



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:30 AM UTC

PDB ID : 7O0U / pdb_00007o0u
EMDB ID : EMD-12679
Title : Cryo-EM structure (model_1a) of the RC-dLH complex from Gemmatimonas phototrophica at 2.4 Å
Authors : Qian, P.; Koblizek, M.
Deposited on : 2021-03-27
Resolution : 2.35 Å (reported)
Based on initial models : 1LGH, 5Y5S, 6ET5

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:

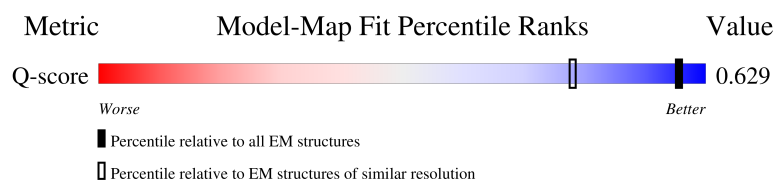
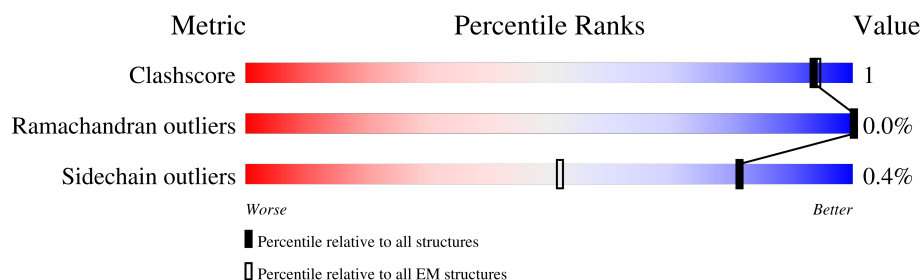
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.35 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.



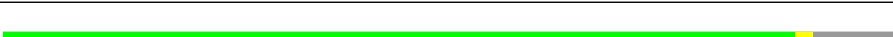
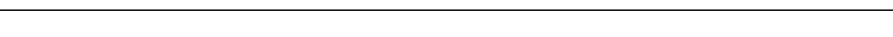
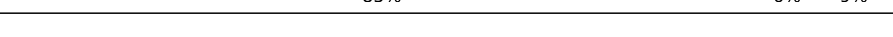
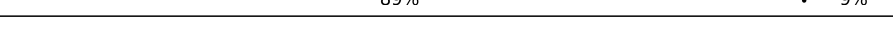
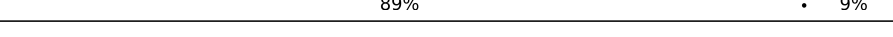
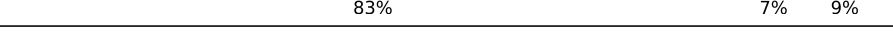
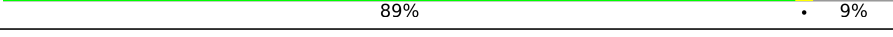
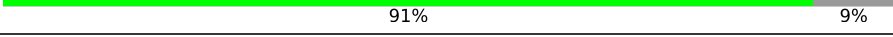
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4607 (1.85 - 2.85)

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	
1	AB	54	
1	AC	54	
1	AD	54	

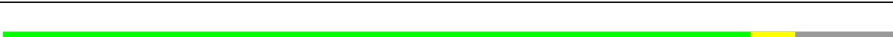
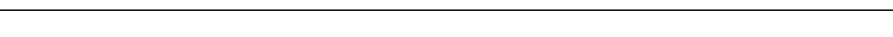
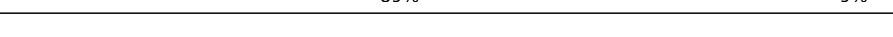
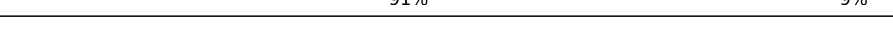
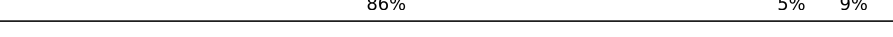
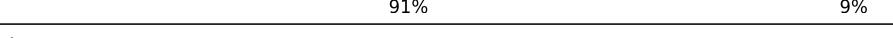
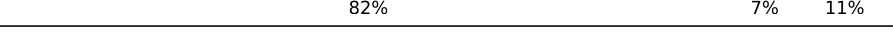
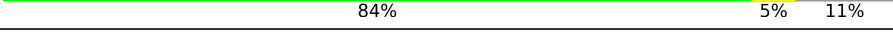
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Mol	Chain	Length	Quality of chain
1	AE	54	 89% 9%
1	AF	54	 89% 9%
1	AG	54	 89% 9%
1	AH	54	 83% 7% 9%
1	AI	54	 89% 9%
1	AJ	54	 87% 9%
1	AK	54	 87% 9%
1	AL	54	 89% 9%
1	AM	54	 87% 9%
1	AN	54	 85% 6% 9%
1	AO	54	 89% 9%
1	AP	54	 89% 9%
1	AQ	54	 87% 9%
1	AR	54	 85% 6% 9%
1	AS	54	 89% 9%
1	AT	54	 89% 9%
1	AU	54	 89% 9%
1	AV	54	 89% 9%
1	AW	54	 83% 7% 9%
1	AX	54	 89% 9%
2	BA	44	 86% 11%
2	BB	44	 91% 9%
2	BC	44	 86% 11%
2	BD	44	 91% 9%
2	BE	44	 91% 9%

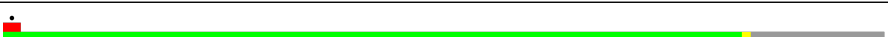
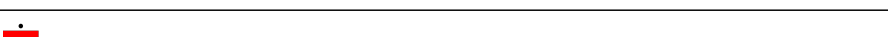
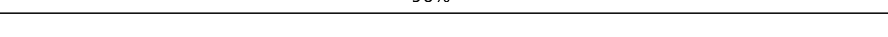
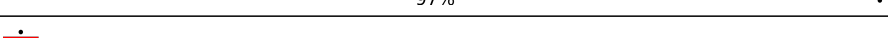
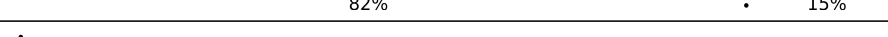
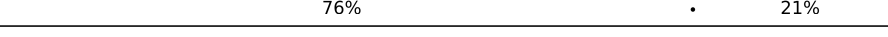
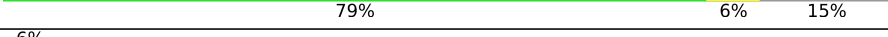
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Mol	Chain	Length	Quality of chain
2	BF	44	
2	BG	44	
2	BH	44	
2	BI	44	
2	BJ	44	
2	BK	44	
2	BL	44	
2	BM	44	
2	BN	44	
2	BO	44	
2	BP	44	
2	BQ	44	
2	BR	44	
2	BS	44	
2	BT	44	
2	BU	44	
2	BV	44	
2	BW	44	
2	BX	44	
2	ba	44	
2	bb	44	
2	bc	44	
2	bd	44	
2	be	44	
2	bf	44	

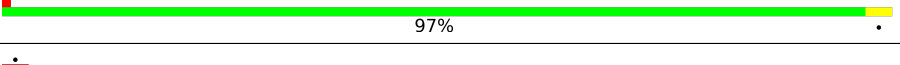
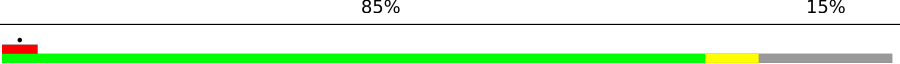
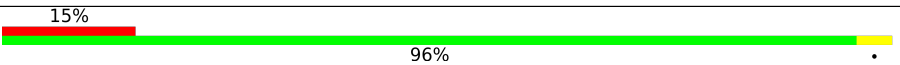
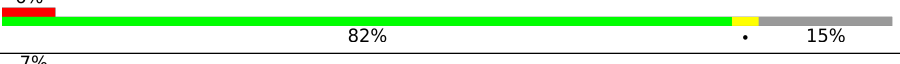
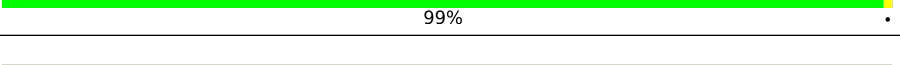
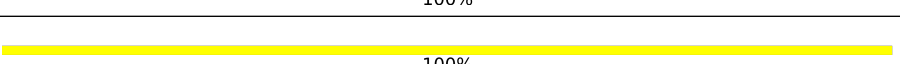
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Mol	Chain	Length	Quality of chain
2	bg	44	 86% • 11%
2	bh	44	 86% • 11%
2	bi	44	 86% • 11%
2	bj	44	 89% 11%
2	bk	44	 86% • 11%
2	bl	44	 89% 11%
2	bm	44	 89% 11%
2	bn	44	 7% 89% • 9%
2	bo	44	 89% 11%
2	bp	44	 5% 89% 11%
3	C	354	 83% • 15%
4	C1	202	 50% 49%
5	H1	67	 85% 7% 7%
6	H2	181	 96% • •
7	L	274	 97% •
8	M	367	 83% 5% 12%
9	aa	71	 6% 82% • 15%
9	ab	71	 82% • 15%
9	ac	71	 76% • 21%
9	ad	71	 79% 6% 15%
9	ae	71	 6% 79% 6% 15%
9	af	71	 77% 7% 15%
9	ag	71	 7% 82% • 15%
9	ah	71	 80% • 15%
9	ai	71	 80% • 15%

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Mol	Chain	Length	Quality of chain
9	aj	71	
9	ak	71	
9	al	71	
9	am	71	
9	an	71	
9	ao	71	
9	ap	71	
10	CG	2	
10	MG	2	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 55758 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	301	Total	C	N	O	S	0	0
			2337	1470	421	427	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 PRCH domain-containing protein.

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

- Molecule 6 is a protein called RC-Hc.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H2	176	Total	C	N	O	S	0	0
			1371	872	234	261	4		

- Molecule 7 is a protein called Photosynthetic reaction center L subunit.

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

- Molecule 8 is a protein called RC-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	323	Total	C	N	O	S	0	0
			2611	1741	427	432	11		

- Molecule 9 is a protein called LHC domain-containing protein.

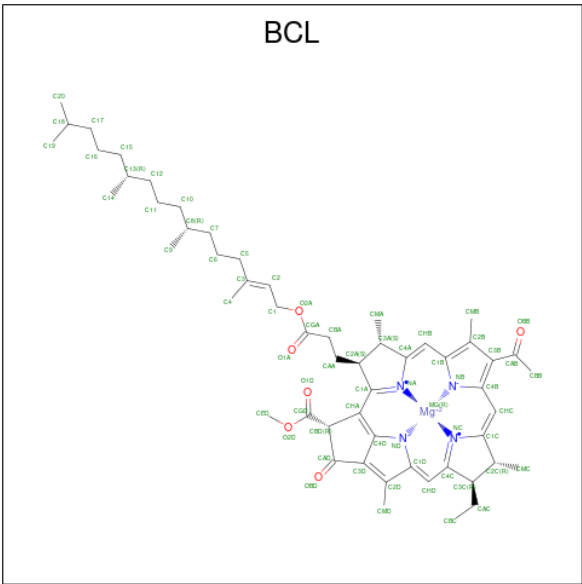
Mol	Chain	Residues	Atoms					AltConf	Trace
9	aa	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ab	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ac	56	Total	C	N	O	S	0	0
			443	290	77	73	3		
9	ad	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ae	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	af	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ag	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ah	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ai	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	aj	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ak	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
9	al	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	am	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	an	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
9	ao	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
9	ap	71	Total	C	N	O	S	0	0
			543	352	95	92	4		

- Molecule 10 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose.



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

- Molecule 11 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	AA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	AC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
11	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BH	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BO	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BP	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BR	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BS	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BT	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BU	1	Total 66	C 55	Mg 1	N 4	O 6	0

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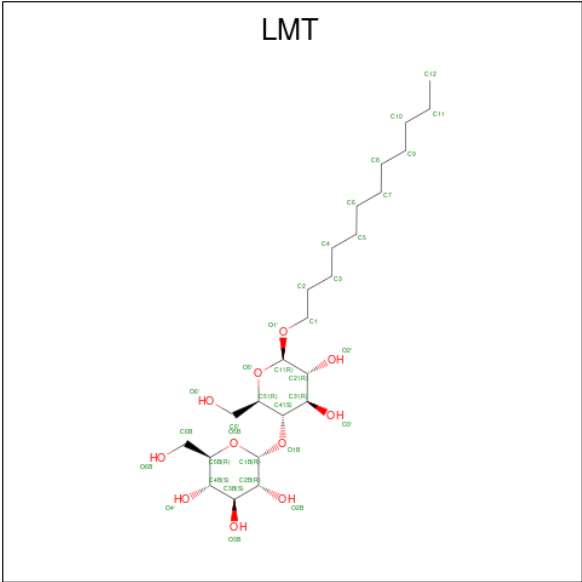
Mol	Chain	Residues	Atoms					AltConf
11	BV	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BW	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BX	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	aa	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ai	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	aj	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ak	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	al	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	am	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	an	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	ao	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ap	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	ba	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bb	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bc	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bd	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	be	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bf	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bg	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bh	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bi	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bj	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bk	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bl	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bm	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bn	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bo	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	bp	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 12 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
12	AA	1	Total	C	O	0
			35	24	11	
12	AB	1	Total	C	O	0
			35	24	11	
12	AD	1	Total	C	O	0
			35	24	11	
12	AE	1	Total	C	O	0
			35	24	11	
12	AE	1	Total	C	O	0
			35	24	11	
12	AG	1	Total	C	O	0
			35	24	11	
12	AH	1	Total	C	O	0
			35	24	11	
12	AH	1	Total	C	O	0
			35	24	11	
12	AI	1	Total	C	O	0
			35	24	11	
12	AJ	1	Total	C	O	0
			35	24	11	
12	AK	1	Total	C	O	0
			35	24	11	
12	AK	1	Total	C	O	0
			35	24	11	
12	AL	1	Total	C	O	0
			35	24	11	
12	AL	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
12	AM	1	Total 35	C 24	O 11	0
12	AN	1	Total 35	C 24	O 11	0
12	AN	1	Total 35	C 24	O 11	0
12	AP	1	Total 35	C 24	O 11	0
12	AQ	1	Total 35	C 24	O 11	0
12	AR	1	Total 35	C 24	O 11	0
12	AS	1	Total 35	C 24	O 11	0
12	AT	1	Total 35	C 24	O 11	0
12	AT	1	Total 35	C 24	O 11	0
12	AV	1	Total 35	C 24	O 11	0
12	AW	1	Total 35	C 24	O 11	0
12	BA	1	Total 35	C 24	O 11	0
12	BA	1	Total 35	C 24	O 11	0
12	BA	1	Total 35	C 24	O 11	0
12	BA	1	Total 35	C 24	O 11	0
12	BB	1	Total 35	C 24	O 11	0
12	BB	1	Total 35	C 24	O 11	0
12	BB	1	Total 35	C 24	O 11	0
12	BC	1	Total 35	C 24	O 11	0
12	BC	1	Total 35	C 24	O 11	0
12	BC	1	Total 35	C 24	O 11	0

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Mol	Chain	Residues	Atoms			AltConf
12	BD	1	Total	C	O	0
			35	24	11	
12	BD	1	Total	C	O	0
			35	24	11	
12	BD	1	Total	C	O	0
			35	24	11	
12	BD	1	Total	C	O	0
			35	24	11	
12	BE	1	Total	C	O	0
			35	24	11	
12	BE	1	Total	C	O	0
			35	24	11	
12	BF	1	Total	C	O	0
			35	24	11	
12	BF	1	Total	C	O	0
			35	24	11	
12	BF	1	Total	C	O	0
			35	24	11	
12	BG	1	Total	C	O	0
			35	24	11	
12	BG	1	Total	C	O	0
			35	24	11	
12	BG	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	BJ	1	Total	C	O	0
			35	24	11	
12	BJ	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
12	BK	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BL	1	Total	C	O	0
			35	24	11	
12	BL	1	Total	C	O	0
			35	24	11	
12	BL	1	Total	C	O	0
			35	24	11	
12	BL	1	Total	C	O	0
			35	24	11	
12	BM	1	Total	C	O	0
			35	24	11	
12	BM	1	Total	C	O	0
			35	24	11	
12	BM	1	Total	C	O	0
			35	24	11	
12	BN	1	Total	C	O	0
			35	24	11	
12	BN	1	Total	C	O	0
			35	24	11	
12	BN	1	Total	C	O	0
			35	24	11	
12	BO	1	Total	C	O	0
			35	24	11	
12	BO	1	Total	C	O	0
			35	24	11	
12	BO	1	Total	C	O	0
			35	24	11	
12	BP	1	Total	C	O	0
			35	24	11	
12	BP	1	Total	C	O	0
			35	24	11	
12	BP	1	Total	C	O	0
			35	24	11	
12	BQ	1	Total	C	O	0
			35	24	11	
12	BQ	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
12	BR	1	Total 35	C 24	O 11	0
12	BR	1	Total 35	C 24	O 11	0
12	BR	1	Total 35	C 24	O 11	0
12	BS	1	Total 35	C 24	O 11	0
12	BS	1	Total 35	C 24	O 11	0
12	BS	1	Total 35	C 24	O 11	0
12	BS	1	Total 35	C 24	O 11	0
12	BT	1	Total 35	C 24	O 11	0
12	BT	1	Total 35	C 24	O 11	0
12	BT	1	Total 35	C 24	O 11	0
12	BU	1	Total 35	C 24	O 11	0
12	BU	1	Total 35	C 24	O 11	0
12	BU	1	Total 35	C 24	O 11	0
12	BV	1	Total 35	C 24	O 11	0
12	BV	1	Total 35	C 24	O 11	0
12	BV	1	Total 35	C 24	O 11	0
12	BW	1	Total 35	C 24	O 11	0
12	BW	1	Total 35	C 24	O 11	0
12	BX	1	Total 35	C 24	O 11	0
12	BX	1	Total 35	C 24	O 11	0
12	H2	1	Total 35	C 24	O 11	0

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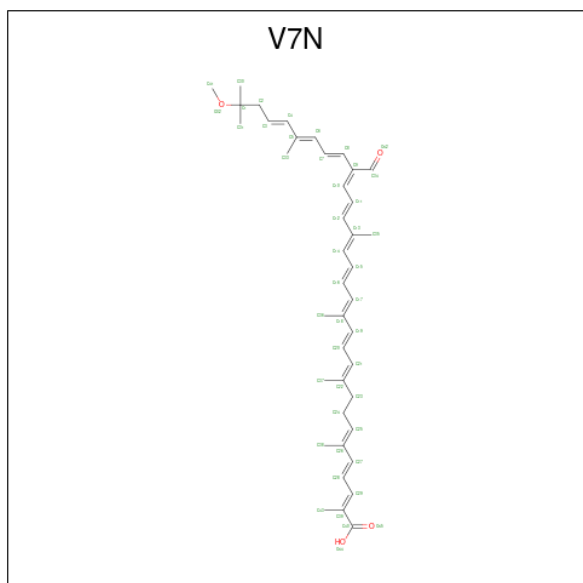
Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	M	1	Total	C	O	0
			35	24	11	
12	ac	1	Total	C	O	0
			35	24	11	
12	ba	1	Total	C	O	0
			35	24	11	
12	bb	1	Total	C	O	0
			35	24	11	
12	bc	1	Total	C	O	0
			35	24	11	
12	bd	1	Total	C	O	0
			35	24	11	
12	be	1	Total	C	O	0
			35	24	11	
12	be	1	Total	C	O	0
			35	24	11	
12	bf	1	Total	C	O	0
			35	24	11	
12	bg	1	Total	C	O	0
			35	24	11	
12	bi	1	Total	C	O	0
			35	24	11	
12	bi	1	Total	C	O	0
			35	24	11	
12	bj	1	Total	C	O	0
			35	24	11	
12	bk	1	Total	C	O	0
			35	24	11	
12	bl	1	Total	C	O	0
			35	24	11	
12	bm	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
12	bn	1	Total	C	O	0
			35	24	11	
12	bo	1	Total	C	O	0
			35	24	11	
12	bo	1	Total	C	O	0
			35	24	11	
12	bp	1	Total	C	O	0
			35	24	11	

- Molecule 13 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-dotriacont-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (CCD ID: V7N) (formula: C₄₁H₅₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	AB	1	Total	C	O	0
			45	41	4	
13	AE	1	Total	C	O	0
			45	41	4	
13	AE	1	Total	C	O	0
			45	41	4	
13	AH	1	Total	C	O	0
			45	41	4	
13	AQ	1	Total	C	O	0
			45	41	4	
13	AT	1	Total	C	O	0
			45	41	4	

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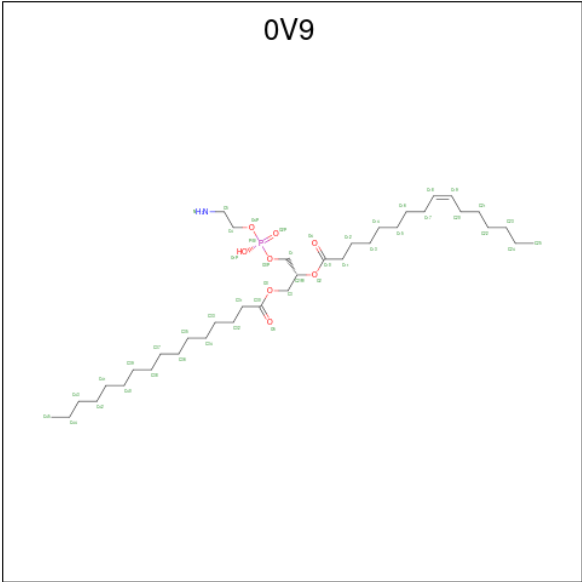
Mol	Chain	Residues	Atoms			AltConf
13	AW	1	Total 45	C 41	O 4	0
13	BB	1	Total 45	C 41	O 4	0
13	BC	1	Total 45	C 41	O 4	0
13	BE	1	Total 45	C 41	O 4	0
13	BG	1	Total 45	C 41	O 4	0
13	BH	1	Total 45	C 41	O 4	0
13	BJ	1	Total 45	C 41	O 4	0
13	BK	1	Total 45	C 41	O 4	0
13	BL	1	Total 45	C 41	O 4	0
13	BM	1	Total 45	C 41	O 4	0
13	BN	1	Total 45	C 41	O 4	0
13	BO	1	Total 45	C 41	O 4	0
13	BP	1	Total 45	C 41	O 4	0
13	BQ	1	Total 45	C 41	O 4	0
13	BS	1	Total 45	C 41	O 4	0
13	BT	1	Total 45	C 41	O 4	0
13	BV	1	Total 45	C 41	O 4	0
13	BW	1	Total 45	C 41	O 4	0
13	af	1	Total 45	C 41	O 4	0
13	aj	1	Total 45	C 41	O 4	0
13	ba	1	Total 45	C 41	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
13	bb	1	Total	C	O	0
			45	41	4	
13	bc	1	Total	C	O	0
			45	41	4	
13	bd	1	Total	C	O	0
			45	41	4	
13	be	1	Total	C	O	0
			45	41	4	
13	bf	1	Total	C	O	0
			45	41	4	
13	bh	1	Total	C	O	0
			45	41	4	
13	bi	1	Total	C	O	0
			45	41	4	
13	bj	1	Total	C	O	0
			45	41	4	
13	bl	1	Total	C	O	0
			45	41	4	
13	bm	1	Total	C	O	0
			45	41	4	
13	bn	1	Total	C	O	0
			45	41	4	
13	bo	1	Total	C	O	0
			45	41	4	
13	bp	1	Total	C	O	0
			45	41	4	

- Molecule 14 is (19R,22S)-25-amino-22-hydroxy-22-oxido-16-oxo-17,21,23-trioxa-22lambda 5-phosphapentacosan-19-yl (9Z)-hexadec-9-enoate (CCD ID: 0V9) (formula: C₃₇H₇₂NO₈P).



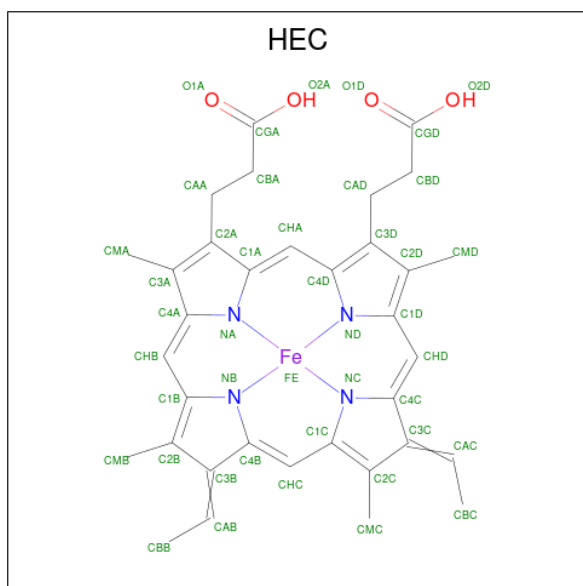
Mol	Chain	Residues	Atoms					AltConf
14	AJ	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	AQ	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	H1	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	aj	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bb	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bb	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bc	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bd	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	be	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bf	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bi	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bi	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bj	1	Total	C	N	O	P	0
			45	35	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
14	bk	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bl	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bm	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bn	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bo	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	bp	1	Total	C	N	O	P	0
			45	35	1	8	1	

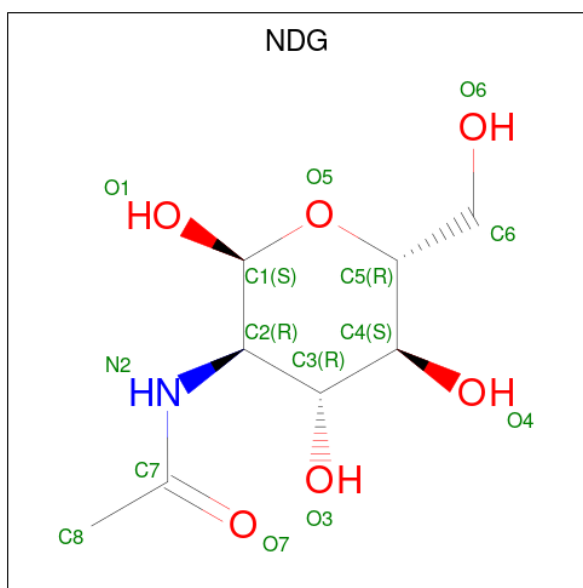
- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

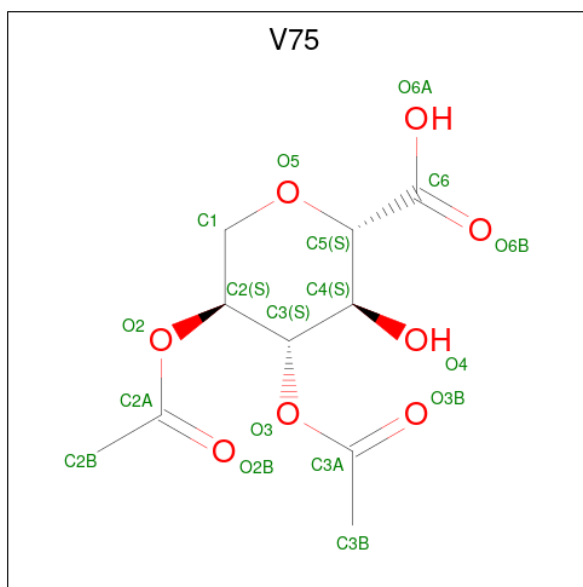
- Molecule 16 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (CCD ID: NDG) (formula:

C₈H₁₅NO₆).



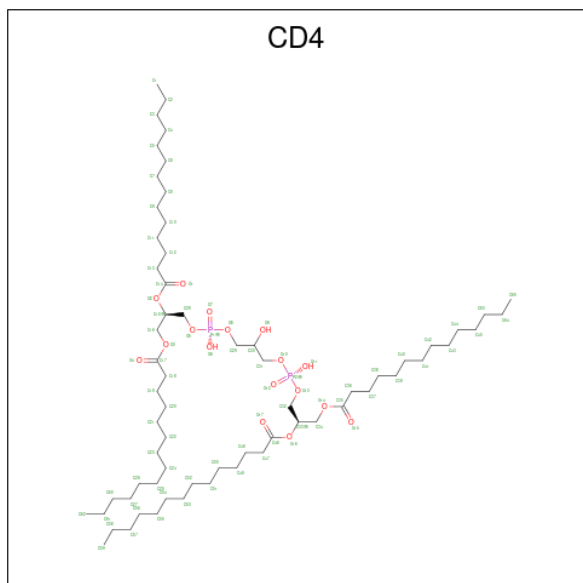
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
16	C	1	14	8	1	5	0
16	C1	1	14	8	1	5	0

- Molecule 17 is (2 {S},3 {S},4 {S},5 {S})-4,5-diacetyloxy-3-oxidanyl-oxane-2-carboxylic acid (CCD ID: V75) (formula: C₁₀H₁₄O₈).



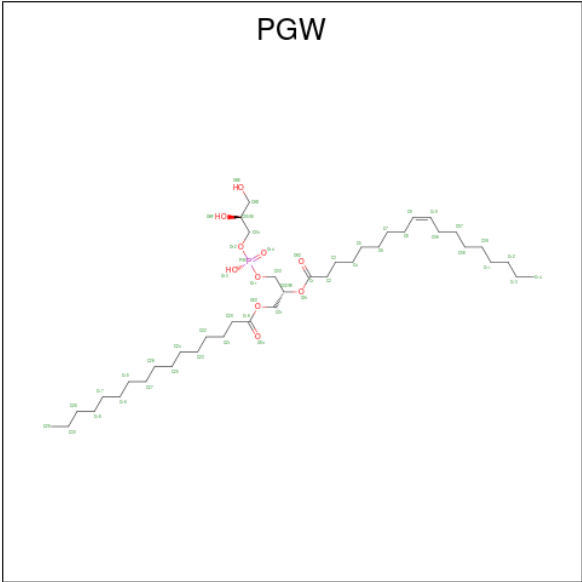
Mol	Chain	Residues	Atoms			AltConf
17	C	1	Total	C	O	0
			18	10	8	
17	M	1	Total	C	O	0
			18	10	8	

- Molecule 18 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriciacont-1-yl tetradecanoate (CCD ID: CD4) (formula: $C_{65}H_{126}O_{17}P_2$).



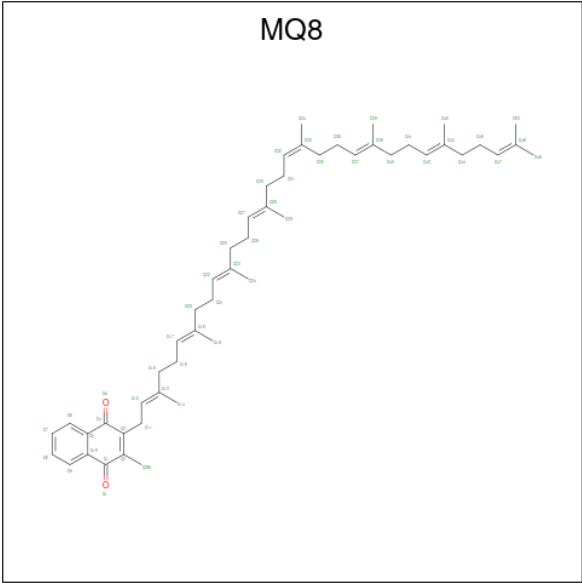
Mol	Chain	Residues	Atoms				AltConf
18	H1	1	Total	C	O	P	0
			84	65	17	2	
18	M	1	Total	C	O	P	0
			84	65	17	2	
18	M	1	Total	C	O	P	0
			84	65	17	2	
18	ad	1	Total	C	O	P	0
			84	65	17	2	
18	ae	1	Total	C	O	P	0
			84	65	17	2	
18	ag	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 19 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: $C_{40}H_{77}O_{10}P$).



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

- Molecule 20 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂) (labeled as "Ligand of Interest" by depositor).



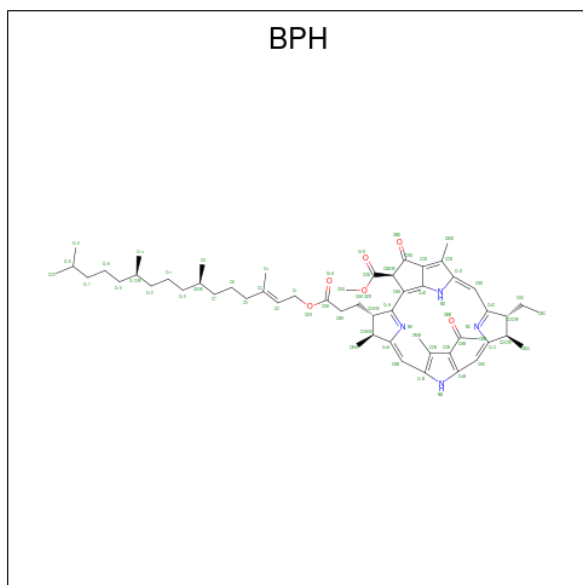
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	L	1	53	51	2	0
20	M	1	53	51	2	0

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Mol	Chain	Residues	Atoms			AltConf
20	ao	1	Total	C	O	0
			53	51	2	

- Molecule 21 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

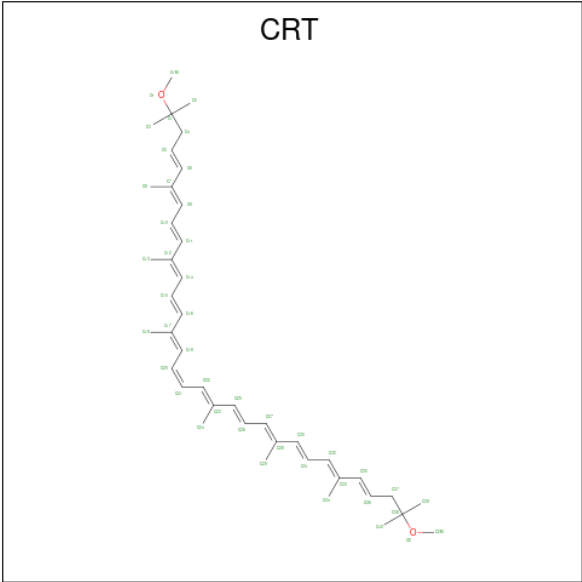


Mol	Chain	Residues	Atoms				AltConf
21	L	1	Total	C	N	O	0
			65	55	4	6	
21	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 22 is FE (III) ION (CCD ID: FE) (formula: Fe).

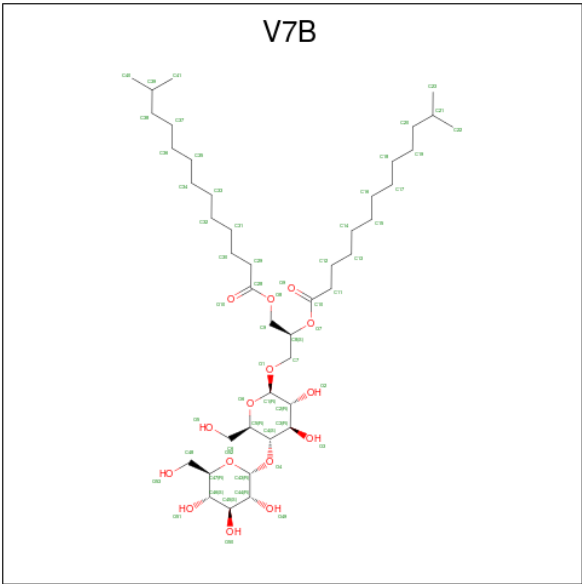
Mol	Chain	Residues	Atoms		AltConf
22	M	1	Total	Fe	0
			1	1	

- Molecule 23 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 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 (CCD ID: V7B) (formula: C₄₃H₈₀O₁₅).



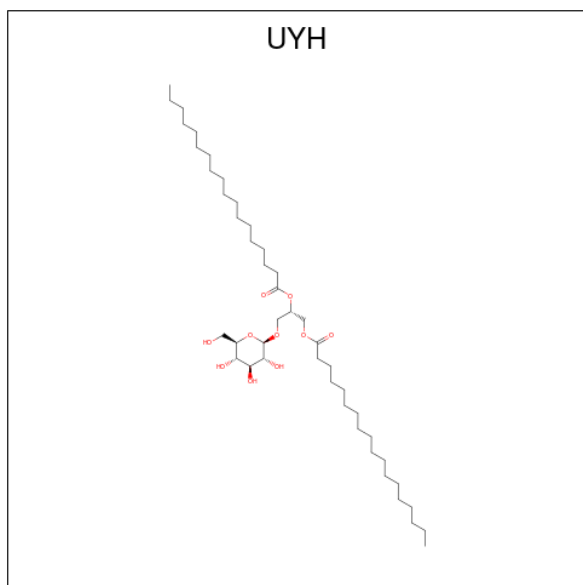
Mol	Chain	Residues	Atoms			AltConf
24	af	1	Total	C	O	0
			58	43	15	

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

- Molecule 25 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 (CCD ID: UYH) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	AA	4	Total	O	0
			4	4	
26	AB	3	Total	O	0
			3	3	
26	AC	1	Total	O	0
			1	1	
26	AD	2	Total	O	0
			2	2	
26	AF	1	Total	O	0
			1	1	
26	AG	6	Total	O	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
26	AH	5	Total 5	O 5	0
26	AI	1	Total 1	O 1	0
26	AJ	6	Total 6	O 6	0
26	AK	4	Total 4	O 4	0
26	AL	1	Total 1	O 1	0
26	AM	2	Total 2	O 2	0
26	AN	3	Total 3	O 3	0
26	AO	1	Total 1	O 1	0
26	AP	3	Total 3	O 3	0
26	AQ	4	Total 4	O 4	0
26	AR	1	Total 1	O 1	0
26	AS	4	Total 4	O 4	0
26	AT	2	Total 2	O 2	0
26	AU	1	Total 1	O 1	0
26	AV	4	Total 4	O 4	0
26	AW	2	Total 2	O 2	0
26	AX	1	Total 1	O 1	0
26	BG	1	Total 1	O 1	0
26	C	82	Total 82	O 82	0
26	C1	35	Total 35	O 35	0
26	H1	9	Total 9	O 9	0

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Mol	Chain	Residues	Atoms		AltConf
26	H2	8	Total 8	O 8	0
26	L	47	Total 47	O 47	0
26	M	59	Total 59	O 59	0
26	aa	5	Total 5	O 5	0
26	ab	5	Total 5	O 5	0
26	ac	6	Total 6	O 6	0
26	ad	10	Total 10	O 10	0
26	ae	14	Total 14	O 14	0
26	af	10	Total 10	O 10	0
26	ag	11	Total 11	O 11	0
26	ah	5	Total 5	O 5	0
26	ai	5	Total 5	O 5	0
26	aj	8	Total 8	O 8	0
26	ak	16	Total 16	O 16	0
26	al	11	Total 11	O 11	0
26	am	10	Total 10	O 10	0
26	an	10	Total 10	O 10	0
26	ao	5	Total 5	O 5	0
26	ap	5	Total 5	O 5	0
26	ba	1	Total 1	O 1	0
26	bb	2	Total 2	O 2	0

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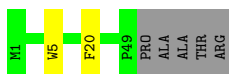
Mol	Chain	Residues	Atoms		AltConf
26	bc	3	Total 3	O 3	0
26	bd	5	Total 5	O 5	0
26	be	6	Total 6	O 6	0
26	bf	2	Total 2	O 2	0
26	bg	3	Total 3	O 3	0
26	bh	4	Total 4	O 4	0
26	bi	3	Total 3	O 3	0
26	bj	1	Total 1	O 1	0
26	bk	5	Total 5	O 5	0
26	bl	2	Total 2	O 2	0
26	bm	5	Total 5	O 5	0
26	bn	3	Total 3	O 3	0
26	bo	5	Total 5	O 5	0
26	bp	2	Total 2	O 2	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.

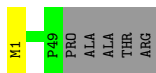
- Molecule 1: LHh-alpha

Chain AA:  87% 9%



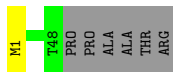
- Molecule 1: LHh-alpha

Chain AB:  89% 9%



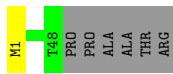
- Molecule 1: LHh-alpha

Chain AC:  87% 11%



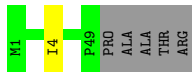
- Molecule 1: LHh-alpha

Chain AD:  87% 11%



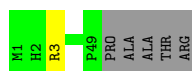
- Molecule 1: LHh-alpha

Chain AE:  89% 9%



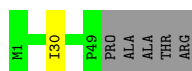
- Molecule 1: LHh-alpha

Chain AF:  89% 9%



• Molecule 1: LHh-alpha

Chain AG:  89% 9%



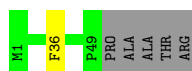
• Molecule 1: LHh-alpha

Chain AH:  83% 7% 9%



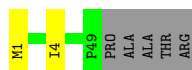
• Molecule 1: LHh-alpha

Chain AI:  89% 9%



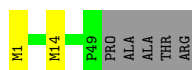
• Molecule 1: LHh-alpha

Chain AJ:  87% 9%



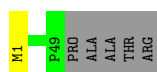
• Molecule 1: LHh-alpha

Chain AK:  87% 9%



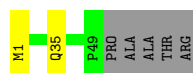
• Molecule 1: LHh-alpha

Chain AL:  89% 9%



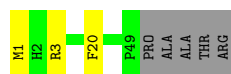
• Molecule 1: LHh-alpha

Chain AM:  87% • 9%



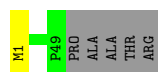
• Molecule 1: LHh-alpha

Chain AN:  85% 6% 9%



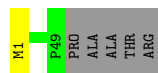
• Molecule 1: LHh-alpha

Chain AO:  89% • 9%



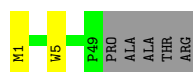
• Molecule 1: LHh-alpha

Chain AP:  89% • 9%



• Molecule 1: LHh-alpha

Chain AQ:  87% • 9%



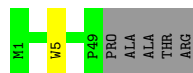
• Molecule 1: LHh-alpha

Chain AR:  85% 6% 9%



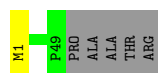
• Molecule 1: LHh-alpha

Chain AS:  89% • 9%



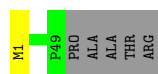
• Molecule 1: LHh-alpha

Chain AT:  89% 9%



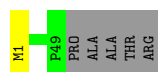
- Molecule 1: LHh-alpha

Chain AU:  89% 9%



- Molecule 1: LHh-alpha

Chain AV:  89% 9%



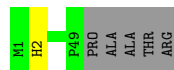
- Molecule 1: LHh-alpha

Chain AW:  83% 7% 9%



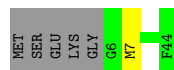
- Molecule 1: LHh-alpha

Chain AX:  89% 9%



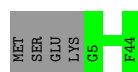
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BA:  86% 11%



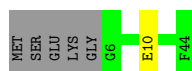
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BB:  91% 9%



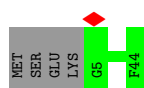
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BC:  86% 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%



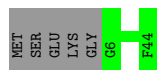
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BF:  84% 5% 11%



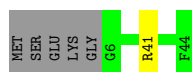
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BG:  89% 11%



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

Chain BH:  86% 11%



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

Chain BI:  89% 9%



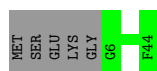
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BJ:  89% 11%



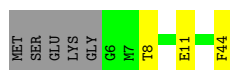
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BK:  89% 11%



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

Chain BL:  82% 7% 11%



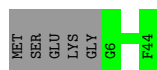
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BM:  89% 11%



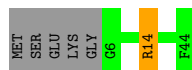
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BN:  89% 11%



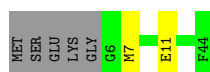
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BO:  86% • 11%



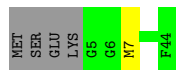
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BP:  84% 5% 11%



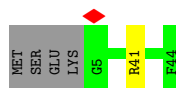
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BQ:  89% 9%



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

Chain BR:  89% 9%



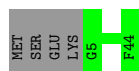
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BS:  89% 9%



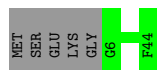
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BT:  91% 9%



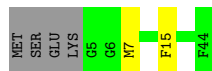
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BU:  89% 11%



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

Chain BV:  86% 5% 9%

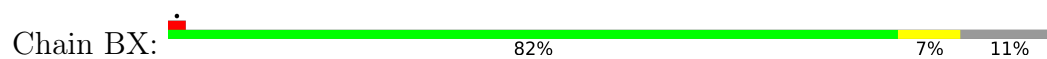


- Molecule 2: Light-harvesting protein B:885 subunit beta

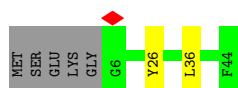
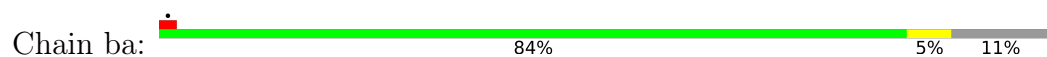
Chain BW:  91% 9%



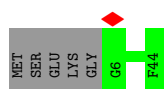
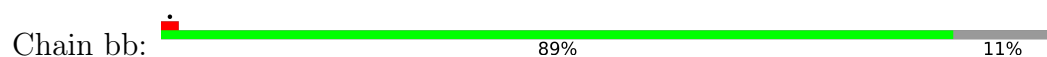
- Molecule 2: Light-harvesting protein B:885 subunit beta



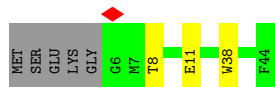
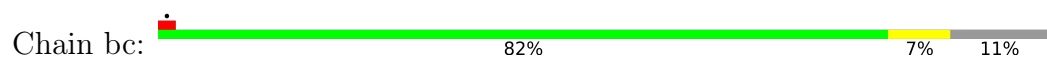
- Molecule 2: Light-harvesting protein B:885 subunit beta



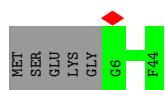
- Molecule 2: Light-harvesting protein B:885 subunit beta



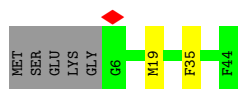
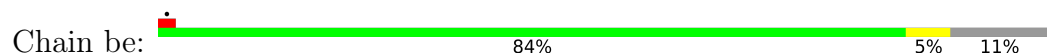
- Molecule 2: Light-harvesting protein B:885 subunit beta



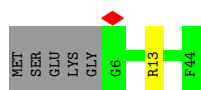
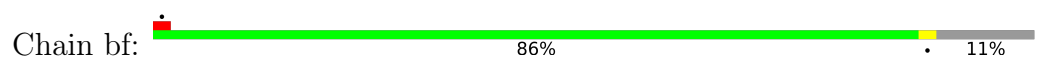
- Molecule 2: Light-harvesting protein B:885 subunit beta



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

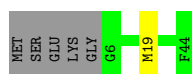


- Molecule 2: Light-harvesting protein B:885 subunit beta



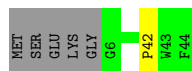
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bg:  86% 11%



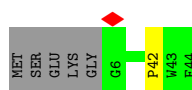
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bh:  86% 11%



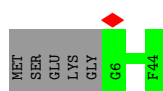
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bi:  86% 11%



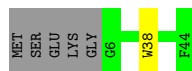
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bj:  89% 11%



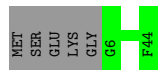
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bk:  86% 11%



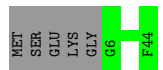
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bl:  89% 11%

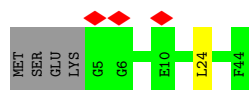
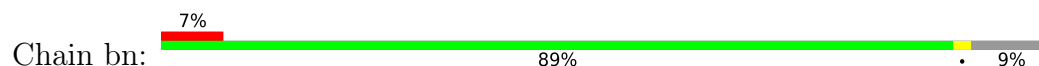


- Molecule 2: Light-harvesting protein B:885 subunit beta

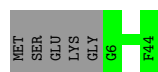
Chain bm:  89% 11%



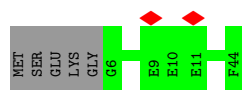
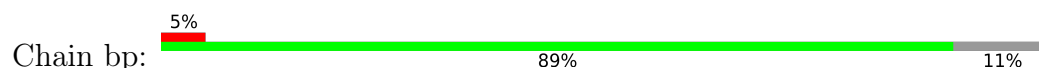
- Molecule 2: Light-harvesting protein B:885 subunit beta



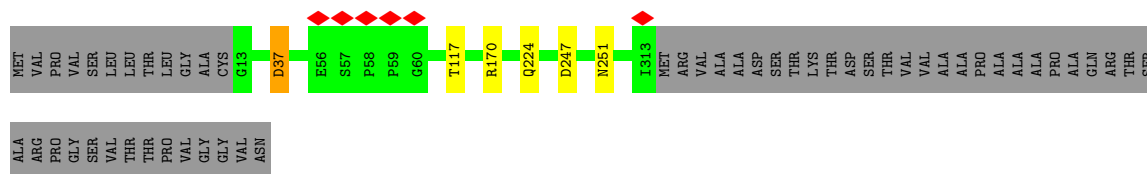
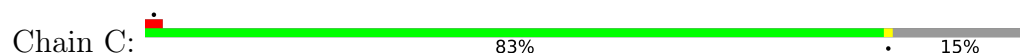
- Molecule 2: Light-harvesting protein B:885 subunit beta



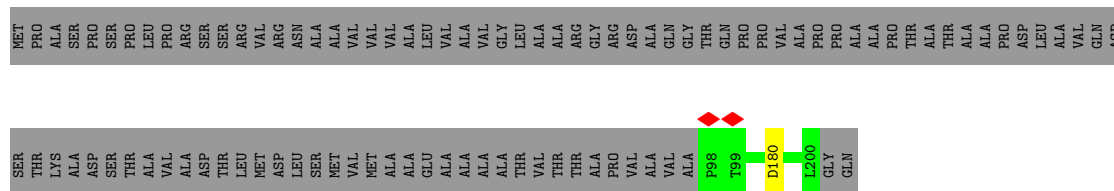
- Molecule 2: Light-harvesting protein B:885 subunit beta



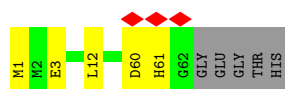
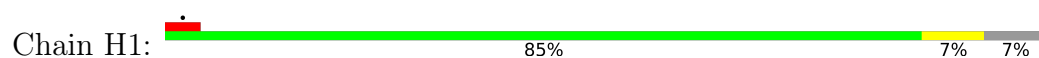
- Molecule 3: MULTIHEME_CYTC domain-containing protein



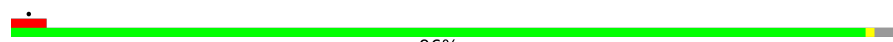
- Molecule 4: RC-S

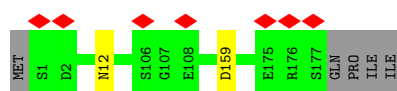


- Molecule 5: PRCH domain-containing protein

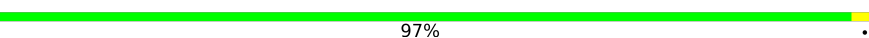


- Molecule 6: RC-Hc

Chain H2:  96%



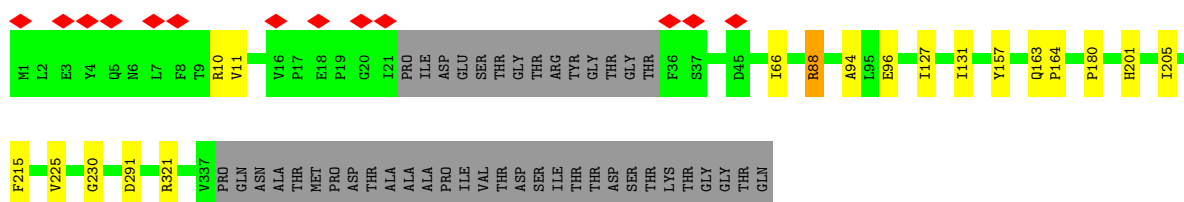
- Molecule 7: Photosynthetic reaction center L subunit

Chain L:  97%



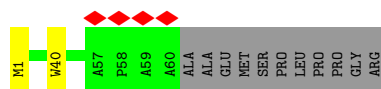
- Molecule 8: RC-M

Chain M:  83% 5% 12%



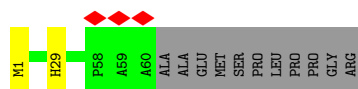
- Molecule 9: LHC domain-containing protein

Chain aa:  6% 82% 15%



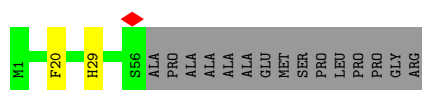
- Molecule 9: LHC domain-containing protein

Chain ab:  82% 15%



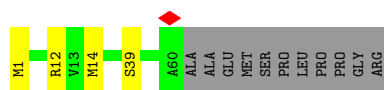
- Molecule 9: LHC domain-containing protein

Chain ac:  76% 21%

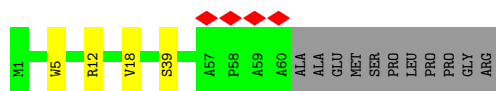
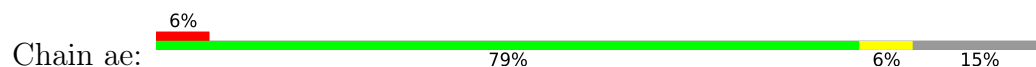


- Molecule 9: LHC domain-containing protein

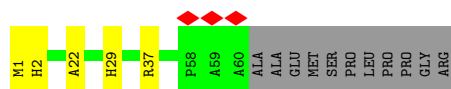
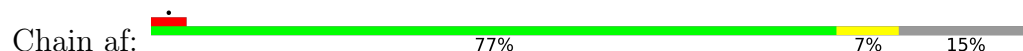
Chain ad:  79% 6% 15%



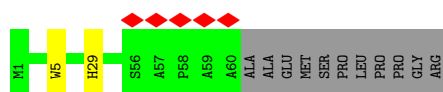
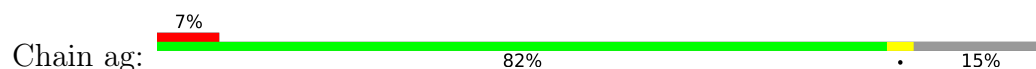
- Molecule 9: LHC domain-containing protein



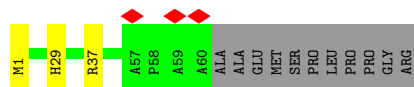
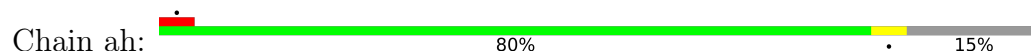
- Molecule 9: LHC domain-containing protein



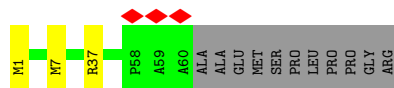
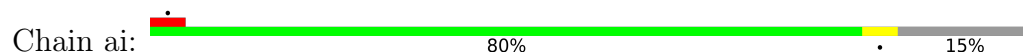
- Molecule 9: LHC domain-containing protein



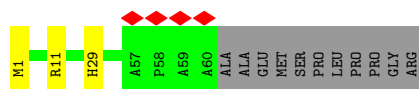
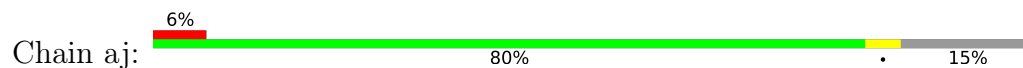
- Molecule 9: LHC domain-containing protein



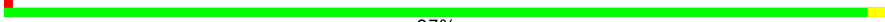
- Molecule 9: LHC domain-containing protein



- Molecule 9: LHC domain-containing protein



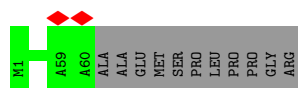
- Molecule 9: LHC domain-containing protein

Chain ak:  97%



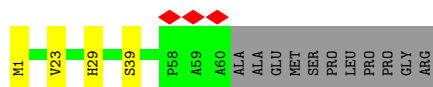
- Molecule 9: LHC domain-containing protein

Chain al:  85% 15%



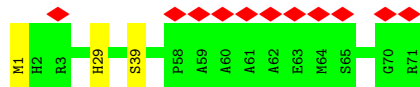
- Molecule 9: LHC domain-containing protein

Chain am:  79% 6% 15%



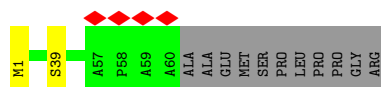
- Molecule 9: LHC domain-containing protein

Chain an:  15% 96%



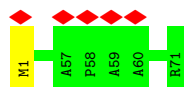
- Molecule 9: LHC domain-containing protein

Chain ao:  6% 82% 15%



- Molecule 9: LHC domain-containing protein

Chain ap:  7% 99%

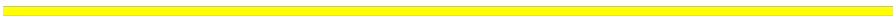


- Molecule 10: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain MG:  100%



- Molecule 10: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain CG:  100%

MAN1
RA12

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	176531	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	0.211	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0238	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: FME, RAM, FE, NDG, BPH, CRT, V7B, V7N, CD4, PGW, 0V9, UYH, MAN, V75, LMT, MQ8, BCL, HEC

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	0.14	0/396	0.50	0/541
1	AB	0.14	0/396	0.48	0/541
1	AC	0.14	0/388	0.45	0/529
1	AD	0.15	0/388	0.51	0/529
1	AE	0.15	0/396	0.49	0/541
1	AF	0.16	0/396	0.50	0/541
1	AG	0.15	0/396	0.48	0/541
1	AH	0.14	0/396	0.47	0/541
1	AI	0.13	0/396	0.44	0/541
1	AJ	0.16	0/396	0.48	0/541
1	AK	0.14	0/396	0.44	0/541
1	AL	0.14	0/396	0.47	0/541
1	AM	0.14	0/396	0.47	0/541
1	AN	0.14	0/396	0.44	0/541
1	AO	0.15	0/396	0.49	0/541
1	AP	0.14	0/396	0.46	0/541
1	AQ	0.15	0/396	0.47	0/541
1	AR	0.14	0/396	0.48	0/541
1	AS	0.15	0/396	0.47	0/541
1	AT	0.14	0/396	0.46	0/541
1	AU	0.14	0/396	0.42	0/541
1	AV	0.15	0/396	0.46	0/541
1	AW	0.14	0/396	0.48	0/541
1	AX	0.15	0/396	0.47	0/541
2	BA	0.13	0/336	0.41	0/456
2	BB	0.13	0/340	0.41	0/461
2	BC	0.11	0/336	0.41	0/456
2	BD	0.12	0/340	0.43	0/461
2	BE	0.13	0/340	0.44	0/461
2	BF	0.11	0/336	0.41	0/456
2	BG	0.13	0/336	0.42	0/456

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BH	0.12	0/336	0.41	0/456
2	BI	0.12	0/340	0.43	0/461
2	BJ	0.12	0/336	0.40	0/456
2	BK	0.12	0/336	0.43	0/456
2	BL	0.12	0/336	0.40	0/456
2	BM	0.12	0/336	0.42	0/456
2	BN	0.12	0/336	0.40	0/456
2	BO	0.13	0/336	0.44	0/456
2	BP	0.14	0/336	0.43	0/456
2	BQ	0.14	0/340	0.49	0/461
2	BR	0.14	0/340	0.45	0/461
2	BS	0.12	0/340	0.43	0/461
2	BT	0.13	0/340	0.42	0/461
2	BU	0.13	0/336	0.41	0/456
2	BV	0.12	0/340	0.40	0/461
2	BW	0.11	0/340	0.42	0/461
2	BX	0.14	0/336	0.45	0/456
2	ba	0.12	0/336	0.38	0/456
2	bb	0.15	0/336	0.41	0/456
2	bc	0.12	0/336	0.36	0/456
2	bd	0.14	0/336	0.41	0/456
2	be	0.15	0/336	0.41	0/456
2	bf	0.14	0/336	0.39	0/456
2	bg	0.13	0/336	0.39	0/456
2	bh	0.15	0/336	0.48	0/456
2	bi	0.14	0/336	0.40	0/456
2	bj	0.14	0/336	0.42	0/456
2	bk	0.15	0/336	0.40	0/456
2	bl	0.15	0/336	0.47	0/456
2	bm	0.13	0/336	0.37	0/456
2	bn	0.14	0/340	0.42	0/461
2	bo	0.13	0/336	0.37	0/456
2	bp	0.15	0/336	0.44	0/456
3	C	0.18	0/2404	0.50	0/3279
4	C1	0.16	0/826	0.46	0/1128
5	H1	0.18	0/531	0.48	0/717
6	H2	0.15	0/1409	0.44	0/1924
7	L	0.15	0/2252	0.46	0/3081
8	M	0.16	0/2699	0.49	0/3691
9	aa	0.15	0/467	0.44	0/638
9	ab	0.16	0/467	0.48	0/638
9	ac	0.15	0/444	0.46	0/605
9	ad	0.16	0/467	0.44	0/638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	ae	0.17	0/467	0.50	0/638
9	af	0.15	0/467	0.47	0/638
9	ag	0.15	0/467	0.45	0/638
9	ah	0.17	0/467	0.48	0/638
9	ai	0.17	0/467	0.47	0/638
9	aj	0.17	0/467	0.50	0/638
9	ak	0.17	0/547	0.51	0/748
9	al	0.15	0/467	0.47	0/638
9	am	0.15	0/467	0.42	0/638
9	an	0.20	0/547	0.51	0/748
9	ao	0.18	0/467	0.54	0/638
9	ap	0.15	0/548	0.44	0/748
All	All	0.15	0/40783	0.46	0/55580

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
2	BF	0	1
2	BO	0	1
8	M	0	2
9	af	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BF	13	ARG	Sidechain
2	BO	14	ARG	Sidechain
8	M	321	ARG	Sidechain
8	M	88	ARG	Sidechain
9	af	37	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	391	0	390	2	0
1	AB	391	0	390	0	0
1	AC	384	0	383	0	0
1	AD	384	0	383	0	0
1	AE	391	0	390	1	0
1	AF	391	0	390	1	0
1	AG	391	0	390	1	0
1	AH	391	0	390	3	0
1	AI	391	0	390	1	0
1	AJ	391	0	390	1	0
1	AK	391	0	390	1	0
1	AL	391	0	390	0	0
1	AM	391	0	390	0	0
1	AN	391	0	390	2	0
1	AO	391	0	390	0	0
1	AP	391	0	390	0	0
1	AQ	391	0	390	1	0
1	AR	391	0	390	2	0
1	AS	391	0	390	2	0
1	AT	391	0	390	0	0
1	AU	391	0	390	0	0
1	AV	391	0	390	0	0
1	AW	391	0	390	2	0
1	AX	391	0	390	1	0
2	BA	323	0	300	1	0
2	BB	327	0	303	0	0
2	BC	323	0	300	0	0
2	BD	327	0	303	0	0
2	BE	327	0	303	0	0
2	BF	323	0	300	1	0
2	BG	323	0	300	0	0
2	BH	323	0	300	1	0
2	BI	327	0	303	1	0
2	BJ	323	0	300	0	0
2	BK	323	0	300	0	0
2	BL	323	0	300	2	0
2	BM	323	0	300	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BN	323	0	300	0	0
2	BO	323	0	300	1	0
2	BP	323	0	300	1	0
2	BQ	327	0	303	1	0
2	BR	327	0	303	1	0
2	BS	327	0	303	2	0
2	BT	327	0	303	0	0
2	BU	323	0	300	0	0
2	BV	327	0	303	1	0
2	BW	327	0	303	0	0
2	BX	323	0	300	2	0
2	ba	323	0	300	3	0
2	bb	323	0	300	0	0
2	bc	323	0	300	3	0
2	bd	323	0	300	0	0
2	be	323	0	300	2	0
2	bf	323	0	300	1	0
2	bg	323	0	300	1	0
2	bh	323	0	300	1	0
2	bi	323	0	300	1	0
2	bj	323	0	300	0	0
2	bk	323	0	300	1	0
2	bl	323	0	300	0	0
2	bm	323	0	300	0	0
2	bn	327	0	303	1	0
2	bo	323	0	300	0	0
2	bp	323	0	300	0	0
3	C	2337	0	2252	5	0
4	C1	806	0	818	1	0
5	H1	522	0	503	2	0
6	H2	1371	0	1332	1	0
7	L	2165	0	2126	3	0
8	M	2611	0	2550	9	0
9	aa	465	0	475	1	0
9	ab	465	0	475	1	0
9	ac	443	0	453	2	0
9	ad	465	0	475	1	0
9	ae	465	0	475	4	0
9	af	465	0	475	3	0
9	ag	465	0	475	2	0
9	ah	465	0	475	2	0
9	ai	465	0	475	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	aj	465	0	475	2	0
9	ak	542	0	553	2	0
9	al	465	0	475	0	0
9	am	465	0	475	2	0
9	an	542	0	553	1	0
9	ao	465	0	475	0	0
9	ap	543	0	553	0	0
10	CG	21	0	18	0	0
10	MG	21	0	18	0	0
11	AA	132	0	148	3	0
11	AB	198	0	222	3	0
11	AC	66	0	74	1	0
11	AD	132	0	148	1	0
11	AE	132	0	148	1	0
11	AF	132	0	148	2	0
11	AG	132	0	148	1	0
11	AH	132	0	148	1	0
11	AI	132	0	148	1	0
11	AJ	132	0	148	1	0
11	AK	132	0	148	3	0
11	AL	132	0	148	1	0
11	AM	132	0	148	2	0
11	AN	198	0	222	3	0
11	AO	66	0	74	1	0
11	AP	132	0	148	1	0
11	AQ	132	0	148	1	0
11	AR	132	0	148	1	0
11	AS	198	0	222	6	0
11	AT	66	0	74	1	0
11	AU	132	0	148	2	0
11	AV	198	0	222	2	0
11	AW	132	0	148	2	0
11	AX	66	0	74	2	0
11	BA	66	0	74	0	0
11	BB	66	0	74	0	0
11	BC	66	0	74	0	0
11	BD	66	0	74	0	0
11	BE	66	0	74	0	0
11	BF	66	0	74	0	0
11	BG	66	0	74	0	0
11	BH	66	0	74	0	0
11	BI	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BJ	66	0	74	0	0
11	BK	66	0	74	0	0
11	BL	66	0	74	1	0
11	BM	66	0	74	0	0
11	BN	66	0	74	0	0
11	BO	66	0	74	0	0
11	BP	66	0	74	0	0
11	BQ	66	0	74	0	0
11	BR	66	0	74	0	0
11	BS	66	0	74	0	0
11	BT	66	0	74	0	0
11	BU	66	0	74	1	0
11	BV	66	0	74	0	0
11	BW	66	0	74	0	0
11	BX	66	0	74	0	0
11	L	132	0	148	3	0
11	M	132	0	148	2	0
11	aa	66	0	74	4	0
11	ab	66	0	74	2	0
11	ac	66	0	74	0	0
11	ad	66	0	74	0	0
11	ae	66	0	74	2	0
11	af	66	0	74	2	0
11	ag	66	0	74	1	0
11	ah	66	0	74	0	0
11	ai	66	0	74	0	0
11	aj	66	0	74	1	0
11	ak	66	0	74	0	0
11	al	66	0	74	0	0
11	am	66	0	74	1	0
11	an	66	0	74	1	0
11	ao	66	0	74	1	0
11	ap	66	0	74	0	0
11	ba	66	0	74	0	0
11	bb	66	0	74	1	0
11	bc	66	0	74	1	0
11	bd	66	0	74	0	0
11	be	66	0	74	0	0
11	bf	66	0	74	1	0
11	bg	66	0	74	1	0
11	bh	66	0	74	1	0
11	bi	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	bj	66	0	74	1	0
11	bk	66	0	74	1	0
11	bl	66	0	74	0	0
11	bm	66	0	74	1	0
11	bn	66	0	74	1	0
11	bo	66	0	74	0	0
11	bp	66	0	74	0	0
12	AA	35	0	44	0	0
12	AB	35	0	45	0	0
12	AD	35	0	46	2	0
12	AE	70	0	91	0	0
12	AG	35	0	45	0	0
12	AH	70	0	90	2	0
12	AI	35	0	45	0	0
12	AJ	35	0	46	0	0
12	AK	70	0	90	1	0
12	AL	70	0	91	0	0
12	AM	35	0	45	0	0
12	AN	70	0	91	0	0
12	AP	35	0	45	1	0
12	AQ	35	0	45	0	0
12	AR	35	0	45	0	0
12	AS	35	0	46	0	0
12	AT	70	0	91	0	0
12	AV	35	0	46	0	0
12	AW	35	0	46	0	0
12	BA	140	0	182	1	0
12	BB	105	0	137	0	0
12	BC	105	0	138	0	0
12	BD	140	0	181	0	0
12	BE	70	0	91	0	0
12	BF	105	0	137	1	0
12	BG	105	0	136	0	0
12	BH	105	0	137	1	0
12	BI	140	0	182	0	0
12	BJ	70	0	92	0	0
12	BK	105	0	137	0	0
12	BL	140	0	181	1	0
12	BM	105	0	137	0	0
12	BN	105	0	138	0	0
12	BO	105	0	135	1	0
12	BP	105	0	136	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	BQ	70	0	92	0	0
12	BR	105	0	136	0	0
12	BS	140	0	181	1	0
12	BT	105	0	137	1	0
12	BU	105	0	137	1	0
12	BV	105	0	137	0	0
12	BW	70	0	92	0	0
12	BX	70	0	92	0	0
12	H2	35	0	46	0	0
12	L	175	0	226	0	0
12	M	35	0	45	0	0
12	ac	35	0	45	0	0
12	ba	35	0	46	0	0
12	bb	35	0	45	0	0
12	bc	35	0	45	0	0
12	bd	35	0	45	0	0
12	be	70	0	91	0	0
12	bf	35	0	46	0	0
12	bg	35	0	45	0	0
12	bi	70	0	92	0	0
12	bj	35	0	45	0	0
12	bk	35	0	45	0	0
12	bl	35	0	46	0	0
12	bm	35	0	45	0	0
12	bn	35	0	45	0	0
12	bo	70	0	91	0	0
12	bp	35	0	46	0	0
13	AB	45	0	0	0	0
13	AE	90	0	0	0	0
13	AH	45	0	0	0	0
13	AQ	45	0	0	0	0
13	AT	45	0	0	0	0
13	AW	45	0	0	0	0
13	BB	45	0	0	0	0
13	BC	45	0	0	0	0
13	BE	45	0	0	0	0
13	BG	45	0	0	0	0
13	BH	45	0	0	0	0
13	BJ	45	0	0	0	0
13	BK	45	0	0	0	0
13	BL	45	0	0	0	0
13	BM	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	BN	45	0	0	0	0
13	BO	45	0	0	0	0
13	BP	45	0	0	0	0
13	BQ	45	0	0	0	0
13	BS	45	0	0	0	0
13	BT	45	0	0	0	0
13	BV	45	0	0	0	0
13	BW	45	0	0	0	0
13	af	45	0	0	0	0
13	aj	45	0	0	0	0
13	ba	45	0	0	0	0
13	bb	45	0	0	0	0
13	bc	45	0	0	0	0
13	bd	45	0	0	0	0
13	be	45	0	0	0	0
13	bf	45	0	0	0	0
13	bh	45	0	0	0	0
13	bi	45	0	0	0	0
13	bj	45	0	0	0	0
13	bl	45	0	0	0	0
13	bm	45	0	0	0	0
13	bn	45	0	0	0	0
13	bo	45	0	0	0	0
13	bp	45	0	0	0	0
14	AJ	45	0	0	0	0
14	AQ	45	0	0	0	0
14	H1	45	0	0	0	0
14	L	45	0	0	0	0
14	aj	45	0	0	0	0
14	bb	90	0	0	0	0
14	bc	45	0	0	0	0
14	bd	45	0	0	0	0
14	be	45	0	0	0	0
14	bf	45	0	0	0	0
14	bi	90	0	0	0	0
14	bj	45	0	0	0	0
14	bk	45	0	0	0	0
14	bl	45	0	0	0	0
14	bm	45	0	0	0	0
14	bn	45	0	0	0	0
14	bo	45	0	0	0	0
14	bp	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	172	0	120	5	0
16	C	14	0	12	0	0
16	C1	14	0	12	0	0
17	C	18	0	0	0	0
17	M	18	0	0	0	0
18	H1	84	0	124	1	0
18	M	168	0	248	0	0
18	ad	84	0	124	1	0
18	ae	84	0	124	2	0
18	ag	84	0	124	0	0
19	H1	51	0	76	2	0
20	L	53	0	72	1	0
20	M	53	0	72	0	0
20	ao	53	0	72	1	0
21	L	65	0	76	1	0
21	M	65	0	76	2	0
22	M	1	0	0	0	0
23	M	44	0	60	1	0
24	af	58	0	0	0	0
24	ag	58	0	0	0	0
25	ai	55	0	0	0	0
26	AA	4	0	0	0	0
26	AB	3	0	0	0	0
26	AC	1	0	0	0	0
26	AD	2	0	0	0	0
26	AF	1	0	0	0	0
26	AG	6	0	0	0	0
26	AH	5	0	0	0	0
26	AI	1	0	0	0	0
26	AJ	6	0	0	0	0
26	AK	4	0	0	0	0
26	AL	1	0	0	0	0
26	AM	2	0	0	0	0
26	AN	3	0	0	0	0
26	AO	1	0	0	0	0
26	AP	3	0	0	0	0
26	AQ	4	0	0	0	0
26	AR	1	0	0	0	0
26	AS	4	0	0	0	0
26	AT	2	0	0	0	0
26	AU	1	0	0	0	0
26	AV	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	AW	2	0	0	0	0
26	AX	1	0	0	0	0
26	BG	1	0	0	0	0
26	C	82	0	0	1	0
26	C1	35	0	0	0	0
26	H1	9	0	0	0	0
26	H2	8	0	0	0	0
26	L	47	0	0	0	0
26	M	59	0	0	0	0
26	aa	5	0	0	0	0
26	ab	5	0	0	0	0
26	ac	6	0	0	0	0
26	ad	10	0	0	0	0
26	ae	14	0	0	0	0
26	af	10	0	0	0	0
26	ag	11	0	0	0	0
26	ah	5	0	0	0	0
26	ai	5	0	0	0	0
26	aj	8	0	0	0	0
26	ak	16	0	0	0	0
26	al	11	0	0	0	0
26	am	10	0	0	0	0
26	an	10	0	0	0	0
26	ao	5	0	0	0	0
26	ap	5	0	0	0	0
26	ba	1	0	0	0	0
26	bb	2	0	0	0	0
26	bc	3	0	0	0	0
26	bd	5	0	0	0	0
26	be	6	0	0	0	0
26	bf	2	0	0	0	0
26	bg	3	0	0	0	0
26	bh	4	0	0	0	0
26	bi	3	0	0	0	0
26	bj	1	0	0	0	0
26	bk	5	0	0	0	0
26	bl	2	0	0	0	0
26	bm	5	0	0	0	0
26	bn	3	0	0	0	0
26	bo	5	0	0	0	0
26	bp	2	0	0	0	0
All	All	55758	0	53786	140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 140 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:5:TRP:HH2	11:AS:104:BCL:H143	1.47	0.78
11:AS:104:BCL:H141	2:BS:19:MET:HE2	1.71	0.72
12:AP:103:LMT:H6D	2:bk:38:TRP:HE1	1.57	0.69
11:AA:1001:BCL:H191	2:ba:36:LEU:HD11	1.78	0.65
21:M:404:BPH:HHC	21:M:404:BPH:HBB3	1.82	0.62

There are no symmetry-related clashes.

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%)	47 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AM	47/54 (87%)	47 (100%)	0	0	100	100
1	AN	47/54 (87%)	47 (100%)	0	0	100	100
1	AO	47/54 (87%)	47 (100%)	0	0	100	100
1	AP	47/54 (87%)	47 (100%)	0	0	100	100
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%)	46 (98%)	1 (2%)	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%)	37 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	38 (100%)	0	0	100	100
2	BW	38/44 (86%)	38 (100%)	0	0	100	100
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%)	36 (97%)	1 (3%)	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%)	37 (100%)	0	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%)	36 (97%)	1 (3%)	0	100	100
3	C	299/354 (84%)	284 (95%)	15 (5%)	0	100	100
4	C1	101/202 (50%)	98 (97%)	3 (3%)	0	100	100
5	H1	60/67 (90%)	60 (100%)	0	0	100	100
6	H2	174/181 (96%)	169 (97%)	5 (3%)	0	100	100
7	L	271/274 (99%)	264 (97%)	6 (2%)	1 (0%)	30	34
8	M	319/367 (87%)	310 (97%)	9 (3%)	0	100	100
9	aa	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
9	ab	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
9	ac	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
9	ad	58/71 (82%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	ae	58/71 (82%)	58 (100%)	0	0	100	100
9	af	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
9	ag	58/71 (82%)	58 (100%)	0	0	100	100
9	ah	58/71 (82%)	58 (100%)	0	0	100	100
9	ai	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
9	aj	58/71 (82%)	58 (100%)	0	0	100	100
9	ak	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
9	al	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
9	am	58/71 (82%)	58 (100%)	0	0	100	100
9	an	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
9	ao	58/71 (82%)	58 (100%)	0	0	100	100
9	ap	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
All	All	4798/5637 (85%)	4740 (99%)	57 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AG	38/41 (93%)	38 (100%)	0	100	100
1	AH	38/41 (93%)	38 (100%)	0	100	100
1	AI	38/41 (93%)	38 (100%)	0	100	100
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%)	37 (97%)	1 (3%)	40	54
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%)	30 (97%)	1 (3%)	34	46
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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%)	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
3	C	246/285 (86%)	245 (100%)	1 (0%)	84	91
4	C1	88/156 (56%)	88 (100%)	0	100	100
5	H1	50/53 (94%)	49 (98%)	1 (2%)	48	63
6	H2	146/151 (97%)	145 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	L	215/216 (100%)	213 (99%)	2 (1%)	70	82
8	M	263/298 (88%)	260 (99%)	3 (1%)	65	79
9	aa	46/54 (85%)	46 (100%)	0	100	100
9	ab	46/54 (85%)	46 (100%)	0	100	100
9	ac	45/54 (83%)	45 (100%)	0	100	100
9	ad	46/54 (85%)	44 (96%)	2 (4%)	26	34
9	ae	46/54 (85%)	45 (98%)	1 (2%)	45	59
9	af	46/54 (85%)	46 (100%)	0	100	100
9	ag	46/54 (85%)	46 (100%)	0	100	100
9	ah	46/54 (85%)	46 (100%)	0	100	100
9	ai	46/54 (85%)	46 (100%)	0	100	100
9	aj	46/54 (85%)	46 (100%)	0	100	100
9	ak	54/54 (100%)	54 (100%)	0	100	100
9	al	46/54 (85%)	46 (100%)	0	100	100
9	am	46/54 (85%)	45 (98%)	1 (2%)	45	59
9	an	54/54 (100%)	53 (98%)	1 (2%)	50	65
9	ao	46/54 (85%)	45 (98%)	1 (2%)	45	59
9	ap	54/54 (100%)	54 (100%)	0	100	100
All	All	3917/4407 (89%)	3901 (100%)	16 (0%)	81	91

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	an	39	SER
9	am	39	SER
8	M	215	PHE
9	ae	39	SER
8	M	96	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	32	ASN
3	C	44	GLN
9	ah	36	GLN

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Mol	Chain	Res	Type
7	L	104	GLN
8	M	325	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 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	$\# Z > 2$
9	FME	am	1	9	8,9,10	0.97	0	8,9,11	1.01	1 (12%)
1	FME	AM	1	1	8,9,10	0.96	0	8,9,11	0.96	1 (12%)
9	FME	ah	1	9	8,9,10	0.94	0	8,9,11	1.01	1 (12%)
8	FME	M	1	8	8,9,10	0.95	0	8,9,11	0.78	0
1	FME	AA	1	1	8,9,10	0.96	0	8,9,11	0.95	0
9	FME	ac	1	9	8,9,10	1.00	0	8,9,11	0.66	0
1	FME	AB	1	1	8,9,10	0.95	0	8,9,11	1.05	1 (12%)
1	FME	AE	1	1	8,9,10	0.96	0	8,9,11	0.90	0
1	FME	AR	1	1	8,9,10	0.99	0	8,9,11	0.78	0
1	FME	AV	1	1	8,9,10	0.94	0	8,9,11	1.10	1 (12%)
1	FME	AF	1	1	8,9,10	0.97	0	8,9,11	0.89	0
1	FME	AX	1	1	8,9,10	0.99	0	8,9,11	0.84	0
9	FME	al	1	9	8,9,10	0.94	0	8,9,11	0.95	0
9	FME	ap	1	9	8,9,10	0.90	0	8,9,11	1.28	2 (25%)
1	FME	AH	1	1	8,9,10	0.96	0	8,9,11	0.97	1 (12%)
1	FME	AJ	1	1	8,9,10	0.95	0	8,9,11	1.00	1 (12%)
1	FME	AP	1	1	8,9,10	0.96	0	8,9,11	1.04	1 (12%)
9	FME	aj	1	9	8,9,10	0.95	0	8,9,11	1.11	1 (12%)
1	FME	AD	1	1	8,9,10	0.96	0	8,9,11	1.27	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	AN	1	1	8,9,10	0.93	0	8,9,11	1.33	2 (25%)
1	FME	AS	1	1	8,9,10	1.00	0	8,9,11	0.85	0
9	FME	ao	1	9	8,9,10	0.93	0	8,9,11	1.07	1 (12%)
9	FME	ag	1	9	8,9,10	0.97	0	8,9,11	0.89	0
9	FME	ab	1	9	8,9,10	0.92	0	8,9,11	1.16	1 (12%)
5	FME	H1	1	5	8,9,10	0.96	0	8,9,11	1.04	1 (12%)
9	FME	ae	1	9	8,9,10	0.97	0	8,9,11	0.88	0
1	FME	AL	1	1	8,9,10	0.95	0	8,9,11	0.98	1 (12%)
1	FME	AQ	1	1	8,9,10	0.95	0	8,9,11	1.05	1 (12%)
9	FME	aa	1	9	8,9,10	0.96	0	8,9,11	0.98	1 (12%)
1	FME	AW	1	1	8,9,10	0.95	0	8,9,11	0.97	1 (12%)
9	FME	ak	1	9	8,9,10	0.98	0	8,9,11	0.93	0
9	FME	ai	1	9	8,9,10	0.96	0	8,9,11	1.09	1 (12%)
9	FME	ad	1	9	8,9,10	0.94	0	8,9,11	1.05	1 (12%)
1	FME	AC	1	1	8,9,10	0.97	0	8,9,11	1.00	1 (12%)
1	FME	AO	1	1	8,9,10	0.94	0	8,9,11	1.28	2 (25%)
1	FME	AI	1	1	8,9,10	0.98	0	8,9,11	0.86	0
9	FME	af	1	9	8,9,10	0.97	0	8,9,11	0.98	1 (12%)
1	FME	AG	1	1	8,9,10	0.98	0	8,9,11	0.92	0
9	FME	an	1	9	8,9,10	0.96	0	8,9,11	1.01	1 (12%)
1	FME	AK	1	1	8,9,10	0.94	0	8,9,11	1.11	1 (12%)
1	FME	AT	1	1	8,9,10	0.96	0	8,9,11	1.03	1 (12%)
1	FME	AU	1	1	8,9,10	0.95	0	8,9,11	0.96	1 (12%)

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
9	FME	am	1	9	-	0/7/9/11	-
1	FME	AM	1	1	-	1/7/9/11	-
9	FME	ah	1	9	-	0/7/9/11	-
8	FME	M	1	8	-	2/7/9/11	-
1	FME	AA	1	1	-	1/7/9/11	-
9	FME	ac	1	9	-	0/7/9/11	-
1	FME	AB	1	1	-	0/7/9/11	-
1	FME	AE	1	1	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AR	1	1	-	2/7/9/11	-
1	FME	AV	1	1	-	2/7/9/11	-
1	FME	AF	1	1	-	0/7/9/11	-
1	FME	AX	1	1	-	0/7/9/11	-
9	FME	al	1	9	-	3/7/9/11	-
9	FME	ap	1	9	-	1/7/9/11	-
1	FME	AH	1	1	-	1/7/9/11	-
1	FME	AJ	1	1	-	2/7/9/11	-
1	FME	AP	1	1	-	1/7/9/11	-
9	FME	aj	1	9	-	0/7/9/11	-
1	FME	AD	1	1	-	0/7/9/11	-
1	FME	AN	1	1	-	0/7/9/11	-
1	FME	AS	1	1	-	1/7/9/11	-
9	FME	ao	1	9	-	0/7/9/11	-
9	FME	ag	1	9	-	1/7/9/11	-
9	FME	ab	1	9	-	4/7/9/11	-
5	FME	H1	1	5	-	2/7/9/11	-
9	FME	ae	1	9	-	2/7/9/11	-
1	FME	AL	1	1	-	1/7/9/11	-
1	FME	AQ	1	1	-	0/7/9/11	-
9	FME	aa	1	9	-	2/7/9/11	-
1	FME	AW	1	1	-	0/7/9/11	-
9	FME	ak	1	9	-	2/7/9/11	-
9	FME	ai	1	9	-	0/7/9/11	-
9	FME	ad	1	9	-	0/7/9/11	-
1	FME	AC	1	1	-	1/7/9/11	-
1	FME	AO	1	1	-	2/7/9/11	-
1	FME	AI	1	1	-	1/7/9/11	-
9	FME	af	1	9	-	0/7/9/11	-
1	FME	AG	1	1	-	2/7/9/11	-
9	FME	an	1	9	-	2/7/9/11	-
1	FME	AK	1	1	-	0/7/9/11	-
1	FME	AT	1	1	-	0/7/9/11	-
1	FME	AU	1	1	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AN	1	FME	C-CA-N	2.81	114.92	109.50
9	ab	1	FME	CA-N-CN	2.63	126.86	122.82
1	AD	1	FME	C-CA-N	2.59	114.50	109.50
1	AO	1	FME	C-CA-N	2.48	114.28	109.50
1	AV	1	FME	C-CA-N	2.44	114.21	109.50

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H1	1	FME	CB-CA-N-CN
9	aa	1	FME	N-CA-CB-CG
9	ab	1	FME	CB-CA-N-CN
9	ab	1	FME	N-CA-CB-CG
9	ae	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	$\# Z > 2$
10	MAN	CG	1	10,17,3	11,11,12	0.82	1 (9%)	15,15,17	1.05	1 (6%)
10	RAM	CG	2	10	10,10,11	1.67	3 (30%)	14,14,16	1.02	1 (7%)
10	MAN	MG	1	10,17,8	11,11,12	0.75	0	15,15,17	0.96	1 (6%)
10	RAM	MG	2	10	10,10,11	1.63	2 (20%)	14,14,16	1.94	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
10	MAN	CG	1	10,17,3	-	2/2/19/22	0/1/1/1
10	RAM	CG	2	10	-	-	0/1/1/1
10	MAN	MG	1	10,17,8	-	0/2/19/22	0/1/1/1
10	RAM	MG	2	10	-	-	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)
10	CG	2	RAM	O5-C1	3.97	1.50	1.43
10	MG	2	RAM	O5-C1	3.66	1.49	1.43
10	MG	2	RAM	C2-C3	-2.49	1.48	1.52
10	CG	2	RAM	C2-C3	-2.22	1.49	1.52
10	CG	2	RAM	O5-C5	2.11	1.47	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	MG	2	RAM	C3-C4-C5	3.88	115.72	109.81
10	MG	2	RAM	C6-C5-C4	-3.82	106.10	113.08
10	MG	2	RAM	O5-C5-C4	3.68	116.18	109.55
10	CG	1	MAN	C1-O5-C5	2.96	116.15	112.19
10	MG	1	MAN	C1-O5-C5	2.30	115.28	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

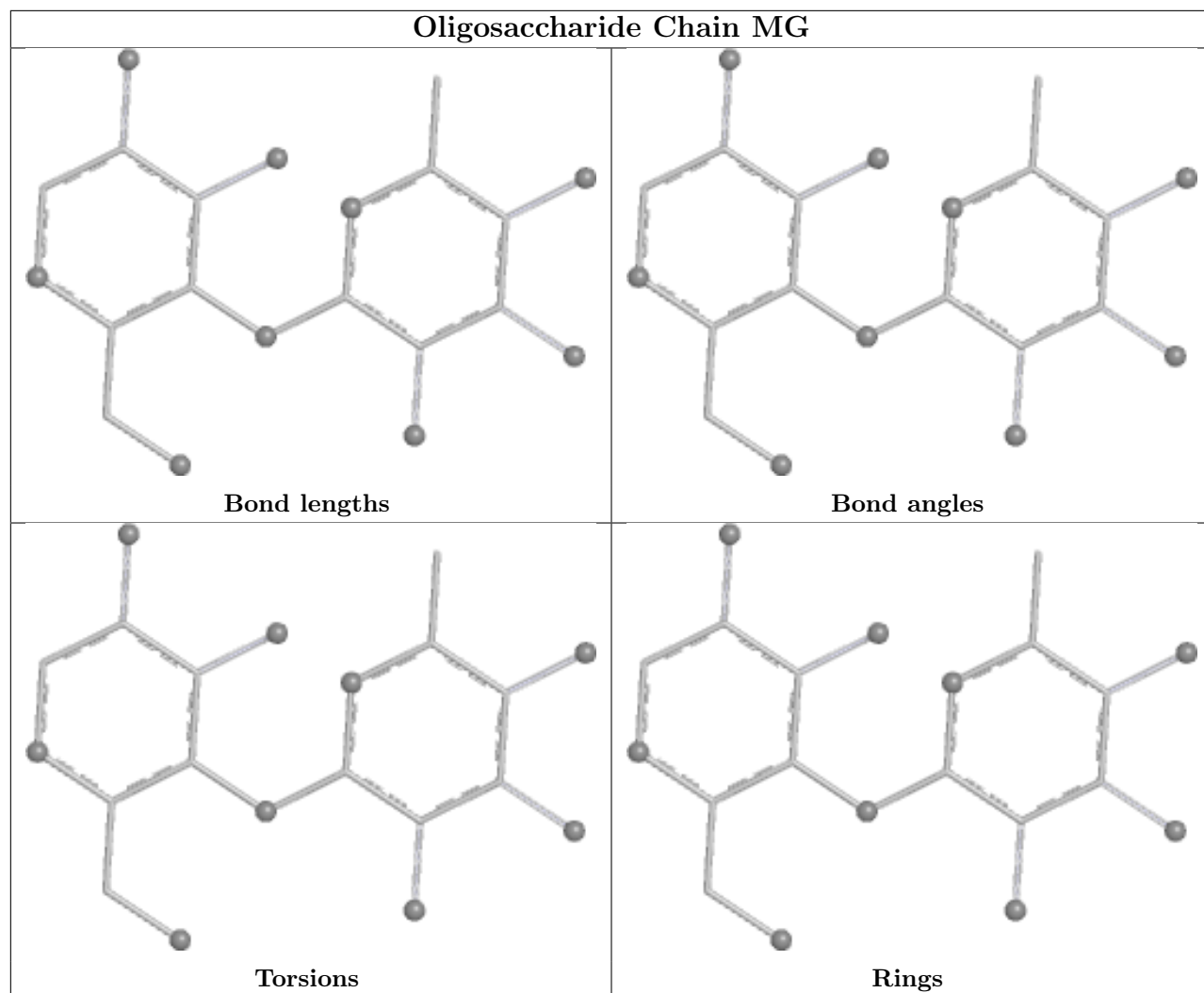
Mol	Chain	Res	Type	Atoms
10	CG	1	MAN	O5-C5-C6-O6
10	CG	1	MAN	C4-C5-C6-O6

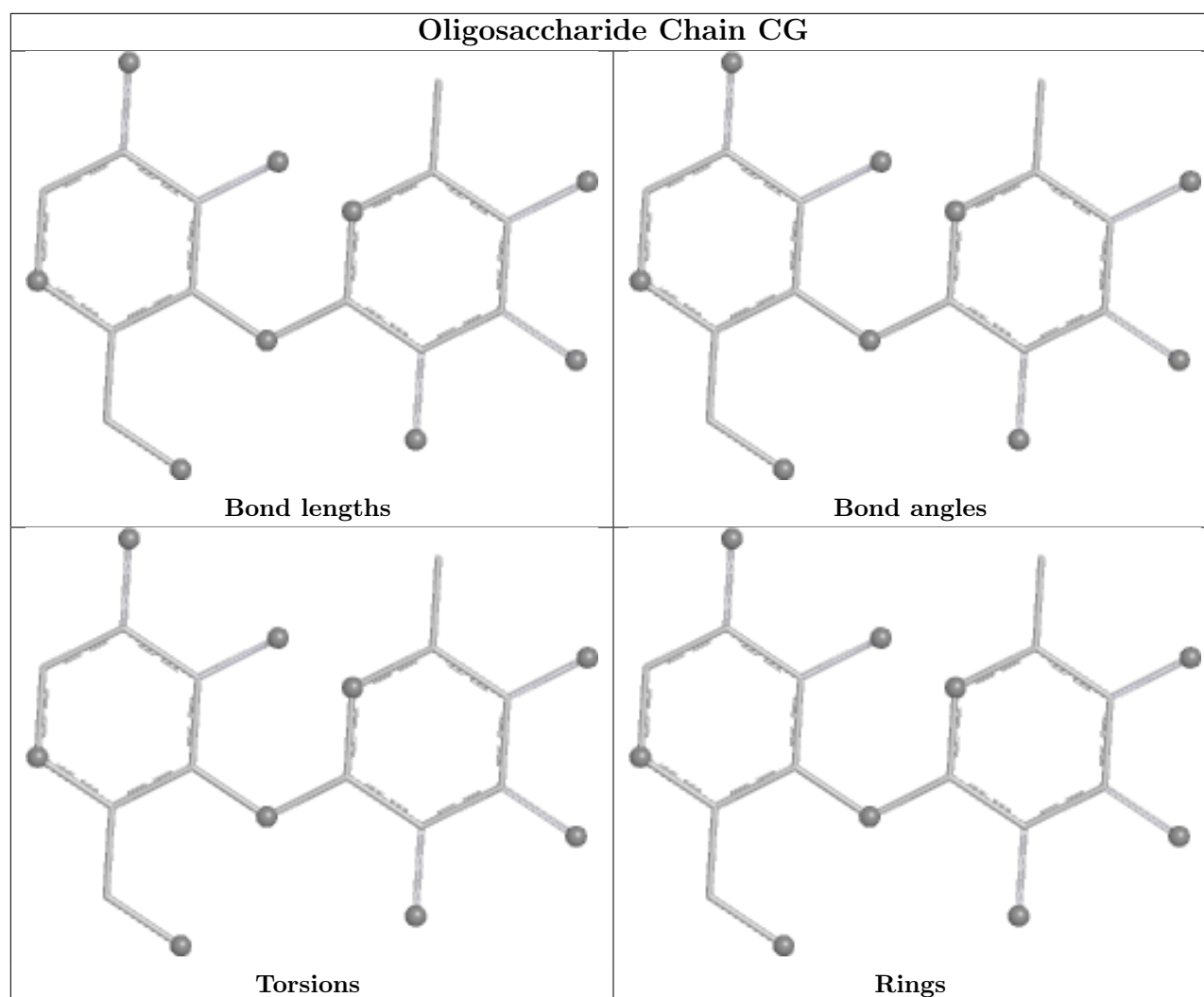
There are no ring outliers.

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.

