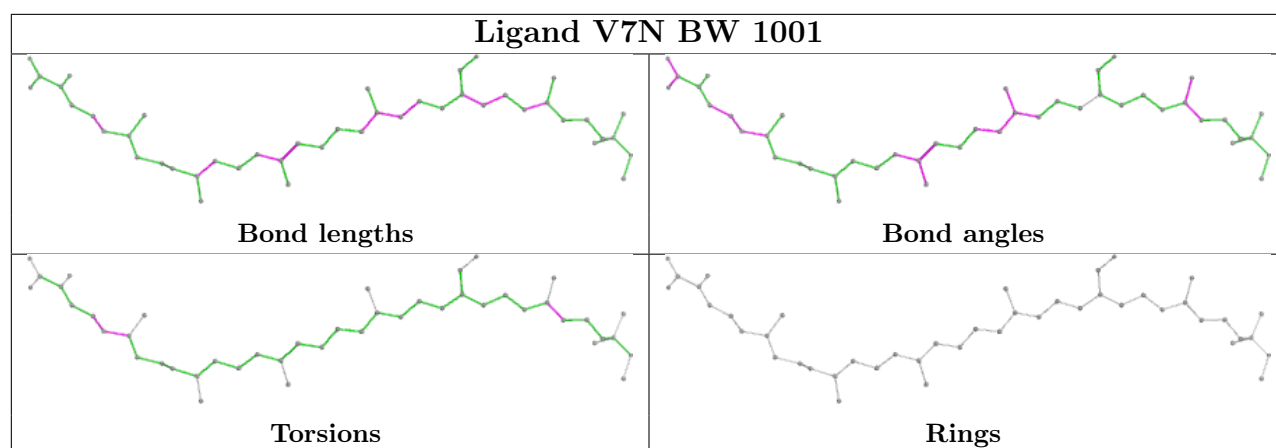


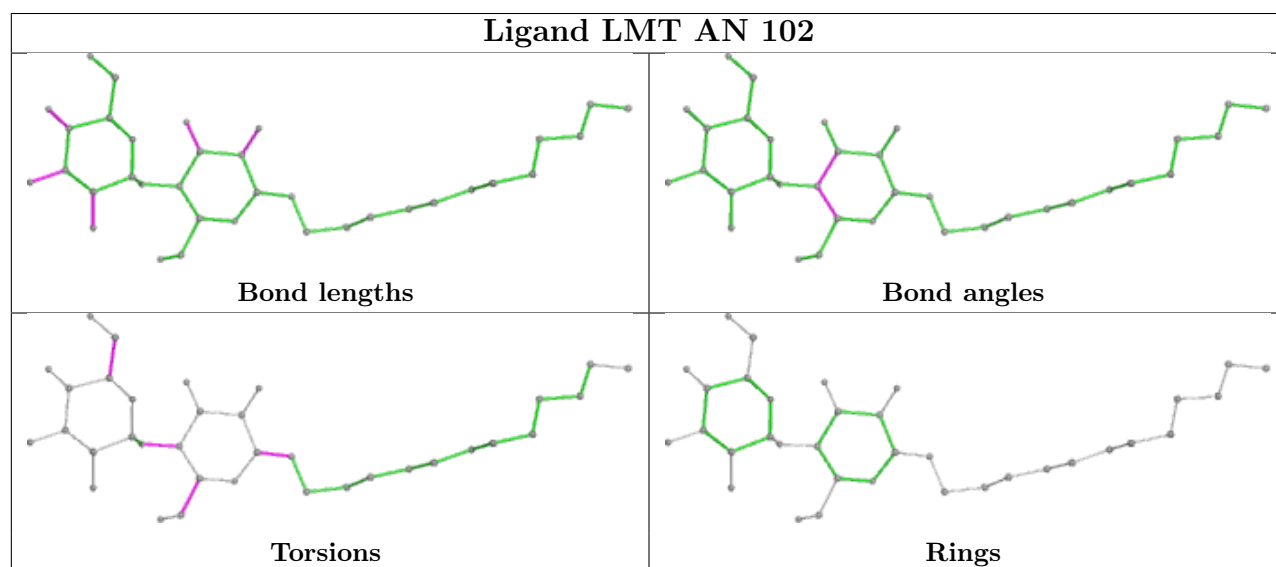
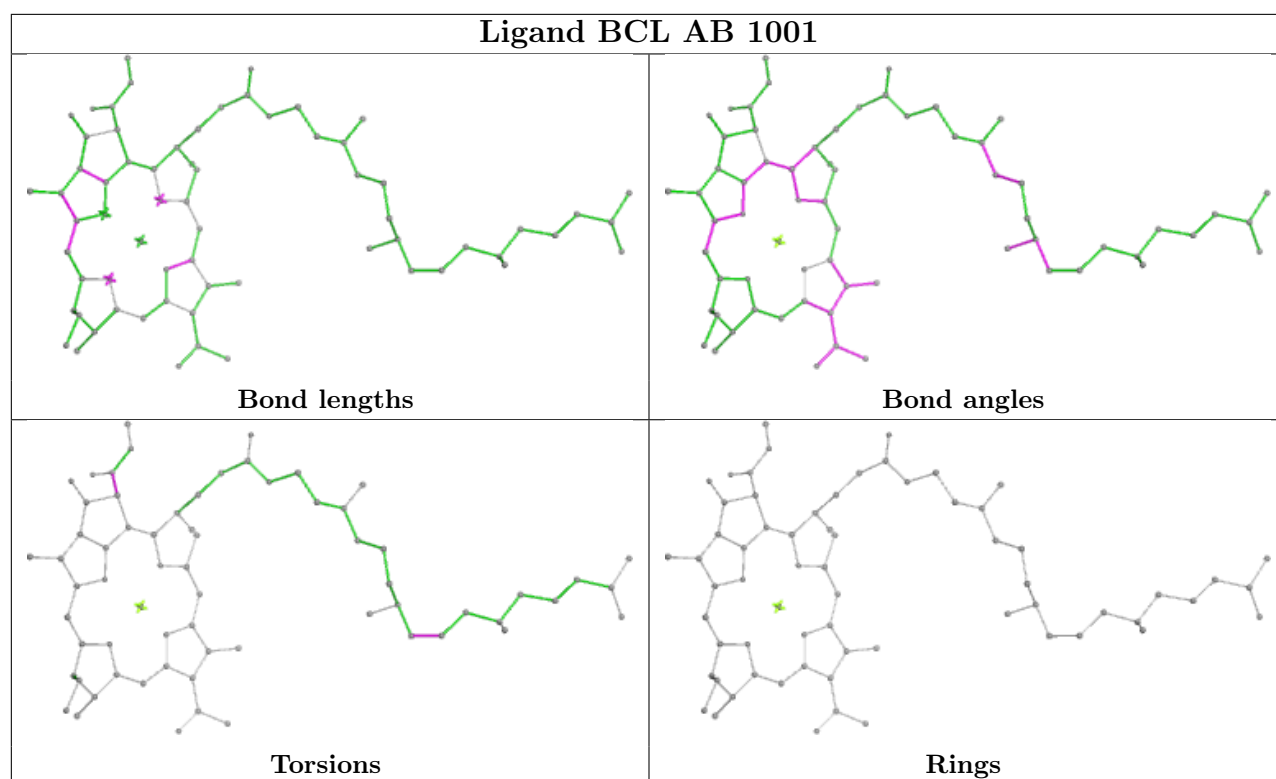




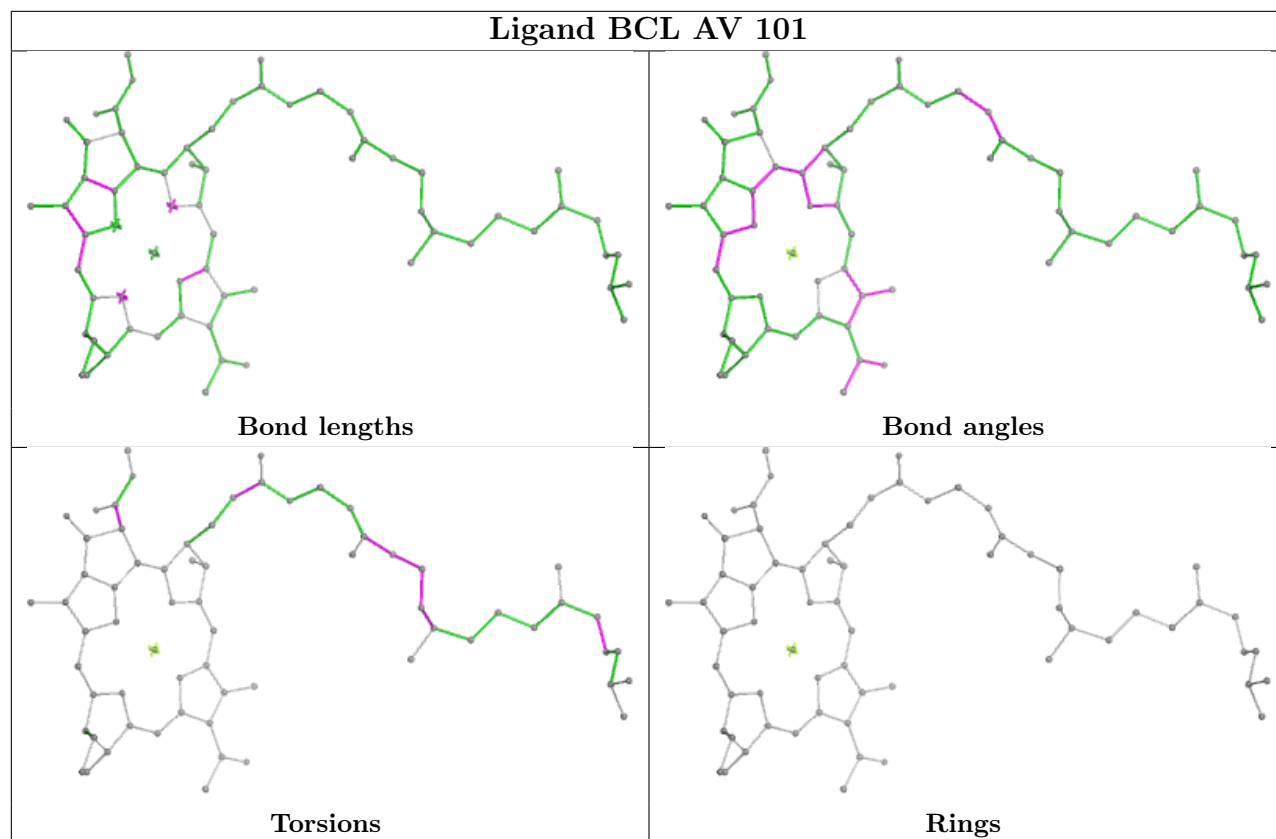




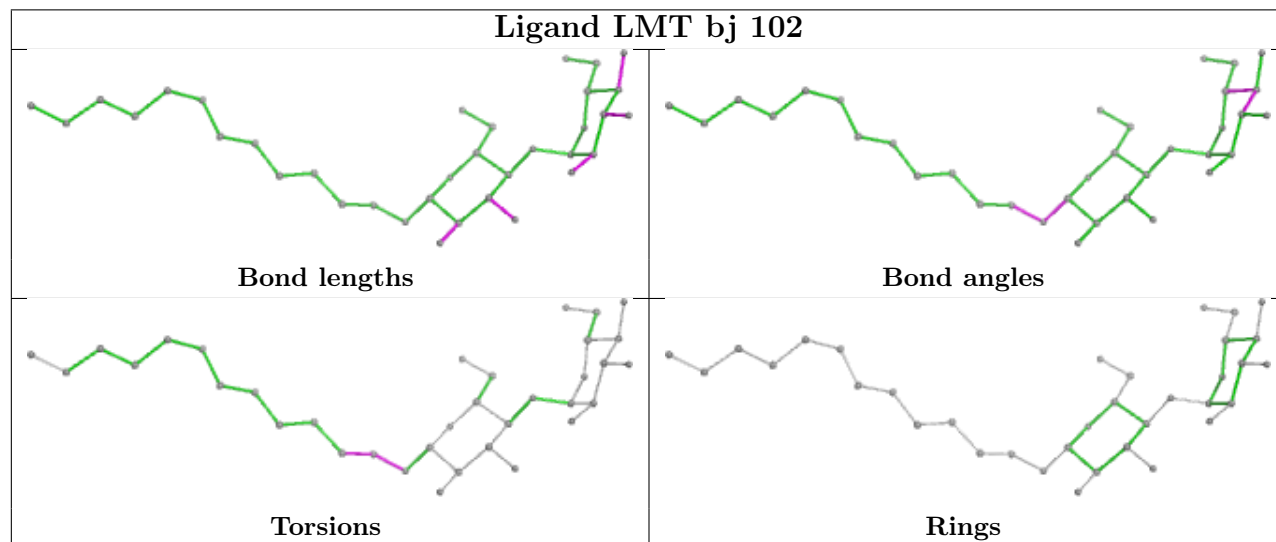




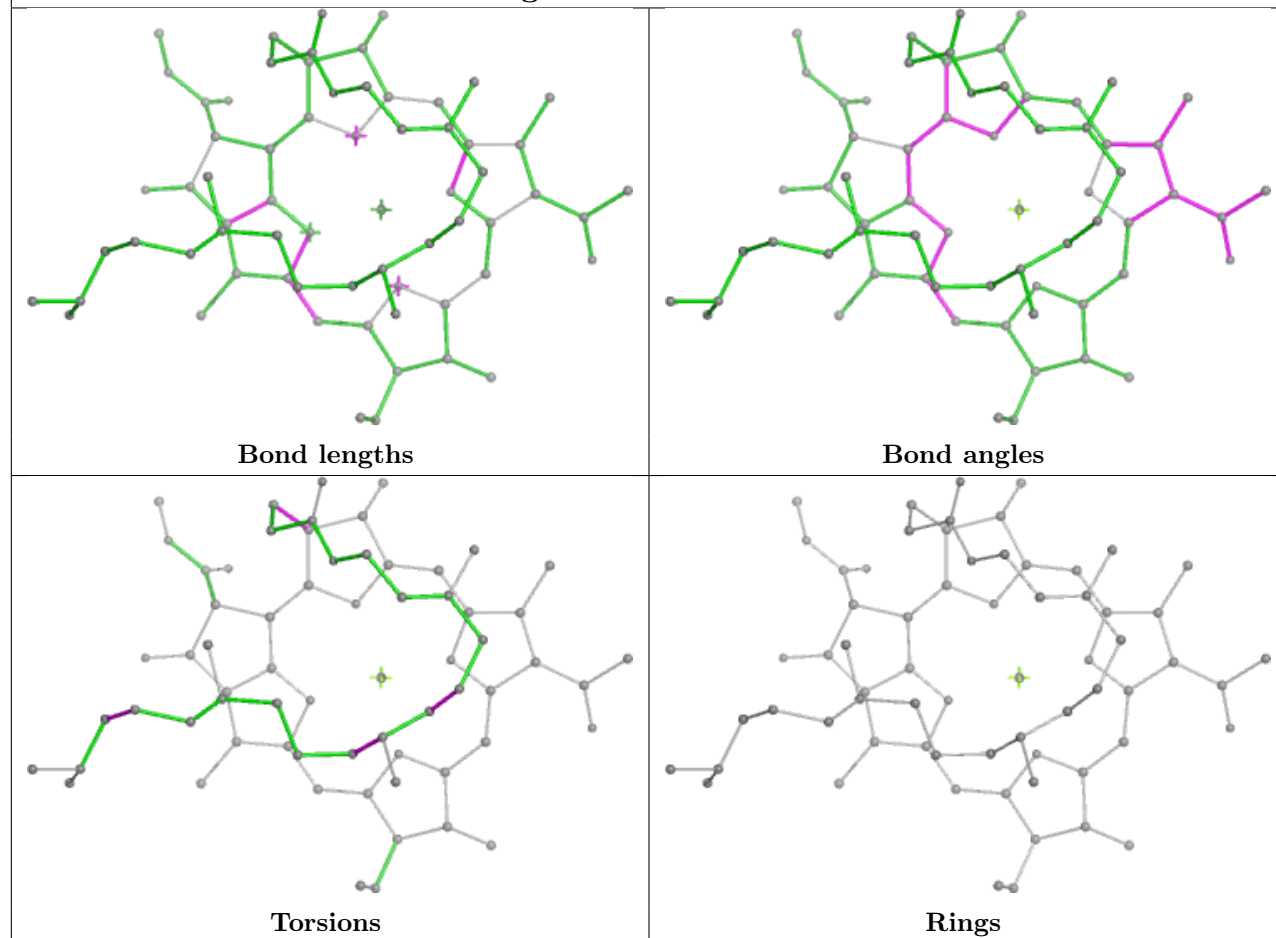
Ligand BCL AV 101



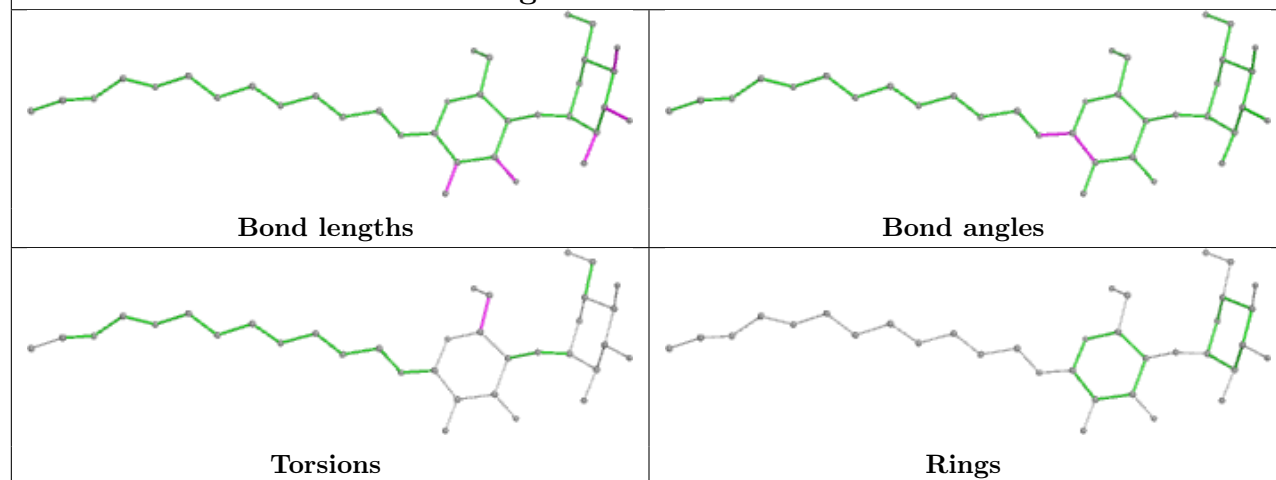
Ligand LMT bj 102

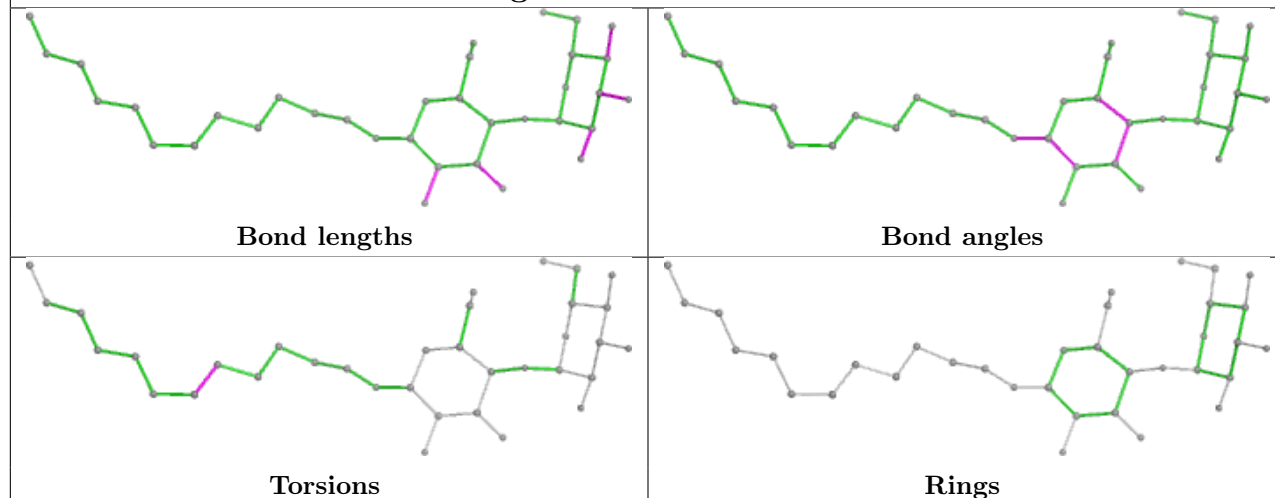
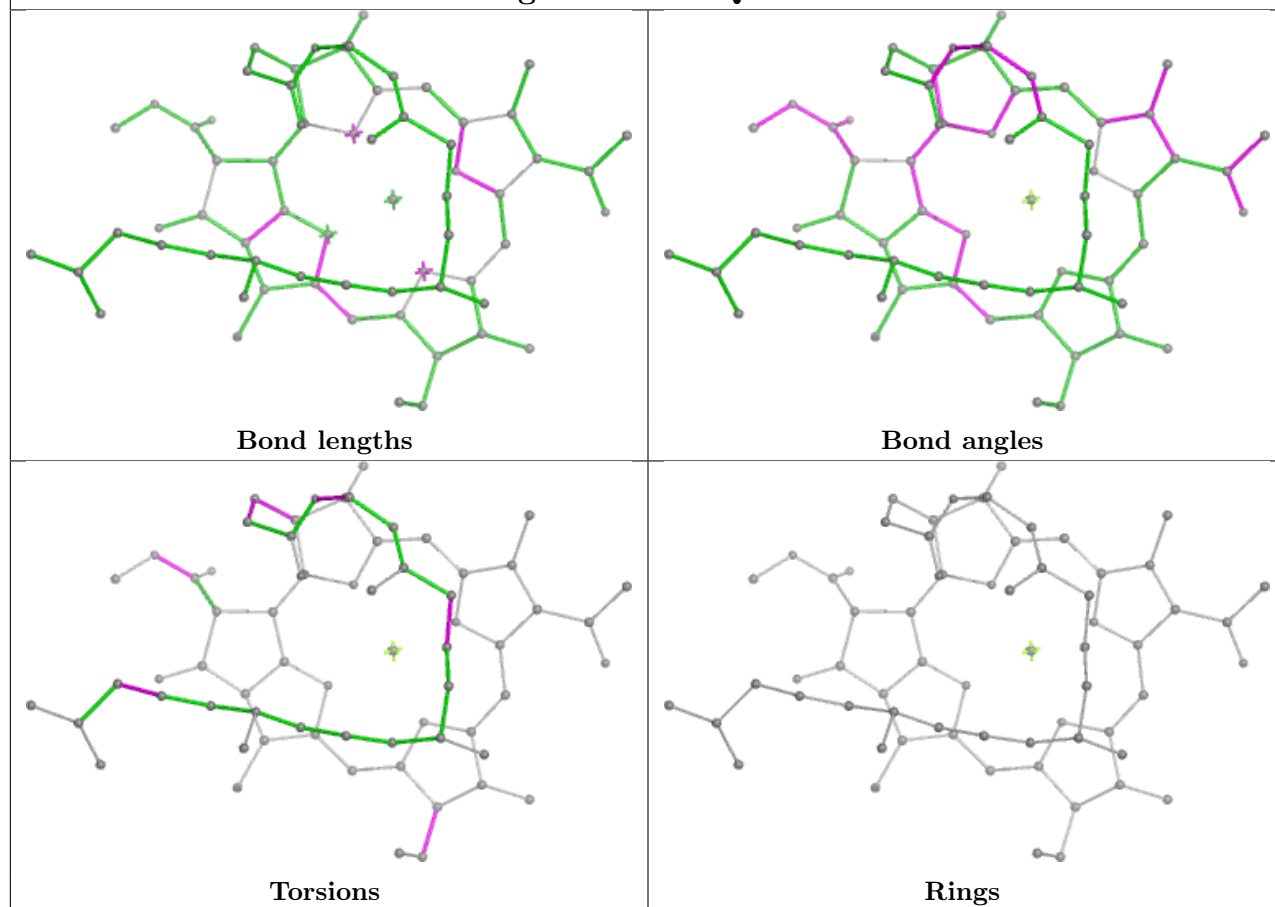


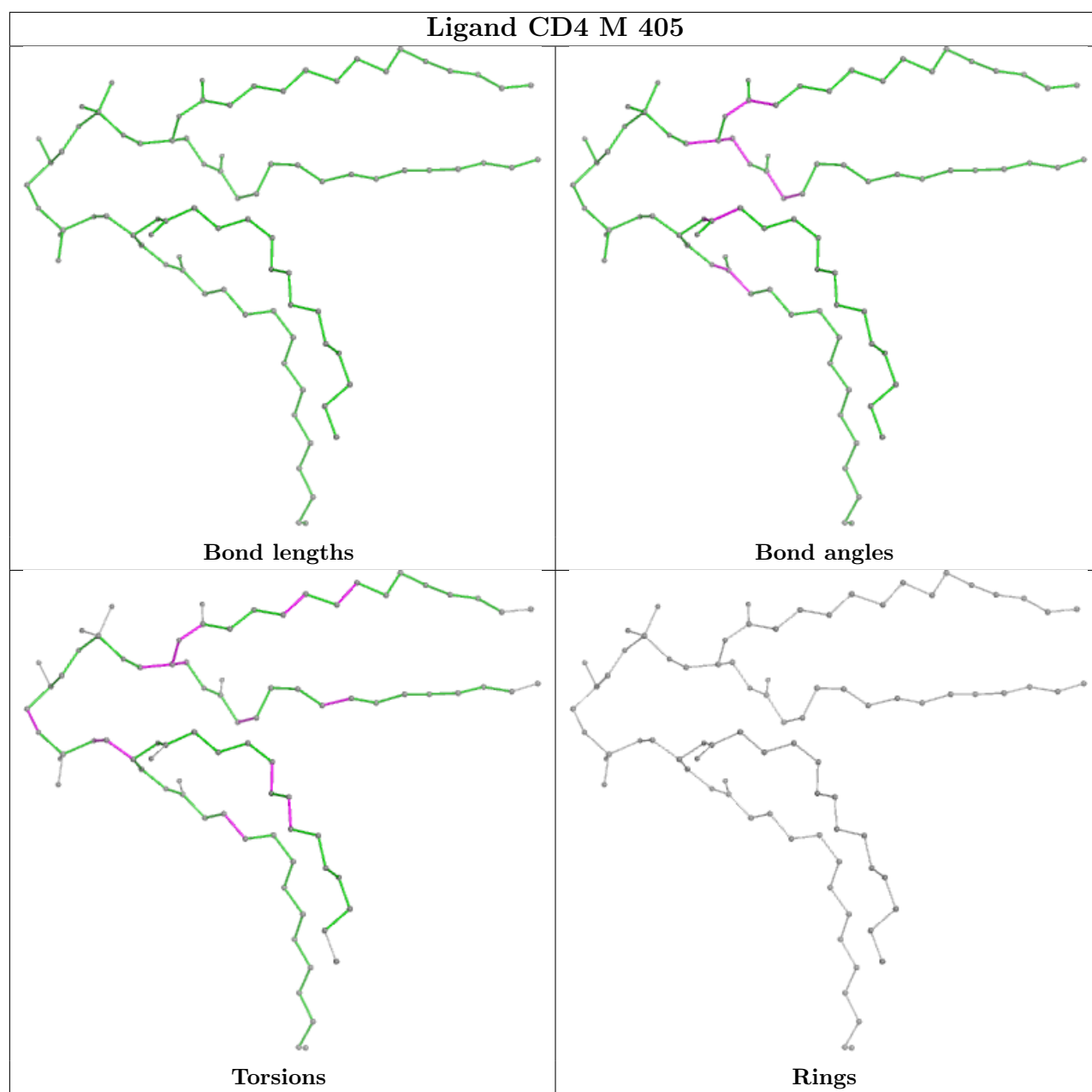
Ligand BCL AV 103



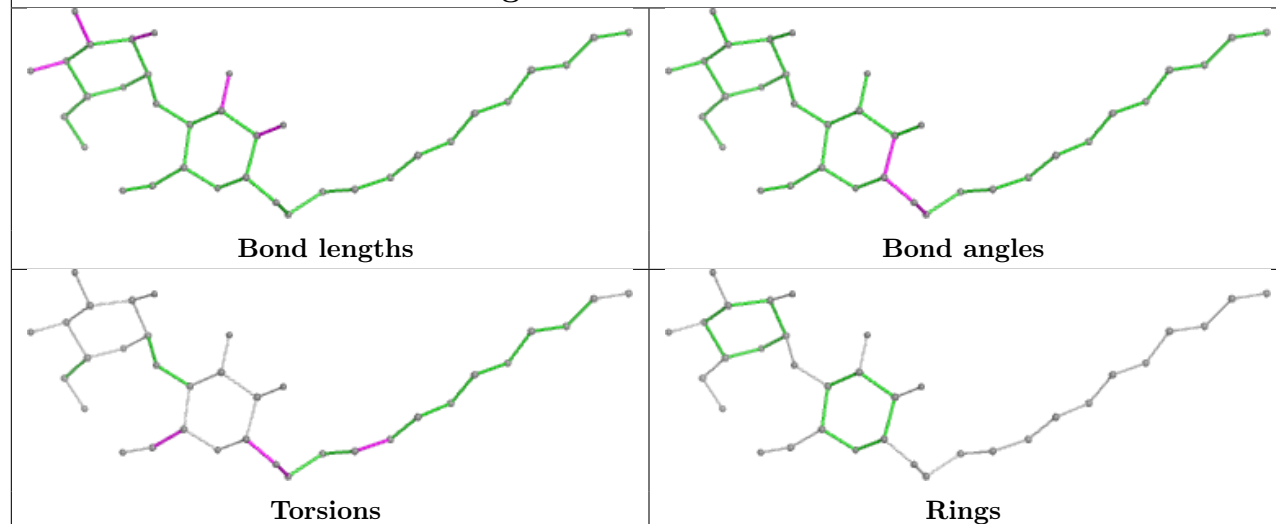
Ligand LMT AJ 101



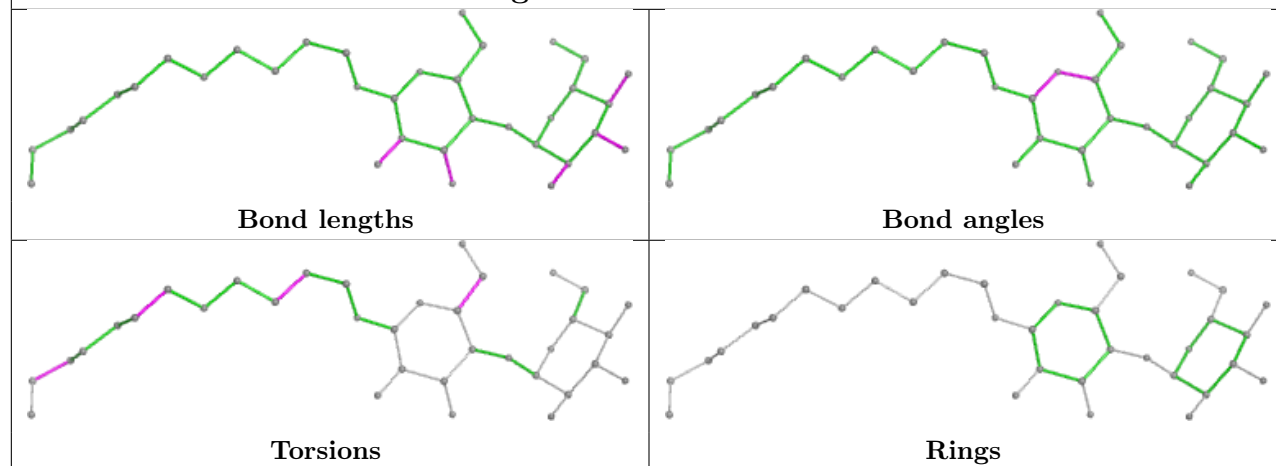
Ligand LMT BJ 1002**Ligand BCL AQ 104**

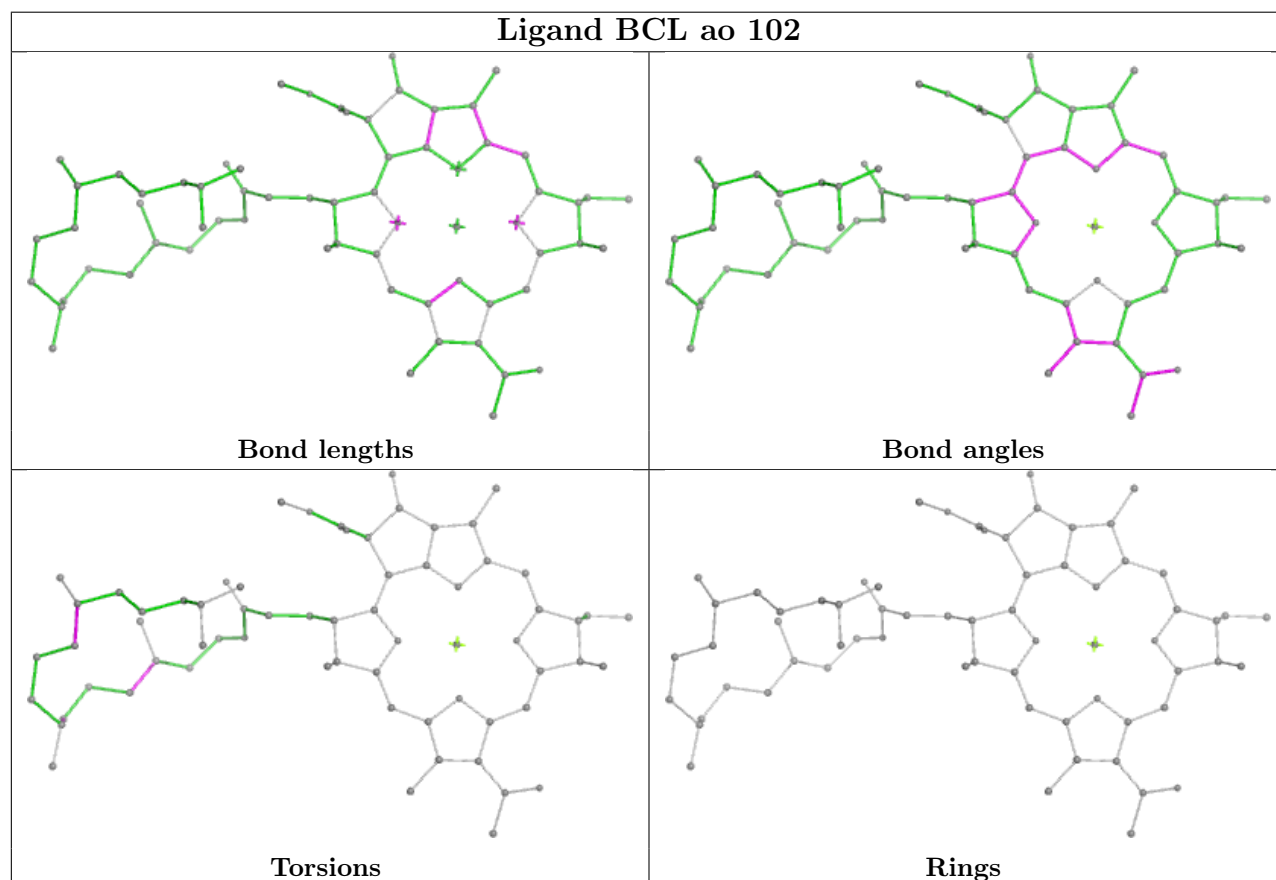
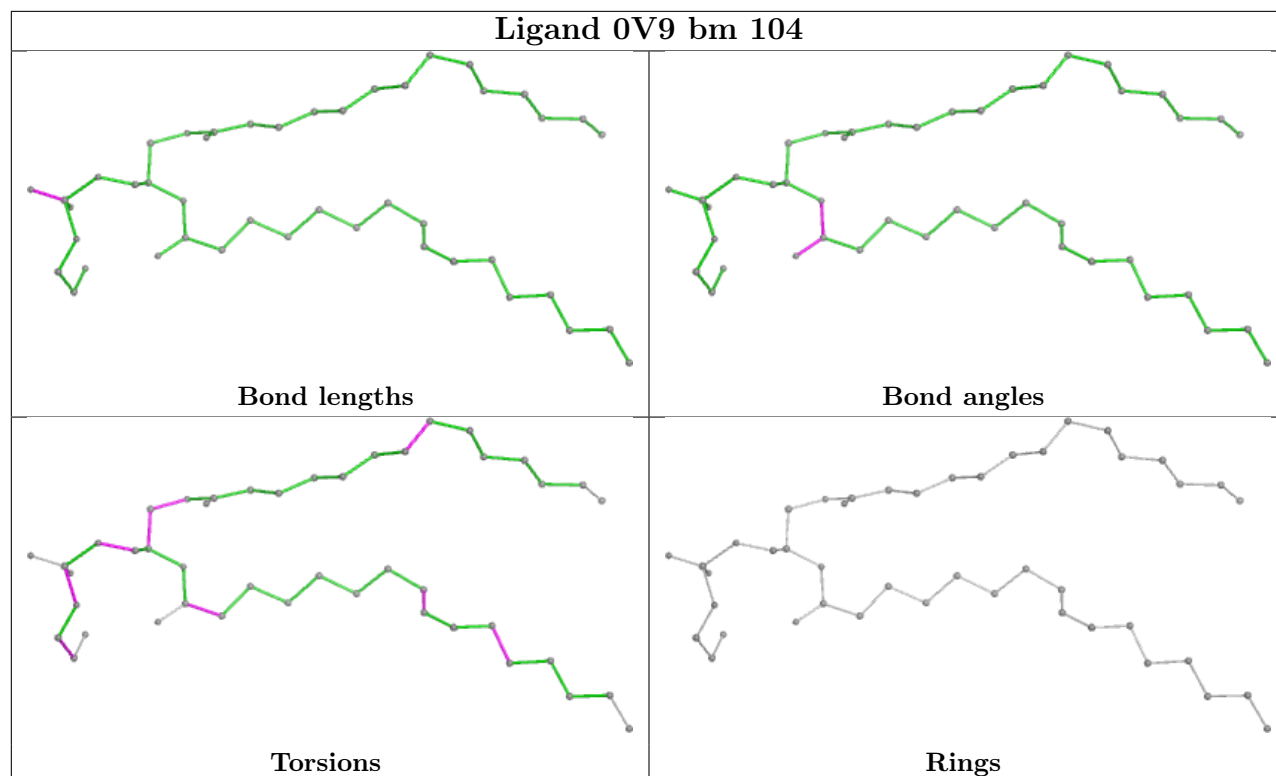


Ligand LMT BW 1004

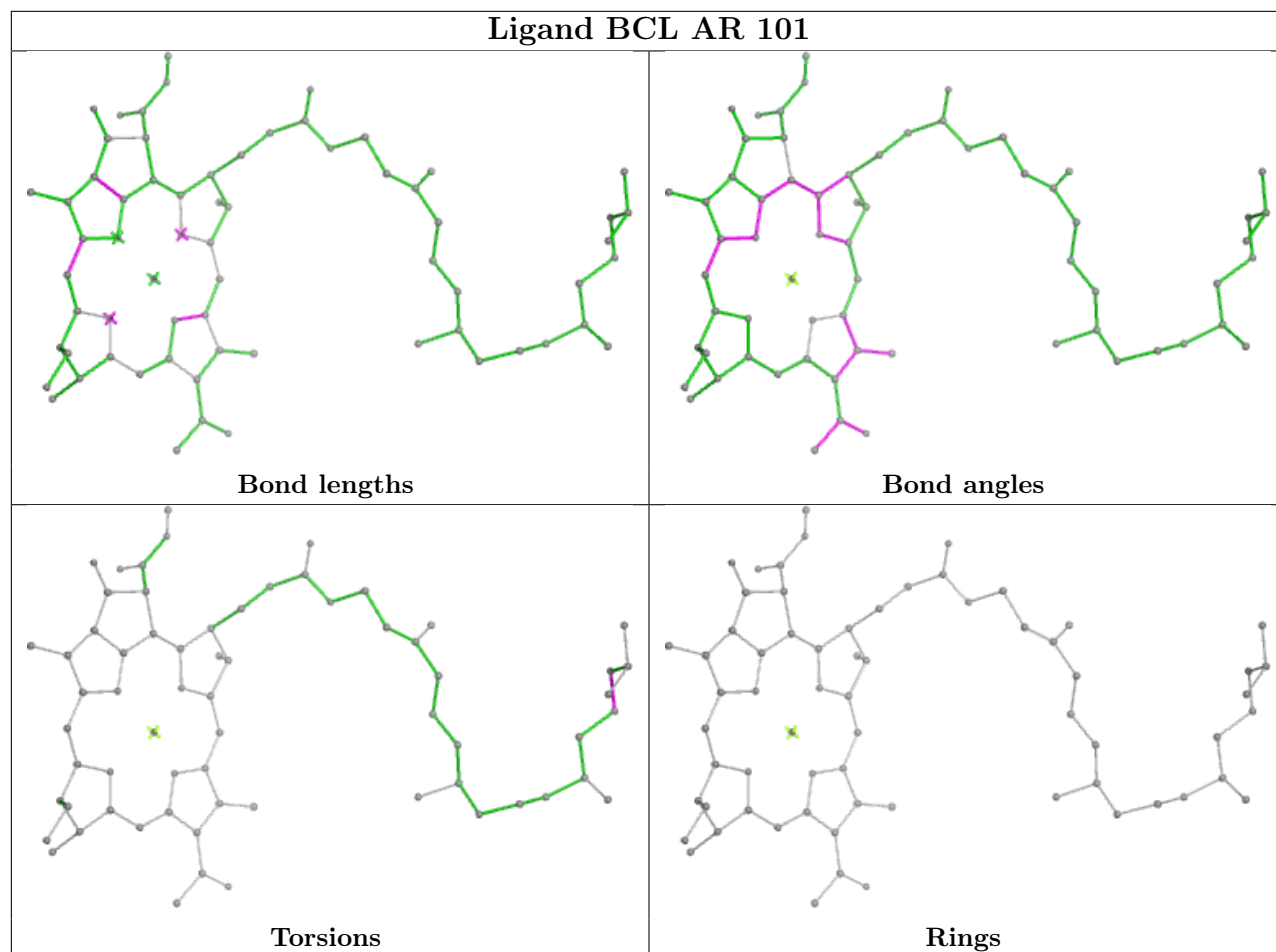


Ligand LMT BJ 1006

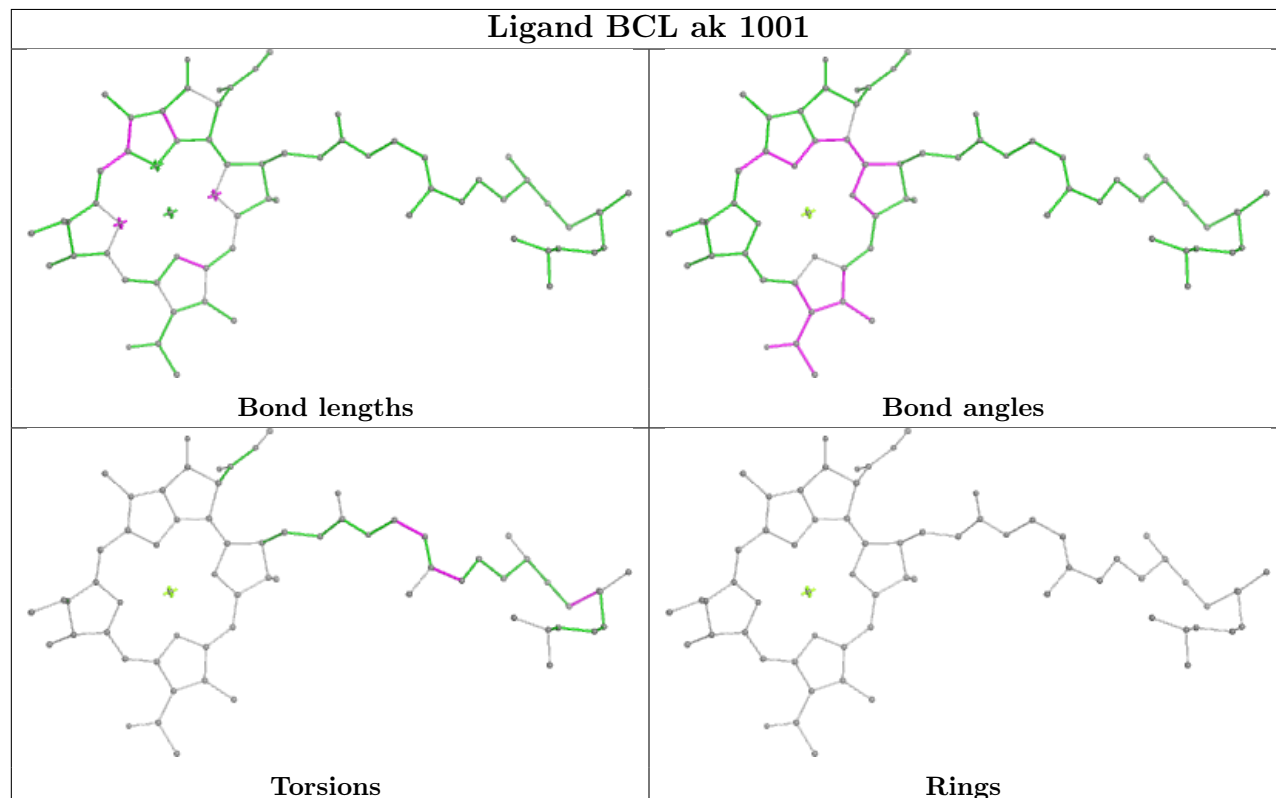


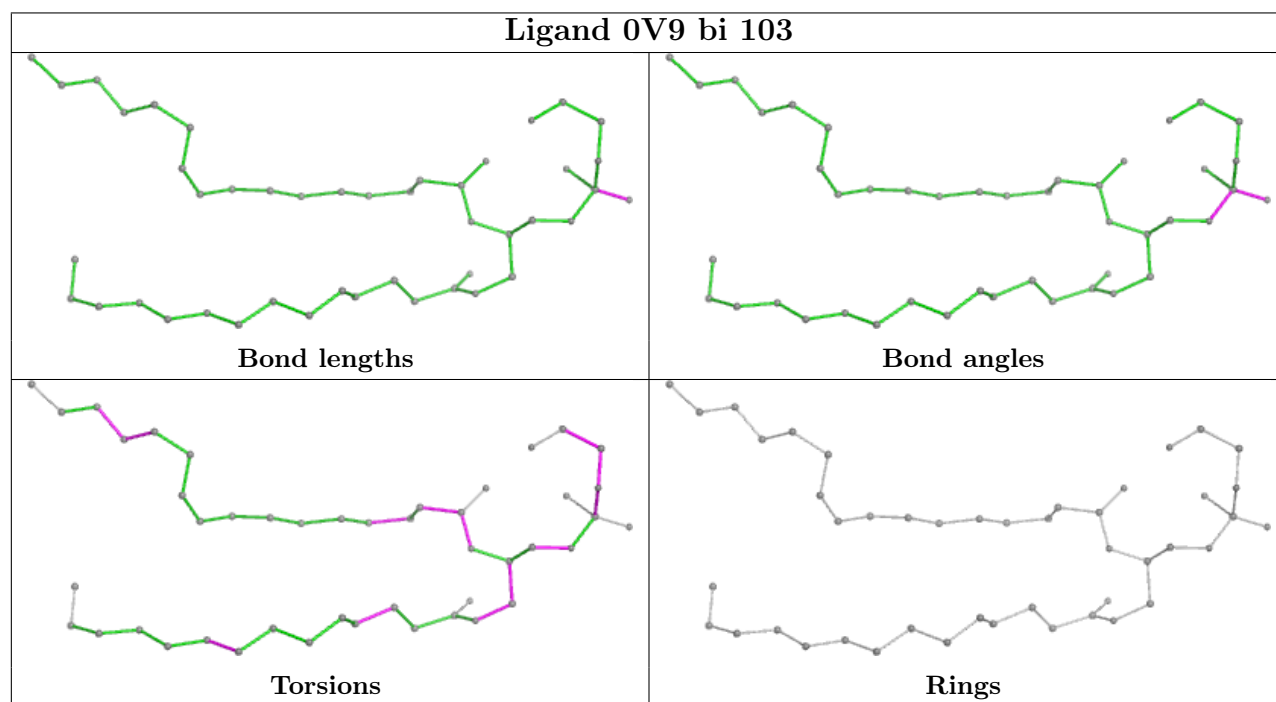
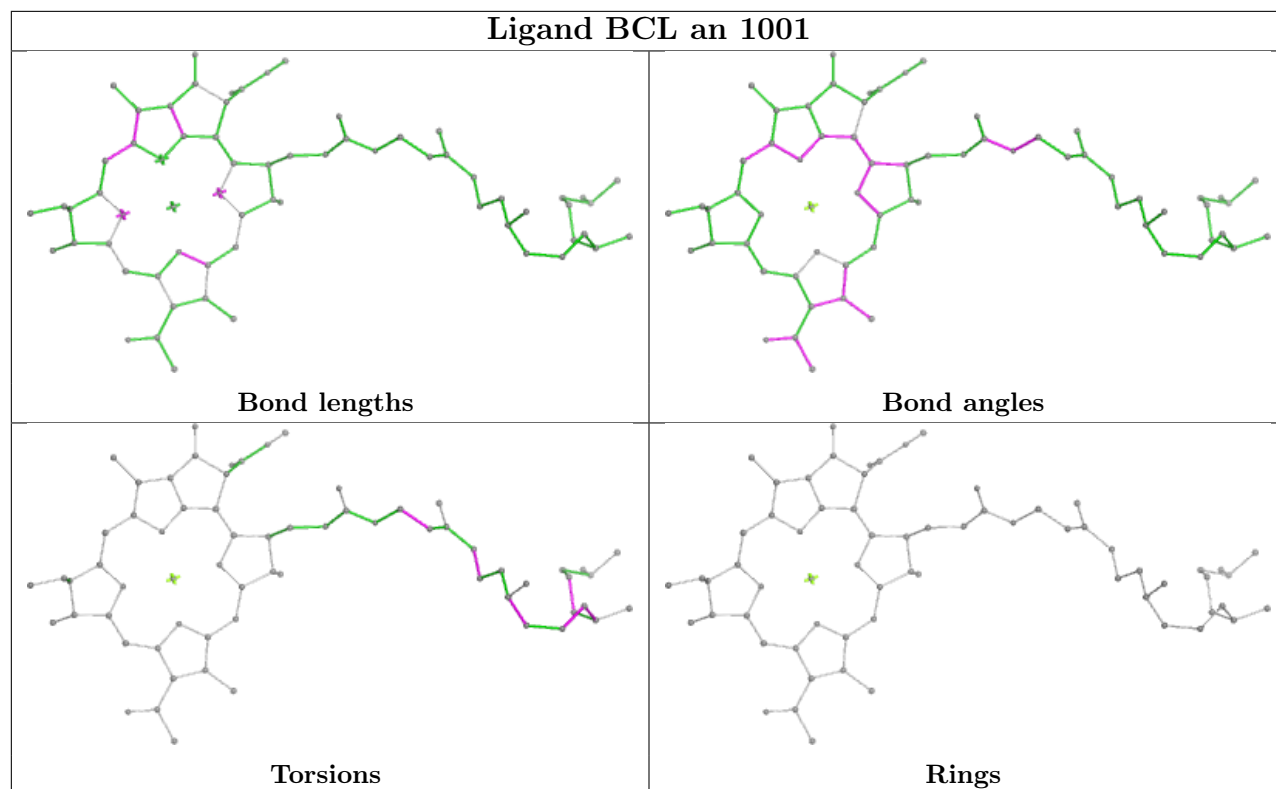


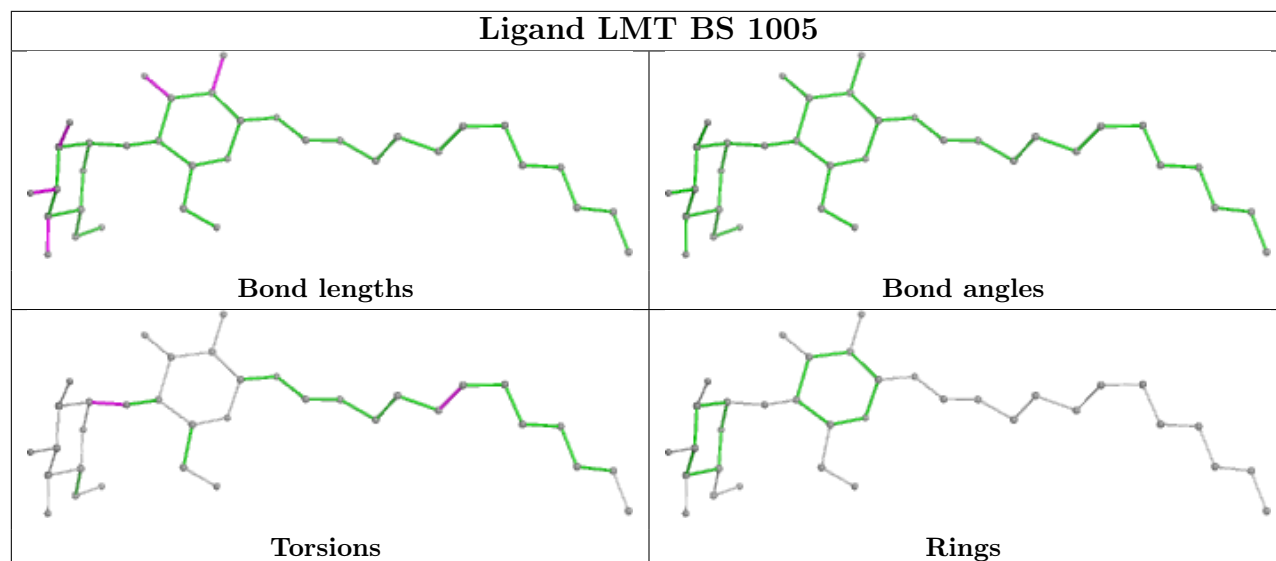
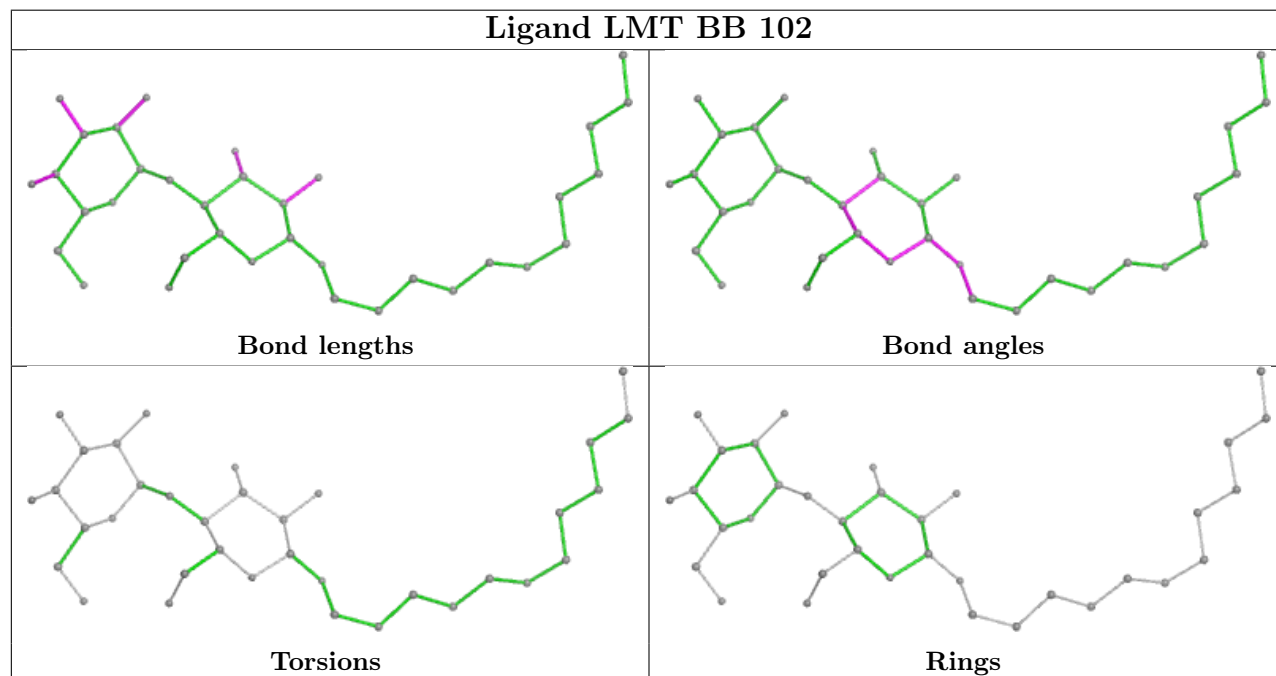
Ligand BCL AR 101

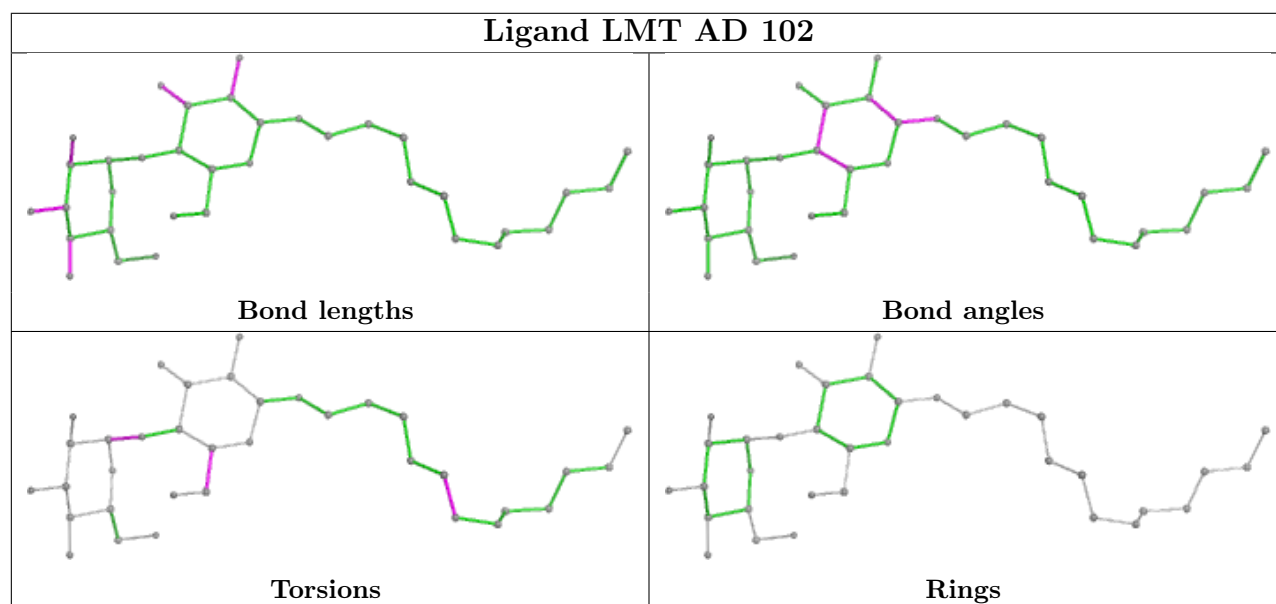
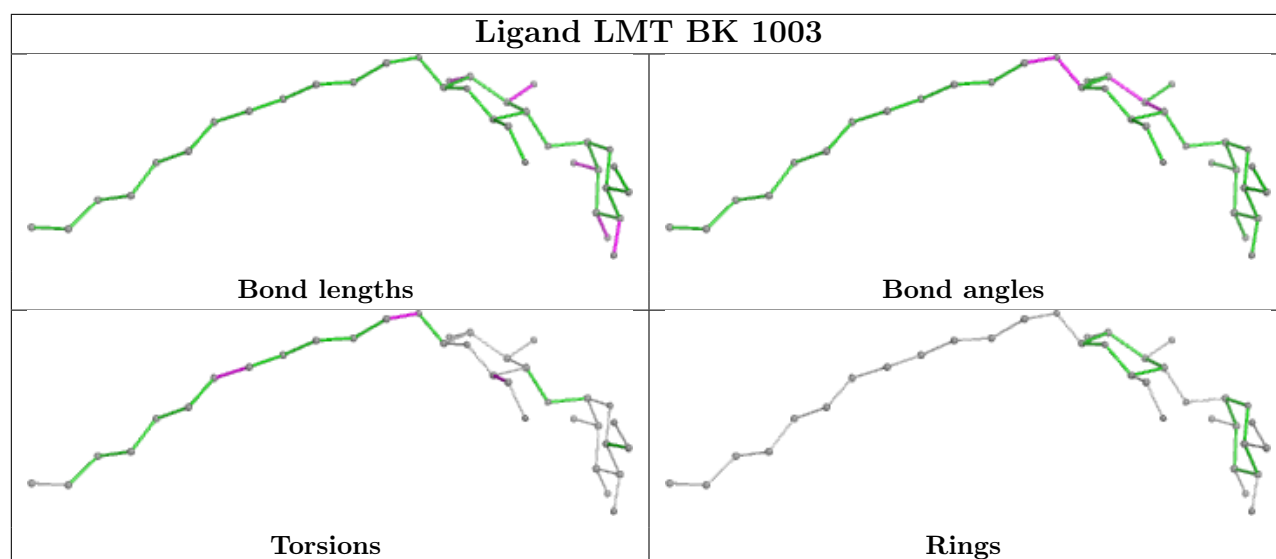


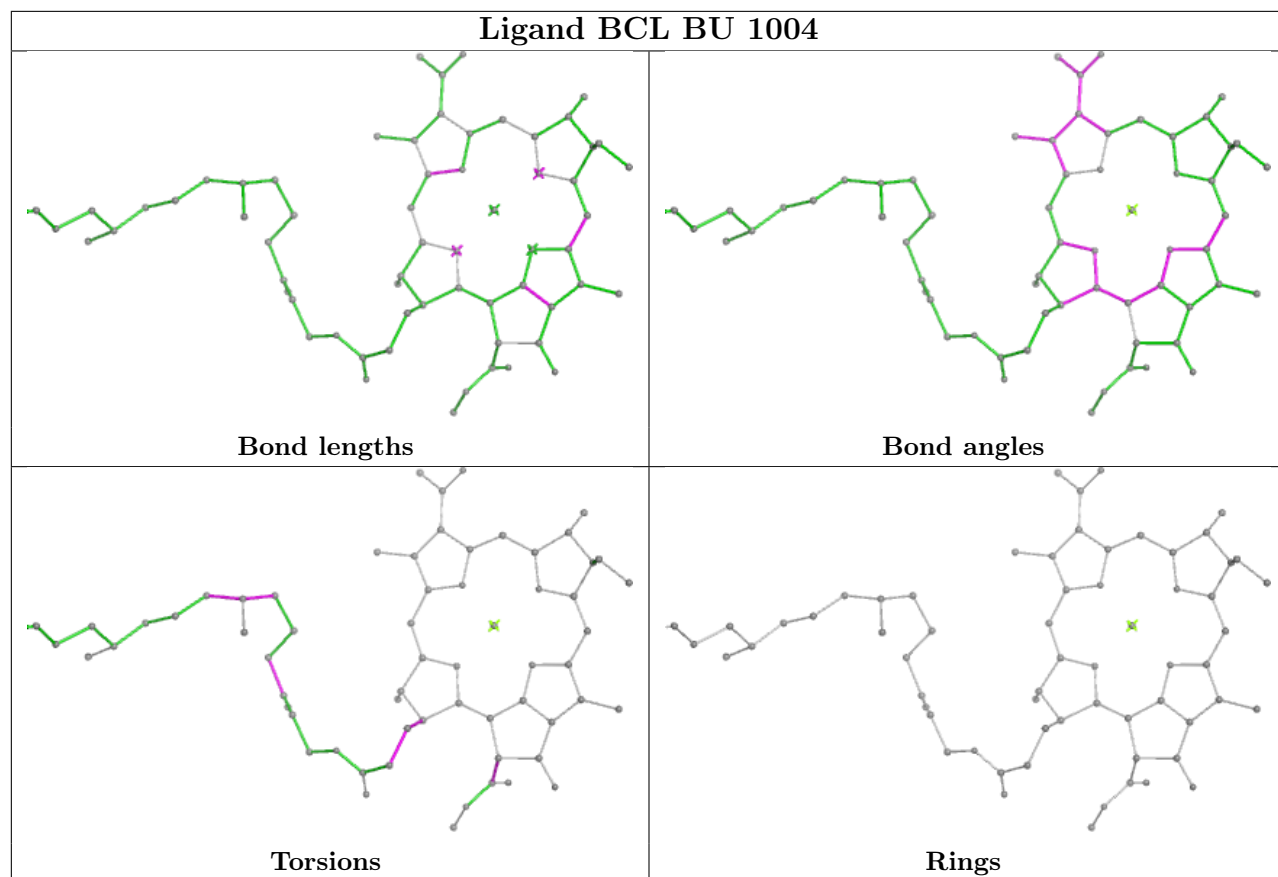
Ligand BCL ak 1001

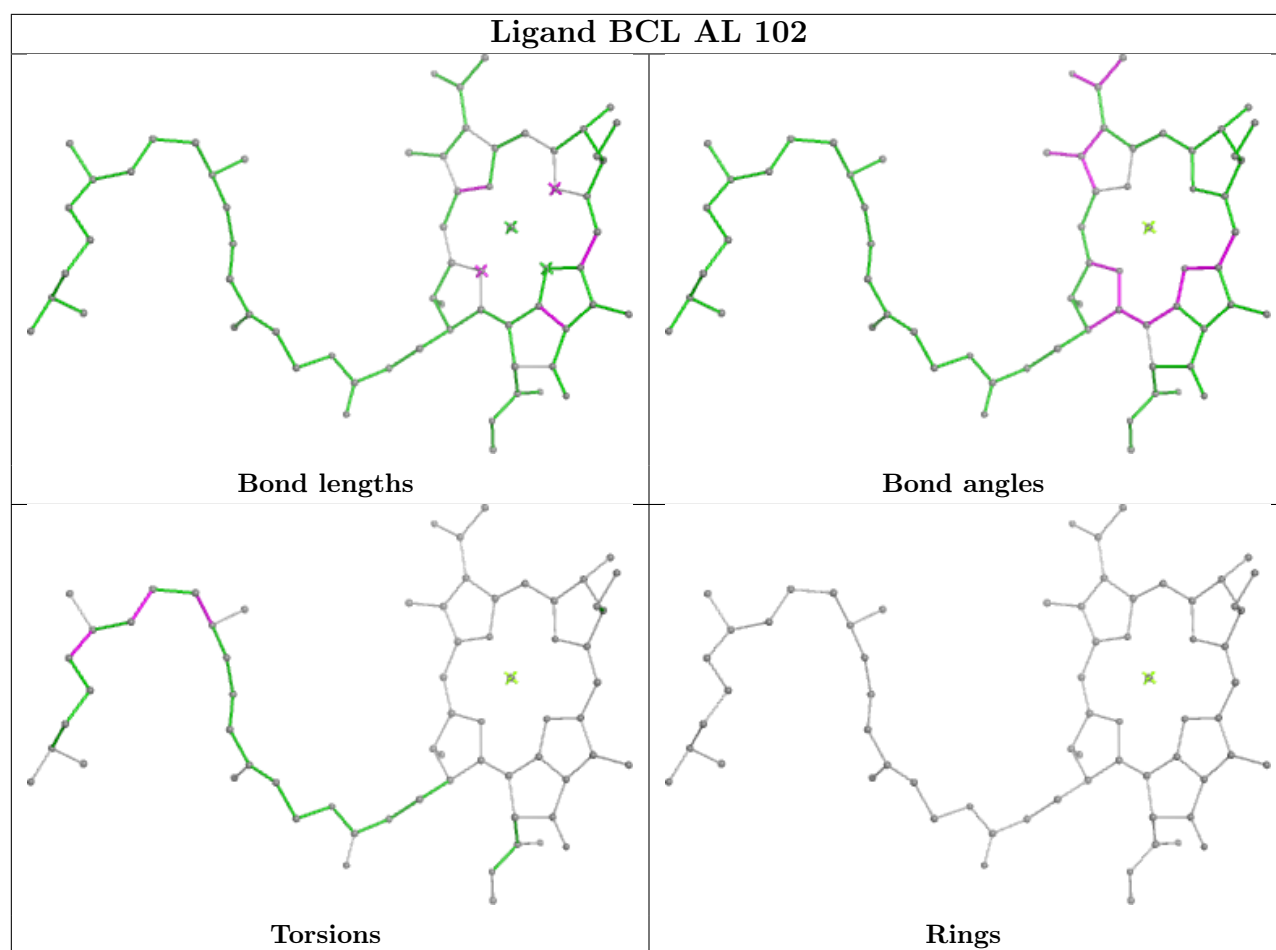


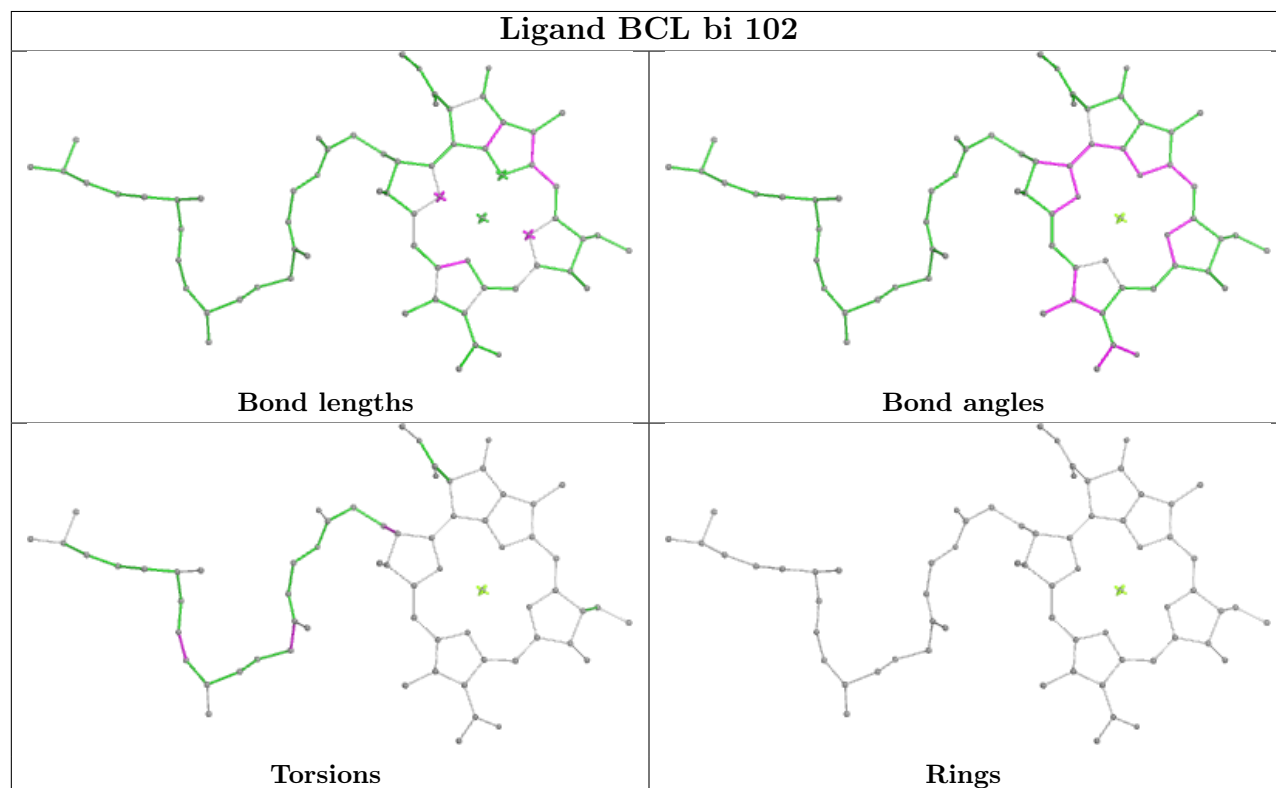
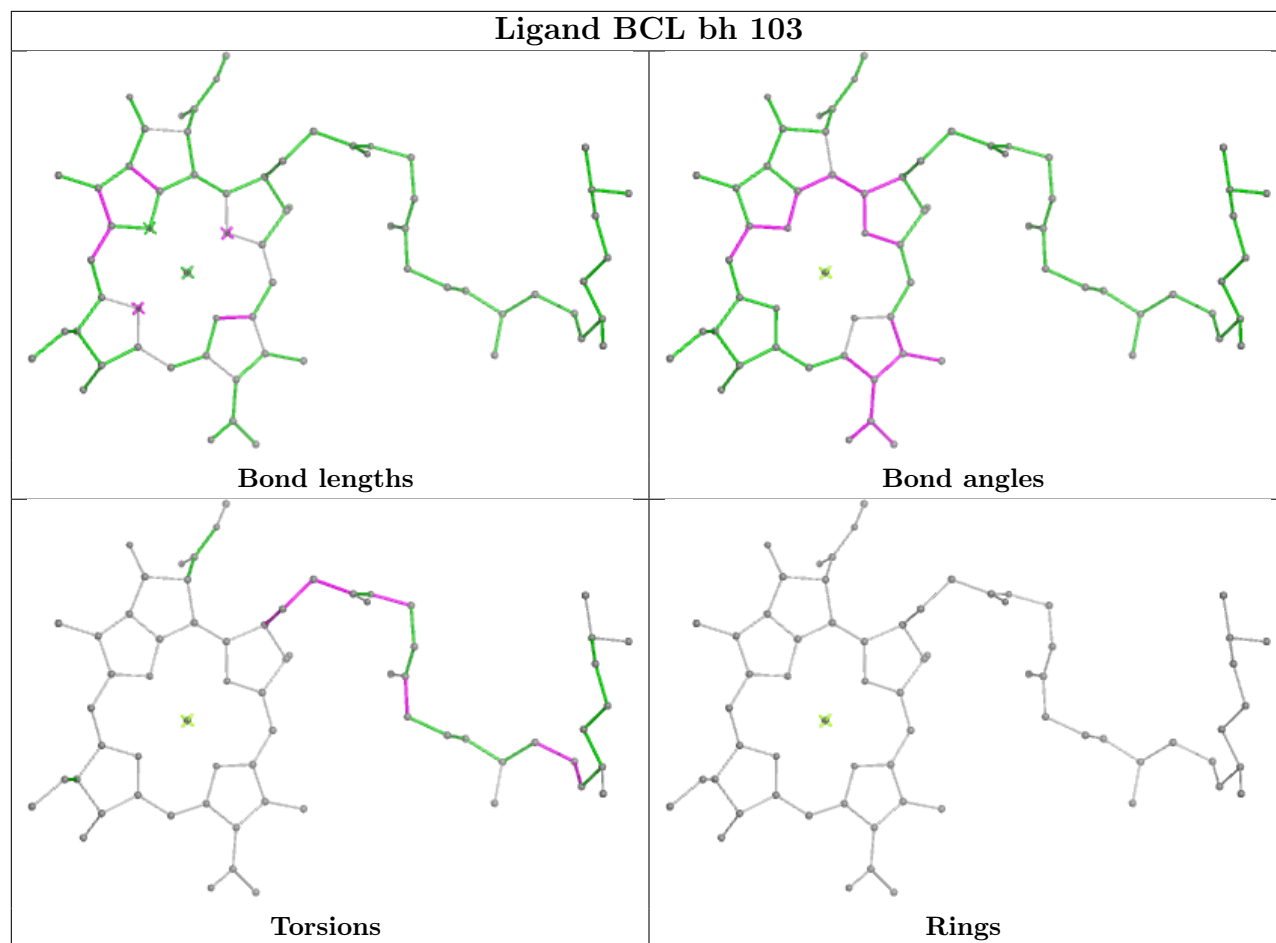


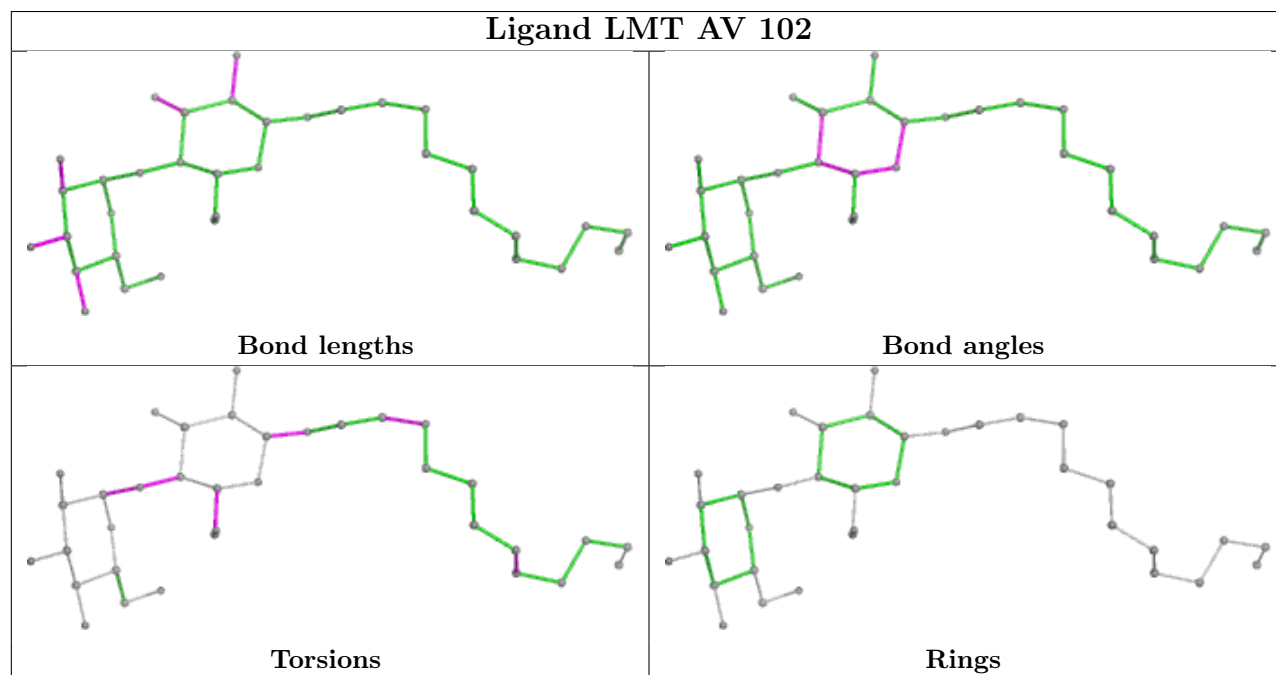
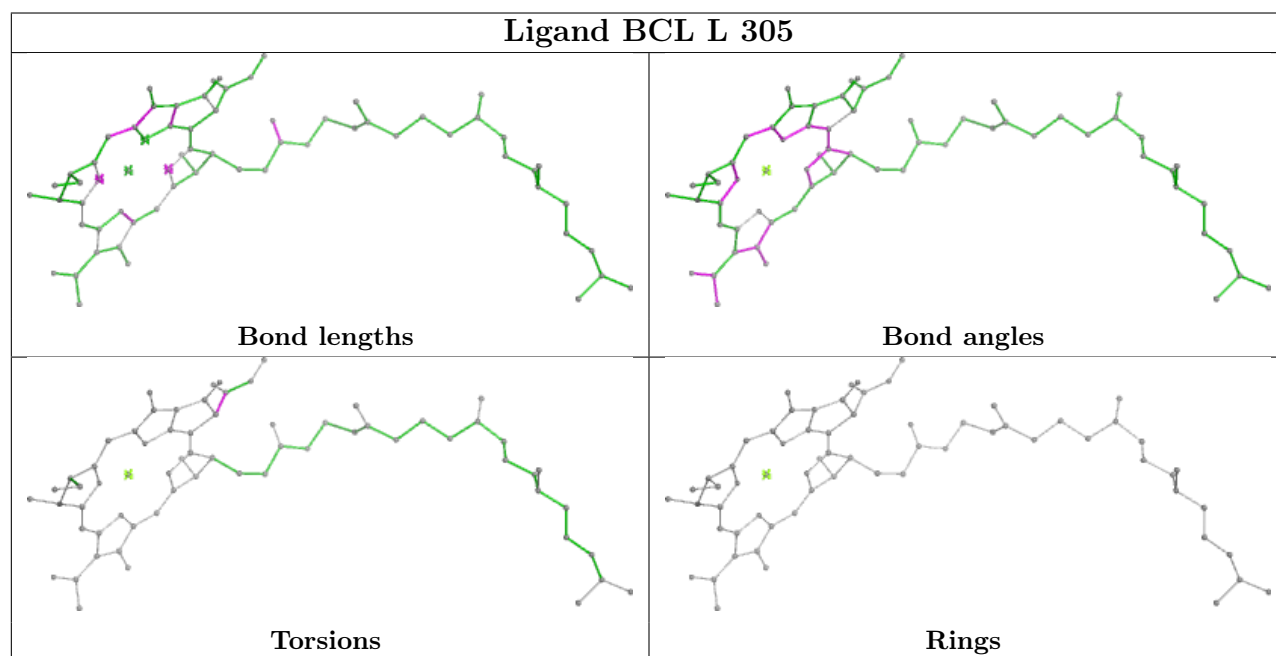
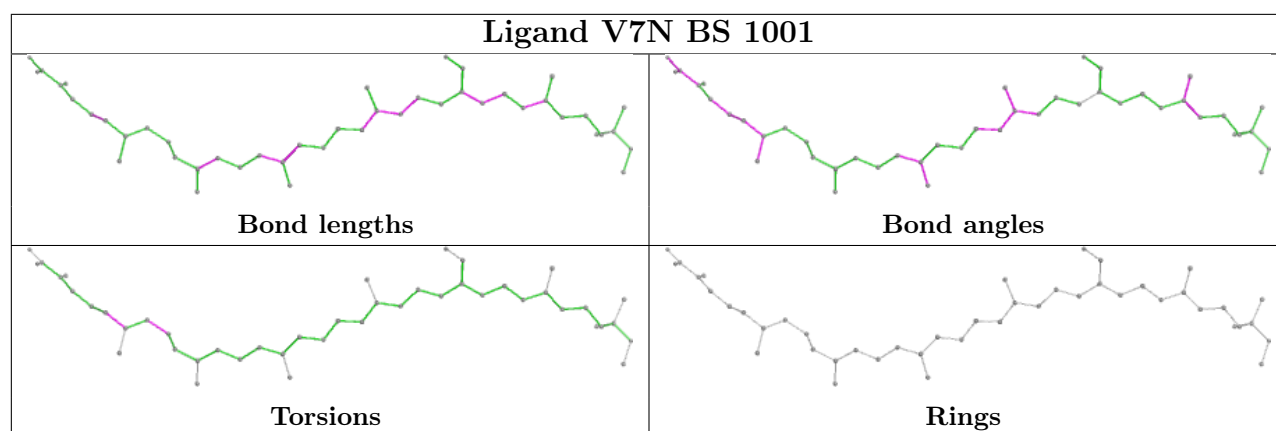
Ligand LMT BS 1005**Ligand LMT BB 102**

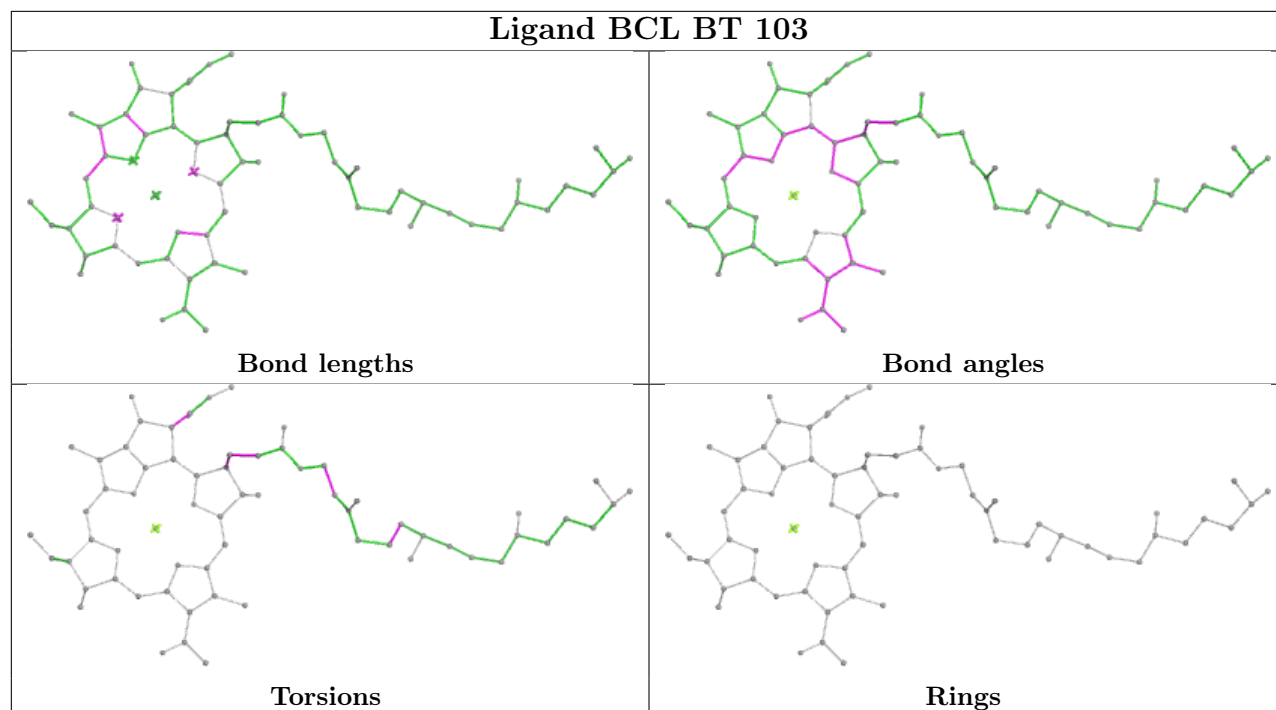
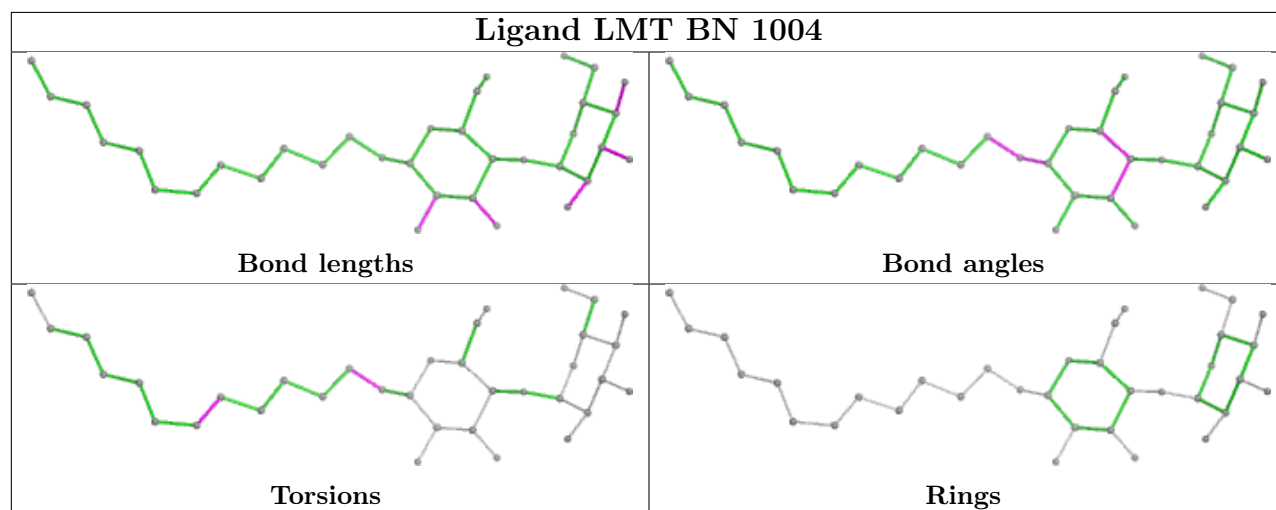




