



wwPDB EM Validation Summary Report ⓘ

Sep 11, 2026 – 06:45 am BST

PDB ID : 7O0X / pdb_00007o0x
EMDB ID : EMD-12682
Title : Cryo-EM structure (model_2b) of the RC-dLH complex from Gemmatimonas phototrophica at 2.44 Å
Authors : Qian, P.; Koblizek, M.
Deposited on : 2021-03-28
Resolution : 2.44 Å (reported)
Based on initial models : 6ET5, 1LGH, 5Y5S

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

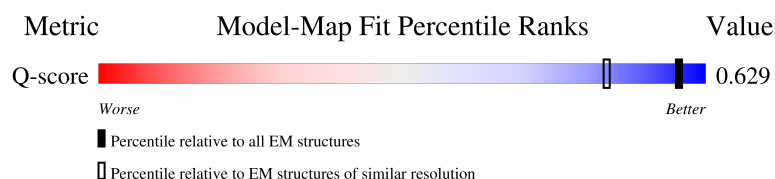
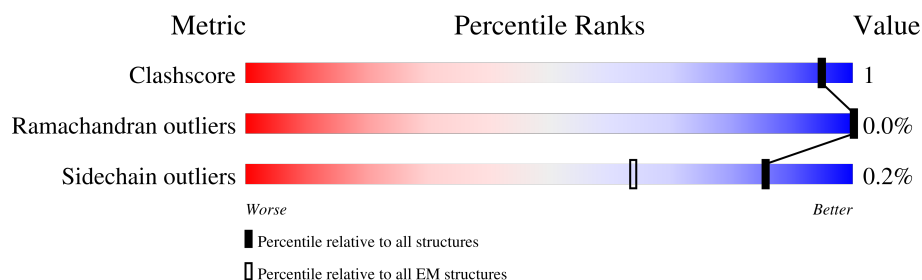
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.44 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.



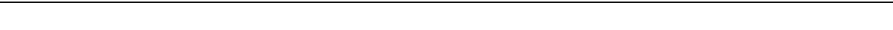
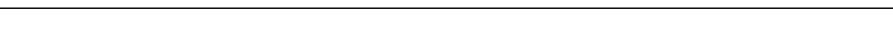
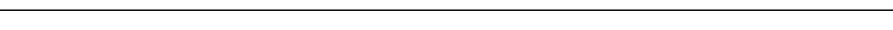
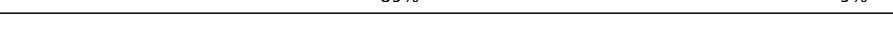
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5856 (1.94 - 2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	54	89% 9%
1	AB	54	87% 9%
1	AC	54	81% 7% 11%
1	AD	54	87% 11%

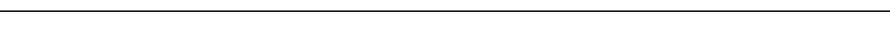
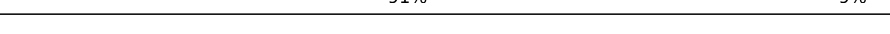
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Mol	Chain	Length	Quality of chain
1	AE	54	 89% 9%
1	AF	54	 87% 9%
1	AG	54	 89% 9%
1	AH	54	 87% 9%
1	AI	54	 89% 9%
1	AJ	54	 89% 9%
1	AK	54	 89% 9%
1	AL	54	 89% 9%
1	AM	54	 89% 9%
1	AN	54	 85% 9%
1	AO	54	 89% 9%
1	AP	54	 87% 9%
1	AQ	54	 87% 9%
1	AR	54	 89% 9%
1	AS	54	 85% 6% 9%
1	AT	54	 87% 9%
1	AU	54	 91% 9%
1	AV	54	 89% 9%
1	AW	54	 91% 9%
1	AX	54	 89% 9%
2	BA	44	 89% 11%
2	BB	44	 86% 5% 9%
2	BC	44	 86% 11%
2	BD	44	 91% 9%
2	BE	44	 91% 9%

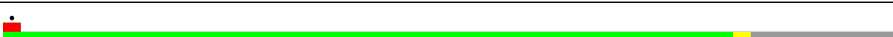
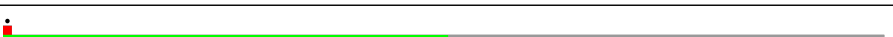
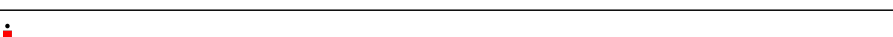
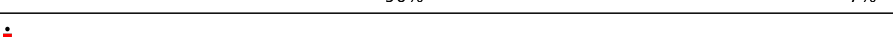
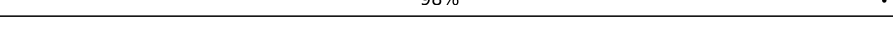
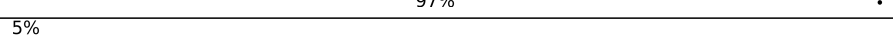
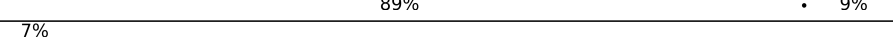
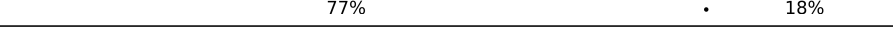
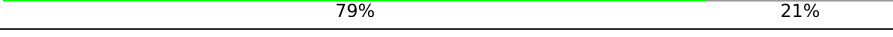
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Mol	Chain	Length	Quality of chain
2	BF	44	
2	BG	44	
2	BH	44	
2	BI	44	
2	BJ	44	
2	BK	44	
2	BL	44	
2	BM	44	
2	BN	44	
2	BO	44	
2	BP	44	
2	BQ	44	
2	BR	44	
2	BS	44	
2	BT	44	
2	BU	44	
2	BV	44	
2	BW	44	
2	BX	44	
2	ba	44	
2	bb	44	
2	bc	44	
2	bd	44	
2	be	44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

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Mol	Chain	Length	Quality of chain
2	bg	44	
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	
3	C	354	
4	C1	202	
5	C2	125	
6	H1	67	
7	H2	181	
8	L	274	
9	M	367	
10	aa	71	
11	ab	71	
11	ac	71	
11	ad	71	
11	ae	71	
11	af	71	
11	ag	71	
11	ah	71	

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Mol	Chain	Length	Quality of chain
11	ai	71	
11	aj	71	
11	ak	71	
11	al	71	
11	am	71	
11	an	71	
11	ao	71	
11	ap	71	
12	CG	2	
12	MG	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	HEC	C	1001	X	-	-	-
16	HEC	C	1002	X	-	-	-
16	HEC	C	1003	X	-	-	-
16	HEC	C	1004	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 56446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called LHH-alpha.

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

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

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

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

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

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

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

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

- Molecule 4 is a protein called RC-S.

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

- Molecule 5 is a protein called RC-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C2	99	Total	C	N	O	S	0	0
			766	483	148	132	3		

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

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

- Molecule 7 is a protein called RC-Hc.

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

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

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

- Molecule 9 is a protein called RC-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	335	Total	C	N	O	S	0	0
			2694	1789	442	453	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aa	55	Total	C	N	O	S	0	0
			433	284	76	71	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	ab	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	ac	56	Total	C	N	O	S	0	0
			443	290	77	73	3		
11	ad	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ae	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	af	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	ag	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
11	ah	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ai	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	aj	60	Total	C	N	O	S	0	0
			465	304	81	77	3		

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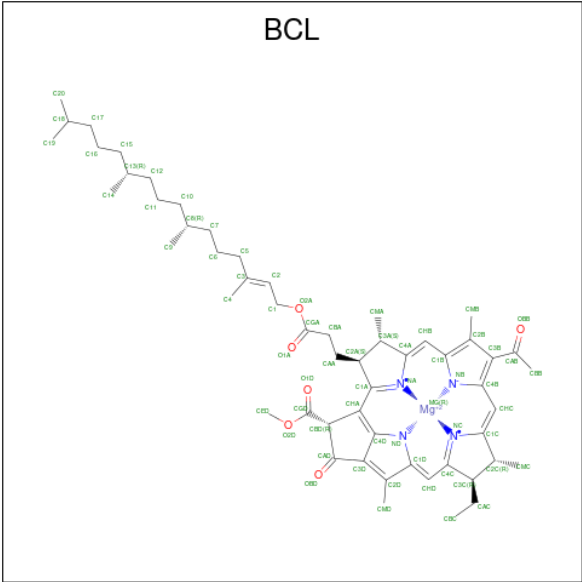
Mol	Chain	Residues	Atoms					AltConf	Trace
11	ak	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
11	al	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	am	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	an	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
11	ao	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
11	ap	71	Total	C	N	O	S	0	0
			543	352	95	92	4		

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



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

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



Mol	Chain	Residues	Atoms					AltConf
13	AA	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AA	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0

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

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

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

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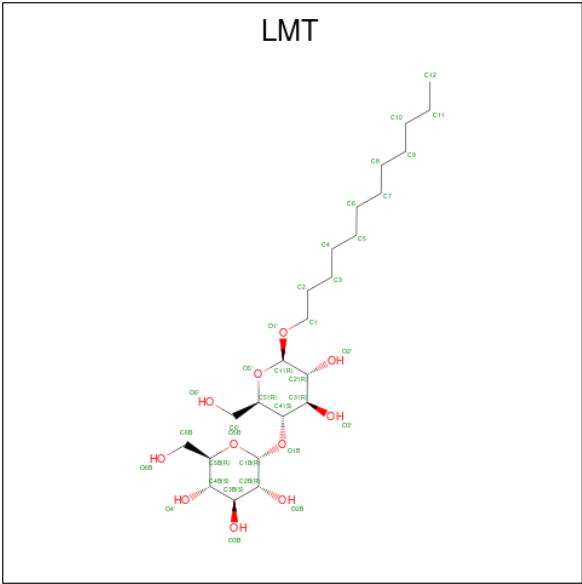
Mol	Chain	Residues	Atoms					AltConf
13	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	ai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

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

- Molecule 14 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

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Mol	Chain	Residues	Atoms			AltConf
14	AB	1	Total	C	O	0
			35	24	11	
14	AB	1	Total	C	O	0
			35	24	11	
14	AD	1	Total	C	O	0
			35	24	11	
14	AD	1	Total	C	O	0
			35	24	11	
14	AF	1	Total	C	O	0
			35	24	11	
14	AG	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			35	24	11	
14	AH	1	Total	C	O	0
			35	24	11	
14	AI	1	Total	C	O	0
			35	24	11	
14	AJ	1	Total	C	O	0
			35	24	11	
14	AK	1	Total	C	O	0
			35	24	11	
14	AL	1	Total	C	O	0
			35	24	11	
14	AN	1	Total	C	O	0
			35	24	11	
14	AN	1	Total	C	O	0
			35	24	11	
14	AO	1	Total	C	O	0
			35	24	11	
14	AP	1	Total	C	O	0
			35	24	11	
14	AR	1	Total	C	O	0
			35	24	11	
14	AS	1	Total	C	O	0
			35	24	11	
14	AT	1	Total	C	O	0
			35	24	11	
14	AU	1	Total	C	O	0
			35	24	11	

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

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

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

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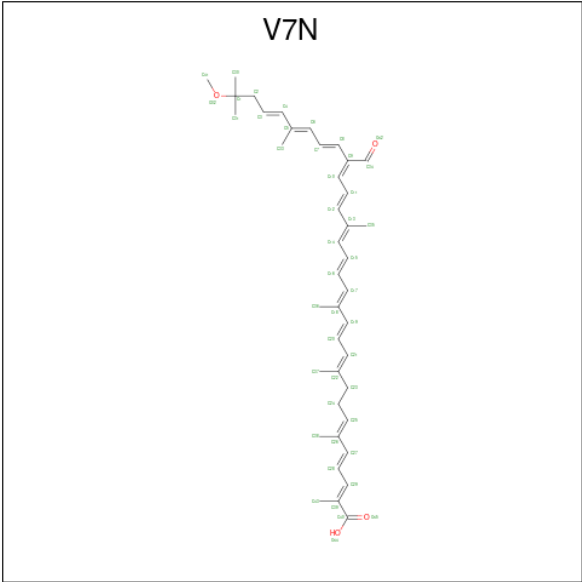
Mol	Chain	Residues	Atoms			AltConf
14	BU	1	Total	C	O	0
			35	24	11	
14	BU	1	Total	C	O	0
			35	24	11	
14	BU	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BV	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BW	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	BX	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	M	1	Total	C	O	0
			35	24	11	
14	ac	1	Total	C	O	0
			35	24	11	
14	bb	1	Total	C	O	0
			35	24	11	
14	bc	1	Total	C	O	0
			35	24	11	
14	bd	1	Total	C	O	0
			35	24	11	

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

- Molecule 15 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-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
15	AE	1	Total	C	O	0
			45	41	4	
15	AH	1	Total	C	O	0
			45	41	4	
15	AT	1	Total	C	O	0
			45	41	4	
15	BA	1	Total	C	O	0
			45	41	4	
15	BB	1	Total	C	O	0
			45	41	4	
15	BC	1	Total	C	O	0
			45	41	4	
15	BD	1	Total	C	O	0
			45	41	4	
15	BE	1	Total	C	O	0
			45	41	4	
15	BG	1	Total	C	O	0
			45	41	4	
15	BH	1	Total	C	O	0
			45	41	4	
15	BJ	1	Total	C	O	0
			45	41	4	
15	BK	1	Total	C	O	0
			45	41	4	
15	BL	1	Total	C	O	0
			45	41	4	
15	BM	1	Total	C	O	0
			45	41	4	

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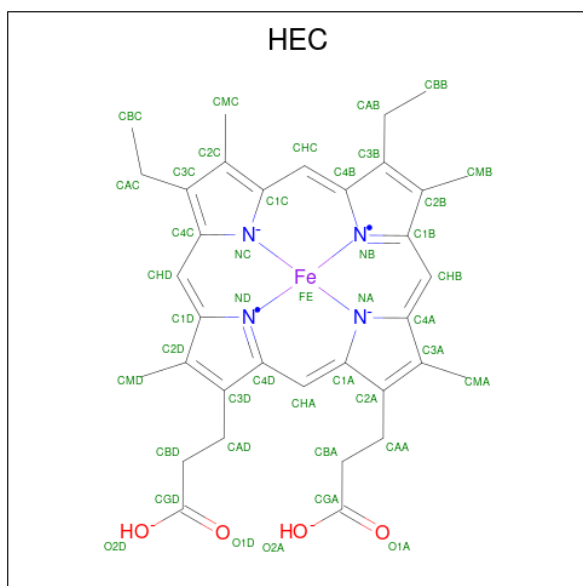
Mol	Chain	Residues	Atoms			AltConf
15	BN	1	Total 45	C 41	O 4	0
15	BO	1	Total 45	C 41	O 4	0
15	BP	1	Total 45	C 41	O 4	0
15	BQ	1	Total 45	C 41	O 4	0
15	BR	1	Total 45	C 41	O 4	0
15	BS	1	Total 45	C 41	O 4	0
15	BT	1	Total 45	C 41	O 4	0
15	BV	1	Total 45	C 41	O 4	0
15	BW	1	Total 45	C 41	O 4	0
15	BX	1	Total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

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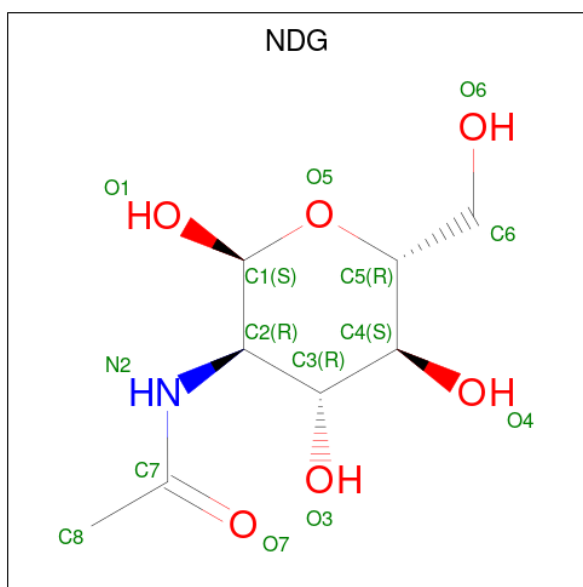
Mol	Chain	Residues	Atoms			AltConf
15	bl	1	Total	C	O	0
			45	41	4	
15	bm	1	Total	C	O	0
			45	41	4	
15	bn	1	Total	C	O	0
			45	41	4	
15	bo	1	Total	C	O	0
			45	41	4	
15	bp	1	Total	C	O	0
			45	41	4	

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



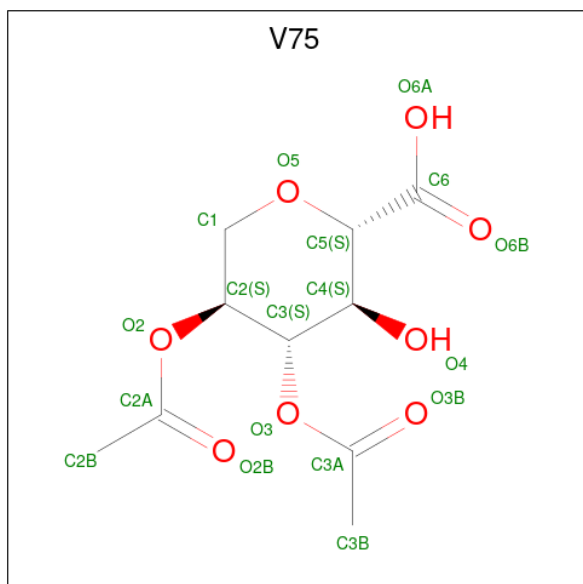
Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



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

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



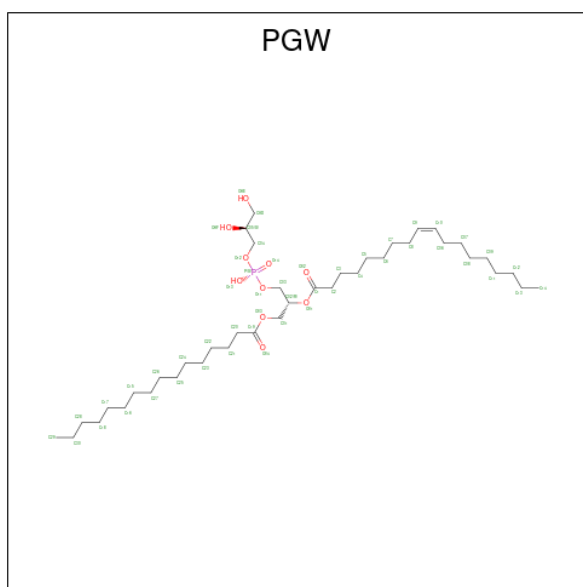
Mol	Chain	Residues	Atoms			AltConf
18	C	1	Total	C	O	0
			18	10	8	

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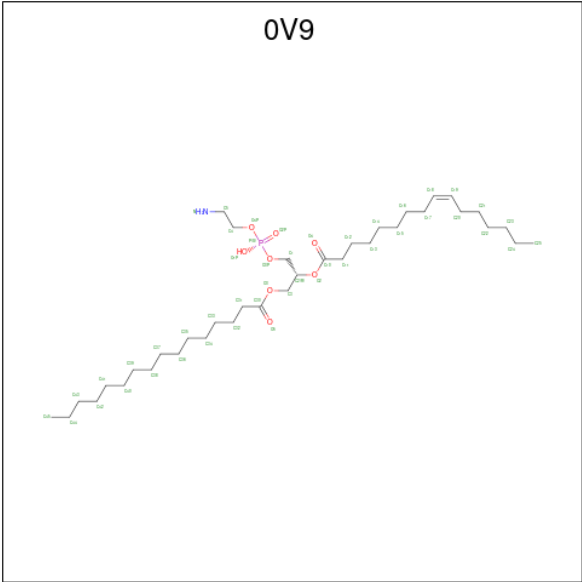
Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	C	O	0
			18	10	8	

- 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: C₄₀H₇₇O₁₀P).



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

- Molecule 20 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) (labeled as "Ligand of Interest" by depositor).



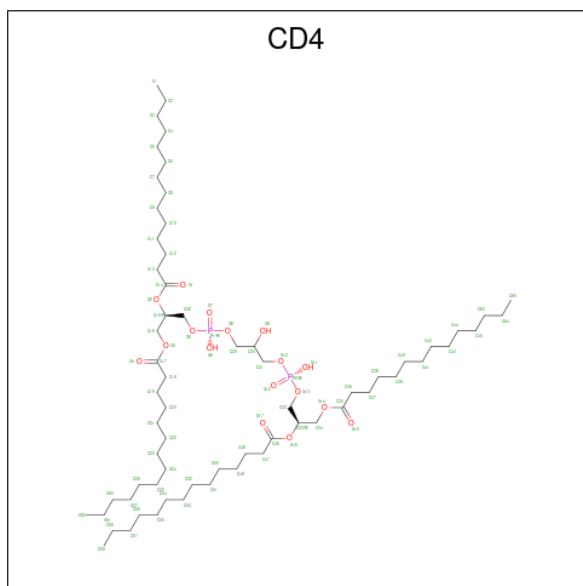
Mol	Chain	Residues	Atoms					AltConf
20	H1	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	aj	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	ba	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	ba	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bb	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bc	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	be	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	be	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bf	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bg	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bh	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bi	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bj	1	Total	C	N	O	P	0
			45	35	1	8	1	

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

- Molecule 21 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: $C_{65}H_{126}O_{17}P_2$).



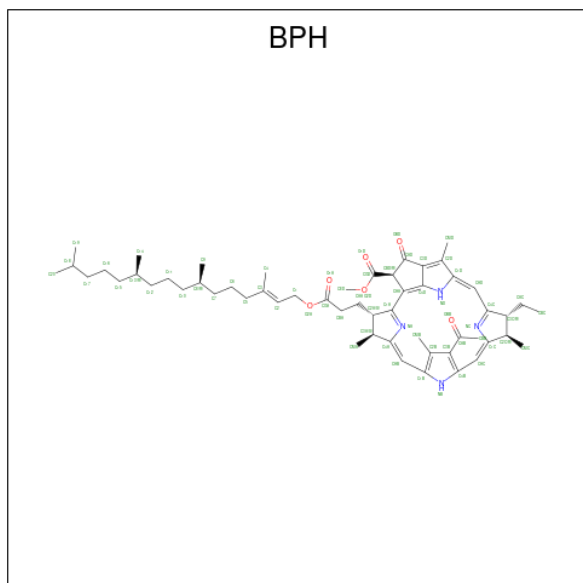
Mol	Chain	Residues	Atoms				AltConf
21	H1	1	Total	C	O	P	0
			84	65	17	2	
21	M	1	Total	C	O	P	0
			84	65	17	2	
21	ad	1	Total	C	O	P	0
			84	65	17	2	
21	af	1	Total	C	O	P	0
			84	65	17	2	

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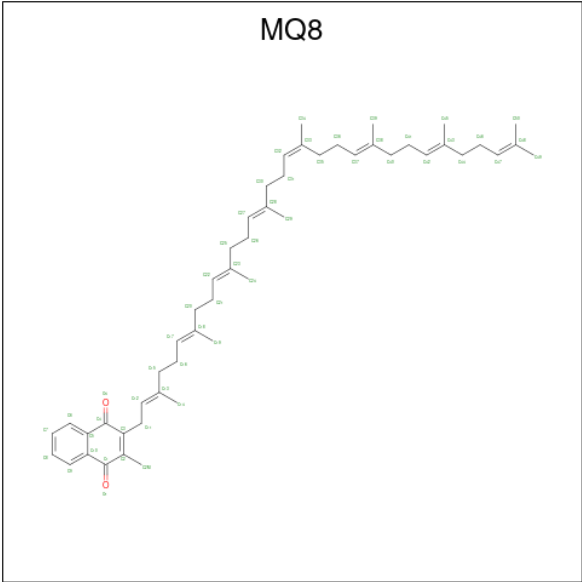
Mol	Chain	Residues	Atoms				AltConf
21	af	1	Total	C	O	P	0
			84	65	17	2	
21	ai	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 22 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
22	L	1	Total	C	N	O	0
			65	55	4	6	
22	M	1	Total	C	N	O	0
			65	55	4	6	

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

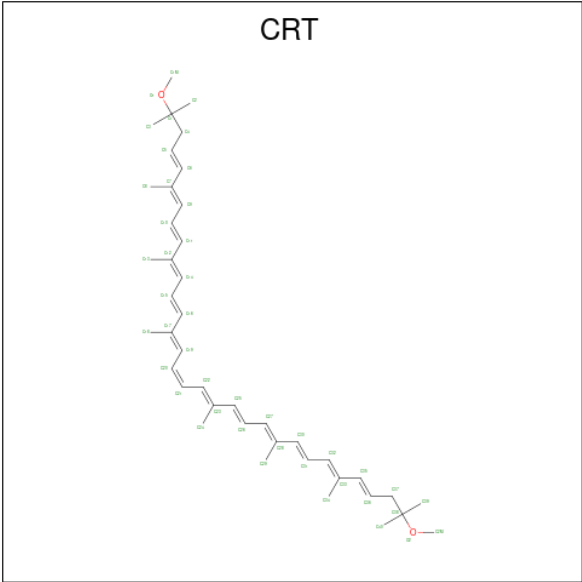


Mol	Chain	Residues	Atoms			AltConf
23	L	1	Total	C	O	0
			53	51	2	
23	M	1	Total	C	O	0
			53	51	2	
23	an	1	Total	C	O	0
			53	51	2	

- Molecule 24 is FE (III) ION (CCD ID: FE) (formula: Fe).

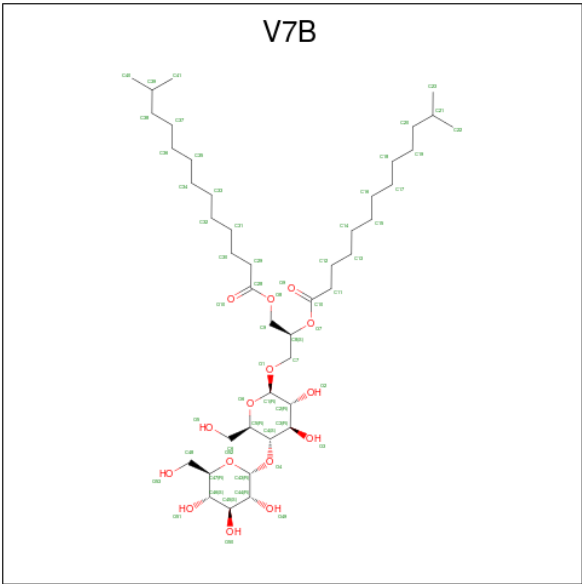
Mol	Chain	Residues	Atoms		AltConf
24	M	1	Total	Fe	0
			1	1	

- Molecule 25 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



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

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



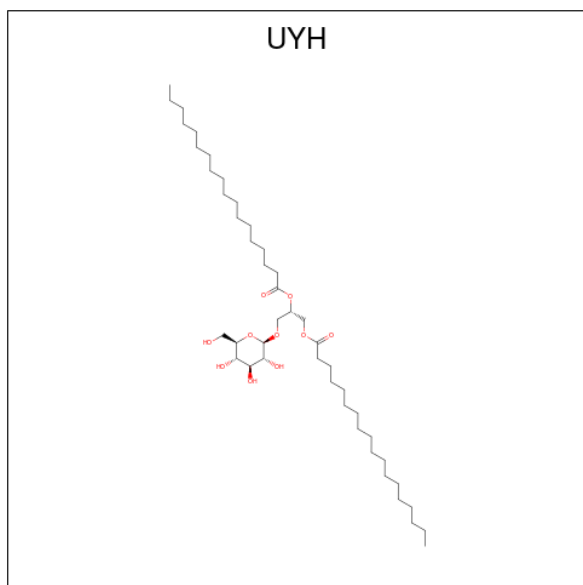
Mol	Chain	Residues	Atoms			AltConf
26	af	1	Total	C	O	0
			58	43	15	

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

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



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	AA	3	Total	O	0
			3	3	
28	AB	3	Total	O	0
			3	3	
28	AC	2	Total	O	0
			2	2	
28	AD	5	Total	O	0
			5	5	
28	AG	2	Total	O	0
			2	2	
28	AH	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
28	AI	3	Total 3	O 3	0
28	AJ	6	Total 6	O 6	0
28	AK	3	Total 3	O 3	0
28	AL	3	Total 3	O 3	0
28	AM	4	Total 4	O 4	0
28	AN	3	Total 3	O 3	0
28	AO	2	Total 2	O 2	0
28	AP	3	Total 3	O 3	0
28	AQ	5	Total 5	O 5	0
28	AR	2	Total 2	O 2	0
28	AS	5	Total 5	O 5	0
28	AT	7	Total 7	O 7	0
28	AV	6	Total 6	O 6	0
28	AW	6	Total 6	O 6	0
28	AX	5	Total 5	O 5	0
28	BD	1	Total 1	O 1	0
28	BE	1	Total 1	O 1	0
28	BF	1	Total 1	O 1	0
28	BO	1	Total 1	O 1	0
28	BW	1	Total 1	O 1	0
28	C	98	Total 98	O 98	0

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Mol	Chain	Residues	Atoms		AltConf
28	C1	48	Total 48	O 48	0
28	C2	3	Total 3	O 3	0
28	H1	9	Total 9	O 9	0
28	H2	35	Total 35	O 35	0
28	L	53	Total 53	O 53	0
28	M	59	Total 59	O 59	0
28	aa	3	Total 3	O 3	0
28	ab	3	Total 3	O 3	0
28	ac	4	Total 4	O 4	0
28	ad	9	Total 9	O 9	0
28	ae	7	Total 7	O 7	0
28	af	7	Total 7	O 7	0
28	ag	7	Total 7	O 7	0
28	ah	6	Total 6	O 6	0
28	ai	3	Total 3	O 3	0
28	aj	6	Total 6	O 6	0
28	ak	14	Total 14	O 14	0
28	al	8	Total 8	O 8	0
28	am	8	Total 8	O 8	0
28	an	5	Total 5	O 5	0
28	ao	2	Total 2	O 2	0

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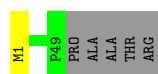
Mol	Chain	Residues	Atoms		AltConf
28	ap	8	Total 8	O 8	0
28	bb	2	Total 2	O 2	0
28	bc	2	Total 2	O 2	0
28	bd	1	Total 1	O 1	0
28	be	1	Total 1	O 1	0
28	bf	1	Total 1	O 1	0
28	bg	1	Total 1	O 1	0
28	bh	2	Total 2	O 2	0
28	bi	3	Total 3	O 3	0
28	bk	4	Total 4	O 4	0
28	bl	3	Total 3	O 3	0
28	bm	4	Total 4	O 4	0
28	bn	3	Total 3	O 3	0
28	bo	2	Total 2	O 2	0
28	bp	1	Total 1	O 1	0

3 Residue-property plots [i](#)

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

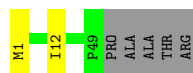
- Molecule 1: LHh-alpha

Chain AA:  89% 9%



- Molecule 1: LHh-alpha

Chain AB:  87% 9%



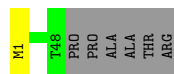
- Molecule 1: LHh-alpha

Chain AC:  81% 7% 11%



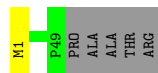
- Molecule 1: LHh-alpha

Chain AD:  87% 11%



- Molecule 1: LHh-alpha

Chain AE:  89% 9%



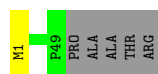
- Molecule 1: LHh-alpha

Chain AF:  87% 9%



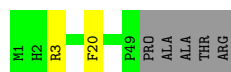
• Molecule 1: LHh-alpha

Chain AG:  89% 9%



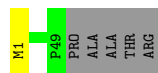
• Molecule 1: LHh-alpha

Chain AH:  87% 9%



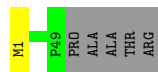
• Molecule 1: LHh-alpha

Chain AI:  89% 9%



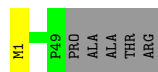
• Molecule 1: LHh-alpha

Chain AJ:  89% 9%



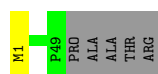
• Molecule 1: LHh-alpha

Chain AK:  89% 9%



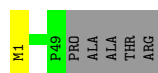
• Molecule 1: LHh-alpha

Chain AL:  89% 9%



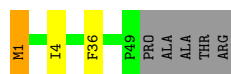
• Molecule 1: LHh-alpha

Chain AM:  89% 9%



- Molecule 1: LHh-alpha

Chain AN:  85% 9%



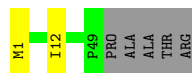
- Molecule 1: LHh-alpha

Chain AO:  89% 9%



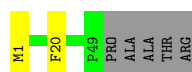
- Molecule 1: LHh-alpha

Chain AP:  87% 9%



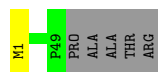
- Molecule 1: LHh-alpha

Chain AQ:  87% 9%



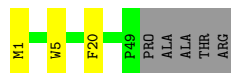
- Molecule 1: LHh-alpha

Chain AR:  89% 9%



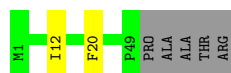
- Molecule 1: LHh-alpha

Chain AS:  85% 6% 9%



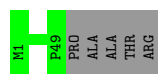
- Molecule 1: LHh-alpha

Chain AT:  87% 9%



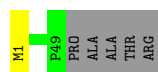
- Molecule 1: LHh-alpha

Chain AU:  91% 9%



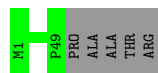
- Molecule 1: LHh-alpha

Chain AV:  89% 9%



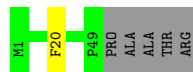
- Molecule 1: LHh-alpha

Chain AW:  91% 9%



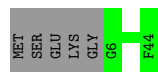
- Molecule 1: LHh-alpha

Chain AX:  89% 9%



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

Chain BA:  89% 11%



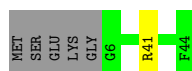
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BB:  86% 5% 9%



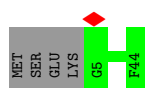
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BC:  86% 11%



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

Chain BD:  91% 9%



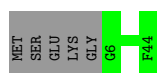
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BE:  91% 9%



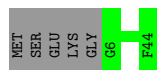
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BF:  89% 11%



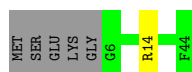
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BG:  89% 11%



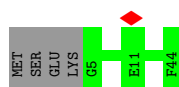
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BH:  86% 11%



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

Chain BI:  91% 9%



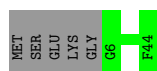
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BJ:  89% 11%



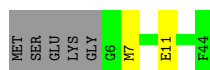
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BK:  89% 11%



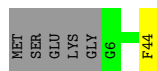
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BL:  84% 5% 11%



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

Chain BM:  86% • 11%



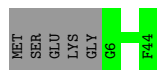
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BN:  84% 5% 11%



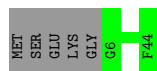
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BO:  89% 11%



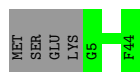
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BP:  89% 11%



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

Chain BQ:  91% 9%



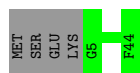
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BR:  91% 9%



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

Chain BS:  91% 9%



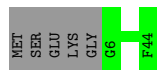
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BT:  91% 9%



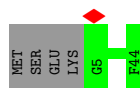
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BU:  89% 11%



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

Chain BV:  91% 9%



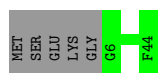
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BW:  89% 9%



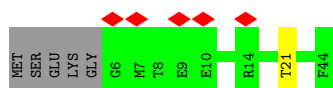
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BX:  89% 11%



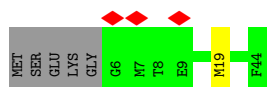
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain ba:  11% 86% 11%



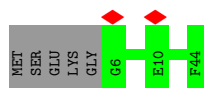
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bb:  7% 86% 11%



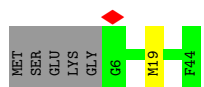
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bc:  5% 89% 11%



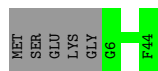
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bd:  86% 11%



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

Chain be:  89% 11%



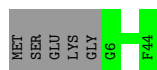
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bf:  86% 11%



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

Chain bg:  89% 11%



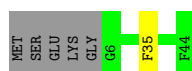
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bh:  86% 11%



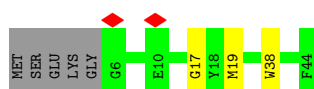
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bi:  86% 11%



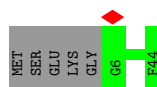
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bj:  82% 7% 11% 5%



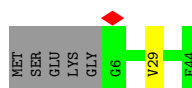
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bk:  89% 11%



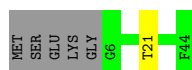
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bl:  86% 11%

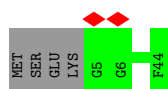
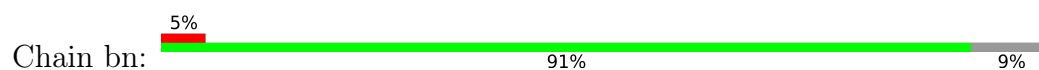


- Molecule 2: Light-harvesting protein B:885 subunit beta

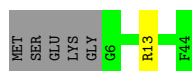
Chain bm:  86% 11%



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



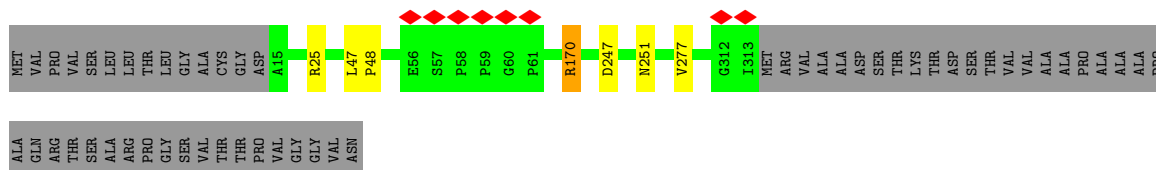
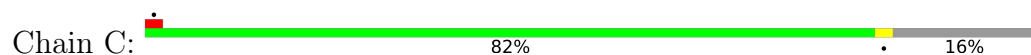
- Molecule 2: Light-harvesting protein B:885 subunit beta



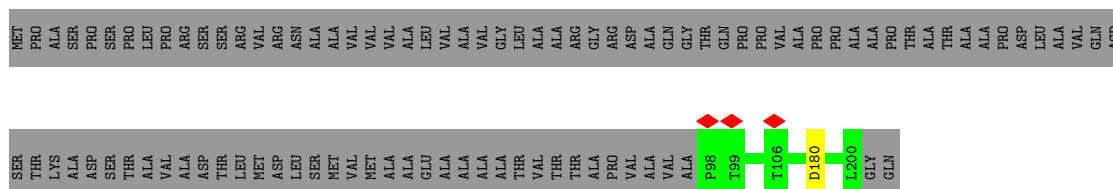
- Molecule 2: Light-harvesting protein B:885 subunit beta



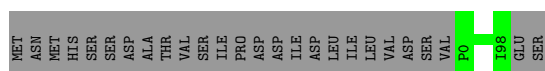
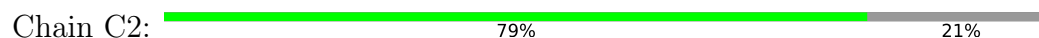
- Molecule 3: MULTHEME_CYTC domain-containing protein



- Molecule 4: RC-S

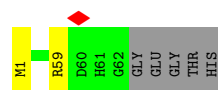


- Molecule 5: RC-U

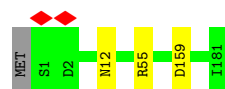


- Molecule 6: PRCH domain-containing protein





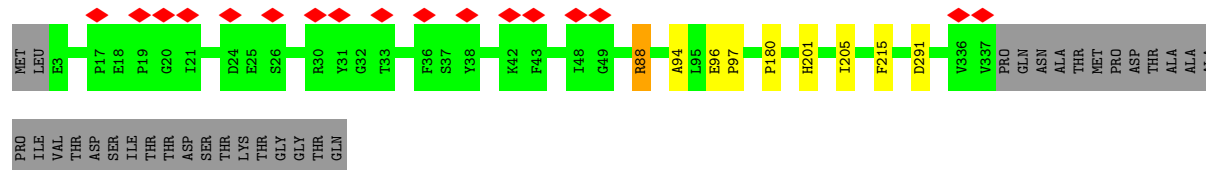
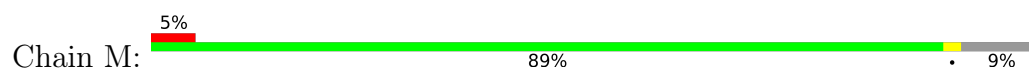
- Molecule 7: RC-Hc



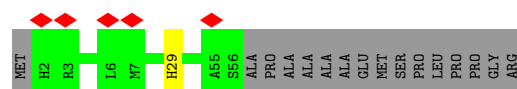
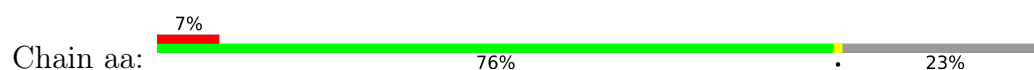
- Molecule 8: Photosynthetic reaction center L subunit



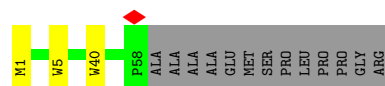
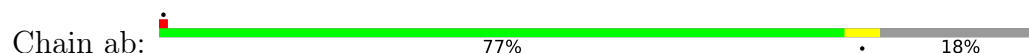
- Molecule 9: RC-M



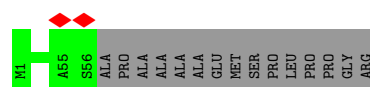
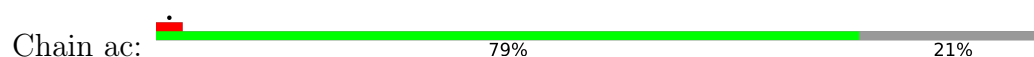
- Molecule 10: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein

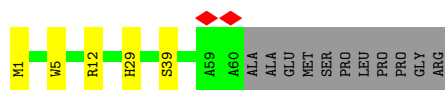


- Molecule 11: LHC domain-containing protein



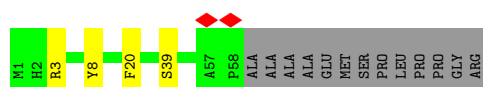
- Molecule 11: LHC domain-containing protein

Chain ad:  77% 7% 15%



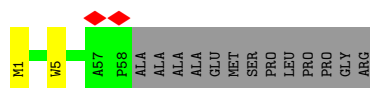
- Molecule 11: LHC domain-containing protein

Chain ae:  76% 6% 18%



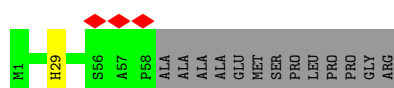
- Molecule 11: LHC domain-containing protein

Chain af:  79% 0% 18%



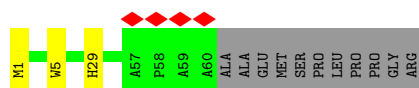
- Molecule 11: LHC domain-containing protein

Chain ag:  80% 0% 18%



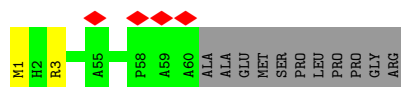
- Molecule 11: LHC domain-containing protein

Chain ah:  6% 80% 0% 15%



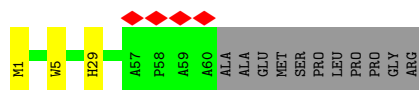
- Molecule 11: LHC domain-containing protein

Chain ai:  6% 82% 0% 15%

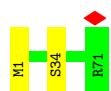


- Molecule 11: LHC domain-containing protein

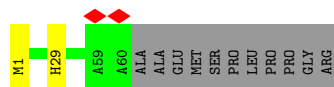
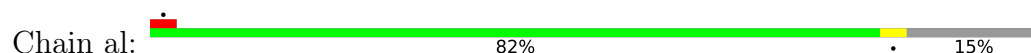
Chain aj:  6% 80% 0% 15%



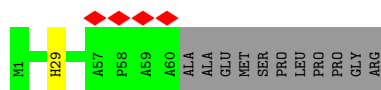
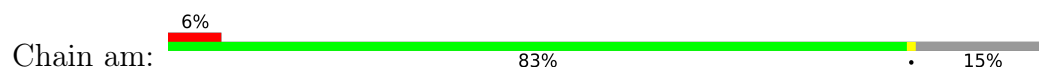
- Molecule 11: LHC domain-containing protein



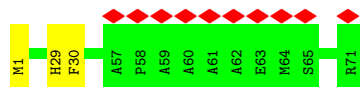
- Molecule 11: LHC domain-containing protein



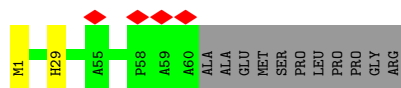
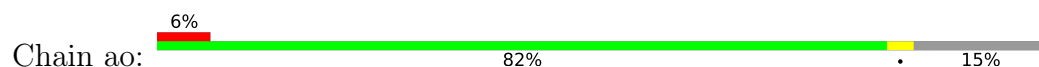
- Molecule 11: LHC domain-containing protein



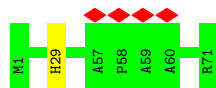
- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein



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

Chain MG:  100%

MAN1
MAN2

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

Chain CG:  100%

MAN1
MAN2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73853	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	0.204	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0292	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: RAM, FME, MQ8, FE, CRT, MAN, CD4, NDG, PGW, BCL, BPH, HEC, V7N, UYH, LMT, V75, 0V9, V7B

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	0.45	0/541
1	AB	0.15	0/396	0.46	0/541
1	AC	0.14	0/388	0.48	0/529
1	AD	0.14	0/388	0.47	0/529
1	AE	0.15	0/396	0.45	0/541
1	AF	0.15	0/396	0.45	0/541
1	AG	0.15	0/396	0.46	0/541
1	AH	0.14	0/396	0.45	0/541
1	AI	0.14	0/396	0.44	0/541
1	AJ	0.16	0/396	0.47	0/541
1	AK	0.15	0/396	0.48	0/541
1	AL	0.14	0/396	0.48	0/541
1	AM	0.13	0/396	0.44	0/541
1	AN	0.14	0/396	0.46	0/541
1	AO	0.15	0/396	0.47	0/541
1	AP	0.15	0/396	0.46	0/541
1	AQ	0.14	0/396	0.46	0/541
1	AR	0.14	0/396	0.43	0/541
1	AS	0.14	0/396	0.48	0/541
1	AT	0.14	0/396	0.48	0/541
1	AU	0.14	0/396	0.46	0/541
1	AV	0.14	0/396	0.47	0/541
1	AW	0.14	0/396	0.50	0/541
1	AX	0.15	0/396	0.47	0/541
2	BA	0.12	0/336	0.42	0/456
2	BB	0.12	0/340	0.41	0/461
2	BC	0.12	0/336	0.42	0/456
2	BD	0.13	0/340	0.42	0/461
2	BE	0.11	0/340	0.39	0/461
2	BF	0.13	0/336	0.42	0/456
2	BG	0.13	0/336	0.40	0/456

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BH	0.12	0/336	0.39	0/456
2	BI	0.11	0/340	0.40	0/461
2	BJ	0.12	0/336	0.39	0/456
2	BK	0.13	0/336	0.43	0/456
2	BL	0.14	0/336	0.47	0/456
2	BM	0.13	0/336	0.43	0/456
2	BN	0.13	0/336	0.43	0/456
2	BO	0.12	0/336	0.46	0/456
2	BP	0.13	0/336	0.43	0/456
2	BQ	0.13	0/340	0.43	0/461
2	BR	0.14	0/340	0.46	0/461
2	BS	0.12	0/340	0.42	0/461
2	BT	0.14	0/340	0.47	0/461
2	BU	0.12	0/336	0.43	0/456
2	BV	0.13	0/340	0.42	0/461
2	BW	0.12	0/340	0.43	0/461
2	BX	0.13	0/336	0.41	0/456
2	ba	0.14	0/336	0.45	0/456
2	bb	0.12	0/336	0.41	0/456
2	bc	0.14	0/336	0.45	0/456
2	bd	0.15	0/336	0.41	0/456
2	be	0.14	0/336	0.47	0/456
2	bf	0.13	0/336	0.38	0/456
2	bg	0.13	0/336	0.42	0/456
2	bh	0.13	0/336	0.42	0/456
2	bi	0.15	0/336	0.45	0/456
2	bj	0.16	0/336	0.48	0/456
2	bk	0.16	0/336	0.47	0/456
2	bl	0.14	0/336	0.43	0/456
2	bm	0.13	0/336	0.42	0/456
2	bn	0.14	0/340	0.42	0/461
2	bo	0.13	0/336	0.41	0/456
2	bp	0.13	0/336	0.43	0/456
3	C	0.19	0/2392	0.50	0/3263
4	C1	0.17	0/826	0.48	0/1128
5	C2	0.15	0/787	0.47	0/1075
6	H1	0.16	0/531	0.43	0/717
7	H2	0.16	0/1443	0.47	0/1970
8	L	0.16	0/2252	0.47	0/3081
9	M	0.17	0/2795	0.50	0/3824
10	aa	0.16	0/444	0.47	0/605
11	ab	0.15	0/457	0.43	0/624
11	ac	0.18	0/444	0.53	0/605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	ad	0.16	0/467	0.42	0/638
11	ae	0.16	0/457	0.45	0/624
11	af	0.15	0/457	0.42	0/624
11	ag	0.17	0/457	0.50	0/624
11	ah	0.18	0/467	0.49	0/638
11	ai	0.17	0/467	0.48	0/638
11	aj	0.16	0/467	0.45	0/638
11	ak	0.18	0/547	0.47	0/748
11	al	0.17	0/467	0.48	0/638
11	am	0.17	0/467	0.48	0/638
11	an	0.18	0/547	0.48	0/748
11	ao	0.17	0/467	0.51	0/638
11	ap	0.17	0/548	0.47	0/748
All	All	0.15	0/41625	0.46	0/56729

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AH	0	1
2	BH	0	1
2	bo	0	1
3	C	0	1
6	H1	0	1
7	H2	0	1
8	L	0	1
9	M	0	1
11	ae	0	1
11	ai	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AH	3	ARG	Sidechain
2	BH	14	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	170	ARG	Sidechain
6	H1	59	ARG	Sidechain
7	H2	55	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	0	0
1	AB	391	0	390	1	0
1	AC	384	0	383	2	0
1	AD	384	0	383	0	0
1	AE	391	0	390	0	0
1	AF	391	0	390	1	0
1	AG	391	0	390	0	0
1	AH	391	0	390	1	0
1	AI	391	0	390	0	0
1	AJ	391	0	390	0	0
1	AK	391	0	390	0	0
1	AL	391	0	390	0	0
1	AM	391	0	390	0	0
1	AN	391	0	390	3	0
1	AO	391	0	390	1	0
1	AP	391	0	390	1	0
1	AQ	391	0	390	2	0
1	AR	391	0	390	0	0
1	AS	391	0	390	3	0
1	AT	391	0	390	2	0
1	AU	391	0	390	0	0
1	AV	391	0	390	0	0
1	AW	391	0	390	0	0
1	AX	391	0	390	1	0
2	BA	323	0	300	0	0
2	BB	327	0	303	1	0
2	BC	323	0	300	1	0
2	BD	327	0	303	0	0
2	BE	327	0	303	0	0
2	BF	323	0	300	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BG	323	0	300	0	0
2	BH	323	0	300	0	0
2	BI	327	0	303	0	0
2	BJ	323	0	300	0	0
2	BK	323	0	300	0	0
2	BL	323	0	300	1	0
2	BM	323	0	300	1	0
2	BN	323	0	300	1	0
2	BO	323	0	300	0	0
2	BP	323	0	300	0	0
2	BQ	327	0	303	0	0
2	BR	327	0	303	0	0
2	BS	327	0	303	0	0
2	BT	327	0	303	0	0
2	BU	323	0	300	0	0
2	BV	327	0	303	0	0
2	BW	327	0	303	1	0
2	BX	323	0	300	0	0
2	ba	323	0	300	1	0
2	bb	323	0	300	1	0
2	bc	323	0	300	0	0
2	bd	323	0	300	1	0
2	be	323	0	300	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	323	0	300	1	0
2	bj	323	0	300	3	0
2	bk	323	0	300	0	0
2	bl	323	0	300	1	0
2	bm	323	0	300	1	0
2	bn	327	0	303	0	0
2	bo	323	0	300	0	0
2	bp	323	0	300	0	0
3	C	2325	0	2245	3	0
4	C1	806	0	818	1	0
5	C2	766	0	751	0	0
6	H1	522	0	503	0	0
7	H2	1404	0	1369	1	0
8	L	2165	0	2126	4	0
9	M	2694	0	2621	4	0
10	aa	433	0	442	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	ab	455	0	465	2	0
11	ac	443	0	453	0	0
11	ad	465	0	475	3	0
11	ae	455	0	465	2	0
11	af	455	0	465	1	0
11	ag	455	0	465	1	0
11	ah	465	0	475	2	0
11	ai	465	0	475	0	0
11	aj	465	0	475	2	0
11	ak	542	0	553	0	0
11	al	465	0	475	1	0
11	am	465	0	475	1	0
11	an	542	0	553	2	0
11	ao	465	0	475	1	0
11	ap	543	0	553	1	0
12	CG	21	0	18	0	0
12	MG	21	0	18	0	0
13	AA	132	0	148	3	0
13	AB	132	0	148	1	0
13	AC	132	0	148	2	0
13	AD	132	0	148	1	0
13	AE	132	0	148	2	0
13	AF	132	0	148	2	0
13	AG	132	0	148	2	0
13	AH	132	0	148	1	0
13	AI	132	0	148	2	0
13	AJ	132	0	148	1	0
13	AK	132	0	148	2	0
13	AL	132	0	148	2	0
13	AM	132	0	148	1	0
13	AN	132	0	148	1	0
13	AO	132	0	148	2	0
13	AP	132	0	148	2	0
13	AQ	198	0	222	3	0
13	AR	66	0	74	1	0
13	AS	198	0	222	7	0
13	AT	66	0	74	1	0
13	AU	132	0	148	3	0
13	AV	132	0	148	0	0
13	AW	198	0	222	3	0
13	AX	66	0	74	1	0
13	BA	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	BB	66	0	74	0	0
13	BC	66	0	74	0	0
13	BD	66	0	74	1	0
13	BE	66	0	74	0	0
13	BF	66	0	74	0	0
13	BG	66	0	74	0	0
13	BH	66	0	74	0	0
13	BI	66	0	74	1	0
13	BJ	66	0	74	0	0
13	BK	66	0	74	0	0
13	BL	66	0	74	0	0
13	BM	66	0	74	0	0
13	BN	66	0	74	2	0
13	BO	66	0	74	0	0
13	BP	66	0	74	0	0
13	BQ	66	0	74	0	0
13	BR	66	0	74	0	0
13	BS	66	0	74	0	0
13	BT	66	0	74	0	0
13	BU	66	0	74	0	0
13	BV	66	0	74	0	0
13	BW	66	0	74	0	0
13	BX	66	0	74	0	0
13	L	132	0	148	2	0
13	M	132	0	148	3	0
13	aa	66	0	74	2	0
13	ab	66	0	74	3	0
13	ac	66	0	74	1	0
13	ad	66	0	74	0	0
13	ae	66	0	74	1	0
13	af	66	0	74	2	0
13	ag	66	0	74	1	0
13	ah	66	0	74	0	0
13	ai	66	0	74	1	0
13	aj	66	0	74	0	0
13	ak	66	0	74	0	0
13	al	66	0	74	1	0
13	am	66	0	74	0	0
13	an	66	0	74	1	0
13	ao	66	0	74	1	0
13	ap	66	0	74	0	0
13	ba	66	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	bb	66	0	74	0	0
13	bc	66	0	74	0	0
13	bd	66	0	74	1	0
13	be	66	0	74	0	0
13	bf	66	0	74	1	0
13	bg	66	0	74	1	0
13	bh	66	0	74	1	0
13	bi	66	0	74	0	0
13	bj	66	0	74	1	0
13	bk	66	0	74	1	0
13	bl	66	0	74	1	0
13	bm	66	0	74	2	0
13	bn	66	0	74	1	0
13	bo	66	0	74	1	0
13	bp	66	0	74	1	0
14	AA	35	0	46	0	0
14	AB	70	0	91	0	0
14	AD	70	0	91	0	0
14	AF	35	0	46	0	0
14	AG	35	0	45	0	0
14	AH	105	0	138	0	0
14	AI	35	0	45	0	0
14	AJ	35	0	45	0	0
14	AK	35	0	45	1	0
14	AL	35	0	46	0	0
14	AN	70	0	92	0	0
14	AO	35	0	46	1	0
14	AP	35	0	46	1	0
14	AR	35	0	46	0	0
14	AS	35	0	45	0	0
14	AT	35	0	46	0	0
14	AU	35	0	44	0	0
14	AV	35	0	46	0	0
14	AW	35	0	45	0	0
14	BA	140	0	183	0	0
14	BB	70	0	92	0	0
14	BC	70	0	91	0	0
14	BD	140	0	181	1	0
14	BE	140	0	182	1	0
14	BF	105	0	136	0	0
14	BG	70	0	91	1	0
14	BH	105	0	135	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	BI	140	0	183	0	0
14	BJ	70	0	92	0	0
14	BK	140	0	182	0	0
14	BL	105	0	136	0	0
14	BM	70	0	92	0	0
14	BN	140	0	183	1	0
14	BO	70	0	90	0	0
14	BP	140	0	182	0	0
14	BQ	70	0	92	0	0
14	BR	140	0	181	0	0
14	BS	105	0	138	0	0
14	BT	105	0	137	1	0
14	BU	105	0	137	0	0
14	BV	70	0	92	0	0
14	BW	140	0	182	1	0
14	BX	70	0	91	0	0
14	L	175	0	228	1	0
14	M	35	0	45	0	0
14	ac	35	0	45	0	0
14	bb	35	0	45	0	0
14	bc	35	0	46	0	0
14	bd	35	0	45	0	0
14	bf	70	0	90	0	0
14	bg	35	0	45	0	0
14	bh	70	0	92	0	0
14	bj	35	0	45	0	0
14	bk	35	0	45	0	0
14	bl	70	0	92	0	0
14	bm	35	0	46	0	0
14	bn	35	0	45	0	0
14	bo	35	0	45	0	0
14	bp	35	0	46	0	0
15	AE	45	0	0	0	0
15	AH	45	0	0	0	0
15	AT	45	0	0	0	0
15	BA	45	0	0	0	0
15	BB	45	0	0	0	0
15	BC	45	0	0	0	0
15	BD	45	0	0	0	0
15	BE	45	0	0	0	0
15	BG	45	0	0	0	0
15	BH	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	BJ	45	0	0	0	0
15	BK	45	0	0	0	0
15	BL	45	0	0	0	0
15	BM	45	0	0	0	0
15	BN	45	0	0	0	0
15	BO	45	0	0	0	0
15	BP	45	0	0	0	0
15	BQ	45	0	0	0	0
15	BR	45	0	0	0	0
15	BS	45	0	0	0	0
15	BT	45	0	0	0	0
15	BV	45	0	0	0	0
15	BW	45	0	0	0	0
15	BX	45	0	0	0	0
15	ba	45	0	0	0	0
15	bb	45	0	0	0	0
15	bc	45	0	0	0	0
15	bd	45	0	0	0	0
15	be	45	0	0	0	0
15	bf	45	0	0	0	0
15	bg	45	0	0	0	0
15	bh	45	0	0	0	0
15	bi	45	0	0	0	0
15	bj	45	0	0	0	0
15	bk	45	0	0	0	0
15	bl	45	0	0	0	0
15	bm	45	0	0	0	0
15	bn	45	0	0	0	0
15	bo	45	0	0	0	0
15	bp	45	0	0	0	0
16	C	172	0	120	4	0
17	C	14	0	12	0	0
17	C1	14	0	12	0	0
18	C	18	0	0	0	0
18	M	18	0	0	0	0
19	H1	51	0	76	0	0
20	H1	45	0	0	0	0
20	L	45	0	0	0	0
20	aj	45	0	0	0	0
20	ba	90	0	0	0	0
20	bb	45	0	0	0	0
20	bc	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	be	90	0	0	0	0
20	bf	45	0	0	0	0
20	bg	45	0	0	0	0
20	bh	45	0	0	0	0
20	bi	45	0	0	0	0
20	bj	45	0	0	0	0
20	bk	90	0	0	0	0
20	bl	45	0	0	0	0
20	bm	45	0	0	0	0
20	bn	45	0	0	0	0
20	bo	45	0	0	0	0
21	H1	84	0	124	0	0
21	M	84	0	124	0	0
21	ad	84	0	124	0	0
21	af	168	0	248	1	0
21	ai	84	0	124	0	0
22	L	65	0	76	2	0
22	M	65	0	76	3	0
23	L	53	0	72	1	0
23	M	53	0	72	1	0
23	an	53	0	72	2	0
24	M	1	0	0	0	0
25	M	44	0	60	1	0
26	af	58	0	0	0	0
26	ag	58	0	0	0	0
27	ai	55	0	0	0	0
28	AA	3	0	0	0	0
28	AB	3	0	0	0	0
28	AC	2	0	0	0	0
28	AD	5	0	0	0	0
28	AG	2	0	0	0	0
28	AH	3	0	0	0	0
28	AI	3	0	0	0	0
28	AJ	6	0	0	0	0
28	AK	3	0	0	0	0
28	AL	3	0	0	0	0
28	AM	4	0	0	0	0
28	AN	3	0	0	0	0
28	AO	2	0	0	0	0
28	AP	3	0	0	0	0
28	AQ	5	0	0	0	0
28	AR	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AS	5	0	0	0	0
28	AT	7	0	0	0	0
28	AV	6	0	0	0	0
28	AW	6	0	0	0	0
28	AX	5	0	0	0	0
28	BD	1	0	0	0	0
28	BE	1	0	0	0	0
28	BF	1	0	0	0	0
28	BO	1	0	0	0	0
28	BW	1	0	0	0	0
28	C	98	0	0	1	0
28	C1	48	0	0	0	0
28	C2	3	0	0	0	0
28	H1	9	0	0	0	0
28	H2	35	0	0	0	0
28	L	53	0	0	0	0
28	M	59	0	0	0	0
28	aa	3	0	0	0	0
28	ab	3	0	0	0	0
28	ac	4	0	0	0	0
28	ad	9	0	0	0	0
28	ae	7	0	0	0	0
28	af	7	0	0	0	0
28	ag	7	0	0	0	0
28	ah	6	0	0	0	0
28	ai	3	0	0	0	0
28	aj	6	0	0	0	0
28	ak	14	0	0	0	0
28	al	8	0	0	0	0
28	am	8	0	0	0	0
28	an	5	0	0	0	0
28	ao	2	0	0	0	0
28	ap	8	0	0	0	0
28	bb	2	0	0	0	0
28	bc	2	0	0	0	0
28	bd	1	0	0	0	0
28	be	1	0	0	0	0
28	bf	1	0	0	0	0
28	bg	1	0	0	0	0
28	bh	2	0	0	0	0
28	bi	3	0	0	0	0
28	bk	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	bl	3	0	0	0	0
28	bm	4	0	0	0	0
28	bn	3	0	0	0	0
28	bo	2	0	0	0	0
28	bp	1	0	0	0	0
All	All	56446	0	54391	126	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 126 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)
14:AP:102:LMT:H6D	2:bj:38:TRP:HE1	1.59	0.66
13:AA:1001:BCL:H193	1:AX:20:PHE:HB2	1.80	0.61
22:M:406:BPH:HHC	22:M:406:BPH:HBB3	1.83	0.61
13:ag:1001:BCL:H143	13:bf:105:BCL:H41	1.83	0.60
13:M:403:BCL:HHC	13:M:403:BCL:HBB2	1.85	0.57

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	46 (98%)	1 (2%)	0	100	100
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%)	46 (98%)	1 (2%)	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%)	47 (100%)	0	0	100	100
1	AU	47/54 (87%)	47 (100%)	0	0	100	100
1	AV	47/54 (87%)	47 (100%)	0	0	100	100
1	AW	47/54 (87%)	46 (98%)	1 (2%)	0	100	100
1	AX	47/54 (87%)	47 (100%)	0	0	100	100
2	BA	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	BB	38/44 (86%)	37 (97%)	1 (3%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BM	37/44 (84%)	37 (100%)	0	0	100	100
2	BN	37/44 (84%)	37 (100%)	0	0	100	100
2	BO	37/44 (84%)	37 (100%)	0	0	100	100
2	BP	37/44 (84%)	37 (100%)	0	0	100	100
2	BQ	38/44 (86%)	38 (100%)	0	0	100	100
2	BR	38/44 (86%)	38 (100%)	0	0	100	100
2	BS	38/44 (86%)	38 (100%)	0	0	100	100
2	BT	38/44 (86%)	38 (100%)	0	0	100	100
2	BU	37/44 (84%)	37 (100%)	0	0	100	100
2	BV	38/44 (86%)	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%)	37 (100%)	0	0	100	100
2	bc	37/44 (84%)	37 (100%)	0	0	100	100
2	bd	37/44 (84%)	37 (100%)	0	0	100	100
2	be	37/44 (84%)	37 (100%)	0	0	100	100
2	bf	37/44 (84%)	37 (100%)	0	0	100	100
2	bg	37/44 (84%)	37 (100%)	0	0	100	100
2	bh	37/44 (84%)	37 (100%)	0	0	100	100
2	bi	37/44 (84%)	37 (100%)	0	0	100	100
2	bj	37/44 (84%)	37 (100%)	0	0	100	100
2	bk	37/44 (84%)	36 (97%)	1 (3%)	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	38/44 (86%)	37 (97%)	1 (3%)	0	100	100
2	bo	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	bp	37/44 (84%)	37 (100%)	0	0	100	100
3	C	297/354 (84%)	283 (95%)	13 (4%)	1 (0%)	36	44
4	C1	101/202 (50%)	97 (96%)	4 (4%)	0	100	100
5	C2	97/125 (78%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H1	60/67 (90%)	60 (100%)	0	0	100	100
7	H2	178/181 (98%)	173 (97%)	5 (3%)	0	100	100
8	L	271/274 (99%)	263 (97%)	8 (3%)	0	100	100
9	M	333/367 (91%)	324 (97%)	9 (3%)	0	100	100
10	aa	53/71 (75%)	53 (100%)	0	0	100	100
11	ab	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	ac	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
11	ad	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ae	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	af	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	ag	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
11	ah	58/71 (82%)	58 (100%)	0	0	100	100
11	ai	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
11	aj	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ak	69/71 (97%)	66 (96%)	3 (4%)	0	100	100
11	al	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	am	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	an	69/71 (97%)	64 (93%)	5 (7%)	0	100	100
11	ao	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
11	ap	69/71 (97%)	69 (100%)	0	0	100	100
All	All	4898/5762 (85%)	4828 (99%)	69 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	38/41 (93%)	38 (100%)	0	100	100
1	AB	38/41 (93%)	38 (100%)	0	100	100
1	AC	37/41 (90%)	37 (100%)	0	100	100
1	AD	37/41 (90%)	37 (100%)	0	100	100
1	AE	38/41 (93%)	38 (100%)	0	100	100
1	AF	38/41 (93%)	38 (100%)	0	100	100
1	AG	38/41 (93%)	38 (100%)	0	100	100
1	AH	38/41 (93%)	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%)	38 (100%)	0	100	100
1	AN	38/41 (93%)	38 (100%)	0	100	100
1	AO	38/41 (93%)	38 (100%)	0	100	100
1	AP	38/41 (93%)	38 (100%)	0	100	100
1	AQ	38/41 (93%)	38 (100%)	0	100	100
1	AR	38/41 (93%)	38 (100%)	0	100	100
1	AS	38/41 (93%)	38 (100%)	0	100	100
1	AT	38/41 (93%)	38 (100%)	0	100	100
1	AU	38/41 (93%)	38 (100%)	0	100	100
1	AV	38/41 (93%)	38 (100%)	0	100	100
1	AW	38/41 (93%)	38 (100%)	0	100	100
1	AX	38/41 (93%)	38 (100%)	0	100	100
2	BA	31/35 (89%)	31 (100%)	0	100	100
2	BB	31/35 (89%)	31 (100%)	0	100	100
2	BC	31/35 (89%)	31 (100%)	0	100	100
2	BD	31/35 (89%)	31 (100%)	0	100	100
2	BE	31/35 (89%)	31 (100%)	0	100	100
2	BF	31/35 (89%)	31 (100%)	0	100	100
2	BG	31/35 (89%)	31 (100%)	0	100	100
2	BH	31/35 (89%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	bp	31/35 (89%)	31 (100%)	0	100	100
3	C	245/285 (86%)	244 (100%)	1 (0%)	84	89
4	C1	88/156 (56%)	88 (100%)	0	100	100
5	C2	70/95 (74%)	70 (100%)	0	100	100
6	H1	50/53 (94%)	50 (100%)	0	100	100
7	H2	150/151 (99%)	149 (99%)	1 (1%)	76	83
8	L	215/216 (100%)	213 (99%)	2 (1%)	70	80
9	M	273/299 (91%)	271 (99%)	2 (1%)	76	83
10	aa	45/55 (82%)	45 (100%)	0	100	100
11	ab	46/54 (85%)	46 (100%)	0	100	100
11	ac	45/54 (83%)	45 (100%)	0	100	100
11	ad	46/54 (85%)	45 (98%)	1 (2%)	45	59
11	ae	46/54 (85%)	45 (98%)	1 (2%)	45	59
11	af	46/54 (85%)	46 (100%)	0	100	100
11	ag	46/54 (85%)	46 (100%)	0	100	100
11	ah	46/54 (85%)	46 (100%)	0	100	100
11	ai	46/54 (85%)	46 (100%)	0	100	100
11	aj	46/54 (85%)	46 (100%)	0	100	100
11	ak	54/54 (100%)	53 (98%)	1 (2%)	50	63
11	al	46/54 (85%)	46 (100%)	0	100	100
11	am	46/54 (85%)	46 (100%)	0	100	100
11	an	54/54 (100%)	54 (100%)	0	100	100
11	ao	46/54 (85%)	46 (100%)	0	100	100
11	ap	54/54 (100%)	54 (100%)	0	100	100
All	All	3999/4504 (89%)	3990 (100%)	9 (0%)	85	92

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	ae	39	SER
11	ak	34	SER
8	L	249	VAL
9	M	215	PHE
9	M	291	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
8	L	116	HIS
2	bc	16	HIS
11	ag	50	GLN
3	C	183	GLN
8	L	104	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	AI	1	1	8,9,10	0.95	0	7,9,11	0.98	1 (14%)
1	FME	AD	1	1	8,9,10	0.92	0	7,9,11	1.12	1 (14%)
11	FME	ad	1	11	8,9,10	0.90	0	7,9,11	1.31	1 (14%)
11	FME	aj	1	11	8,9,10	0.92	0	7,9,11	1.14	1 (14%)
11	FME	ah	1	11	8,9,10	0.92	0	7,9,11	1.21	1 (14%)
6	FME	H1	1	6	8,9,10	0.92	0	7,9,11	1.13	1 (14%)
1	FME	AA	1	1	8,9,10	0.93	0	7,9,11	1.08	1 (14%)
1	FME	AT	1	1	8,9,10	0.94	0	7,9,11	0.90	0
1	FME	AC	1	1	8,9,10	0.91	0	7,9,11	1.37	2 (28%)
1	FME	AF	1	1	8,9,10	0.91	0	7,9,11	1.36	2 (28%)
11	FME	ai	1	11	8,9,10	0.95	0	7,9,11	1.17	1 (14%)
11	FME	ao	1	11	8,9,10	0.94	0	7,9,11	1.06	1 (14%)
1	FME	AV	1	1	8,9,10	0.96	0	7,9,11	0.95	1 (14%)
11	FME	al	1	11	8,9,10	0.94	0	7,9,11	1.14	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	AU	1	1	8,9,10	0.96	0	7,9,11	0.95	0
1	FME	AW	1	1	8,9,10	0.89	0	7,9,11	0.96	0
11	FME	an	1	11	8,9,10	0.96	0	7,9,11	1.03	1 (14%)
1	FME	AE	1	1	8,9,10	0.93	0	7,9,11	1.08	1 (14%)
1	FME	AH	1	1	8,9,10	0.93	0	7,9,11	0.97	0
11	FME	ac	1	11	8,9,10	0.96	0	7,9,11	1.02	0
1	FME	AP	1	1	8,9,10	0.91	0	7,9,11	1.04	1 (14%)
11	FME	am	1	11	8,9,10	0.93	0	7,9,11	0.70	0
11	FME	af	1	11	8,9,10	0.91	0	7,9,11	1.29	1 (14%)
11	FME	ag	1	11	8,9,10	0.90	0	7,9,11	1.01	0
1	FME	AN	1	1	8,9,10	0.91	0	7,9,11	1.10	1 (14%)
11	FME	ap	1	11	8,9,10	0.92	0	7,9,11	0.99	0
1	FME	AG	1	1	8,9,10	0.89	0	7,9,11	1.22	1 (14%)
1	FME	AB	1	1	8,9,10	0.91	0	7,9,11	1.08	1 (14%)
1	FME	AJ	1	1	8,9,10	0.93	0	7,9,11	1.04	1 (14%)
1	FME	AO	1	1	8,9,10	0.94	0	7,9,11	0.95	0
1	FME	AR	1	1	8,9,10	0.94	0	7,9,11	0.96	1 (14%)
11	FME	ak	1	11	8,9,10	0.94	0	7,9,11	1.02	1 (14%)
1	FME	AS	1	1	8,9,10	0.93	0	7,9,11	1.15	1 (14%)
11	FME	ae	1	11	8,9,10	0.92	0	7,9,11	0.91	0
1	FME	AL	1	1	8,9,10	0.93	0	7,9,11	1.09	1 (14%)
1	FME	AQ	1	1	8,9,10	0.91	0	7,9,11	1.21	1 (14%)
1	FME	AM	1	1	8,9,10	0.93	0	7,9,11	1.01	1 (14%)
1	FME	AK	1	1	8,9,10	0.92	0	7,9,11	1.10	1 (14%)
11	FME	ab	1	11	8,9,10	0.91	0	7,9,11	1.30	1 (14%)
1	FME	AX	1	1	8,9,10	0.97	0	7,9,11	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AI	1	1	-	0/7/9/11	-
1	FME	AD	1	1	-	1/7/9/11	-
11	FME	ad	1	11	-	2/7/9/11	-
11	FME	aj	1	11	-	0/7/9/11	-
11	FME	ah	1	11	-	1/7/9/11	-
6	FME	H1	1	6	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AA	1	1	-	1/7/9/11	-
1	FME	AT	1	1	-	1/7/9/11	-
1	FME	AC	1	1	-	0/7/9/11	-
1	FME	AF	1	1	-	1/7/9/11	-
11	FME	ai	1	11	-	0/7/9/11	-
11	FME	ao	1	11	-	0/7/9/11	-
1	FME	AV	1	1	-	0/7/9/11	-
11	FME	al	1	11	-	0/7/9/11	-
1	FME	AU	1	1	-	0/7/9/11	-
1	FME	AW	1	1	-	3/7/9/11	-
11	FME	an	1	11	-	0/7/9/11	-
1	FME	AE	1	1	-	0/7/9/11	-
1	FME	AH	1	1	-	0/7/9/11	-
11	FME	ac	1	11	-	1/7/9/11	-
1	FME	AP	1	1	-	1/7/9/11	-
11	FME	am	1	11	-	1/7/9/11	-
11	FME	af	1	11	-	0/7/9/11	-
11	FME	ag	1	11	-	1/7/9/11	-
1	FME	AN	1	1	-	2/7/9/11	-
11	FME	ap	1	11	-	1/7/9/11	-
1	FME	AG	1	1	-	1/7/9/11	-
1	FME	AB	1	1	-	2/7/9/11	-
1	FME	AJ	1	1	-	0/7/9/11	-
1	FME	AO	1	1	-	0/7/9/11	-
1	FME	AR	1	1	-	0/7/9/11	-
11	FME	ak	1	11	-	1/7/9/11	-
1	FME	AS	1	1	-	1/7/9/11	-
11	FME	ae	1	11	-	0/7/9/11	-
1	FME	AL	1	1	-	0/7/9/11	-
1	FME	AQ	1	1	-	1/7/9/11	-
1	FME	AM	1	1	-	2/7/9/11	-
1	FME	AK	1	1	-	1/7/9/11	-
11	FME	ab	1	11	-	0/7/9/11	-
1	FME	AX	1	1	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	ad	1	FME	C-CA-N	2.85	114.88	109.73
11	af	1	FME	C-CA-N	2.85	114.87	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	ab	1	FME	C-CA-N	2.77	114.72	109.73
11	ah	1	FME	C-CA-N	2.64	114.49	109.73
1	AC	1	FME	C-CA-N	2.58	114.39	109.73

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	ah	1	FME	O-C-CA-CB
1	AB	1	FME	O-C-CA-CB
1	AK	1	FME	O-C-CA-CB
1	AM	1	FME	O-C-CA-CB
1	AN	1	FME	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AN	1	FME	1	0

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	MAN	CG	1	18,3,12	11,11,12	0.81	1 (9%)	15,15,17	1.06	1 (6%)
12	RAM	CG	2	12	10,10,11	1.76	2 (20%)	14,14,16	0.81	0
12	MAN	MG	1	18,12,9	11,11,12	0.92	0	15,15,17	1.15	1 (6%)
12	RAM	MG	2	12	10,10,11	1.85	3 (30%)	14,14,16	2.17	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	MG	2	RAM	O5-C1	4.43	1.50	1.43
12	CG	2	RAM	O5-C1	4.34	1.50	1.43
12	MG	2	RAM	C2-C3	-2.66	1.48	1.52
12	CG	2	RAM	C2-C3	-2.38	1.49	1.52
12	CG	1	MAN	O5-C1	-2.23	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	MG	2	RAM	O5-C5-C4	4.15	116.97	109.52
12	MG	2	RAM	C6-C5-C4	-4.12	105.45	113.07
12	MG	2	RAM	C3-C4-C5	3.84	115.76	109.77
12	MG	1	MAN	C1-O5-C5	3.37	116.76	112.19
12	MG	2	RAM	C1-C2-C3	2.59	112.85	109.67

There are no chirality outliers.

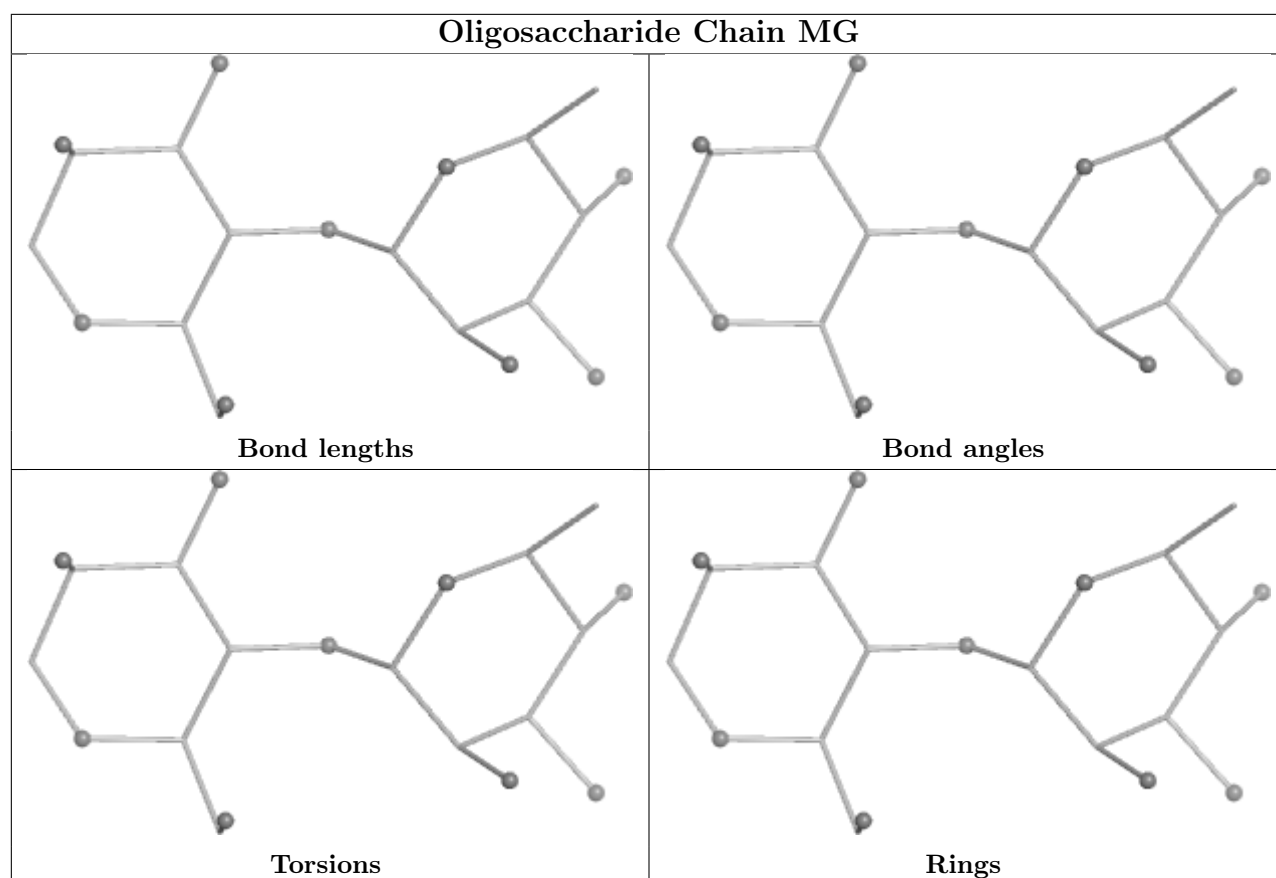
All (2) torsion outliers are listed below:

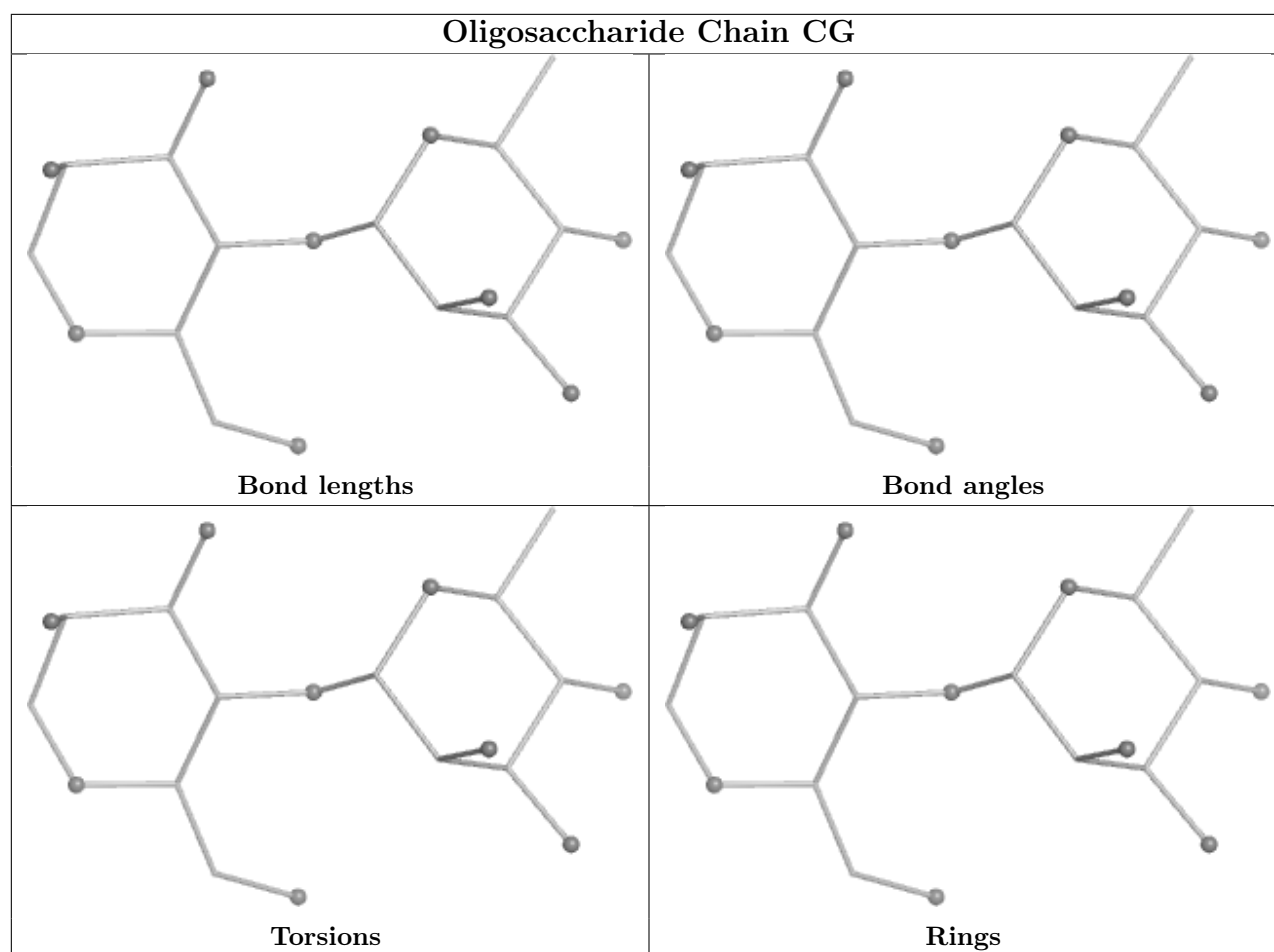
Mol	Chain	Res	Type	Atoms
12	CG	1	MAN	O5-C5-C6-O6
12	CG	1	MAN	C4-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 1 is monoatomic - leaving 311 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	0V9	bk	104	-	44,44,46	0.73	1 (2%)	47,49,51	0.98	3 (6%)
13	BCL	bj	104	2	69,74,74	1.14	5 (7%)	83,115,115	1.39	12 (14%)
13	BCL	AG	102	-	69,74,74	1.15	5 (7%)	83,115,115	1.47	12 (14%)
15	V7N	BK	1001	-	43,44,44	2.03	10 (23%)	44,54,54	1.52	9 (20%)
20	0V9	bl	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	L	303	8	69,74,74	1.14	6 (8%)	83,115,115	1.36	12 (14%)
14	LMT	BU	1001	-	36,36,36	1.07	4 (11%)	47,47,47	0.89	1 (2%)
15	V7N	bf	102	-	43,44,44	2.06	11 (25%)	44,54,54	1.52	9 (20%)
13	BCL	AK	102	1	69,74,74	1.18	6 (8%)	83,115,115	1.40	10 (12%)
14	LMT	BQ	1002	-	36,36,36	1.10	4 (11%)	47,47,47	0.91	3 (6%)
14	LMT	BR	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	1 (2%)
13	BCL	AD	1002	1	69,74,74	1.15	6 (8%)	83,115,115	1.43	11 (13%)
13	BCL	am	1001	11	69,74,74	1.15	5 (7%)	83,115,115	1.41	11 (13%)
17	NDG	C	1005	18	14,14,15	0.64	0	17,19,21	1.05	2 (11%)
13	BCL	AU	103	1	69,74,74	1.17	6 (8%)	83,115,115	1.41	10 (12%)
14	LMT	M	402	-	36,36,36	1.11	5 (13%)	47,47,47	0.92	2 (4%)
20	0V9	be	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	0
14	LMT	AW	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.95	3 (6%)
13	BCL	ag	1001	11	69,74,74	1.16	5 (7%)	83,115,115	1.42	12 (14%)
14	LMT	AB	104	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	2 (4%)
16	HEC	C	1001	3	50,50,50	1.74	7 (14%)	68,82,82	1.64	10 (14%)
20	0V9	H1	1002	-	44,44,46	0.76	1 (2%)	47,49,51	0.82	2 (4%)
14	LMT	L	306	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
13	BCL	ak	1001	11	69,74,74	1.14	5 (7%)	83,115,115	1.41	12 (14%)
14	LMT	BN	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
14	LMT	BF	102	-	36,36,36	1.09	5 (13%)	47,47,47	0.99	2 (4%)
20	0V9	bk	102	-	44,44,46	0.77	1 (2%)	47,49,51	0.80	1 (2%)
14	LMT	BD	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	2 (4%)
14	LMT	BF	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.10	3 (6%)
14	LMT	bp	101	-	36,36,36	1.10	4 (11%)	47,47,47	1.09	3 (6%)
14	LMT	BN	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.96	2 (4%)
15	V7N	AT	103	-	43,44,44	2.15	10 (23%)	44,54,54	1.64	10 (22%)
14	LMT	BU	1003	-	36,36,36	1.09	5 (13%)	47,47,47	1.03	3 (6%)
15	V7N	BJ	1001	-	43,44,44	2.00	10 (23%)	44,54,54	1.55	9 (20%)
14	LMT	AU	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.83	0
13	BCL	AR	101	1	69,74,74	1.17	6 (8%)	83,115,115	1.38	10 (12%)
15	V7N	AE	1003	-	43,44,44	2.04	10 (23%)	44,54,54	1.54	8 (18%)
14	LMT	AD	1004	-	36,36,36	1.10	4 (11%)	47,47,47	0.86	2 (4%)
13	BCL	AP	101	1	69,74,74	1.16	6 (8%)	83,115,115	1.41	10 (12%)
14	LMT	BU	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	AI	101	-	36,36,36	1.09	4 (11%)	47,47,47	0.82	0
14	LMT	bl	104	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	BM	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
21	CD4	H1	1003	-	83,83,83	0.46	0	89,95,95	0.94	3 (3%)
13	BCL	AS	102	28	69,74,74	1.17	5 (7%)	83,115,115	1.48	11 (13%)
14	LMT	AO	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	0
14	LMT	BS	1004	-	36,36,36	1.09	4 (11%)	47,47,47	0.88	1 (2%)
21	CD4	M	404	-	83,83,83	0.46	0	89,95,95	1.06	5 (5%)
14	LMT	AT	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	2 (4%)
13	BCL	ai	102	11	69,74,74	1.14	5 (7%)	83,115,115	1.46	13 (15%)
14	LMT	BG	1003	-	36,36,36	1.10	4 (11%)	47,47,47	0.84	1 (2%)
15	V7N	bc	104	-	43,44,44	2.05	11 (25%)	44,54,54	1.62	9 (20%)
14	LMT	BC	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.89	1 (2%)
13	BCL	AE	1002	1	69,74,74	1.16	6 (8%)	83,115,115	1.39	10 (12%)
13	BCL	AP	103	28	69,74,74	1.18	5 (7%)	83,115,115	1.47	12 (14%)
13	BCL	AK	103	-	69,74,74	1.16	5 (7%)	83,115,115	1.41	12 (14%)
14	LMT	L	304	-	36,36,36	1.05	4 (11%)	47,47,47	0.93	1 (2%)
20	OV9	bj	103	-	44,44,46	0.78	1 (2%)	47,49,51	0.92	2 (4%)
14	LMT	bf	104	-	36,36,36	1.11	5 (13%)	47,47,47	0.85	2 (4%)
13	BCL	ba	103	2	69,74,74	1.17	5 (7%)	83,115,115	1.39	12 (14%)
15	V7N	BW	1001	-	43,44,44	1.99	10 (23%)	44,54,54	1.52	9 (20%)
14	LMT	BP	1002	-	36,36,36	1.09	4 (11%)	47,47,47	0.91	1 (2%)
14	LMT	bh	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.98	1 (2%)
14	LMT	BJ	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.80	1 (2%)
13	BCL	BI	104	2	69,74,74	1.14	5 (7%)	83,115,115	1.44	11 (13%)
13	BCL	AI	103	1	69,74,74	1.16	6 (8%)	83,115,115	1.40	10 (12%)
14	LMT	AN	101	-	36,36,36	1.09	4 (11%)	47,47,47	1.00	3 (6%)
13	BCL	AL	101	1	69,74,74	1.16	6 (8%)	83,115,115	1.40	10 (12%)
14	LMT	BT	1005	-	36,36,36	1.07	5 (13%)	47,47,47	0.97	2 (4%)
15	V7N	BL	1001	-	43,44,44	2.05	10 (23%)	44,54,54	1.50	8 (18%)
13	BCL	bf	105	2	69,74,74	1.15	5 (7%)	83,115,115	1.36	12 (14%)
13	BCL	aa	1001	10	69,74,74	1.19	6 (8%)	83,115,115	1.44	11 (13%)
15	V7N	BC	101	-	43,44,44	2.04	9 (20%)	44,54,54	1.59	8 (18%)
14	LMT	BR	1006	-	36,36,36	1.10	5 (13%)	47,47,47	1.02	2 (4%)
15	V7N	BA	101	-	43,44,44	2.00	10 (23%)	44,54,54	1.58	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	BR	1003	2	69,74,74	1.15	6 (8%)	83,115,115	1.39	10 (12%)
15	V7N	bl	102	-	43,44,44	2.06	10 (23%)	44,54,54	1.54	9 (20%)
13	BCL	AT	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.42	10 (12%)
14	LMT	BK	1006	-	36,36,36	1.09	5 (13%)	47,47,47	1.00	2 (4%)
13	BCL	bc	103	2	69,74,74	1.17	5 (7%)	83,115,115	1.39	13 (15%)
13	BCL	AS	104	28	69,74,74	1.16	6 (8%)	83,115,115	1.58	14 (16%)
13	BCL	BJ	1004	2	69,74,74	1.15	5 (7%)	83,115,115	1.48	13 (15%)
13	BCL	AQ	102	28	69,74,74	1.16	5 (7%)	83,115,115	1.42	12 (14%)
14	LMT	BO	1003	-	36,36,36	1.06	5 (13%)	47,47,47	0.93	2 (4%)
14	LMT	BH	1005	-	36,36,36	1.12	5 (13%)	47,47,47	0.90	2 (4%)
13	BCL	AW	101	28	69,74,74	1.17	6 (8%)	83,115,115	1.45	13 (15%)
14	LMT	AL	102	-	36,36,36	1.09	4 (11%)	47,47,47	0.82	0
14	LMT	BJ	1002	-	36,36,36	1.06	5 (13%)	47,47,47	1.02	2 (4%)
14	LMT	BQ	1004	-	36,36,36	1.11	5 (13%)	47,47,47	0.89	2 (4%)
13	BCL	bg	104	2	69,74,74	1.13	5 (7%)	83,115,115	1.35	11 (13%)
13	BCL	AH	101	-	69,74,74	1.16	6 (8%)	83,115,115	1.48	12 (14%)
13	BCL	al	1001	11	69,74,74	1.17	5 (7%)	83,115,115	1.44	11 (13%)
20	0V9	be	102	-	44,44,46	0.77	1 (2%)	47,49,51	0.95	3 (6%)
14	LMT	BE	106	-	36,36,36	1.12	5 (13%)	47,47,47	0.93	2 (4%)
22	BPH	L	301	-	59,70,70	1.06	4 (6%)	61,101,101	1.86	9 (14%)
17	NDG	C1	301	18	14,14,15	0.66	0	17,19,21	0.87	1 (5%)
14	LMT	BD	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	1 (2%)
26	V7B	af	101	-	59,59,59	0.87	3 (5%)	75,75,75	1.12	5 (6%)
14	LMT	BV	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.88	1 (2%)
14	LMT	BB	103	-	36,36,36	1.10	5 (13%)	47,47,47	0.98	2 (4%)
13	BCL	BV	1004	2	69,74,74	1.14	6 (8%)	83,115,115	1.41	12 (14%)
15	V7N	BB	101	-	43,44,44	1.99	10 (23%)	44,54,54	1.58	8 (18%)
15	V7N	BG	1001	-	43,44,44	2.05	10 (23%)	44,54,54	1.57	8 (18%)
20	0V9	ba	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.90	1 (2%)
15	V7N	BP	1001	-	43,44,44	1.98	10 (23%)	44,54,54	1.67	11 (25%)
14	LMT	bl	101	-	36,36,36	1.10	4 (11%)	47,47,47	1.06	5 (10%)
13	BCL	AC	1002	-	69,74,74	1.18	5 (7%)	83,115,115	1.45	13 (15%)
14	LMT	BC	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	1 (2%)
13	BCL	AJ	101	1	69,74,74	1.18	6 (8%)	83,115,115	1.39	10 (12%)
13	BCL	BN	1006	2	69,74,74	1.13	5 (7%)	83,115,115	1.48	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	AG	101	-	36,36,36	1.13	5 (13%)	47,47,47	1.09	3 (6%)
15	V7N	bb	101	-	43,44,44	2.09	10 (23%)	44,54,54	1.74	9 (20%)
15	V7N	BE	101	-	43,44,44	2.06	11 (25%)	44,54,54	1.47	8 (18%)
13	BCL	BD	106	2	69,74,74	1.15	6 (8%)	83,115,115	1.42	11 (13%)
14	LMT	BA	106	-	36,36,36	1.07	5 (13%)	47,47,47	1.02	3 (6%)
14	LMT	AK	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.95	1 (2%)
13	BCL	BP	1004	2	69,74,74	1.13	5 (7%)	83,115,115	1.48	13 (15%)
13	BCL	AD	1001	28	69,74,74	1.15	5 (7%)	83,115,115	1.45	11 (13%)
14	LMT	BK	1005	-	36,36,36	1.11	5 (13%)	47,47,47	0.95	2 (4%)
15	V7N	AH	105	-	43,44,44	2.04	9 (20%)	44,54,54	1.46	8 (18%)
20	0V9	bh	104	-	44,44,46	0.73	1 (2%)	47,49,51	0.83	2 (4%)
14	LMT	BX	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.87	2 (4%)
15	V7N	BT	1001	-	43,44,44	2.04	10 (23%)	44,54,54	1.51	9 (20%)
14	LMT	AH	104	-	36,36,36	1.10	4 (11%)	47,47,47	0.81	0
13	BCL	BC	103	2	69,74,74	1.13	5 (7%)	83,115,115	1.40	11 (13%)
21	CD4	ai	103	-	83,83,83	0.49	0	89,95,95	1.07	7 (7%)
13	BCL	AE	1001	-	69,74,74	1.16	6 (8%)	83,115,115	1.40	12 (14%)
14	LMT	BL	1002	-	36,36,36	1.08	4 (11%)	47,47,47	1.07	3 (6%)
15	V7N	BO	1001	-	43,44,44	2.03	10 (23%)	44,54,54	1.46	8 (18%)
14	LMT	BI	105	-	36,36,36	1.10	5 (13%)	47,47,47	0.89	1 (2%)
13	BCL	bm	103	2	69,74,74	1.16	5 (7%)	83,115,115	1.39	12 (14%)
14	LMT	AA	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.99	1 (2%)
13	BCL	AJ	102	28	69,74,74	1.17	5 (7%)	83,115,115	1.56	15 (18%)
20	0V9	bo	104	-	44,44,46	0.74	1 (2%)	47,49,51	0.82	1 (2%)
13	BCL	bo	102	2	69,74,74	1.14	6 (8%)	83,115,115	1.35	11 (13%)
14	LMT	L	302	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	1 (2%)
14	LMT	bk	101	-	36,36,36	1.08	5 (13%)	47,47,47	0.97	2 (4%)
13	BCL	AF	1001	1	69,74,74	1.17	5 (7%)	83,115,115	1.46	12 (14%)
20	0V9	bb	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.86	1 (2%)
14	LMT	AN	103	-	36,36,36	1.05	5 (13%)	47,47,47	0.97	2 (4%)
20	0V9	bm	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.91	1 (2%)
15	V7N	bd	101	-	43,44,44	2.02	9 (20%)	44,54,54	1.52	9 (20%)
14	LMT	BA	102	-	36,36,36	1.09	4 (11%)	47,47,47	0.93	2 (4%)
19	PGW	H1	1001	-	50,50,50	0.46	0	53,56,56	1.04	3 (5%)
13	BCL	BQ	1003	2	69,74,74	1.13	5 (7%)	83,115,115	1.40	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	V7N	bk	103	-	43,44,44	2.14	10 (23%)	44,54,54	1.43	7 (15%)
14	LMT	BD	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.86	1 (2%)
13	BCL	AN	102	28	69,74,74	1.17	5 (7%)	83,115,115	1.45	12 (14%)
14	LMT	BP	1003	-	36,36,36	1.10	5 (13%)	47,47,47	0.86	1 (2%)
13	BCL	BB	104	2	69,74,74	1.14	6 (8%)	83,115,115	1.47	13 (15%)
13	BCL	AM	102	1	69,74,74	1.18	6 (8%)	83,115,115	1.39	10 (12%)
13	BCL	AB	101	1	69,74,74	1.14	6 (8%)	83,115,115	1.47	12 (14%)
13	BCL	AW	104	-	69,74,74	1.16	5 (7%)	83,115,115	1.55	15 (18%)
13	BCL	bp	103	2	69,74,74	1.17	6 (8%)	83,115,115	1.39	12 (14%)
14	LMT	BW	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.88	0
14	LMT	BB	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.84	1 (2%)
13	BCL	M	403	9	69,74,74	1.13	5 (7%)	83,115,115	1.42	9 (10%)
14	LMT	bb	102	-	36,36,36	1.13	5 (13%)	47,47,47	0.93	3 (6%)
13	BCL	BO	1004	2	69,74,74	1.13	6 (8%)	83,115,115	1.41	11 (13%)
14	LMT	BF	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	1 (2%)
13	BCL	BH	1003	2	69,74,74	1.14	5 (7%)	83,115,115	1.49	13 (15%)
14	LMT	L	307	-	36,36,36	1.08	4 (11%)	47,47,47	0.95	2 (4%)
13	BCL	bn	103	2	69,74,74	1.15	6 (8%)	83,115,115	1.36	10 (12%)
13	BCL	BX	1004	2	69,74,74	1.13	5 (7%)	83,115,115	1.39	12 (14%)
14	LMT	BE	102	-	36,36,36	1.09	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	bg	103	-	36,36,36	1.08	5 (13%)	47,47,47	1.01	2 (4%)
14	LMT	BI	103	-	36,36,36	1.11	5 (13%)	47,47,47	0.89	1 (2%)
13	BCL	BK	1003	2	69,74,74	1.13	5 (7%)	83,115,115	1.42	11 (13%)
13	BCL	AU	102	-	69,74,74	1.16	5 (7%)	83,115,115	1.56	15 (18%)
15	V7N	BV	1001	-	43,44,44	2.05	10 (23%)	44,54,54	1.48	9 (20%)
14	LMT	AF	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.88	1 (2%)
20	0V9	L	310	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	1 (2%)
15	V7N	BS	1001	-	43,44,44	1.99	10 (23%)	44,54,54	1.62	10 (22%)
13	BCL	bd	103	2	69,74,74	1.16	6 (8%)	83,115,115	1.40	11 (13%)
14	LMT	BL	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.94	2 (4%)
13	BCL	AL	103	-	69,74,74	1.19	5 (7%)	83,115,115	1.56	14 (16%)
13	BCL	ad	102	11	69,74,74	1.15	6 (8%)	83,115,115	1.43	11 (13%)
13	BCL	ae	1001	11	69,74,74	1.15	6 (8%)	83,115,115	1.43	11 (13%)
14	LMT	AS	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.94	2 (4%)
14	LMT	ac	101	-	36,36,36	1.10	4 (11%)	47,47,47	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	bm	104	-	36,36,36	1.08	4 (11%)	47,47,47	0.96	2 (4%)
13	BCL	AS	101	1	69,74,74	1.17	6 (8%)	83,115,115	1.38	10 (12%)
13	BCL	af	102	11	69,74,74	1.18	5 (7%)	83,115,115	1.41	11 (13%)
15	V7N	bj	101	-	43,44,44	2.05	9 (20%)	44,54,54	1.52	8 (18%)
15	V7N	BM	1001	-	43,44,44	1.99	10 (23%)	44,54,54	1.71	9 (20%)
15	V7N	BR	1001	-	43,44,44	2.02	9 (20%)	44,54,54	1.73	11 (25%)
13	BCL	AN	104	1	69,74,74	1.17	6 (8%)	83,115,115	1.40	10 (12%)
13	BCL	AQ	101	1	69,74,74	1.16	6 (8%)	83,115,115	1.42	10 (12%)
21	CD4	af	104	-	83,83,83	0.49	0	89,95,95	1.04	4 (4%)
15	V7N	be	101	-	43,44,44	1.99	10 (23%)	44,54,54	1.60	8 (18%)
13	BCL	AA	1002	28	69,74,74	1.16	5 (7%)	83,115,115	1.47	13 (15%)
14	LMT	BR	1005	-	36,36,36	1.10	5 (13%)	47,47,47	0.89	0
14	LMT	BT	1002	-	36,36,36	1.12	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	BP	1006	-	36,36,36	1.07	4 (11%)	47,47,47	0.99	2 (4%)
14	LMT	bh	101	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	3 (6%)
14	LMT	BA	105	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	2 (4%)
13	BCL	BS	1005	2	69,74,74	1.14	5 (7%)	83,115,115	1.48	12 (14%)
14	LMT	BG	1002	-	36,36,36	1.09	4 (11%)	47,47,47	0.82	0
14	LMT	bc	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.05	4 (8%)
20	0V9	aj	101	-	44,44,46	0.76	1 (2%)	47,49,51	0.85	2 (4%)
14	LMT	AH	106	-	36,36,36	1.11	5 (13%)	47,47,47	1.07	5 (10%)
25	CRT	M	408	-	41,43,43	0.55	0	50,54,54	0.65	0
14	LMT	L	305	-	36,36,36	1.11	5 (13%)	47,47,47	0.83	0
14	LMT	BS	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.88	0
15	V7N	bg	101	-	43,44,44	2.07	10 (23%)	44,54,54	1.65	10 (22%)
13	BCL	be	104	2	69,74,74	1.14	5 (7%)	83,115,115	1.35	11 (13%)
13	BCL	BF	104	2	69,74,74	1.14	5 (7%)	83,115,115	1.38	11 (13%)
13	BCL	bk	105	2	69,74,74	1.14	5 (7%)	83,115,115	1.50	15 (18%)
23	MQ8	L	309	-	54,54,54	0.62	0	66,69,69	0.83	3 (4%)
23	MQ8	M	407	-	54,54,54	0.63	0	66,69,69	0.63	0
13	BCL	BU	1004	2	69,74,74	1.14	6 (8%)	83,115,115	1.42	10 (12%)
14	LMT	BI	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	1 (2%)
13	BCL	an	102	11	69,74,74	1.16	6 (8%)	83,115,115	1.41	11 (13%)
20	0V9	bi	102	-	44,44,46	0.76	1 (2%)	47,49,51	0.82	2 (4%)
14	LMT	BN	1005	-	36,36,36	1.09	5 (13%)	47,47,47	0.93	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	V7N	BQ	1001	-	43,44,44	2.01	9 (20%)	44,54,54	1.51	9 (20%)
13	BCL	BA	104	2	69,74,74	1.12	5 (7%)	83,115,115	1.62	13 (15%)
16	HEC	C	1004	3	50,50,50	1.73	6 (12%)	68,82,82	1.57	10 (14%)
13	BCL	BM	1004	2	69,74,74	1.18	6 (8%)	83,115,115	1.48	12 (14%)
21	CD4	af	103	-	83,83,83	0.49	0	89,95,95	1.07	5 (5%)
15	V7N	bp	102	-	43,44,44	2.10	10 (23%)	44,54,54	1.54	8 (18%)
14	LMT	BH	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.87	0
14	LMT	BE	105	-	36,36,36	1.07	5 (13%)	47,47,47	0.88	1 (2%)
27	UYH	ai	101	-	55,55,55	2.11	14 (25%)	63,63,63	1.01	3 (4%)
14	LMT	bo	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.88	1 (2%)
20	OV9	bc	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.89	3 (6%)
14	LMT	bd	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.86	1 (2%)
14	LMT	BN	1004	-	36,36,36	1.11	5 (13%)	47,47,47	0.86	0
13	BCL	AF	1002	-	69,74,74	1.17	5 (7%)	83,115,115	1.47	11 (13%)
14	LMT	BE	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.85	1 (2%)
13	BCL	M	405	9	69,74,74	1.13	5 (7%)	83,115,115	1.46	11 (13%)
13	BCL	AO	101	-	69,74,74	1.21	5 (7%)	83,115,115	1.41	12 (14%)
14	LMT	AJ	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
23	MQ8	an	101	-	54,54,54	0.63	0	66,69,69	1.15	7 (10%)
15	V7N	BH	1001	-	43,44,44	2.05	11 (25%)	44,54,54	1.63	11 (25%)
15	V7N	bh	102	-	43,44,44	2.03	9 (20%)	44,54,54	1.56	8 (18%)
14	LMT	BI	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.82	0
14	LMT	bn	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.86	1 (2%)
13	BCL	ac	102	11	69,74,74	1.16	5 (7%)	83,115,115	1.41	11 (13%)
13	BCL	aj	102	11	69,74,74	1.15	5 (7%)	83,115,115	1.51	14 (16%)
14	LMT	AD	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.95	3 (6%)
13	BCL	AV	103	28	69,74,74	1.17	6 (8%)	83,115,115	1.44	12 (14%)
13	BCL	BT	1004	2	69,74,74	1.14	5 (7%)	83,115,115	1.51	15 (18%)
14	LMT	AV	101	-	36,36,36	1.12	4 (11%)	47,47,47	1.02	3 (6%)
14	LMT	BW	1005	-	36,36,36	1.08	5 (13%)	47,47,47	1.40	4 (8%)
14	LMT	bf	101	-	36,36,36	1.14	5 (13%)	47,47,47	0.92	2 (4%)
14	LMT	BW	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.92	0
21	CD4	ad	101	-	83,83,83	0.47	0	89,95,95	1.07	5 (5%)
13	BCL	AG	103	1	69,74,74	1.17	6 (8%)	83,115,115	1.41	10 (12%)
13	BCL	AI	102	-	69,74,74	1.19	5 (7%)	83,115,115	1.43	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMT	BP	1005	-	36,36,36	1.08	5 (13%)	47,47,47	0.82	1 (2%)
15	V7N	BX	1001	-	43,44,44	2.05	10 (23%)	44,54,54	1.56	8 (18%)
15	V7N	bm	101	-	43,44,44	2.04	9 (20%)	44,54,54	1.56	9 (20%)
20	0V9	bn	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.92	2 (4%)
13	BCL	AB	103	28	69,74,74	1.16	5 (7%)	83,115,115	1.54	14 (16%)
13	BCL	bl	105	2	69,74,74	1.16	6 (8%)	83,115,115	1.34	11 (13%)
13	BCL	BE	104	2	69,74,74	1.14	5 (7%)	83,115,115	1.52	14 (16%)
13	BCL	AM	101	28	69,74,74	1.19	6 (8%)	83,115,115	1.51	14 (16%)
14	LMT	BS	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.92	2 (4%)
14	LMT	BK	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.93	2 (4%)
14	LMT	AR	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.06	3 (6%)
14	LMT	BK	1004	-	36,36,36	1.08	5 (13%)	47,47,47	1.12	3 (6%)
14	LMT	BT	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.85	1 (2%)
14	LMT	BW	1006	-	36,36,36	1.07	4 (11%)	47,47,47	1.15	4 (8%)
13	BCL	L	308	8	69,74,74	1.12	5 (7%)	83,115,115	1.39	8 (9%)
22	BPH	M	406	-	59,70,70	1.05	4 (6%)	61,101,101	1.89	9 (14%)
13	BCL	BG	1004	2	69,74,74	1.16	5 (7%)	83,115,115	1.46	12 (14%)
14	LMT	AH	103	-	36,36,36	1.12	5 (13%)	47,47,47	0.80	0
15	V7N	bn	101	-	43,44,44	2.09	9 (20%)	44,54,54	1.53	10 (22%)
13	BCL	ab	1001	11	69,74,74	1.19	6 (8%)	83,115,115	1.44	12 (14%)
14	LMT	BR	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.98	2 (4%)
20	0V9	ba	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.87	1 (2%)
20	0V9	bf	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.88	3 (6%)
15	V7N	bo	101	-	43,44,44	2.07	12 (27%)	44,54,54	1.52	9 (20%)
18	V75	M	409	12,17	18,18,18	1.64	5 (27%)	21,25,25	1.72	2 (9%)
13	BCL	AC	1001	1	69,74,74	1.17	6 (8%)	83,115,115	1.39	10 (12%)
13	BCL	AV	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.39	10 (12%)
20	0V9	bg	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	2 (4%)
13	BCL	ao	1001	11	69,74,74	1.15	5 (7%)	83,115,115	1.42	11 (13%)
13	BCL	AO	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.40	10 (12%)
13	BCL	AH	102	1	69,74,74	1.16	5 (7%)	83,115,115	1.41	10 (12%)
14	LMT	BV	1002	-	36,36,36	1.11	5 (13%)	47,47,47	0.88	1 (2%)
13	BCL	bb	103	2	69,74,74	1.14	5 (7%)	83,115,115	1.35	11 (13%)
13	BCL	AA	1001	1	69,74,74	1.17	6 (8%)	83,115,115	1.44	11 (13%)
14	LMT	BX	1003	-	36,36,36	1.07	5 (13%)	47,47,47	0.93	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	AW	103	1	69,74,74	1.18	6 (8%)	83,115,115	1.42	10 (12%)
13	BCL	bi	103	2	69,74,74	1.12	5 (7%)	83,115,115	1.38	13 (15%)
13	BCL	AQ	103	-	69,74,74	1.20	5 (7%)	83,115,115	1.65	14 (16%)
14	LMT	AP	102	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	0
14	LMT	BM	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.86	1 (2%)
14	LMT	bj	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.90	2 (4%)
14	LMT	BA	103	-	36,36,36	1.07	5 (13%)	47,47,47	0.93	2 (4%)
13	BCL	ap	1001	11	69,74,74	1.17	6 (8%)	83,115,115	1.39	11 (13%)
15	V7N	BN	1001	-	43,44,44	2.00	10 (23%)	44,54,54	1.82	10 (22%)
13	BCL	bh	105	2	69,74,74	1.13	5 (7%)	83,115,115	1.36	12 (14%)
14	LMT	BL	1005	-	36,36,36	1.06	5 (13%)	47,47,47	1.00	2 (4%)
15	V7N	ba	101	-	43,44,44	2.09	10 (23%)	44,54,54	1.53	9 (20%)
26	V7B	ag	1002	-	59,59,59	0.93	5 (8%)	75,75,75	1.29	8 (10%)
13	BCL	ah	1001	11	69,74,74	1.16	5 (7%)	83,115,115	1.40	11 (13%)
14	LMT	AB	102	-	36,36,36	1.11	4 (11%)	47,47,47	0.82	2 (4%)
14	LMT	BH	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.91	1 (2%)
16	HEC	C	1003	3	50,50,50	1.73	7 (14%)	68,82,82	1.66	10 (14%)
18	V75	C	1006	12,17	18,18,18	1.59	5 (27%)	21,25,25	1.70	2 (9%)
14	LMT	BO	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.87	1 (2%)
13	BCL	BL	1004	2	69,74,74	1.12	5 (7%)	83,115,115	1.40	11 (13%)
13	BCL	AX	101	1	69,74,74	1.19	7 (10%)	83,115,115	1.44	10 (12%)
14	LMT	BD	105	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	2 (4%)
15	V7N	bi	101	-	43,44,44	2.06	10 (23%)	44,54,54	1.53	9 (20%)
15	V7N	BD	101	-	43,44,44	2.00	9 (20%)	44,54,54	1.68	10 (22%)
16	HEC	C	1002	3	50,50,50	1.73	5 (10%)	68,82,82	1.53	12 (17%)
13	BCL	BW	1003	2	69,74,74	1.16	6 (8%)	83,115,115	1.45	12 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	0V9	bk	104	-	-	11/48/48/50	-
13	BCL	bj	104	2	-	10/41/137/137	-
13	BCL	AG	102	-	-	12/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	V7N	BK	1001	-	-	3/53/53/53	-
20	0V9	bl	103	-	-	12/48/48/50	-
13	BCL	L	303	8	-	4/41/137/137	-
14	LMT	BU	1001	-	-	5/21/61/61	0/2/2/2
15	V7N	bf	102	-	-	3/53/53/53	-
13	BCL	AK	102	1	-	1/41/137/137	-
14	LMT	BQ	1002	-	-	1/21/61/61	0/2/2/2
14	LMT	BR	1002	-	-	5/21/61/61	0/2/2/2
13	BCL	AD	1002	1	-	2/41/137/137	-
13	BCL	am	1001	11	-	2/41/137/137	-
17	NDG	C	1005	18	-	0/6/23/26	0/1/1/1
13	BCL	AU	103	1	-	4/41/137/137	-
14	LMT	M	402	-	-	3/21/61/61	0/2/2/2
20	0V9	be	103	-	-	12/48/48/50	-
14	LMT	AW	102	-	-	3/21/61/61	0/2/2/2
16	HEC	C	1001	3	1/1/3/7	9/14/54/54	-
13	BCL	ag	1001	11	-	5/41/137/137	-
14	LMT	AB	104	-	-	7/21/61/61	0/2/2/2
20	0V9	H1	1002	-	-	10/48/48/50	-
14	LMT	L	306	-	-	3/21/61/61	0/2/2/2
13	BCL	ak	1001	11	-	6/41/137/137	-
14	LMT	BN	1003	-	-	5/21/61/61	0/2/2/2
14	LMT	BF	102	-	-	5/21/61/61	0/2/2/2
20	0V9	bk	102	-	-	12/48/48/50	-
14	LMT	BD	102	-	-	3/21/61/61	0/2/2/2
14	LMT	BF	101	-	-	3/21/61/61	0/2/2/2
14	LMT	bp	101	-	-	9/21/61/61	0/2/2/2
14	LMT	BN	1002	-	-	8/21/61/61	0/2/2/2
15	V7N	AT	103	-	-	6/53/53/53	-
14	LMT	BU	1003	-	-	4/21/61/61	0/2/2/2
15	V7N	BJ	1001	-	-	4/53/53/53	-
14	LMT	AU	101	-	-	5/21/61/61	0/2/2/2
13	BCL	AR	101	1	-	3/41/137/137	-
15	V7N	AE	1003	-	-	3/53/53/53	-
14	LMT	AD	1004	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	AP	101	1	-	5/41/137/137	-
14	LMT	BU	1002	-	-	1/21/61/61	0/2/2/2
14	LMT	AI	101	-	-	4/21/61/61	0/2/2/2
14	LMT	bl	104	-	-	3/21/61/61	0/2/2/2
14	LMT	BM	1003	-	-	2/21/61/61	0/2/2/2
21	CD4	H1	1003	-	-	17/94/94/94	-
13	BCL	AS	102	28	-	7/41/137/137	-
14	LMT	AO	103	-	-	4/21/61/61	0/2/2/2
14	LMT	BS	1004	-	-	3/21/61/61	0/2/2/2
21	CD4	M	404	-	-	21/94/94/94	-
14	LMT	AT	101	-	-	3/21/61/61	0/2/2/2
13	BCL	ai	102	11	-	6/41/137/137	-
14	LMT	BG	1003	-	-	4/21/61/61	0/2/2/2
15	V7N	bc	104	-	-	9/53/53/53	-
14	LMT	BC	104	-	-	6/21/61/61	0/2/2/2
13	BCL	AE	1002	1	-	1/41/137/137	-
13	BCL	AP	103	28	-	6/41/137/137	-
13	BCL	AK	103	-	-	14/41/137/137	-
14	LMT	L	304	-	-	3/21/61/61	0/2/2/2
20	0V9	bj	103	-	-	6/48/48/50	-
14	LMT	bf	104	-	-	6/21/61/61	0/2/2/2
13	BCL	ba	103	2	-	10/41/137/137	-
15	V7N	BW	1001	-	-	5/53/53/53	-
14	LMT	BP	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	bh	103	-	-	1/21/61/61	0/2/2/2
14	LMT	BJ	1003	-	-	2/21/61/61	0/2/2/2
13	BCL	BI	104	2	-	12/41/137/137	-
13	BCL	AI	103	1	-	6/41/137/137	-
14	LMT	AN	101	-	-	2/21/61/61	0/2/2/2
13	BCL	AL	101	1	-	1/41/137/137	-
14	LMT	BT	1005	-	-	6/21/61/61	0/2/2/2
15	V7N	BL	1001	-	-	7/53/53/53	-
13	BCL	bf	105	2	-	3/41/137/137	-
13	BCL	aa	1001	10	-	3/41/137/137	-
15	V7N	BC	101	-	-	3/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BR	1006	-	-	2/21/61/61	0/2/2/2
15	V7N	BA	101	-	-	4/53/53/53	-
13	BCL	BR	1003	2	-	7/41/137/137	-
15	V7N	bl	102	-	-	8/53/53/53	-
13	BCL	AT	102	1	-	1/41/137/137	-
14	LMT	BK	1006	-	-	3/21/61/61	0/2/2/2
13	BCL	bc	103	2	-	7/41/137/137	-
13	BCL	AS	104	28	-	9/41/137/137	-
13	BCL	BJ	1004	2	-	8/41/137/137	-
13	BCL	AQ	102	28	-	6/41/137/137	-
14	LMT	BO	1003	-	-	4/21/61/61	0/2/2/2
14	LMT	BH	1005	-	-	4/21/61/61	0/2/2/2
13	BCL	AW	101	28	-	8/41/137/137	-
14	LMT	AL	102	-	-	5/21/61/61	0/2/2/2
14	LMT	BJ	1002	-	-	6/21/61/61	0/2/2/2
14	LMT	BQ	1004	-	-	3/21/61/61	0/2/2/2
13	BCL	bg	104	2	-	8/41/137/137	-
13	BCL	AH	101	-	-	12/41/137/137	-
13	BCL	al	1001	11	-	6/41/137/137	-
20	0V9	be	102	-	-	16/48/48/50	-
14	LMT	BE	106	-	-	2/21/61/61	0/2/2/2
22	BPH	L	301	-	-	3/37/105/105	0/5/6/6
17	NDG	C1	301	18	-	0/6/23/26	0/1/1/1
14	LMT	BD	103	-	-	4/21/61/61	0/2/2/2
26	V7B	af	101	-	-	14/48/88/88	0/2/2/2
14	LMT	BV	1003	-	-	1/21/61/61	0/2/2/2
14	LMT	BB	103	-	-	5/21/61/61	0/2/2/2
13	BCL	BV	1004	2	-	9/41/137/137	-
15	V7N	BB	101	-	-	3/53/53/53	-
15	V7N	BG	1001	-	-	5/53/53/53	-
20	0V9	ba	104	-	-	12/48/48/50	-
15	V7N	BP	1001	-	-	4/53/53/53	-
14	LMT	bl	101	-	-	2/21/61/61	0/2/2/2
13	BCL	AC	1002	-	-	10/41/137/137	-
14	LMT	BC	102	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	AJ	101	1	-	0/41/137/137	-
13	BCL	BN	1006	2	-	9/41/137/137	-
14	LMT	AG	101	-	-	6/21/61/61	0/2/2/2
15	V7N	bb	101	-	-	17/53/53/53	-
15	V7N	BE	101	-	-	3/53/53/53	-
13	BCL	BD	106	2	-	6/41/137/137	-
14	LMT	BA	106	-	-	7/21/61/61	0/2/2/2
14	LMT	AK	101	-	-	5/21/61/61	0/2/2/2
13	BCL	BP	1004	2	-	8/41/137/137	-
13	BCL	AD	1001	28	-	5/41/137/137	-
14	LMT	BK	1005	-	-	2/21/61/61	0/2/2/2
15	V7N	AH	105	-	-	6/53/53/53	-
20	0V9	bh	104	-	-	11/48/48/50	-
14	LMT	BX	1002	-	-	3/21/61/61	0/2/2/2
15	V7N	BT	1001	-	-	3/53/53/53	-
14	LMT	AH	104	-	-	2/21/61/61	0/2/2/2
13	BCL	BC	103	2	-	3/41/137/137	-
21	CD4	ai	103	-	-	19/94/94/94	-
13	BCL	AE	1001	-	-	11/41/137/137	-
14	LMT	BL	1002	-	-	10/21/61/61	0/2/2/2
15	V7N	BO	1001	-	-	6/53/53/53	-
14	LMT	BI	105	-	-	2/21/61/61	0/2/2/2
13	BCL	bm	103	2	-	8/41/137/137	-
14	LMT	AA	1003	-	-	7/21/61/61	0/2/2/2
13	BCL	AJ	102	28	-	11/41/137/137	-
20	0V9	bo	104	-	-	8/48/48/50	-
13	BCL	bo	102	2	-	4/41/137/137	-
14	LMT	L	302	-	-	6/21/61/61	0/2/2/2
14	LMT	bk	101	-	-	7/21/61/61	0/2/2/2
13	BCL	AF	1001	1	-	7/41/137/137	-
20	0V9	bb	104	-	-	10/48/48/50	-
14	LMT	AN	103	-	-	6/21/61/61	0/2/2/2
20	0V9	bm	102	-	-	11/48/48/50	-
15	V7N	bd	101	-	-	5/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BA	102	-	-	2/21/61/61	0/2/2/2
19	PGW	H1	1001	-	-	15/55/55/55	-
13	BCL	BQ	1003	2	-	7/41/137/137	-
15	V7N	bk	103	-	-	8/53/53/53	-
14	LMT	BD	104	-	-	2/21/61/61	0/2/2/2
13	BCL	AN	102	28	-	6/41/137/137	-
14	LMT	BP	1003	-	-	5/21/61/61	0/2/2/2
13	BCL	BB	104	2	-	7/41/137/137	-
13	BCL	AM	102	1	-	6/41/137/137	-
13	BCL	AB	101	1	-	2/41/137/137	-
13	BCL	AW	104	-	-	14/41/137/137	-
13	BCL	bp	103	2	-	11/41/137/137	-
14	LMT	BW	1004	-	-	4/21/61/61	0/2/2/2
14	LMT	BB	102	-	-	3/21/61/61	0/2/2/2
13	BCL	M	403	9	-	9/41/137/137	-
14	LMT	bb	102	-	-	6/21/61/61	0/2/2/2
13	BCL	BO	1004	2	-	8/41/137/137	-
14	LMT	BF	103	-	-	1/21/61/61	0/2/2/2
13	BCL	BH	1003	2	-	9/41/137/137	-
14	LMT	L	307	-	-	6/21/61/61	0/2/2/2
13	BCL	bn	103	2	-	5/41/137/137	-
13	BCL	BX	1004	2	-	6/41/137/137	-
14	LMT	BE	102	-	-	5/21/61/61	0/2/2/2
14	LMT	bg	103	-	-	6/21/61/61	0/2/2/2
14	LMT	BI	103	-	-	2/21/61/61	0/2/2/2
13	BCL	BK	1003	2	-	12/41/137/137	-
13	BCL	AU	102	-	-	7/41/137/137	-
15	V7N	BV	1001	-	-	5/53/53/53	-
14	LMT	AF	1003	-	-	5/21/61/61	0/2/2/2
20	0V9	L	310	-	-	10/48/48/50	-
15	V7N	BS	1001	-	-	6/53/53/53	-
13	BCL	bd	103	2	-	4/41/137/137	-
14	LMT	BL	1003	-	-	4/21/61/61	0/2/2/2
13	BCL	AL	103	-	-	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	ad	102	11	-	6/41/137/137	-
13	BCL	ae	1001	11	-	9/41/137/137	-
14	LMT	AS	103	-	-	8/21/61/61	0/2/2/2
14	LMT	ac	101	-	-	4/21/61/61	0/2/2/2
14	LMT	bm	104	-	-	7/21/61/61	0/2/2/2
13	BCL	AS	101	1	-	7/41/137/137	-
13	BCL	af	102	11	-	3/41/137/137	-
15	V7N	bj	101	-	-	2/53/53/53	-
15	V7N	BM	1001	-	-	7/53/53/53	-
15	V7N	BR	1001	-	-	5/53/53/53	-
13	BCL	AN	104	1	-	1/41/137/137	-
13	BCL	AQ	101	1	-	3/41/137/137	-
21	CD4	af	104	-	-	20/94/94/94	-
15	V7N	be	101	-	-	6/53/53/53	-
13	BCL	AA	1002	28	-	9/41/137/137	-
14	LMT	BR	1005	-	-	3/21/61/61	0/2/2/2
14	LMT	BT	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	BP	1006	-	-	3/21/61/61	0/2/2/2
14	LMT	bh	101	-	-	9/21/61/61	0/2/2/2
14	LMT	BA	105	-	-	4/21/61/61	0/2/2/2
13	BCL	BS	1005	2	-	8/41/137/137	-
14	LMT	BG	1002	-	-	4/21/61/61	0/2/2/2
14	LMT	bc	101	-	-	11/21/61/61	0/2/2/2
20	0V9	aj	101	-	-	16/48/48/50	-
14	LMT	AH	106	-	-	3/21/61/61	0/2/2/2
25	CRT	M	408	-	-	3/51/51/51	-
14	LMT	L	305	-	-	7/21/61/61	0/2/2/2
14	LMT	BS	1003	-	-	6/21/61/61	0/2/2/2
15	V7N	bg	101	-	-	6/53/53/53	-
13	BCL	be	104	2	-	6/41/137/137	-
13	BCL	BF	104	2	-	6/41/137/137	-
13	BCL	bk	105	2	-	8/41/137/137	-
23	MQ8	L	309	-	-	10/47/67/67	0/2/2/2
23	MQ8	M	407	-	-	0/47/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	BU	1004	2	-	12/41/137/137	-
14	LMT	BI	101	-	-	2/21/61/61	0/2/2/2
13	BCL	an	102	11	-	3/41/137/137	-
20	0V9	bi	102	-	-	7/48/48/50	-
14	LMT	BN	1005	-	-	2/21/61/61	0/2/2/2
15	V7N	BQ	1001	-	-	4/53/53/53	-
13	BCL	BA	104	2	-	9/41/137/137	-
16	HEC	C	1004	3	1/1/3/7	4/14/54/54	-
13	BCL	BM	1004	2	-	3/41/137/137	-
21	CD4	af	103	-	-	30/94/94/94	-
15	V7N	bp	102	-	-	5/53/53/53	-
14	LMT	BH	1002	-	-	2/21/61/61	0/2/2/2
14	LMT	BE	105	-	-	2/21/61/61	0/2/2/2
27	UYH	ai	101	-	-	9/50/70/70	0/1/1/1
14	LMT	bo	103	-	-	3/21/61/61	0/2/2/2
20	0V9	bc	102	-	-	15/48/48/50	-
14	LMT	bd	102	-	-	8/21/61/61	0/2/2/2
14	LMT	BN	1004	-	-	4/21/61/61	0/2/2/2
13	BCL	AF	1002	-	-	10/41/137/137	-
14	LMT	BE	103	-	-	3/21/61/61	0/2/2/2
13	BCL	M	405	9	-	4/41/137/137	-
13	BCL	AO	101	-	-	11/41/137/137	-
14	LMT	AJ	103	-	-	2/21/61/61	0/2/2/2
23	MQ8	an	101	-	-	4/47/67/67	0/2/2/2
15	V7N	BH	1001	-	-	4/53/53/53	-
15	V7N	bh	102	-	-	5/53/53/53	-
14	LMT	BI	102	-	-	4/21/61/61	0/2/2/2
14	LMT	bn	102	-	-	2/21/61/61	0/2/2/2
13	BCL	ac	102	11	-	2/41/137/137	-
13	BCL	aj	102	11	-	5/41/137/137	-
14	LMT	AD	1003	-	-	6/21/61/61	0/2/2/2
13	BCL	AV	103	28	-	6/41/137/137	-
13	BCL	BT	1004	2	-	9/41/137/137	-
14	LMT	AV	101	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	BW	1005	-	-	6/21/61/61	0/2/2/2
14	LMT	bf	101	-	-	7/21/61/61	0/2/2/2
14	LMT	BW	1002	-	-	3/21/61/61	0/2/2/2
21	CD4	ad	101	-	-	21/94/94/94	-
13	BCL	AG	103	1	-	5/41/137/137	-
13	BCL	AI	102	-	-	8/41/137/137	-
14	LMT	BP	1005	-	-	4/21/61/61	0/2/2/2
15	V7N	BX	1001	-	-	5/53/53/53	-
15	V7N	bm	101	-	-	4/53/53/53	-
20	0V9	bn	104	-	-	12/48/48/50	-
13	BCL	AB	103	28	-	7/41/137/137	-
13	BCL	bl	105	2	-	8/41/137/137	-
13	BCL	BE	104	2	-	3/41/137/137	-
13	BCL	AM	101	28	-	10/41/137/137	-
14	LMT	BS	1002	-	-	3/21/61/61	0/2/2/2
14	LMT	BK	1002	-	-	5/21/61/61	0/2/2/2
14	LMT	AR	102	-	-	11/21/61/61	0/2/2/2
14	LMT	BK	1004	-	-	7/21/61/61	0/2/2/2
14	LMT	BT	1003	-	-	4/21/61/61	0/2/2/2
14	LMT	BW	1006	-	-	9/21/61/61	0/2/2/2
13	BCL	L	308	8	-	3/41/137/137	-
22	BPH	M	406	-	-	4/37/105/105	0/5/6/6
13	BCL	BG	1004	2	-	12/41/137/137	-
14	LMT	AH	103	-	-	3/21/61/61	0/2/2/2
15	V7N	bn	101	-	-	5/53/53/53	-
13	BCL	ab	1001	11	-	4/41/137/137	-
14	LMT	BR	1004	-	-	7/21/61/61	0/2/2/2
20	0V9	ba	102	-	-	8/48/48/50	-
20	0V9	bf	103	-	-	11/48/48/50	-
15	V7N	bo	101	-	-	3/53/53/53	-
18	V75	M	409	12,17	-	0/12/29/29	0/1/1/1
13	BCL	AC	1001	1	-	6/41/137/137	-
13	BCL	AV	102	1	-	3/41/137/137	-
20	0V9	bg	102	-	-	15/48/48/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	ao	1001	11	-	7/41/137/137	-
13	BCL	AO	102	1	-	3/41/137/137	-
13	BCL	AH	102	1	-	0/41/137/137	-
14	LMT	BV	1002	-	-	2/21/61/61	0/2/2/2
13	BCL	bb	103	2	-	5/41/137/137	-
13	BCL	AA	1001	1	-	3/41/137/137	-
14	LMT	BX	1003	-	-	8/21/61/61	0/2/2/2
13	BCL	AW	103	1	-	4/41/137/137	-
13	BCL	bi	103	2	-	6/41/137/137	-
13	BCL	AQ	103	-	-	10/41/137/137	-
14	LMT	AP	102	-	-	7/21/61/61	0/2/2/2
14	LMT	BM	1002	-	-	1/21/61/61	0/2/2/2
14	LMT	bj	102	-	-	5/21/61/61	0/2/2/2
14	LMT	BA	103	-	-	7/21/61/61	0/2/2/2
13	BCL	ap	1001	11	-	11/41/137/137	-
15	V7N	BN	1001	-	-	8/53/53/53	-
13	BCL	bh	105	2	-	6/41/137/137	-
14	LMT	BL	1005	-	-	5/21/61/61	0/2/2/2
15	V7N	ba	101	-	-	7/53/53/53	-
26	V7B	ag	1002	-	-	15/48/88/88	0/2/2/2
13	BCL	ah	1001	11	-	7/41/137/137	-
14	LMT	AB	102	-	-	3/21/61/61	0/2/2/2
14	LMT	BH	1004	-	-	4/21/61/61	0/2/2/2
16	HEC	C	1003	3	1/1/3/7	6/14/54/54	-
18	V75	C	1006	12,17	-	1/12/29/29	0/1/1/1
14	LMT	BO	1002	-	-	5/21/61/61	0/2/2/2
13	BCL	BL	1004	2	-	6/41/137/137	-
13	BCL	AX	101	1	-	4/41/137/137	-
14	LMT	BD	105	-	-	8/21/61/61	0/2/2/2
15	V7N	bi	101	-	-	3/53/53/53	-
15	V7N	BD	101	-	-	3/53/53/53	-
16	HEC	C	1002	3	1/1/3/7	8/14/54/54	-
13	BCL	BW	1003	2	-	5/41/137/137	-

