



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 09:05 pm BST

PDB ID : 7O0V / pdb_00007o0v
EMDB ID : EMD-12680
Title : Cryo-EM structure (model_2a) of the RC-dLH complex from Gemmatimonas phototrophica at 2.5 Å
Authors : Qian, P.; Koblizek, M.
Deposited on : 2021-03-27
Resolution : 2.50 Å (reported)
Based on initial models : 5Y5S, 1LGH, 6ET5

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

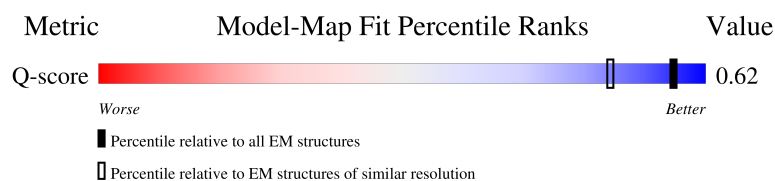
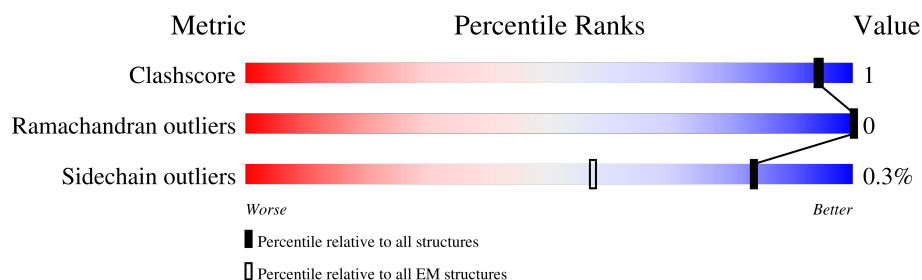
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.50 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	7115 (2.00 - 3.00)

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	 85% 6% 9%
1	AB	54	 83% 7% 9%
1	AE	54	 87% 9%
1	AF	54	 89% 9%

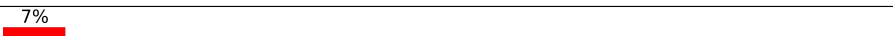
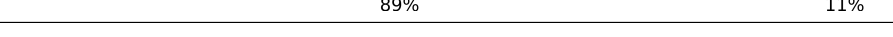
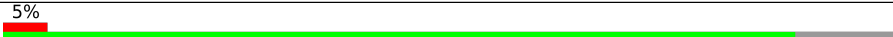
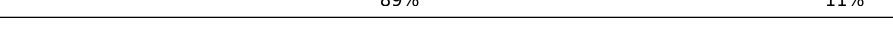
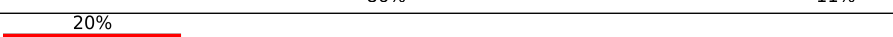
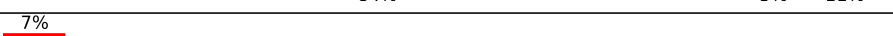
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AG	54	
1	AH	54	
1	AI	54	
1	AJ	54	
1	AK	54	
1	AL	54	
1	AM	54	
1	AN	54	
1	AO	54	
1	AP	54	
1	AQ	54	
1	AR	54	
1	AS	54	
1	AT	54	
1	AU	54	
1	AV	54	
1	AW	54	
1	AX	54	
2	AC	54	
2	AD	54	
3	BA	44	
3	BC	44	
3	BF	44	
3	BG	44	
3	BH	44	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	BJ	44	
3	BK	44	
3	BL	44	
3	BM	44	
3	BN	44	
3	BO	44	
3	BP	44	
3	BU	44	
3	BX	44	
3	ba	44	
3	bb	44	
3	bc	44	
3	bd	44	
3	be	44	
3	bf	44	
3	bg	44	
3	bh	44	
3	bi	44	
3	bj	44	
3	bk	44	
3	bl	44	
3	bm	44	
3	bo	44	
3	bp	44	
4	BB	43	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	BD	43	
4	BE	43	
4	BI	43	
4	BQ	43	
4	BR	43	
4	BS	43	
4	BT	43	
4	BV	43	
4	BW	43	
4	bn	43	
5	C	354	
6	C1	202	
7	H1	67	
8	H2	181	
9	L	274	
10	M	367	
11	aa	71	
12	ab	71	
12	ac	71	
12	ad	71	
12	ae	71	
12	af	71	
12	ag	71	
12	ah	71	
12	ai	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	aj	71	
12	ak	71	
12	al	71	
12	am	71	
12	an	71	
12	ao	71	
12	ap	71	
13	CG	2	
13	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
17	HEC	C	401	X	-	-	-
17	HEC	C	402	X	-	-	-
17	HEC	C	403	X	-	-	-
17	HEC	C	404	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 55475 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	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		
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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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 LHH-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	48	Total	C	N	O	S	0	0
			384	256	64	60	4		
2	AD	48	Total	C	N	O	S	0	0
			384	256	64	60	4		

- Molecule 3 is a protein called Light-harvesting protein B:885 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BA	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BC	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BF	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BG	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BH	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BJ	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BK	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BL	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BM	39	Total	C	N	O	S	0	0
			323	213	55	53	2		
3	BN	39	Total	C	N	O	S	0	0
			323	213	55	53	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BO	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	BP	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	BU	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	BX	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	ba	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bb	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bc	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bd	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	be	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bf	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bg	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bh	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bi	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bj	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bk	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bl	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bm	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bo	39	Total 323	C 213	N 55	O 53	S 2	0	0
3	bp	39	Total 323	C 213	N 55	O 53	S 2	0	0

- Molecule 4 is a protein called Light-harvesting protein B:885 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BB	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BD	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BE	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BI	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BQ	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BR	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BS	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BT	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BV	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	BW	40	Total	C	N	O	S	0	0
			327	215	56	54	2		
4	bn	40	Total	C	N	O	S	0	0
			327	215	56	54	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	?	-	LYS	deletion	UNP A0A143BHS8
BD	?	-	LYS	deletion	UNP A0A143BHS8
BE	?	-	LYS	deletion	UNP A0A143BHS8
BI	?	-	LYS	deletion	UNP A0A143BHS8
BQ	?	-	LYS	deletion	UNP A0A143BHS8
BR	?	-	LYS	deletion	UNP A0A143BHS8
BS	?	-	LYS	deletion	UNP A0A143BHS8
BT	?	-	LYS	deletion	UNP A0A143BHS8
BV	?	-	LYS	deletion	UNP A0A143BHS8
BW	?	-	LYS	deletion	UNP A0A143BHS8
bn	?	-	LYS	deletion	UNP A0A143BHS8

- Molecule 5 is a protein called MULTIHEME_CYTC domain-containing protein.

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

- Molecule 6 is a protein called RC-S.

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

- Molecule 7 is a protein called PRCH domain-containing protein.

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

- Molecule 8 is a protein called RC-Hc.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H2	174	Total	C	N	O	S	0	0
			1354	863	229	258	4		

- Molecule 9 is a protein called Photosynthetic reaction center L subunit.

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

- Molecule 10 is a protein called RC-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	315	Total	C	N	O	S	0	0
			2536	1691	417	418	10		

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

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

- Molecule 12 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	ab	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	ac	56	Total	C	N	O	S	0	0
			443	290	77	73	3		

Continued on next page...

Continued from previous page...

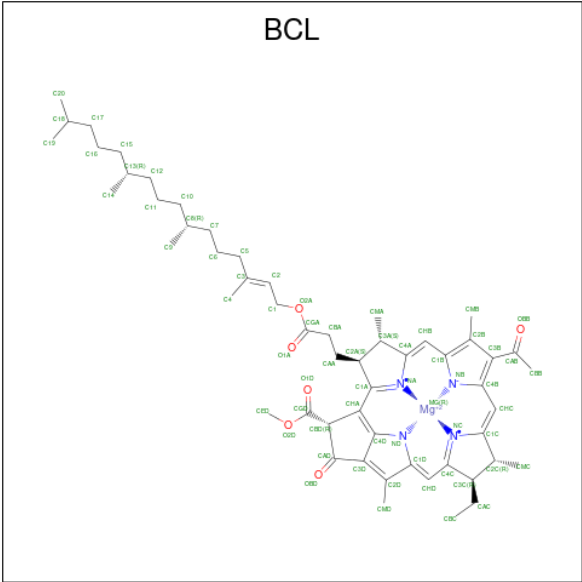
Mol	Chain	Residues	Atoms					AltConf	Trace
12	ad	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ae	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	af	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	ag	58	Total	C	N	O	S	0	0
			455	298	79	75	3		
12	ah	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ai	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	aj	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ak	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
12	al	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	am	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	an	71	Total	C	N	O	S	0	0
			542	352	95	91	4		
12	ao	60	Total	C	N	O	S	0	0
			465	304	81	77	3		
12	ap	71	Total	C	N	O	S	0	0
			543	352	95	92	4		

- Molecule 13 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose.



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

- Molecule 14 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

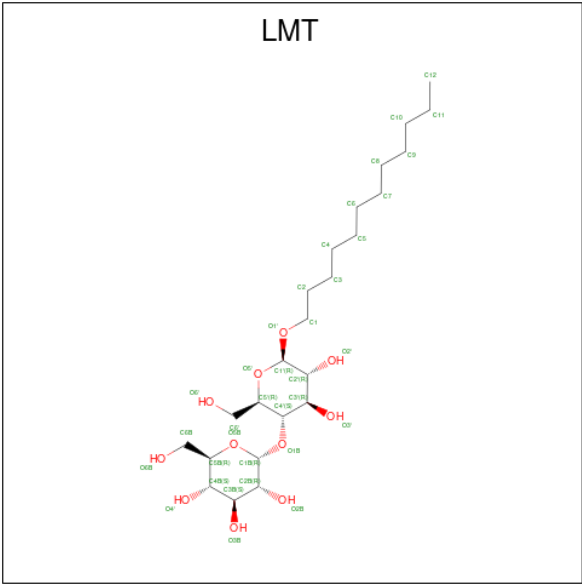
Mol	Chain	Residues	Atoms					AltConf
14	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	ai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

Continued on next page...

Continued from previous page...

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

- Molecule 15 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
15	AA	1	Total	C	O	0
			35	24	11	
15	AC	1	Total	C	O	0
			35	24	11	
15	AD	1	Total	C	O	0
			35	24	11	
15	AD	1	Total	C	O	0
			35	24	11	
15	AE	1	Total	C	O	0
			35	24	11	
15	AF	1	Total	C	O	0
			35	24	11	
15	AG	1	Total	C	O	0
			35	24	11	
15	AH	1	Total	C	O	0
			35	24	11	
15	AH	1	Total	C	O	0
			35	24	11	
15	AI	1	Total	C	O	0
			35	24	11	
15	AJ	1	Total	C	O	0
			35	24	11	
15	AJ	1	Total	C	O	0
			35	24	11	
15	AL	1	Total	C	O	0
			35	24	11	
15	AN	1	Total	C	O	0
			35	24	11	
15	AP	1	Total	C	O	0
			35	24	11	
15	AP	1	Total	C	O	0
			35	24	11	
15	AQ	1	Total	C	O	0
			35	24	11	
15	AS	1	Total	C	O	0
			35	24	11	
15	AT	1	Total	C	O	0
			35	24	11	
15	AU	1	Total	C	O	0
			35	24	11	
15	AX	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
15	BA	1	Total 35	C 24	O 11	0
15	BA	1	Total 35	C 24	O 11	0
15	BA	1	Total 35	C 24	O 11	0
15	BB	1	Total 35	C 24	O 11	0
15	BB	1	Total 35	C 24	O 11	0
15	BB	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BC	1	Total 35	C 24	O 11	0
15	BD	1	Total 35	C 24	O 11	0
15	BD	1	Total 35	C 24	O 11	0
15	BD	1	Total 35	C 24	O 11	0
15	BE	1	Total 35	C 24	O 11	0
15	BE	1	Total 35	C 24	O 11	0
15	BF	1	Total 35	C 24	O 11	0
15	BF	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0
15	BG	1	Total 35	C 24	O 11	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

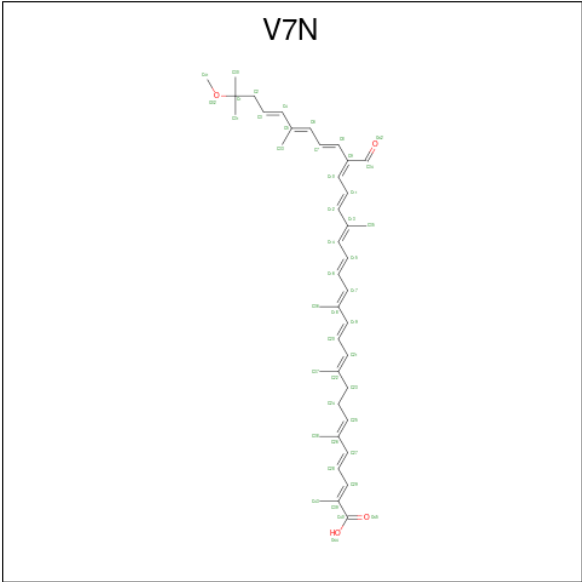
Mol	Chain	Residues	Atoms			AltConf
15	BV	1	Total	C	O	0
			35	24	11	
15	BV	1	Total	C	O	0
			35	24	11	
15	BV	1	Total	C	O	0
			35	24	11	
15	BV	1	Total	C	O	0
			35	24	11	
15	BW	1	Total	C	O	0
			35	24	11	
15	BW	1	Total	C	O	0
			35	24	11	
15	BW	1	Total	C	O	0
			35	24	11	
15	BX	1	Total	C	O	0
			35	24	11	
15	BX	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	L	1	Total	C	O	0
			35	24	11	
15	M	1	Total	C	O	0
			35	24	11	
15	ab	1	Total	C	O	0
			35	24	11	
15	bb	1	Total	C	O	0
			35	24	11	
15	bc	1	Total	C	O	0
			35	24	11	
15	bd	1	Total	C	O	0
			35	24	11	
15	be	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

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

- Molecule 16 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-dotriaconta-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (CCD ID: V7N) (formula: C₄₁H₅₄O₄).



Mol	Chain	Residues	Atoms			AltConf
16	AE	1	Total	C	O	0
			45	41	4	
16	AO	1	Total	C	O	0
			45	41	4	
16	AS	1	Total	C	O	0
			45	41	4	
16	BA	1	Total	C	O	0
			45	41	4	
16	BB	1	Total	C	O	0
			45	41	4	
16	BC	1	Total	C	O	0
			45	41	4	
16	BD	1	Total	C	O	0
			45	41	4	
16	BE	1	Total	C	O	0
			45	41	4	
16	BG	1	Total	C	O	0
			45	41	4	
16	BH	1	Total	C	O	0
			45	41	4	
16	BI	1	Total	C	O	0
			45	41	4	
16	BJ	1	Total	C	O	0
			45	41	4	
16	BK	1	Total	C	O	0
			45	41	4	
16	BL	1	Total	C	O	0
			45	41	4	

Continued on next page...

Continued from previous page...

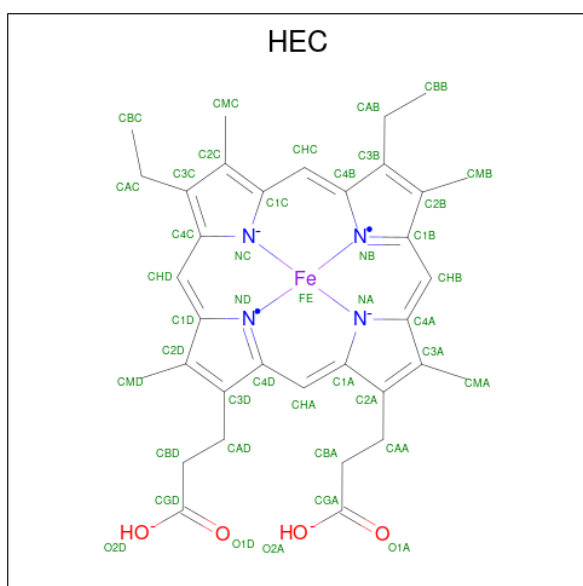
Mol	Chain	Residues	Atoms			AltConf
16	BM	1	Total 45	C 41	O 4	0
16	BO	1	Total 45	C 41	O 4	0
16	BP	1	Total 45	C 41	O 4	0
16	BQ	1	Total 45	C 41	O 4	0
16	BR	1	Total 45	C 41	O 4	0
16	BS	1	Total 45	C 41	O 4	0
16	BU	1	Total 45	C 41	O 4	0
16	BV	1	Total 45	C 41	O 4	0
16	BW	1	Total 45	C 41	O 4	0
16	BX	1	Total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

Continued on next page...

Continued from previous page...

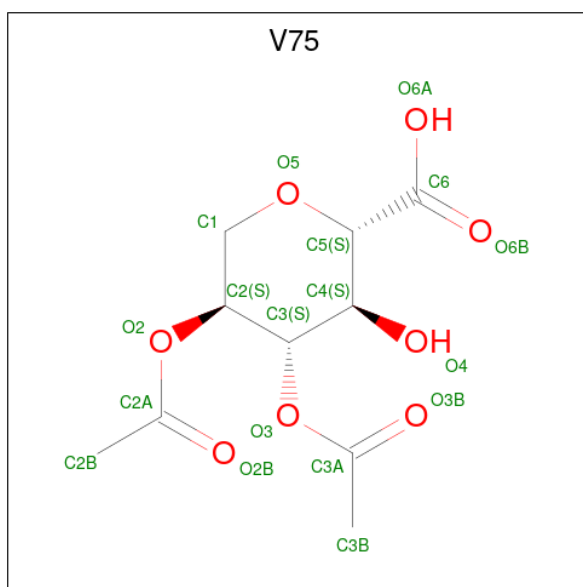
Mol	Chain	Residues	Atoms			AltConf
16	bl	1	Total	C	O	0
			45	41	4	
16	bm	1	Total	C	O	0
			45	41	4	
16	bn	1	Total	C	O	0
			45	41	4	
16	bo	1	Total	C	O	0
			45	41	4	
16	bp	1	Total	C	O	0
			45	41	4	

- Molecule 17 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



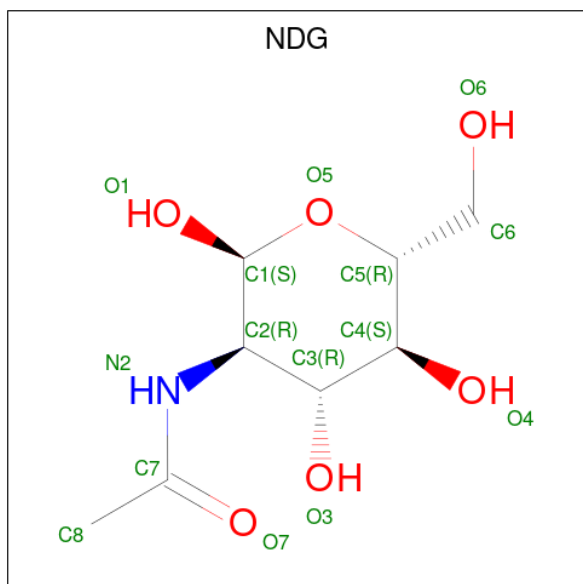
Mol	Chain	Residues	Atoms					AltConf
17	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
17	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
17	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
17	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 18 is (2 {S},3 {S},4 {S},5 {S})-4,5-diacetyloxy-3-oxidanyl-oxane-2-carboxylic acid (CCD ID: V75) (formula: $C_{10}H_{14}O_8$).



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

- Molecule 19 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



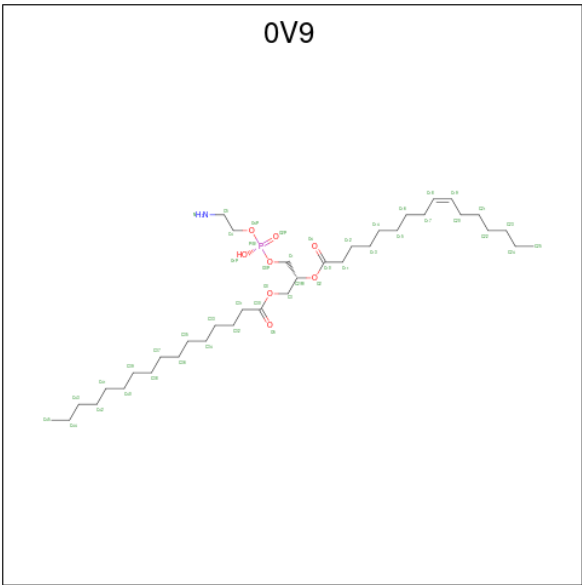
Mol	Chain	Residues	Atoms				AltConf
19	C	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

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

- 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).



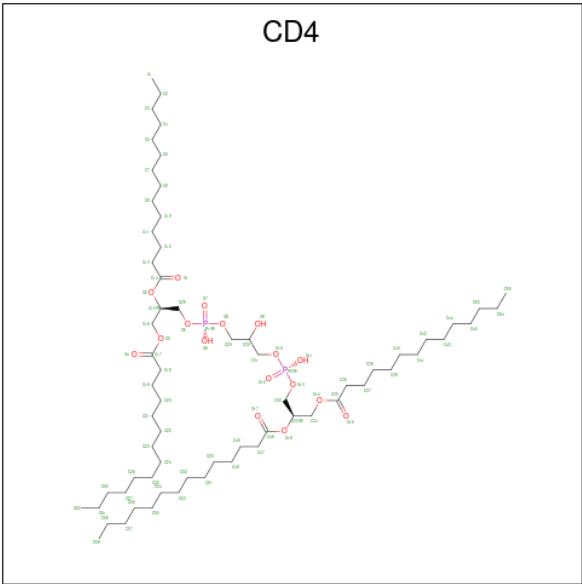
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	C1	1	45	35	1	8	1	0
20	H1	1	45	35	1	8	1	0
20	aj	1	45	35	1	8	1	0
20	ba	1	45	35	1	8	1	0
20	bb	1	45	35	1	8	1	0
20	bc	1	45	35	1	8	1	0
20	be	1	45	35	1	8	1	0
20	be	1	45	35	1	8	1	0
20	bg	1	45	35	1	8	1	0

Continued on next page...

Continued from previous page...

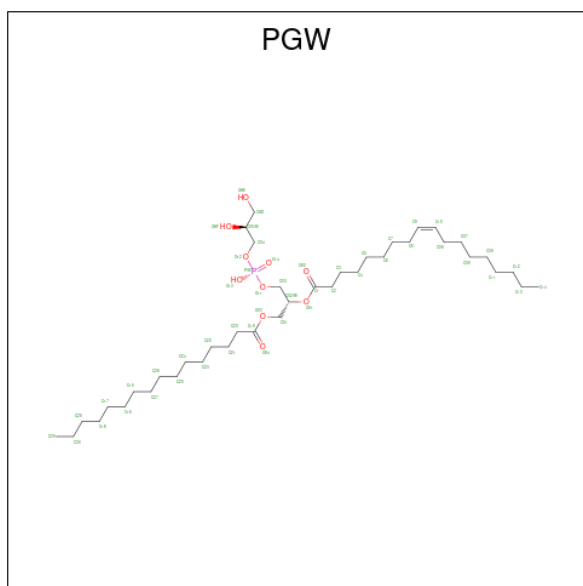
Mol	Chain	Residues	Atoms					AltConf
20	bg	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bh	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bi	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bj	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bk	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bk	1	Total	C	N	O	P	0
			45	35	1	8	1	
20	bl	1	Total	C	N	O	P	0
			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	
20	bp	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-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).



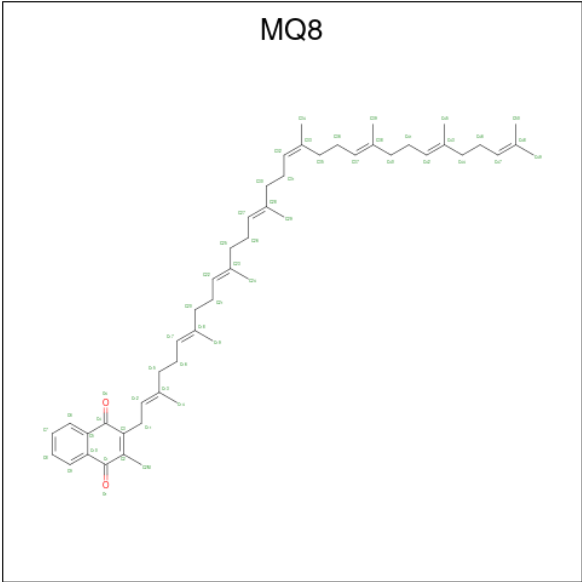
Mol	Chain	Residues	Atoms				AltConf
21	H1	1	Total	C	O	P	0
			84	65	17	2	
21	H1	1	Total	C	O	P	0
			84	65	17	2	
21	M	1	Total	C	O	P	0
			84	65	17	2	
21	ae	1	Total	C	O	P	0
			84	65	17	2	
21	af	1	Total	C	O	P	0
			84	65	17	2	
21	aj	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 22 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).



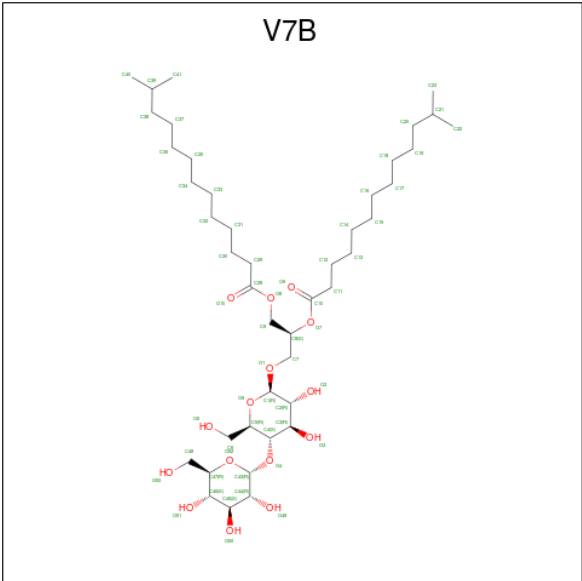
Mol	Chain	Residues	Atoms				AltConf
22	H1	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 23 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



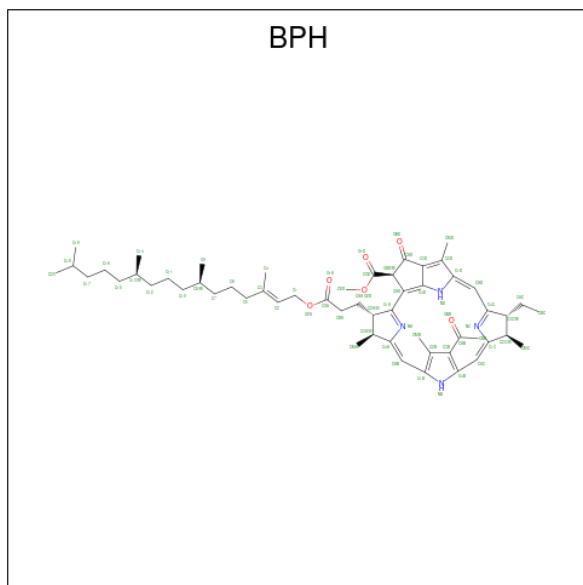
Mol	Chain	Residues	Atoms			AltConf
23	L	1	Total	C	O	0
			53	51	2	
23	M	1	Total	C	O	0
			53	51	2	
23	ao	1	Total	C	O	0
			53	51	2	

- Molecule 24 is [(2 {S})-3-[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-5-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]oxy-2-(12-methyltridecanoyloxy)propyl] 12-methyltridecanoate (CCD ID: V7B) (formula: C₄₃H₈₀O₁₅).



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

- Molecule 25 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

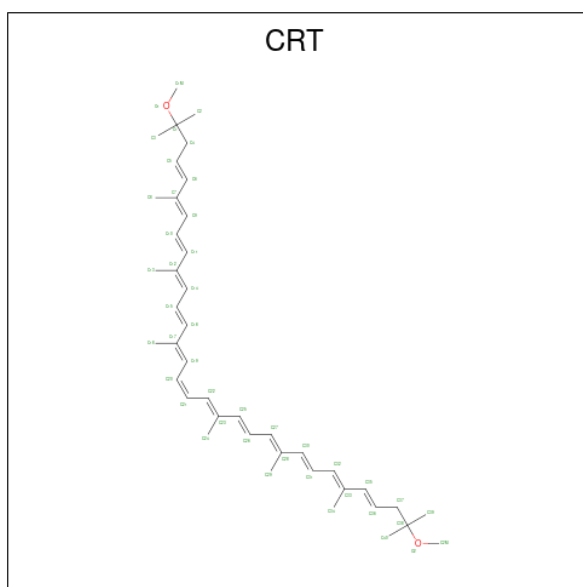


Mol	Chain	Residues	Atoms				AltConf
25	L	1	Total	C	N	O	0
			65	55	4	6	
25	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 26 is FE (III) ION (CCD ID: FE) (formula: Fe).

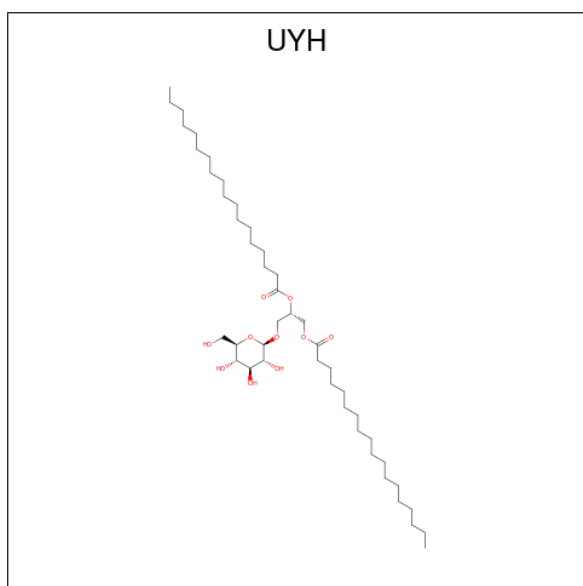
Mol	Chain	Residues	Atoms		AltConf
26	M	1	Total	Fe	0
			1	1	

- Molecule 27 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



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

- Molecule 28 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: $C_{45}H_{86}O_{10}$).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	AltConf
29	AA	2	Total O 2 2	0
29	AB	3	Total O 3 3	0
29	AC	3	Total O 3 3	0
29	AD	1	Total O 1 1	0
29	AE	3	Total O 3 3	0
29	AF	2	Total O 2 2	0
29	AG	5	Total O 5 5	0
29	AH	1	Total O 1 1	0
29	AI	3	Total O 3 3	0
29	AJ	5	Total O 5 5	0
29	AK	4	Total O 4 4	0
29	AL	2	Total O 2 2	0
29	AM	6	Total O 6 6	0
29	AN	4	Total O 4 4	0
29	AO	4	Total O 4 4	0
29	AP	4	Total O 4 4	0
29	AQ	4	Total O 4 4	0
29	AS	6	Total O 6 6	0
29	AT	2	Total O 2 2	0
29	AU	1	Total O 1 1	0
29	AV	6	Total O 6 6	0
29	AW	2	Total O 2 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
29	AX	3	Total O 3 3	0
29	BB	1	Total O 1 1	0
29	BI	1	Total O 1 1	0
29	BJ	1	Total O 1 1	0
29	BO	1	Total O 1 1	0
29	BP	1	Total O 1 1	0
29	C	86	Total O 86 86	0
29	C1	42	Total O 42 42	0
29	H1	17	Total O 17 17	0
29	H2	9	Total O 9 9	0
29	L	51	Total O 51 51	0
29	M	58	Total O 58 58	0
29	aa	3	Total O 3 3	0
29	ab	3	Total O 3 3	0
29	ac	3	Total O 3 3	0
29	ad	6	Total O 6 6	0
29	ae	10	Total O 10 10	0
29	af	11	Total O 11 11	0
29	ag	7	Total O 7 7	0
29	ah	6	Total O 6 6	0
29	ai	5	Total O 5 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
29	aj	7	Total 7	O 7	0
29	ak	13	Total 13	O 13	0
29	al	5	Total 5	O 5	0
29	am	5	Total 5	O 5	0
29	an	9	Total 9	O 9	0
29	ao	5	Total 5	O 5	0
29	ap	11	Total 11	O 11	0
29	ba	3	Total 3	O 3	0
29	bb	4	Total 4	O 4	0
29	bc	2	Total 2	O 2	0
29	bd	3	Total 3	O 3	0
29	be	4	Total 4	O 4	0
29	bf	1	Total 1	O 1	0
29	bg	2	Total 2	O 2	0
29	bh	2	Total 2	O 2	0
29	bi	2	Total 2	O 2	0
29	bj	3	Total 3	O 3	0
29	bk	3	Total 3	O 3	0
29	bl	3	Total 3	O 3	0
29	bm	2	Total 2	O 2	0
29	bn	1	Total 1	O 1	0

Continued on next page...

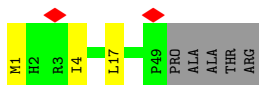
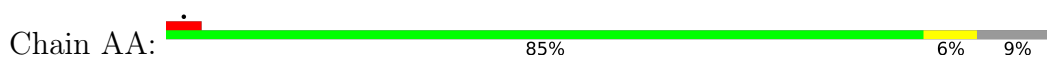
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
29	bo	1	Total	O	0
			1	1	

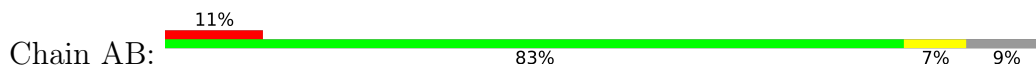
3 Residue-property plots [i](#)

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.

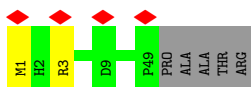
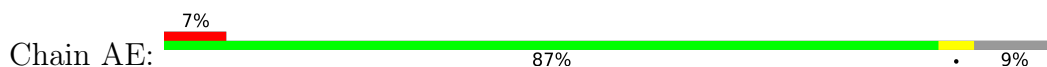
- Molecule 1: LHh-alpha



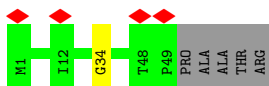
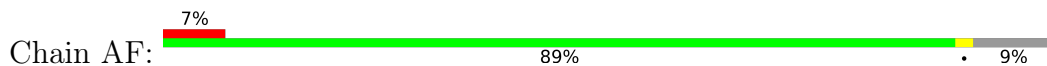
- Molecule 1: LHh-alpha



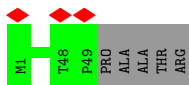
- Molecule 1: LHh-alpha



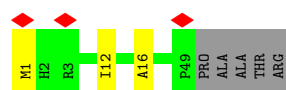
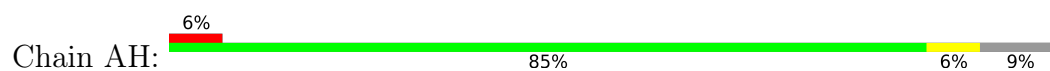
- Molecule 1: LHh-alpha



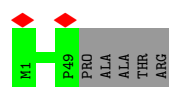
- Molecule 1: LHh-alpha



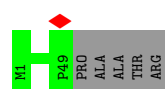
● Molecule 1: LHh-alpha



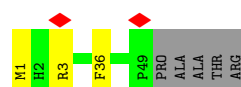
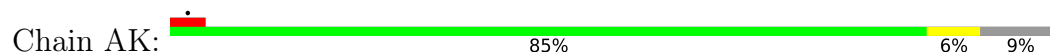
● Molecule 1: LHh-alpha



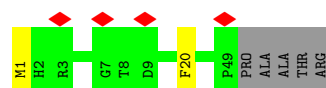
● Molecule 1: LHh-alpha



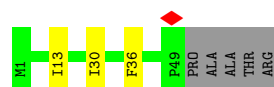
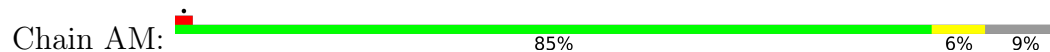
● Molecule 1: LHh-alpha



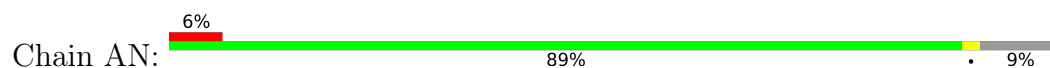
● Molecule 1: LHh-alpha

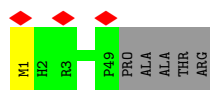


● Molecule 1: LHh-alpha

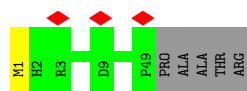
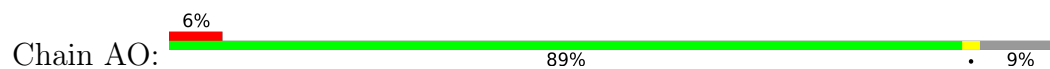


● Molecule 1: LHh-alpha

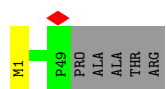




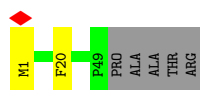
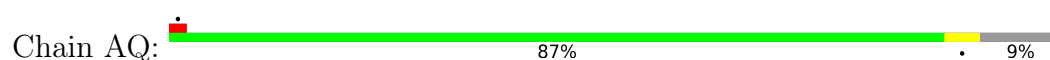
- Molecule 1: LHh-alpha



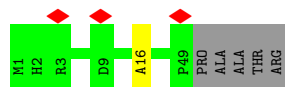
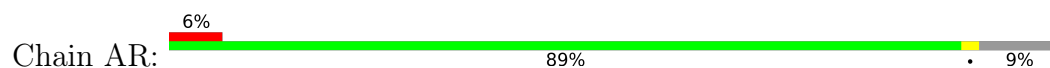
- Molecule 1: LHh-alpha



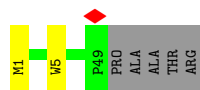
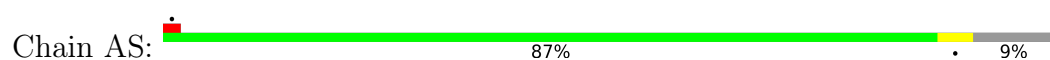
- Molecule 1: LHh-alpha



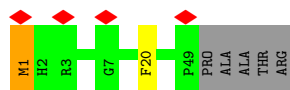
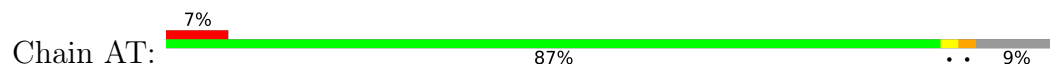
- Molecule 1: LHh-alpha



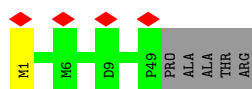
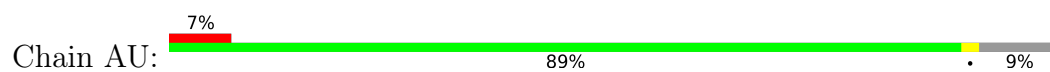
- Molecule 1: LHh-alpha



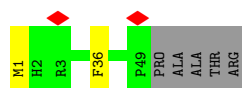
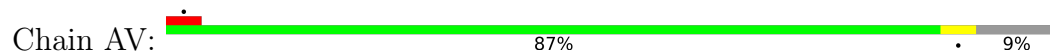
- Molecule 1: LHh-alpha



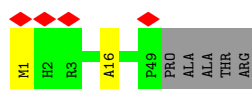
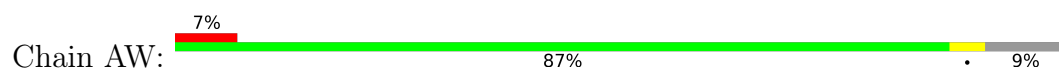
- Molecule 1: LHh-alpha



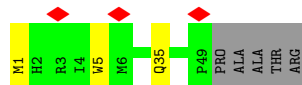
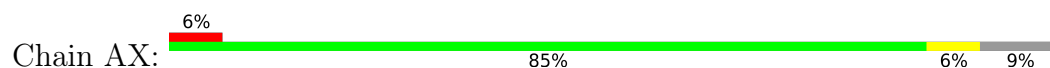
- Molecule 1: LHH-alpha



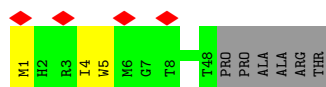
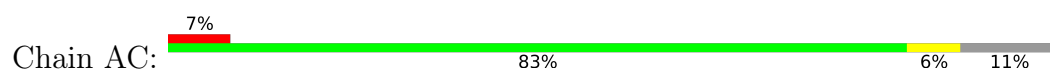
- Molecule 1: LHH-alpha



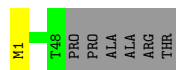
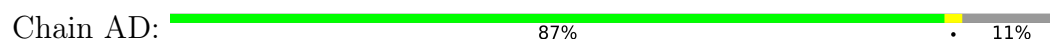
- Molecule 1: LHH-alpha



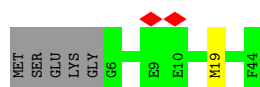
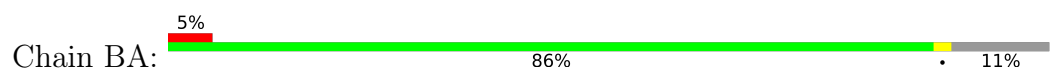
- Molecule 2: LHH-alpha



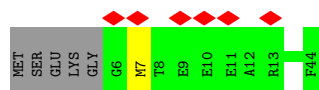
- Molecule 2: LHH-alpha



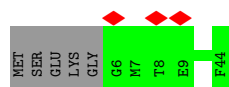
- Molecule 3: Light-harvesting protein B:885 subunit beta



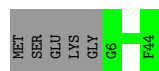
- Molecule 3: Light-harvesting protein B:885 subunit beta



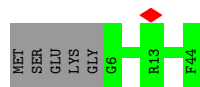
- Molecule 3: Light-harvesting protein B:885 subunit beta



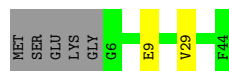
- Molecule 3: Light-harvesting protein B:885 subunit beta



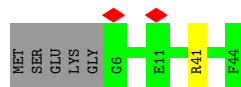
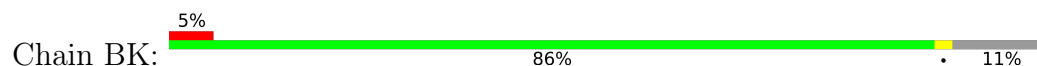
- Molecule 3: Light-harvesting protein B:885 subunit beta



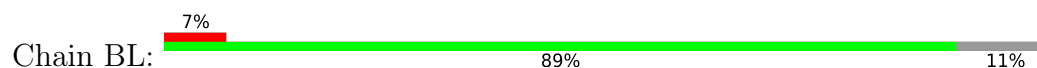
- Molecule 3: Light-harvesting protein B:885 subunit beta

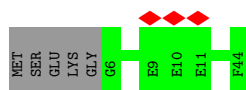


- Molecule 3: Light-harvesting protein B:885 subunit beta

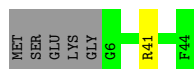
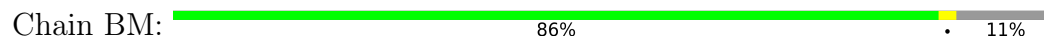


- Molecule 3: Light-harvesting protein B:885 subunit beta

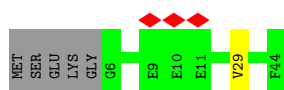
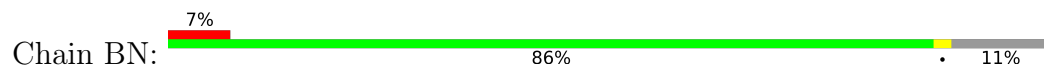




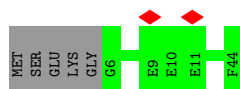
- Molecule 3: Light-harvesting protein B:885 subunit beta



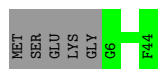
- Molecule 3: Light-harvesting protein B:885 subunit beta



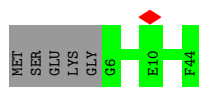
- Molecule 3: Light-harvesting protein B:885 subunit beta



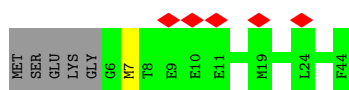
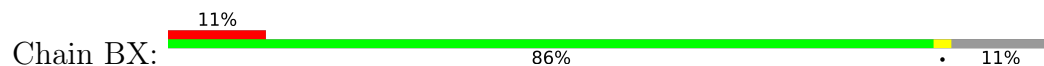
- Molecule 3: Light-harvesting protein B:885 subunit beta



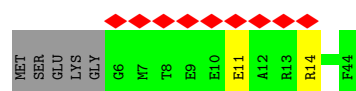
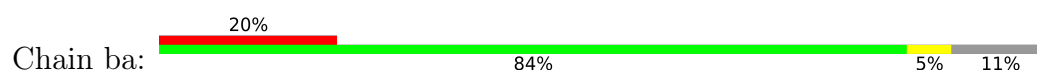
- Molecule 3: Light-harvesting protein B:885 subunit beta



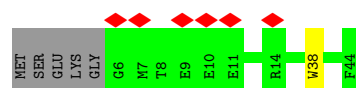
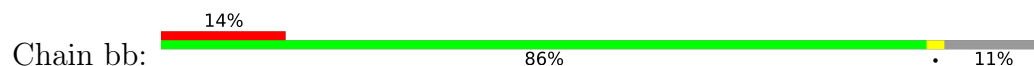
- Molecule 3: Light-harvesting protein B:885 subunit beta



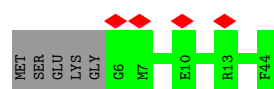
- Molecule 3: Light-harvesting protein B:885 subunit beta



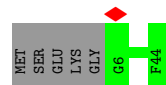
- Molecule 3: Light-harvesting protein B:885 subunit beta



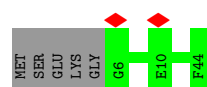
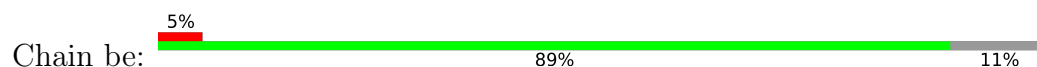
- Molecule 3: Light-harvesting protein B:885 subunit beta



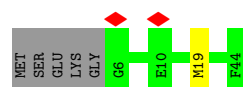
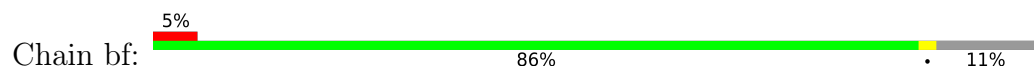
- Molecule 3: Light-harvesting protein B:885 subunit beta



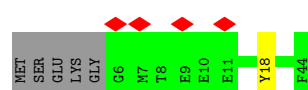
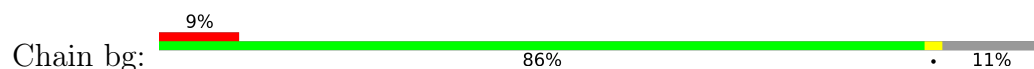
- Molecule 3: Light-harvesting protein B:885 subunit beta



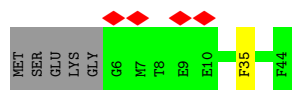
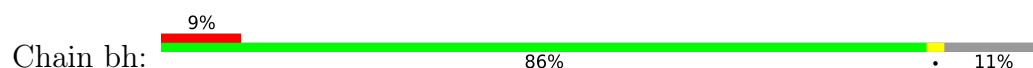
- Molecule 3: Light-harvesting protein B:885 subunit beta



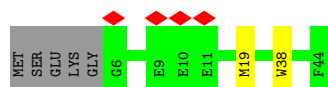
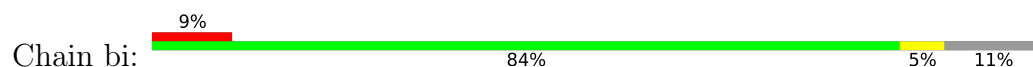
- Molecule 3: Light-harvesting protein B:885 subunit beta



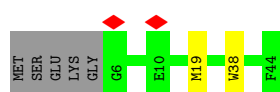
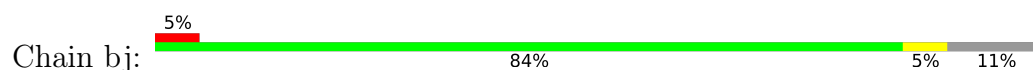
- Molecule 3: Light-harvesting protein B:885 subunit beta



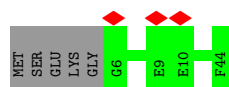
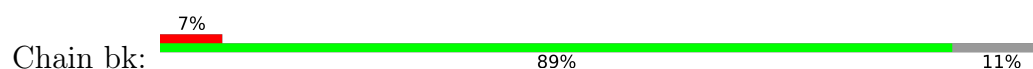
- Molecule 3: Light-harvesting protein B:885 subunit beta



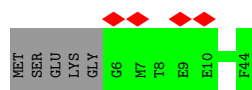
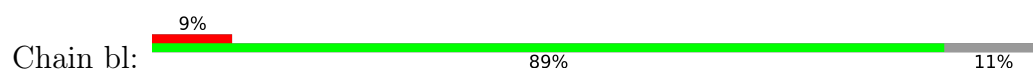
- Molecule 3: Light-harvesting protein B:885 subunit beta



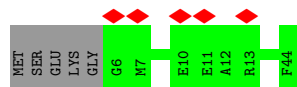
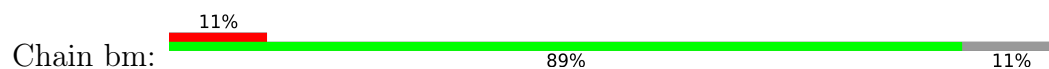
- Molecule 3: Light-harvesting protein B:885 subunit beta



- Molecule 3: Light-harvesting protein B:885 subunit beta

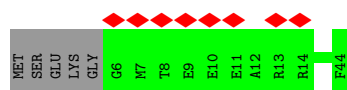


- Molecule 3: Light-harvesting protein B:885 subunit beta

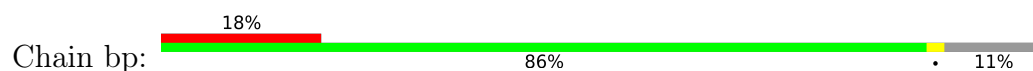


- Molecule 3: Light-harvesting protein B:885 subunit beta

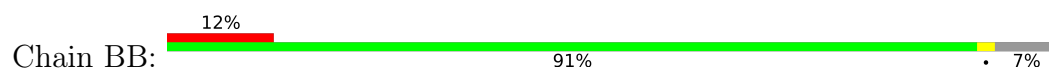




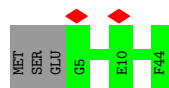
- Molecule 3: Light-harvesting protein B:885 subunit beta



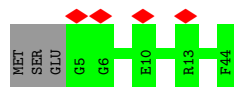
- Molecule 4: Light-harvesting protein B:885 subunit beta



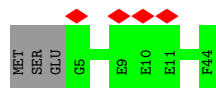
- Molecule 4: Light-harvesting protein B:885 subunit beta



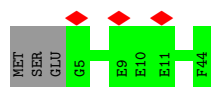
- Molecule 4: Light-harvesting protein B:885 subunit beta



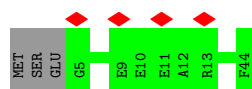
- Molecule 4: Light-harvesting protein B:885 subunit beta



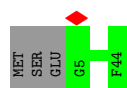
- Molecule 4: Light-harvesting protein B:885 subunit beta



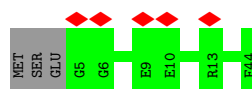
- Molecule 4: Light-harvesting protein B:885 subunit beta



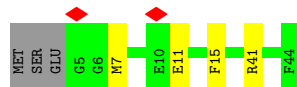
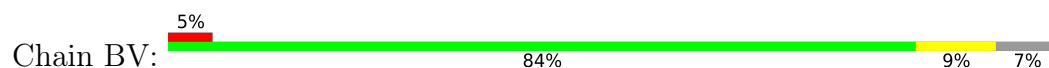
- Molecule 4: Light-harvesting protein B:885 subunit beta



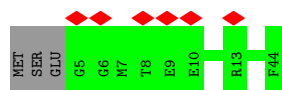
- Molecule 4: Light-harvesting protein B:885 subunit beta



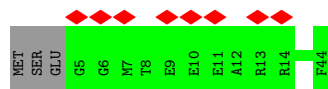
- Molecule 4: Light-harvesting protein B:885 subunit beta



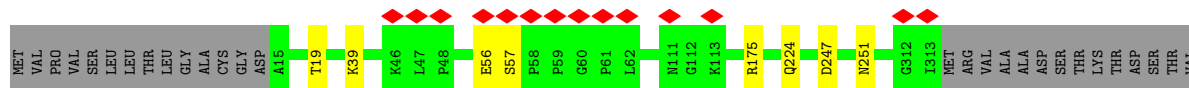
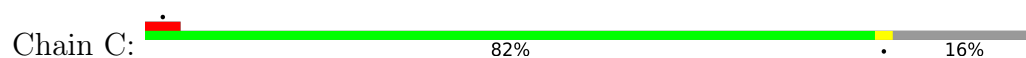
- Molecule 4: Light-harvesting protein B:885 subunit beta



- Molecule 4: Light-harvesting protein B:885 subunit beta



- Molecule 5: MULTHEME_CYTC domain-containing protein



VAL
ALA
ALA
PRO
ALA
ALA
ALA
PRO
ALA
Gln
ARG
THR
SER
ALA
ARG
PRO
GLY
SER
VAL
THR
THR
PRO
VAL
GLY
GLY
VAL
ASN

• Molecule 6: RC-S

Chain C1: 50% 49%

MET
PRO
ALA
SER
PRO
SER
PRO
LEU
PRO
ARG
SER
SER
GLY
VAL
ASP
ARG
ASN
ALA
ALA
VAL
VAL
VAL
VAL
ALA
LEU
VAL
VAL
ALA
ALA
ARG
GLY
ASP
ALA
GLN
GLY
THR
GLN
PRO
PRO
VAL
ALA
PRO
PRO
ALA
ALA
THR
THR
ALA
ALA
PRO
ASP
LEU
VAL
ASP

SER
THR
LYS
ALA
ASP
SER
THR
ALA
VAL
ALA
ASP
THR
LEU
MET
LEU
SER
MET
MET
MET
ALA
GLU
GLU
ALA
ALA
ALA
ALA
THR
THR
THR
ALA
PRO
VAL
VAL
ALA
P98
T99
A100
D104
P105
T106
T107
S154
D180
L200
GLY
GLN

• Molecule 7: PRCH domain-containing protein

Chain H1: 9% 91% 7%

M1
Q9
H58
R59
D60
H61
G62
GLY
GLY
THR
THR
HIS

• Molecule 8: RC-Hc

Chain H2: 13% 96% 7%

MET
S1
D2
D57
A63
K64
G65
D66
K79
L104
A105
S106
G107
E108
R109
R110
M122
F123
G124
L125
W126
D129
D150
D159
E175
ARG
SER
GLN
PRO
ILE
ILE

• Molecule 9: Photosynthetic reaction center L subunit

Chain L: 97%

MET
A1
L77
L91
Y128
H144
F181
V197
C247
I248
V249
K273

• Molecule 10: RC-M

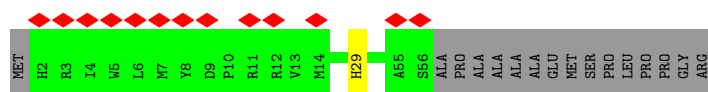
Chain M: 6% 83% 14%

MET
LEU
GLU
TYR
ASN
GLN
LEU
PHE
T9
R10
R14
T15
P16
E18
P19
G20
T21
PRO
ILE
ASP
GLU
SER
THR
GLY
THR
THR
ARG
TVR
GLY
THR
THR
F36
S37
Y38
L39
A40
G41
K42
F43
G44
D45
A46
Q47
R88
E96
P97
M142
H201
T206
F215
A259

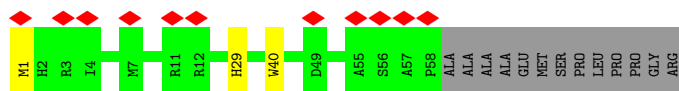
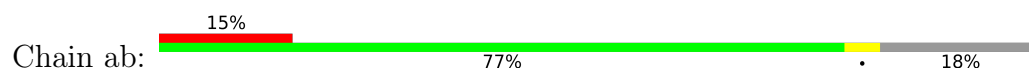
D291
V336
V337
PRO
GLN
ASN
ALA
THR
MET
PRO
ASP
THR
ALA
ALA
ALA
PRO
ILE
VAL
THR
ASP
SER
ILE
THR
THR
ASP
SER
THR
LYS
THR
GLY
GLY
THR
GLN

• Molecule 11: LHC domain-containing protein

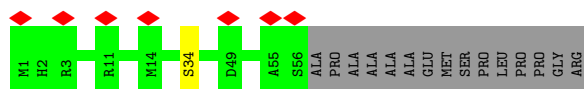
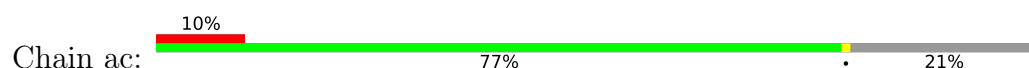
Chain aa: 18% 76% 23%



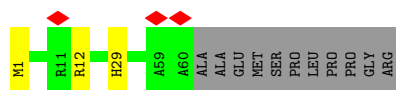
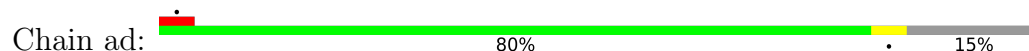
- Molecule 12: LHC domain-containing protein



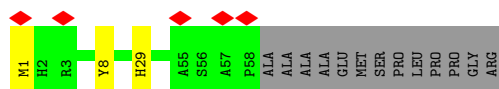
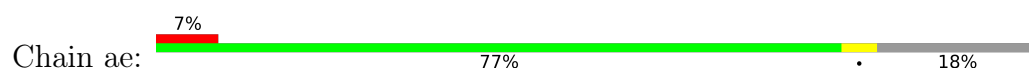
- Molecule 12: LHC domain-containing protein



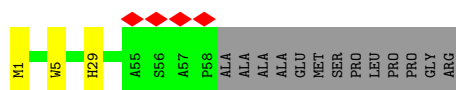
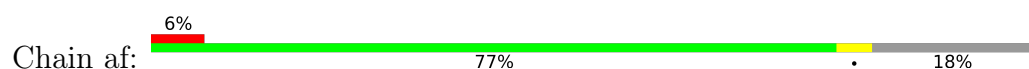
- Molecule 12: LHC domain-containing protein



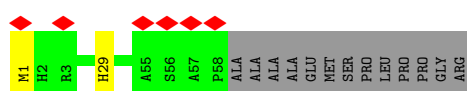
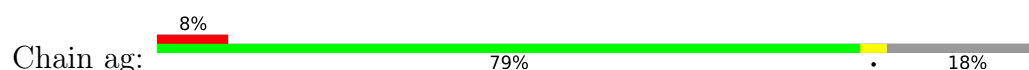
- Molecule 12: LHC domain-containing protein



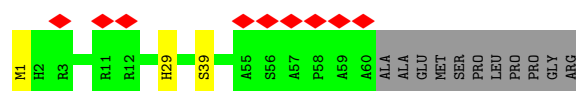
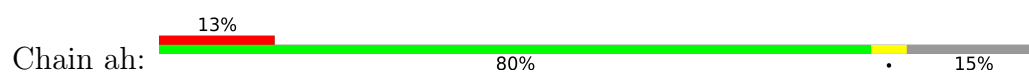
- Molecule 12: LHC domain-containing protein



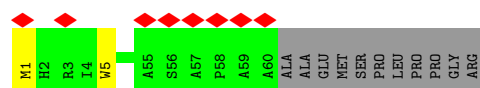
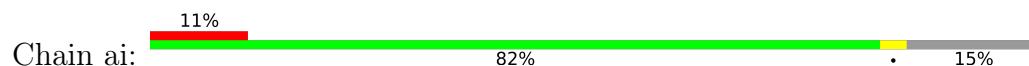
- Molecule 12: LHC domain-containing protein



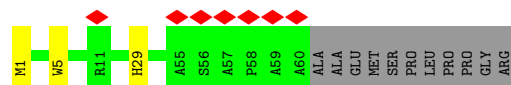
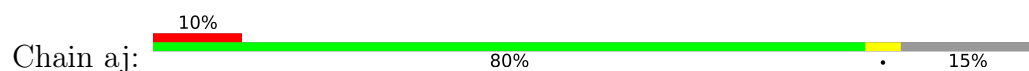
- Molecule 12: LHC domain-containing protein



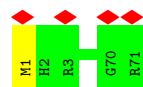
- Molecule 12: LHC domain-containing protein



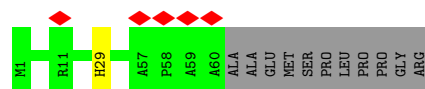
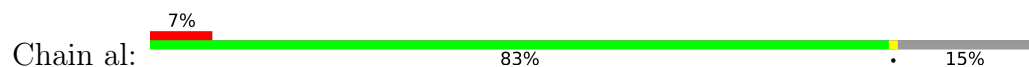
- Molecule 12: LHC domain-containing protein



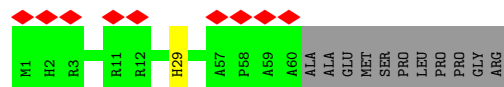
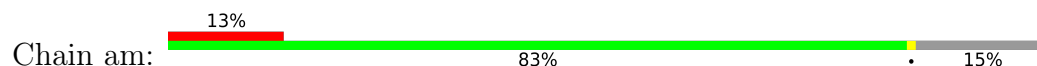
- Molecule 12: LHC domain-containing protein



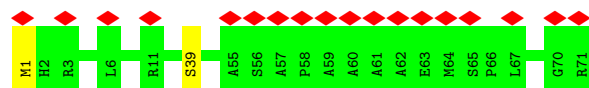
- Molecule 12: LHC domain-containing protein



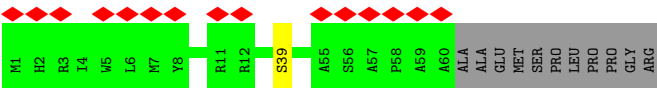
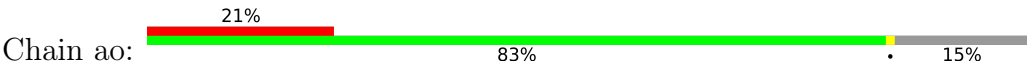
- Molecule 12: LHC domain-containing protein



- Molecule 12: LHC domain-containing protein



• Molecule 12: LHC domain-containing protein



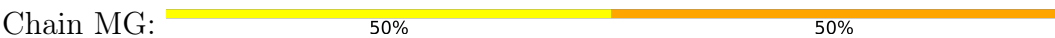
• Molecule 12: LHC domain-containing protein



• Molecule 13: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose



• Molecule 13: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103156	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	0.192	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0348	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: V75, BCL, V7N, MAN, BPH, 0V9, V7B, FE, RAM, LMT, HEC, MQ8, CRT, UYH, FME, CD4, PGW, NDG

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	0.47	0/541
1	AB	0.14	0/396	0.44	0/541
1	AE	0.14	0/396	0.45	0/541
1	AF	0.17	0/396	0.49	0/541
1	AG	0.14	0/396	0.45	0/541
1	AH	0.14	0/396	0.49	0/541
1	AI	0.14	0/396	0.46	0/541
1	AJ	0.14	0/396	0.47	0/541
1	AK	0.14	0/396	0.47	0/541
1	AL	0.14	0/396	0.44	0/541
1	AM	0.14	0/396	0.47	0/541
1	AN	0.14	0/396	0.45	0/541
1	AO	0.14	0/396	0.46	0/541
1	AP	0.15	0/396	0.49	0/541
1	AQ	0.13	0/396	0.43	0/541
1	AR	0.14	0/396	0.42	0/541
1	AS	0.14	0/396	0.45	0/541
1	AT	0.15	0/396	0.47	0/541
1	AU	0.14	0/396	0.44	0/541
1	AV	0.14	0/396	0.47	0/541
1	AW	0.14	0/396	0.43	0/541
1	AX	0.14	0/396	0.46	0/541
2	AC	0.13	0/388	0.44	0/529
2	AD	0.14	0/388	0.47	0/529
3	BA	0.11	0/336	0.37	0/456
3	BC	0.11	0/336	0.38	0/456
3	BF	0.12	0/336	0.43	0/456
3	BG	0.13	0/336	0.43	0/456
3	BH	0.12	0/336	0.40	0/456
3	BJ	0.12	0/336	0.39	0/456
3	BK	0.13	0/336	0.42	0/456

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	BL	0.12	0/336	0.42	0/456
3	BM	0.13	0/336	0.43	0/456
3	BN	0.13	0/336	0.44	0/456
3	BO	0.11	0/336	0.41	0/456
3	BP	0.12	0/336	0.47	0/456
3	BU	0.11	0/336	0.40	0/456
3	BX	0.12	0/336	0.44	0/456
3	ba	0.13	0/336	0.40	0/456
3	bb	0.13	0/336	0.42	0/456
3	bc	0.15	0/336	0.45	0/456
3	bd	0.13	0/336	0.40	0/456
3	be	0.14	0/336	0.41	0/456
3	bf	0.13	0/336	0.38	0/456
3	bg	0.13	0/336	0.43	0/456
3	bh	0.12	0/336	0.37	0/456
3	bi	0.13	0/336	0.39	0/456
3	bj	0.13	0/336	0.46	0/456
3	bk	0.16	0/336	0.48	0/456
3	bl	0.13	0/336	0.43	0/456
3	bm	0.14	0/336	0.44	0/456
3	bo	0.13	0/336	0.45	0/456
3	bp	0.14	0/336	0.42	0/456
4	BB	0.12	0/340	0.47	0/461
4	BD	0.12	0/340	0.41	0/461
4	BE	0.11	0/340	0.37	0/461
4	BI	0.11	0/340	0.41	0/461
4	BQ	0.13	0/340	0.48	0/461
4	BR	0.12	0/340	0.40	0/461
4	BS	0.13	0/340	0.43	0/461
4	BT	0.14	0/340	0.46	0/461
4	BV	0.11	0/340	0.36	0/461
4	BW	0.13	0/340	0.44	0/461
4	bn	0.13	0/340	0.39	0/461
5	C	0.18	0/2392	0.49	0/3263
6	C1	0.16	0/826	0.44	0/1128
7	H1	0.16	0/531	0.44	0/717
8	H2	0.15	0/1392	0.45	0/1902
9	L	0.15	0/2252	0.46	0/3081
10	M	0.16	0/2632	0.48	0/3600
11	aa	0.15	0/444	0.46	0/605
12	ab	0.15	0/457	0.44	0/624
12	ac	0.14	0/444	0.46	0/605
12	ad	0.15	0/467	0.44	0/638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	ae	0.17	0/457	0.47	0/624
12	af	0.15	0/457	0.44	0/624
12	ag	0.16	0/457	0.47	0/624
12	ah	0.16	0/467	0.46	0/638
12	ai	0.16	0/467	0.46	0/638
12	aj	0.15	0/467	0.47	0/638
12	ak	0.16	0/547	0.44	0/748
12	al	0.15	0/467	0.44	0/638
12	am	0.18	0/467	0.51	0/638
12	an	0.20	0/547	0.51	0/748
12	ao	0.16	0/467	0.47	0/638
12	ap	0.15	0/548	0.44	0/748
All	All	0.15	0/40624	0.45	0/55362

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AE	0	1
1	AK	0	1
10	M	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AE	3	ARG	Sidechain
1	AK	3	ARG	Sidechain
10	M	88	ARG	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	391	0	390	2	0
1	AB	391	0	390	3	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	1	0
1	AL	391	0	390	1	0
1	AM	391	0	390	3	0
1	AN	391	0	390	0	0
1	AO	391	0	390	0	0
1	AP	391	0	390	0	0
1	AQ	391	0	390	2	0
1	AR	391	0	390	1	0
1	AS	391	0	390	2	0
1	AT	391	0	390	2	0
1	AU	391	0	390	0	0
1	AV	391	0	390	1	0
1	AW	391	0	390	1	0
1	AX	391	0	390	1	0
2	AC	384	0	383	2	0
2	AD	384	0	383	0	0
3	BA	323	0	300	1	0
3	BC	323	0	300	1	0
3	BF	323	0	300	0	0
3	BG	323	0	300	0	0
3	BH	323	0	300	0	0
3	BJ	323	0	300	1	0
3	BK	323	0	300	1	0
3	BL	323	0	300	0	0
3	BM	323	0	300	1	0
3	BN	323	0	300	1	0
3	BO	323	0	300	0	0
3	BP	323	0	300	0	0
3	BU	323	0	300	0	0
3	BX	323	0	300	1	0
3	ba	323	0	300	1	0
3	bb	323	0	300	1	0
3	bc	323	0	300	0	0
3	bd	323	0	300	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	be	323	0	300	0	0
3	bf	323	0	300	1	0
3	bg	323	0	300	1	0
3	bh	323	0	300	1	0
3	bi	323	0	300	2	0
3	bj	323	0	300	2	0
3	bk	323	0	300	0	0
3	bl	323	0	300	0	0
3	bm	323	0	300	0	0
3	bo	323	0	300	0	0
3	bp	323	0	300	1	0
4	BB	327	0	303	1	0
4	BD	327	0	303	0	0
4	BE	327	0	303	0	0
4	BI	327	0	303	0	0
4	BQ	327	0	303	0	0
4	BR	327	0	303	0	0
4	BS	327	0	303	0	0
4	BT	327	0	303	0	0
4	BV	327	0	303	3	0
4	BW	327	0	303	0	0
4	bn	327	0	303	0	0
5	C	2325	0	2245	5	0
6	C1	806	0	818	1	0
7	H1	522	0	503	1	0
8	H2	1354	0	1314	0	0
9	L	2165	0	2126	6	0
10	M	2536	0	2479	7	0
11	aa	433	0	442	1	0
12	ab	455	0	465	2	0
12	ac	443	0	453	1	0
12	ad	465	0	475	2	0
12	ae	455	0	465	2	0
12	af	455	0	465	2	0
12	ag	455	0	465	1	0
12	ah	465	0	475	1	0
12	ai	465	0	475	1	0
12	aj	465	0	475	2	0
12	ak	542	0	553	0	0
12	al	465	0	475	1	0
12	am	465	0	475	1	0
12	an	542	0	553	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	ao	465	0	475	0	0
12	ap	543	0	553	1	0
13	CG	21	0	18	0	0
13	MG	21	0	18	1	0
14	AA	132	0	148	2	0
14	AB	132	0	148	2	0
14	AC	198	0	222	3	0
14	AD	66	0	74	0	0
14	AE	198	0	222	1	0
14	AF	66	0	74	2	0
14	AG	132	0	148	1	0
14	AH	132	0	148	2	0
14	AI	132	0	148	3	0
14	AJ	132	0	148	1	0
14	AK	132	0	148	1	0
14	AL	132	0	148	1	0
14	AM	132	0	148	2	0
14	AN	198	0	222	2	0
14	AO	66	0	74	1	0
14	AP	132	0	148	1	0
14	AQ	132	0	148	1	0
14	AR	132	0	148	3	0
14	AS	198	0	222	4	0
14	AT	66	0	74	1	0
14	AU	132	0	148	2	0
14	AV	198	0	222	2	0
14	AW	66	0	74	3	0
14	AX	132	0	148	3	0
14	BA	66	0	74	0	0
14	BB	66	0	74	0	0
14	BC	66	0	74	0	0
14	BD	66	0	74	0	0
14	BE	66	0	74	0	0
14	BF	66	0	73	0	0
14	BG	66	0	74	0	0
14	BH	66	0	74	0	0
14	BI	66	0	74	2	0
14	BJ	66	0	74	0	0
14	BK	66	0	74	0	0
14	BL	66	0	74	0	0
14	BM	66	0	74	1	0
14	BN	66	0	74	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	BO	66	0	74	0	0
14	BP	66	0	74	0	0
14	BQ	66	0	74	0	0
14	BR	66	0	74	0	0
14	BS	66	0	74	1	0
14	BT	66	0	74	0	0
14	BU	66	0	74	1	0
14	BV	66	0	74	0	0
14	BW	66	0	74	0	0
14	BX	66	0	74	0	0
14	L	132	0	148	2	0
14	M	132	0	148	2	0
14	aa	66	0	74	1	0
14	ab	66	0	74	2	0
14	ac	66	0	74	1	0
14	ad	66	0	74	0	0
14	ae	66	0	74	1	0
14	af	66	0	74	2	0
14	ag	66	0	74	1	0
14	ah	66	0	74	1	0
14	ai	66	0	74	1	0
14	aj	66	0	74	0	0
14	ak	66	0	74	0	0
14	al	66	0	74	0	0
14	am	66	0	74	1	0
14	an	66	0	74	0	0
14	ao	66	0	74	1	0
14	ap	66	0	74	0	0
14	ba	66	0	74	1	0
14	bb	66	0	74	1	0
14	bc	66	0	74	0	0
14	bd	66	0	74	1	0
14	be	66	0	74	1	0
14	bf	66	0	74	2	0
14	bg	66	0	74	1	0
14	bh	66	0	74	1	0
14	bi	66	0	74	0	0
14	bj	66	0	74	1	0
14	bk	66	0	74	0	0
14	bl	66	0	74	1	0
14	bm	66	0	74	1	0
14	bn	66	0	74	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bo	66	0	74	0	0
14	bp	66	0	74	1	0
15	AA	70	0	91	0	0
15	AC	35	0	46	0	0
15	AD	70	0	91	1	0
15	AE	35	0	45	0	0
15	AF	35	0	46	1	0
15	AG	35	0	46	0	0
15	AH	70	0	91	1	0
15	AI	35	0	45	0	0
15	AJ	70	0	91	0	0
15	AL	35	0	45	0	0
15	AN	35	0	46	0	0
15	AP	70	0	92	1	0
15	AQ	35	0	46	0	0
15	AS	35	0	45	0	0
15	AT	35	0	45	0	0
15	AU	35	0	45	0	0
15	AX	35	0	46	0	0
15	BA	105	0	136	1	0
15	BB	105	0	136	0	0
15	BC	140	0	184	0	0
15	BD	105	0	137	0	0
15	BE	70	0	92	0	0
15	BF	70	0	92	0	0
15	BG	140	0	183	1	0
15	BH	105	0	136	1	0
15	BI	140	0	182	0	0
15	BJ	70	0	91	0	0
15	BK	140	0	182	0	0
15	BL	105	0	137	0	0
15	BM	70	0	92	0	0
15	BN	140	0	183	0	0
15	BO	70	0	92	1	0
15	BP	105	0	137	0	0
15	BQ	105	0	136	0	0
15	BR	105	0	136	1	0
15	BS	140	0	182	0	0
15	BT	105	0	138	1	0
15	BU	70	0	91	0	0
15	BV	140	0	183	2	0
15	BW	105	0	134	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	BX	70	0	91	0	0
15	L	210	0	273	0	0
15	M	35	0	45	0	0
15	ab	35	0	46	0	0
15	bb	35	0	45	0	0
15	bc	35	0	45	1	0
15	bd	35	0	45	0	0
15	be	35	0	46	0	0
15	bf	35	0	45	0	0
15	bg	35	0	46	0	0
15	bh	70	0	90	0	0
15	bi	35	0	46	1	0
15	bj	35	0	45	0	0
15	bl	70	0	91	0	0
15	bm	70	0	92	0	0
15	bn	70	0	91	0	0
15	bo	70	0	91	1	0
16	AE	45	0	0	0	0
16	AO	45	0	0	0	0
16	AS	45	0	0	0	0
16	BA	45	0	0	0	0
16	BB	45	0	0	0	0
16	BC	45	0	0	0	0
16	BD	45	0	0	0	0
16	BE	45	0	0	0	0
16	BG	45	0	0	0	0
16	BH	45	0	0	0	0
16	BI	45	0	0	0	0
16	BJ	45	0	0	0	0
16	BK	45	0	0	0	0
16	BL	45	0	0	0	0
16	BM	45	0	0	0	0
16	BO	45	0	0	0	0
16	BP	45	0	0	0	0
16	BQ	45	0	0	0	0
16	BR	45	0	0	0	0
16	BS	45	0	0	0	0
16	BU	45	0	0	0	0
16	BV	45	0	0	1	0
16	BW	45	0	0	0	0
16	BX	45	0	0	0	0
16	ba	45	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	bb	45	0	0	0	0
16	bc	45	0	0	0	0
16	bd	45	0	0	0	0
16	be	45	0	0	0	0
16	bf	45	0	0	0	0
16	bg	45	0	0	1	0
16	bh	45	0	0	0	0
16	bi	45	0	0	0	0
16	bj	45	0	0	0	0
16	bk	45	0	0	0	0
16	bl	45	0	0	0	0
16	bm	45	0	0	0	0
16	bn	45	0	0	0	0
16	bo	45	0	0	0	0
16	bp	45	0	0	0	0
17	C	172	0	120	4	0
18	C	18	0	0	0	0
18	M	18	0	0	0	0
19	C	14	0	12	0	0
19	C1	14	0	12	0	0
20	C1	45	0	0	0	0
20	H1	45	0	0	0	0
20	aj	45	0	0	0	0
20	ba	45	0	0	0	0
20	bb	45	0	0	0	0
20	bc	45	0	0	0	0
20	be	90	0	0	0	0
20	bg	90	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	1	0
20	bn	45	0	0	0	0
20	bo	45	0	0	0	0
20	bp	45	0	0	0	0
21	H1	168	0	248	0	0
21	M	84	0	124	0	0
21	ae	84	0	124	1	0
21	af	84	0	124	1	0
21	aj	84	0	124	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H1	51	0	76	1	0
23	L	53	0	72	1	0
23	M	53	0	72	2	0
23	ao	53	0	72	0	0
24	L	58	0	0	0	0
24	ag	58	0	0	0	0
25	L	65	0	76	2	0
25	M	65	0	76	3	0
26	M	1	0	0	0	0
27	M	44	0	60	2	0
28	ai	55	0	0	0	0
29	AA	2	0	0	0	0
29	AB	3	0	0	0	0
29	AC	3	0	0	0	0
29	AD	1	0	0	0	0
29	AE	3	0	0	0	0
29	AF	2	0	0	0	0
29	AG	5	0	0	0	0
29	AH	1	0	0	0	0
29	AI	3	0	0	0	0
29	AJ	5	0	0	0	0
29	AK	4	0	0	0	0
29	AL	2	0	0	0	0
29	AM	6	0	0	0	0
29	AN	4	0	0	0	0
29	AO	4	0	0	0	0
29	AP	4	0	0	0	0
29	AQ	4	0	0	0	0
29	AS	6	0	0	0	0
29	AT	2	0	0	0	0
29	AU	1	0	0	0	0
29	AV	6	0	0	0	0
29	AW	2	0	0	0	0
29	AX	3	0	0	0	0
29	BB	1	0	0	0	0
29	BI	1	0	0	0	0
29	BJ	1	0	0	0	0
29	BO	1	0	0	0	0
29	BP	1	0	0	0	0
29	C	86	0	0	0	0
29	C1	42	0	0	0	0
29	H1	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	H2	9	0	0	0	0
29	L	51	0	0	0	0
29	M	58	0	0	0	0
29	aa	3	0	0	0	0
29	ab	3	0	0	0	0
29	ac	3	0	0	0	0
29	ad	6	0	0	0	0
29	ae	10	0	0	0	0
29	af	11	0	0	0	0
29	ag	7	0	0	0	0
29	ah	6	0	0	0	0
29	ai	5	0	0	0	0
29	aj	7	0	0	0	0
29	ak	13	0	0	0	0
29	al	5	0	0	0	0
29	am	5	0	0	0	0
29	an	9	0	0	0	0
29	ao	5	0	0	0	0
29	ap	11	0	0	0	0
29	ba	3	0	0	0	0
29	bb	4	0	0	0	0
29	bc	2	0	0	0	0
29	bd	3	0	0	0	0
29	be	4	0	0	0	0
29	bf	1	0	0	0	0
29	bg	2	0	0	0	0
29	bh	2	0	0	0	0
29	bi	2	0	0	0	0
29	bj	3	0	0	0	0
29	bk	3	0	0	0	0
29	bl	3	0	0	0	0
29	bm	2	0	0	0	0
29	bn	1	0	0	0	0
29	bo	1	0	0	0	0
All	All	55475	0	53489	135	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 135 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:5:TRP:HH2	14:AS:104:BCL:H143	1.51	0.76
14:BI:1003:BCL:H112	14:BI:1003:BCL:H41	1.75	0.68
14:AA:1001:BCL:H191	3:bp:36:LEU:HD11	1.77	0.67
12:ad:12:ARG:HG3	21:ae:101:CD4:H52	1.78	0.64
14:ag:1001:BCL:H143	14:bf:103:BCL:H41	1.83	0.60

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	AE	47/54 (87%)	47 (100%)	0	0	100	100
1	AF	47/54 (87%)	47 (100%)	0	0	100	100
1	AG	47/54 (87%)	47 (100%)	0	0	100	100
1	AH	47/54 (87%)	47 (100%)	0	0	100	100
1	AI	47/54 (87%)	47 (100%)	0	0	100	100
1	AJ	47/54 (87%)	47 (100%)	0	0	100	100
1	AK	47/54 (87%)	47 (100%)	0	0	100	100
1	AL	47/54 (87%)	47 (100%)	0	0	100	100
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	46 (98%)	1 (2%)	0	100	100
2	AC	46/54 (85%)	46 (100%)	0	0	100	100
2	AD	46/54 (85%)	46 (100%)	0	0	100	100
3	BA	37/44 (84%)	37 (100%)	0	0	100	100
3	BC	37/44 (84%)	37 (100%)	0	0	100	100
3	BF	37/44 (84%)	37 (100%)	0	0	100	100
3	BG	37/44 (84%)	37 (100%)	0	0	100	100
3	BH	37/44 (84%)	37 (100%)	0	0	100	100
3	BJ	37/44 (84%)	37 (100%)	0	0	100	100
3	BK	37/44 (84%)	37 (100%)	0	0	100	100
3	BL	37/44 (84%)	37 (100%)	0	0	100	100
3	BM	37/44 (84%)	37 (100%)	0	0	100	100
3	BN	37/44 (84%)	37 (100%)	0	0	100	100
3	BO	37/44 (84%)	37 (100%)	0	0	100	100
3	BP	37/44 (84%)	37 (100%)	0	0	100	100
3	BU	37/44 (84%)	37 (100%)	0	0	100	100
3	BX	37/44 (84%)	37 (100%)	0	0	100	100
3	ba	37/44 (84%)	37 (100%)	0	0	100	100
3	bb	37/44 (84%)	37 (100%)	0	0	100	100
3	bc	37/44 (84%)	37 (100%)	0	0	100	100
3	bd	37/44 (84%)	37 (100%)	0	0	100	100
3	be	37/44 (84%)	37 (100%)	0	0	100	100
3	bf	37/44 (84%)	37 (100%)	0	0	100	100
3	bg	37/44 (84%)	37 (100%)	0	0	100	100
3	bh	37/44 (84%)	37 (100%)	0	0	100	100
3	bi	37/44 (84%)	37 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	bj	37/44 (84%)	37 (100%)	0	0	100	100
3	bk	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
3	bl	37/44 (84%)	37 (100%)	0	0	100	100
3	bm	37/44 (84%)	37 (100%)	0	0	100	100
3	bo	37/44 (84%)	37 (100%)	0	0	100	100
3	bp	37/44 (84%)	37 (100%)	0	0	100	100
4	BB	38/43 (88%)	38 (100%)	0	0	100	100
4	BD	38/43 (88%)	38 (100%)	0	0	100	100
4	BE	38/43 (88%)	38 (100%)	0	0	100	100
4	BI	38/43 (88%)	38 (100%)	0	0	100	100
4	BQ	38/43 (88%)	38 (100%)	0	0	100	100
4	BR	38/43 (88%)	38 (100%)	0	0	100	100
4	BS	38/43 (88%)	38 (100%)	0	0	100	100
4	BT	38/43 (88%)	38 (100%)	0	0	100	100
4	BV	38/43 (88%)	38 (100%)	0	0	100	100
4	BW	38/43 (88%)	38 (100%)	0	0	100	100
4	bn	38/43 (88%)	38 (100%)	0	0	100	100
5	C	297/354 (84%)	285 (96%)	12 (4%)	0	100	100
6	C1	101/202 (50%)	100 (99%)	1 (1%)	0	100	100
7	H1	60/67 (90%)	60 (100%)	0	0	100	100
8	H2	172/181 (95%)	169 (98%)	3 (2%)	0	100	100
9	L	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
10	M	311/367 (85%)	298 (96%)	13 (4%)	0	100	100
11	aa	53/71 (75%)	53 (100%)	0	0	100	100
12	ab	56/71 (79%)	56 (100%)	0	0	100	100
12	ac	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
12	ad	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
12	ae	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
12	af	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
12	ag	56/71 (79%)	56 (100%)	0	0	100	100
12	ah	58/71 (82%)	57 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	ai	58/71 (82%)	58 (100%)	0	0	100	100
12	aj	58/71 (82%)	58 (100%)	0	0	100	100
12	ak	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
12	al	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
12	am	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
12	an	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
12	ao	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
12	ap	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
All	All	4773/5626 (85%)	4717 (99%)	56 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AE	38/41 (93%)	38 (100%)	0	100	100
1	AF	38/41 (93%)	38 (100%)	0	100	100
1	AG	38/41 (93%)	38 (100%)	0	100	100
1	AH	38/41 (93%)	37 (97%)	1 (3%)	40	68
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	37 (97%)	1 (3%)	40	68
2	AC	37/41 (90%)	37 (100%)	0	100	100
2	AD	37/41 (90%)	37 (100%)	0	100	100
3	BA	31/35 (89%)	31 (100%)	0	100	100
3	BC	31/35 (89%)	31 (100%)	0	100	100
3	BF	31/35 (89%)	31 (100%)	0	100	100
3	BG	31/35 (89%)	31 (100%)	0	100	100
3	BH	31/35 (89%)	31 (100%)	0	100	100
3	BJ	31/35 (89%)	30 (97%)	1 (3%)	34	62
3	BK	31/35 (89%)	31 (100%)	0	100	100
3	BL	31/35 (89%)	31 (100%)	0	100	100
3	BM	31/35 (89%)	31 (100%)	0	100	100
3	BN	31/35 (89%)	31 (100%)	0	100	100
3	BO	31/35 (89%)	31 (100%)	0	100	100
3	BP	31/35 (89%)	31 (100%)	0	100	100
3	BU	31/35 (89%)	31 (100%)	0	100	100
3	BX	31/35 (89%)	31 (100%)	0	100	100
3	ba	31/35 (89%)	31 (100%)	0	100	100
3	bb	31/35 (89%)	31 (100%)	0	100	100
3	bc	31/35 (89%)	31 (100%)	0	100	100
3	bd	31/35 (89%)	31 (100%)	0	100	100
3	be	31/35 (89%)	31 (100%)	0	100	100
3	bf	31/35 (89%)	31 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	bg	31/35 (89%)	31 (100%)	0	100	100
3	bh	31/35 (89%)	31 (100%)	0	100	100
3	bi	31/35 (89%)	31 (100%)	0	100	100
3	bj	31/35 (89%)	31 (100%)	0	100	100
3	bk	31/35 (89%)	31 (100%)	0	100	100
3	bl	31/35 (89%)	31 (100%)	0	100	100
3	bm	31/35 (89%)	31 (100%)	0	100	100
3	bo	31/35 (89%)	31 (100%)	0	100	100
3	bp	31/35 (89%)	31 (100%)	0	100	100
4	BB	31/34 (91%)	31 (100%)	0	100	100
4	BD	31/34 (91%)	31 (100%)	0	100	100
4	BE	31/34 (91%)	31 (100%)	0	100	100
4	BI	31/34 (91%)	31 (100%)	0	100	100
4	BQ	31/34 (91%)	31 (100%)	0	100	100
4	BR	31/34 (91%)	31 (100%)	0	100	100
4	BS	31/34 (91%)	31 (100%)	0	100	100
4	BT	31/34 (91%)	31 (100%)	0	100	100
4	BV	31/34 (91%)	31 (100%)	0	100	100
4	BW	31/34 (91%)	31 (100%)	0	100	100
4	bn	31/34 (91%)	31 (100%)	0	100	100
5	C	245/285 (86%)	244 (100%)	1 (0%)	84	93
6	C1	88/156 (56%)	88 (100%)	0	100	100
7	H1	50/53 (94%)	50 (100%)	0	100	100
8	H2	144/151 (95%)	143 (99%)	1 (1%)	76	89
9	L	215/216 (100%)	213 (99%)	2 (1%)	70	87
10	M	256/299 (86%)	254 (99%)	2 (1%)	73	88
11	aa	45/55 (82%)	45 (100%)	0	100	100
12	ab	46/54 (85%)	46 (100%)	0	100	100
12	ac	45/54 (83%)	45 (100%)	0	100	100
12	ad	46/54 (85%)	46 (100%)	0	100	100
12	ae	46/54 (85%)	46 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	af	46/54 (85%)	46 (100%)	0	100	100
12	ag	46/54 (85%)	46 (100%)	0	100	100
12	ah	46/54 (85%)	45 (98%)	1 (2%)	45	73
12	ai	46/54 (85%)	46 (100%)	0	100	100
12	aj	46/54 (85%)	46 (100%)	0	100	100
12	ak	54/54 (100%)	54 (100%)	0	100	100
12	al	46/54 (85%)	46 (100%)	0	100	100
12	am	46/54 (85%)	46 (100%)	0	100	100
12	an	54/54 (100%)	53 (98%)	1 (2%)	50	76
12	ao	46/54 (85%)	45 (98%)	1 (2%)	45	73
12	ap	54/54 (100%)	54 (100%)	0	100	100
All	All	3906/4398 (89%)	3894 (100%)	12 (0%)	84	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	M	215	PHE
10	M	291	ASP
12	ao	39	SER
12	ah	39	SER
5	C	39	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
12	ae	36	GLN
12	ai	50	GLN
5	C	183	GLN
5	C	189	ASN
6	C1	158	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	$\# Z > 2$
12	FME	am	1	12	8,9,10	0.91	0	7,9,11	0.96	0
7	FME	H1	1	7	8,9,10	0.92	0	7,9,11	0.89	0
12	FME	ac	1	12	8,9,10	0.91	0	7,9,11	0.90	0
12	FME	ad	1	12	8,9,10	0.90	0	7,9,11	1.09	1 (14%)
1	FME	AG	1	1	8,9,10	0.92	0	7,9,11	1.01	0
12	FME	ai	1	12	8,9,10	0.93	0	7,9,11	0.98	1 (14%)
12	FME	ae	1	12	8,9,10	0.93	0	7,9,11	1.17	1 (14%)
12	FME	ag	1	12	8,9,10	0.92	0	7,9,11	1.04	1 (14%)
12	FME	ah	1	12	8,9,10	0.93	0	7,9,11	1.09	1 (14%)
1	FME	AM	1	1	8,9,10	0.94	0	7,9,11	0.97	0
12	FME	ab	1	12	8,9,10	0.90	0	7,9,11	1.17	1 (14%)
1	FME	AJ	1	1	8,9,10	0.97	0	7,9,11	0.76	0
1	FME	AE	1	1	8,9,10	0.90	0	7,9,11	1.03	1 (14%)
12	FME	aj	1	12	8,9,10	0.93	0	7,9,11	1.06	1 (14%)
12	FME	an	1	12	8,9,10	0.94	0	7,9,11	1.17	1 (14%)
1	FME	AS	1	1	8,9,10	0.93	0	7,9,11	1.13	1 (14%)
12	FME	al	1	12	8,9,10	0.93	0	7,9,11	1.01	0
1	FME	AK	1	1	8,9,10	0.91	0	7,9,11	1.05	1 (14%)
1	FME	AL	1	1	8,9,10	0.92	0	7,9,11	1.19	1 (14%)
1	FME	AN	1	1	8,9,10	0.94	0	7,9,11	1.05	1 (14%)
2	FME	AD	1	2	8,9,10	0.94	0	7,9,11	1.03	1 (14%)
12	FME	af	1	12	8,9,10	0.93	0	7,9,11	1.08	1 (14%)
12	FME	ao	1	12	8,9,10	0.92	0	7,9,11	1.01	0
1	FME	AO	1	1	8,9,10	0.92	0	7,9,11	1.01	1 (14%)
1	FME	AI	1	1	8,9,10	0.95	0	7,9,11	0.93	0
1	FME	AB	1	1	8,9,10	0.93	0	7,9,11	1.01	1 (14%)
1	FME	AH	1	1	8,9,10	0.93	0	7,9,11	1.06	1 (14%)
1	FME	AP	1	1	8,9,10	0.92	0	7,9,11	1.01	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	AV	1	1	8,9,10	0.93	0	7,9,11	1.02	1 (14%)
1	FME	AU	1	1	8,9,10	0.92	0	7,9,11	0.99	1 (14%)
1	FME	AW	1	1	8,9,10	0.91	0	7,9,11	1.09	1 (14%)
1	FME	AQ	1	1	8,9,10	0.92	0	7,9,11	1.14	1 (14%)
1	FME	AT	1	1	8,9,10	0.92	0	7,9,11	0.98	1 (14%)
1	FME	AX	1	1	8,9,10	0.91	0	7,9,11	1.27	1 (14%)
12	FME	ap	1	12	8,9,10	0.95	0	7,9,11	0.93	0
12	FME	ak	1	12	8,9,10	0.95	0	7,9,11	1.09	1 (14%)
1	FME	AR	1	1	8,9,10	0.93	0	7,9,11	0.93	0
1	FME	AF	1	1	8,9,10	0.95	0	7,9,11	0.91	0
2	FME	AC	1	2	8,9,10	0.94	0	7,9,11	1.07	1 (14%)
1	FME	AA	1	1	8,9,10	0.94	0	7,9,11	0.98	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	am	1	12	-	2/7/9/11	-
7	FME	H1	1	7	-	0/7/9/11	-
12	FME	ac	1	12	-	1/7/9/11	-
12	FME	ad	1	12	-	0/7/9/11	-
1	FME	AG	1	1	-	0/7/9/11	-
12	FME	ai	1	12	-	0/7/9/11	-
12	FME	ae	1	12	-	1/7/9/11	-
12	FME	ag	1	12	-	0/7/9/11	-
12	FME	ah	1	12	-	0/7/9/11	-
1	FME	AM	1	1	-	1/7/9/11	-
12	FME	ab	1	12	-	1/7/9/11	-
1	FME	AJ	1	1	-	1/7/9/11	-
1	FME	AE	1	1	-	1/7/9/11	-
12	FME	aj	1	12	-	1/7/9/11	-
12	FME	an	1	12	-	1/7/9/11	-
1	FME	AS	1	1	-	0/7/9/11	-
12	FME	al	1	12	-	2/7/9/11	-
1	FME	AK	1	1	-	0/7/9/11	-
1	FME	AL	1	1	-	1/7/9/11	-
1	FME	AN	1	1	-	1/7/9/11	-
2	FME	AD	1	2	-	0/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	af	1	12	-	2/7/9/11	-
12	FME	ao	1	12	-	1/7/9/11	-
1	FME	AO	1	1	-	0/7/9/11	-
1	FME	AI	1	1	-	1/7/9/11	-
1	FME	AB	1	1	-	1/7/9/11	-
1	FME	AH	1	1	-	0/7/9/11	-
1	FME	AP	1	1	-	1/7/9/11	-
1	FME	AV	1	1	-	0/7/9/11	-
1	FME	AU	1	1	-	1/7/9/11	-
1	FME	AW	1	1	-	0/7/9/11	-
1	FME	AQ	1	1	-	0/7/9/11	-
1	FME	AT	1	1	-	0/7/9/11	-
1	FME	AX	1	1	-	1/7/9/11	-
12	FME	ap	1	12	-	1/7/9/11	-
12	FME	ak	1	12	-	2/7/9/11	-
1	FME	AR	1	1	-	0/7/9/11	-
1	FME	AF	1	1	-	1/7/9/11	-
2	FME	AC	1	2	-	0/7/9/11	-
1	FME	AA	1	1	-	1/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AX	1	FME	C-CA-N	2.67	114.55	109.73
12	ab	1	FME	C-CA-N	2.61	114.44	109.73
1	AL	1	FME	C-CA-N	2.50	114.23	109.73
1	AQ	1	FME	C-CA-N	2.40	114.06	109.73
12	an	1	FME	C-CA-N	2.40	114.06	109.73

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	ab	1	FME	O-C-CA-CB
12	ac	1	FME	O-C-CA-CB
12	af	1	FME	O-C-CA-CB
12	ak	1	FME	O-C-CA-CB
12	am	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AT	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
13	MAN	CG	1	5,18,13	11,11,12	0.82	1 (9%)	15,15,17	1.02	0
13	RAM	CG	2	13	10,10,11	1.71	2 (20%)	14,14,16	0.98	0
13	MAN	MG	1	18,10,13	11,11,12	0.72	0	15,15,17	1.06	1 (6%)
13	RAM	MG	2	13	10,10,11	1.50	2 (20%)	14,14,16	1.35	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	CG	1	5,18,13	-	1/2/19/22	0/1/1/1
13	RAM	CG	2	13	-	-	0/1/1/1
13	MAN	MG	1	18,10,13	-	0/2/19/22	0/1/1/1
13	RAM	MG	2	13	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	CG	2	RAM	O5-C1	4.19	1.50	1.43
13	MG	2	RAM	O5-C1	3.45	1.49	1.43
13	CG	2	RAM	C2-C3	-2.28	1.49	1.52
13	CG	1	MAN	O5-C1	-2.16	1.40	1.43
13	MG	2	RAM	C2-C3	-2.09	1.49	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	MG	2	RAM	C1-C2-C3	2.71	113.00	109.67
13	MG	2	RAM	C6-C5-C4	-2.59	108.29	113.07
13	MG	1	MAN	C1-O5-C5	2.30	115.31	112.19
13	MG	2	RAM	C1-O5-C5	-2.21	107.77	112.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

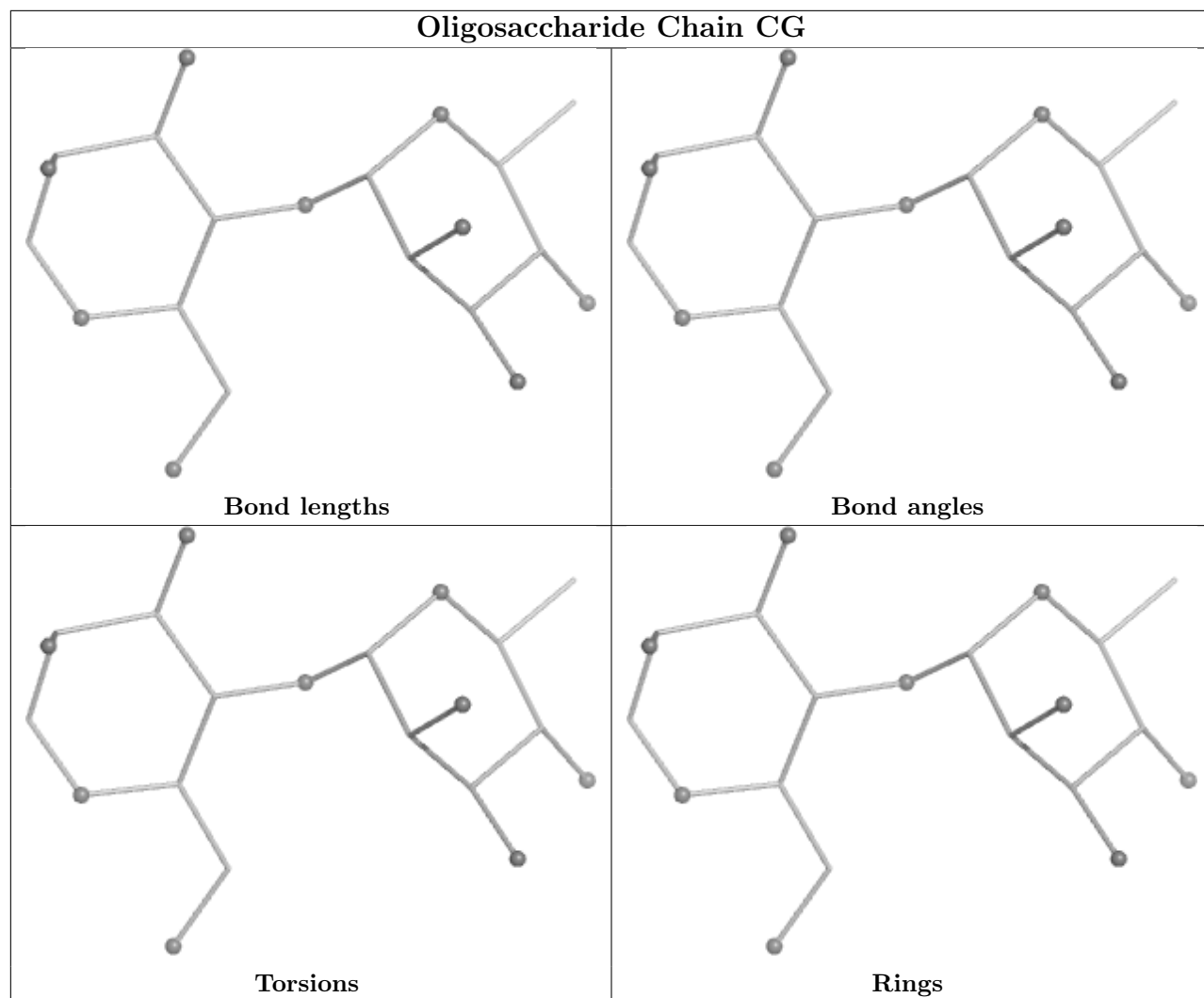
Mol	Chain	Res	Type	Atoms
13	CG	1	MAN	O5-C5-C6-O6