Oligosaccharide Chain MG





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	$\# Z > 2$
12	LMT	bg	1001	-	36,36,36	1.09	4 (11%)	47,47,47	0.84	1 (2%)
11	BCL	AN	102	26	69,74,74	1.16	6 (8%)	79,115,115	1.36	9 (11%)
11	BCL	AX	101	-	69,74,74	1.17	6 (8%)	79,115,115	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LMT	ac	1001	-	36,36,36	1.06	4 (11%)	47,47,47	0.93	3 (6%)
13	V7N	bj	101	-	44,44,44	1.66	6 (13%)	48,54,54	1.56	9 (18%)
12	LMT	BP	1003	-	36,36,36	1.05	4 (11%)	47,47,47	1.01	2 (4%)
14	0V9	bj	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.86	2 (4%)
12	LMT	BD	104	-	36,36,36	1.06	4 (11%)	47,47,47	0.85	0
11	BCL	bg	1002	-	69,74,74	1.12	5 (7%)	79,115,115	1.32	10 (12%)
13	V7N	AE	105	-	44,44,44	1.66	8 (18%)	48,54,54	1.62	9 (18%)
13	V7N	BE	101	-	44,44,44	1.67	6 (13%)	48,54,54	1.59	11 (22%)
11	BCL	AC	1001	-	69,74,74	1.15	5 (7%)	79,115,115	1.29	7 (8%)
12	LMT	AK	101	-	36,36,36	1.04	4 (11%)	47,47,47	1.02	4 (8%)
11	BCL	AF	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	7 (8%)
12	LMT	AQ	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.98	2 (4%)
12	LMT	BV	1004	-	36,36,36	1.06	4 (11%)	47,47,47	0.93	3 (6%)
11	BCL	BM	1004	-	69,74,74	1.12	5 (7%)	79,115,115	1.37	11 (13%)
12	LMT	ba	101	-	36,36,36	1.04	4 (11%)	47,47,47	0.93	1 (2%)
14	0V9	bo	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.89	2 (4%)
11	BCL	AM	101	26	69,74,74	1.14	6 (8%)	79,115,115	1.55	13 (16%)
13	V7N	bn	101	-	44,44,44	1.72	7 (15%)	48,54,54	1.55	9 (18%)
18	CD4	M	409	-	83,83,83	0.47	0	89,95,95	1.03	5 (5%)
14	0V9	L	310	-	44,44,46	0.76	1 (2%)	47,49,51	0.83	2 (4%)
13	V7N	ba	102	-	44,44,44	1.72	7 (15%)	48,54,54	1.62	11 (22%)
13	V7N	bm	101	-	44,44,44	1.68	7 (15%)	48,54,54	1.59	11 (22%)
11	BCL	AV	104	26	69,74,74	1.18	7 (10%)	79,115,115	1.56	13 (16%)
11	BCL	BA	103	-	69,74,74	1.12	5 (7%)	79,115,115	1.28	9 (11%)
11	BCL	AB	105	-	69,74,74	1.21	5 (7%)	79,115,115	1.28	10 (12%)
12	LMT	BL	1006	-	36,36,36	1.05	4 (11%)	47,47,47	1.03	2 (4%)
11	BCL	AV	102	26	69,74,74	1.15	5 (7%)	79,115,115	1.37	9 (11%)
11	BCL	AH	101	-	69,74,74	1.14	5 (7%)	79,115,115	1.28	7 (8%)
12	LMT	BM	1005	-	36,36,36	1.04	4 (11%)	47,47,47	0.87	1 (2%)
11	BCL	AM	102	-	69,74,74	1.13	5 (7%)	79,115,115	1.31	7 (8%)
12	LMT	bd	102	-	36,36,36	1.05	4 (11%)	47,47,47	0.86	1 (2%)
12	LMT	BX	102	-	36,36,36	1.05	4 (11%)	47,47,47	0.92	3 (6%)
12	LMT	BO	1002	-	36,36,36	1.03	3 (8%)	47,47,47	0.88	1 (2%)
12	LMT	BQ	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.84	0
12	LMT	BL	1004	-	36,36,36	1.04	4 (11%)	47,47,47	0.95	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LMT	BD	102	-	36,36,36	1.05	4 (11%)	47,47,47	0.88	0
11	BCL	AI	103	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	8 (10%)
11	BCL	AW	103	-	69,74,74	1.16	5 (7%)	79,115,115	1.47	12 (15%)
11	BCL	AU	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.38	12 (15%)
11	BCL	al	1001	-	69,74,74	1.14	5 (7%)	79,115,115	1.29	9 (11%)
14	0V9	bi	105	-	44,44,46	0.76	1 (2%)	47,49,51	0.99	3 (6%)
11	BCL	ab	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.83	10 (12%)
12	LMT	BO	1004	-	36,36,36	1.07	4 (11%)	47,47,47	0.85	1 (2%)
11	BCL	AW	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.33	7 (8%)
12	LMT	bo	103	-	36,36,36	1.07	4 (11%)	47,47,47	0.94	1 (2%)
11	BCL	ag	102	-	69,74,74	1.13	5 (7%)	79,115,115	1.31	9 (11%)
12	LMT	BK	1004	-	36,36,36	1.03	4 (11%)	47,47,47	1.04	3 (6%)
12	LMT	AJ	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.88	1 (2%)
14	0V9	bc	103	-	44,44,46	0.77	1 (2%)	47,49,51	0.96	3 (6%)
11	BCL	AJ	101	26	69,74,74	1.17	6 (8%)	79,115,115	1.53	12 (15%)
11	BCL	bc	104	-	69,74,74	1.13	5 (7%)	79,115,115	1.35	11 (13%)
12	LMT	BK	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.87	1 (2%)
24	V7B	af	101	-	59,59,59	0.90	3 (5%)	75,75,75	1.09	5 (6%)
11	BCL	AQ	101	26	69,74,74	1.16	6 (8%)	79,115,115	1.77	13 (16%)
15	HEC	C	403	3	46,50,50	1.84	4 (8%)	58,82,82	1.66	7 (12%)
12	LMT	bn	103	-	36,36,36	1.03	4 (11%)	47,47,47	1.23	5 (10%)
12	LMT	BT	1003	-	36,36,36	1.01	4 (11%)	47,47,47	0.96	3 (6%)
11	BCL	AN	105	-	69,74,74	1.21	5 (7%)	79,115,115	1.35	10 (12%)
12	LMT	BS	1005	-	36,36,36	1.07	4 (11%)	47,47,47	0.87	1 (2%)
11	BCL	AR	101	-	69,74,74	1.14	6 (8%)	79,115,115	1.37	10 (12%)
12	LMT	BF	103	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	2 (4%)
15	HEC	C	401	3	46,50,50	1.84	5 (10%)	58,82,82	1.58	5 (8%)
13	V7N	bb	101	-	44,44,44	1.68	7 (15%)	48,54,54	1.59	11 (22%)
11	BCL	BE	103	-	69,74,74	1.13	5 (7%)	79,115,115	1.35	11 (13%)
11	BCL	BW	1002	-	69,74,74	1.14	5 (7%)	79,115,115	1.53	12 (15%)
11	BCL	ao	102	-	69,74,74	1.12	5 (7%)	79,115,115	1.32	9 (11%)
12	LMT	BL	1003	-	36,36,36	1.08	4 (11%)	47,47,47	0.96	2 (4%)
12	LMT	BV	1003	-	36,36,36	1.03	4 (11%)	47,47,47	0.91	2 (4%)
14	0V9	AJ	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.84	2 (4%)
17	V75	M	410	10,16	18,18,18	1.62	5 (27%)	21,25,25	1.72	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AL	102	-	69,74,74	1.16	5 (7%)	79,115,115	1.33	7 (8%)
12	LMT	AK	104	-	36,36,36	1.06	4 (11%)	47,47,47	1.00	2 (4%)
12	LMT	BA	102	-	36,36,36	1.04	4 (11%)	47,47,47	0.91	1 (2%)
14	0V9	bp	103	-	44,44,46	0.77	1 (2%)	47,49,51	0.87	3 (6%)
18	CD4	H1	1001	-	83,83,83	0.48	0	89,95,95	1.02	5 (5%)
11	BCL	bj	104	-	69,74,74	1.12	5 (7%)	79,115,115	1.39	11 (13%)
11	BCL	bh	102	-	69,74,74	1.12	6 (8%)	79,115,115	1.31	10 (12%)
13	V7N	BT	1001	-	44,44,44	1.67	8 (18%)	48,54,54	1.56	8 (16%)
12	LMT	BO	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.91	1 (2%)
12	LMT	AN	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.92	2 (4%)
14	0V9	bd	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.94	3 (6%)
13	V7N	BQ	1001	-	44,44,44	1.66	7 (15%)	48,54,54	1.67	13 (27%)
25	UYH	ai	102	-	55,55,55	2.15	15 (27%)	63,63,63	1.19	6 (9%)
12	LMT	BT	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.99	2 (4%)
12	LMT	L	306	-	36,36,36	1.08	4 (11%)	47,47,47	0.98	2 (4%)
11	BCL	aj	102	-	69,74,74	1.13	5 (7%)	79,115,115	1.32	10 (12%)
12	LMT	BF	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.90	2 (4%)
11	BCL	an	1001	-	69,74,74	1.13	5 (7%)	79,115,115	1.30	9 (11%)
12	LMT	BI	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.91	1 (2%)
12	LMT	L	305	-	36,36,36	1.08	4 (11%)	47,47,47	0.84	1 (2%)
11	BCL	bn	104	-	69,74,74	1.12	5 (7%)	79,115,115	1.25	10 (12%)
16	NDG	C	405	17	14,14,15	0.66	0	17,19,21	1.10	1 (5%)
13	V7N	bl	101	-	44,44,44	1.68	7 (15%)	48,54,54	1.70	14 (29%)
11	BCL	AG	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.29	7 (8%)
12	LMT	H2	201	-	36,36,36	1.06	4 (11%)	47,47,47	0.92	1 (2%)
11	BCL	BN	1004	-	69,74,74	1.13	5 (7%)	79,115,115	1.38	11 (13%)
12	LMT	BW	1003	-	36,36,36	1.06	4 (11%)	47,47,47	1.10	3 (6%)
13	V7N	be	102	-	44,44,44	1.67	7 (15%)	48,54,54	1.72	11 (22%)
11	BCL	ac	1002	-	69,74,74	1.13	5 (7%)	79,115,115	1.30	9 (11%)
12	LMT	bk	1001	-	36,36,36	1.08	4 (11%)	47,47,47	0.87	1 (2%)
12	LMT	bi	104	-	36,36,36	1.06	4 (11%)	47,47,47	0.87	1 (2%)
14	0V9	bi	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.86	1 (2%)
13	V7N	af	103	-	44,44,44	1.68	7 (15%)	48,54,54	1.71	12 (25%)
11	BCL	bo	105	-	69,74,74	1.12	5 (7%)	79,115,115	1.26	10 (12%)
11	BCL	ad	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.34	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	BJ	1004	-	69,74,74	1.10	5 (7%)	79,115,115	1.31	9 (11%)
11	BCL	AU	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	7 (8%)
12	LMT	AB	104	-	36,36,36	1.06	4 (11%)	47,47,47	1.03	2 (4%)
18	CD4	ae	102	-	83,83,83	0.49	0	89,95,95	1.14	7 (7%)
11	BCL	AK	103	26	69,74,74	1.16	6 (8%)	79,115,115	1.43	10 (12%)
12	LMT	M	408	-	36,36,36	1.05	4 (11%)	47,47,47	0.94	3 (6%)
14	0V9	bb	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.85	1 (2%)
13	V7N	BM	1001	-	44,44,44	1.66	6 (13%)	48,54,54	1.76	14 (29%)
13	V7N	BS	1001	-	44,44,44	1.65	6 (13%)	48,54,54	1.69	12 (25%)
11	BCL	af	102	-	69,74,74	1.13	5 (7%)	79,115,115	1.33	10 (12%)
11	BCL	AN	103	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	7 (8%)
12	LMT	be	103	-	36,36,36	1.08	4 (11%)	47,47,47	0.85	1 (2%)
12	LMT	BU	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.92	2 (4%)
12	LMT	BC	104	-	36,36,36	1.05	4 (11%)	47,47,47	1.01	1 (2%)
11	BCL	bb	103	-	69,74,74	1.11	5 (7%)	79,115,115	1.44	11 (13%)
12	LMT	BD	105	-	36,36,36	1.08	4 (11%)	47,47,47	0.93	2 (4%)
11	BCL	AB	102	26	69,74,74	1.14	5 (7%)	79,115,115	1.37	10 (12%)
12	LMT	BE	102	-	36,36,36	1.05	4 (11%)	47,47,47	1.01	1 (2%)
12	LMT	be	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.91	2 (4%)
12	LMT	AT	102	-	36,36,36	1.00	4 (11%)	47,47,47	1.12	3 (6%)
12	LMT	bo	101	-	36,36,36	1.05	4 (11%)	47,47,47	0.85	1 (2%)
11	BCL	AI	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.51	13 (16%)
13	V7N	bc	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.56	9 (18%)
13	V7N	BB	101	-	44,44,44	1.66	8 (18%)	48,54,54	1.51	10 (20%)
11	BCL	AD	101	26	69,74,74	1.14	5 (7%)	79,115,115	1.47	13 (16%)
11	BCL	BC	105	-	69,74,74	1.14	5 (7%)	79,115,115	1.33	10 (12%)
12	LMT	BI	103	-	36,36,36	1.05	4 (11%)	47,47,47	1.04	2 (4%)
11	BCL	ai	101	-	69,74,74	1.14	5 (7%)	79,115,115	1.32	9 (11%)
13	V7N	bo	102	-	44,44,44	1.70	8 (18%)	48,54,54	1.61	12 (25%)
12	LMT	bi	101	-	36,36,36	1.09	4 (11%)	47,47,47	1.01	4 (8%)
18	CD4	M	402	-	83,83,83	0.48	0	89,95,95	1.09	7 (7%)
11	BCL	L	304	-	69,74,74	1.13	5 (7%)	79,115,115	1.28	9 (11%)
13	V7N	AH	104	-	44,44,44	1.67	7 (15%)	48,54,54	1.71	13 (27%)
12	LMT	BL	1002	-	36,36,36	1.08	4 (11%)	47,47,47	0.91	1 (2%)
20	MQ8	ao	101	-	54,54,54	0.64	0	67,69,69	1.00	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	BQ	1002	-	69,74,74	1.12	5 (7%)	79,115,115	1.35	10 (12%)
17	V75	C	406	10,16	18,18,18	1.59	4 (22%)	21,25,25	1.72	3 (14%)
11	BCL	AE	102	-	69,74,74	1.13	6 (8%)	79,115,115	1.43	14 (17%)
11	BCL	AA	1002	26	69,74,74	1.15	6 (8%)	79,115,115	1.38	10 (12%)
11	BCL	AA	1001	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	7 (8%)
11	BCL	bi	106	-	69,74,74	1.12	5 (7%)	79,115,115	1.30	10 (12%)
11	BCL	ah	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.34	10 (12%)
14	OV9	bl	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.93	2 (4%)
12	LMT	BP	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	1 (2%)
12	LMT	L	307	-	36,36,36	1.04	4 (11%)	47,47,47	1.00	3 (6%)
12	LMT	AH	105	-	36,36,36	1.08	4 (11%)	47,47,47	0.94	2 (4%)
20	MQ8	M	407	-	54,54,54	0.64	0	67,69,69	0.72	1 (1%)
13	V7N	bf	101	-	44,44,44	1.66	7 (15%)	48,54,54	1.59	10 (20%)
11	BCL	AG	102	26	69,74,74	1.13	6 (8%)	79,115,115	1.51	12 (15%)
12	LMT	BD	101	-	36,36,36	1.04	4 (11%)	47,47,47	1.03	3 (6%)
11	BCL	AO	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.30	7 (8%)
11	BCL	BV	1002	-	69,74,74	1.11	5 (7%)	79,115,115	1.29	9 (11%)
16	NDG	C1	301	17	14,14,15	0.67	0	17,19,21	1.07	2 (11%)
11	BCL	BI	102	-	69,74,74	1.12	5 (7%)	79,115,115	1.33	9 (11%)
11	BCL	be	105	-	69,74,74	1.11	5 (7%)	79,115,115	1.26	9 (11%)
12	LMT	AI	102	-	36,36,36	1.03	4 (11%)	47,47,47	0.83	1 (2%)
12	LMT	AW	102	-	36,36,36	1.09	4 (11%)	47,47,47	0.87	1 (2%)
13	V7N	AW	104	-	44,44,44	1.68	7 (15%)	48,54,54	1.61	11 (22%)
11	BCL	BU	1001	-	69,74,74	1.11	5 (7%)	79,115,115	1.28	8 (10%)
11	BCL	bp	104	-	69,74,74	1.14	5 (7%)	79,115,115	1.45	10 (12%)
13	V7N	BC	101	-	44,44,44	1.66	6 (13%)	48,54,54	1.55	11 (22%)
13	V7N	aj	103	-	44,44,44	1.69	8 (18%)	48,54,54	1.69	13 (27%)
11	BCL	bf	103	-	69,74,74	1.13	5 (7%)	79,115,115	1.38	12 (15%)
11	BCL	ap	1001	-	69,74,74	1.15	5 (7%)	79,115,115	1.38	10 (12%)
12	LMT	AV	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.95	2 (4%)
13	V7N	BN	1001	-	44,44,44	1.65	7 (15%)	48,54,54	1.60	10 (20%)
12	LMT	BA	101	-	36,36,36	1.04	4 (11%)	47,47,47	0.93	1 (2%)
11	BCL	BX	103	-	69,74,74	1.12	5 (7%)	79,115,115	1.31	9 (11%)
12	LMT	BR	104	-	36,36,36	1.05	4 (11%)	47,47,47	1.02	2 (4%)
12	LMT	bl	102	-	36,36,36	1.04	4 (11%)	47,47,47	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGW	H1	1003	-	50,50,50	0.46	0	53,56,56	0.94	3 (5%)
11	BCL	AH	102	26	69,74,74	1.15	6 (8%)	79,115,115	1.46	14 (17%)
12	LMT	BQ	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.92	1 (2%)
11	BCL	AP	101	26	69,74,74	1.13	6 (8%)	79,115,115	1.50	11 (13%)
14	0V9	H1	1002	-	44,44,46	0.77	1 (2%)	47,49,51	0.86	0
12	LMT	BB	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.78	1 (2%)
14	0V9	bn	102	-	44,44,46	0.76	1 (2%)	47,49,51	0.83	1 (2%)
14	0V9	be	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.97	3 (6%)
12	LMT	L	301	-	36,36,36	1.11	4 (11%)	47,47,47	0.85	0
12	LMT	BT	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.85	0
12	LMT	BH	1002	-	36,36,36	1.08	4 (11%)	47,47,47	0.99	2 (4%)
14	0V9	bk	1003	-	44,44,46	0.77	1 (2%)	47,49,51	0.95	2 (4%)
12	LMT	BI	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.86	2 (4%)
11	BCL	BR	102	-	69,74,74	1.12	5 (7%)	79,115,115	1.38	11 (13%)
12	LMT	BC	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.82	2 (4%)
13	V7N	bd	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.64	12 (25%)
11	BCL	AT	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	7 (8%)
12	LMT	BX	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.90	2 (4%)
21	BPH	M	404	-	59,70,70	1.11	3 (5%)	59,101,101	1.88	12 (20%)
12	LMT	BJ	1002	-	36,36,36	1.03	4 (11%)	47,47,47	0.92	2 (4%)
11	BCL	ba	103	-	69,74,74	1.13	5 (7%)	79,115,115	1.26	9 (11%)
12	LMT	bf	102	-	36,36,36	1.04	4 (11%)	47,47,47	1.00	1 (2%)
12	LMT	BI	105	-	36,36,36	1.06	4 (11%)	47,47,47	0.93	2 (4%)
11	BCL	AS	101	-	69,74,74	1.18	5 (7%)	79,115,115	1.34	9 (11%)
12	LMT	BW	1004	-	36,36,36	1.06	4 (11%)	47,47,47	1.00	3 (6%)
11	BCL	AD	102	-	69,74,74	1.14	5 (7%)	79,115,115	1.36	10 (12%)
11	BCL	bk	1002	-	69,74,74	1.12	5 (7%)	79,115,115	1.39	12 (15%)
13	V7N	BL	1001	-	44,44,44	1.65	8 (18%)	48,54,54	1.61	11 (22%)
13	V7N	bh	101	-	44,44,44	1.67	7 (15%)	48,54,54	1.58	10 (20%)
11	BCL	BF	102	-	69,74,74	1.10	5 (7%)	79,115,115	1.30	9 (11%)
13	V7N	bp	101	-	44,44,44	1.69	7 (15%)	48,54,54	1.65	12 (25%)
13	V7N	AQ	104	-	44,44,44	1.67	8 (18%)	48,54,54	1.75	14 (29%)
12	LMT	BG	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.88	2 (4%)
12	LMT	BS	1004	-	36,36,36	1.05	4 (11%)	47,47,47	0.92	2 (4%)
12	LMT	bj	102	-	36,36,36	1.06	4 (11%)	47,47,47	0.95	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AS	102	26	69,74,74	1.12	5 (7%)	79,115,115	1.32	10 (12%)
11	BCL	AF	101	-	69,74,74	1.19	6 (8%)	79,115,115	1.37	10 (12%)
12	LMT	BB	104	-	36,36,36	1.06	4 (11%)	47,47,47	1.09	2 (4%)
12	LMT	bc	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.83	1 (2%)
24	V7B	ag	103	-	59,59,59	0.89	4 (6%)	75,75,75	1.01	4 (5%)
12	LMT	AP	103	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	0
11	BCL	AQ	102	-	69,74,74	1.17	5 (7%)	79,115,115	1.31	7 (8%)
12	LMT	BB	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.90	2 (4%)
11	BCL	ae	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.34	9 (11%)
13	V7N	BH	1001	-	44,44,44	1.67	7 (15%)	48,54,54	1.56	11 (22%)
11	BCL	bd	103	-	69,74,74	1.14	5 (7%)	79,115,115	1.41	13 (16%)
12	LMT	AE	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.97	2 (4%)
12	LMT	AH	103	-	36,36,36	1.07	4 (11%)	47,47,47	0.95	2 (4%)
13	V7N	BP	1001	-	44,44,44	1.67	7 (15%)	48,54,54	1.62	13 (27%)
12	LMT	AR	103	-	36,36,36	1.03	4 (11%)	47,47,47	0.94	2 (4%)
11	BCL	M	403	-	69,74,74	1.14	5 (7%)	79,115,115	1.36	9 (11%)
11	BCL	BD	103	-	69,74,74	1.12	5 (7%)	79,115,115	1.32	9 (11%)
12	LMT	AT	104	-	36,36,36	1.05	4 (11%)	47,47,47	1.05	1 (2%)
13	V7N	BW	1001	-	44,44,44	1.65	7 (15%)	48,54,54	1.57	11 (22%)
13	V7N	AB	101	-	44,44,44	1.68	8 (18%)	48,54,54	1.63	14 (29%)
11	BCL	AR	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.31	7 (8%)
11	BCL	am	1001	-	69,74,74	1.13	5 (7%)	79,115,115	1.32	9 (11%)
11	BCL	BG	1003	-	69,74,74	1.13	5 (7%)	79,115,115	1.33	10 (12%)
12	LMT	BN	1005	-	36,36,36	1.04	5 (13%)	47,47,47	0.92	2 (4%)
12	LMT	BH	1003	-	36,36,36	1.04	4 (11%)	47,47,47	0.95	1 (2%)
11	BCL	bm	103	-	69,74,74	1.12	5 (7%)	79,115,115	1.28	10 (12%)
12	LMT	bb	105	-	36,36,36	1.06	4 (11%)	47,47,47	0.92	2 (4%)
12	LMT	BC	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.88	1 (2%)
12	LMT	BM	1002	-	36,36,36	1.04	4 (11%)	47,47,47	1.02	2 (4%)
12	LMT	AN	101	-	36,36,36	1.05	4 (11%)	47,47,47	0.93	2 (4%)
12	LMT	bm	102	-	36,36,36	1.05	4 (11%)	47,47,47	0.89	2 (4%)
12	LMT	BR	103	-	36,36,36	1.01	4 (11%)	47,47,47	0.92	1 (2%)
12	LMT	BJ	1003	-	36,36,36	1.05	4 (11%)	47,47,47	0.91	1 (2%)
12	LMT	AS	103	-	36,36,36	1.08	4 (11%)	47,47,47	1.04	3 (6%)
21	BPH	L	309	-	59,70,70	1.12	4 (6%)	59,101,101	1.84	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AL	103	-	69,74,74	1.17	5 (7%)	79,115,115	1.61	13 (16%)
11	BCL	M	406	-	69,74,74	1.13	5 (7%)	79,115,115	1.30	8 (10%)
12	LMT	AL	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.96	1 (2%)
12	LMT	BN	1002	-	36,36,36	1.03	4 (11%)	47,47,47	0.85	1 (2%)
13	V7N	BO	1001	-	44,44,44	1.67	7 (15%)	48,54,54	1.66	12 (25%)
12	LMT	BV	1005	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	3 (6%)
14	0V9	bf	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.88	3 (6%)
12	LMT	BA	105	-	36,36,36	1.05	4 (11%)	47,47,47	1.09	2 (4%)
12	LMT	AD	103	-	36,36,36	1.05	4 (11%)	47,47,47	0.94	3 (6%)
13	V7N	AT	103	-	44,44,44	1.68	7 (15%)	48,54,54	1.52	9 (18%)
13	V7N	BK	1001	-	44,44,44	1.65	6 (13%)	48,54,54	1.56	10 (20%)
15	HEC	C	404	3	46,50,50	1.84	5 (10%)	58,82,82	1.68	7 (12%)
11	BCL	BB	105	-	69,74,74	1.12	5 (7%)	79,115,115	1.35	9 (11%)
14	0V9	aj	101	-	44,44,46	0.76	1 (2%)	47,49,51	0.83	1 (2%)
18	CD4	ag	101	-	83,83,83	0.47	0	89,95,95	1.07	4 (4%)
11	BCL	AK	102	-	69,74,74	1.16	5 (7%)	79,115,115	1.29	7 (8%)
12	LMT	AA	1003	-	36,36,36	1.07	4 (11%)	47,47,47	1.08	3 (6%)
12	LMT	BG	1002	-	36,36,36	1.05	4 (11%)	47,47,47	1.02	3 (6%)
13	V7N	BJ	1001	-	44,44,44	1.65	8 (18%)	48,54,54	1.61	10 (20%)
13	V7N	bi	102	-	44,44,44	1.68	7 (15%)	48,54,54	1.60	12 (25%)
12	LMT	BS	1002	-	36,36,36	1.06	4 (11%)	47,47,47	0.91	1 (2%)
12	LMT	BP	1005	-	36,36,36	1.07	5 (13%)	47,47,47	1.00	4 (8%)
12	LMT	AE	106	-	36,36,36	1.06	4 (11%)	47,47,47	0.91	0
11	BCL	BO	1005	-	69,74,74	1.11	5 (7%)	79,115,115	1.28	9 (11%)
12	LMT	L	308	-	36,36,36	1.04	4 (11%)	47,47,47	0.87	1 (2%)
11	BCL	aa	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.31	7 (8%)
11	BCL	BK	1005	-	69,74,74	1.14	5 (7%)	79,115,115	1.42	11 (13%)
23	CRT	M	405	-	43,43,43	0.60	0	48,54,54	0.88	3 (6%)
12	LMT	BE	104	-	36,36,36	1.07	4 (11%)	47,47,47	1.29	6 (12%)
12	LMT	BG	1005	-	36,36,36	1.07	4 (11%)	47,47,47	0.81	1 (2%)
12	LMT	BF	104	-	36,36,36	1.06	4 (11%)	47,47,47	1.13	4 (8%)
12	LMT	BM	1003	-	36,36,36	1.07	4 (11%)	47,47,47	0.94	1 (2%)
14	0V9	AQ	105	-	44,44,46	0.76	1 (2%)	47,49,51	0.80	1 (2%)
12	LMT	AM	103	-	36,36,36	1.05	4 (11%)	47,47,47	0.95	2 (4%)
11	BCL	BL	1005	-	69,74,74	1.11	5 (7%)	79,115,115	1.28	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LMT	bp	102	-	36,36,36	1.04	4 (11%)	47,47,47	0.88	2 (4%)
13	V7N	BG	1001	-	44,44,44	1.66	8 (18%)	48,54,54	1.56	8 (16%)
14	0V9	bb	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.86	2 (4%)
12	LMT	BA	104	-	36,36,36	1.05	4 (11%)	47,47,47	0.87	0
14	0V9	bm	104	-	44,44,46	0.77	1 (2%)	47,49,51	0.89	2 (4%)
11	BCL	AV	101	-	69,74,74	1.15	5 (7%)	79,115,115	1.28	7 (8%)
11	BCL	BP	1002	-	69,74,74	1.12	5 (7%)	79,115,115	1.36	10 (12%)
11	BCL	bl	104	-	69,74,74	1.14	6 (8%)	79,115,115	1.36	9 (11%)
20	MQ8	L	302	-	54,54,54	0.66	0	67,69,69	0.71	1 (1%)
12	LMT	BR	101	-	36,36,36	1.05	4 (11%)	47,47,47	0.91	0
11	BCL	BS	1006	-	69,74,74	1.20	6 (8%)	79,115,115	1.70	12 (15%)
11	BCL	BH	1004	-	69,74,74	1.11	5 (7%)	79,115,115	1.38	11 (13%)
12	LMT	BU	1002	-	36,36,36	1.03	4 (11%)	47,47,47	1.04	2 (4%)
15	HEC	C	402	3	46,50,50	1.83	5 (10%)	58,82,82	1.67	6 (10%)
11	BCL	AP	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.37	9 (11%)
11	BCL	ak	101	-	69,74,74	1.14	5 (7%)	79,115,115	1.32	9 (11%)
12	LMT	BN	1003	-	36,36,36	1.06	4 (11%)	47,47,47	1.01	2 (4%)
11	BCL	BT	1002	-	69,74,74	1.14	5 (7%)	79,115,115	1.39	11 (13%)
12	LMT	BU	1004	-	36,36,36	1.05	4 (11%)	47,47,47	1.07	4 (8%)
11	BCL	AJ	102	-	69,74,74	1.16	5 (7%)	79,115,115	1.32	7 (8%)
18	CD4	ad	101	-	83,83,83	0.49	0	89,95,95	1.03	6 (6%)
12	LMT	BH	1005	-	36,36,36	1.07	4 (11%)	47,47,47	0.92	1 (2%)
12	LMT	BK	1002	-	36,36,36	1.06	4 (11%)	47,47,47	0.94	2 (4%)
13	V7N	BV	1001	-	44,44,44	1.68	7 (15%)	48,54,54	1.72	12 (25%)
12	LMT	AG	103	-	36,36,36	1.07	4 (11%)	47,47,47	1.02	3 (6%)
11	BCL	AB	103	-	69,74,74	1.11	5 (7%)	79,115,115	1.38	11 (13%)
11	BCL	L	303	-	69,74,74	1.11	5 (7%)	79,115,115	1.28	7 (8%)
12	LMT	AL	101	-	36,36,36	1.05	4 (11%)	47,47,47	0.85	0
11	BCL	AS	104	26	69,74,74	1.16	6 (8%)	79,115,115	1.54	14 (17%)
11	BCL	AE	103	-	69,74,74	1.15	5 (7%)	79,115,115	1.32	7 (8%)
12	LMT	BS	1003	-	36,36,36	1.03	4 (11%)	47,47,47	0.92	1 (2%)
13	V7N	AE	101	-	44,44,44	1.69	7 (15%)	48,54,54	1.44	6 (12%)

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	LMT	bg	1001	-	-	8/21/61/61	0/2/2/2
11	BCL	AN	102	26	-	3/41/137/137	-
11	BCL	AX	101	-	-	4/41/137/137	-
12	LMT	ac	1001	-	-	4/21/61/61	0/2/2/2
13	V7N	bj	101	-	-	7/53/53/53	-
12	LMT	BP	1003	-	-	5/21/61/61	0/2/2/2
14	0V9	bj	103	-	-	9/48/48/50	-
12	LMT	BD	104	-	-	5/21/61/61	0/2/2/2
11	BCL	bg	1002	-	-	7/41/137/137	-
13	V7N	AE	105	-	-	7/53/53/53	-
13	V7N	BE	101	-	-	5/53/53/53	-
11	BCL	AC	1001	-	-	4/41/137/137	-
12	LMT	AK	101	-	-	6/21/61/61	0/2/2/2
11	BCL	AF	102	-	-	3/41/137/137	-
12	LMT	AQ	103	-	-	4/21/61/61	0/2/2/2
12	LMT	BV	1004	-	-	3/21/61/61	0/2/2/2
11	BCL	BM	1004	-	-	3/41/137/137	-
12	LMT	ba	101	-	-	5/21/61/61	0/2/2/2
14	0V9	bo	104	-	-	10/48/48/50	-
11	BCL	AM	101	26	-	5/41/137/137	-
13	V7N	bn	101	-	-	8/53/53/53	-
18	CD4	M	409	-	-	20/94/94/94	-
14	0V9	L	310	-	-	9/48/48/50	-
13	V7N	ba	102	-	-	7/53/53/53	-
13	V7N	bm	101	-	-	4/53/53/53	-
11	BCL	AV	104	26	-	10/41/137/137	-
11	BCL	BA	103	-	-	5/41/137/137	-
11	BCL	AB	105	-	-	6/41/137/137	-
12	LMT	BL	1006	-	-	5/21/61/61	0/2/2/2
11	BCL	AV	102	26	-	3/41/137/137	-
11	BCL	AH	101	-	-	0/41/137/137	-
12	LMT	BM	1005	-	-	4/21/61/61	0/2/2/2
11	BCL	AM	102	-	-	2/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	bd	102	-	-	7/21/61/61	0/2/2/2
12	LMT	BX	102	-	-	7/21/61/61	0/2/2/2
12	LMT	BO	1002	-	-	4/21/61/61	0/2/2/2
12	LMT	BQ	1003	-	-	5/21/61/61	0/2/2/2
12	LMT	BL	1004	-	-	4/21/61/61	0/2/2/2
12	LMT	BD	102	-	-	1/21/61/61	0/2/2/2
11	BCL	AI	103	-	-	2/41/137/137	-
11	BCL	AW	103	-	-	8/41/137/137	-
11	BCL	AU	101	-	-	4/41/137/137	-
11	BCL	al	1001	-	-	4/41/137/137	-
14	0V9	bi	105	-	-	9/48/48/50	-
11	BCL	ab	101	-	-	6/41/137/137	-
12	LMT	BO	1004	-	-	2/21/61/61	0/2/2/2
11	BCL	AW	101	-	-	2/41/137/137	-
12	LMT	bo	103	-	-	9/21/61/61	0/2/2/2
11	BCL	ag	102	-	-	3/41/137/137	-
12	LMT	BK	1004	-	-	6/21/61/61	0/2/2/2
12	LMT	AJ	103	-	-	6/21/61/61	0/2/2/2
14	0V9	bc	103	-	-	12/48/48/50	-
11	BCL	AJ	101	26	-	5/41/137/137	-
11	BCL	bc	104	-	-	6/41/137/137	-
12	LMT	BK	1003	-	-	2/21/61/61	0/2/2/2
24	V7B	af	101	-	-	7/48/88/88	0/2/2/2
11	BCL	AQ	101	26	-	7/41/137/137	-
15	HEC	C	403	3	-	4/14/54/54	-
12	LMT	bn	103	-	-	8/21/61/61	0/2/2/2
12	LMT	BT	1003	-	-	7/21/61/61	0/2/2/2
11	BCL	AN	105	-	-	6/41/137/137	-
12	LMT	BS	1005	-	-	4/21/61/61	0/2/2/2
11	BCL	AR	101	-	-	7/41/137/137	-
12	LMT	BF	103	-	-	7/21/61/61	0/2/2/2
15	HEC	C	401	3	-	6/14/54/54	-
13	V7N	bb	101	-	-	10/53/53/53	-
11	BCL	BE	103	-	-	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	BW	1002	-	-	6/41/137/137	-
11	BCL	ao	102	-	-	6/41/137/137	-
12	LMT	BL	1003	-	-	5/21/61/61	0/2/2/2
12	LMT	BV	1003	-	-	4/21/61/61	0/2/2/2
14	0V9	AJ	104	-	-	19/48/48/50	-
17	V75	M	410	10,16	-	0/12/29/29	0/1/1/1
11	BCL	AL	102	-	-	6/41/137/137	-
12	LMT	AK	104	-	-	5/21/61/61	0/2/2/2
12	LMT	BA	102	-	-	5/21/61/61	0/2/2/2
14	0V9	bp	103	-	-	12/48/48/50	-
18	CD4	H1	1001	-	-	23/94/94/94	-
11	BCL	bj	104	-	-	7/41/137/137	-
11	BCL	bh	102	-	-	12/41/137/137	-
13	V7N	BT	1001	-	-	3/53/53/53	-
12	LMT	BO	1003	-	-	5/21/61/61	0/2/2/2
12	LMT	AN	104	-	-	0/21/61/61	0/2/2/2
14	0V9	bd	104	-	-	7/48/48/50	-
13	V7N	BQ	1001	-	-	8/53/53/53	-
25	UYH	ai	102	-	-	11/50/70/70	0/1/1/1
12	LMT	BT	1005	-	-	4/21/61/61	0/2/2/2
12	LMT	L	306	-	-	4/21/61/61	0/2/2/2
11	BCL	aj	102	-	-	7/41/137/137	-
12	LMT	BF	101	-	-	4/21/61/61	0/2/2/2
11	BCL	an	1001	-	-	3/41/137/137	-
12	LMT	BI	101	-	-	5/21/61/61	0/2/2/2
12	LMT	L	305	-	-	1/21/61/61	0/2/2/2
11	BCL	bn	104	-	-	9/41/137/137	-
16	NDG	C	405	17	-	0/6/23/26	0/1/1/1
13	V7N	bl	101	-	-	7/53/53/53	-
11	BCL	AG	101	-	-	1/41/137/137	-
12	LMT	H2	201	-	-	4/21/61/61	0/2/2/2
11	BCL	BN	1004	-	-	8/41/137/137	-
12	LMT	BW	1003	-	-	4/21/61/61	0/2/2/2
13	V7N	be	102	-	-	4/53/53/53	-
11	BCL	ac	1002	-	-	3/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	bk	1001	-	-	7/21/61/61	0/2/2/2
12	LMT	bi	104	-	-	4/21/61/61	0/2/2/2
14	0V9	bi	103	-	-	9/48/48/50	-
13	V7N	af	103	-	-	7/53/53/53	-
11	BCL	bo	105	-	-	4/41/137/137	-
11	BCL	ad	102	-	-	7/41/137/137	-
11	BCL	BJ	1004	-	-	7/41/137/137	-
11	BCL	AU	102	-	-	2/41/137/137	-
12	LMT	AB	104	-	-	2/21/61/61	0/2/2/2
18	CD4	ae	102	-	-	23/94/94/94	-
11	BCL	AK	103	26	-	10/41/137/137	-
12	LMT	M	408	-	-	4/21/61/61	0/2/2/2
14	0V9	bb	102	-	-	11/48/48/50	-
13	V7N	BM	1001	-	-	4/53/53/53	-
13	V7N	BS	1001	-	-	4/53/53/53	-
11	BCL	af	102	-	-	7/41/137/137	-
11	BCL	AN	103	-	-	4/41/137/137	-
12	LMT	be	103	-	-	5/21/61/61	0/2/2/2
12	LMT	BU	1003	-	-	2/21/61/61	0/2/2/2
12	LMT	BC	104	-	-	4/21/61/61	0/2/2/2
11	BCL	bb	103	-	-	9/41/137/137	-
12	LMT	BD	105	-	-	4/21/61/61	0/2/2/2
11	BCL	AB	102	26	-	3/41/137/137	-
12	LMT	BE	102	-	-	5/21/61/61	0/2/2/2
12	LMT	be	101	-	-	3/21/61/61	0/2/2/2
12	LMT	AT	102	-	-	6/21/61/61	0/2/2/2
12	LMT	bo	101	-	-	1/21/61/61	0/2/2/2
11	BCL	AI	101	-	-	7/41/137/137	-
13	V7N	bc	101	-	-	6/53/53/53	-
13	V7N	BB	101	-	-	9/53/53/53	-
11	BCL	AD	101	26	-	11/41/137/137	-
11	BCL	BC	105	-	-	1/41/137/137	-
12	LMT	BI	103	-	-	7/21/61/61	0/2/2/2
11	BCL	ai	101	-	-	5/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	V7N	bo	102	-	-	8/53/53/53	-
12	LMT	bi	101	-	-	1/21/61/61	0/2/2/2
18	CD4	M	402	-	-	15/94/94/94	-
11	BCL	L	304	-	-	3/41/137/137	-
13	V7N	AH	104	-	-	6/53/53/53	-
12	LMT	BL	1002	-	-	5/21/61/61	0/2/2/2
20	MQ8	ao	101	-	-	10/47/67/67	0/2/2/2
11	BCL	BQ	1002	-	-	7/41/137/137	-
17	V75	C	406	10,16	-	0/12/29/29	0/1/1/1
11	BCL	AE	102	-	-	11/41/137/137	-
11	BCL	AA	1002	26	-	5/41/137/137	-
11	BCL	AA	1001	-	-	1/41/137/137	-
11	BCL	bi	106	-	-	10/41/137/137	-
11	BCL	ah	1001	-	-	5/41/137/137	-
14	0V9	bl	103	-	-	8/48/48/50	-
12	LMT	BP	1004	-	-	0/21/61/61	0/2/2/2
12	LMT	L	307	-	-	2/21/61/61	0/2/2/2
12	LMT	AH	105	-	-	7/21/61/61	0/2/2/2
20	MQ8	M	407	-	-	3/47/67/67	0/2/2/2
13	V7N	bf	101	-	-	5/53/53/53	-
11	BCL	AG	102	26	-	8/41/137/137	-
12	LMT	BD	101	-	-	8/21/61/61	0/2/2/2
11	BCL	AO	101	-	-	1/41/137/137	-
11	BCL	BV	1002	-	-	7/41/137/137	-
16	NDG	C1	301	17	-	0/6/23/26	0/1/1/1
11	BCL	BI	102	-	-	9/41/137/137	-
11	BCL	be	105	-	-	4/41/137/137	-
12	LMT	AI	102	-	-	3/21/61/61	0/2/2/2
12	LMT	AW	102	-	-	1/21/61/61	0/2/2/2
13	V7N	AW	104	-	-	6/53/53/53	-
11	BCL	BU	1001	-	-	6/41/137/137	-
11	BCL	bp	104	-	-	8/41/137/137	-
13	V7N	BC	101	-	-	6/53/53/53	-
13	V7N	aj	103	-	-	5/53/53/53	-
11	BCL	bf	103	-	-	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	ap	1001	-	-	5/41/137/137	-
12	LMT	AV	103	-	-	7/21/61/61	0/2/2/2
13	V7N	BN	1001	-	-	4/53/53/53	-
12	LMT	BA	101	-	-	4/21/61/61	0/2/2/2
11	BCL	BX	103	-	-	7/41/137/137	-
12	LMT	BR	104	-	-	6/21/61/61	0/2/2/2
12	LMT	bl	102	-	-	5/21/61/61	0/2/2/2
19	PGW	H1	1003	-	-	17/55/55/55	-
11	BCL	AH	102	26	-	10/41/137/137	-
12	LMT	BQ	1004	-	-	0/21/61/61	0/2/2/2
11	BCL	AP	101	26	-	4/41/137/137	-
14	0V9	H1	1002	-	-	10/48/48/50	-
12	LMT	BB	103	-	-	3/21/61/61	0/2/2/2
14	0V9	bn	102	-	-	11/48/48/50	-
14	0V9	be	104	-	-	9/48/48/50	-
12	LMT	L	301	-	-	3/21/61/61	0/2/2/2
12	LMT	BT	1004	-	-	5/21/61/61	0/2/2/2
12	LMT	BH	1002	-	-	3/21/61/61	0/2/2/2
14	0V9	bk	1003	-	-	16/48/48/50	-
12	LMT	BI	104	-	-	2/21/61/61	0/2/2/2
11	BCL	BR	102	-	-	4/41/137/137	-
12	LMT	BC	103	-	-	2/21/61/61	0/2/2/2
13	V7N	bd	101	-	-	4/53/53/53	-
11	BCL	AT	101	-	-	0/41/137/137	-
12	LMT	BX	101	-	-	4/21/61/61	0/2/2/2
21	BPH	M	404	-	-	5/37/105/105	0/5/6/6
12	LMT	BJ	1002	-	-	8/21/61/61	0/2/2/2
11	BCL	ba	103	-	-	2/41/137/137	-
12	LMT	bf	102	-	-	8/21/61/61	0/2/2/2
12	LMT	BI	105	-	-	1/21/61/61	0/2/2/2
11	BCL	AS	101	-	-	3/41/137/137	-
12	LMT	BW	1004	-	-	4/21/61/61	0/2/2/2
11	BCL	AD	102	-	-	1/41/137/137	-
11	BCL	bk	1002	-	-	7/41/137/137	-
13	V7N	BL	1001	-	-	4/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	V7N	bh	101	-	-	5/53/53/53	-
11	BCL	BF	102	-	-	10/41/137/137	-
13	V7N	bp	101	-	-	5/53/53/53	-
13	V7N	AQ	104	-	-	6/53/53/53	-
12	LMT	BG	1004	-	-	2/21/61/61	0/2/2/2
12	LMT	BS	1004	-	-	5/21/61/61	0/2/2/2
12	LMT	bj	102	-	-	4/21/61/61	0/2/2/2
11	BCL	AS	102	26	-	7/41/137/137	-
11	BCL	AF	101	-	-	8/41/137/137	-
12	LMT	BB	104	-	-	3/21/61/61	0/2/2/2
12	LMT	bc	102	-	-	6/21/61/61	0/2/2/2
24	V7B	ag	103	-	-	13/48/88/88	0/2/2/2
12	LMT	AP	103	-	-	7/21/61/61	0/2/2/2
11	BCL	AQ	102	-	-	2/41/137/137	-
12	LMT	BB	102	-	-	1/21/61/61	0/2/2/2
11	BCL	ae	101	-	-	7/41/137/137	-
13	V7N	BH	1001	-	-	4/53/53/53	-
11	BCL	bd	103	-	-	10/41/137/137	-
12	LMT	AE	104	-	-	5/21/61/61	0/2/2/2
12	LMT	AH	103	-	-	6/21/61/61	0/2/2/2
13	V7N	BP	1001	-	-	5/53/53/53	-
12	LMT	AR	103	-	-	6/21/61/61	0/2/2/2
11	BCL	M	403	-	-	2/41/137/137	-
11	BCL	BD	103	-	-	4/41/137/137	-
12	LMT	AT	104	-	-	7/21/61/61	0/2/2/2
13	V7N	BW	1001	-	-	6/53/53/53	-
13	V7N	AB	101	-	-	5/53/53/53	-
11	BCL	AR	102	-	-	5/41/137/137	-
11	BCL	am	1001	-	-	8/41/137/137	-
11	BCL	BG	1003	-	-	9/41/137/137	-
12	LMT	BN	1005	-	-	1/21/61/61	0/2/2/2
12	LMT	BH	1003	-	-	4/21/61/61	0/2/2/2
11	BCL	bm	103	-	-	7/41/137/137	-
12	LMT	bb	105	-	-	6/21/61/61	0/2/2/2
12	LMT	BC	102	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	BM	1002	-	-	5/21/61/61	0/2/2/2
12	LMT	AN	101	-	-	8/21/61/61	0/2/2/2
12	LMT	bm	102	-	-	2/21/61/61	0/2/2/2
12	LMT	BR	103	-	-	7/21/61/61	0/2/2/2
12	LMT	BJ	1003	-	-	2/21/61/61	0/2/2/2
12	LMT	AS	103	-	-	8/21/61/61	0/2/2/2
21	BPH	L	309	-	-	3/37/105/105	0/5/6/6
11	BCL	AL	103	-	-	7/41/137/137	-
11	BCL	M	406	-	-	7/41/137/137	-
12	LMT	AL	104	-	-	7/21/61/61	0/2/2/2
12	LMT	BN	1002	-	-	4/21/61/61	0/2/2/2
13	V7N	BO	1001	-	-	8/53/53/53	-
12	LMT	BV	1005	-	-	2/21/61/61	0/2/2/2
14	0V9	bf	104	-	-	13/48/48/50	-
12	LMT	BA	105	-	-	6/21/61/61	0/2/2/2
12	LMT	AD	103	-	-	5/21/61/61	0/2/2/2
13	V7N	AT	103	-	-	8/53/53/53	-
13	V7N	BK	1001	-	-	6/53/53/53	-
15	HEC	C	404	3	-	8/14/54/54	-
11	BCL	BB	105	-	-	8/41/137/137	-
14	0V9	aj	101	-	-	11/48/48/50	-
18	CD4	ag	101	-	-	16/94/94/94	-
11	BCL	AK	102	-	-	0/41/137/137	-
12	LMT	AA	1003	-	-	8/21/61/61	0/2/2/2
12	LMT	BG	1002	-	-	8/21/61/61	0/2/2/2
13	V7N	BJ	1001	-	-	3/53/53/53	-
13	V7N	bi	102	-	-	5/53/53/53	-
12	LMT	BS	1002	-	-	5/21/61/61	0/2/2/2
12	LMT	BP	1005	-	-	5/21/61/61	0/2/2/2
12	LMT	AE	106	-	-	3/21/61/61	0/2/2/2
11	BCL	BO	1005	-	-	6/41/137/137	-
12	LMT	L	308	-	-	3/21/61/61	0/2/2/2
11	BCL	aa	1001	-	-	4/41/137/137	-
11	BCL	BK	1005	-	-	6/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CRT	M	405	-	-	6/51/51/51	-
12	LMT	BE	104	-	-	4/21/61/61	0/2/2/2
12	LMT	BG	1005	-	-	1/21/61/61	0/2/2/2
12	LMT	BF	104	-	-	6/21/61/61	0/2/2/2
12	LMT	BM	1003	-	-	2/21/61/61	0/2/2/2
14	0V9	AQ	105	-	-	10/48/48/50	-
12	LMT	AM	103	-	-	5/21/61/61	0/2/2/2
11	BCL	BL	1005	-	-	7/41/137/137	-
12	LMT	bp	102	-	-	4/21/61/61	0/2/2/2
13	V7N	BG	1001	-	-	2/53/53/53	-
14	0V9	bb	104	-	-	5/48/48/50	-
12	LMT	BA	104	-	-	6/21/61/61	0/2/2/2
14	0V9	bm	104	-	-	12/48/48/50	-
11	BCL	AV	101	-	-	2/41/137/137	-
11	BCL	BP	1002	-	-	7/41/137/137	-
11	BCL	bl	104	-	-	6/41/137/137	-
20	MQ8	L	302	-	-	10/47/67/67	0/2/2/2
12	LMT	BR	101	-	-	5/21/61/61	0/2/2/2
11	BCL	BS	1006	-	-	7/41/137/137	-
11	BCL	BH	1004	-	-	5/41/137/137	-
12	LMT	BU	1002	-	-	5/21/61/61	0/2/2/2
15	HEC	C	402	3	-	9/14/54/54	-
11	BCL	AP	102	-	-	5/41/137/137	-
11	BCL	ak	101	-	-	11/41/137/137	-
12	LMT	BN	1003	-	-	5/21/61/61	0/2/2/2
11	BCL	BT	1002	-	-	7/41/137/137	-
12	LMT	BU	1004	-	-	5/21/61/61	0/2/2/2
11	BCL	AJ	102	-	-	4/41/137/137	-
18	CD4	ad	101	-	-	15/94/94/94	-
12	LMT	BH	1005	-	-	5/21/61/61	0/2/2/2
12	LMT	BK	1002	-	-	6/21/61/61	0/2/2/2
13	V7N	BV	1001	-	-	4/53/53/53	-
12	LMT	AG	103	-	-	8/21/61/61	0/2/2/2
11	BCL	AB	103	-	-	1/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	L	303	-	-	4/41/137/137	-
12	LMT	AL	101	-	-	5/21/61/61	0/2/2/2
11	BCL	AS	104	26	-	4/41/137/137	-
11	BCL	AE	103	-	-	1/41/137/137	-
12	LMT	BS	1003	-	-	6/21/61/61	0/2/2/2
13	V7N	AE	101	-	-	1/53/53/53	-

The worst 5 of 1413 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bn	101	V7N	C28-C27	6.98	1.52	1.34
13	ba	102	V7N	C28-C27	6.96	1.52	1.34
13	AE	101	V7N	C28-C27	6.91	1.52	1.34
13	BH	1001	V7N	C28-C27	6.90	1.52	1.34
13	AW	104	V7N	C28-C27	6.90	1.52	1.34

The worst 5 of 1854 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	M	404	BPH	C4D-CHA-CBD	-10.45	103.44	108.45
11	ab	101	BCL	C1-C2-C3	10.30	143.08	126.20
21	L	309	BPH	C4D-CHA-CBD	-9.74	103.78	108.45
11	BS	1006	BCL	C1-O2A-CGA	8.62	137.53	116.65
11	AQ	101	BCL	C1-O2A-CGA	7.61	135.08	116.65

There are no chirality outliers.

5 of 1803 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AD	101	BCL	C3A-C2A-CAA-CBA
11	AE	102	BCL	C3A-C2A-CAA-CBA
11	AF	101	BCL	C1A-C2A-CAA-CBA
11	AF	101	BCL	CAD-CBD-CGD-O2D
11	AH	102	BCL	C3A-C2A-CAA-CBA

There are no ring outliers.

89 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AN	102	BCL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AX	101	BCL	2	0
11	bg	1002	BCL	1	0
11	AC	1001	BCL	1	0
12	AK	101	LMT	1	0
11	AF	102	BCL	1	0
11	AM	101	BCL	1	0
11	AV	104	BCL	1	0
12	BL	1006	LMT	1	0
11	AH	101	BCL	1	0
11	AM	102	BCL	1	0
12	BO	1002	LMT	1	0
11	AI	103	BCL	1	0
11	AW	103	BCL	1	0
11	AU	101	BCL	1	0
11	ab	101	BCL	2	0
12	BO	1004	LMT	1	0
11	AW	101	BCL	1	0
11	ag	102	BCL	1	0
11	bc	104	BCL	1	0
15	C	403	HEC	1	0
12	BT	1003	LMT	1	0
11	AN	105	BCL	1	0
12	BS	1005	LMT	1	0
12	BF	103	LMT	1	0
15	C	401	HEC	1	0
11	ao	102	BCL	1	0
11	AL	102	BCL	1	0
18	H1	1001	CD4	1	0
11	bj	104	BCL	1	0
11	bh	102	BCL	1	0
11	aj	102	BCL	1	0
11	an	1001	BCL	1	0
11	bn	104	BCL	1	0
11	AG	101	BCL	1	0
11	AU	102	BCL	1	0
18	ae	102	CD4	2	0
11	AK	103	BCL	2	0
11	af	102	BCL	2	0
11	AN	103	BCL	1	0
11	bb	103	BCL	1	0
11	AB	102	BCL	2	0
11	L	304	BCL	1	0

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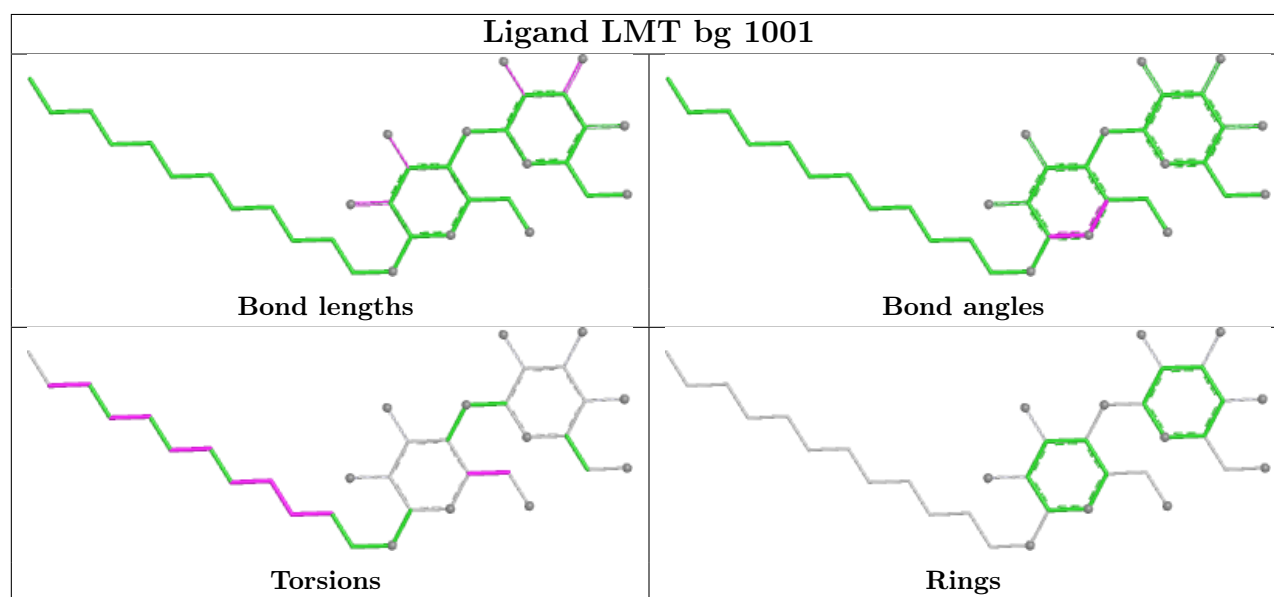
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	ao	101	MQ8	1	0
11	AA	1001	BCL	3	0
12	BP	1004	LMT	1	0
12	AH	105	LMT	1	0
11	AO	101	BCL	1	0
11	BU	1001	BCL	1	0
11	bf	103	BCL	1	0
19	H1	1003	PGW	2	0
12	BT	1004	LMT	1	0
11	AT	101	BCL	1	0
21	M	404	BPH	2	0
11	AS	101	BCL	1	0
11	AD	102	BCL	1	0
11	bk	1002	BCL	1	0
11	AF	101	BCL	1	0
12	AP	103	LMT	1	0
11	AQ	102	BCL	1	0
11	ae	101	BCL	2	0
12	AH	103	LMT	1	0
11	AR	102	BCL	1	0
11	am	1001	BCL	1	0
12	BH	1003	LMT	1	0
11	bm	103	BCL	1	0
21	L	309	BPH	1	0
11	M	406	BCL	2	0
12	AD	103	LMT	2	0
15	C	404	HEC	1	0
11	AK	102	BCL	1	0
12	BP	1005	LMT	1	0
11	aa	1001	BCL	4	0
23	M	405	CRT	1	0
11	BL	1005	BCL	1	0
12	BA	104	LMT	1	0
11	AV	101	BCL	1	0
20	L	302	MQ8	1	0
12	BU	1002	LMT	1	0
15	C	402	HEC	2	0
11	AP	102	BCL	1	0
11	AJ	102	BCL	1	0
18	ad	101	CD4	1	0
12	BH	1005	LMT	1	0
11	AB	103	BCL	1	0

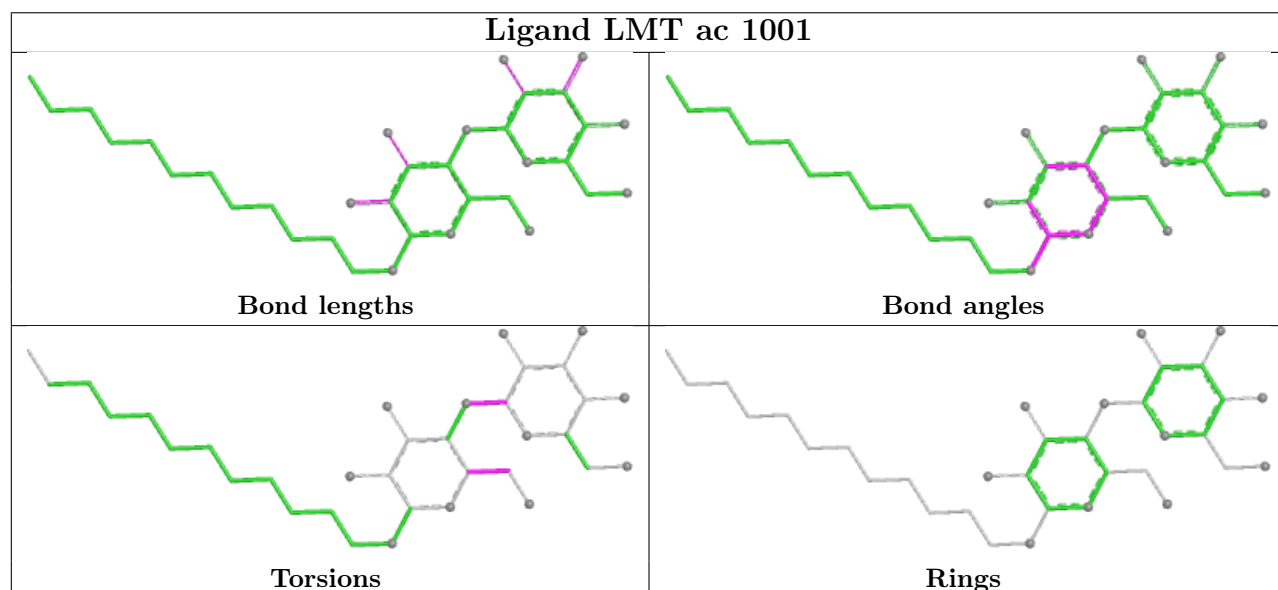
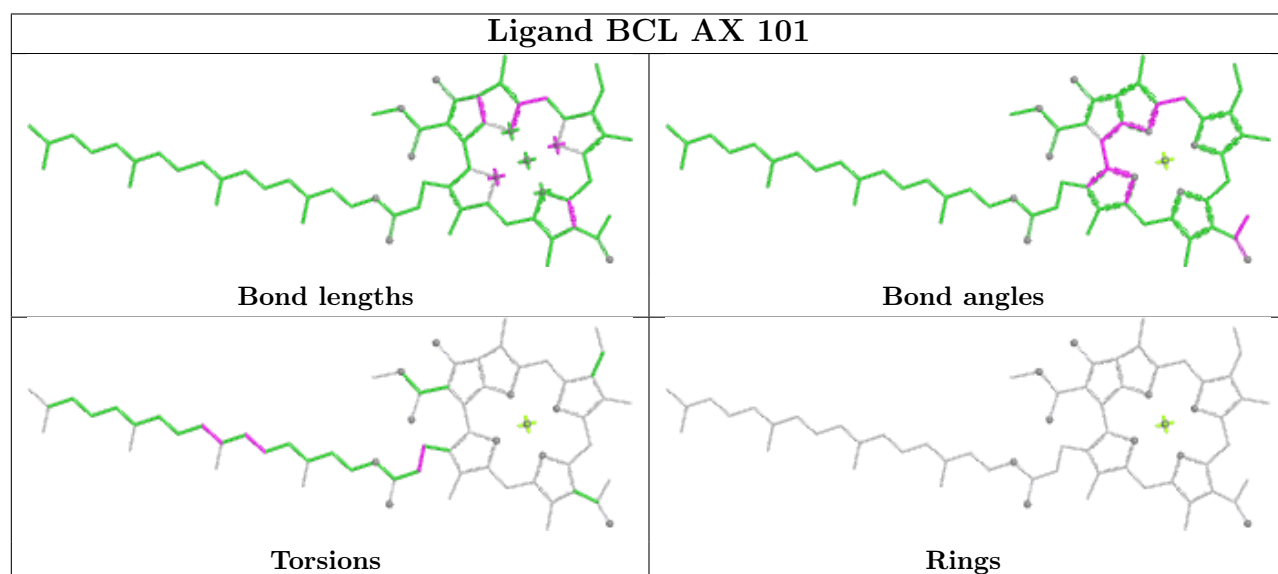
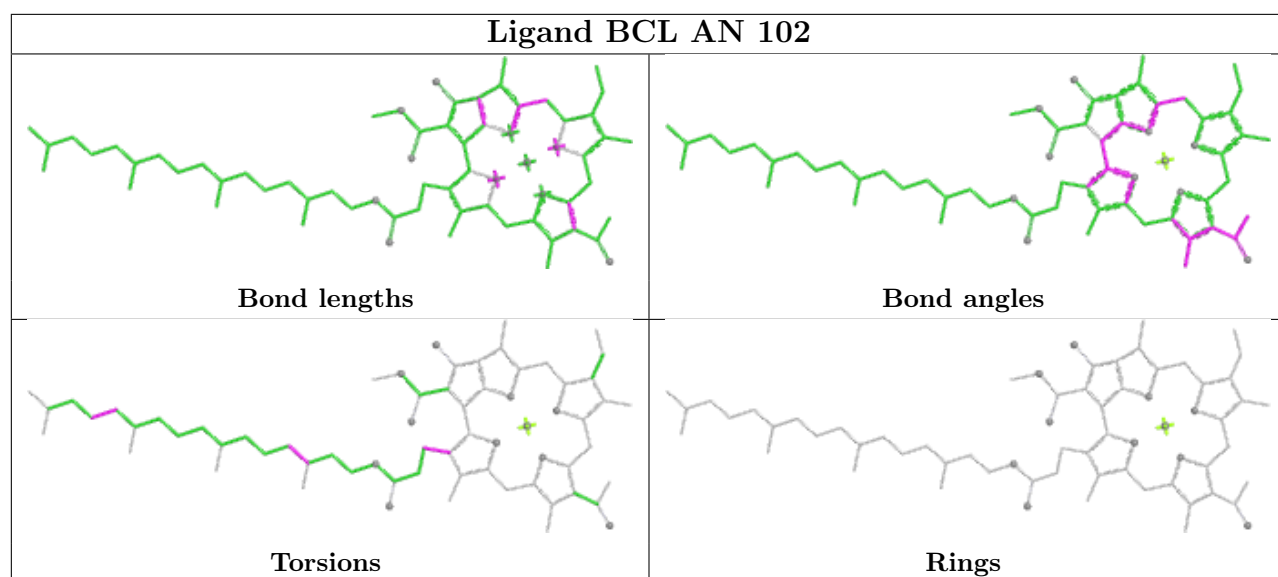
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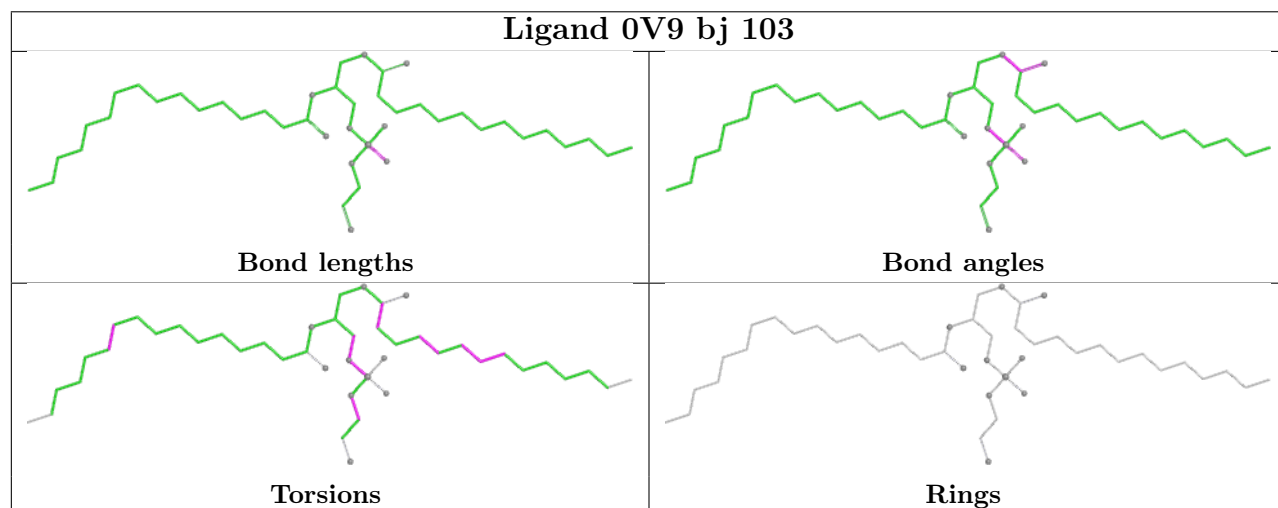
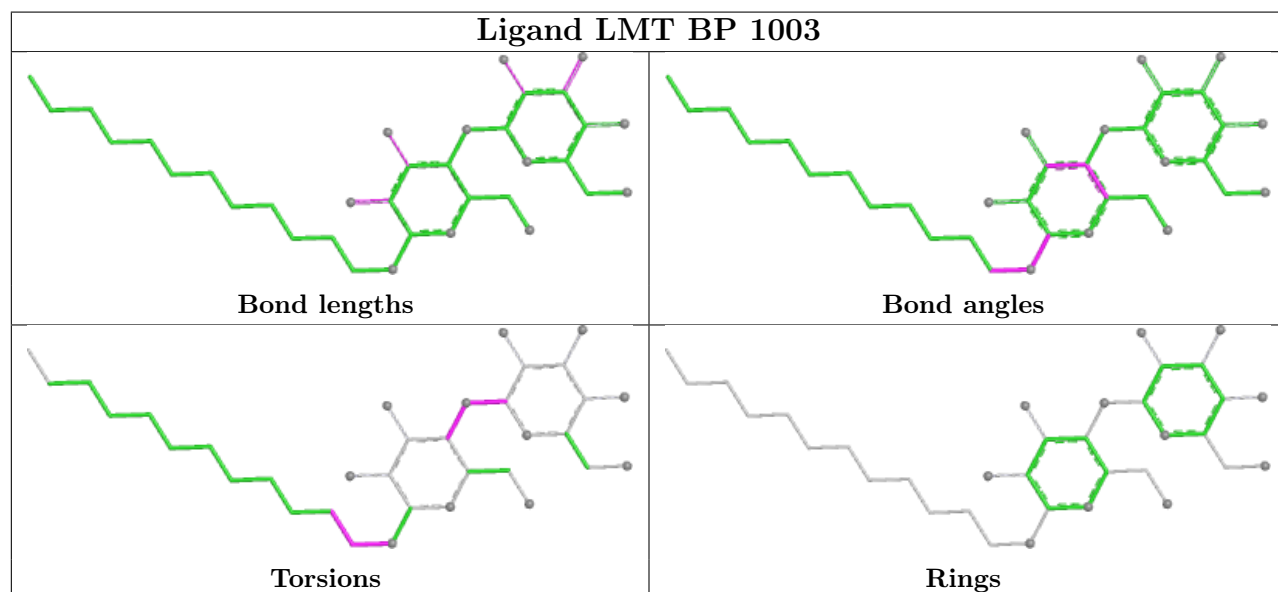
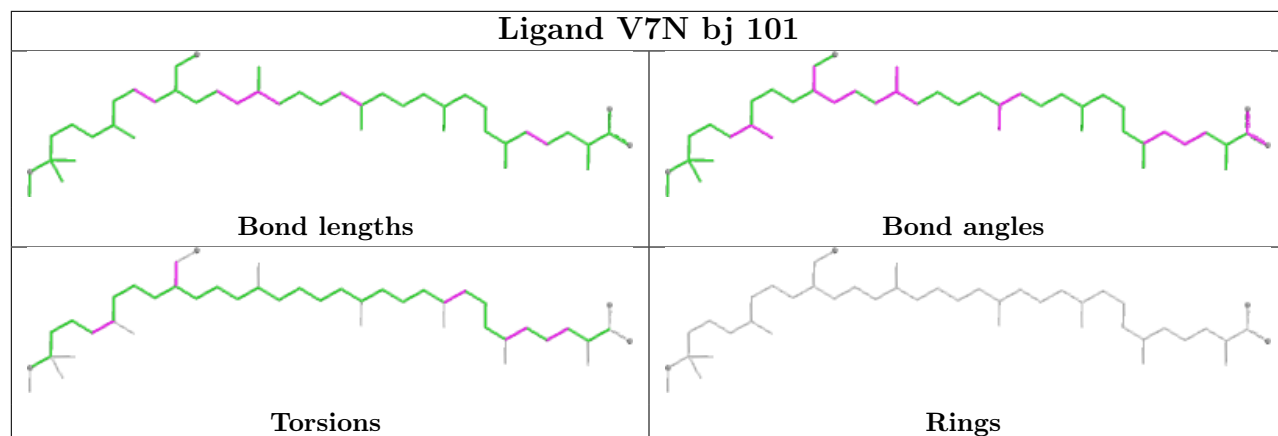
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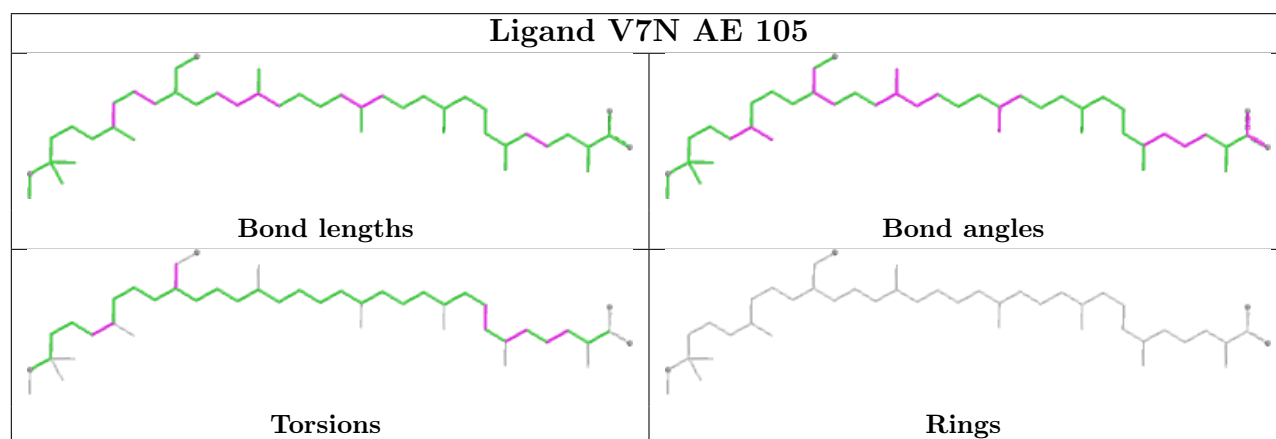
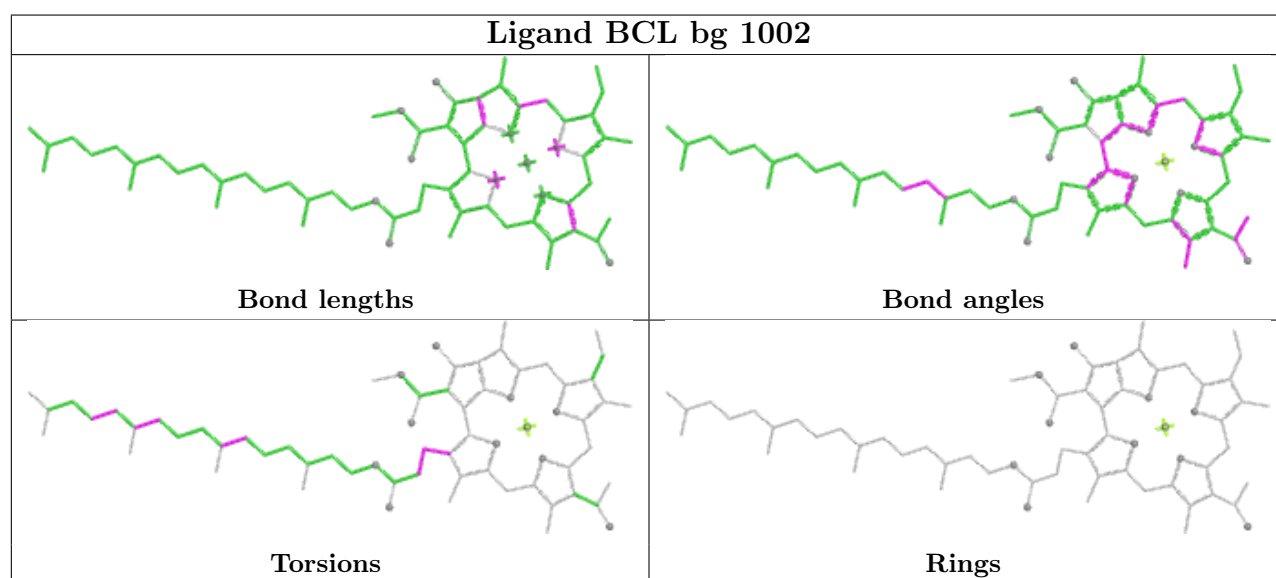
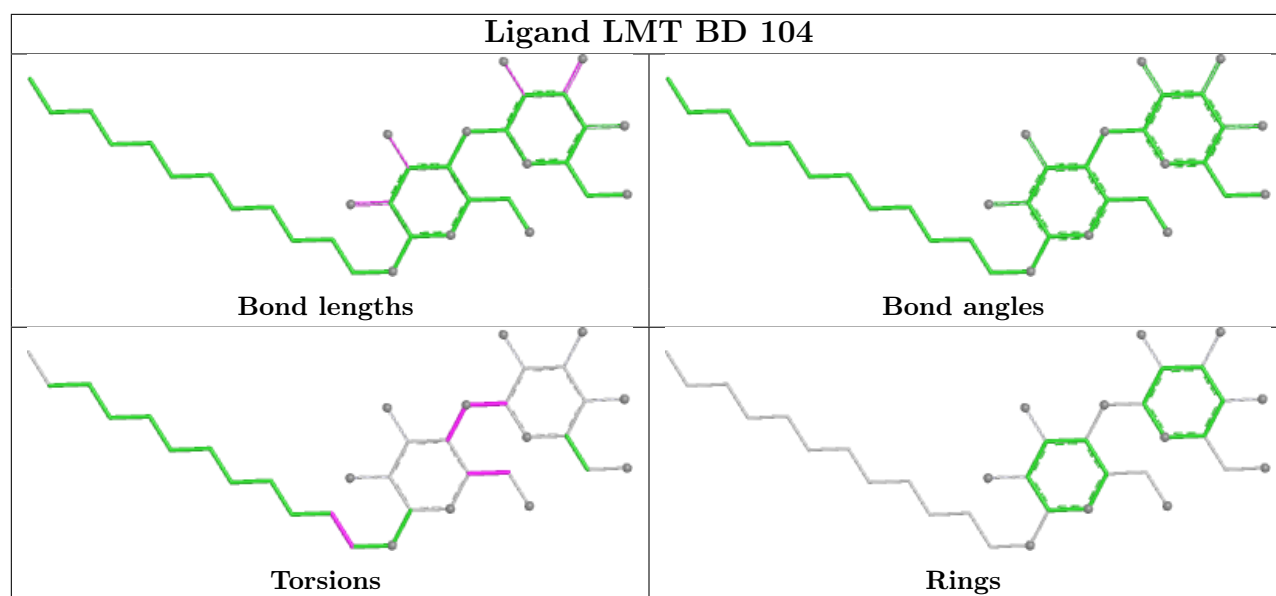
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	303	BCL	2	0
11	AS	104	BCL	5	0
11	AE	103	BCL	1	0
12	BS	1003	LMT	1	0

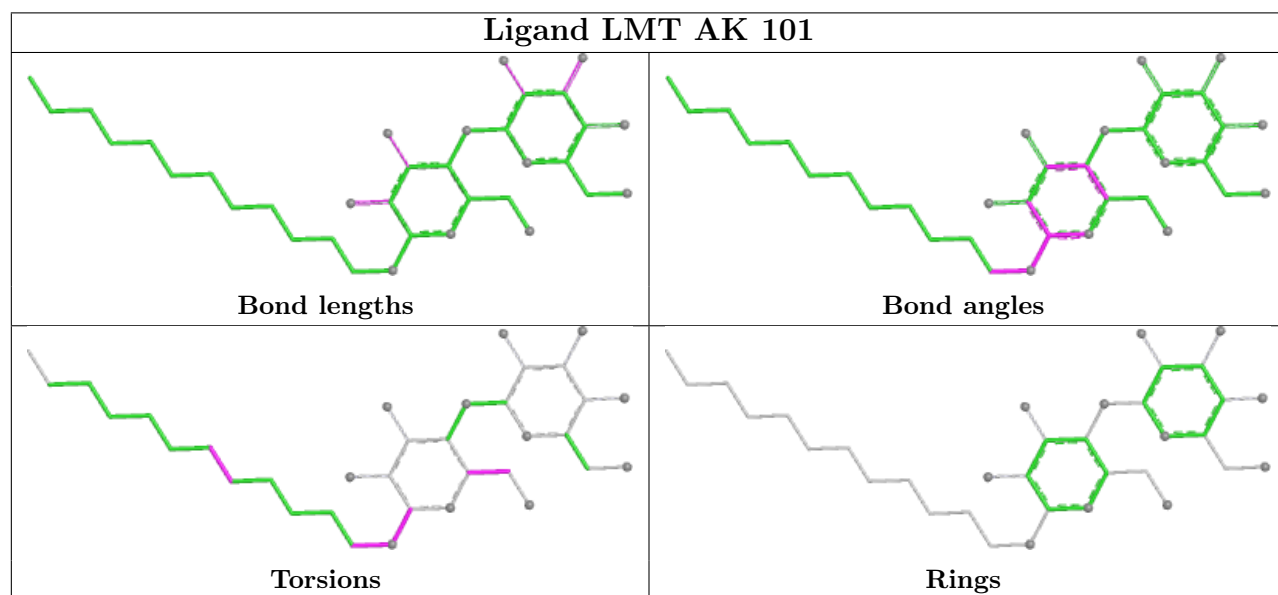
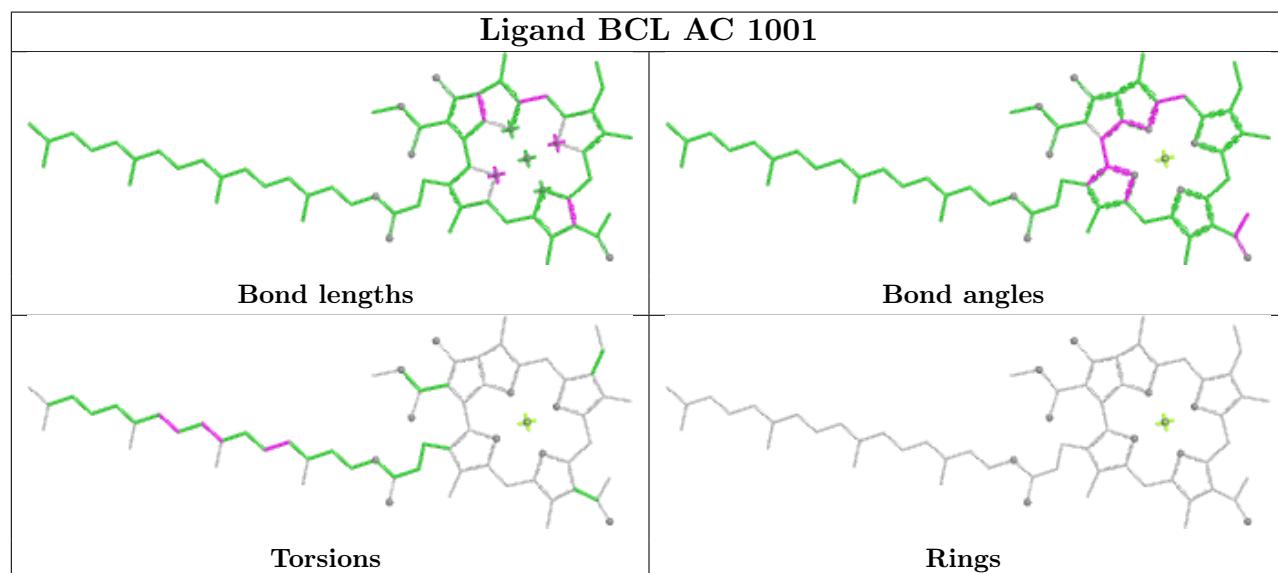
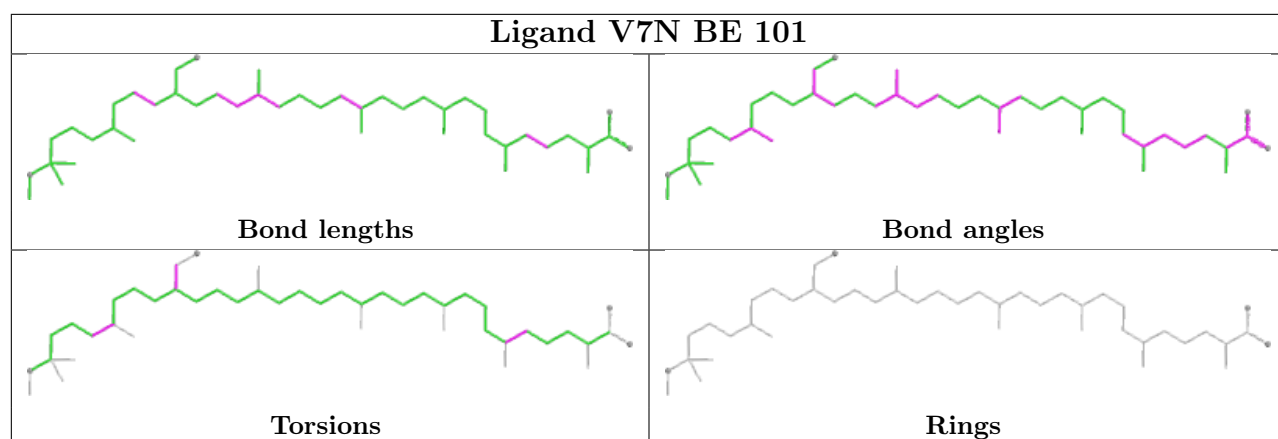
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

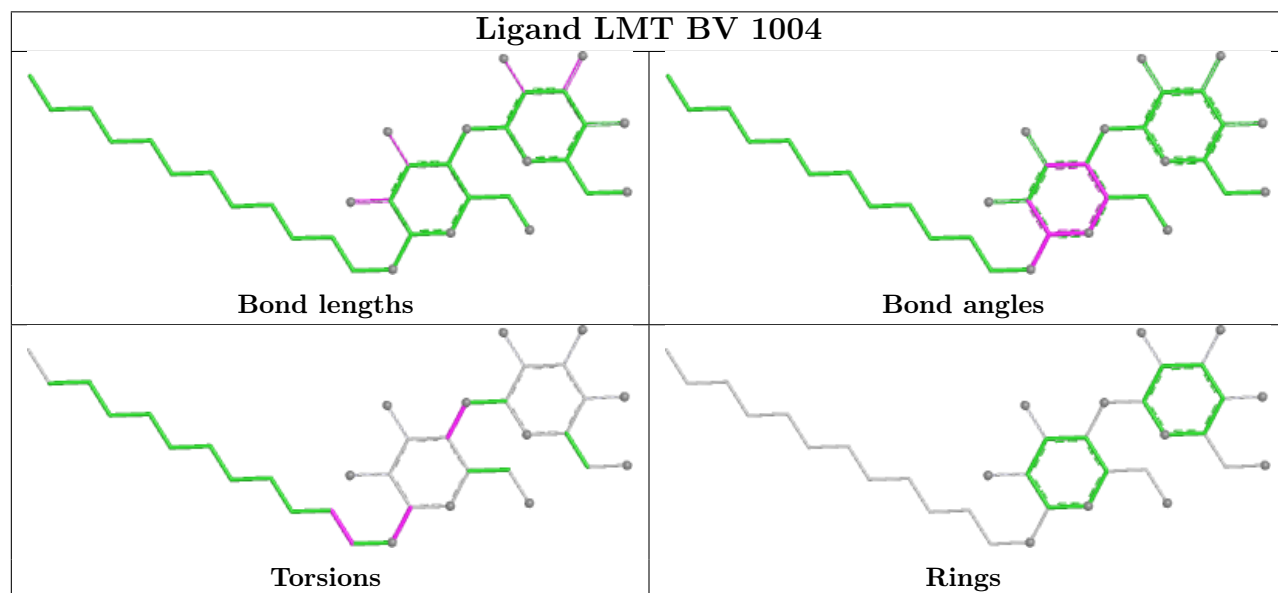
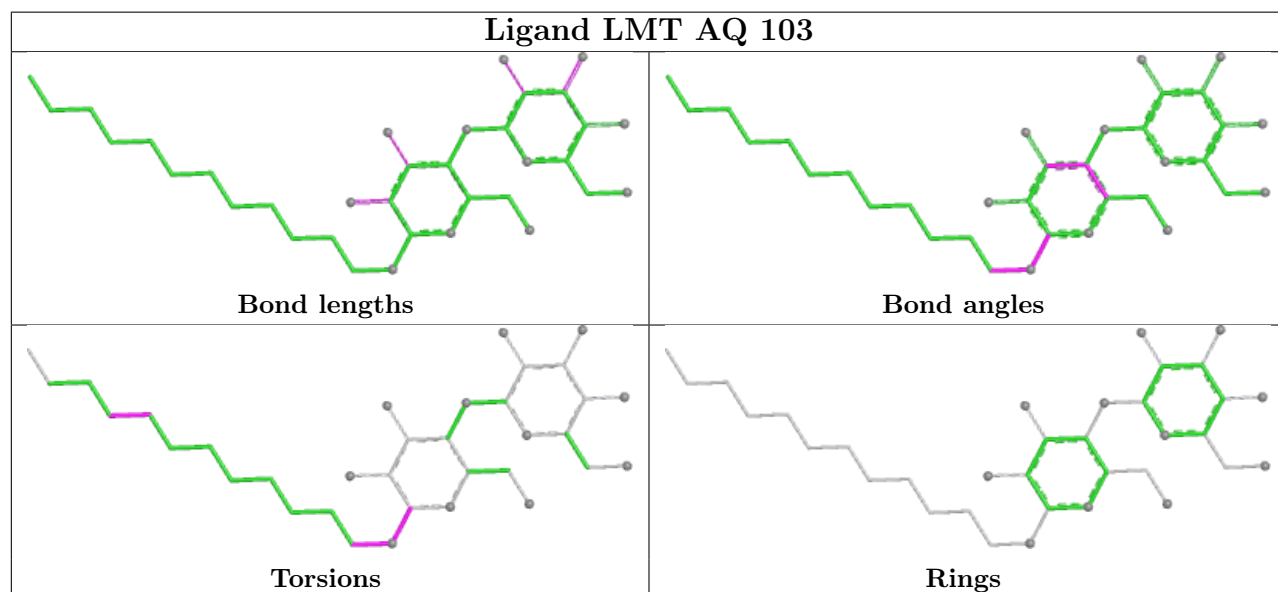
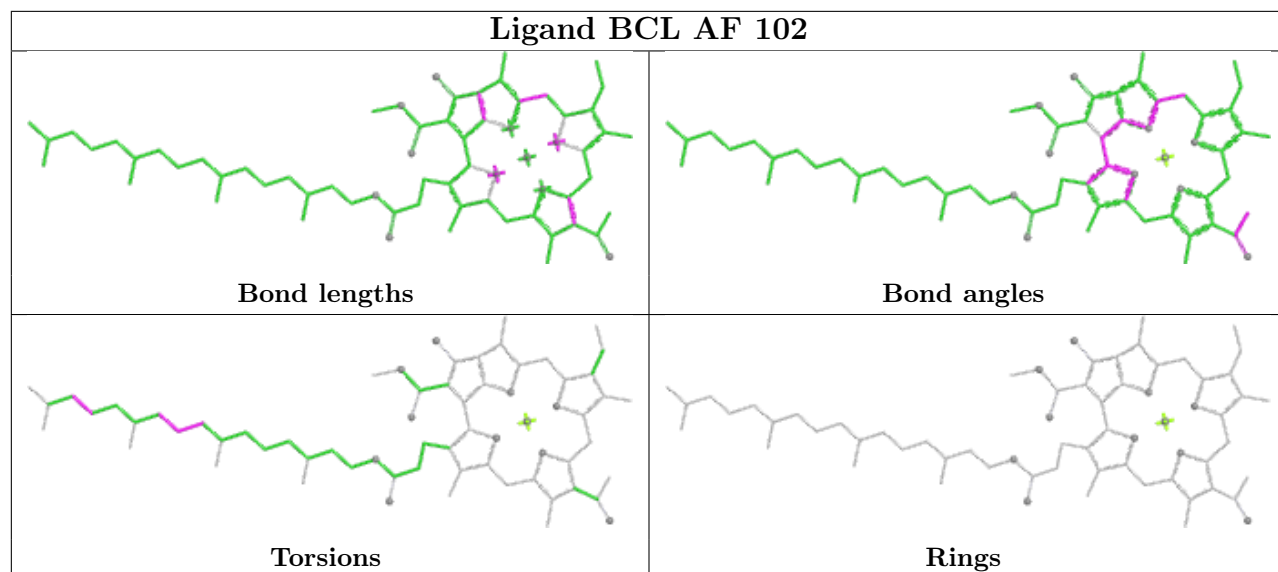


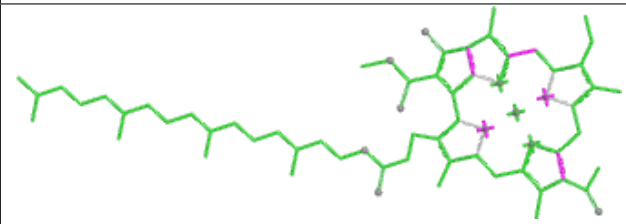
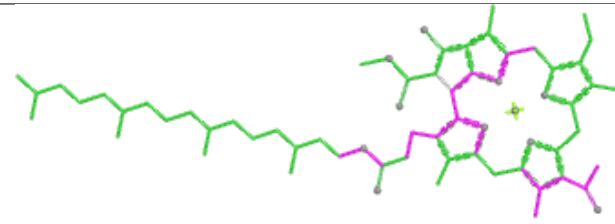
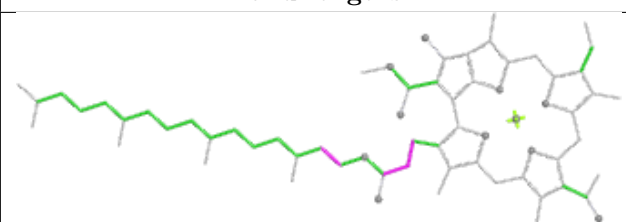
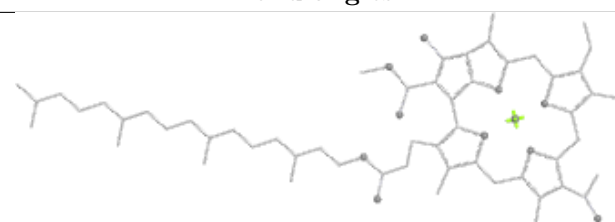


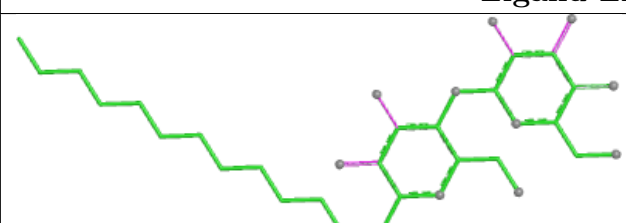
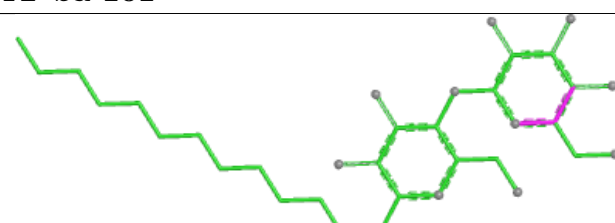
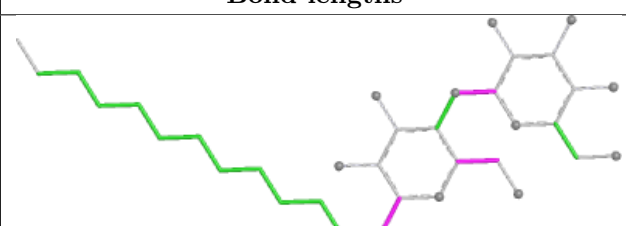
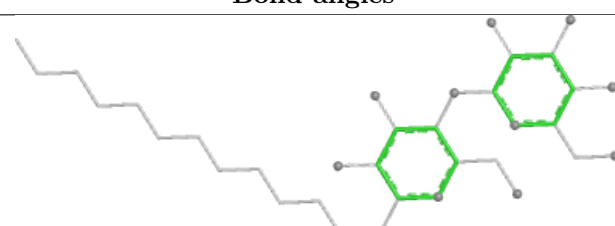


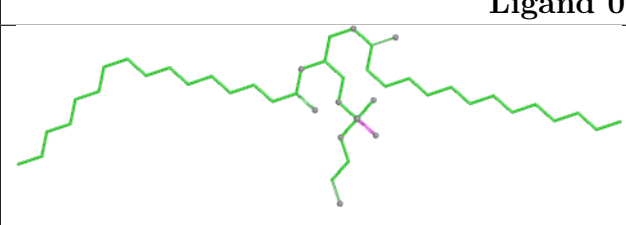
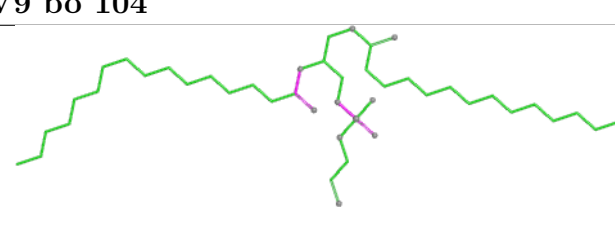
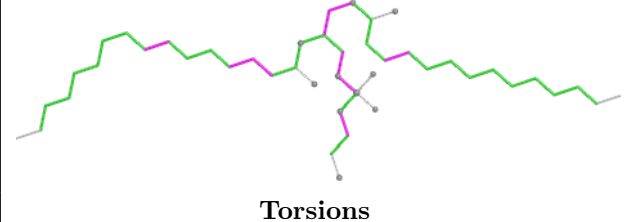
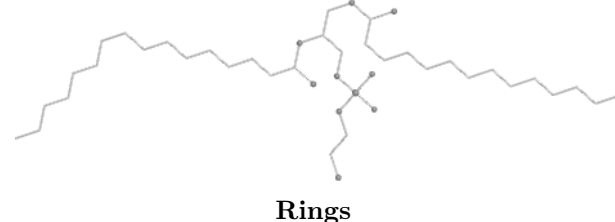


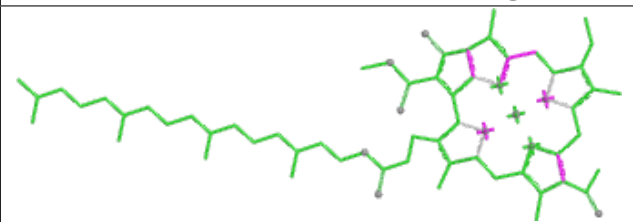
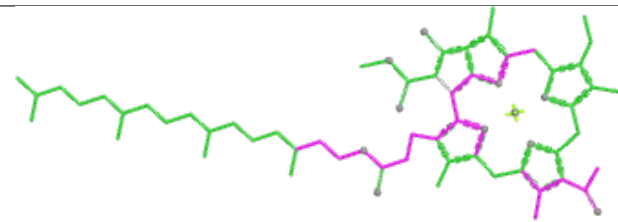
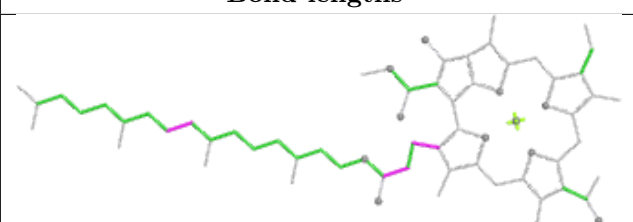
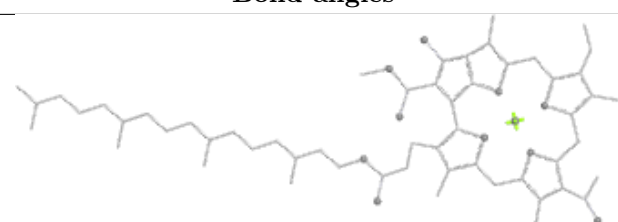


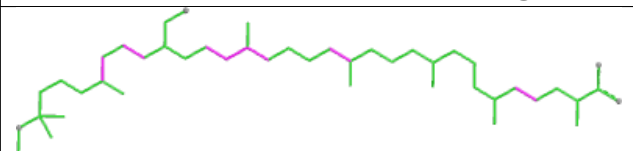
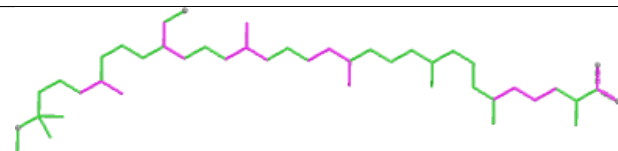
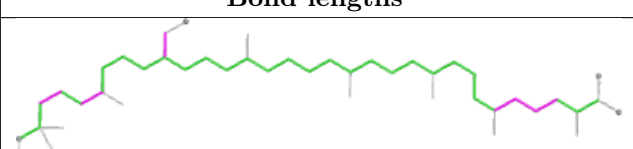
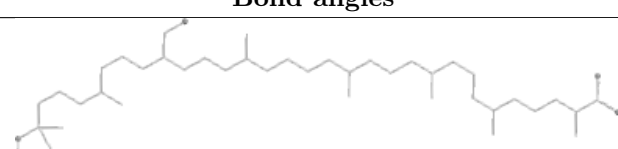