The worst 5 of 1635 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	1002	HEC	C3D-C2D	7.86	1.53	1.36
16	C	1001	HEC	C3D-C2D	7.79	1.53	1.36
16	C	1004	HEC	C3D-C2D	7.77	1.53	1.36
16	C	1003	HEC	C3D-C2D	7.76	1.53	1.36
15	ba	101	V7N	C28-C27	7.01	1.52	1.34

The worst 5 of 1957 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	M	406	BPH	C4D-CHA-CBD	-10.58	103.73	108.52
22	L	301	BPH	C4D-CHA-CBD	-10.29	103.86	108.52
13	BA	104	BCL	C1-C2-C3	6.57	137.41	126.04
13	AQ	103	BCL	C1-O2A-CGA	6.47	133.42	116.44
15	bb	101	V7N	C28-C27-C26	-6.45	108.29	126.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	1001	HEC	NA
16	C	1002	HEC	NA
16	C	1003	HEC	NA
16	C	1004	HEC	NA

5 of 1883 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	AB	103	BCL	C1A-C2A-CAA-CBA
13	AB	103	BCL	C3A-C2A-CAA-CBA
13	AD	1001	BCL	C3A-C2A-CAA-CBA
13	AF	1002	BCL	C1A-C2A-CAA-CBA
13	AG	102	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

88 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	bj	104	BCL	1	0
13	AG	102	BCL	1	0
13	AK	102	BCL	1	0
13	AD	1002	BCL	1	0
13	AU	103	BCL	2	0
13	ag	1001	BCL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	1001	HEC	1	0
14	BN	1002	LMT	1	0
13	AR	101	BCL	1	0
13	AP	101	BCL	1	0
14	AO	103	LMT	1	0
13	ai	102	BCL	1	0
14	BG	1003	LMT	1	0
13	AE	1002	BCL	2	0
13	AP	103	BCL	1	0
13	AK	103	BCL	1	0
13	ba	103	BCL	1	0
13	BI	104	BCL	1	0
13	AI	103	BCL	1	0
13	AL	101	BCL	1	0
14	BT	1005	LMT	1	0
13	bf	105	BCL	1	0
13	aa	1001	BCL	2	0
13	AT	102	BCL	1	0
13	AS	104	BCL	6	0
13	AW	101	BCL	2	0
13	bg	104	BCL	1	0
13	al	1001	BCL	1	0
22	L	301	BPH	2	0
13	AC	1002	BCL	1	0
13	AJ	101	BCL	1	0
13	BN	1006	BCL	2	0
13	BD	106	BCL	1	0
14	AK	101	LMT	1	0
13	bm	103	BCL	2	0
13	bo	102	BCL	1	0
14	L	302	LMT	1	0
13	AF	1001	BCL	2	0
14	BD	104	LMT	1	0
13	AM	102	BCL	1	0
13	AB	101	BCL	1	0
13	bp	103	BCL	1	0
13	M	403	BCL	3	0
14	L	307	LMT	1	0
13	bn	103	BCL	1	0
13	AU	102	BCL	2	0
13	bd	103	BCL	1	0
13	AL	103	BCL	1	0

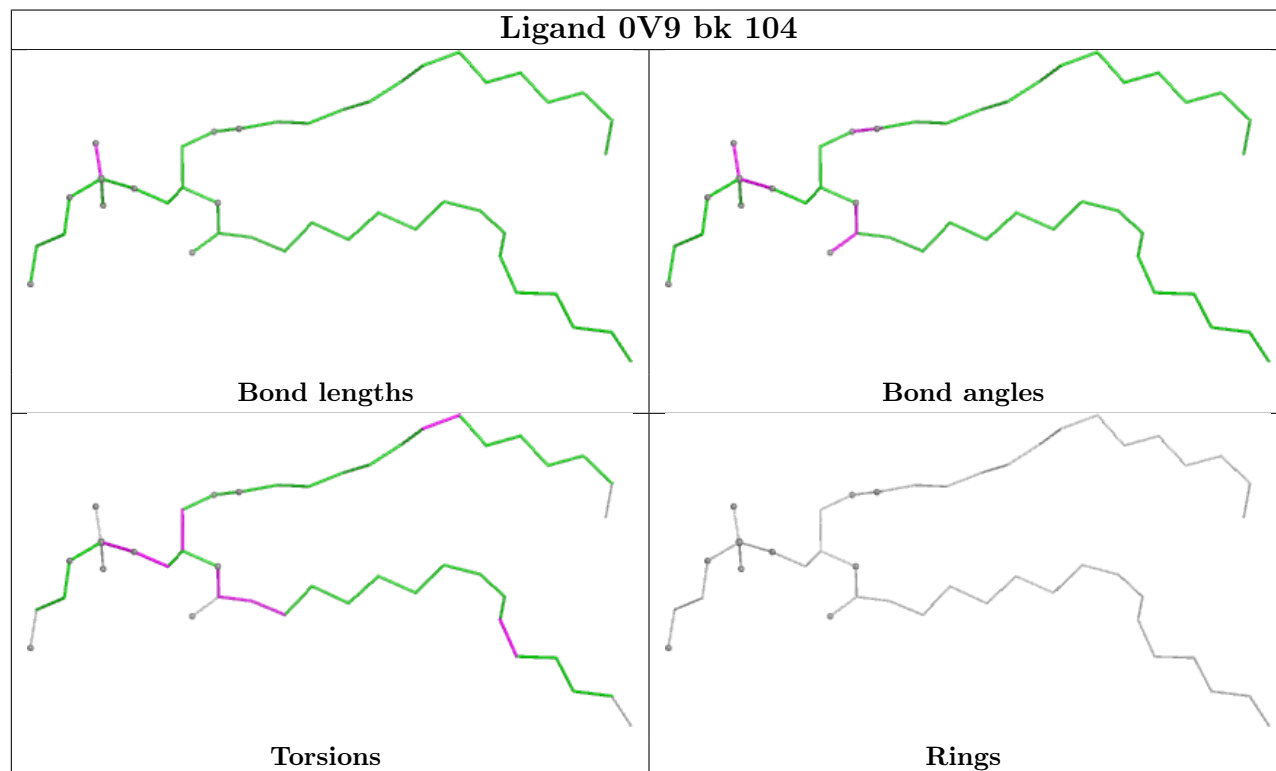
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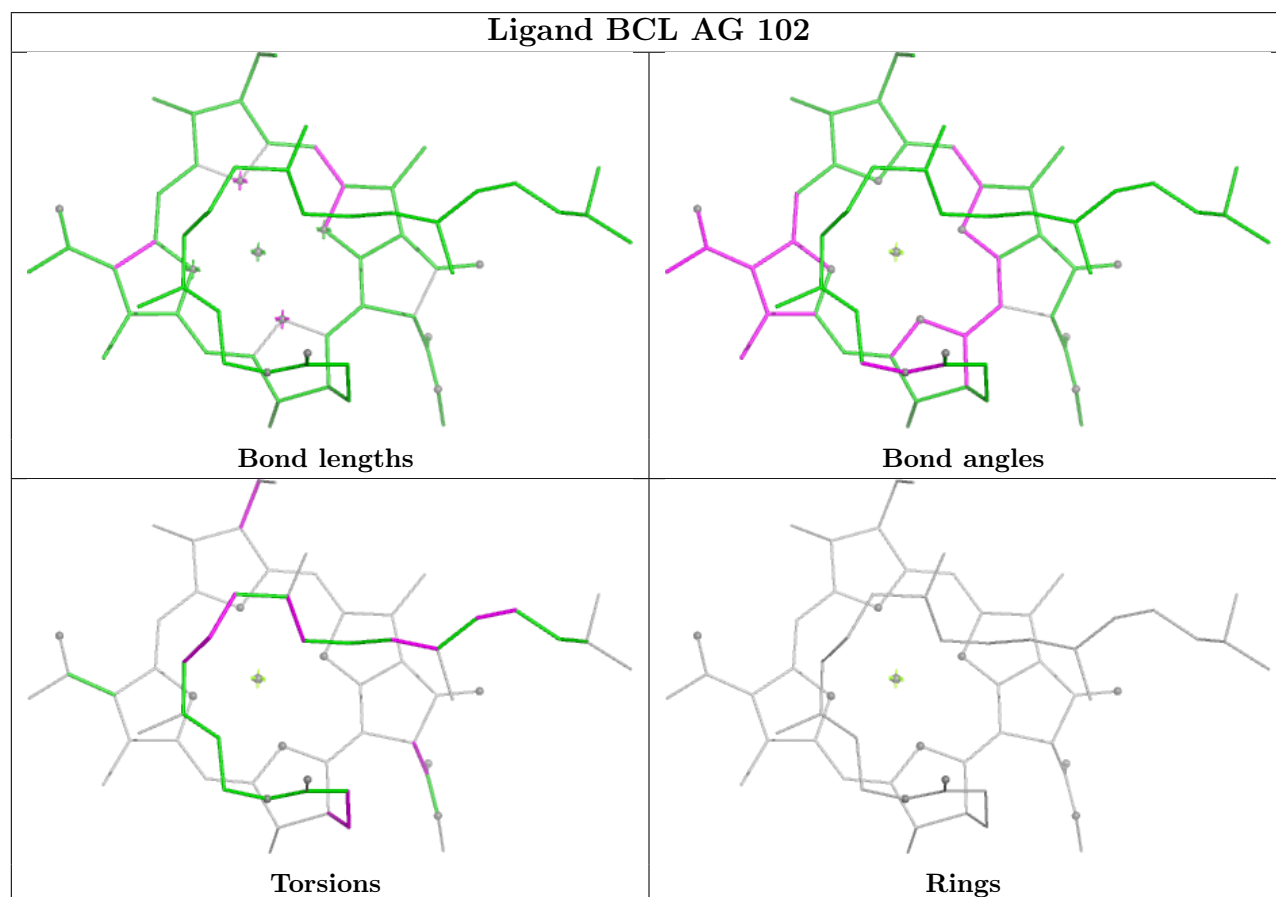
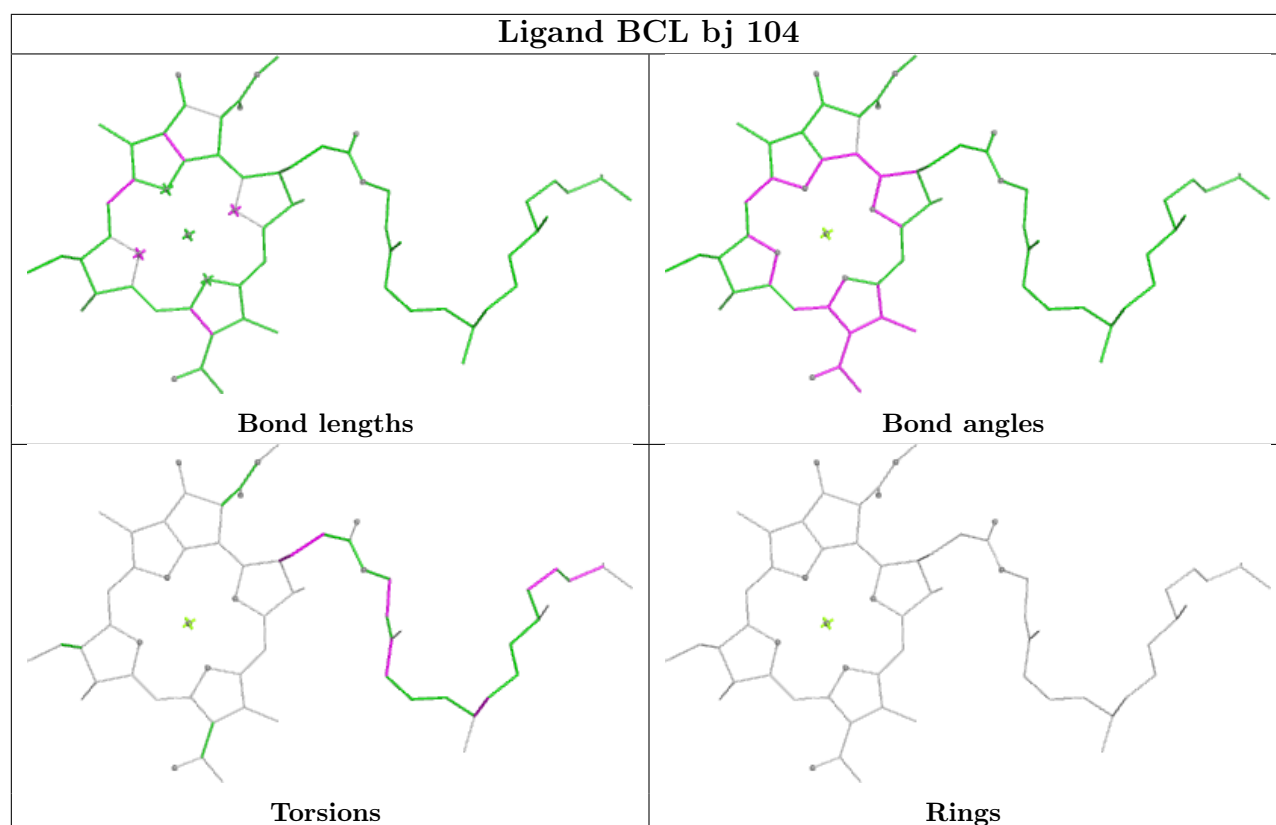
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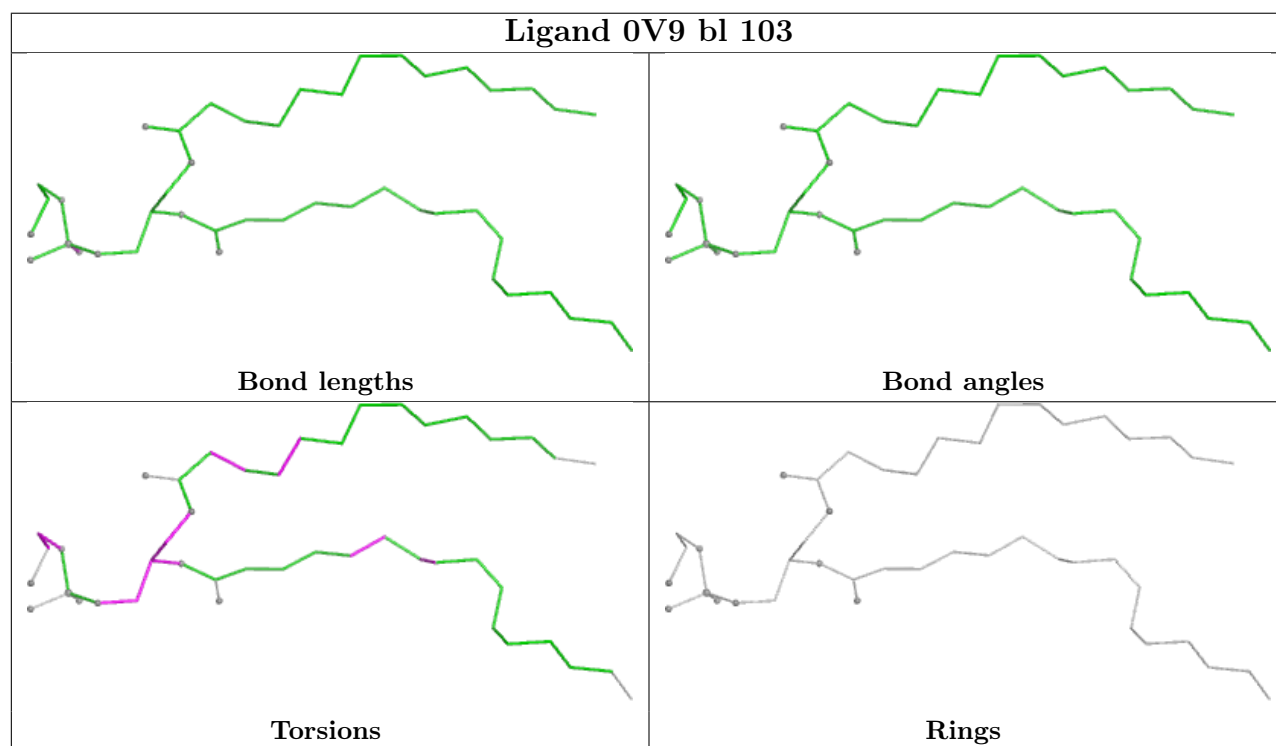
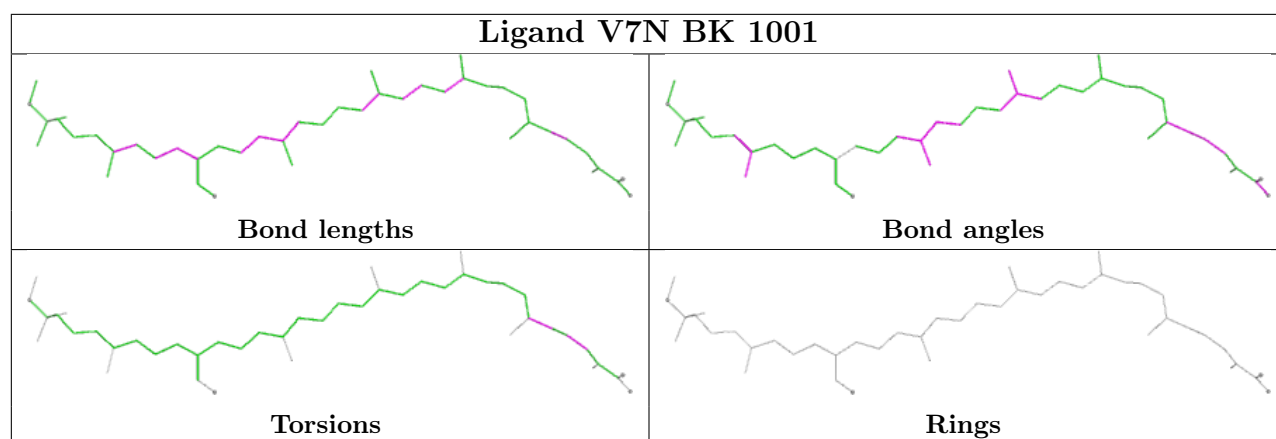
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	ae	1001	BCL	1	0
13	AS	101	BCL	1	0
13	af	102	BCL	2	0
13	AN	104	BCL	1	0
13	AQ	101	BCL	1	0
14	BG	1002	LMT	1	0
25	M	408	CRT	1	0
13	bk	105	BCL	1	0
23	L	309	MQ8	1	0
23	M	407	MQ8	1	0
13	an	102	BCL	1	0
16	C	1004	HEC	1	0
21	af	103	CD4	1	0
14	BE	105	LMT	1	0
13	AF	1002	BCL	1	0
14	BE	103	LMT	1	0
13	M	405	BCL	2	0
13	AO	101	BCL	1	0
23	an	101	MQ8	2	0
13	ac	102	BCL	1	0
14	BW	1005	LMT	1	0
13	AG	103	BCL	1	0
13	AI	102	BCL	1	0
13	bl	105	BCL	1	0
14	BT	1003	LMT	1	0
13	L	308	BCL	2	0
22	M	406	BPH	3	0
13	ab	1001	BCL	3	0
13	AC	1001	BCL	1	0
13	ao	1001	BCL	1	0
13	AO	102	BCL	1	0
13	AH	102	BCL	1	0
13	AA	1001	BCL	3	0
13	AW	103	BCL	1	0
13	AQ	103	BCL	2	0
14	AP	102	LMT	1	0
13	bh	105	BCL	1	0
16	C	1003	HEC	1	0
13	AX	101	BCL	1	0
16	C	1002	HEC	1	0

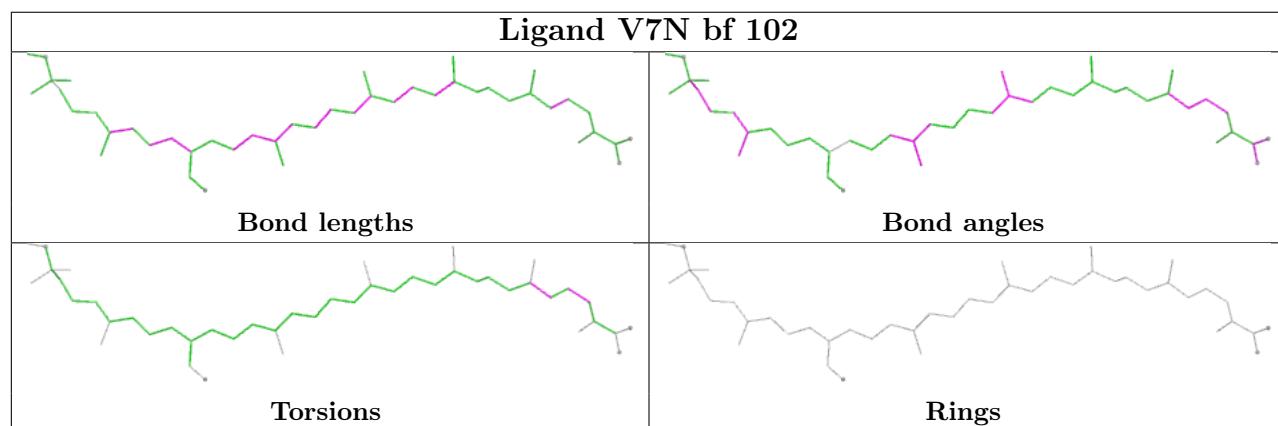
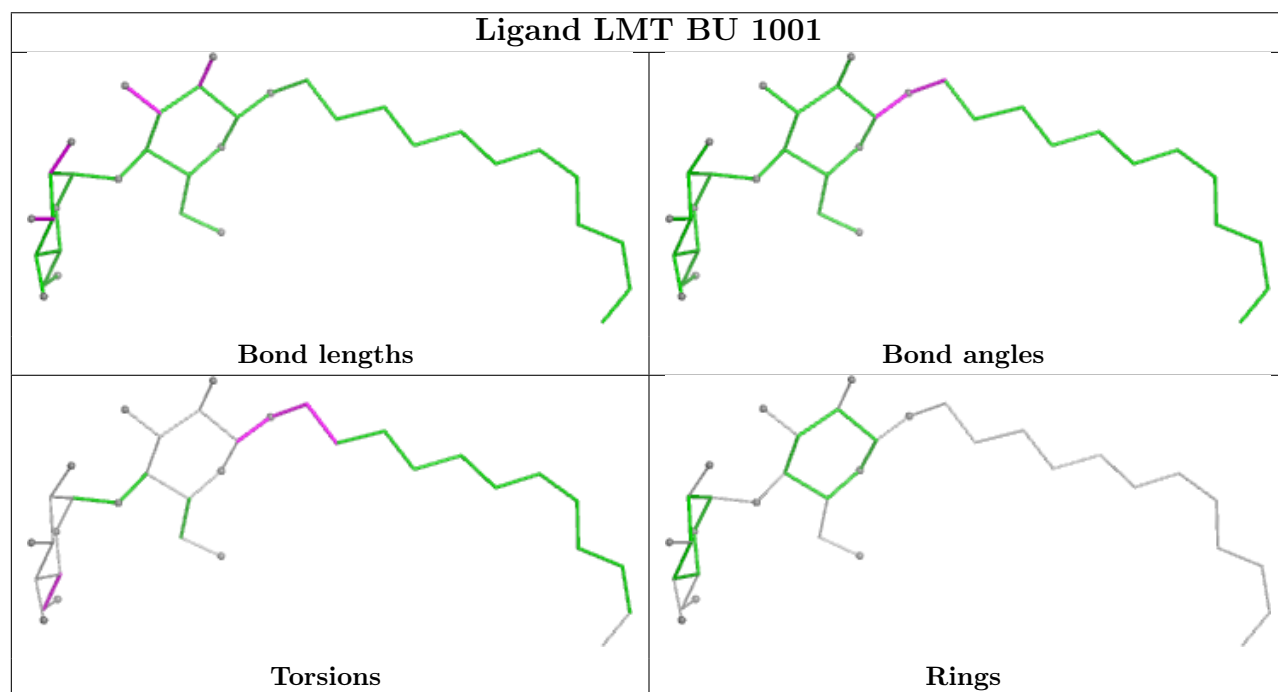
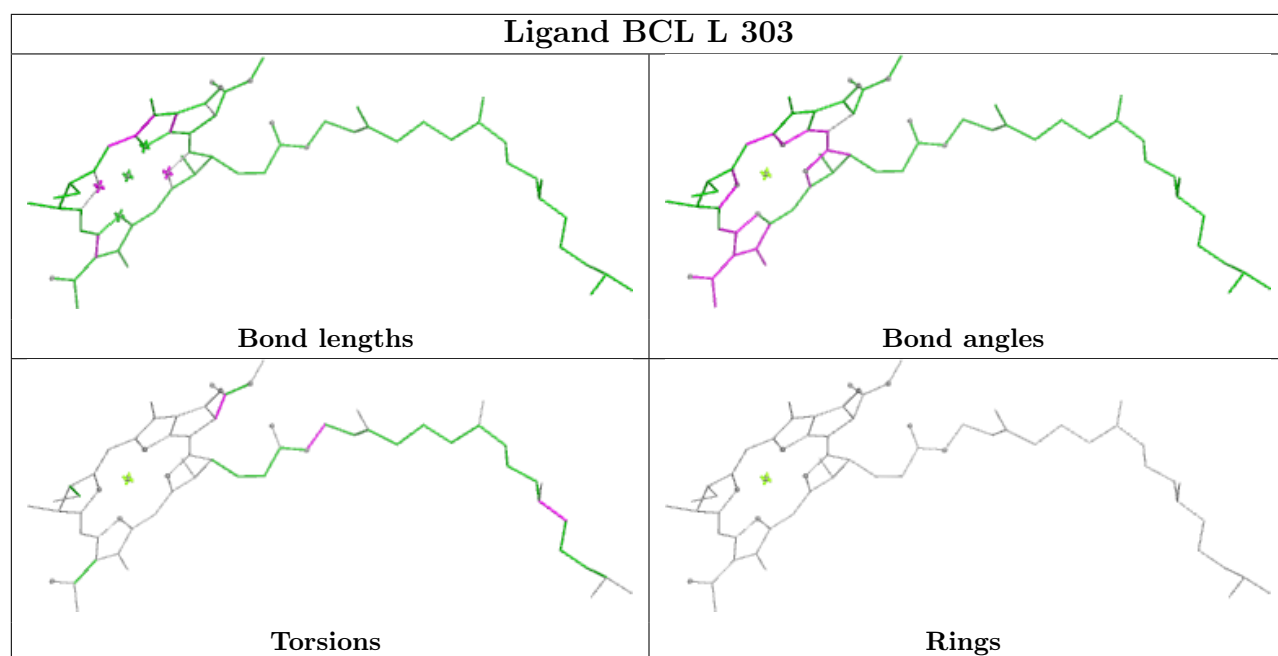
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

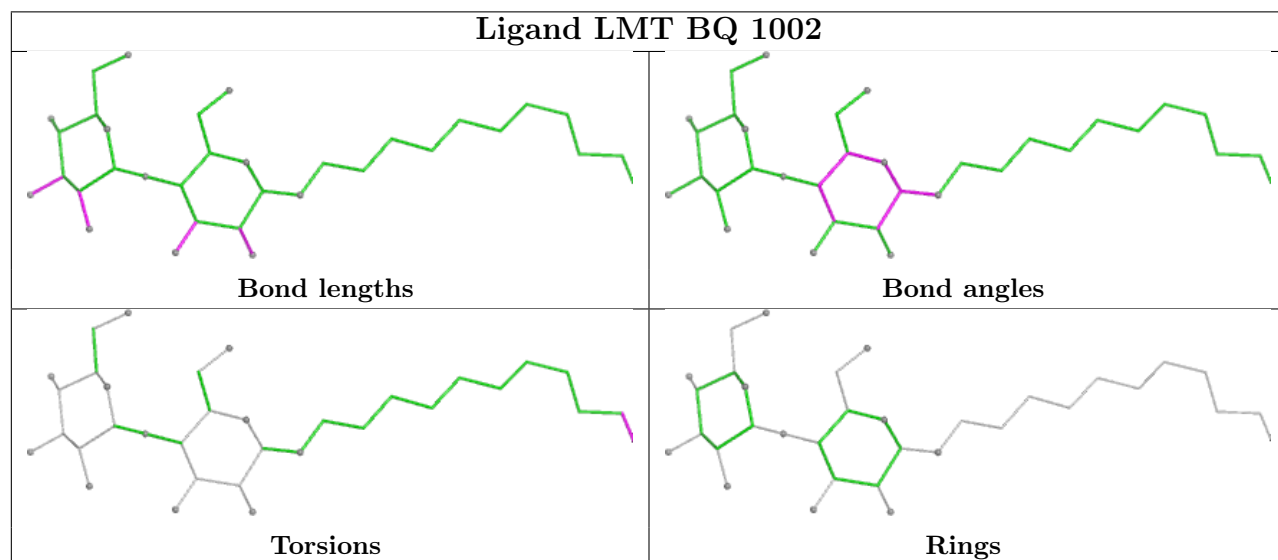
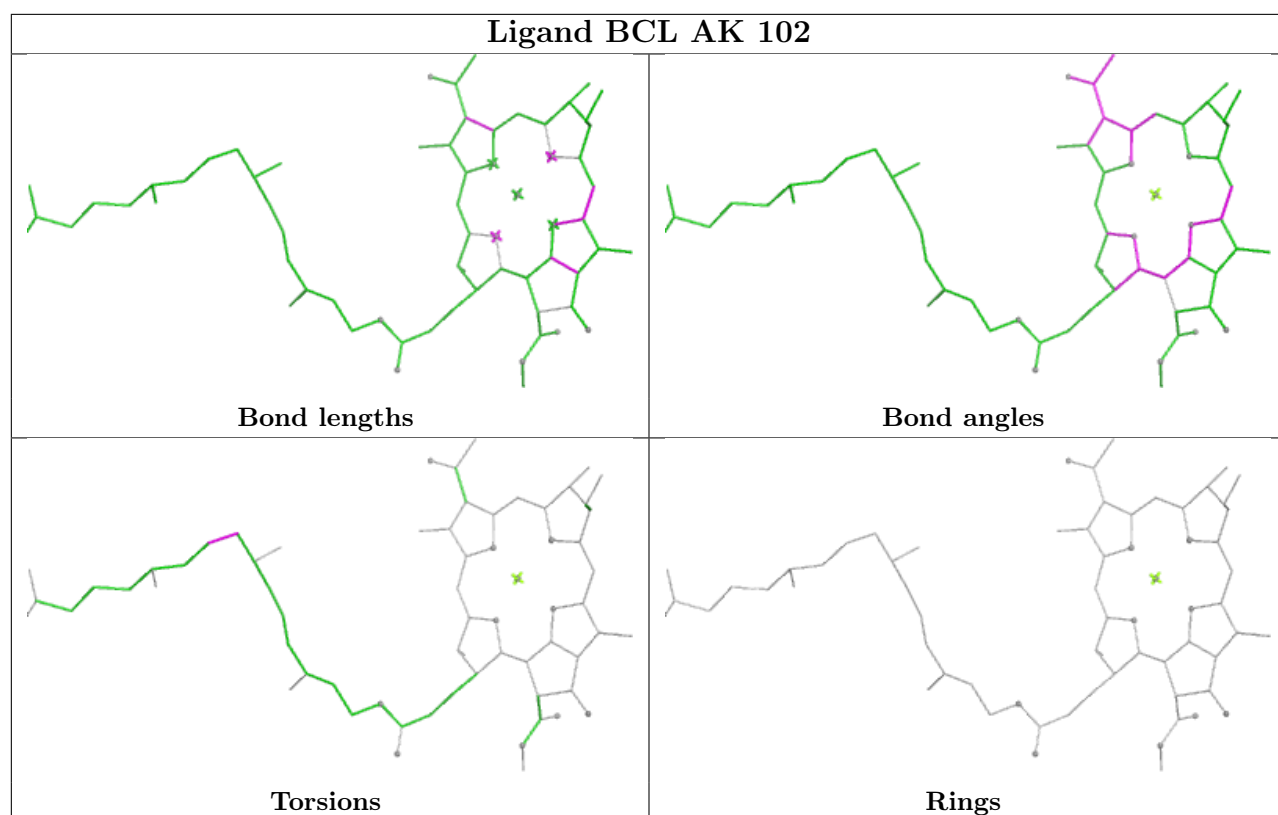
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

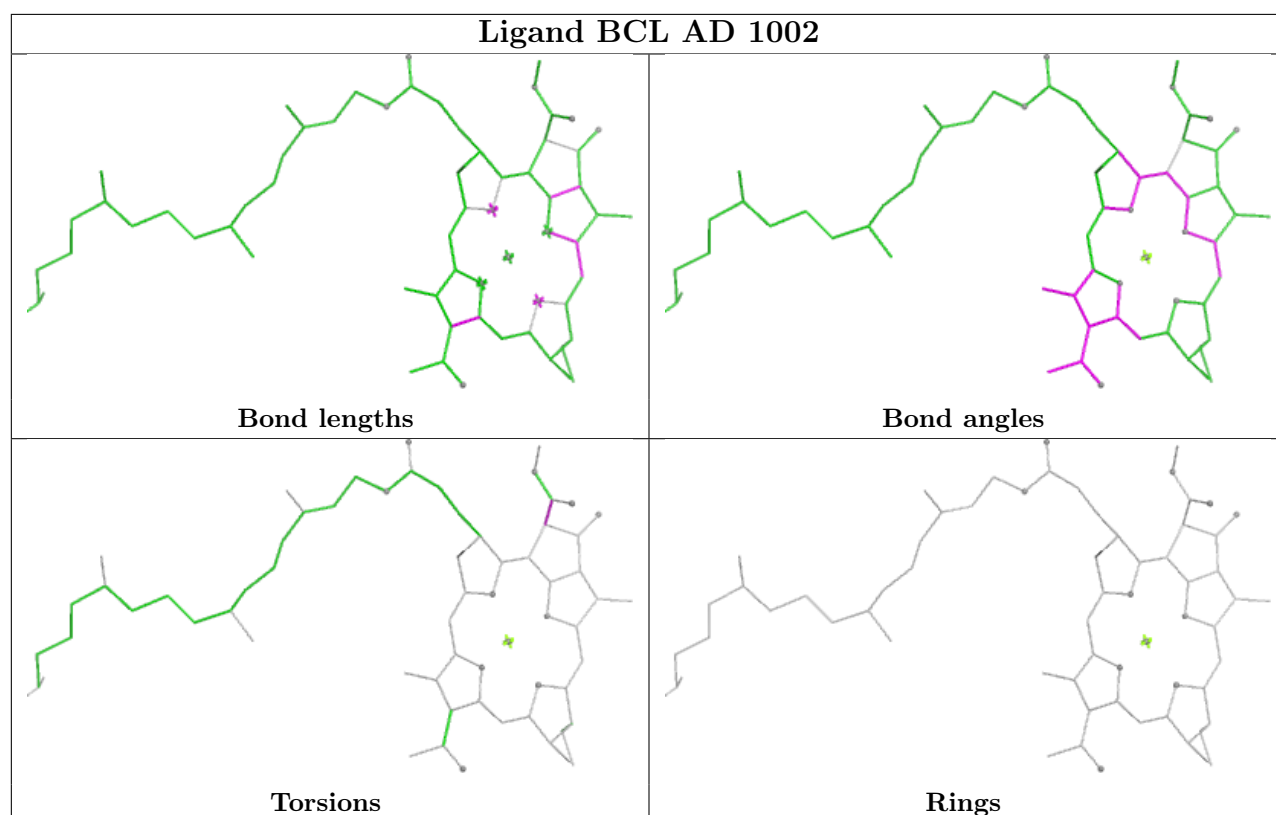
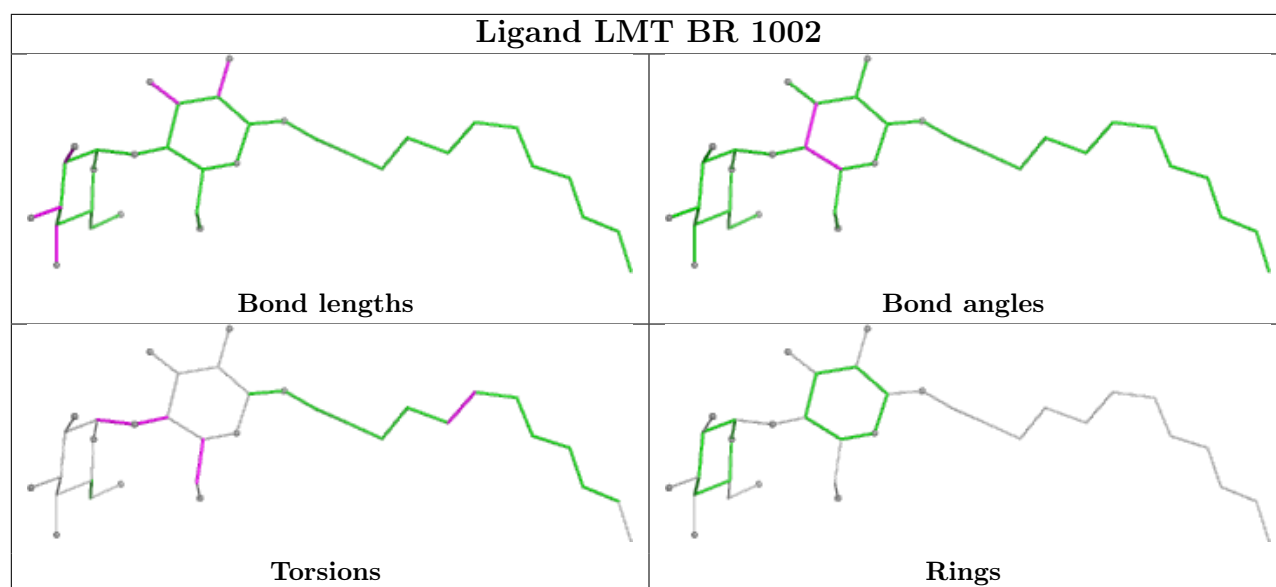


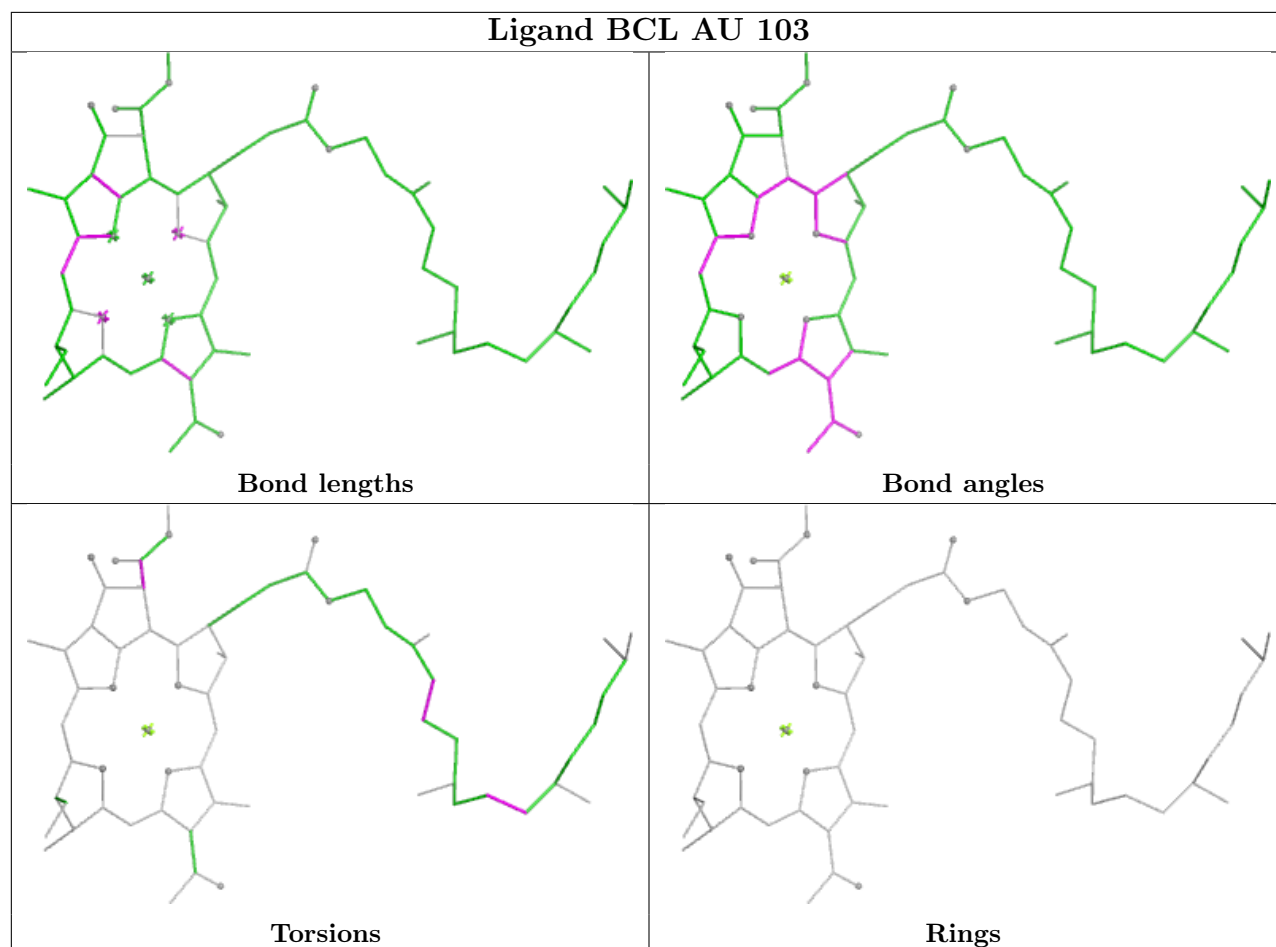
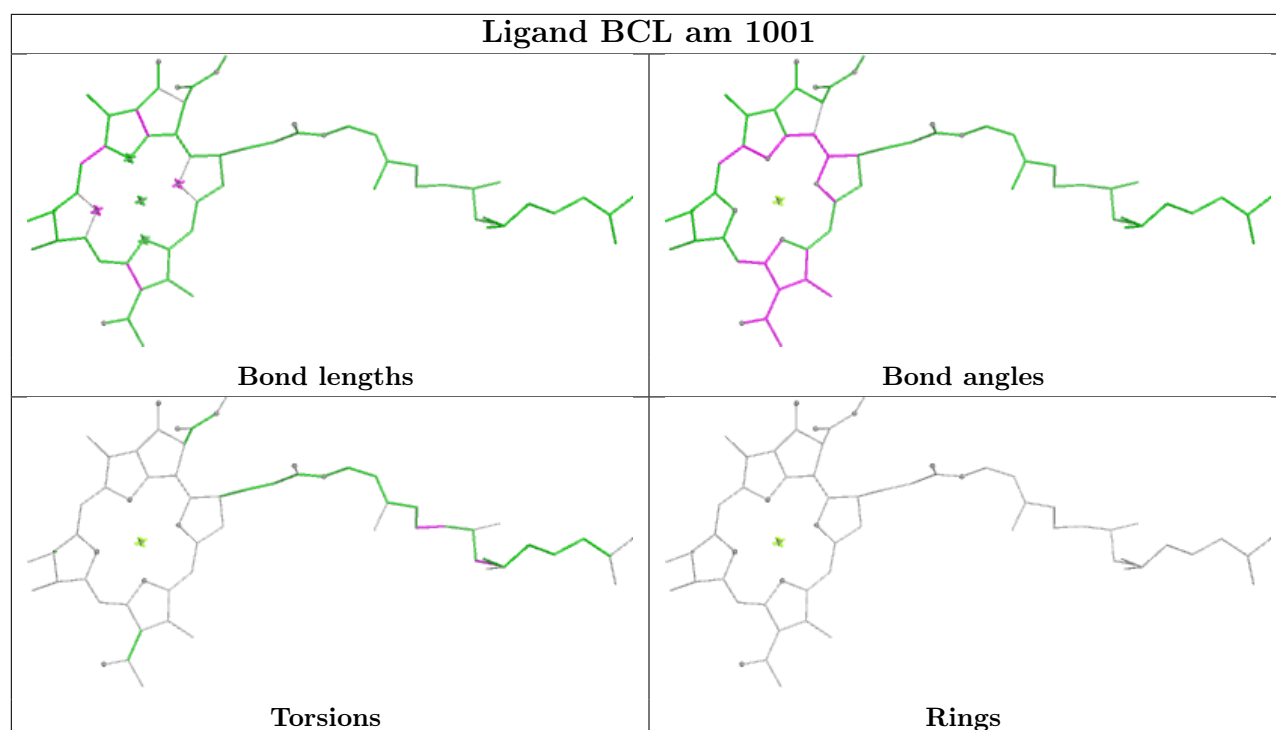


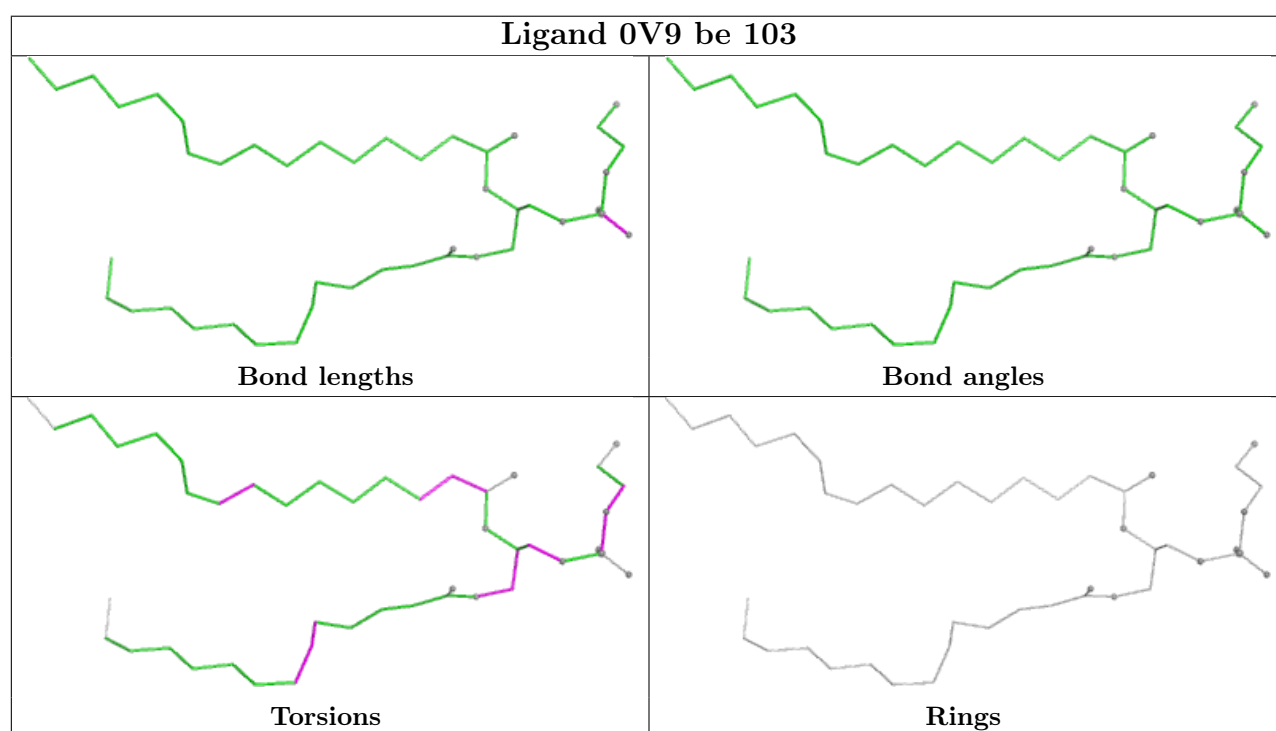
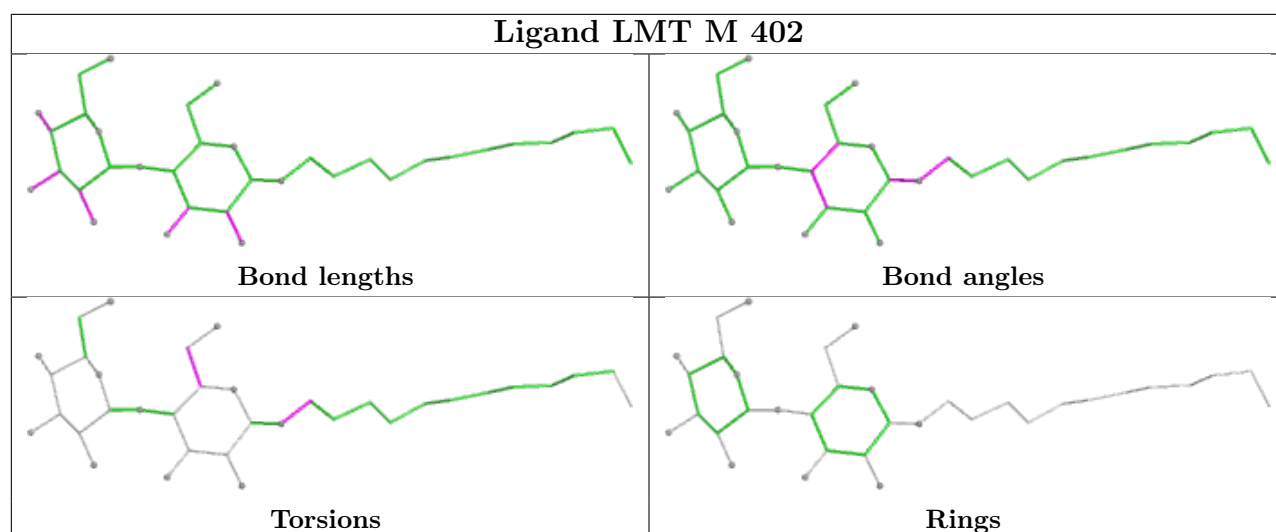


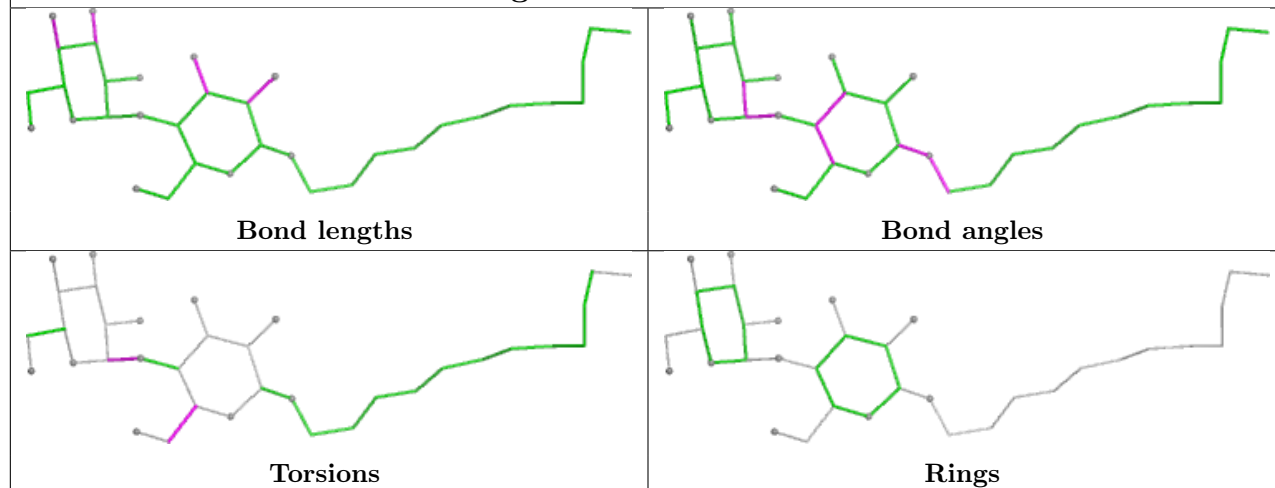
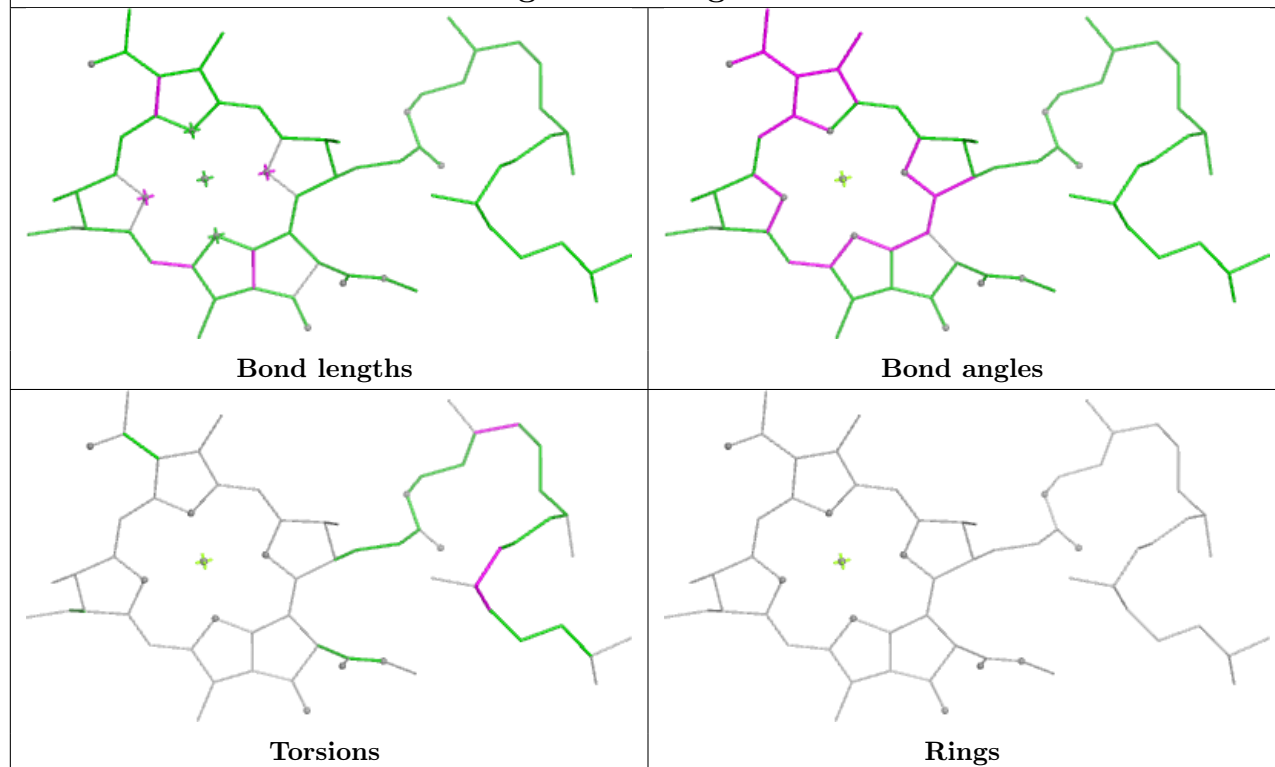


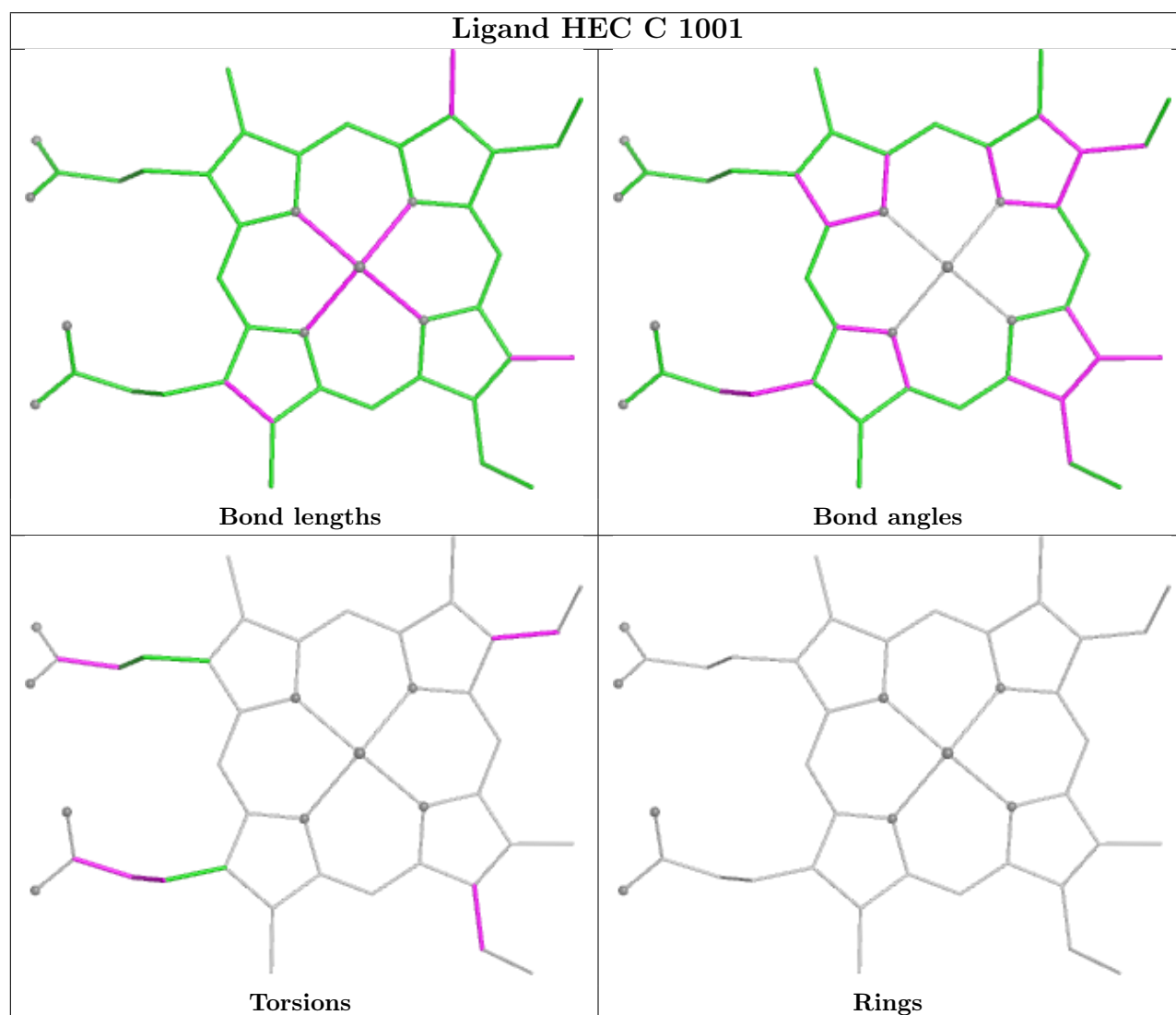
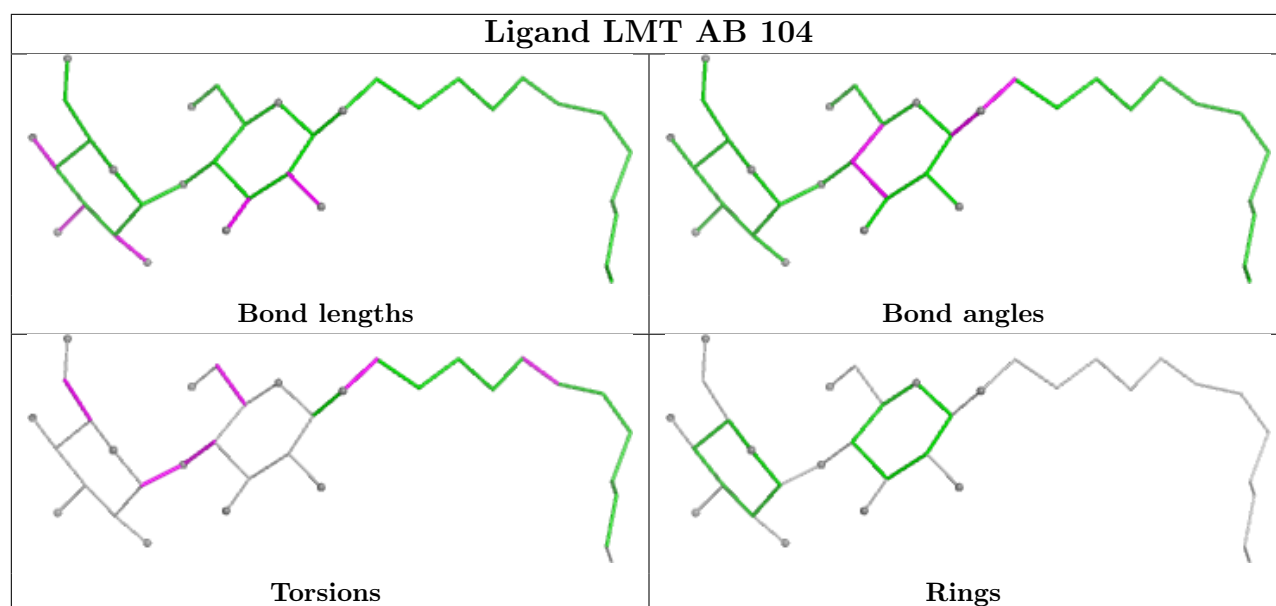


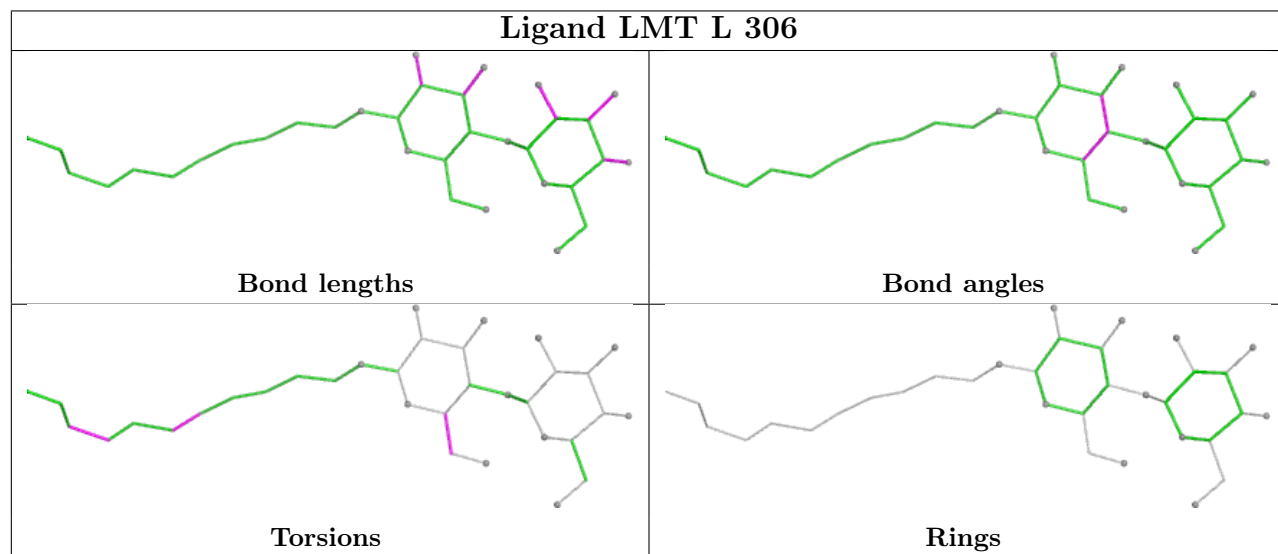
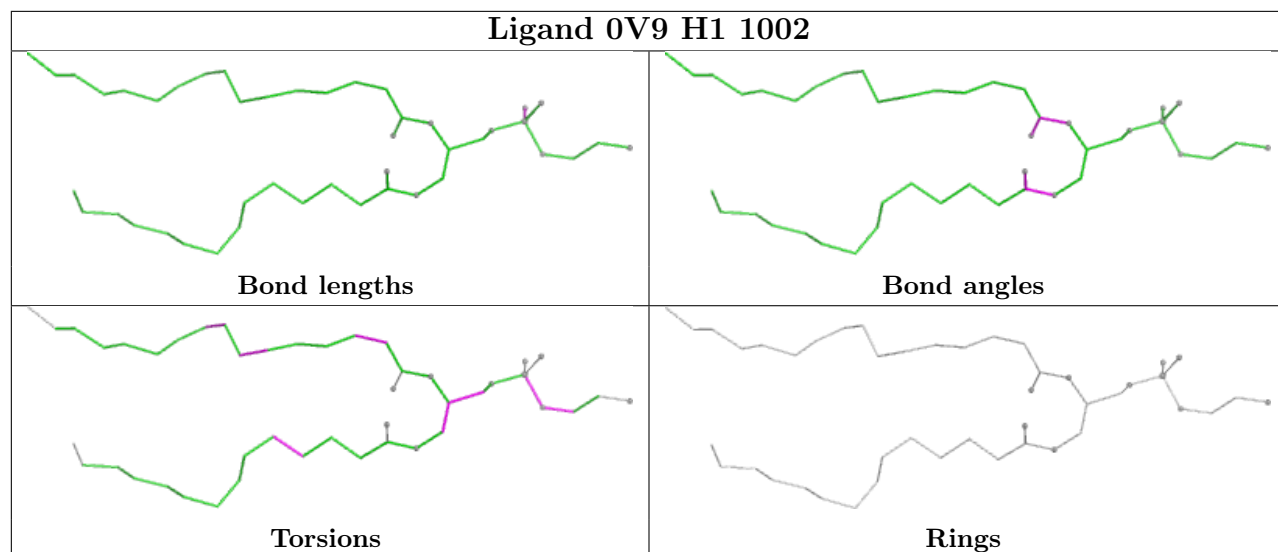


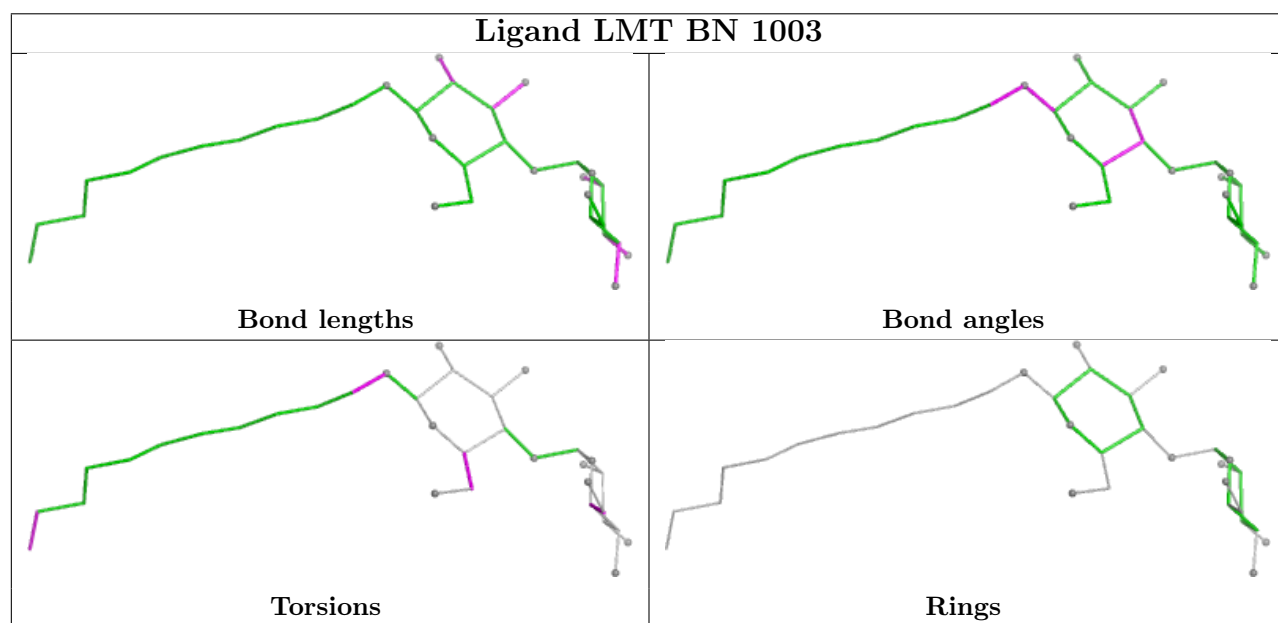
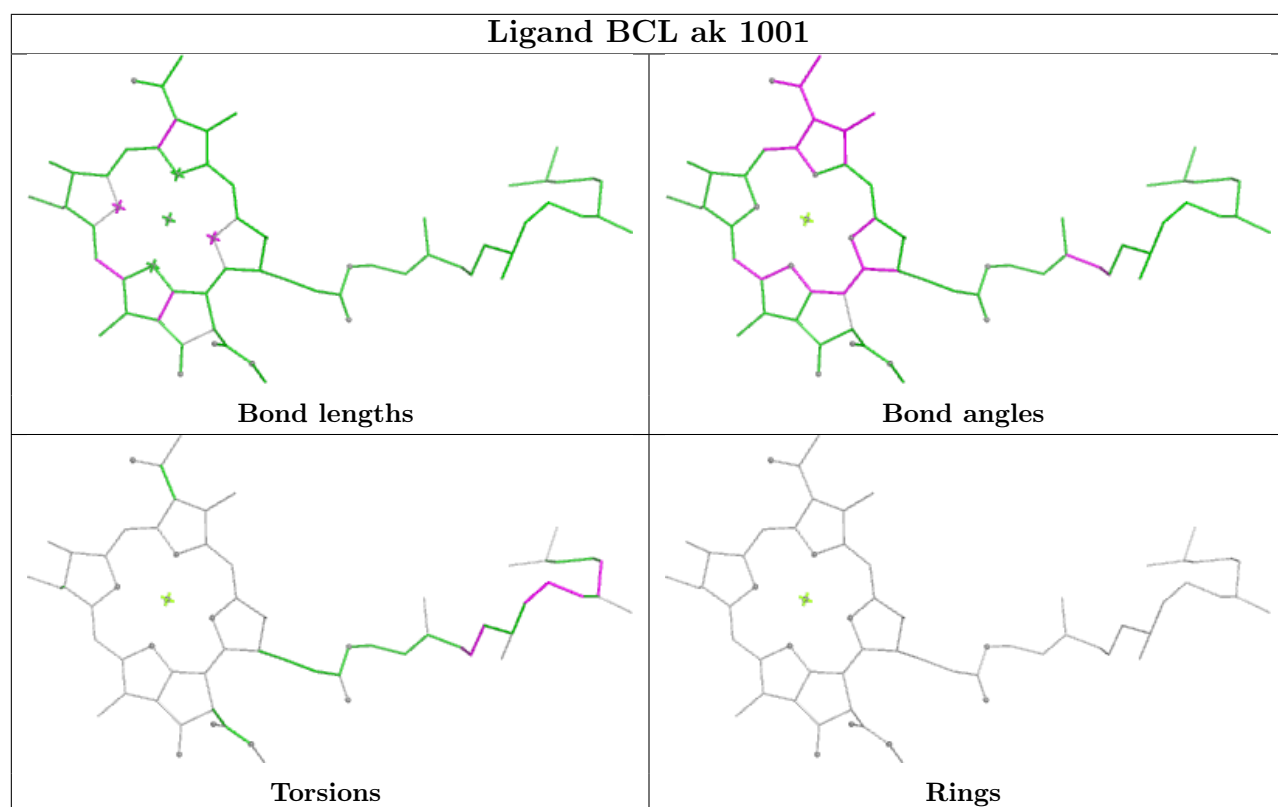


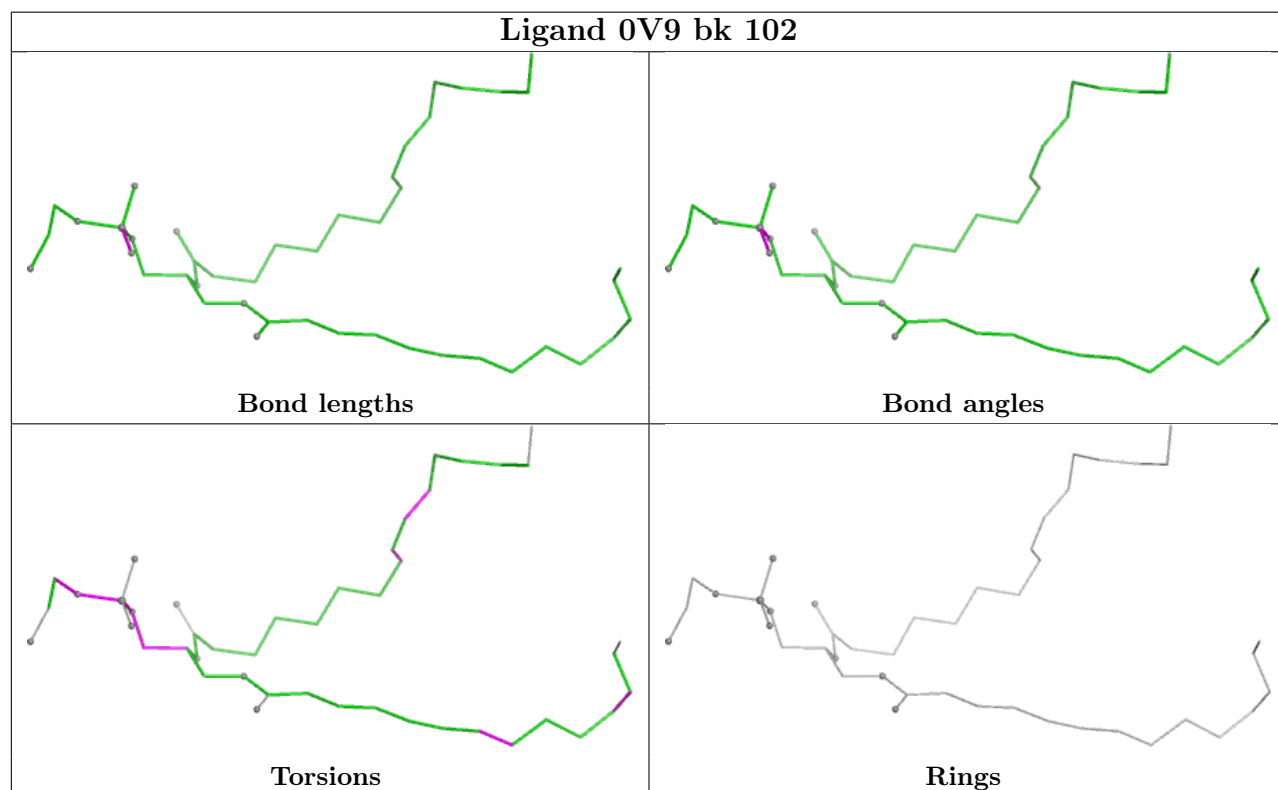
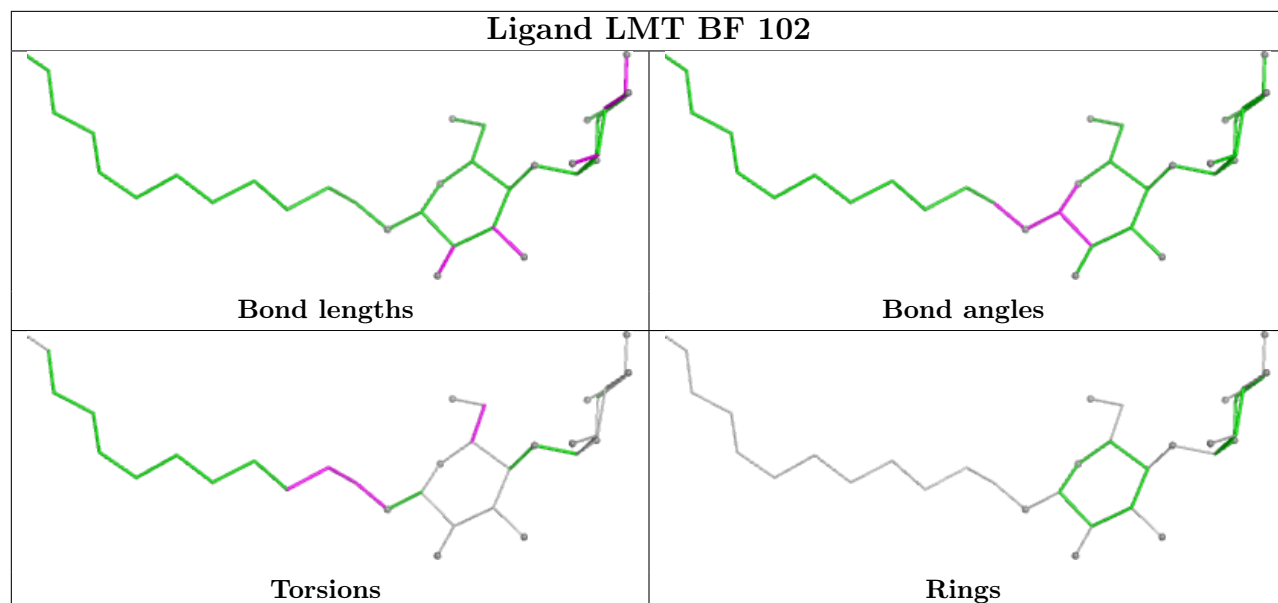


Ligand LMT AW 102**Ligand BCL ag 1001**

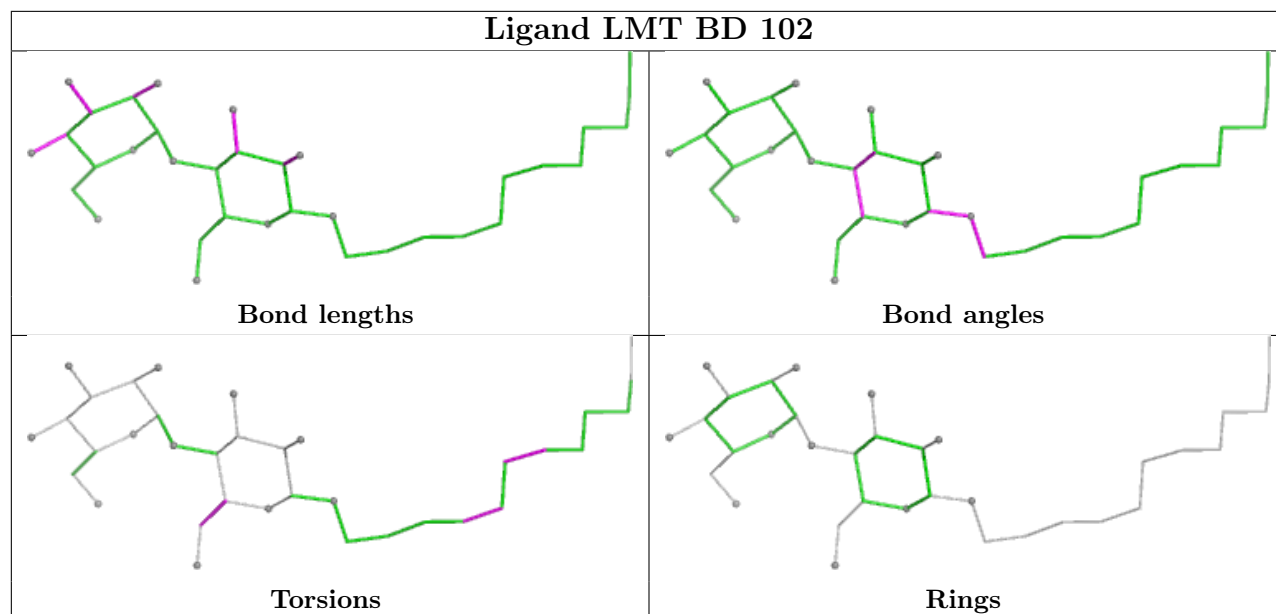




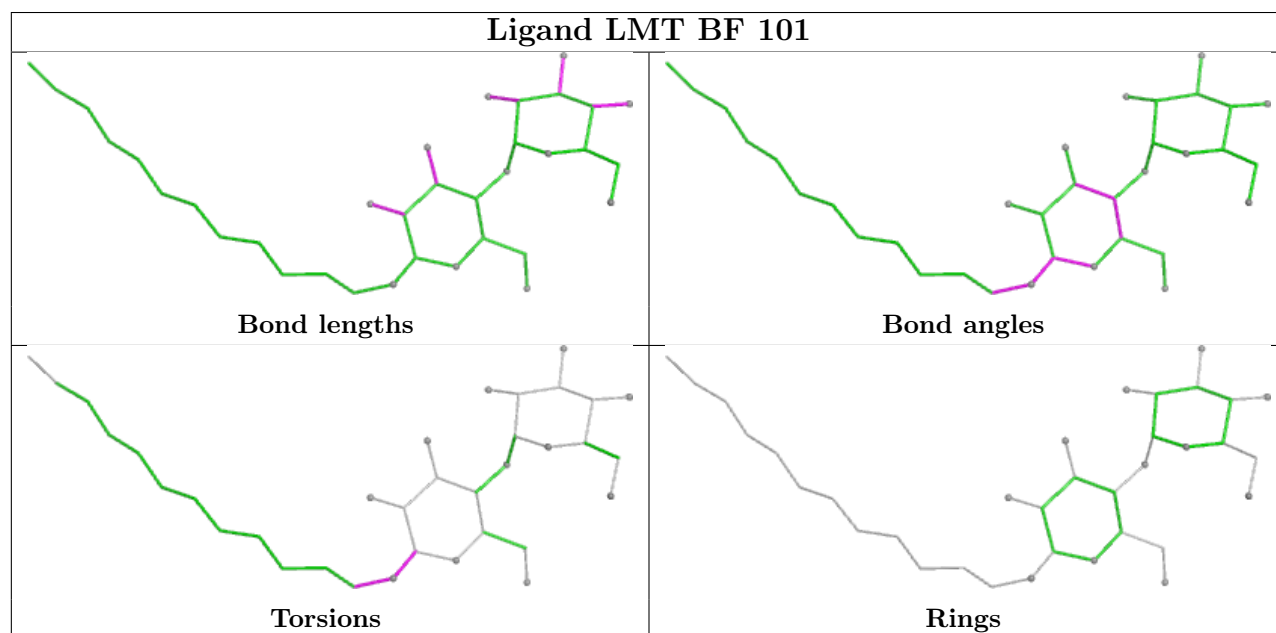


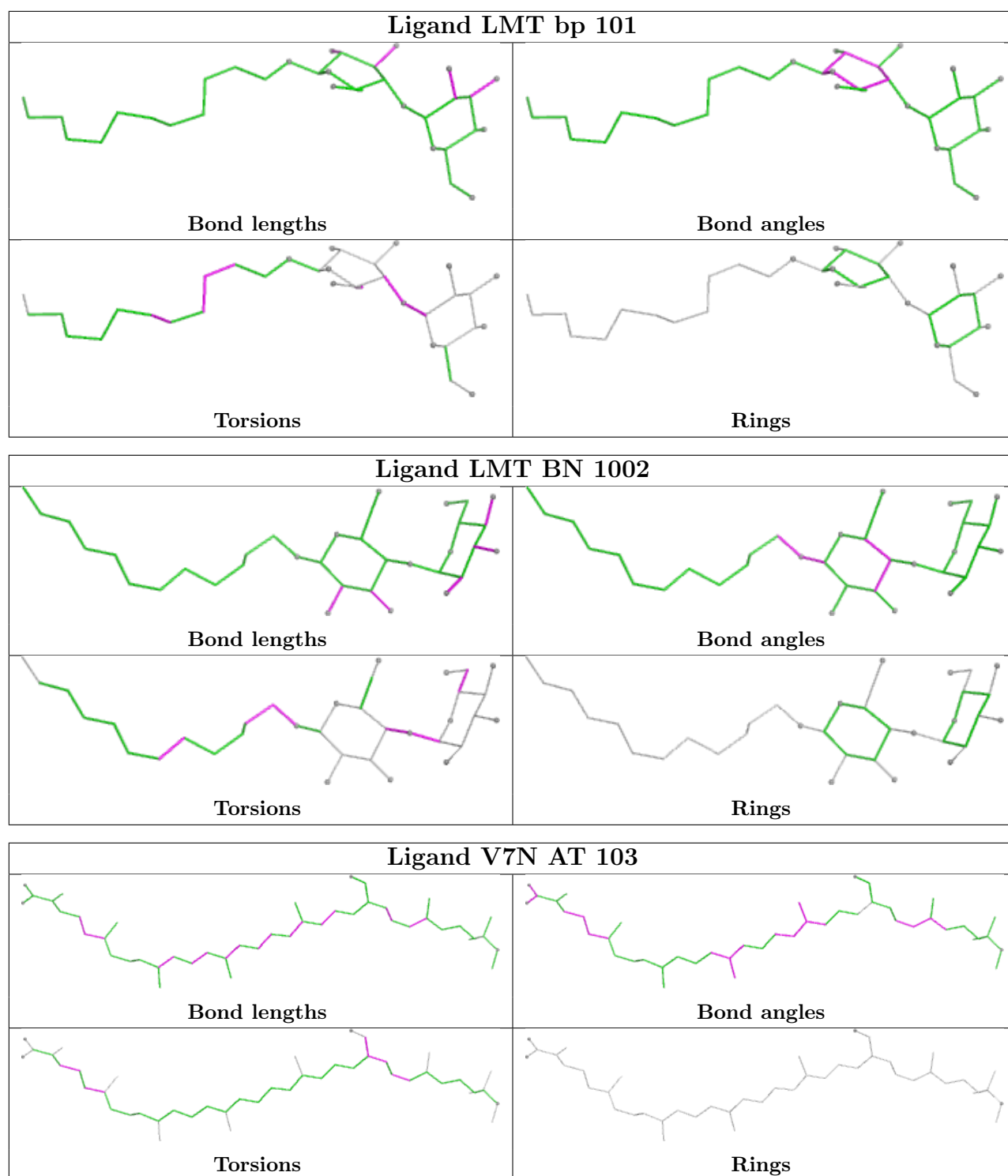


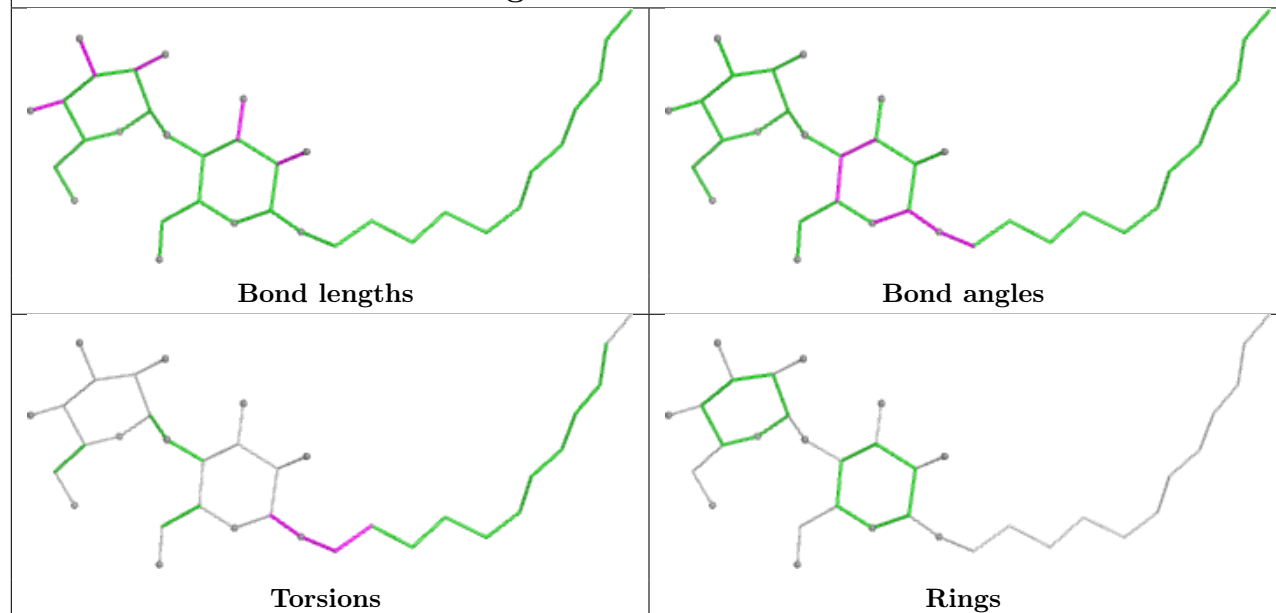
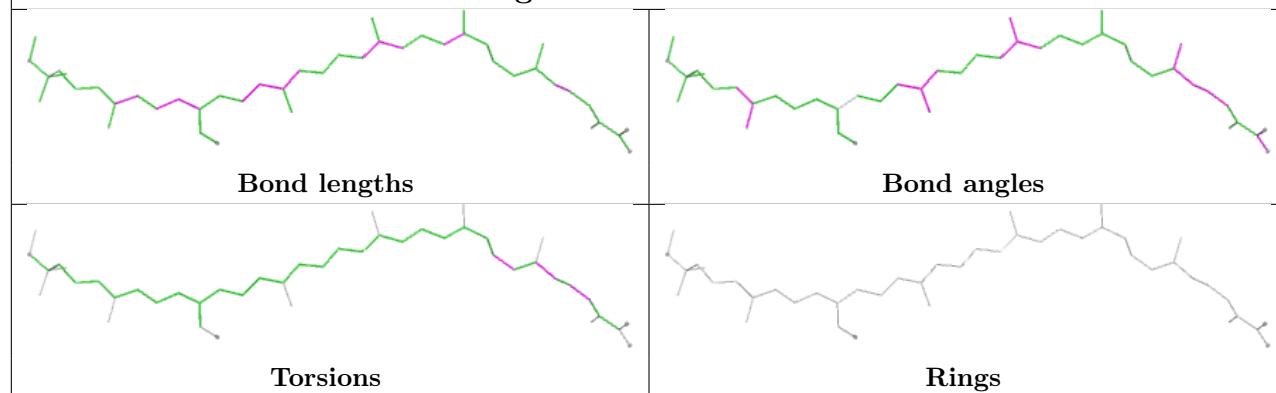
Ligand LMT BD 102

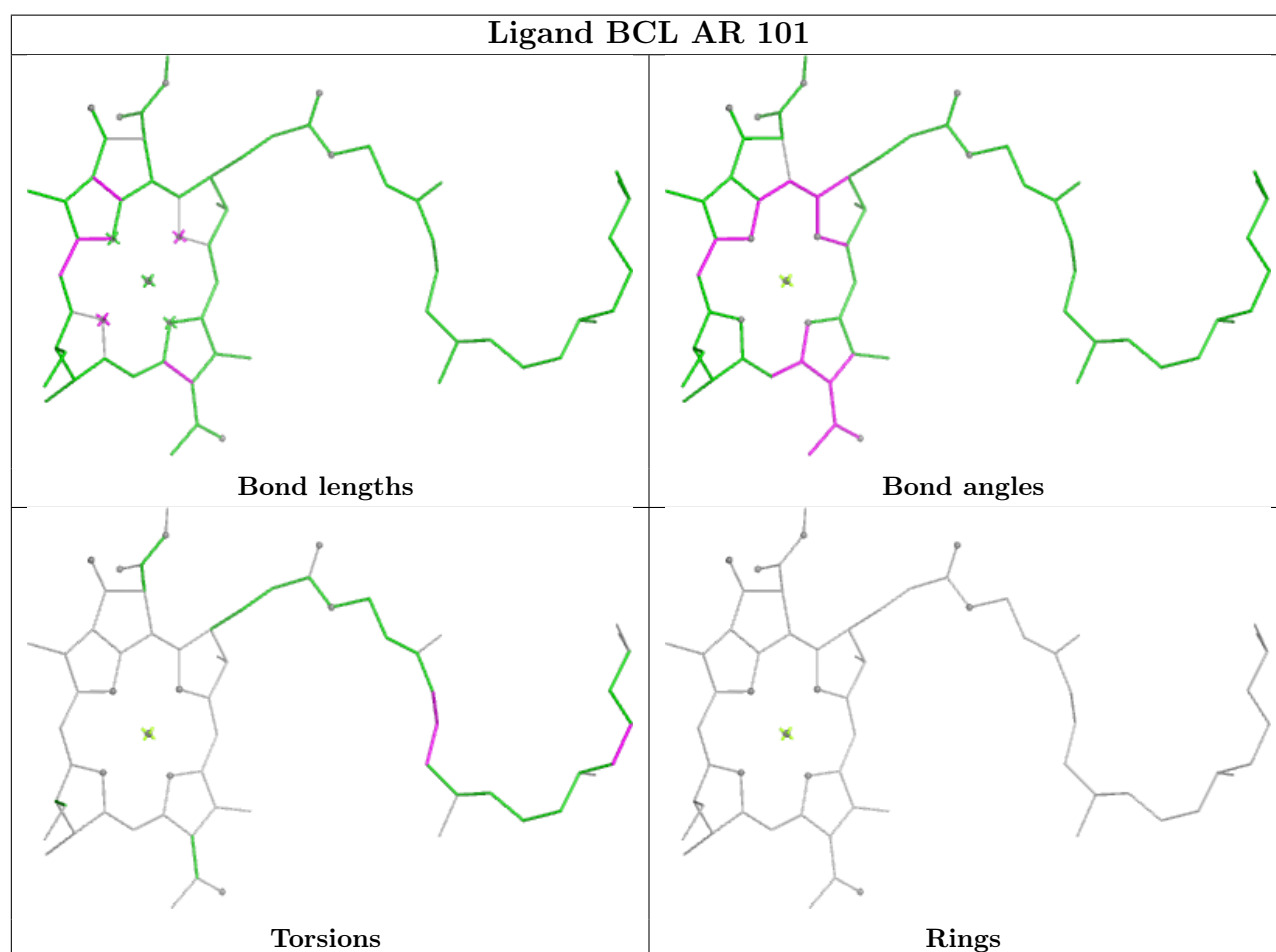
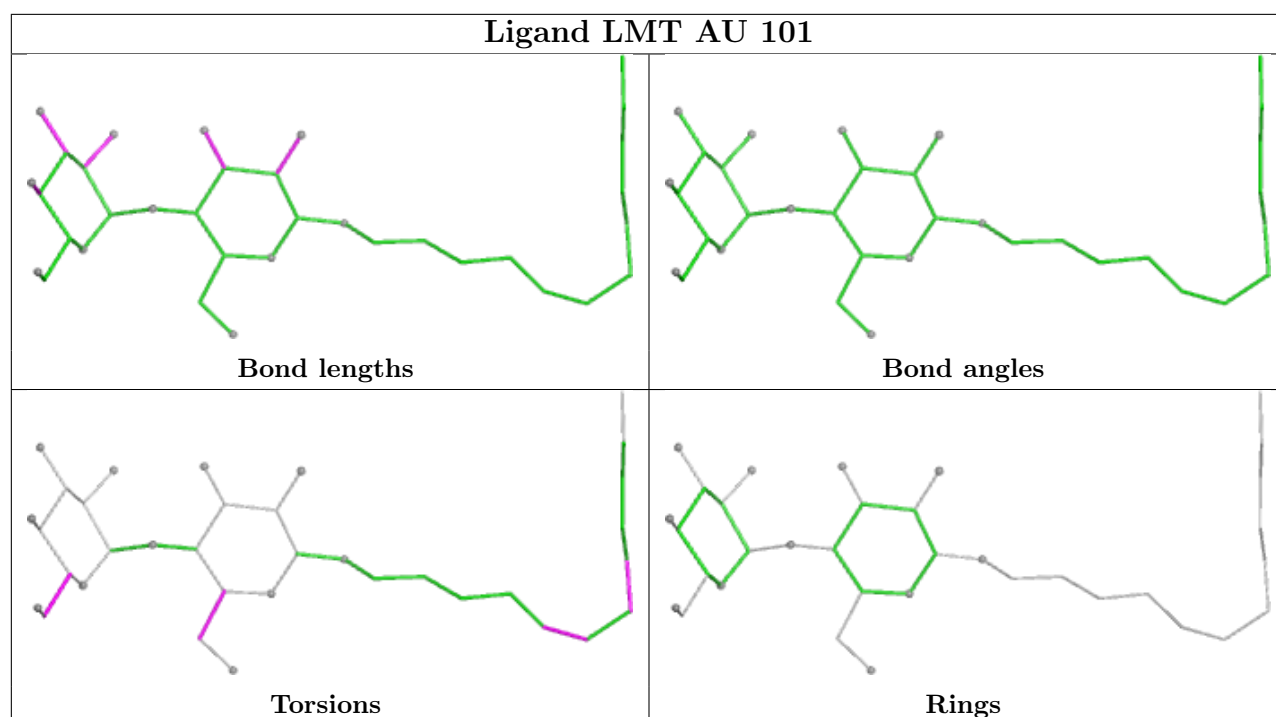


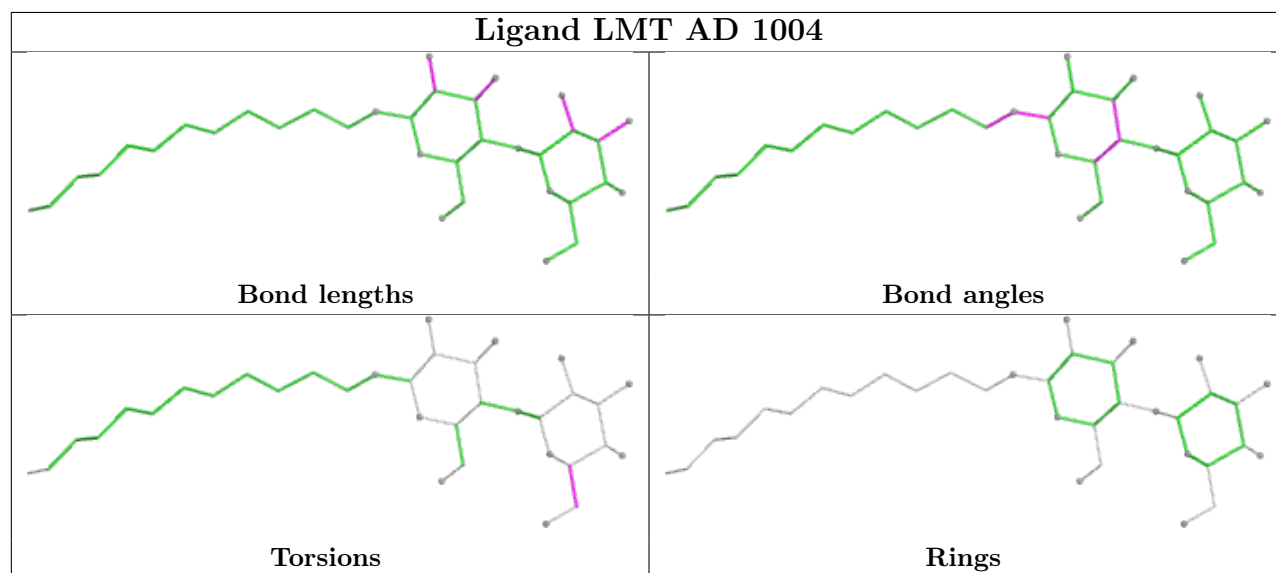
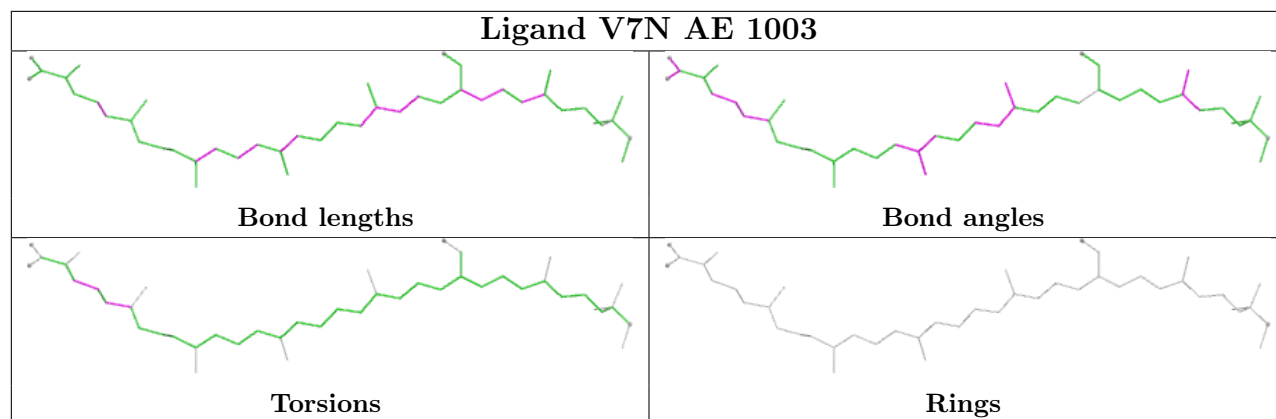
Ligand LMT BF 101