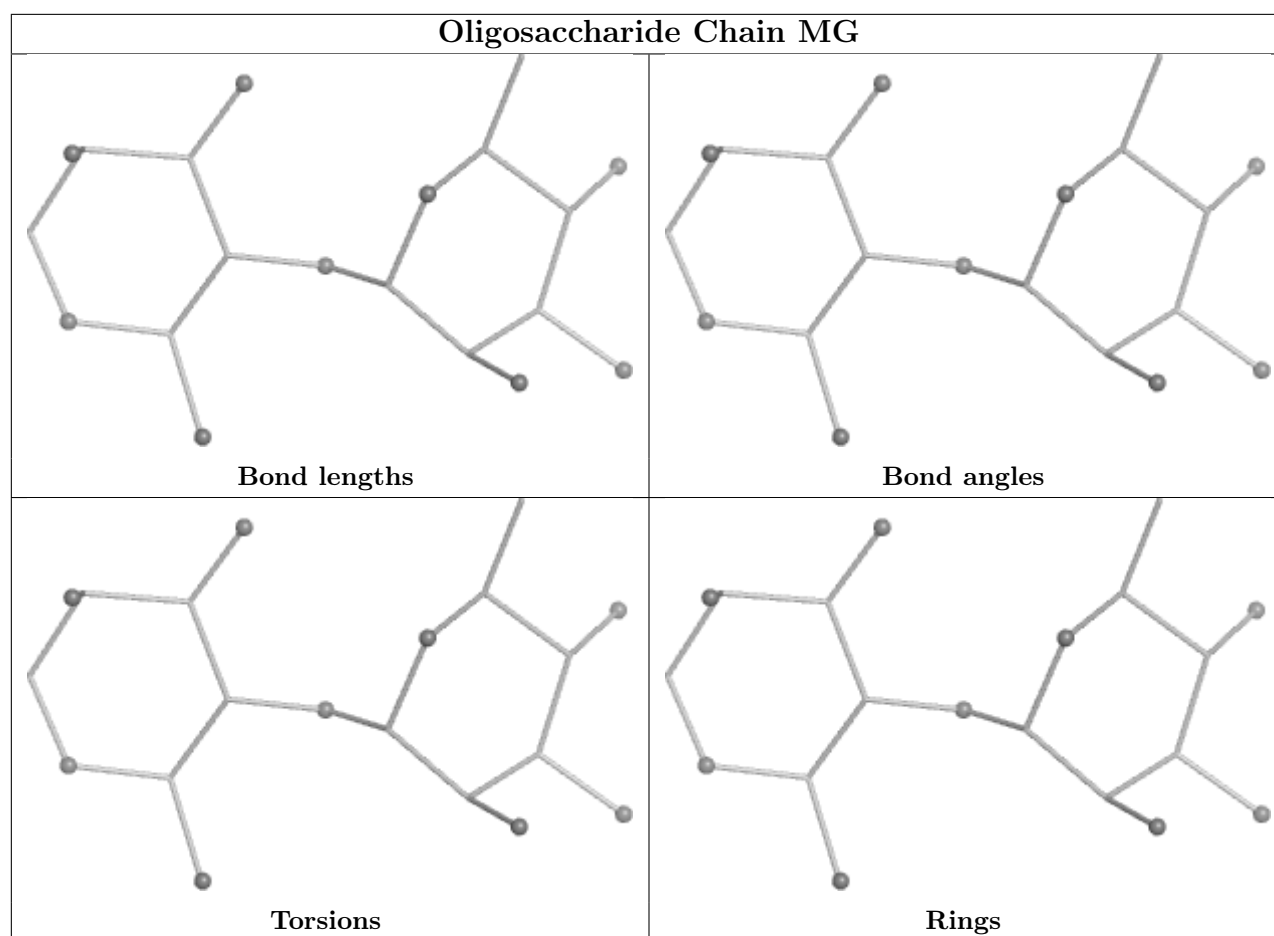
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	MG	2	RAM	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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 1 is monoatomic - leaving 312 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	$\# Z > 2$
17	HEC	C	404	5	50,50,50	1.72	7 (14%)	68,82,82	1.55	10 (14%)
16	V7N	BU	1001	-	43,44,44	2.12	9 (20%)	44,54,54	1.67	6 (13%)
16	V7N	BI	1001	-	43,44,44	2.03	9 (20%)	44,54,54	1.49	9 (20%)
15	LMT	AX	101	-	36,36,36	1.06	4 (11%)	47,47,47	0.96	3 (6%)
15	LMT	BI	1005	-	36,36,36	1.09	5 (13%)	47,47,47	0.82	0
15	LMT	BT	102	-	36,36,36	1.05	5 (13%)	47,47,47	1.01	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCL	AB	1001	1	69,74,74	1.14	6 (8%)	83,115,115	1.47	12 (14%)
15	LMT	AE	1002	-	36,36,36	1.08	4 (11%)	47,47,47	1.03	4 (8%)
14	BCL	bb	104	3	69,74,74	1.13	5 (7%)	83,115,115	1.35	11 (13%)
14	BCL	bk	102	3	69,74,74	1.15	5 (7%)	83,115,115	1.39	12 (14%)
14	BCL	AK	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.39	10 (12%)
21	CD4	H1	102	-	83,83,83	0.46	0	89,95,95	1.01	5 (5%)
16	V7N	BG	1001	-	43,44,44	2.00	10 (23%)	44,54,54	1.59	10 (22%)
14	BCL	BC	104	3	69,74,74	1.13	6 (8%)	83,115,115	1.52	13 (15%)
14	BCL	ae	102	12	69,74,74	1.15	6 (8%)	83,115,115	1.45	12 (14%)
14	BCL	AC	103	29	69,74,74	1.15	6 (8%)	83,115,115	1.41	12 (14%)
15	LMT	BK	1003	-	36,36,36	1.08	4 (11%)	47,47,47	1.10	4 (8%)
20	0V9	H1	101	-	44,44,46	0.76	1 (2%)	47,49,51	0.79	3 (6%)
14	BCL	BF	102	3	69,74,74	1.13	6 (8%)	83,115,115	2.00	14 (16%)
15	LMT	BS	1002	-	36,36,36	1.08	4 (11%)	47,47,47	0.91	2 (4%)
15	LMT	BW	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.90	1 (2%)
16	V7N	BH	1001	-	43,44,44	2.04	10 (23%)	44,54,54	1.66	11 (25%)
15	LMT	BR	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.95	3 (6%)
14	BCL	BI	1003	4	69,74,74	1.37	8 (11%)	83,115,115	1.84	15 (18%)
16	V7N	bo	102	-	43,44,44	2.10	11 (25%)	44,54,54	1.47	9 (20%)
15	LMT	BK	1002	-	36,36,36	1.10	5 (13%)	47,47,47	1.00	3 (6%)
20	0V9	bl	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.90	3 (6%)
27	CRT	M	404	-	41,43,43	0.56	0	50,54,54	0.91	3 (6%)
15	LMT	bi	102	-	36,36,36	1.08	4 (11%)	47,47,47	0.90	0
14	BCL	AR	101	1	69,74,74	1.17	6 (8%)	83,115,115	1.41	10 (12%)
14	BCL	AS	102	29	69,74,74	1.15	5 (7%)	83,115,115	1.42	12 (14%)
16	V7N	BO	1001	-	43,44,44	2.08	9 (20%)	44,54,54	1.63	11 (25%)
14	BCL	ao	102	12	69,74,74	1.18	6 (8%)	83,115,115	1.44	12 (14%)
14	BCL	AW	101	1	69,74,74	1.17	6 (8%)	83,115,115	1.42	10 (12%)
14	BCL	AA	1002	29	69,74,74	1.15	6 (8%)	83,115,115	1.48	14 (16%)
20	0V9	bp	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.91	3 (6%)
16	V7N	BK	1001	-	43,44,44	2.05	10 (23%)	44,54,54	1.53	9 (20%)
15	LMT	BK	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.94	2 (4%)
15	LMT	L	1007	-	36,36,36	1.10	5 (13%)	47,47,47	0.83	1 (2%)
14	BCL	BD	105	4	69,74,74	1.13	6 (8%)	83,115,115	1.40	11 (13%)
14	BCL	AU	103	-	69,74,74	1.15	5 (7%)	83,115,115	1.48	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	0V9	C1	1001	-	44,44,46	0.74	1 (2%)	47,49,51	0.81	2 (4%)
15	LMT	L	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.97	1 (2%)
14	BCL	AN	101	-	69,74,74	1.17	5 (7%)	83,115,115	1.42	11 (13%)
14	BCL	AL	101	-	69,74,74	1.20	5 (7%)	83,115,115	1.74	16 (19%)
15	LMT	L	1003	-	36,36,36	1.11	5 (13%)	47,47,47	0.80	0
15	LMT	BV	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.94	1 (2%)
20	0V9	bm	102	-	44,44,46	0.74	1 (2%)	47,49,51	0.83	1 (2%)
15	LMT	BW	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.89	1 (2%)
15	LMT	AF	1002	-	36,36,36	1.10	4 (11%)	47,47,47	0.85	0
14	BCL	BV	1005	4	69,74,74	1.12	5 (7%)	83,115,115	1.39	11 (13%)
24	V7B	L	1006	-	59,59,59	0.89	3 (5%)	75,75,75	1.04	5 (6%)
14	BCL	AF	1001	1	69,74,74	1.17	6 (8%)	83,115,115	1.43	10 (12%)
15	LMT	bo	105	-	36,36,36	1.12	5 (13%)	47,47,47	1.01	3 (6%)
14	BCL	AV	103	29	69,74,74	1.16	6 (8%)	83,115,115	1.47	11 (13%)
15	LMT	BO	1002	-	36,36,36	1.06	4 (11%)	47,47,47	0.90	1 (2%)
14	BCL	ak	1001	12	69,74,74	1.16	6 (8%)	83,115,115	1.40	11 (13%)
15	LMT	AN	103	-	36,36,36	1.10	5 (13%)	47,47,47	0.94	2 (4%)
16	V7N	BV	1001	-	43,44,44	2.02	9 (20%)	44,54,54	1.53	9 (20%)
14	BCL	AG	101	29	69,74,74	1.14	6 (8%)	83,115,115	1.63	15 (18%)
20	0V9	be	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.87	2 (4%)
15	LMT	AP	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.09	4 (8%)
14	BCL	BO	1004	3	69,74,74	1.13	6 (8%)	83,115,115	1.47	13 (15%)
15	LMT	bh	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.92	1 (2%)
15	LMT	BF	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.90	2 (4%)
14	BCL	AC	102	2	69,74,74	1.17	6 (8%)	83,115,115	1.39	10 (12%)
22	PGW	H1	103	-	50,50,50	0.46	0	53,56,56	1.01	3 (5%)
21	CD4	H1	104	-	83,83,83	0.49	0	89,95,95	1.05	4 (4%)
15	LMT	bg	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.91	2 (4%)
16	V7N	bh	102	-	43,44,44	2.04	10 (23%)	44,54,54	1.56	8 (18%)
15	LMT	BH	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.95	2 (4%)
14	BCL	AE	1003	29	69,74,74	1.15	5 (7%)	83,115,115	1.40	10 (12%)
15	LMT	BG	1006	-	36,36,36	1.08	5 (13%)	47,47,47	0.86	1 (2%)
15	LMT	AA	1003	-	36,36,36	1.10	5 (13%)	47,47,47	1.03	2 (4%)
16	V7N	bl	102	-	43,44,44	2.05	10 (23%)	44,54,54	1.56	10 (22%)
16	V7N	BJ	1001	-	43,44,44	2.00	9 (20%)	44,54,54	1.57	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LMT	BJ	1004	-	36,36,36	1.09	5 (13%)	47,47,47	0.84	1 (2%)
16	V7N	bj	101	-	43,44,44	2.04	9 (20%)	44,54,54	1.62	10 (22%)
14	BCL	AA	1001	1	69,74,74	1.18	6 (8%)	83,115,115	1.41	10 (12%)
14	BCL	BG	1004	3	69,74,74	1.13	6 (8%)	83,115,115	1.39	9 (10%)
14	BCL	AH	101	-	69,74,74	1.16	5 (7%)	83,115,115	1.51	13 (15%)
14	BCL	BA	103	3	69,74,74	1.13	5 (7%)	83,115,115	1.60	12 (14%)
15	LMT	BE	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	3 (6%)
15	LMT	BA	104	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	2 (4%)
15	LMT	BM	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.85	0
15	LMT	BI	1006	-	36,36,36	1.07	4 (11%)	47,47,47	1.05	2 (4%)
20	0V9	ba	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.79	1 (2%)
15	LMT	BN	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.99	2 (4%)
14	BCL	AN	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.40	10 (12%)
15	LMT	BA	105	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	1 (2%)
16	V7N	AE	1005	-	43,44,44	2.05	10 (23%)	44,54,54	1.64	8 (18%)
14	BCL	AS	103	1	69,74,74	1.16	6 (8%)	83,115,115	1.41	10 (12%)
20	0V9	bk	103	-	44,44,46	0.77	1 (2%)	47,49,51	0.76	2 (4%)
14	BCL	AU	102	1	69,74,74	1.16	6 (8%)	83,115,115	1.40	10 (12%)
15	LMT	BH	1004	-	36,36,36	1.11	5 (13%)	47,47,47	0.88	0
16	V7N	BL	1001	-	43,44,44	2.01	9 (20%)	44,54,54	1.58	10 (22%)
16	V7N	AO	1001	-	43,44,44	2.01	10 (23%)	44,54,54	1.68	10 (22%)
15	LMT	BS	1004	-	36,36,36	1.07	5 (13%)	47,47,47	0.91	2 (4%)
14	BCL	ap	1001	12	69,74,74	1.16	6 (8%)	83,115,115	1.45	13 (15%)
16	V7N	BA	101	-	43,44,44	2.05	9 (20%)	44,54,54	1.45	8 (18%)
15	LMT	bd	103	-	36,36,36	1.11	5 (13%)	47,47,47	0.87	2 (4%)
23	MQ8	L	1001	-	54,54,54	0.60	0	66,69,69	0.87	1 (1%)
14	BCL	AB	1002	29	69,74,74	1.14	5 (7%)	83,115,115	1.51	12 (14%)
15	LMT	BD	103	-	36,36,36	1.07	5 (13%)	47,47,47	1.06	2 (4%)
20	0V9	bg	102	-	44,44,46	0.76	1 (2%)	47,49,51	1.08	3 (6%)
14	BCL	BB	103	4	69,74,74	1.13	5 (7%)	83,115,115	1.45	11 (13%)
17	HEC	C	403	5	50,50,50	1.71	7 (14%)	68,82,82	1.61	10 (14%)
15	LMT	AT	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.20	3 (6%)
16	V7N	BC	101	-	43,44,44	2.08	11 (25%)	44,54,54	1.49	9 (20%)
14	BCL	AS	104	29	69,74,74	1.21	5 (7%)	83,115,115	1.54	13 (15%)
14	BCL	BW	1003	4	69,74,74	1.14	6 (8%)	83,115,115	1.45	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LMT	AQ	103	-	36,36,36	1.09	5 (13%)	47,47,47	1.02	3 (6%)
21	CD4	aj	102	-	83,83,83	0.50	0	89,95,95	1.21	8 (8%)
16	V7N	BS	1001	-	43,44,44	2.03	9 (20%)	44,54,54	1.53	9 (20%)
14	BCL	AV	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.37	10 (12%)
20	0V9	be	102	-	44,44,46	0.75	1 (2%)	47,49,51	0.91	2 (4%)
15	LMT	BR	1005	-	36,36,36	1.06	4 (11%)	47,47,47	0.86	0
14	BCL	M	408	10	69,74,74	1.15	5 (7%)	83,115,115	1.46	10 (12%)
15	LMT	BC	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.85	1 (2%)
15	LMT	BI	1004	-	36,36,36	1.09	5 (13%)	47,47,47	0.91	2 (4%)
15	LMT	BR	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.98	2 (4%)
20	0V9	bc	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.94	3 (6%)
15	LMT	BI	1002	-	36,36,36	1.08	5 (13%)	47,47,47	0.96	2 (4%)
14	BCL	AM	102	29	69,74,74	1.18	6 (8%)	83,115,115	1.49	14 (16%)
15	LMT	bm	105	-	36,36,36	1.08	4 (11%)	47,47,47	0.87	2 (4%)
15	LMT	AC	104	-	36,36,36	1.09	5 (13%)	47,47,47	0.96	2 (4%)
15	LMT	AD	101	-	36,36,36	1.07	5 (13%)	47,47,47	1.00	3 (6%)
14	BCL	AK	101	29	69,74,74	1.18	6 (8%)	83,115,115	1.46	11 (13%)
14	BCL	bd	102	3	69,74,74	1.15	5 (7%)	83,115,115	1.36	12 (14%)
16	V7N	bd	101	-	43,44,44	2.08	11 (25%)	44,54,54	1.51	9 (20%)
18	V75	M	409	19,13	18,18,18	1.63	5 (27%)	21,25,25	1.69	2 (9%)
14	BCL	BL	1003	3	69,74,74	1.12	5 (7%)	83,115,115	1.45	12 (14%)
16	V7N	bf	101	-	43,44,44	2.06	11 (25%)	44,54,54	1.55	8 (18%)
18	V75	C	405	19,13	18,18,18	1.59	4 (22%)	21,25,25	1.70	3 (14%)
14	BCL	bi	104	3	69,74,74	1.13	5 (7%)	83,115,115	1.39	12 (14%)
15	LMT	BM	1004	-	36,36,36	1.08	4 (11%)	47,47,47	0.87	2 (4%)
14	BCL	AL	103	1	69,74,74	1.18	6 (8%)	83,115,115	1.41	10 (12%)
14	BCL	af	101	12	69,74,74	1.16	6 (8%)	83,115,115	1.41	11 (13%)
14	BCL	M	405	10	69,74,74	1.14	6 (8%)	83,115,115	1.45	11 (13%)
15	LMT	AP	104	-	36,36,36	1.08	5 (13%)	47,47,47	0.94	1 (2%)
14	BCL	BJ	1002	3	69,74,74	1.11	5 (7%)	83,115,115	1.43	10 (12%)
15	LMT	AJ	103	-	36,36,36	1.09	4 (11%)	47,47,47	1.20	5 (10%)
15	LMT	bm	103	-	36,36,36	1.06	4 (11%)	47,47,47	0.95	3 (6%)
14	BCL	L	1002	9	69,74,74	1.12	6 (8%)	83,115,115	1.38	9 (10%)
16	V7N	bn	102	-	43,44,44	2.11	11 (25%)	44,54,54	1.56	8 (18%)
16	V7N	bb	101	-	43,44,44	2.06	10 (23%)	44,54,54	1.64	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCL	aj	103	12	69,74,74	1.16	5 (7%)	83,115,115	1.42	11 (13%)
24	V7B	ag	1002	-	59,59,59	0.88	4 (6%)	75,75,75	1.03	4 (5%)
14	BCL	BP	1005	3	69,74,74	1.13	5 (7%)	83,115,115	1.40	12 (14%)
14	BCL	be	105	3	69,74,74	1.15	5 (7%)	83,115,115	1.38	11 (13%)
14	BCL	bo	103	3	69,74,74	1.13	5 (7%)	83,115,115	1.38	12 (14%)
16	V7N	BR	1001	-	43,44,44	2.05	10 (23%)	44,54,54	1.65	10 (22%)
15	LMT	L	1005	-	36,36,36	1.05	5 (13%)	47,47,47	0.89	0
14	BCL	AH	103	1	69,74,74	1.17	6 (8%)	83,115,115	1.44	10 (12%)
15	LMT	BL	1005	-	36,36,36	1.09	5 (13%)	47,47,47	0.94	1 (2%)
15	LMT	AD	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.97	2 (4%)
16	V7N	BX	1001	-	43,44,44	2.01	9 (20%)	44,54,54	1.61	9 (20%)
15	LMT	BX	1004	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	2 (4%)
15	LMT	BV	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.85	0
14	BCL	ag	1001	12	69,74,74	1.16	5 (7%)	83,115,115	1.41	11 (13%)
23	MQ8	ao	101	-	54,54,54	0.60	0	66,69,69	1.03	2 (3%)
14	BCL	BM	1002	3	69,74,74	1.14	5 (7%)	83,115,115	1.39	11 (13%)
15	LMT	BQ	1005	-	36,36,36	1.09	4 (11%)	47,47,47	0.87	1 (2%)
14	BCL	BS	1003	4	69,74,74	1.14	5 (7%)	83,115,115	1.49	11 (13%)
15	LMT	BH	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.94	2 (4%)
16	V7N	ba	101	-	43,44,44	2.09	9 (20%)	44,54,54	1.84	13 (29%)
14	BCL	bj	103	3	69,74,74	1.14	5 (7%)	83,115,115	1.41	12 (14%)
14	BCL	L	1010	9	69,74,74	1.14	6 (8%)	83,115,115	1.36	12 (14%)
20	0V9	aj	101	-	44,44,46	0.76	1 (2%)	47,49,51	0.82	1 (2%)
15	LMT	BB	104	-	36,36,36	1.09	5 (13%)	47,47,47	0.88	1 (2%)
14	BCL	an	1001	12	69,74,74	1.15	5 (7%)	83,115,115	1.39	11 (13%)
15	LMT	BC	102	-	36,36,36	1.09	5 (13%)	47,47,47	0.87	1 (2%)
16	V7N	bk	101	-	43,44,44	2.05	10 (23%)	44,54,54	1.50	8 (18%)
15	LMT	M	403	-	36,36,36	1.10	5 (13%)	47,47,47	0.88	2 (4%)
14	BCL	AJ	102	29	69,74,74	1.16	5 (7%)	83,115,115	1.48	15 (18%)
14	BCL	ac	1001	12	69,74,74	1.14	6 (8%)	83,115,115	1.44	11 (13%)
14	BCL	ab	102	12	69,74,74	1.19	6 (8%)	83,115,115	1.42	11 (13%)
21	CD4	af	102	-	83,83,83	0.47	0	89,95,95	1.13	6 (6%)
15	LMT	BL	1004	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	3 (6%)
15	LMT	BO	1003	-	36,36,36	1.10	4 (11%)	47,47,47	0.83	0
14	BCL	AE	1001	1	69,74,74	1.17	6 (8%)	83,115,115	1.40	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CD4	M	402	-	83,83,83	0.48	0	89,95,95	1.07	5 (5%)
14	BCL	AE	1004	-	69,74,74	1.19	5 (7%)	83,115,115	1.47	11 (13%)
15	LMT	bn	105	-	36,36,36	1.11	5 (13%)	47,47,47	0.98	2 (4%)
20	0V9	bb	103	-	44,44,46	0.75	1 (2%)	47,49,51	0.82	1 (2%)
14	BCL	bf	103	3	69,74,74	1.16	5 (7%)	83,115,115	1.40	13 (15%)
15	LMT	BJ	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.88	1 (2%)
15	LMT	AG	103	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	1 (2%)
15	LMT	BU	1002	-	36,36,36	1.08	4 (11%)	47,47,47	0.92	1 (2%)
14	BCL	ai	101	12	69,74,74	1.13	5 (7%)	83,115,115	1.56	12 (14%)
15	LMT	BB	102	-	36,36,36	1.09	4 (11%)	47,47,47	0.93	2 (4%)
14	BCL	AT	101	1	69,74,74	1.18	6 (8%)	83,115,115	1.40	10 (12%)
15	LMT	BN	105	-	36,36,36	1.07	5 (13%)	47,47,47	0.89	1 (2%)
20	0V9	bh	103	-	44,44,46	0.76	1 (2%)	47,49,51	0.95	3 (6%)
15	LMT	bf	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.82	0
15	LMT	BG	1002	-	36,36,36	1.06	5 (13%)	47,47,47	1.11	5 (10%)
17	HEC	C	401	5	50,50,50	1.74	7 (14%)	68,82,82	1.65	11 (16%)
14	BCL	AR	102	-	69,74,74	1.18	6 (8%)	83,115,115	1.53	17 (20%)
28	UYH	ai	102	-	55,55,55	2.08	14 (25%)	63,63,63	0.99	2 (3%)
15	LMT	BV	1002	-	36,36,36	1.10	5 (13%)	47,47,47	0.88	2 (4%)
15	LMT	BC	106	-	36,36,36	1.08	4 (11%)	47,47,47	0.81	1 (2%)
15	LMT	bc	104	-	36,36,36	1.11	4 (11%)	47,47,47	0.96	3 (6%)
14	BCL	AI	102	1	69,74,74	1.16	6 (8%)	83,115,115	1.43	10 (12%)
16	V7N	AS	105	-	43,44,44	2.04	9 (20%)	44,54,54	1.71	7 (15%)
15	LMT	BW	1005	-	36,36,36	1.13	5 (13%)	47,47,47	0.99	1 (2%)
15	LMT	ab	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.90	1 (2%)
15	LMT	AU	101	-	36,36,36	1.08	5 (13%)	47,47,47	0.84	0
15	LMT	AL	102	-	36,36,36	1.09	4 (11%)	47,47,47	0.83	0
16	V7N	BM	1001	-	43,44,44	2.00	9 (20%)	44,54,54	1.68	11 (25%)
15	LMT	BK	1005	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
15	LMT	AH	104	-	36,36,36	1.08	5 (13%)	47,47,47	1.08	3 (6%)
15	LMT	BG	1005	-	36,36,36	1.07	4 (11%)	47,47,47	0.85	0
14	BCL	BX	1002	3	69,74,74	1.13	5 (7%)	83,115,115	1.50	14 (16%)
15	LMT	BB	105	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	1 (2%)
14	BCL	BR	1004	4	69,74,74	1.13	5 (7%)	83,115,115	1.43	11 (13%)
15	LMT	bn	101	-	36,36,36	1.10	5 (13%)	47,47,47	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	HEC	C	402	5	50,50,50	1.73	6 (12%)	68,82,82	1.60	10 (14%)
15	LMT	BT	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.86	2 (4%)
15	LMT	L	1011	-	36,36,36	1.08	5 (13%)	47,47,47	0.93	2 (4%)
20	OV9	bk	104	-	44,44,46	0.74	1 (2%)	47,49,51	0.86	1 (2%)
19	NDG	C1	1002	18	14,14,15	0.63	0	17,19,21	0.95	1 (5%)
15	LMT	L	1008	-	36,36,36	1.08	4 (11%)	47,47,47	0.94	2 (4%)
23	MQ8	M	407	-	54,54,54	0.64	0	66,69,69	0.93	4 (6%)
14	BCL	AX	102	-	69,74,74	1.17	5 (7%)	83,115,115	1.54	15 (18%)
15	LMT	bl	105	-	36,36,36	1.10	5 (13%)	47,47,47	0.84	2 (4%)
14	BCL	BU	1004	3	69,74,74	1.12	6 (8%)	83,115,115	1.42	10 (12%)
14	BCL	bg	105	3	69,74,74	1.13	5 (7%)	83,115,115	1.35	12 (14%)
15	LMT	BN	101	-	36,36,36	1.08	5 (13%)	47,47,47	0.89	1 (2%)
15	LMT	AH	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.99	3 (6%)
15	LMT	BE	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.89	1 (2%)
15	LMT	AS	101	-	36,36,36	1.09	5 (13%)	47,47,47	0.95	2 (4%)
14	BCL	AV	101	29	69,74,74	1.14	5 (7%)	83,115,115	1.44	12 (14%)
14	BCL	bm	104	3	69,74,74	1.11	6 (8%)	83,115,115	1.43	15 (18%)
15	LMT	bh	104	-	36,36,36	1.09	5 (13%)	47,47,47	0.93	2 (4%)
14	BCL	AP	103	29	69,74,74	1.17	5 (7%)	83,115,115	1.44	11 (13%)
14	BCL	BE	104	4	69,74,74	1.15	5 (7%)	83,115,115	1.47	14 (16%)
15	LMT	BT	104	-	36,36,36	1.12	5 (13%)	47,47,47	0.85	0
14	BCL	AI	103	-	69,74,74	1.16	5 (7%)	83,115,115	1.57	15 (18%)
16	V7N	BQ	1001	-	43,44,44	2.04	9 (20%)	44,54,54	1.50	9 (20%)
16	V7N	bg	101	-	43,44,44	2.06	11 (25%)	44,54,54	1.66	8 (18%)
15	LMT	be	104	-	36,36,36	1.09	5 (13%)	47,47,47	0.94	2 (4%)
14	BCL	AM	101	1	69,74,74	1.16	6 (8%)	83,115,115	1.40	10 (12%)
15	LMT	BN	104	-	36,36,36	1.09	5 (13%)	47,47,47	0.82	0
15	LMT	bj	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.92	2 (4%)
14	BCL	bh	105	3	69,74,74	1.14	5 (7%)	83,115,115	1.42	12 (14%)
14	BCL	AP	102	1	69,74,74	1.16	6 (8%)	83,115,115	1.44	11 (13%)
14	BCL	AJ	101	1	69,74,74	1.16	5 (7%)	83,115,115	1.41	10 (12%)
14	BCL	bn	103	4	69,74,74	1.13	6 (8%)	83,115,115	1.36	11 (13%)
21	CD4	ae	101	-	83,83,83	0.47	0	89,95,95	1.06	3 (3%)
14	BCL	AC	101	-	69,74,74	1.20	6 (8%)	83,115,115	1.48	14 (16%)
15	LMT	BV	1006	-	36,36,36	1.08	5 (13%)	47,47,47	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCL	ba	103	3	69,74,74	1.15	5 (7%)	83,115,115	1.36	12 (14%)
14	BCL	AX	103	1	69,74,74	1.18	6 (8%)	83,115,115	1.43	10 (12%)
14	BCL	ah	1001	12	69,74,74	1.18	6 (8%)	83,115,115	1.43	12 (14%)
16	V7N	BW	1001	-	43,44,44	2.03	9 (20%)	44,54,54	1.50	9 (20%)
16	V7N	BD	101	-	43,44,44	2.02	9 (20%)	44,54,54	1.50	9 (20%)
16	V7N	BE	101	-	43,44,44	2.05	10 (23%)	44,54,54	1.52	9 (20%)
14	BCL	bl	104	3	69,74,74	1.14	6 (8%)	83,115,115	1.37	12 (14%)
14	BCL	BH	1005	3	69,74,74	1.14	5 (7%)	83,115,115	1.45	12 (14%)
20	0V9	bn	104	-	44,44,46	0.76	1 (2%)	47,49,51	0.88	2 (4%)
15	LMT	BX	1003	-	36,36,36	1.06	5 (13%)	47,47,47	0.95	2 (4%)
20	0V9	bo	104	-	44,44,46	0.74	1 (2%)	47,49,51	0.90	2 (4%)
15	LMT	BD	104	-	36,36,36	1.10	5 (13%)	47,47,47	0.87	1 (2%)
14	BCL	AD	102	2	69,74,74	1.13	6 (8%)	83,115,115	1.41	11 (13%)
14	BCL	BQ	1003	4	69,74,74	1.14	5 (7%)	83,115,115	1.42	11 (13%)
14	BCL	am	1001	12	69,74,74	1.23	8 (11%)	83,115,115	1.80	14 (16%)
14	BCL	AN	104	-	69,74,74	1.17	5 (7%)	83,115,115	1.50	13 (15%)
16	V7N	bp	101	-	43,44,44	2.09	11 (25%)	44,54,54	1.53	9 (20%)
16	V7N	bi	101	-	43,44,44	2.07	11 (25%)	44,54,54	1.60	12 (27%)
15	LMT	BA	102	-	36,36,36	1.07	4 (11%)	47,47,47	0.93	1 (2%)
15	LMT	BD	102	-	36,36,36	1.08	5 (13%)	47,47,47	0.90	2 (4%)
15	LMT	BP	1004	-	36,36,36	1.07	5 (13%)	47,47,47	0.94	2 (4%)
15	LMT	BC	105	-	36,36,36	1.09	4 (11%)	47,47,47	0.91	1 (2%)
15	LMT	BP	1003	-	36,36,36	1.06	4 (11%)	47,47,47	0.87	1 (2%)
25	BPH	L	1009	-	59,70,70	1.07	4 (6%)	61,101,101	1.82	9 (14%)
16	V7N	bm	101	-	43,44,44	2.09	9 (20%)	44,54,54	1.55	9 (20%)
15	LMT	BL	1002	-	36,36,36	1.07	5 (13%)	47,47,47	1.00	2 (4%)
14	BCL	BT	103	4	69,74,74	1.14	5 (7%)	83,115,115	1.48	13 (15%)
15	LMT	BS	1005	-	36,36,36	1.09	5 (13%)	47,47,47	0.96	3 (6%)
20	0V9	bj	104	-	44,44,46	0.75	1 (2%)	47,49,51	0.91	3 (6%)
15	LMT	AA	1004	-	36,36,36	1.10	5 (13%)	47,47,47	0.93	2 (4%)
14	BCL	bc	102	3	69,74,74	1.18	5 (7%)	83,115,115	1.49	14 (16%)
15	LMT	BQ	1002	-	36,36,36	1.10	4 (11%)	47,47,47	0.86	2 (4%)
14	BCL	BN	103	3	69,74,74	1.31	7 (10%)	83,115,115	1.78	13 (15%)
15	LMT	bb	102	-	36,36,36	1.10	5 (13%)	47,47,47	1.11	4 (8%)
14	BCL	aa	1001	11	69,74,74	1.18	6 (8%)	83,115,115	1.43	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	V7N	BP	1001	-	43,44,44	2.03	9 (20%)	44,54,54	1.51	9 (20%)
15	LMT	bl	101	-	36,36,36	1.08	5 (13%)	47,47,47	1.02	3 (6%)
14	BCL	AQ	101	29	69,74,74	1.17	5 (7%)	83,115,115	1.72	17 (20%)
25	BPH	M	406	-	59,70,70	1.05	4 (6%)	61,101,101	1.90	9 (14%)
20	OV9	bi	103	-	44,44,46	0.74	1 (2%)	47,49,51	0.86	2 (4%)
15	LMT	BG	1003	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	1 (2%)
15	LMT	AJ	104	-	36,36,36	1.08	5 (13%)	47,47,47	0.95	3 (6%)
14	BCL	BK	1006	3	69,74,74	1.13	5 (7%)	83,115,115	1.41	12 (14%)
14	BCL	al	1001	12	69,74,74	1.15	5 (7%)	83,115,115	1.47	12 (14%)
15	LMT	bo	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.88	1 (2%)
16	V7N	bc	101	-	43,44,44	2.04	10 (23%)	44,54,54	1.54	9 (20%)
15	LMT	BP	1002	-	36,36,36	1.09	5 (13%)	47,47,47	0.88	0
19	NDG	C	406	18	14,14,15	0.66	0	17,19,21	0.90	1 (5%)
20	OV9	bg	104	-	44,44,46	0.74	1 (2%)	47,49,51	0.86	3 (6%)
15	LMT	BS	1006	-	36,36,36	1.06	5 (13%)	47,47,47	0.91	2 (4%)
16	V7N	be	101	-	43,44,44	2.02	10 (23%)	44,54,54	1.66	8 (18%)
14	BCL	AG	102	1	69,74,74	1.16	6 (8%)	83,115,115	1.39	10 (12%)
15	LMT	AI	101	-	36,36,36	1.08	4 (11%)	47,47,47	1.12	3 (6%)
15	LMT	BU	1003	-	36,36,36	1.09	5 (13%)	47,47,47	0.81	1 (2%)
15	LMT	BF	103	-	36,36,36	1.08	5 (13%)	47,47,47	0.94	1 (2%)
14	BCL	bp	102	3	69,74,74	1.14	6 (8%)	83,115,115	1.44	12 (14%)
16	V7N	BB	101	-	43,44,44	2.01	9 (20%)	44,54,54	1.59	10 (22%)
14	BCL	AO	1002	1	69,74,74	1.16	6 (8%)	83,115,115	1.37	10 (12%)
14	BCL	ad	1001	12	69,74,74	1.17	6 (8%)	83,115,115	1.42	11 (13%)
15	LMT	BQ	1004	-	36,36,36	1.10	5 (13%)	47,47,47	0.87	1 (2%)
14	BCL	AQ	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.41	10 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEC	C	404	5	1/1/3/7	6/14/54/54	-
16	V7N	BU	1001	-	-	8/53/53/53	-
16	V7N	BI	1001	-	-	5/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	AX	101	-	-	10/21/61/61	0/2/2/2
15	LMT	BI	1005	-	-	1/21/61/61	0/2/2/2
15	LMT	BT	102	-	-	6/21/61/61	0/2/2/2
14	BCL	AB	1001	1	-	4/41/137/137	-
15	LMT	AE	1002	-	-	4/21/61/61	0/2/2/2
14	BCL	bb	104	3	-	7/41/137/137	-
14	BCL	bk	102	3	-	9/41/137/137	-
14	BCL	AK	102	1	-	1/41/137/137	-
21	CD4	H1	102	-	-	22/94/94/94	-
16	V7N	BG	1001	-	-	5/53/53/53	-
14	BCL	BC	104	3	-	9/41/137/137	-
14	BCL	ae	102	12	-	10/41/137/137	-
14	BCL	AC	103	29	-	4/41/137/137	-
15	LMT	BK	1003	-	-	8/21/61/61	0/2/2/2
20	0V9	H1	101	-	-	9/48/48/50	-
14	BCL	BF	102	3	-	9/41/137/137	-
15	LMT	BS	1002	-	-	3/21/61/61	0/2/2/2
15	LMT	BW	1002	-	-	3/21/61/61	0/2/2/2
16	V7N	BH	1001	-	-	5/53/53/53	-
15	LMT	BR	1002	-	-	4/21/61/61	0/2/2/2
14	BCL	BI	1003	4	-	12/41/137/137	-
16	V7N	bo	102	-	-	4/53/53/53	-
15	LMT	BK	1002	-	-	3/21/61/61	0/2/2/2
20	0V9	bl	103	-	-	16/48/48/50	-
27	CRT	M	404	-	-	4/51/51/51	-
15	LMT	bi	102	-	-	3/21/61/61	0/2/2/2
14	BCL	AR	101	1	-	3/41/137/137	-
14	BCL	AS	102	29	-	9/41/137/137	-
16	V7N	BO	1001	-	-	6/53/53/53	-
14	BCL	ao	102	12	-	6/41/137/137	-
14	BCL	AW	101	1	-	1/41/137/137	-
14	BCL	AA	1002	29	-	6/41/137/137	-
20	0V9	bp	103	-	-	13/48/48/50	-
16	V7N	BK	1001	-	-	3/53/53/53	-
15	LMT	BK	1004	-	-	5/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	L	1007	-	-	2/21/61/61	0/2/2/2
14	BCL	BD	105	4	-	5/41/137/137	-
14	BCL	AU	103	-	-	5/41/137/137	-
20	0V9	C1	1001	-	-	13/48/48/50	-
15	LMT	L	1004	-	-	5/21/61/61	0/2/2/2
14	BCL	AN	101	-	-	5/41/137/137	-
14	BCL	AL	101	-	-	11/41/137/137	-
15	LMT	L	1003	-	-	8/21/61/61	0/2/2/2
15	LMT	BV	1004	-	-	4/21/61/61	0/2/2/2
20	0V9	bm	102	-	-	10/48/48/50	-
15	LMT	BW	1004	-	-	4/21/61/61	0/2/2/2
15	LMT	AF	1002	-	-	7/21/61/61	0/2/2/2
14	BCL	BV	1005	4	-	10/41/137/137	-
24	V7B	L	1006	-	-	9/48/88/88	0/2/2/2
14	BCL	AF	1001	1	-	4/41/137/137	-
15	LMT	bo	105	-	-	5/21/61/61	0/2/2/2
14	BCL	AV	103	29	-	11/41/137/137	-
15	LMT	BO	1002	-	-	3/21/61/61	0/2/2/2
14	BCL	ak	1001	12	-	6/41/137/137	-
15	LMT	AN	103	-	-	2/21/61/61	0/2/2/2
16	V7N	BV	1001	-	-	3/53/53/53	-
14	BCL	AG	101	29	-	12/41/137/137	-
20	0V9	be	103	-	-	12/48/48/50	-
15	LMT	AP	101	-	-	5/21/61/61	0/2/2/2
14	BCL	BO	1004	3	-	8/41/137/137	-
15	LMT	bh	101	-	-	6/21/61/61	0/2/2/2
15	LMT	BF	101	-	-	2/21/61/61	0/2/2/2
14	BCL	AC	102	2	-	5/41/137/137	-
22	PGW	H1	103	-	-	15/55/55/55	-
21	CD4	H1	104	-	-	19/94/94/94	-
15	LMT	bg	103	-	-	4/21/61/61	0/2/2/2
16	V7N	bh	102	-	-	5/53/53/53	-
15	LMT	BH	1003	-	-	7/21/61/61	0/2/2/2
14	BCL	AE	1003	29	-	12/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	BG	1006	-	-	1/21/61/61	0/2/2/2
15	LMT	AA	1003	-	-	9/21/61/61	0/2/2/2
16	V7N	bl	102	-	-	4/53/53/53	-
16	V7N	BJ	1001	-	-	4/53/53/53	-
15	LMT	BJ	1004	-	-	1/21/61/61	0/2/2/2
16	V7N	bj	101	-	-	7/53/53/53	-
14	BCL	AA	1001	1	-	5/41/137/137	-
14	BCL	BG	1004	3	-	6/41/137/137	-
14	BCL	AH	101	-	-	7/41/137/137	-
14	BCL	BA	103	3	-	9/41/137/137	-
15	LMT	BE	102	-	-	3/21/61/61	0/2/2/2
15	LMT	BA	104	-	-	7/21/61/61	0/2/2/2
15	LMT	BM	1003	-	-	8/21/61/61	0/2/2/2
15	LMT	BI	1006	-	-	4/21/61/61	0/2/2/2
20	0V9	ba	102	-	-	9/48/48/50	-
15	LMT	BN	102	-	-	3/21/61/61	0/2/2/2
14	BCL	AN	102	1	-	1/41/137/137	-
15	LMT	BA	105	-	-	6/21/61/61	0/2/2/2
16	V7N	AE	1005	-	-	4/53/53/53	-
14	BCL	AS	103	1	-	2/41/137/137	-
20	0V9	bk	103	-	-	10/48/48/50	-
14	BCL	AU	102	1	-	2/41/137/137	-
15	LMT	BH	1004	-	-	3/21/61/61	0/2/2/2
16	V7N	BL	1001	-	-	5/53/53/53	-
16	V7N	AO	1001	-	-	6/53/53/53	-
15	LMT	BS	1004	-	-	6/21/61/61	0/2/2/2
14	BCL	ap	1001	12	-	7/41/137/137	-
16	V7N	BA	101	-	-	3/53/53/53	-
15	LMT	bd	103	-	-	5/21/61/61	0/2/2/2
23	MQ8	L	1001	-	-	8/47/67/67	0/2/2/2
14	BCL	AB	1002	29	-	7/41/137/137	-
15	LMT	BD	103	-	-	7/21/61/61	0/2/2/2
20	0V9	bg	102	-	-	17/48/48/50	-
14	BCL	BB	103	4	-	10/41/137/137	-
17	HEC	C	403	5	1/1/3/7	7/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	AT	102	-	-	3/21/61/61	0/2/2/2
16	V7N	BC	101	-	-	3/53/53/53	-
14	BCL	AS	104	29	-	8/41/137/137	-
14	BCL	BW	1003	4	-	8/41/137/137	-
15	LMT	AQ	103	-	-	7/21/61/61	0/2/2/2
21	CD4	aj	102	-	-	26/94/94/94	-
16	V7N	BS	1001	-	-	4/53/53/53	-
14	BCL	AV	102	1	-	3/41/137/137	-
20	0V9	be	102	-	-	12/48/48/50	-
15	LMT	BR	1005	-	-	6/21/61/61	0/2/2/2
14	BCL	M	408	10	-	3/41/137/137	-
15	LMT	BC	103	-	-	3/21/61/61	0/2/2/2
15	LMT	BI	1004	-	-	3/21/61/61	0/2/2/2
15	LMT	BR	1003	-	-	7/21/61/61	0/2/2/2
20	0V9	bc	103	-	-	11/48/48/50	-
15	LMT	BI	1002	-	-	2/21/61/61	0/2/2/2
14	BCL	AM	102	29	-	8/41/137/137	-
15	LMT	bm	105	-	-	10/21/61/61	0/2/2/2
15	LMT	AC	104	-	-	4/21/61/61	0/2/2/2
15	LMT	AD	101	-	-	8/21/61/61	0/2/2/2
14	BCL	AK	101	29	-	11/41/137/137	-
14	BCL	bd	102	3	-	4/41/137/137	-
16	V7N	bd	101	-	-	3/53/53/53	-
18	V75	M	409	19,13	-	0/12/29/29	0/1/1/1
14	BCL	BL	1003	3	-	3/41/137/137	-
16	V7N	bf	101	-	-	5/53/53/53	-
18	V75	C	405	19,13	-	2/12/29/29	0/1/1/1
14	BCL	bi	104	3	-	6/41/137/137	-
15	LMT	BM	1004	-	-	1/21/61/61	0/2/2/2
14	BCL	AL	103	1	-	4/41/137/137	-
14	BCL	af	101	12	-	3/41/137/137	-
14	BCL	M	405	10	-	2/41/137/137	-
15	LMT	AP	104	-	-	3/21/61/61	0/2/2/2
14	BCL	BJ	1002	3	-	9/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	AJ	103	-	-	9/21/61/61	0/2/2/2
15	LMT	bm	103	-	-	8/21/61/61	0/2/2/2
14	BCL	L	1002	9	-	5/41/137/137	-
16	V7N	bn	102	-	-	3/53/53/53	-
16	V7N	bb	101	-	-	11/53/53/53	-
14	BCL	aj	103	12	-	9/41/137/137	-
24	V7B	ag	1002	-	-	11/48/88/88	0/2/2/2
14	BCL	BP	1005	3	-	6/41/137/137	-
14	BCL	be	105	3	-	8/41/137/137	-
14	BCL	bo	103	3	-	4/41/137/137	-
16	V7N	BR	1001	-	-	6/53/53/53	-
15	LMT	L	1005	-	-	1/21/61/61	0/2/2/2
14	BCL	AH	103	1	-	5/41/137/137	-
15	LMT	BL	1005	-	-	2/21/61/61	0/2/2/2
15	LMT	AD	103	-	-	3/21/61/61	0/2/2/2
16	V7N	BX	1001	-	-	5/53/53/53	-
15	LMT	BX	1004	-	-	5/21/61/61	0/2/2/2
15	LMT	BV	1003	-	-	3/21/61/61	0/2/2/2
14	BCL	ag	1001	12	-	7/41/137/137	-
23	MQ8	ao	101	-	-	11/47/67/67	0/2/2/2
14	BCL	BM	1002	3	-	14/41/137/137	-
15	LMT	BQ	1005	-	-	1/21/61/61	0/2/2/2
14	BCL	BS	1003	4	-	6/41/137/137	-
15	LMT	BH	1002	-	-	4/21/61/61	0/2/2/2
16	V7N	ba	101	-	-	7/53/53/53	-
14	BCL	bj	103	3	-	7/41/137/137	-
14	BCL	L	1010	9	-	4/41/137/137	-
20	0V9	aj	101	-	-	15/48/48/50	-
15	LMT	BB	104	-	-	6/21/61/61	0/2/2/2
14	BCL	an	1001	12	-	9/41/137/137	-
15	LMT	BC	102	-	-	5/21/61/61	0/2/2/2
16	V7N	bk	101	-	-	3/53/53/53	-
15	LMT	M	403	-	-	5/21/61/61	0/2/2/2
14	BCL	AJ	102	29	-	11/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCL	ac	1001	12	-	4/41/137/137	-
14	BCL	ab	102	12	-	6/41/137/137	-
21	CD4	af	102	-	-	22/94/94/94	-
15	LMT	BL	1004	-	-	7/21/61/61	0/2/2/2
15	LMT	BO	1003	-	-	1/21/61/61	0/2/2/2
14	BCL	AE	1001	1	-	1/41/137/137	-
21	CD4	M	402	-	-	22/94/94/94	-
14	BCL	AE	1004	-	-	7/41/137/137	-
15	LMT	bn	105	-	-	5/21/61/61	0/2/2/2
20	0V9	bb	103	-	-	12/48/48/50	-
14	BCL	bf	103	3	-	8/41/137/137	-
15	LMT	BJ	1003	-	-	3/21/61/61	0/2/2/2
15	LMT	AG	103	-	-	10/21/61/61	0/2/2/2
15	LMT	BU	1002	-	-	8/21/61/61	0/2/2/2
14	BCL	ai	101	12	-	11/41/137/137	-
15	LMT	BB	102	-	-	2/21/61/61	0/2/2/2
14	BCL	AT	101	1	-	0/41/137/137	-
15	LMT	BN	105	-	-	3/21/61/61	0/2/2/2
20	0V9	bh	103	-	-	11/48/48/50	-
15	LMT	bf	102	-	-	4/21/61/61	0/2/2/2
15	LMT	BG	1002	-	-	7/21/61/61	0/2/2/2
17	HEC	C	401	5	1/1/3/7	6/14/54/54	-
14	BCL	AR	102	-	-	10/41/137/137	-
28	UYH	ai	102	-	-	7/50/70/70	0/1/1/1
15	LMT	BV	1002	-	-	1/21/61/61	0/2/2/2
15	LMT	BC	106	-	-	3/21/61/61	0/2/2/2
15	LMT	bc	104	-	-	7/21/61/61	0/2/2/2
14	BCL	AI	102	1	-	8/41/137/137	-
16	V7N	AS	105	-	-	5/53/53/53	-
15	LMT	BW	1005	-	-	1/21/61/61	0/2/2/2
15	LMT	ab	101	-	-	3/21/61/61	0/2/2/2
15	LMT	AU	101	-	-	6/21/61/61	0/2/2/2
15	LMT	AL	102	-	-	1/21/61/61	0/2/2/2
16	V7N	BM	1001	-	-	6/53/53/53	-
15	LMT	BK	1005	-	-	4/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	AH	104	-	-	6/21/61/61	0/2/2/2
15	LMT	BG	1005	-	-	3/21/61/61	0/2/2/2
14	BCL	BX	1002	3	-	9/41/137/137	-
15	LMT	BB	105	-	-	5/21/61/61	0/2/2/2
14	BCL	BR	1004	4	-	3/41/137/137	-
15	LMT	bn	101	-	-	9/21/61/61	0/2/2/2
17	HEC	C	402	5	1/1/3/7	4/14/54/54	-
15	LMT	BT	101	-	-	4/21/61/61	0/2/2/2
15	LMT	L	1011	-	-	3/21/61/61	0/2/2/2
20	0V9	bk	104	-	-	13/48/48/50	-
19	NDG	C1	1002	18	-	0/6/23/26	0/1/1/1
15	LMT	L	1008	-	-	6/21/61/61	0/2/2/2
23	MQ8	M	407	-	-	6/47/67/67	0/2/2/2
14	BCL	AX	102	-	-	11/41/137/137	-
15	LMT	bl	105	-	-	2/21/61/61	0/2/2/2
14	BCL	BU	1004	3	-	9/41/137/137	-
14	BCL	bg	105	3	-	5/41/137/137	-
15	LMT	BN	101	-	-	7/21/61/61	0/2/2/2
15	LMT	AH	102	-	-	3/21/61/61	0/2/2/2
15	LMT	BE	103	-	-	5/21/61/61	0/2/2/2
15	LMT	AS	101	-	-	8/21/61/61	0/2/2/2
14	BCL	AV	101	29	-	4/41/137/137	-
14	BCL	bm	104	3	-	8/41/137/137	-
15	LMT	bh	104	-	-	5/21/61/61	0/2/2/2
14	BCL	AP	103	29	-	6/41/137/137	-
14	BCL	BE	104	4	-	7/41/137/137	-
15	LMT	BT	104	-	-	6/21/61/61	0/2/2/2
14	BCL	AI	103	-	-	11/41/137/137	-
16	V7N	BQ	1001	-	-	5/53/53/53	-
16	V7N	bg	101	-	-	6/53/53/53	-
15	LMT	be	104	-	-	10/21/61/61	0/2/2/2
14	BCL	AM	101	1	-	4/41/137/137	-
15	LMT	BN	104	-	-	5/21/61/61	0/2/2/2
15	LMT	bj	102	-	-	6/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCL	bh	105	3	-	6/41/137/137	-
14	BCL	AP	102	1	-	4/41/137/137	-
14	BCL	AJ	101	1	-	0/41/137/137	-
14	BCL	bn	103	4	-	7/41/137/137	-
21	CD4	ae	101	-	-	28/94/94/94	-
14	BCL	AC	101	-	-	10/41/137/137	-
15	LMT	BV	1006	-	-	2/21/61/61	0/2/2/2
14	BCL	ba	103	3	-	2/41/137/137	-
14	BCL	AX	103	1	-	5/41/137/137	-
14	BCL	ah	1001	12	-	2/41/137/137	-
16	V7N	BW	1001	-	-	3/53/53/53	-
16	V7N	BD	101	-	-	3/53/53/53	-
16	V7N	BE	101	-	-	3/53/53/53	-
14	BCL	bl	104	3	-	12/41/137/137	-
14	BCL	BH	1005	3	-	10/41/137/137	-
20	0V9	bn	104	-	-	10/48/48/50	-
15	LMT	BX	1003	-	-	7/21/61/61	0/2/2/2
20	0V9	bo	104	-	-	9/48/48/50	-
15	LMT	BD	104	-	-	3/21/61/61	0/2/2/2
14	BCL	AD	102	2	-	1/41/137/137	-
14	BCL	BQ	1003	4	-	9/41/137/137	-
14	BCL	am	1001	12	-	4/41/137/137	-
14	BCL	AN	104	-	-	9/41/137/137	-
16	V7N	bp	101	-	-	4/53/53/53	-
16	V7N	bi	101	-	-	8/53/53/53	-
15	LMT	BA	102	-	-	4/21/61/61	0/2/2/2
15	LMT	BD	102	-	-	6/21/61/61	0/2/2/2
15	LMT	BP	1004	-	-	2/21/61/61	0/2/2/2
15	LMT	BC	105	-	-	4/21/61/61	0/2/2/2
15	LMT	BP	1003	-	-	3/21/61/61	0/2/2/2
25	BPH	L	1009	-	-	6/37/105/105	0/5/6/6
16	V7N	bm	101	-	-	8/53/53/53	-
15	LMT	BL	1002	-	-	6/21/61/61	0/2/2/2
14	BCL	BT	103	4	-	6/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	BS	1005	-	-	4/21/61/61	0/2/2/2
20	0V9	bj	104	-	-	13/48/48/50	-
15	LMT	AA	1004	-	-	3/21/61/61	0/2/2/2
14	BCL	bc	102	3	-	10/41/137/137	-
15	LMT	BQ	1002	-	-	3/21/61/61	0/2/2/2
14	BCL	BN	103	3	-	11/41/137/137	-
15	LMT	bb	102	-	-	9/21/61/61	0/2/2/2
14	BCL	aa	1001	11	-	7/41/137/137	-
16	V7N	BP	1001	-	-	2/53/53/53	-
15	LMT	bl	101	-	-	8/21/61/61	0/2/2/2
14	BCL	AQ	101	29	-	10/41/137/137	-
25	BPH	M	406	-	-	6/37/105/105	0/5/6/6
20	0V9	bi	103	-	-	10/48/48/50	-
15	LMT	BG	1003	-	-	2/21/61/61	0/2/2/2
15	LMT	AJ	104	-	-	7/21/61/61	0/2/2/2
14	BCL	BK	1006	3	-	8/41/137/137	-
14	BCL	al	1001	12	-	7/41/137/137	-
15	LMT	bo	101	-	-	0/21/61/61	0/2/2/2
16	V7N	bc	101	-	-	4/53/53/53	-
15	LMT	BP	1002	-	-	5/21/61/61	0/2/2/2
19	NDG	C	406	18	-	0/6/23/26	0/1/1/1
20	0V9	bg	104	-	-	9/48/48/50	-
15	LMT	BS	1006	-	-	3/21/61/61	0/2/2/2
16	V7N	be	101	-	-	5/53/53/53	-
14	BCL	AG	102	1	-	5/41/137/137	-
15	LMT	AI	101	-	-	4/21/61/61	0/2/2/2
15	LMT	BU	1003	-	-	2/21/61/61	0/2/2/2
15	LMT	BF	103	-	-	4/21/61/61	0/2/2/2
14	BCL	bp	102	3	-	11/41/137/137	-
16	V7N	BB	101	-	-	5/53/53/53	-
14	BCL	AO	1002	1	-	1/41/137/137	-
14	BCL	ad	1001	12	-	8/41/137/137	-
15	LMT	BQ	1004	-	-	7/21/61/61	0/2/2/2
14	BCL	AQ	102	1	-	0/41/137/137	-

The worst 5 of 1646 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	404	HEC	C3D-C2D	7.80	1.53	1.36
17	C	402	HEC	C3D-C2D	7.74	1.53	1.36
17	C	403	HEC	C3D-C2D	7.74	1.53	1.36
17	C	401	HEC	C3D-C2D	7.69	1.53	1.36
16	bn	102	V7N	C28-C27	7.04	1.52	1.34

The worst 5 of 2002 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BF	102	BCL	C1-C2-C3	12.31	147.32	126.04
25	M	406	BPH	C4D-CHA-CBD	-10.75	103.65	108.52
25	L	1009	BPH	C4D-CHA-CBD	-9.94	104.02	108.52
14	BI	1003	BCL	C1-O2A-CGA	9.20	140.59	116.44
14	am	1001	BCL	C1-C2-C3	9.06	141.72	126.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	C	401	HEC	NA
17	C	402	HEC	NA
17	C	403	HEC	NA
17	C	404	HEC	NA

5 of 1932 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	AA	1002	BCL	CHA-CBD-CGD-O1D
14	AA	1002	BCL	CHA-CBD-CGD-O2D
14	AB	1002	BCL	C1A-C2A-CAA-CBA
14	AB	1002	BCL	C3A-C2A-CAA-CBA
14	AB	1002	BCL	CHA-CBD-CGD-O1D

There are no ring outliers.

100 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	404	HEC	1	0
15	BT	102	LMT	1	0
14	AB	1001	BCL	1	0
14	bb	104	BCL	1	0
14	AK	102	BCL	1	0
14	ae	102	BCL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	AC	103	BCL	1	0
14	BI	1003	BCL	2	0
27	M	404	CRT	2	0
15	bi	102	LMT	1	0
14	AR	101	BCL	1	0
14	AS	102	BCL	1	0
14	ao	102	BCL	1	0
14	AW	101	BCL	3	0
14	AU	103	BCL	1	0
14	AN	101	BCL	1	0
20	bm	102	0V9	1	0
15	AF	1002	LMT	1	0
14	AF	1001	BCL	2	0
14	AV	103	BCL	1	0
15	BO	1002	LMT	1	0
16	BV	1001	V7N	1	0
15	AP	101	LMT	1	0
14	AC	102	BCL	1	0
22	H1	103	PGW	1	0
15	BH	1003	LMT	1	0
15	BG	1006	LMT	1	0
14	AA	1001	BCL	2	0
14	AH	101	BCL	1	0
14	AN	102	BCL	1	0
15	BA	105	LMT	1	0
14	AS	103	BCL	1	0
14	AU	102	BCL	1	0
15	BH	1004	LMT	1	0
23	L	1001	MQ8	1	0
14	AB	1002	BCL	1	0
17	C	403	HEC	1	0
14	AS	104	BCL	2	0
21	aj	102	CD4	1	0
14	AV	102	BCL	1	0
15	BR	1005	LMT	1	0
14	M	408	BCL	2	0
15	BR	1003	LMT	1	0
14	AM	102	BCL	1	0
15	AD	101	LMT	1	0
14	bd	102	BCL	1	0
14	AL	103	BCL	1	0
14	af	101	BCL	2	0

Continued on next page...

Continued from previous page...

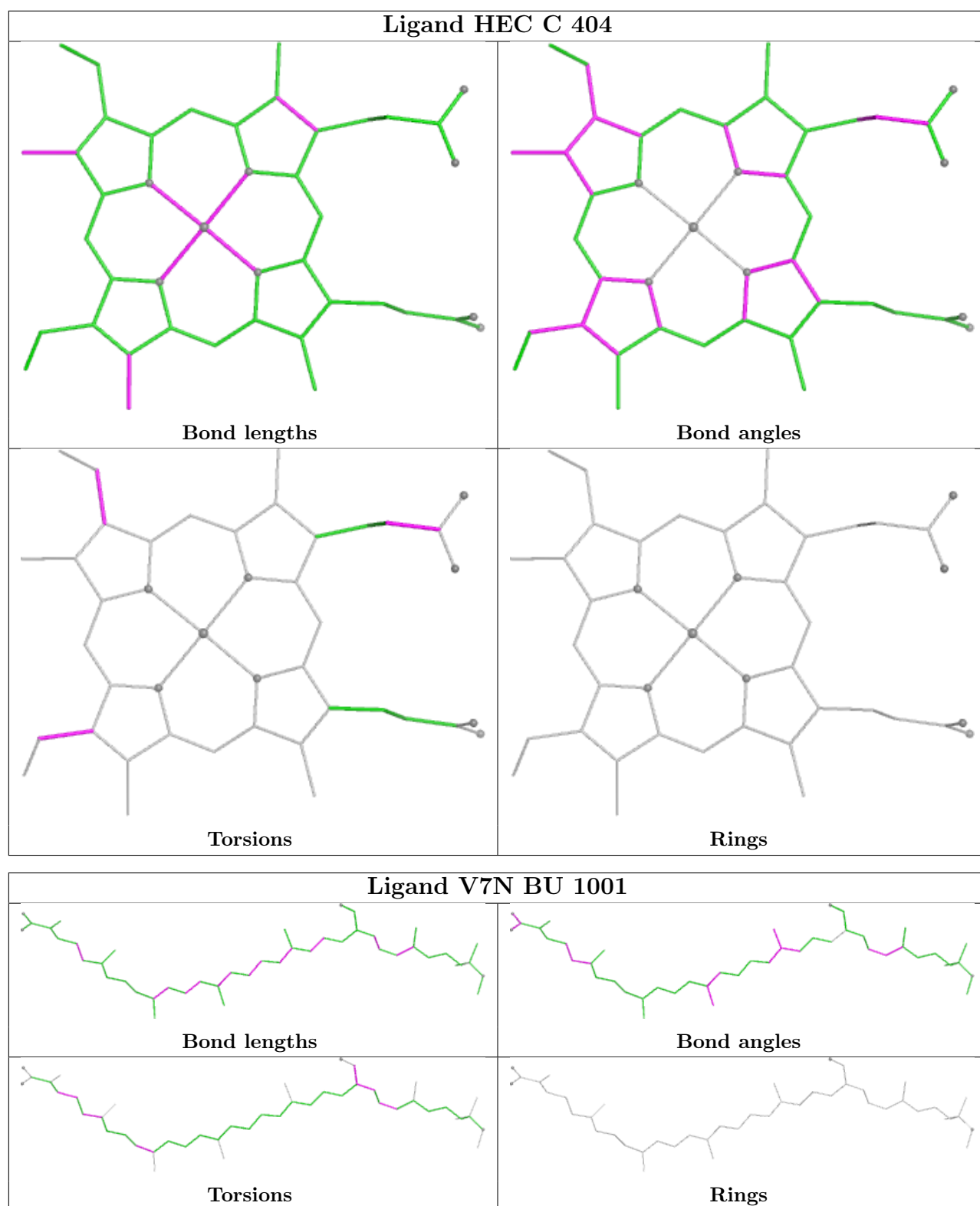
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L	1002	BCL	2	0
14	be	105	BCL	1	0
14	AH	103	BCL	1	0
15	BV	1003	LMT	1	0
14	ag	1001	BCL	1	0
14	BM	1002	BCL	1	0
14	BS	1003	BCL	1	0
14	bj	103	BCL	1	0
14	ac	1001	BCL	1	0
14	ab	102	BCL	2	0
21	af	102	CD4	1	0
15	BO	1003	LMT	1	0
14	AE	1001	BCL	1	0
14	bf	103	BCL	2	0
14	ai	101	BCL	1	0
14	AT	101	BCL	1	0
17	C	401	HEC	1	0
14	AR	102	BCL	2	0
15	BV	1002	LMT	1	0
15	bc	104	LMT	1	0
14	AI	102	BCL	2	0
15	AH	104	LMT	1	0
15	BG	1005	LMT	1	0
17	C	402	HEC	1	0
15	BT	101	LMT	1	0
23	M	407	MQ8	2	0
14	AX	102	BCL	2	0
14	BU	1004	BCL	1	0
14	bg	105	BCL	1	0
14	bm	104	BCL	1	0
14	AI	103	BCL	1	0
16	bg	101	V7N	1	0
14	AM	101	BCL	1	0
14	bh	105	BCL	1	0
14	AP	102	BCL	1	0
14	AJ	101	BCL	1	0
21	ae	101	CD4	1	0
14	AC	101	BCL	1	0
15	BV	1006	LMT	1	0
14	ba	103	BCL	1	0
14	AX	103	BCL	1	0
14	ah	1001	BCL	1	0

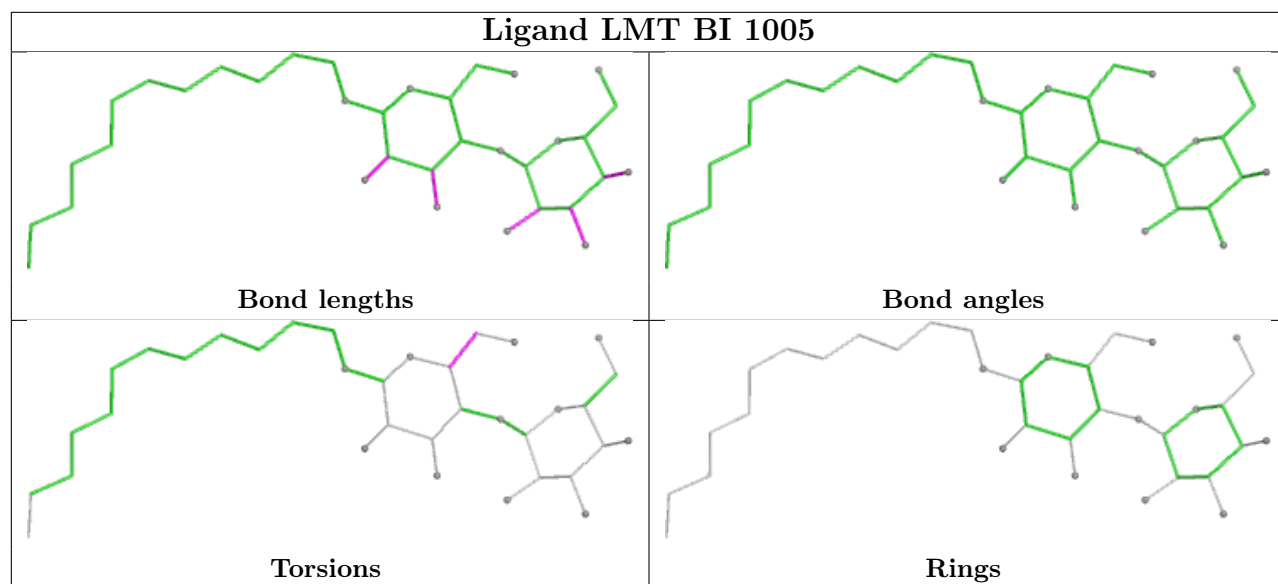
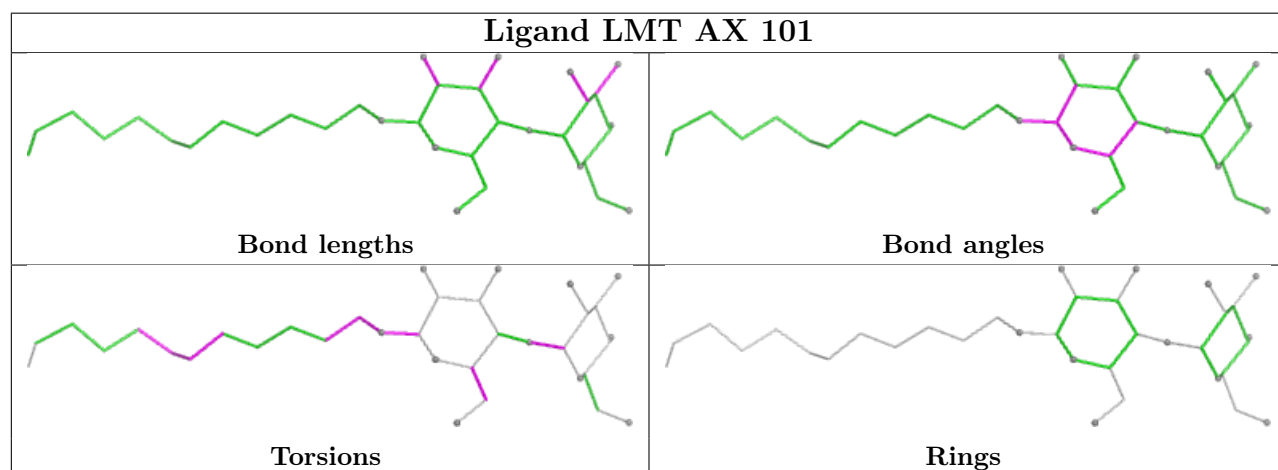
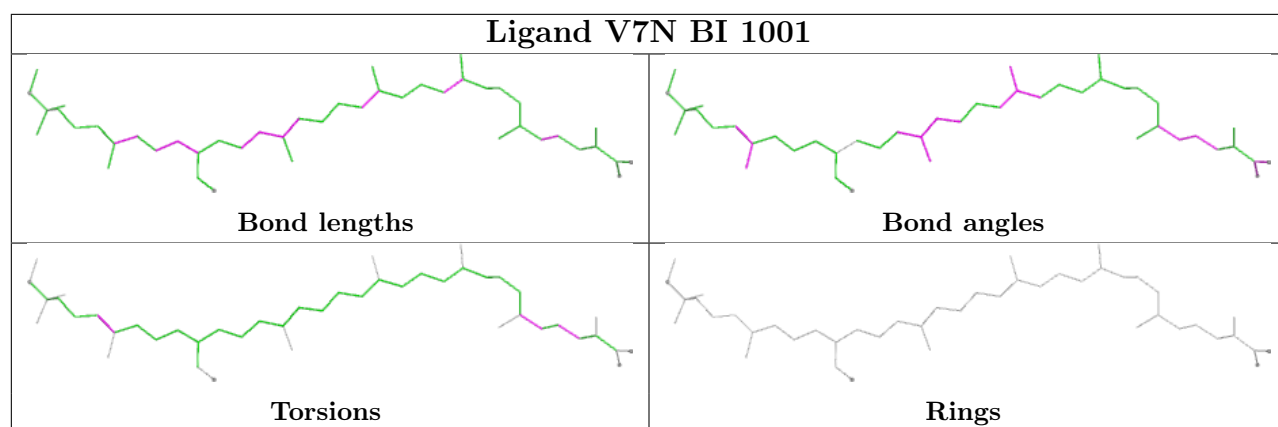
Continued on next page...

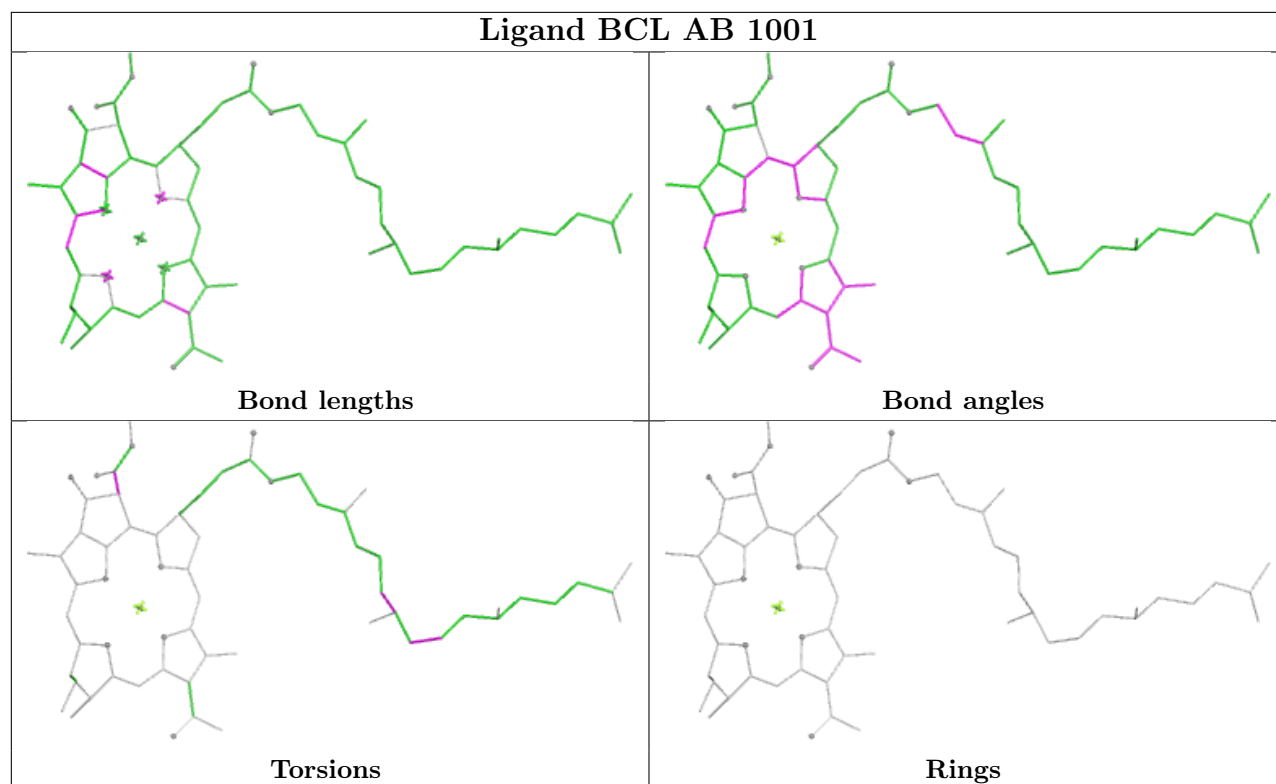
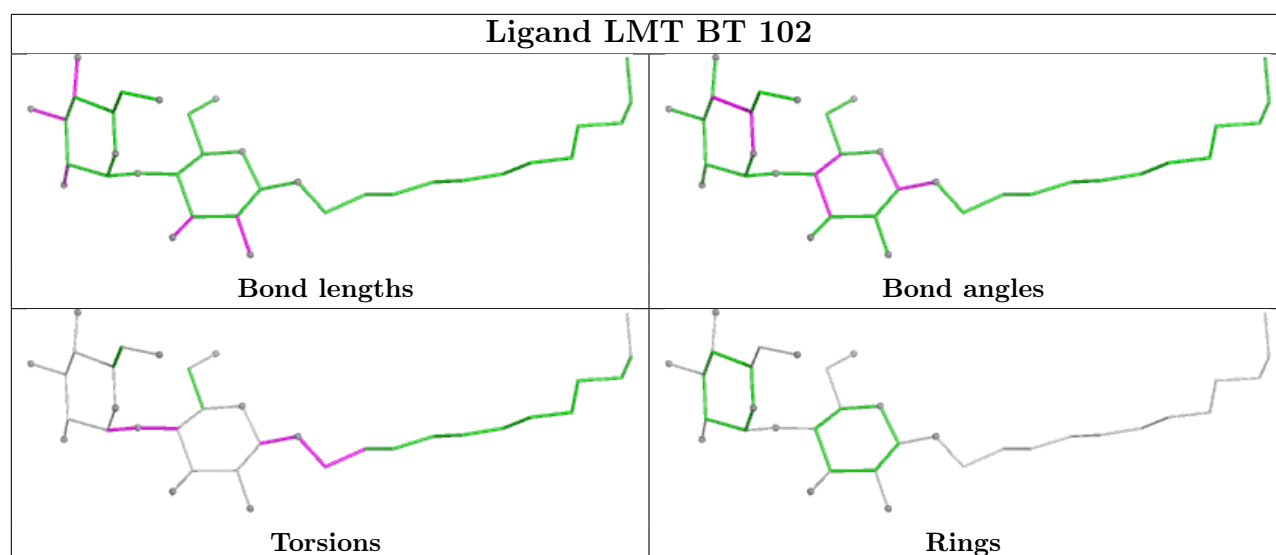
Continued from previous page...

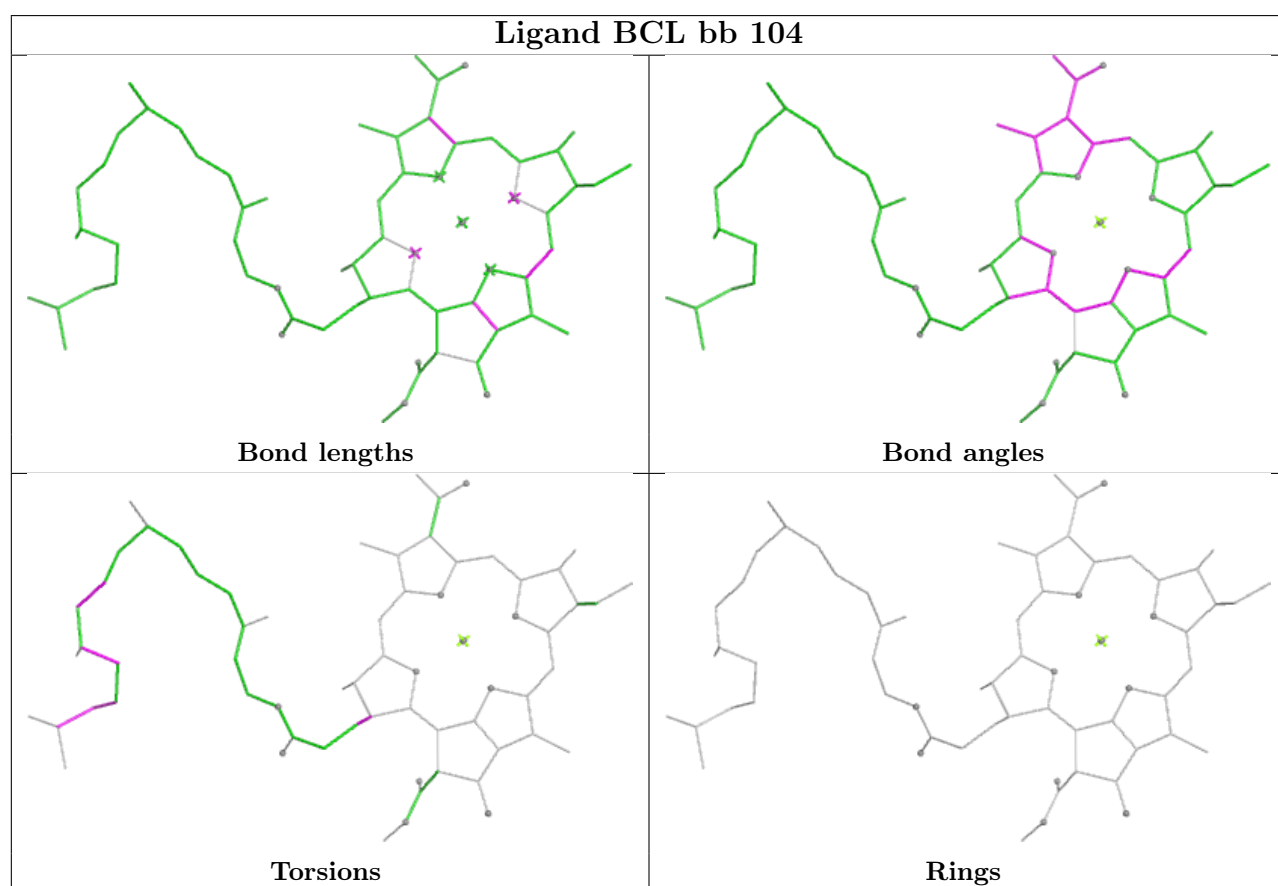
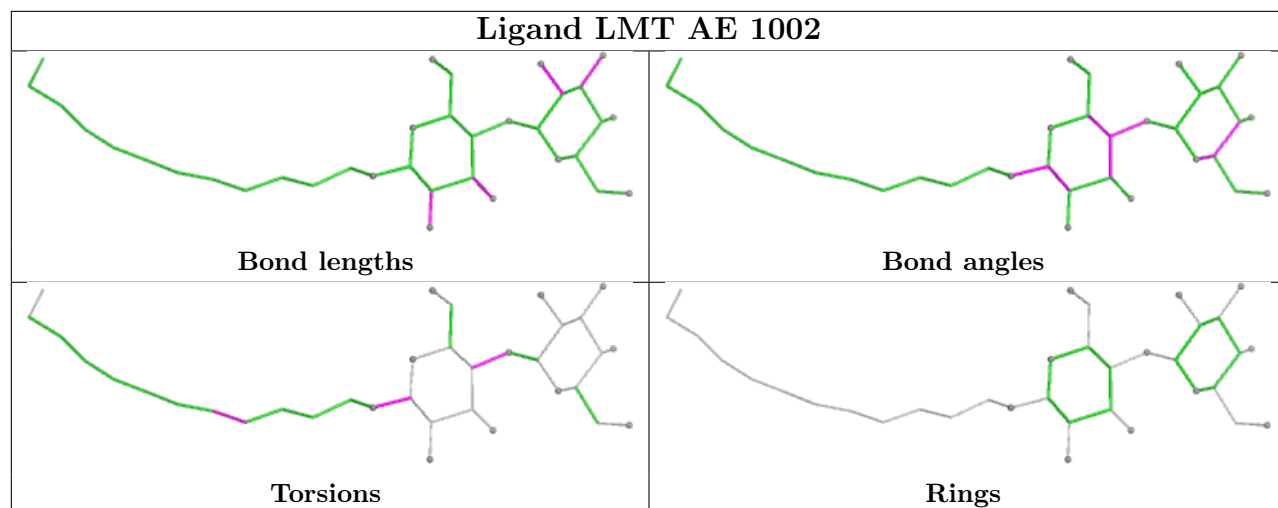
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bl	104	BCL	1	0
14	am	1001	BCL	1	0
25	L	1009	BPH	2	0
14	aa	1001	BCL	1	0
25	M	406	BPH	3	0
15	bo	101	LMT	1	0
14	AG	102	BCL	1	0
14	bp	102	BCL	1	0
14	AO	1002	BCL	1	0
14	AQ	102	BCL	1	0

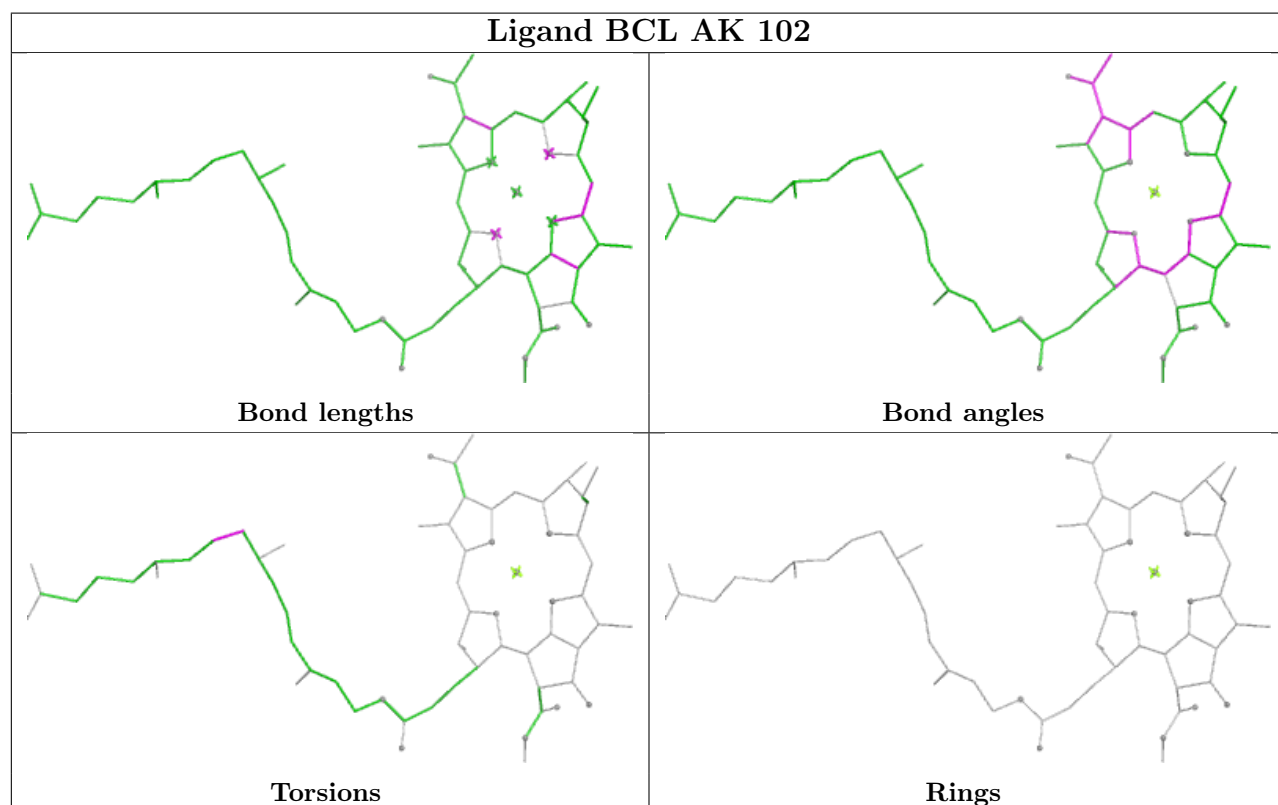
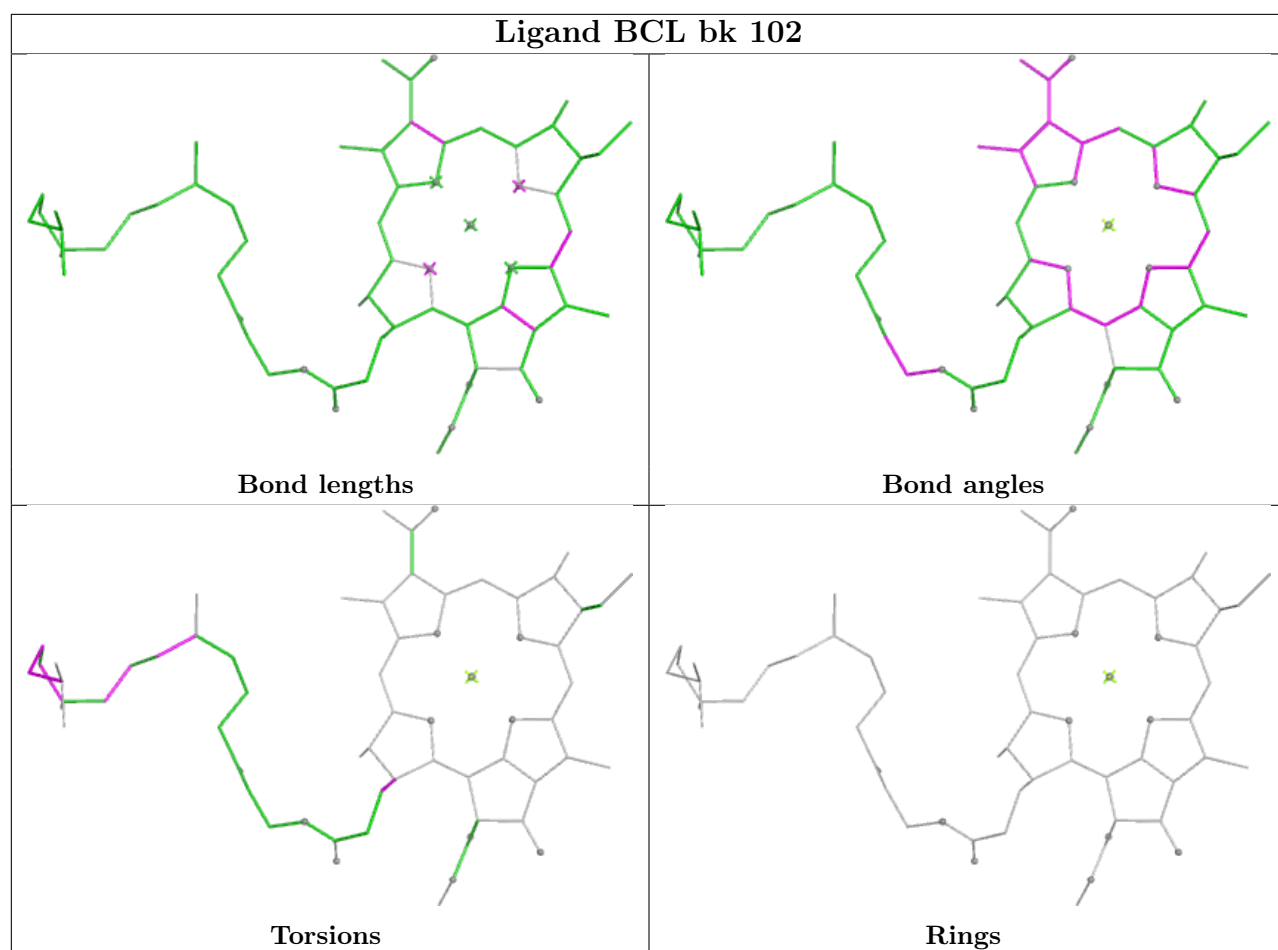
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

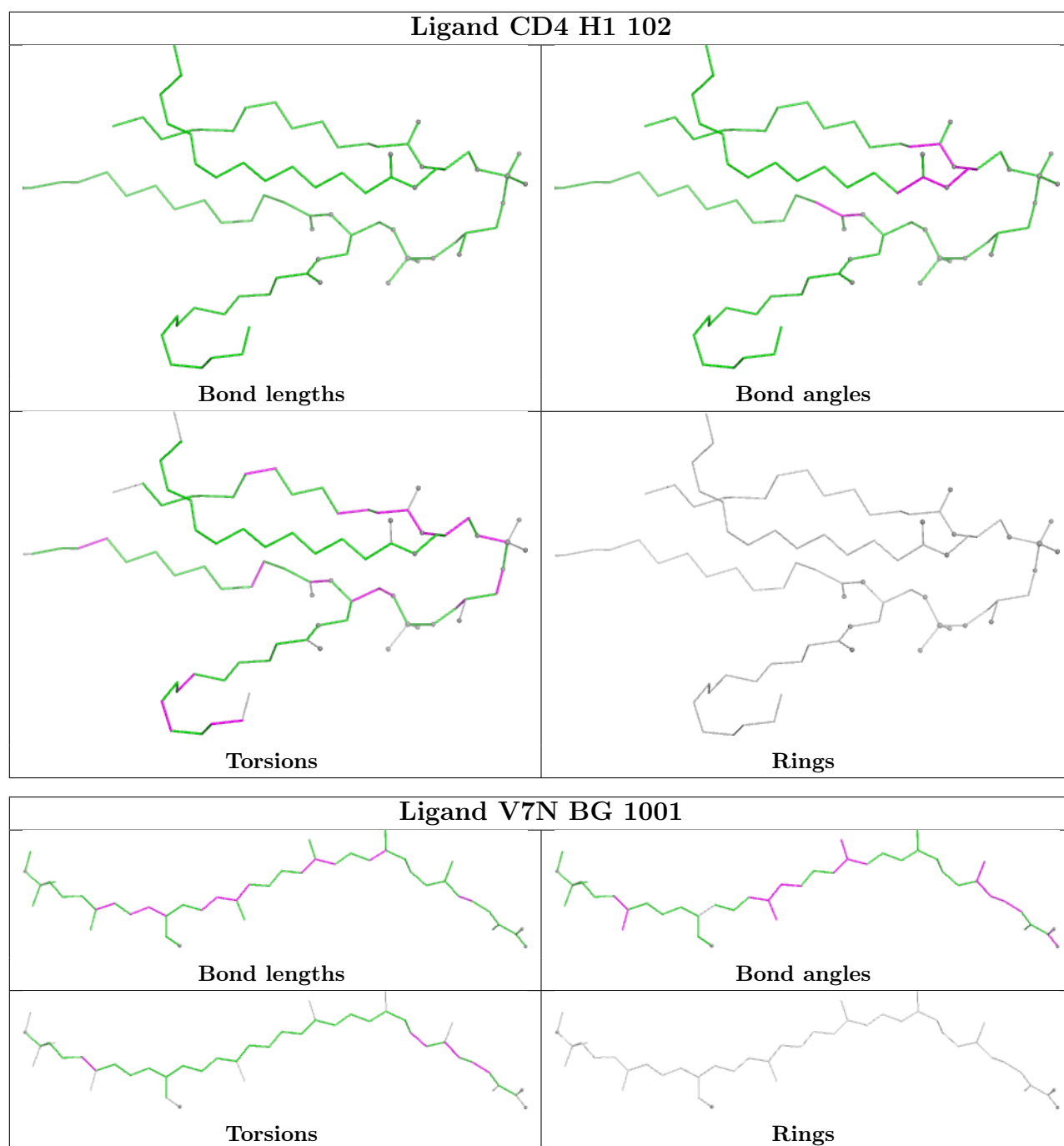


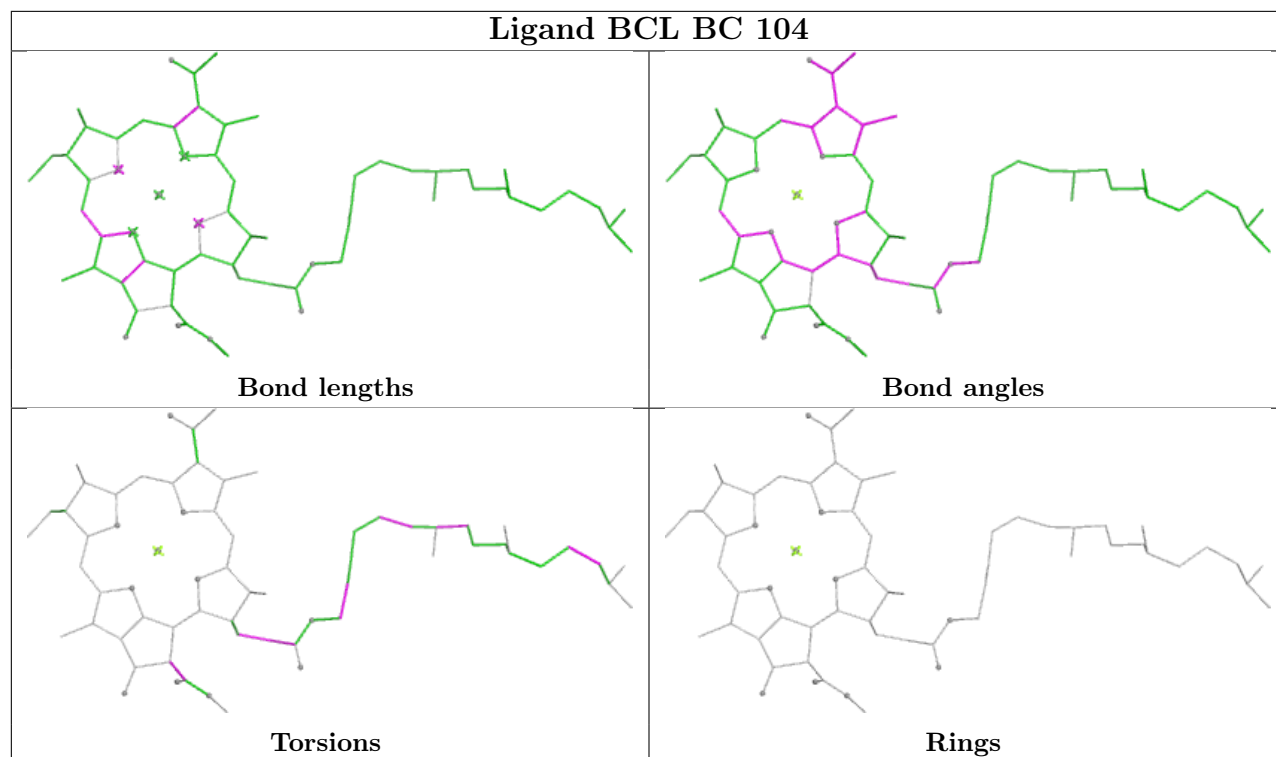
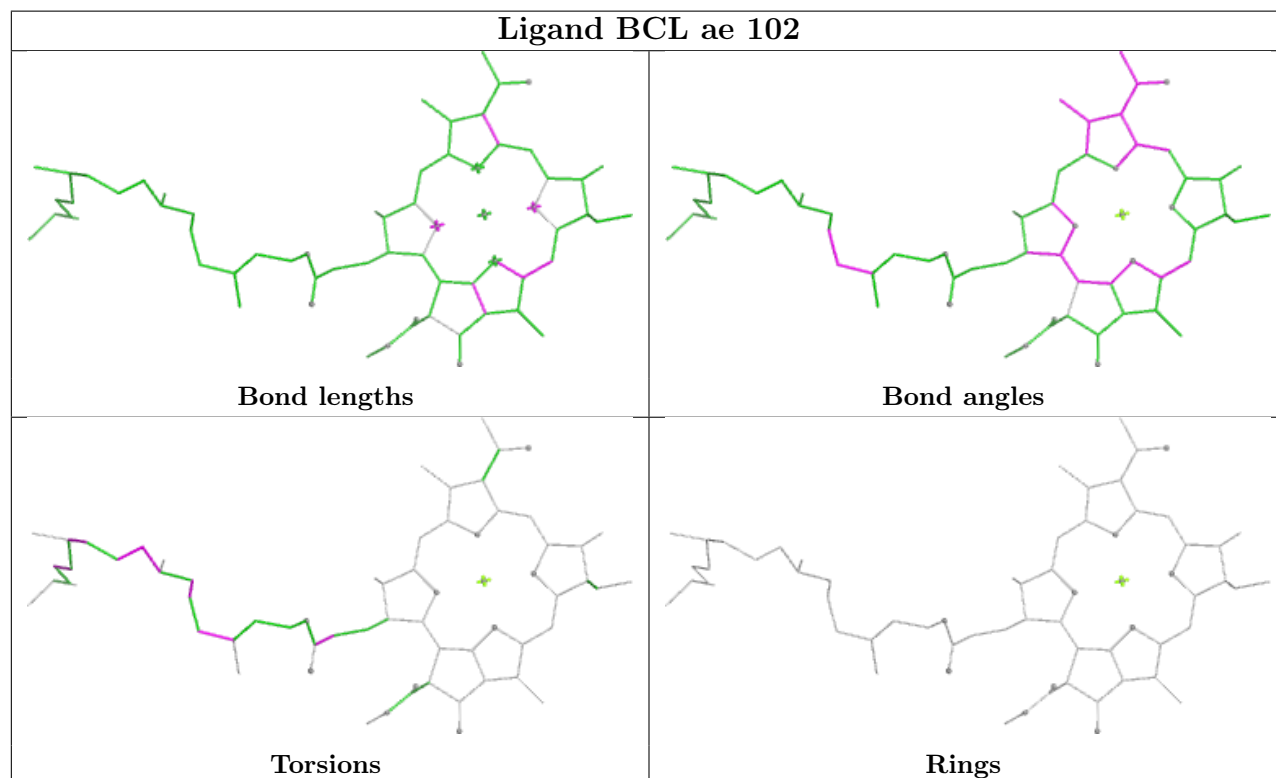


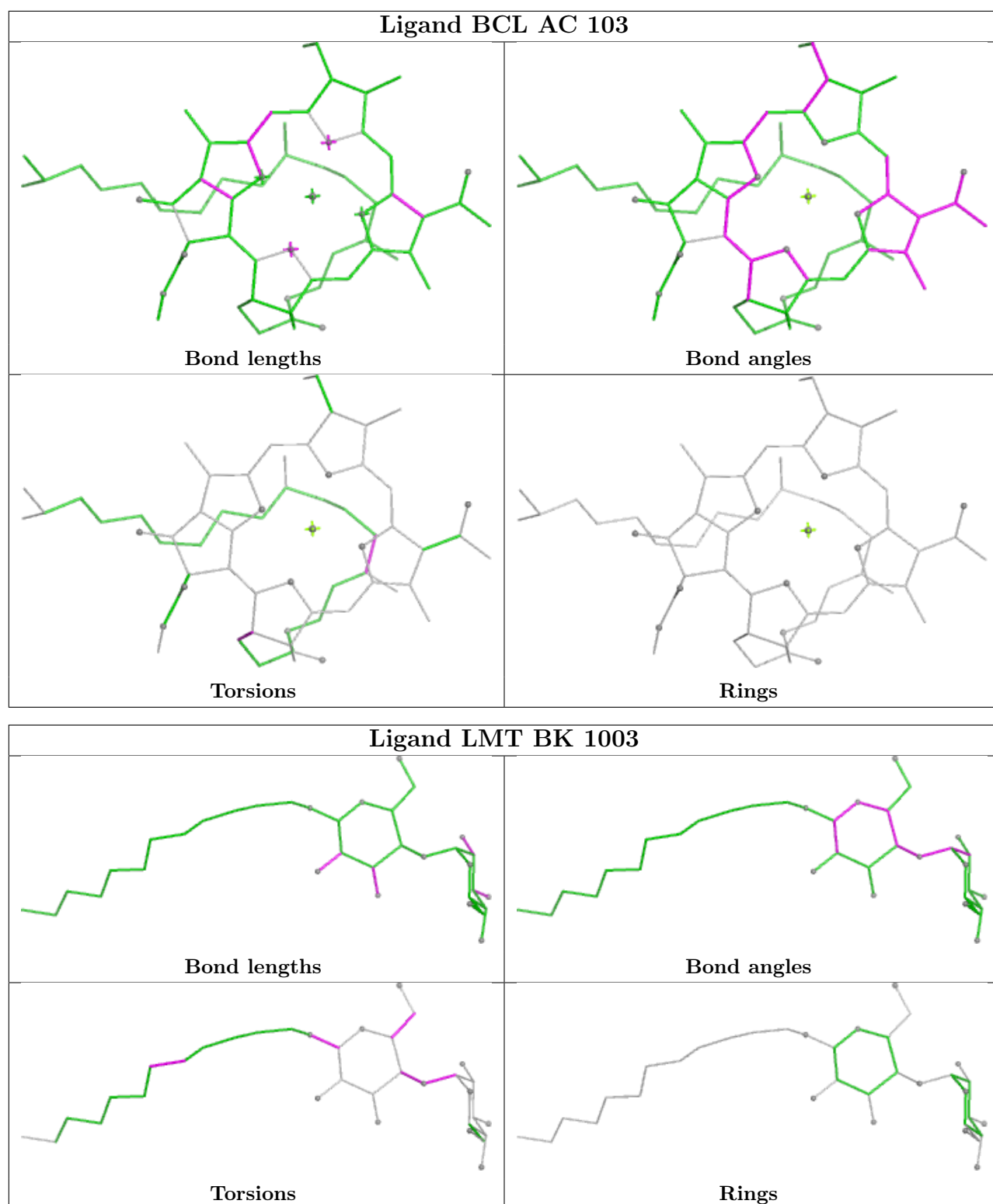


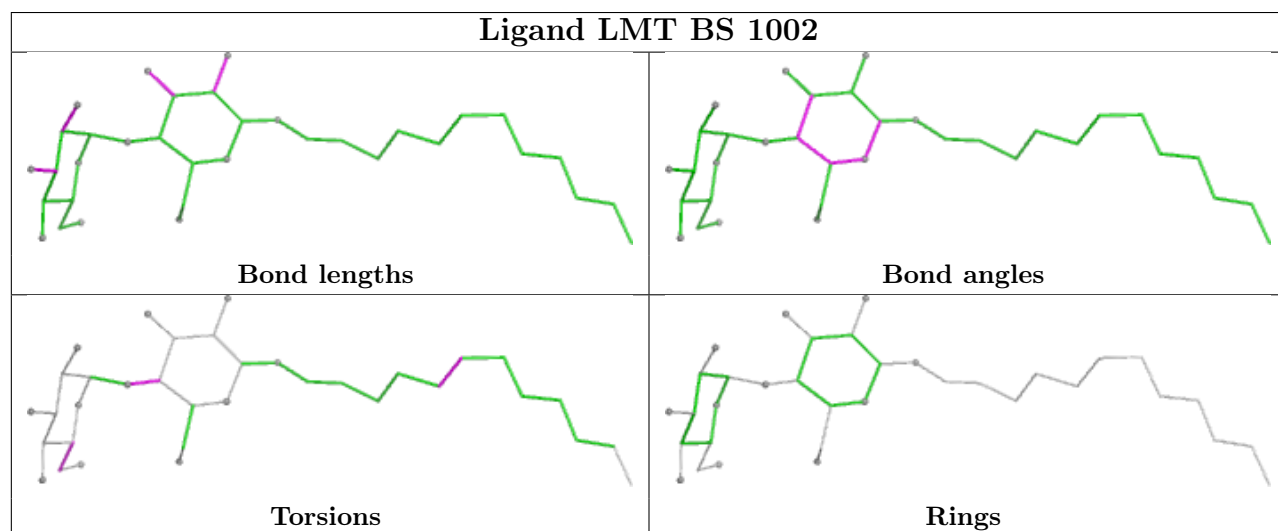
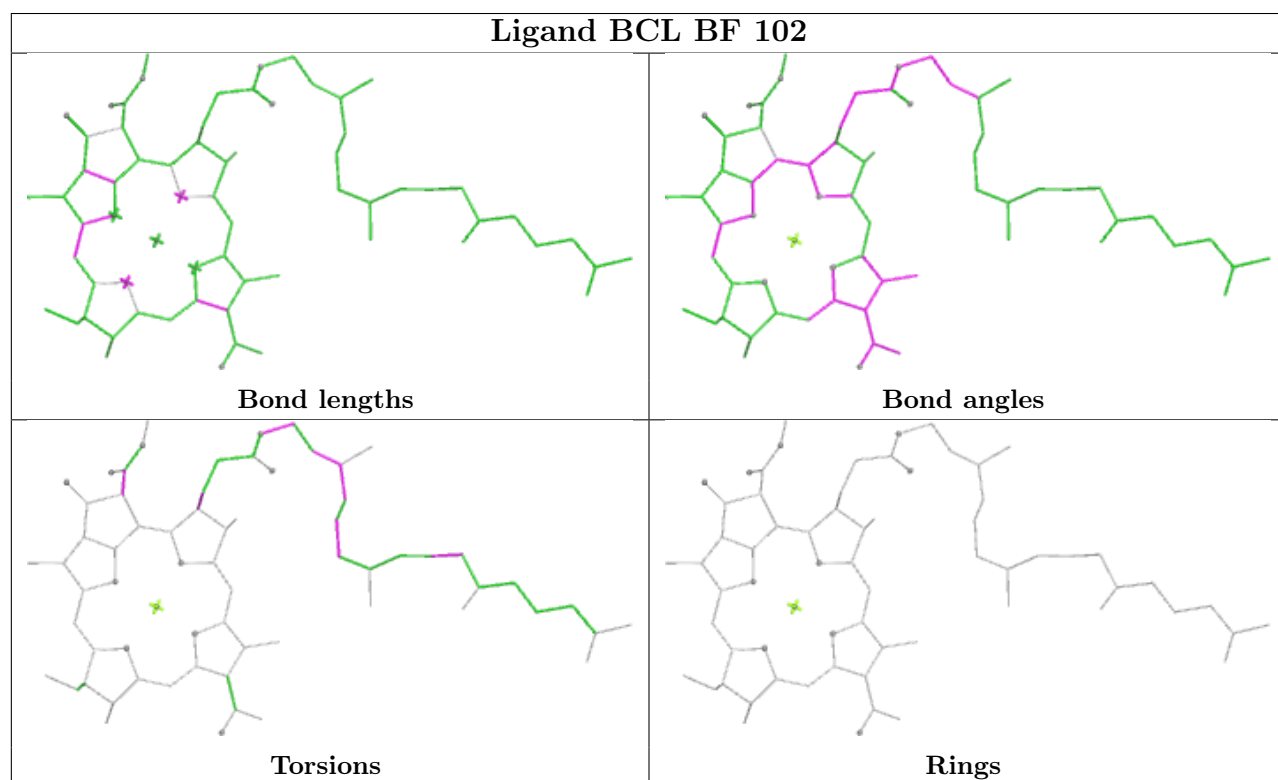
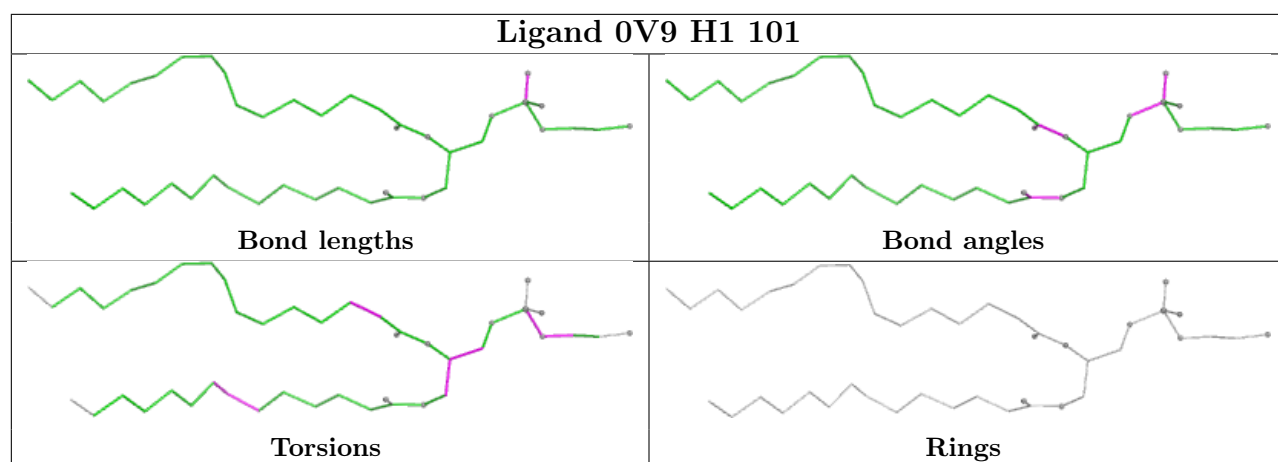


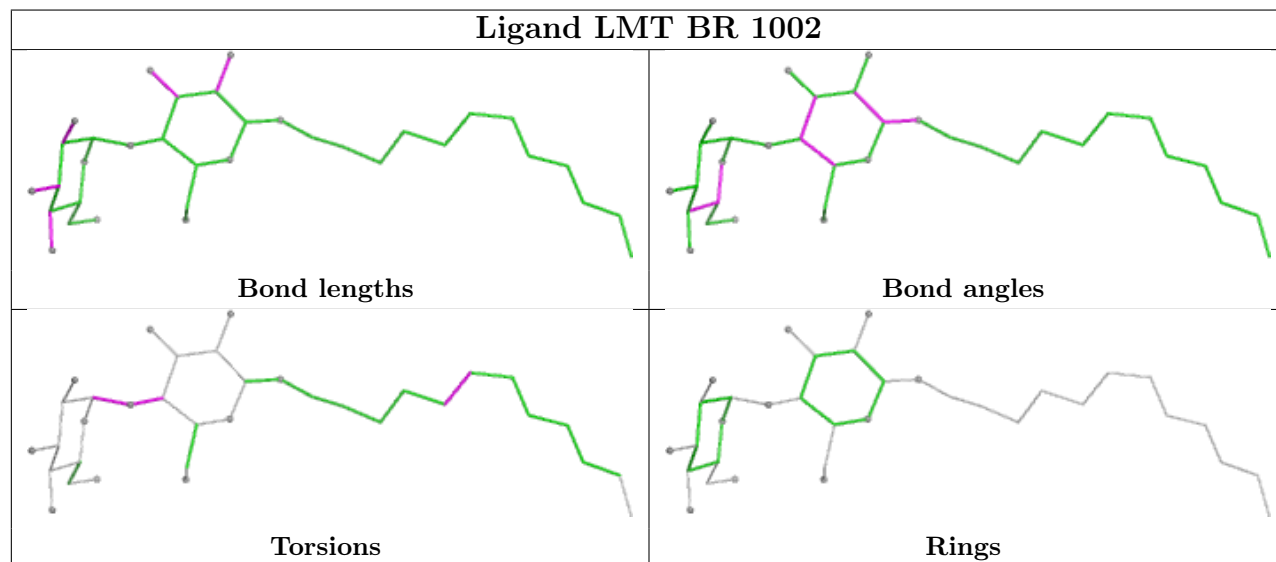
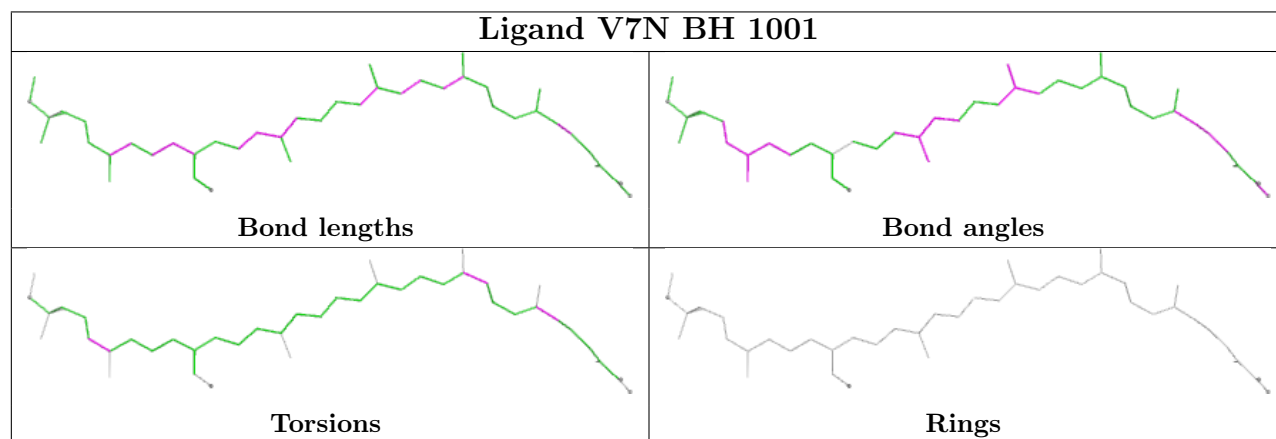
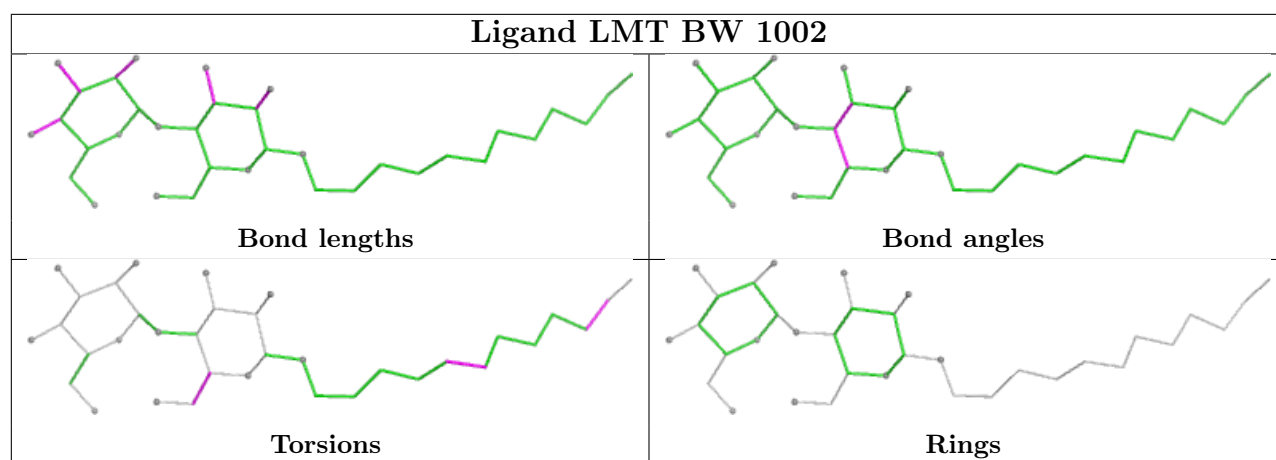


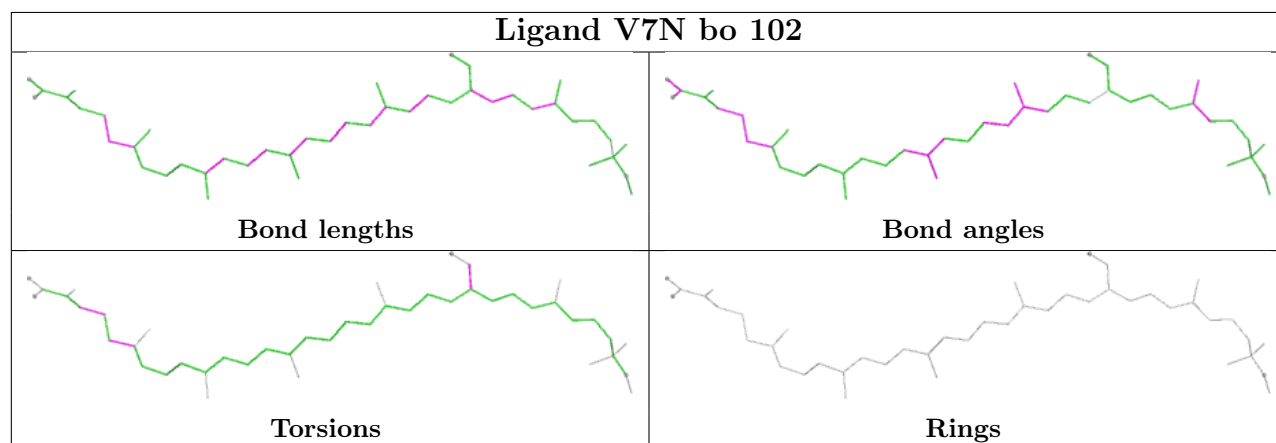
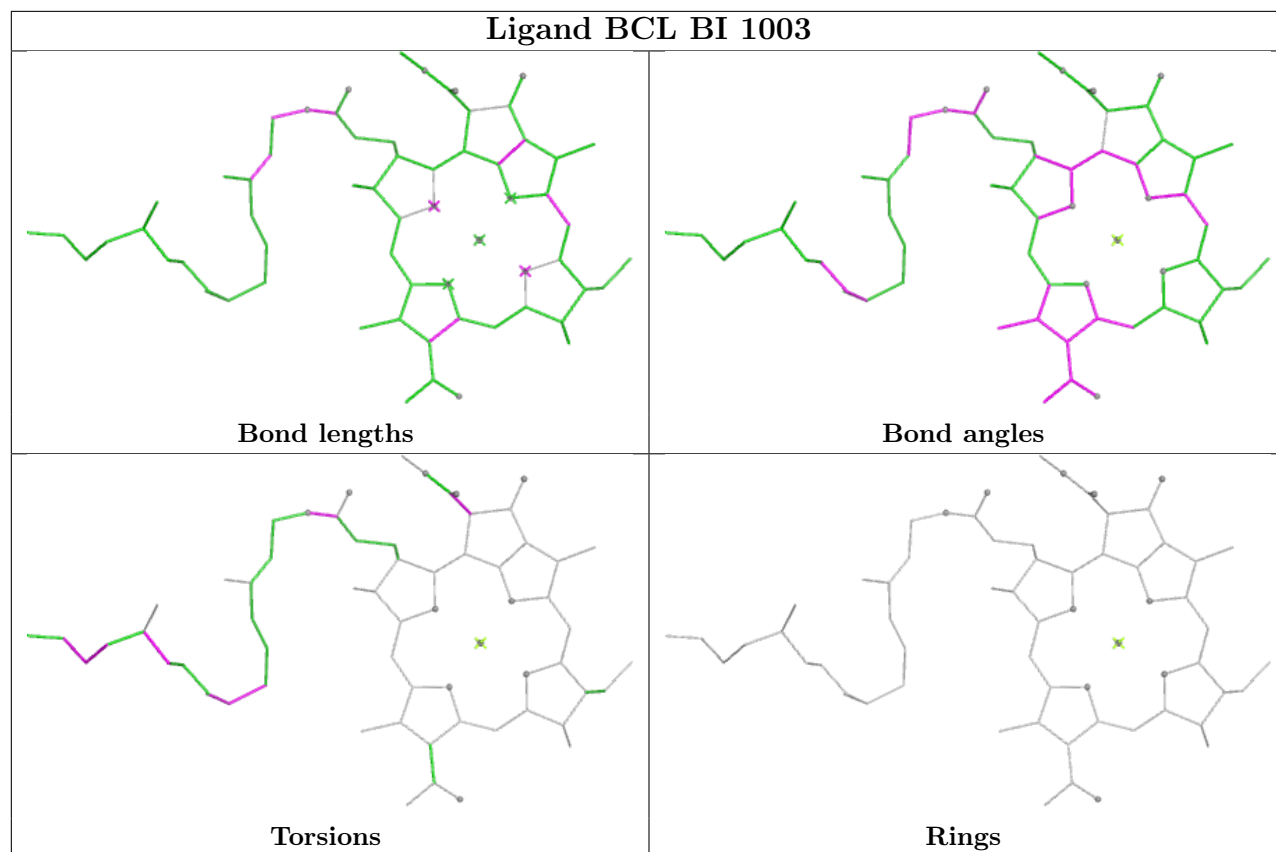


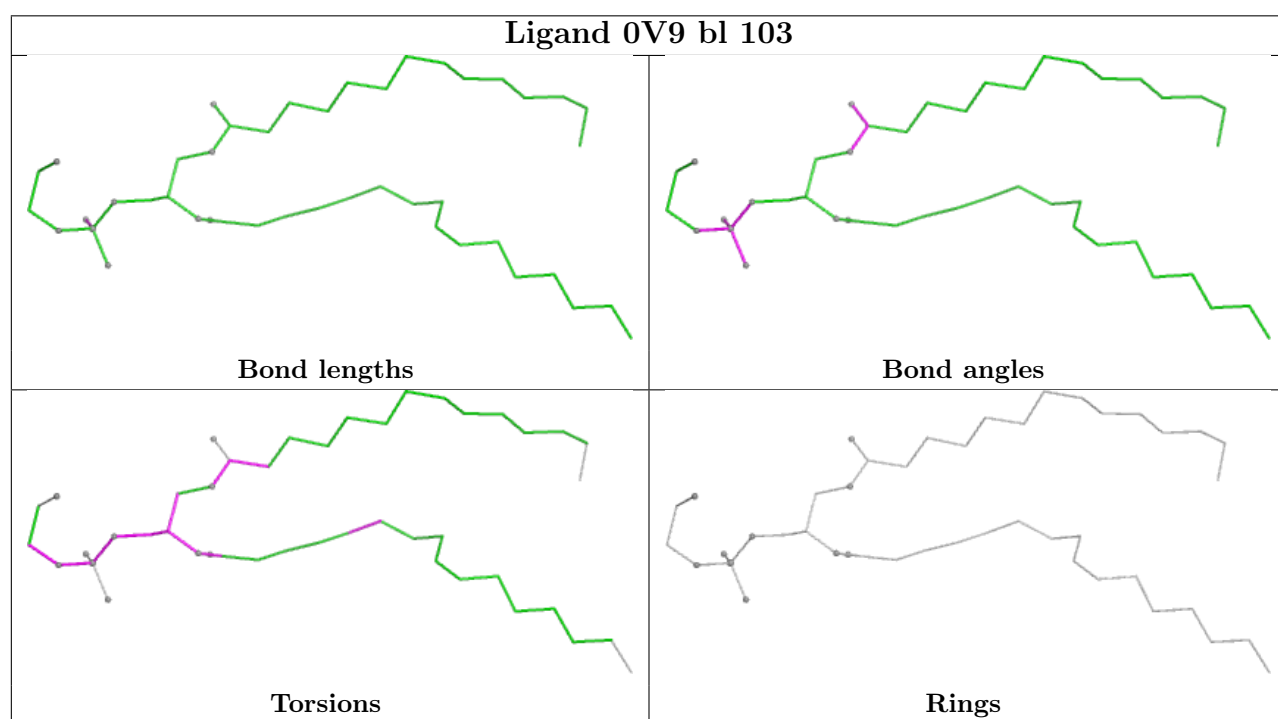
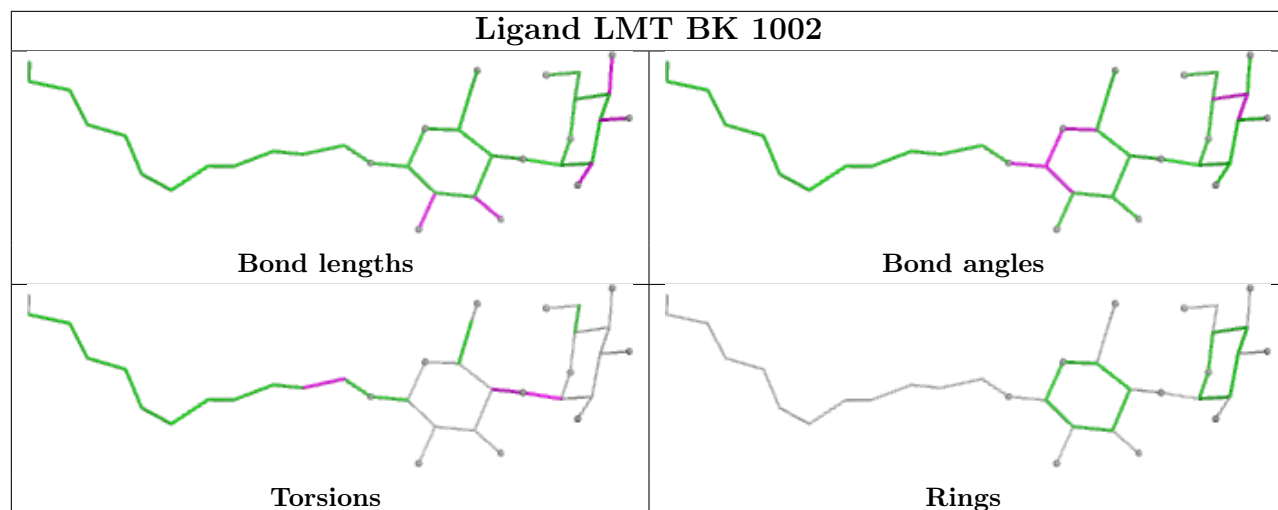
Ligand BCL BC 104**Ligand BCL ae 102**

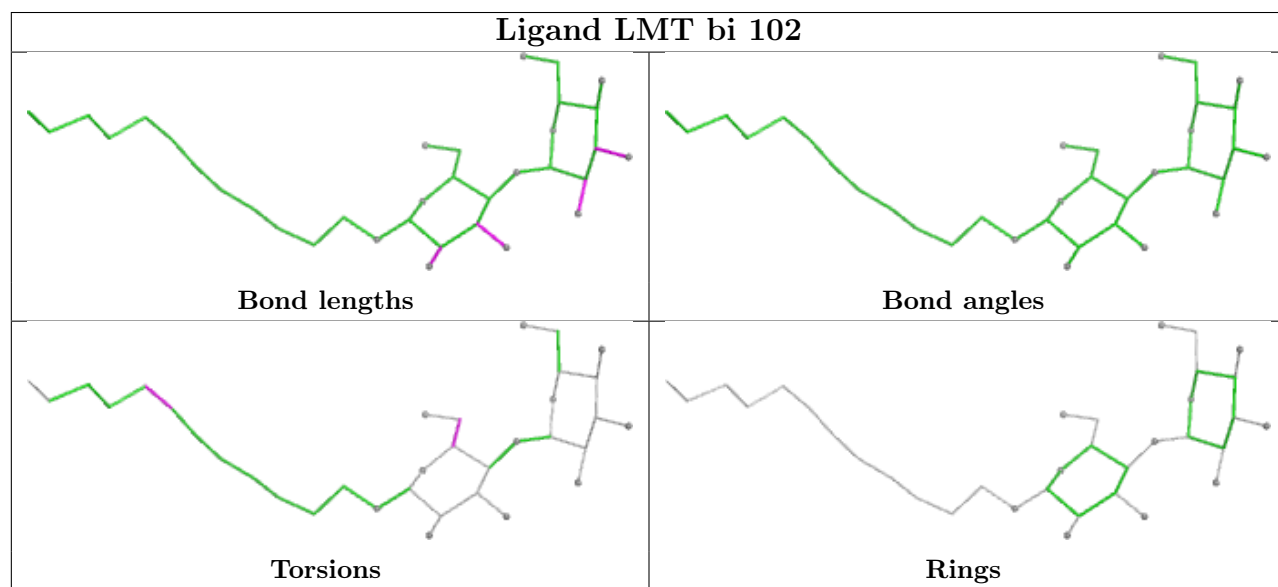
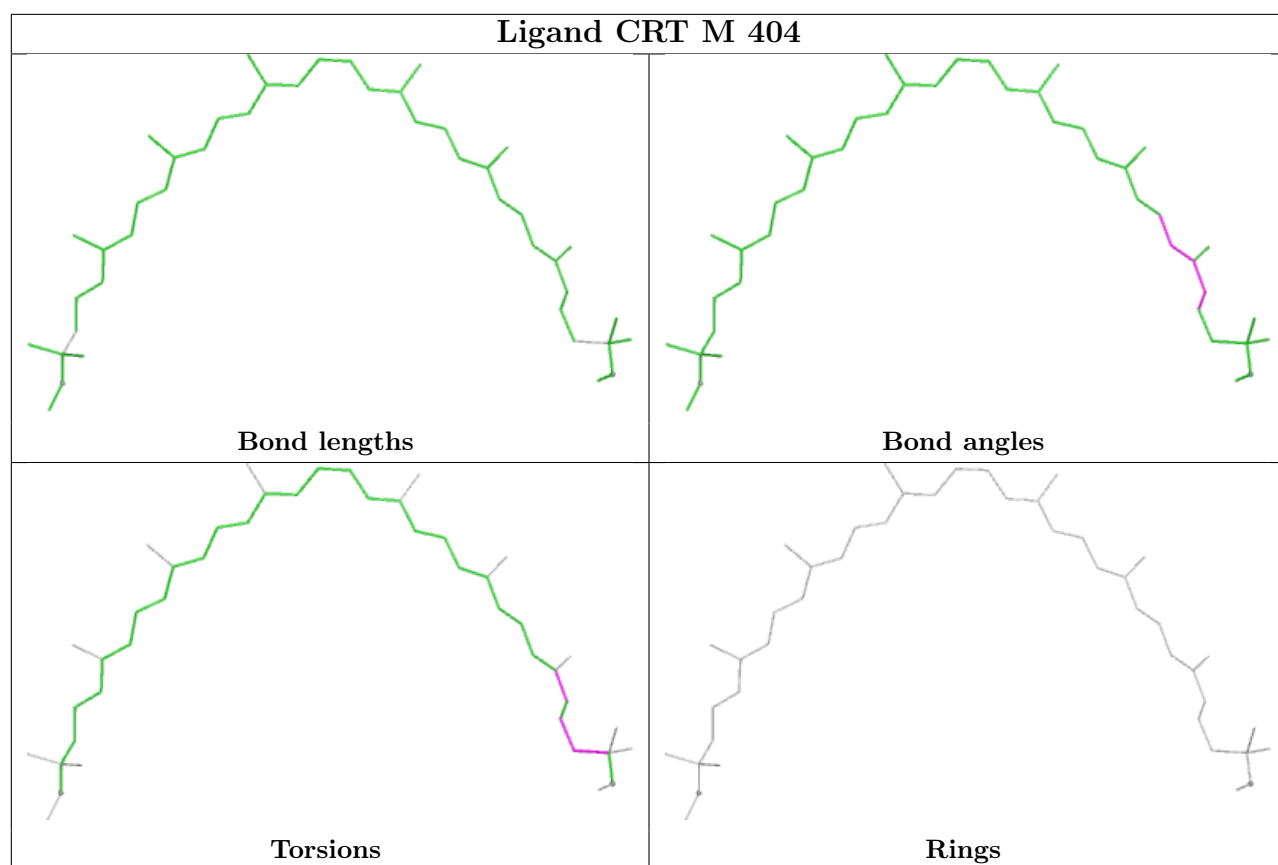


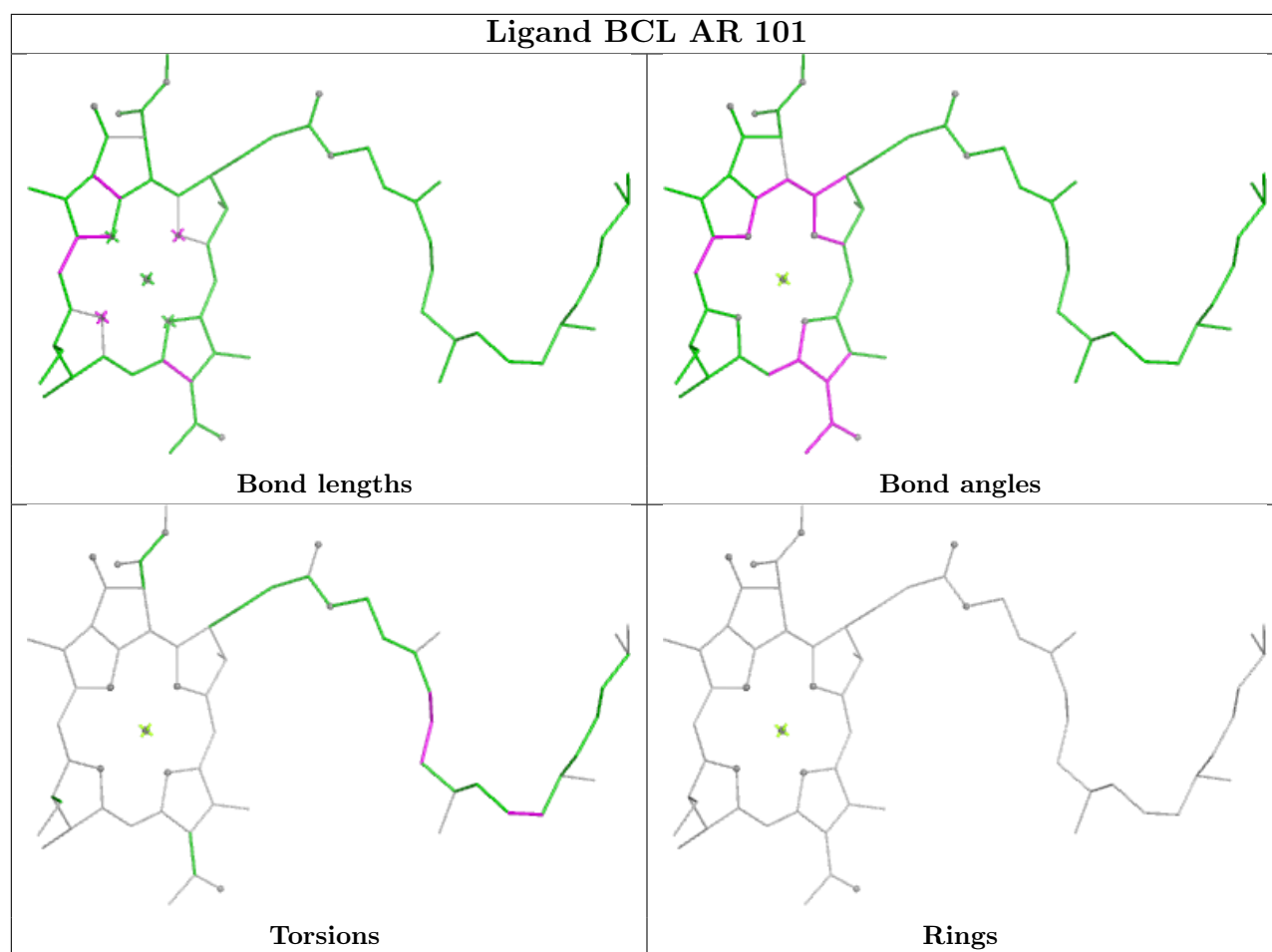




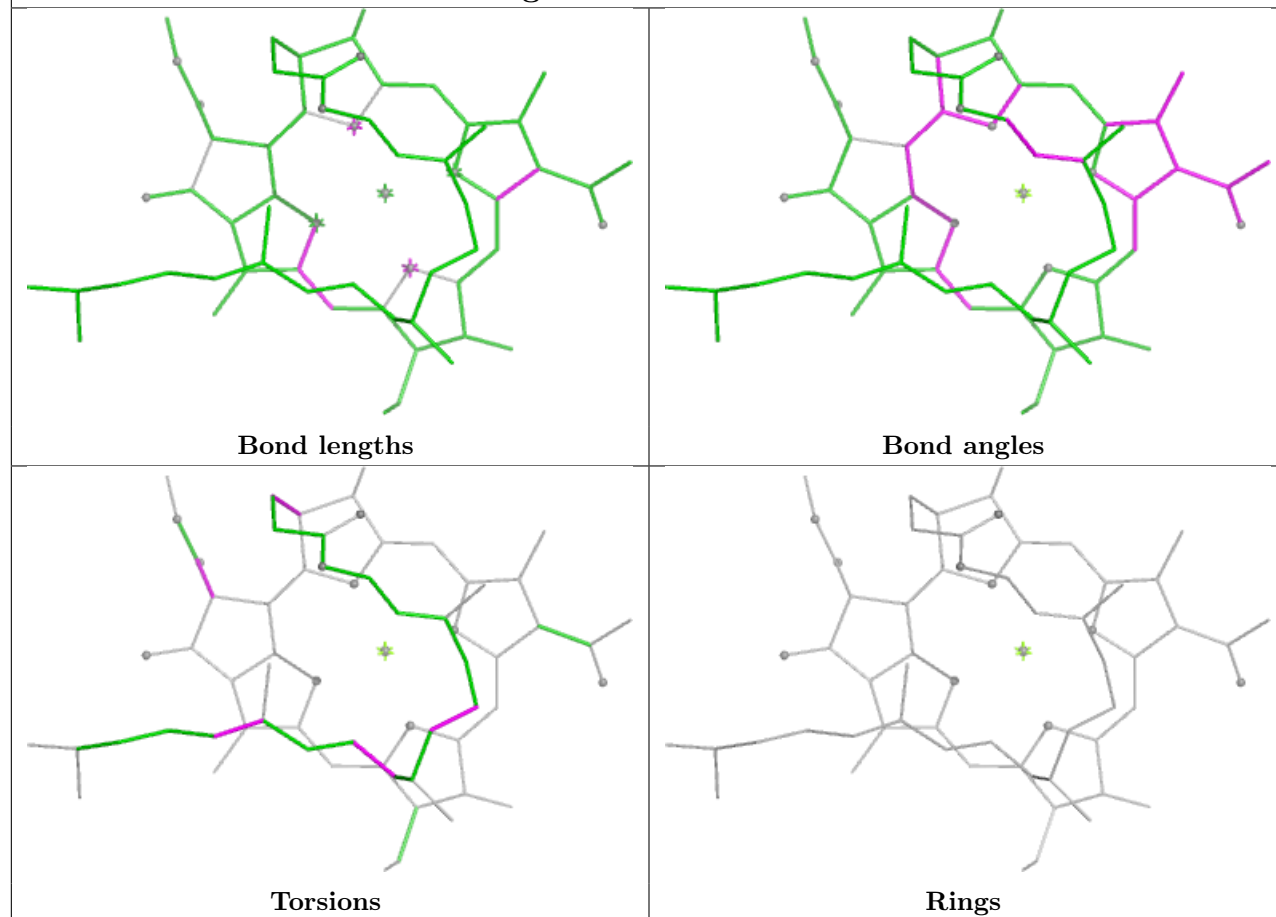




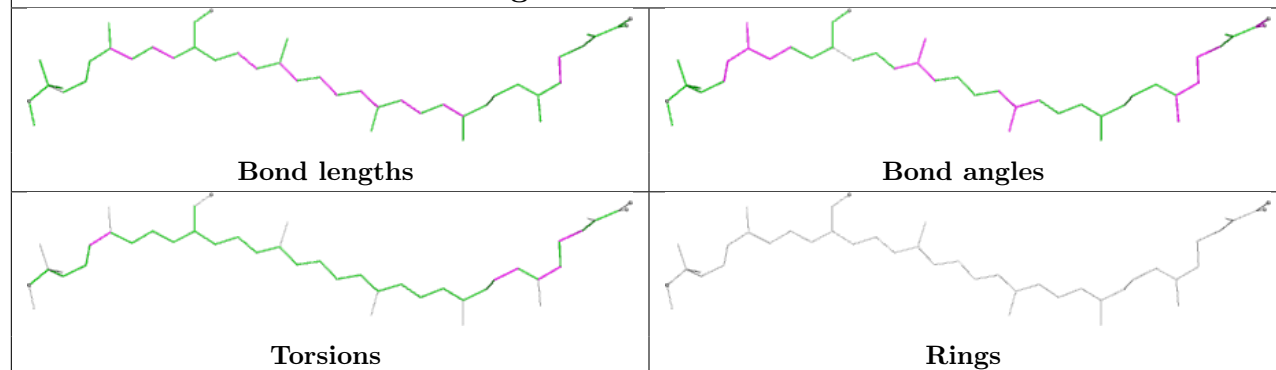


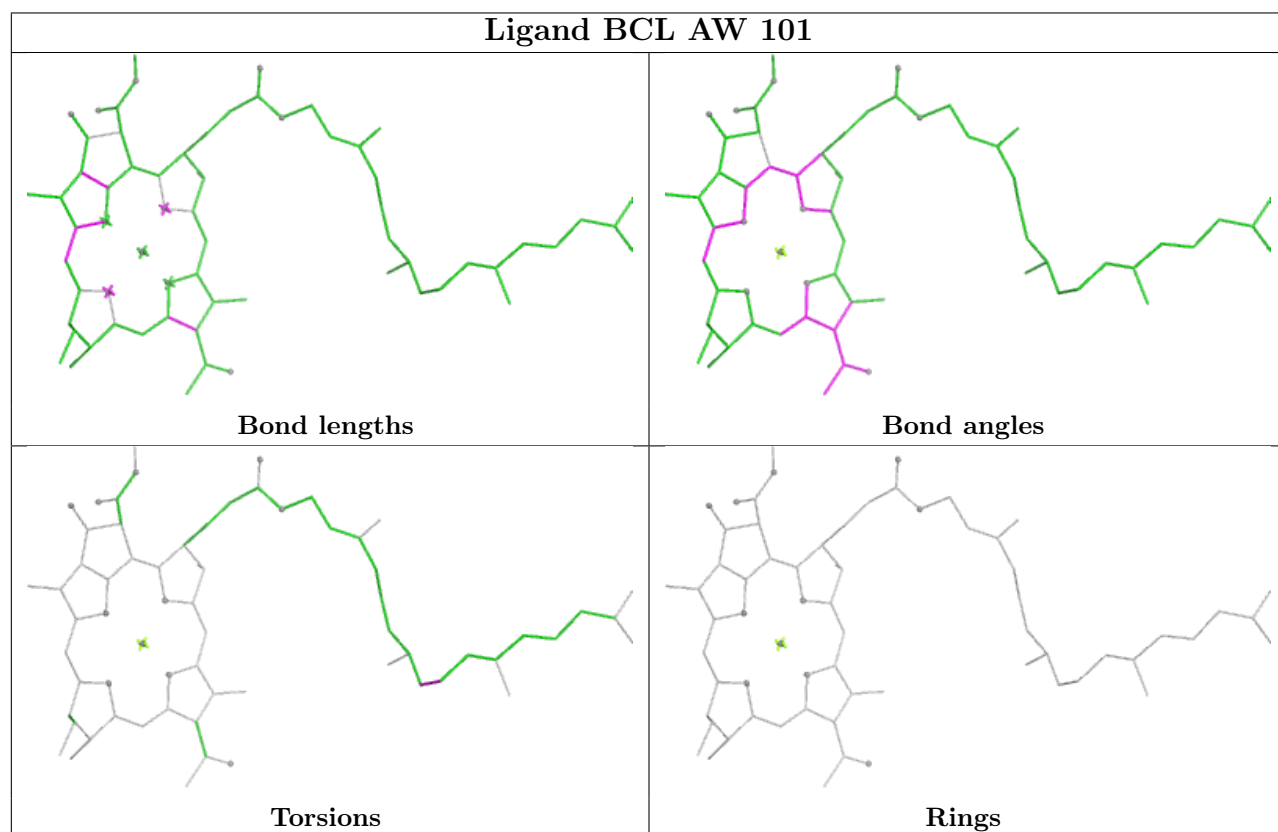
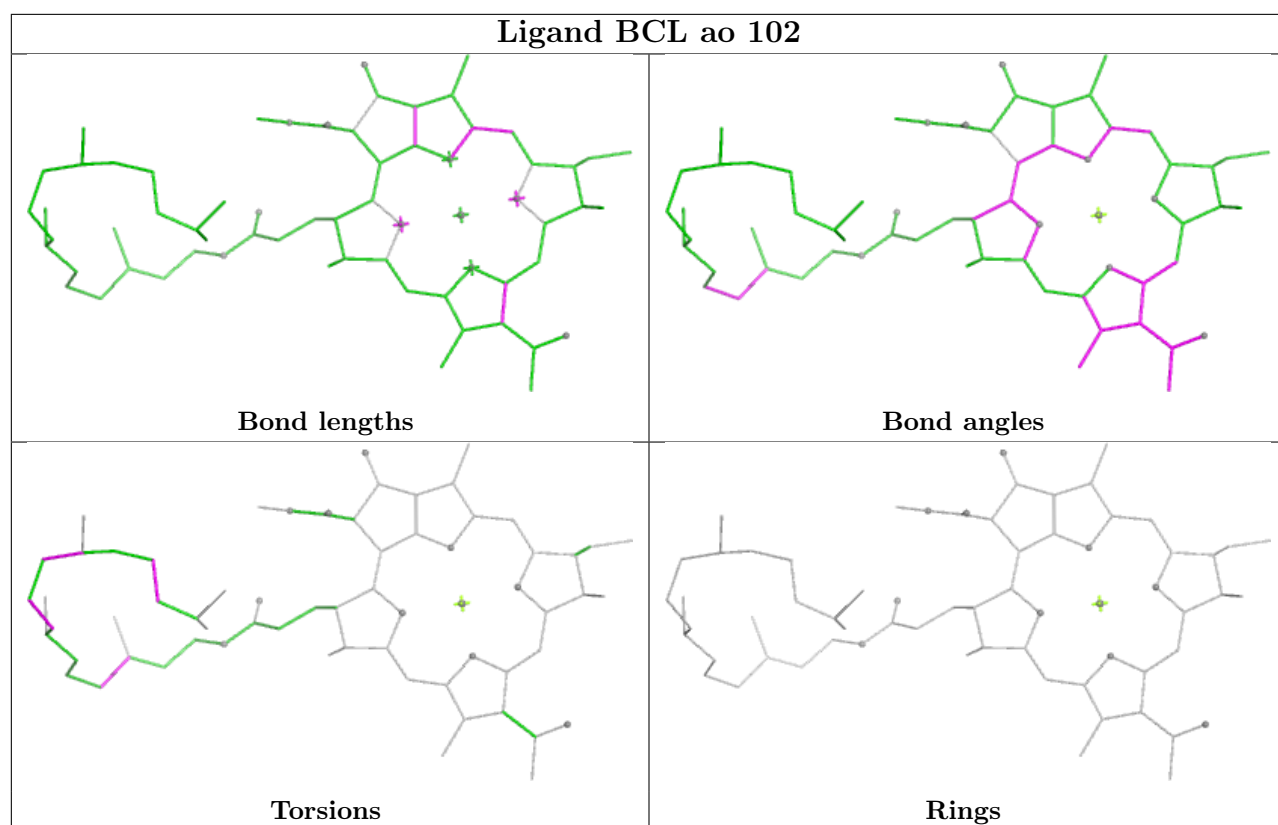