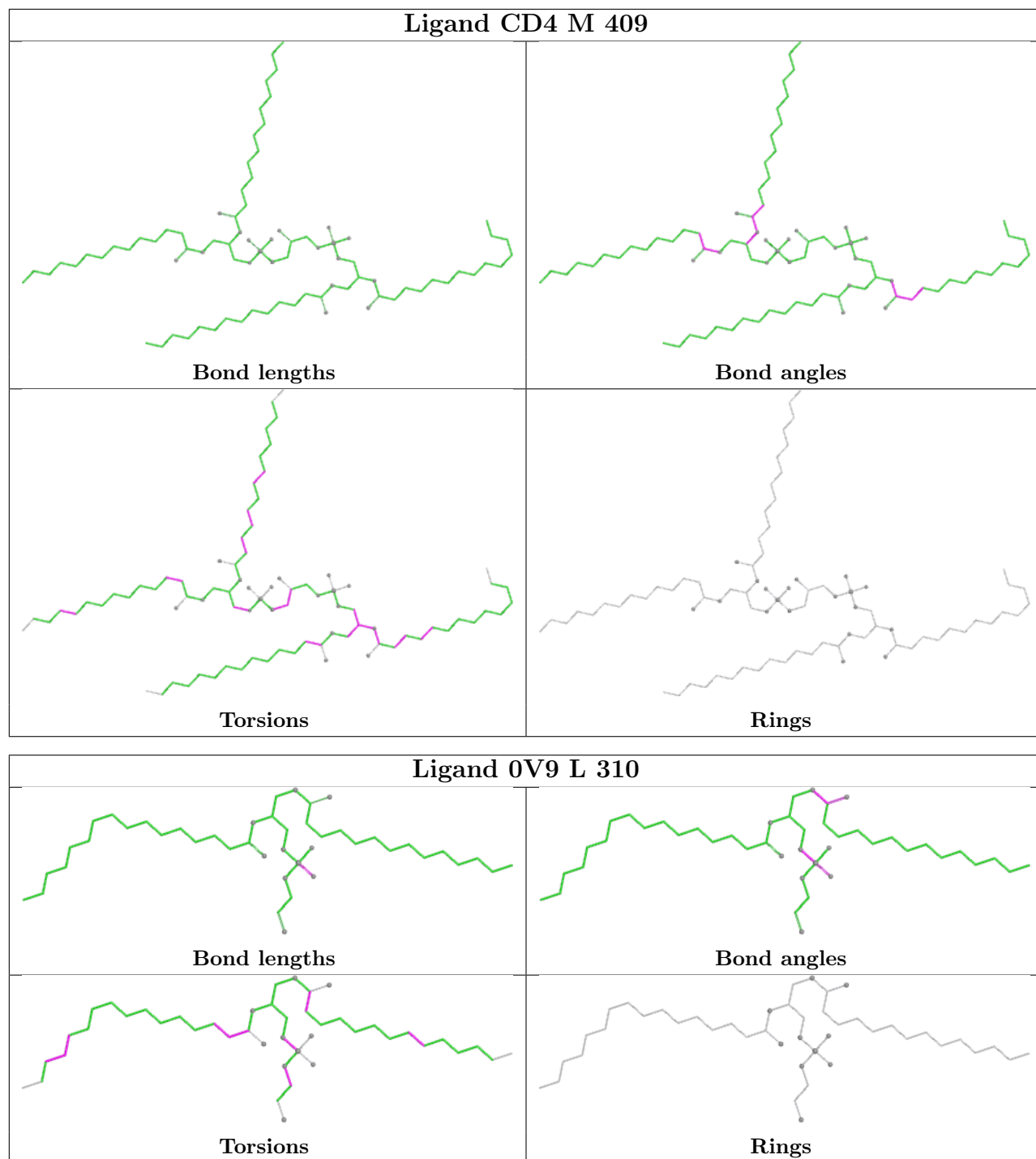
Ligand BCL BM 1004	
	
Bond lengths	Bond angles
	
Torsions	Rings

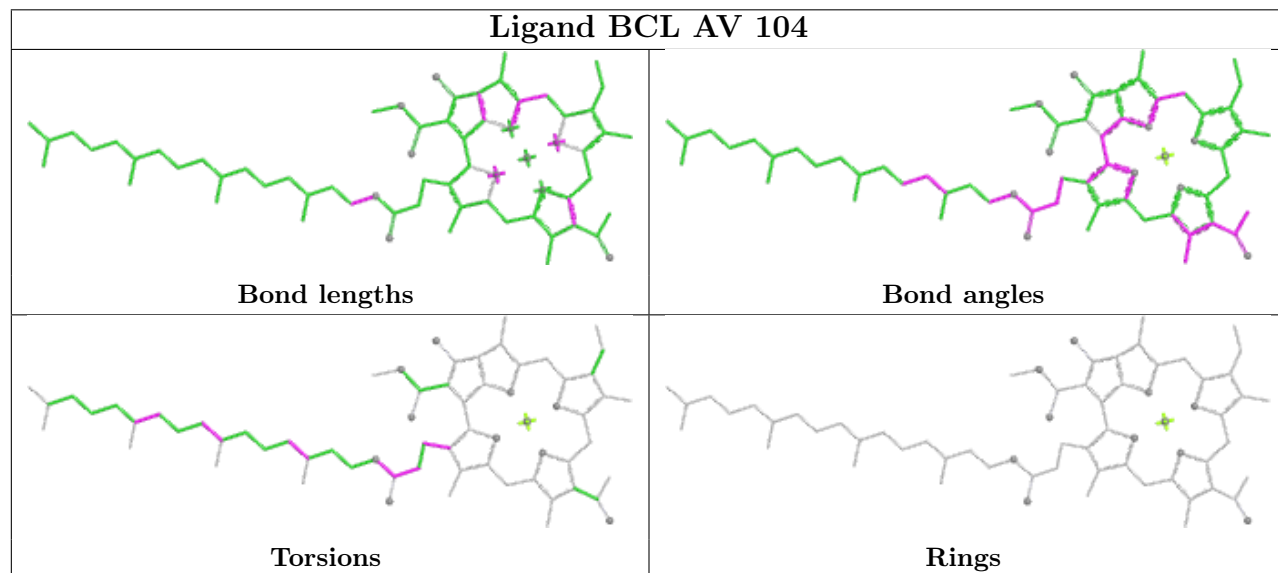
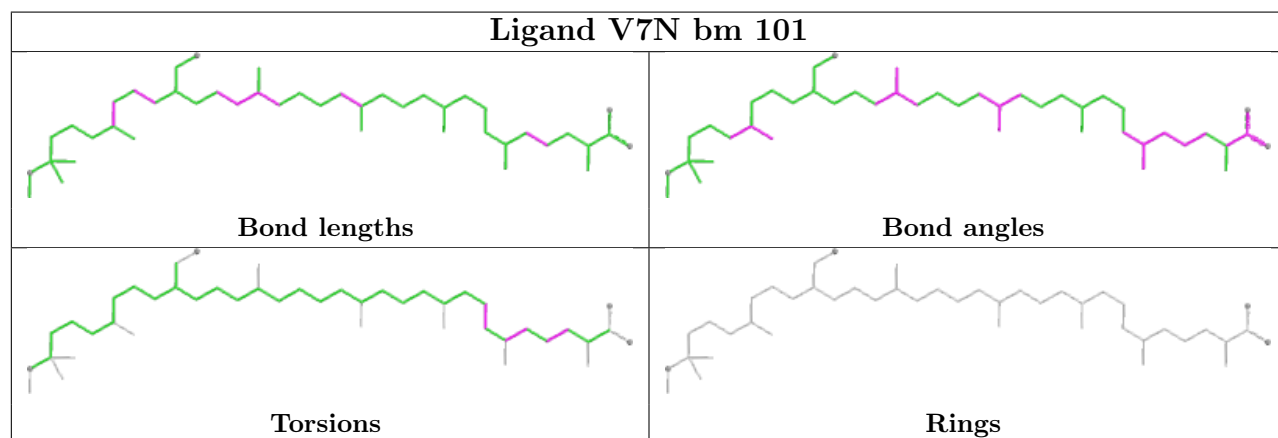
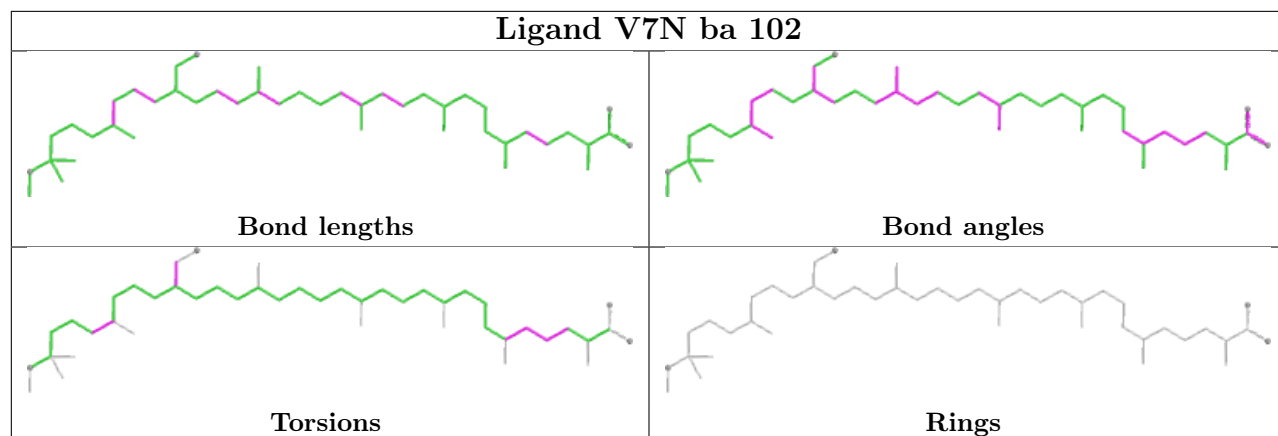
Ligand LMT ba 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

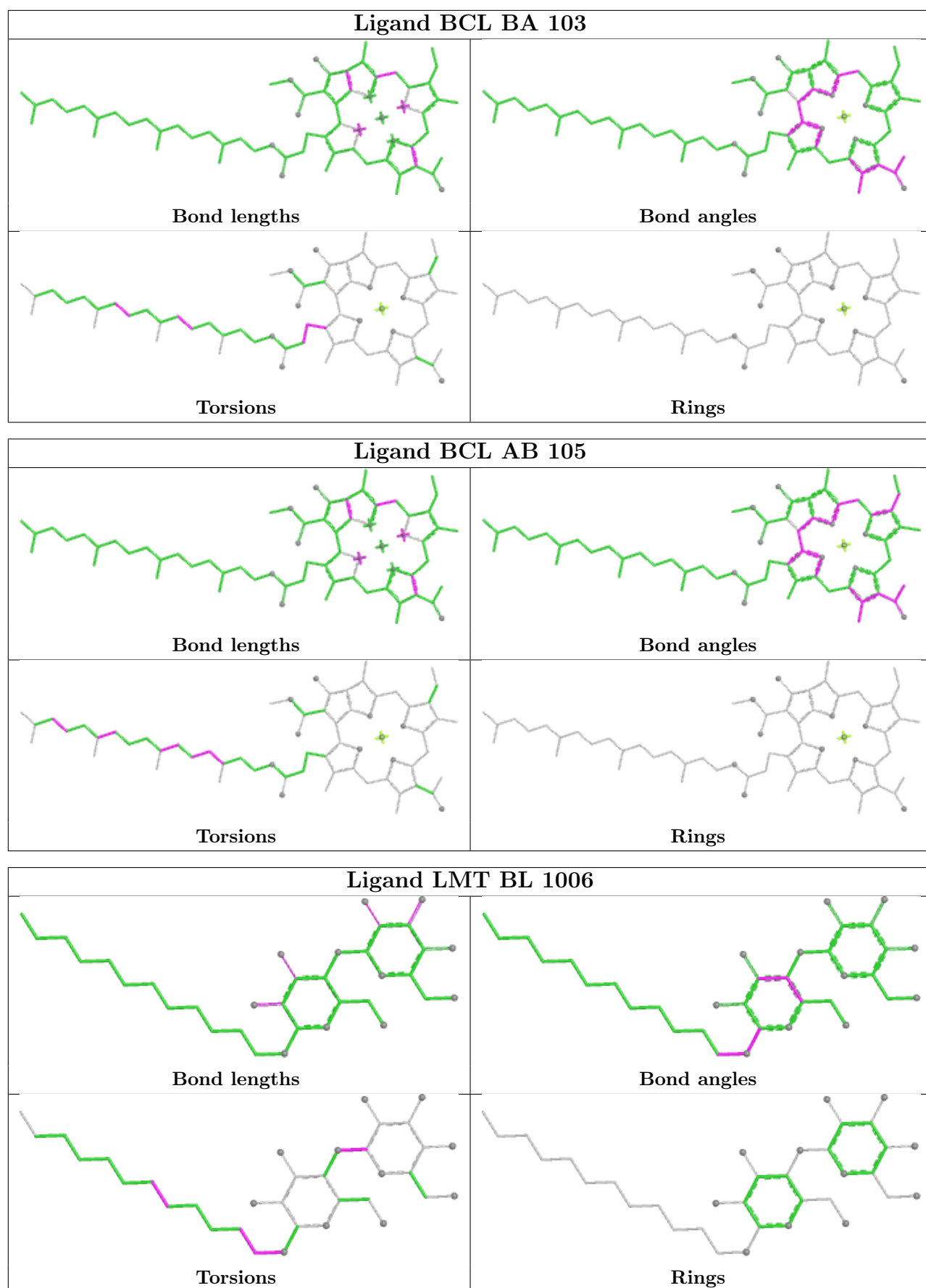
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Bond lengths	Bond angles
	
Torsions	Rings

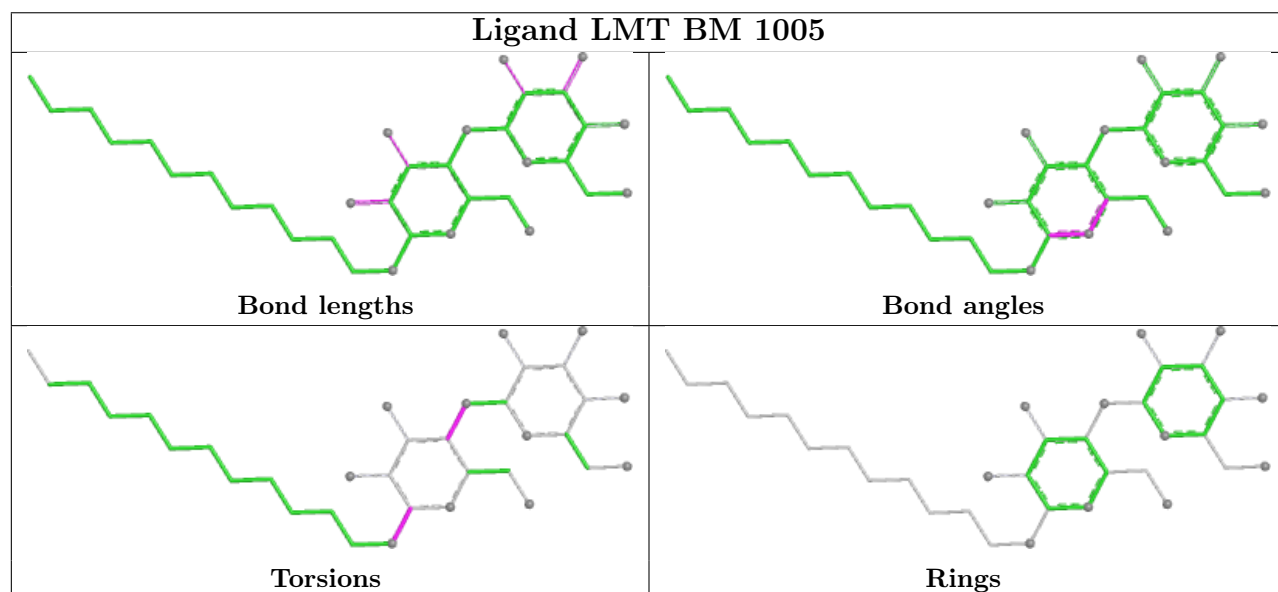
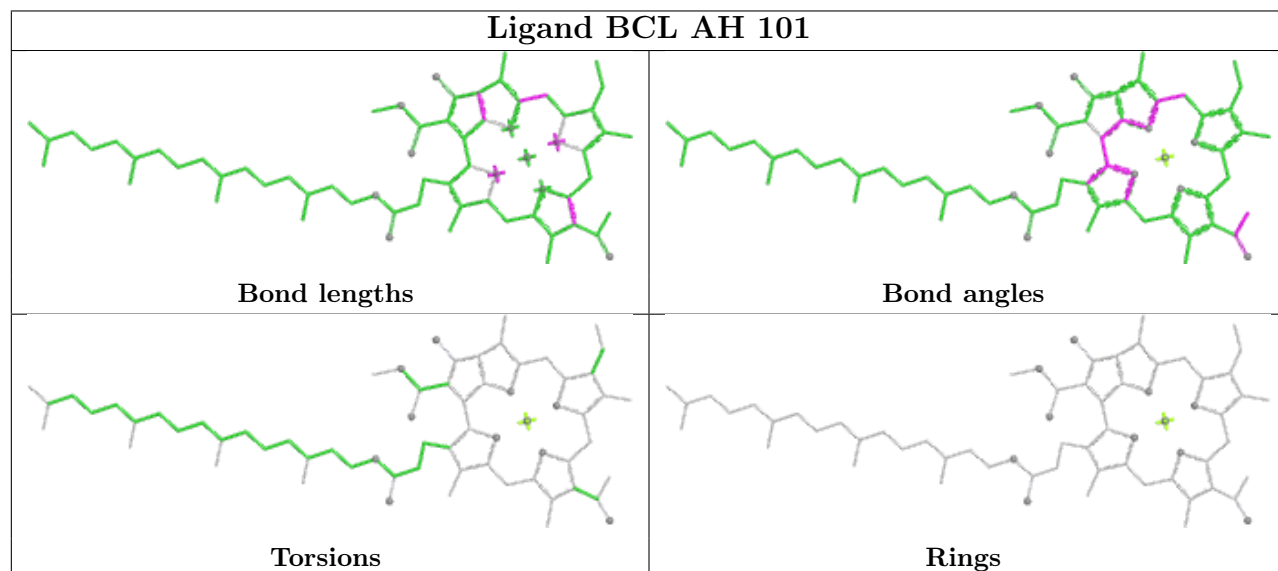
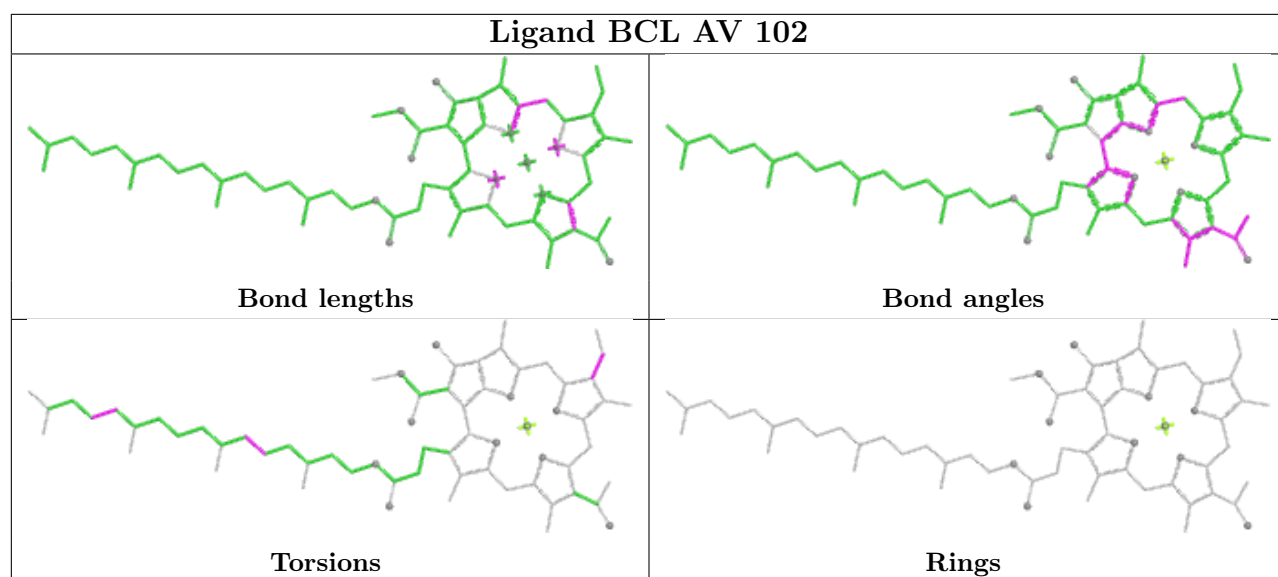
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Bond lengths	Bond angles
	
Torsions	Rings

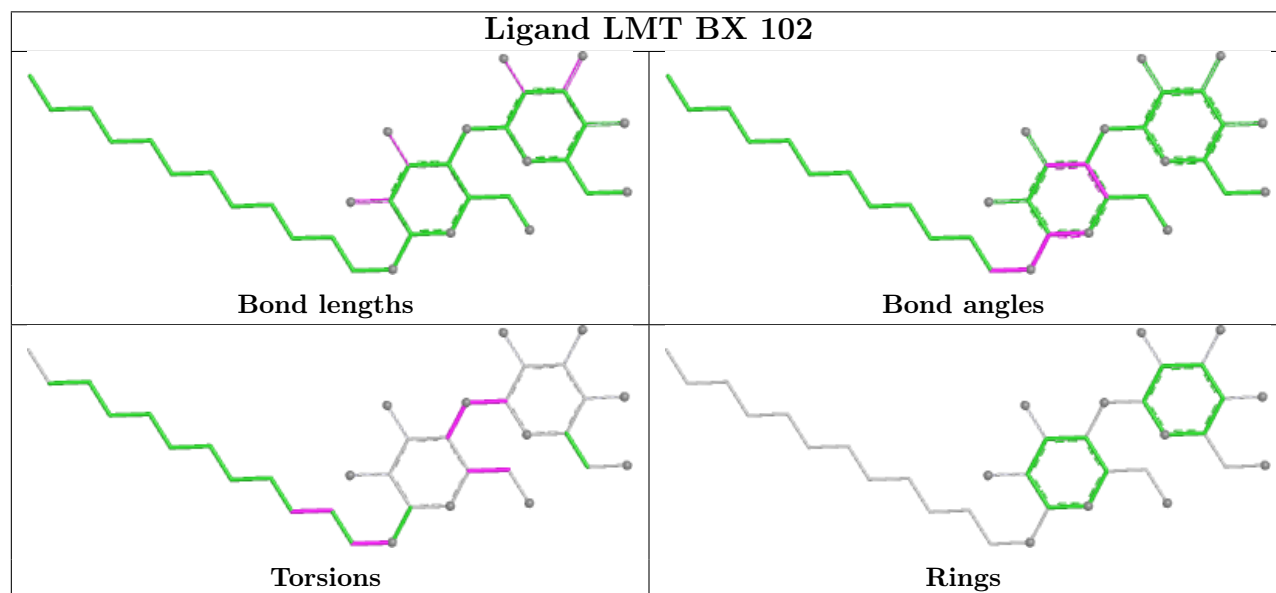
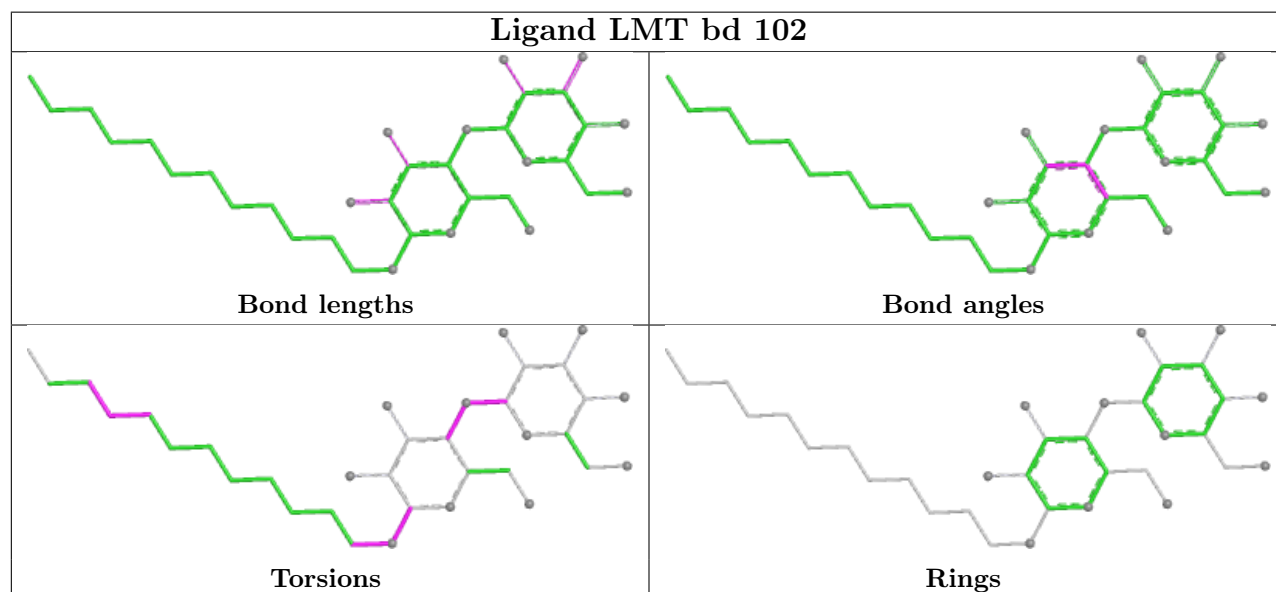
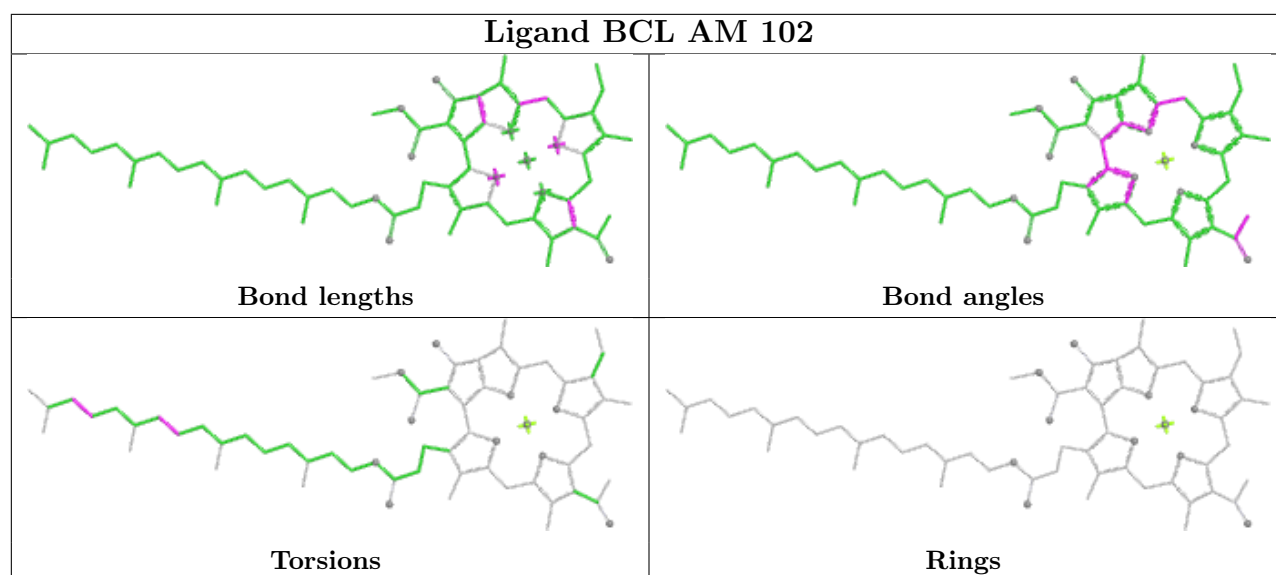
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Bond lengths	Bond angles
	
Torsions	Rings

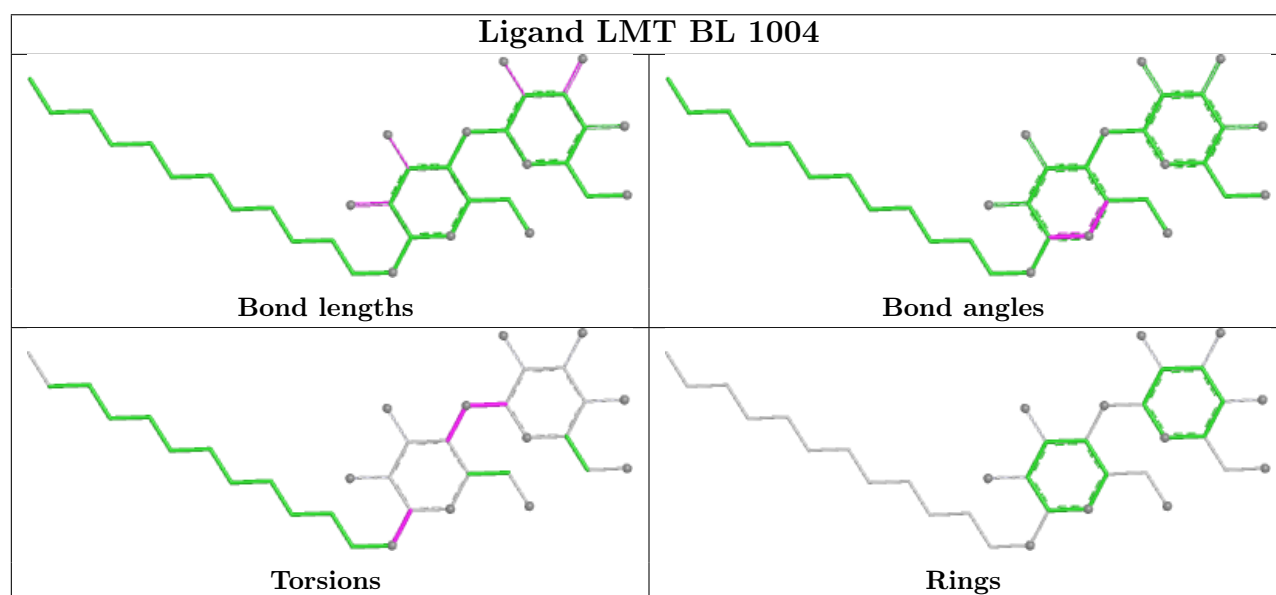
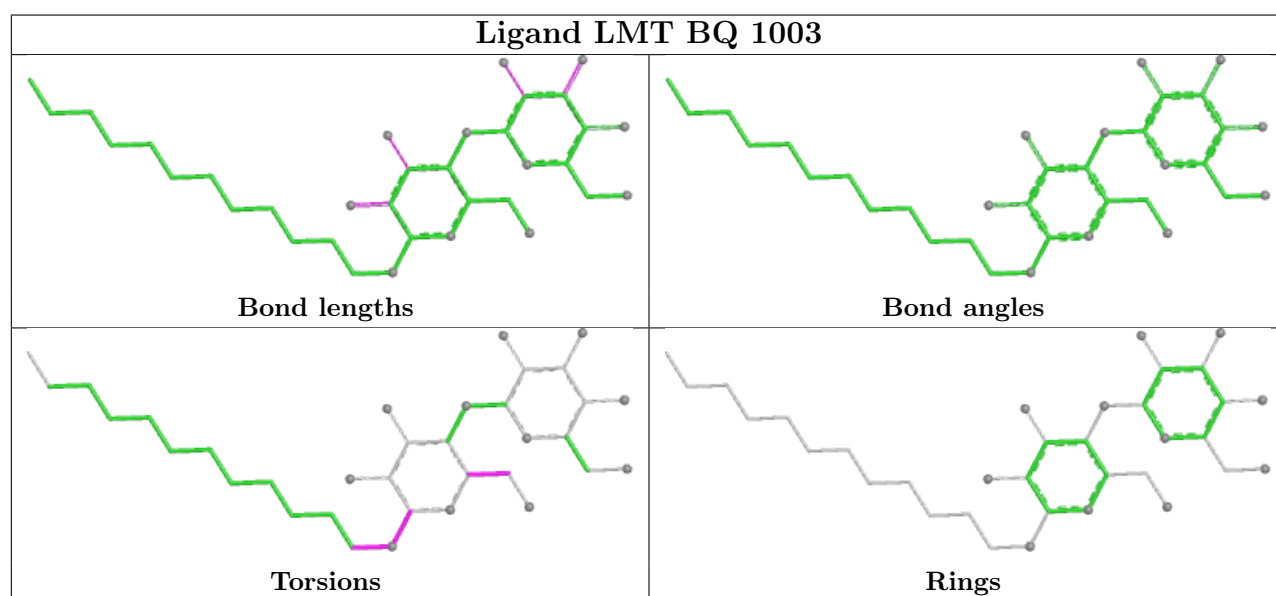
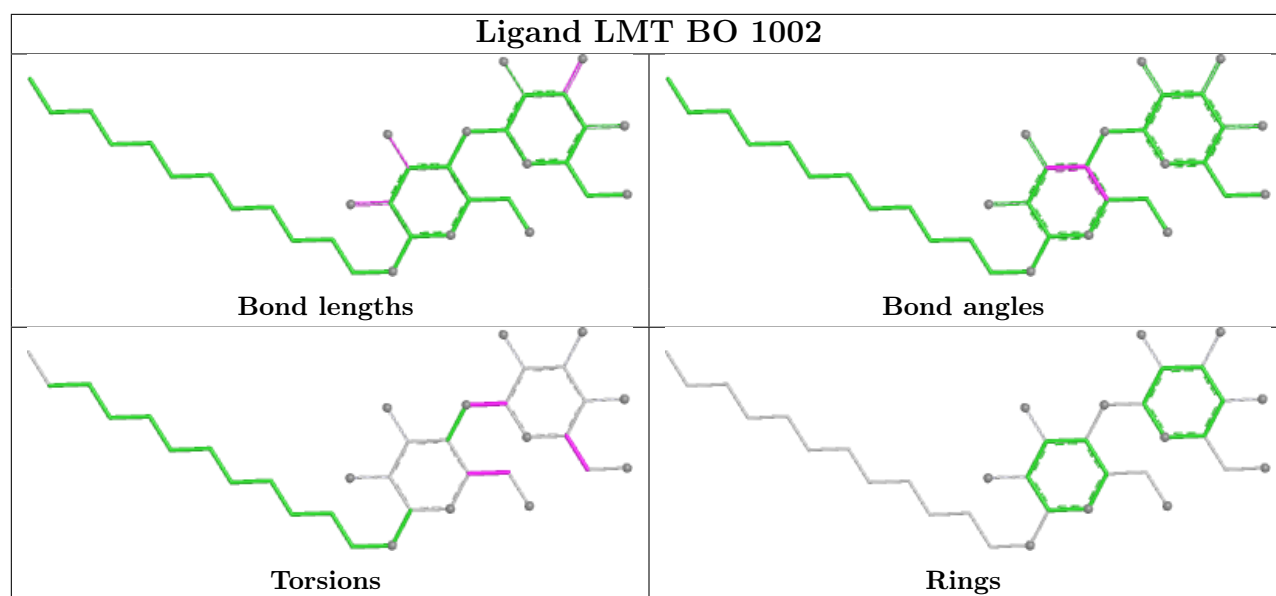


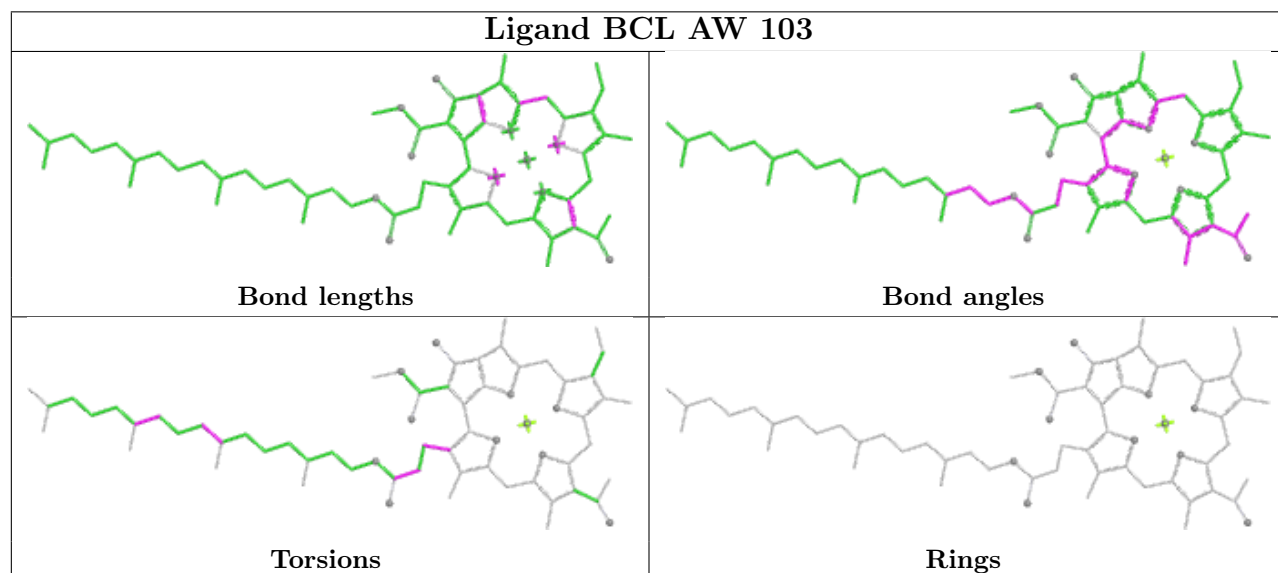
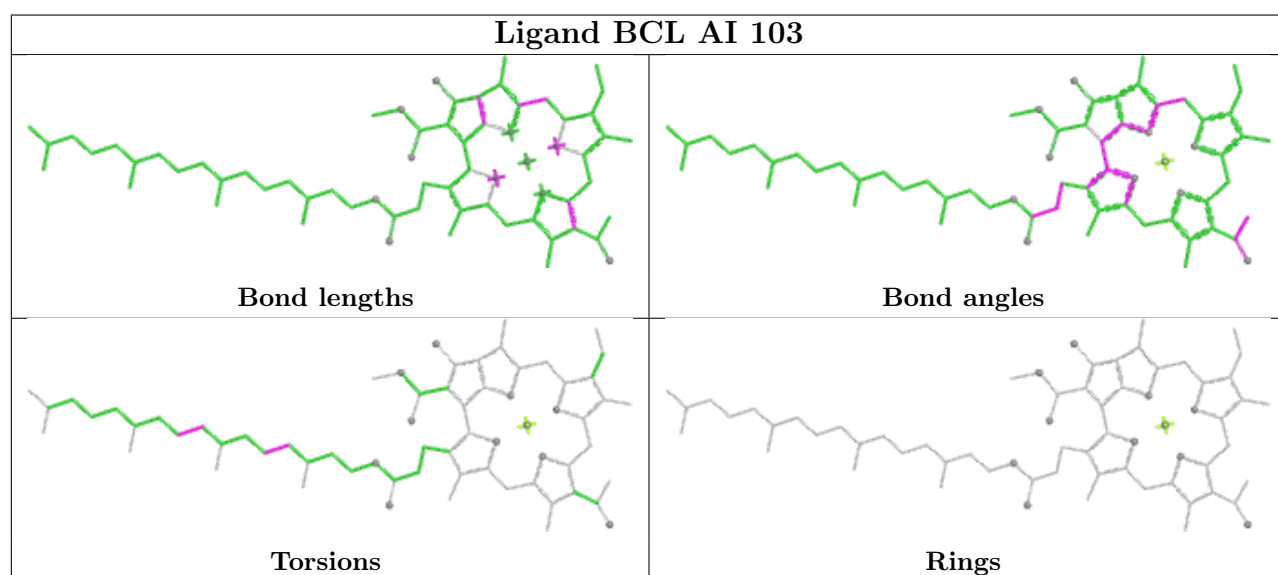
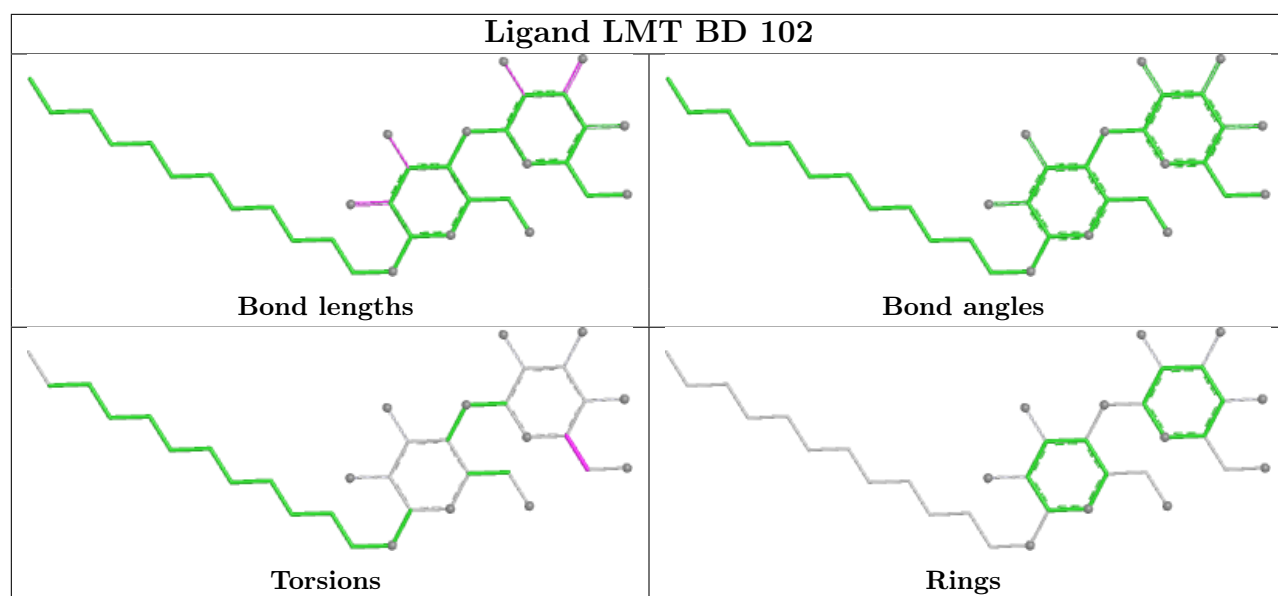


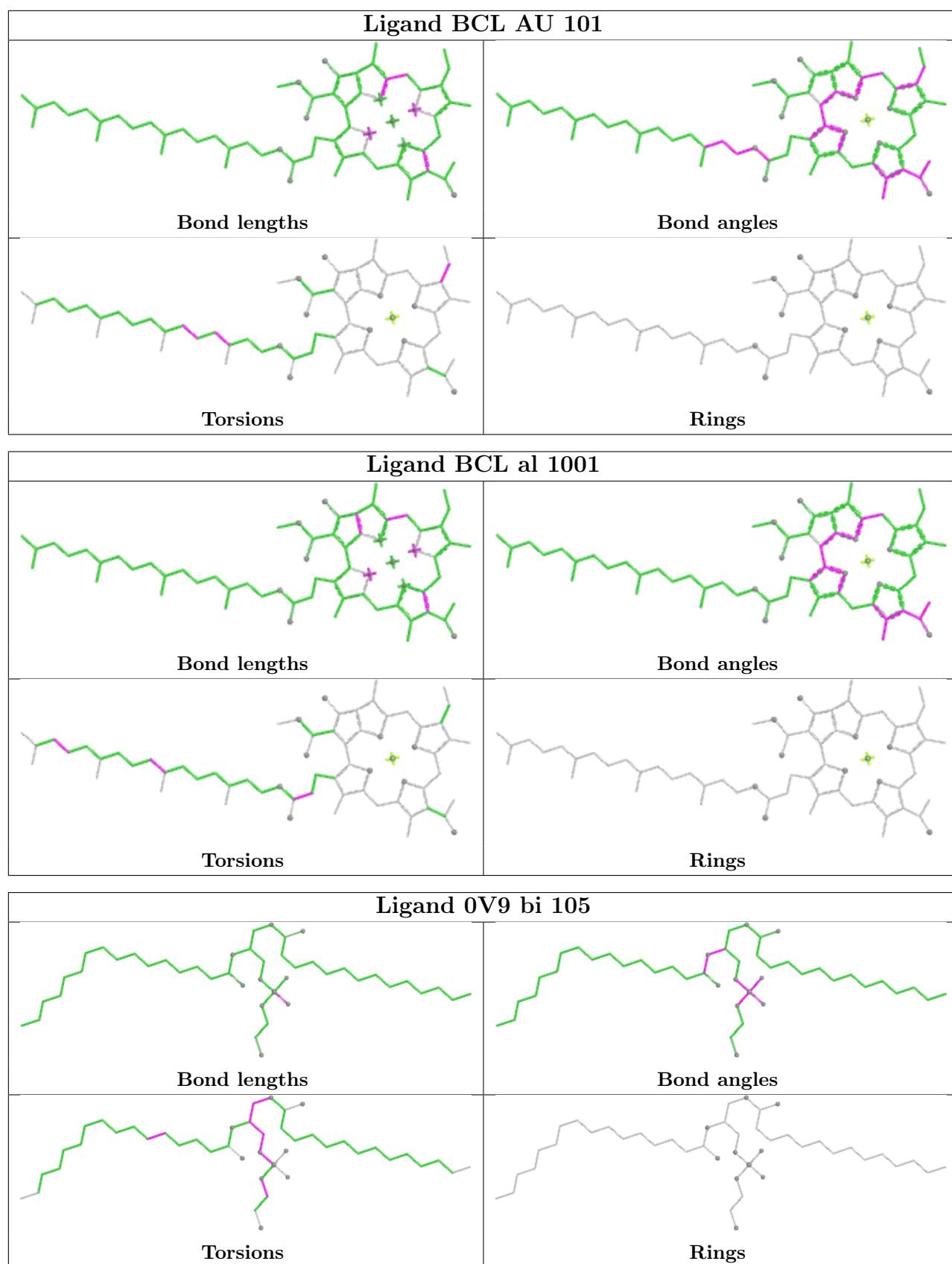


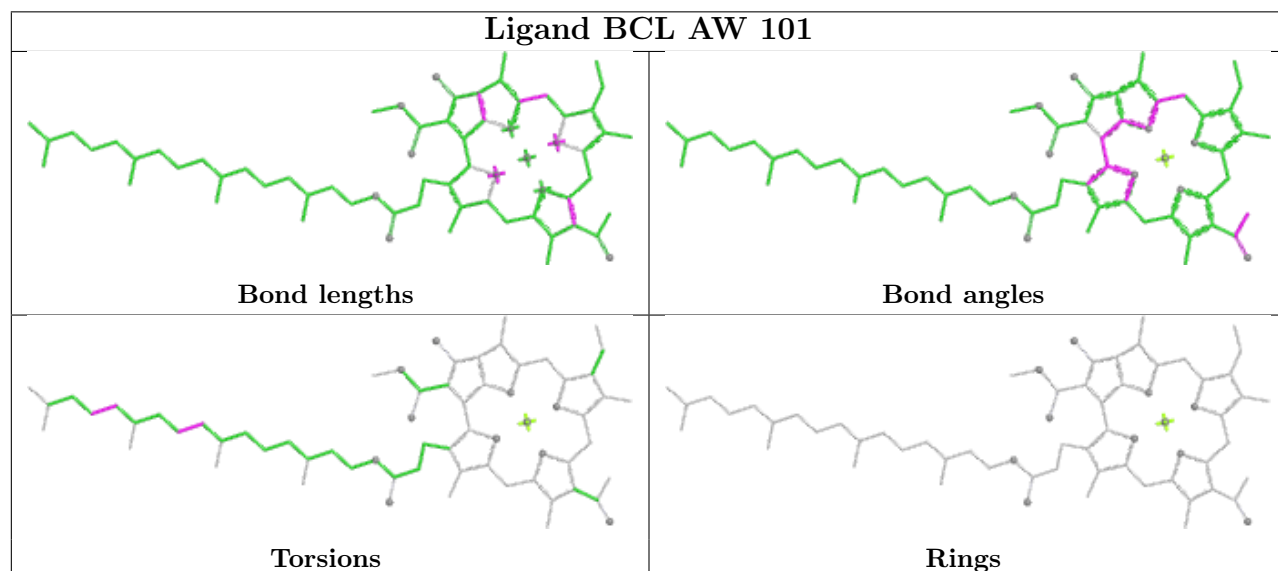
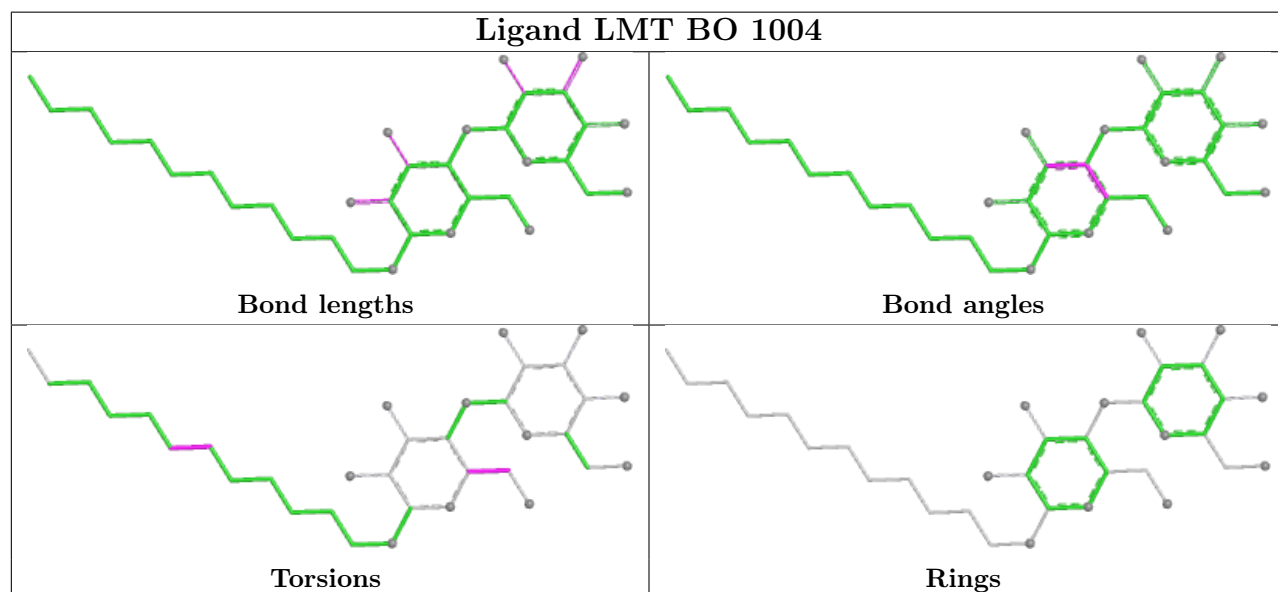
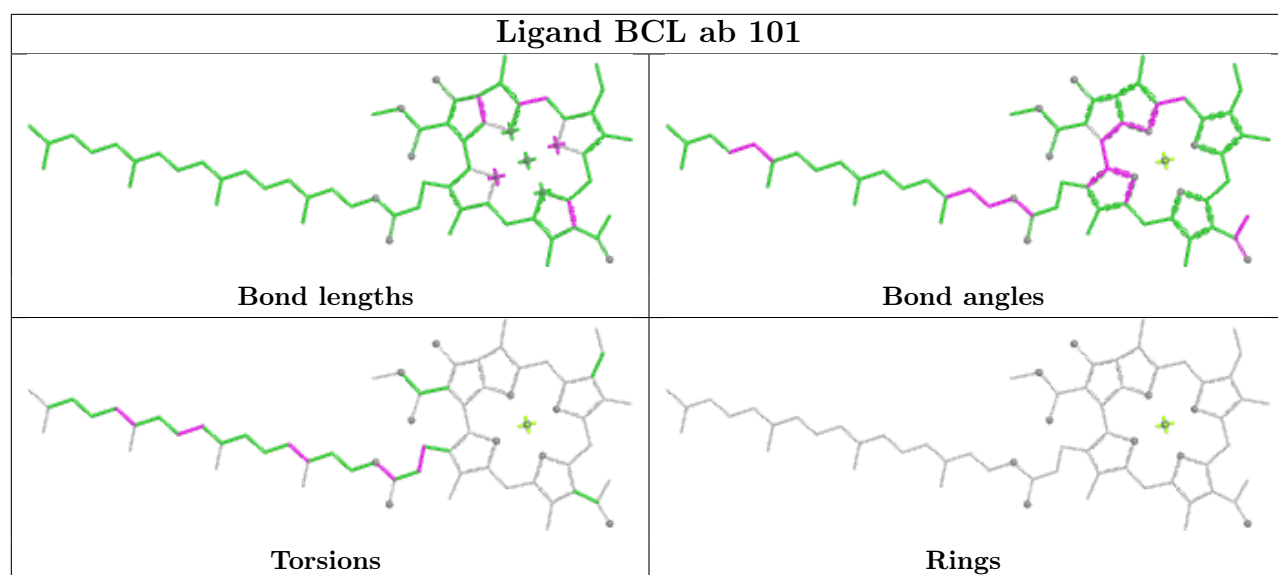


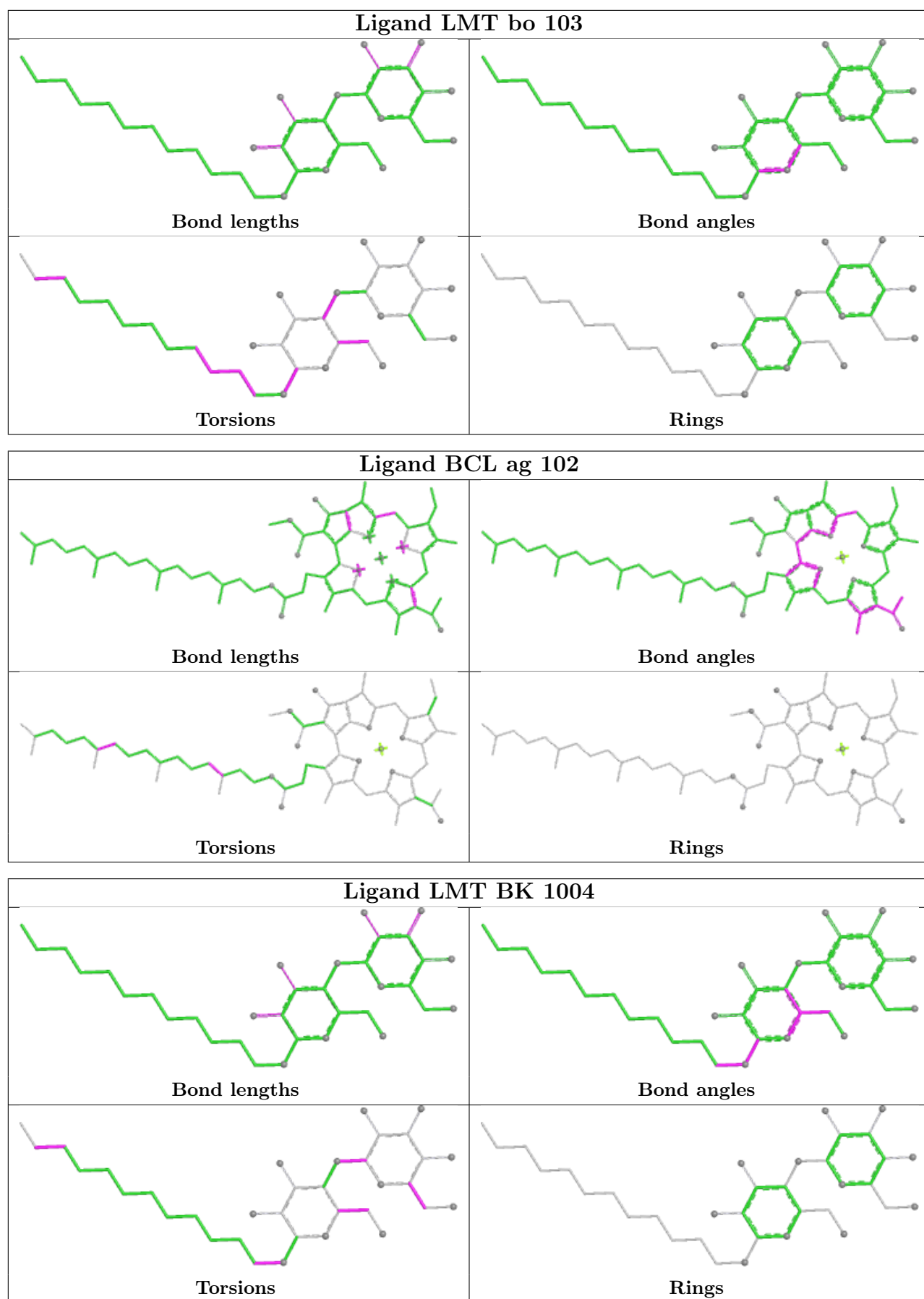


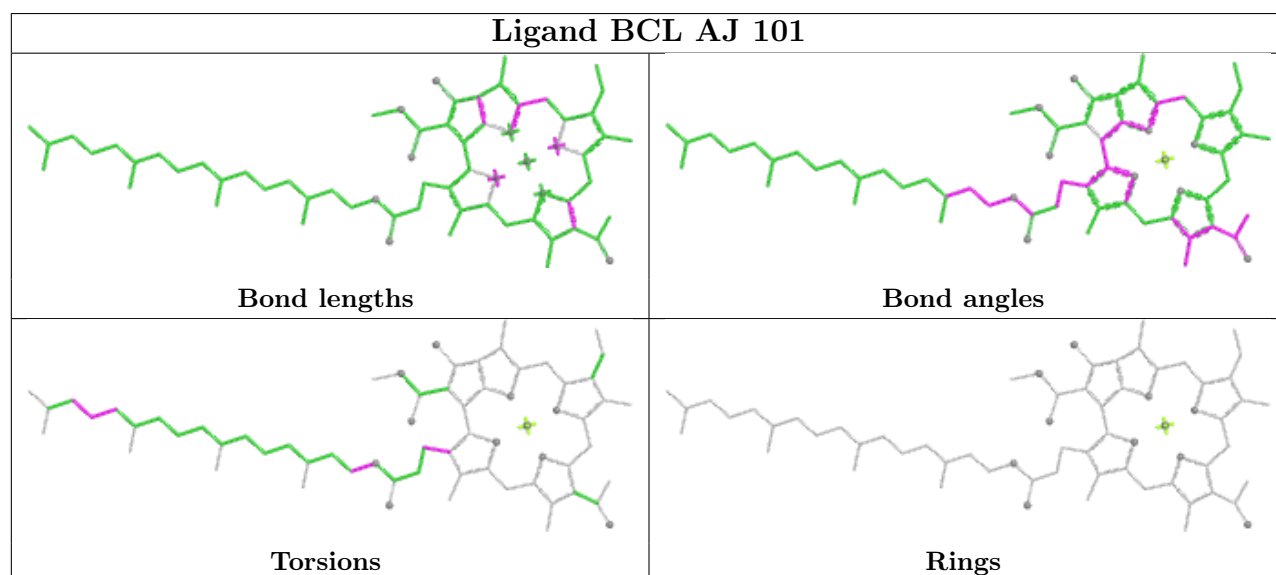
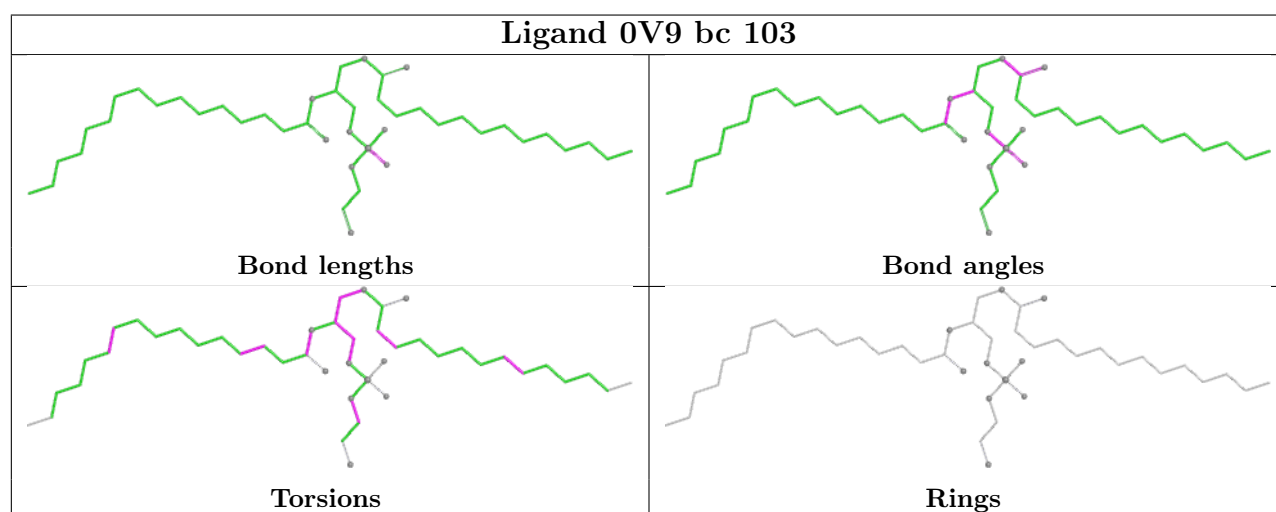
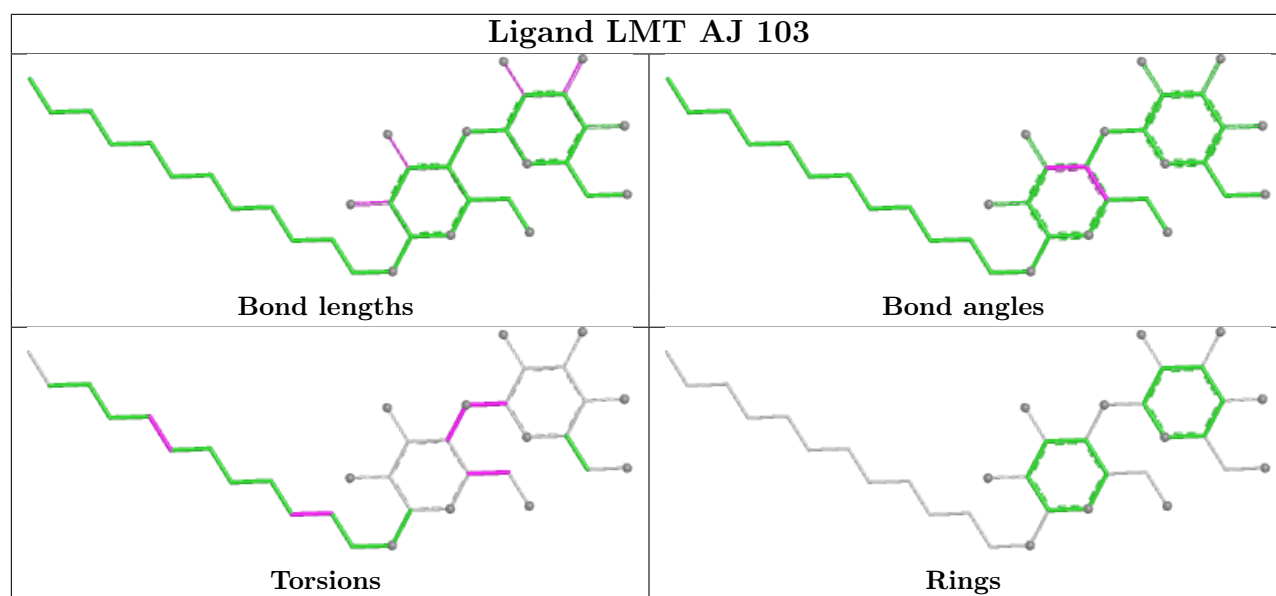


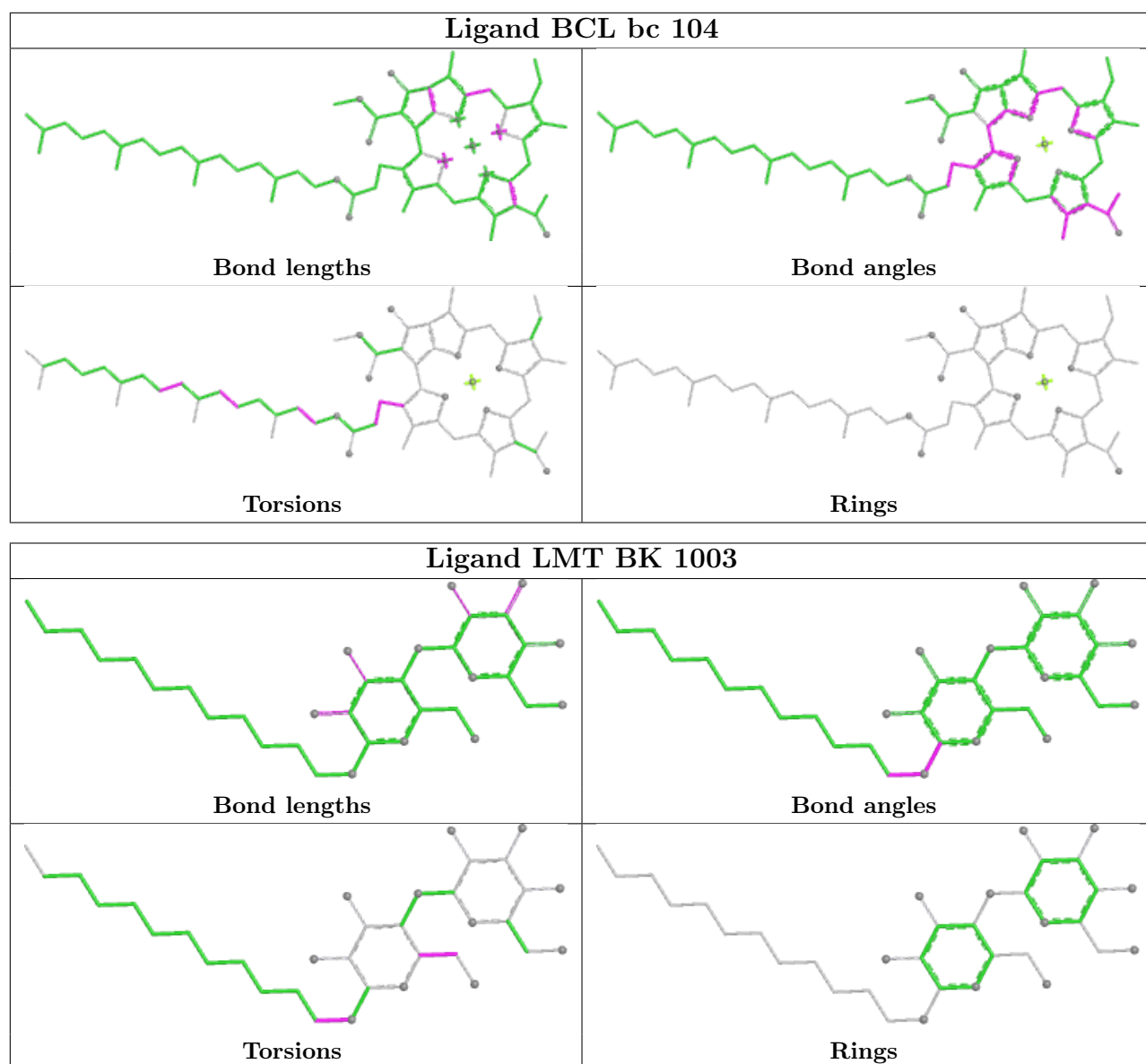


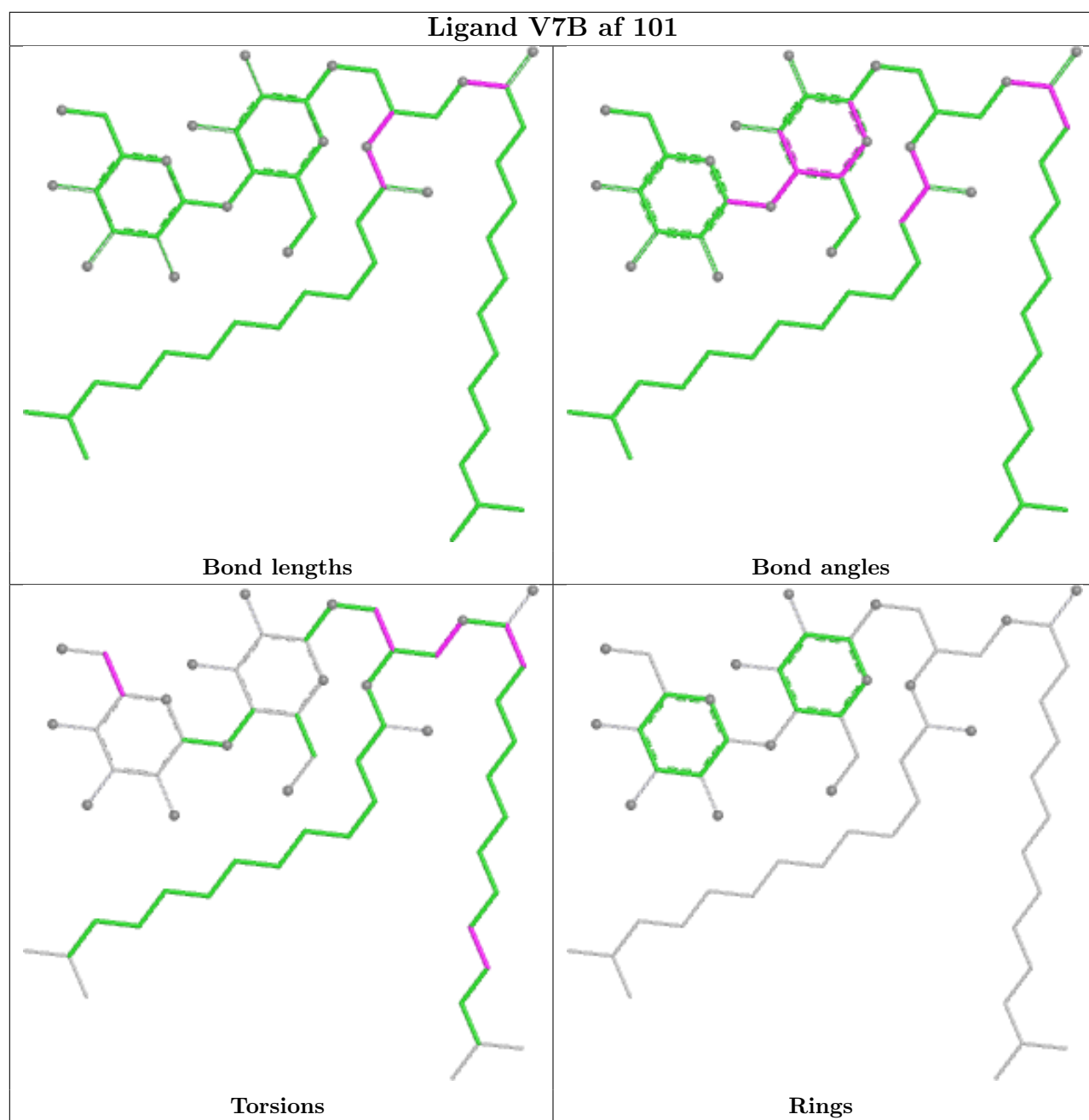


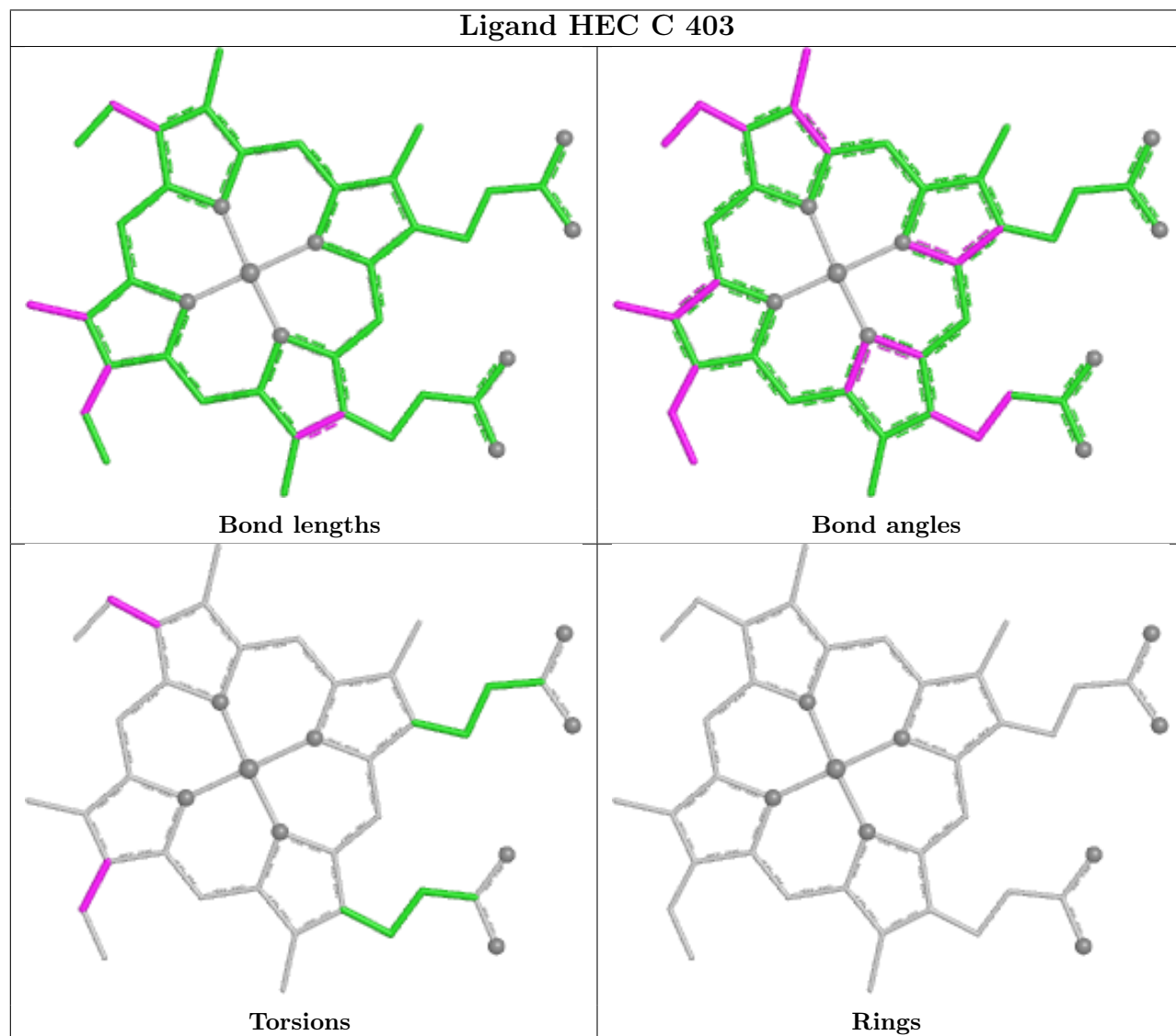
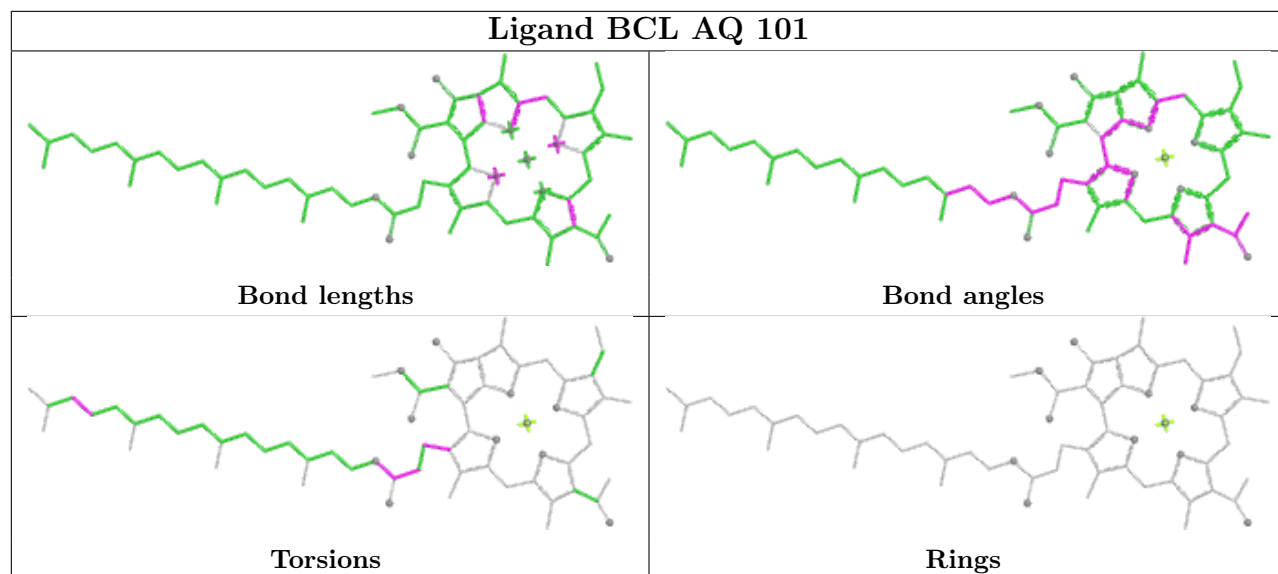


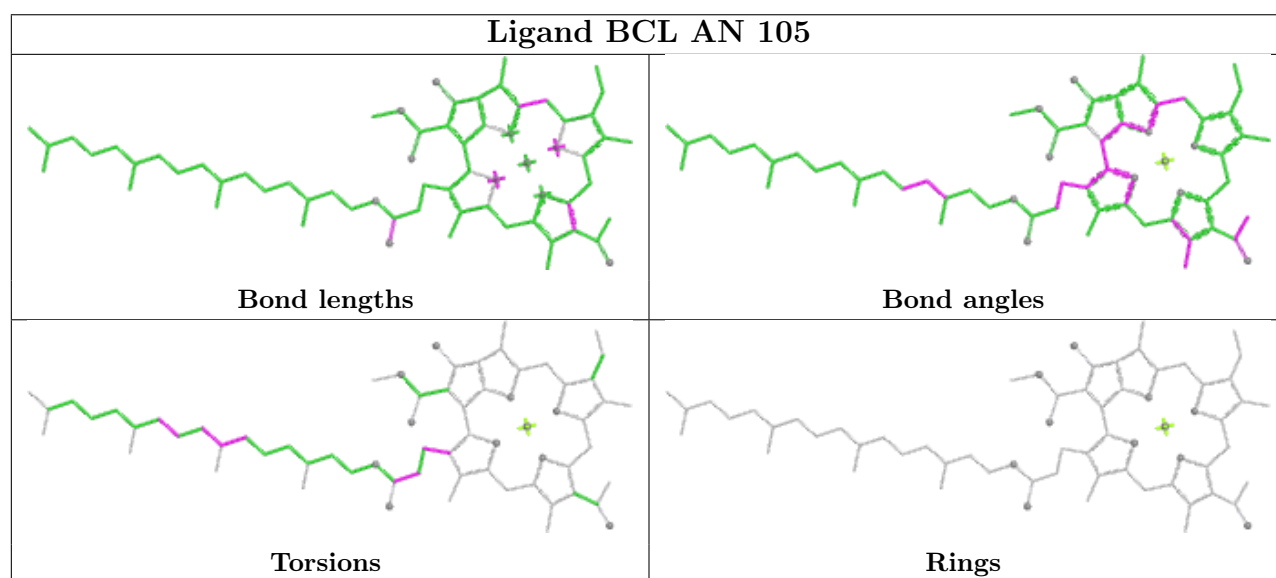
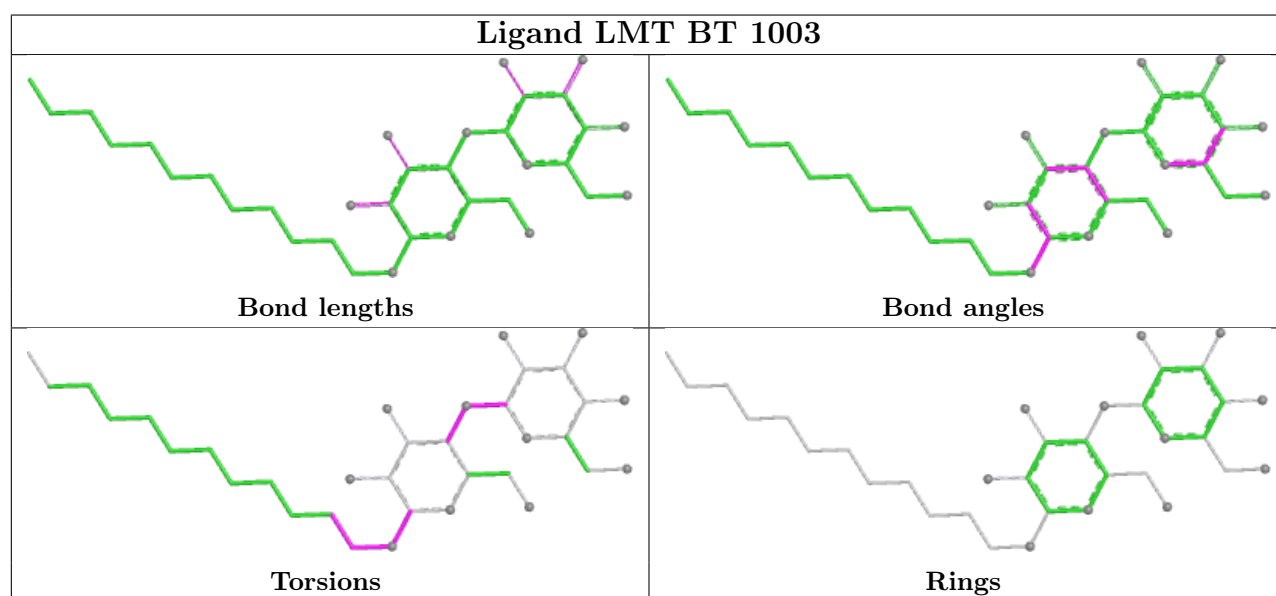
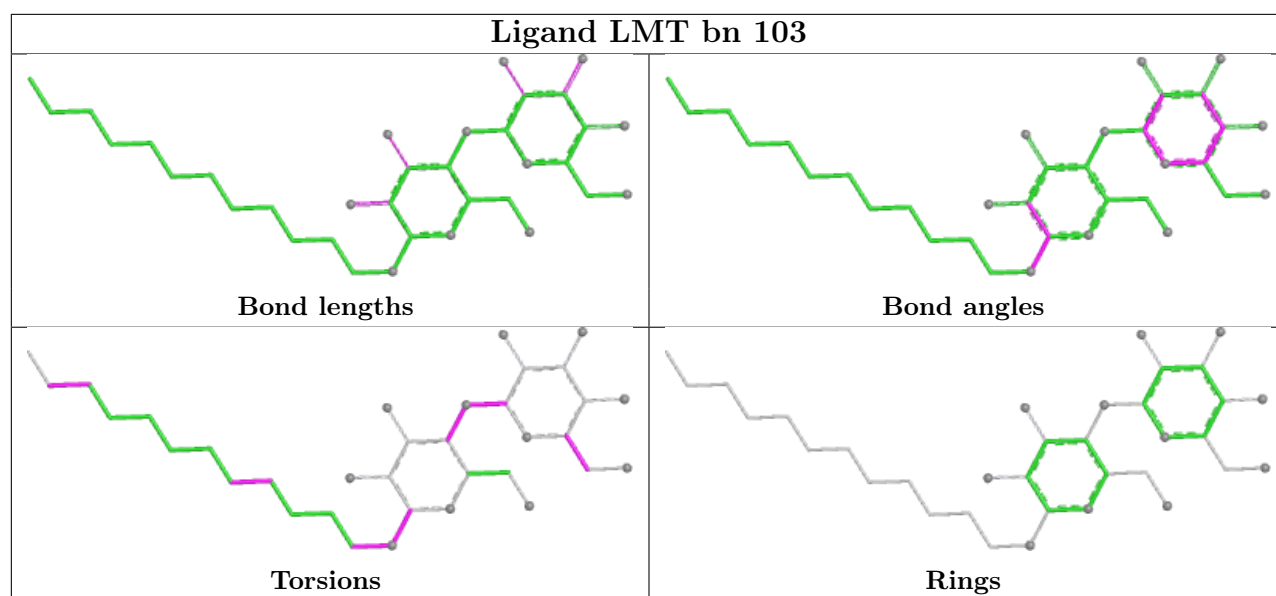


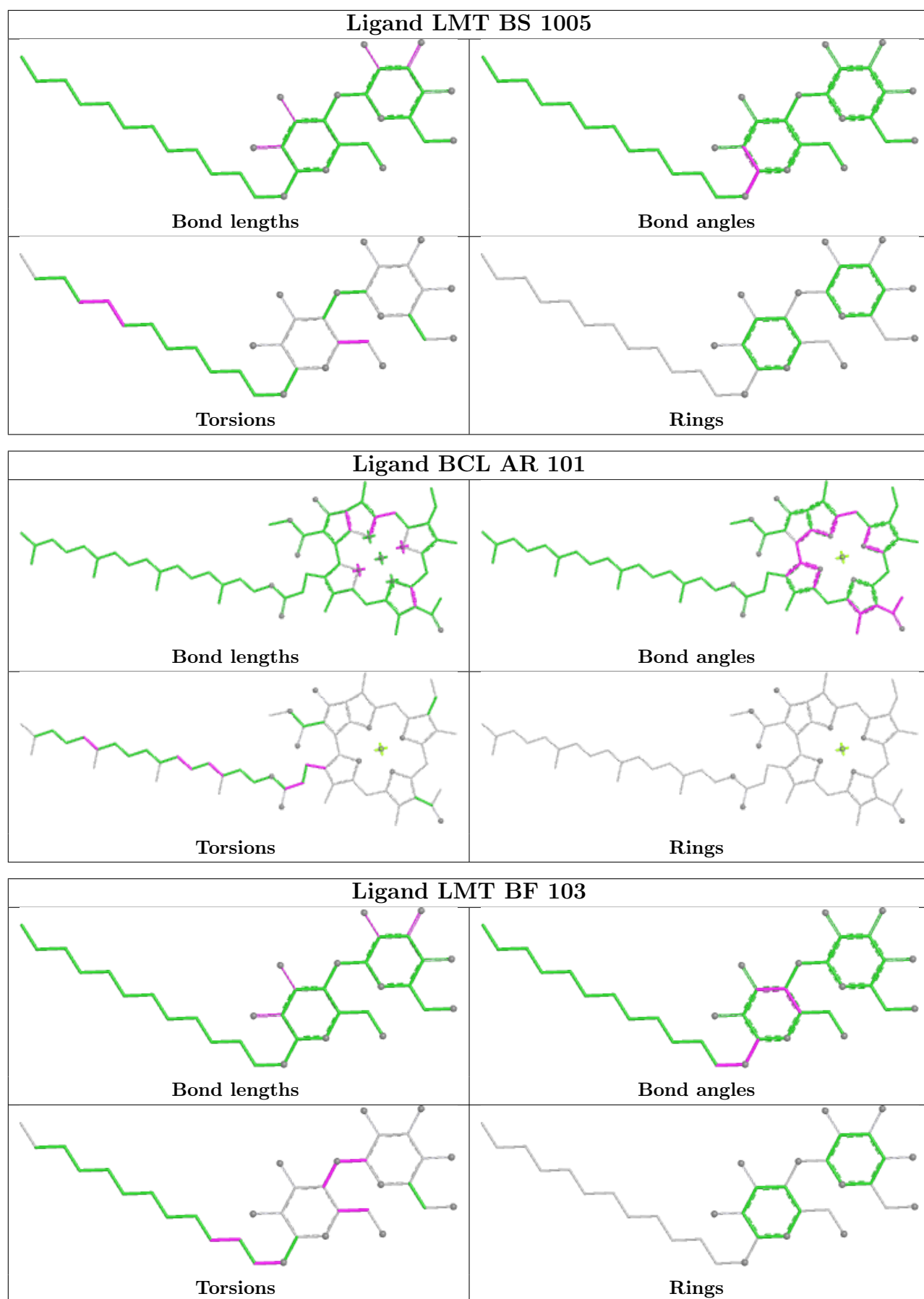




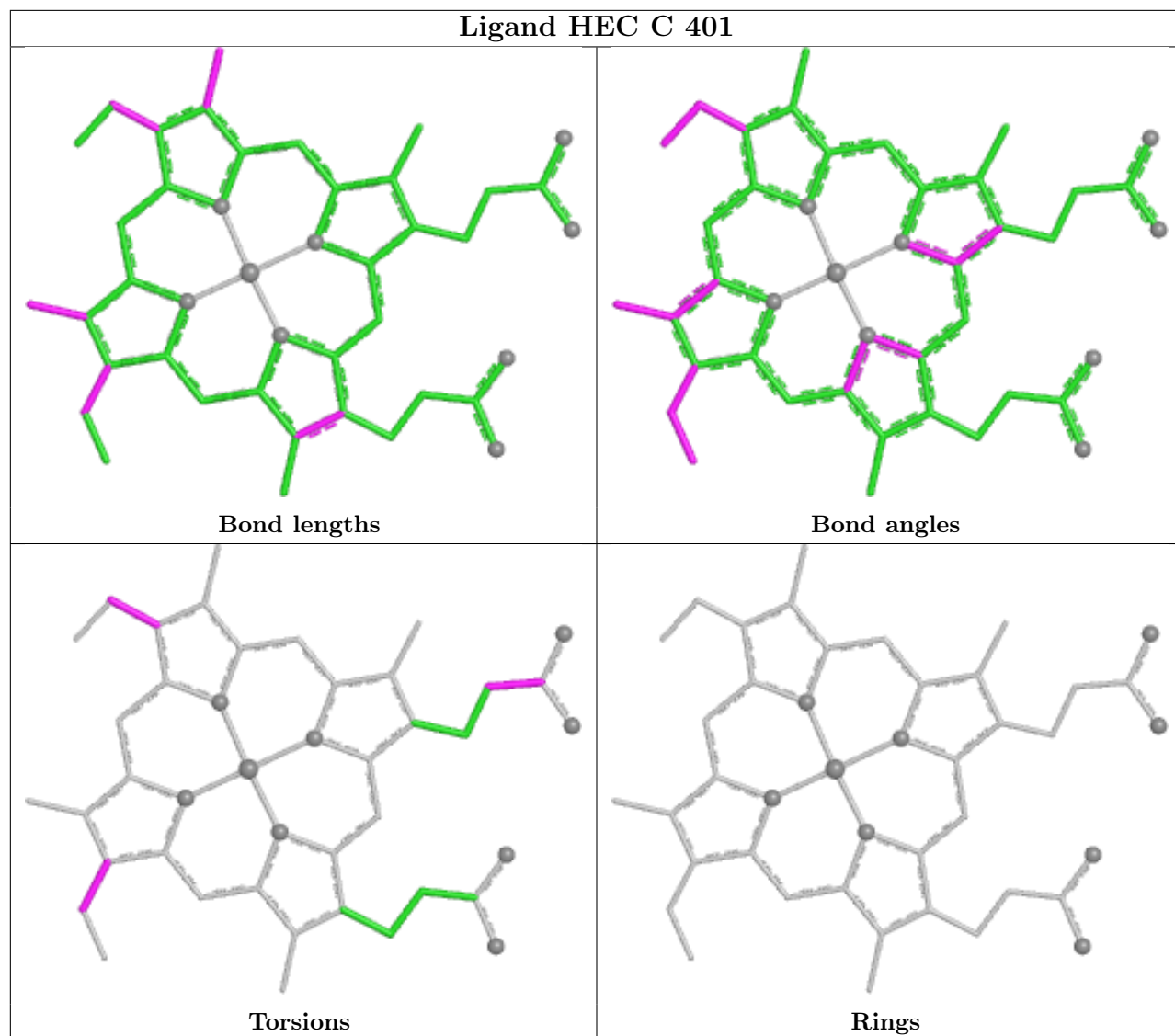




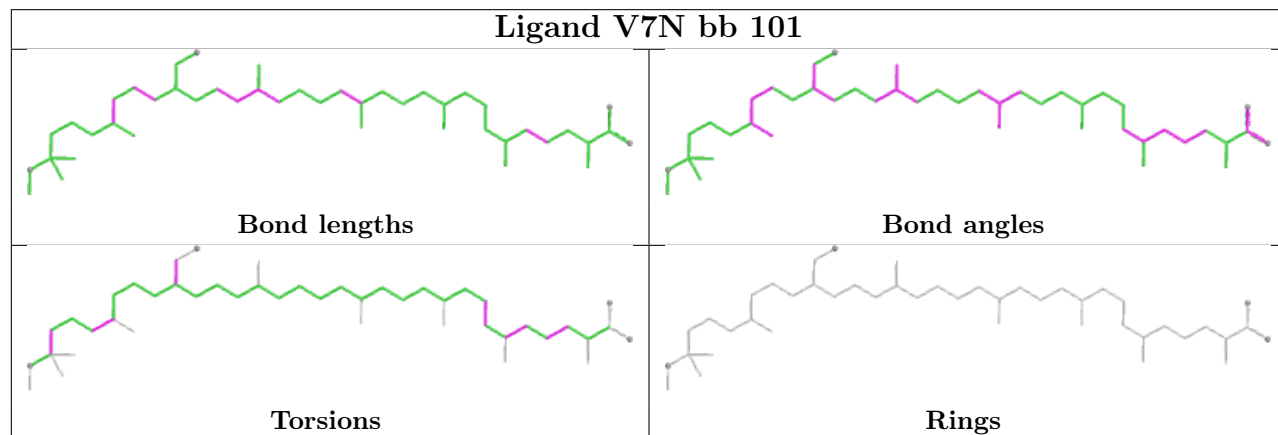


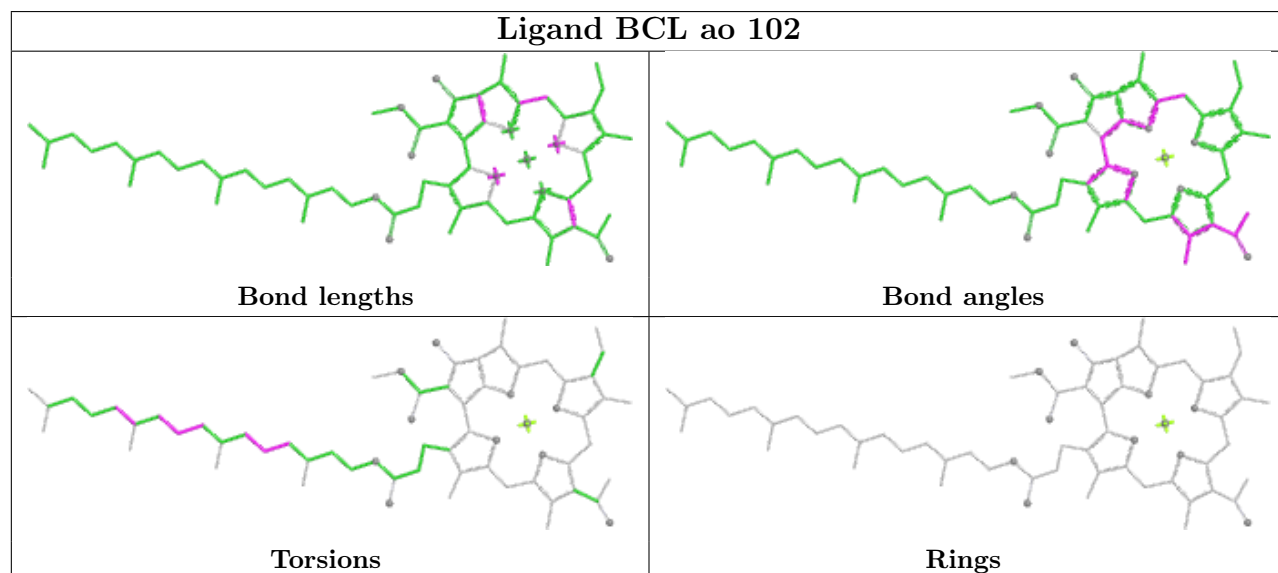
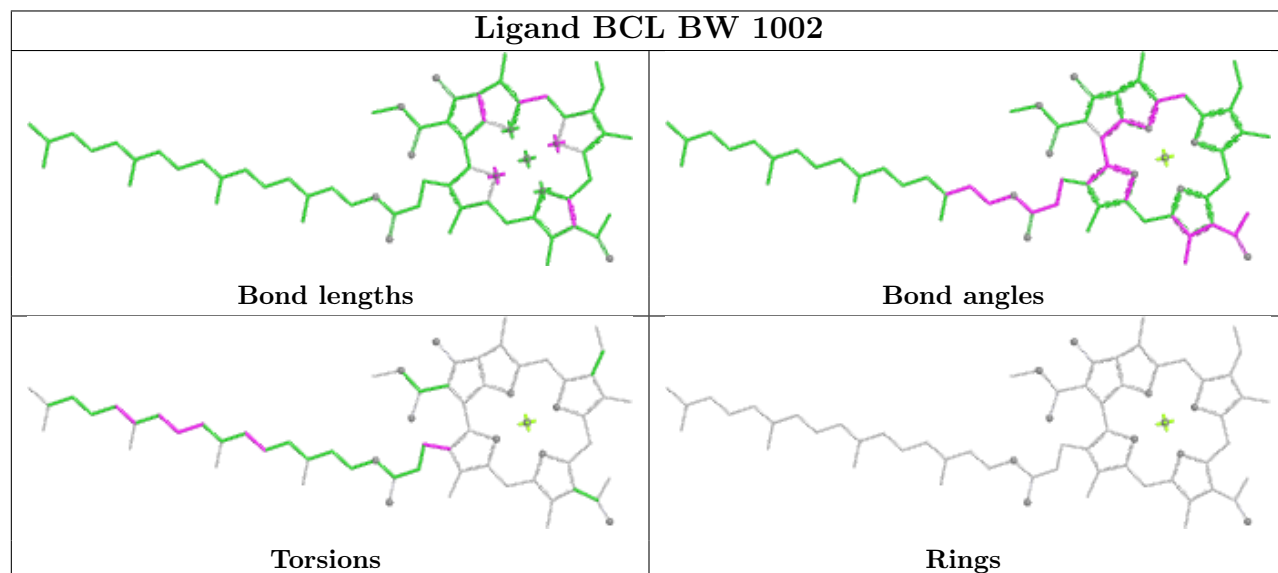
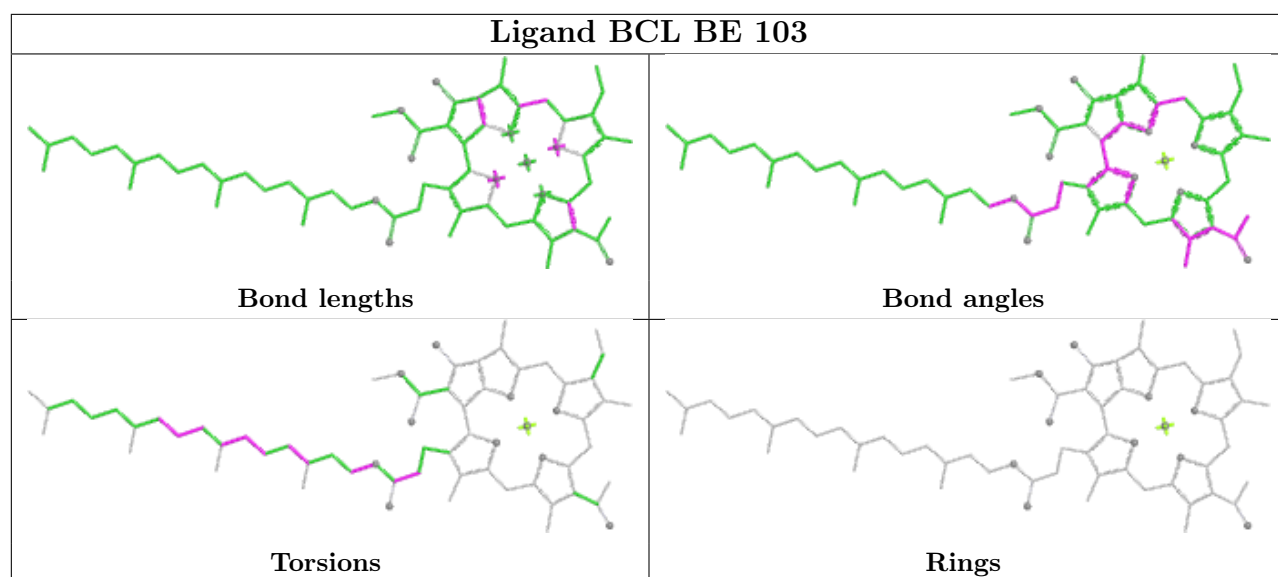