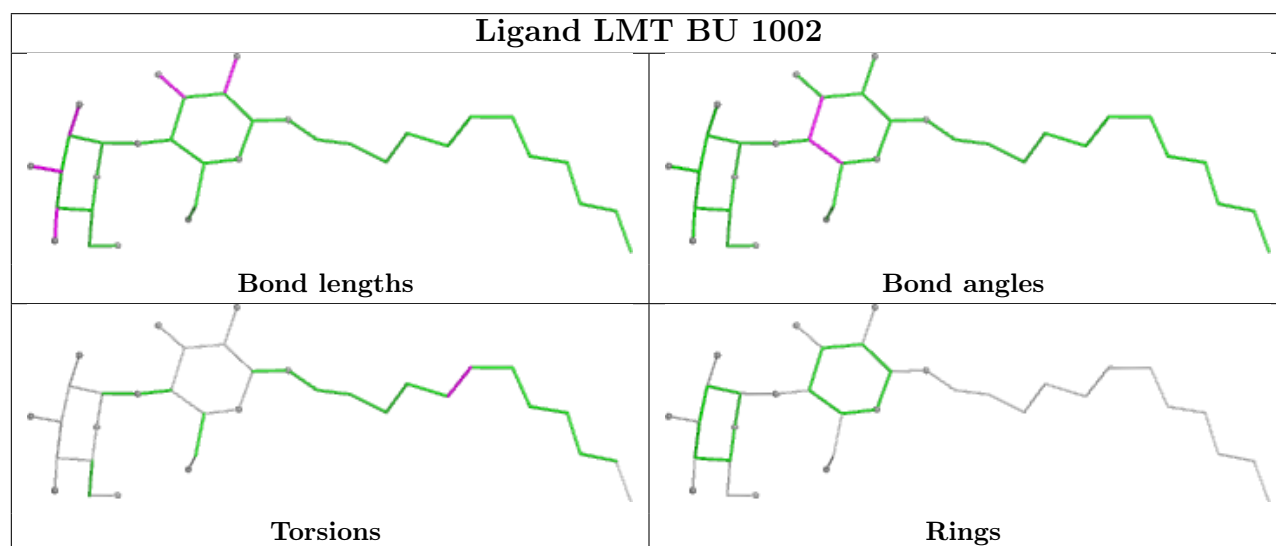
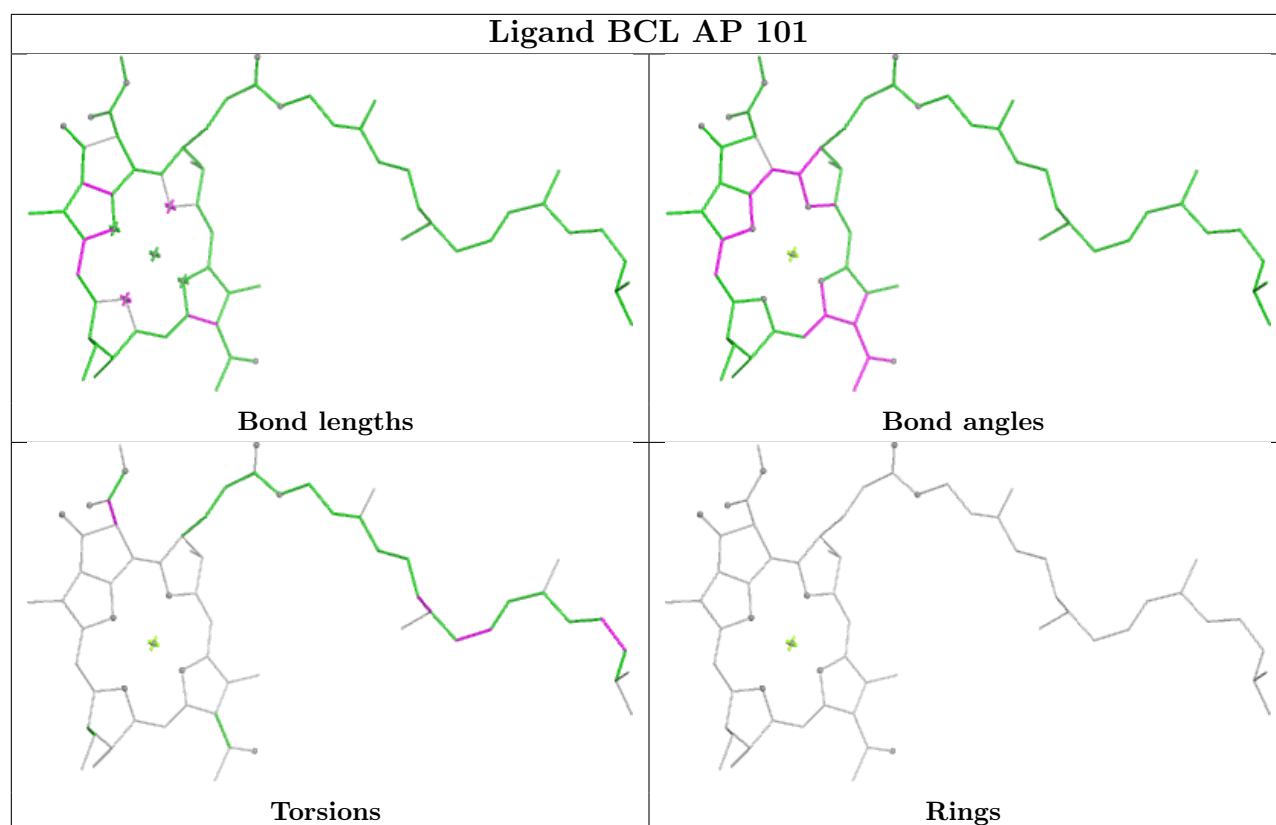


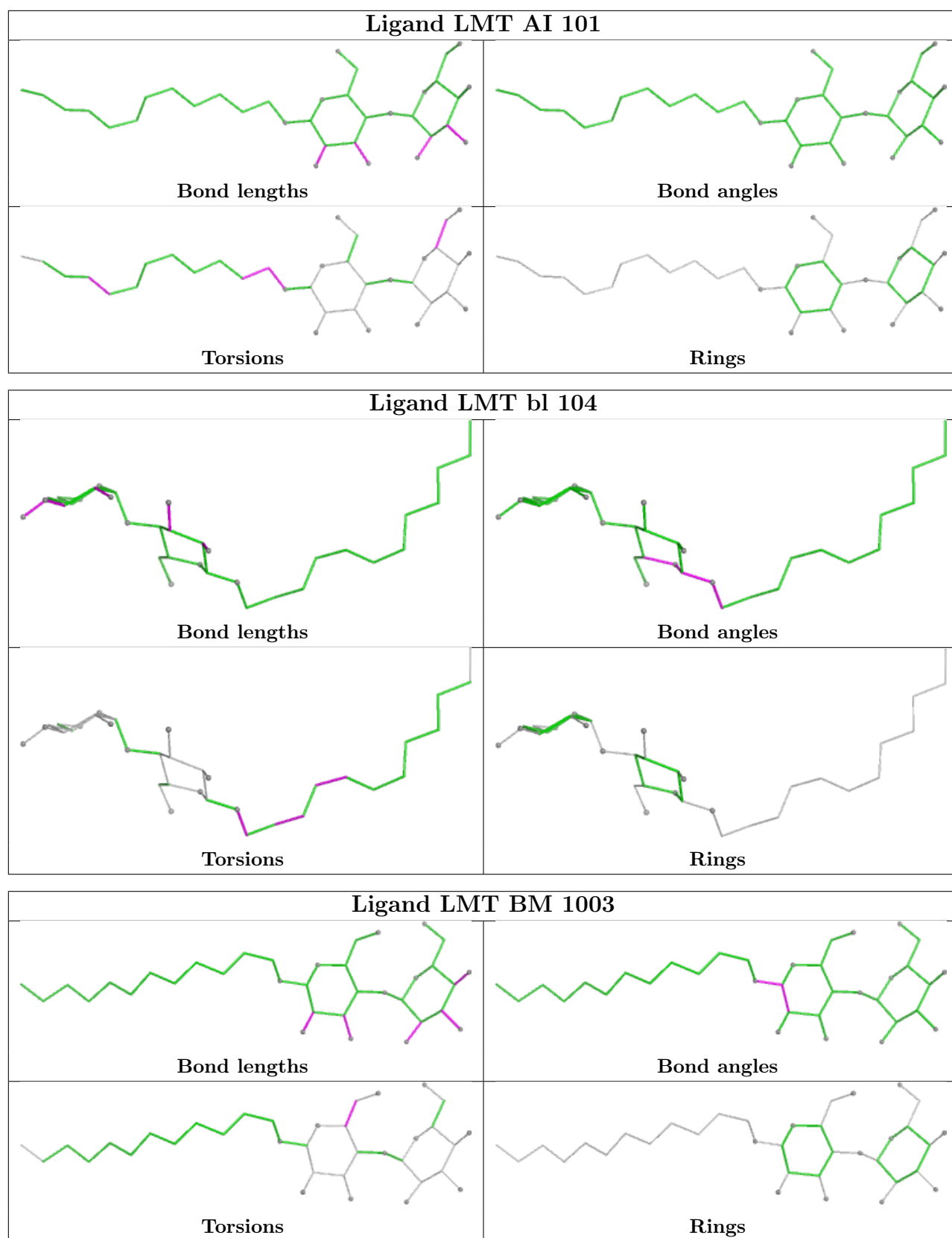


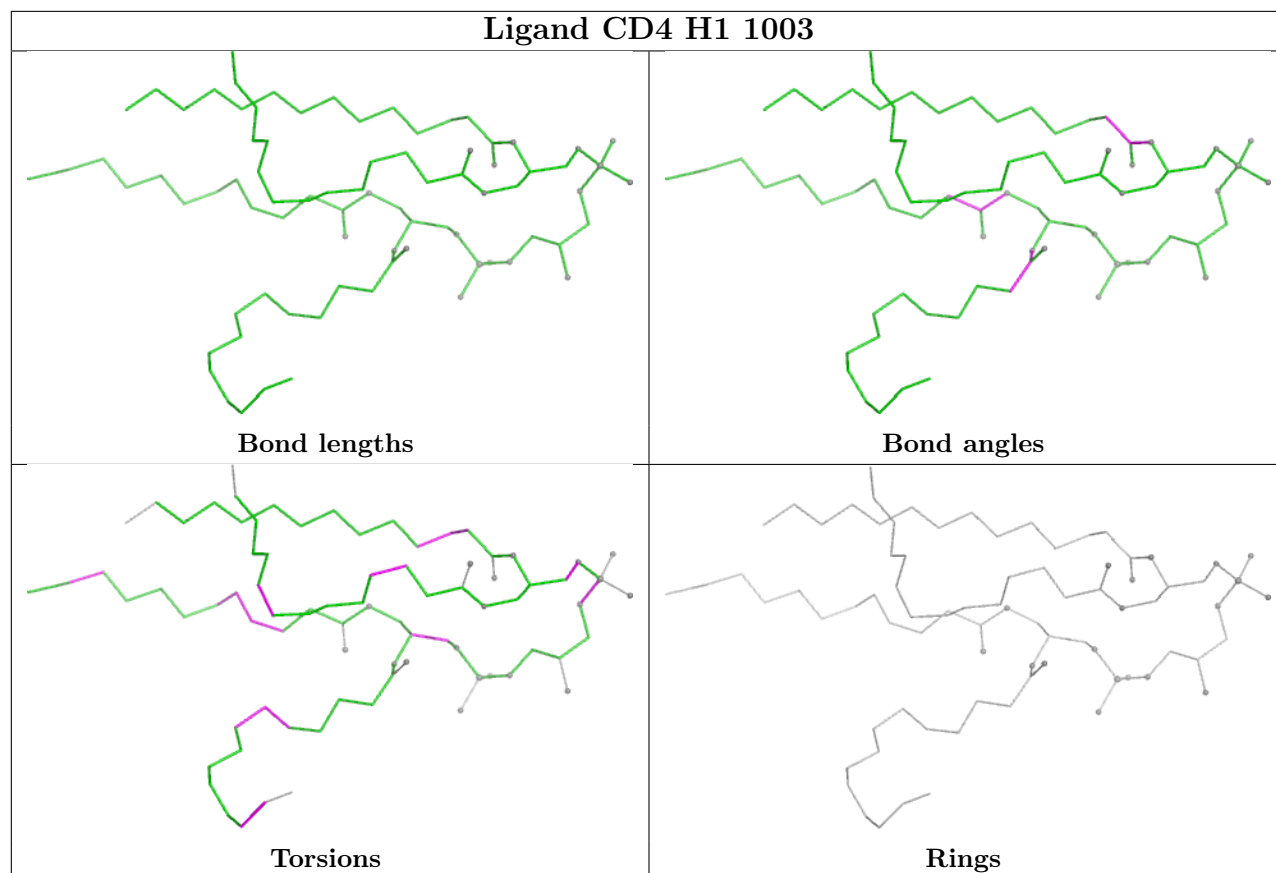
Ligand LMT BU 1003**Ligand V7N BJ 1001**



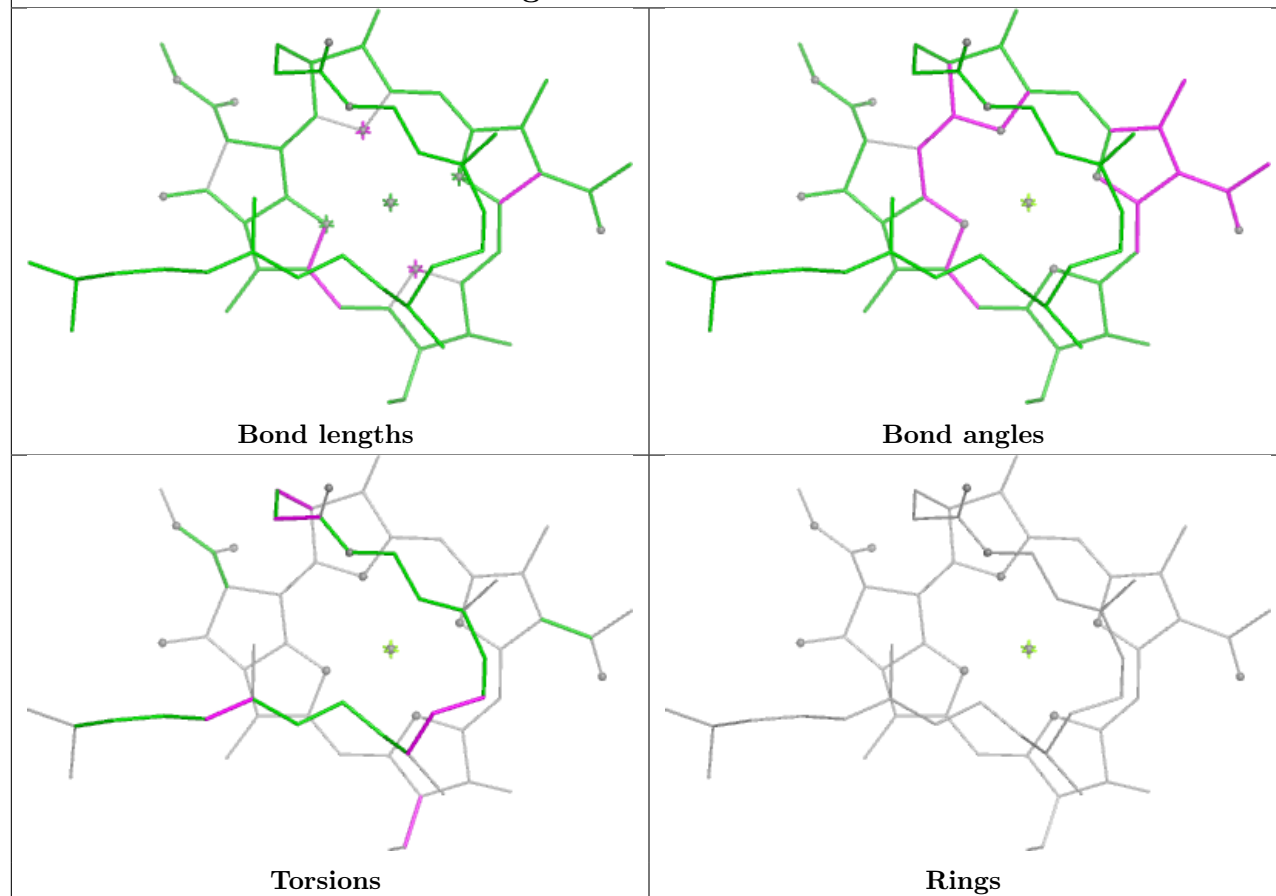




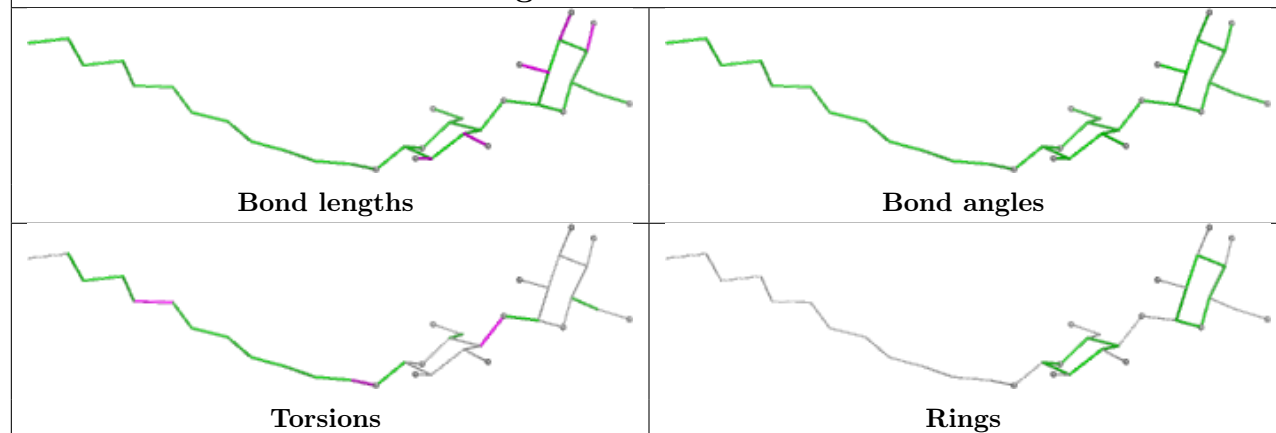


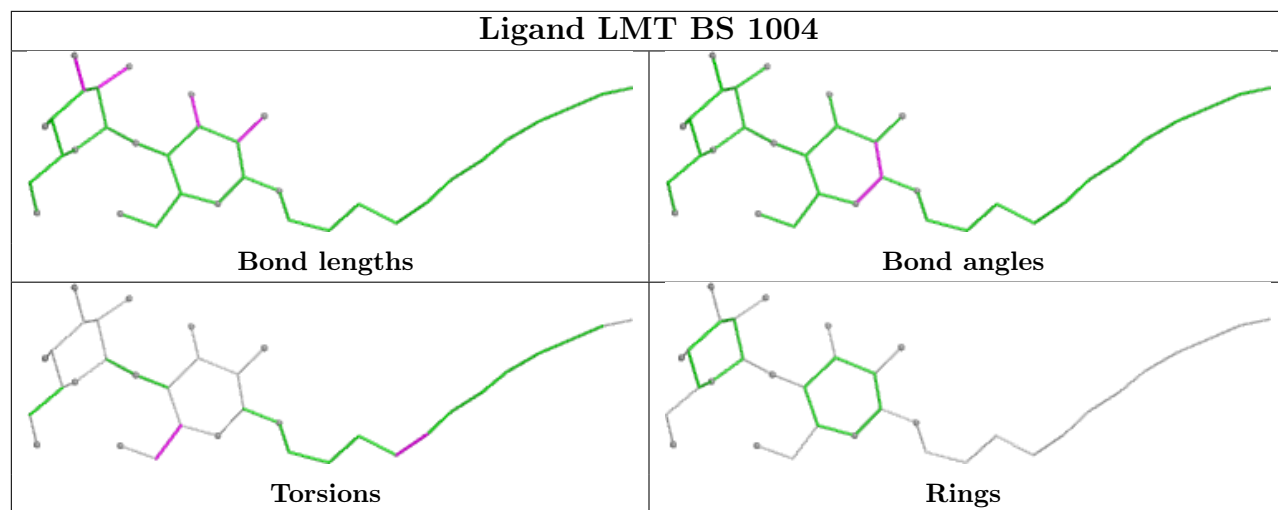


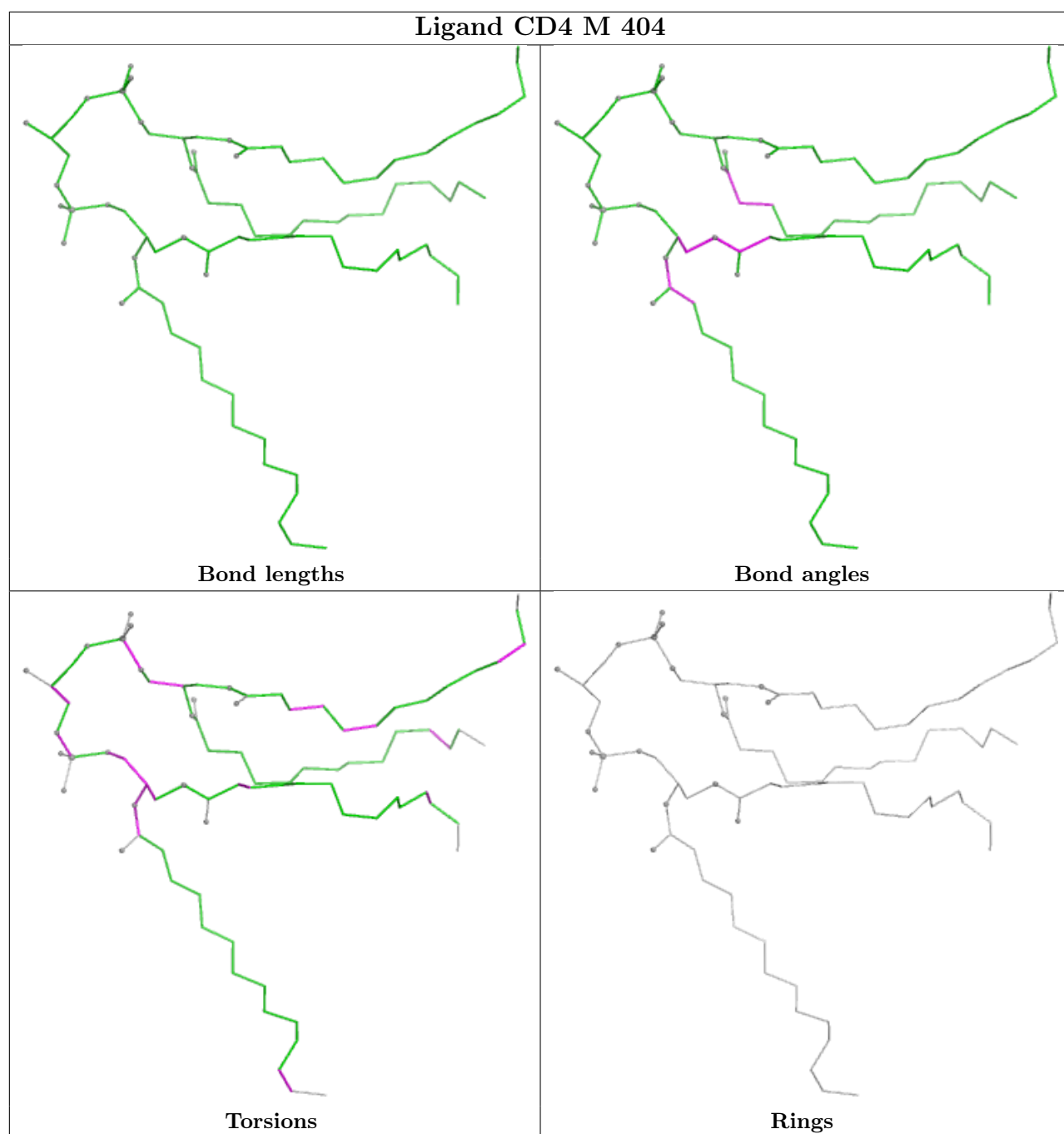
Ligand BCL AS 102

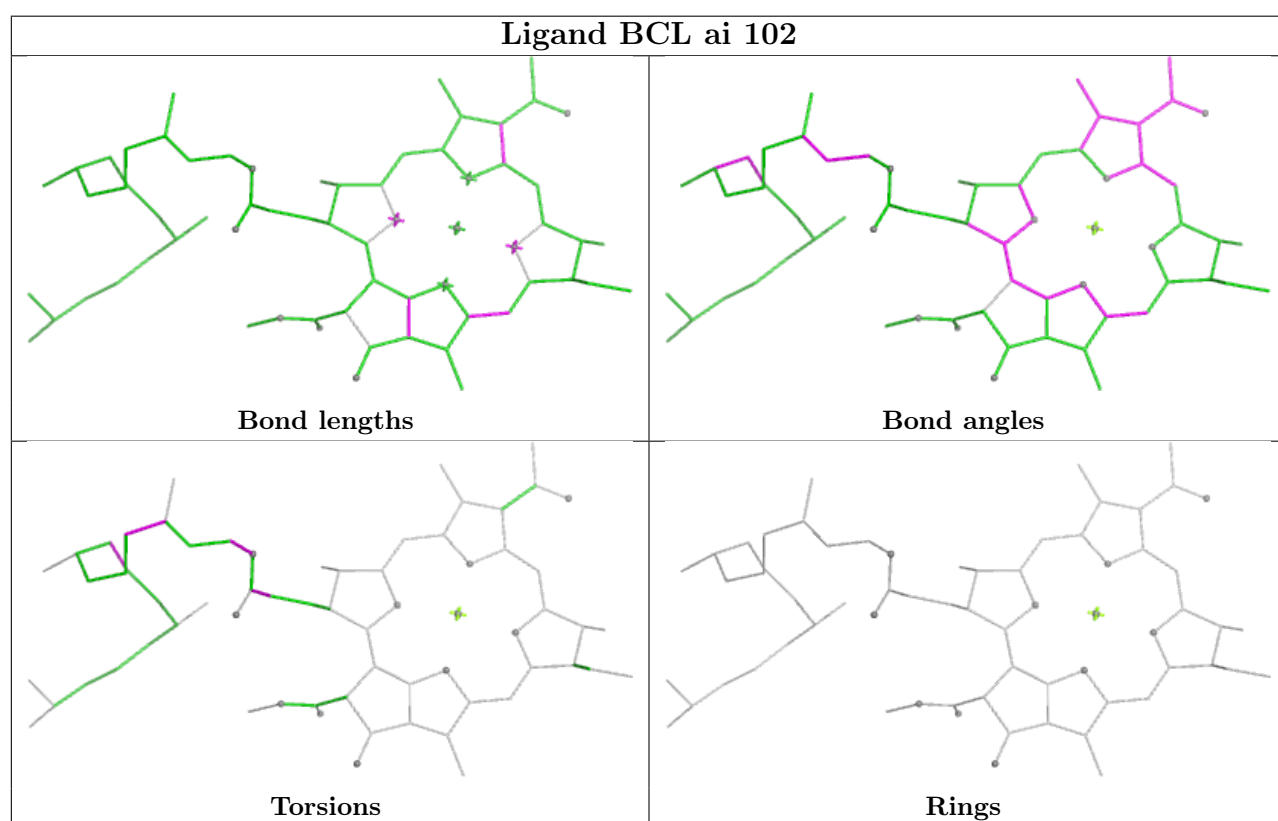
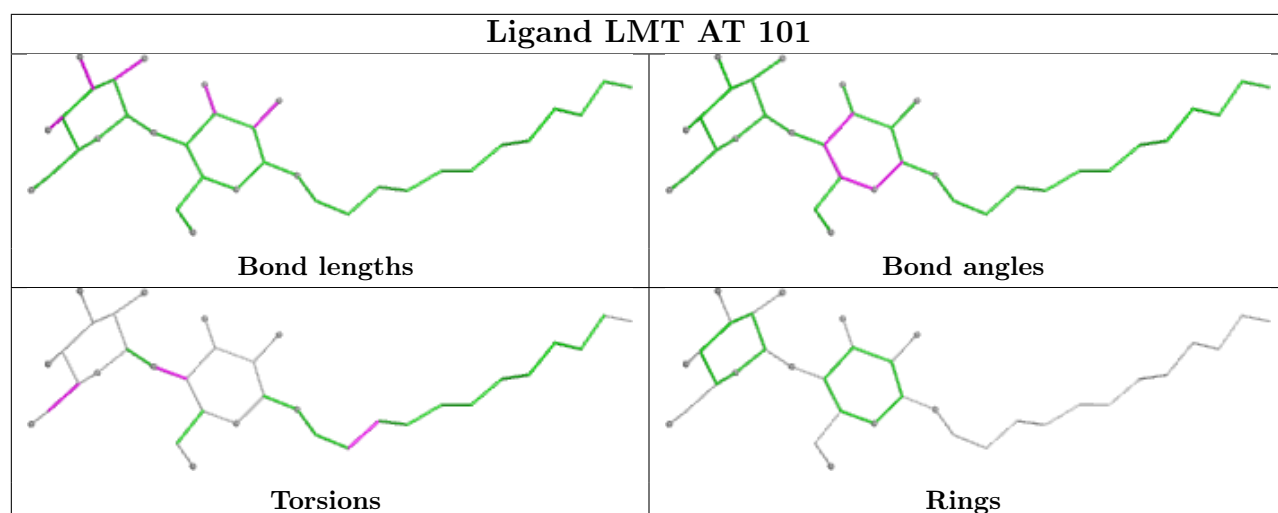


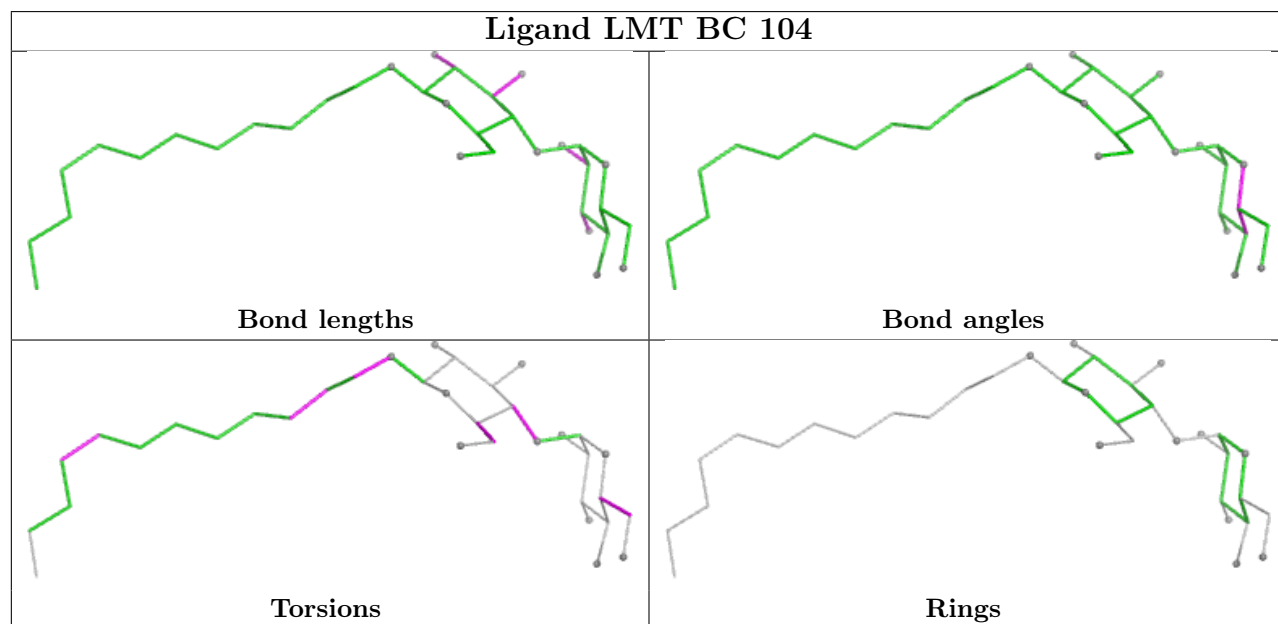
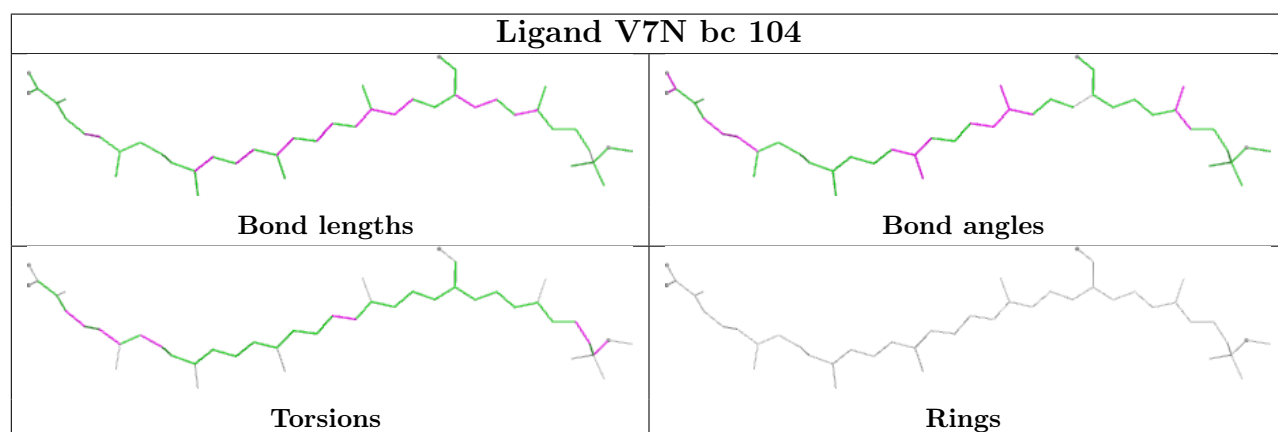
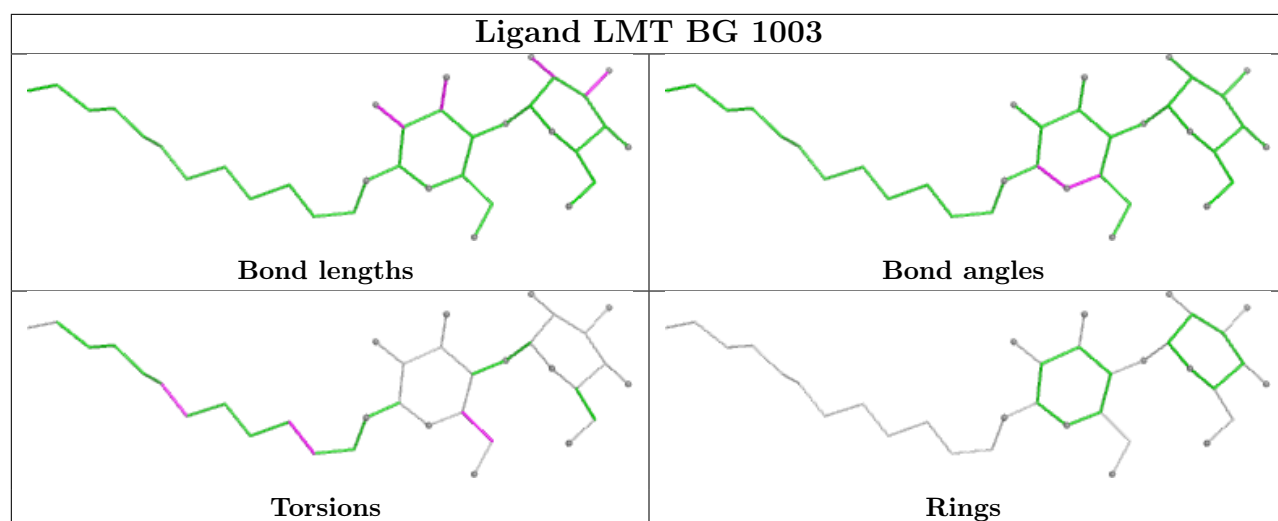
Ligand LMT AO 103

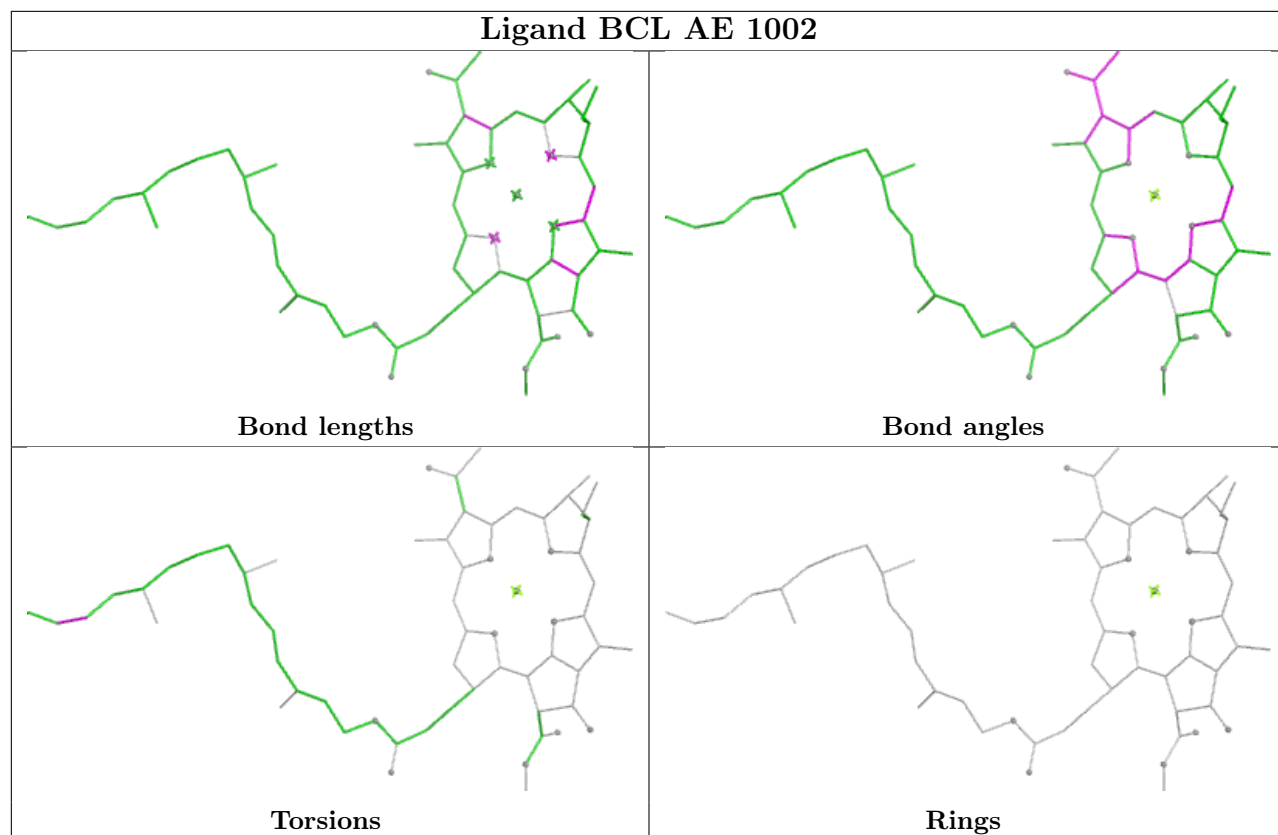
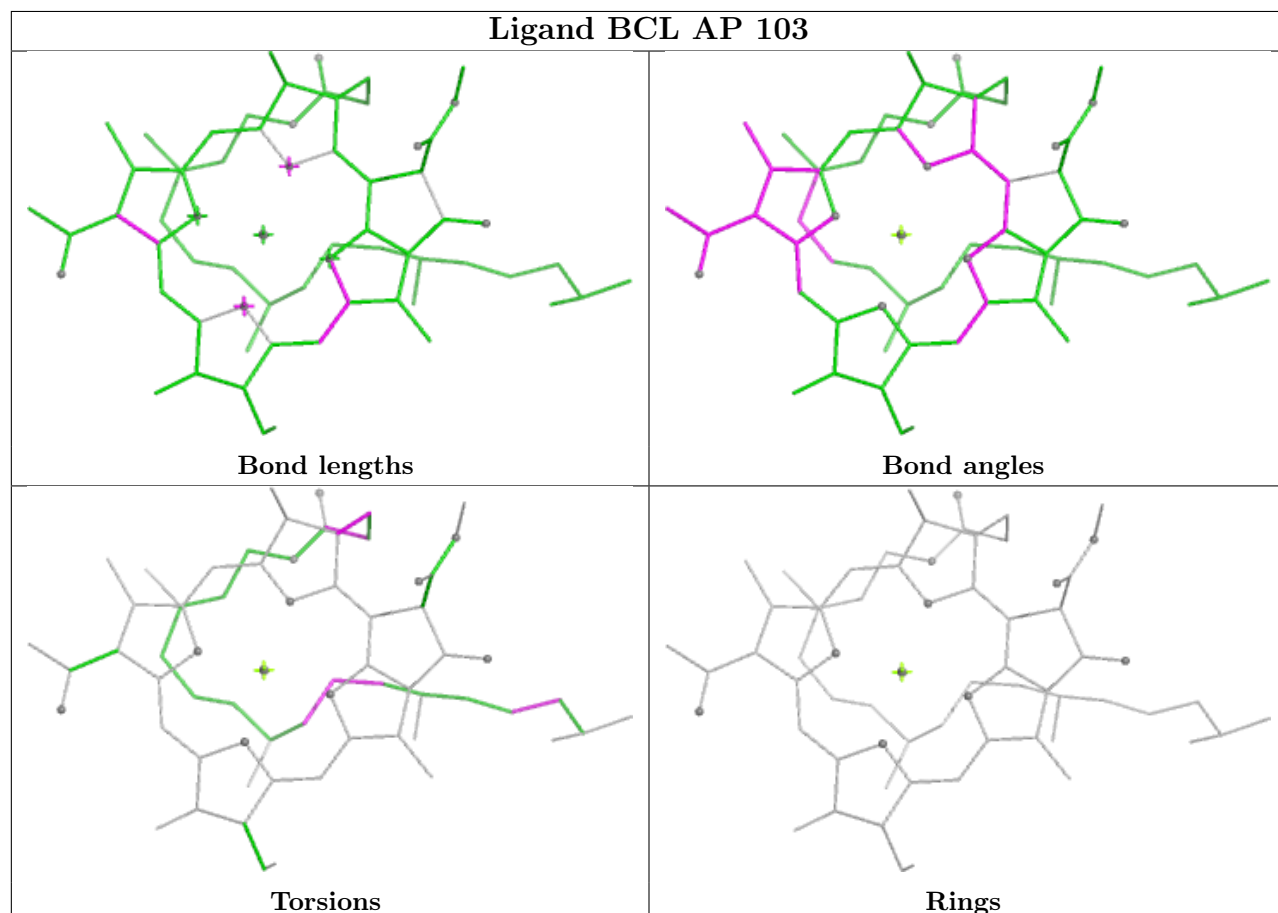




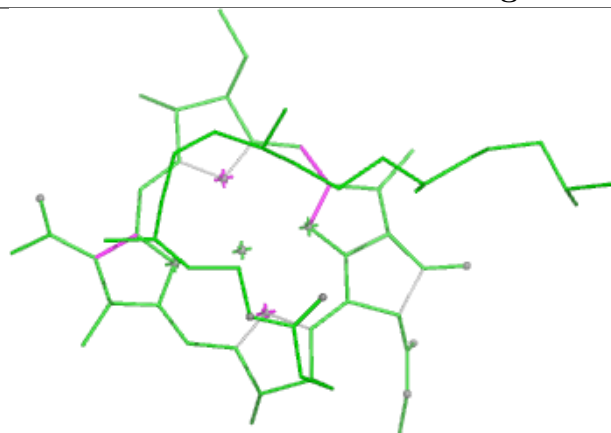




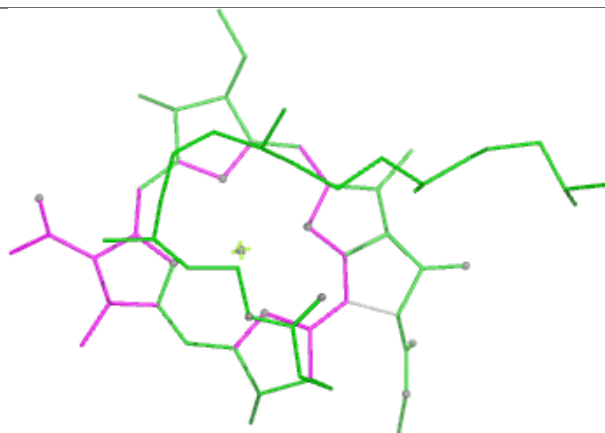


Ligand BCL AE 1002**Ligand BCL AP 103**

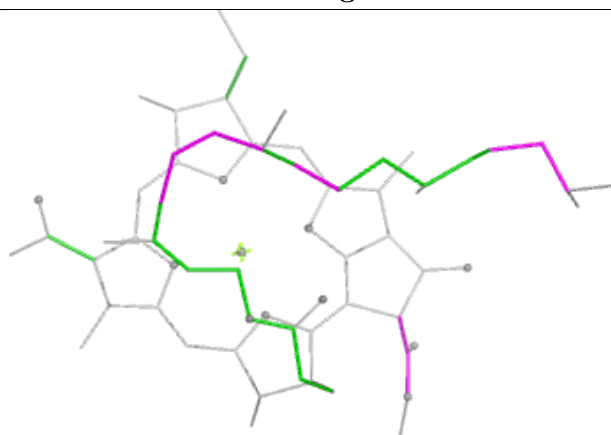
Ligand BCL AK 103



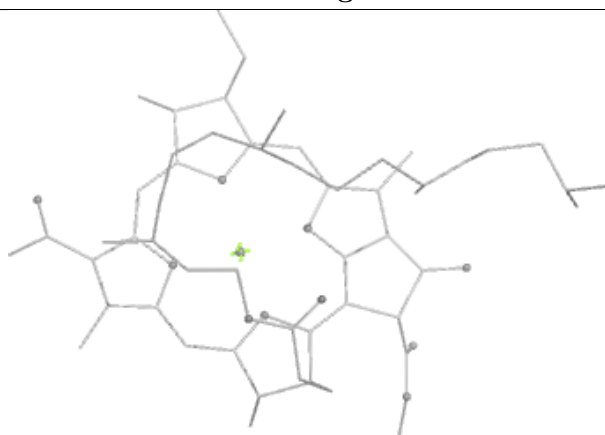
Bond lengths



Bond angles



Torsions



Rings

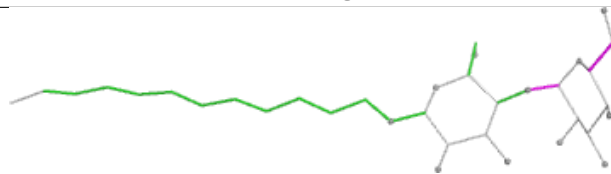
Ligand LMT L 304



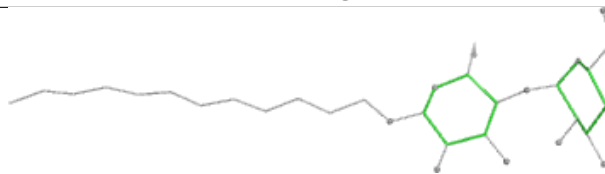
Bond lengths



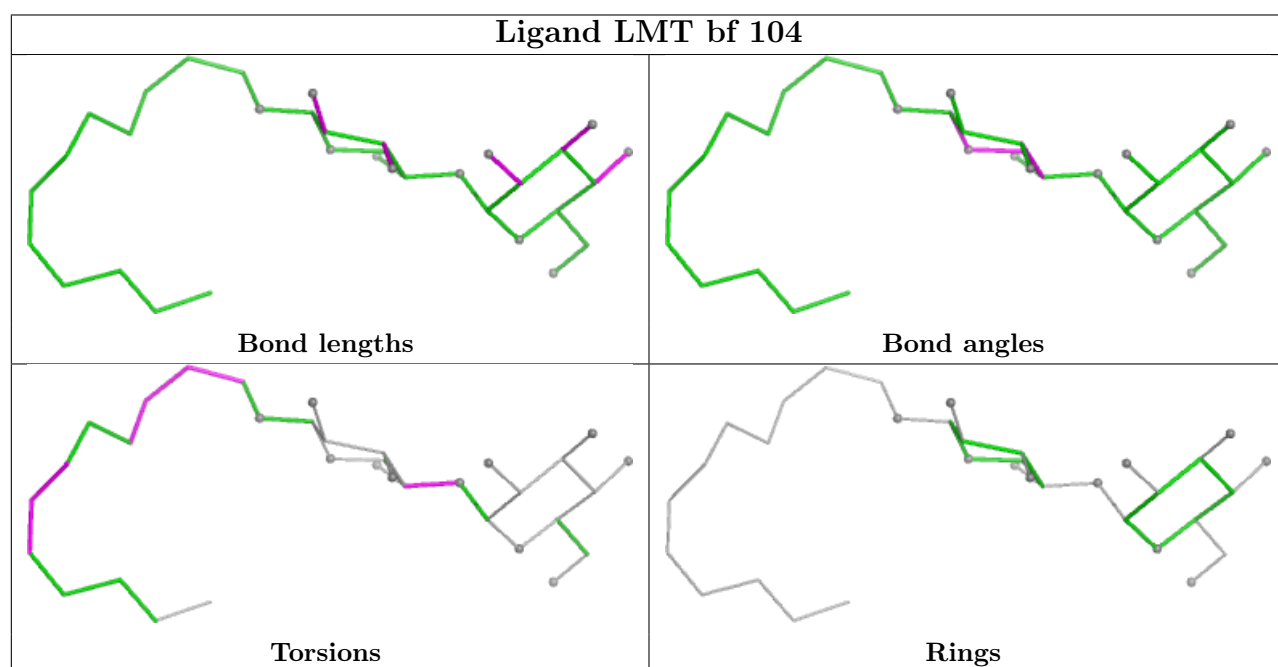
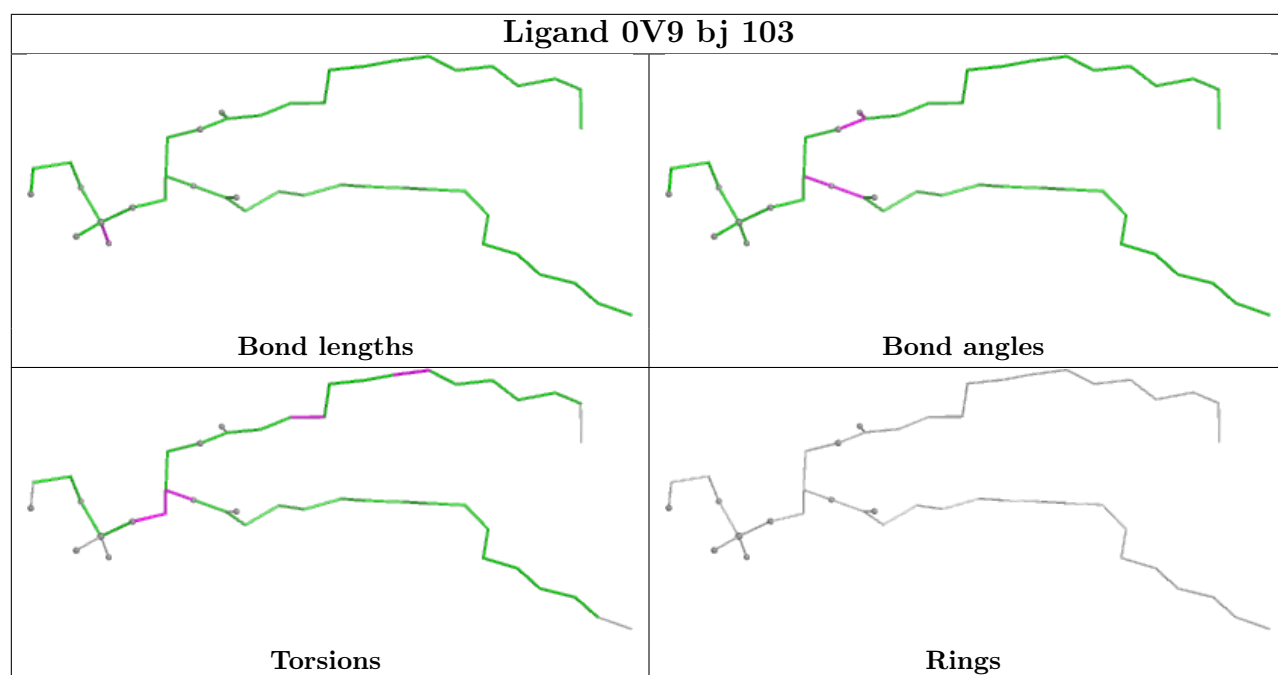
Bond angles

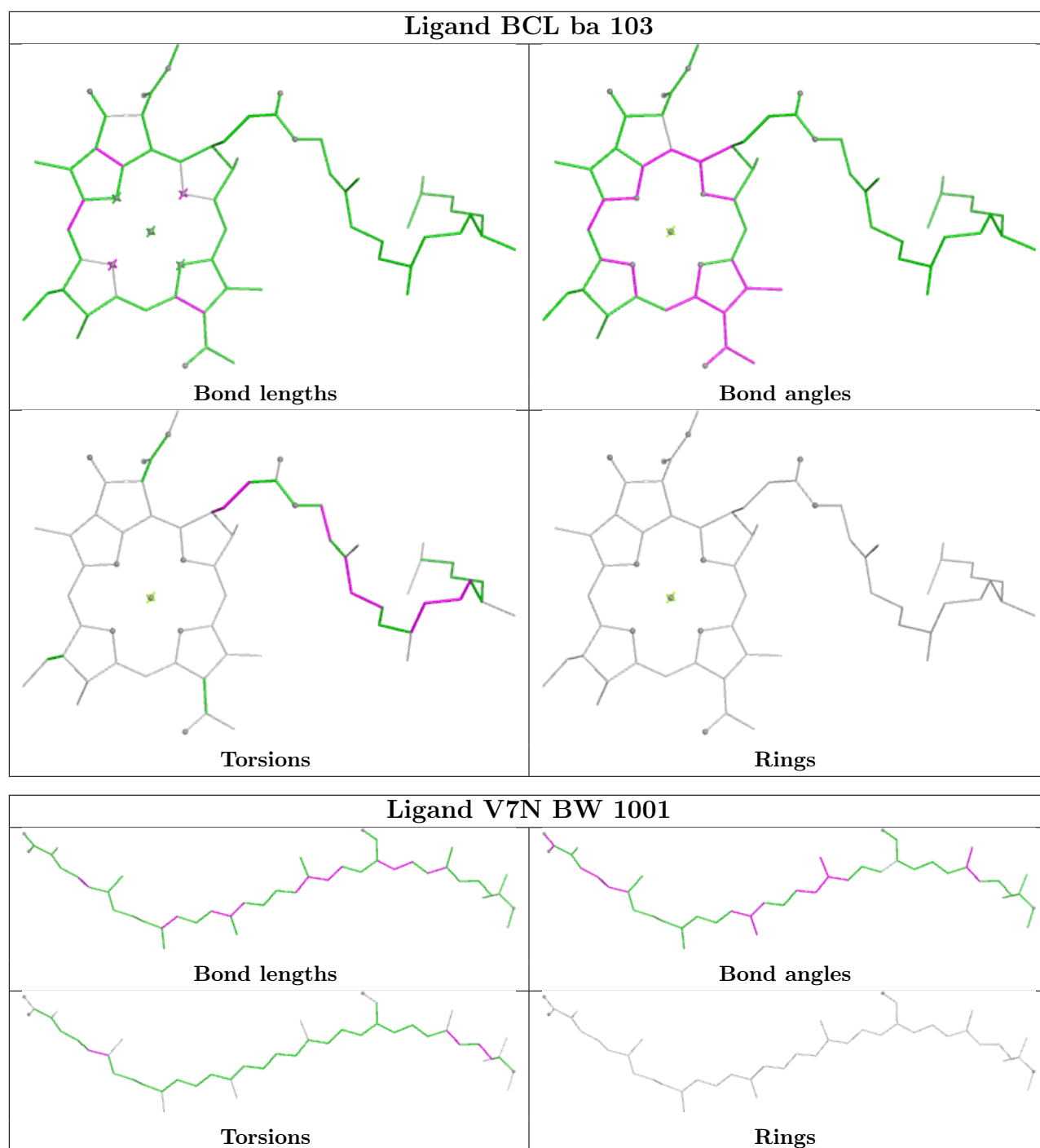


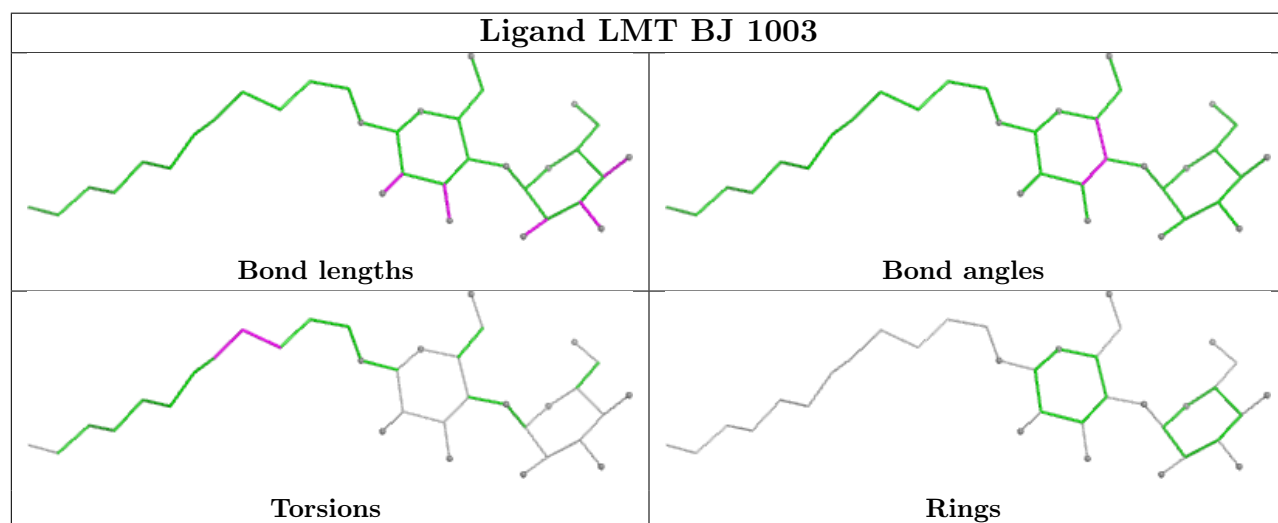
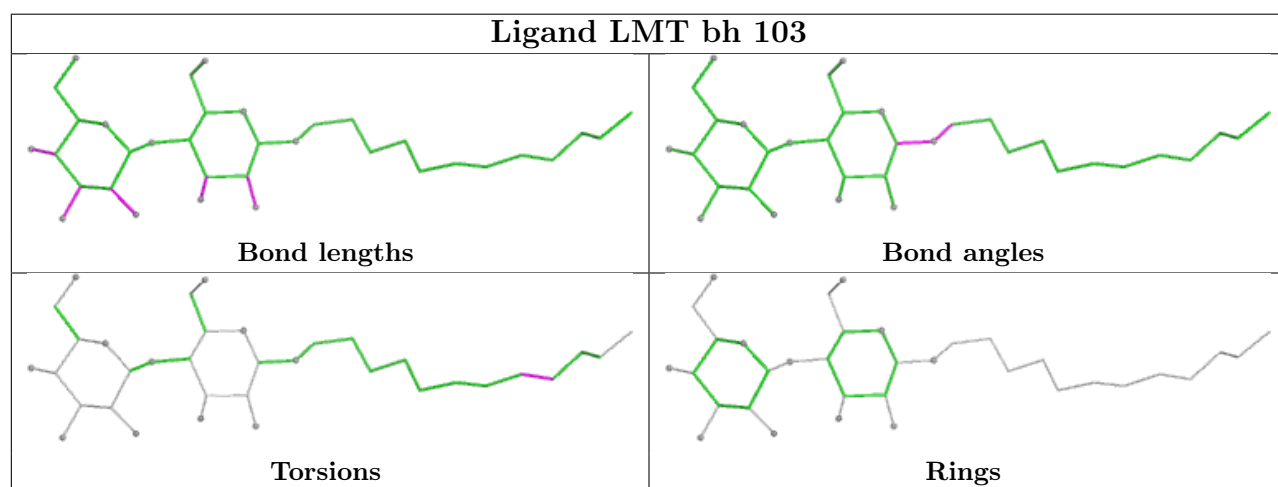
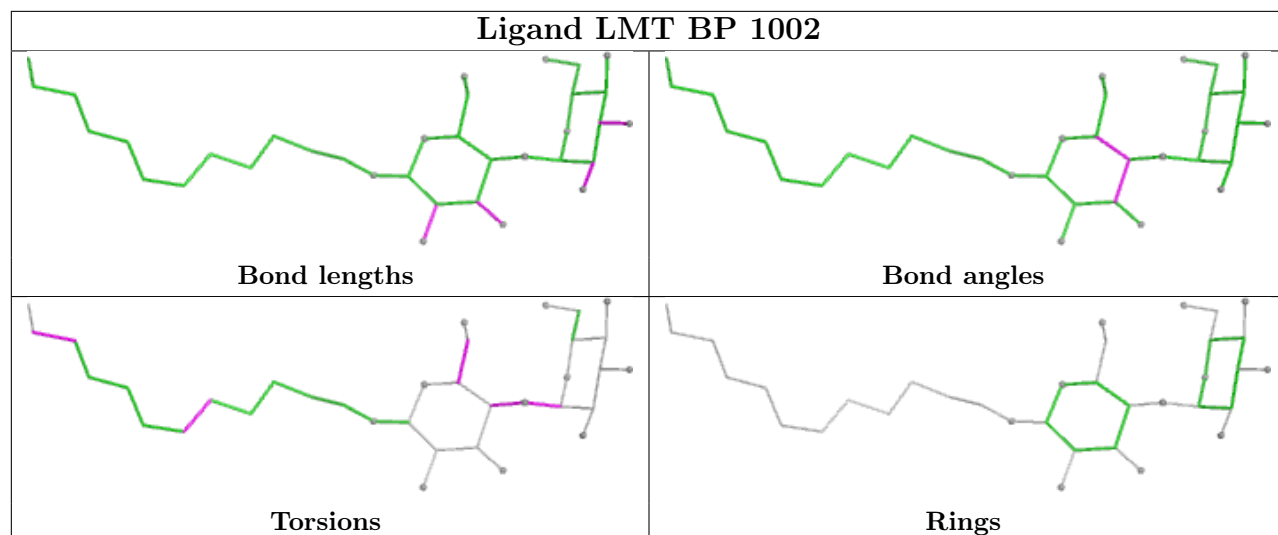
Torsions

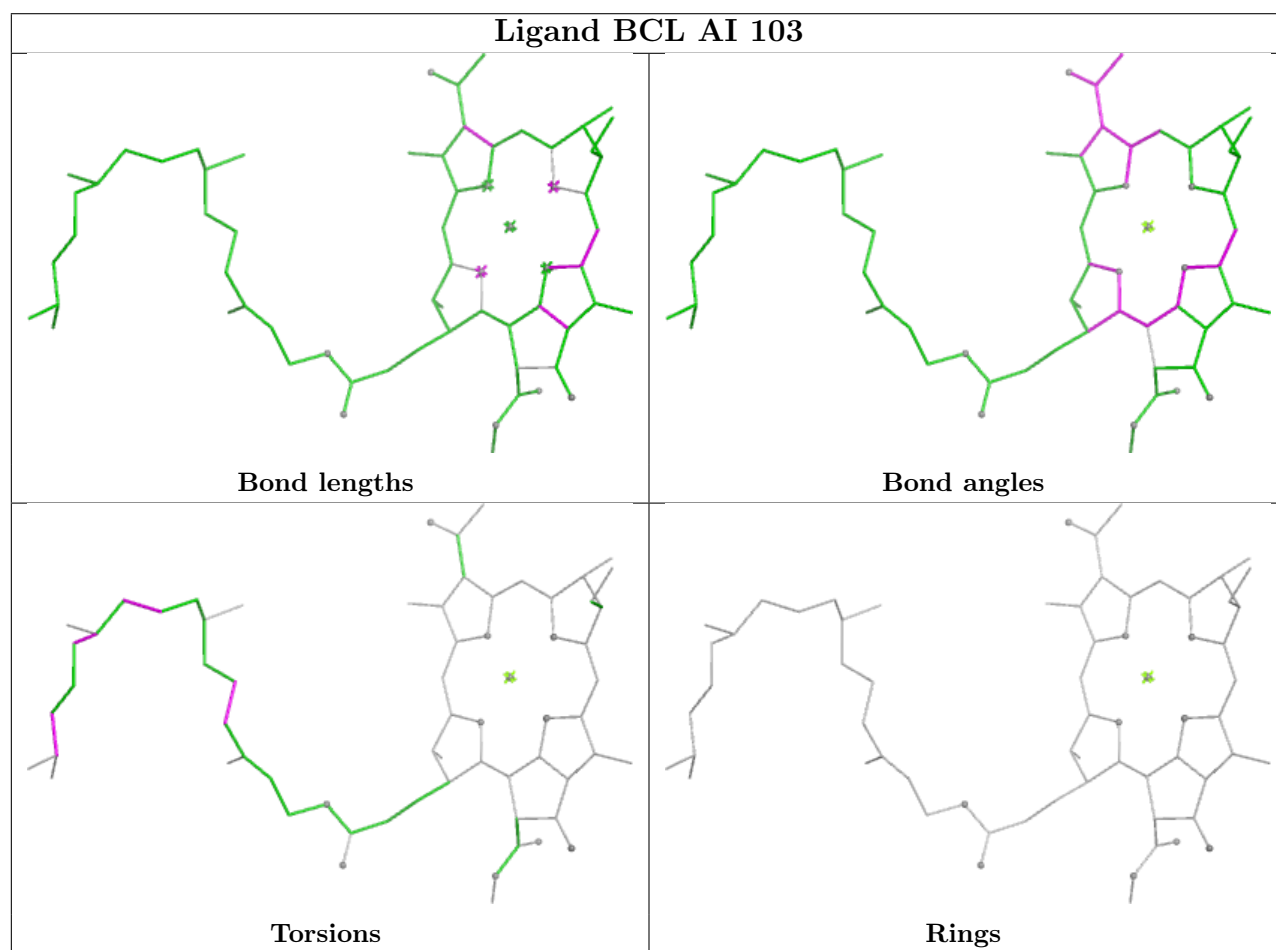
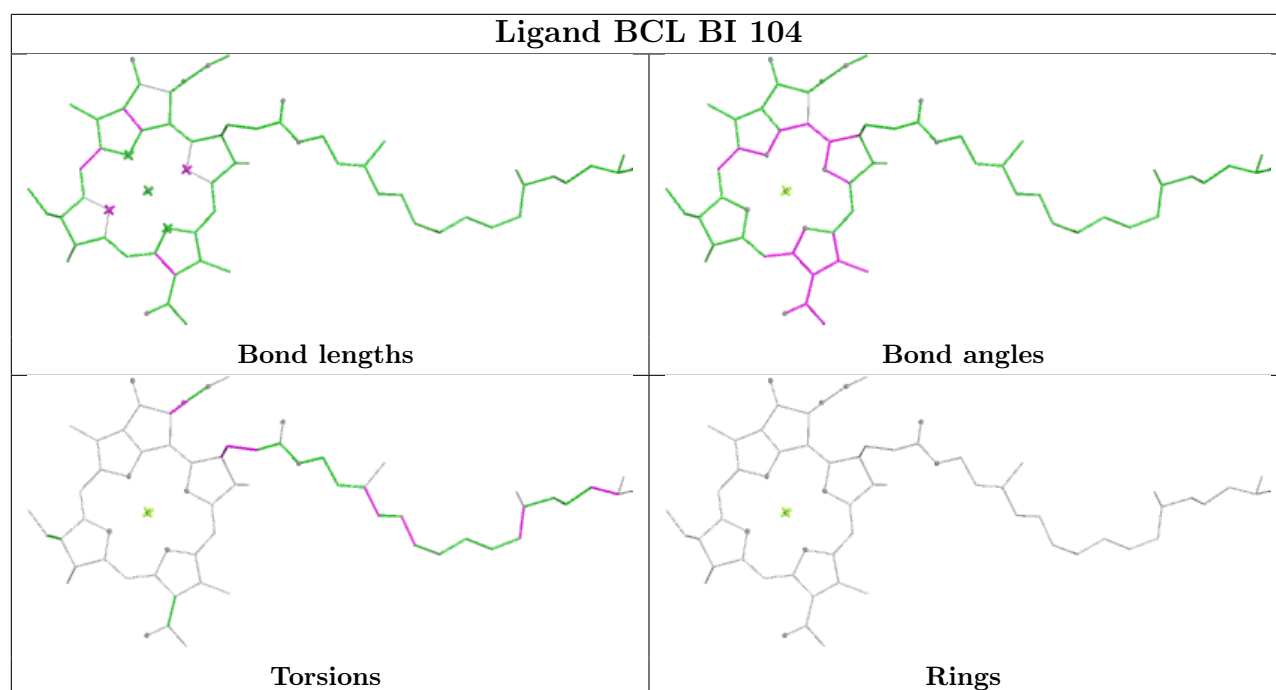


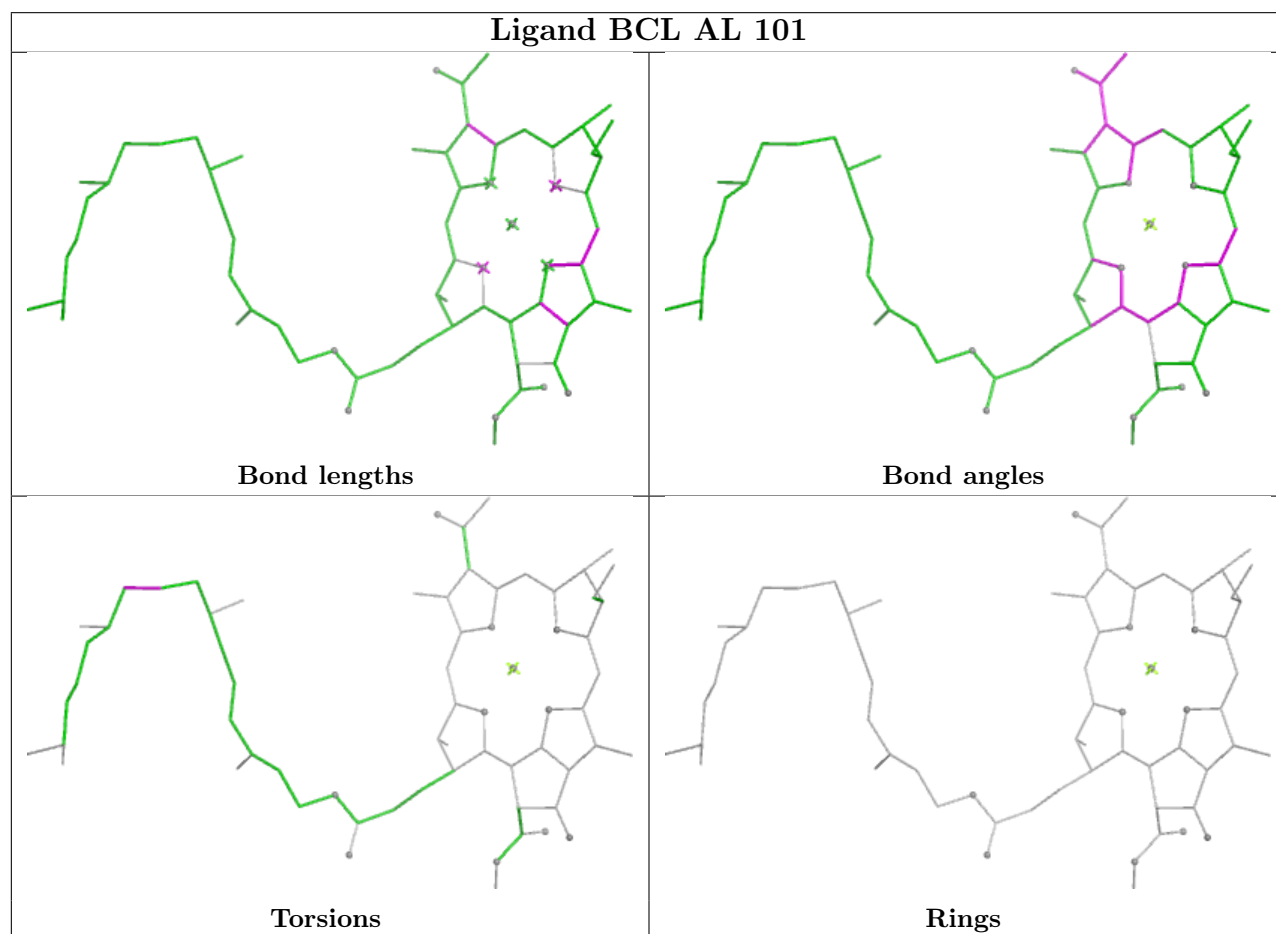
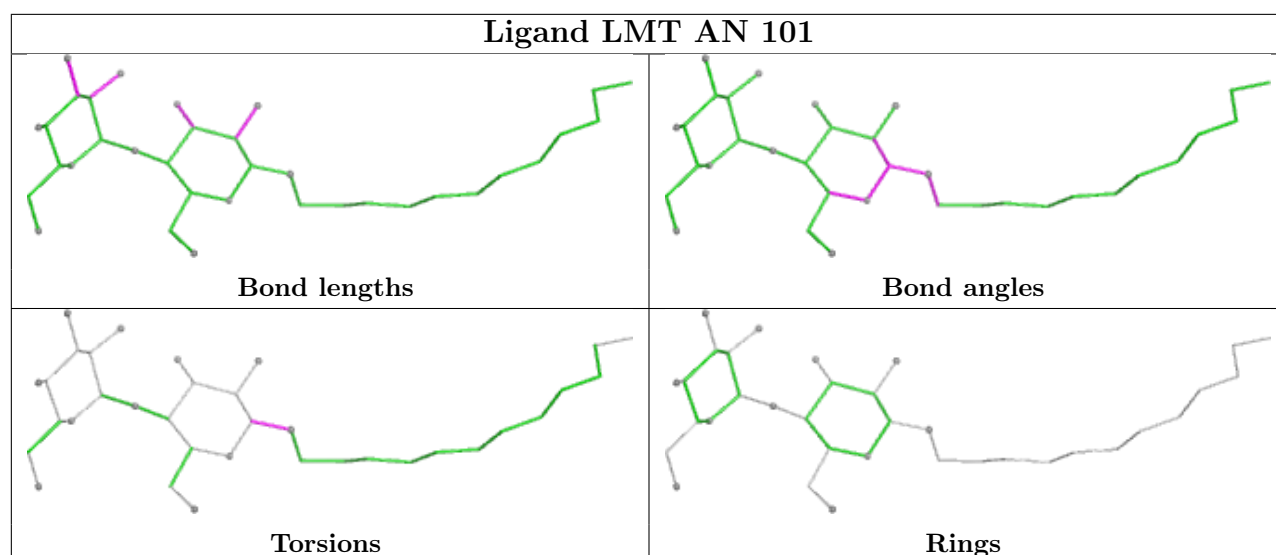
Rings

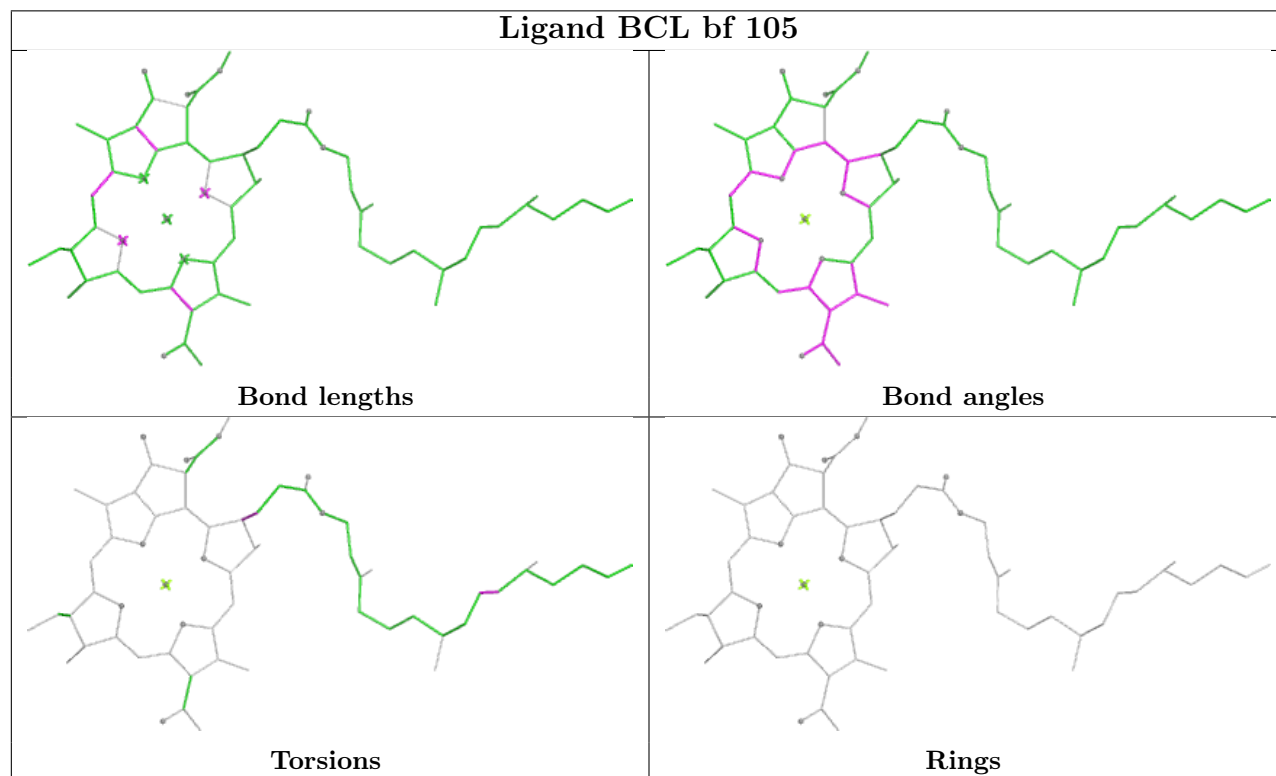
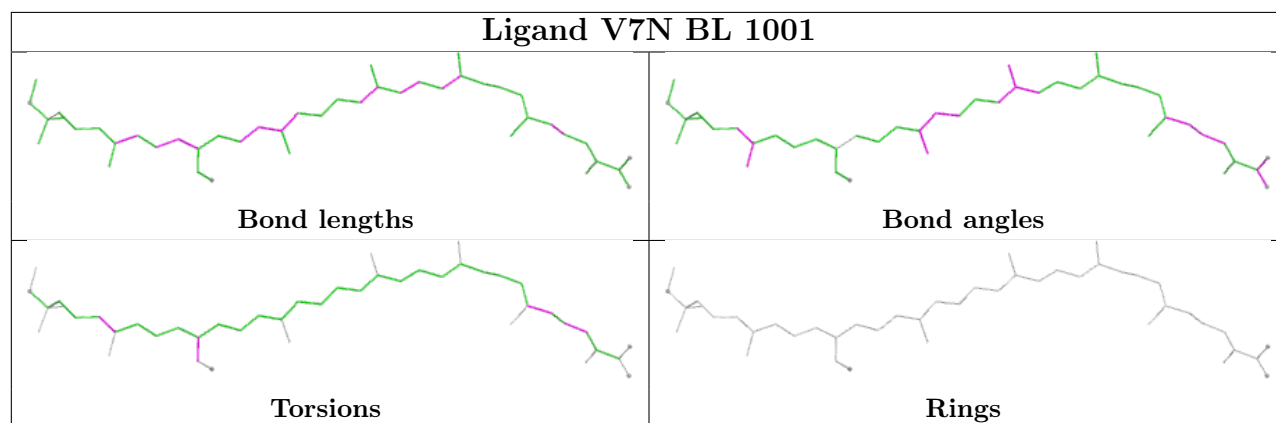
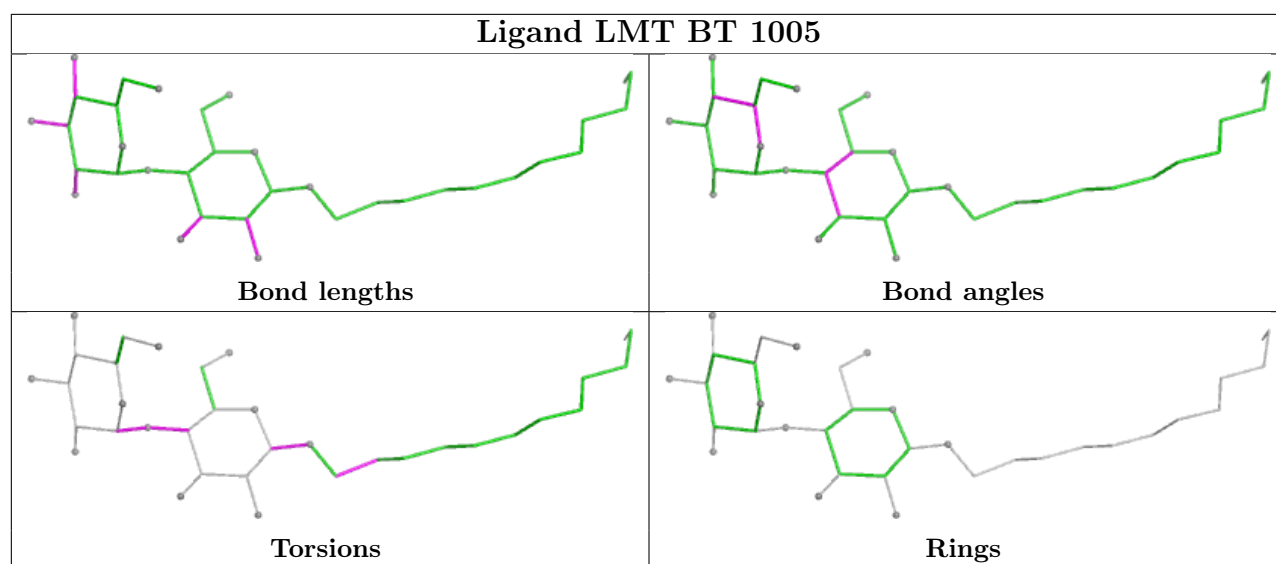


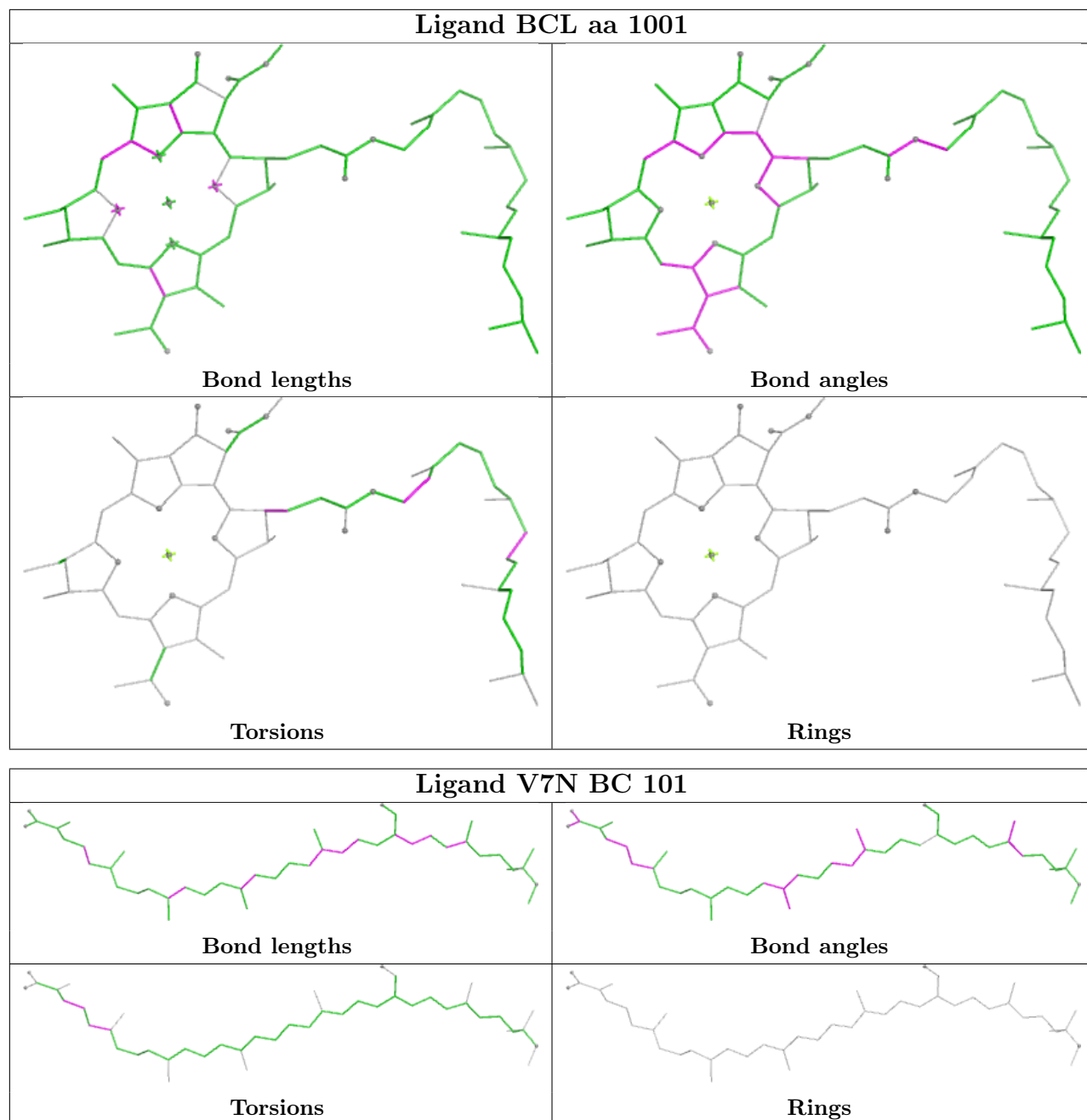


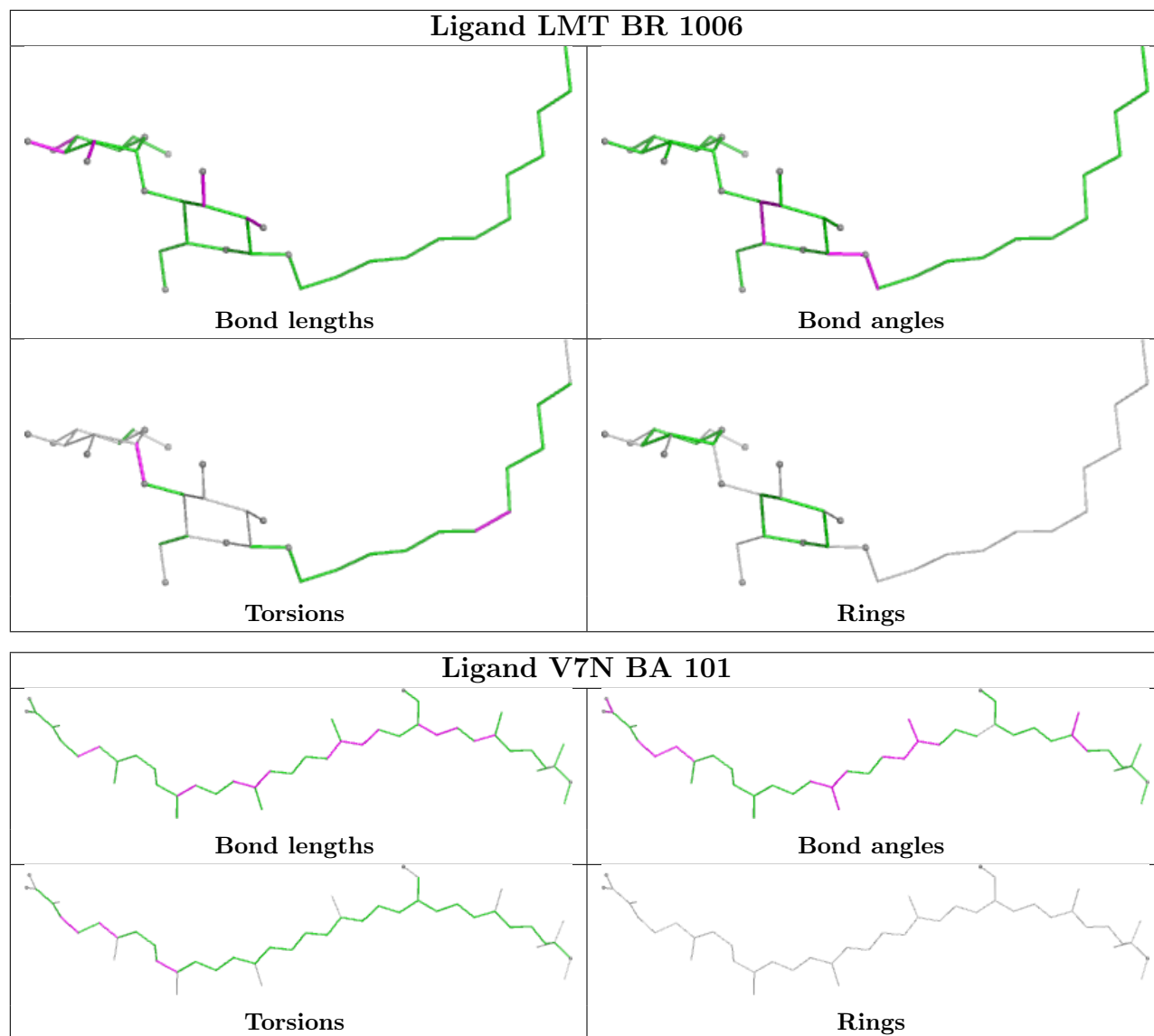




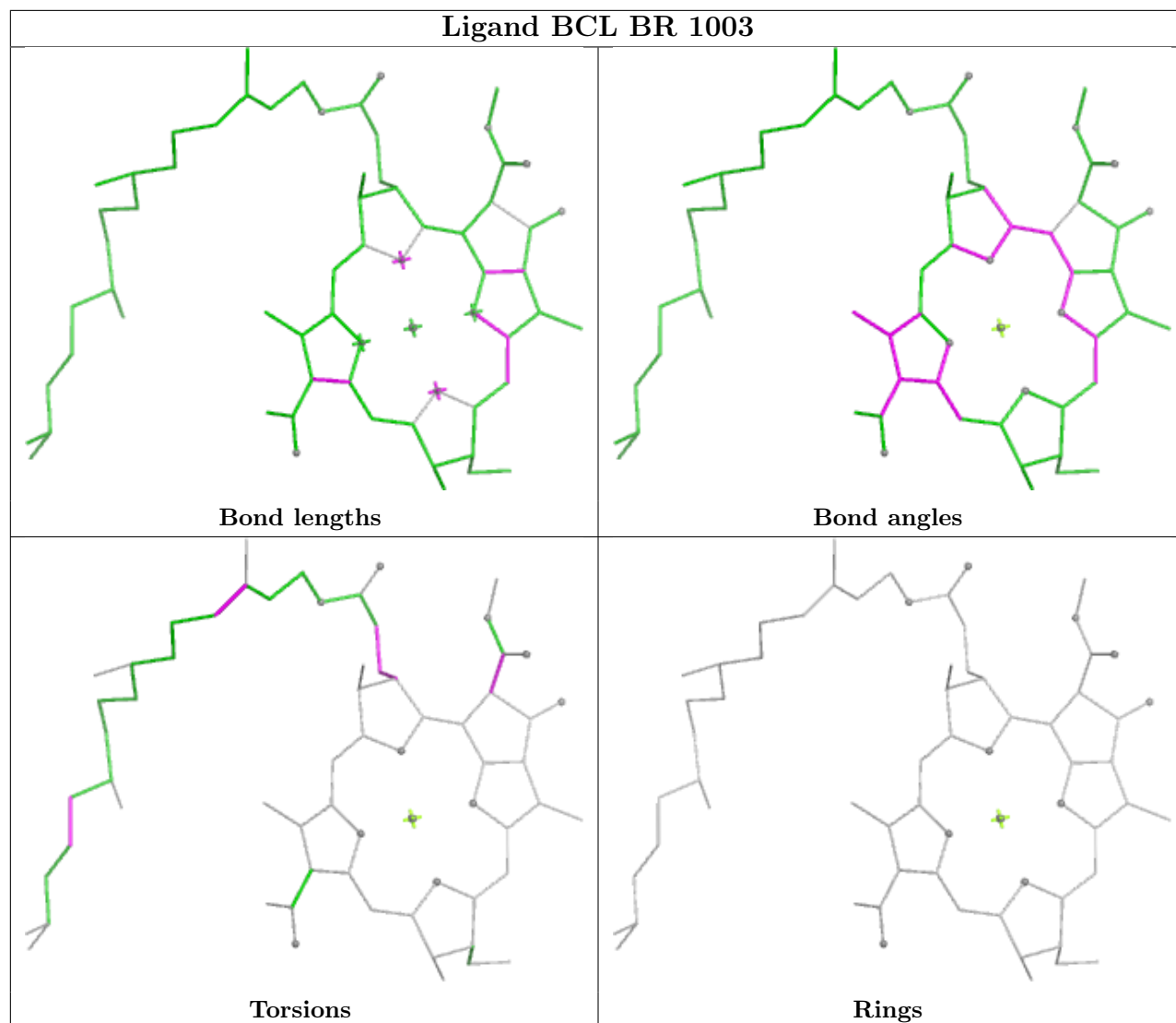




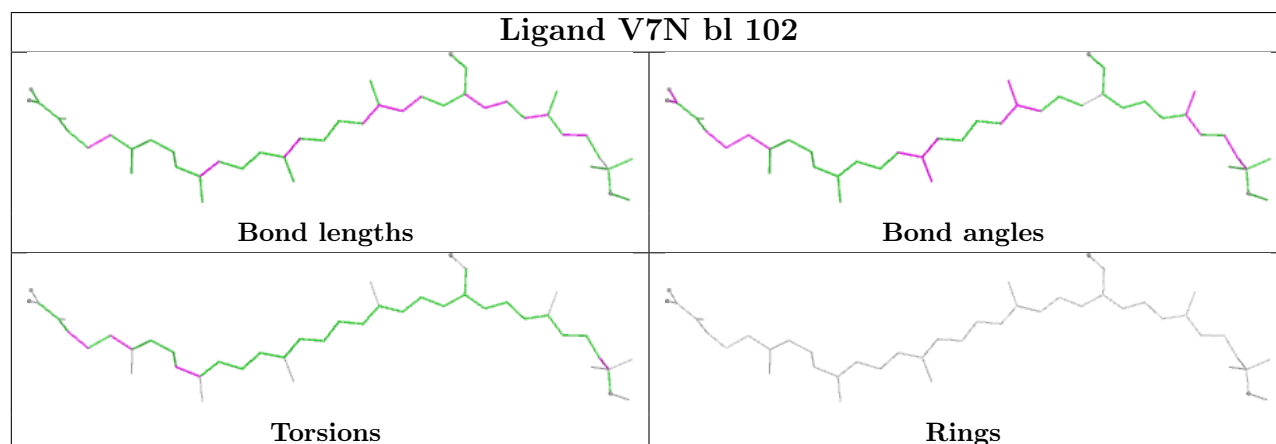


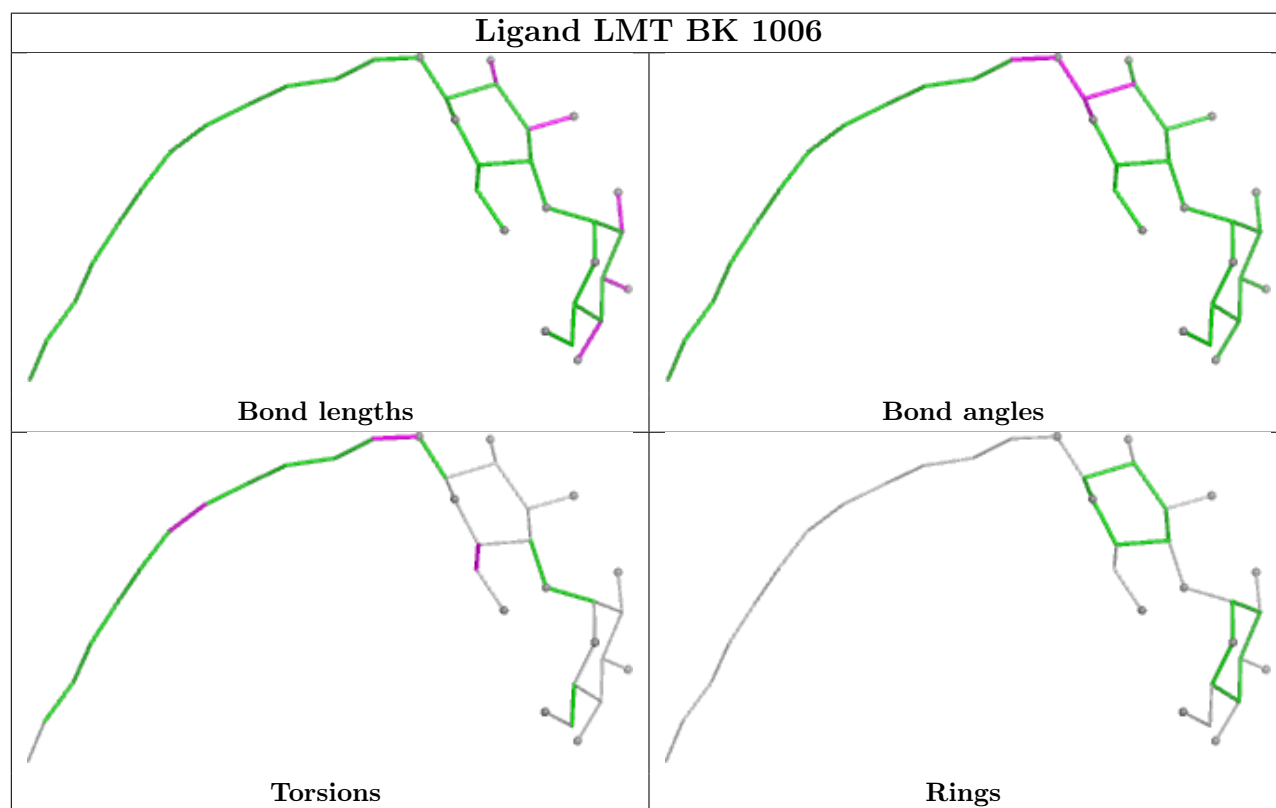
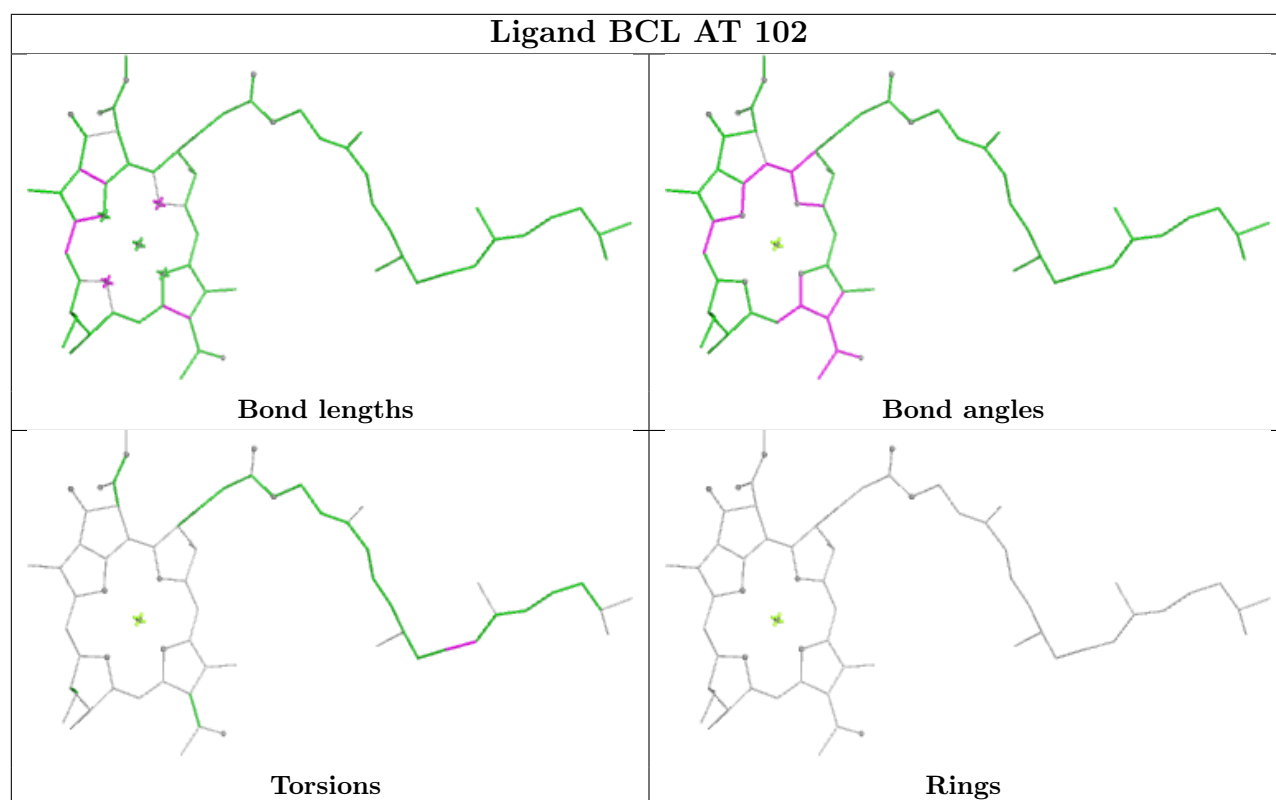


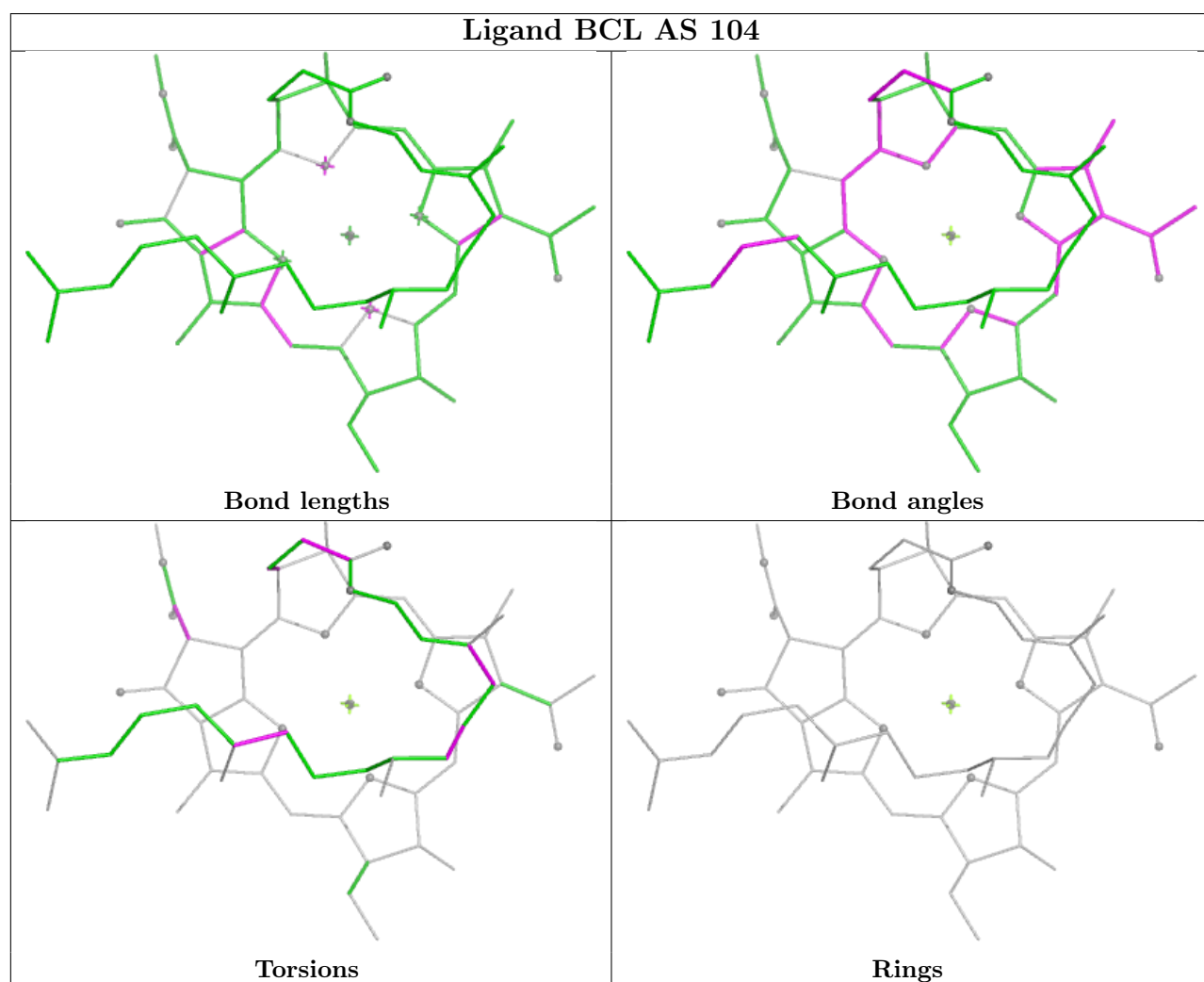
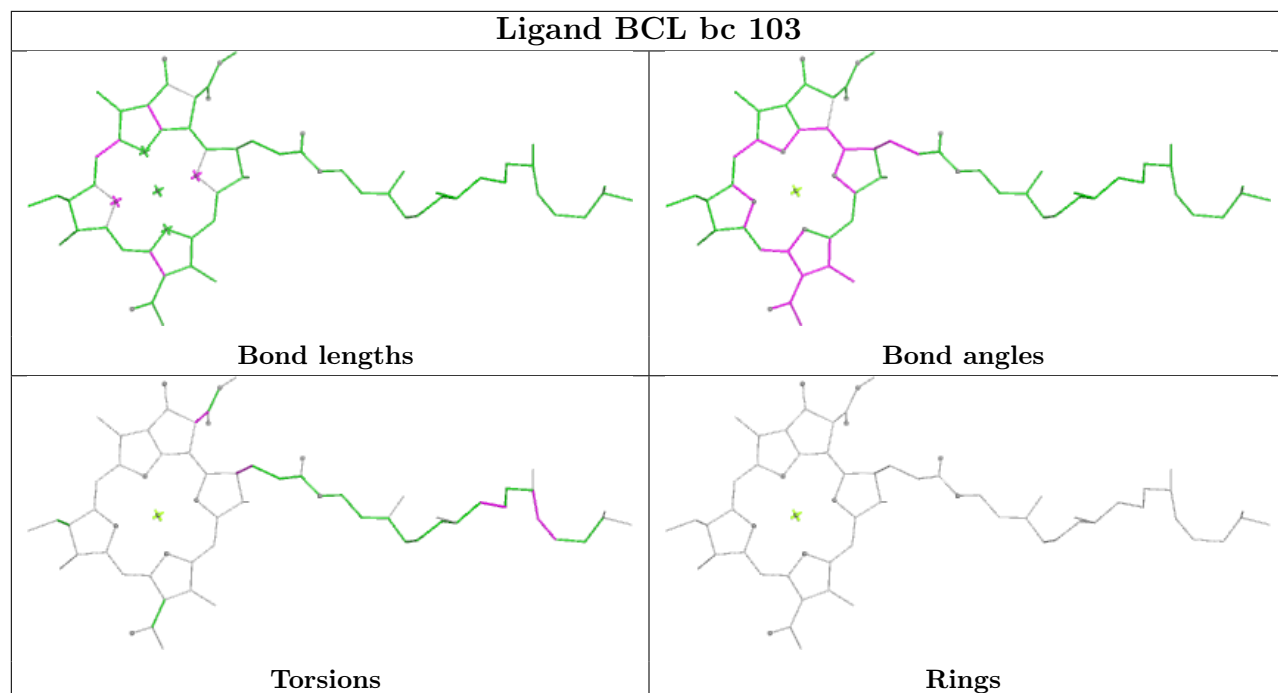
Ligand BCL BR 1003



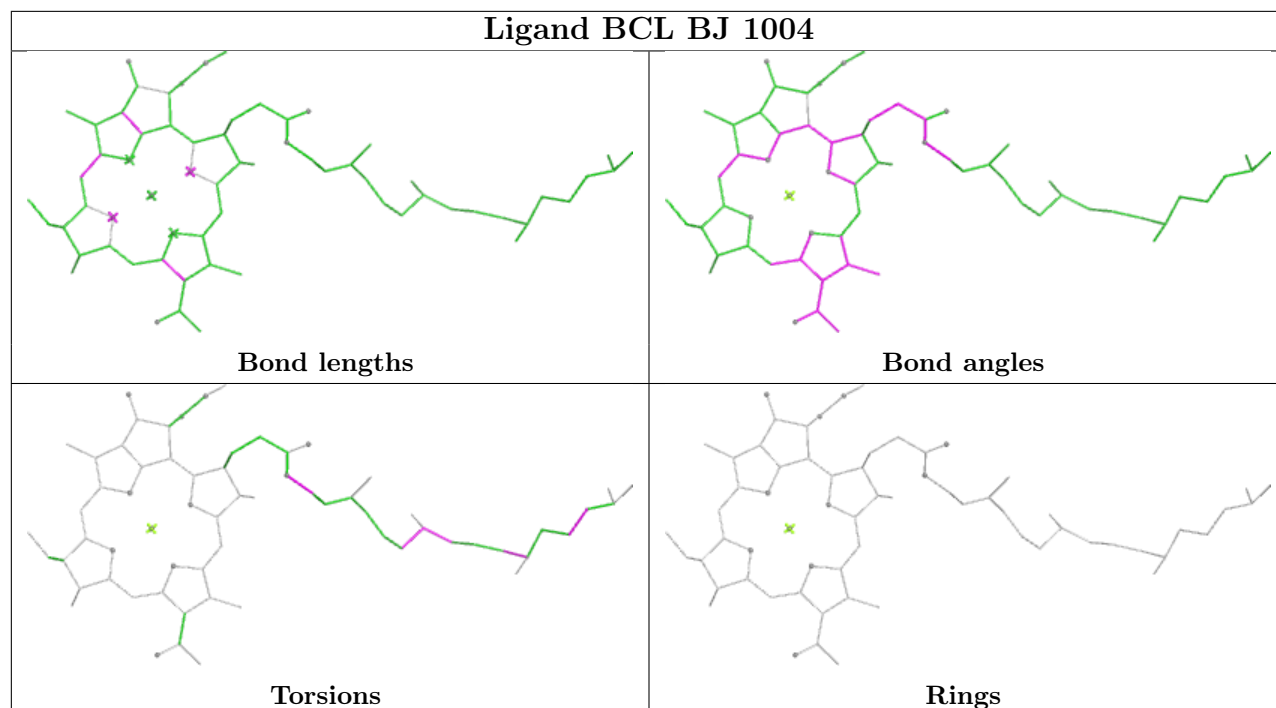
Ligand V7N bl 102



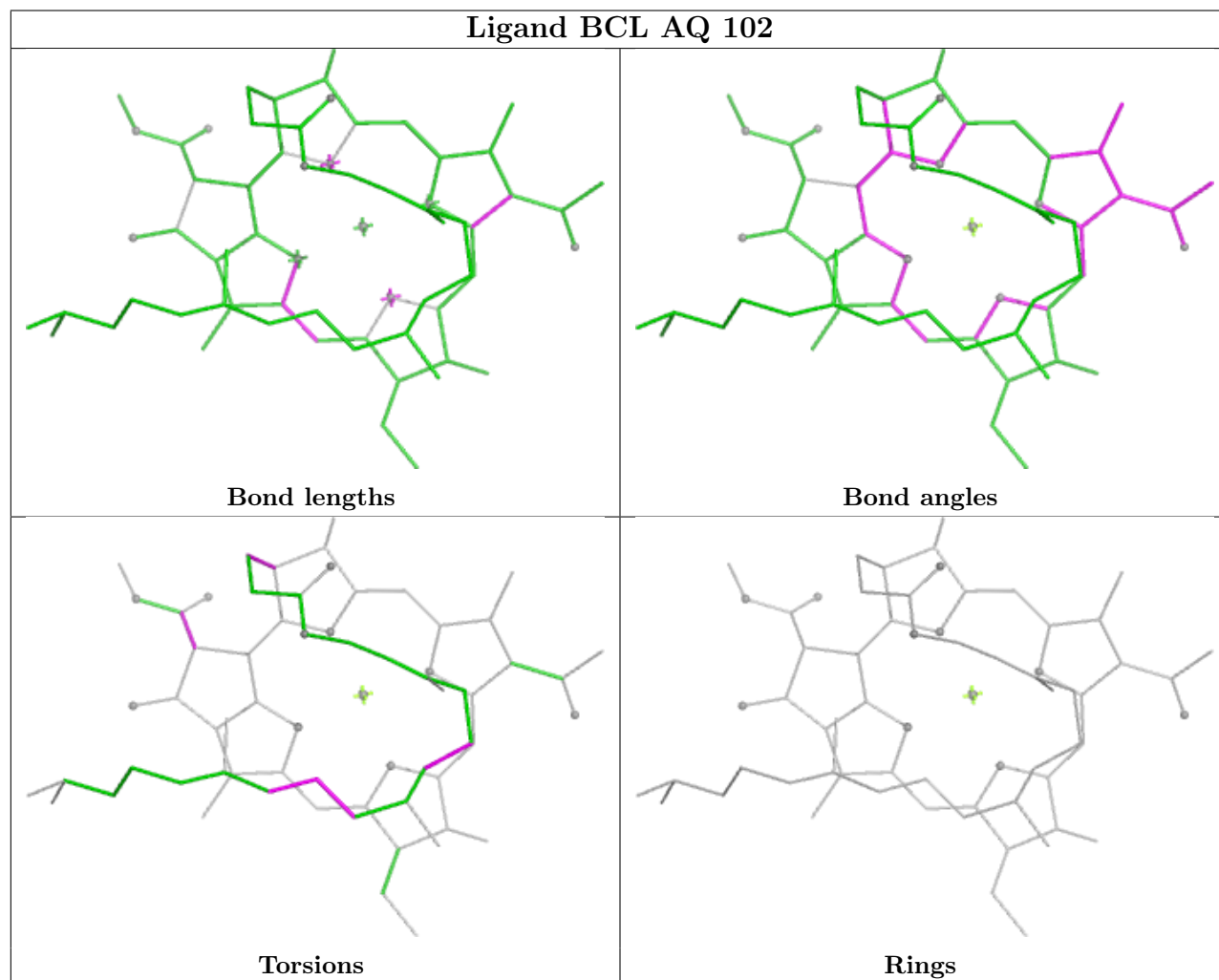


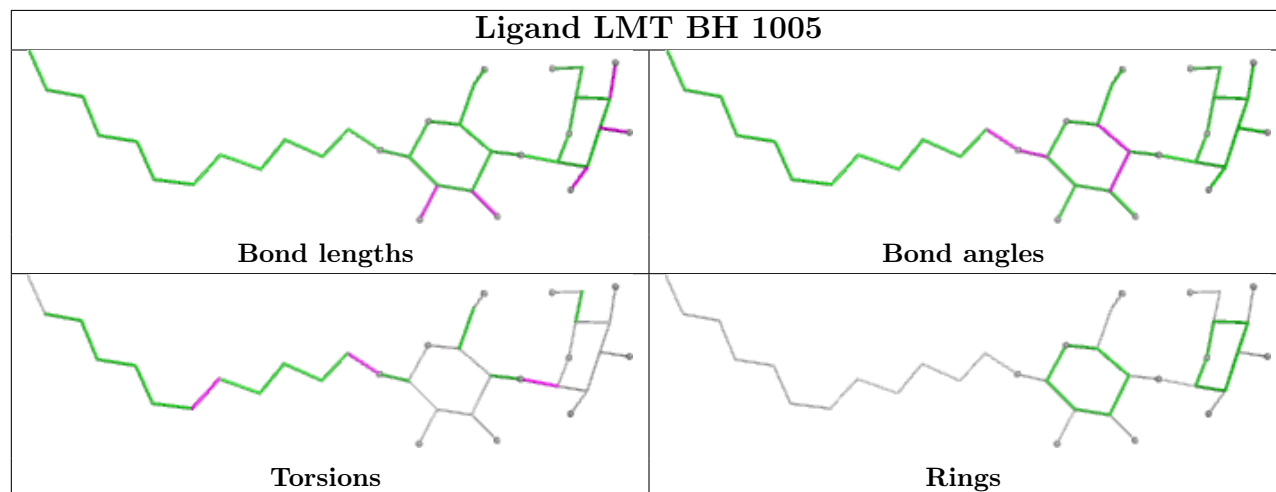
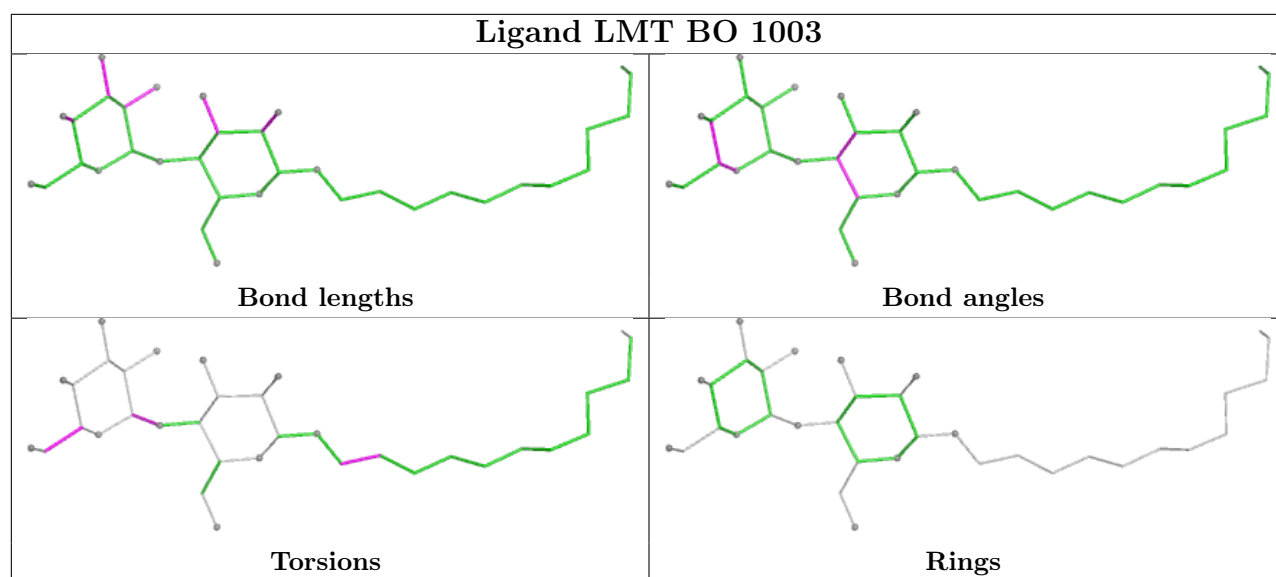