Ligand BCL AS 102

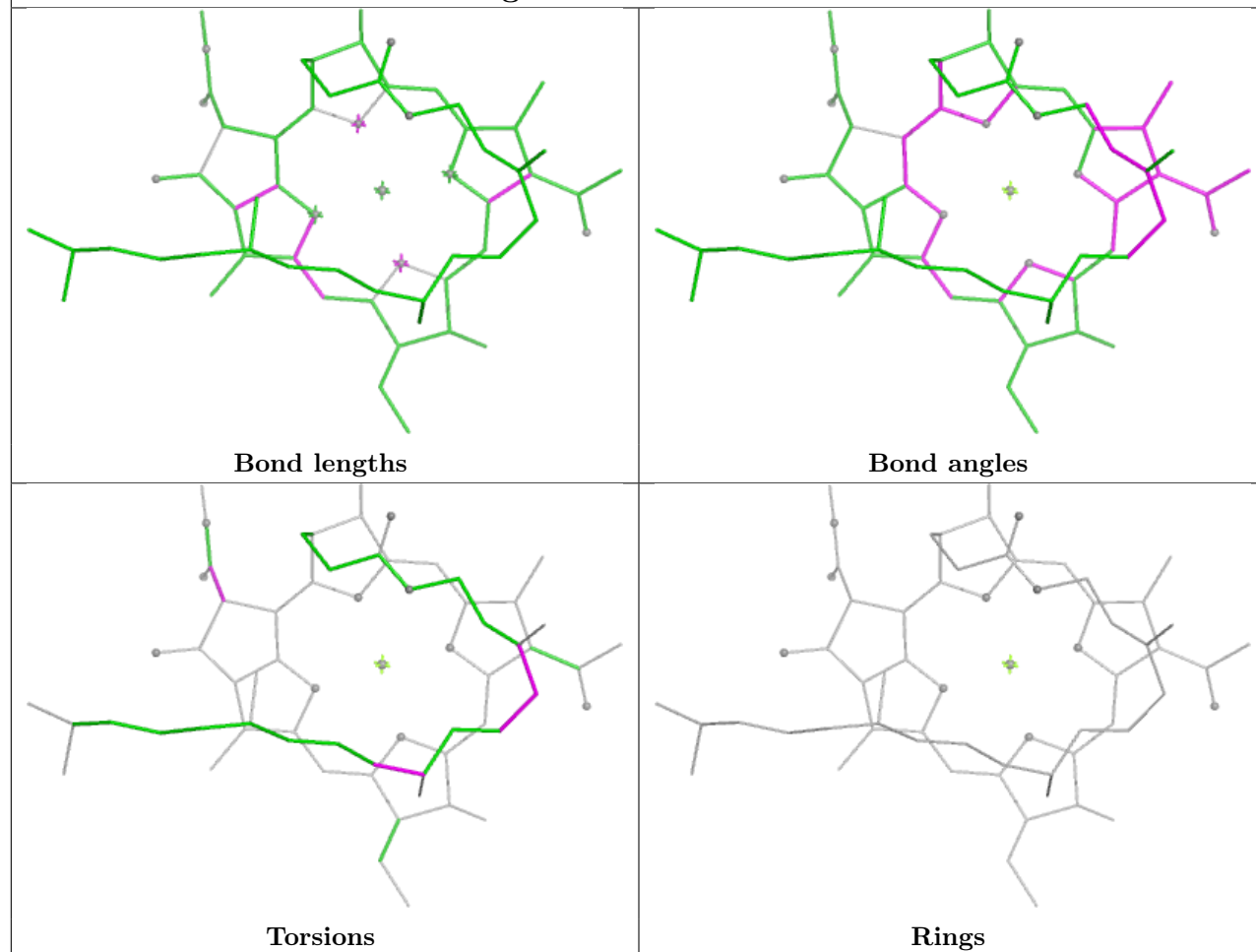


Ligand V7N BO 1001

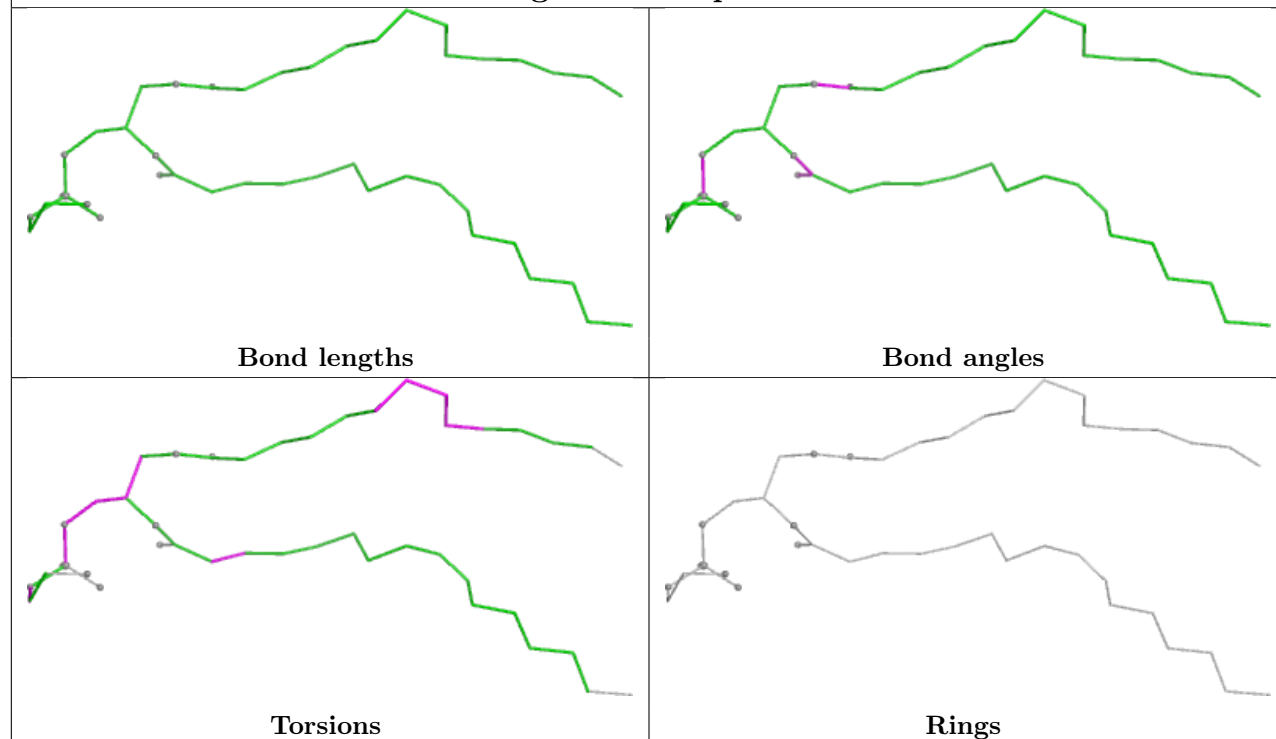


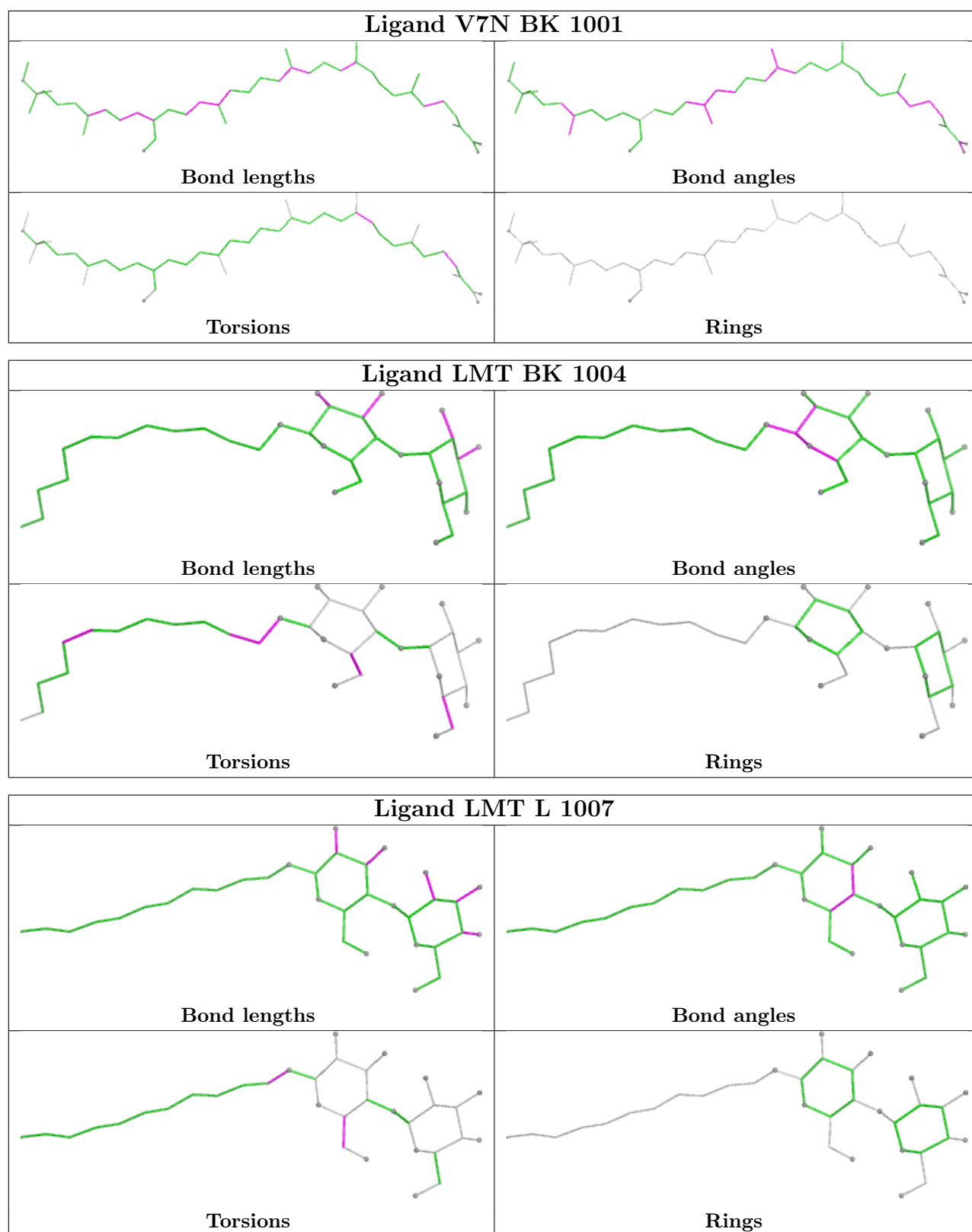


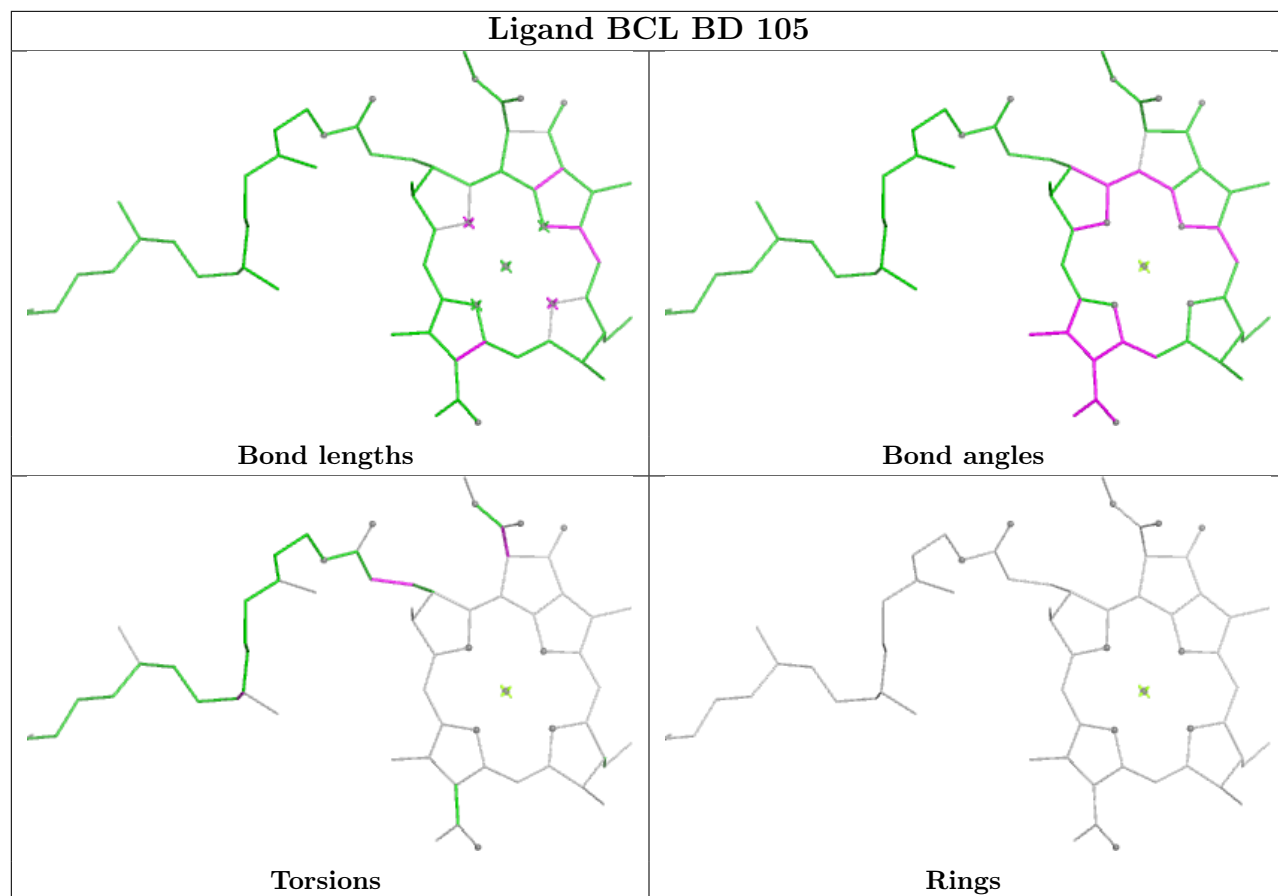
Ligand BCL AA 1002

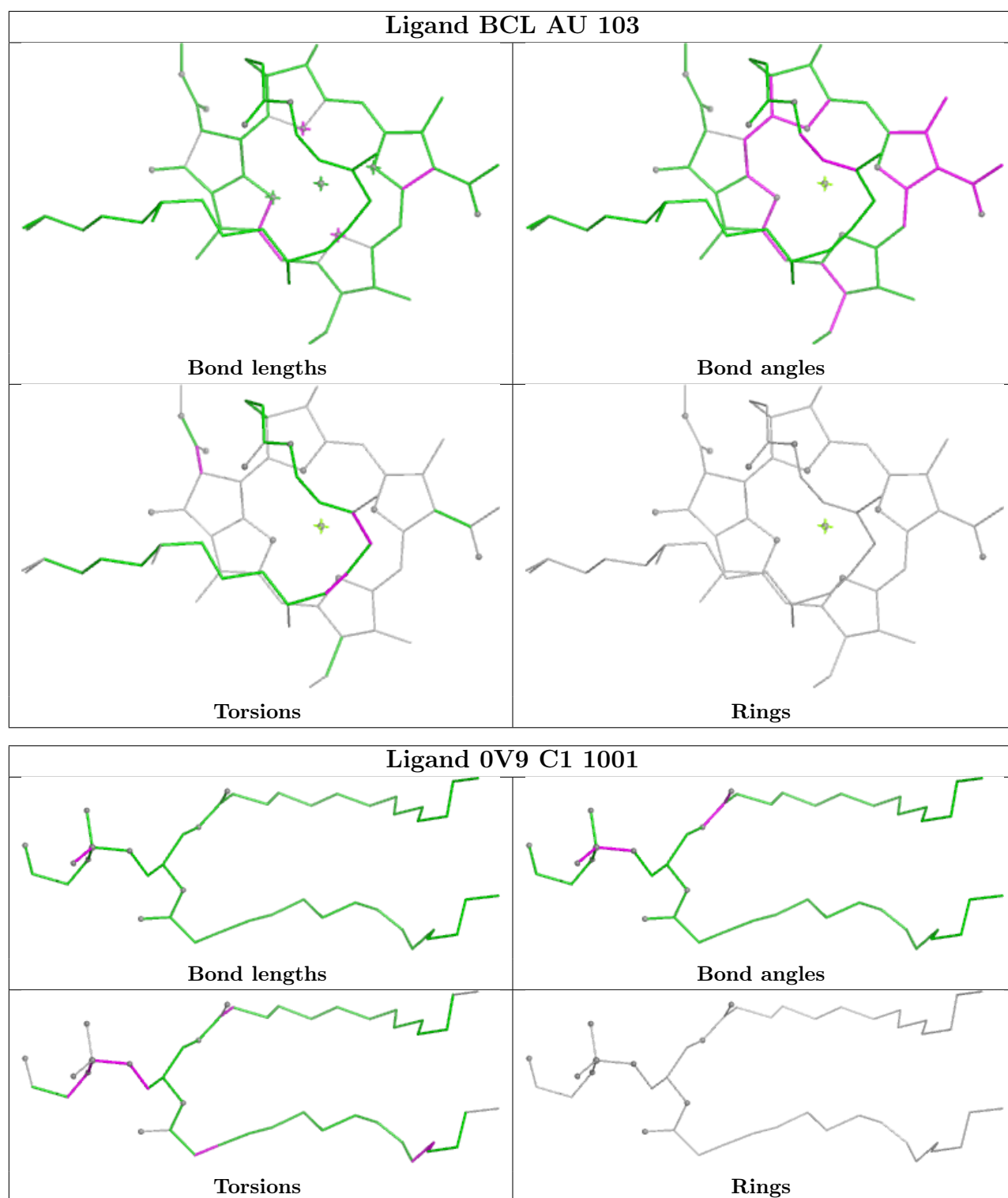


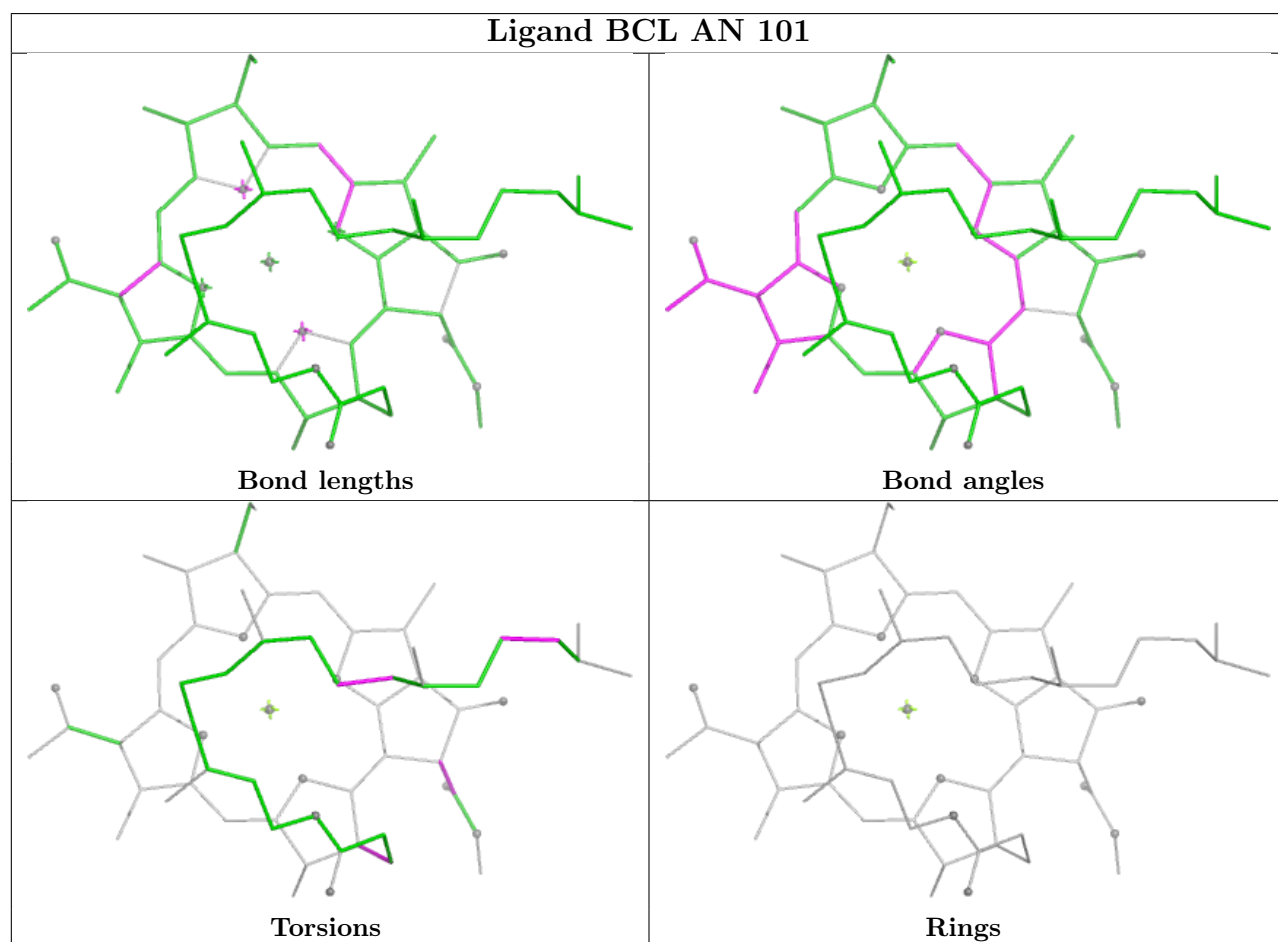
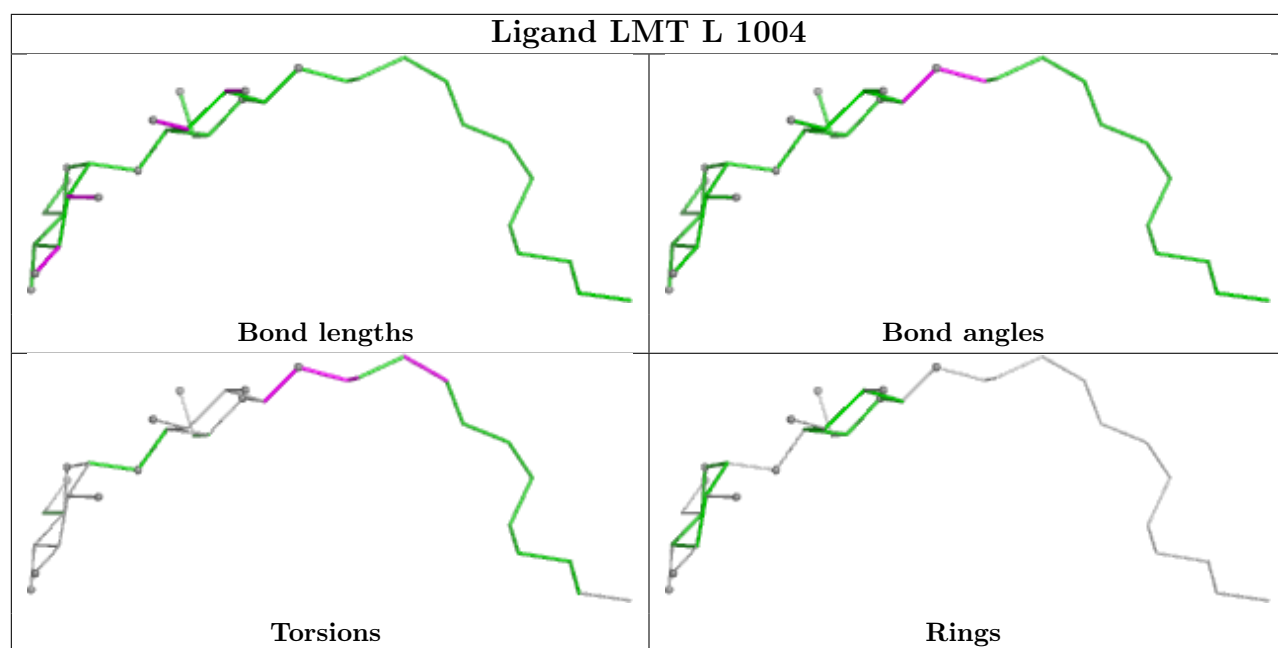
Ligand 0V9 bp 103



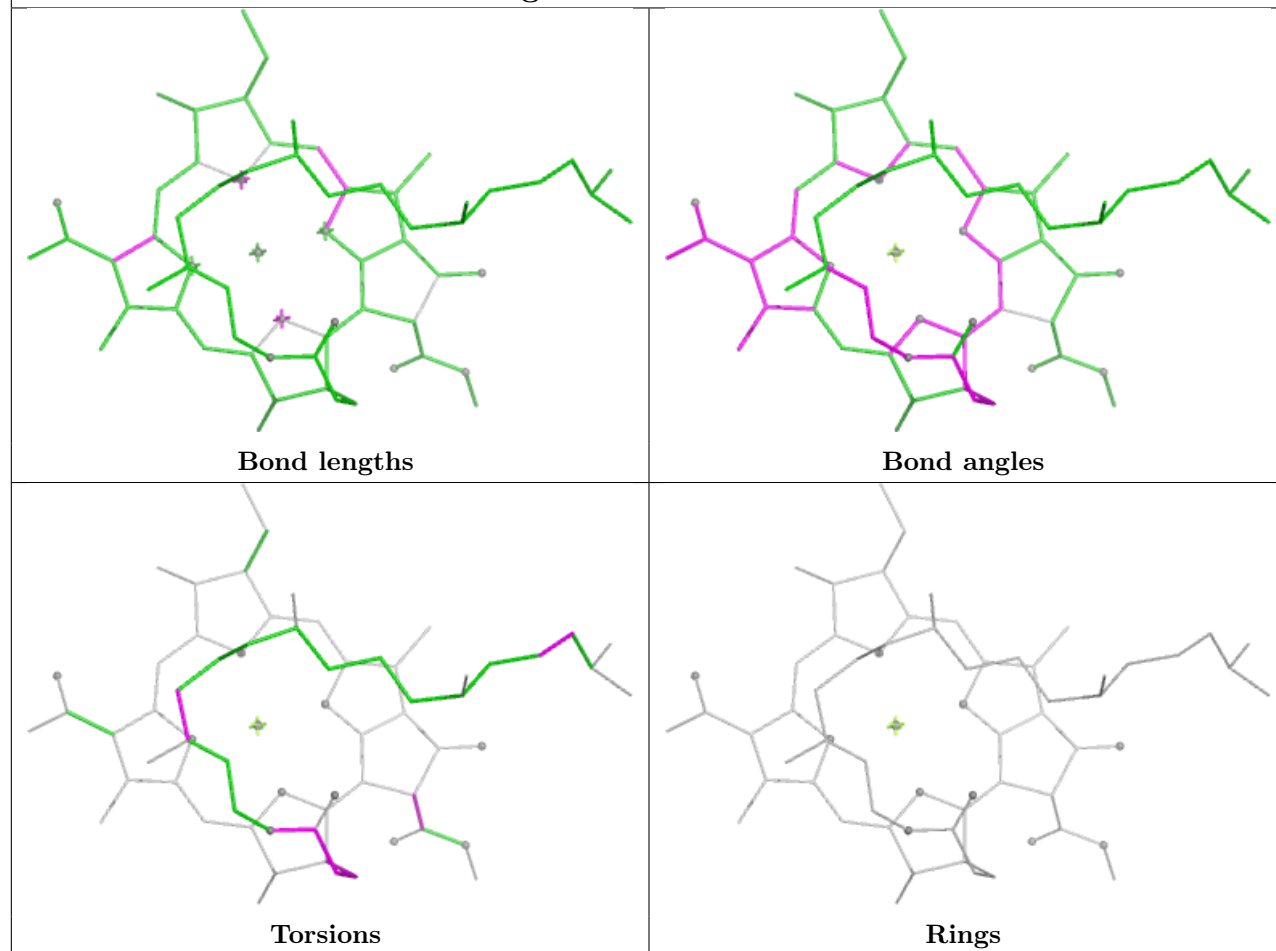




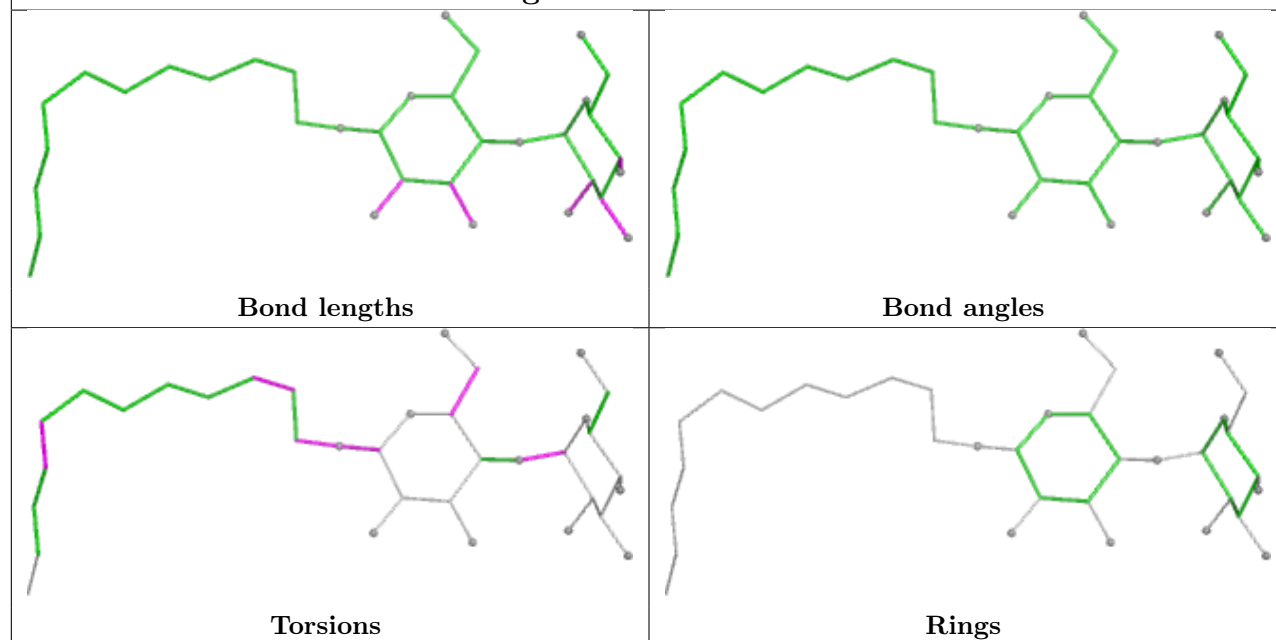


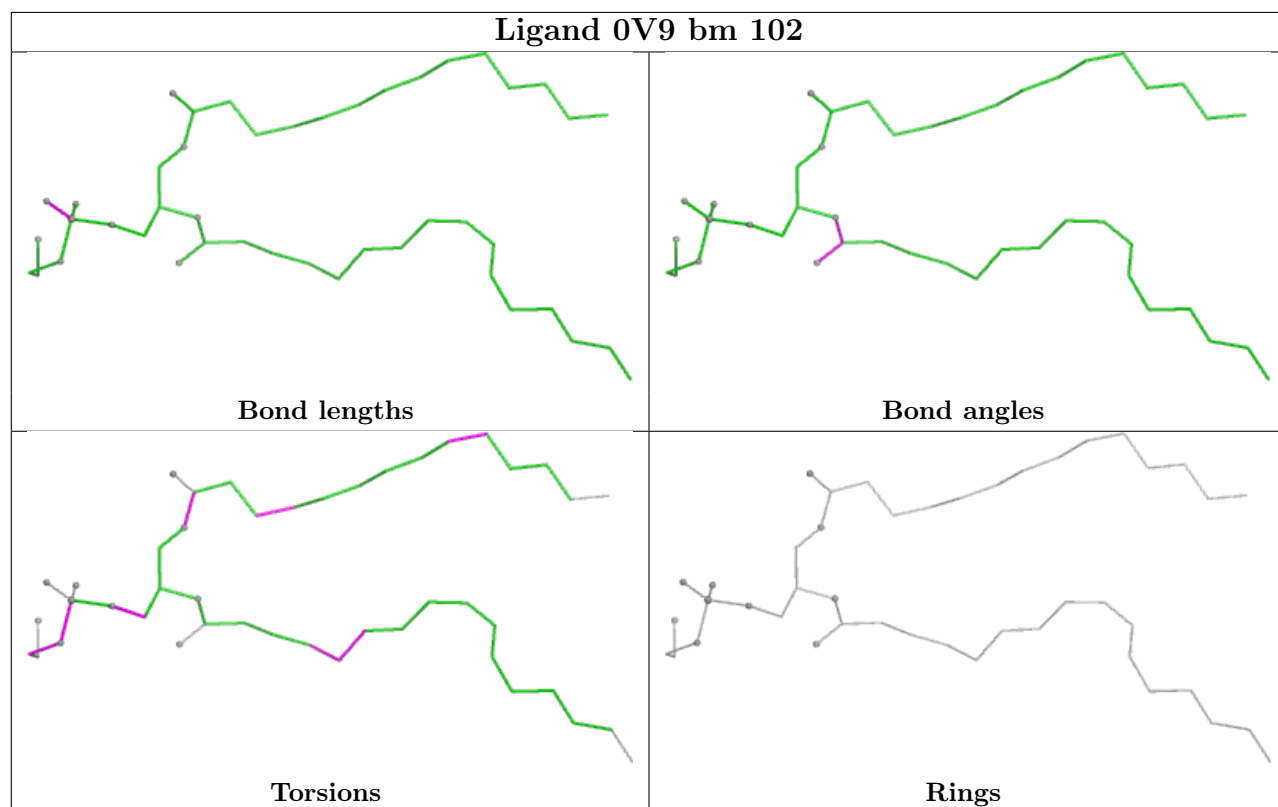
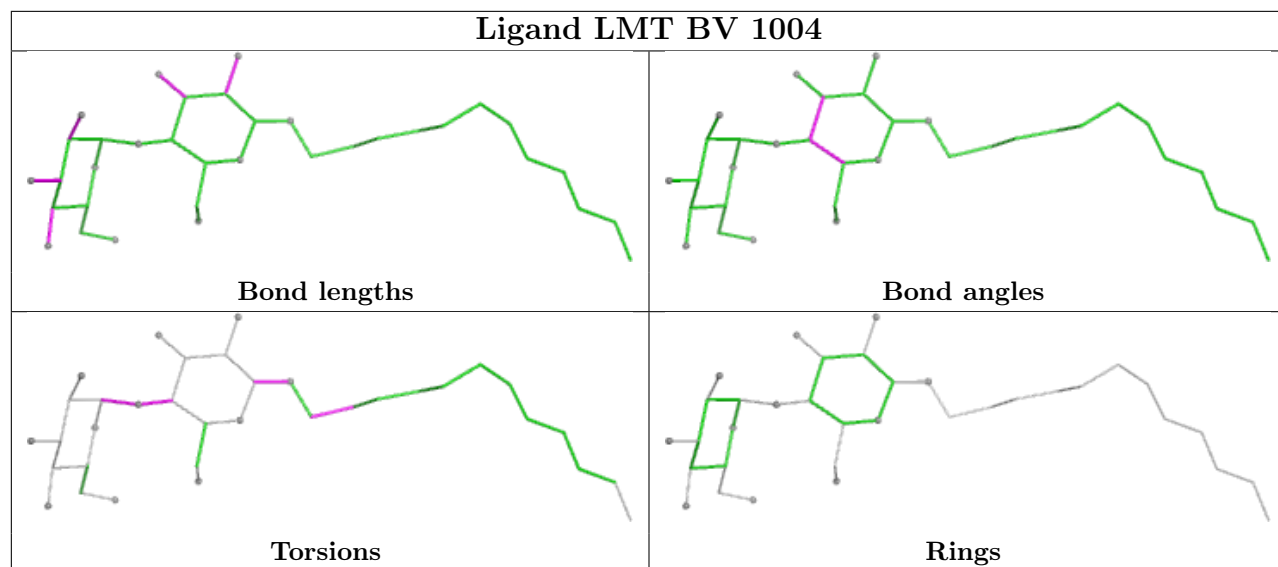


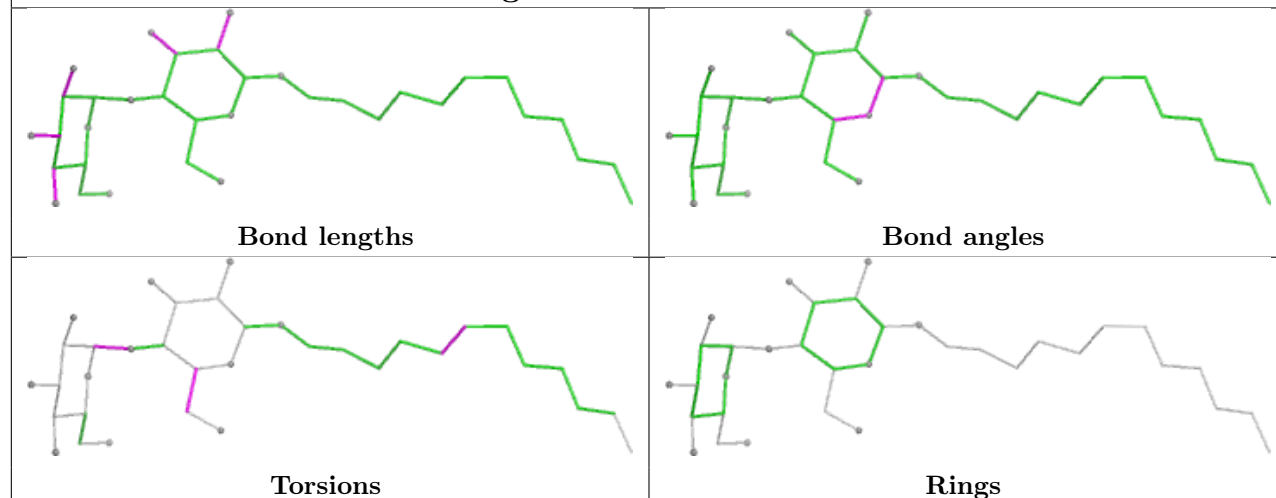
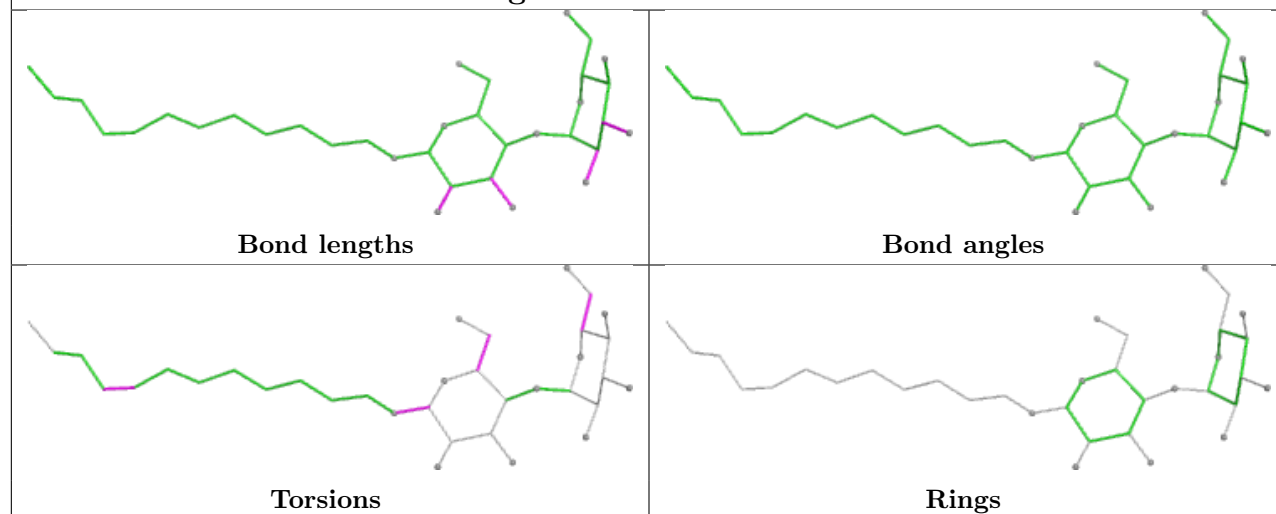
Ligand BCL AL 101

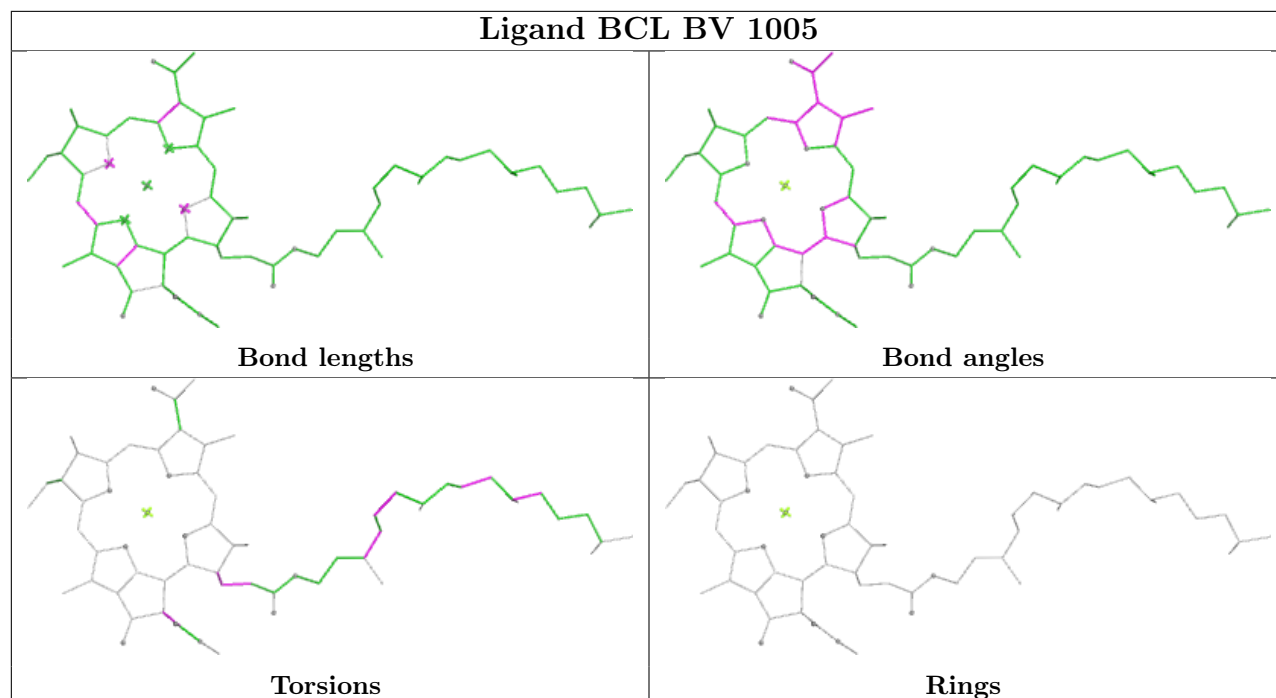
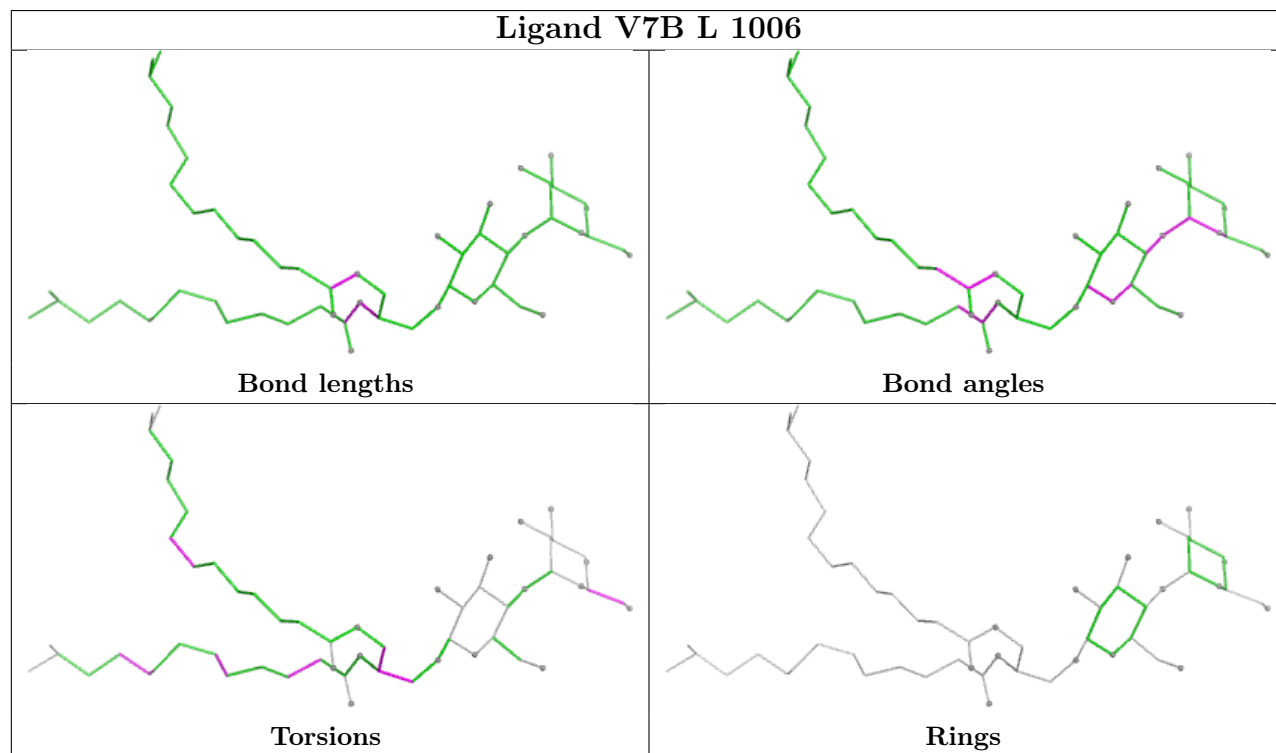


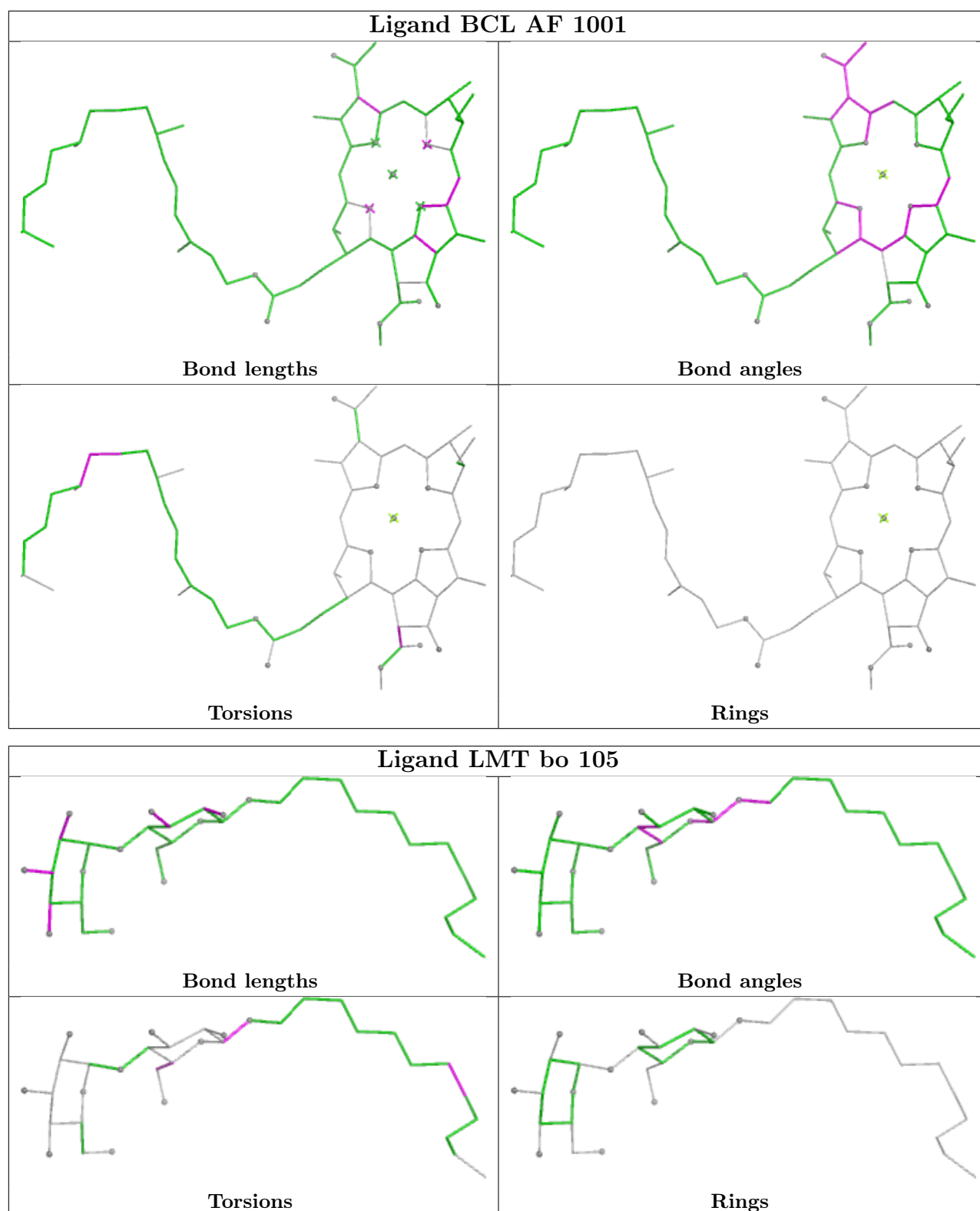
Ligand LMT L 1003

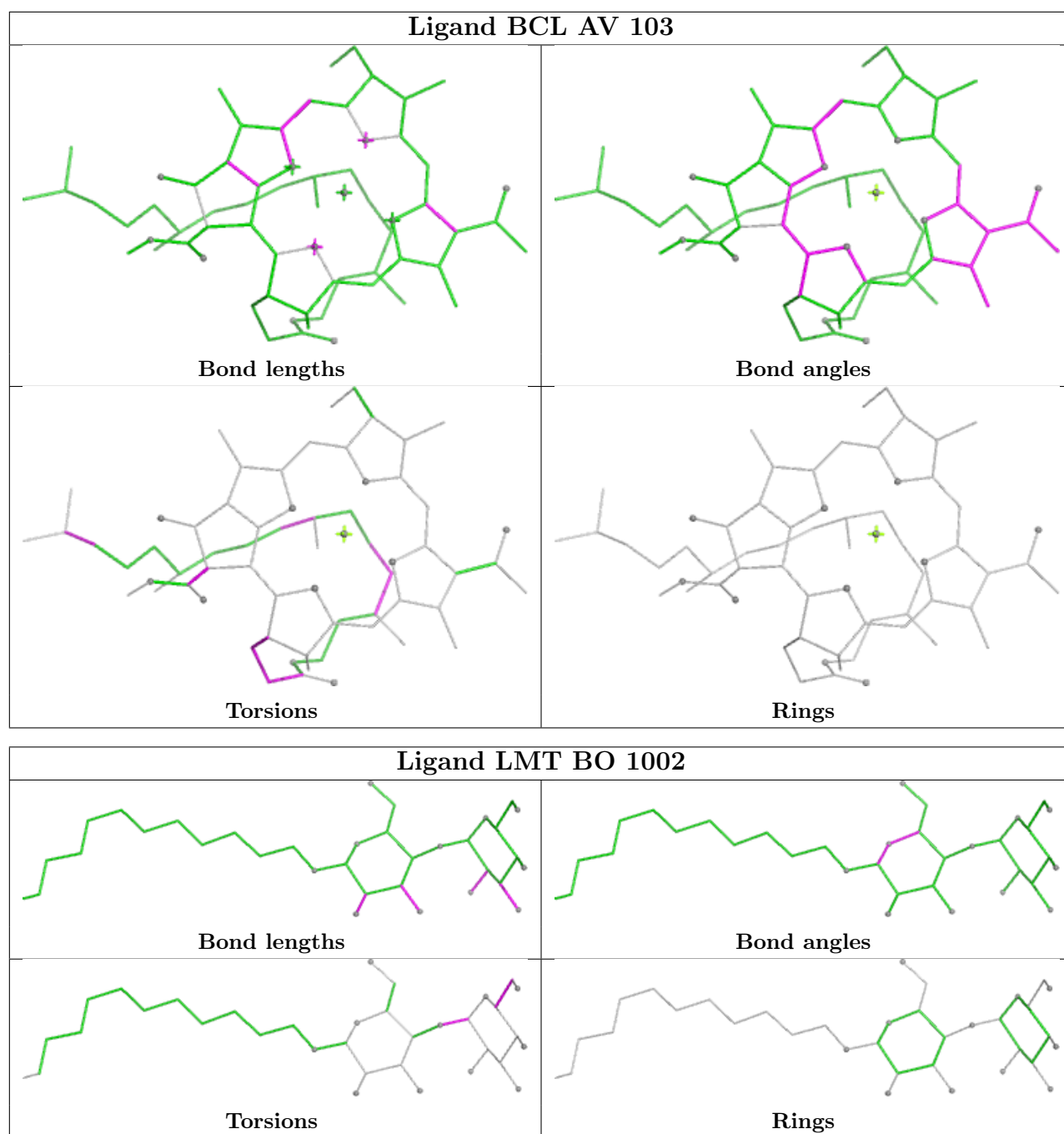


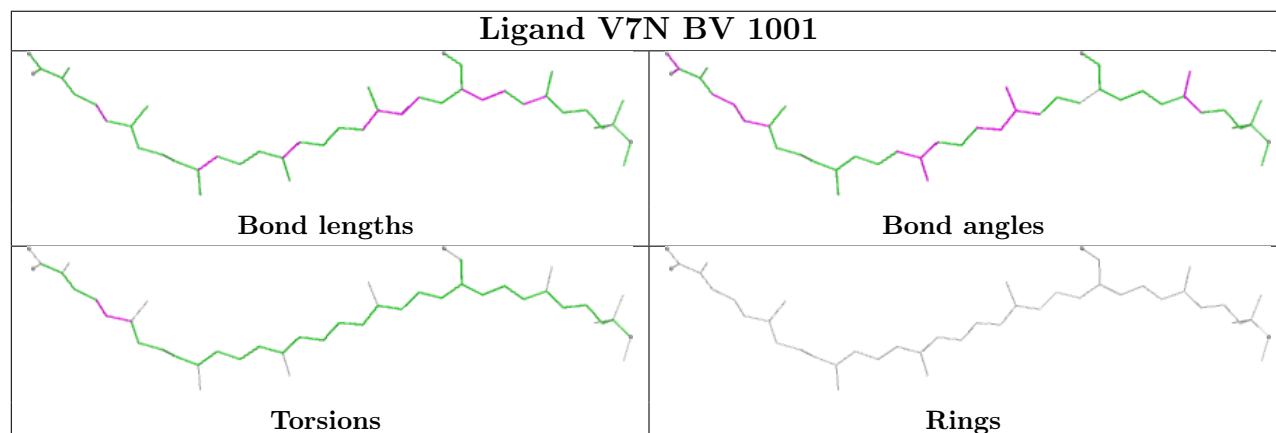
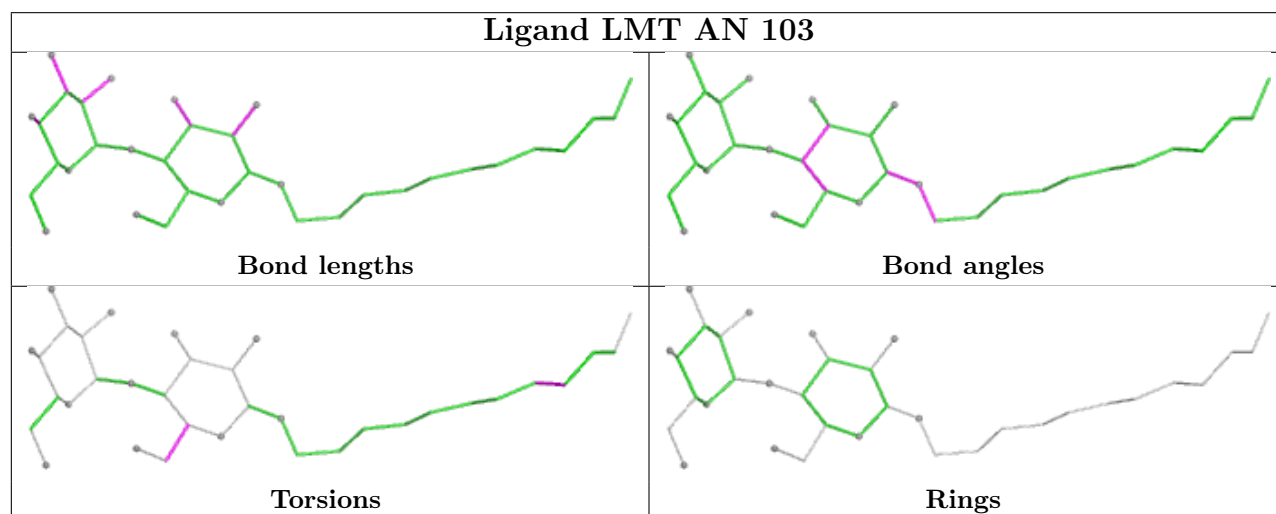
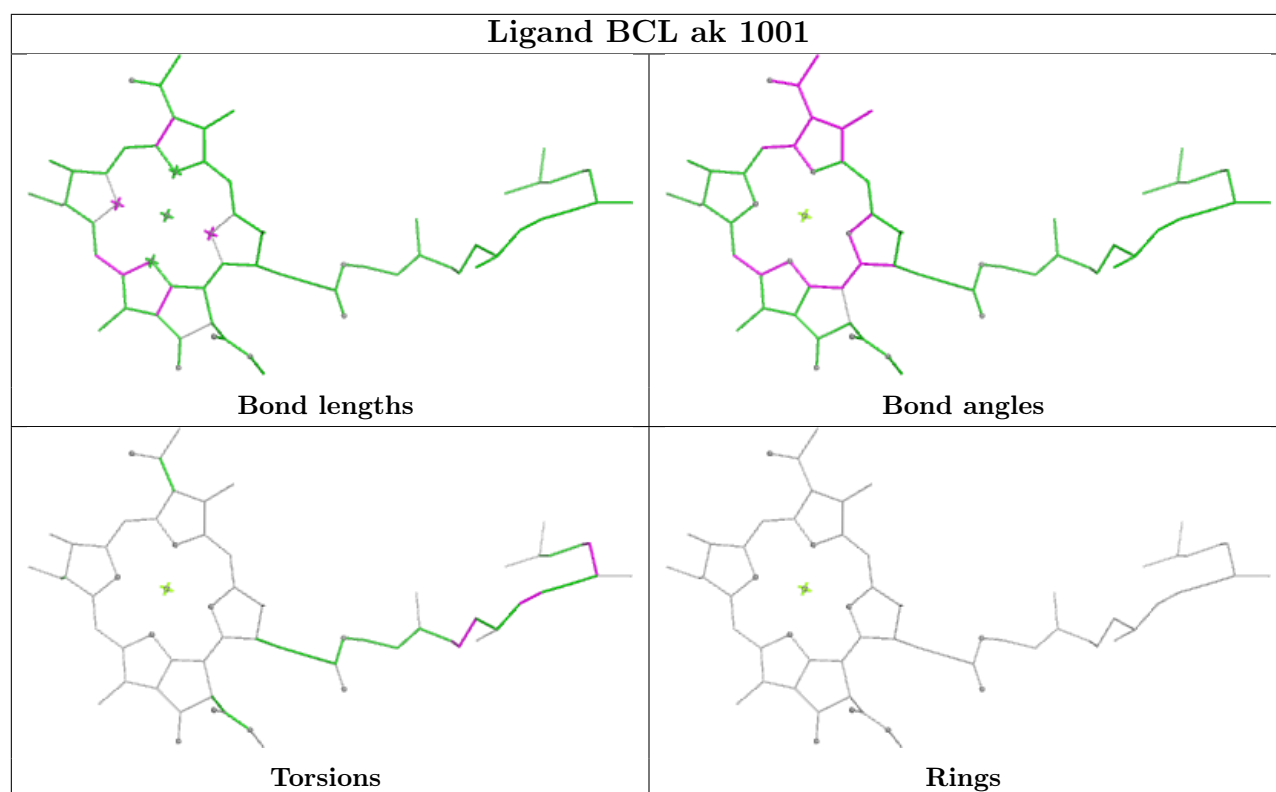


Ligand LMT BW 1004**Ligand LMT AF 1002**

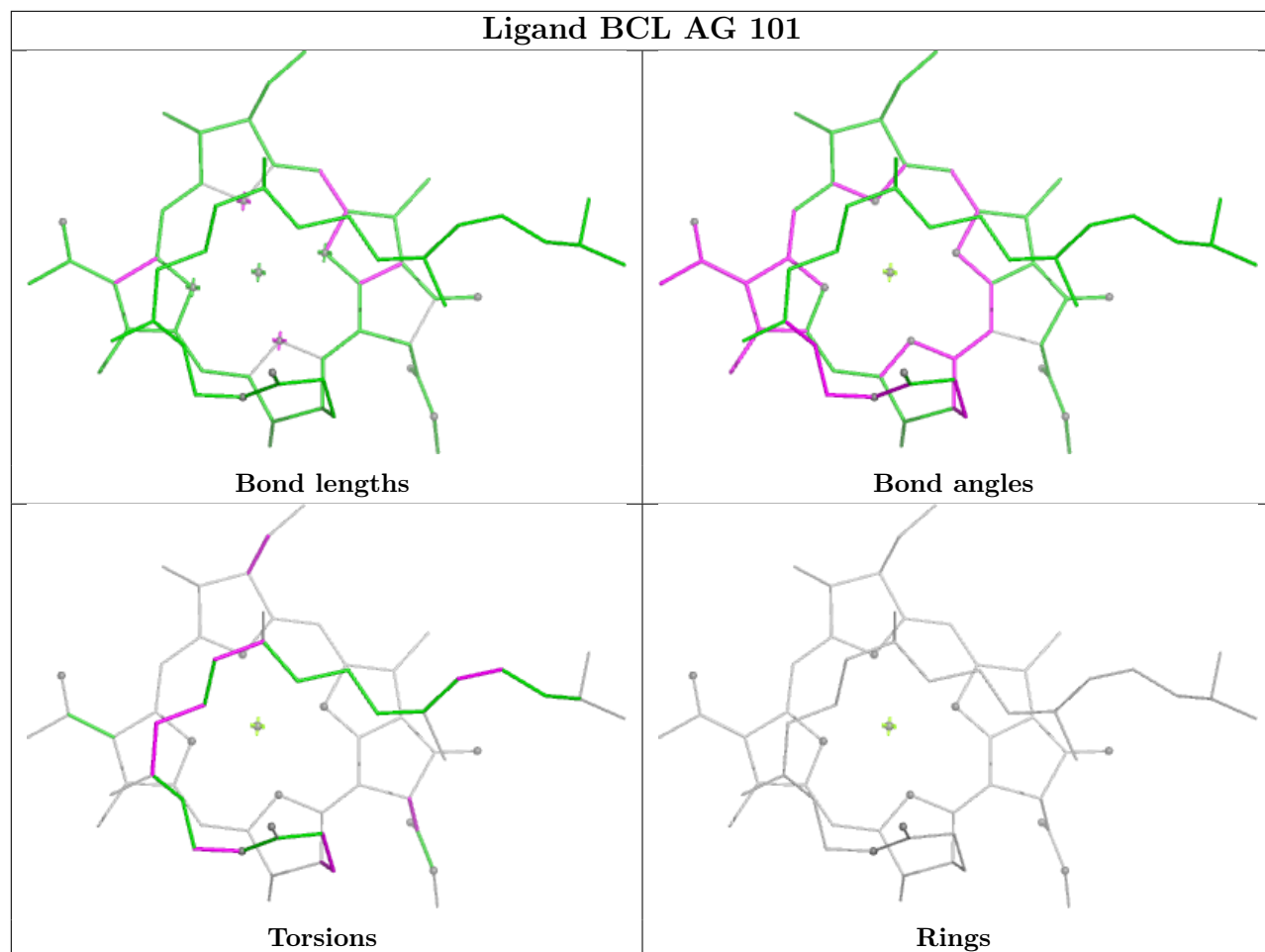
Ligand BCL BV 1005**Ligand V7B L 1006**



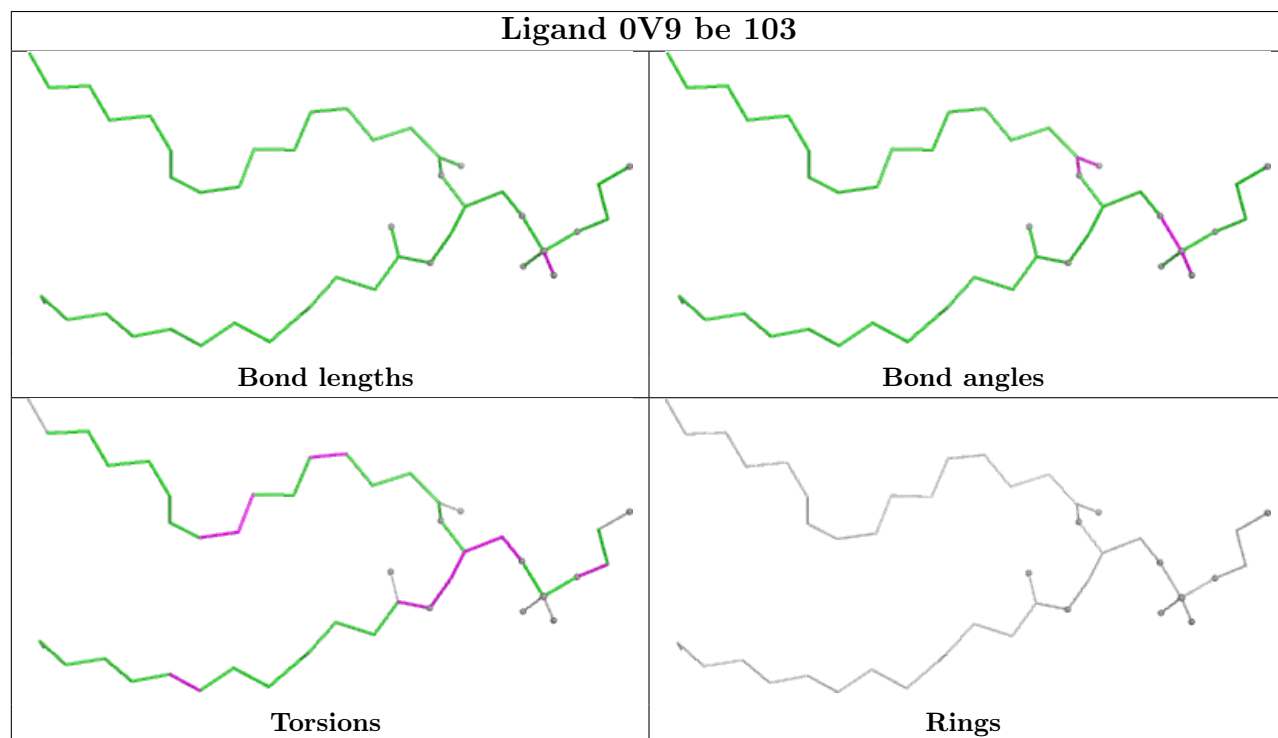


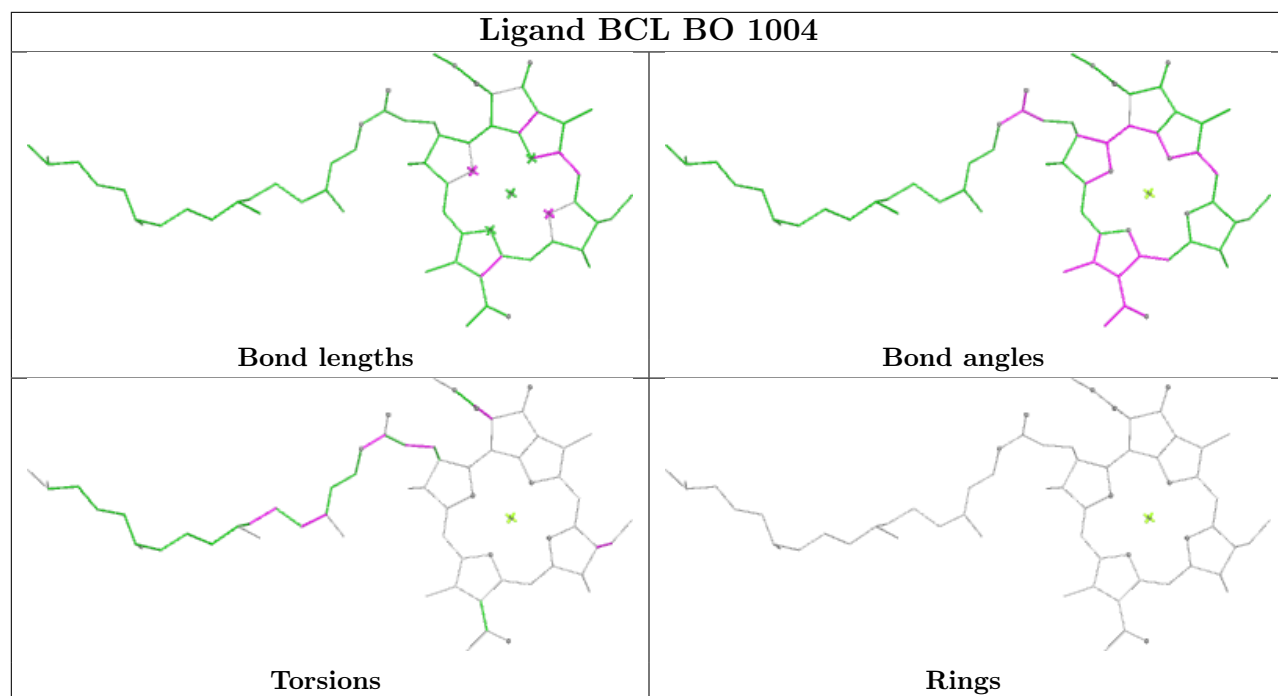
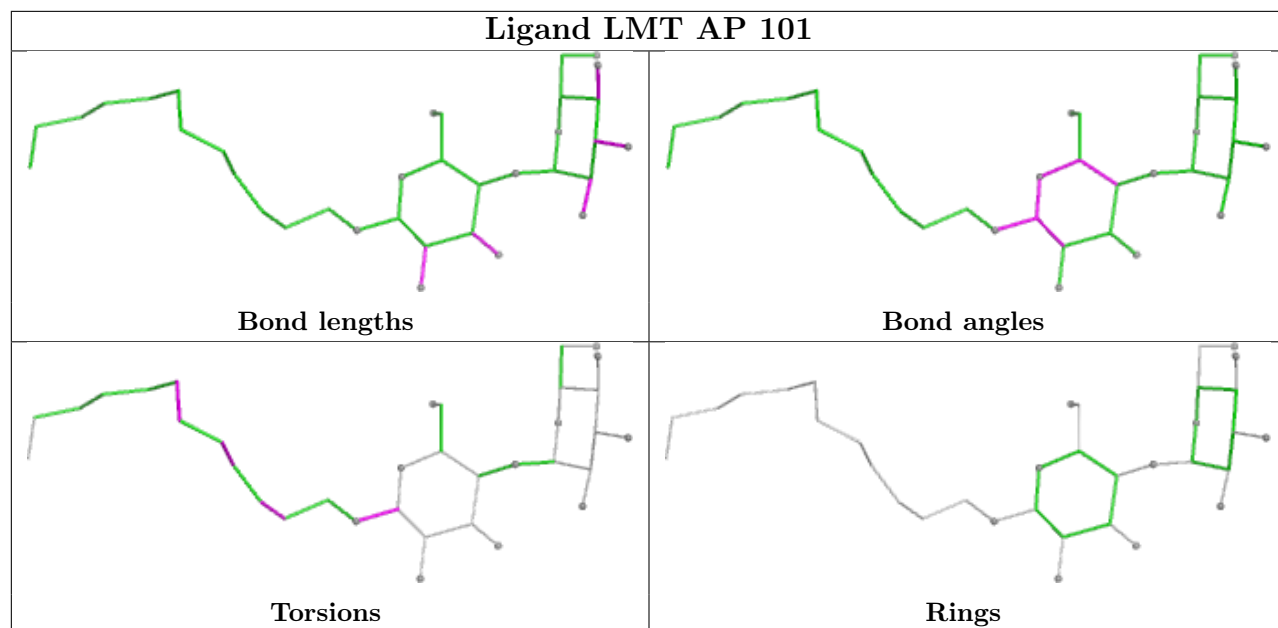


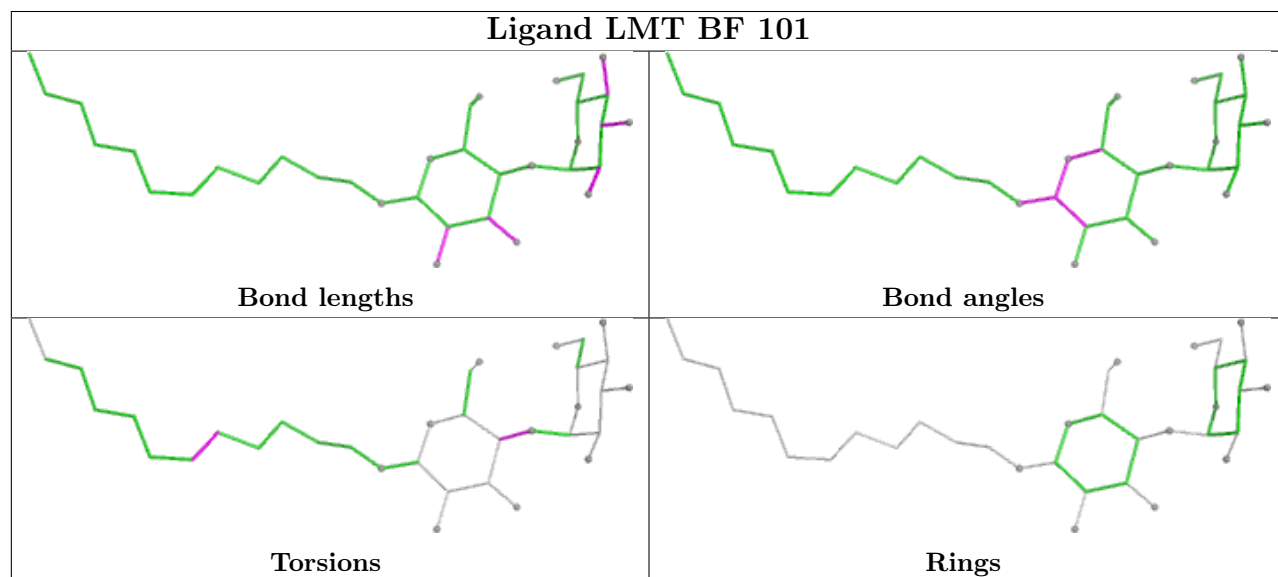
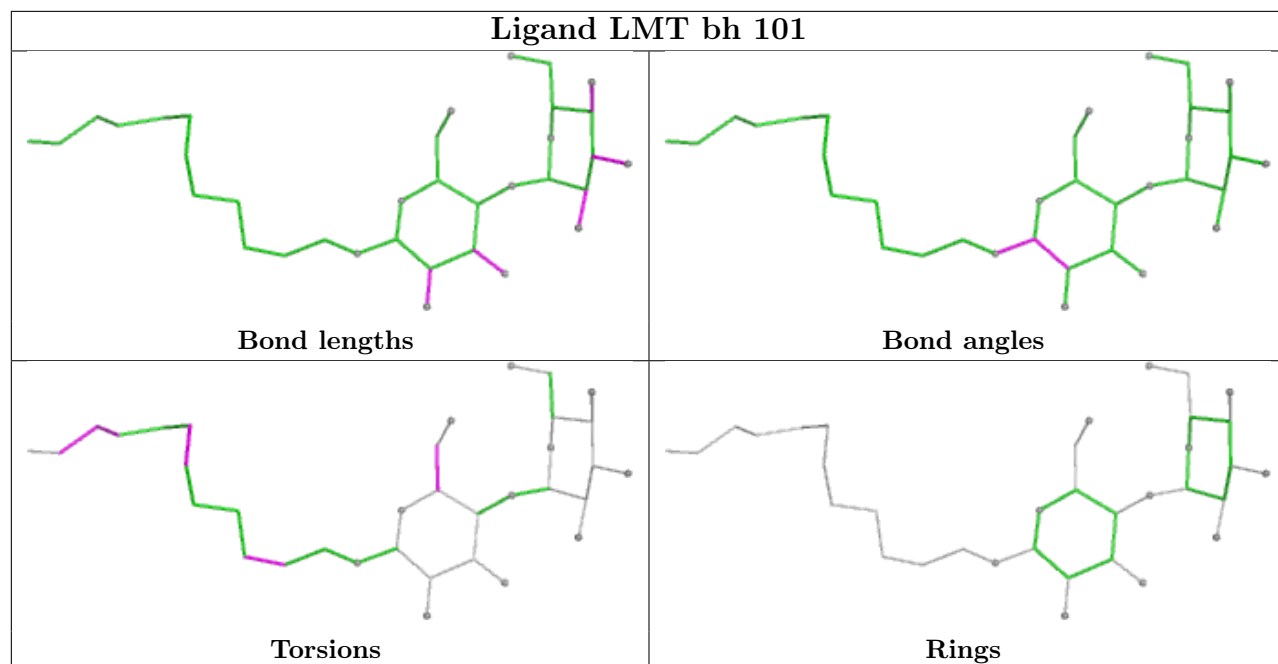
Ligand BCL AG 101

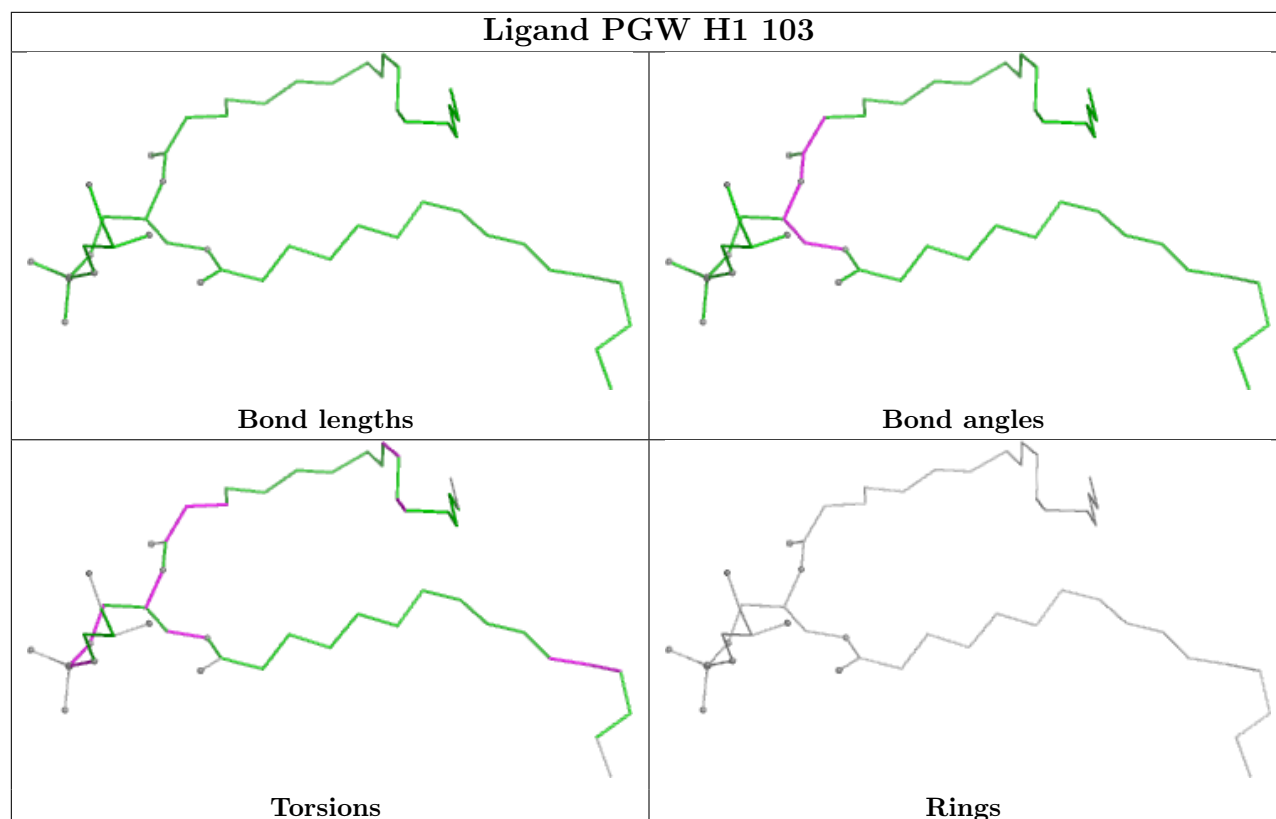
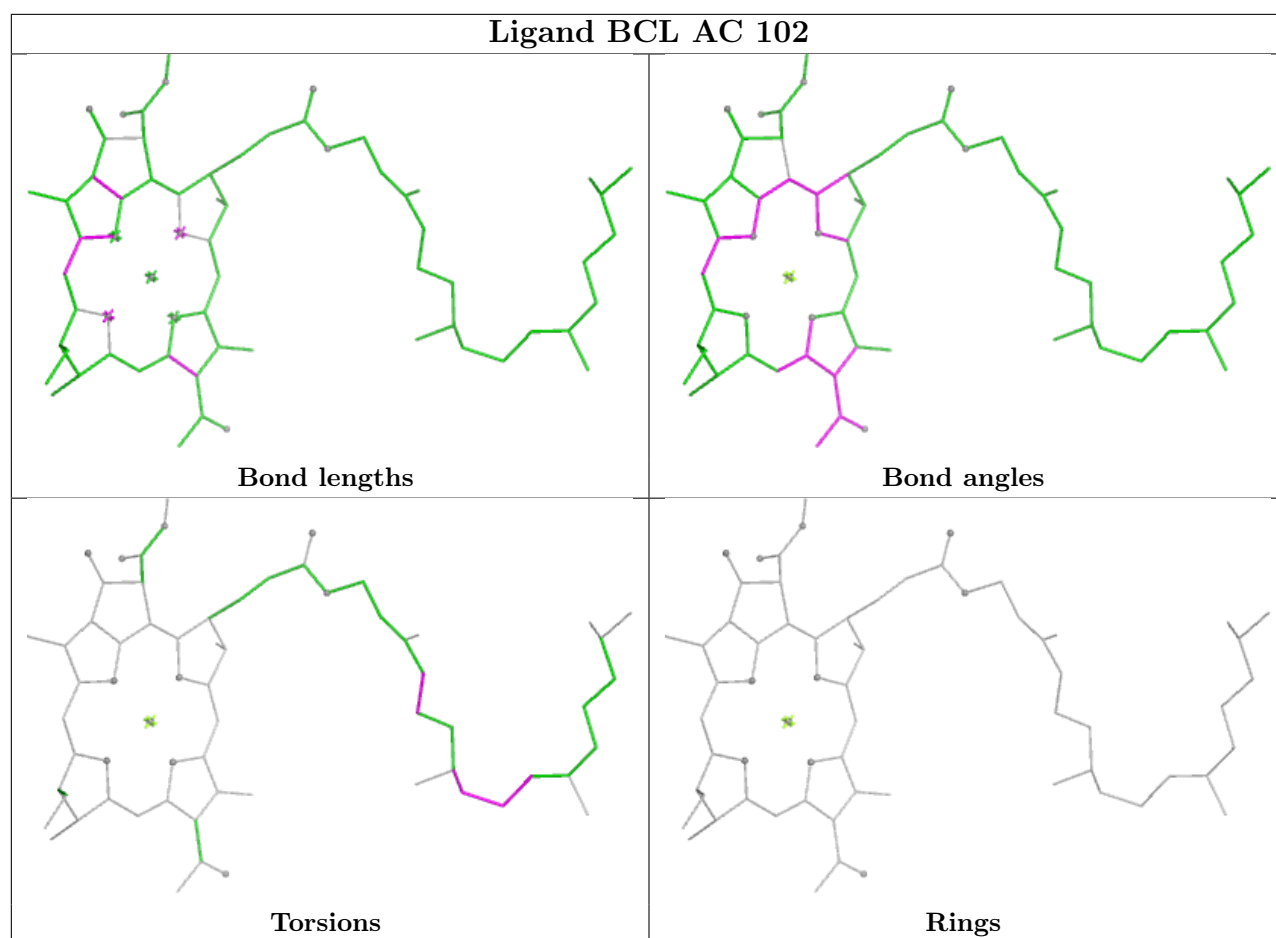


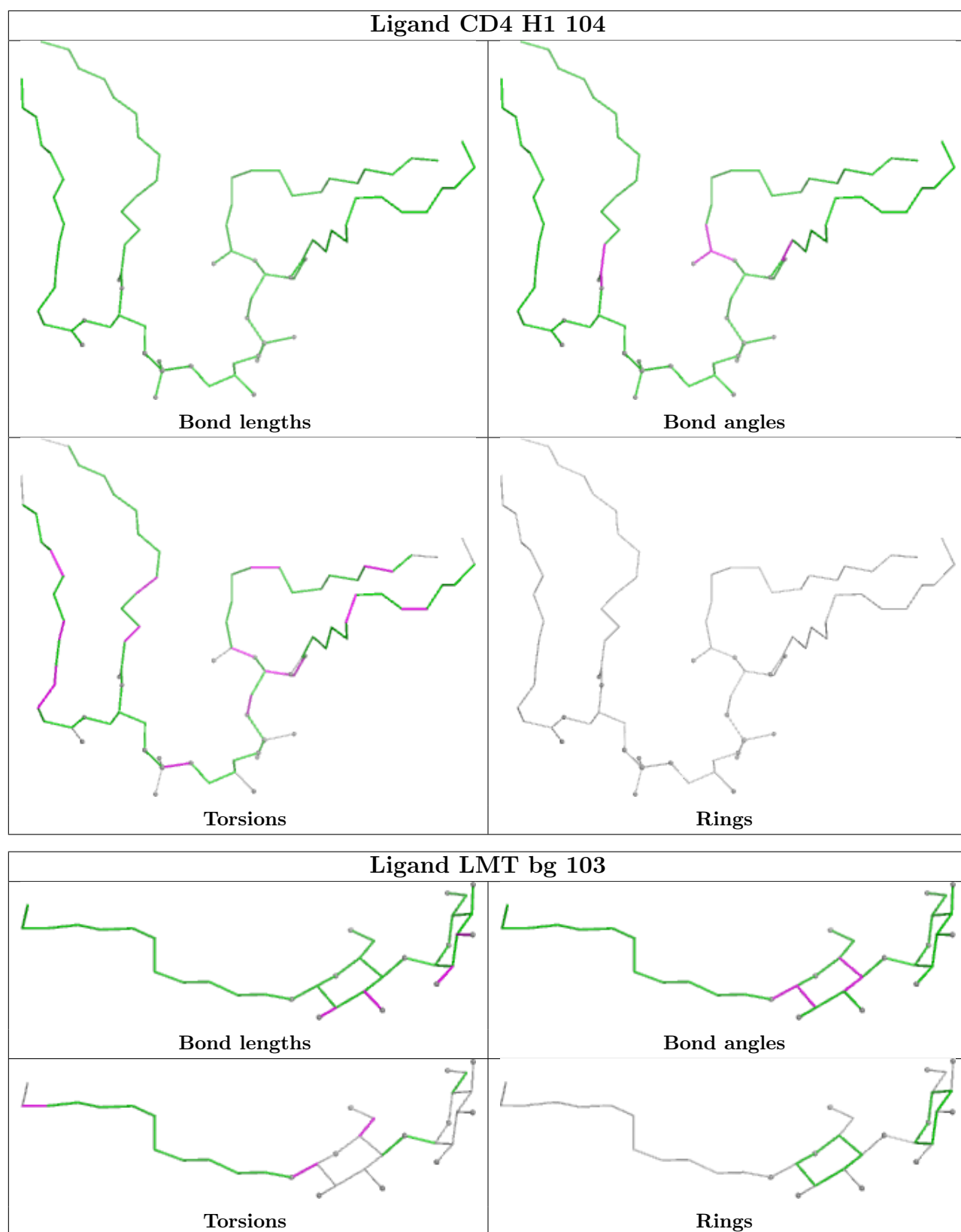
Ligand 0V9 be 103

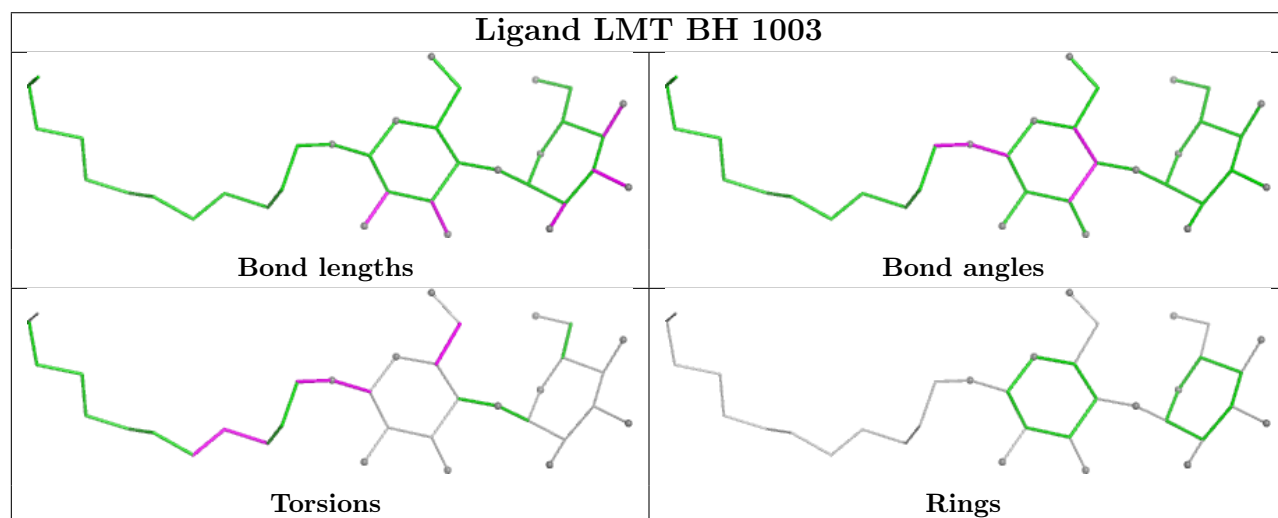
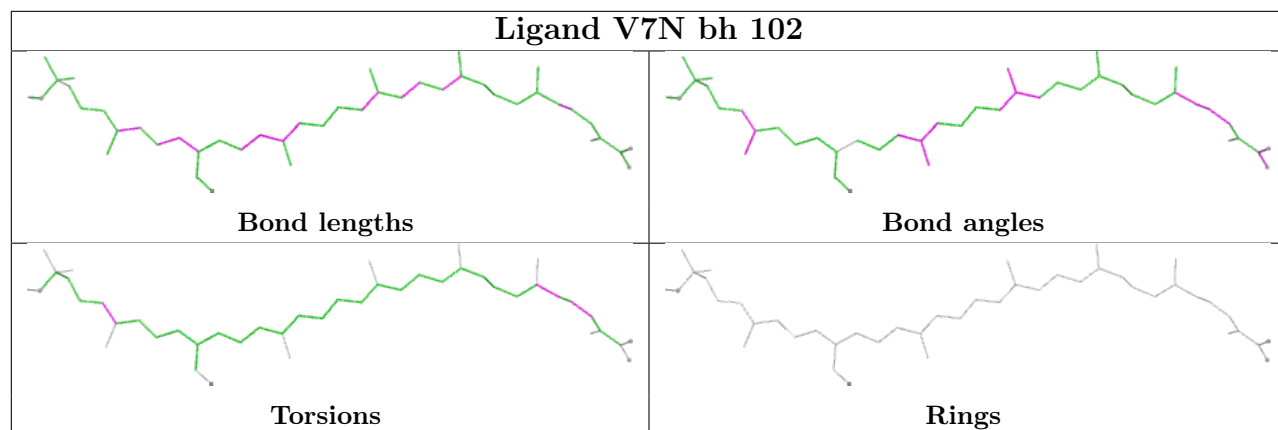




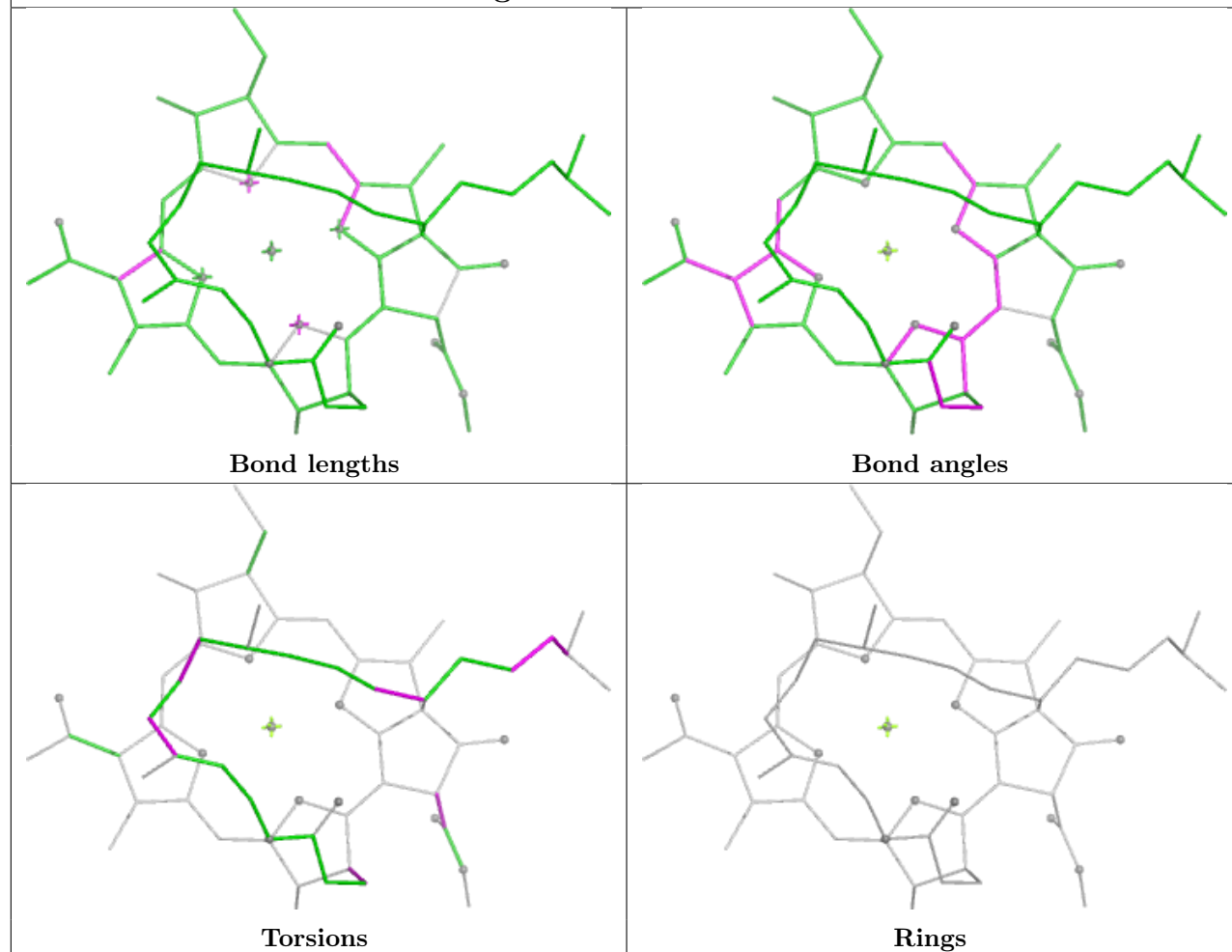




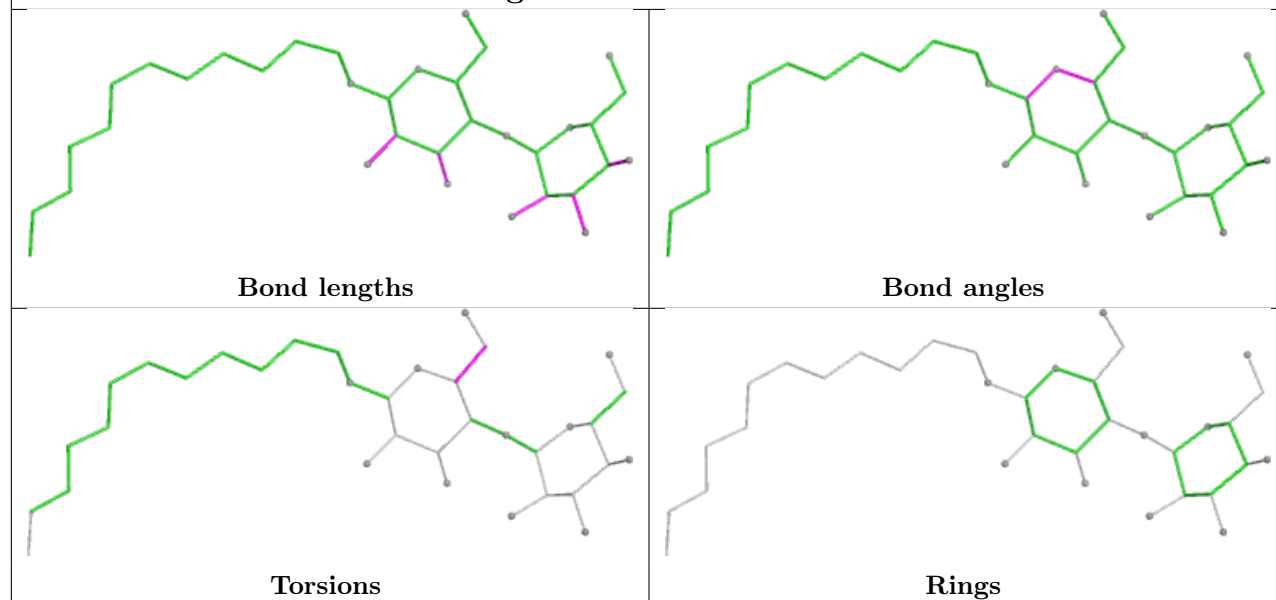


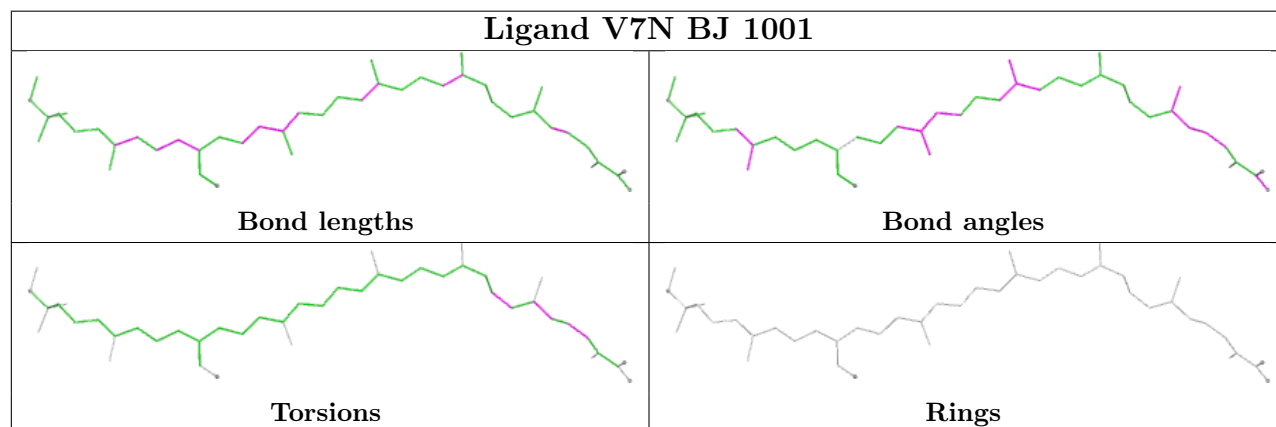
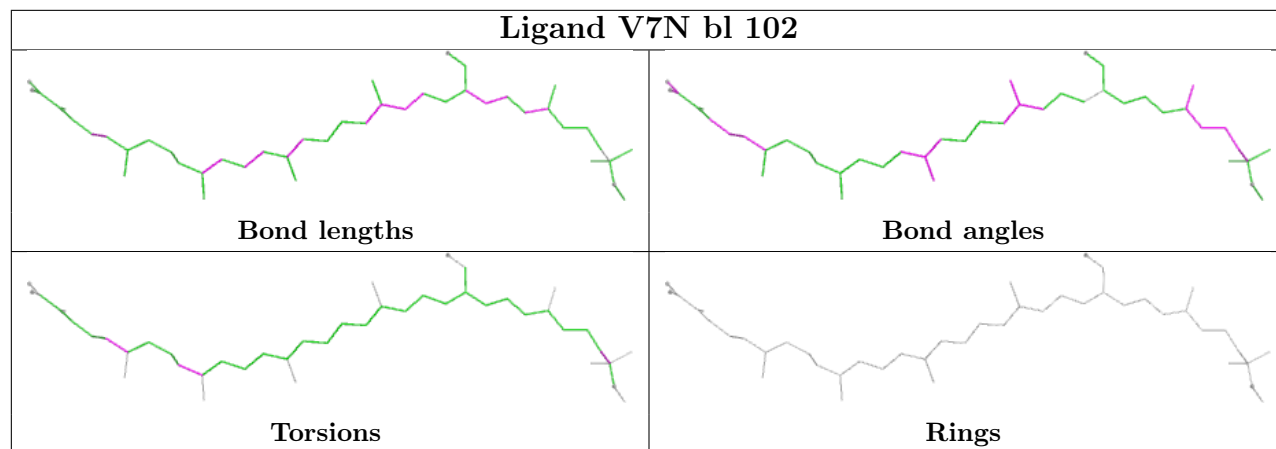
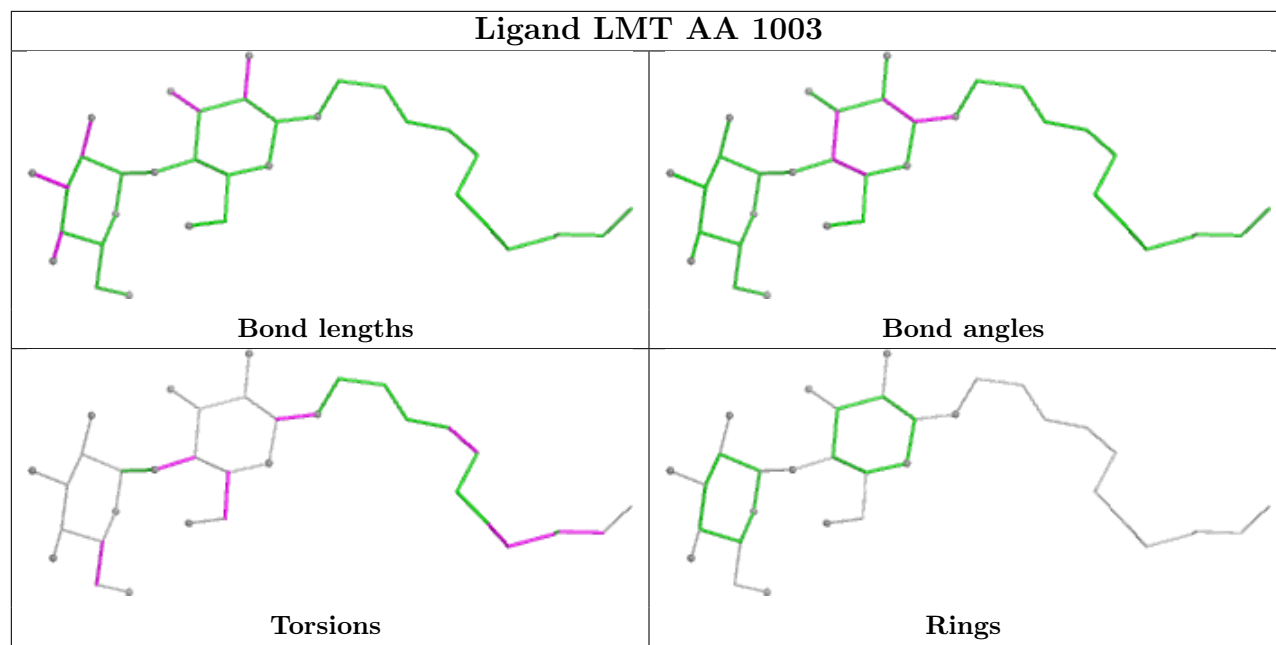


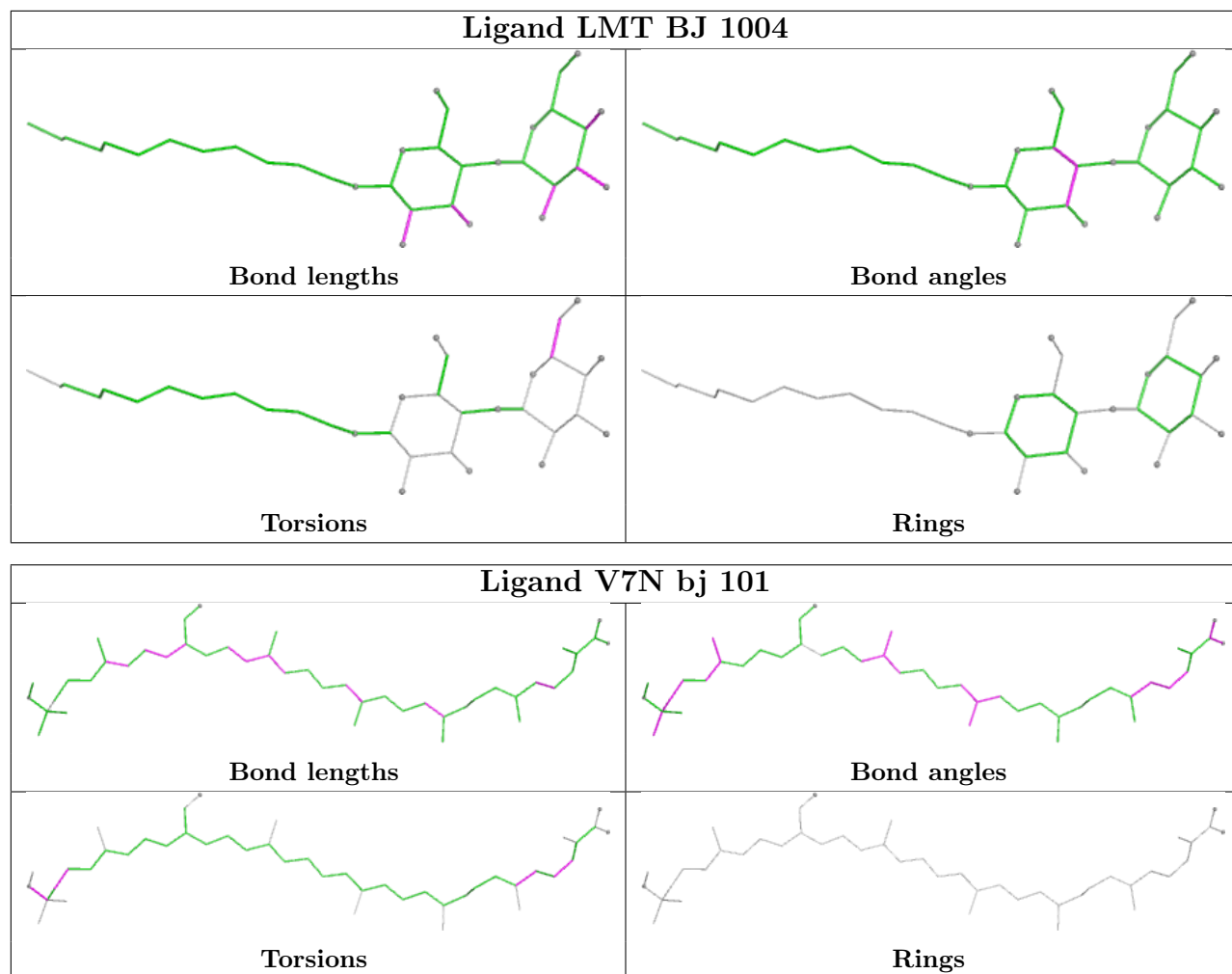
Ligand BCL AE 1003

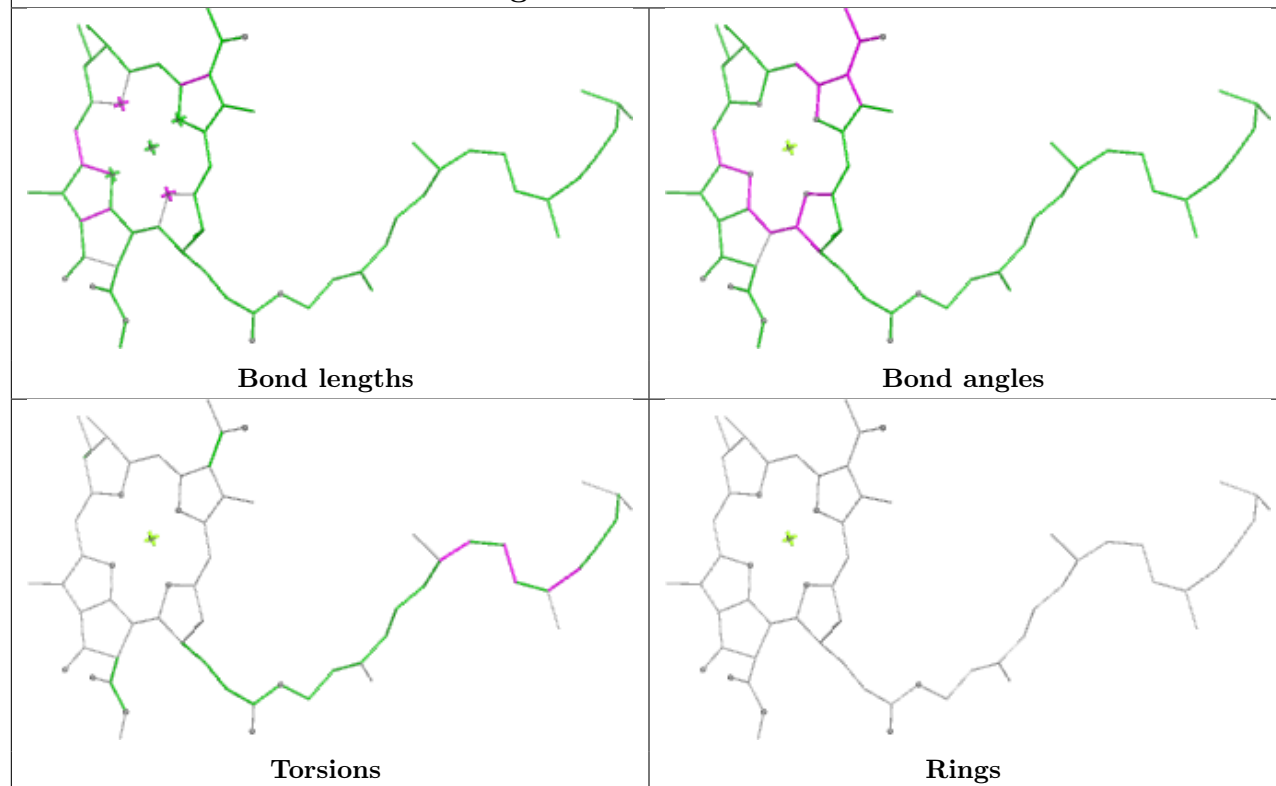
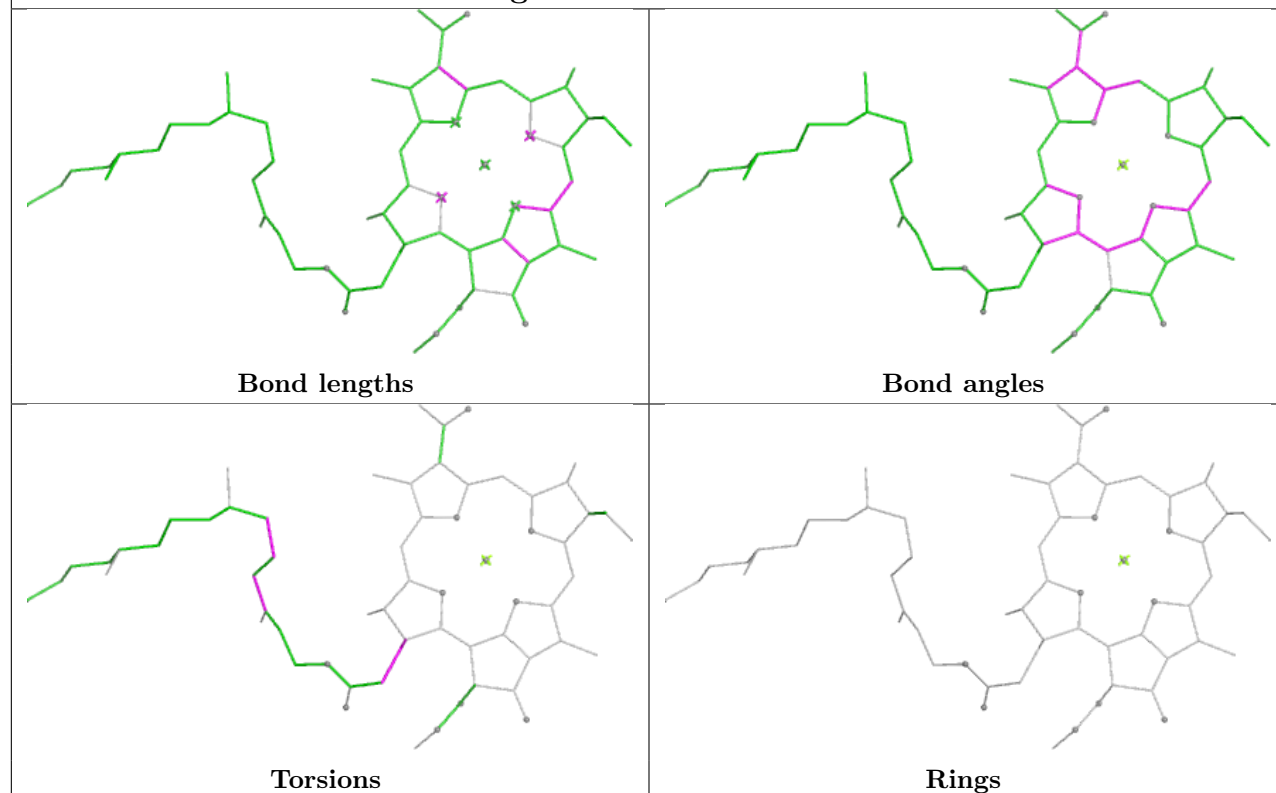


Ligand LMT BG 1006

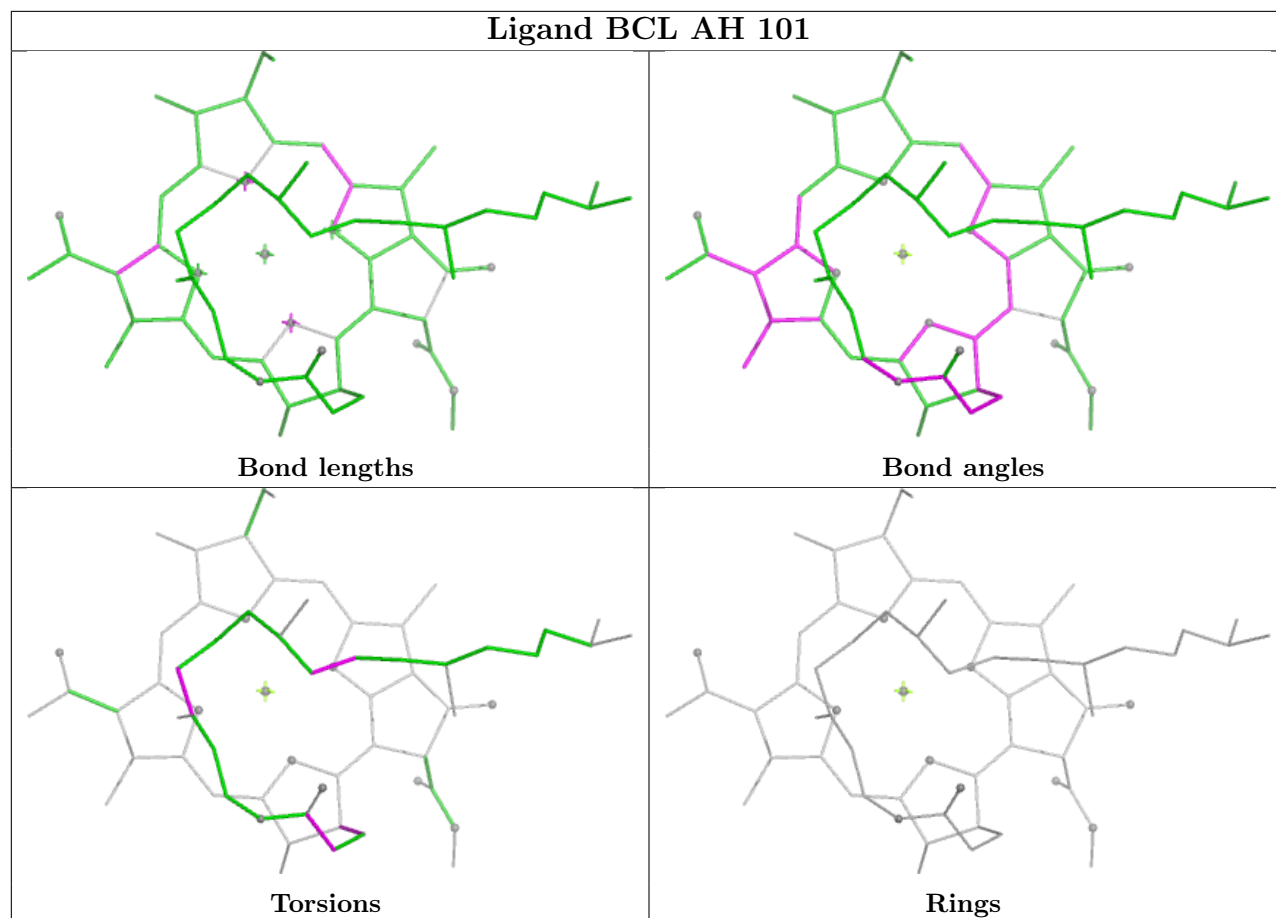




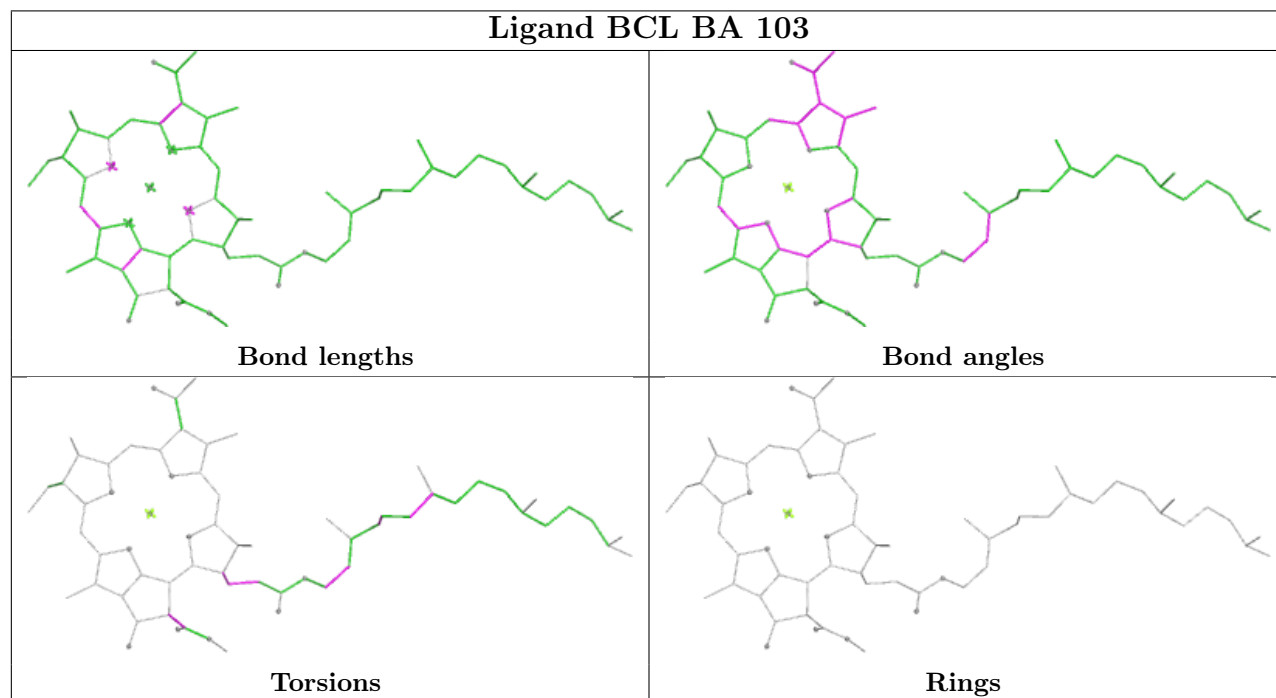


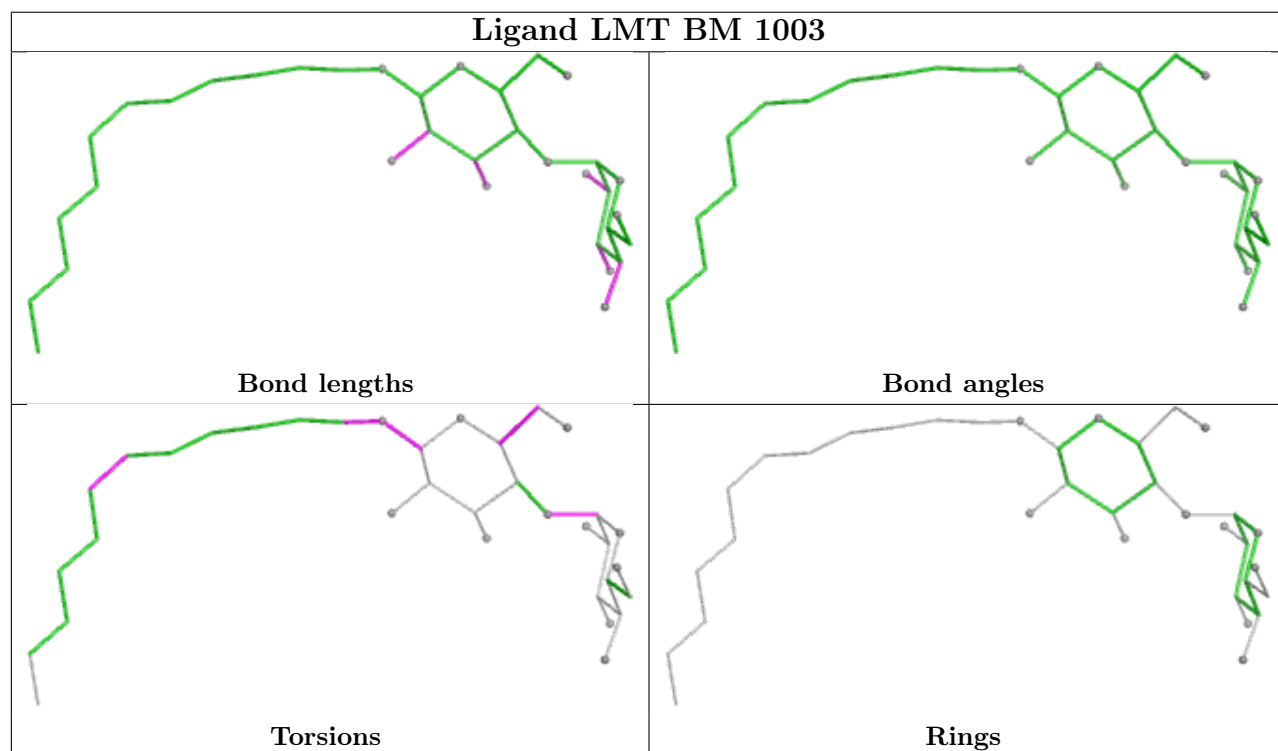
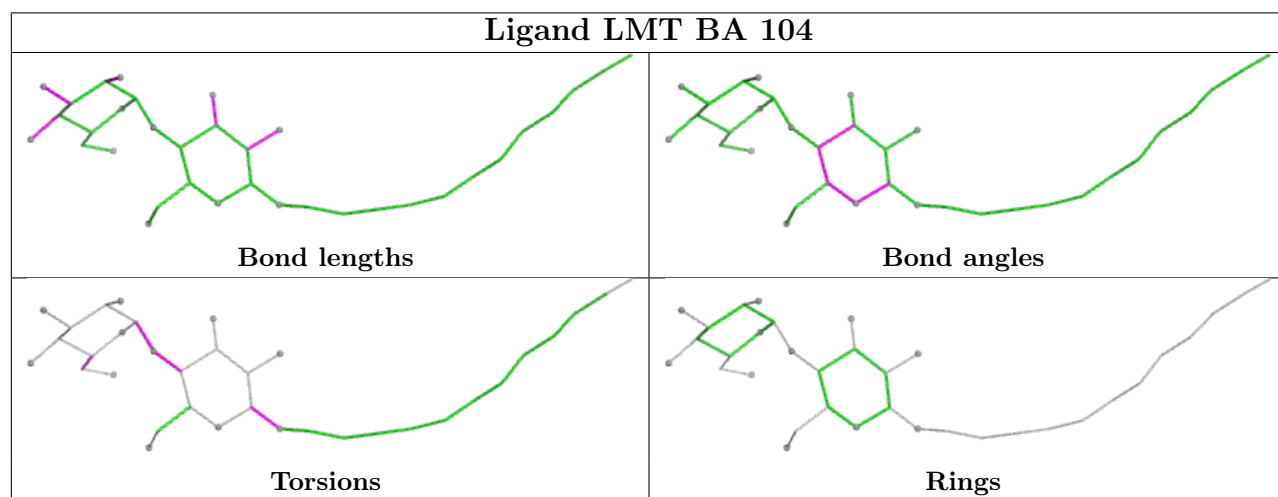
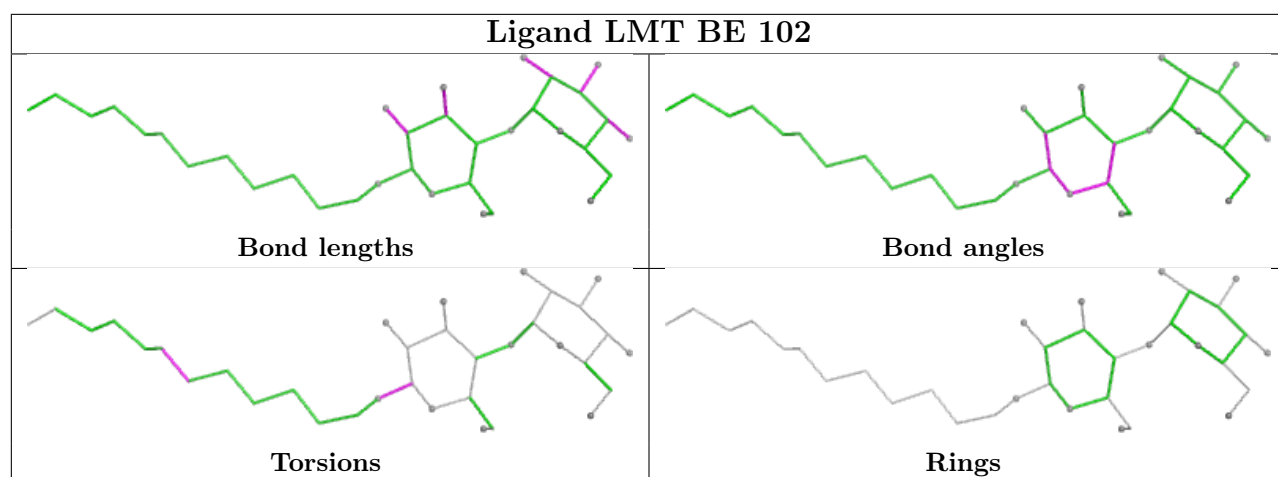
Ligand BCL AA 1001**Ligand BCL BG 1004**