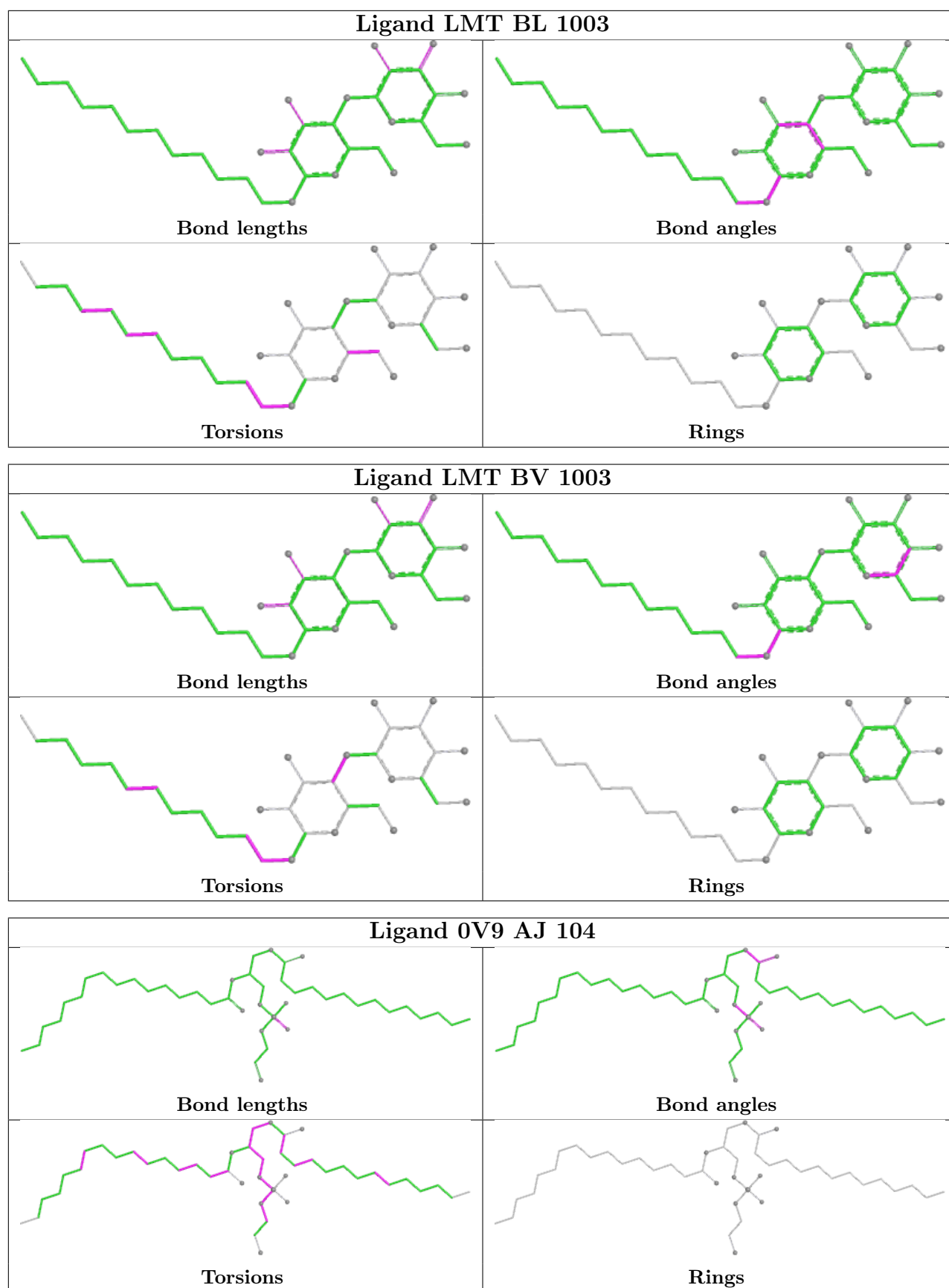
Ligand HEC C 401

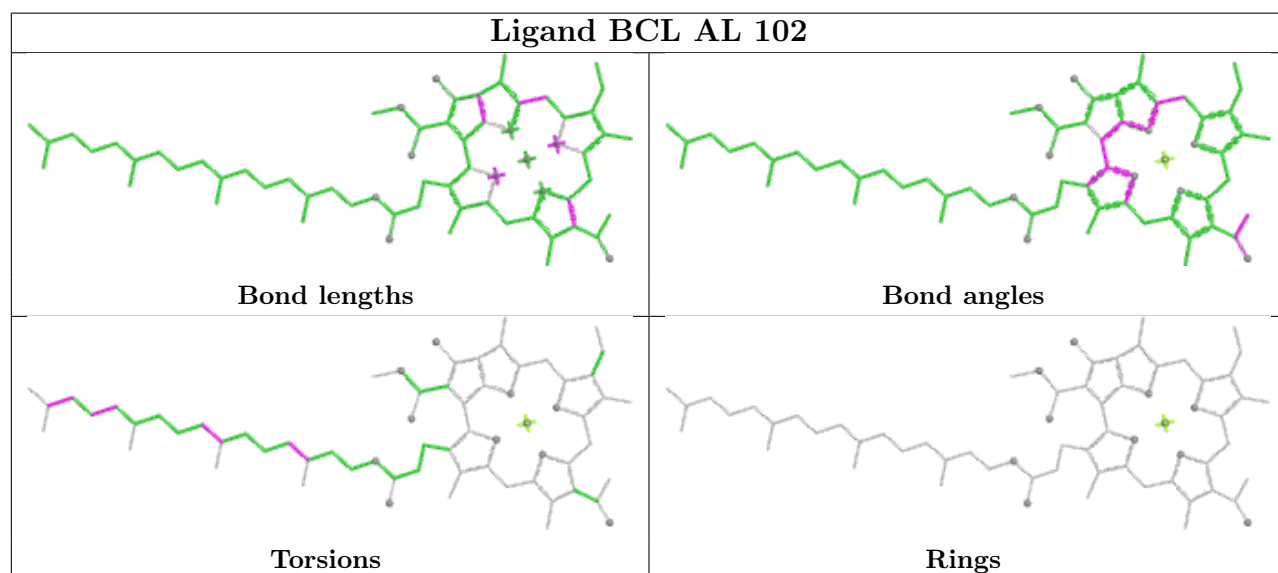
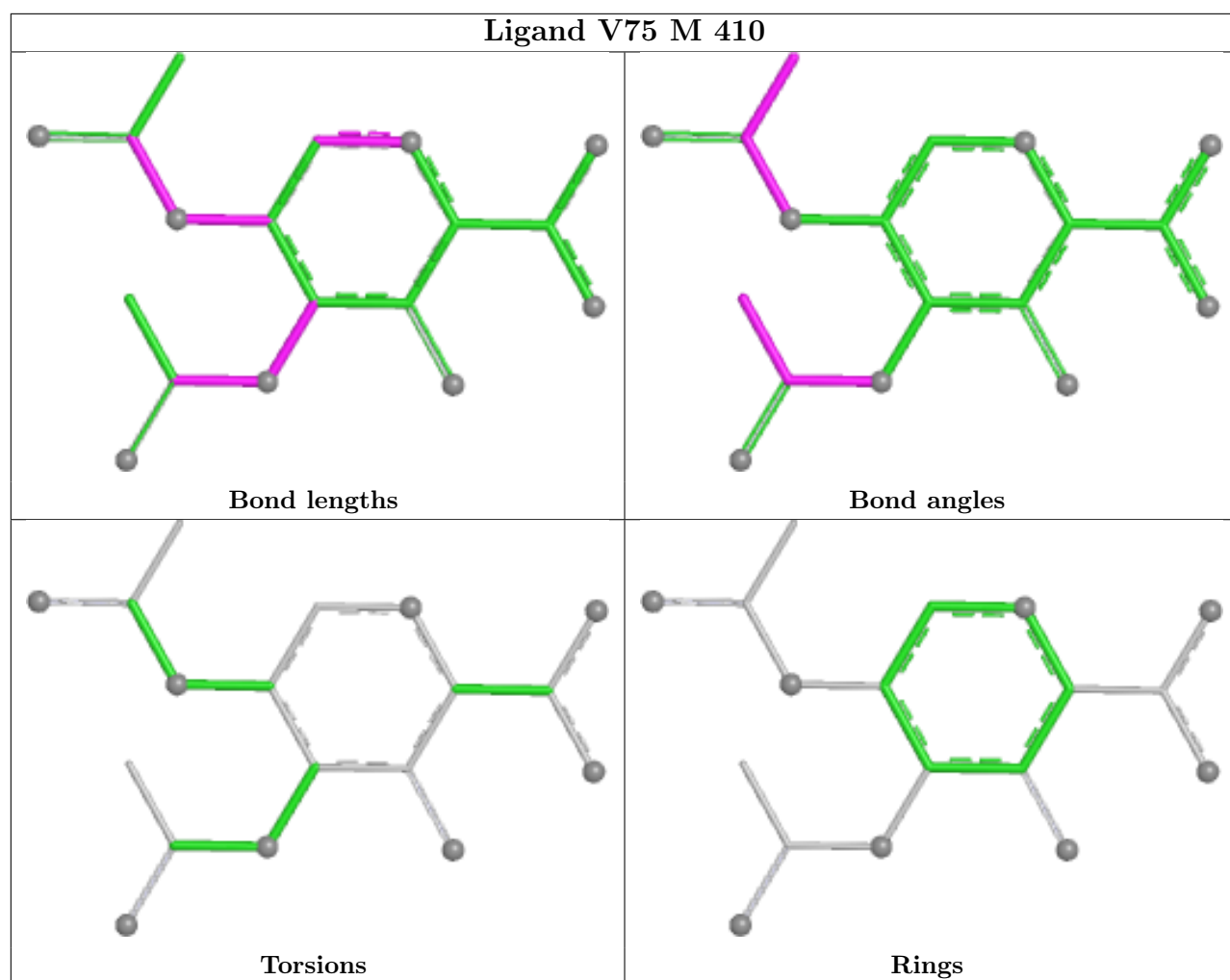


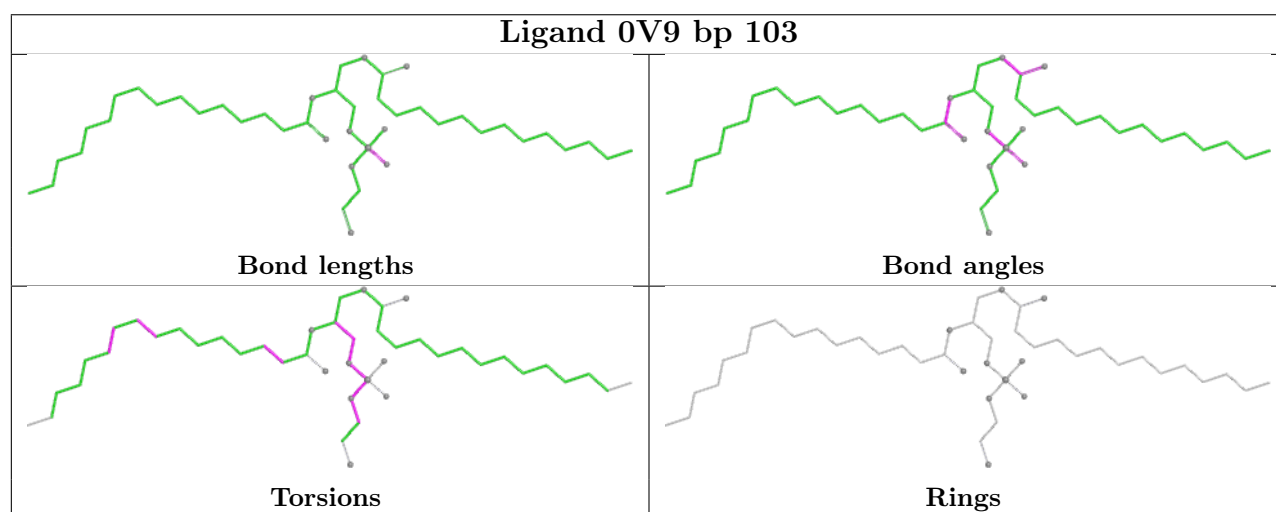
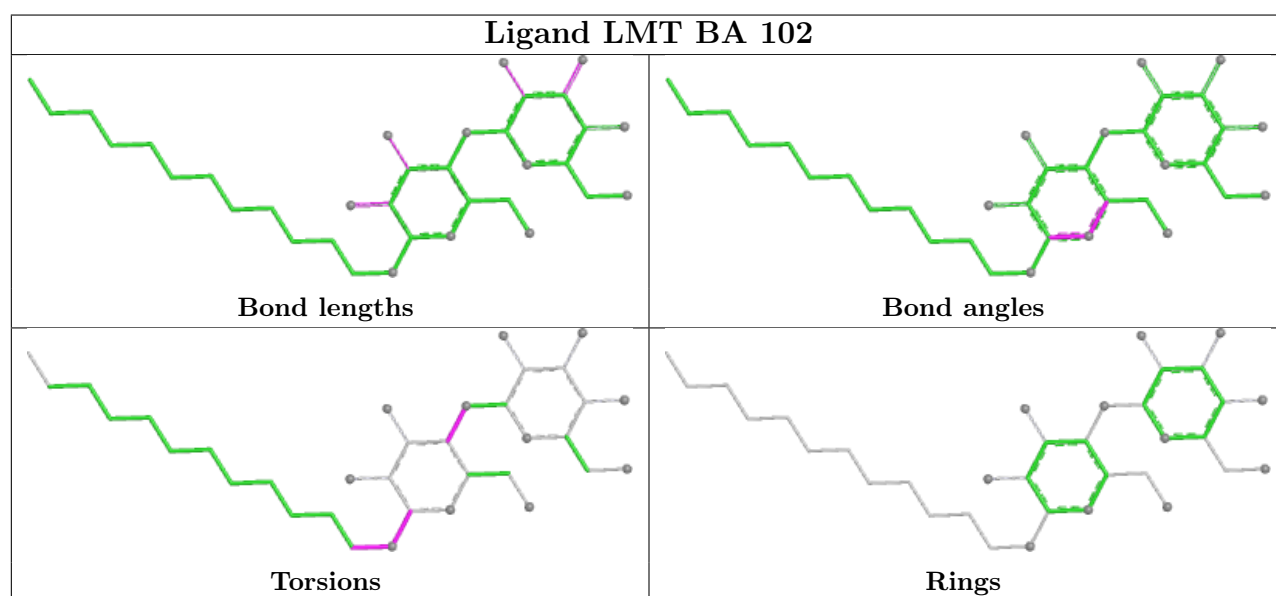
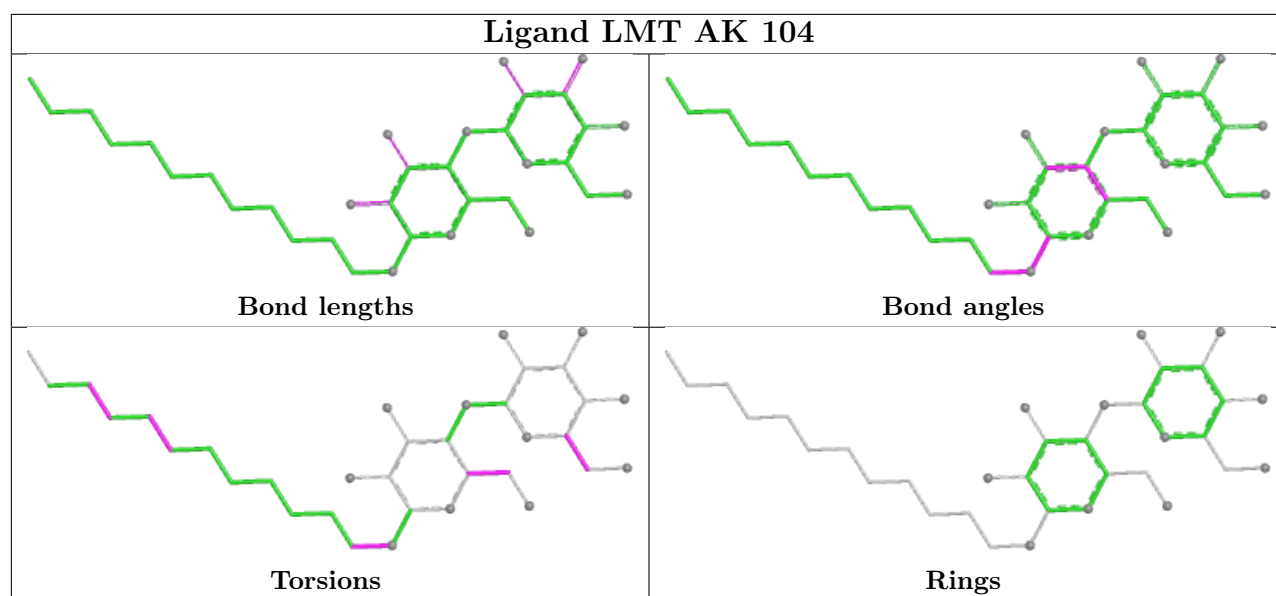
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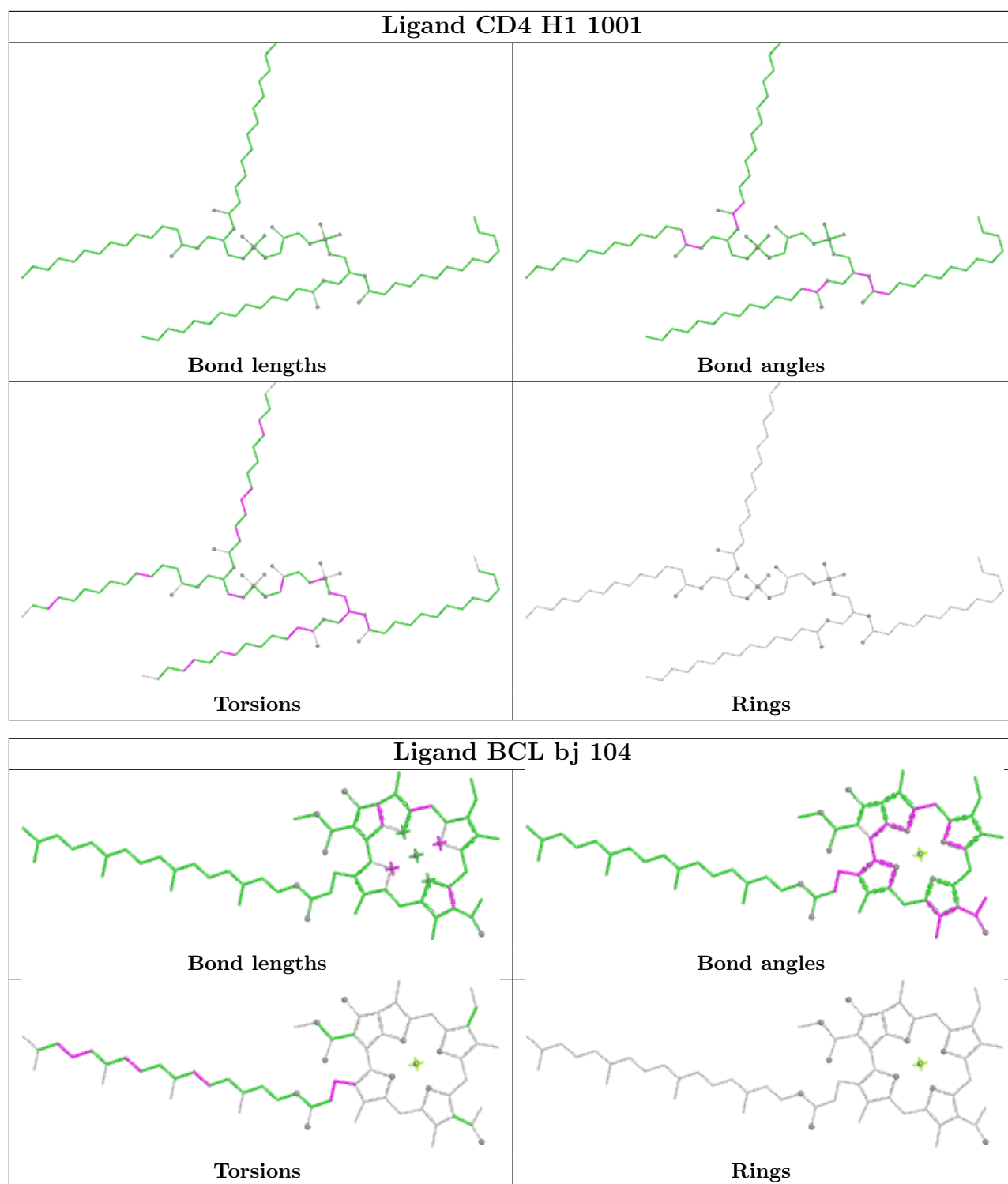


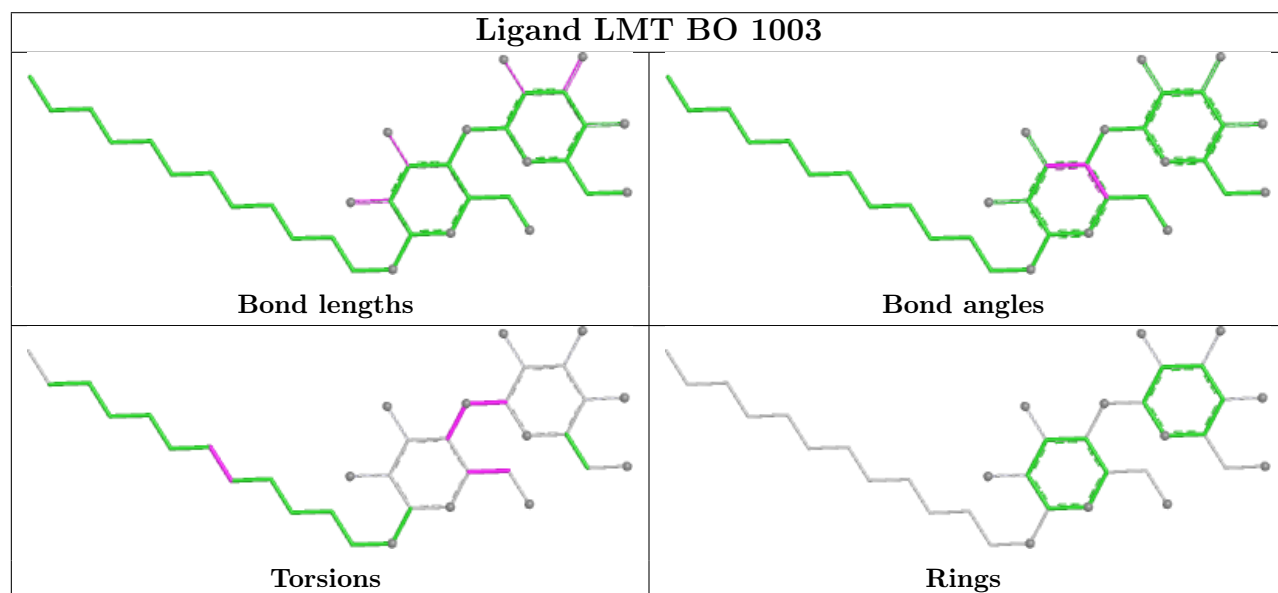
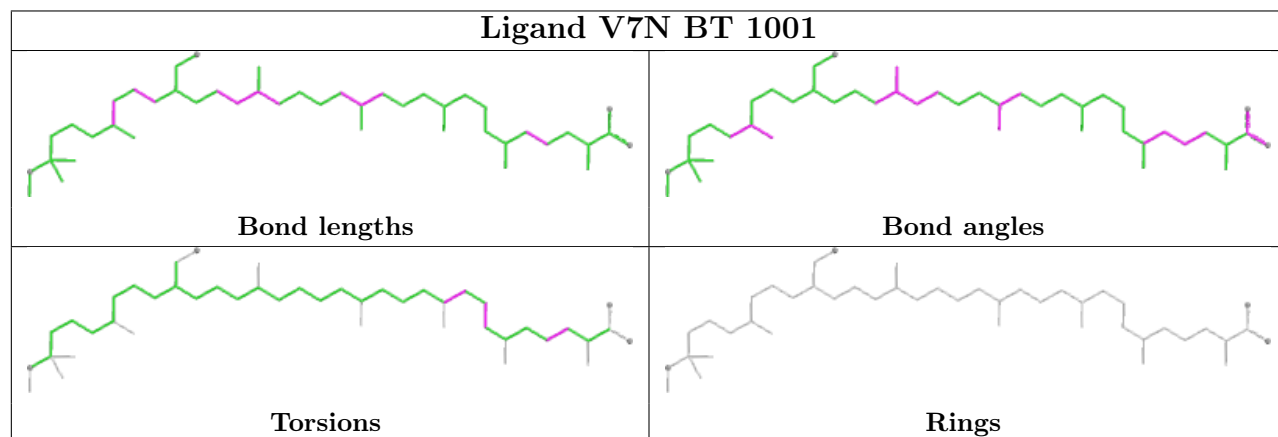
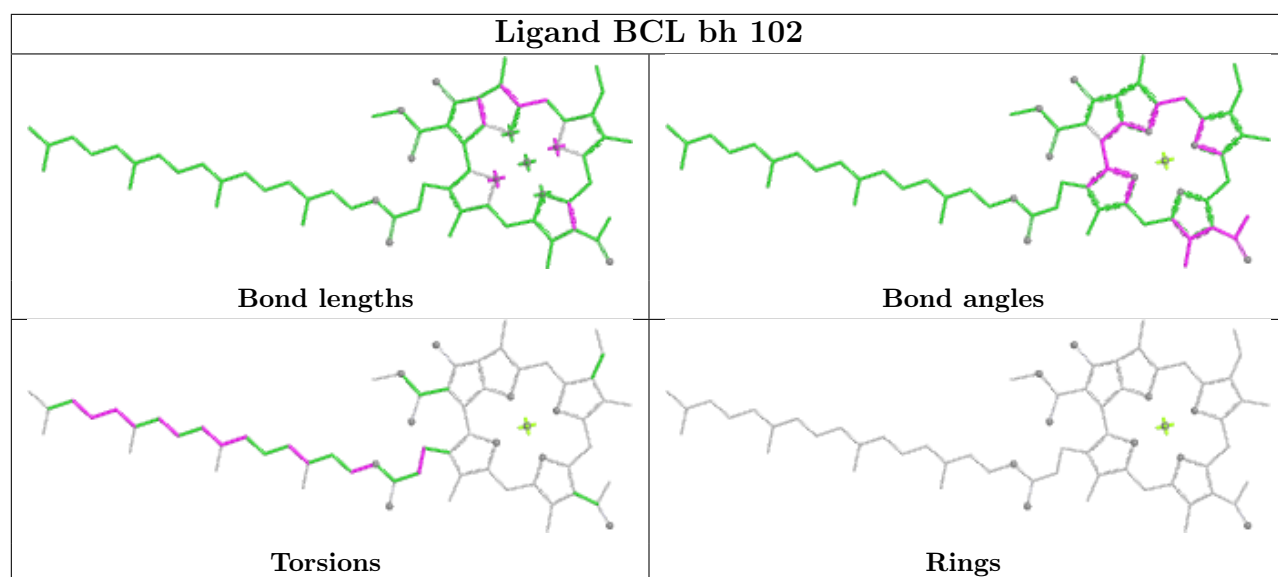


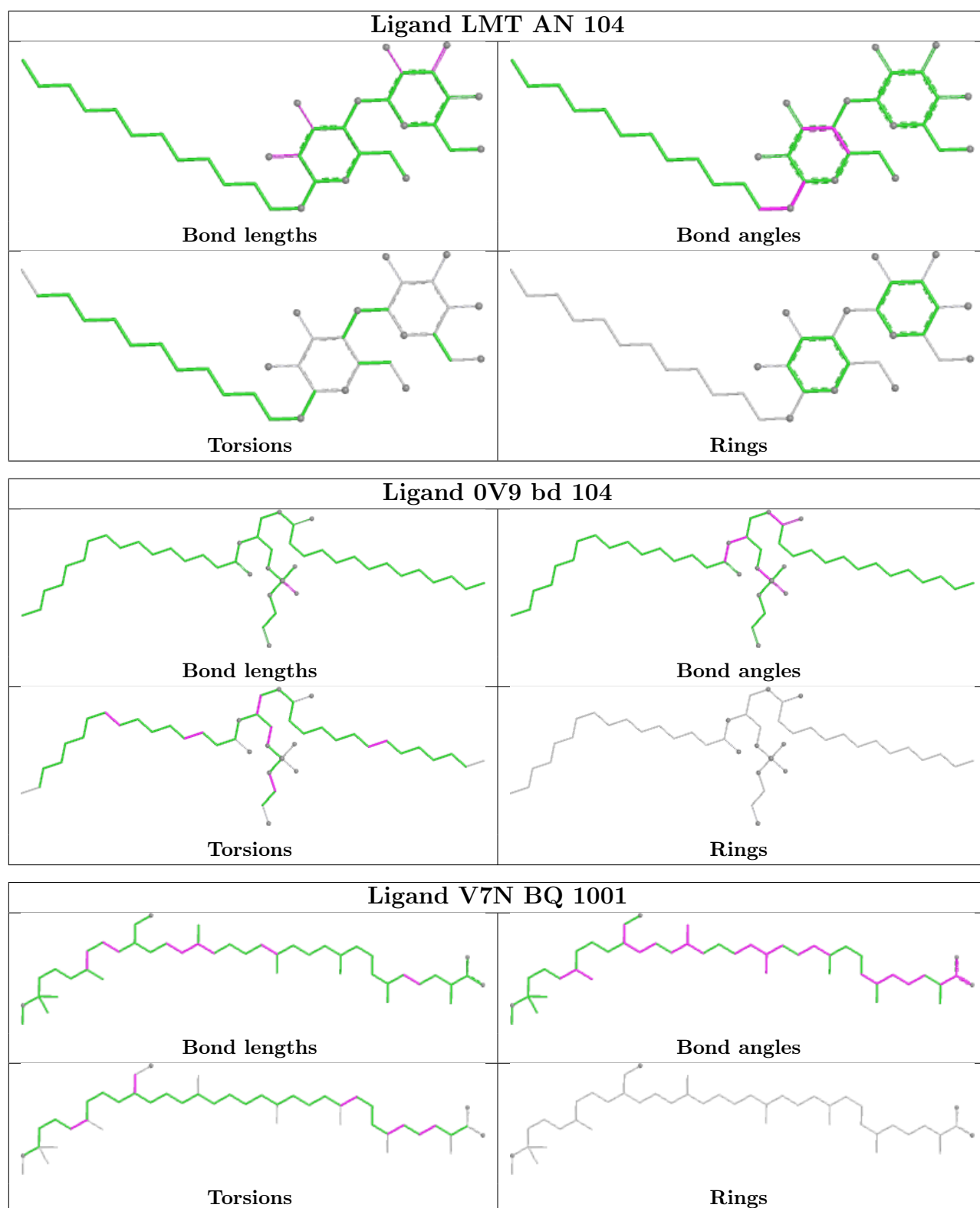


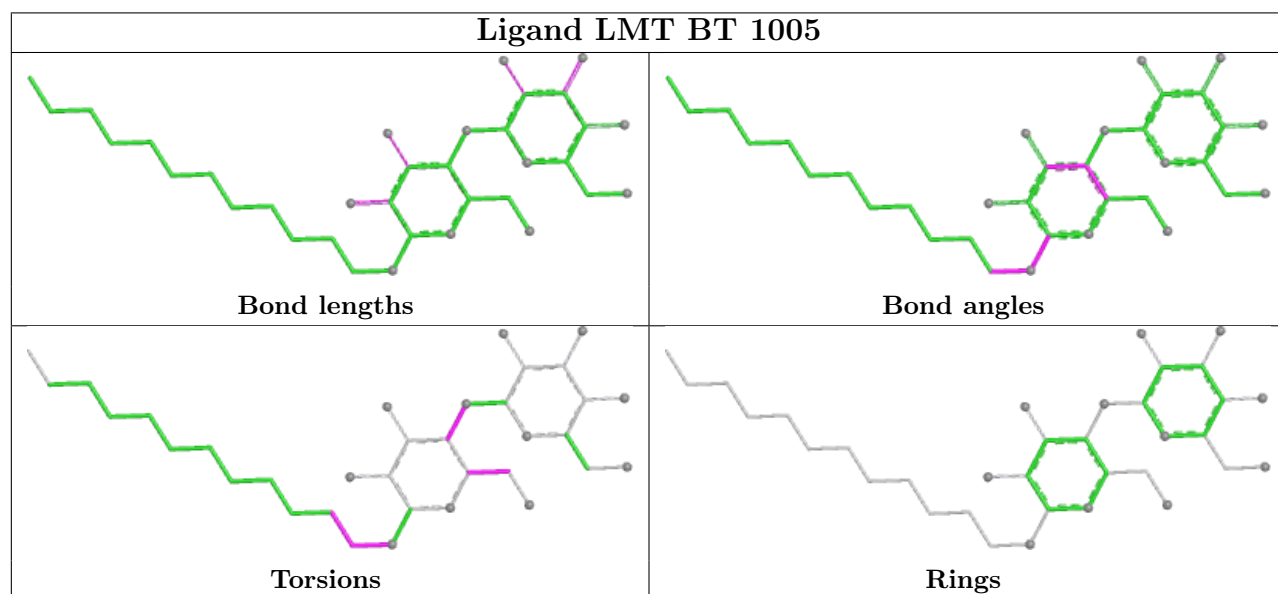
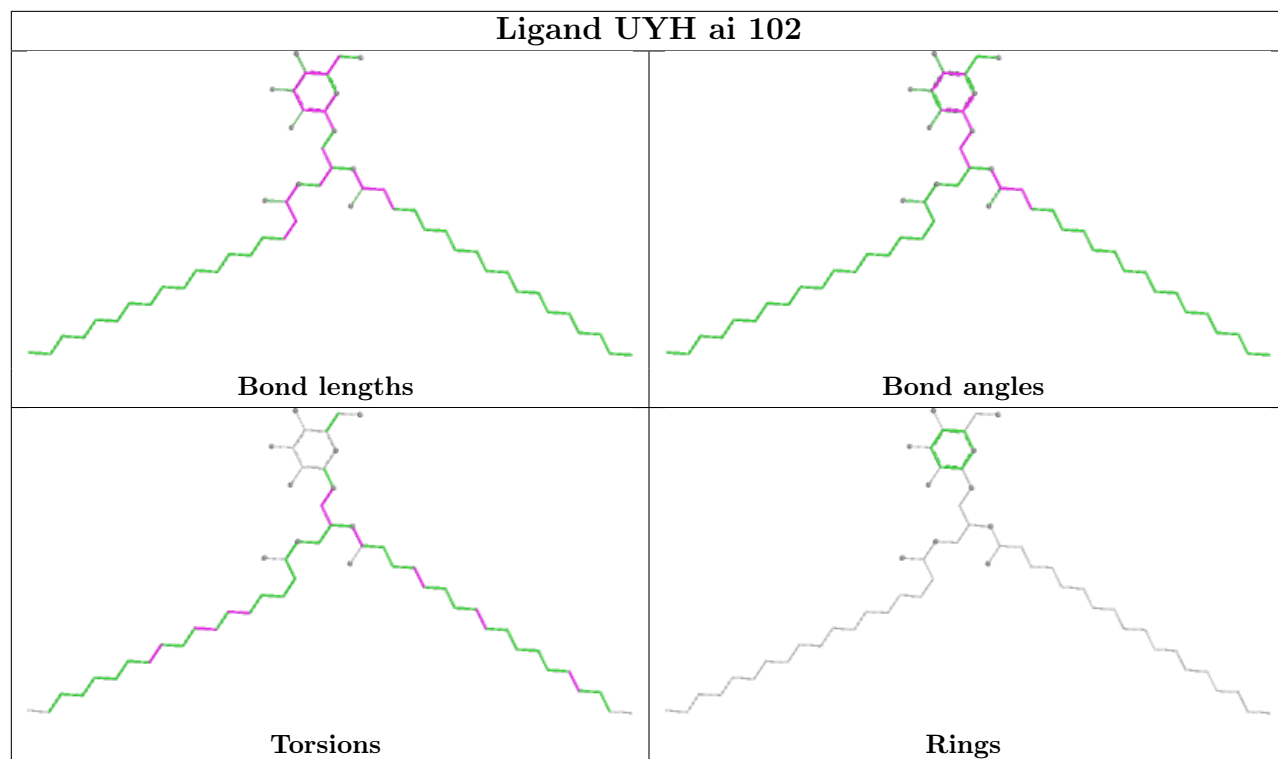


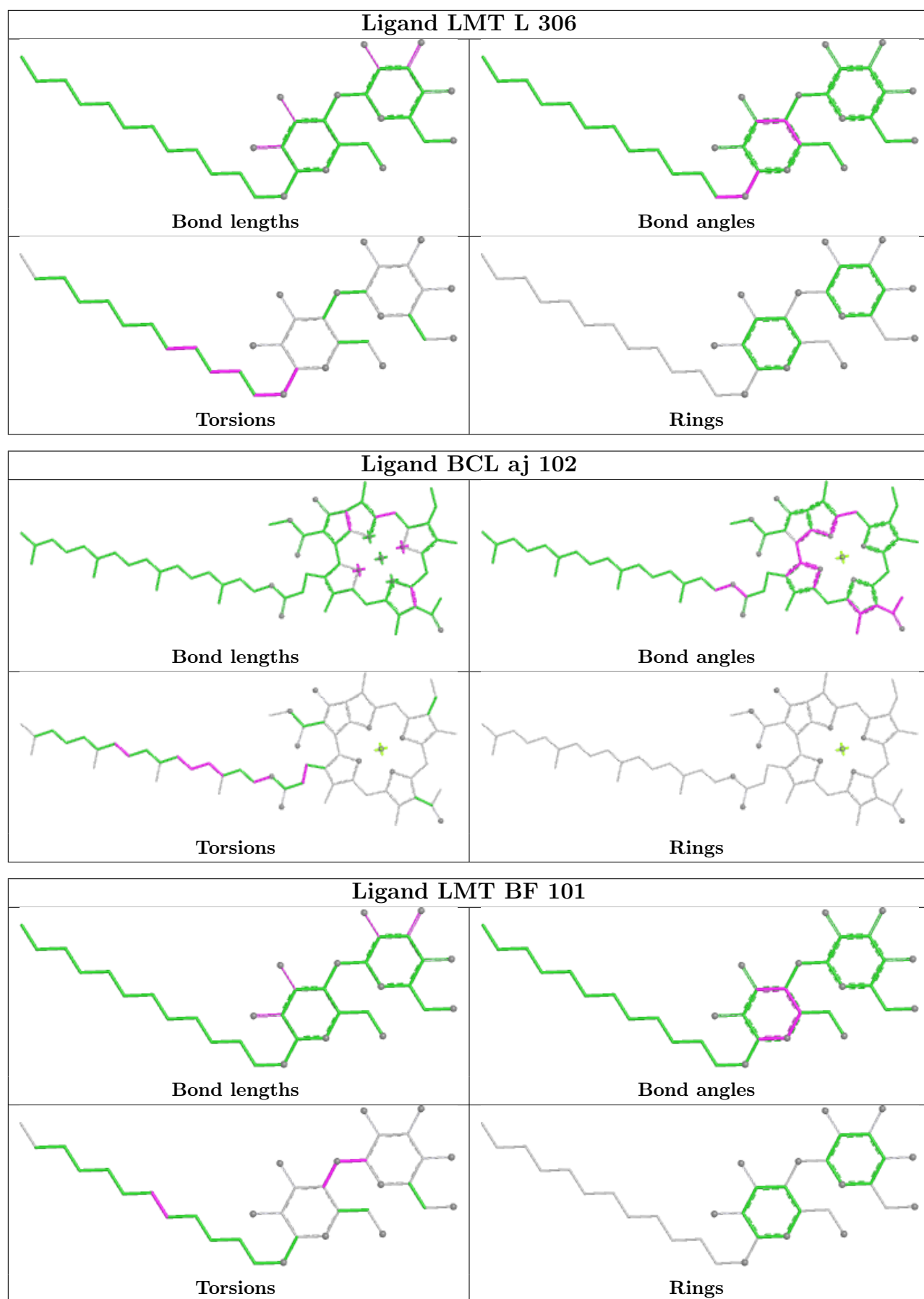


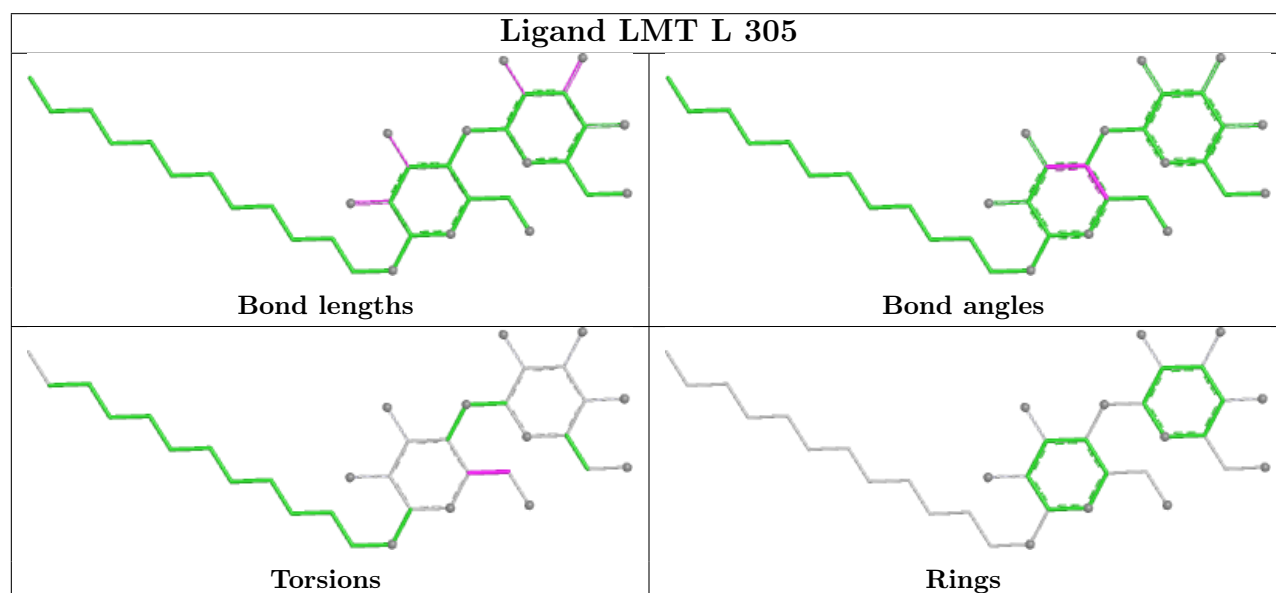
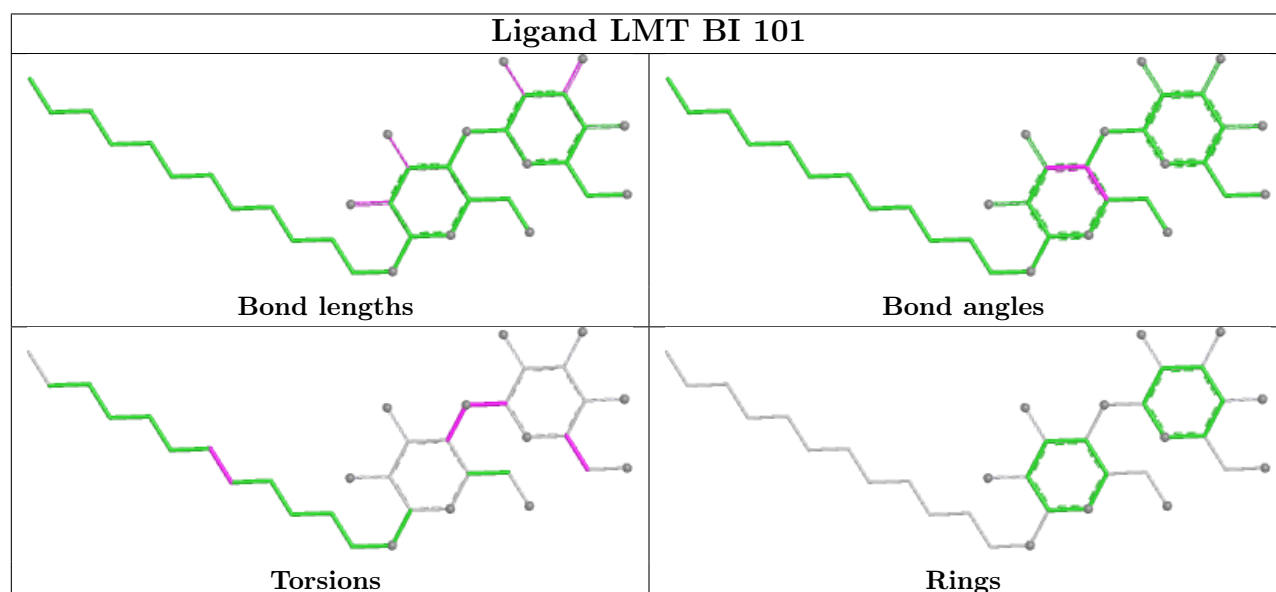
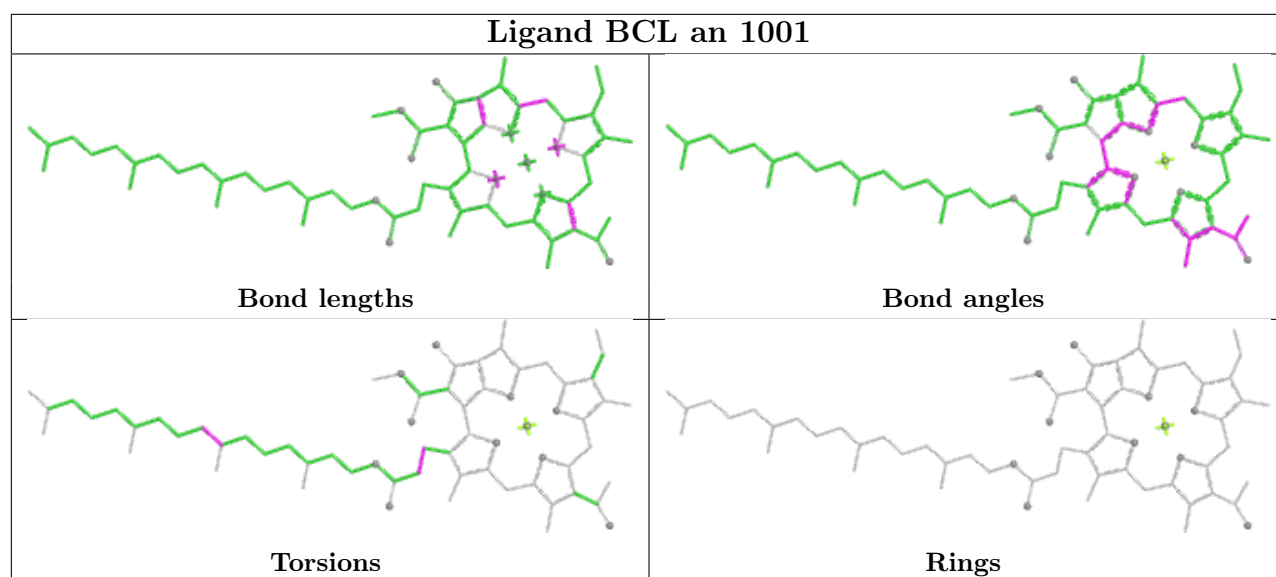


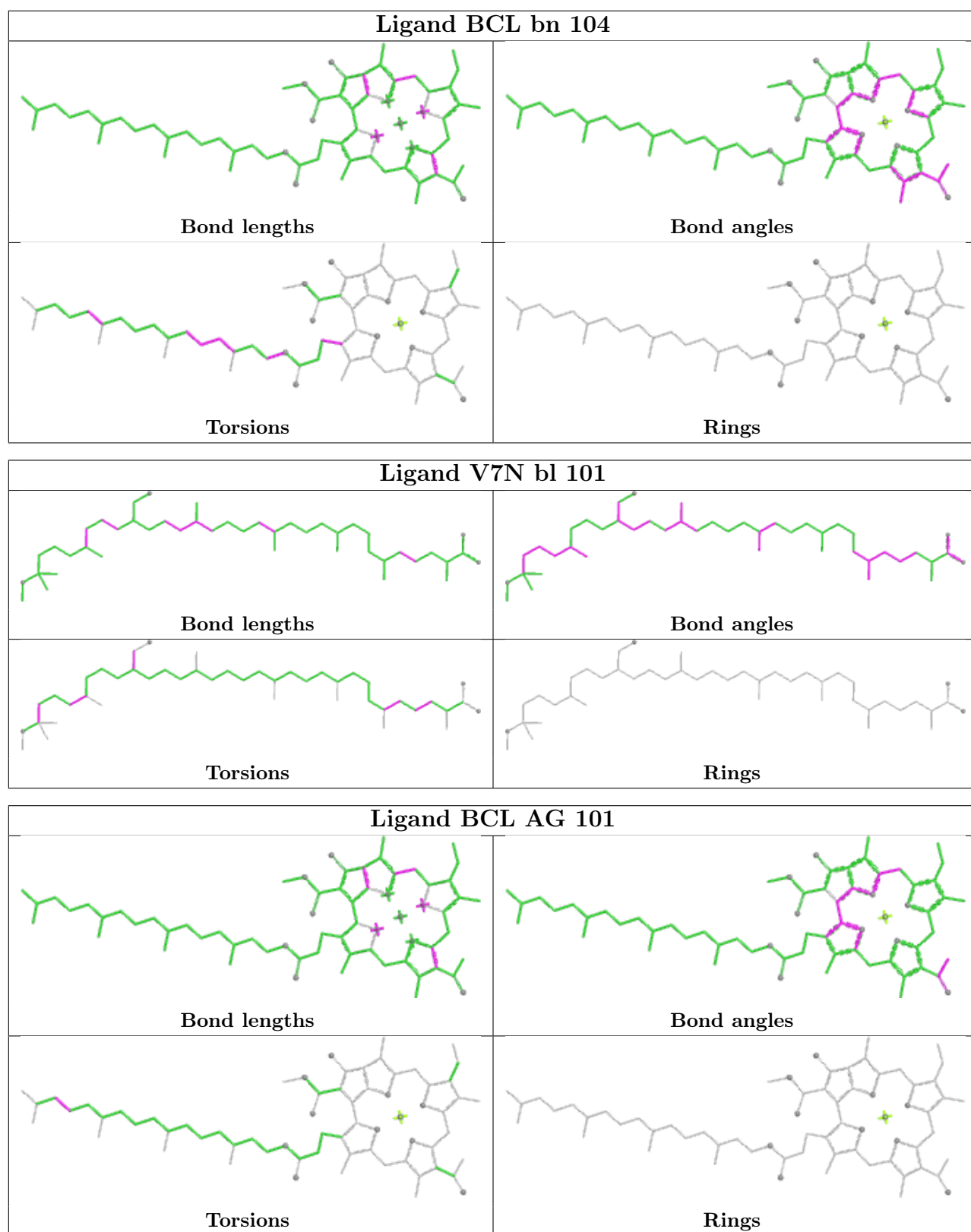


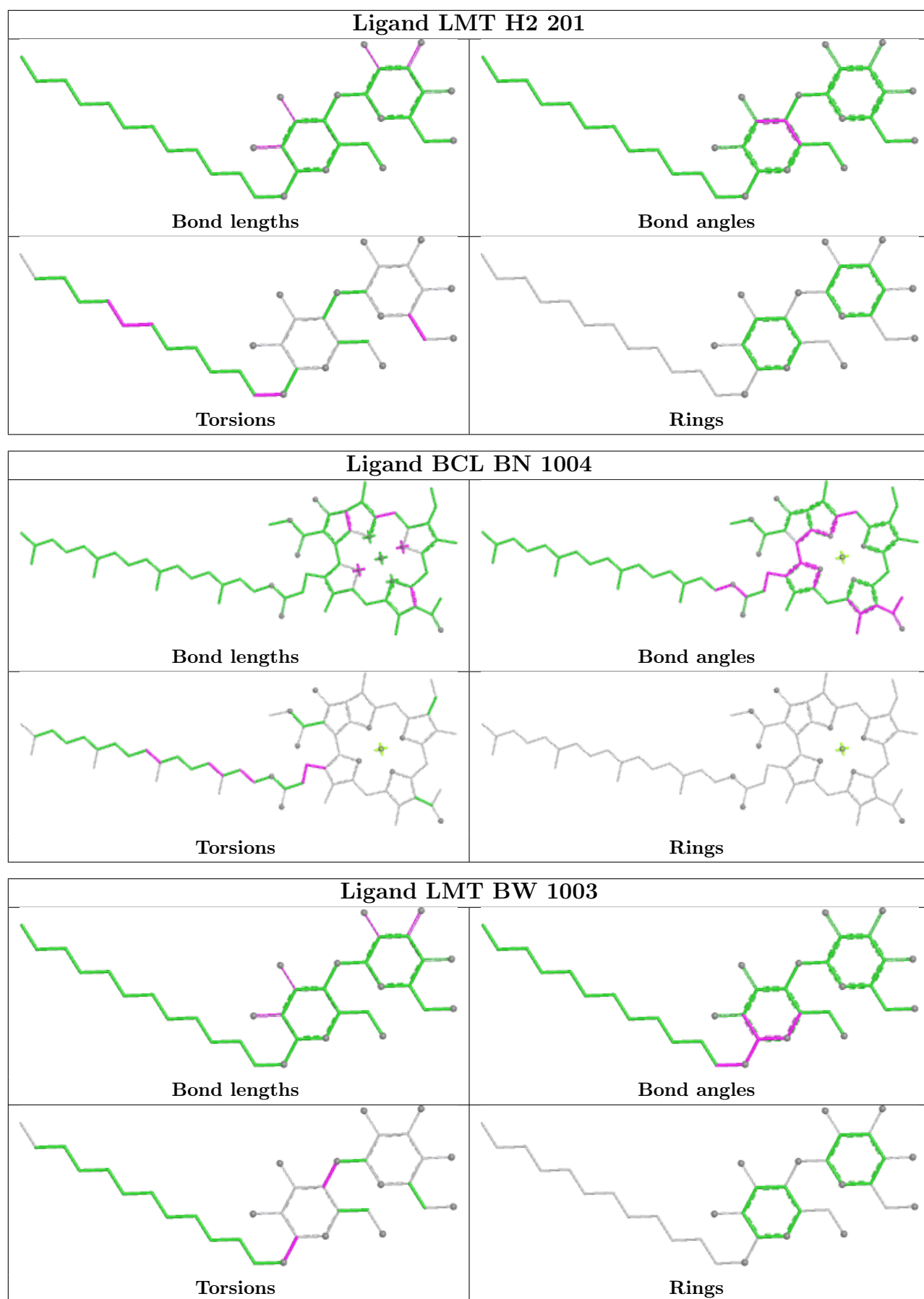


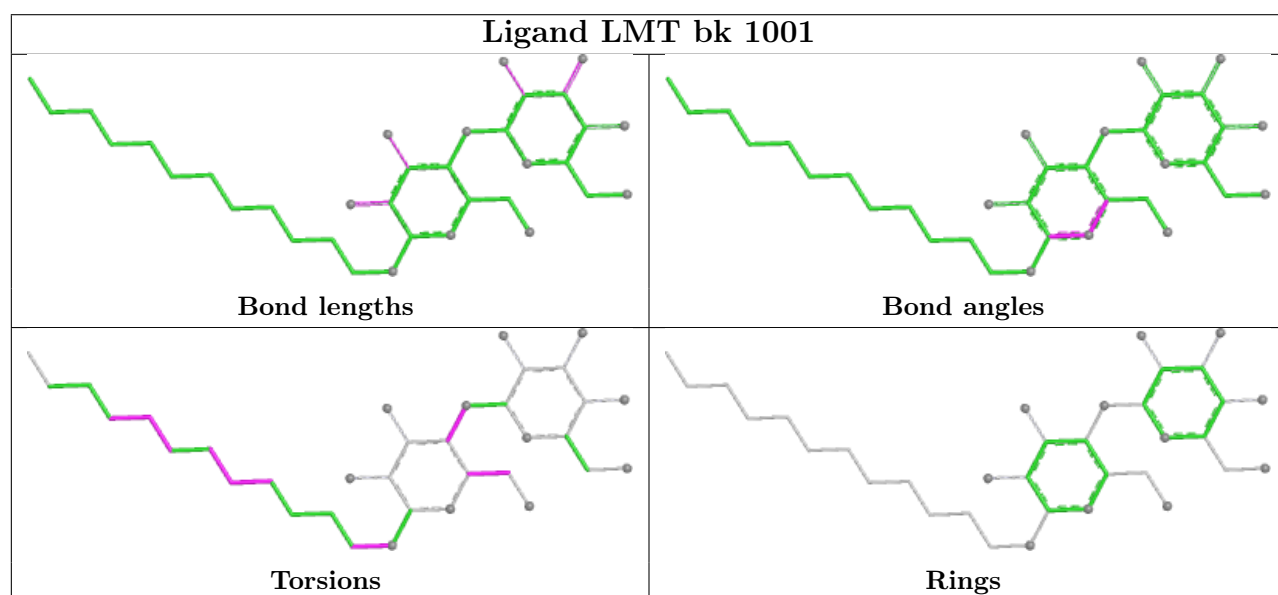
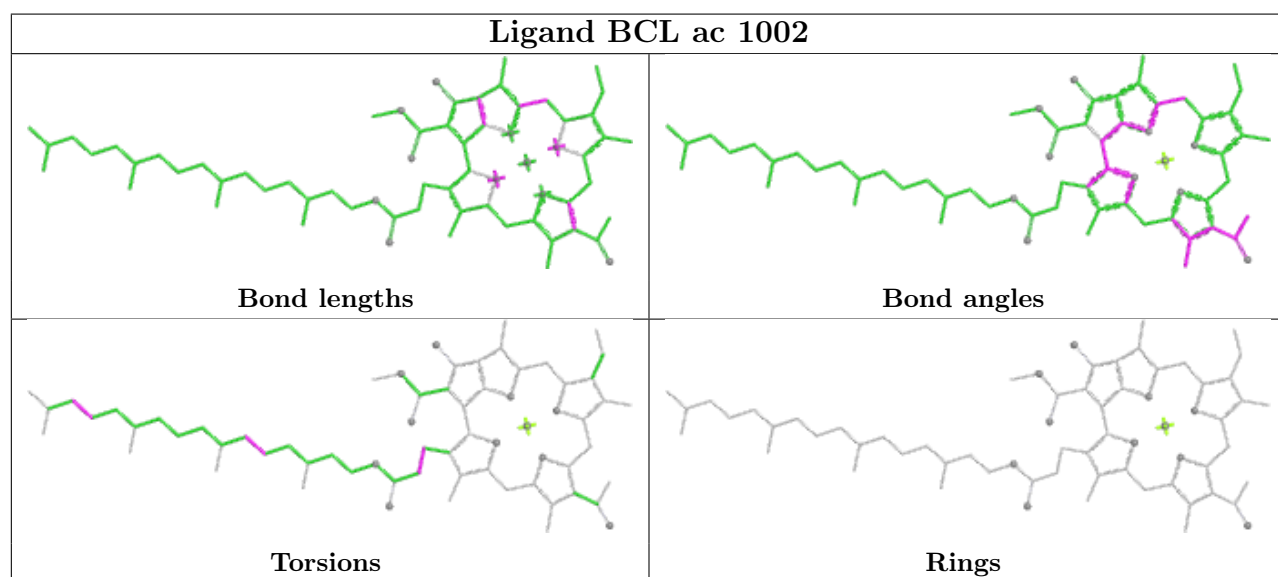
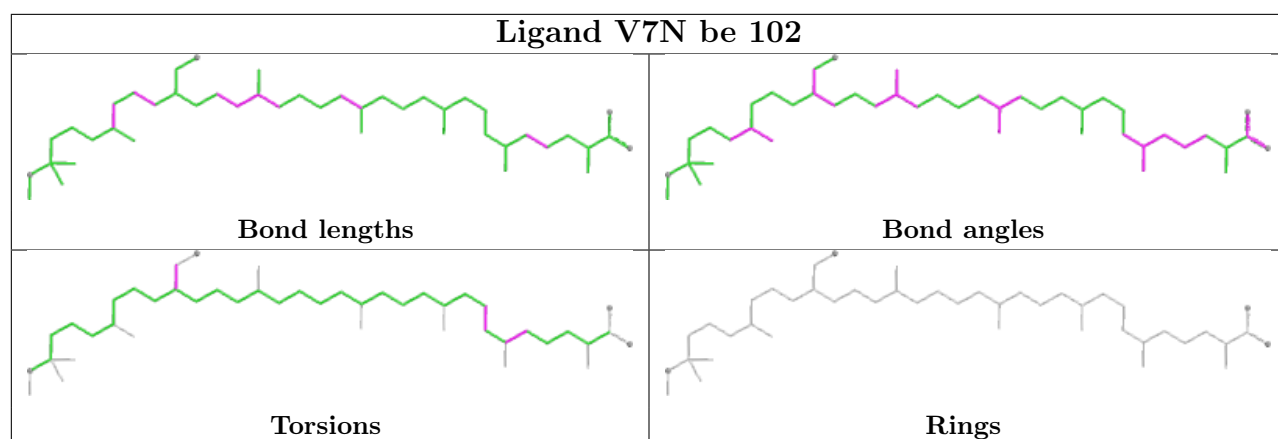


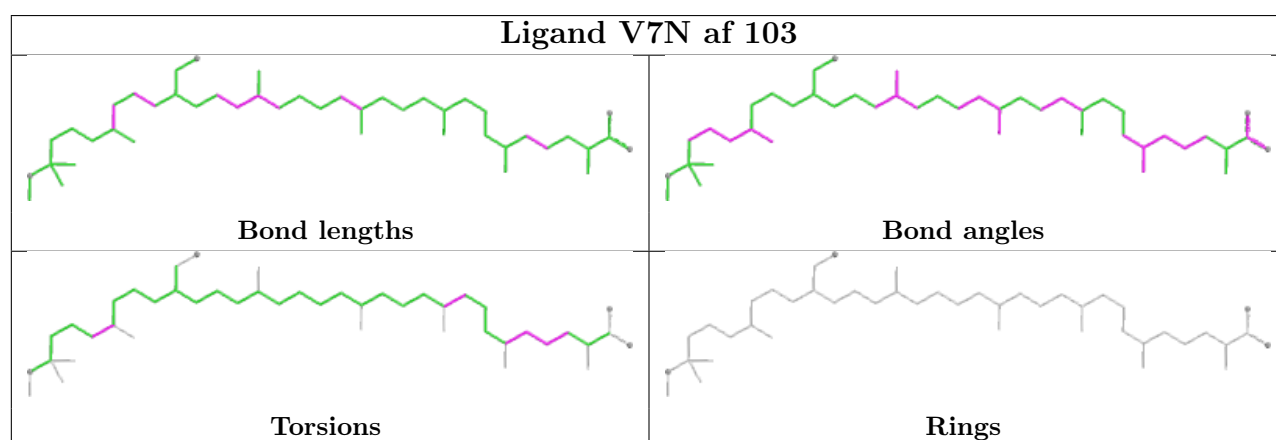
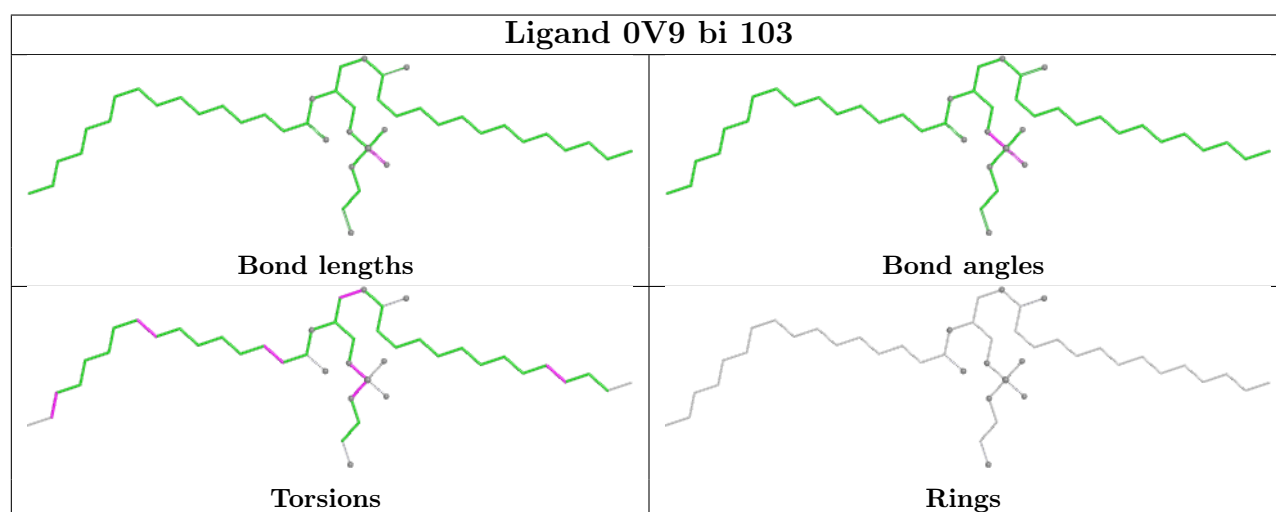
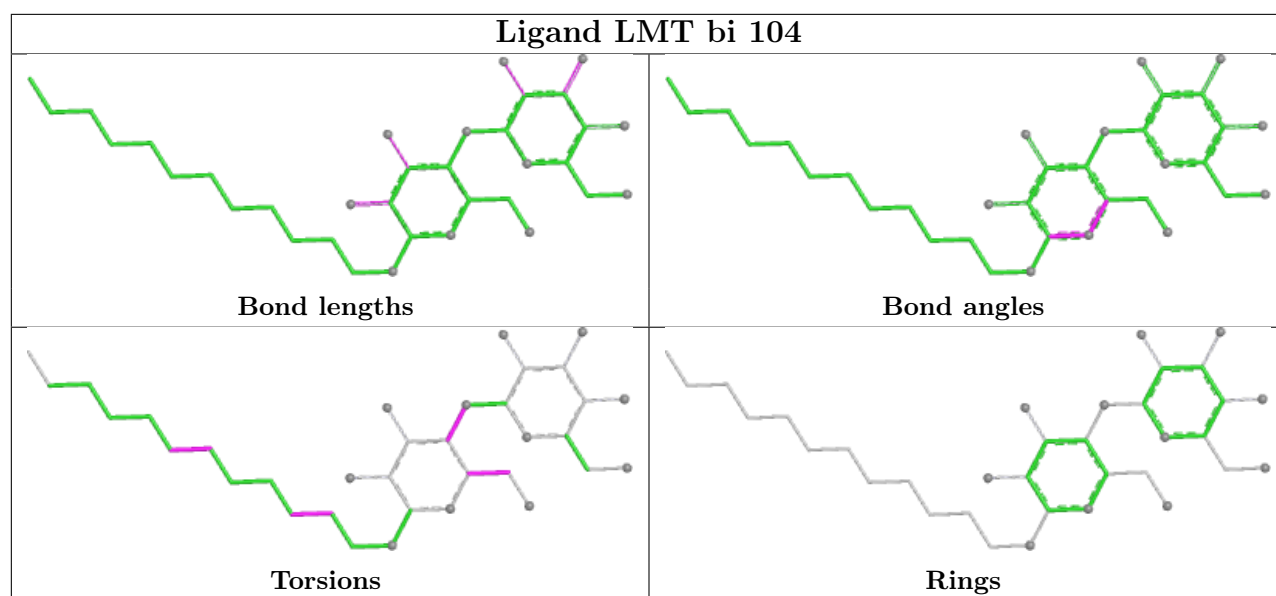


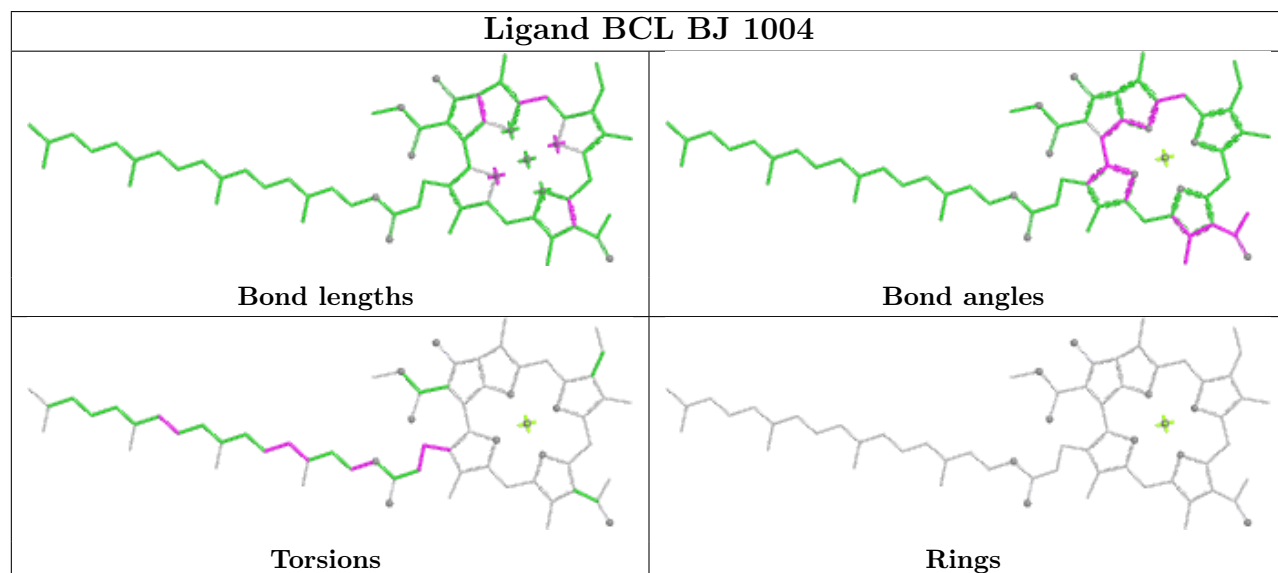
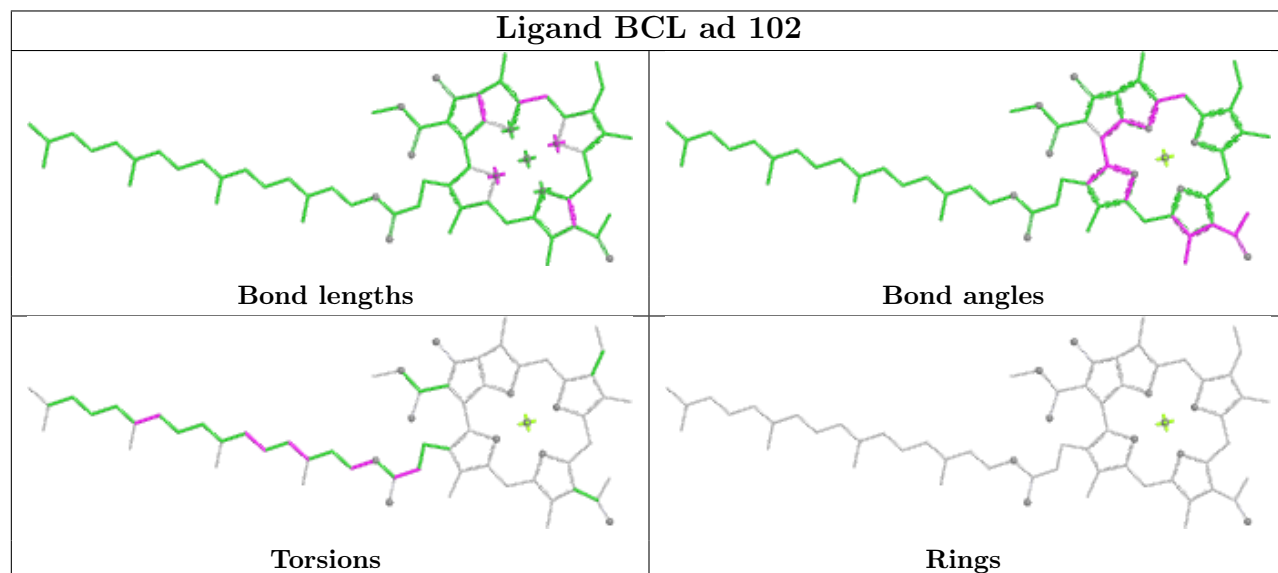
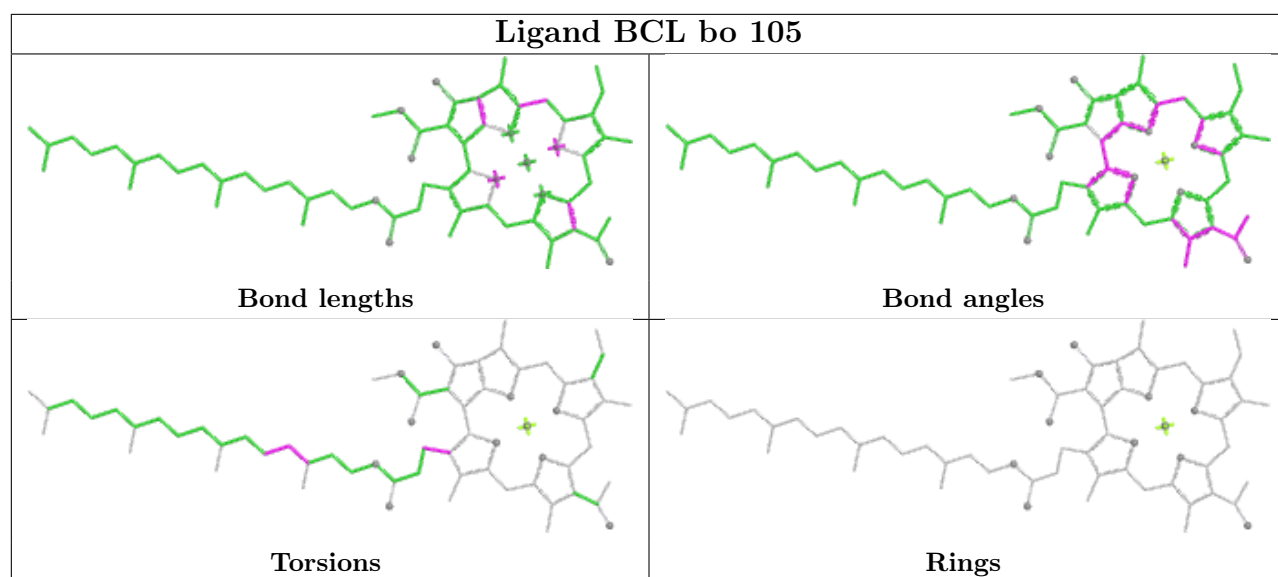


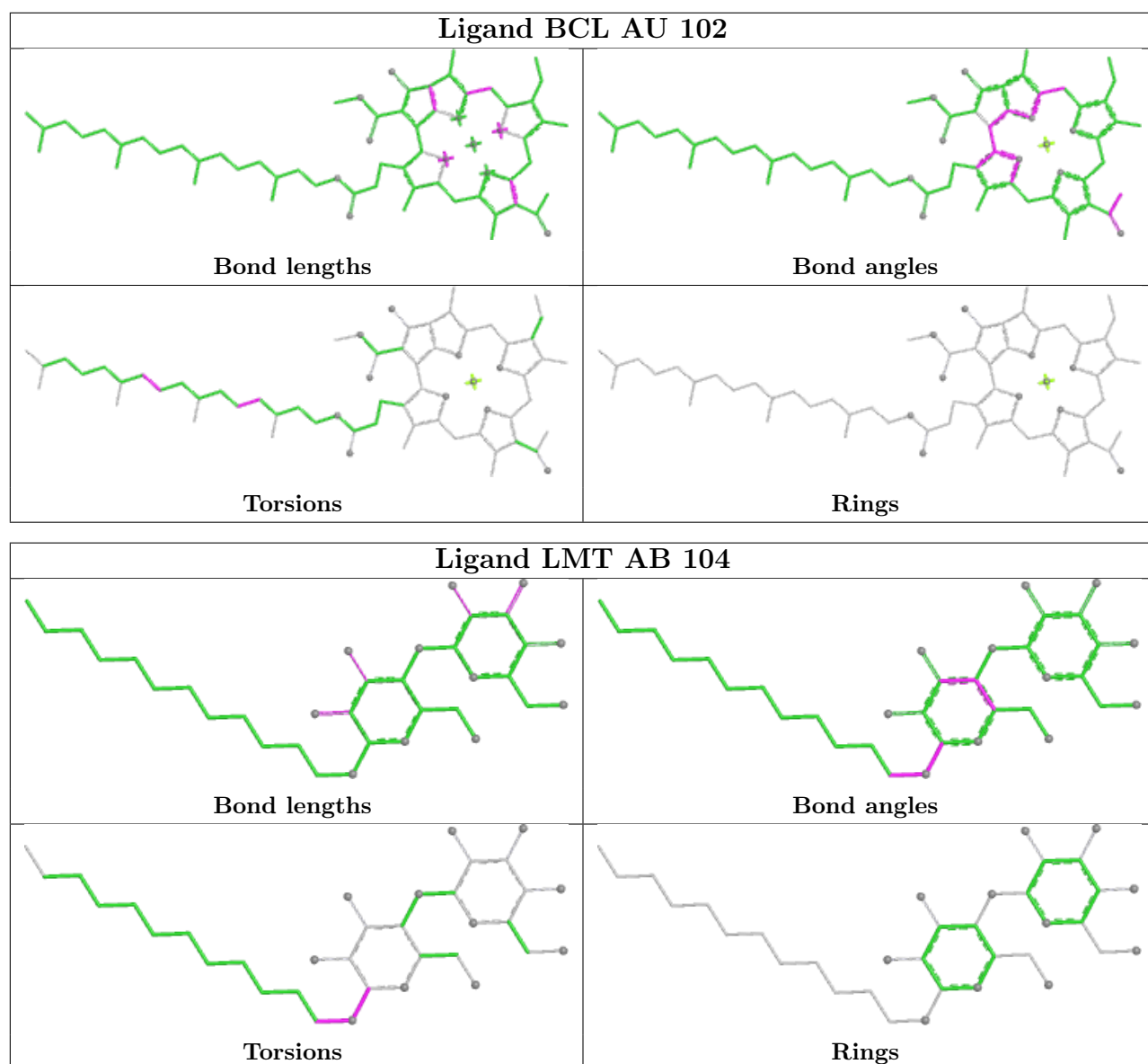


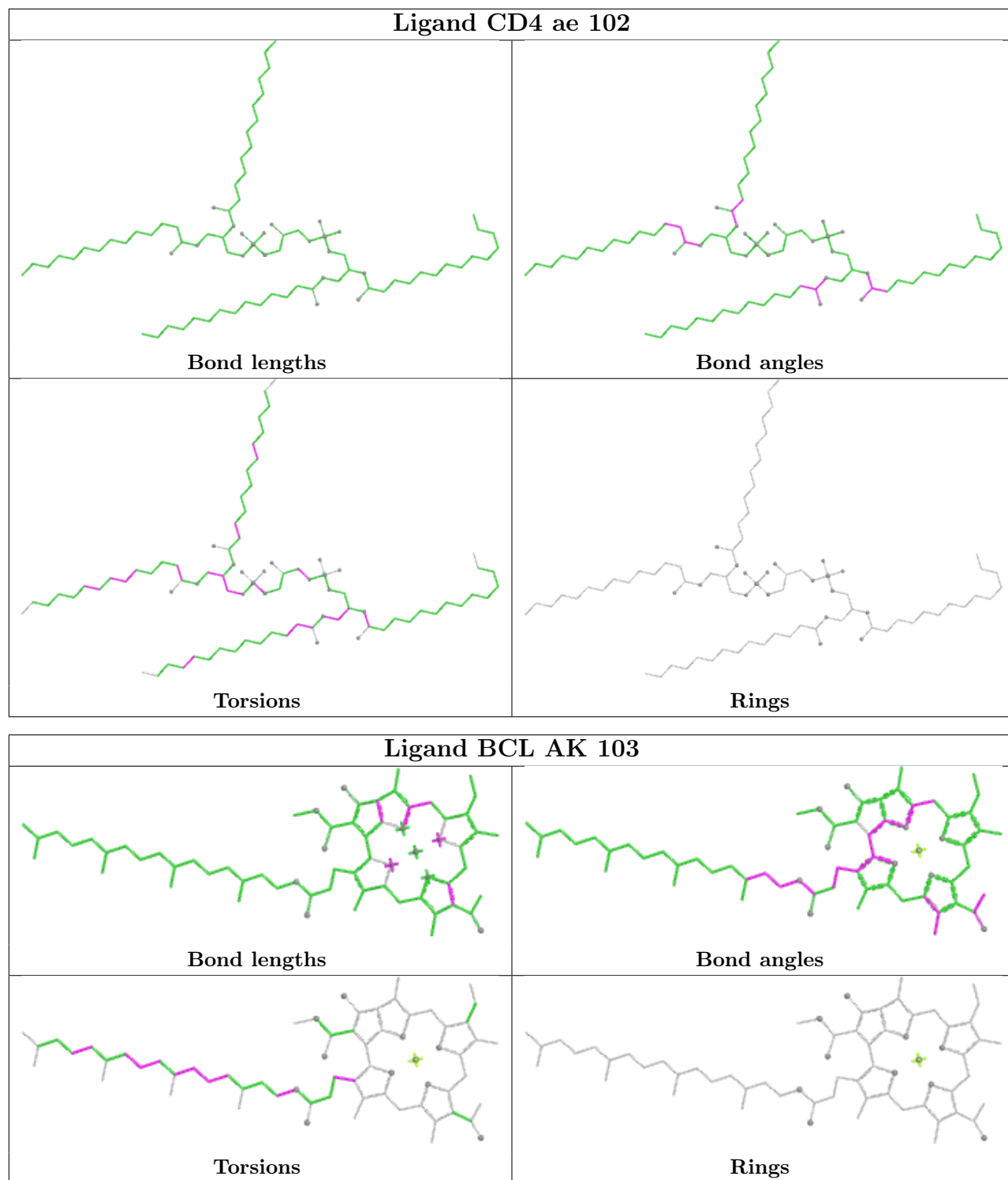


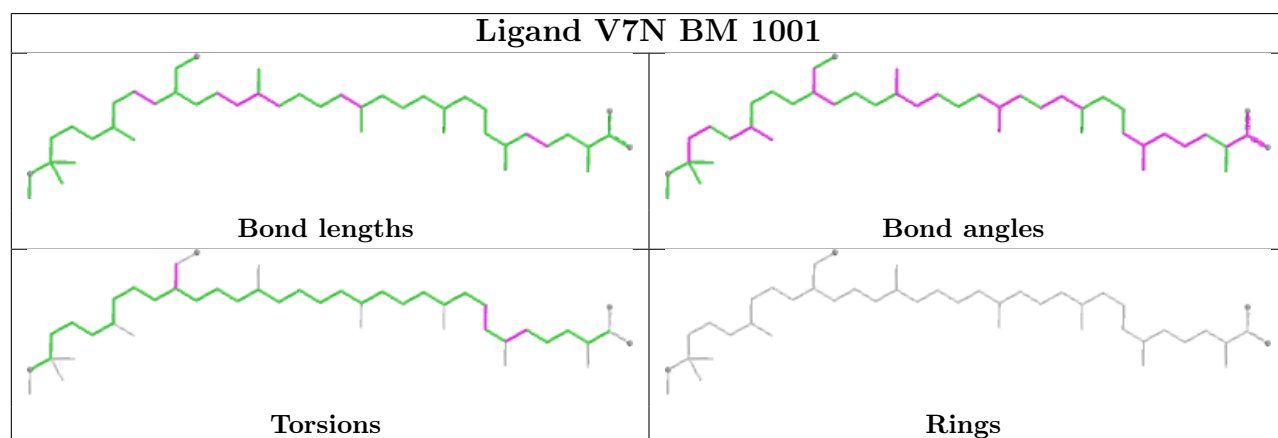
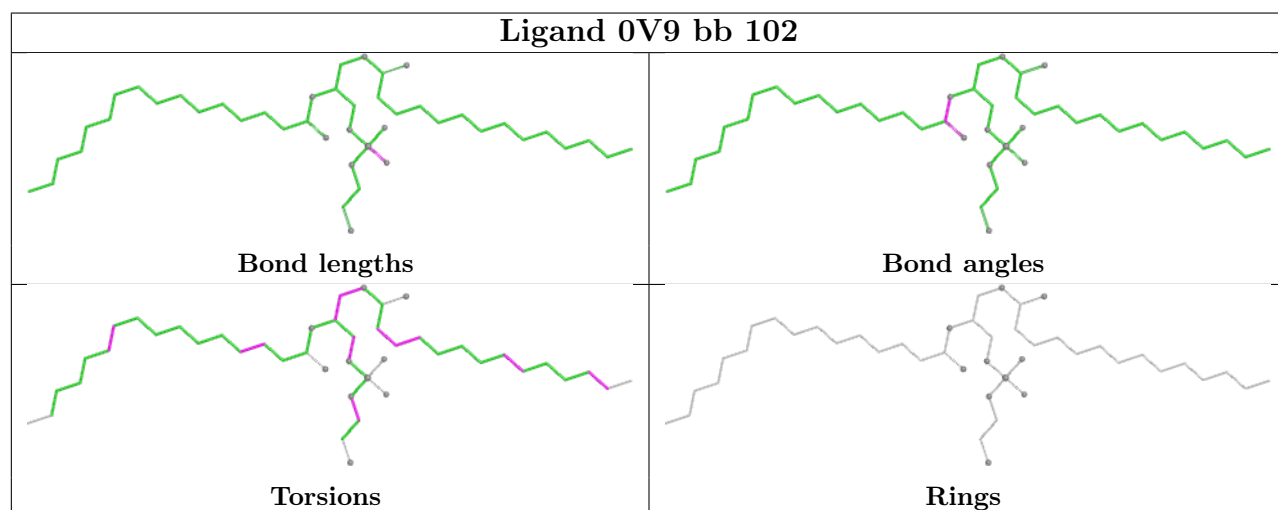
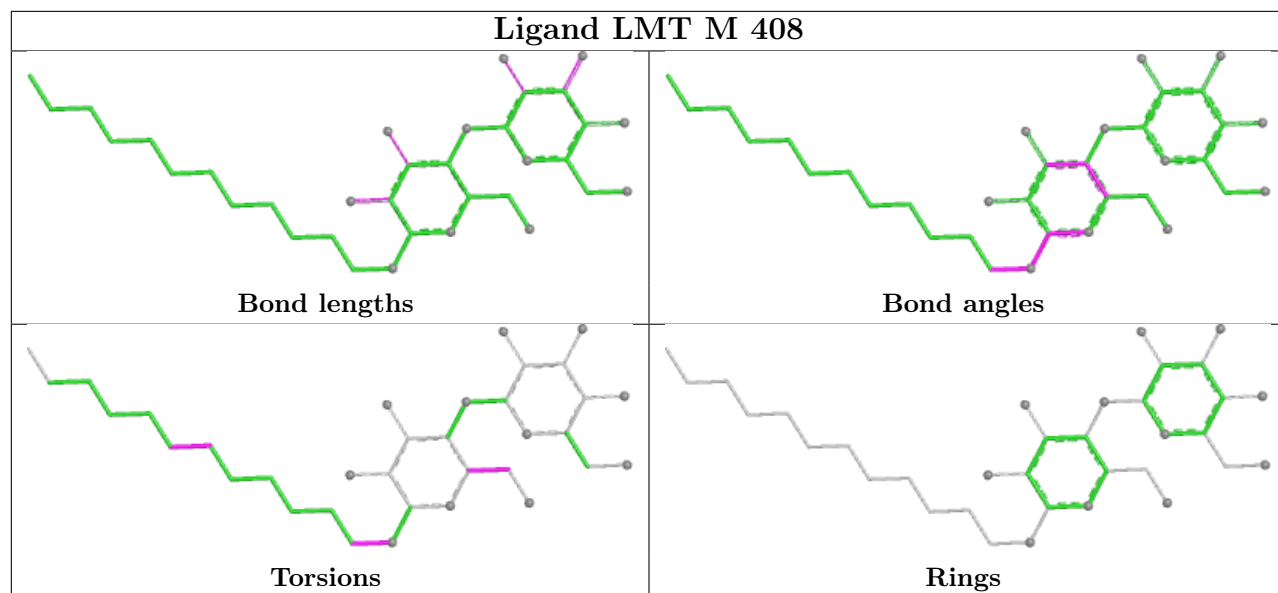


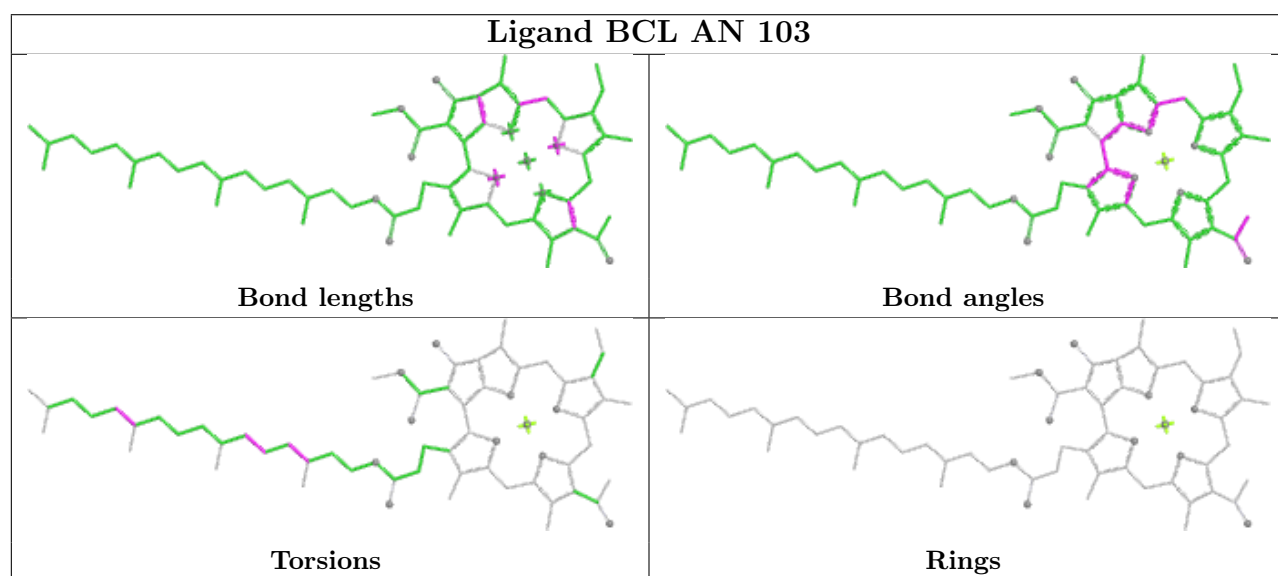
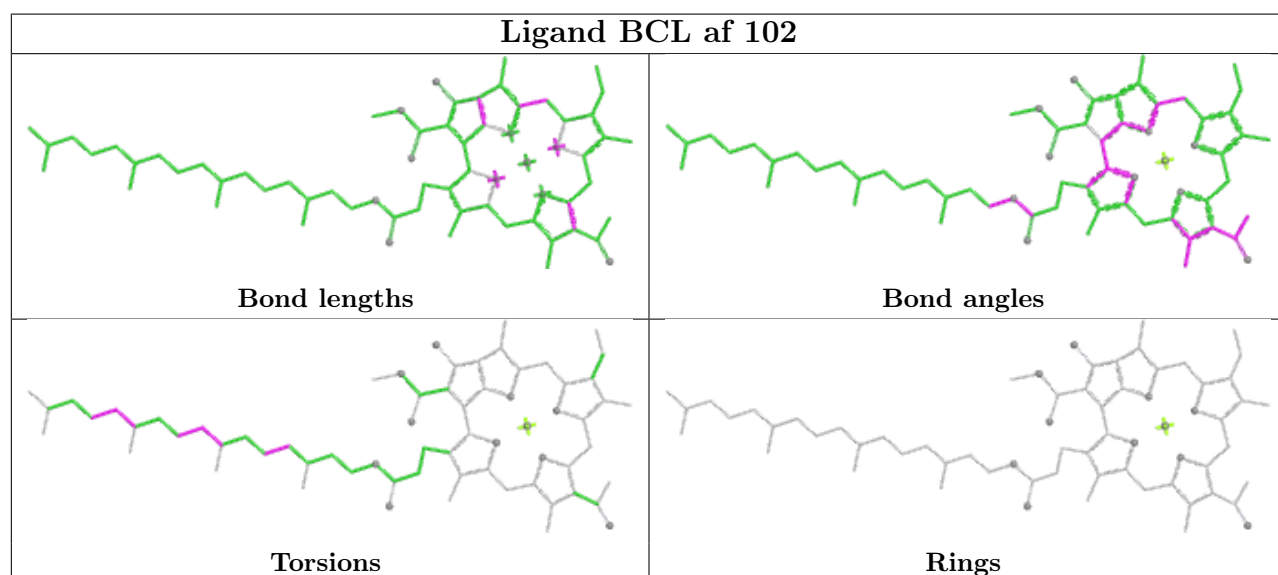
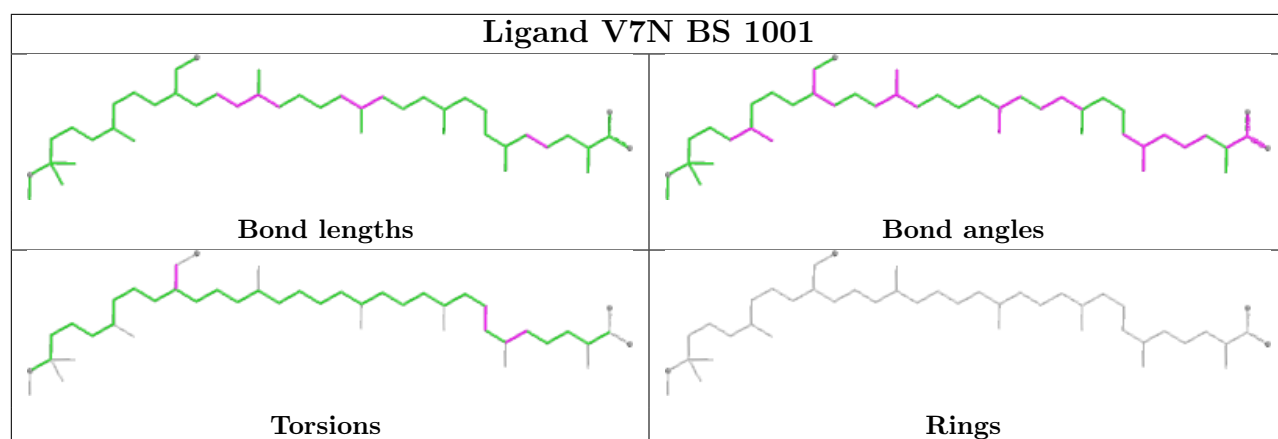


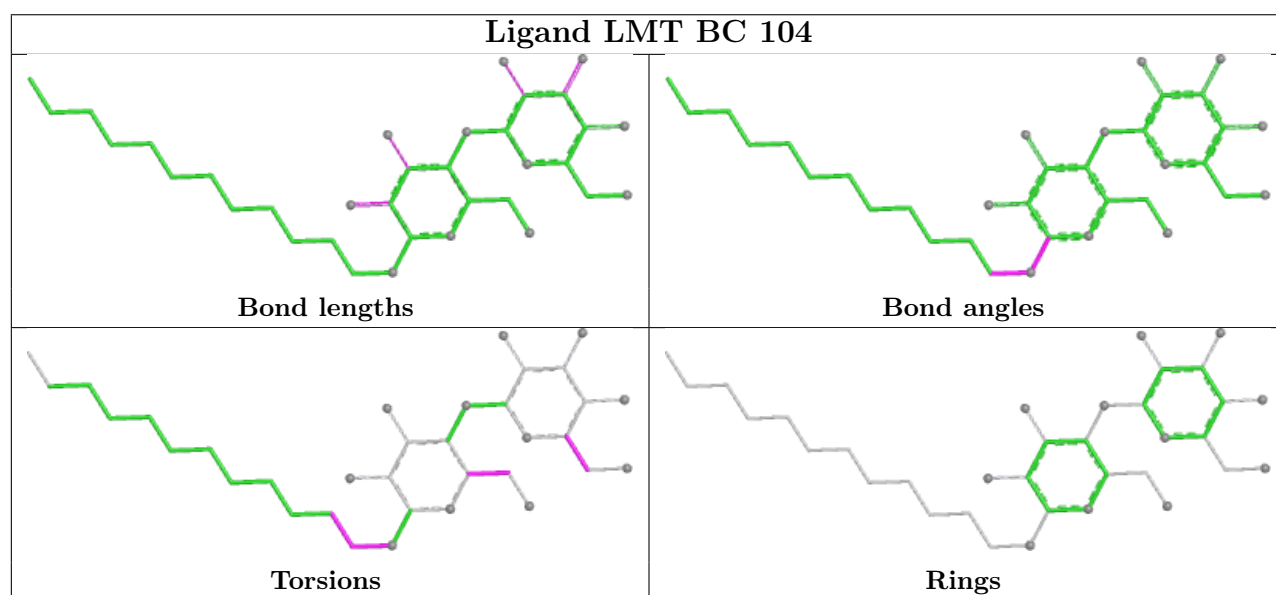
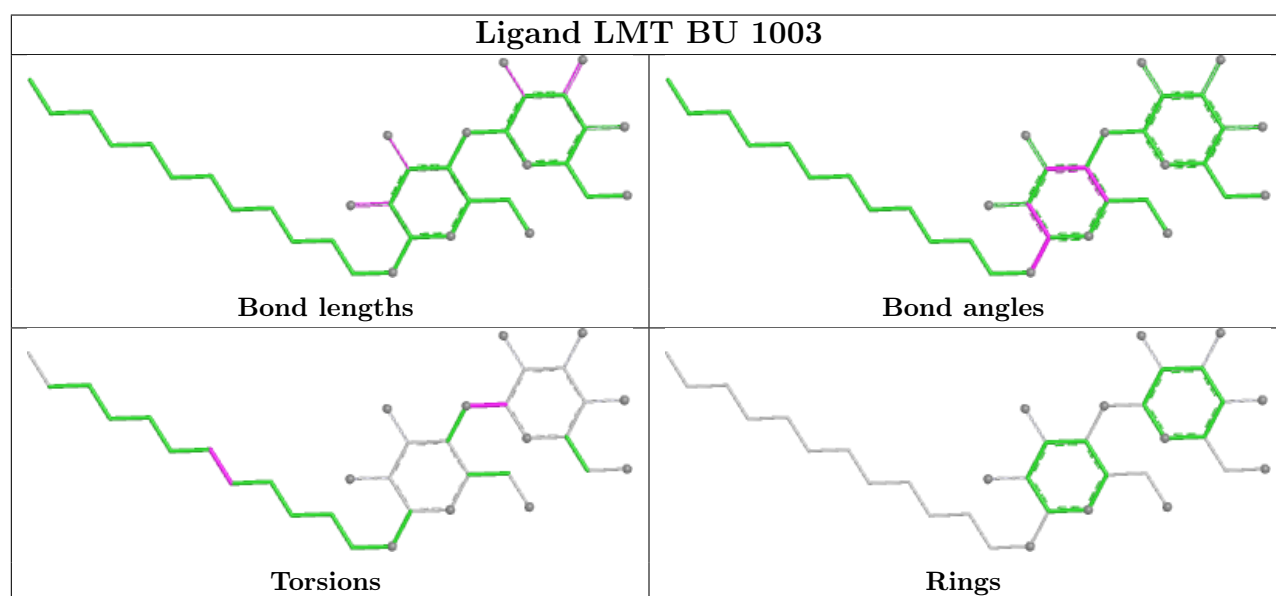
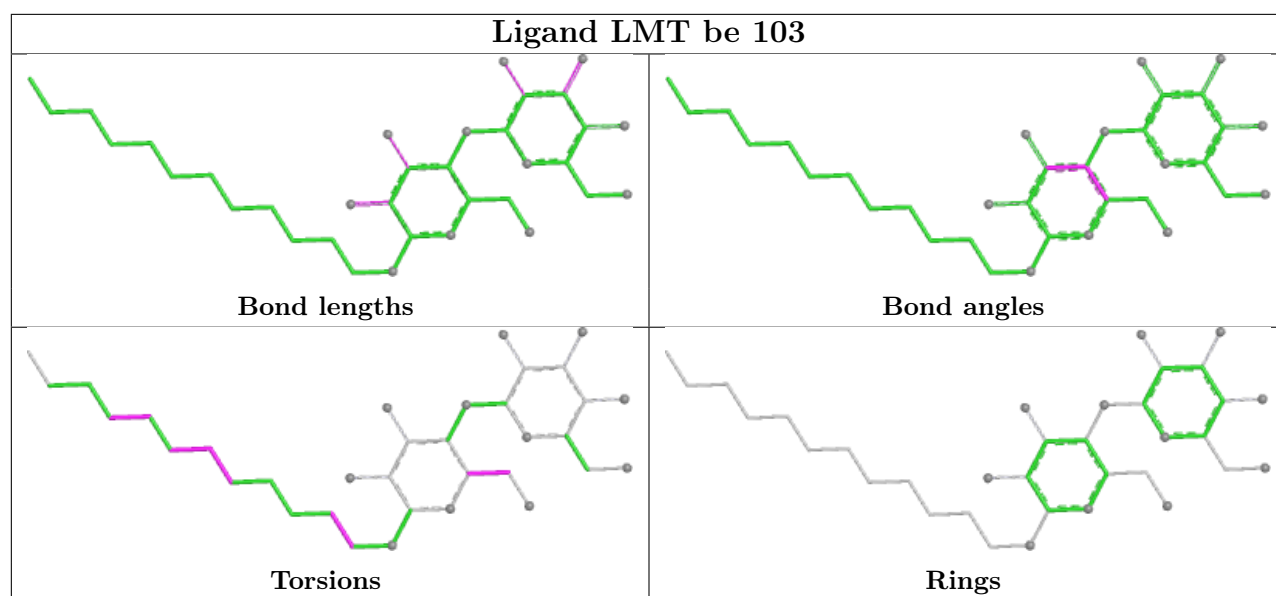