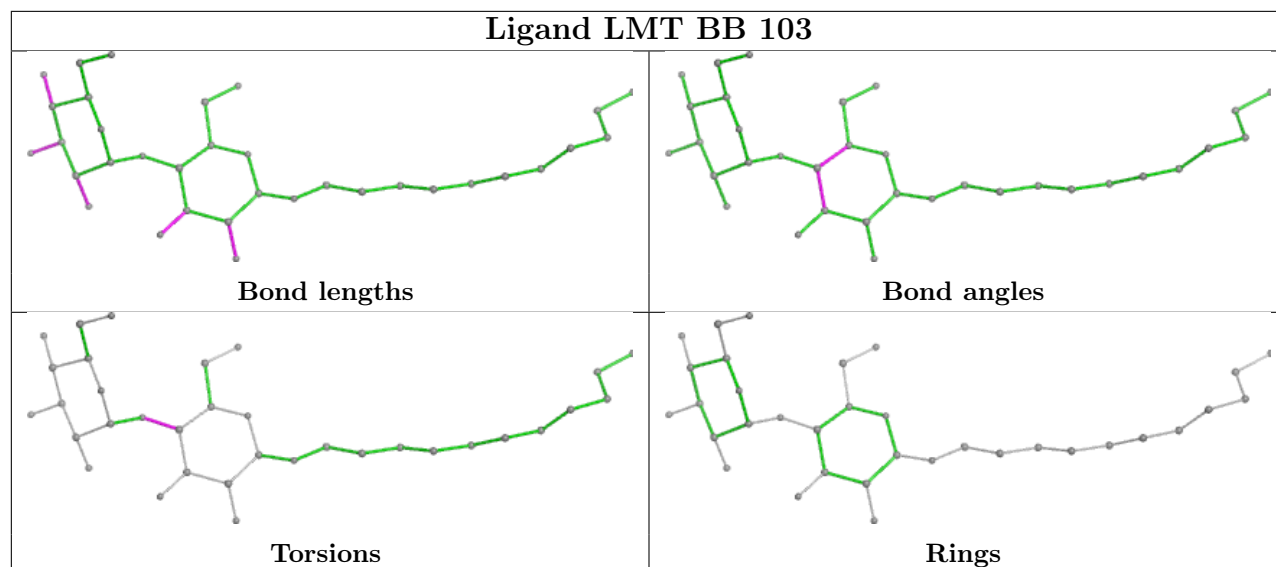




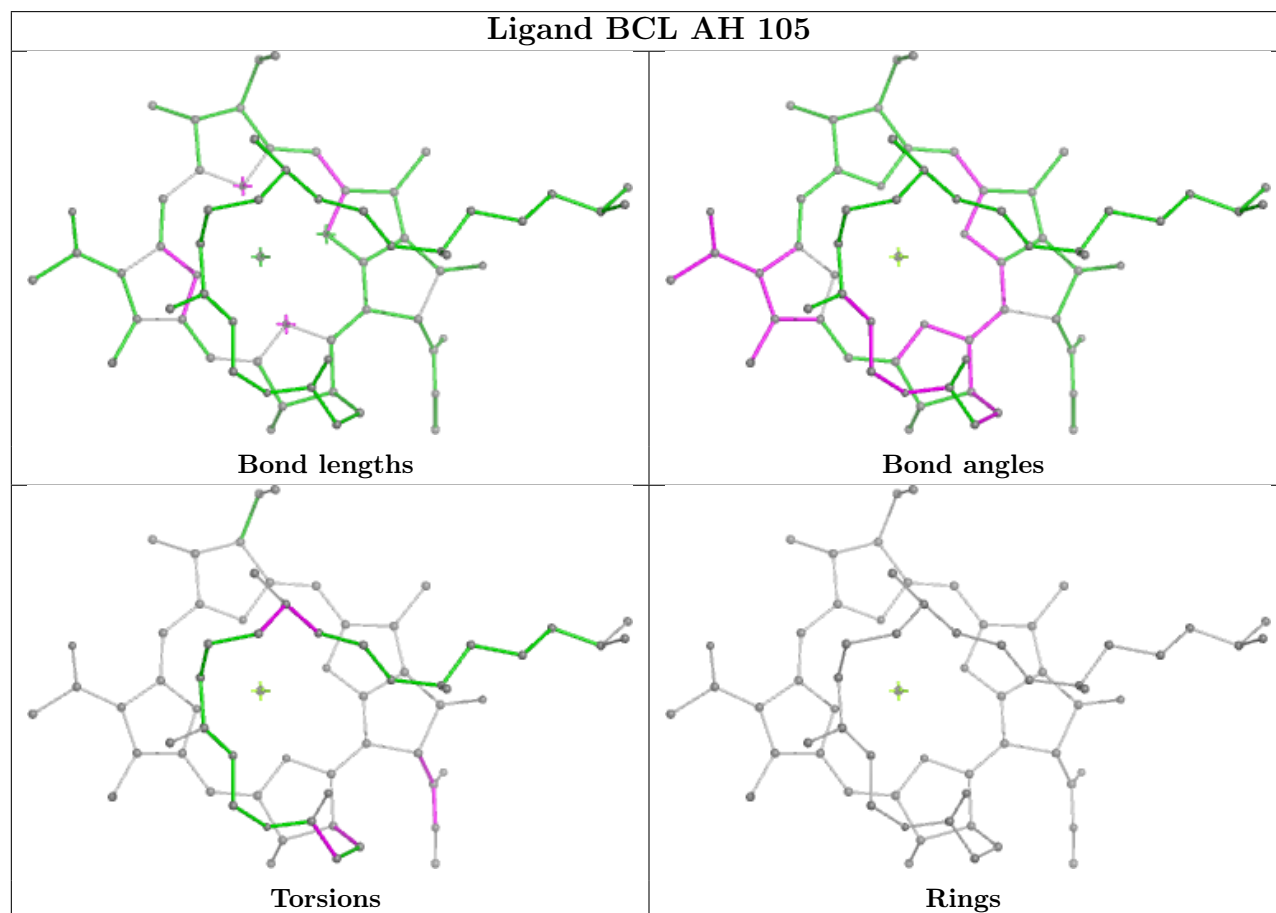


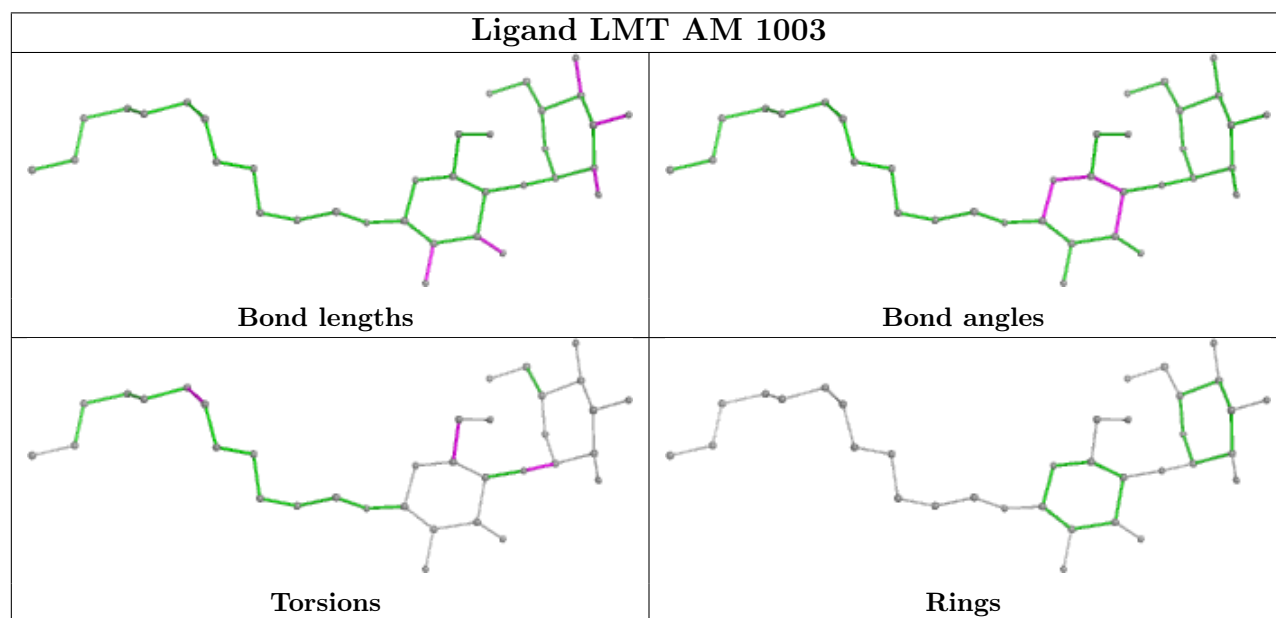
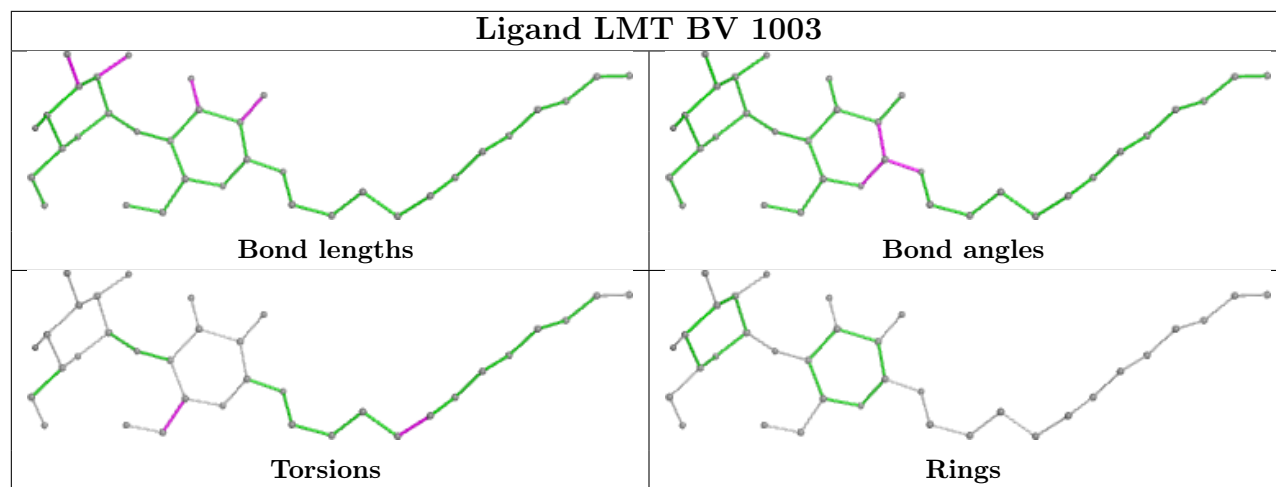
Ligand BCL BT 103**Ligand LMT BN 1004**

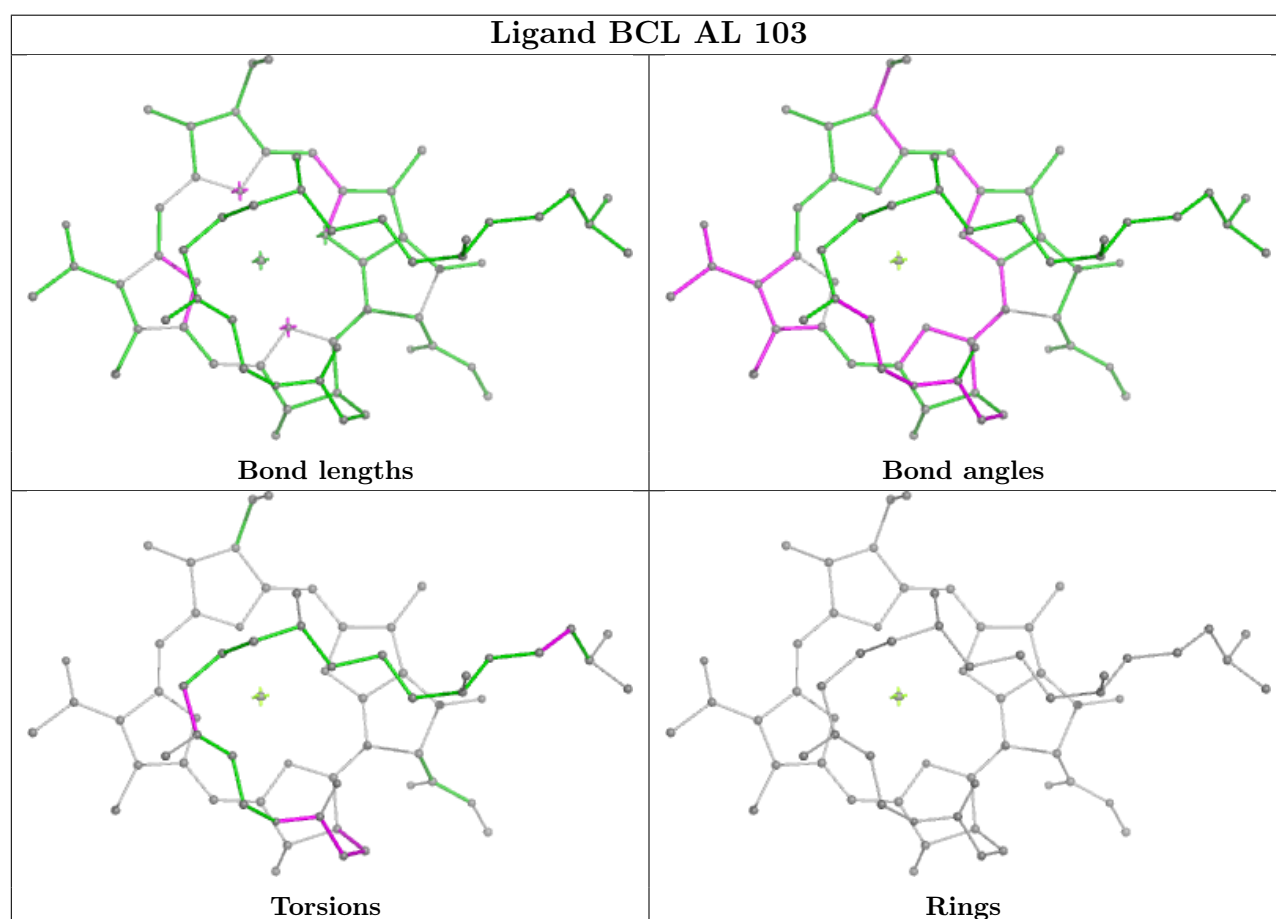
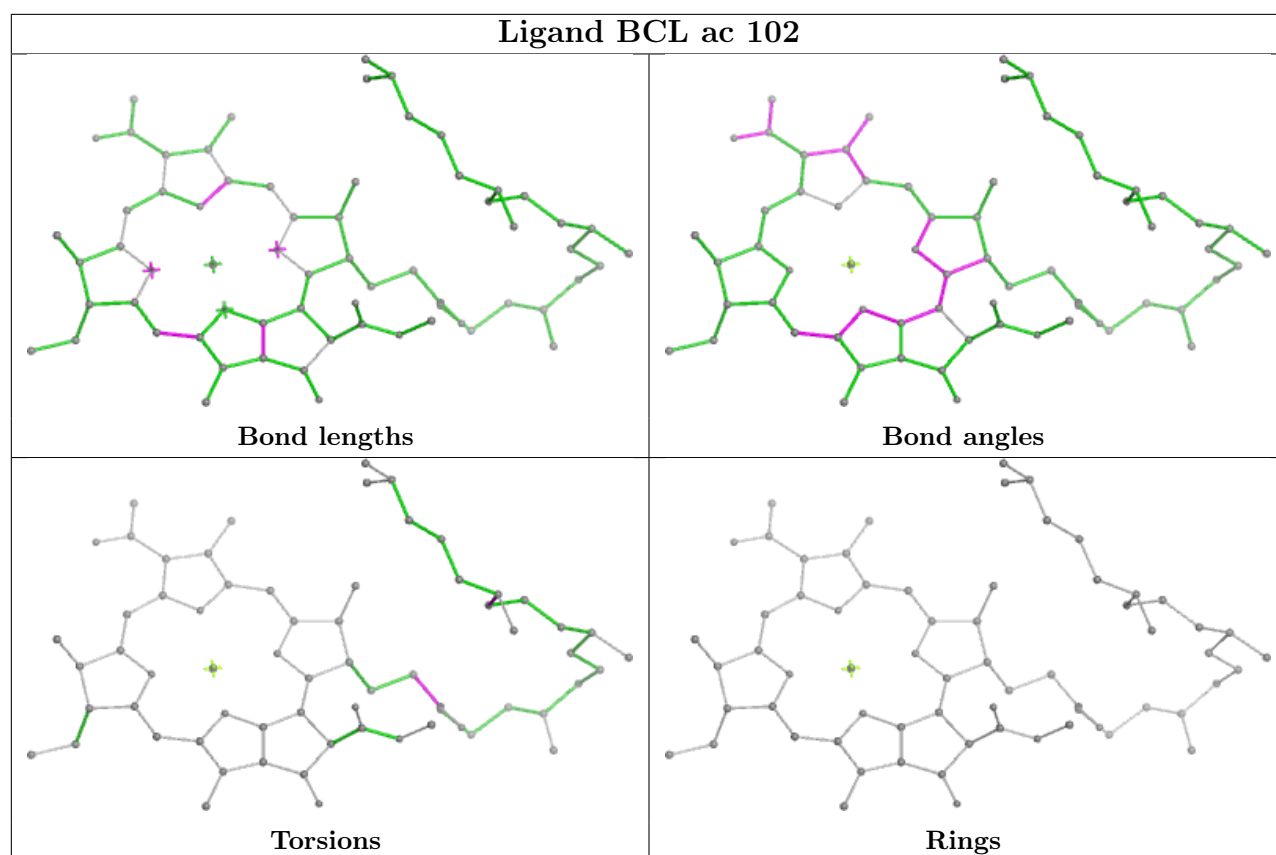
Ligand LMT BB 103

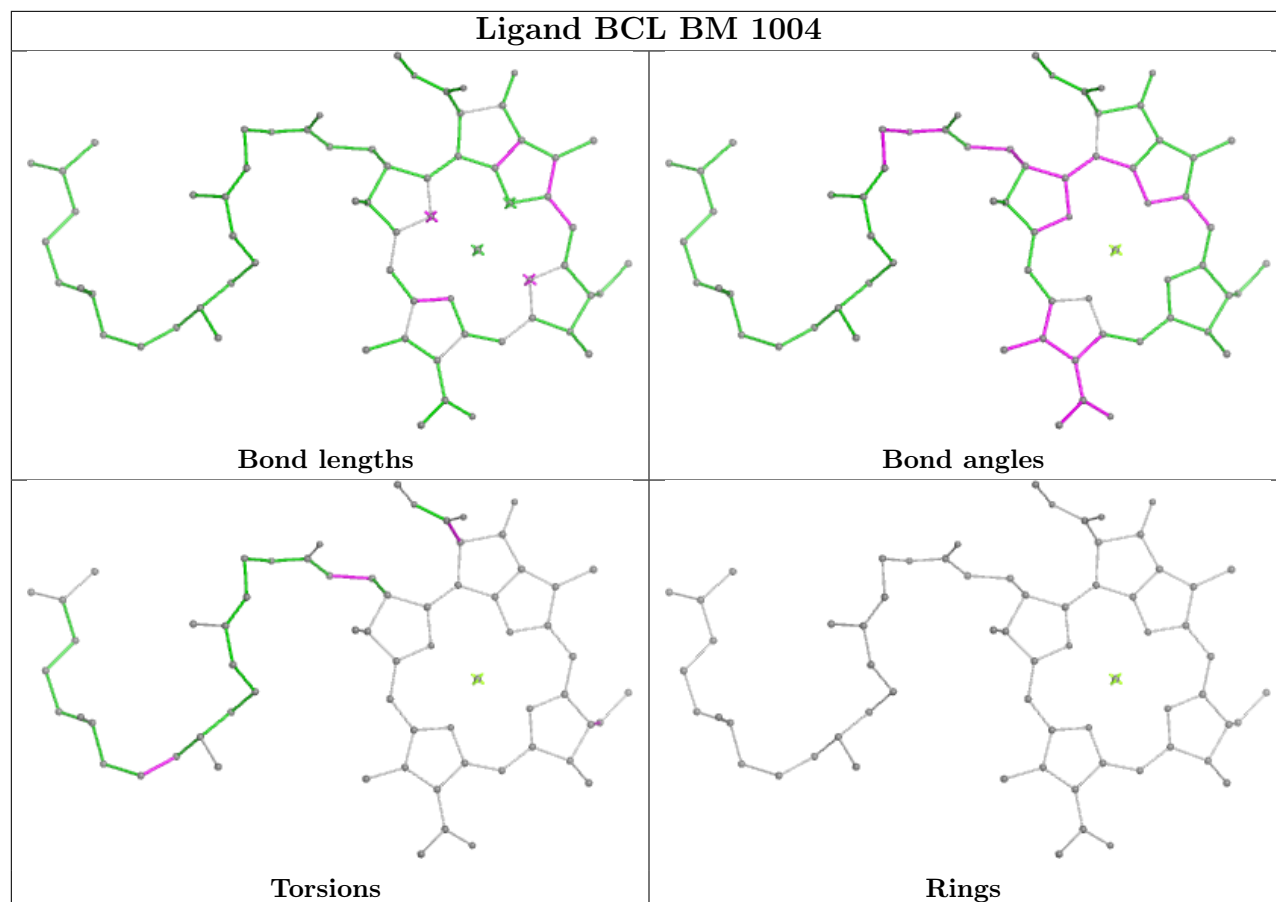
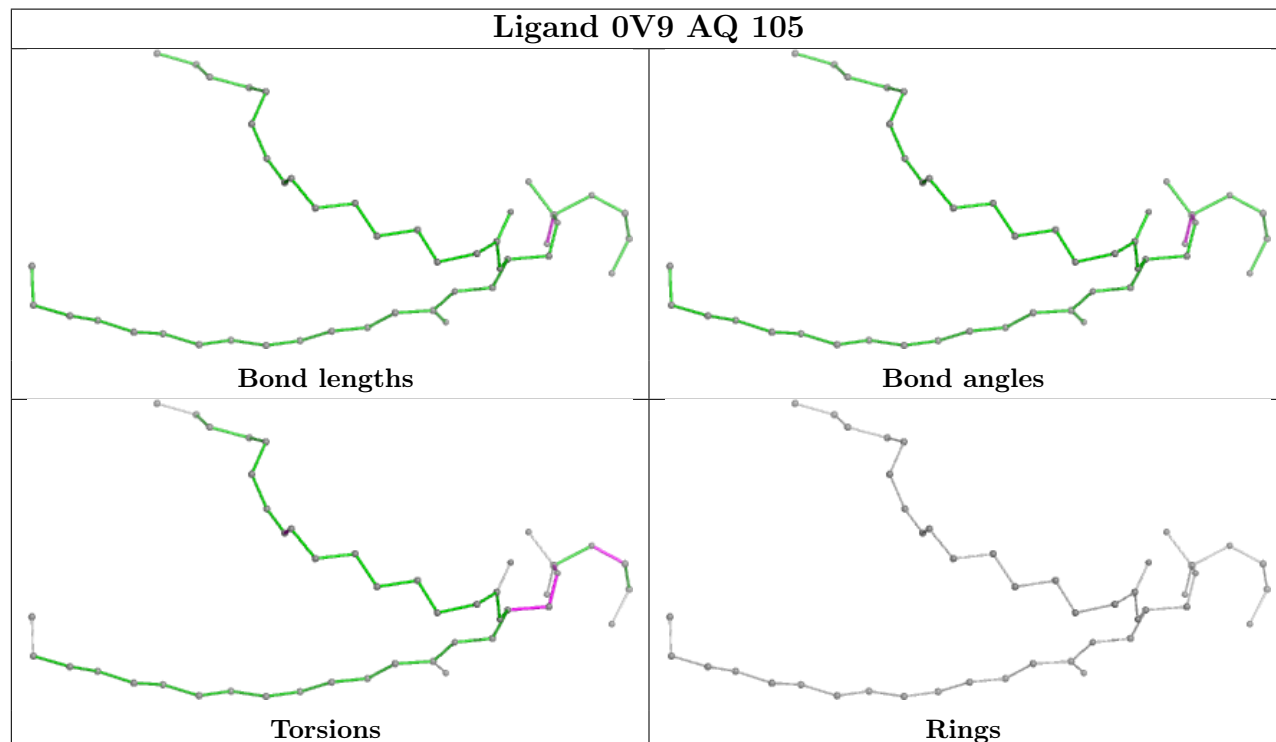


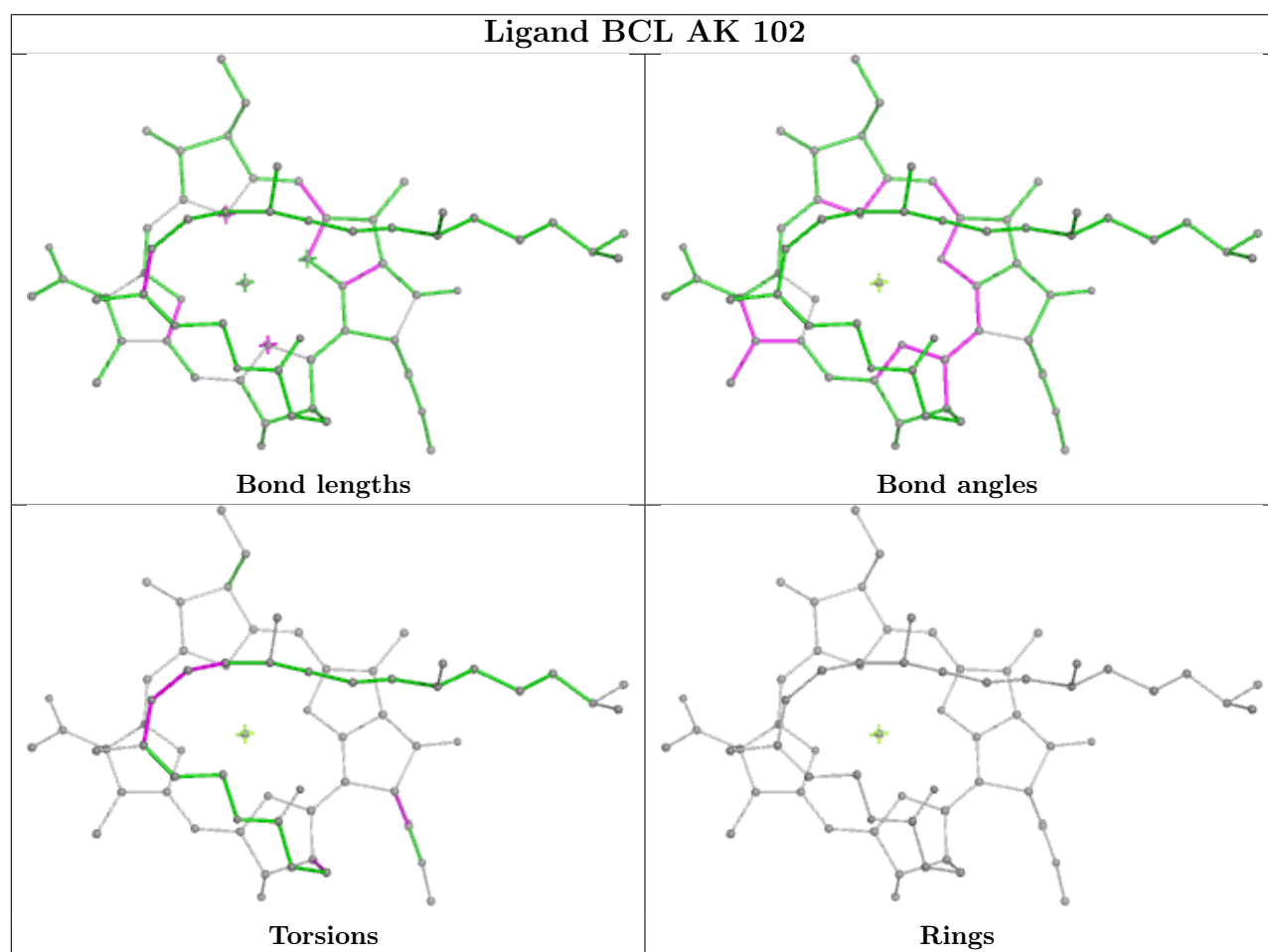
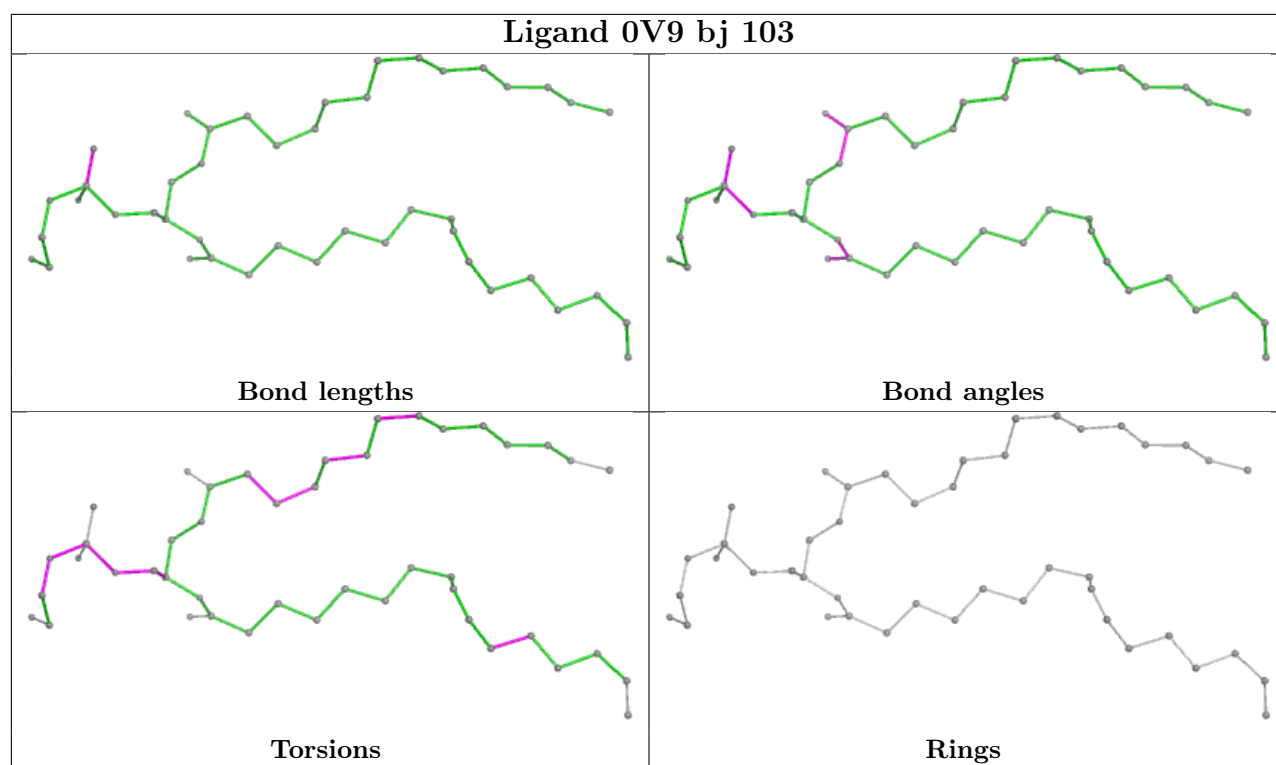
Ligand BCL AH 105

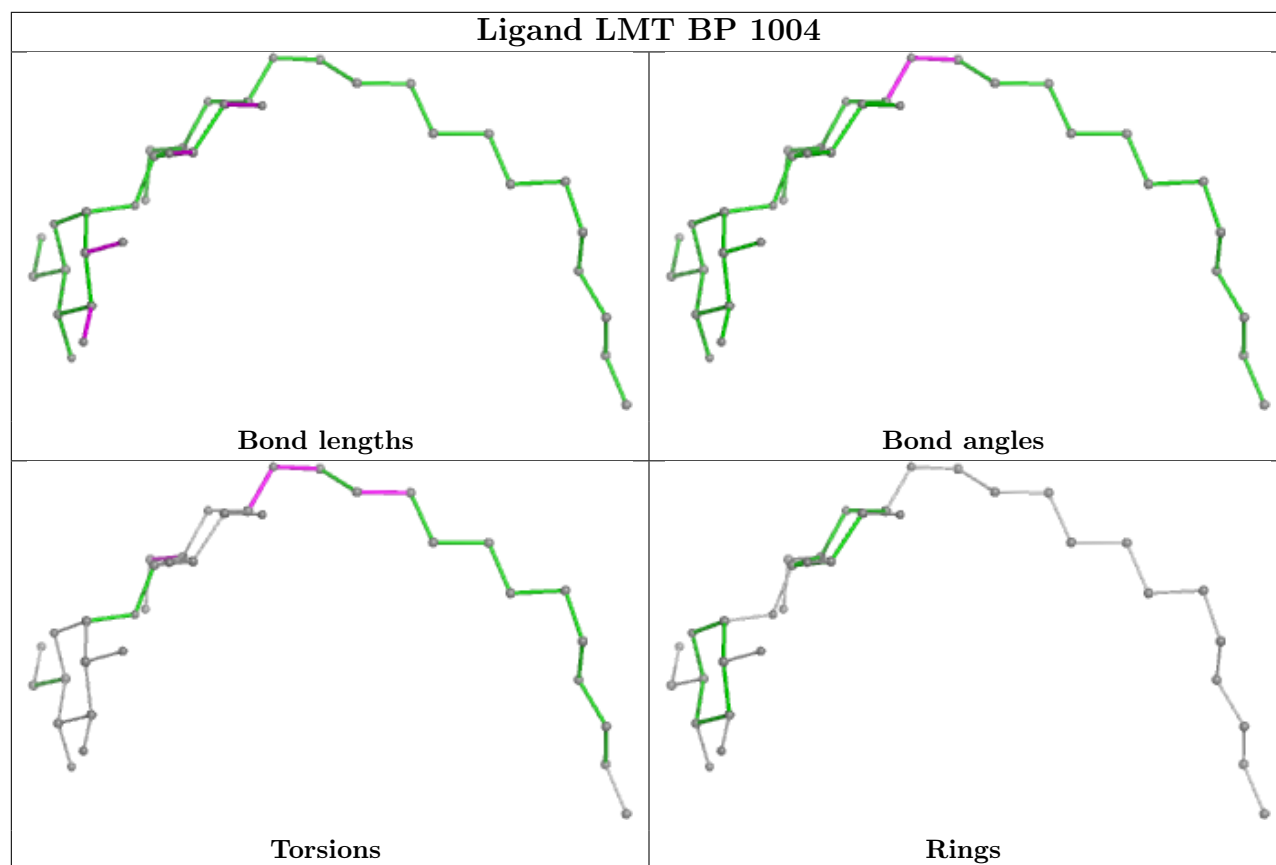
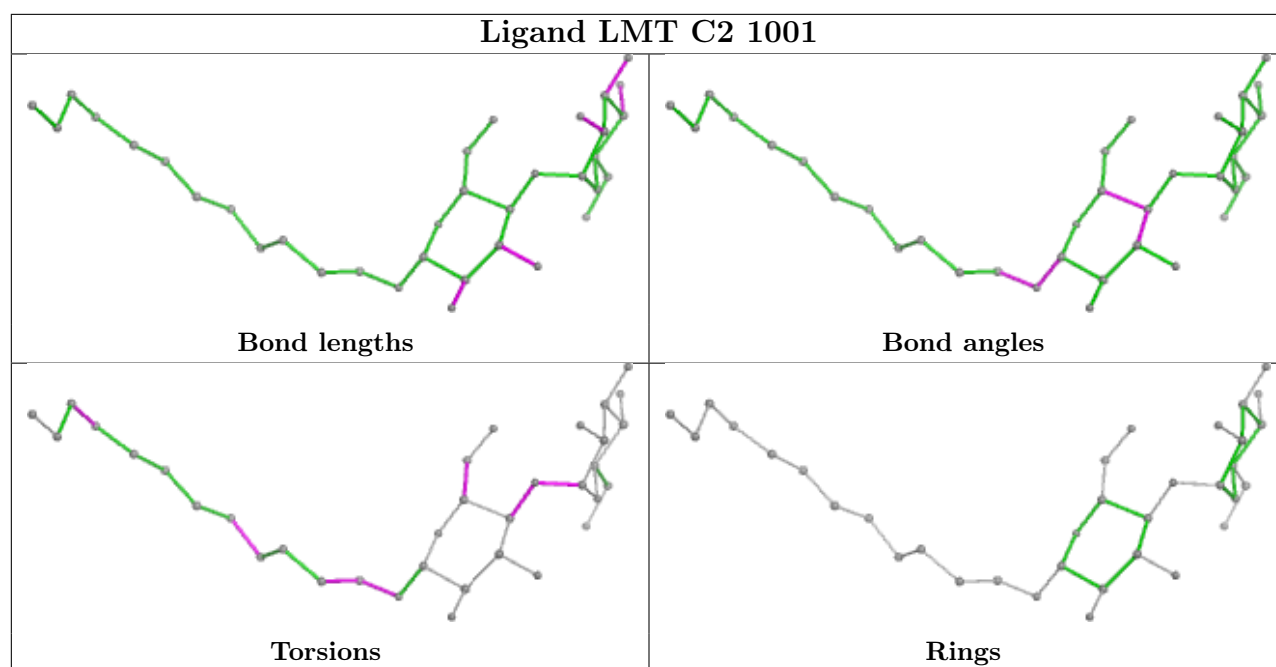


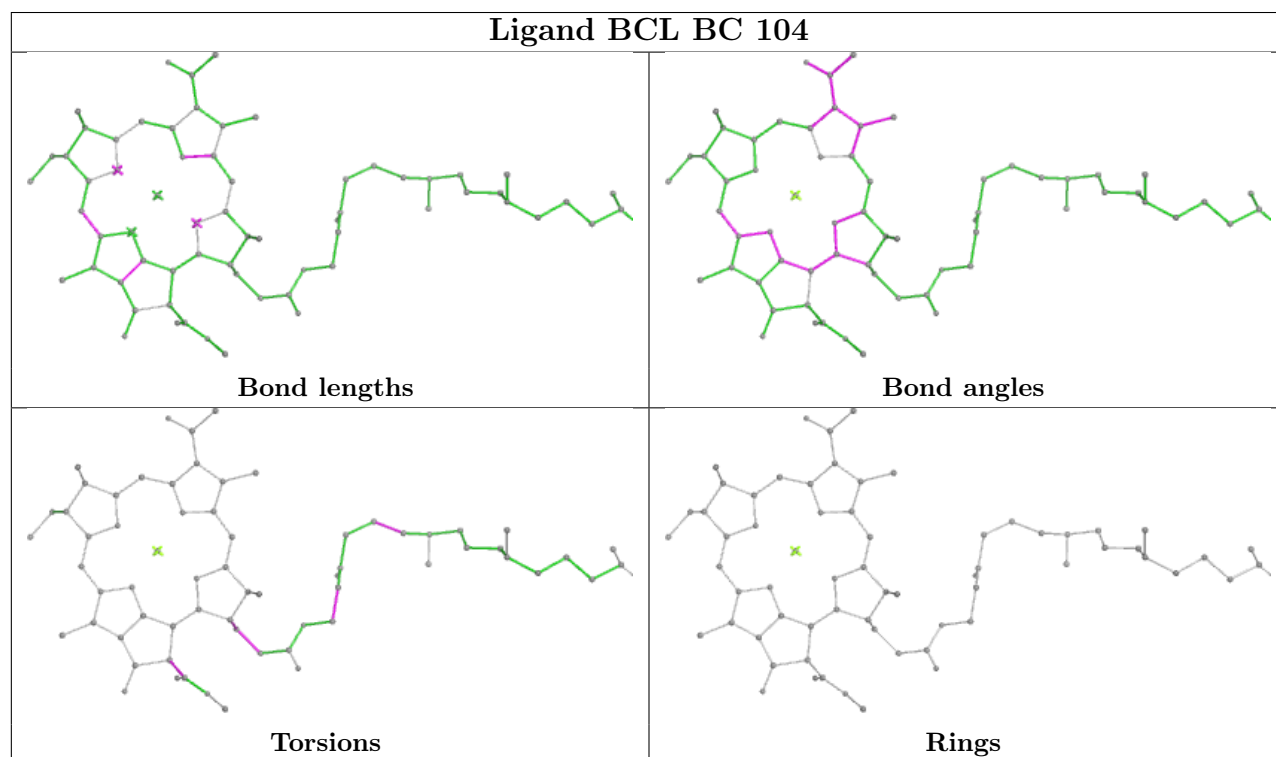
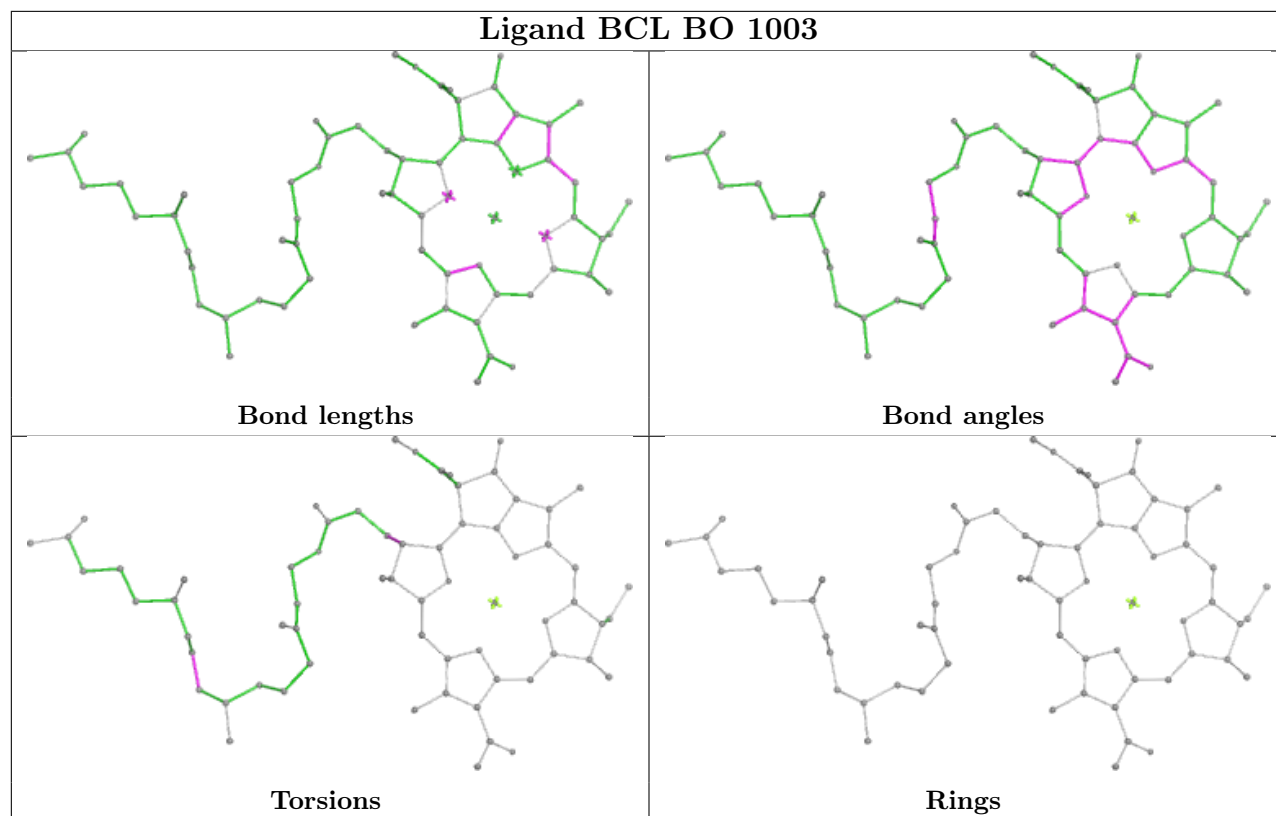


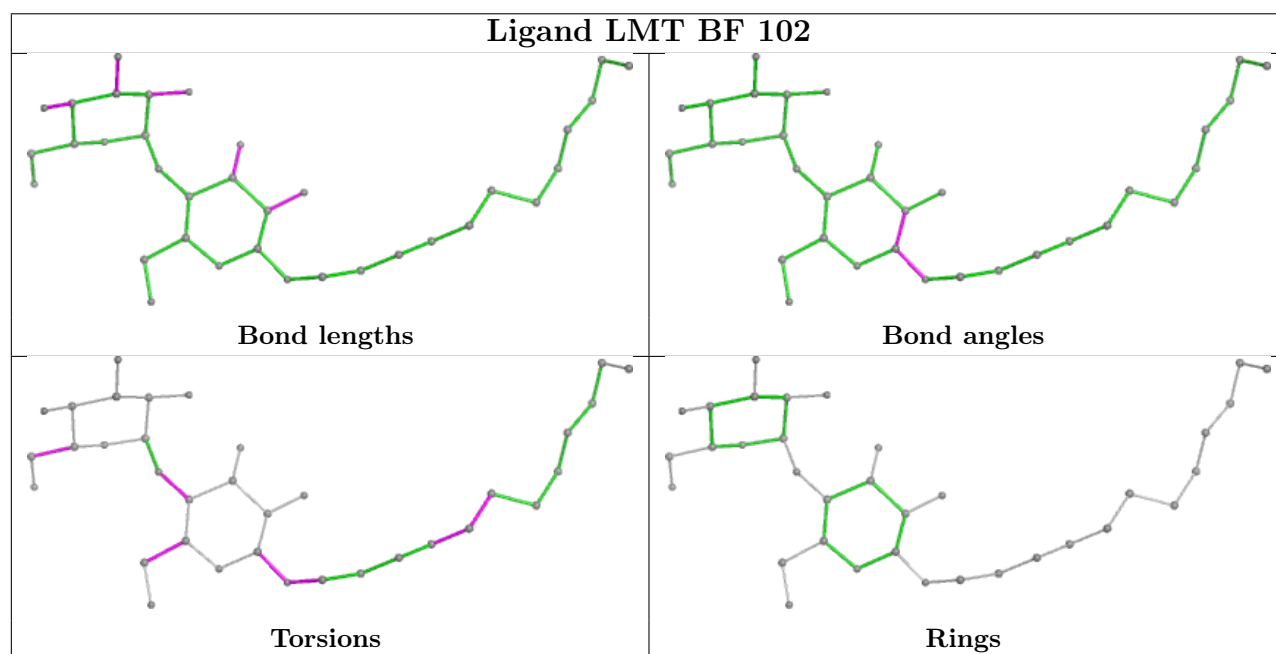
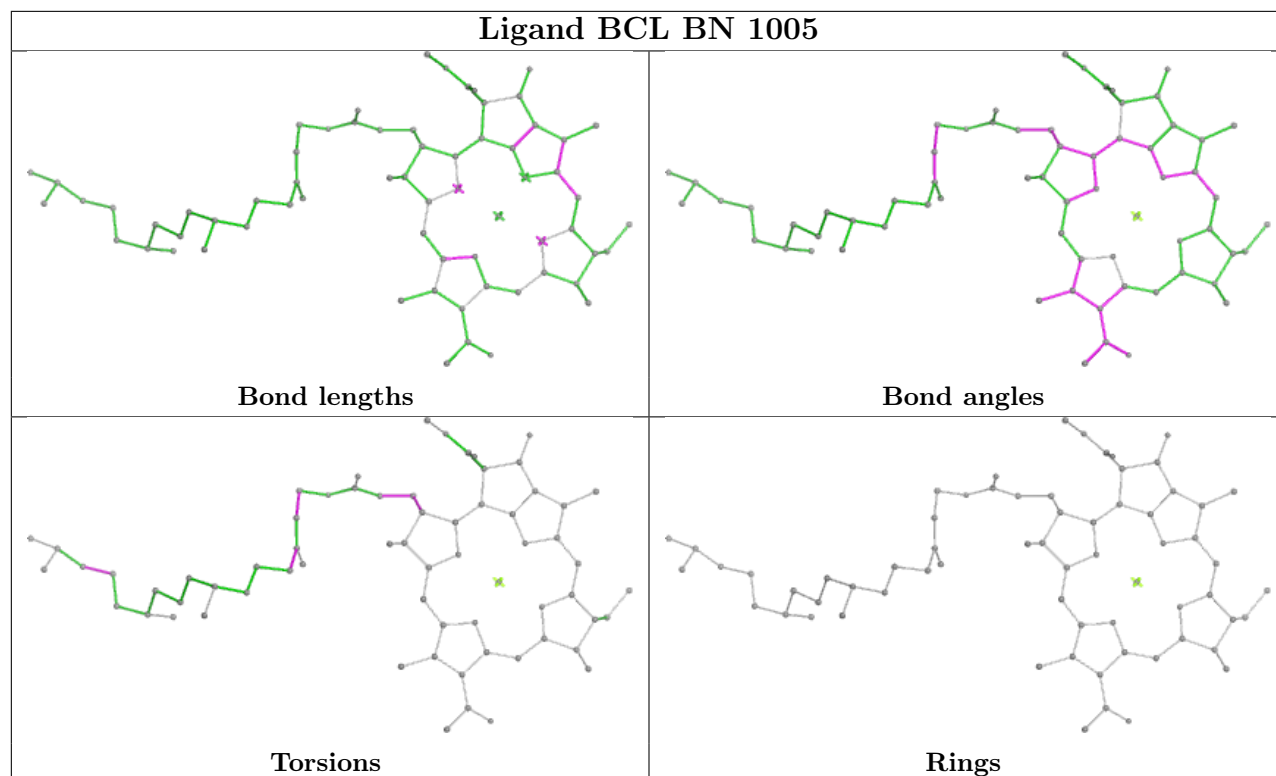


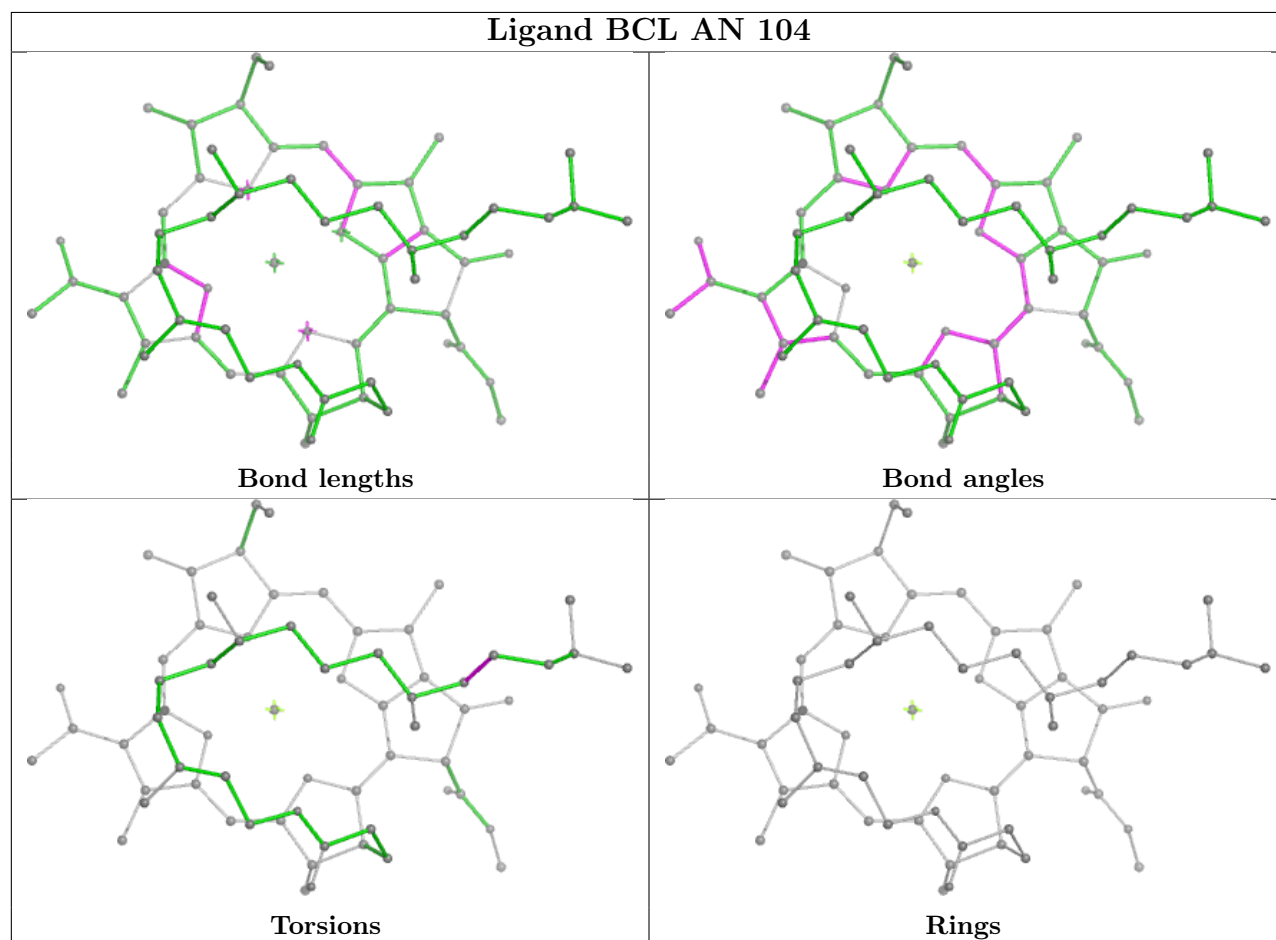
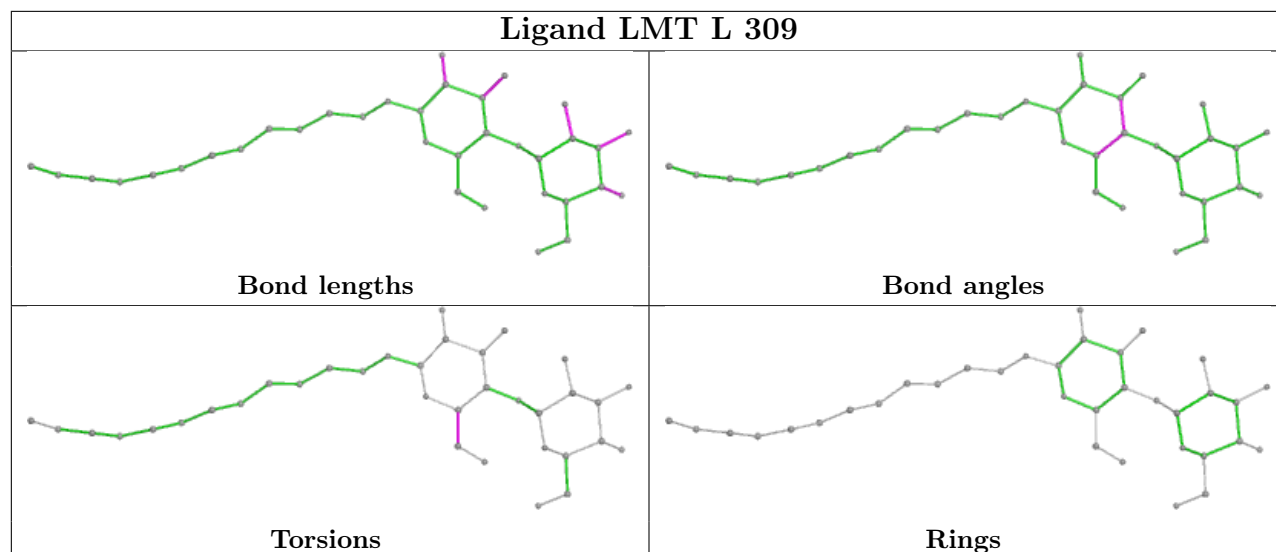
Ligand BCL BM 1004**Ligand 0V9 AQ 105**

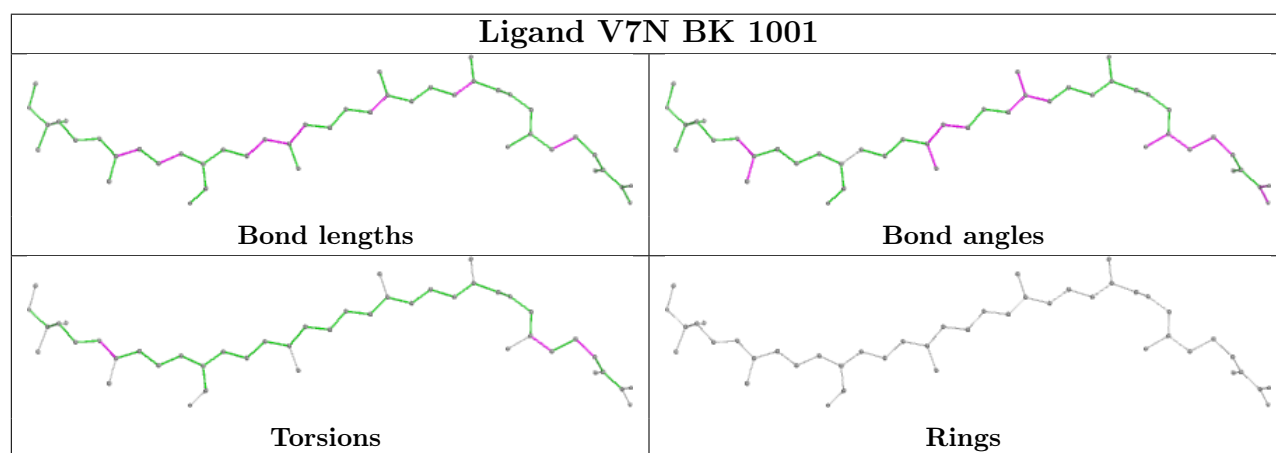
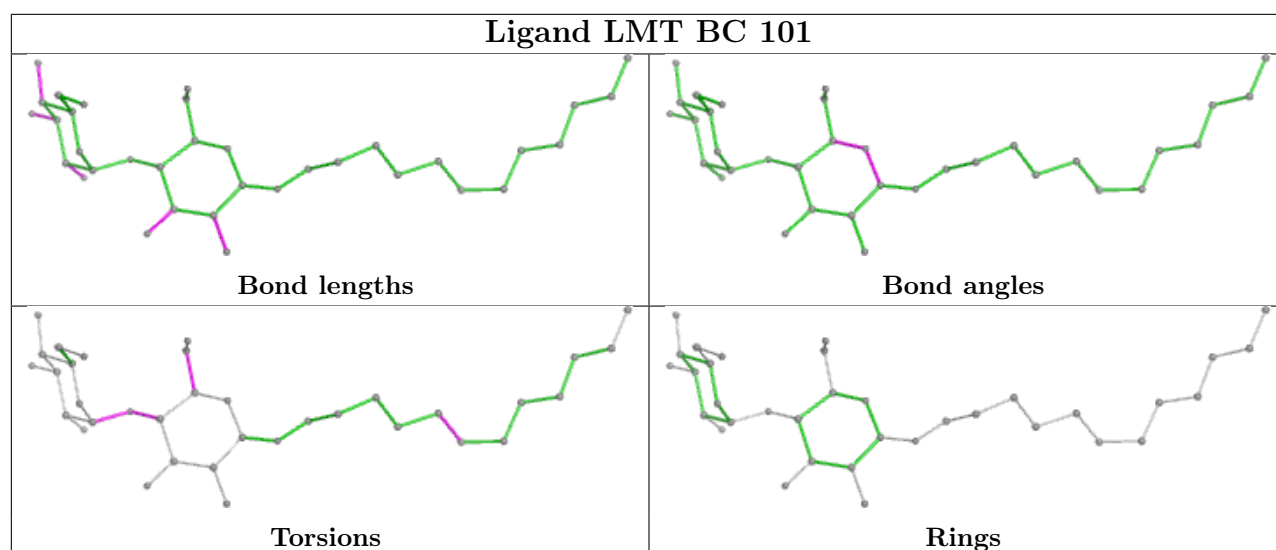




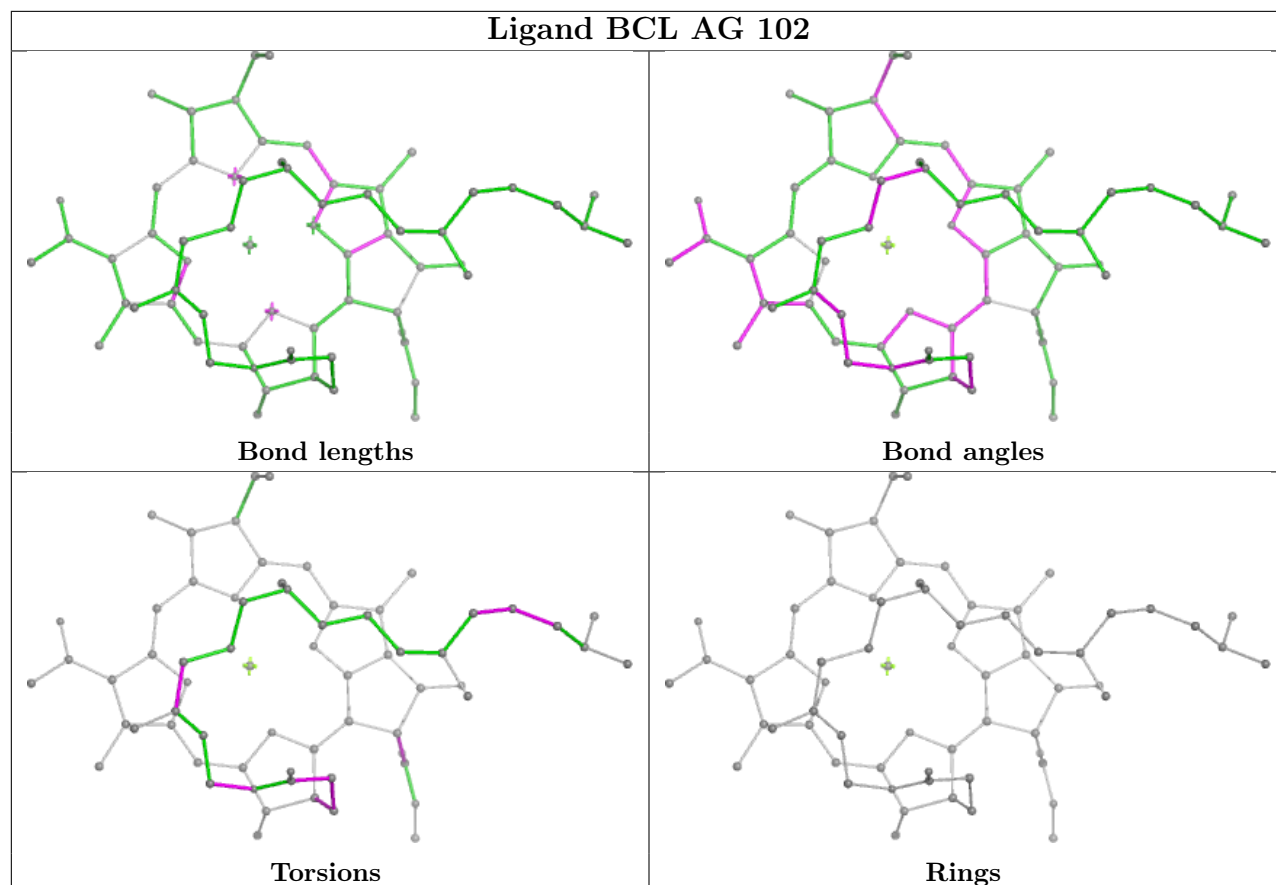




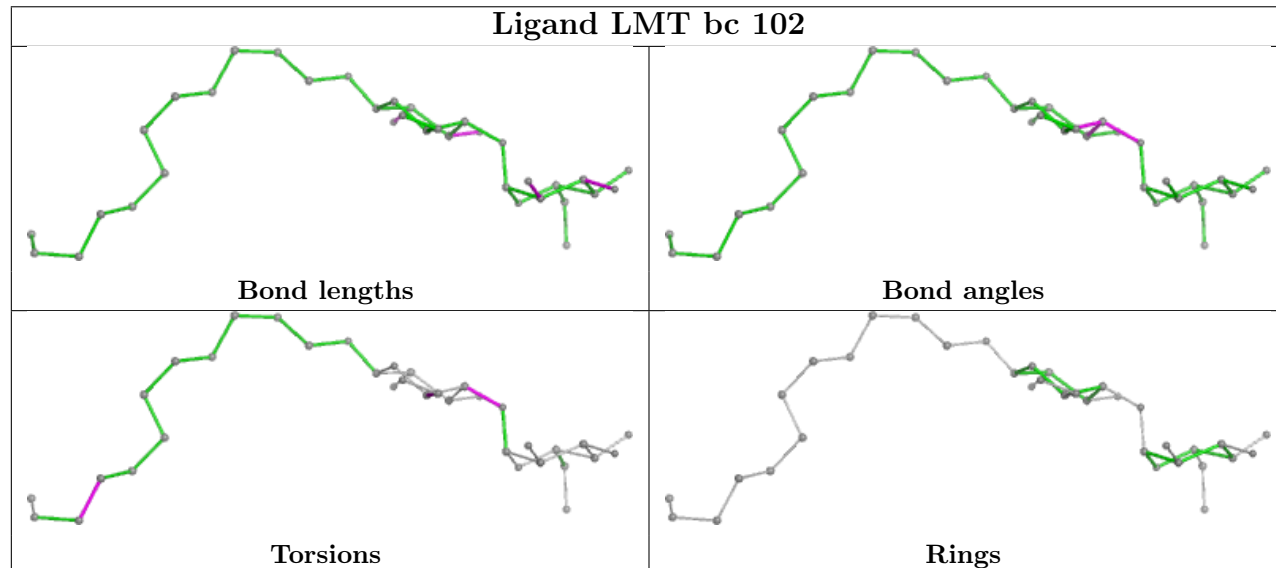


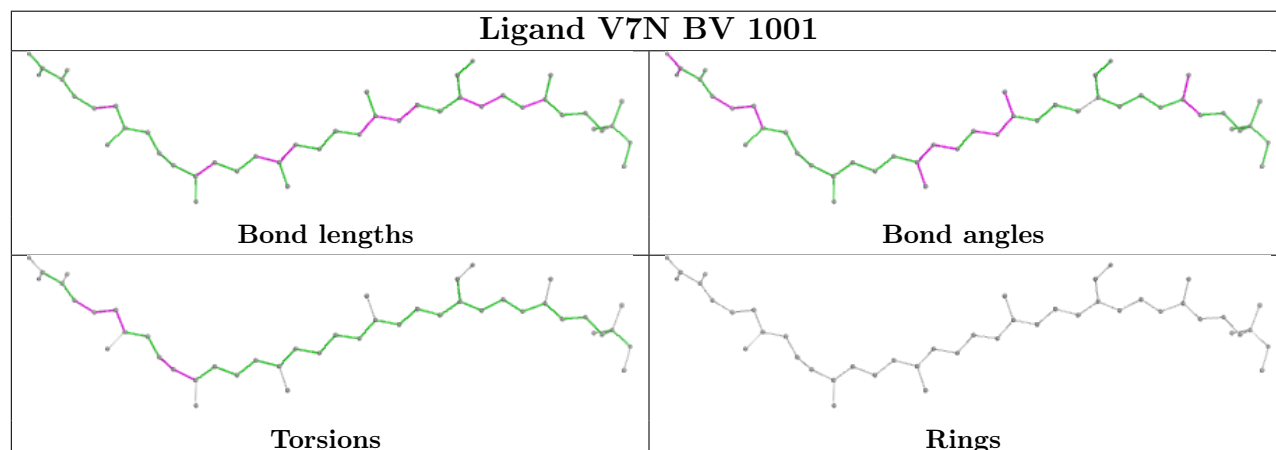
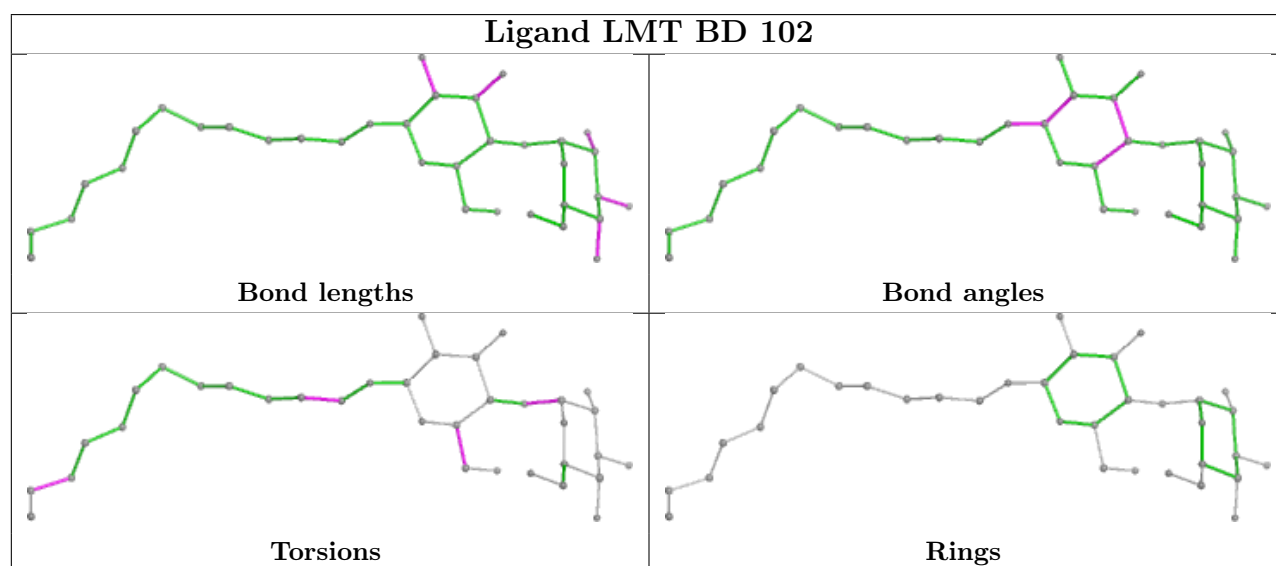
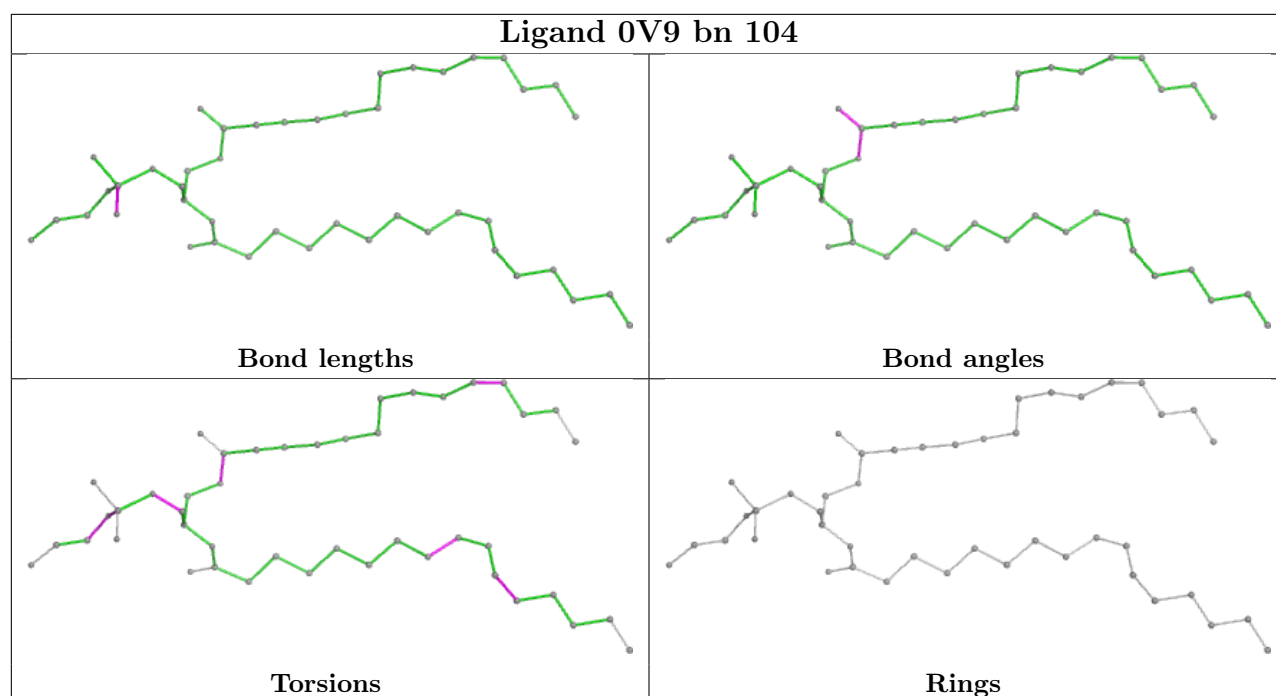


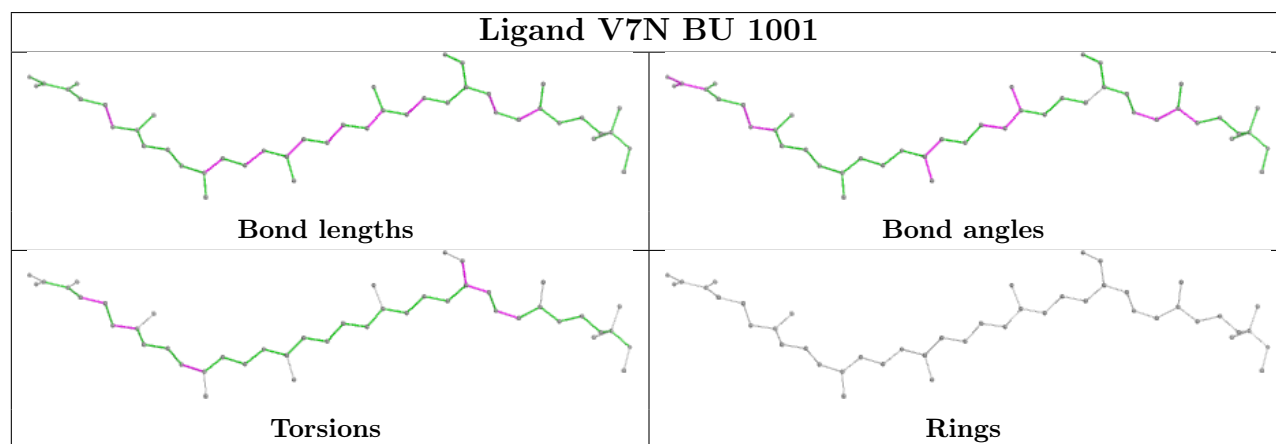
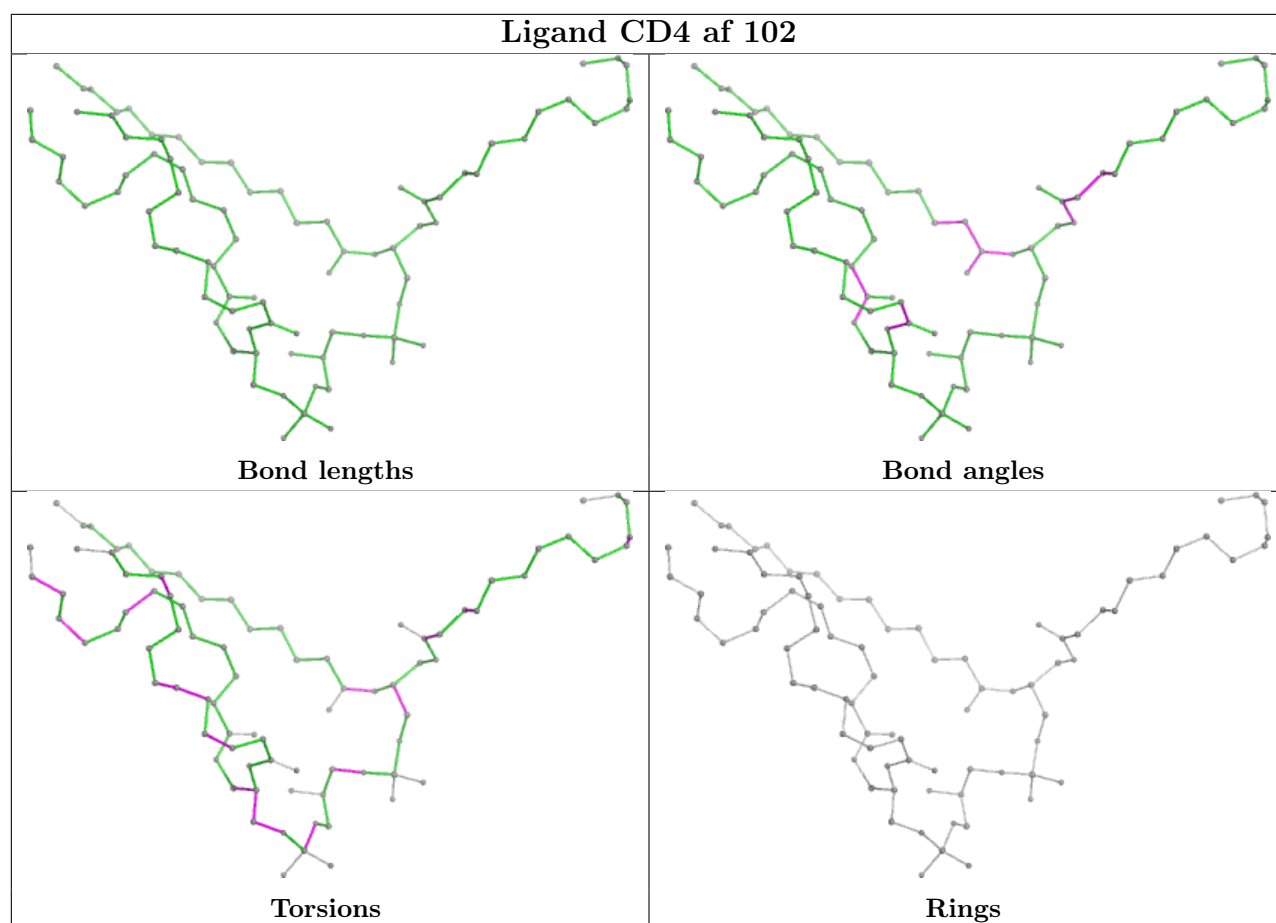
Ligand BCL AG 102

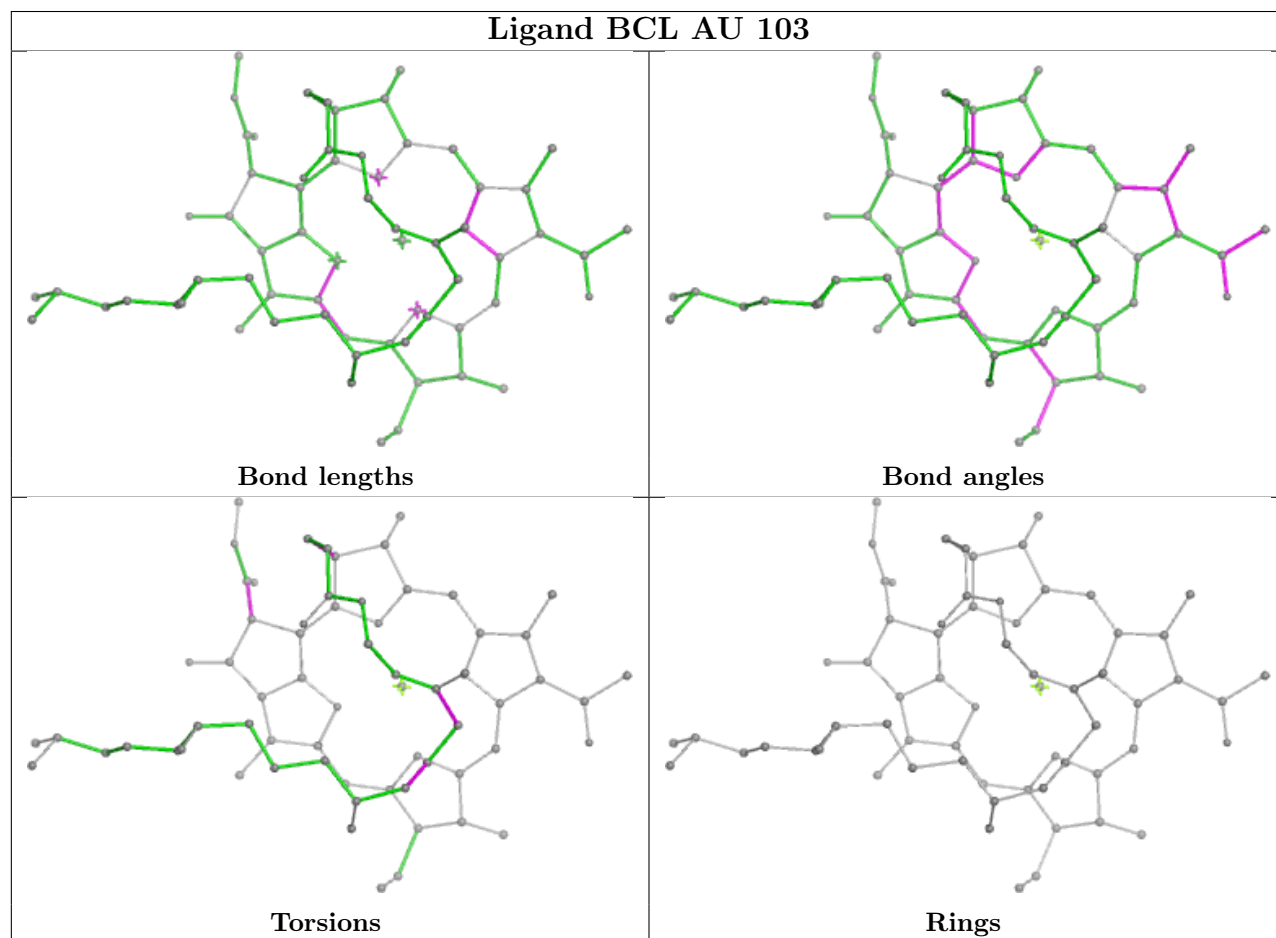
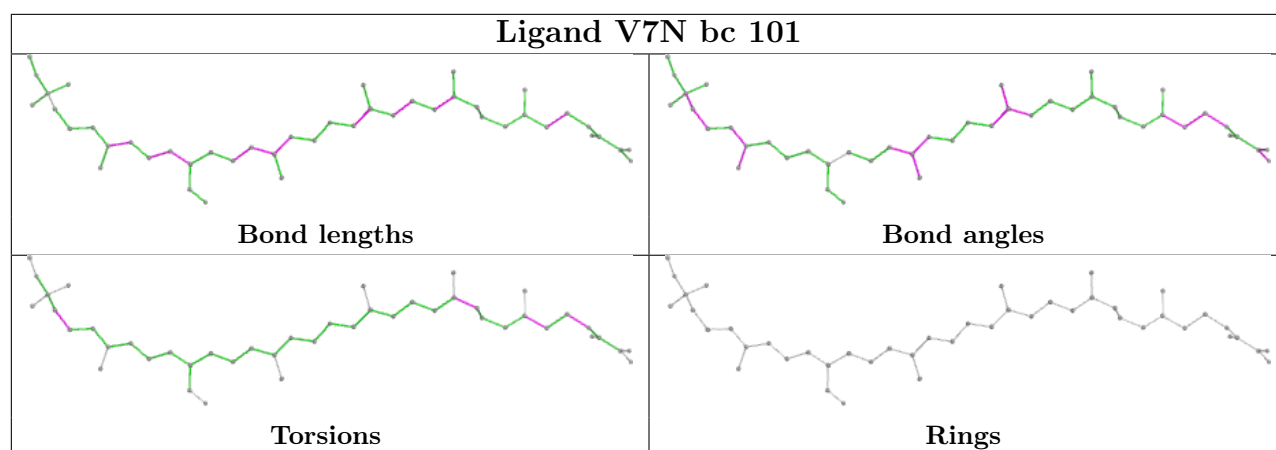


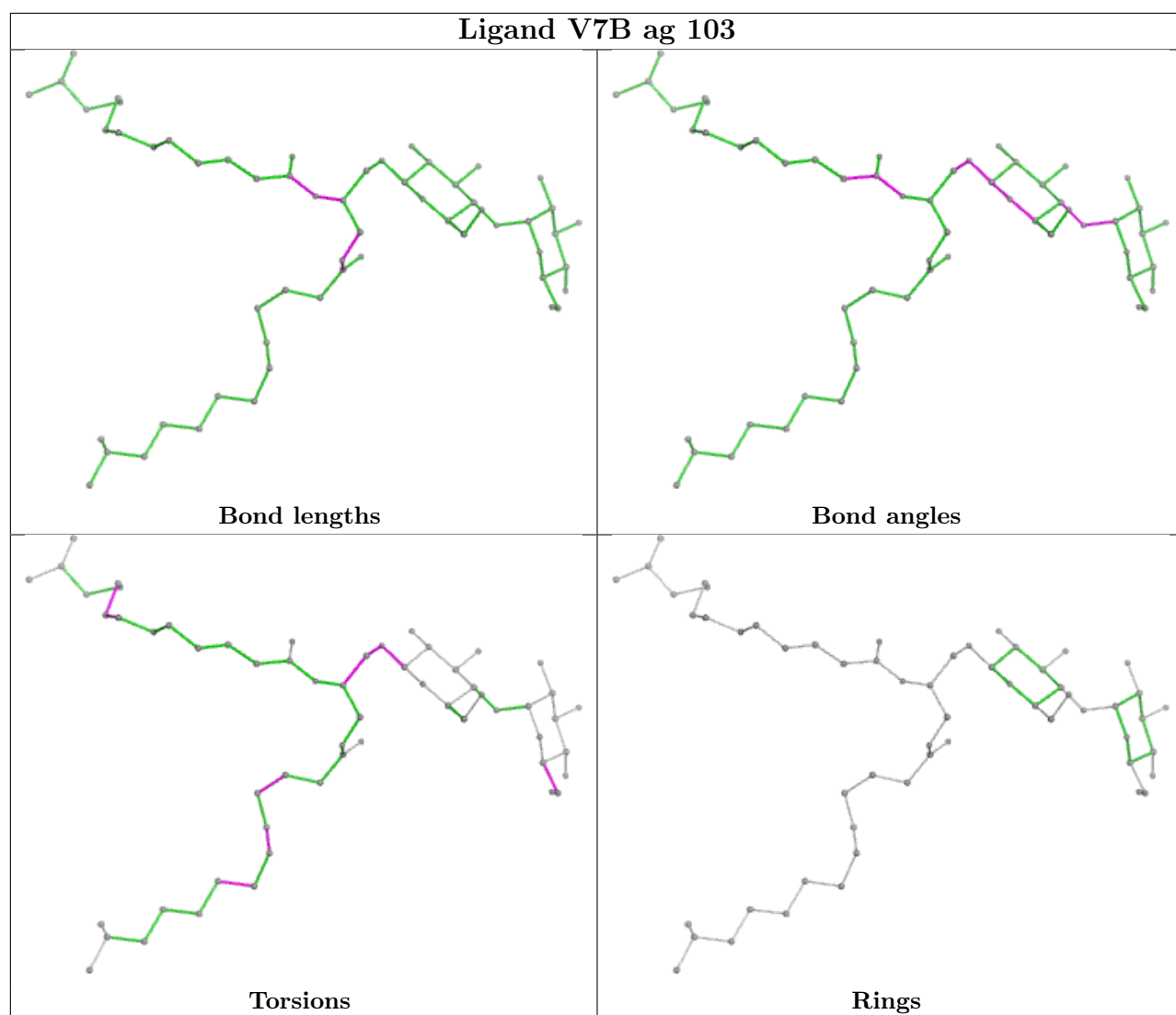
Ligand LMT bc 102

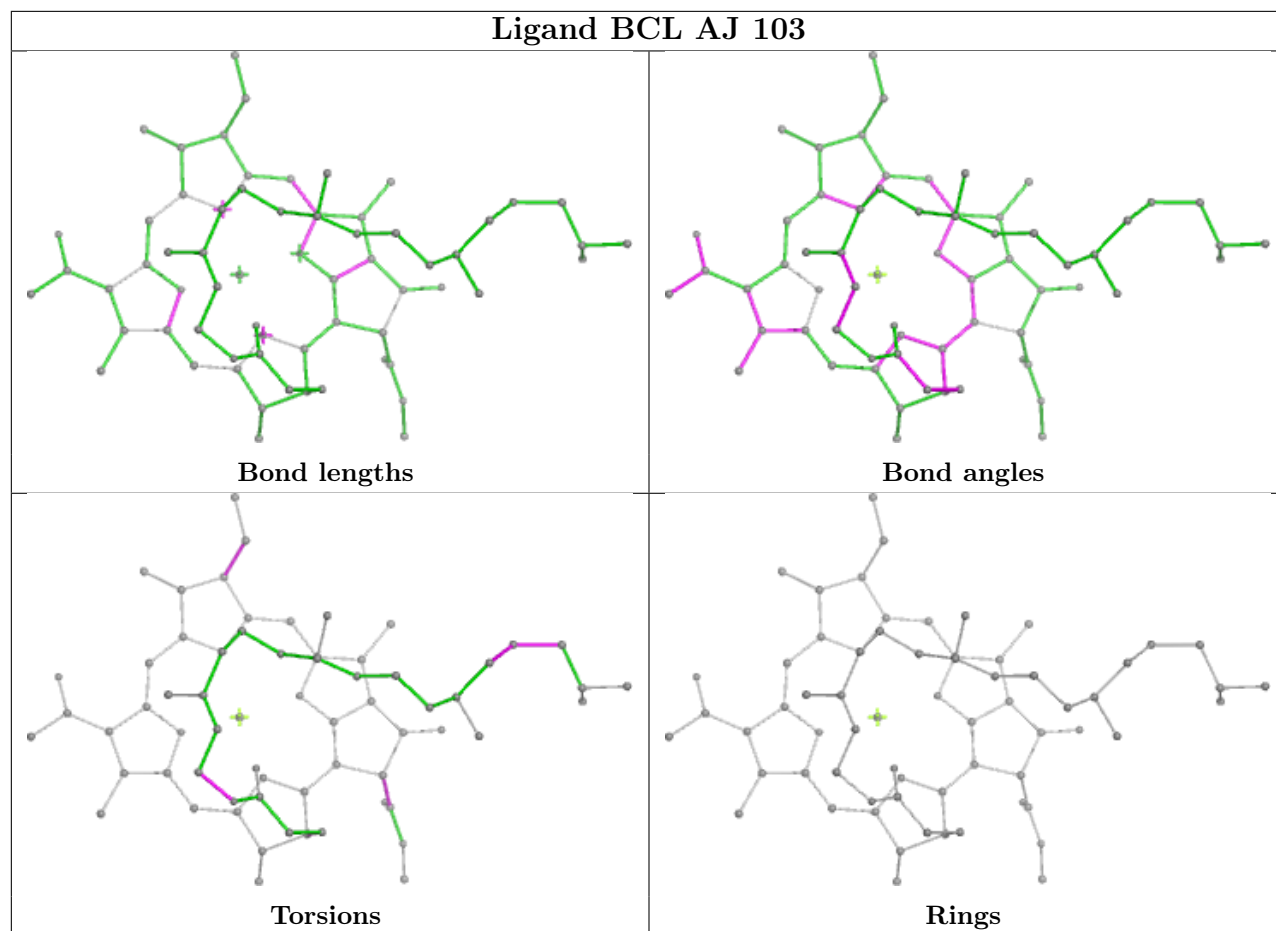
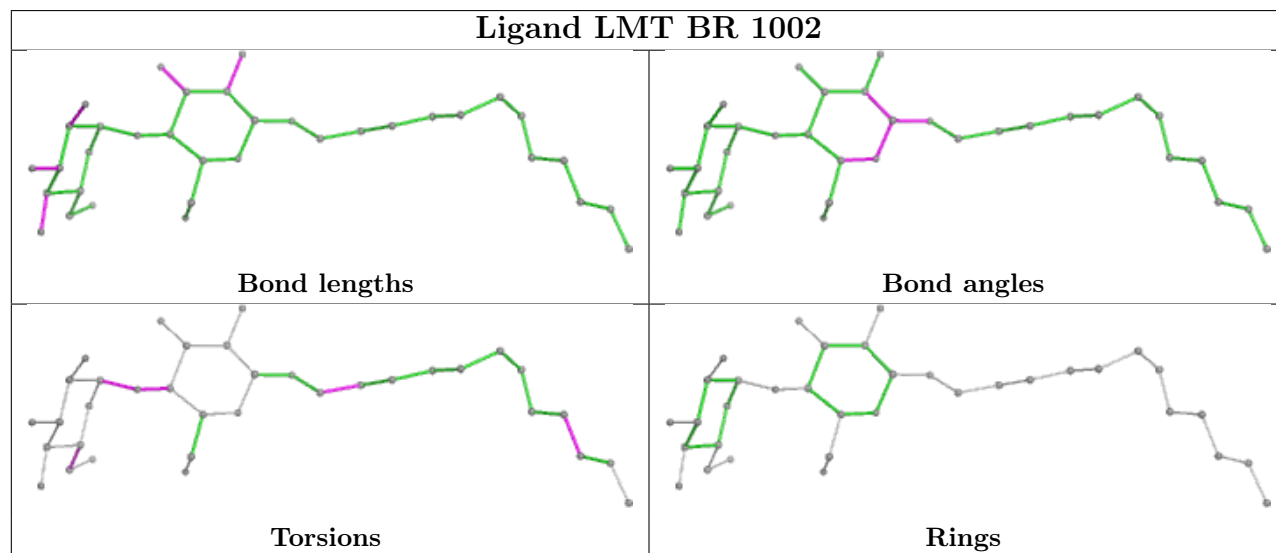