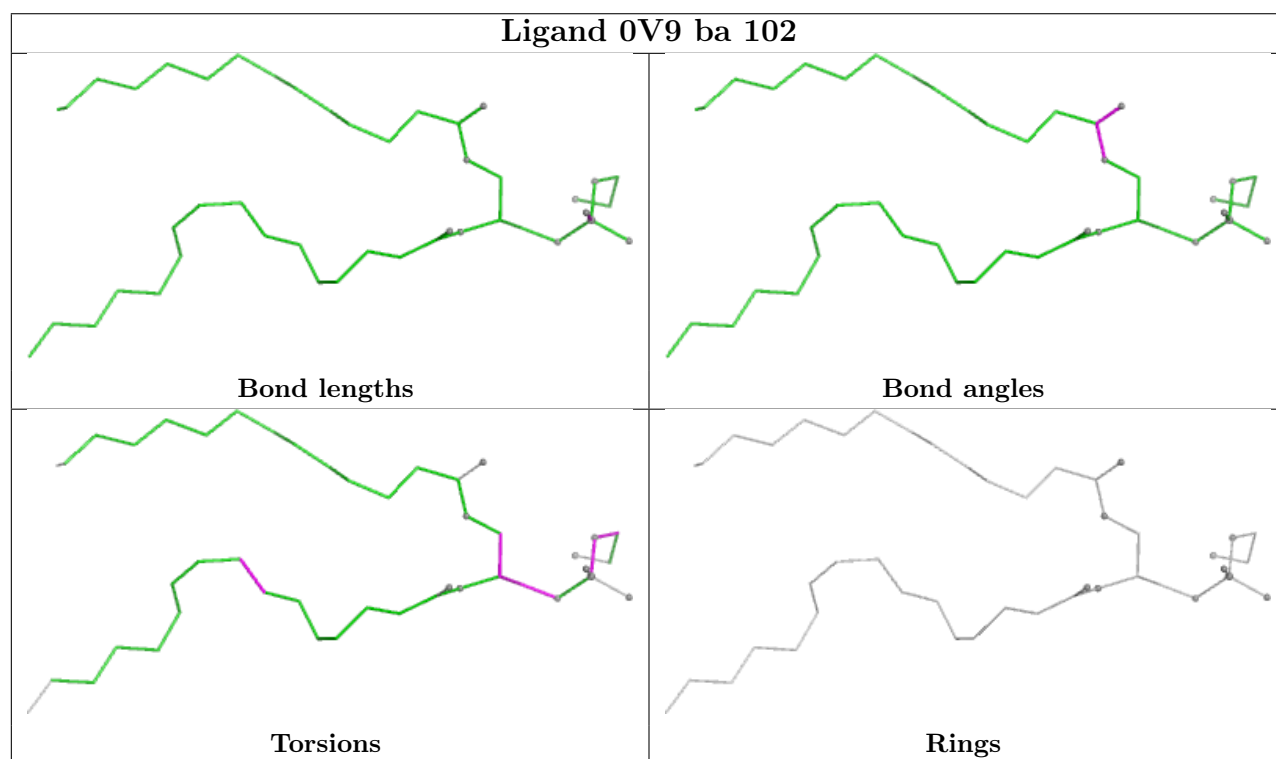
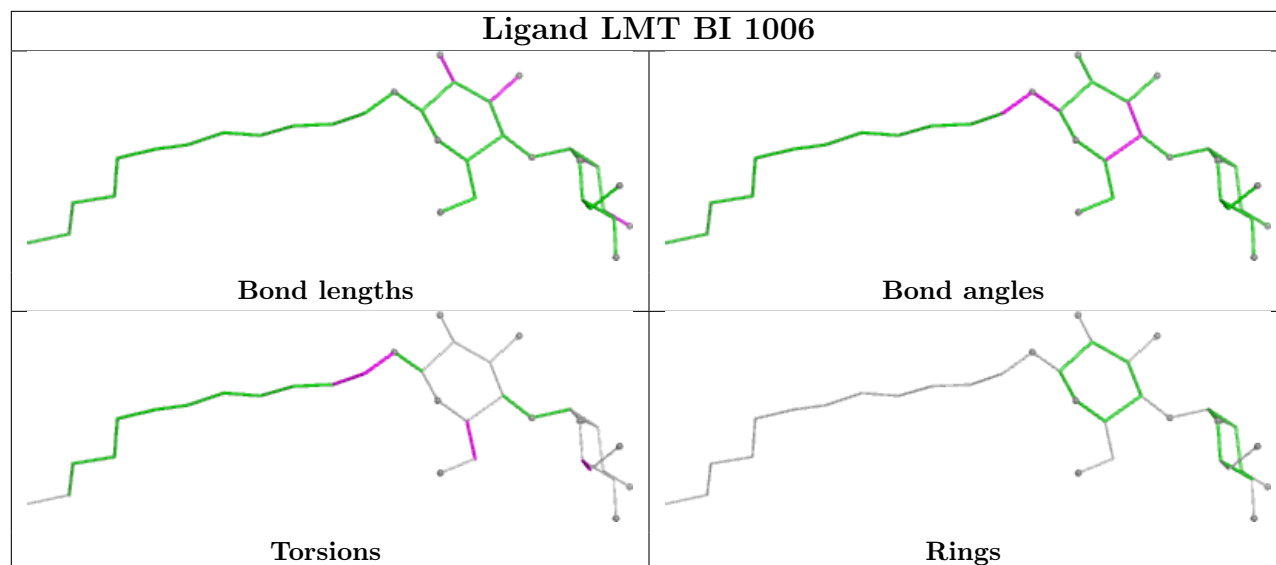
Ligand BCL AH 101

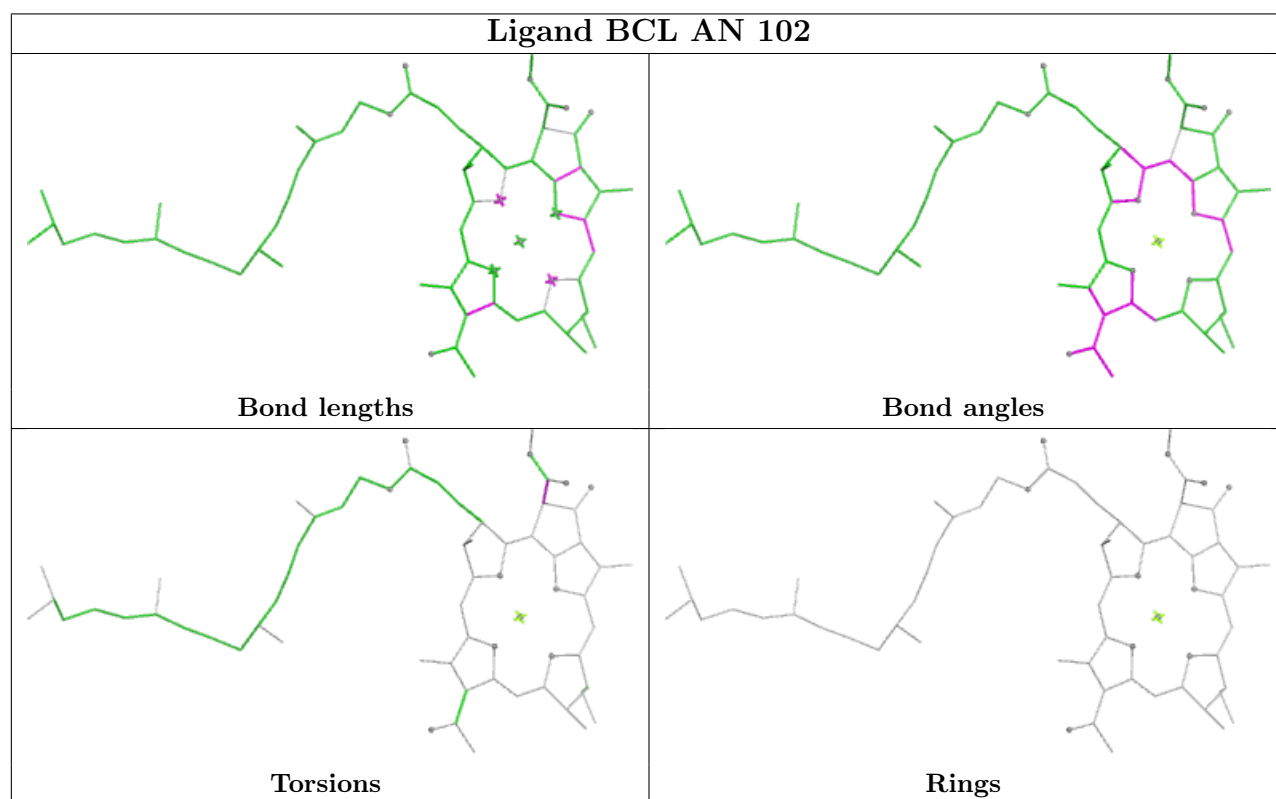
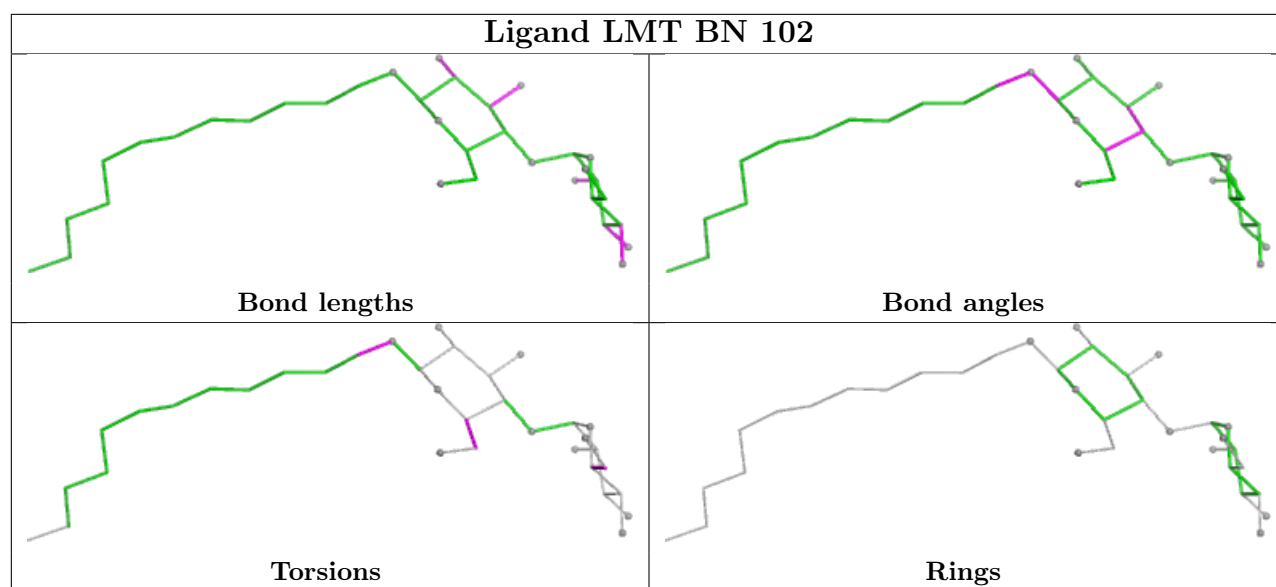


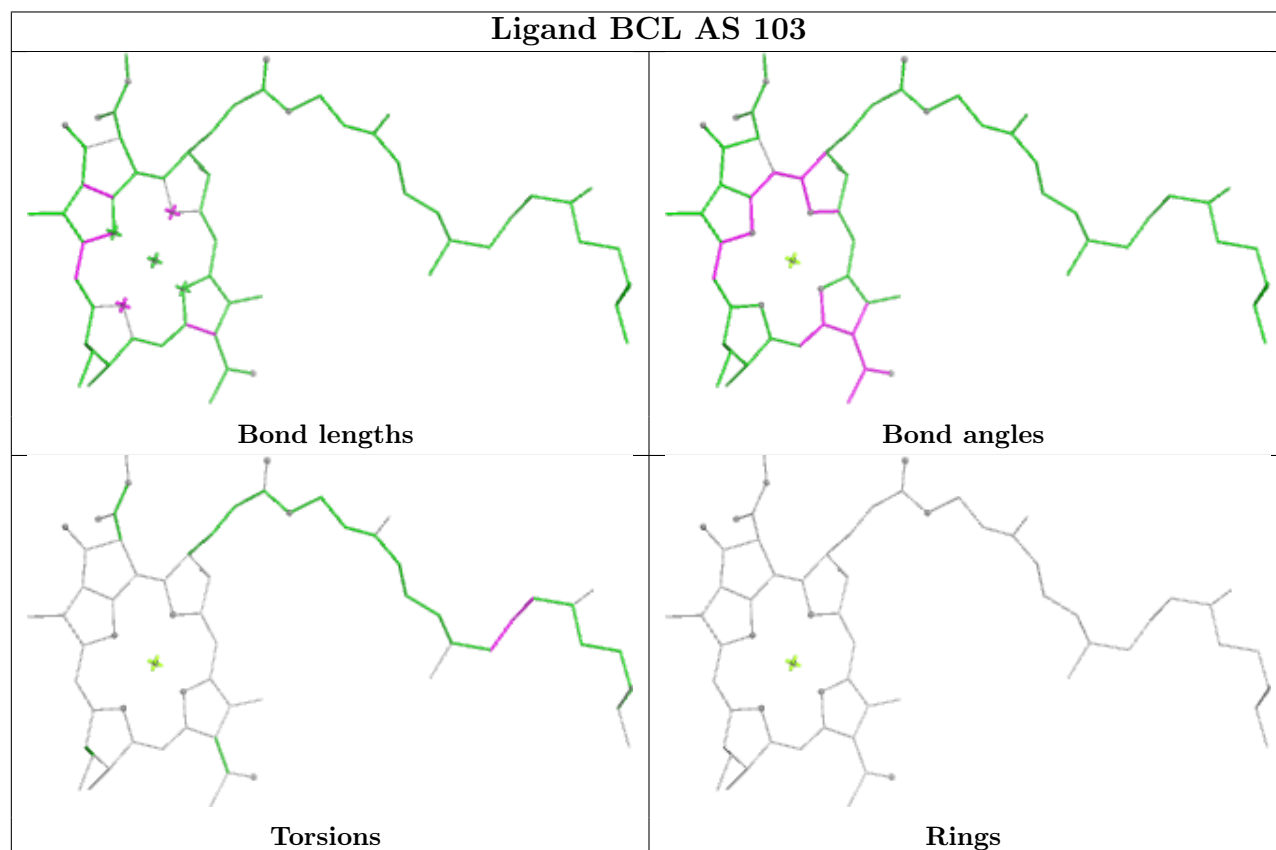
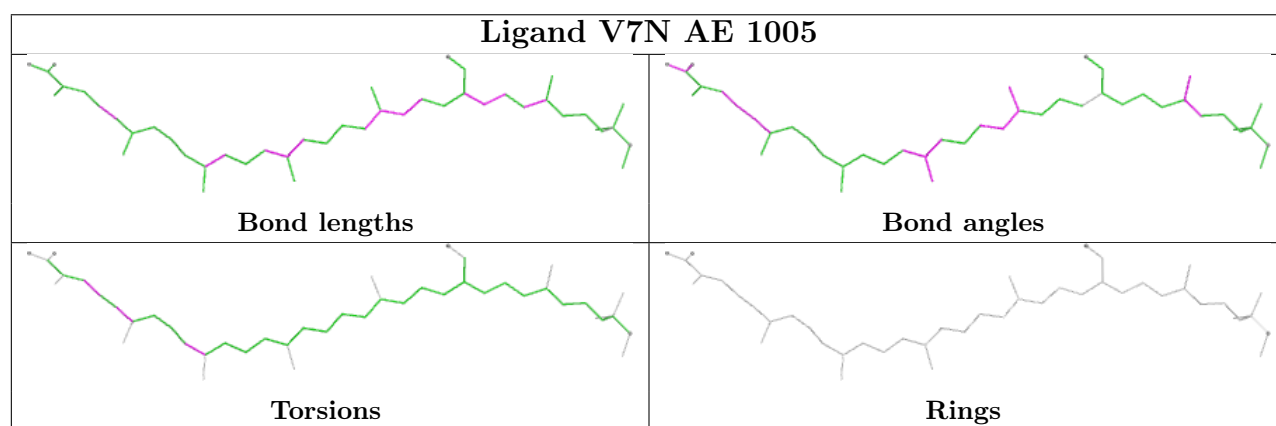
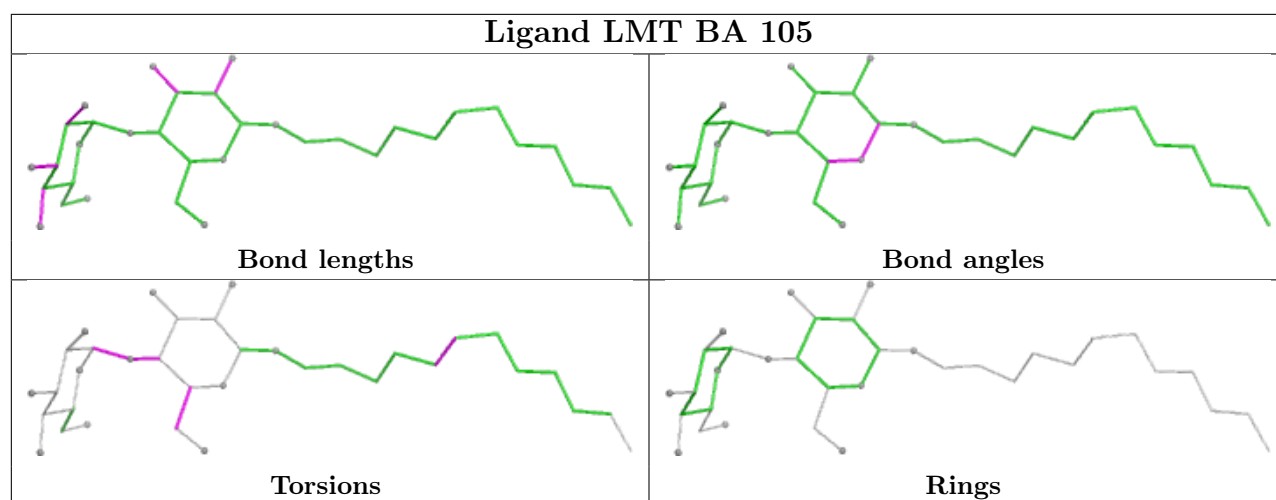
Ligand BCL BA 103

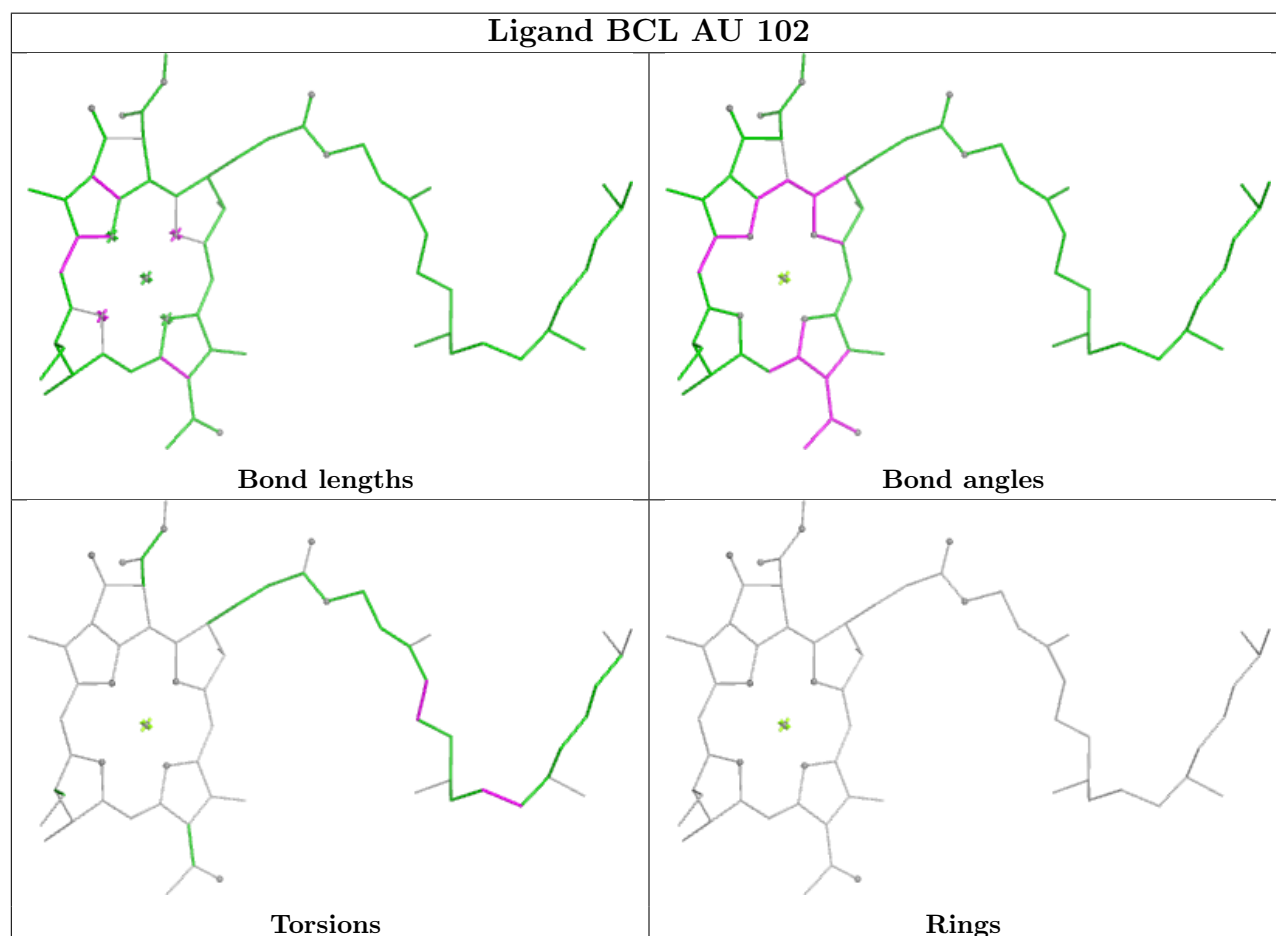
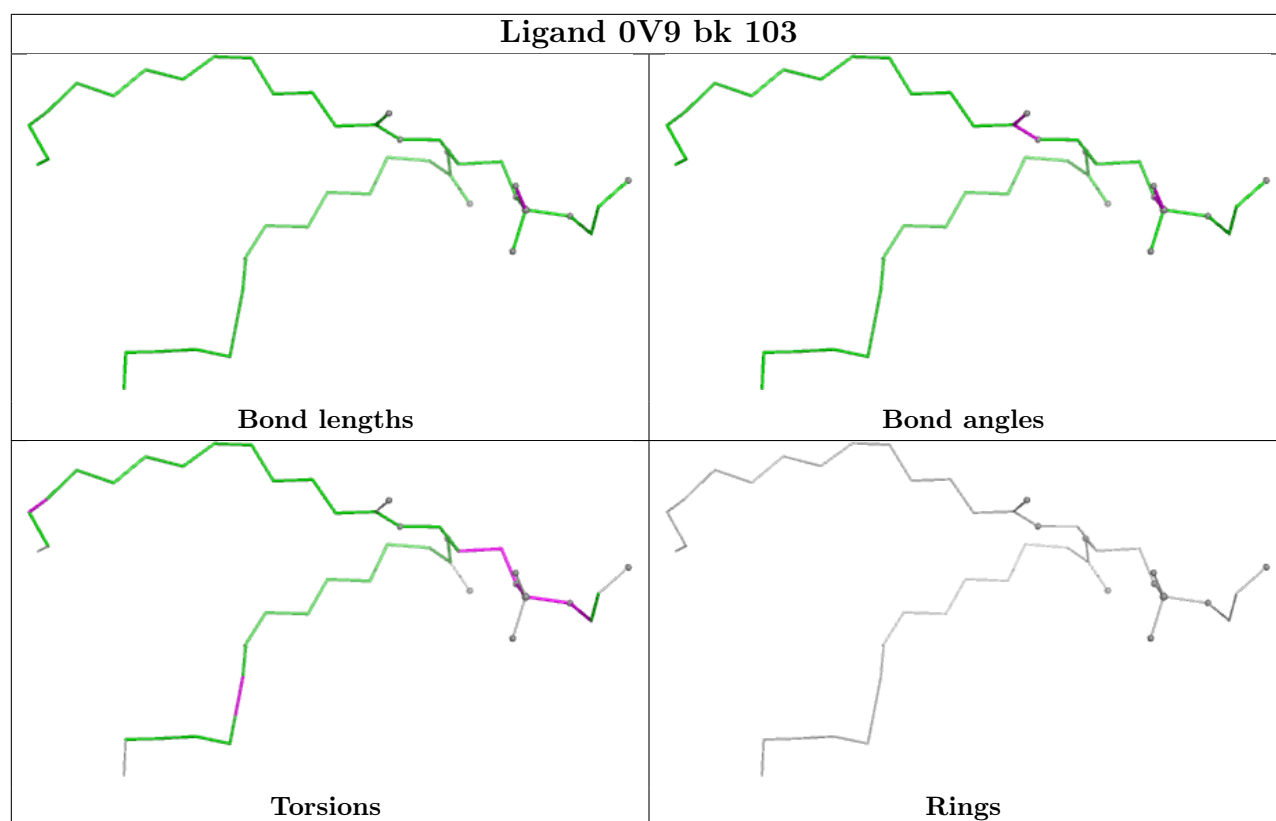


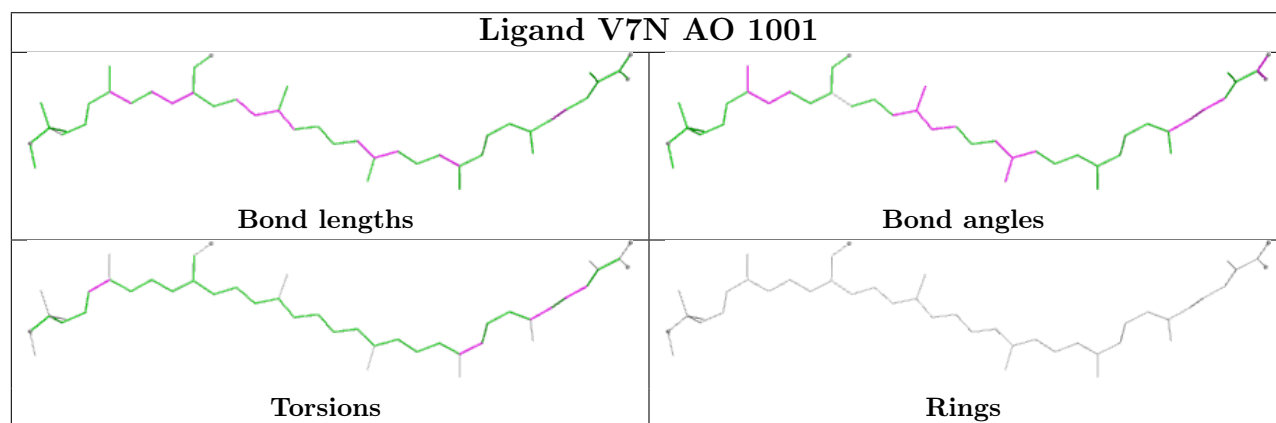
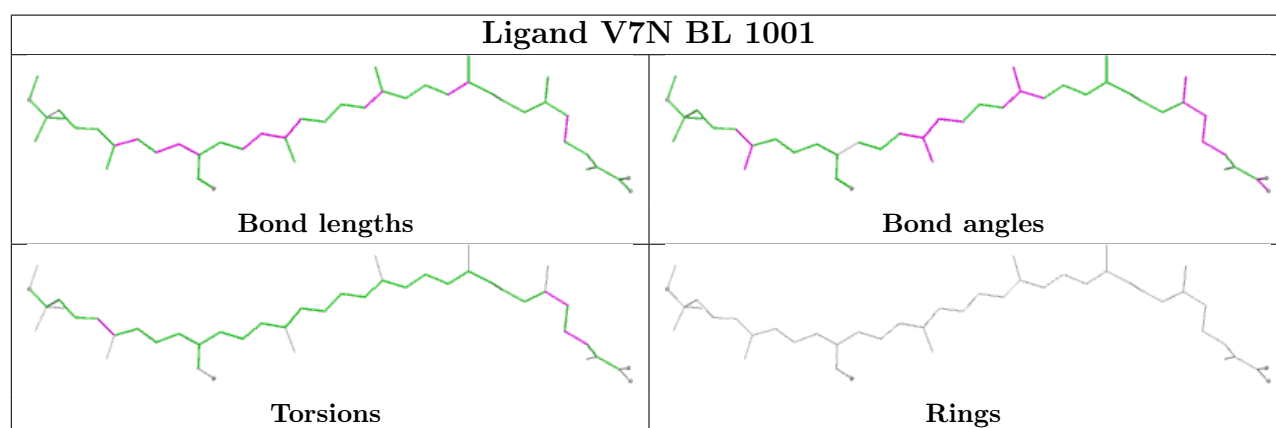
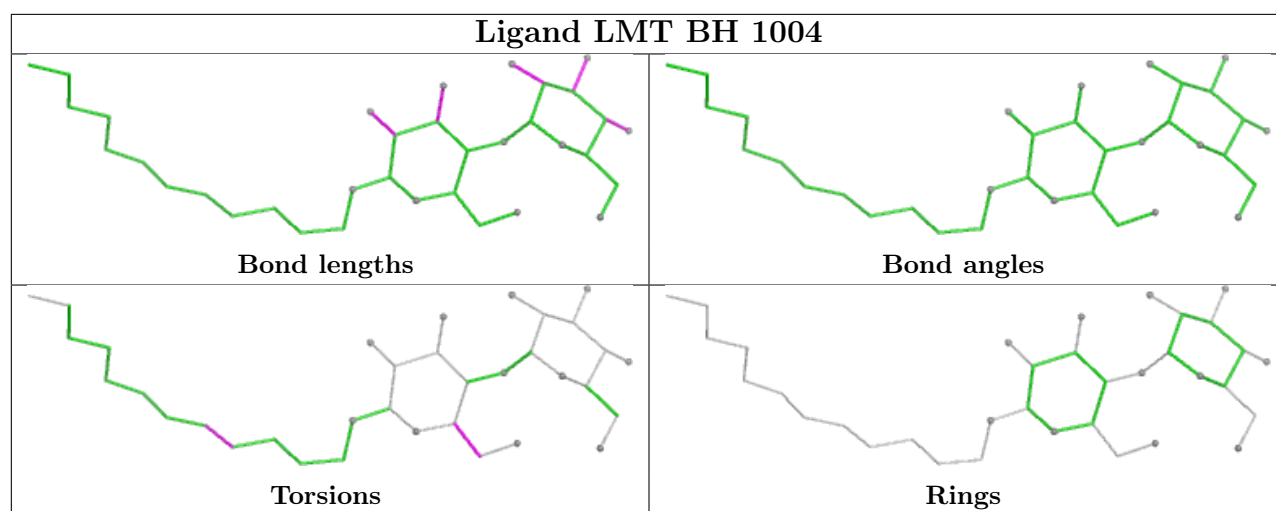


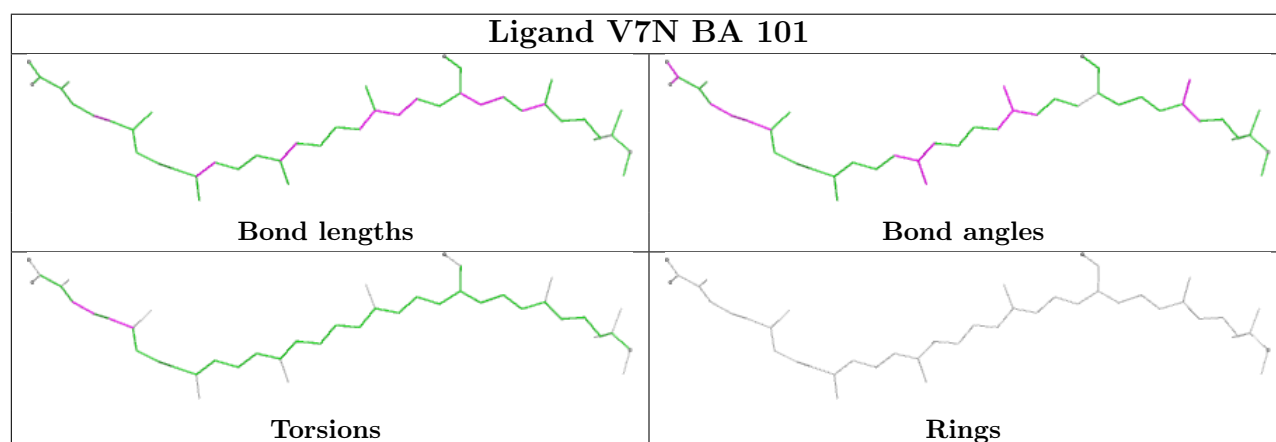
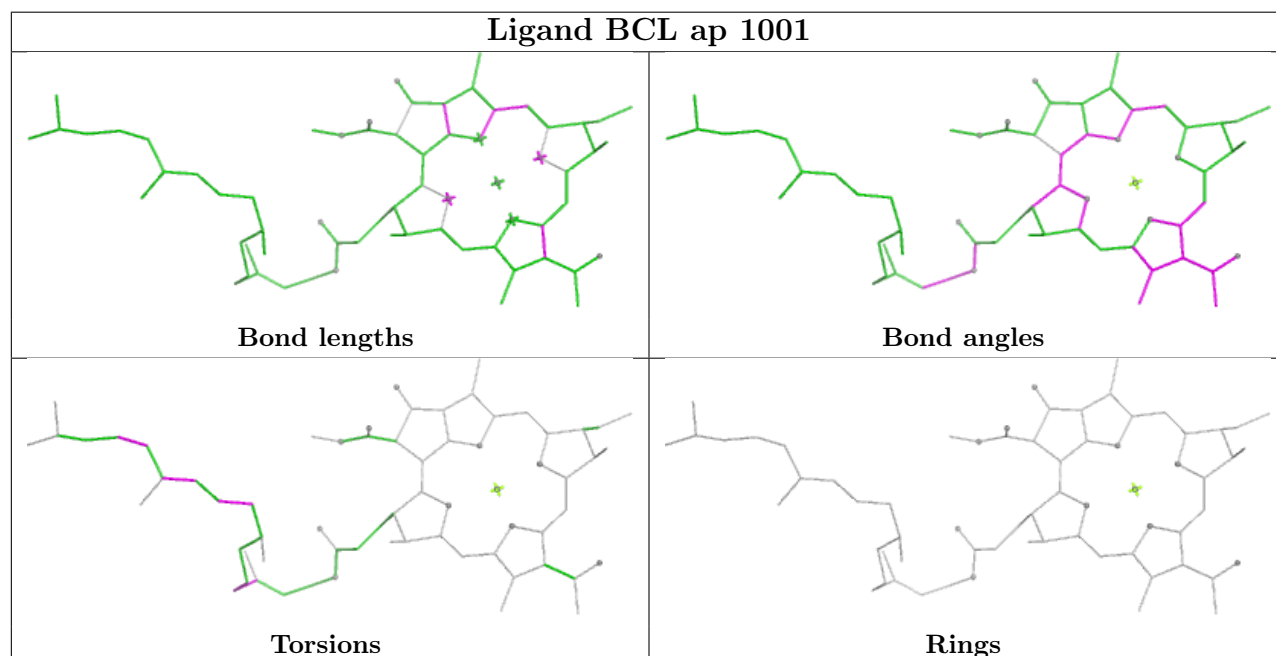
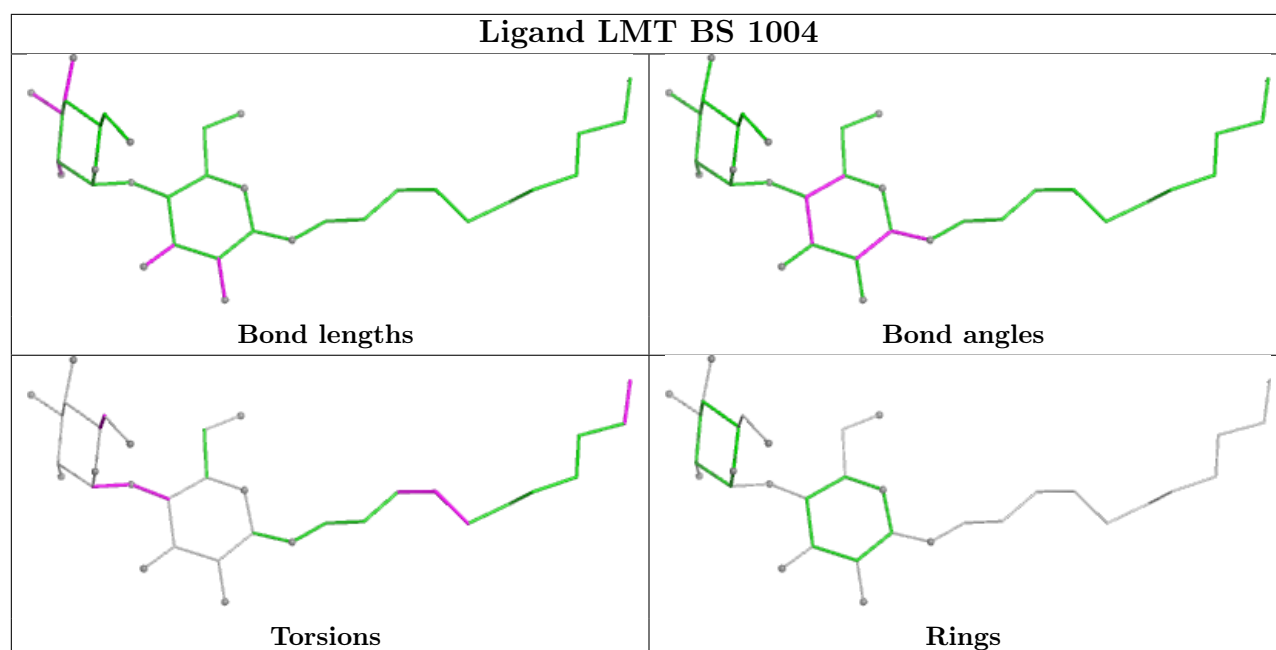


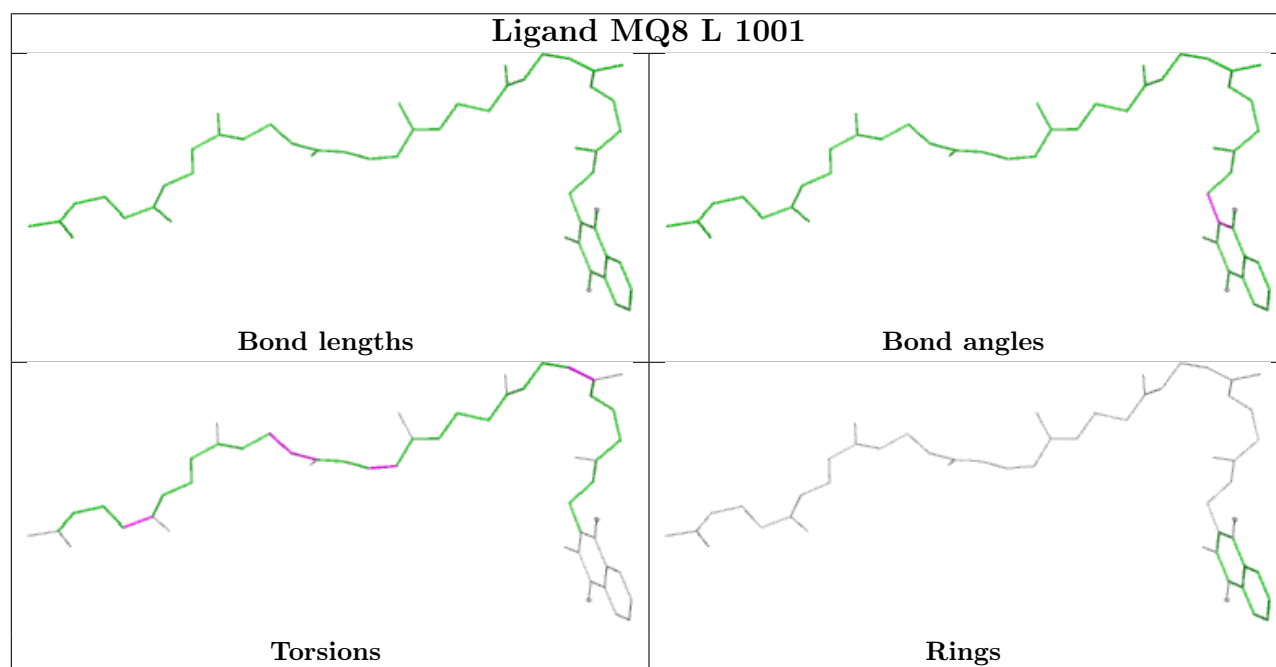
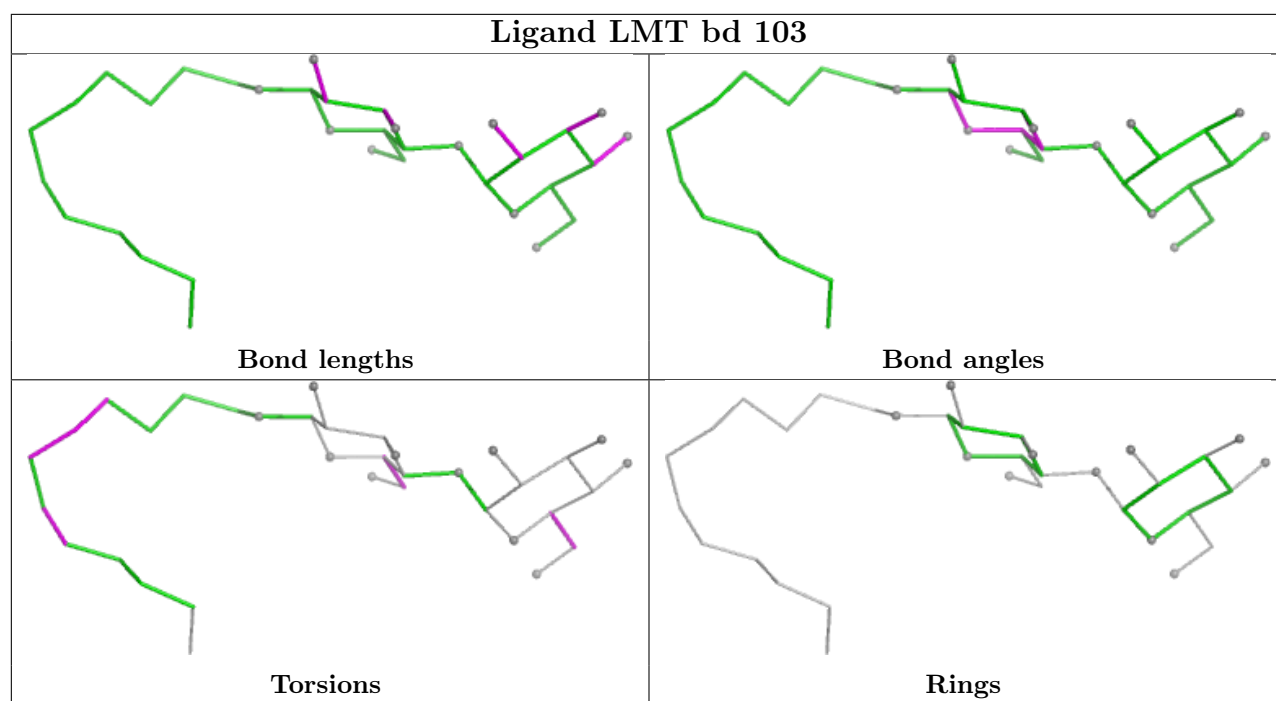




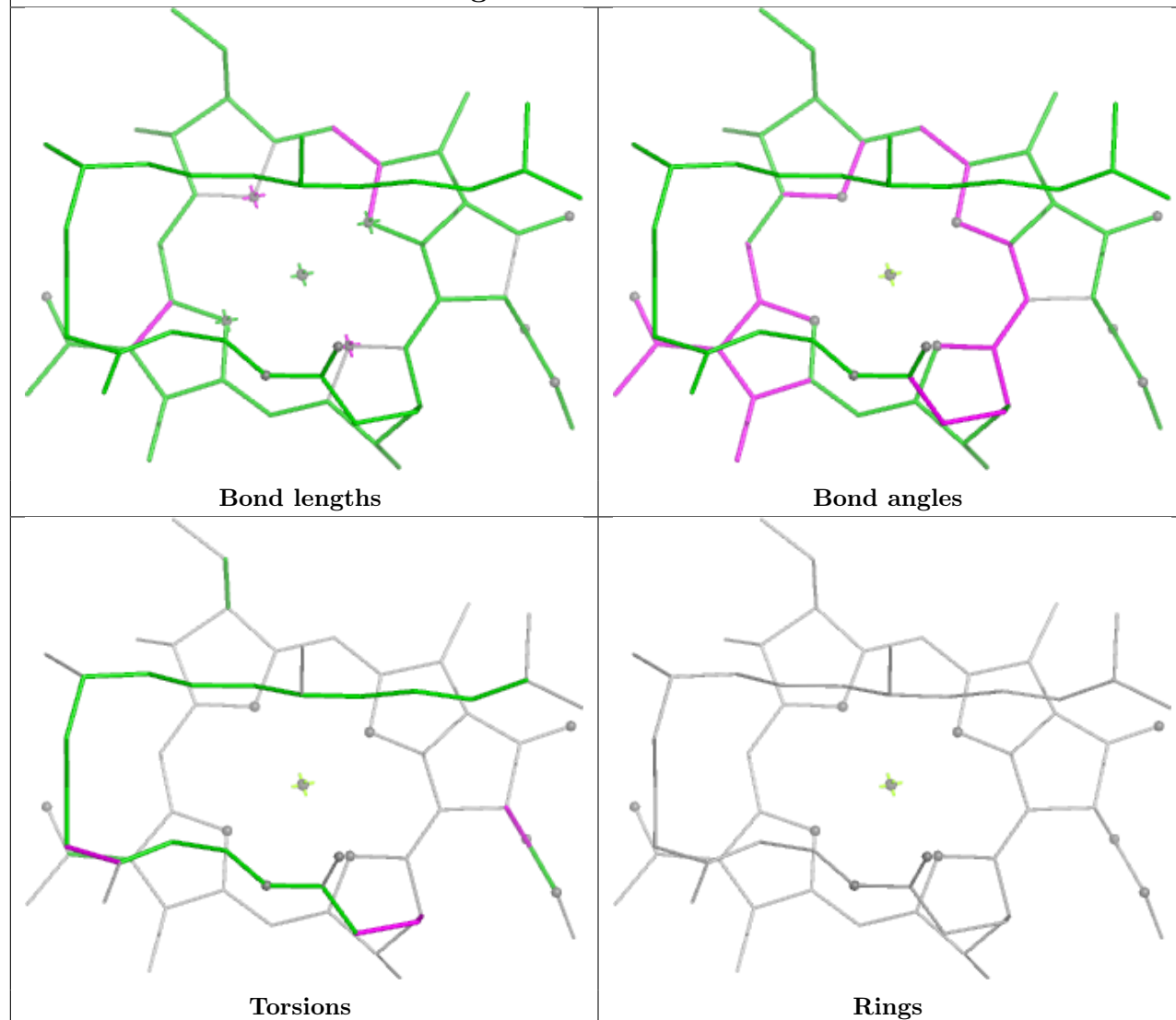




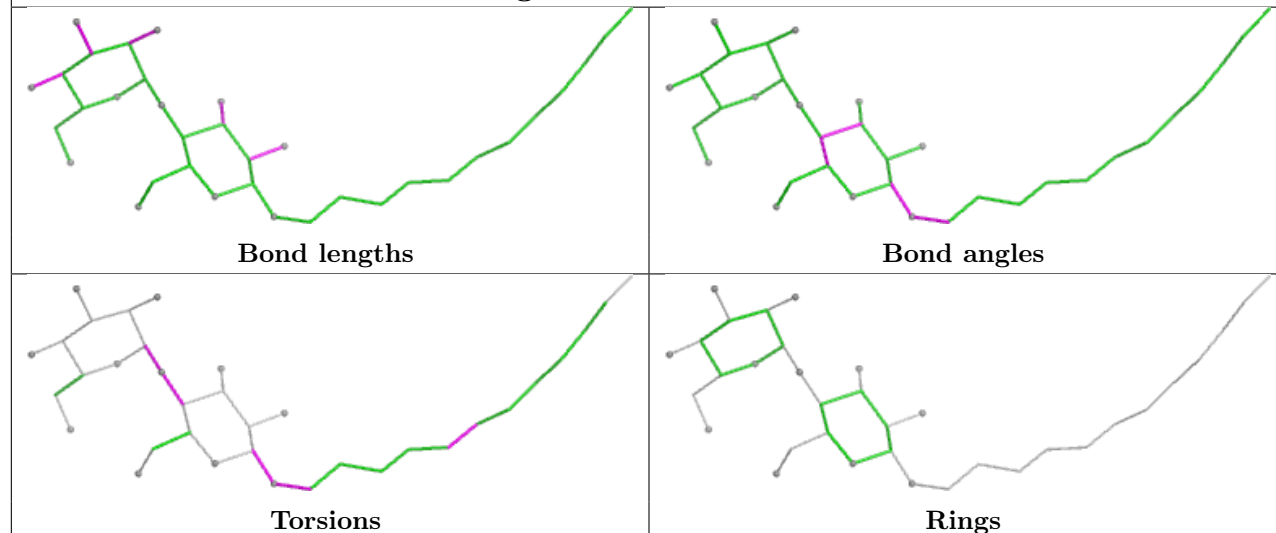


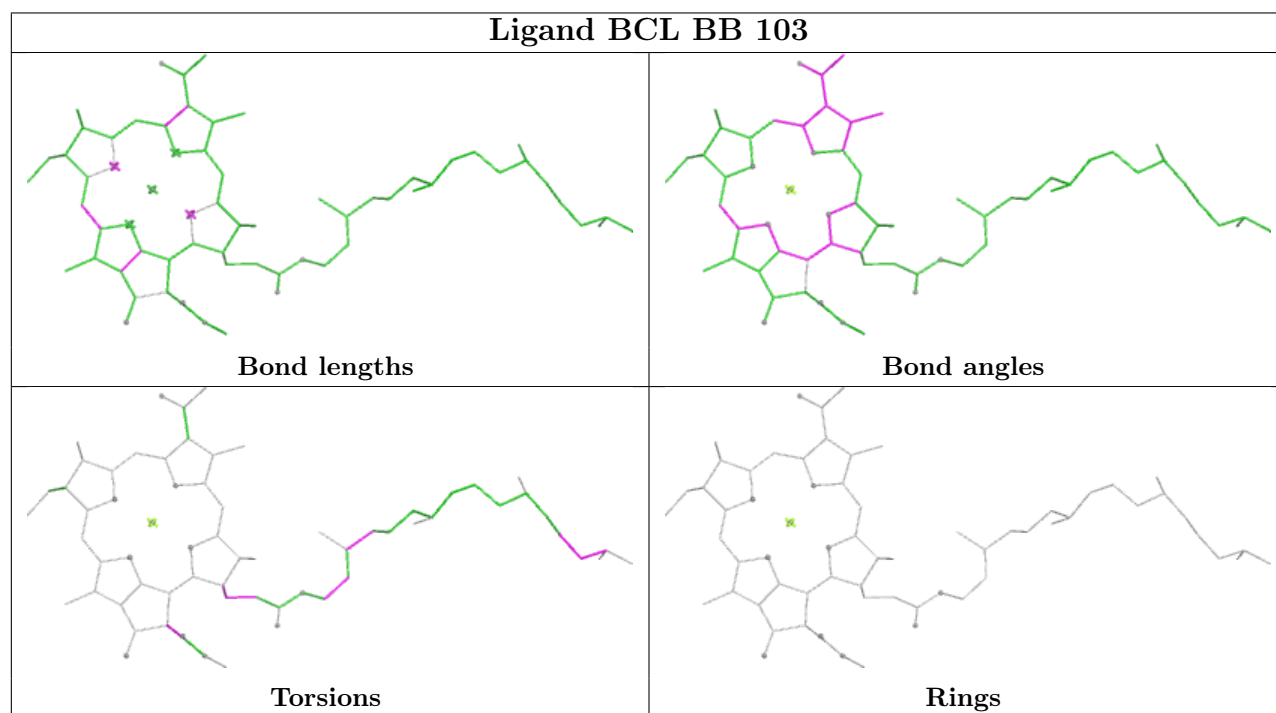
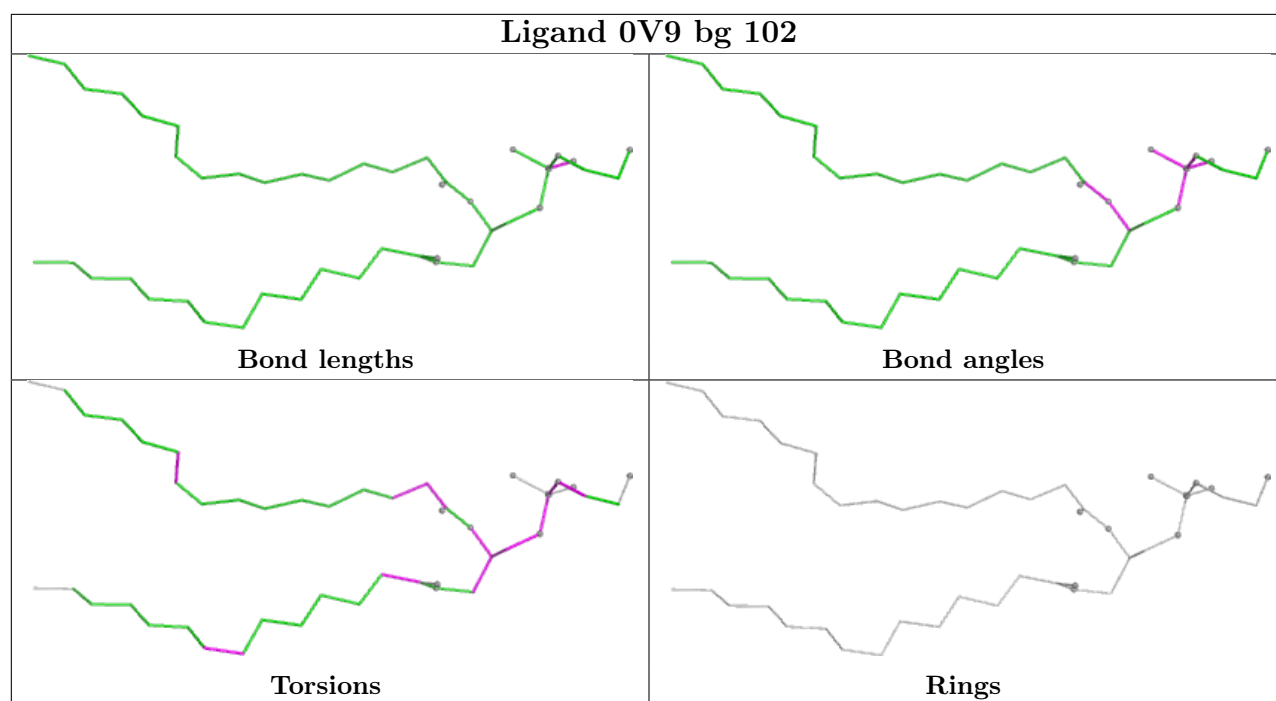


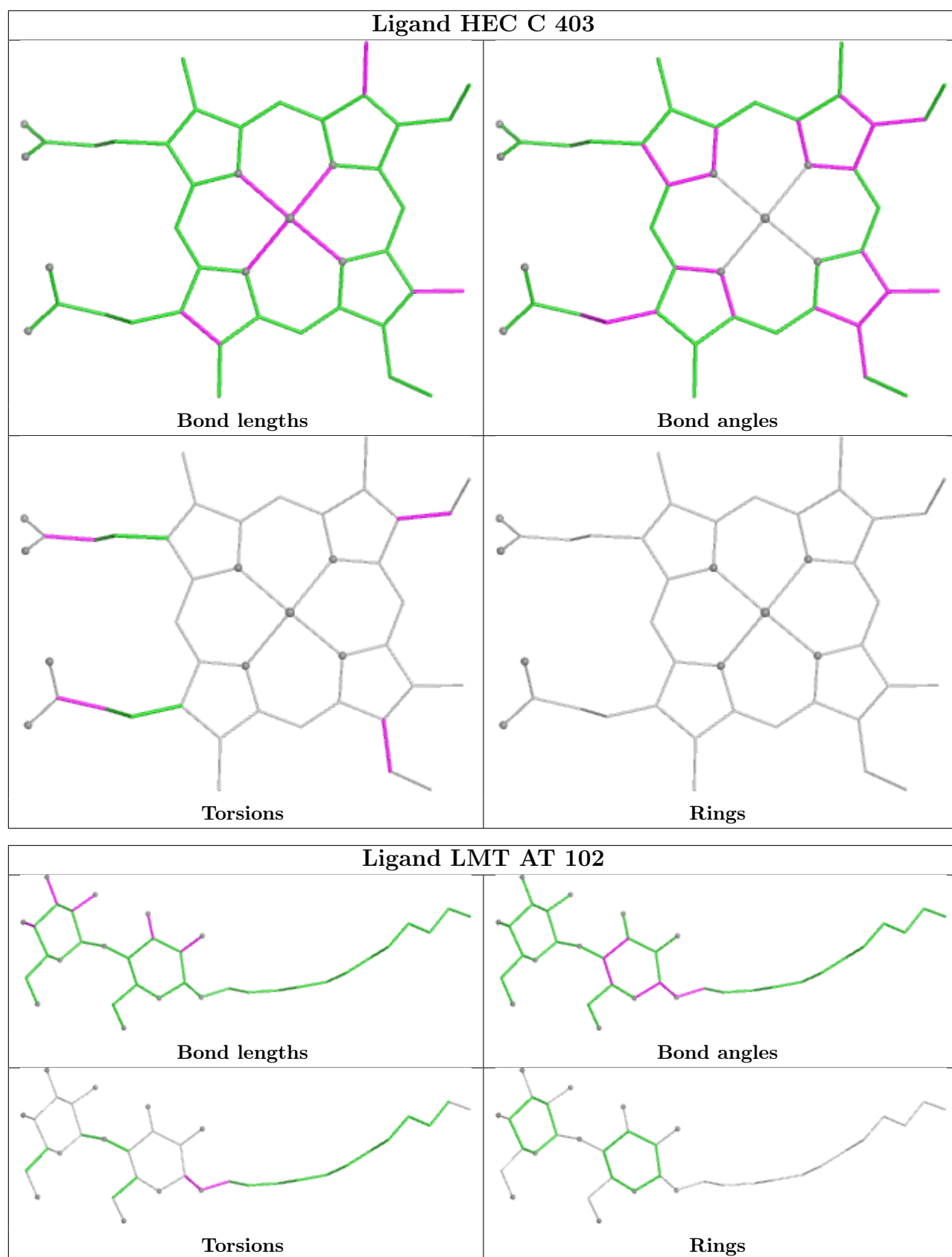
Ligand BCL AB 1002

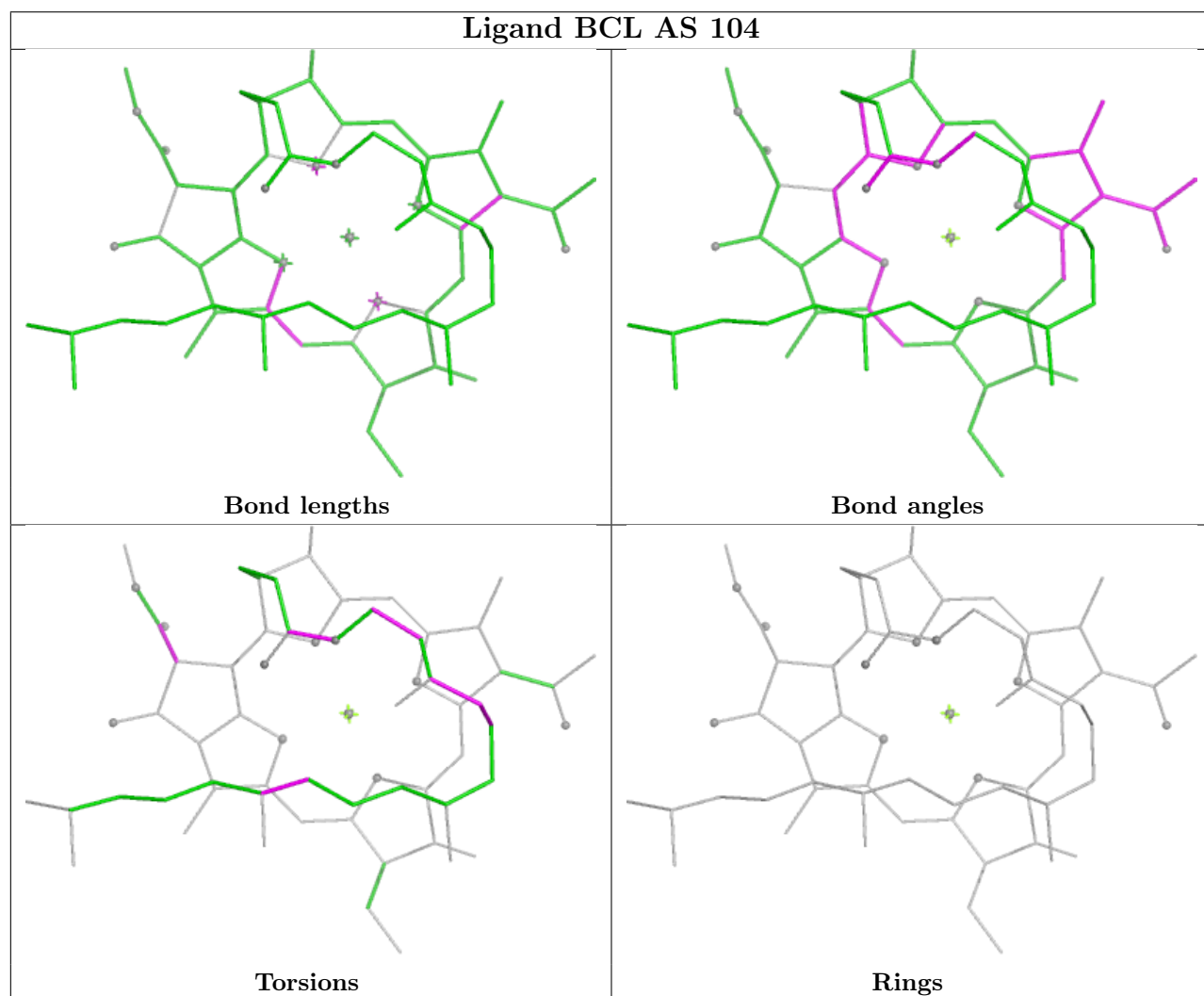
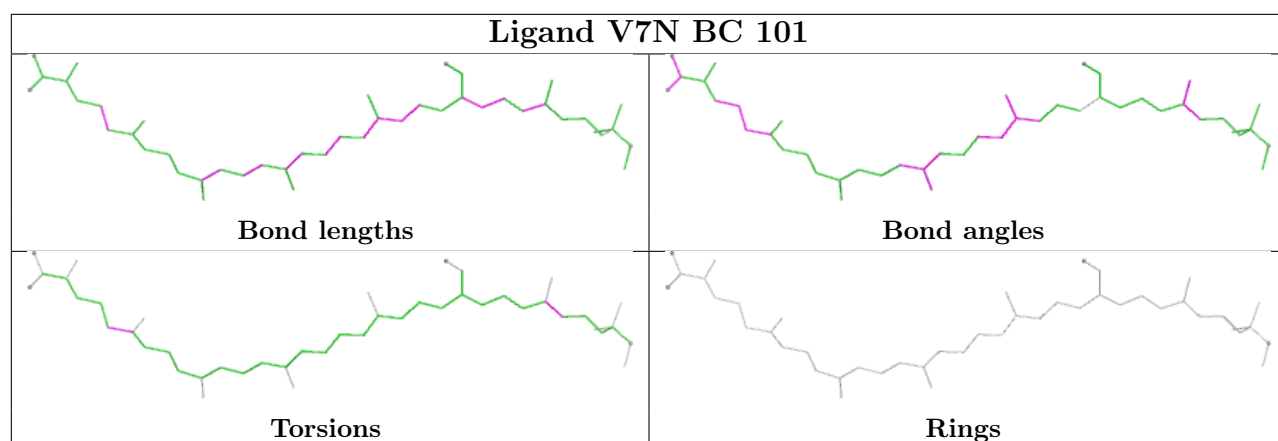


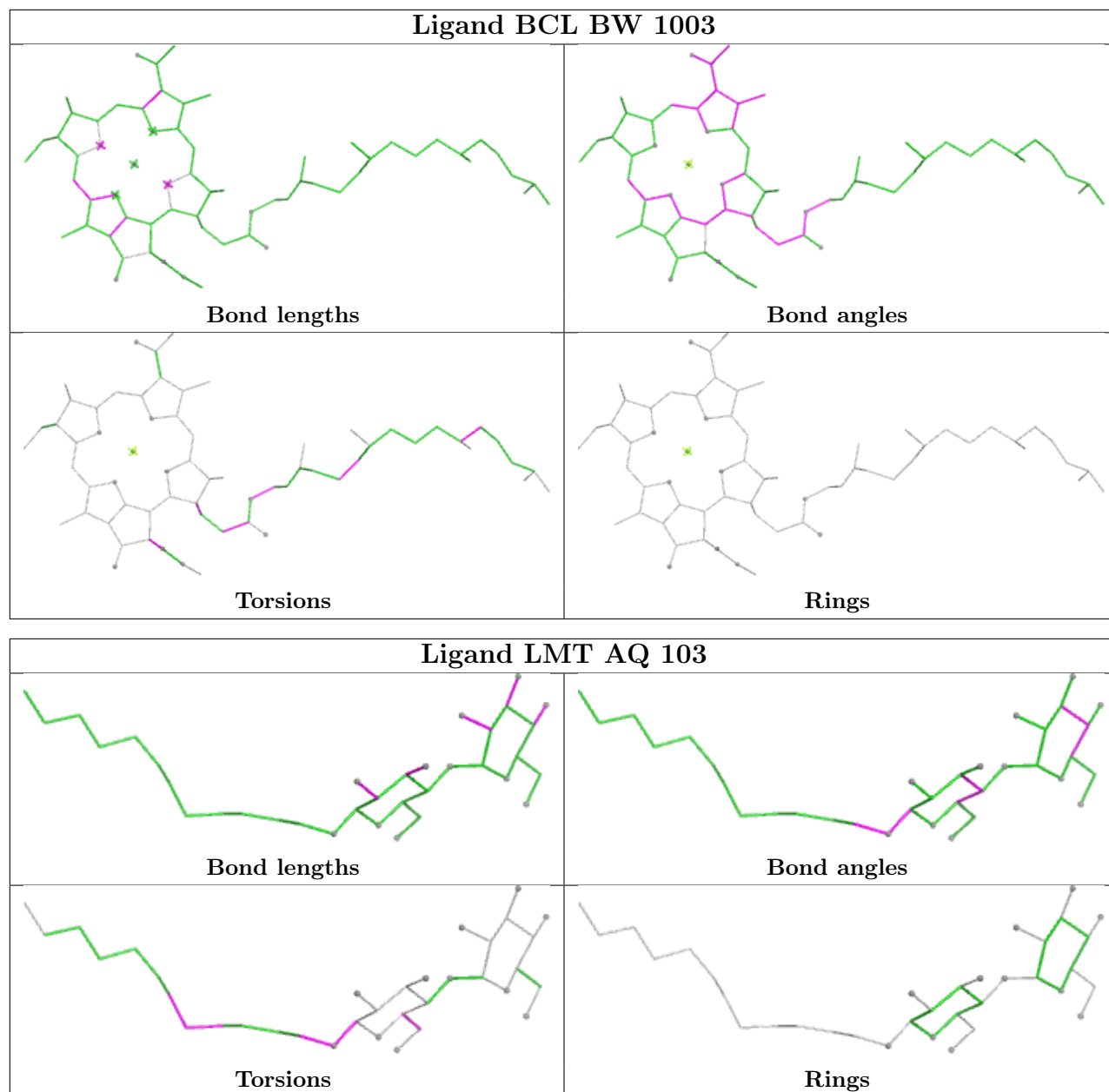
Ligand LMT BD 103

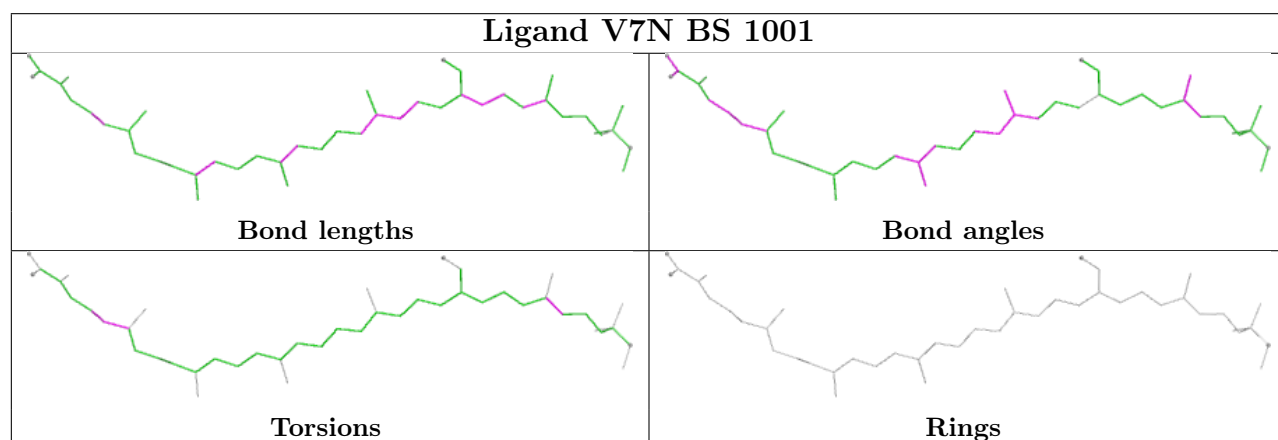
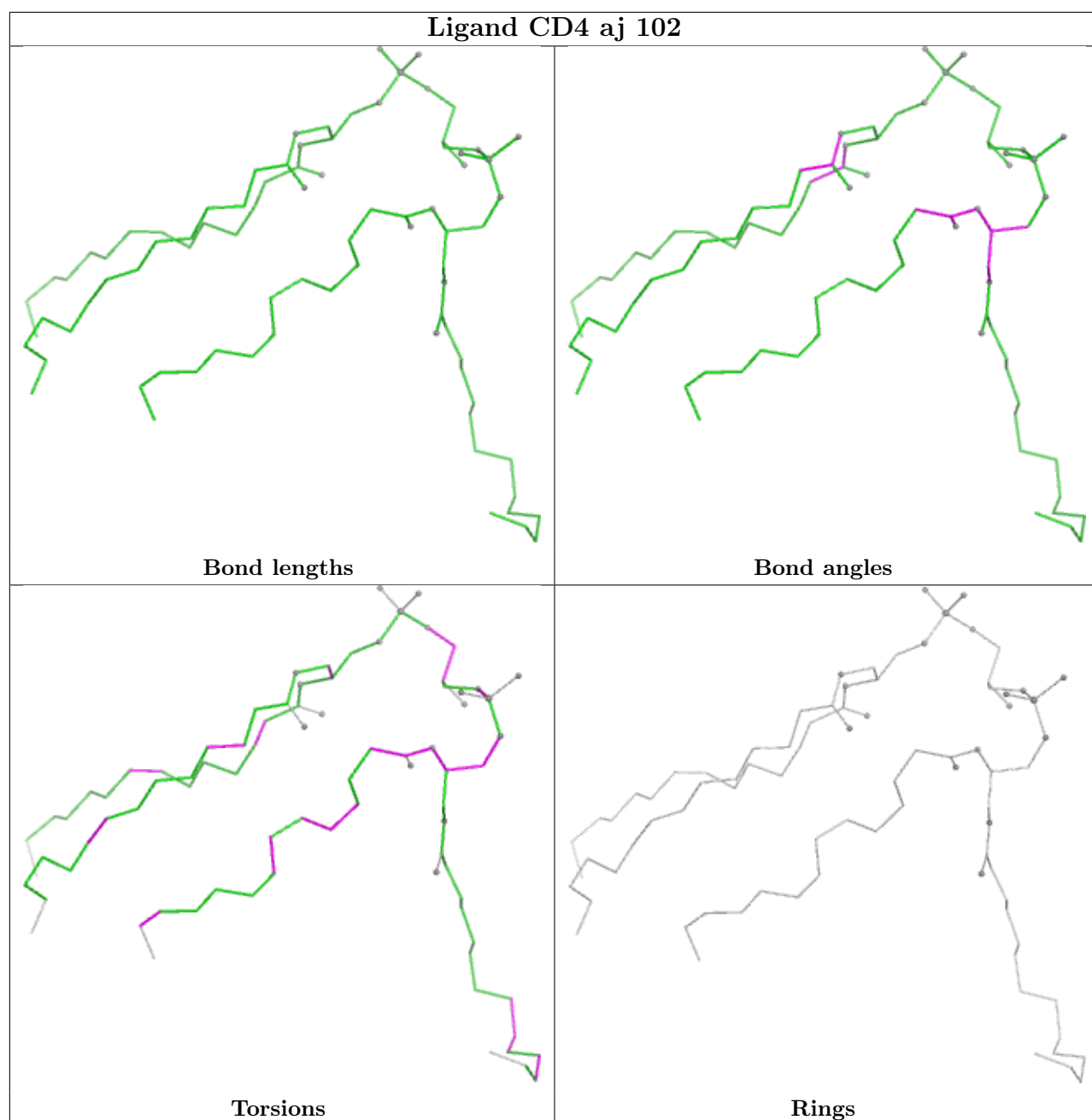


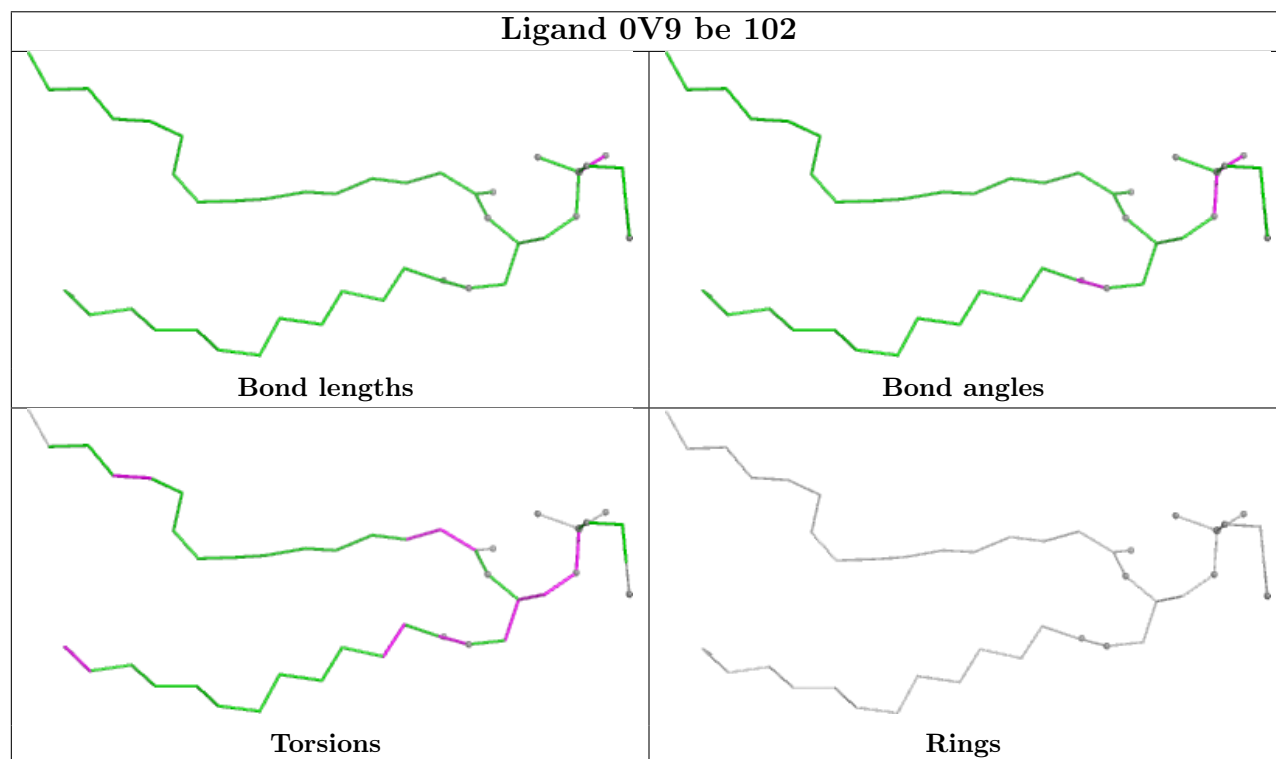
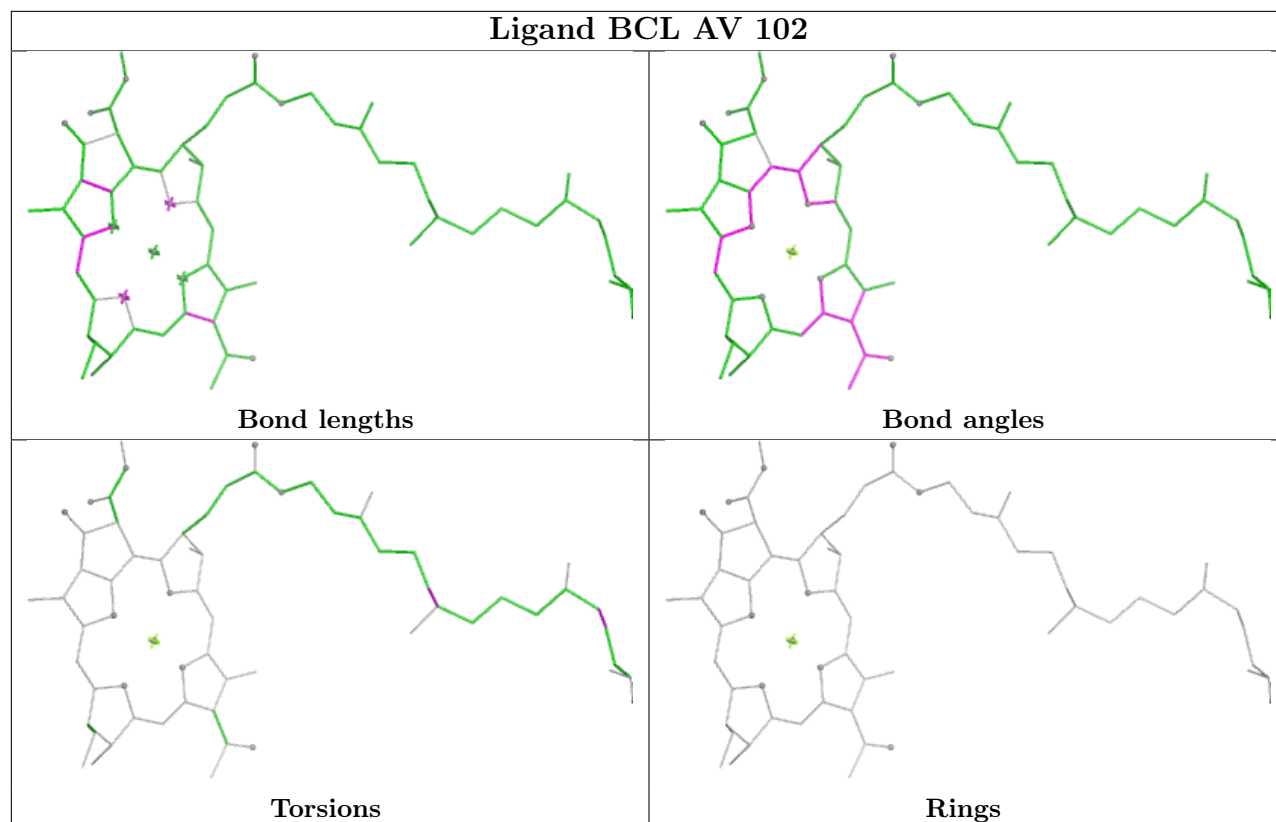




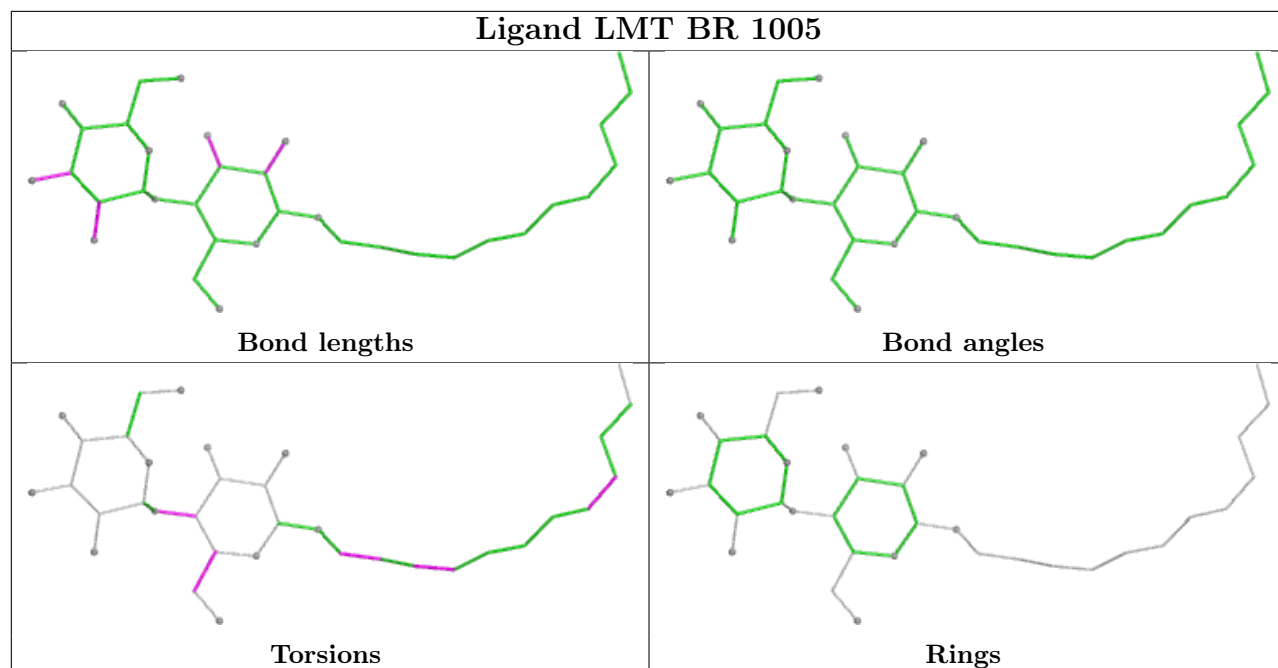




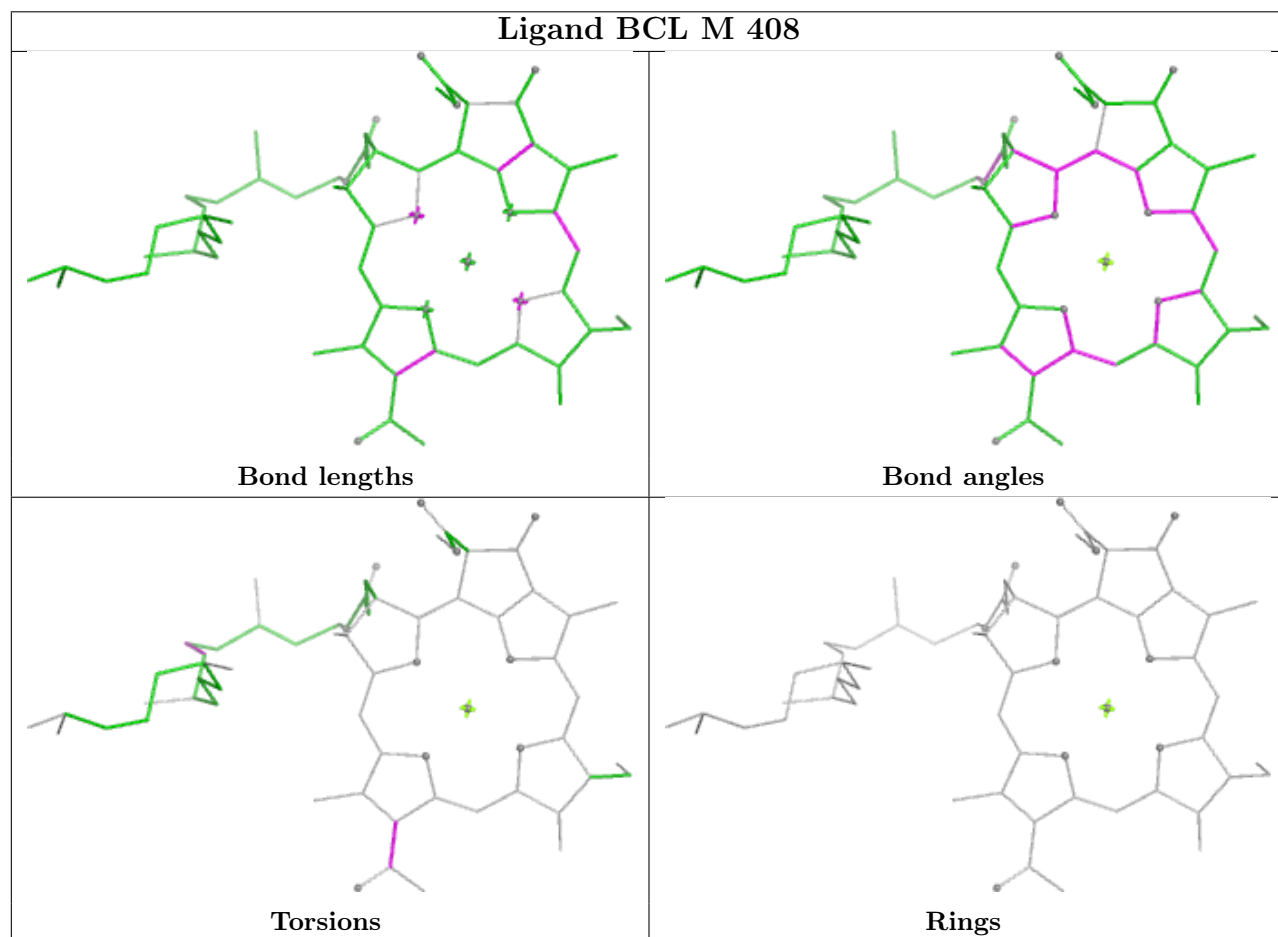


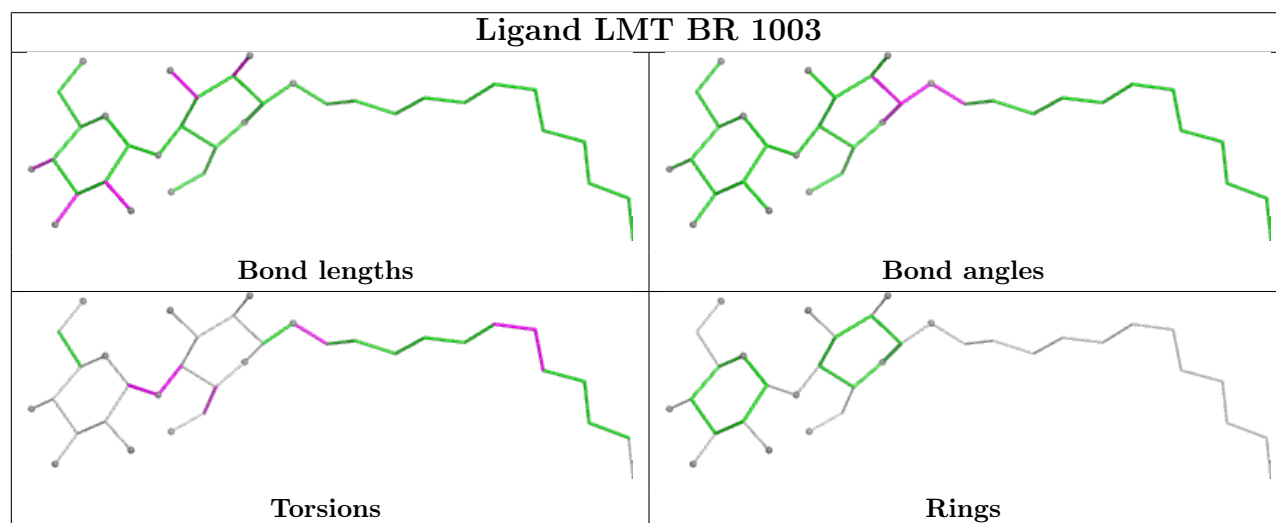
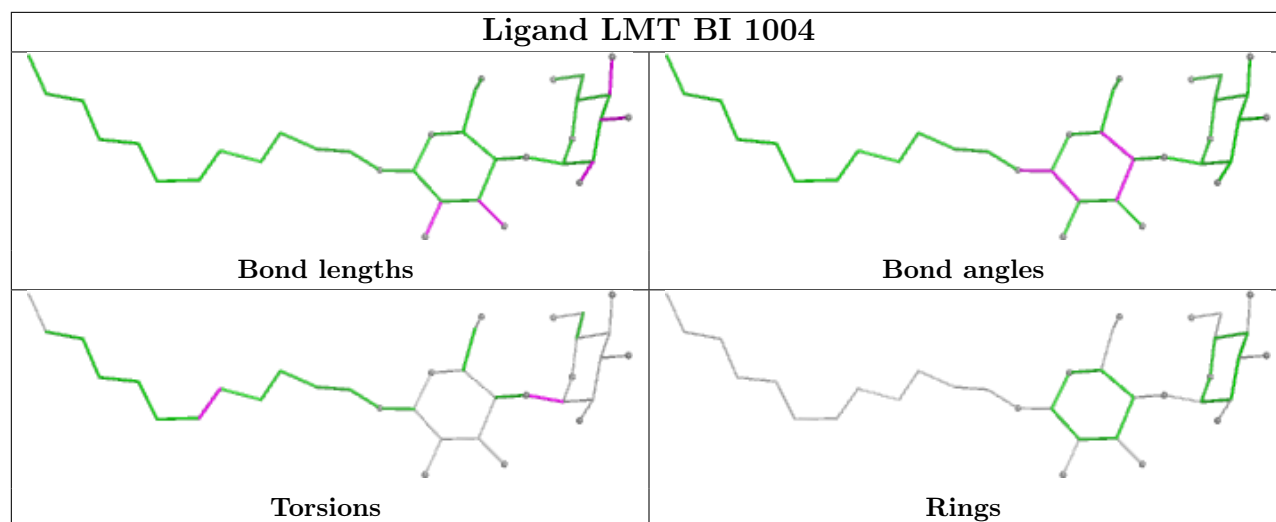
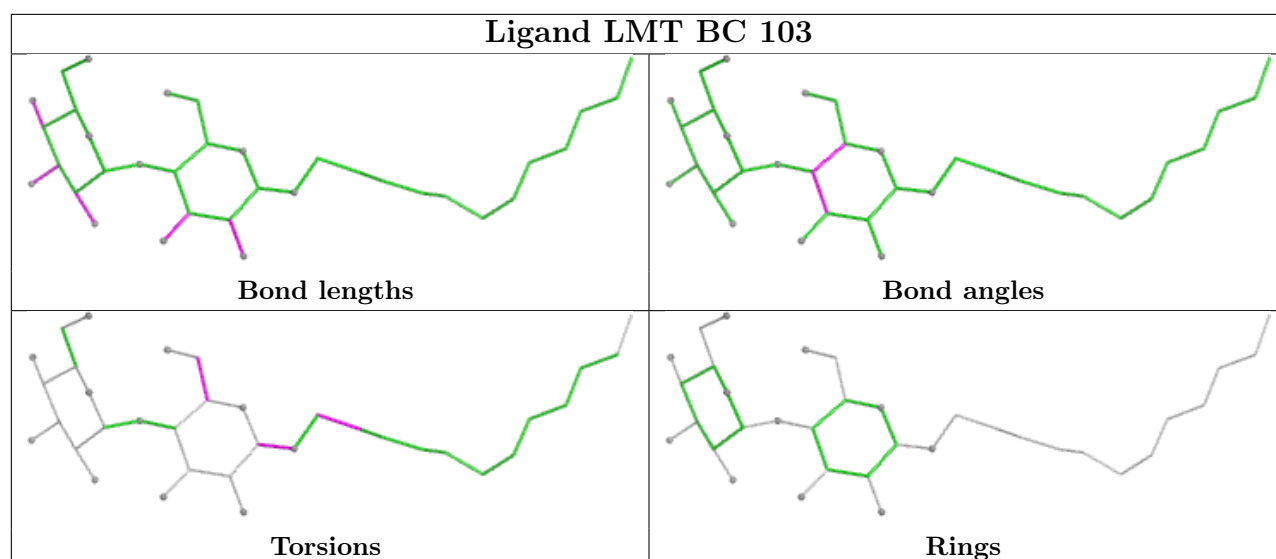


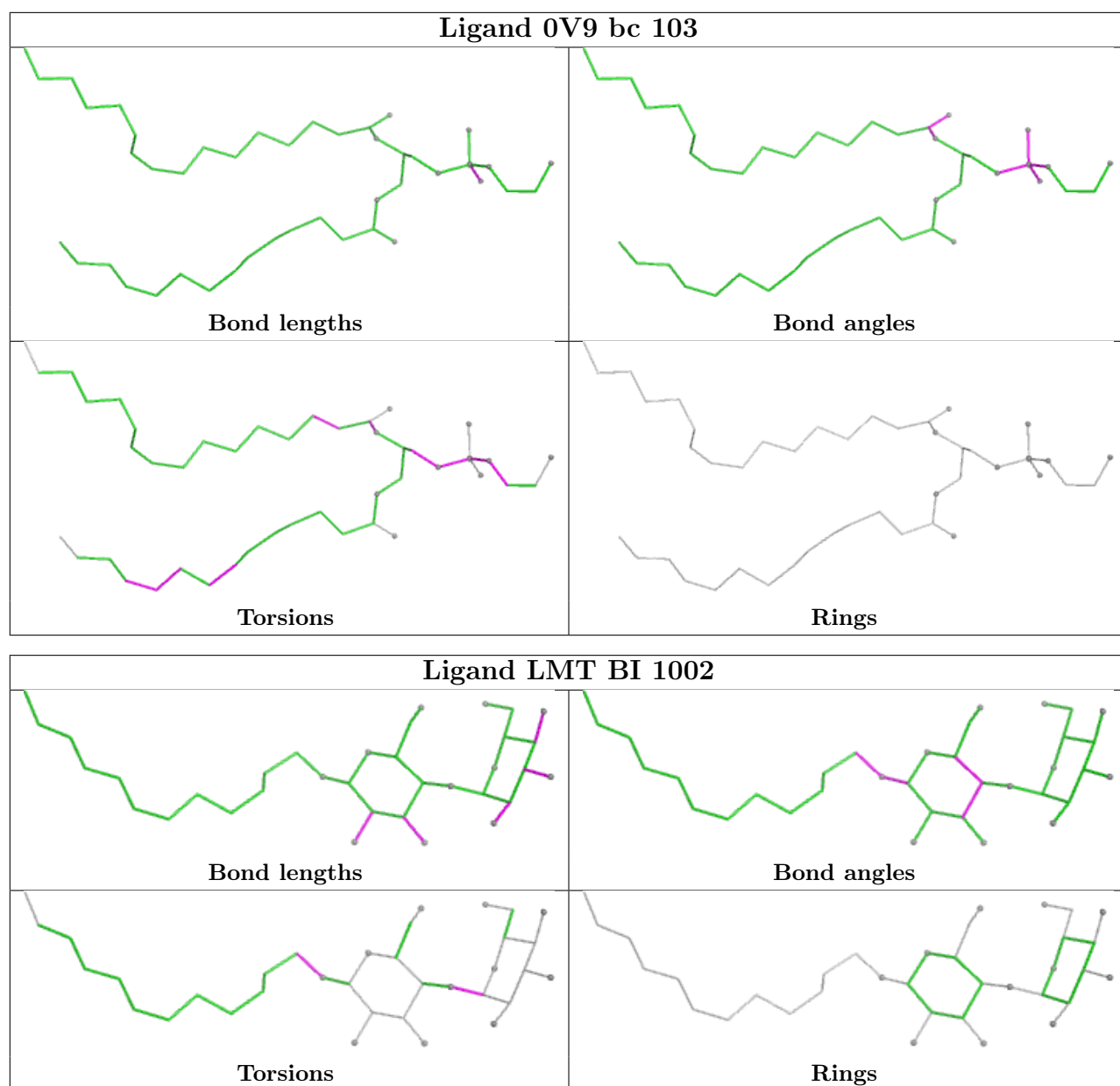
Ligand LMT BR 1005



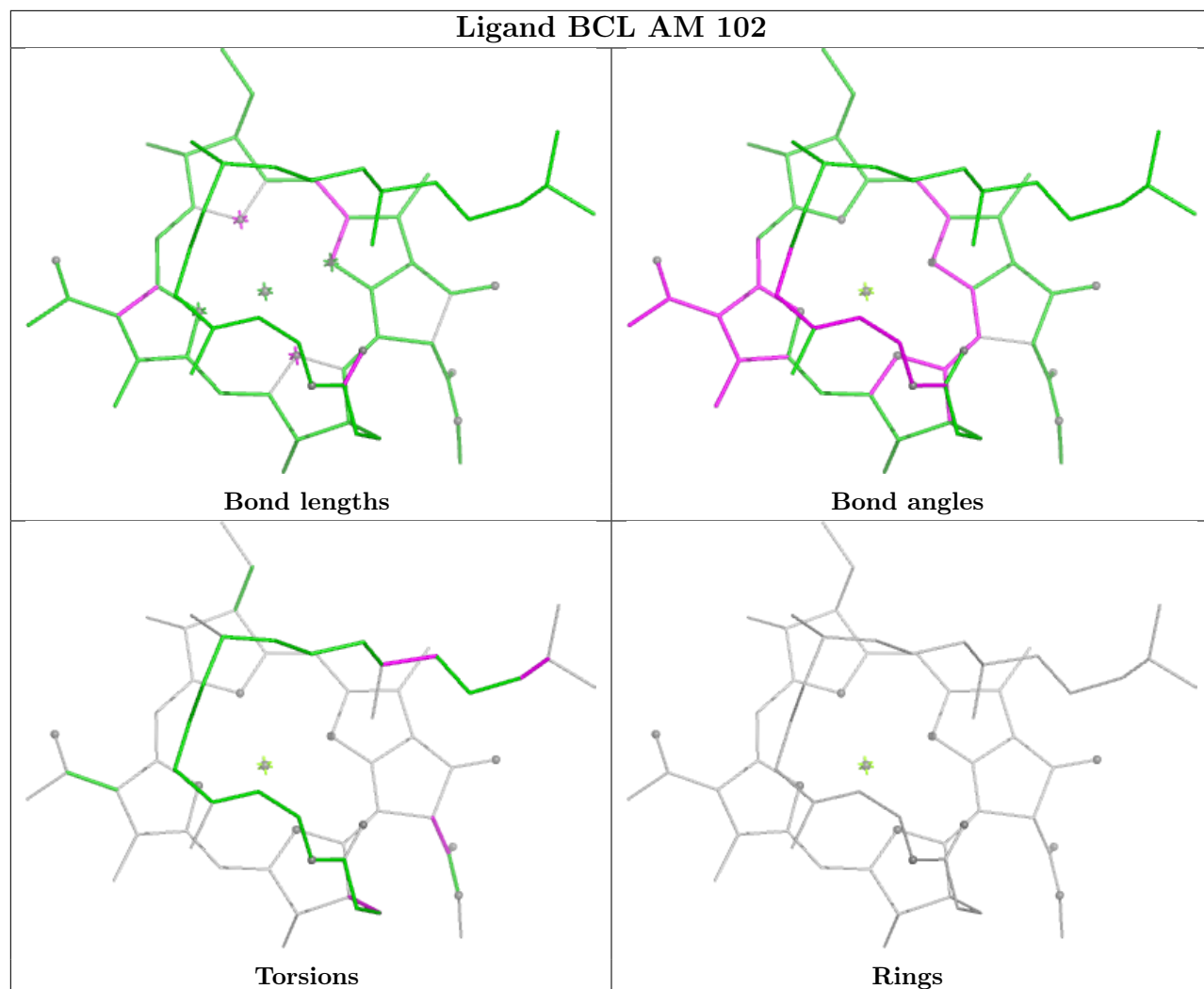
Ligand BCL M 408



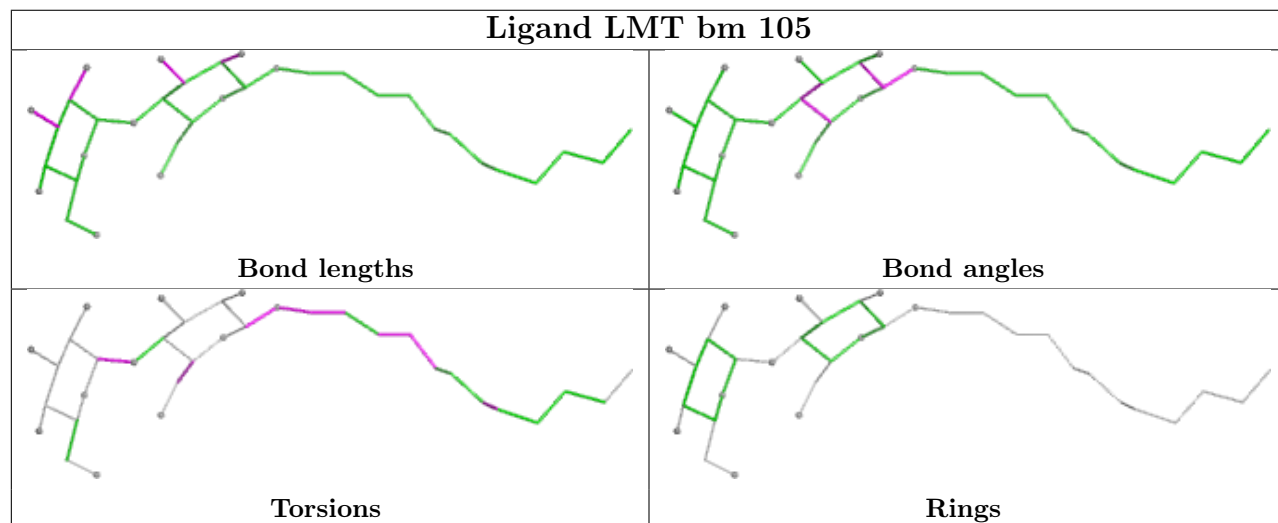


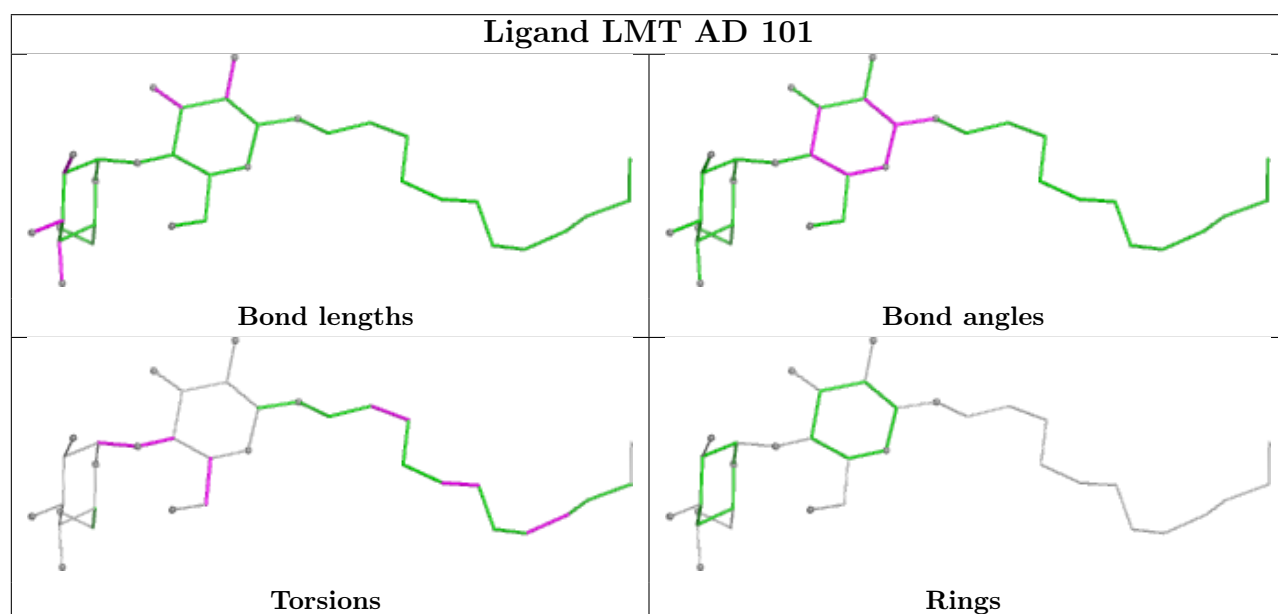
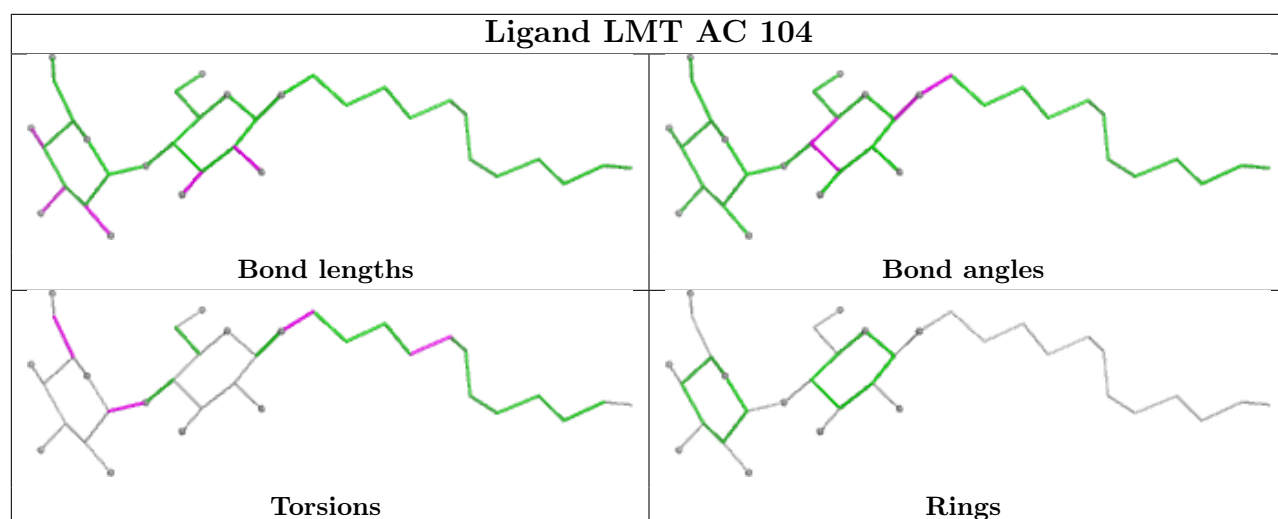


Ligand BCL AM 102

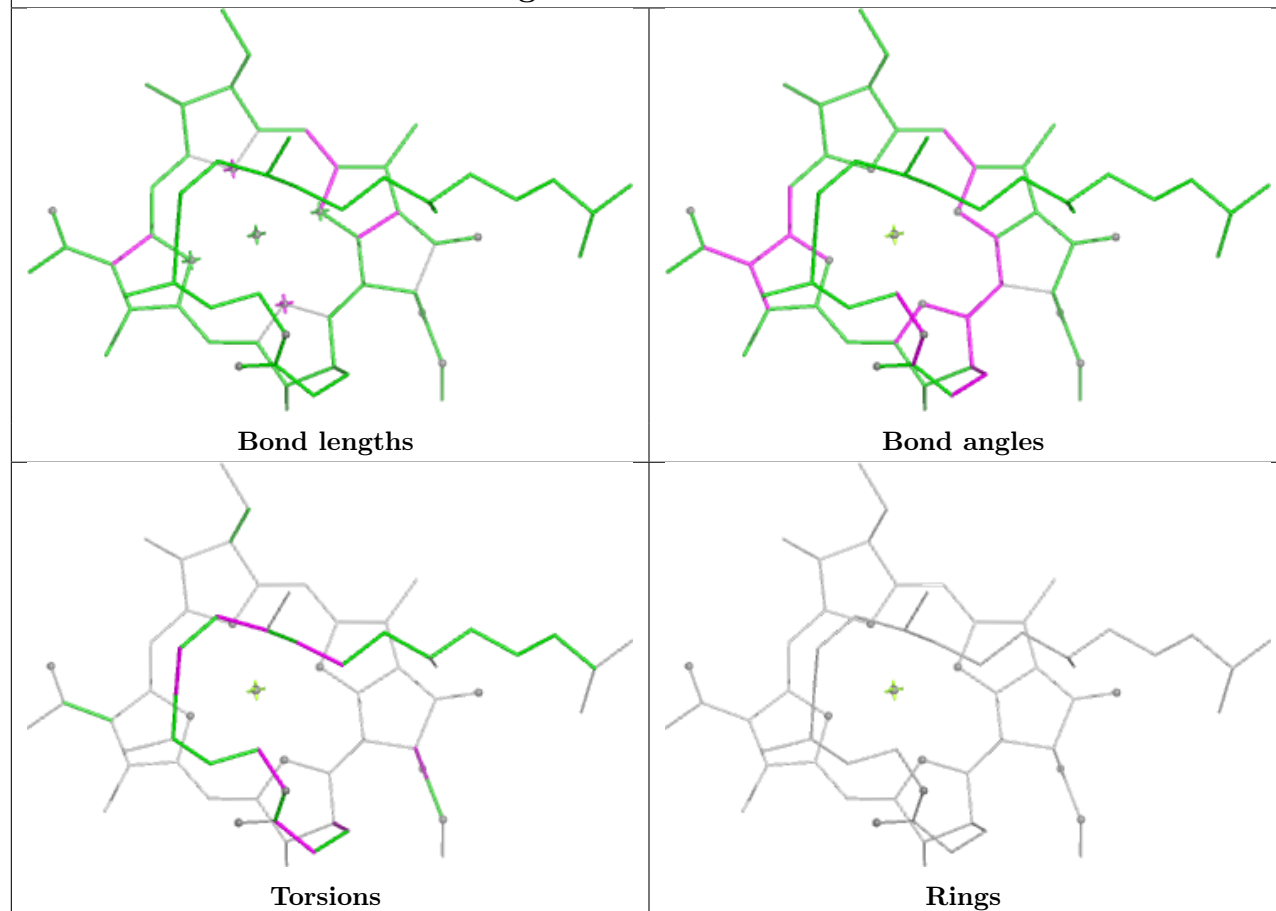


Ligand LMT bm 105

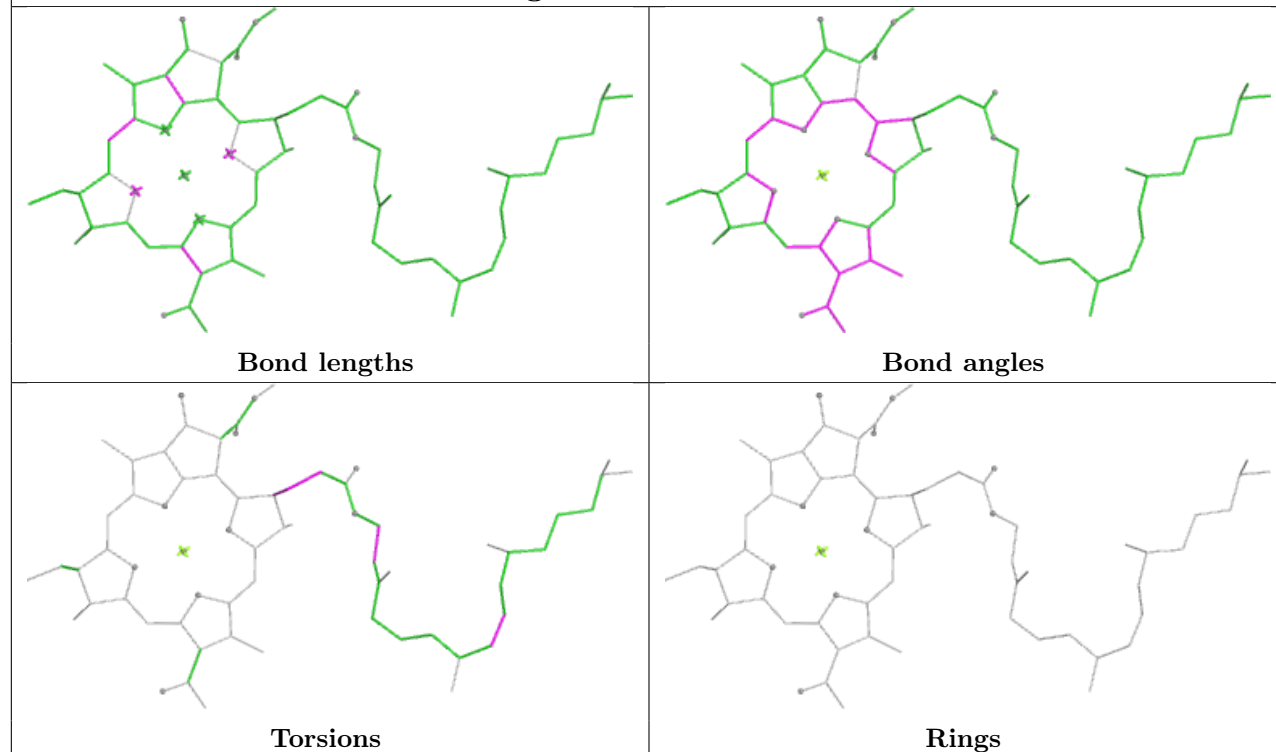


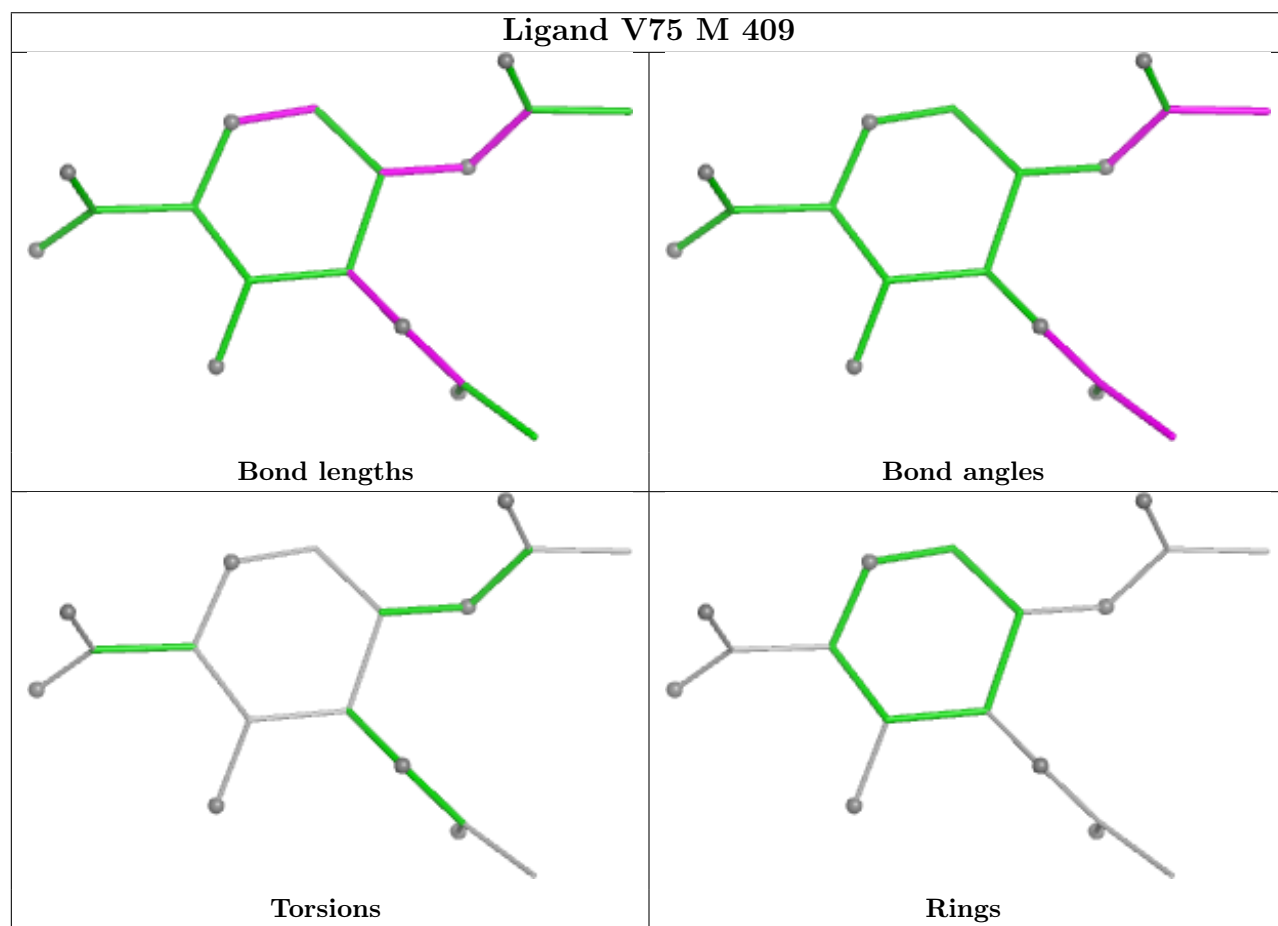
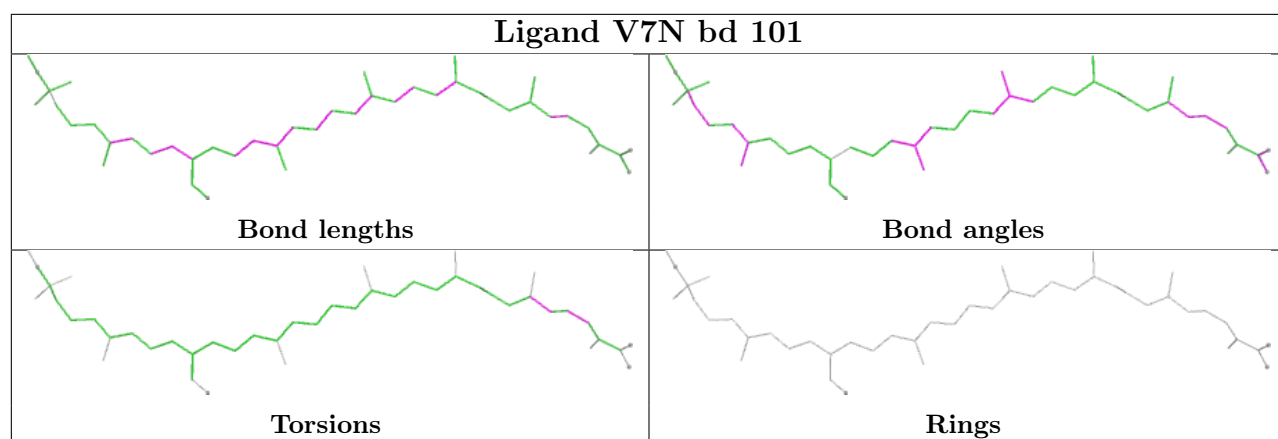