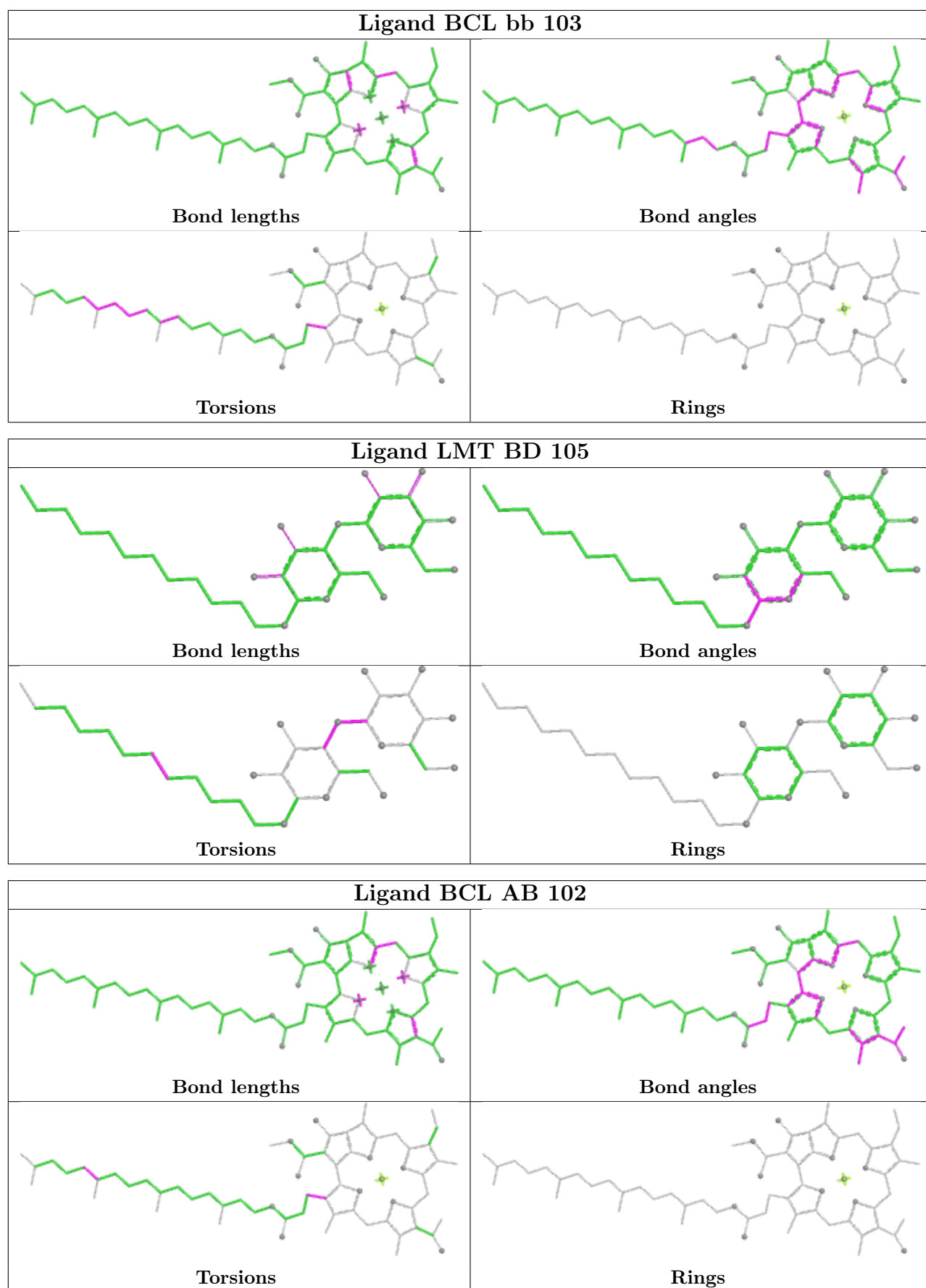


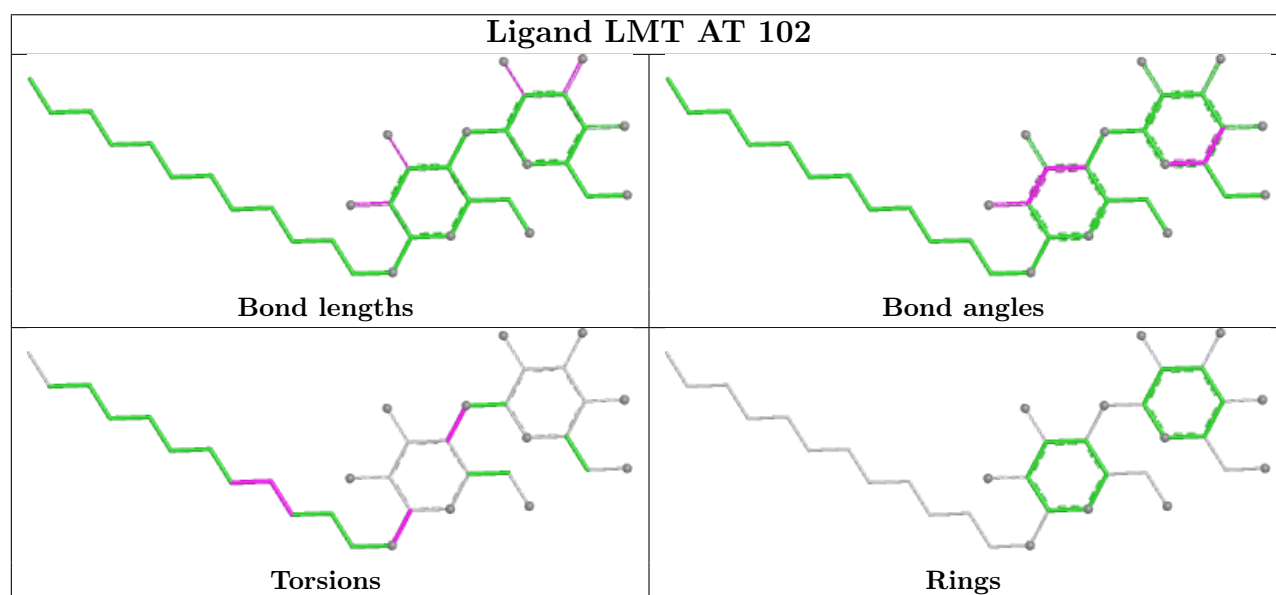
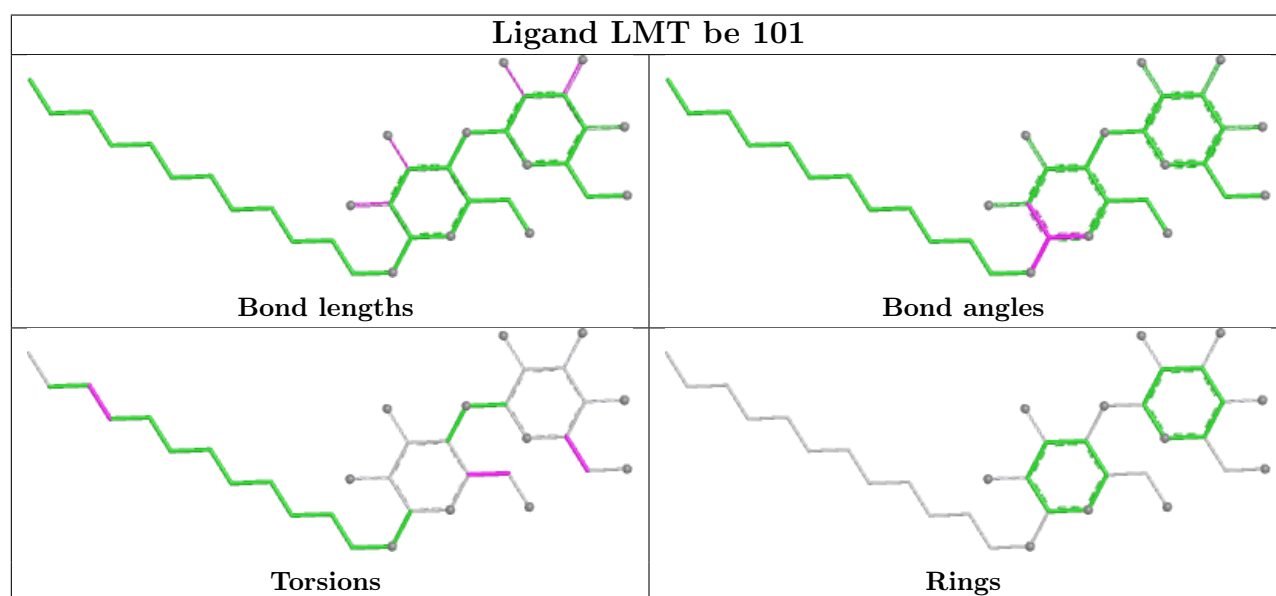
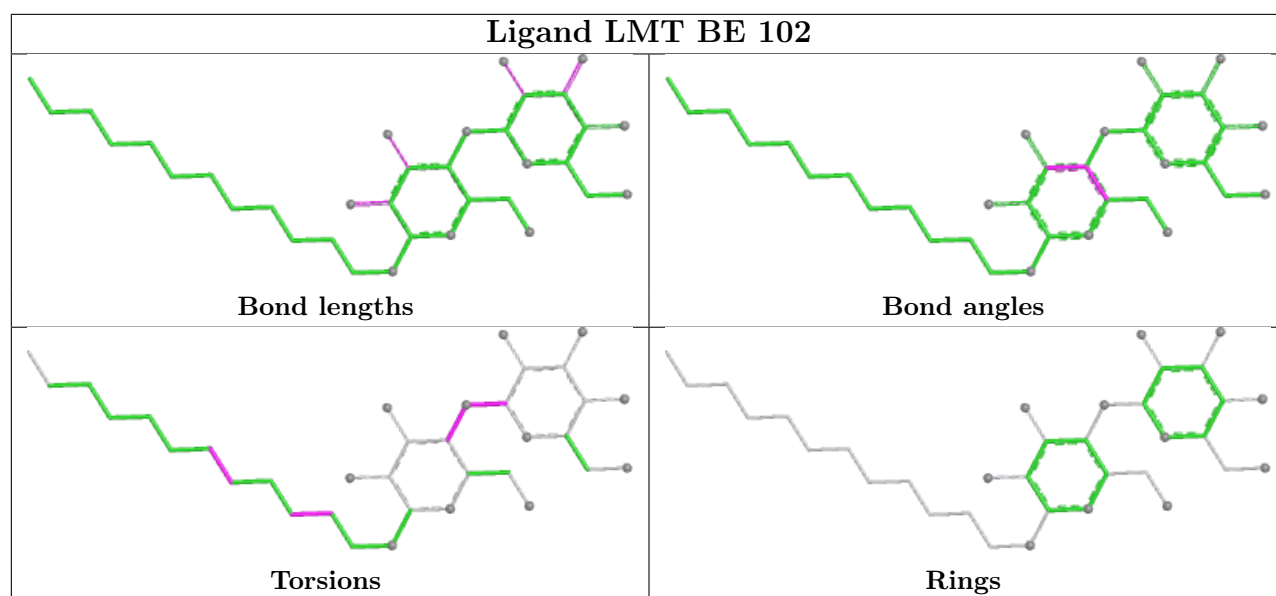


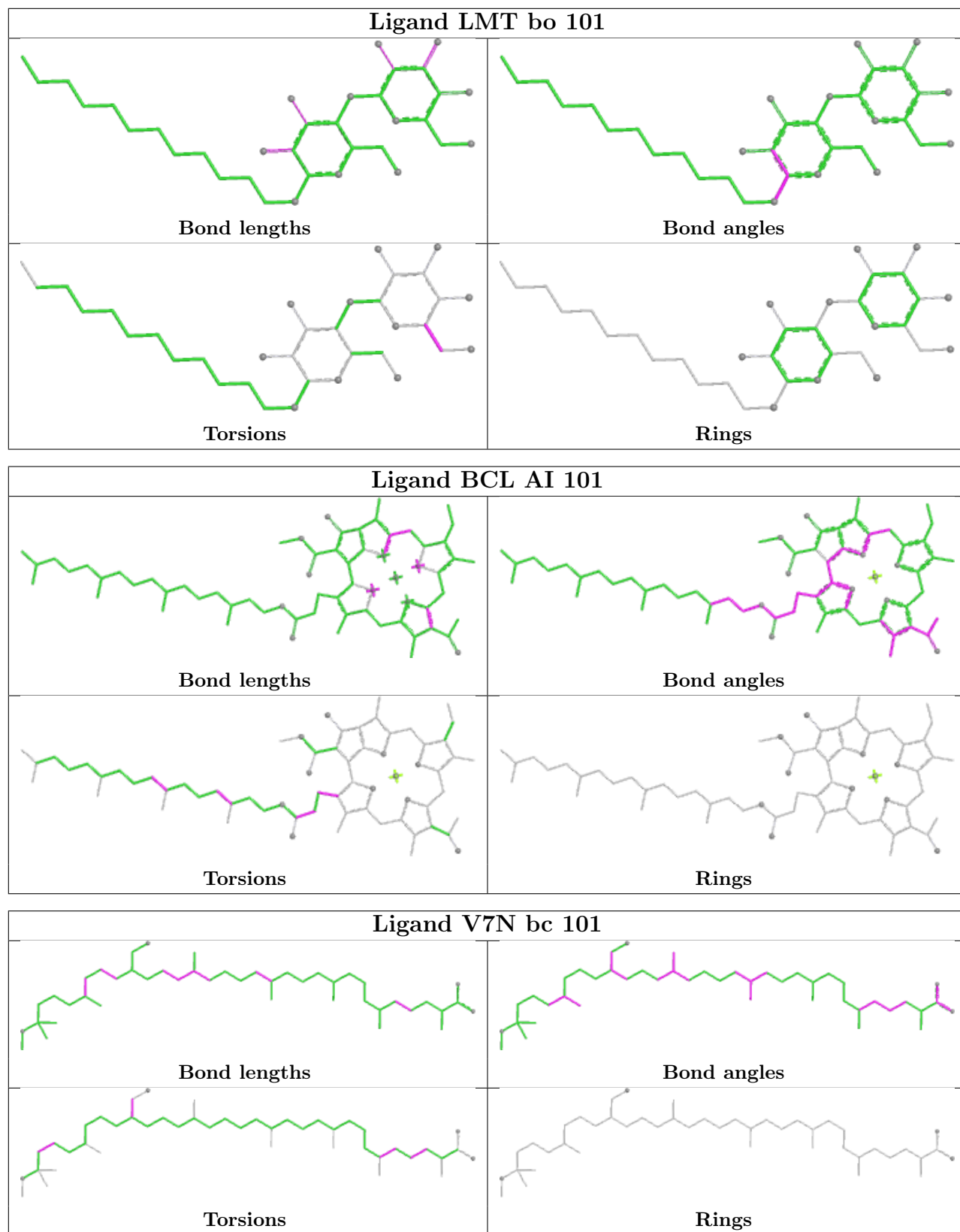


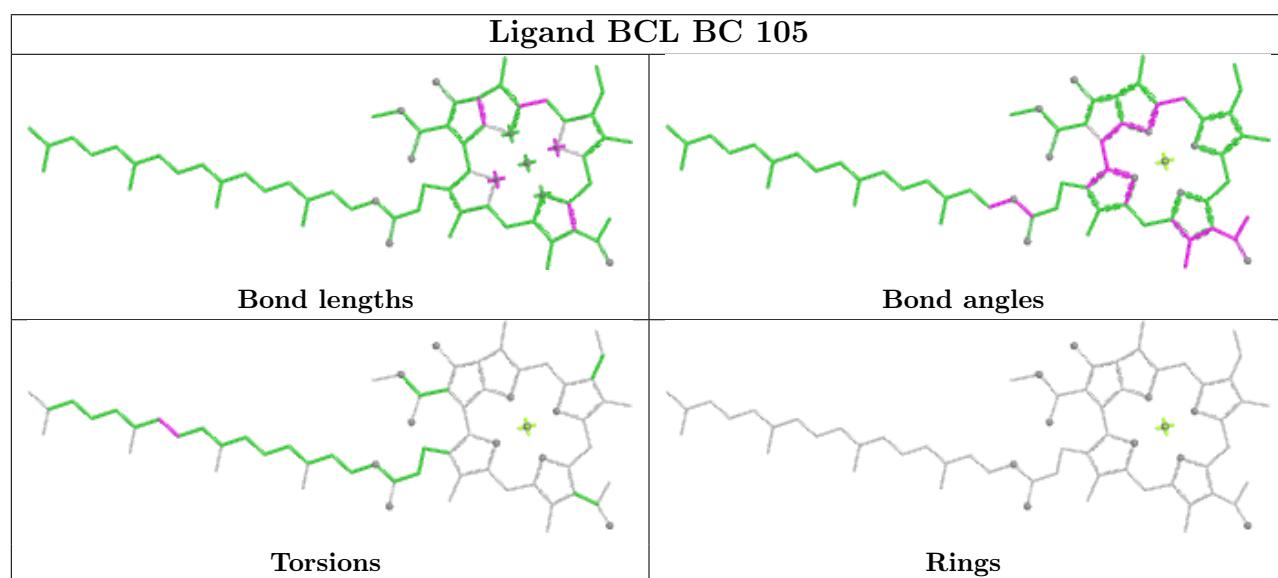
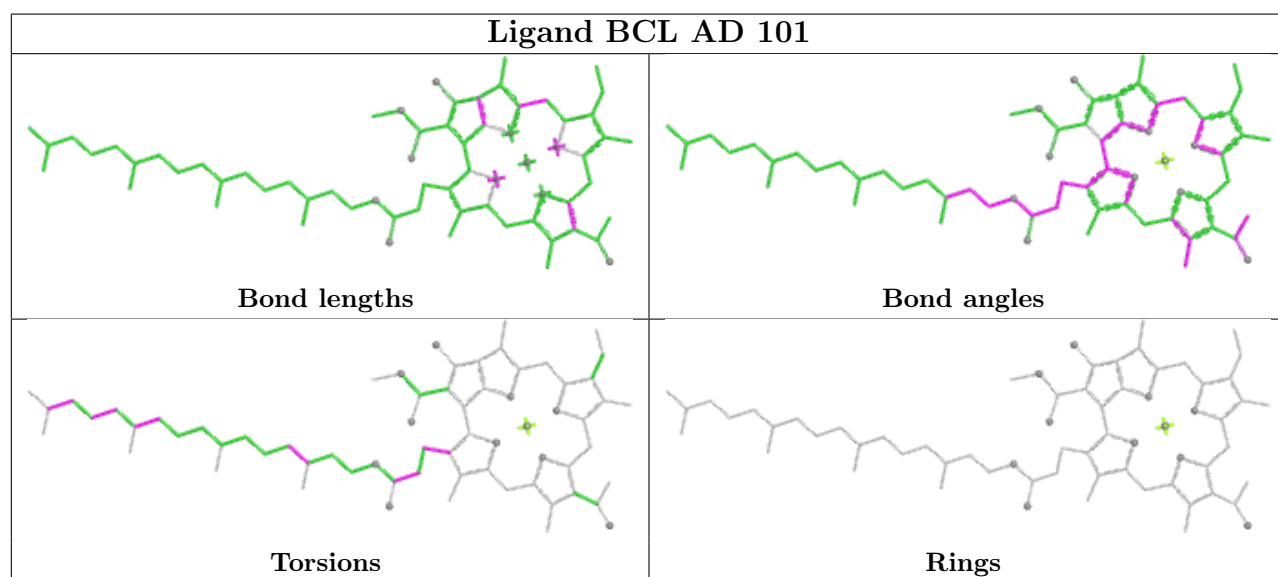
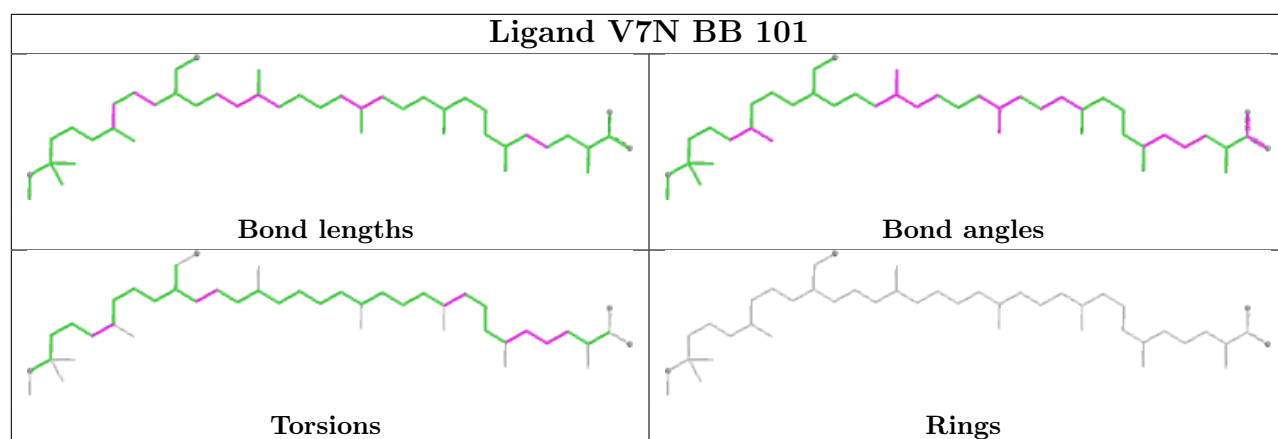


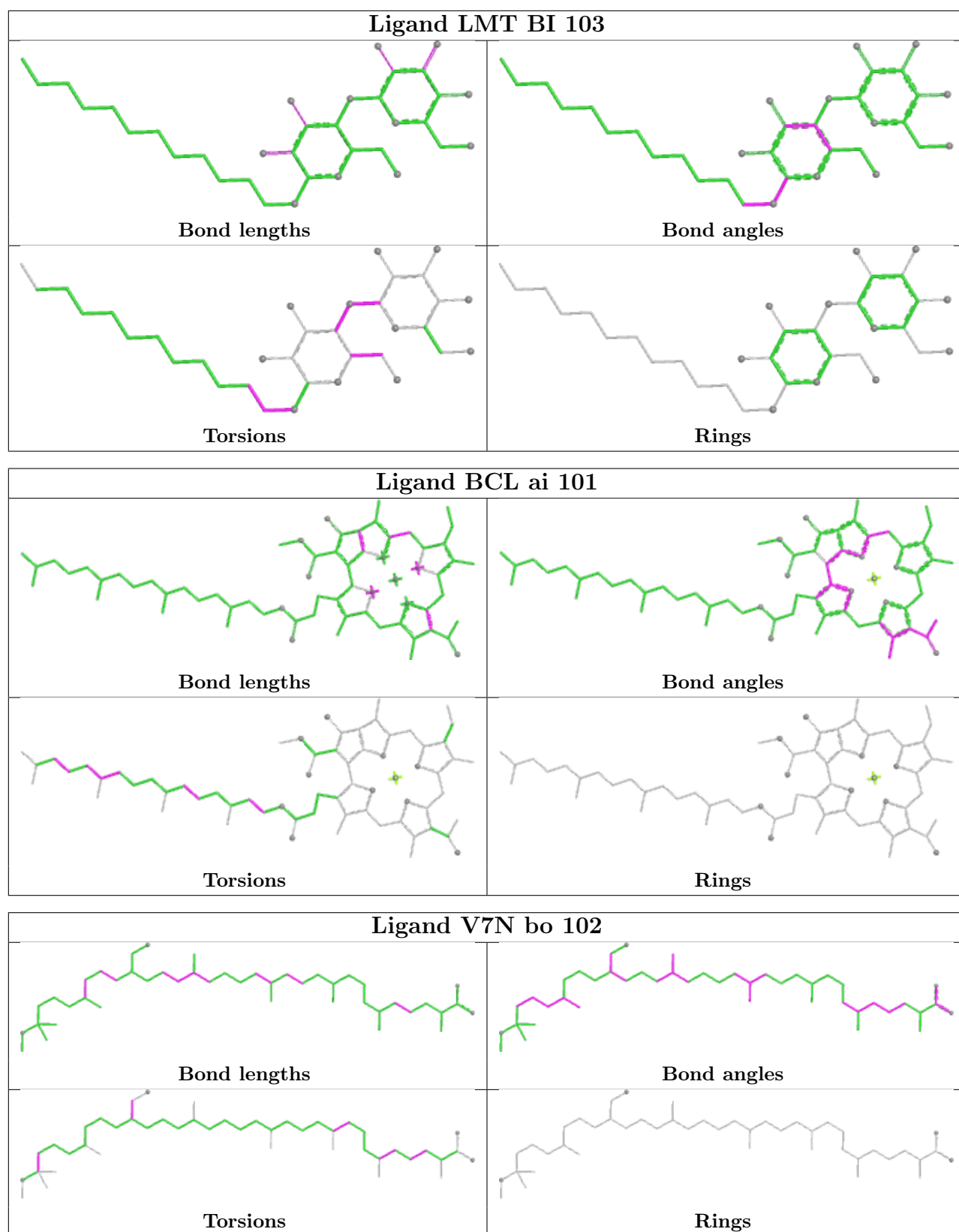


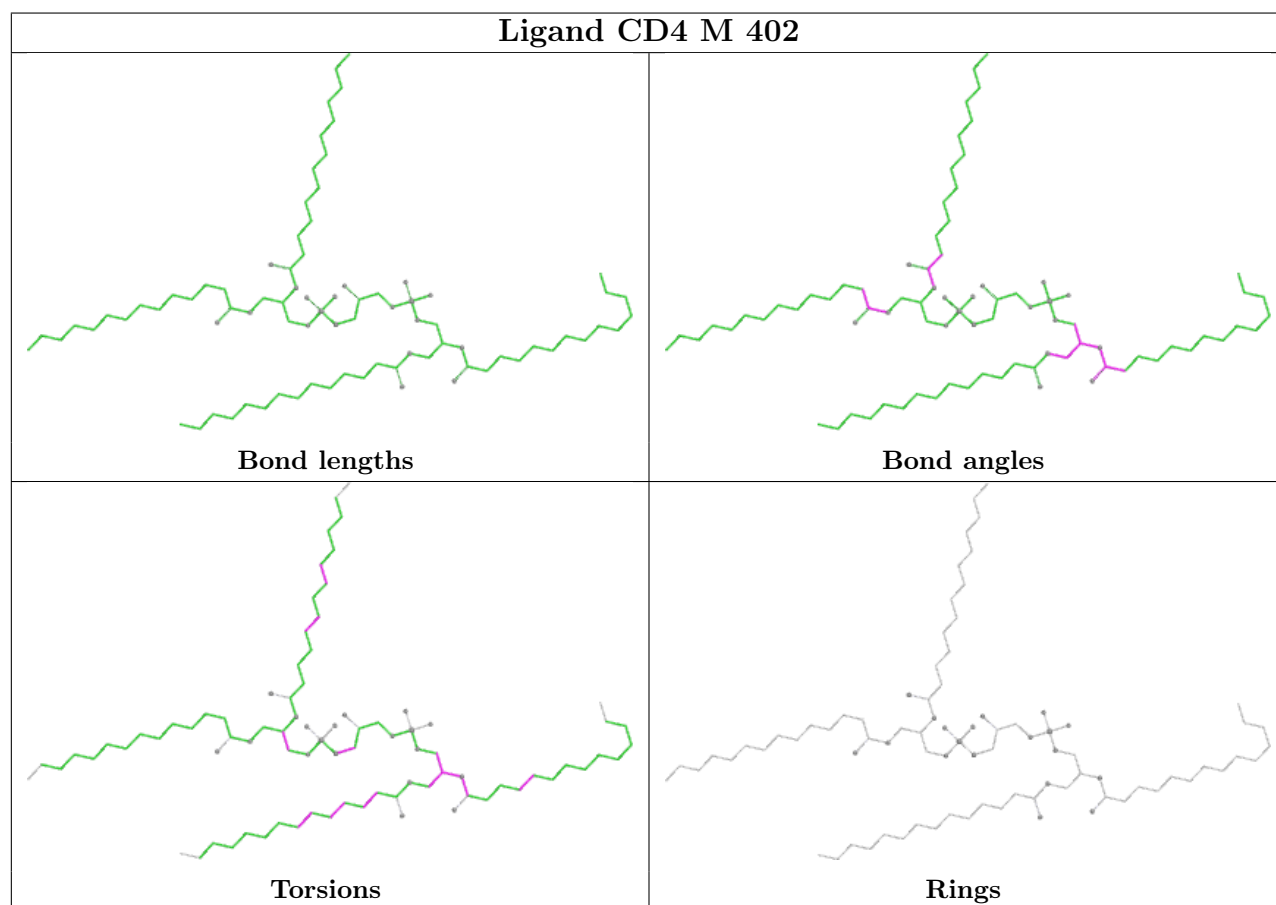
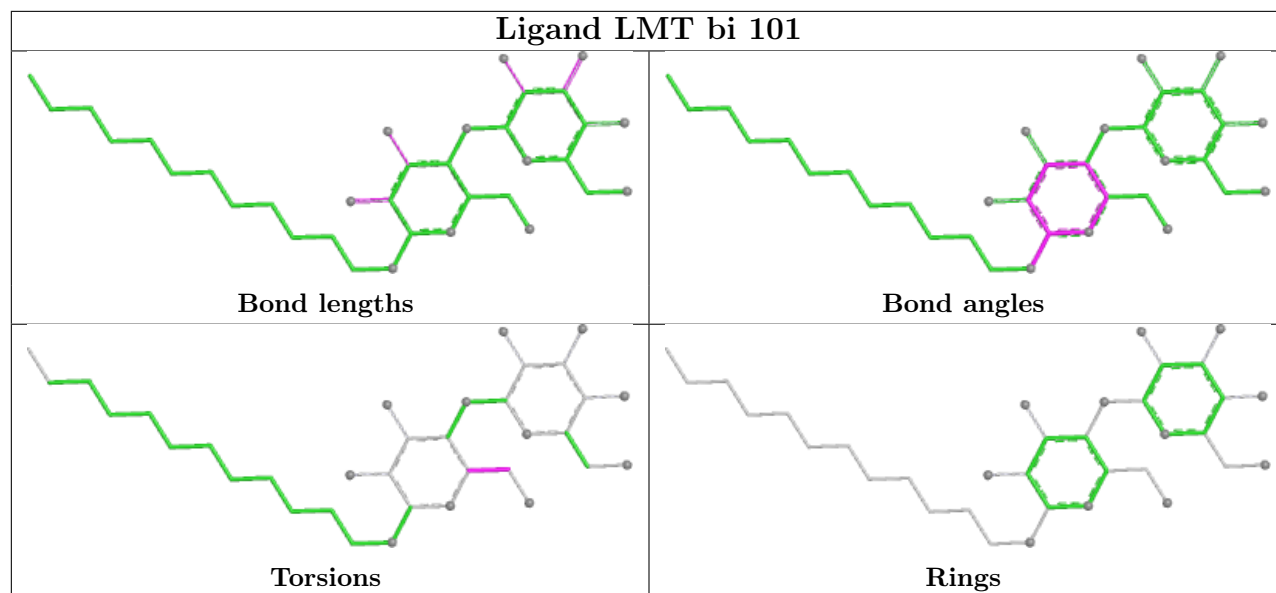


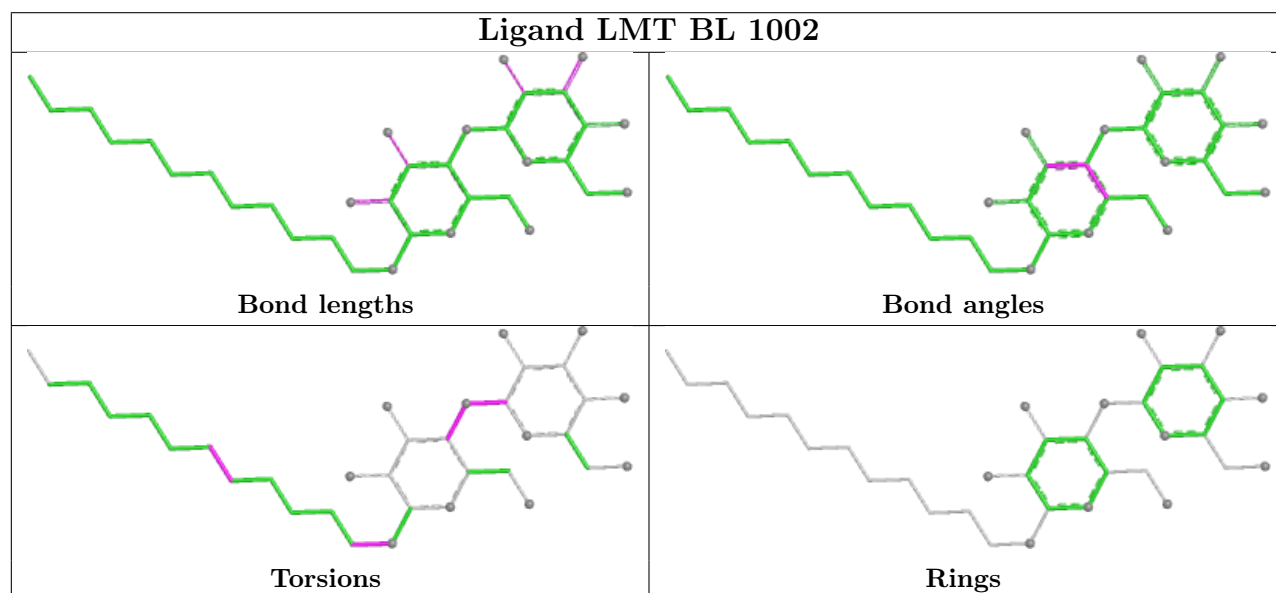
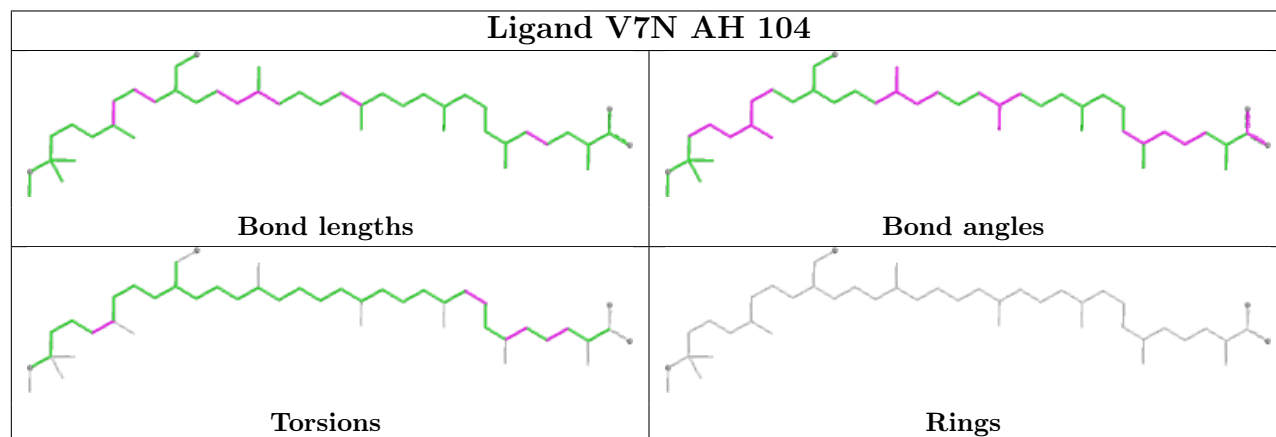
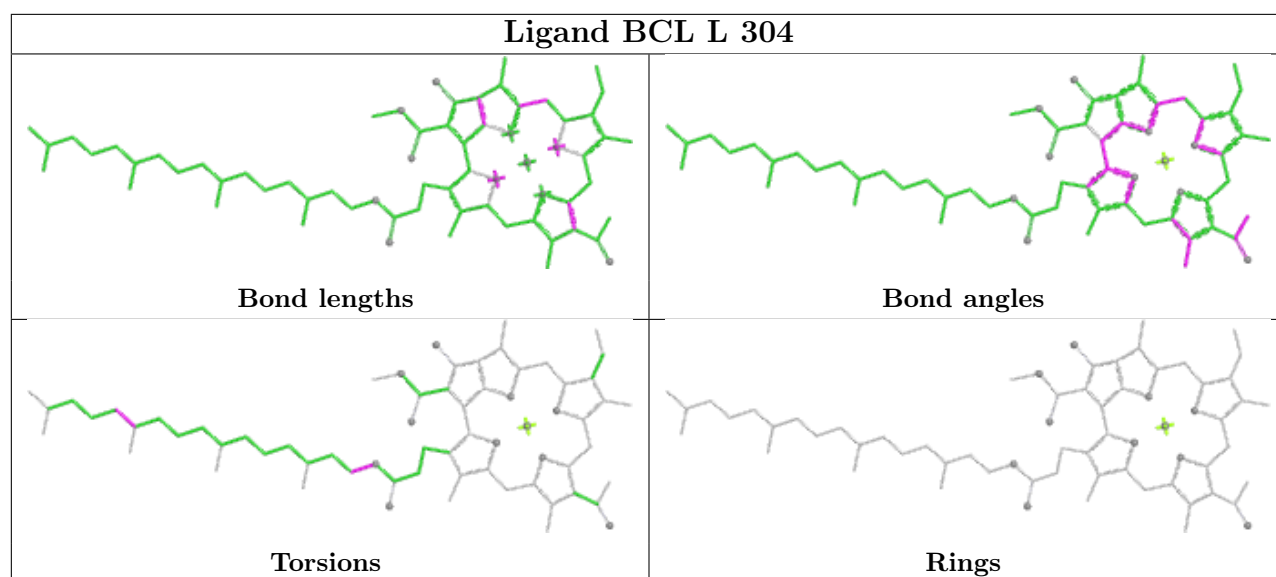


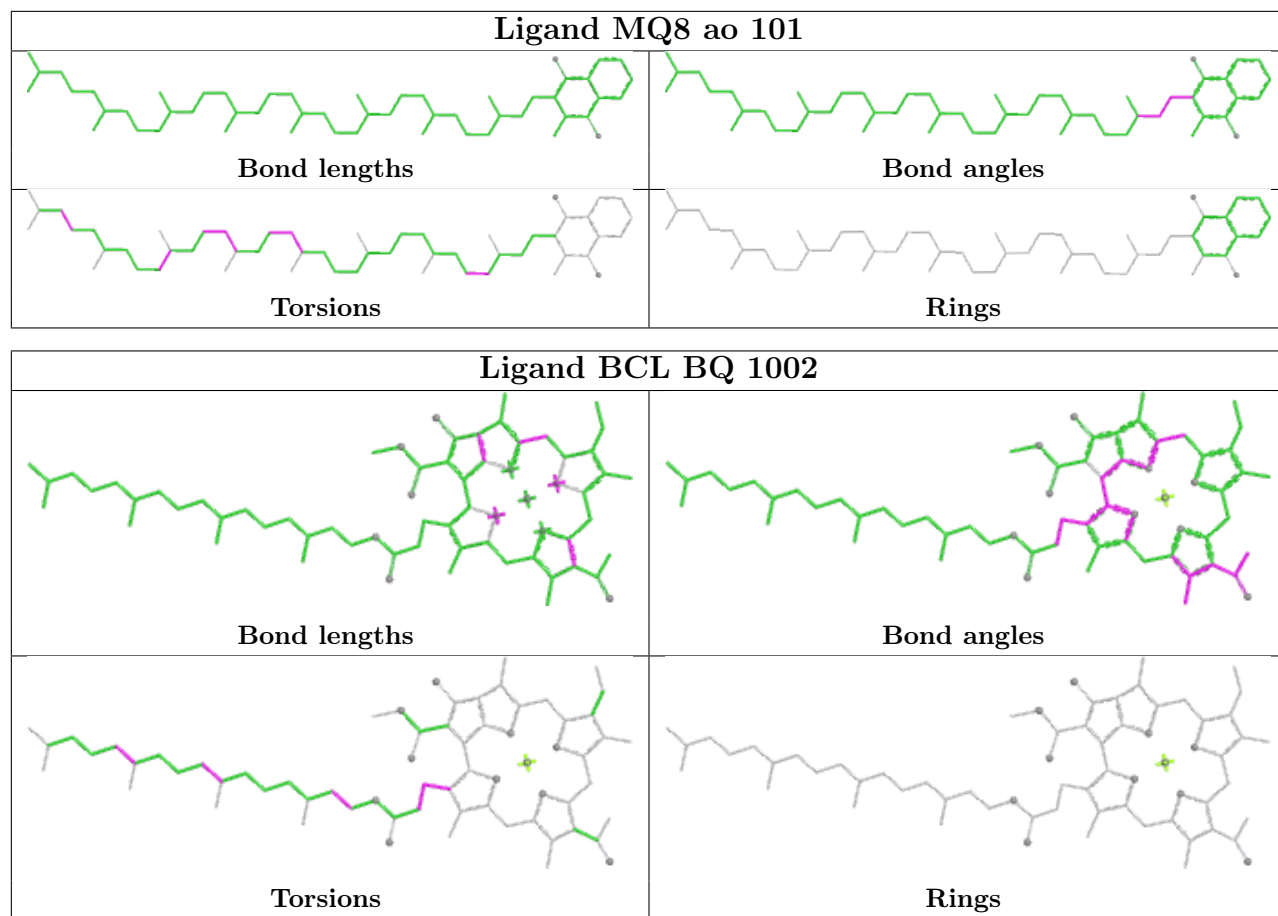




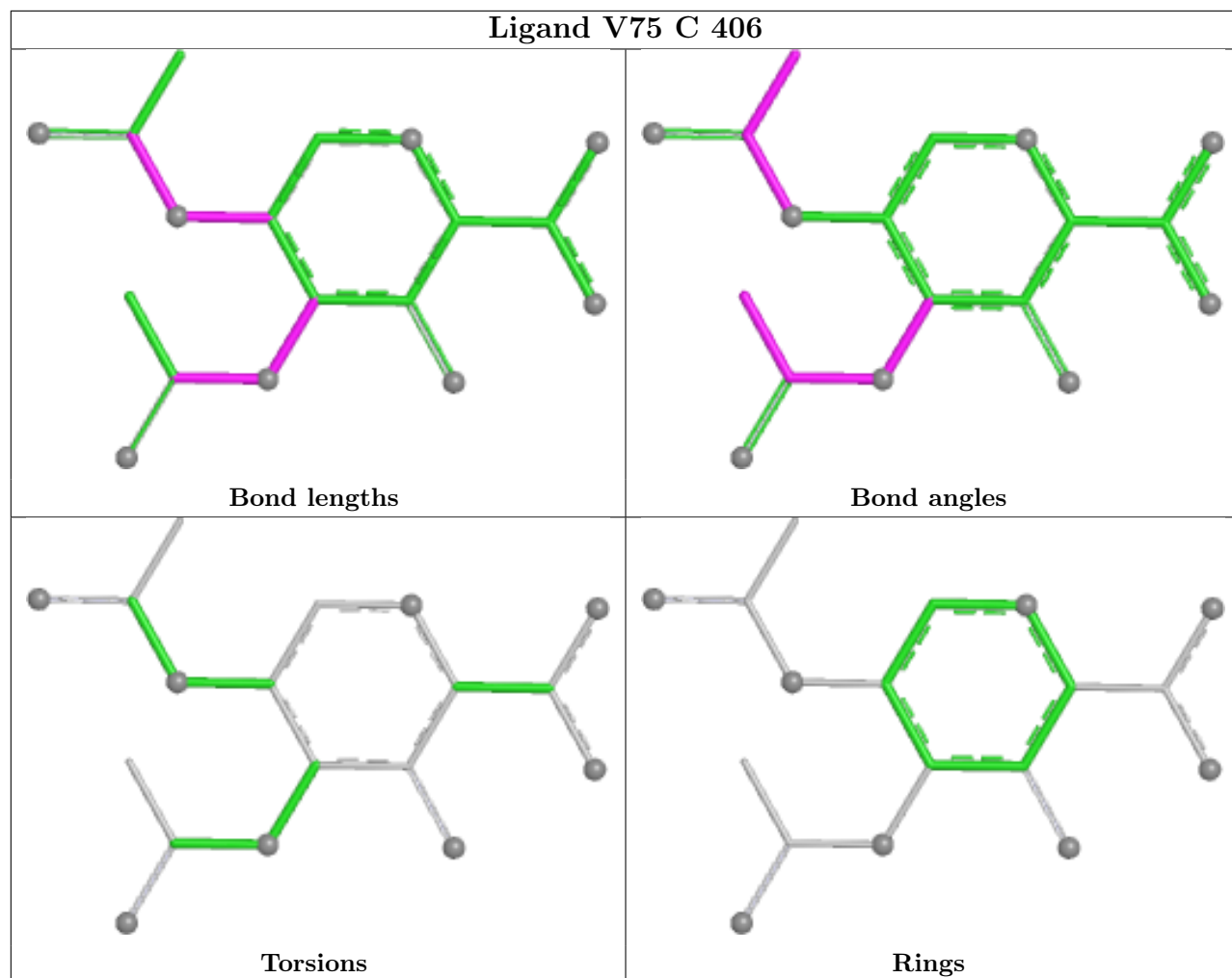




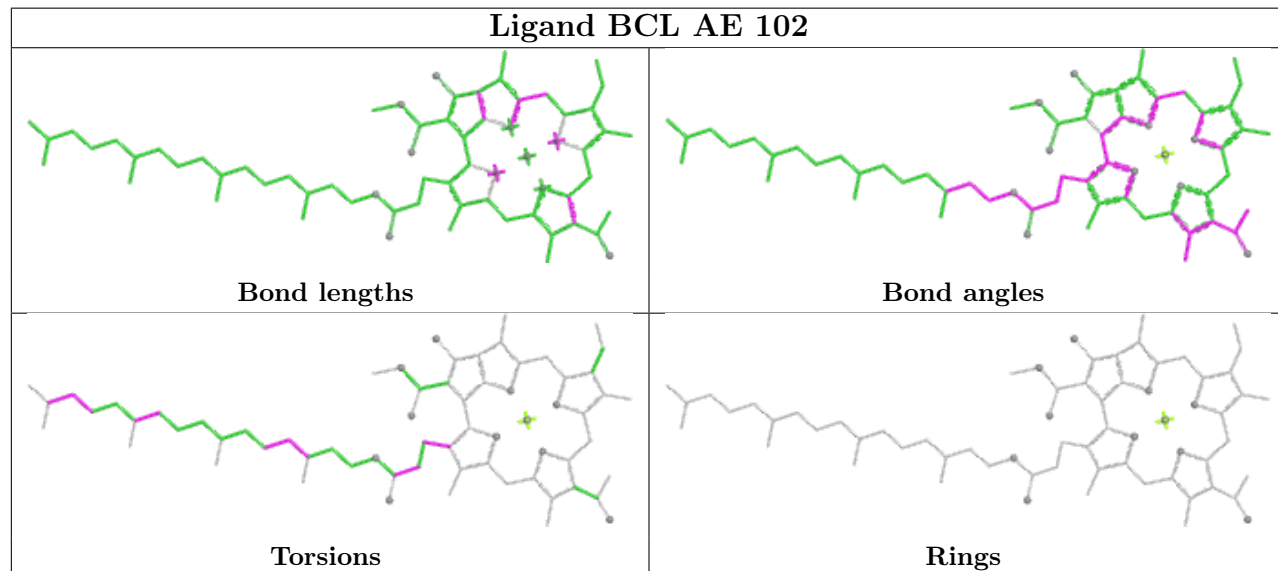


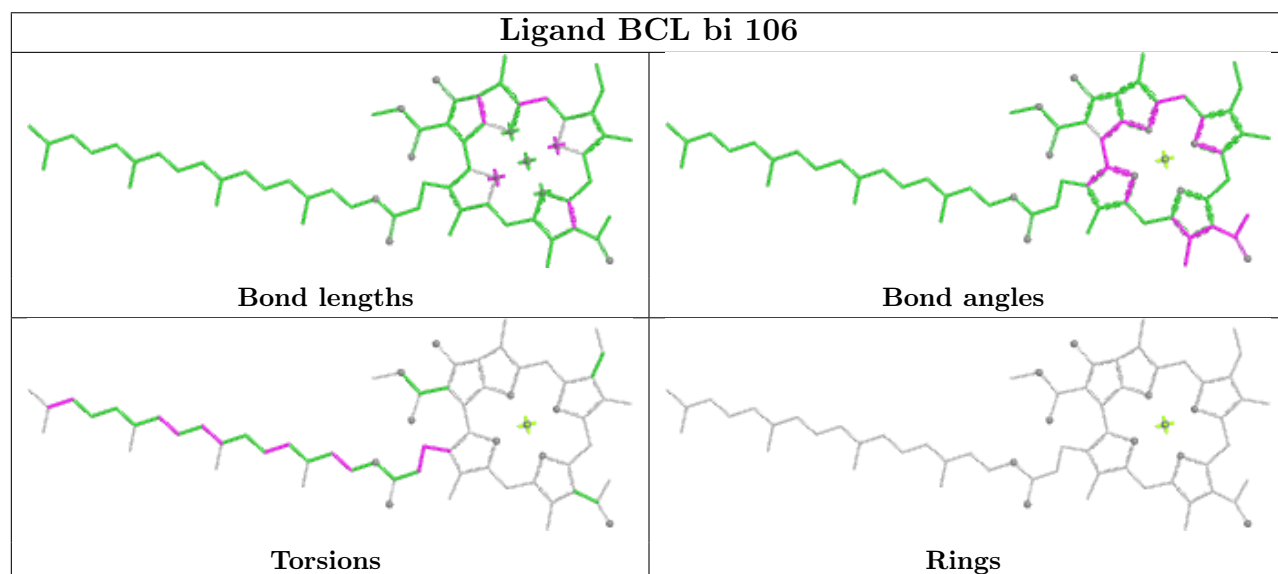
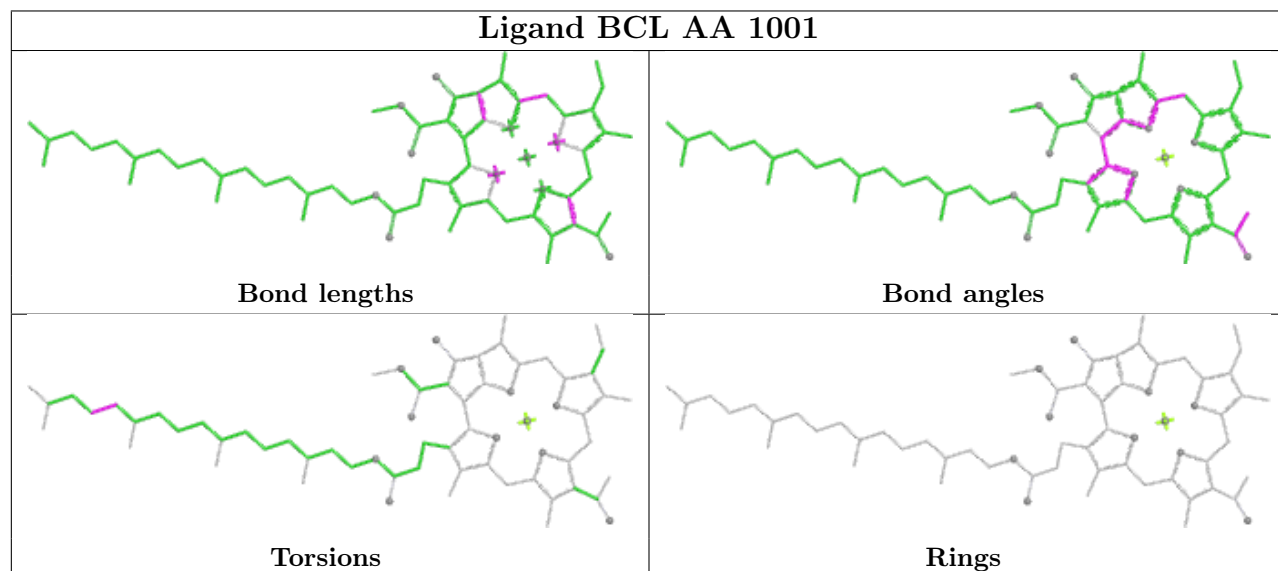
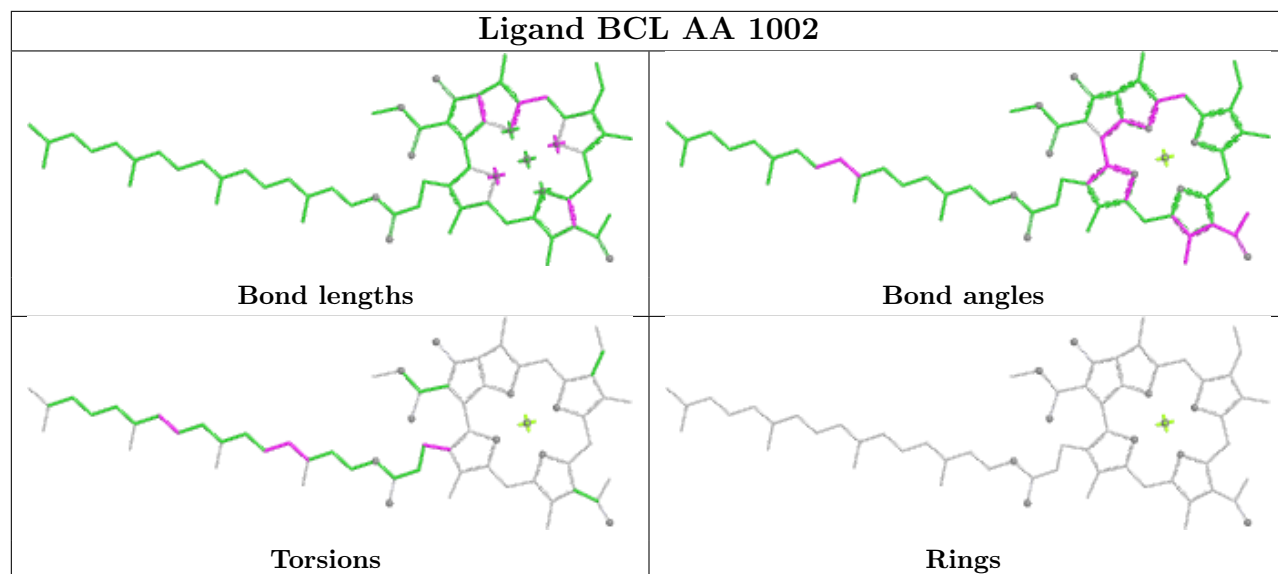


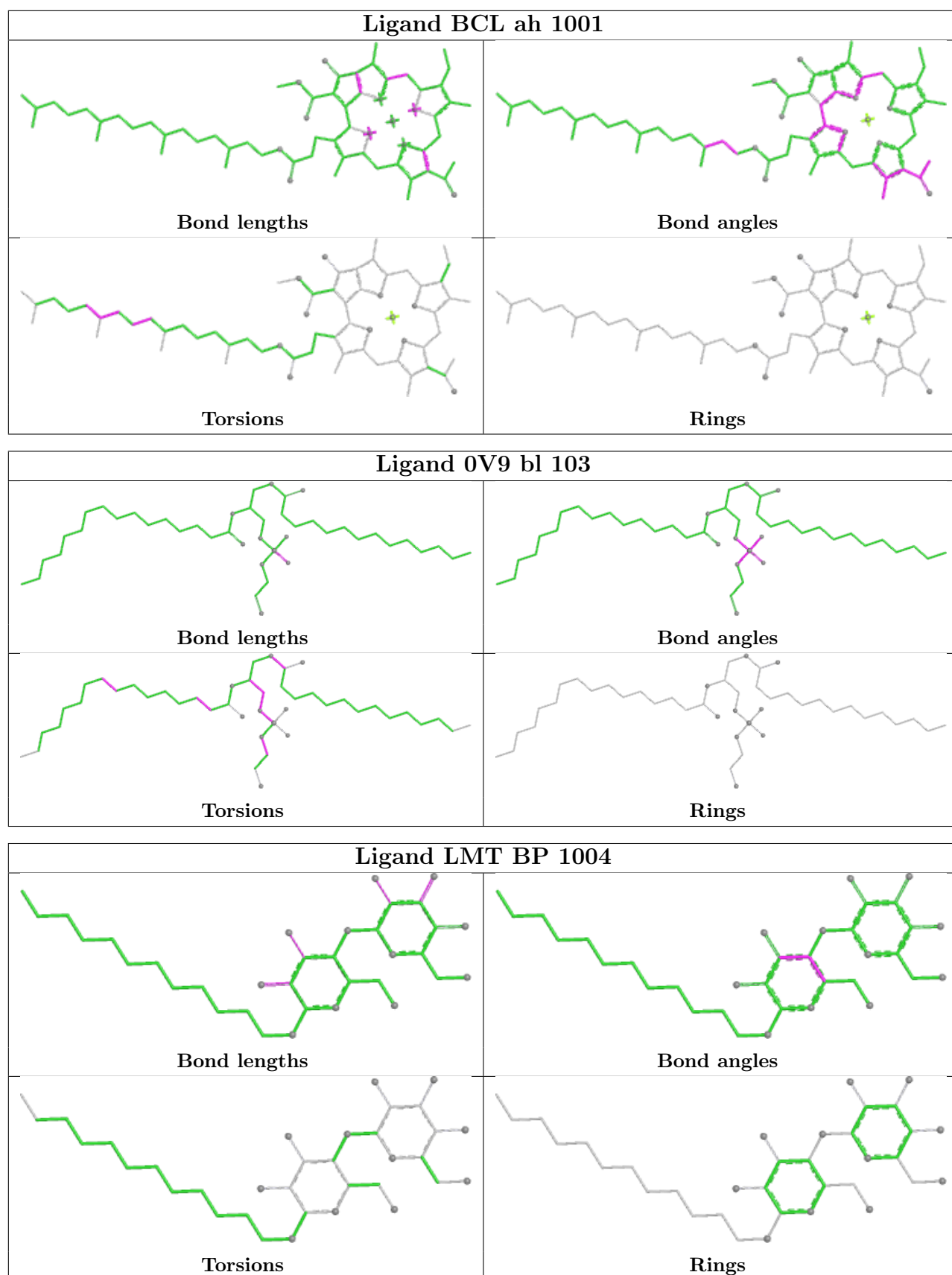
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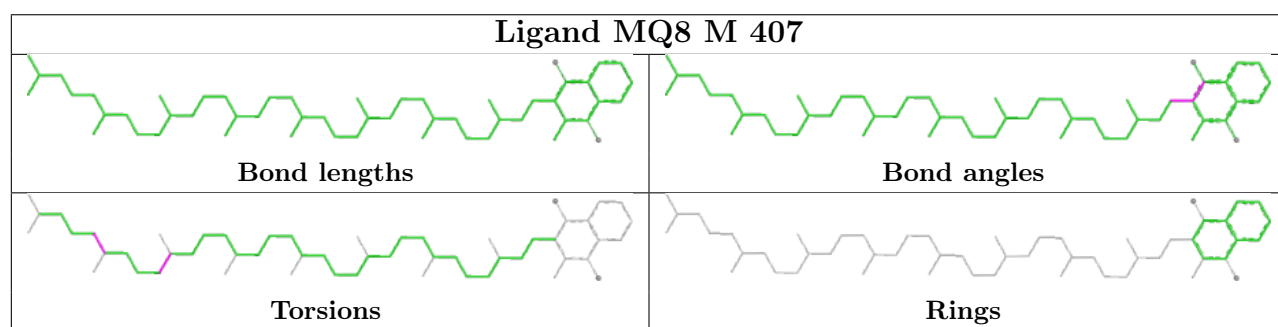
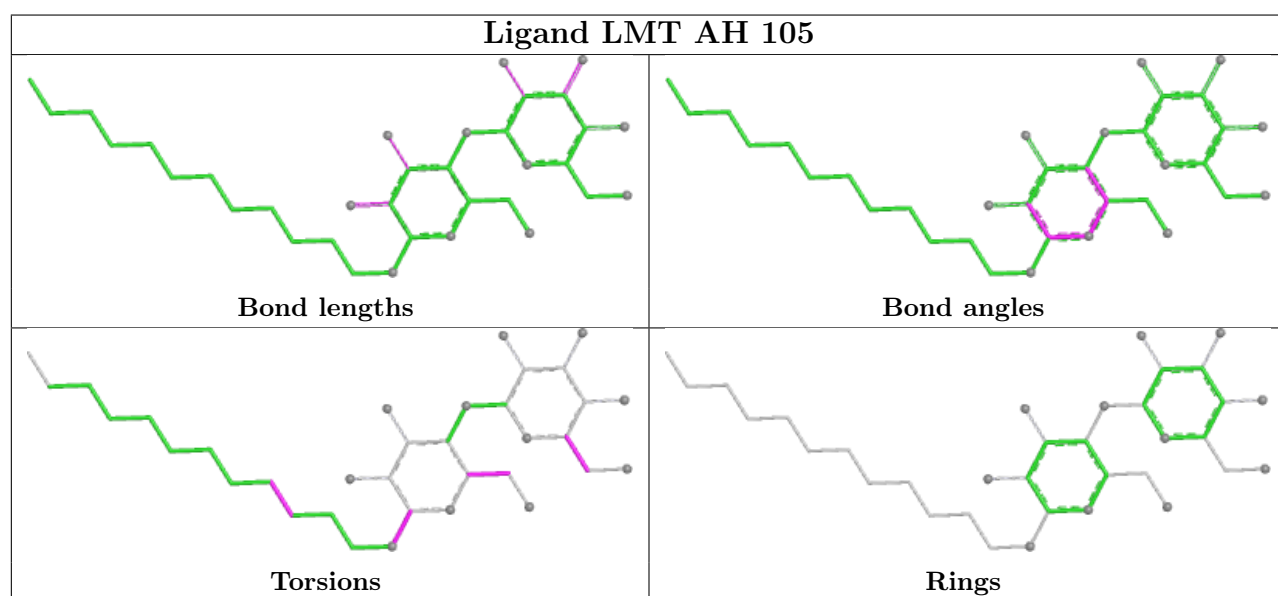
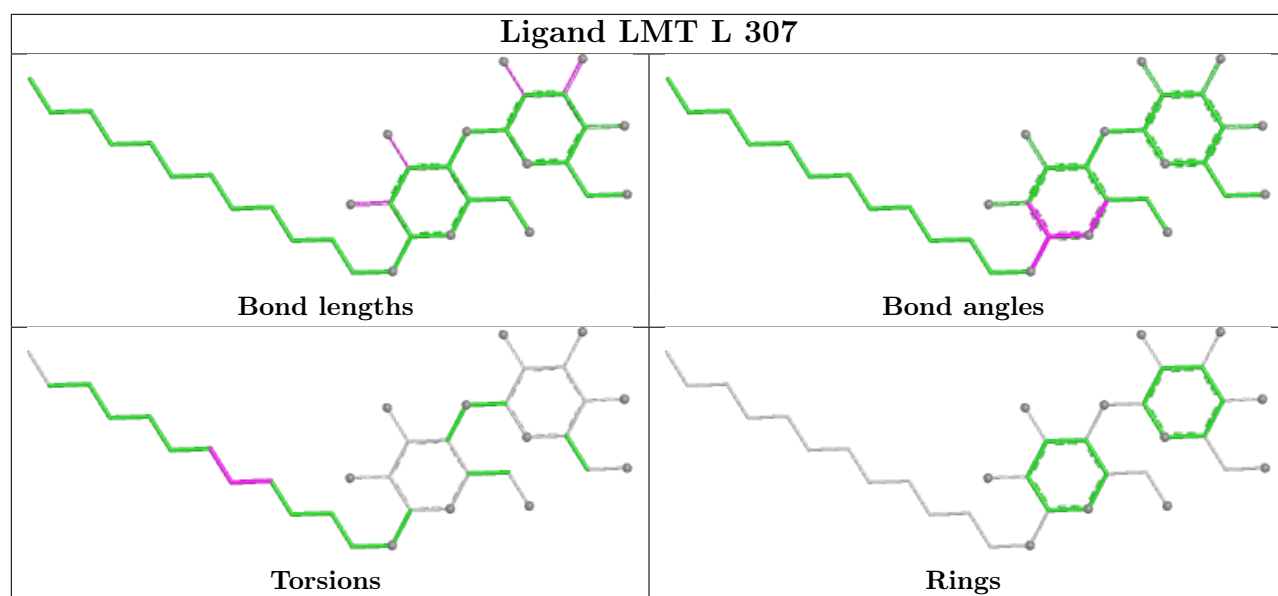


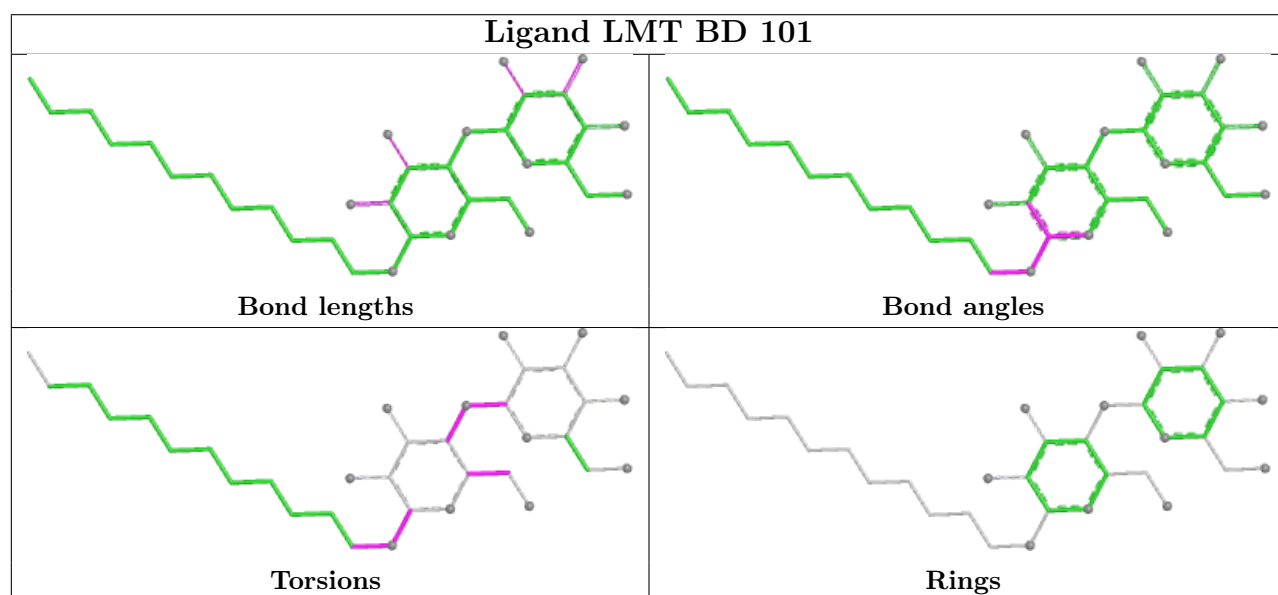
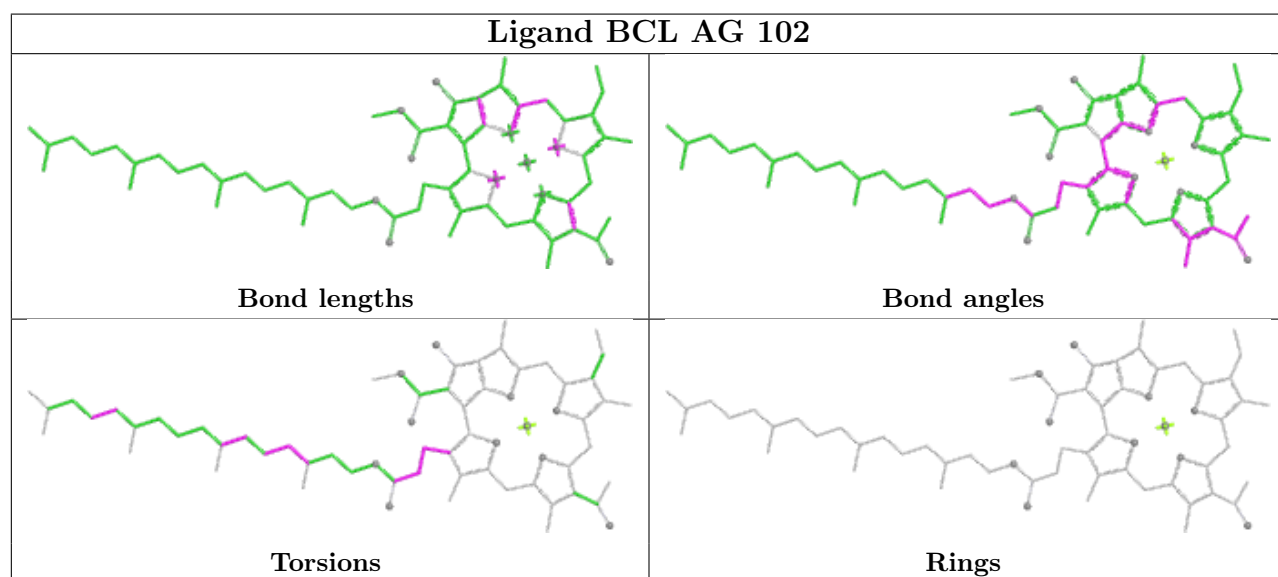
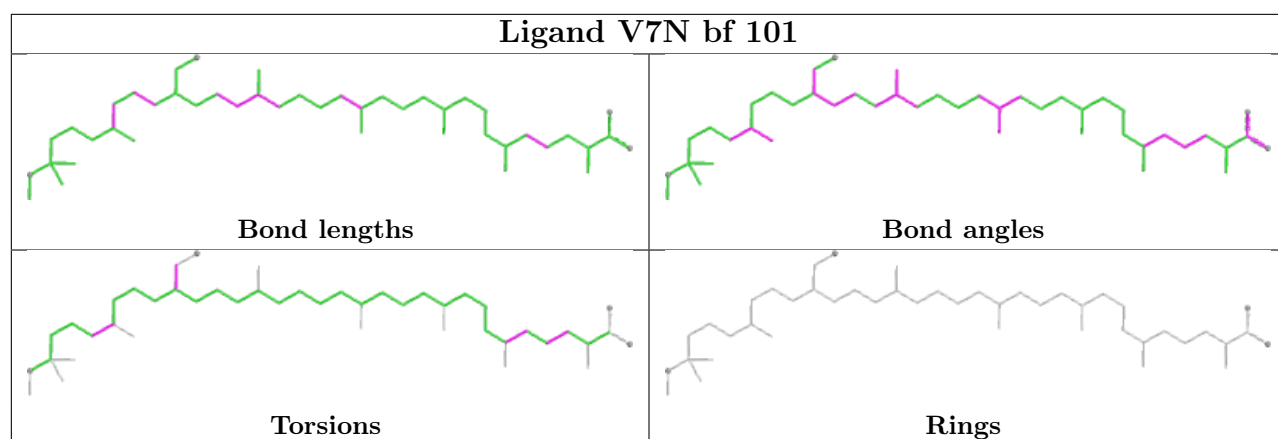
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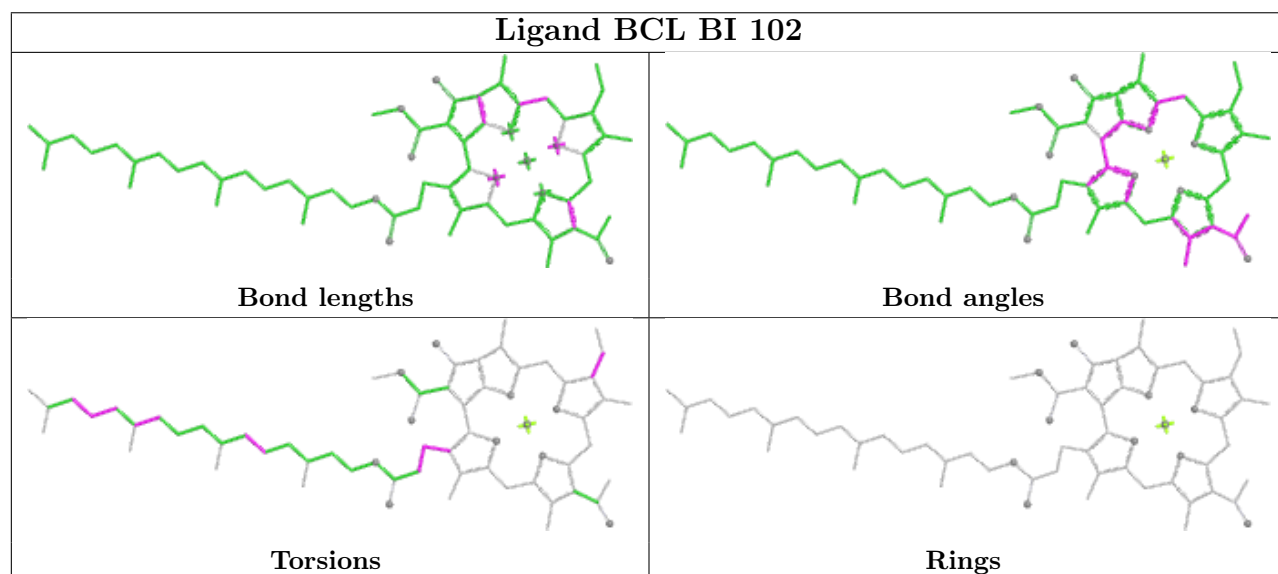
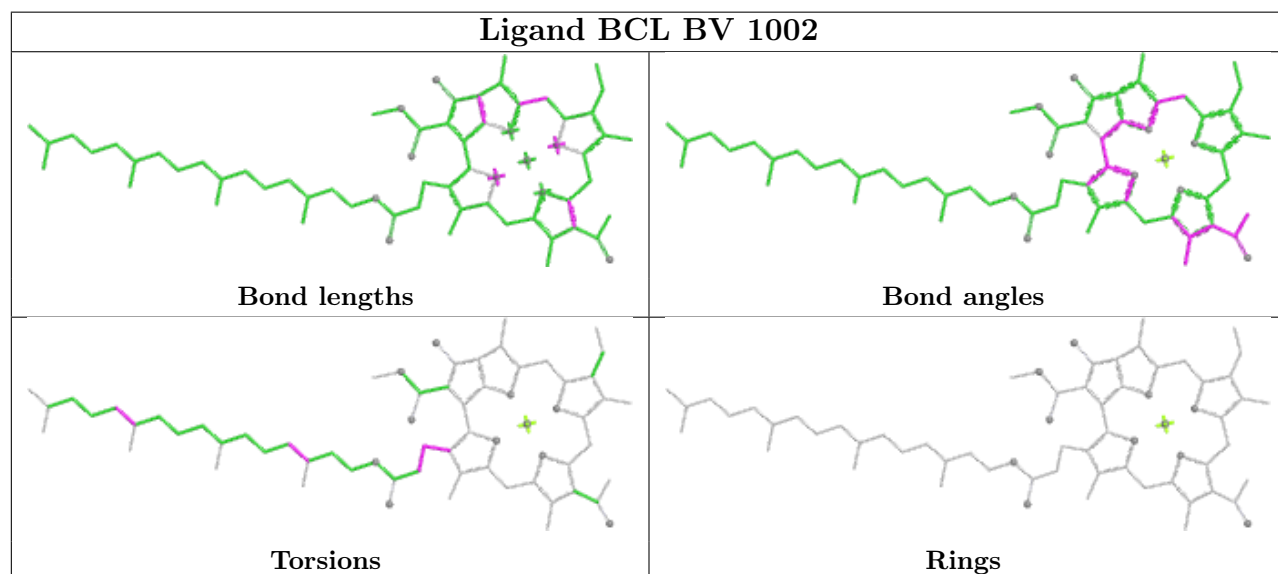
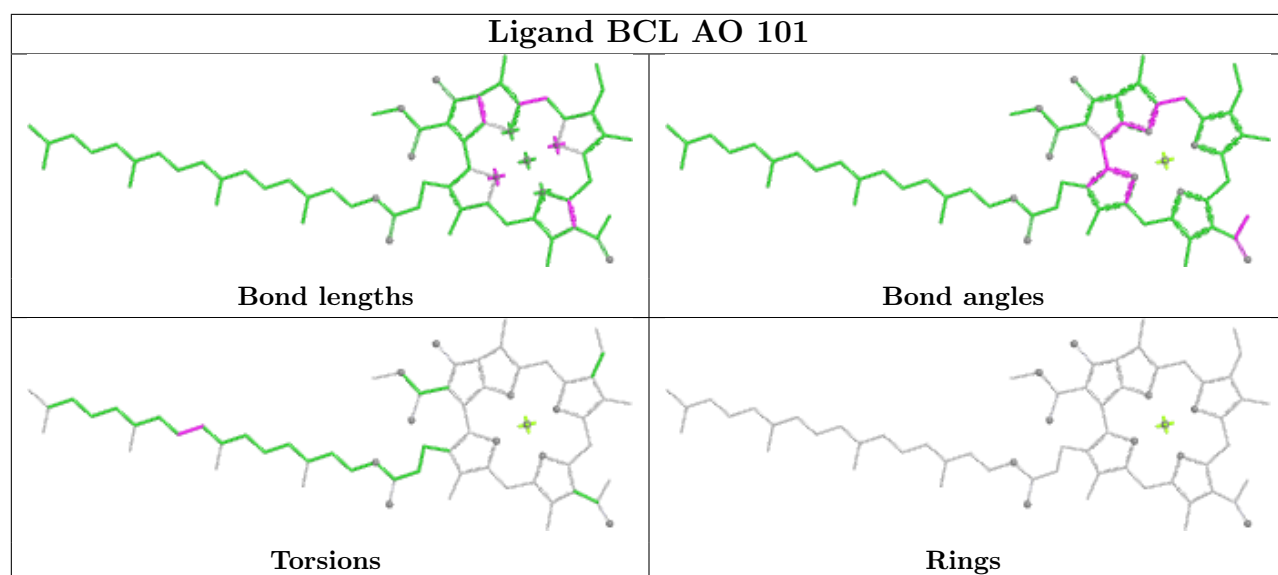


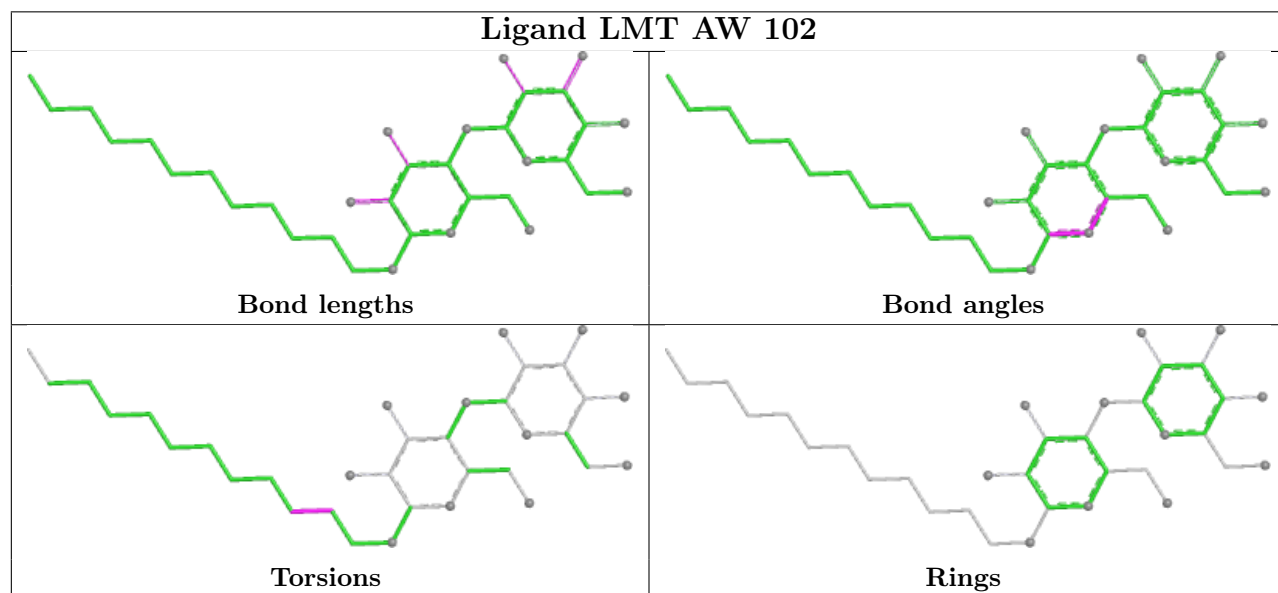
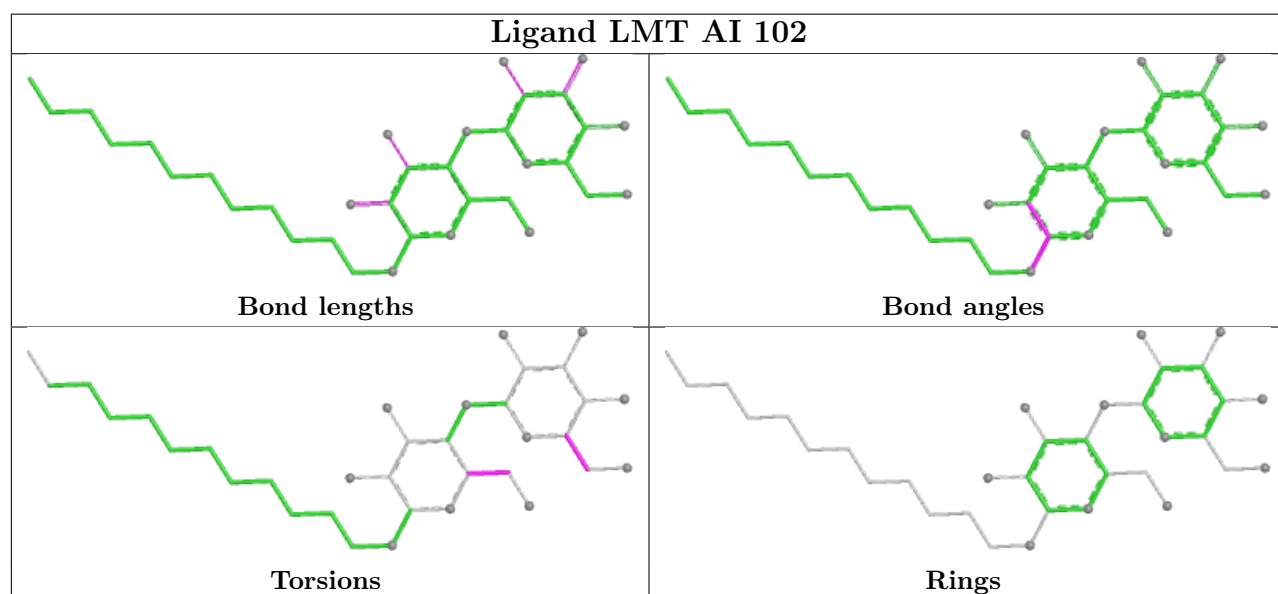
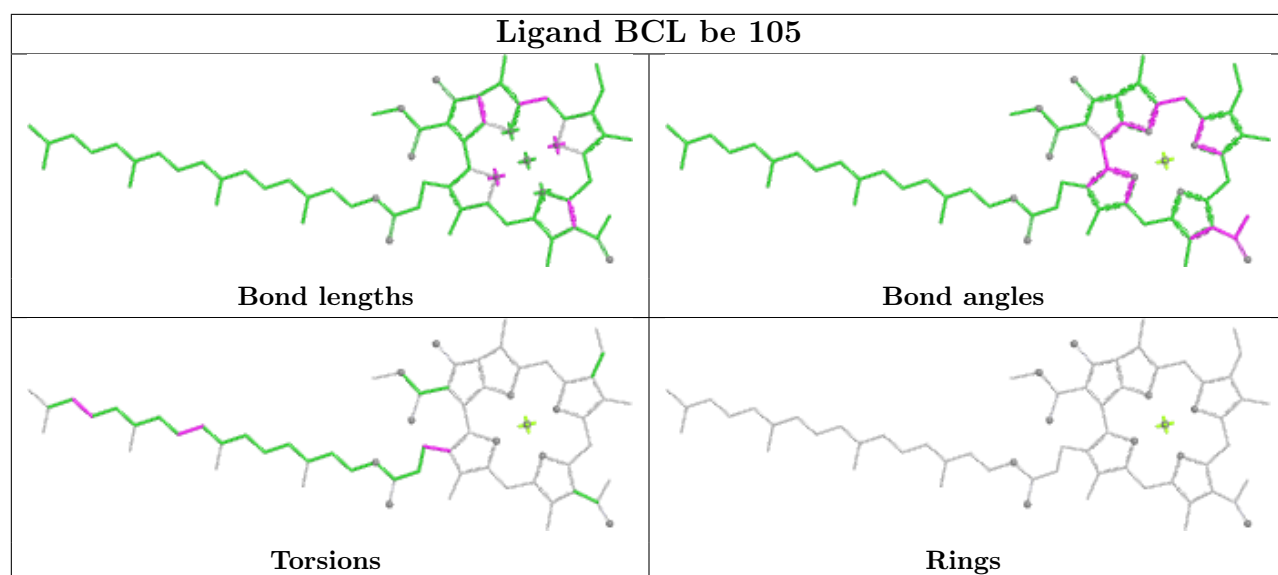


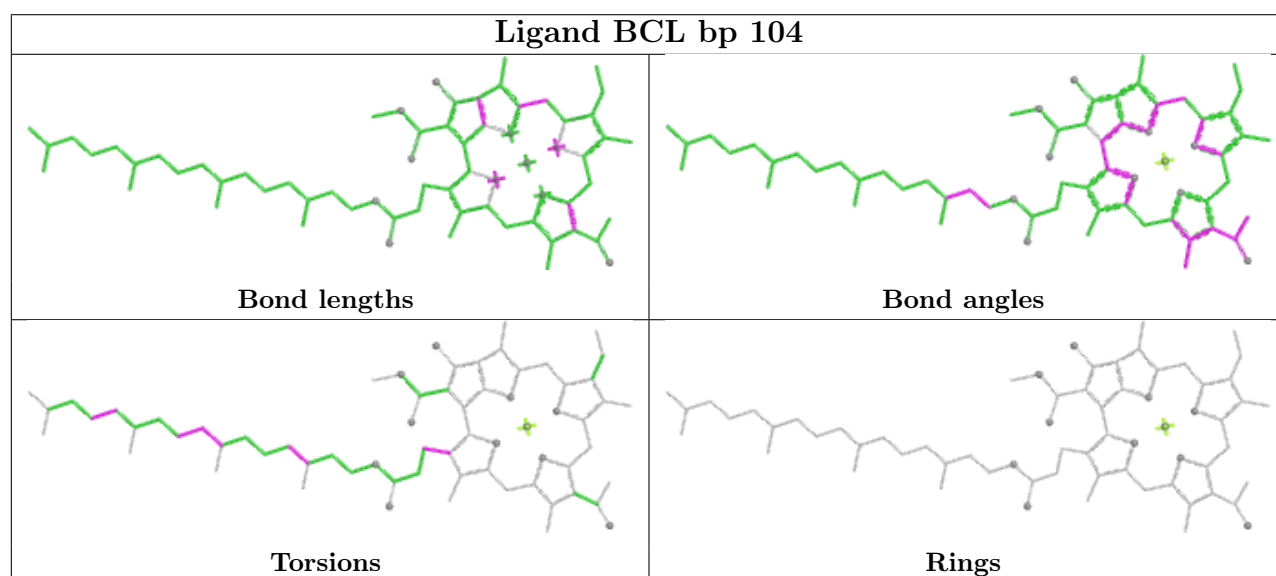
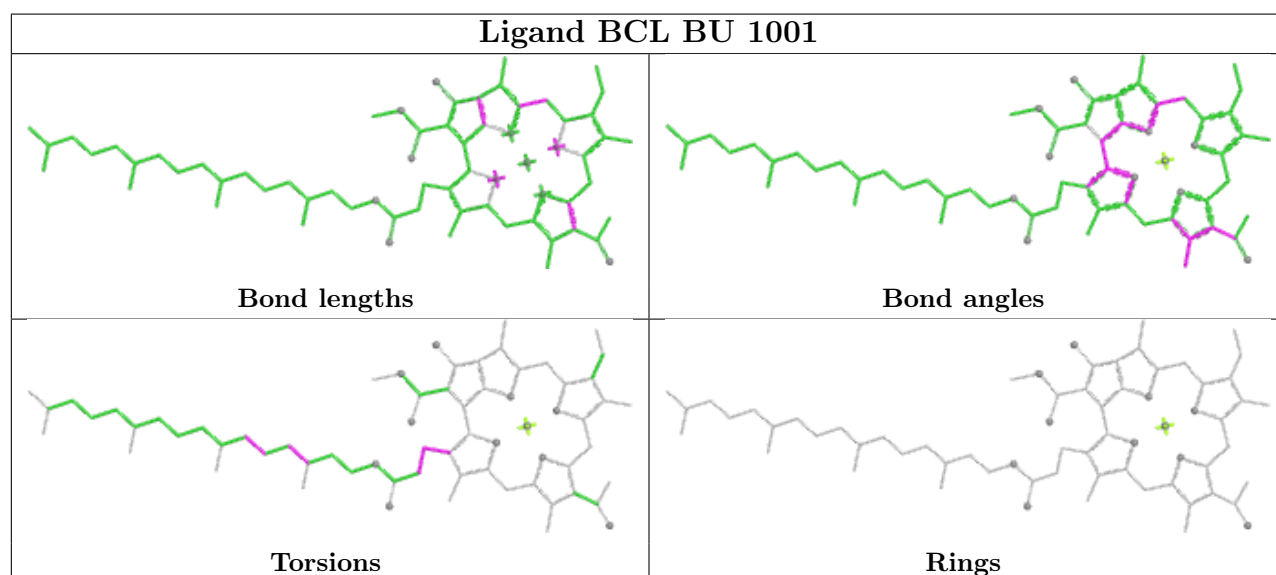
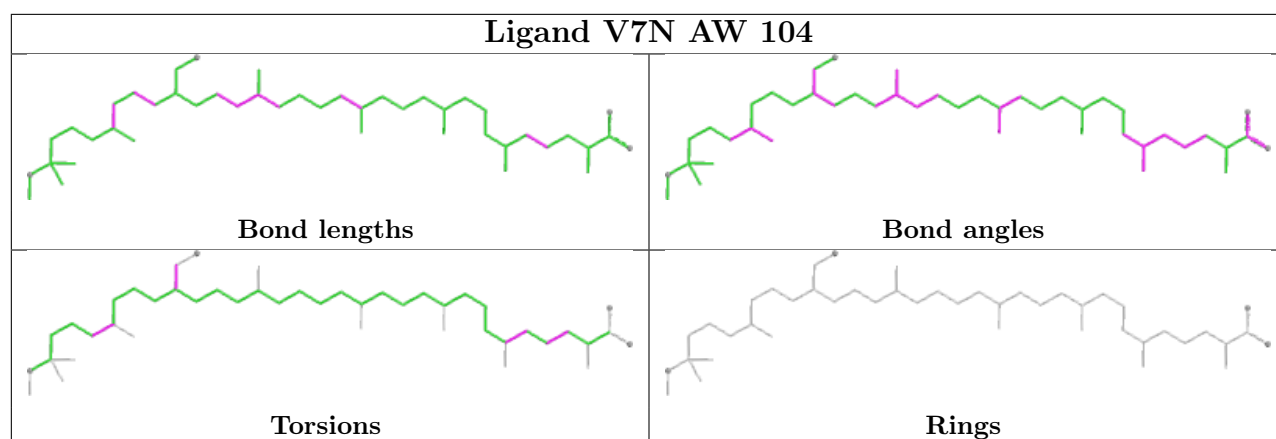


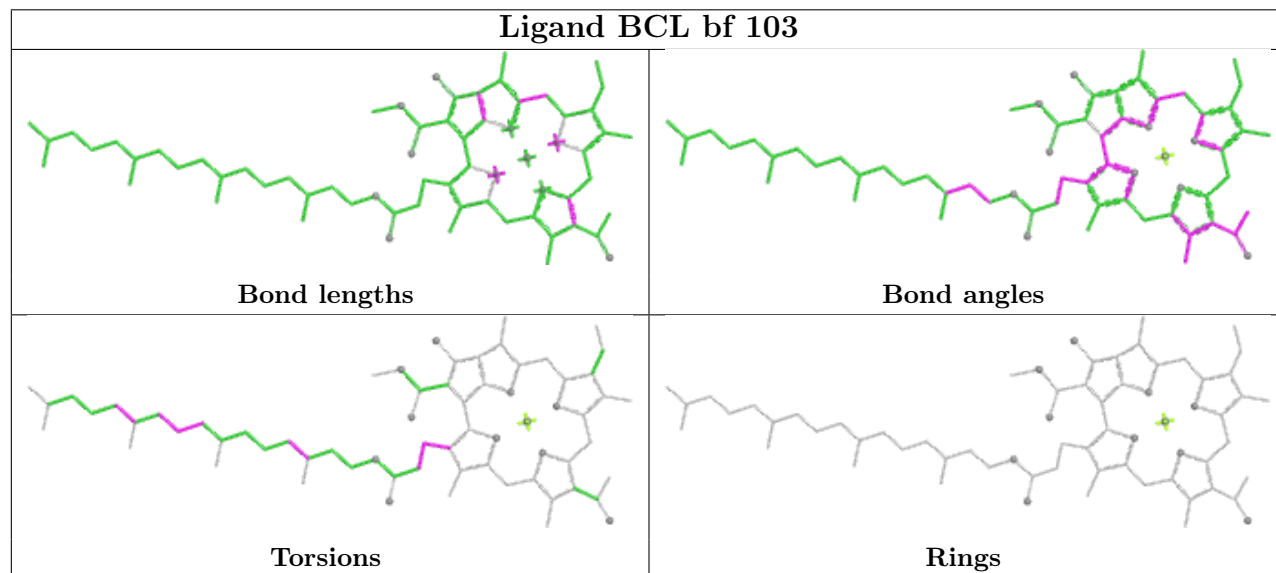
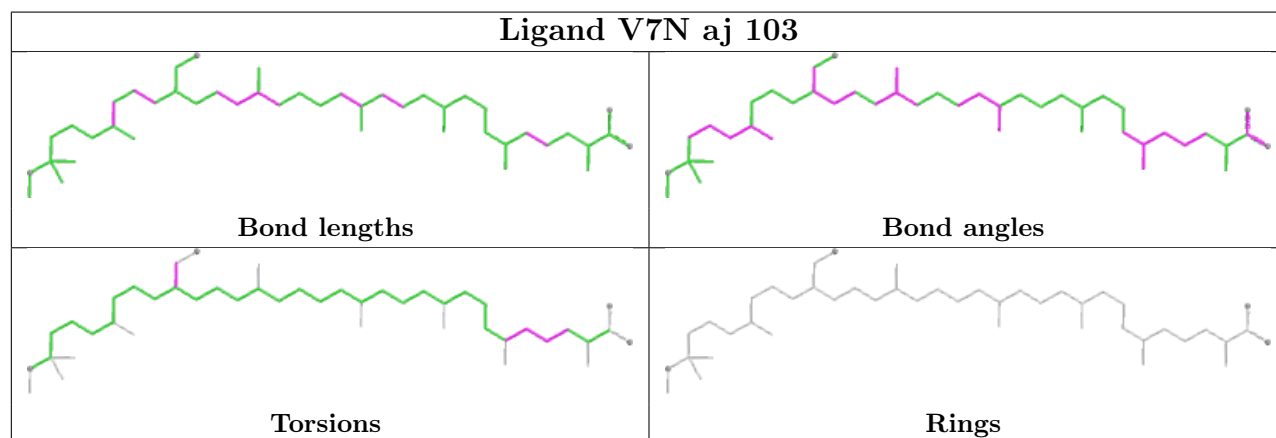
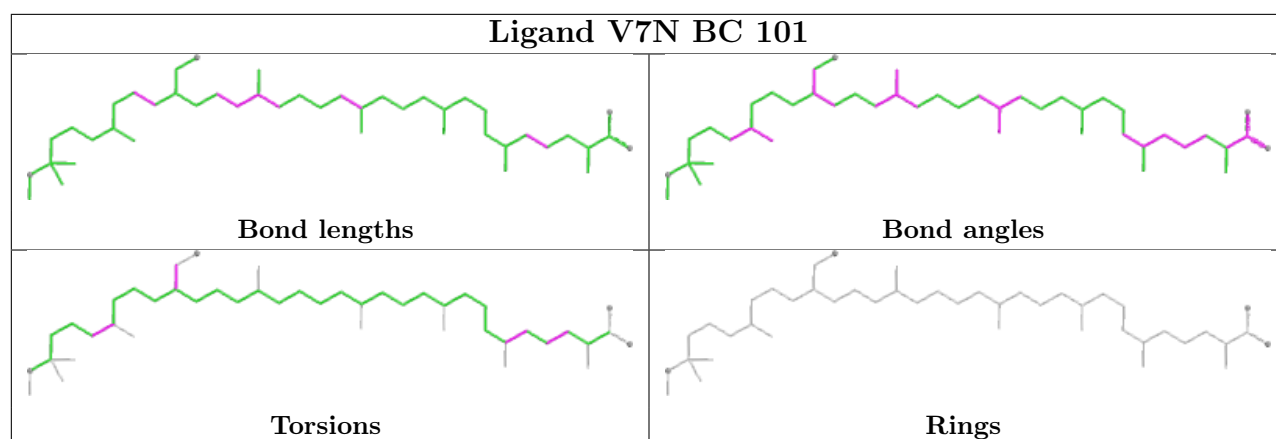