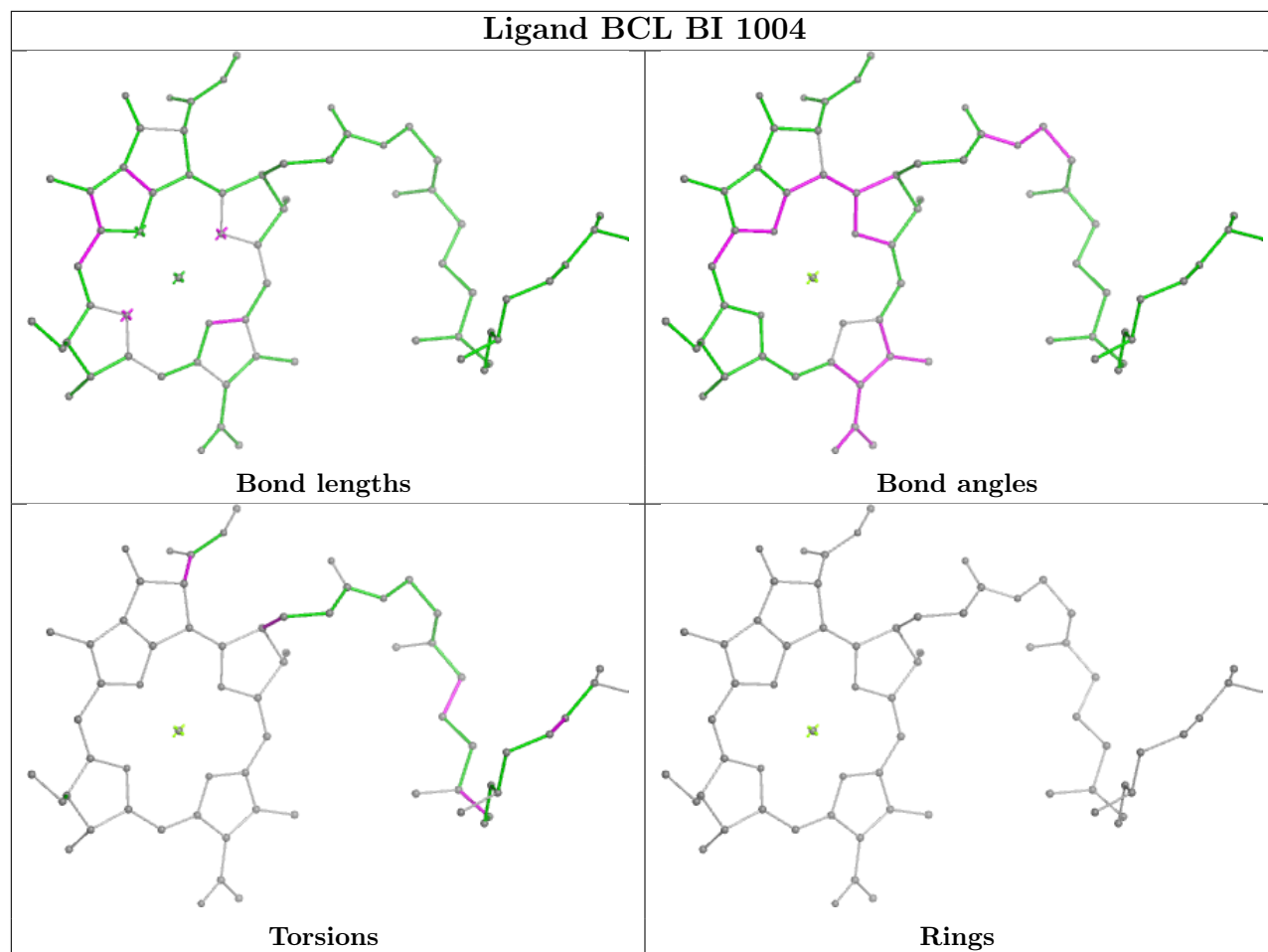


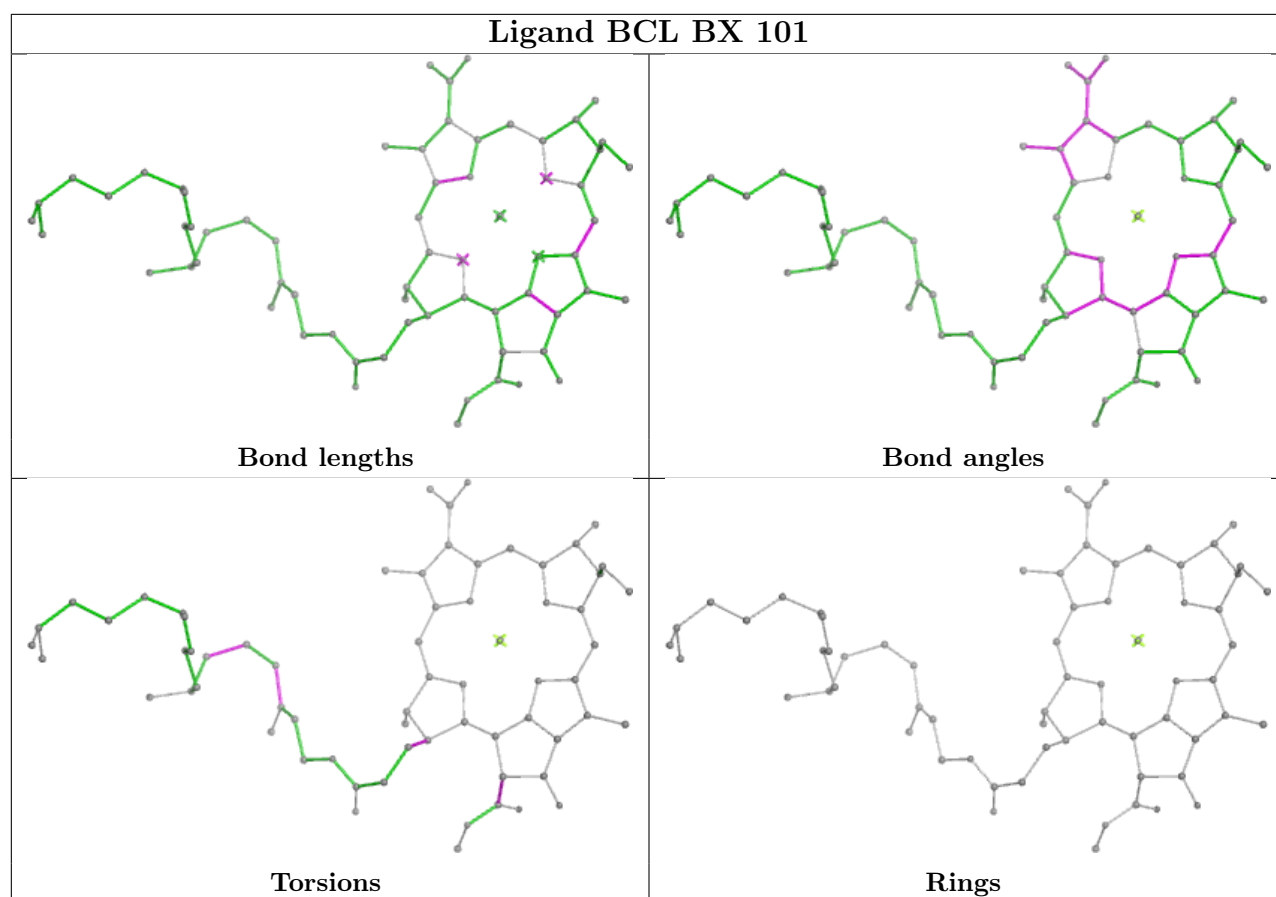




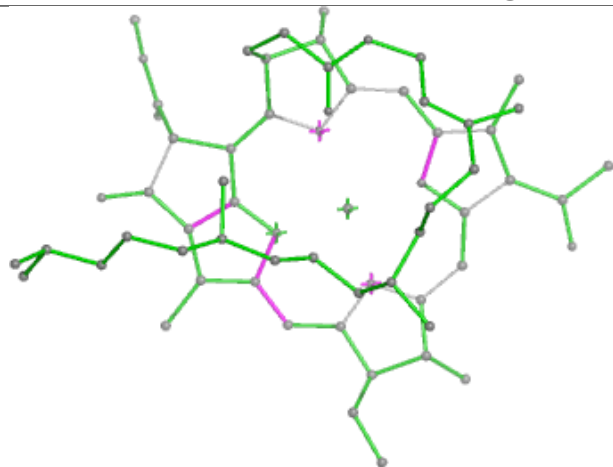
Ligand BCL AJ 103**Ligand LMT BR 1002**

Ligand BCL BI 1004

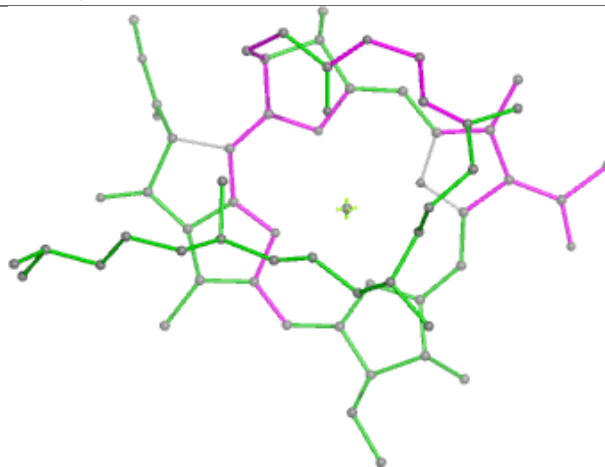




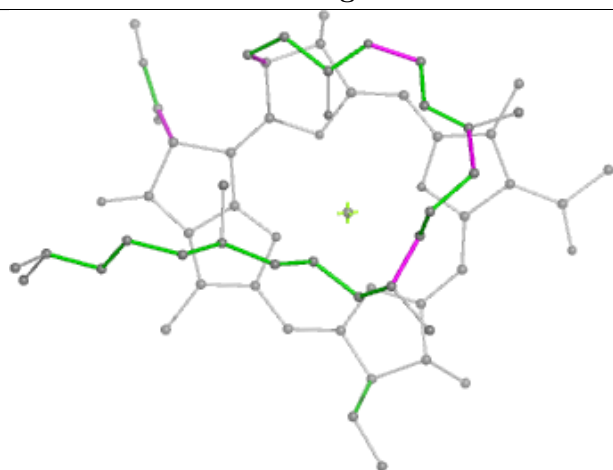
Ligand BCL AQ 102



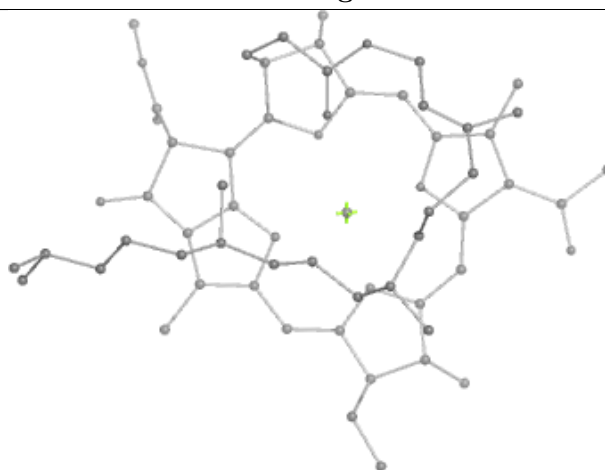
Bond lengths



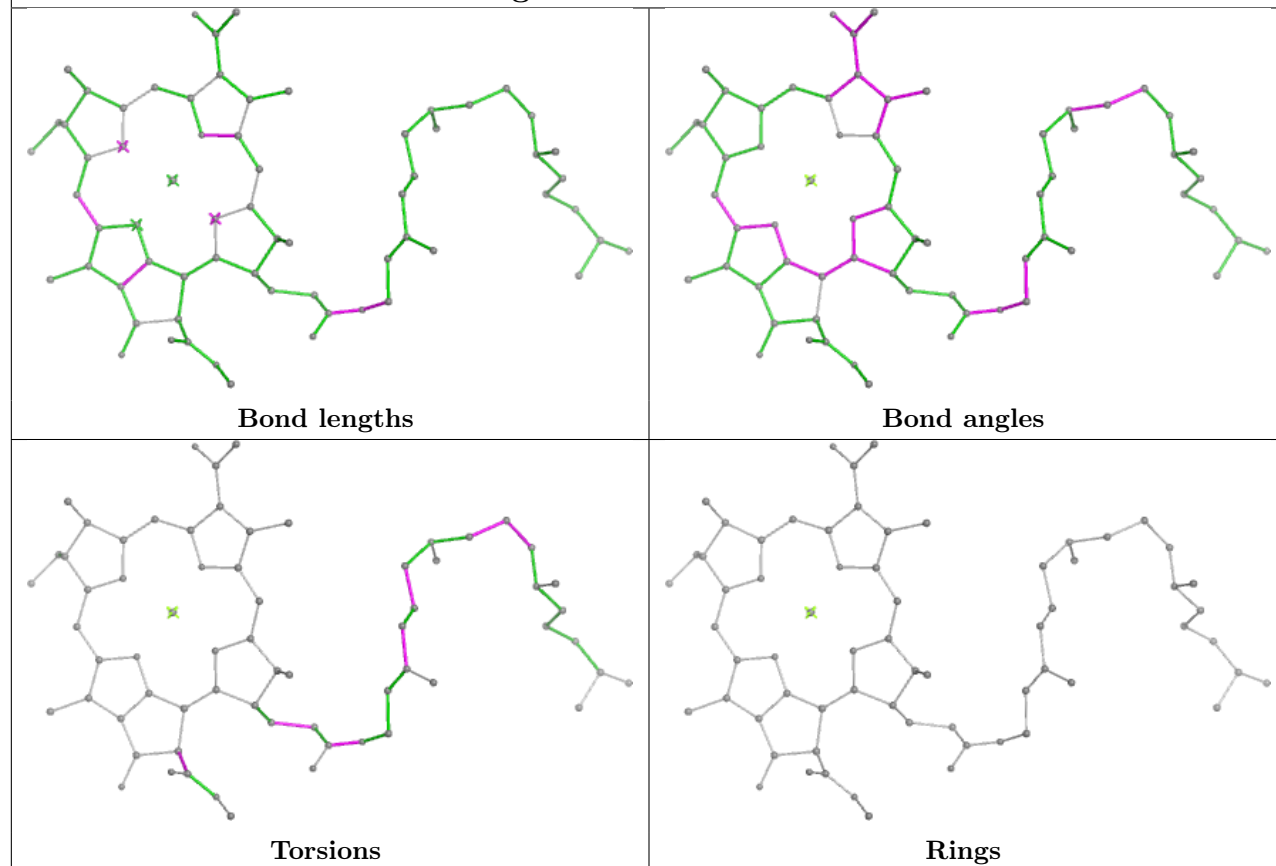
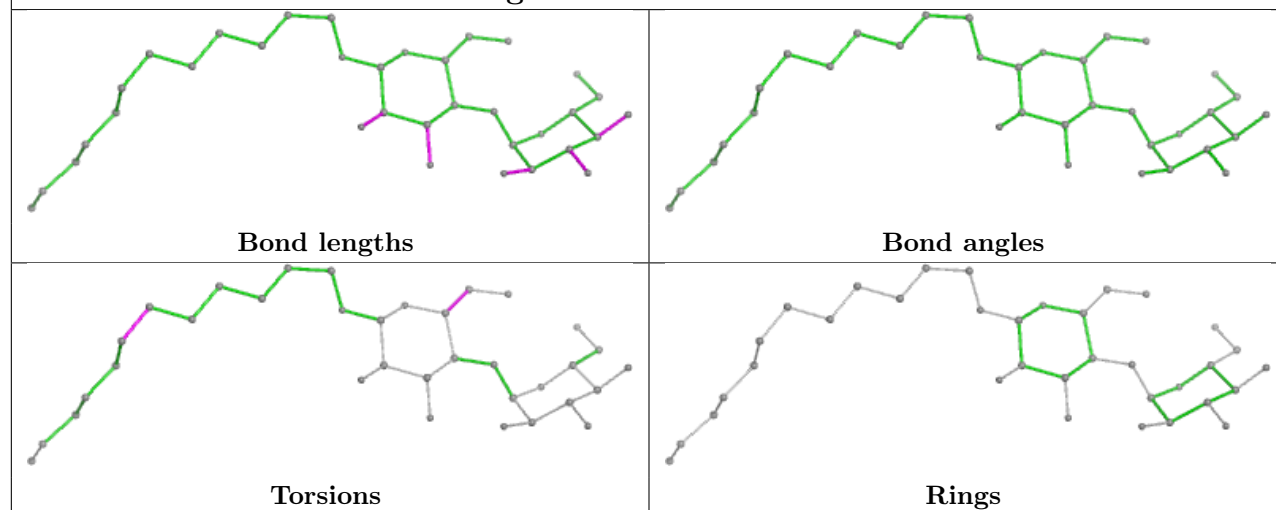
Bond angles

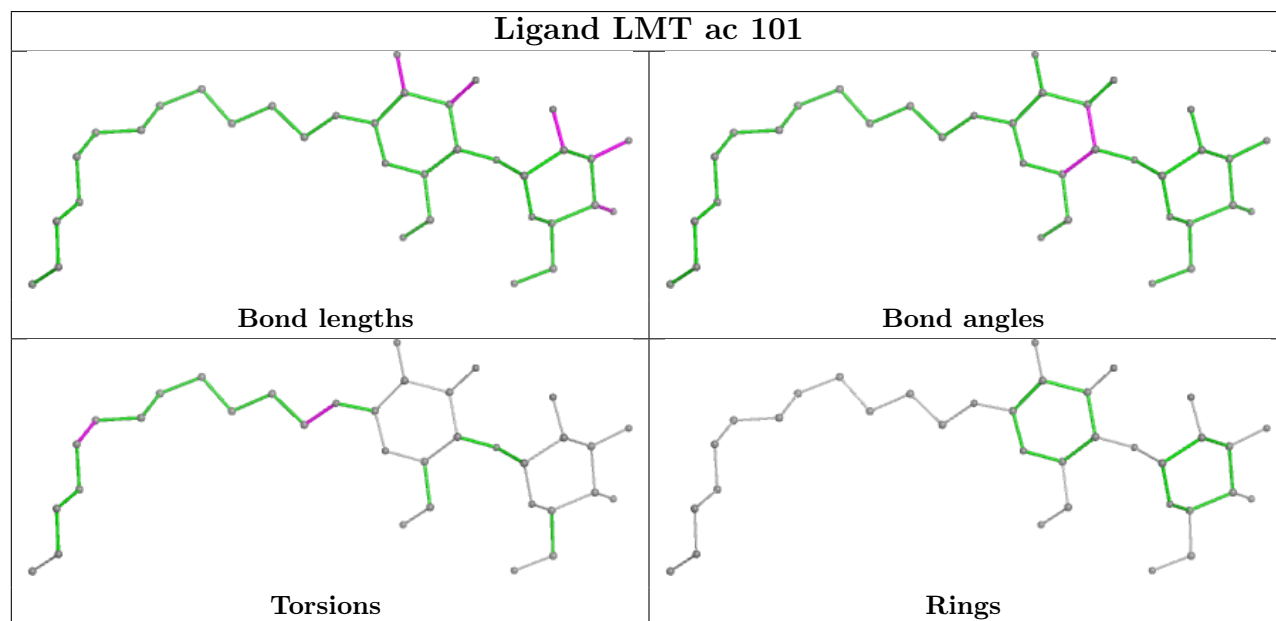
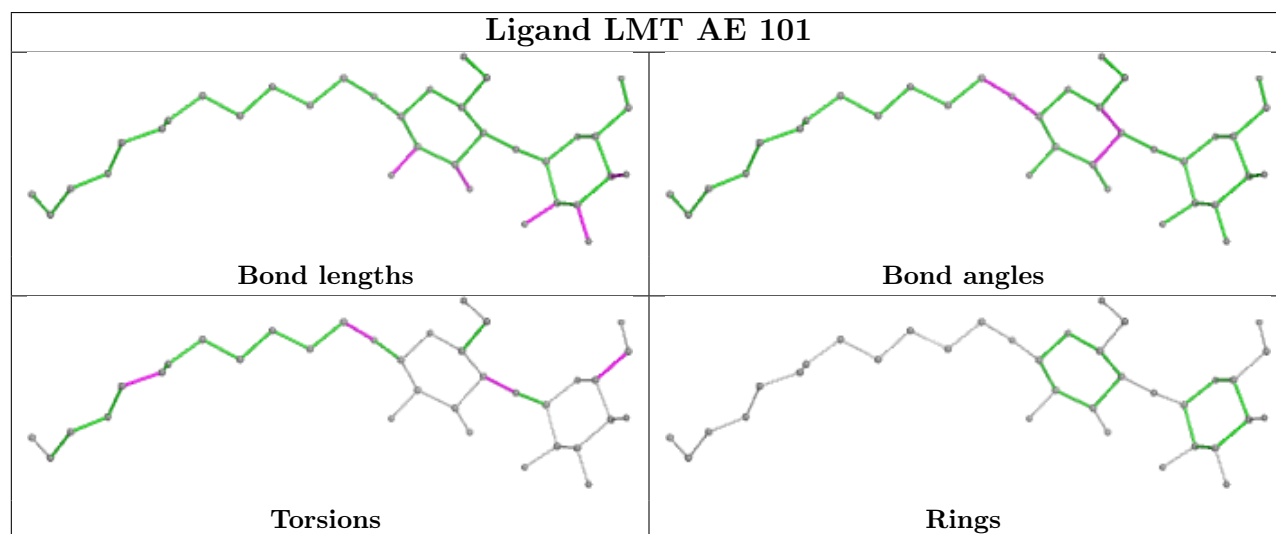
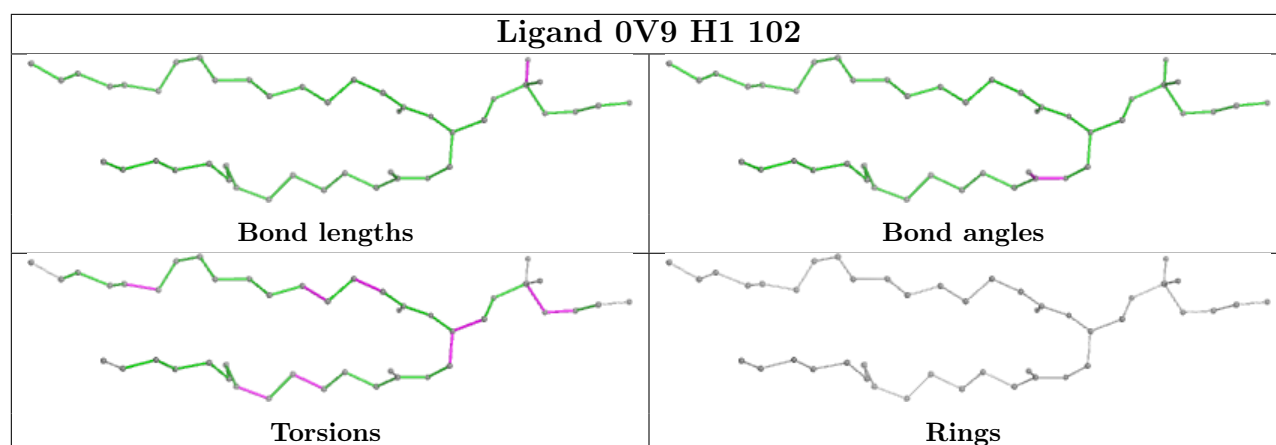


Torsions

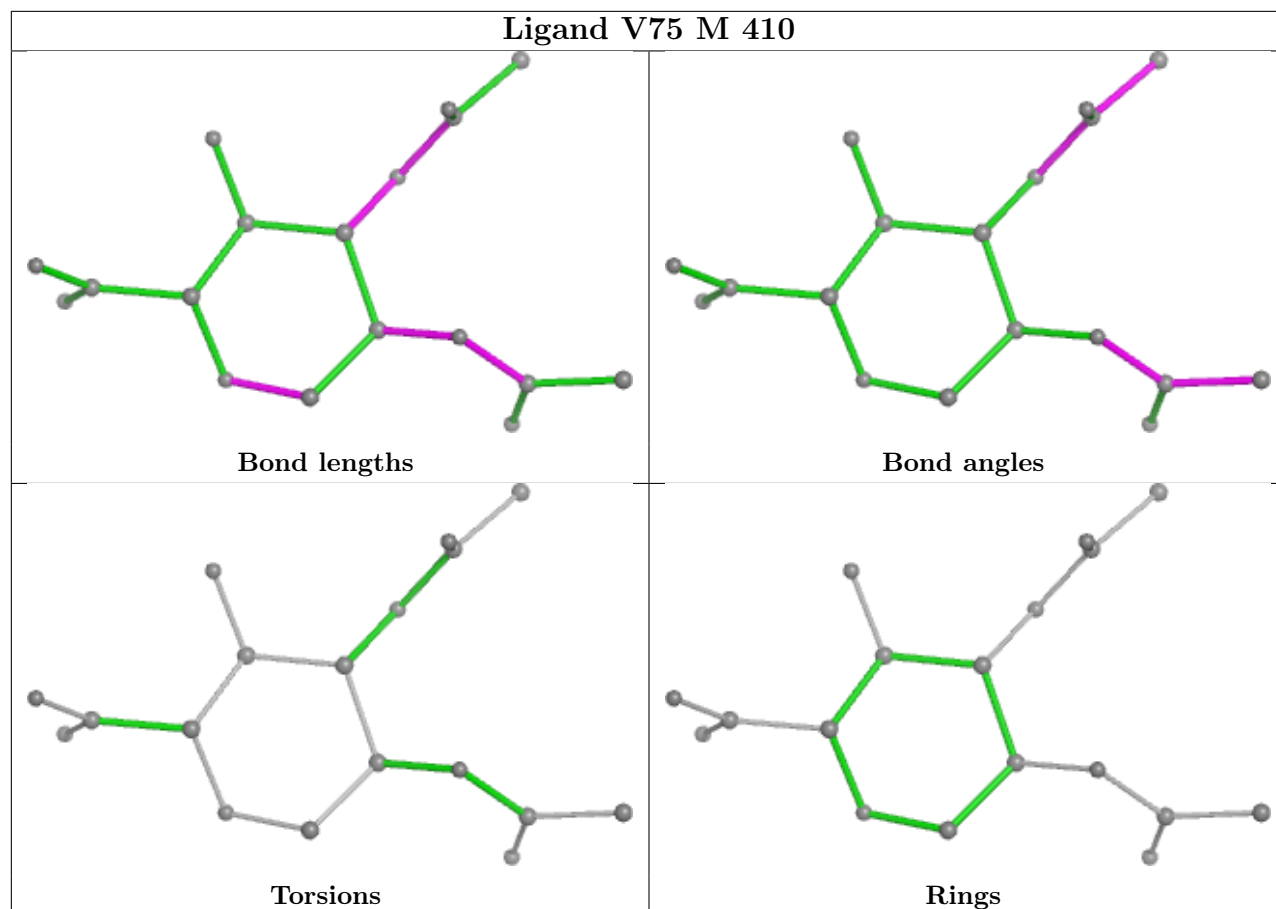


Rings

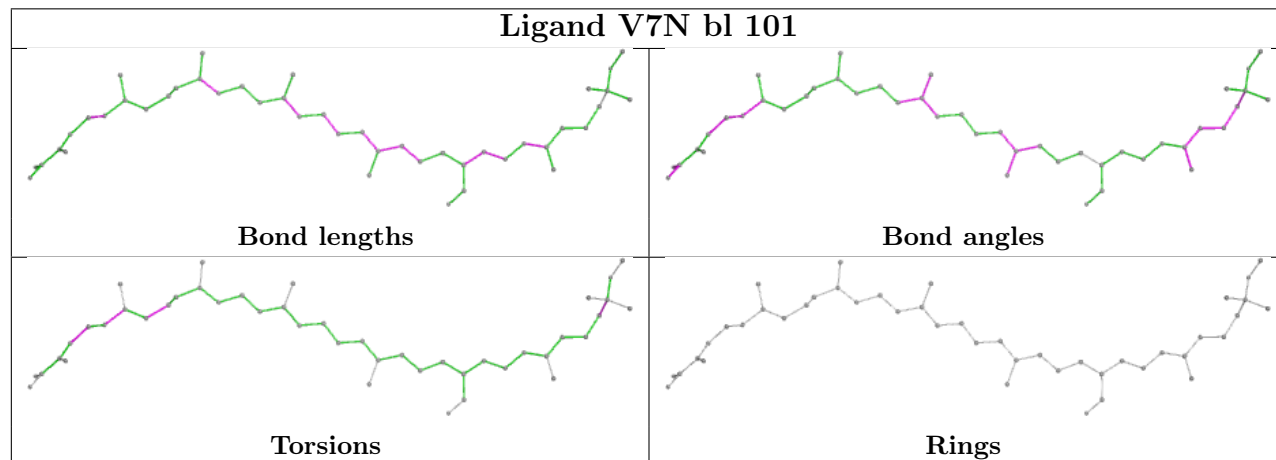
Ligand BCL BP 1003**Ligand LMT BN 1002**

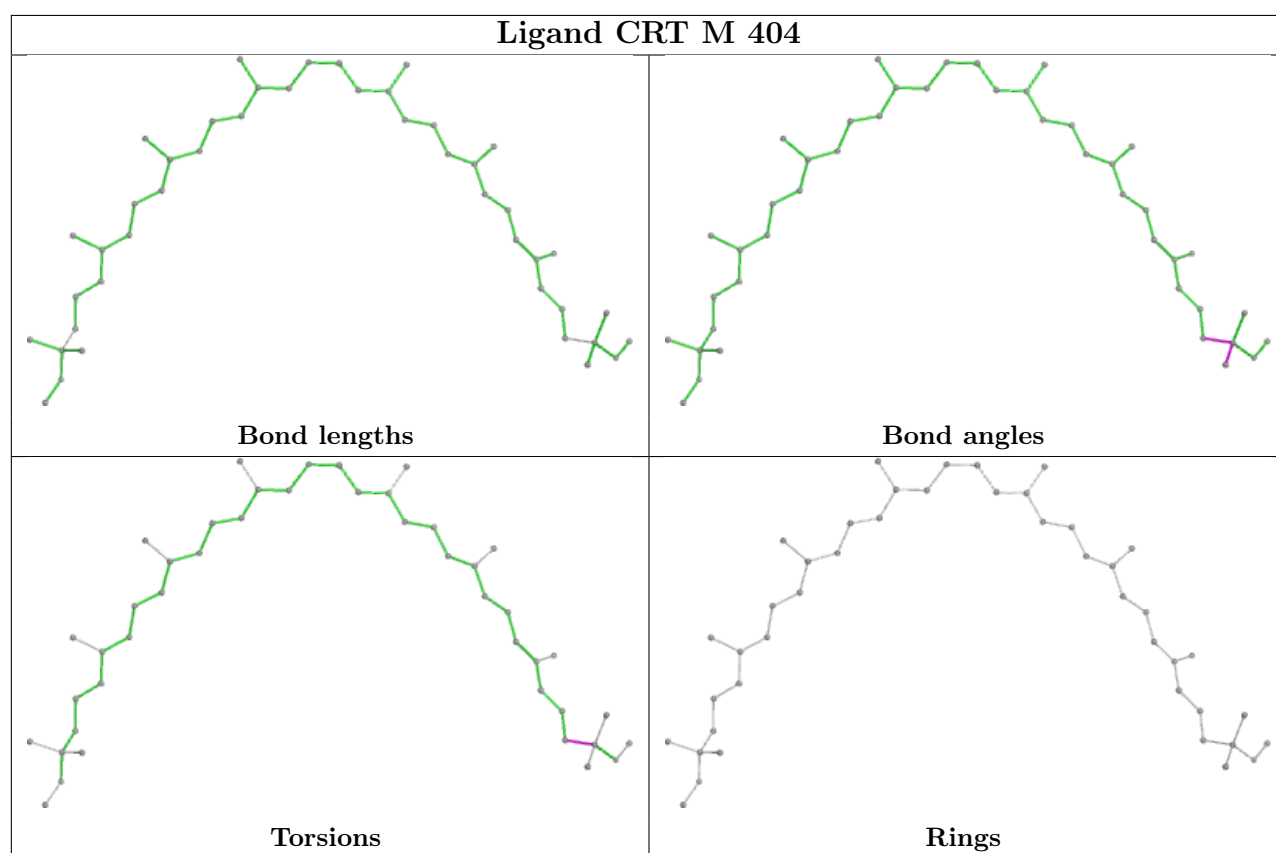
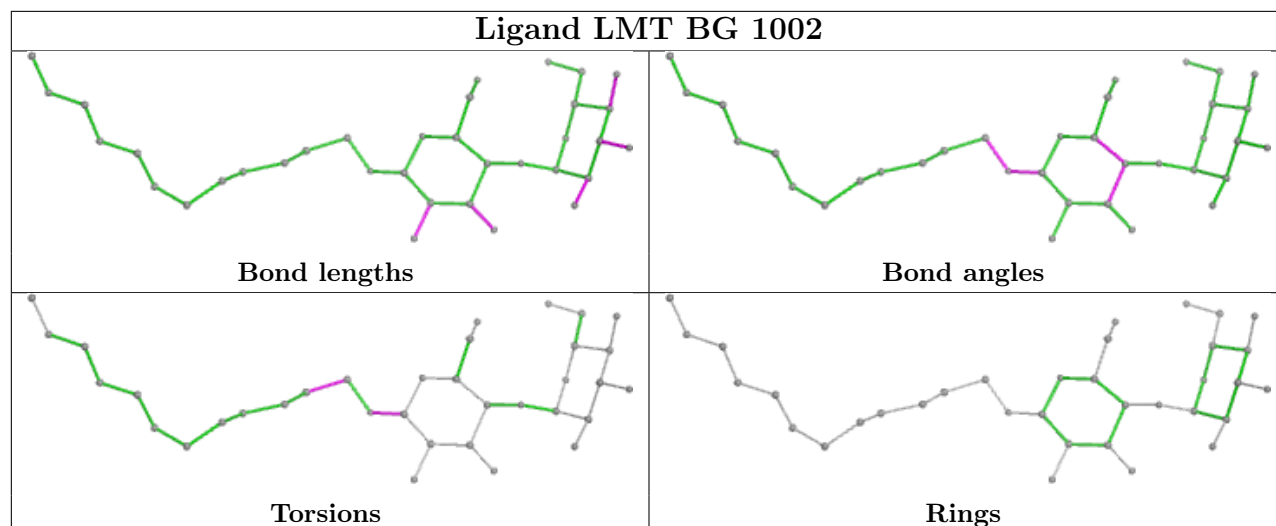


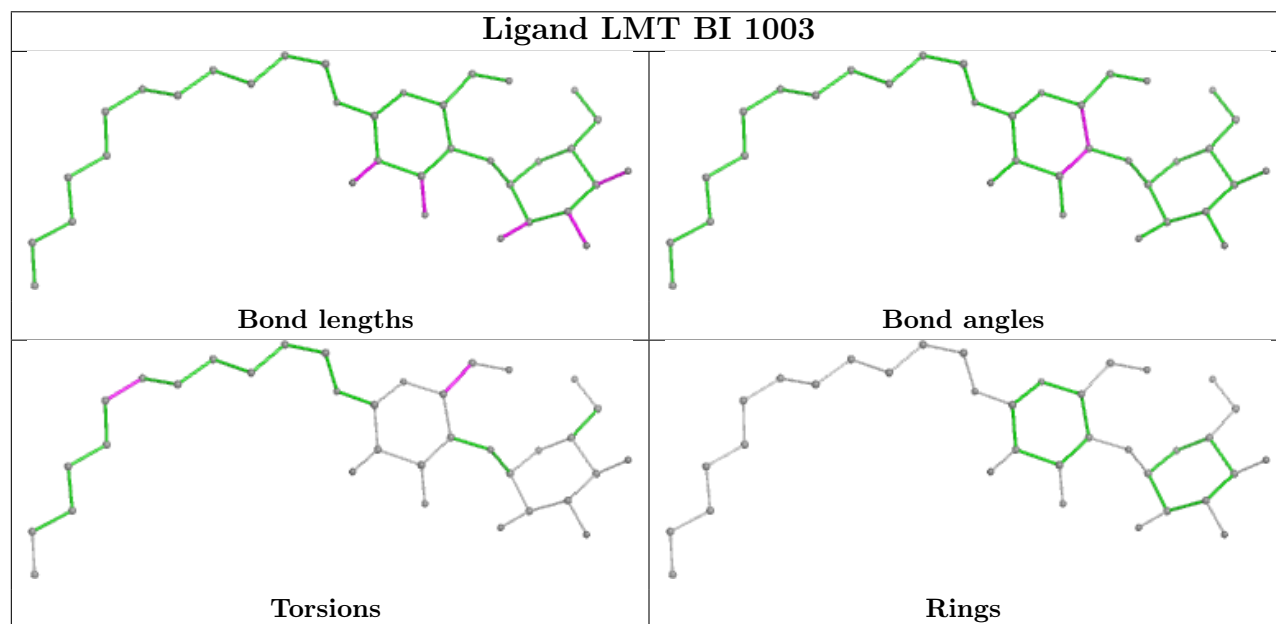
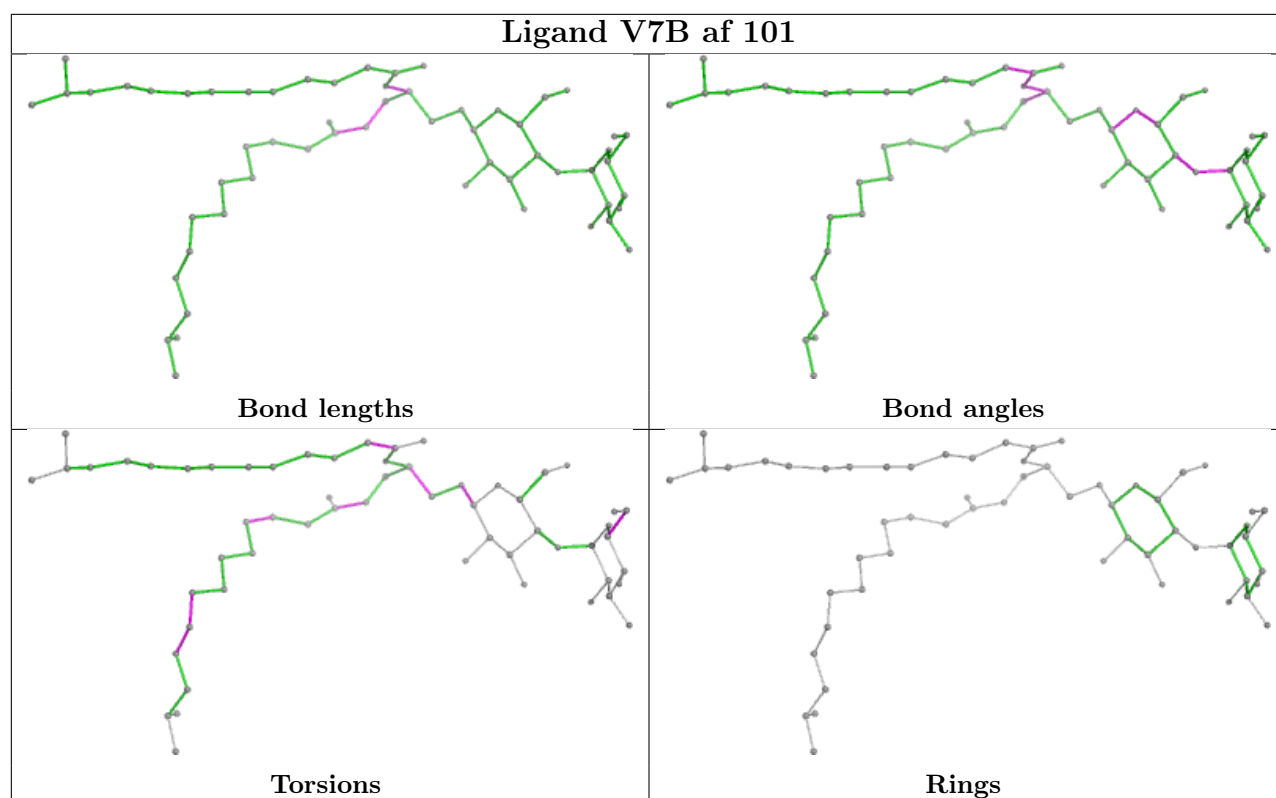
Ligand V75 M 410

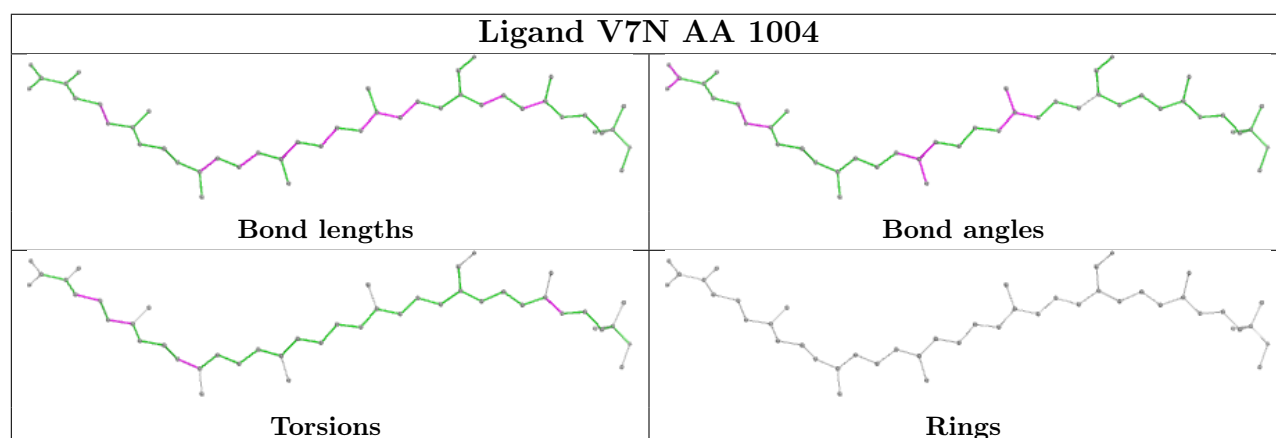
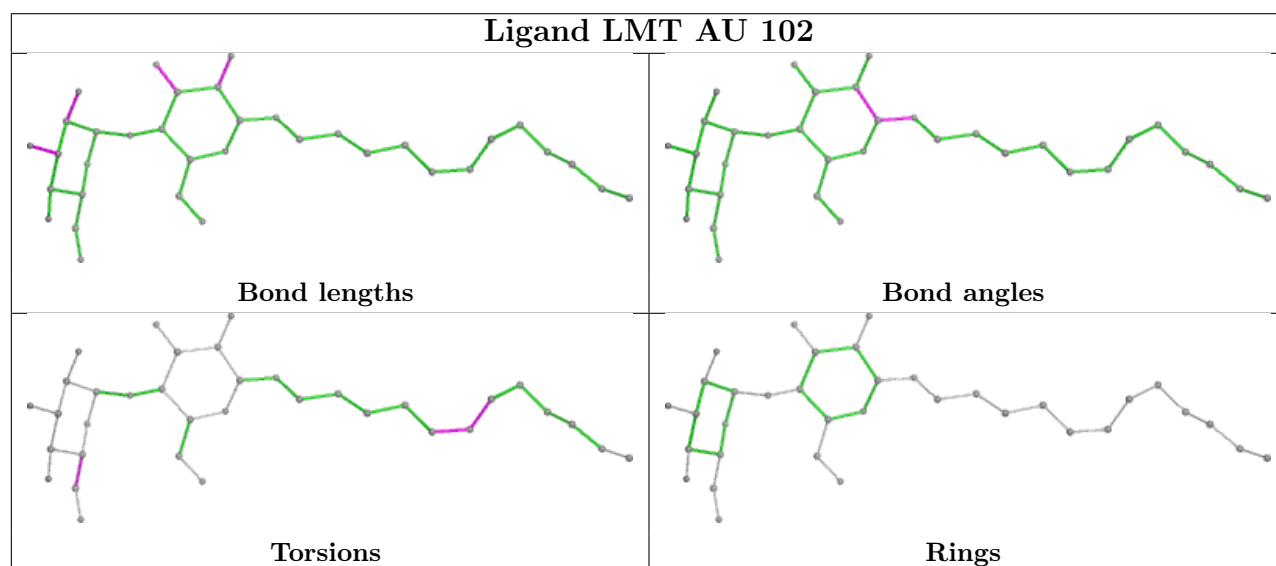
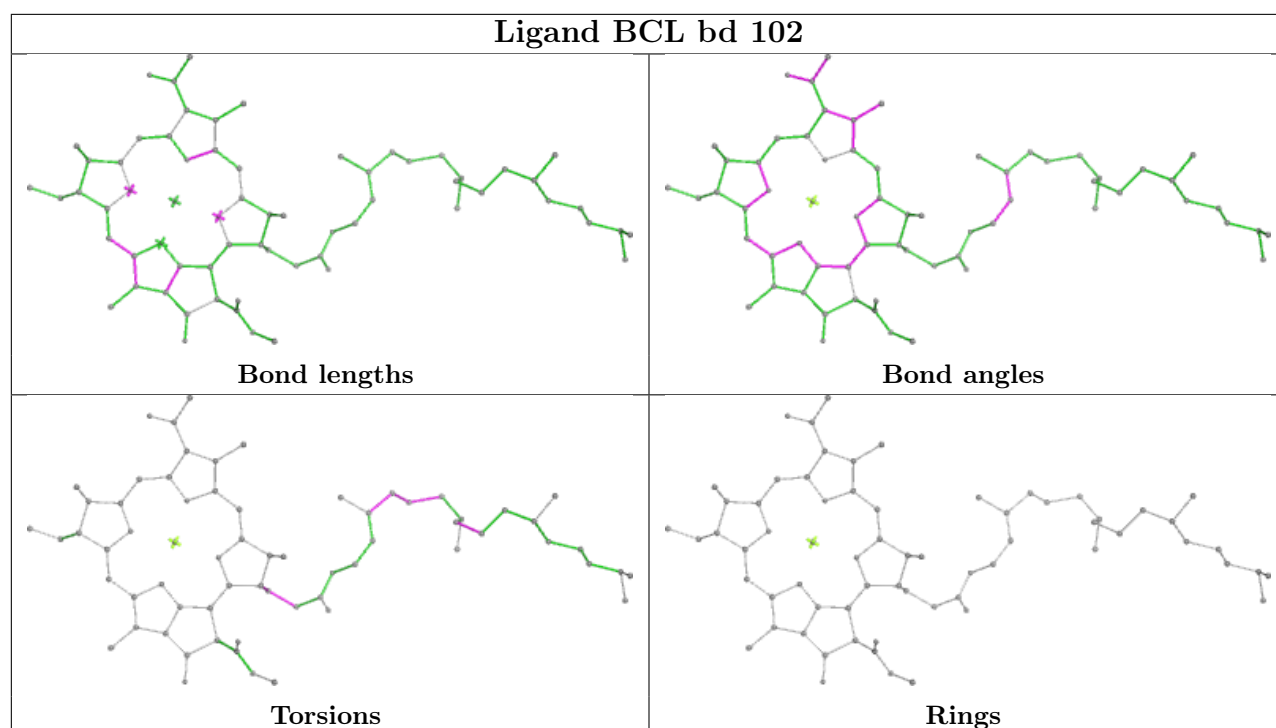


Ligand V7N bl 101

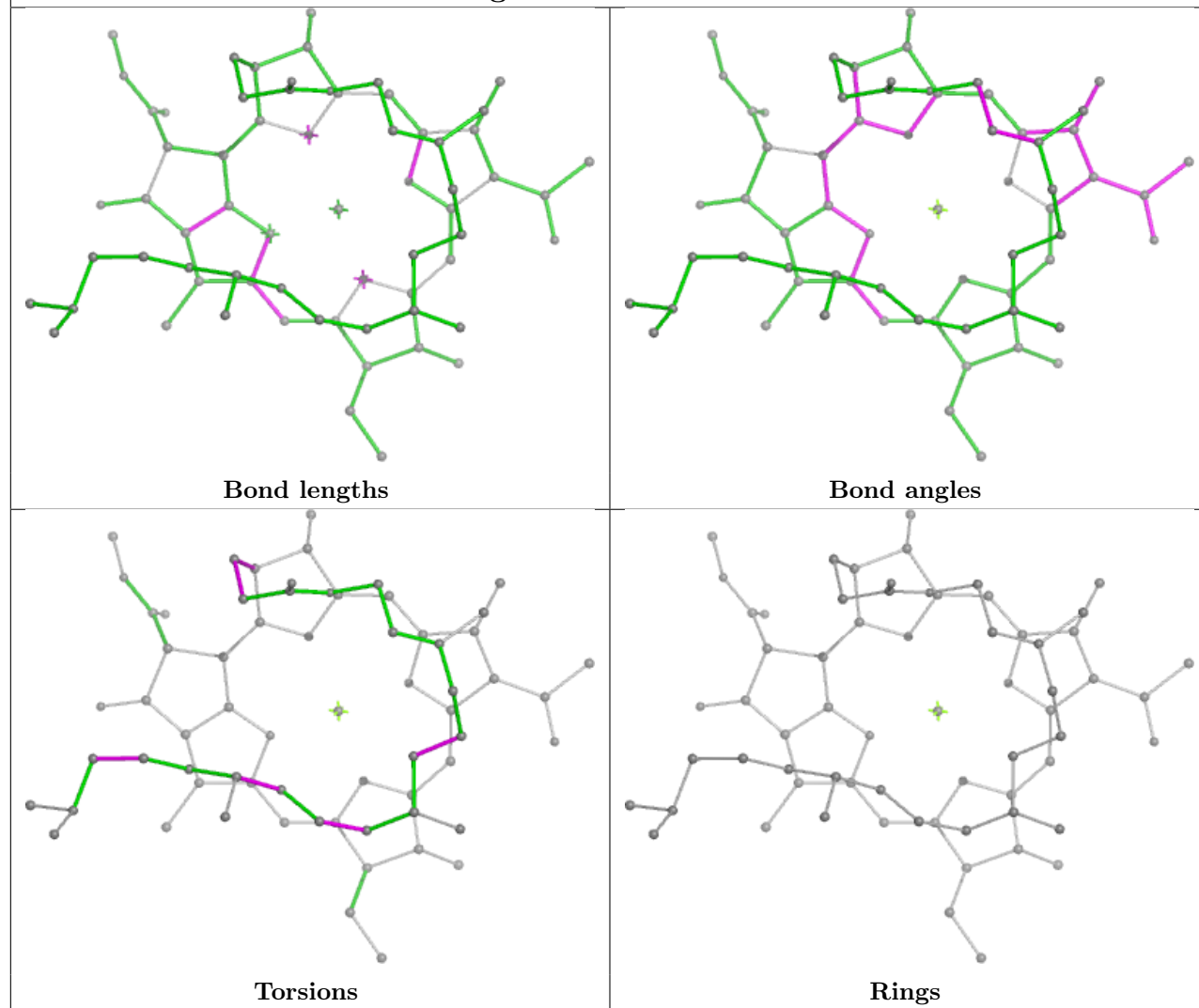




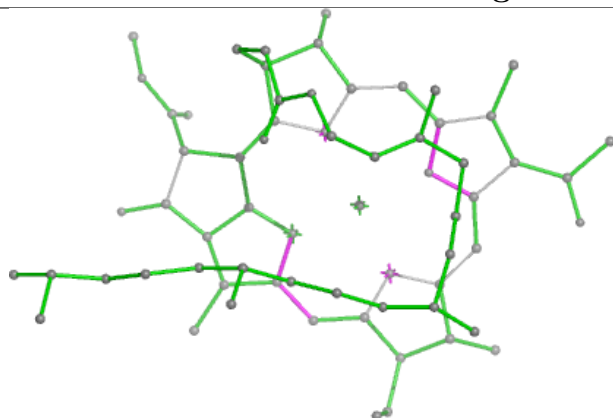




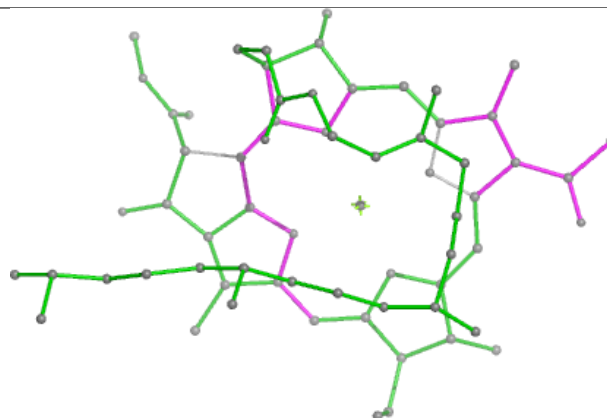
Ligand BCL AT 103



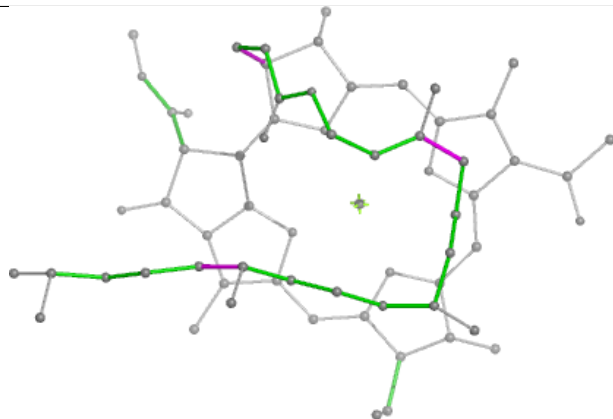
Ligand BCL AB 1002



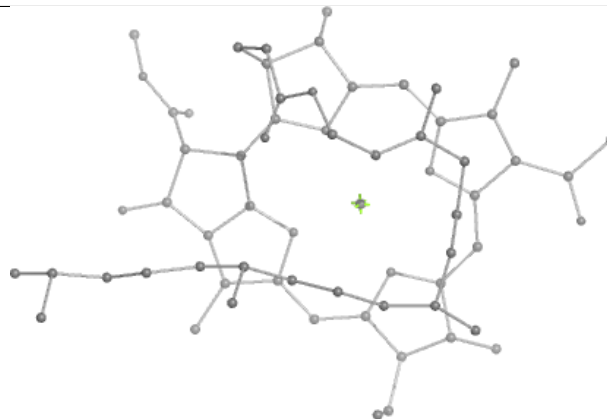
Bond lengths



Bond angles

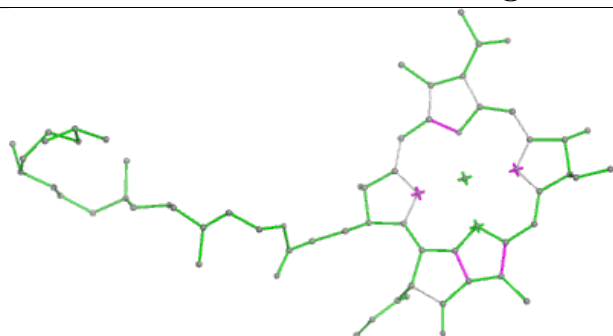


Torsions

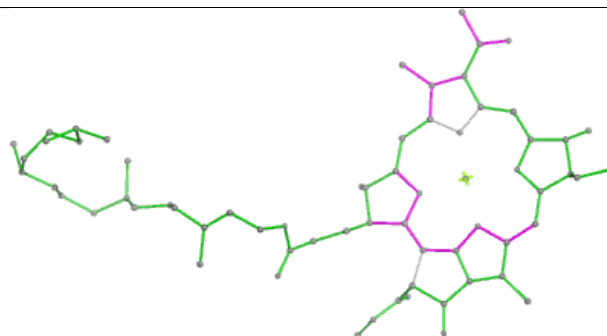


Rings

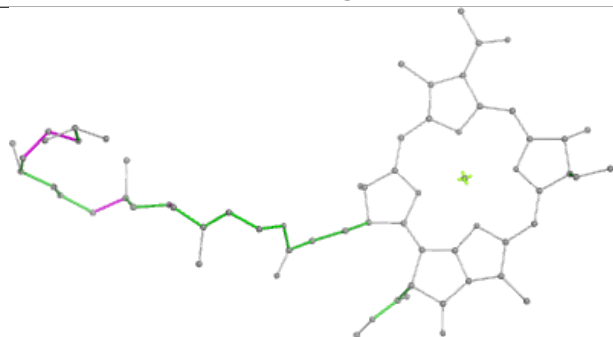
Ligand BCL ae 1001



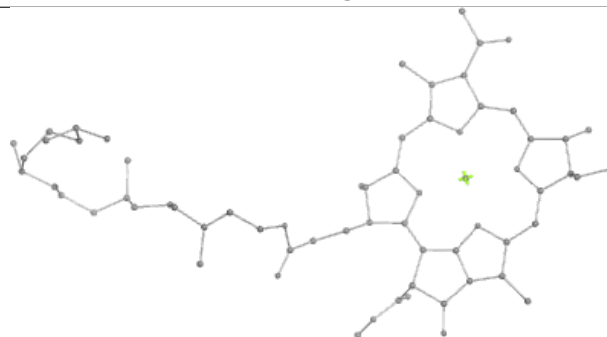
Bond lengths



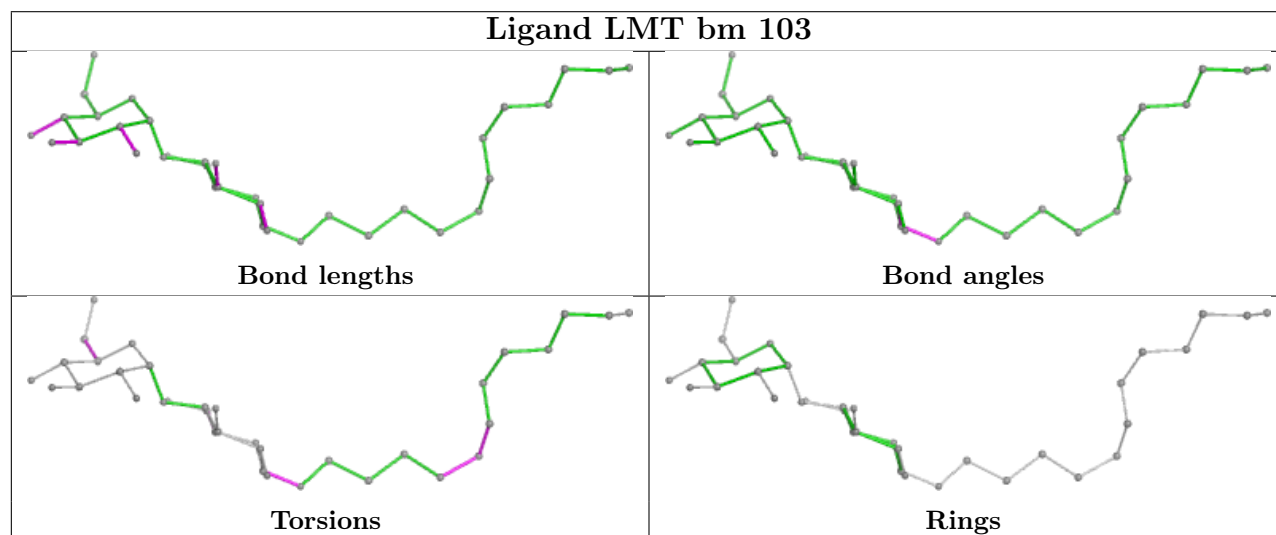
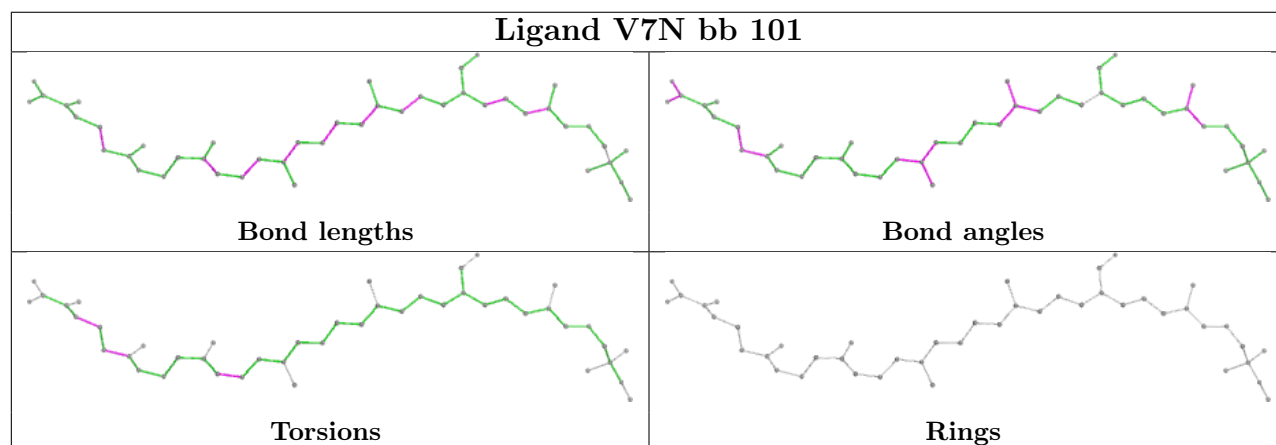
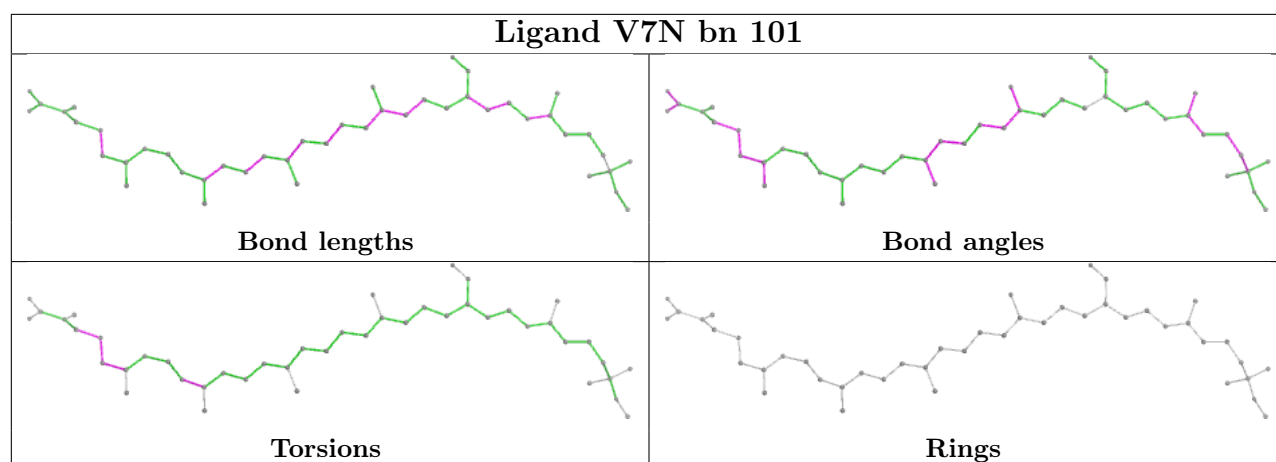
Bond angles

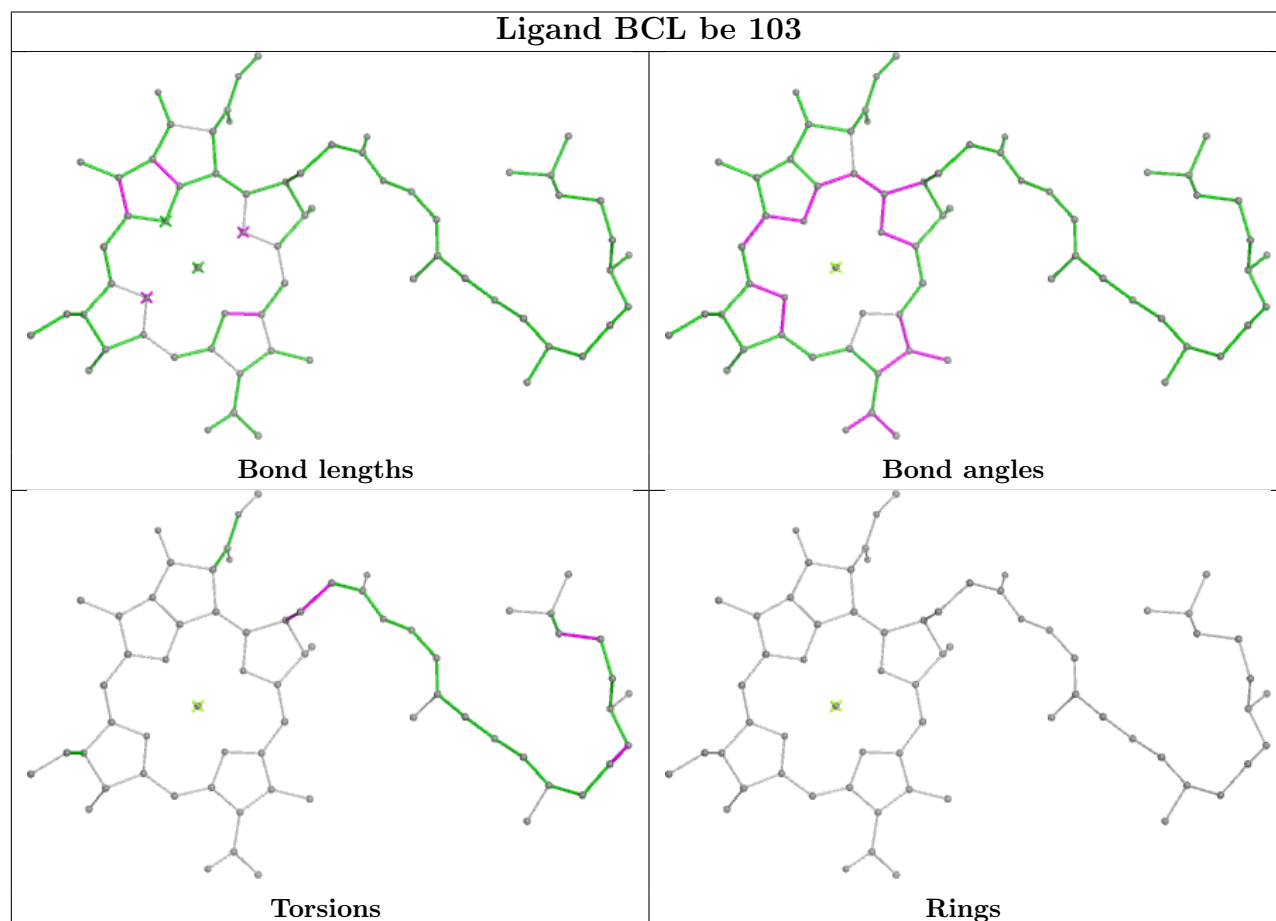
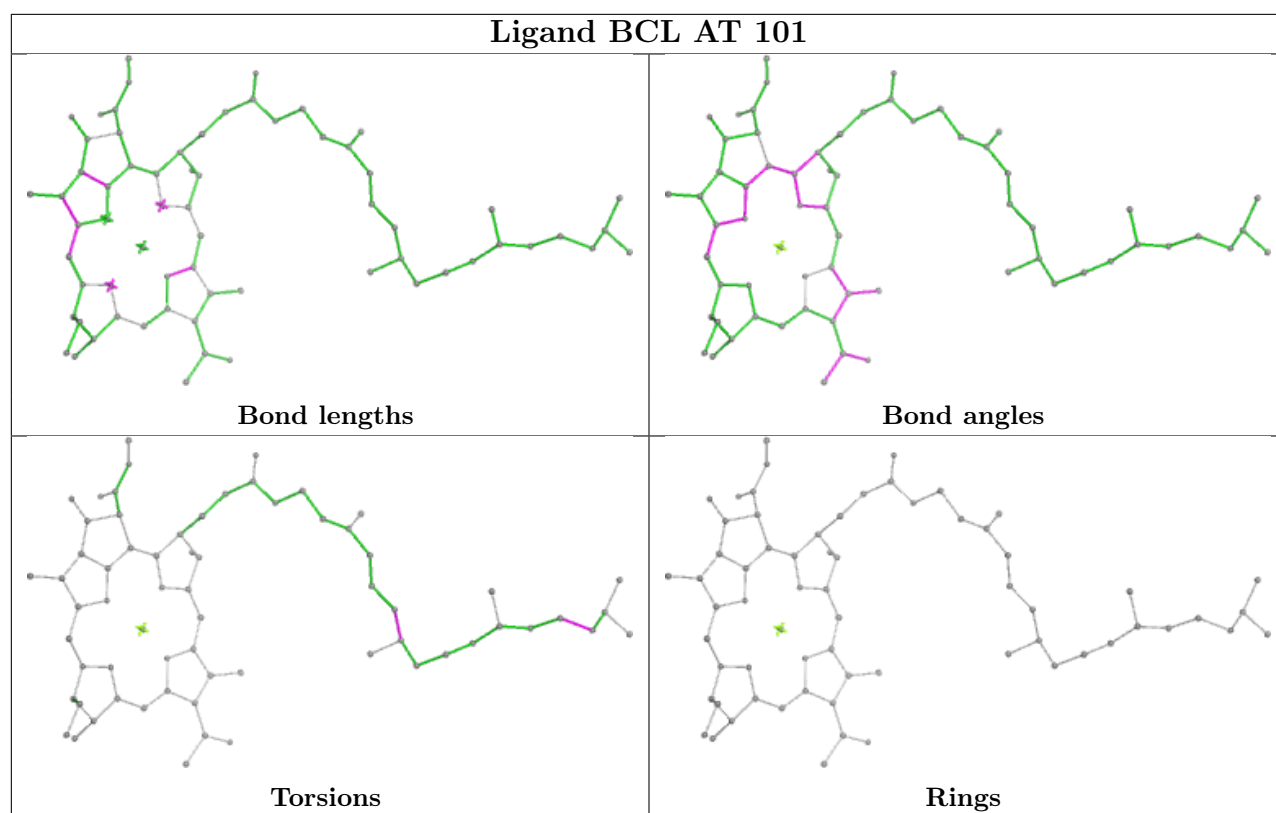


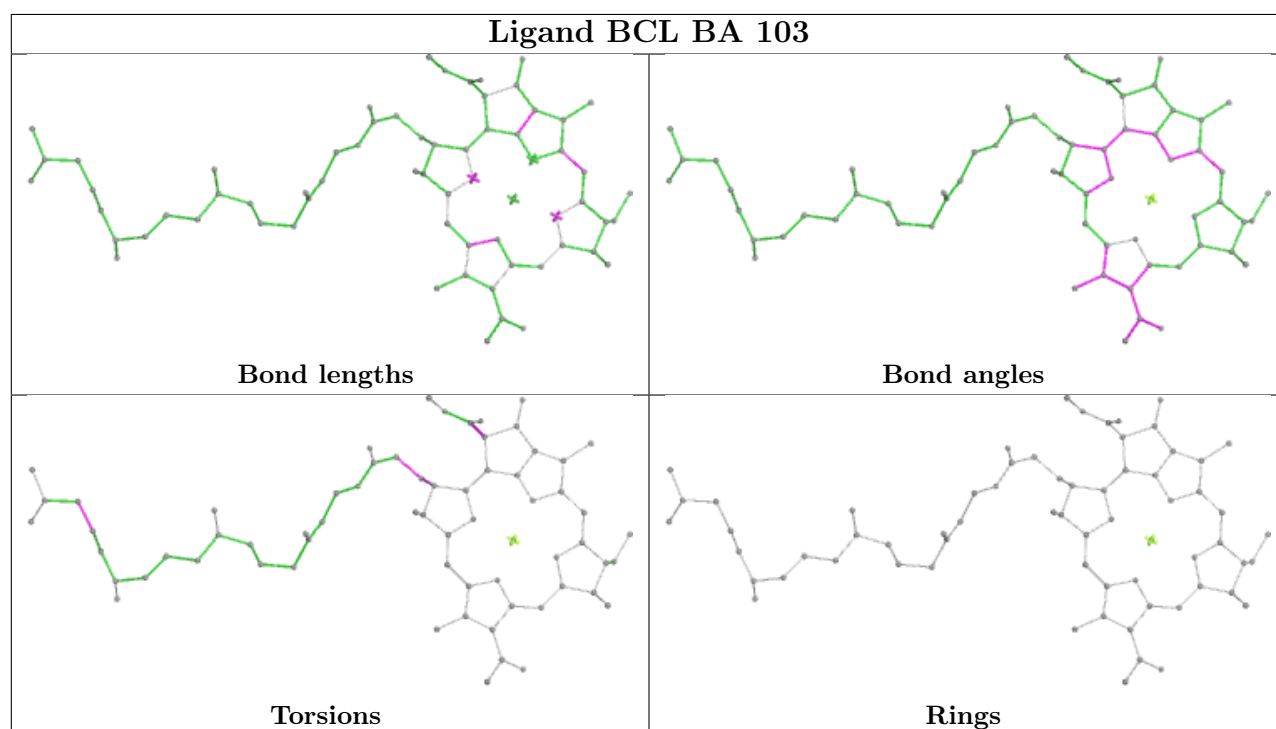
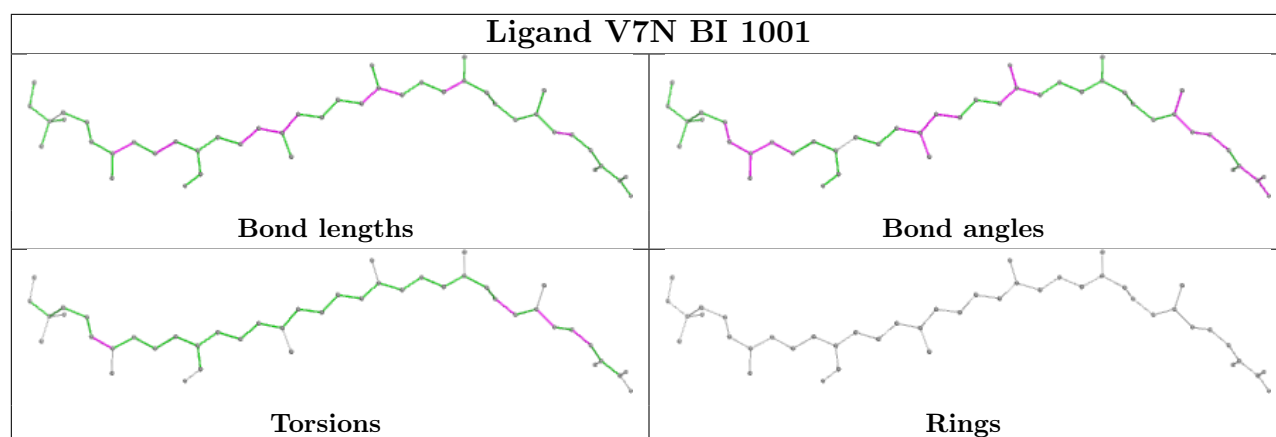
Torsions



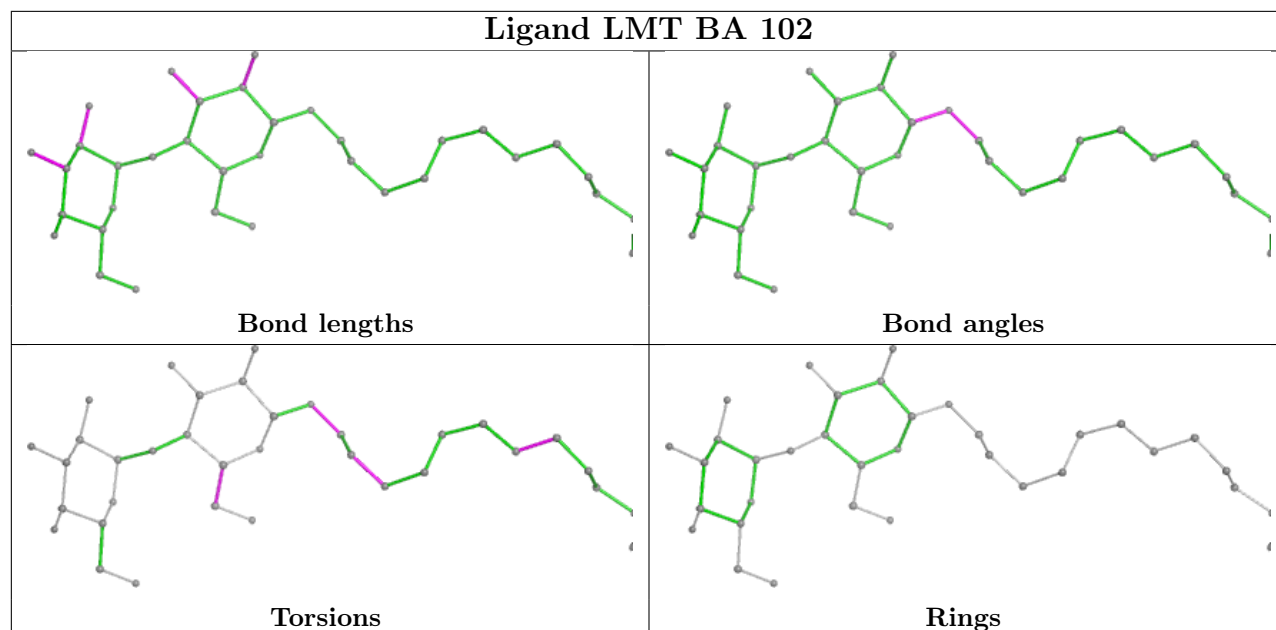
Rings



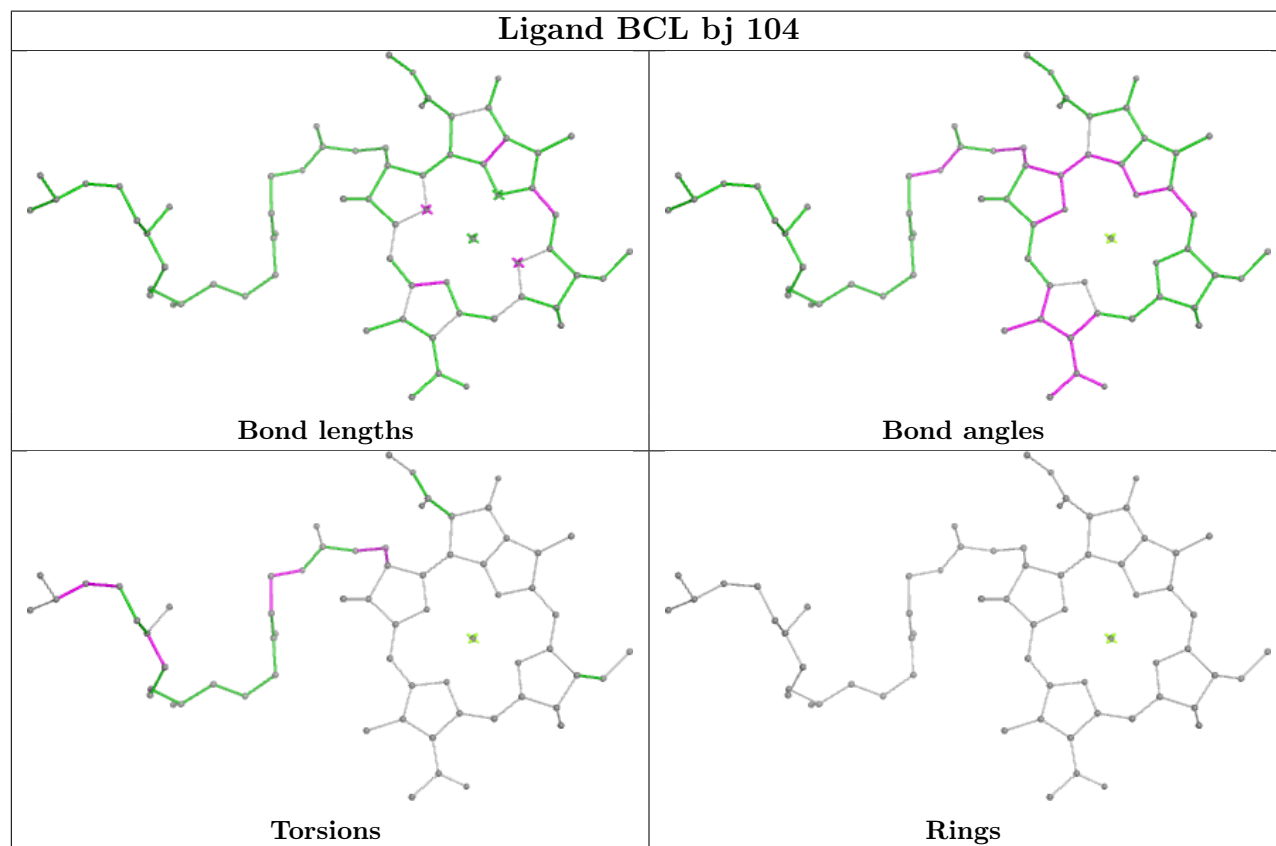


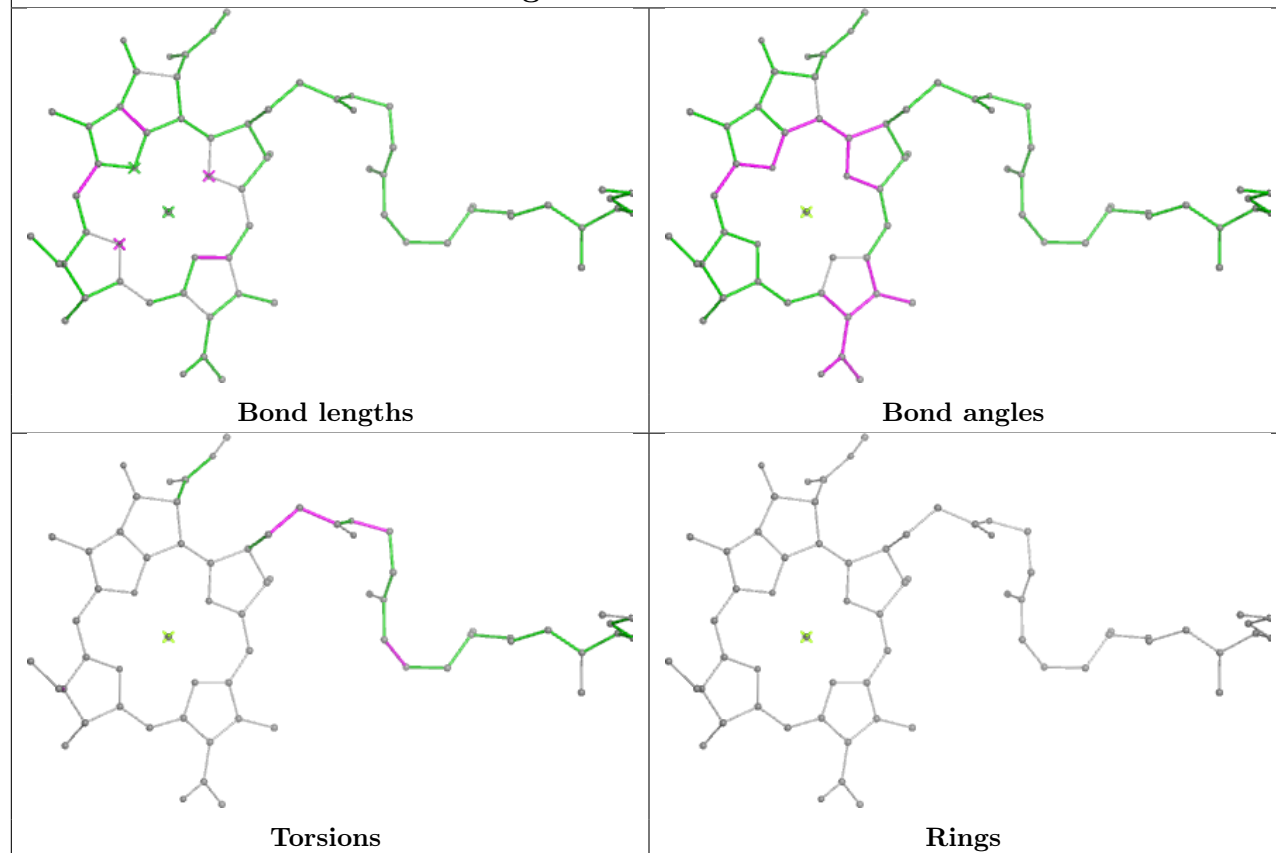
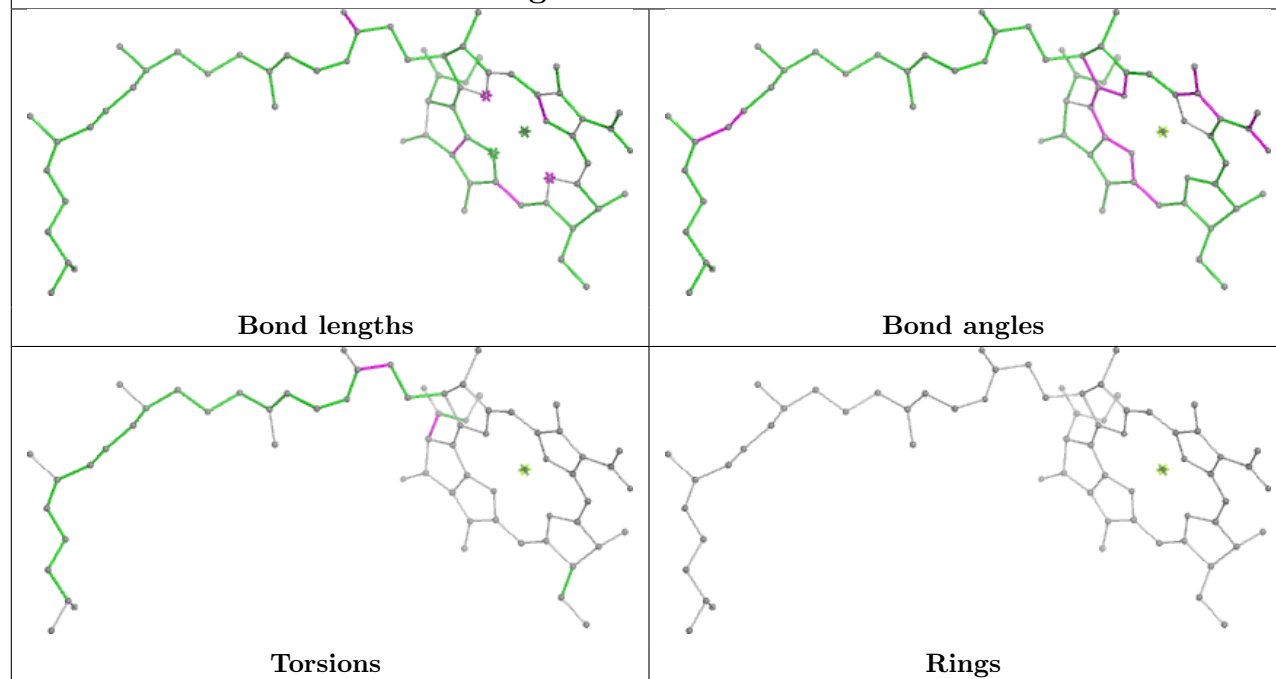


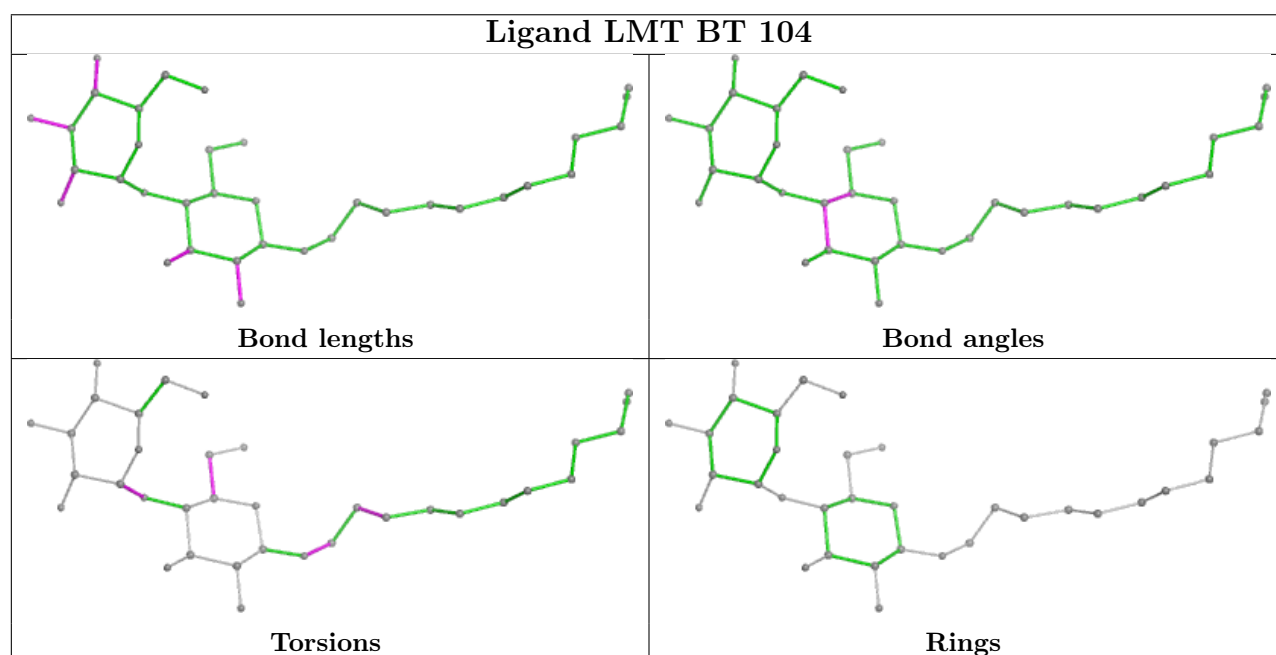
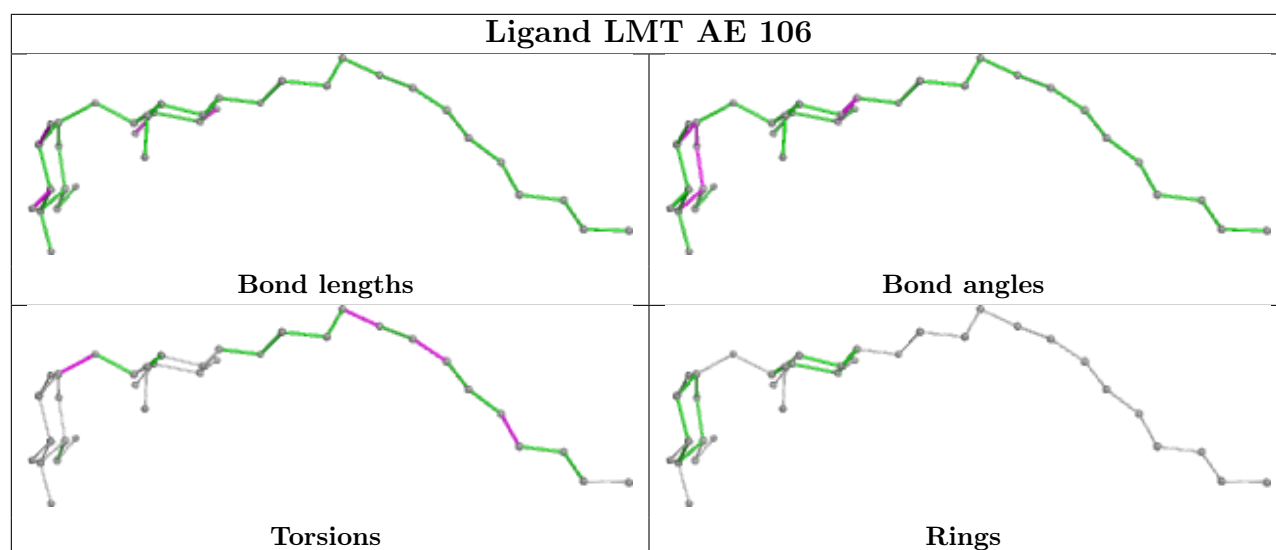
Ligand LMT BA 102