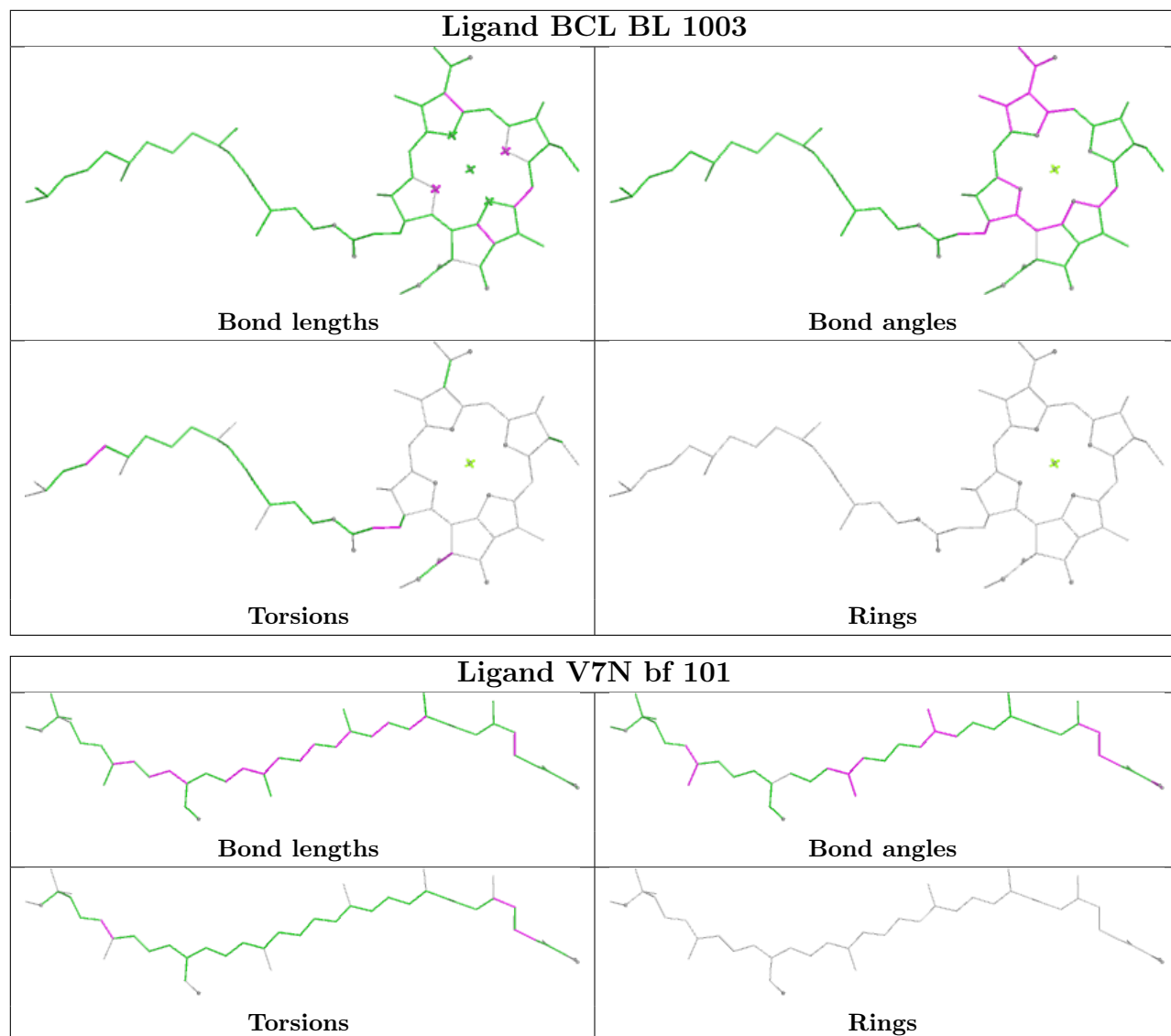
Ligand BCL AK 101

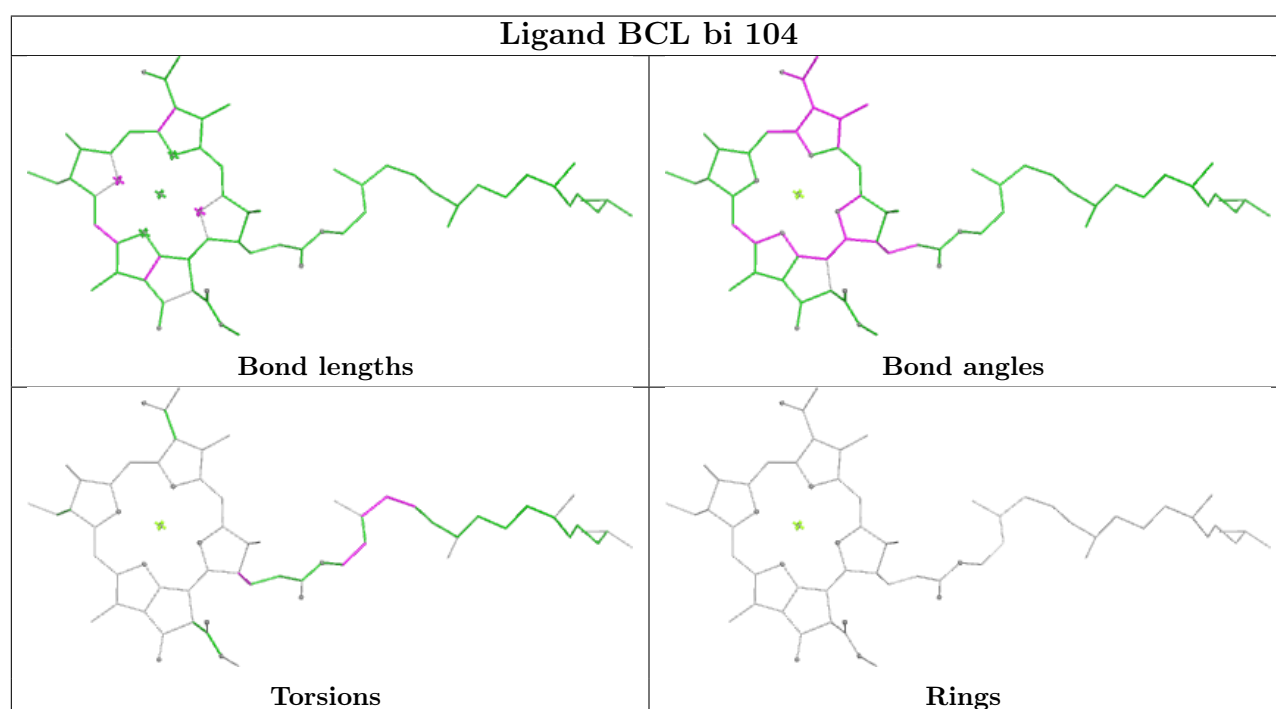
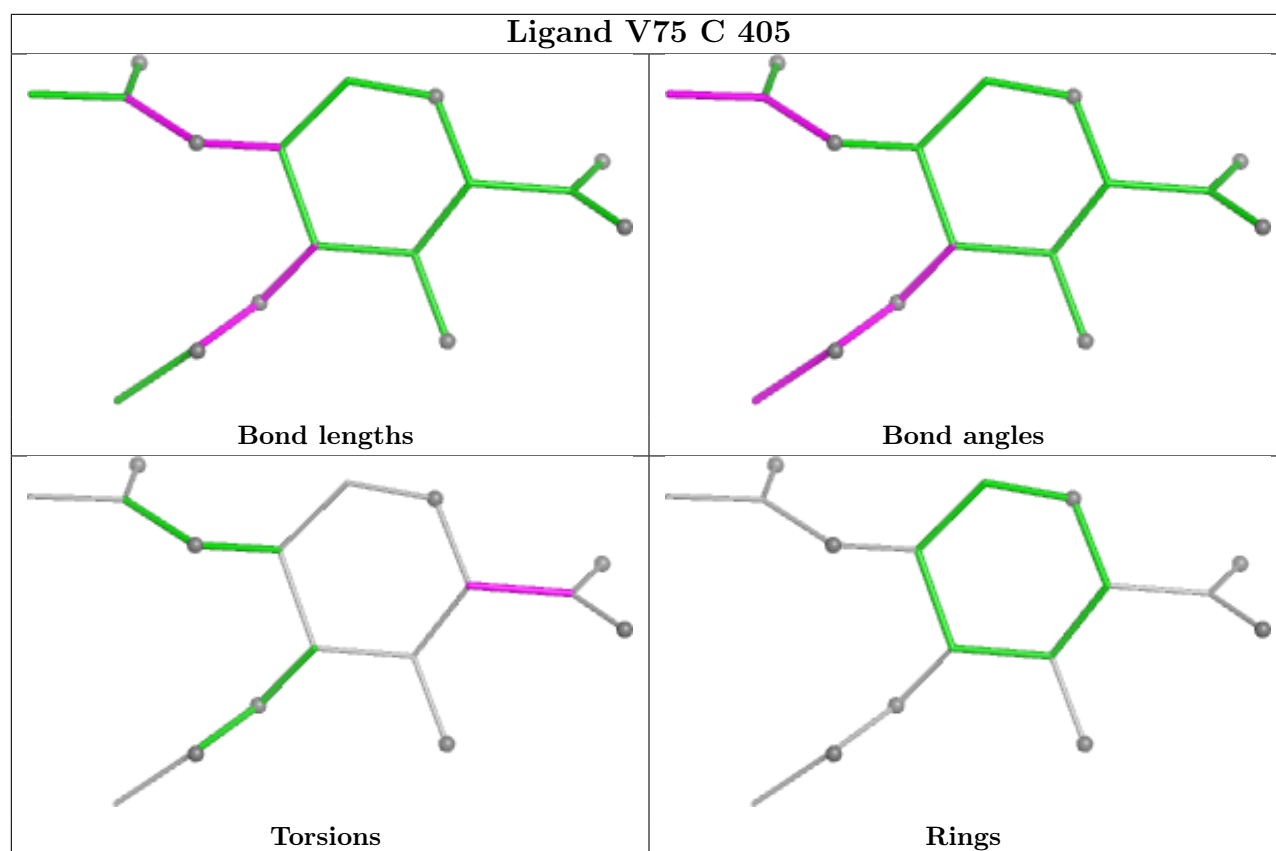


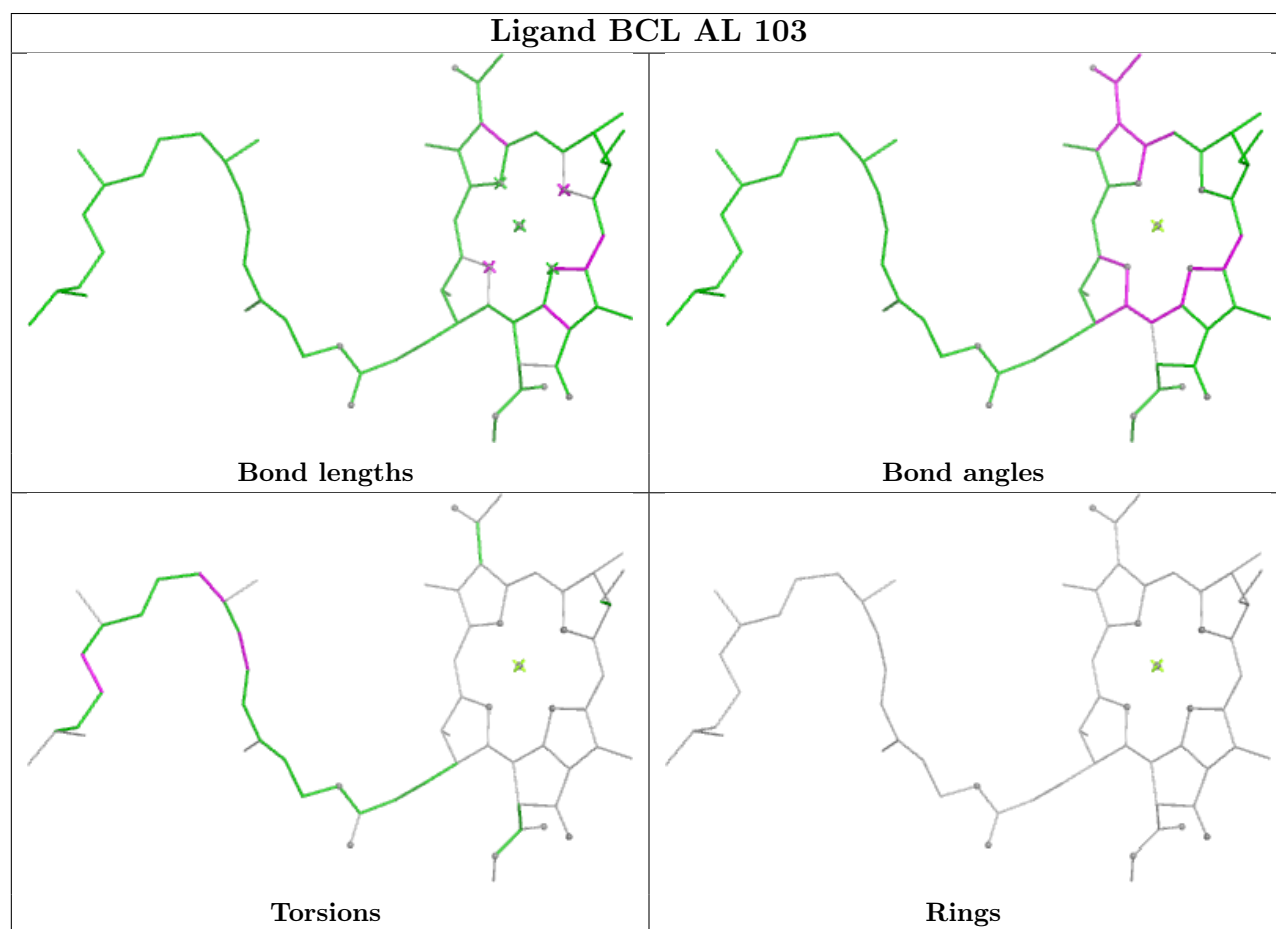
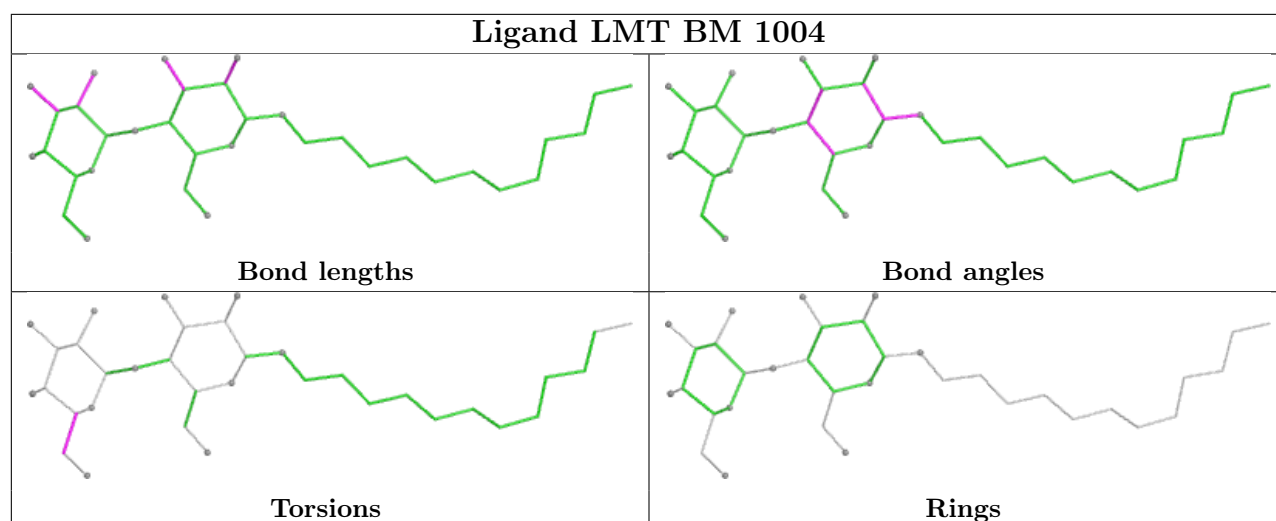
Ligand BCL bd 102

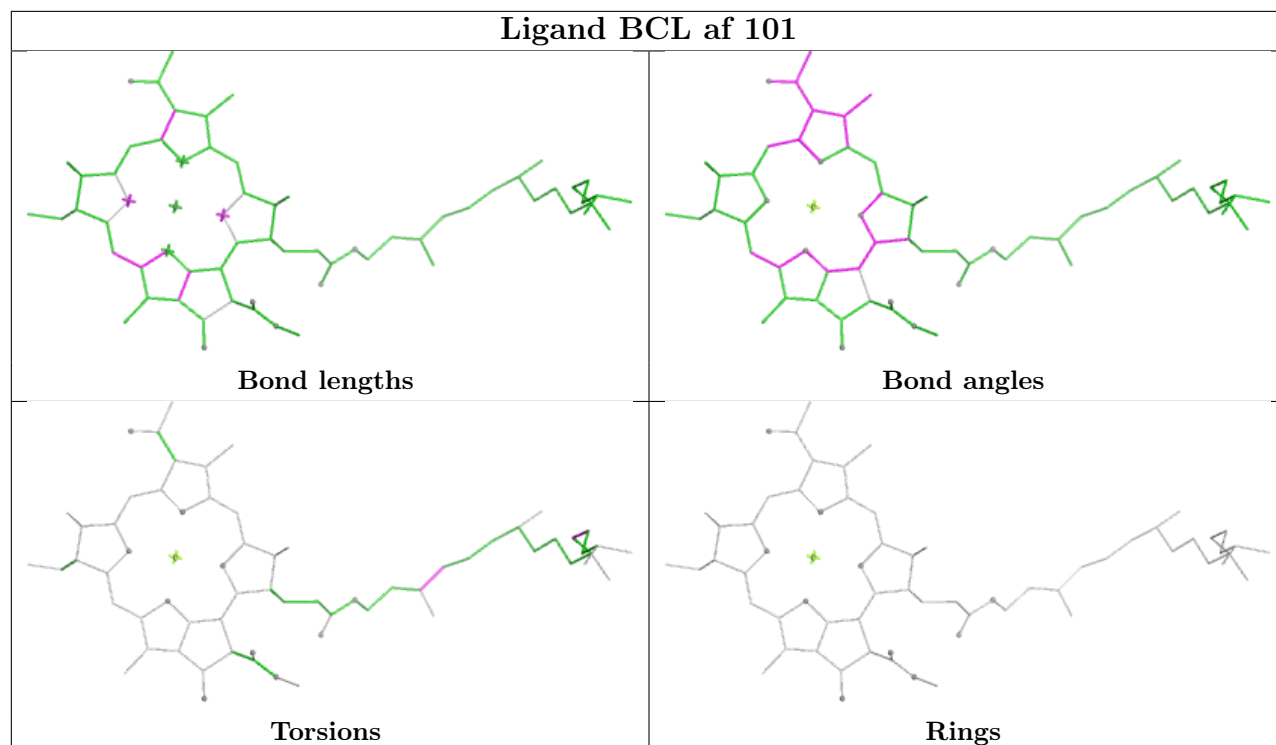
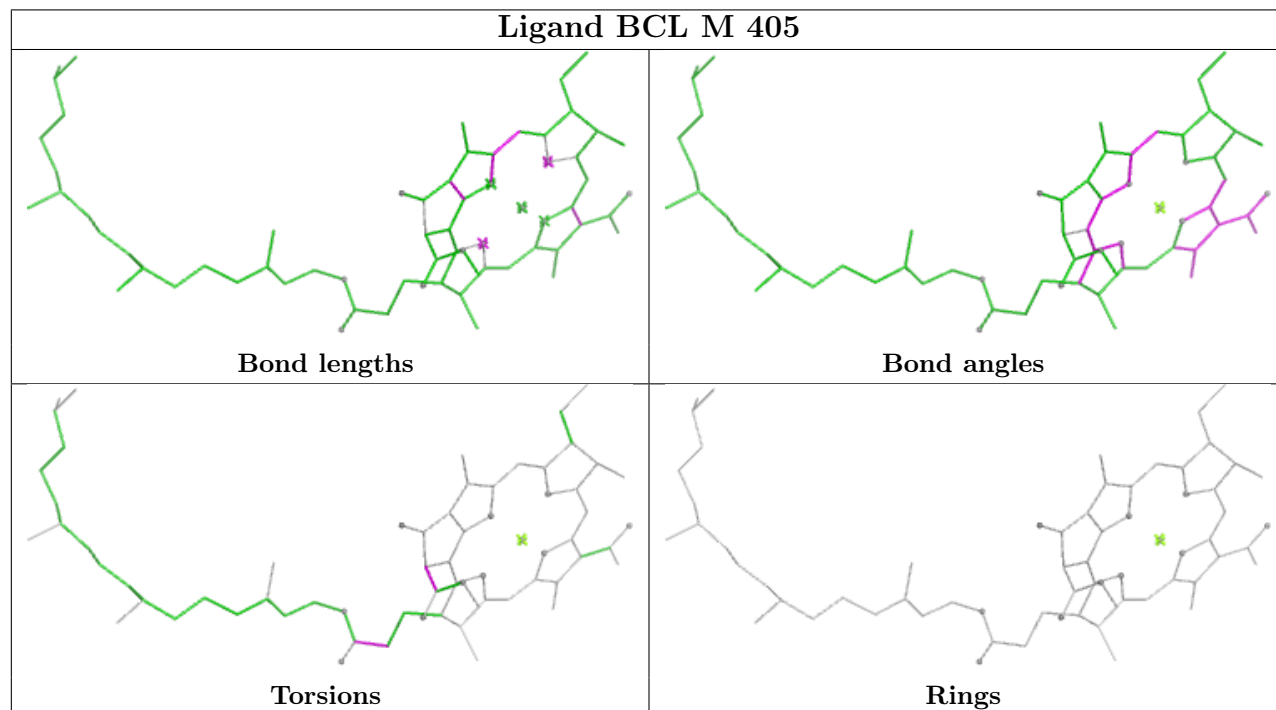


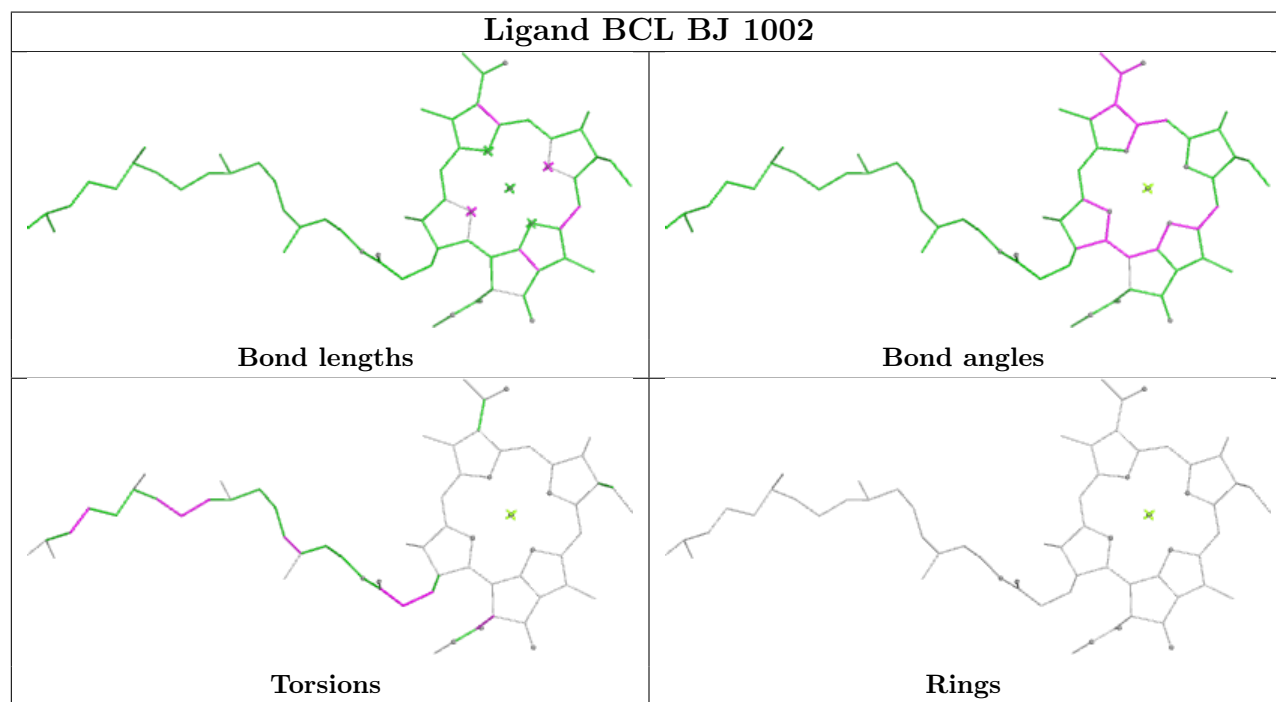
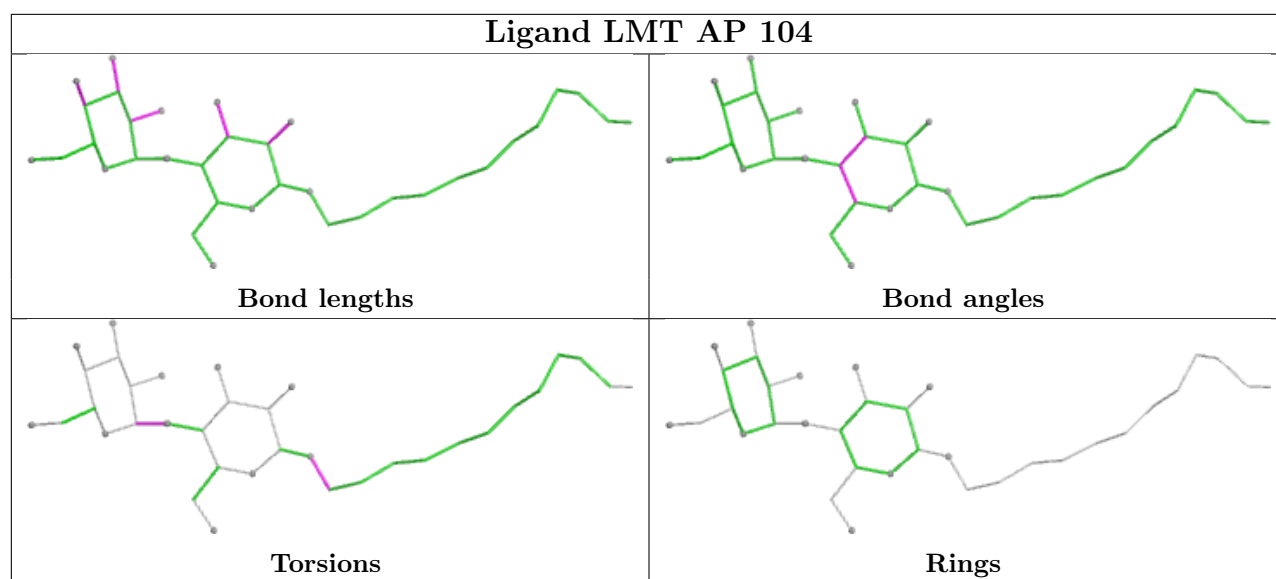


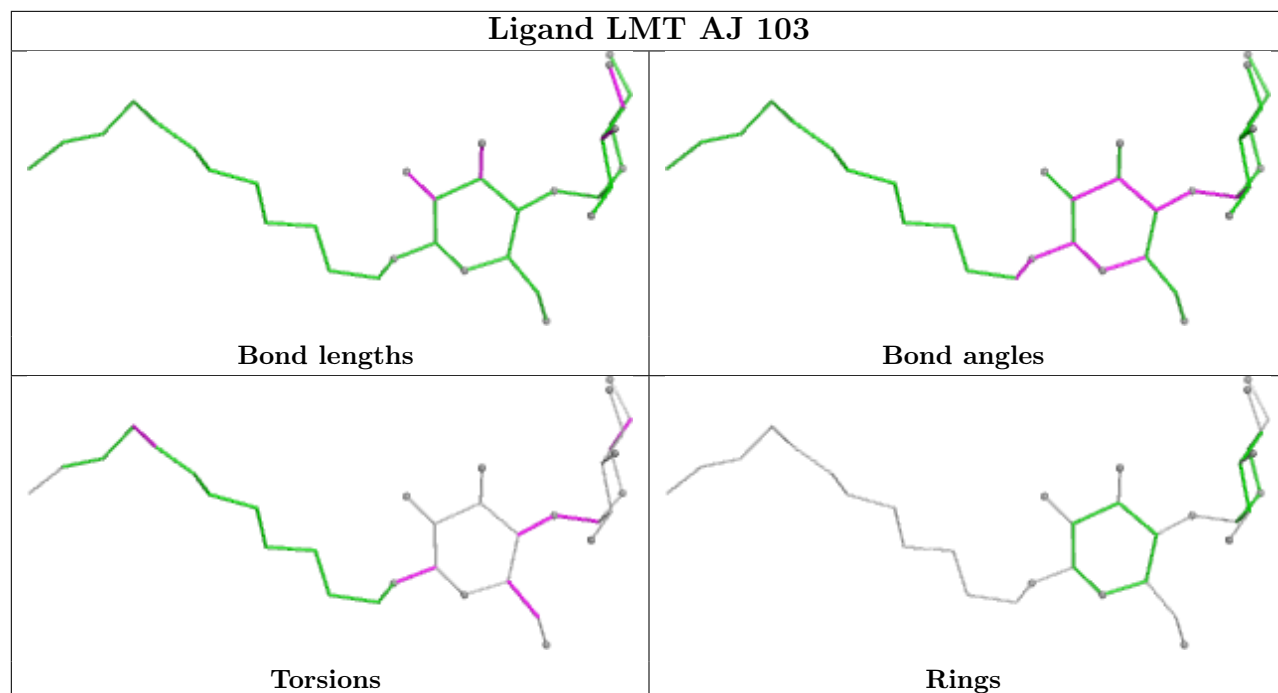
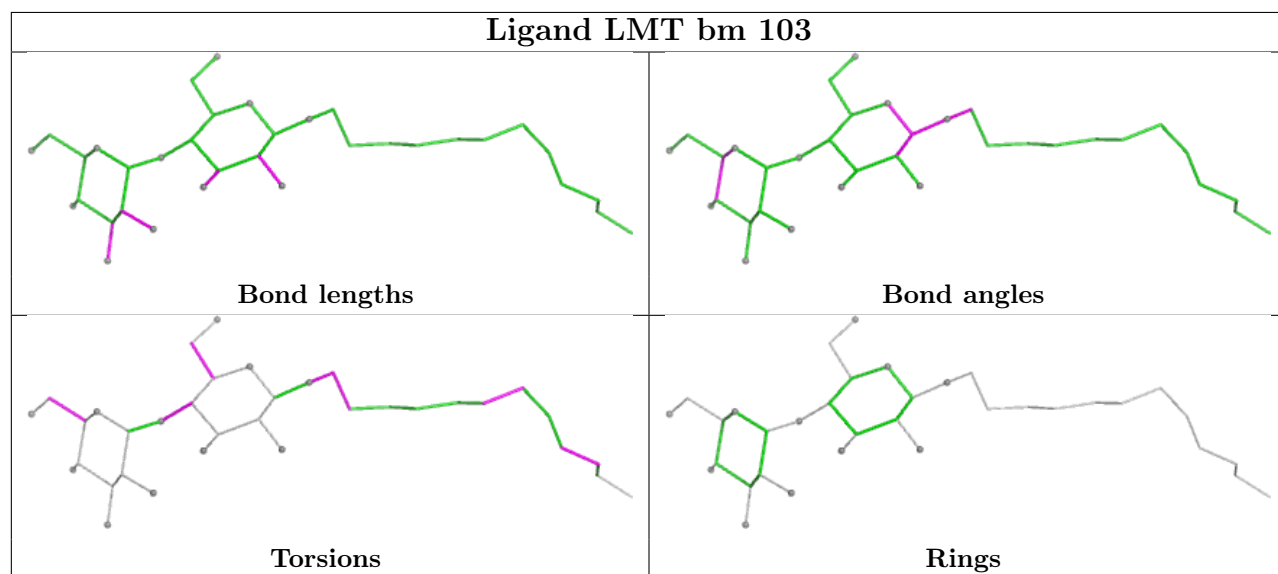


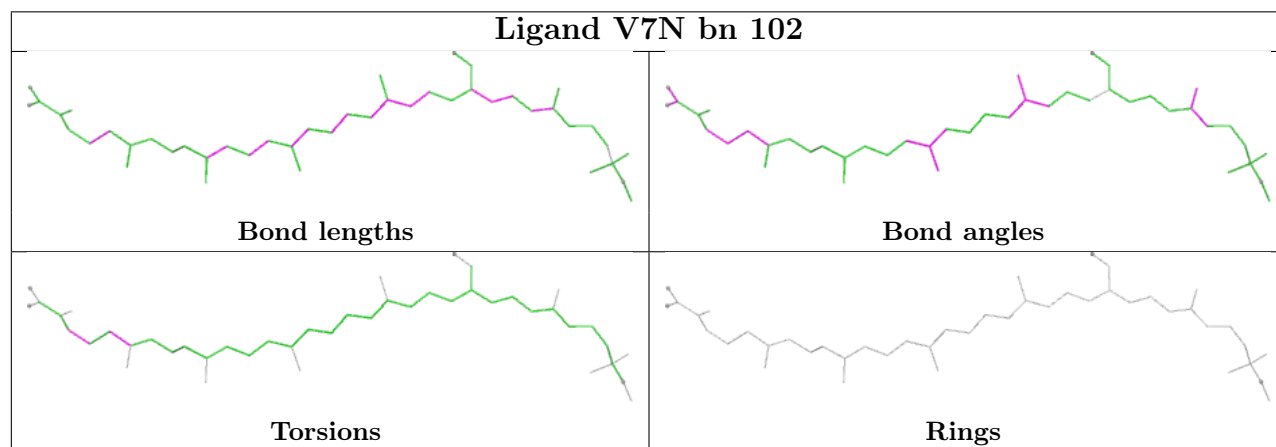
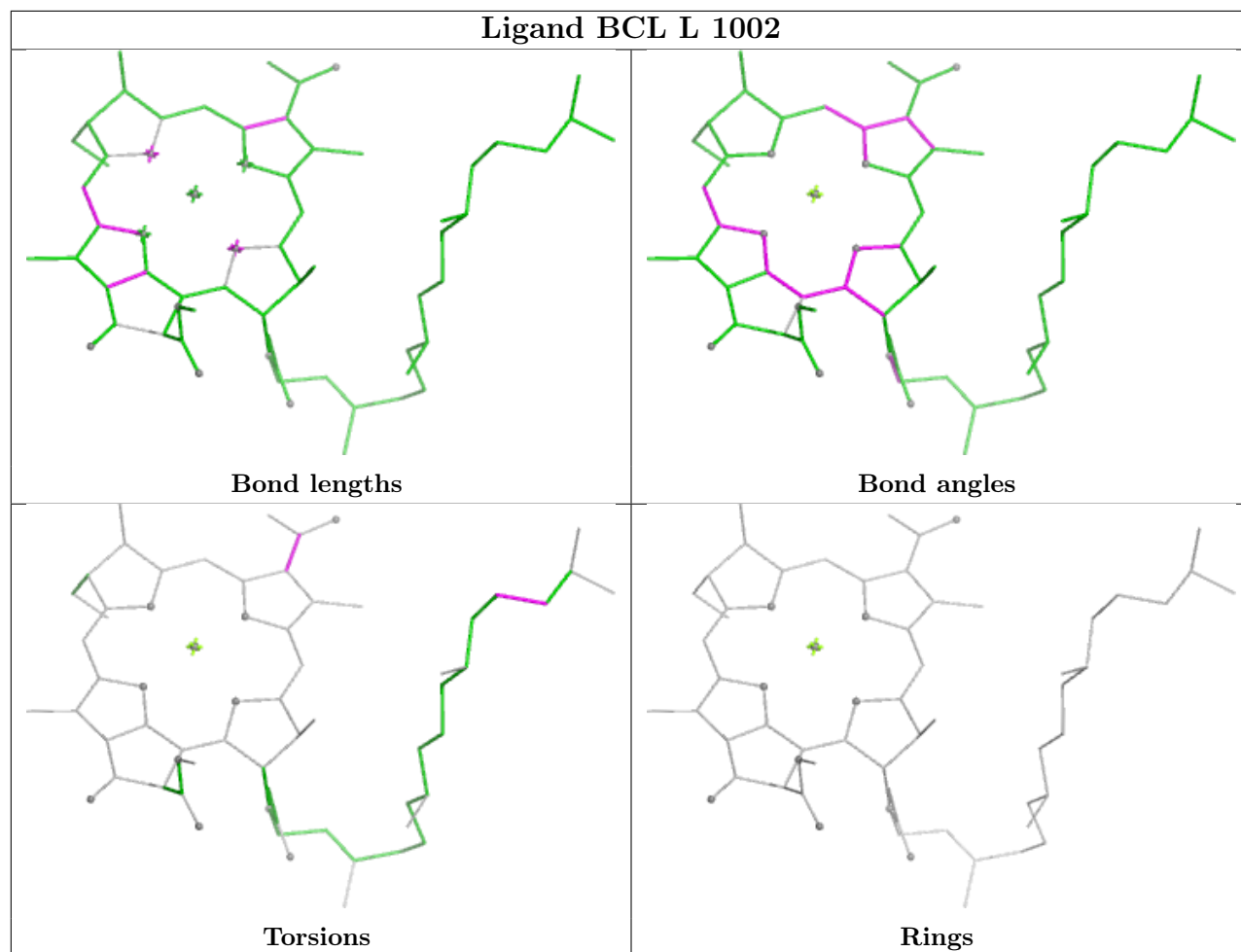


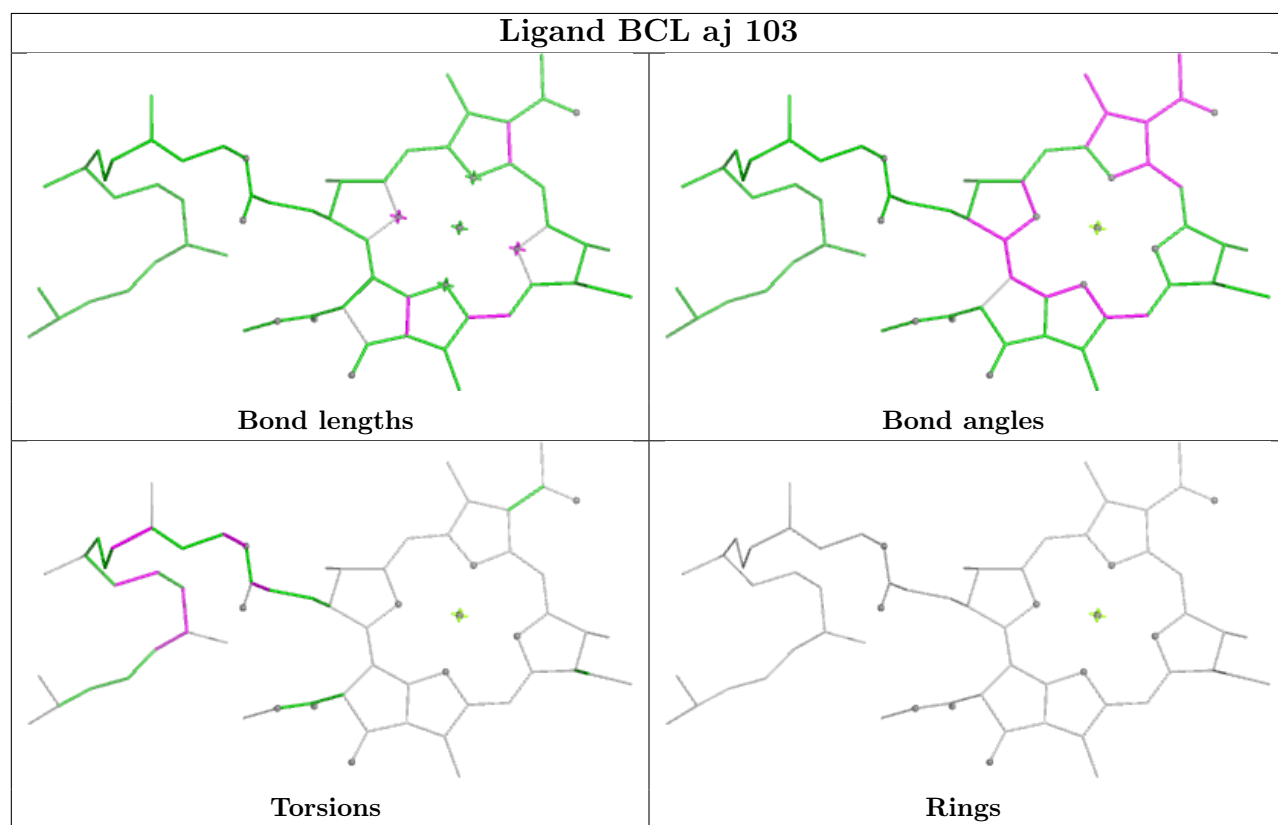
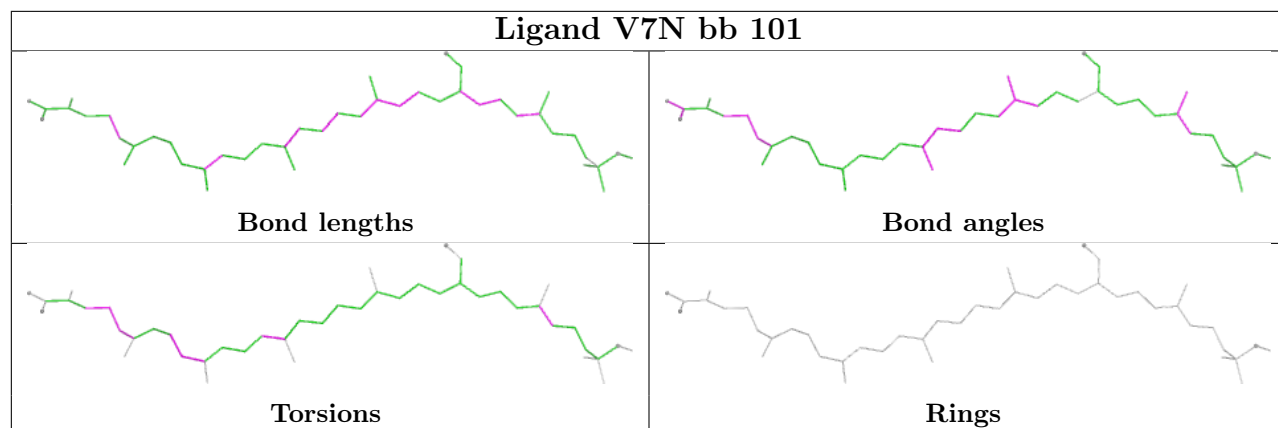


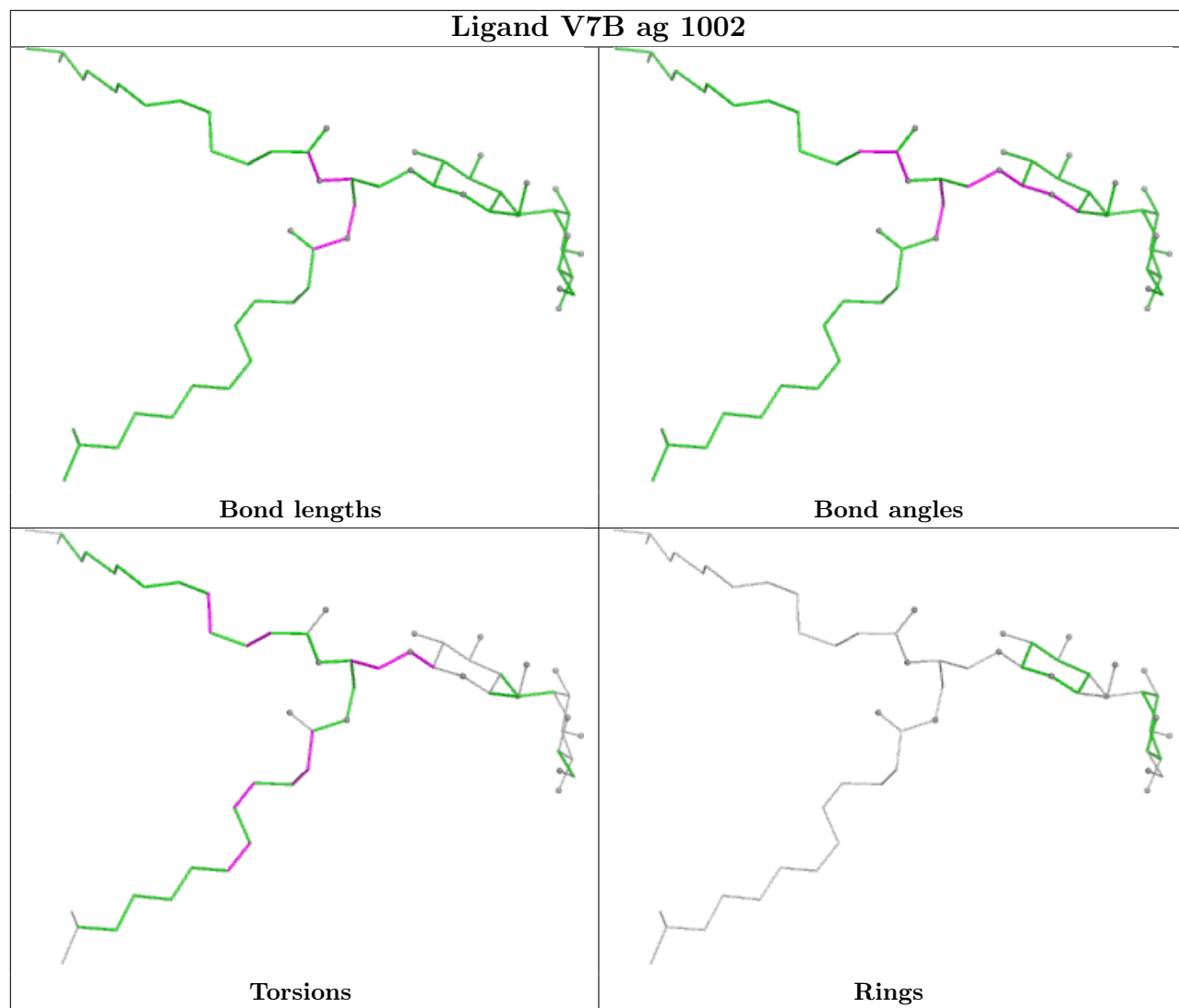
Ligand BCL af 101**Ligand BCL M 405**

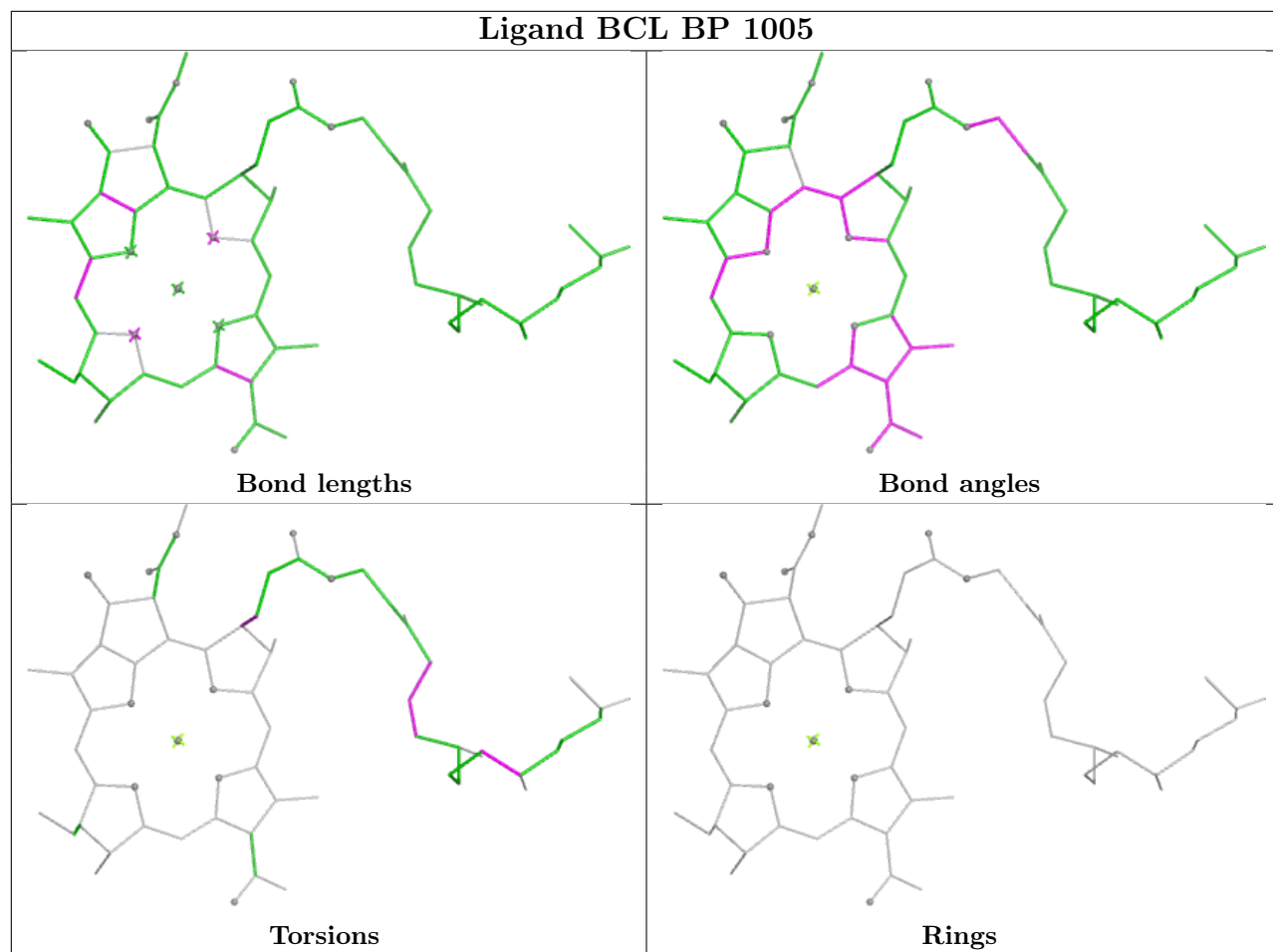


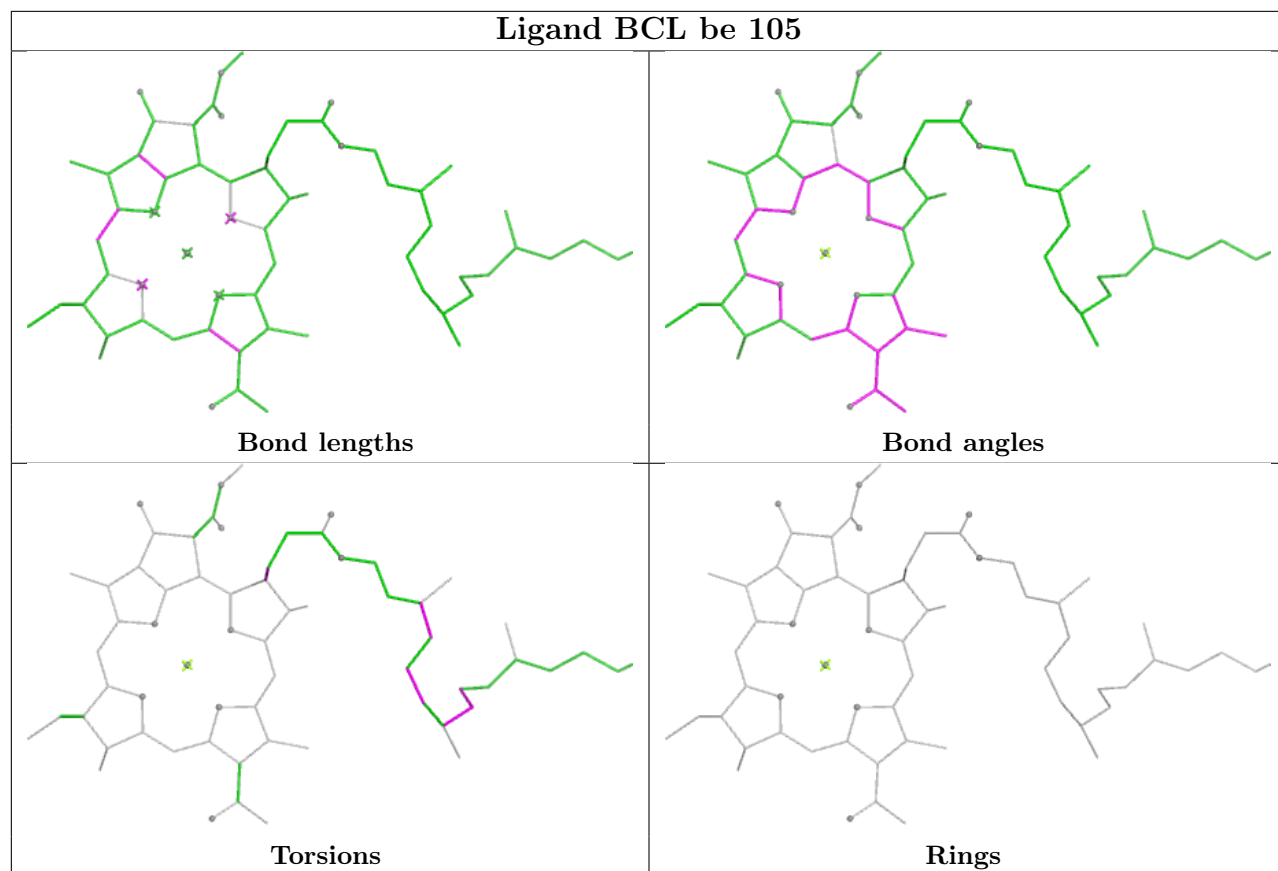
Ligand LMT AJ 103**Ligand LMT bm 103**

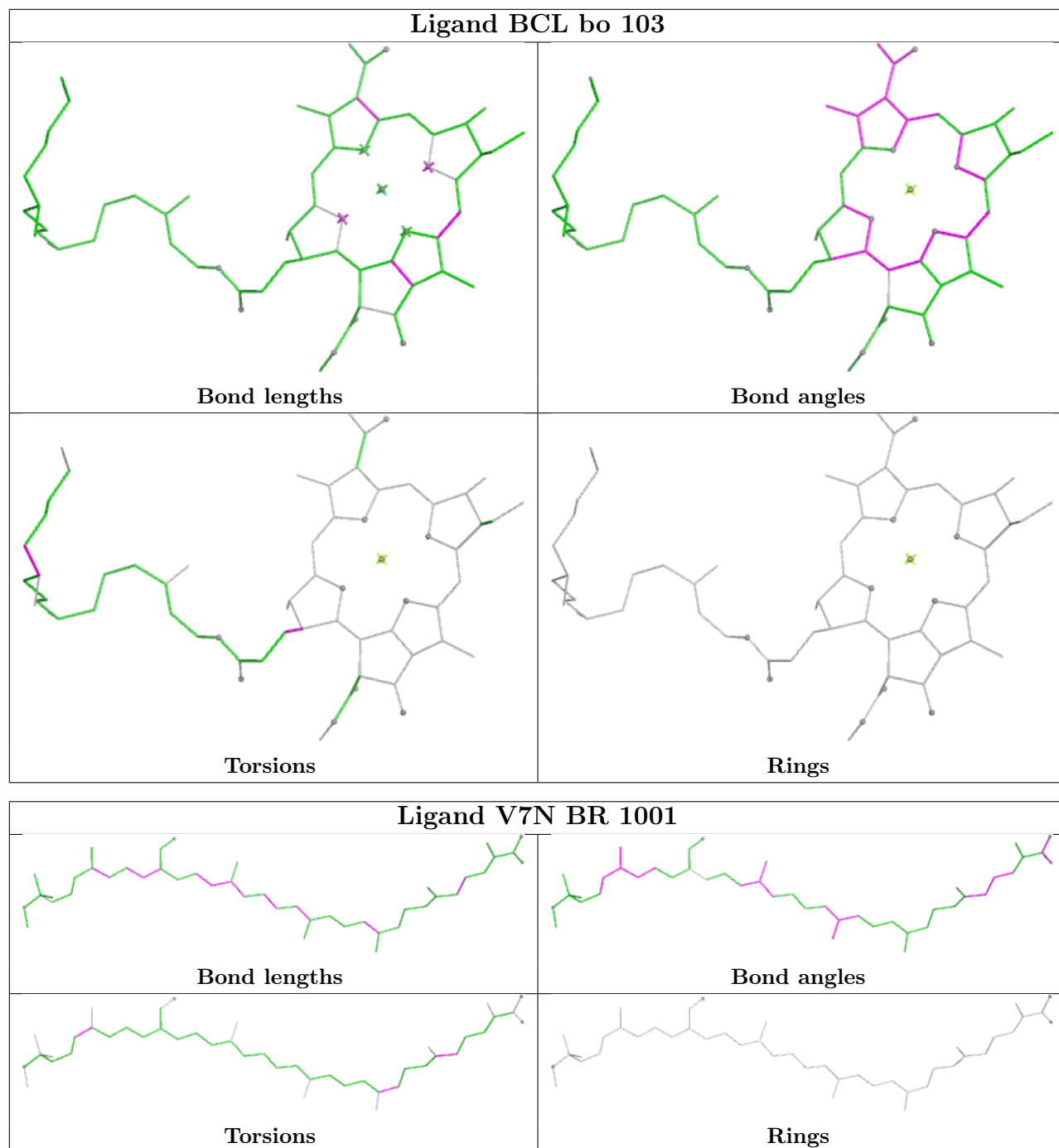


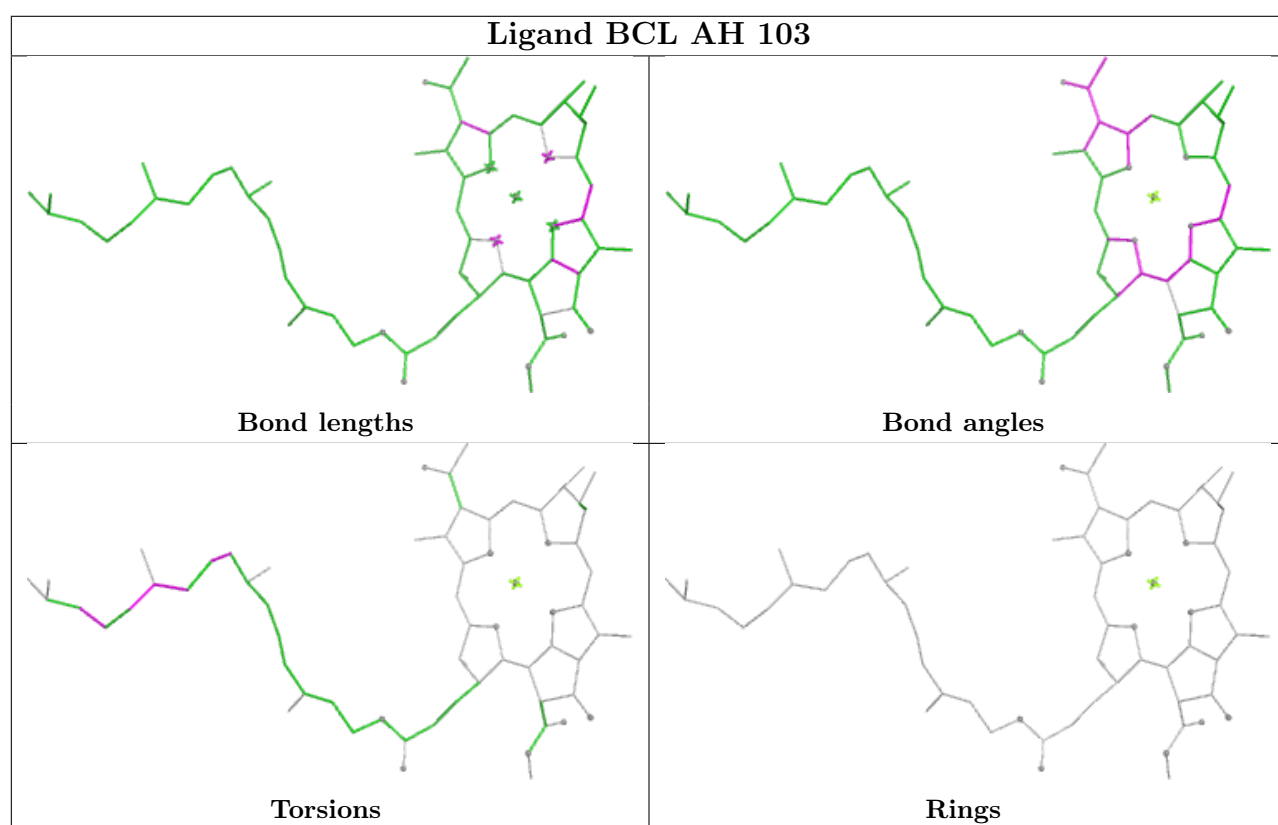
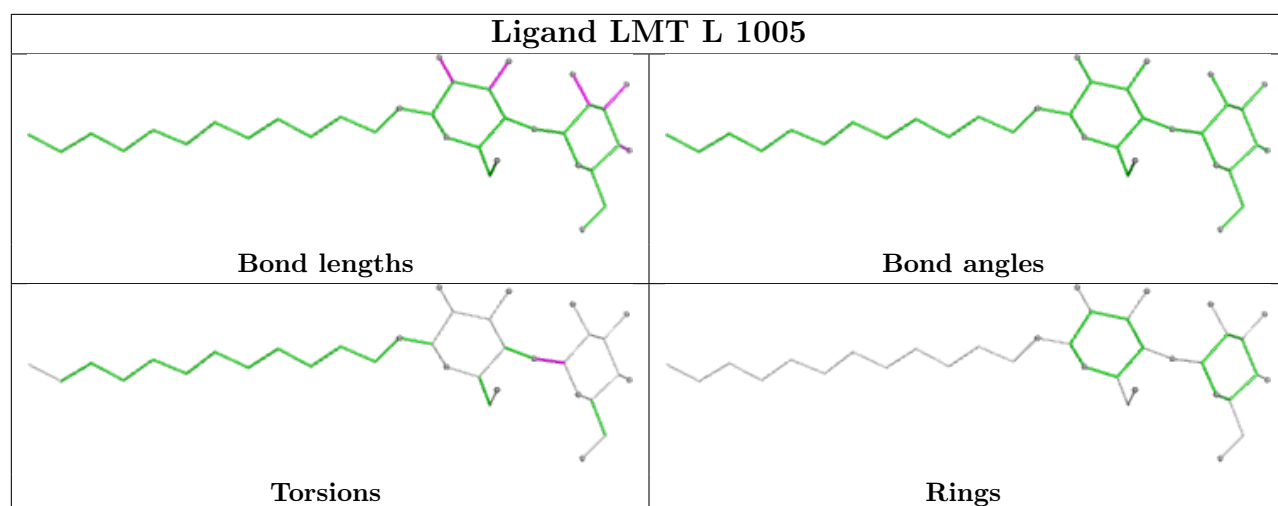


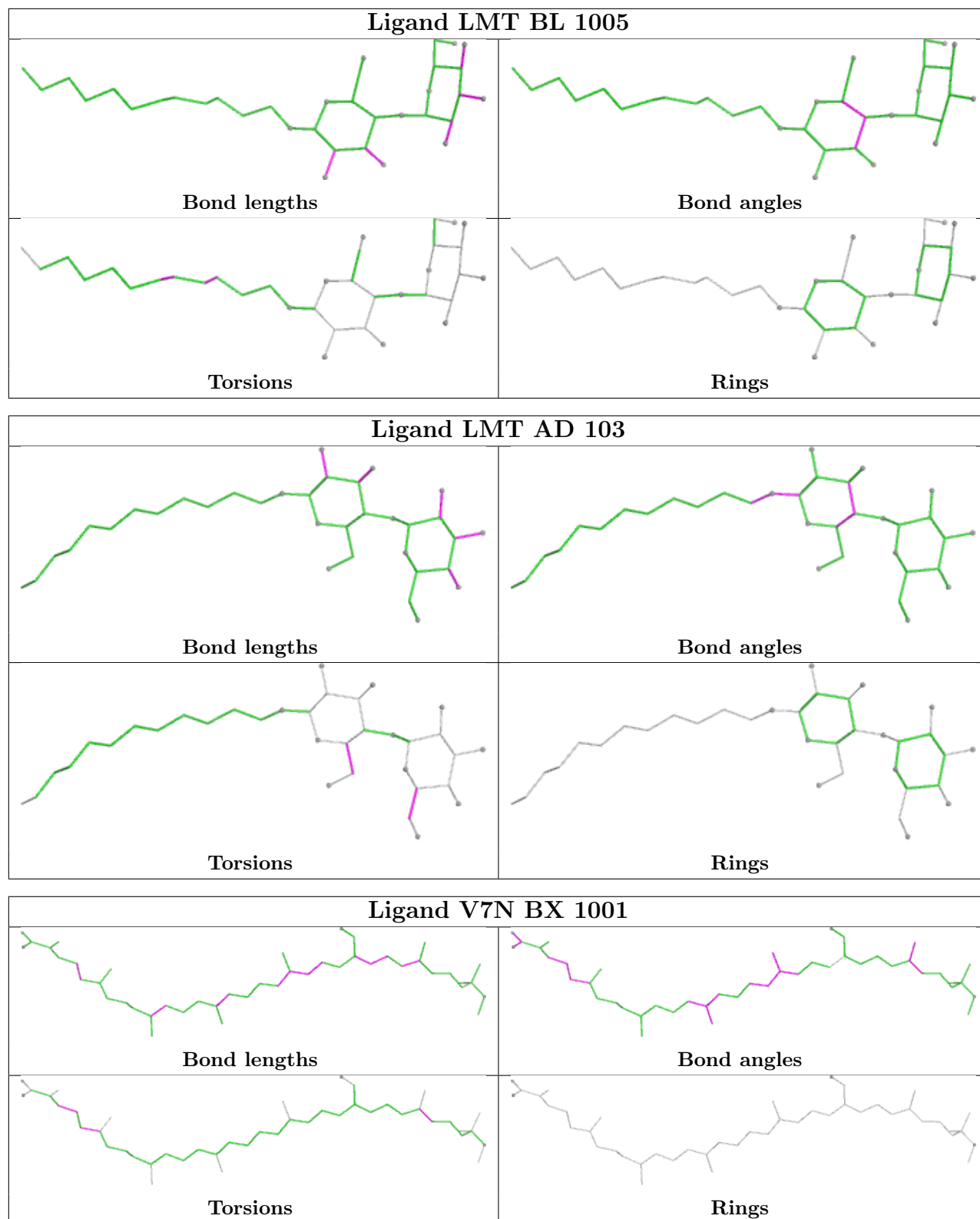


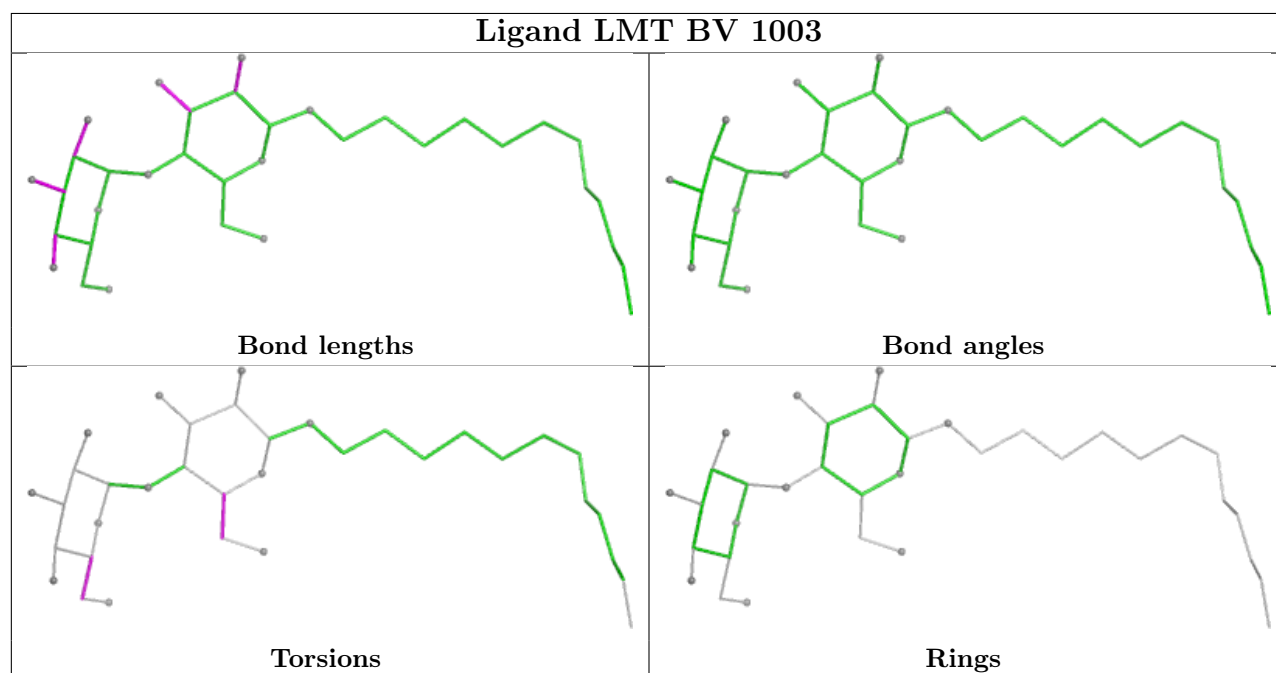
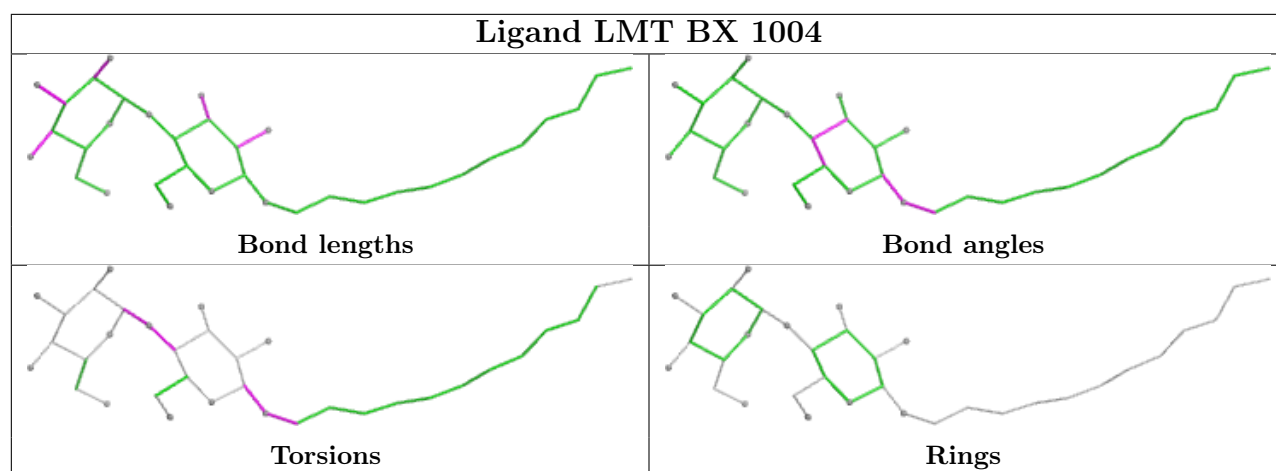


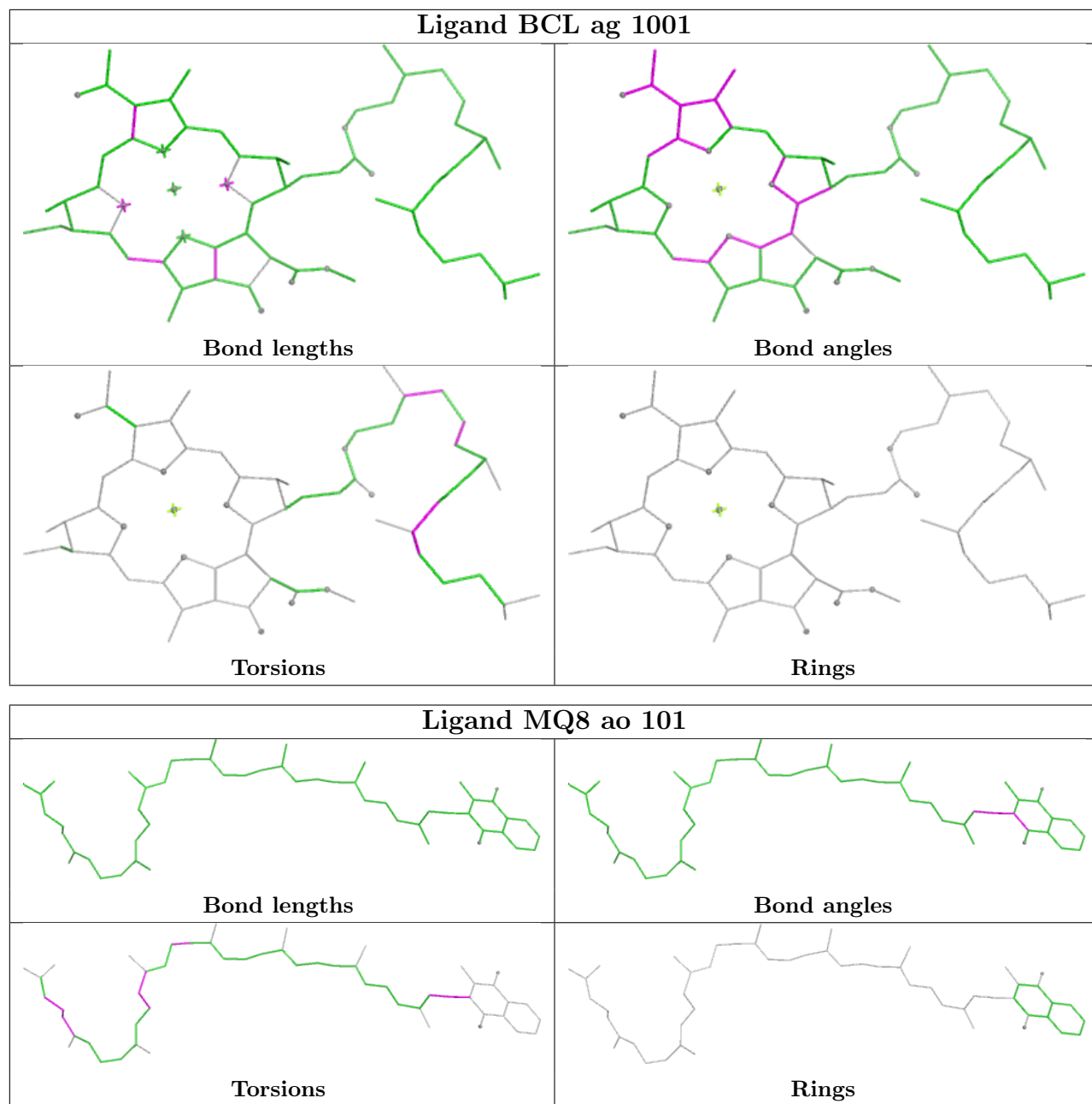


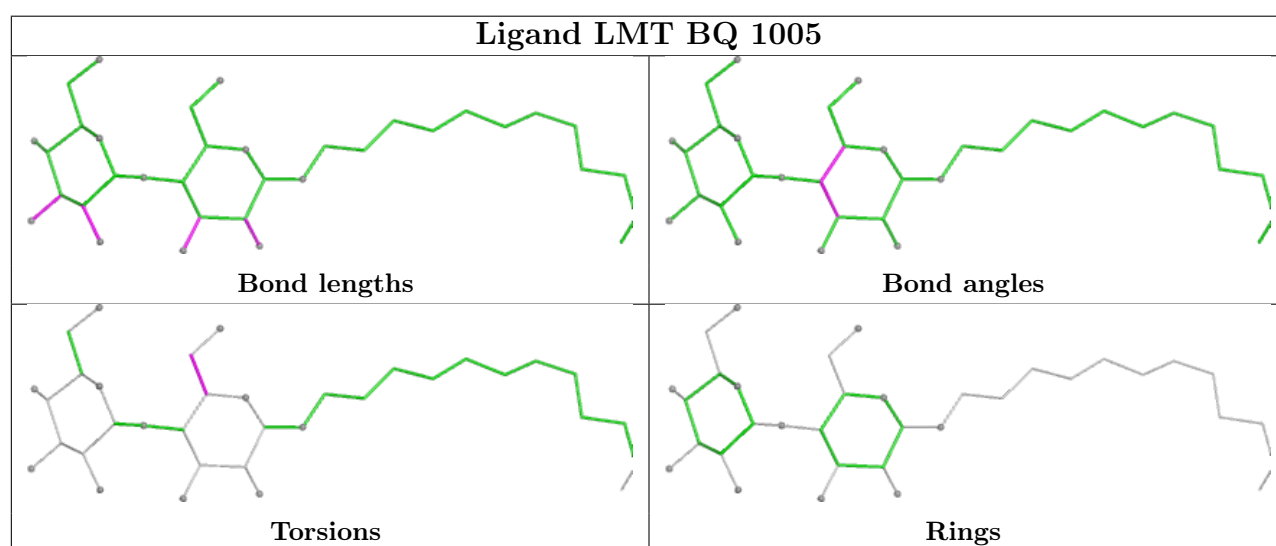
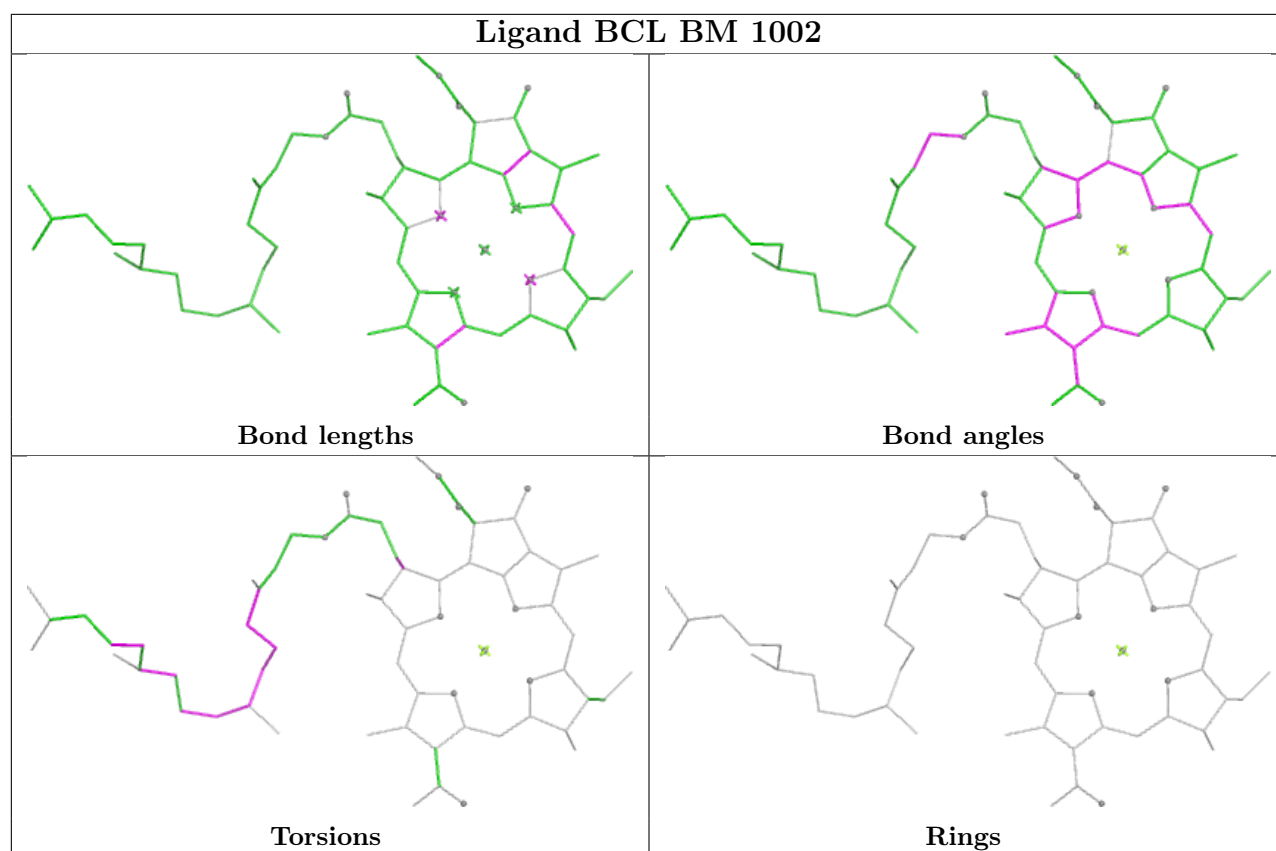


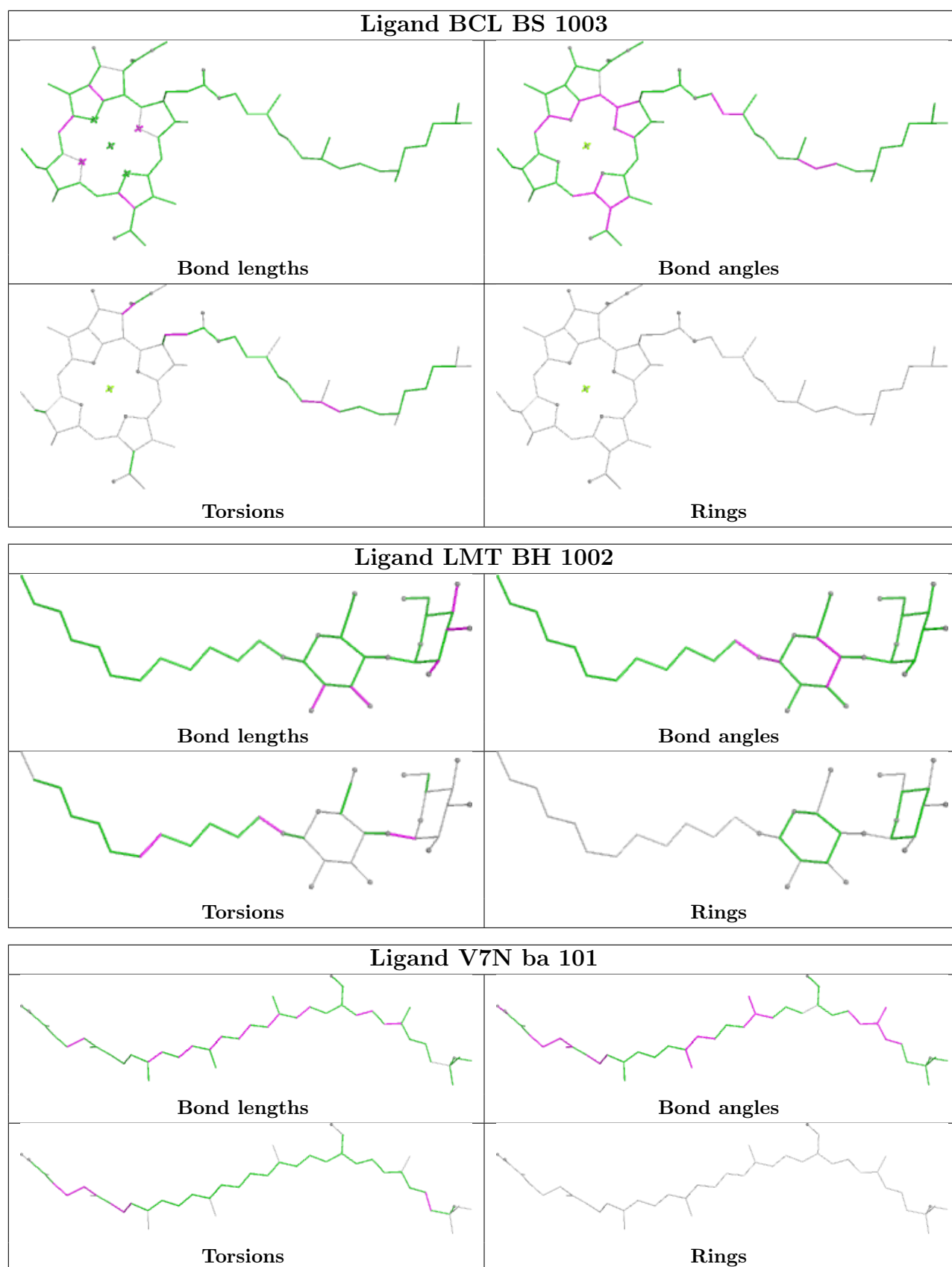


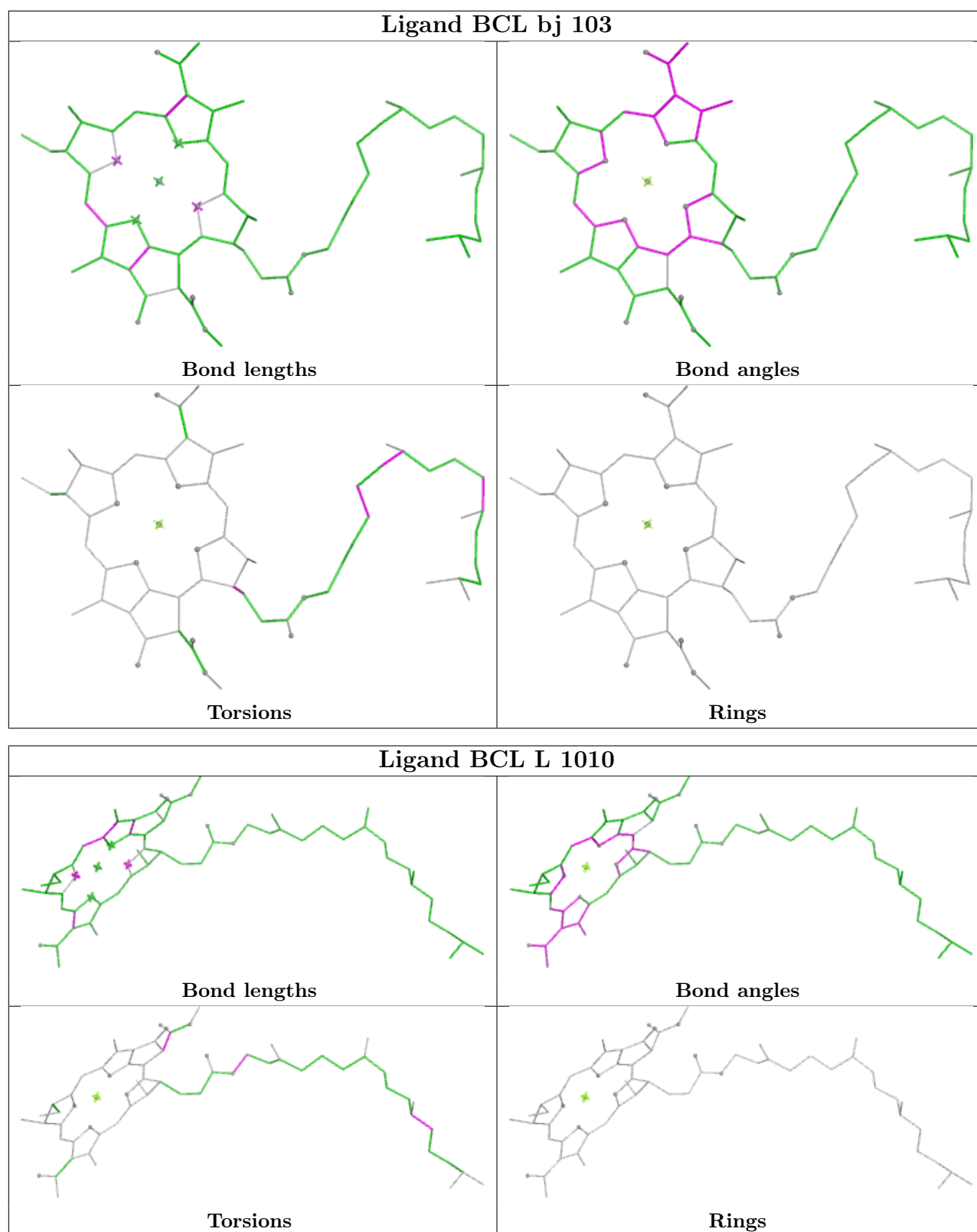


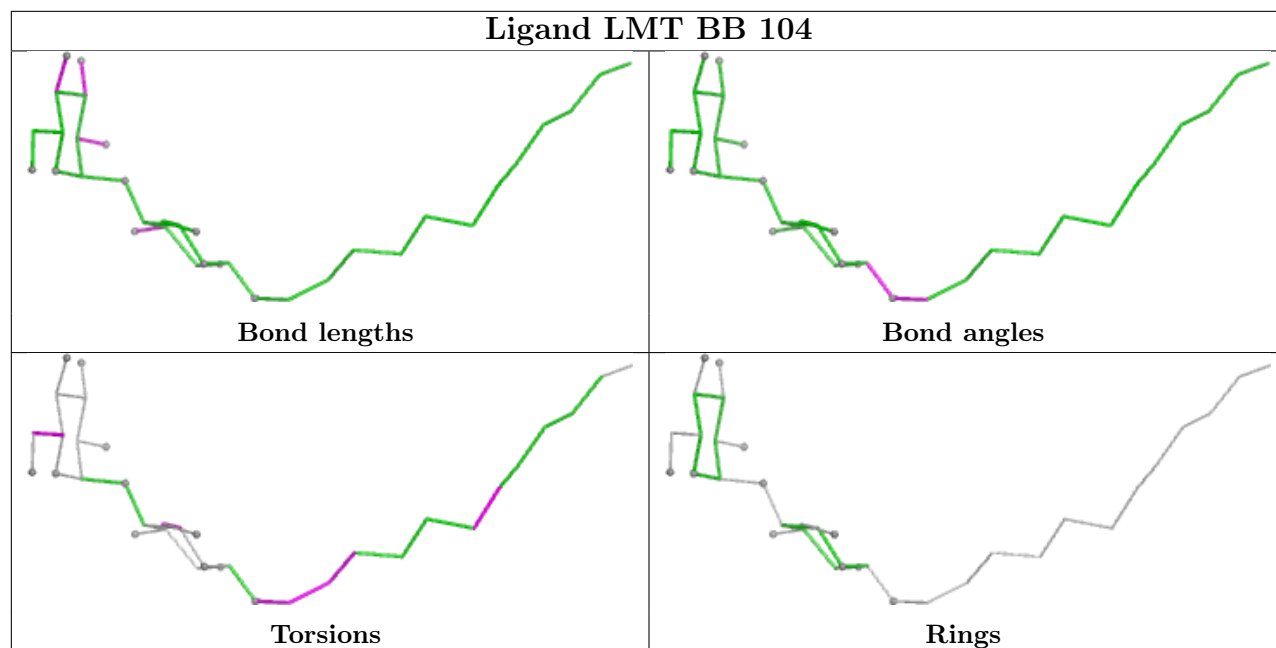
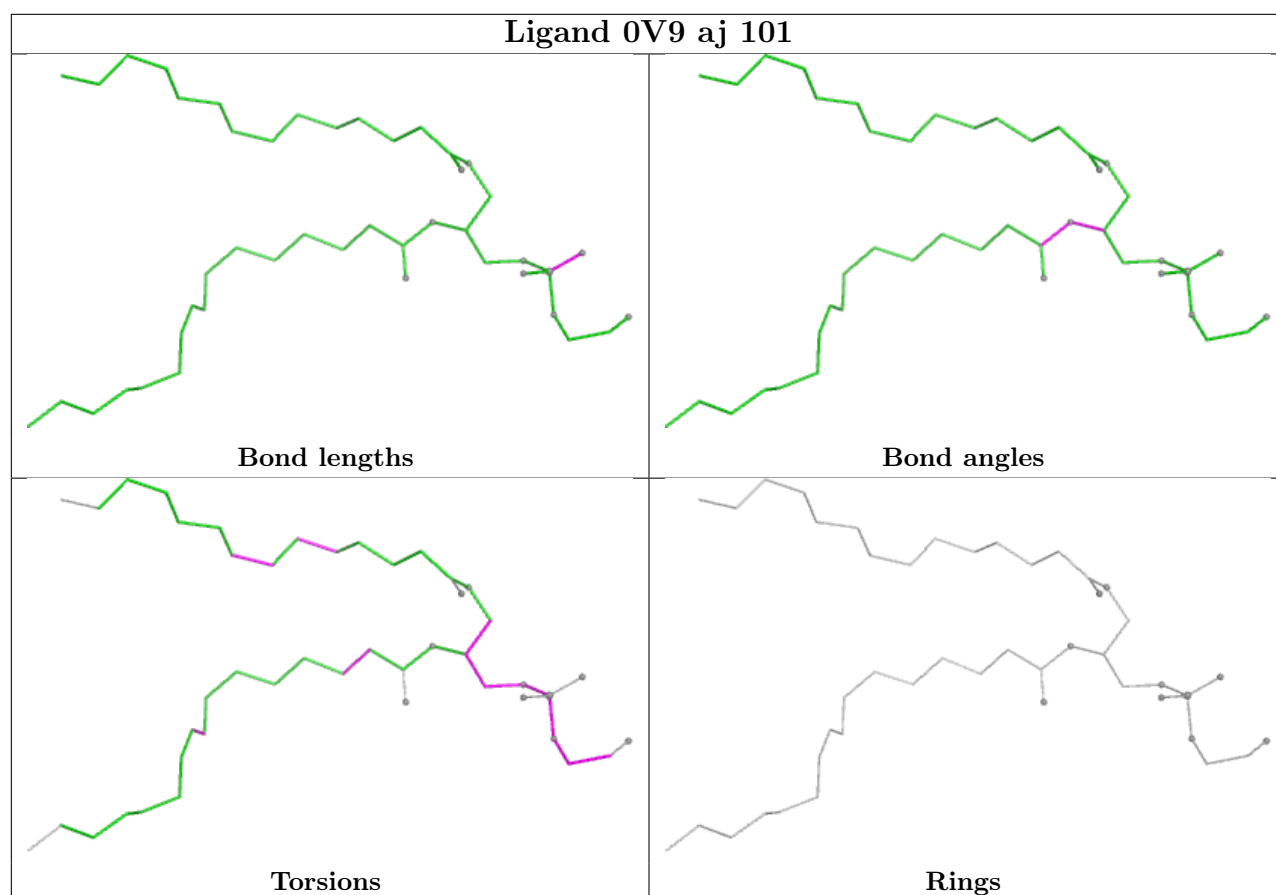


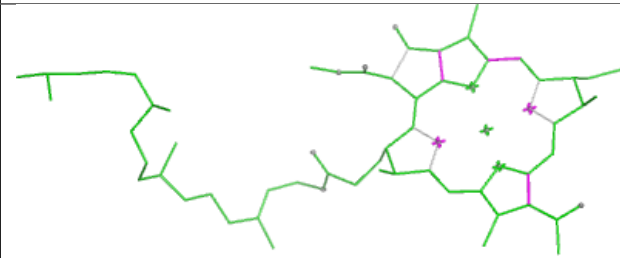
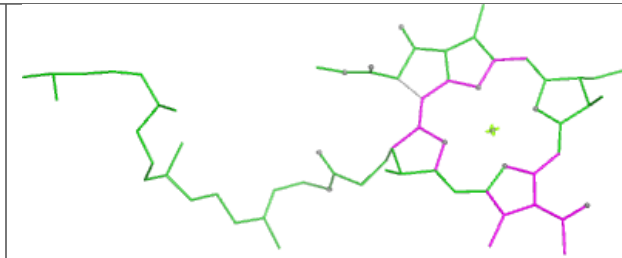
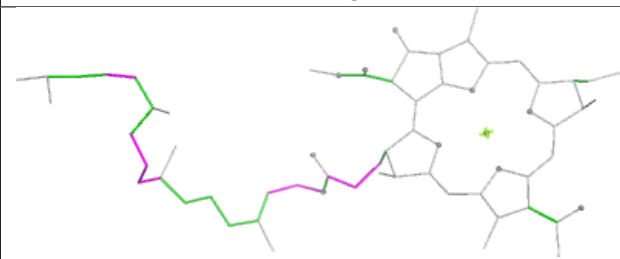
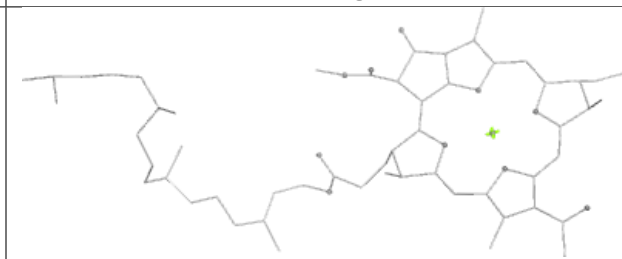


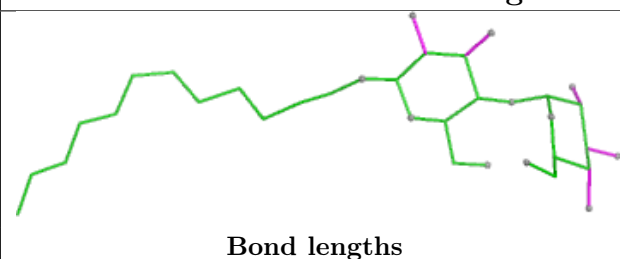
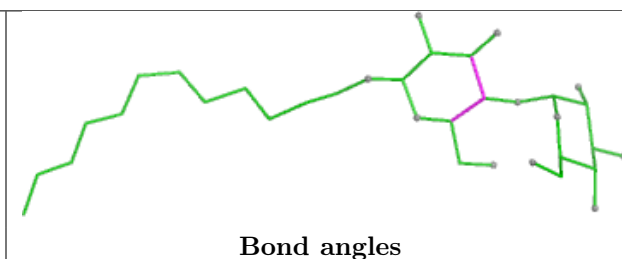
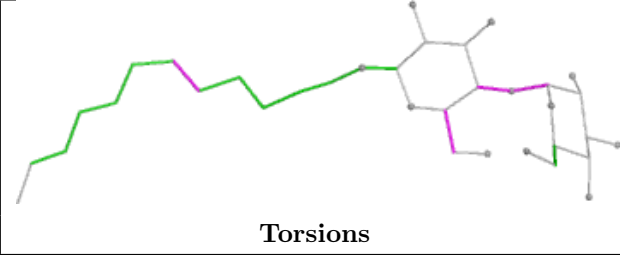
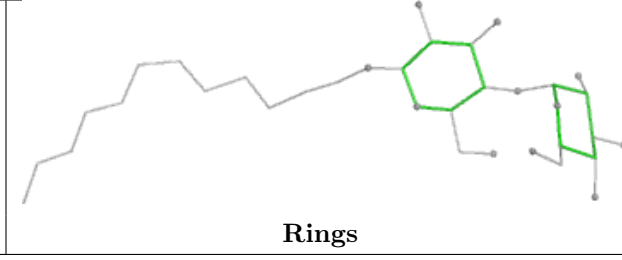


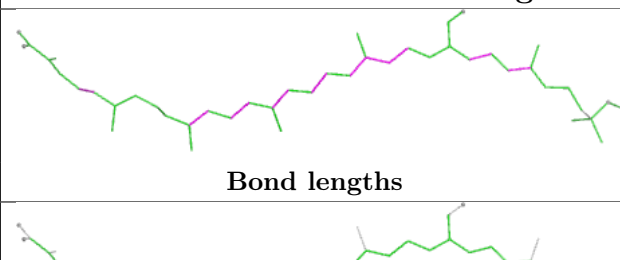
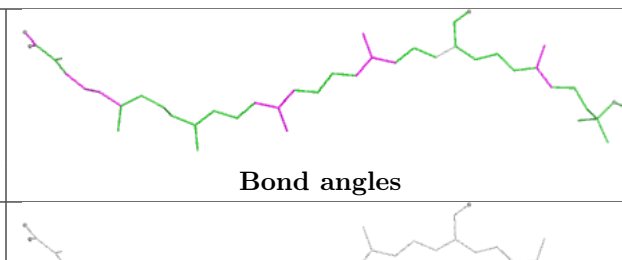


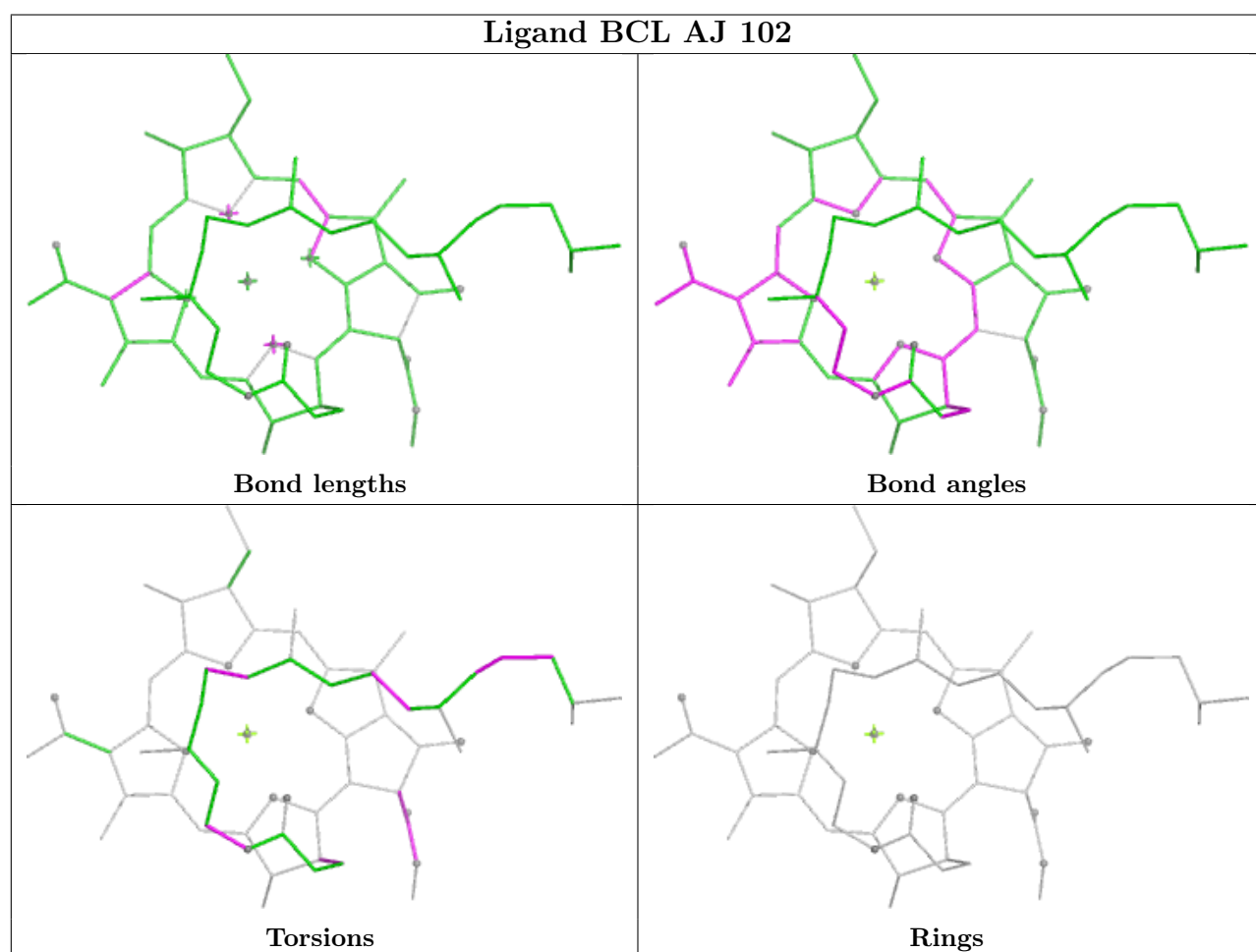
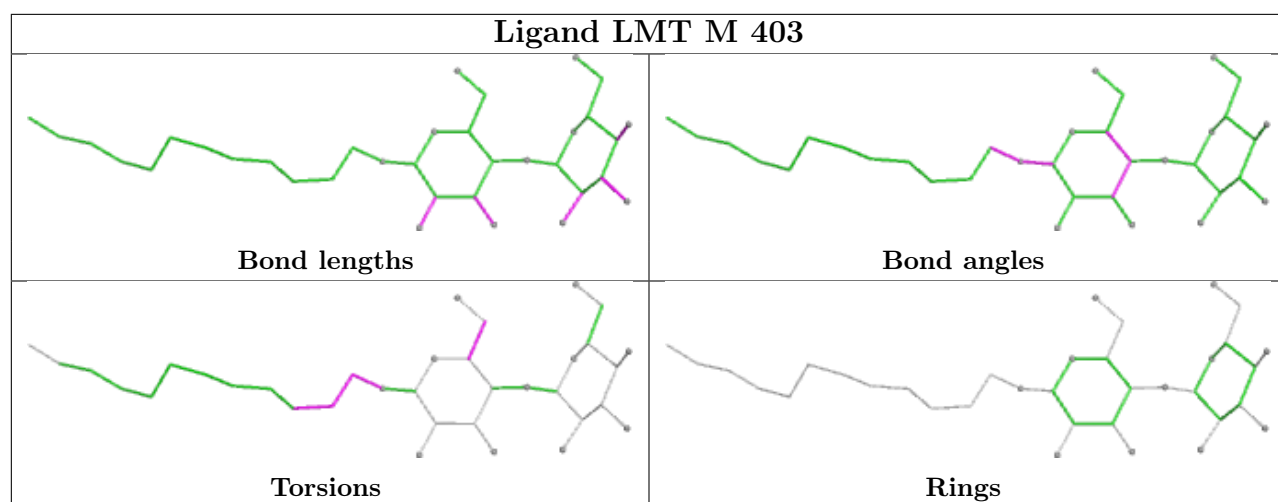


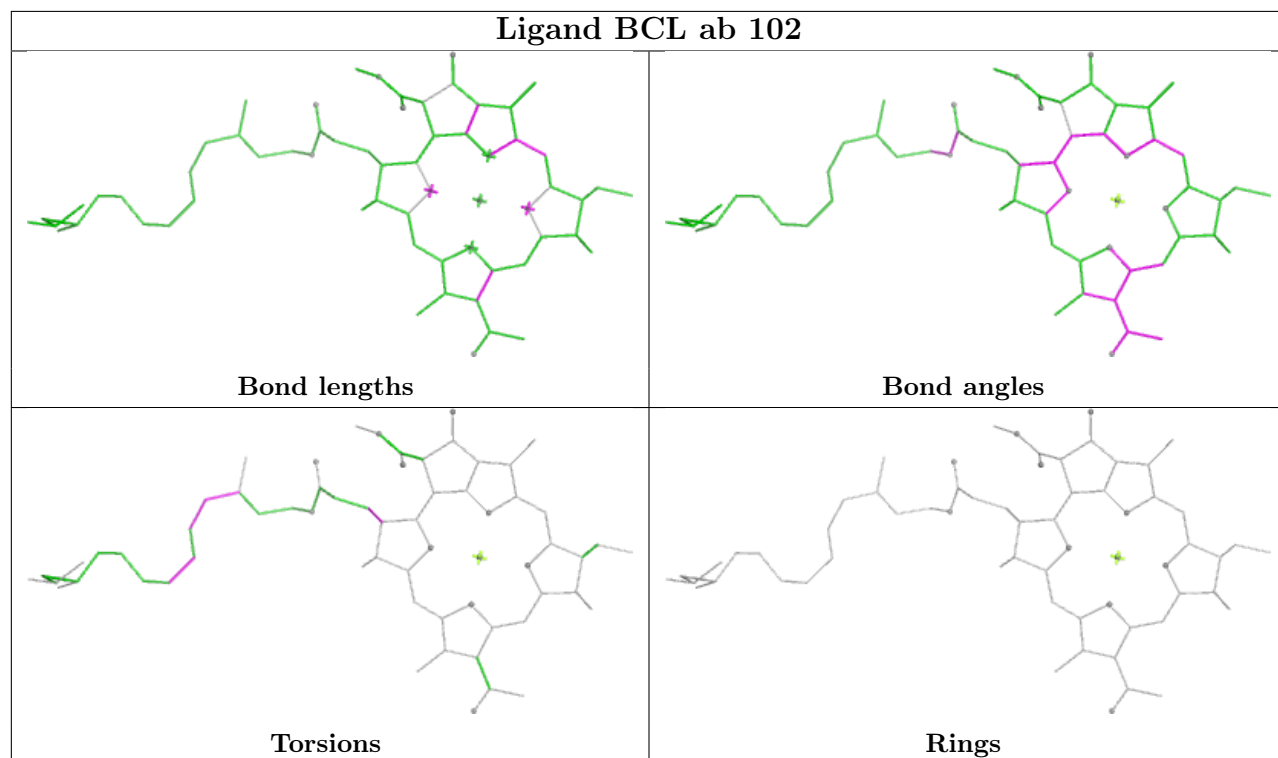
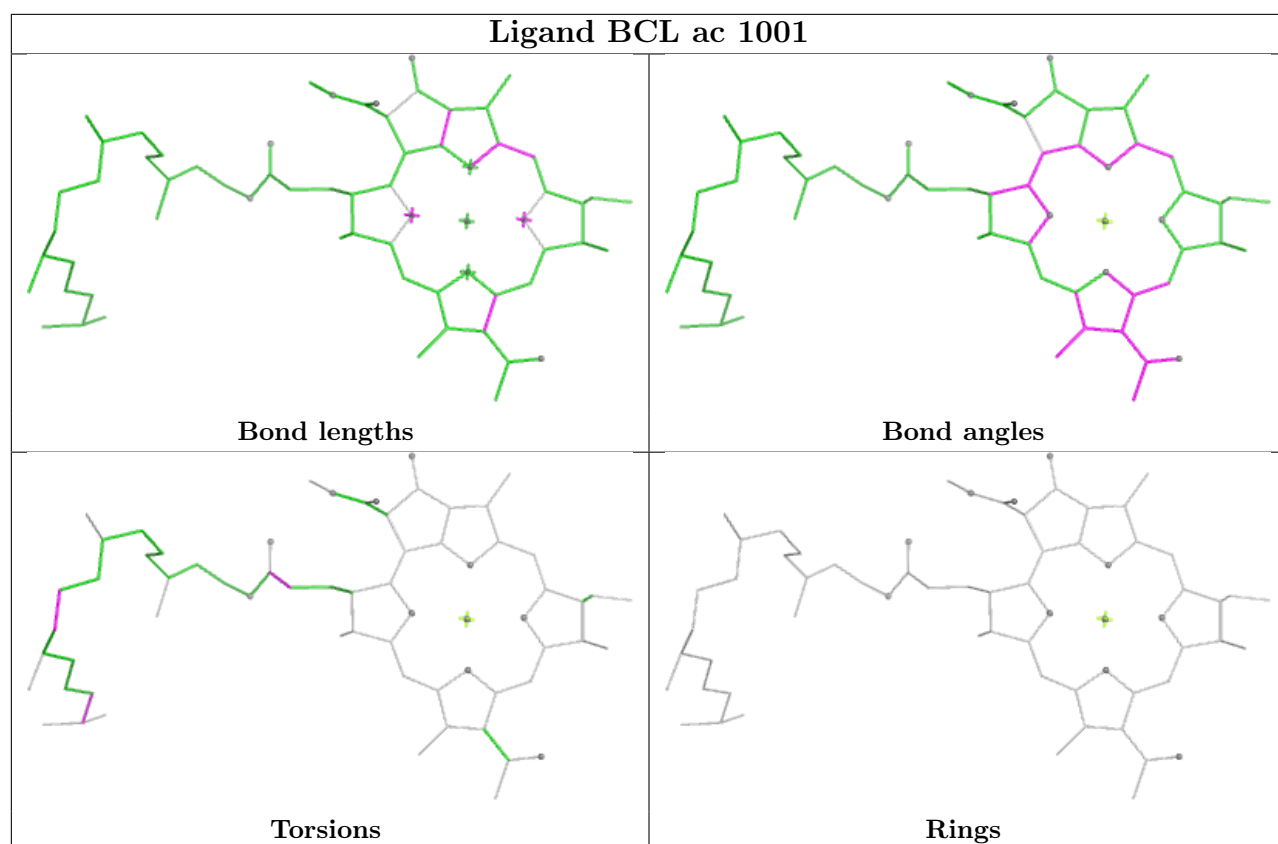


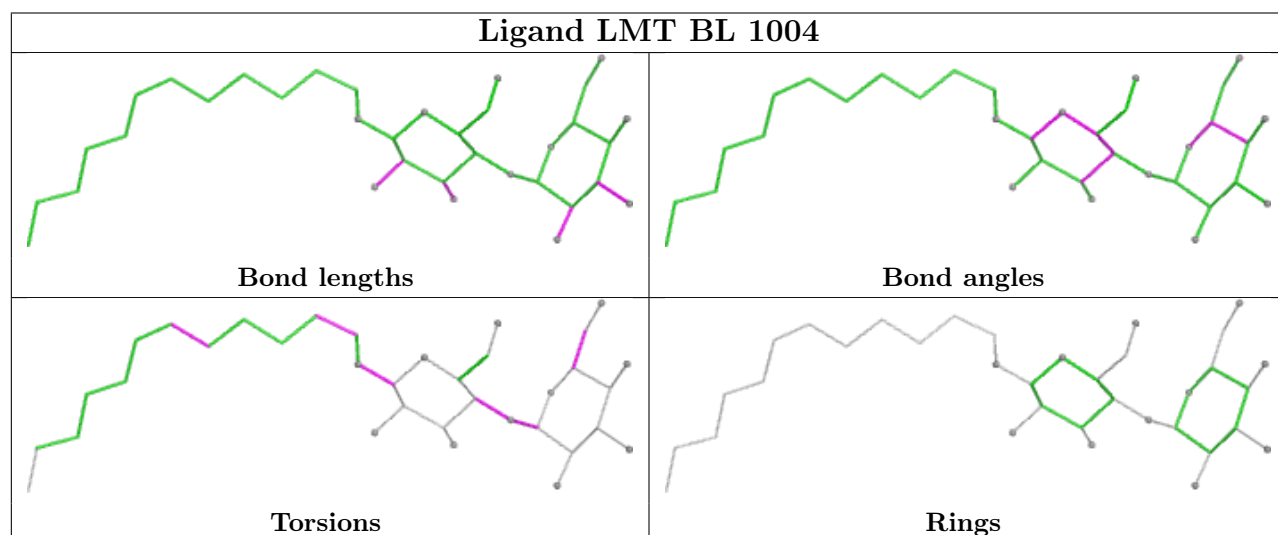
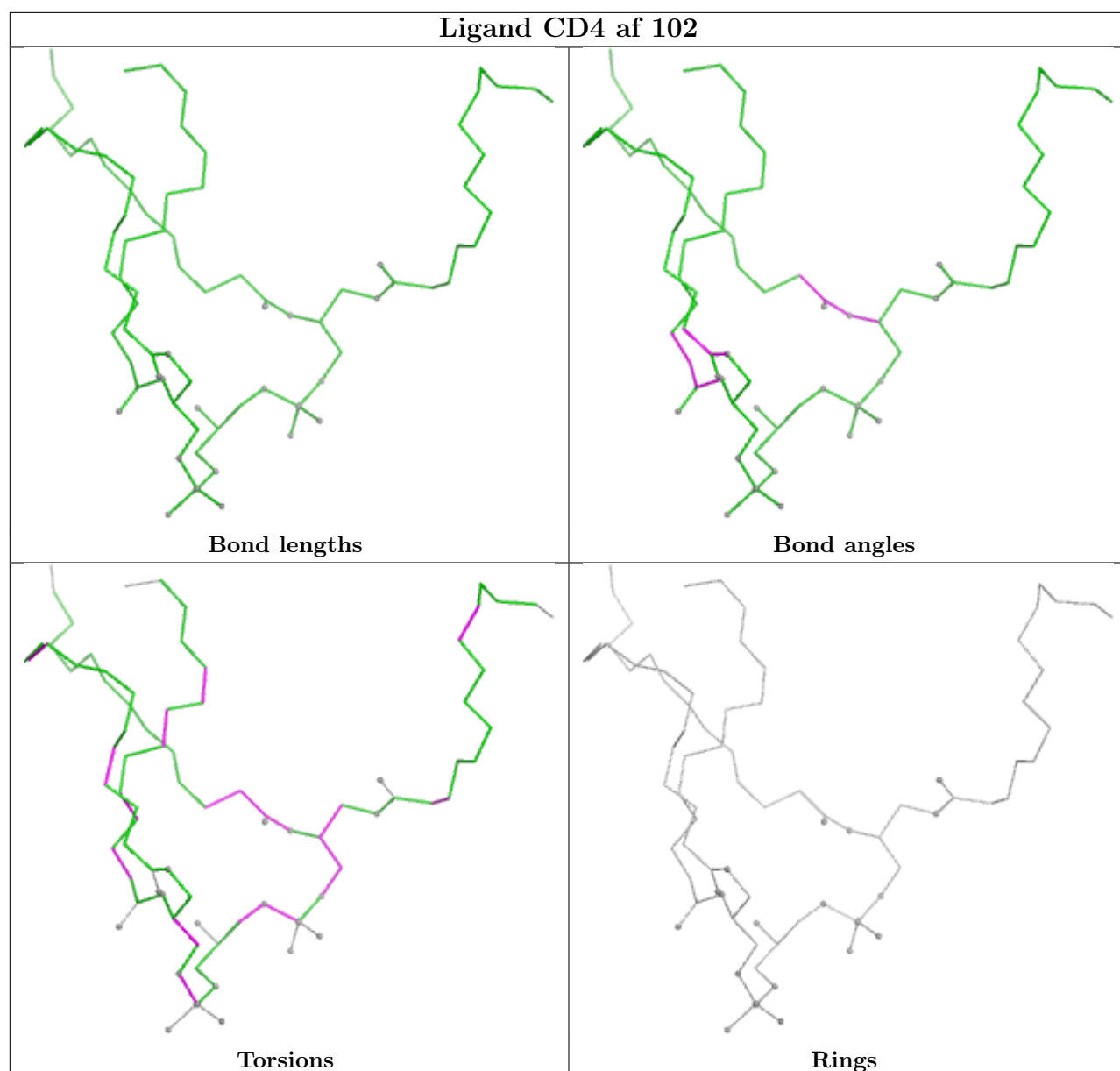
Ligand BCL an 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

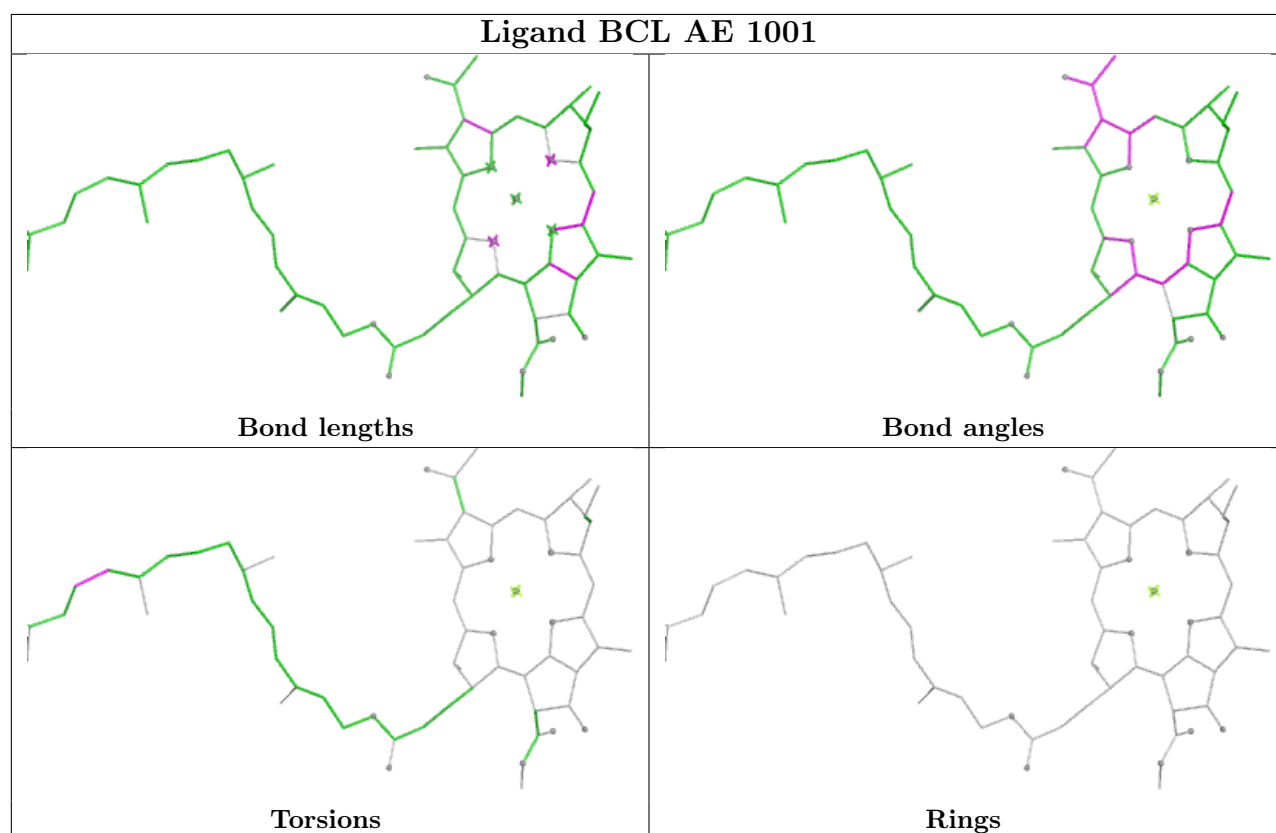
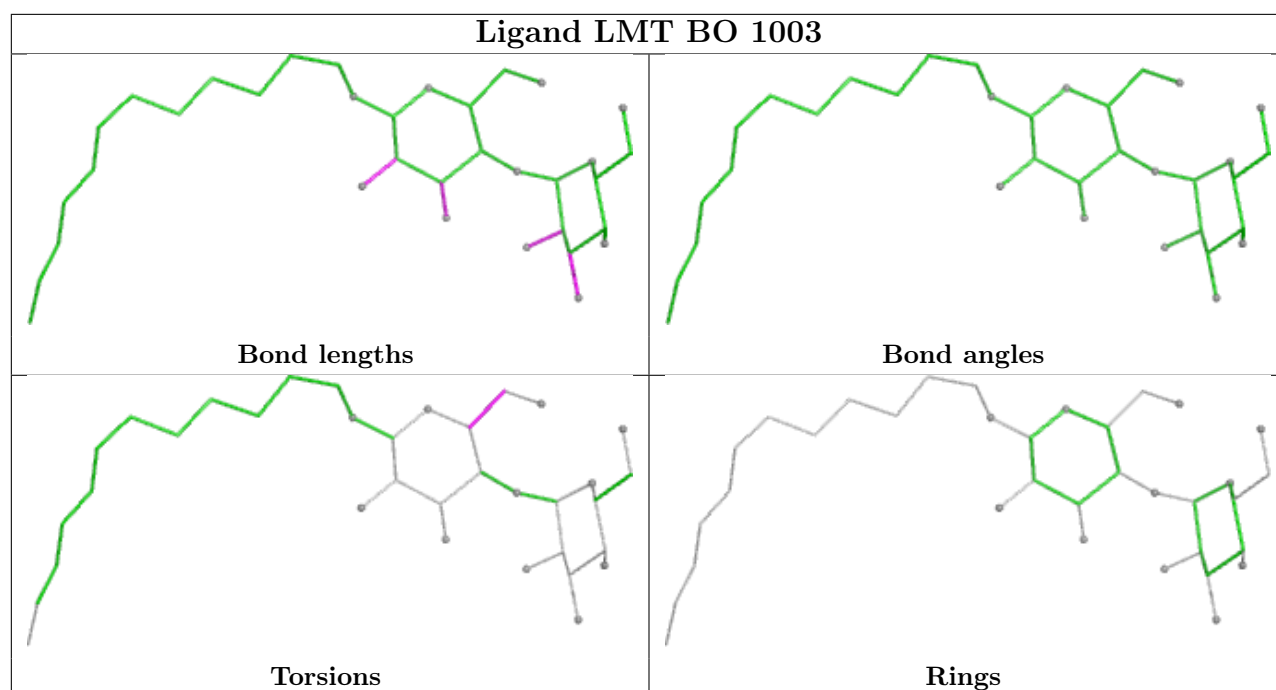
Ligand LMT BC 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