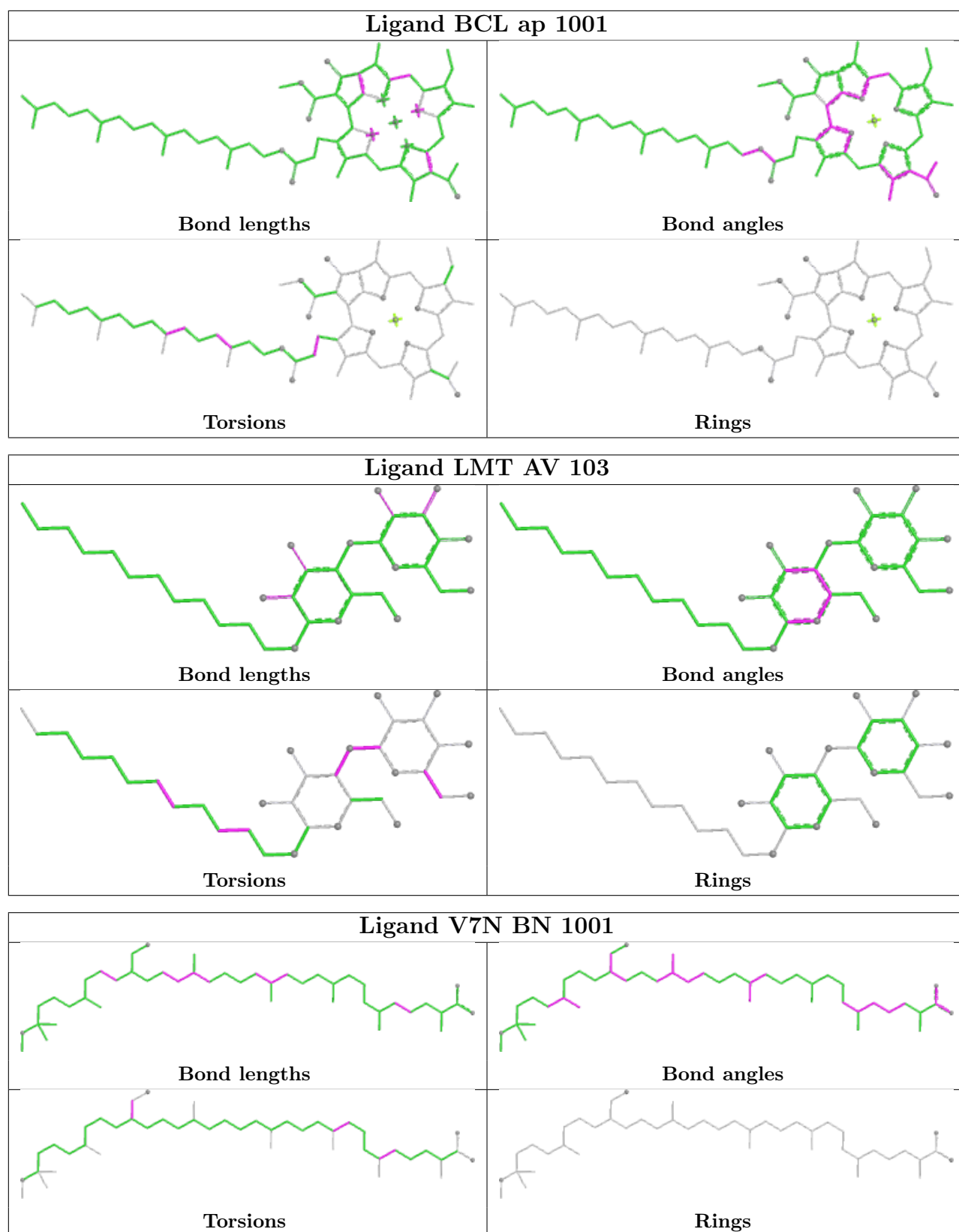


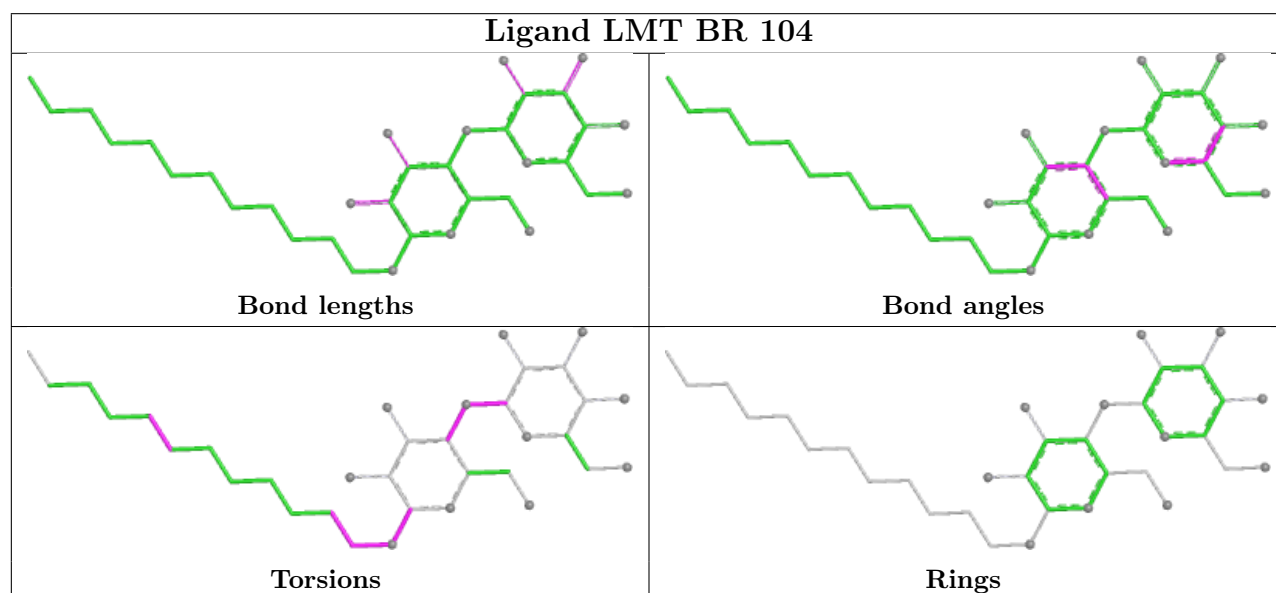
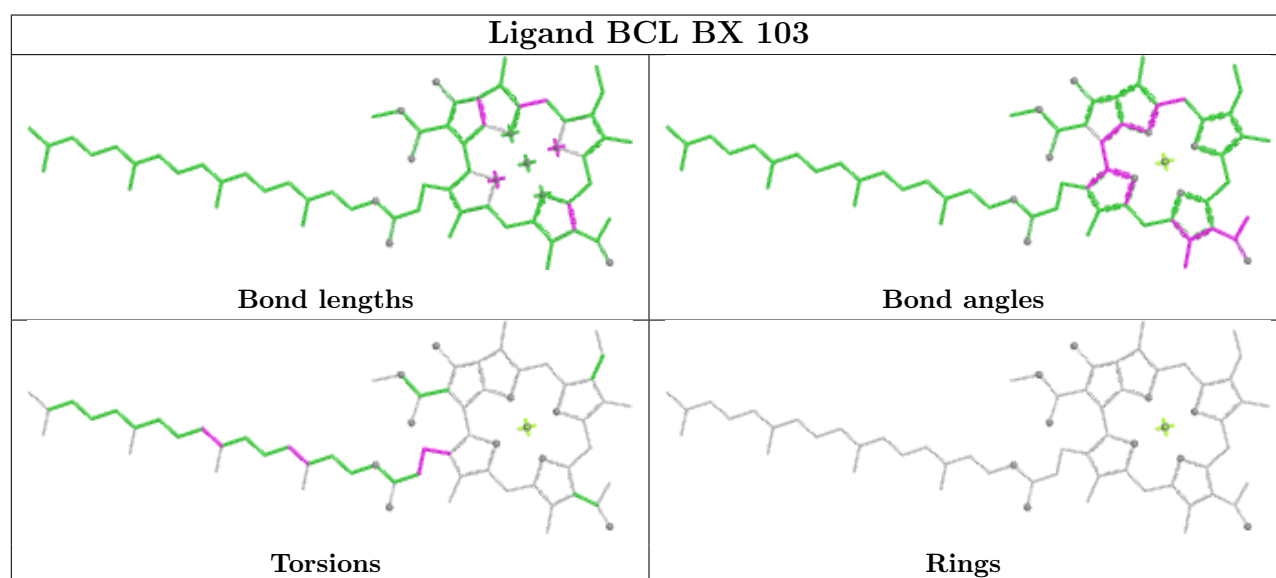
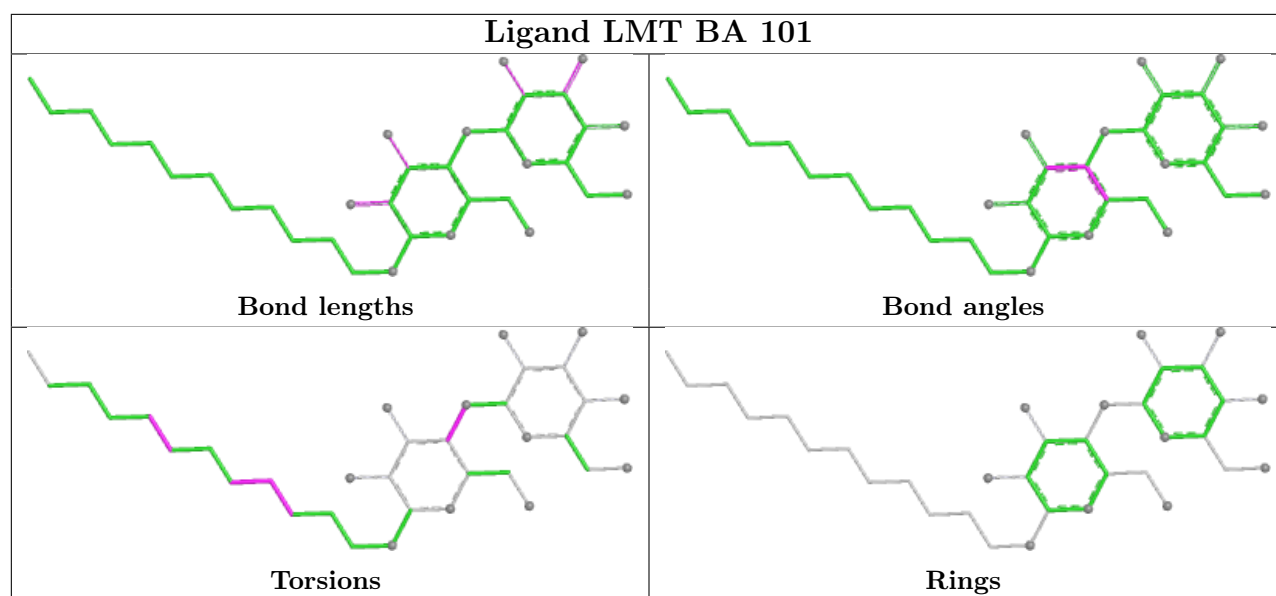


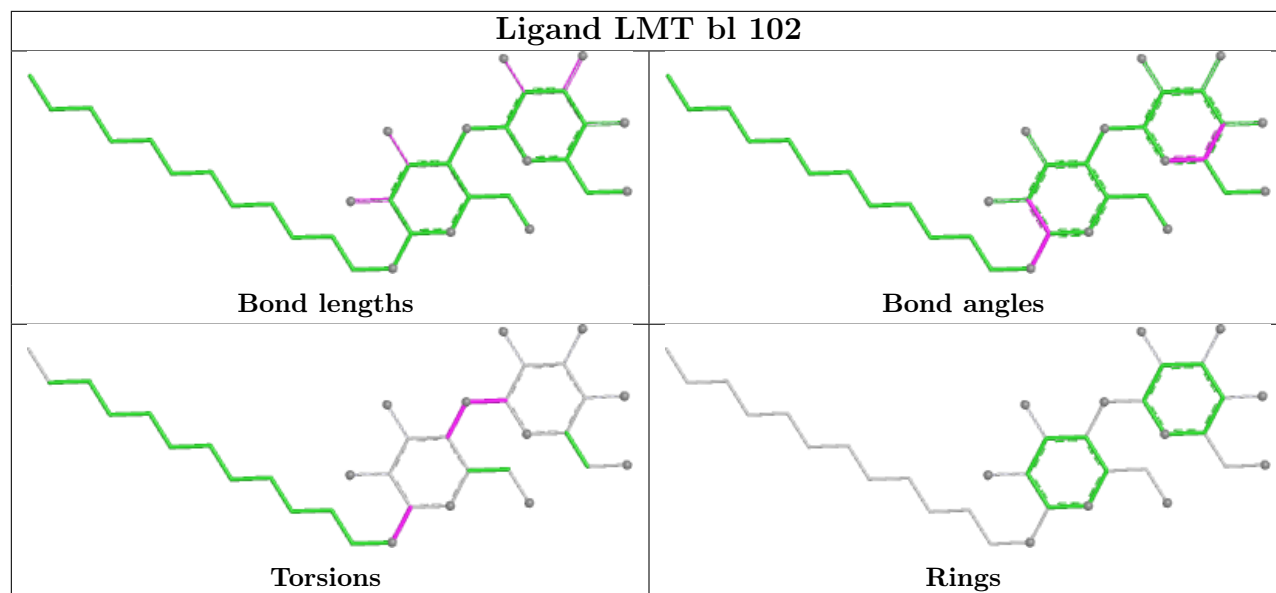




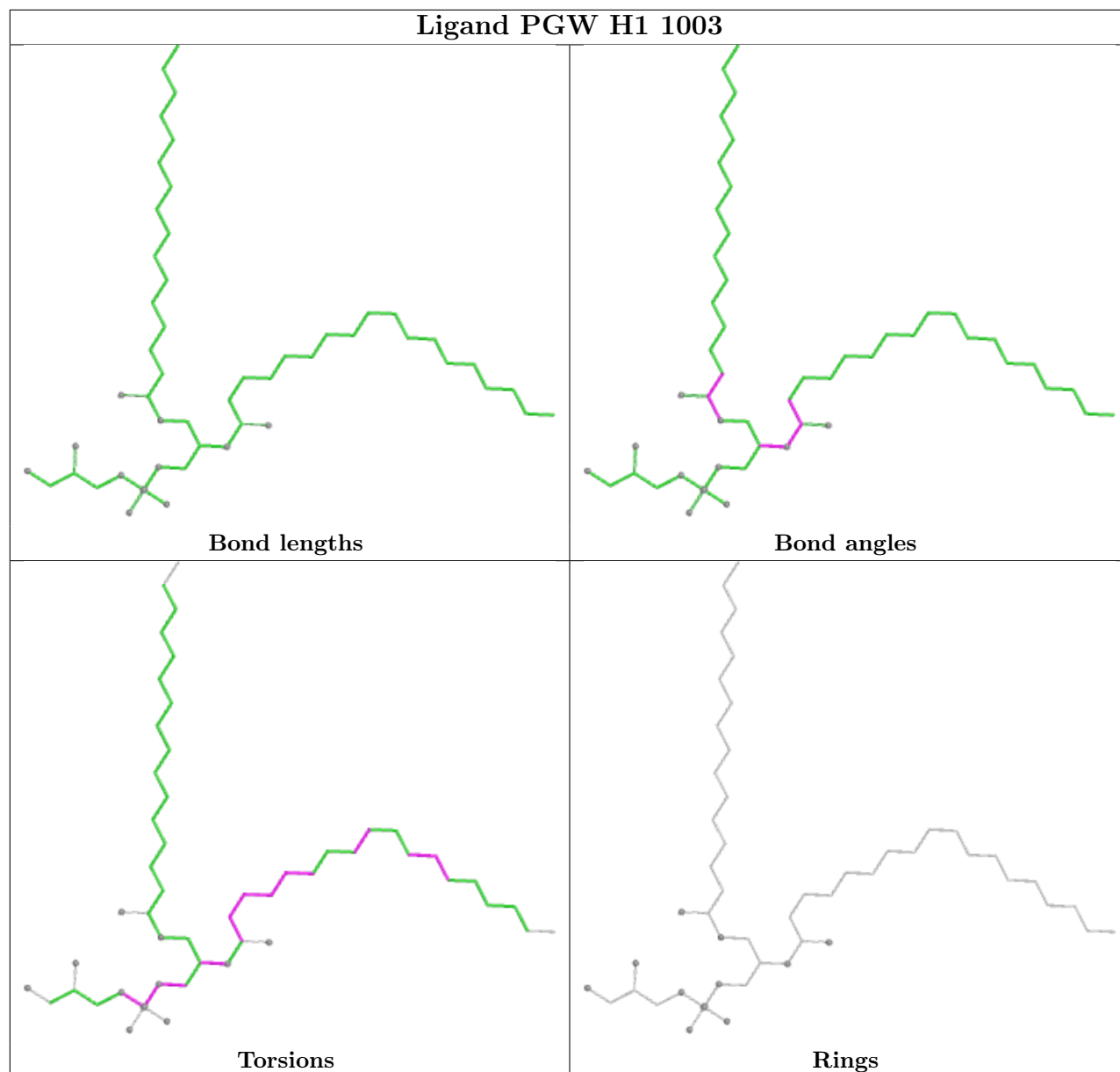




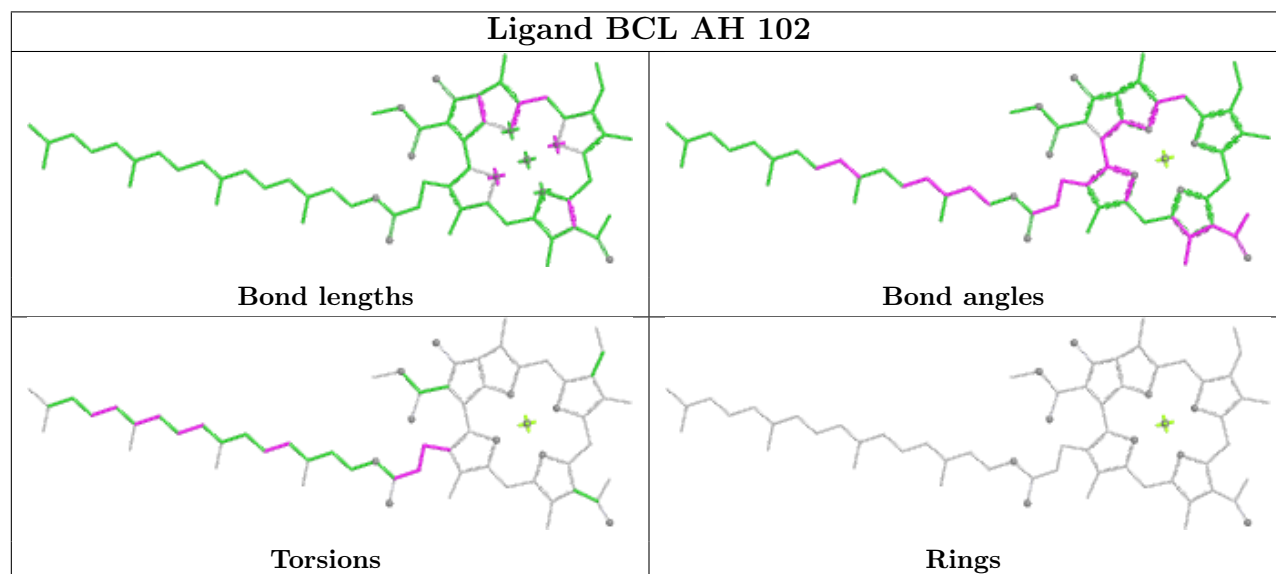


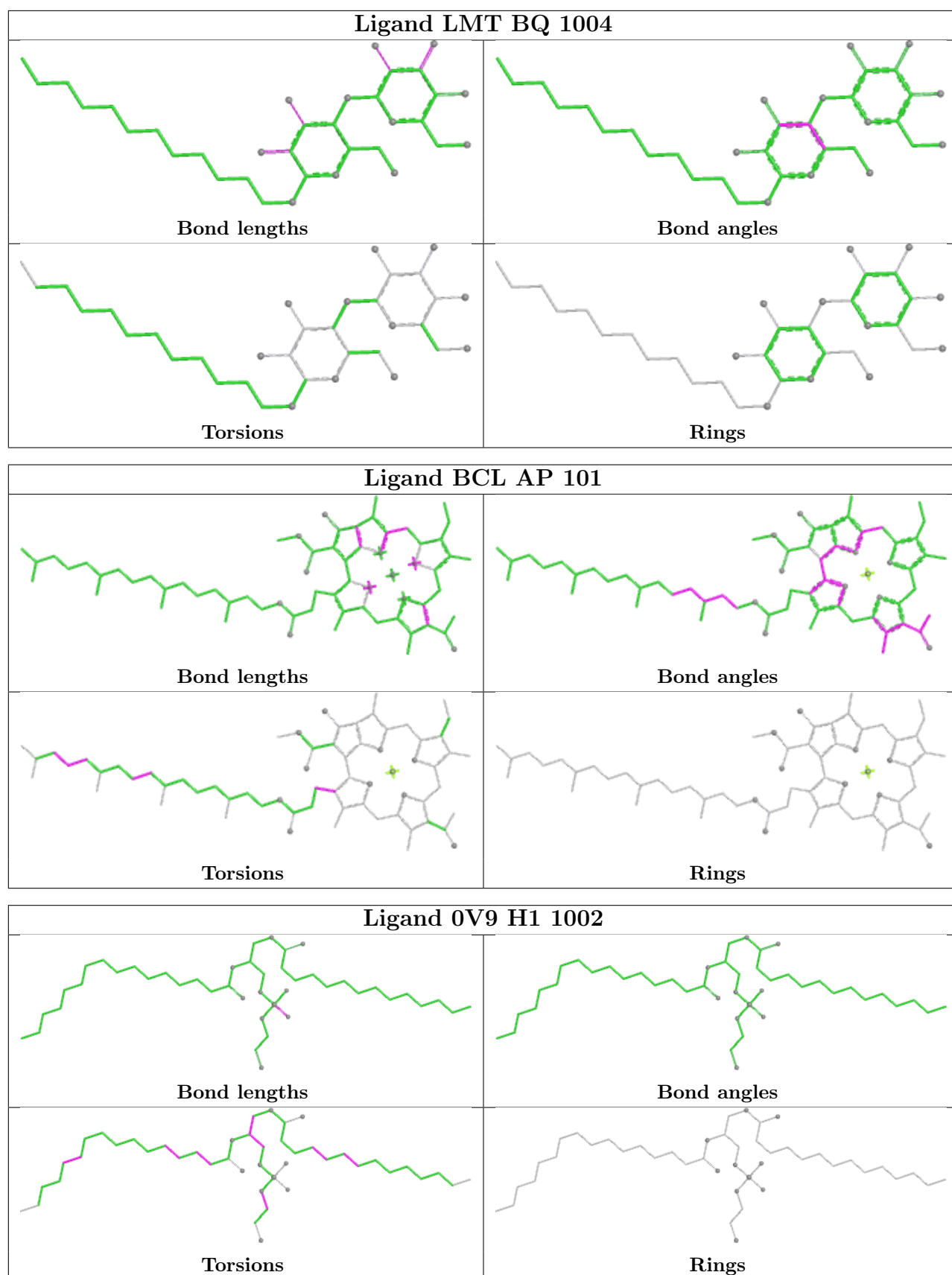


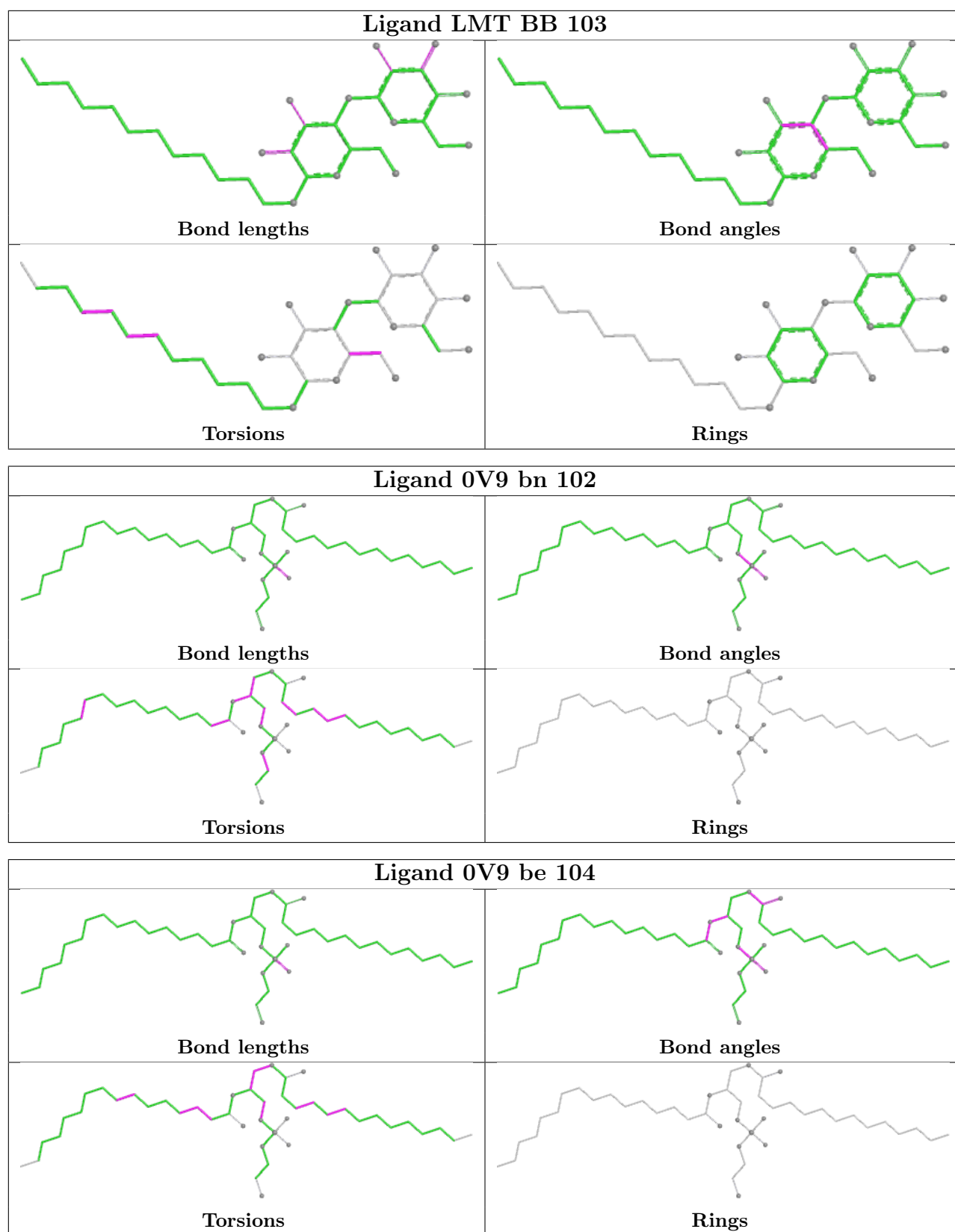
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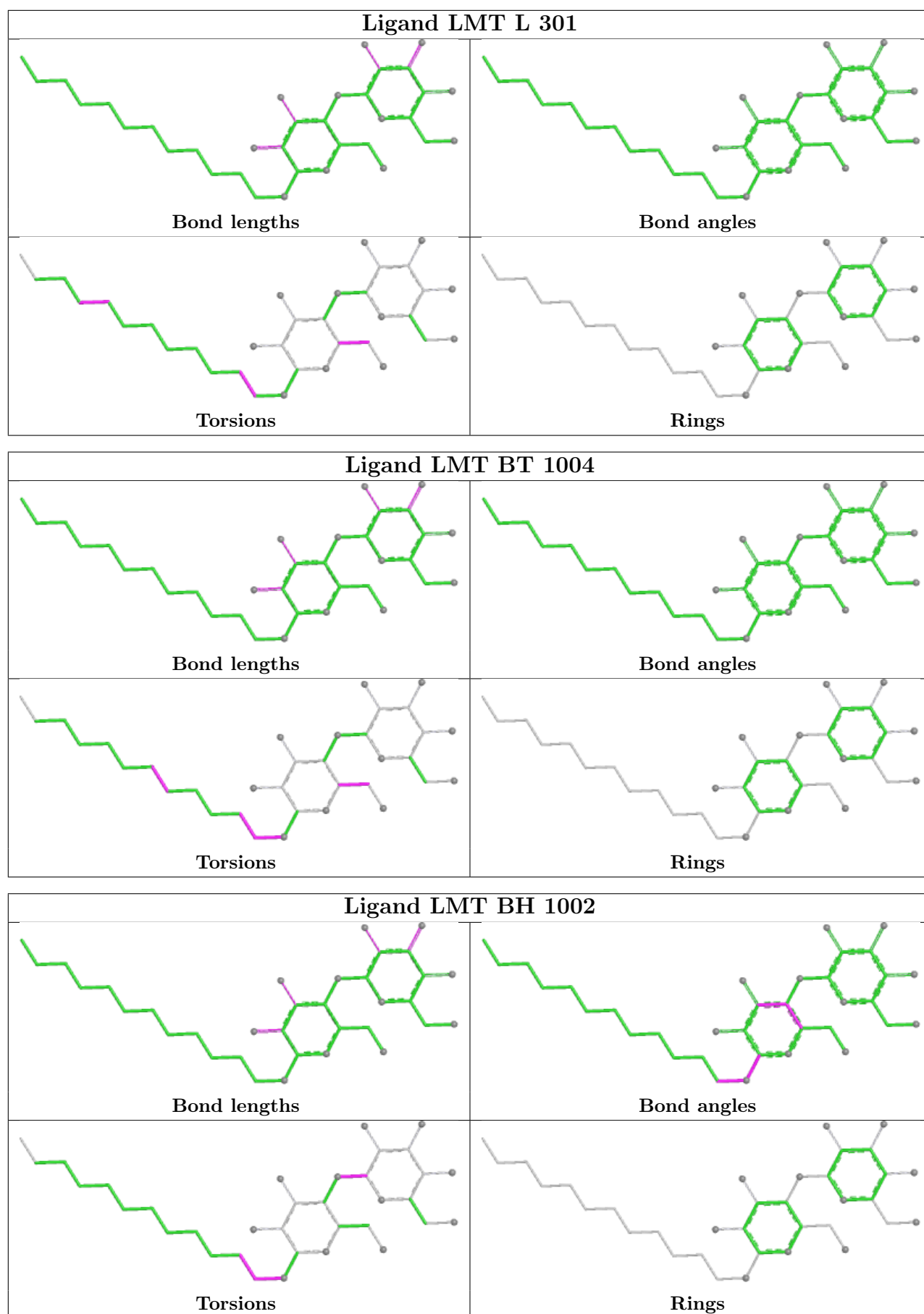


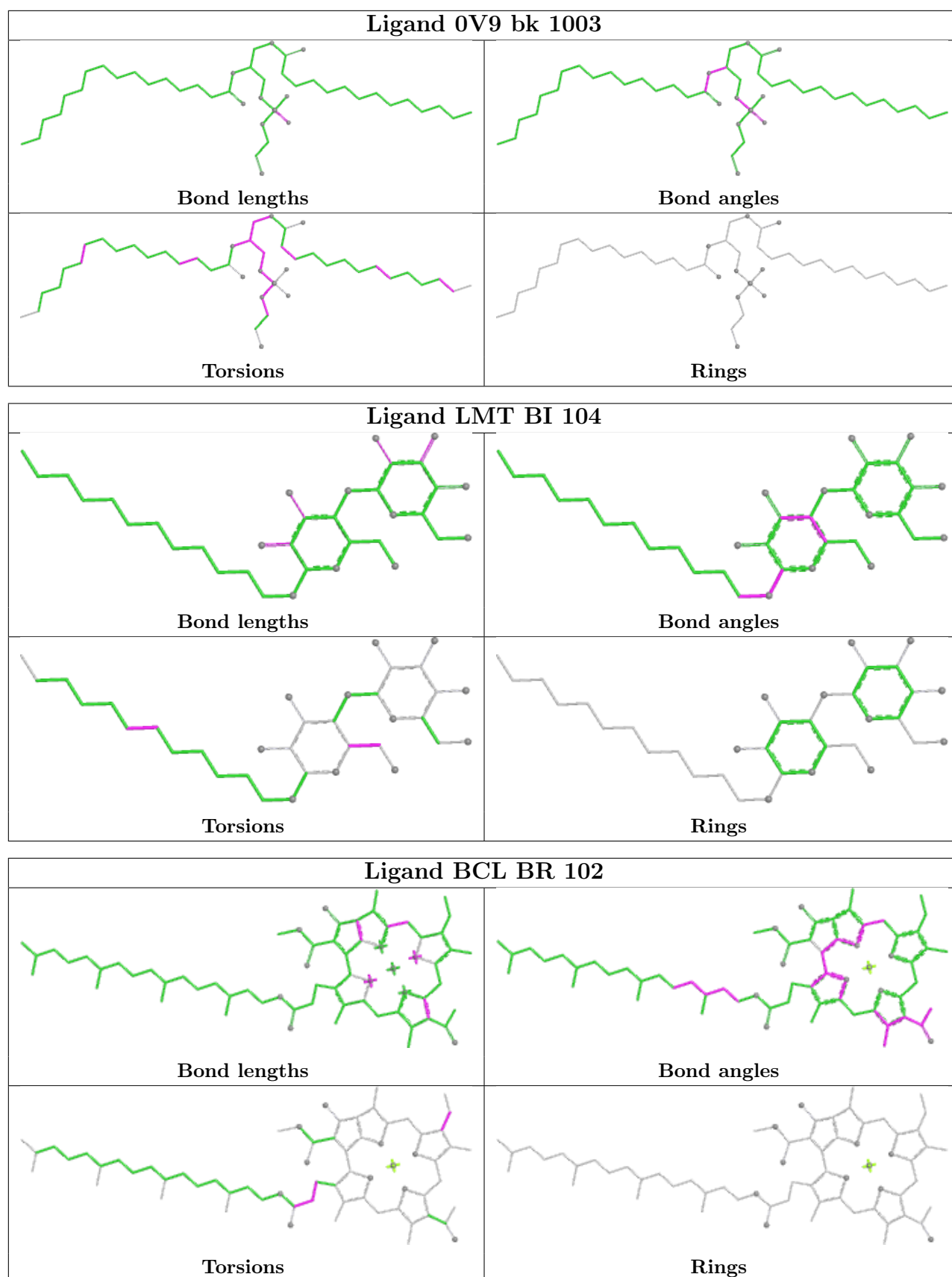
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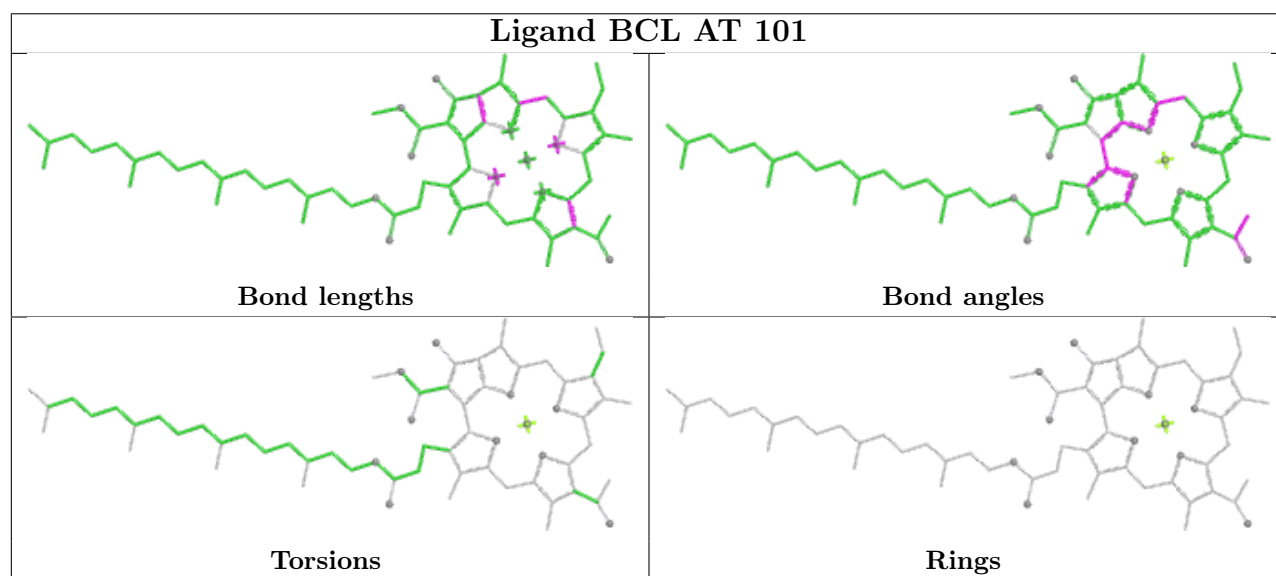
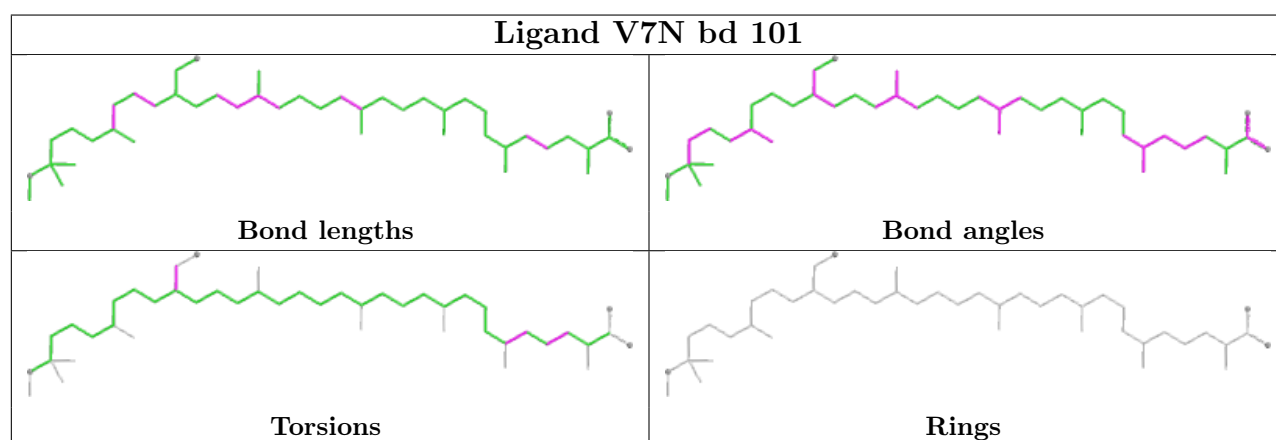
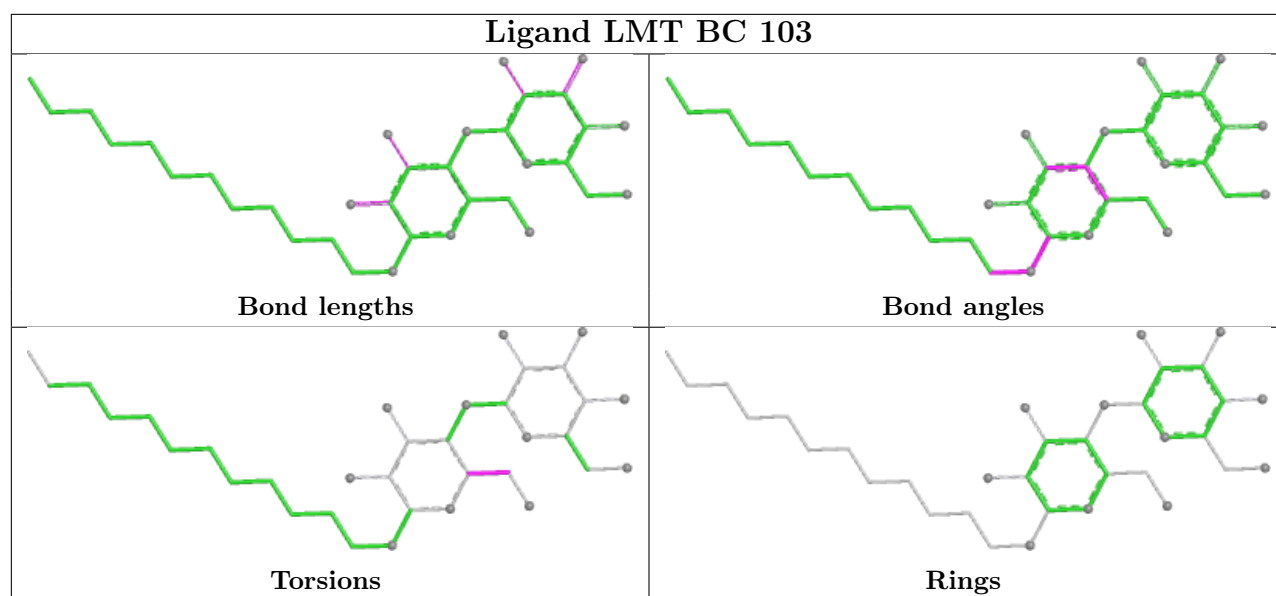


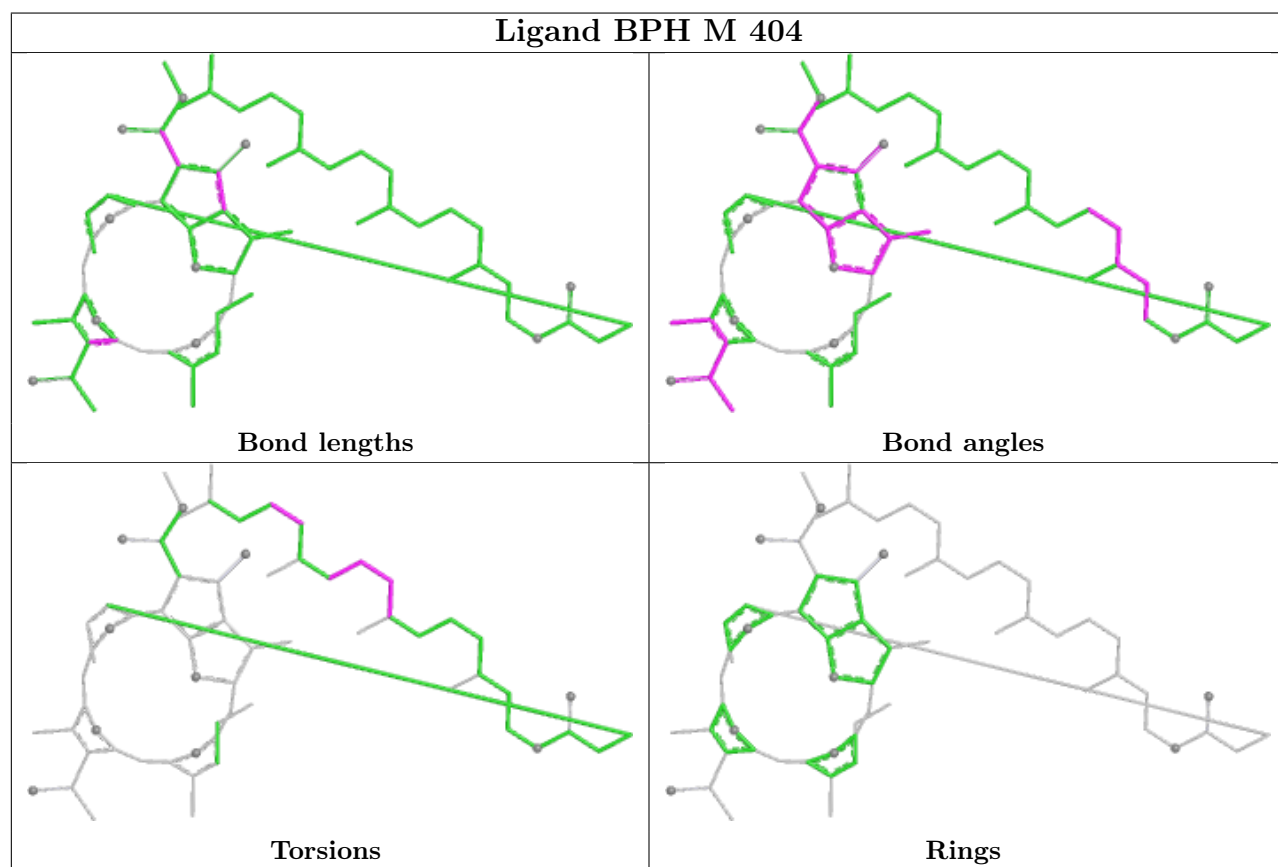
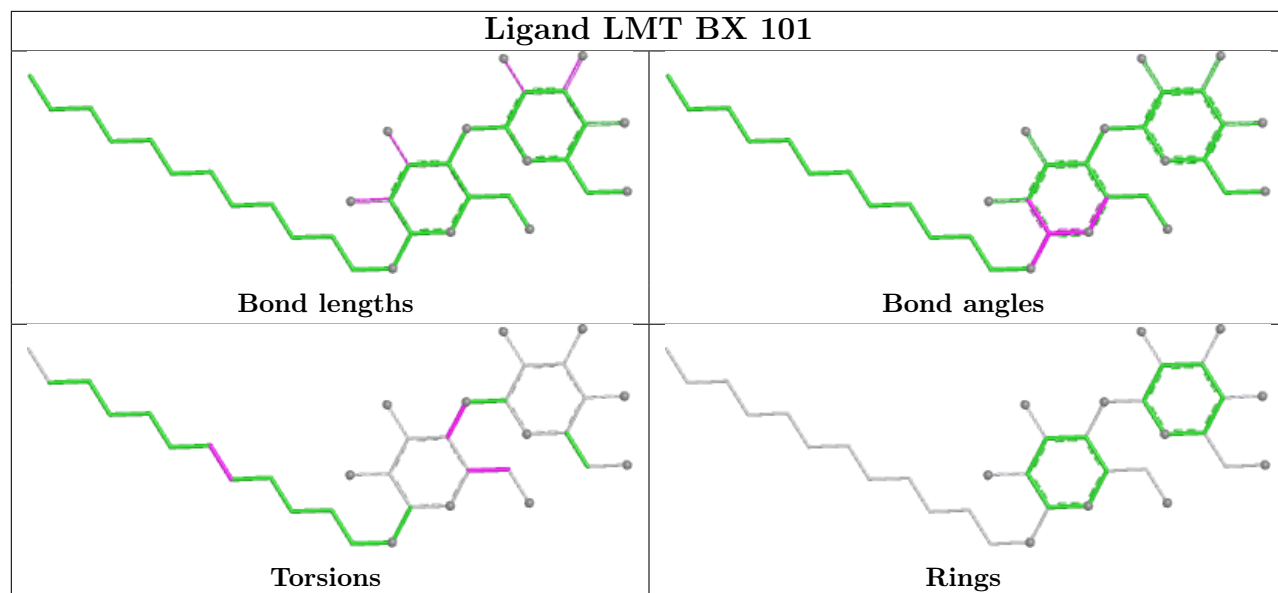


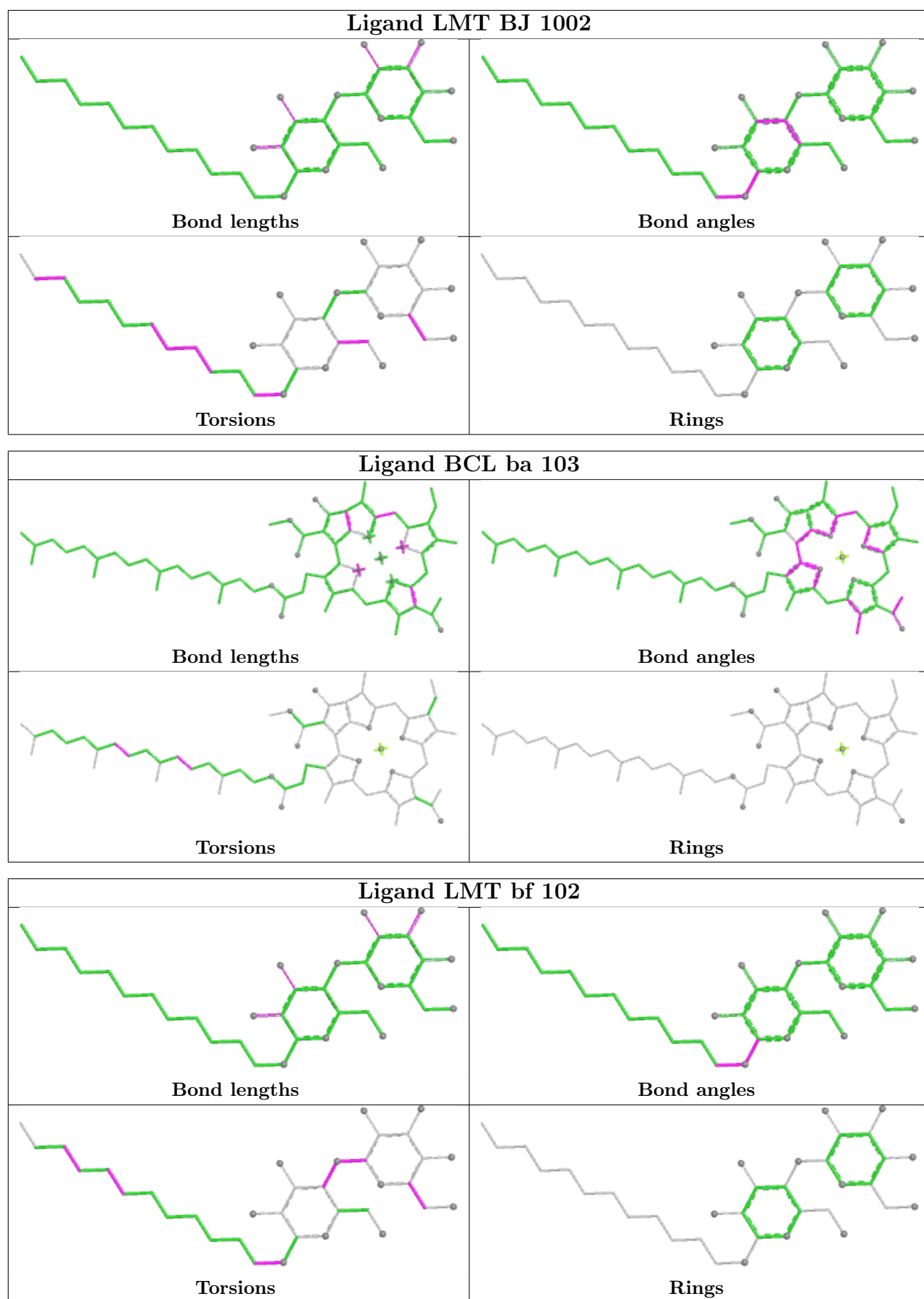


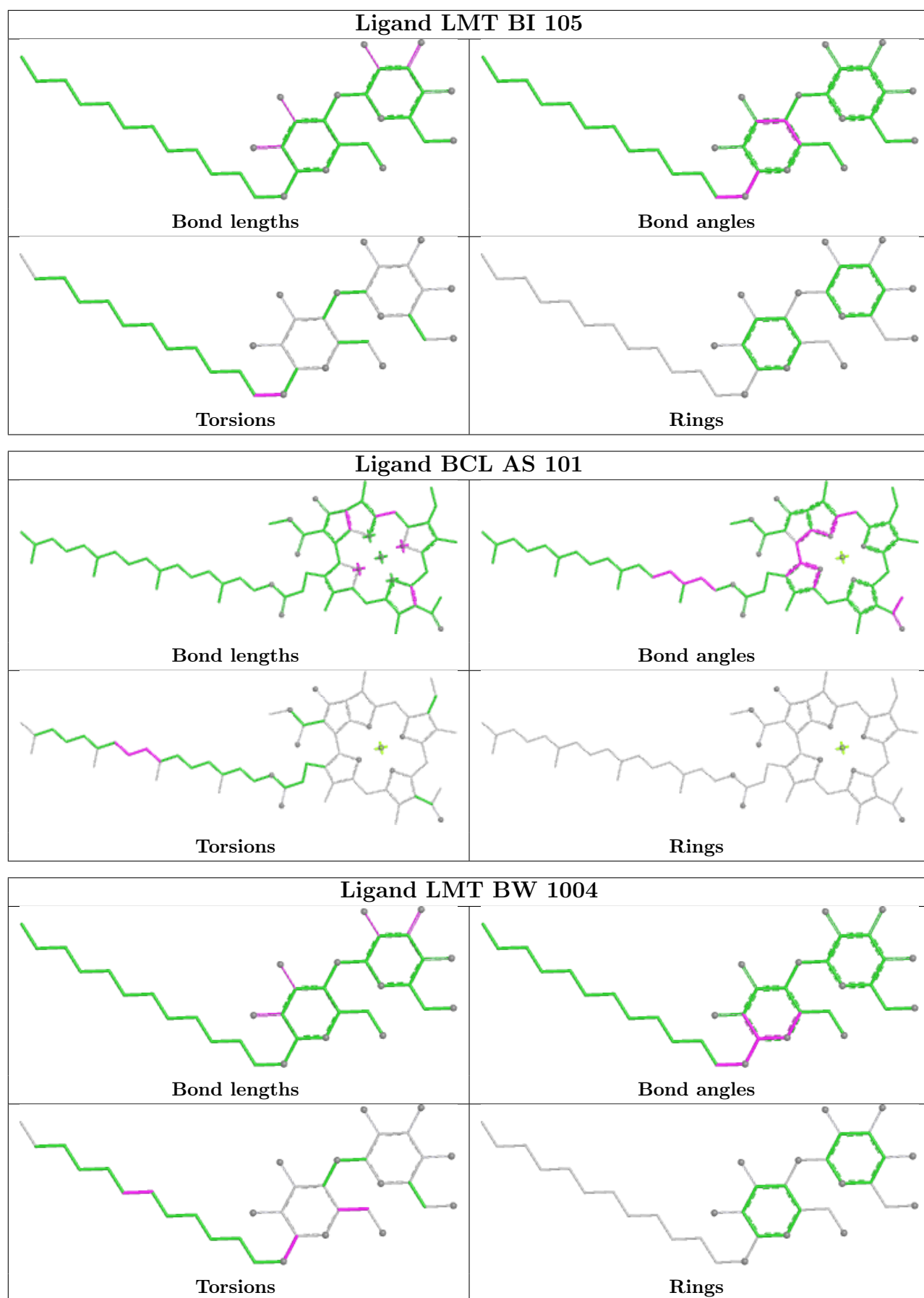


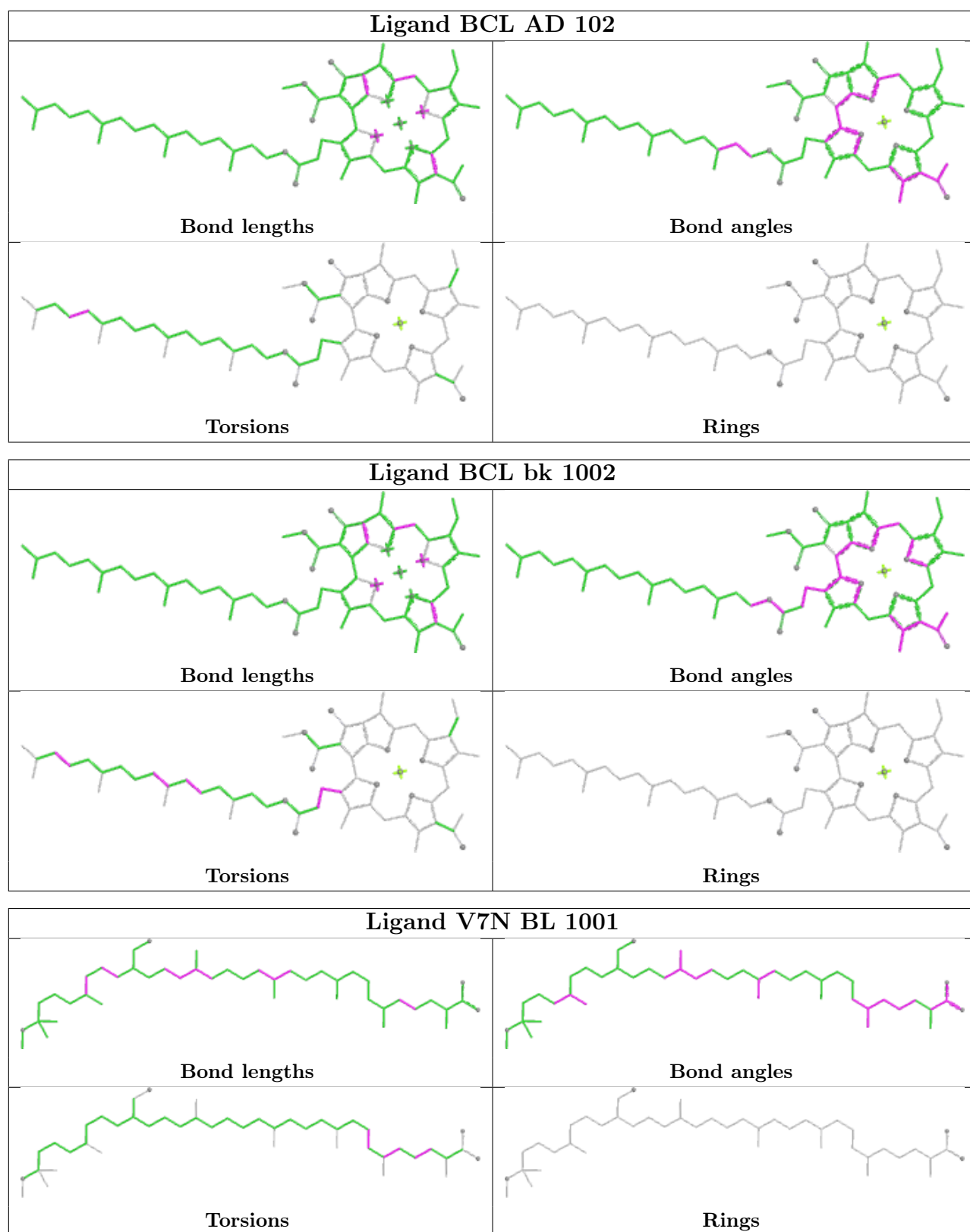


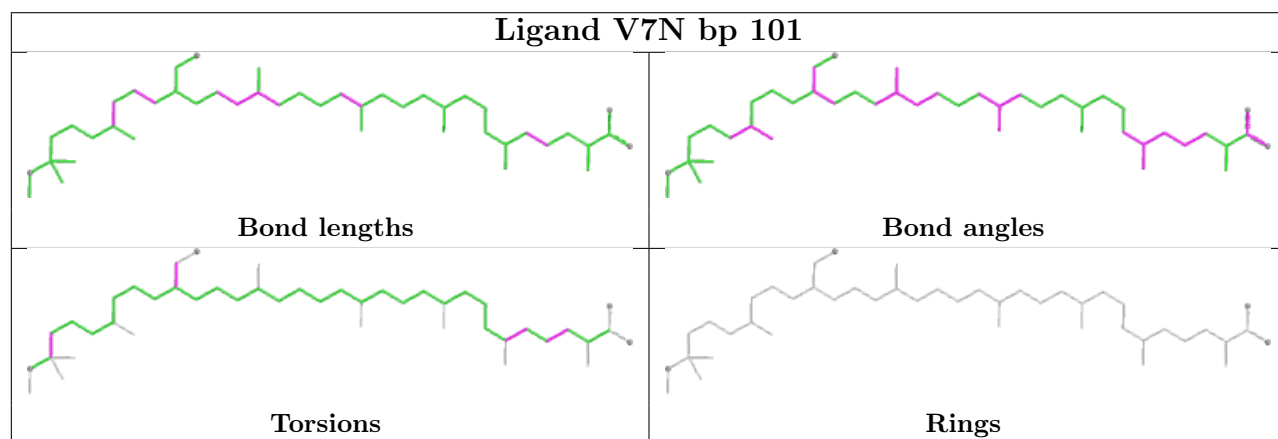
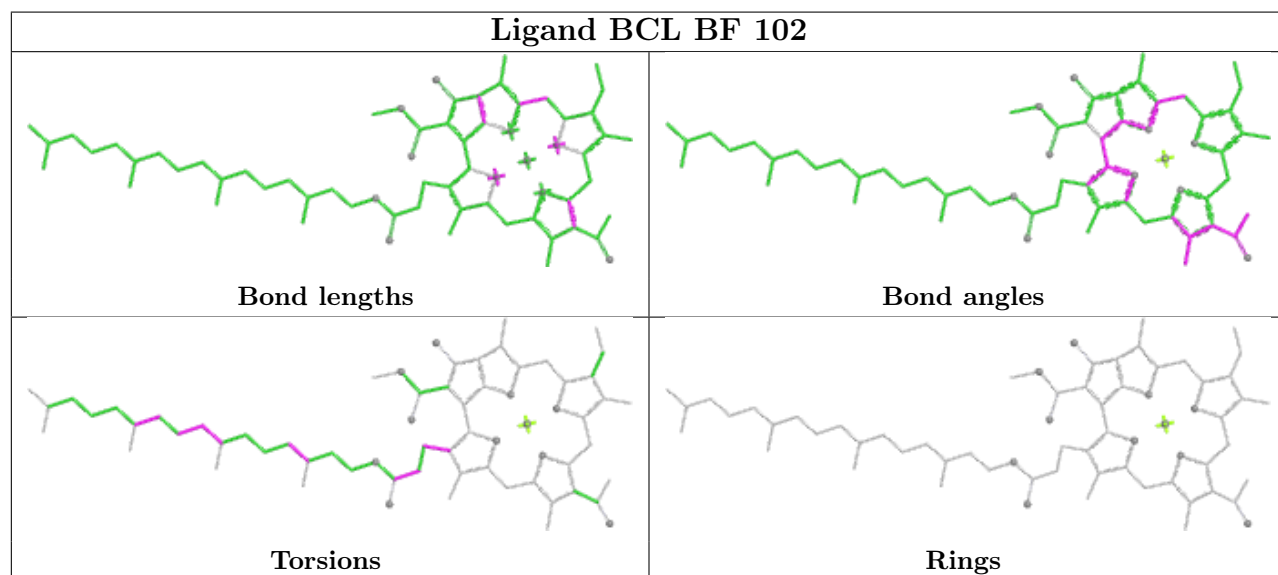
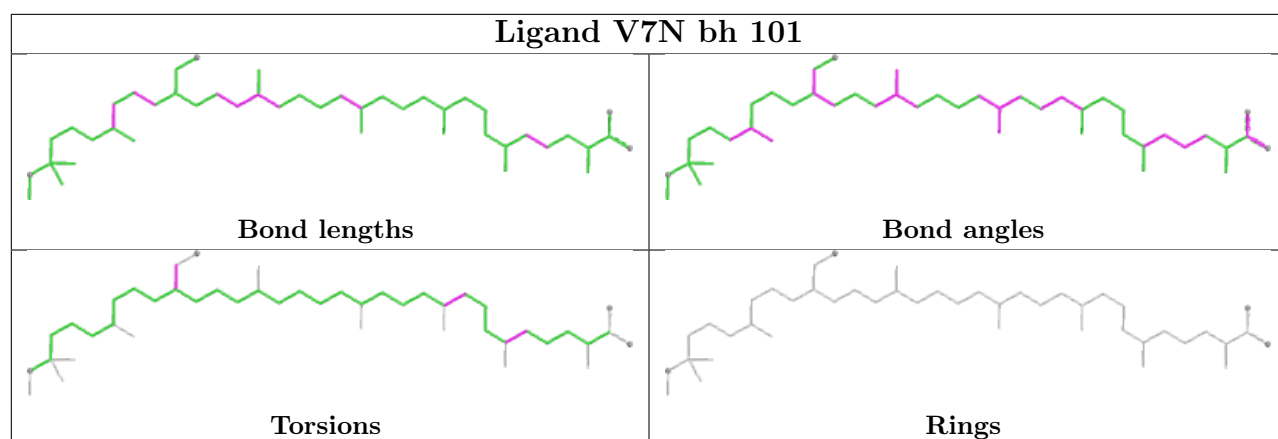


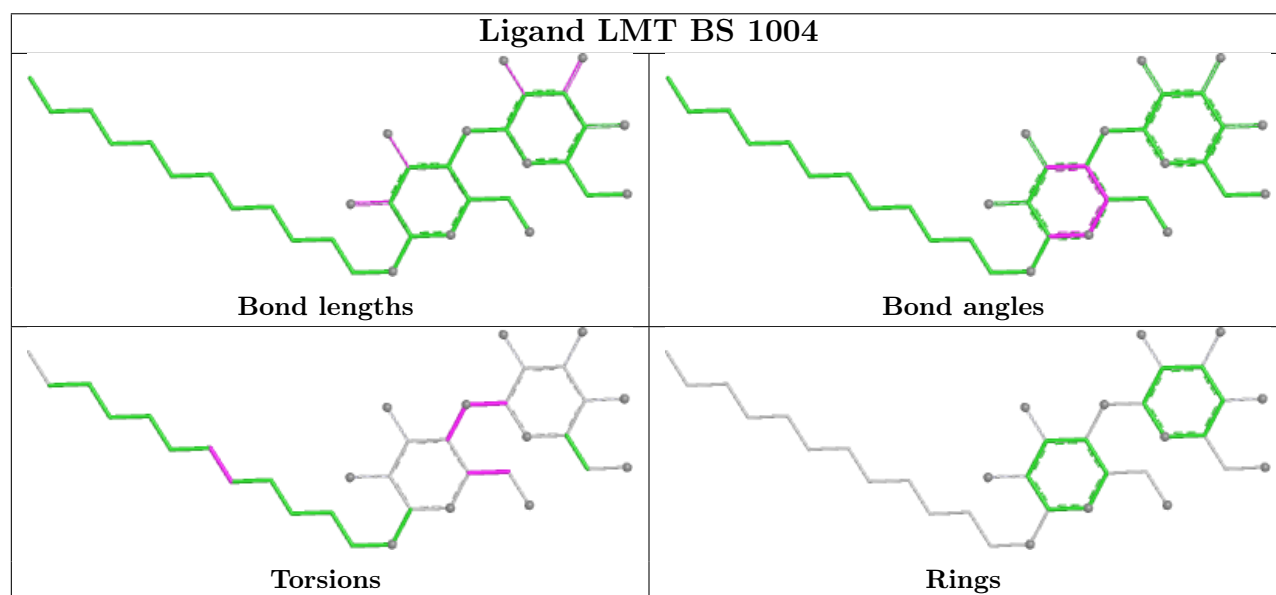
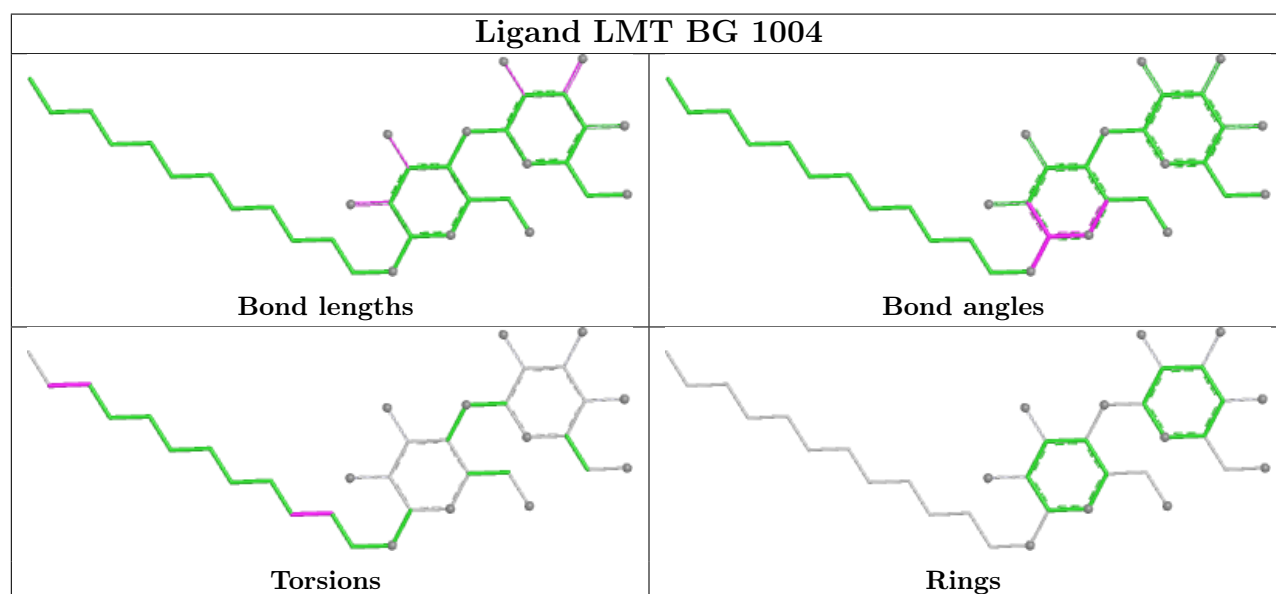
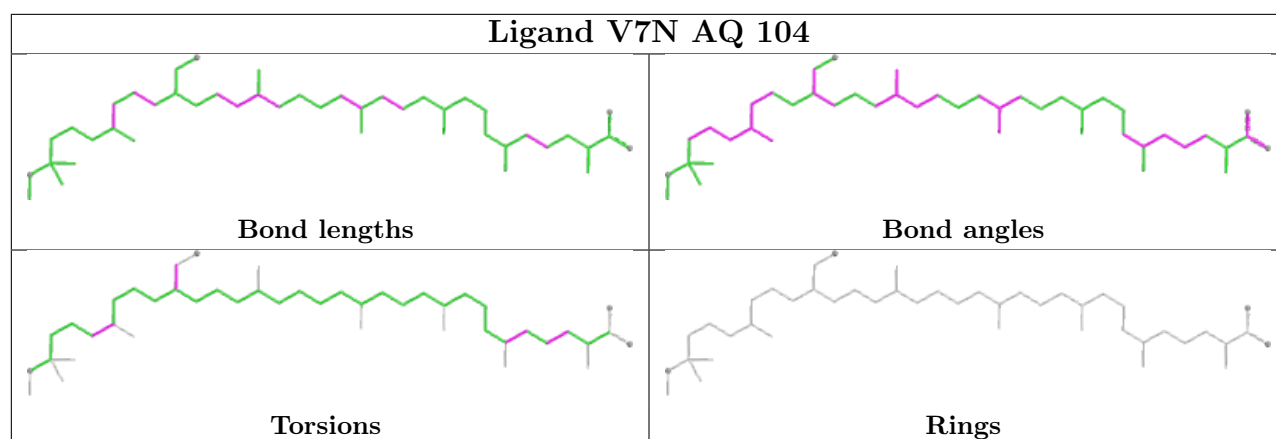


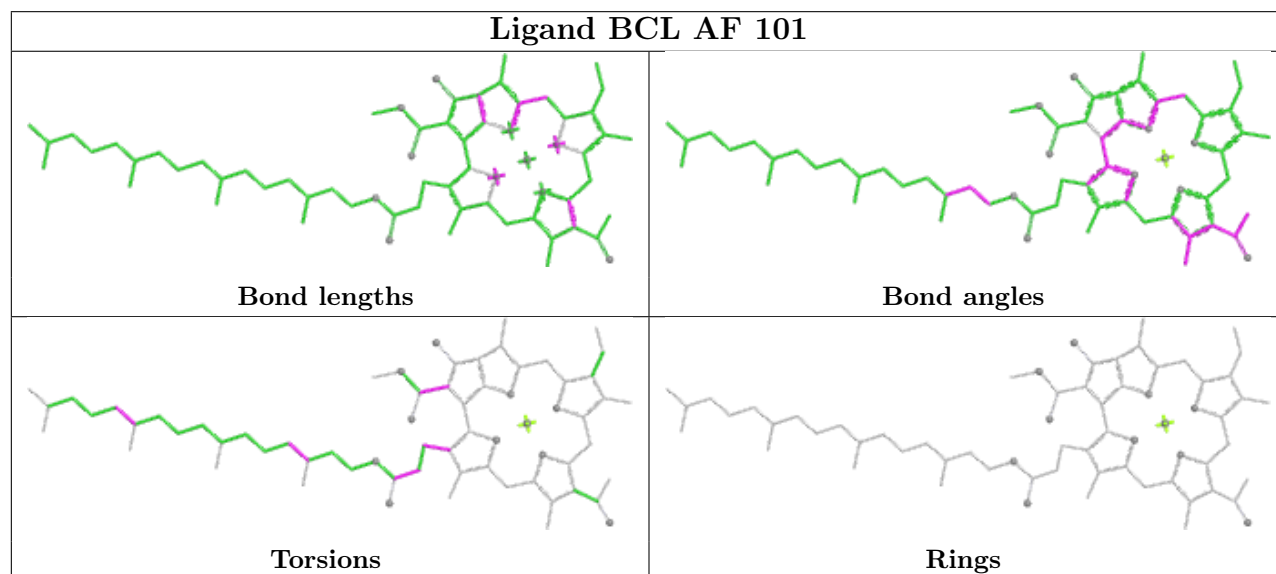
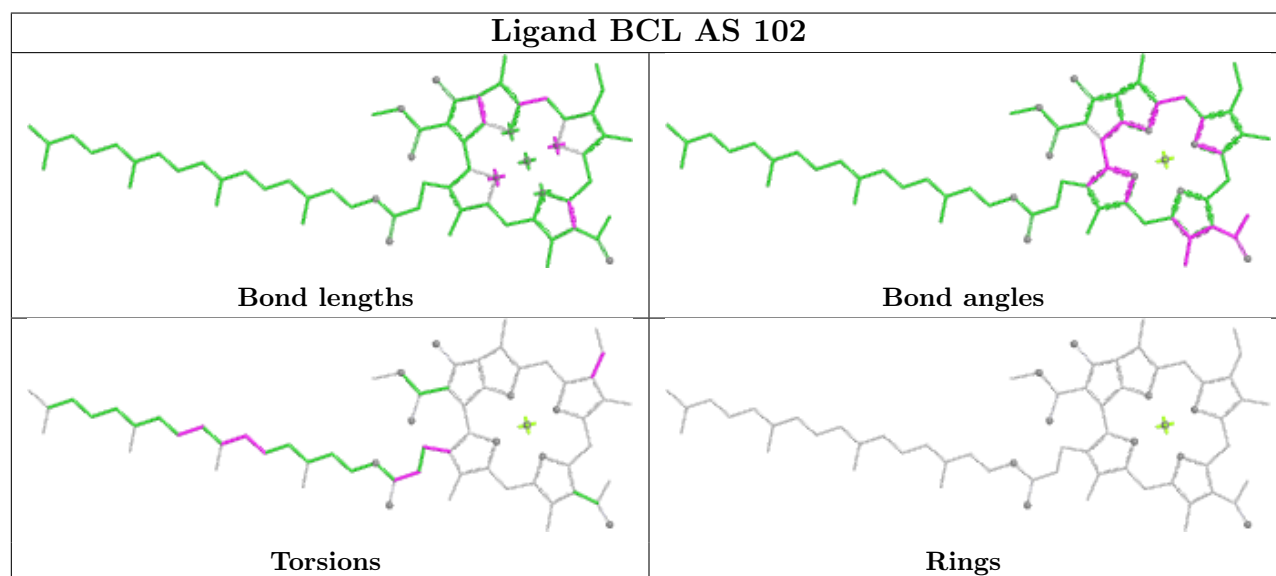
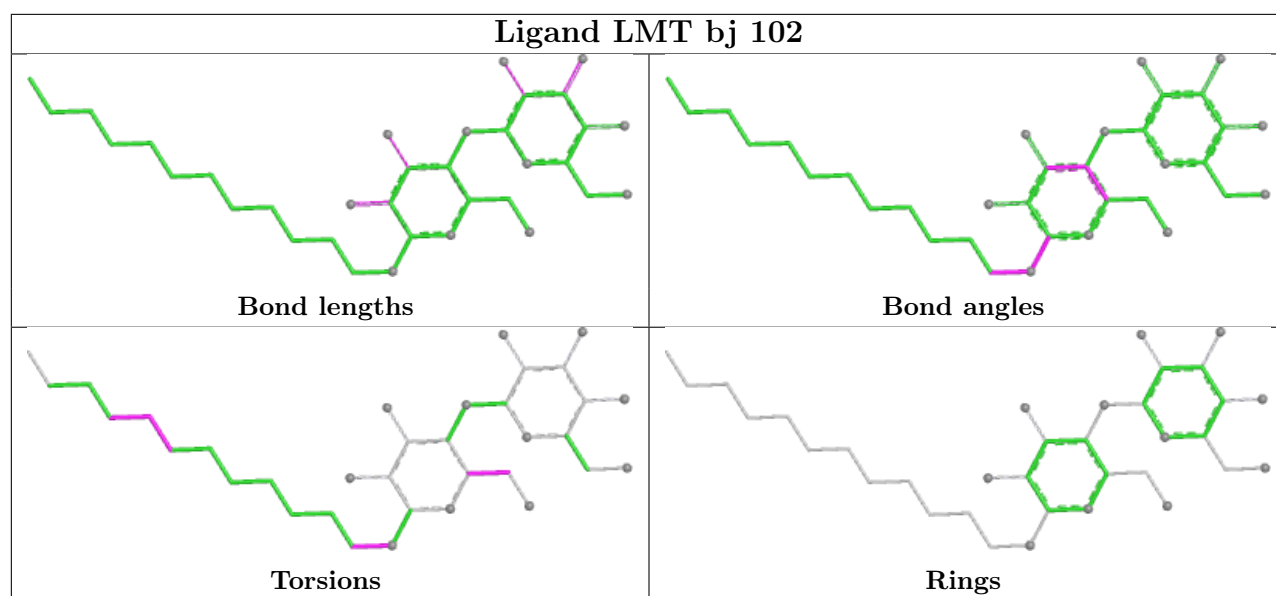


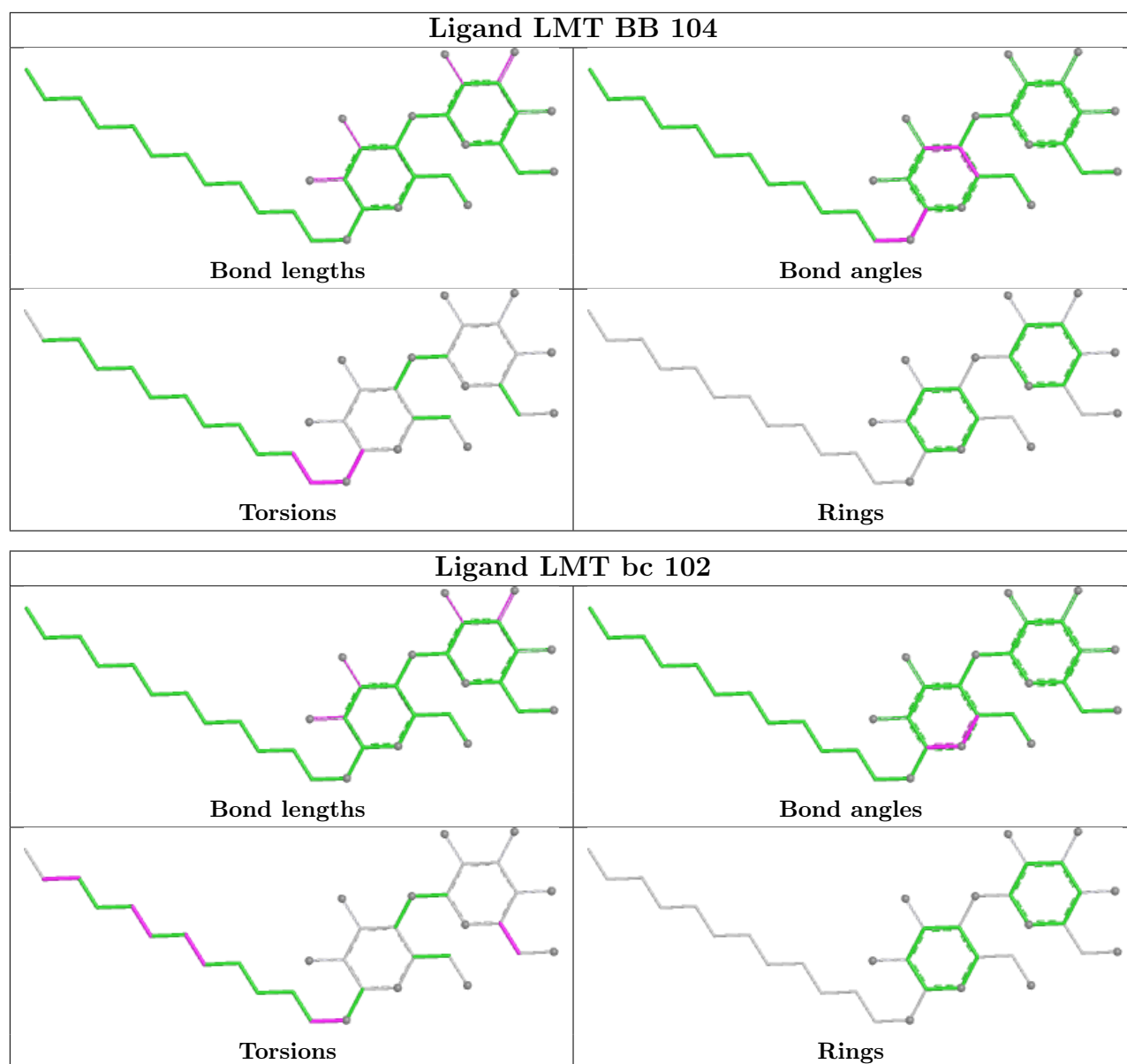


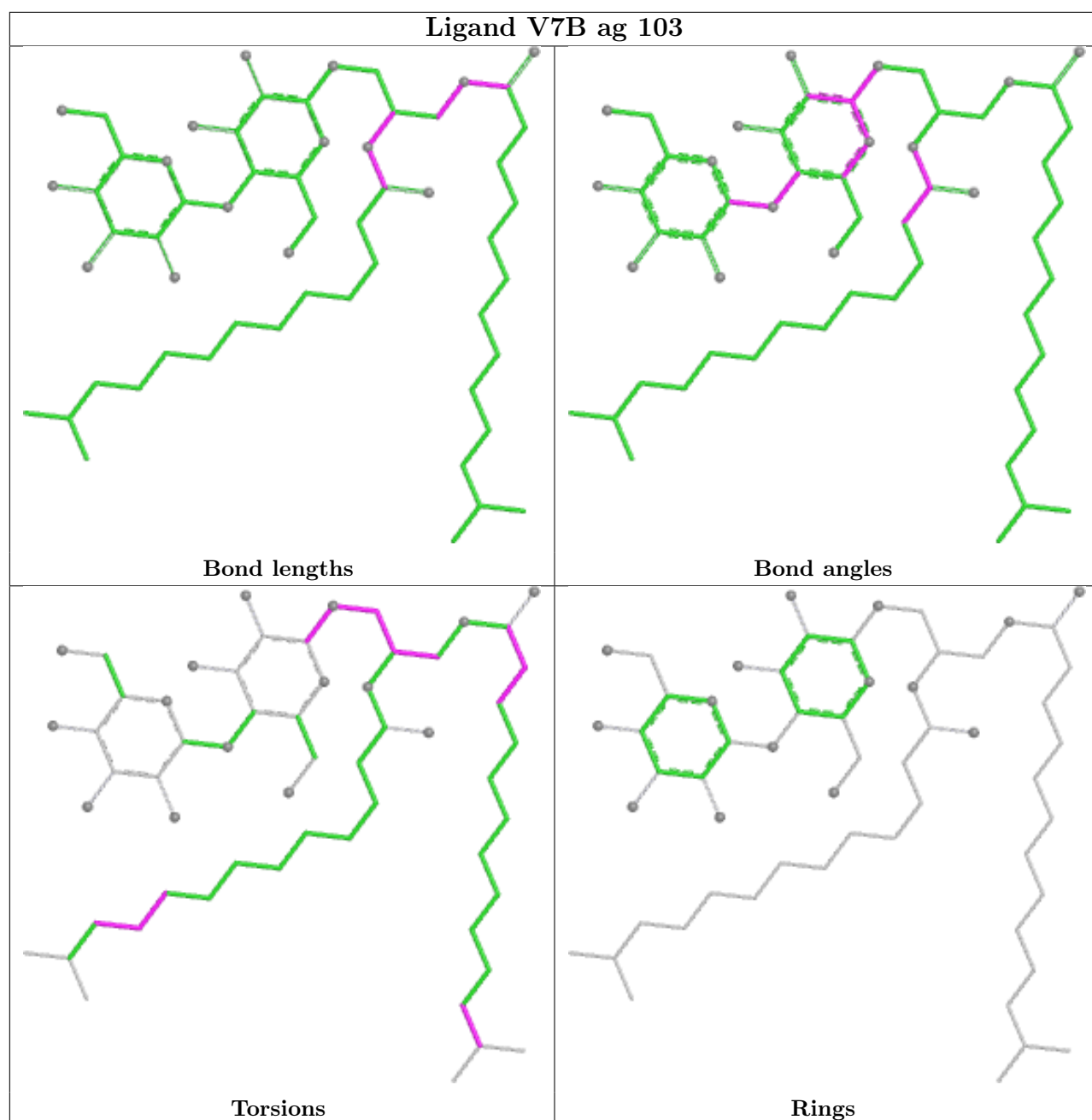


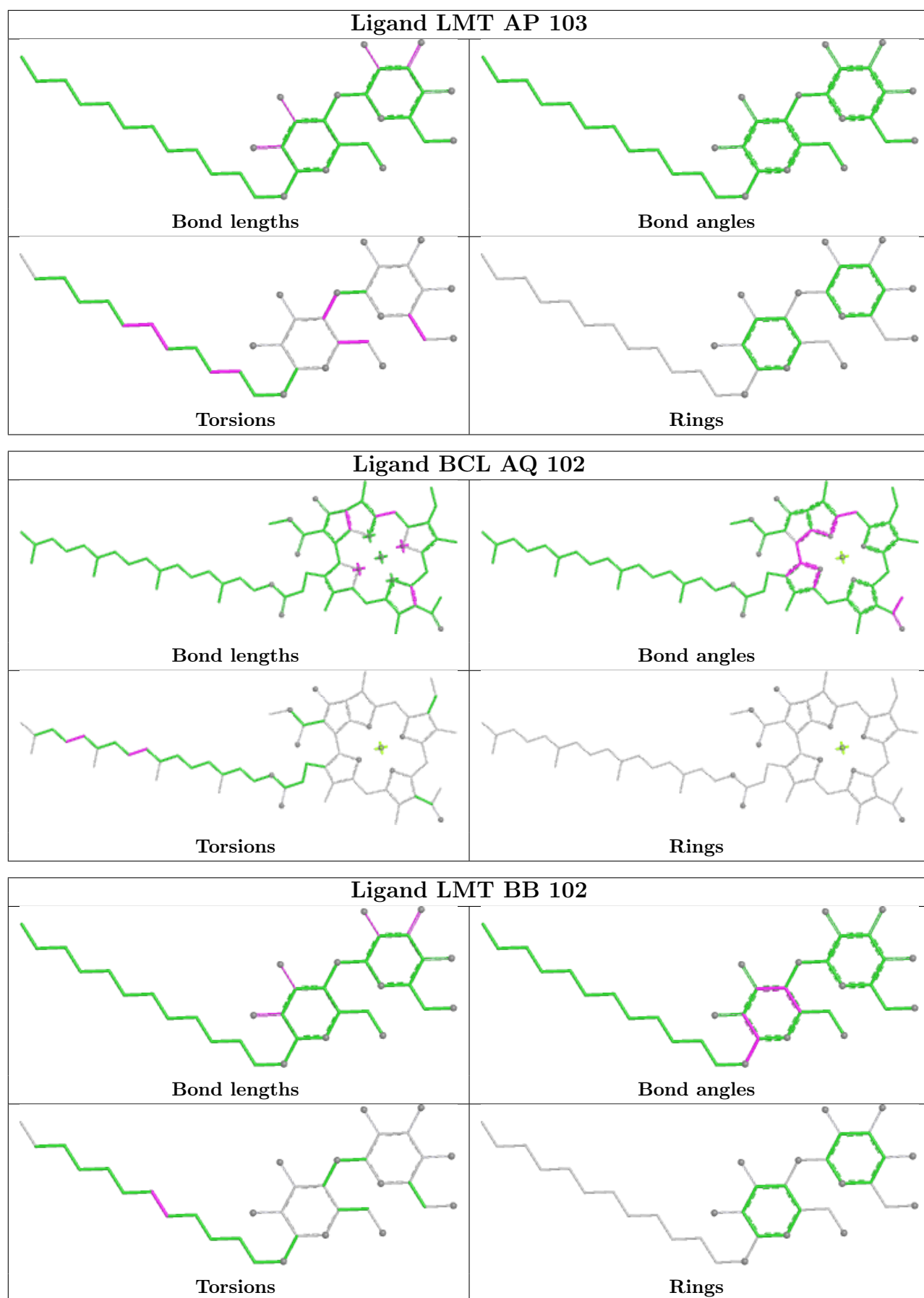


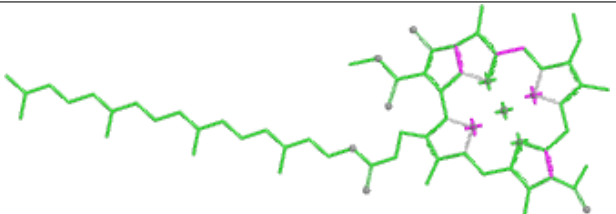
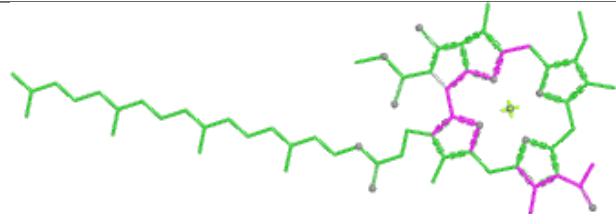
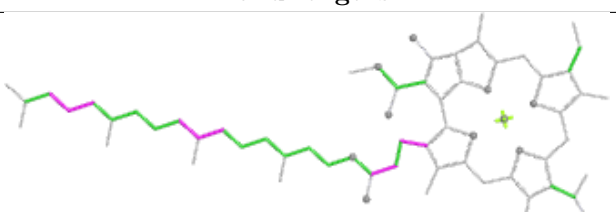
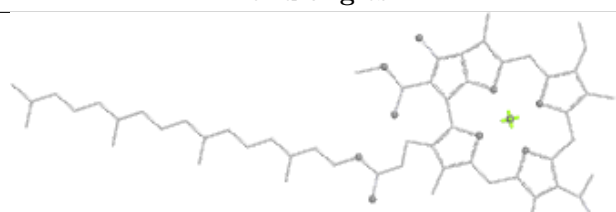


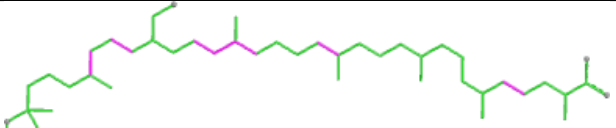
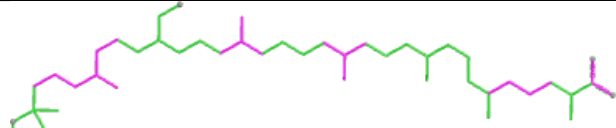
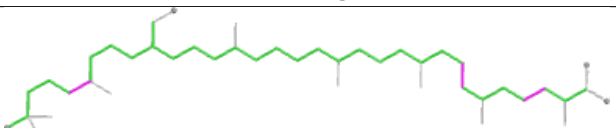
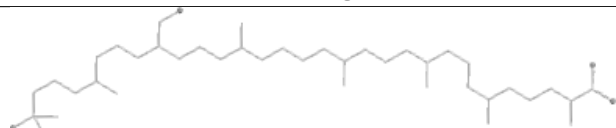


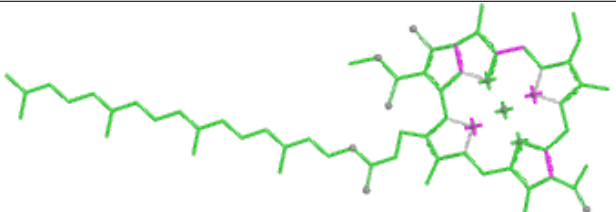
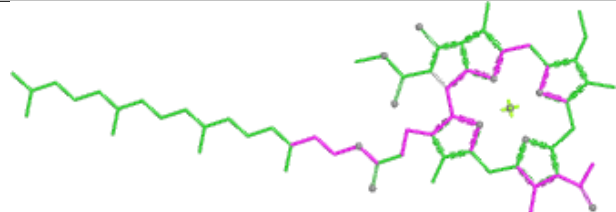
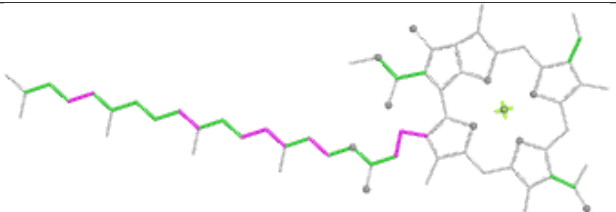
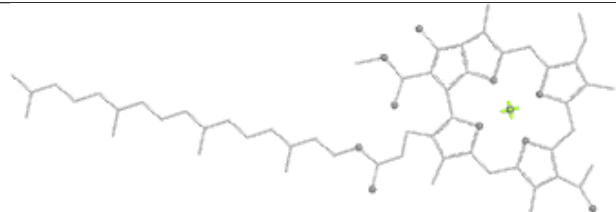


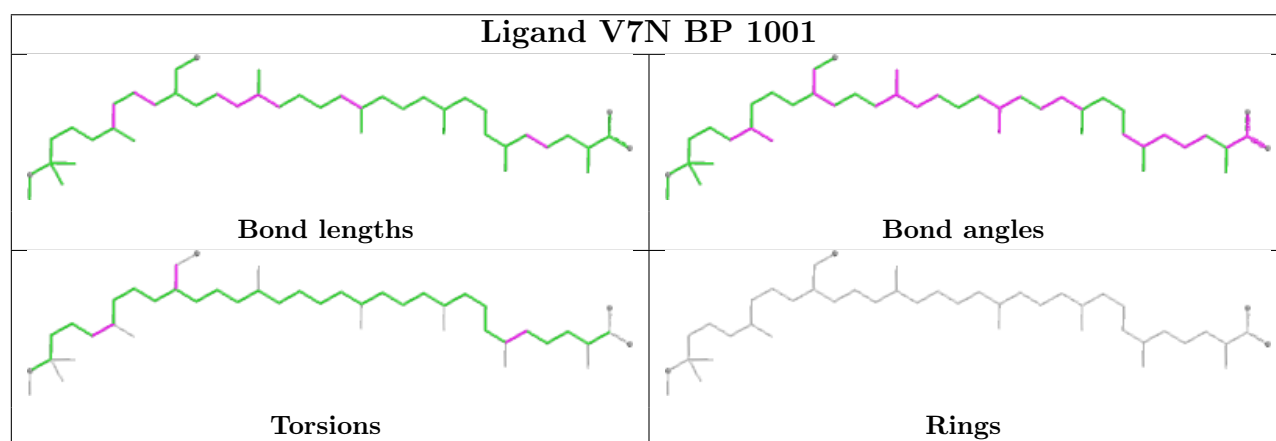
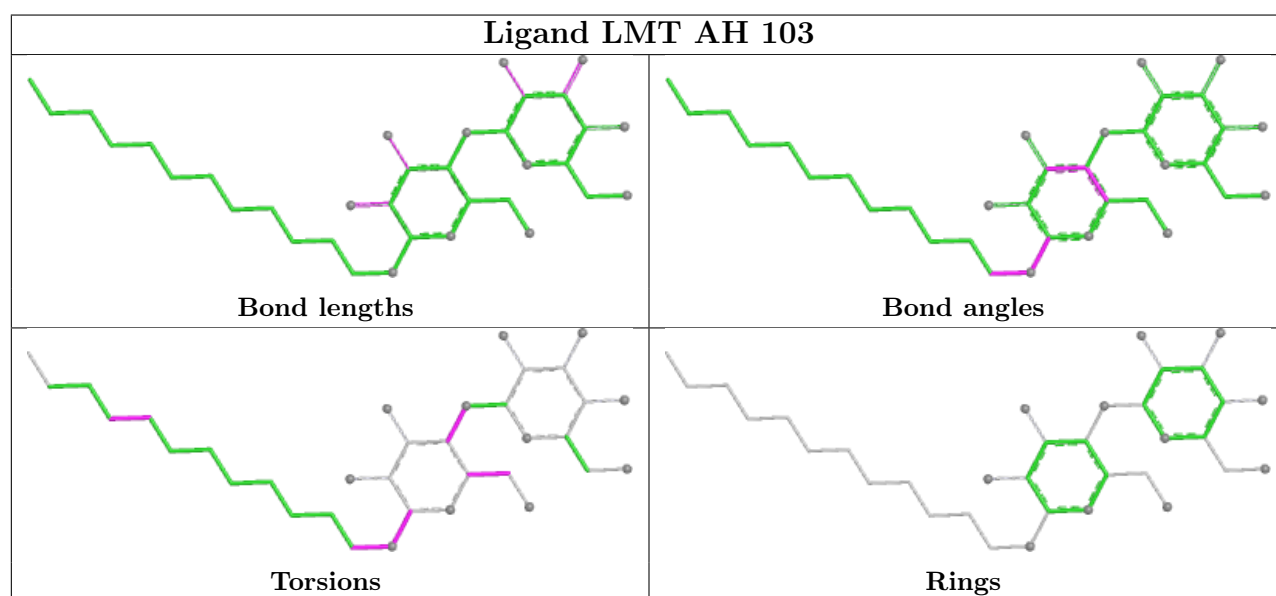
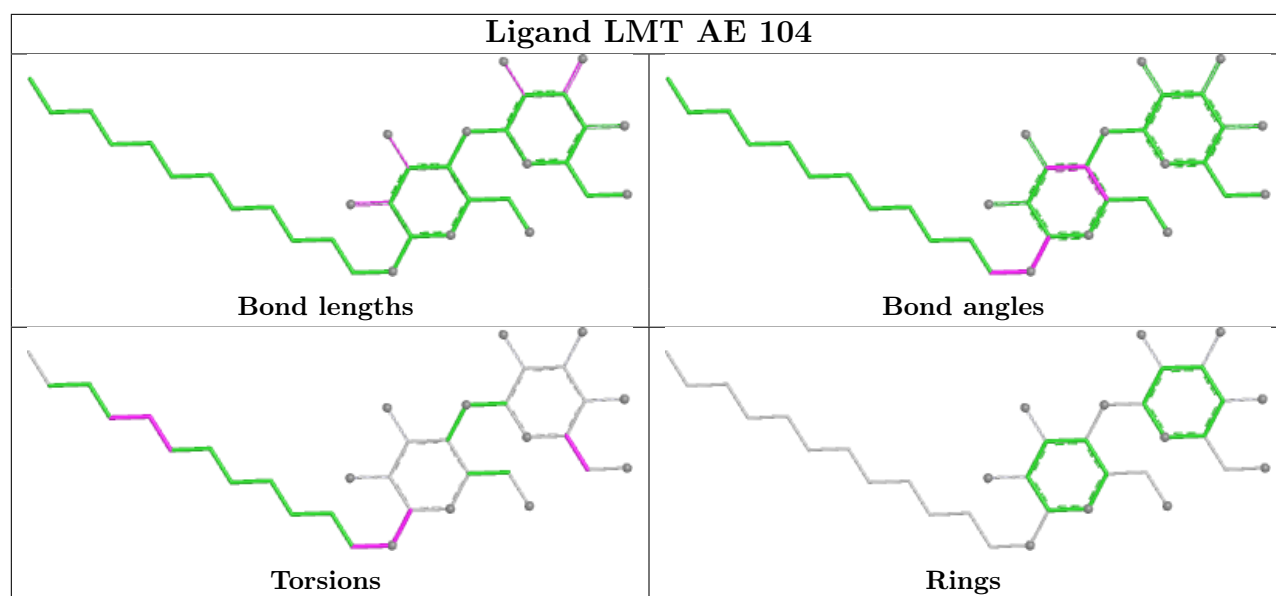


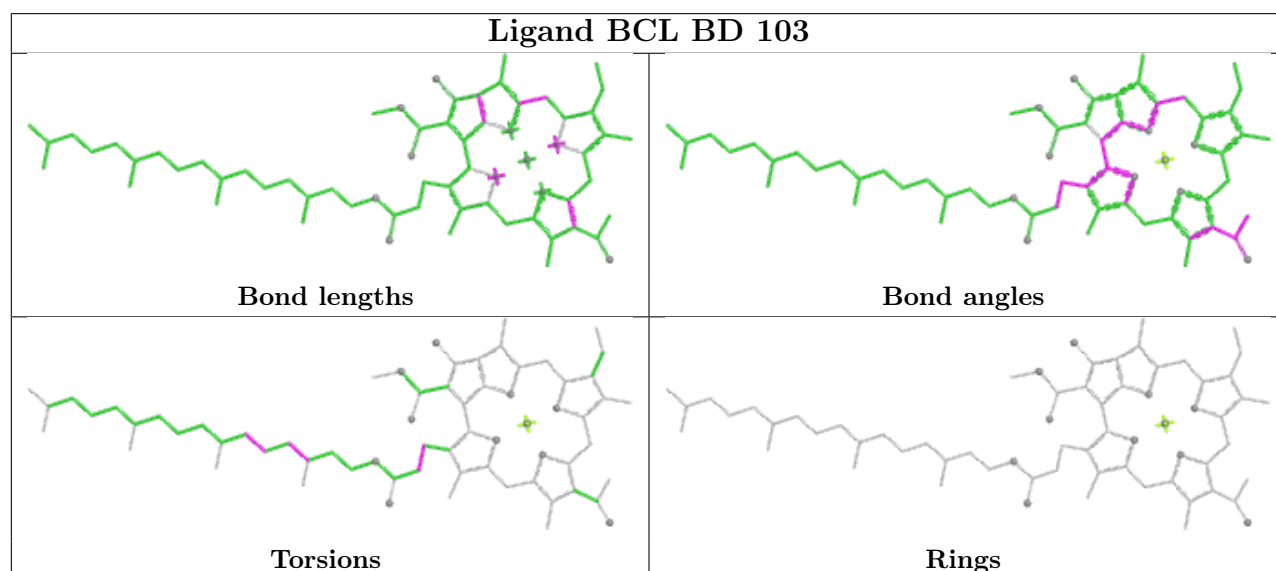
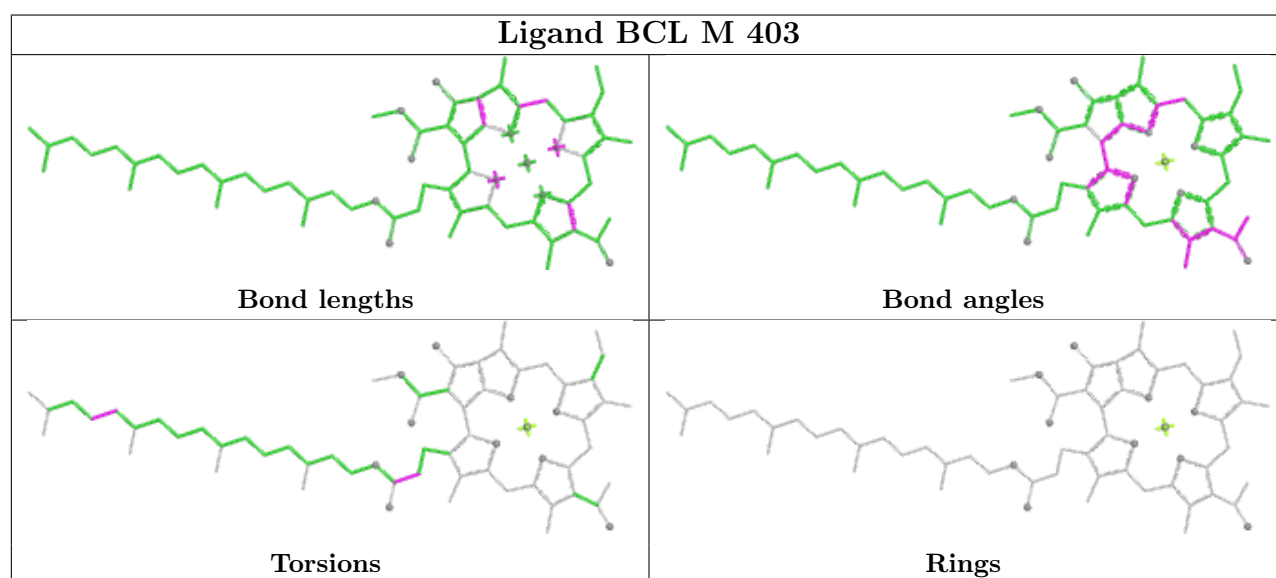
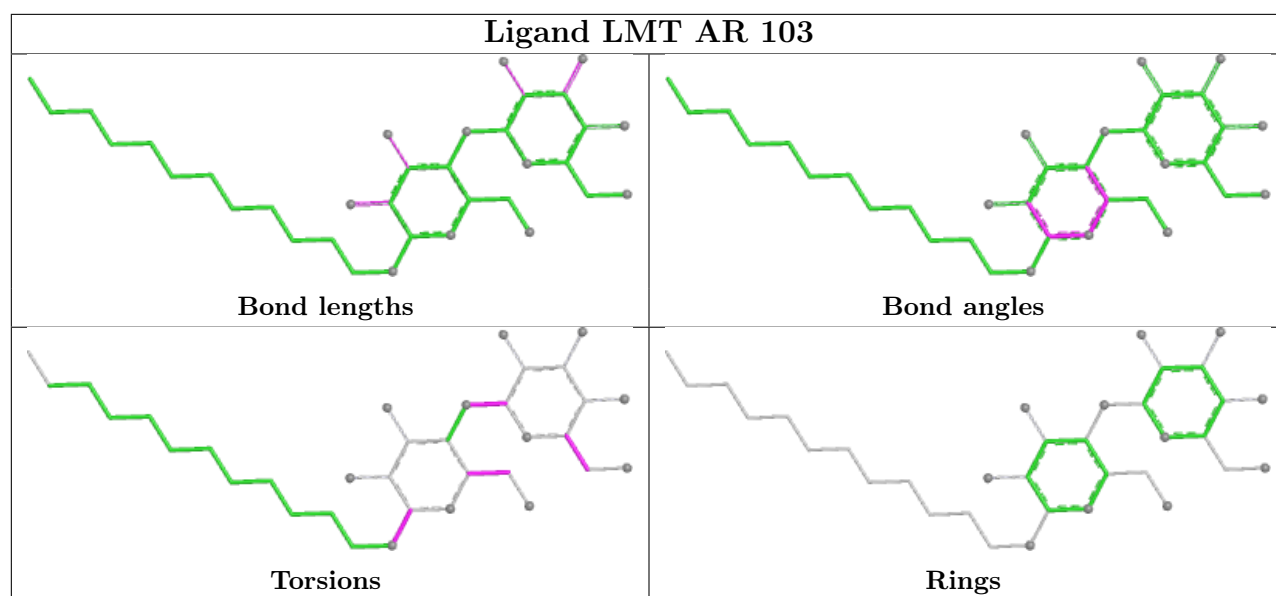