Ligand BCL BJ 1004

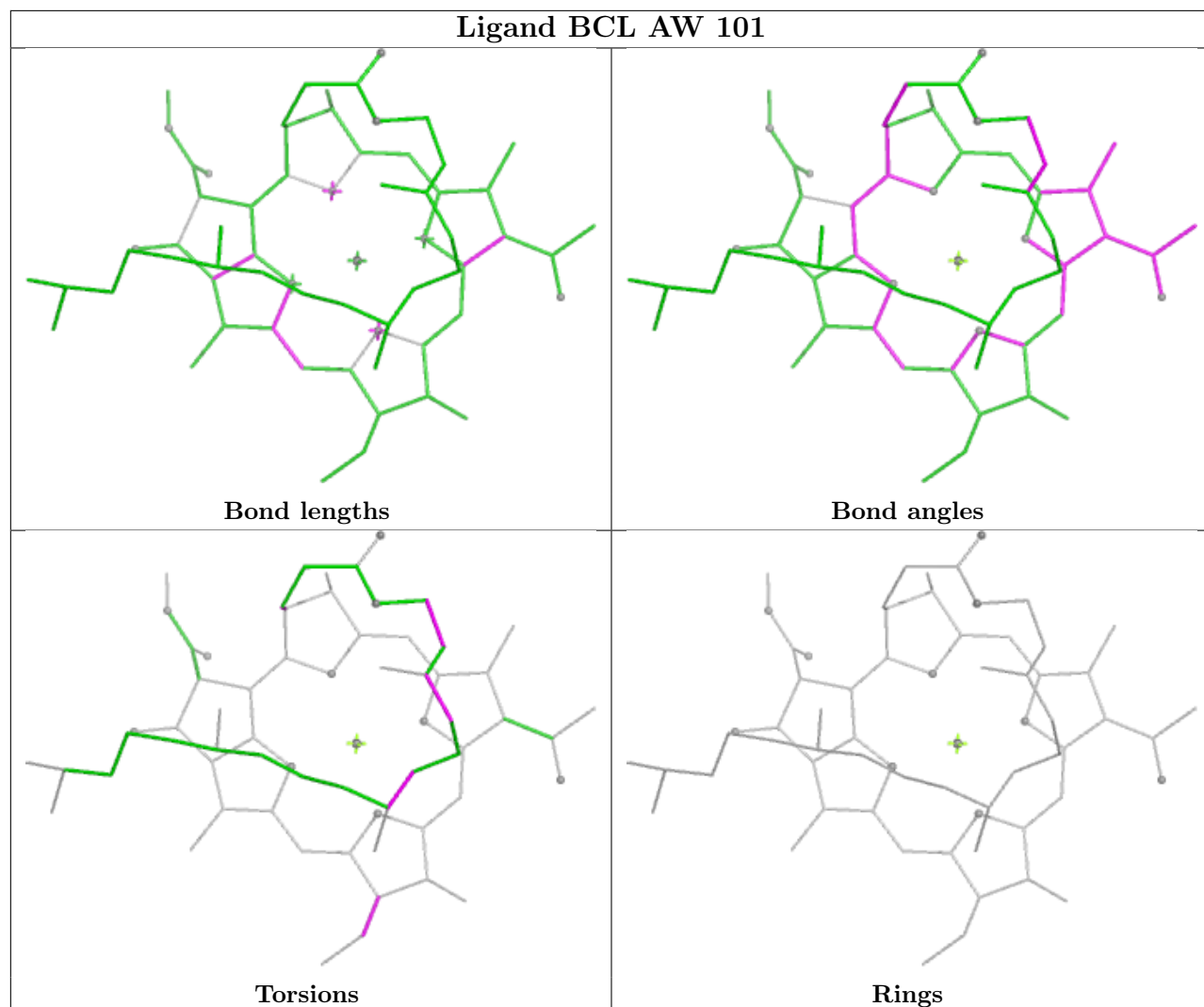


Ligand BCL AQ 102

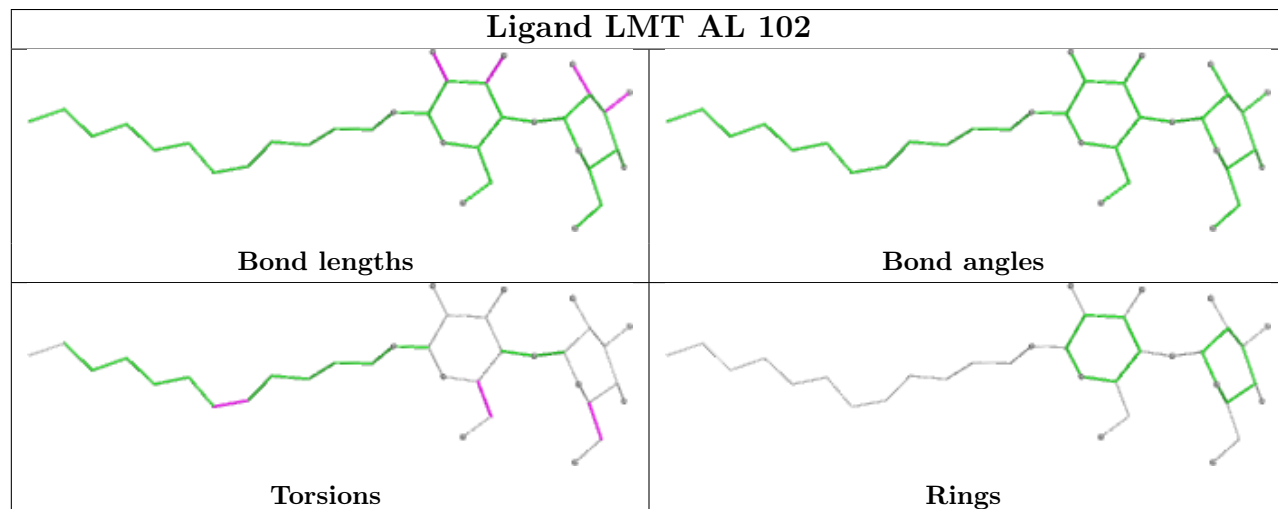


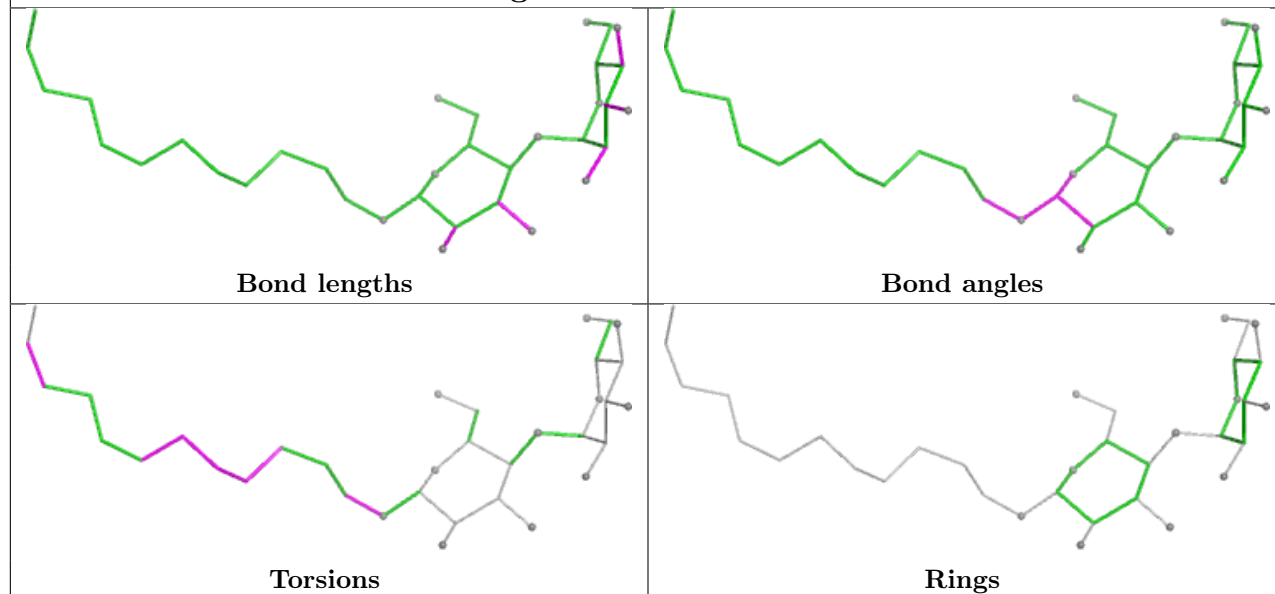
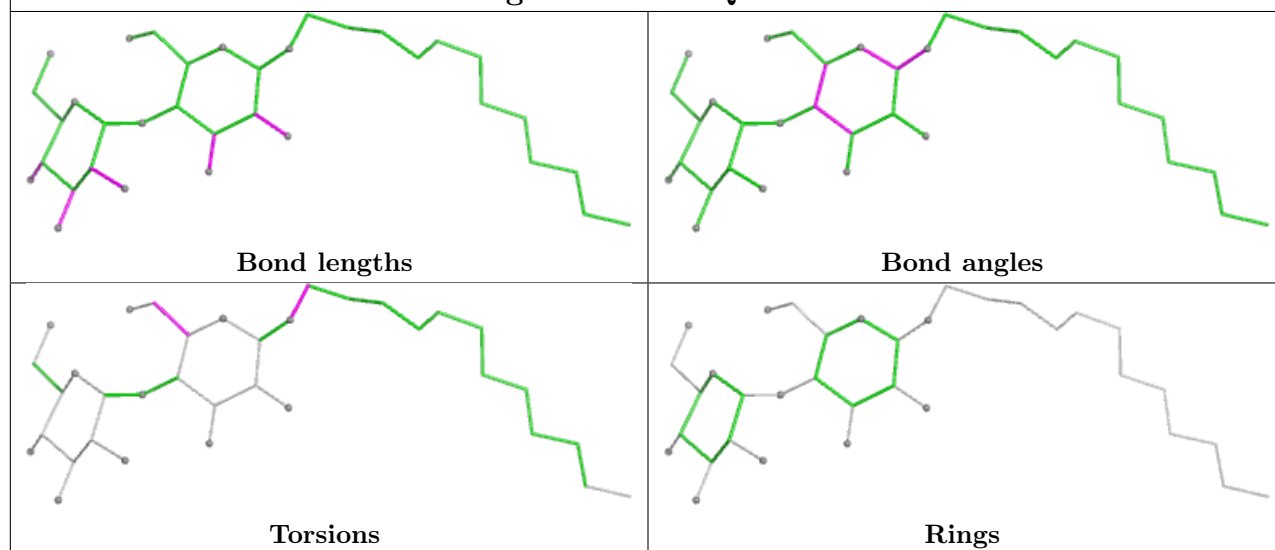


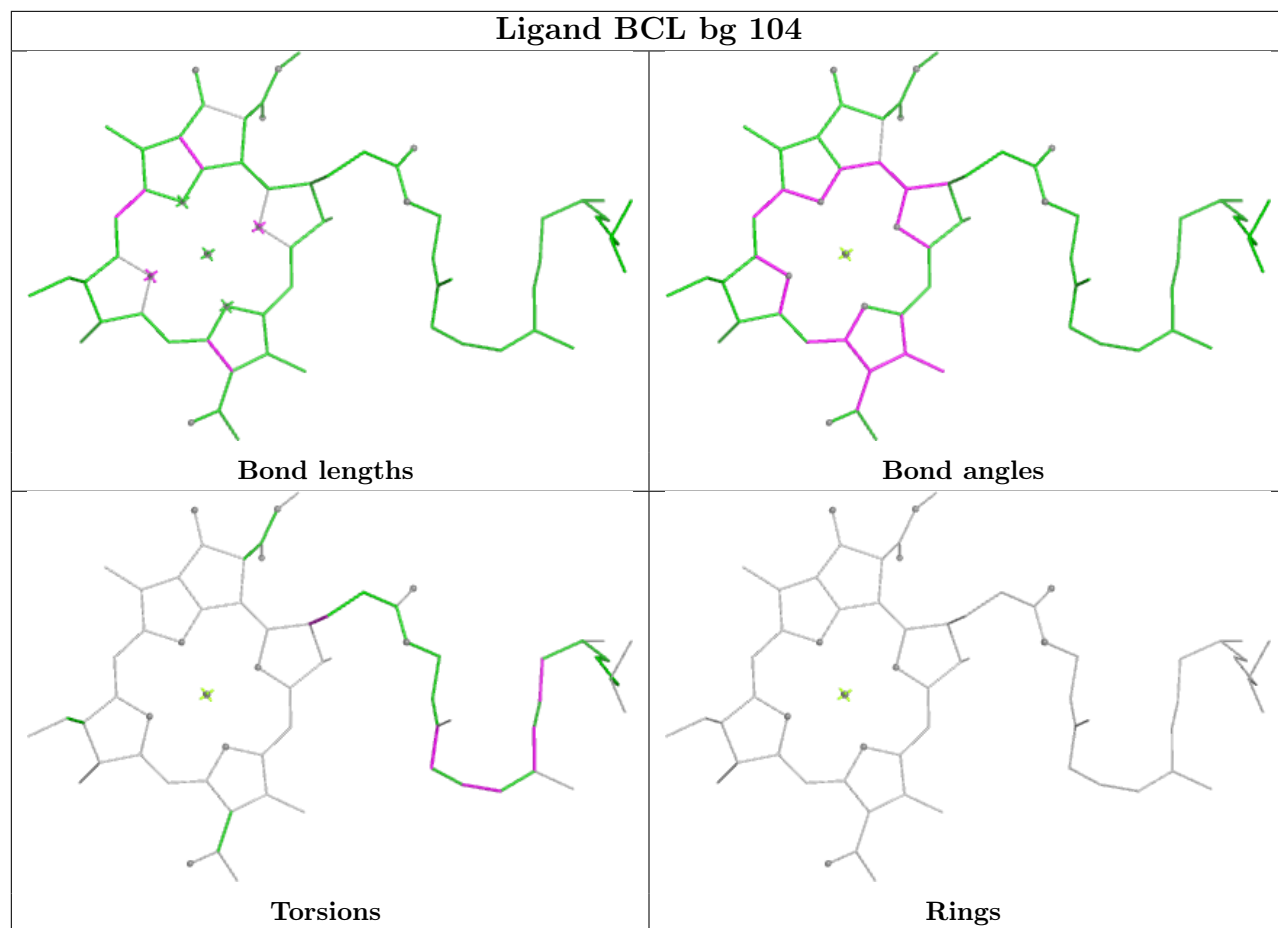
Ligand BCL AW 101



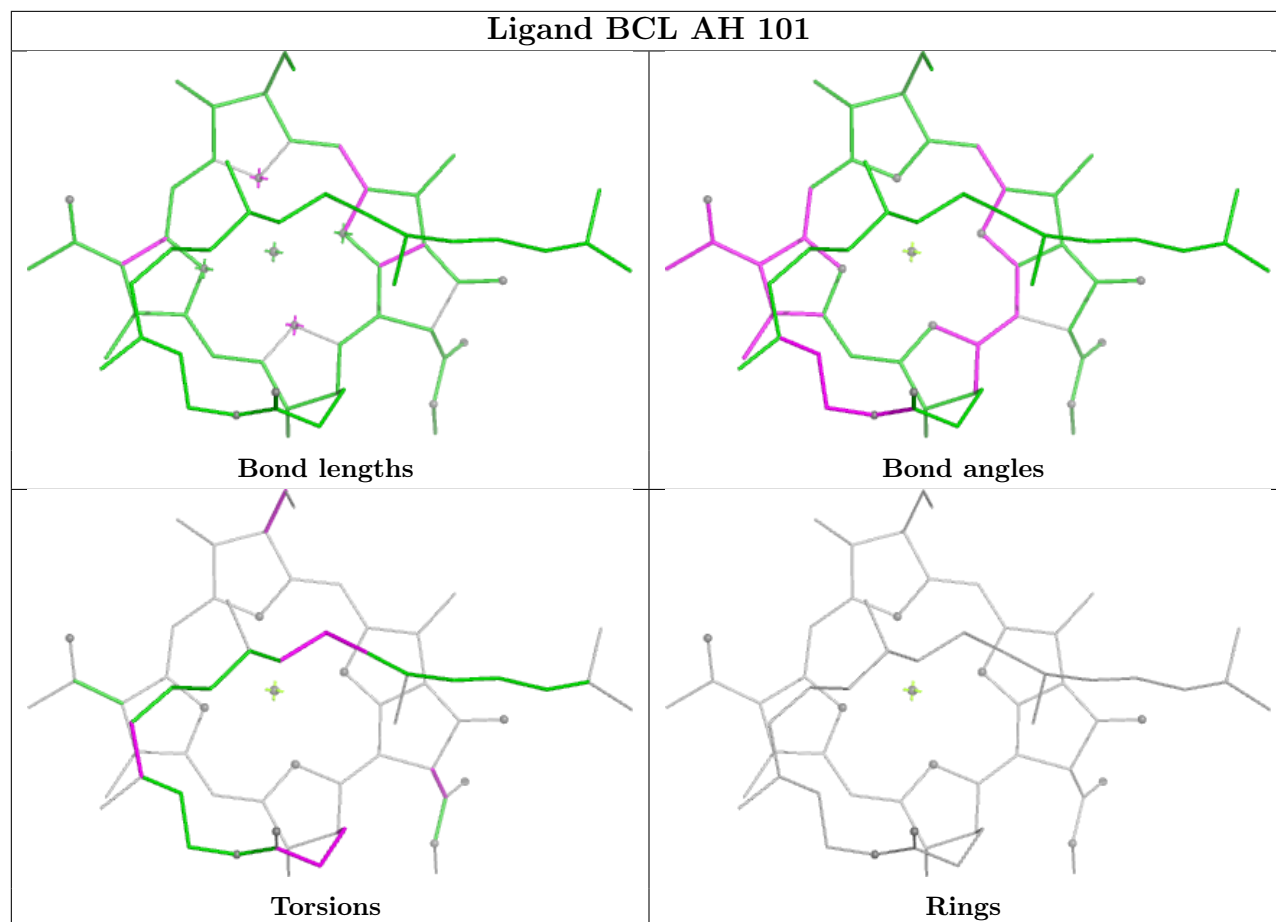
Ligand LMT AL 102



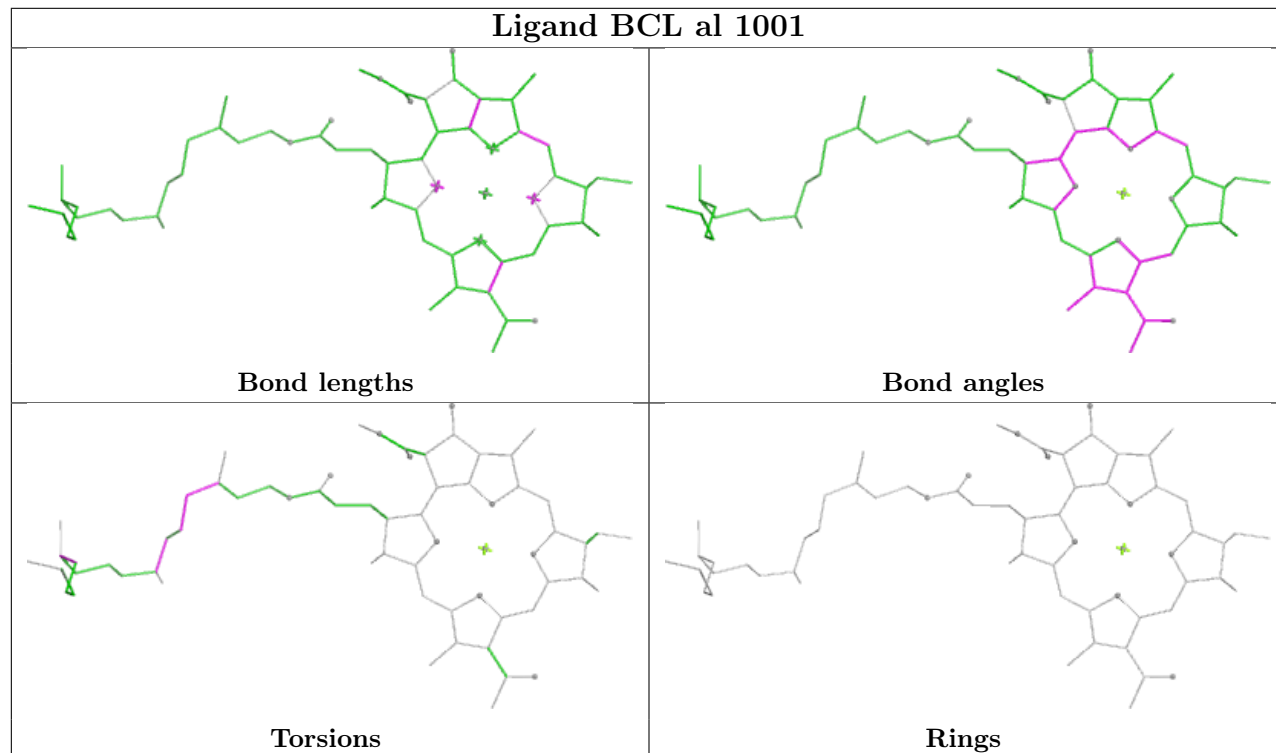
Ligand LMT BJ 1002**Ligand LMT BQ 1004**

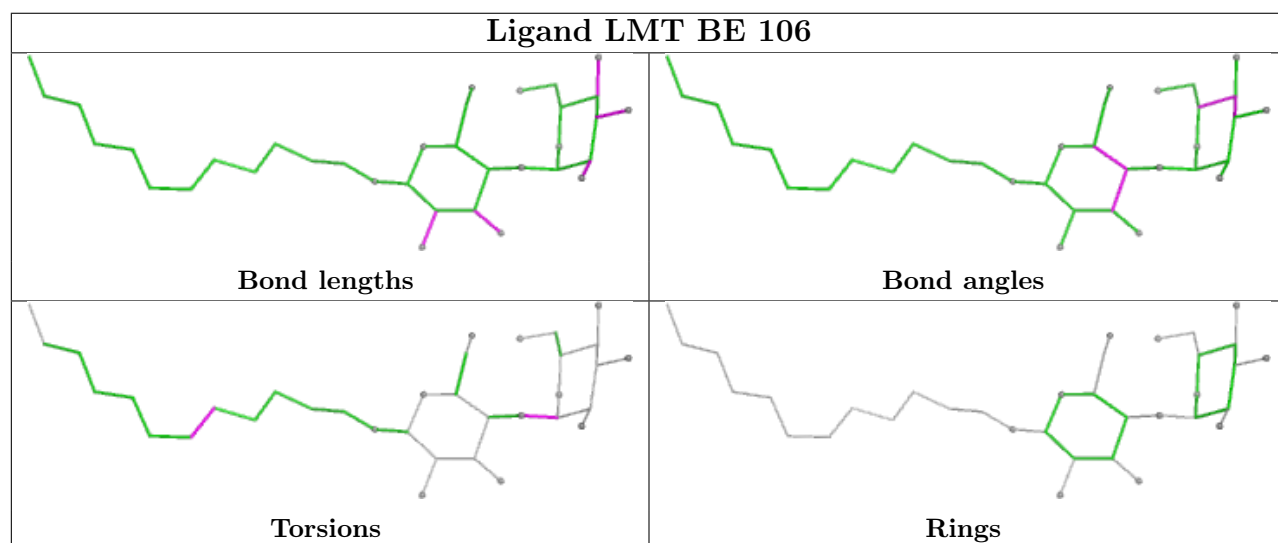
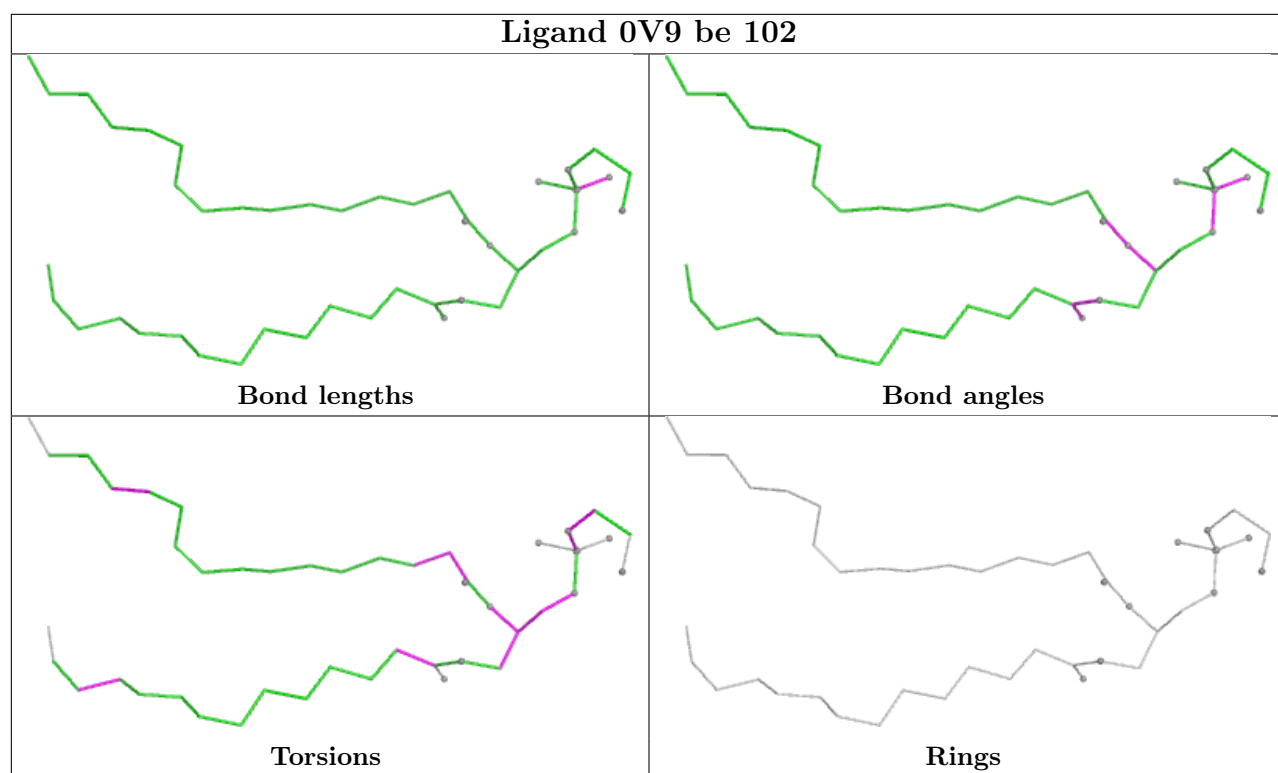


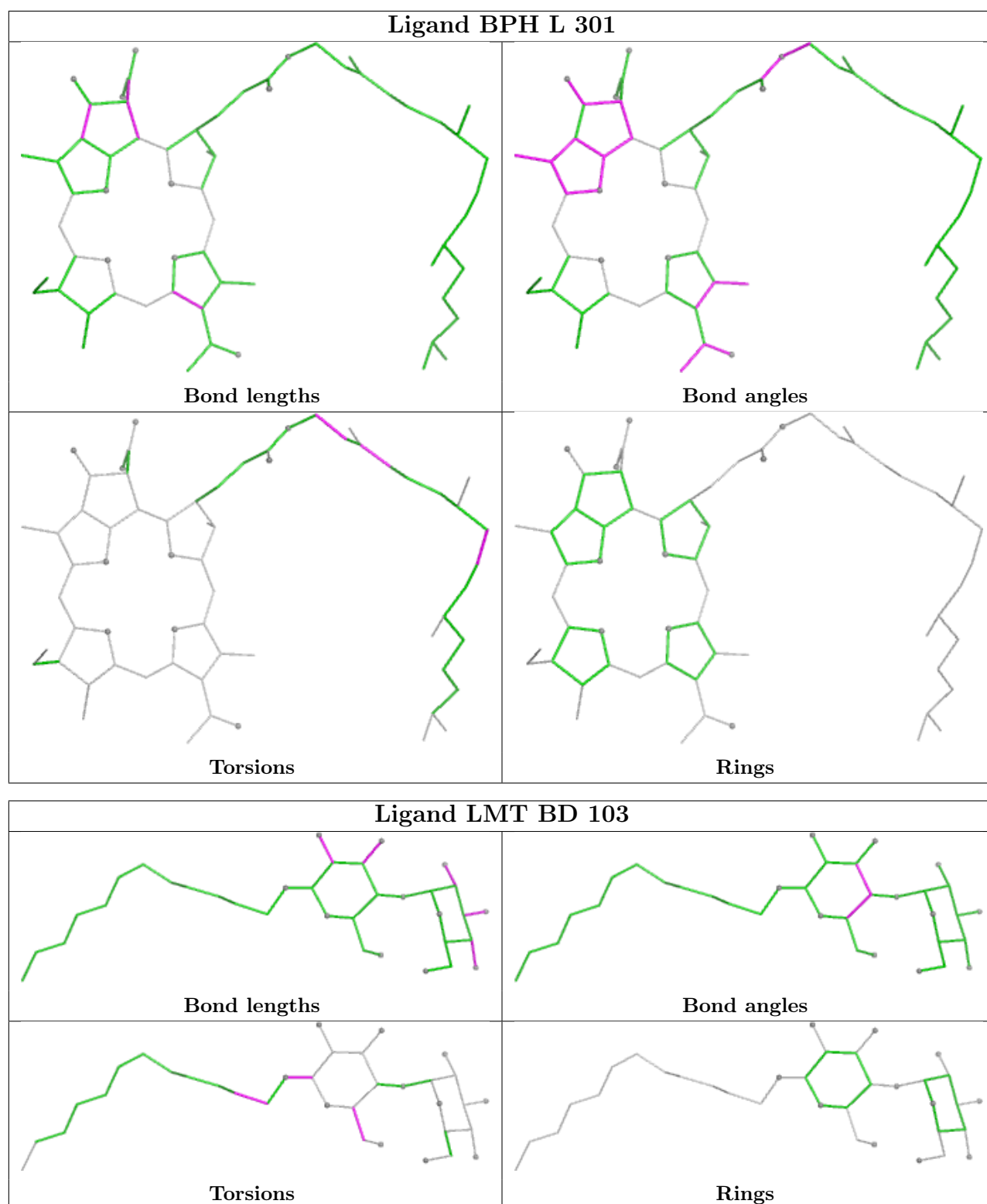
Ligand BCL AH 101

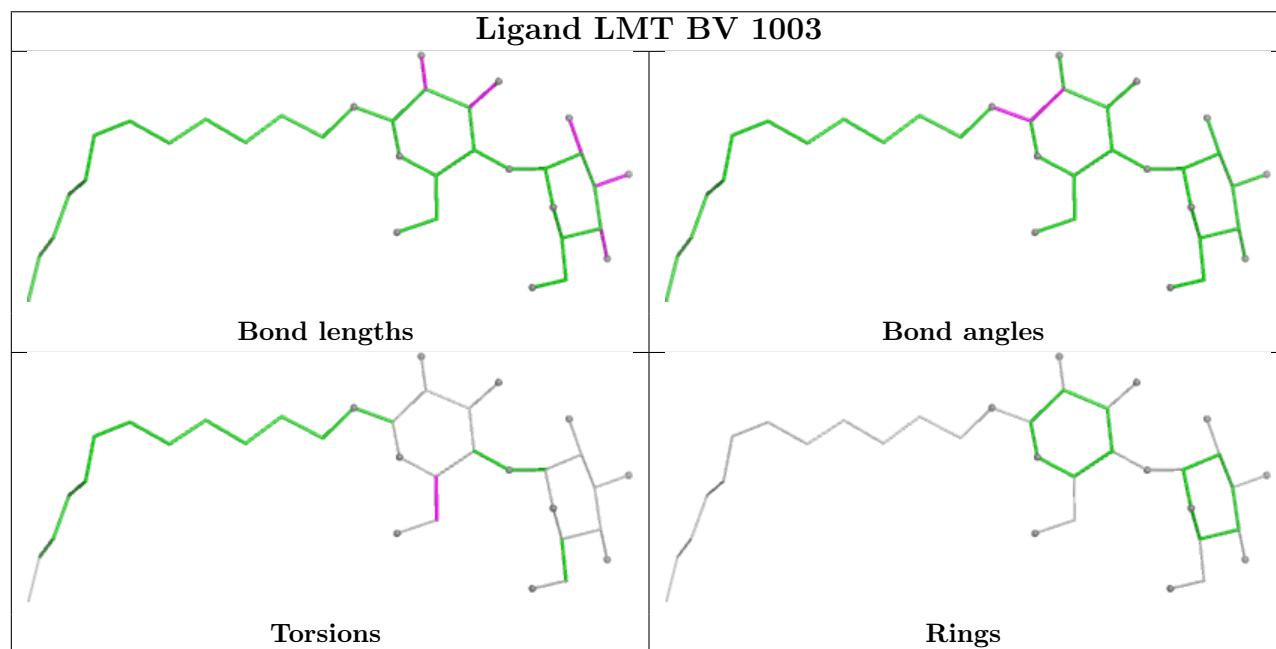
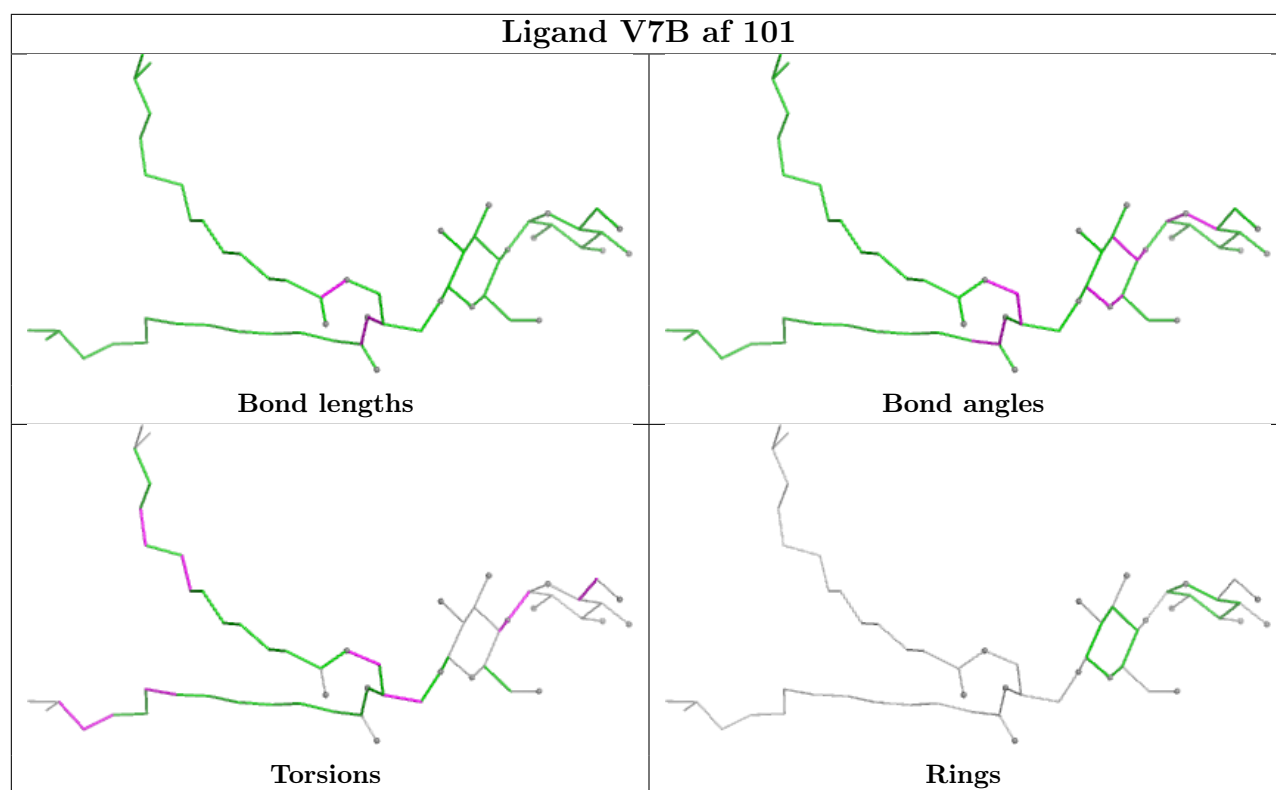


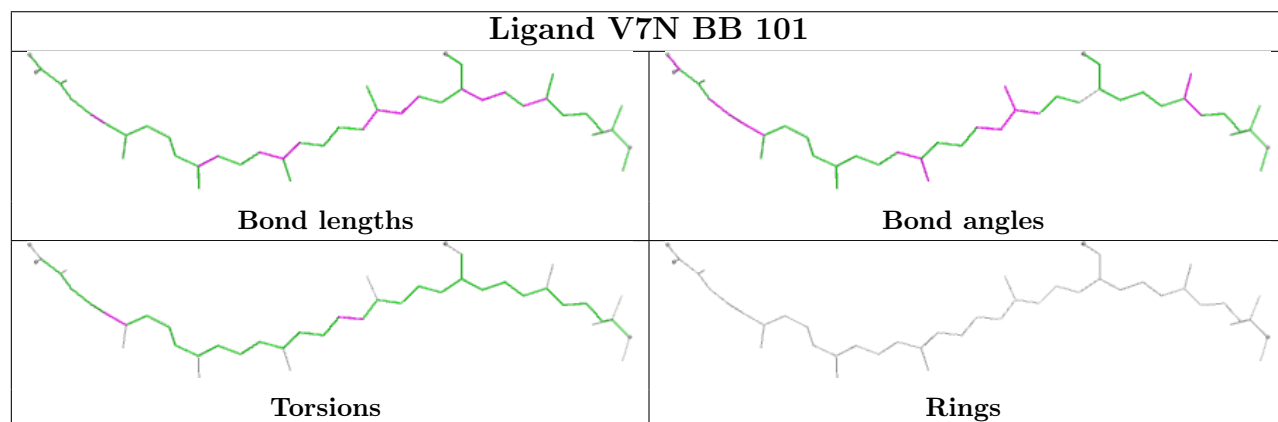
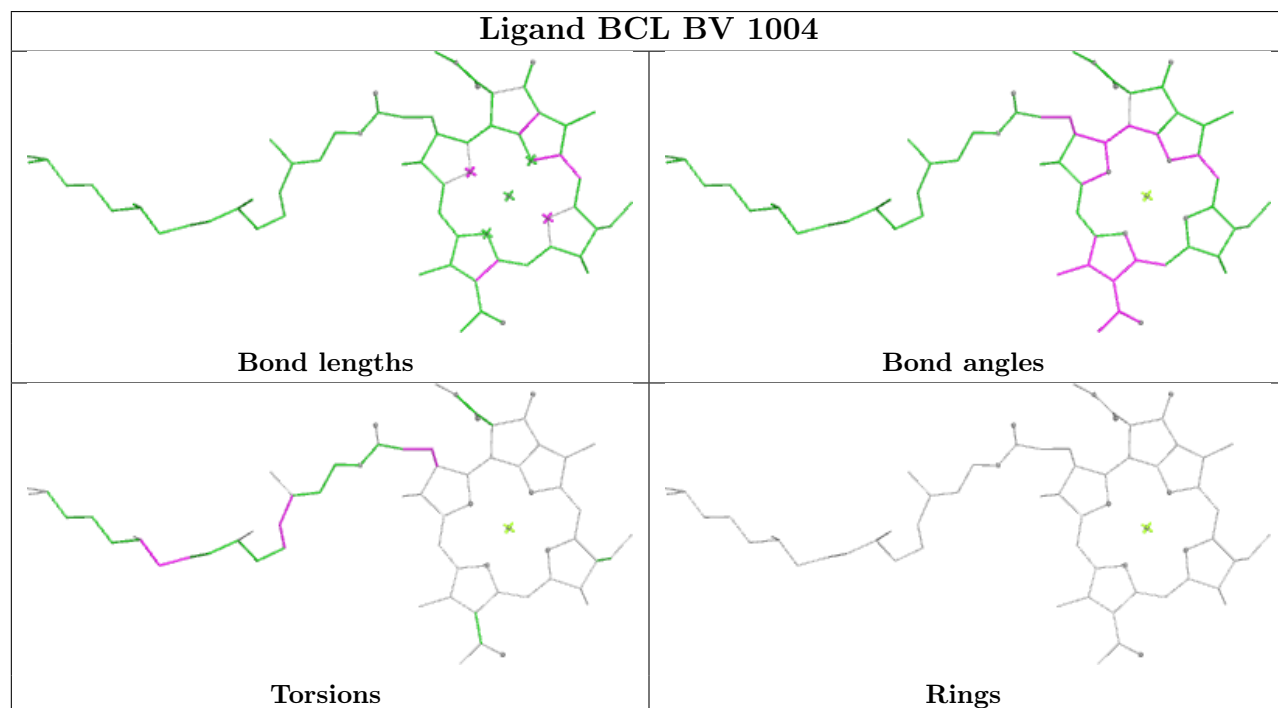
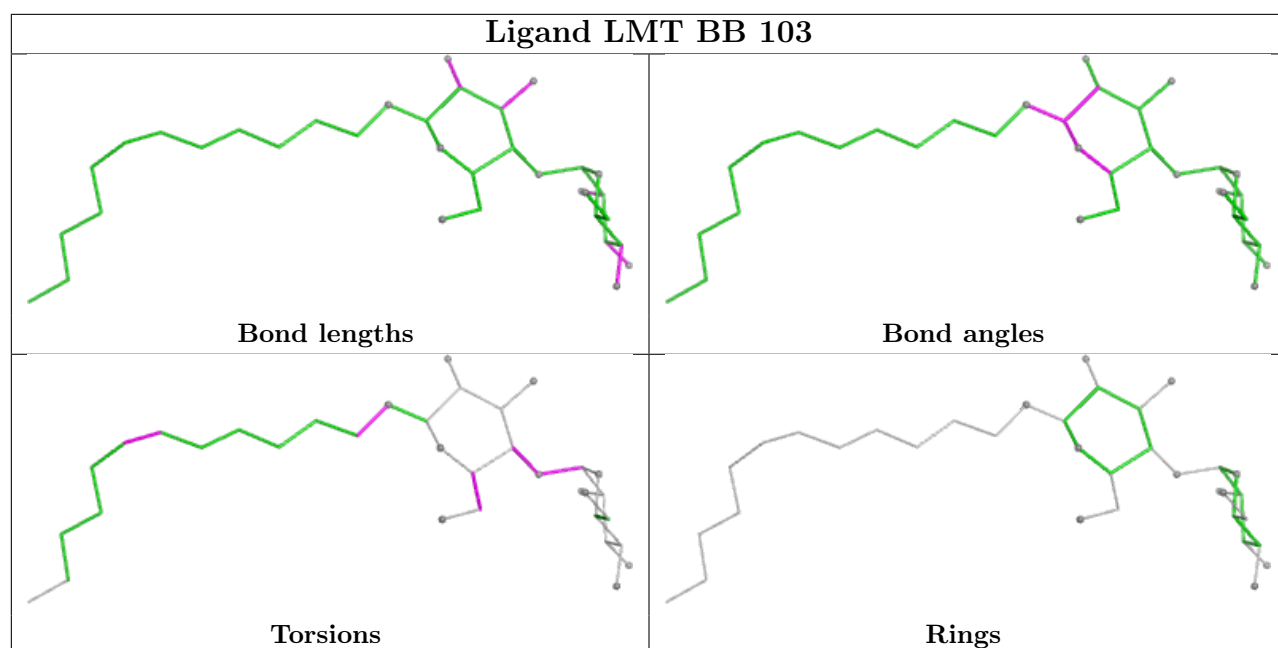
Ligand BCL al 1001

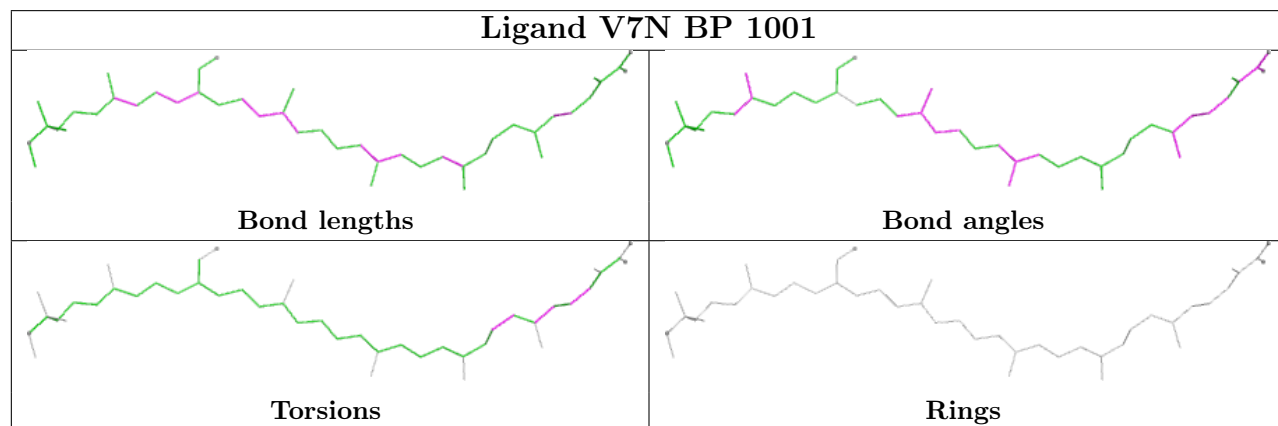
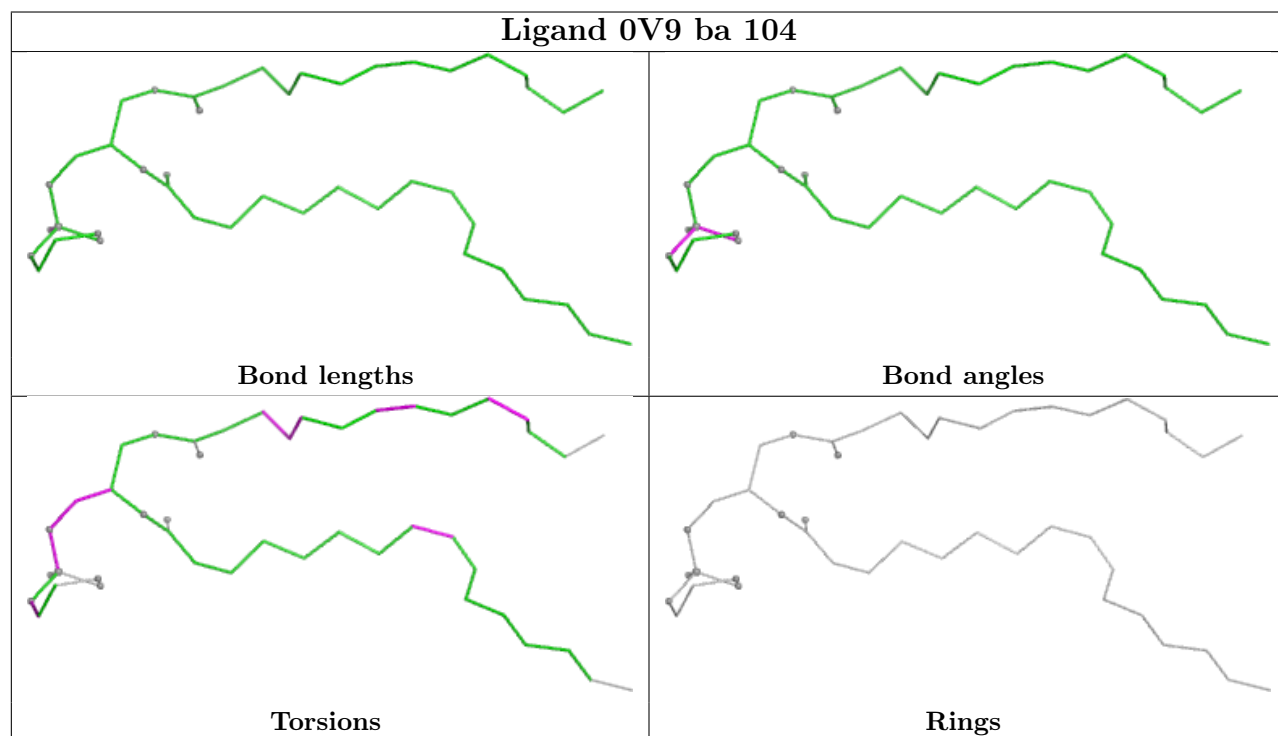
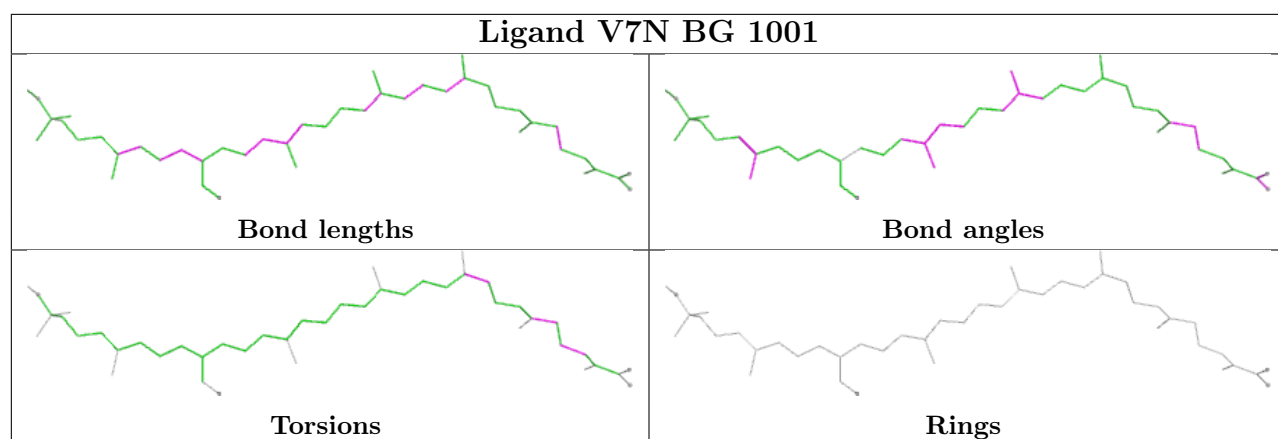


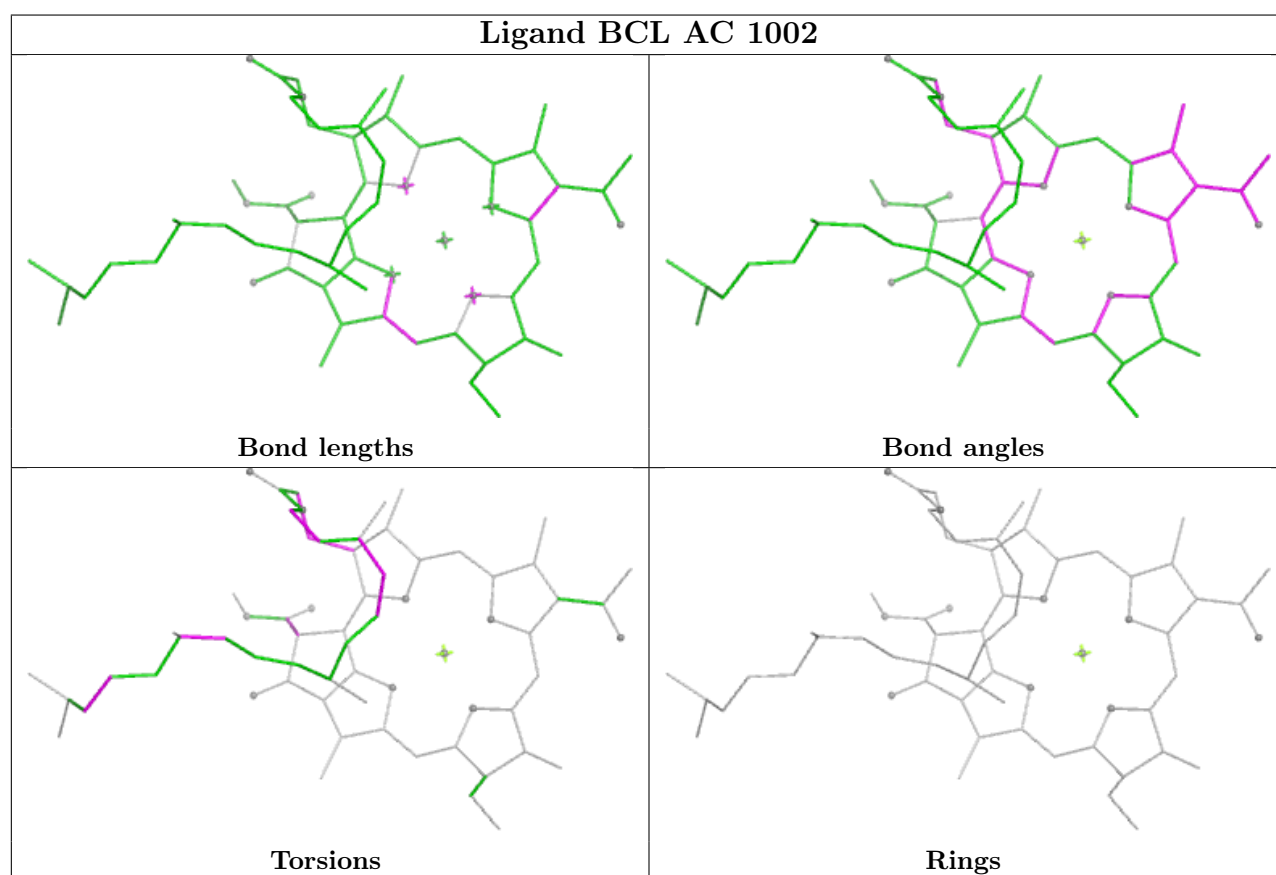
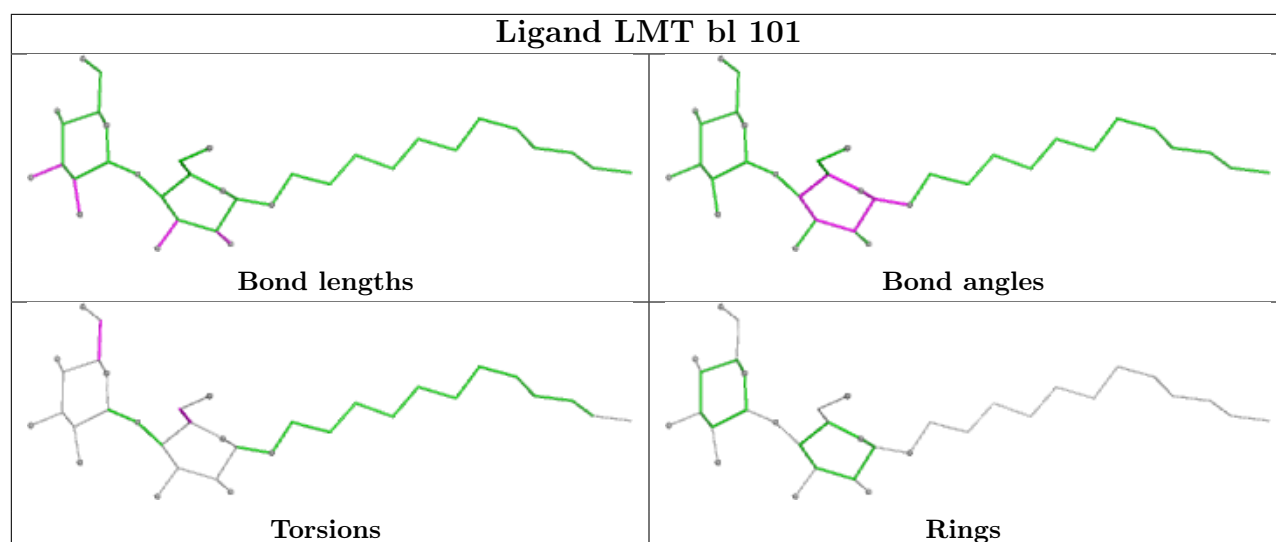


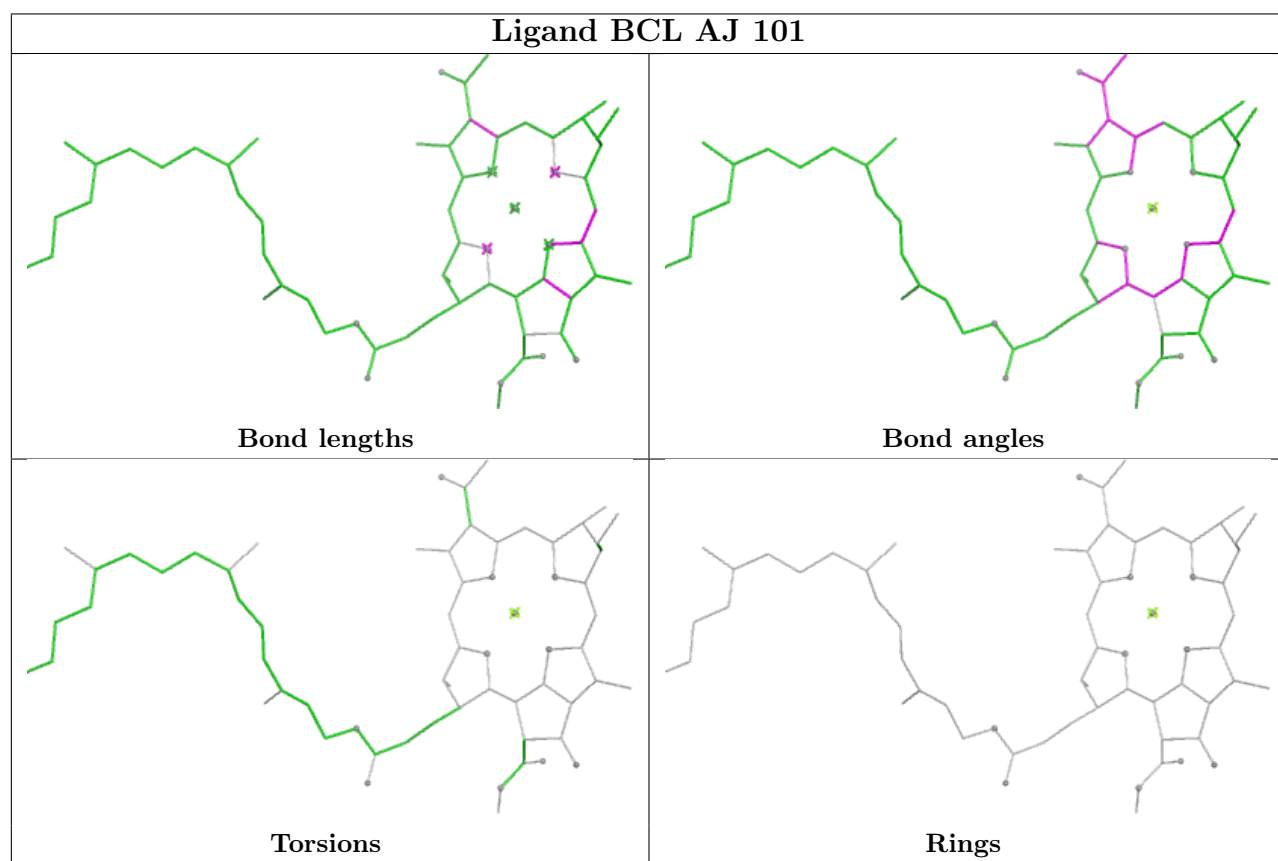
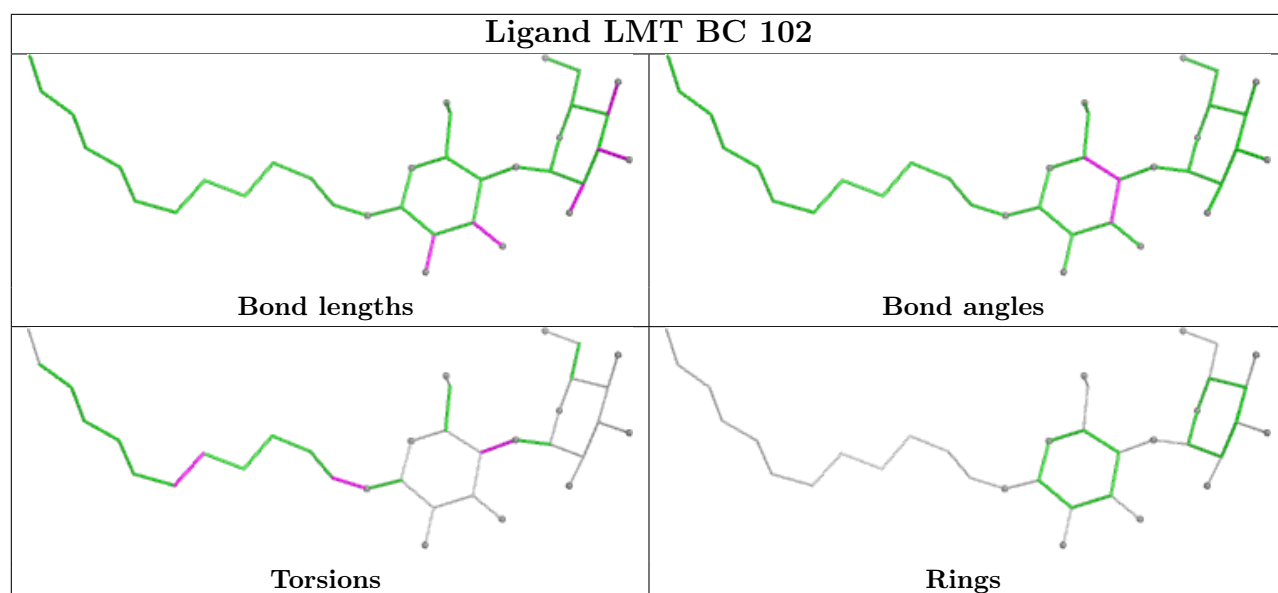


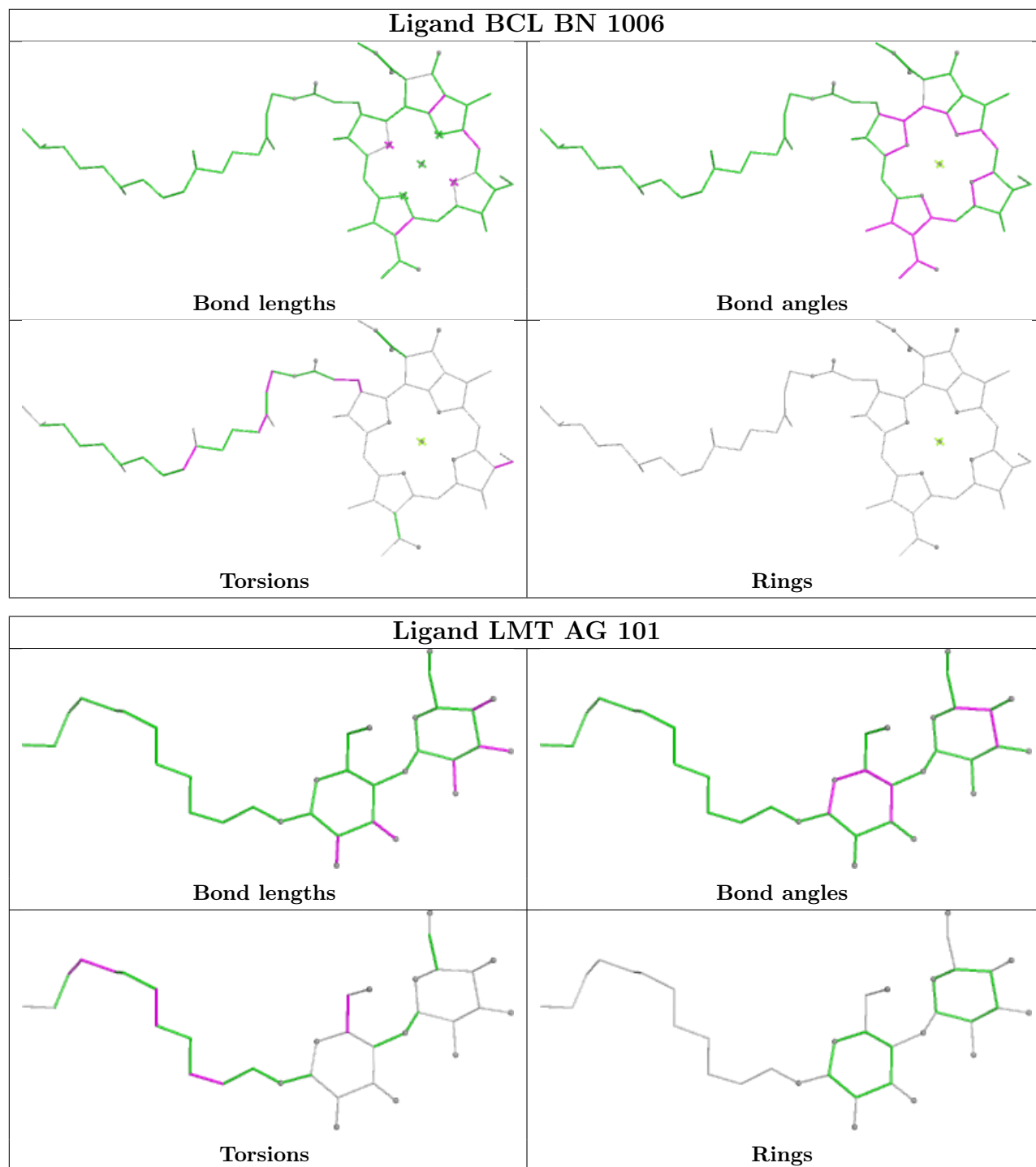


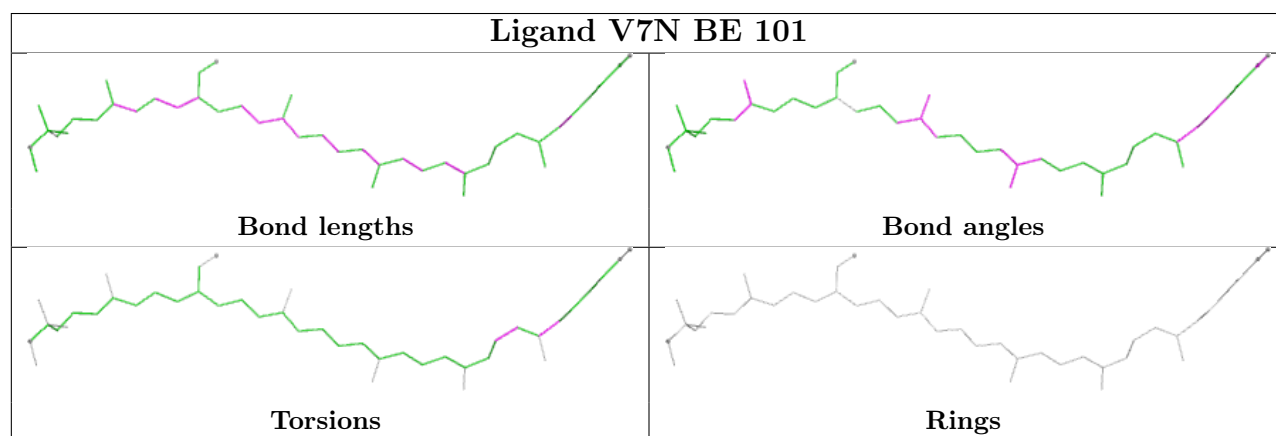
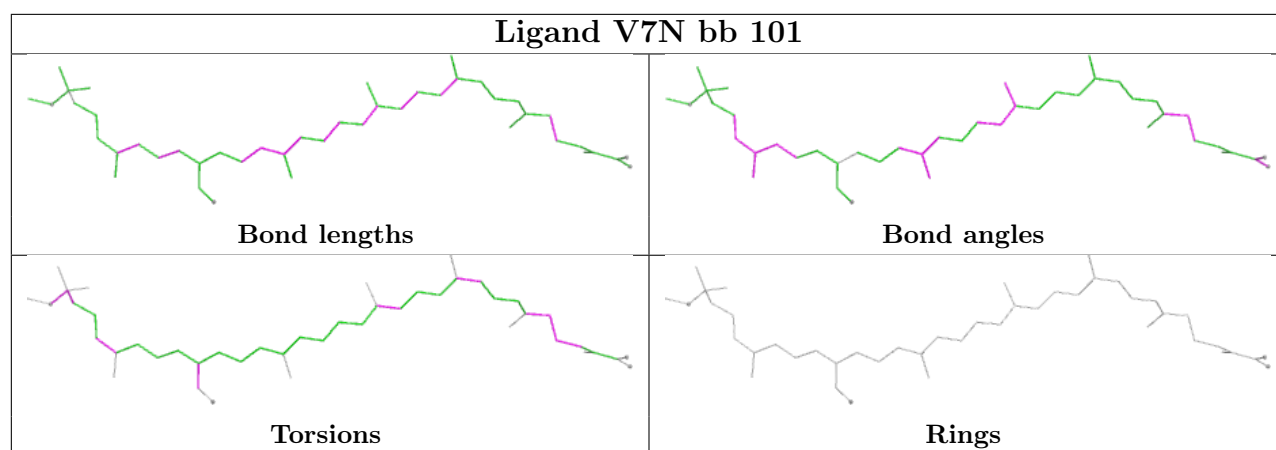


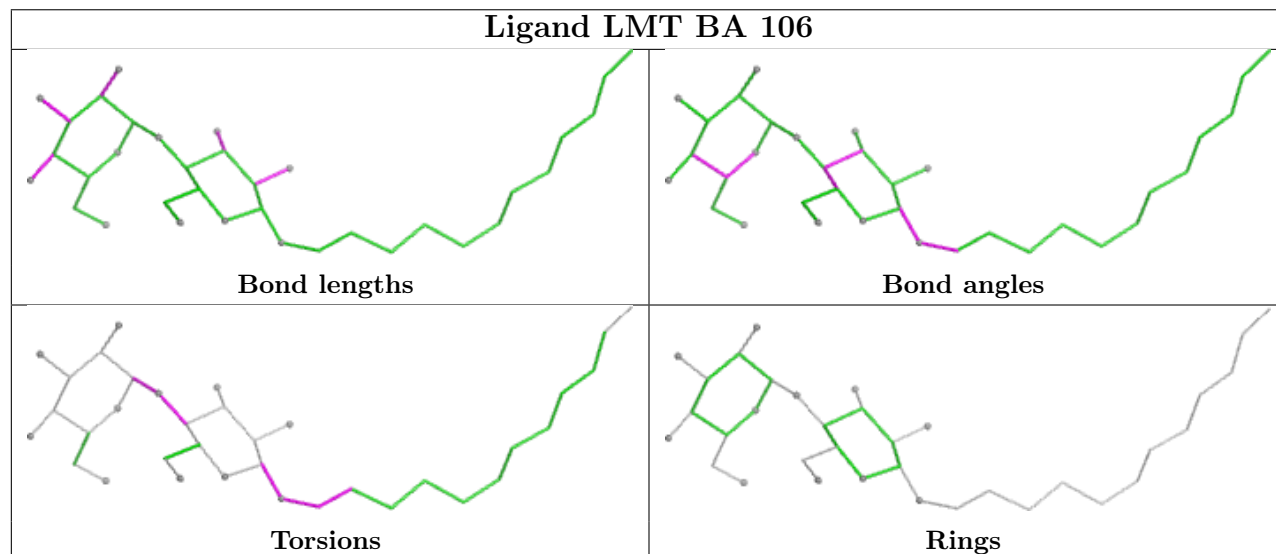
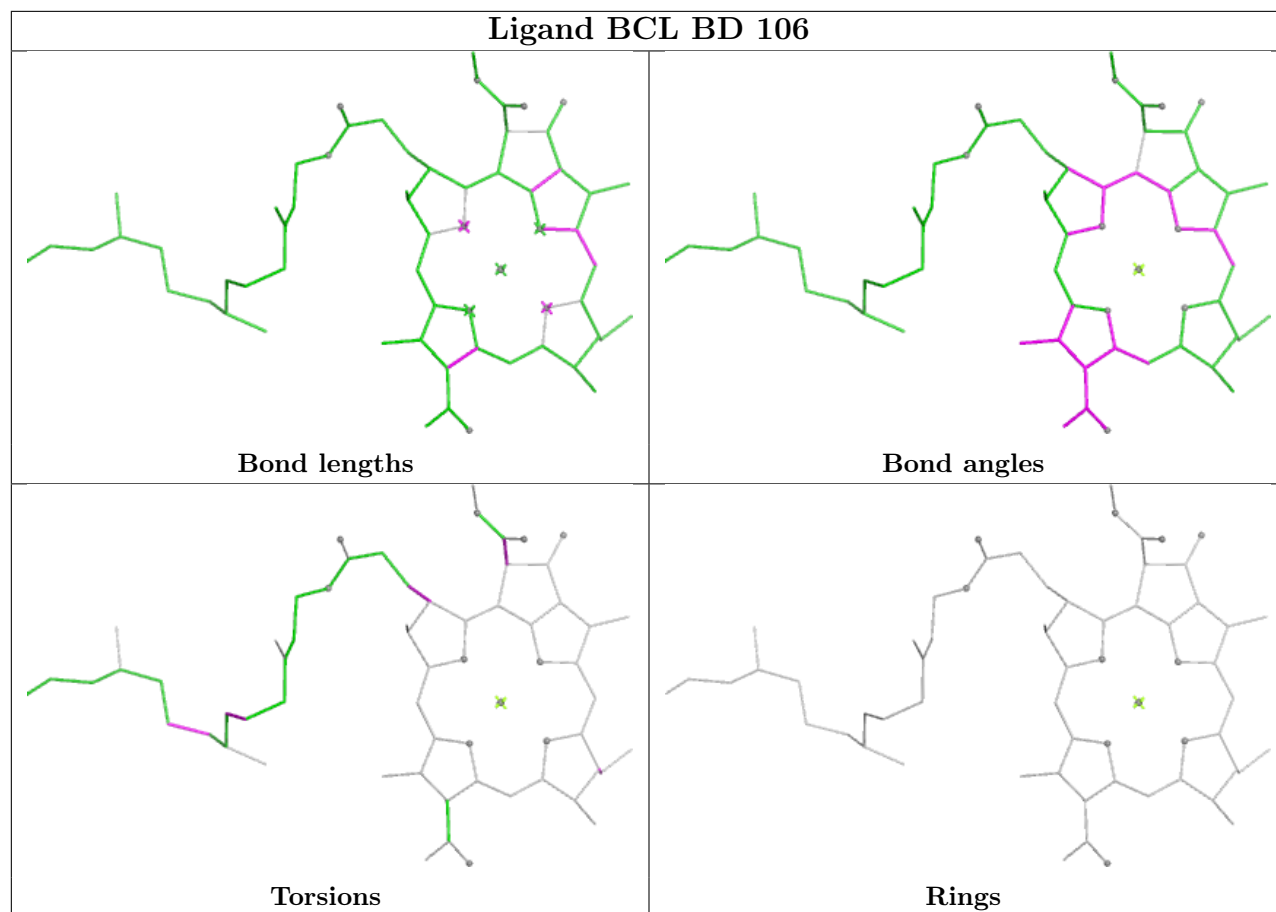


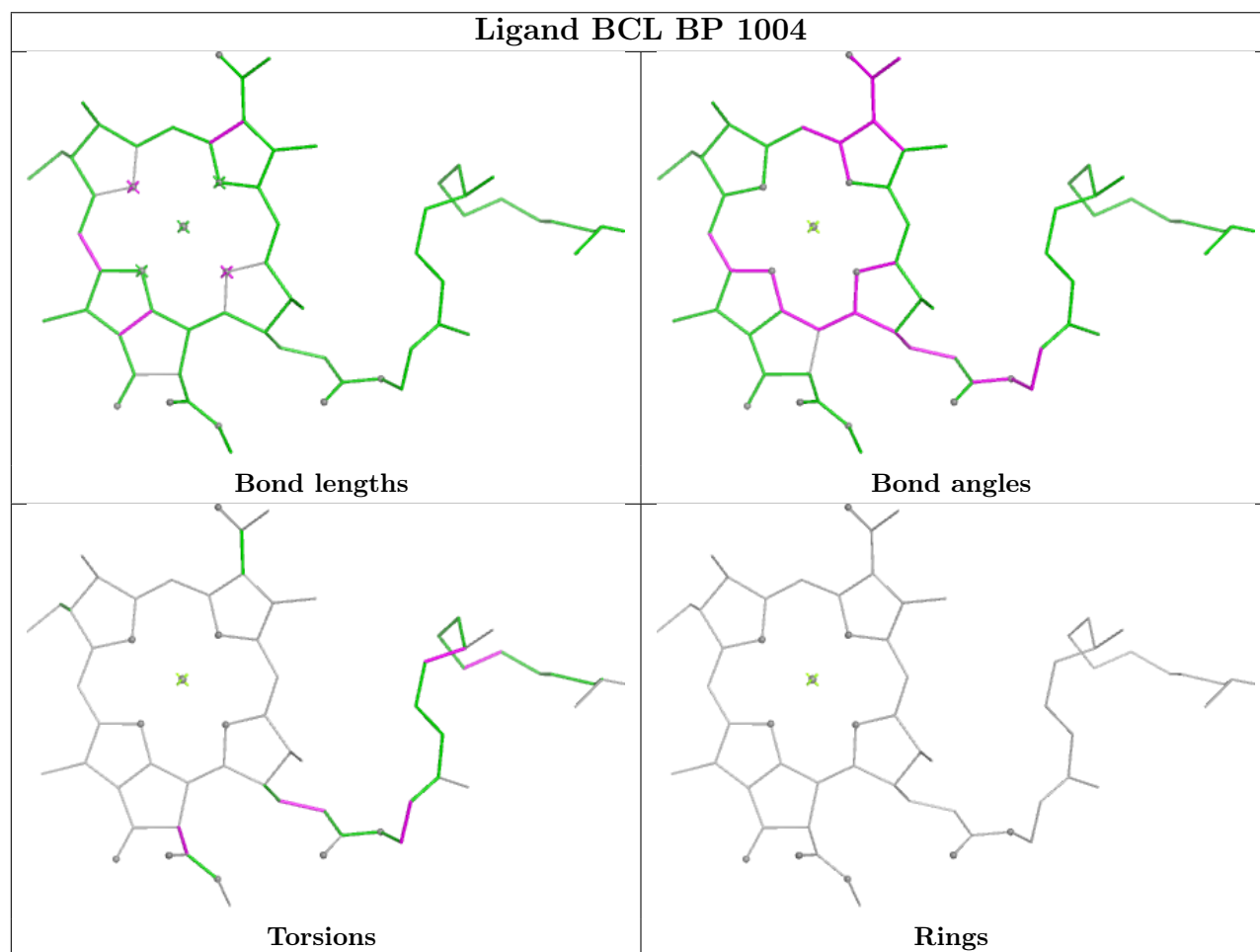
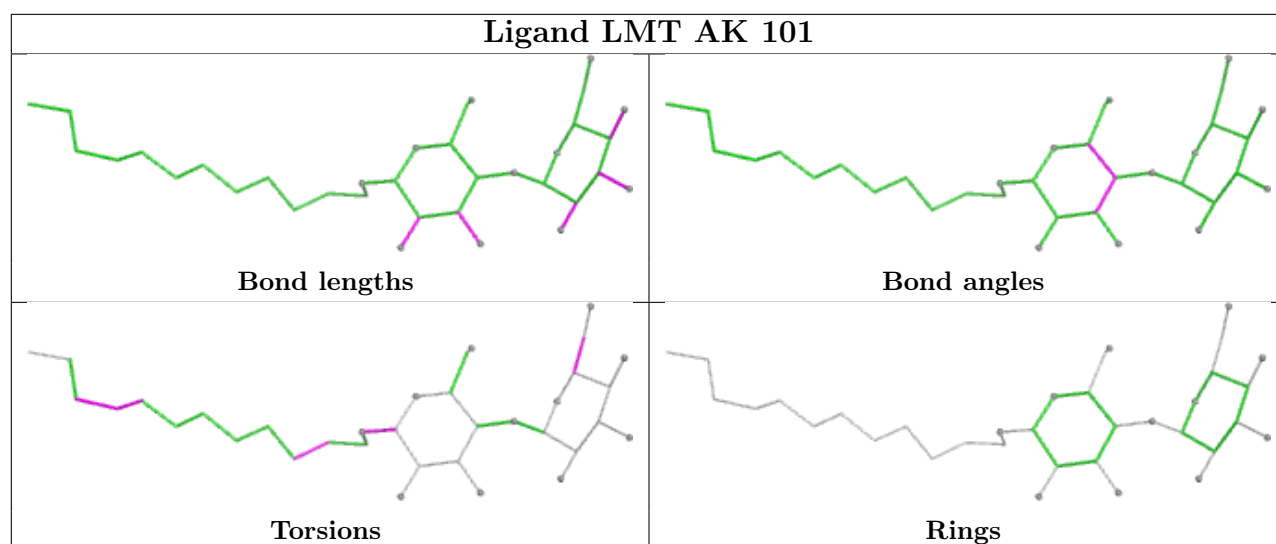


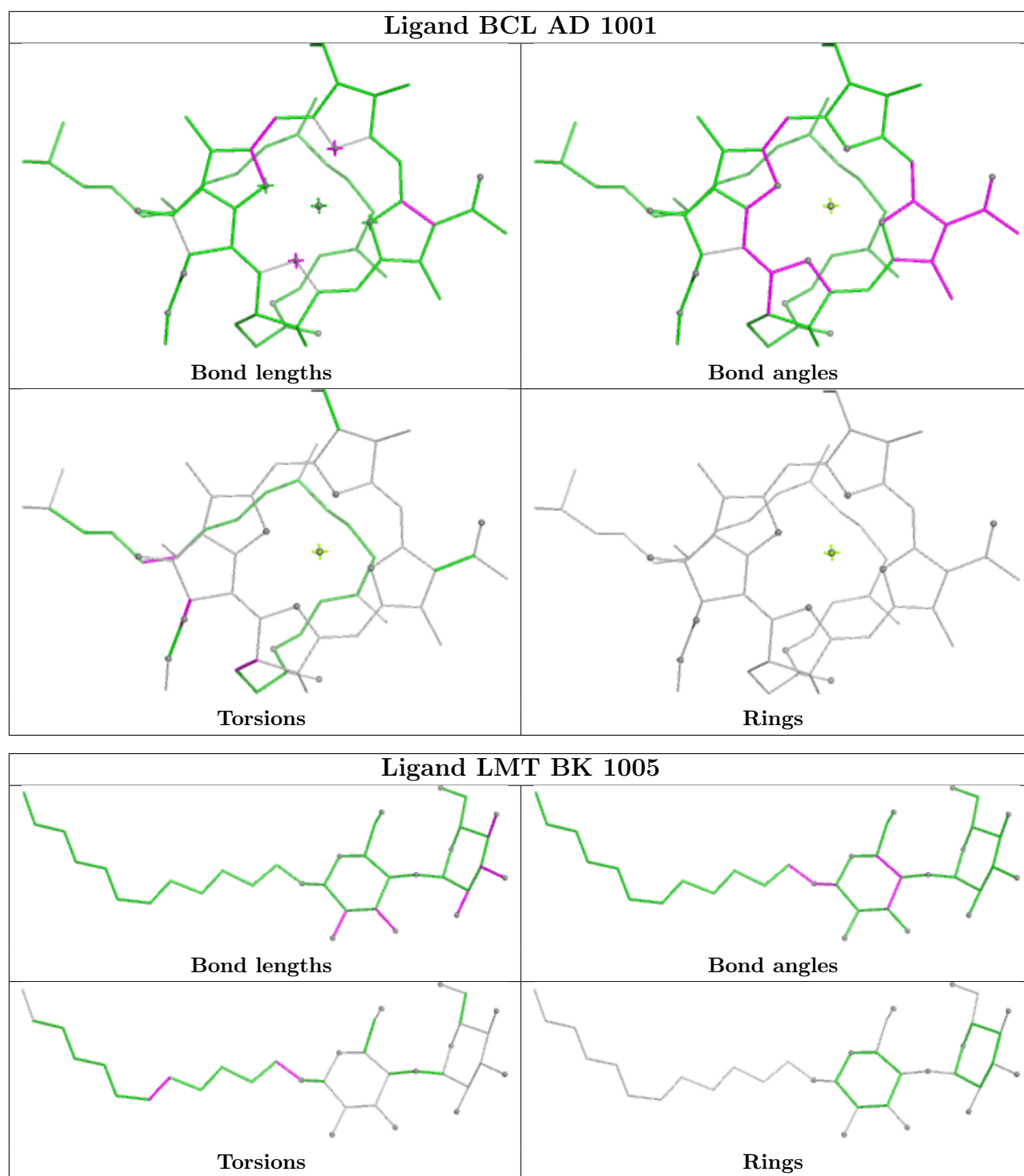


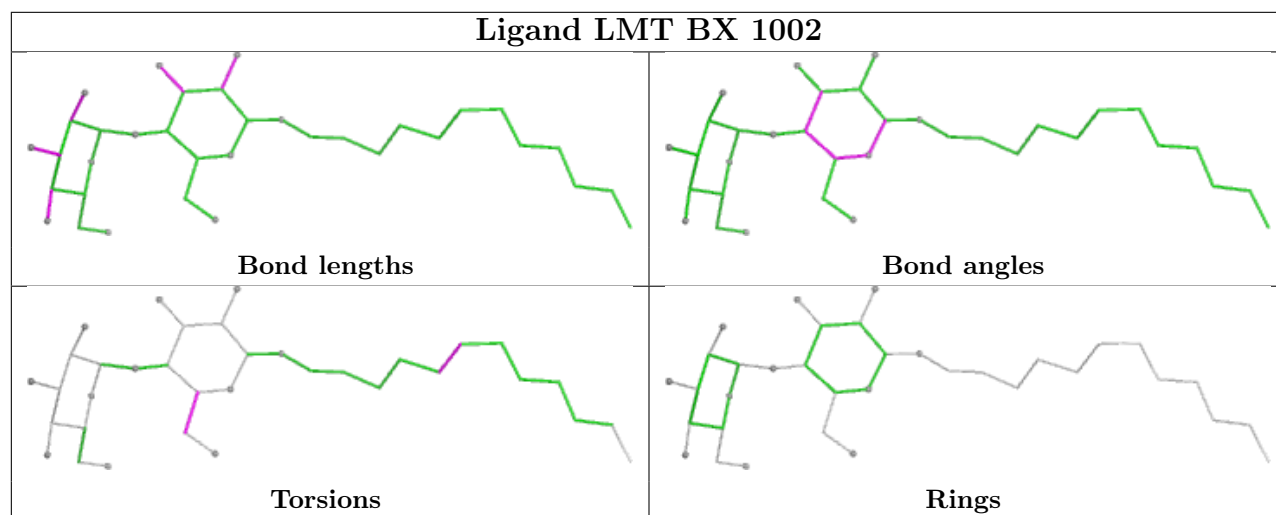
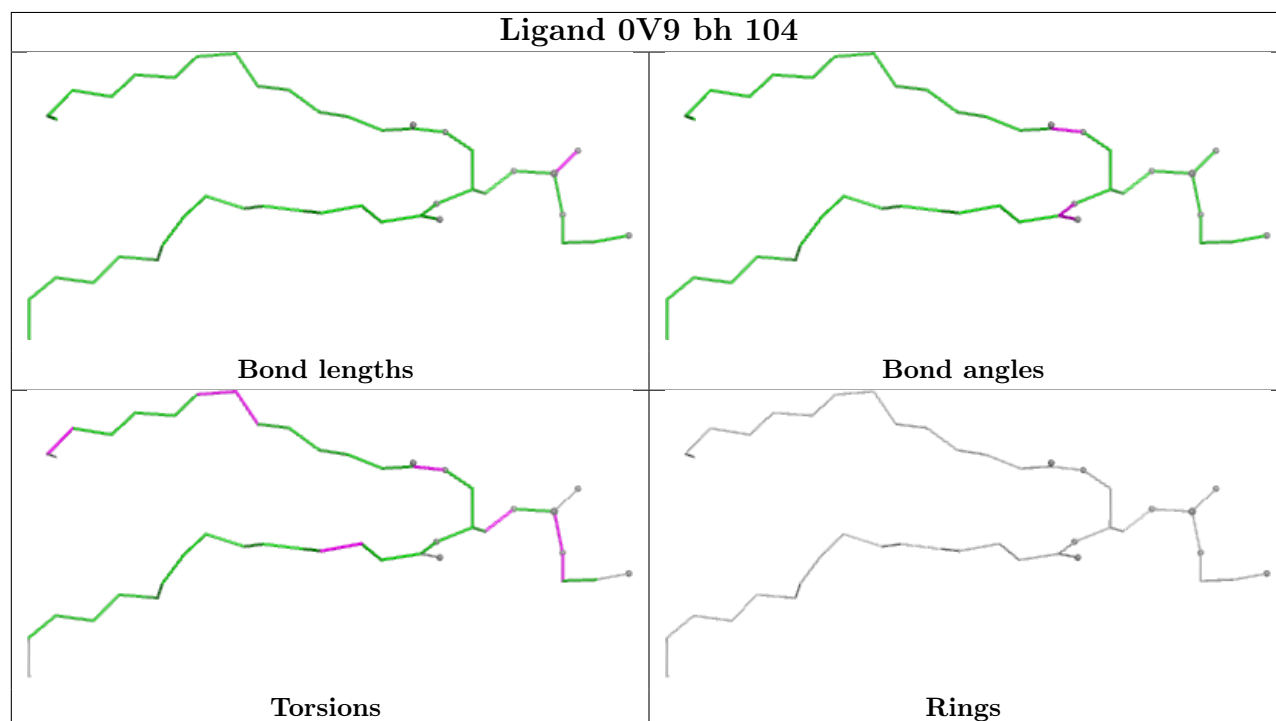
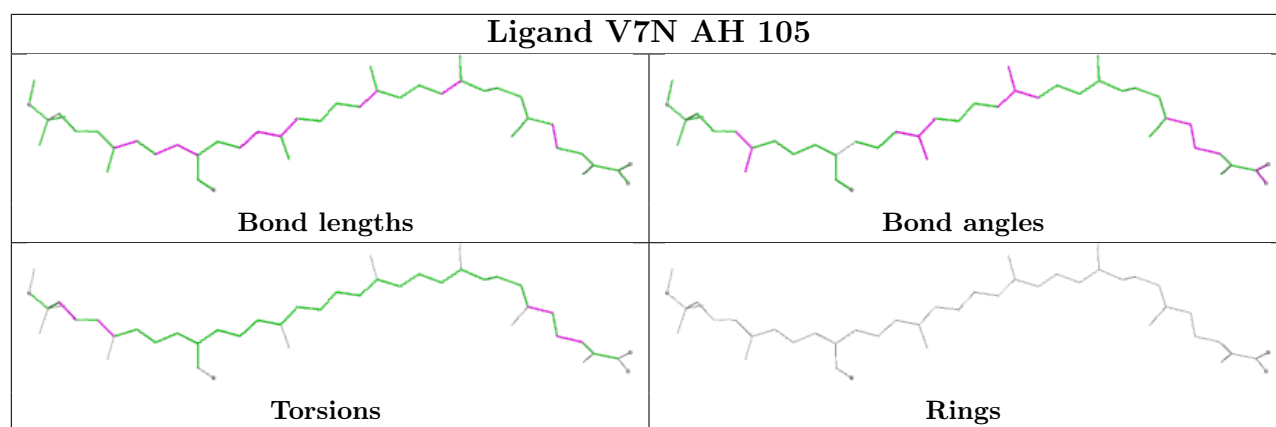


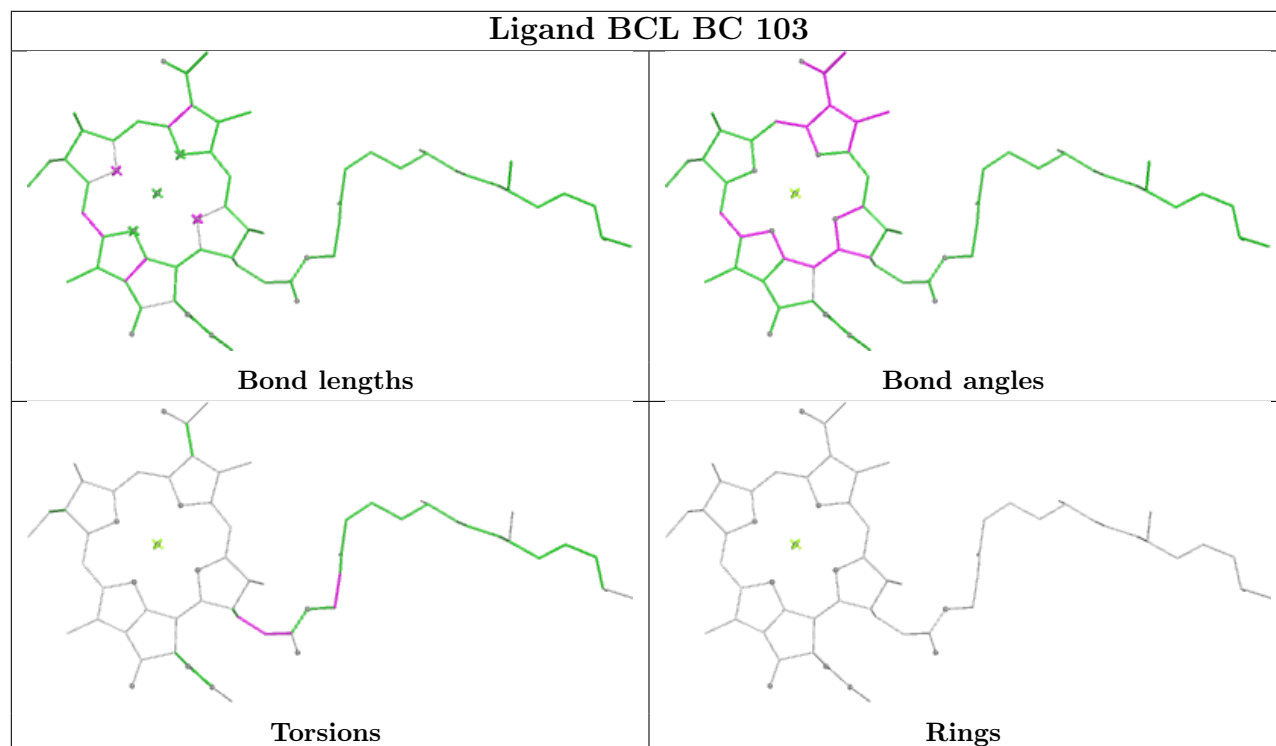
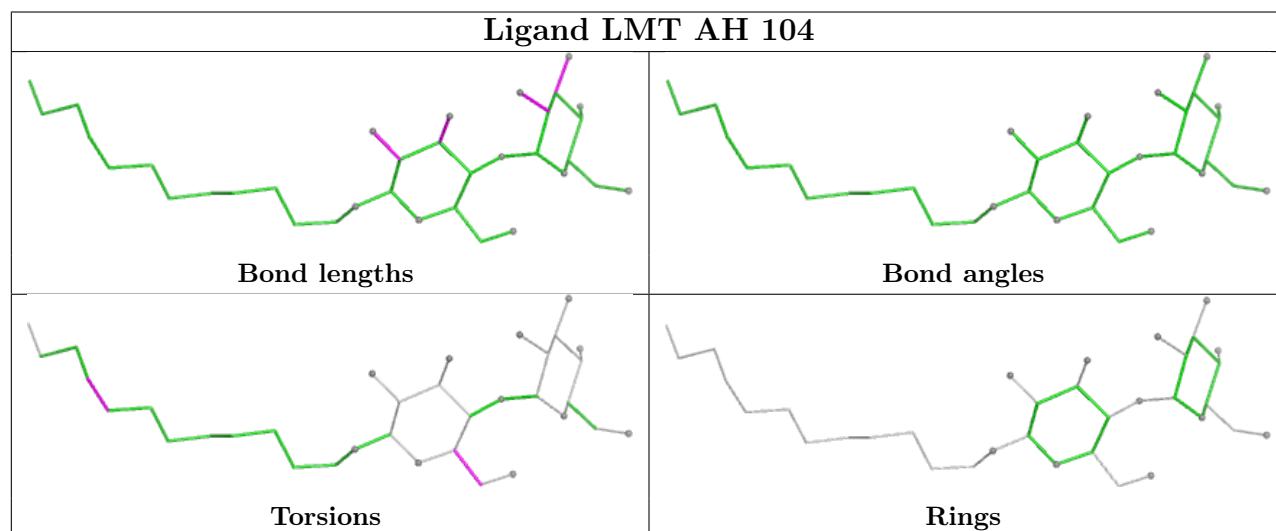
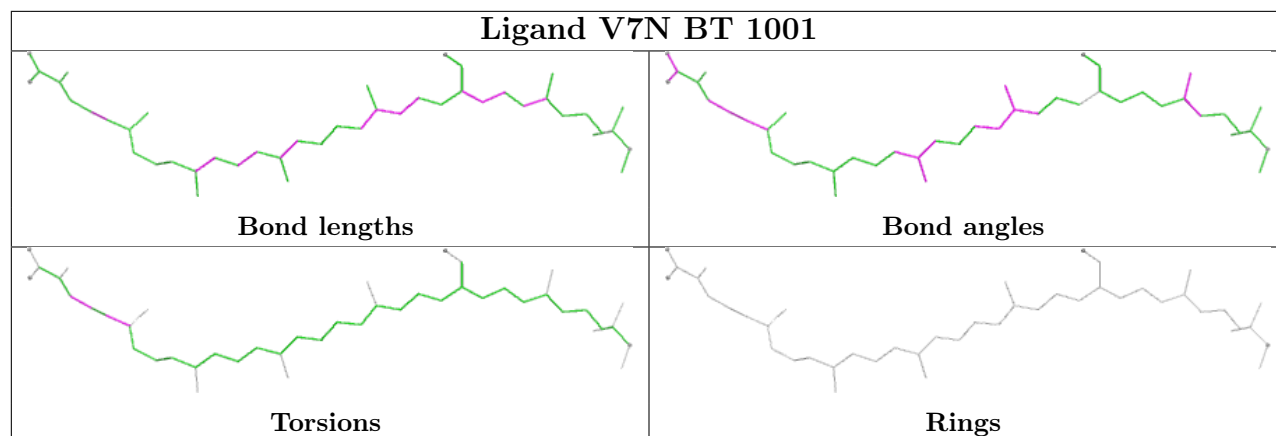


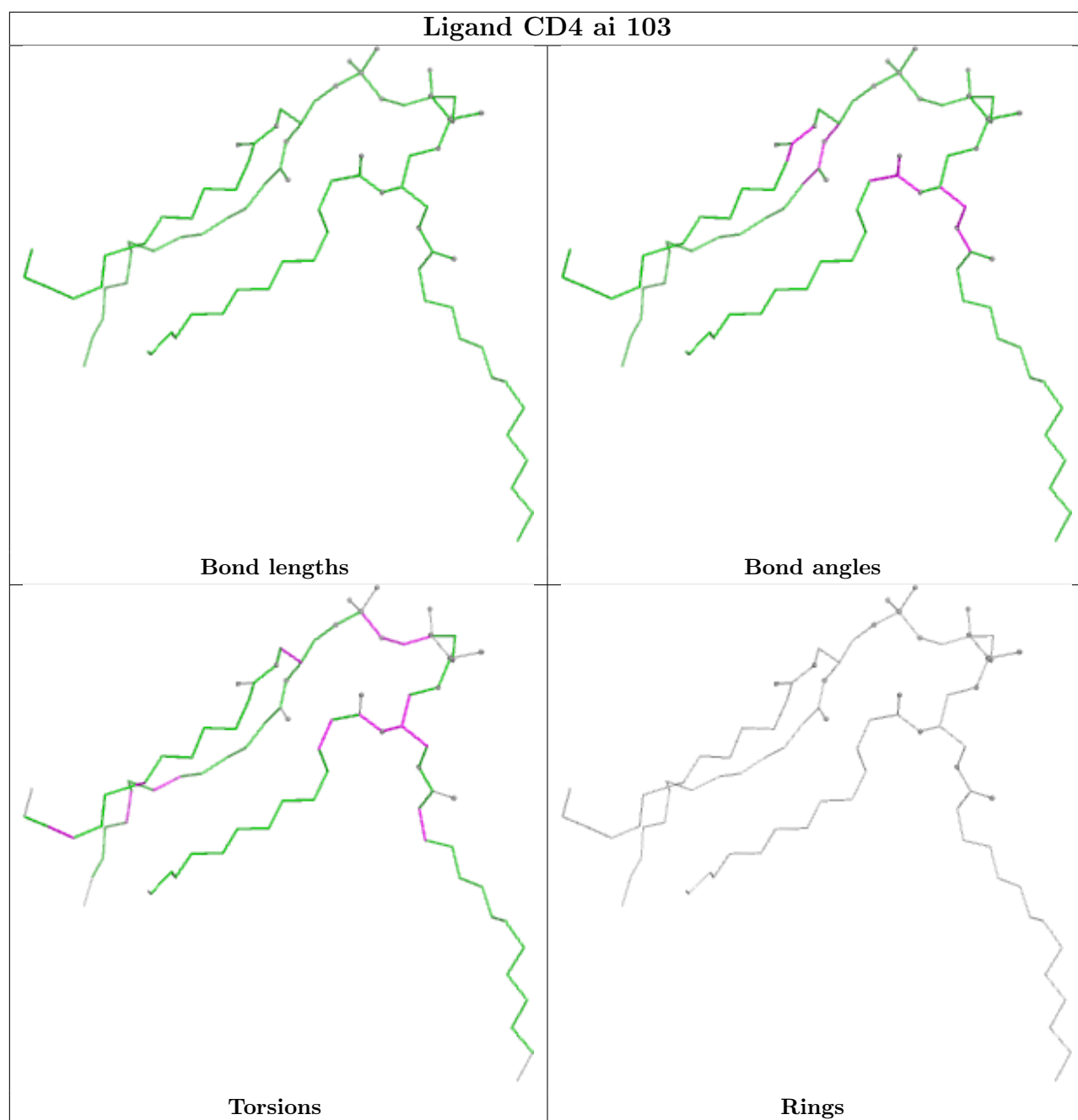




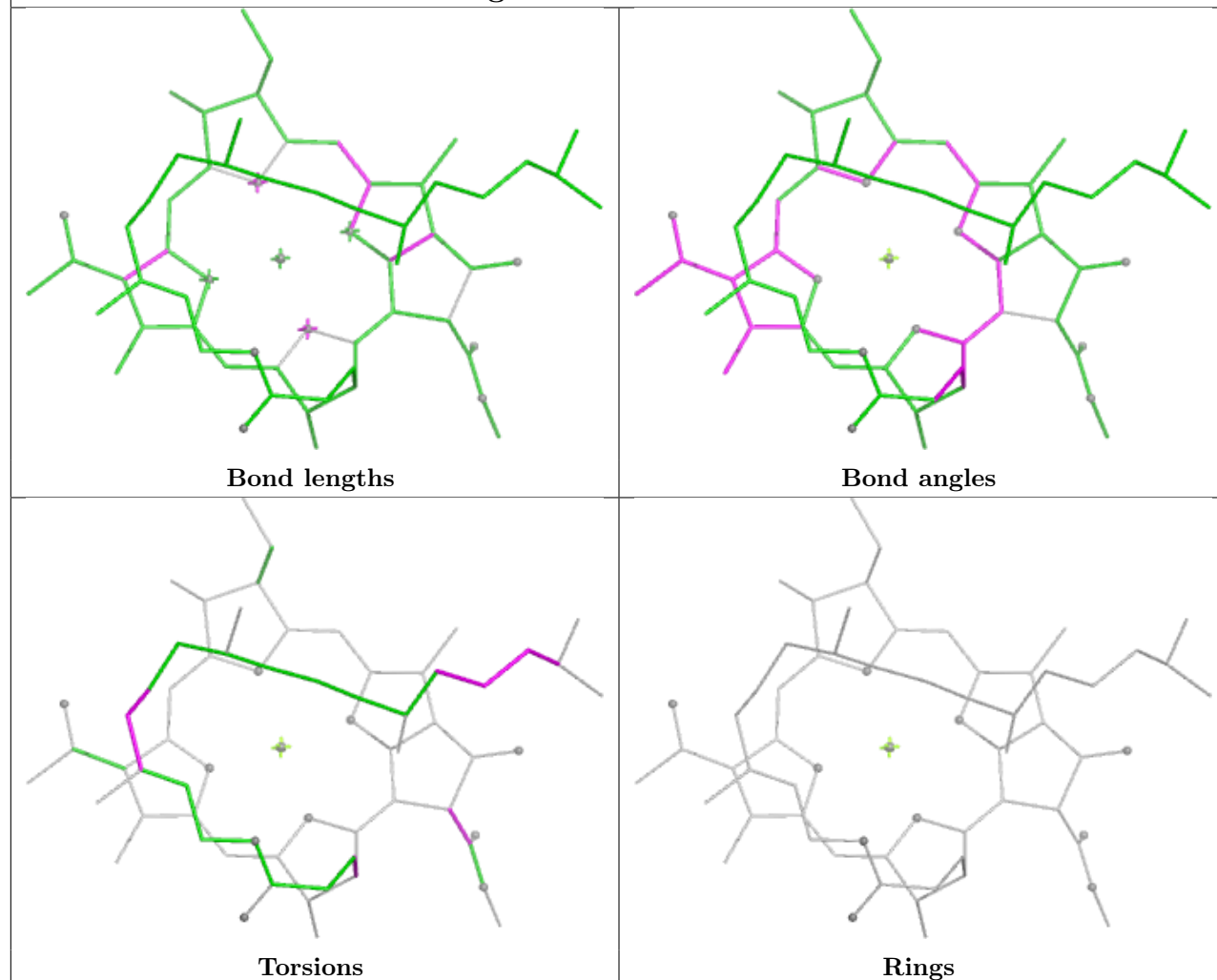




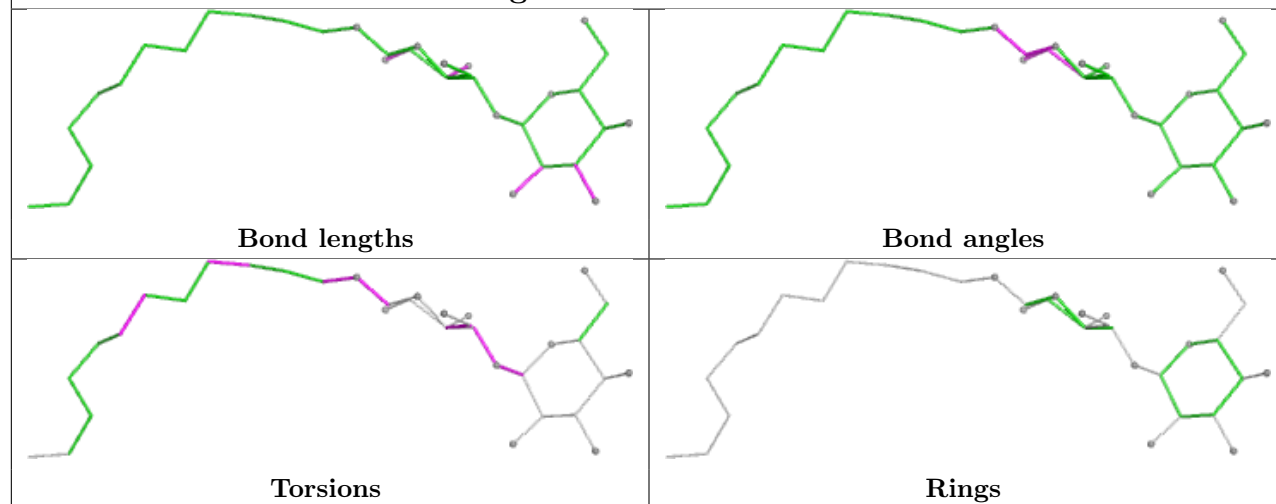


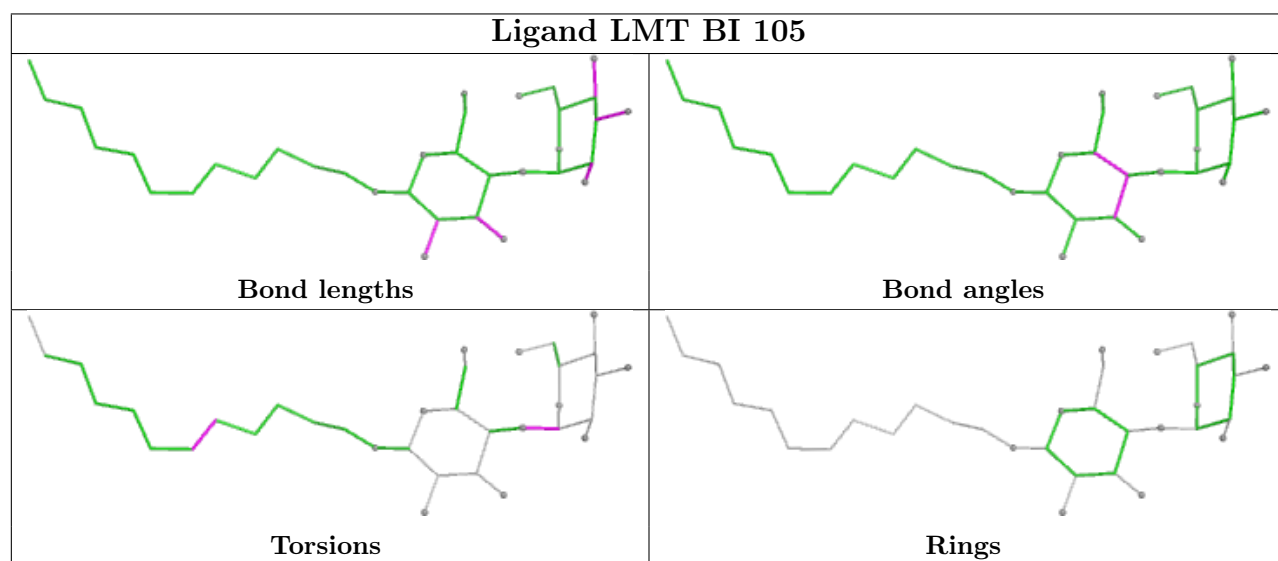
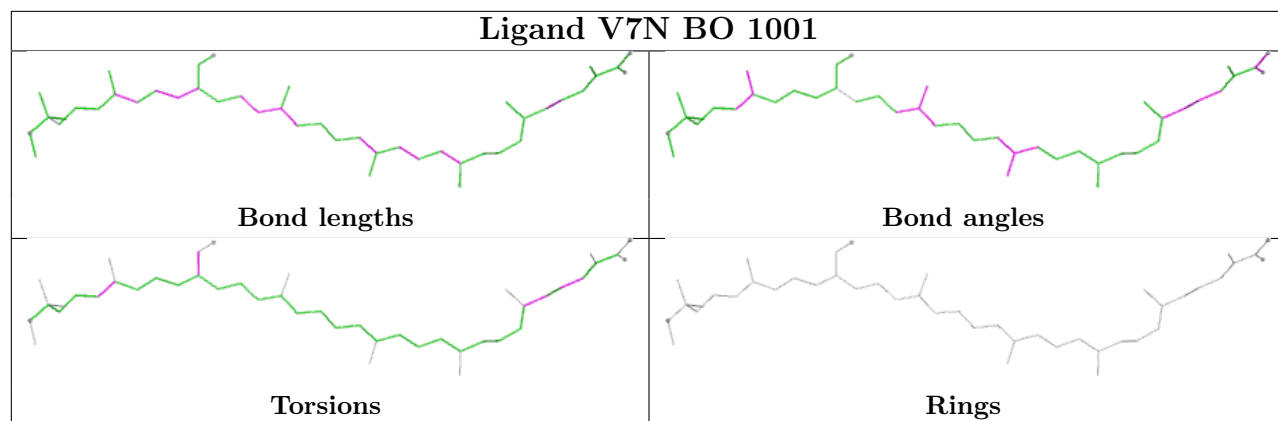


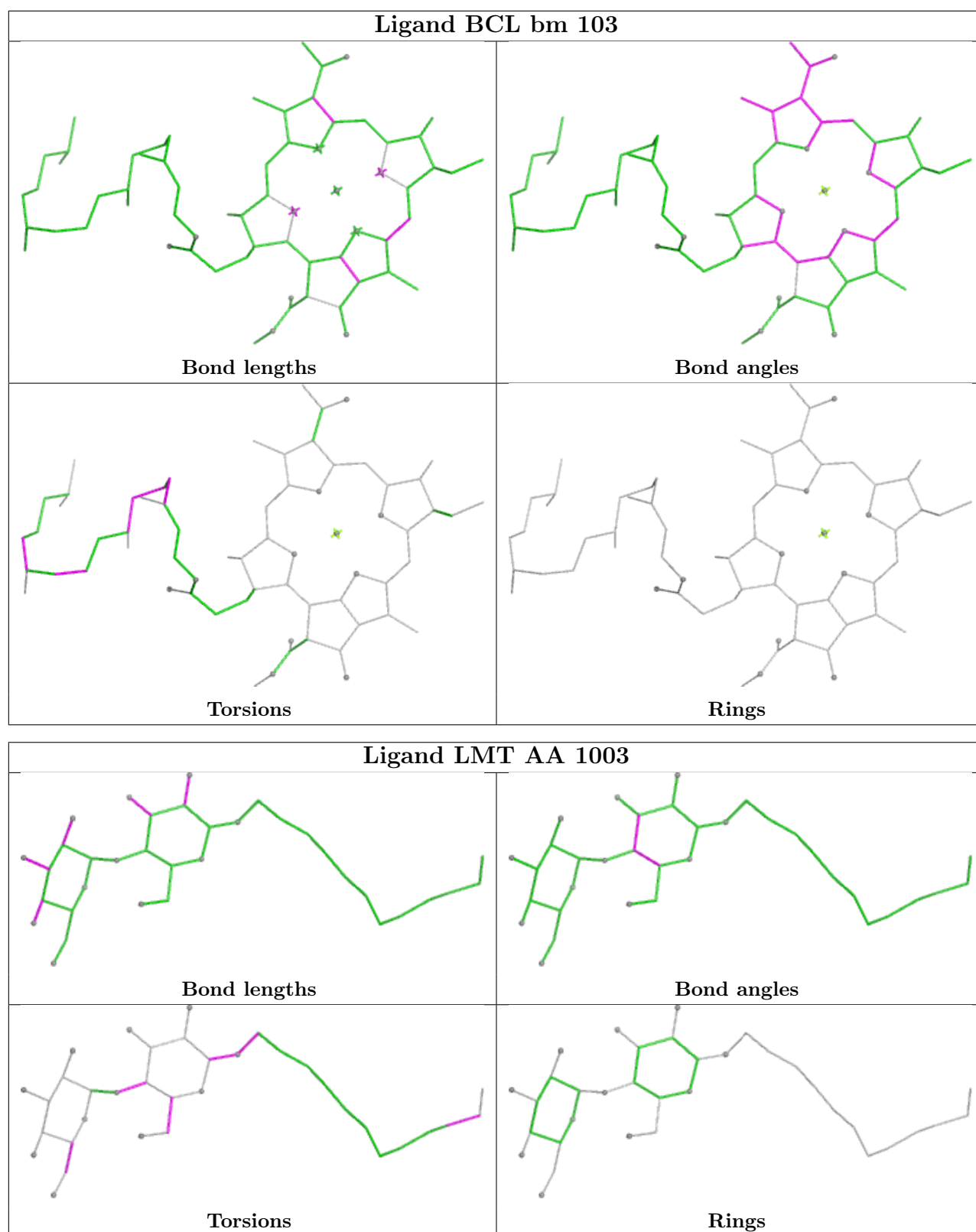
Ligand BCL AE 1001



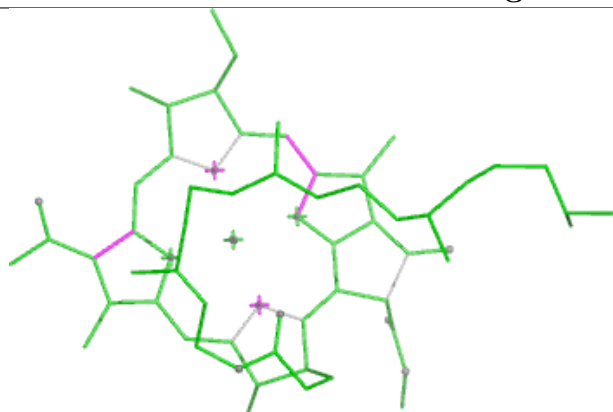
Ligand LMT BL 1002



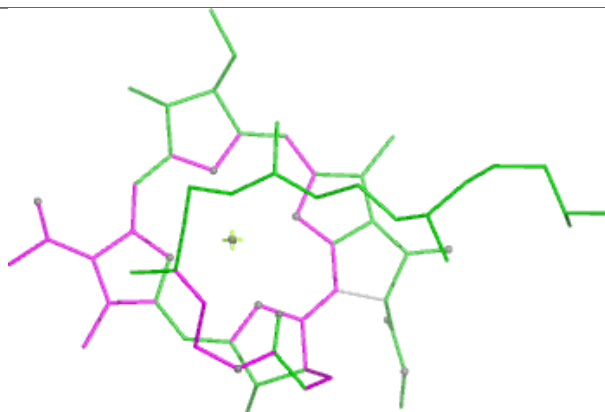




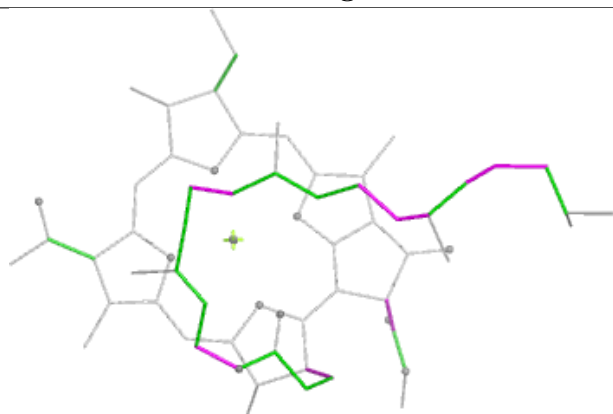
Ligand BCL AJ 102



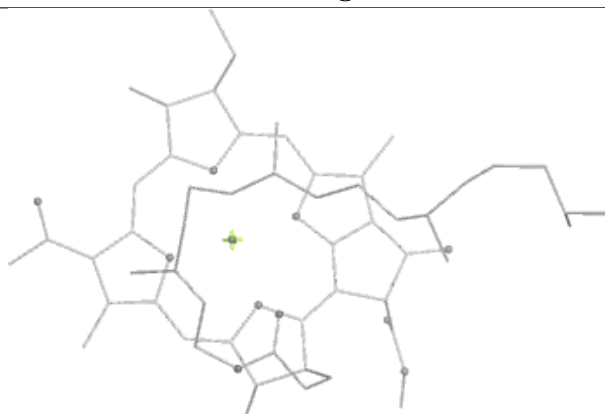
Bond lengths



Bond angles

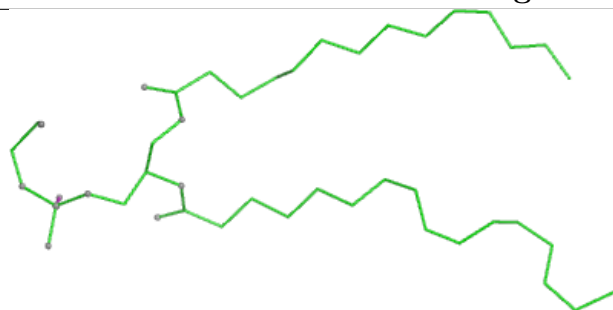


Torsions

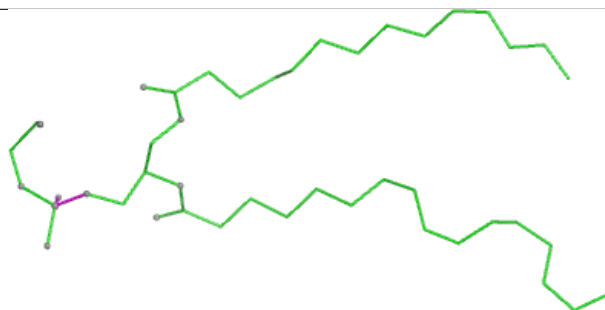


Rings

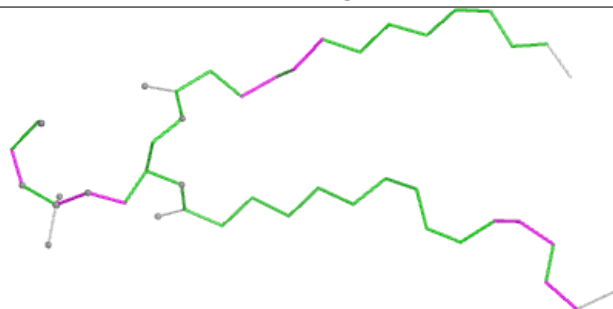
Ligand 0V9 bo 104



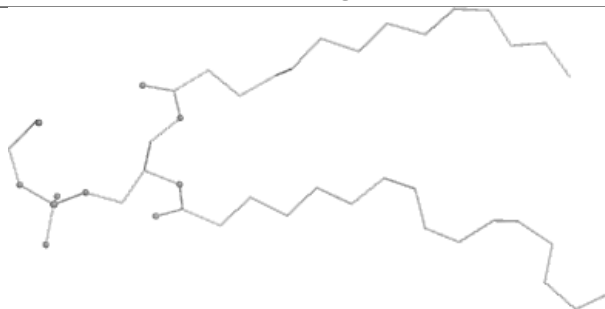
Bond lengths



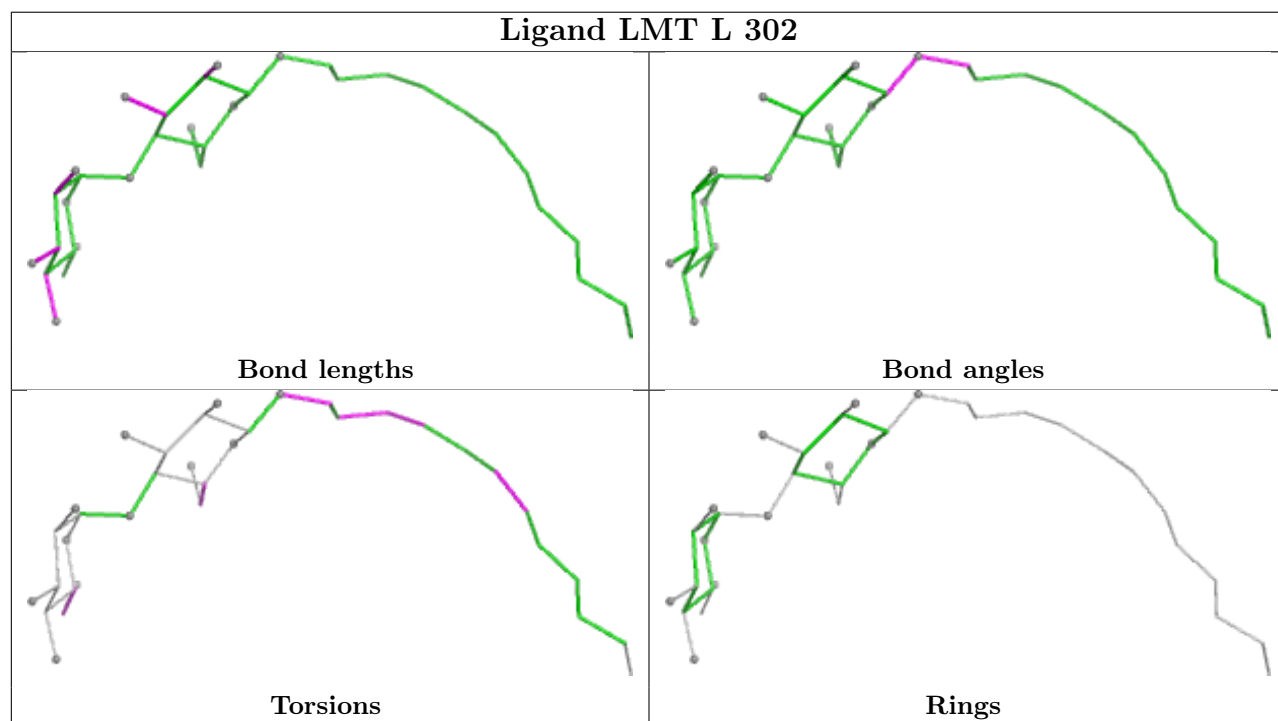
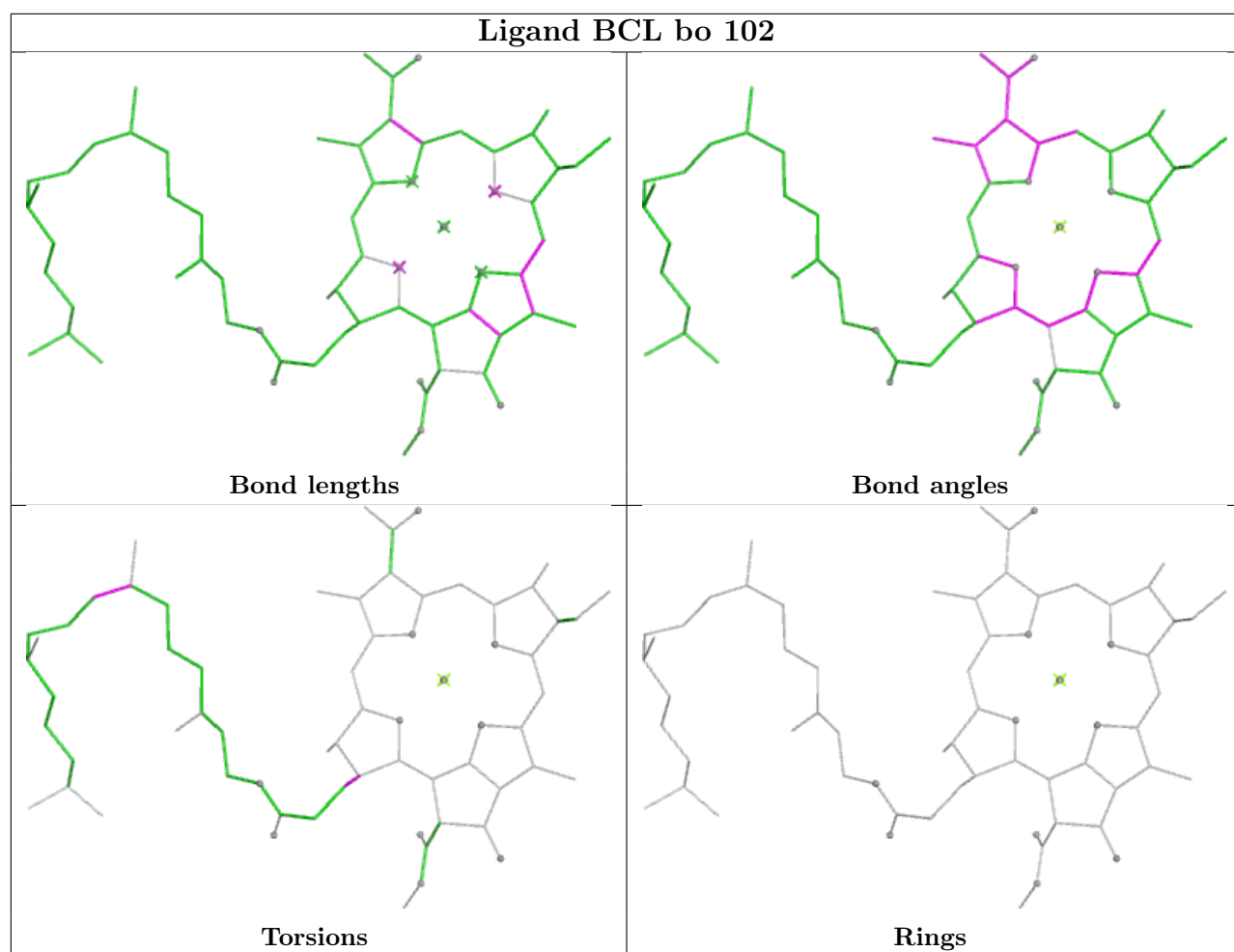
Bond angles