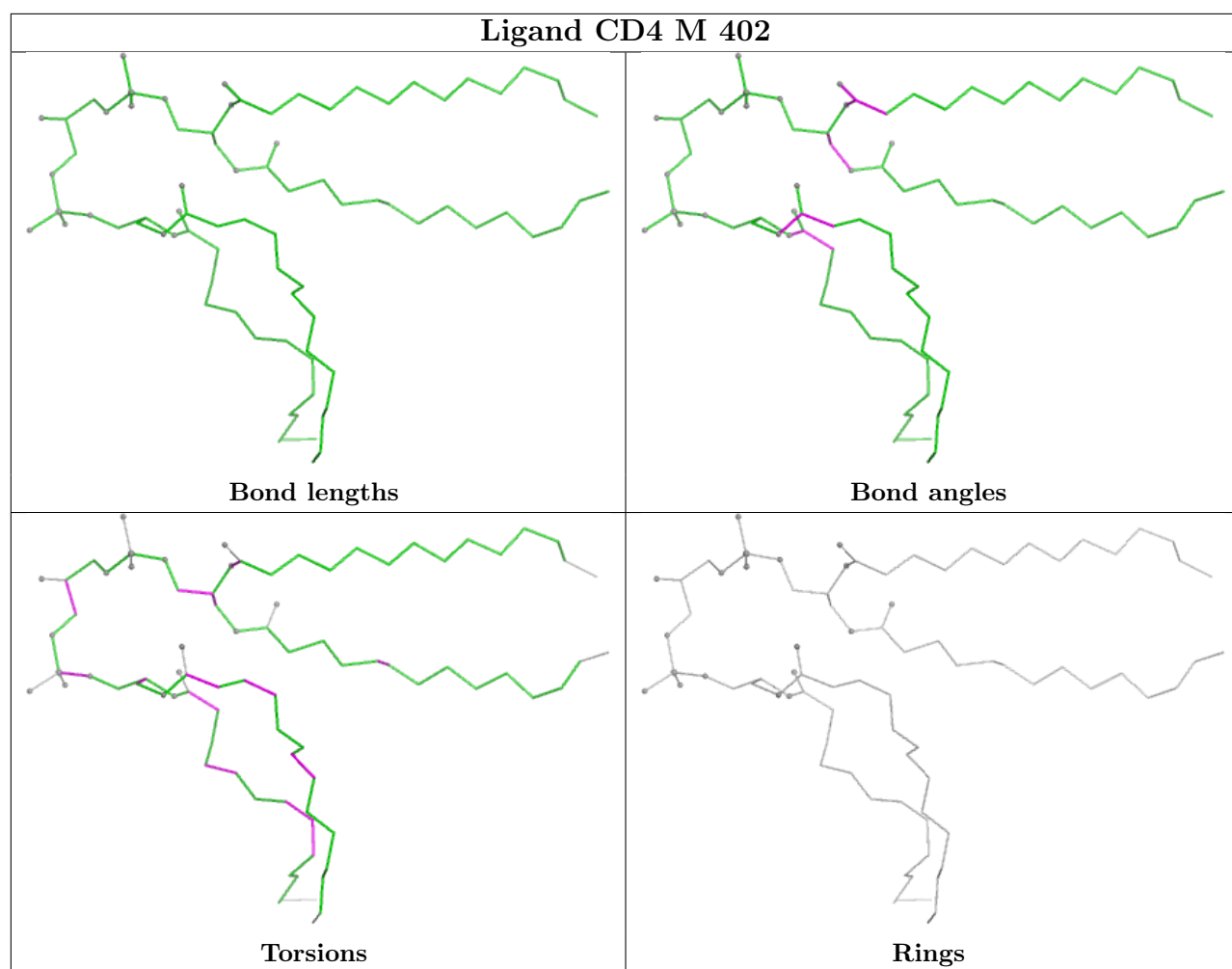
Ligand V7N bk 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

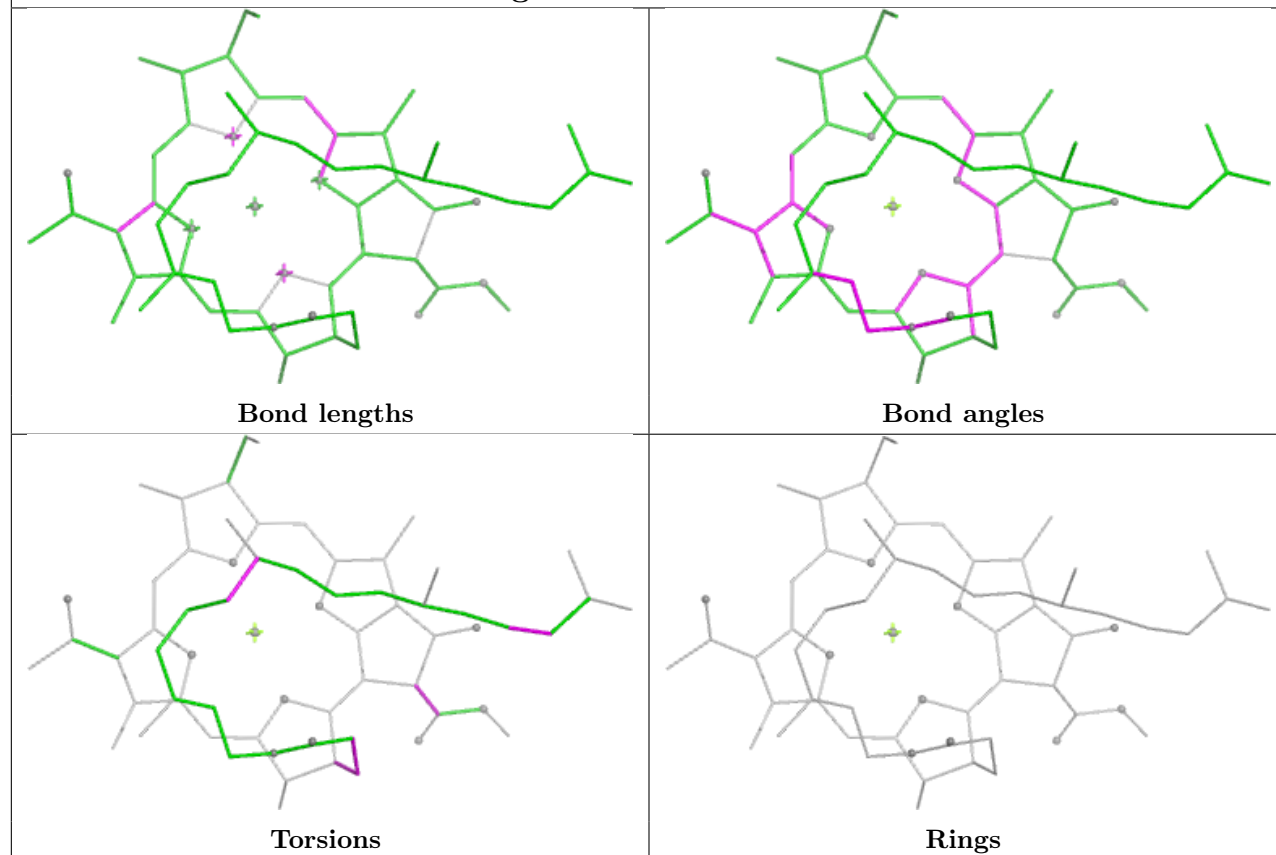
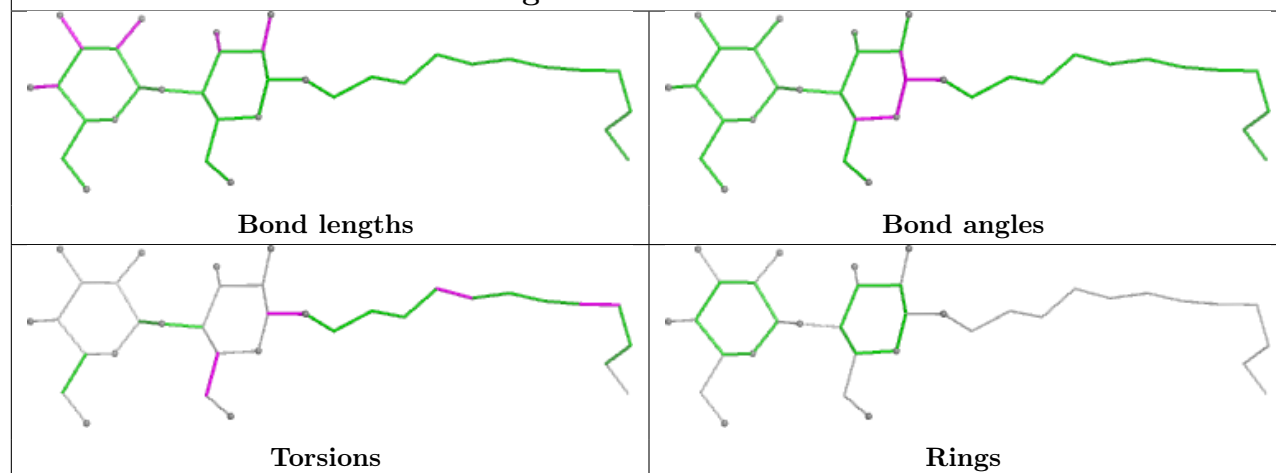


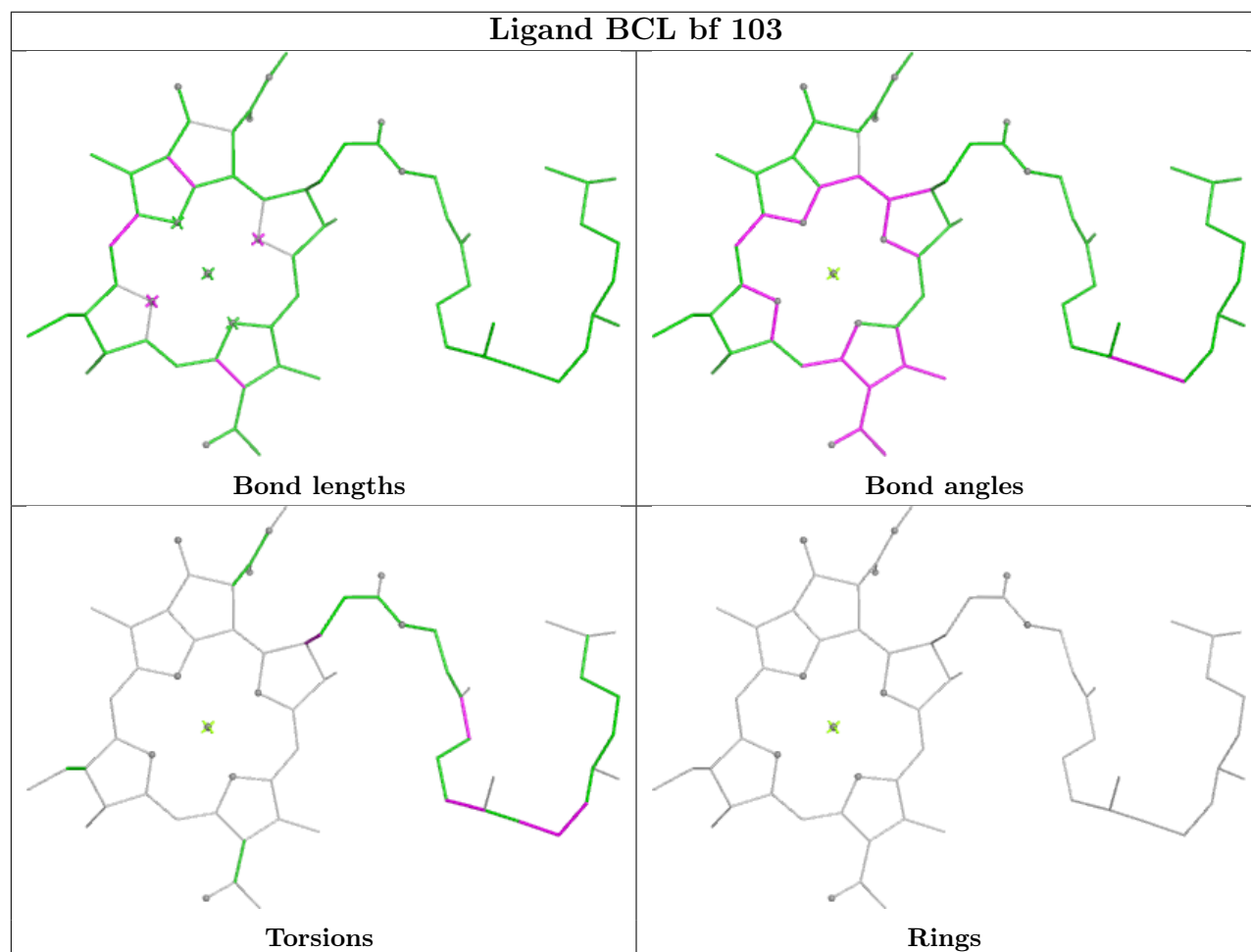
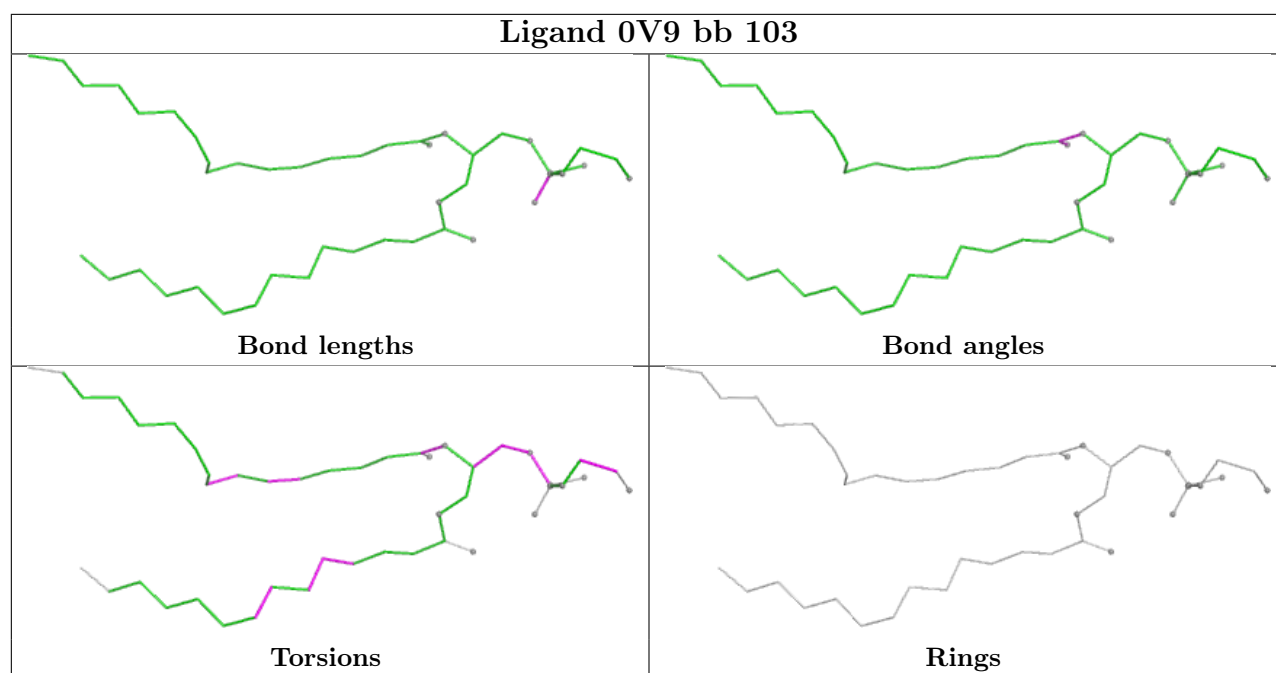


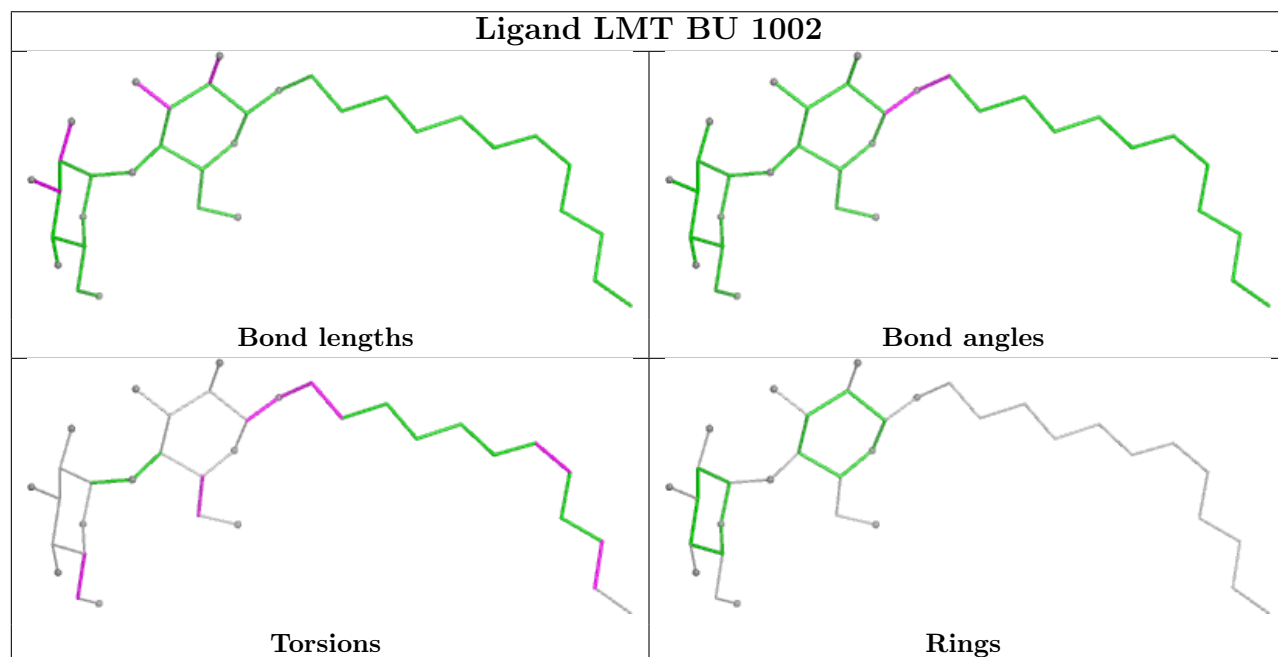
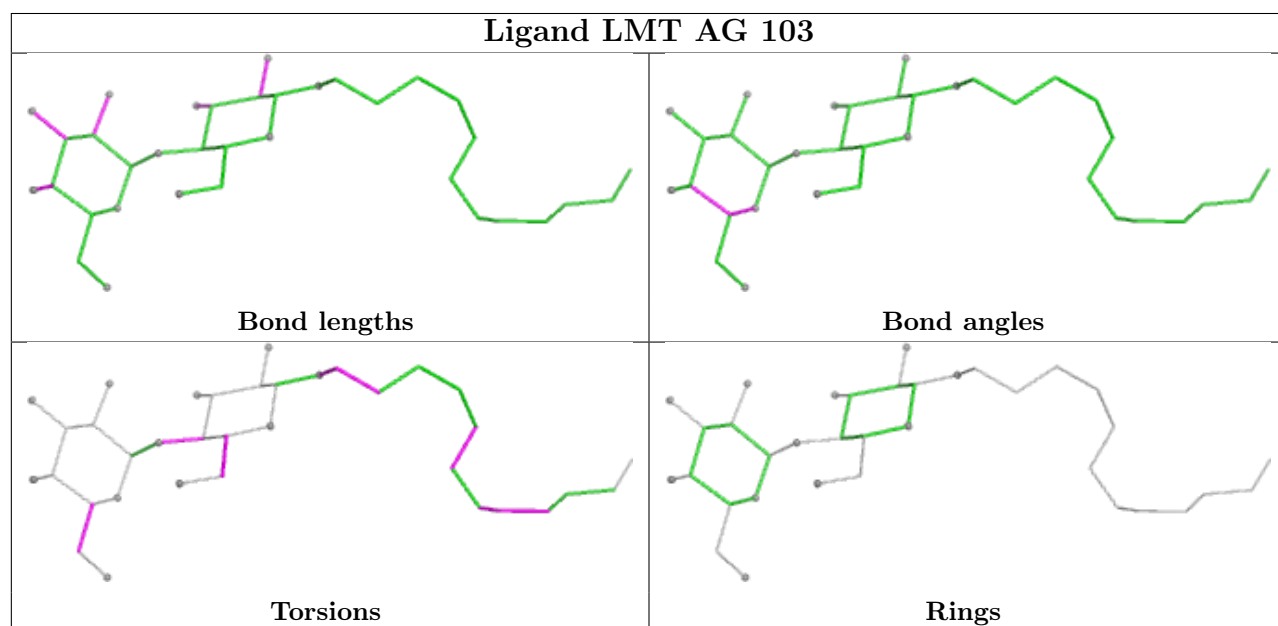
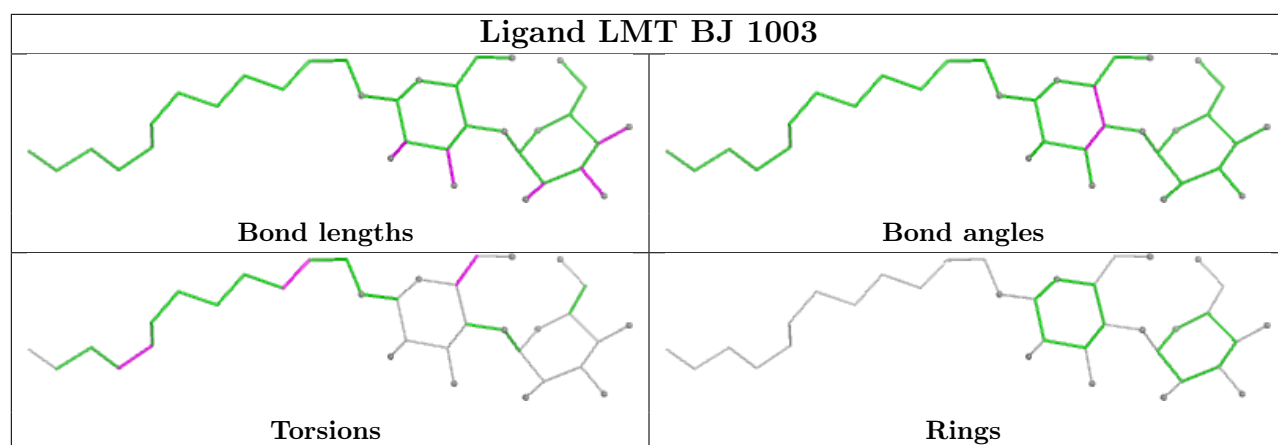


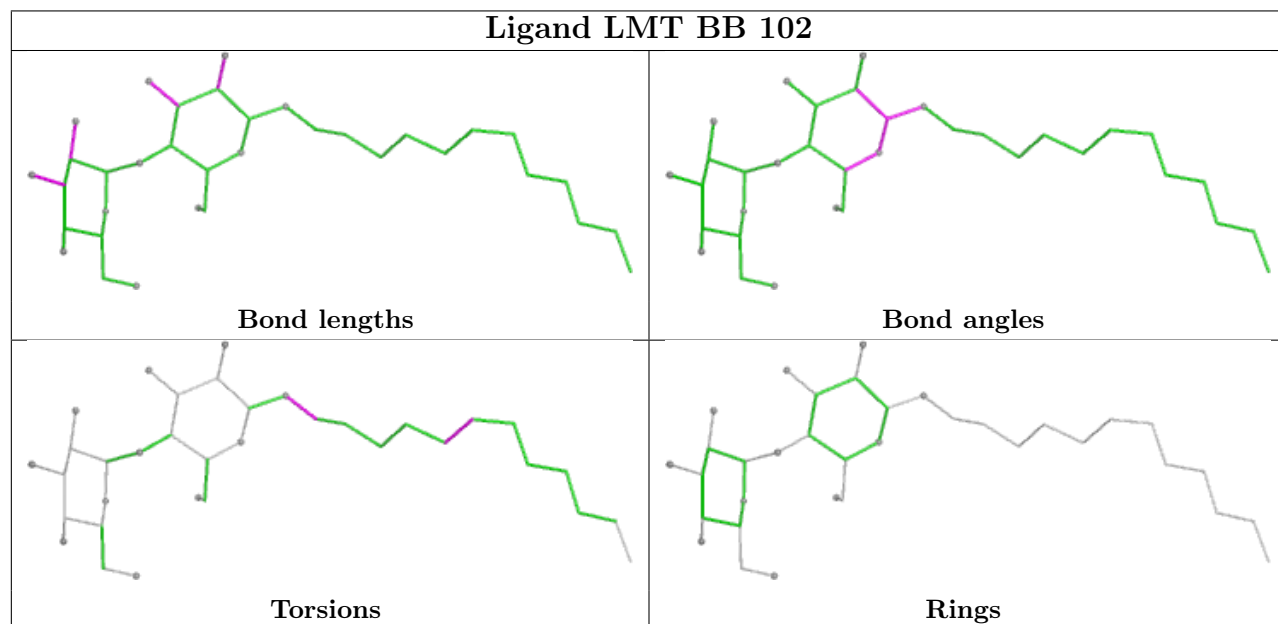
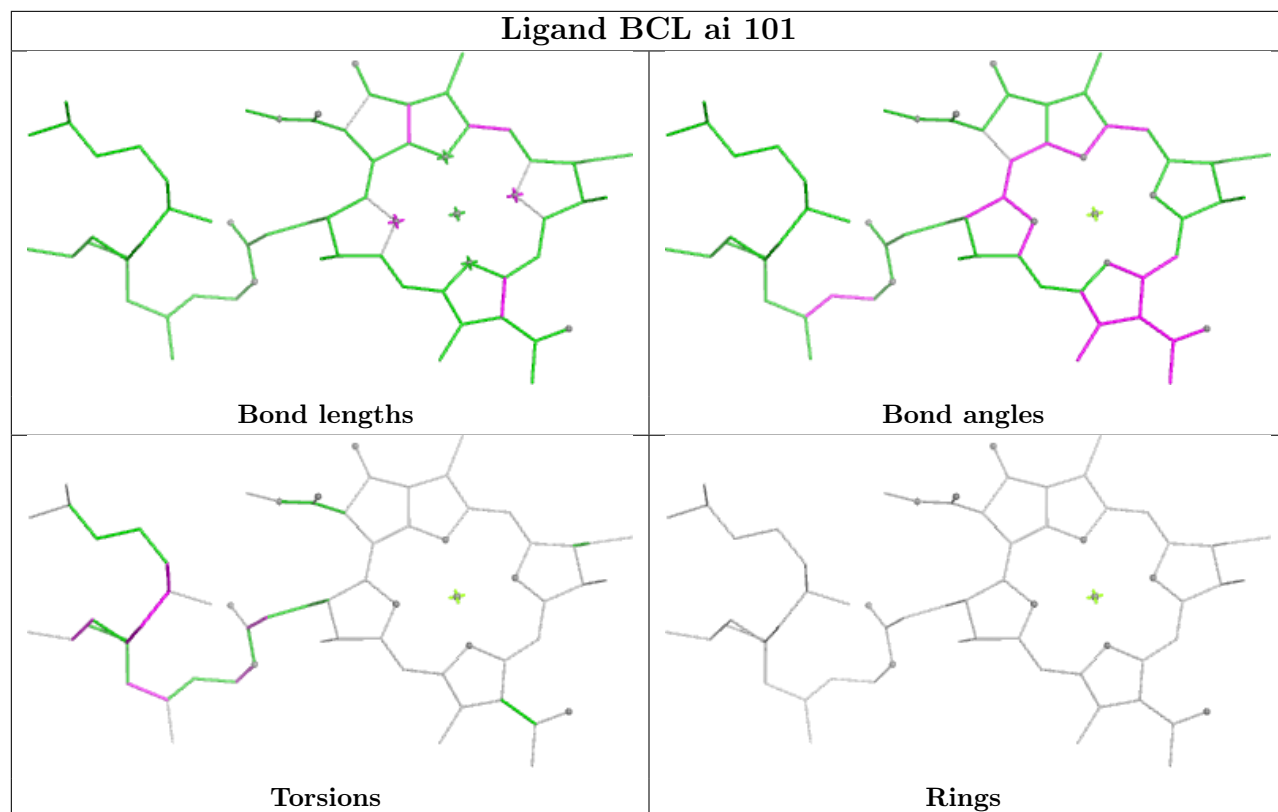


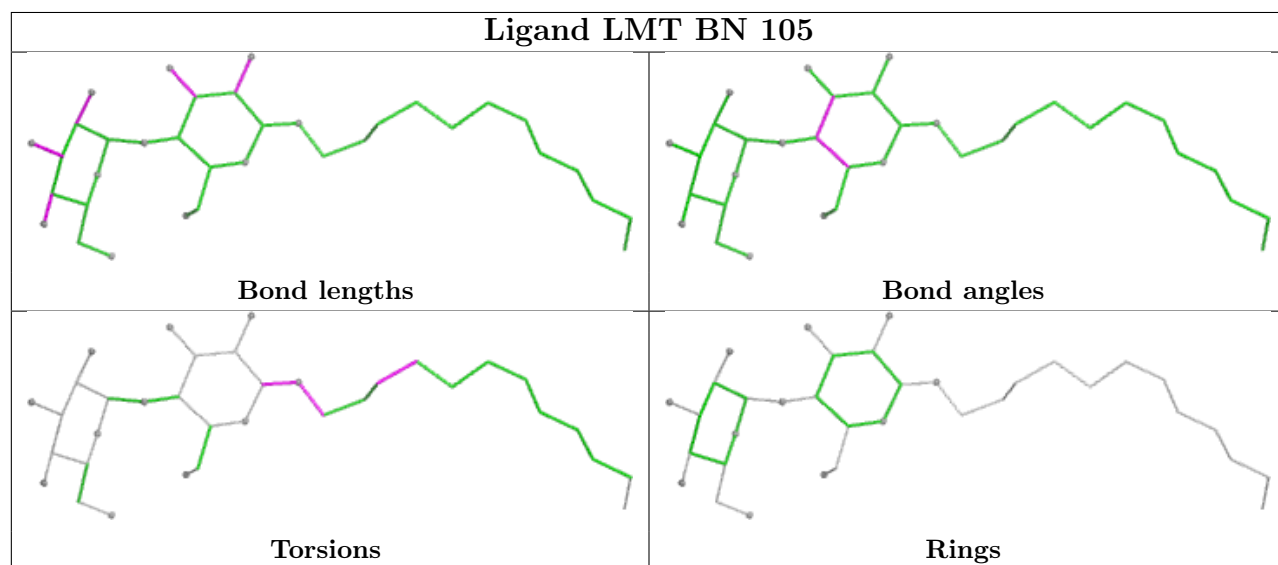
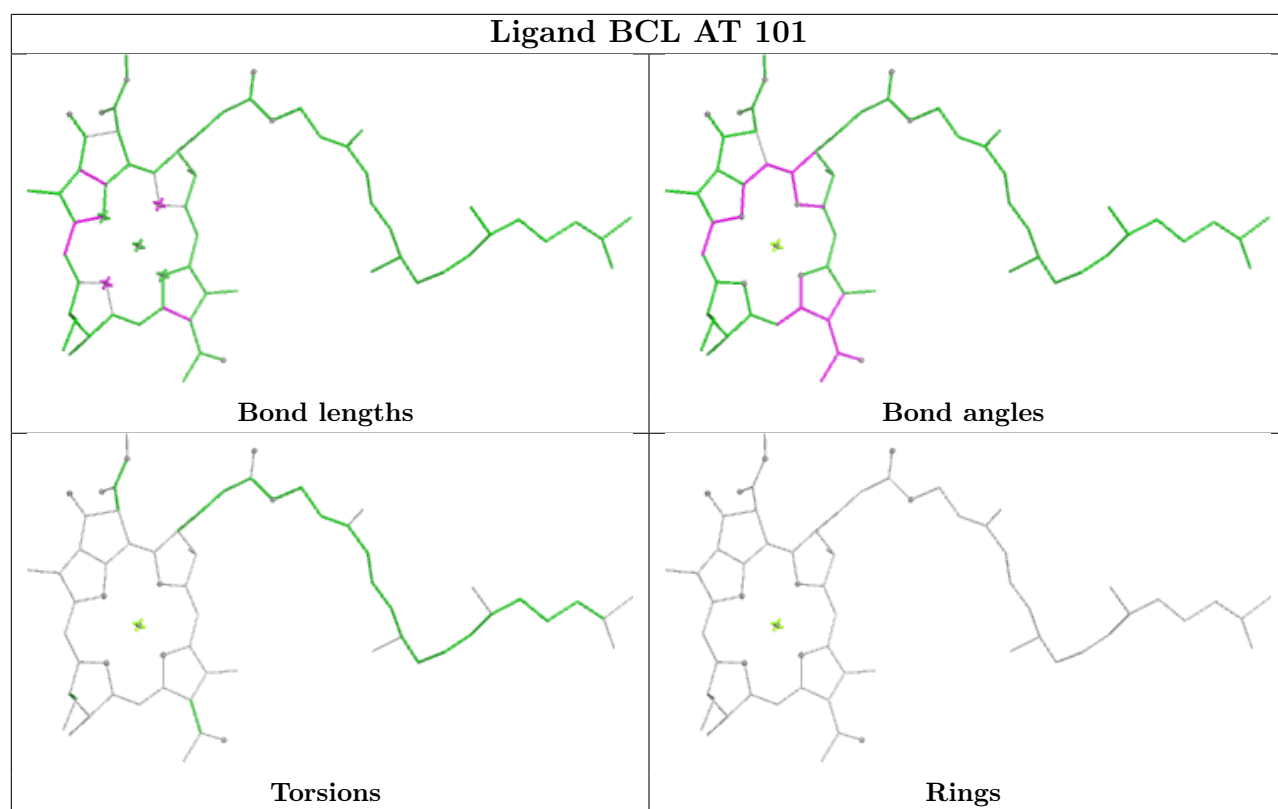


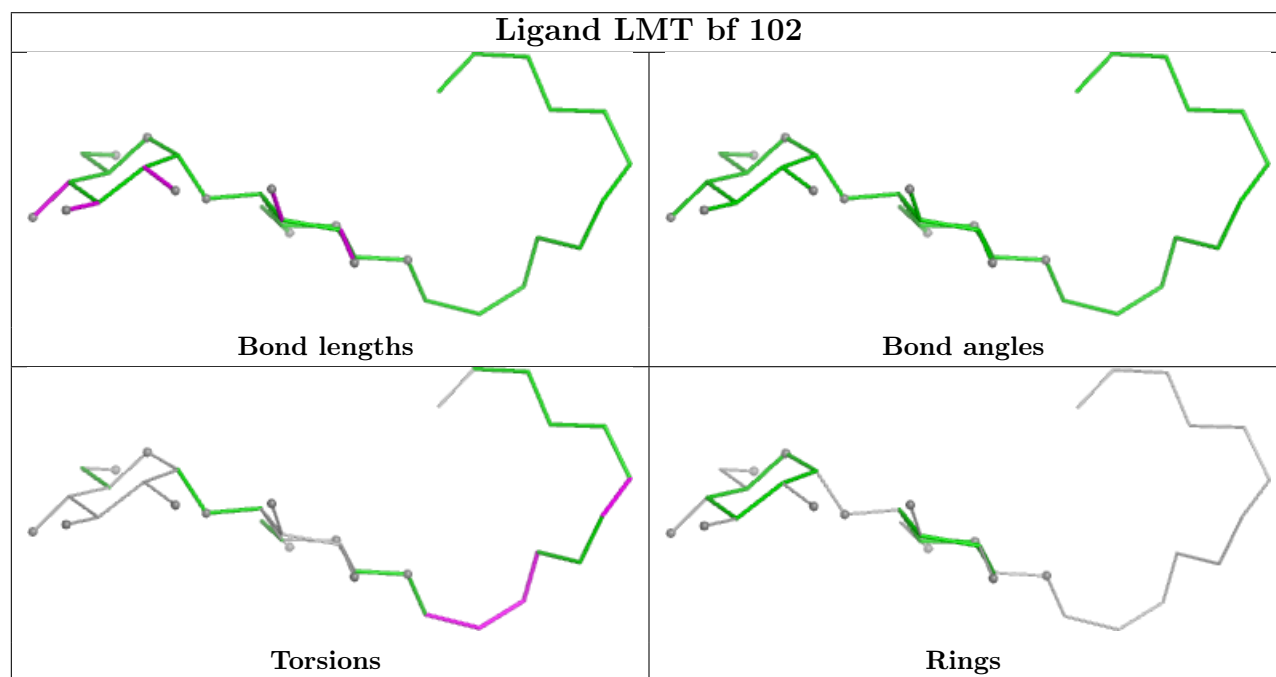
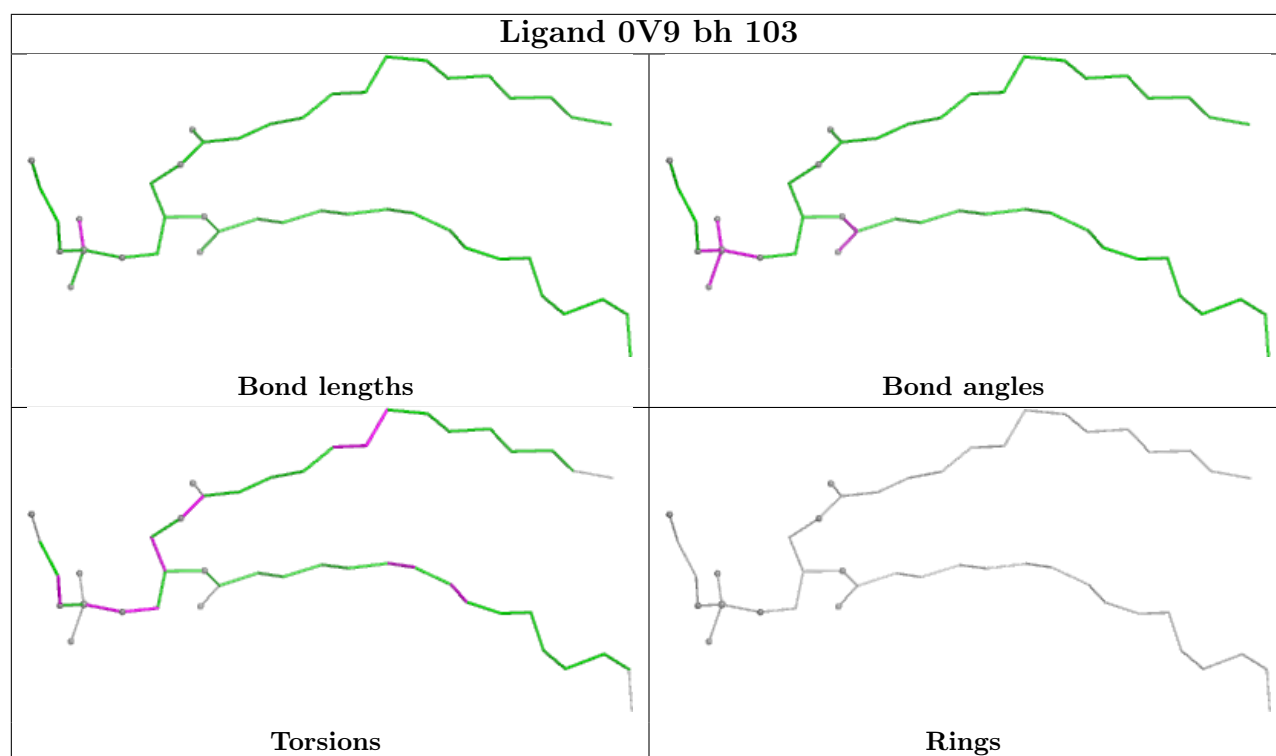
Ligand BCL AE 1004**Ligand LMT bn 105**



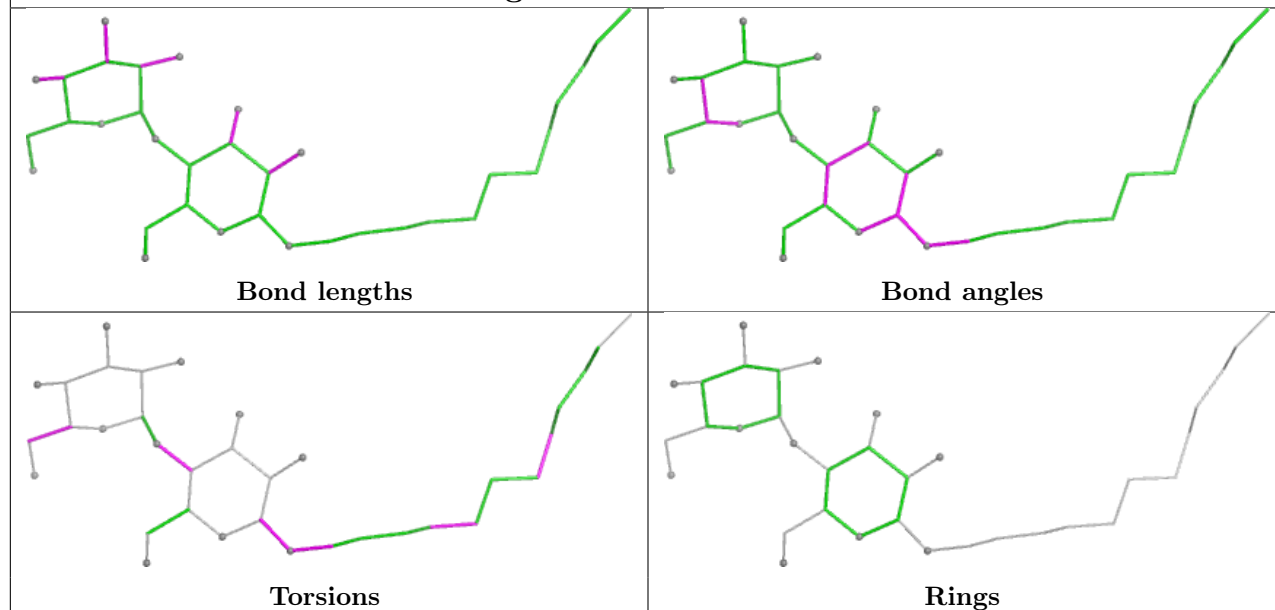




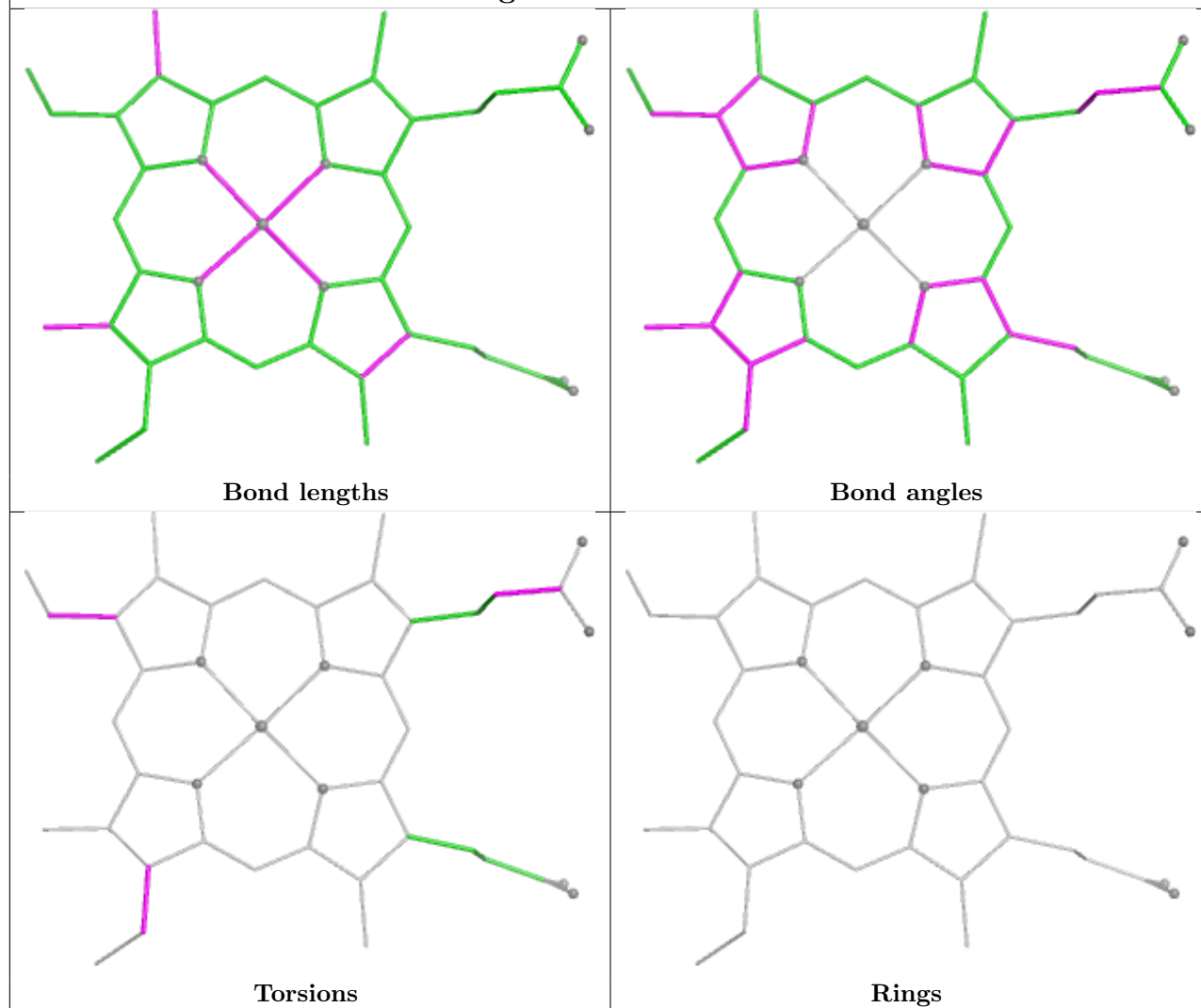


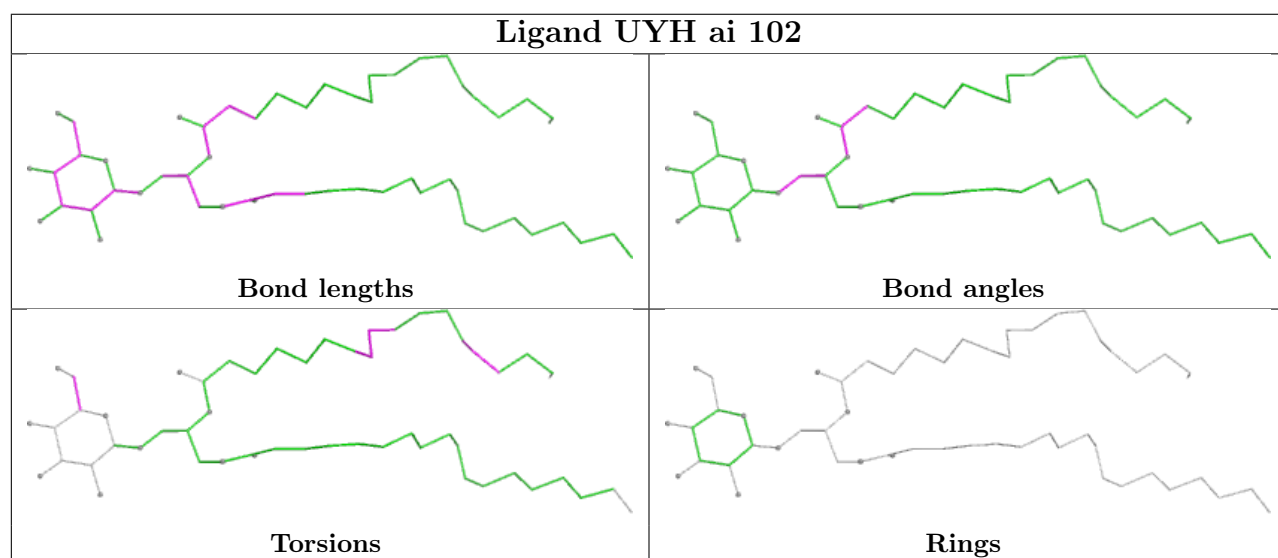
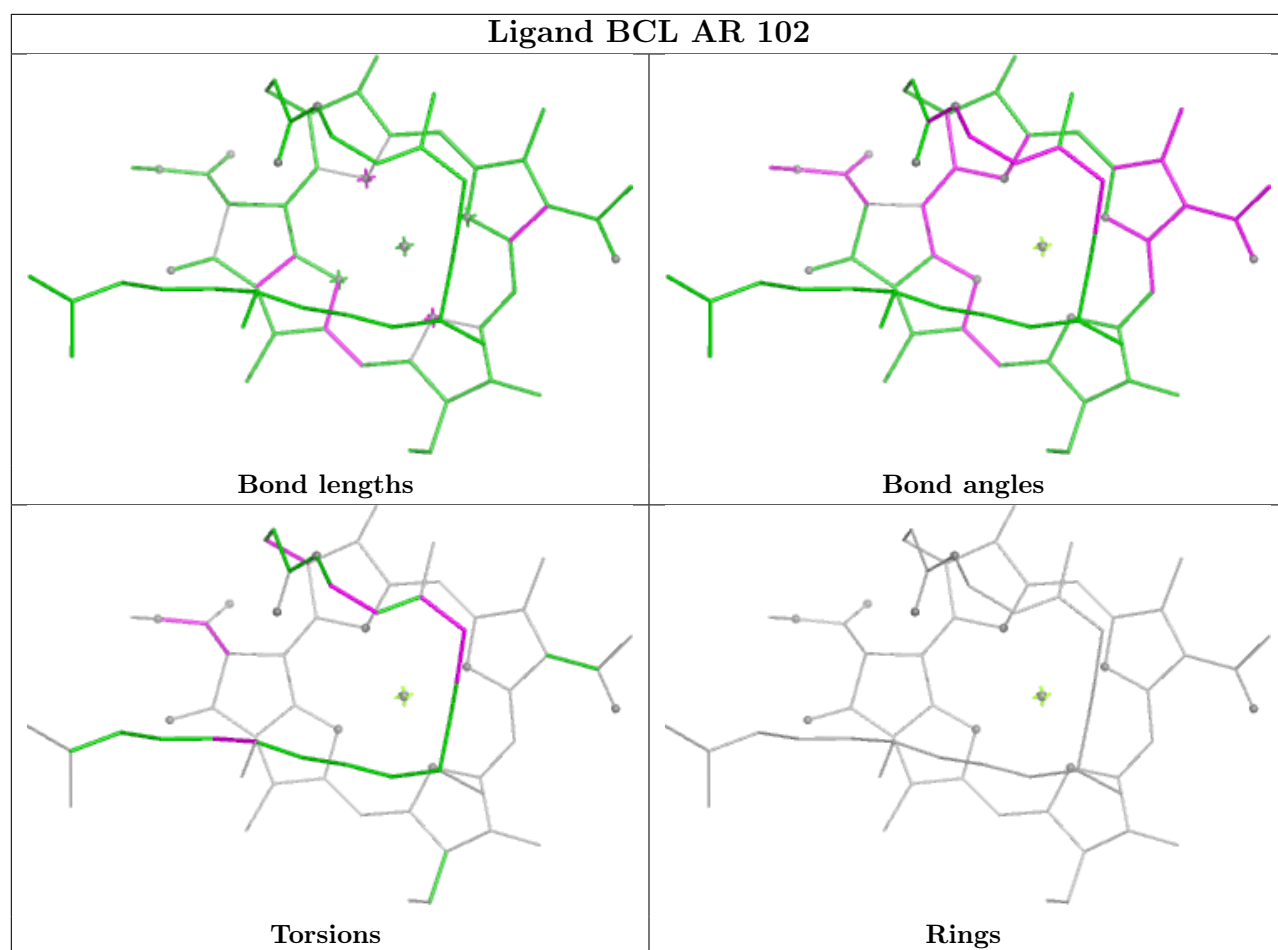


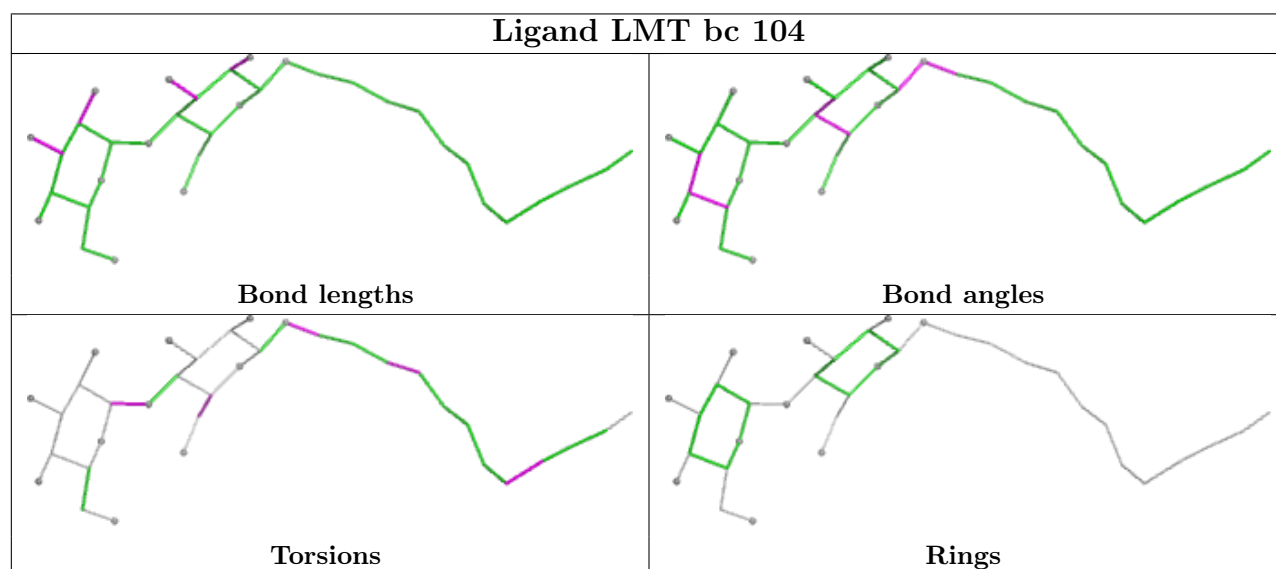
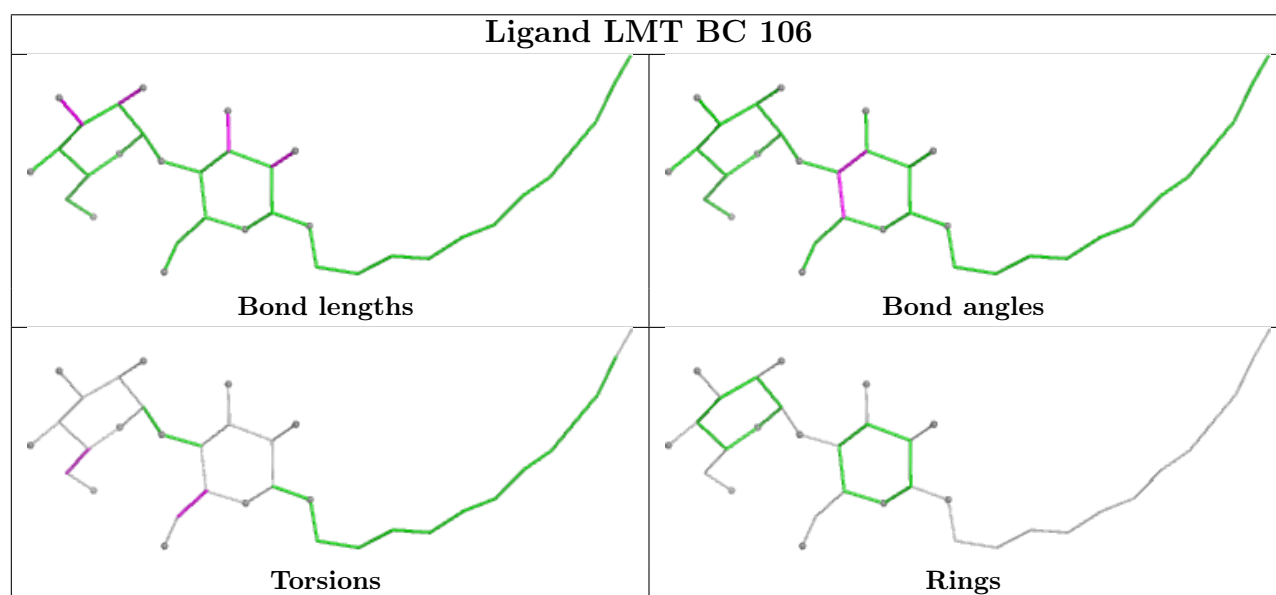
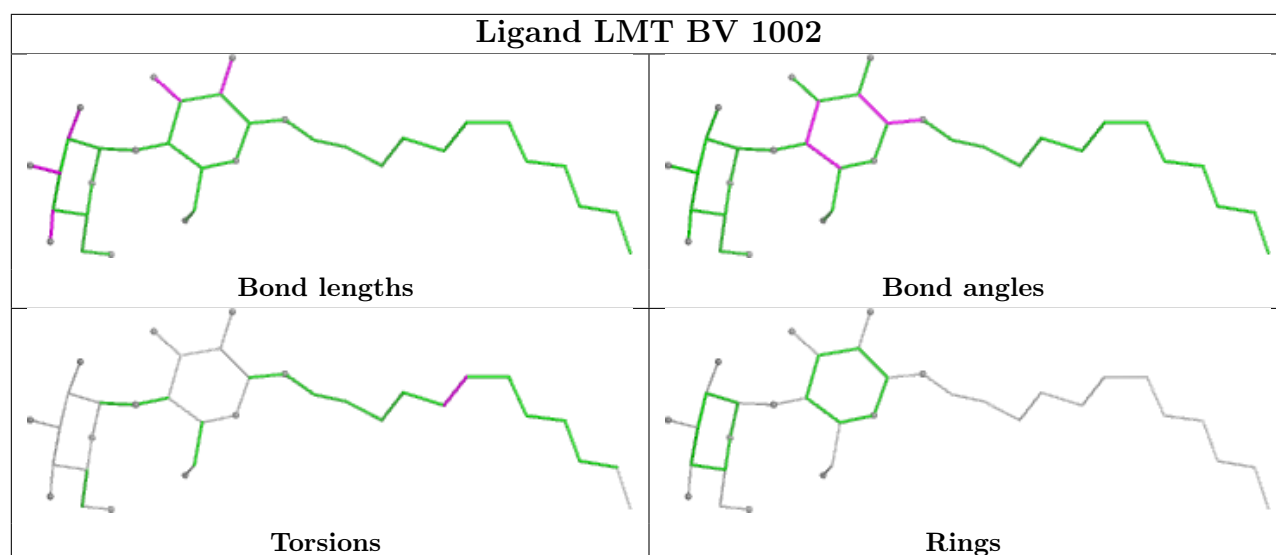
Ligand LMT BG 1002

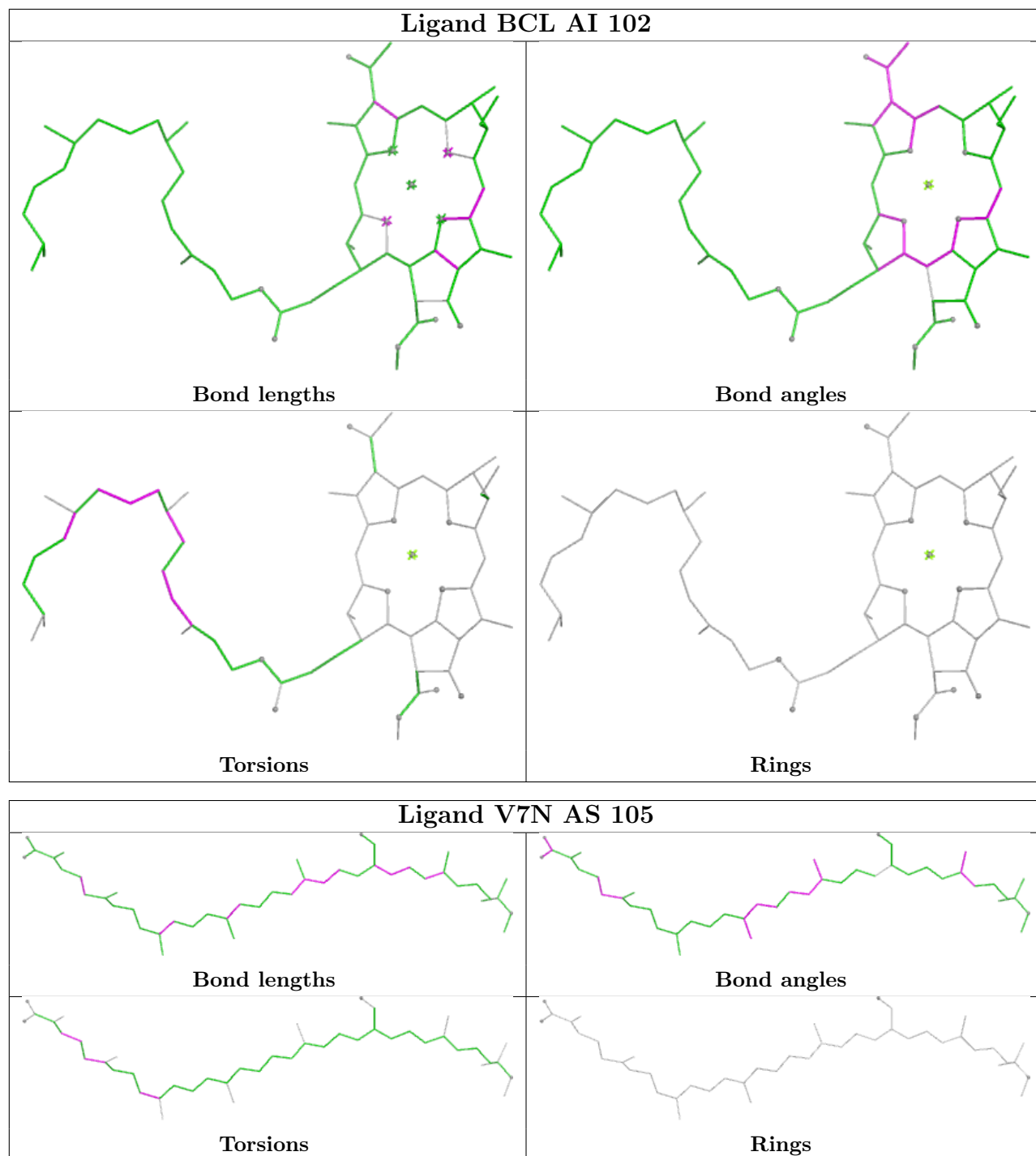


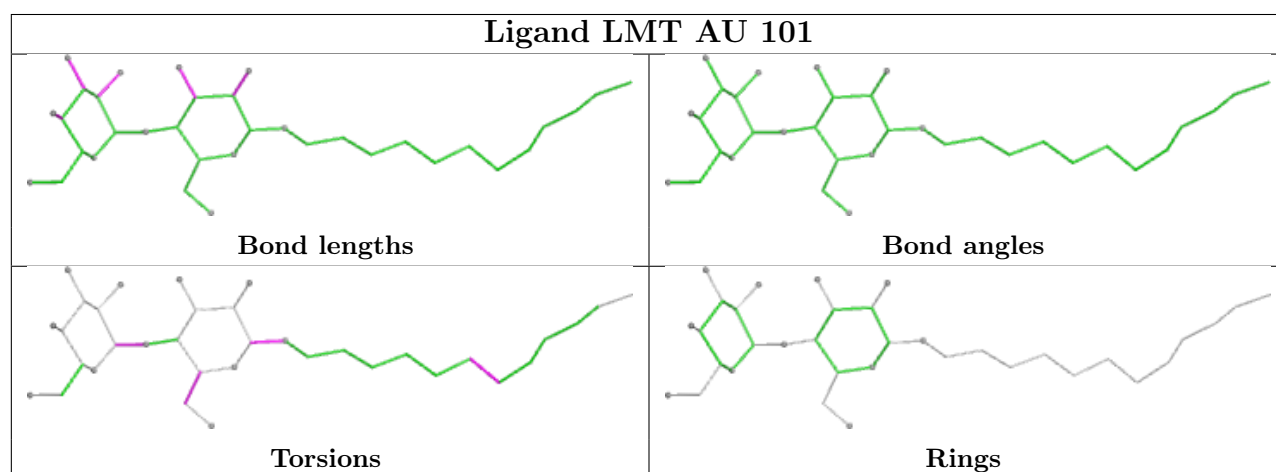
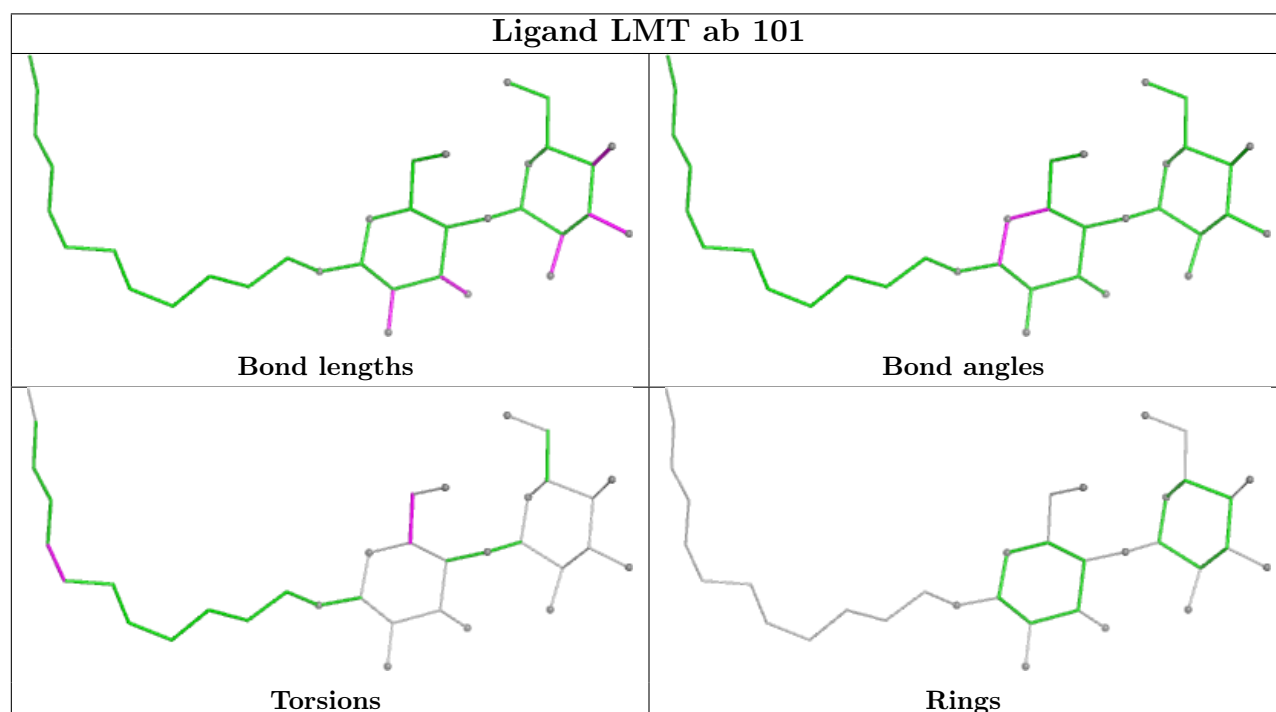
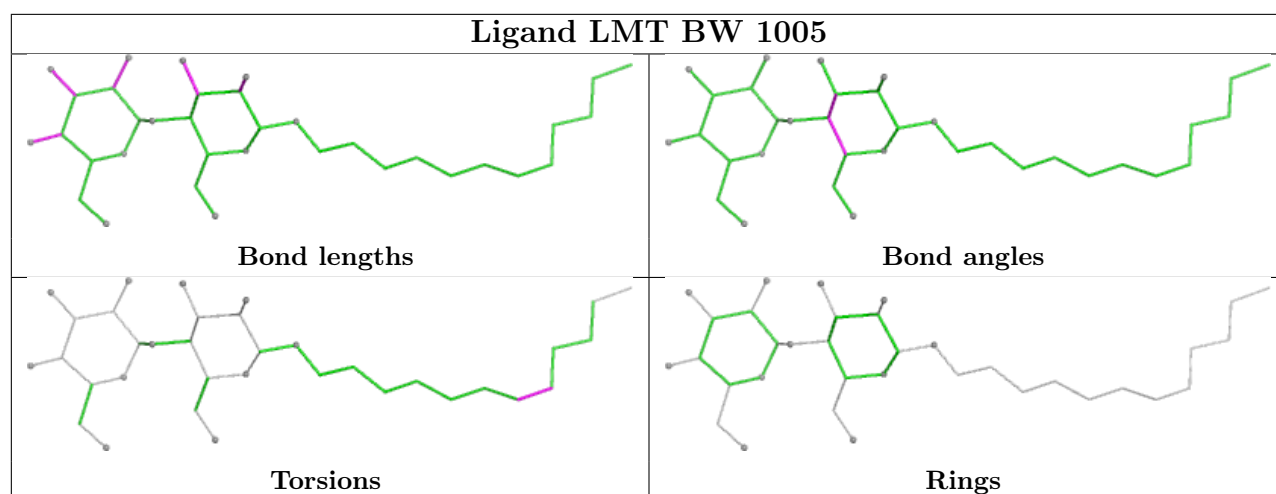
Ligand HEC C 401

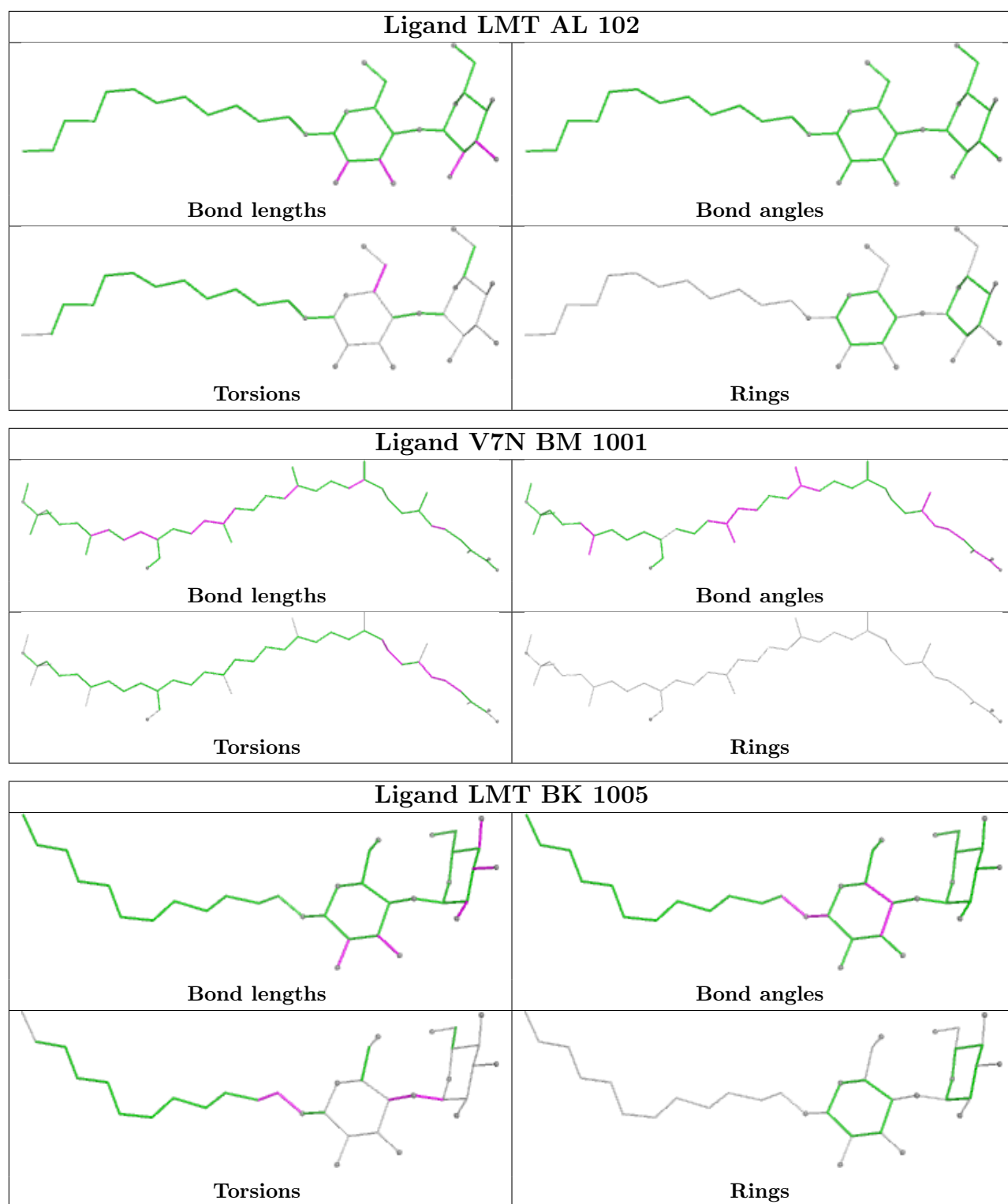


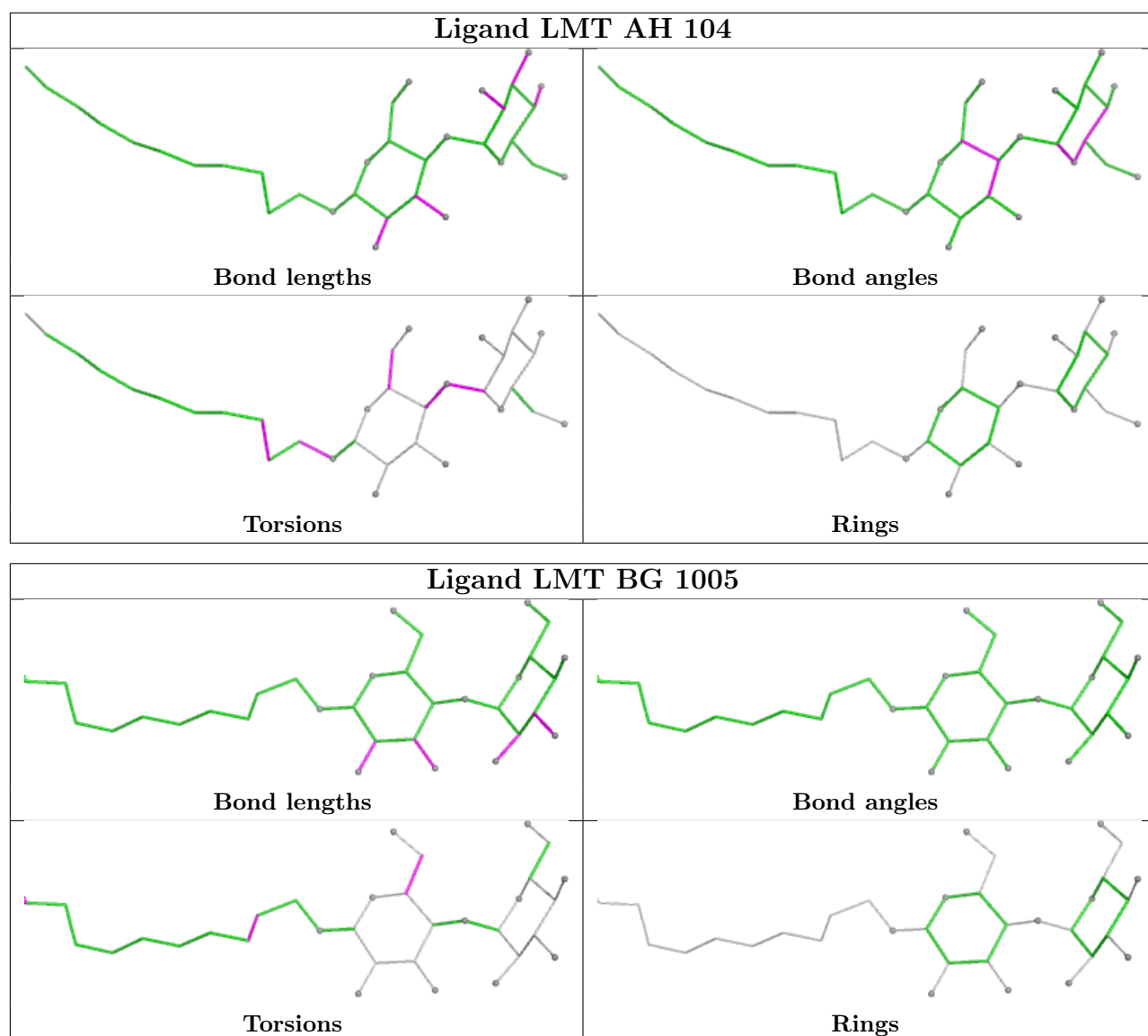


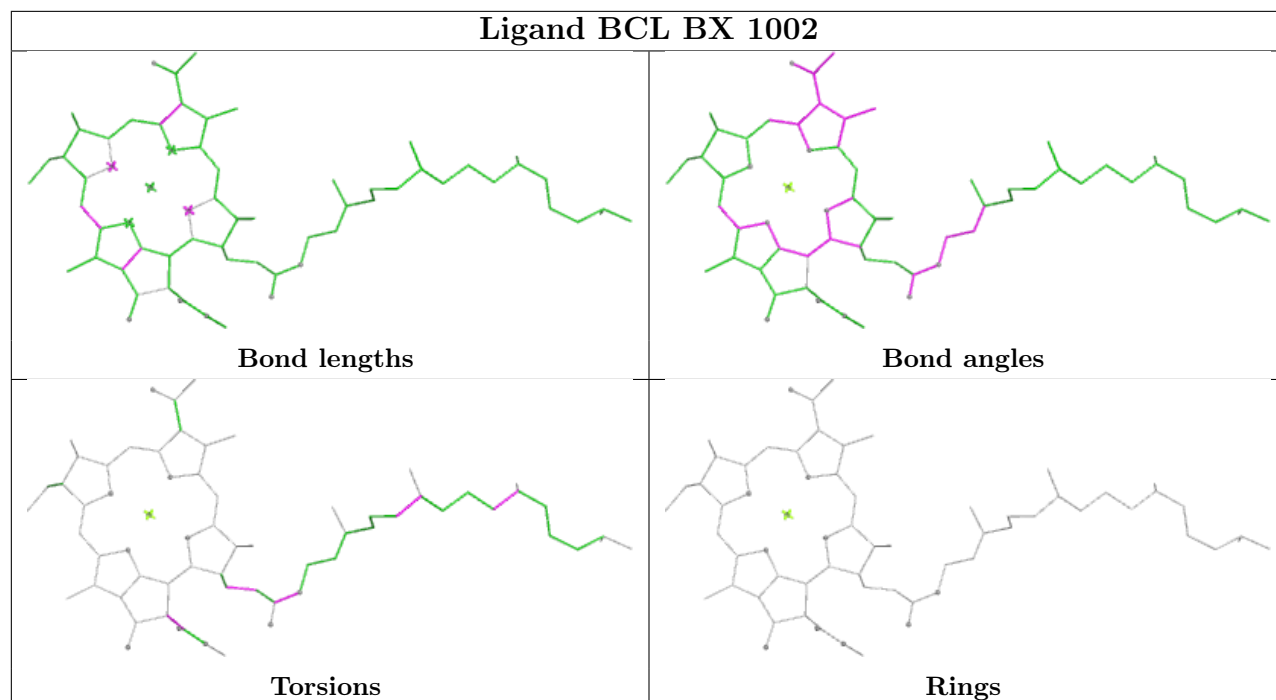
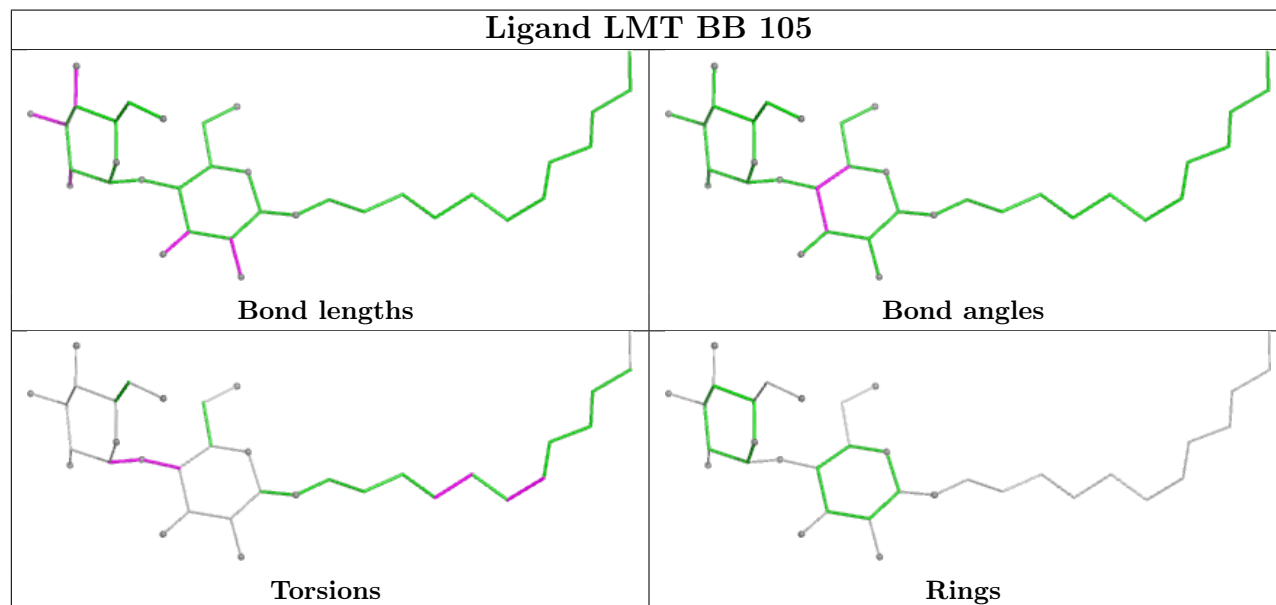


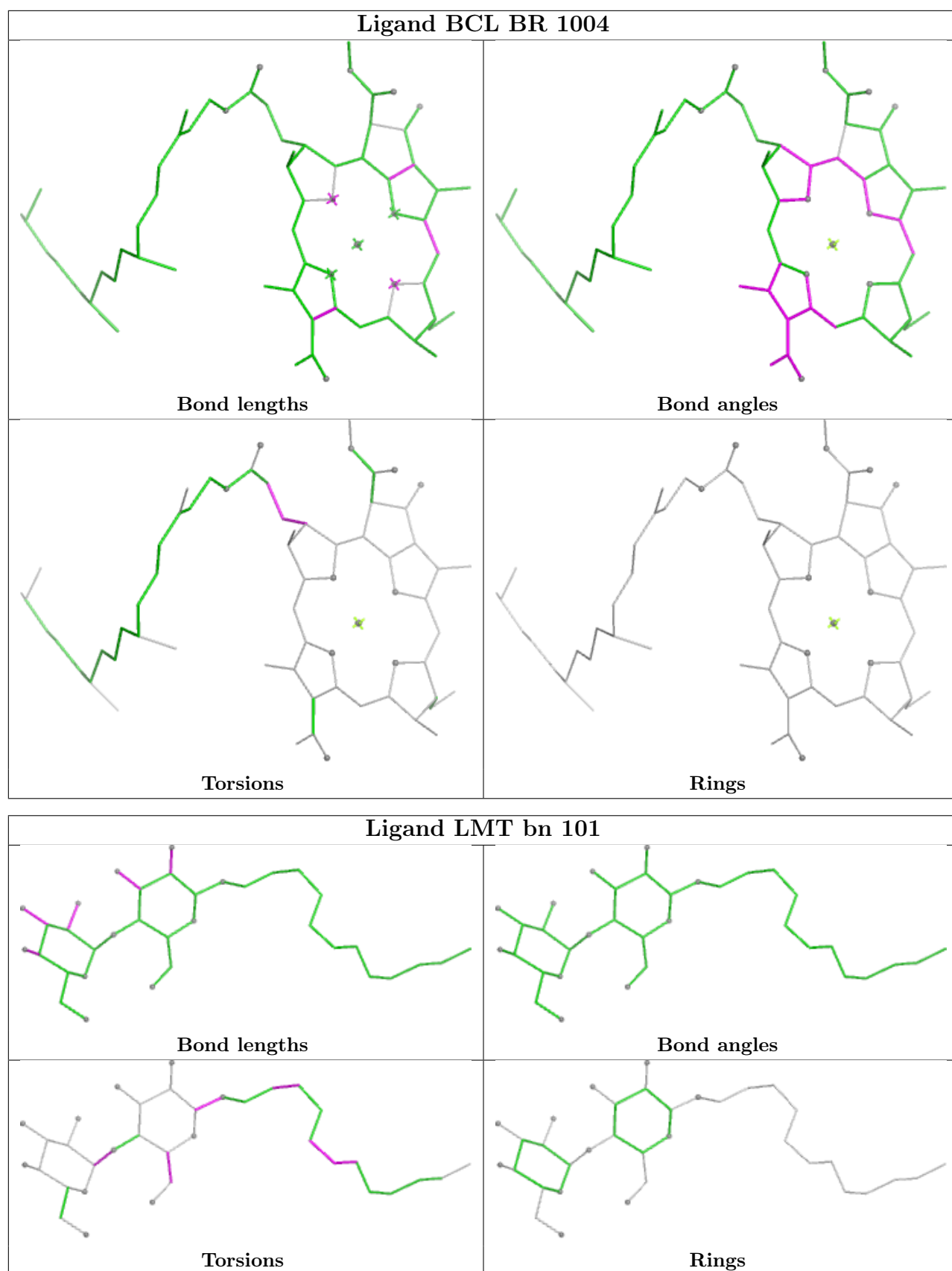


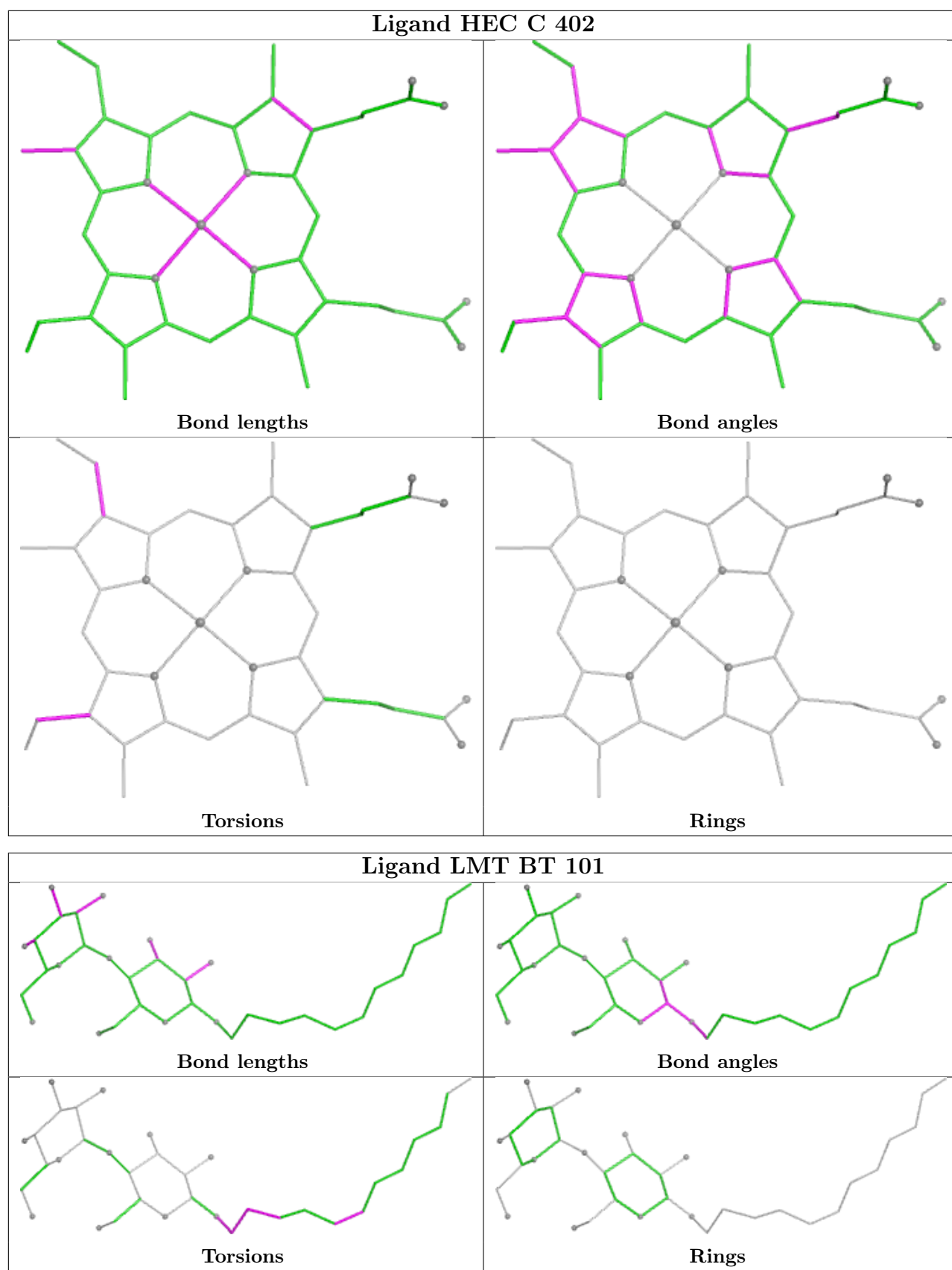


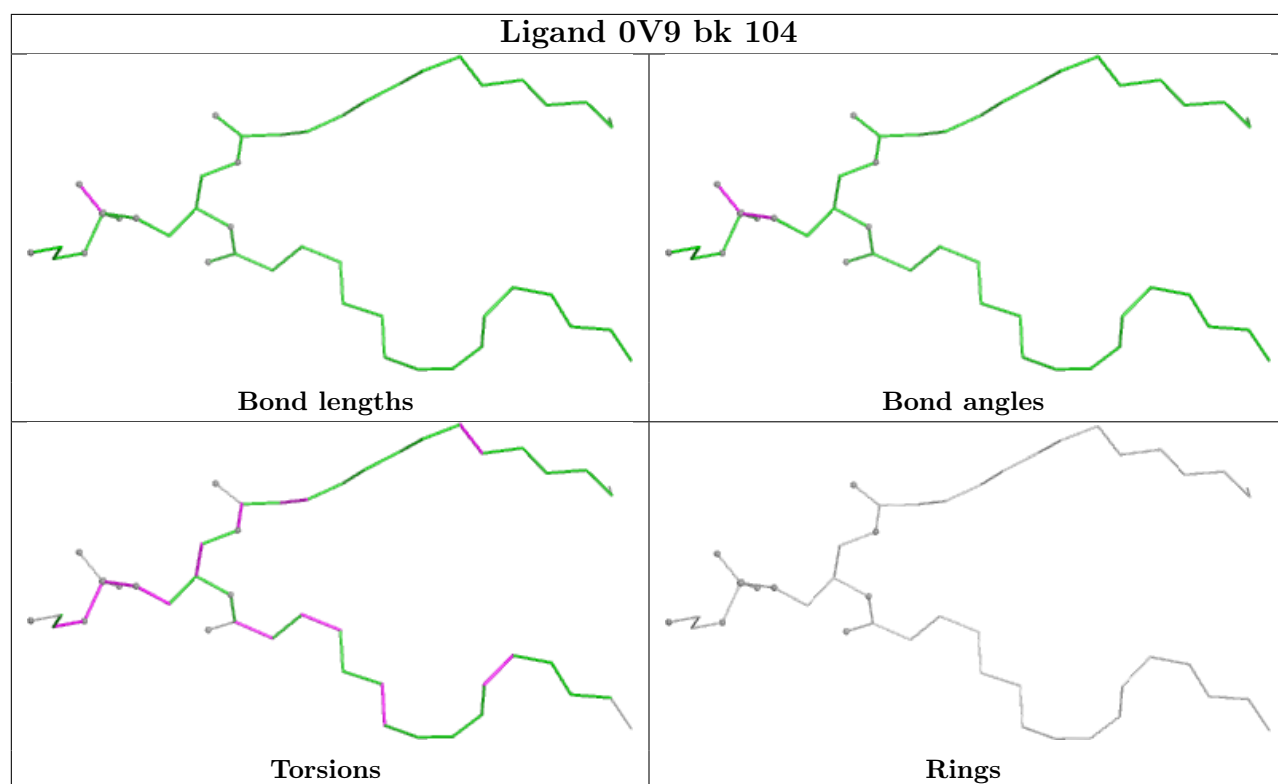
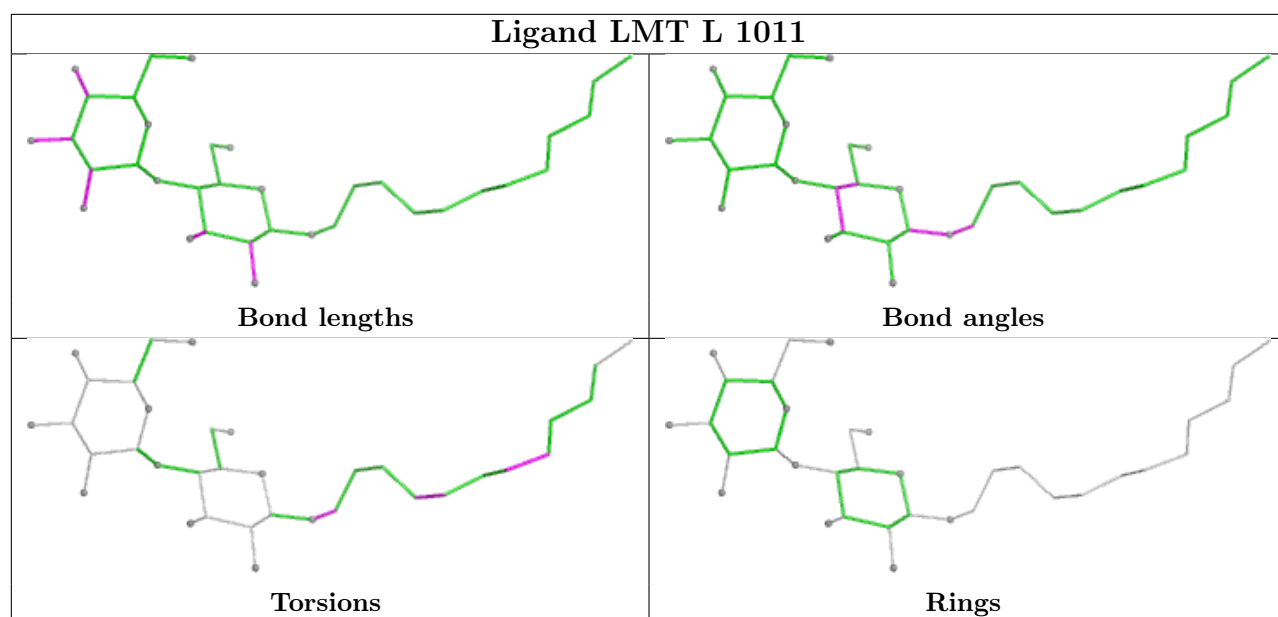


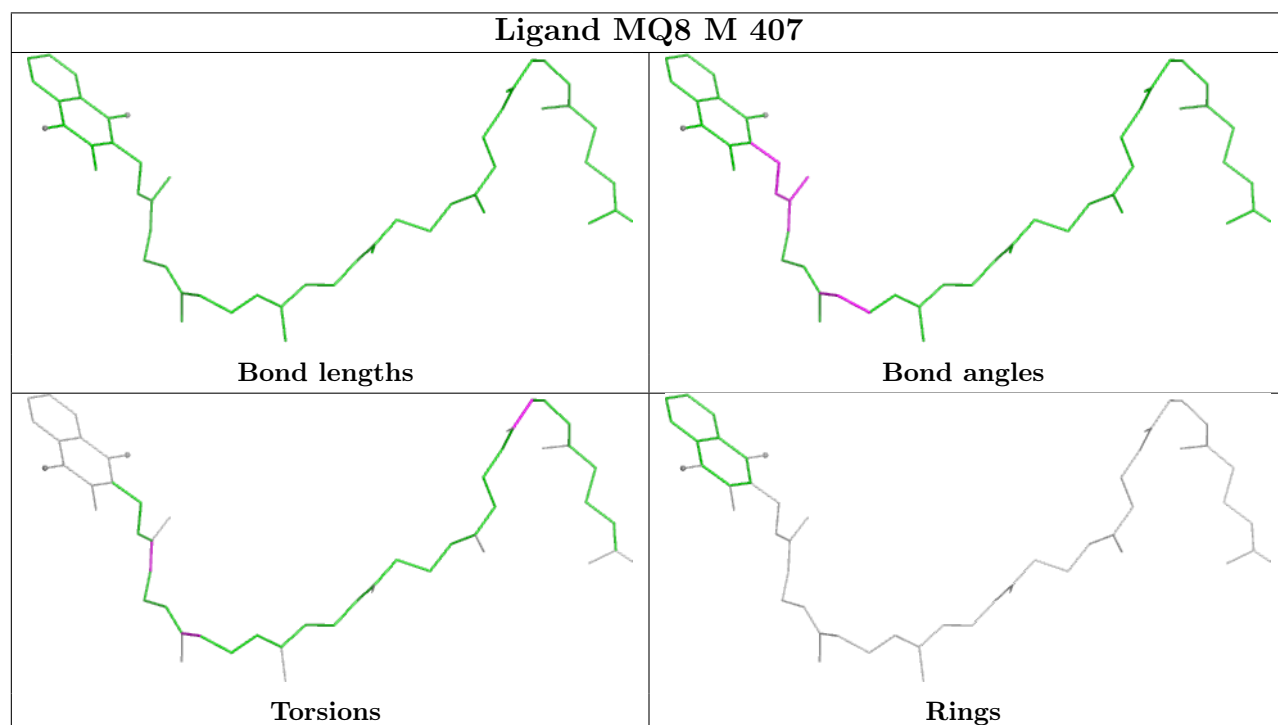
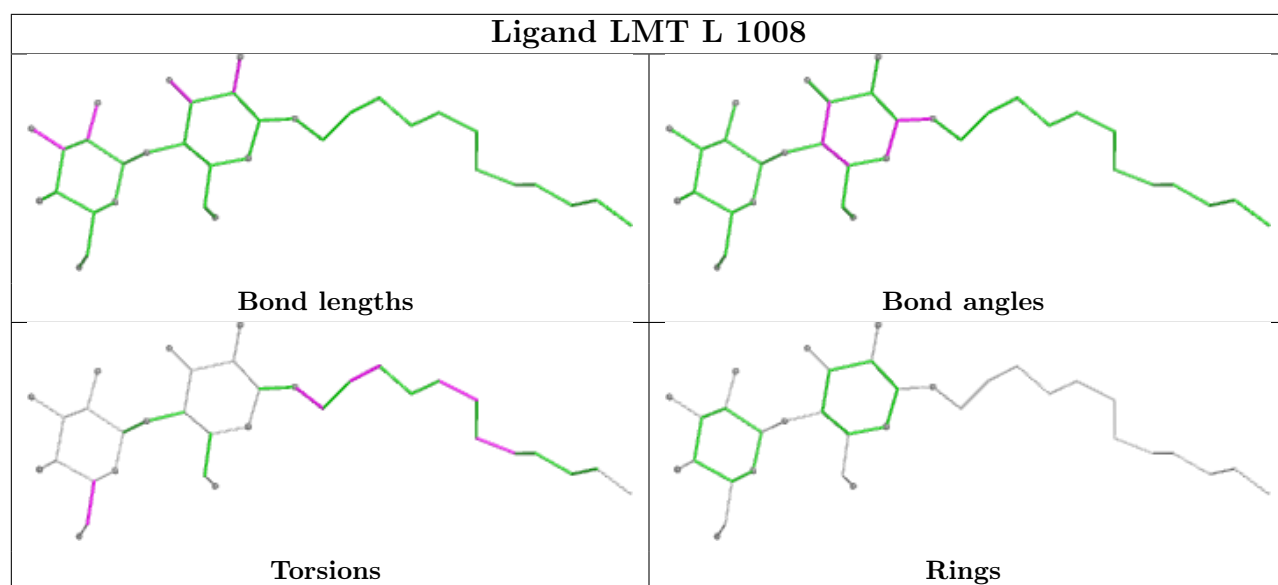


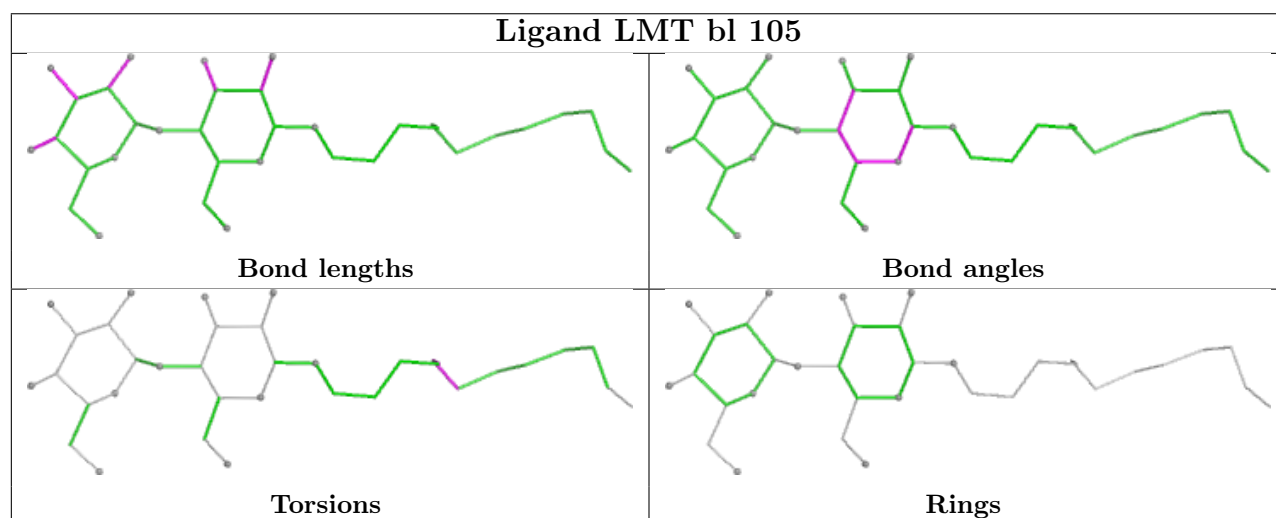
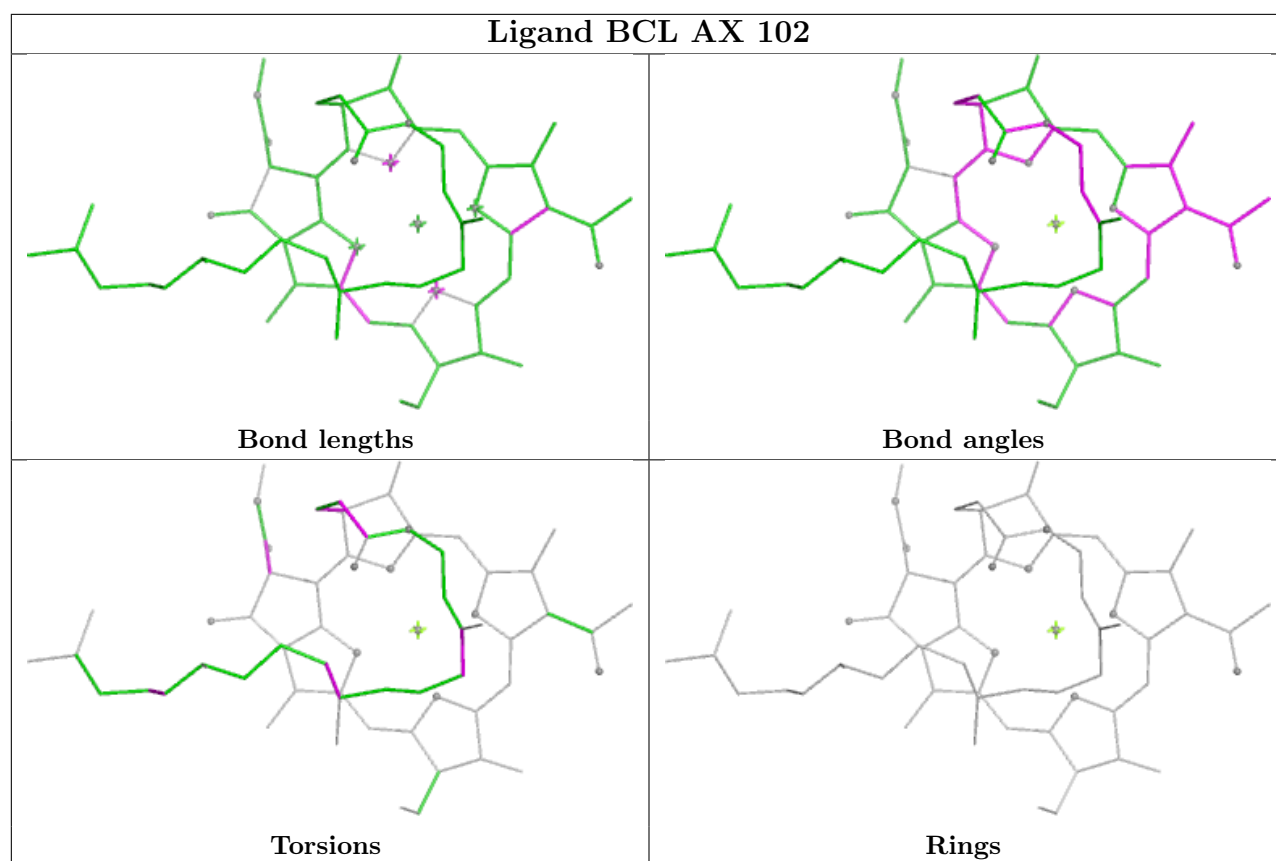
Ligand BCL BX 1002**Ligand LMT BB 105**

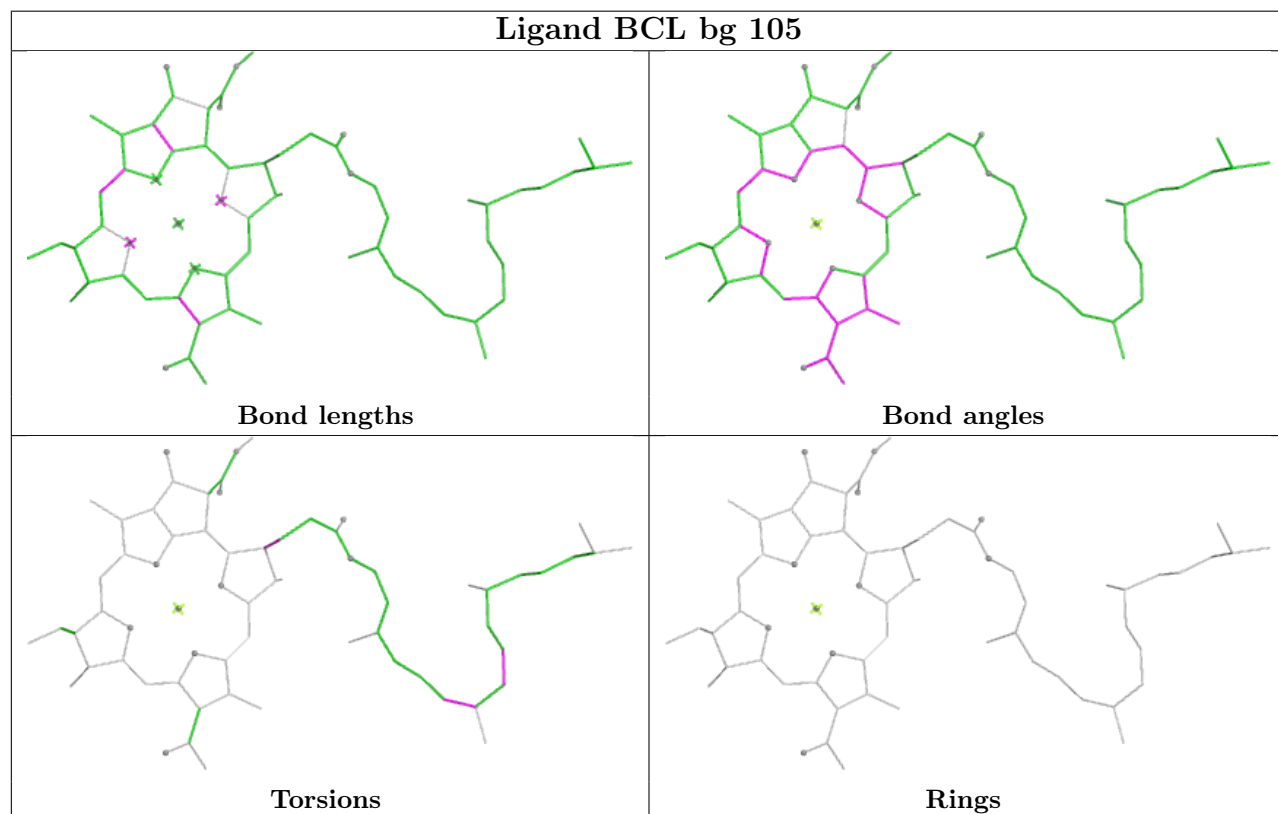
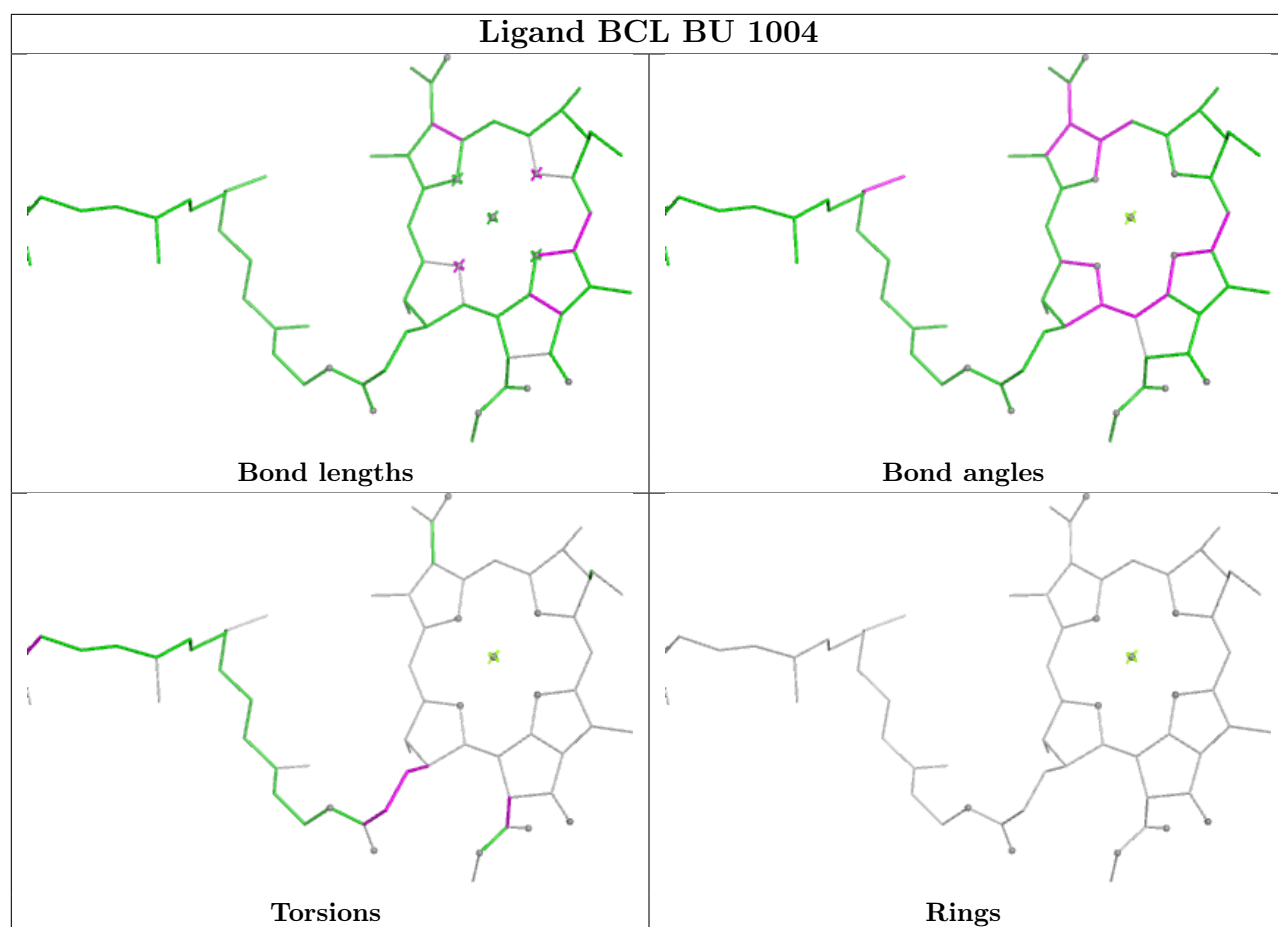


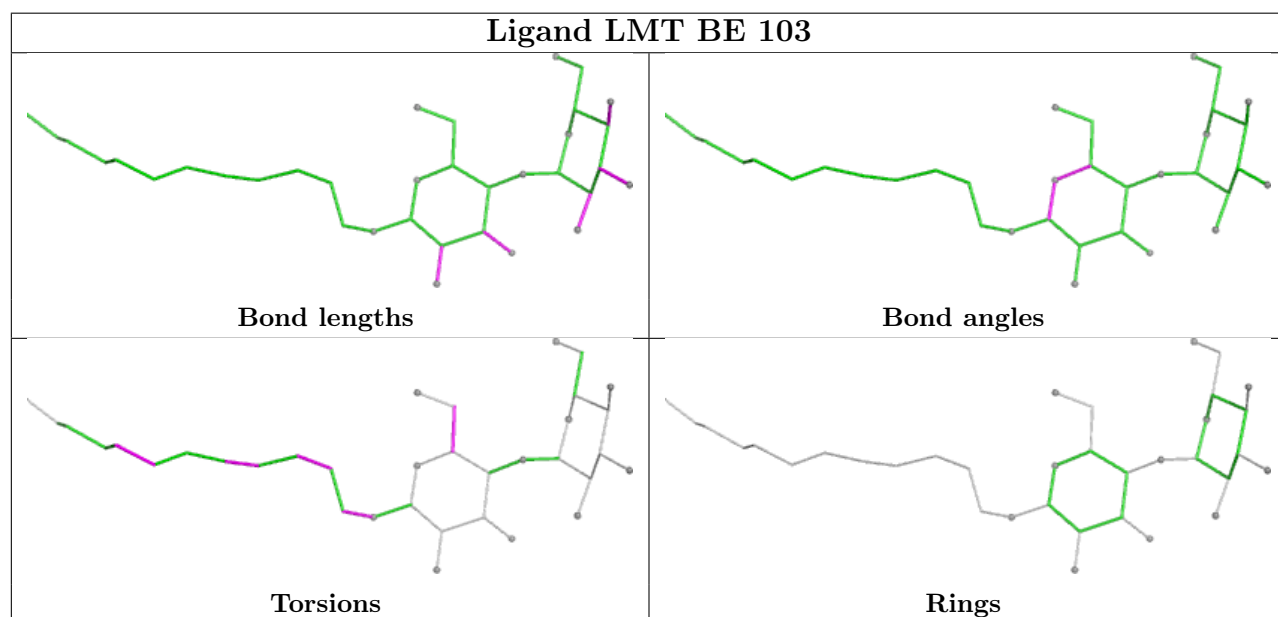
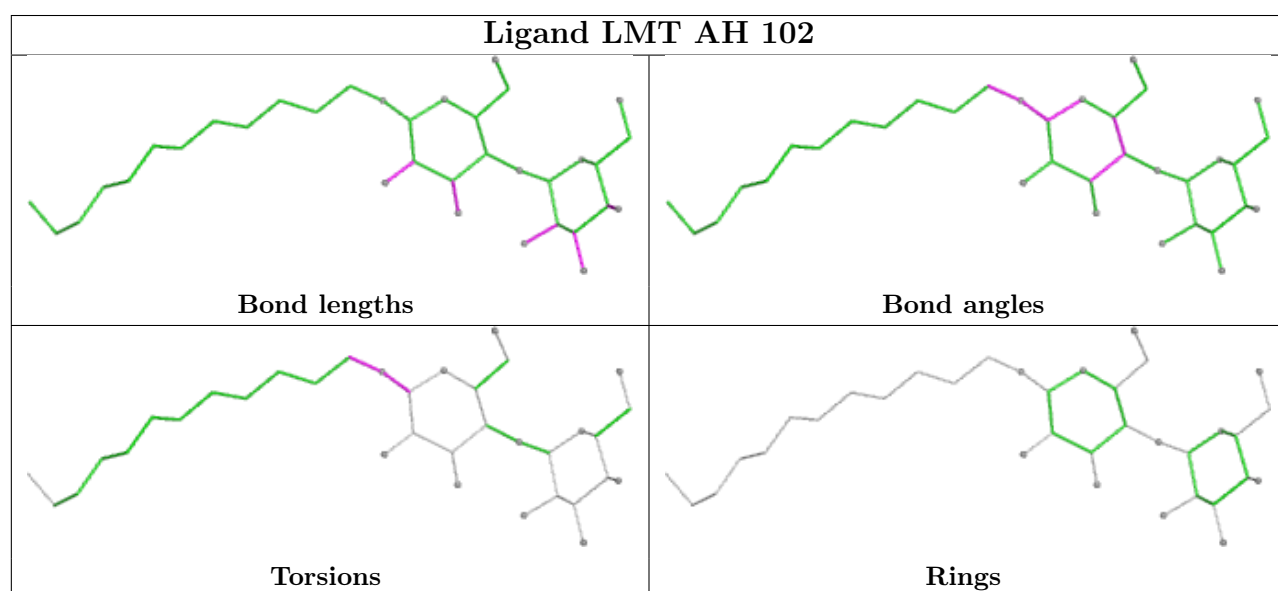
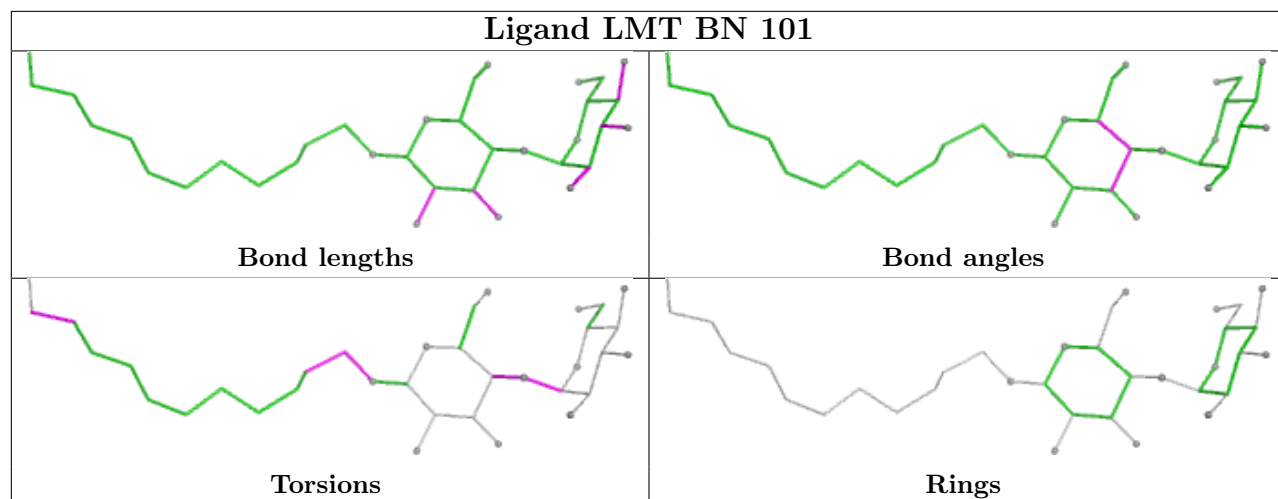