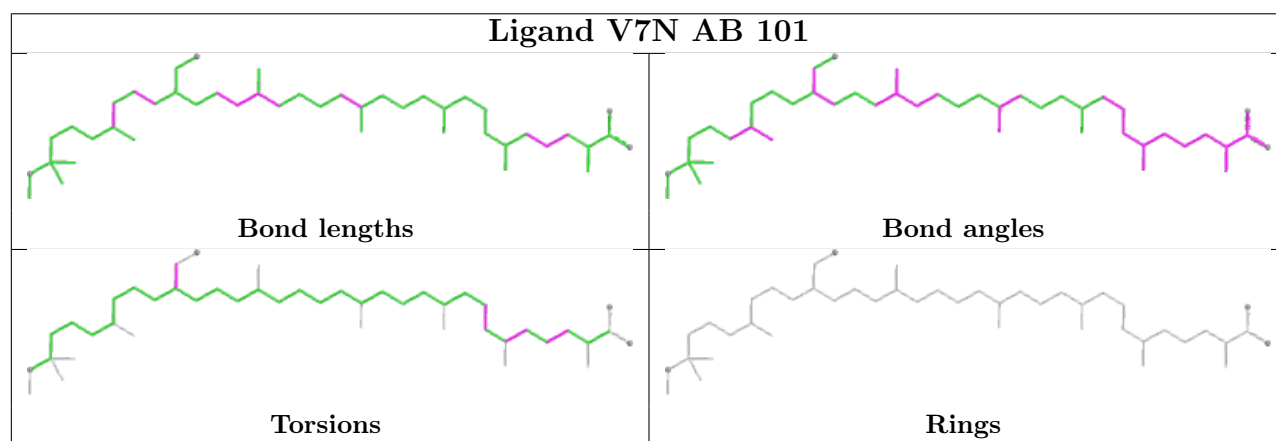
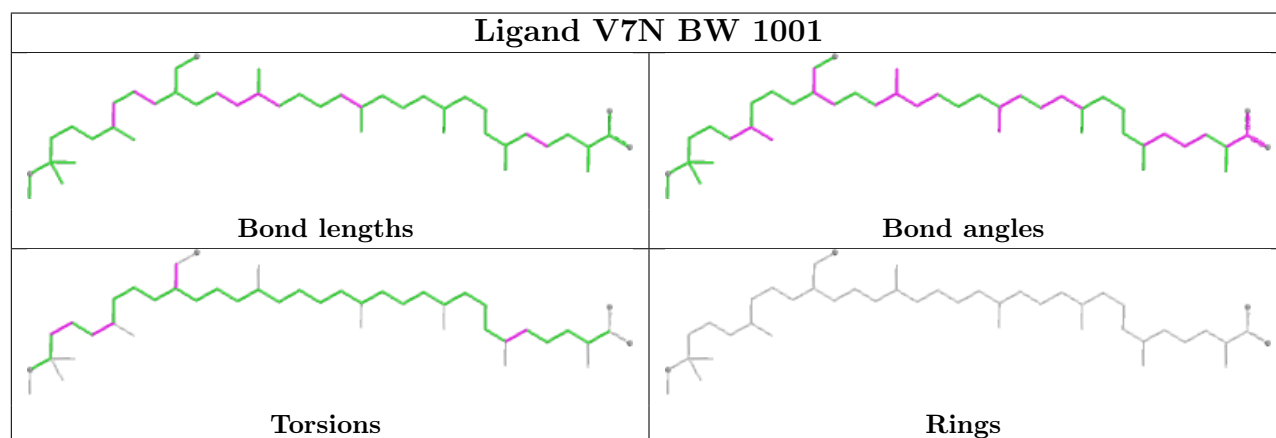
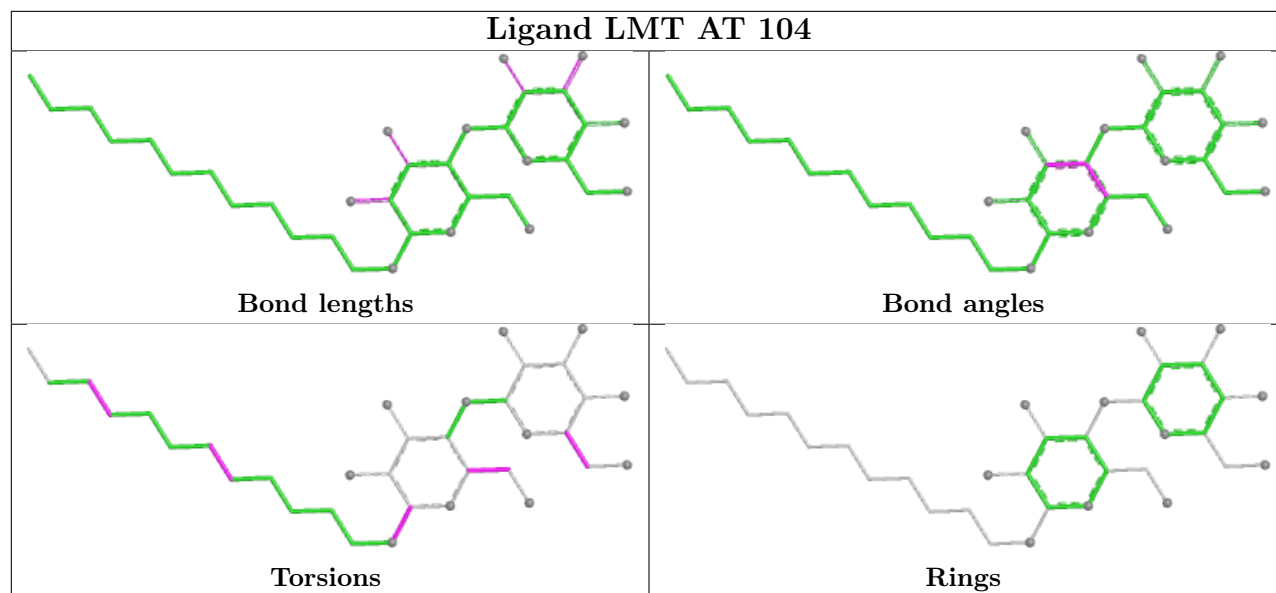
Ligand BCL ae 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

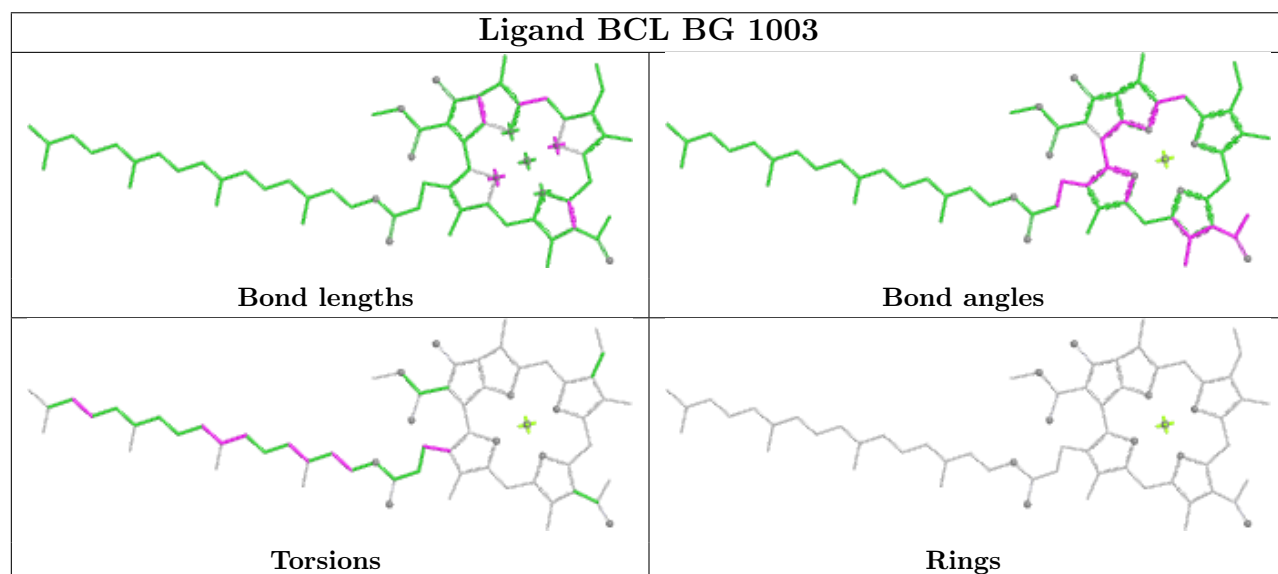
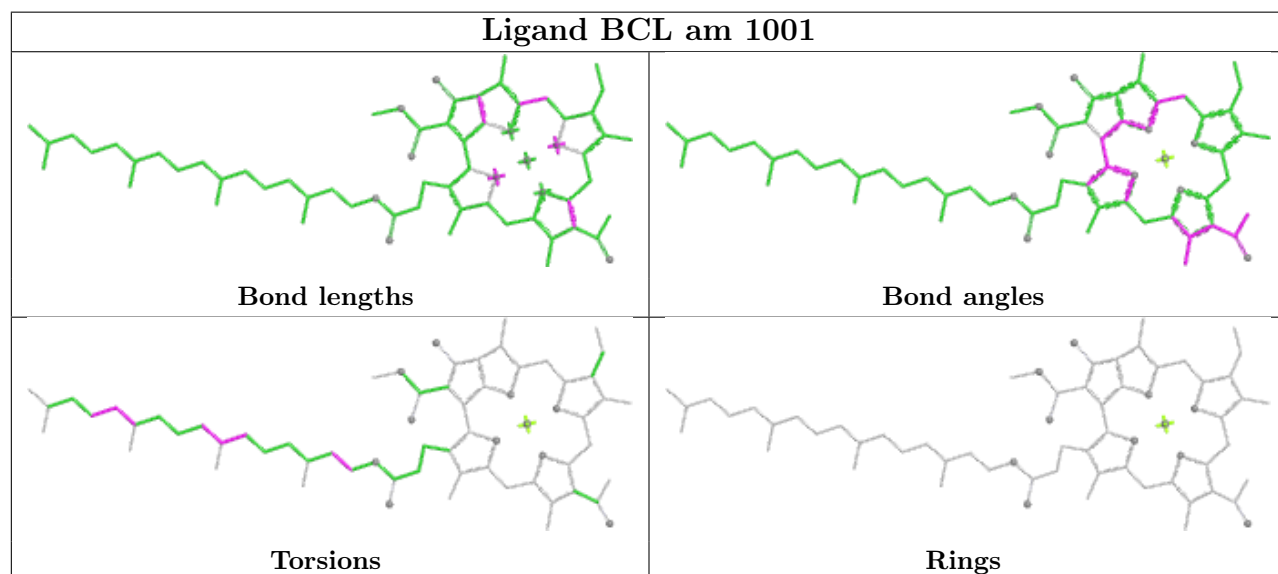
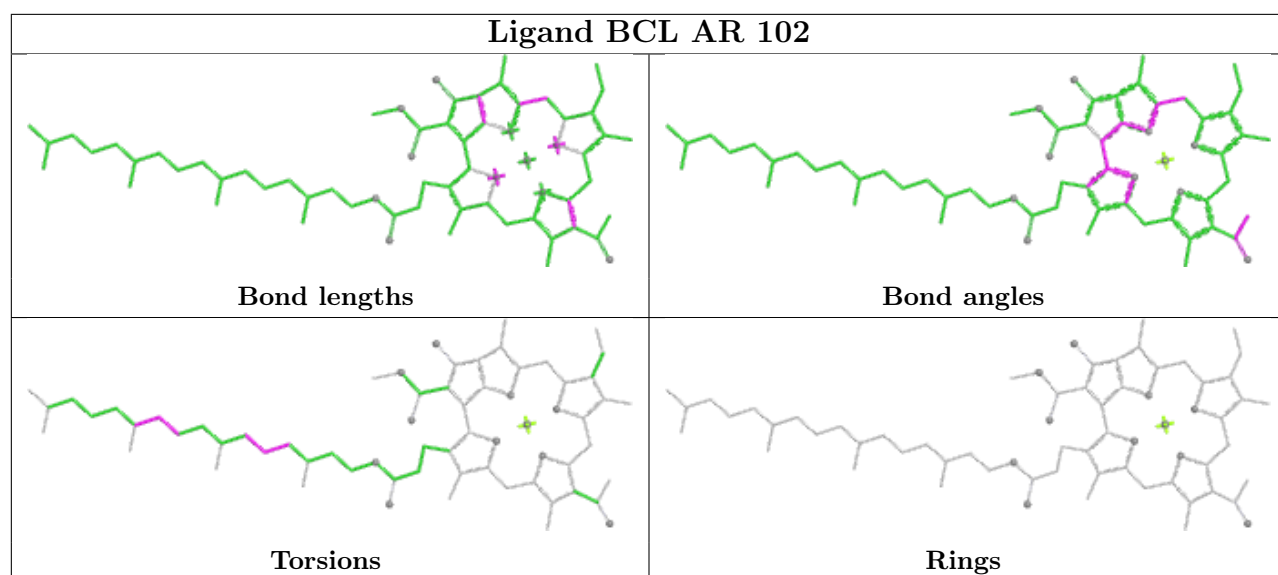
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Bond lengths	Bond angles
	
Torsions	Rings

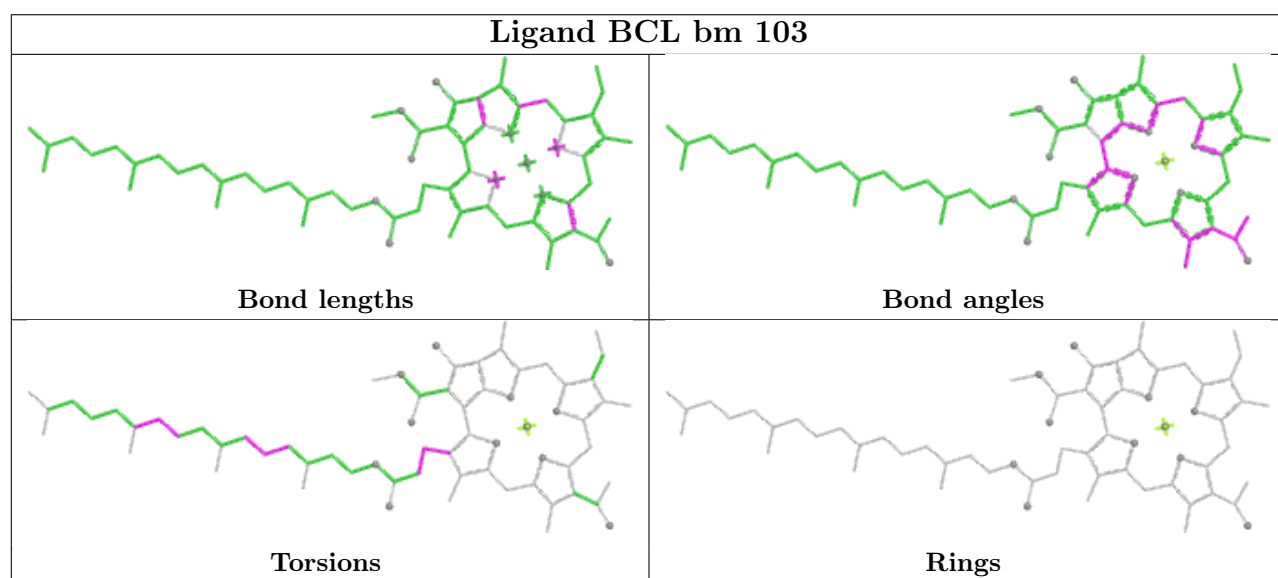
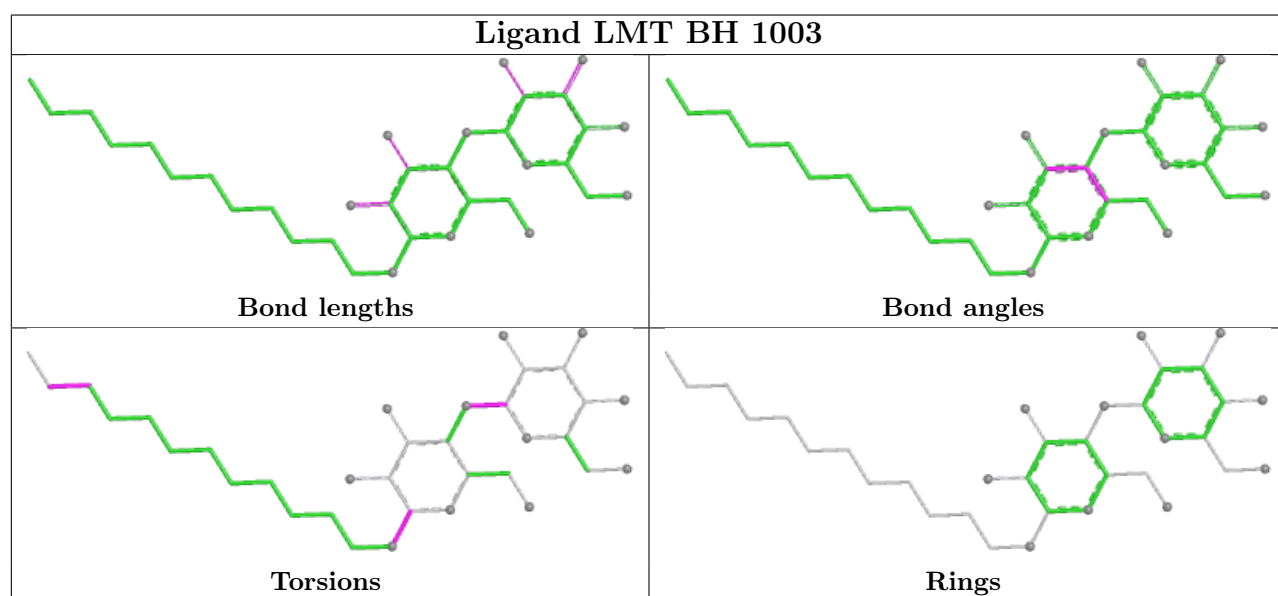
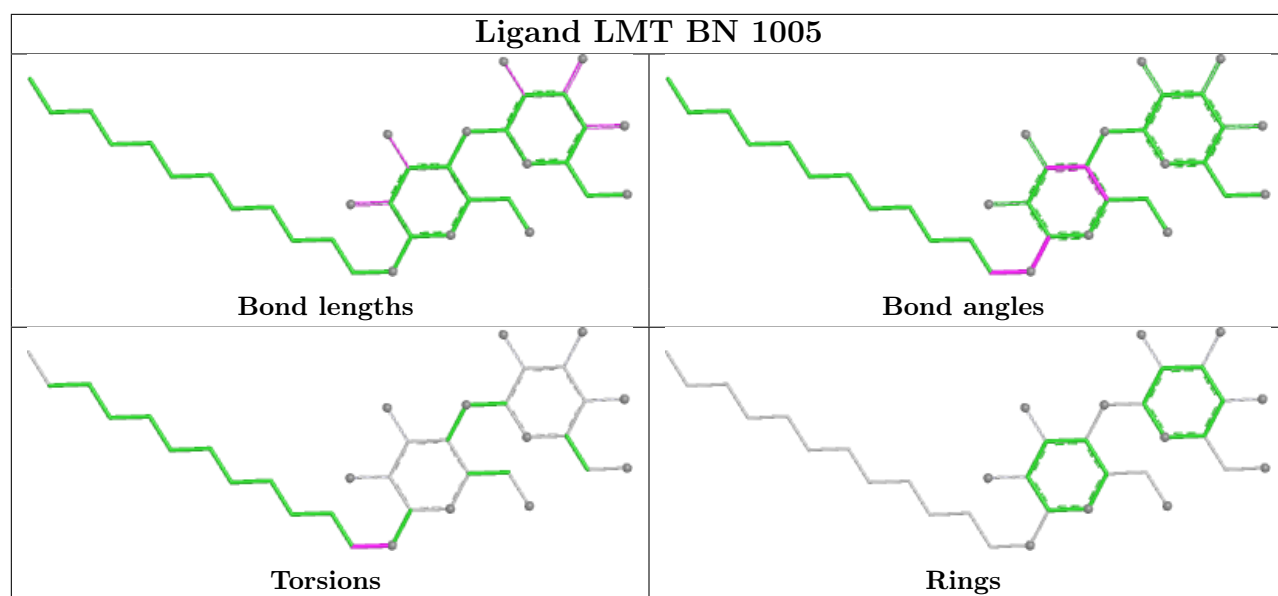
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Bond lengths	Bond angles
	
Torsions	Rings

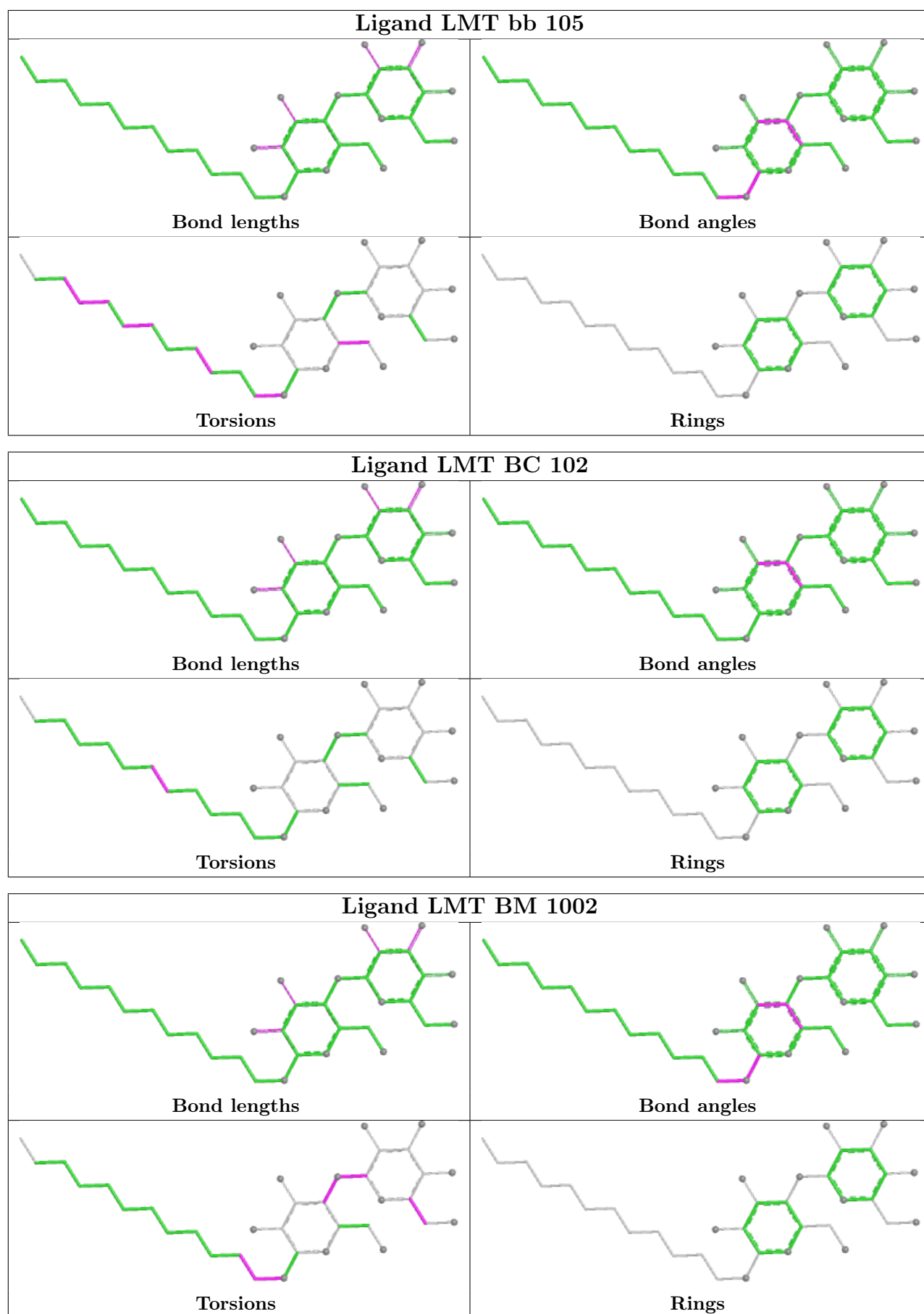


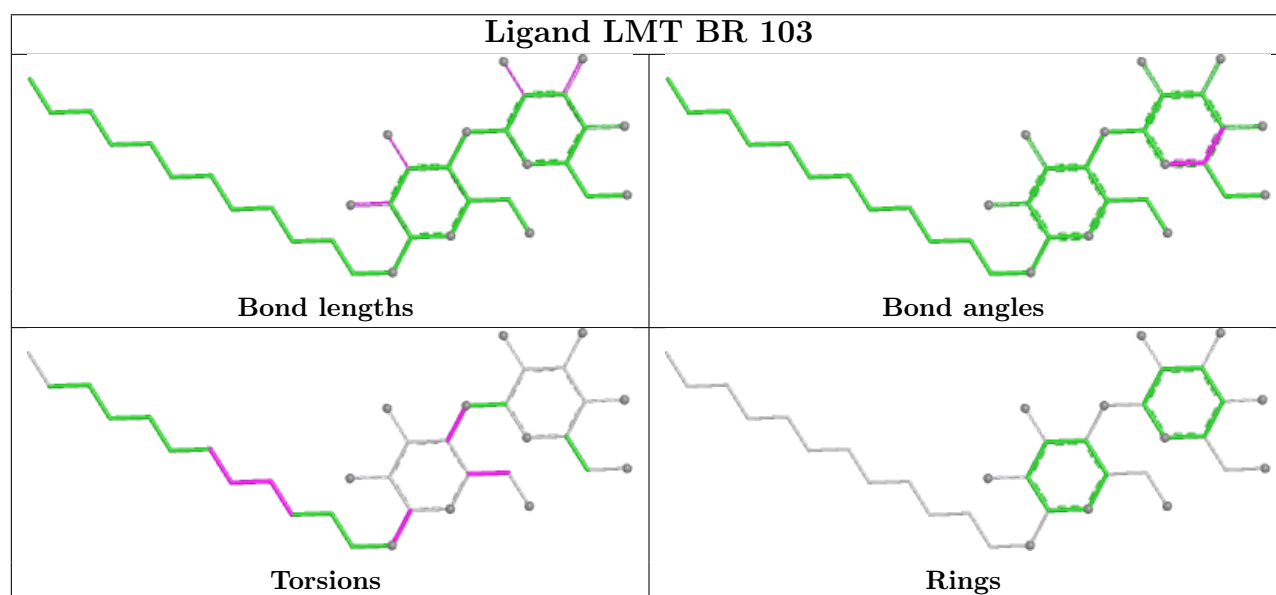
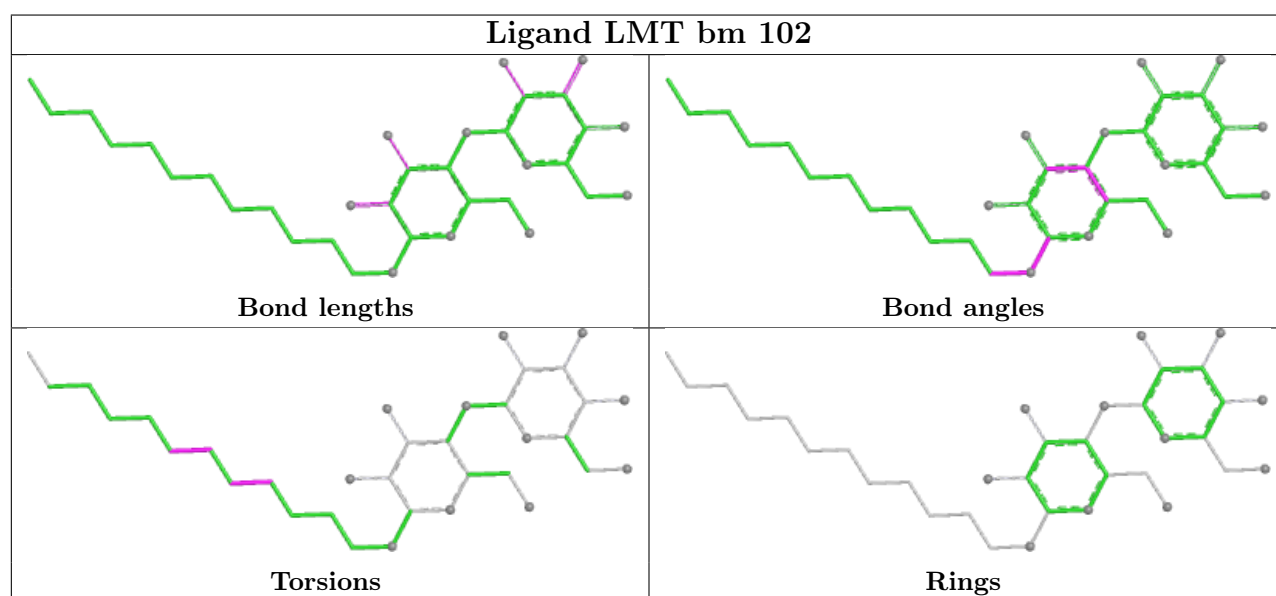
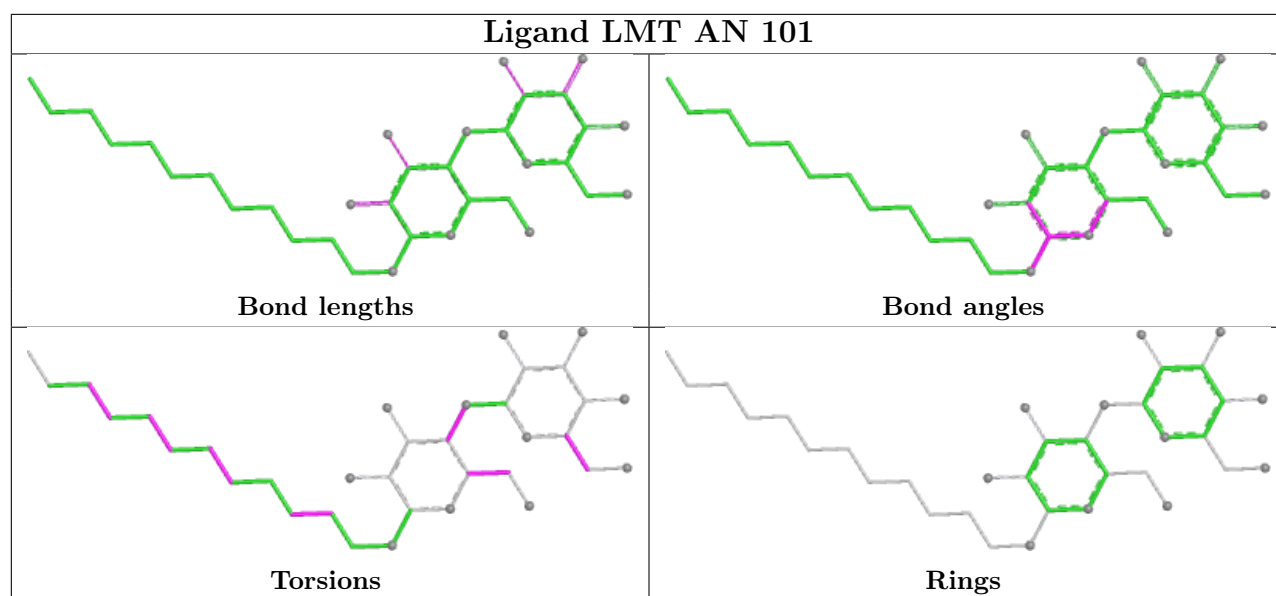


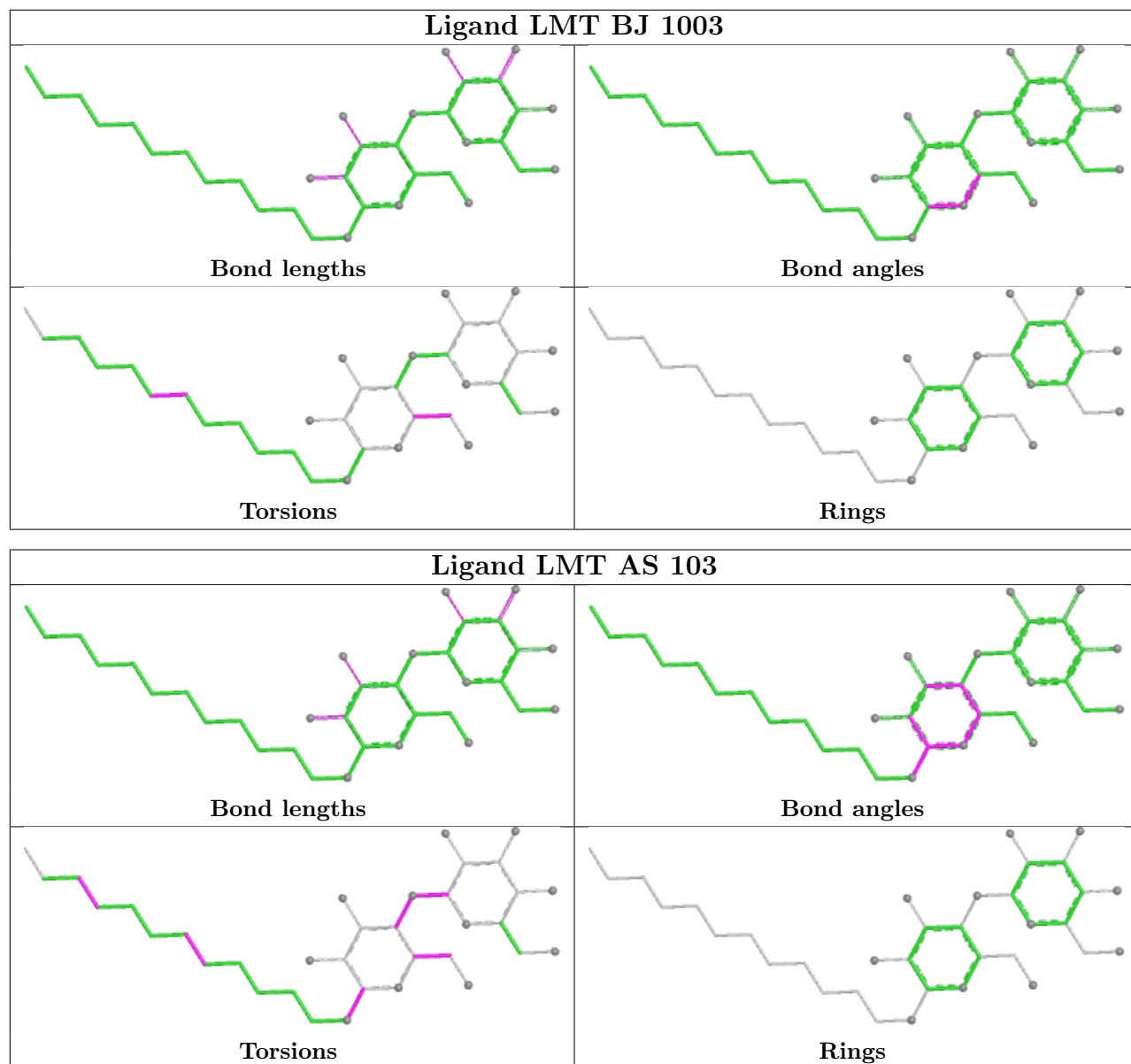


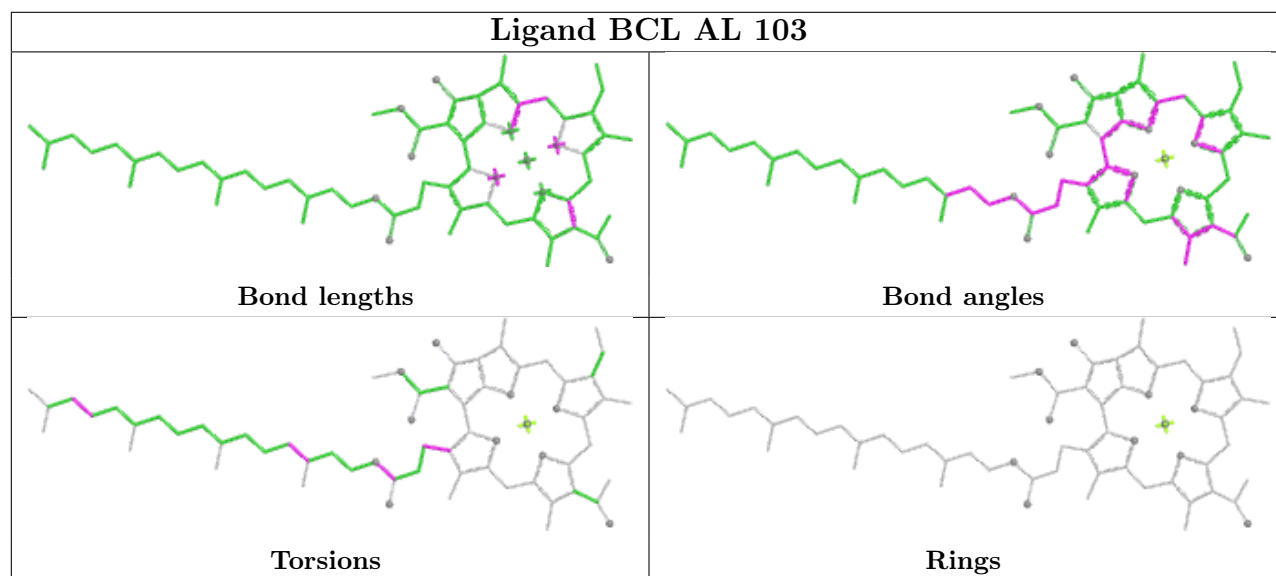
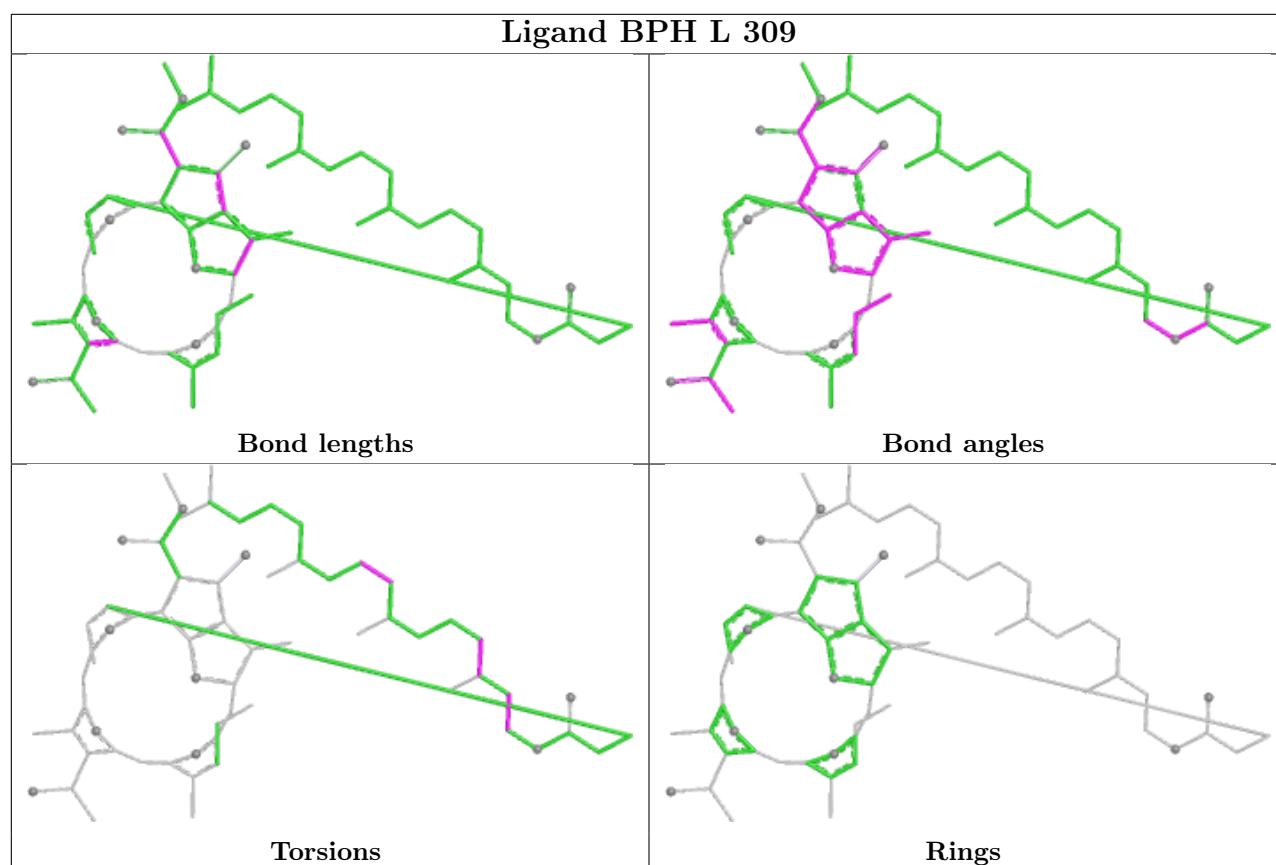


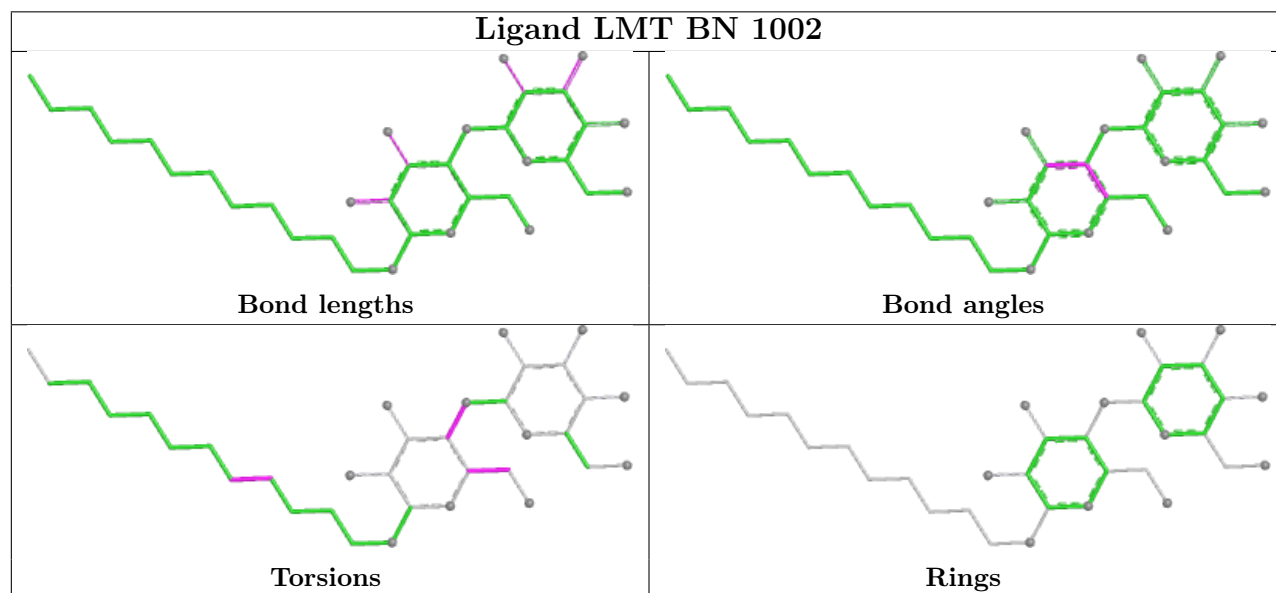
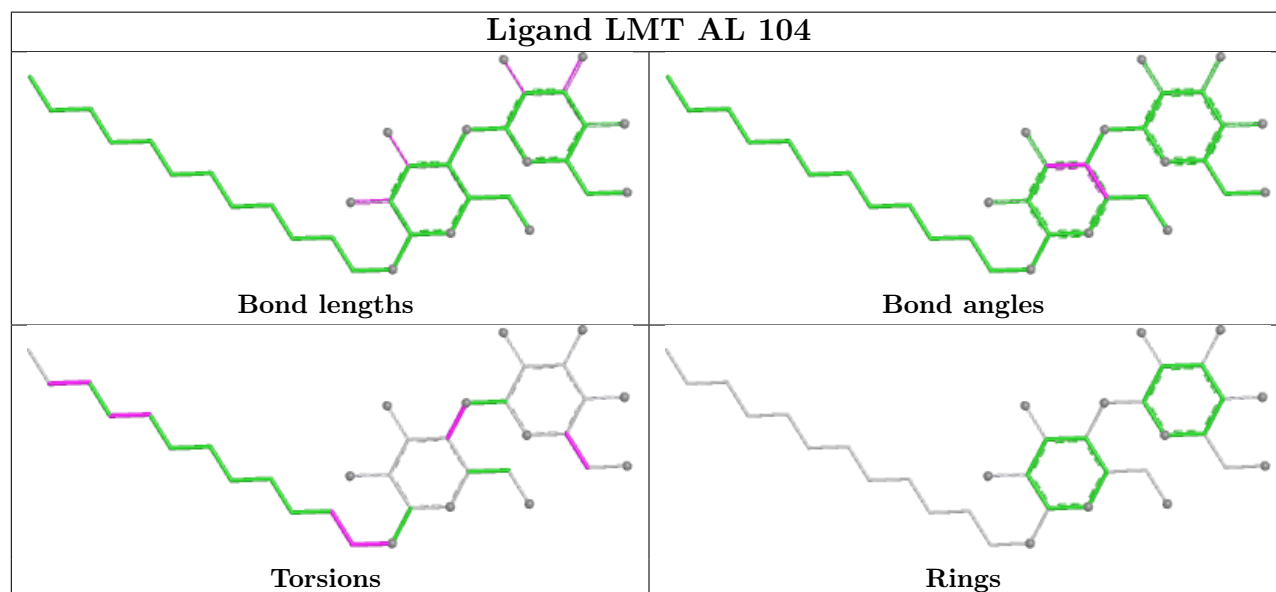
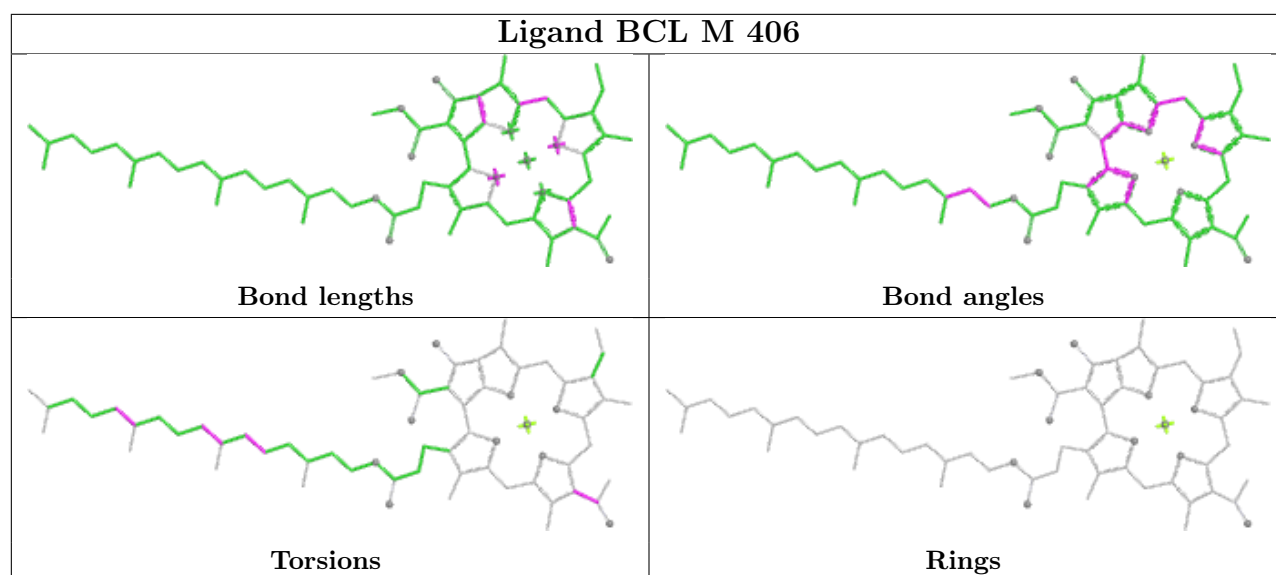


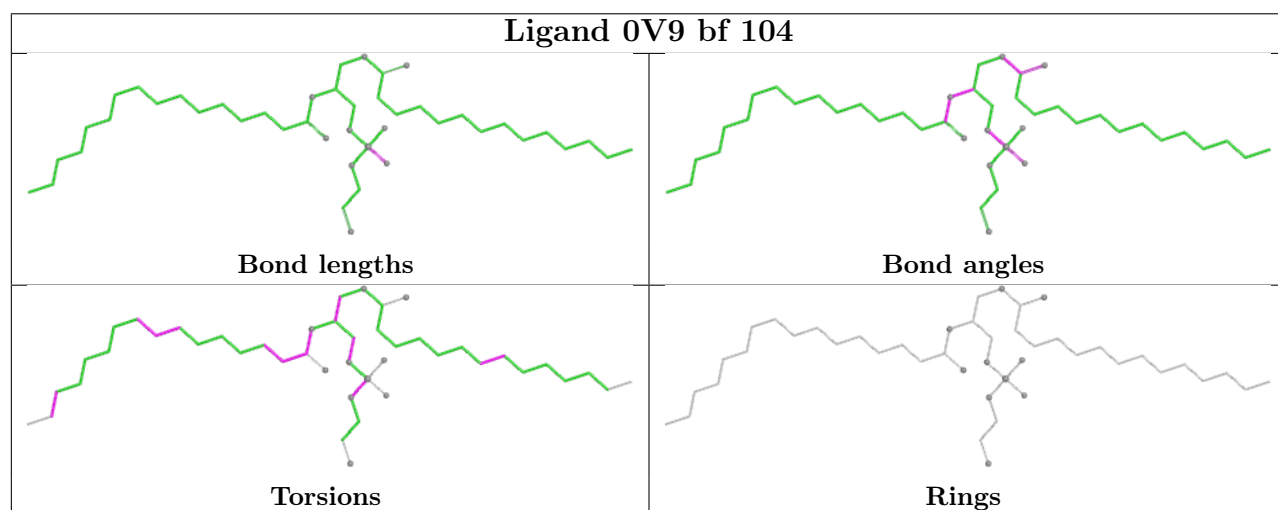
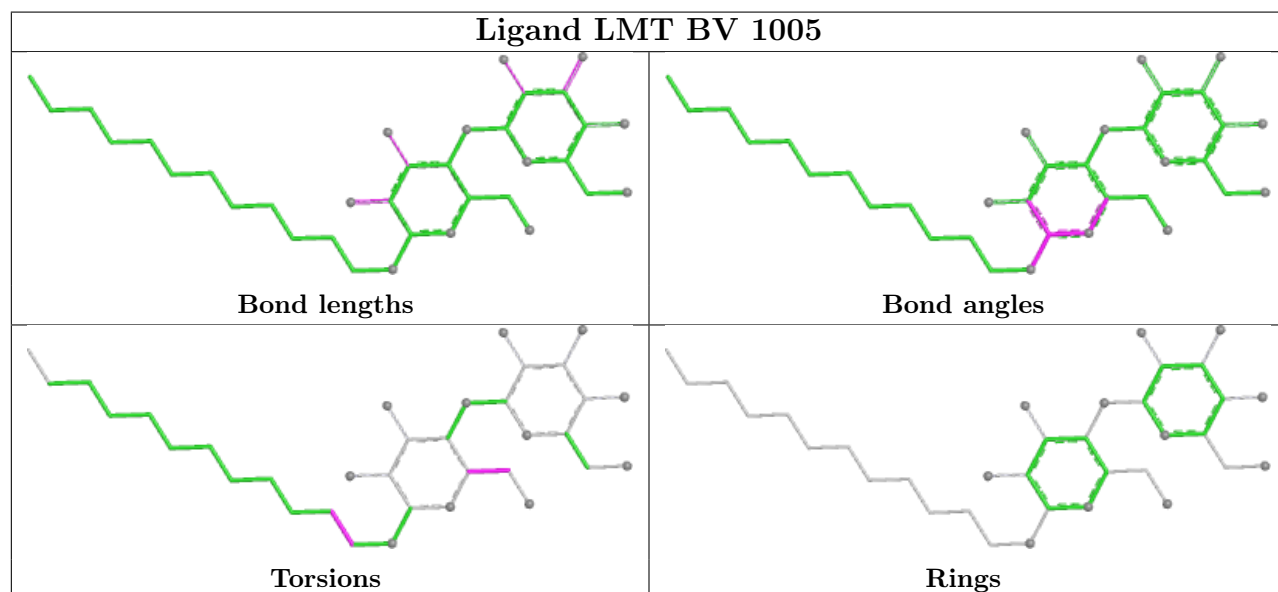
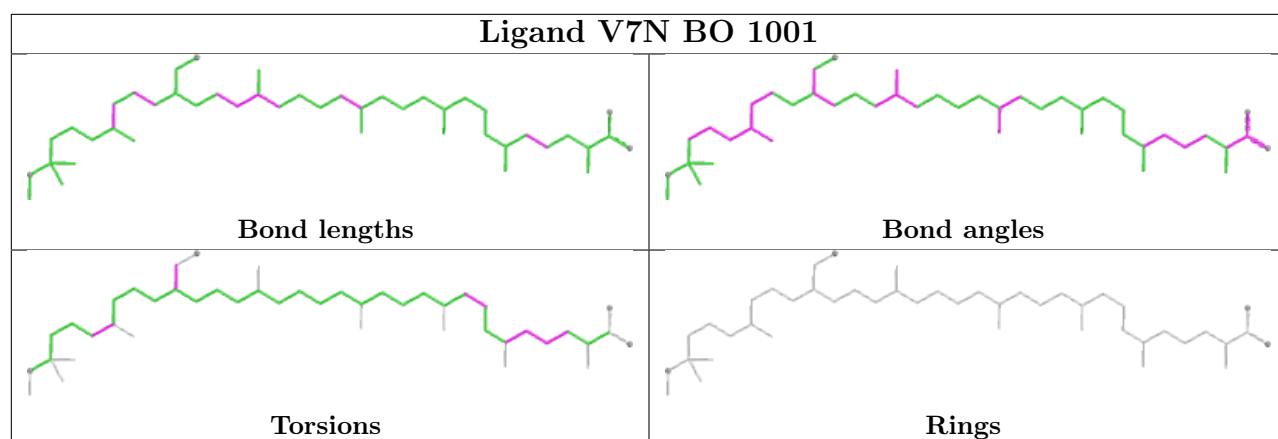


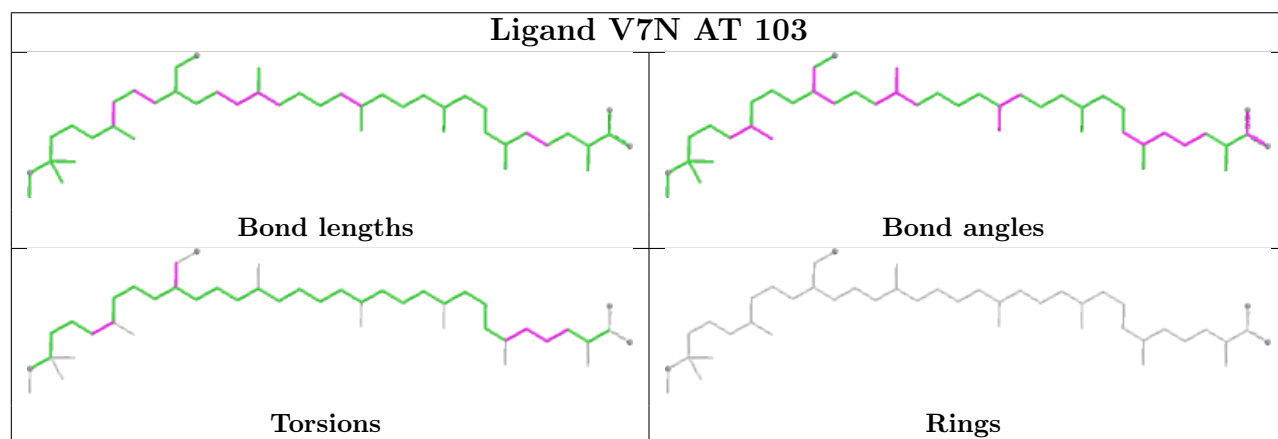
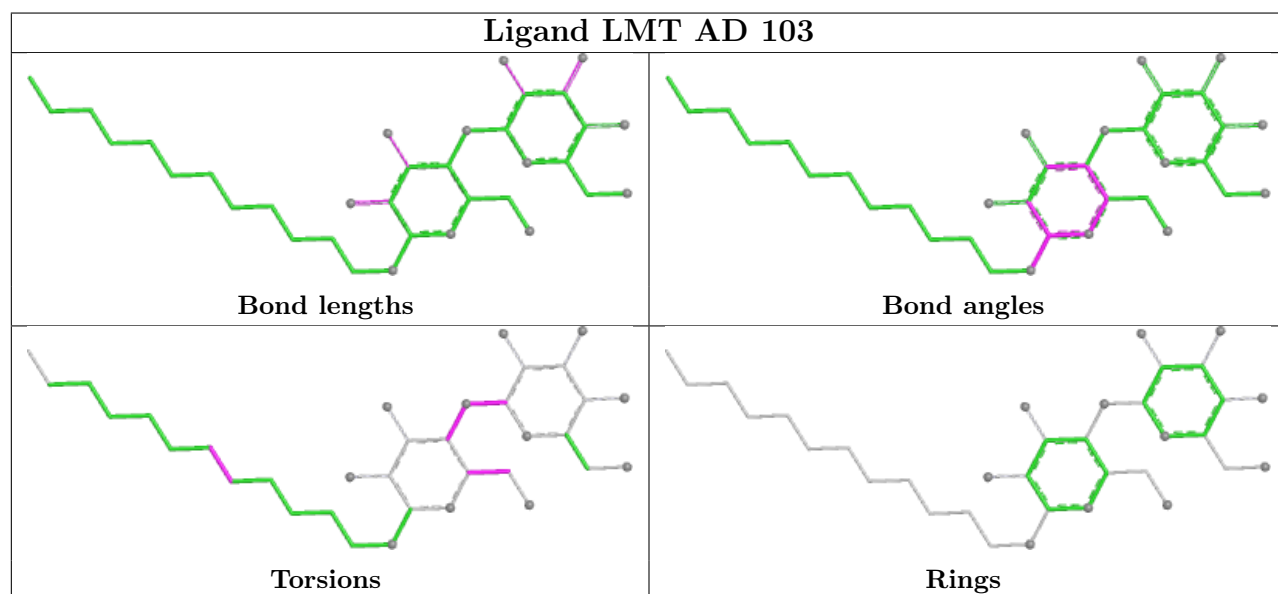
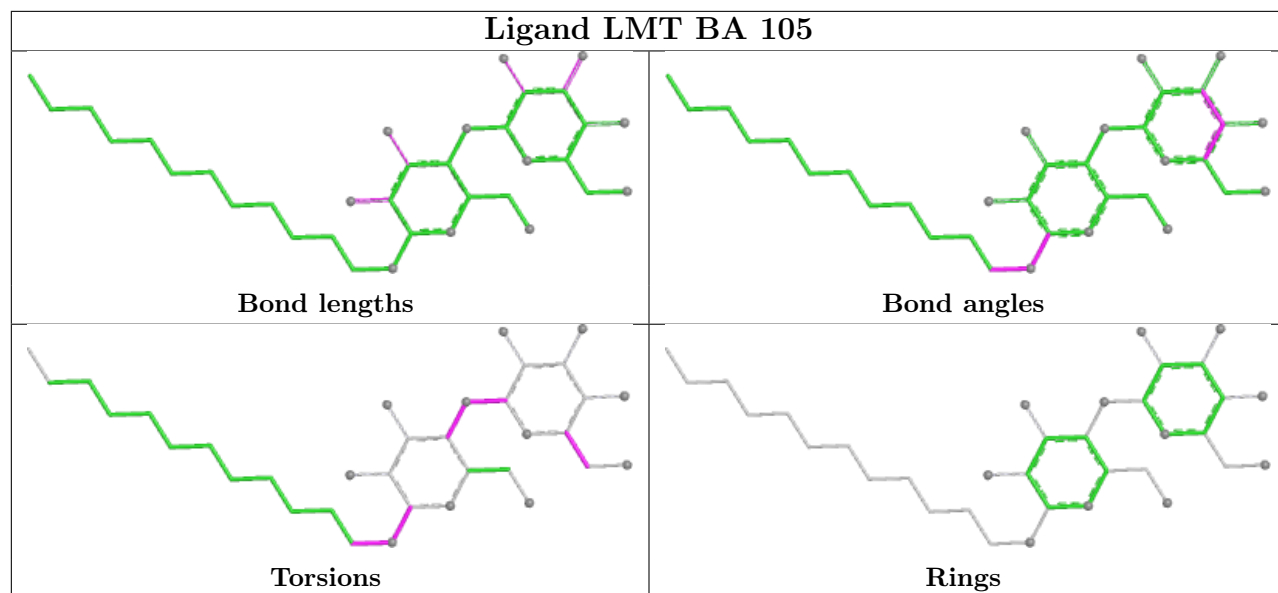


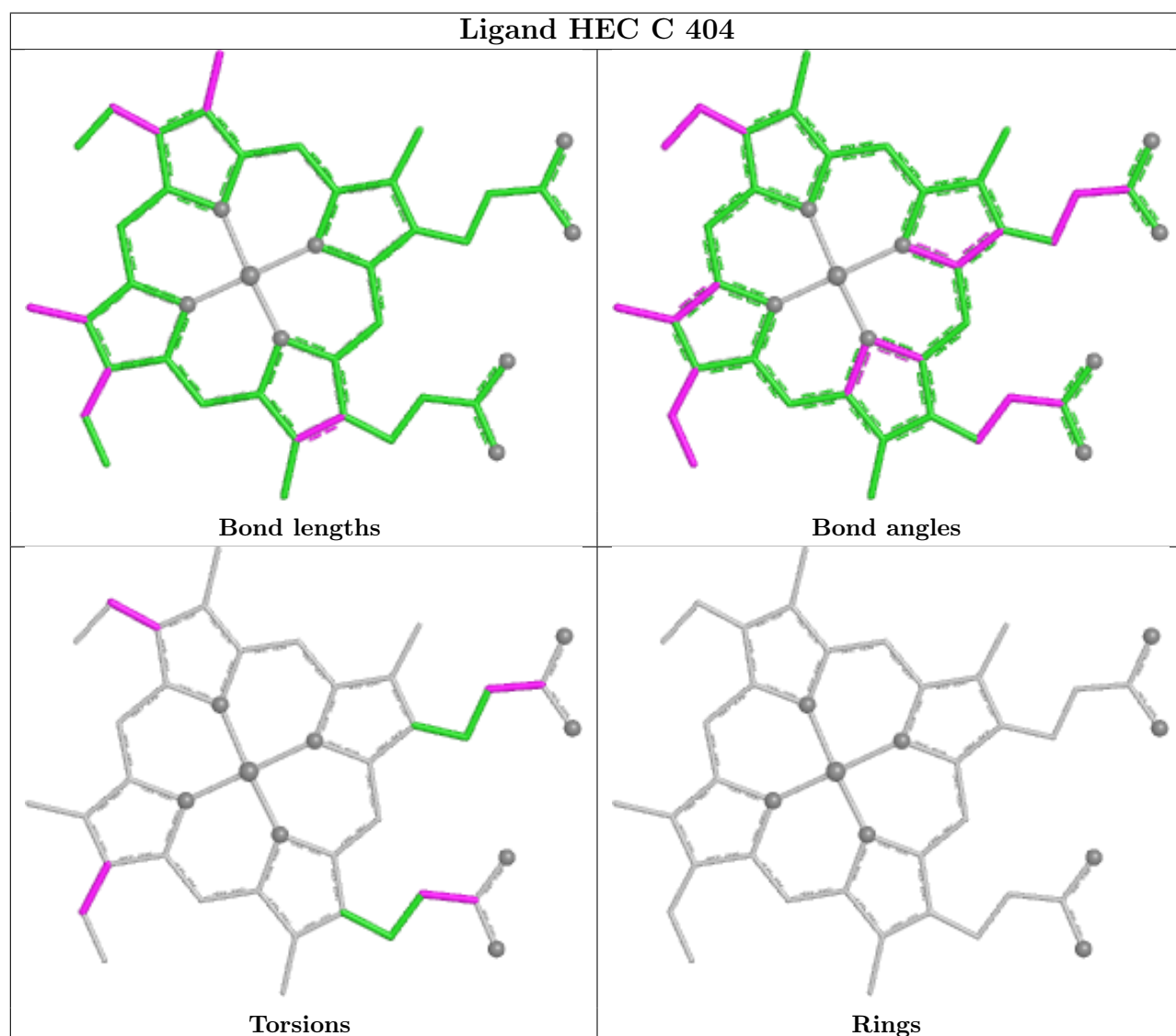
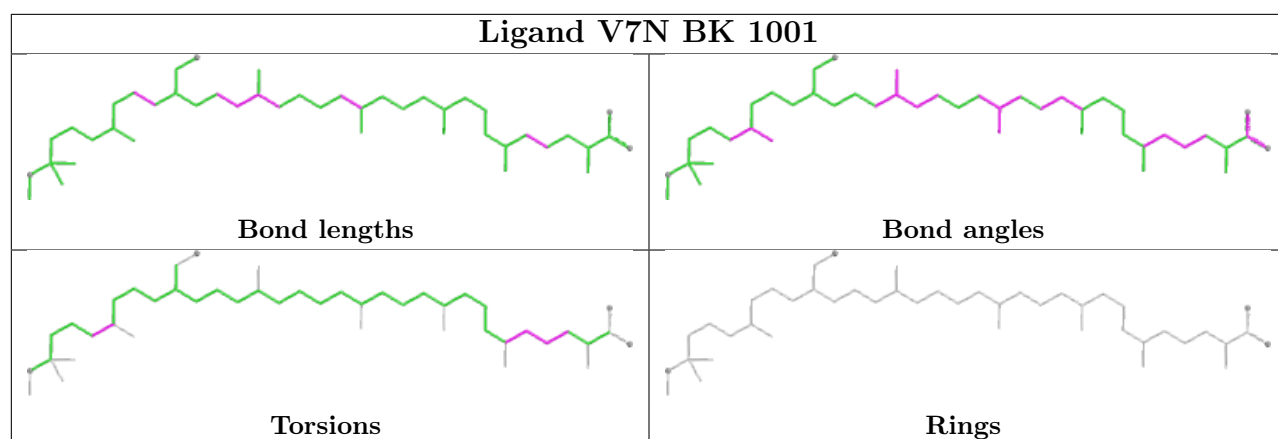


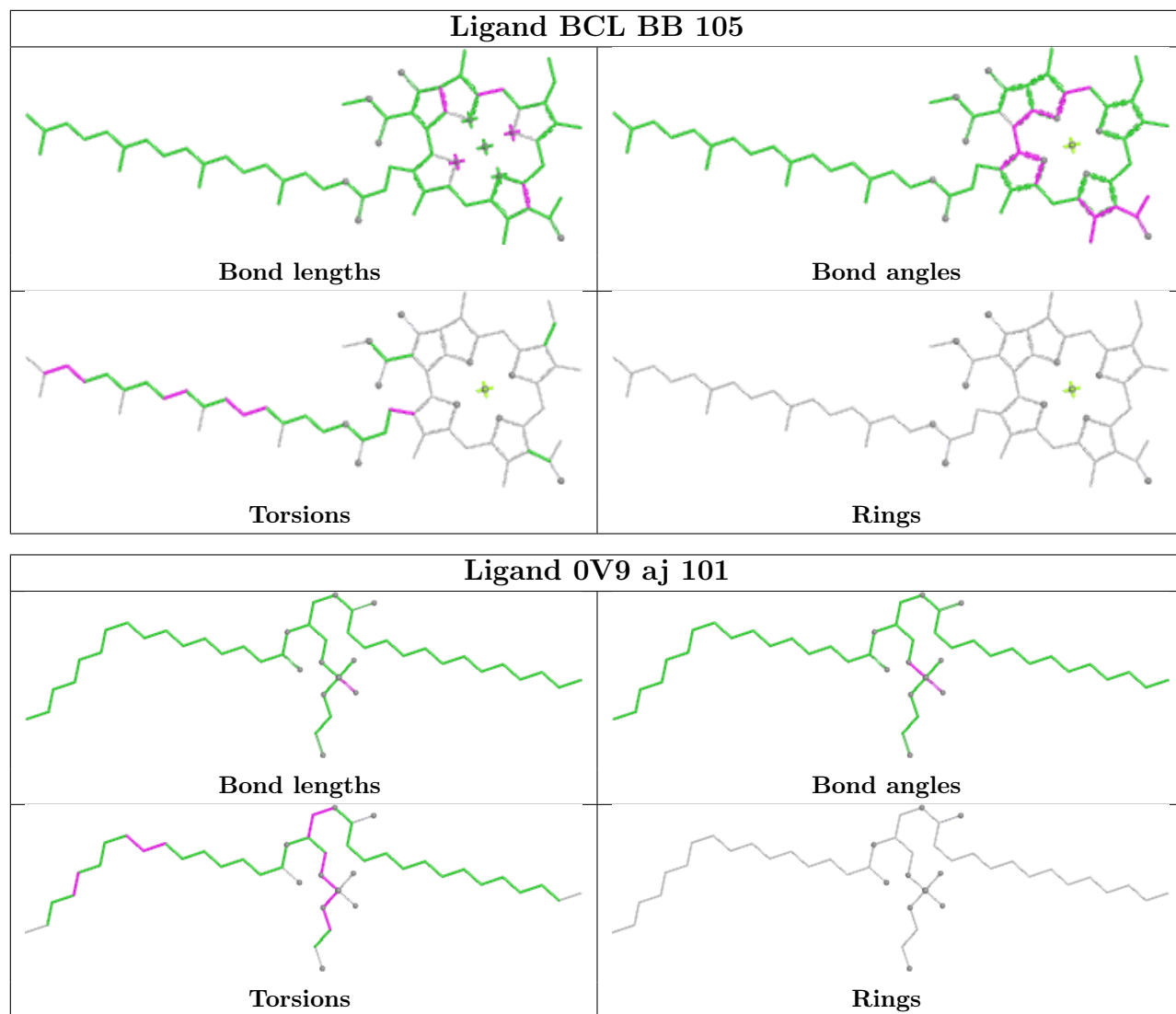


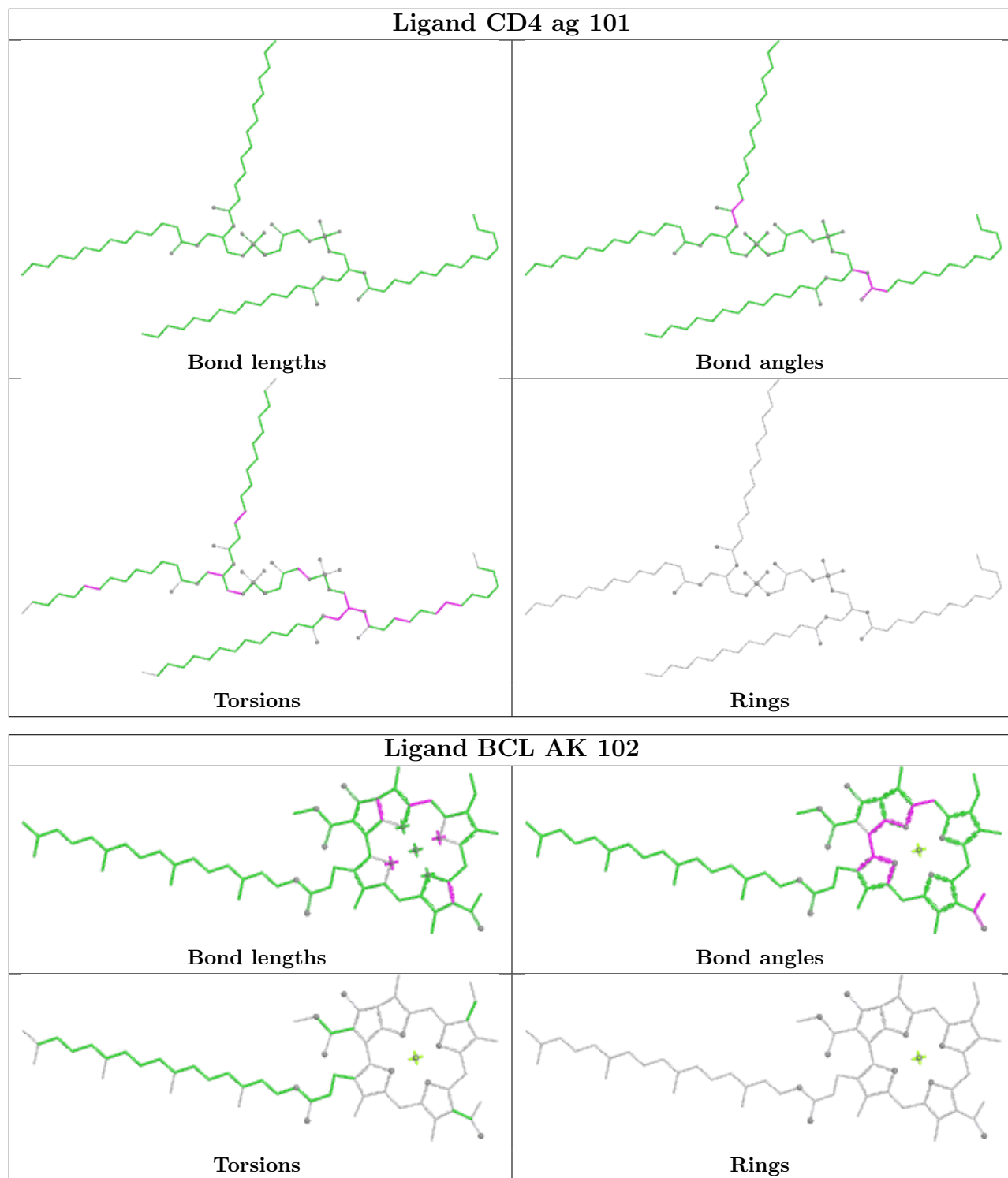


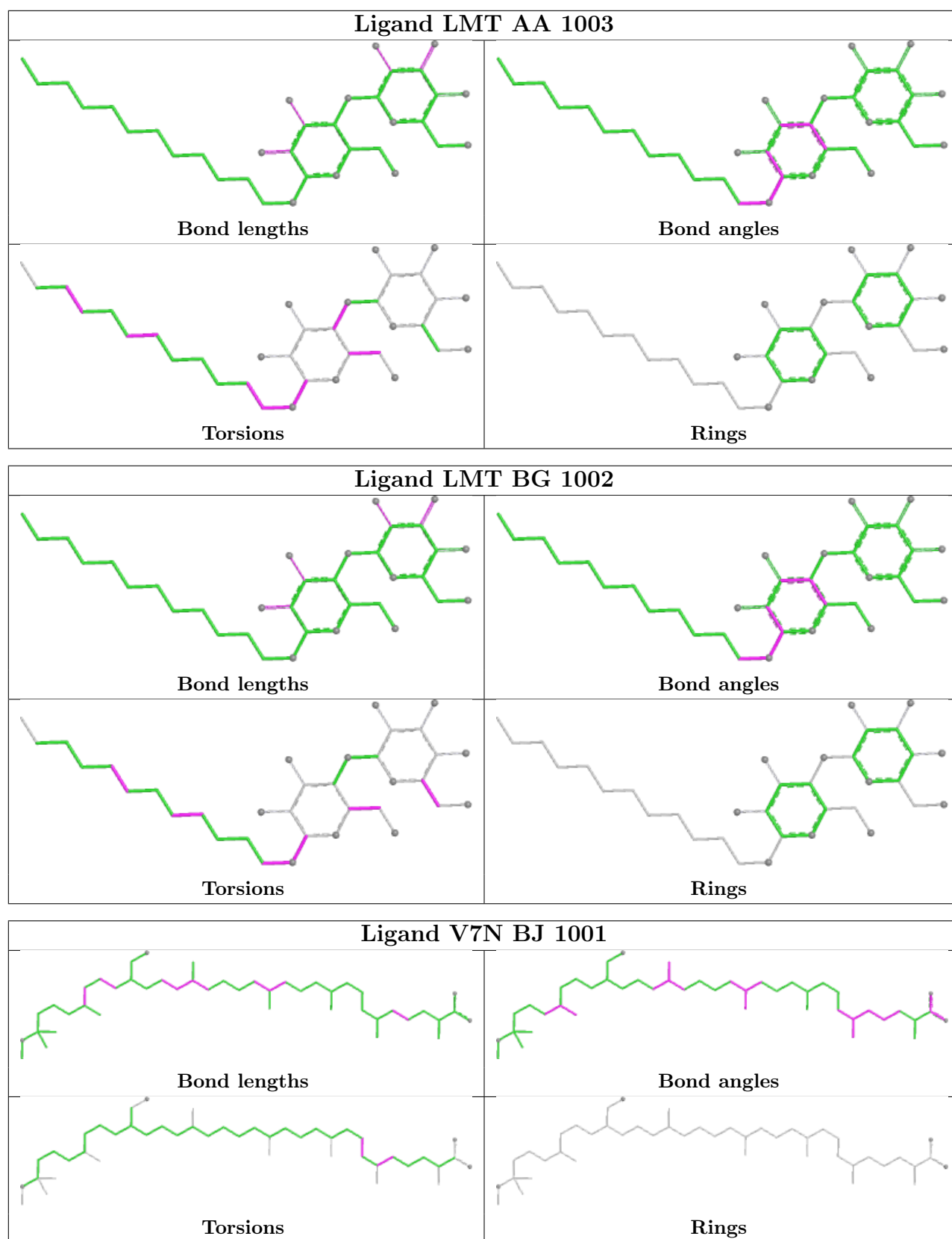


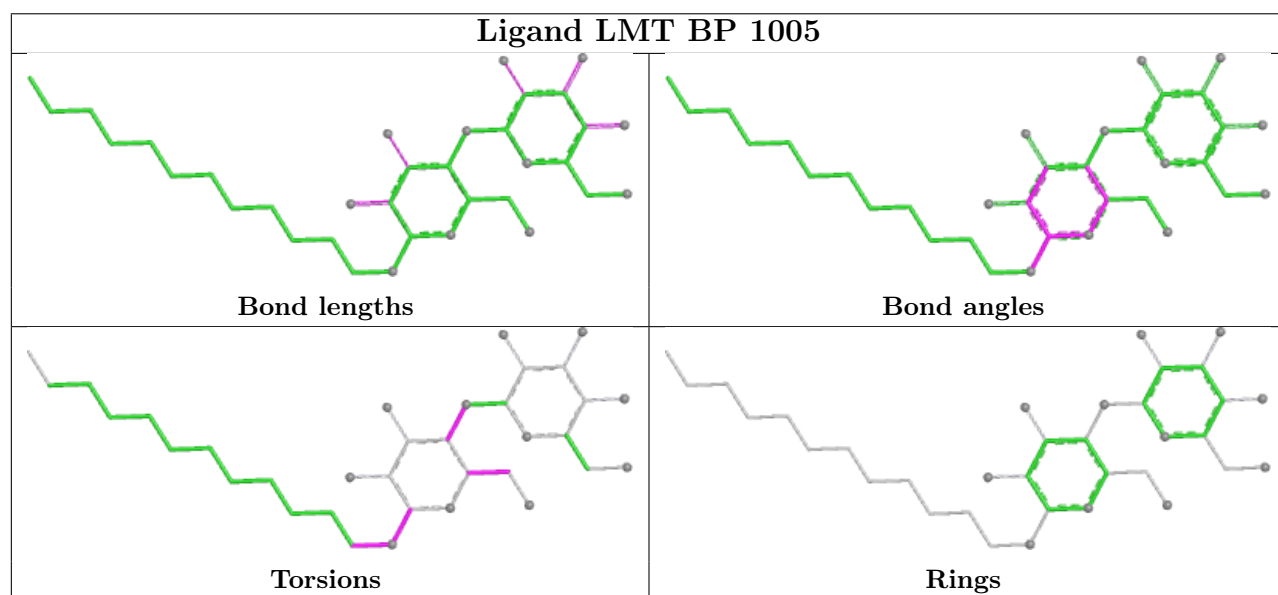
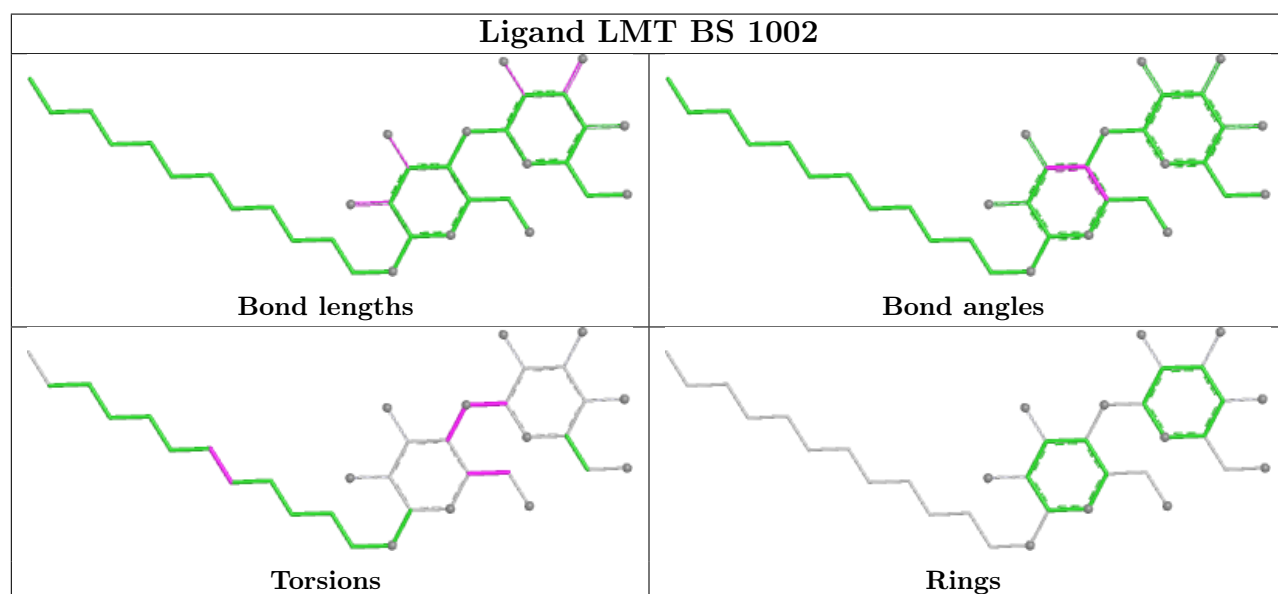
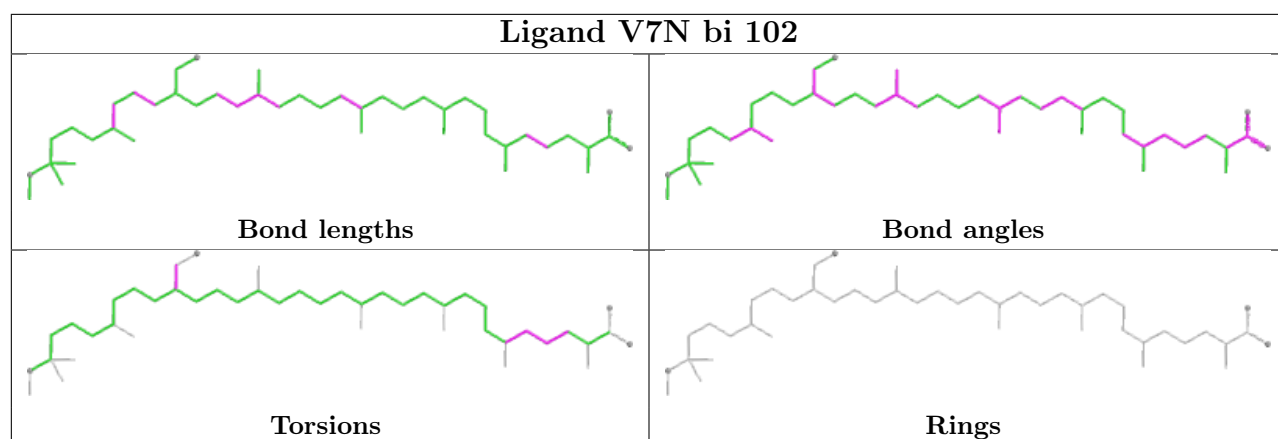


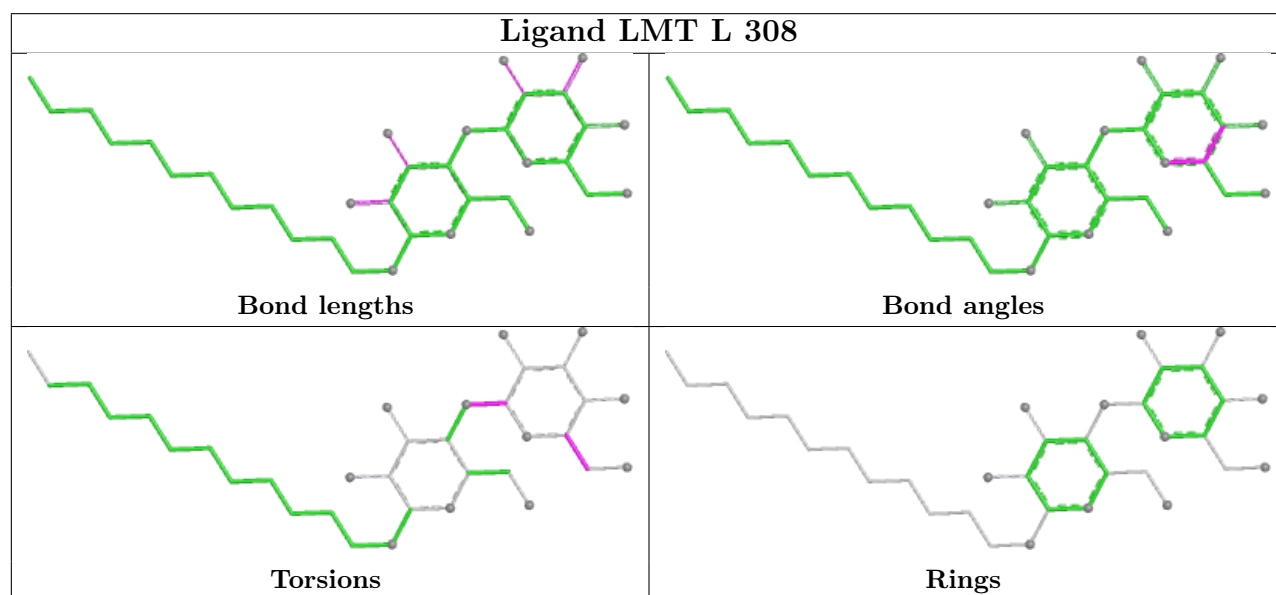
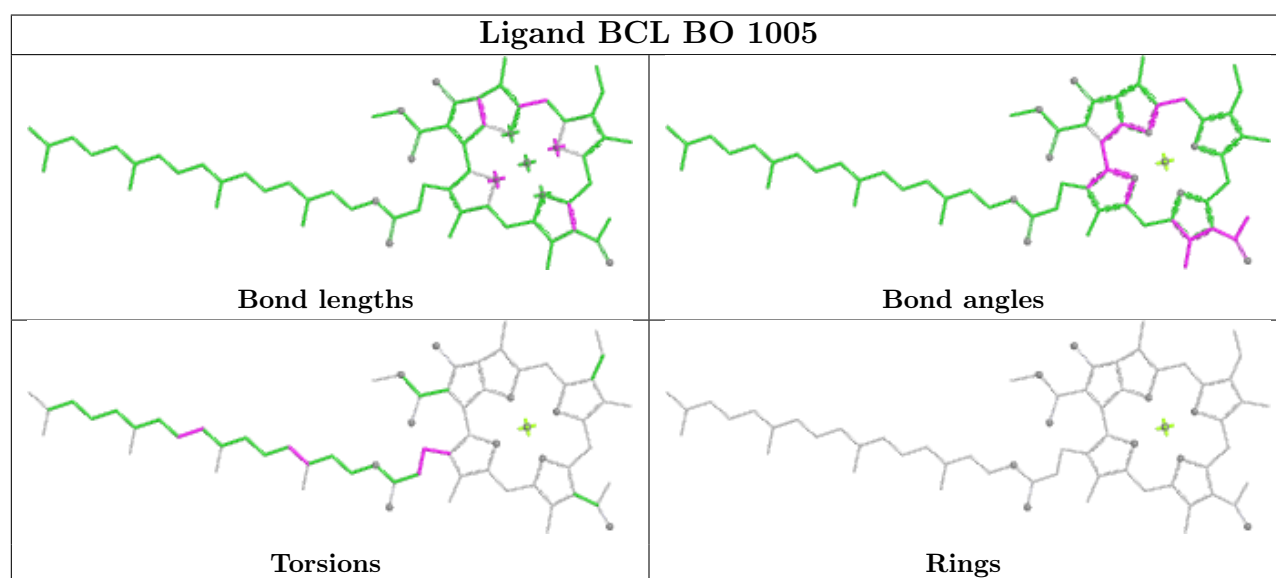
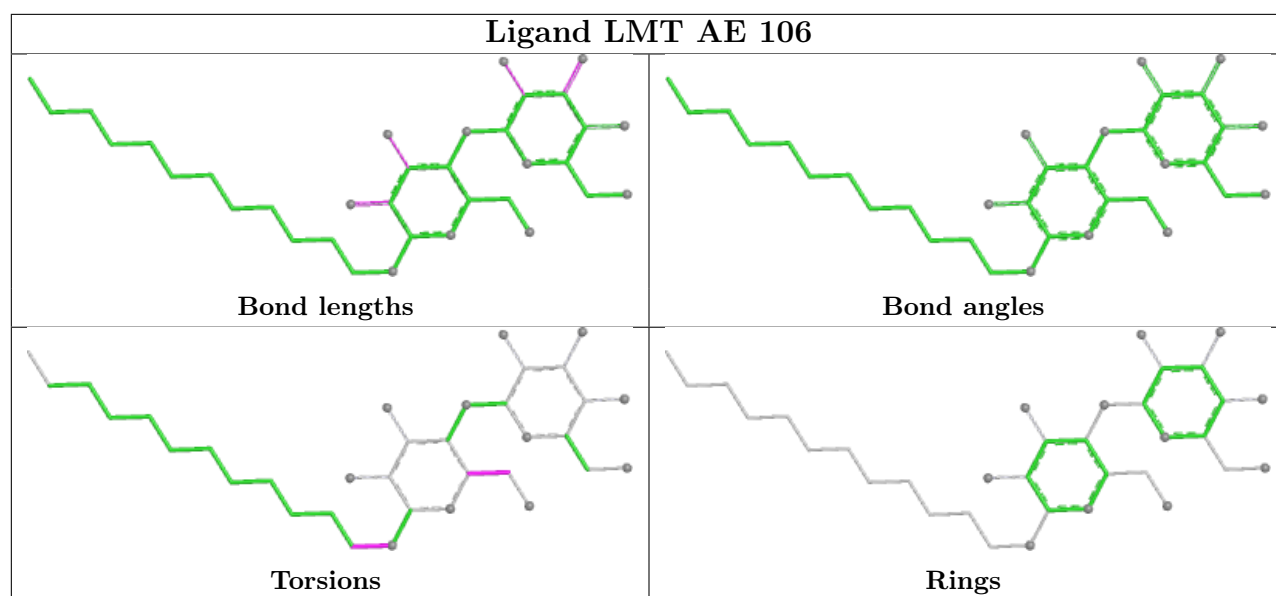


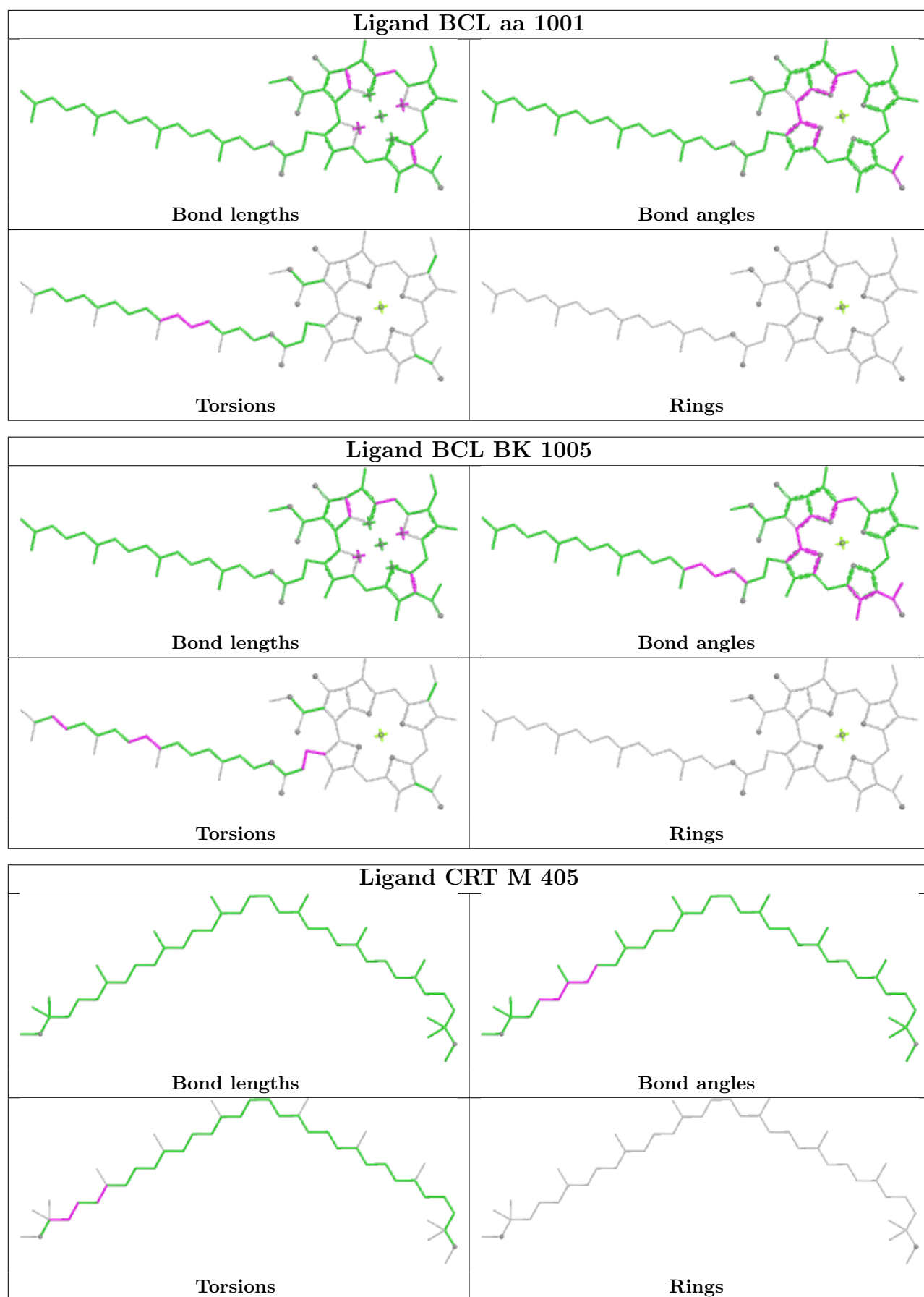


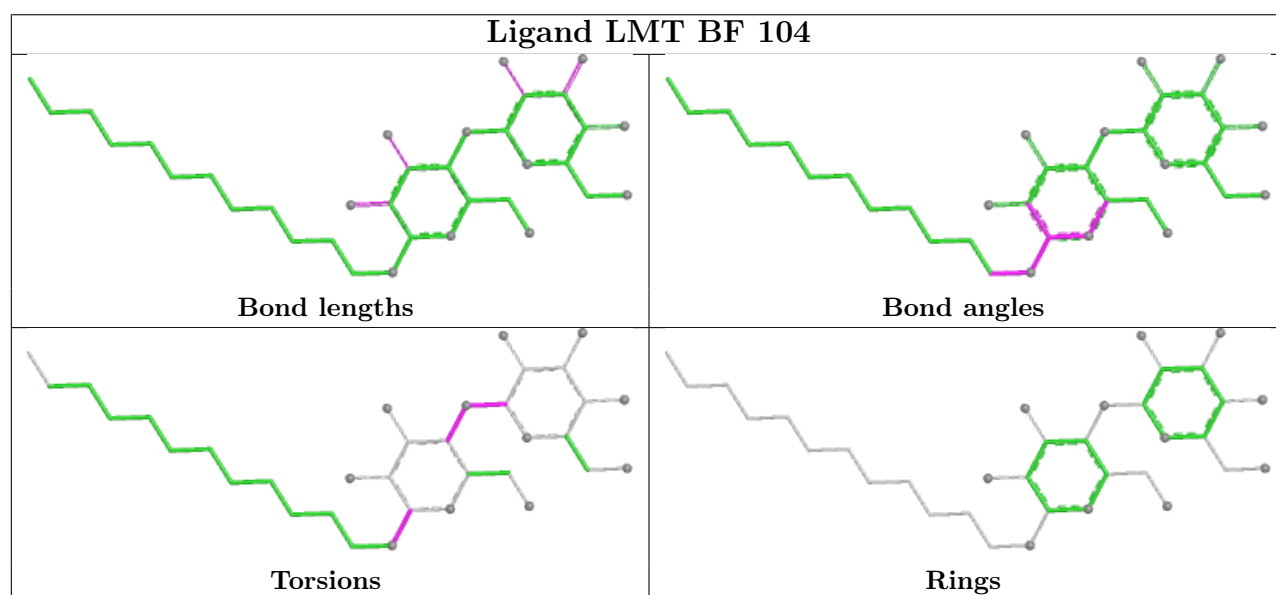
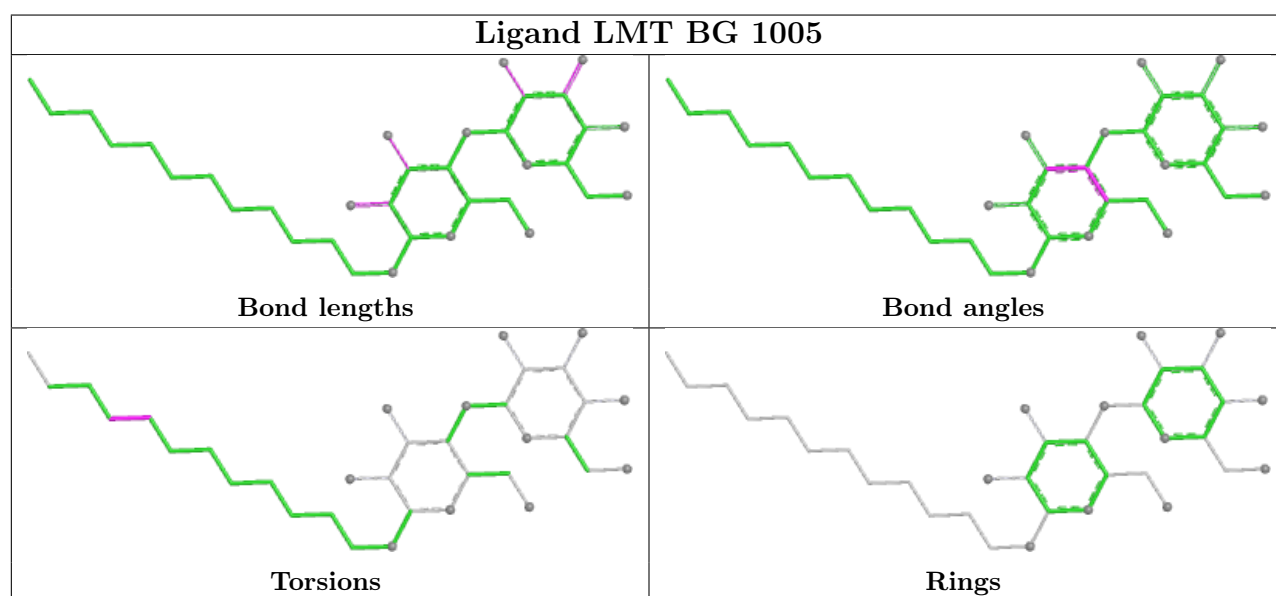
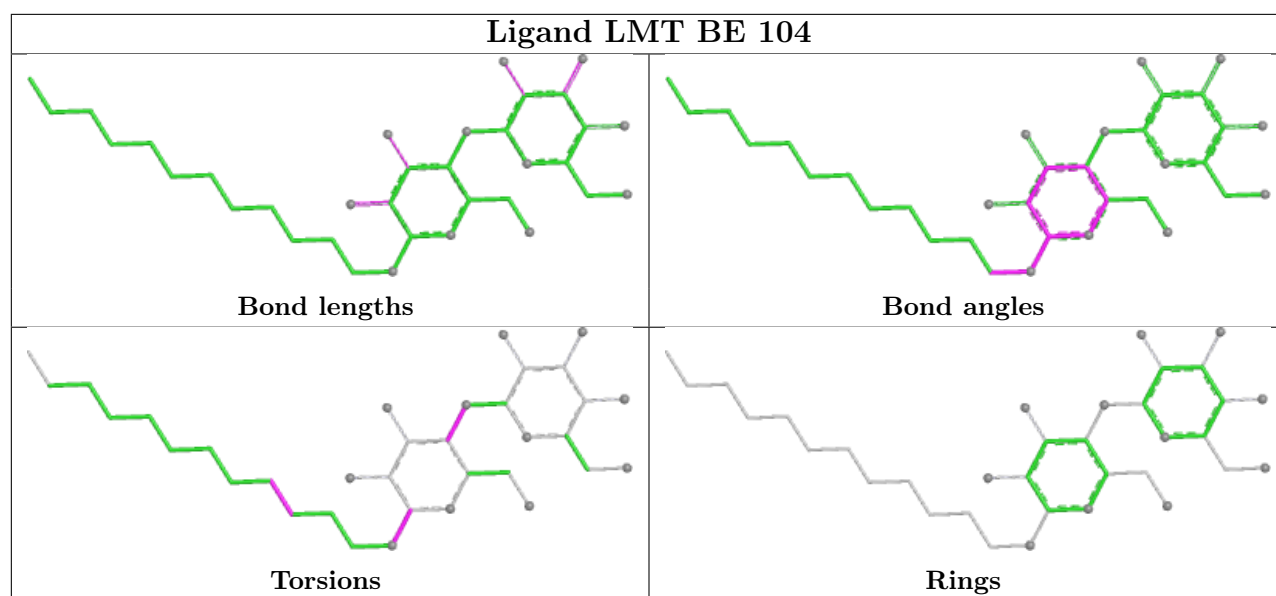