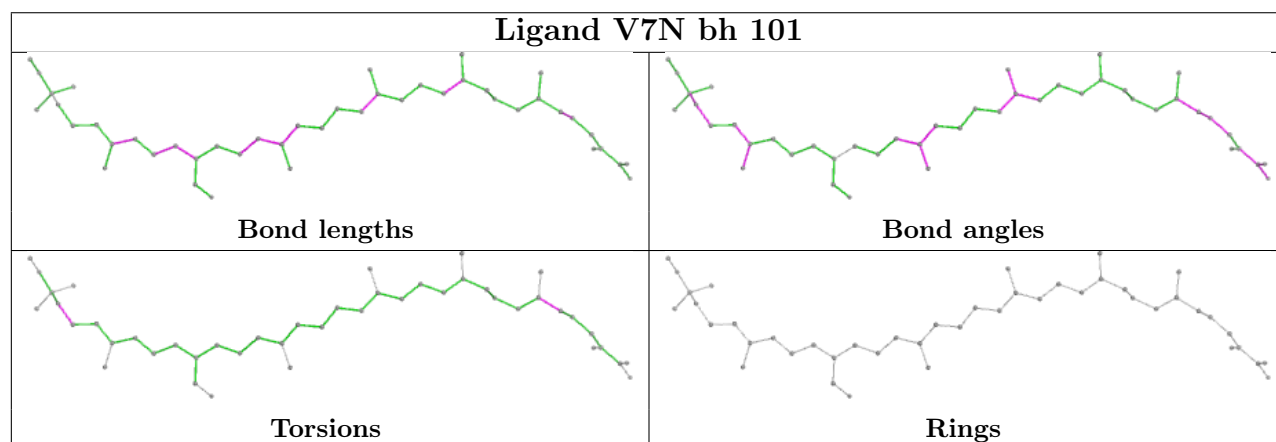
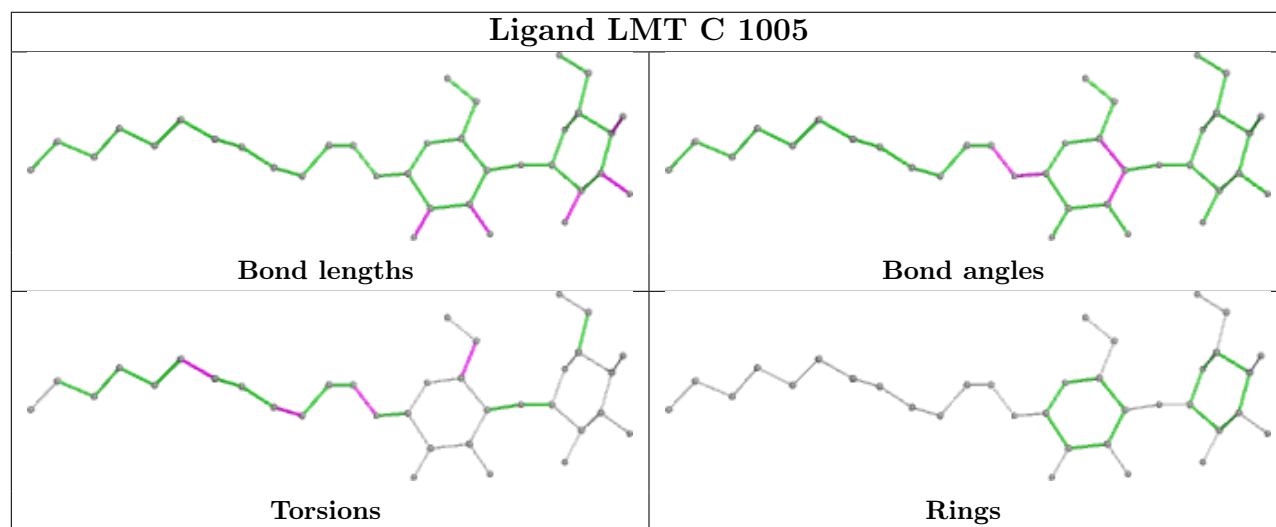
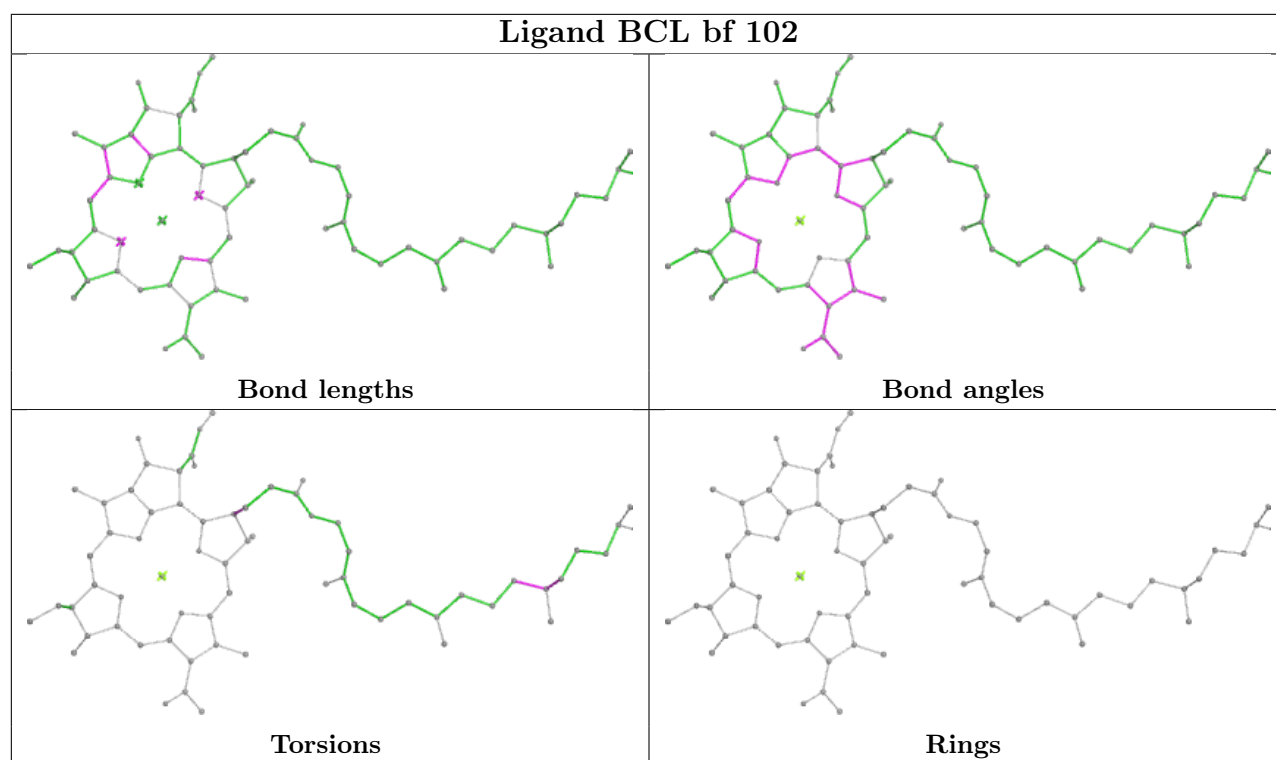


Ligand BCL bj 104

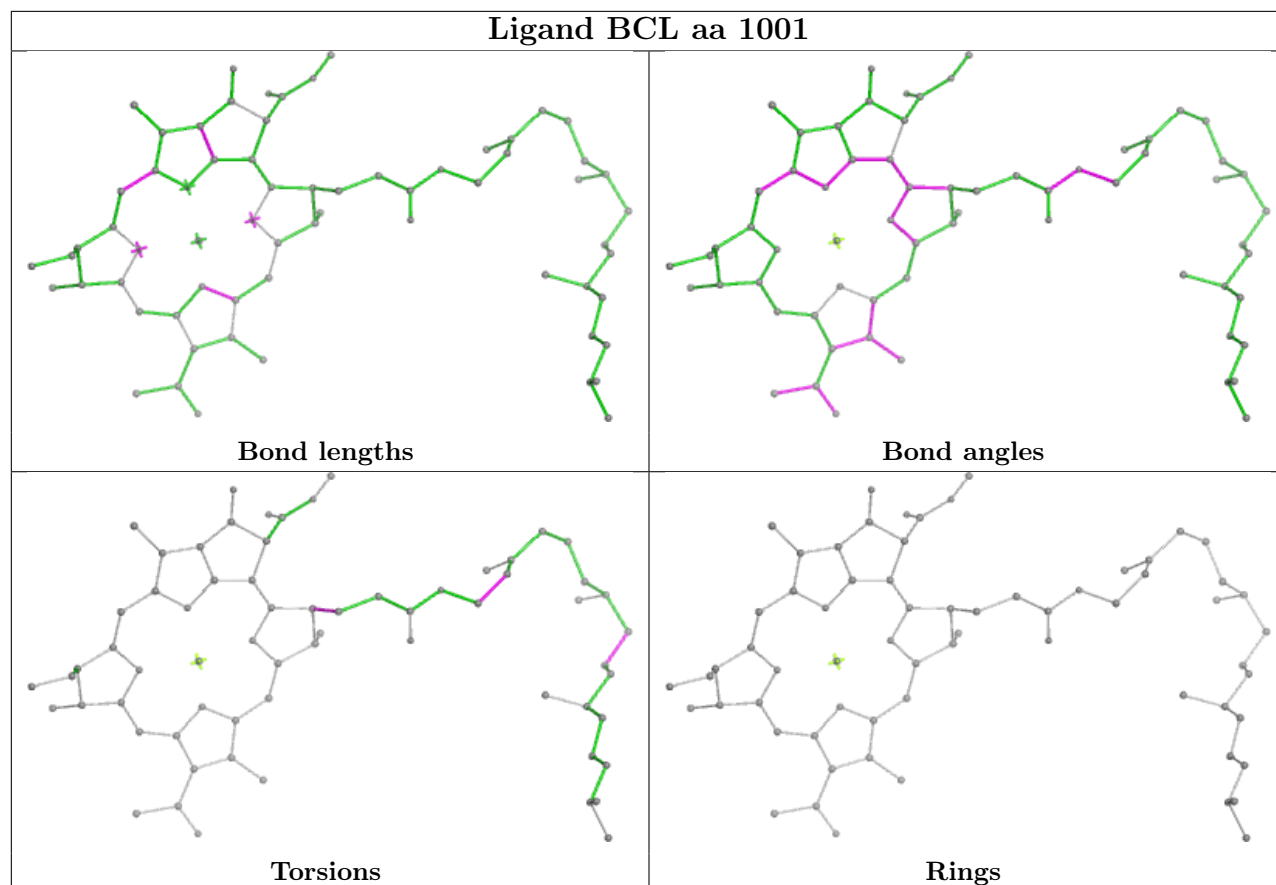


Ligand BCL BL 103**Ligand BCL M 408**

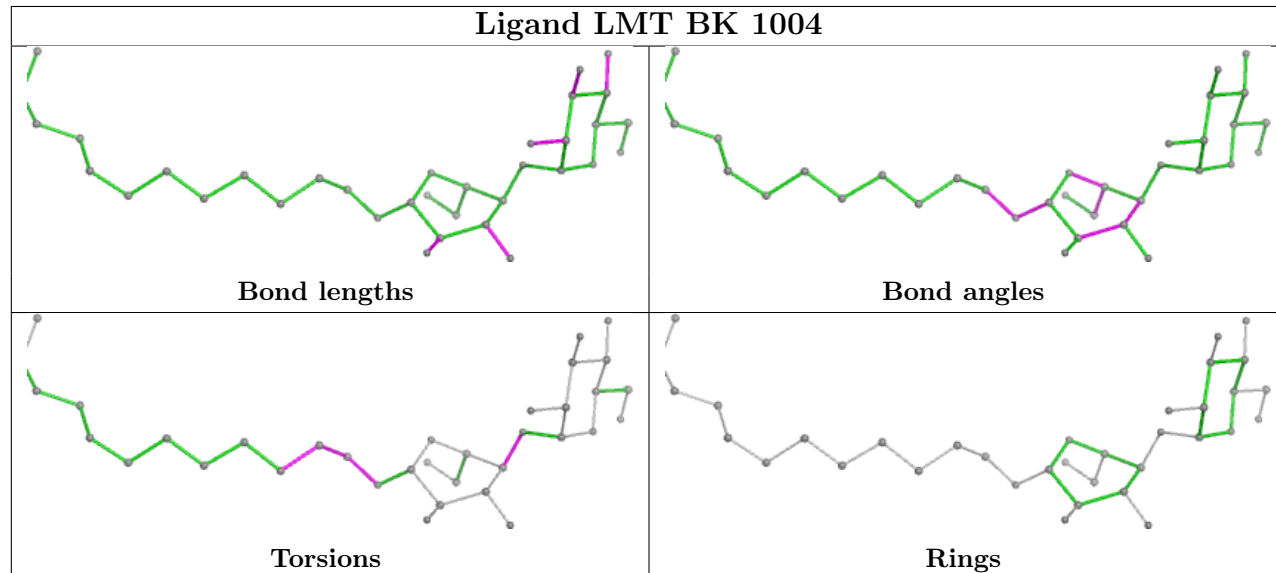


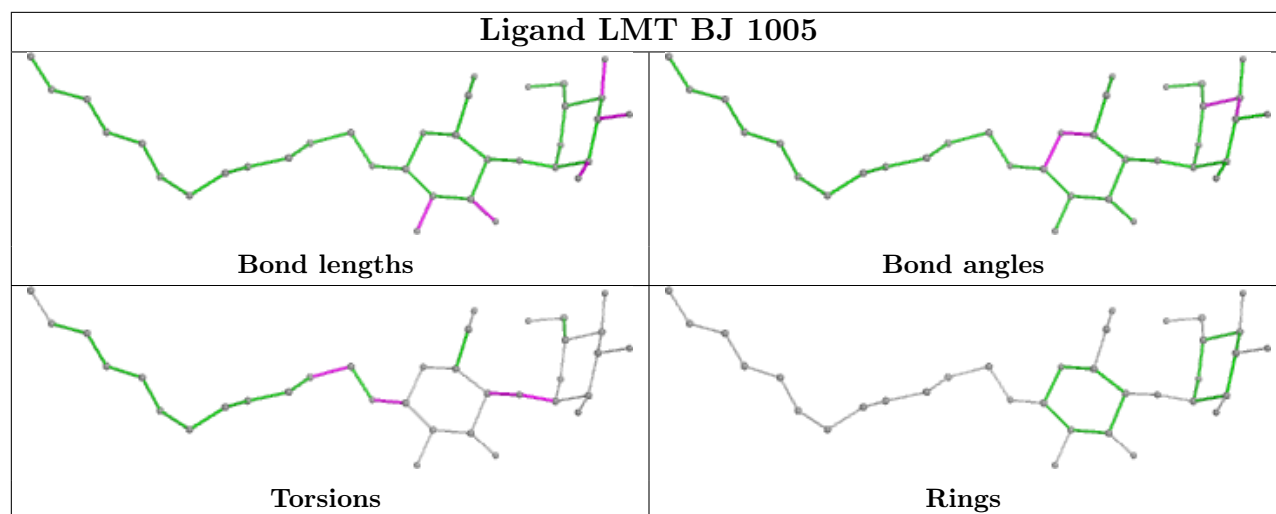
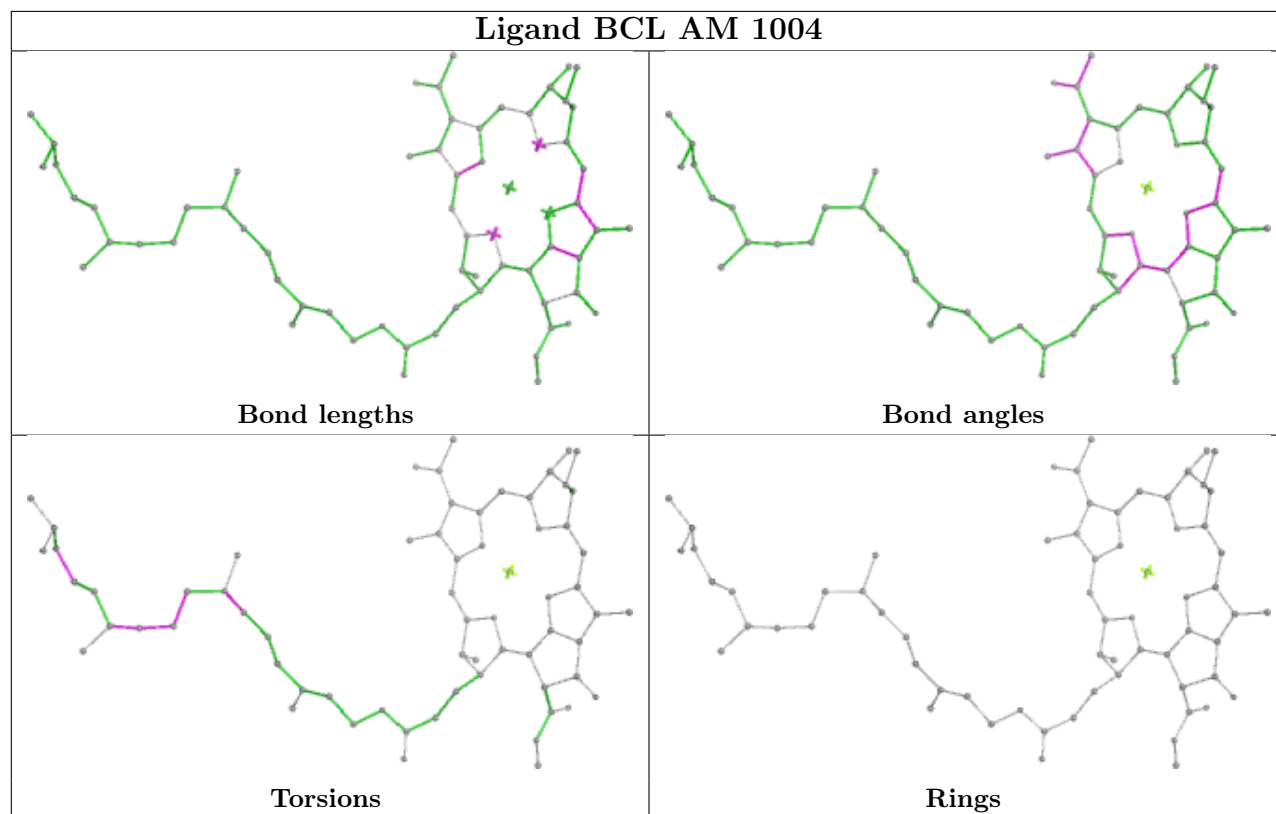


Ligand BCL aa 1001

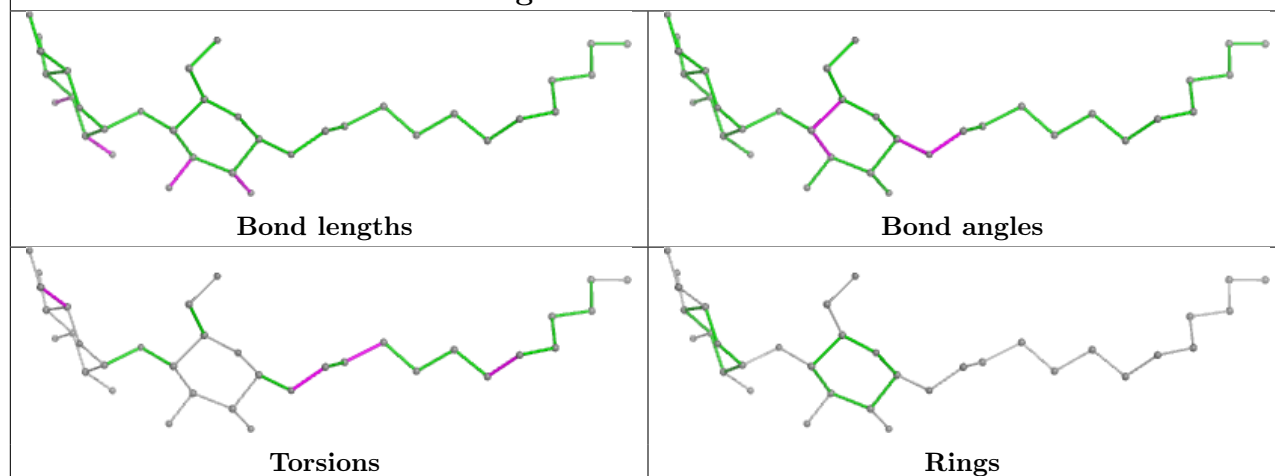


Ligand LMT BK 1004

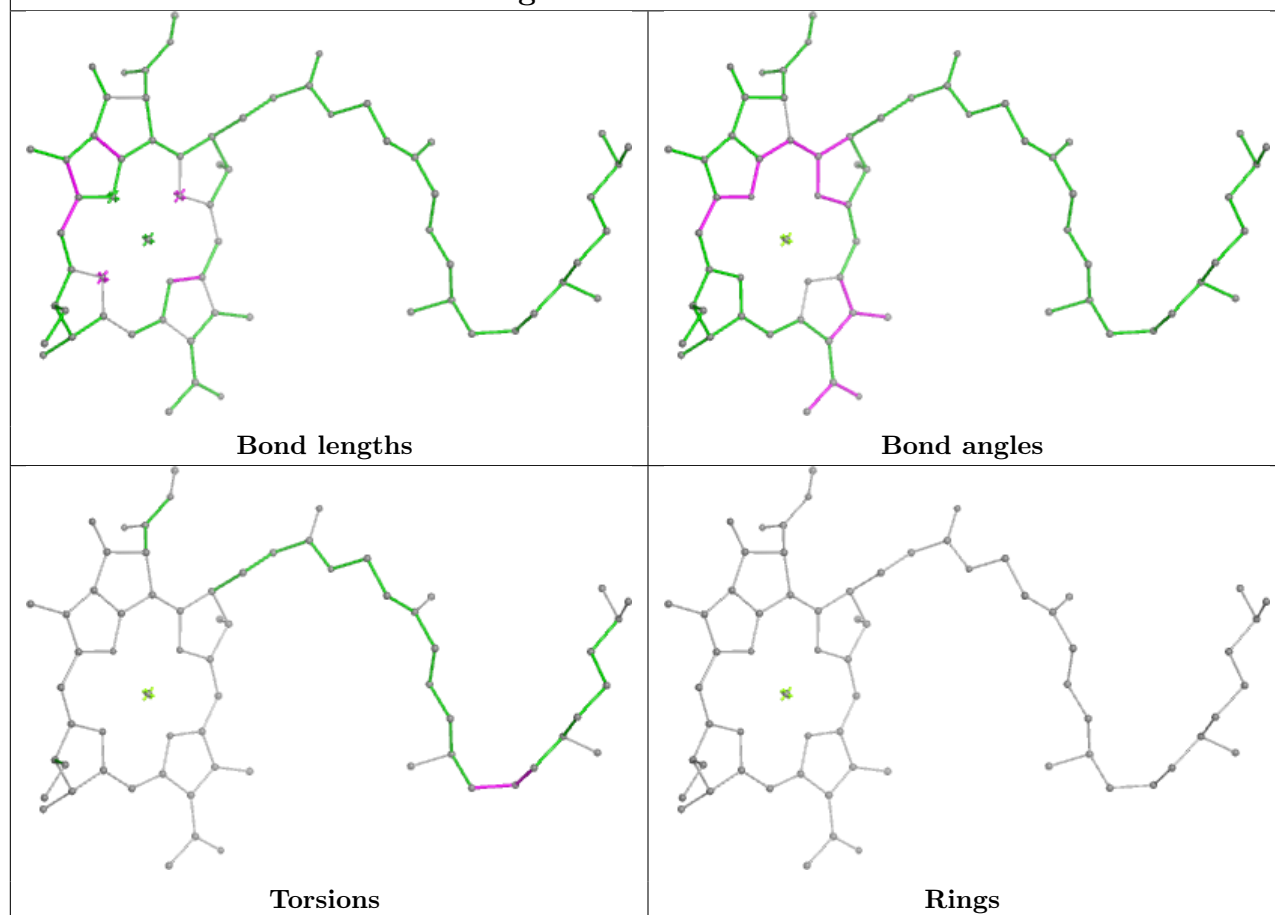




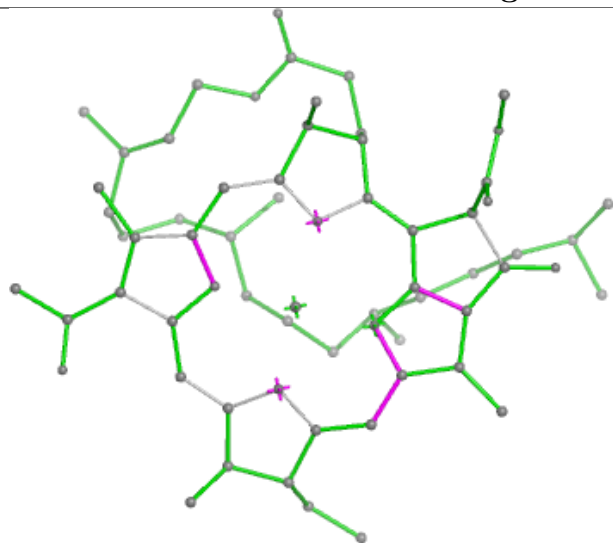
Ligand LMT BC 103



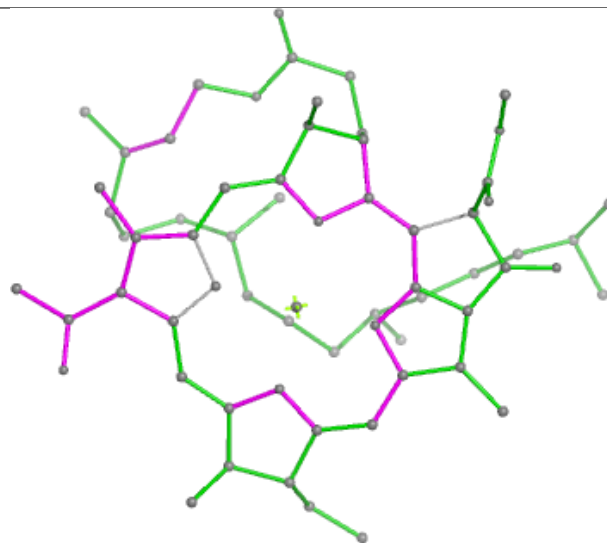
Ligand BCL AU 101



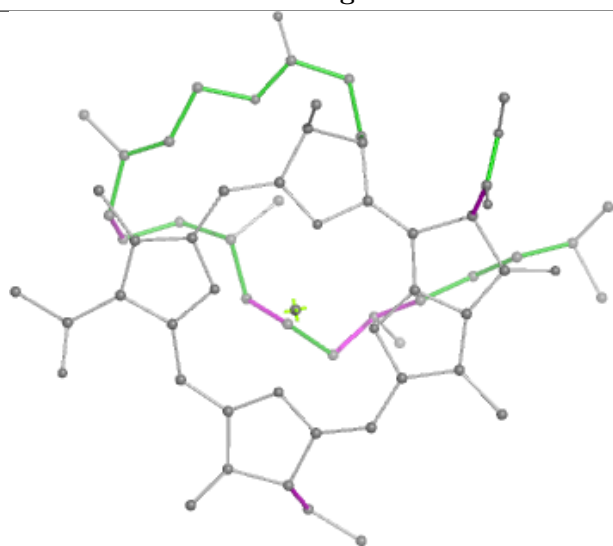
Ligand BCL AD 104



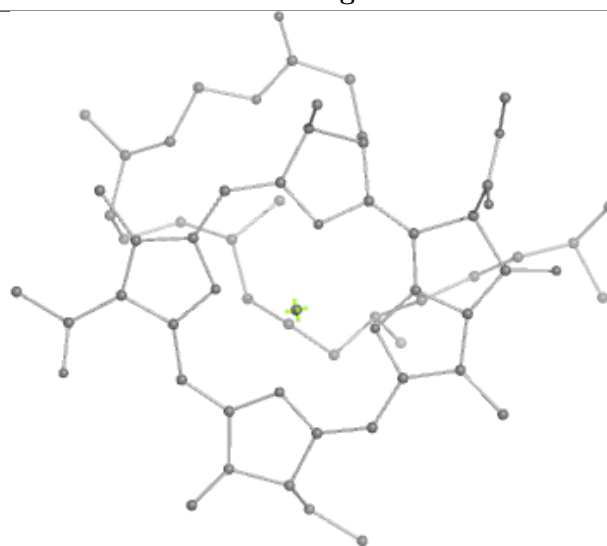
Bond lengths



Bond angles

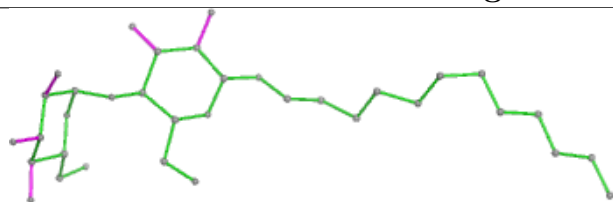


Torsions

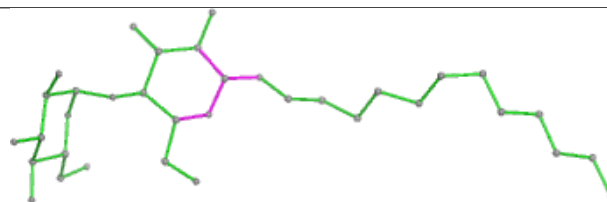


Rings

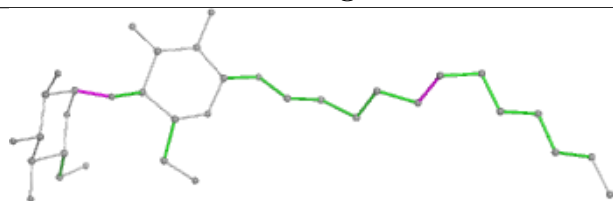
Ligand LMT BW 1006



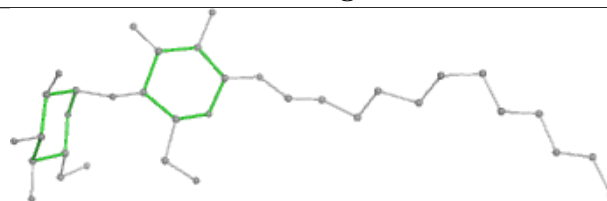
Bond lengths



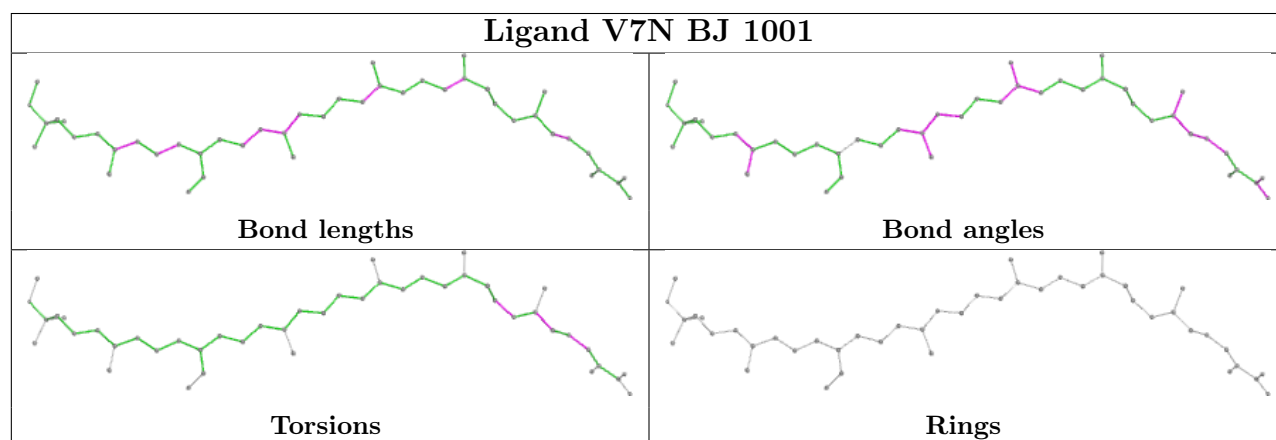
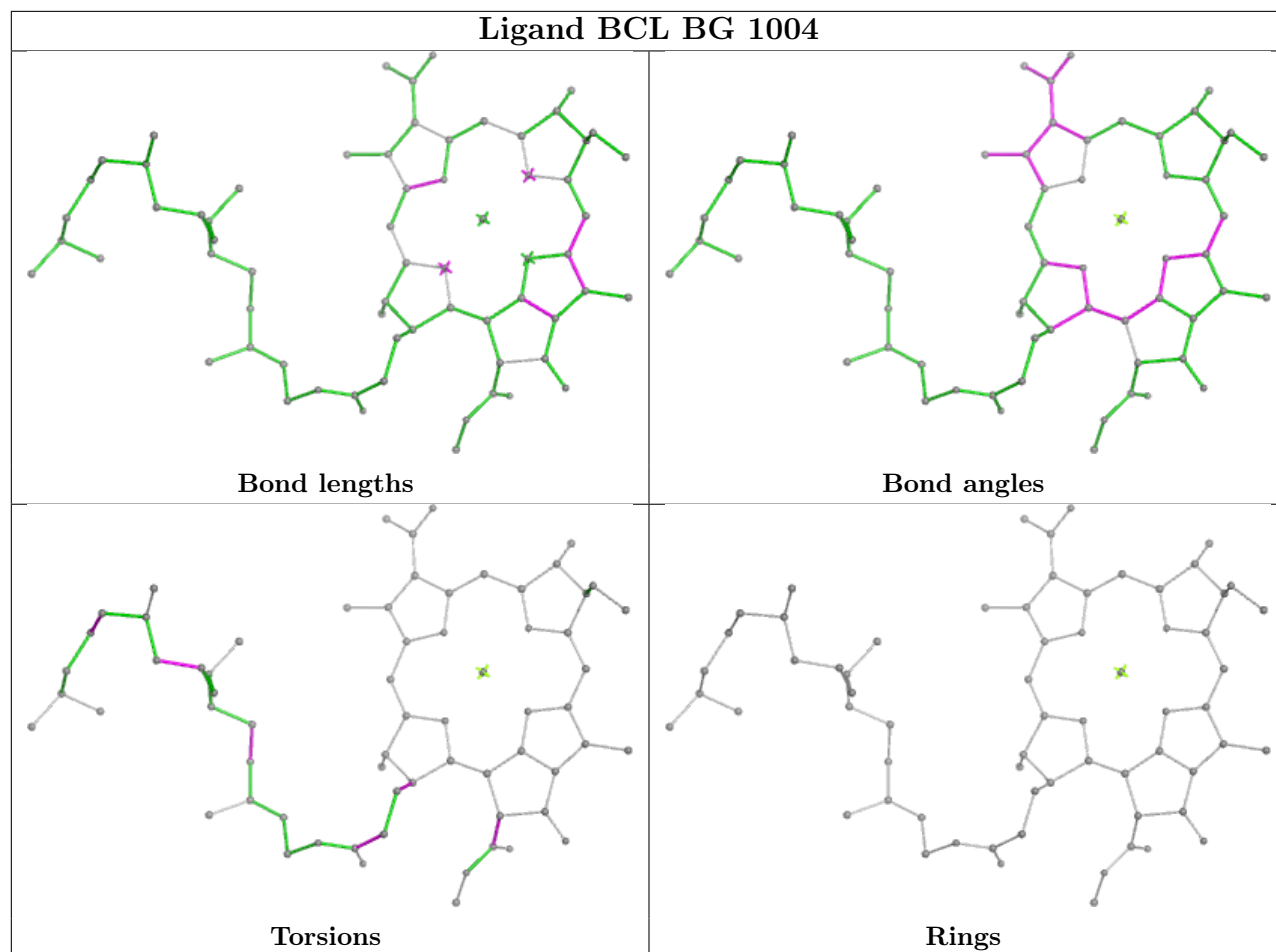
Bond angles

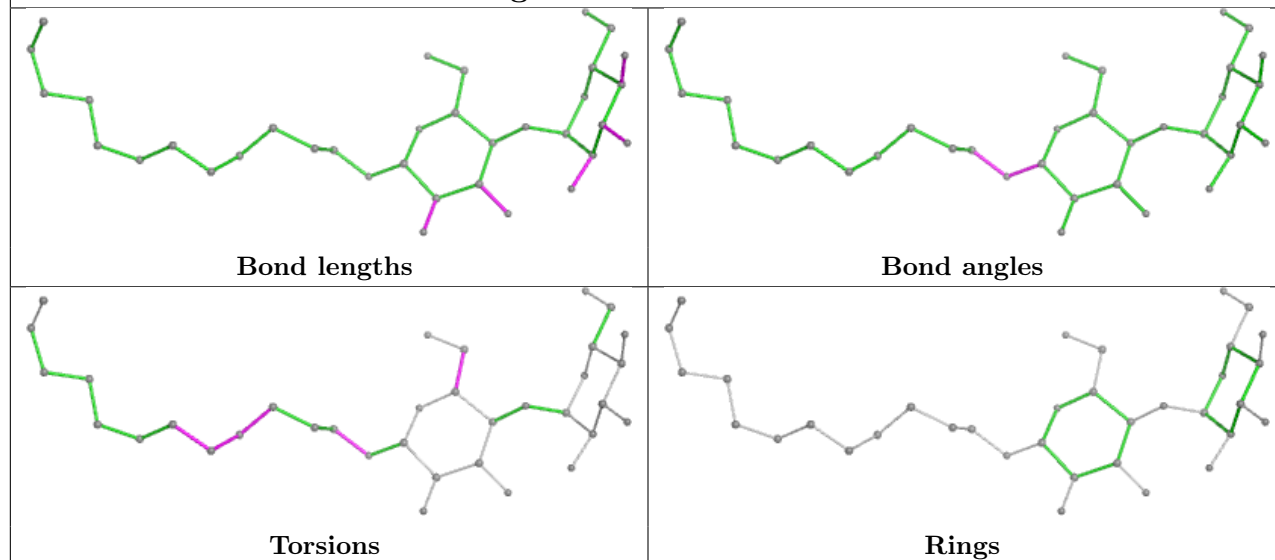
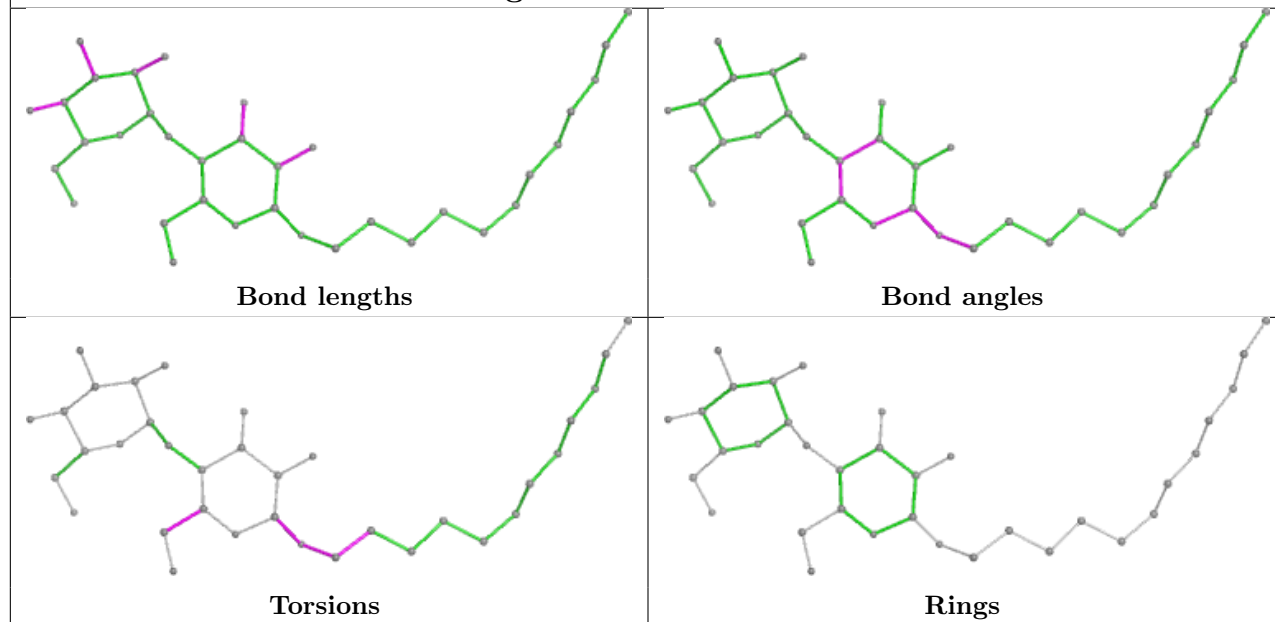


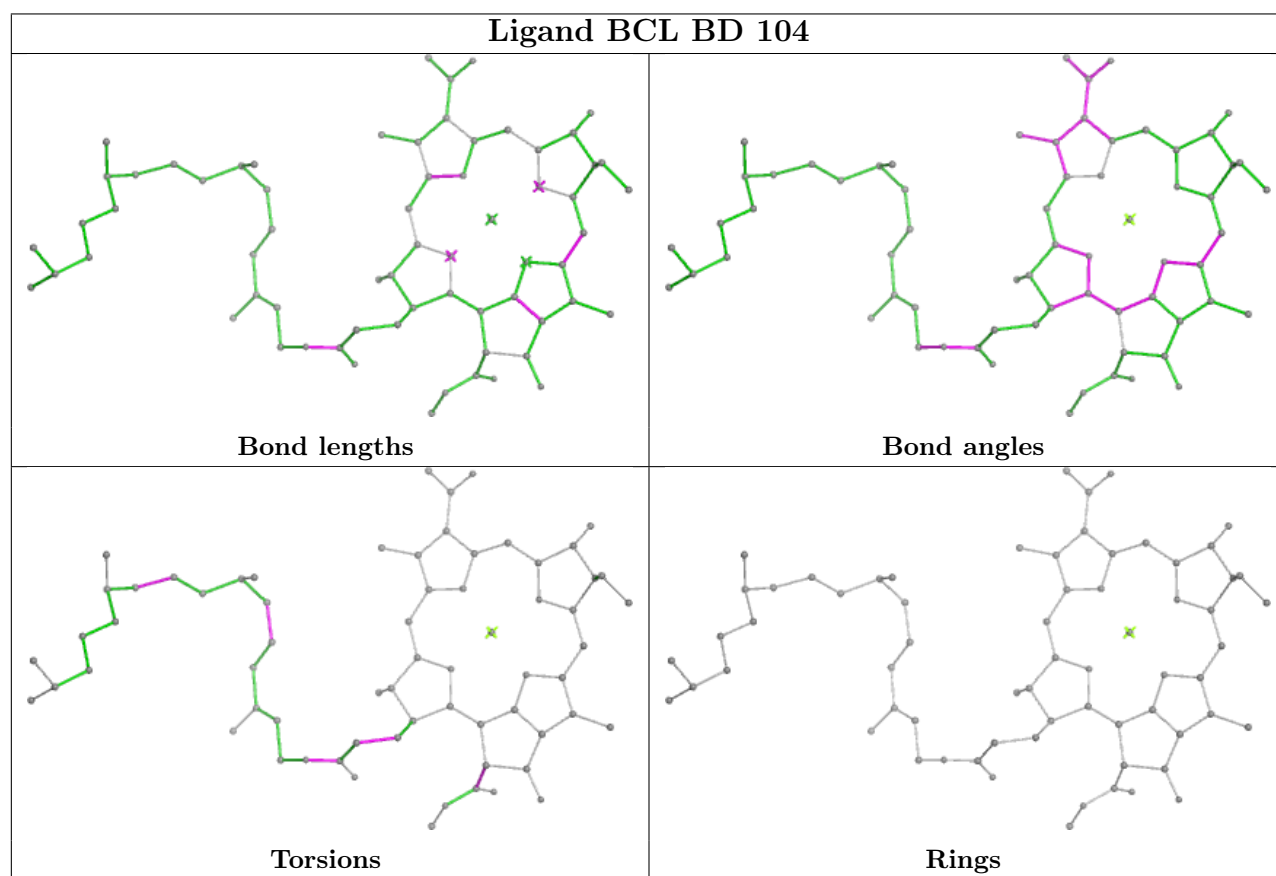
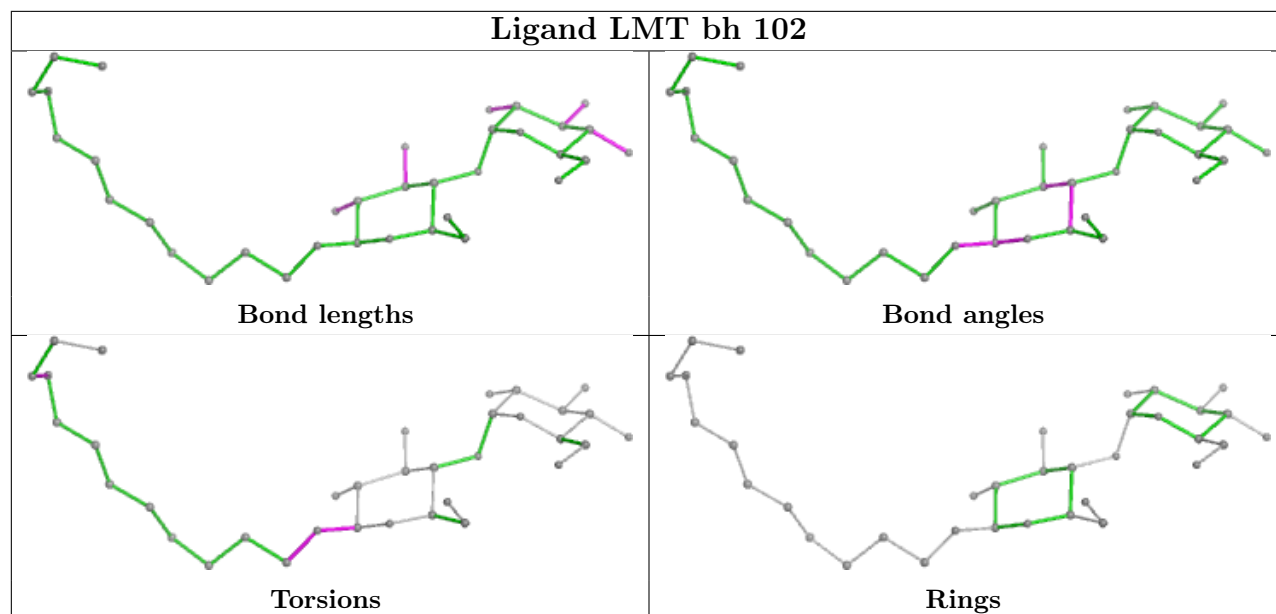
Torsions



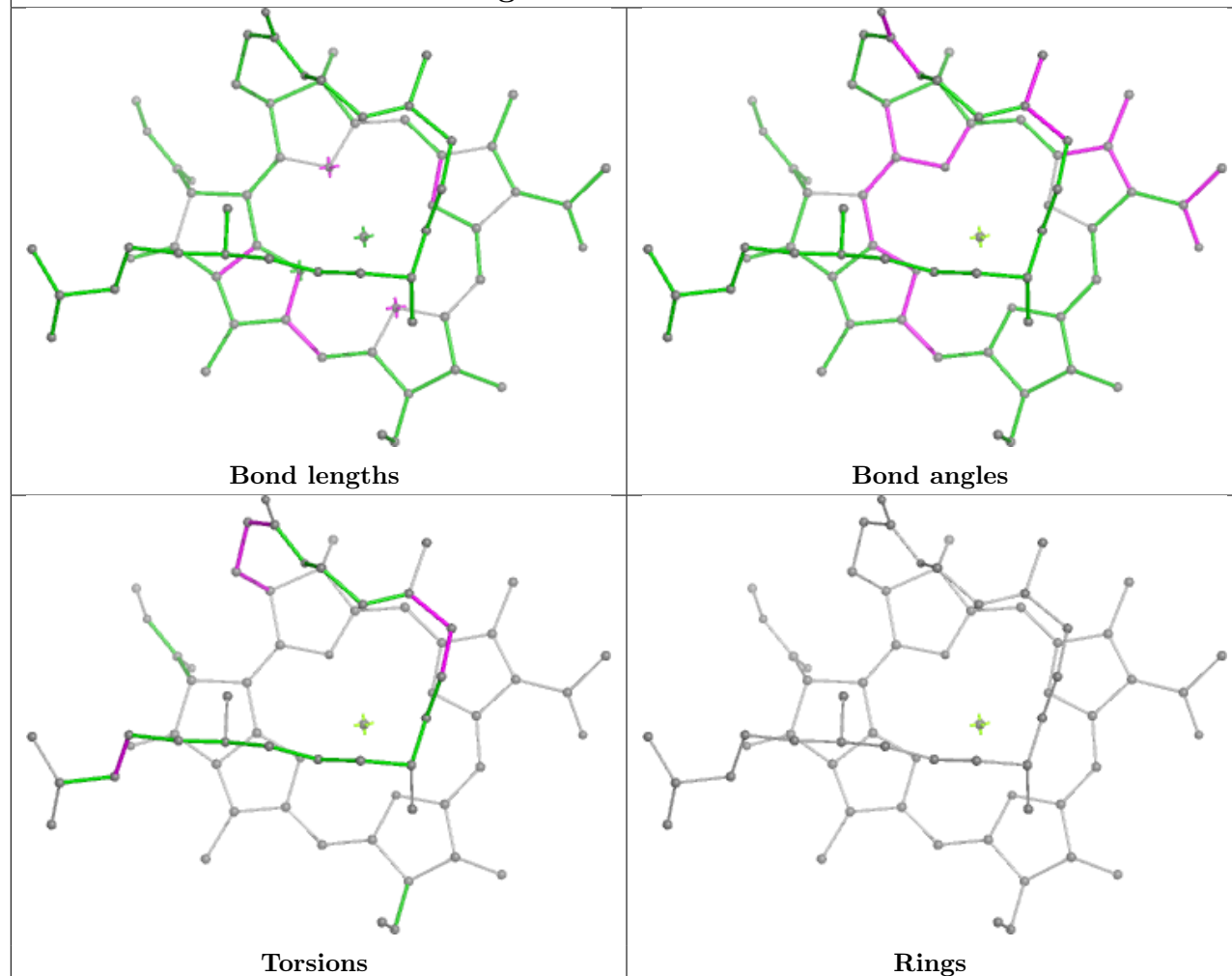
Rings



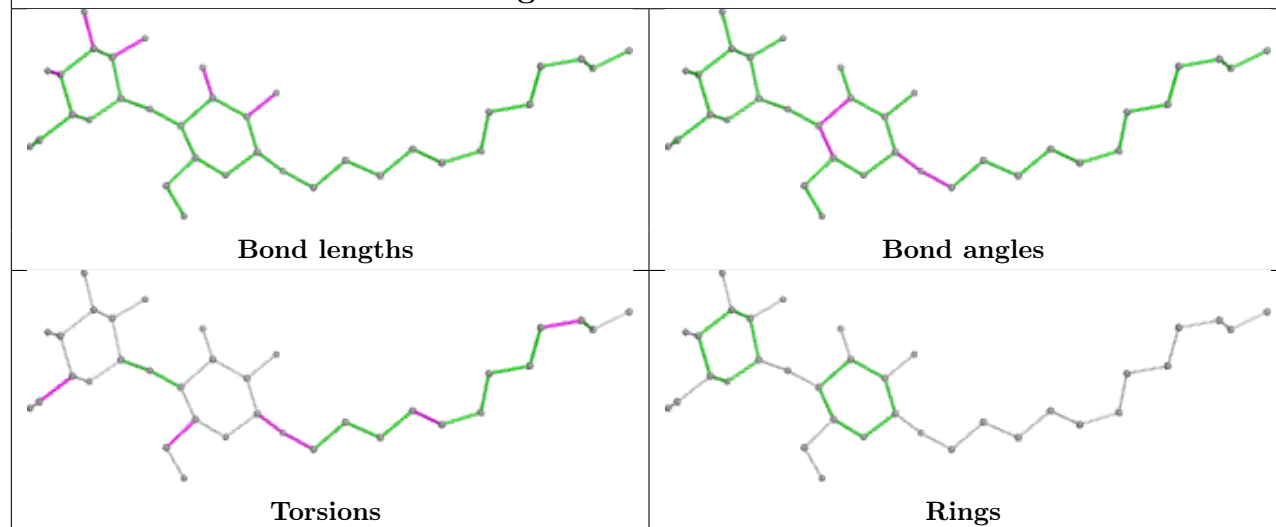
Ligand LMT BJ 1003**Ligand LMT BU 1002**

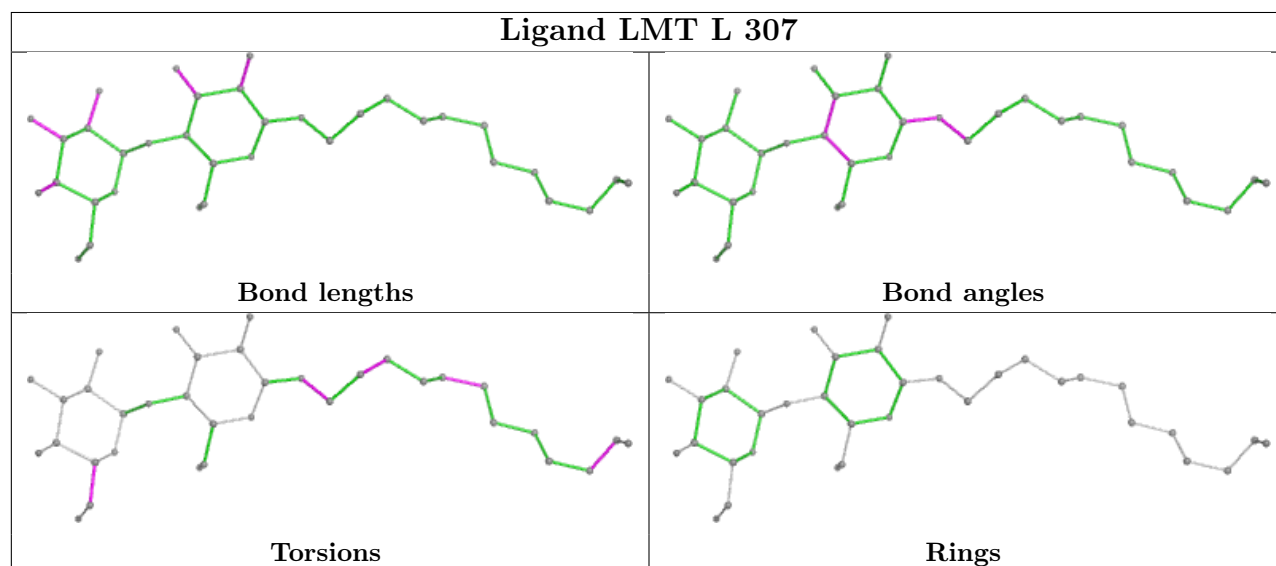
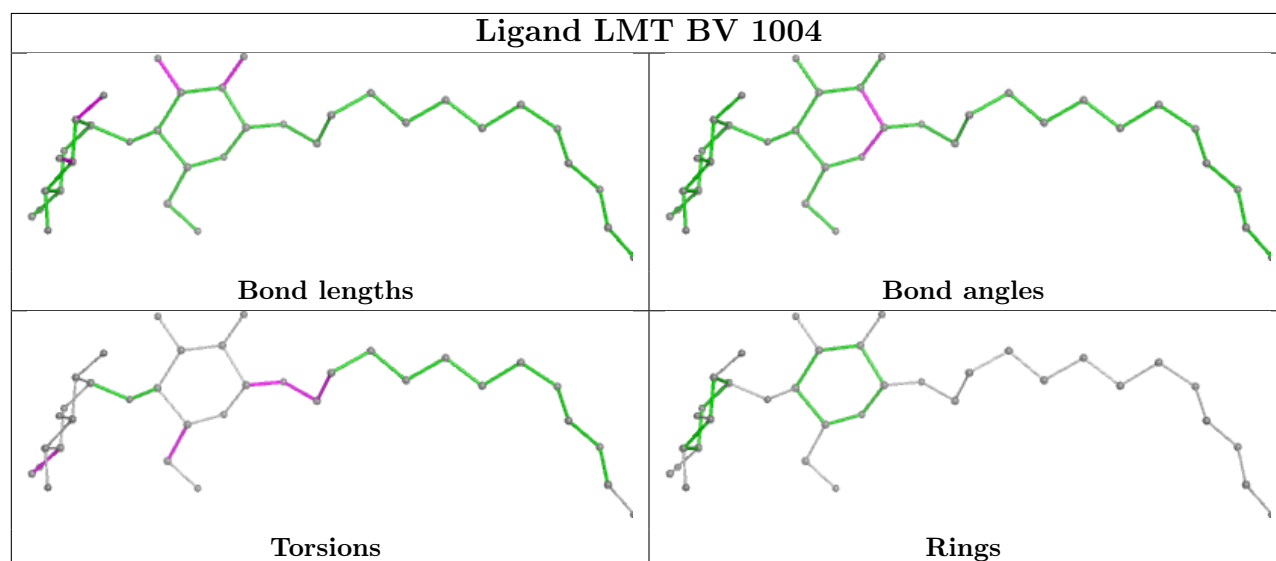
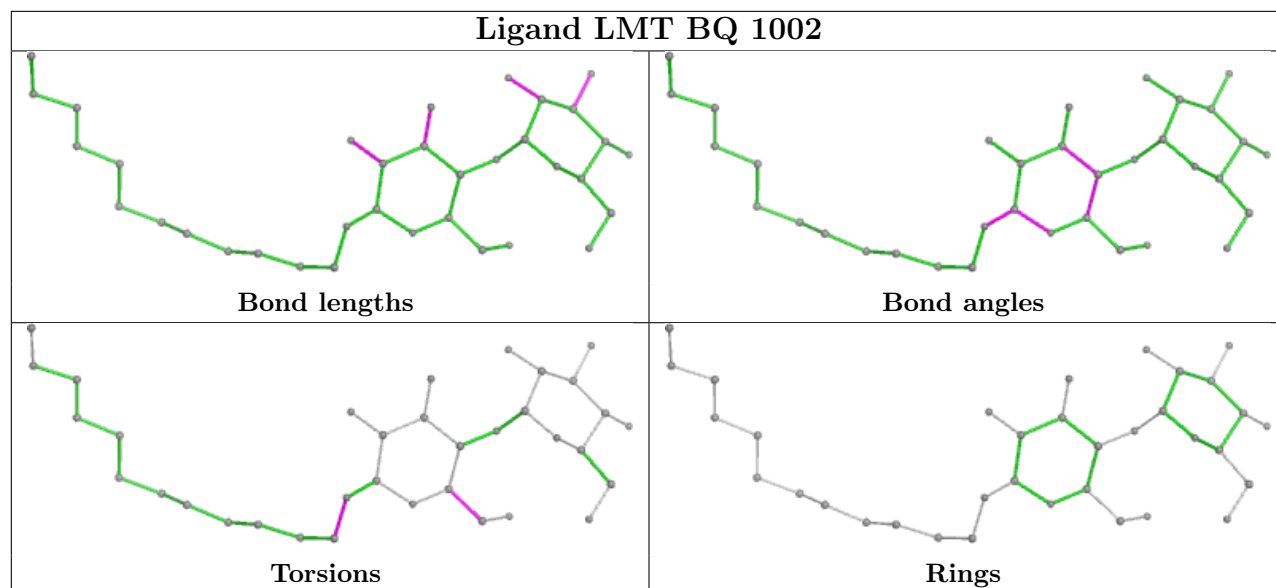


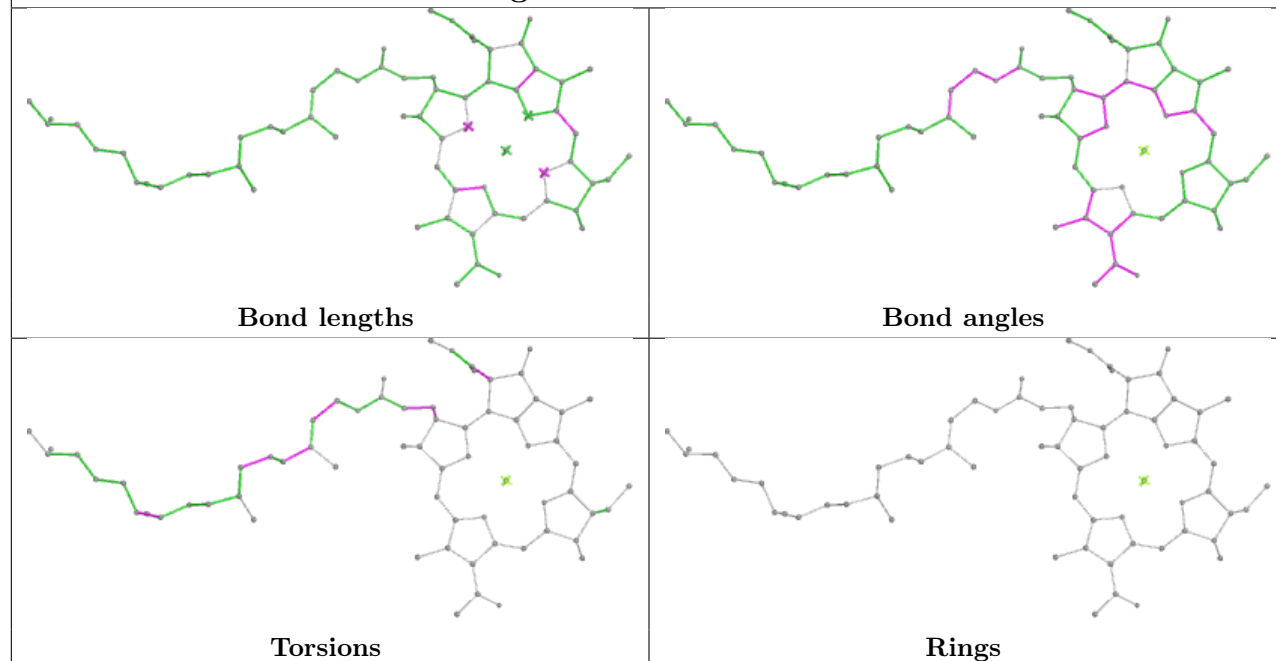
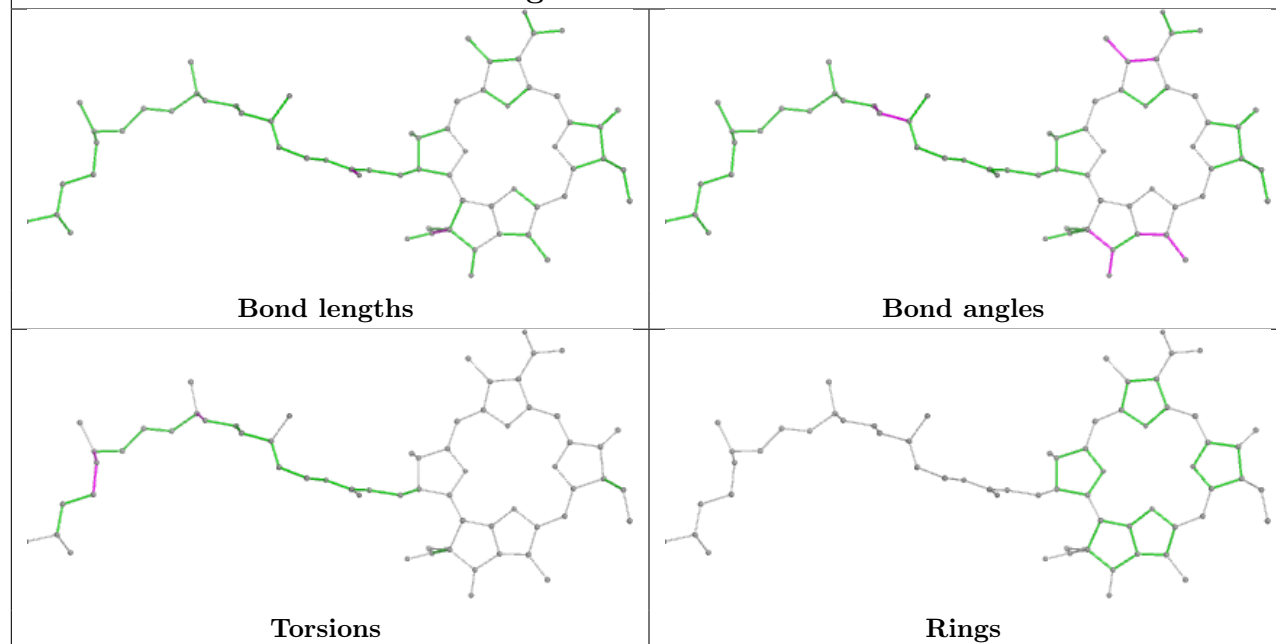
Ligand BCL AW 102

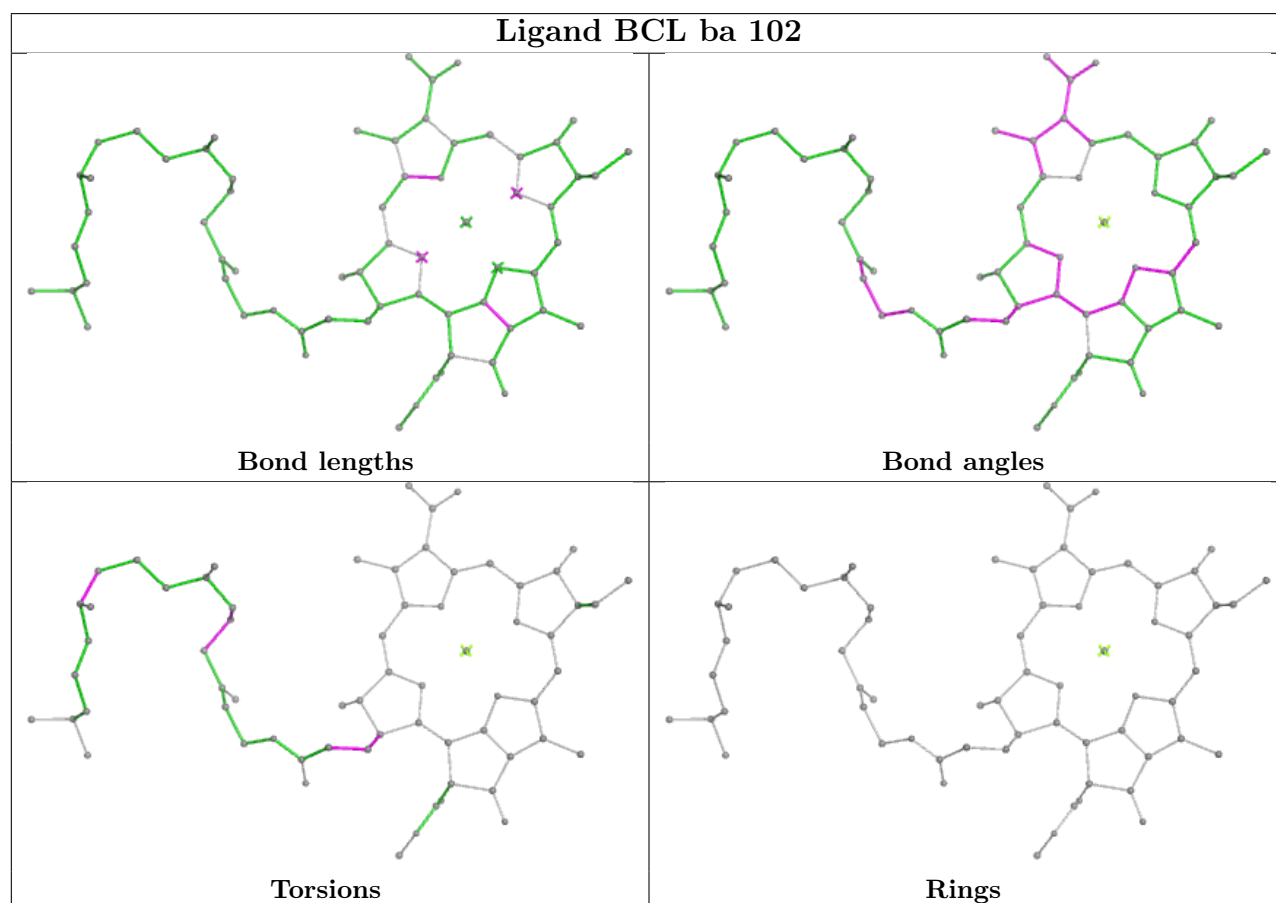
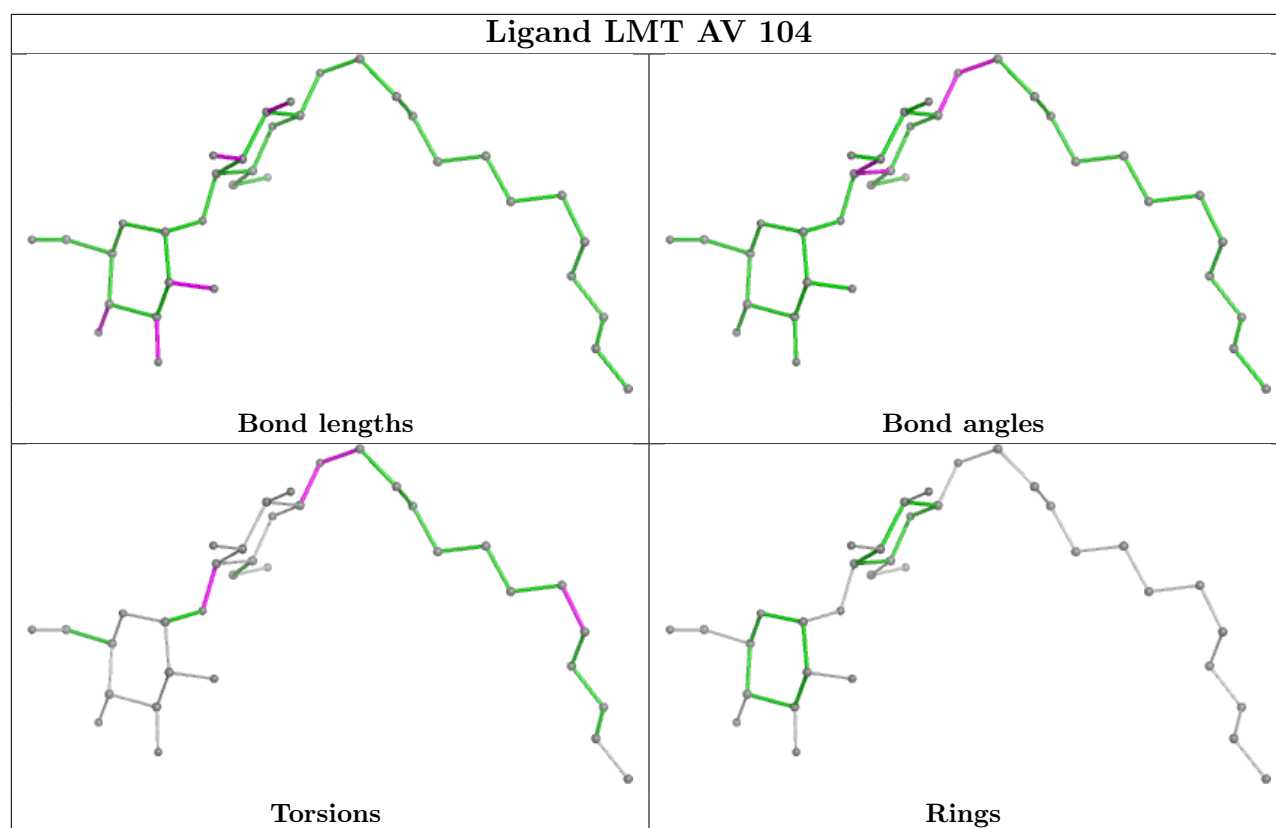


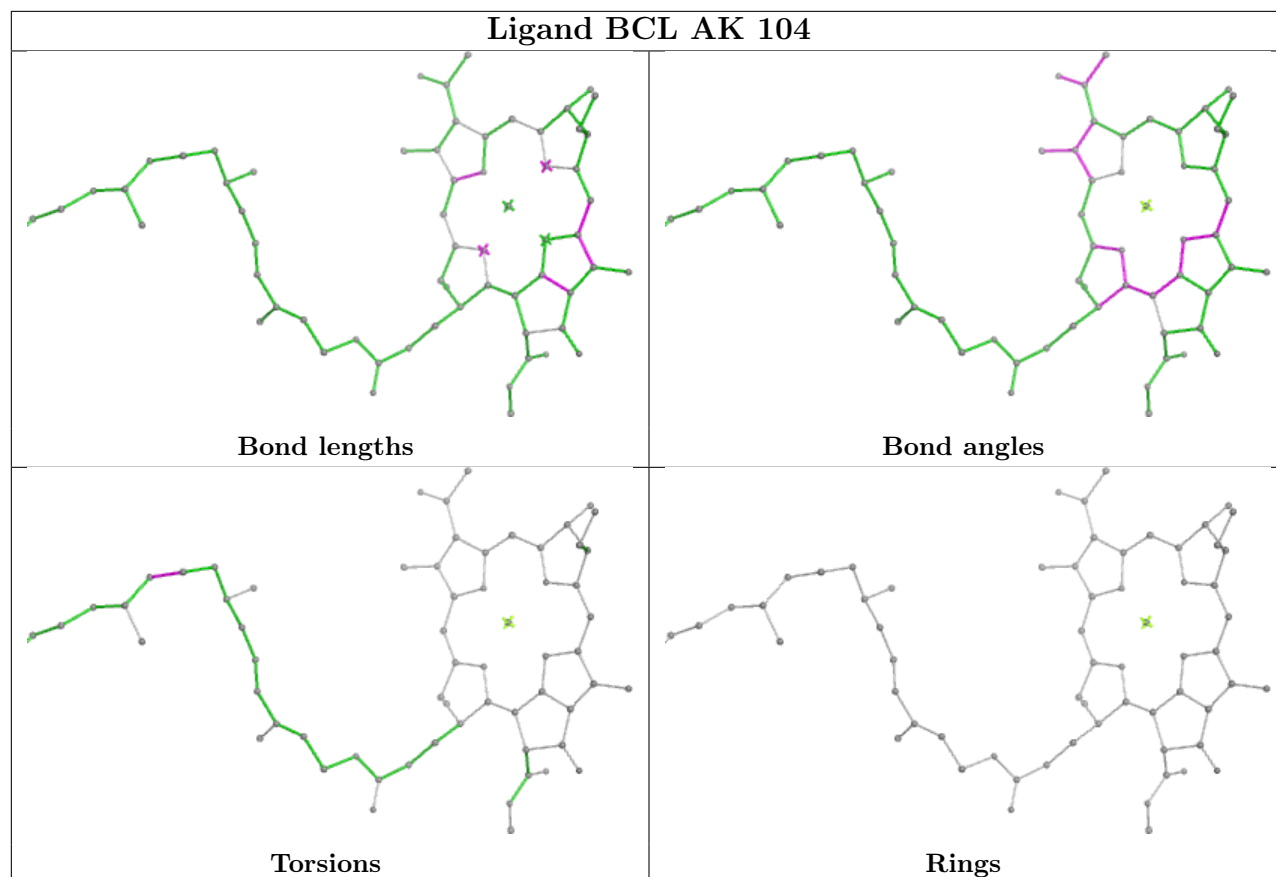
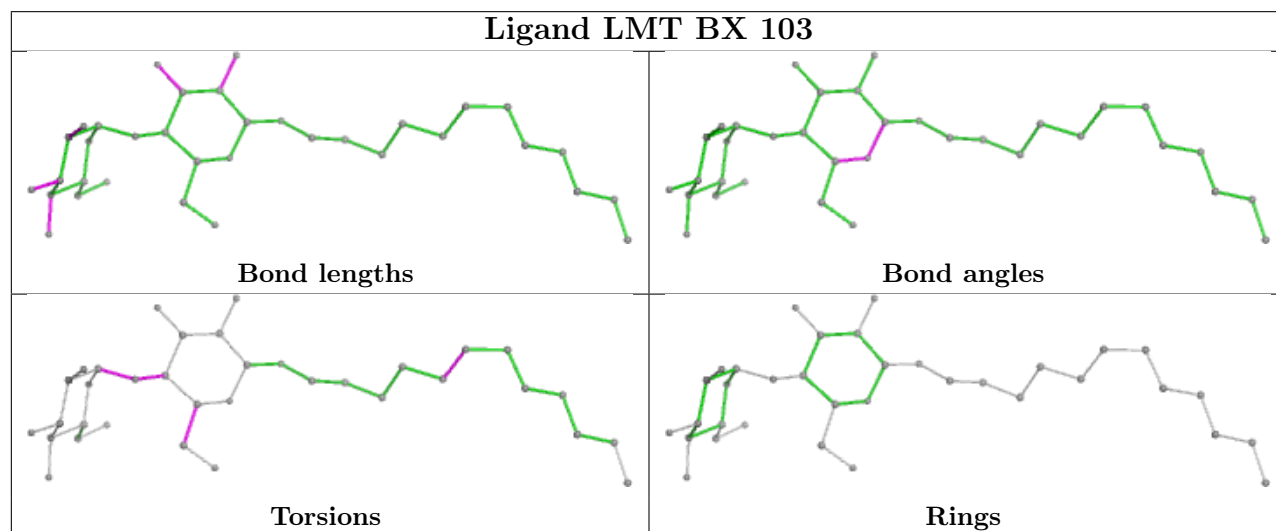
Ligand LMT AT 102

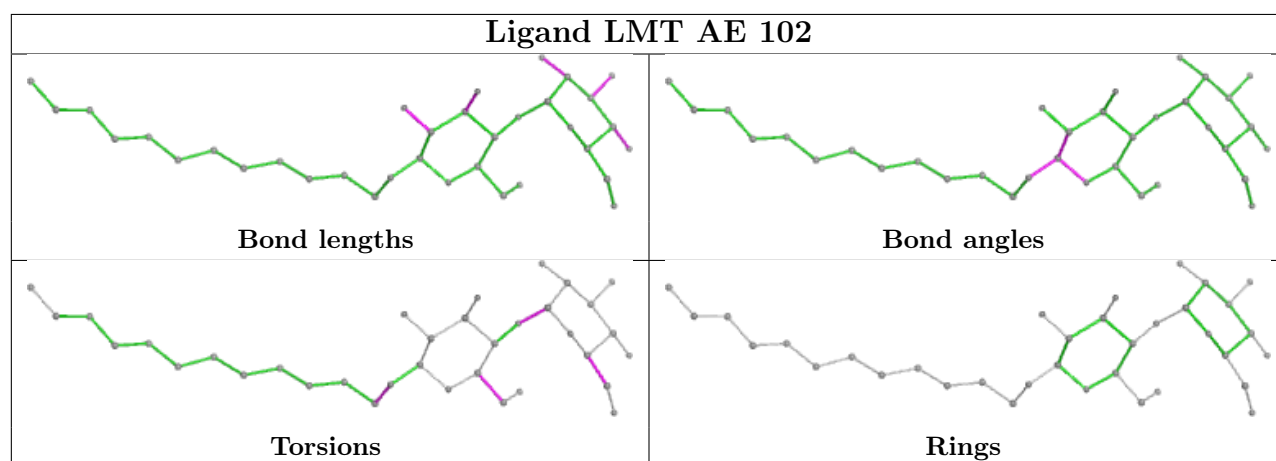
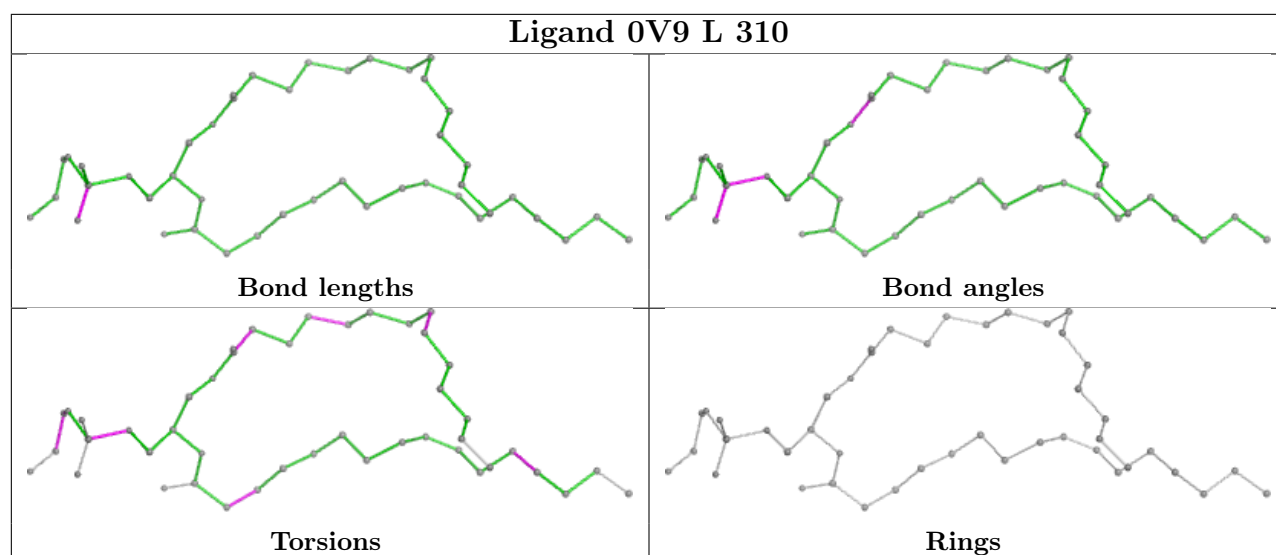




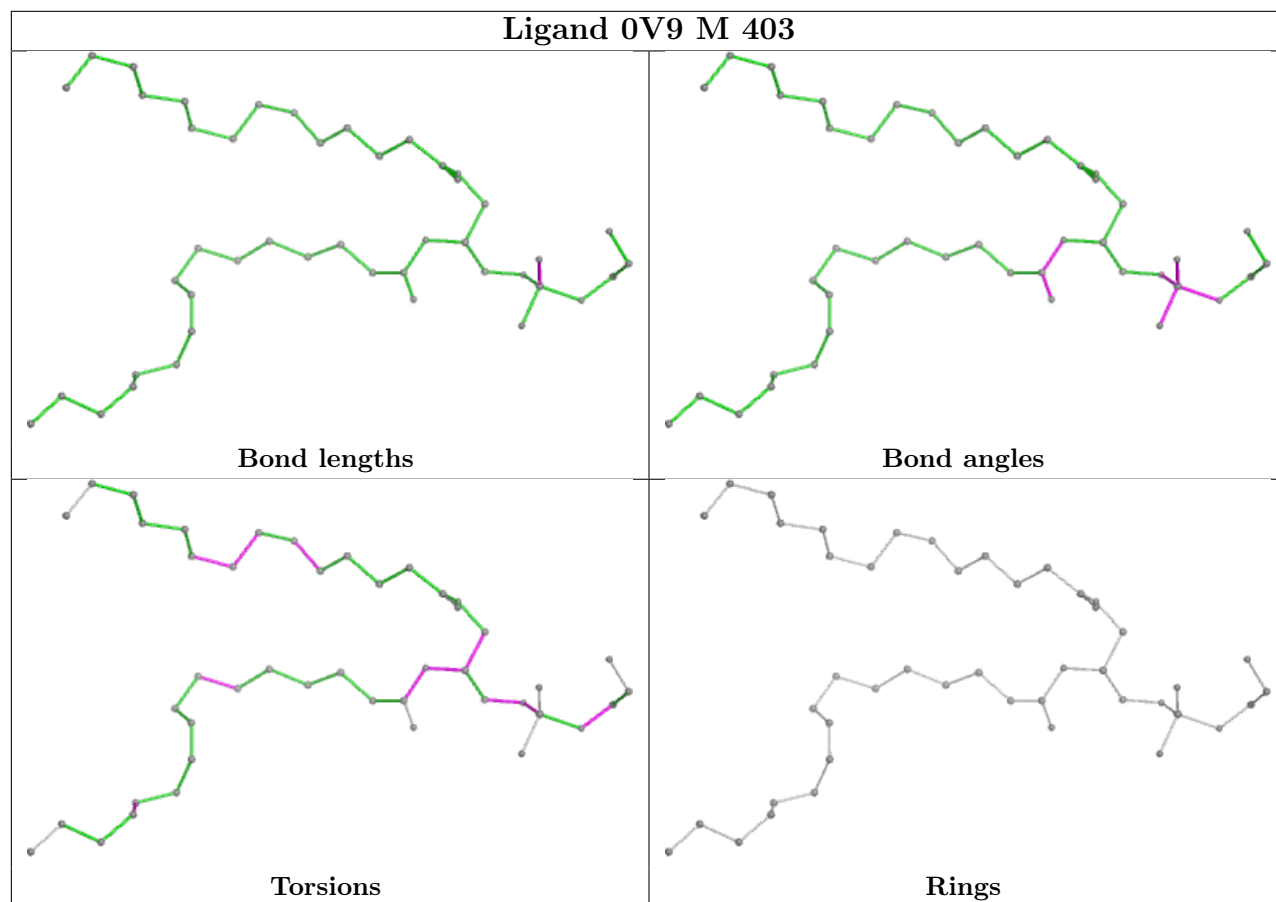
Ligand BCL BK 1002**Ligand BPH M 407**



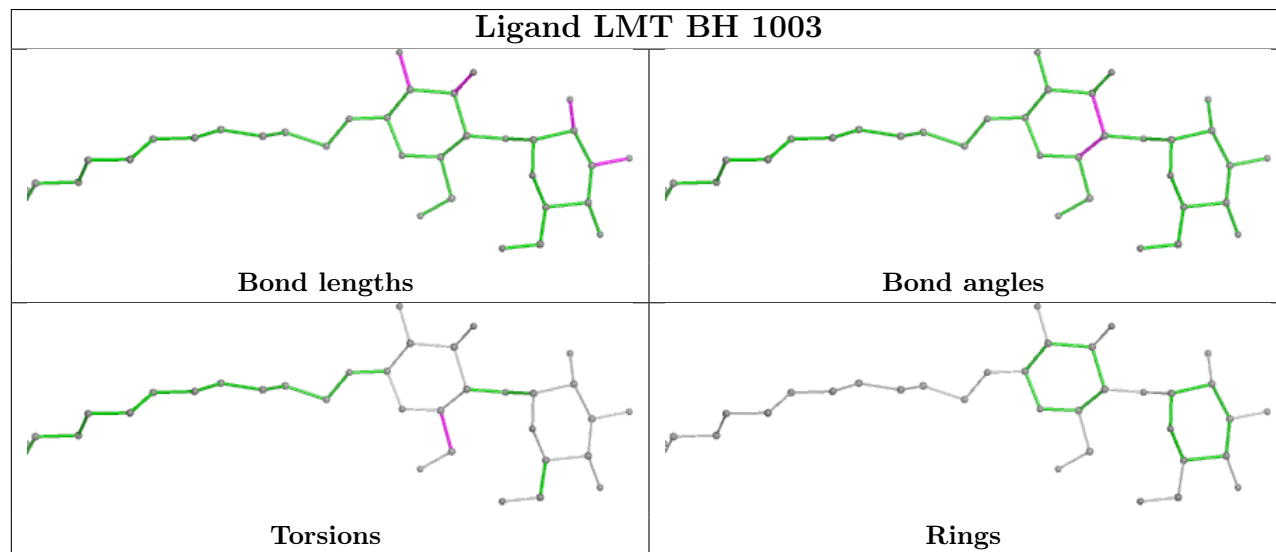
Ligand BCL AK 104**Ligand LMT BX 103**

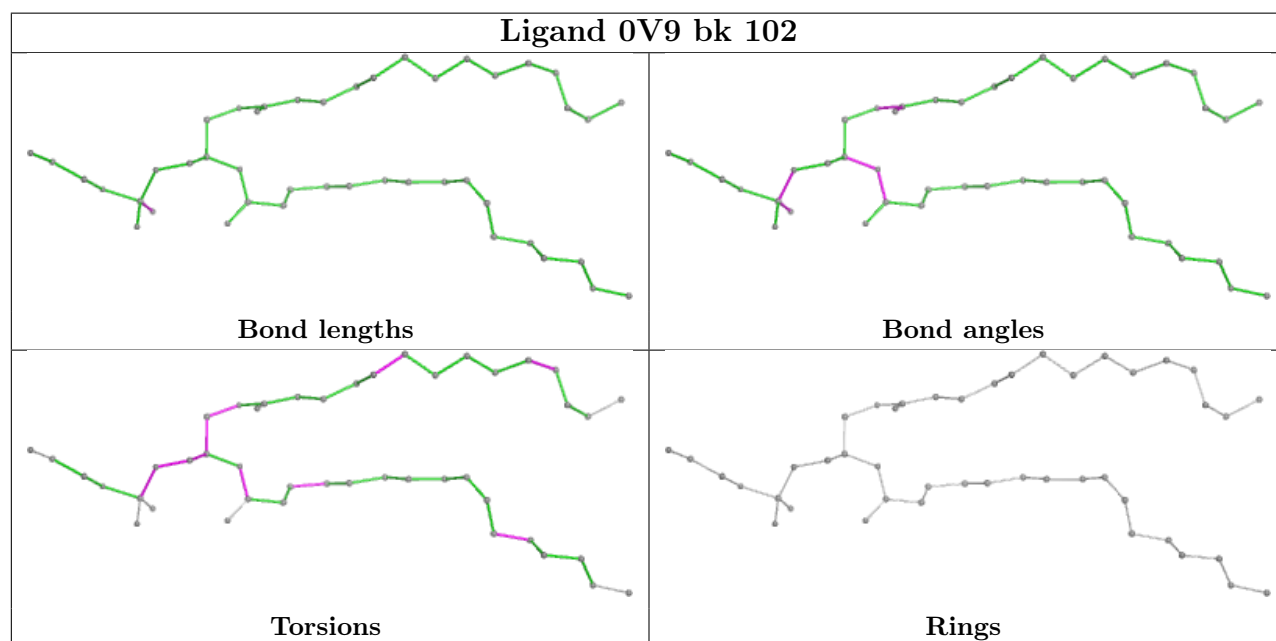
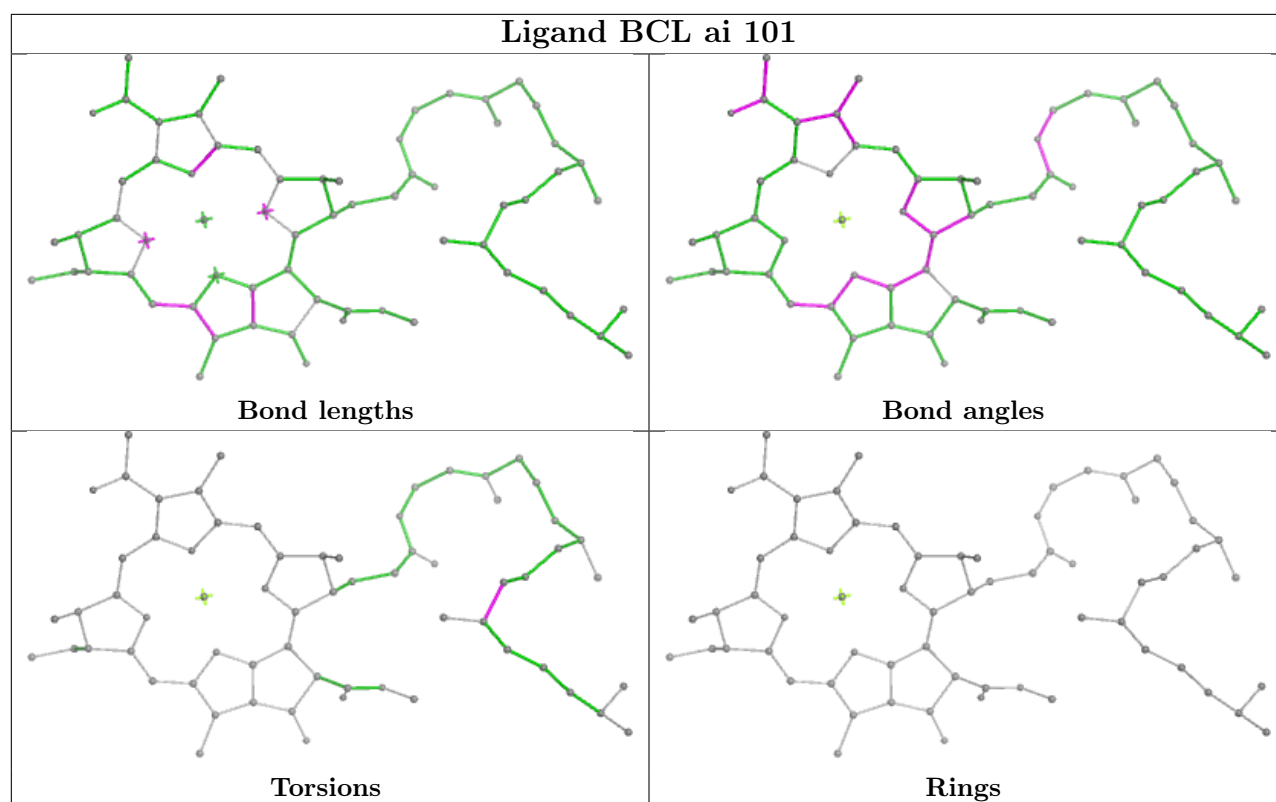