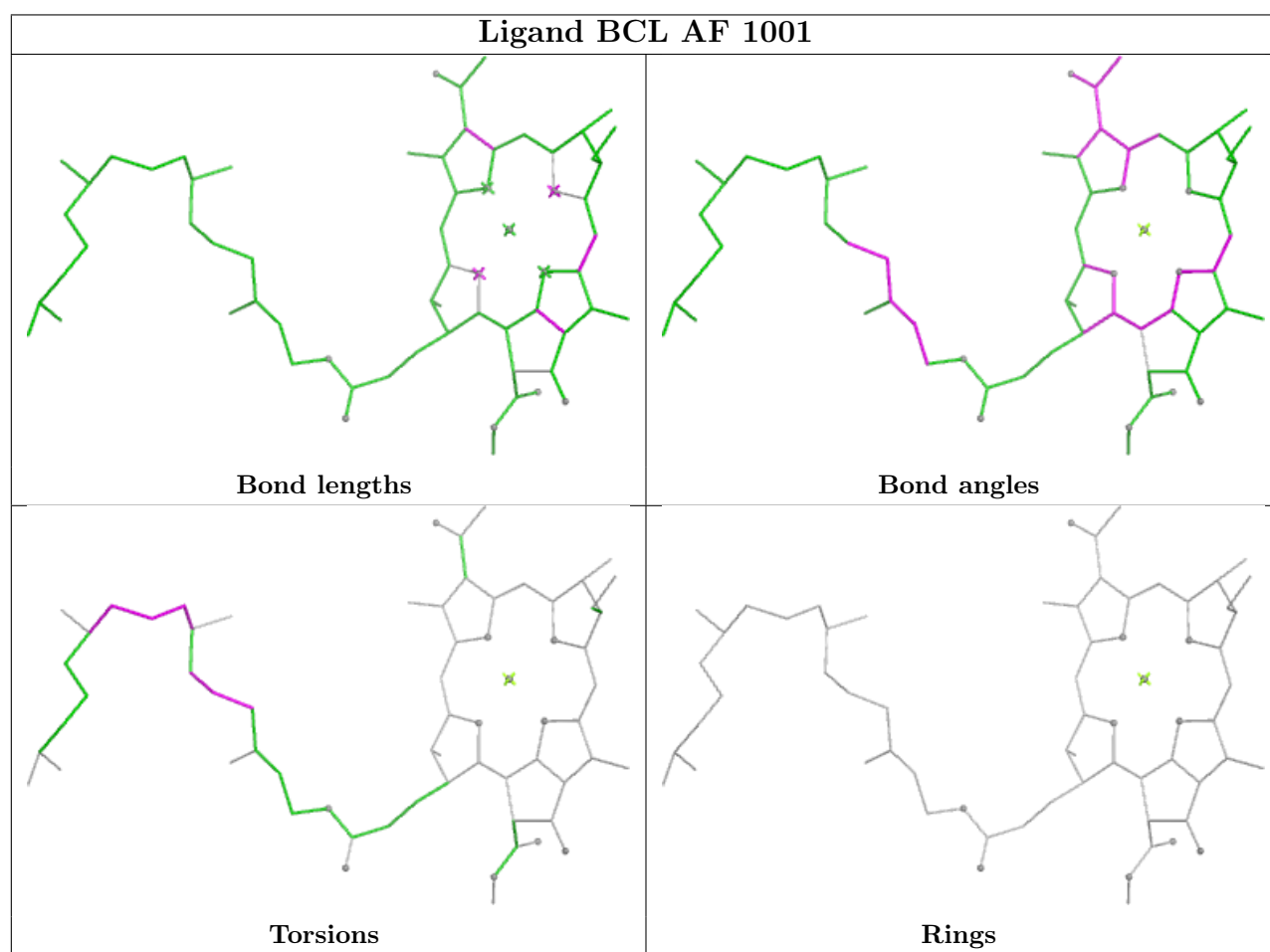
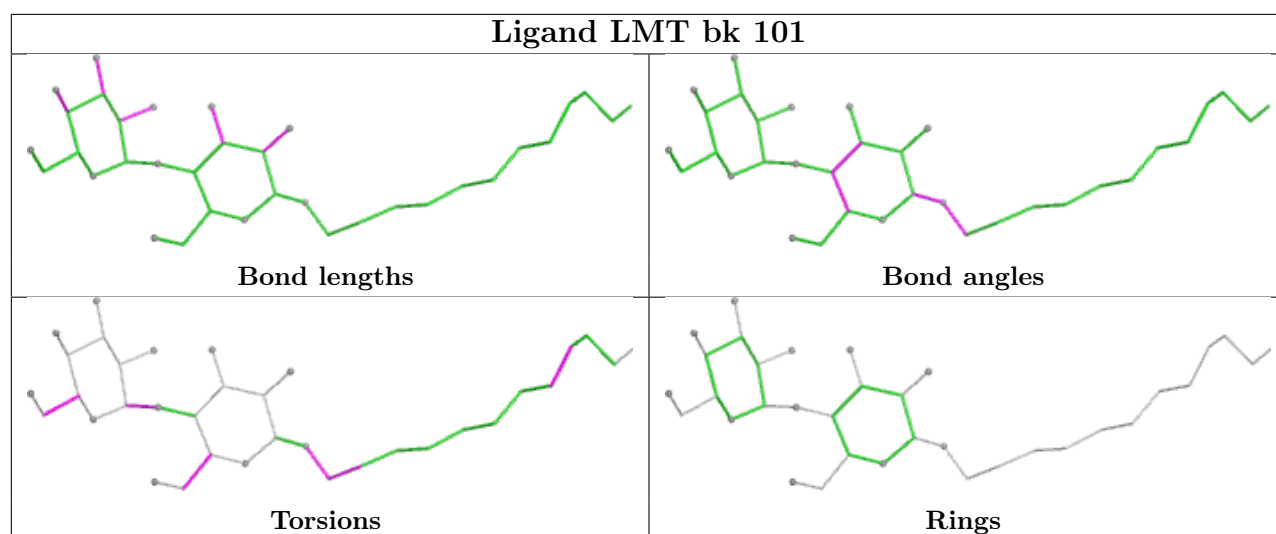


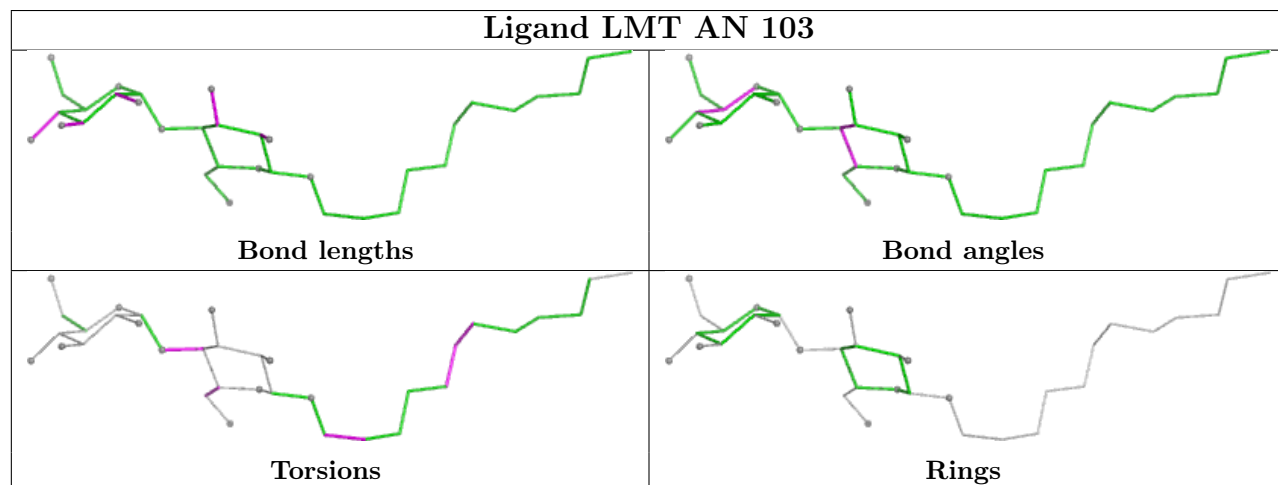
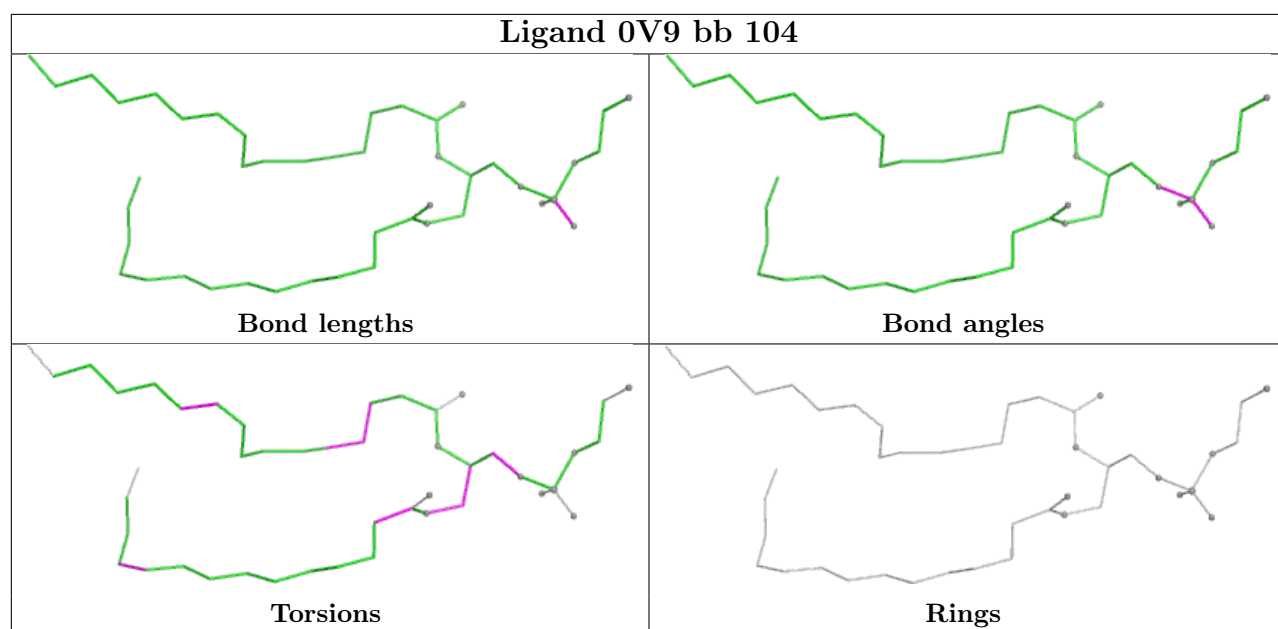
Torsions

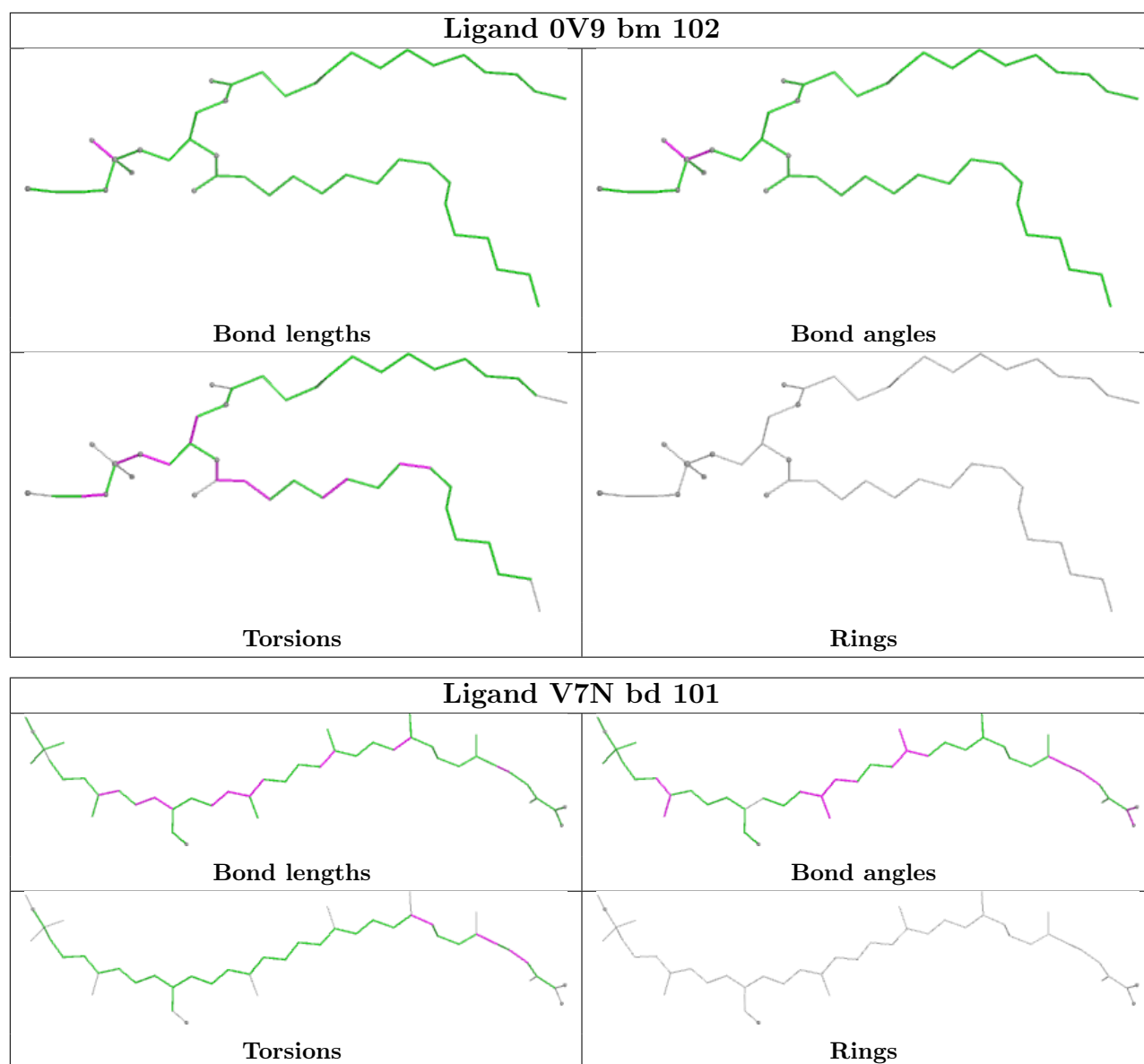


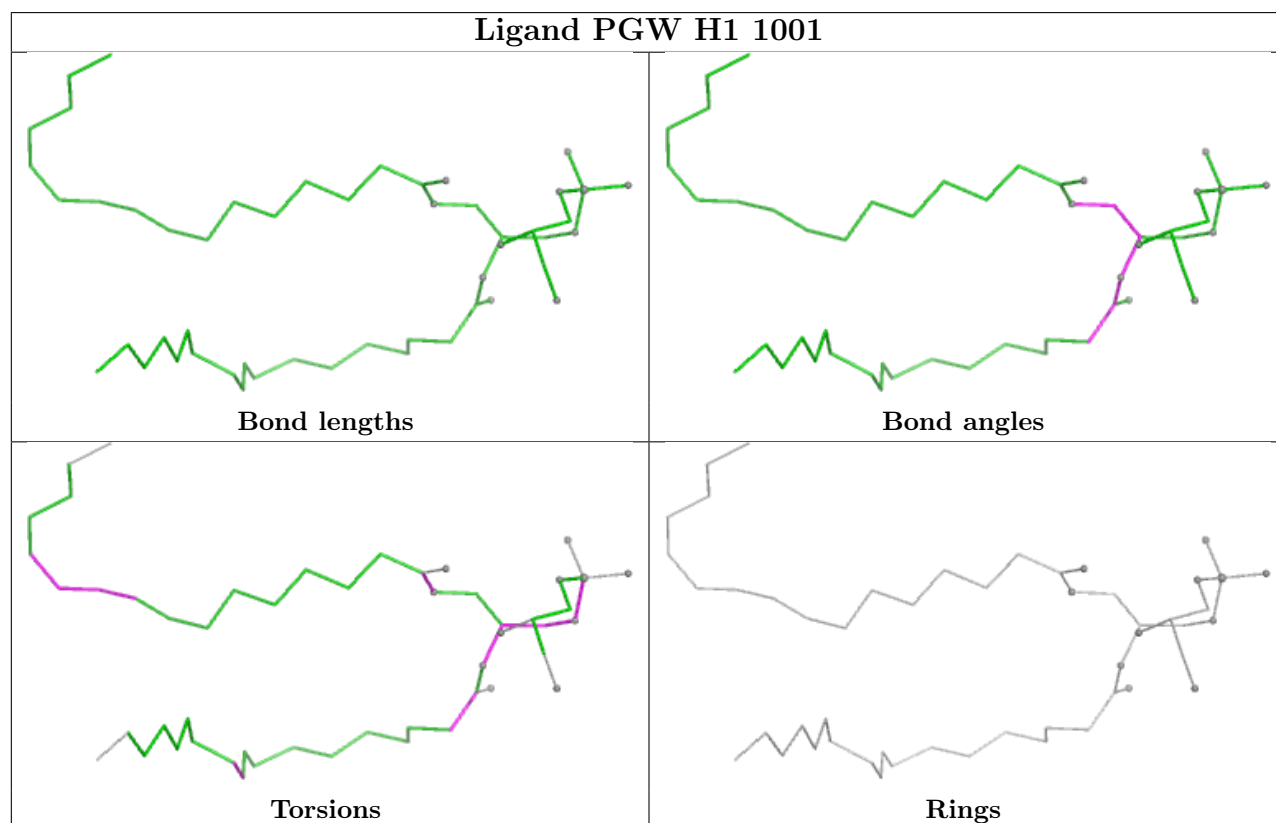
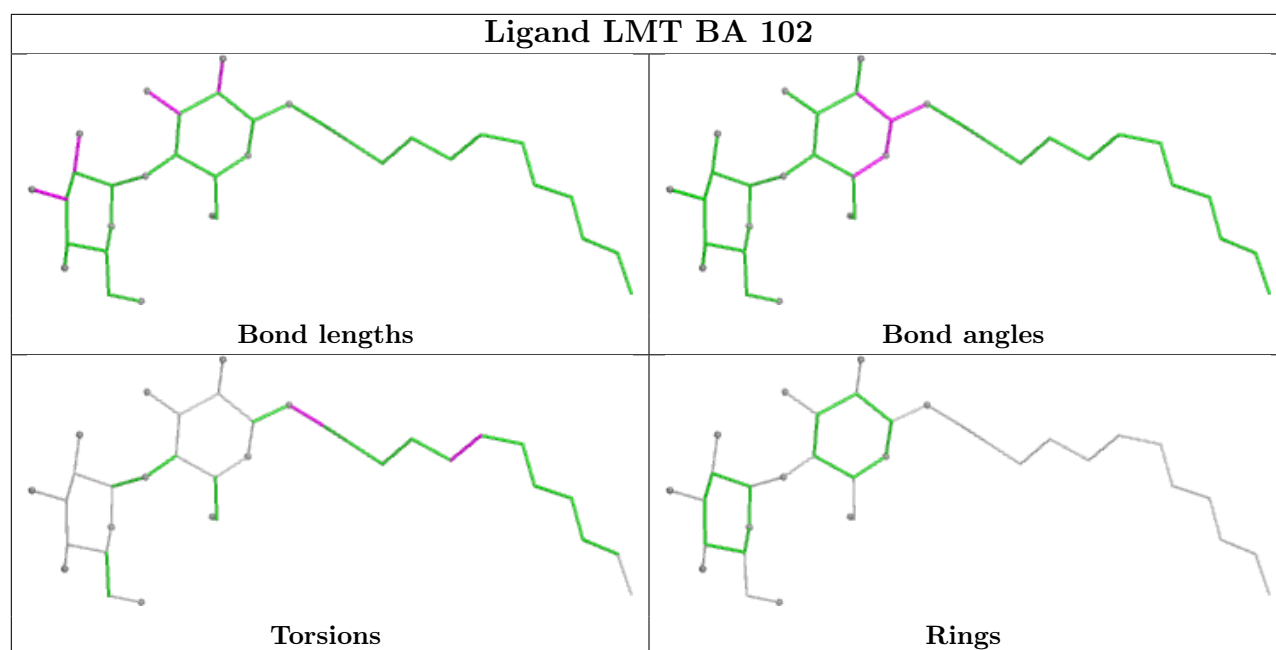
Rings

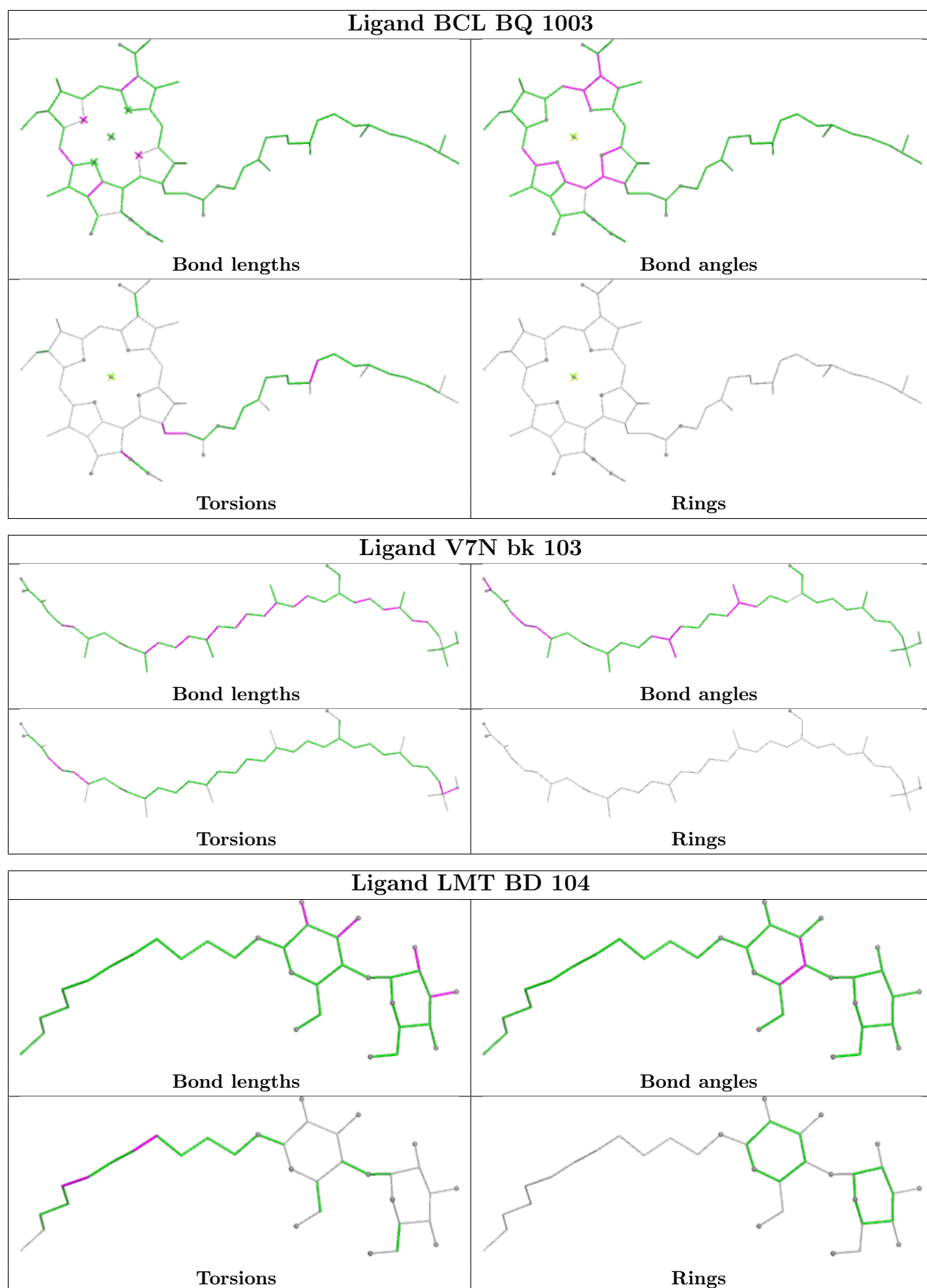




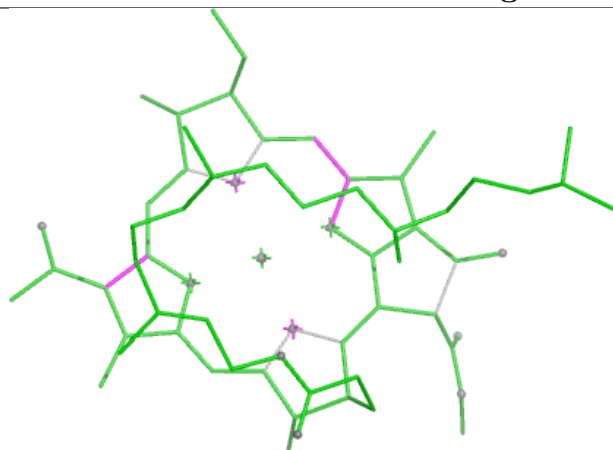




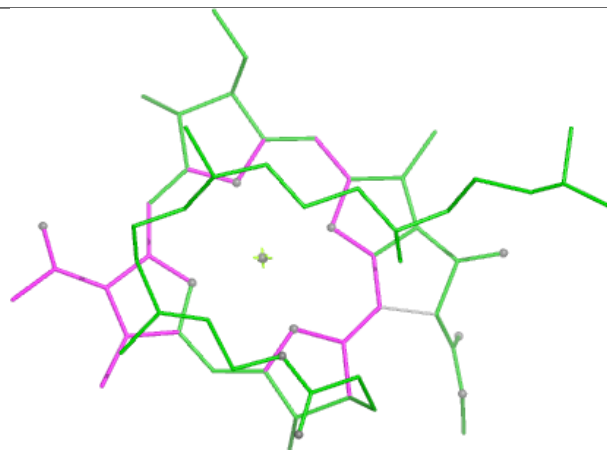




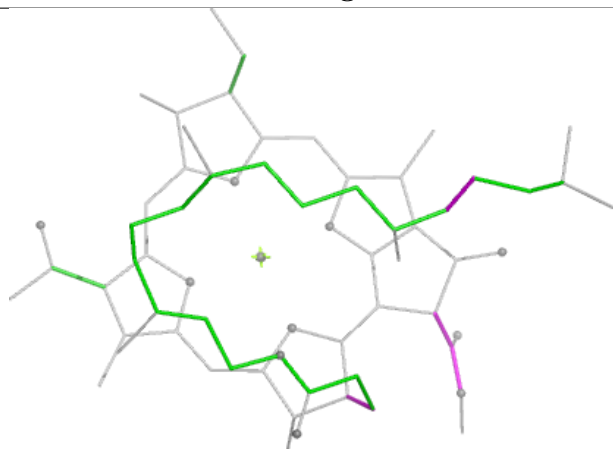
Ligand BCL AN 102



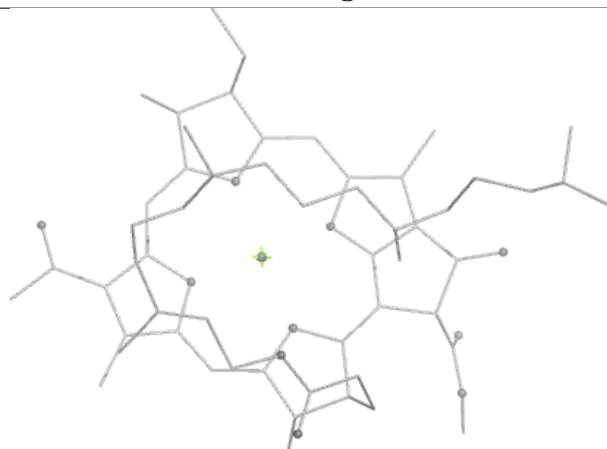
Bond lengths



Bond angles

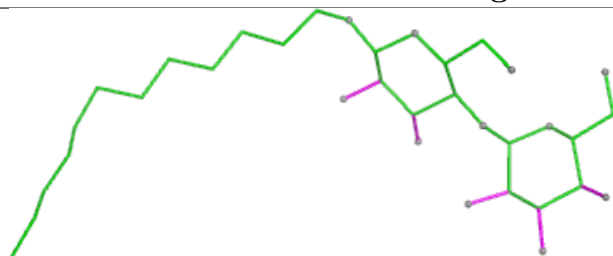


Torsions

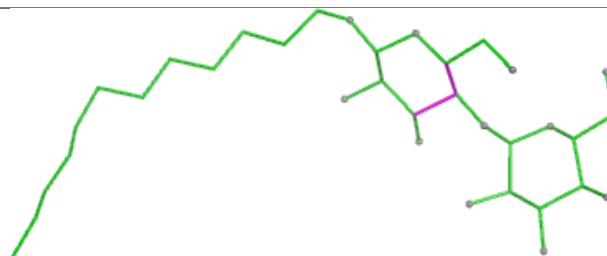


Rings

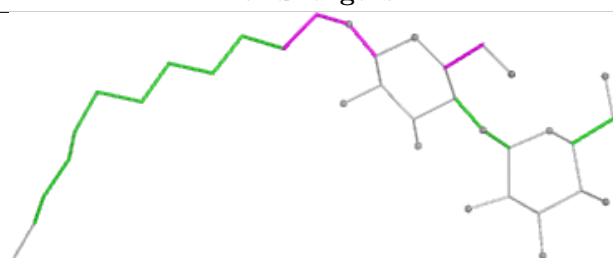
Ligand LMT BP 1003



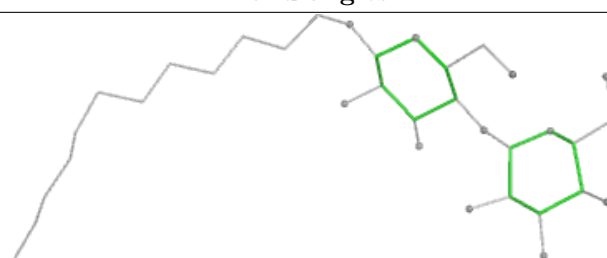
Bond lengths



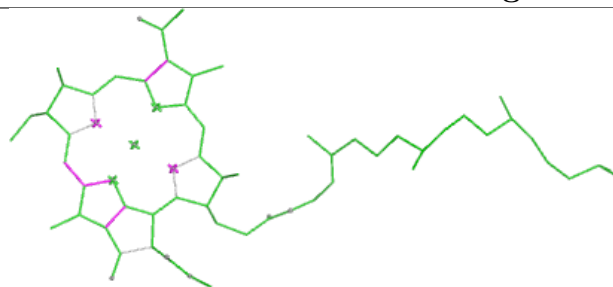
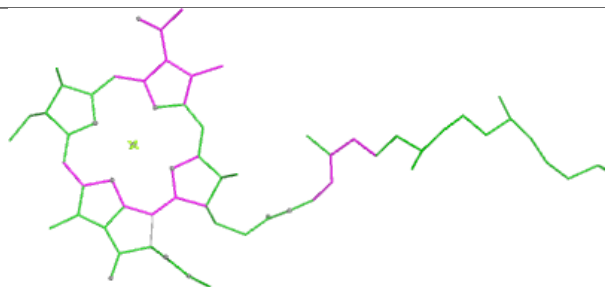
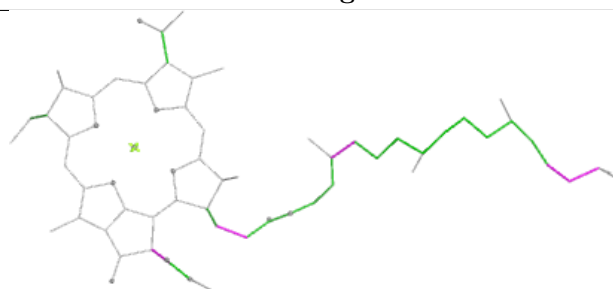
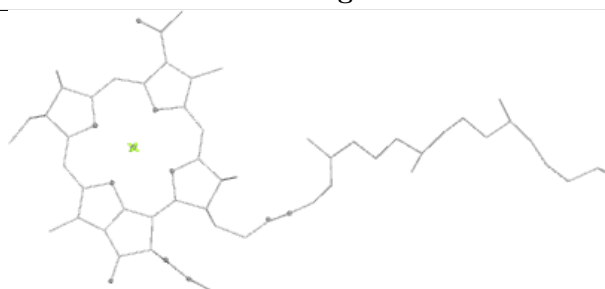
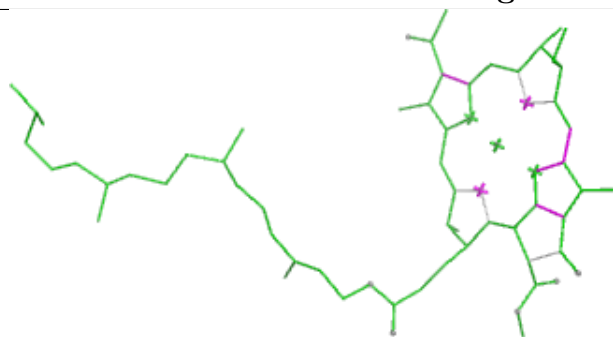
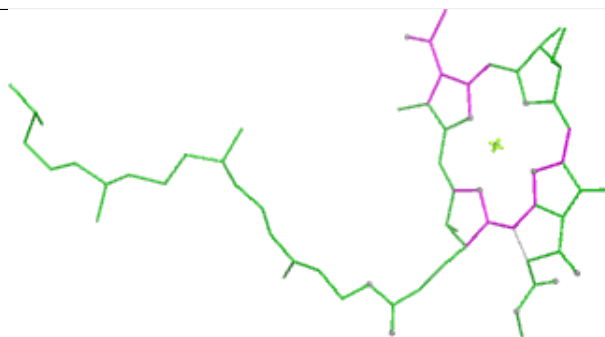
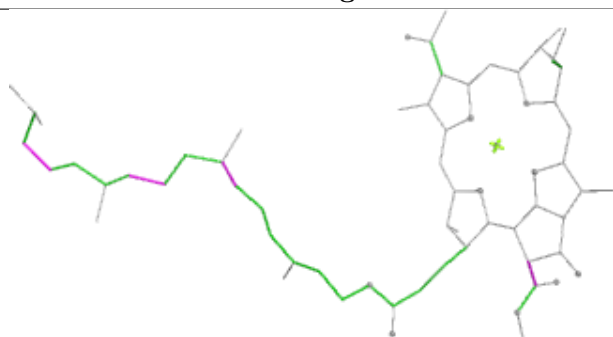
Bond angles

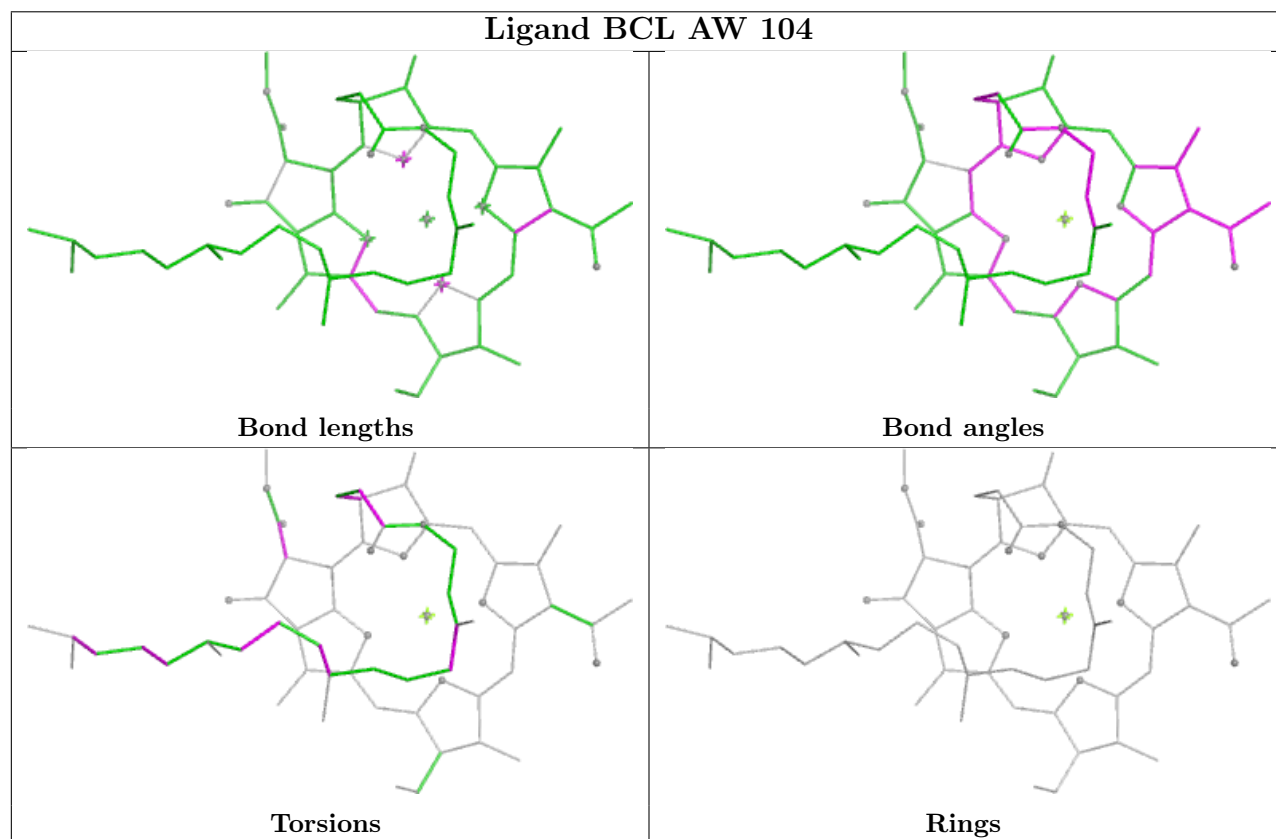
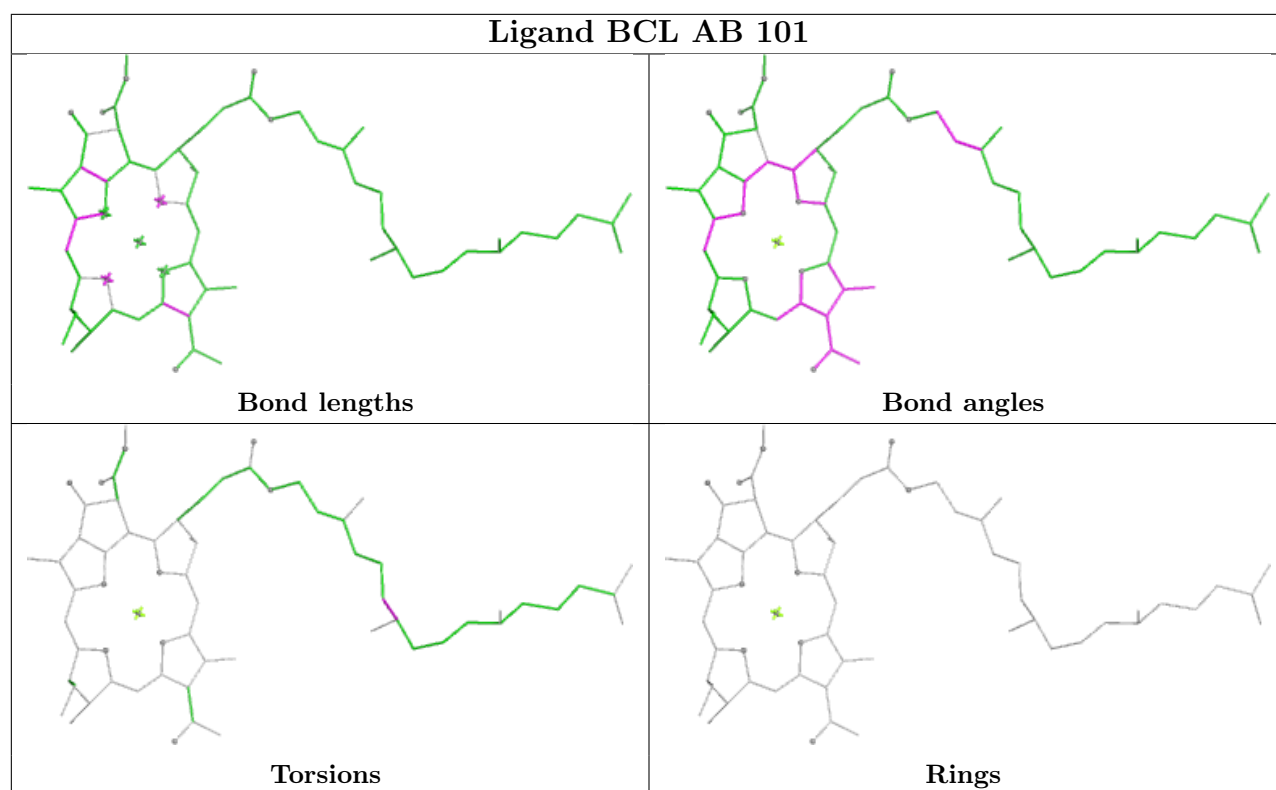


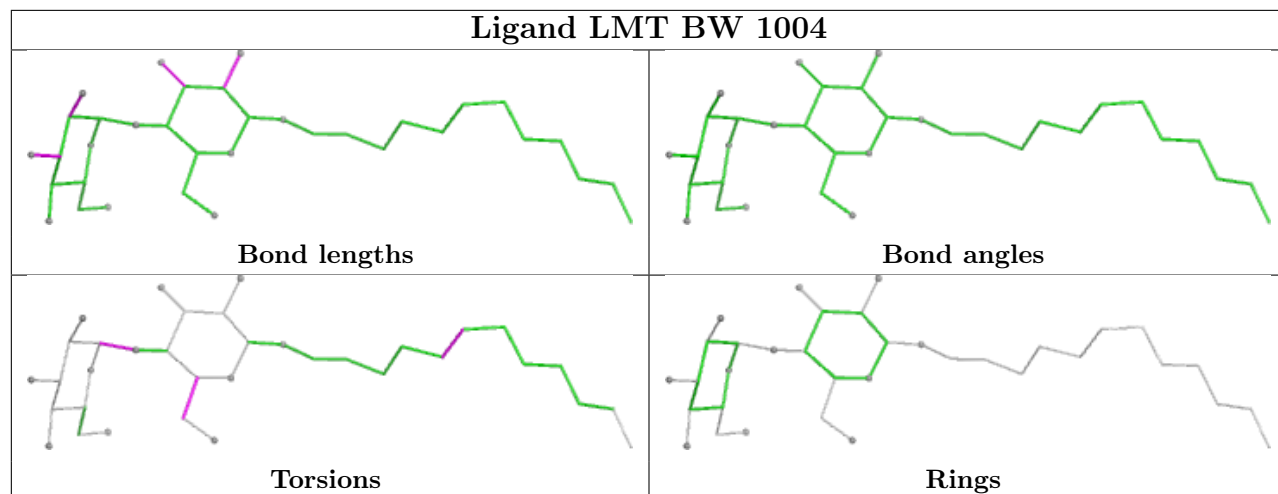
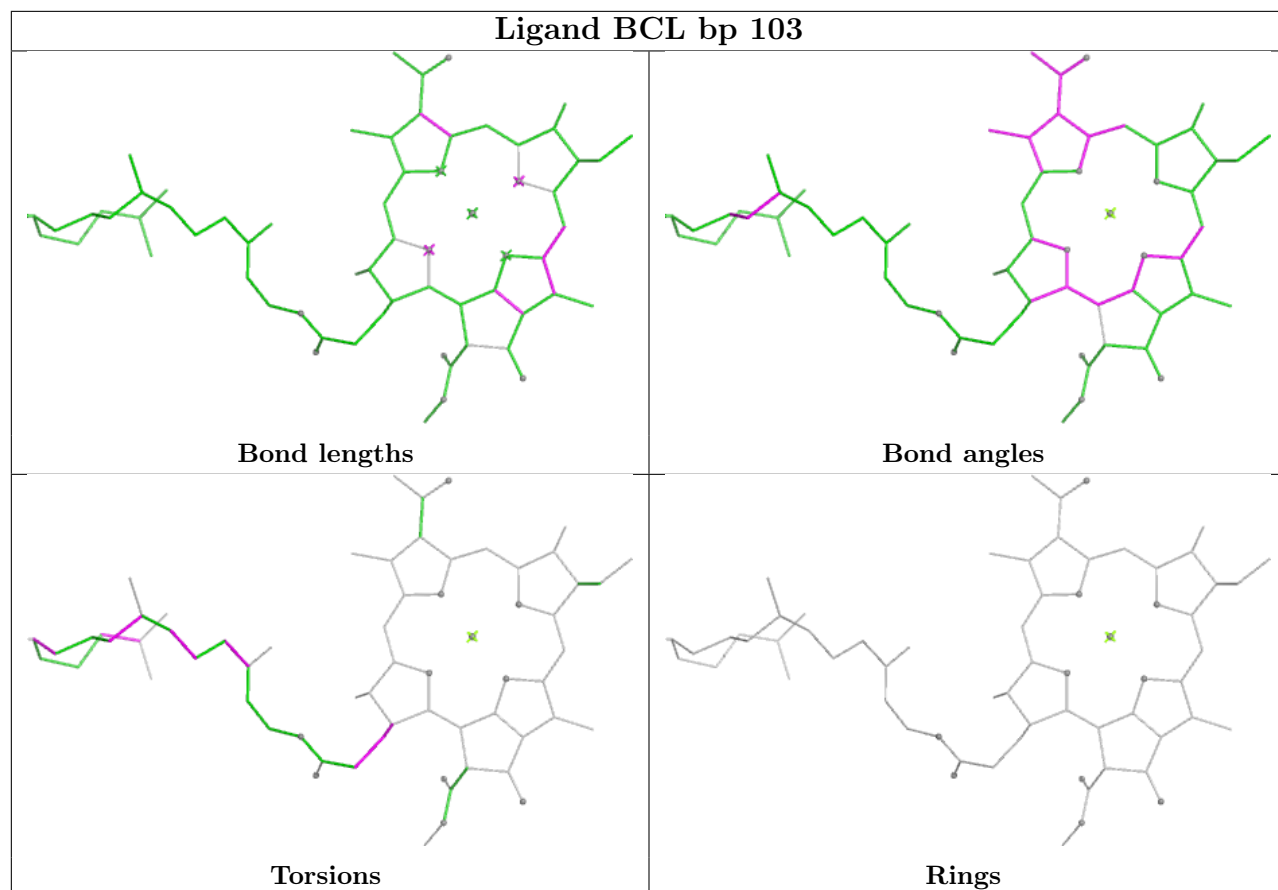
Torsions



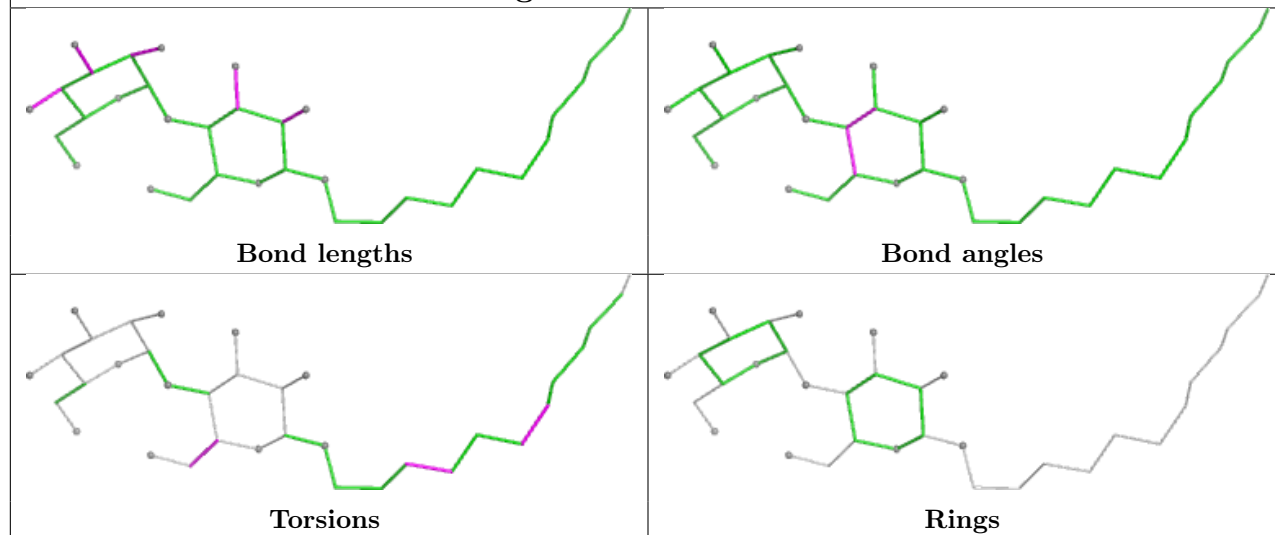
Rings

Ligand BCL BB 104**Bond lengths****Bond angles****Torsions****Rings****Ligand BCL AM 102****Bond lengths****Bond angles****Torsions****Rings**

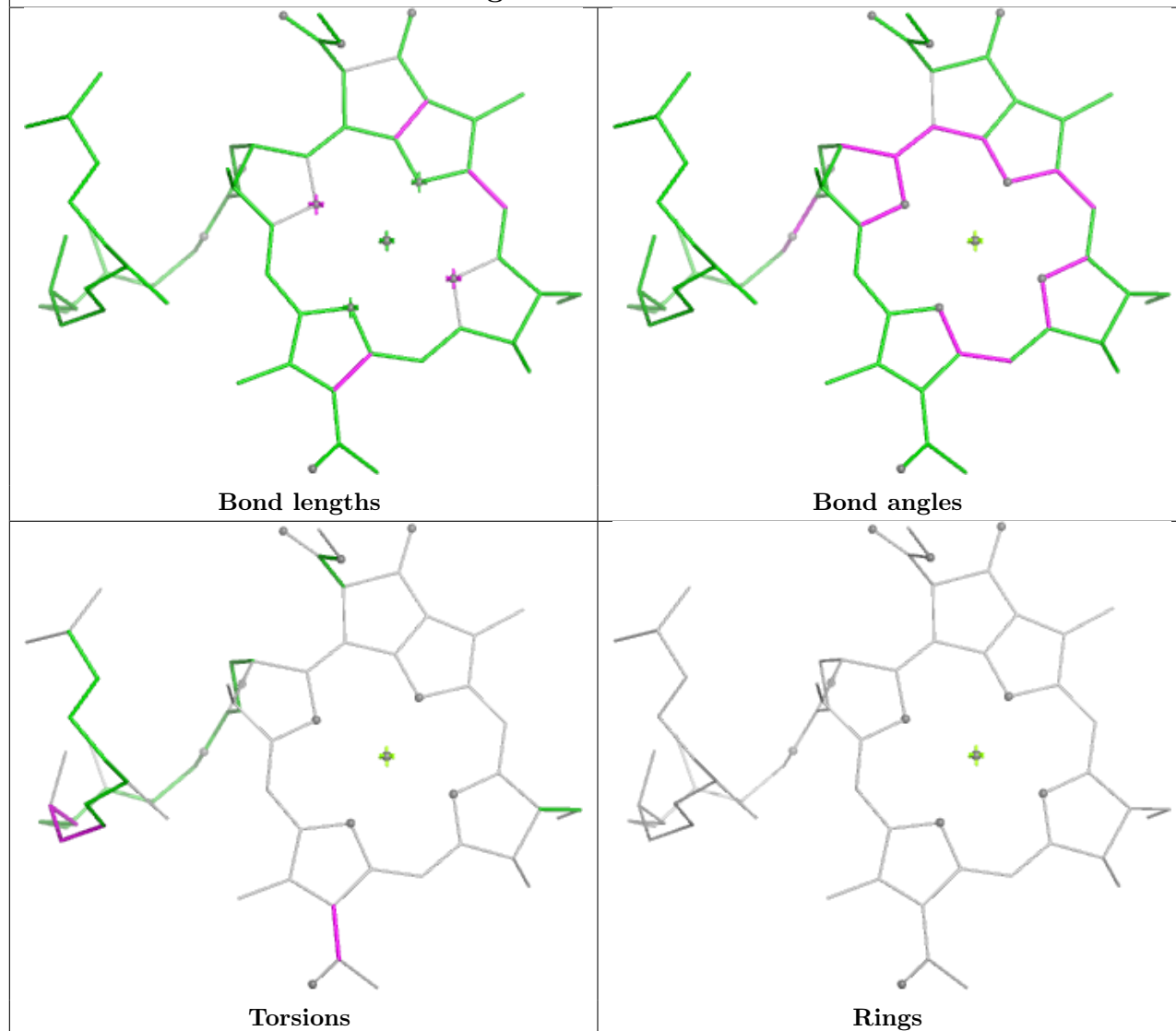


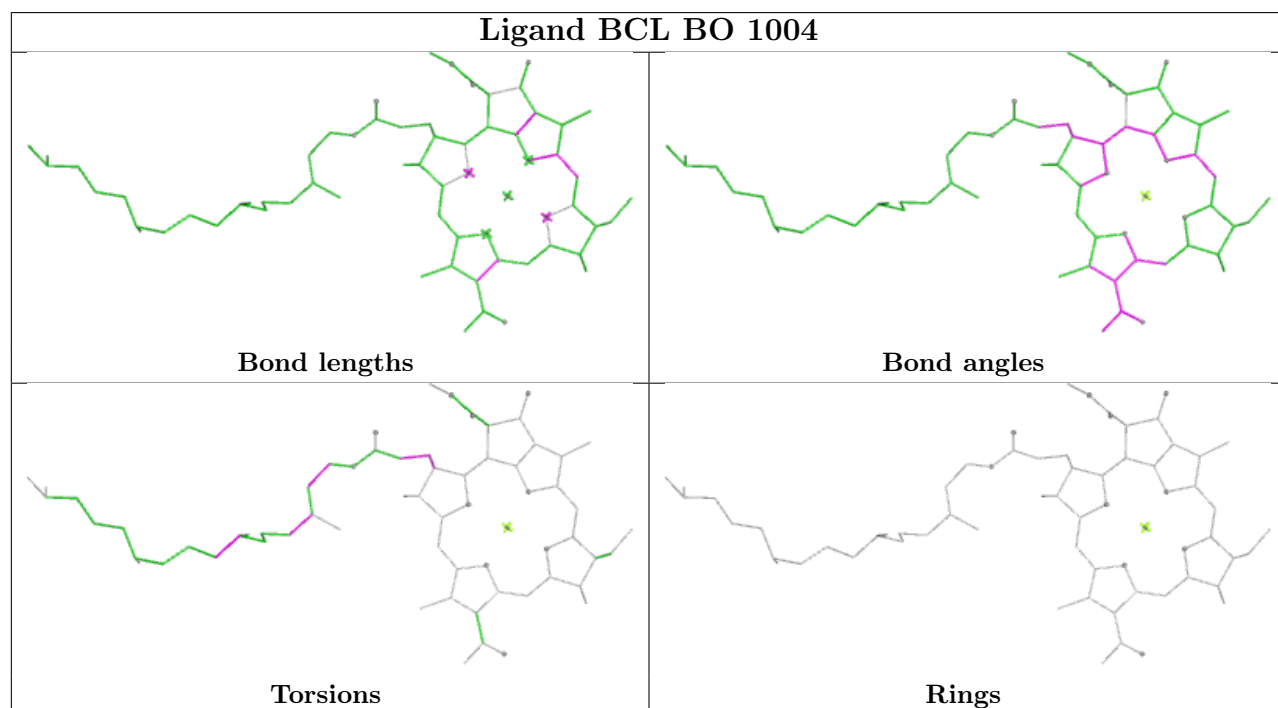
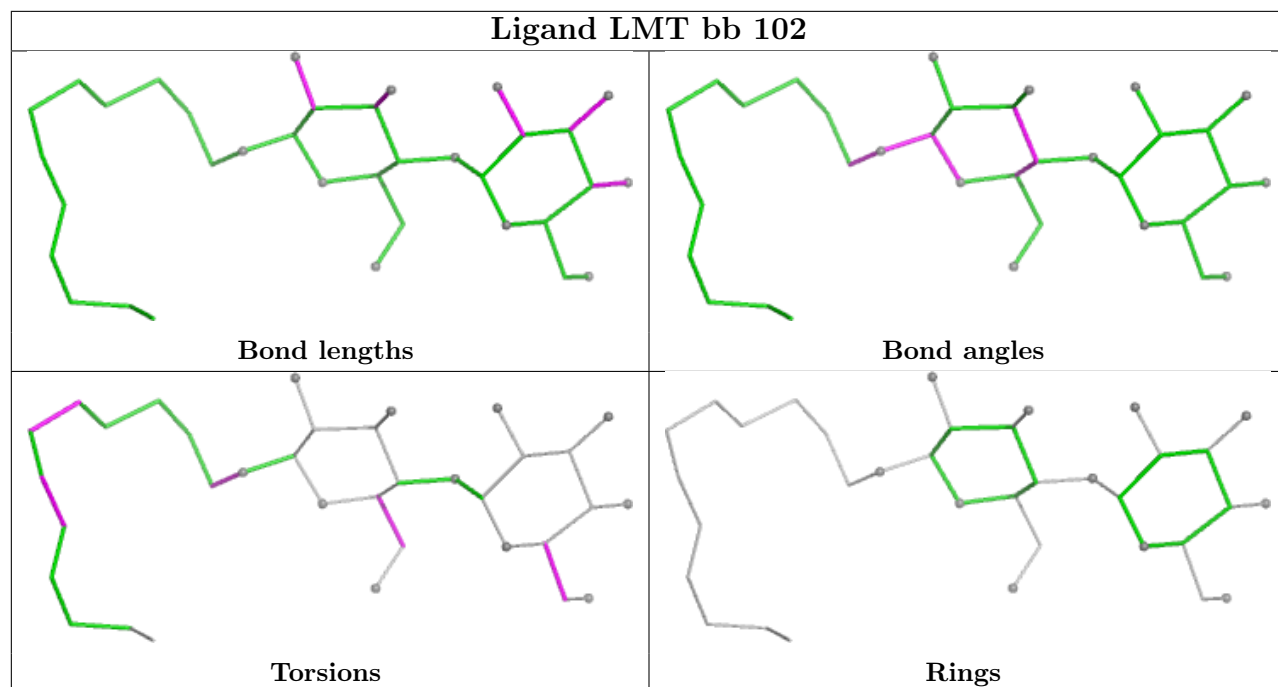


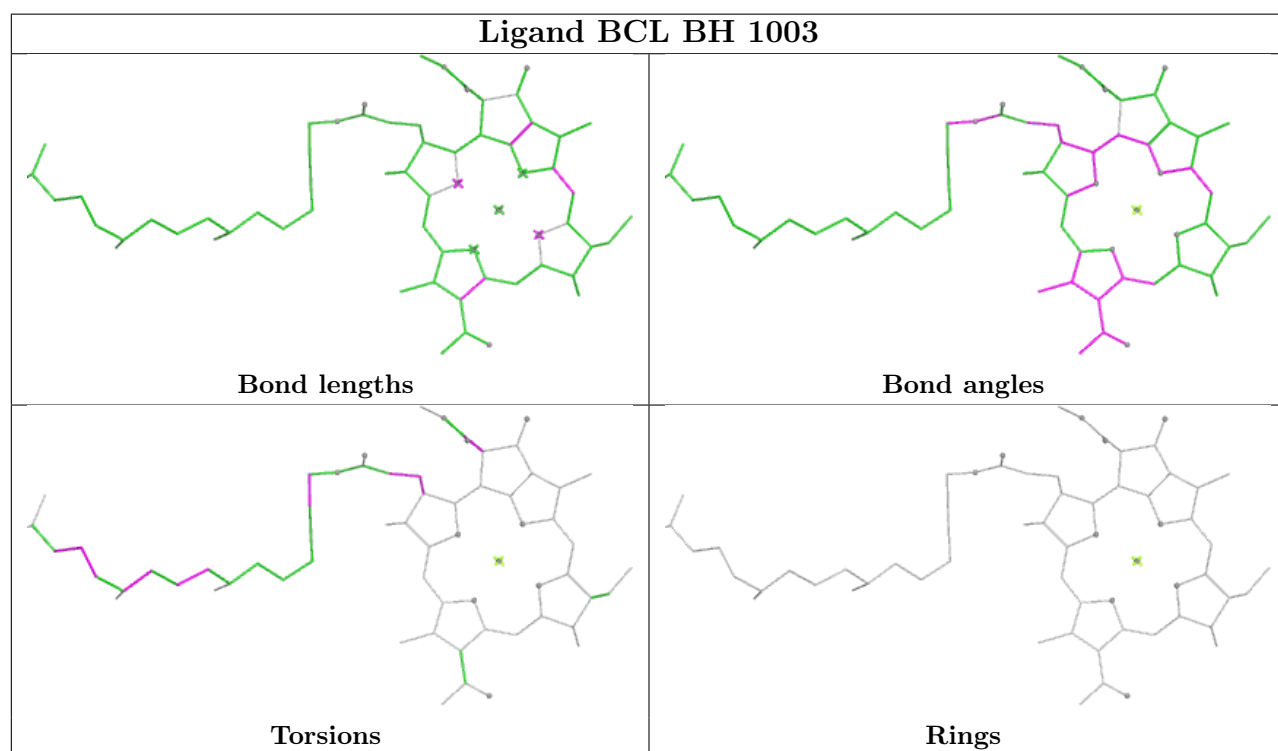
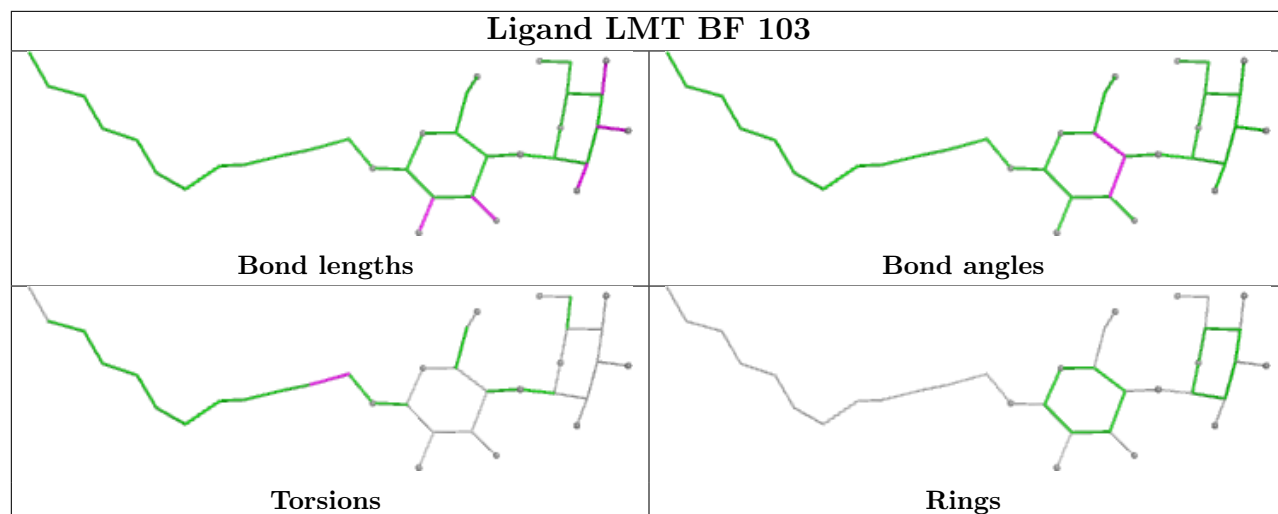
Ligand LMT BB 102

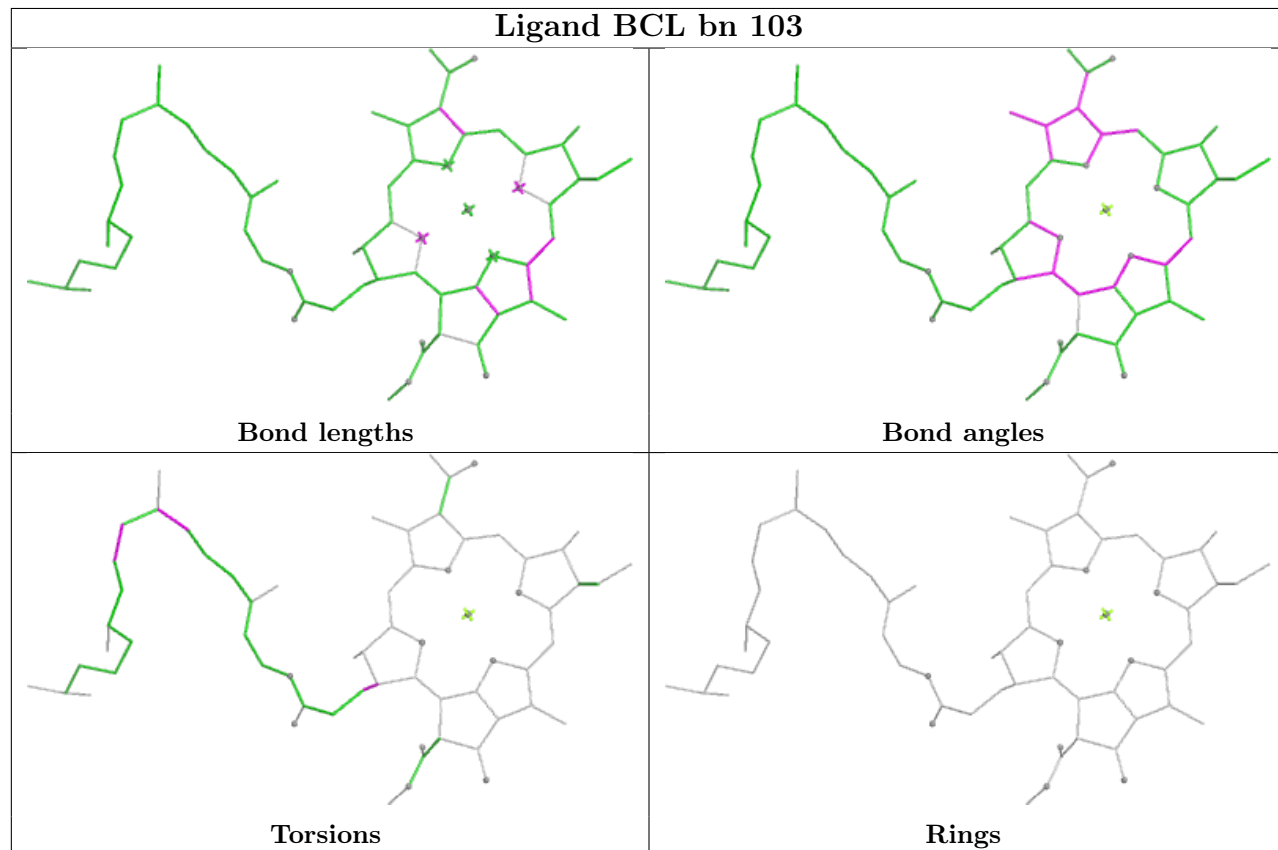
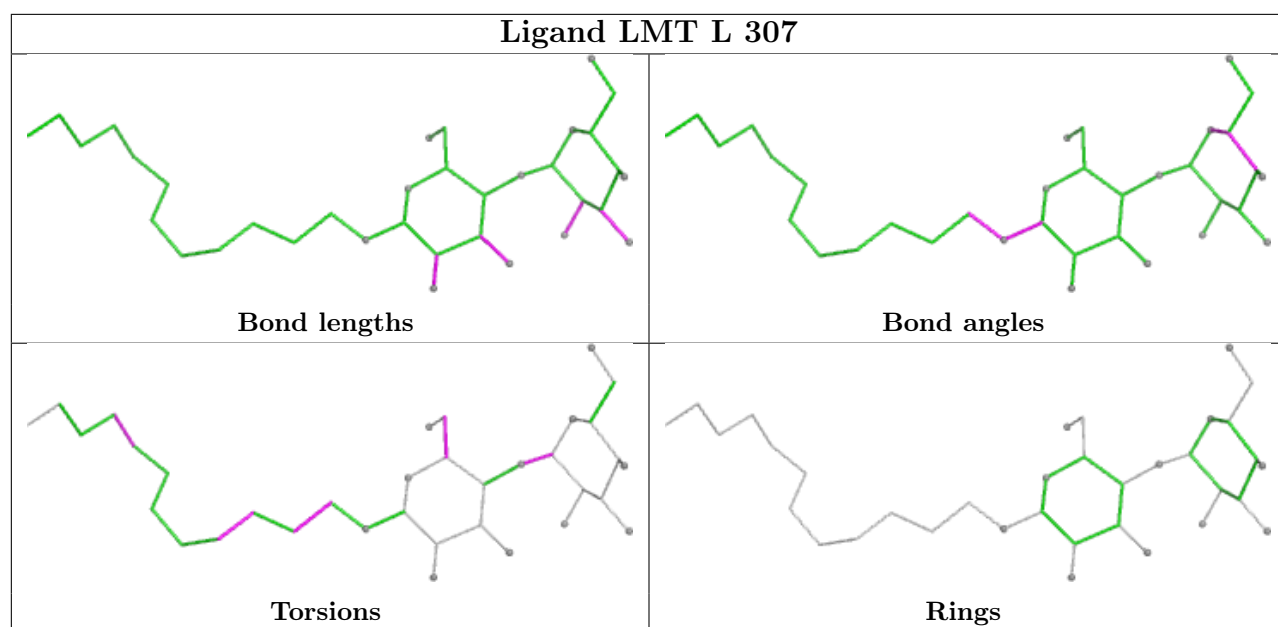


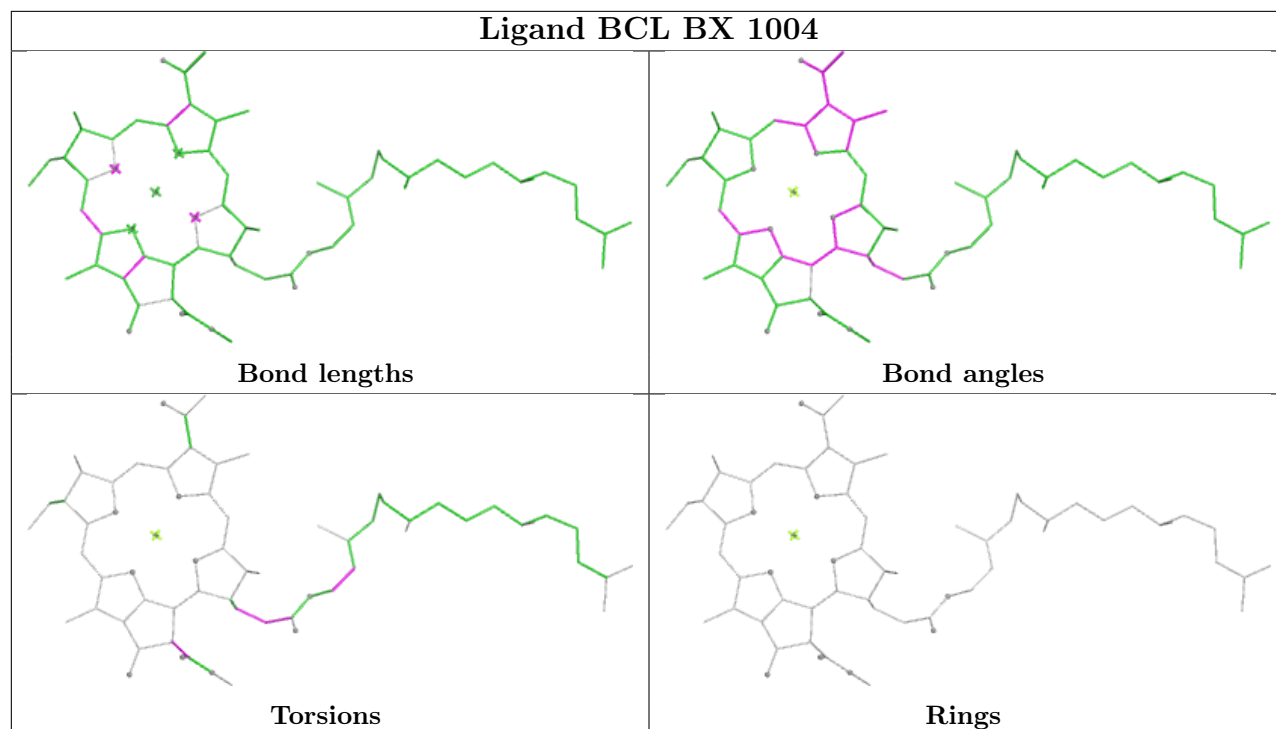
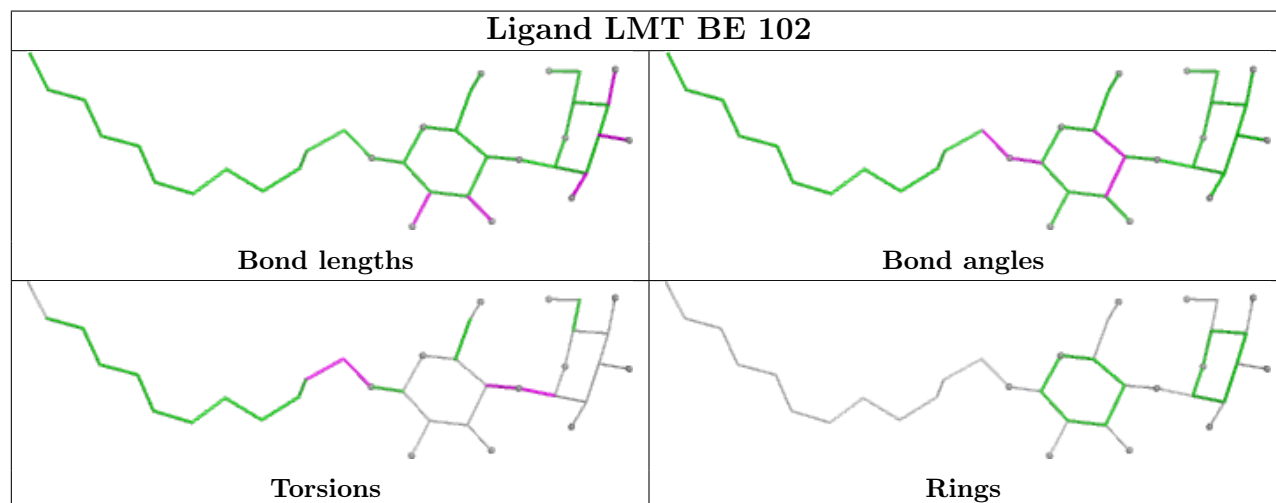
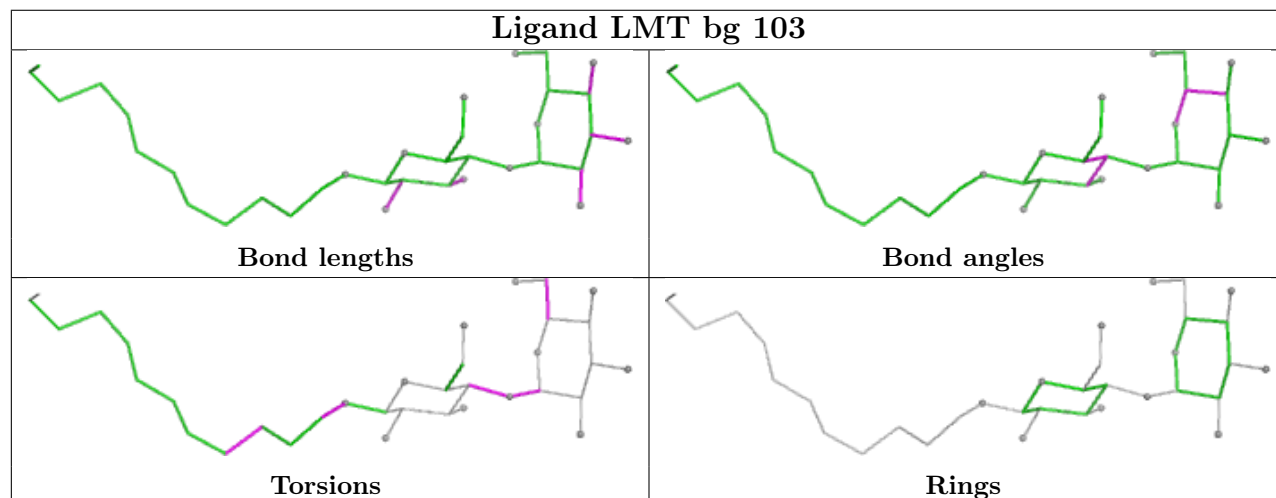
Ligand BCL M 403

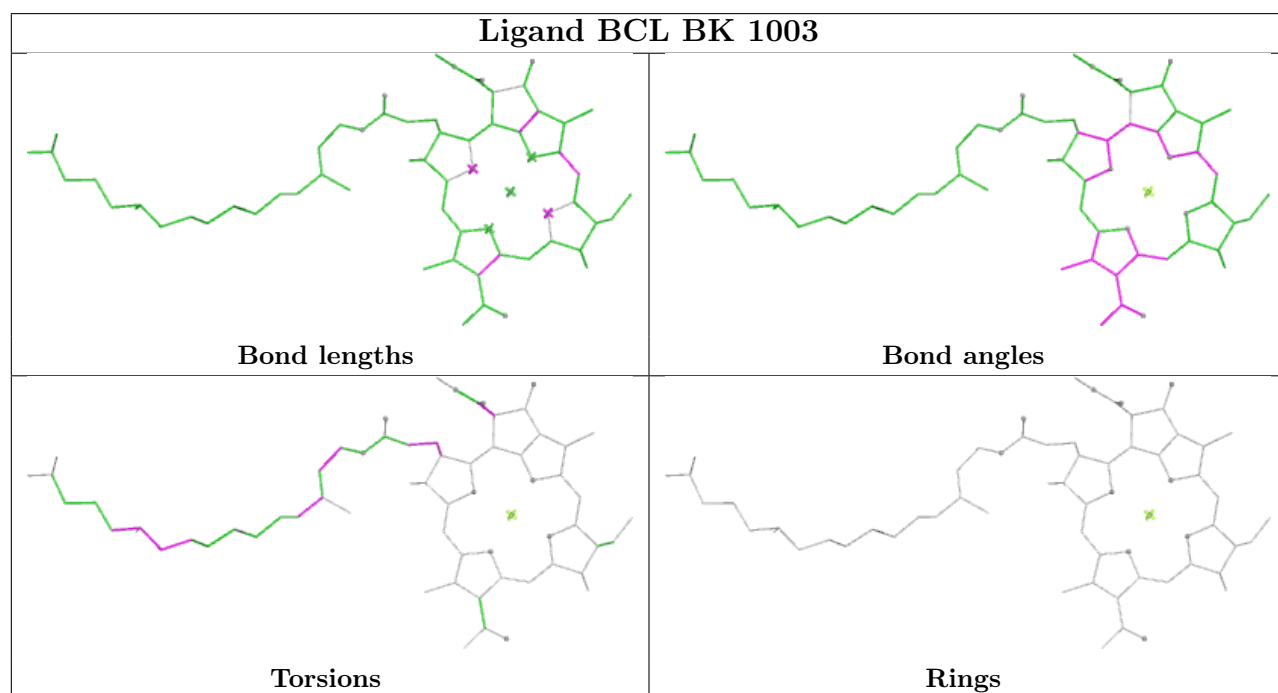
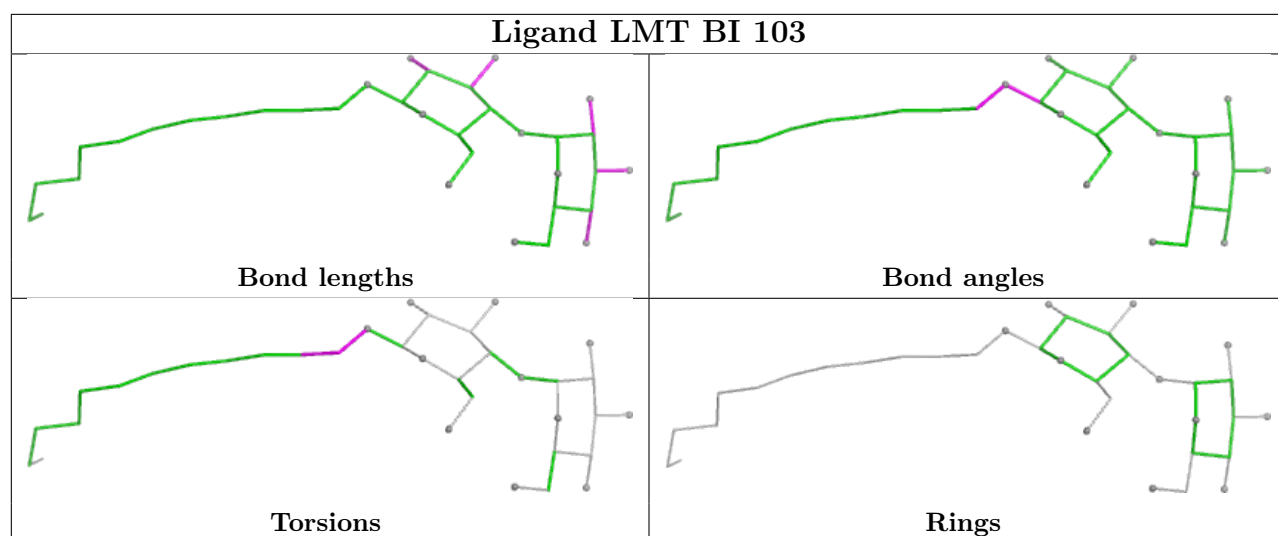


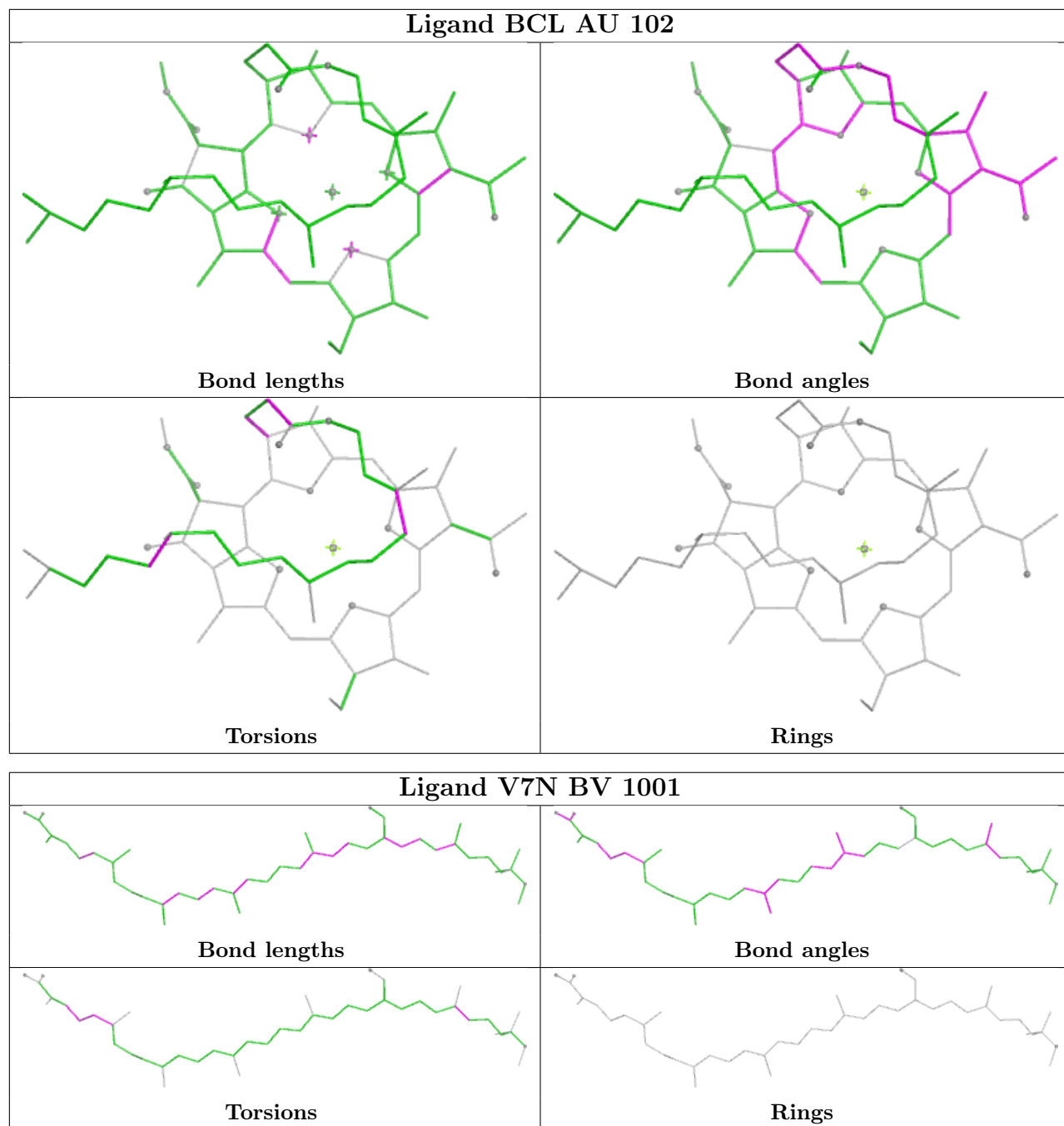


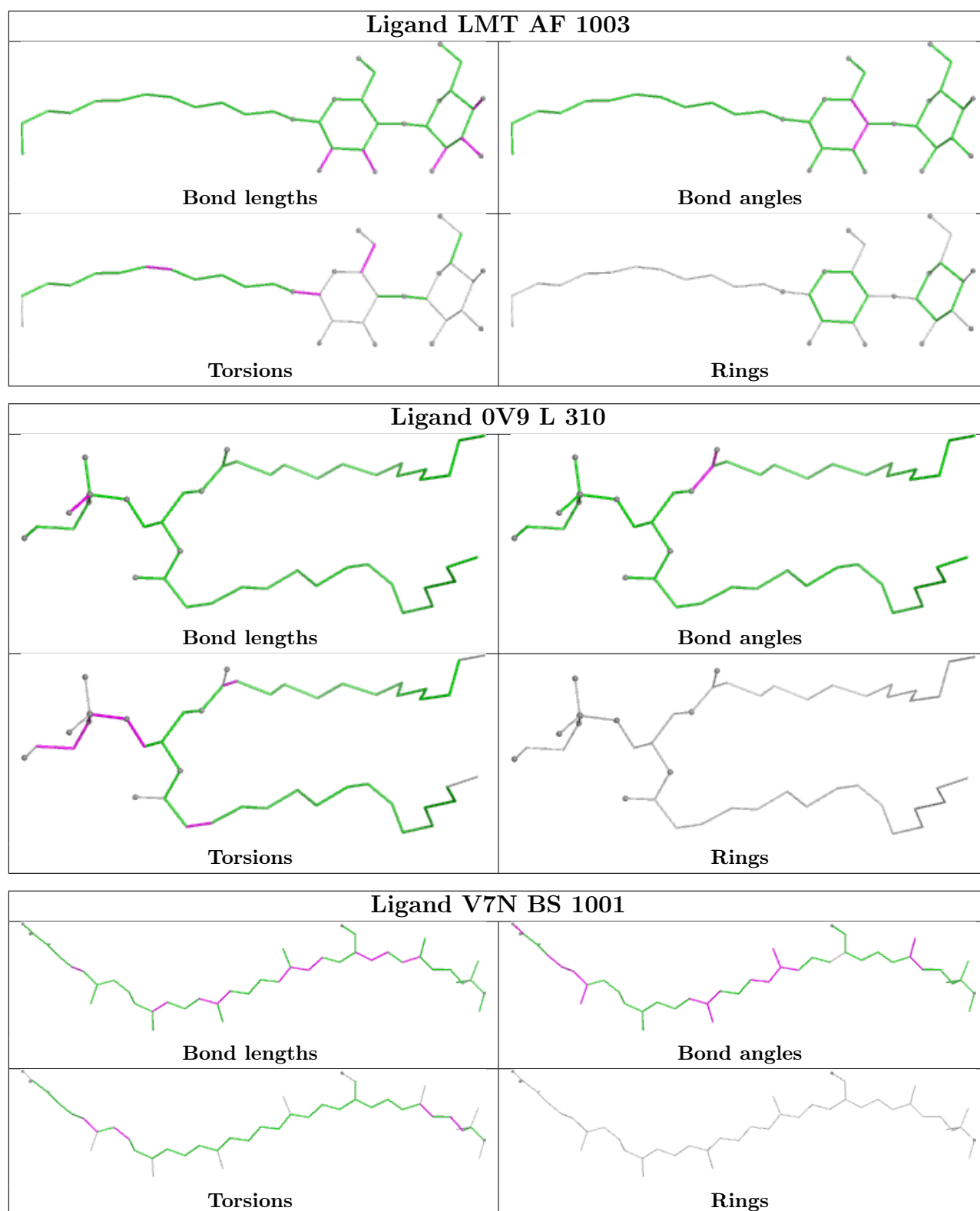


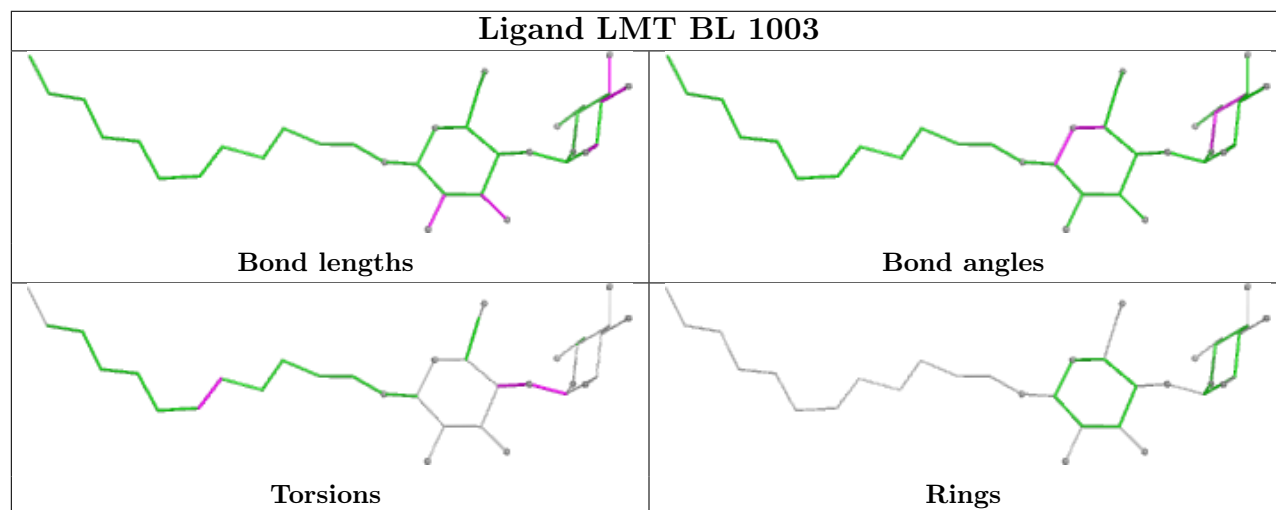
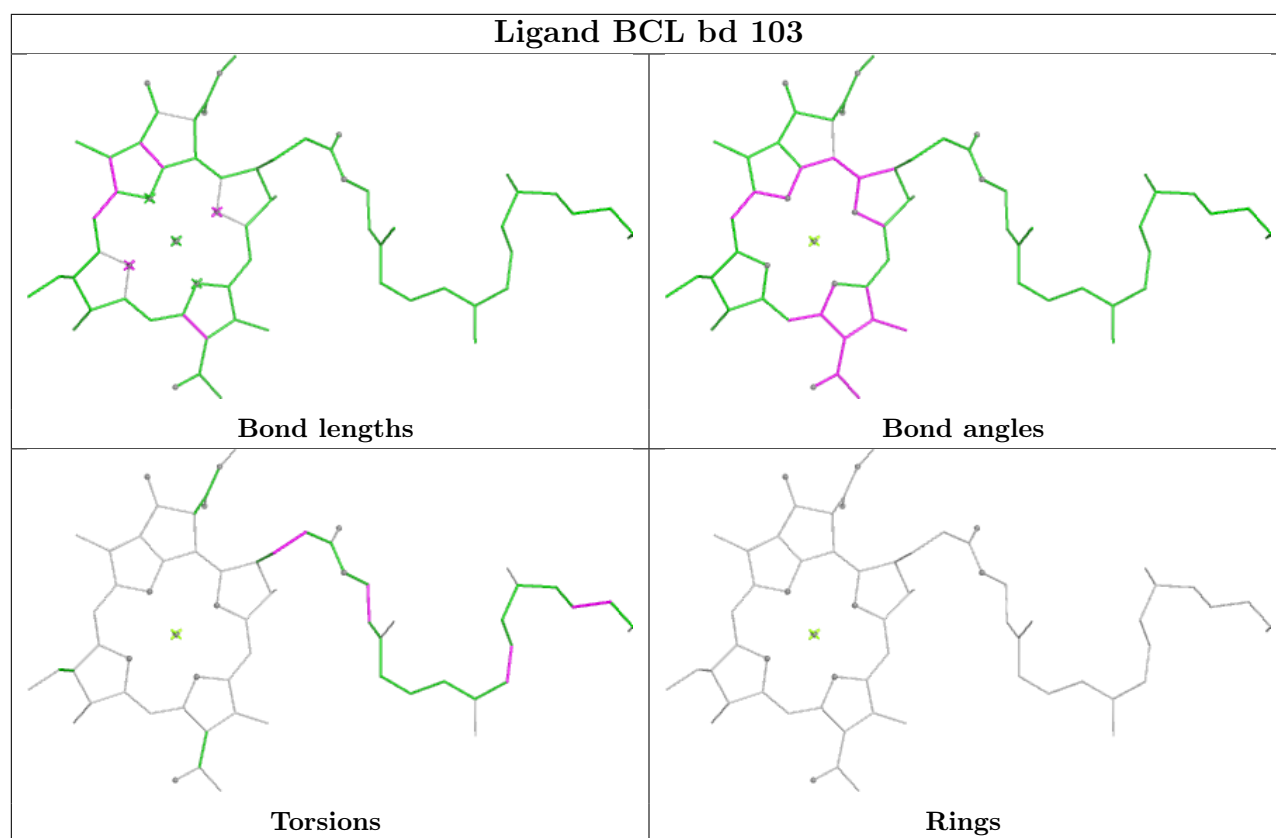


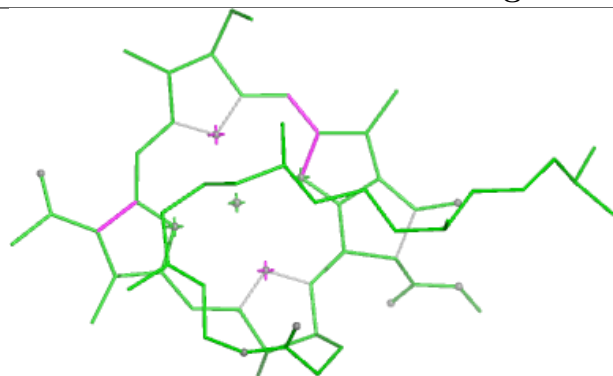
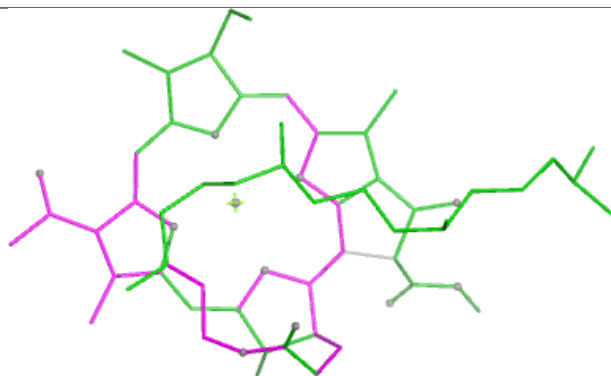
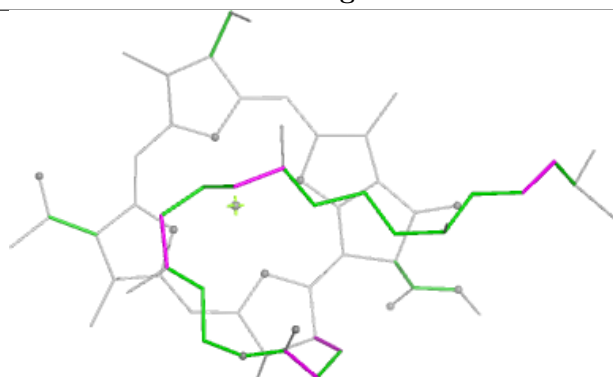
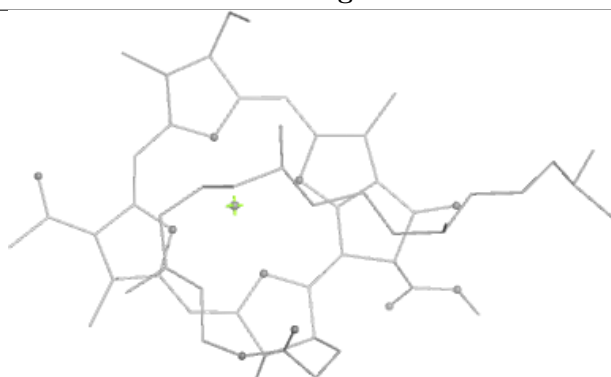
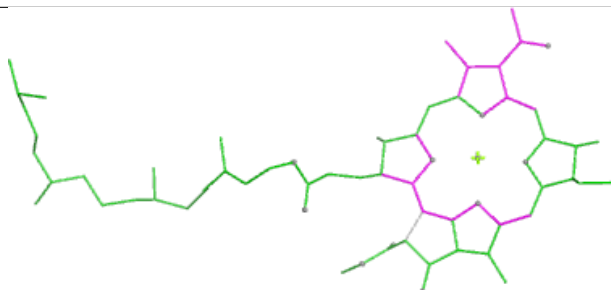
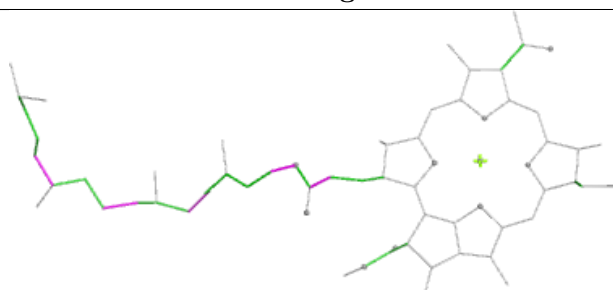
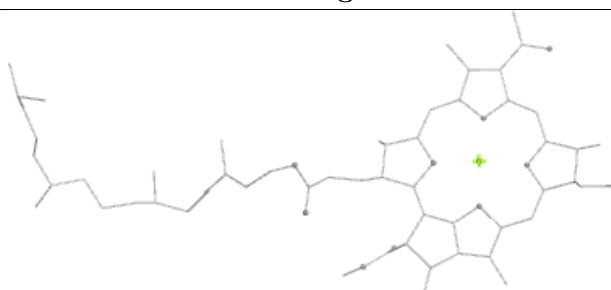
Ligand BCL BX 1004**Ligand LMT BE 102****Ligand LMT bg 103**

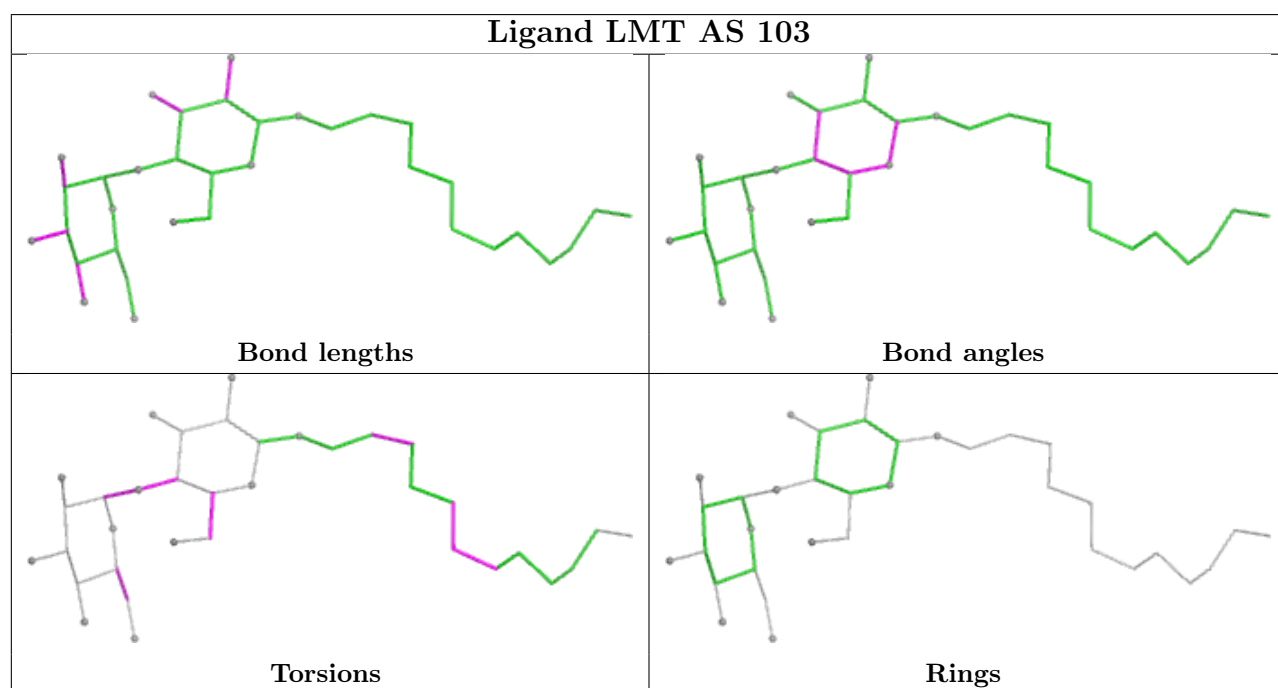
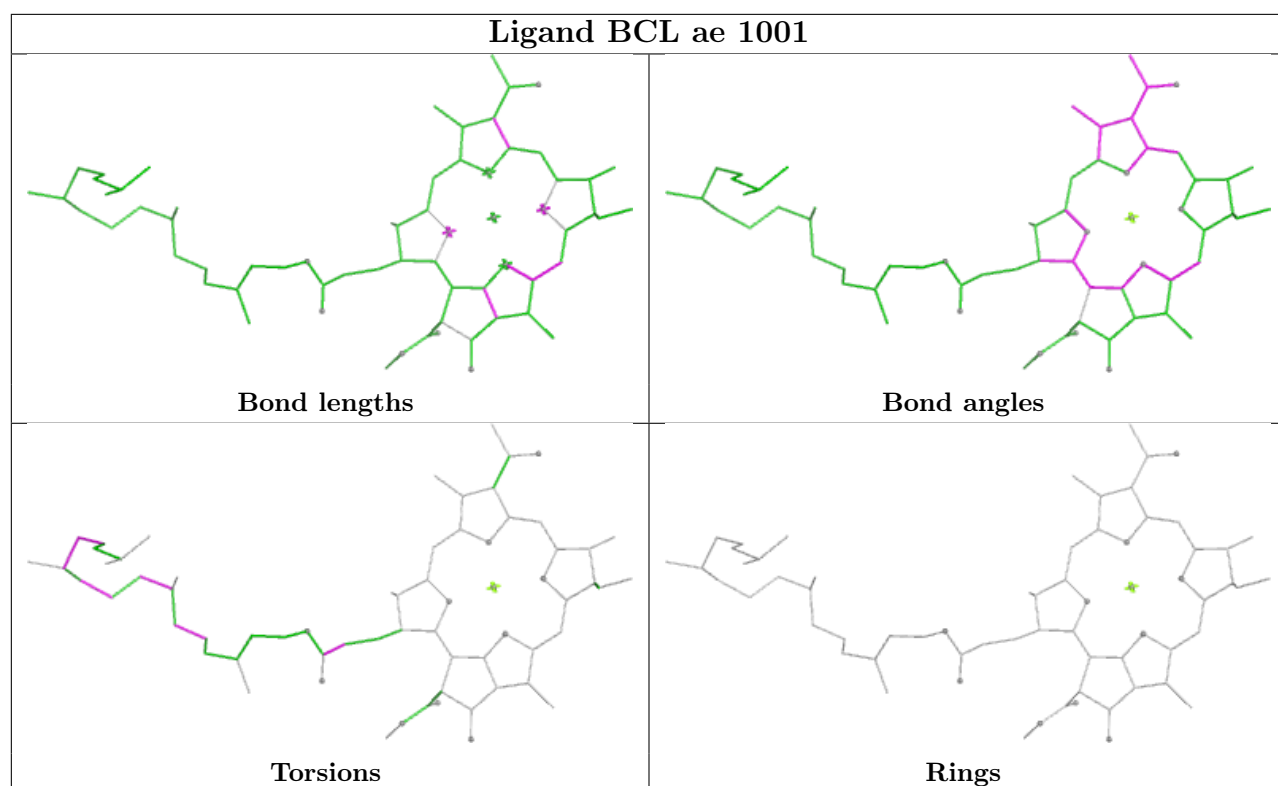


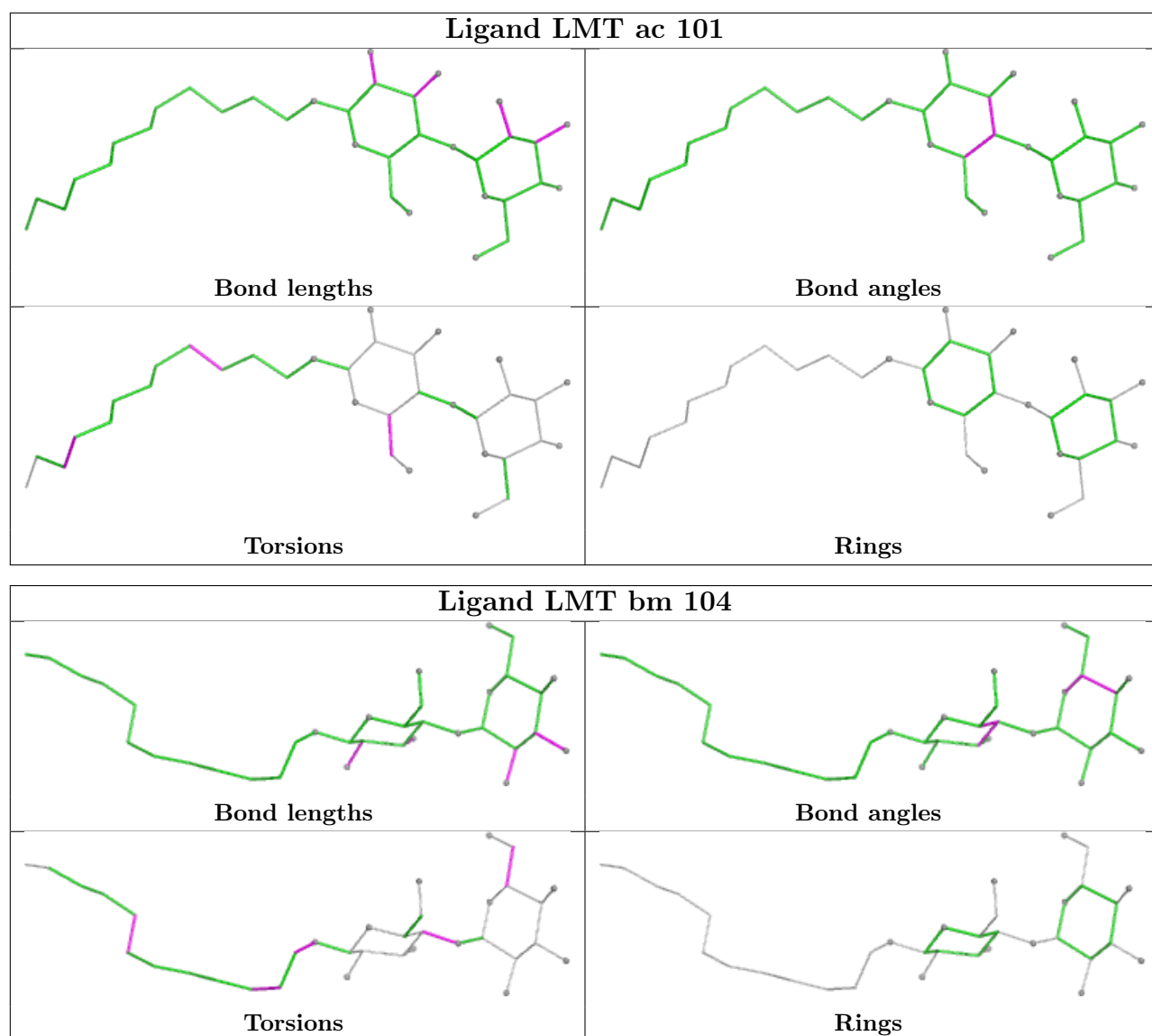


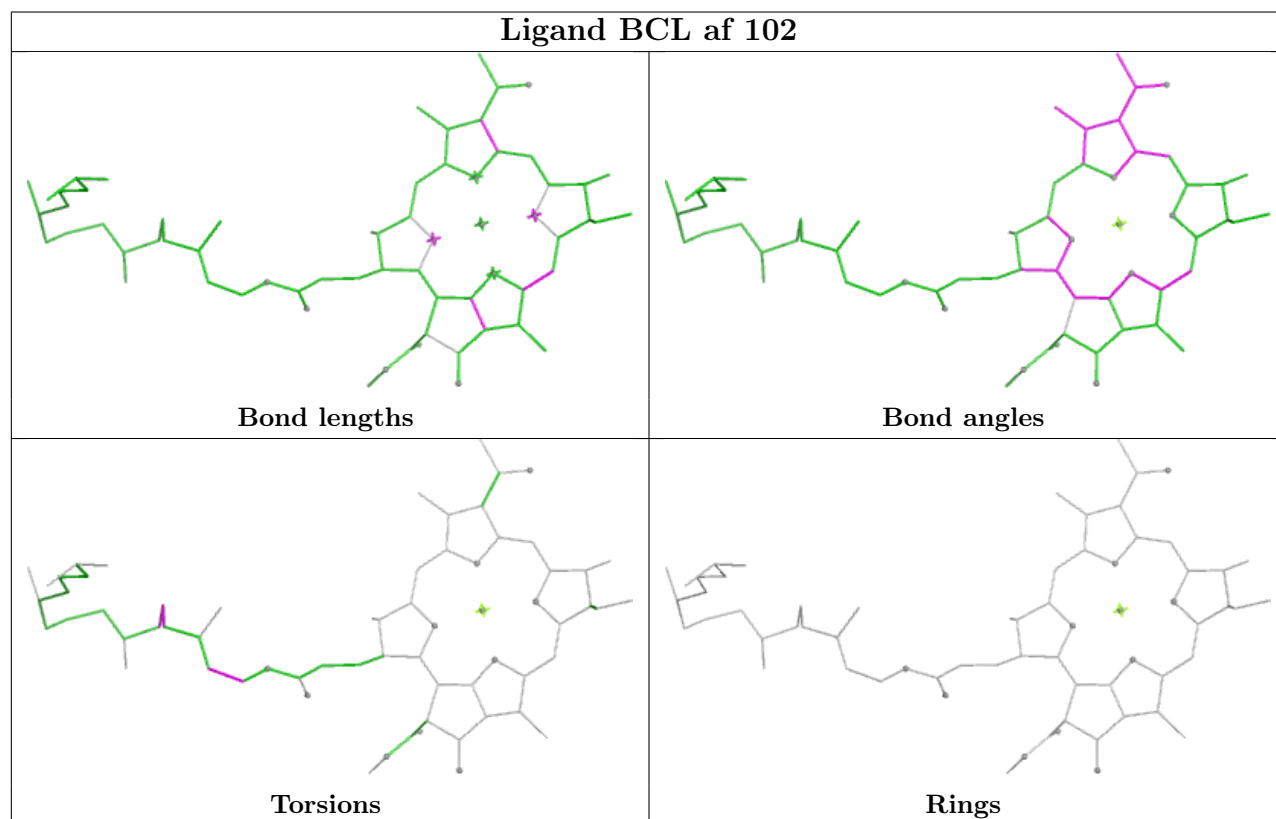
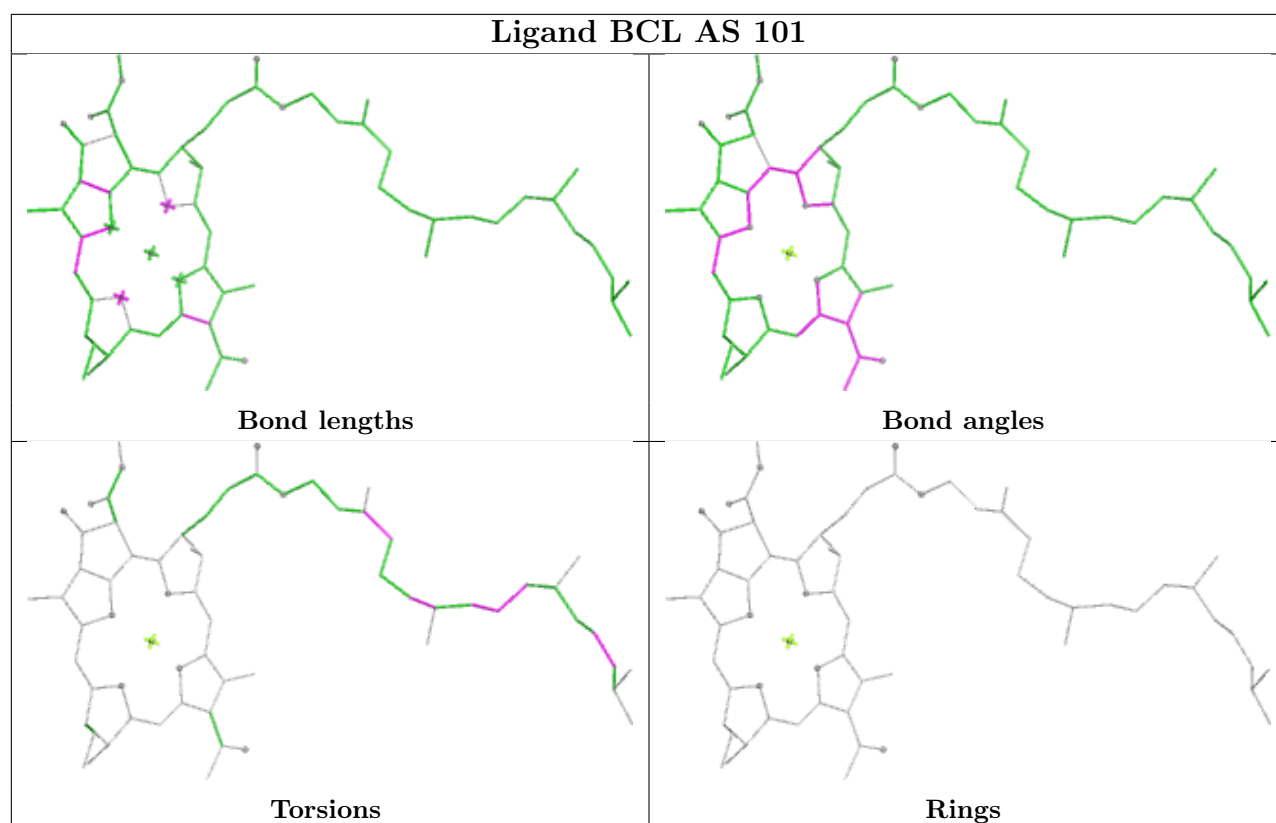