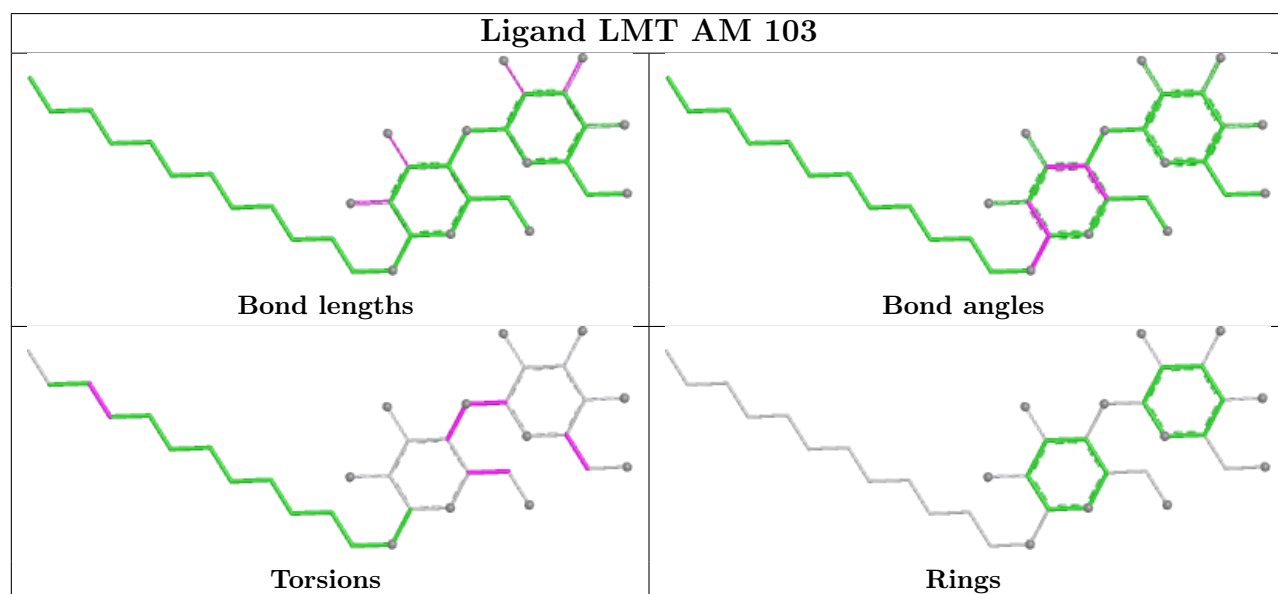
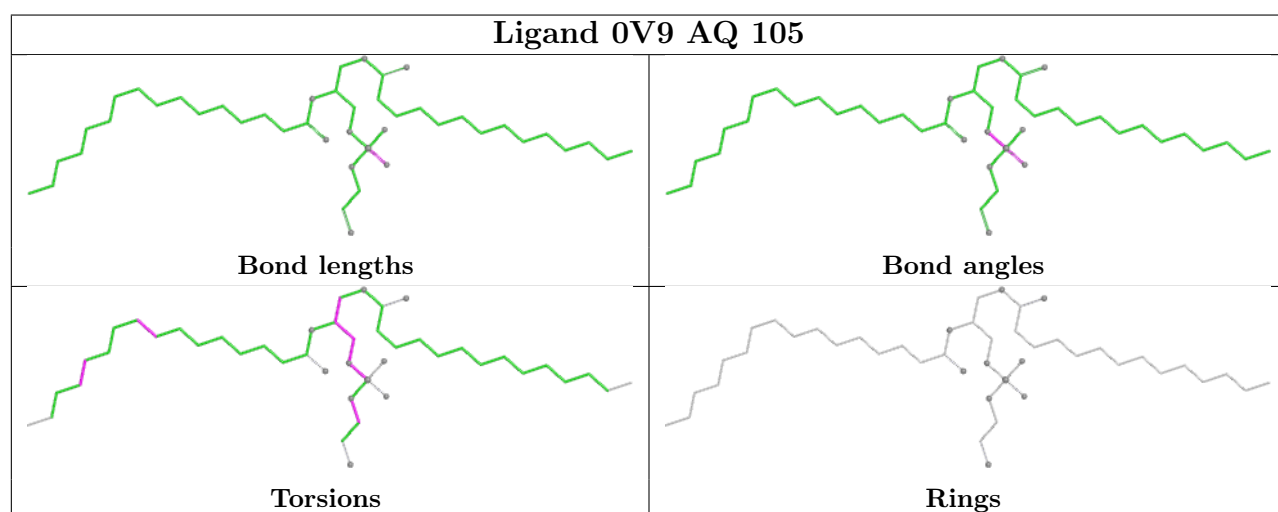
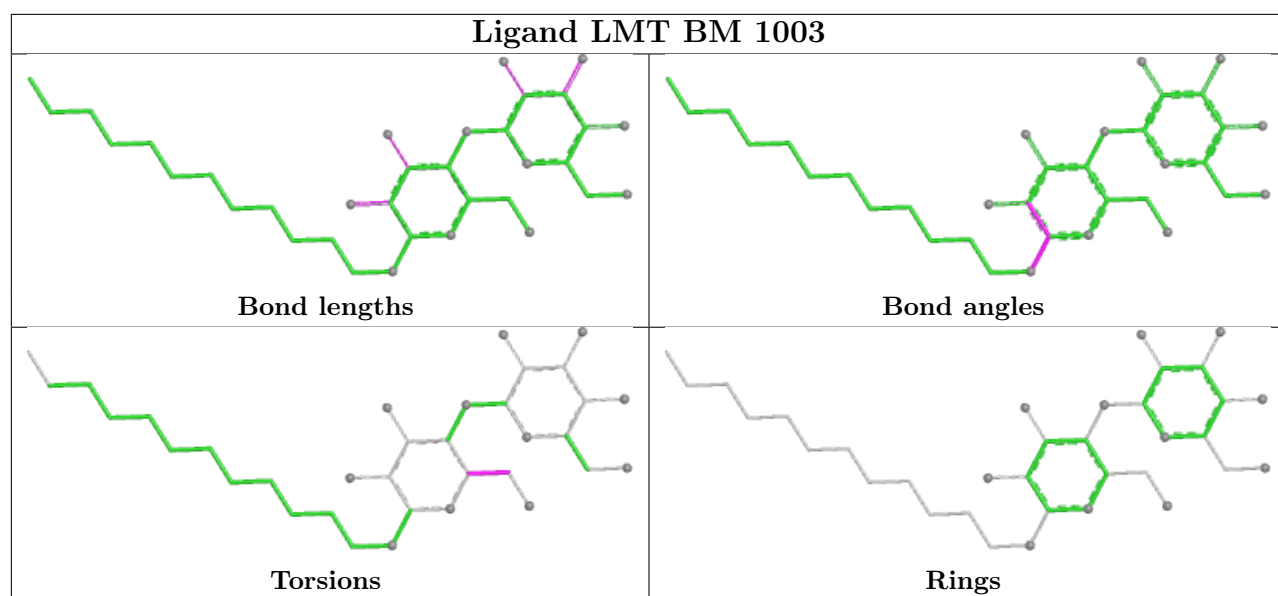


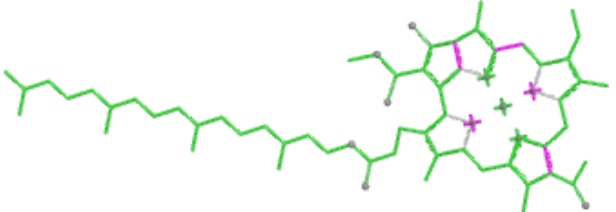
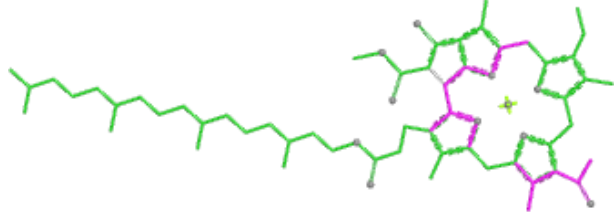
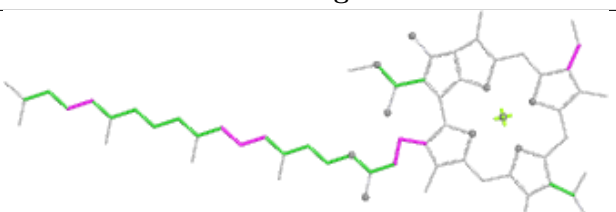
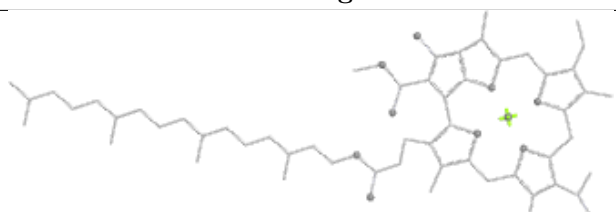
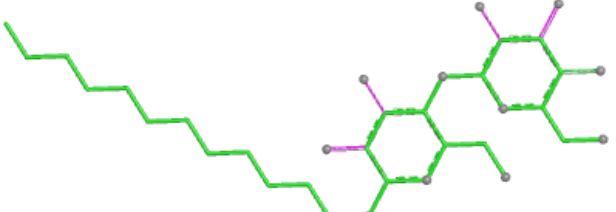
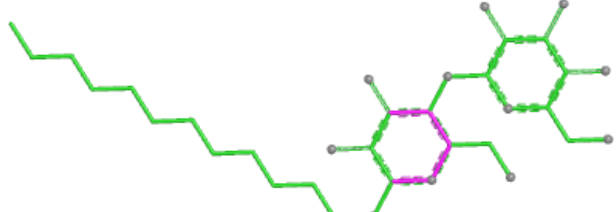
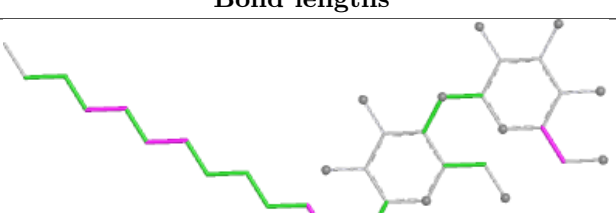
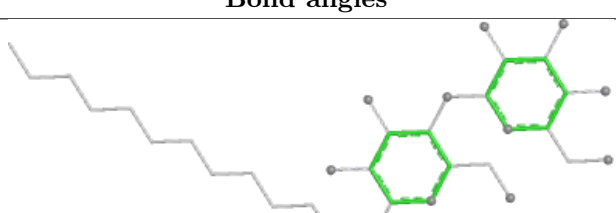
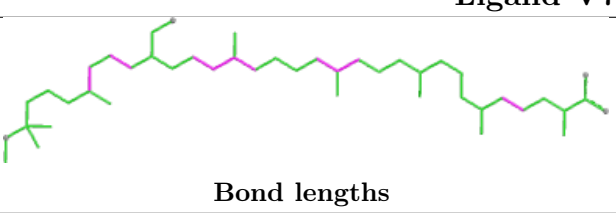
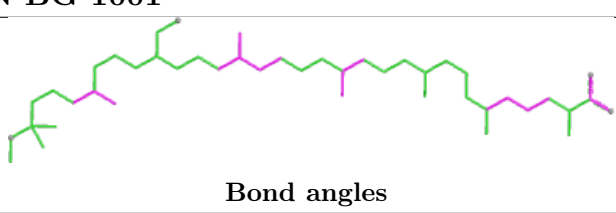
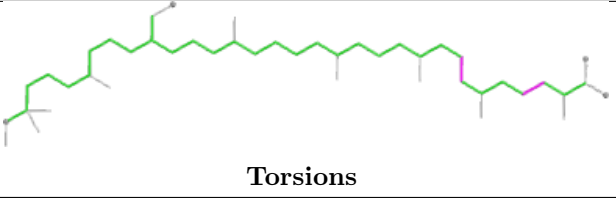
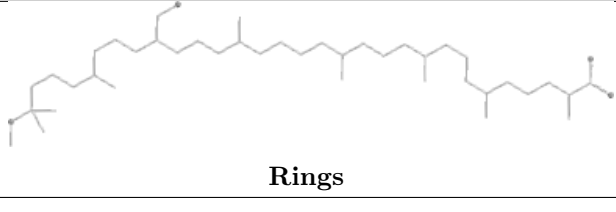


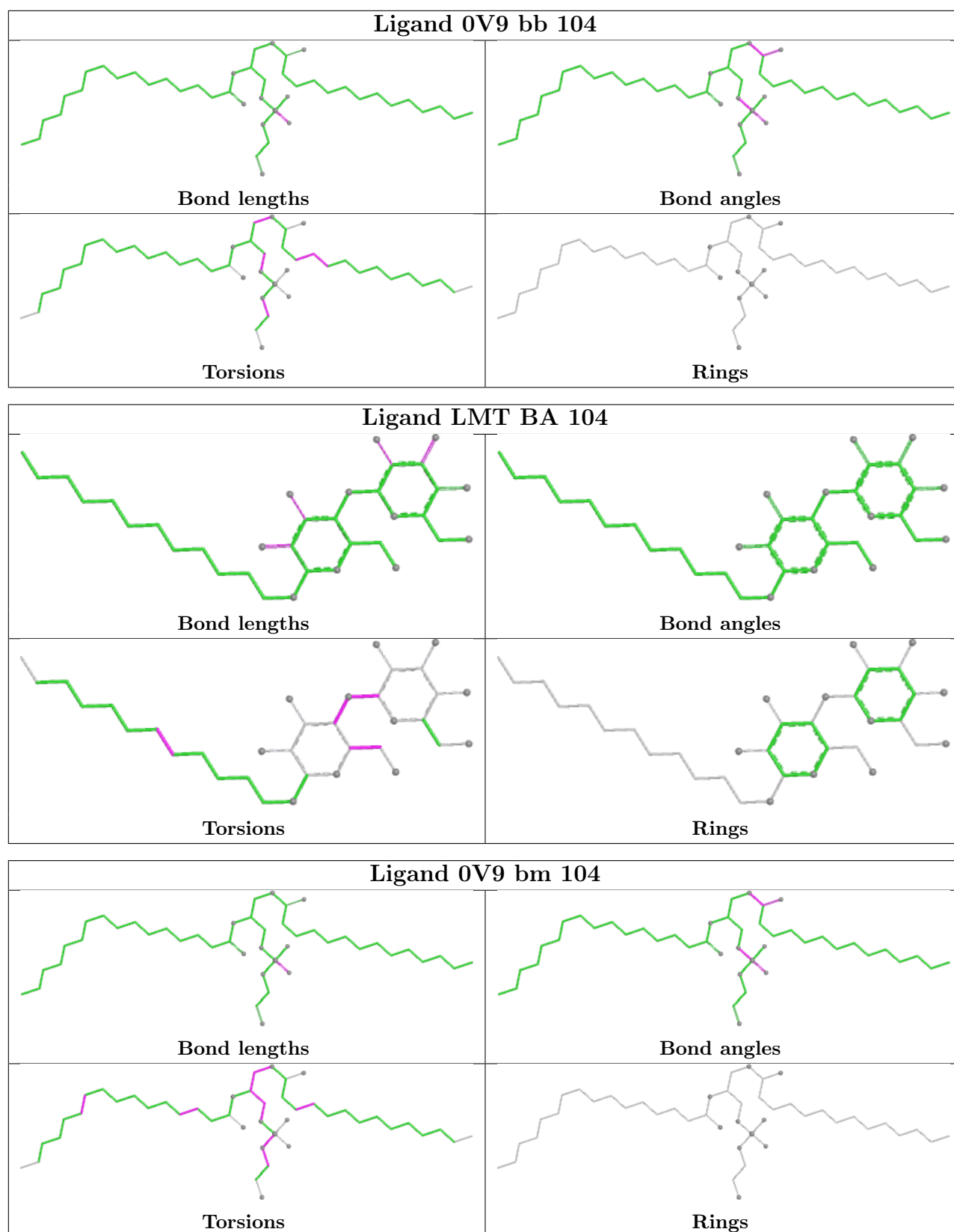


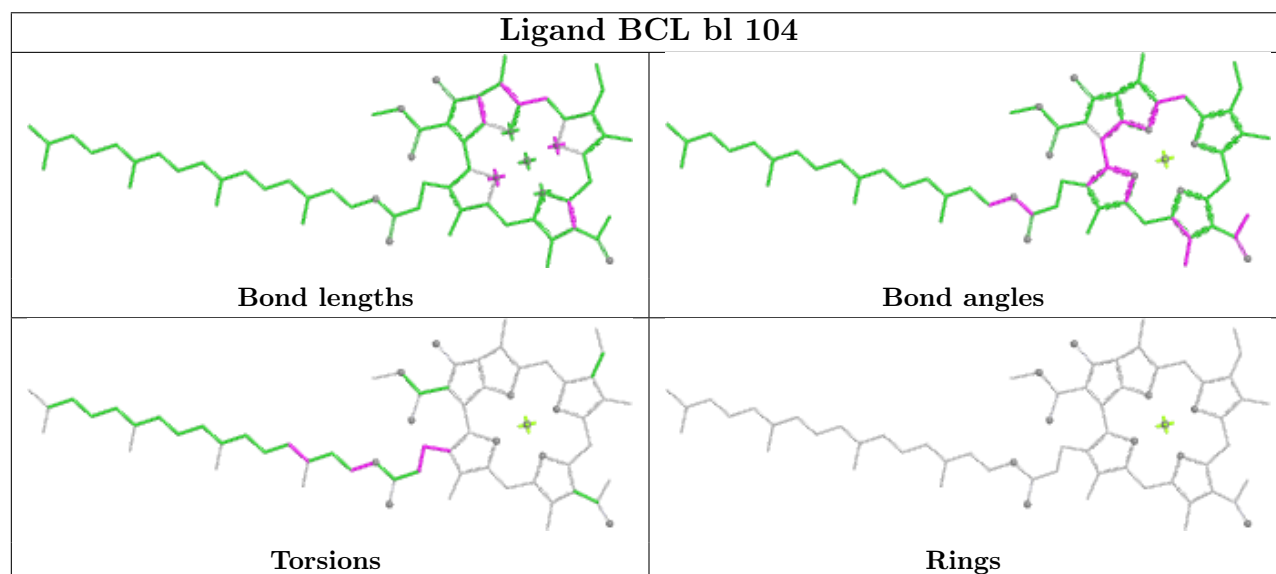
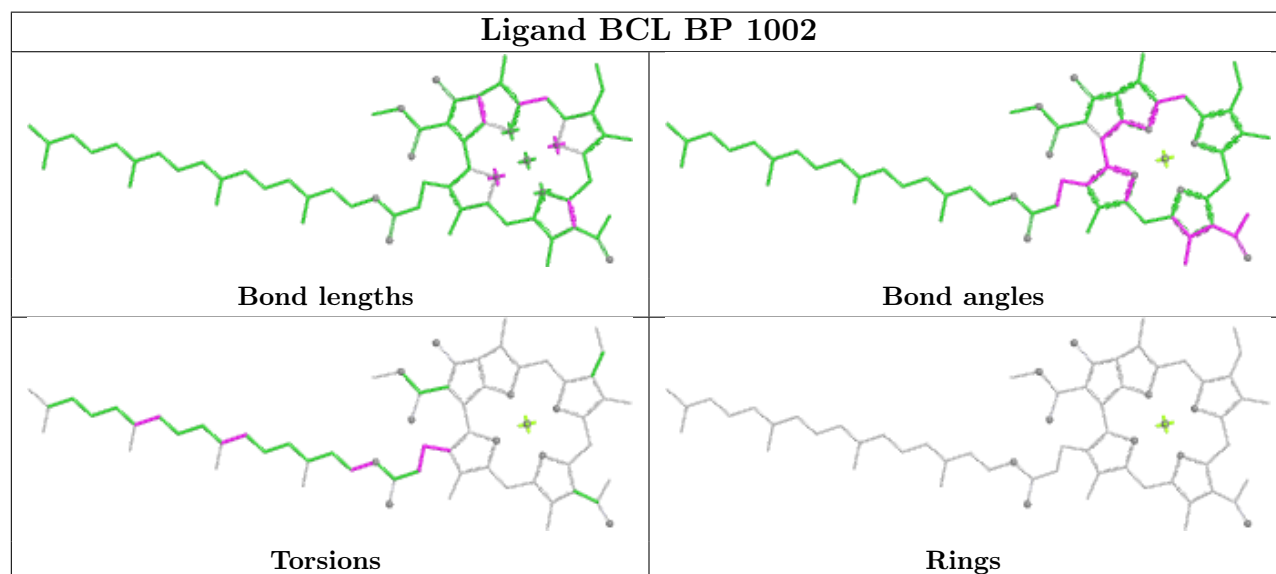
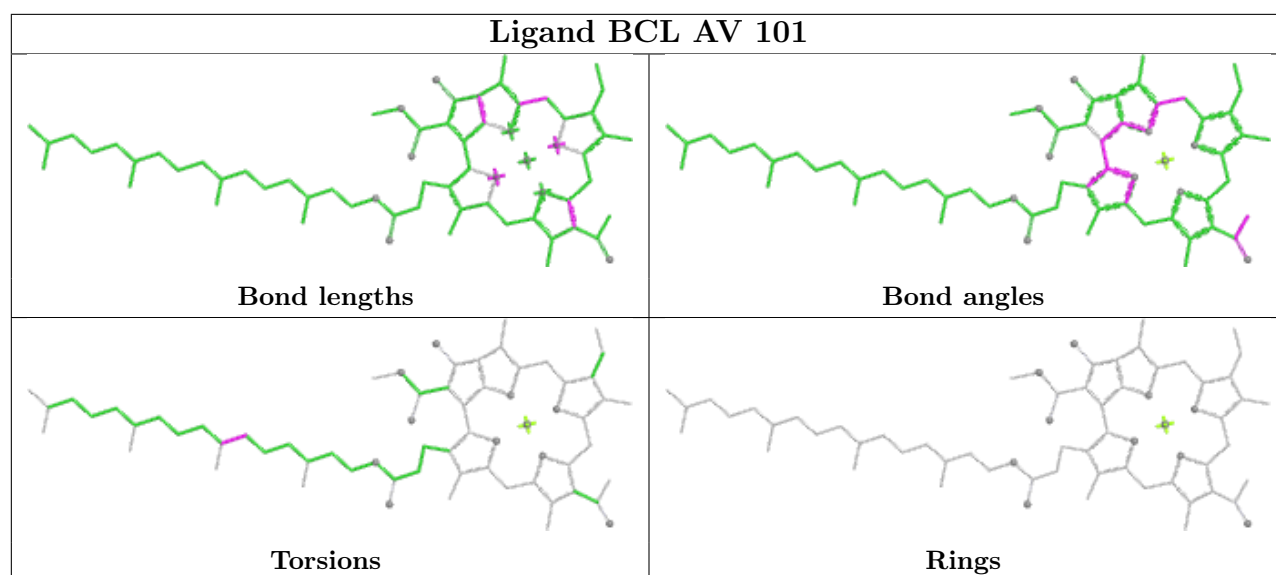


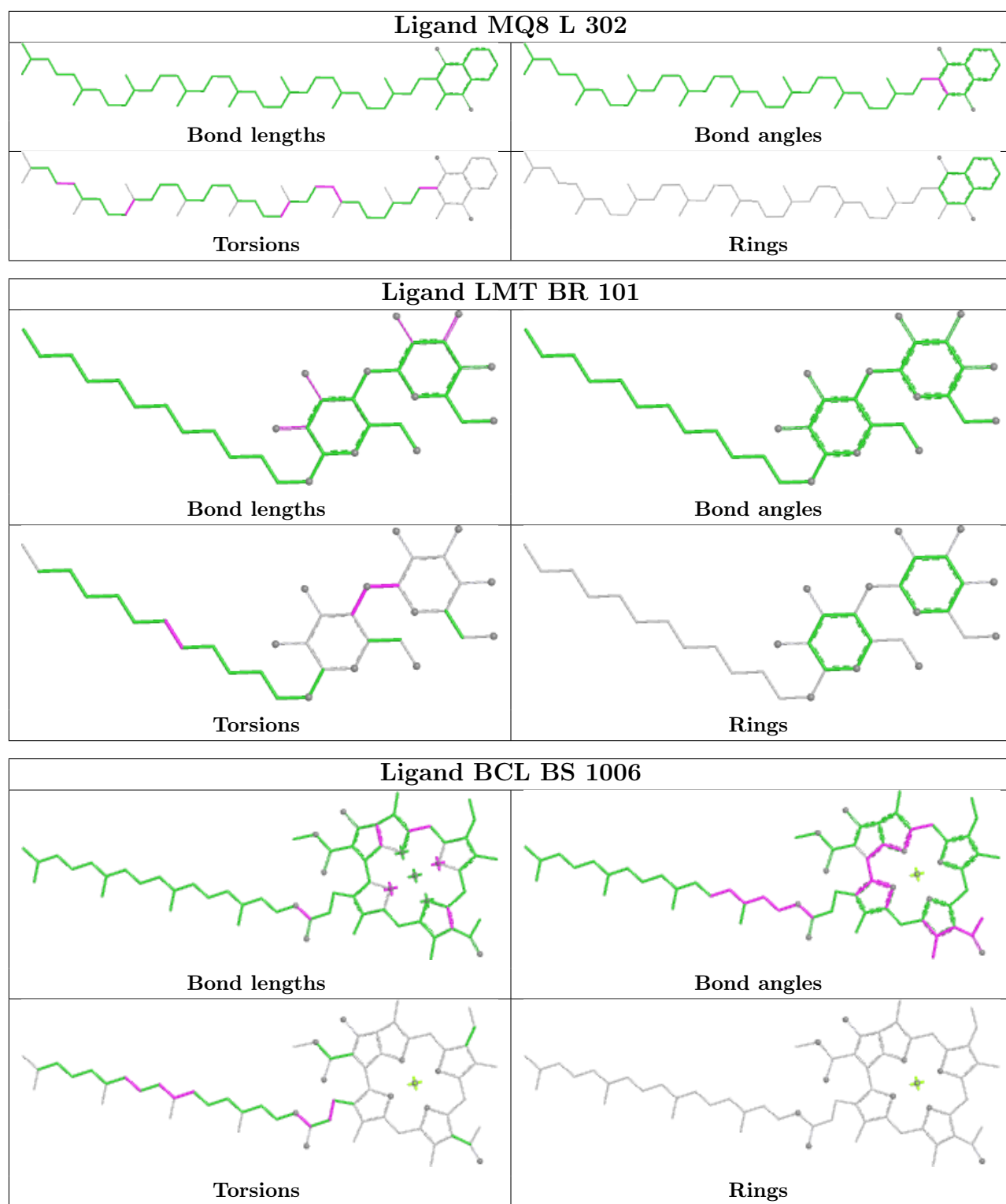


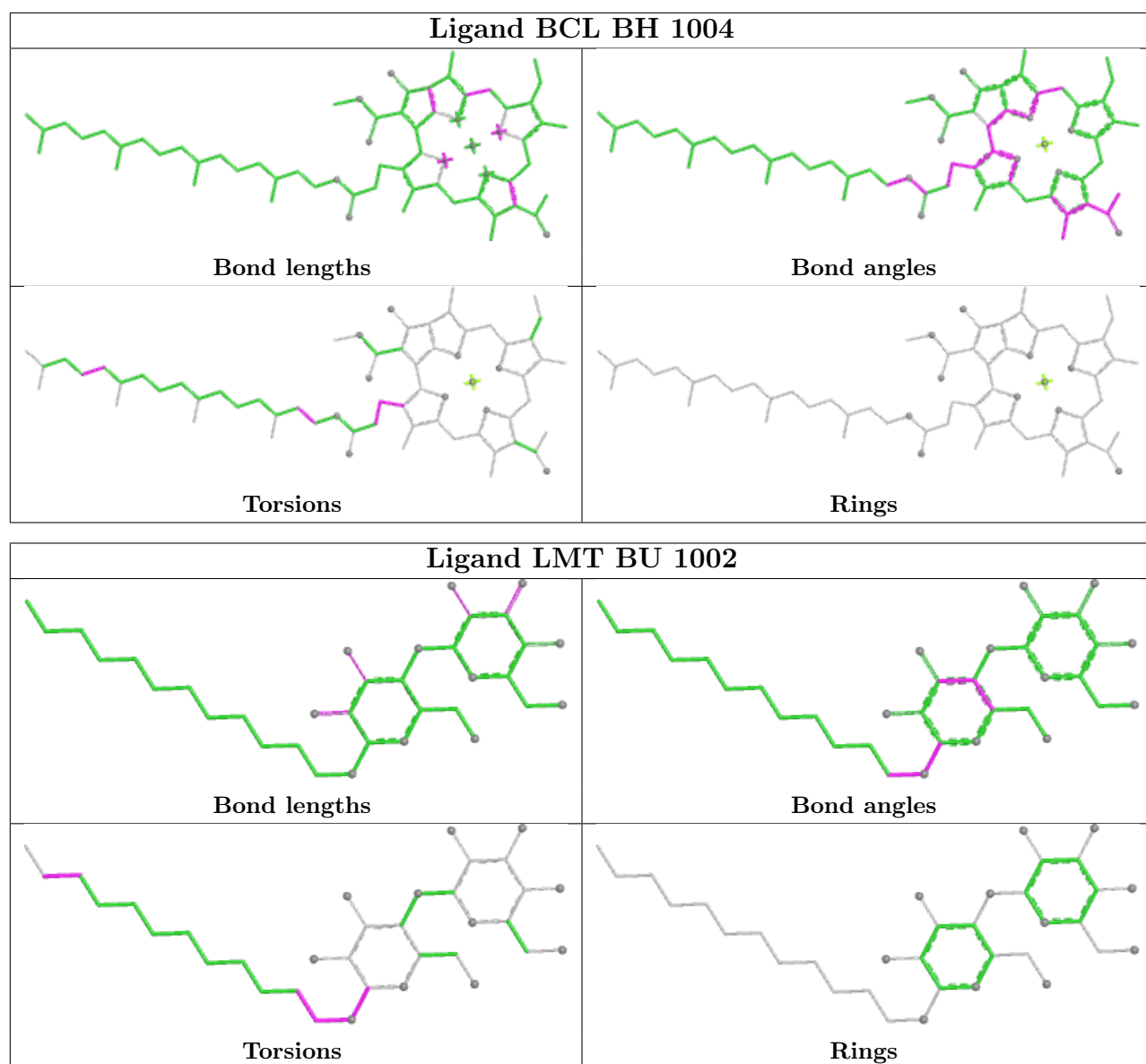


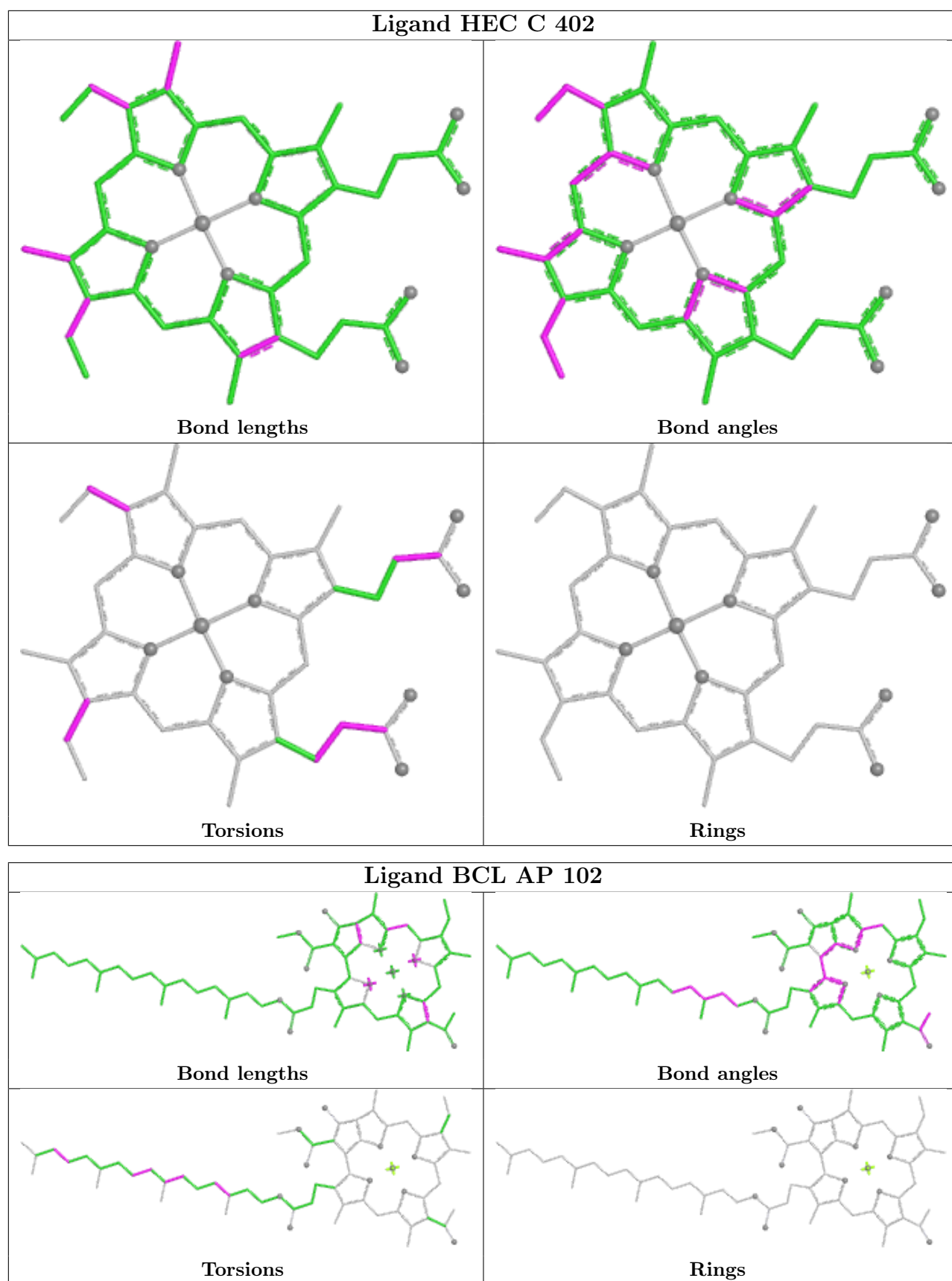
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT bp 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand V7N BG 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

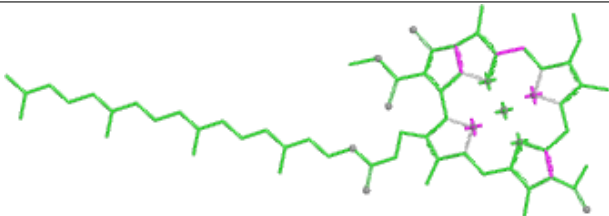
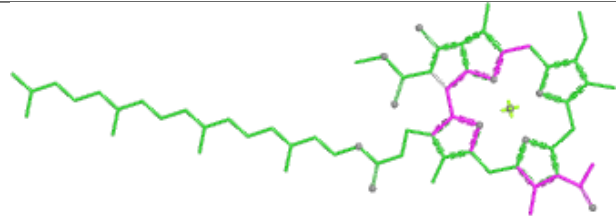
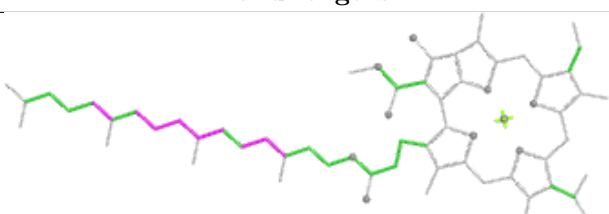
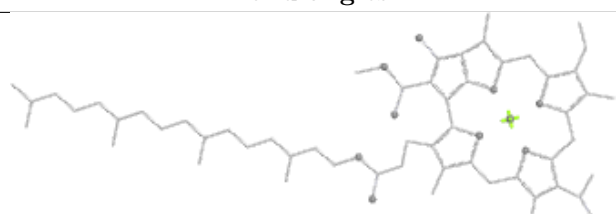


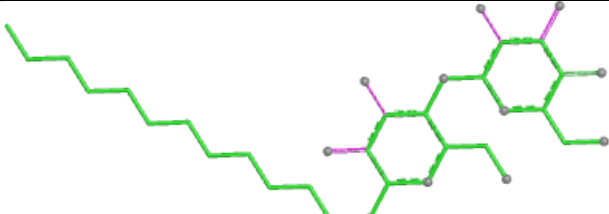
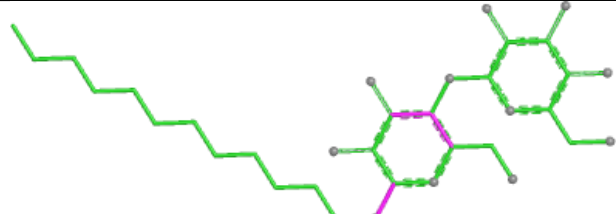
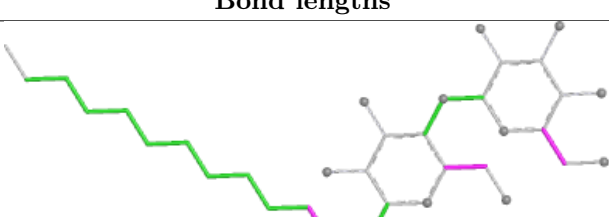
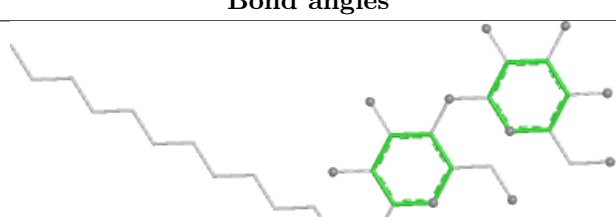


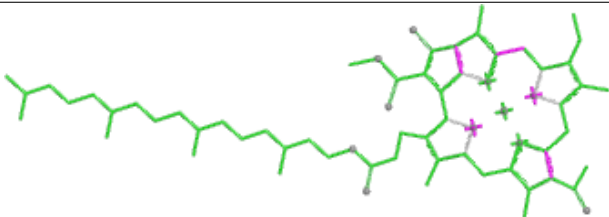
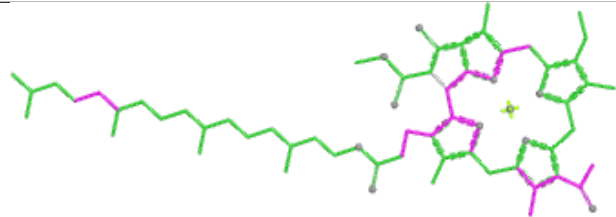
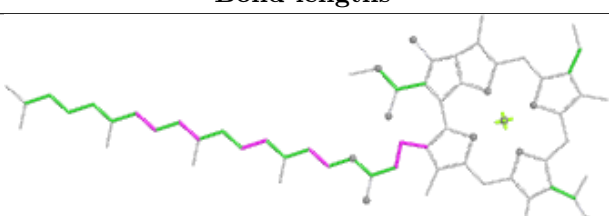
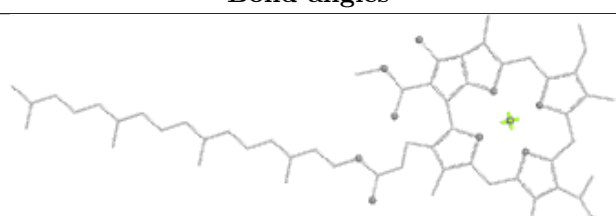


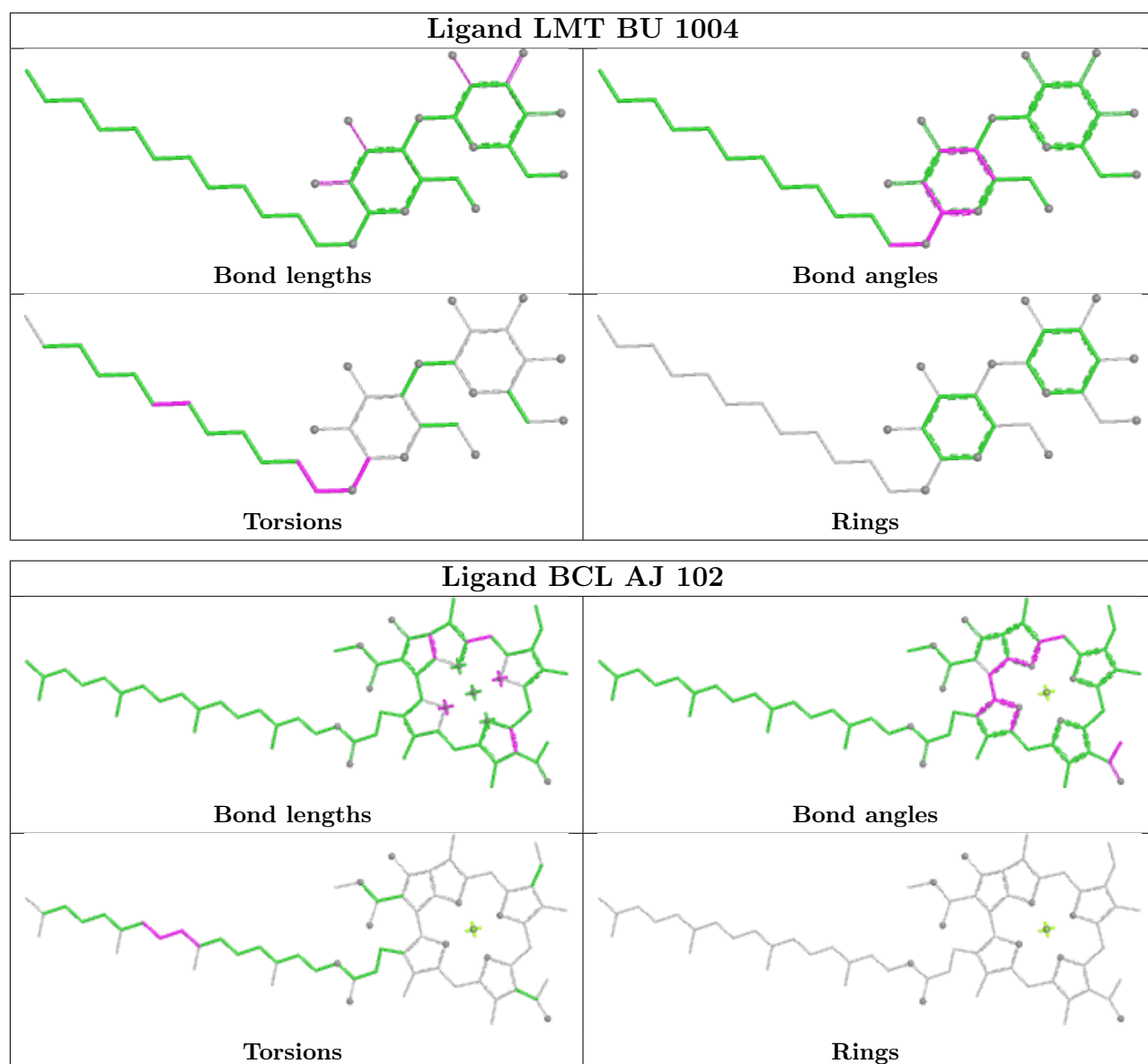


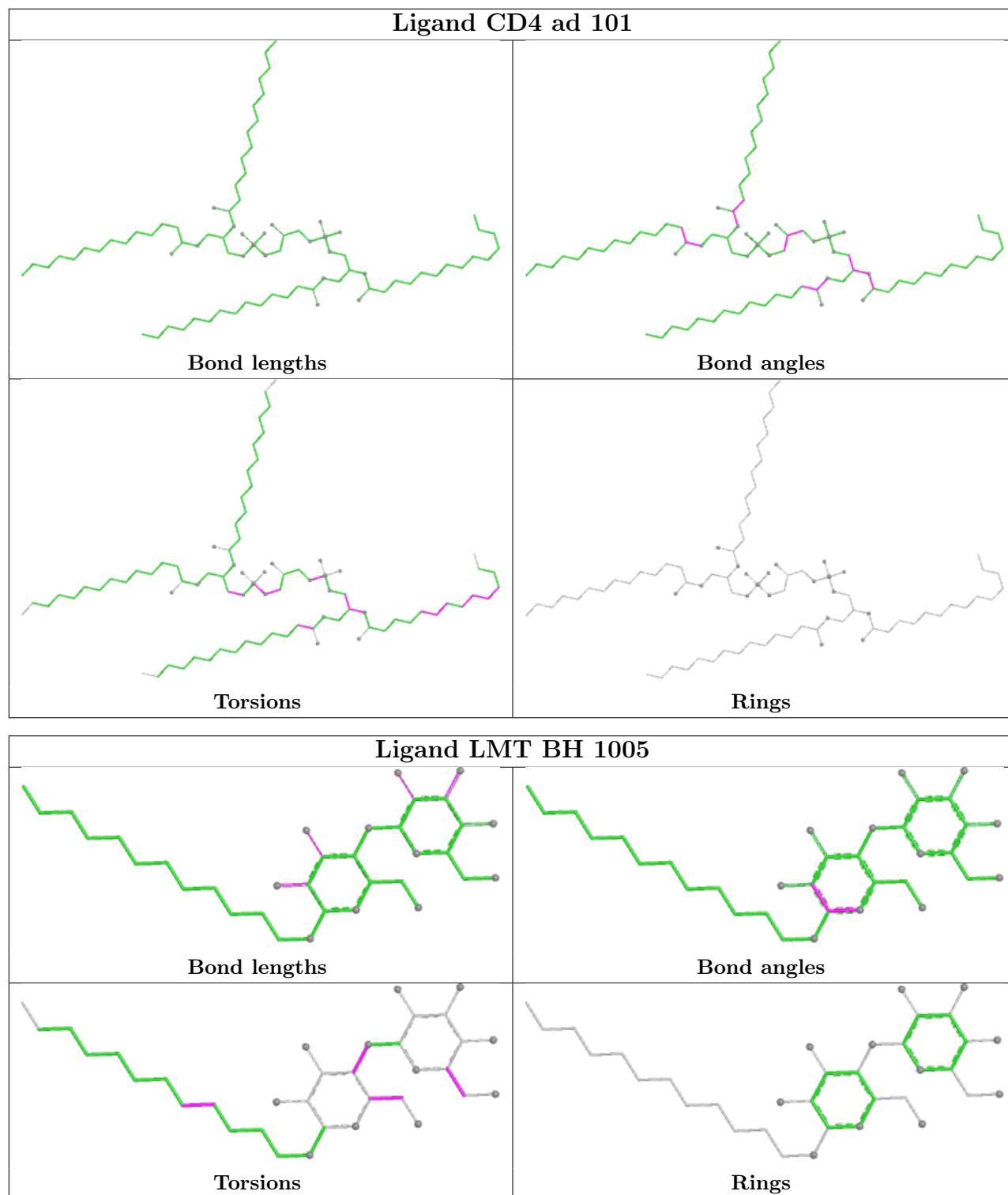


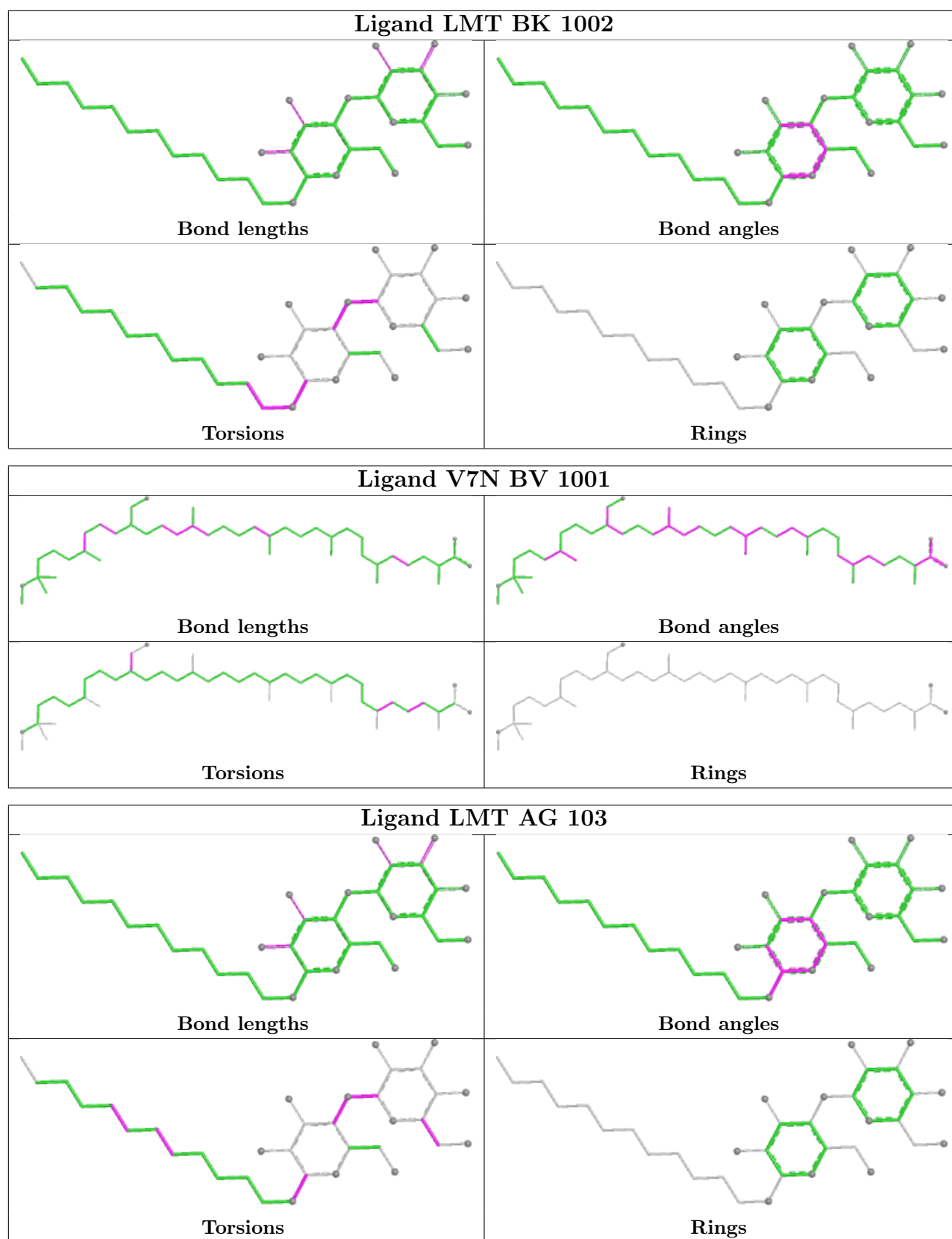
Ligand BCL ak 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

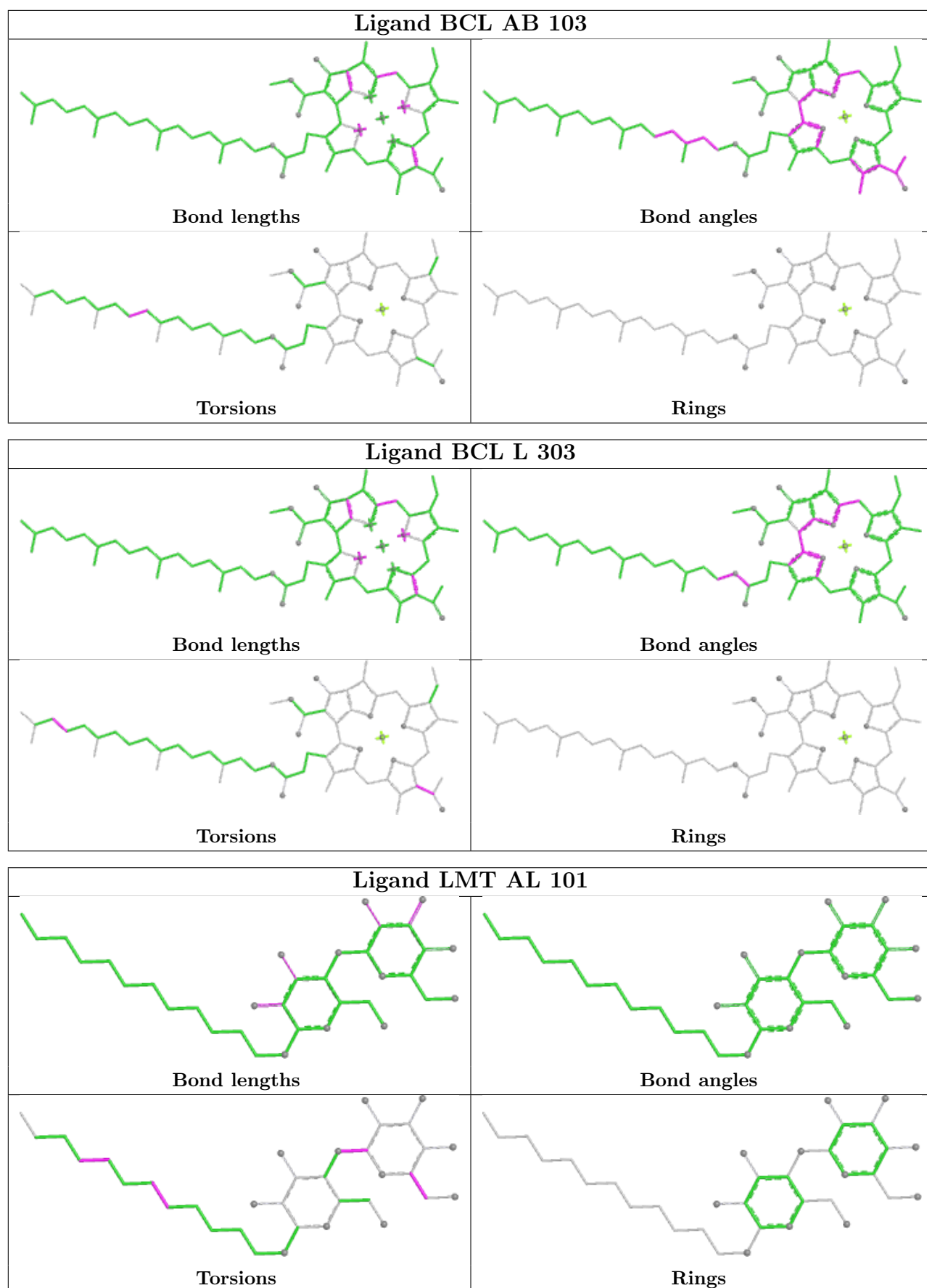
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Bond lengths	Bond angles
	
Torsions	Rings

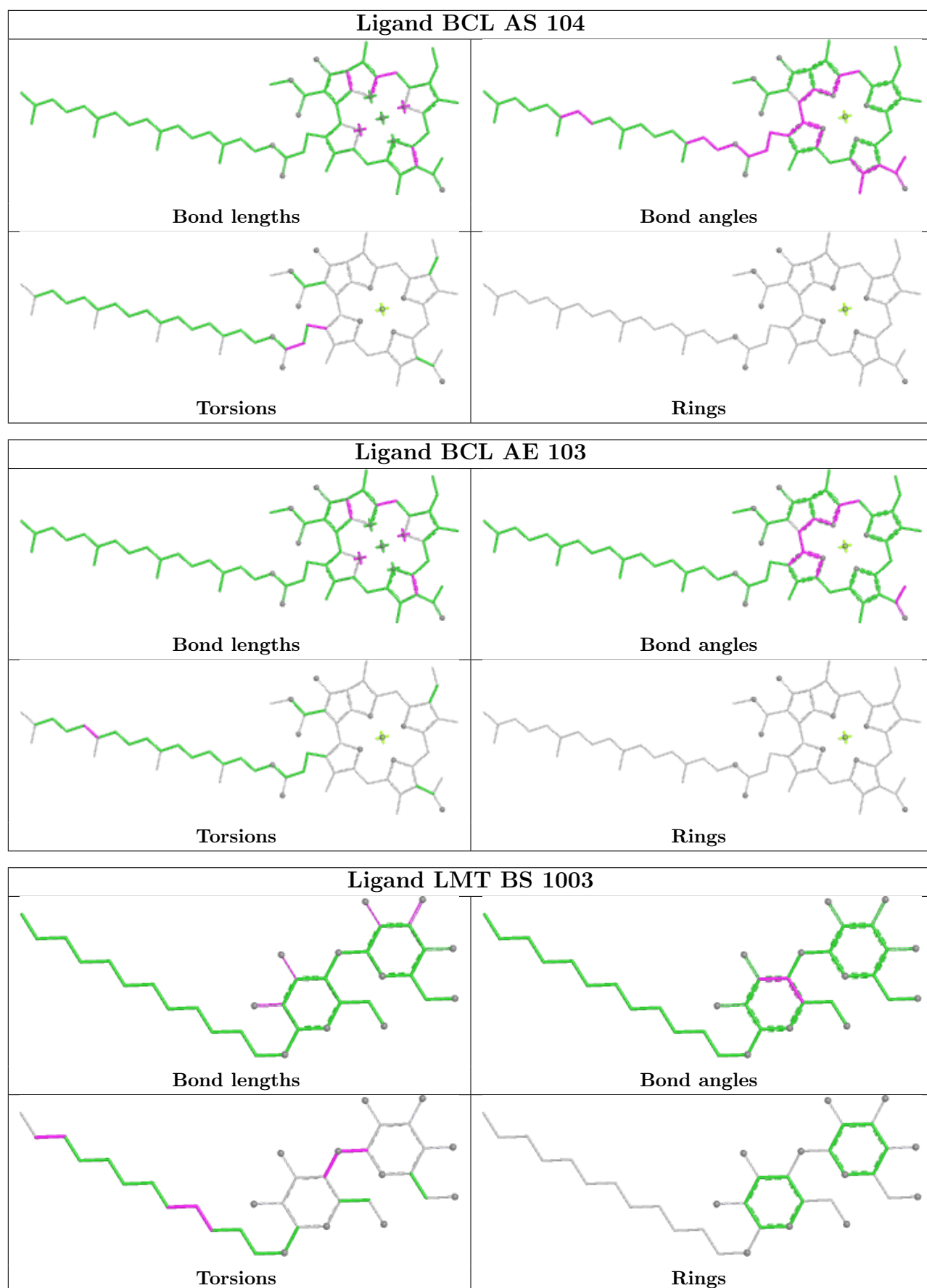
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Bond lengths	Bond angles
	
Torsions	Rings

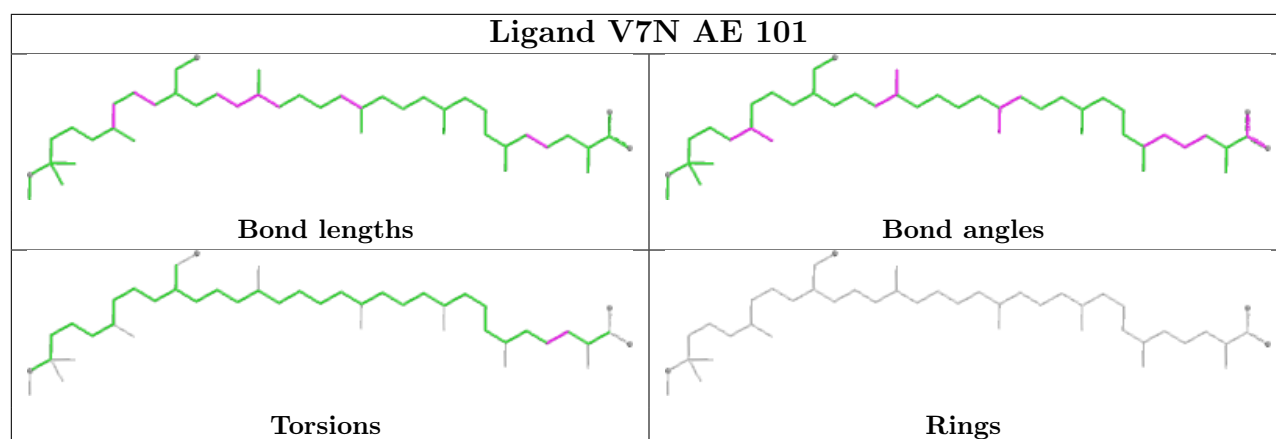












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

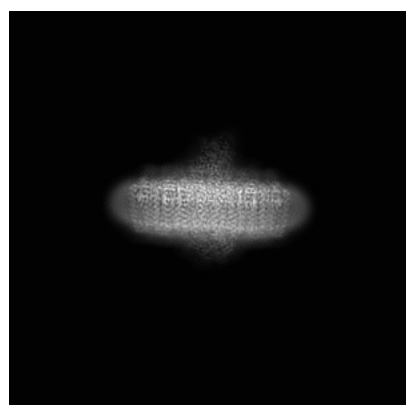
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12679. These allow visual inspection of the internal detail of the map and identification of artifacts.

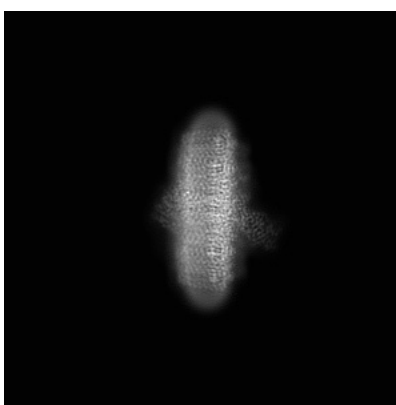
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

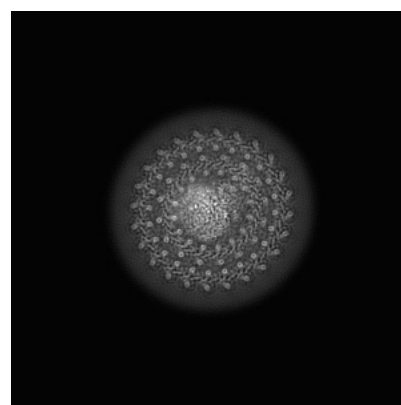
6.1.1 Primary map



X



Y

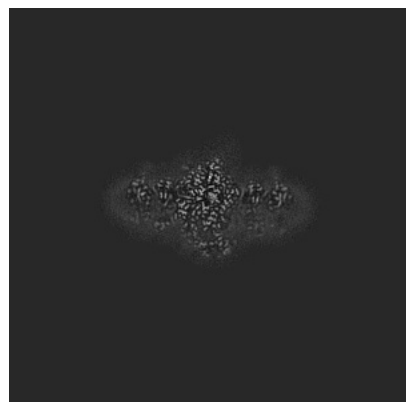


Z

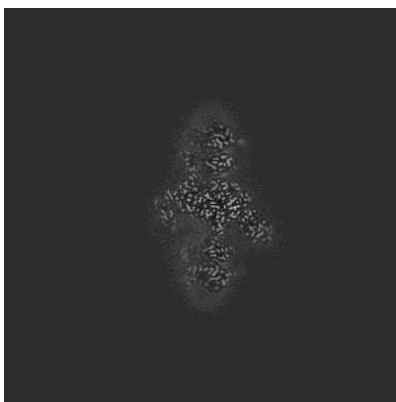
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

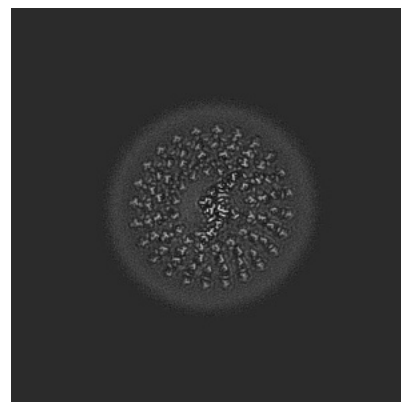
6.2.1 Primary map



X Index: 200



Y Index: 200

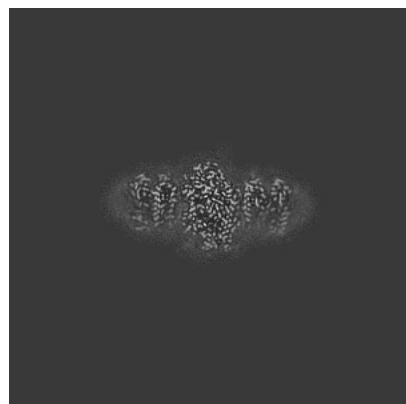


Z Index: 200

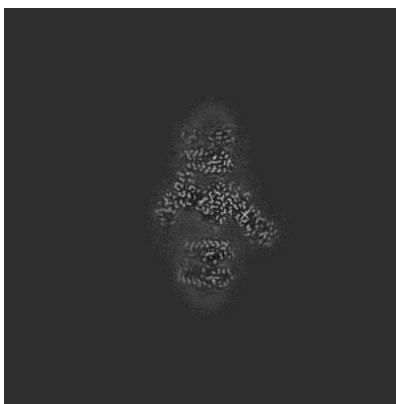
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

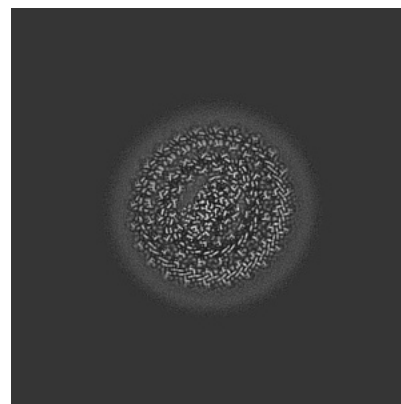
6.3.1 Primary map



X Index: 209



Y Index: 207

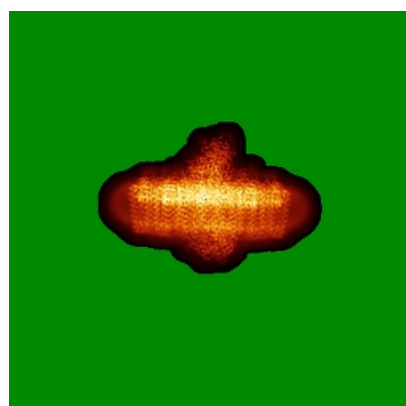


Z Index: 214

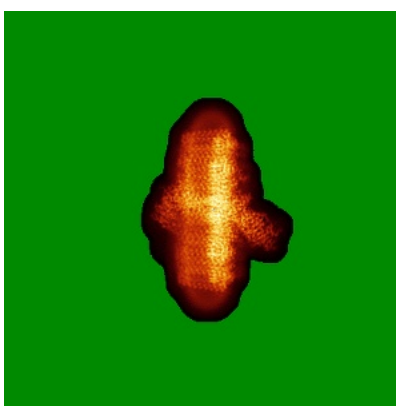
The images above show the largest variance slices of the map in three orthogonal directions.

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

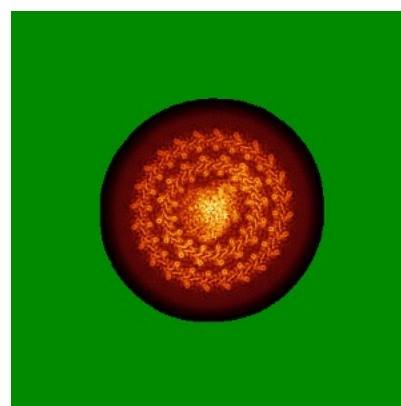
6.4.1 Primary map



X



Y

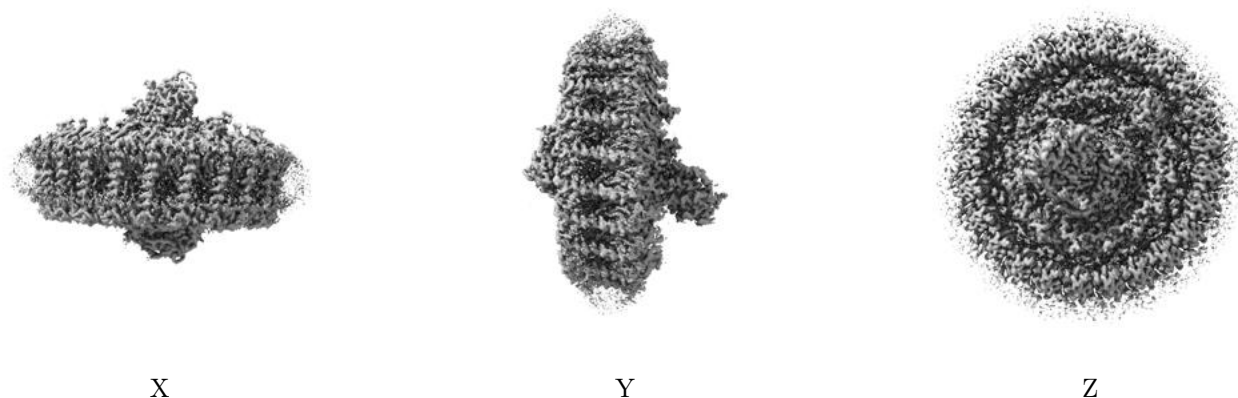


Z

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 0.0238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

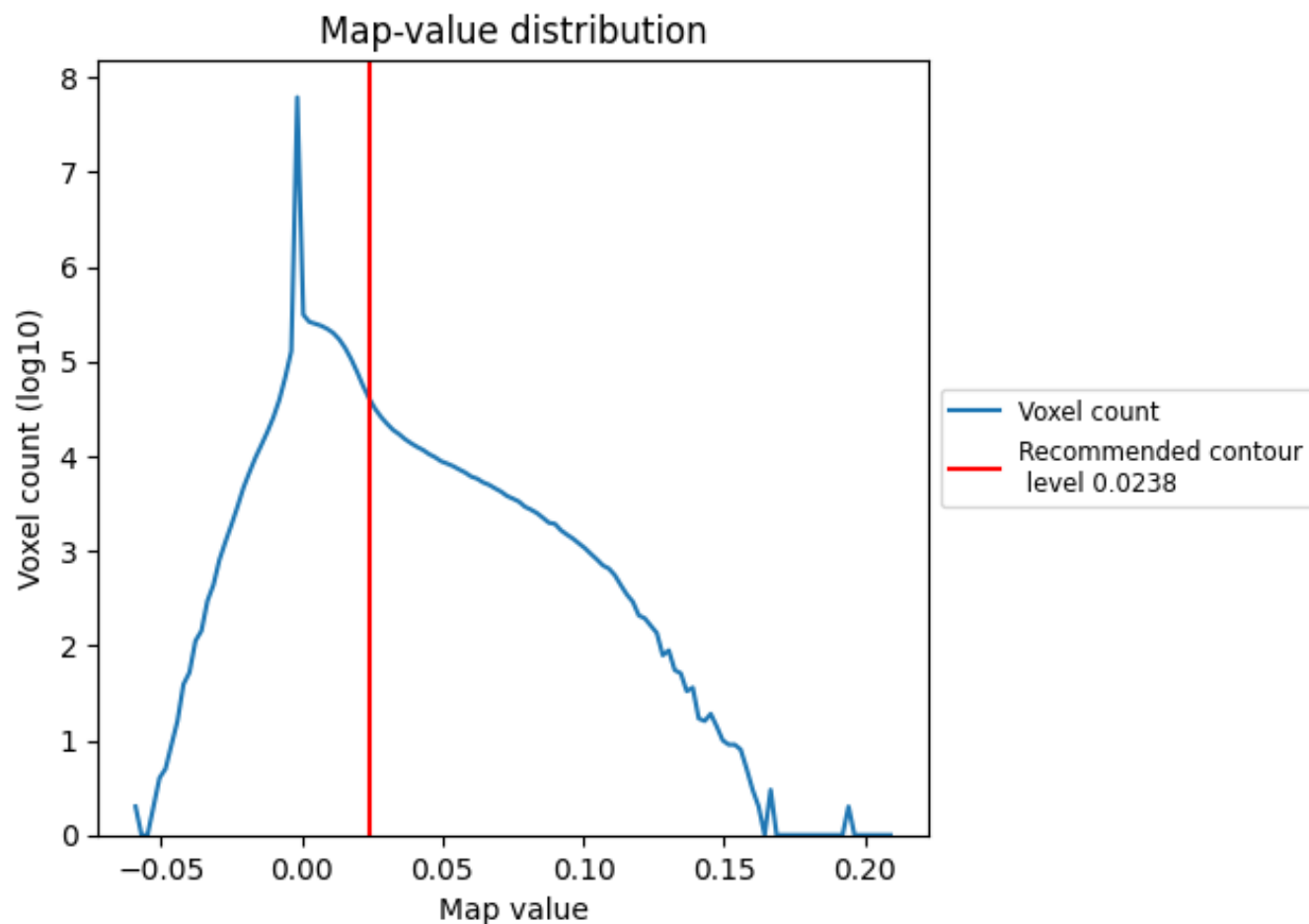
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

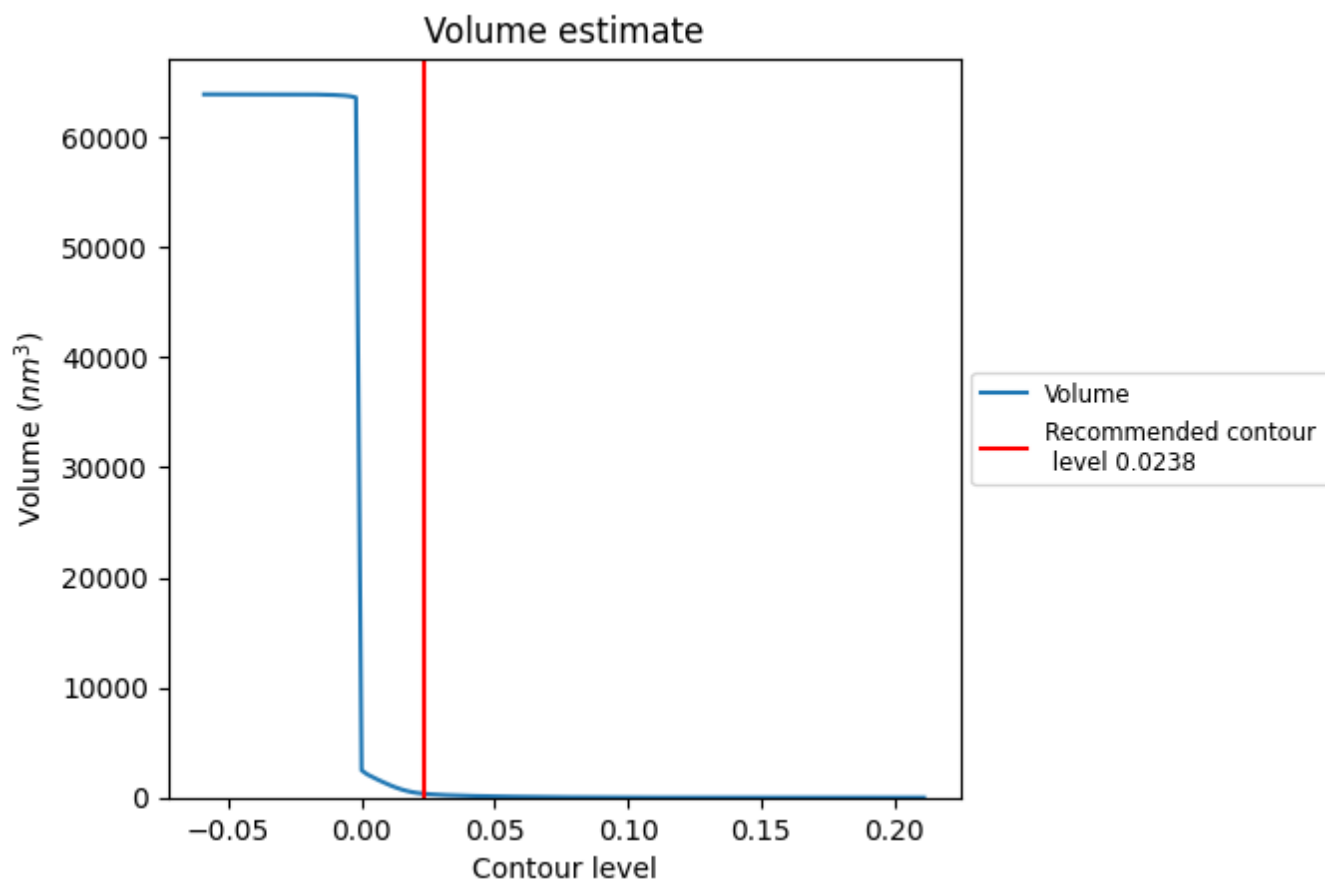
This section contains the results of statistical analysis of the map.

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.

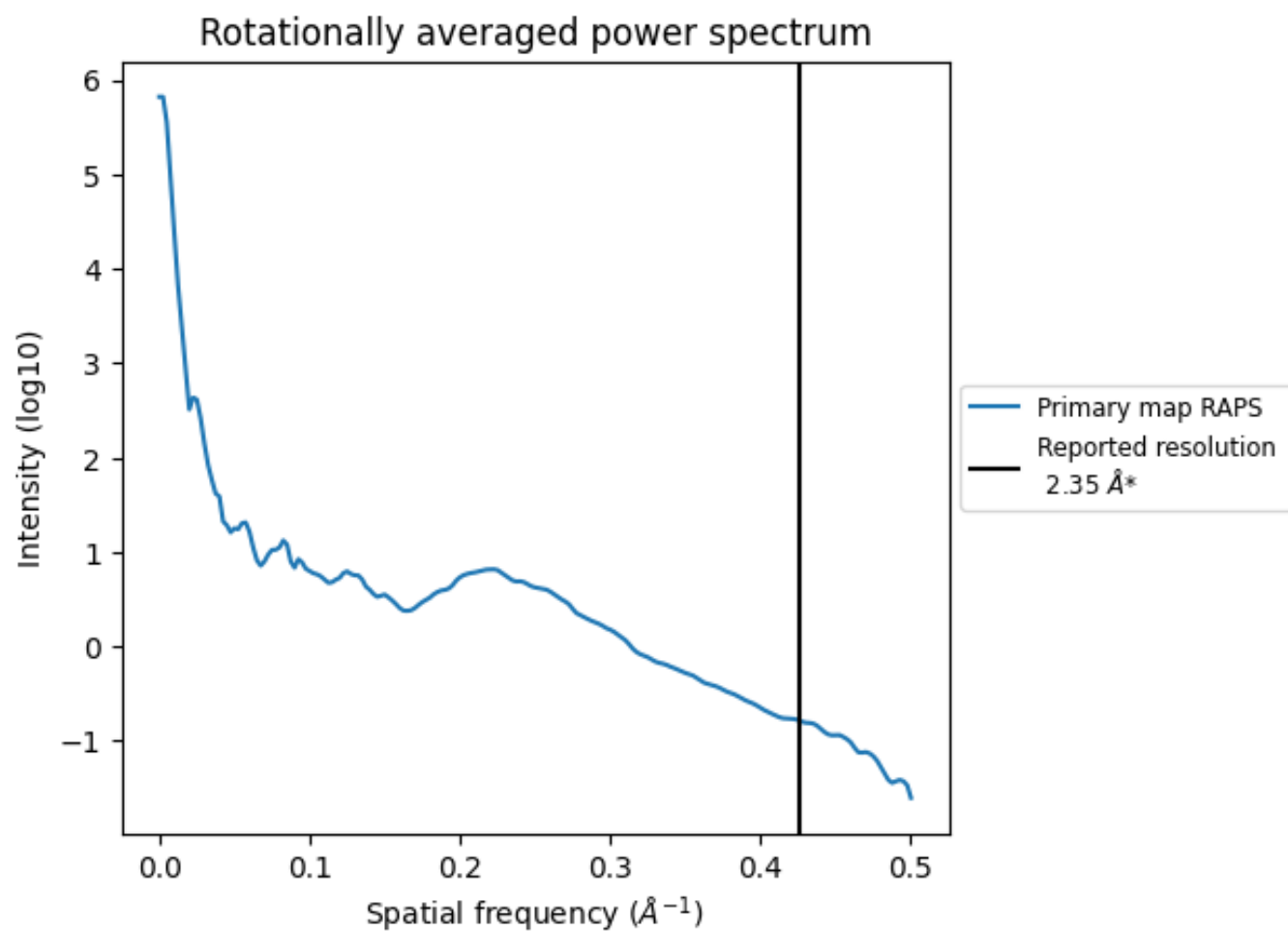
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm^3 ; this corresponds to an approximate mass of 307 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 ⓘ

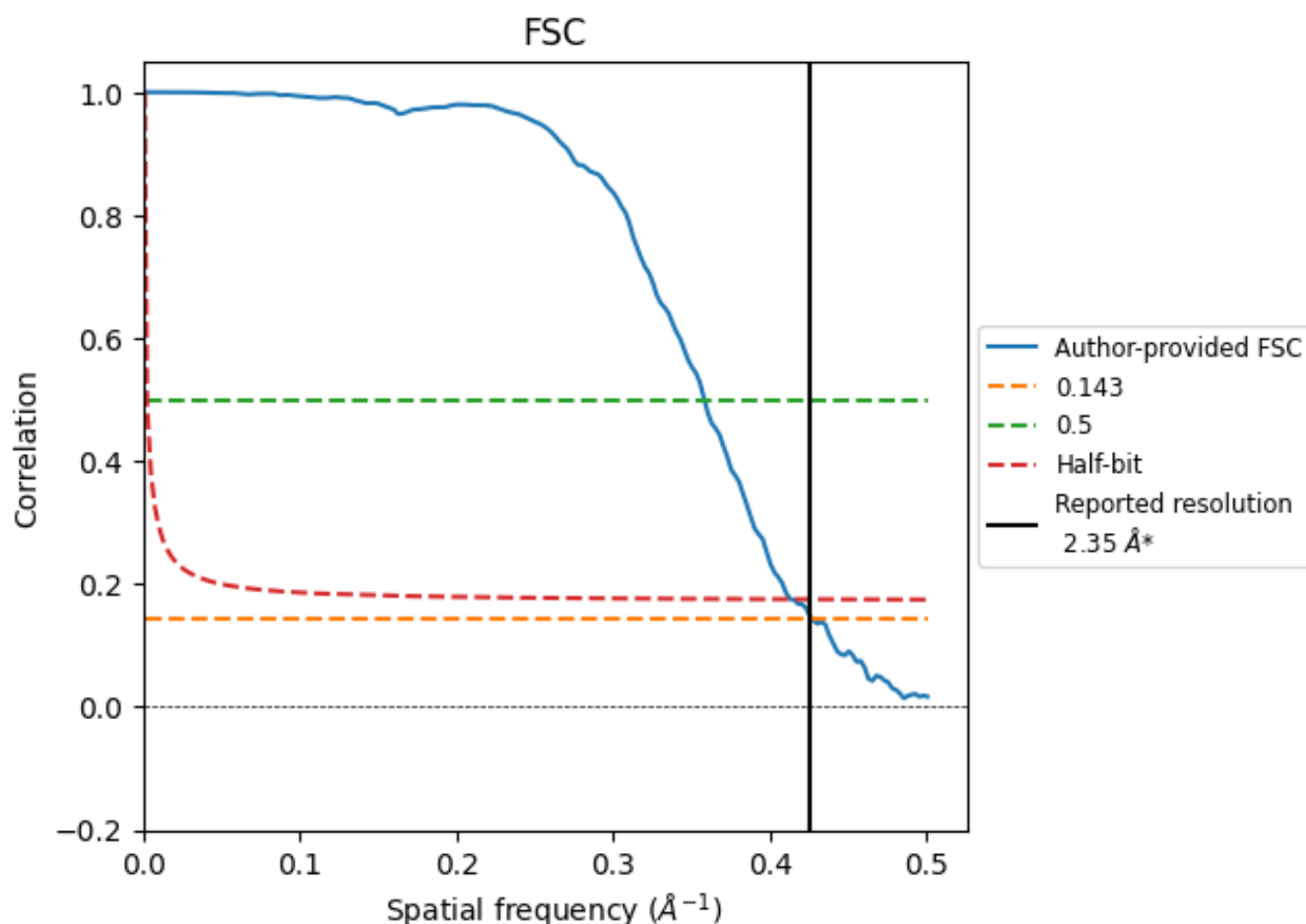


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

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 0.426 Å⁻¹

8.2 Resolution estimates [i](#)

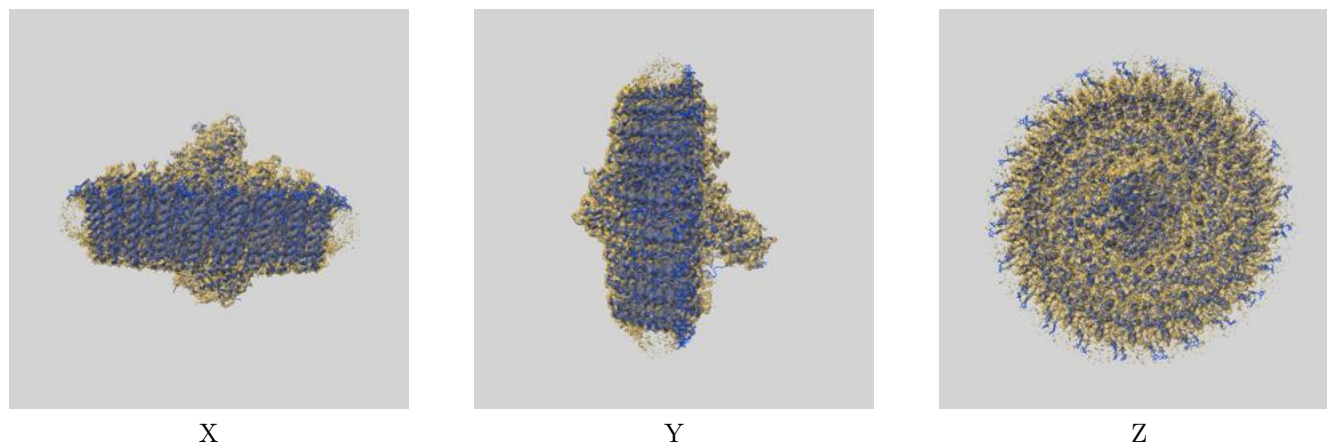
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.34	2.79	2.42
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

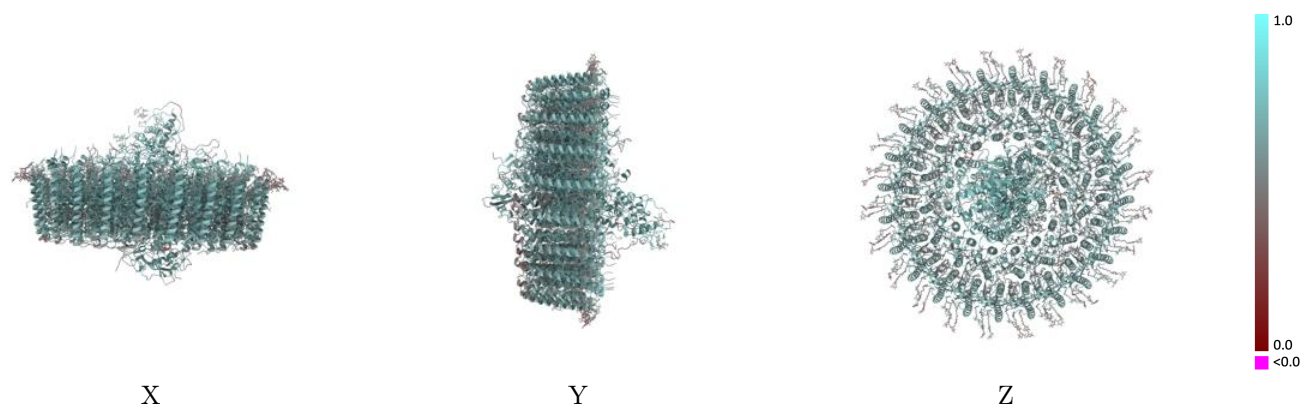
This section contains information regarding the fit between EMDB map EMD-12679 and PDB model 7O0U. Per-residue inclusion information can be found in [section 3](#) on [page 38](#).

9.1 Map-model overlay [i](#)



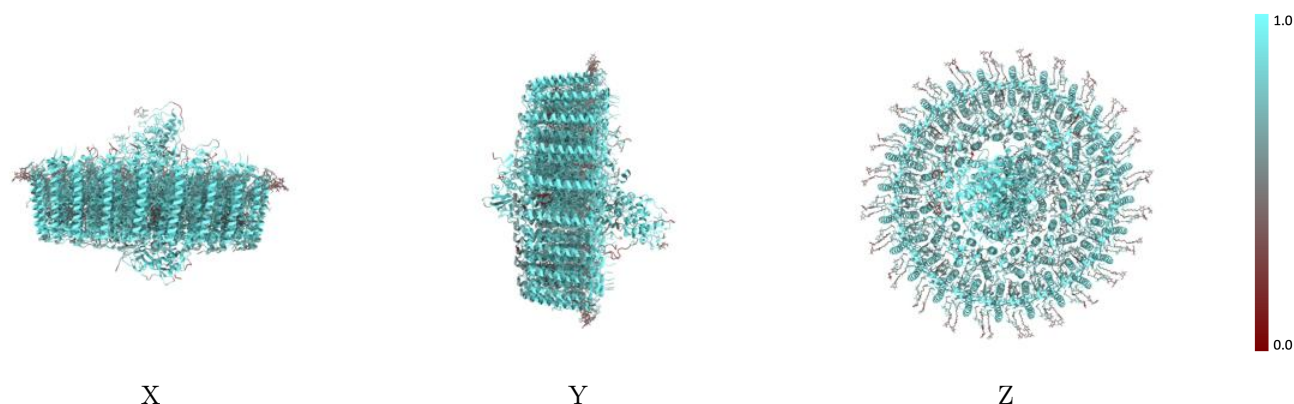
The images above show the 3D surface view of the map at the recommended contour level 0.0238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



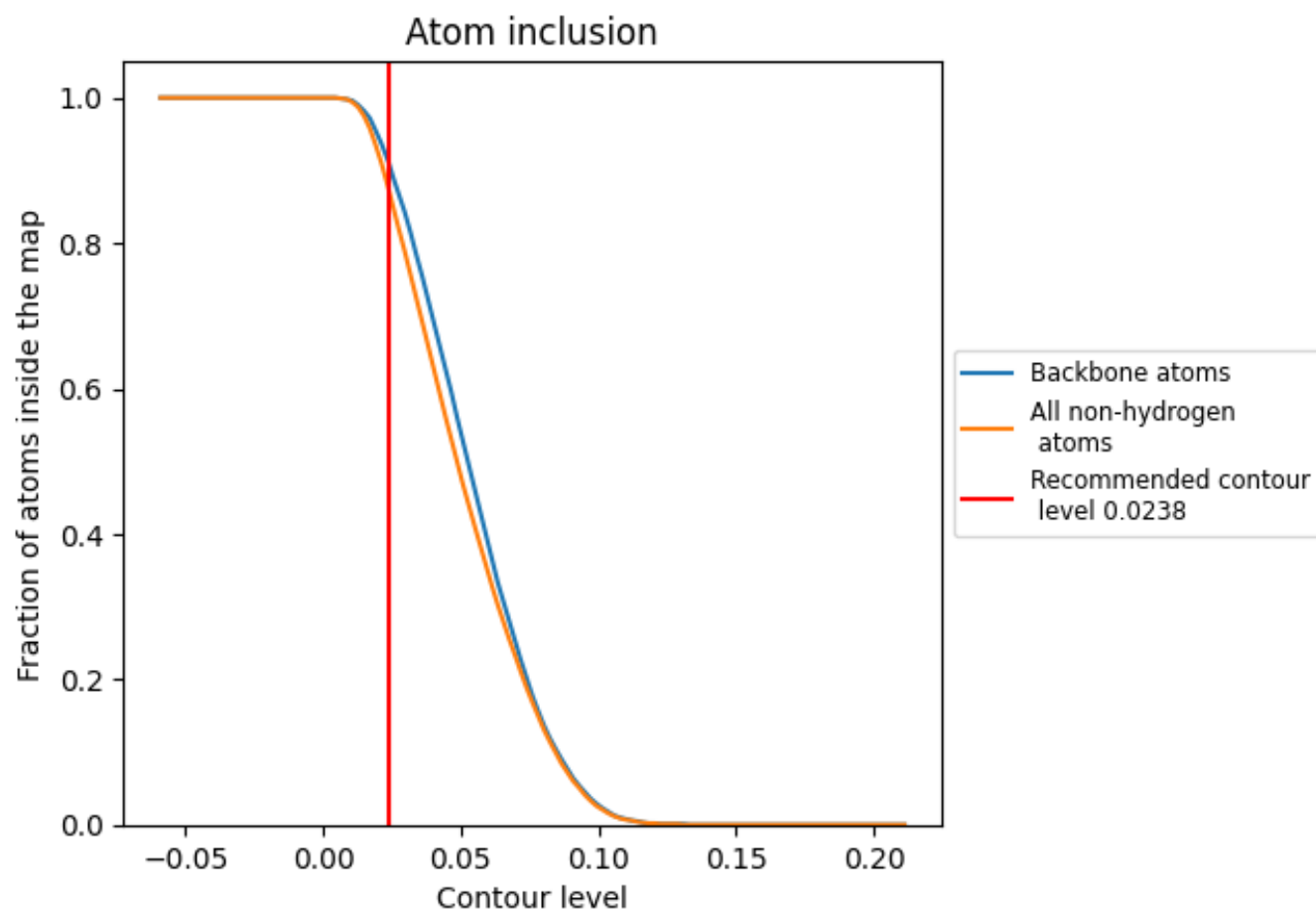
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0238).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.0238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.6290
AA	 0.9010	 0.6220
AB	 0.8030	 0.5930
AC	 0.9450	 0.6330
AD	 0.9230	 0.6400
AE	 0.8790	 0.6220
AF	 0.8660	 0.6200
AG	 0.9470	 0.6570
AH	 0.8960	 0.6300
AI	 0.8450	 0.6110
AJ	 0.9250	 0.6430
AK	 0.8930	 0.6300
AL	 0.8270	 0.5890
AM	 0.9150	 0.6430
AN	 0.8220	 0.5970
AO	 0.9480	 0.6420
AP	 0.9340	 0.6470
AQ	 0.9000	 0.6250
AR	 0.8450	 0.6120
AS	 0.8910	 0.6350
AT	 0.8950	 0.6180
AU	 0.8700	 0.6210
AV	 0.8960	 0.6310
AW	 0.8540	 0.5990
AX	 0.9460	 0.6360
BA	 0.7370	 0.5660
BB	 0.7880	 0.5780
BC	 0.7820	 0.5840
BD	 0.7800	 0.5790
BE	 0.8240	 0.5860
BF	 0.8460	 0.6040
BG	 0.8000	 0.6070
BH	 0.8360	 0.6030
BI	 0.8010	 0.5870
BJ	 0.8320	 0.6100



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Chain	Atom inclusion	Q-score
BK	 0.8320	 0.6100
BL	 0.8030	 0.5840
BM	 0.8170	 0.5930
BN	 0.8190	 0.5900
BO	 0.7980	 0.5860
BP	 0.8260	 0.6020
BQ	 0.8380	 0.6070
BR	 0.8010	 0.5940
BS	 0.7870	 0.5910
BT	 0.8030	 0.5950
BU	 0.7810	 0.5670
BV	 0.8090	 0.5890
BW	 0.8130	 0.5930
BX	 0.8270	 0.5840
C	 0.9410	 0.6750
C1	 0.9310	 0.6730
CG	 0.7140	 0.5680
H1	 0.8800	 0.6510
H2	 0.8770	 0.6140
L	 0.9600	 0.6930
M	 0.9270	 0.6800
MG	 1.0000	 0.6230
aa	 0.8560	 0.6190
ab	 0.8830	 0.6350
ac	 0.9050	 0.6460
ad	 0.9280	 0.6640
ae	 0.8880	 0.6560
af	 0.9080	 0.6530
ag	 0.8400	 0.6230
ah	 0.8890	 0.6340
ai	 0.8720	 0.6320
aj	 0.9160	 0.6430
ak	 0.9540	 0.6680
al	 0.9050	 0.6550
am	 0.9240	 0.6620
an	 0.8030	 0.6070
ao	 0.8500	 0.6020
ap	 0.8390	 0.6030
ba	 0.8520	 0.6190
bb	 0.8400	 0.6080
bc	 0.8960	 0.6360
bd	 0.8900	 0.6440

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Chain	Atom inclusion	Q-score
be	 0.8860	 0.6340
bf	 0.9060	 0.6430
bg	 0.8920	 0.6460
bh	 0.8950	 0.6400
bi	 0.8740	 0.6230
bj	 0.8920	 0.6320
bk	 0.9070	 0.6390
bl	 0.8860	 0.6330
bm	 0.8820	 0.6340
bn	 0.8610	 0.6160
bo	 0.8500	 0.6030
bp	 0.8280	 0.5920