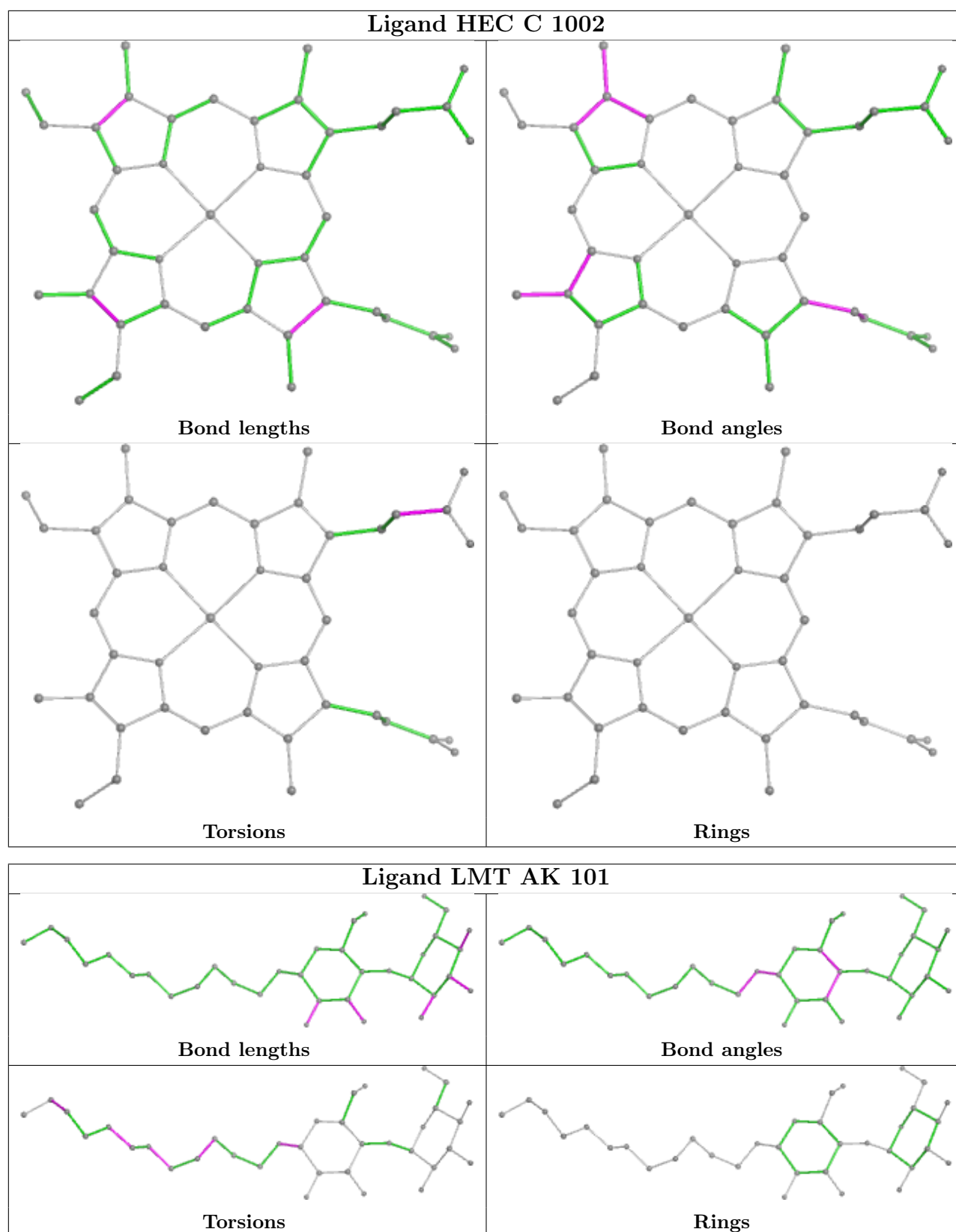
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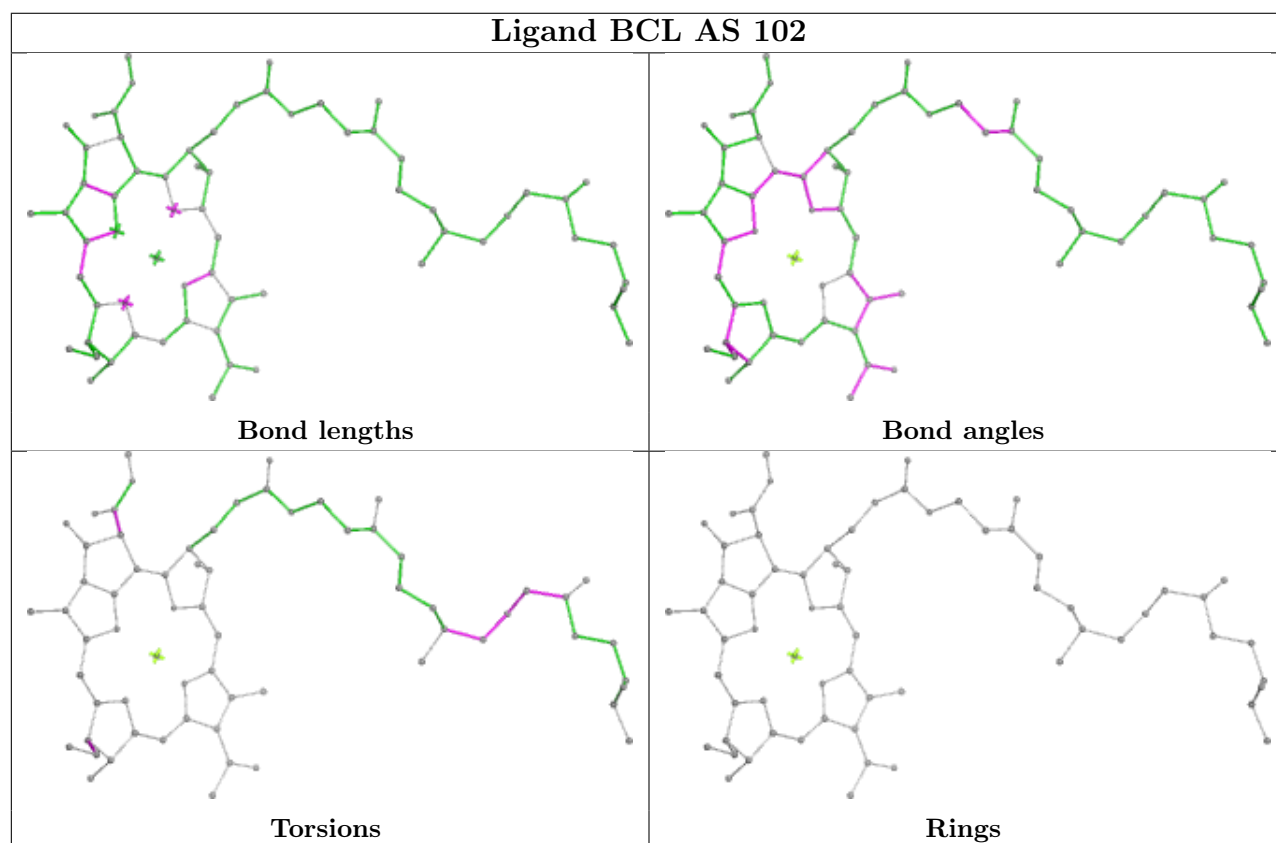
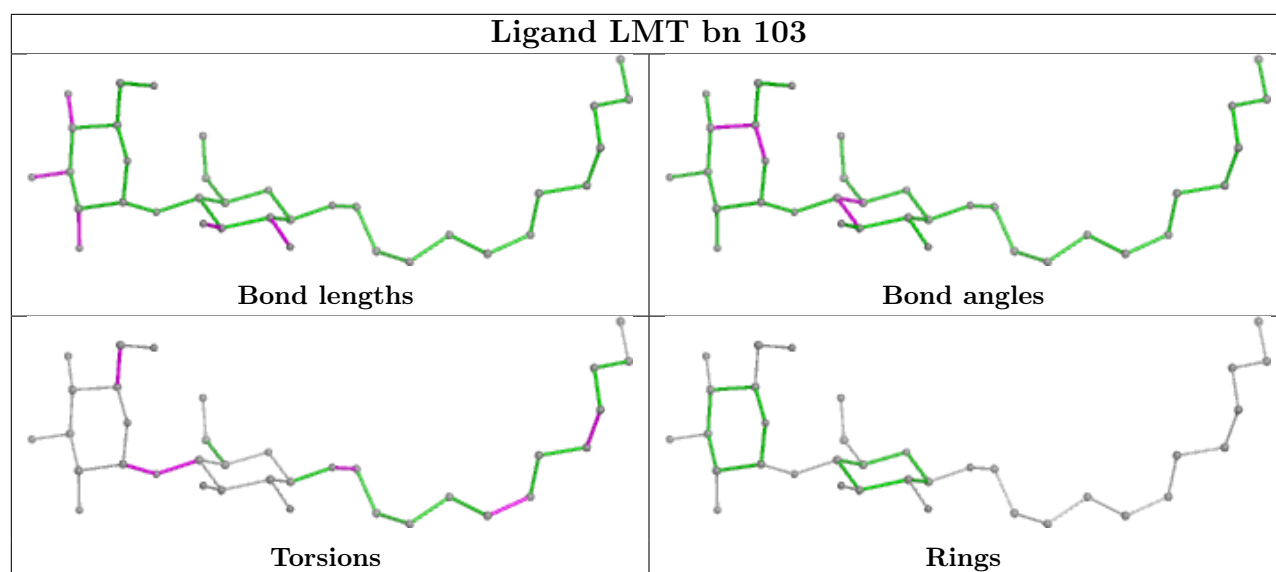


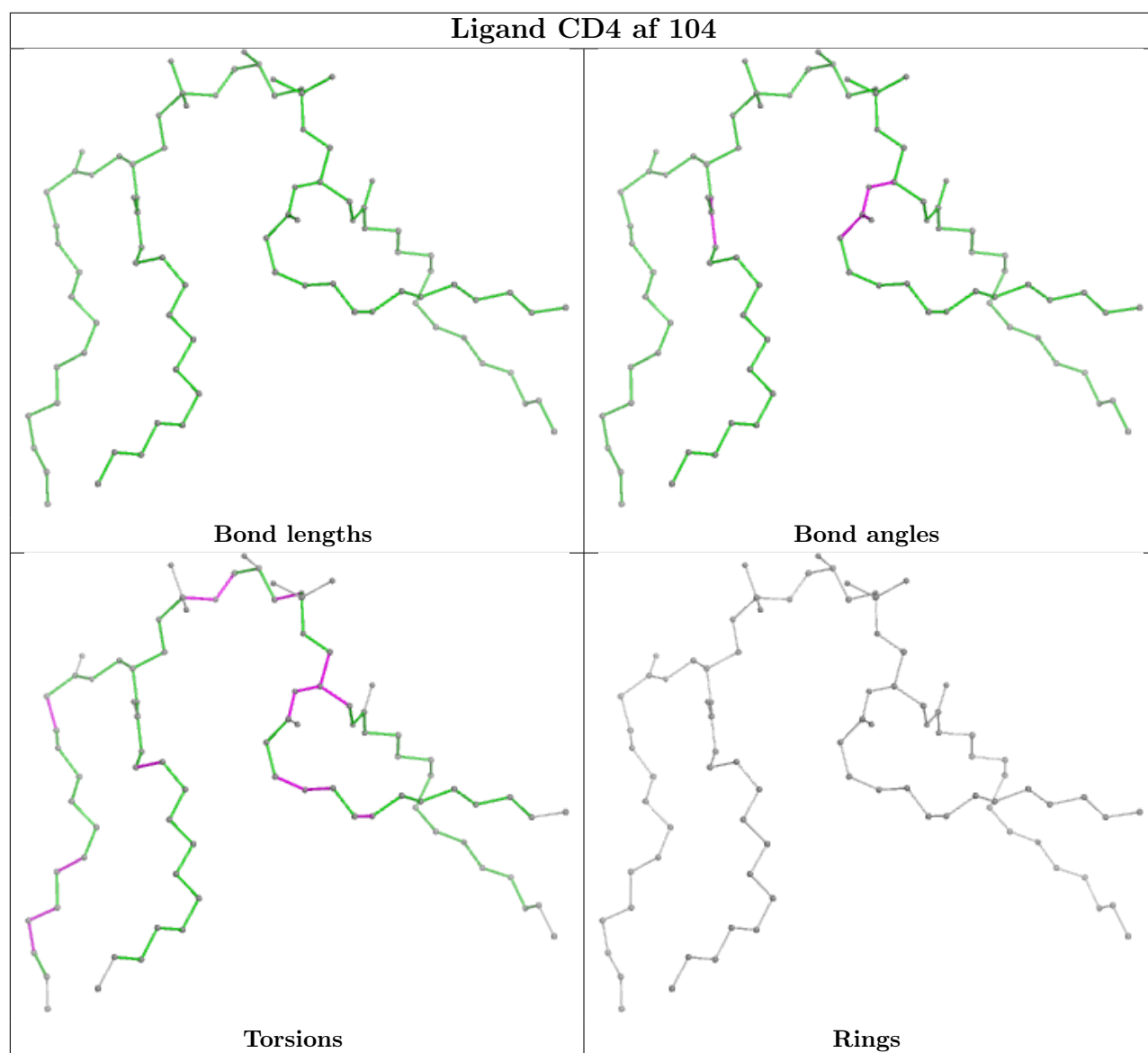
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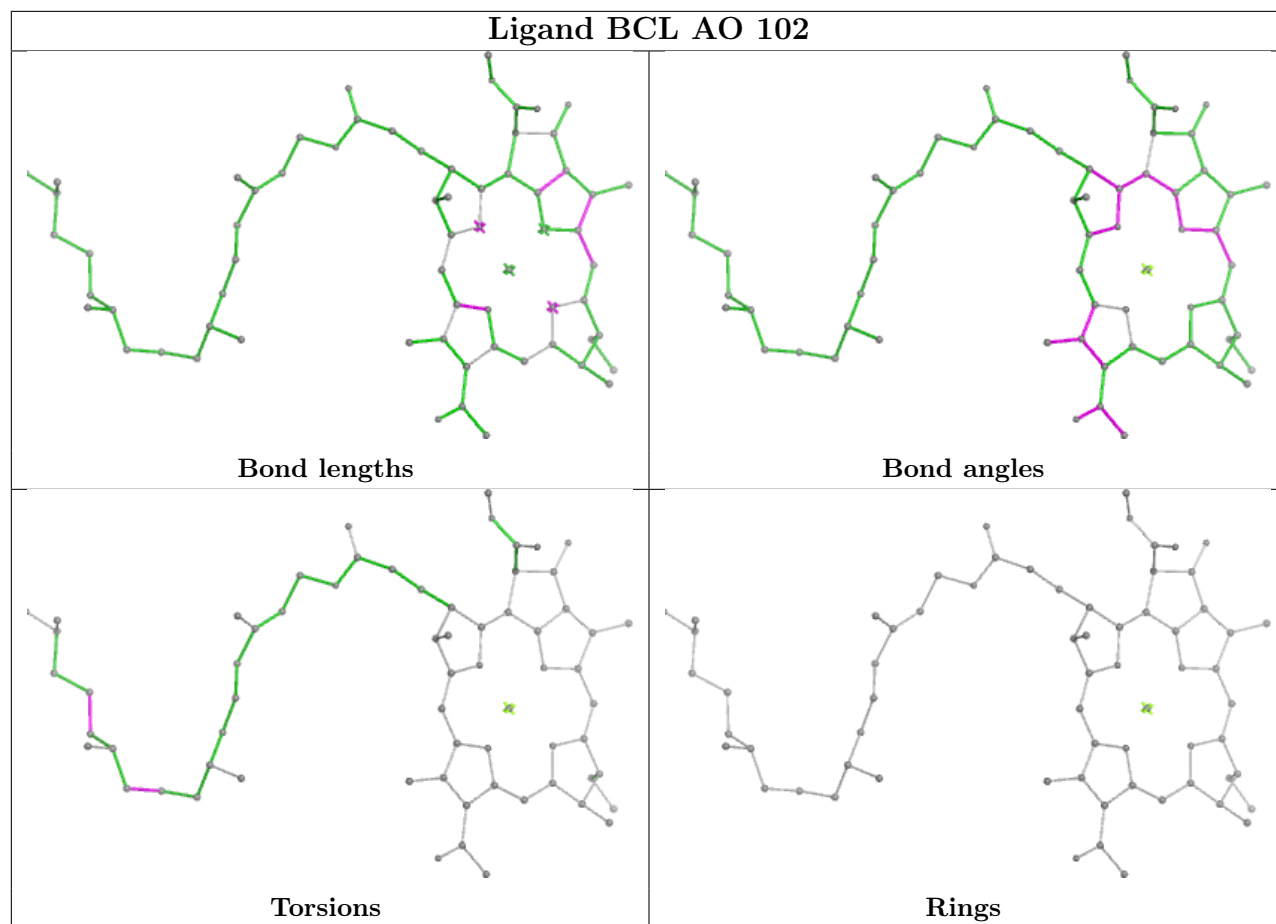




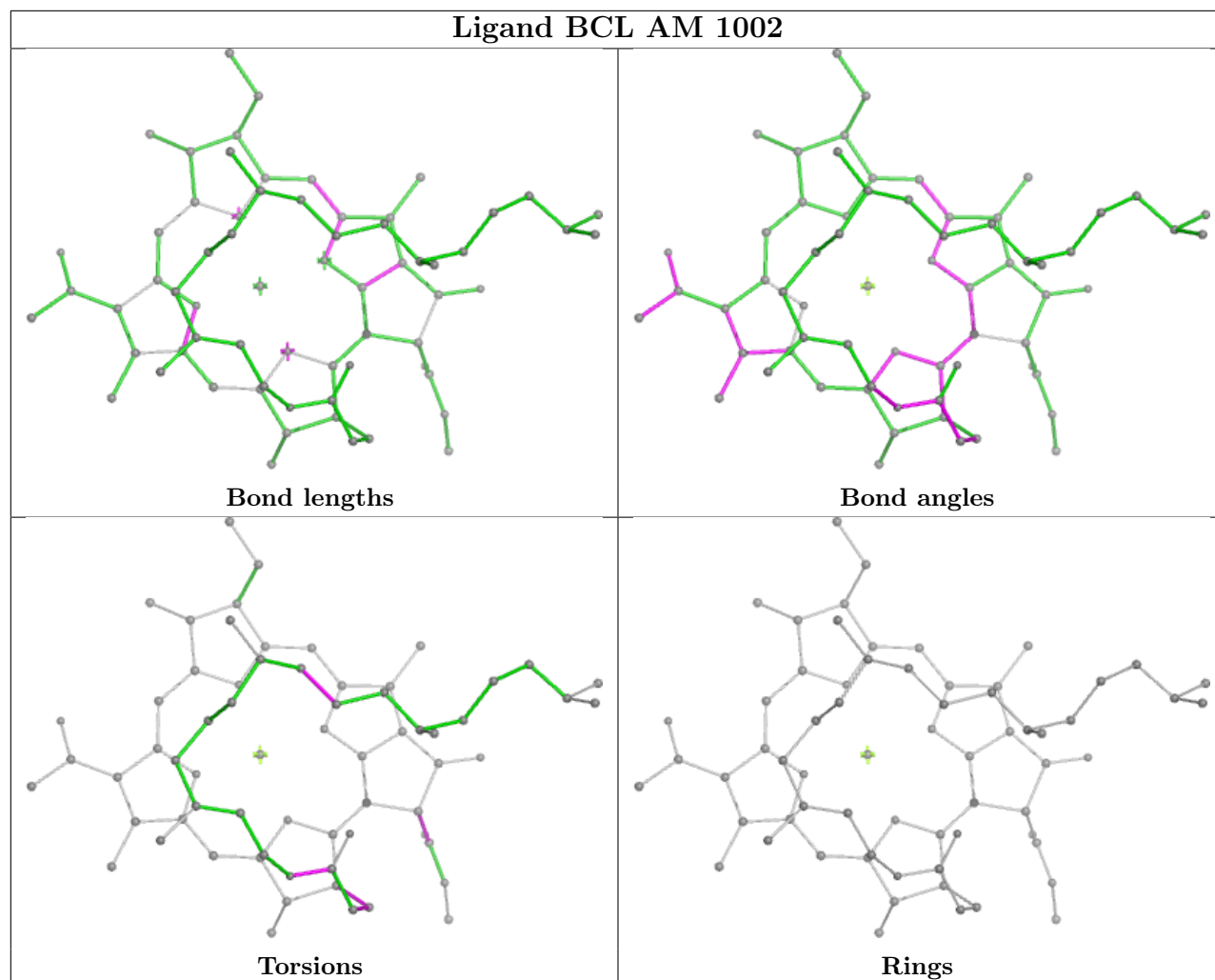




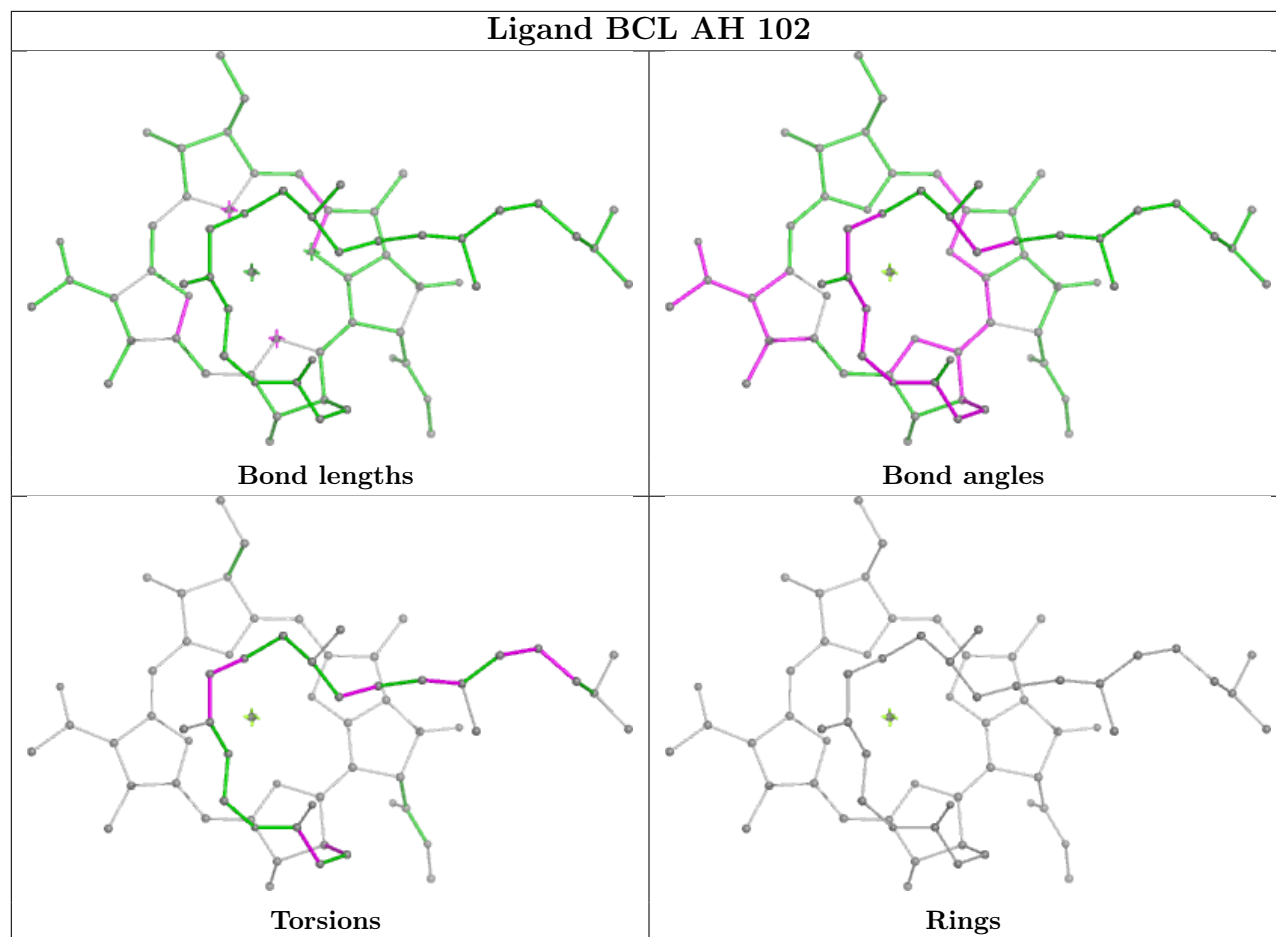




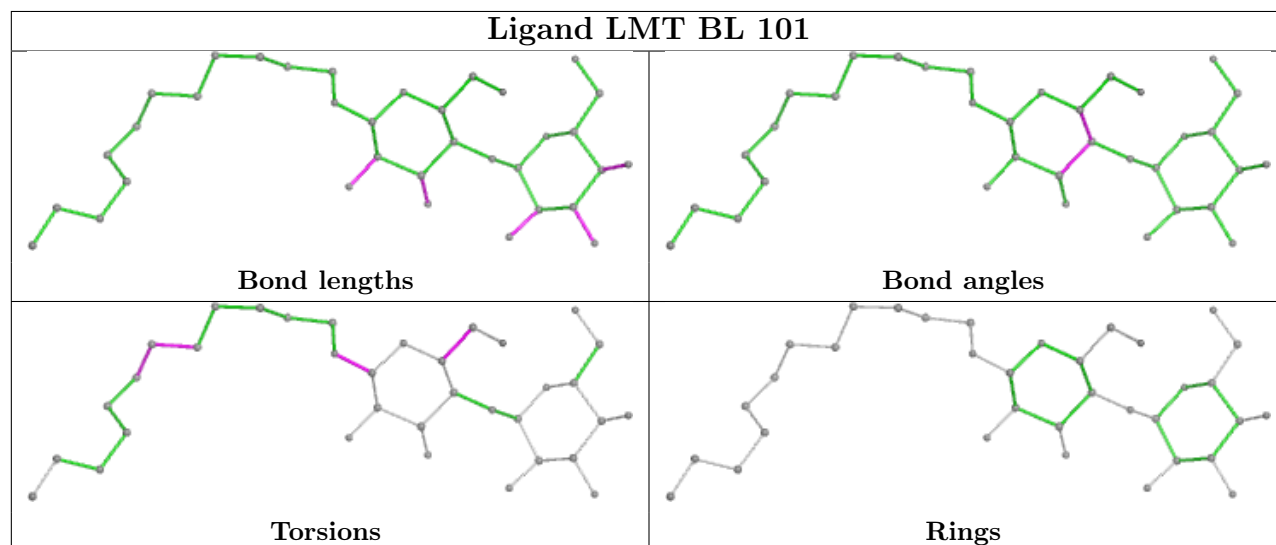
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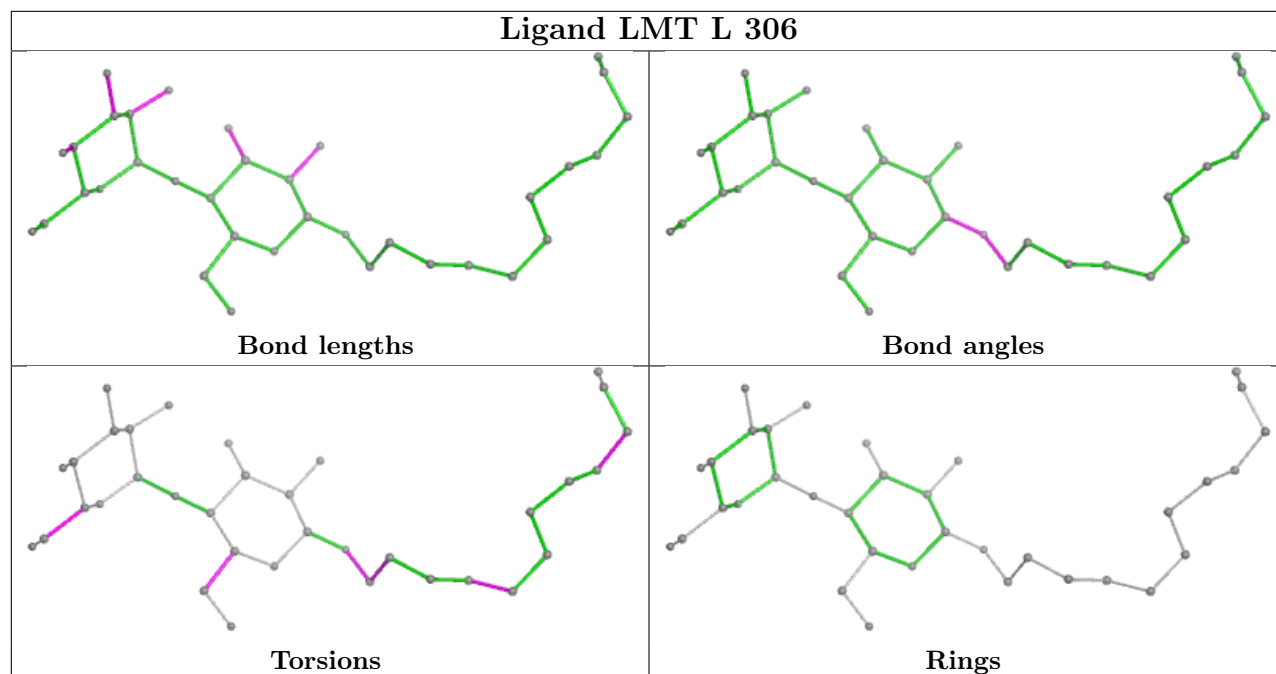
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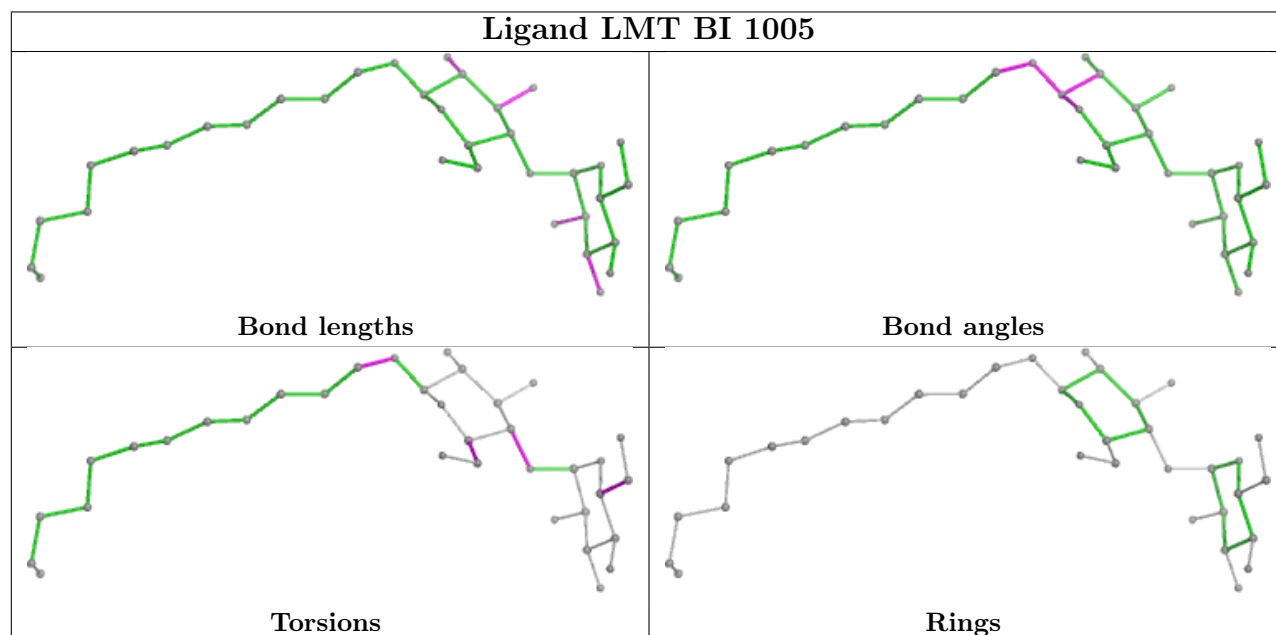
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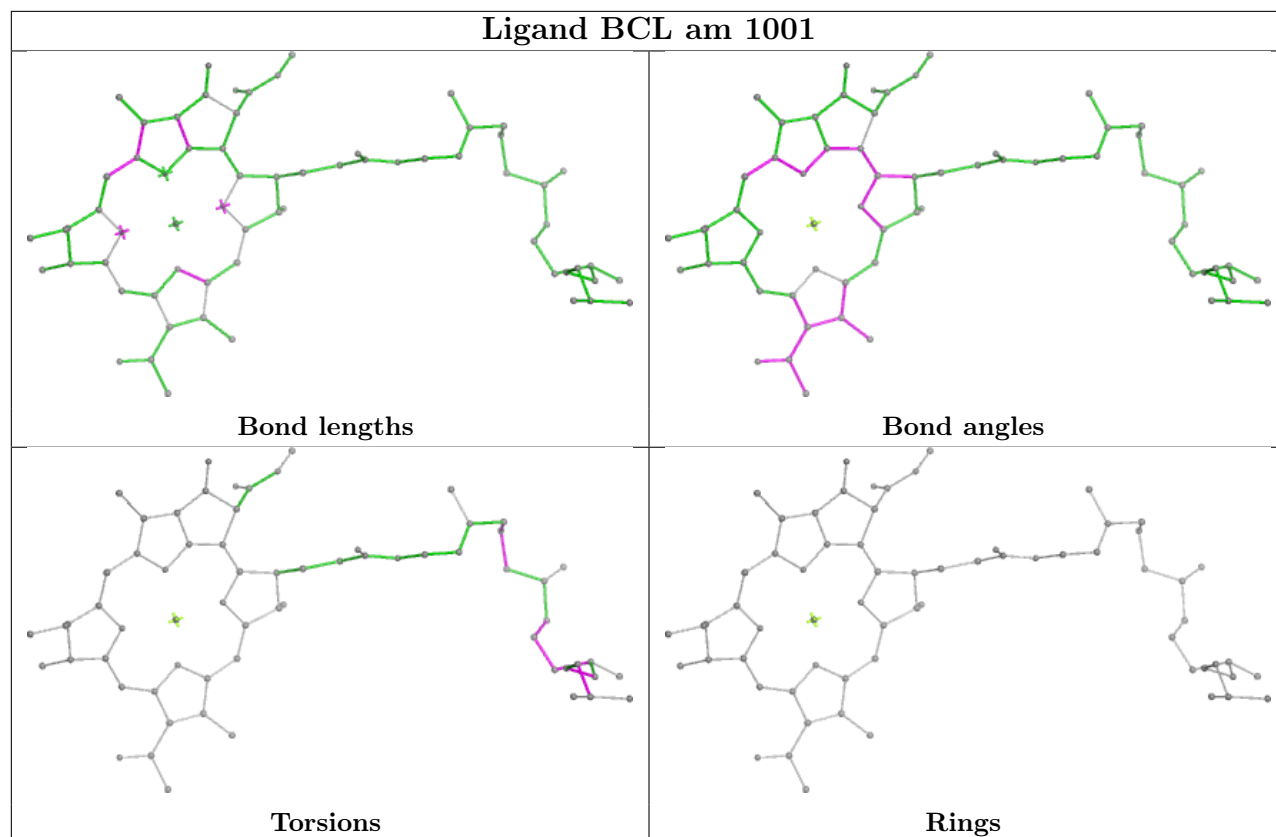
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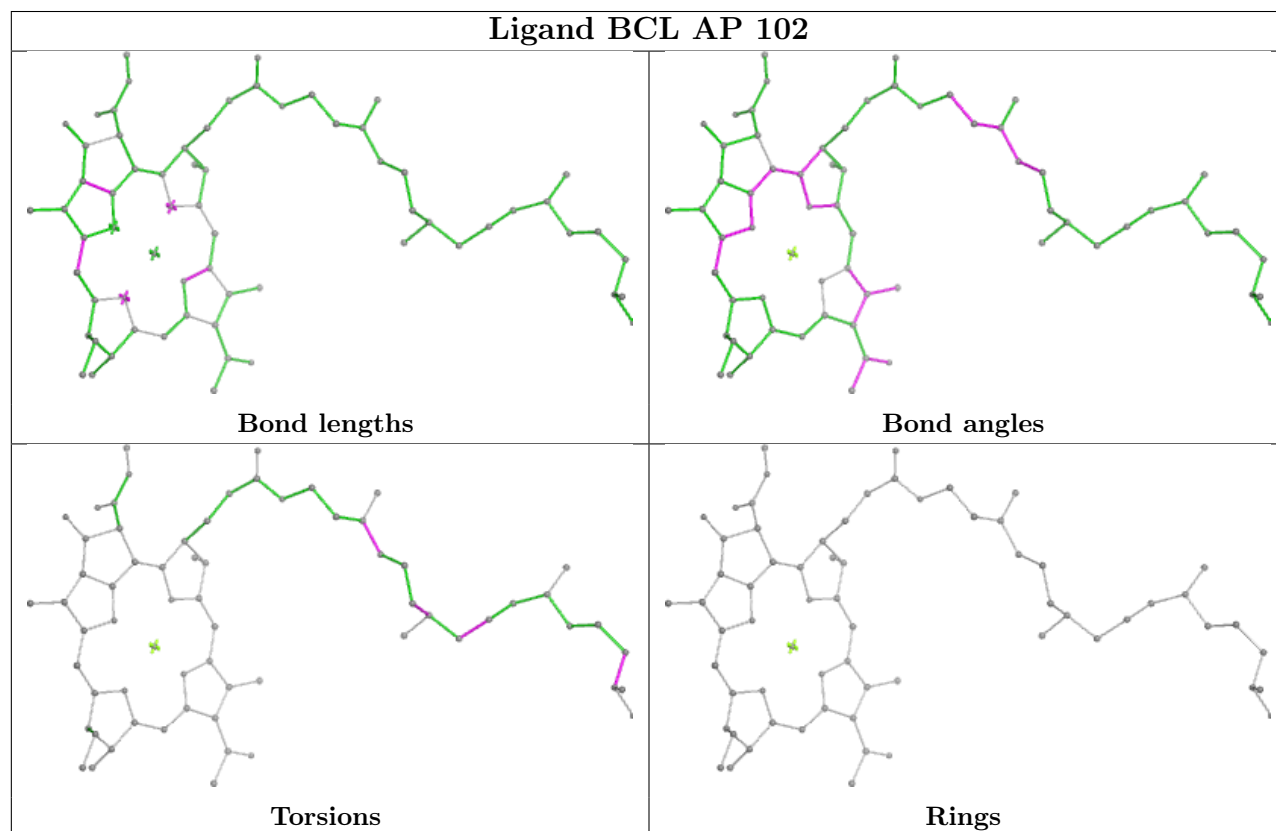
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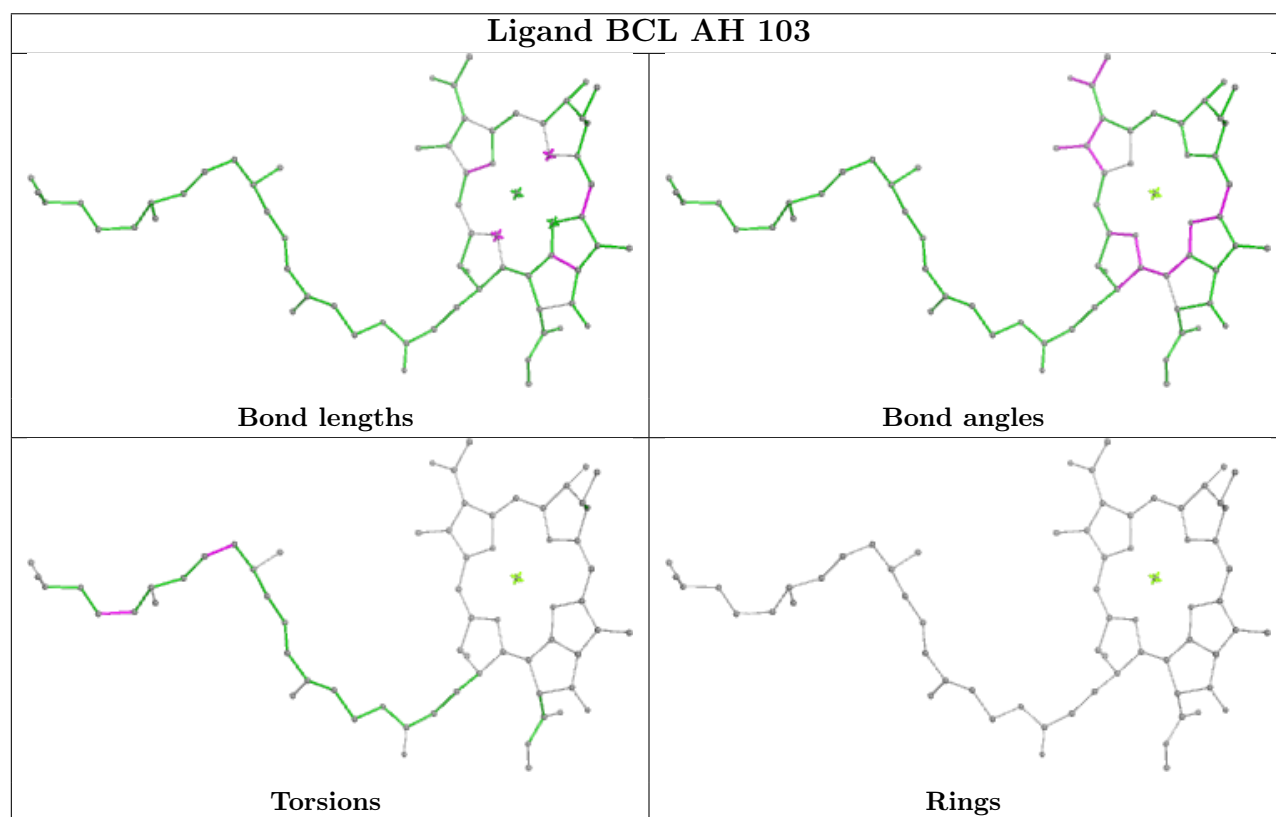
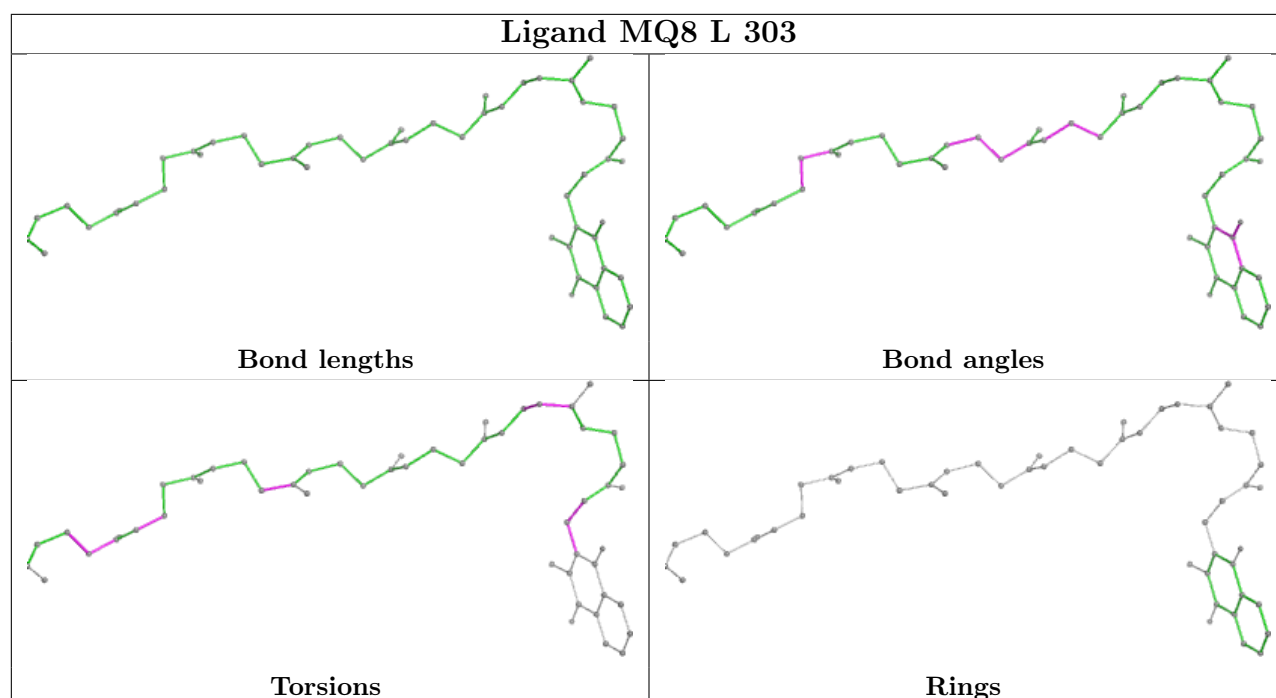


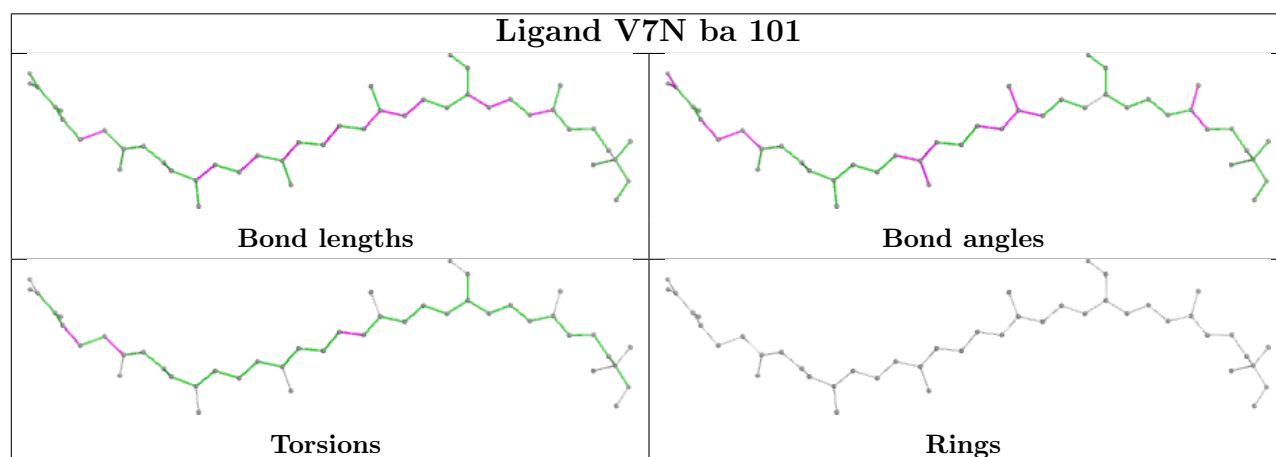
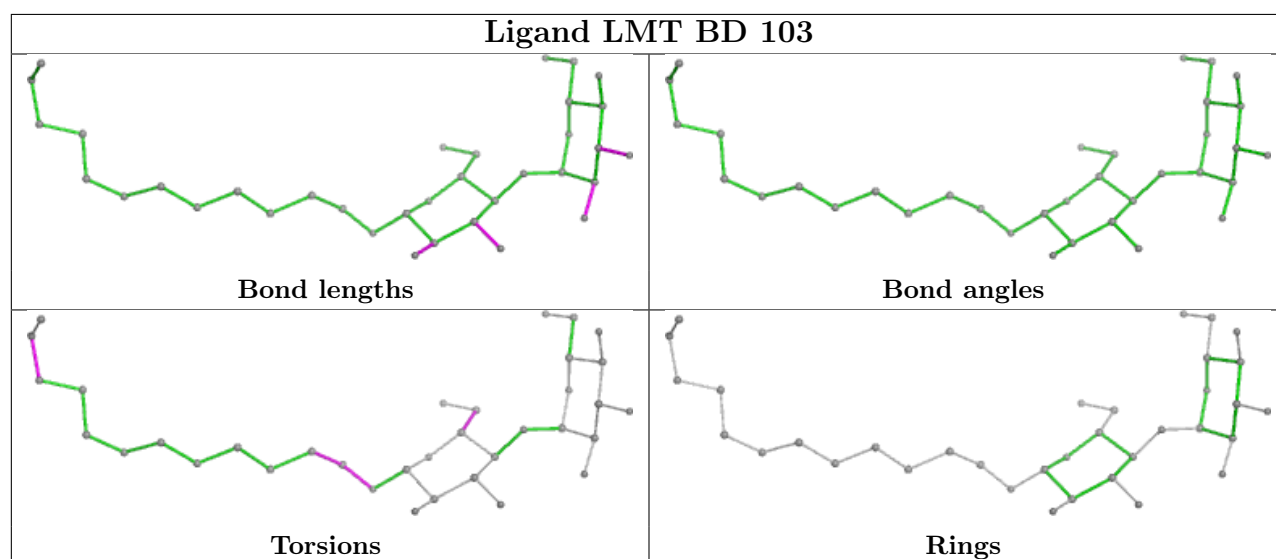
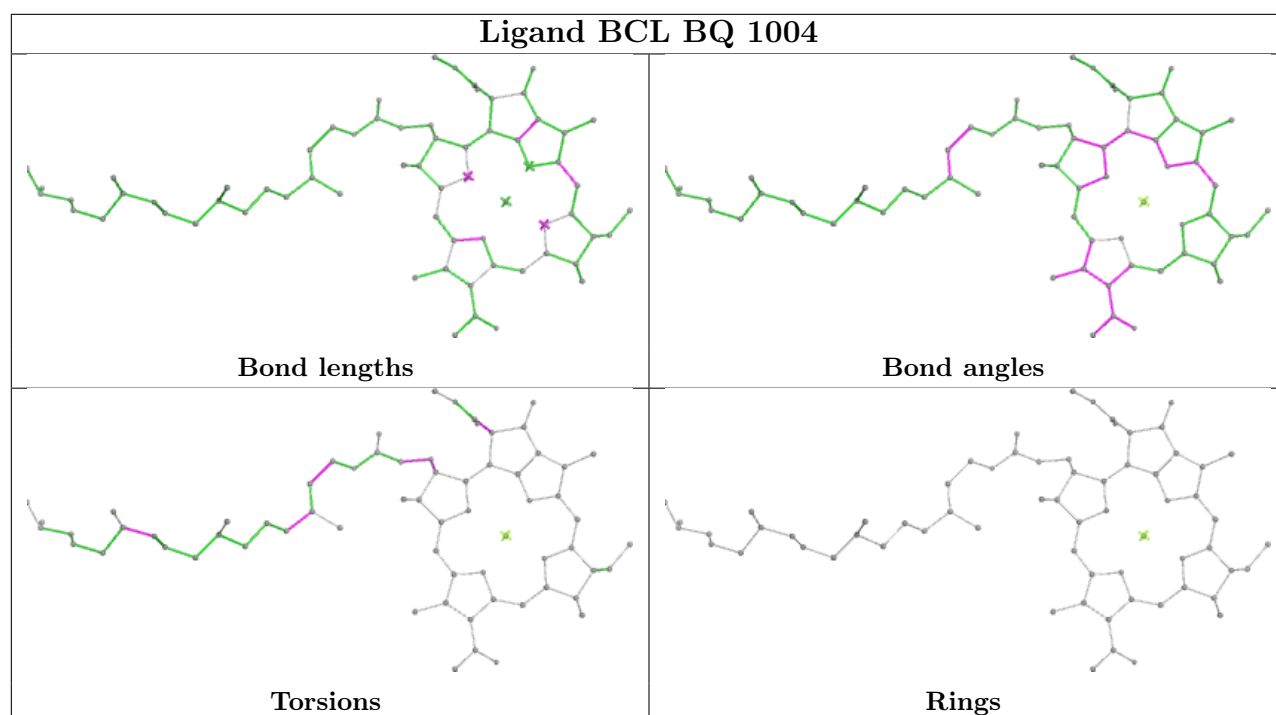
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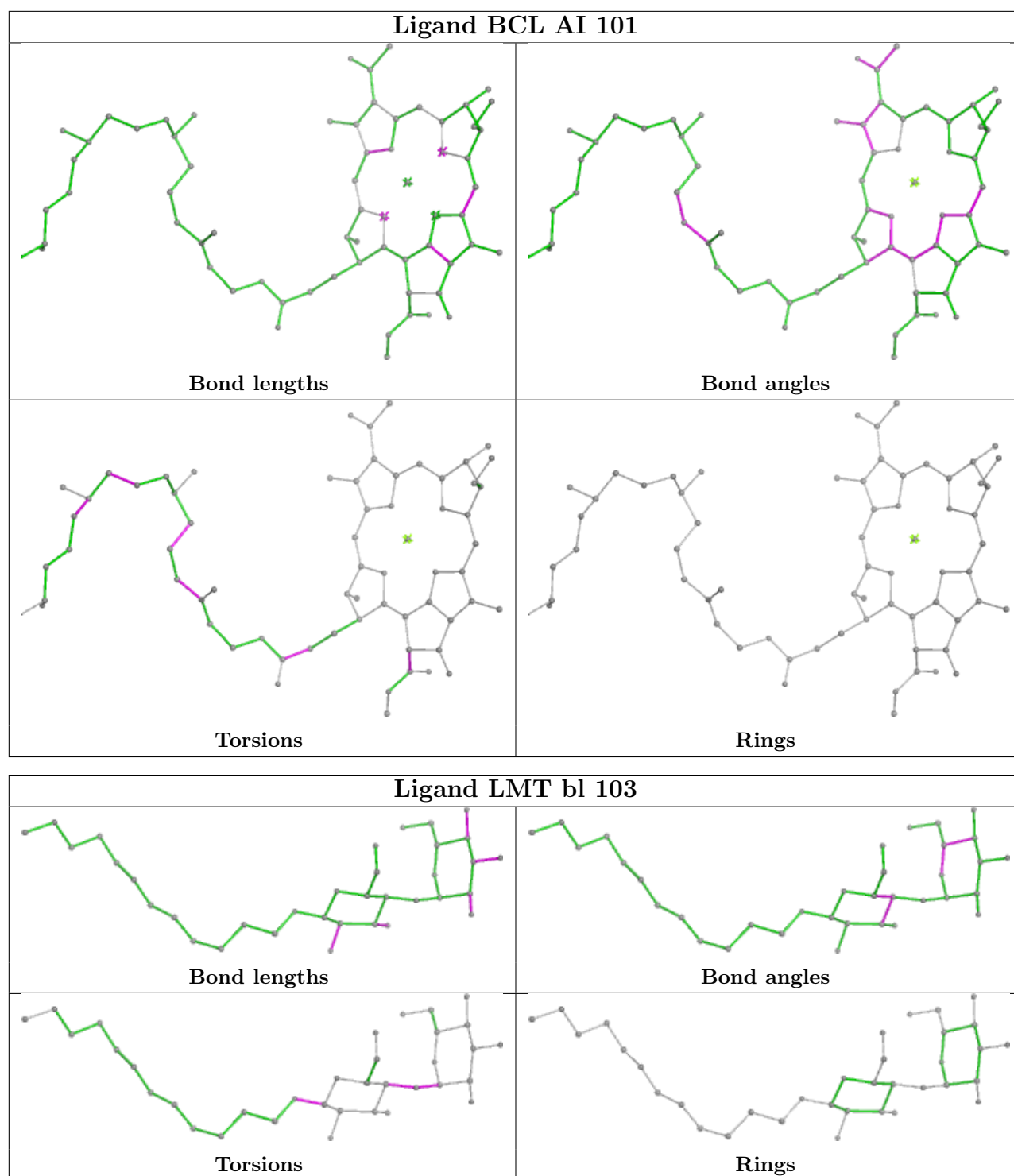


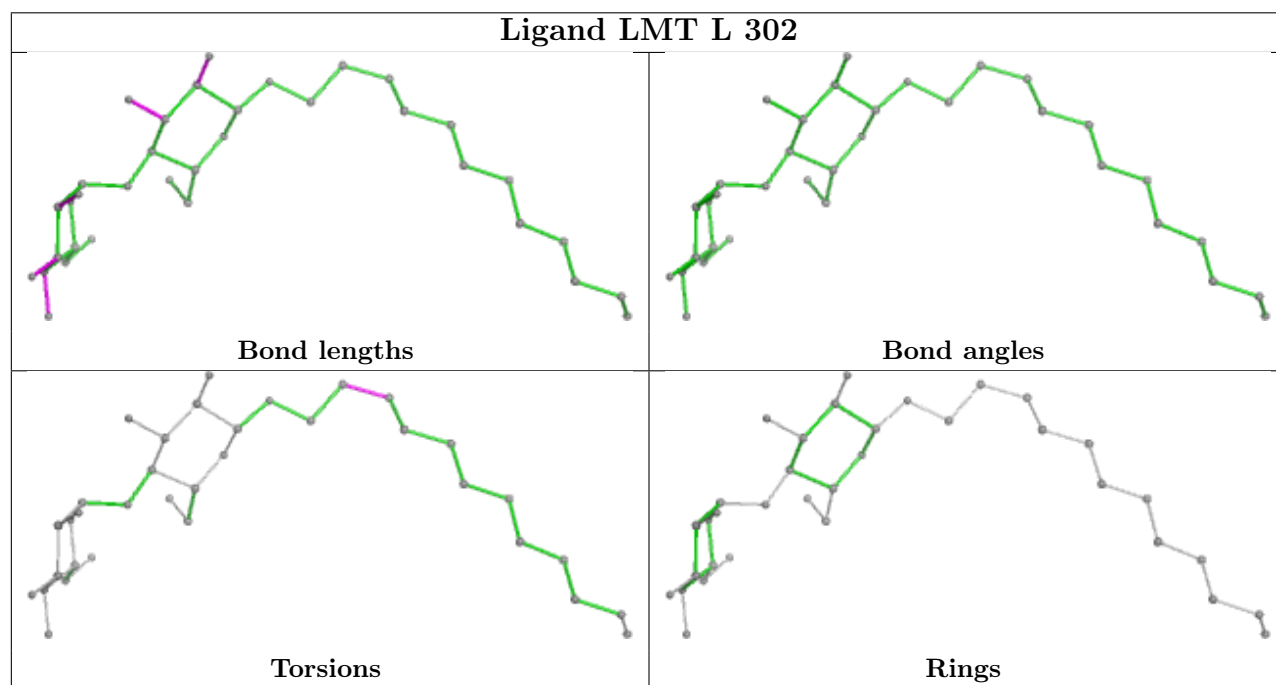
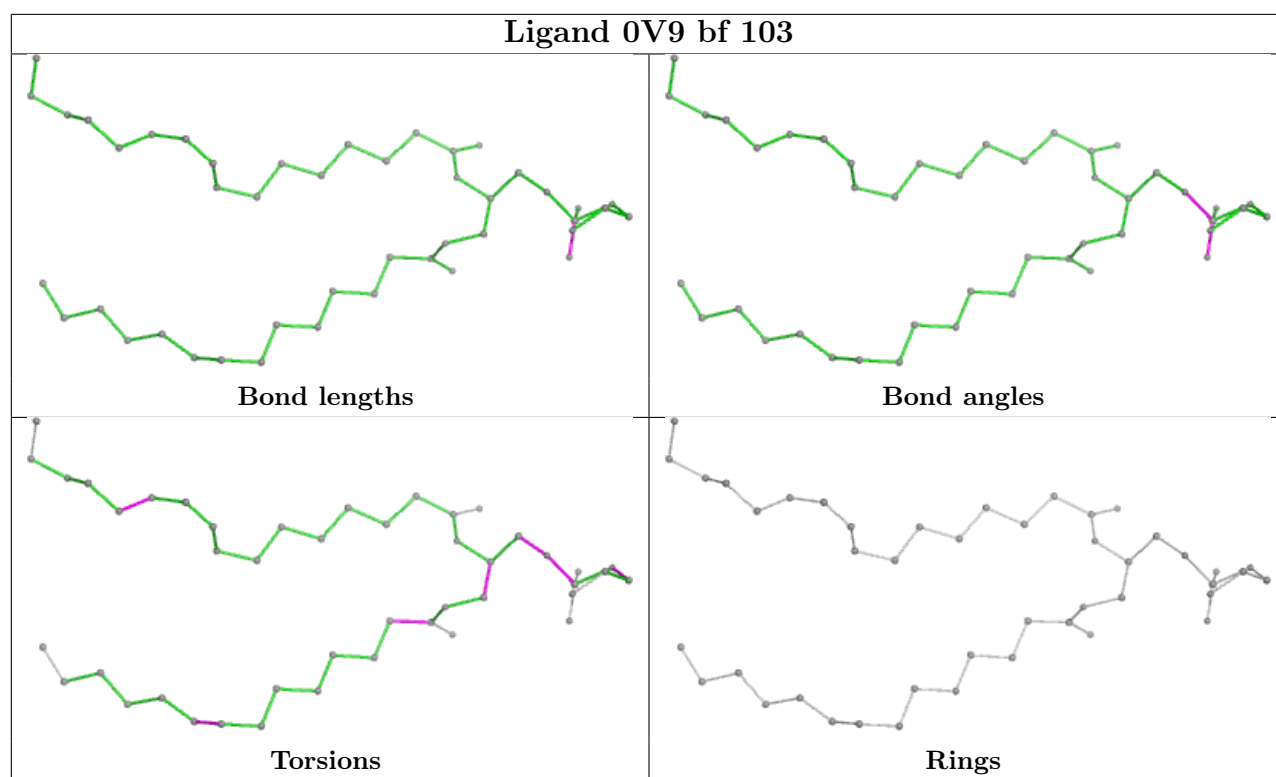
Ligand BCL AP 102



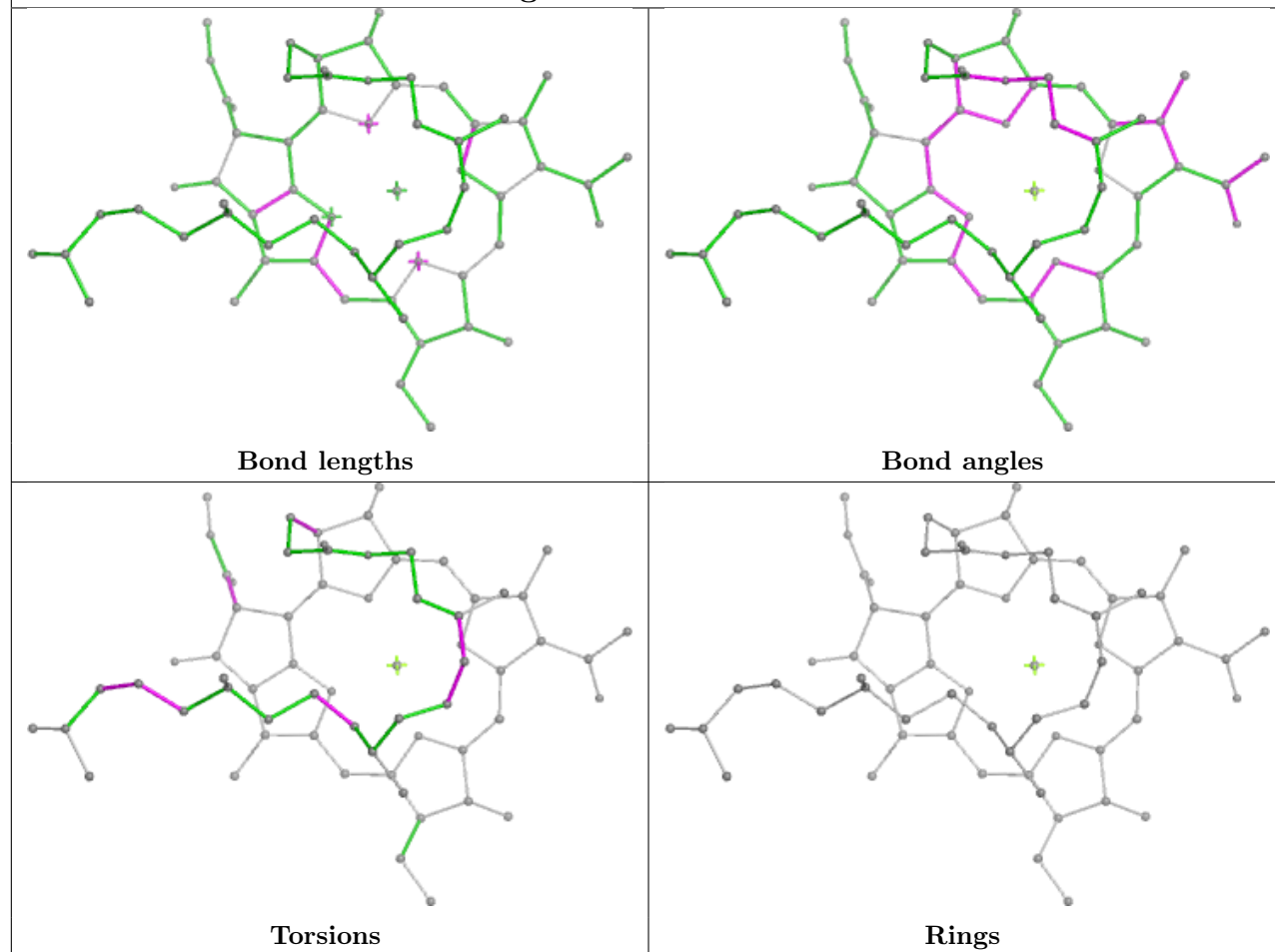




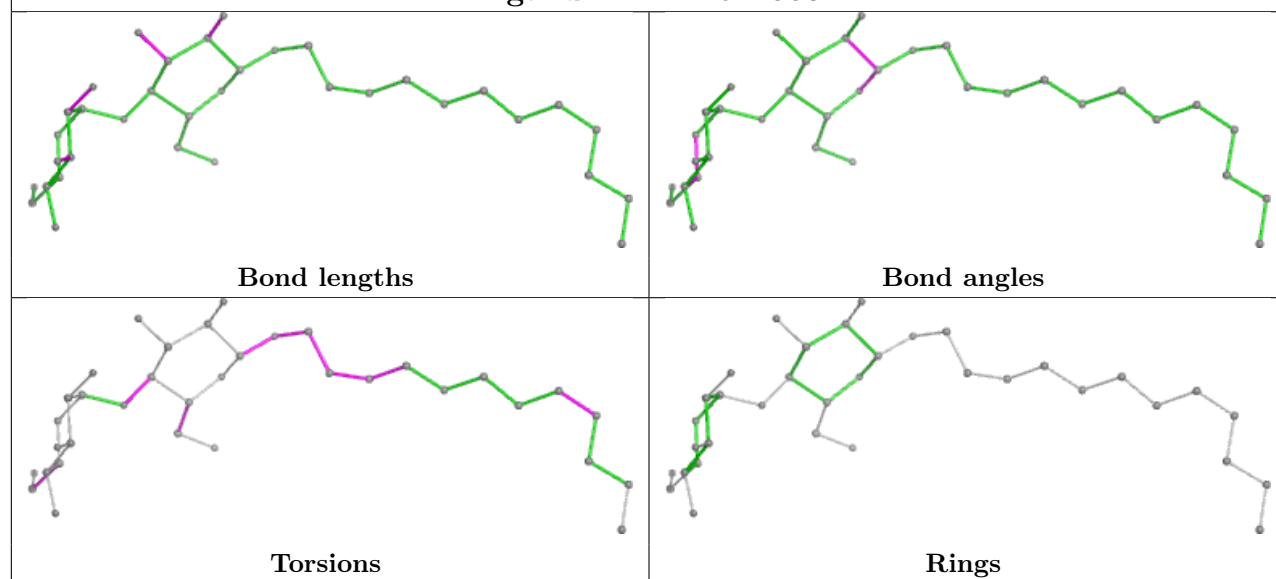




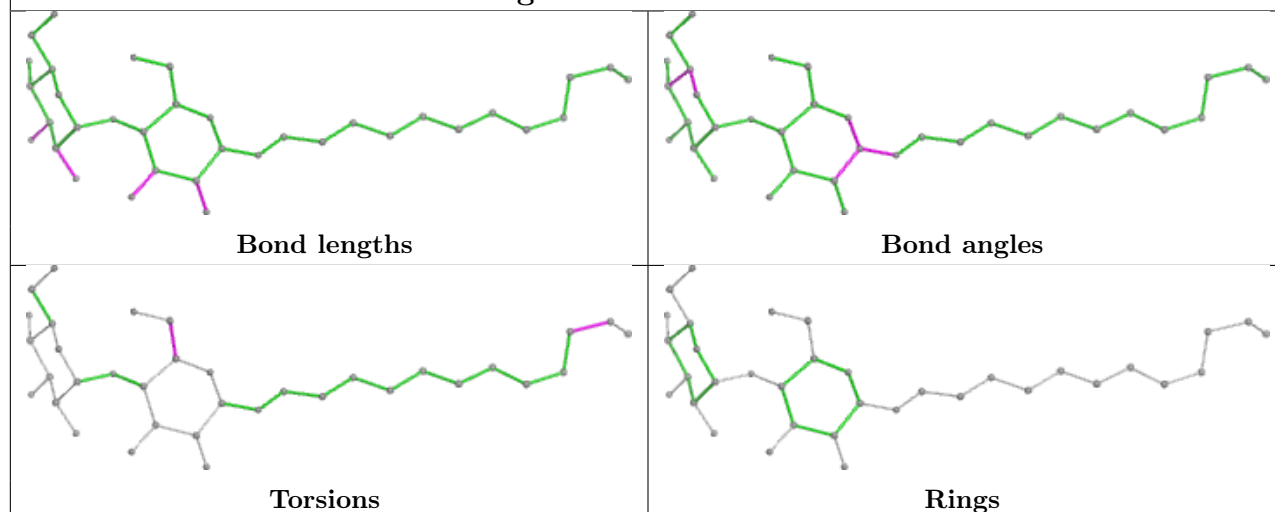
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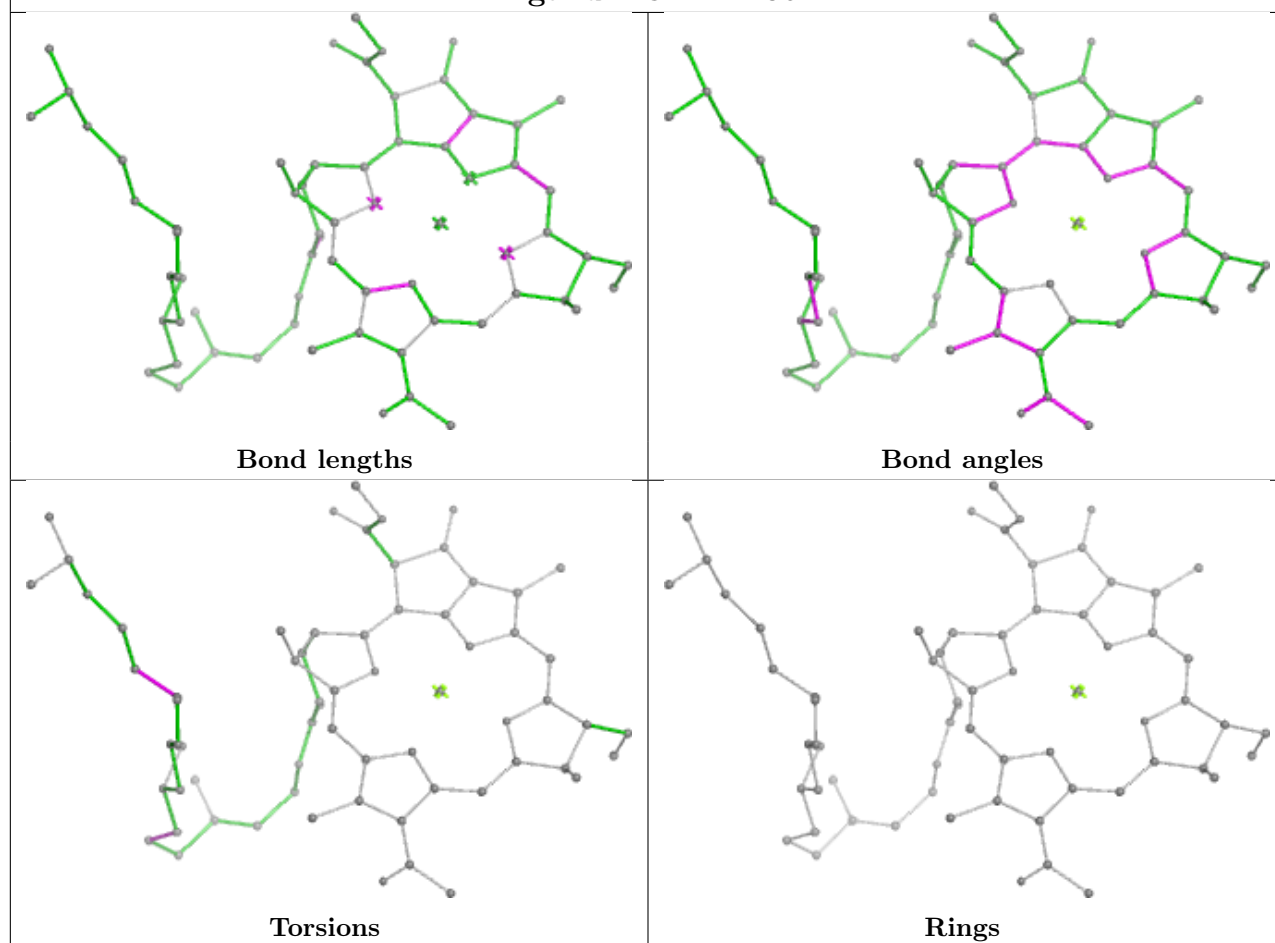
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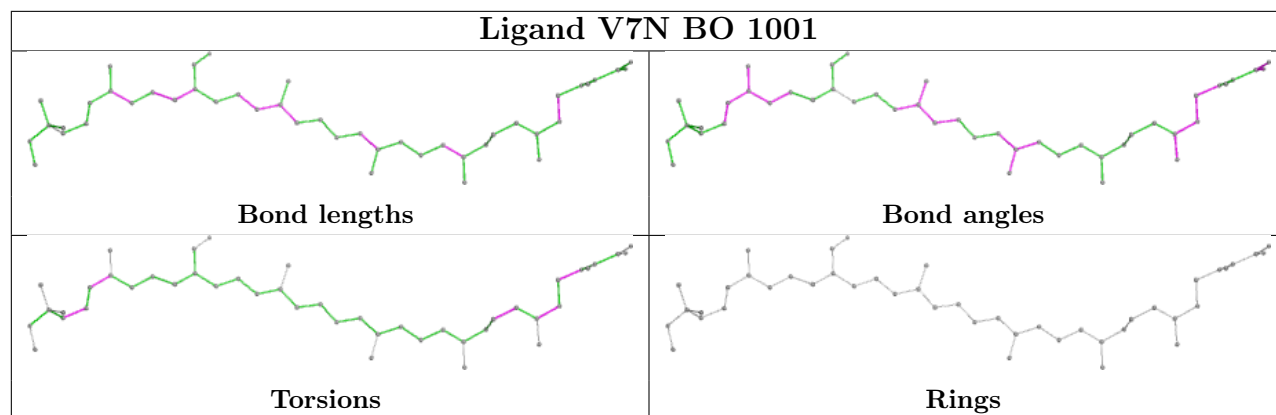
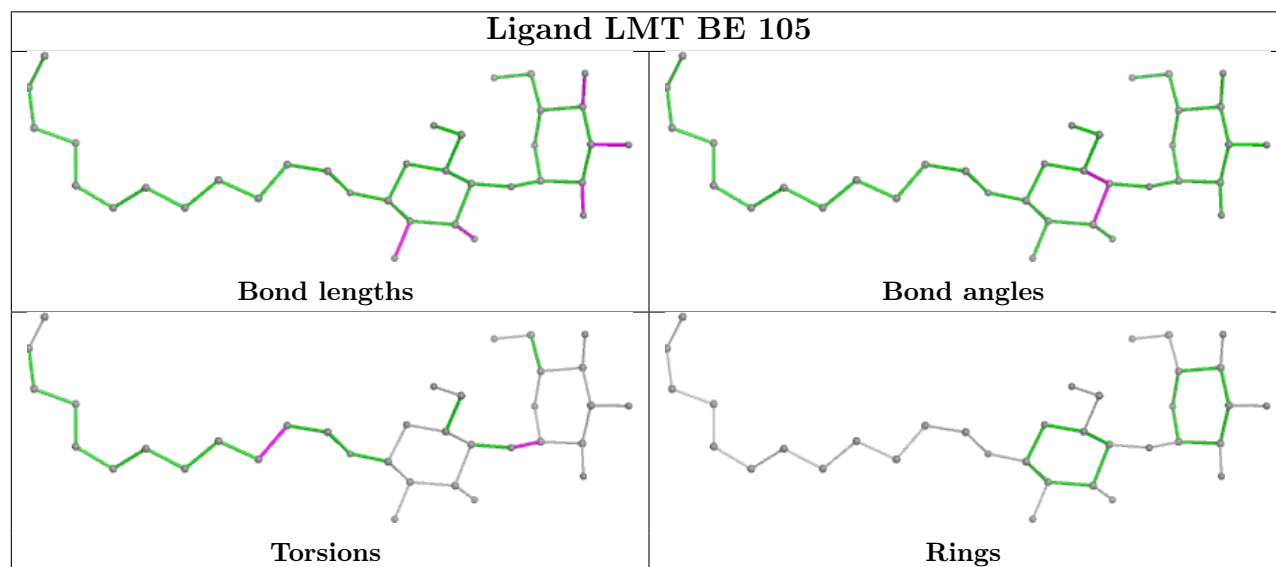
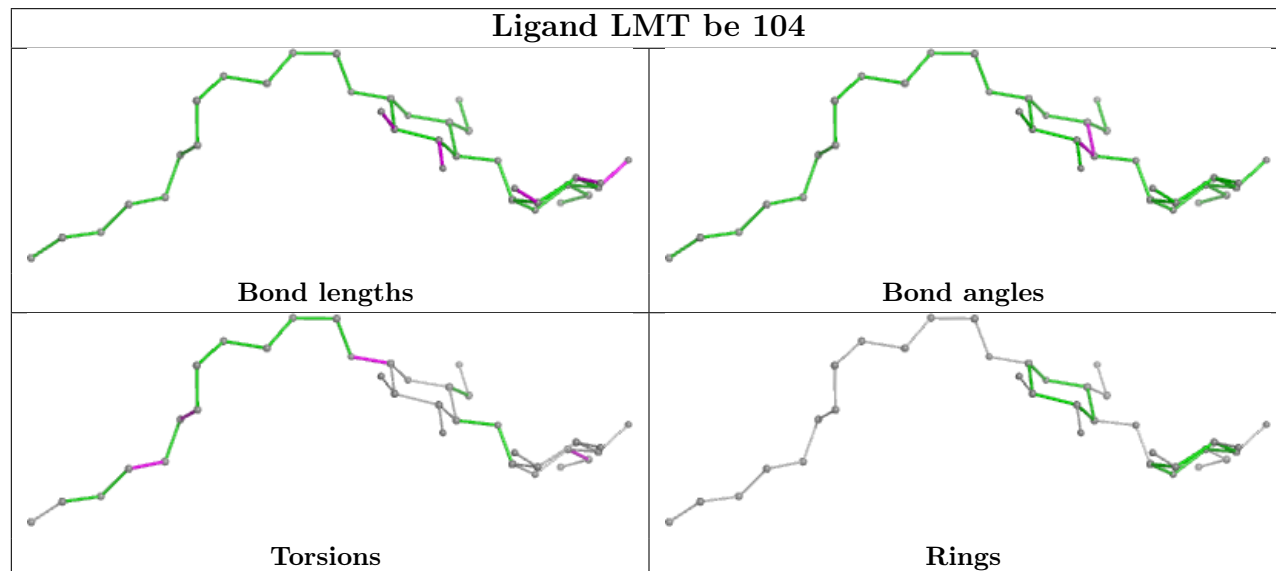


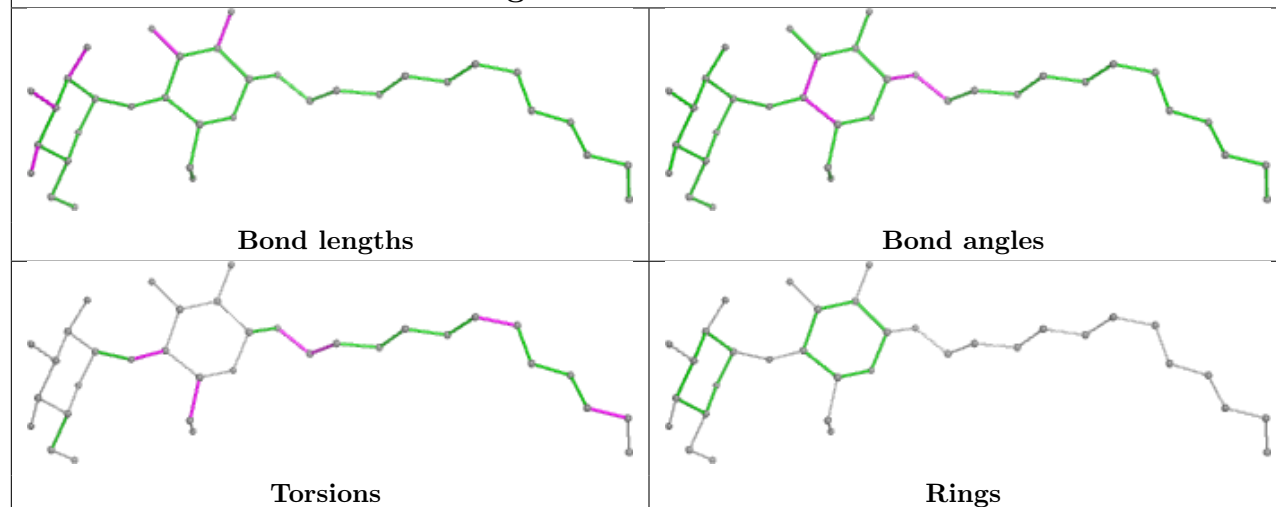
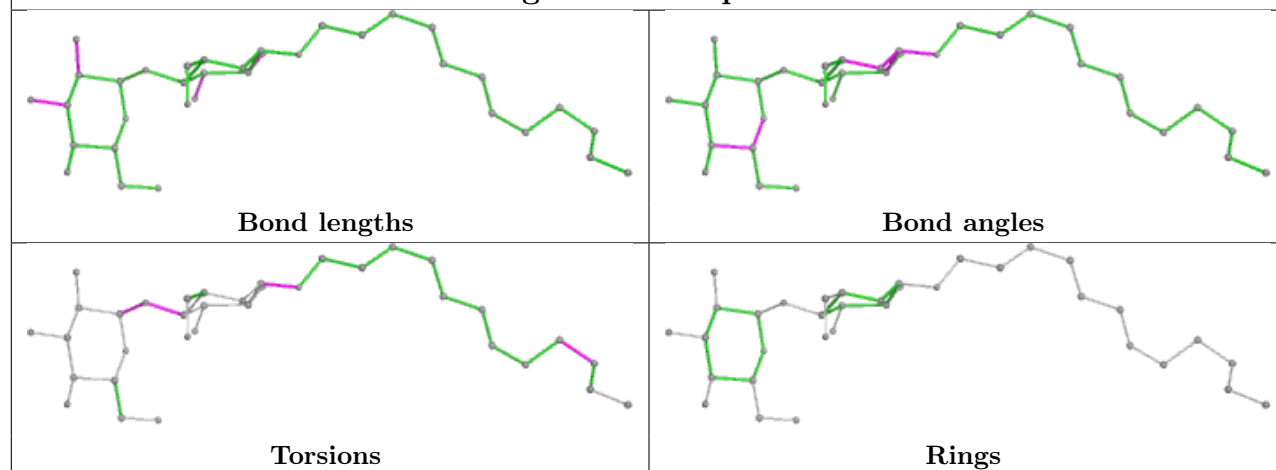
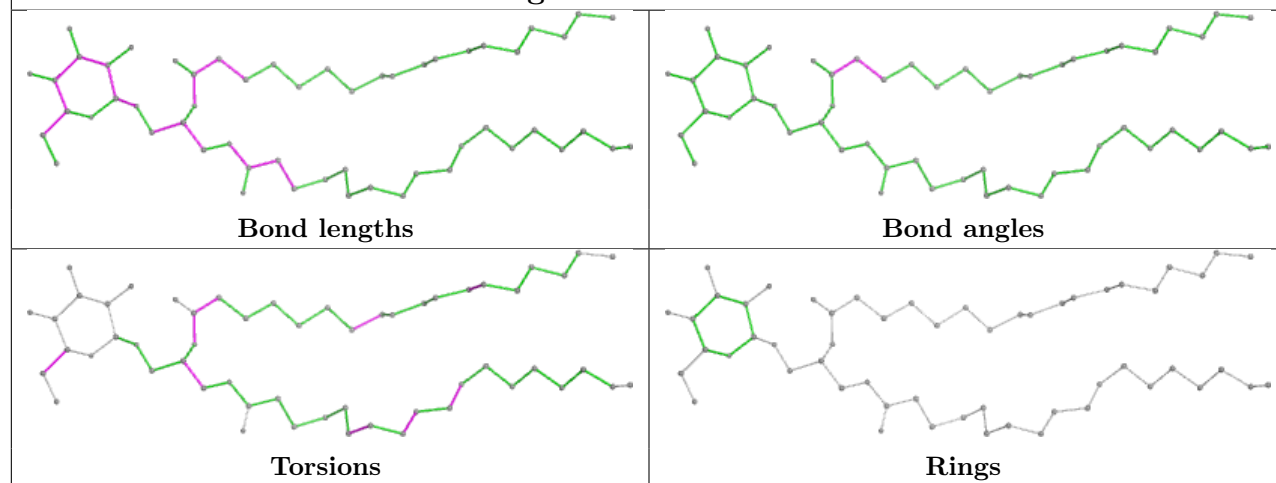
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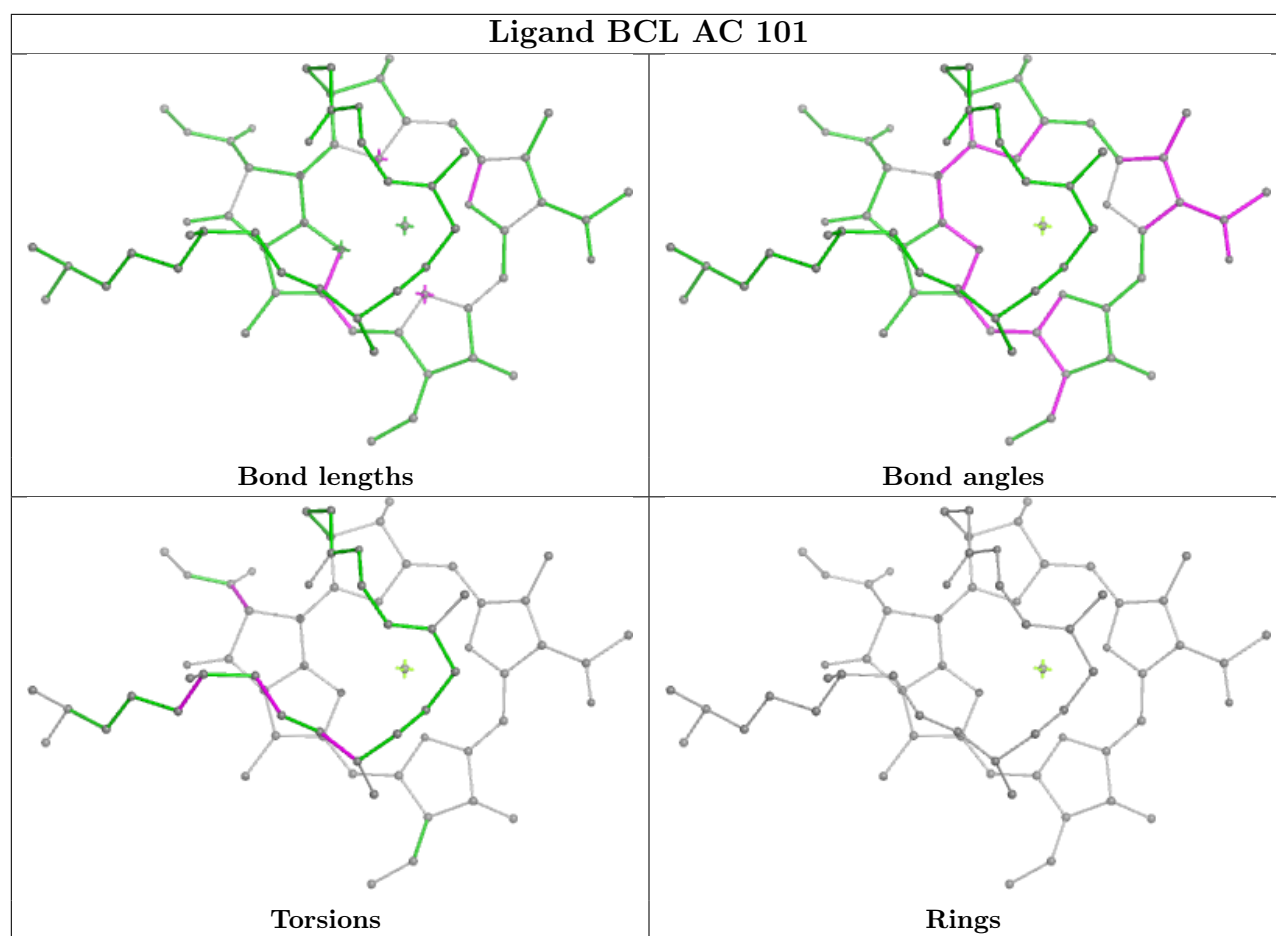


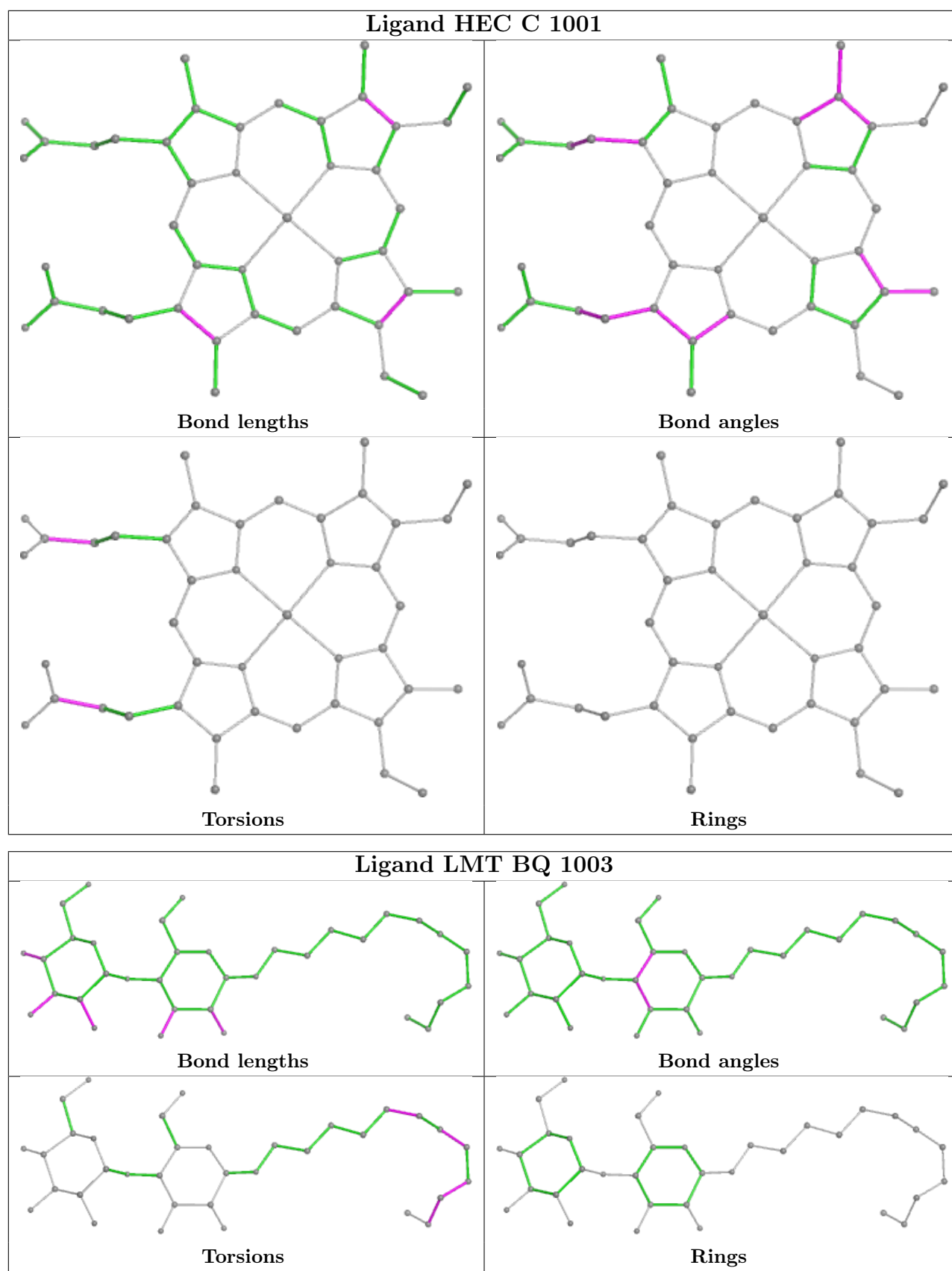
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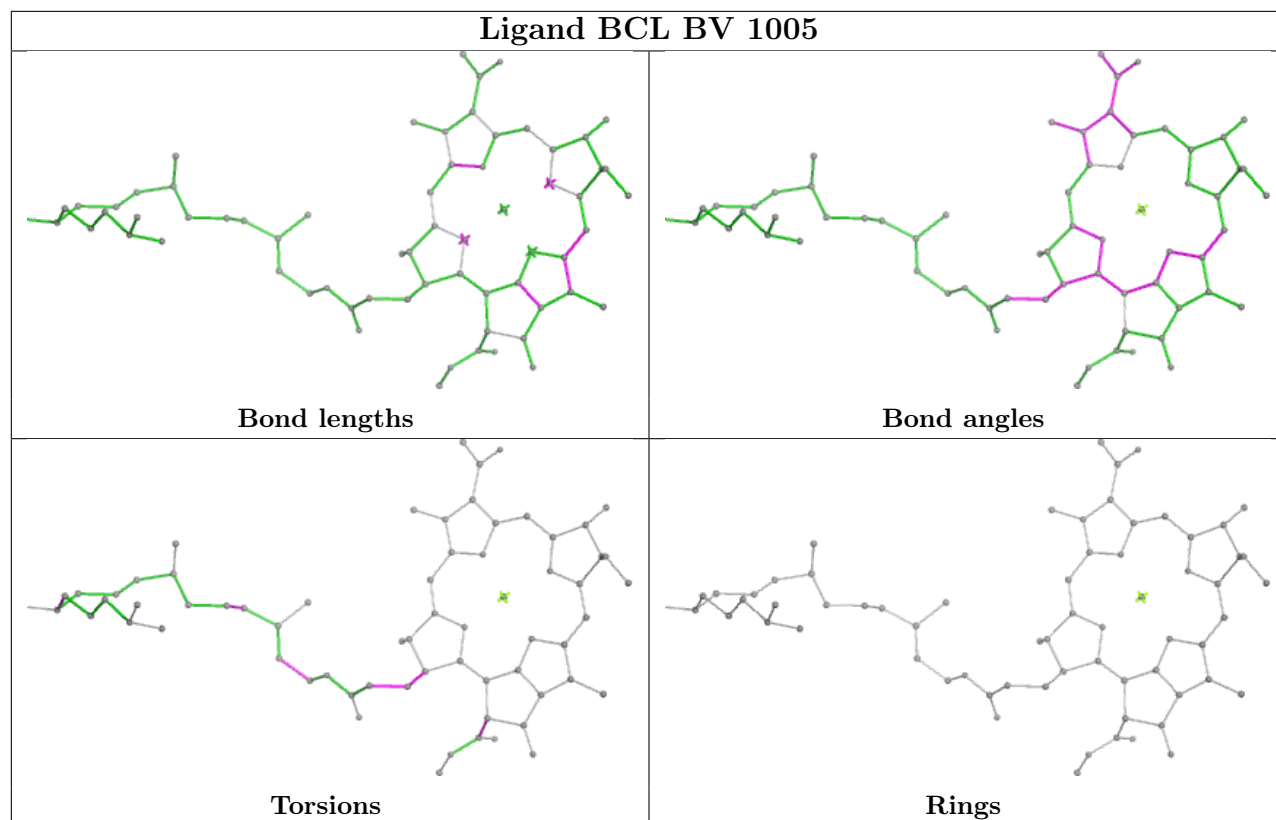