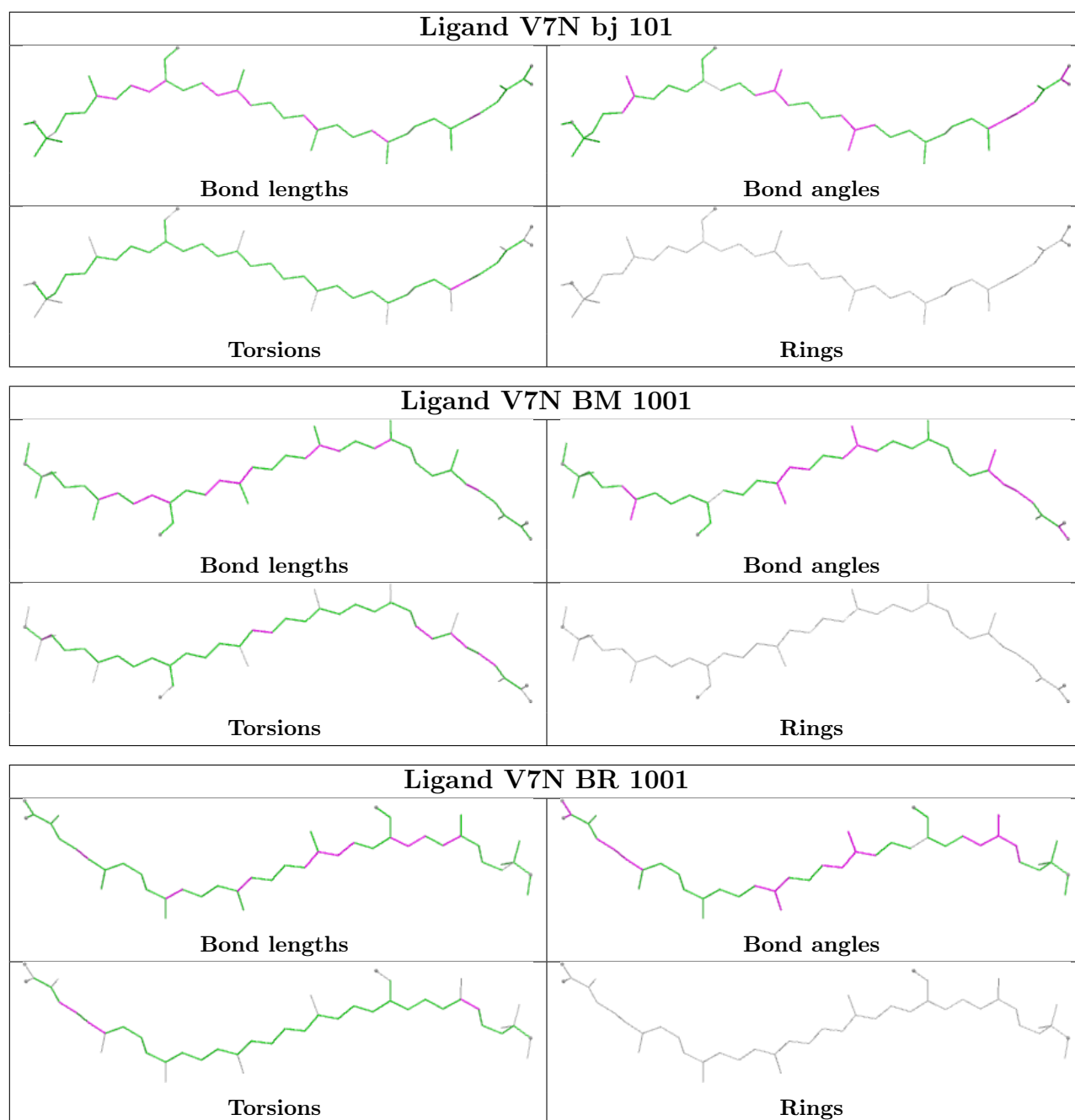


Ligand BCL AL 103**Bond lengths****Bond angles****Torsions****Rings****Ligand BCL ad 102****Bond lengths****Bond angles****Torsions****Rings**

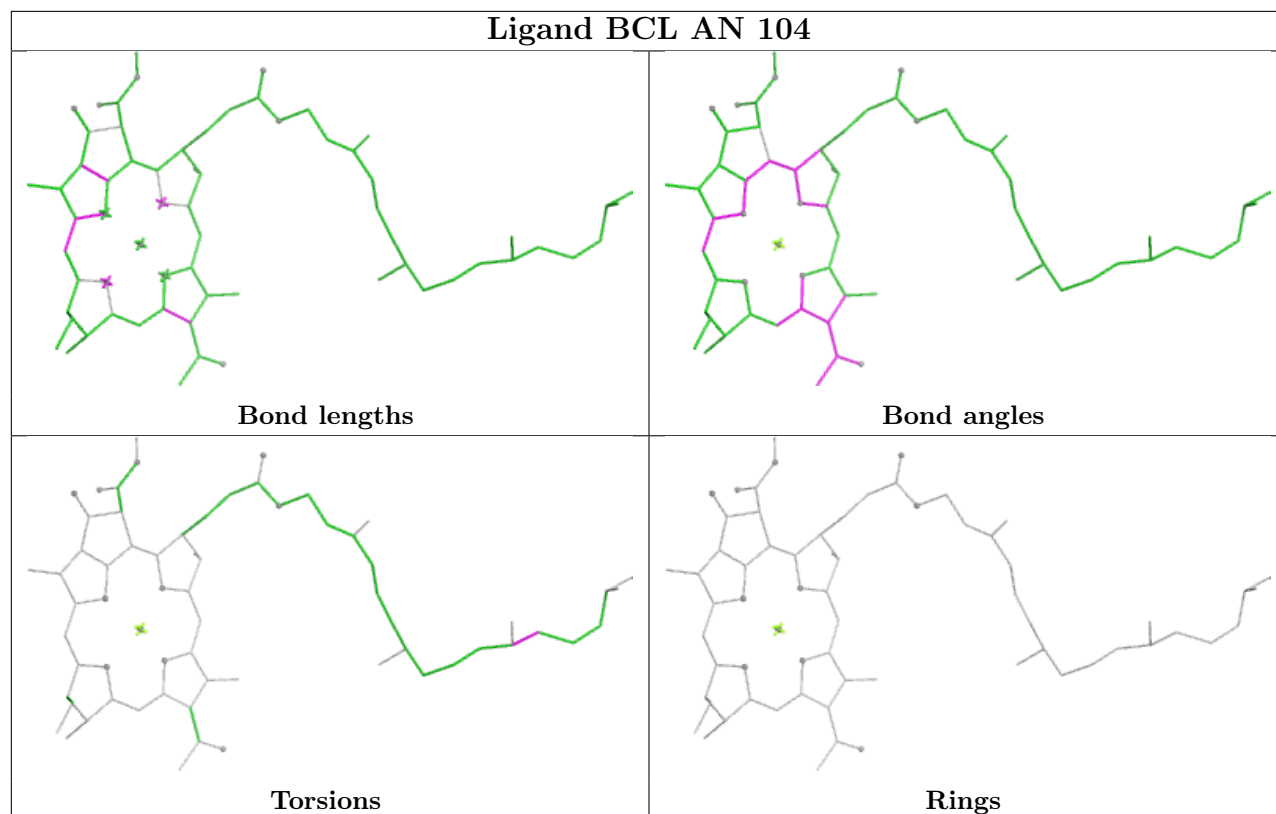




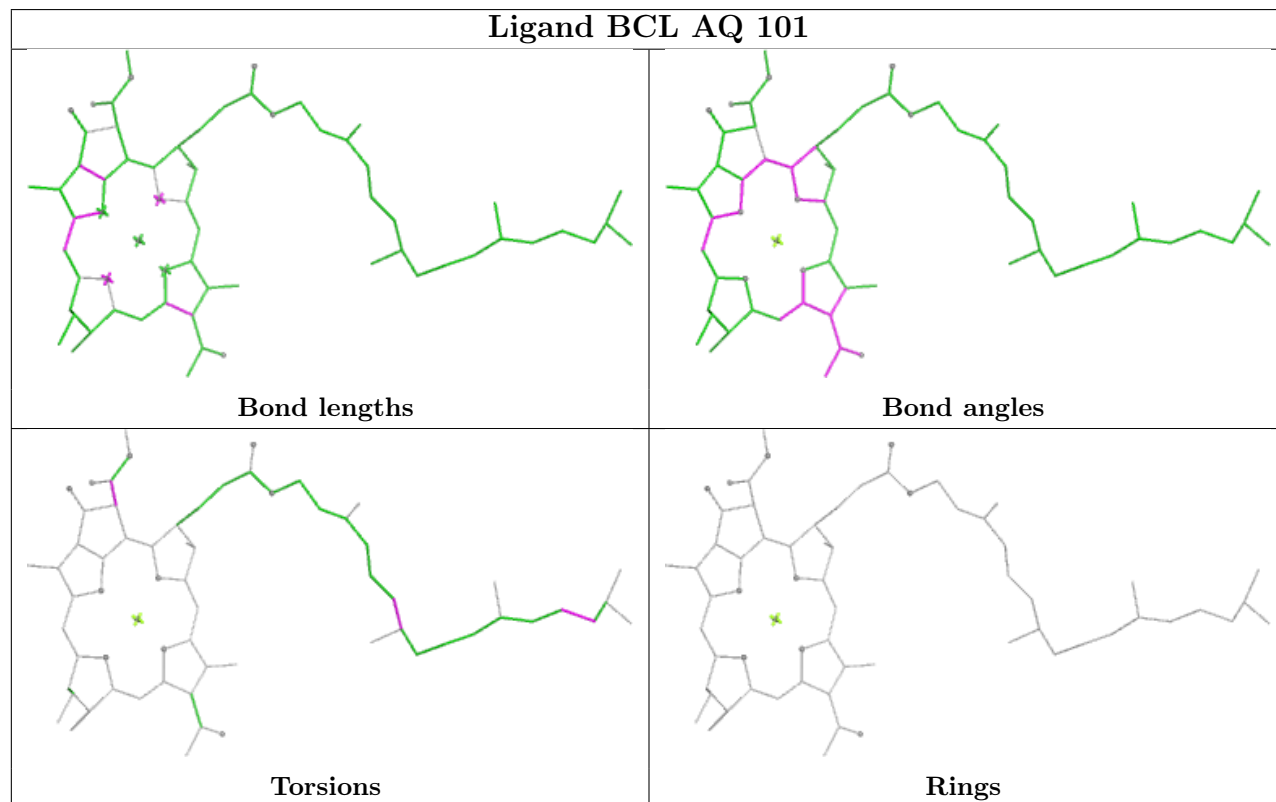


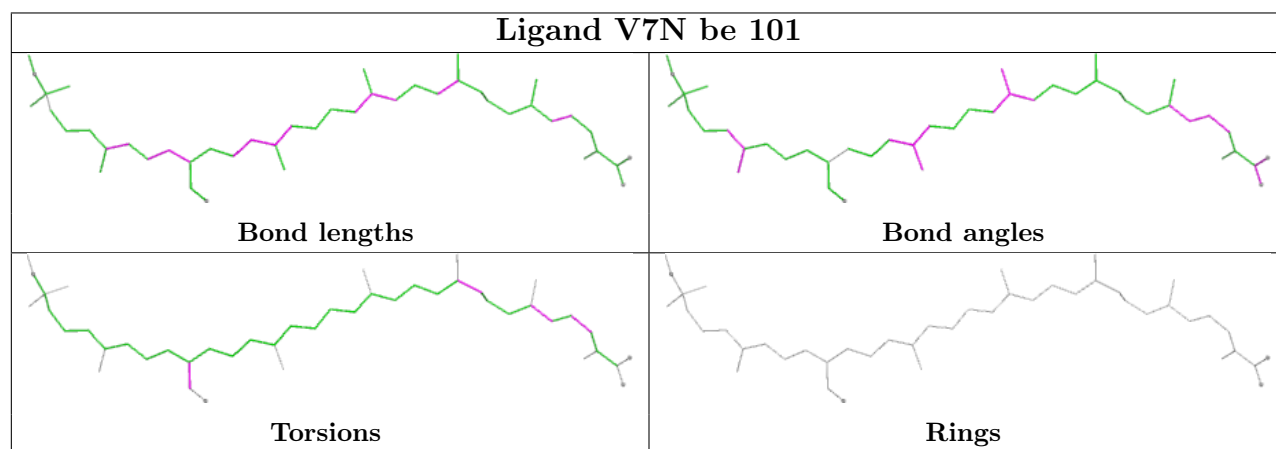
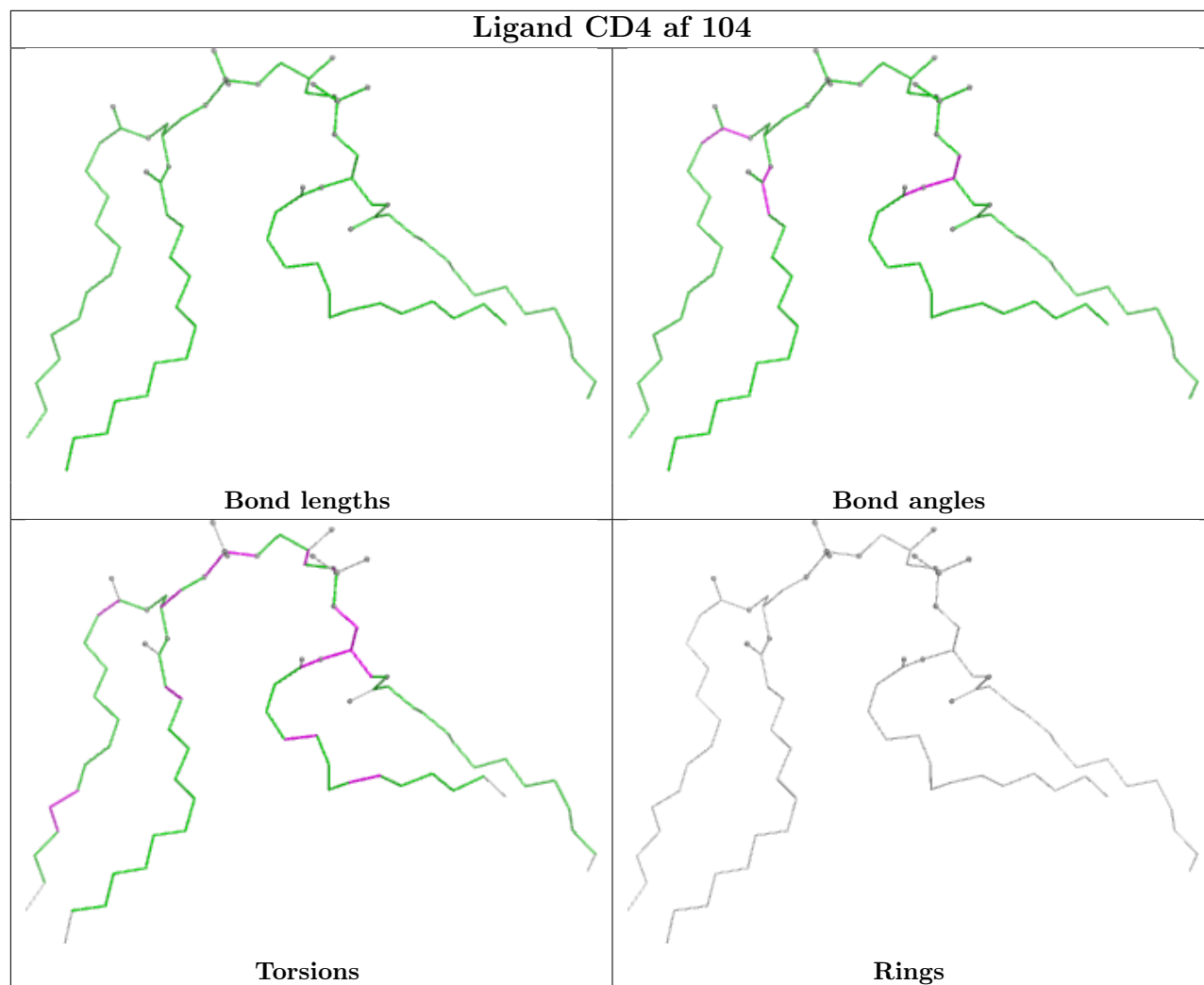


Ligand BCL AN 104

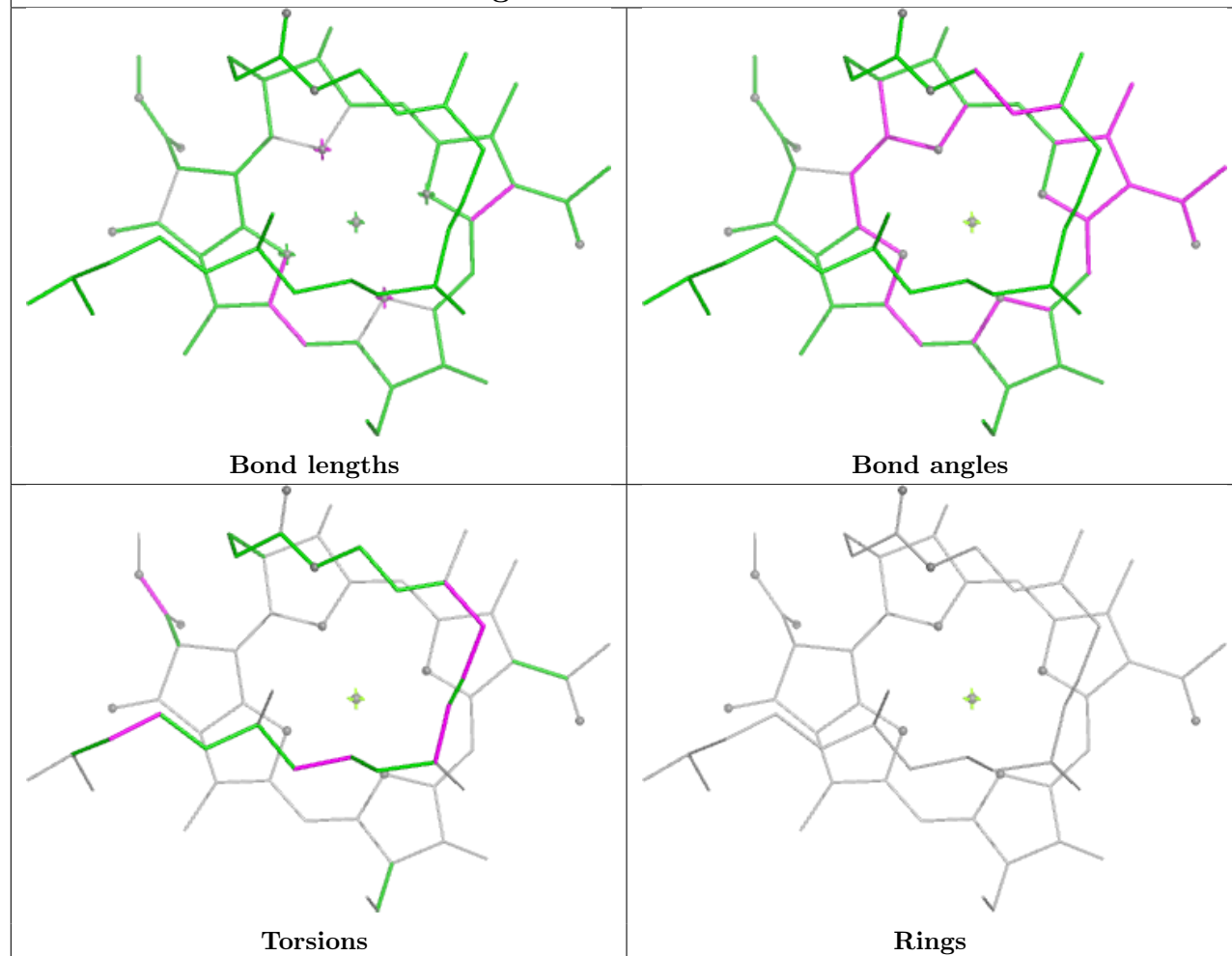


Ligand BCL AQ 101

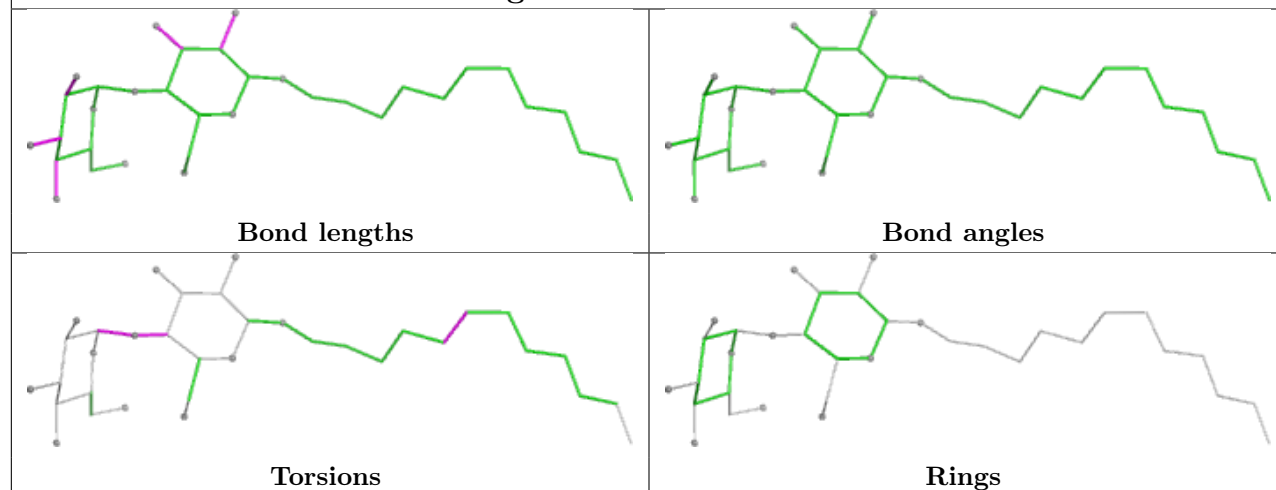


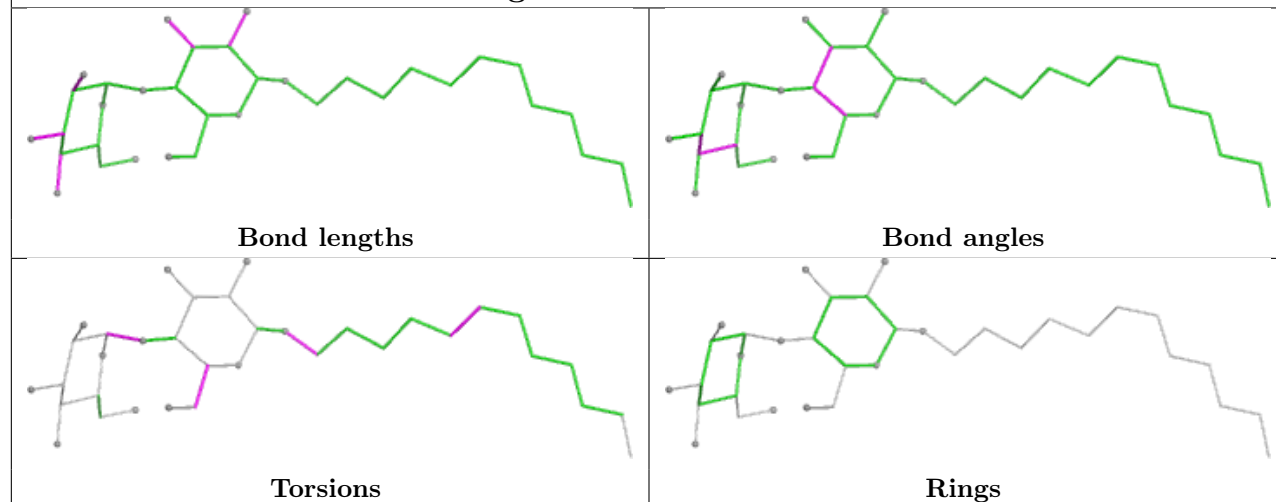
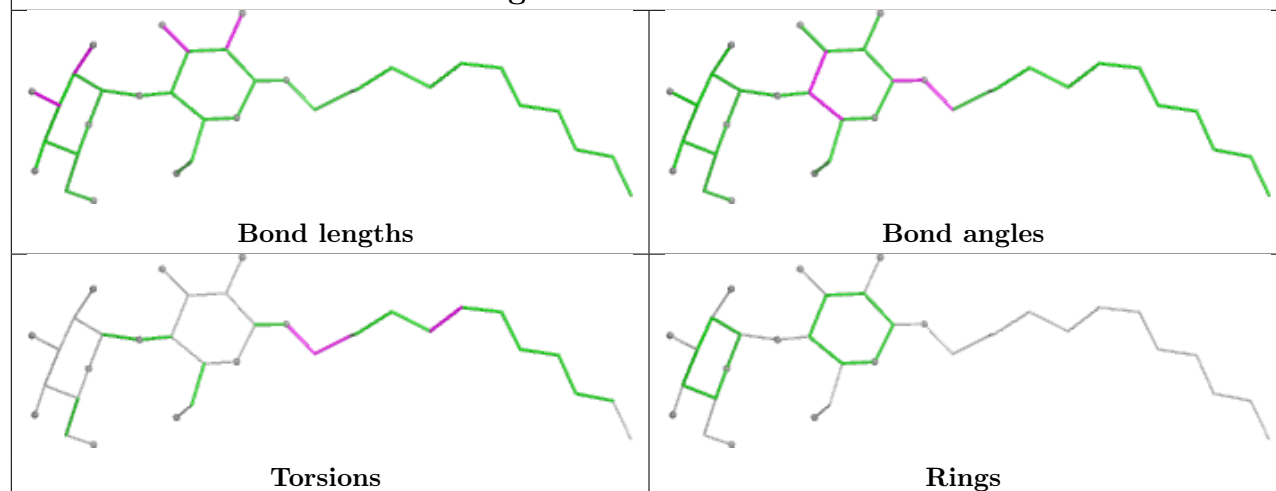
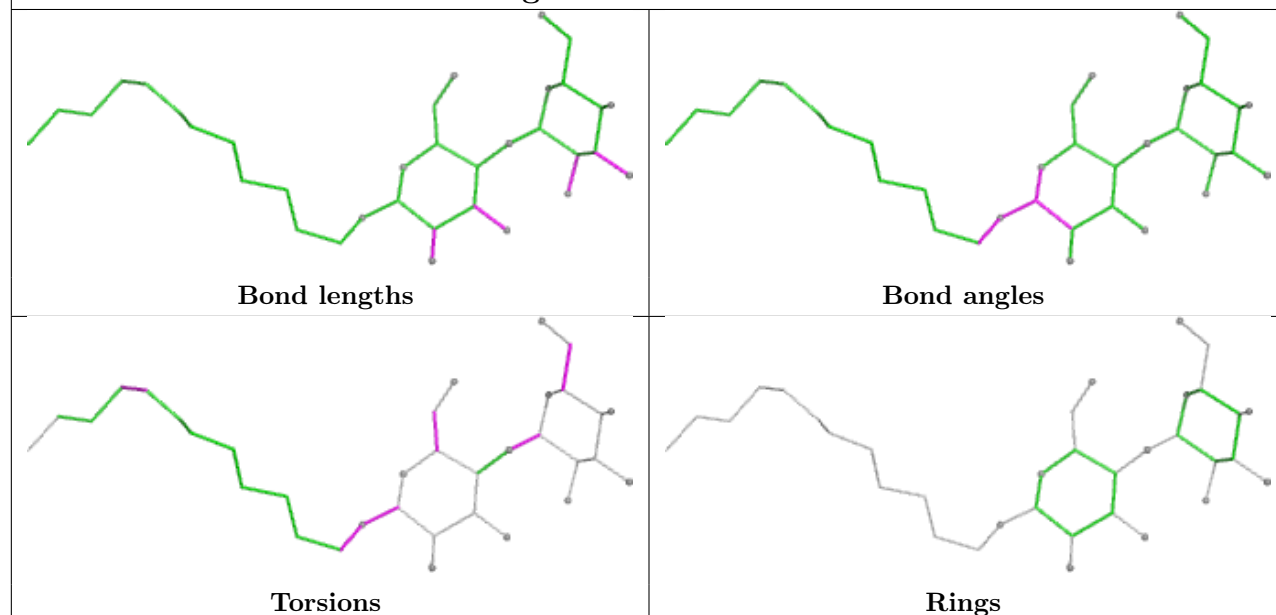


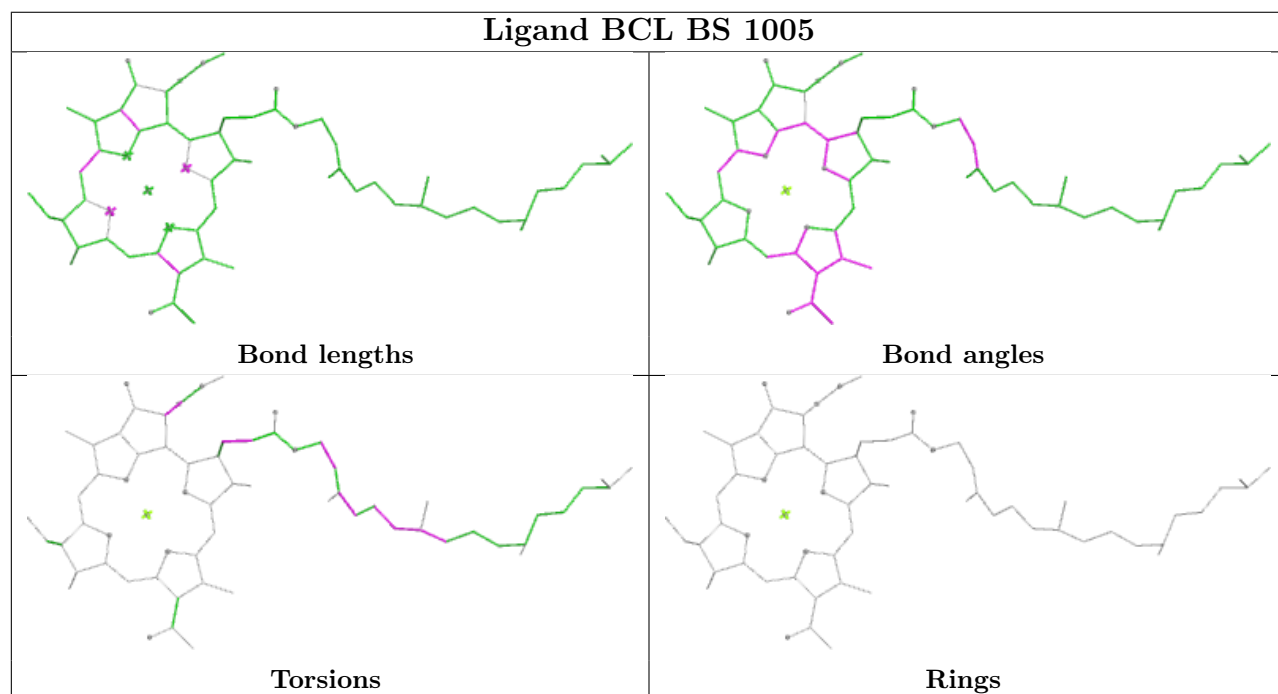
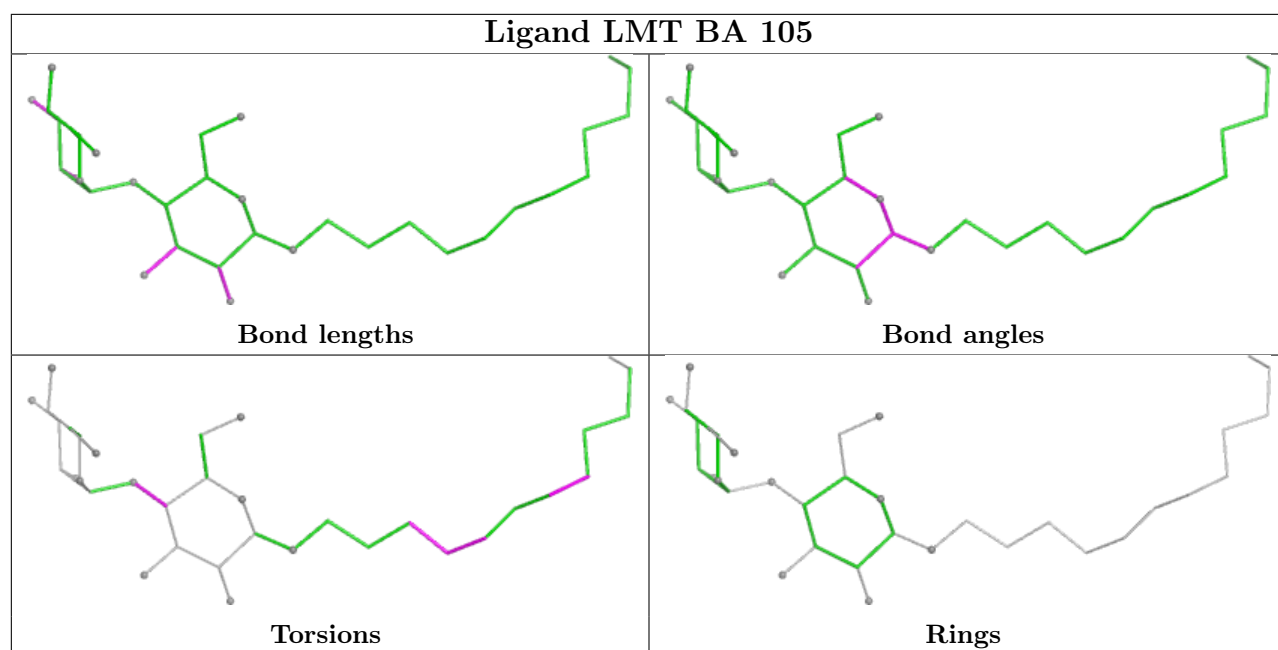
Ligand BCL AA 1002

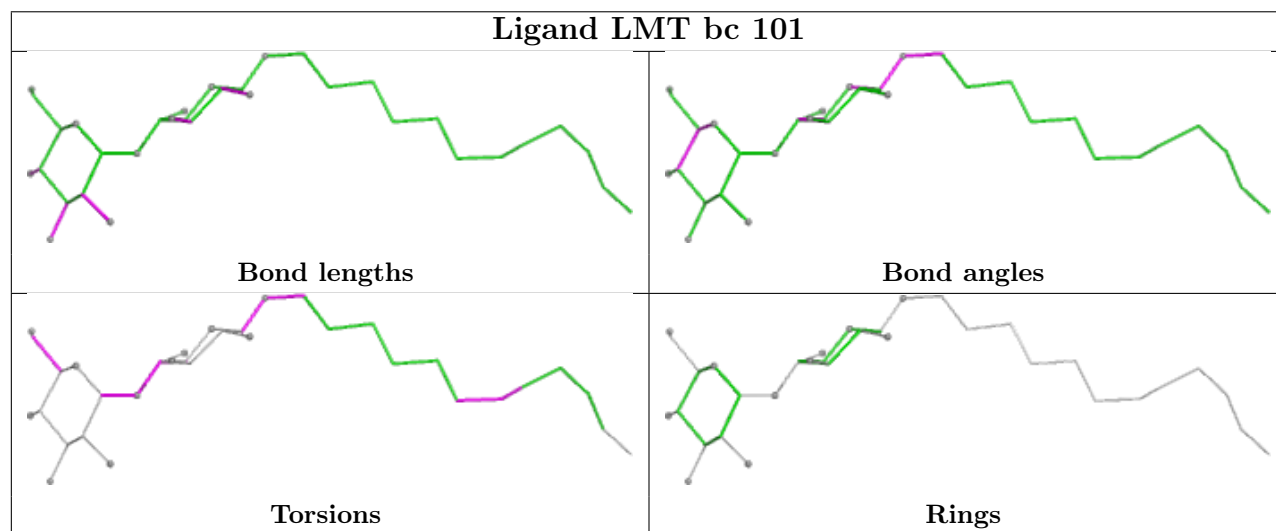
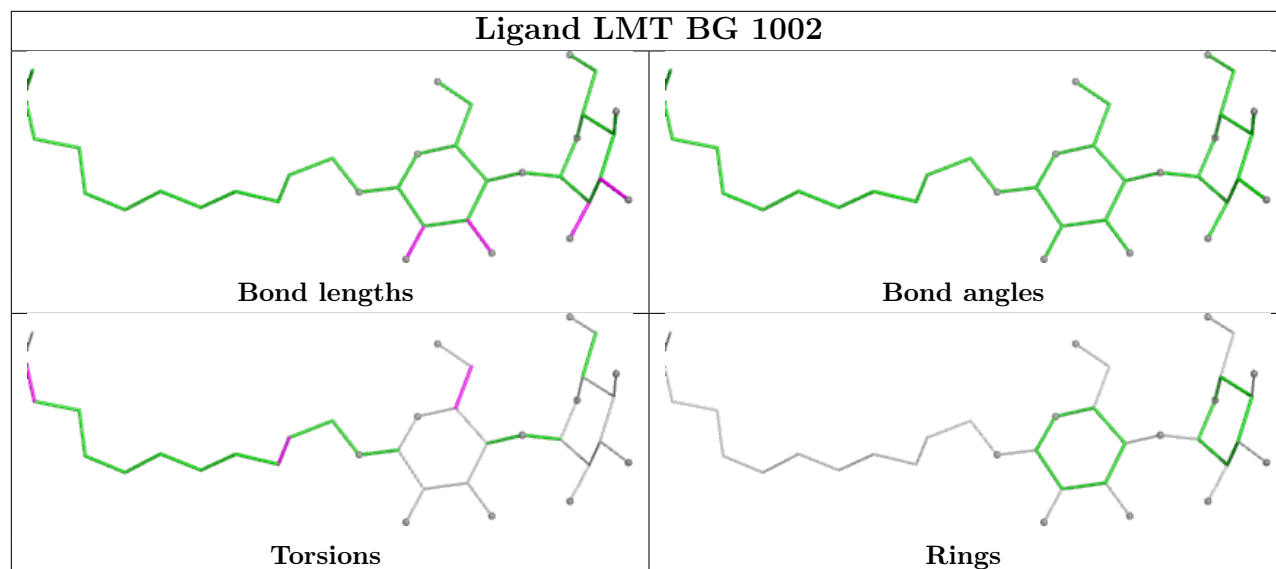


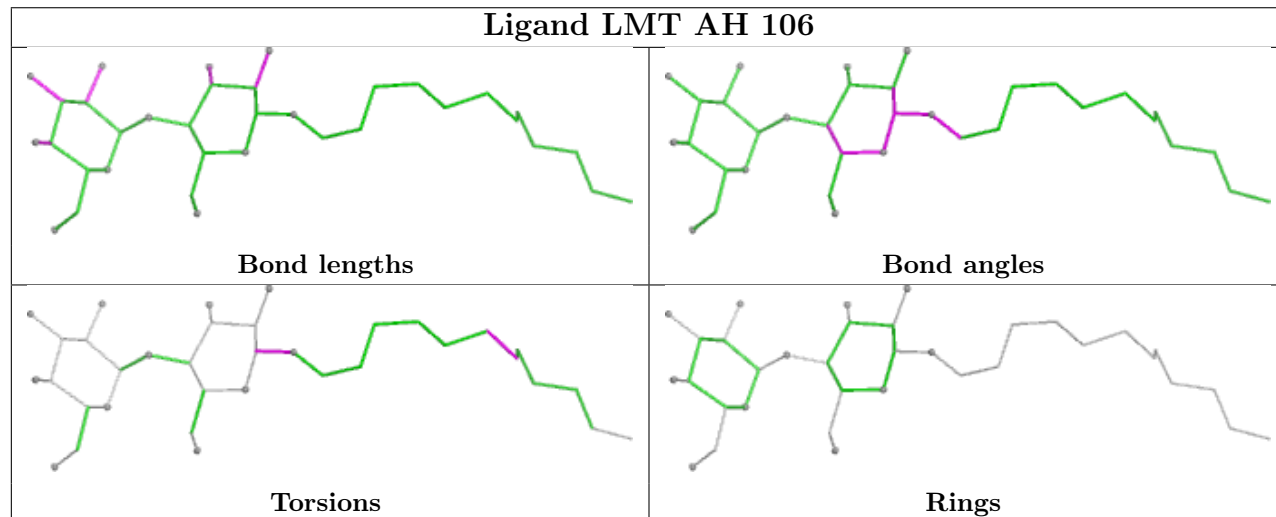
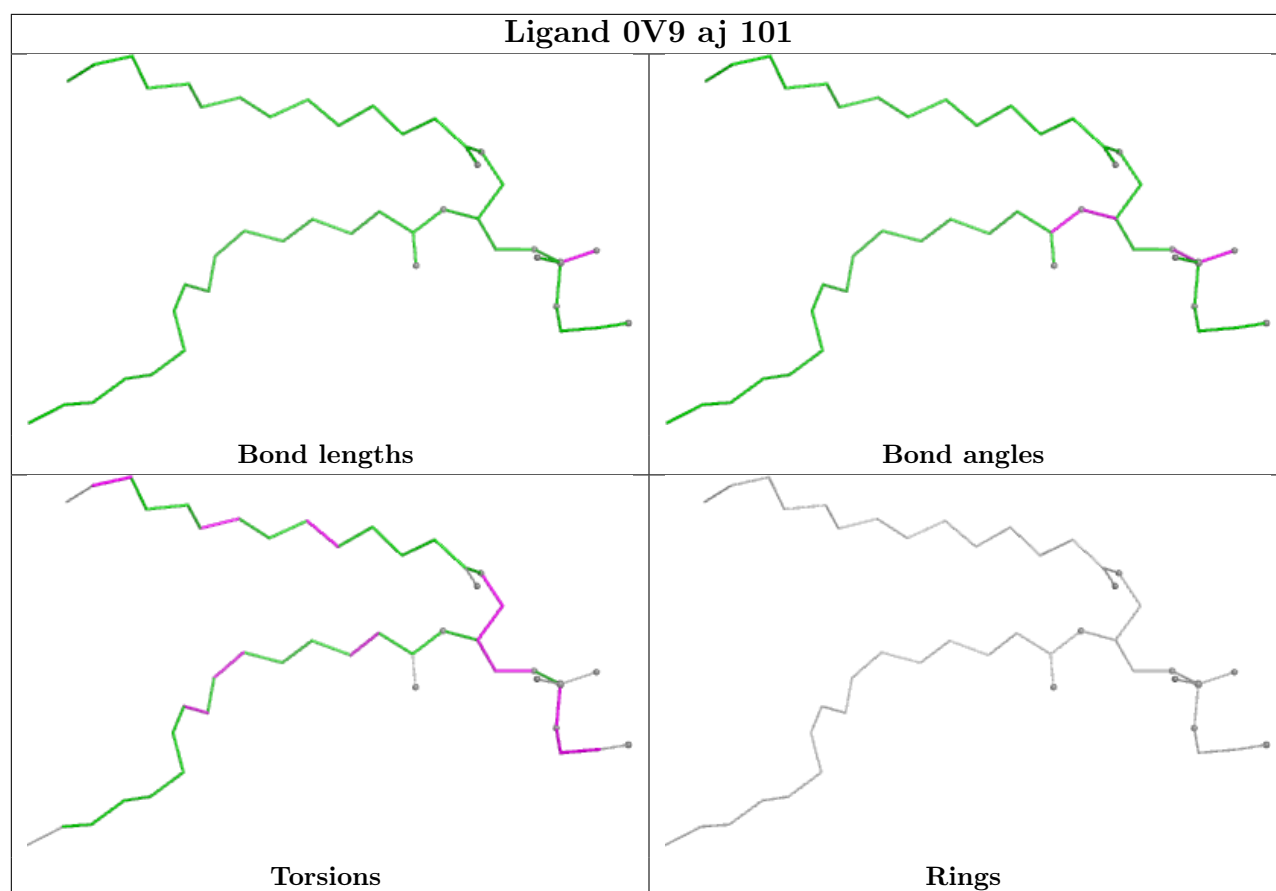
Ligand LMT BR 1005

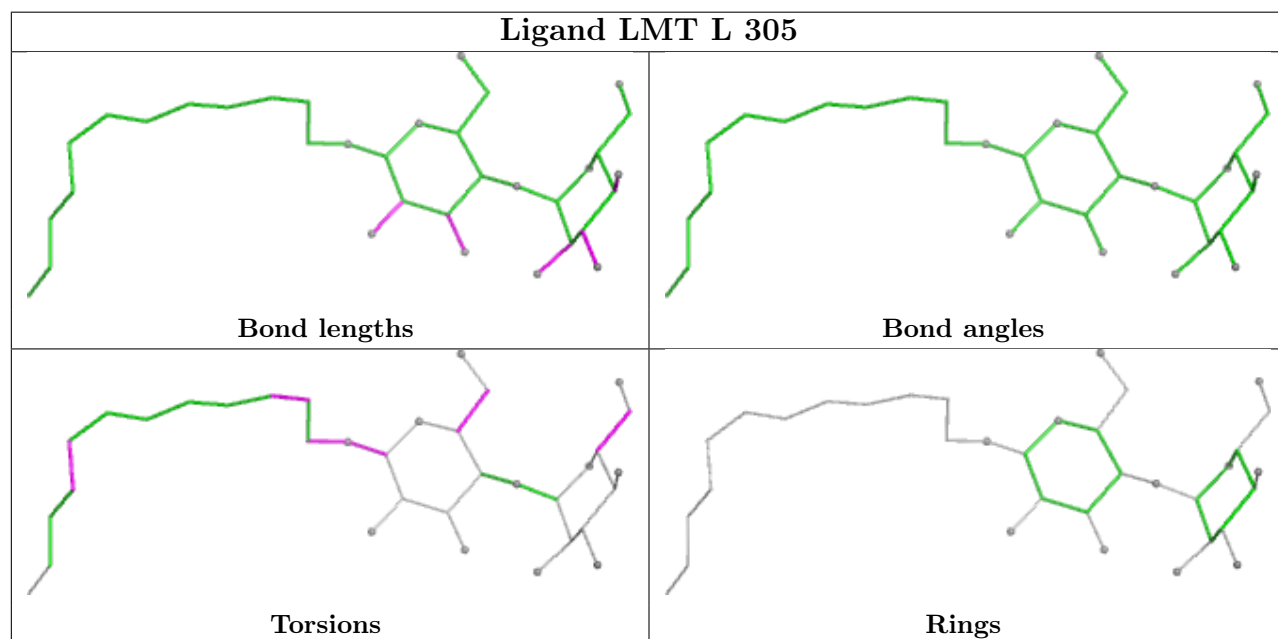
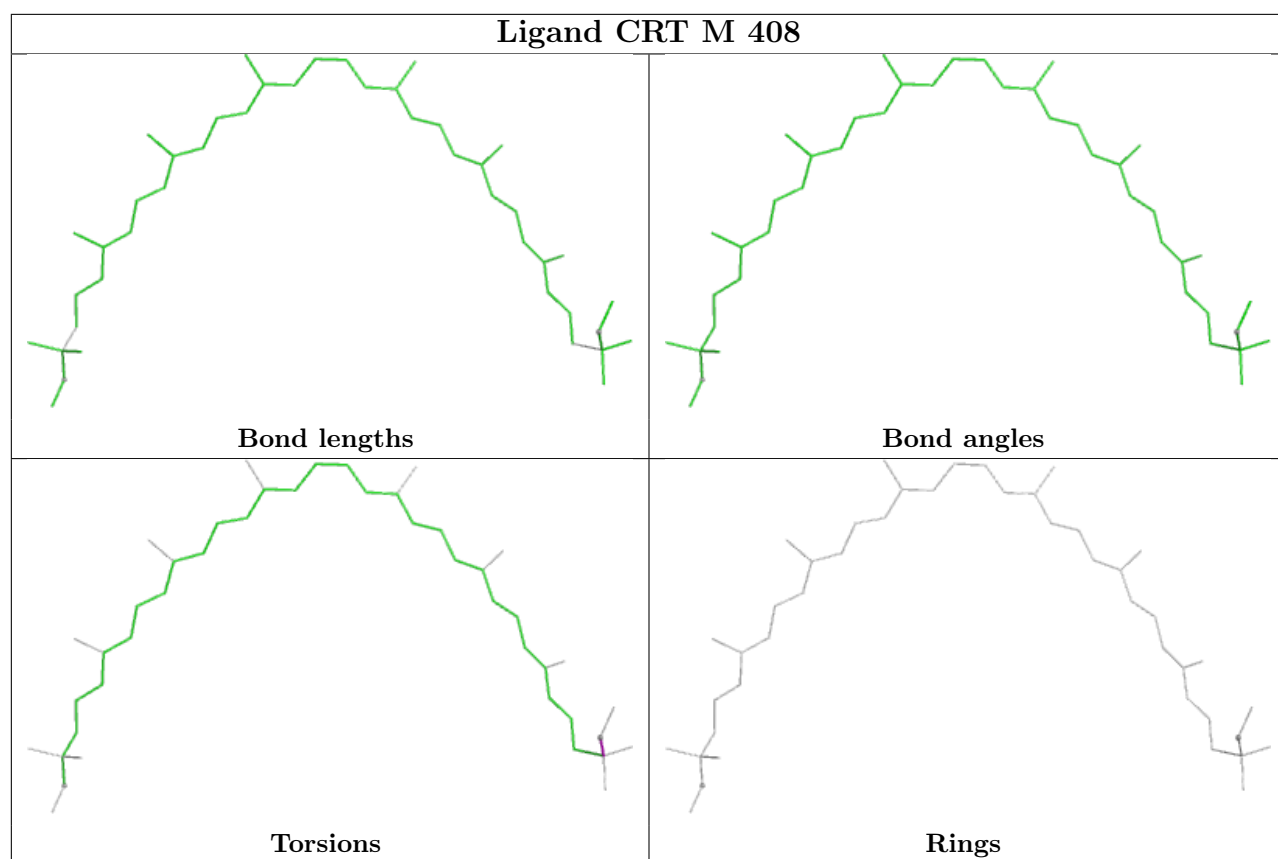


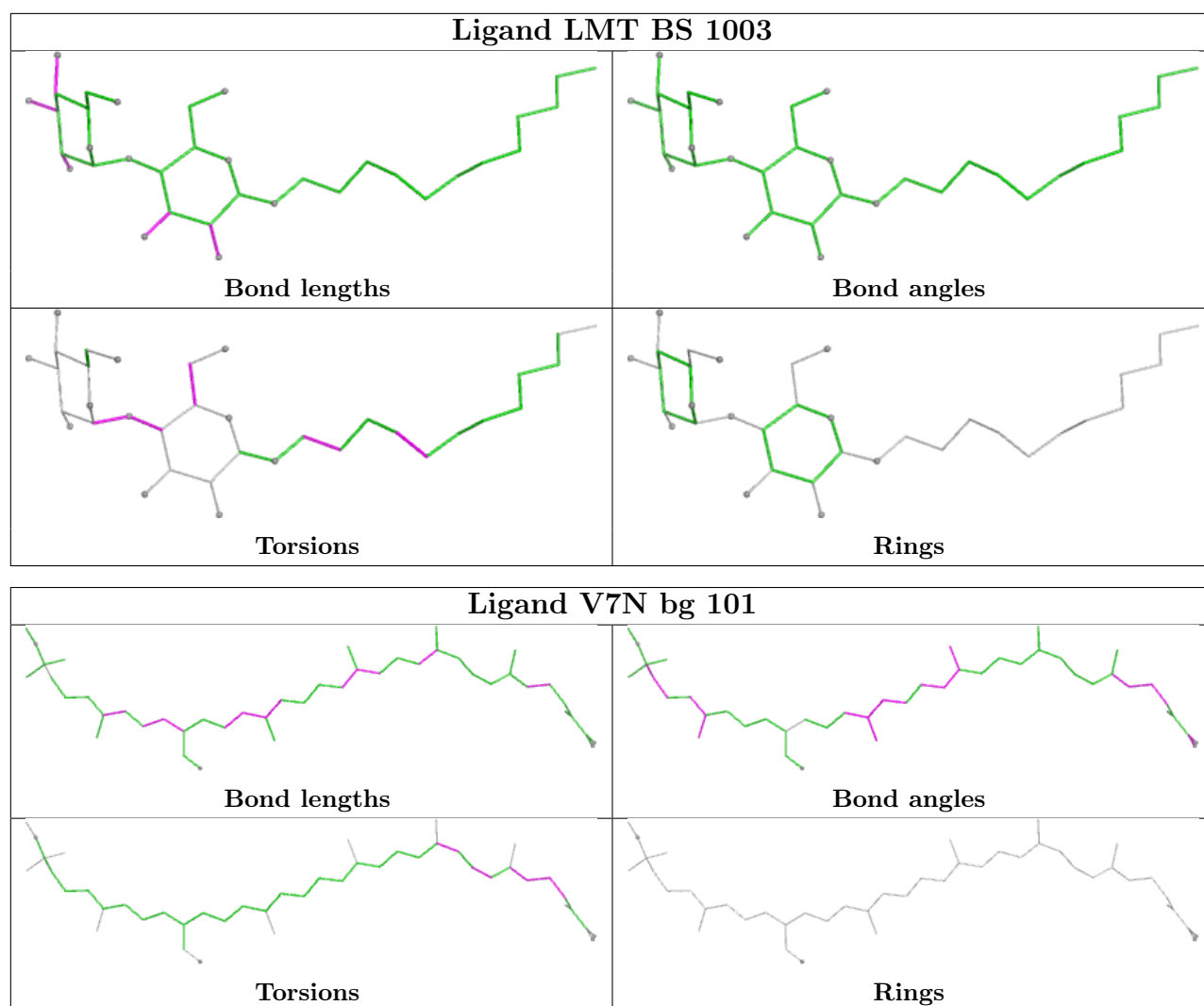
Ligand LMT BT 1002**Ligand LMT BP 1006****Ligand LMT bh 101**

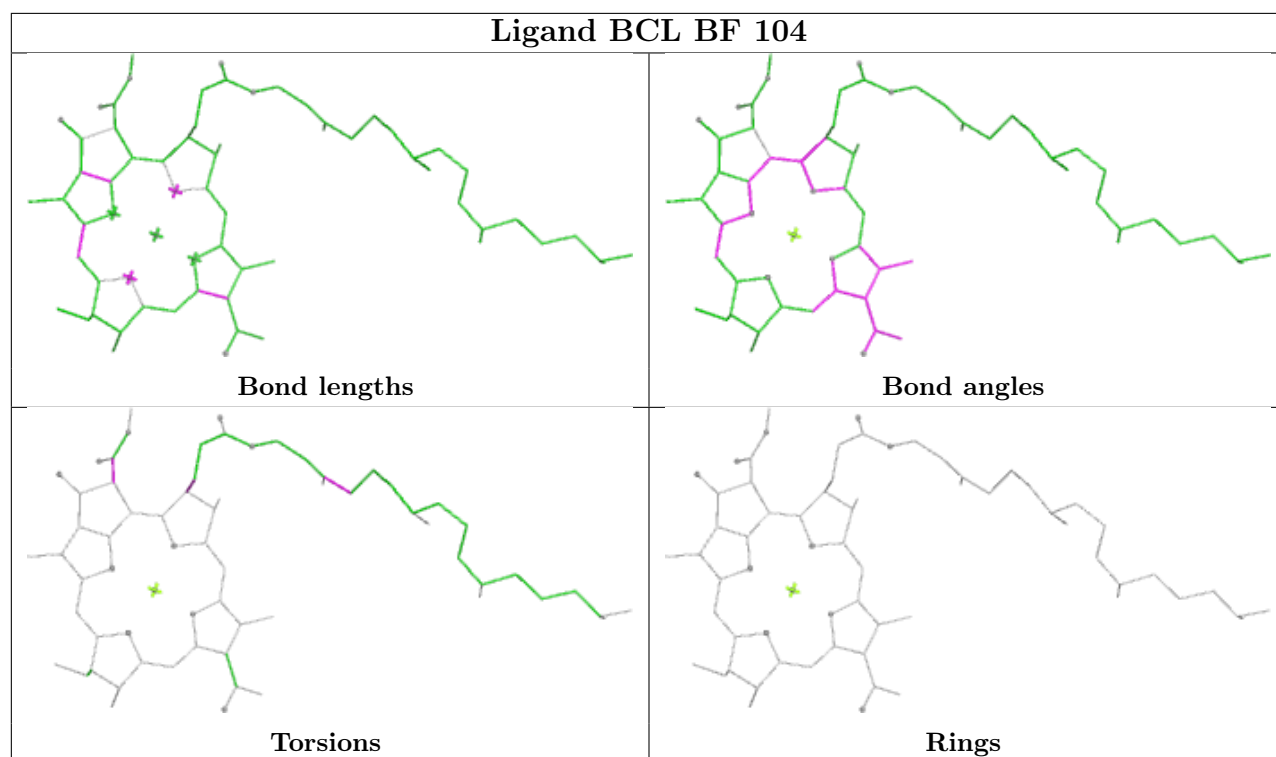
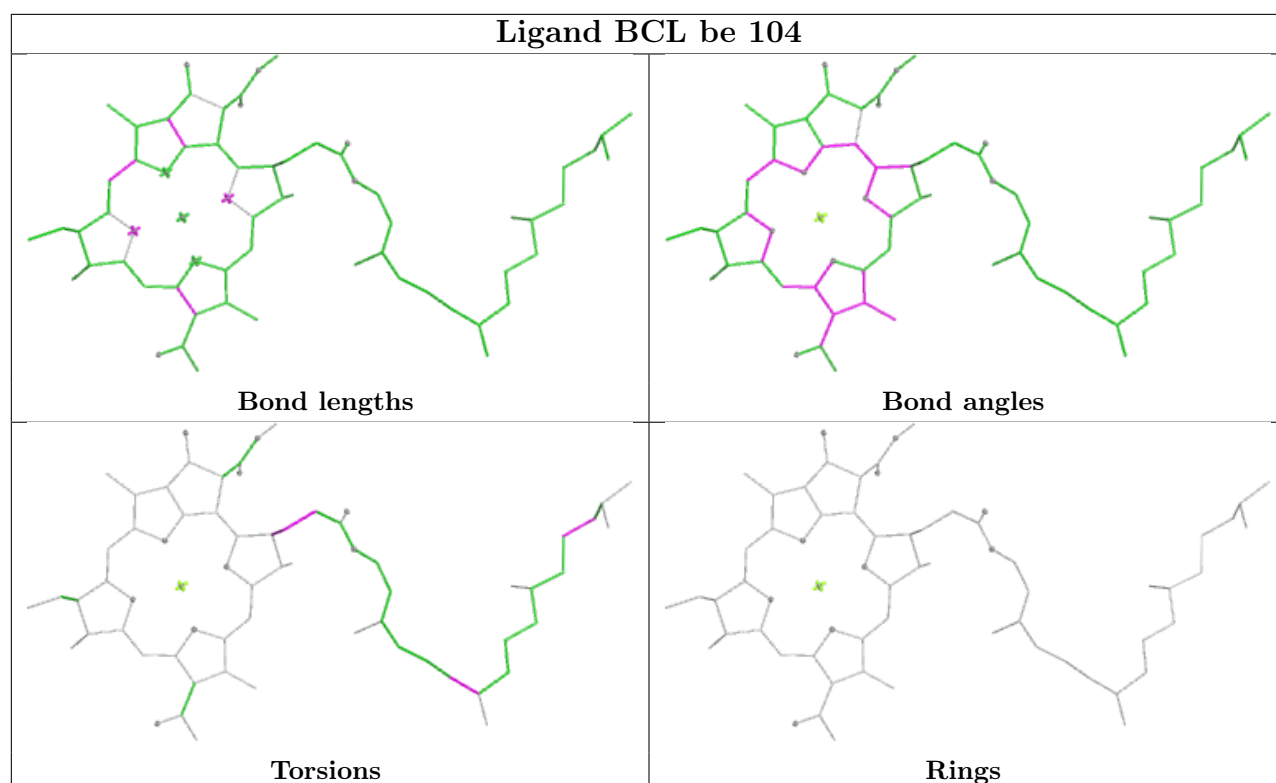


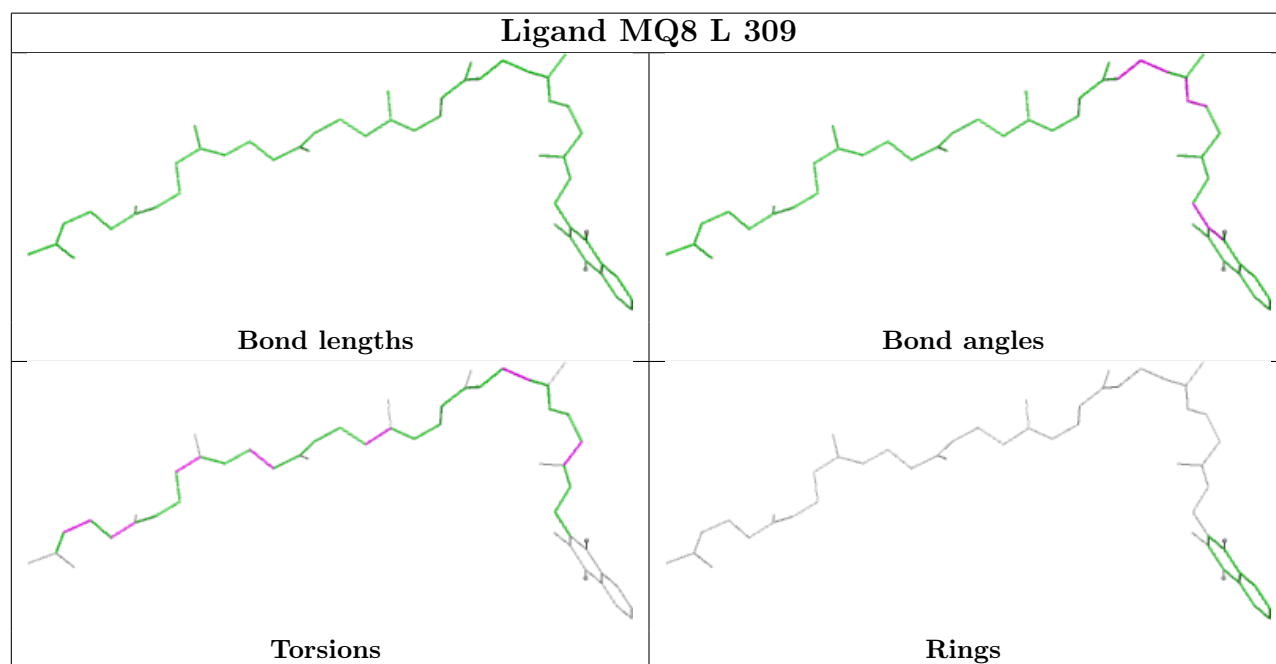
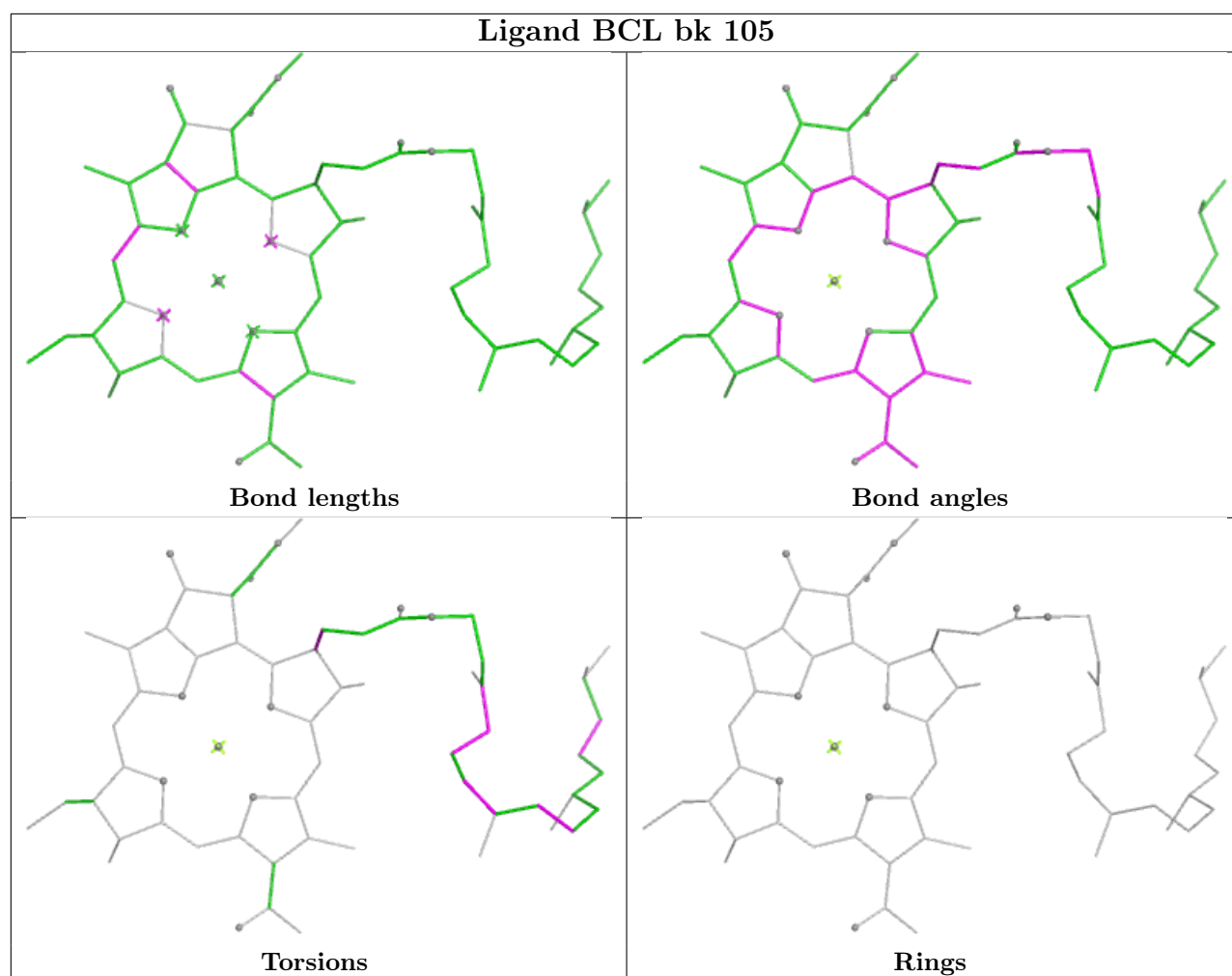


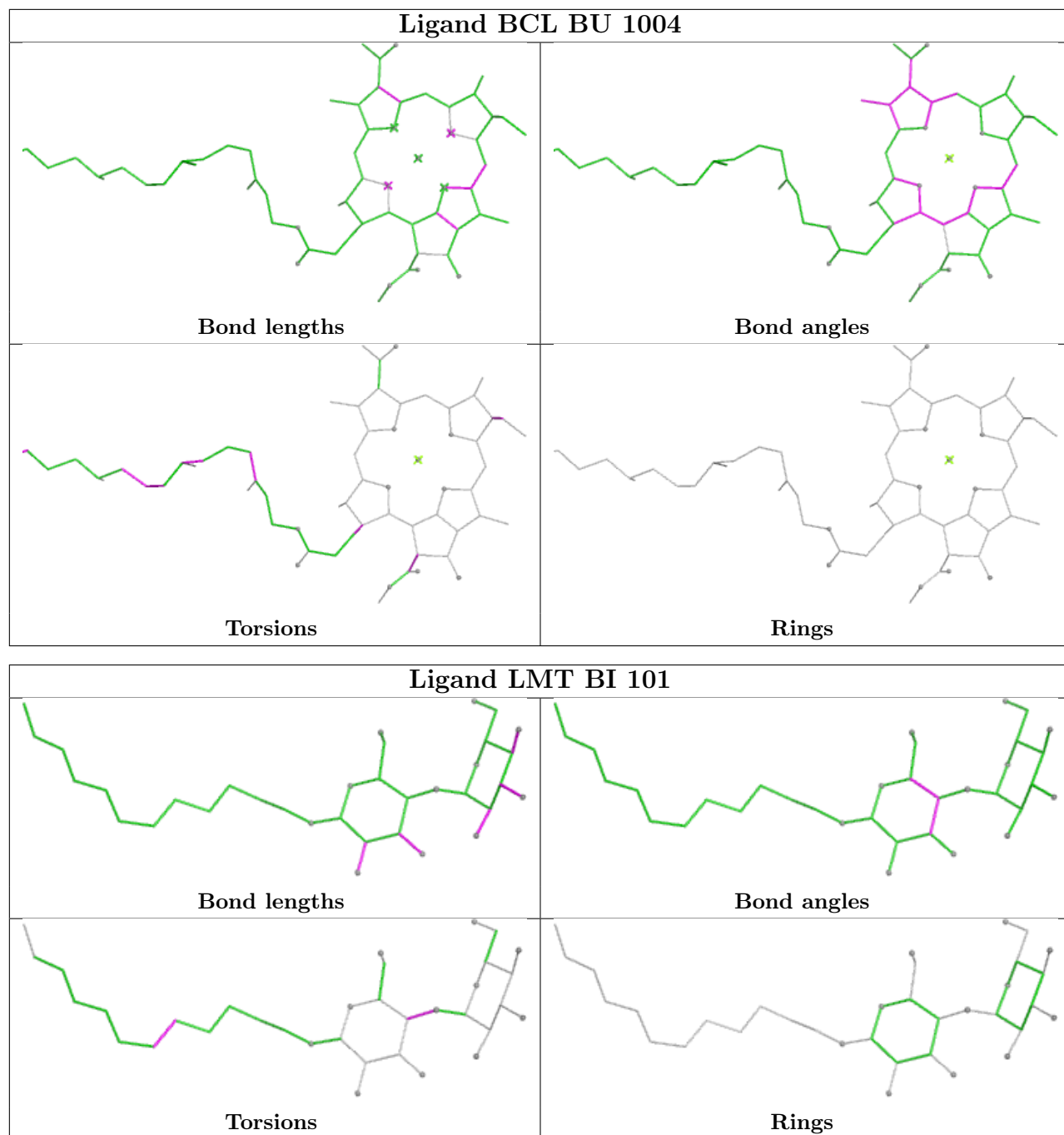


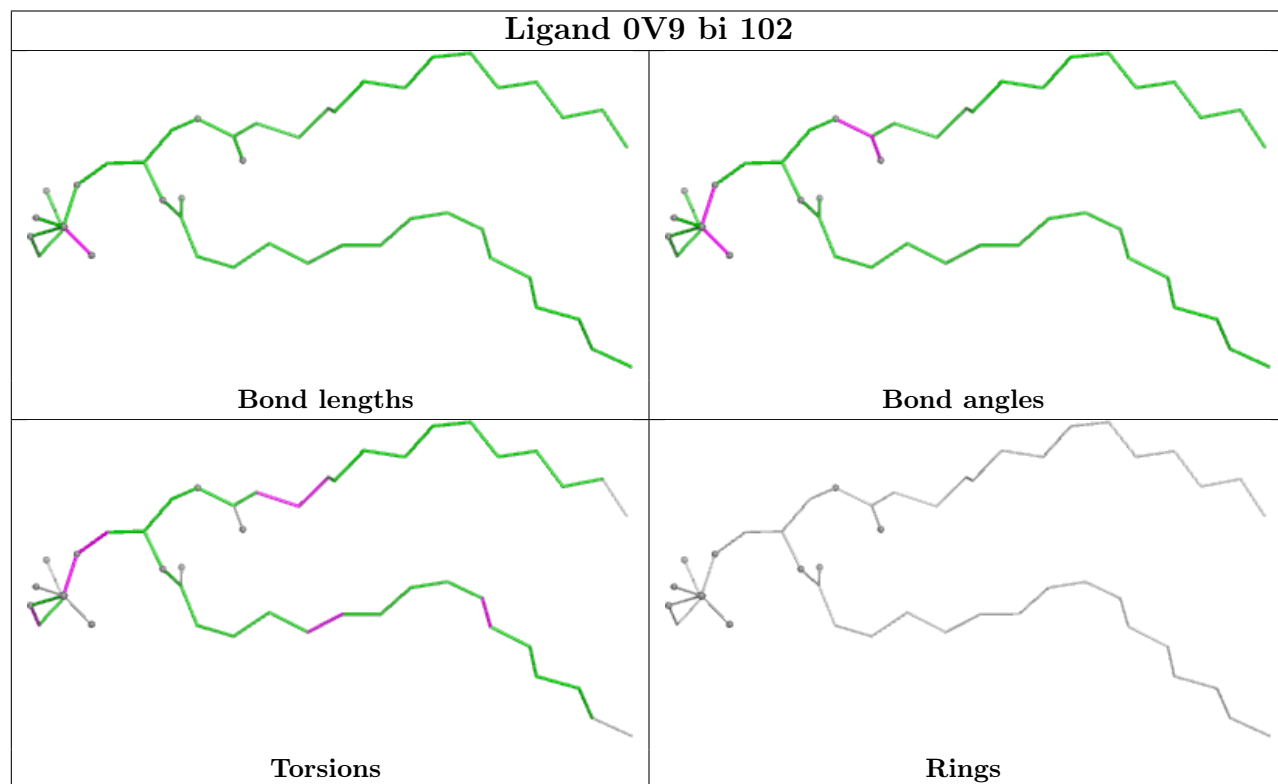
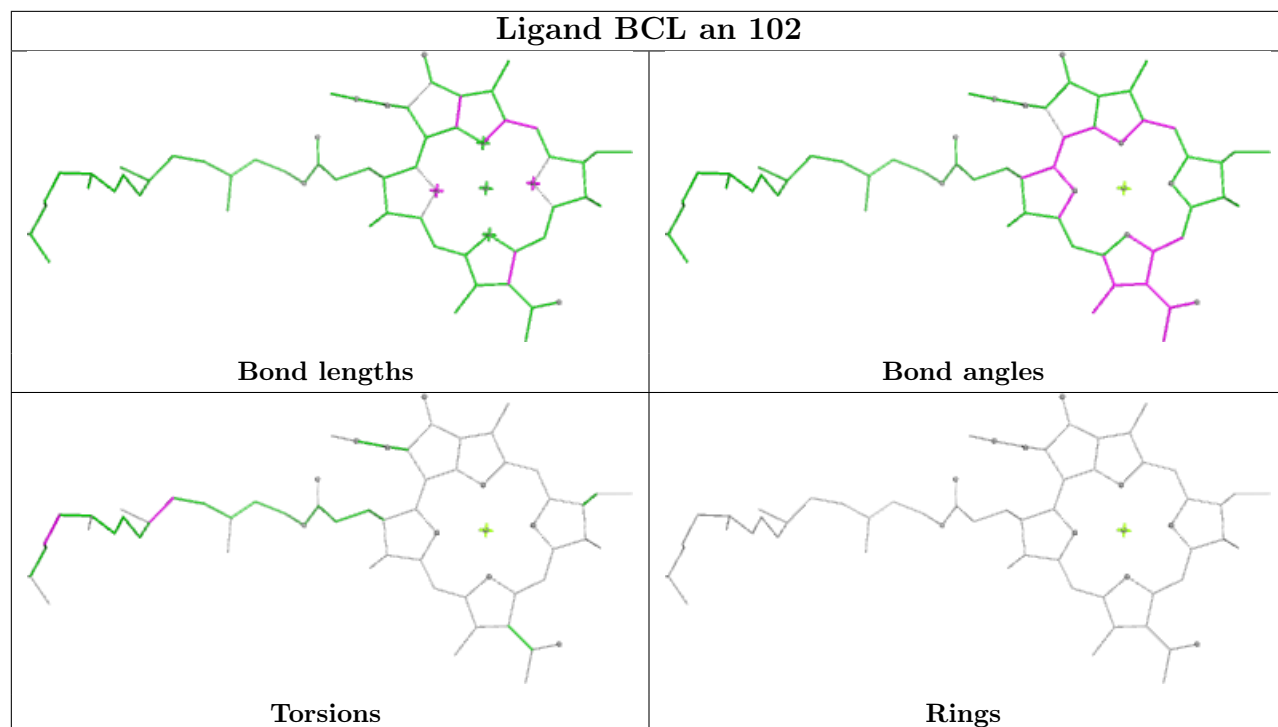


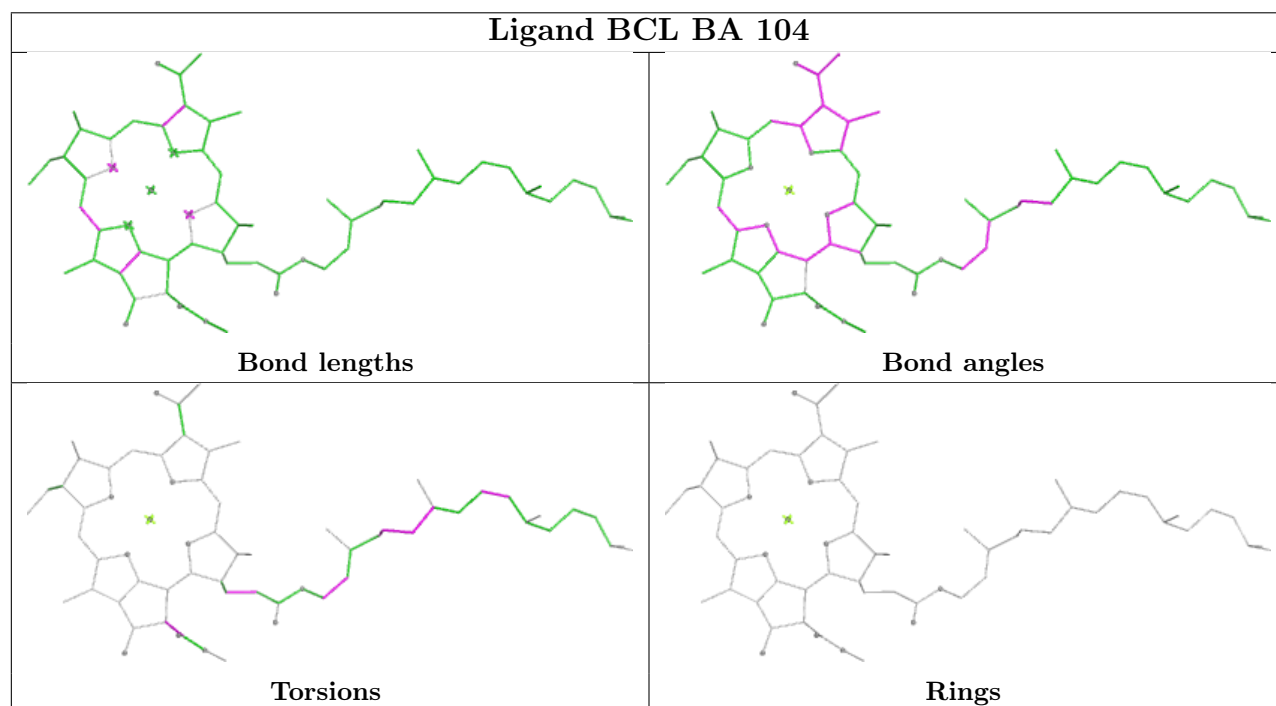
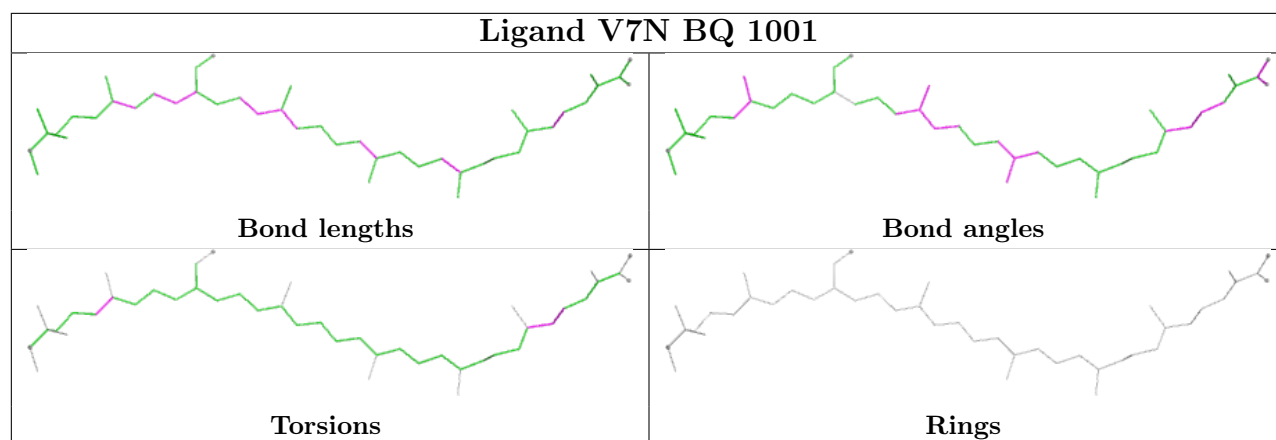
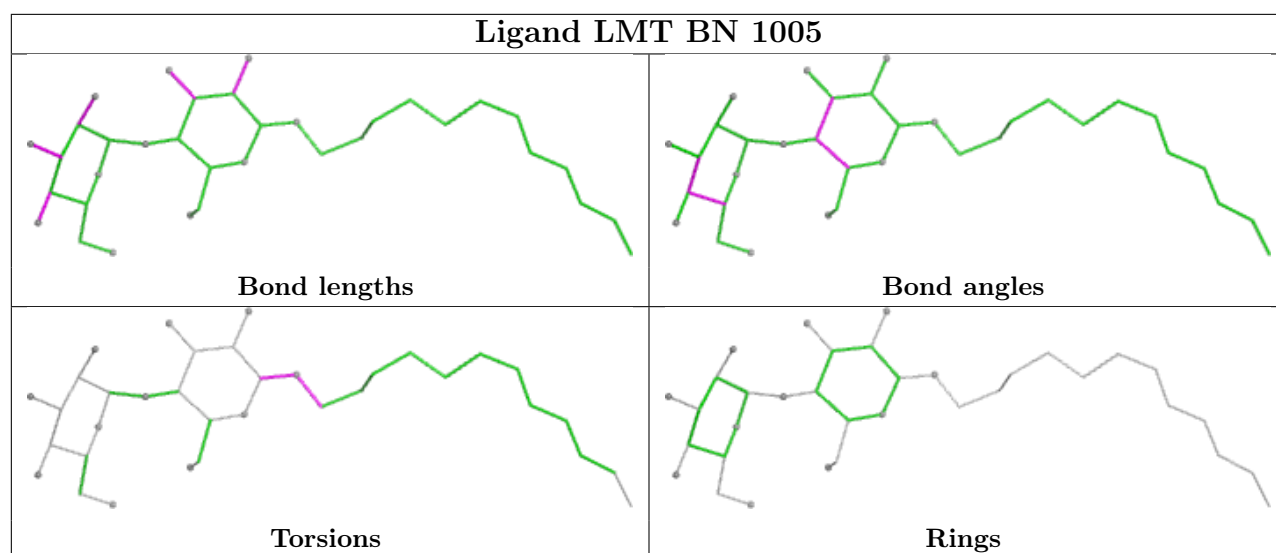


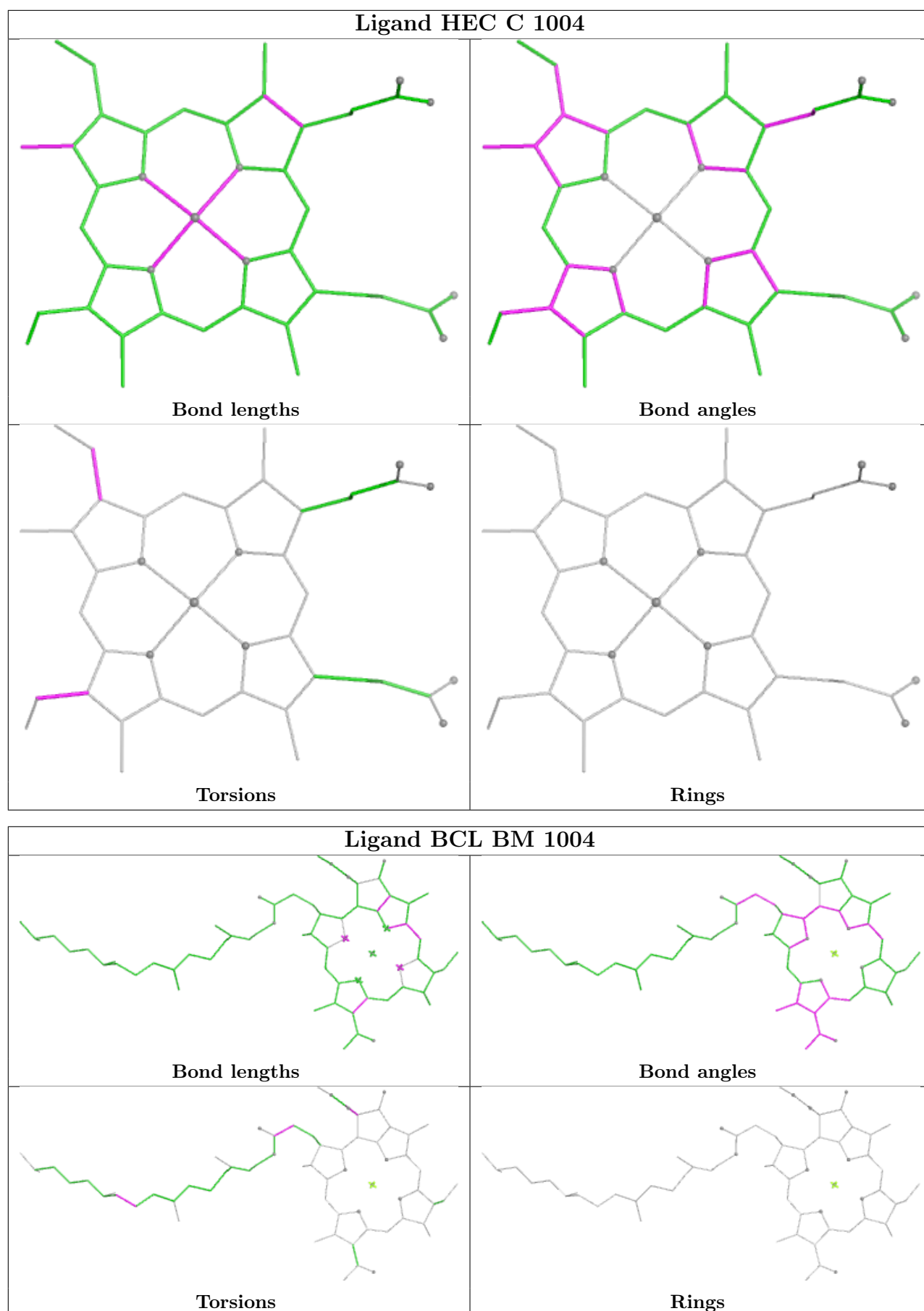


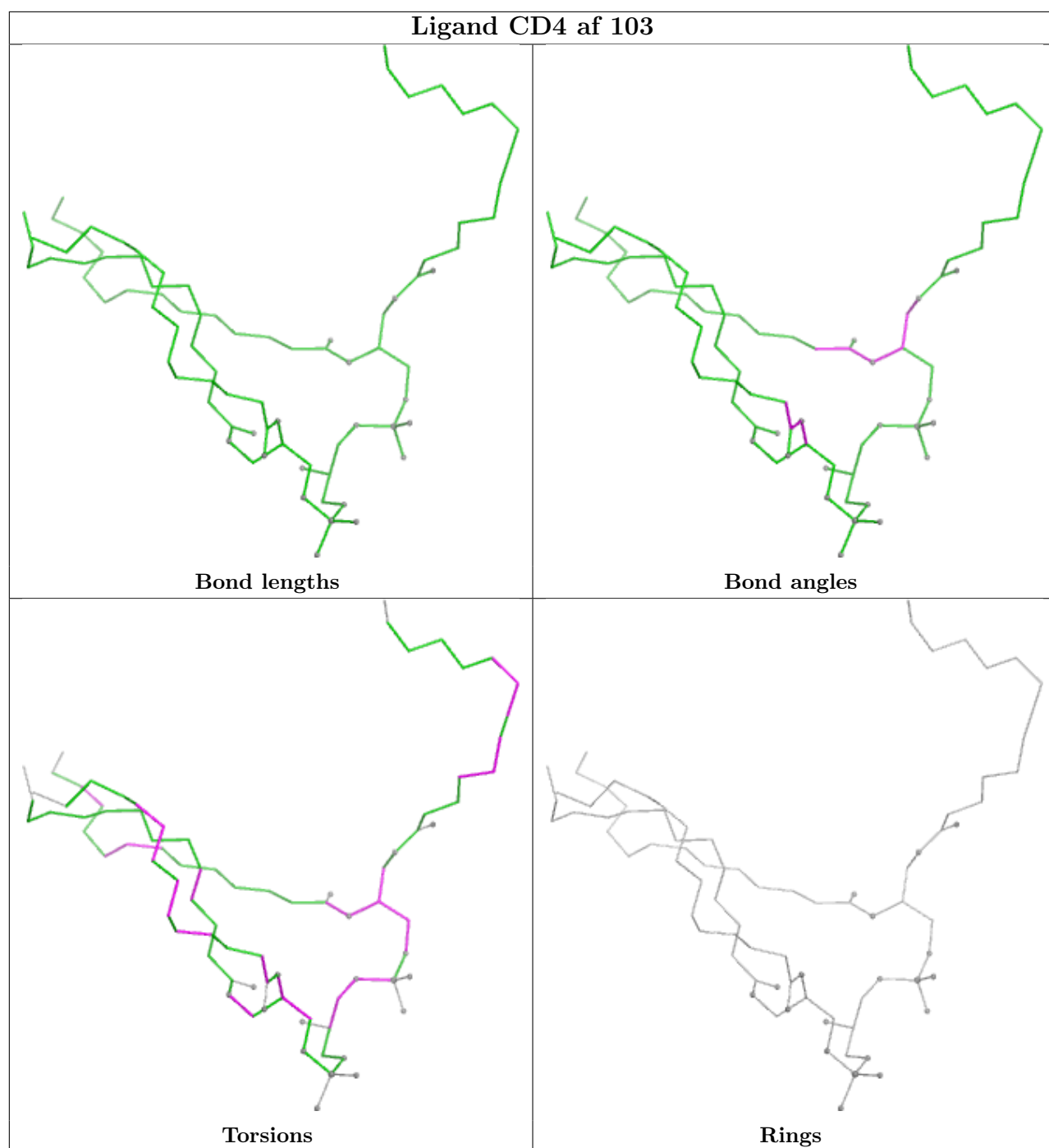


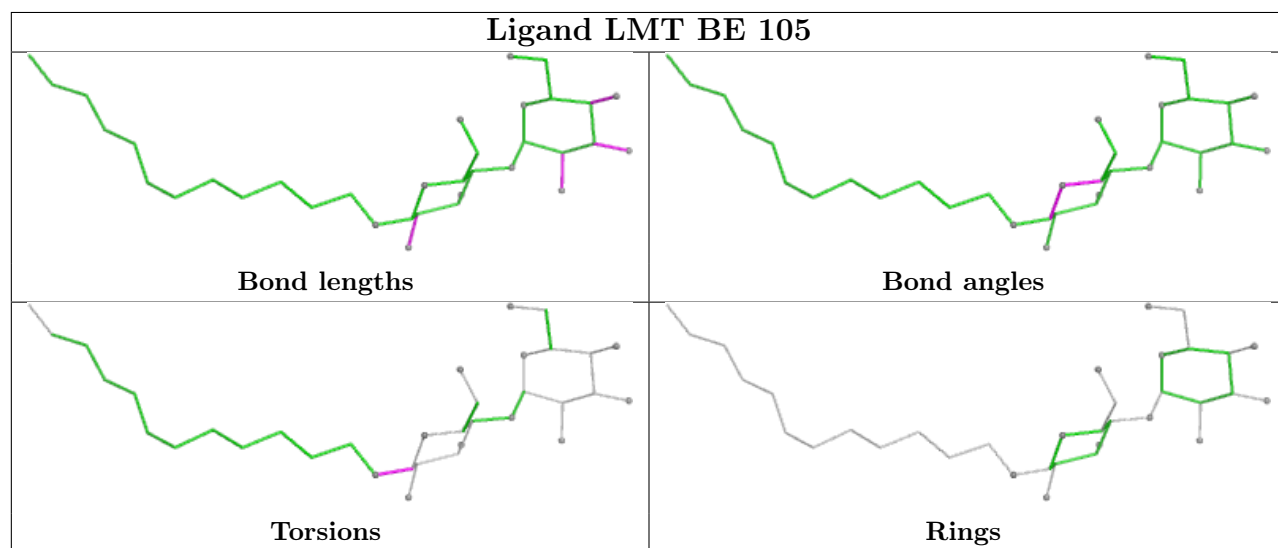
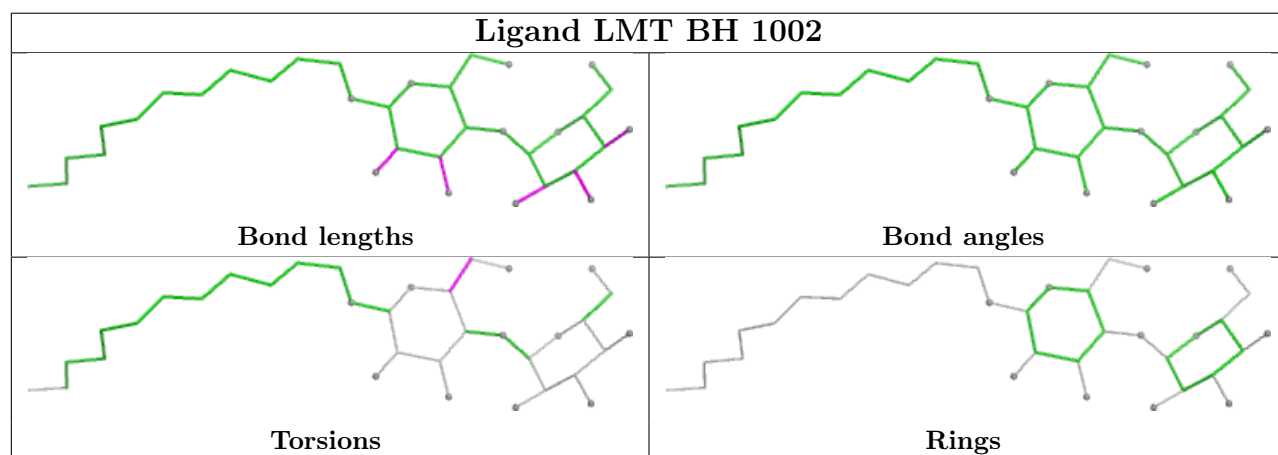
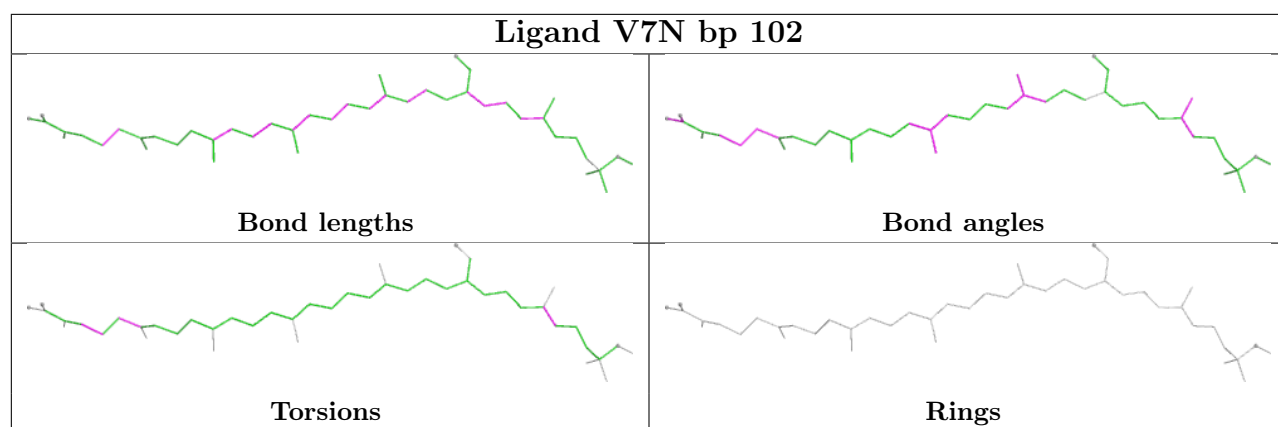


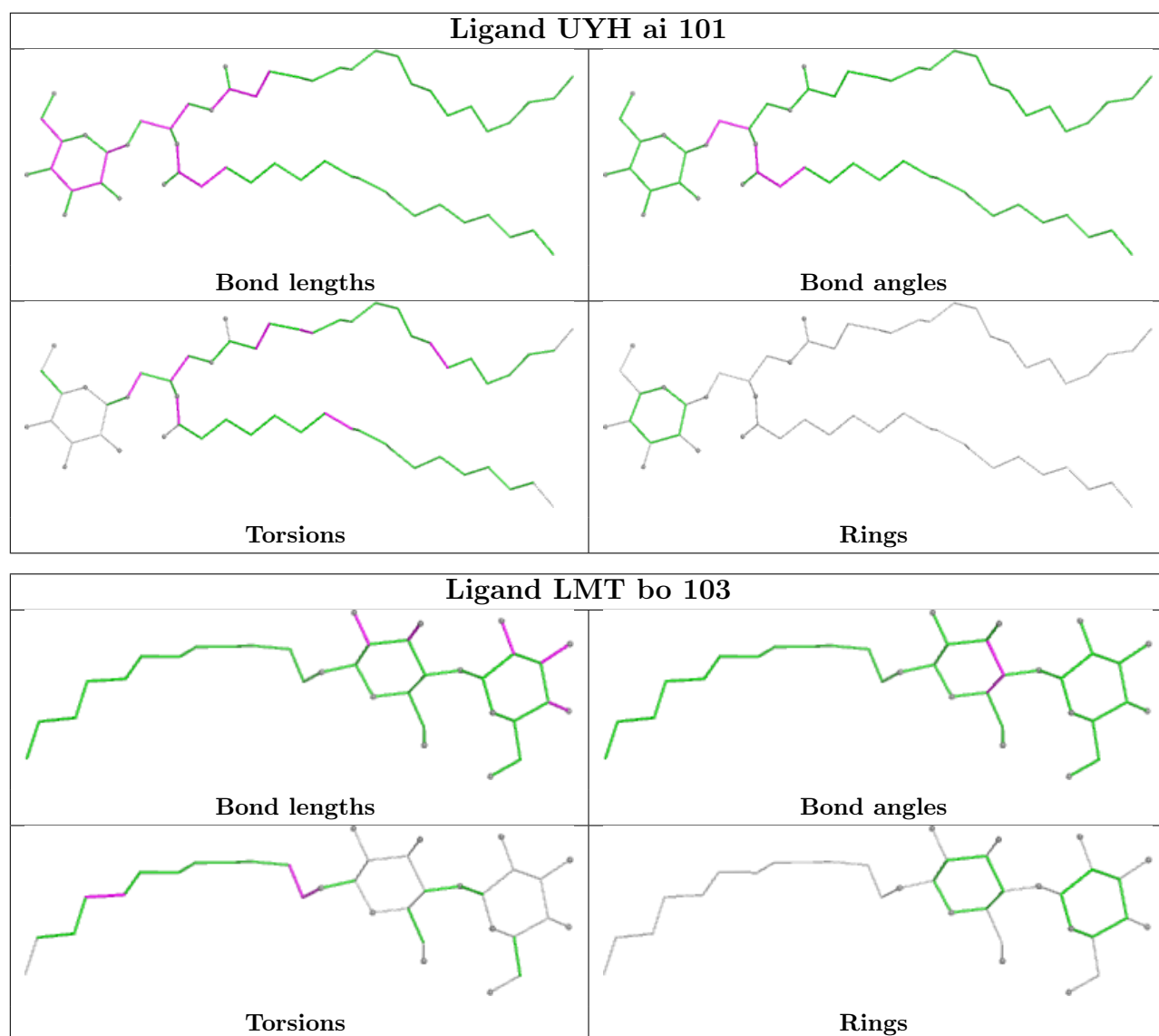


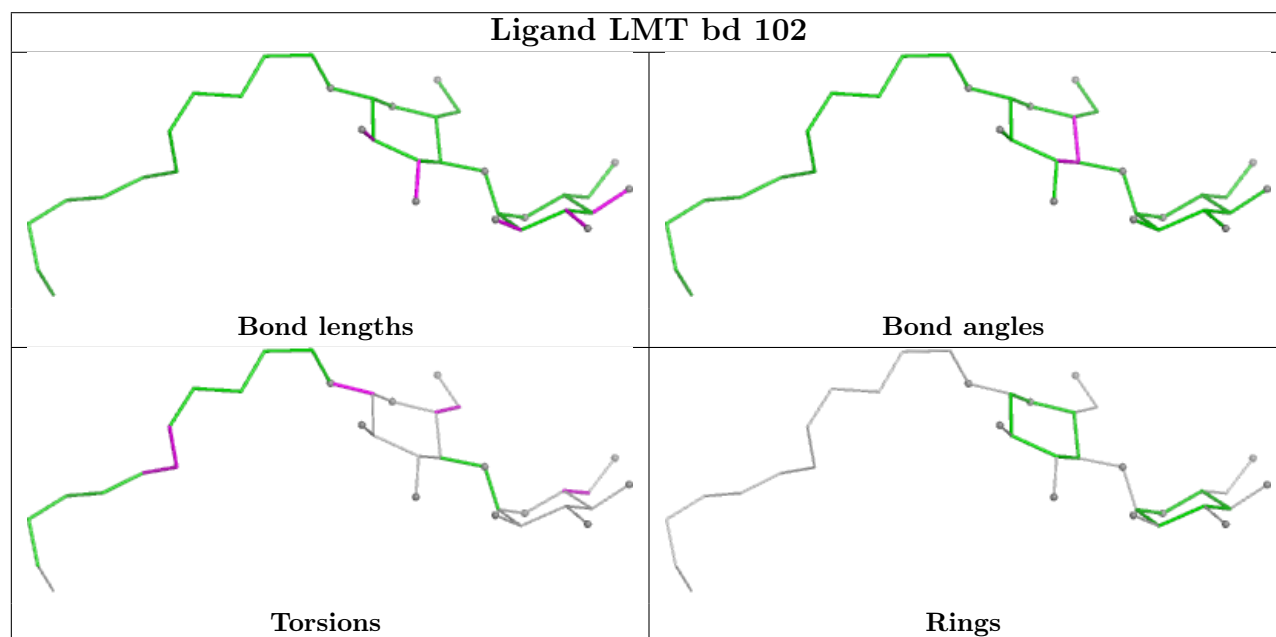
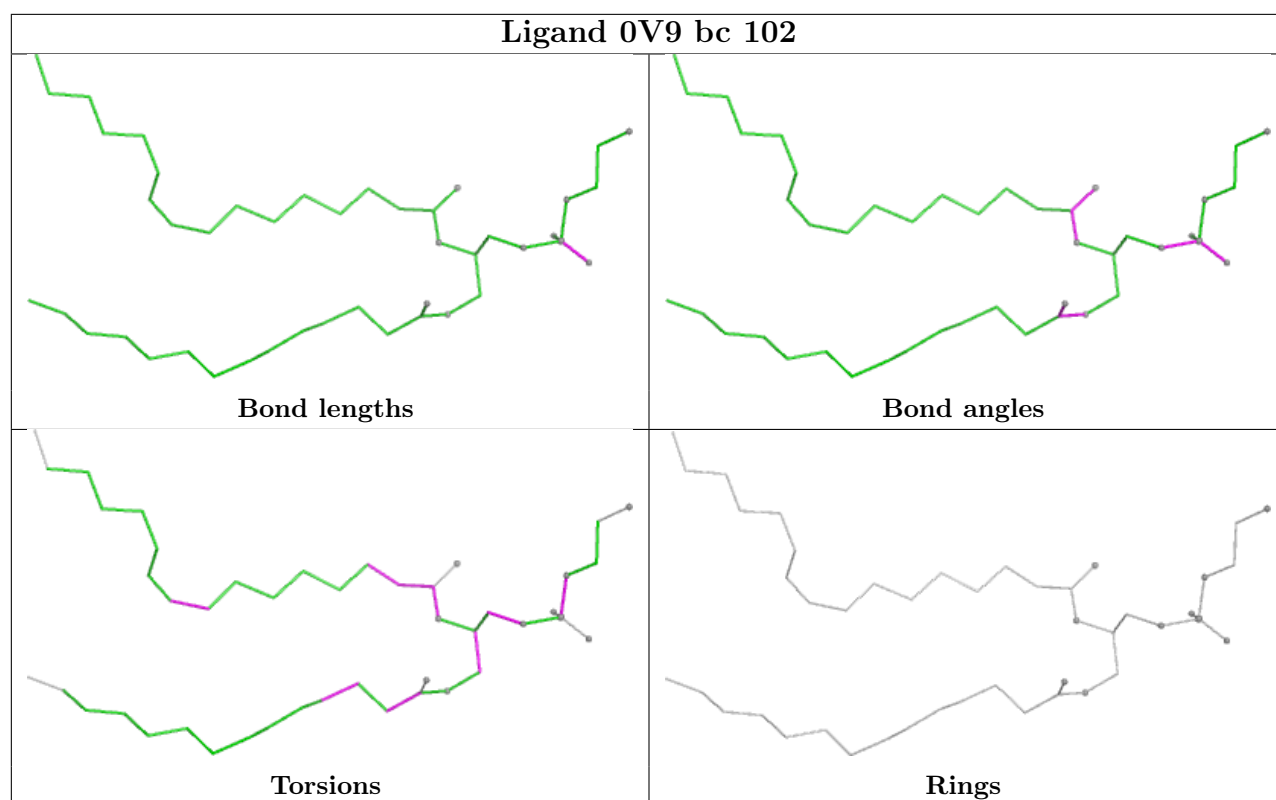


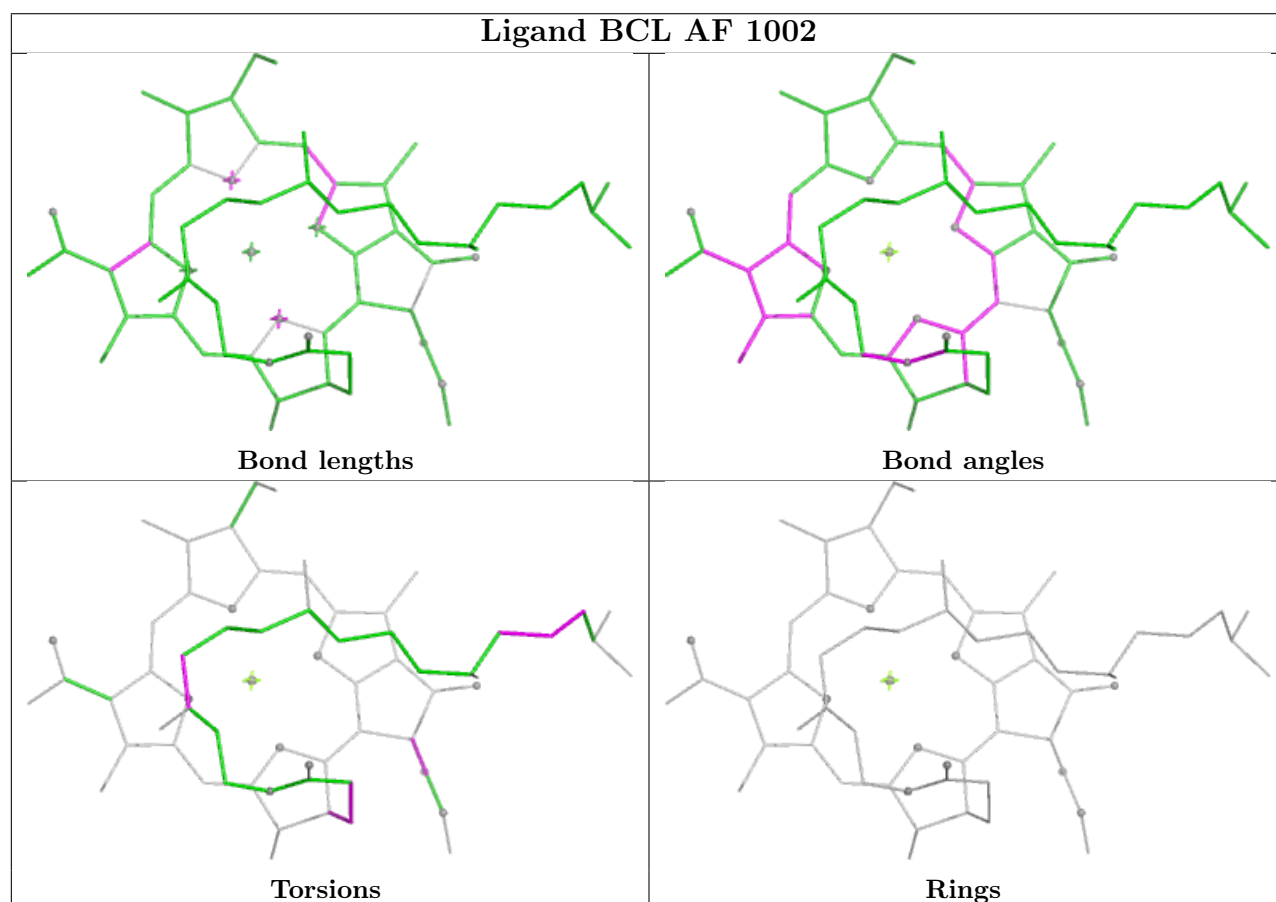
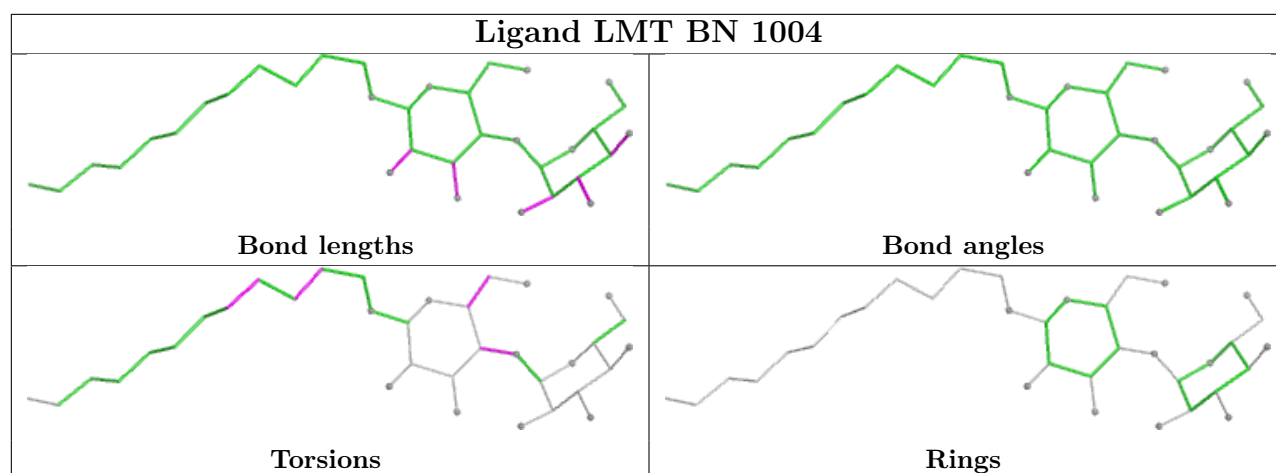


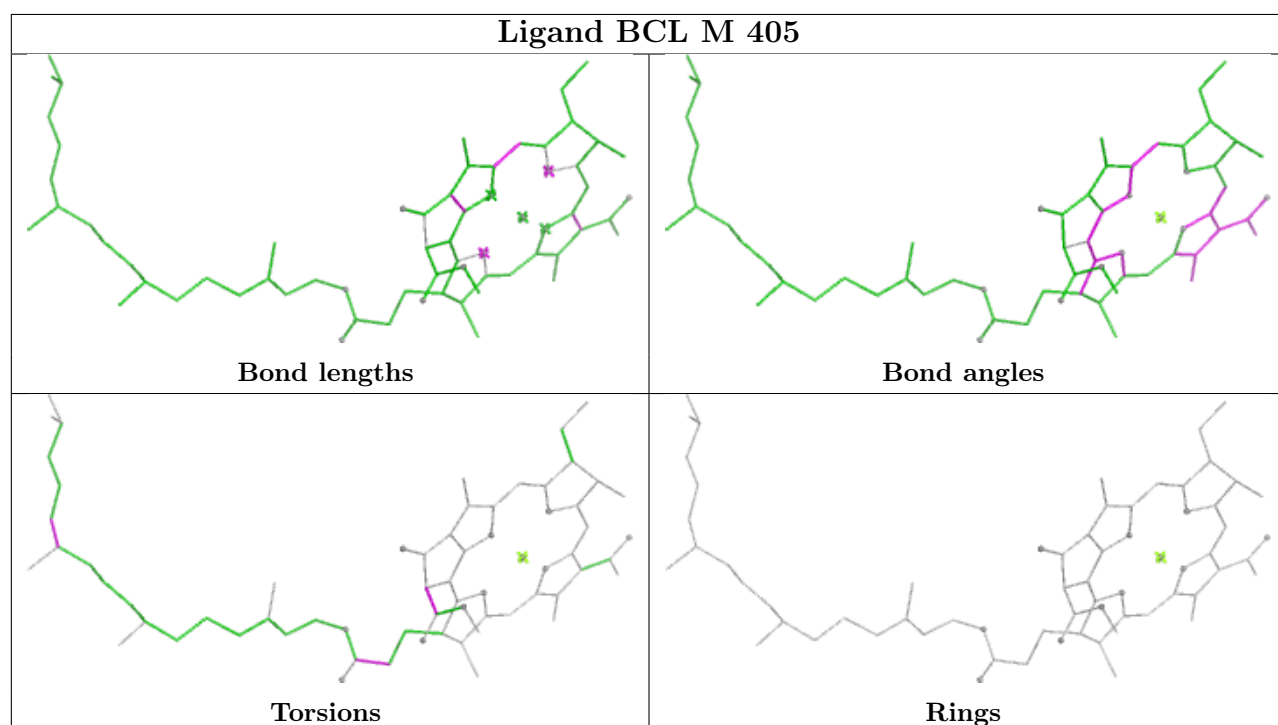
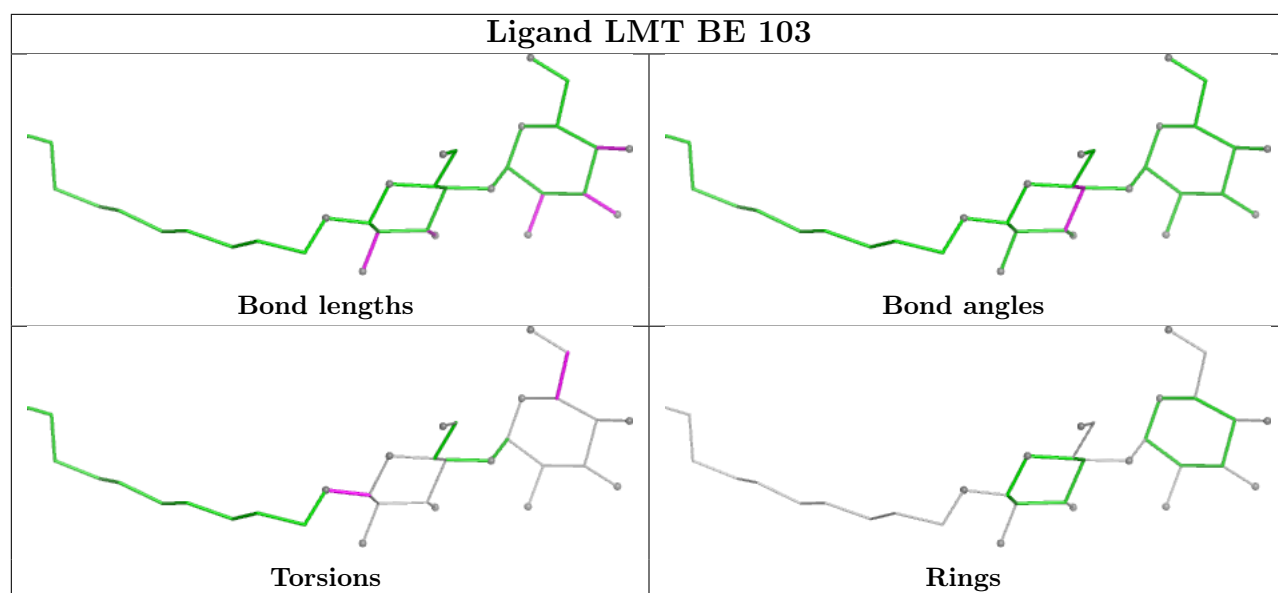