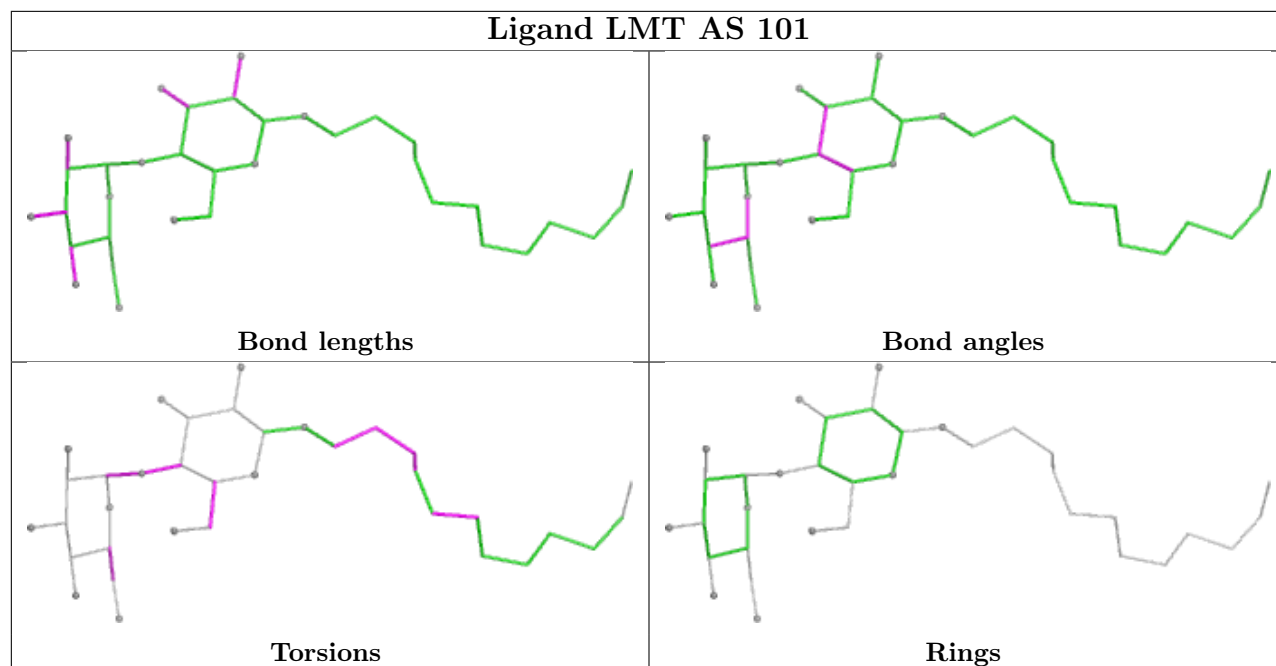




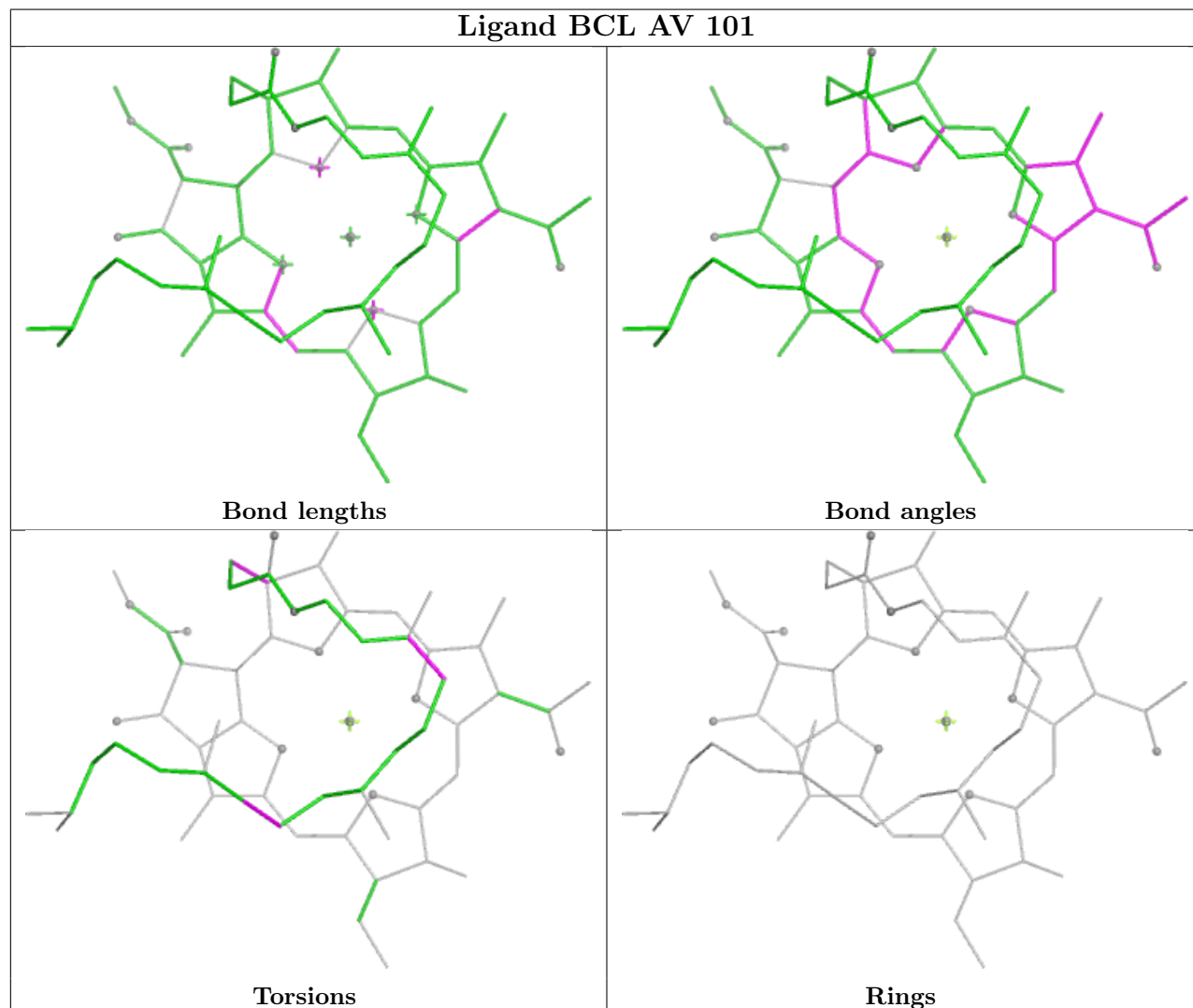


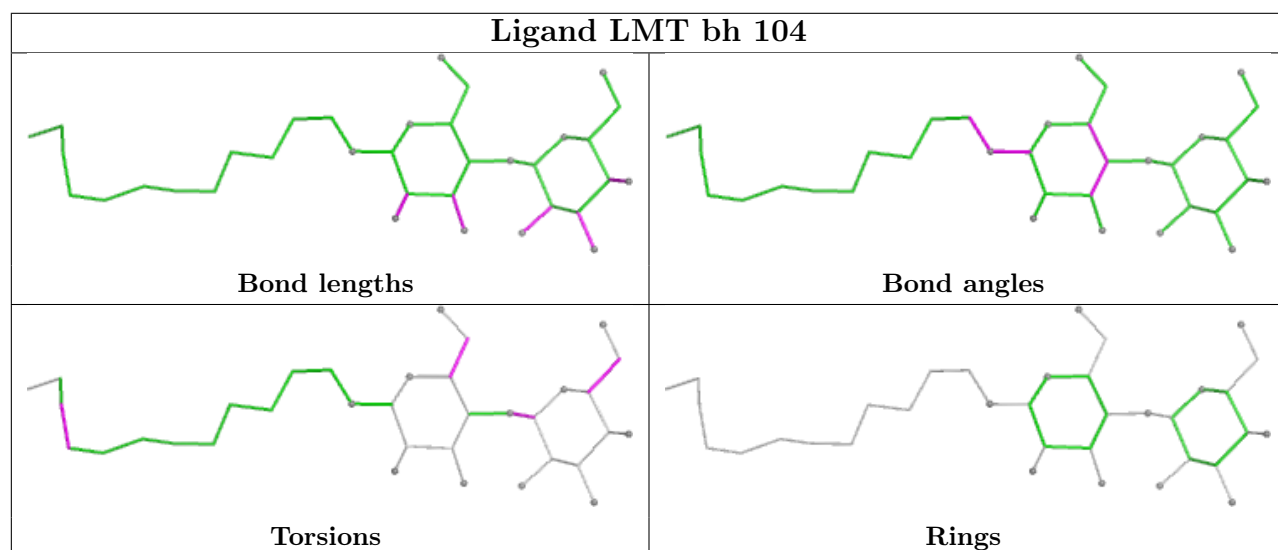
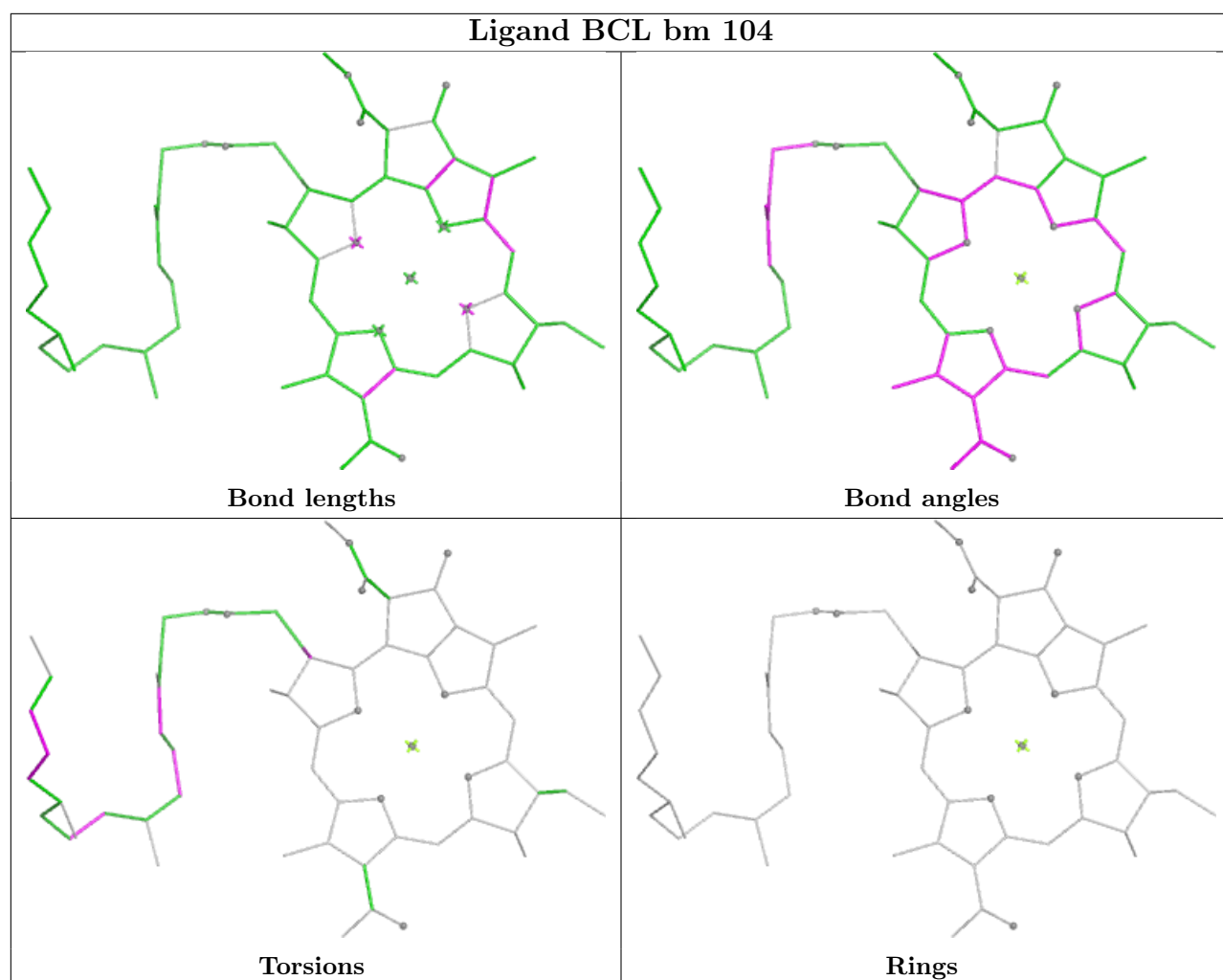


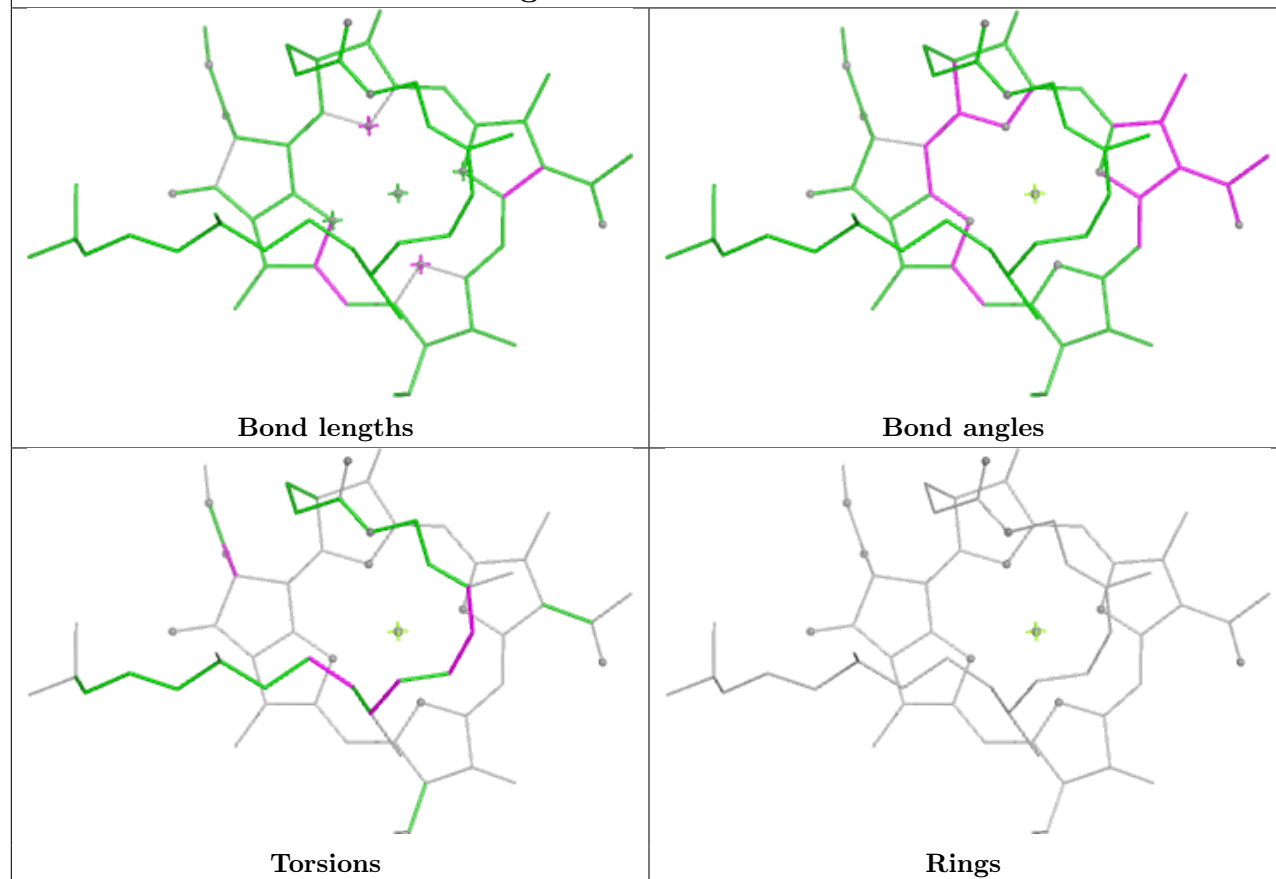
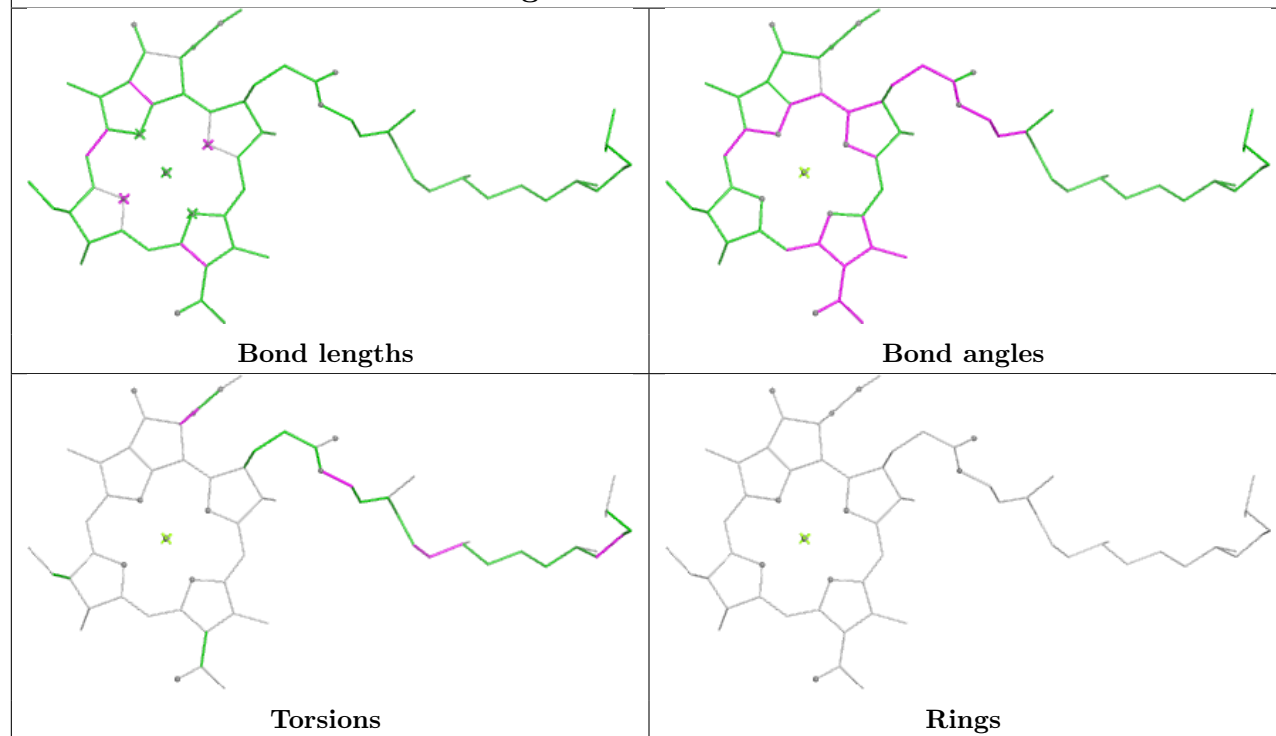
Ligand LMT AS 101



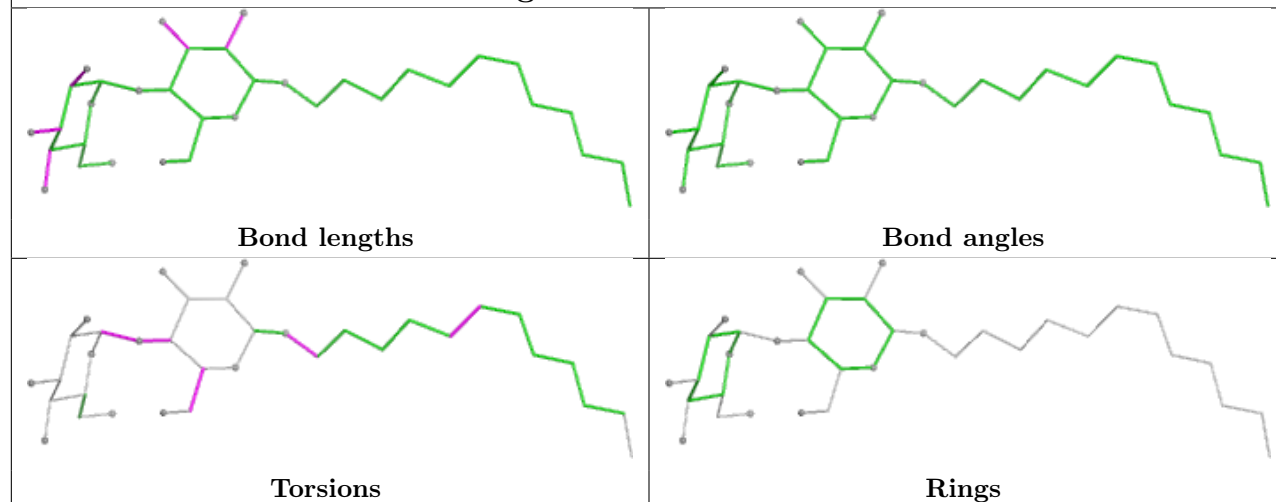
Ligand BCL AV 101



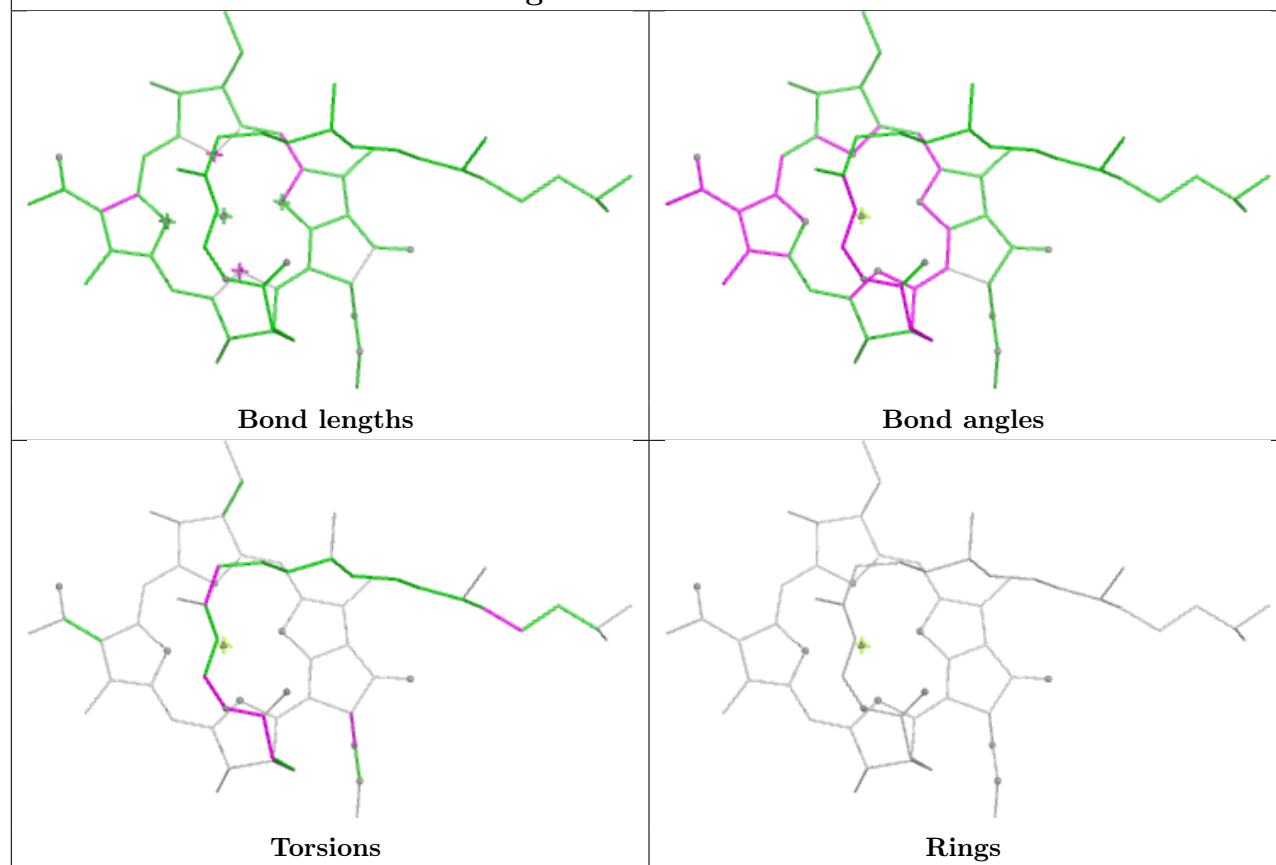


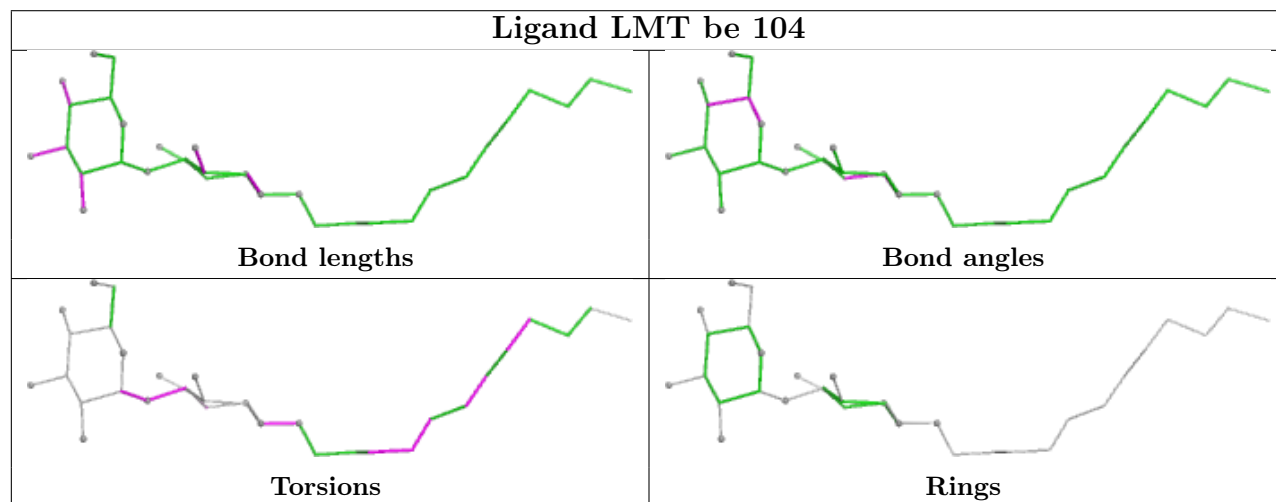
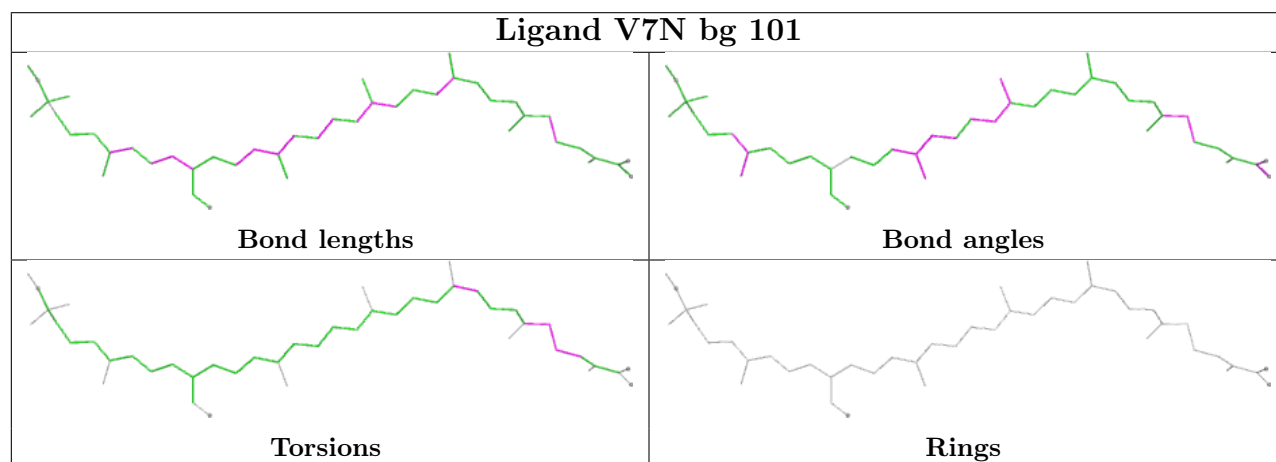
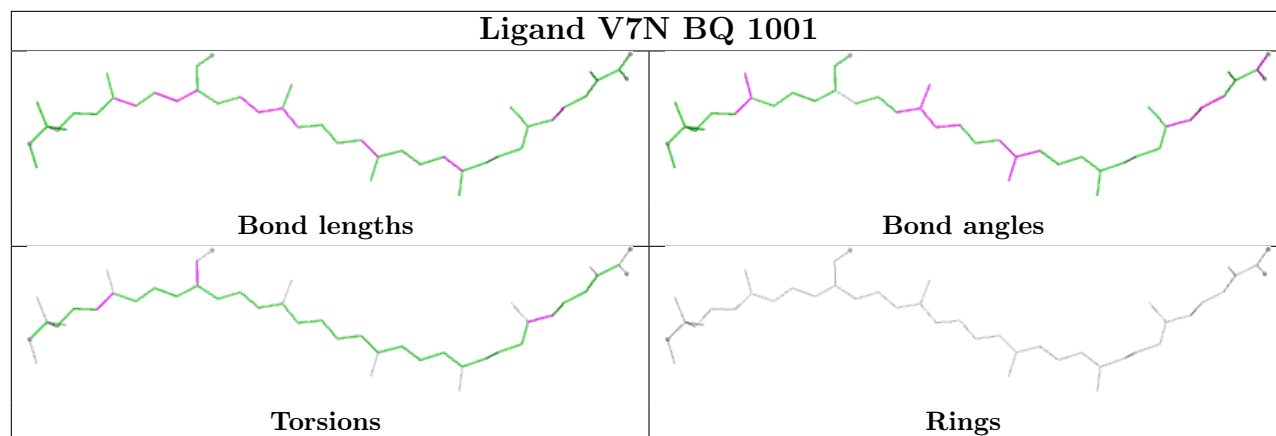
Ligand BCL AP 103**Ligand BCL BE 104**

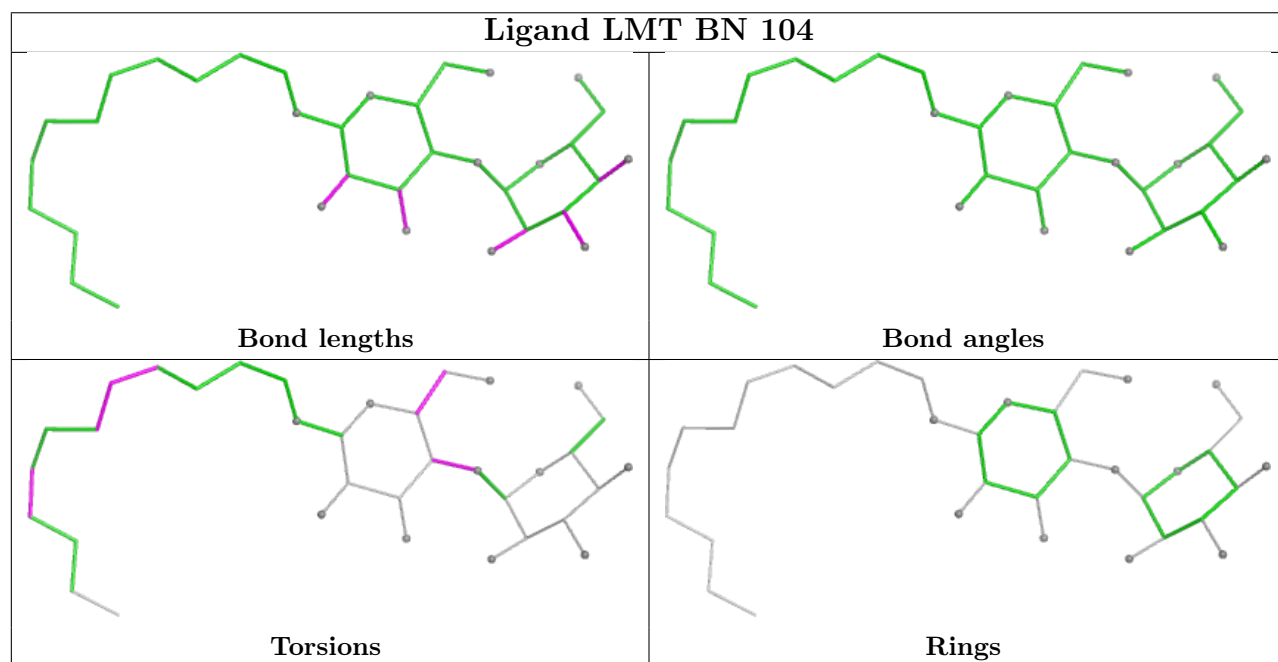
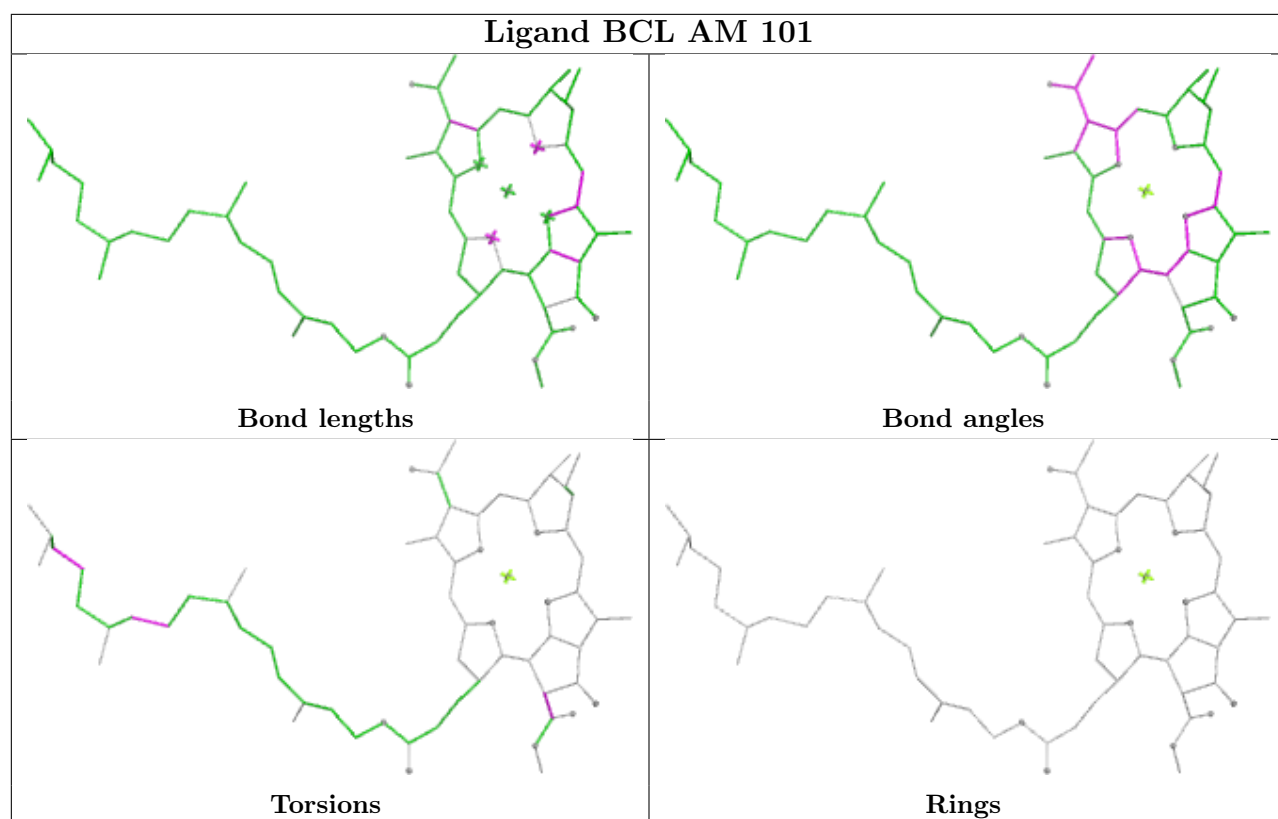
Ligand LMT BT 104

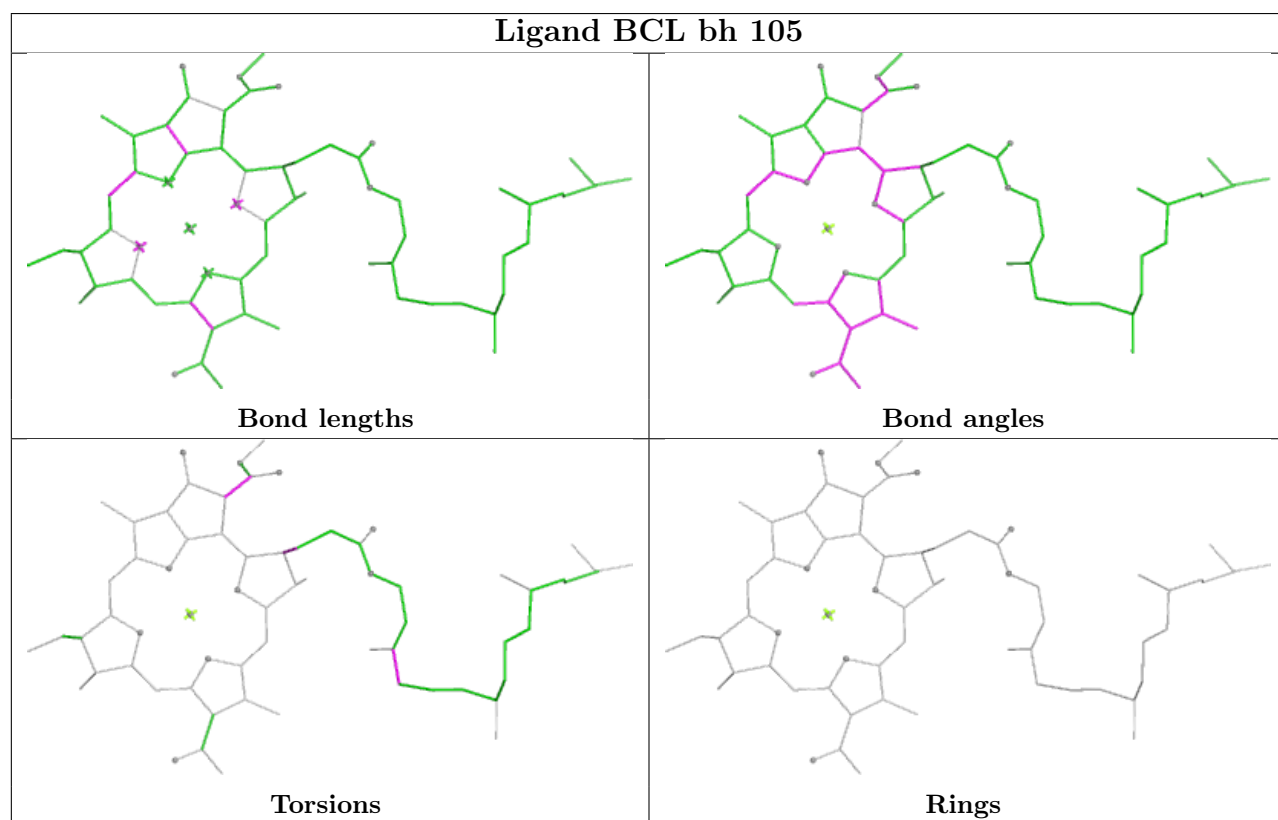
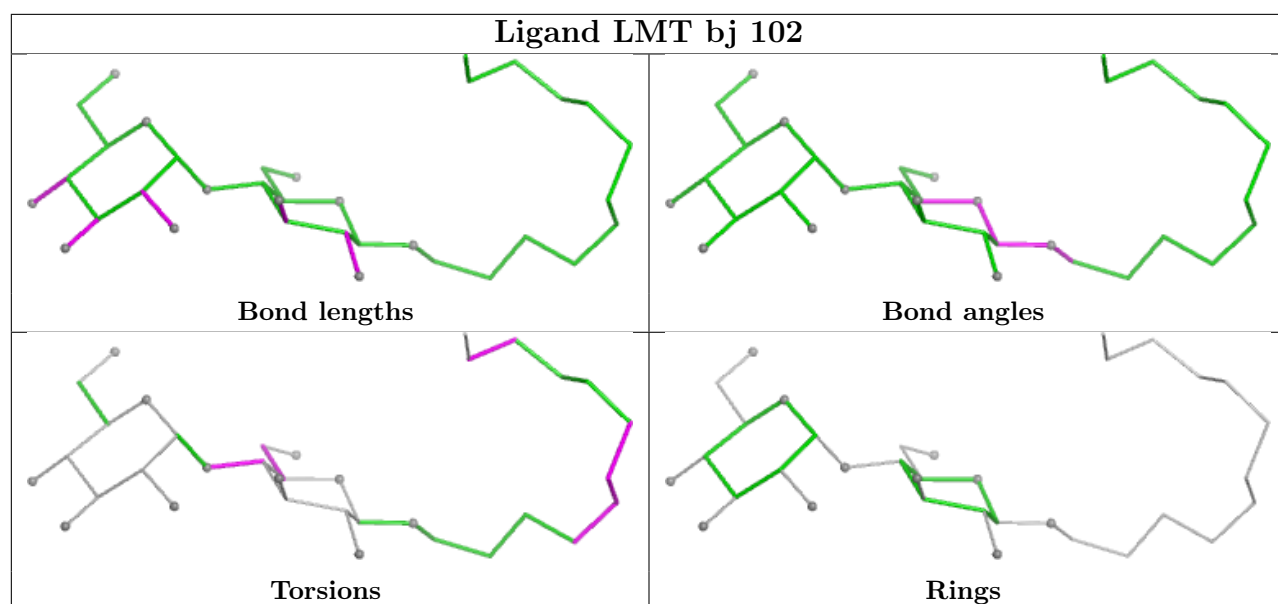


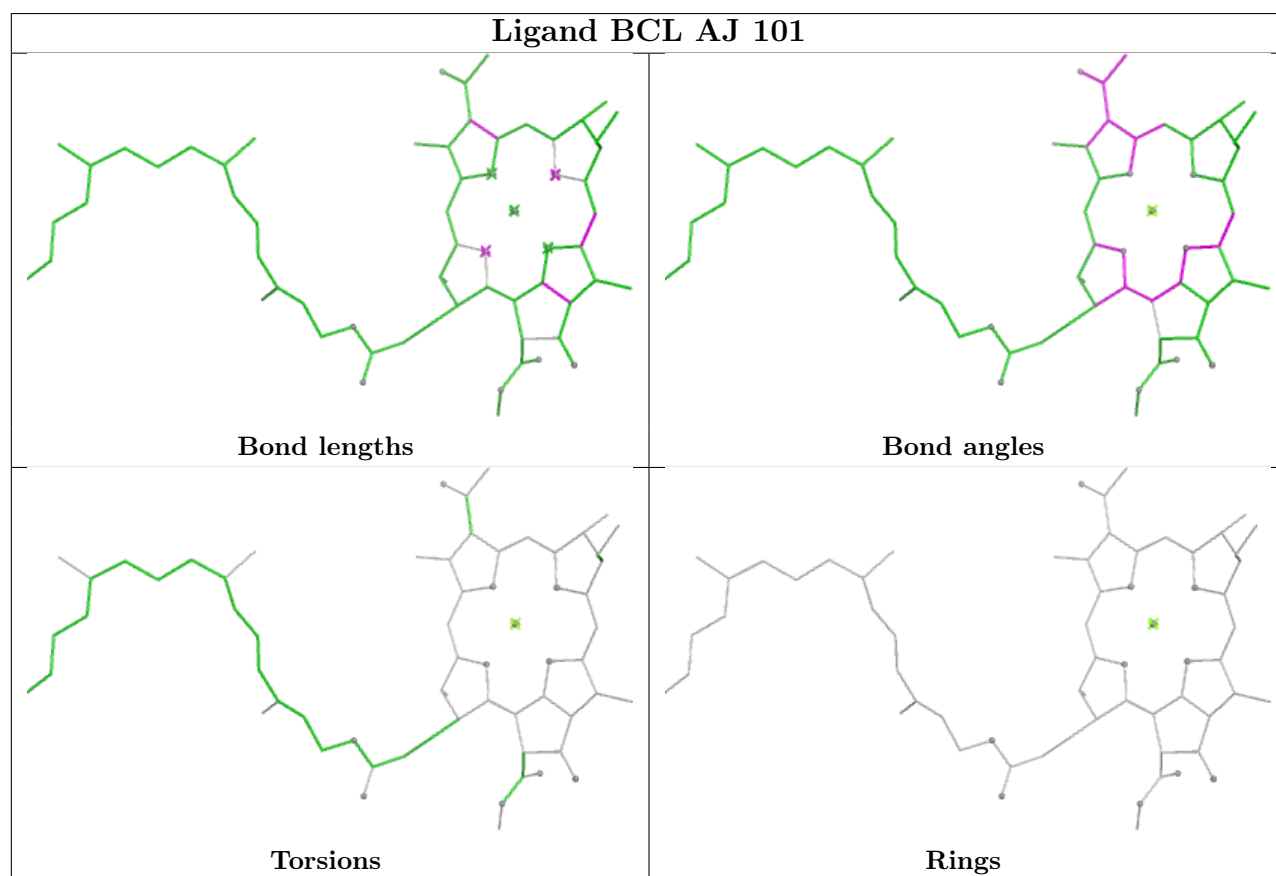
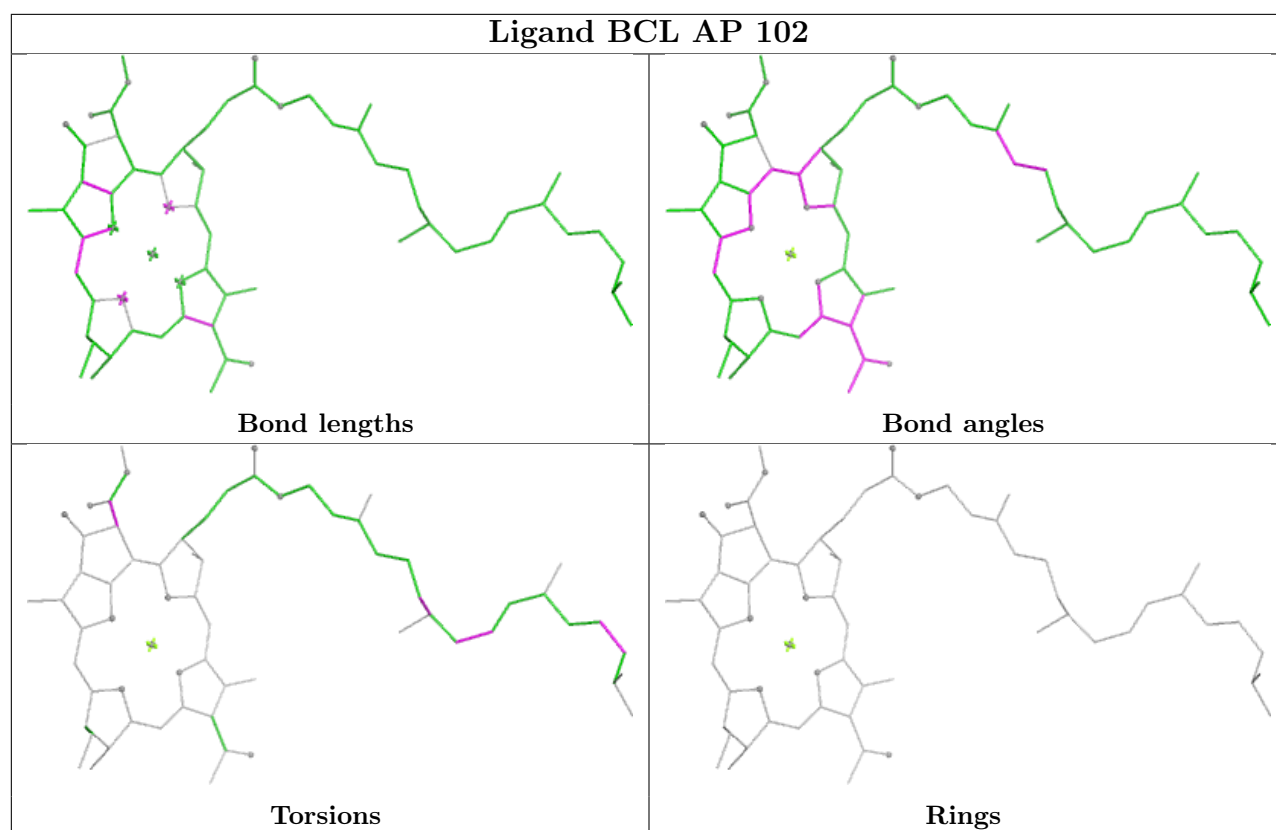
Ligand BCL AI 103

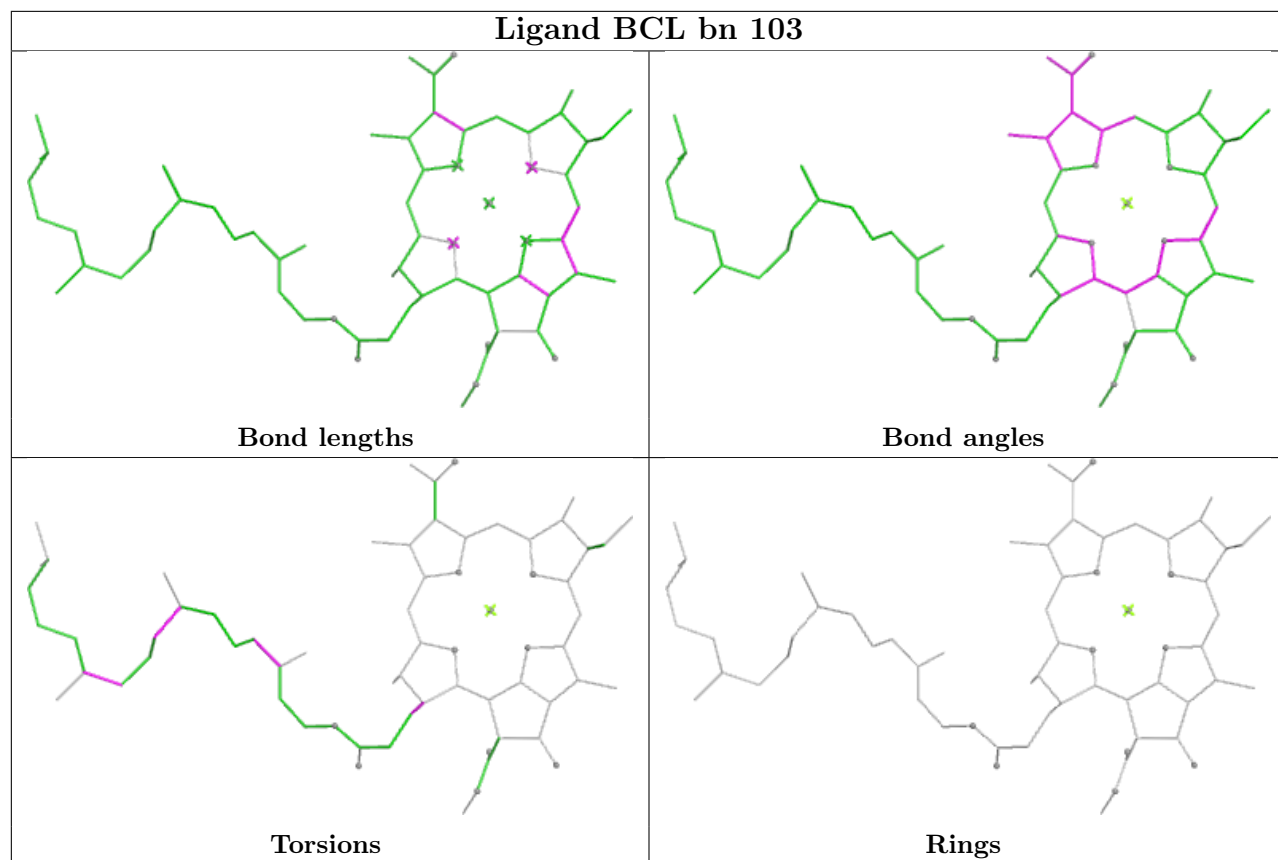


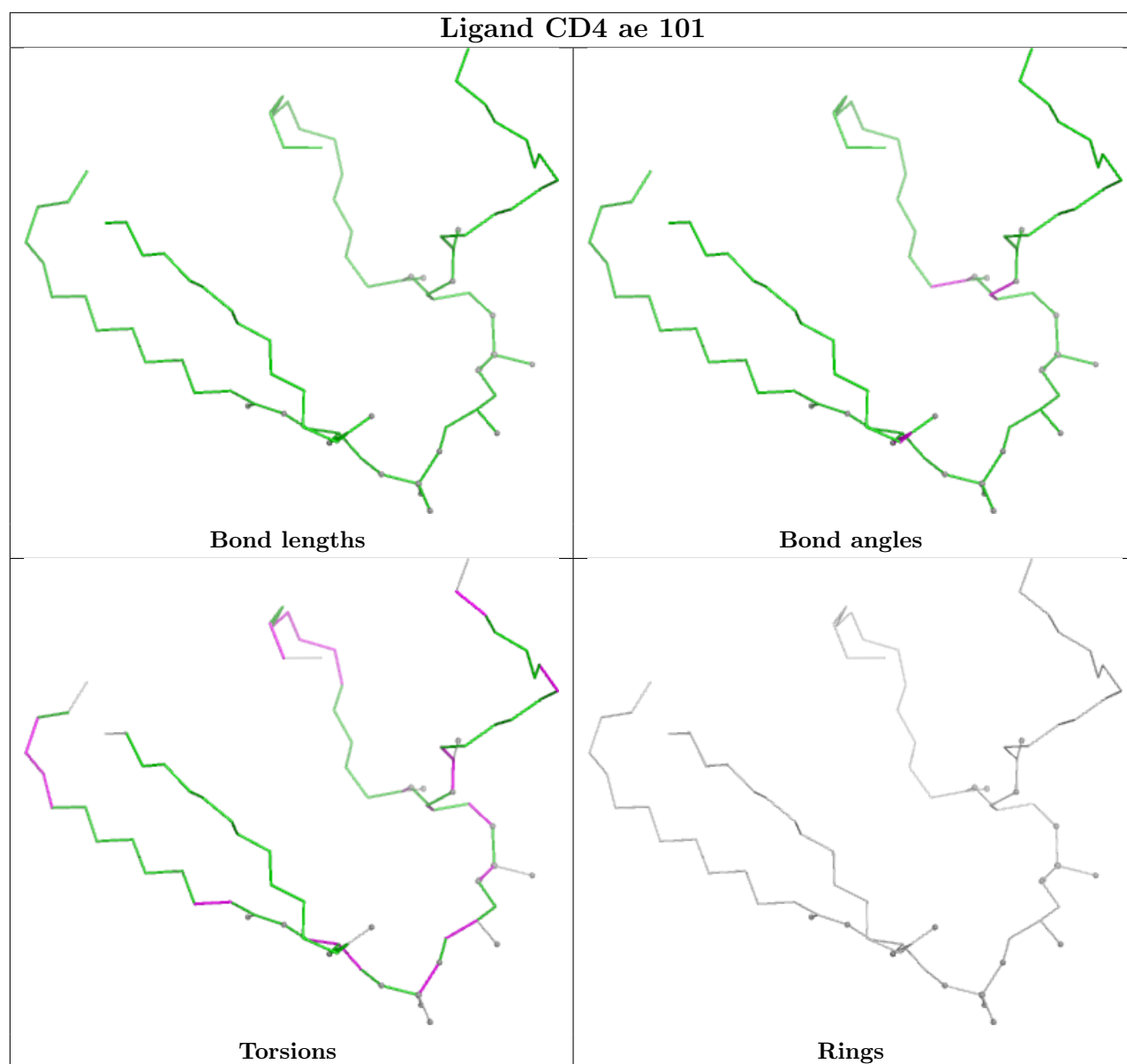


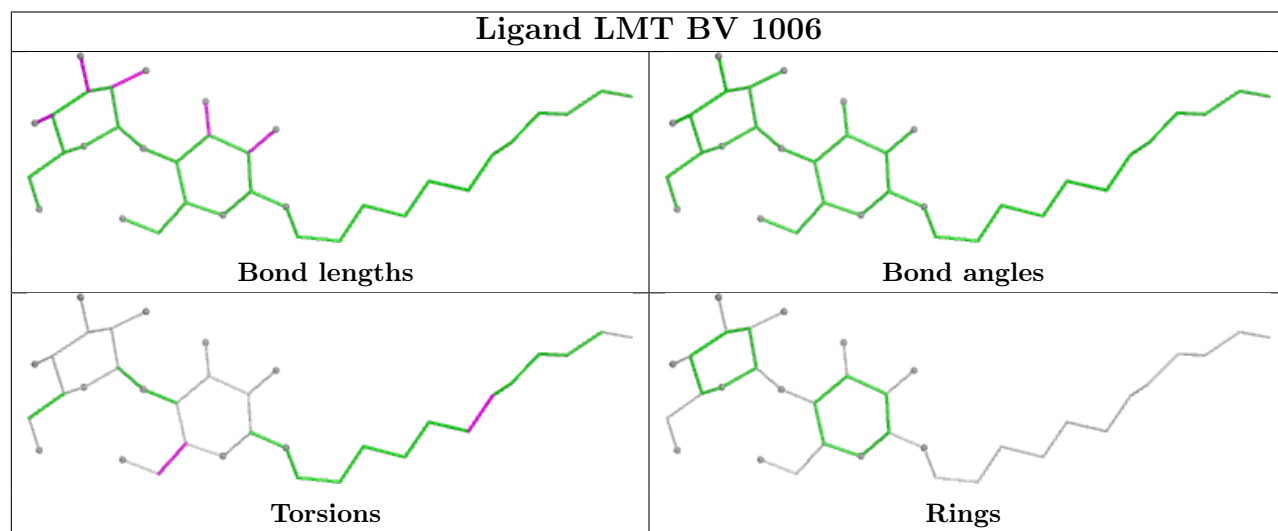
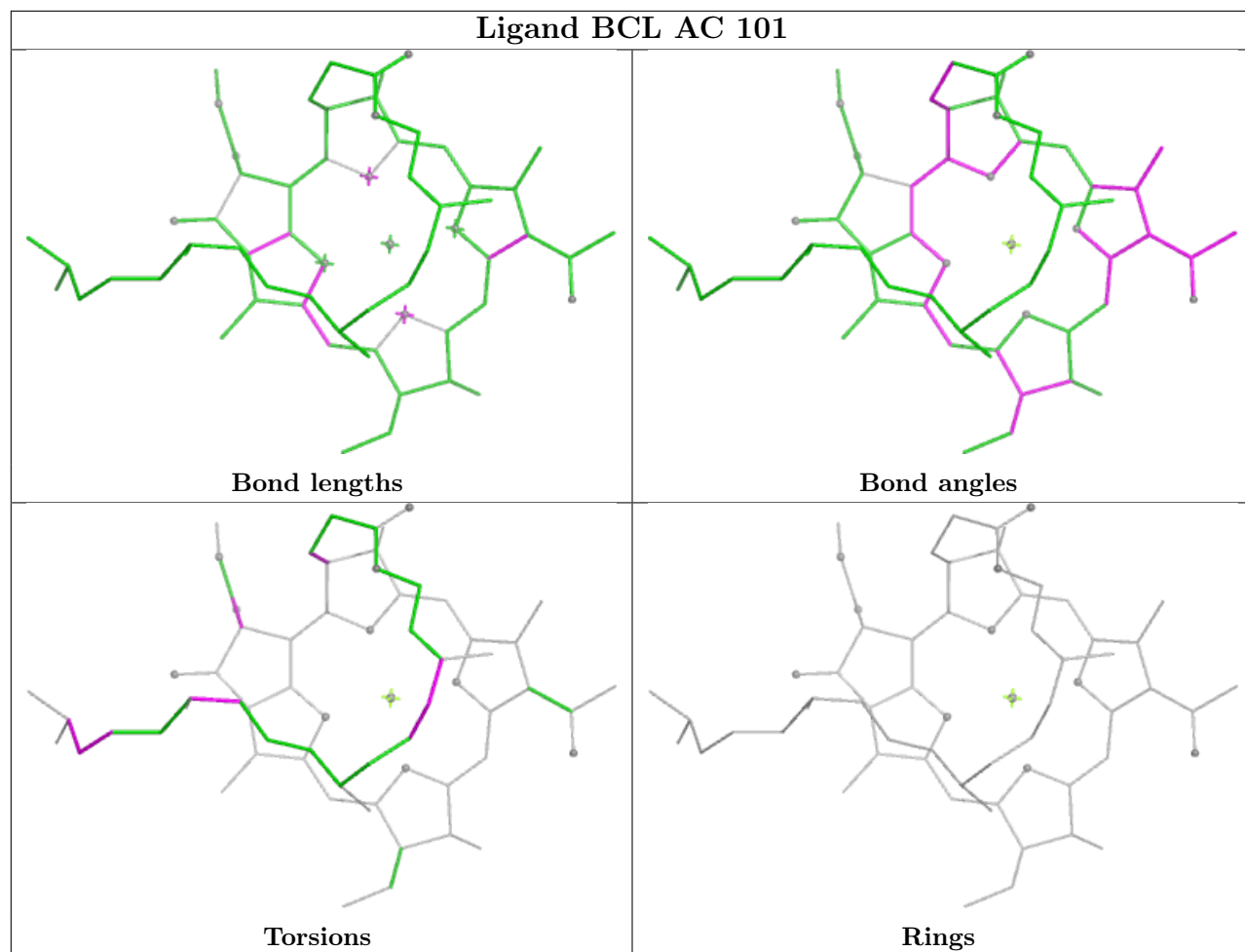


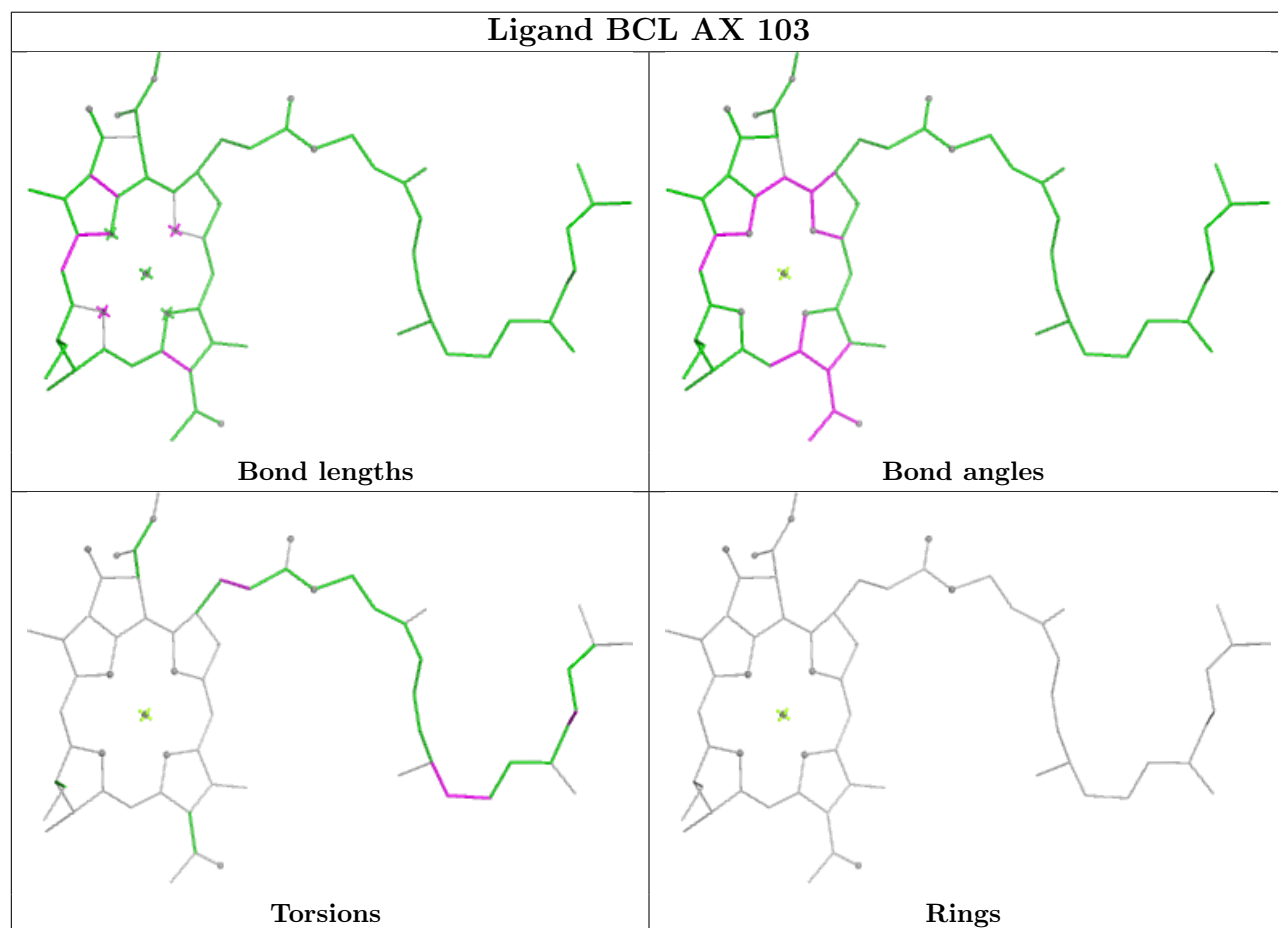
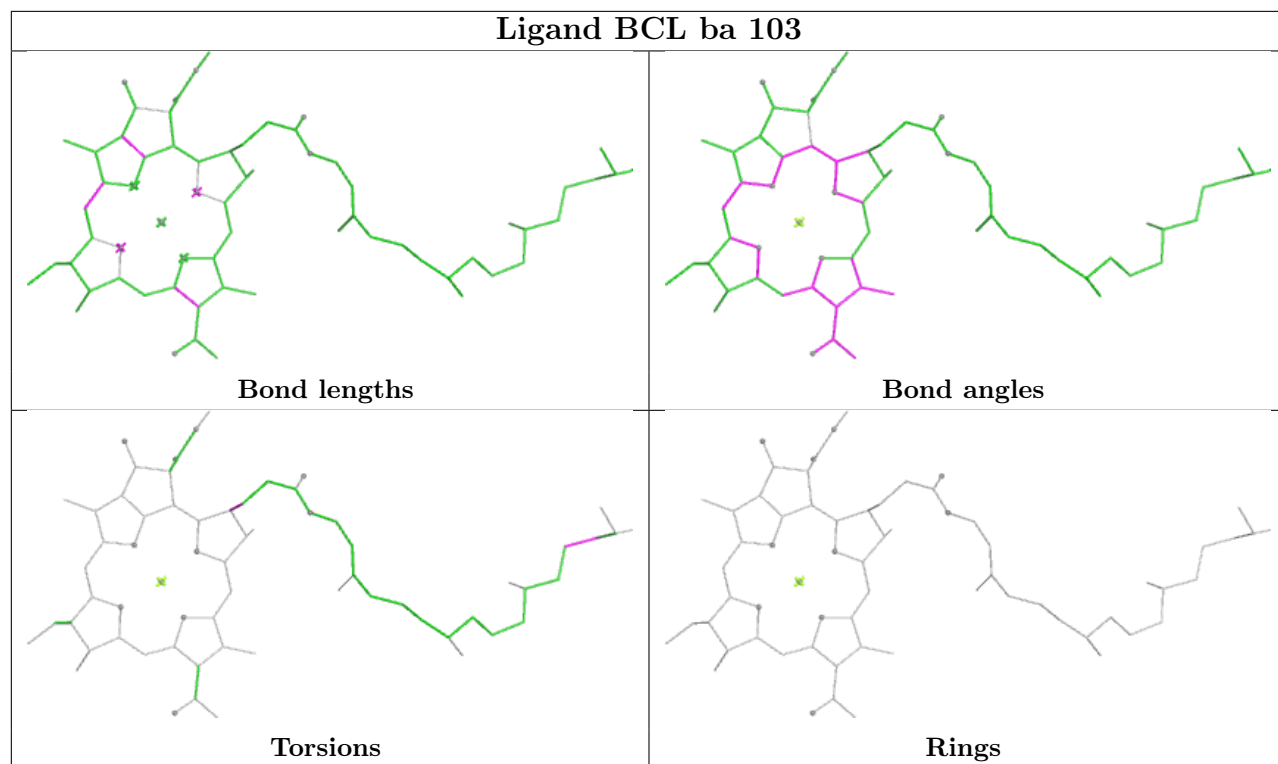


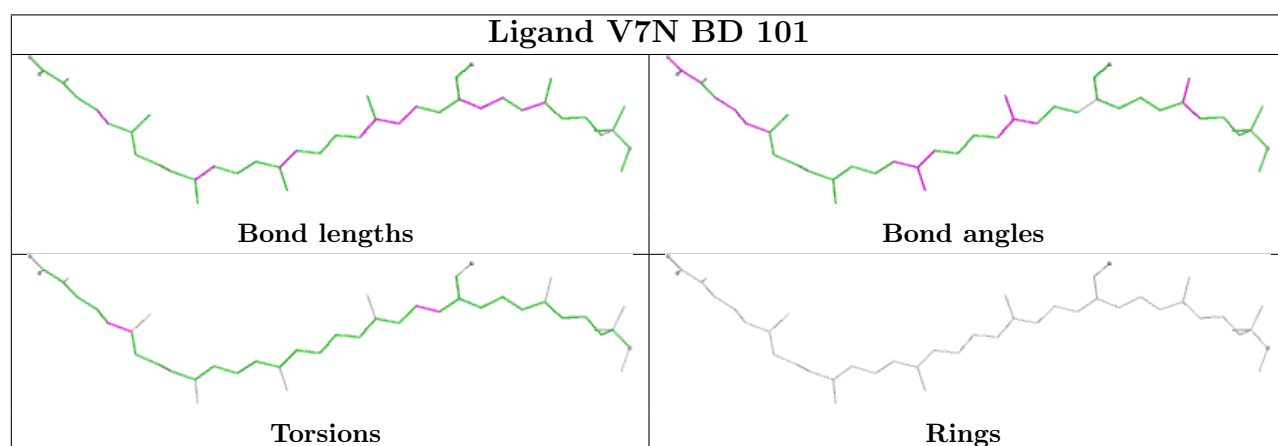
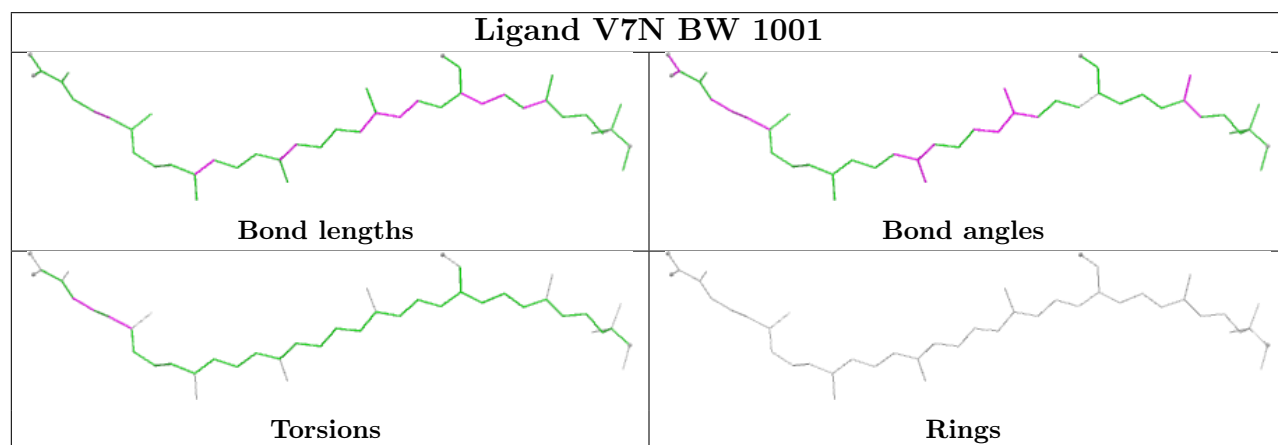
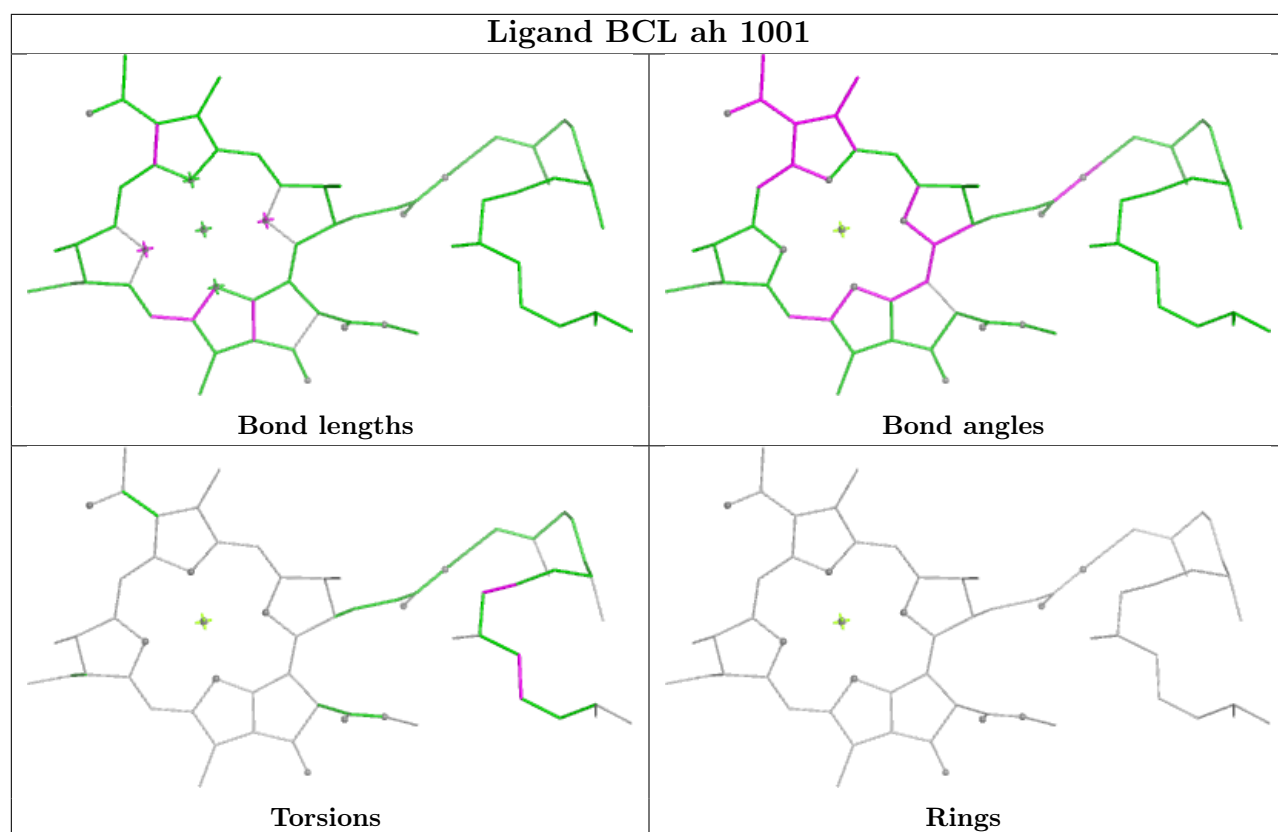


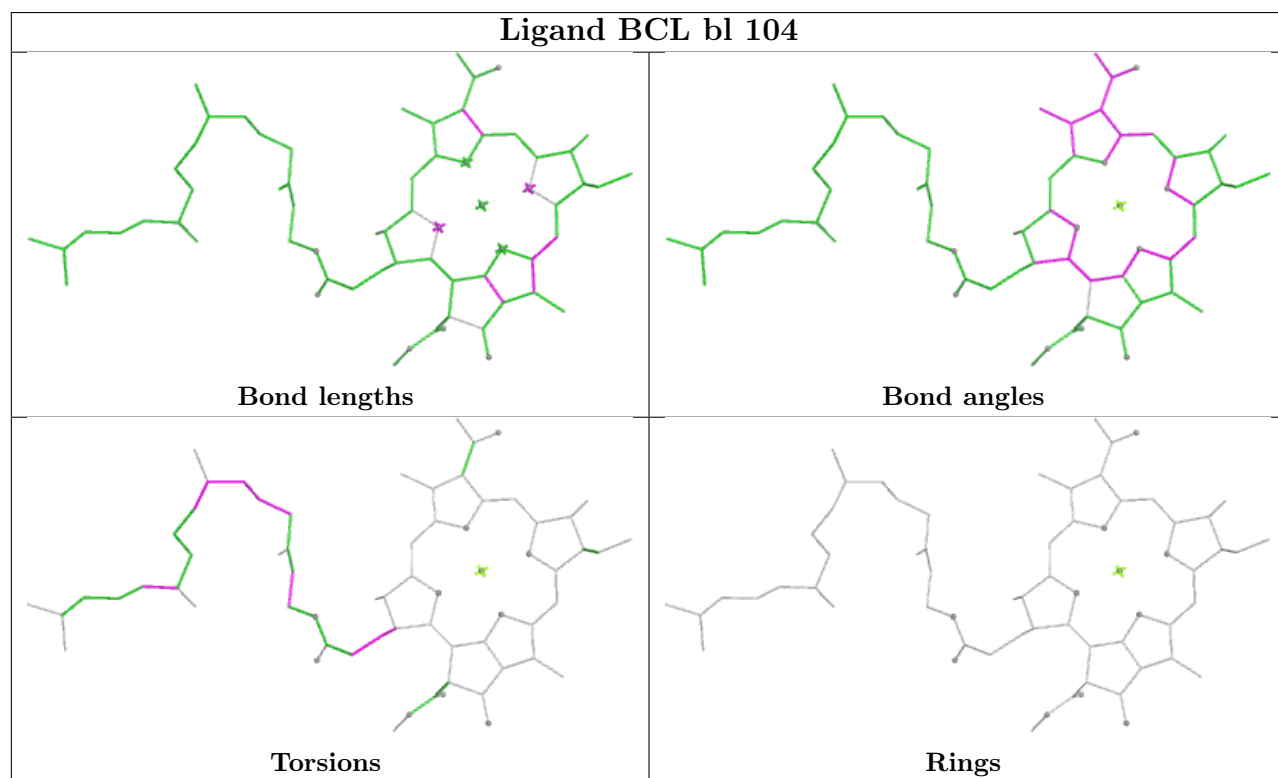
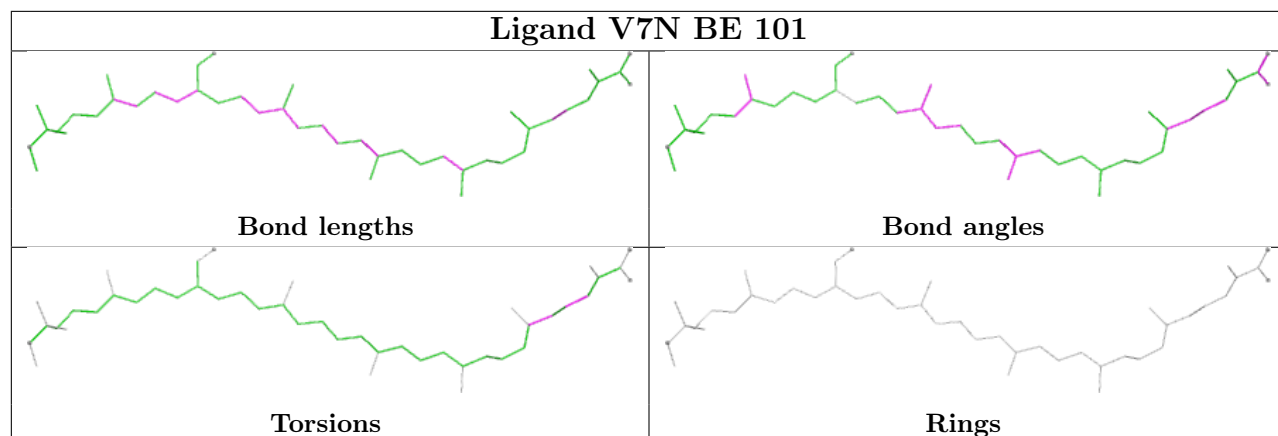


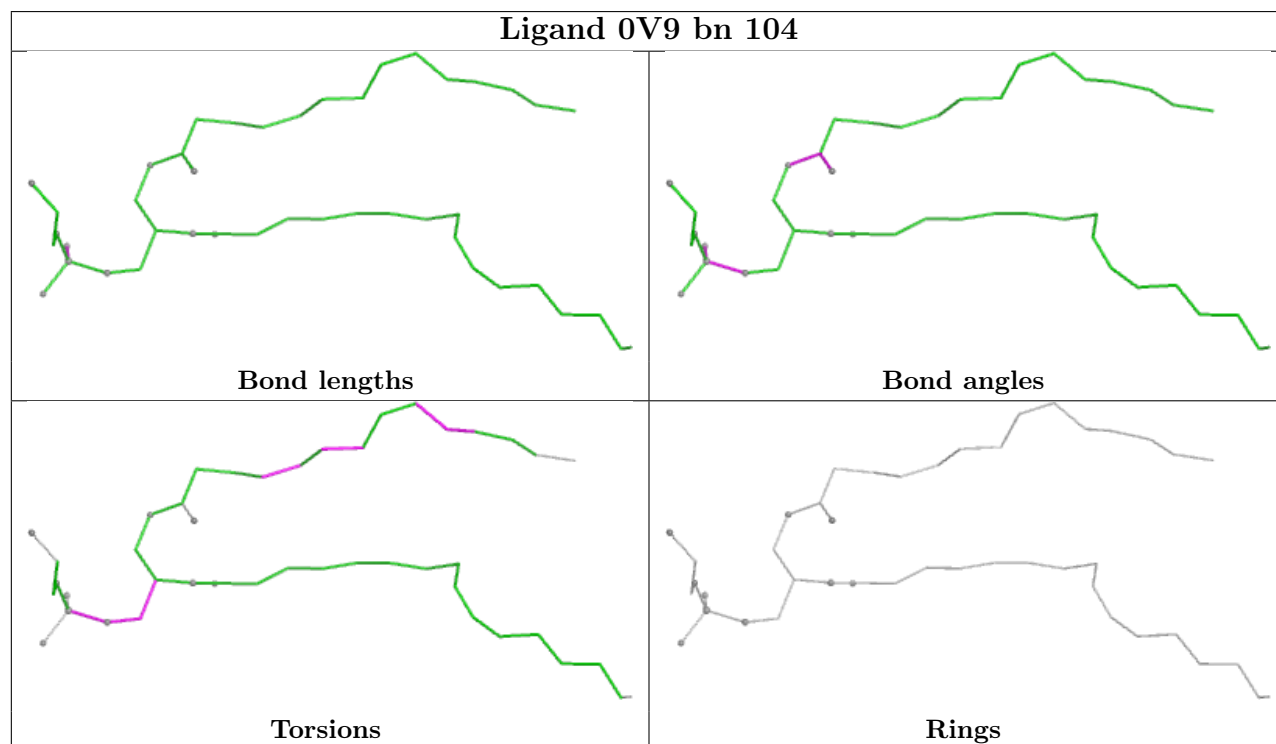
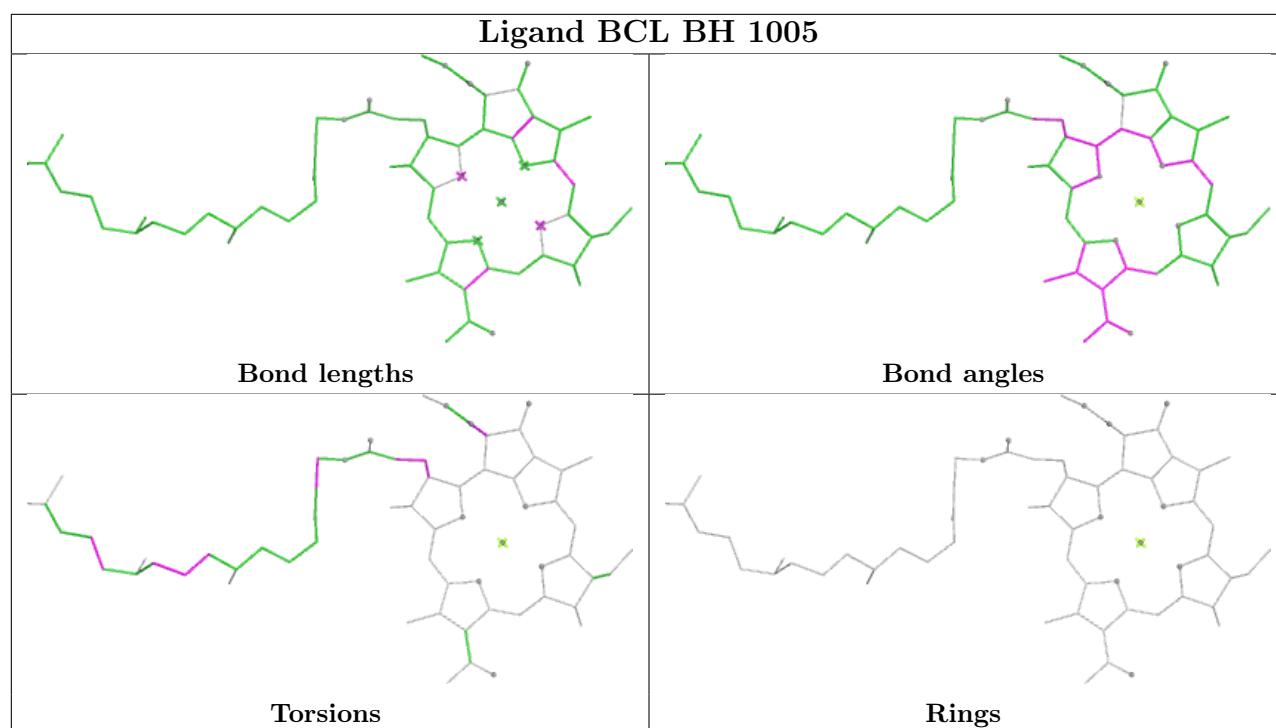


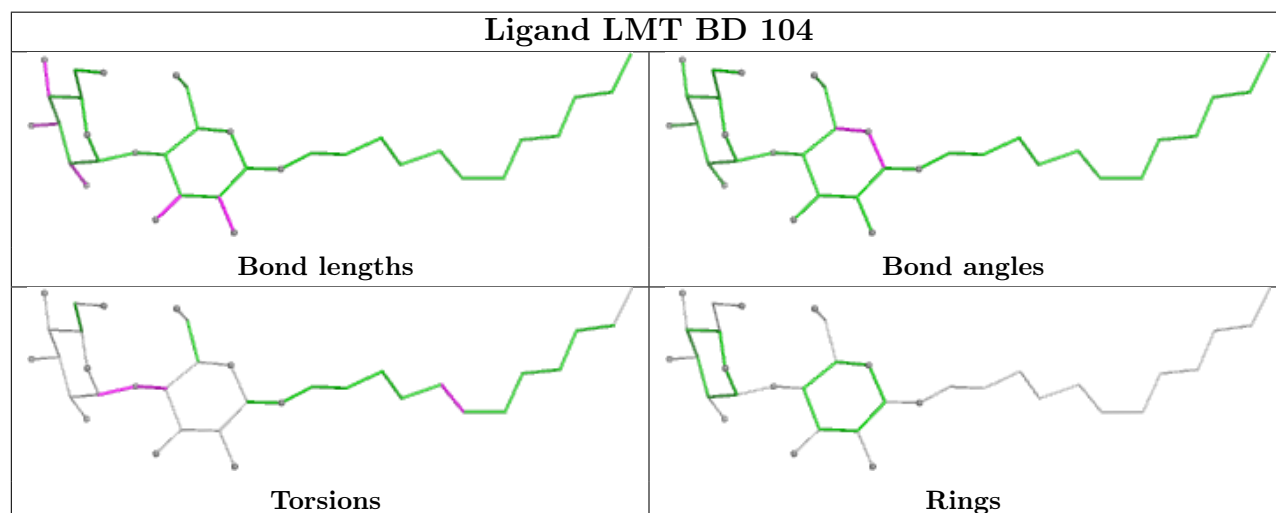
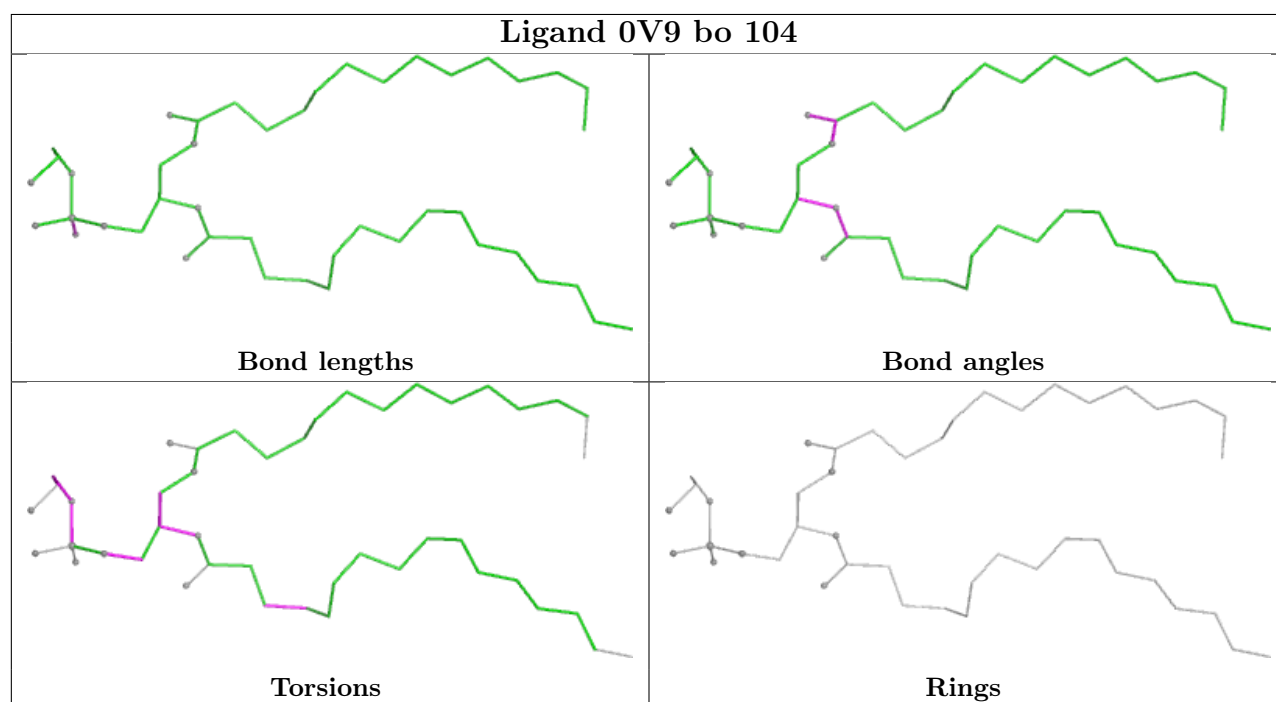
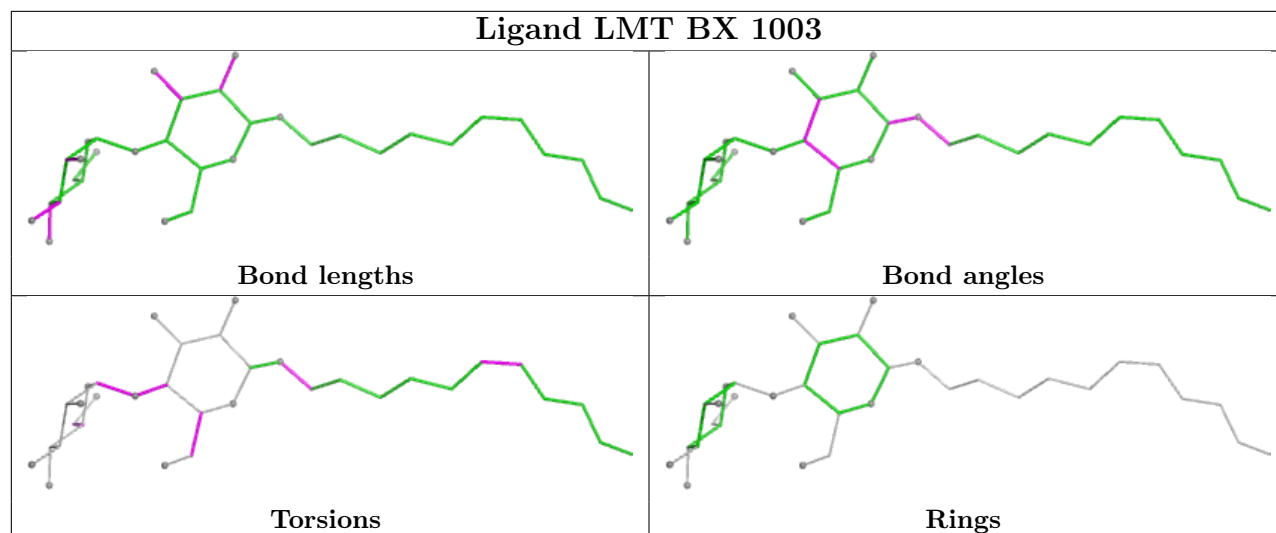


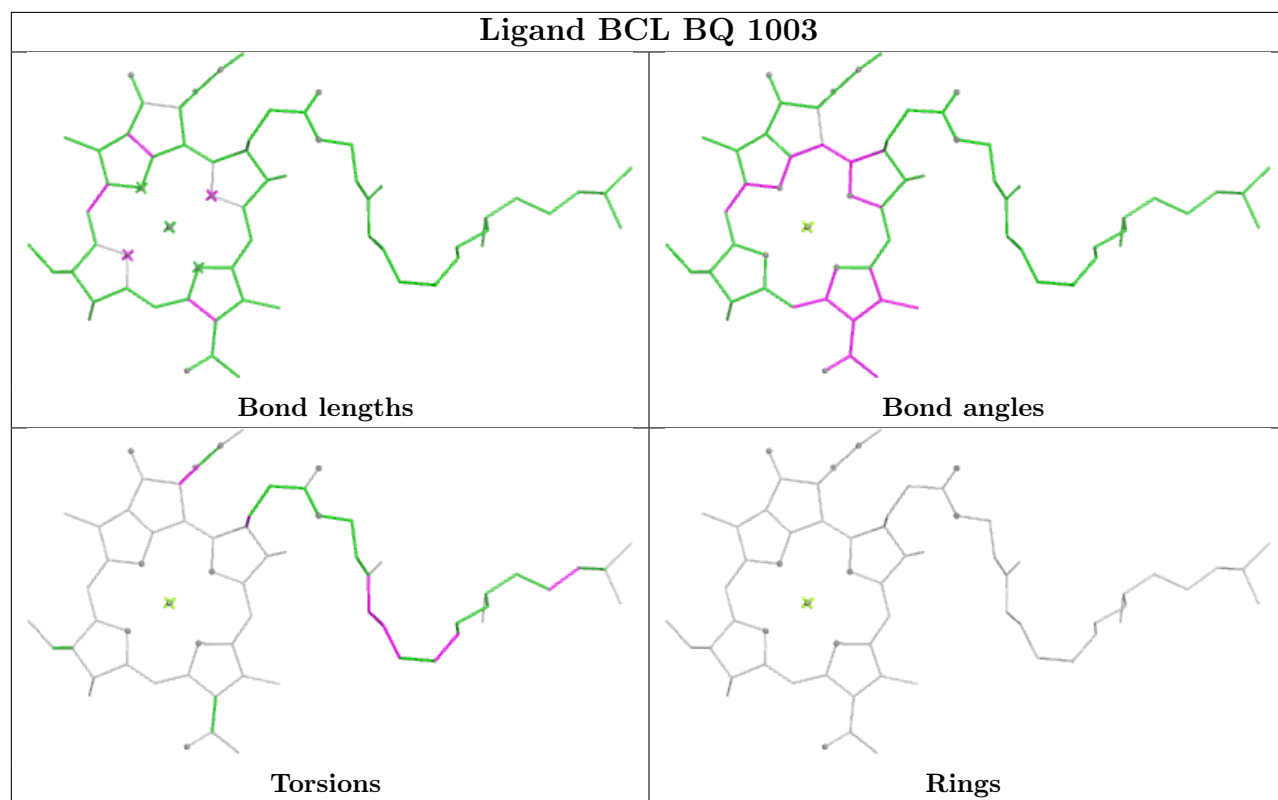
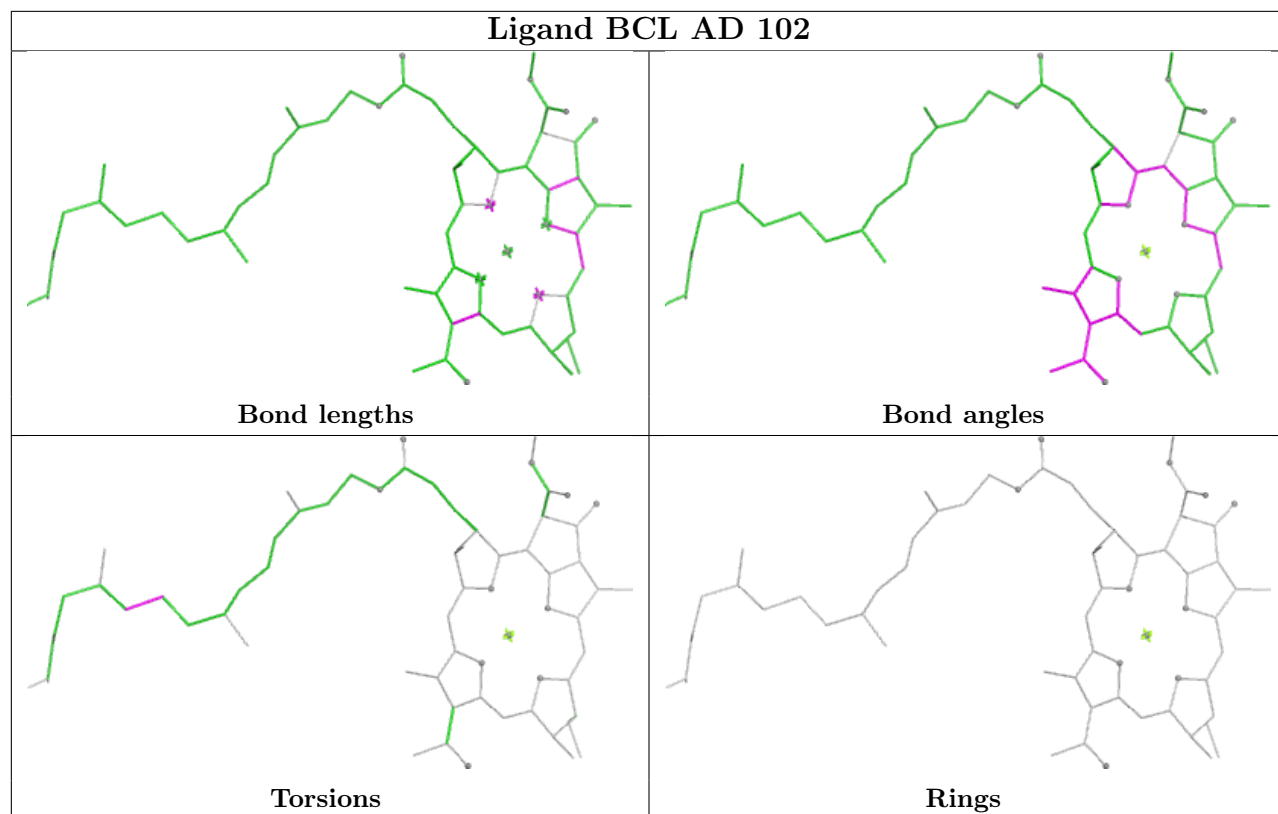


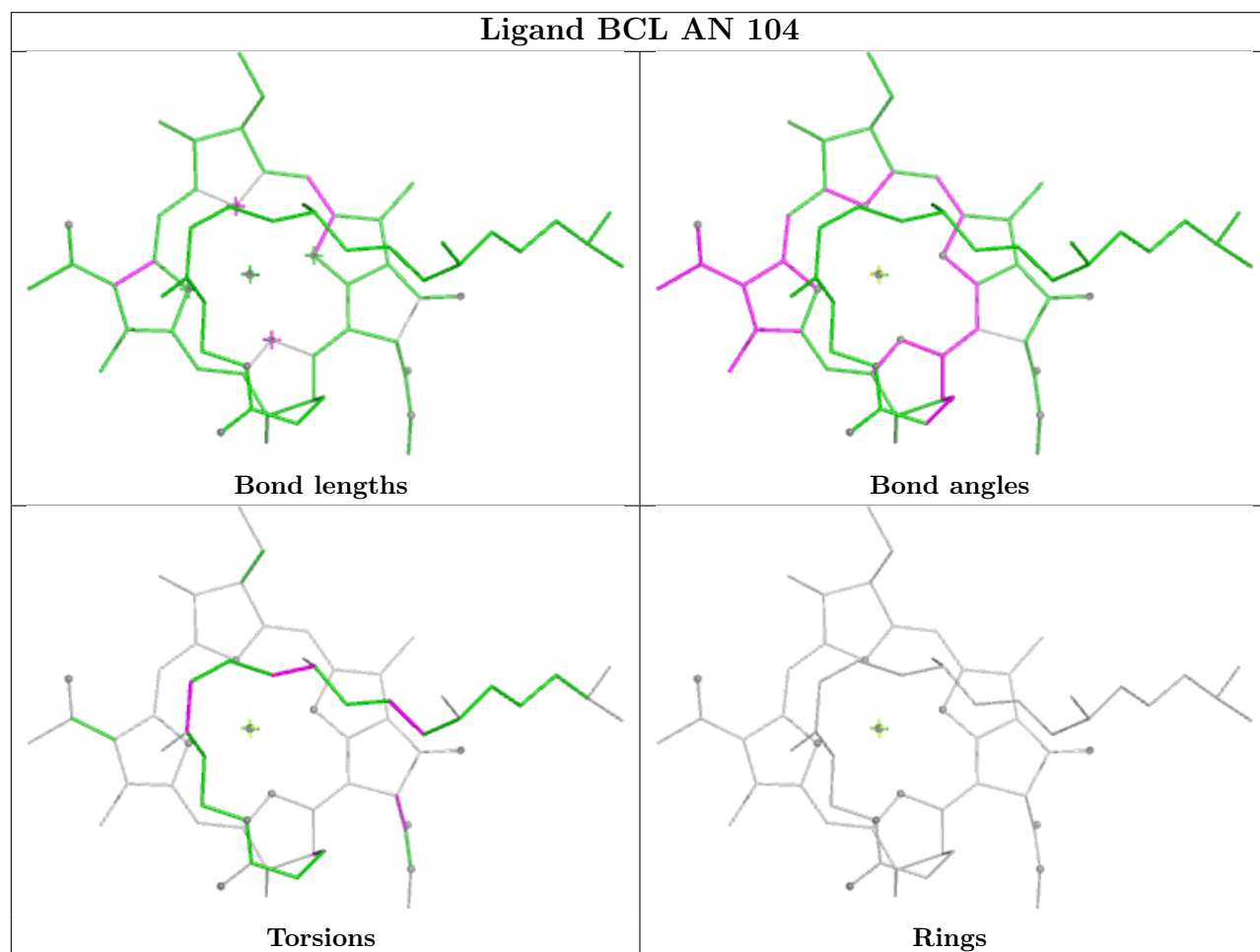
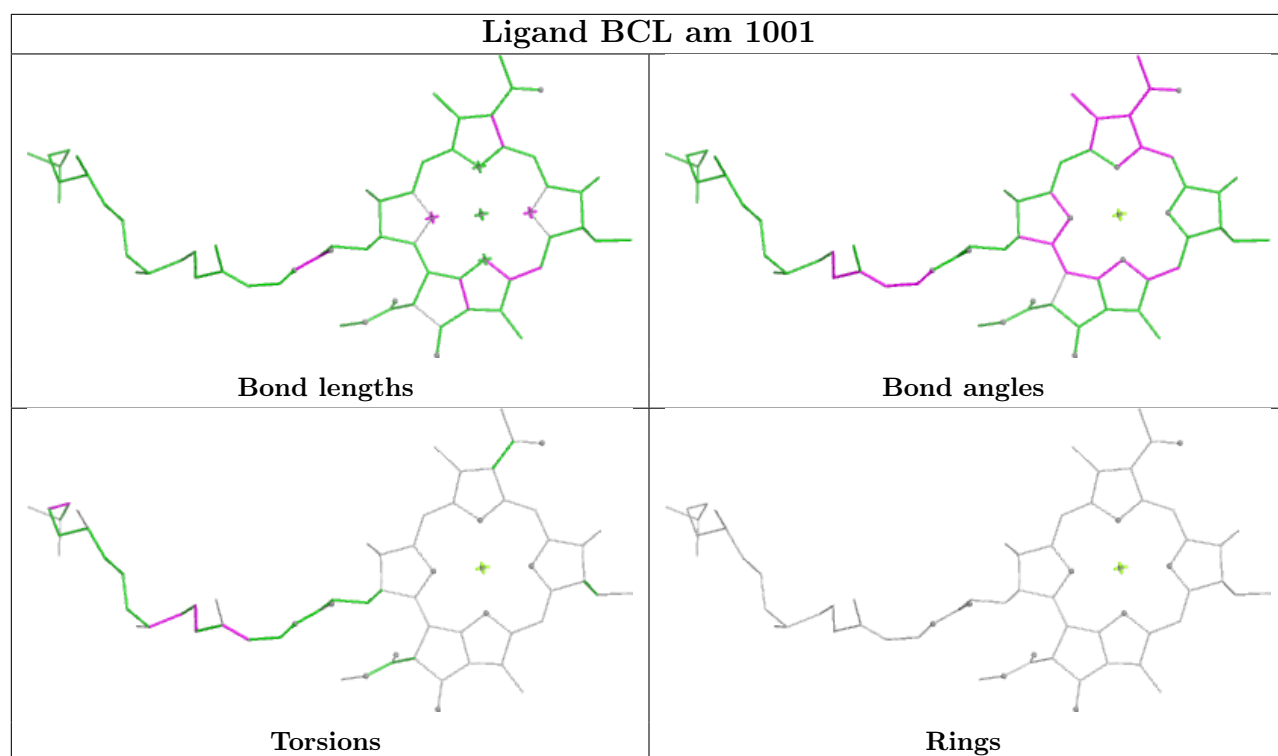


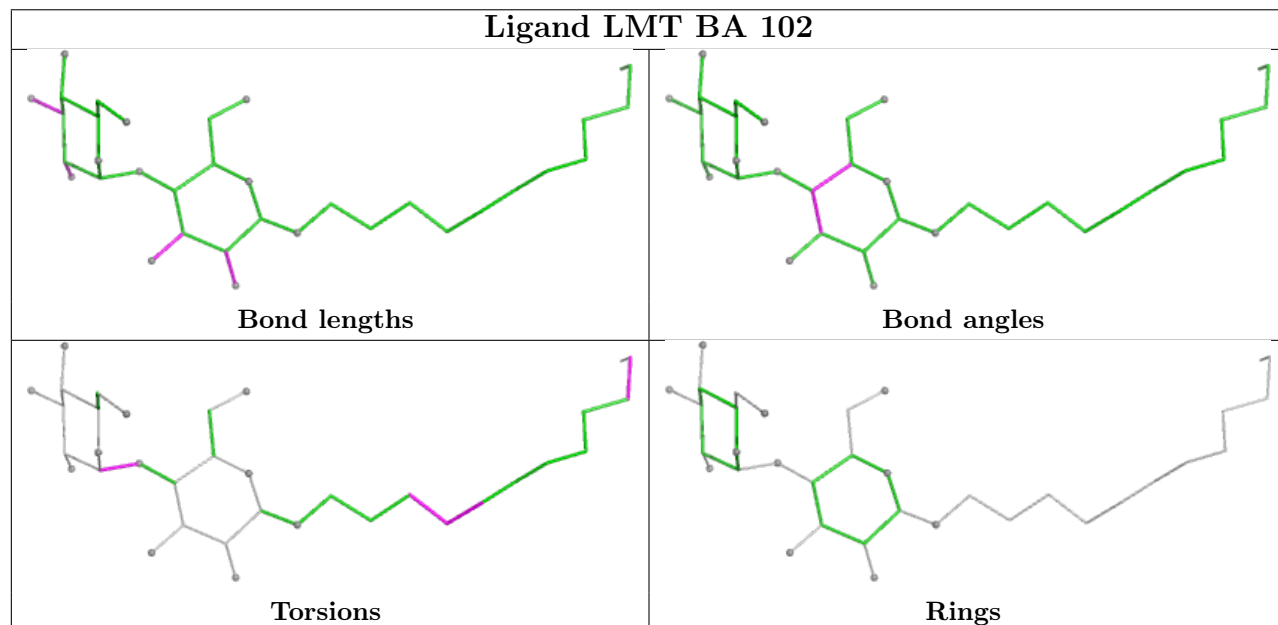
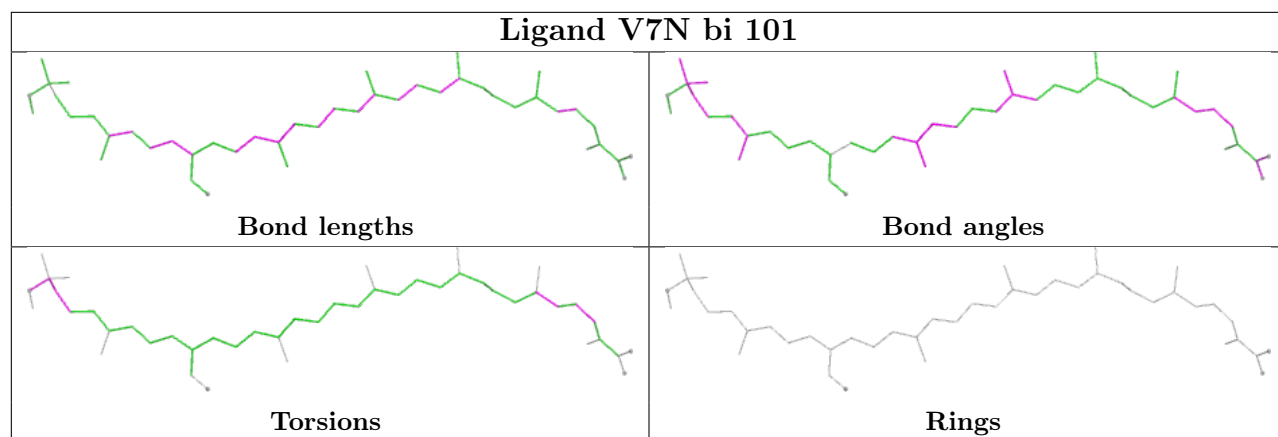
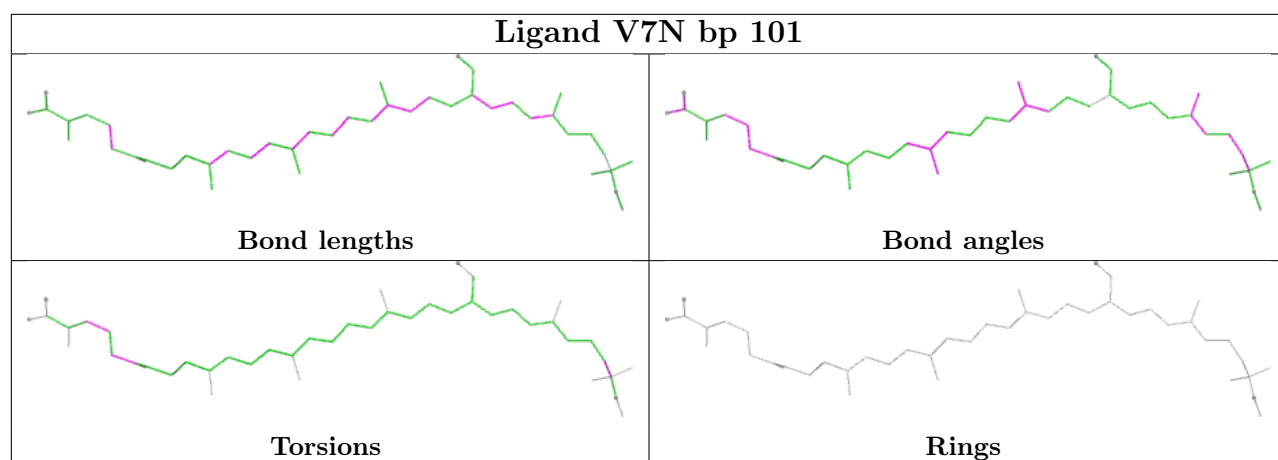


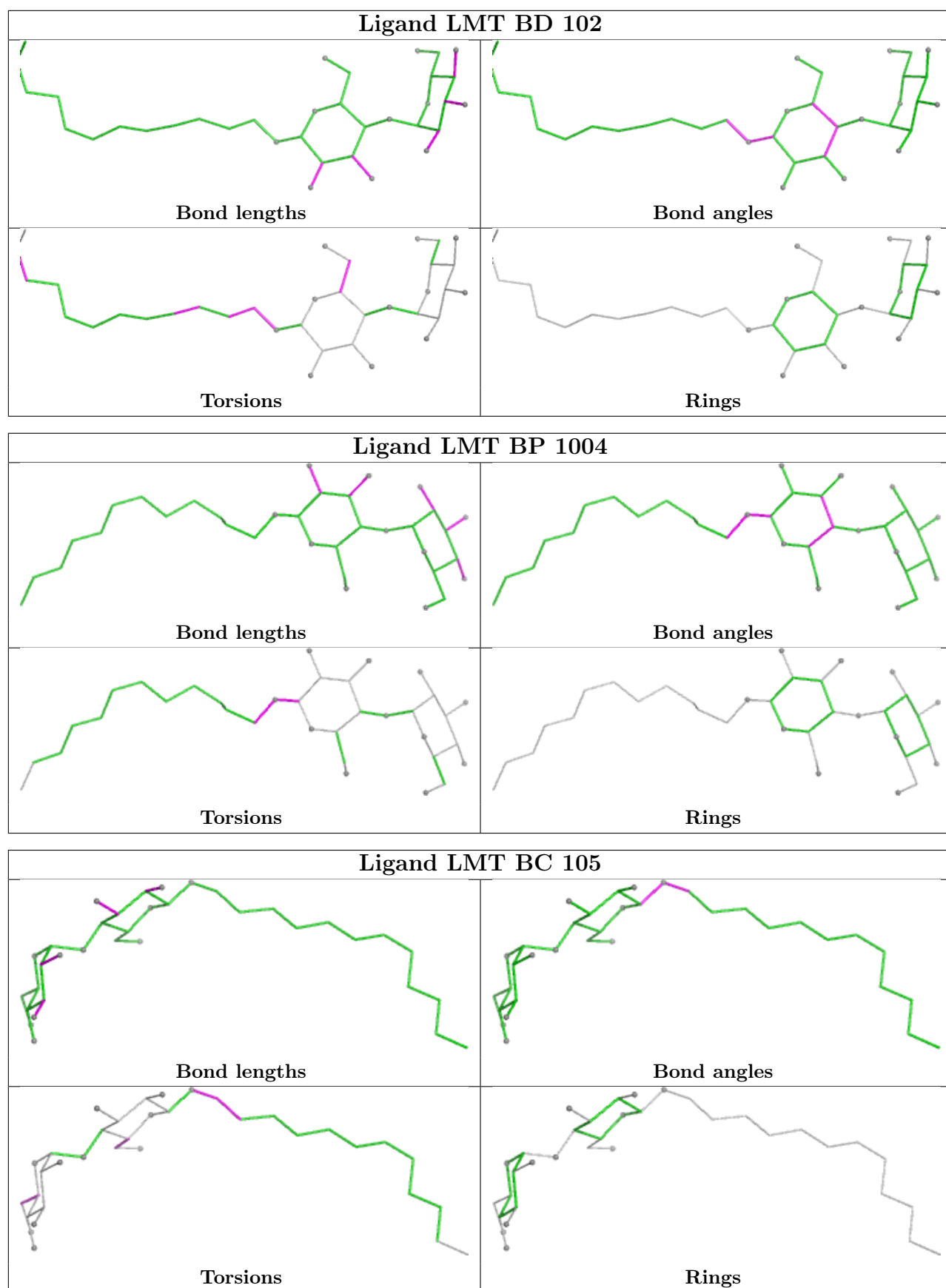


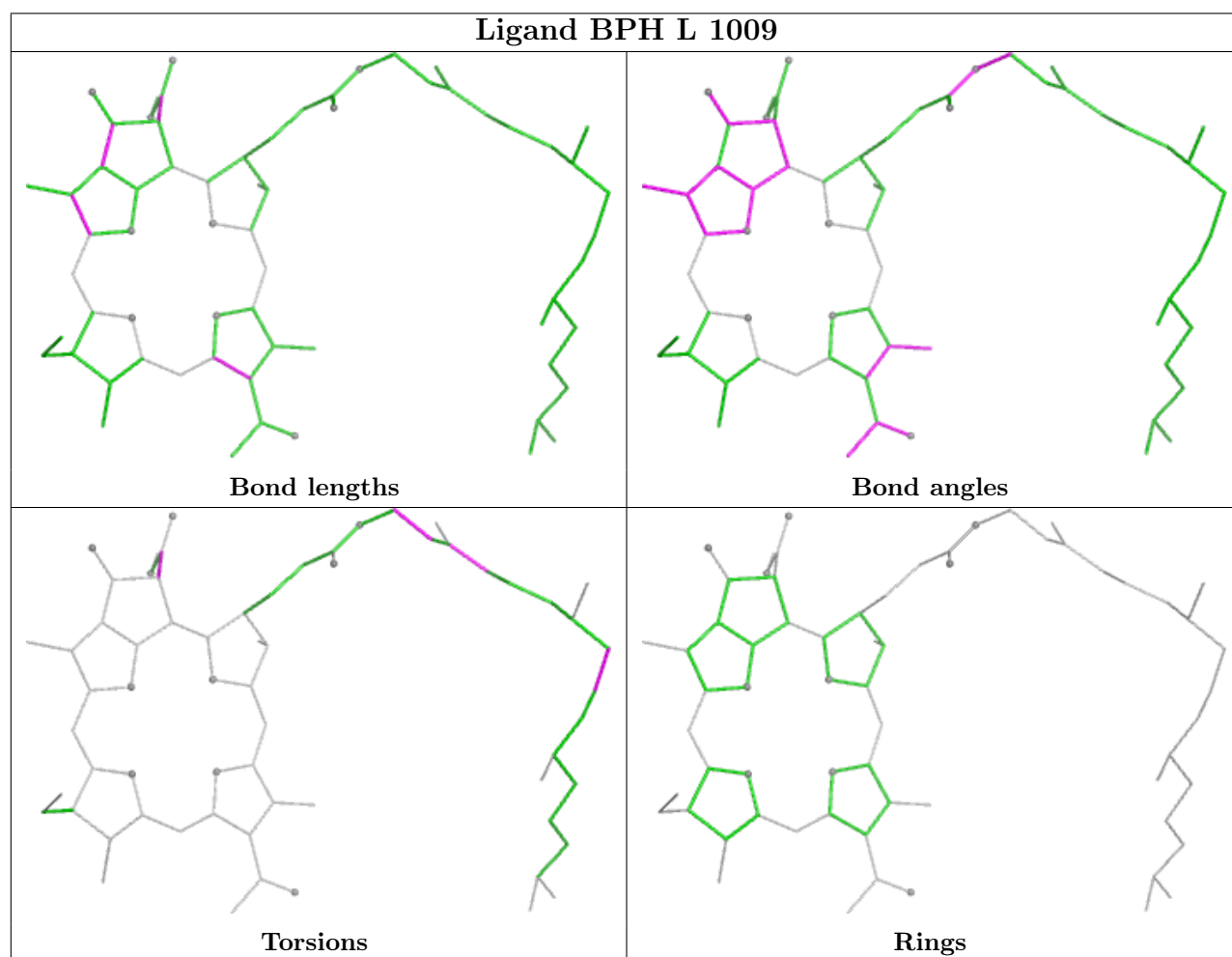
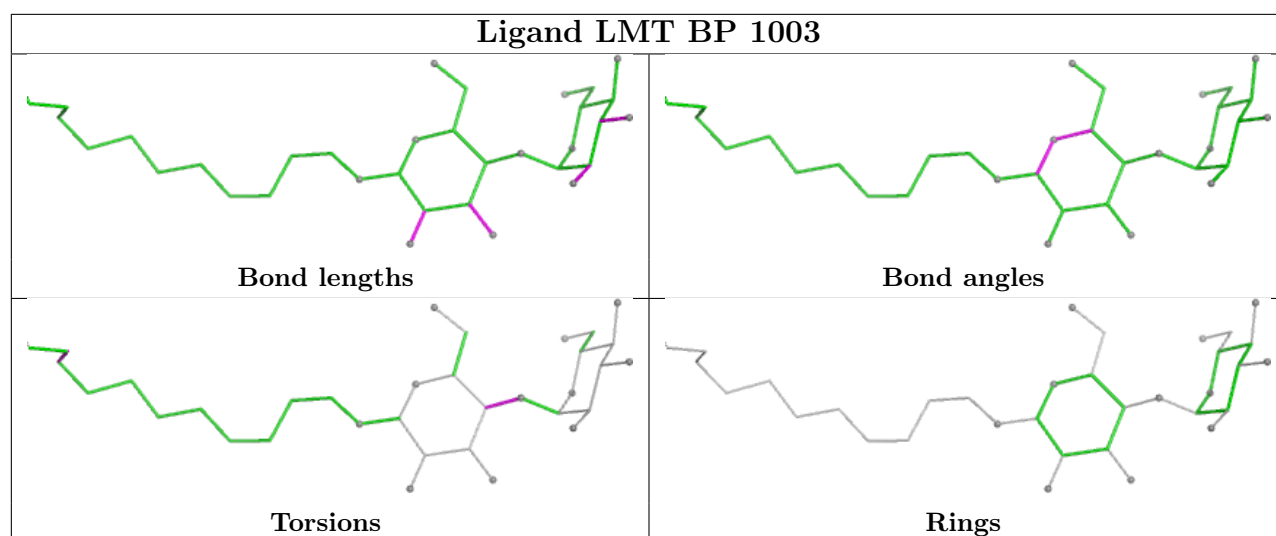