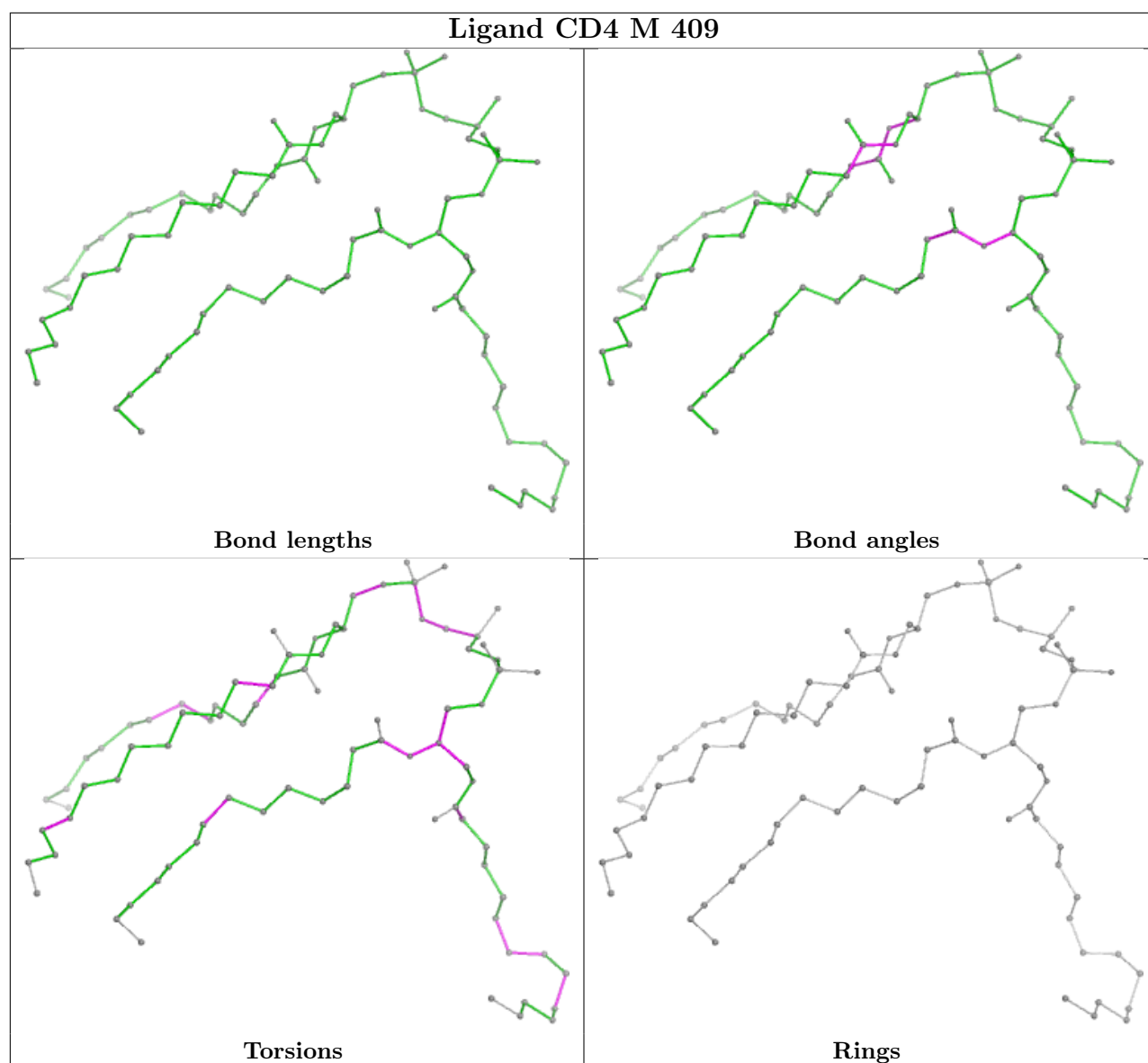
Ligand V7N BO 1001**Ligand LMT BE 105****Ligand LMT be 104**

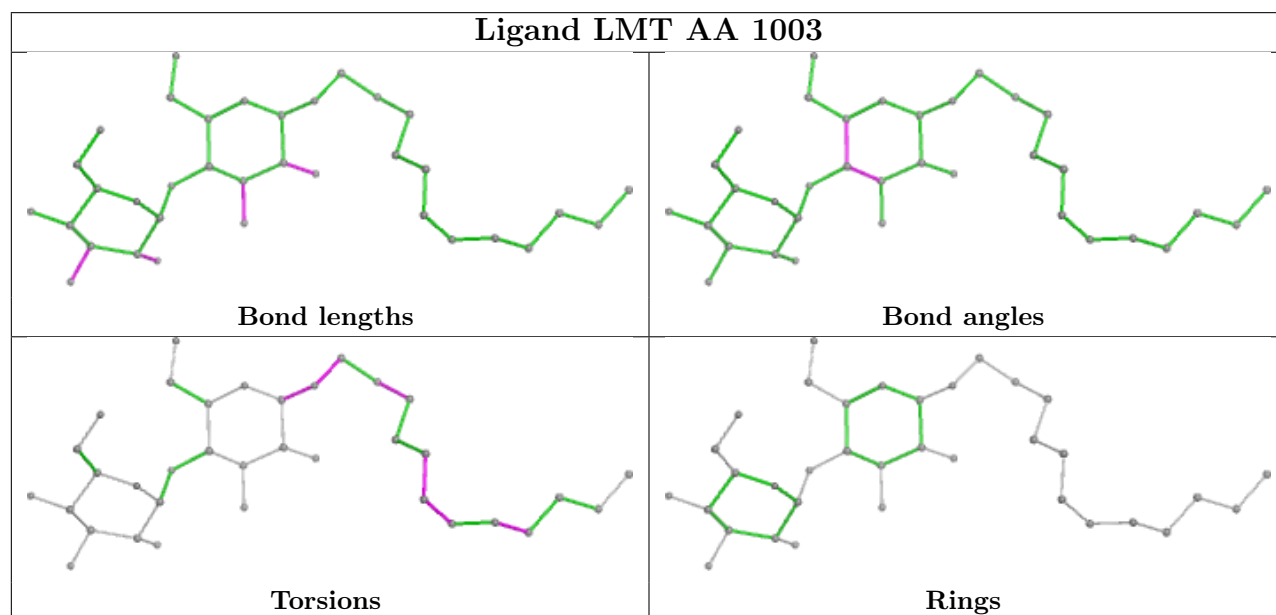
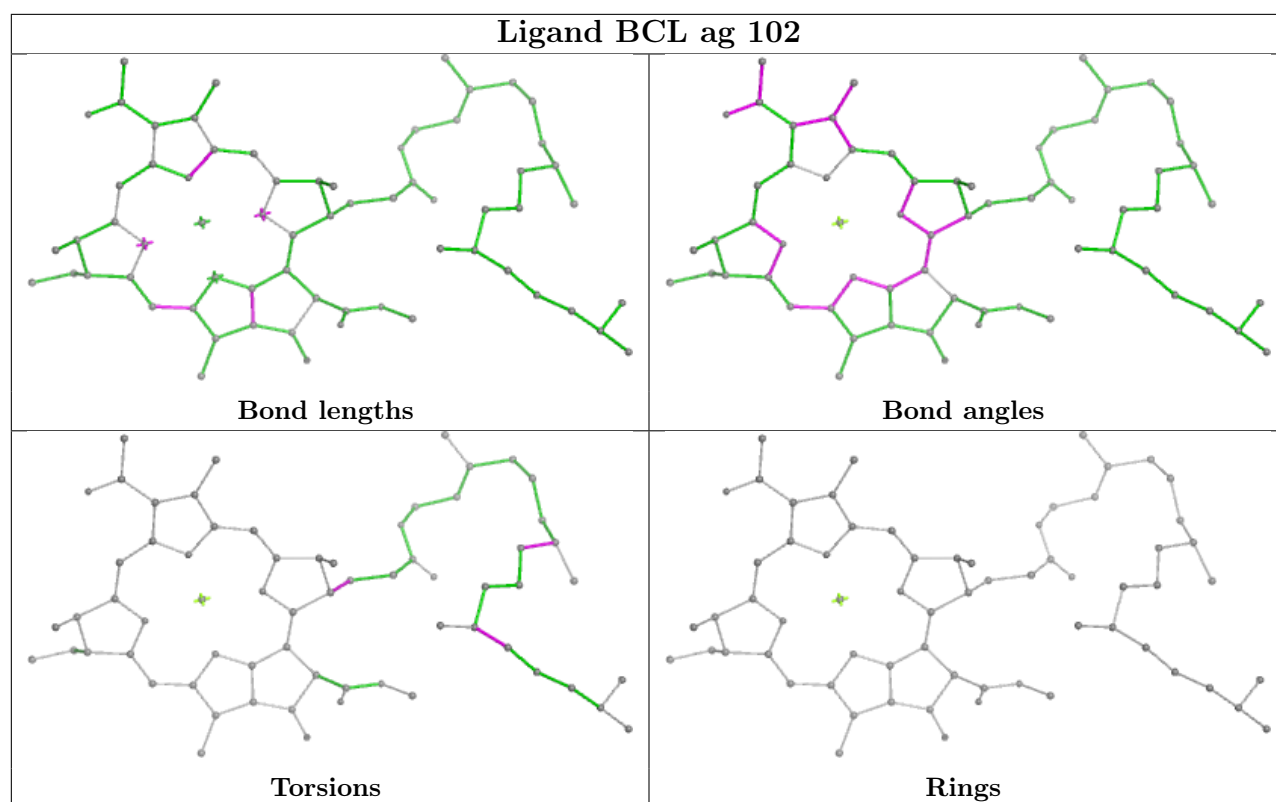
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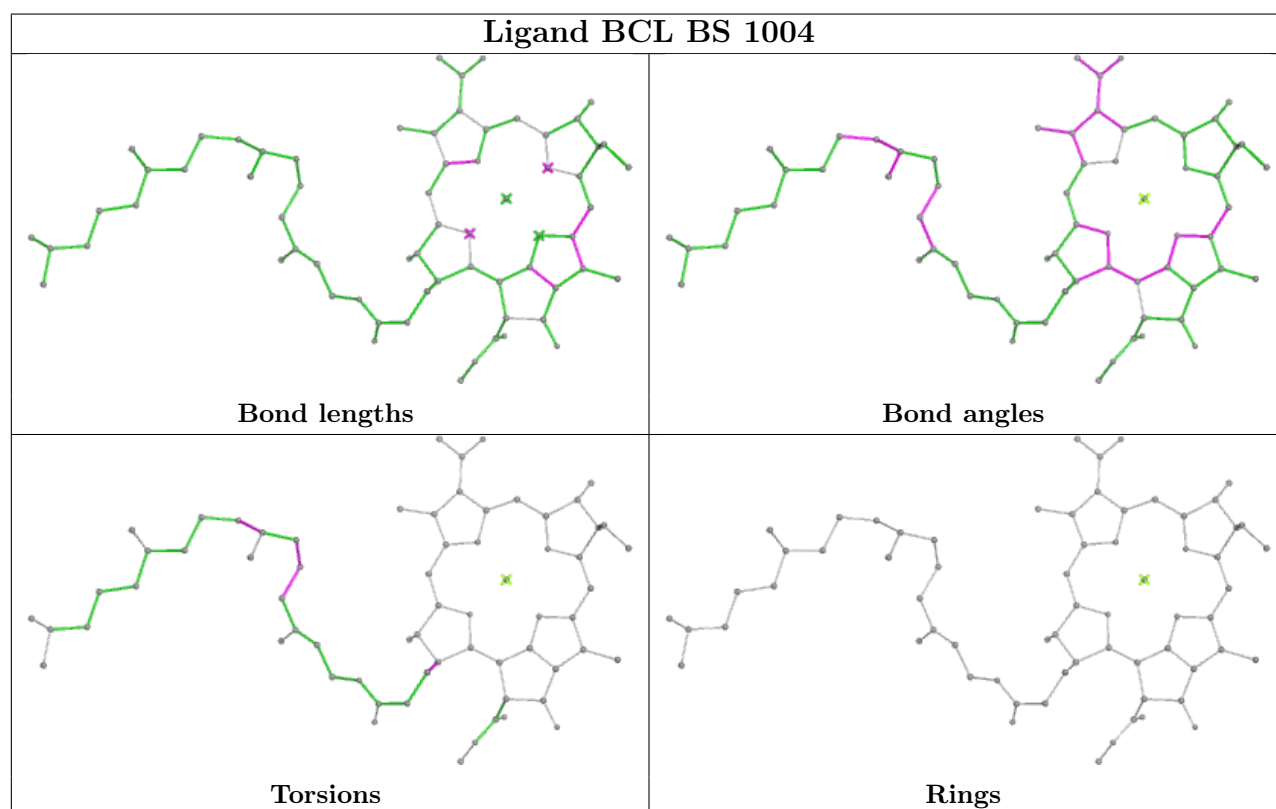
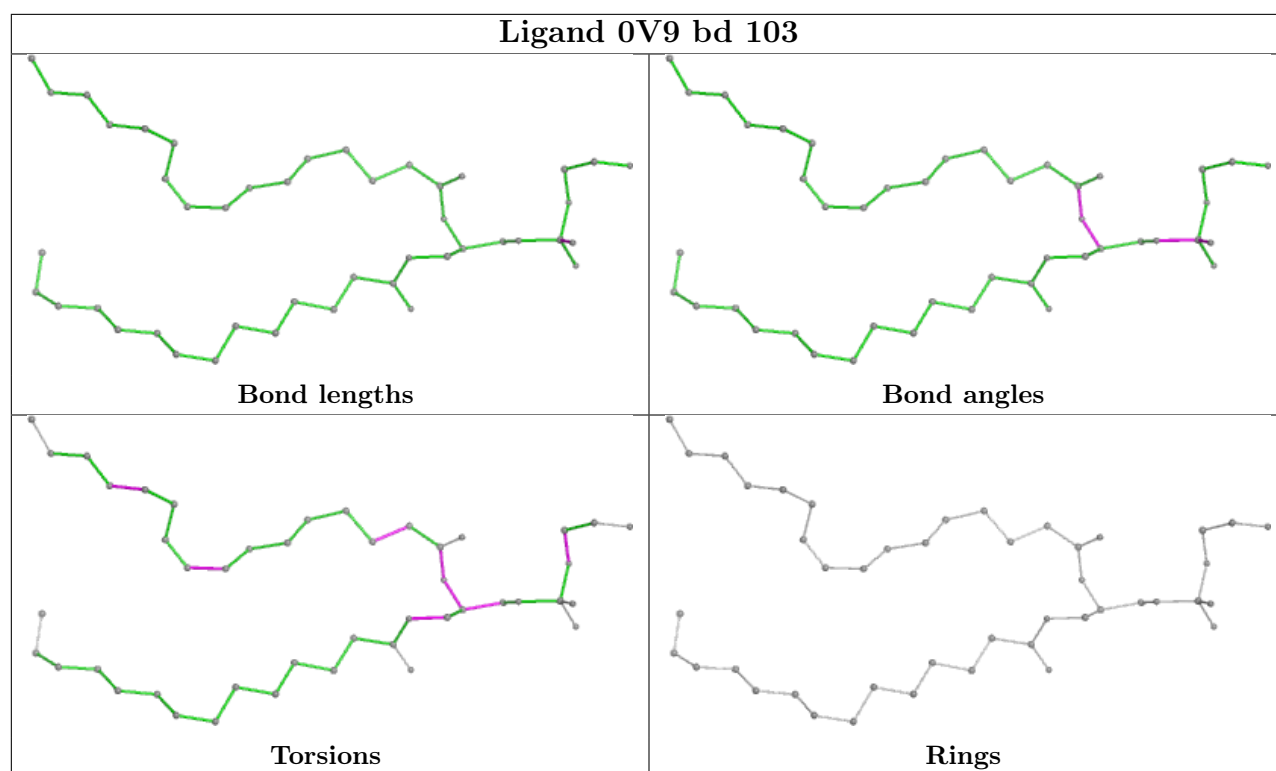


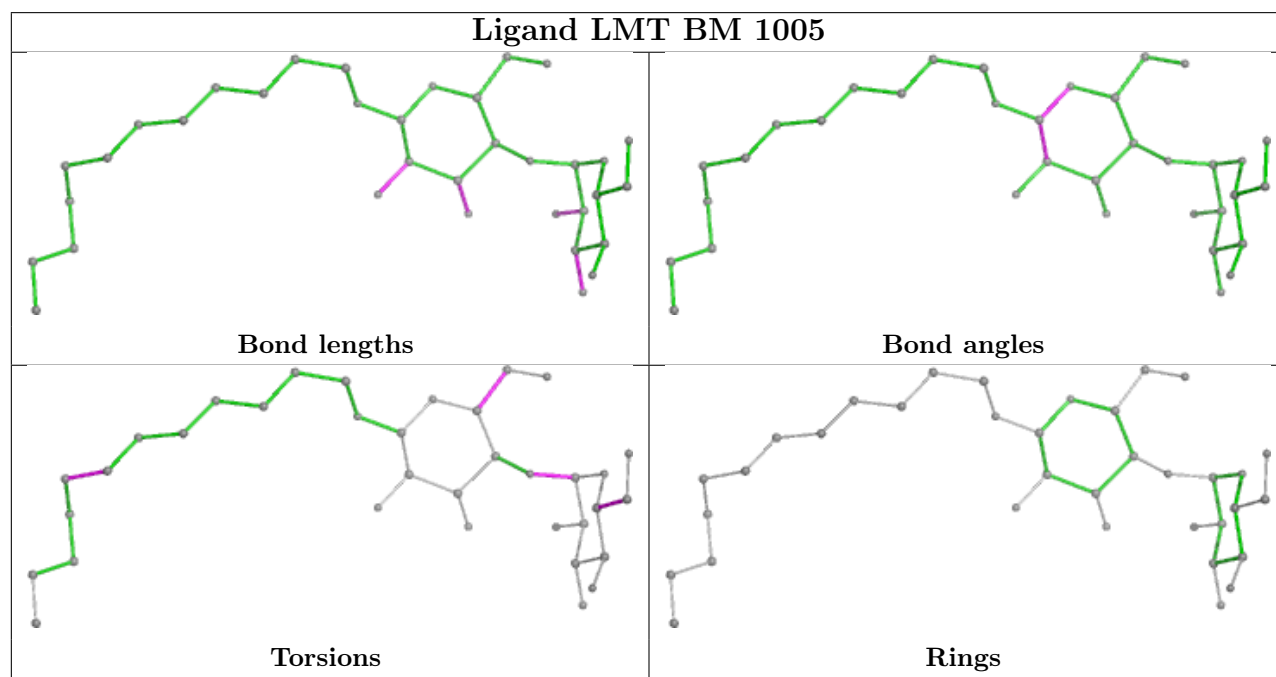
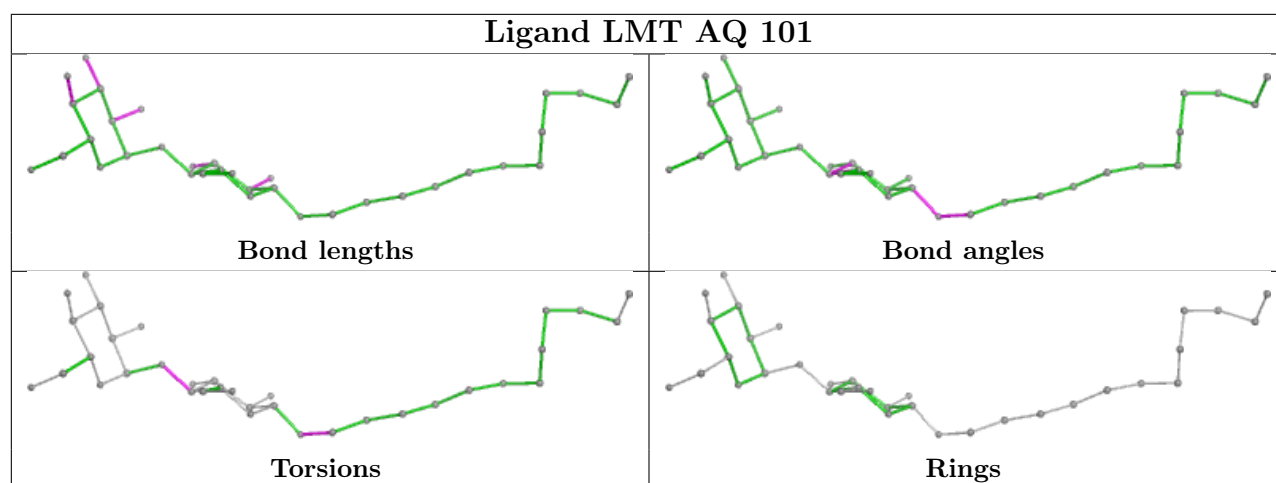


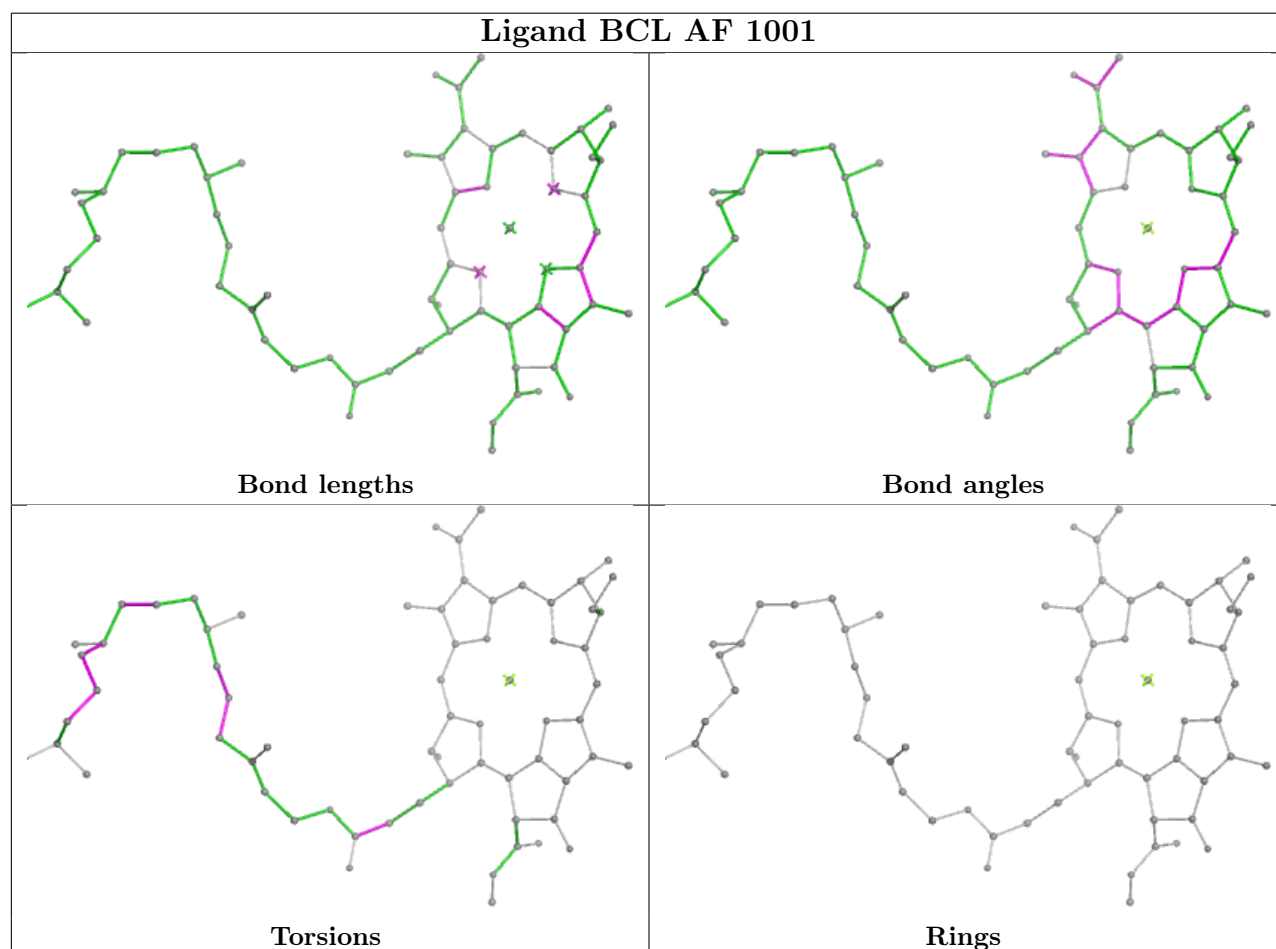
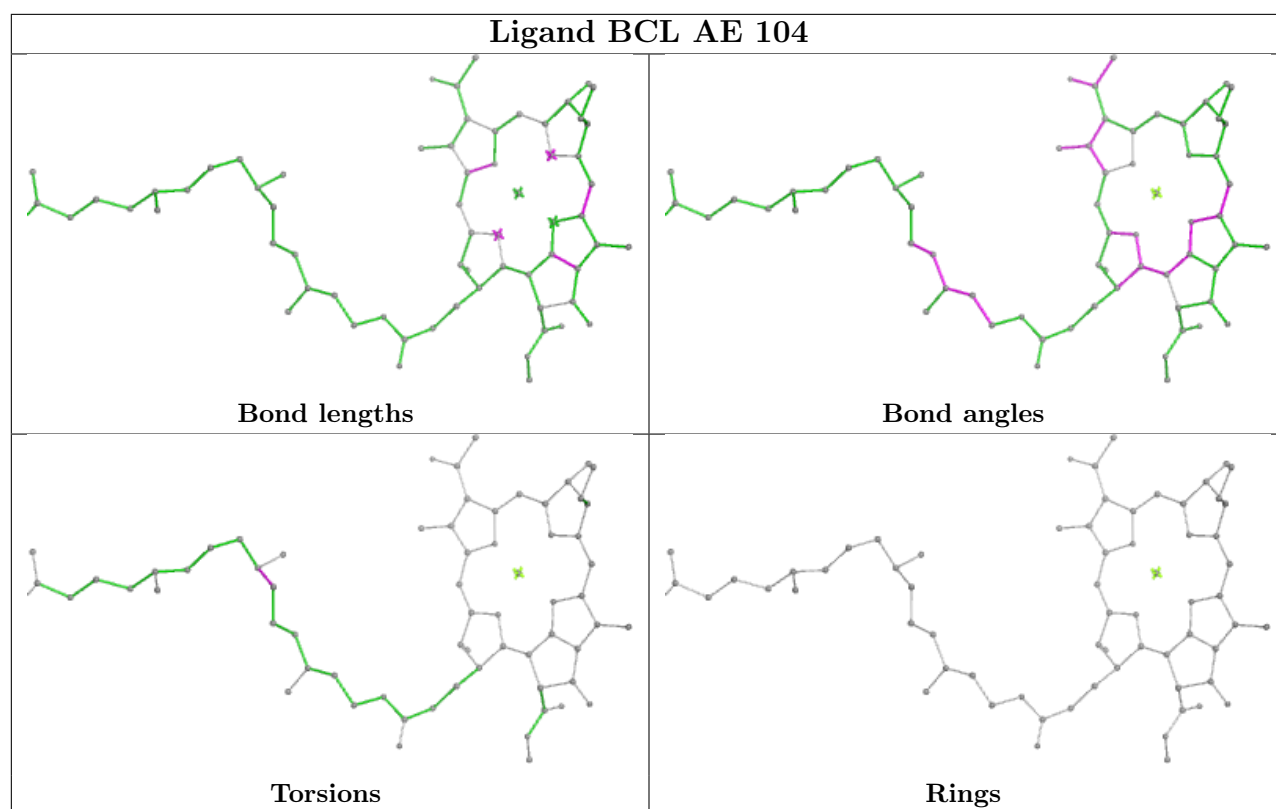


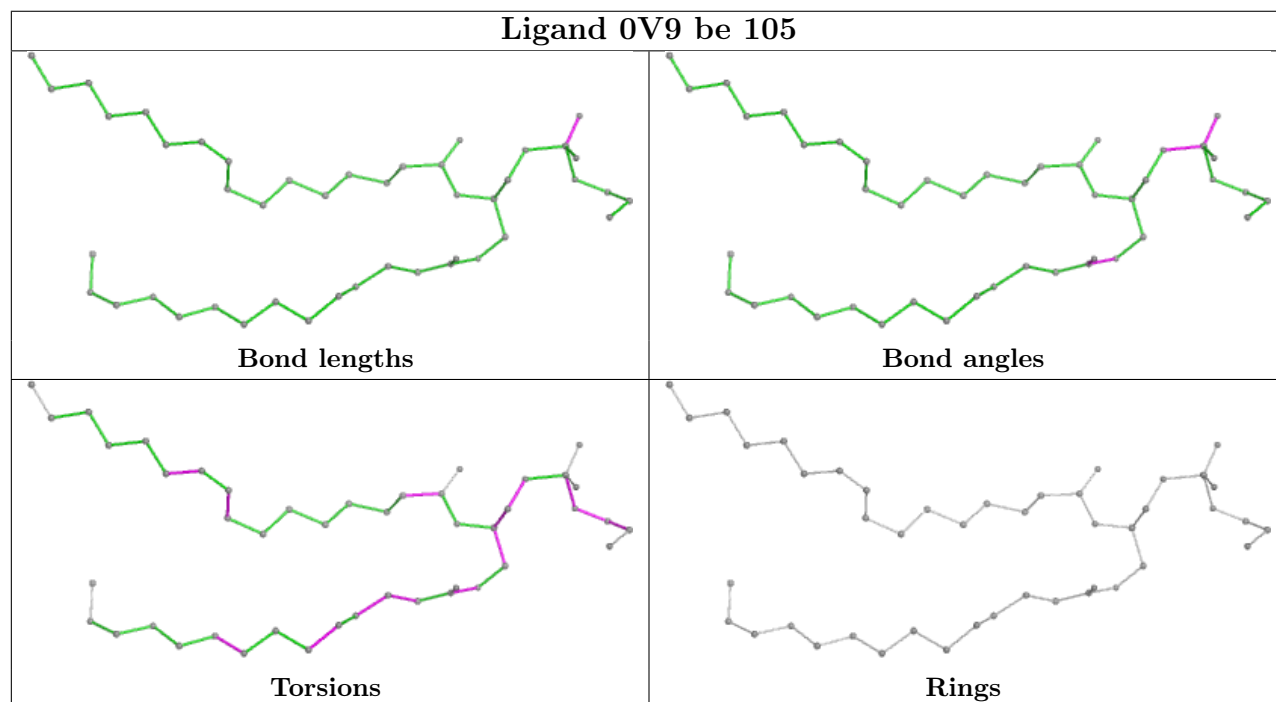
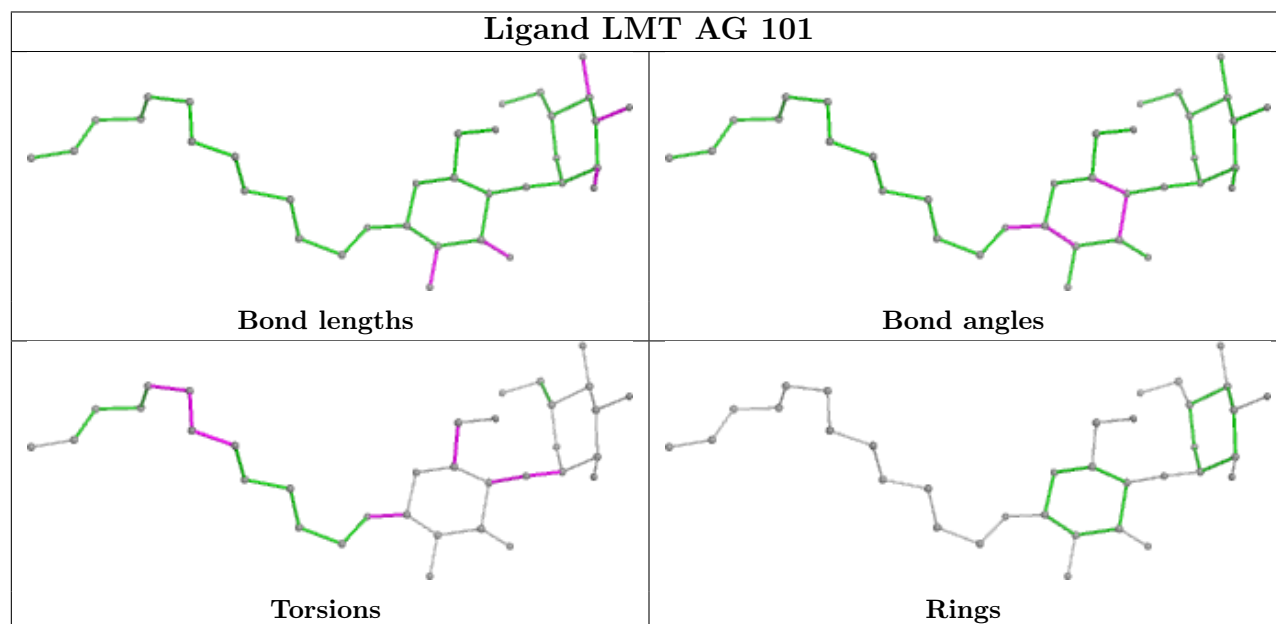
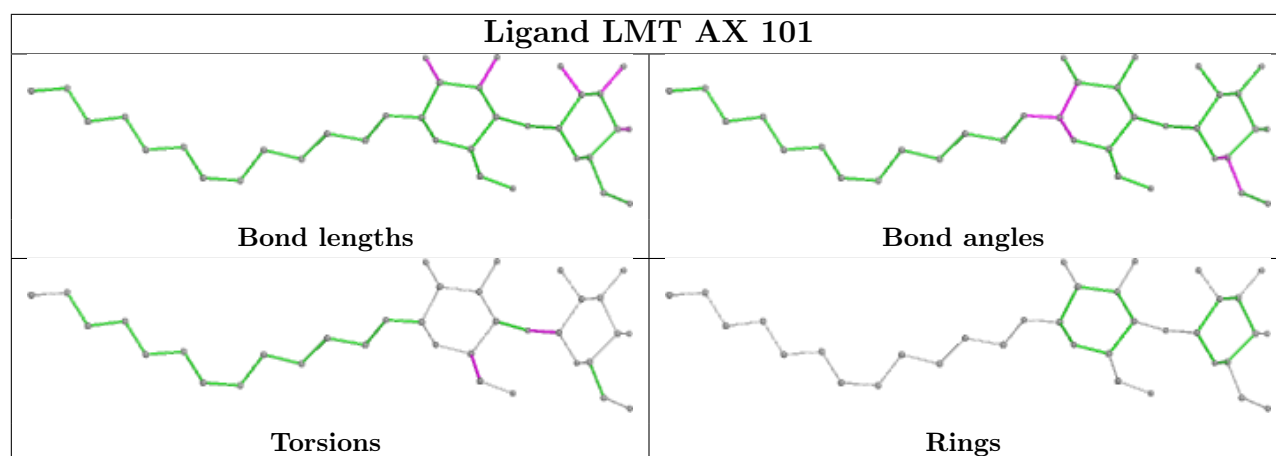


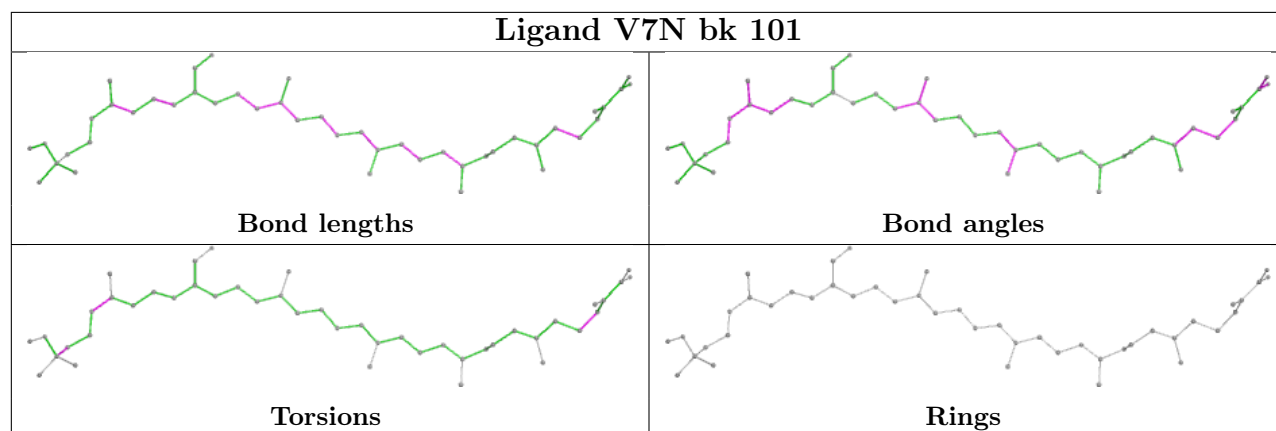
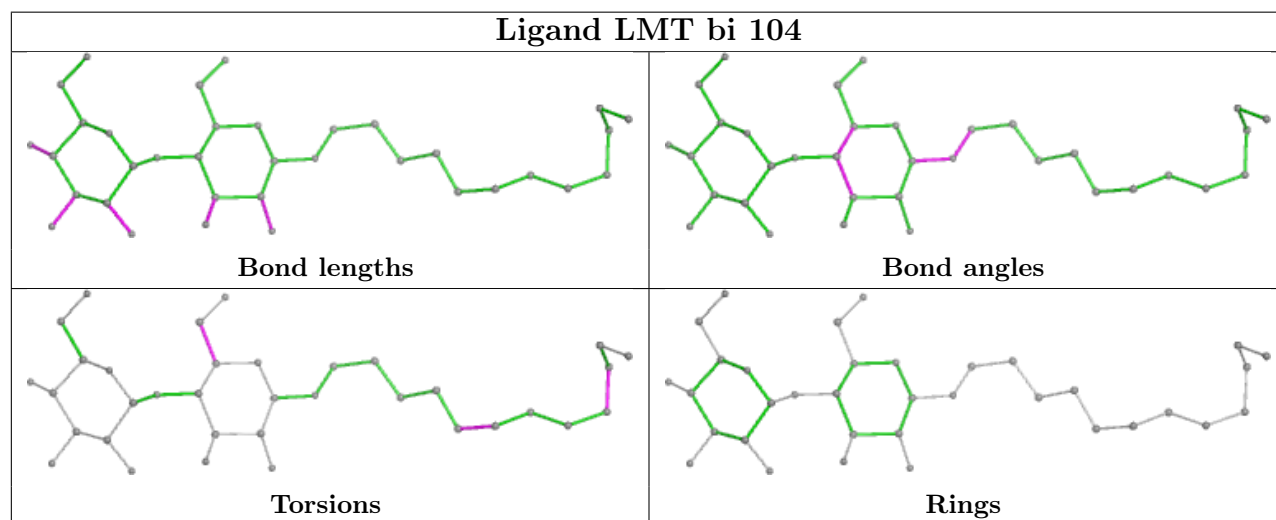
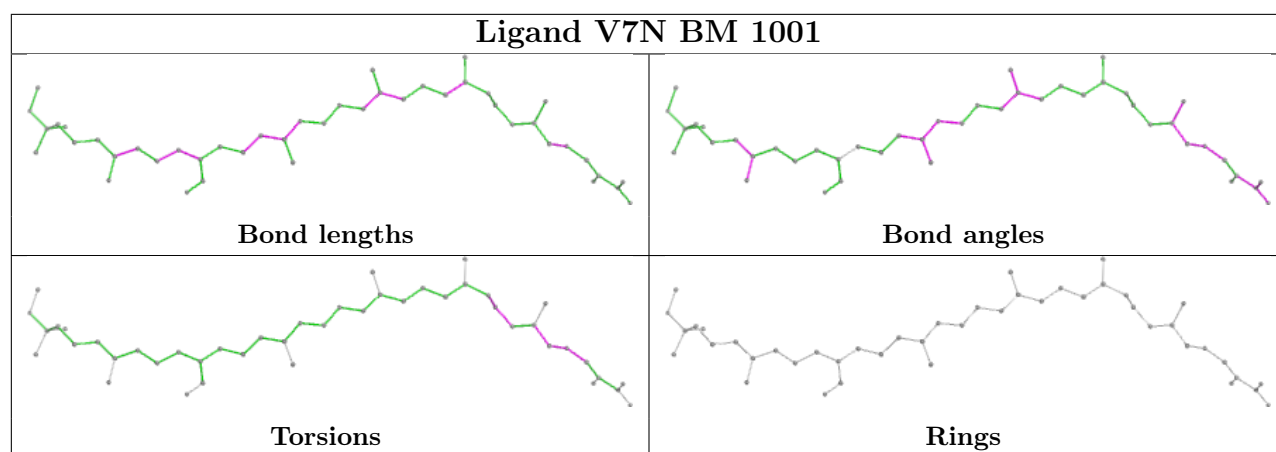


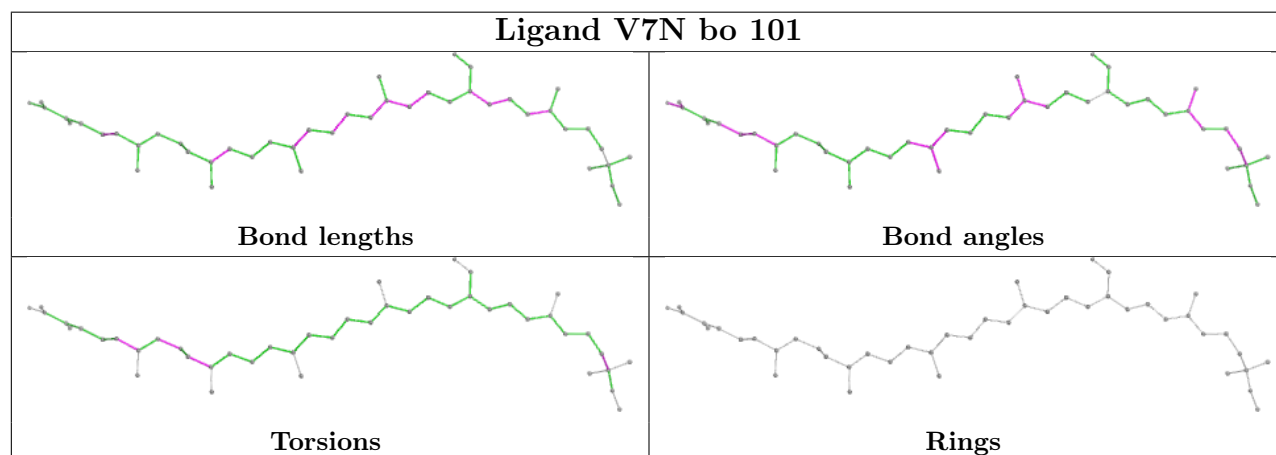
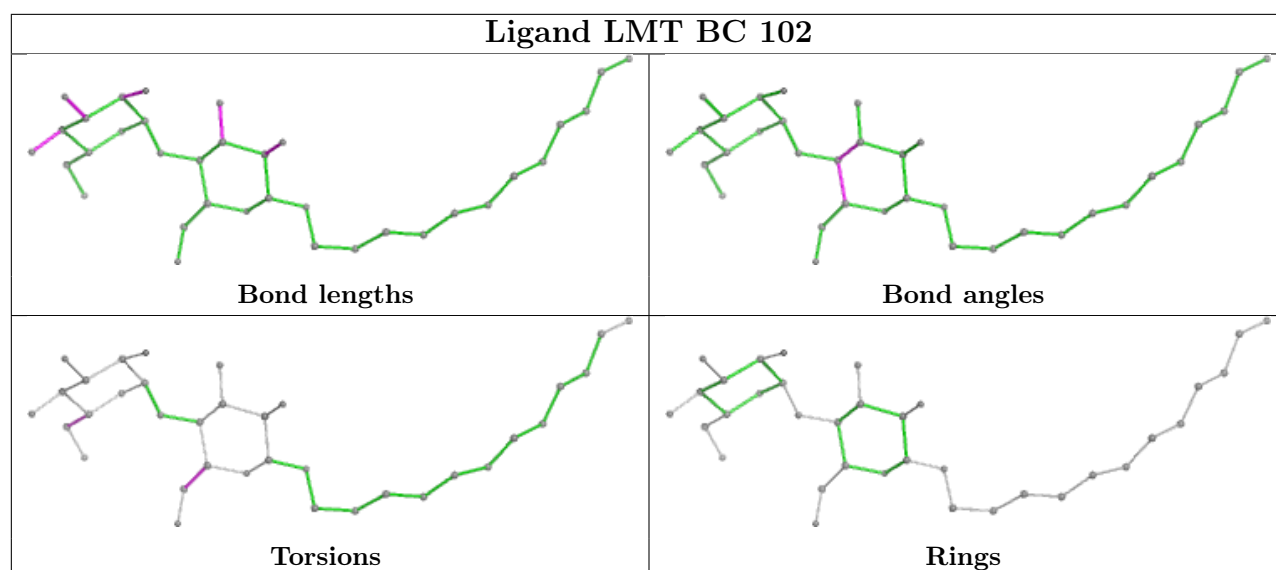


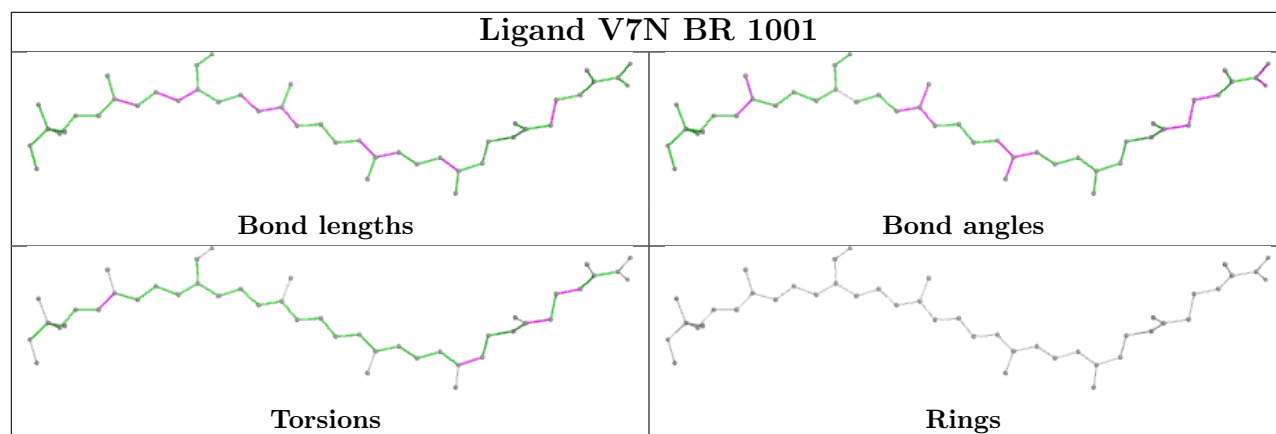
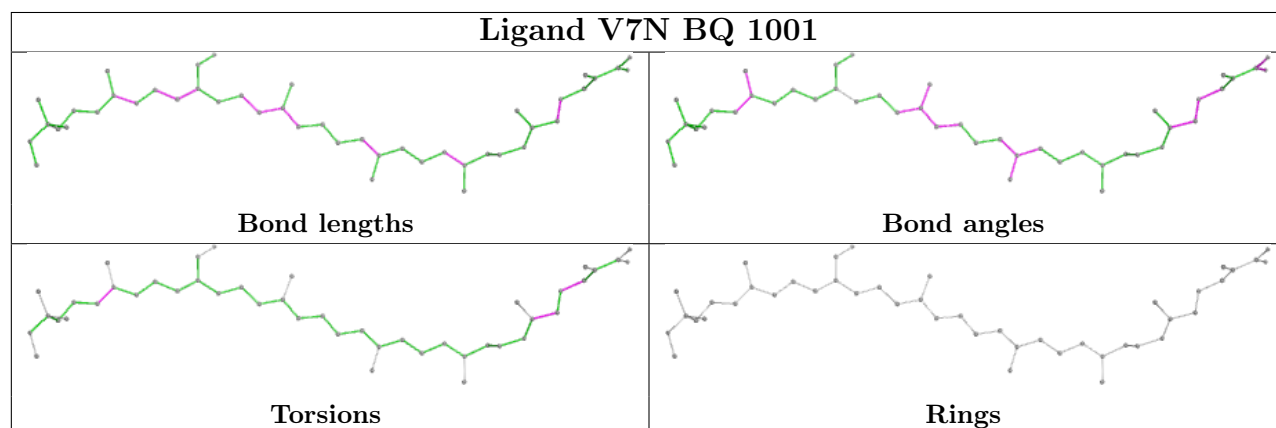
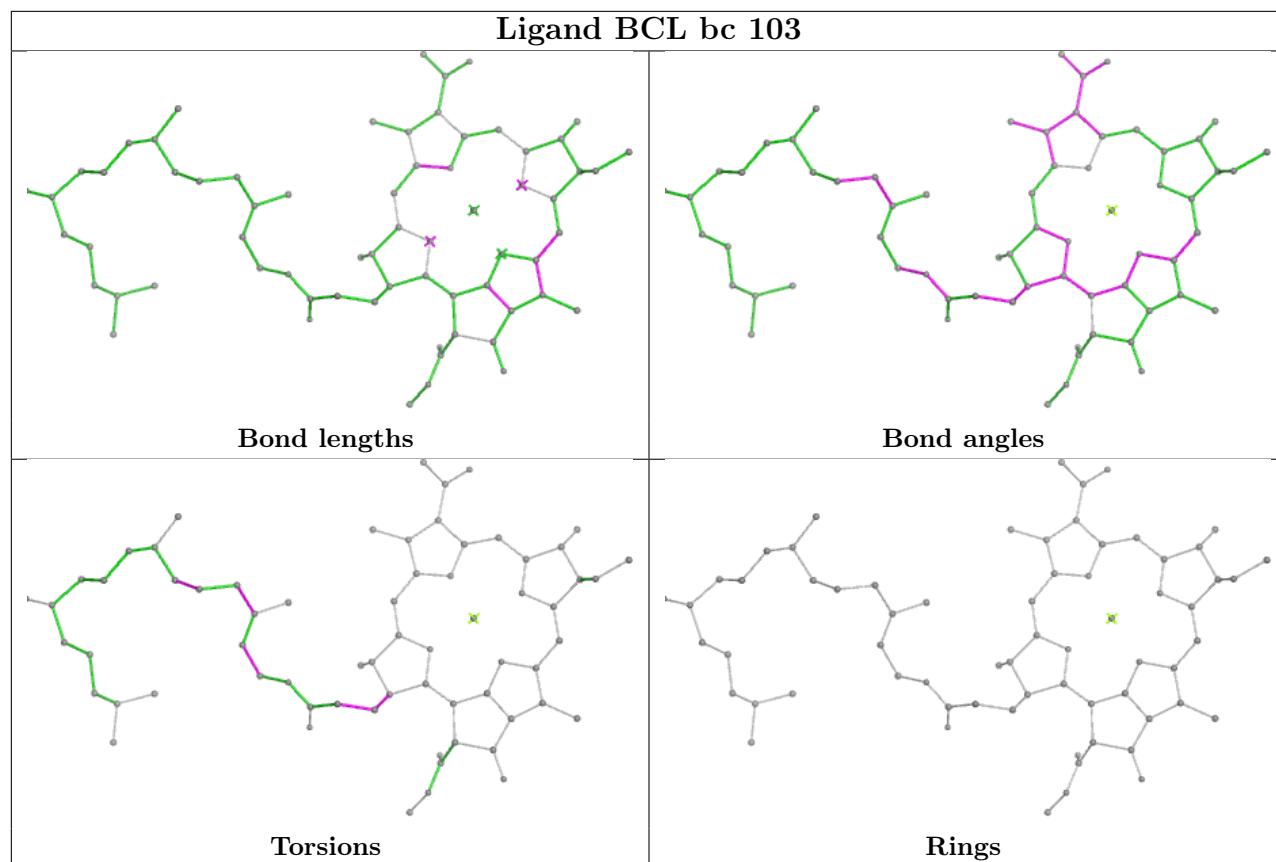


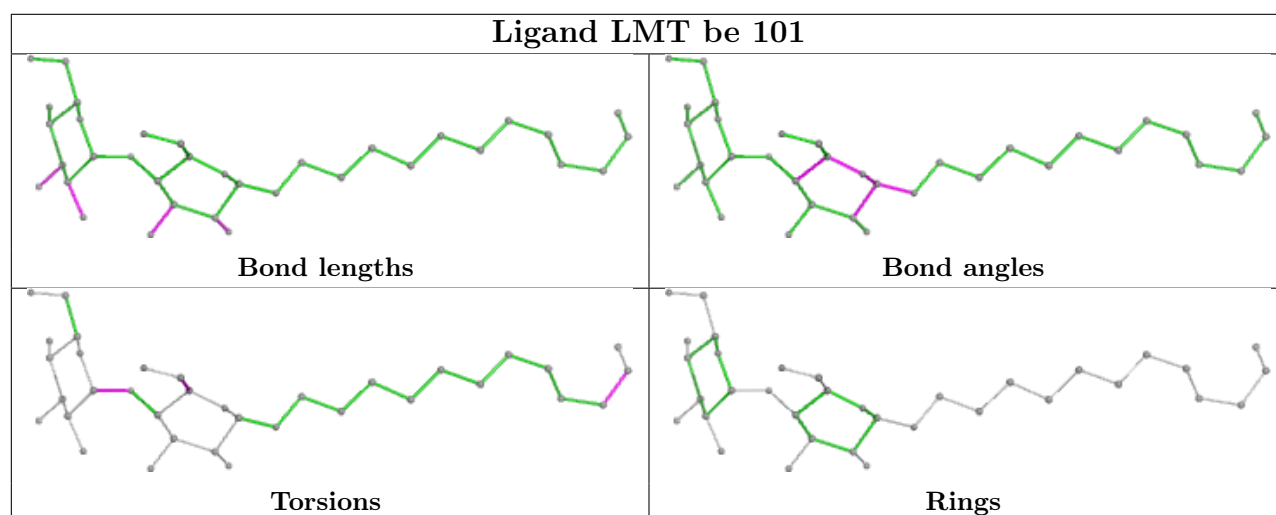
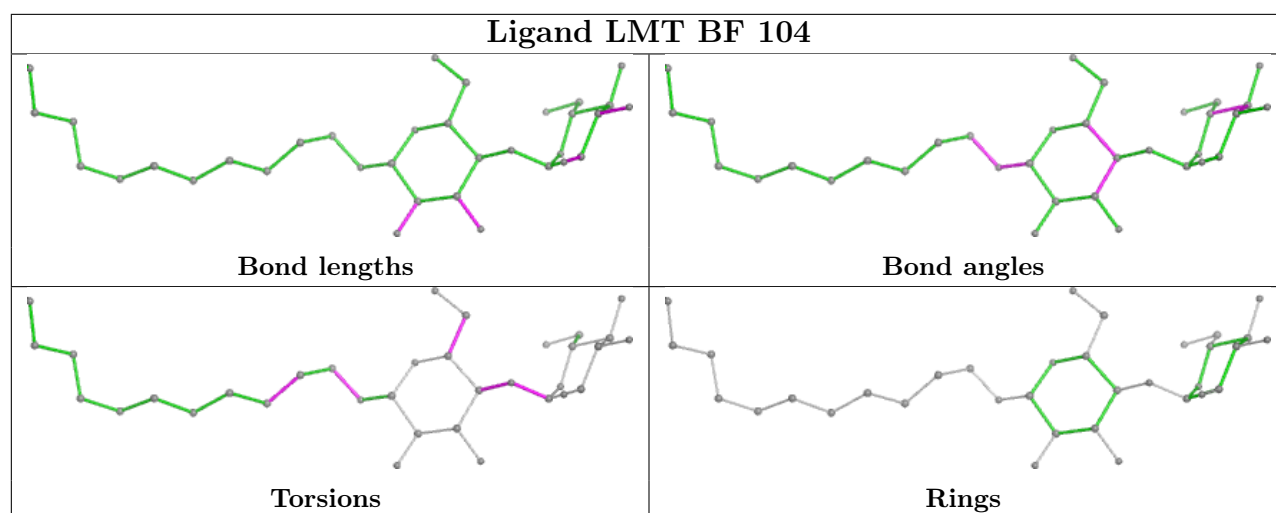


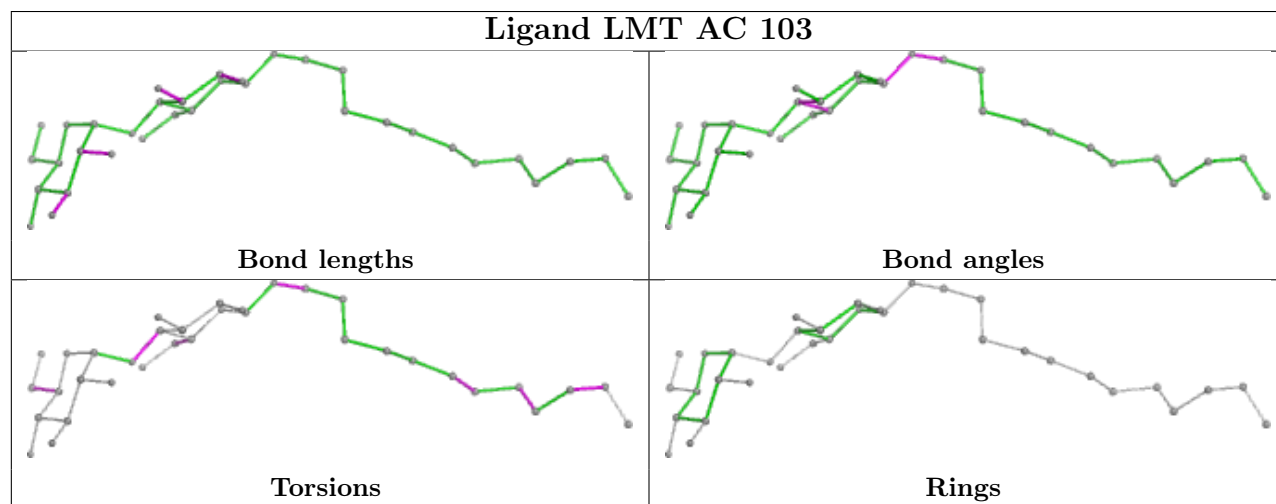
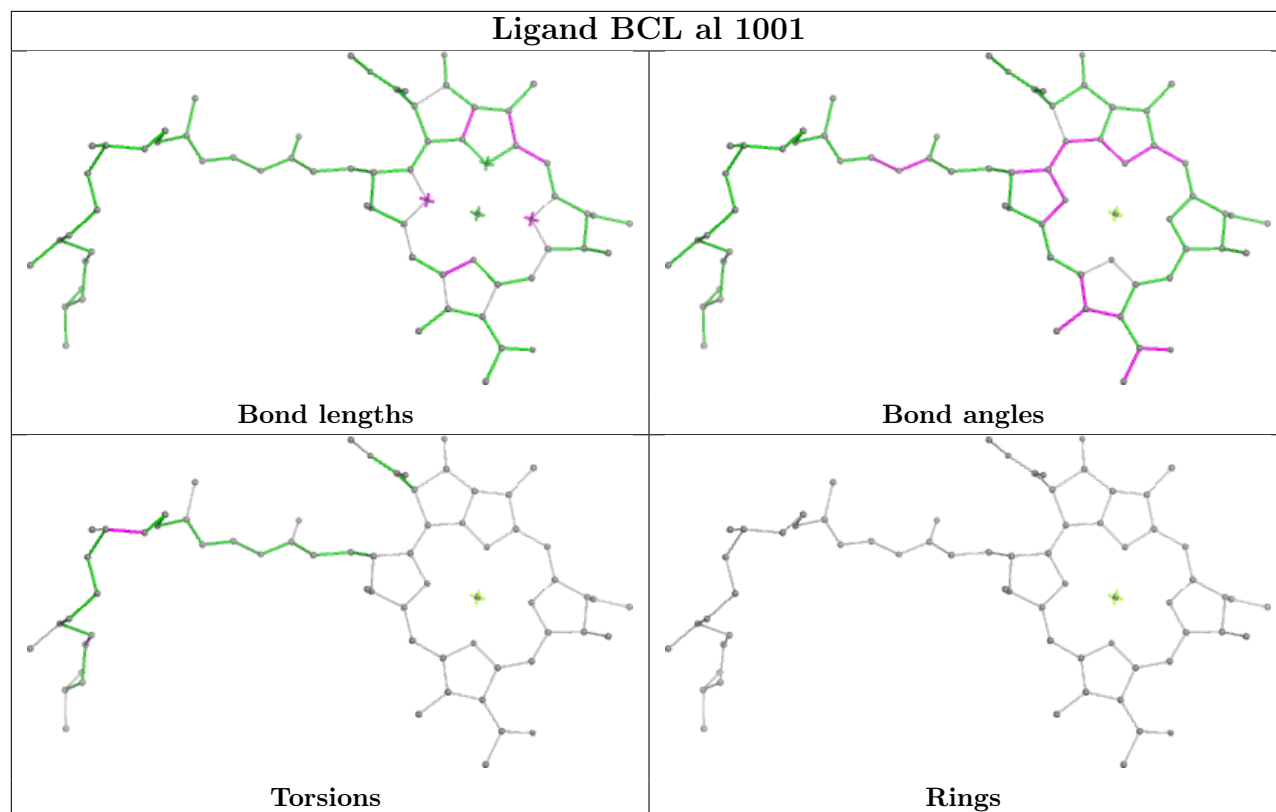


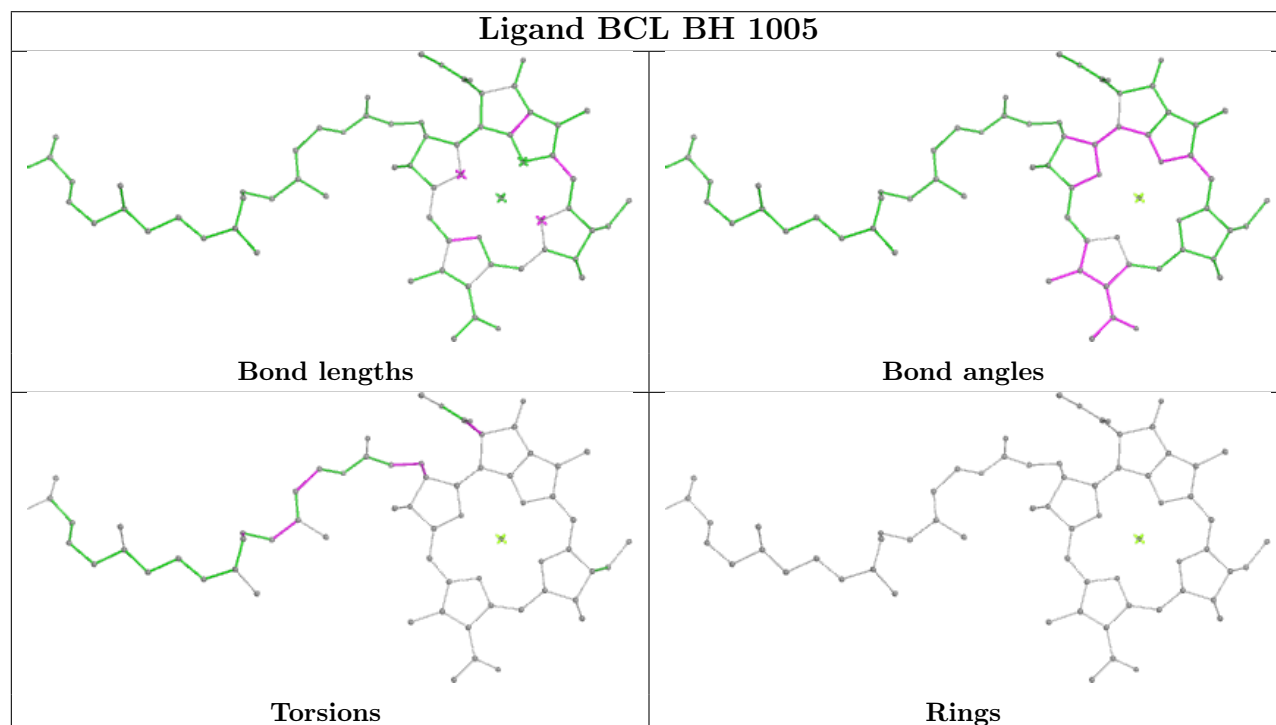
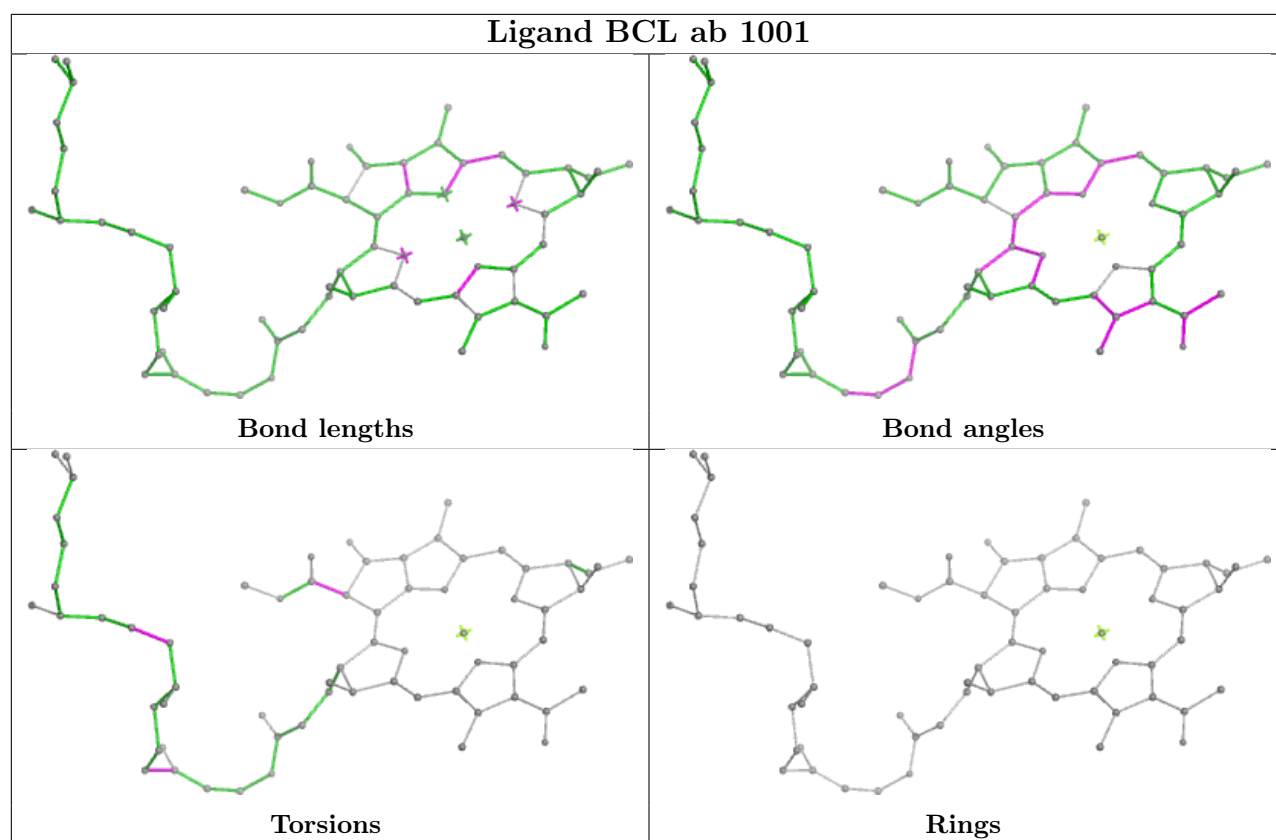


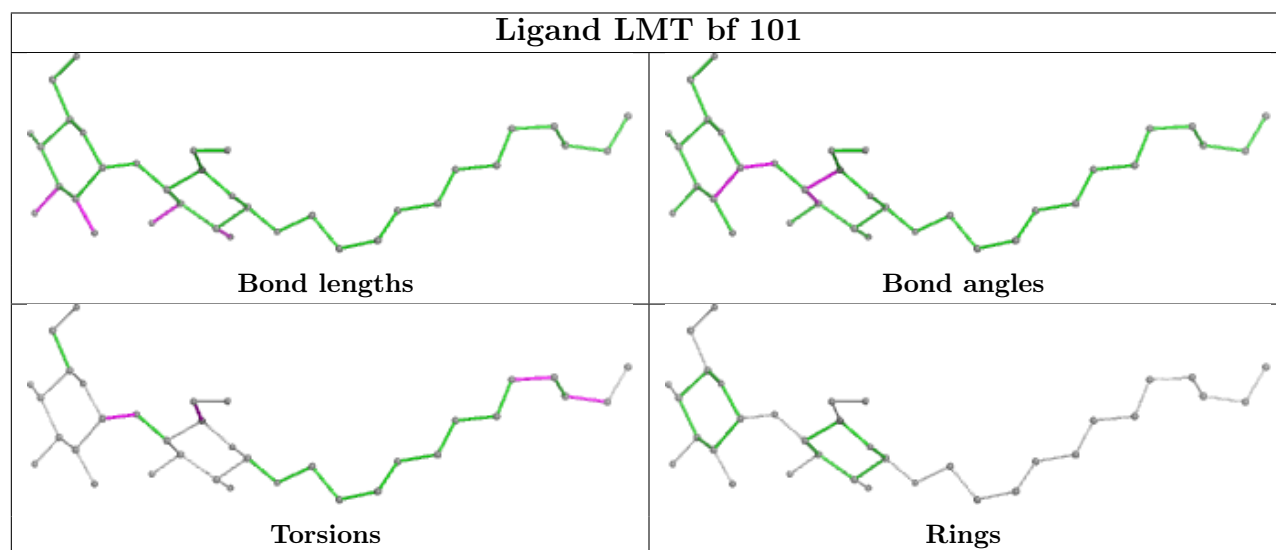
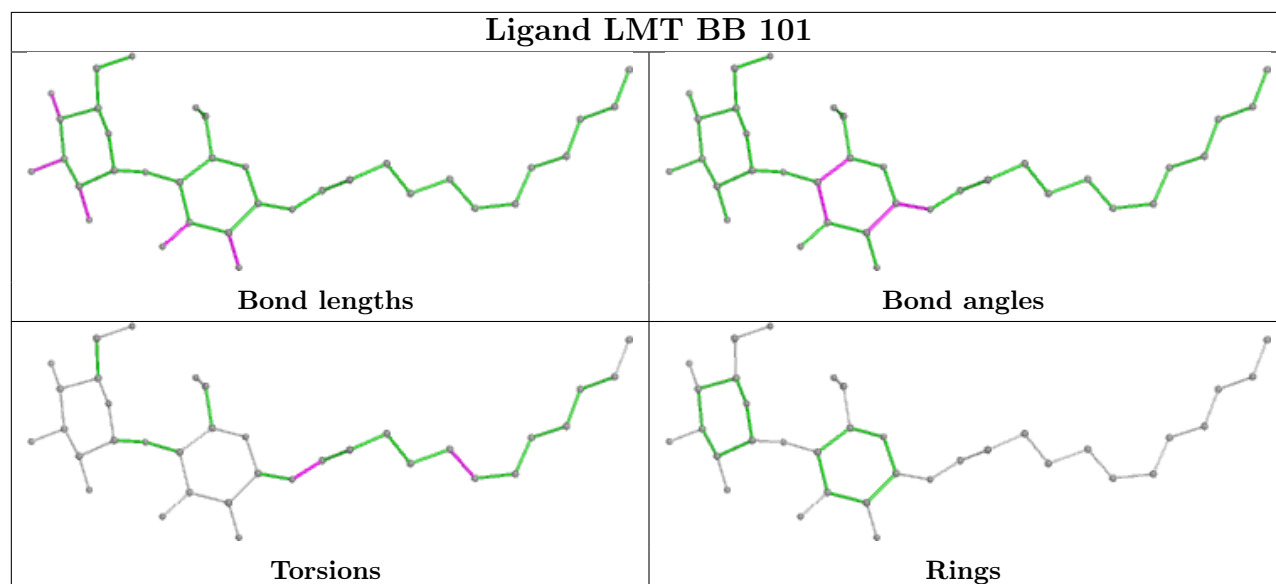
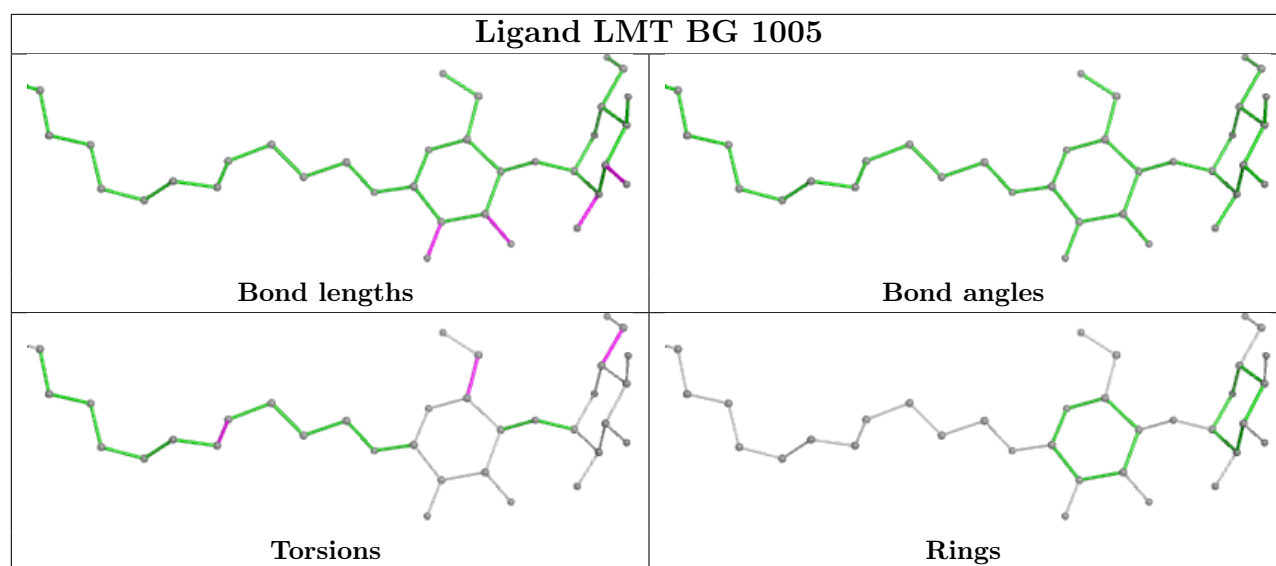


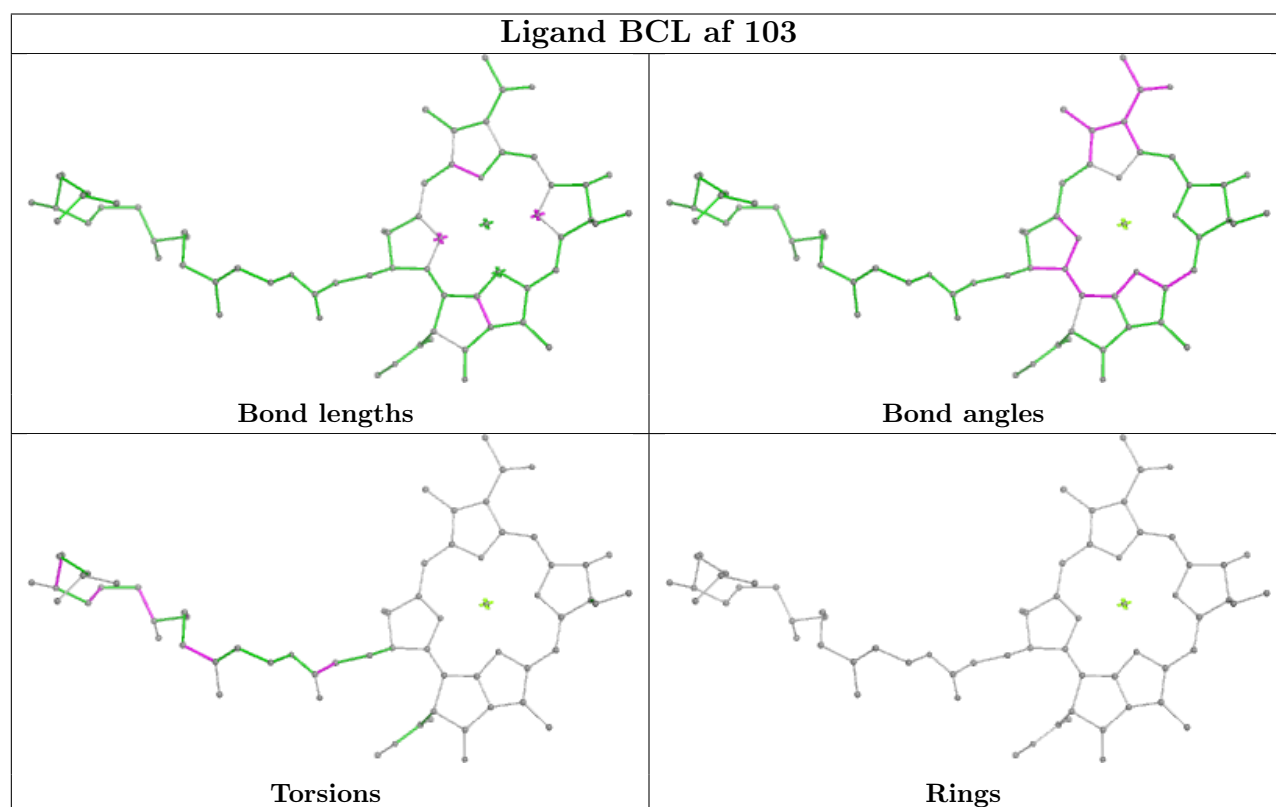
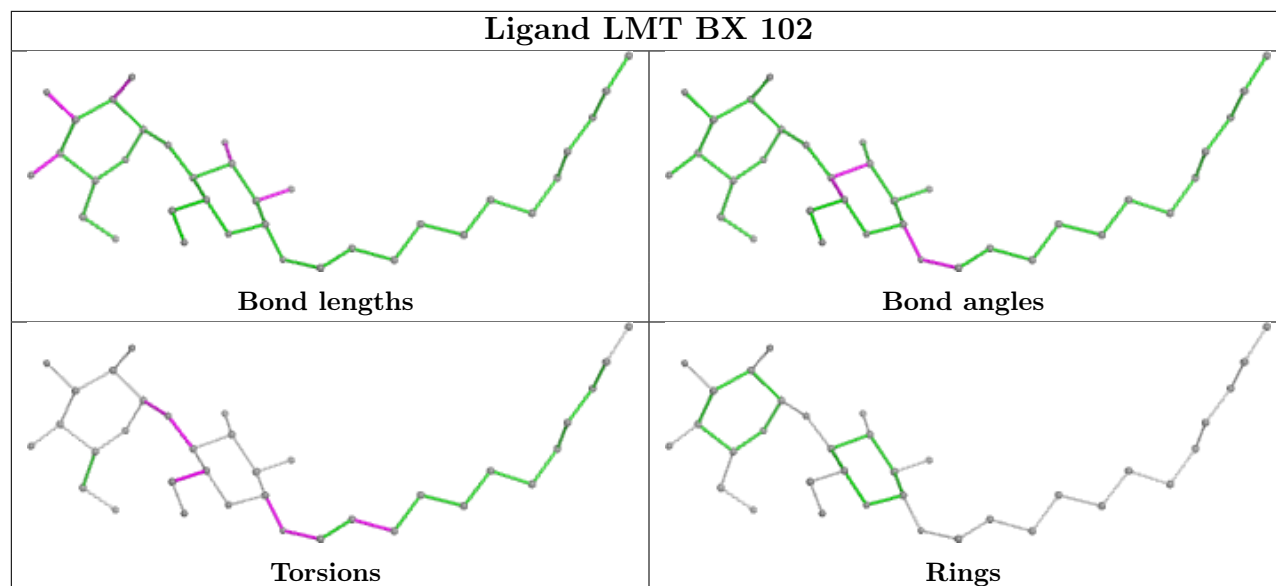


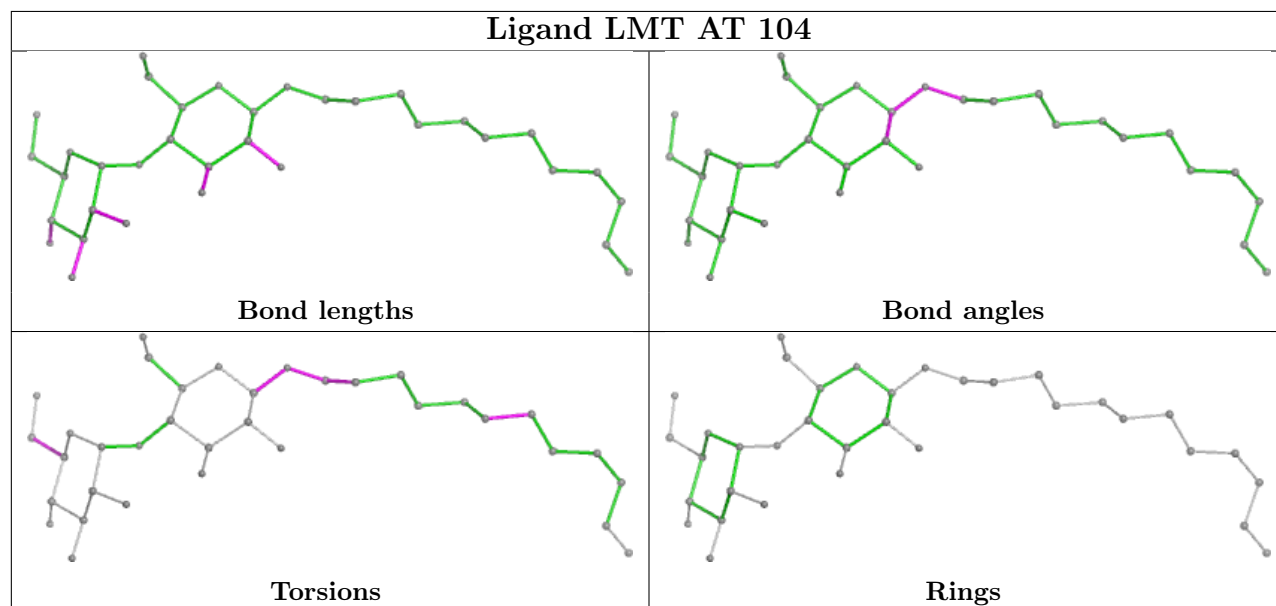
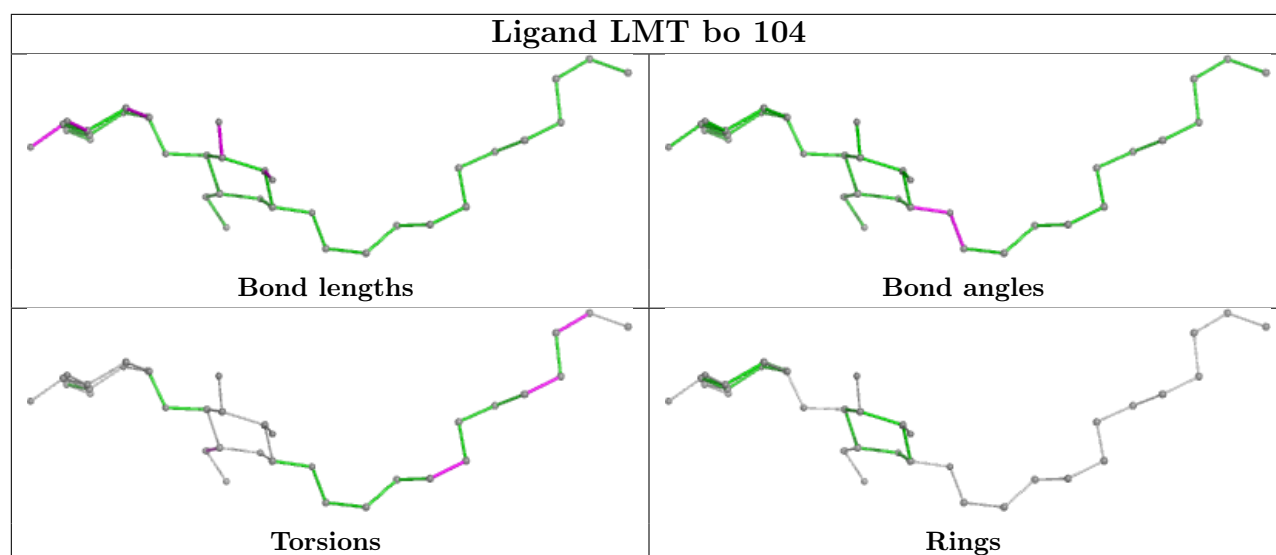


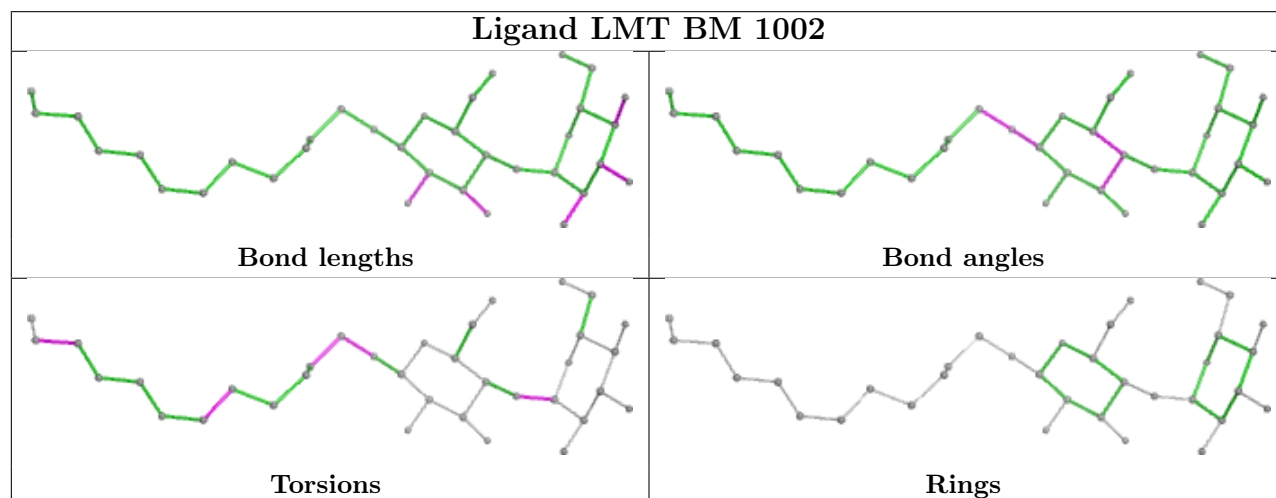
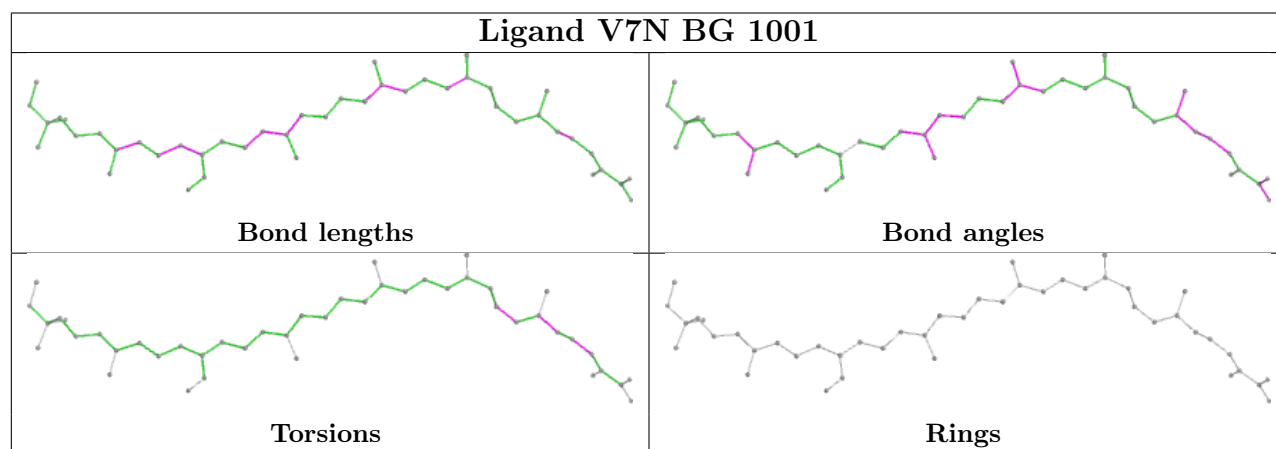
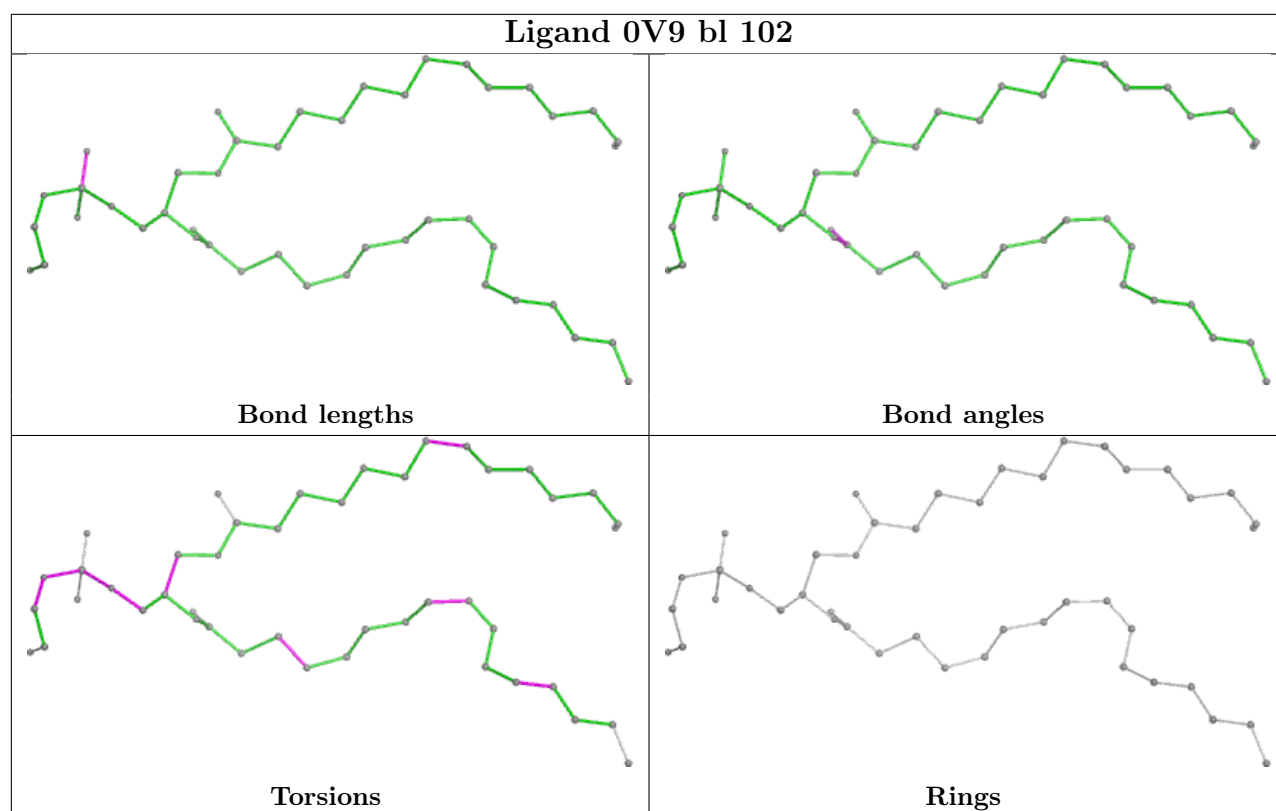