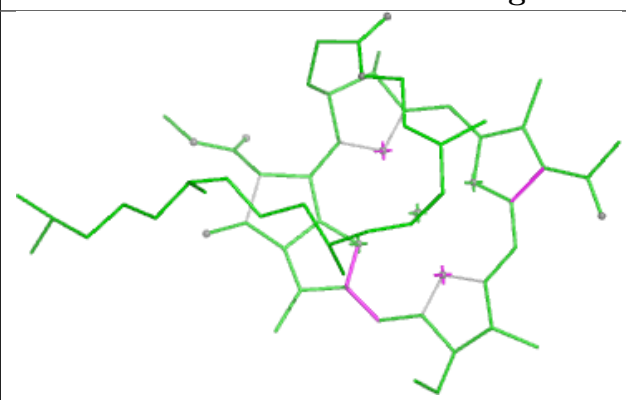
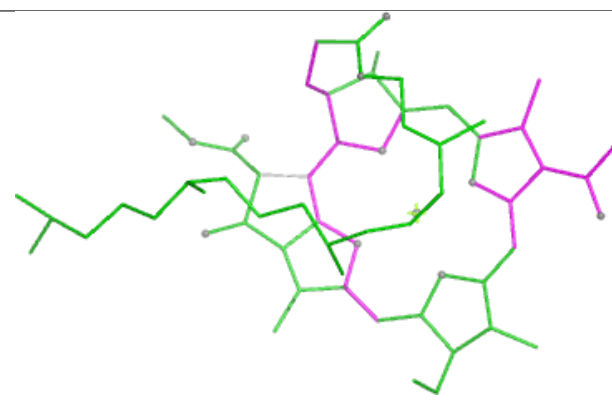
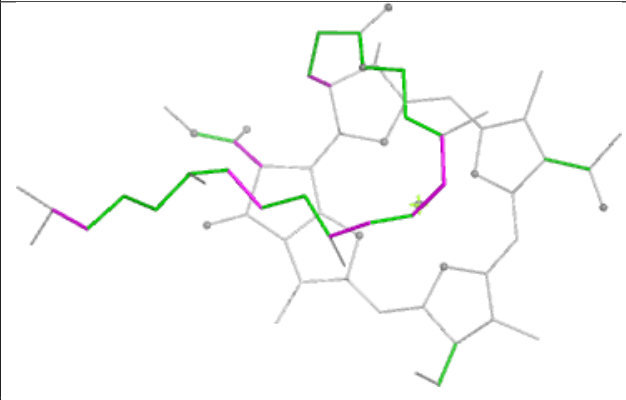
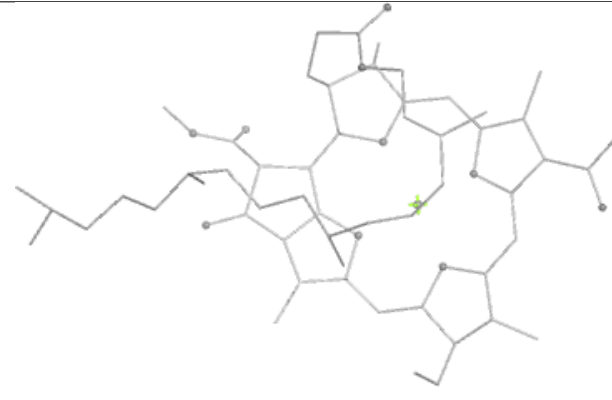


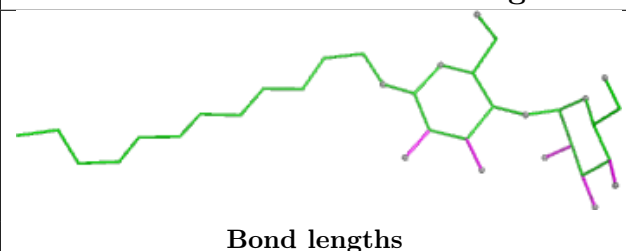
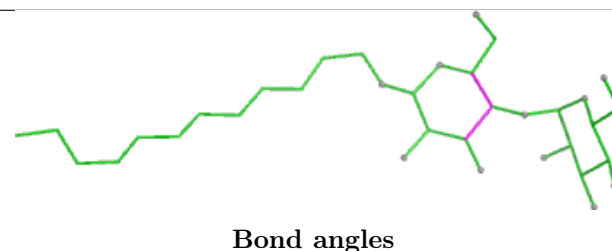
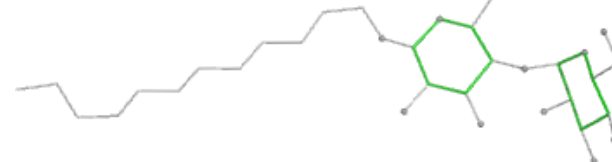


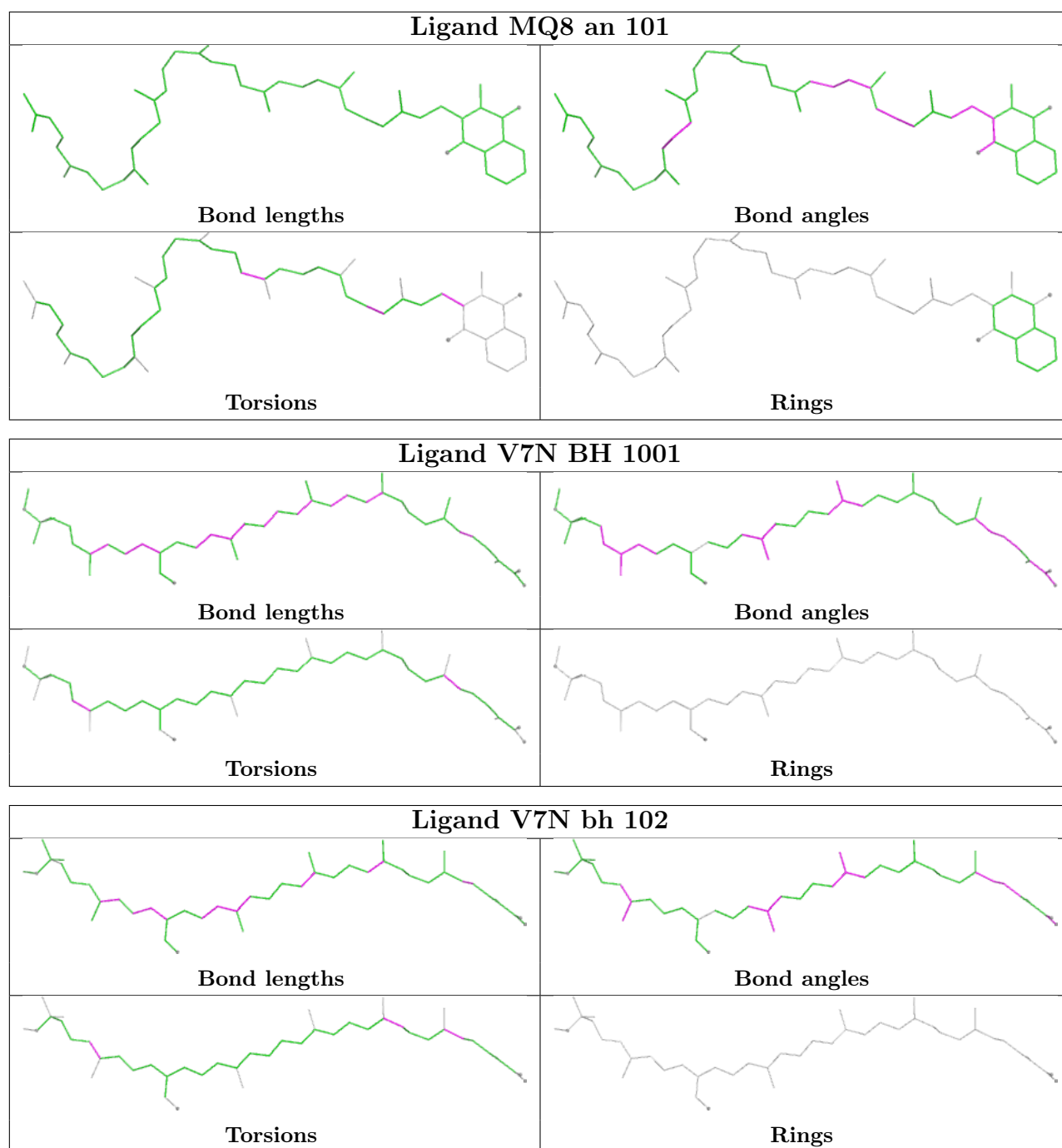


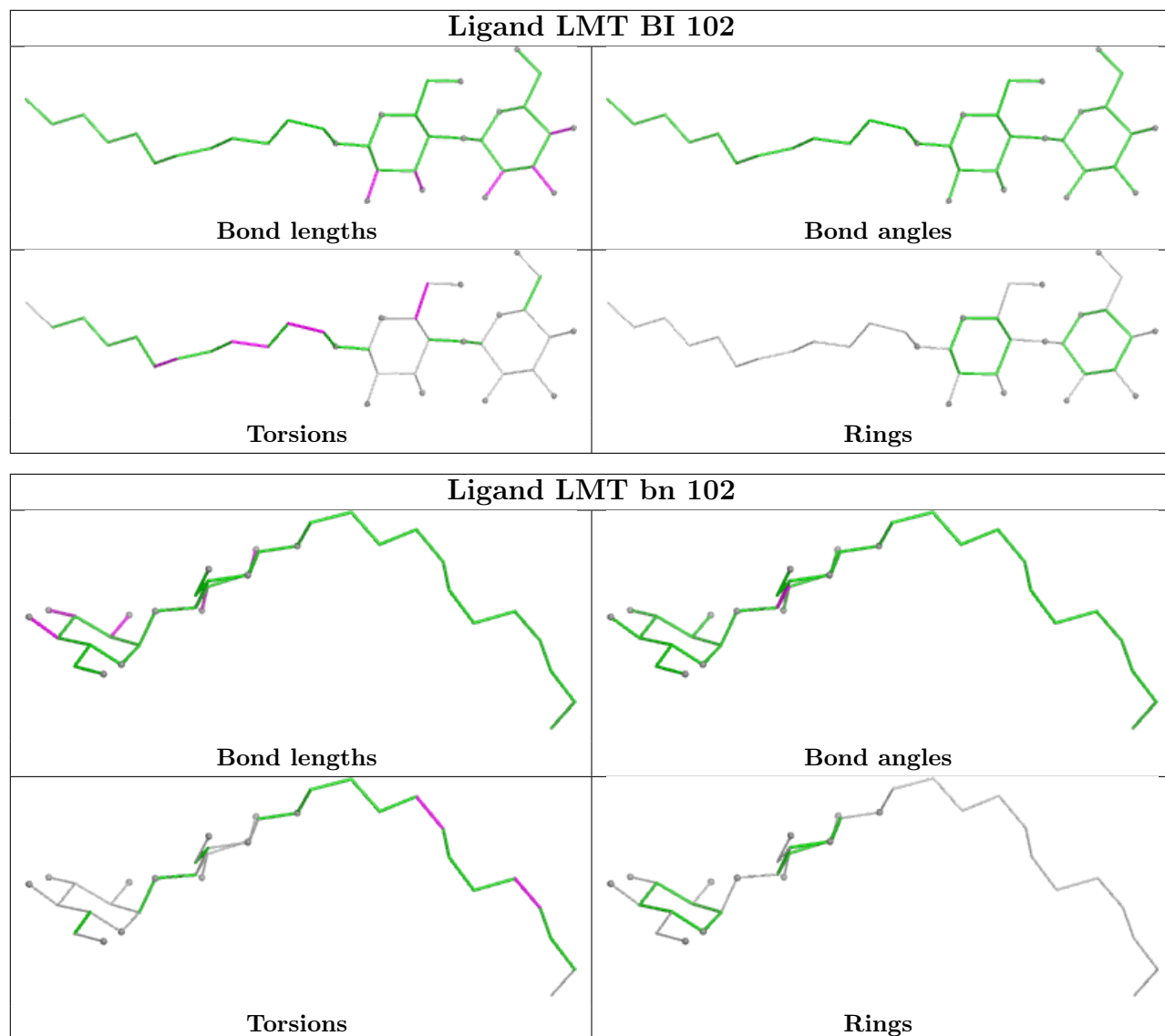


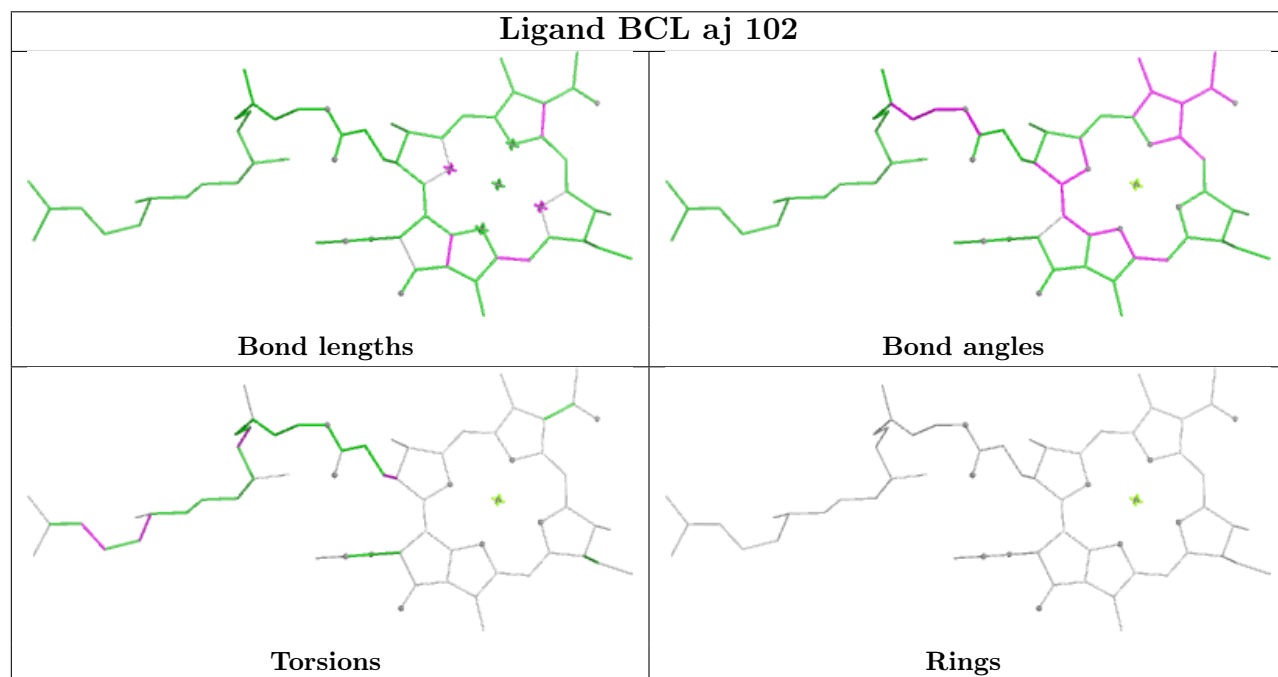
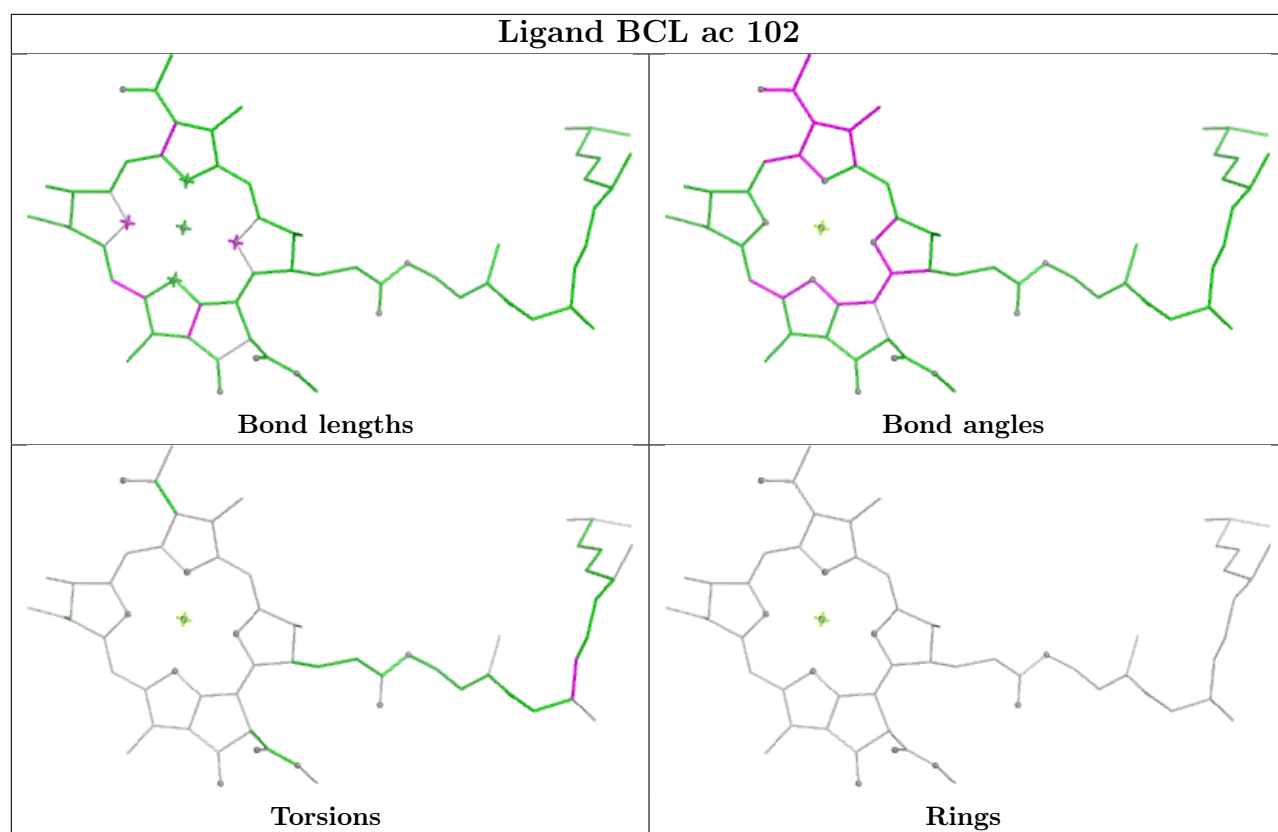


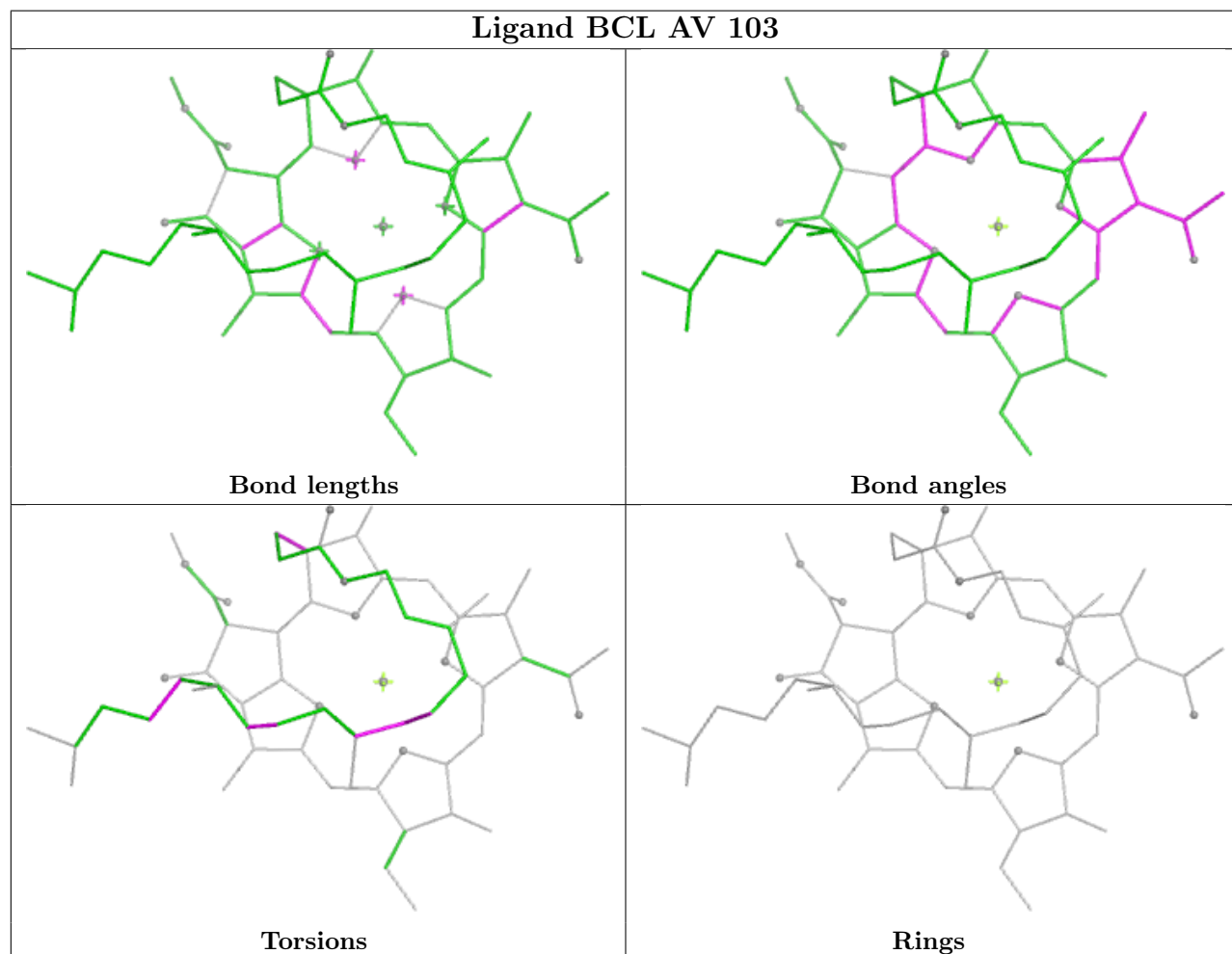
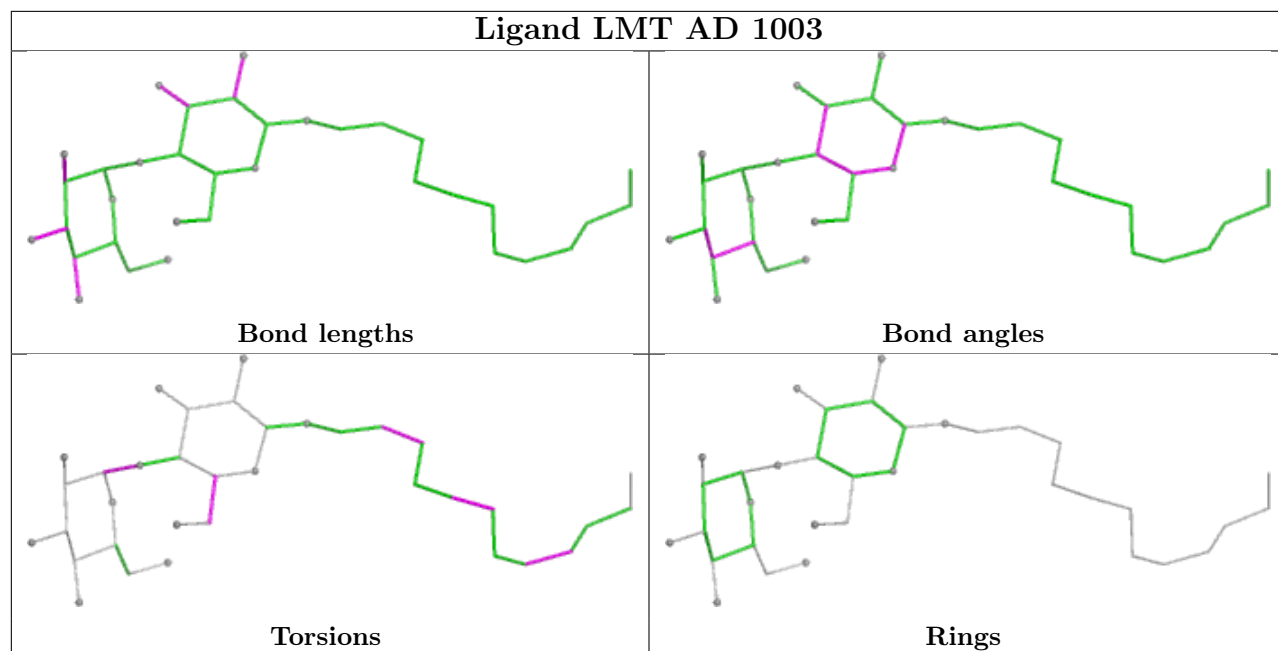
Ligand BCL AO 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT AJ 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

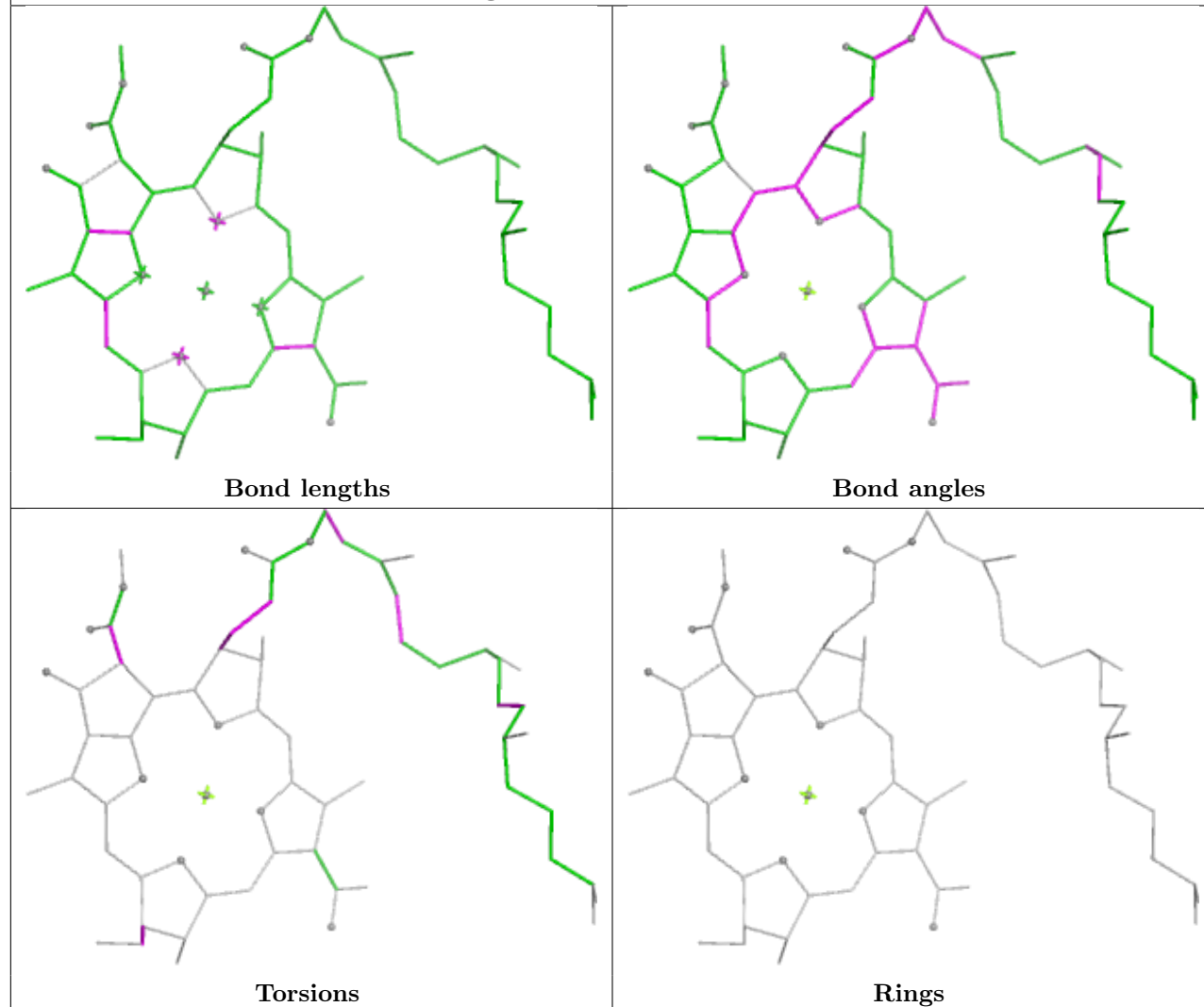




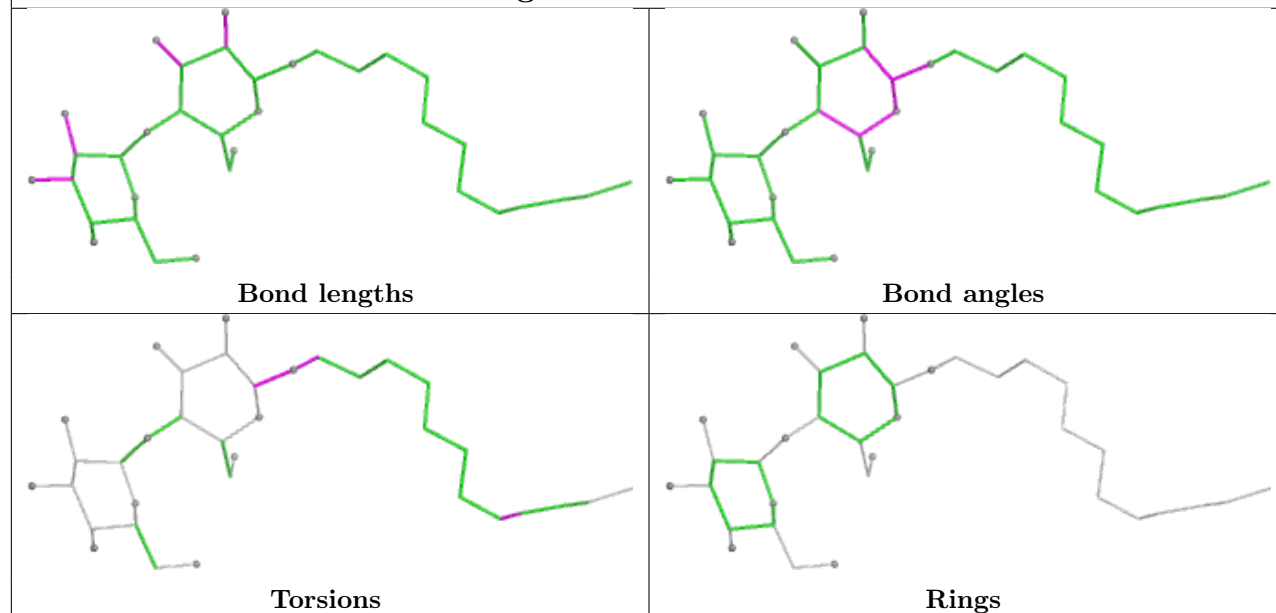


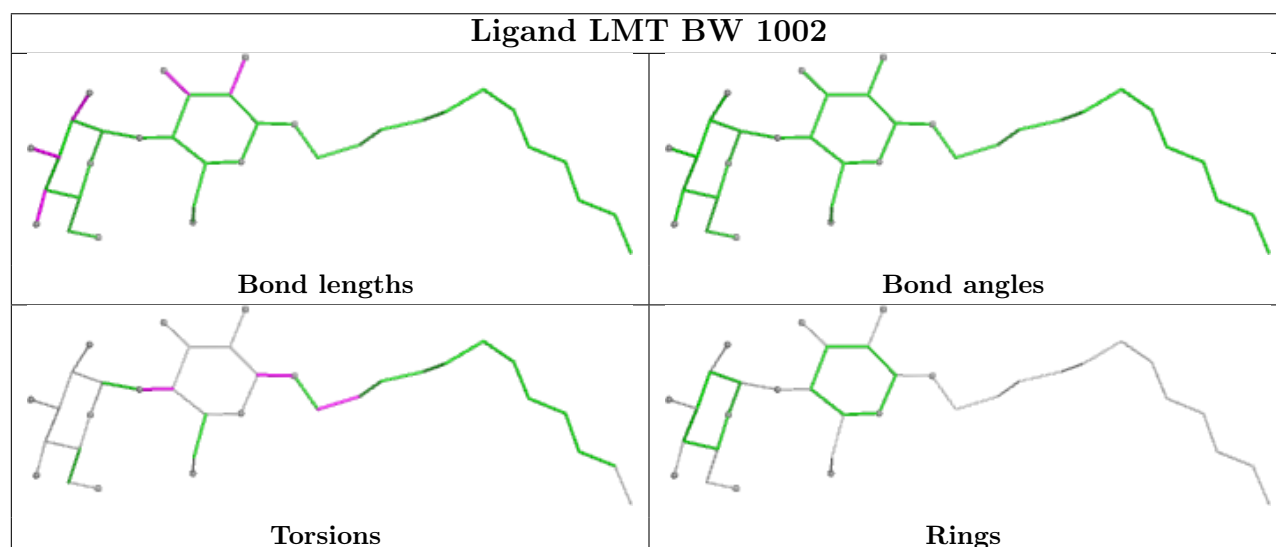
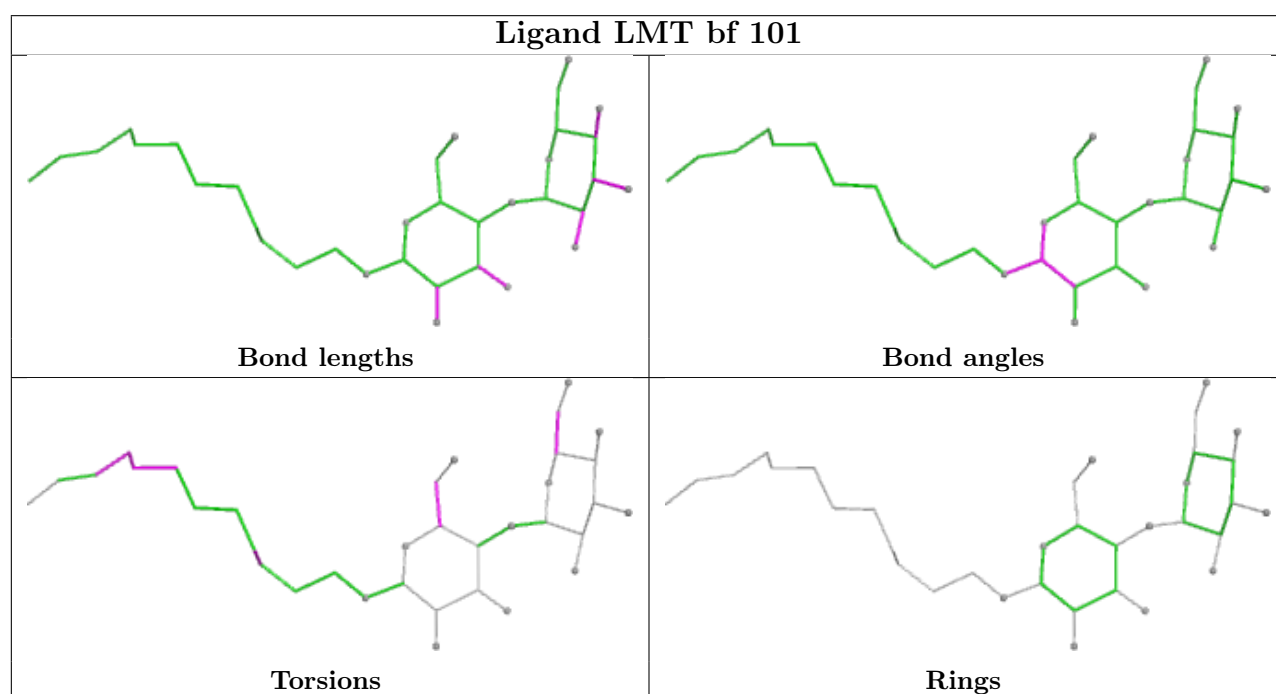
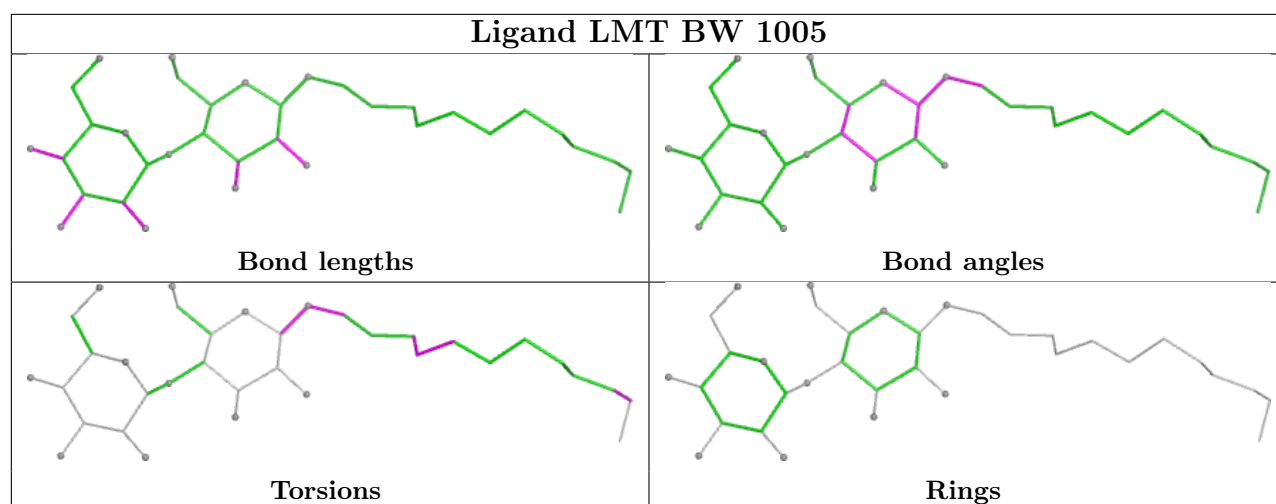


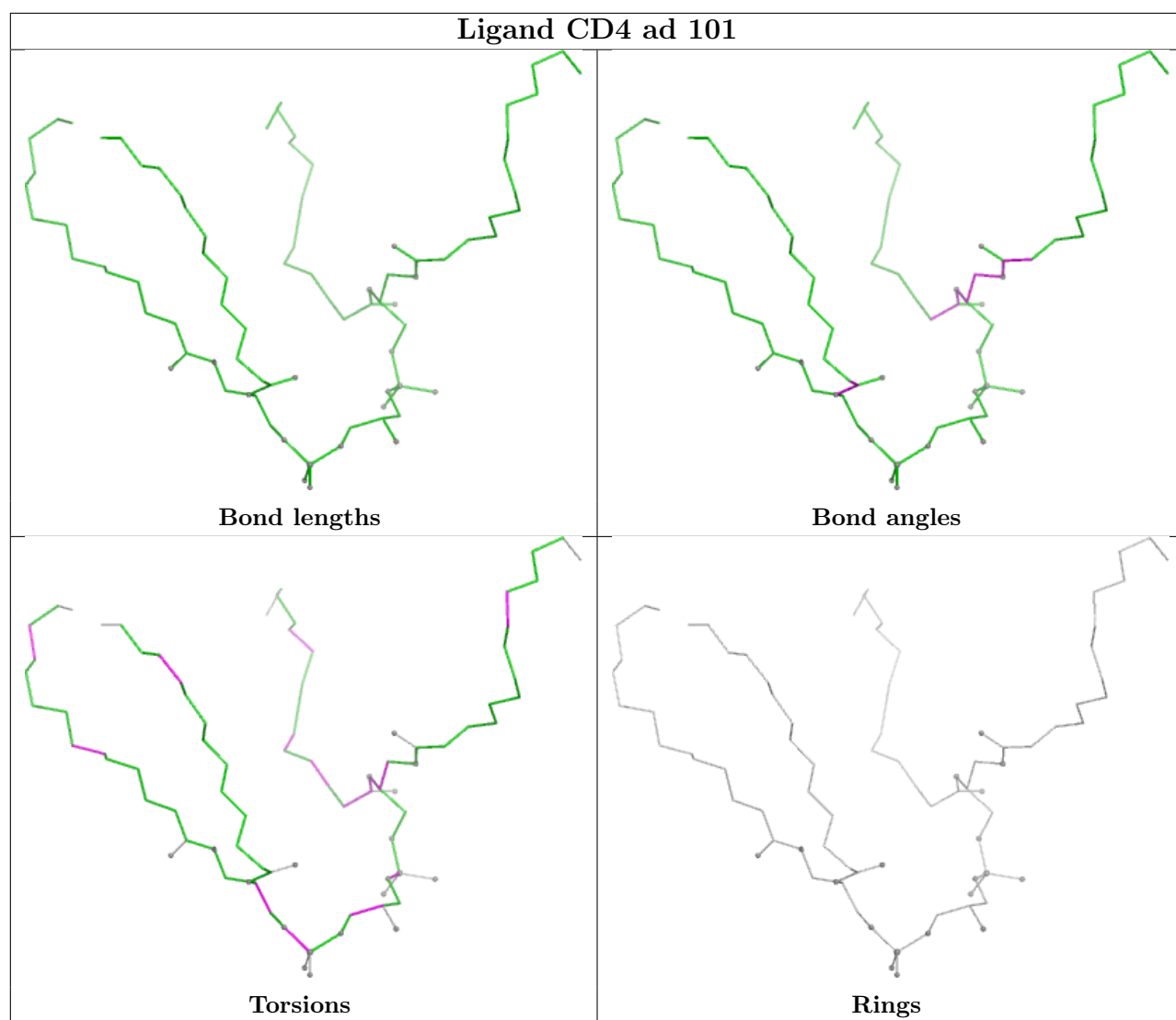
Ligand BCL BT 1004

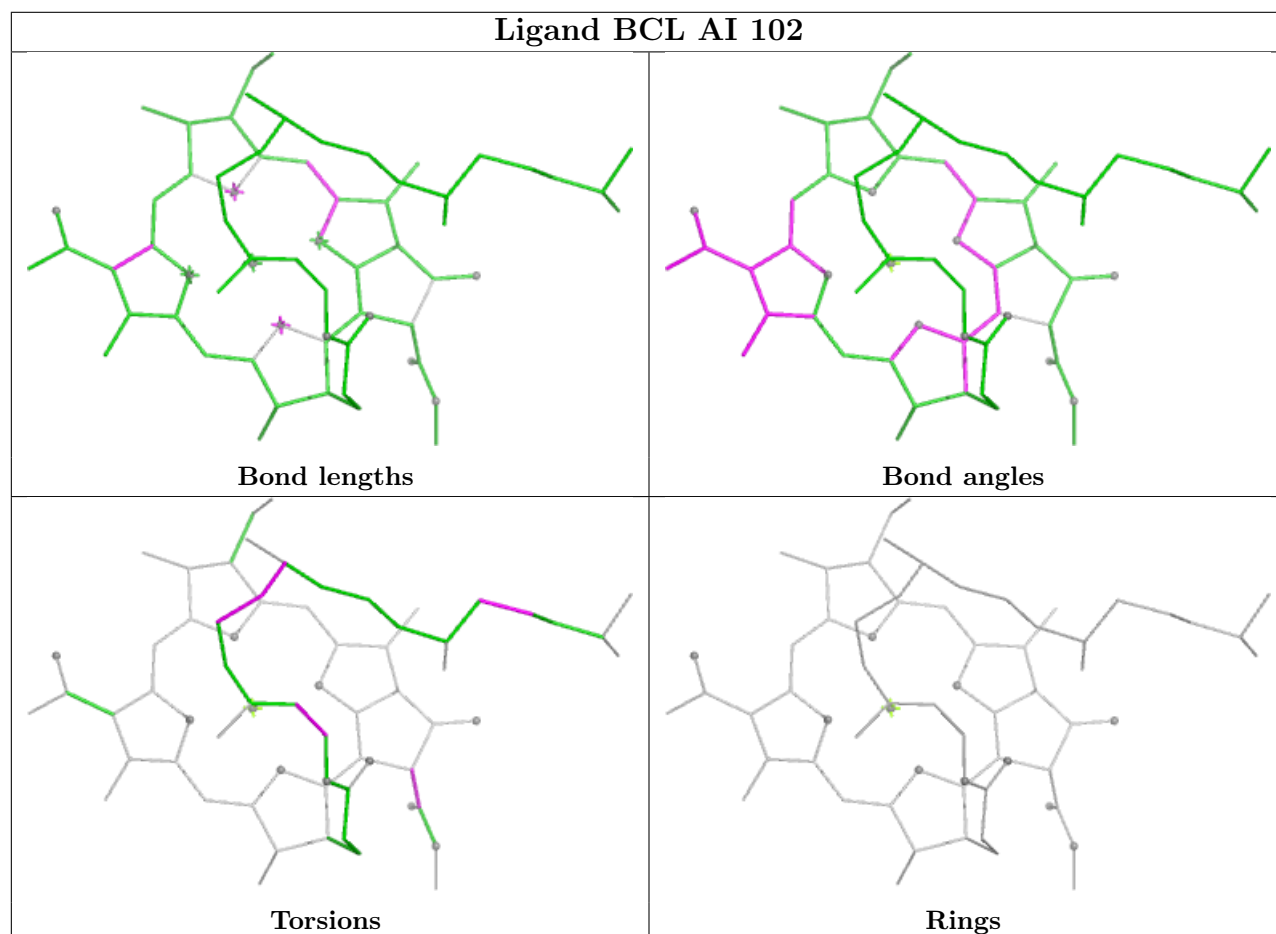
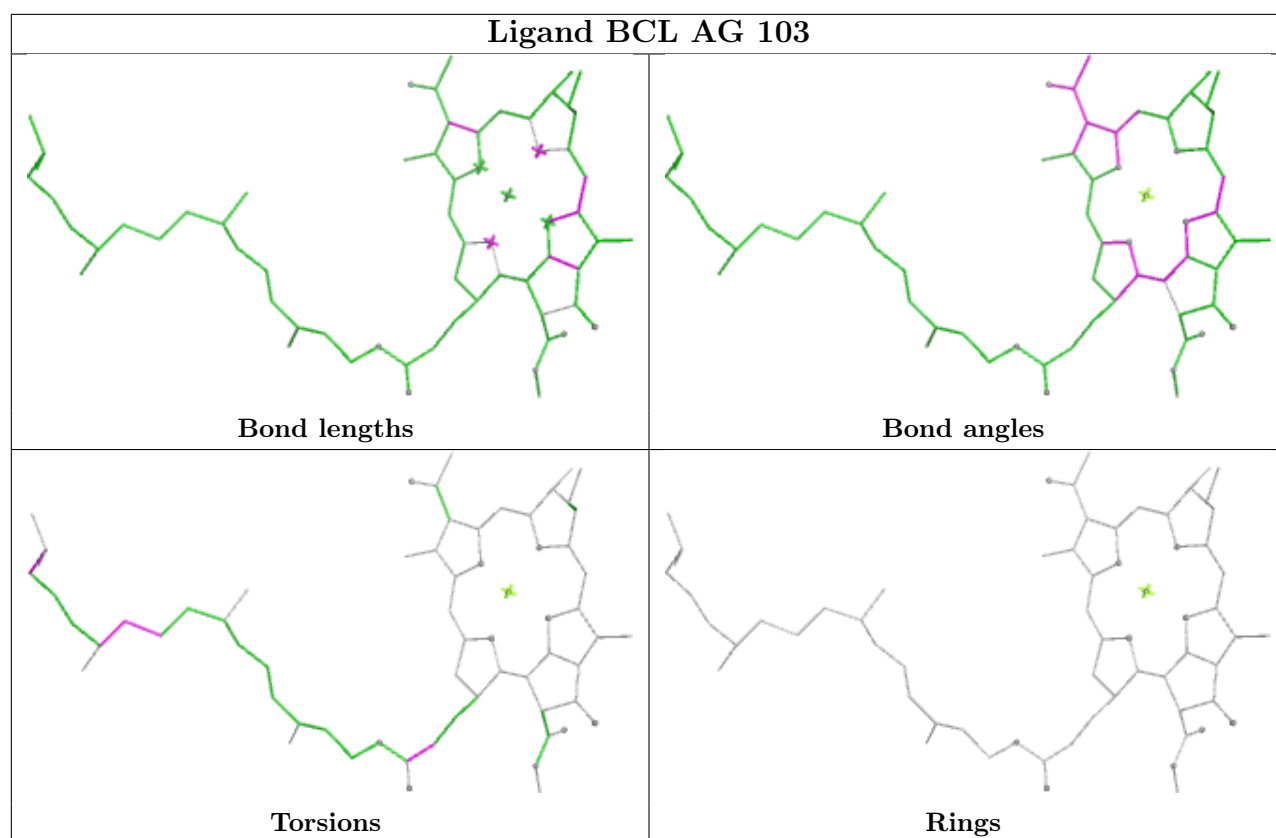


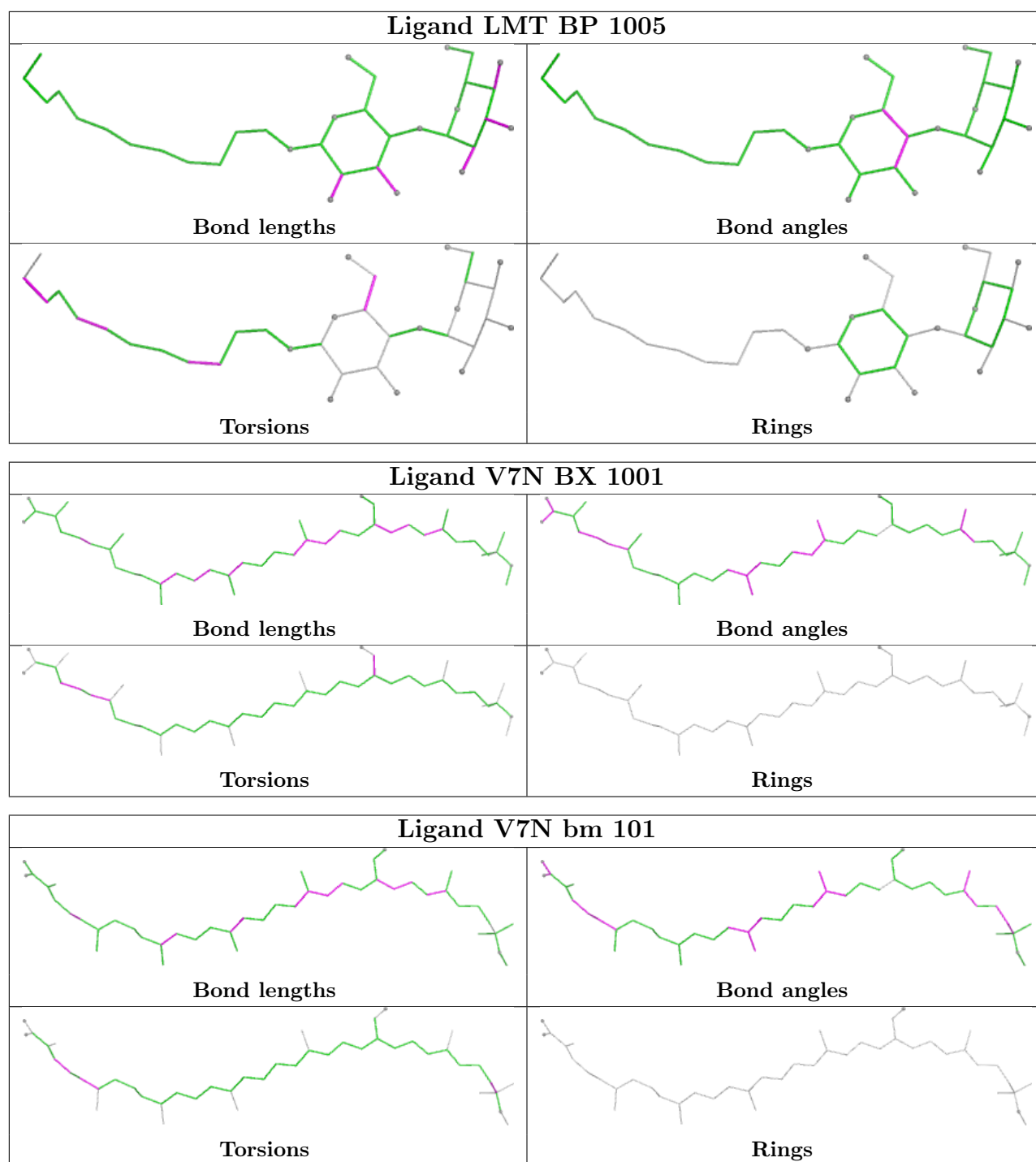
Ligand LMT AV 101

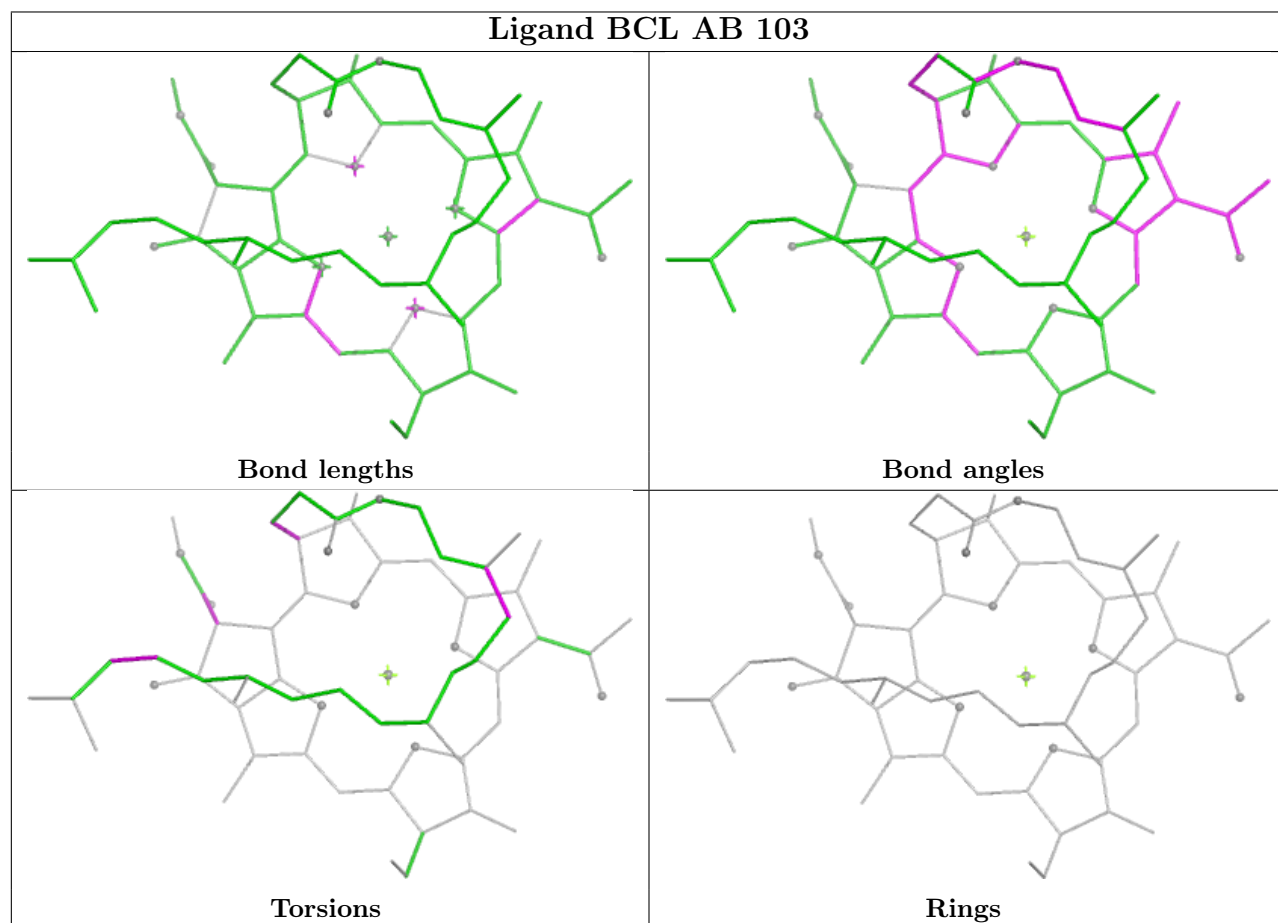
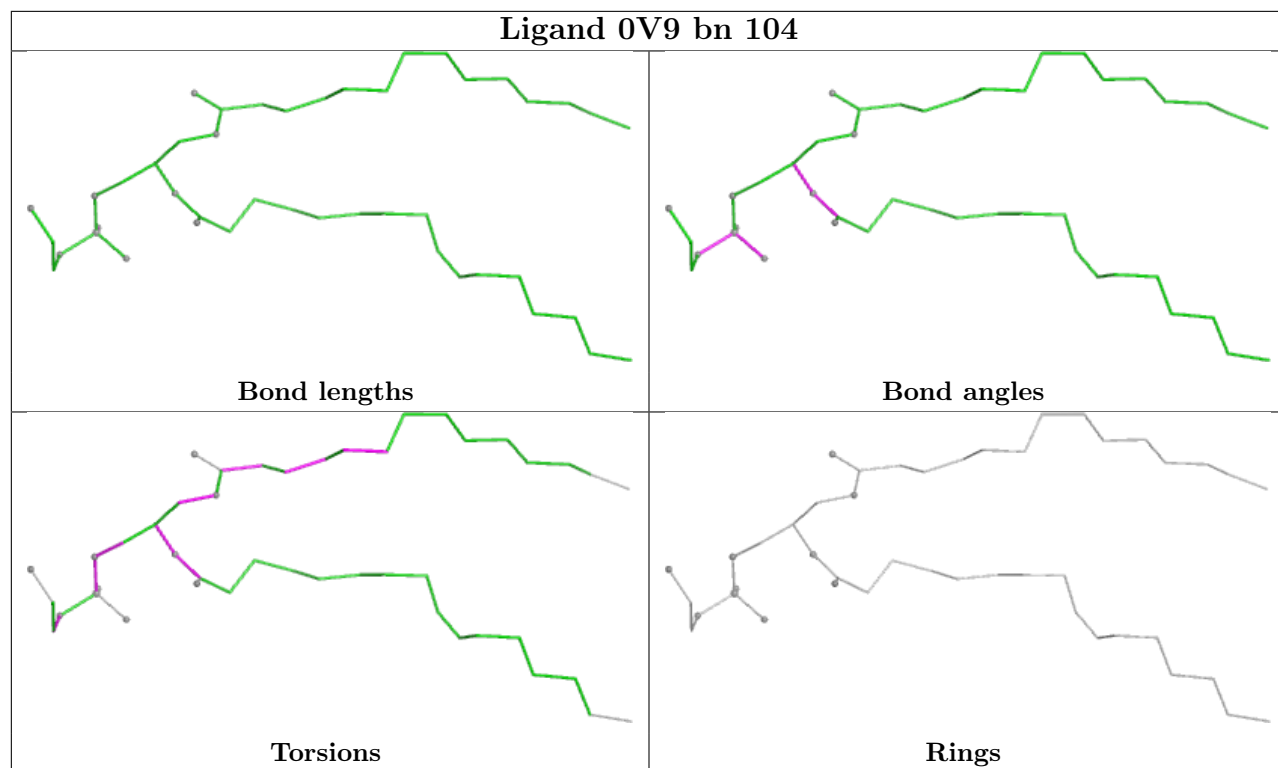


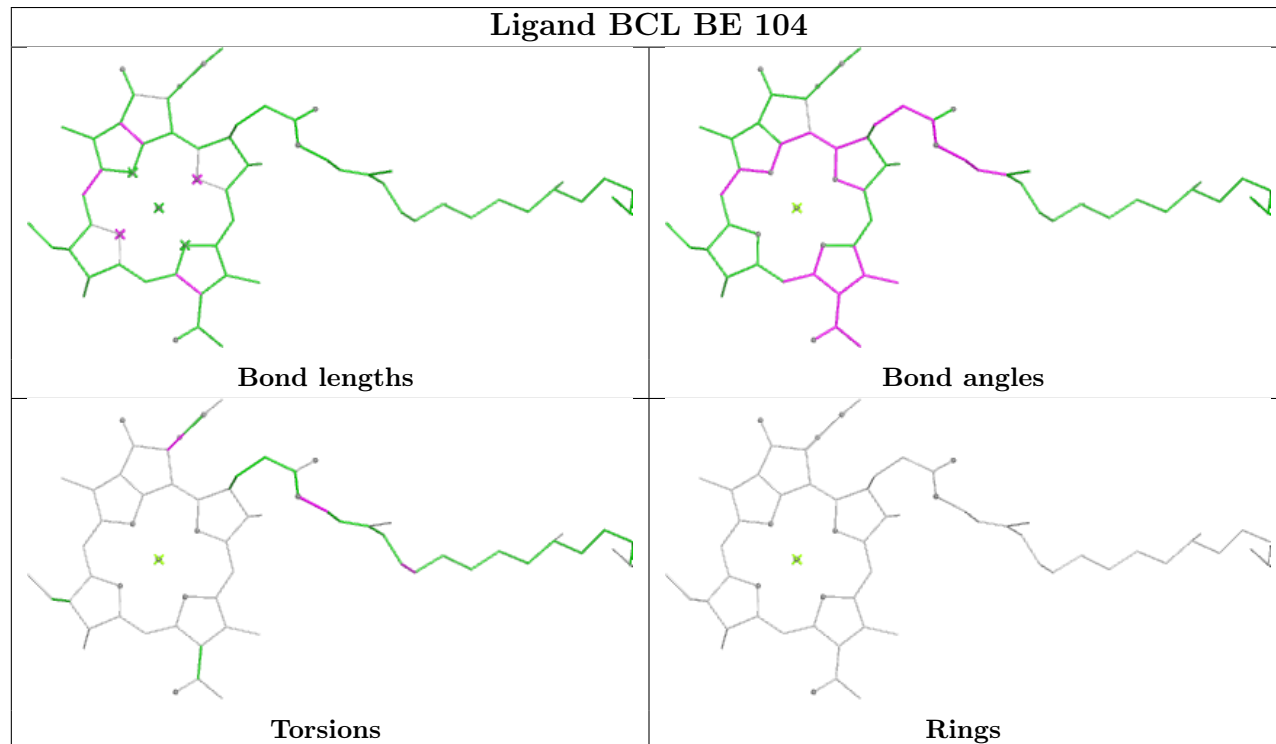
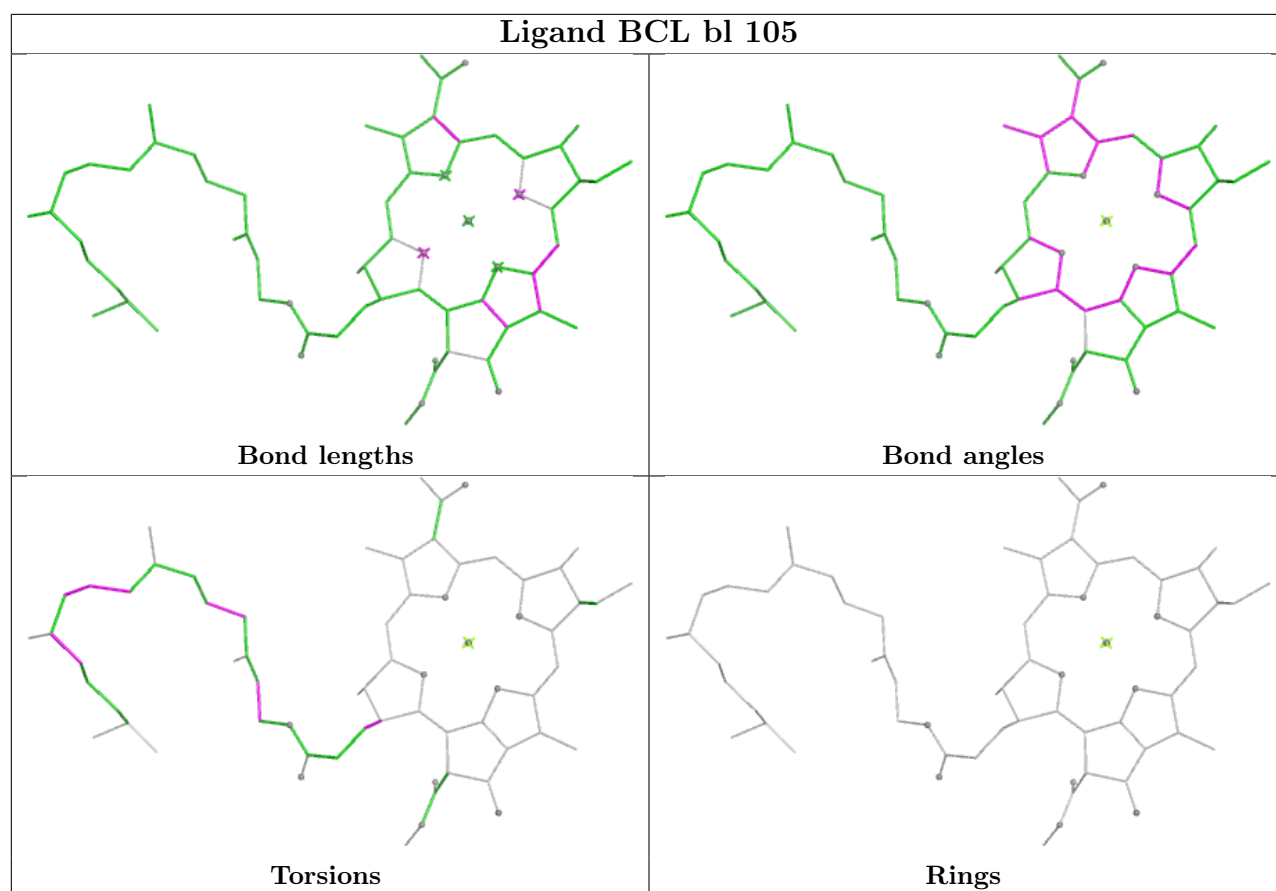




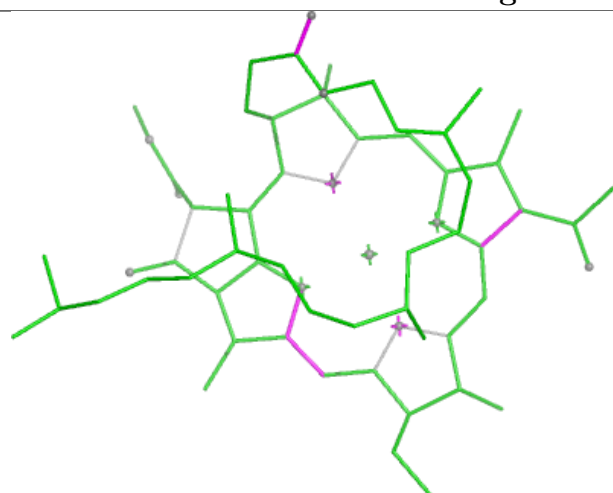




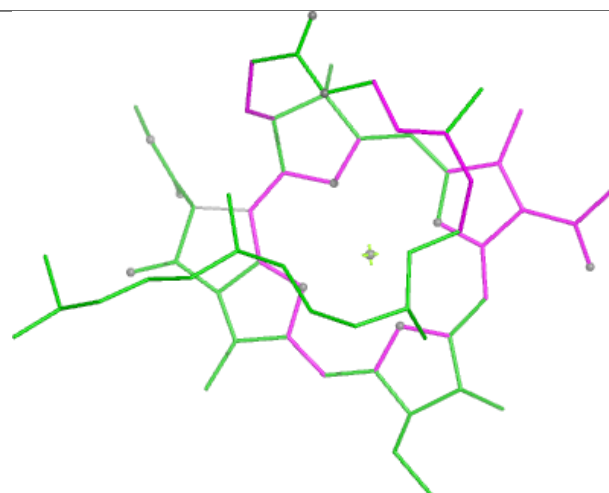




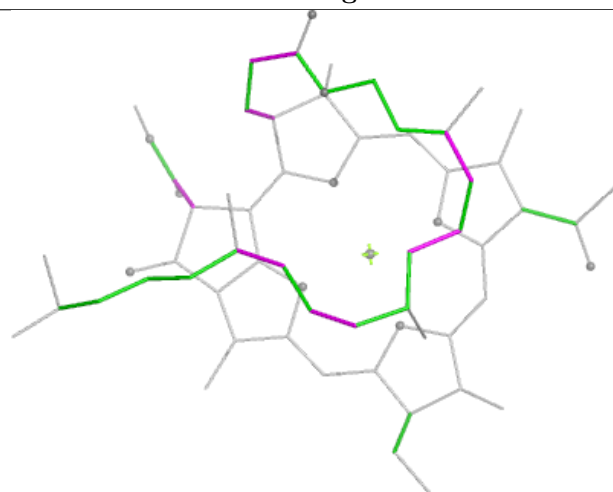
Ligand BCL AM 101



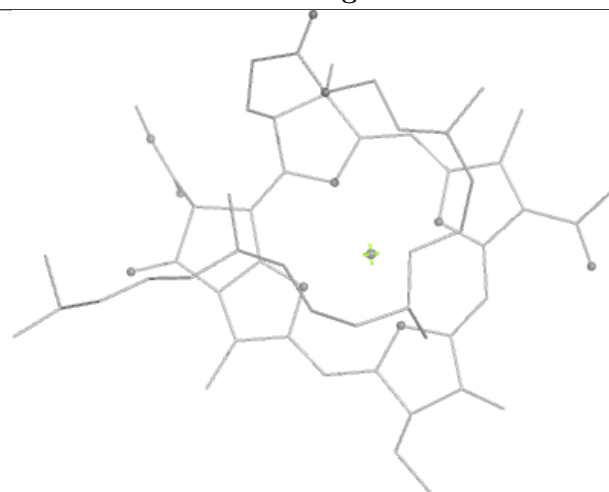
Bond lengths



Bond angles

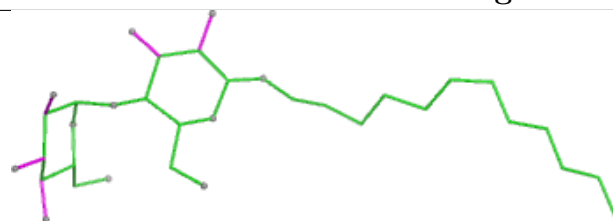


Torsions

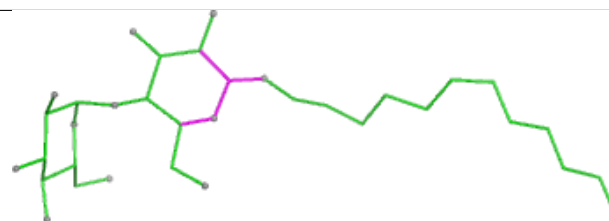


Rings

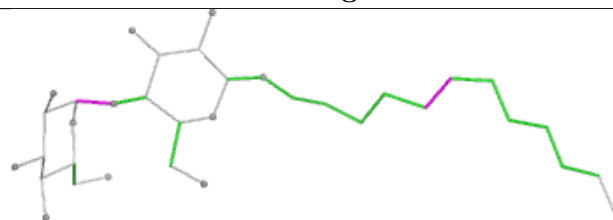
Ligand LMT BS 1002



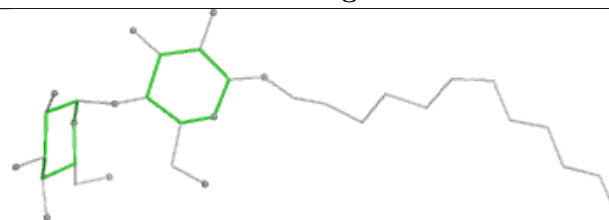
Bond lengths



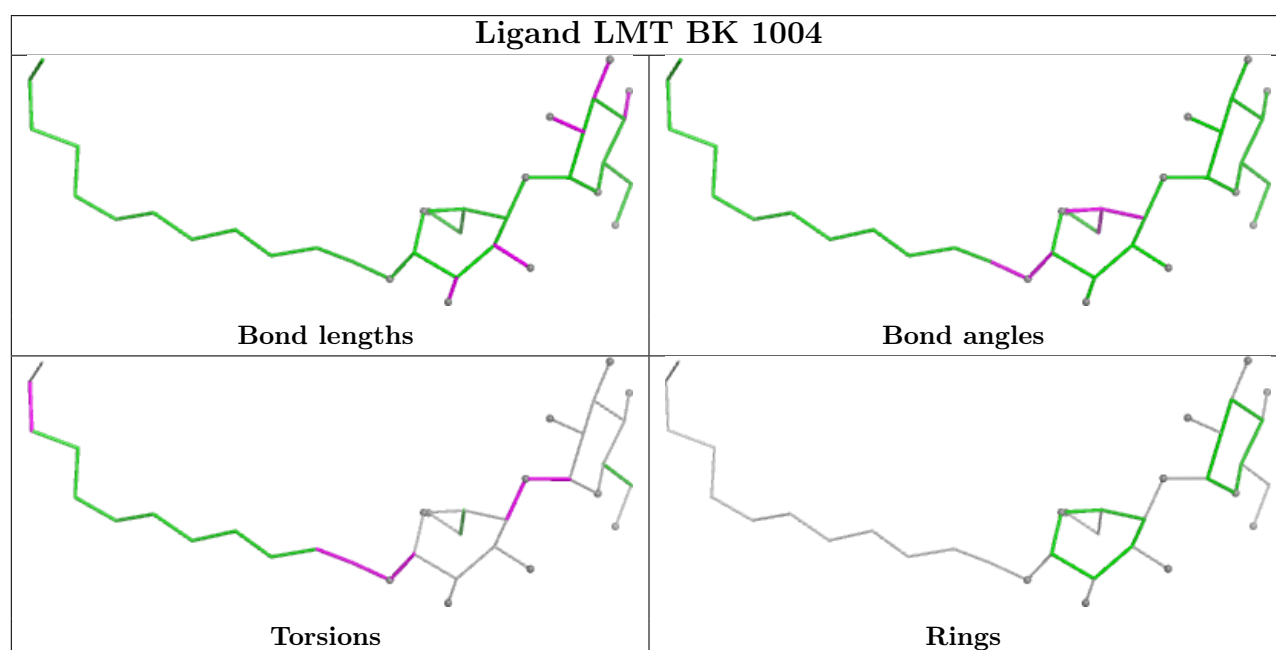
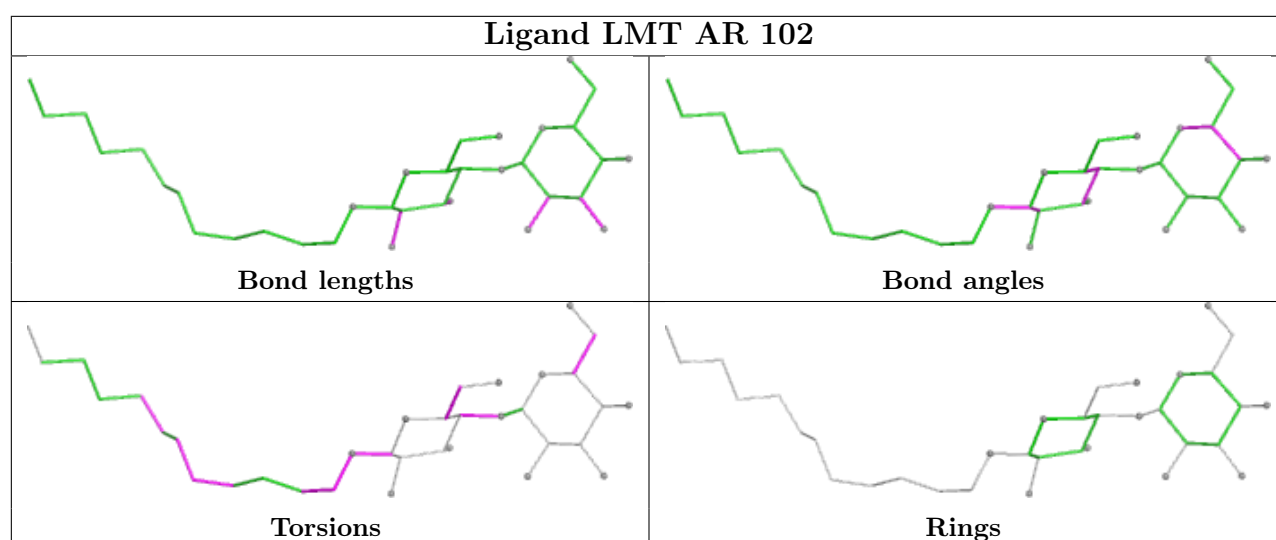
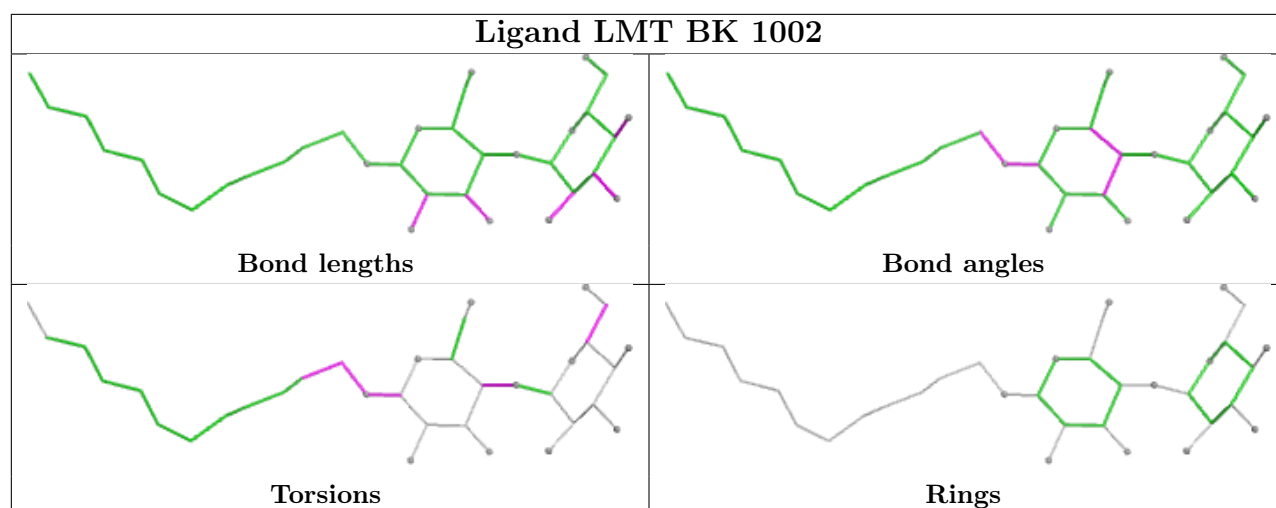
Bond angles

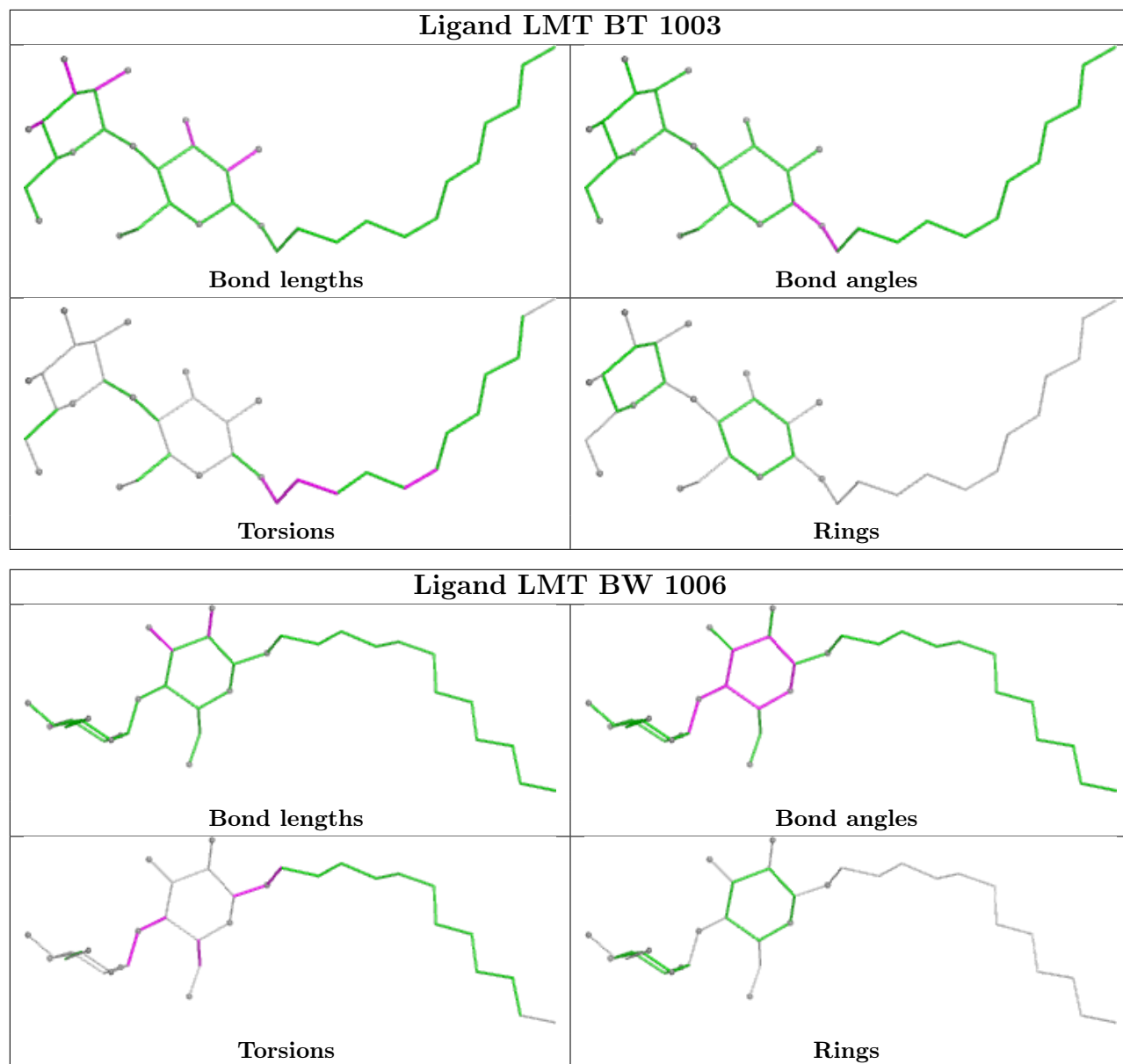


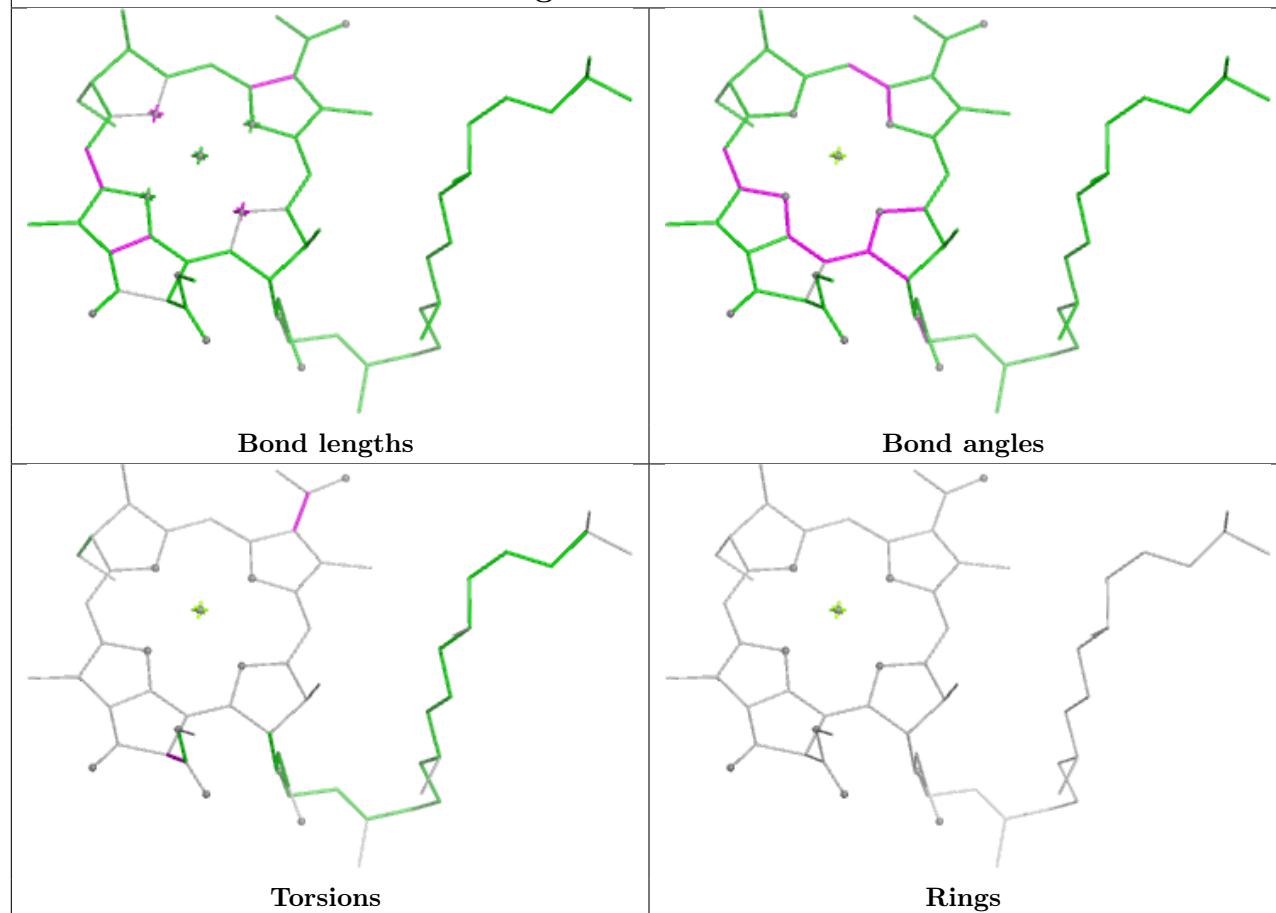
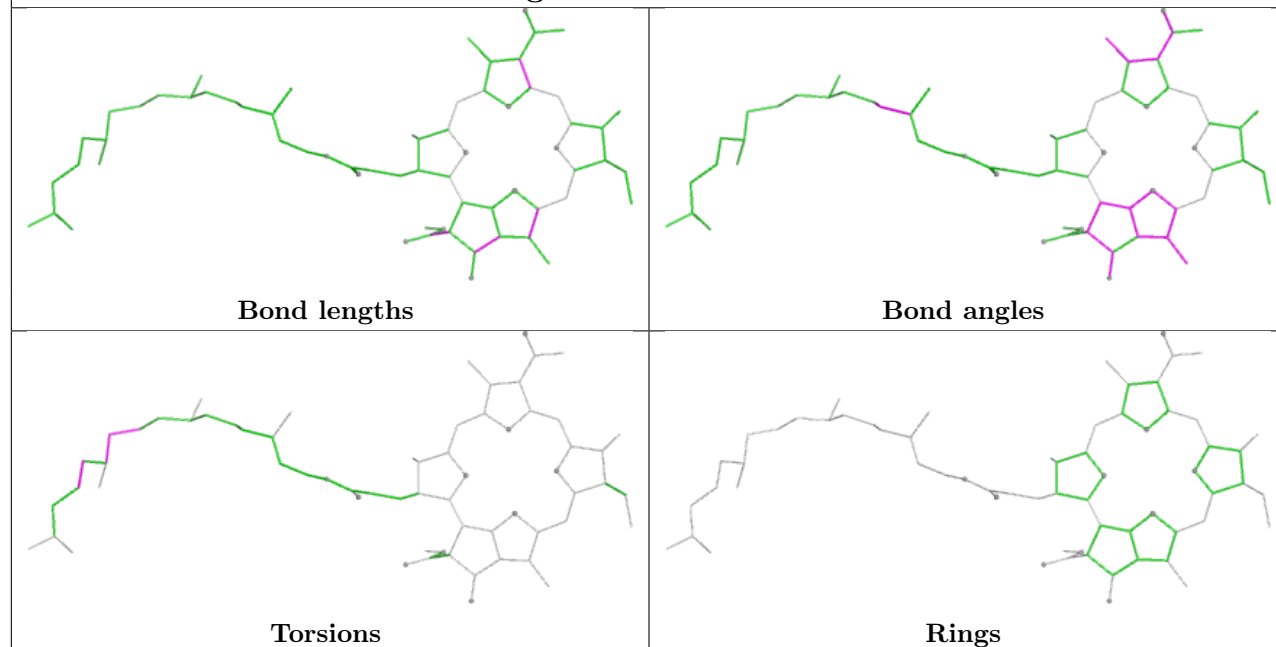
Torsions

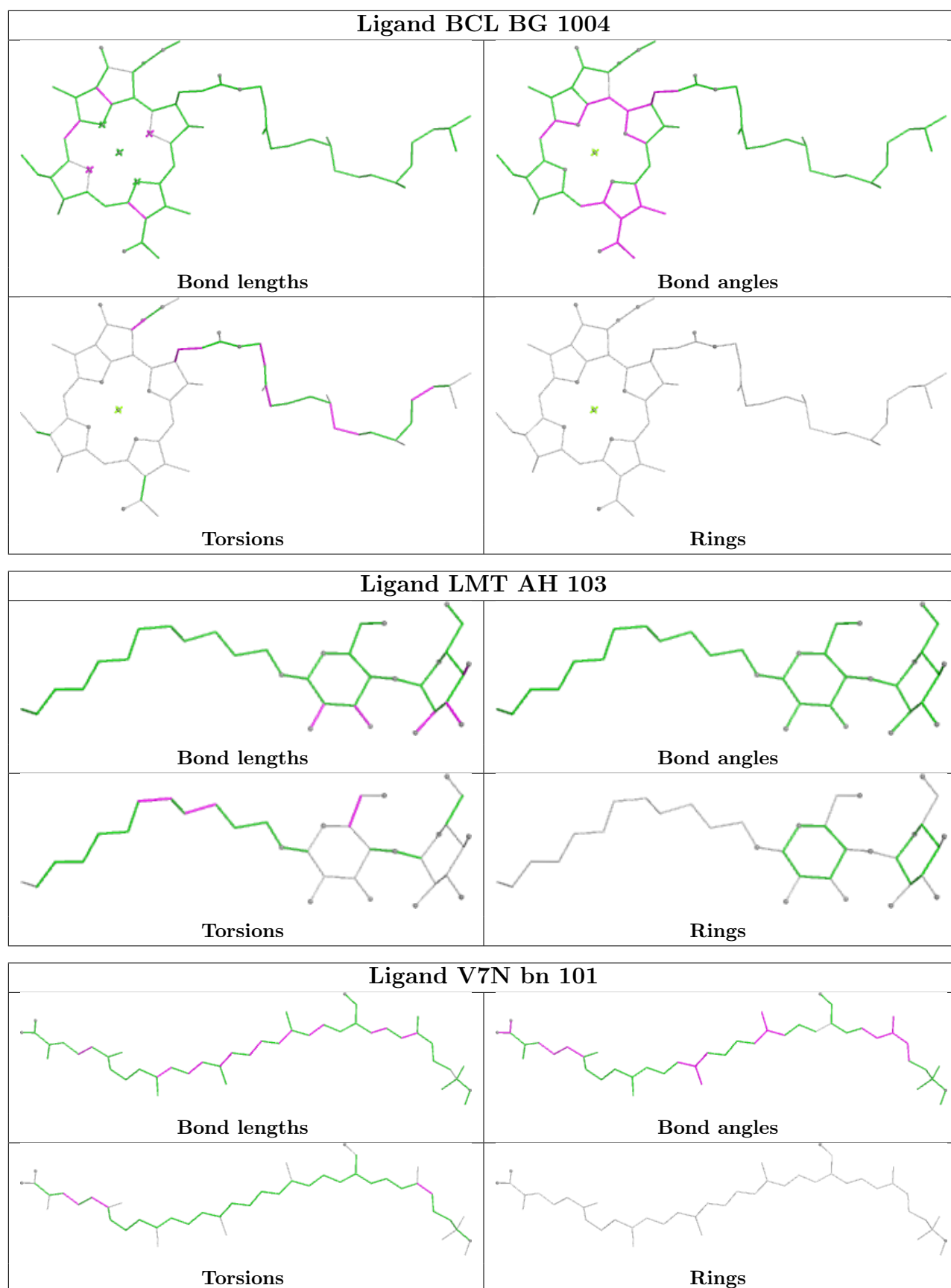


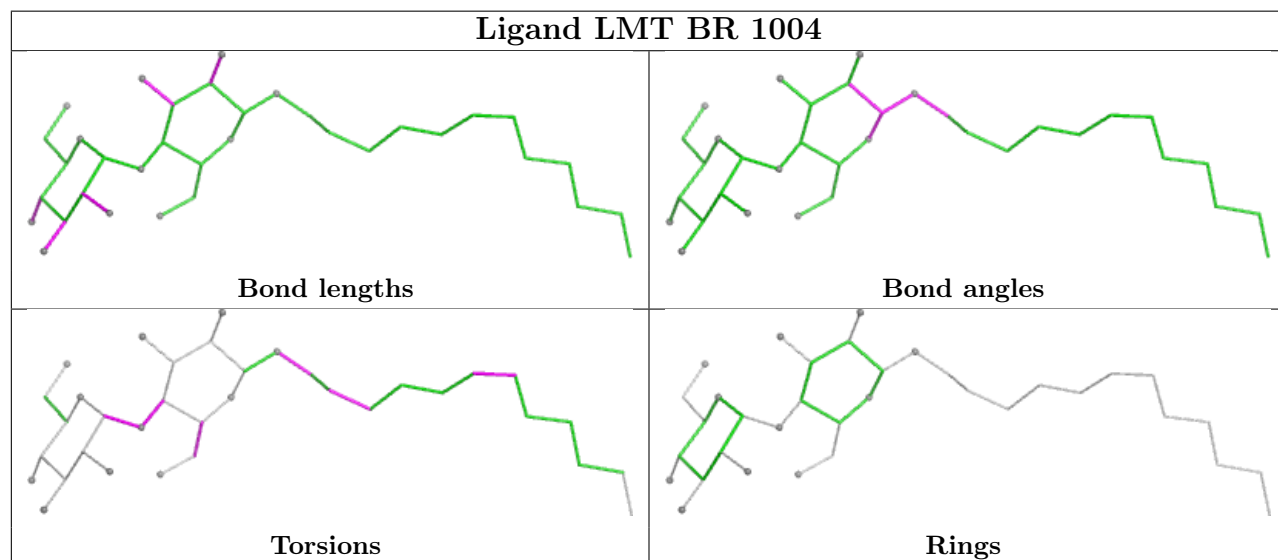
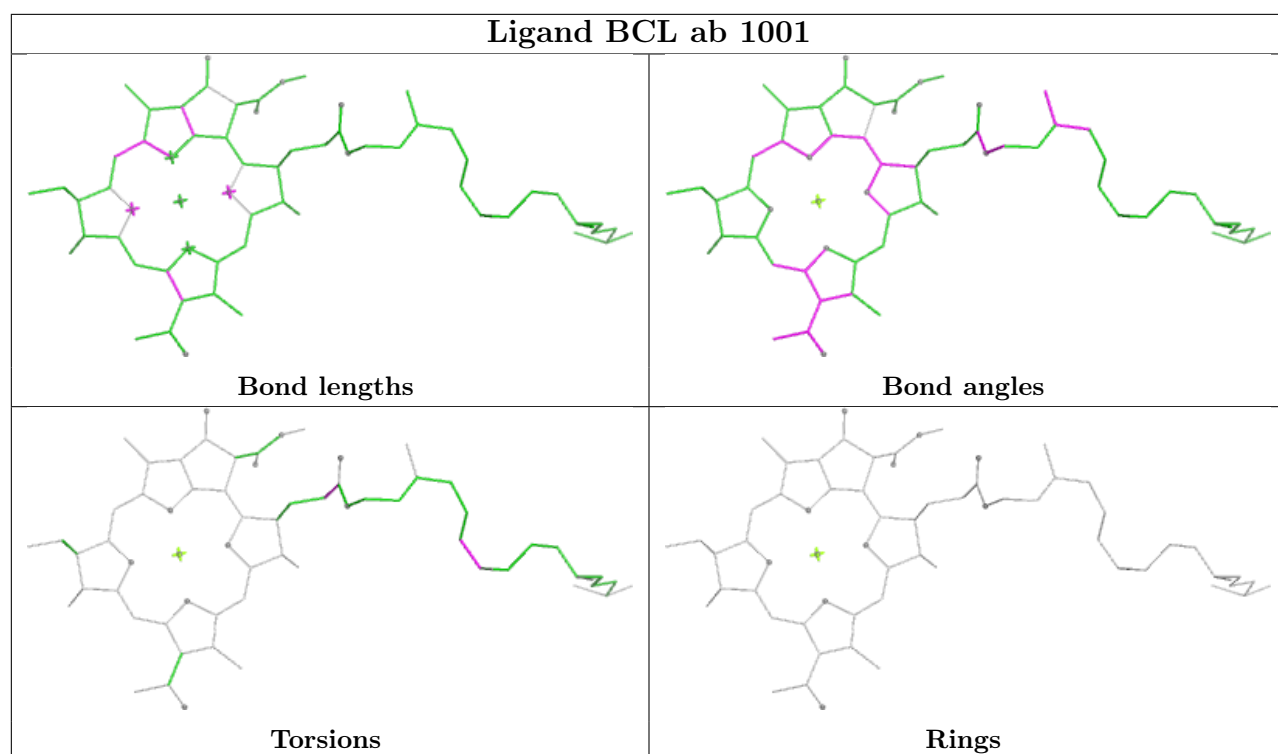
Rings

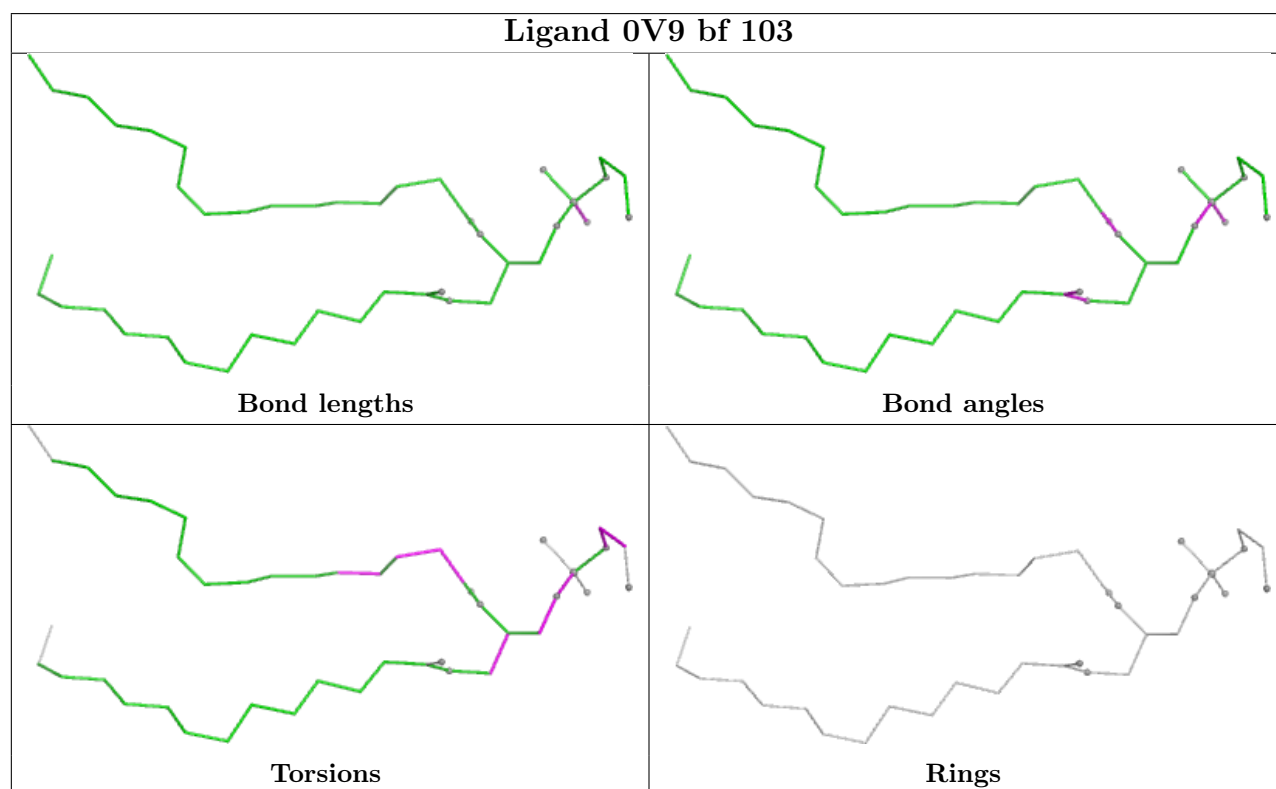
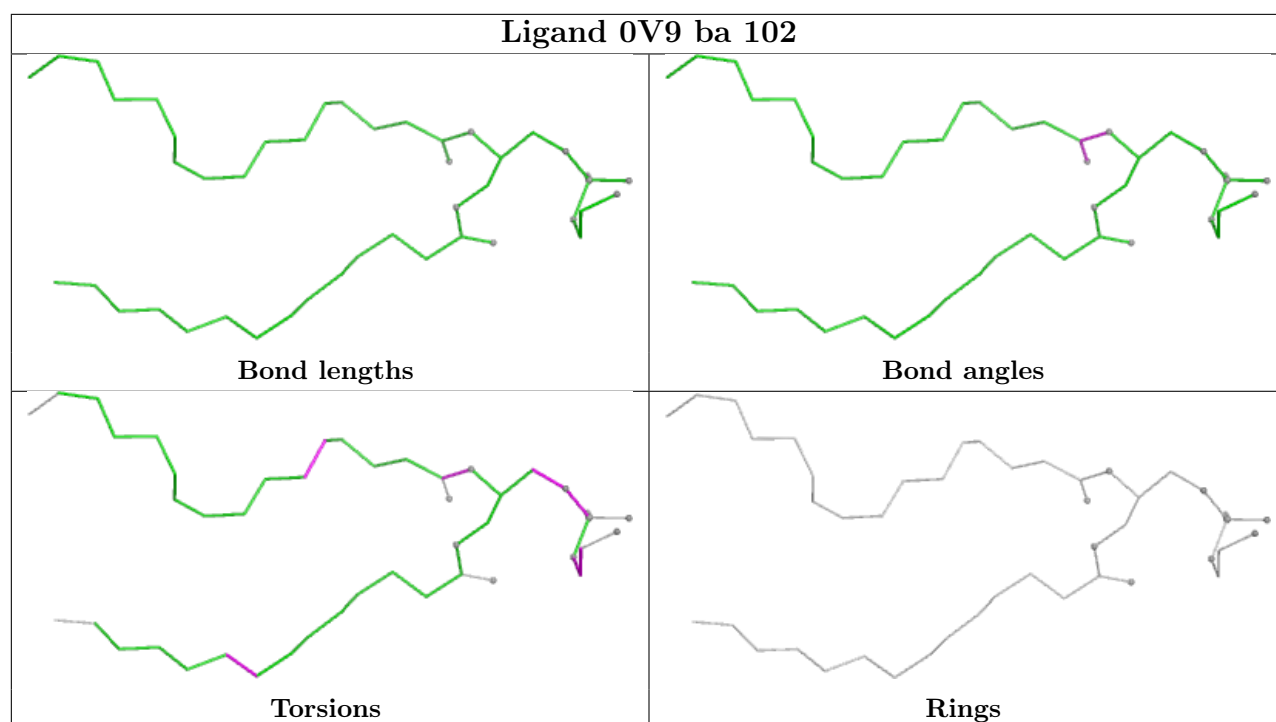


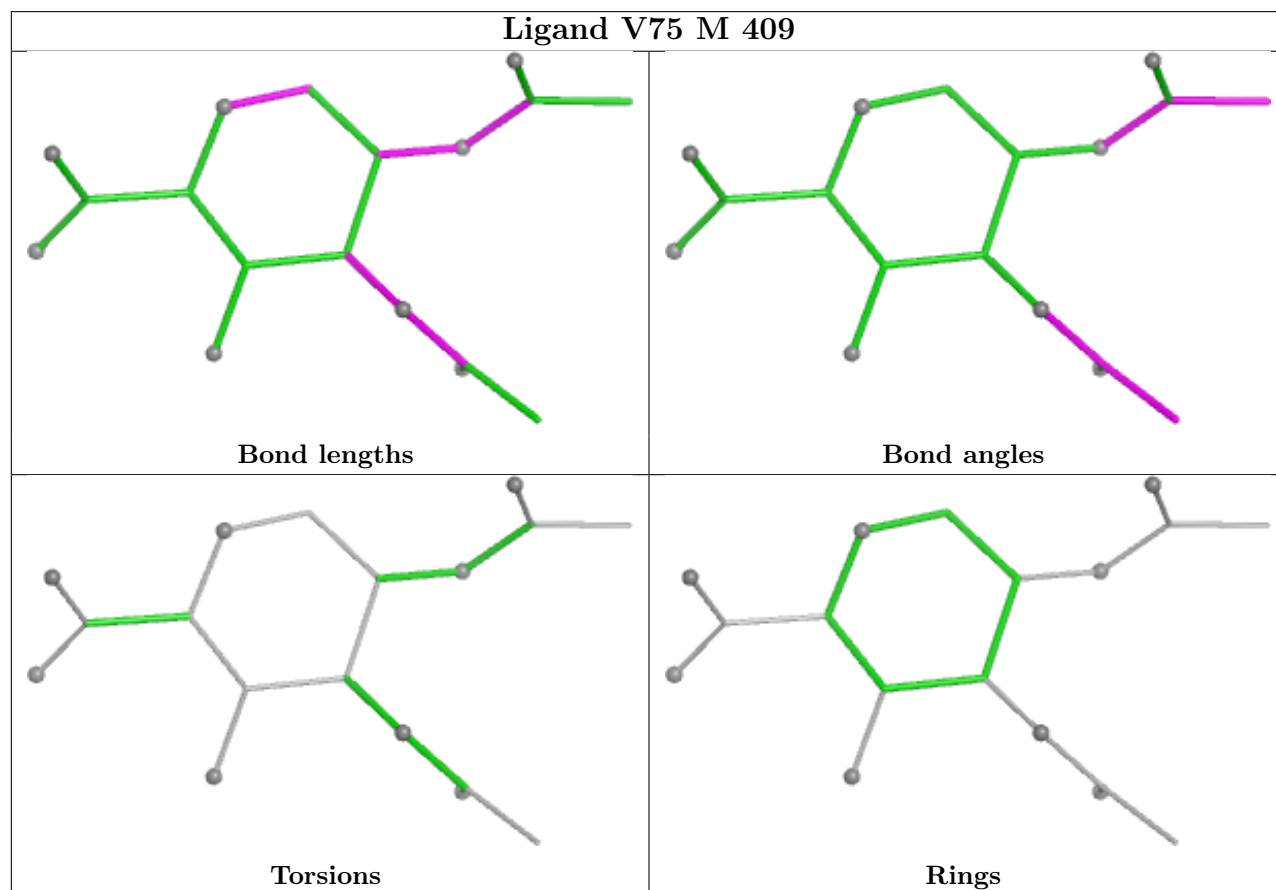
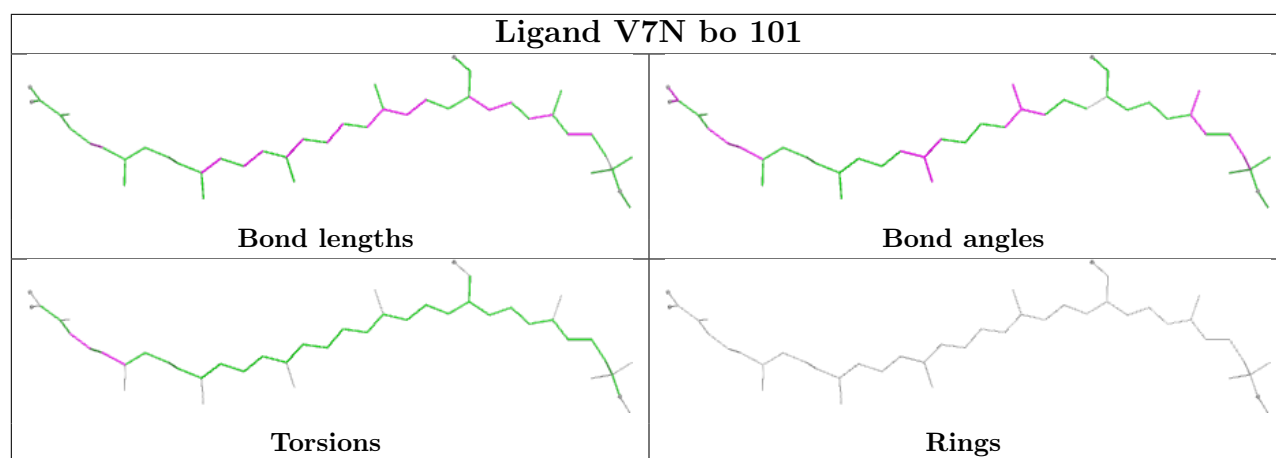


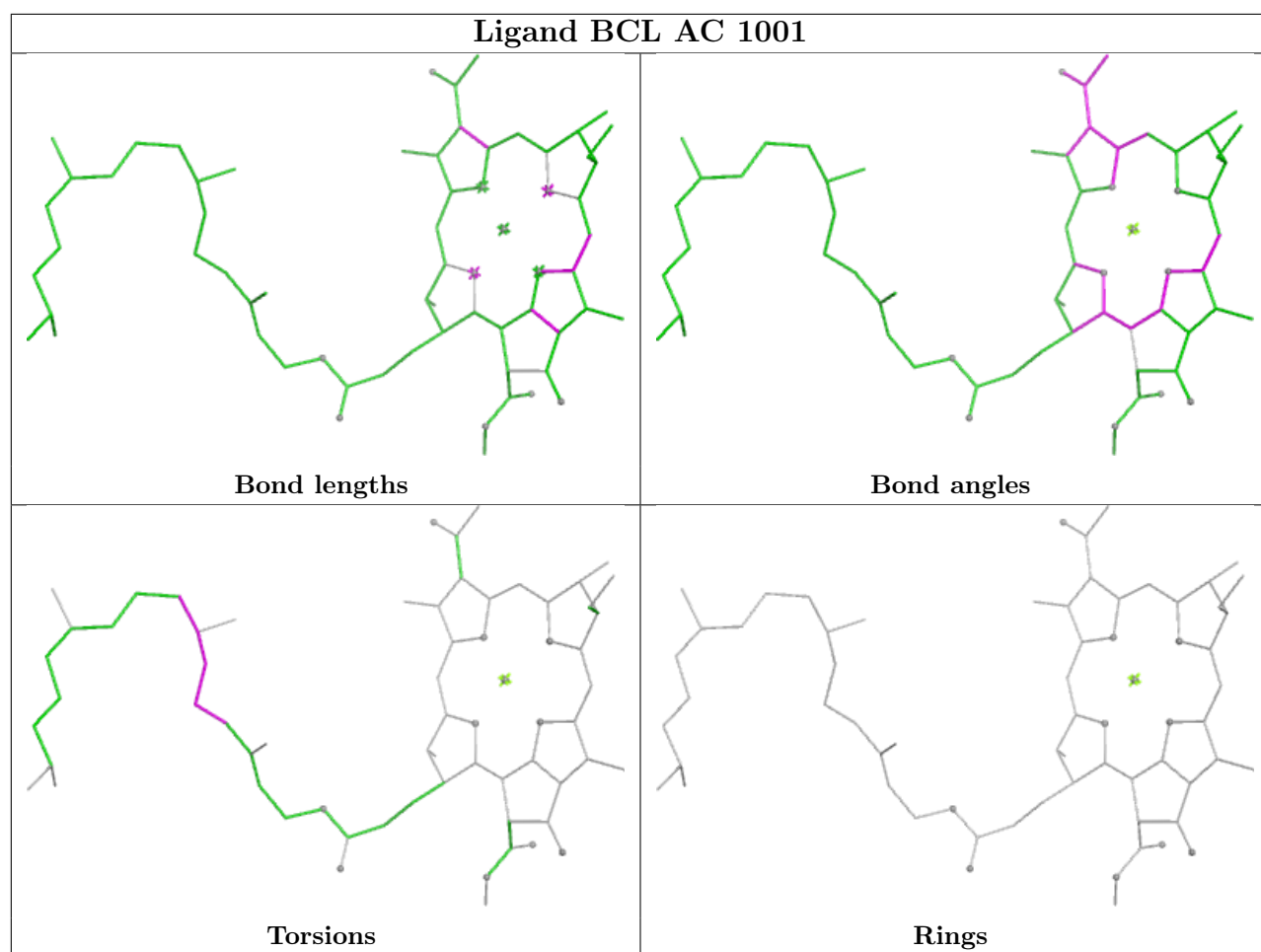
Ligand BCL L 308**Ligand BPH M 406**

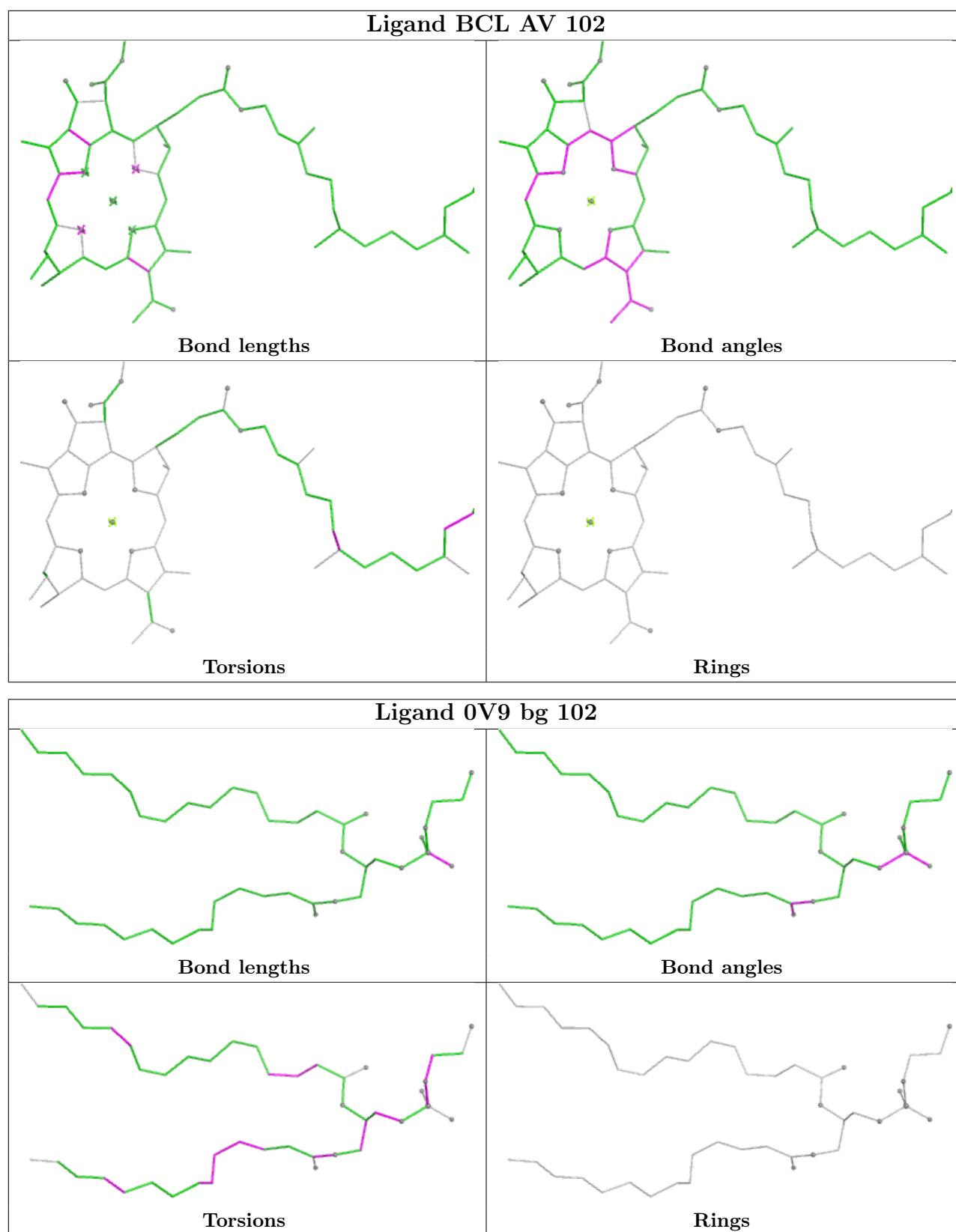


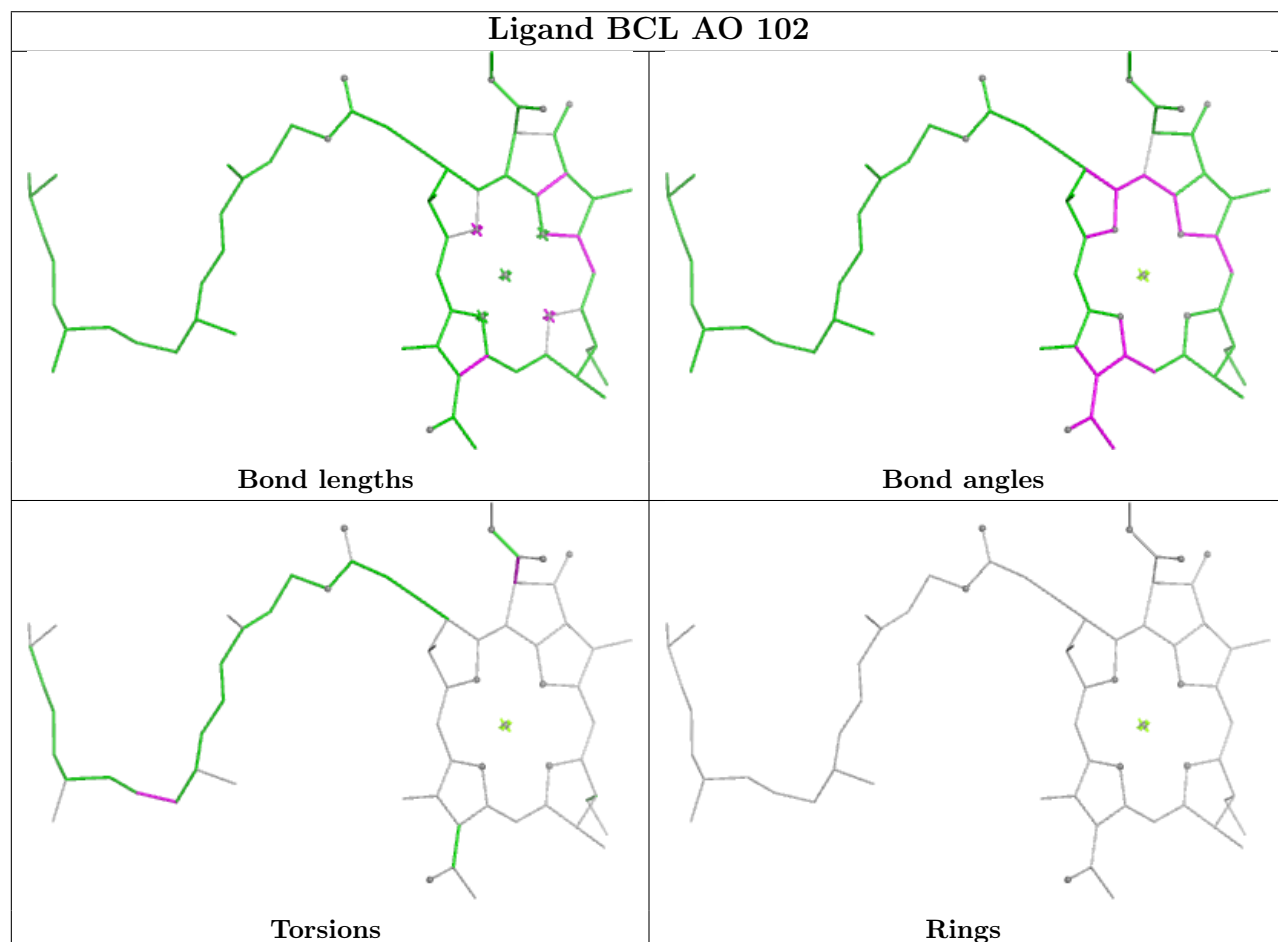
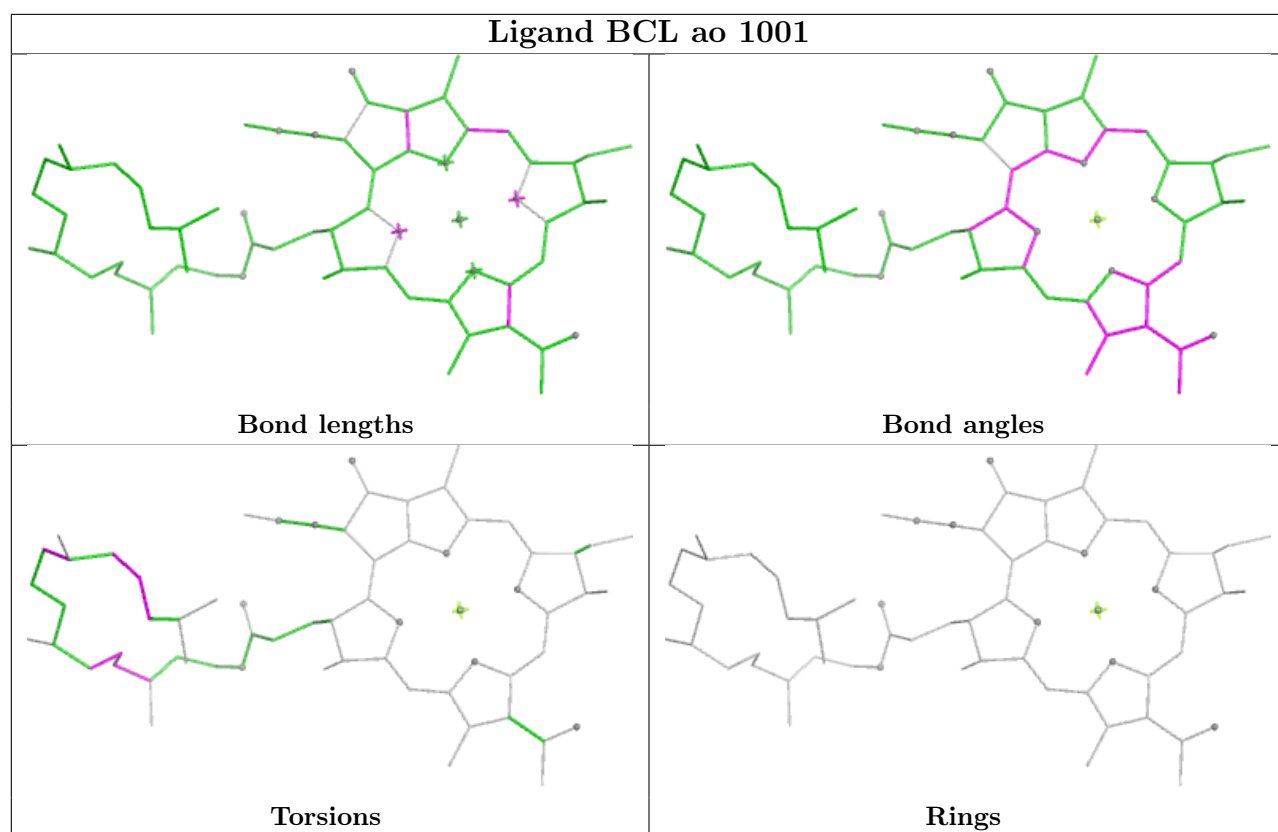