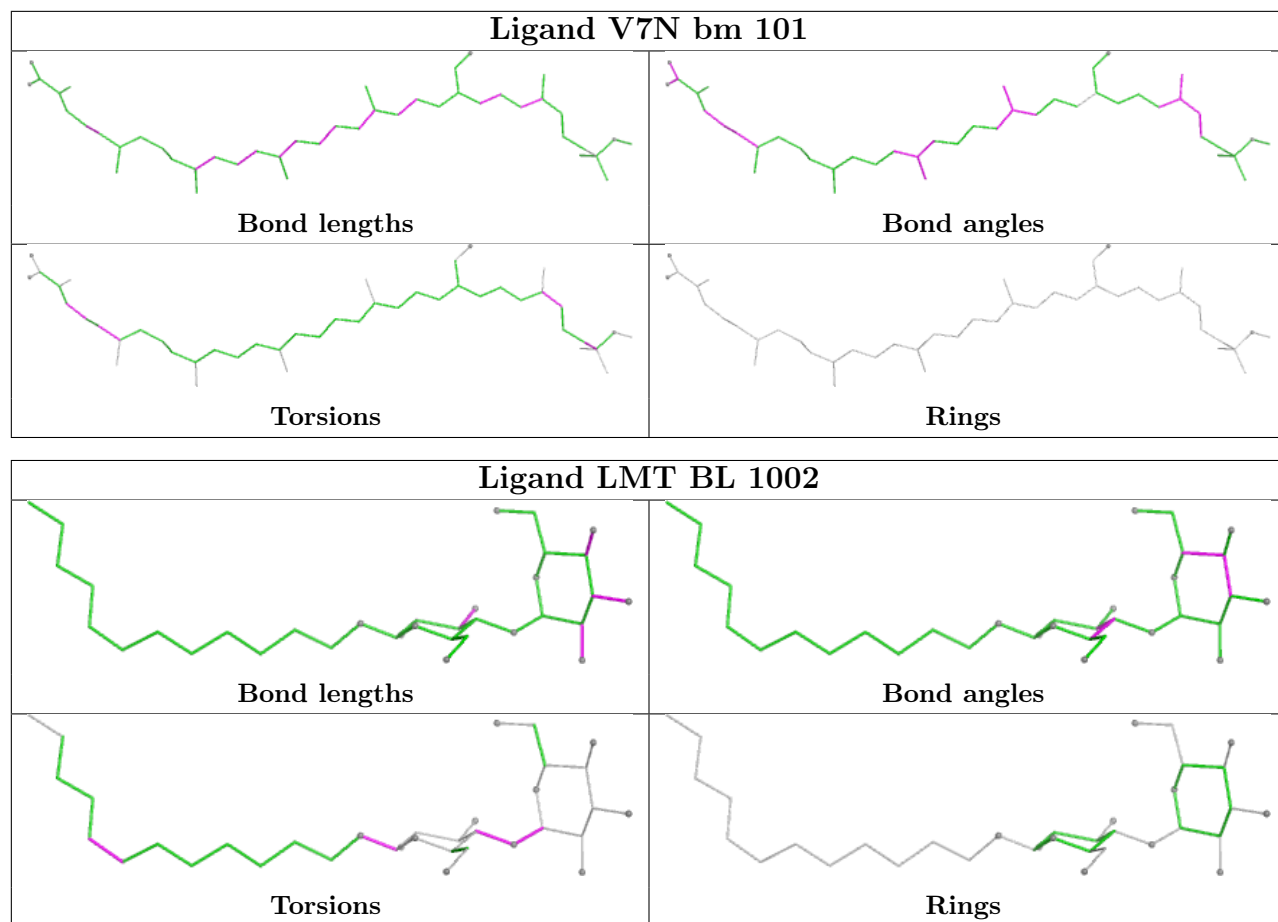


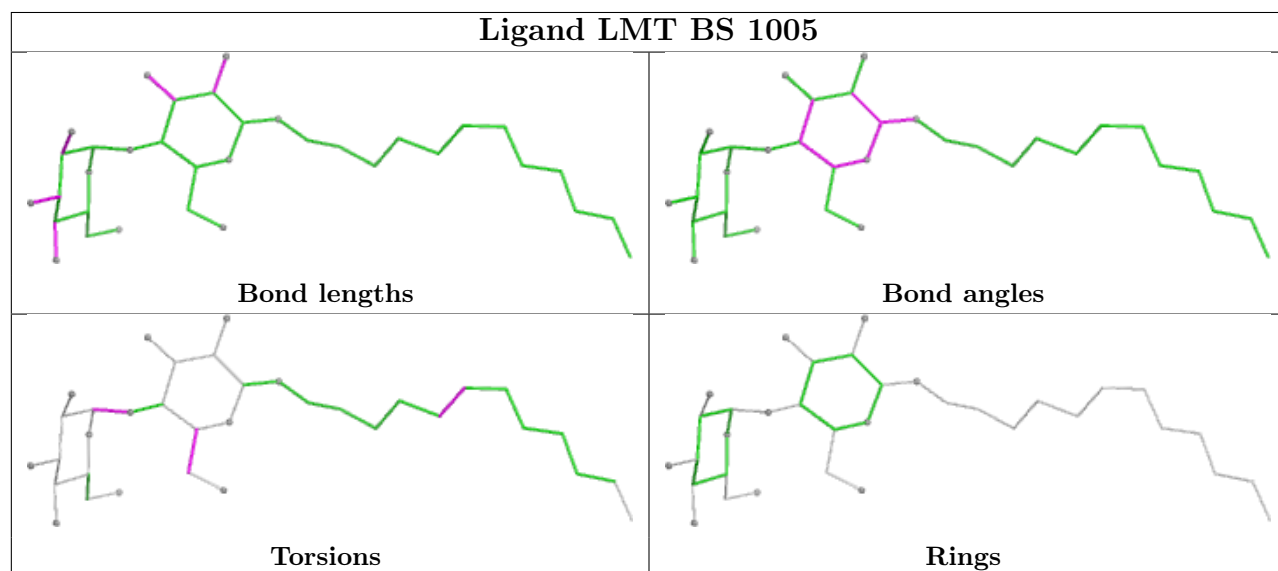
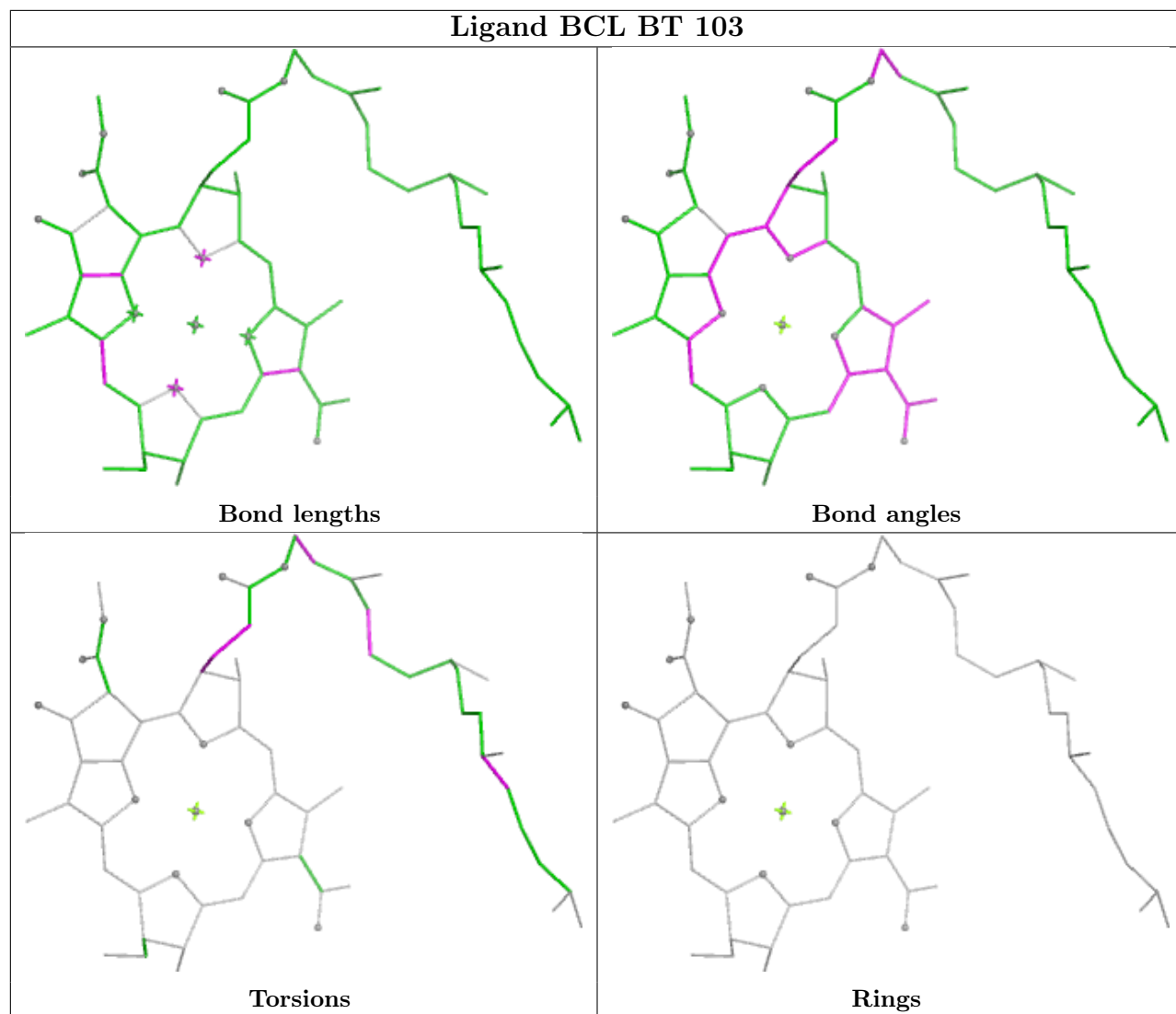


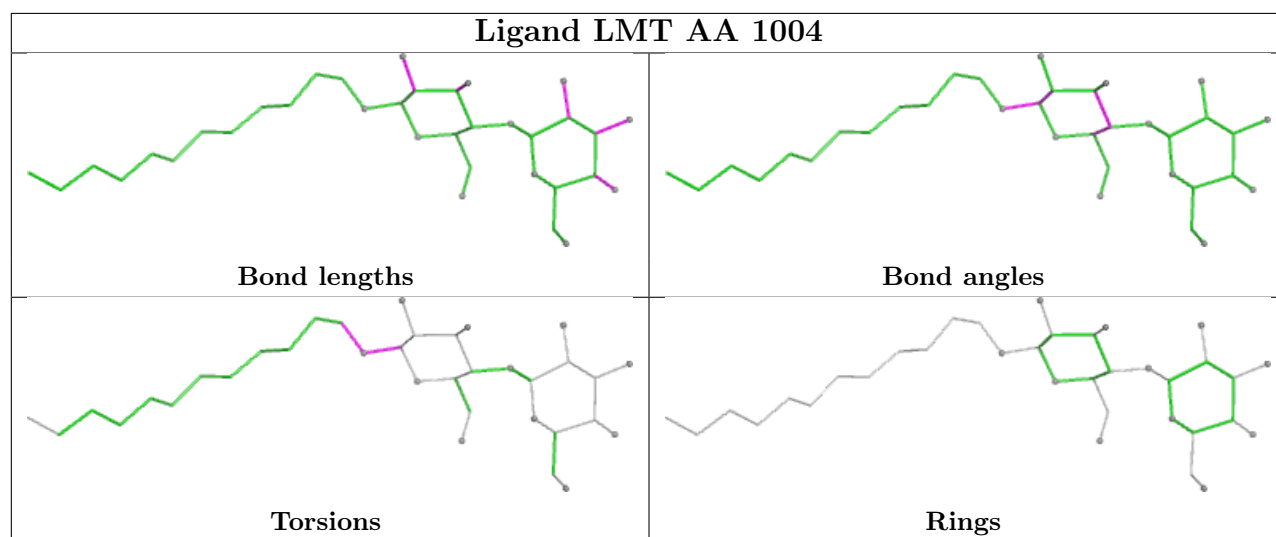
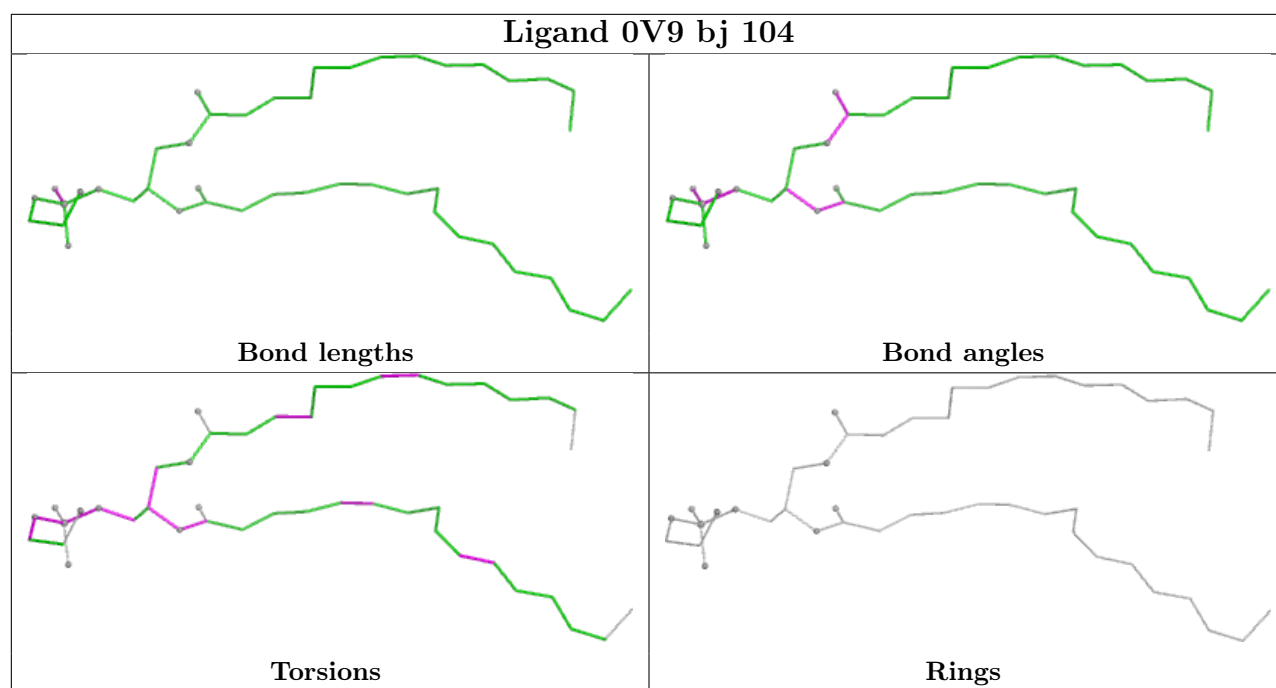


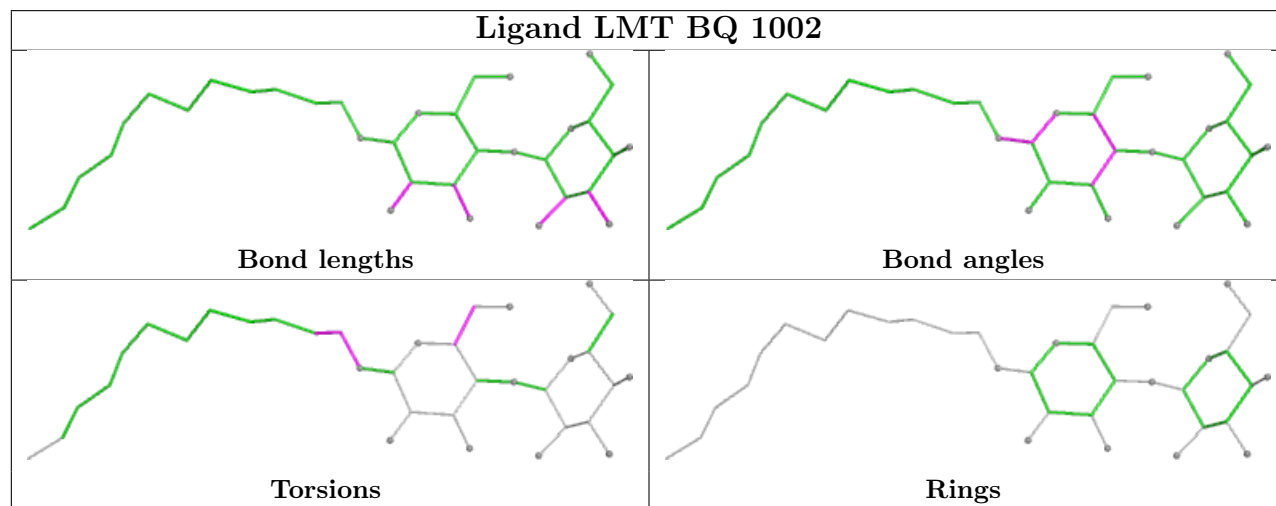
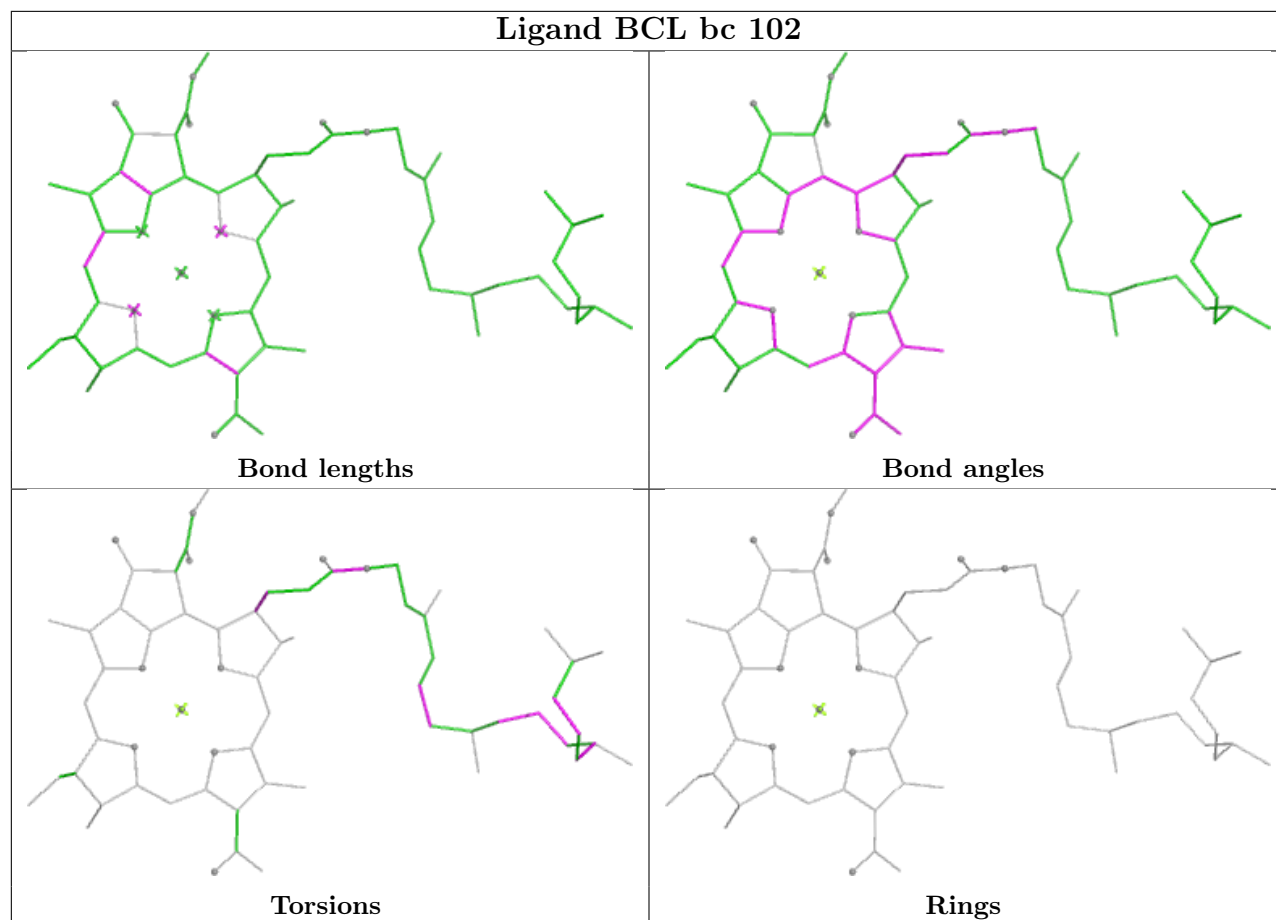


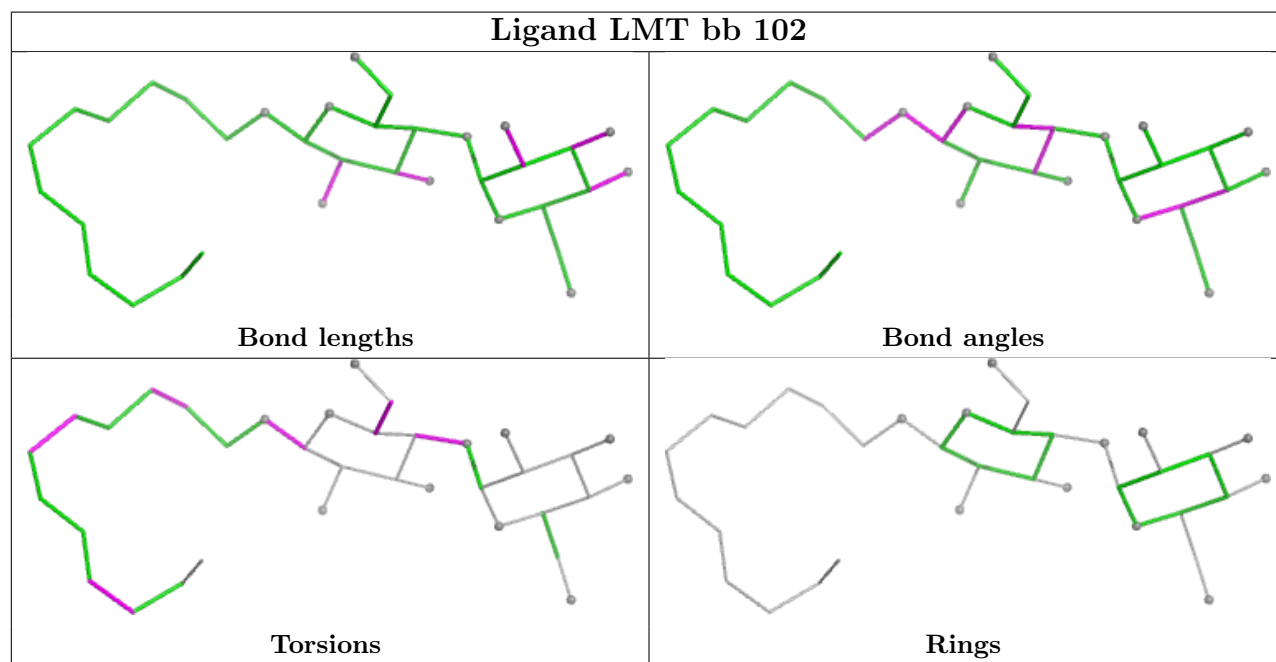
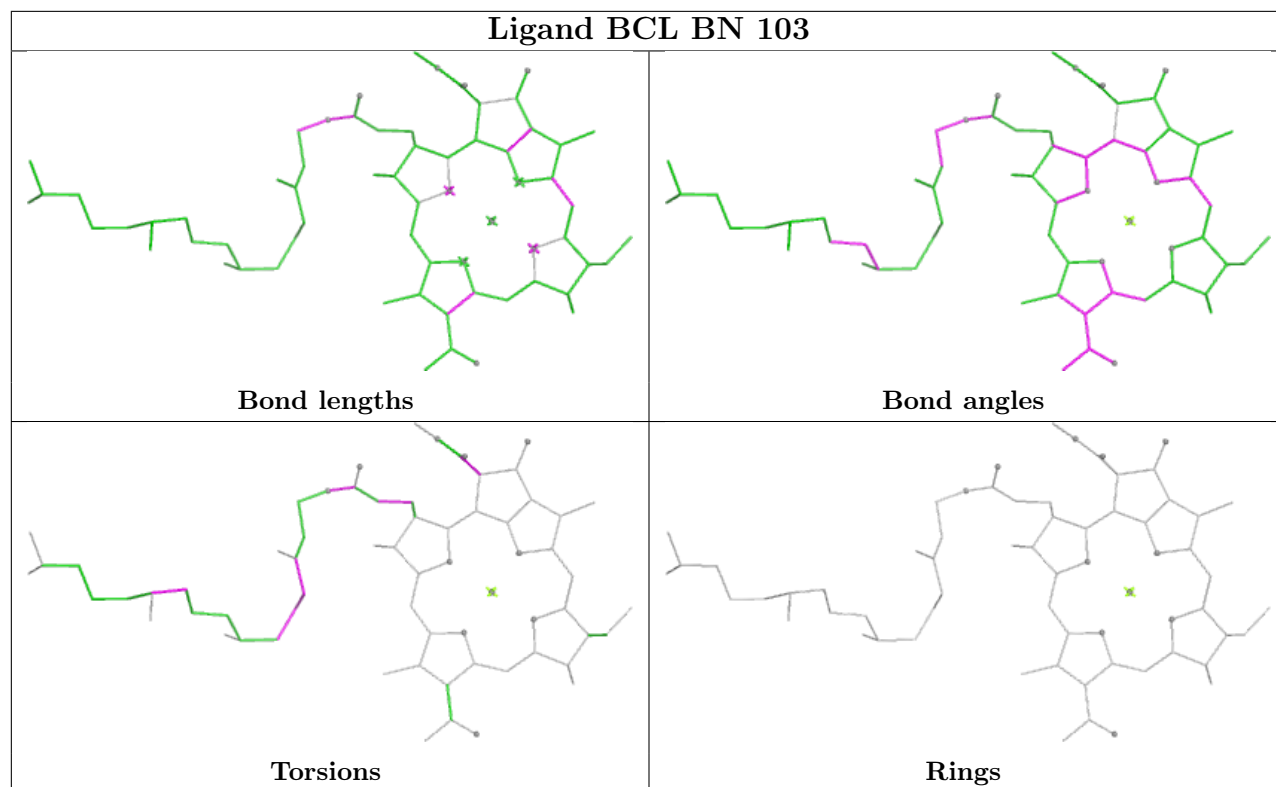


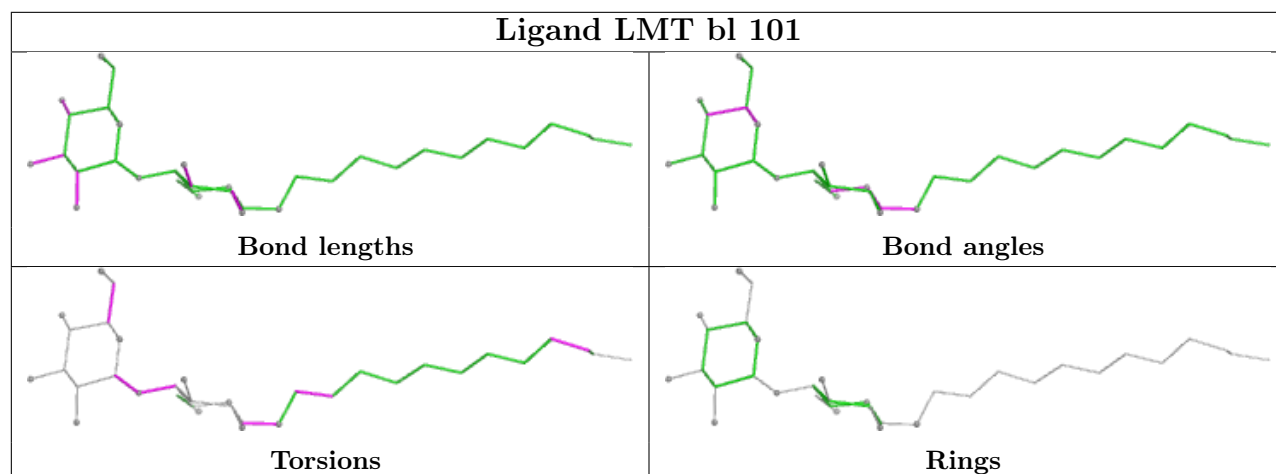
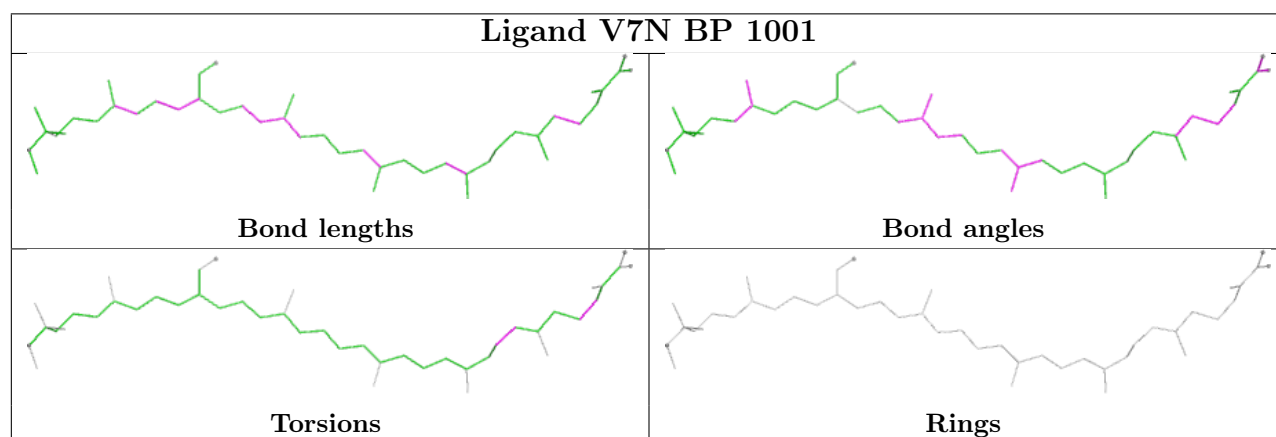
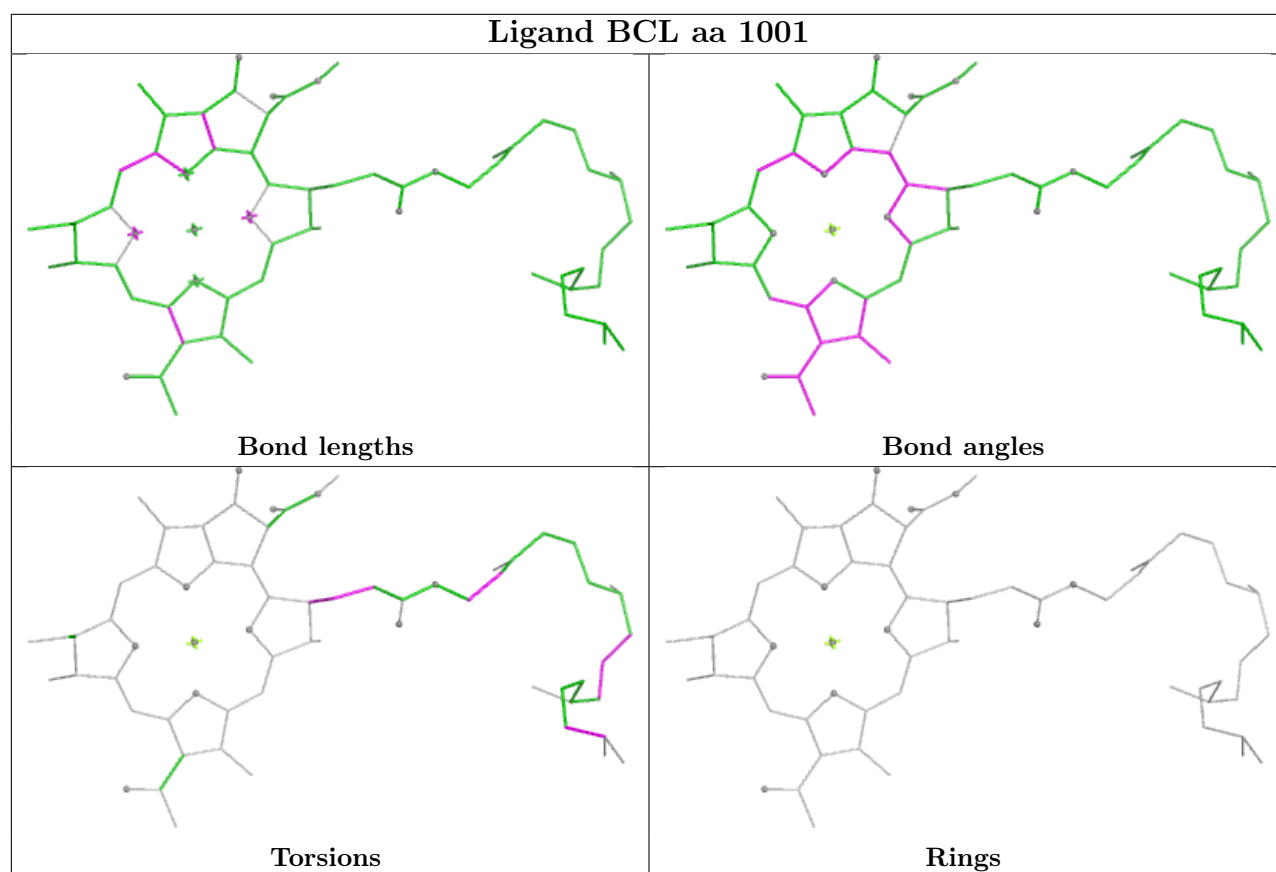




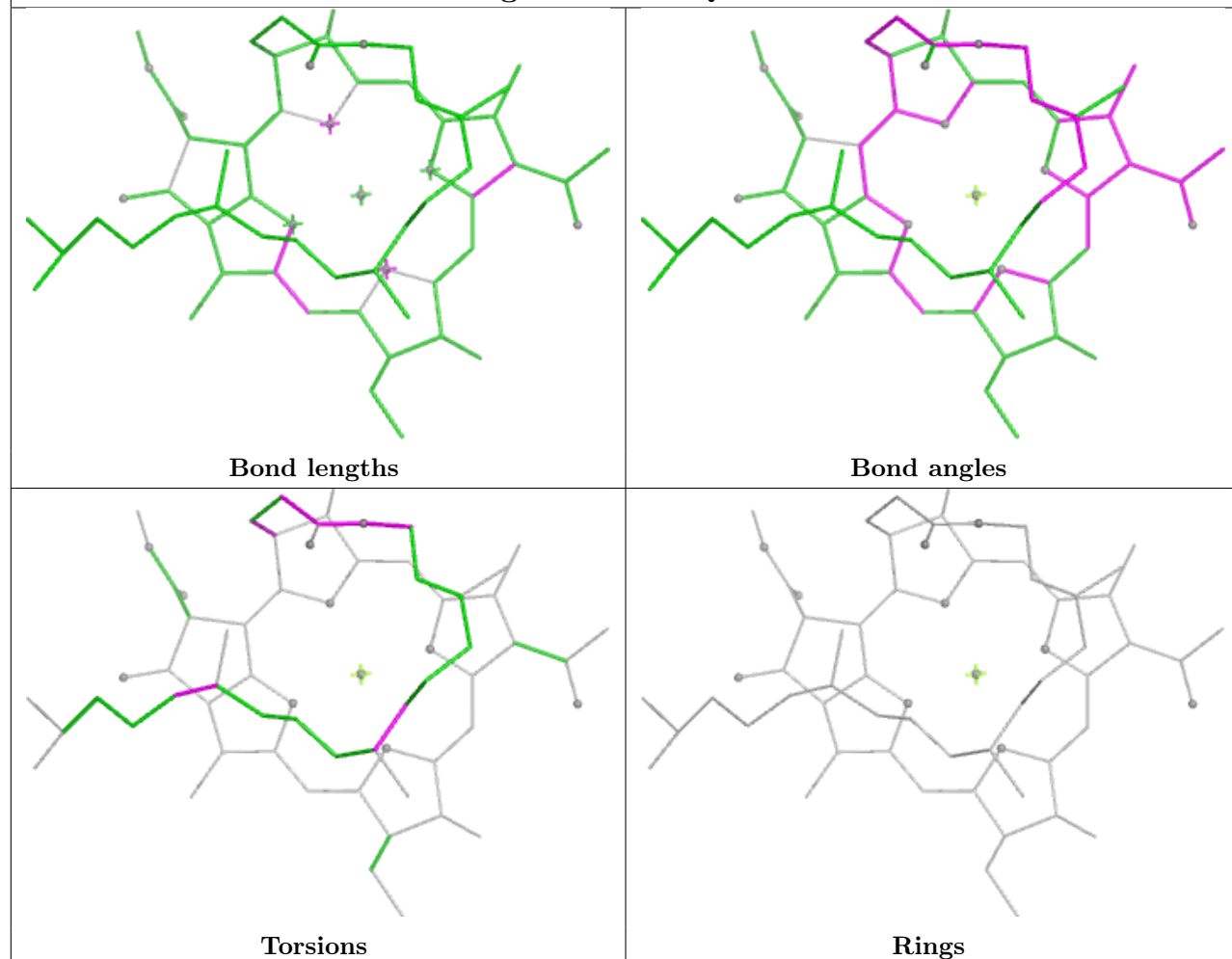




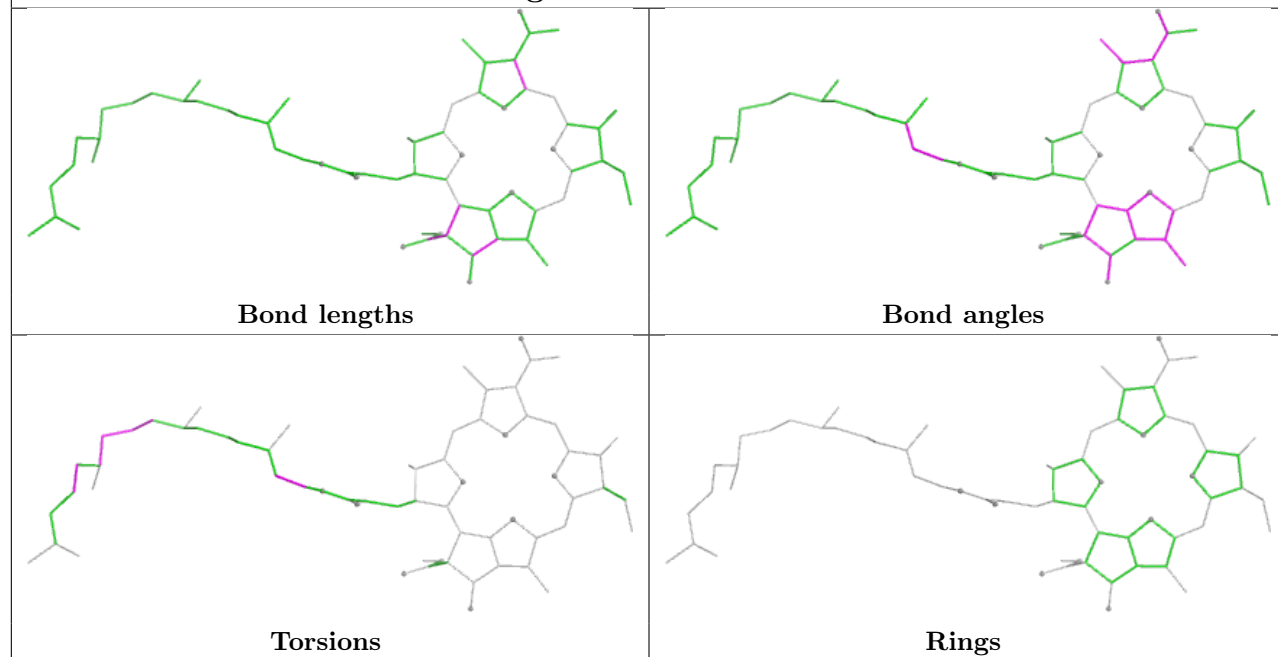


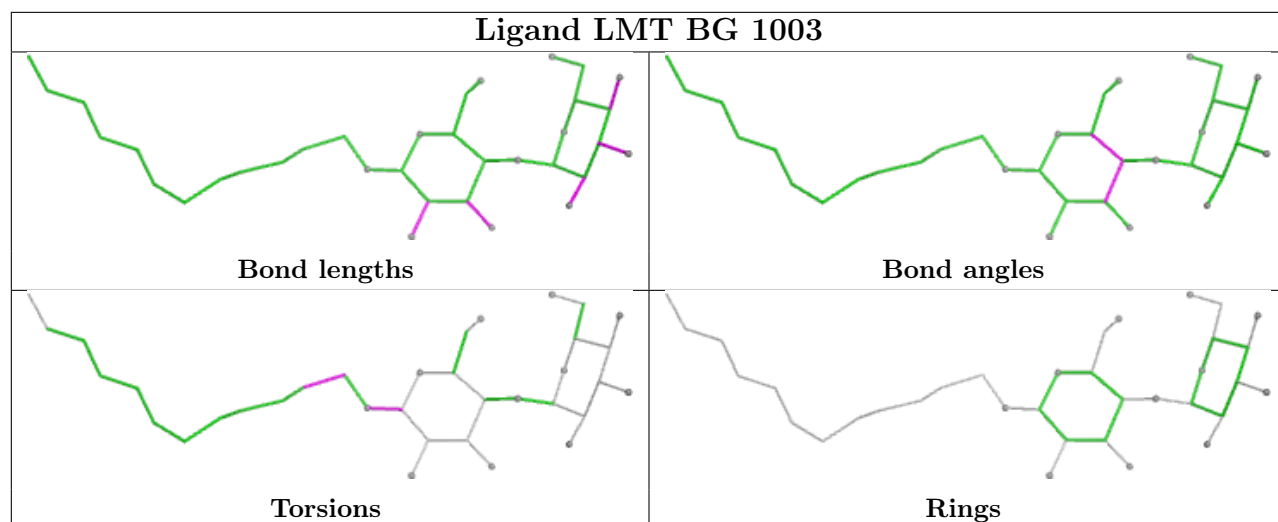
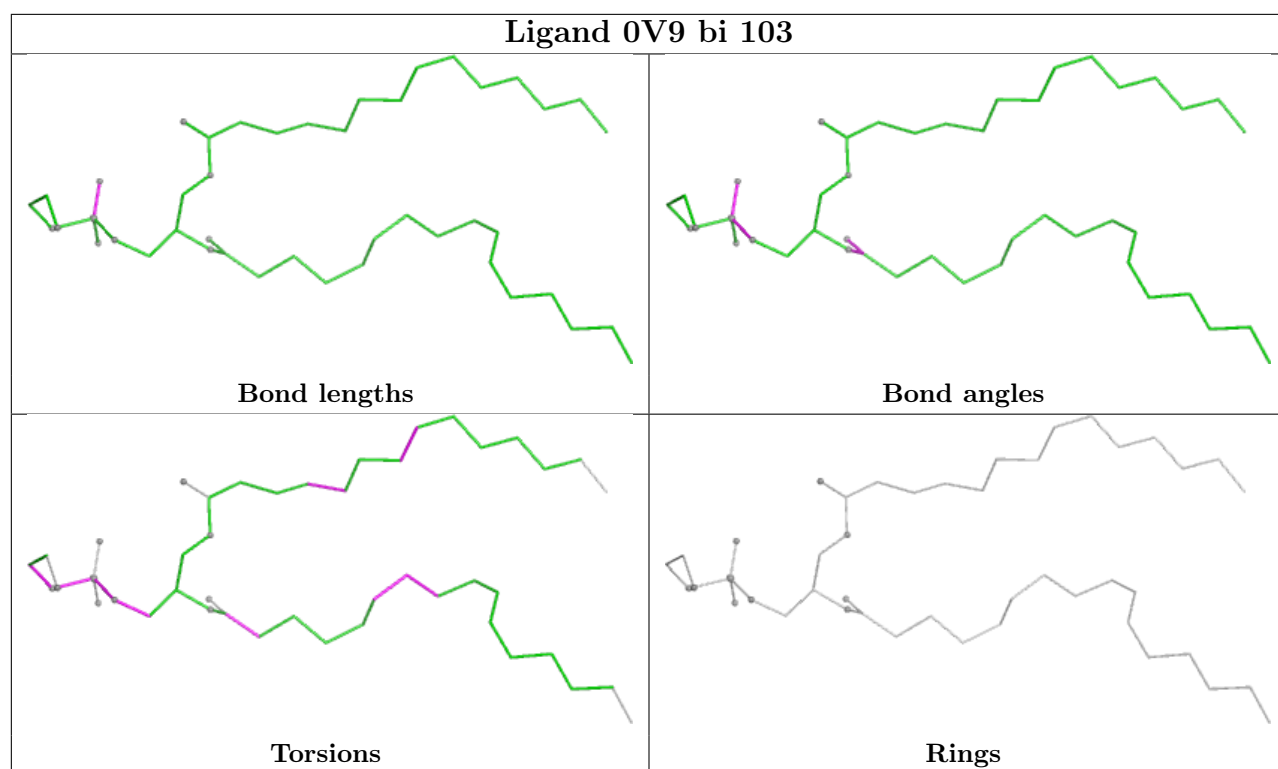


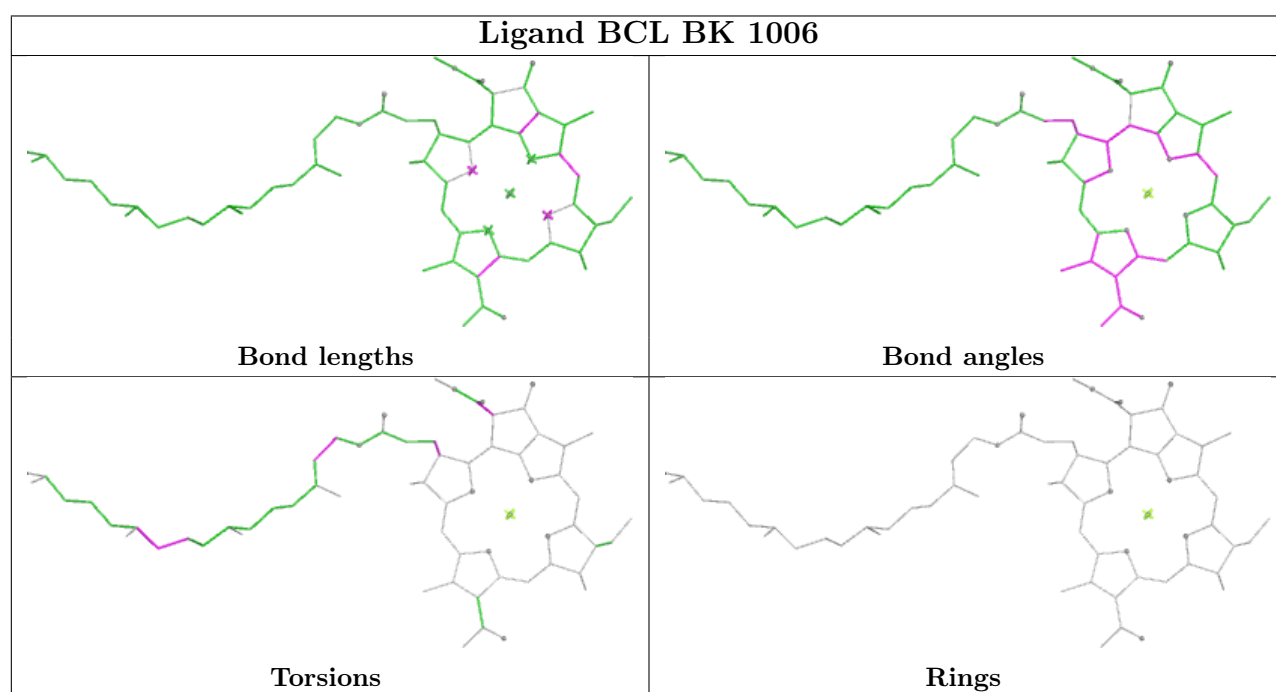
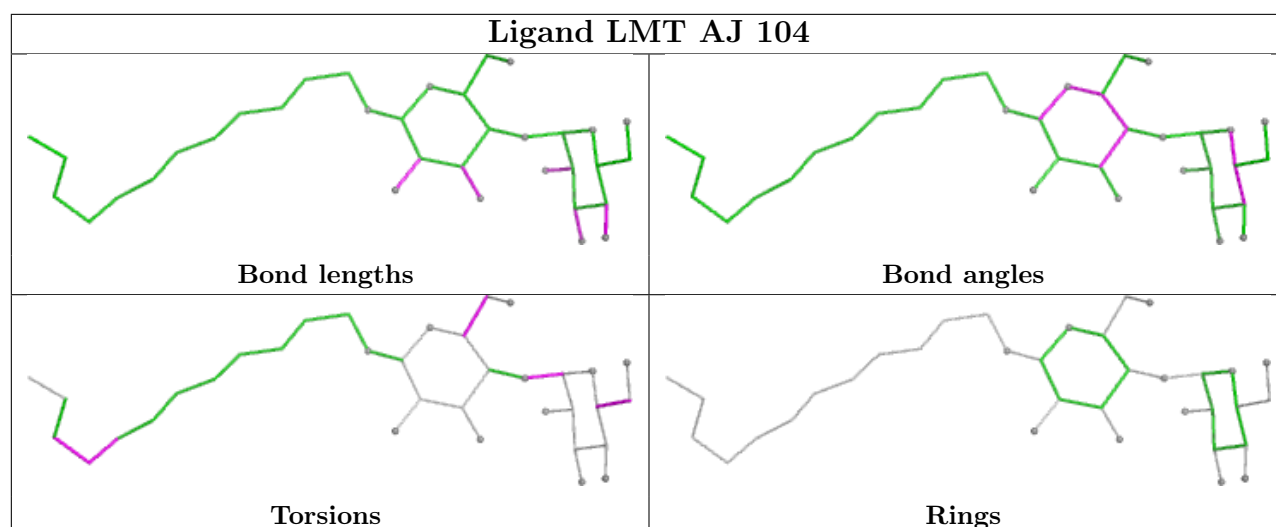
Ligand BCL AQ 101

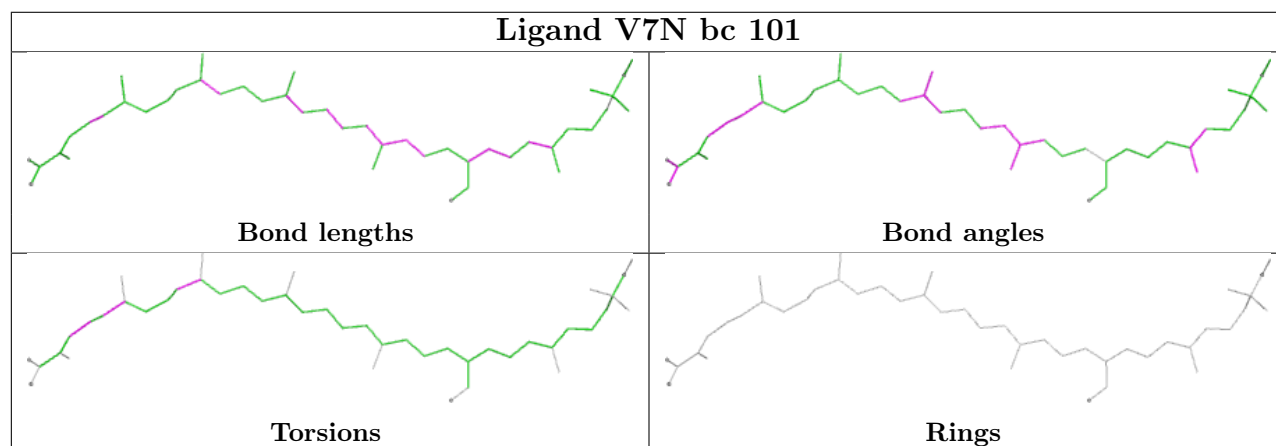
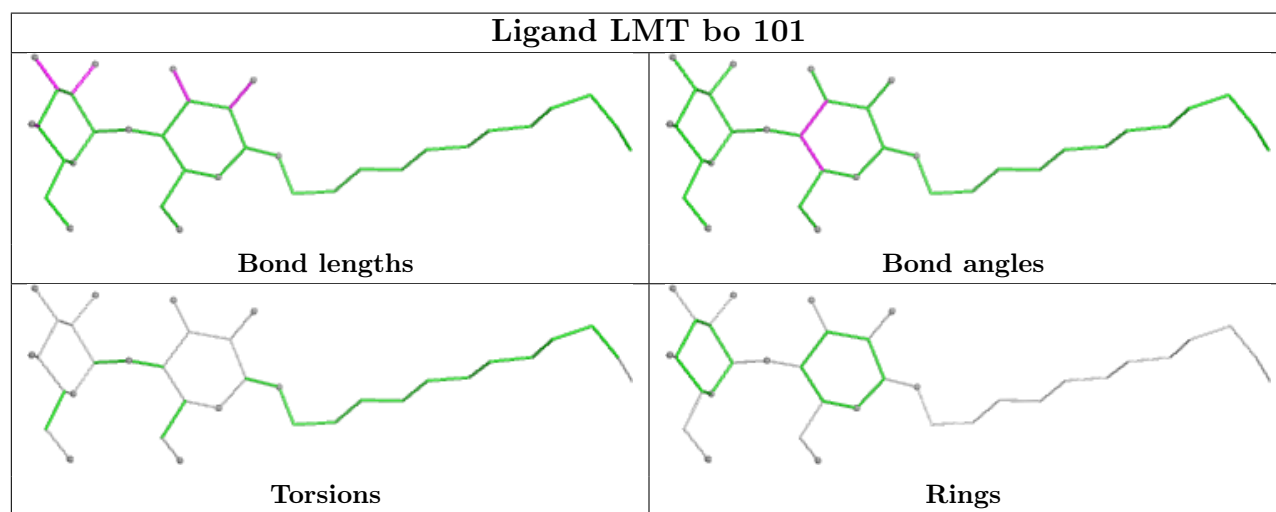
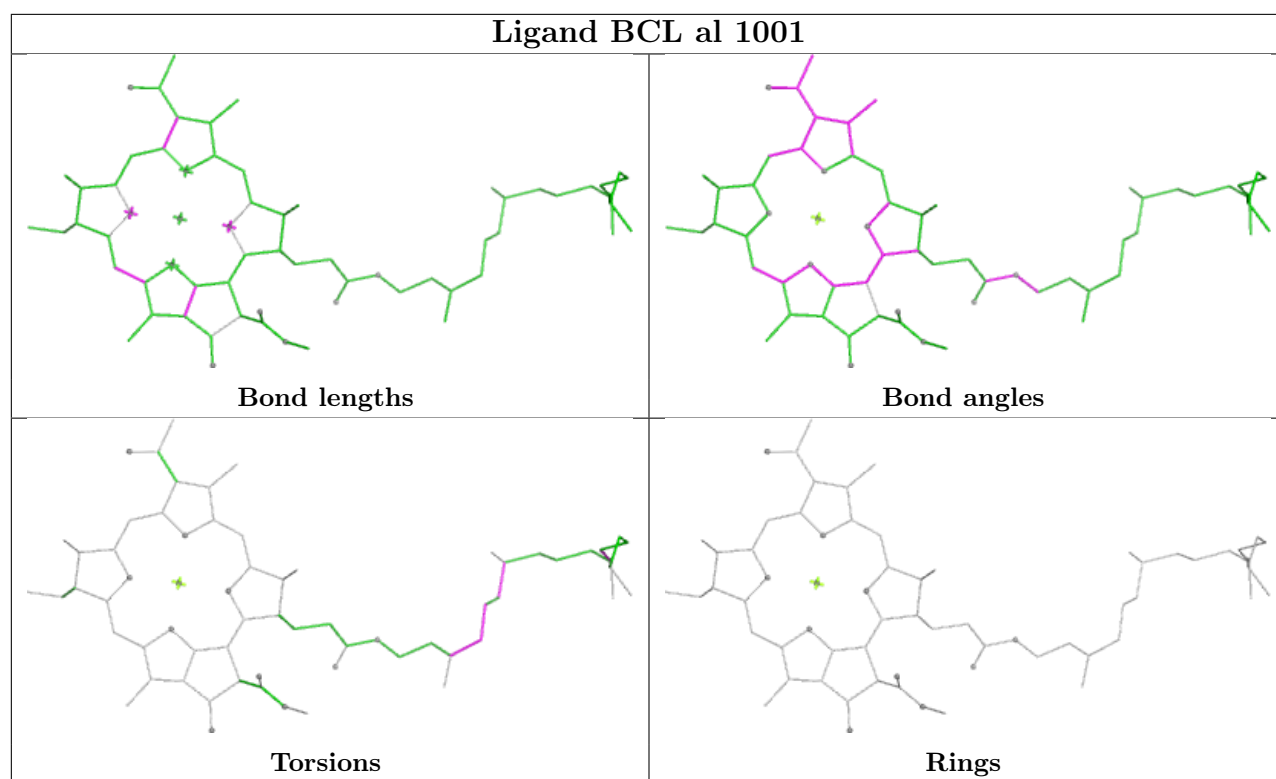


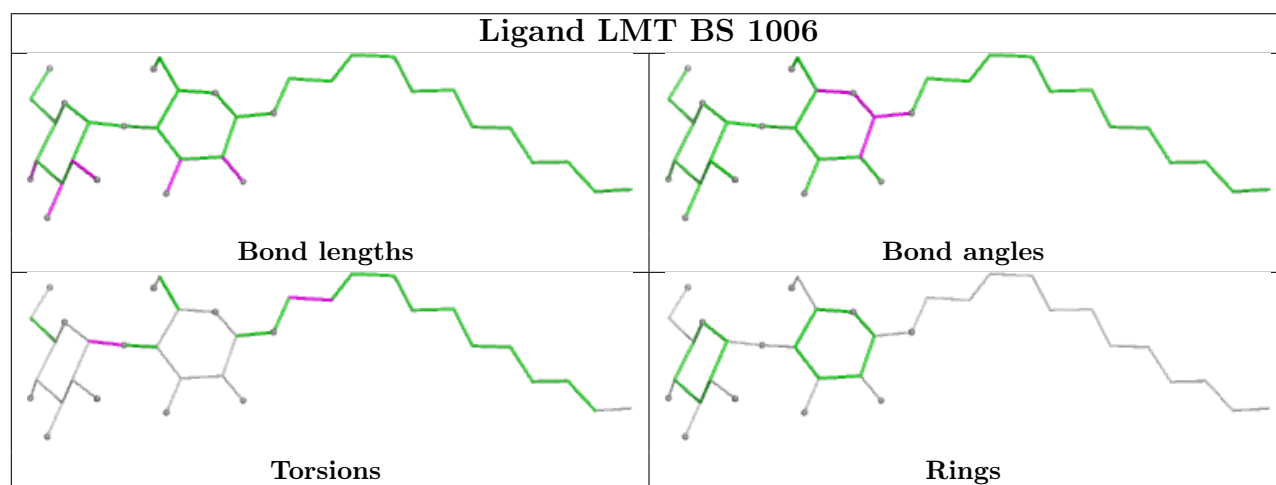
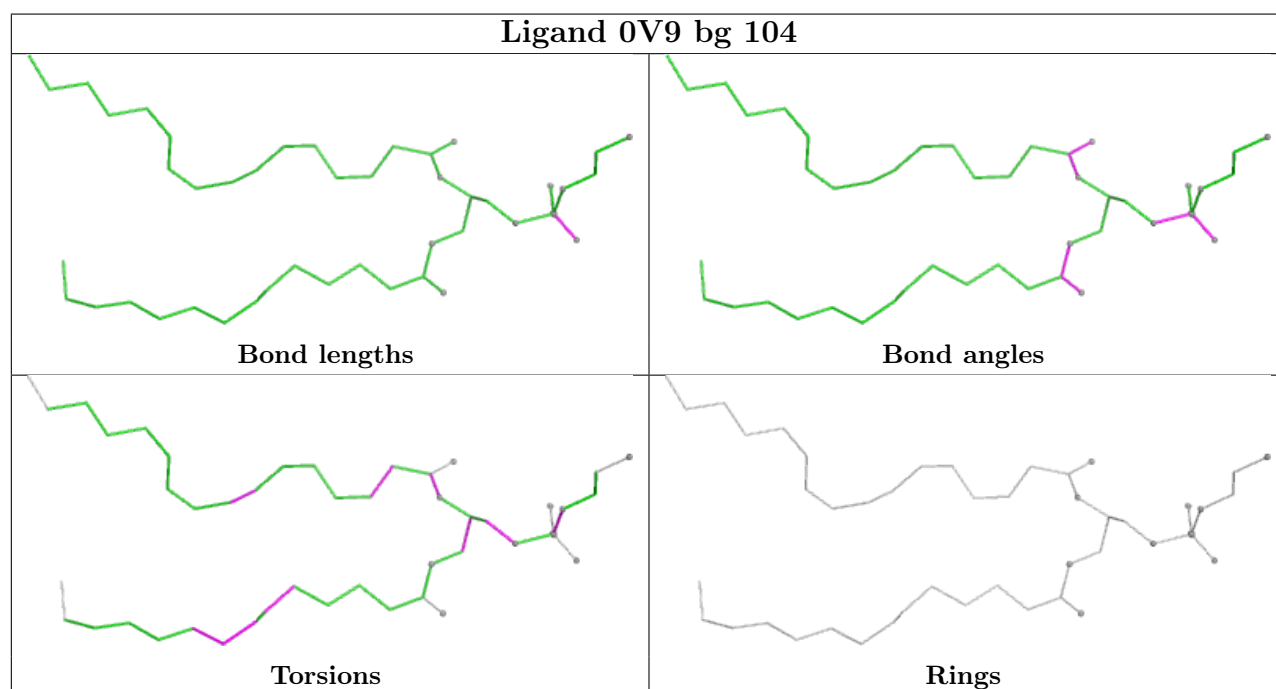
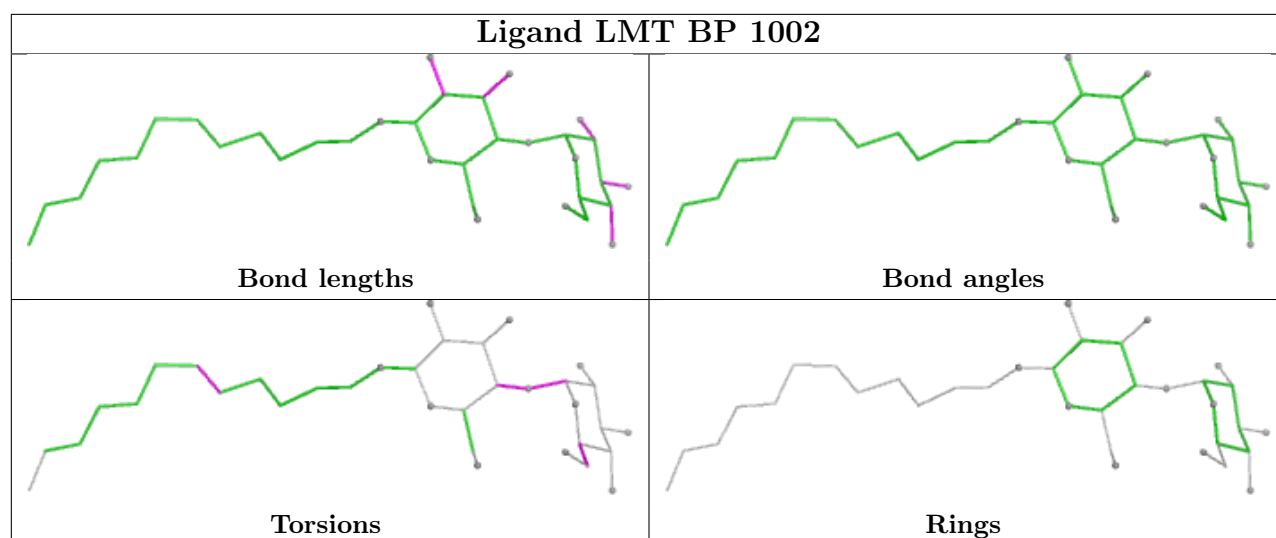
Ligand BPH M 406

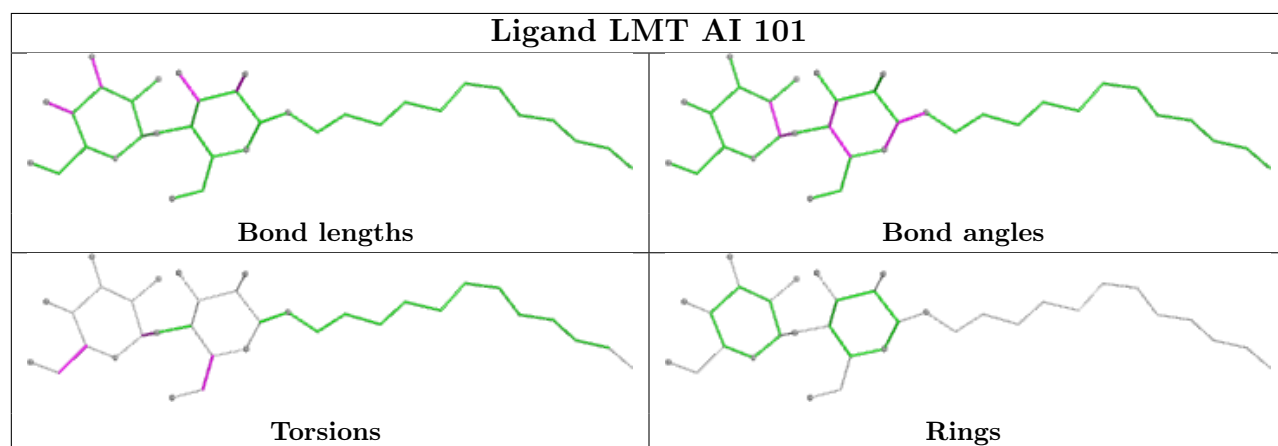
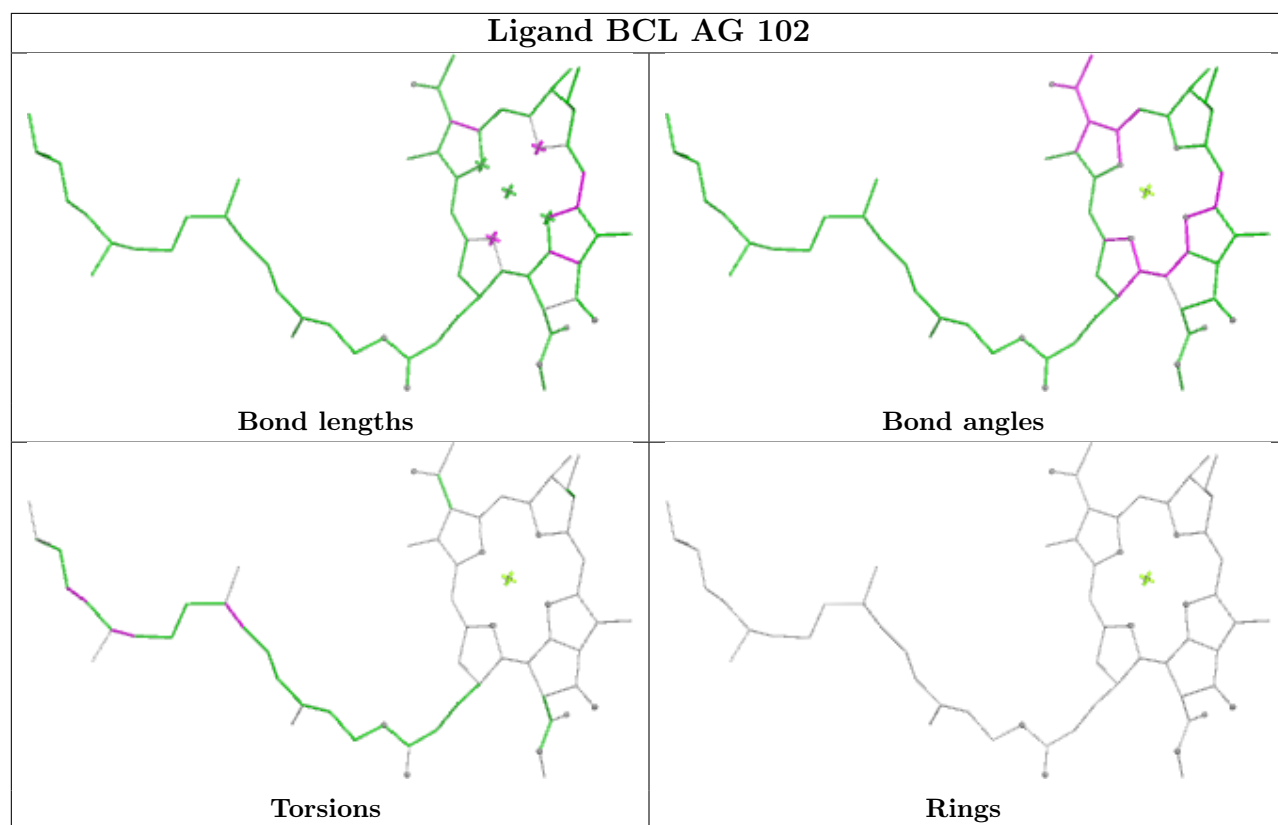
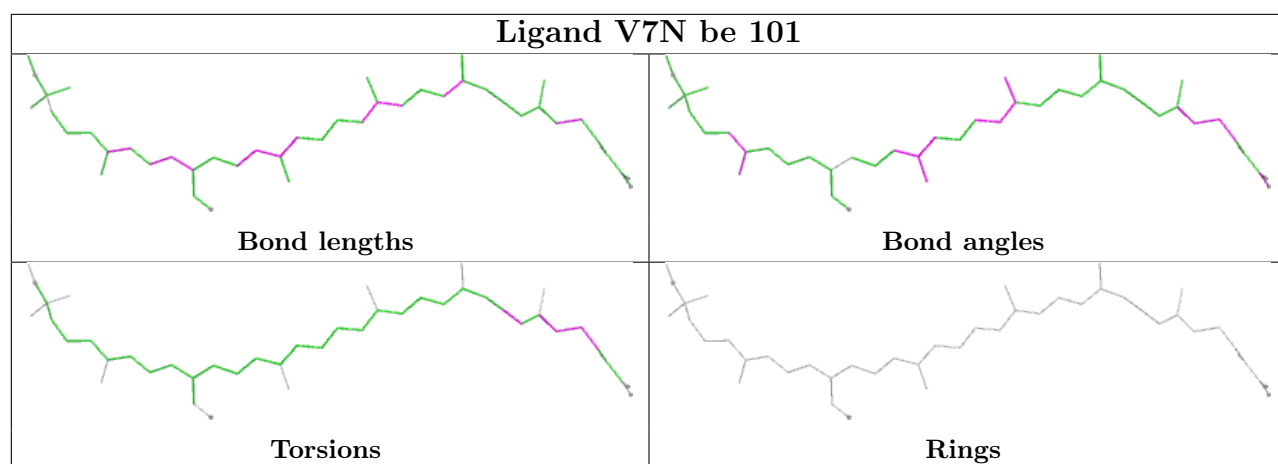




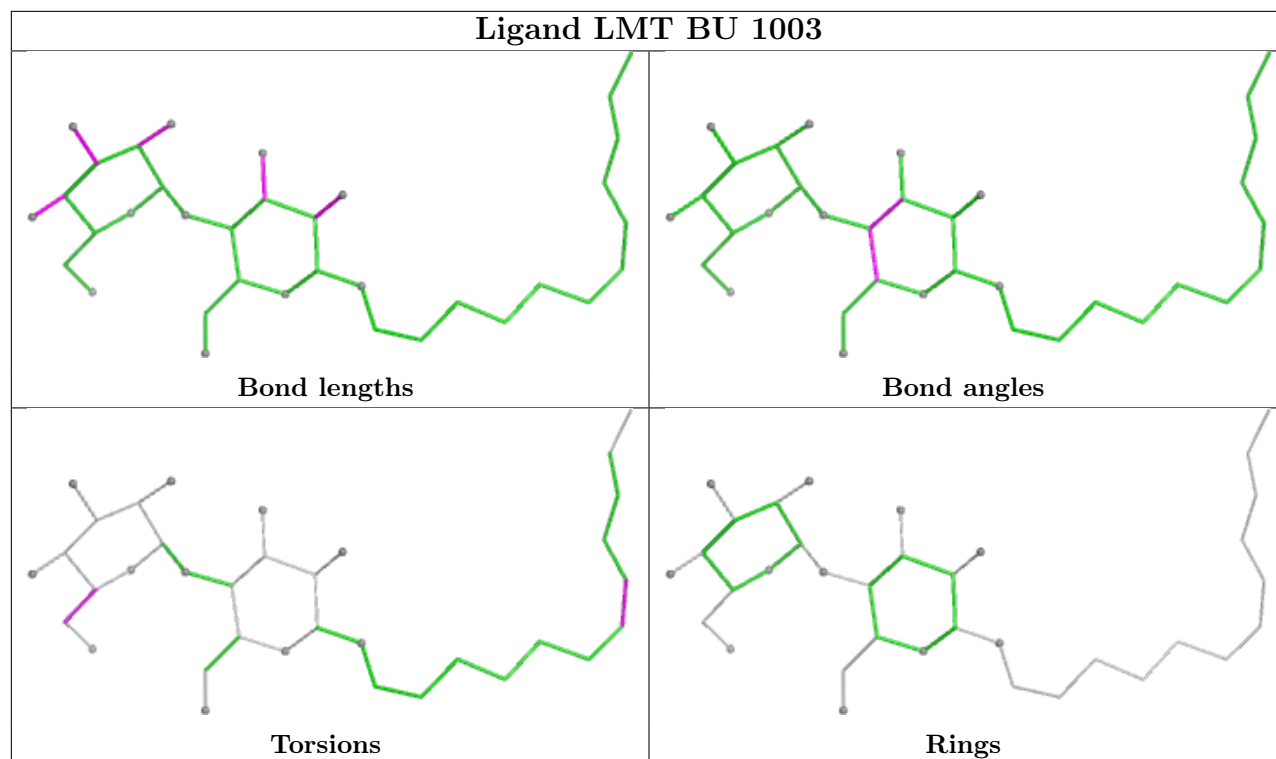




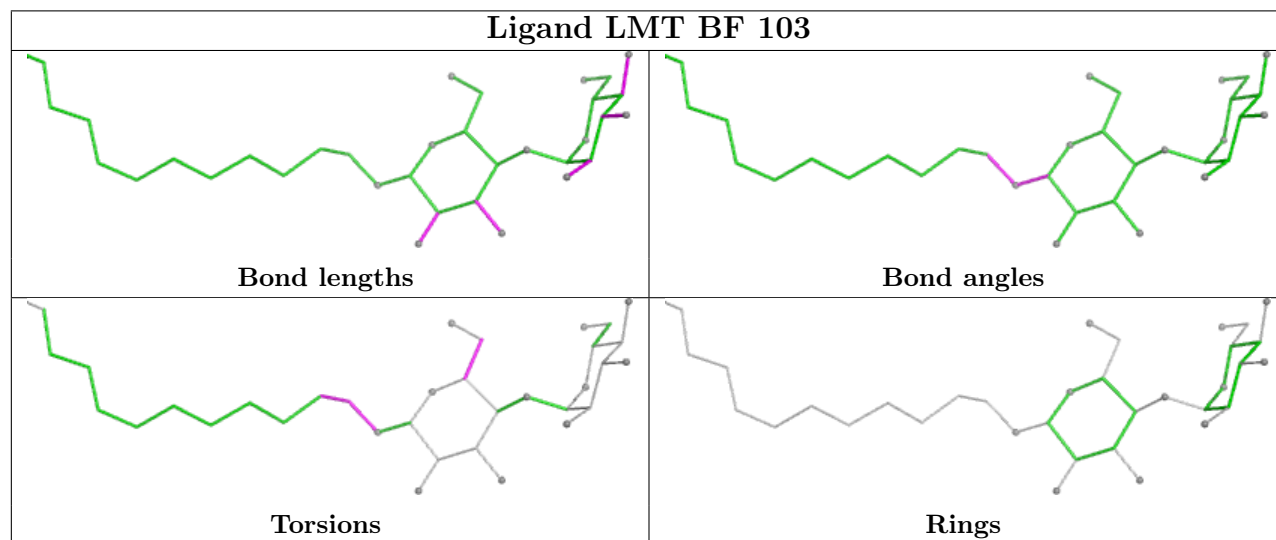


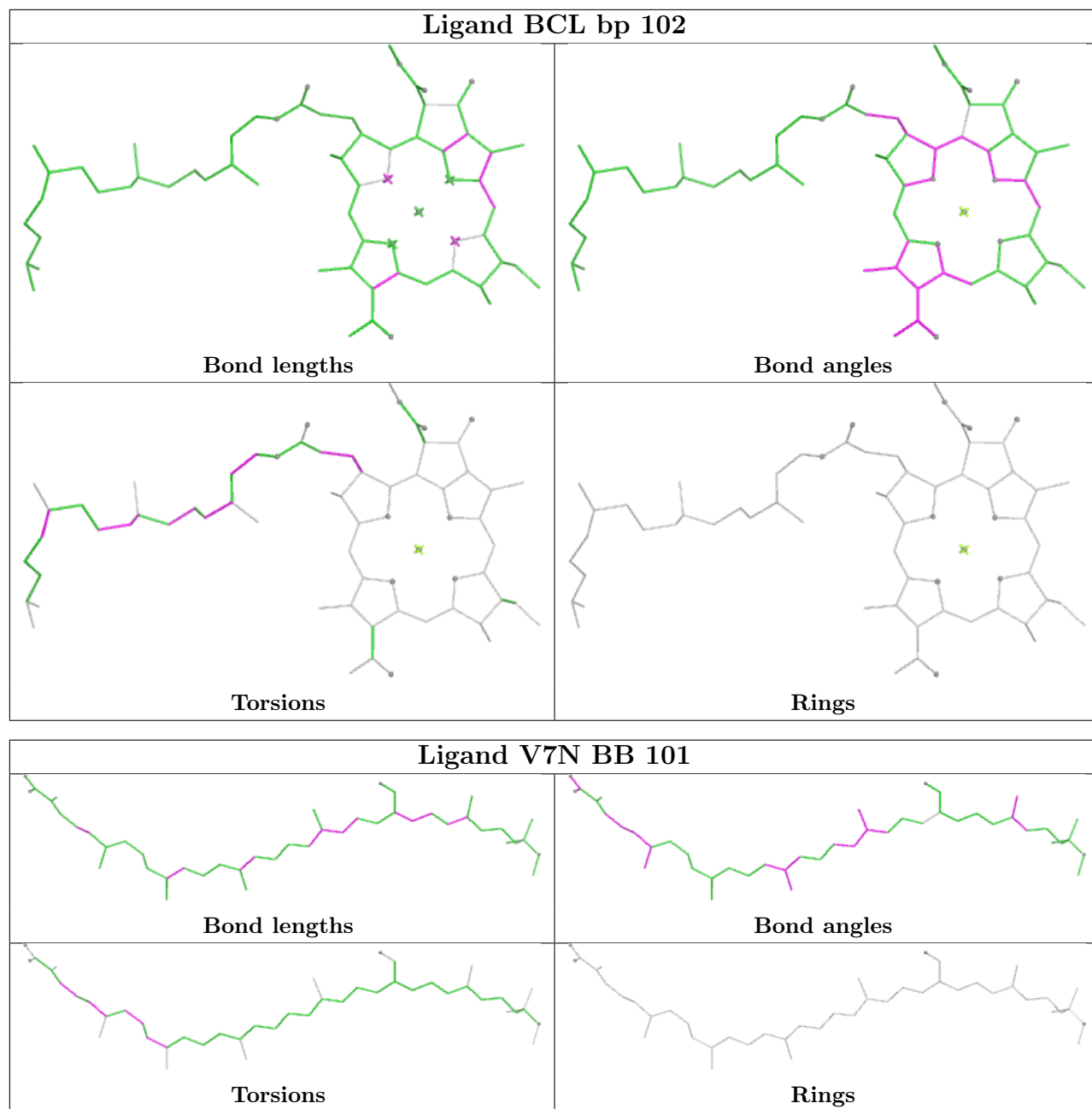


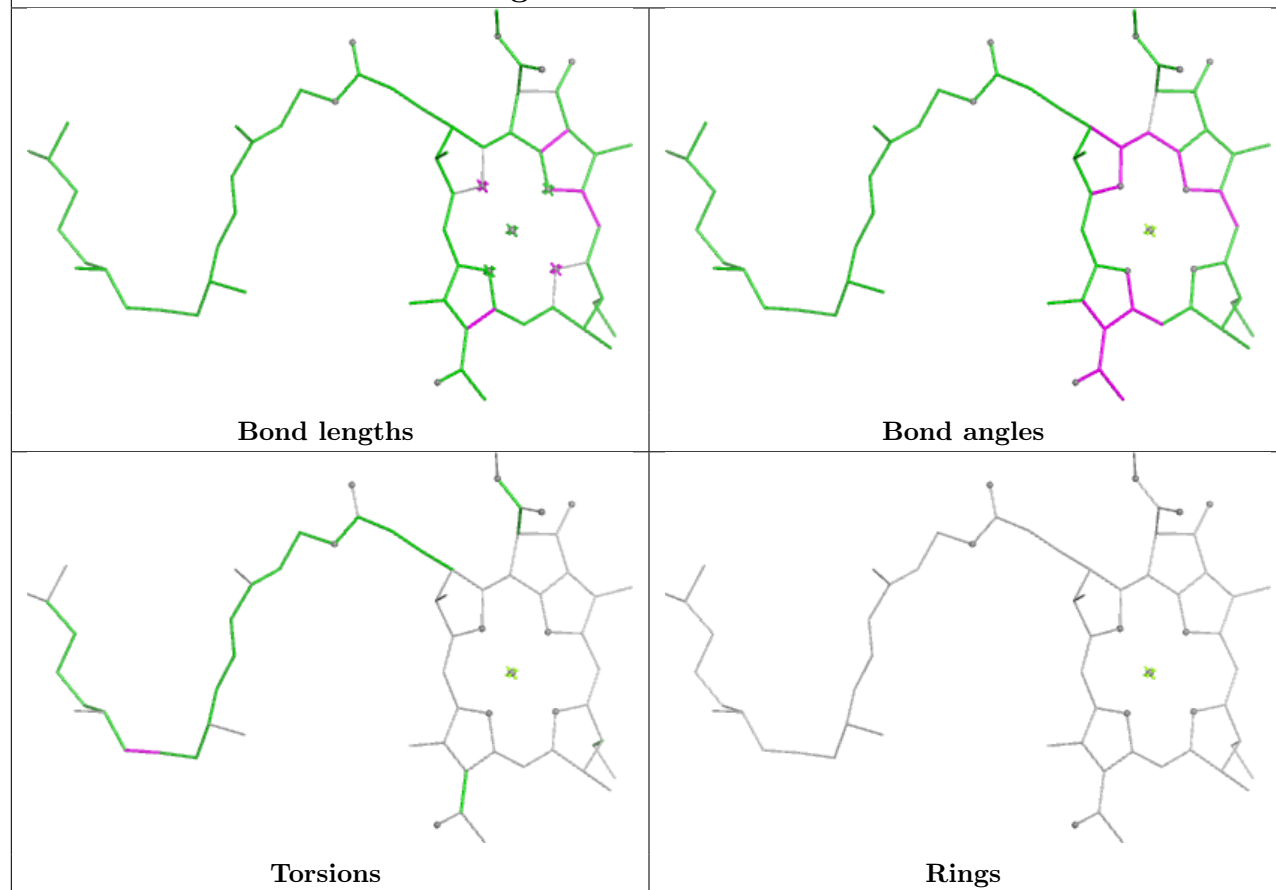
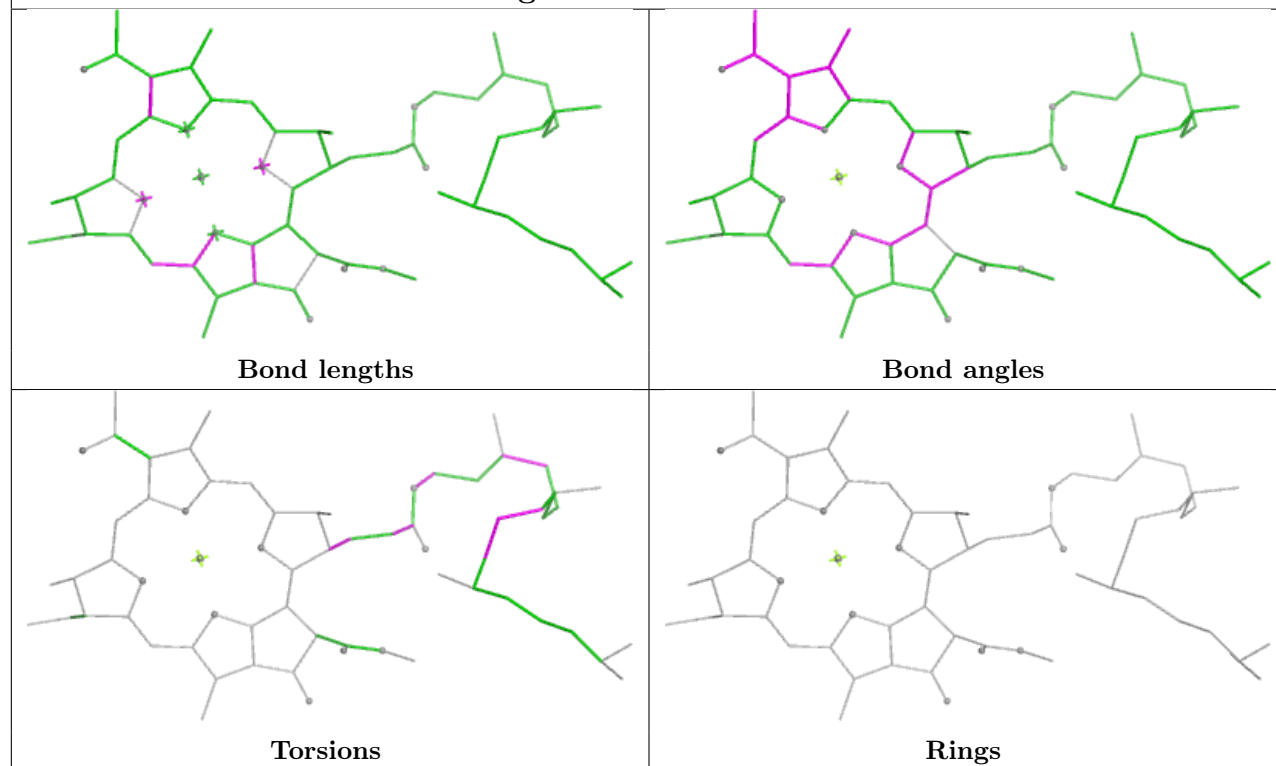
Ligand LMT BU 1003

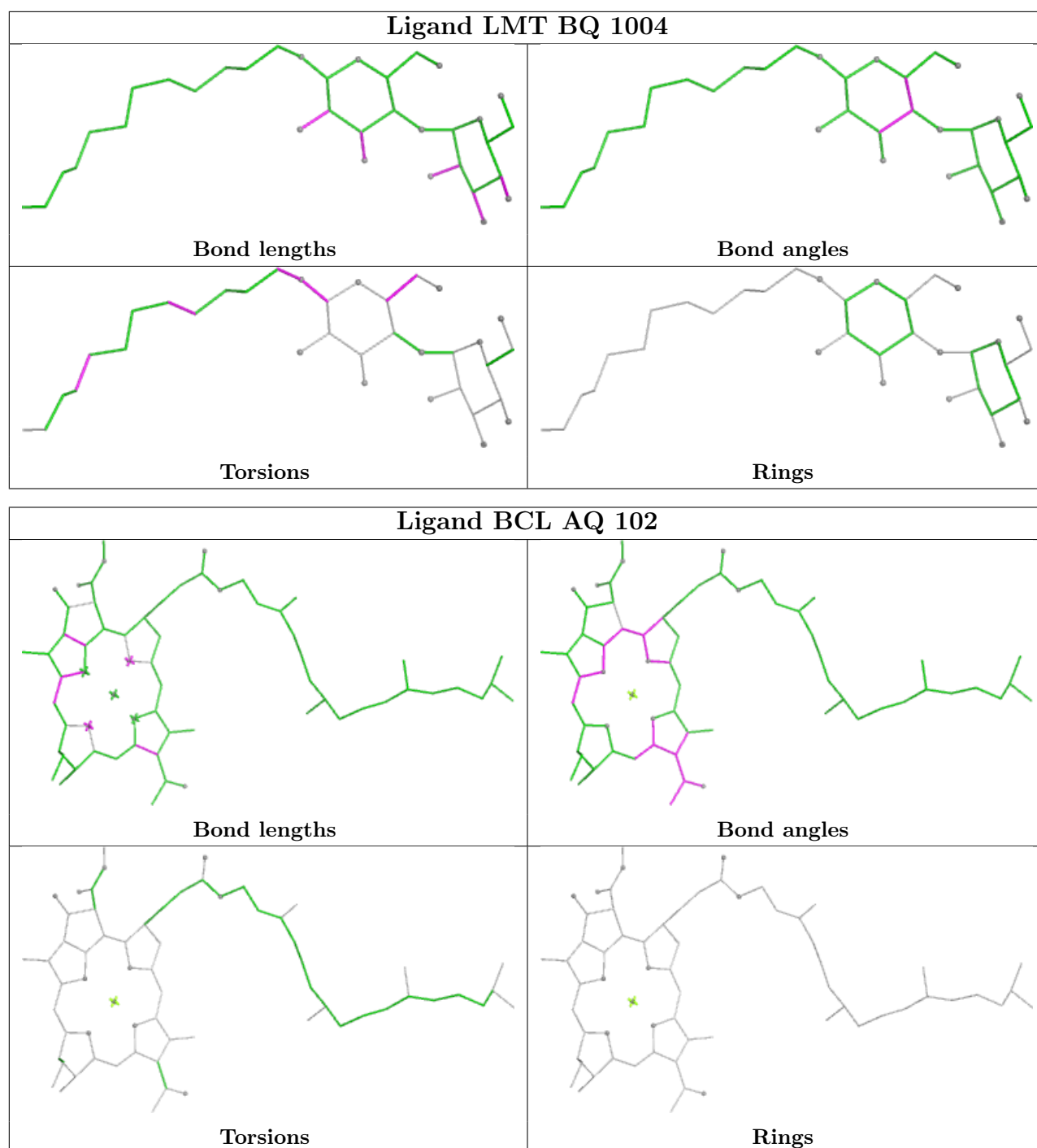


Ligand LMT BF 103





Ligand BCL AO 1002**Ligand BCL ad 1001**



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.

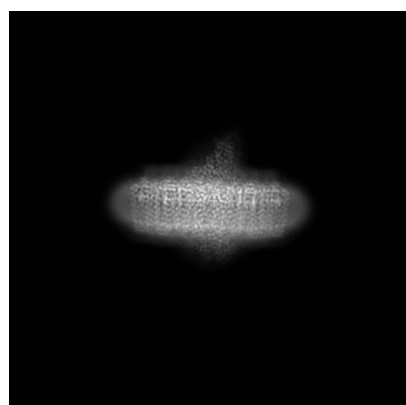
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12680. These allow visual inspection of the internal detail of the map and identification of artifacts.

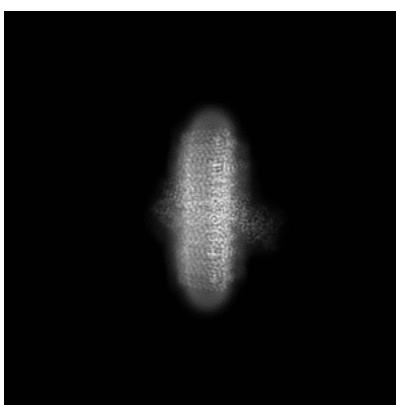
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

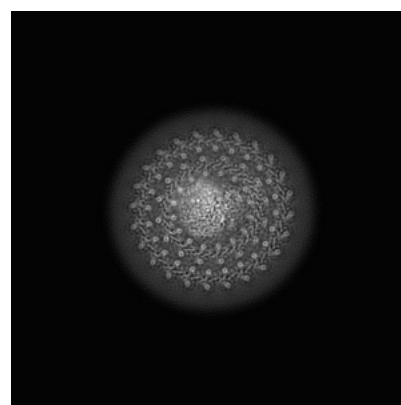
6.1.1 Primary map



X



Y

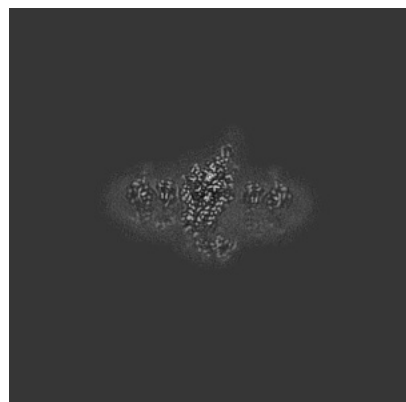


Z

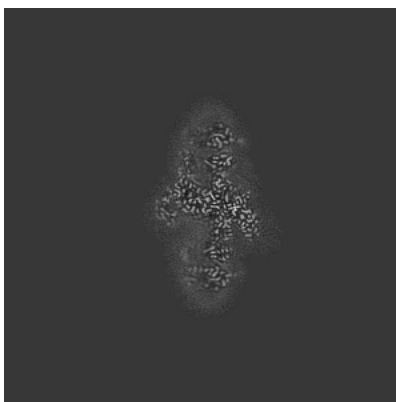
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

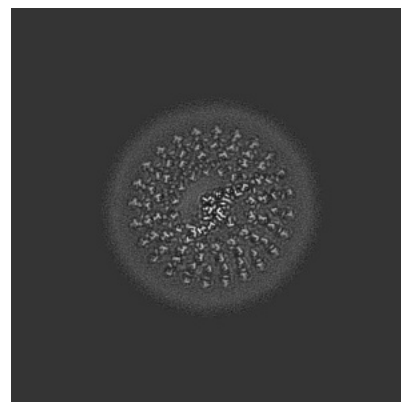
6.2.1 Primary map



X Index: 200



Y Index: 200

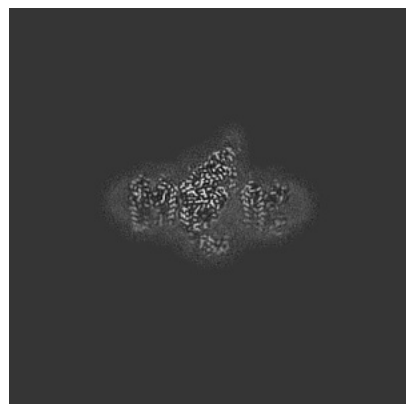


Z Index: 200

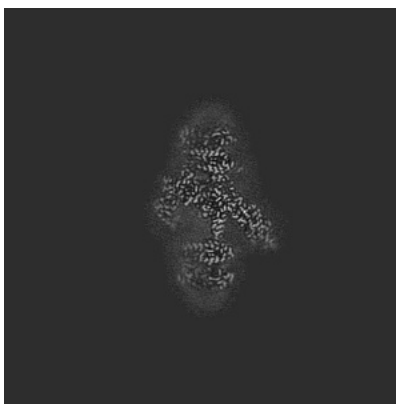
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

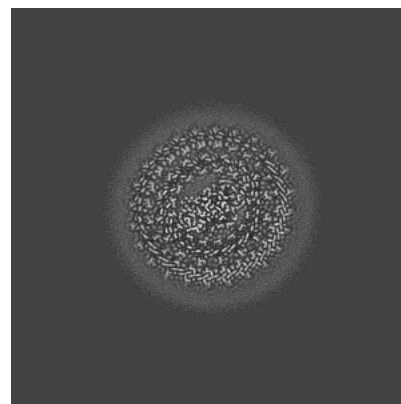
6.3.1 Primary map



X Index: 193



Y Index: 209

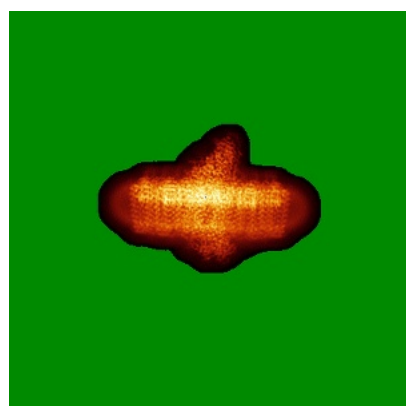


Z Index: 214

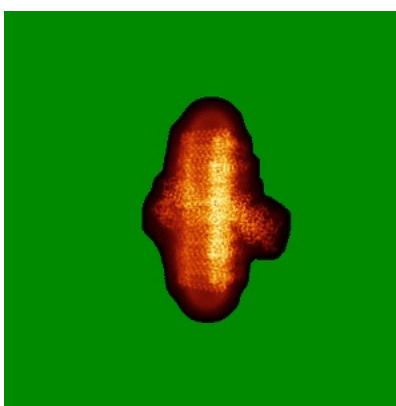
The images above show the largest variance slices of the map in three orthogonal directions.

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

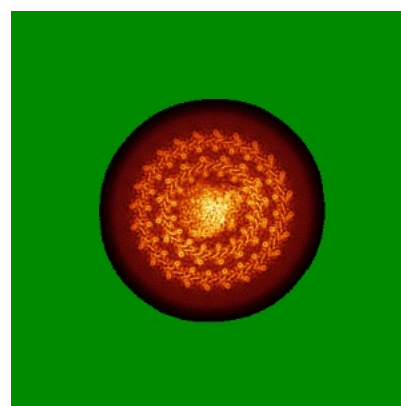
6.4.1 Primary map



X



Y

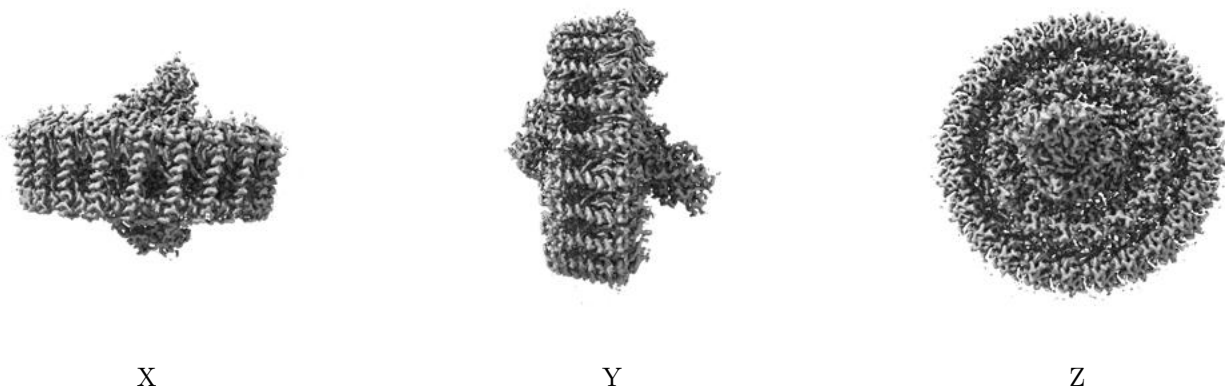


Z

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 0.0348. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

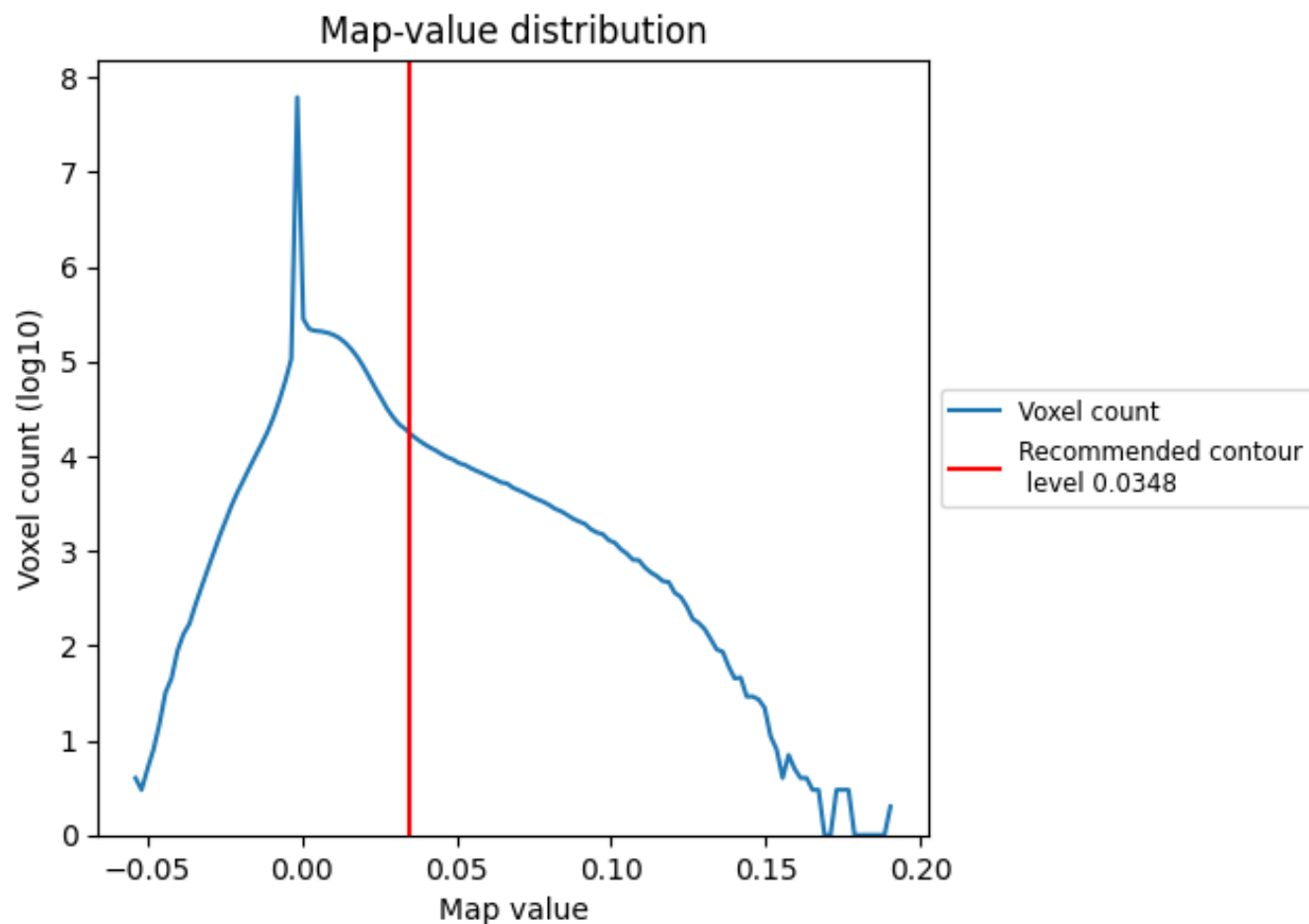
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

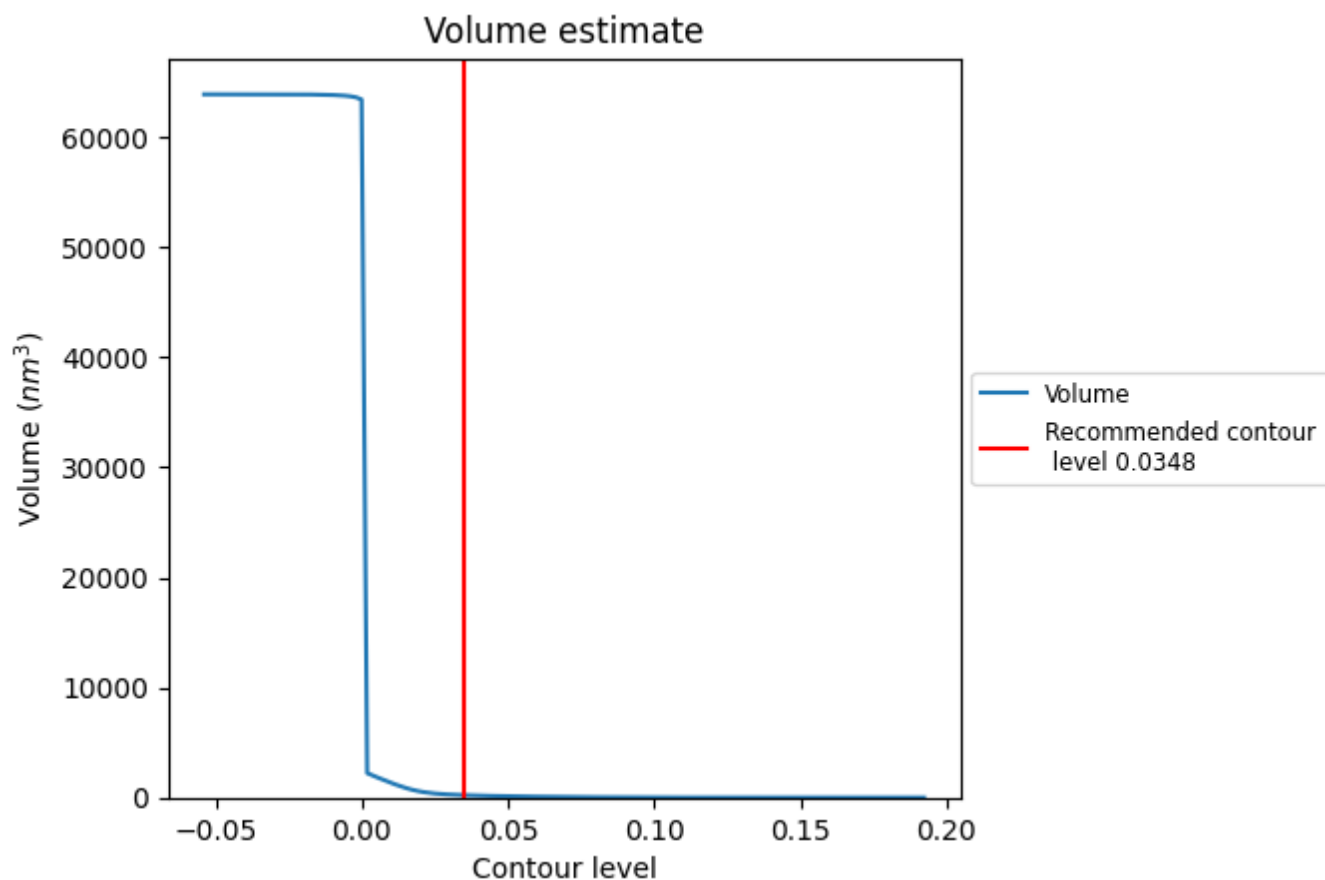
This section contains the results of statistical analysis of the map.

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.

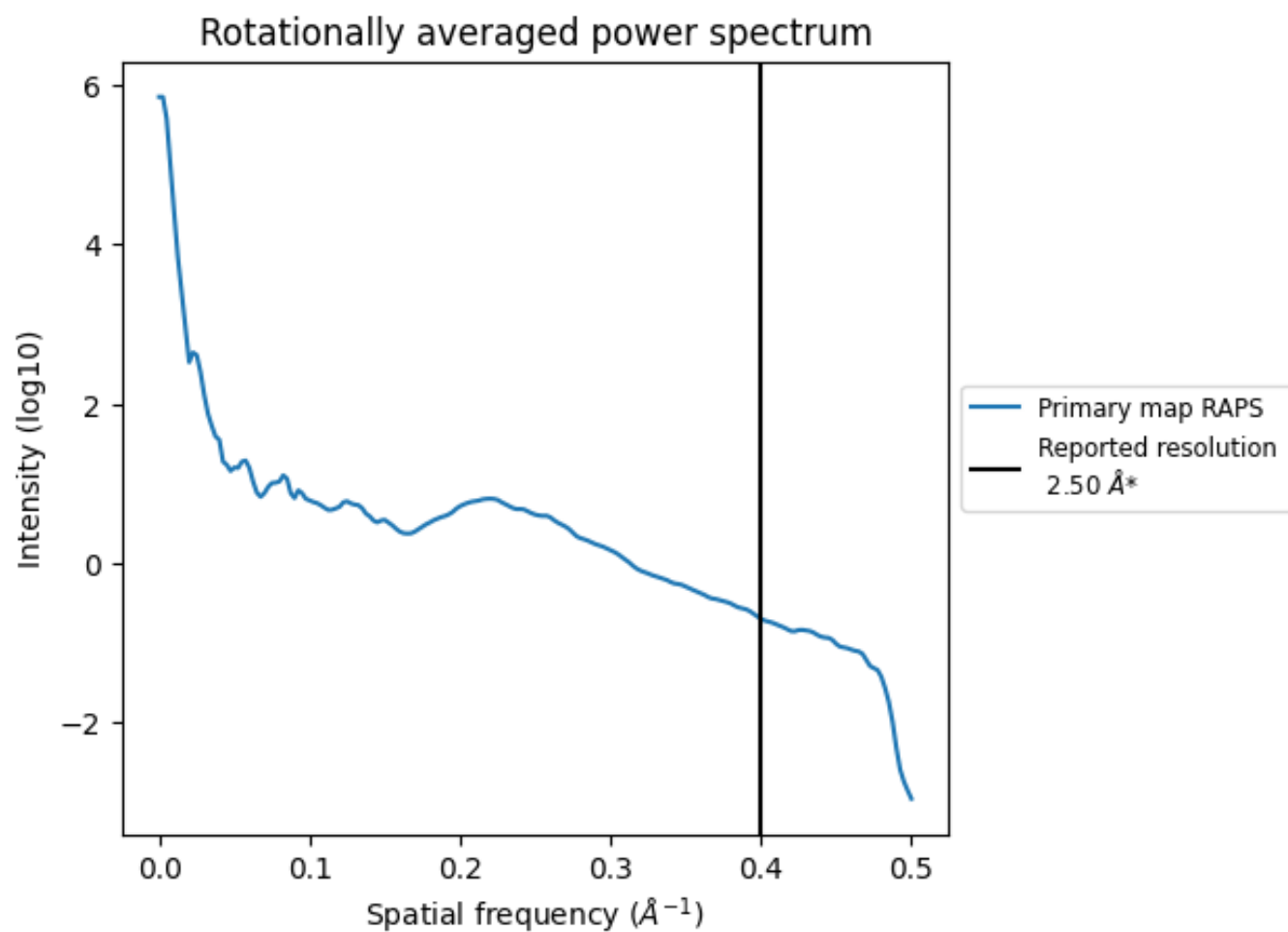
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 198 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 ⓘ

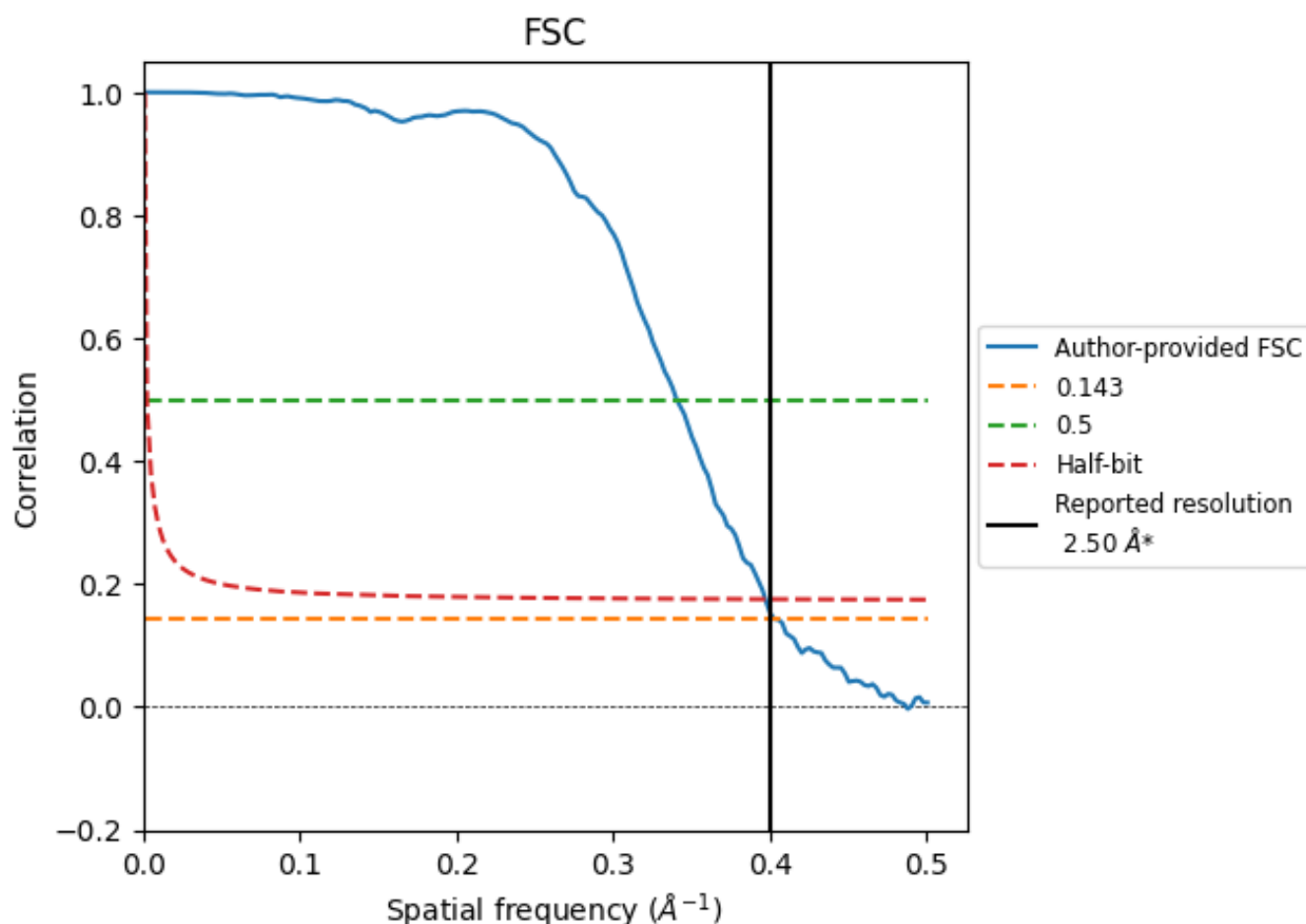


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

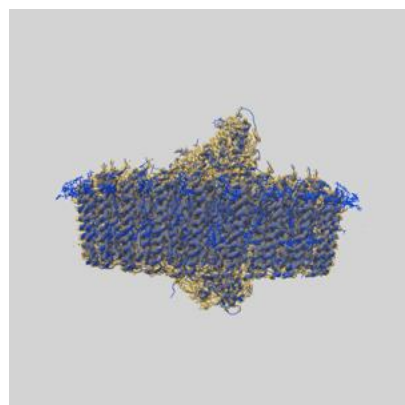
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.94	2.52
Unmasked-calculated*	-	-	-

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

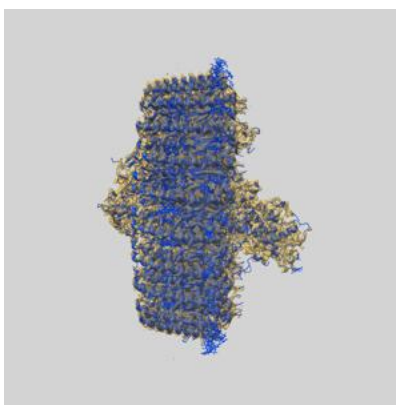
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12680 and PDB model 7O0V. Per-residue inclusion information can be found in [section 3](#) on [page 39](#).

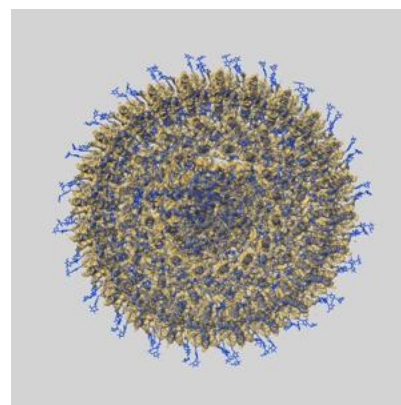
9.1 Map-model overlay [i](#)



X



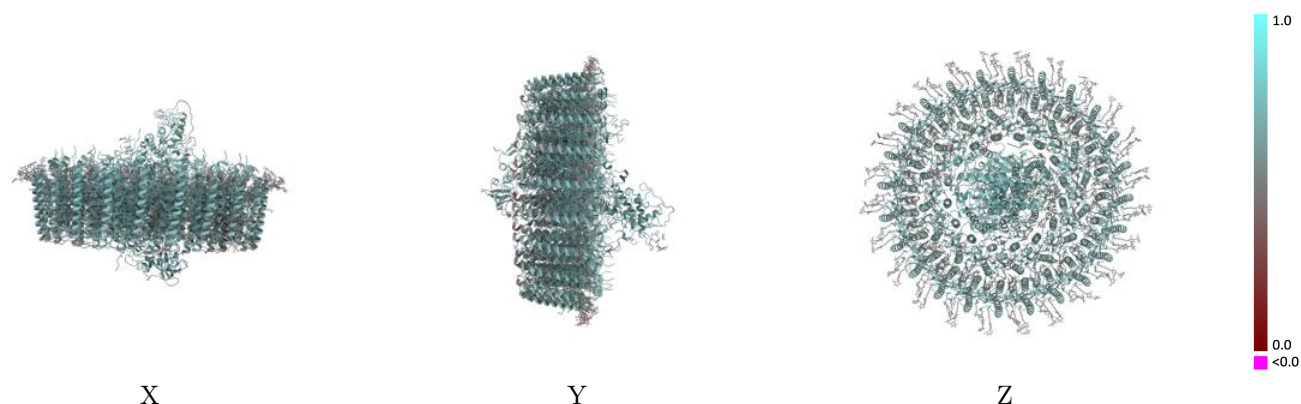
Y



Z

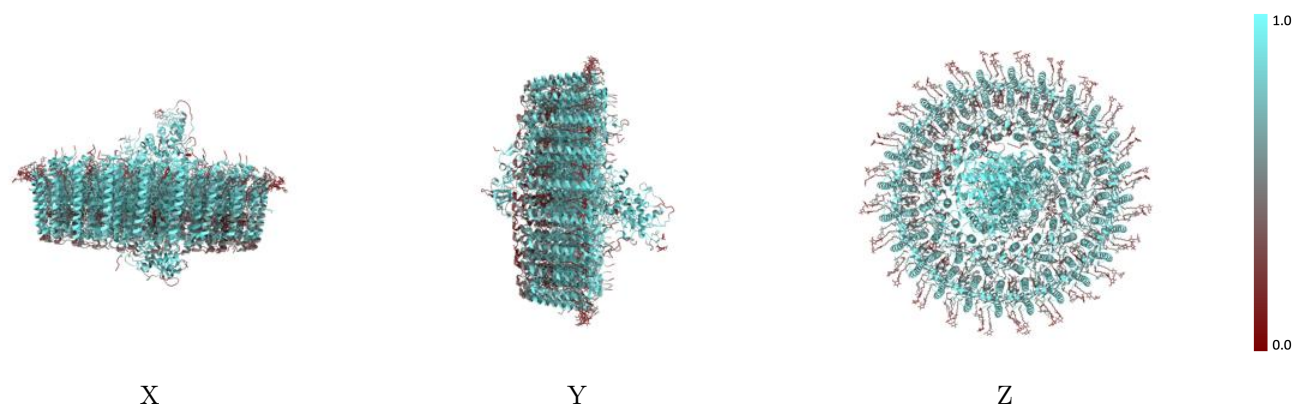
The images above show the 3D surface view of the map at the recommended contour level 0.0348 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



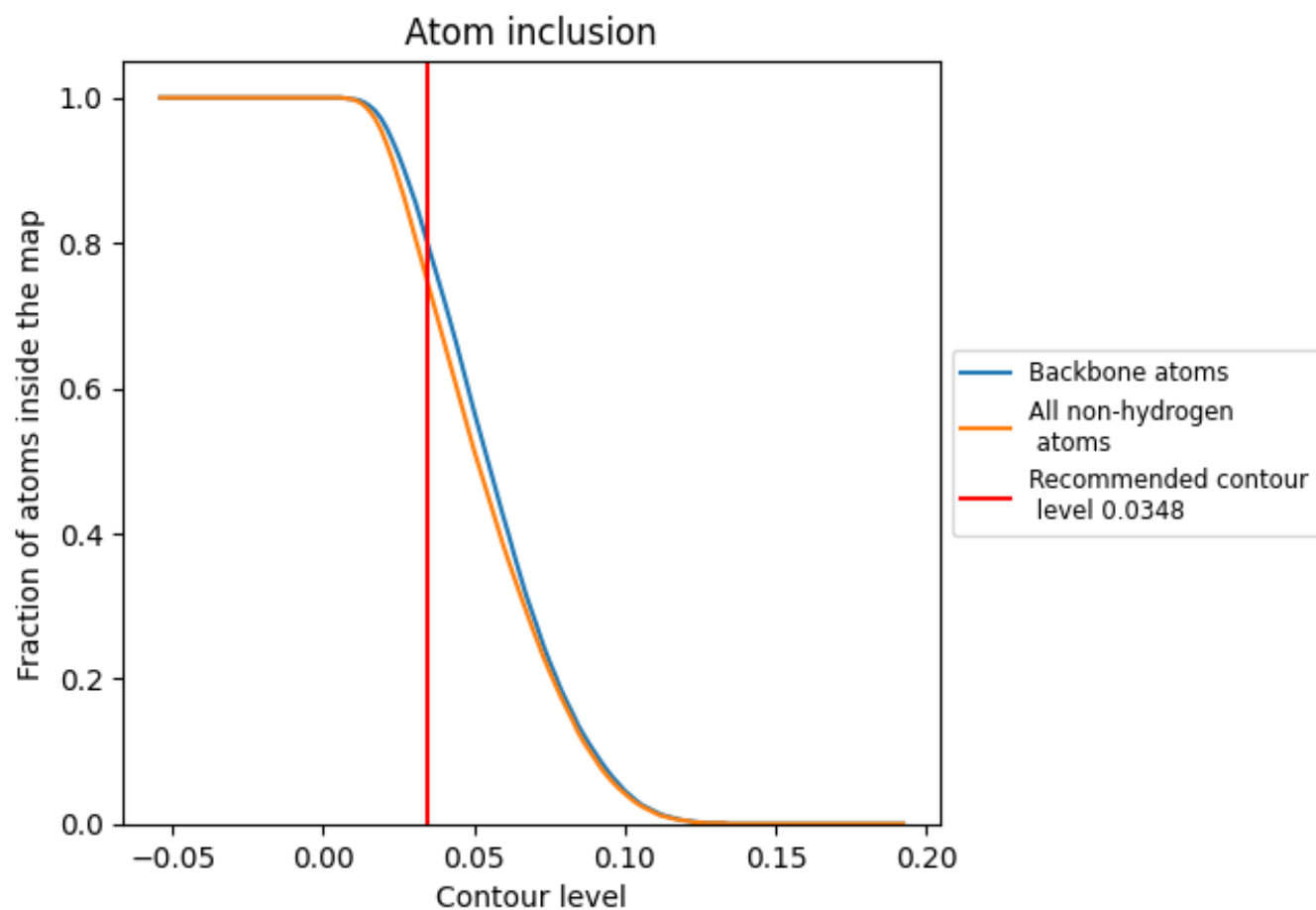
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0348).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.0348) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.6200
AA	 0.7230	 0.6150
AB	 0.7170	 0.6040
AC	 0.5990	 0.5800
AD	 0.7860	 0.6170
AE	 0.6220	 0.5890
AF	 0.7400	 0.6050
AG	 0.7640	 0.6210
AH	 0.7390	 0.6200
AI	 0.7180	 0.6030
AJ	 0.8150	 0.6380
AK	 0.8010	 0.6360
AL	 0.6780	 0.5990
AM	 0.8230	 0.6430
AN	 0.6830	 0.6060
AO	 0.8090	 0.6280
AP	 0.7820	 0.6280
AQ	 0.7570	 0.6270
AR	 0.7300	 0.6120
AS	 0.7340	 0.6230
AT	 0.8230	 0.6390
AU	 0.7020	 0.6020
AV	 0.7300	 0.6250
AW	 0.7940	 0.6240
AX	 0.6650	 0.5980
BA	 0.6340	 0.5780
BB	 0.6040	 0.5650
BC	 0.5730	 0.5530
BD	 0.6160	 0.5740
BE	 0.6370	 0.5800
BF	 0.6580	 0.5810
BG	 0.6600	 0.5800
BH	 0.6700	 0.5930
BI	 0.6500	 0.5940
BJ	 0.7220	 0.6150



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BK	 0.6920	 0.6040
BL	 0.6450	 0.5830
BM	 0.6930	 0.6030
BN	 0.6500	 0.5700
BO	 0.6690	 0.6010
BP	 0.7140	 0.6000
BQ	 0.6610	 0.5810
BR	 0.6510	 0.5920
BS	 0.6680	 0.6050
BT	 0.6460	 0.5780
BU	 0.6500	 0.5840
BV	 0.6480	 0.5810
BW	 0.6310	 0.5720
BX	 0.6140	 0.5720
C	 0.8820	 0.6630
C1	 0.8260	 0.6580
CG	 0.3810	 0.5410
H1	 0.7240	 0.6280
H2	 0.7200	 0.6080
L	 0.9010	 0.6790
M	 0.8970	 0.6830
MG	 0.9520	 0.6170
aa	 0.6690	 0.6100
ab	 0.7090	 0.6210
ac	 0.7750	 0.6250
ad	 0.8850	 0.6710
ae	 0.8320	 0.6540
af	 0.8030	 0.6490
ag	 0.7480	 0.6240
ah	 0.7960	 0.6400
ai	 0.7250	 0.6220
aj	 0.7580	 0.6230
ak	 0.8610	 0.6680
al	 0.8160	 0.6570
am	 0.7500	 0.6230
an	 0.6590	 0.5980
ao	 0.6430	 0.5970
ap	 0.6820	 0.6010
ba	 0.6570	 0.5920
bb	 0.6870	 0.6050
bc	 0.7130	 0.6110
bd	 0.8190	 0.6430

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
be	 0.7810	 0.6270
bf	 0.8240	 0.6480
bg	 0.7550	 0.6200
bh	 0.7470	 0.6210
bi	 0.7510	 0.6130
bj	 0.8060	 0.6370
bk	 0.7620	 0.6300
bl	 0.7150	 0.6170
bm	 0.7080	 0.6000
bn	 0.6730	 0.6000
bo	 0.6440	 0.5970
bp	 0.7050	 0.6030