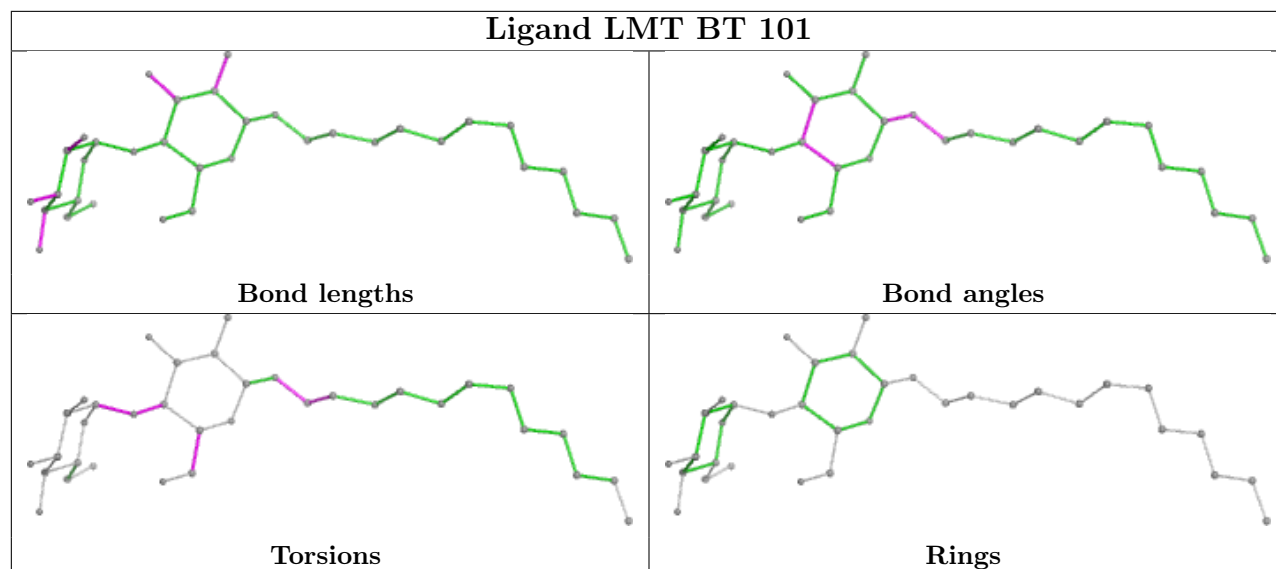




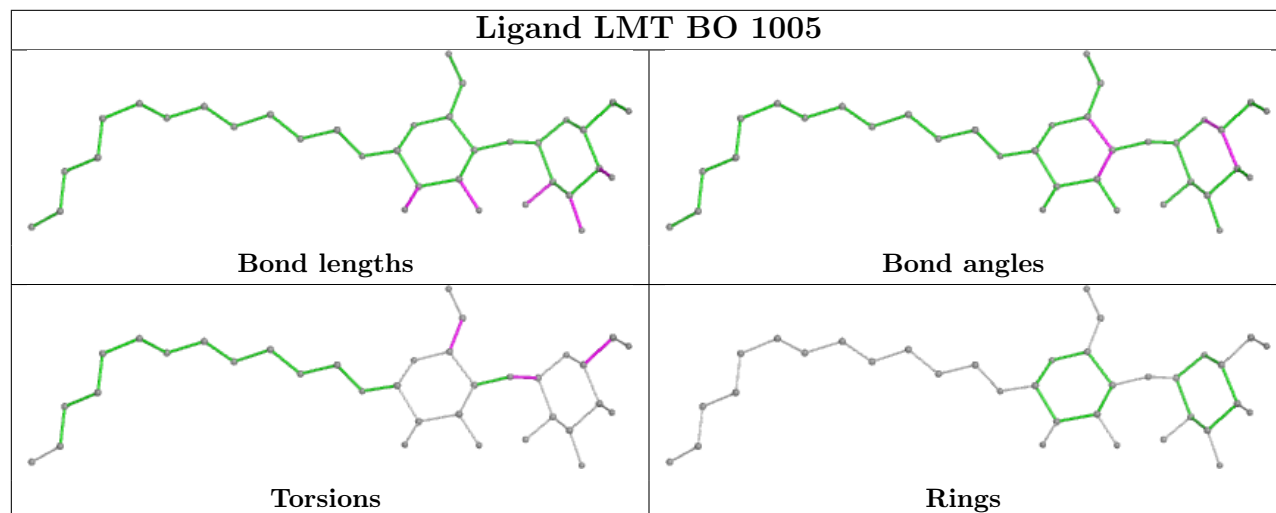


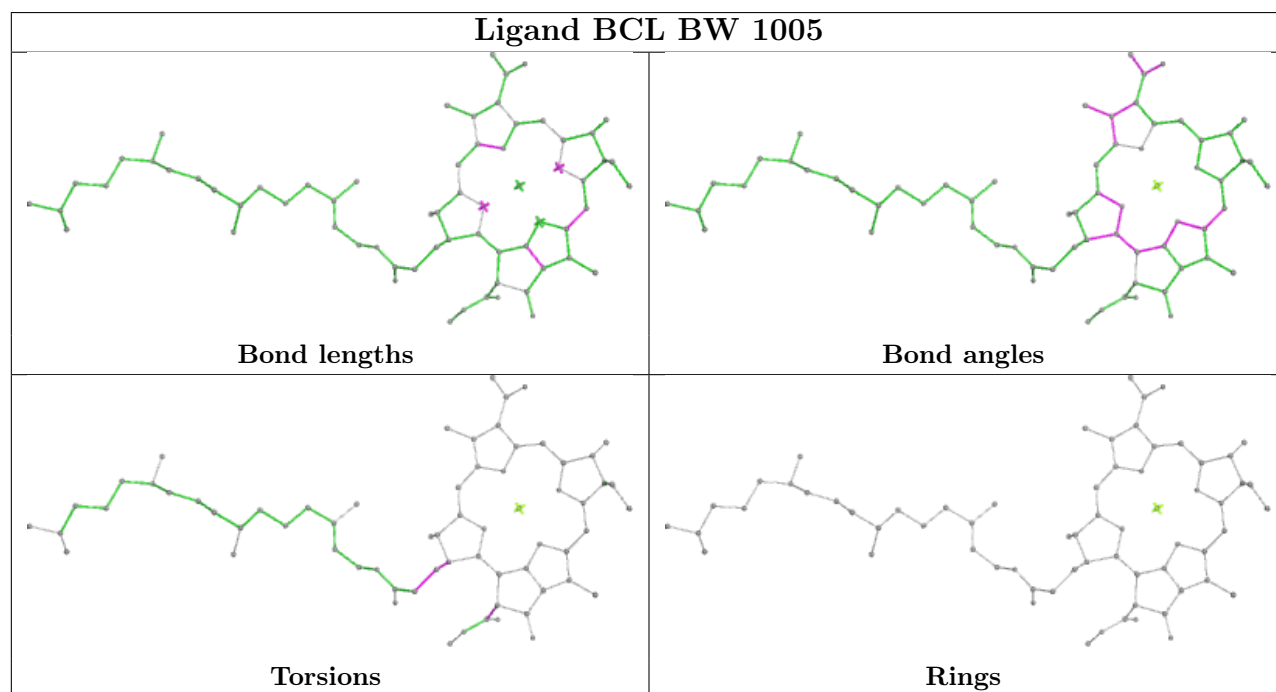
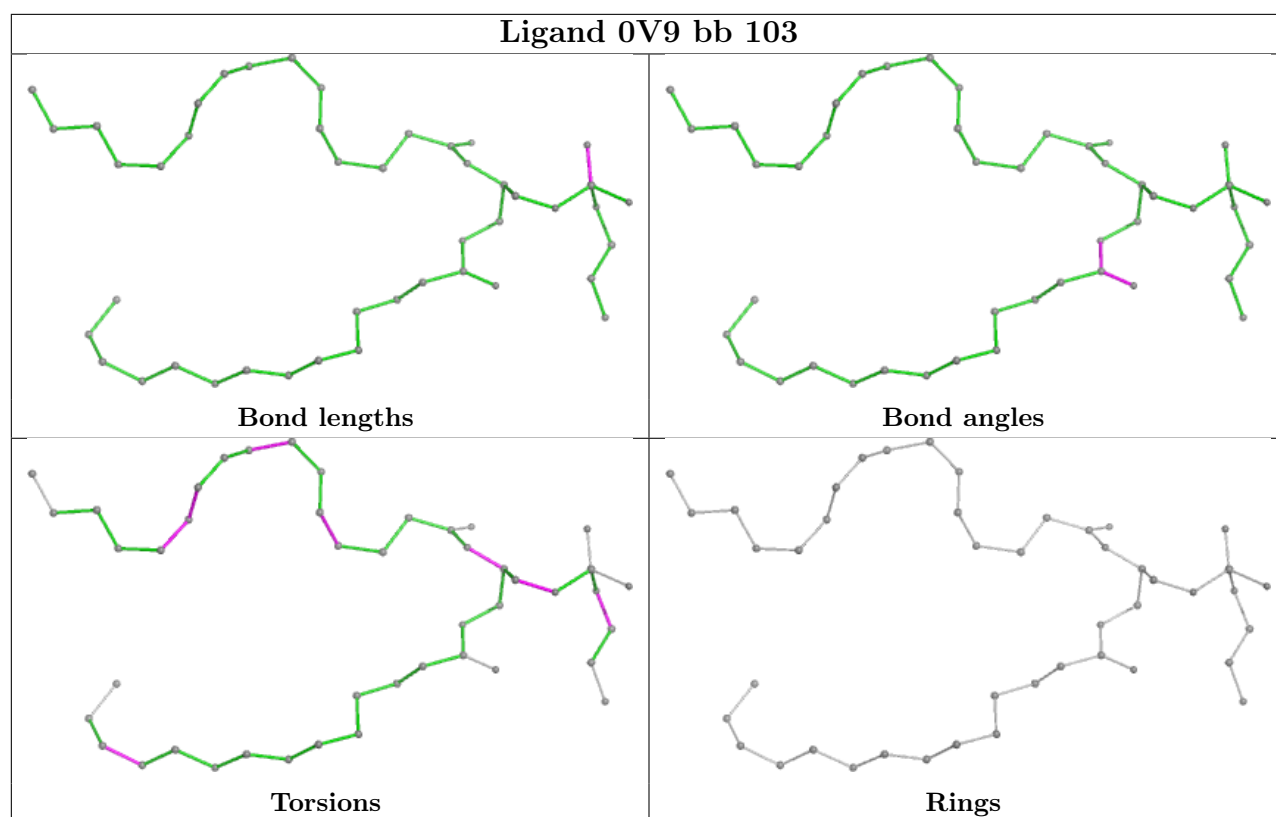


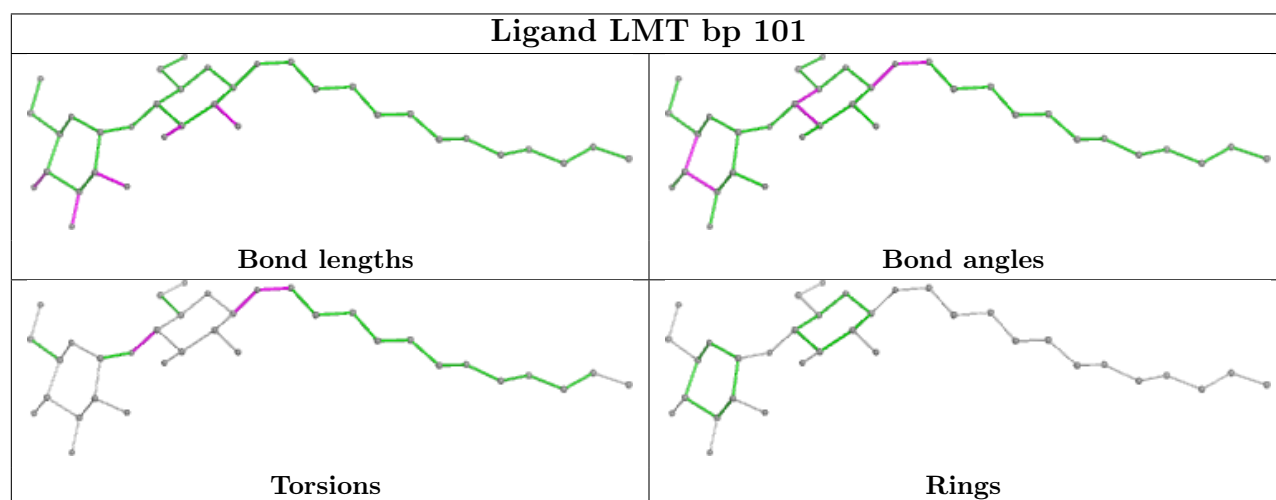
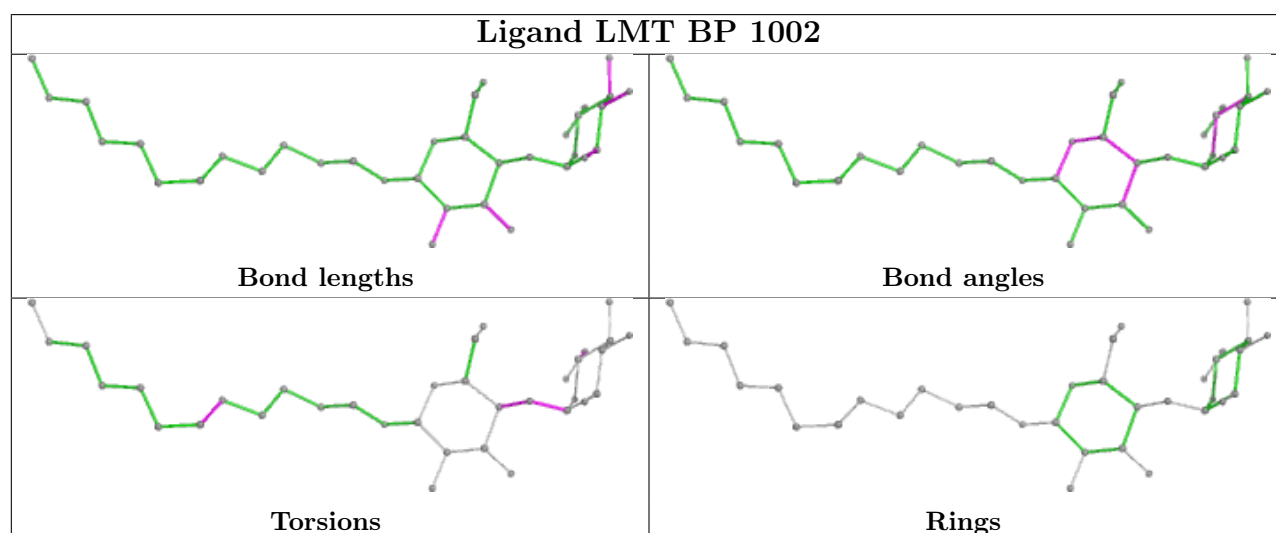
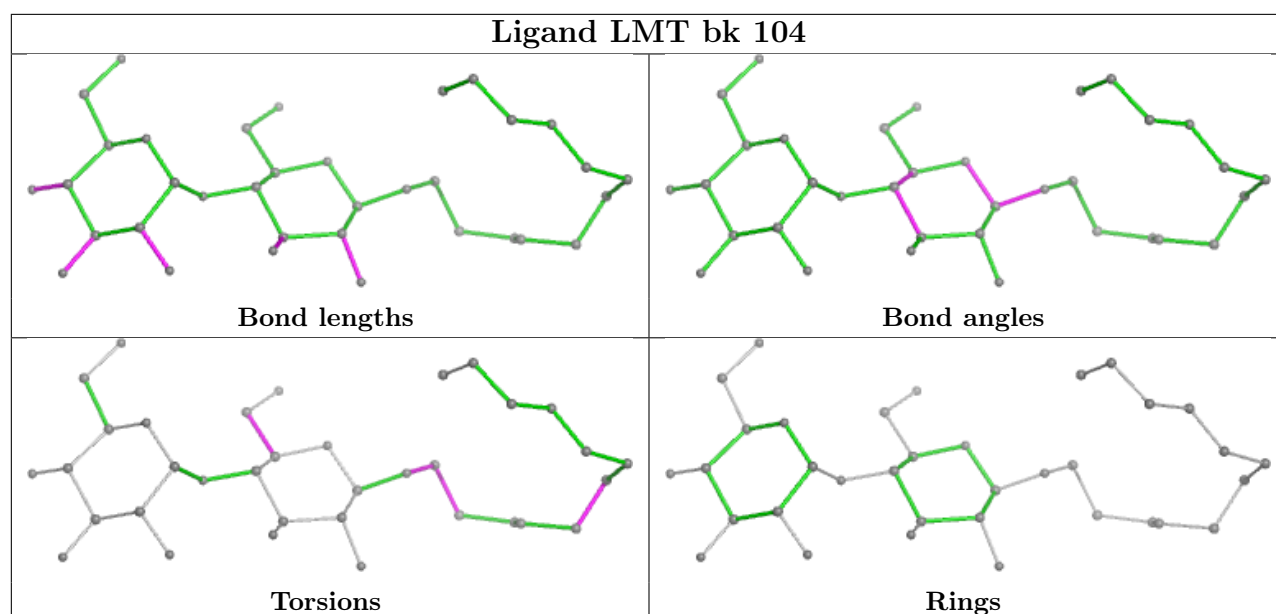
Ligand LMT BT 101

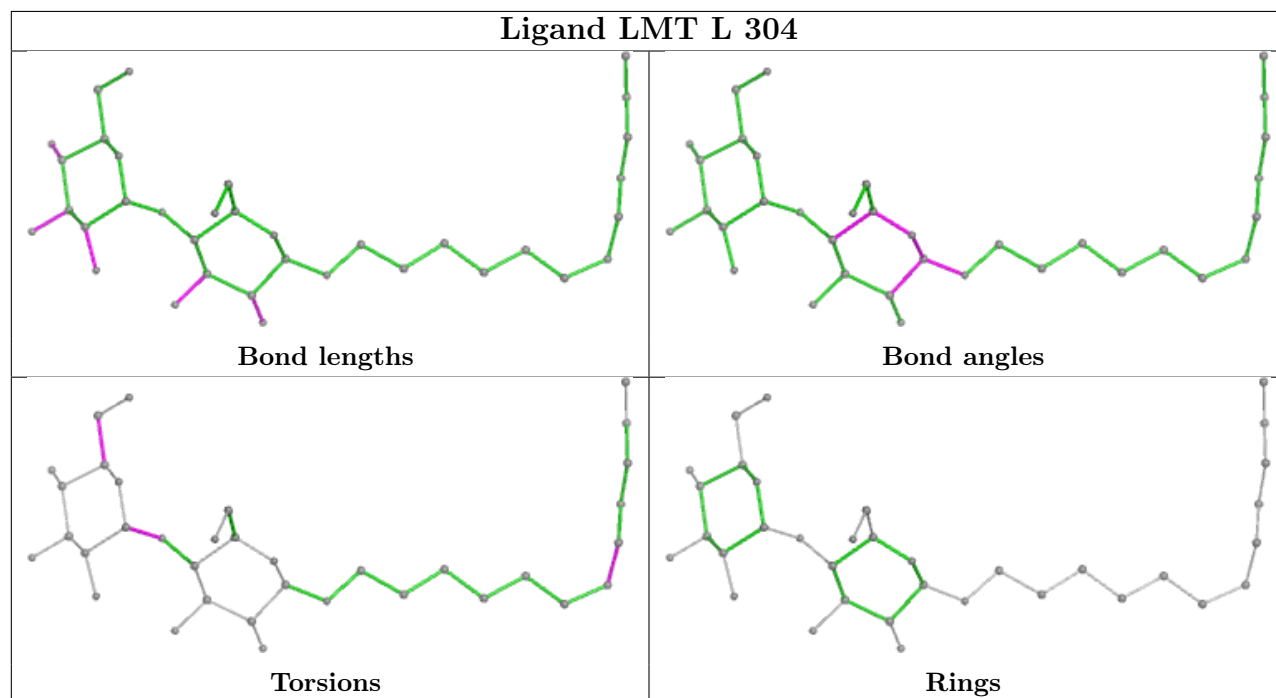
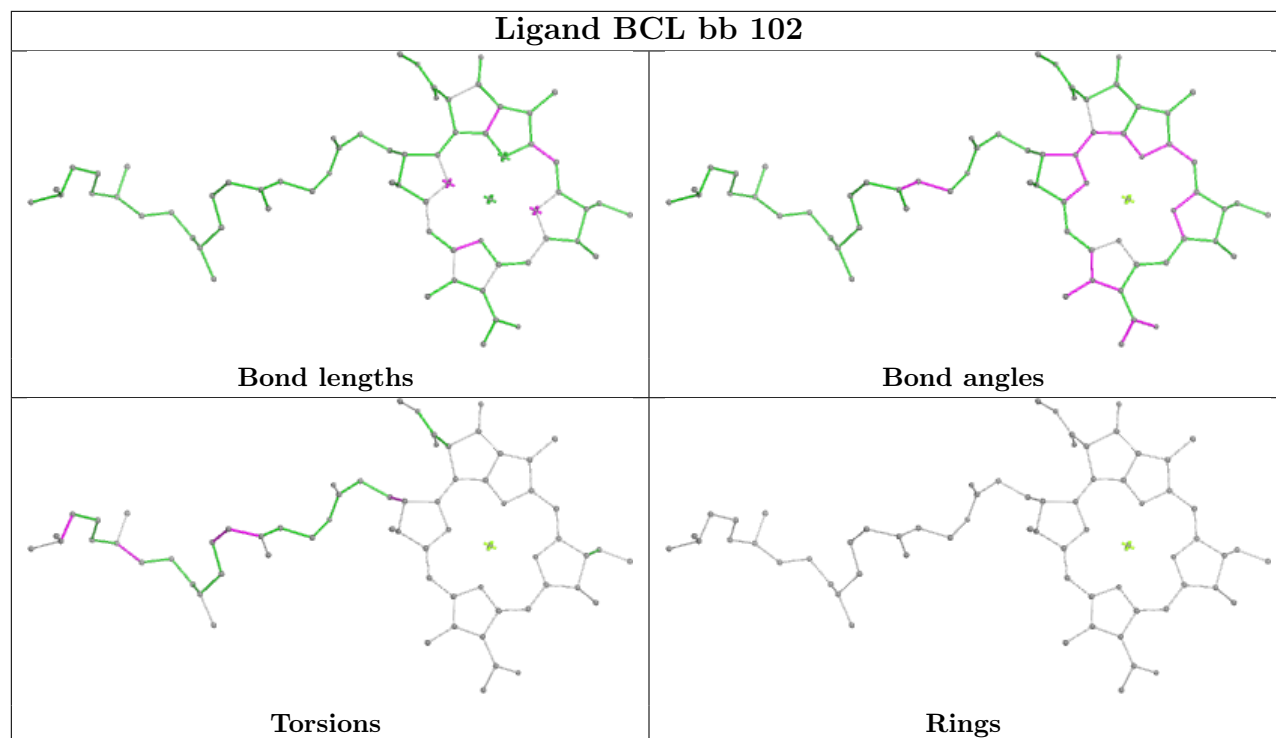


Ligand LMT BO 1005

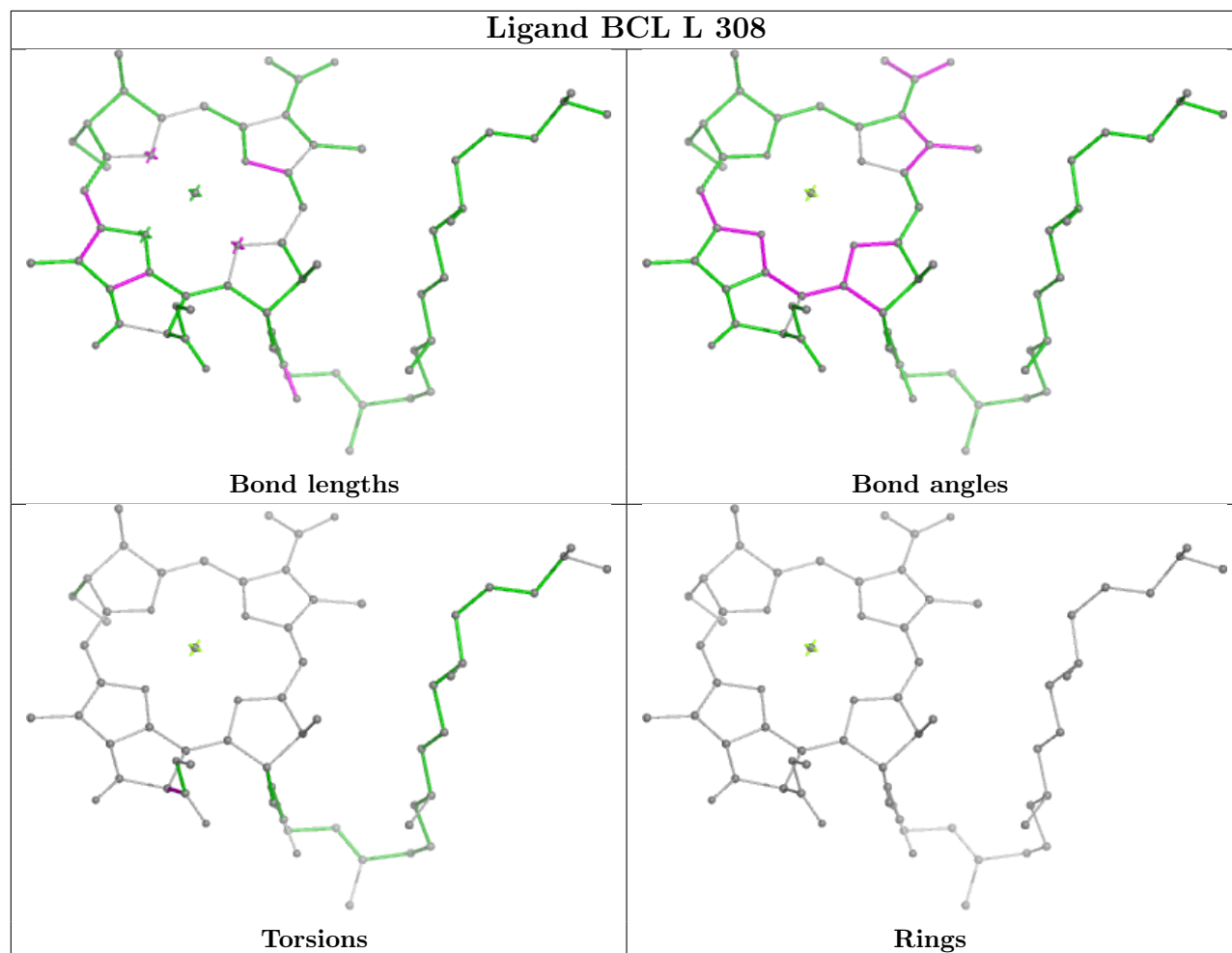


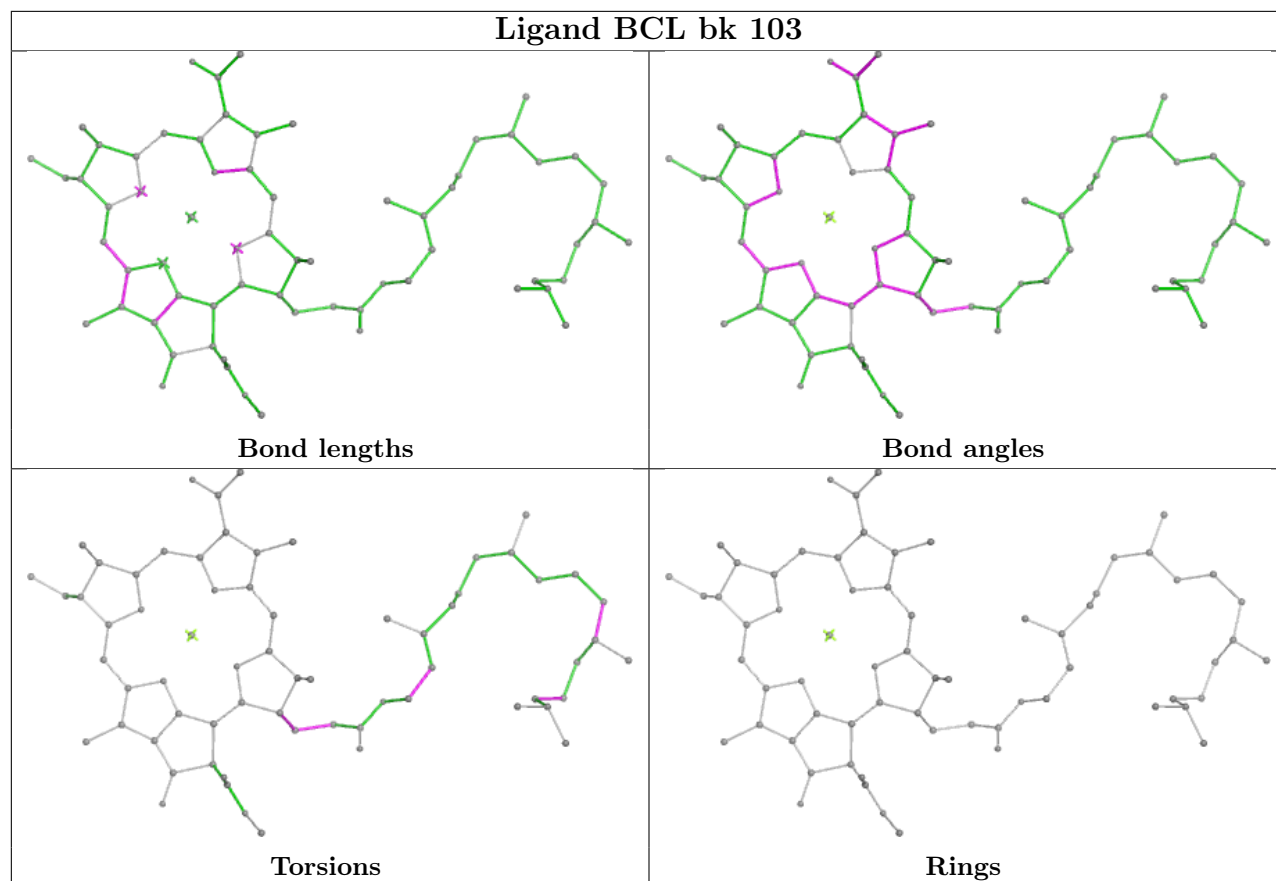




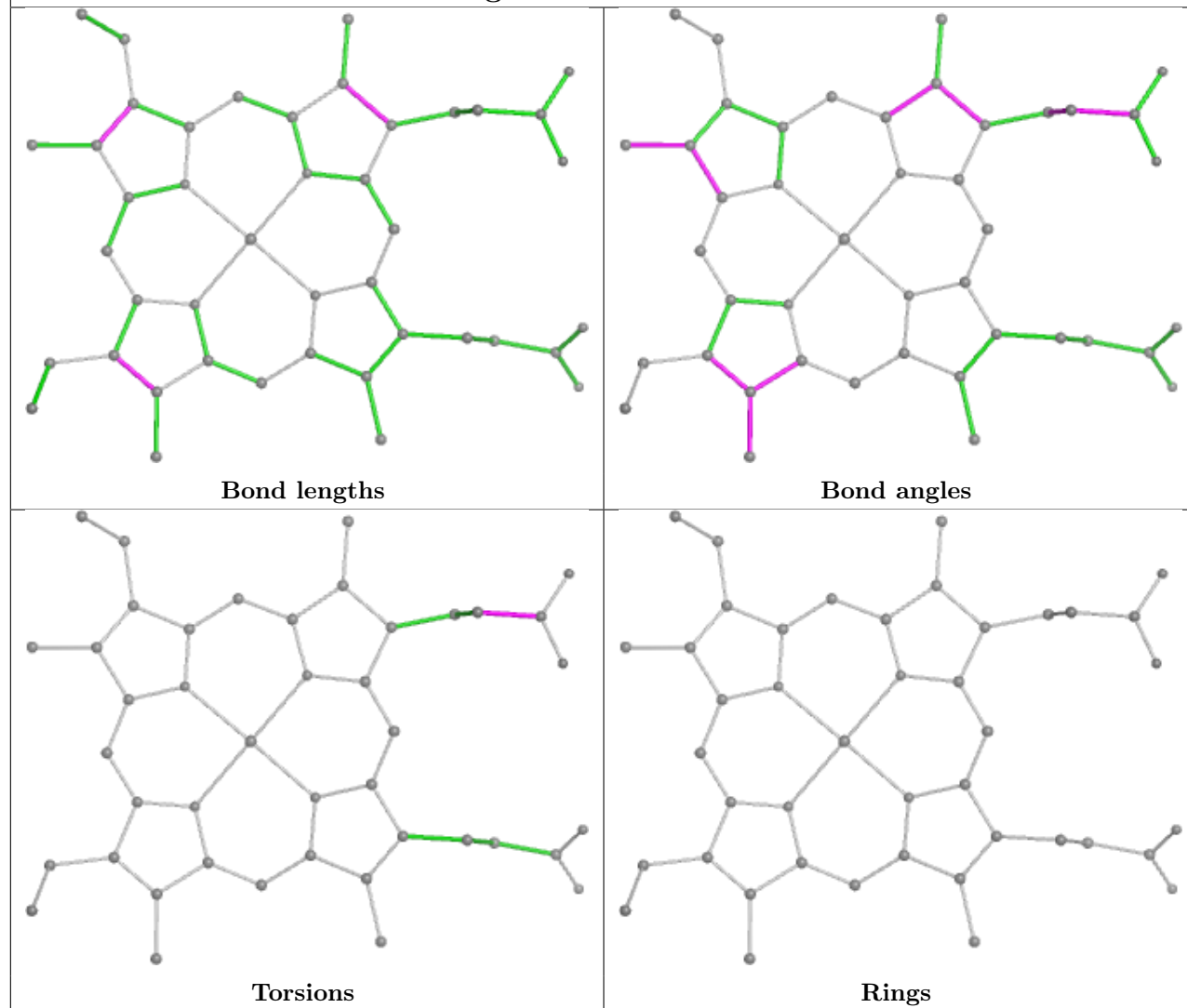


Ligand BCL L 308

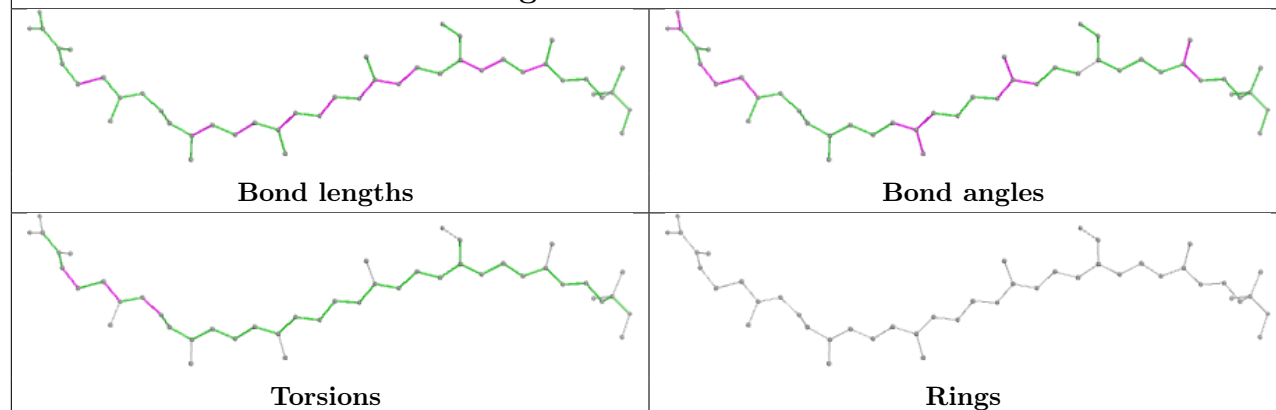


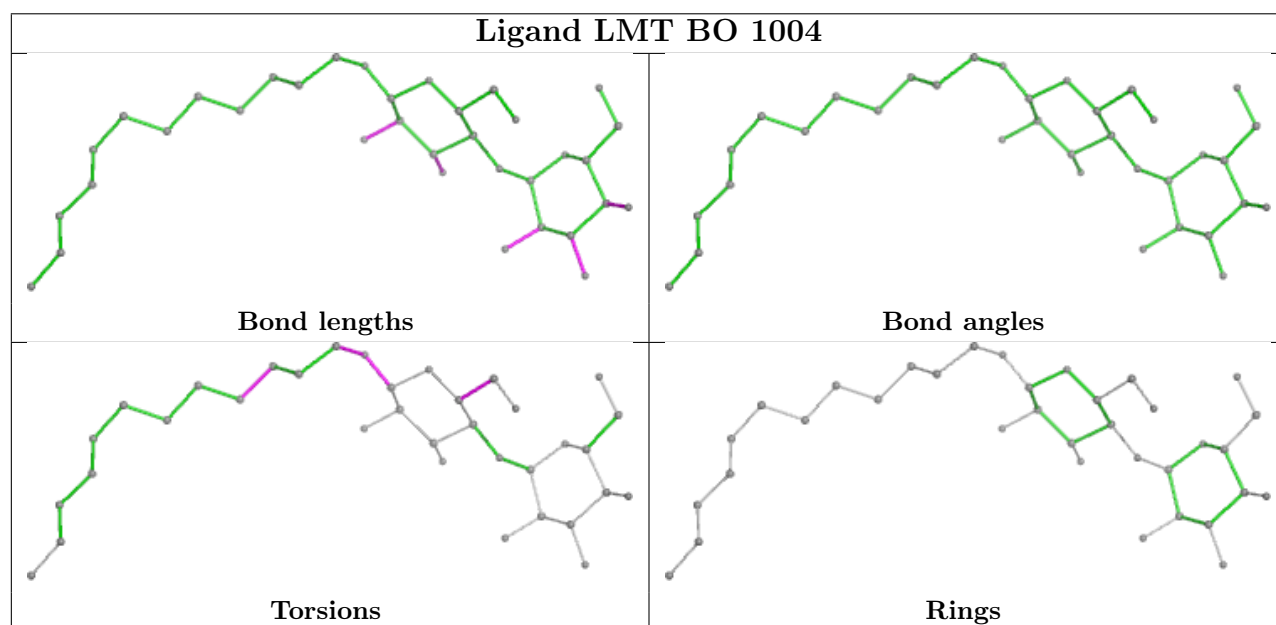
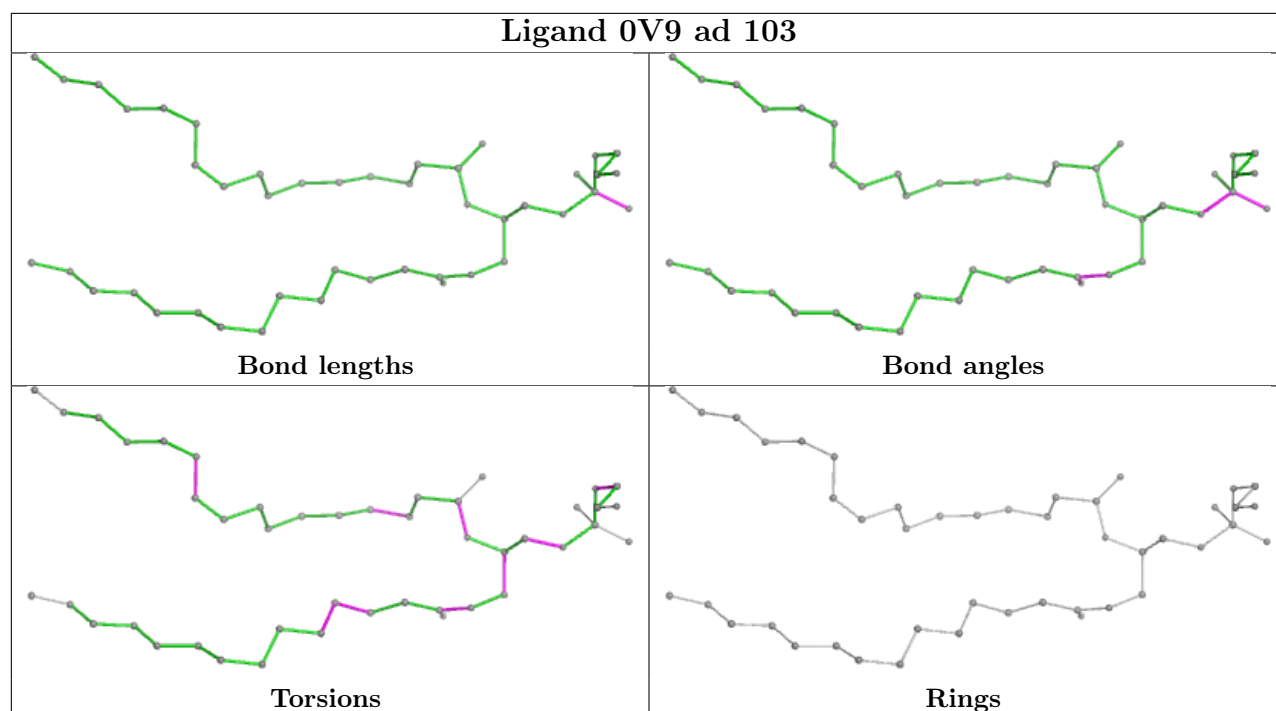
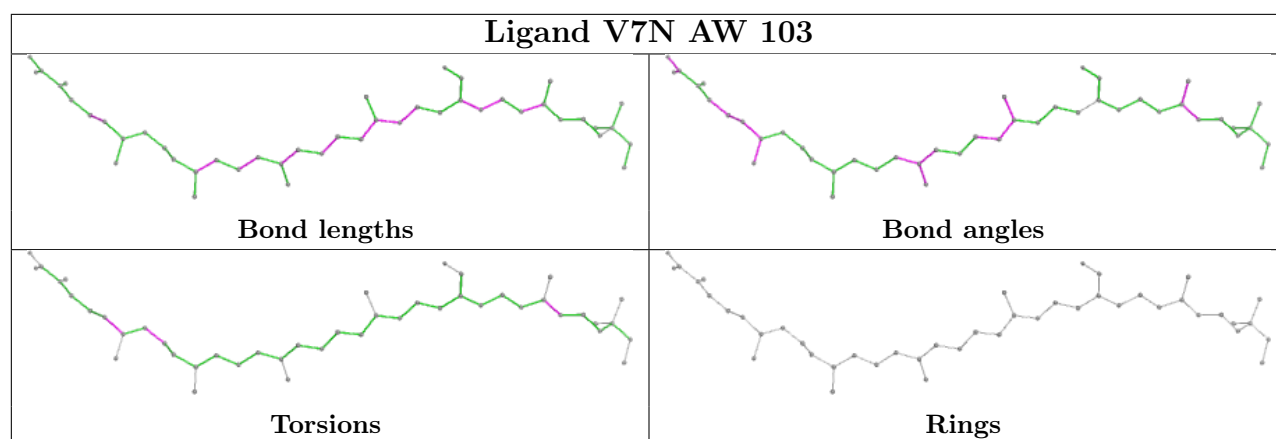


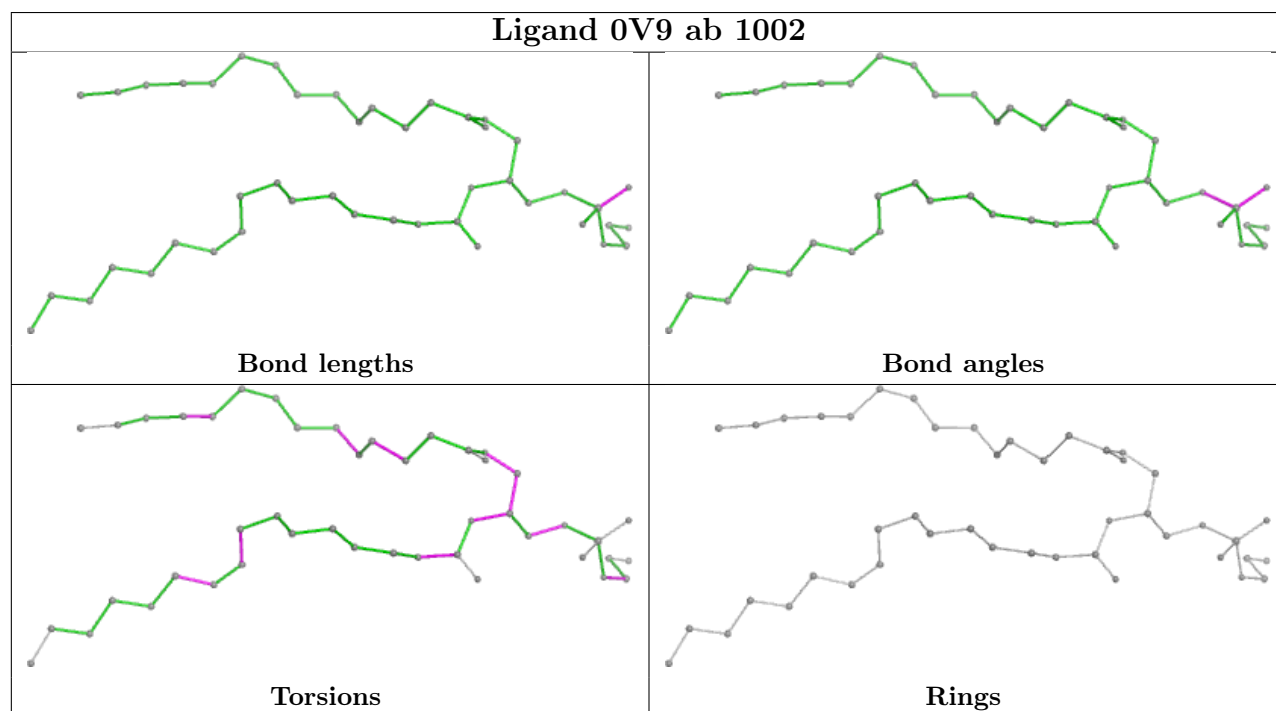
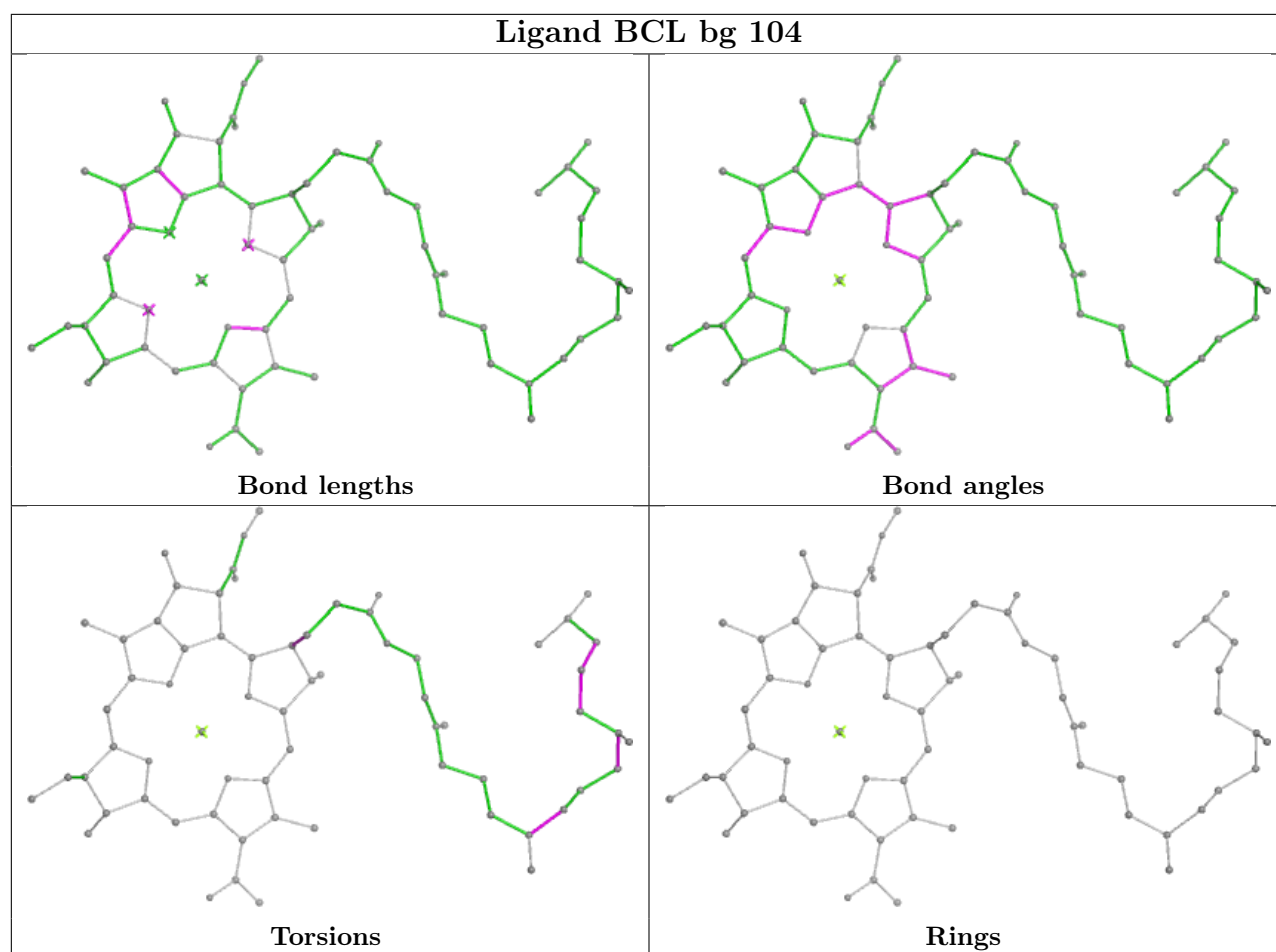
Ligand HEC C 1004

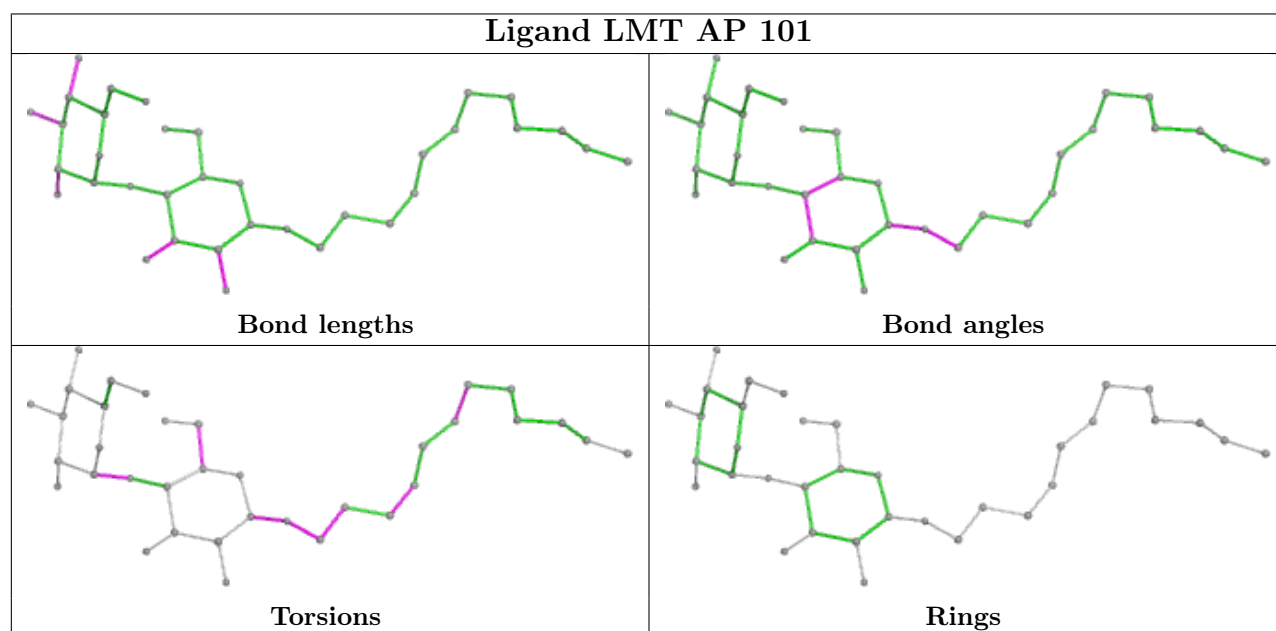
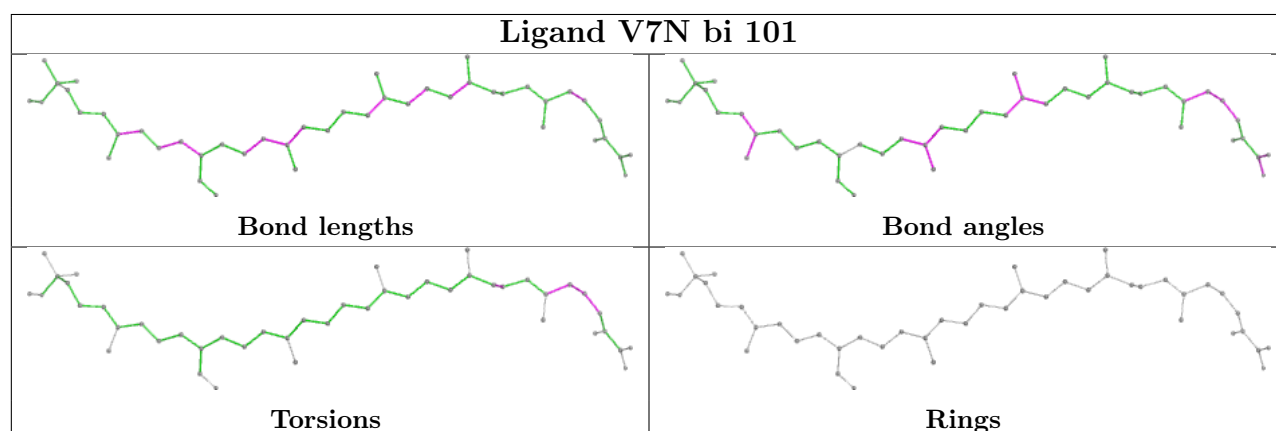
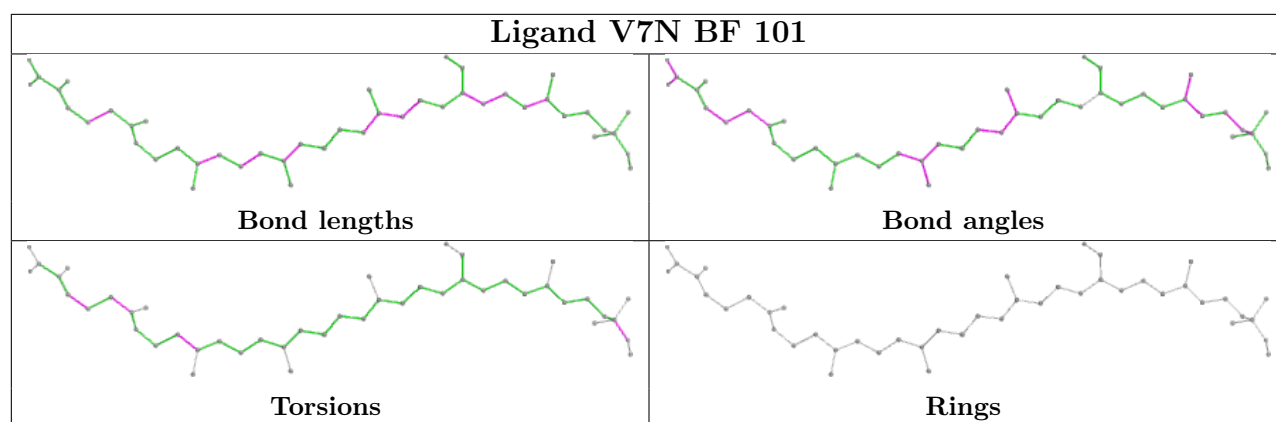


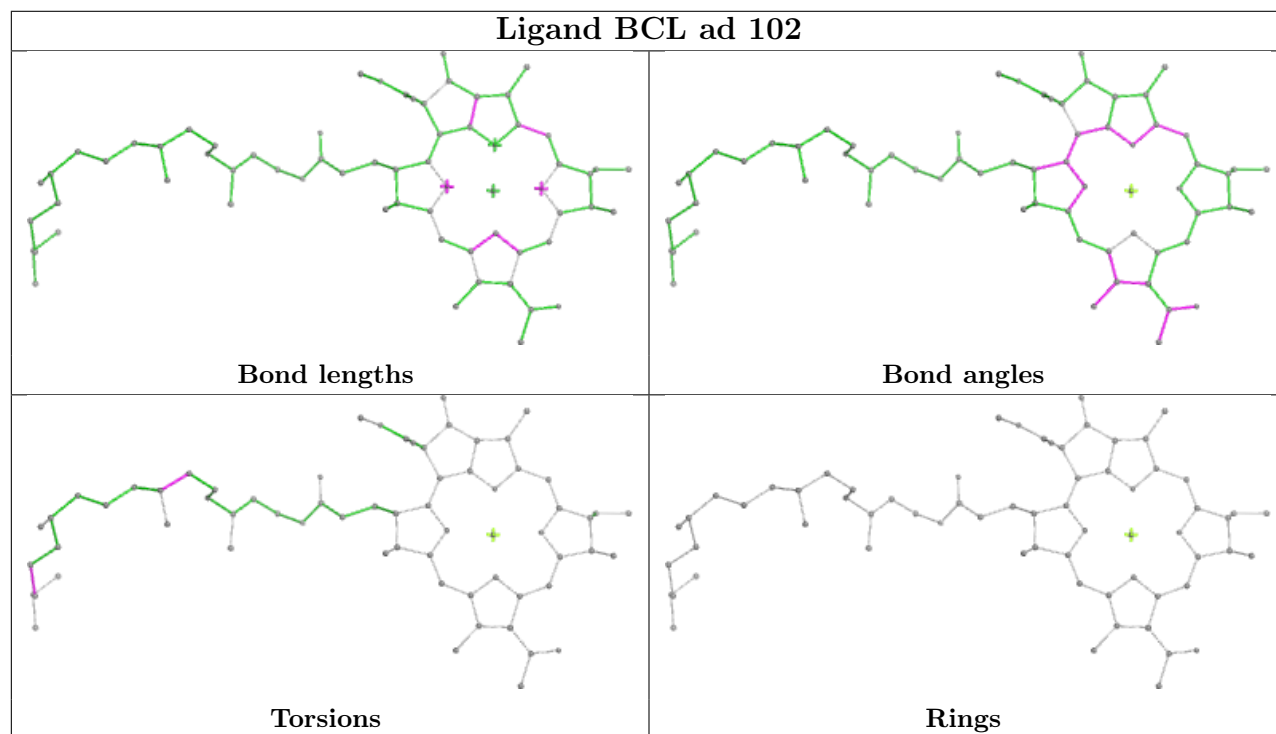
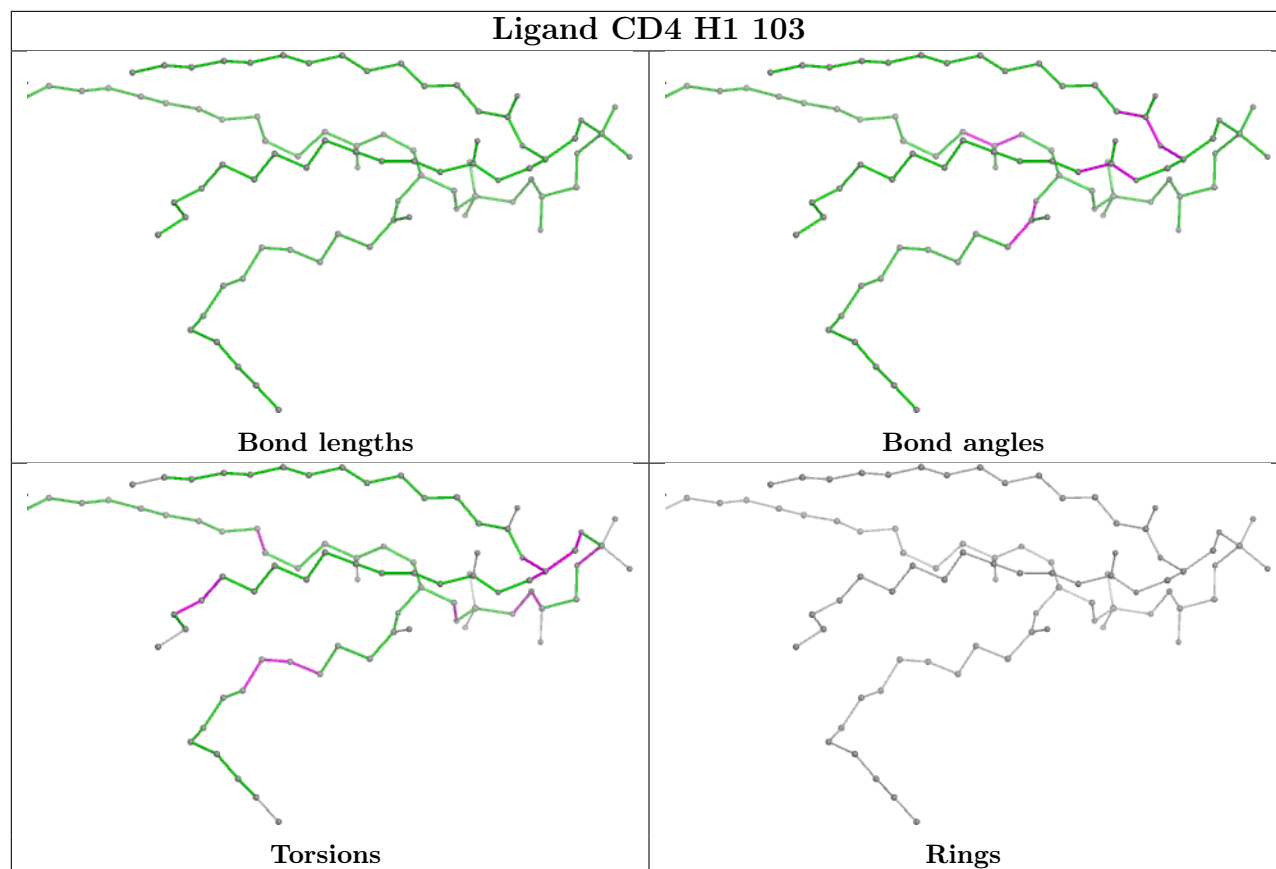
Ligand V7N BD 101

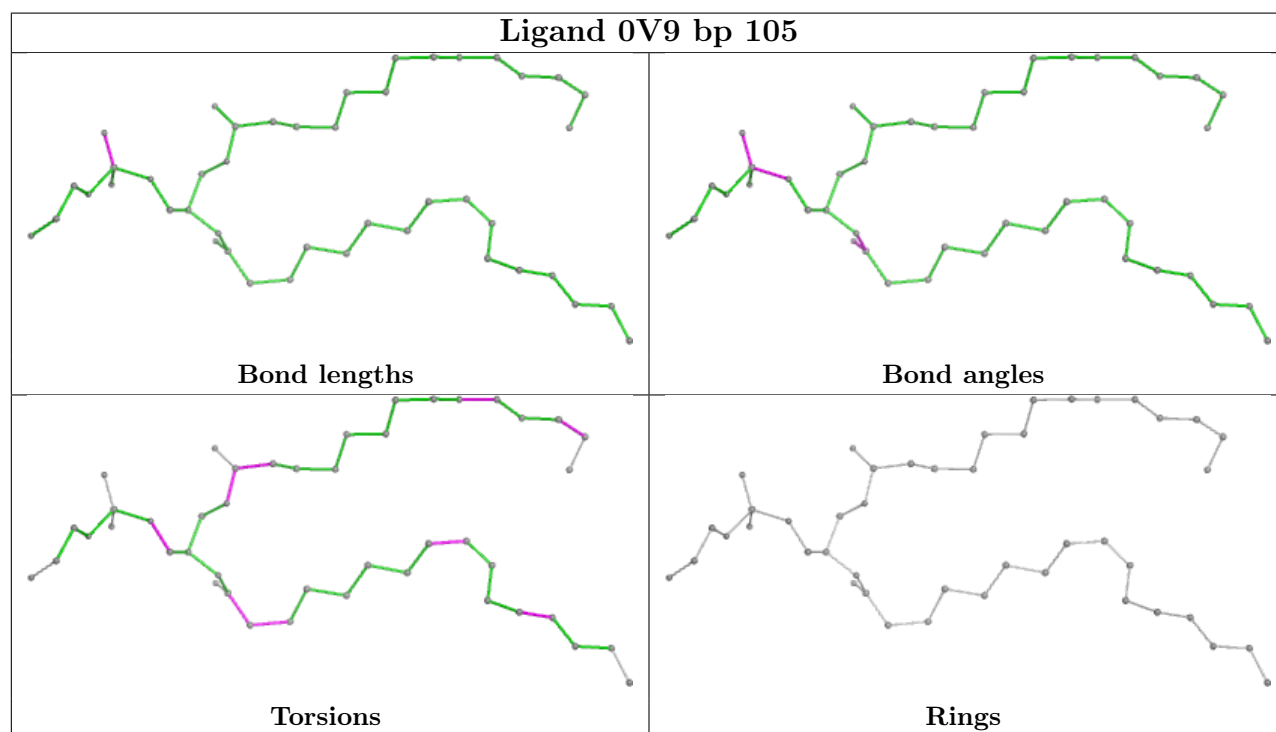
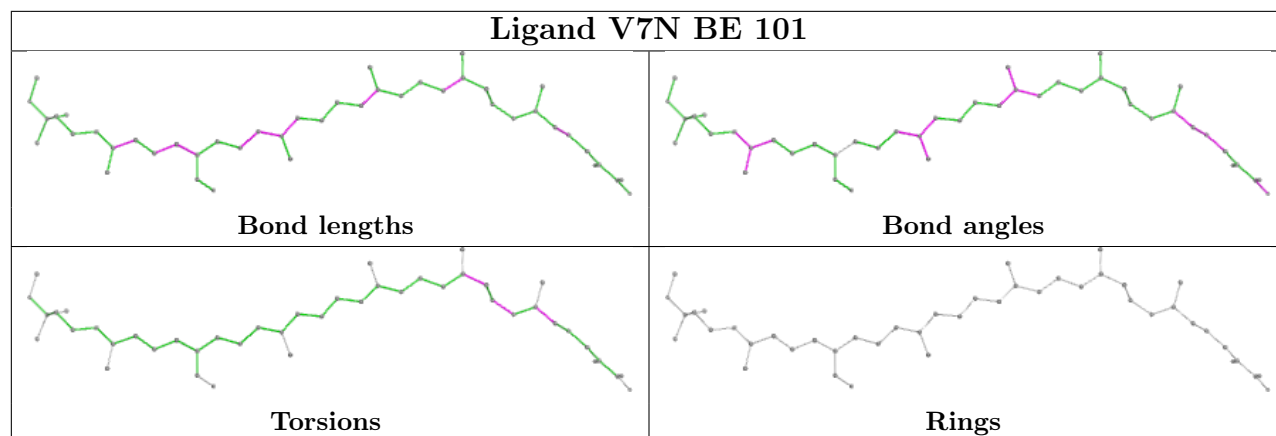


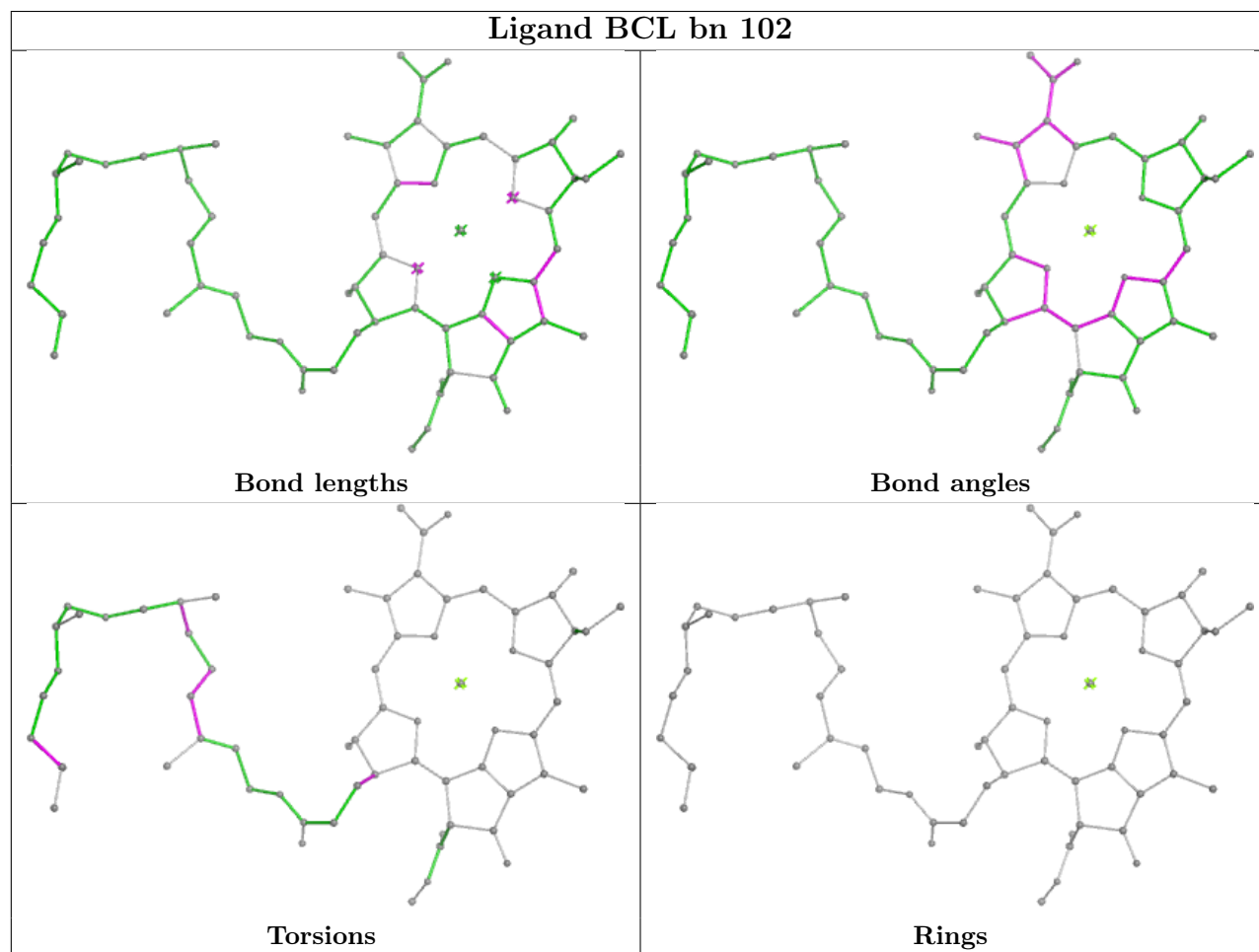
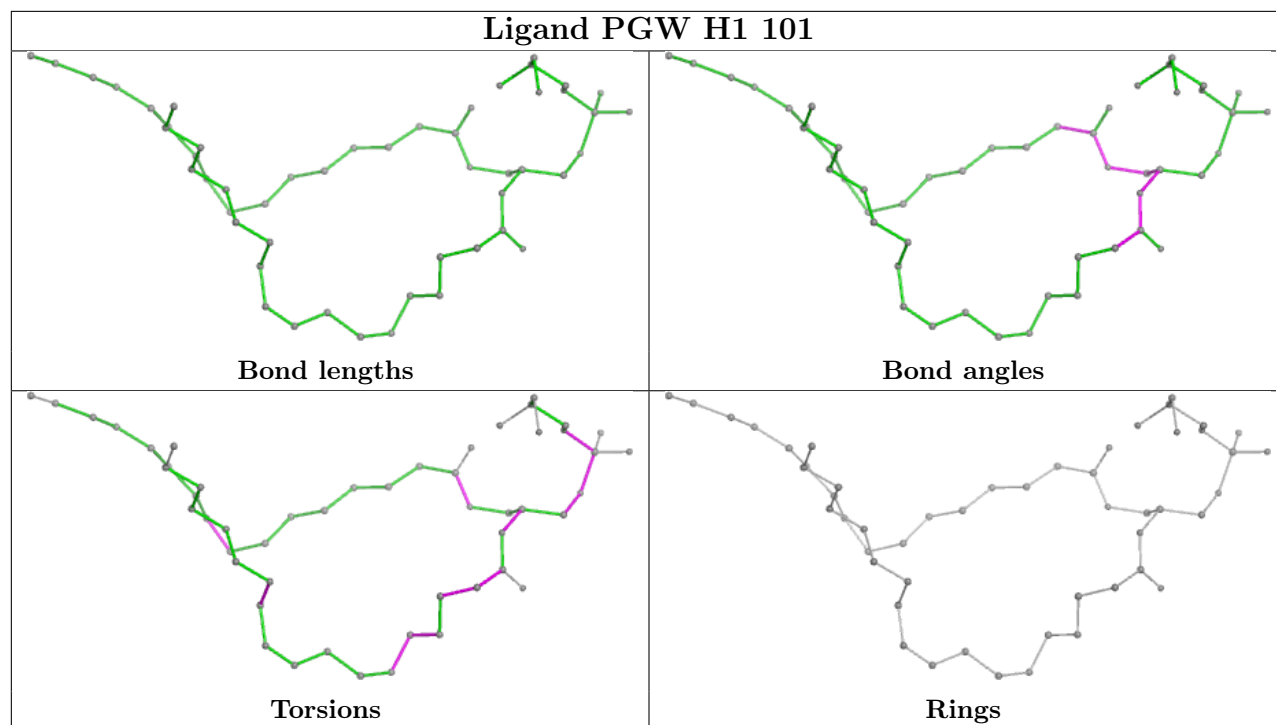


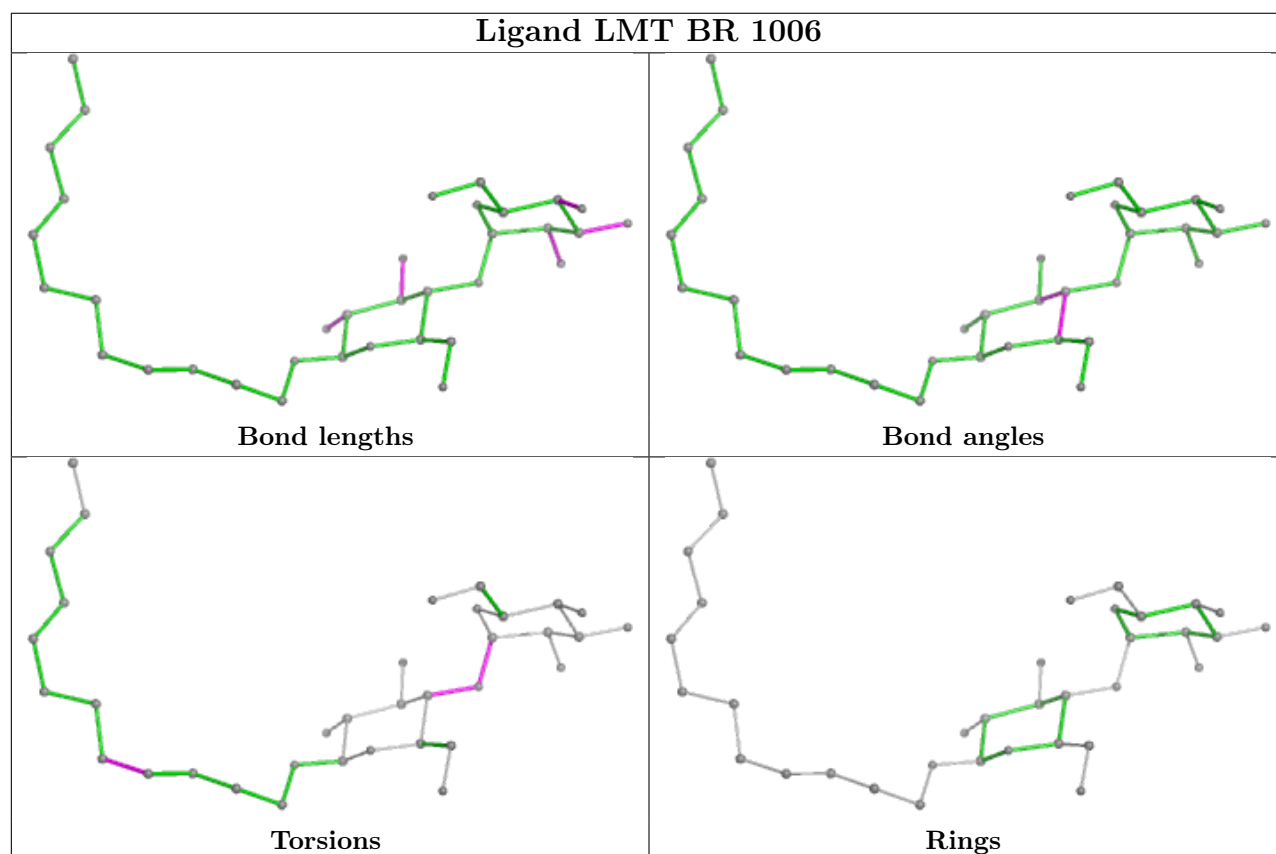
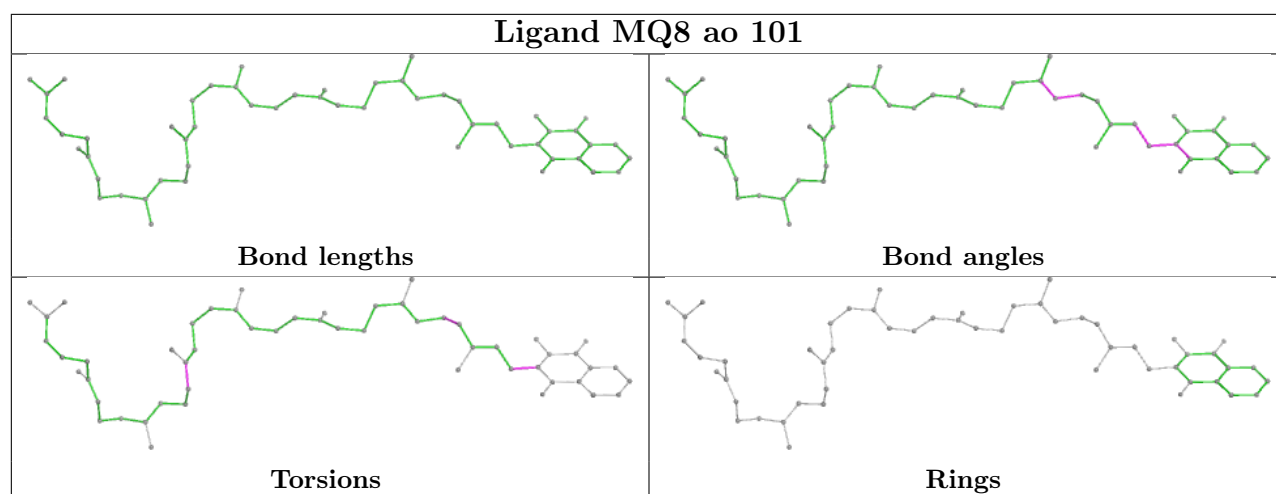


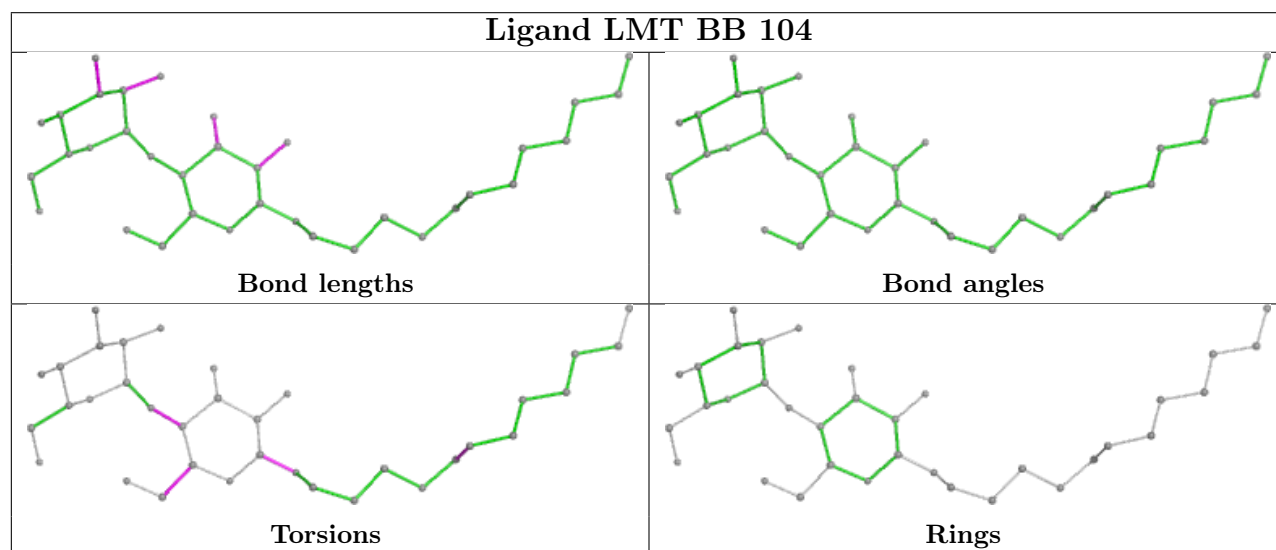
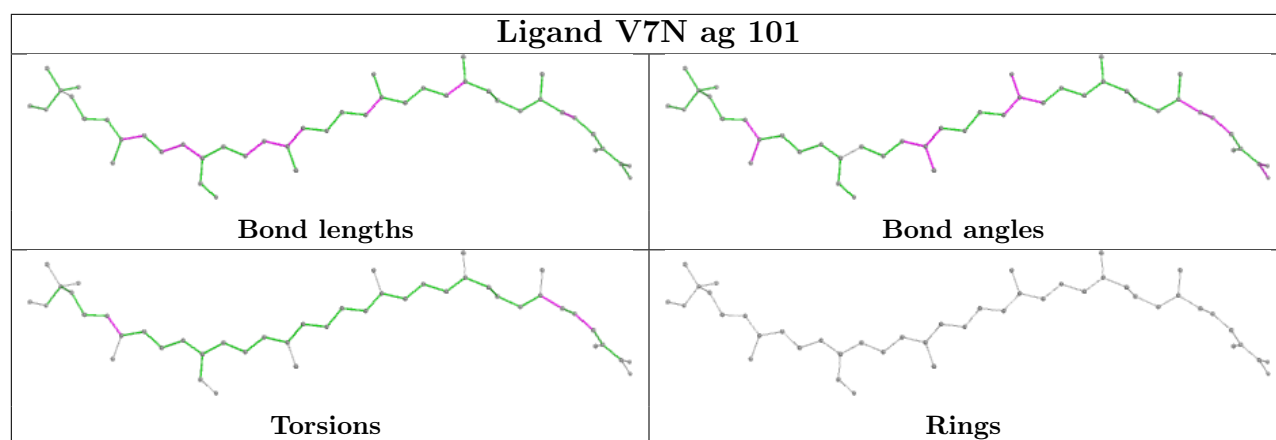
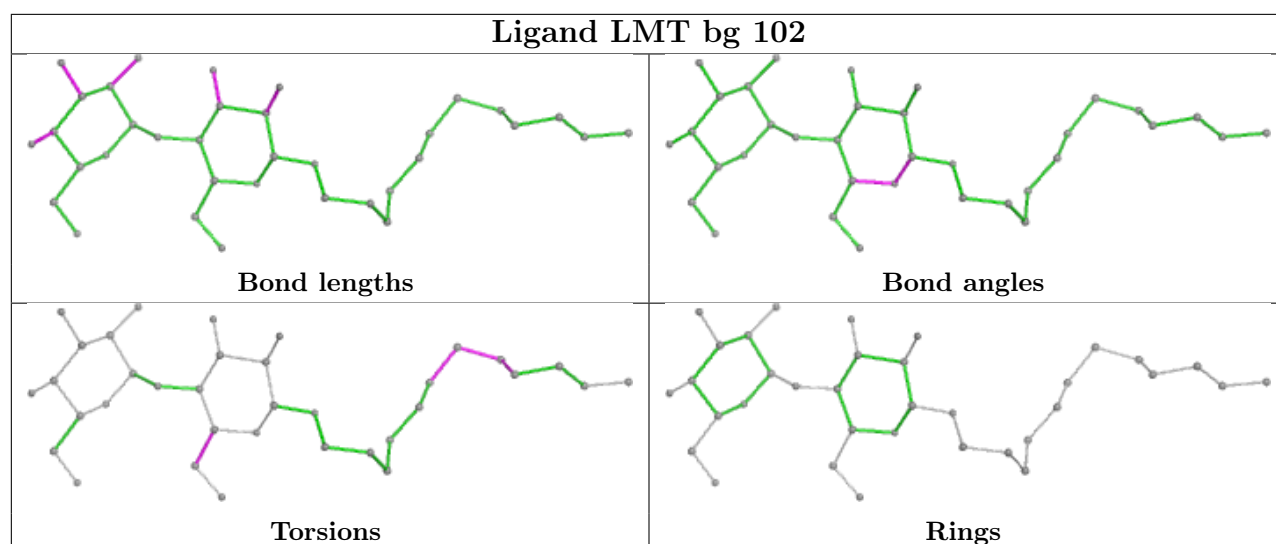


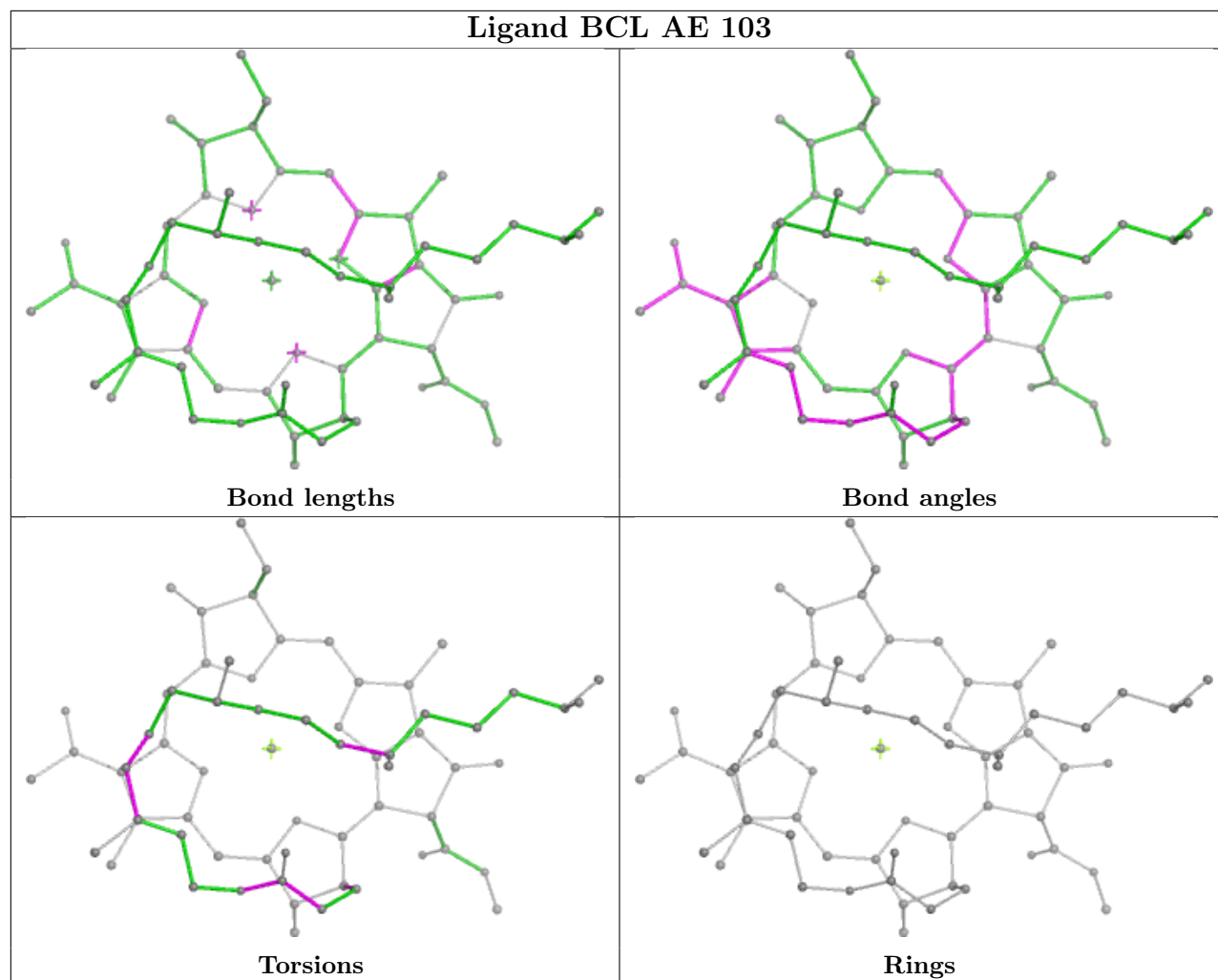
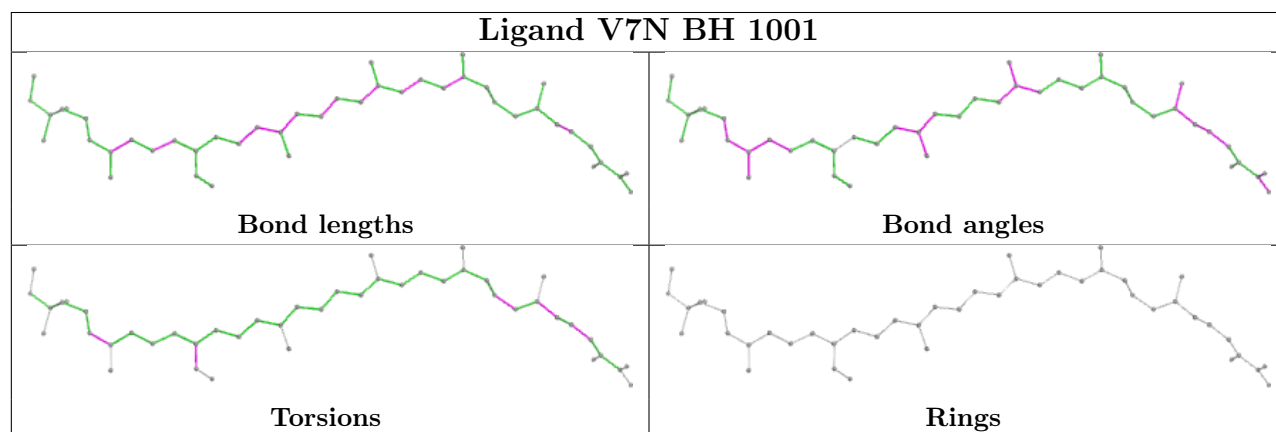