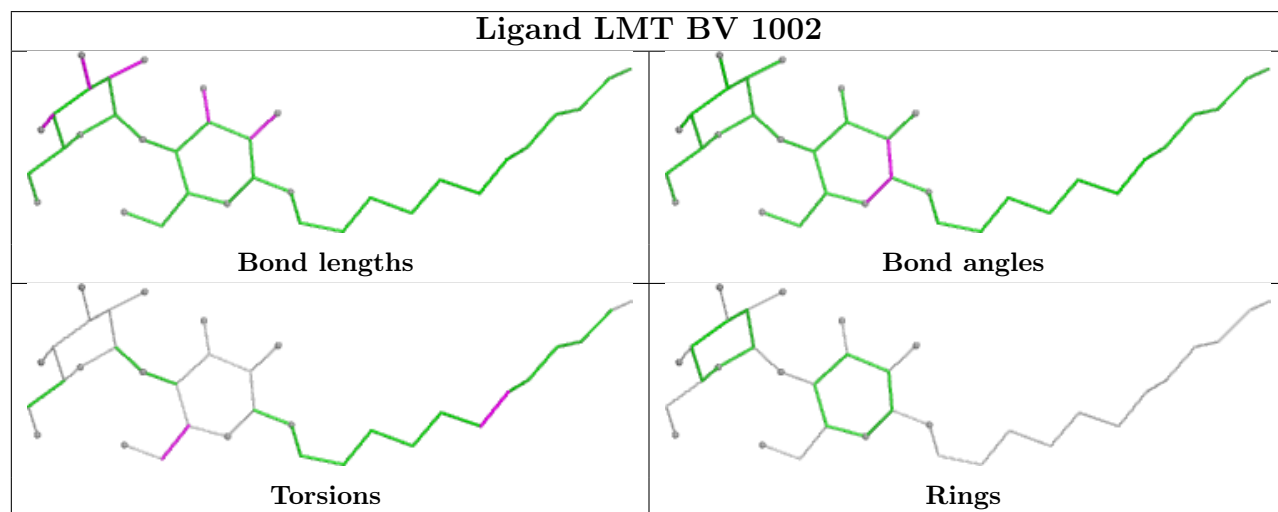
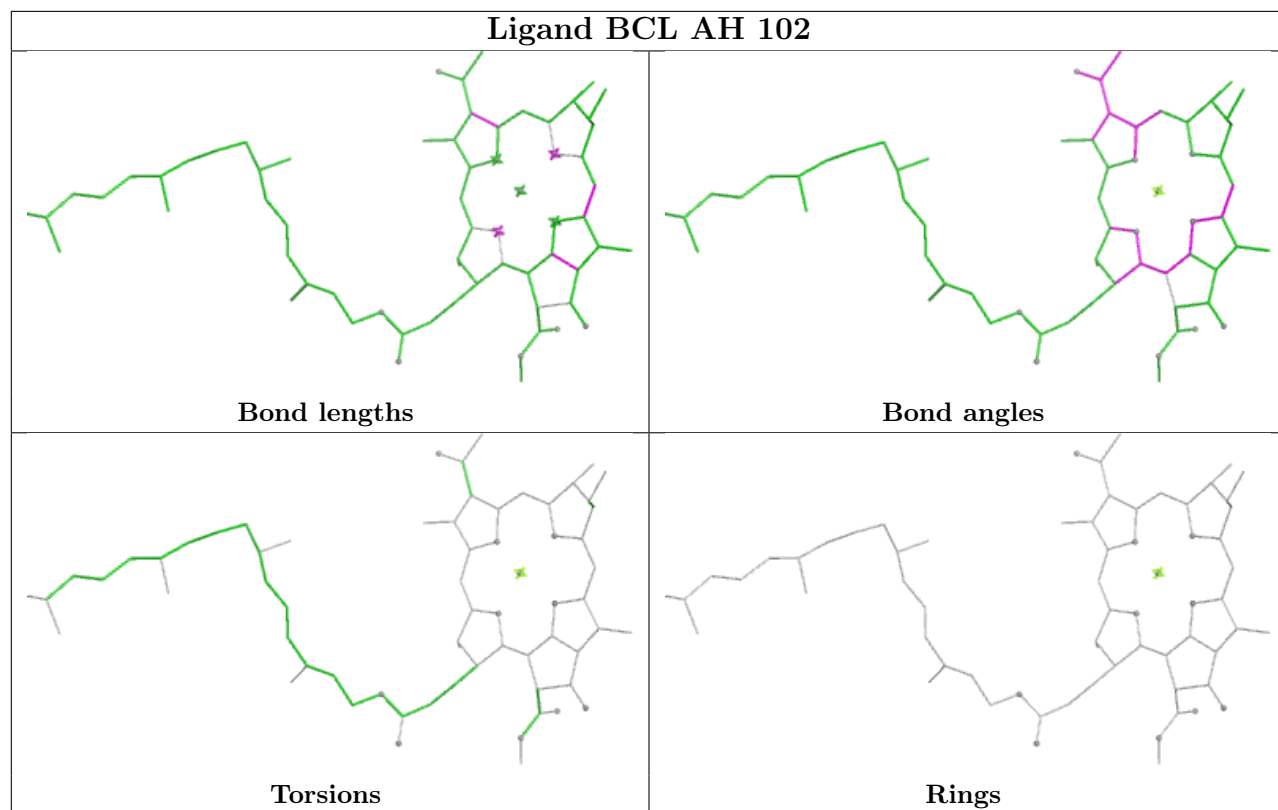


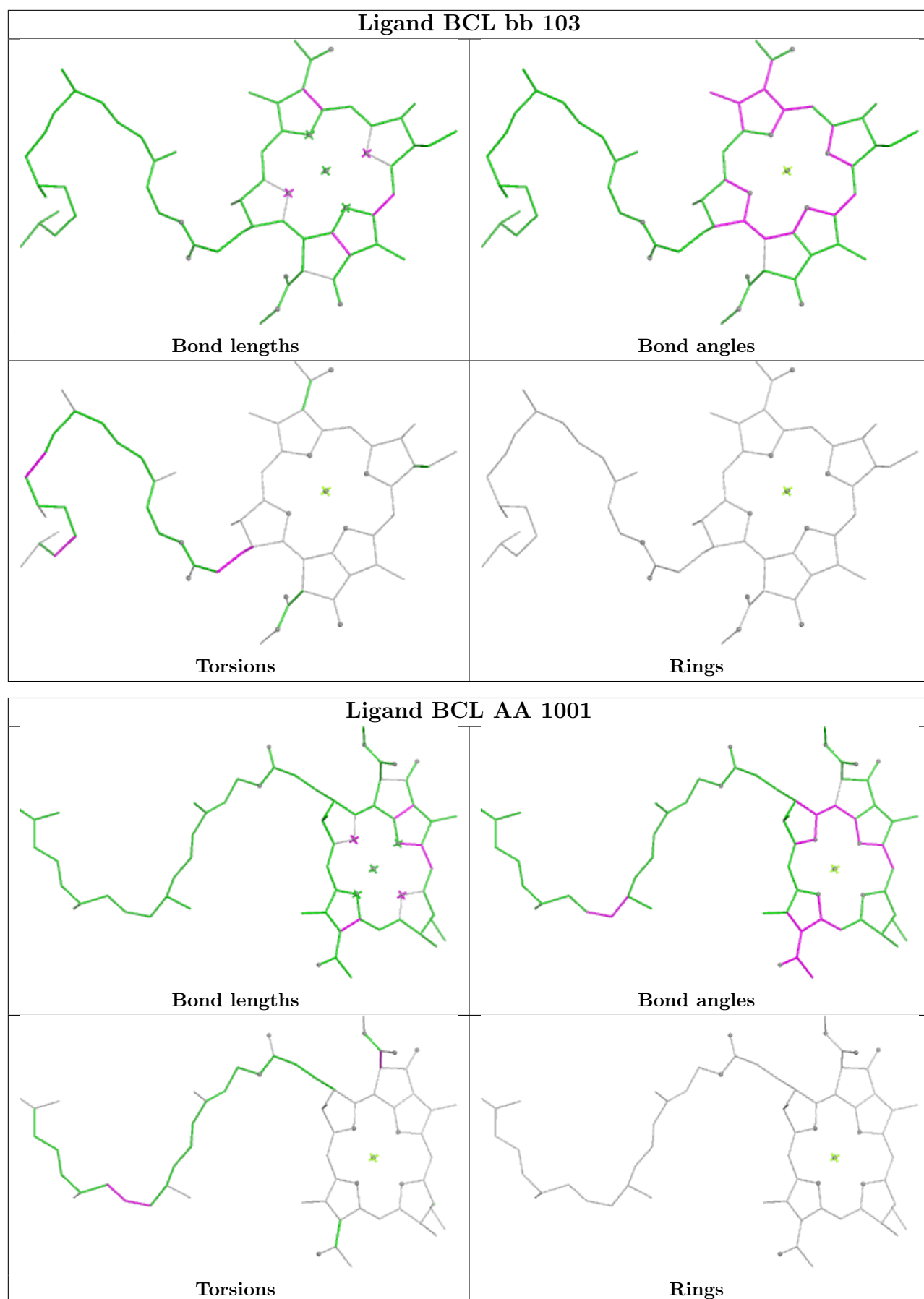


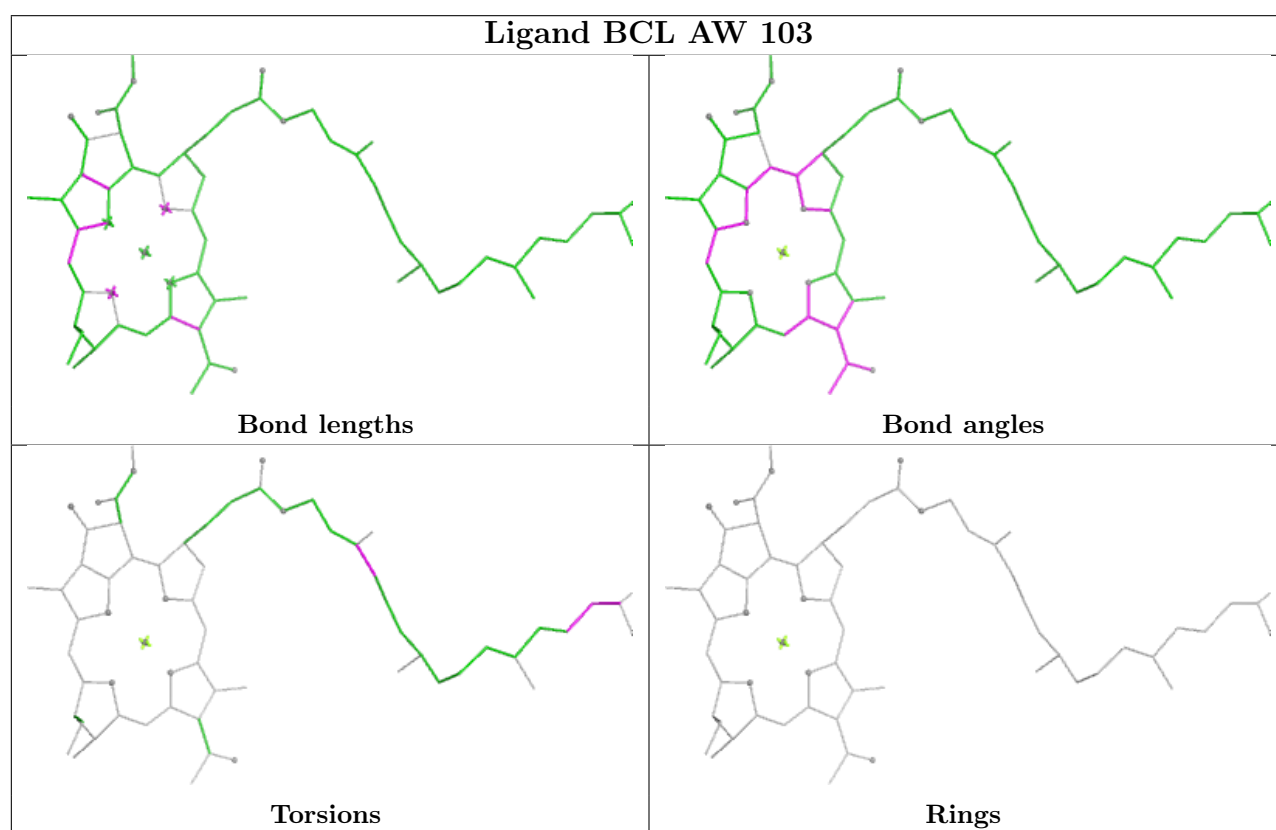
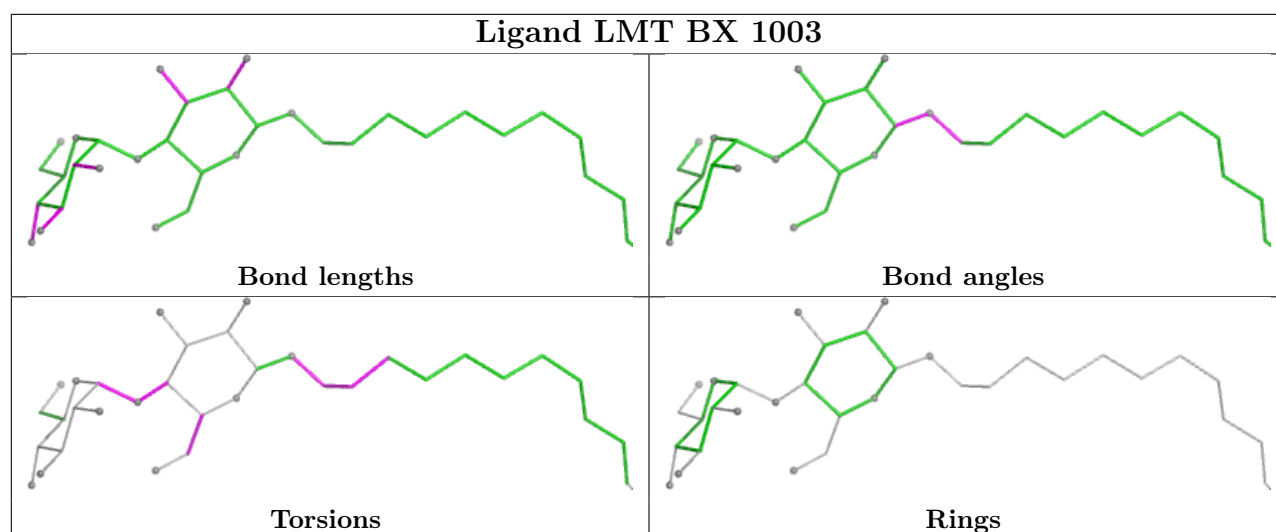


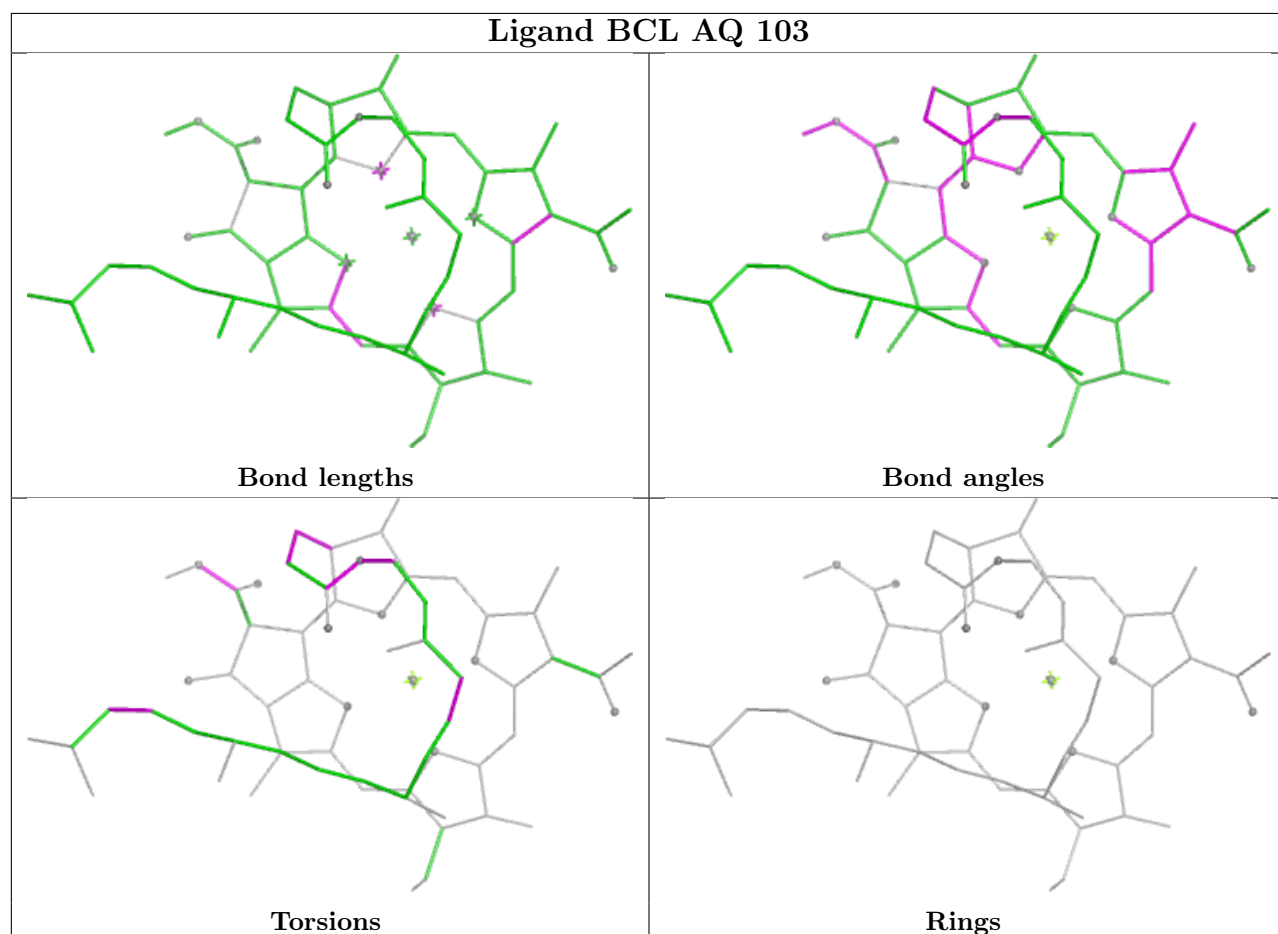
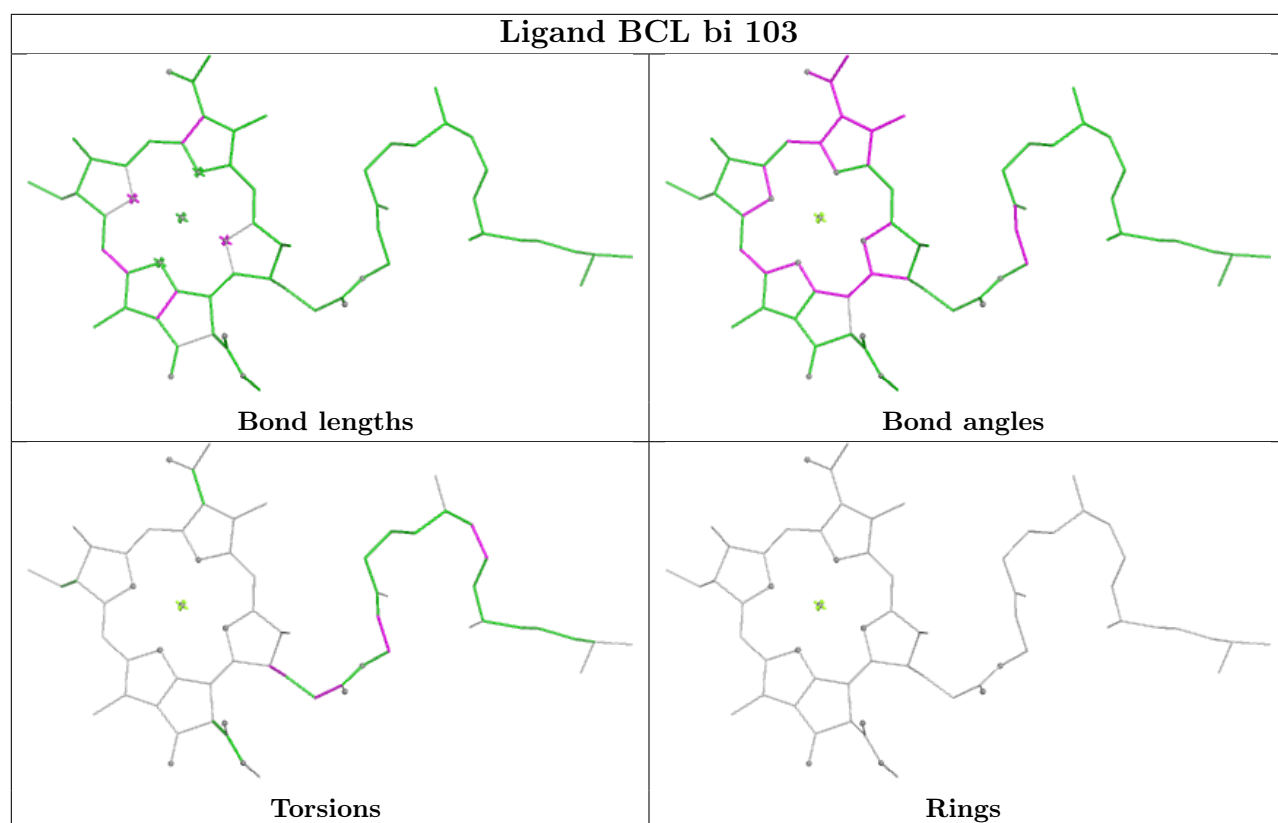


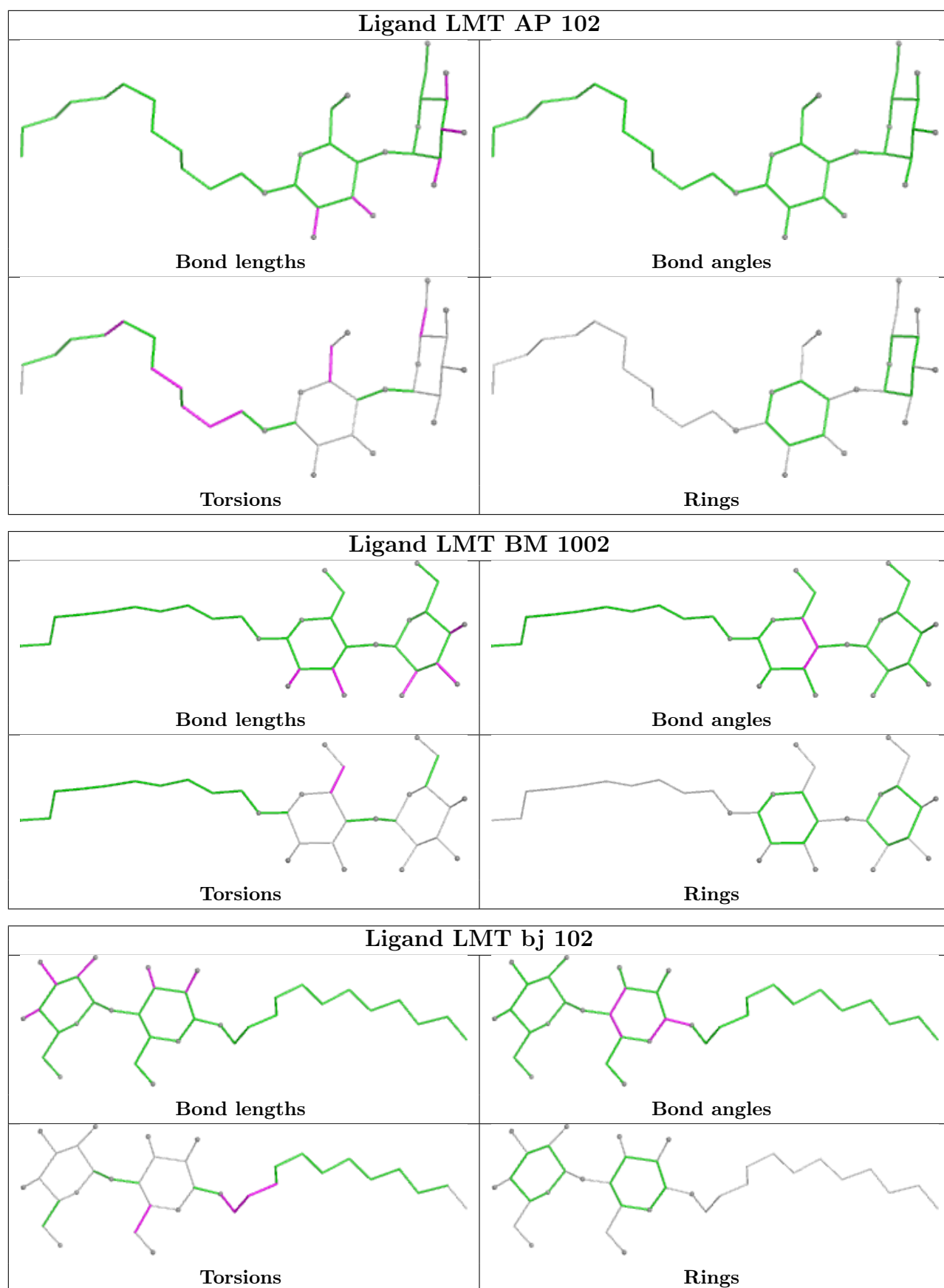


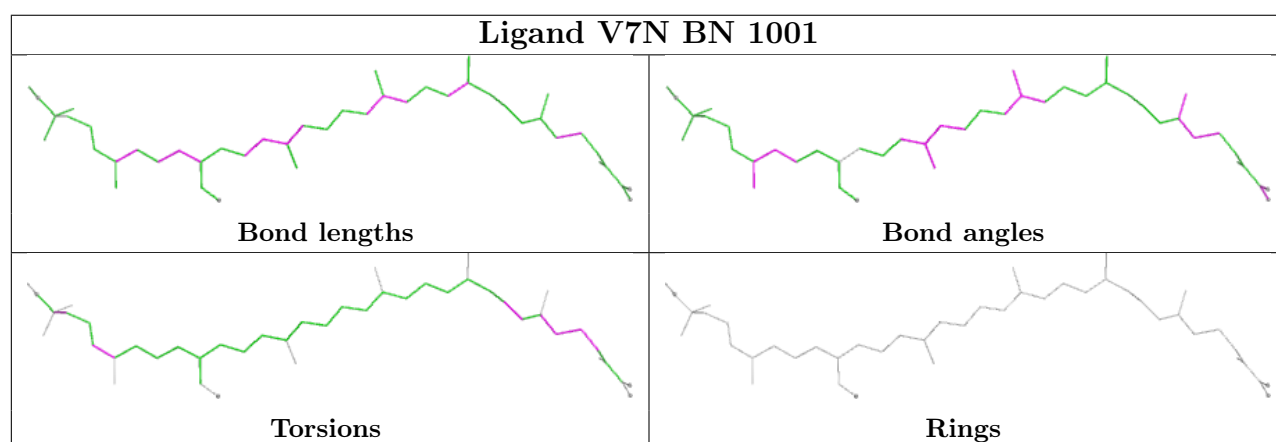
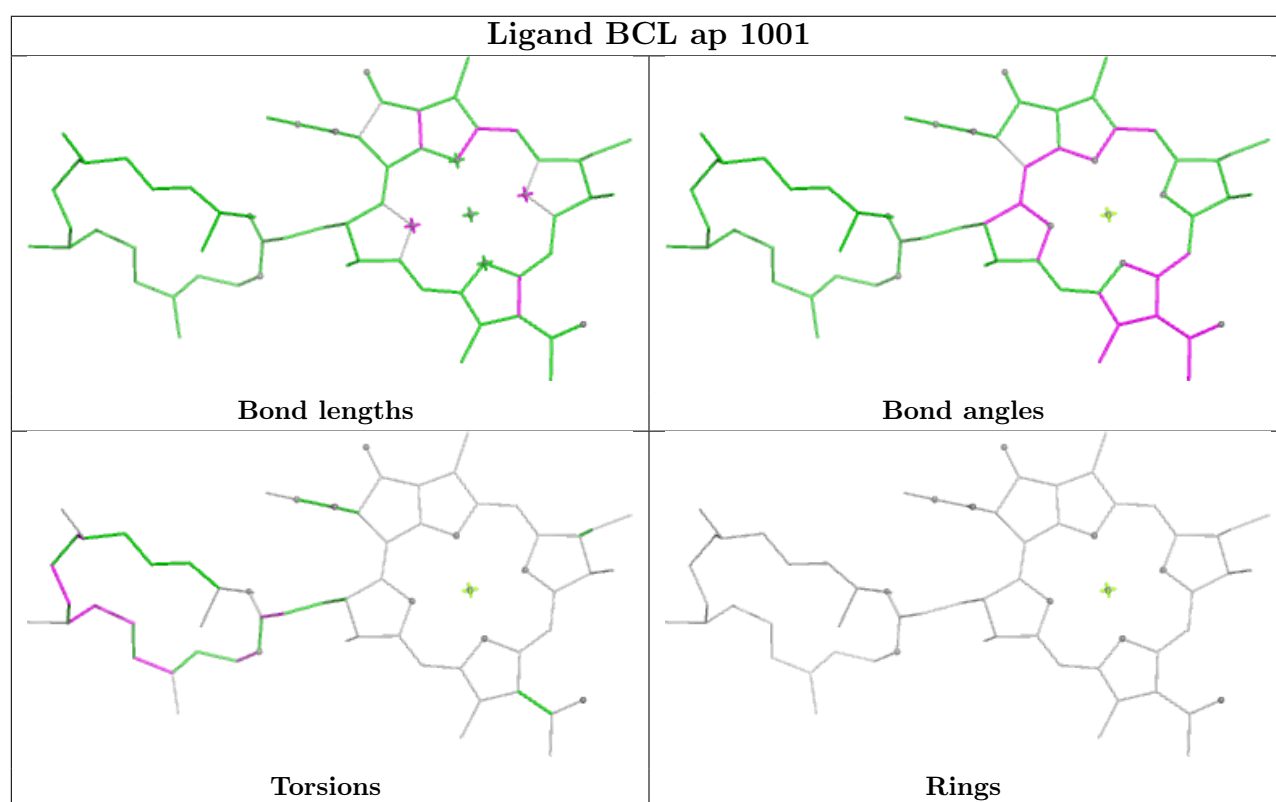
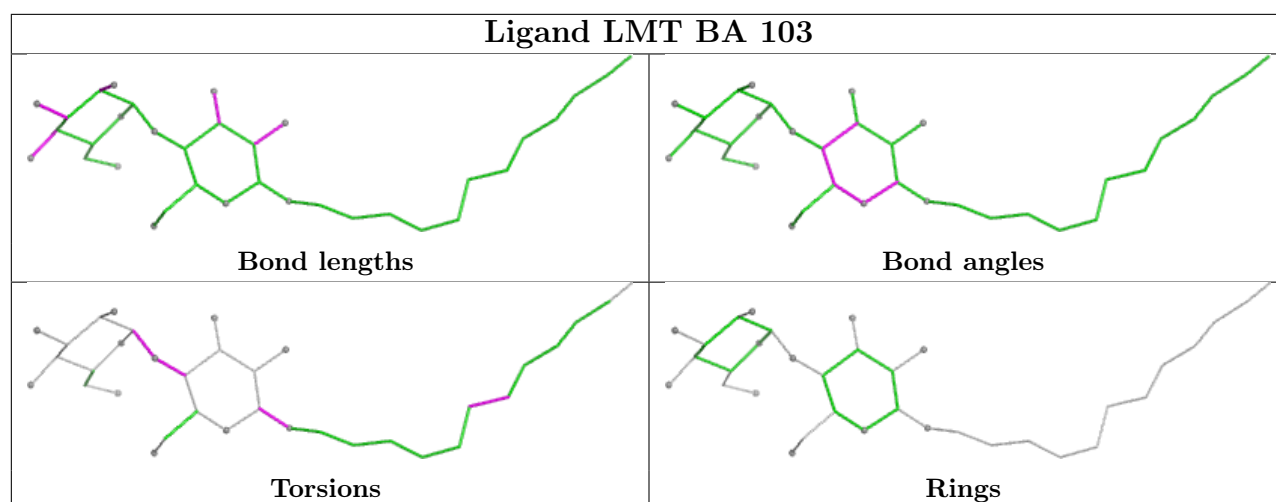


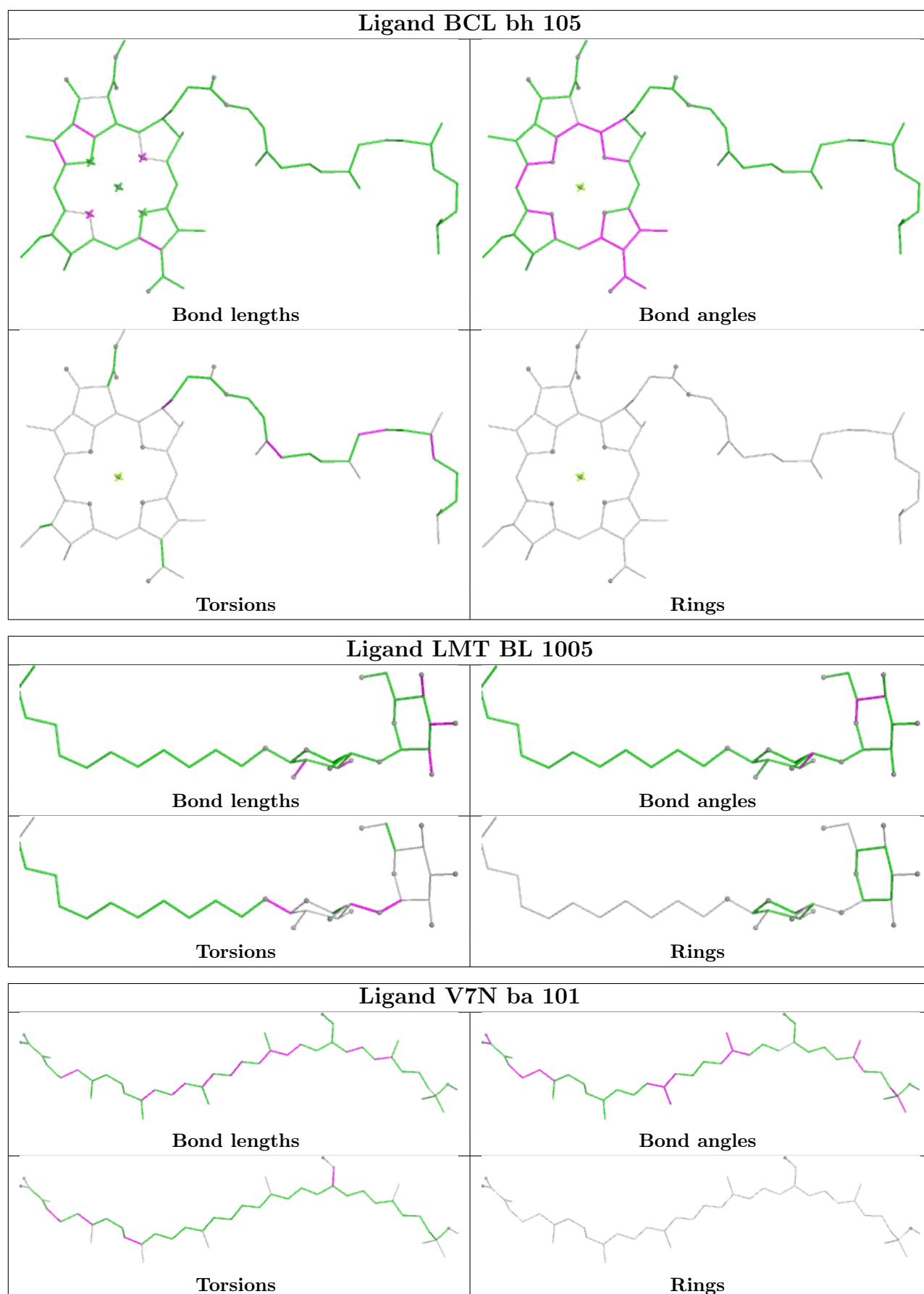


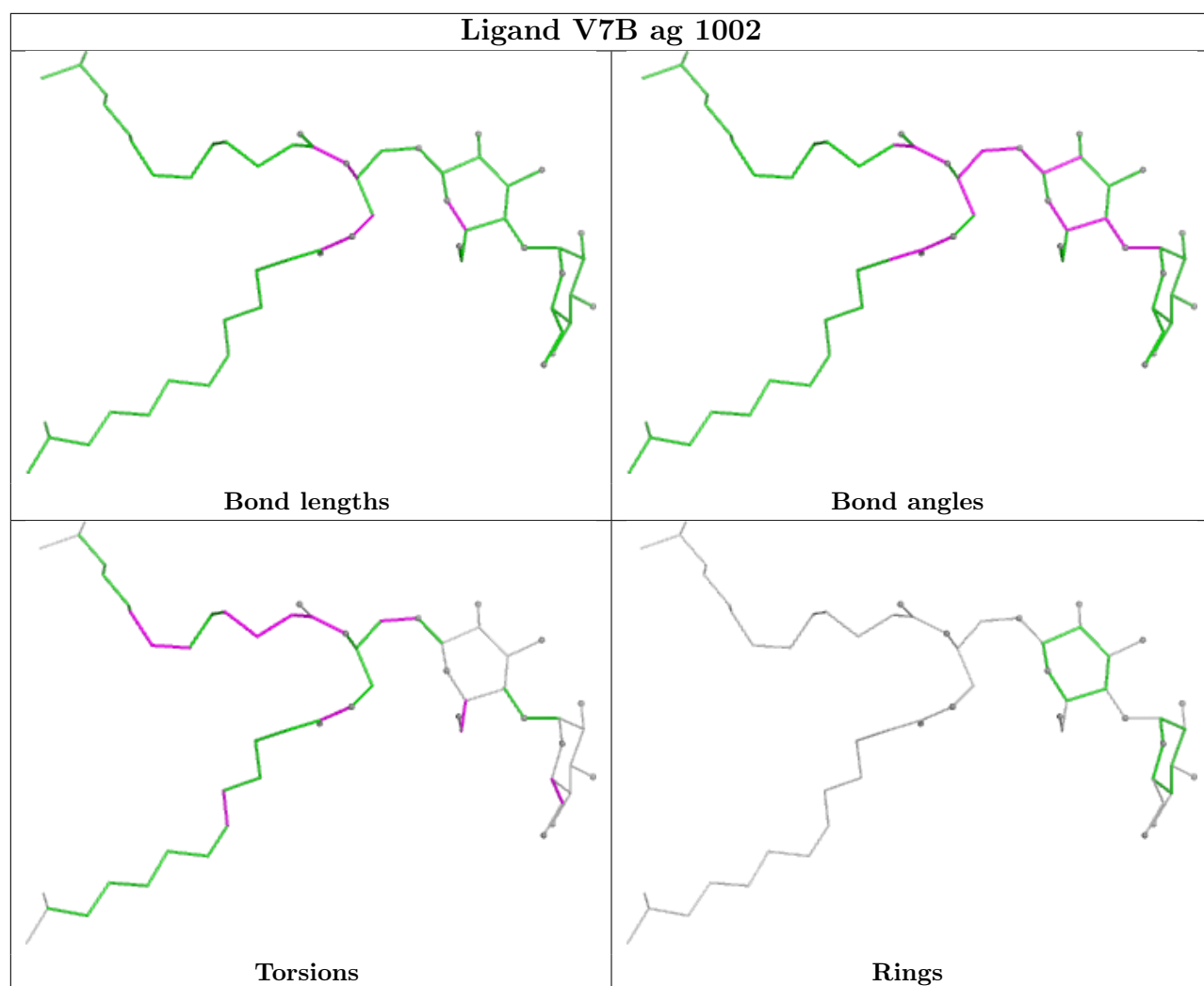


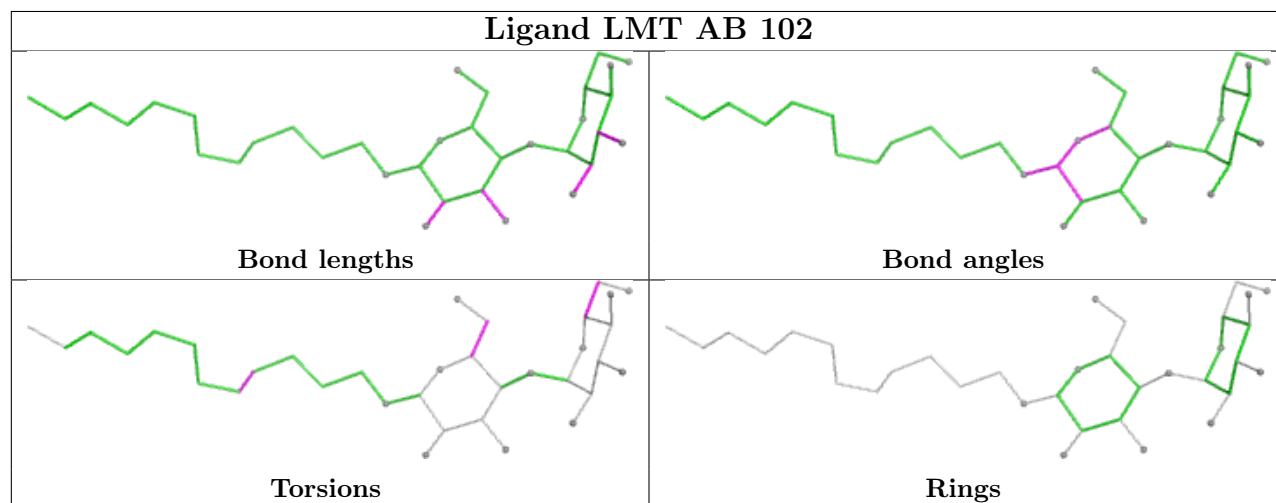
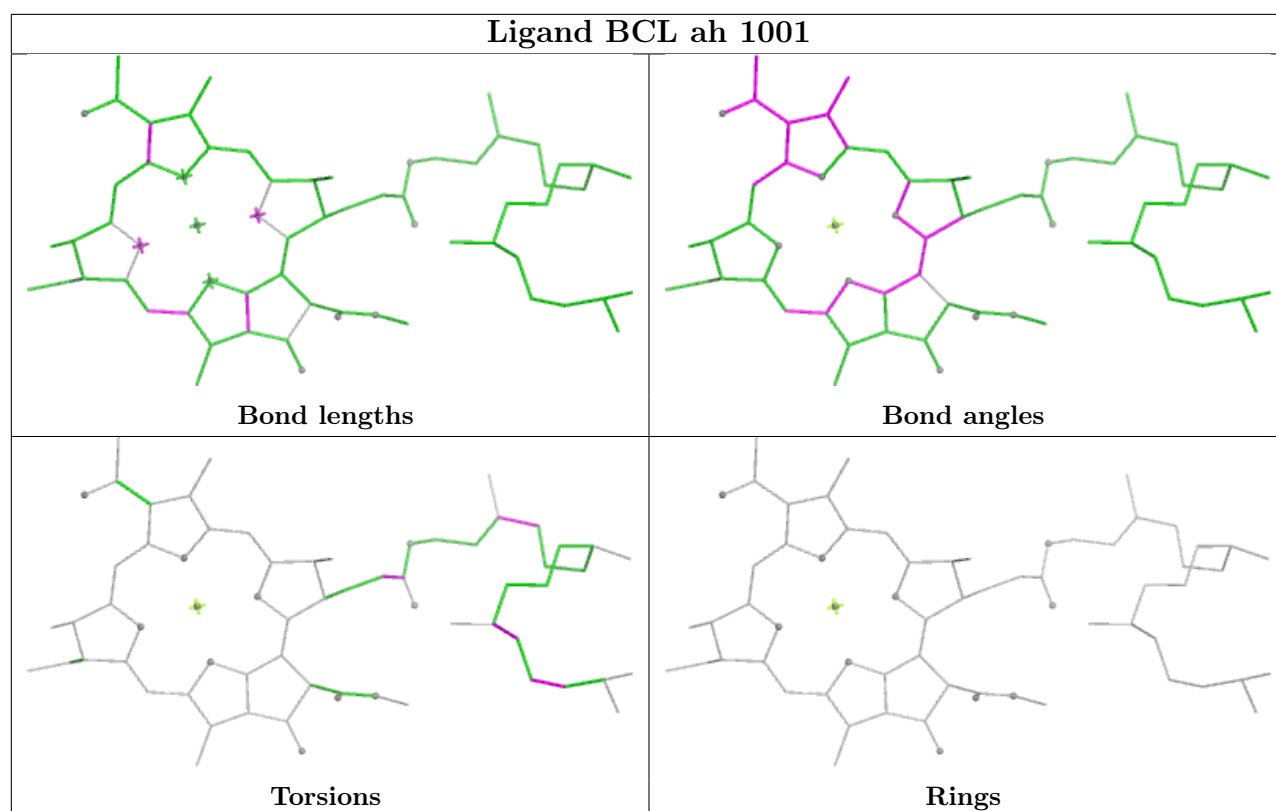


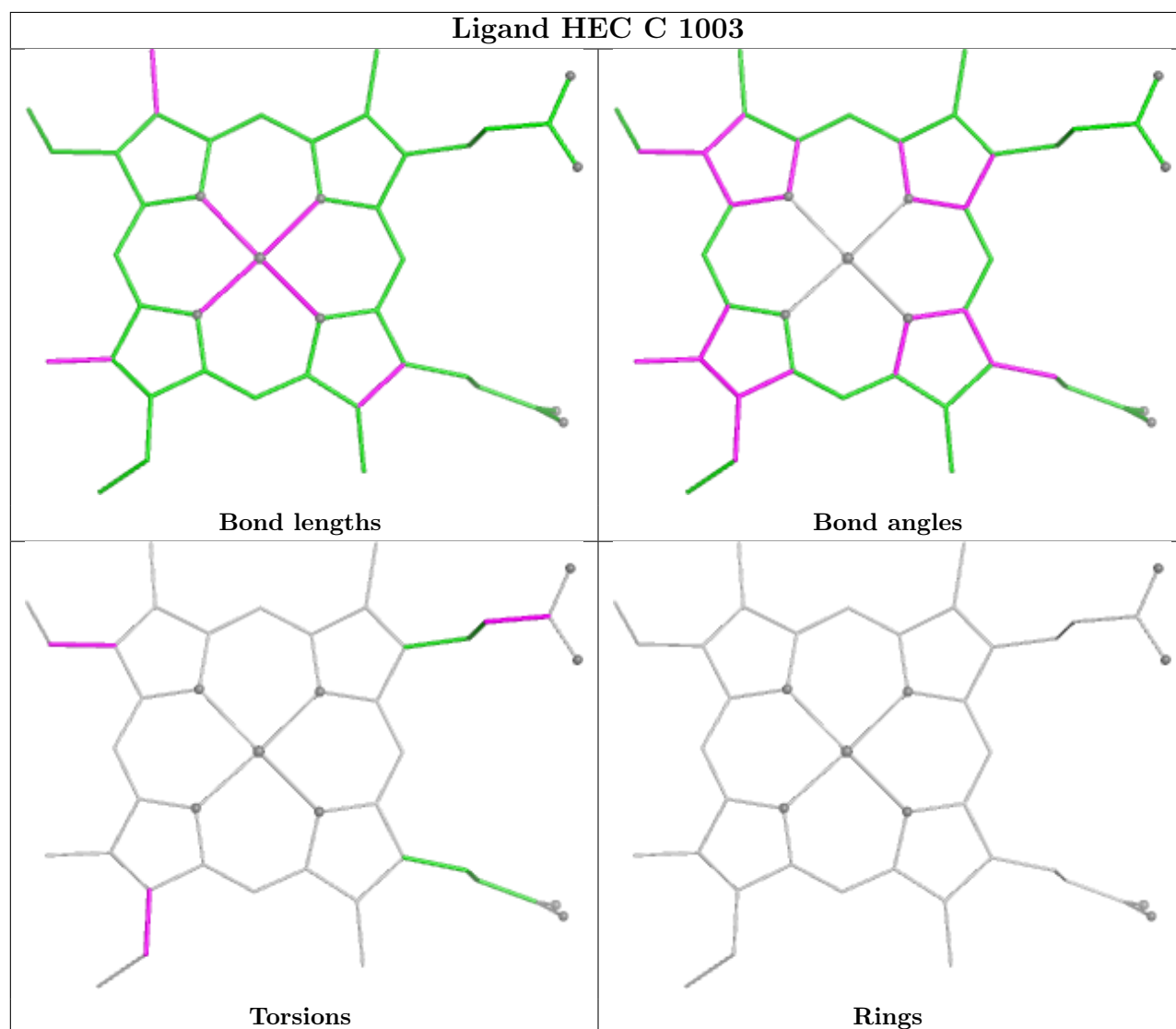
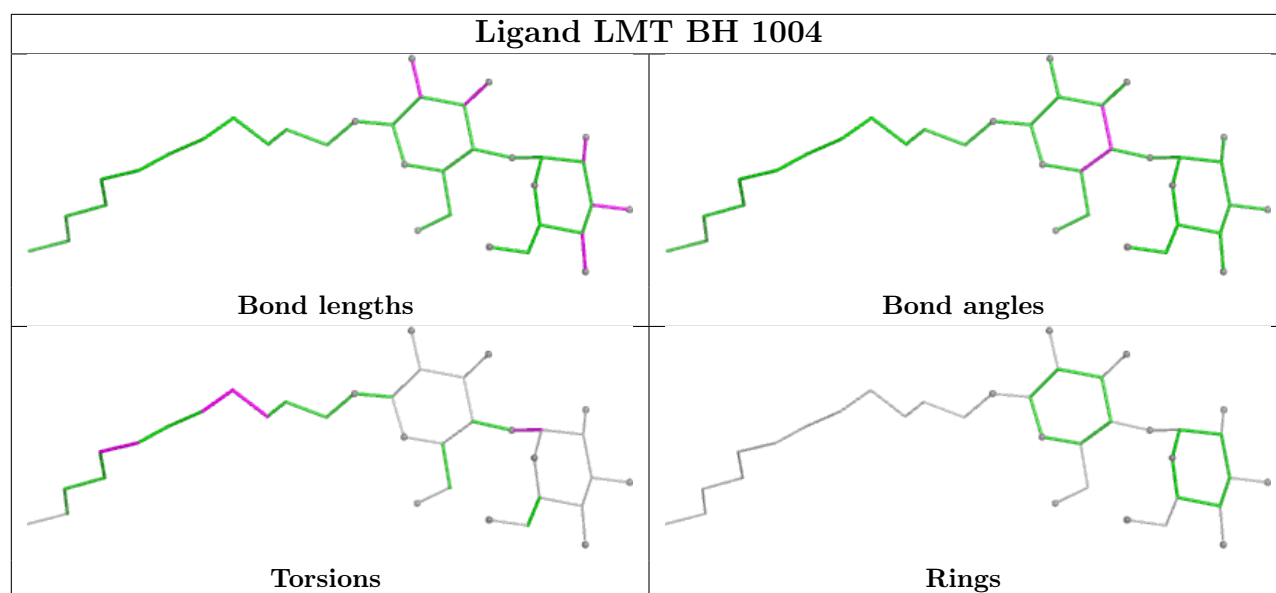


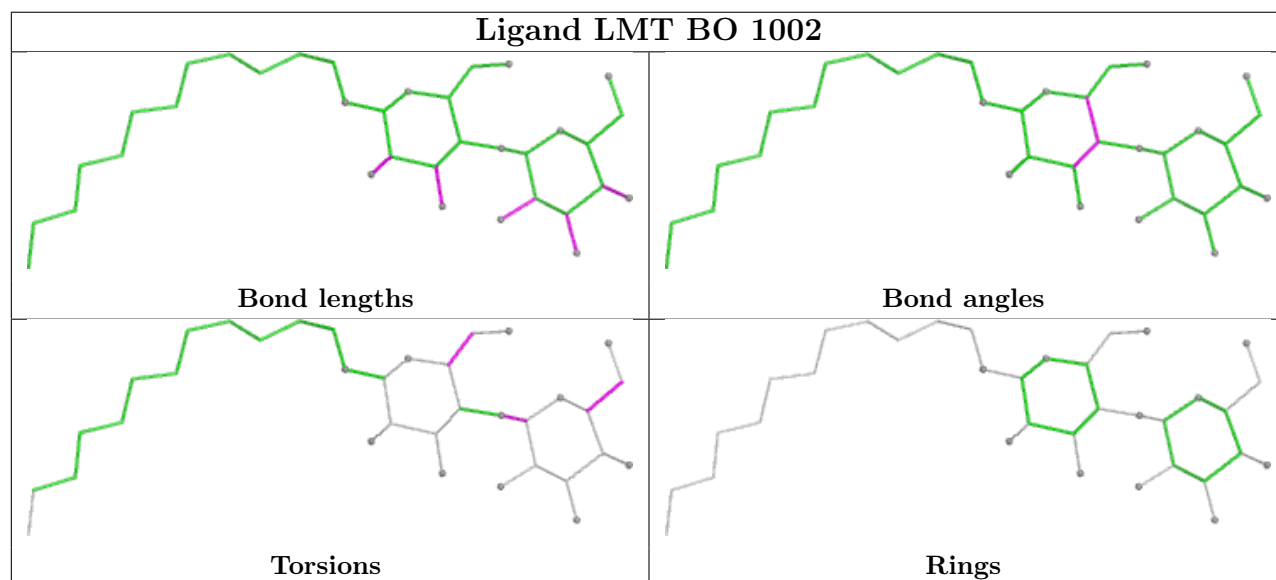
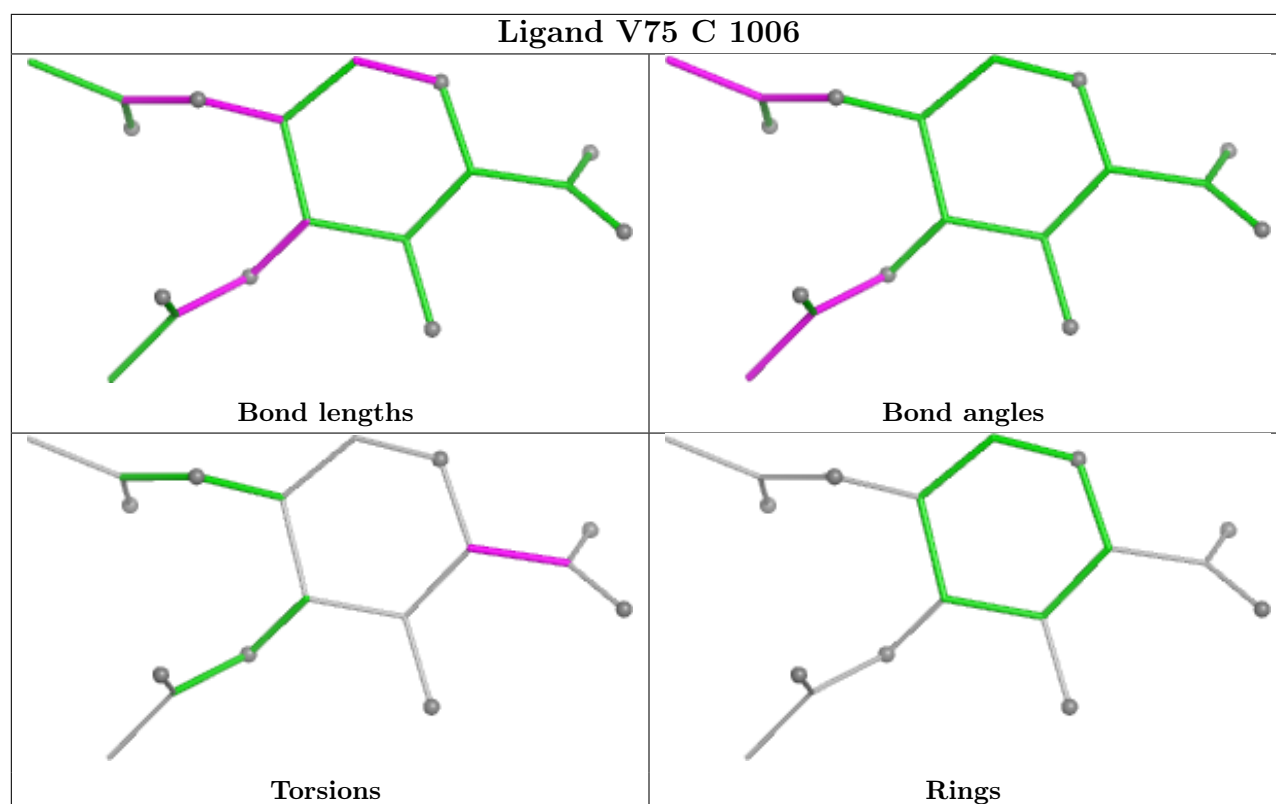


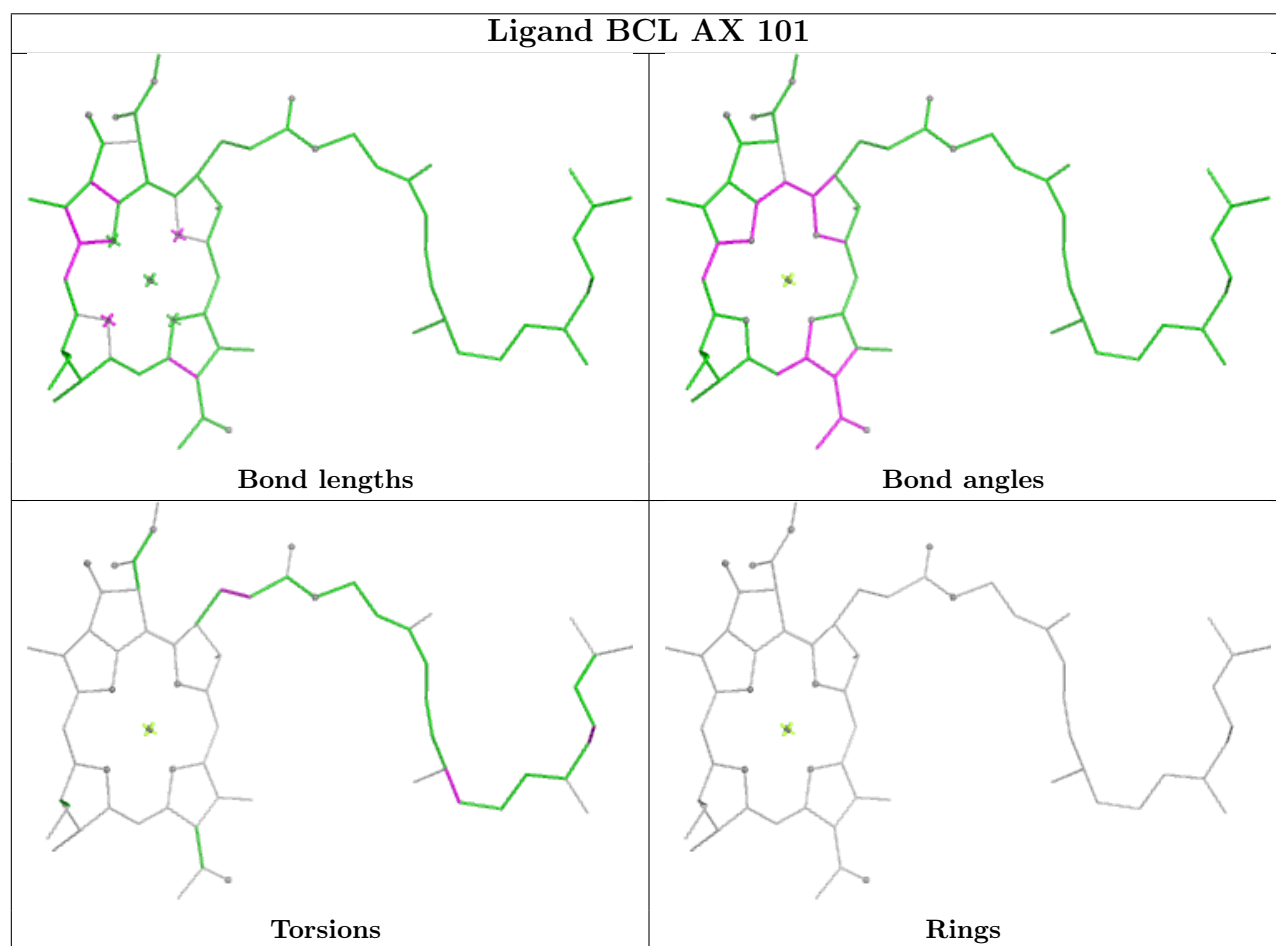
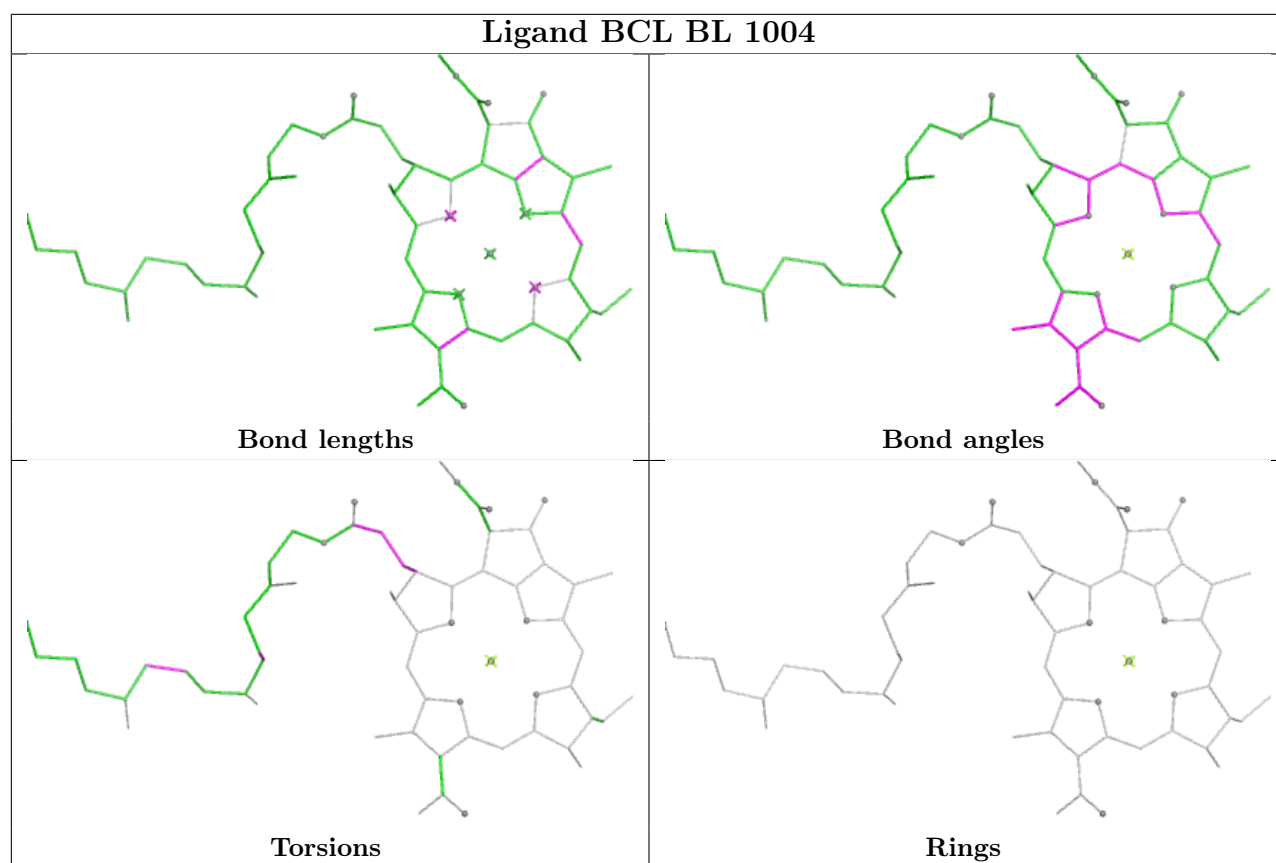


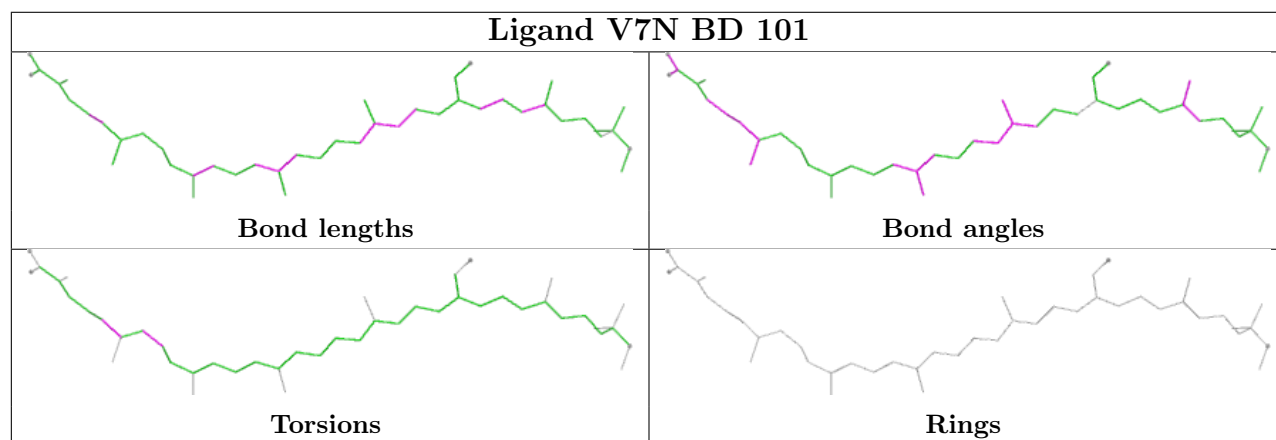
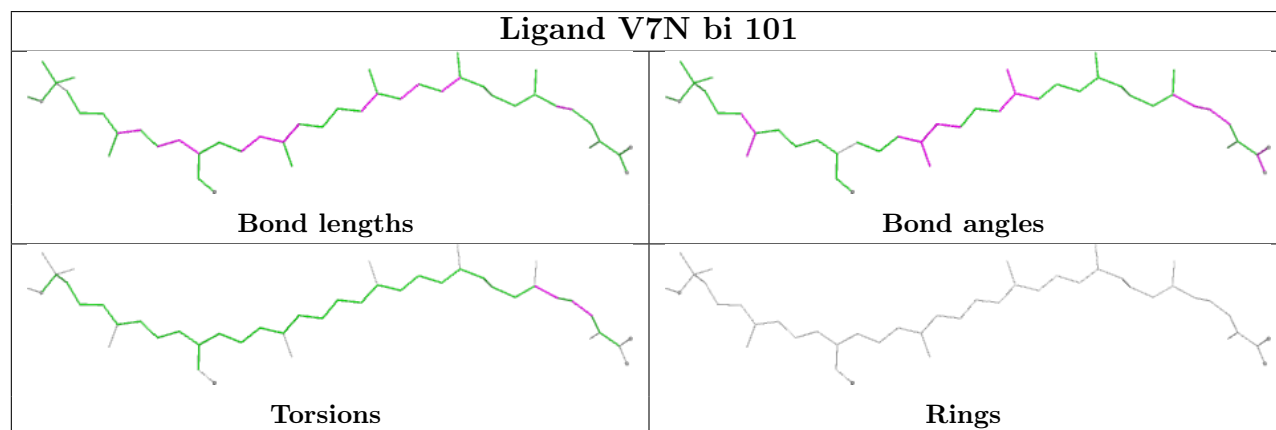
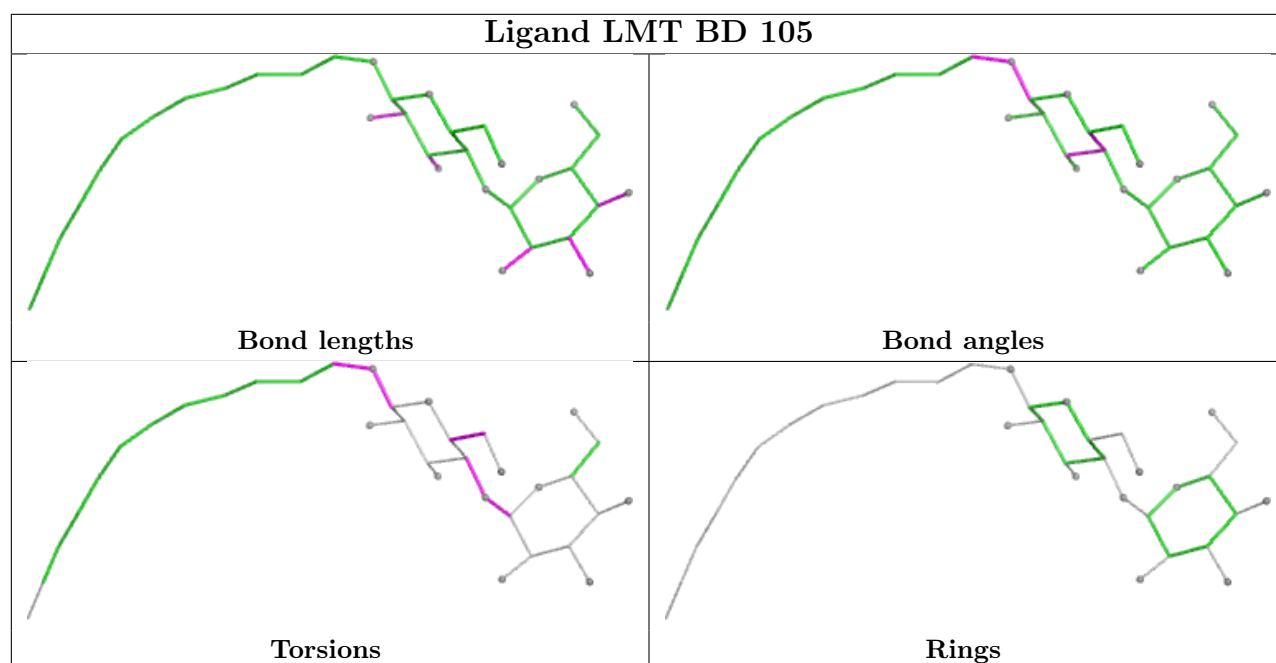




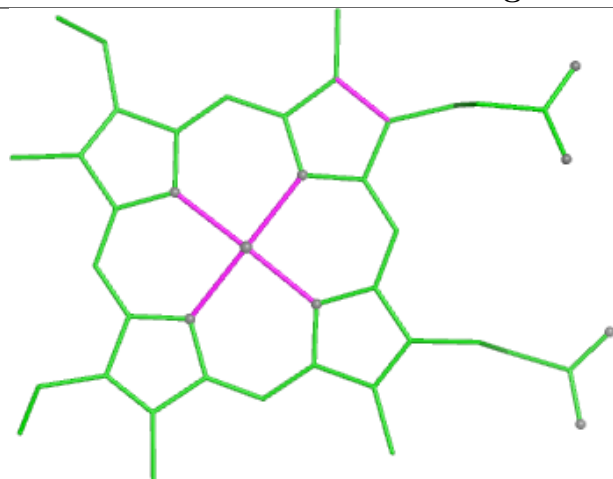




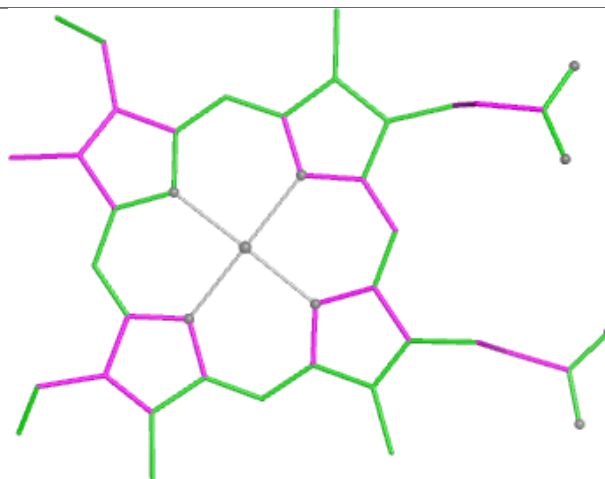




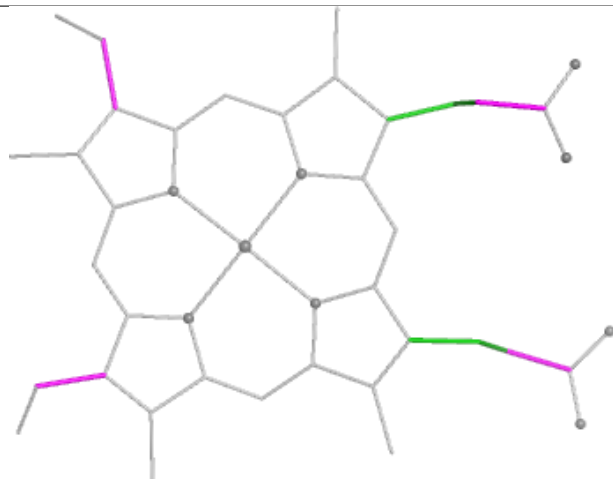
Ligand HEC C 1002



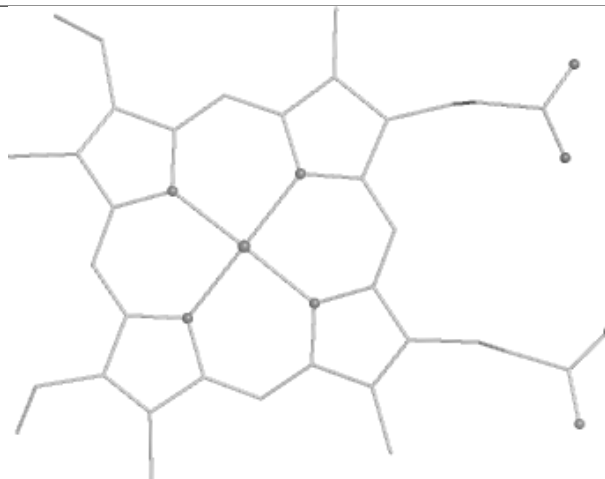
Bond lengths



Bond angles

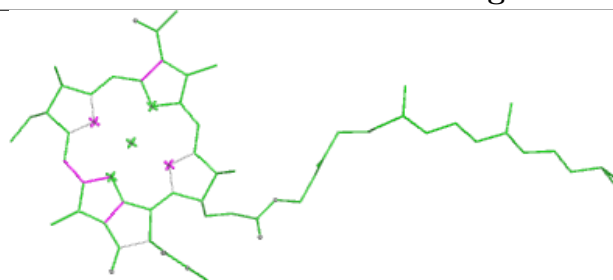


Torsions

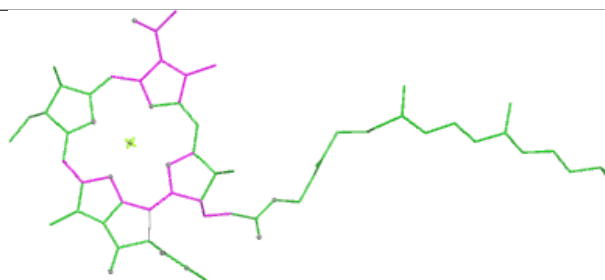


Rings

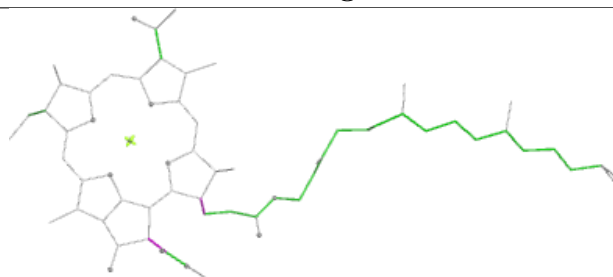
Ligand BCL BW 1003



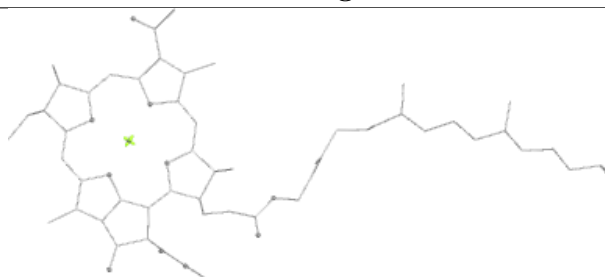
Bond lengths



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.

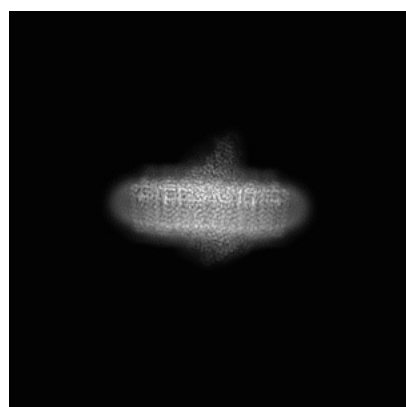
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12682. These allow visual inspection of the internal detail of the map and identification of artifacts.

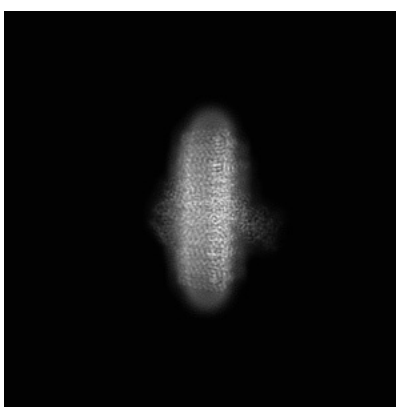
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

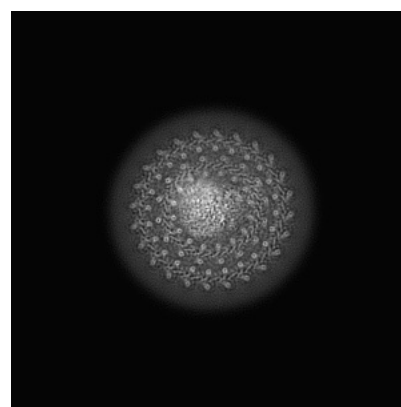
6.1.1 Primary map



X



Y

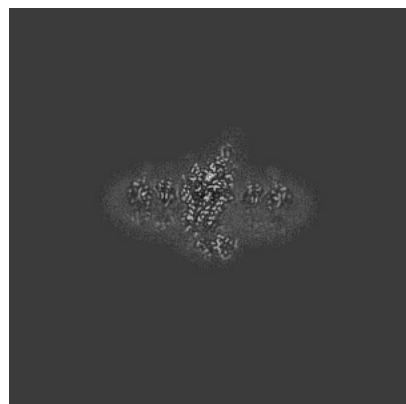


Z

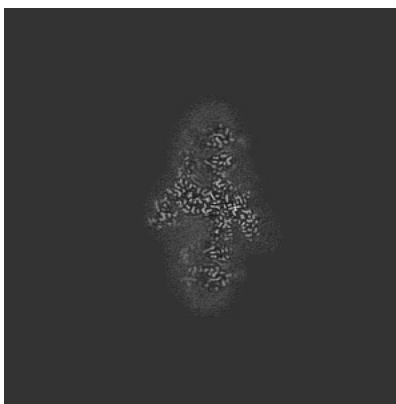
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

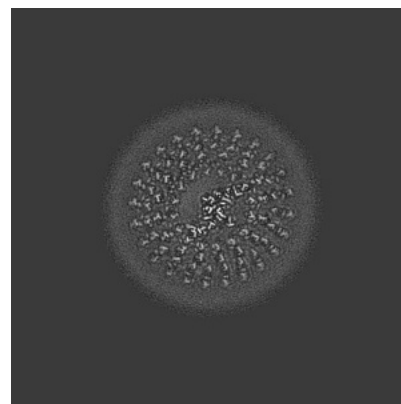
6.2.1 Primary map



X Index: 200



Y Index: 200

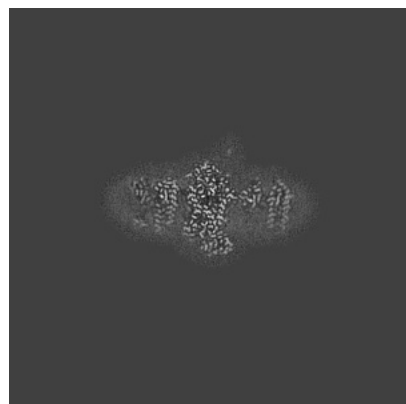


Z Index: 200

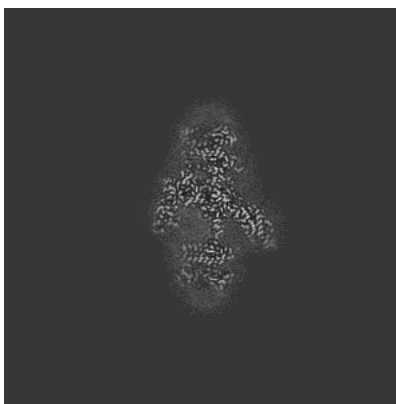
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

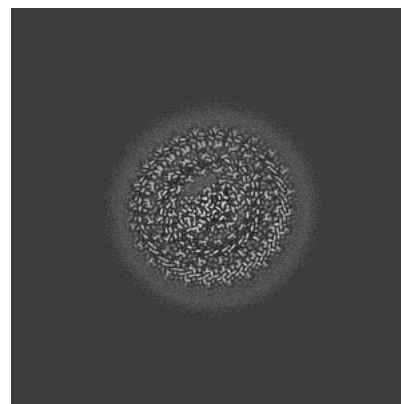
6.3.1 Primary map



X Index: 206



Y Index: 210

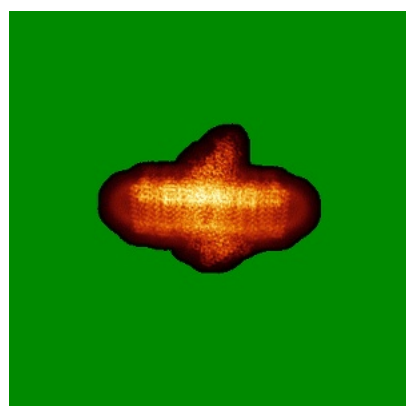


Z Index: 214

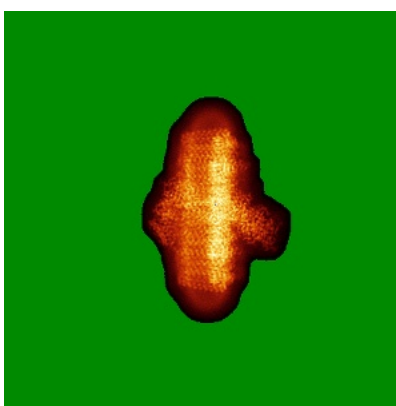
The images above show the largest variance slices of the map in three orthogonal directions.

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

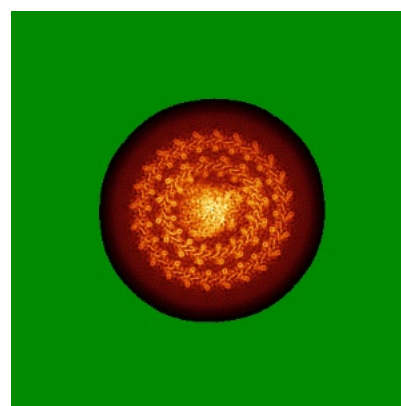
6.4.1 Primary map



X



Y

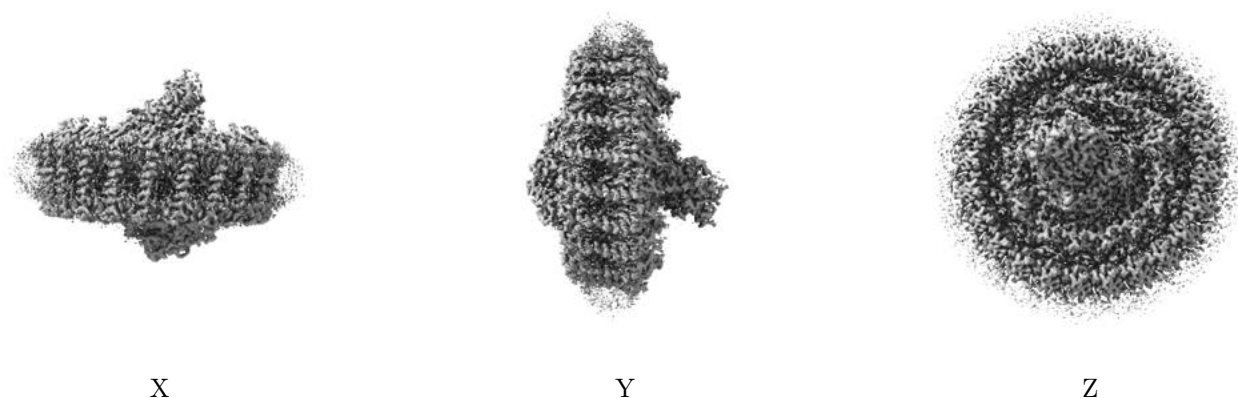


Z

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 0.0292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

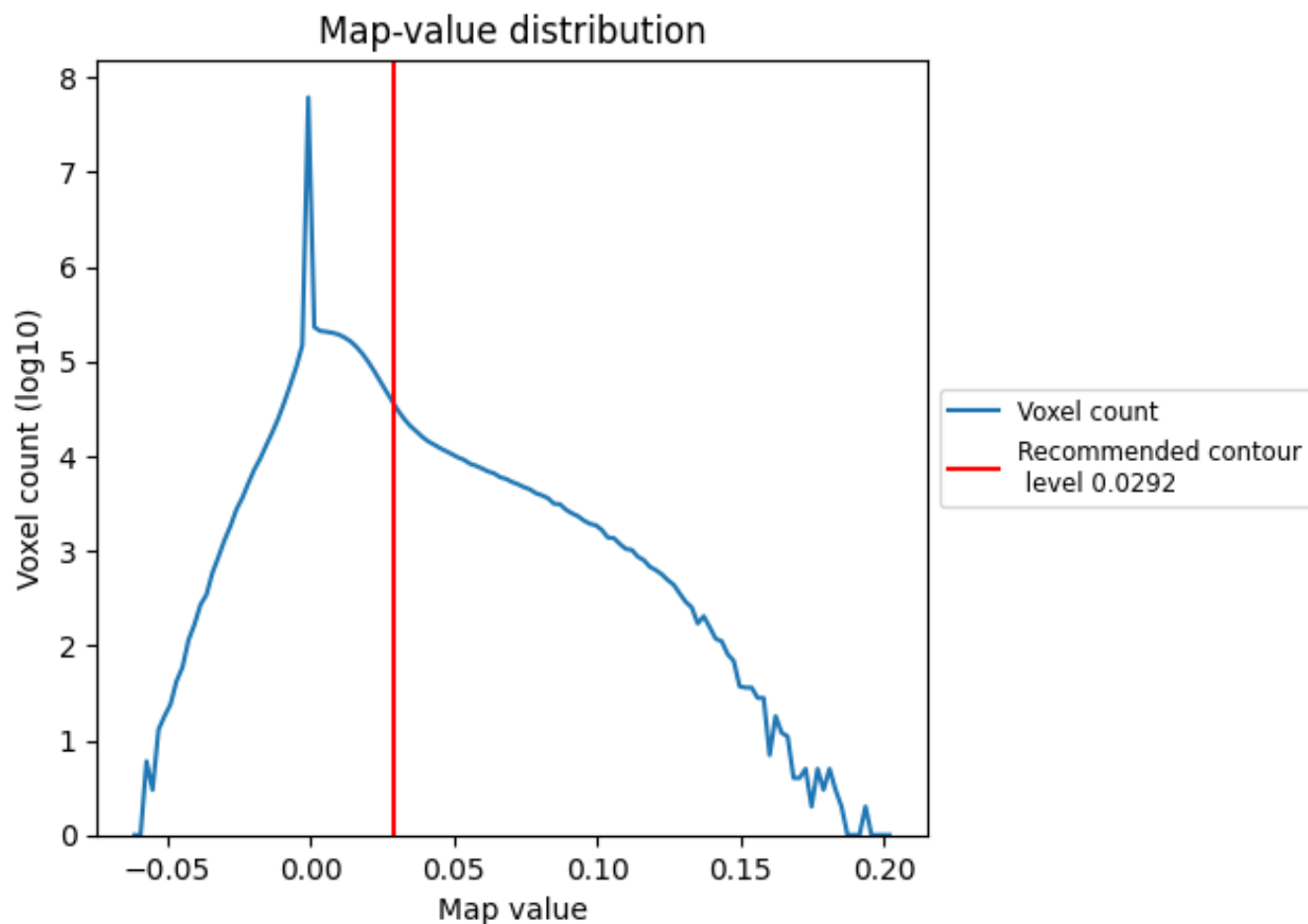
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

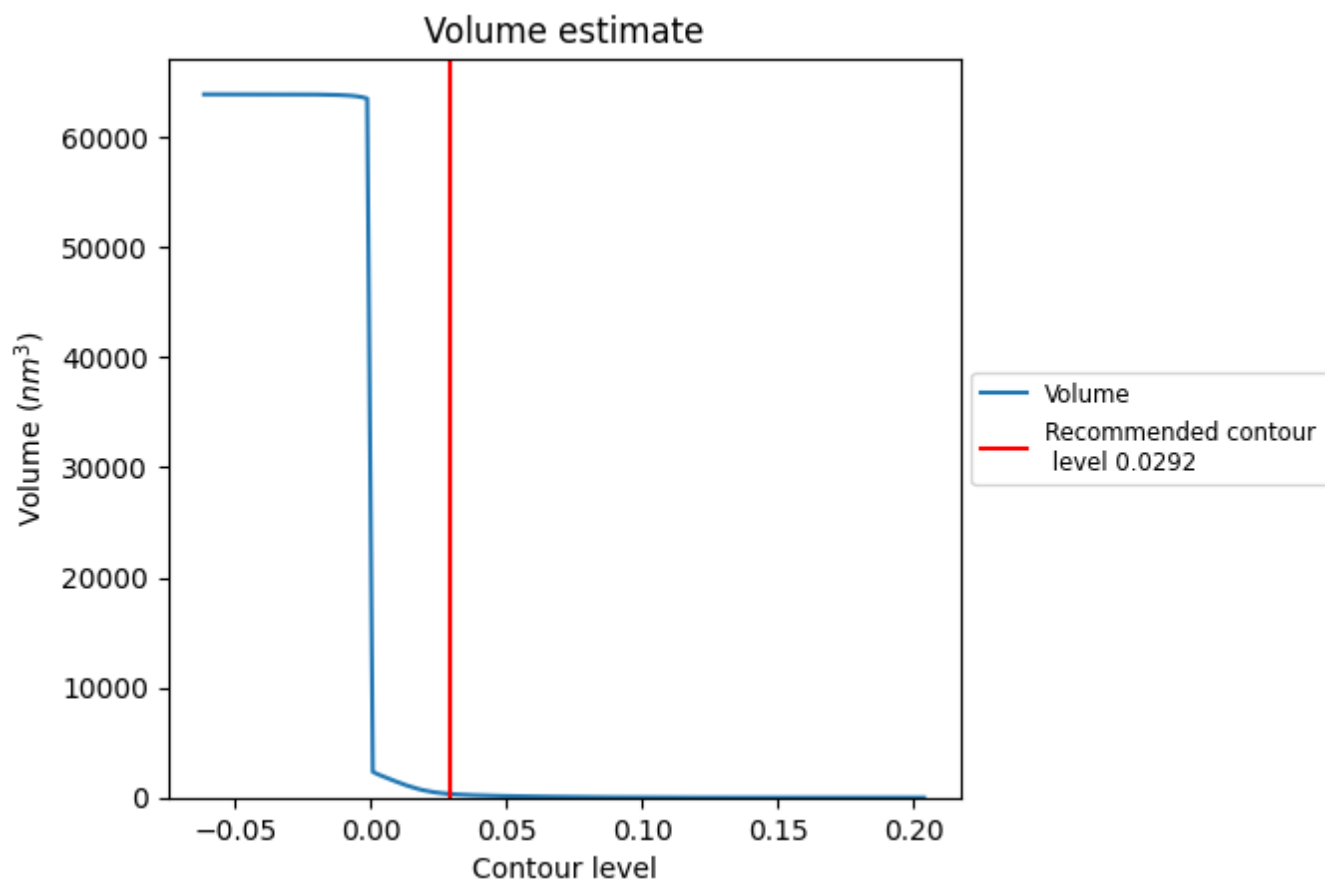
This section contains the results of statistical analysis of the map.

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.

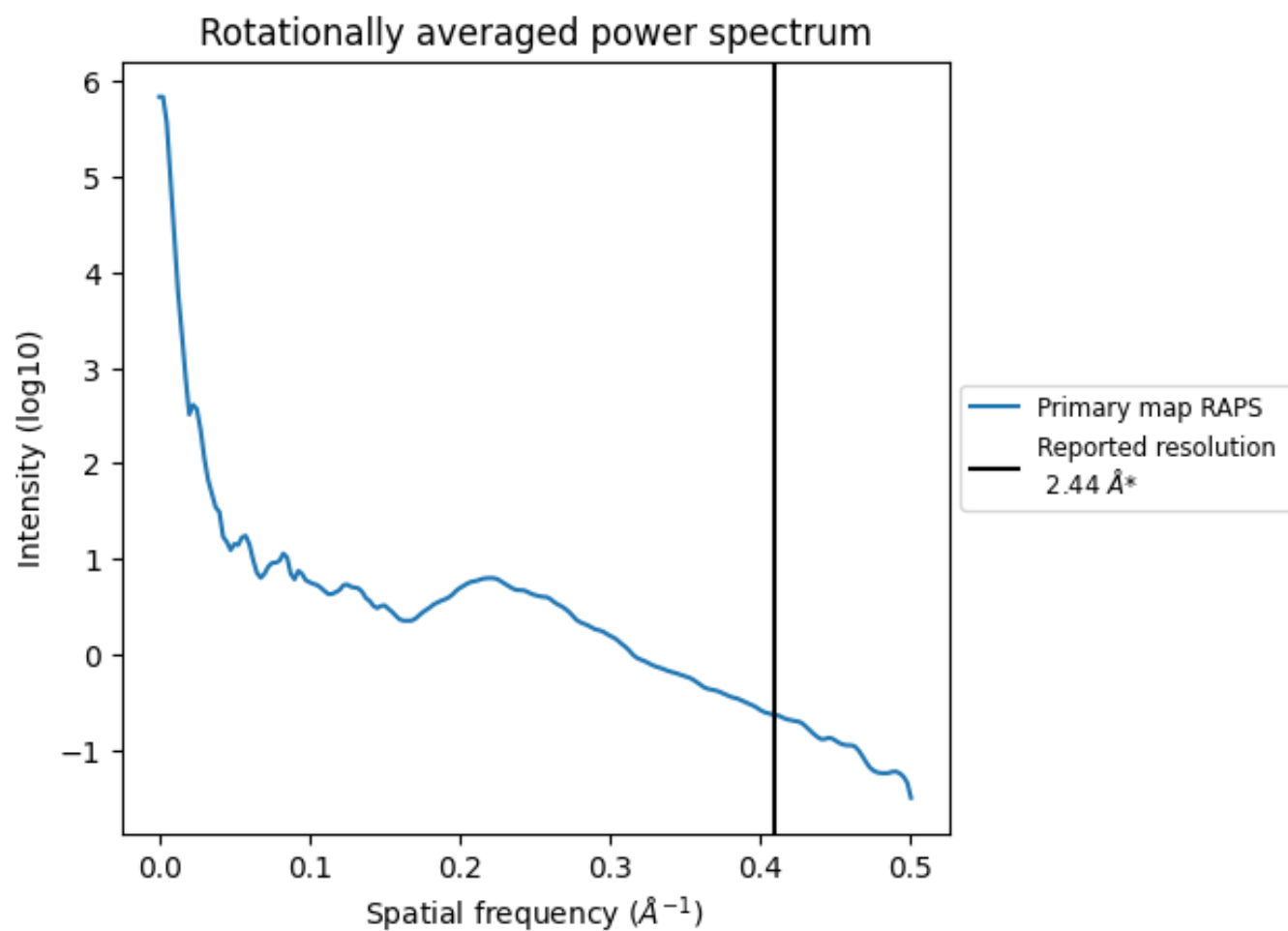
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm³; this corresponds to an approximate mass of 296 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 ⓘ

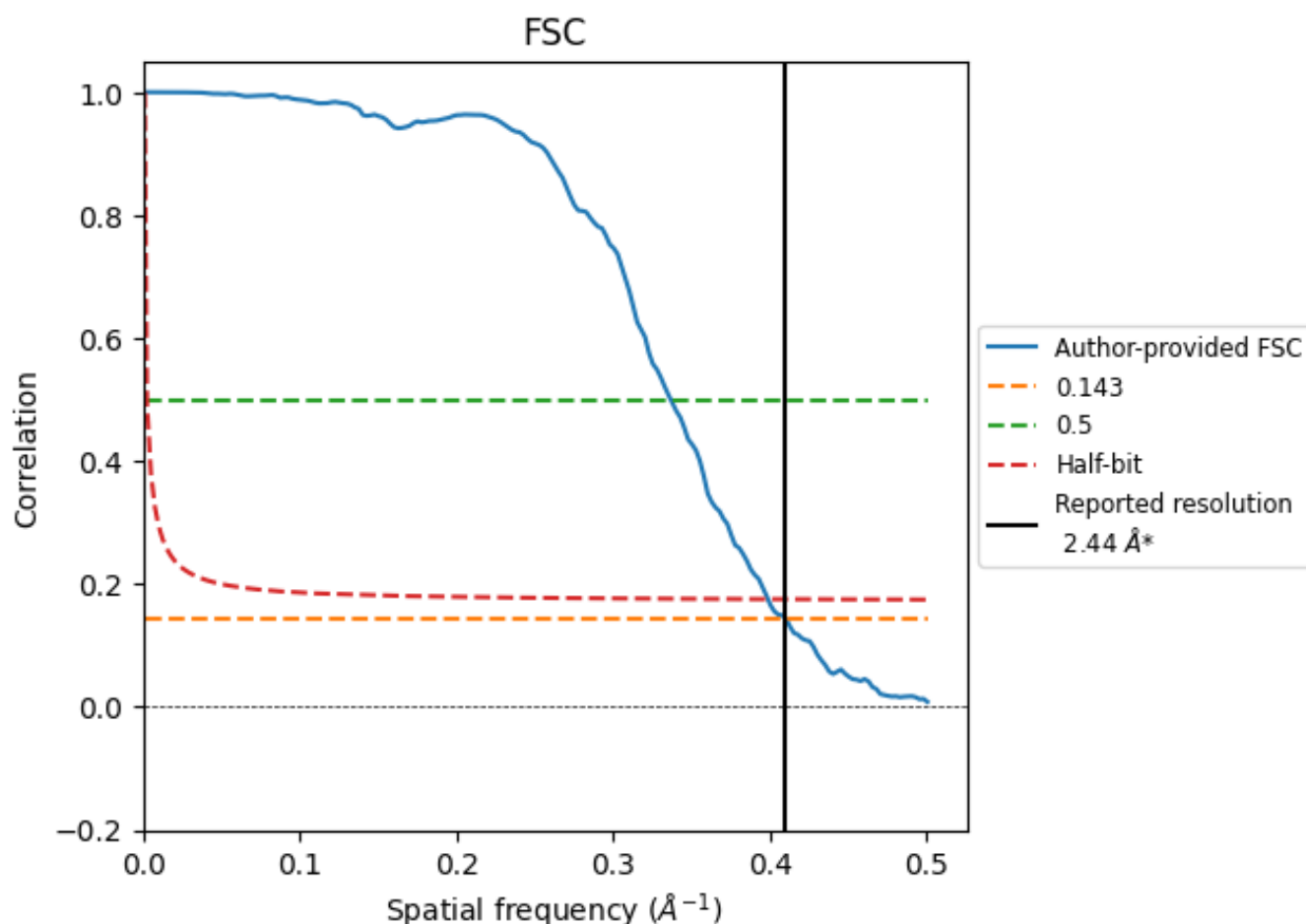


*Reported resolution corresponds to spatial frequency of 0.410 Å⁻¹

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 0.410 Å⁻¹

8.2 Resolution estimates [i](#)

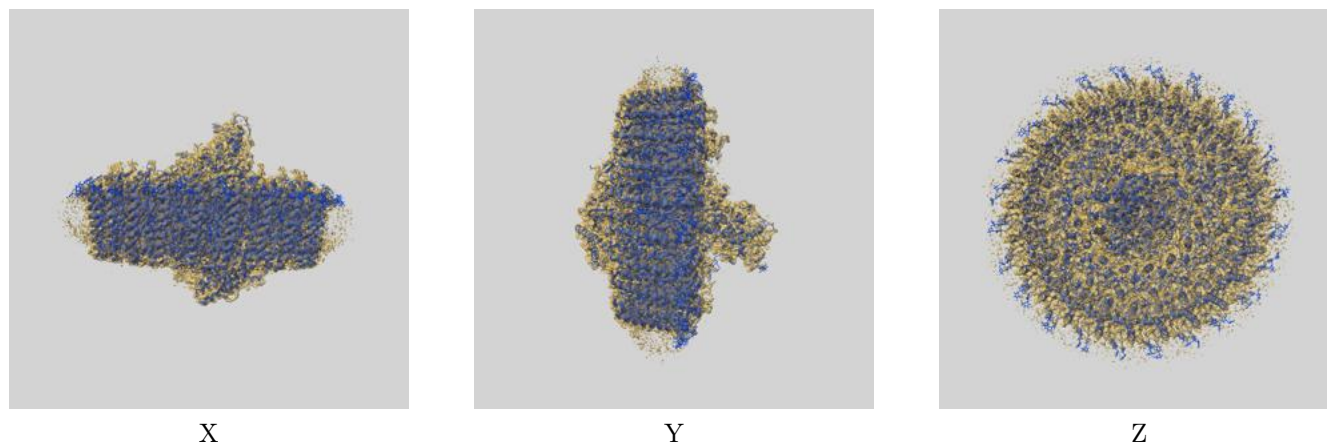
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.97	2.51
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

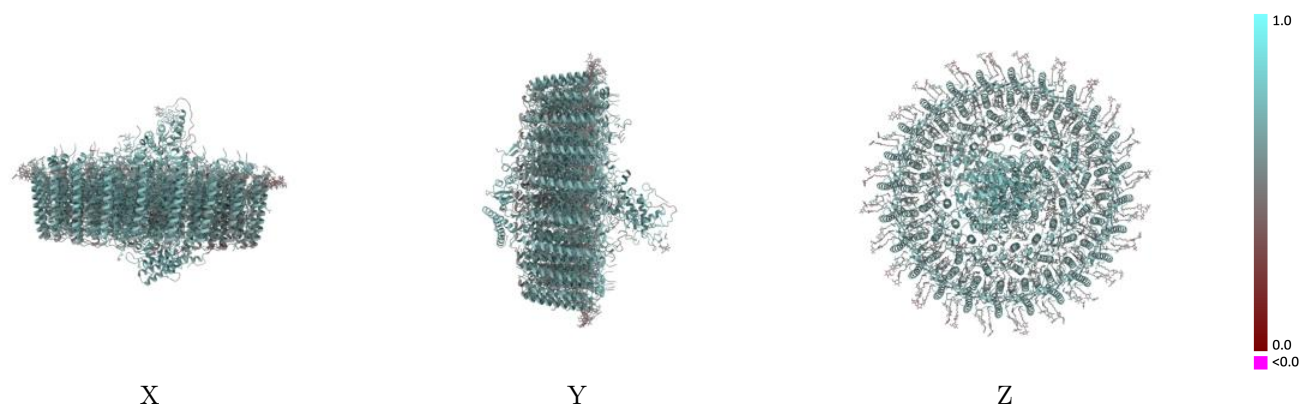
This section contains information regarding the fit between EMDB map EMD-12682 and PDB model 7O0X. Per-residue inclusion information can be found in [section 3](#) on [page 39](#).

9.1 Map-model overlay [i](#)



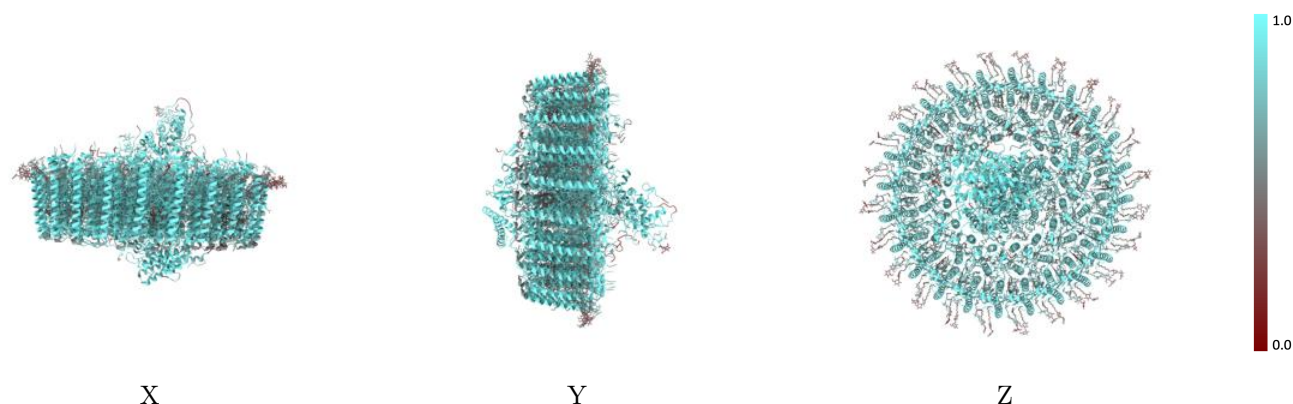
The images above show the 3D surface view of the map at the recommended contour level 0.0292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



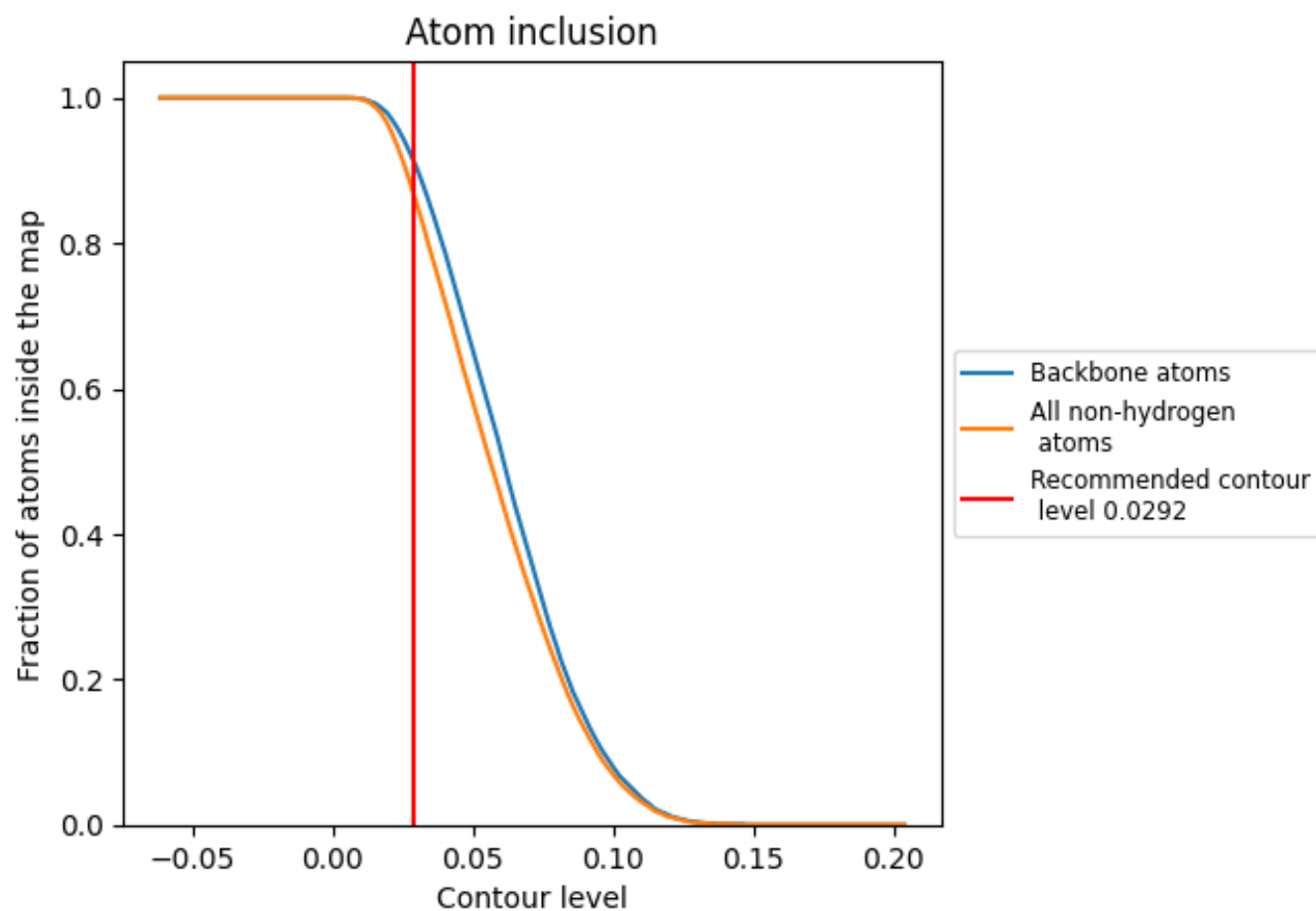
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0292).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.0292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.6290
AA	 0.9120	 0.6400
AB	 0.8220	 0.6000
AC	 0.7940	 0.5860
AD	 0.8440	 0.6100
AE	 0.8500	 0.6240
AF	 0.7610	 0.5730
AG	 0.8890	 0.6320
AH	 0.8500	 0.6170
AI	 0.8360	 0.6050
AJ	 0.9230	 0.6450
AK	 0.8820	 0.6330
AL	 0.8470	 0.6130
AM	 0.9270	 0.6520
AN	 0.8480	 0.6170
AO	 0.8290	 0.6020
AP	 0.9060	 0.6410
AQ	 0.8190	 0.6140
AR	 0.9110	 0.6350
AS	 0.8760	 0.6310
AT	 0.9470	 0.6510
AU	 0.8750	 0.6240
AV	 0.9240	 0.6460
AW	 0.7900	 0.6050
AX	 0.9440	 0.6460
BA	 0.7690	 0.5840
BB	 0.7810	 0.5860
BC	 0.7670	 0.5800
BD	 0.7370	 0.5680
BE	 0.7440	 0.5700
BF	 0.7350	 0.5540
BG	 0.8200	 0.6110
BH	 0.8000	 0.5990
BI	 0.7610	 0.5750
BJ	 0.8360	 0.6130



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Chain	Atom inclusion	Q-score
BK	 0.7910	 0.6010
BL	 0.7730	 0.5990
BM	 0.8200	 0.6030
BN	 0.7850	 0.5910
BO	 0.8020	 0.5910
BP	 0.7820	 0.5940
BQ	 0.8030	 0.5910
BR	 0.7780	 0.5860
BS	 0.7940	 0.5980
BT	 0.7900	 0.5950
BU	 0.7850	 0.5830
BV	 0.8280	 0.6060
BW	 0.7920	 0.5970
BX	 0.8160	 0.6060
C	 0.9290	 0.6680
C1	 0.9220	 0.6700
C2	 0.9240	 0.6370
CG	 0.7620	 0.5010
H1	 0.8990	 0.6520
H2	 0.9290	 0.6570
L	 0.9570	 0.6870
M	 0.9240	 0.6800
MG	 0.9520	 0.6080
aa	 0.8220	 0.6010
ab	 0.8630	 0.6280
ac	 0.8640	 0.6250
ad	 0.9280	 0.6630
ae	 0.9390	 0.6700
af	 0.8540	 0.6360
ag	 0.8790	 0.6330
ah	 0.8990	 0.6420
ai	 0.8320	 0.6150
aj	 0.9110	 0.6490
ak	 0.9560	 0.6680
al	 0.9200	 0.6600
am	 0.8780	 0.6420
an	 0.8070	 0.6170
ao	 0.9150	 0.6620
ap	 0.9050	 0.6340
ba	 0.8050	 0.5900
bb	 0.7840	 0.6010
bc	 0.8660	 0.6240

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Chain	Atom inclusion	Q-score
bd	 0.8920	 0.6470
be	 0.9020	 0.6340
bf	 0.8970	 0.6450
bg	 0.8900	 0.6310
bh	 0.8730	 0.6250
bi	 0.8900	 0.6280
bj	 0.8920	 0.6420
bk	 0.8710	 0.6220
bl	 0.8460	 0.6190
bm	 0.8700	 0.6320
bn	 0.8690	 0.6320
bo	 0.9040	 0.6370
bp	 0.8720	 0.6360