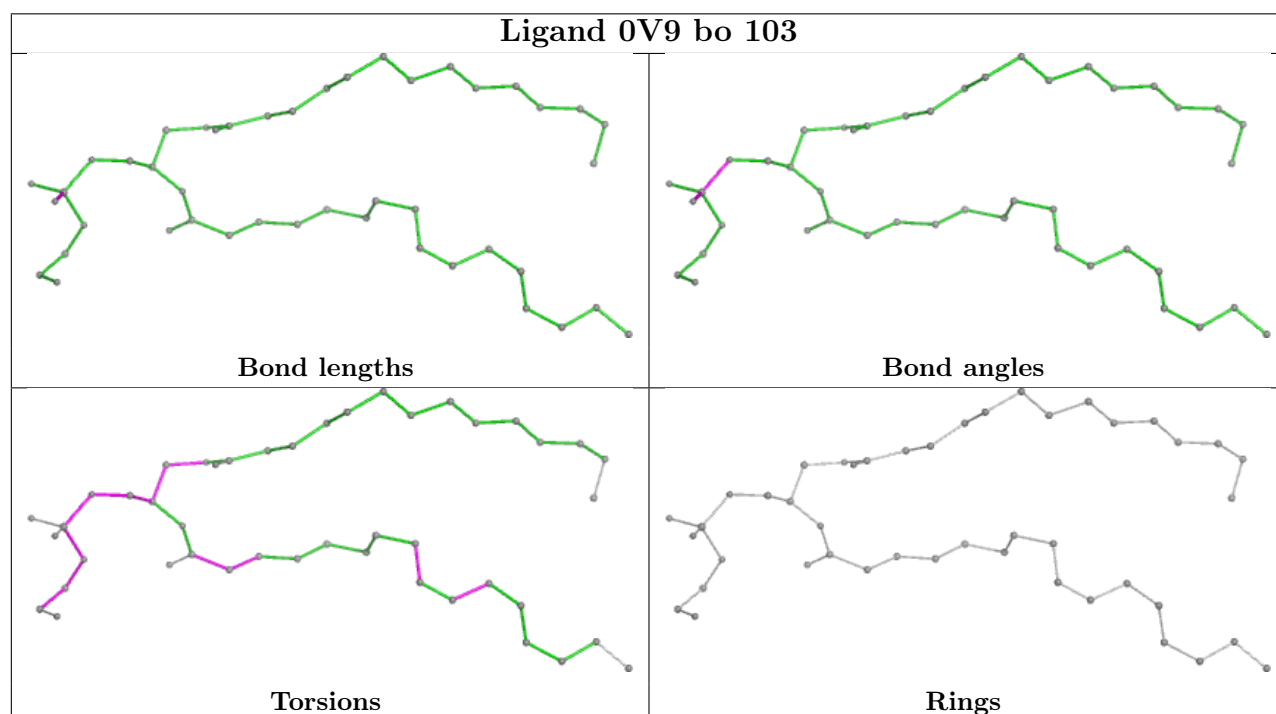
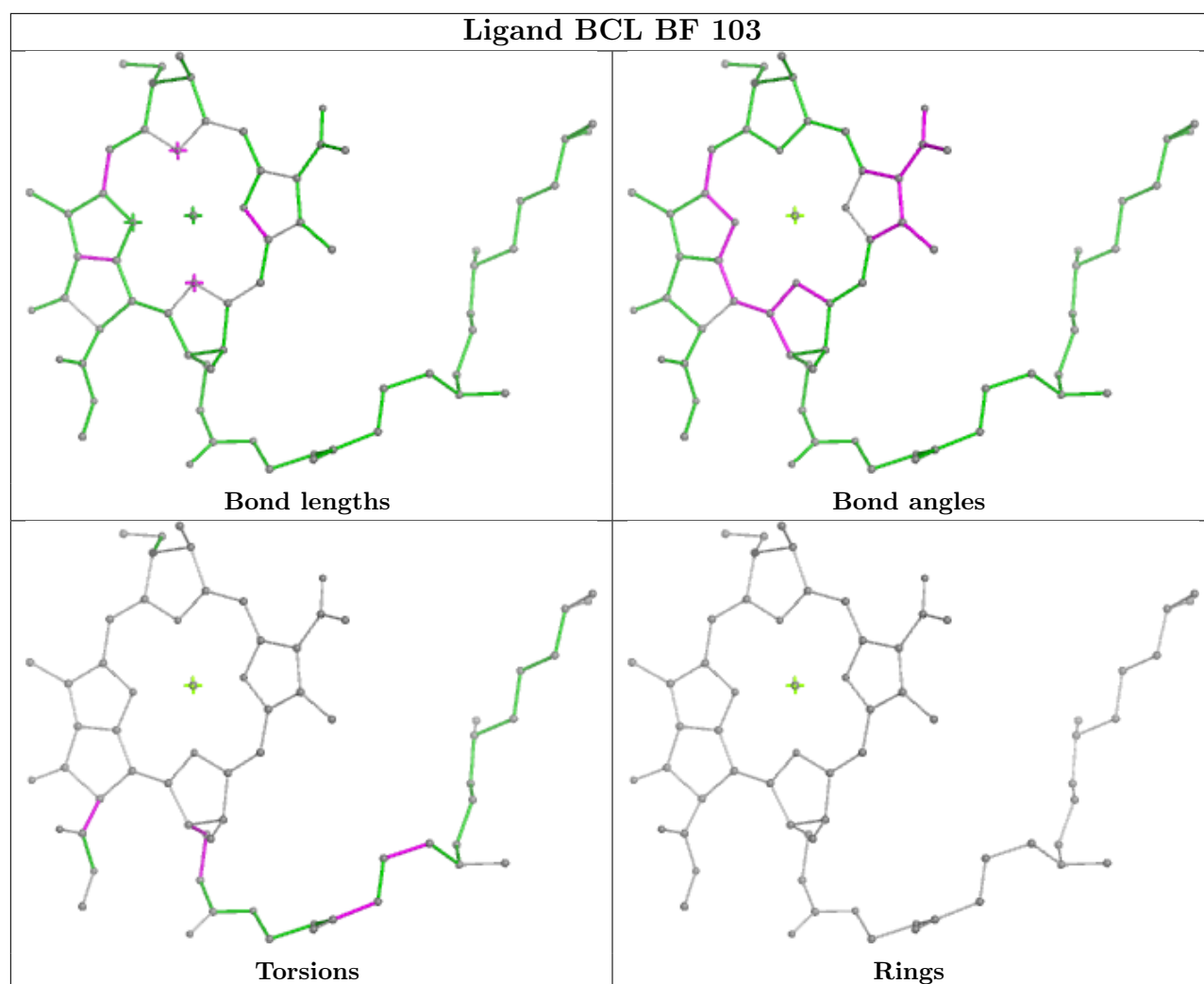


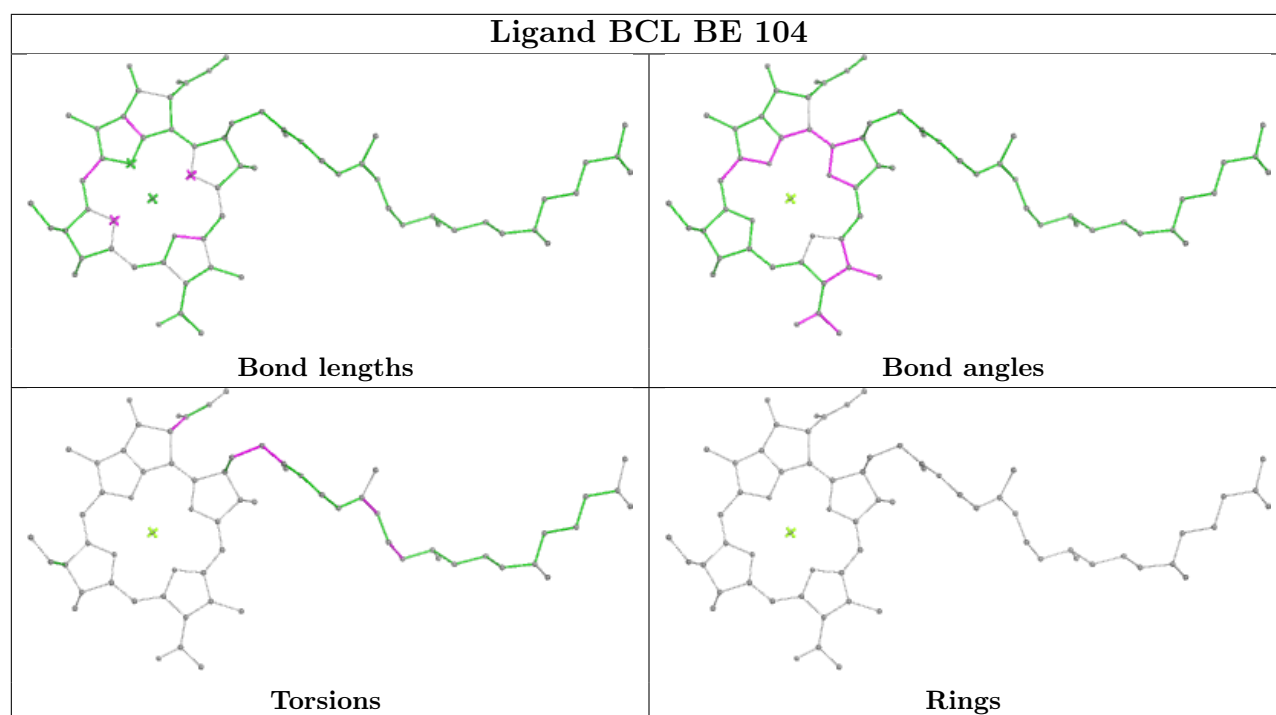




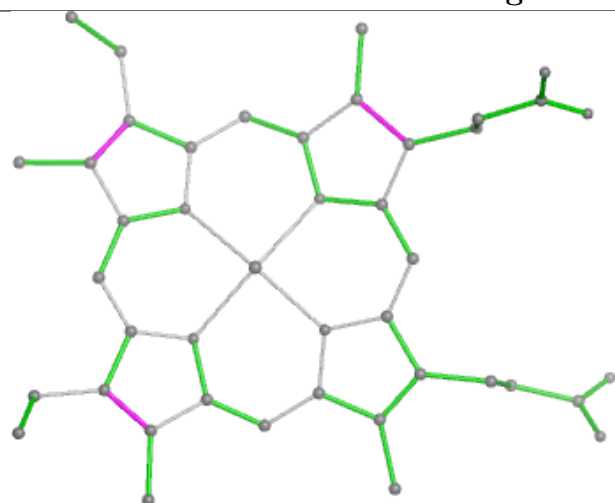


Ligand BCL AE 103**Ligand V7N BH 1001**

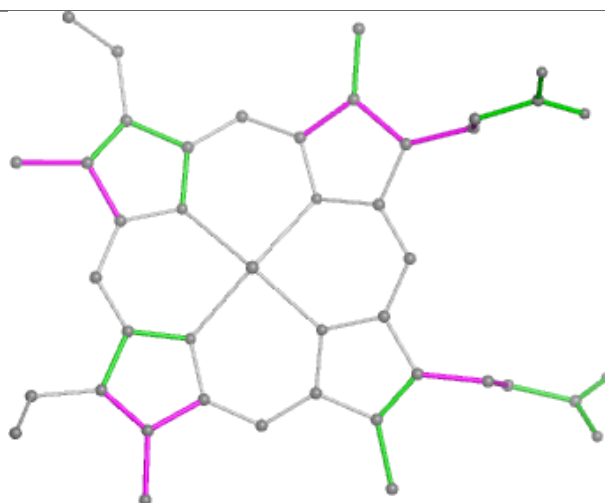




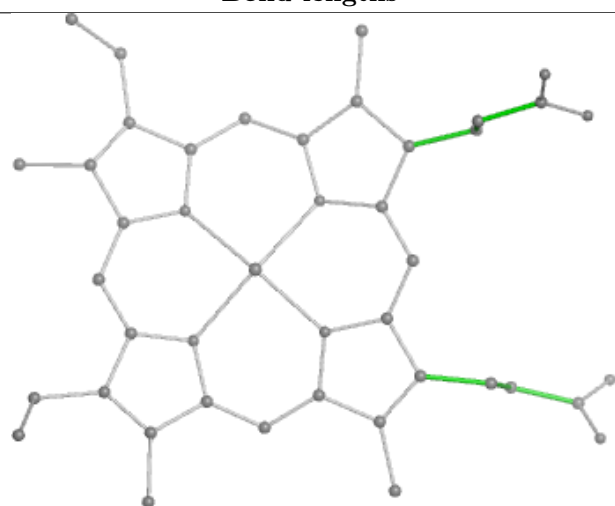
Ligand HEC C 1003



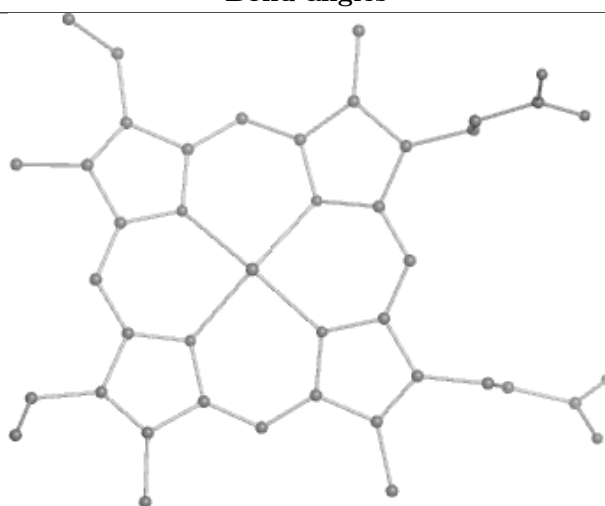
Bond lengths



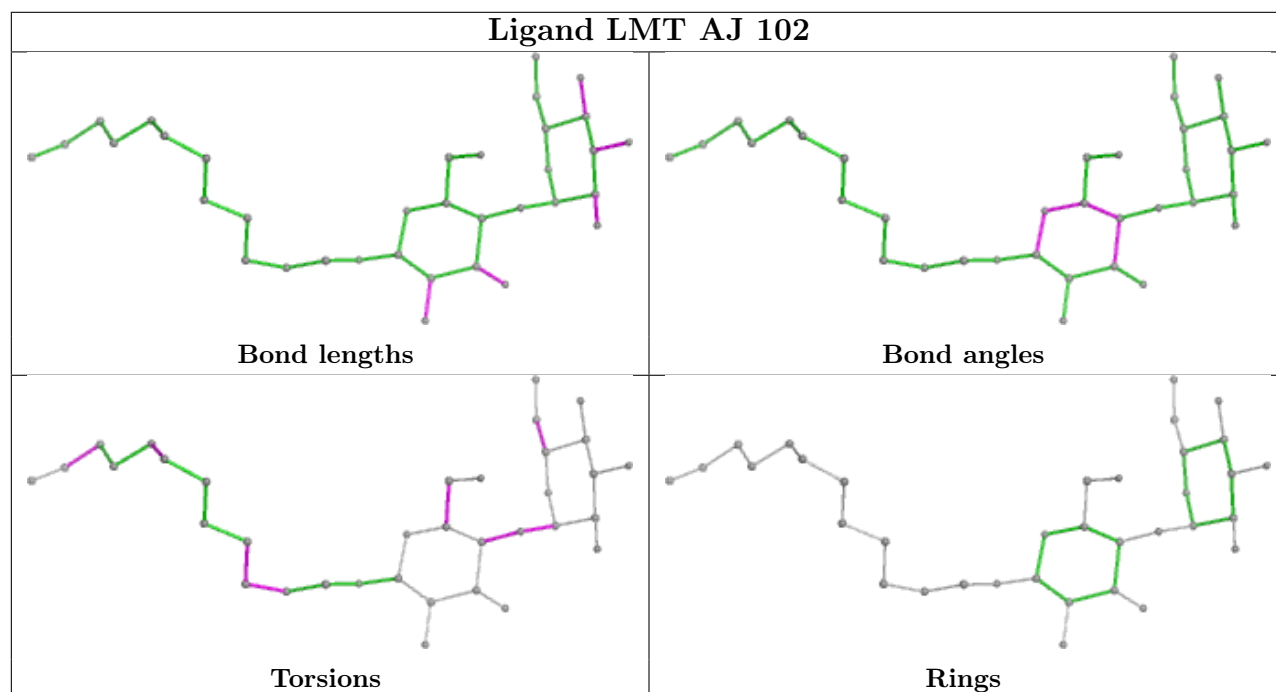
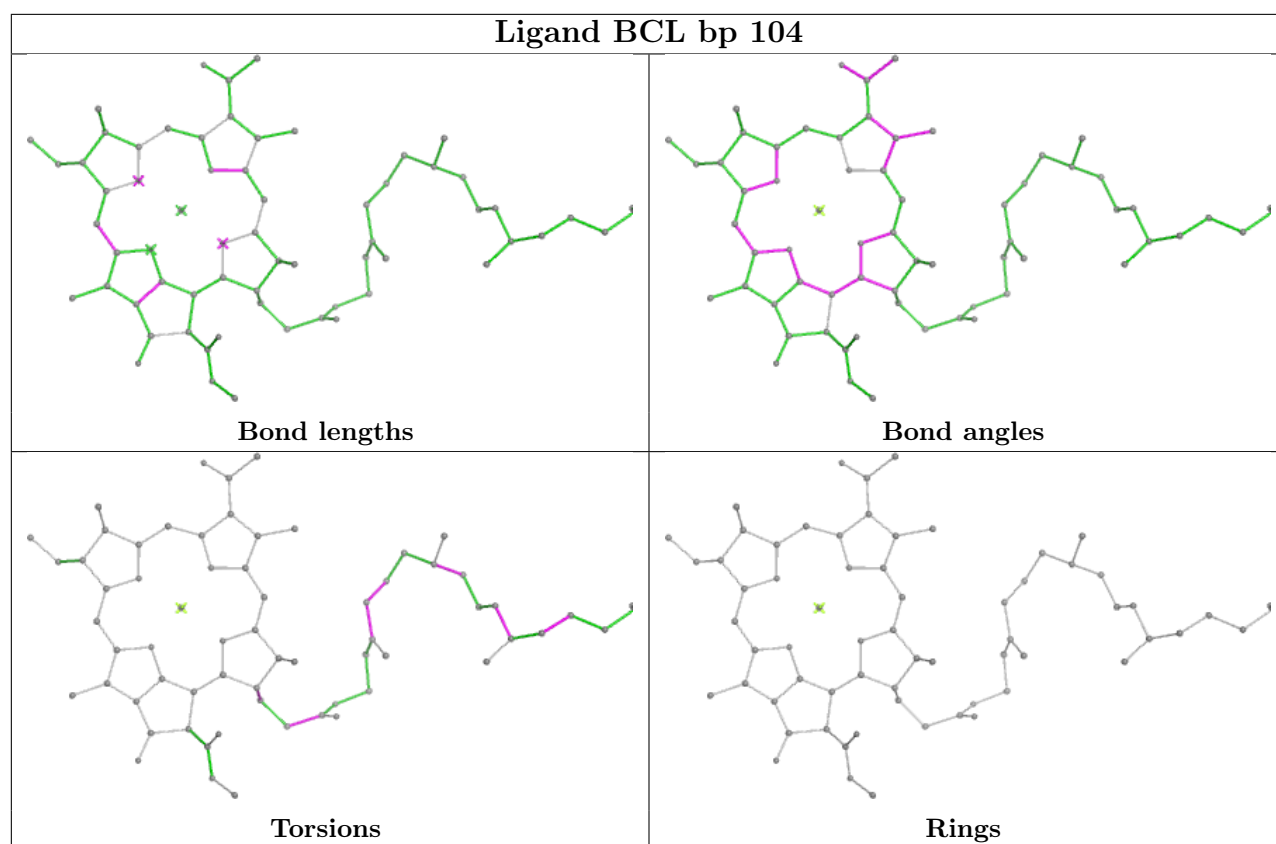
Bond angles

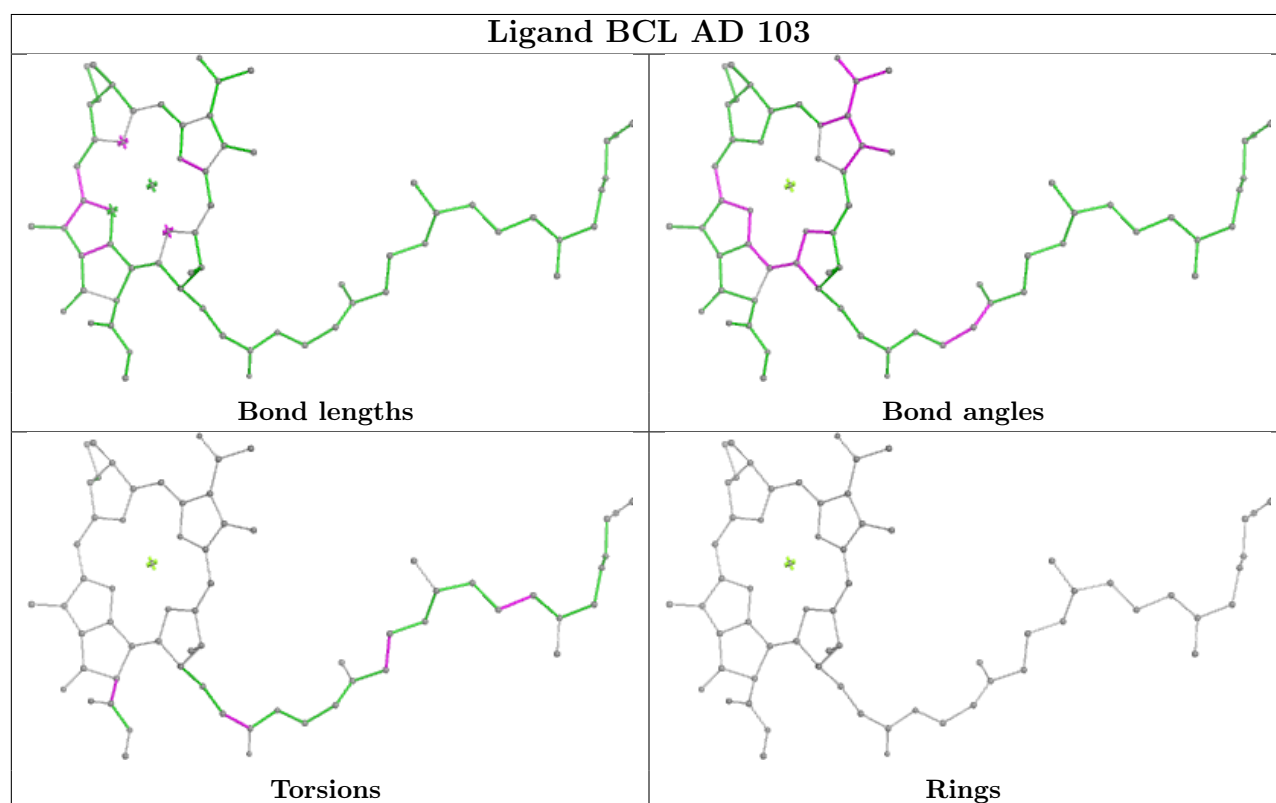
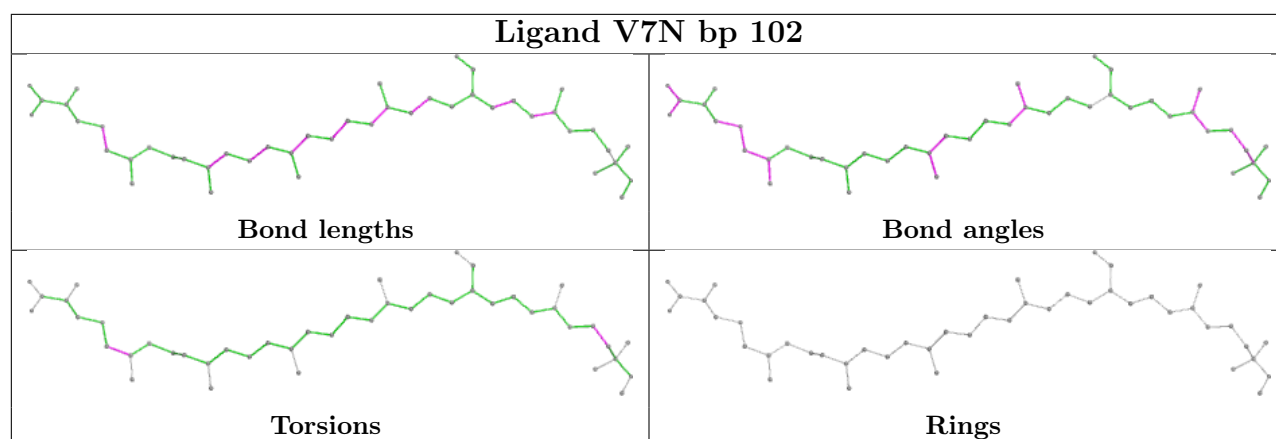


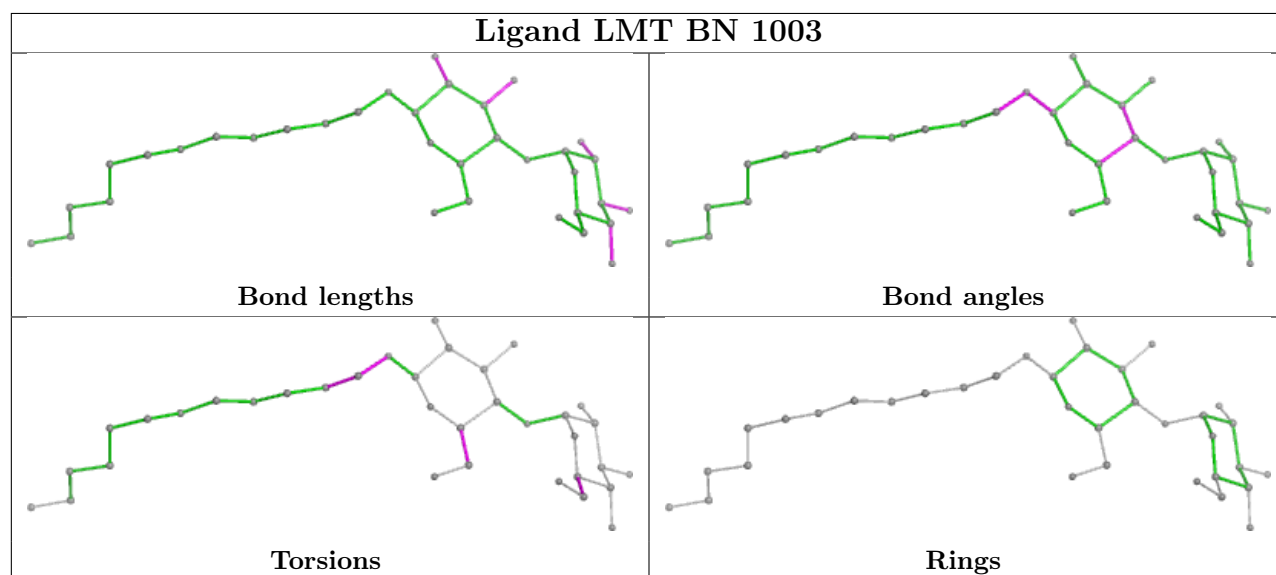
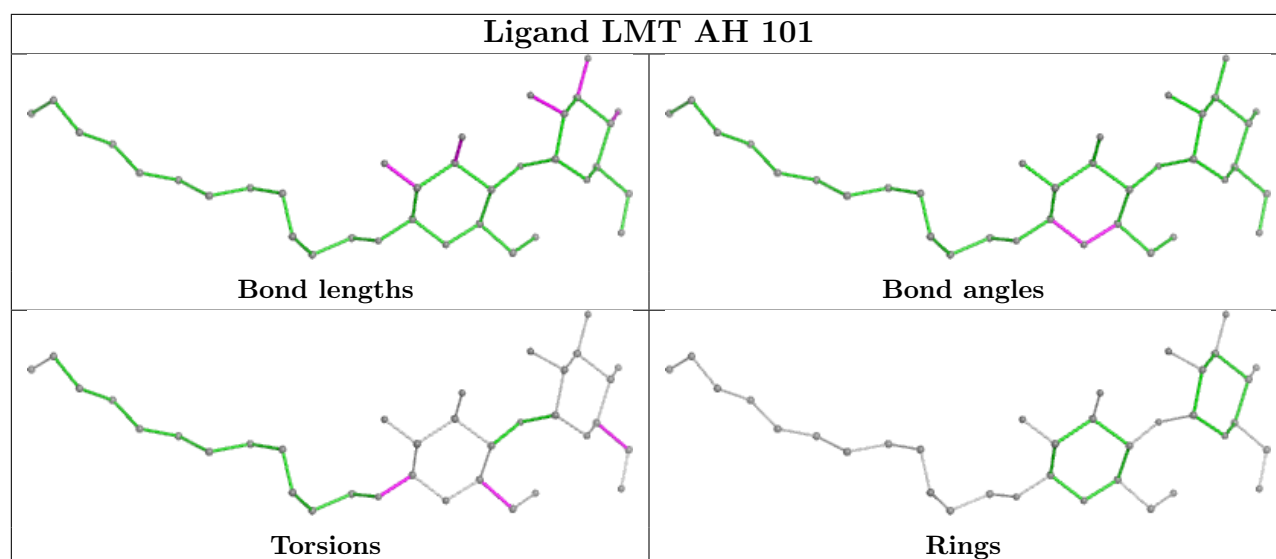
Torsions

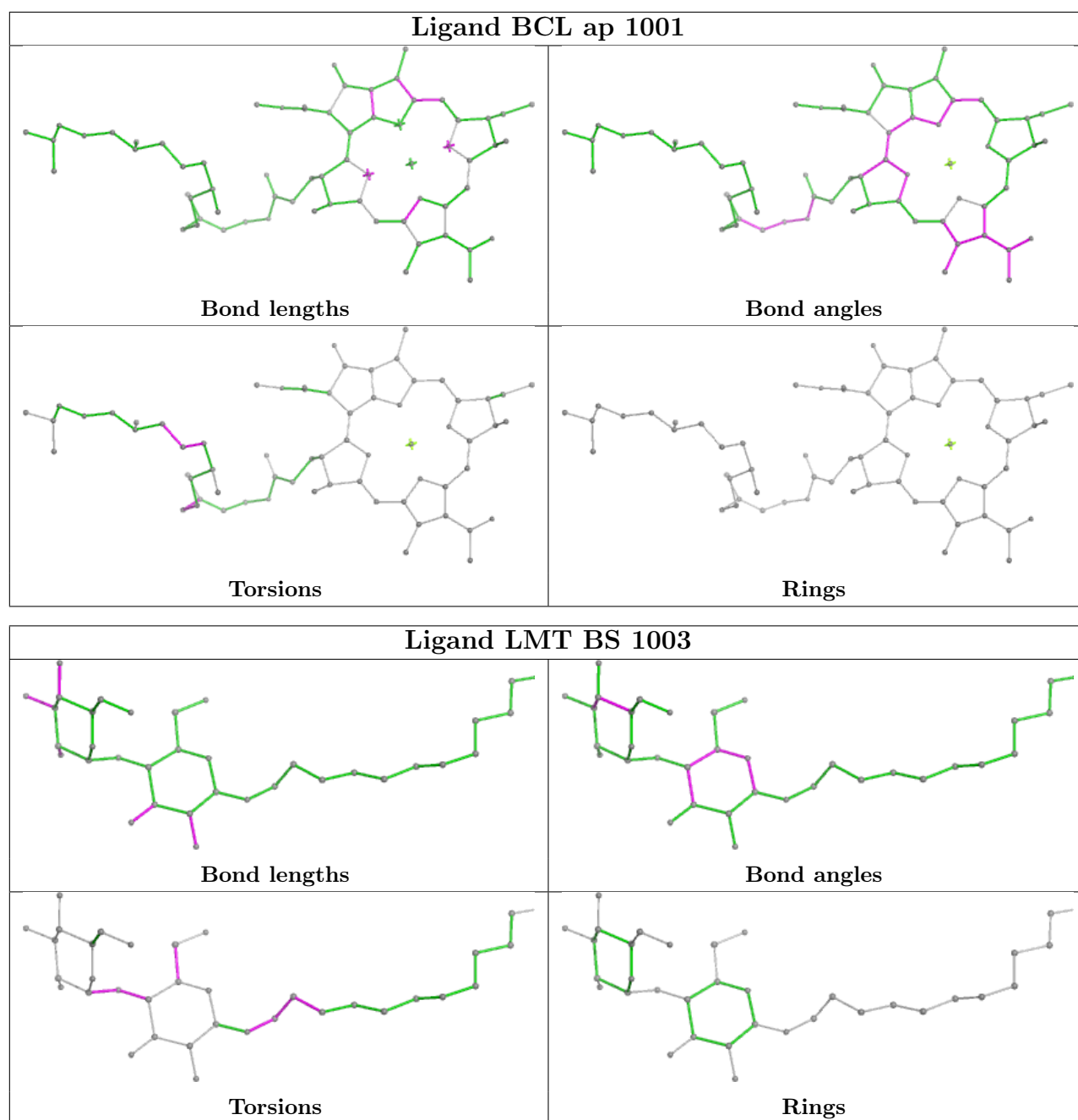


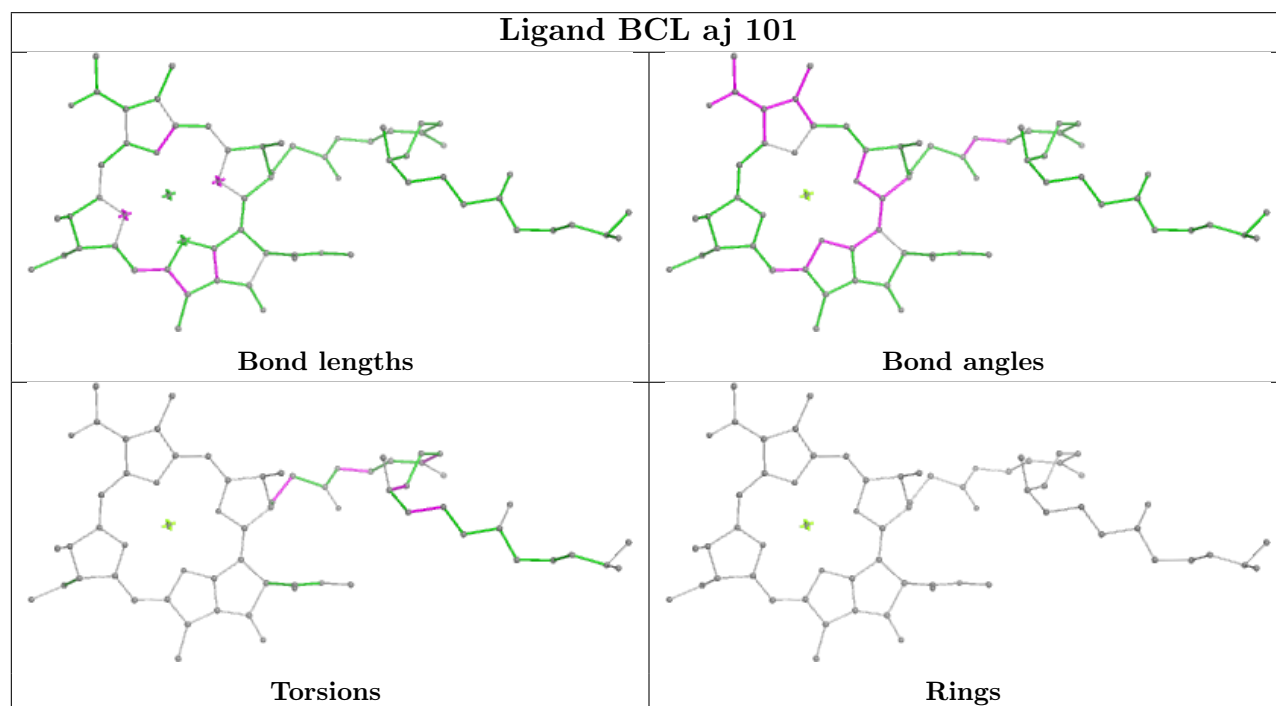
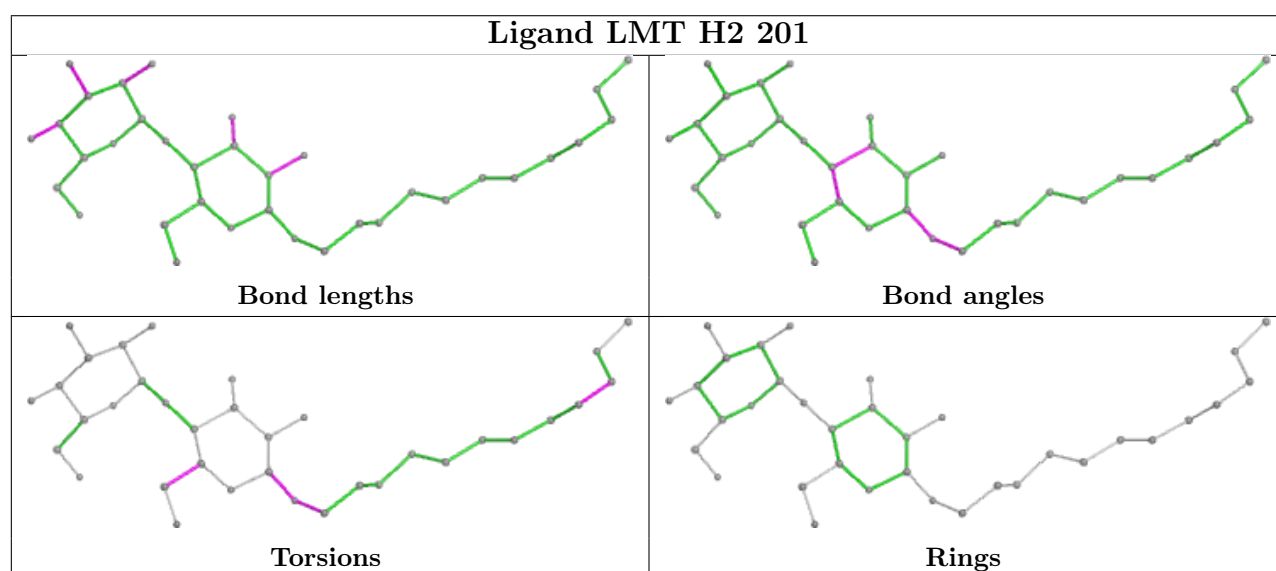
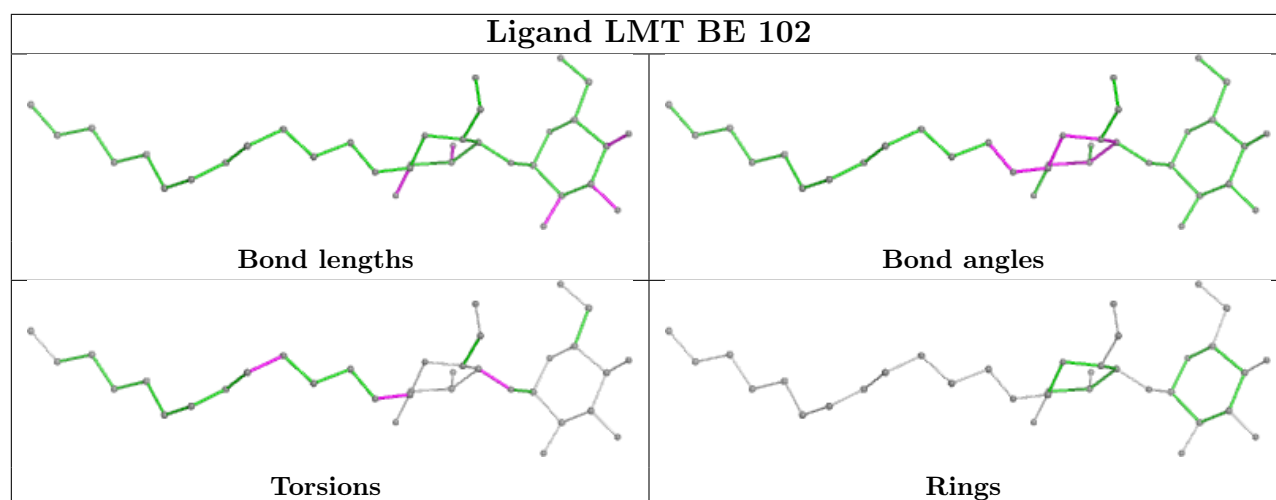
Rings

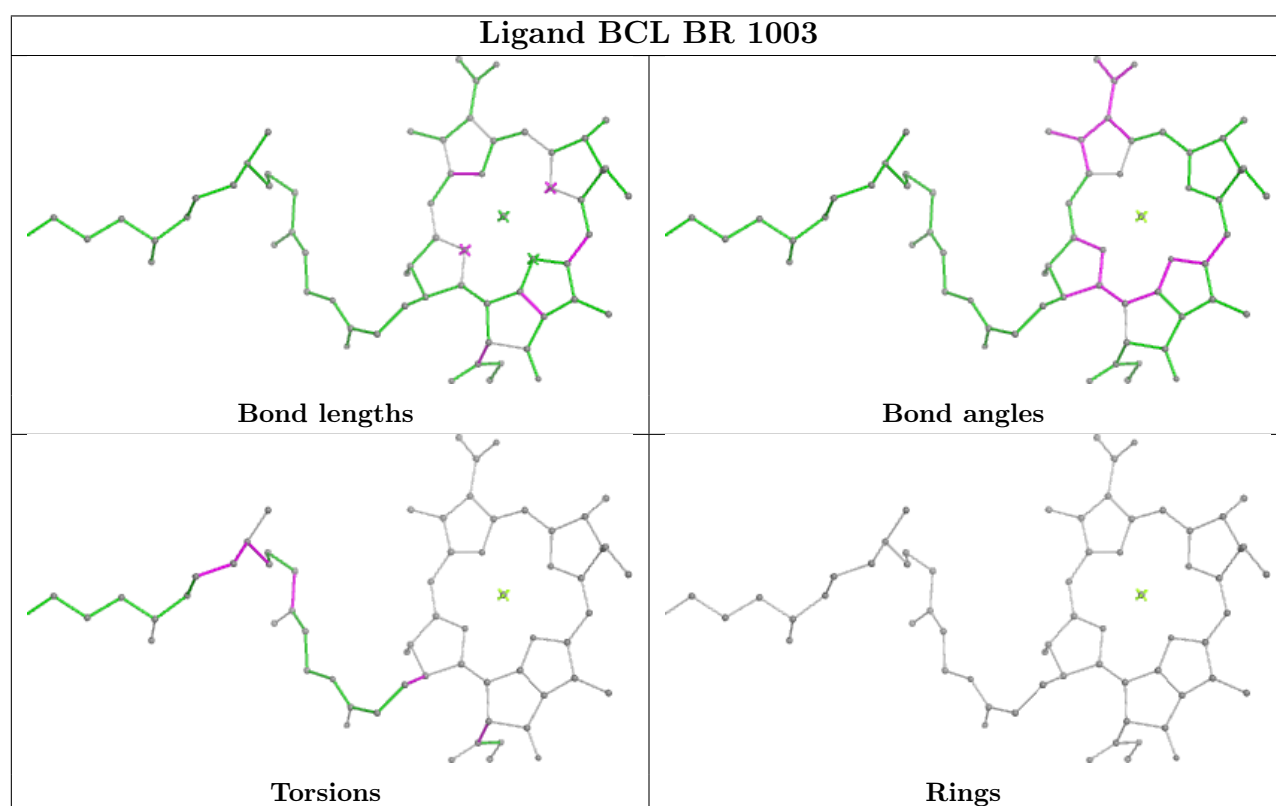
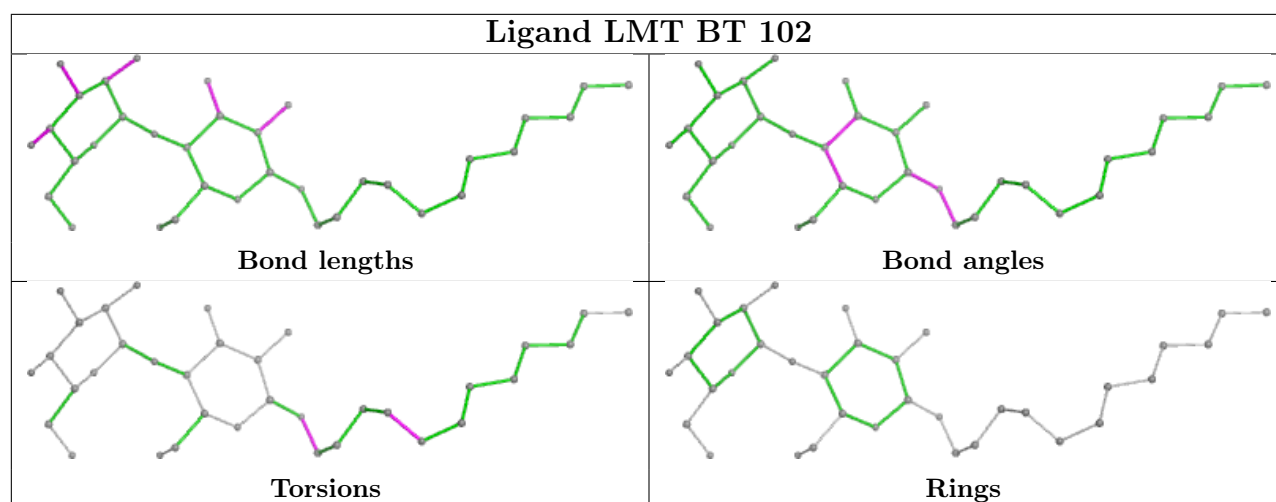




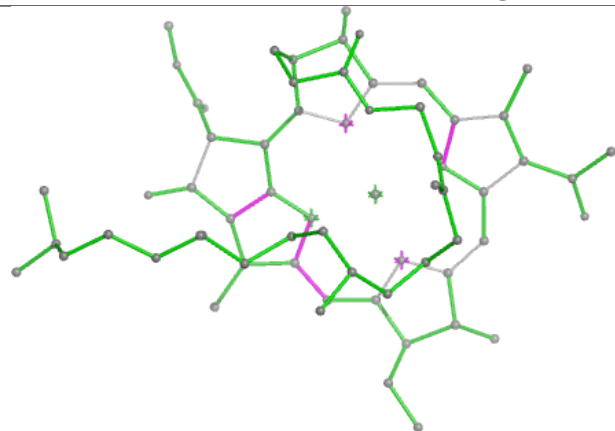




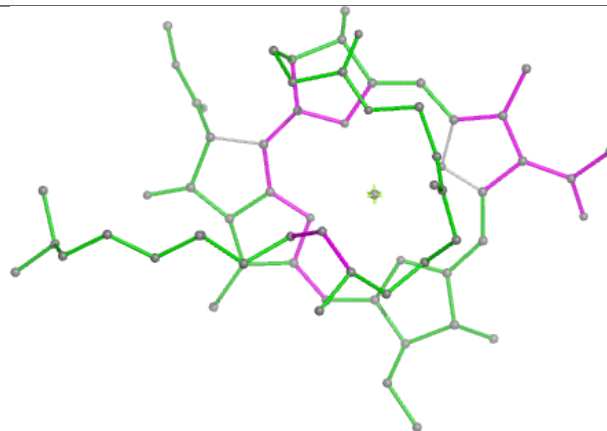




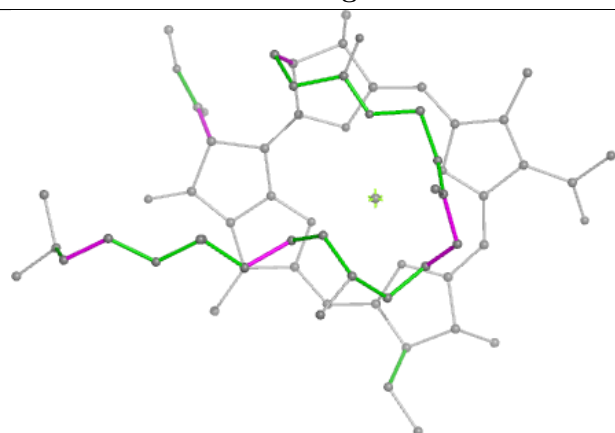
Ligand BCL AA 1002



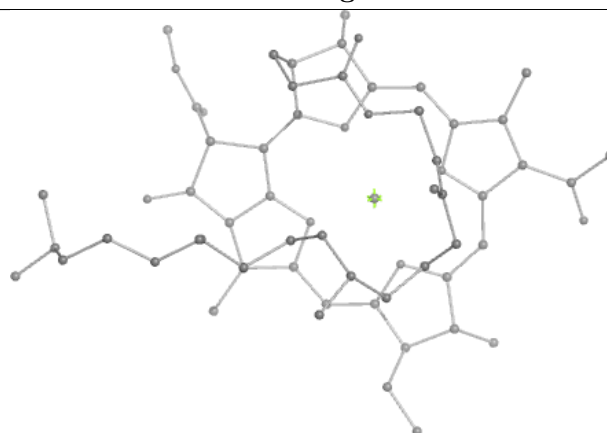
Bond lengths



Bond angles

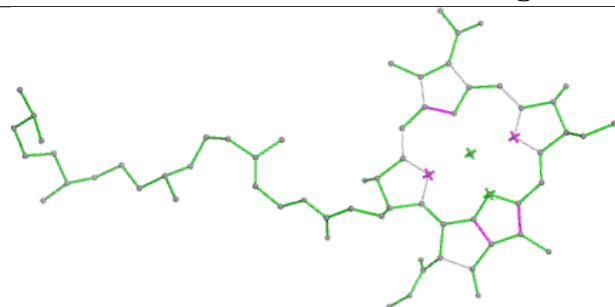


Torsions

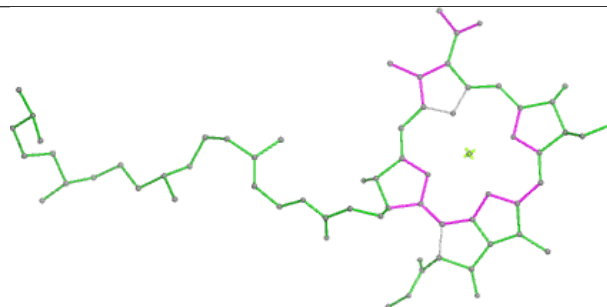


Rings

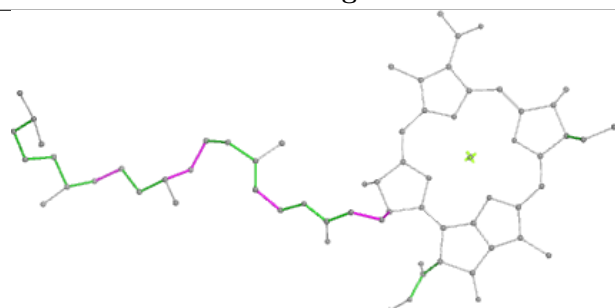
Ligand BCL bl 104



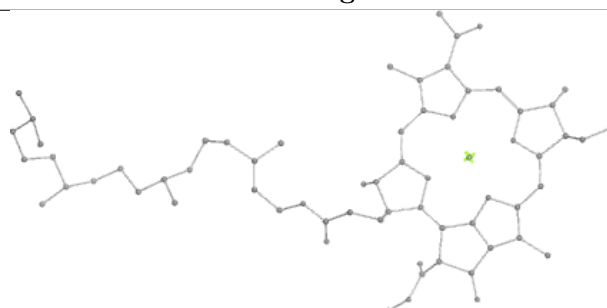
Bond lengths



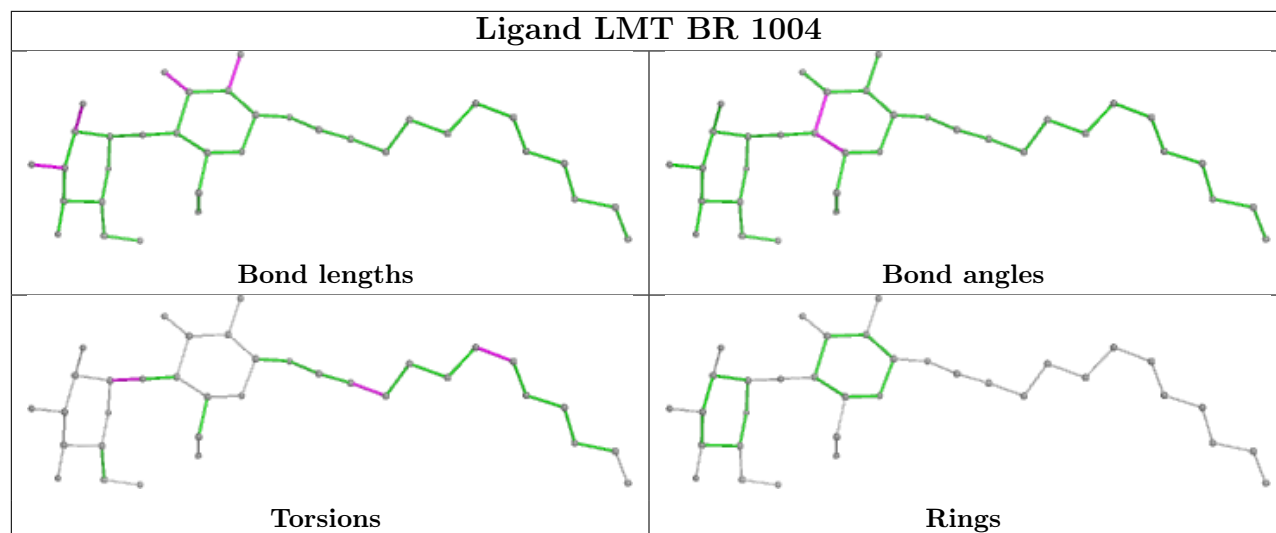
Bond angles



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.

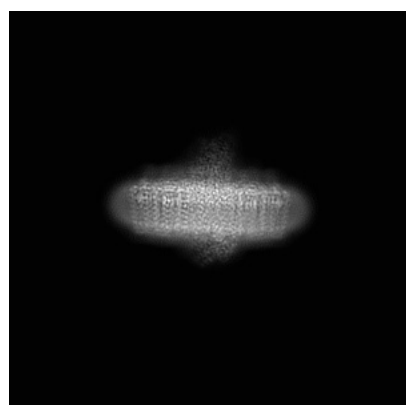
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12681. These allow visual inspection of the internal detail of the map and identification of artifacts.

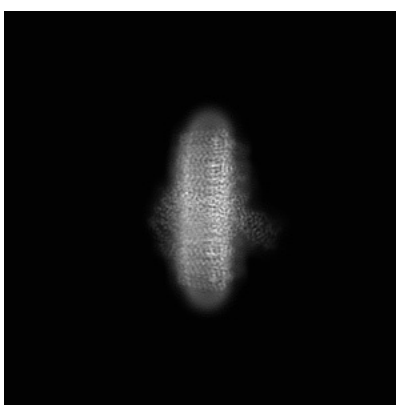
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

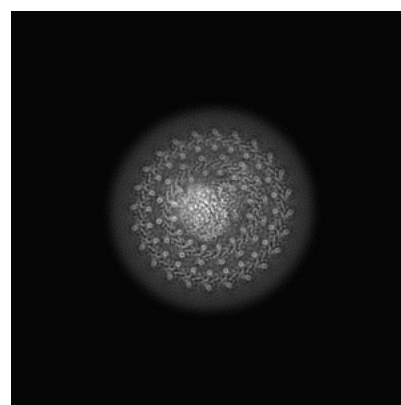
6.1.1 Primary map



X



Y

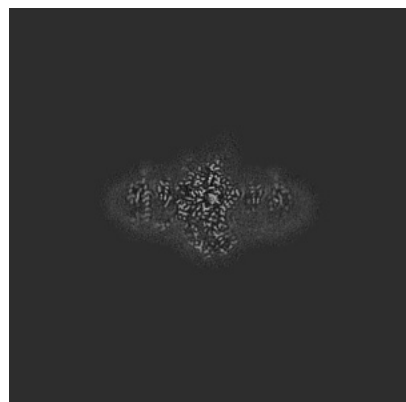


Z

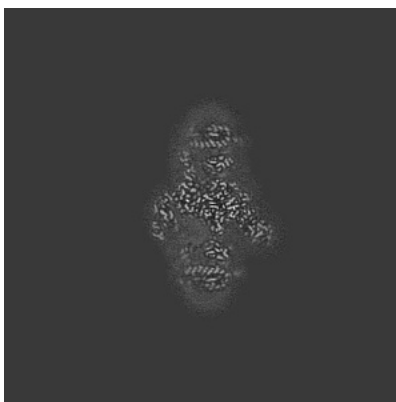
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

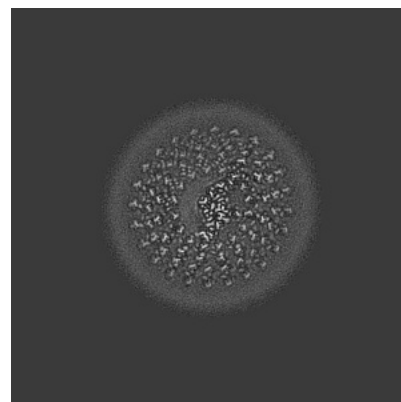
6.2.1 Primary map



X Index: 200



Y Index: 200

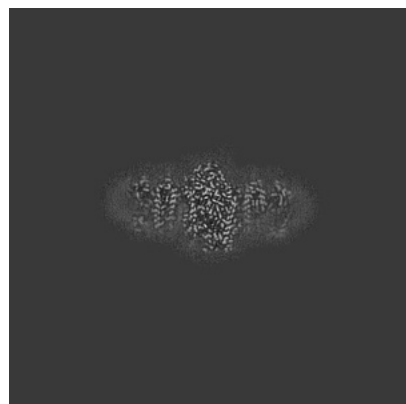


Z Index: 200

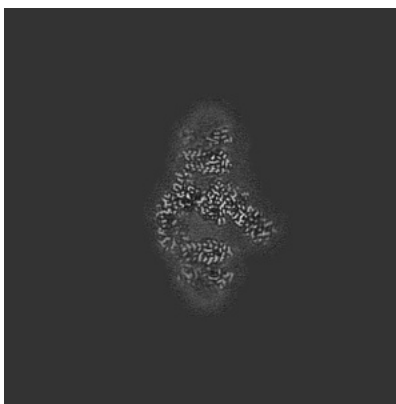
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

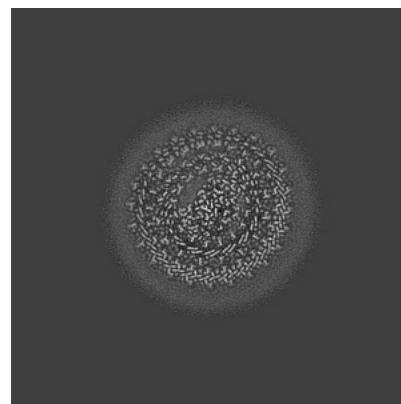
6.3.1 Primary map



X Index: 209



Y Index: 208

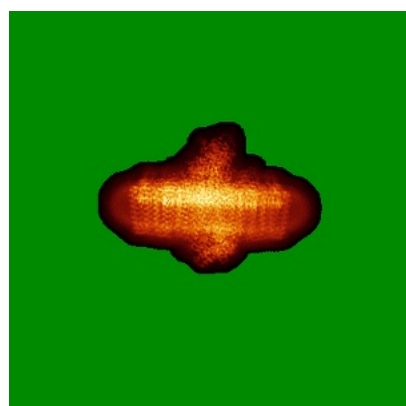


Z Index: 212

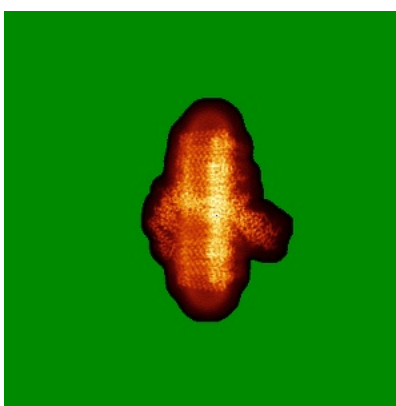
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

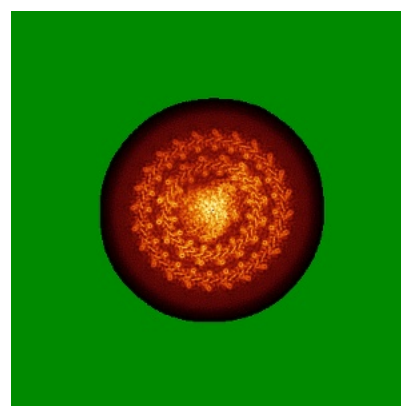
6.4.1 Primary map



X



Y

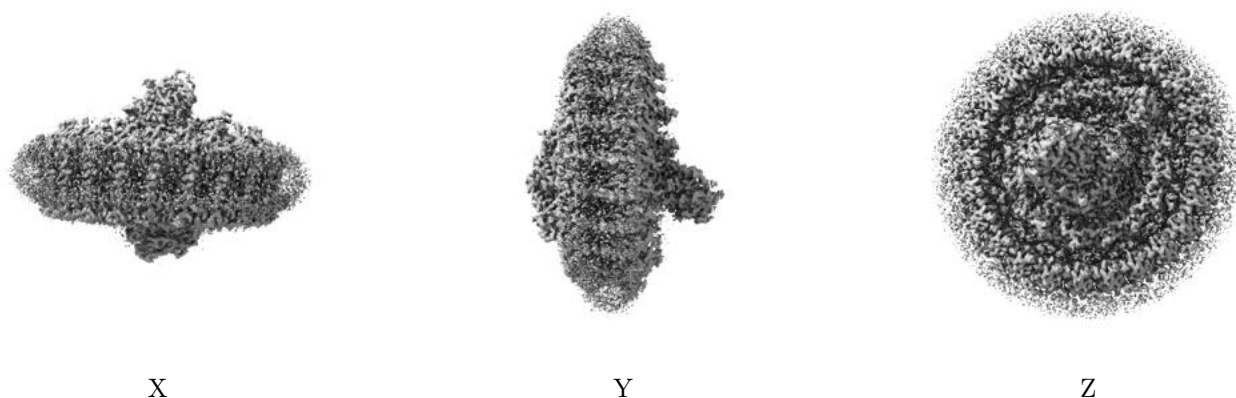


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0233. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

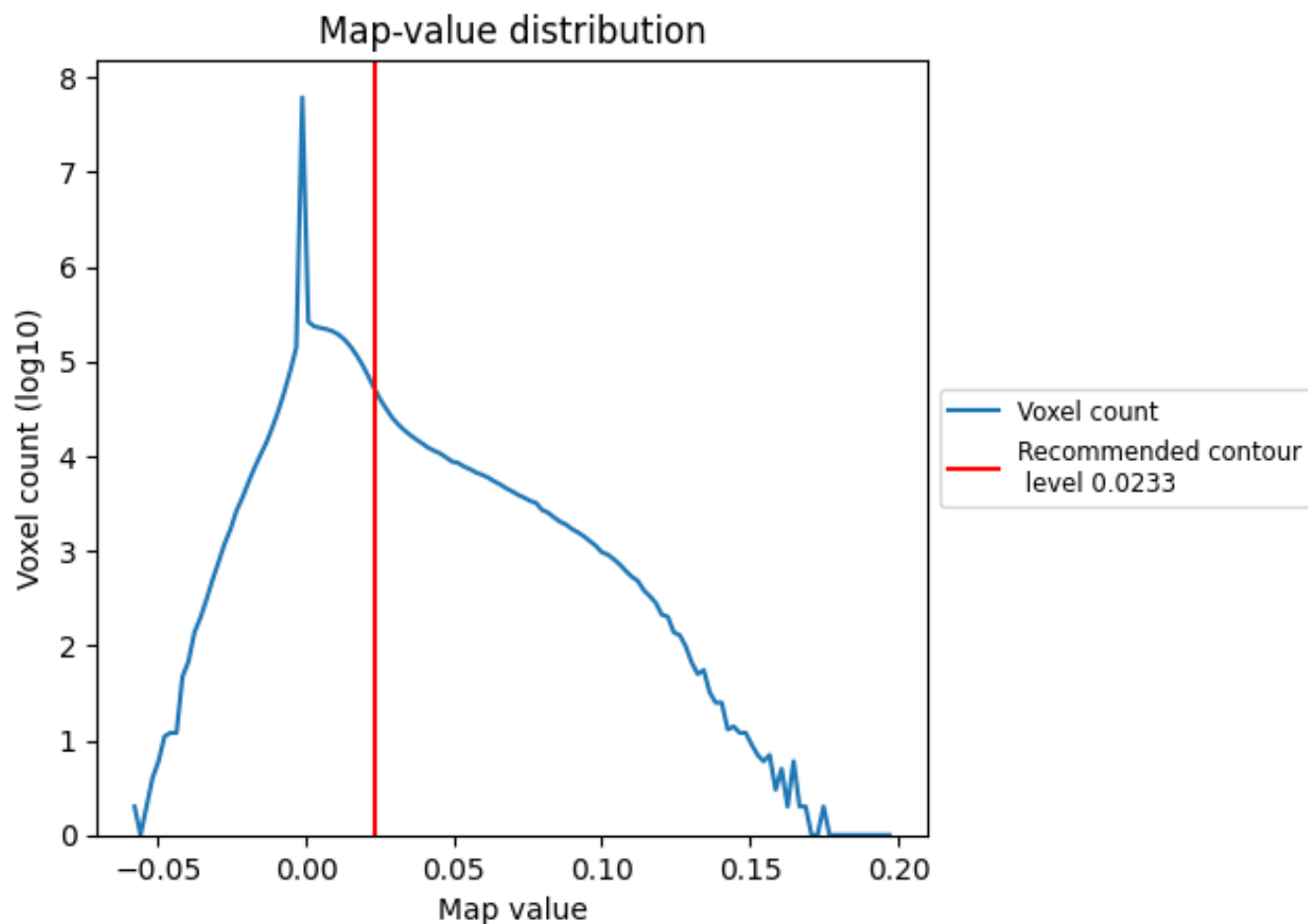
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

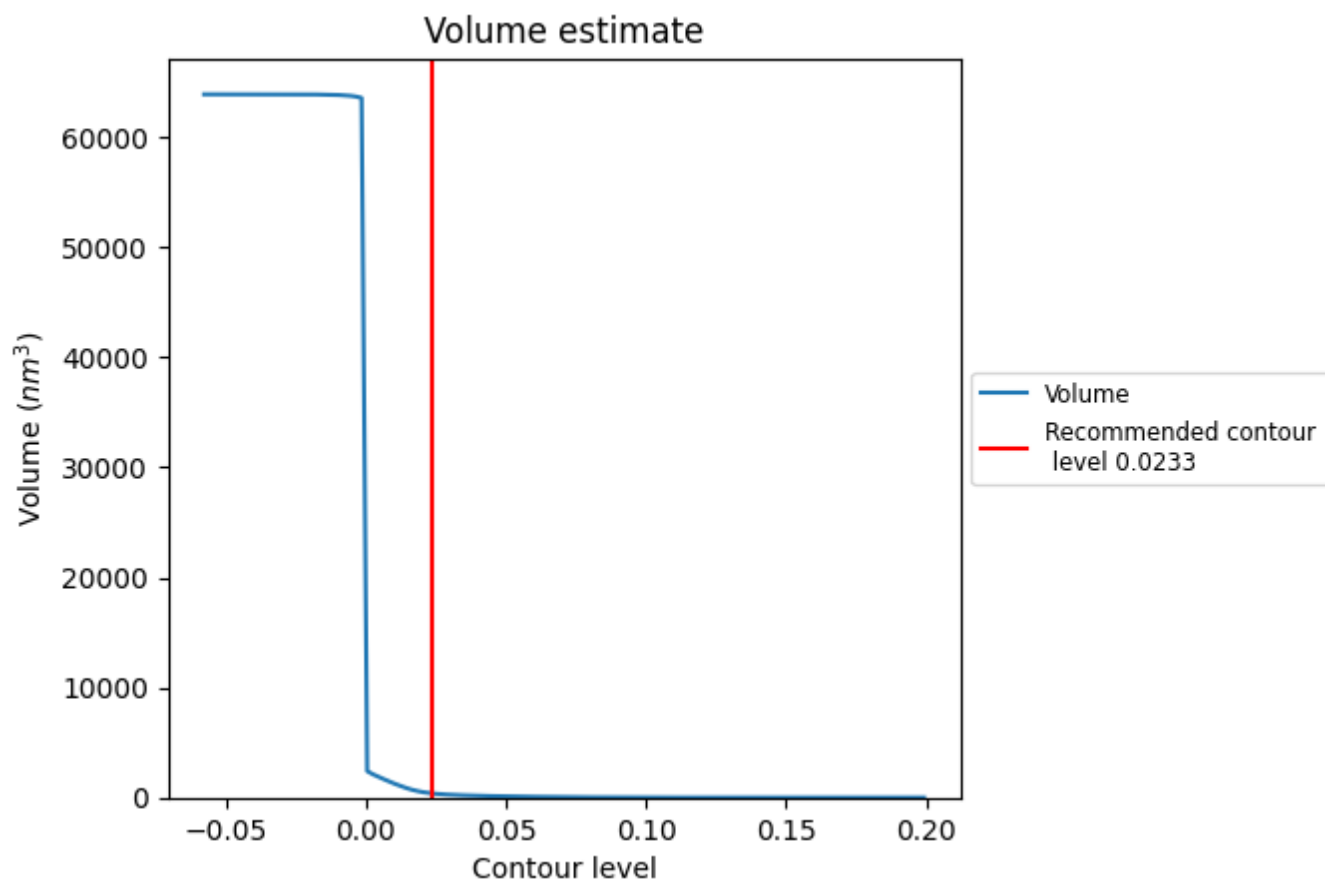
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

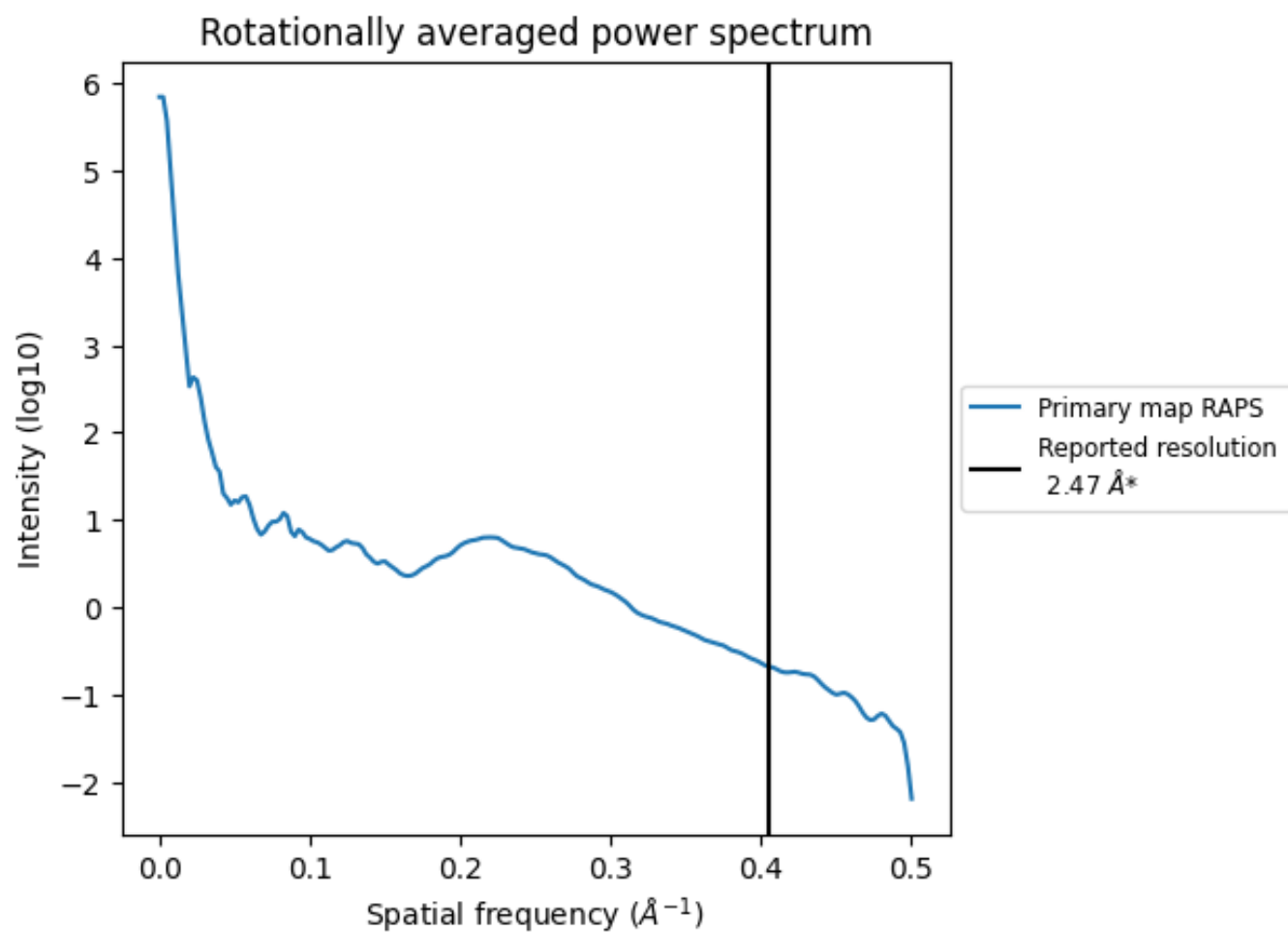
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm^3 ; this corresponds to an approximate mass of 348 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

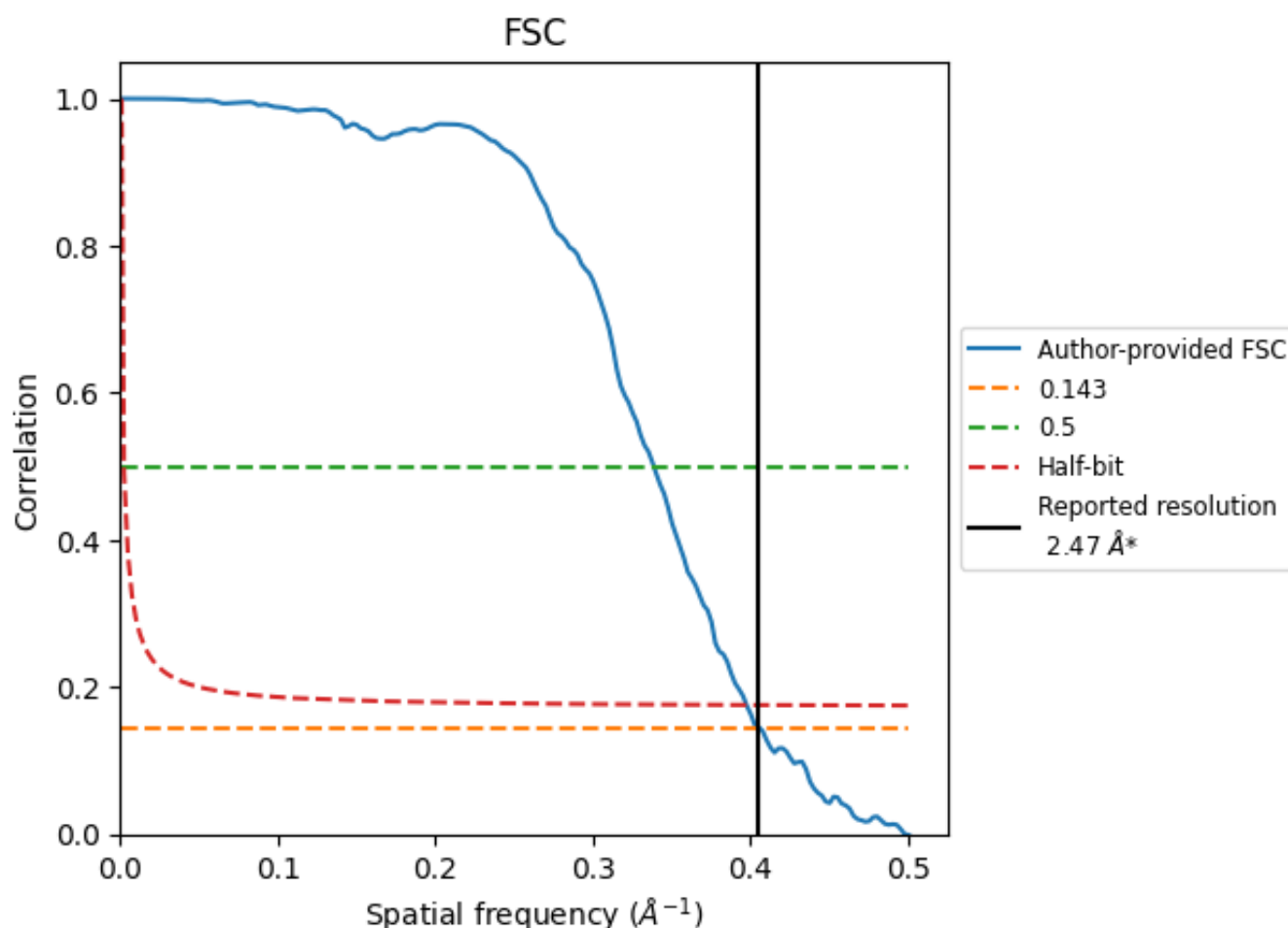


*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

8.2 Resolution estimates [i](#)

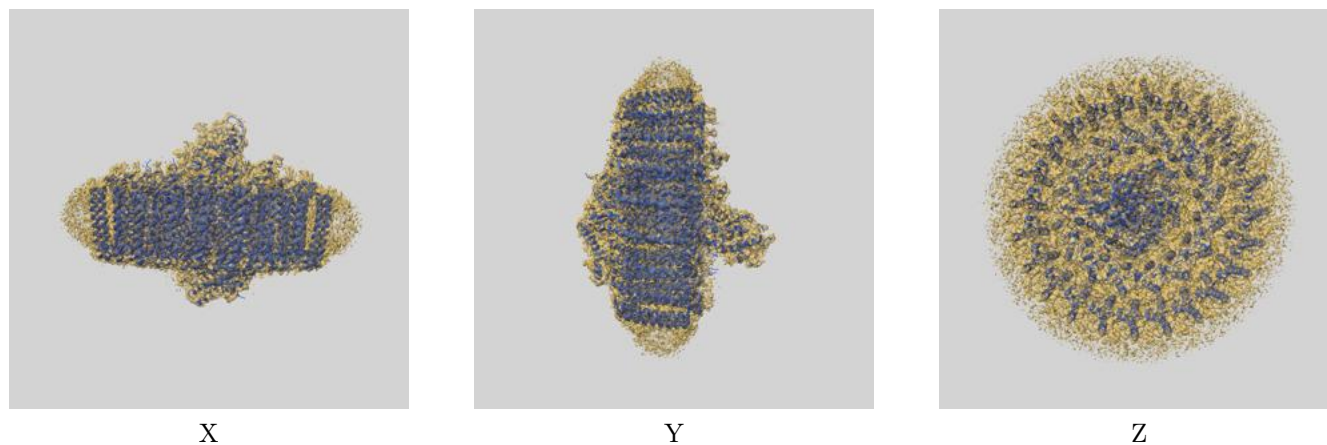
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.46	2.95	2.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

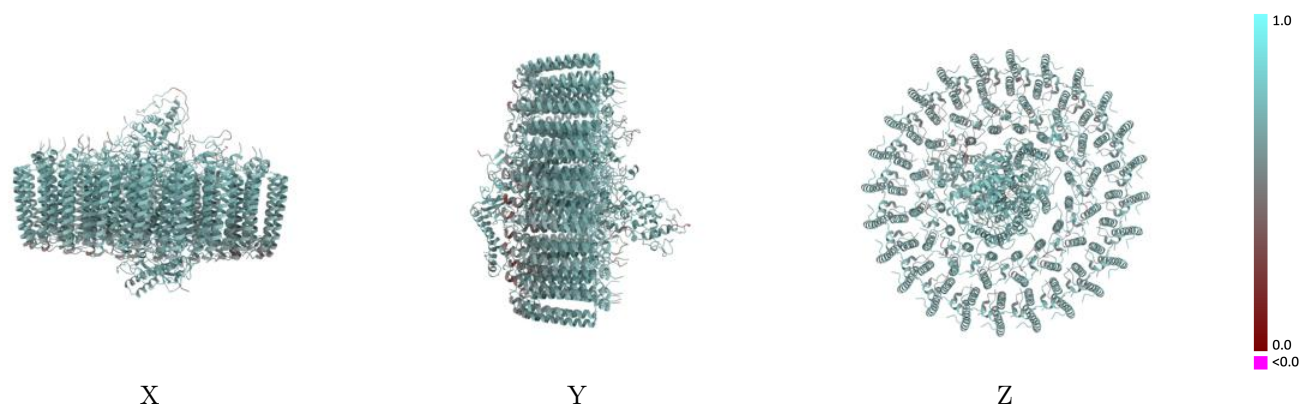
This section contains information regarding the fit between EMDB map EMD-12681 and PDB model 7O0W. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



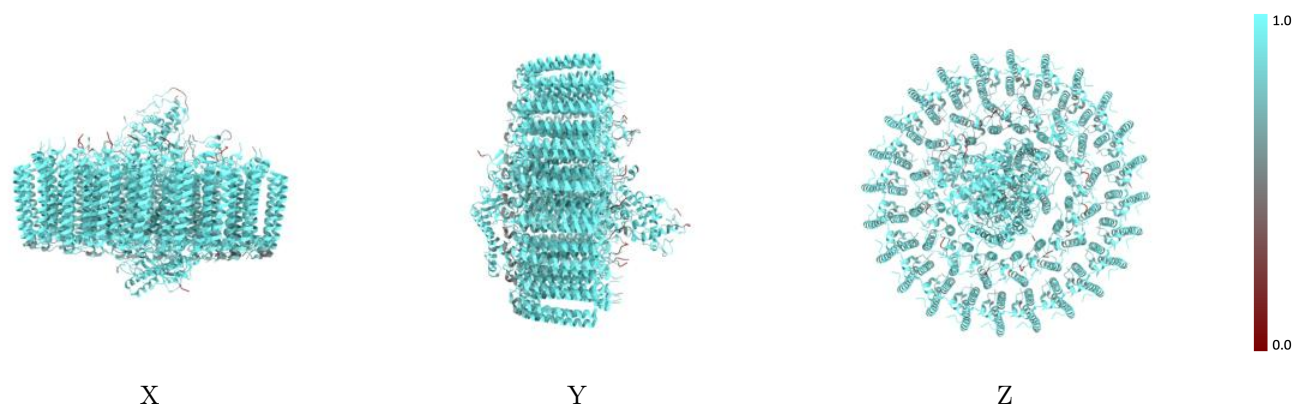
The images above show the 3D surface view of the map at the recommended contour level 0.0233 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



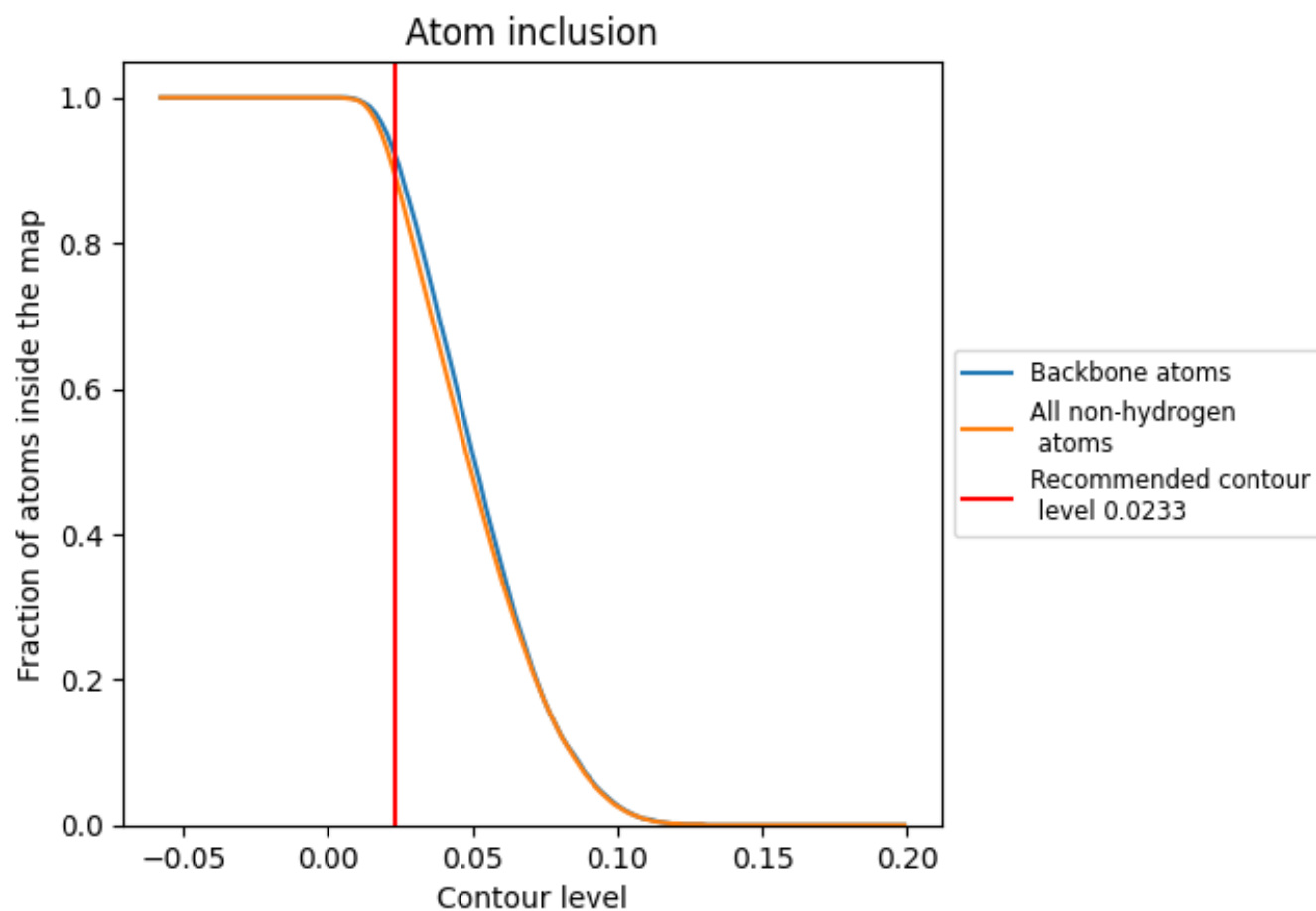
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0233).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.6240
AA	 0.8590	 0.5870
AB	 0.8510	 0.5800
AC	 0.8190	 0.5610
AD	 0.8930	 0.6190
AE	 0.8120	 0.5800
AF	 0.9480	 0.6370
AG	 0.9480	 0.6470
AH	 0.8420	 0.5970
AI	 0.9640	 0.6460
AJ	 0.9310	 0.6380
AK	 0.8930	 0.6160
AL	 0.8730	 0.6060
AM	 0.9460	 0.6460
AN	 0.9070	 0.6210
AO	 0.8760	 0.6080
AP	 0.9500	 0.6410
AQ	 0.8630	 0.6060
AR	 0.9690	 0.6490
AS	 0.9520	 0.6440
AT	 0.9240	 0.6290
AU	 0.9020	 0.6180
AV	 0.9240	 0.6210
AW	 0.9040	 0.6150
AX	 0.8010	 0.5580
BA	 0.8110	 0.5650
BB	 0.7300	 0.5280
BC	 0.7500	 0.5360
BD	 0.7940	 0.5800
BE	 0.8300	 0.5780
BF	 0.8430	 0.5850
BG	 0.8590	 0.6100
BH	 0.8470	 0.5960
BI	 0.8240	 0.5800
BJ	 0.8320	 0.5970





























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Chain	Atom inclusion	Q-score
BK	 0.8510	 0.6060
BL	 0.7970	 0.5640
BM	 0.8320	 0.5950
BN	 0.8320	 0.5890
BO	 0.8380	 0.5820
BP	 0.8350	 0.6010
BQ	 0.8500	 0.6070
BR	 0.8150	 0.5920
BS	 0.8330	 0.6020
BT	 0.8070	 0.5840
BU	 0.8410	 0.5990
BV	 0.8310	 0.5890
BW	 0.7990	 0.5780
BX	 0.7740	 0.5410
C	 0.9440	 0.6660
C1	 0.9470	 0.6680
C2	 0.9200	 0.6080
CG	 0.7620	 0.5370
H1	 0.9080	 0.6510
H2	 0.9400	 0.6490
L	 0.9740	 0.6910
M	 0.9430	 0.6760
MG	 1.0000	 0.6310
aa	 0.8320	 0.5920
ab	 0.8520	 0.5940
ac	 0.9070	 0.6260
ad	 0.9270	 0.6420
ae	 0.9340	 0.6700
af	 0.8780	 0.6230
ag	 0.9010	 0.6380
ah	 0.9030	 0.6230
ai	 0.9100	 0.6400
aj	 0.9220	 0.6500
ak	 0.9630	 0.6660
al	 0.9220	 0.6500
am	 0.9180	 0.6510
an	 0.9440	 0.6490
ao	 0.9010	 0.6270
ap	 0.8950	 0.6050
ba	 0.8640	 0.6070
bb	 0.8530	 0.5940
bc	 0.8810	 0.6240

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Chain	Atom inclusion	Q-score
bd	 0.9090	 0.6420
be	 0.9040	 0.6300
bf	 0.9250	 0.6360
bg	 0.9300	 0.6400
bh	 0.9040	 0.6190
bi	 0.9160	 0.6280
bj	 0.9200	 0.6350
bk	 0.9320	 0.6480
bl	 0.9200	 0.6290
bm	 0.9400	 0.6410
bn	 0.9100	 0.6220
bo	 0.9400	 0.6400
bp	 0.8650	 0.5860