



wwPDB EM Validation Summary Report ⓘ

Oct 20, 2025 – 02:10 pm BST

PDB ID : 9H19 / pdb_00009h19
EMDB ID : EMD-51760
Title : Cryo-EM structure of RC-dLH complex model I from Gem. groenlandica strain TET16
Authors : Gardiner, A.; Qian, P.; Koblizek, M.; Jing, Y.; Joosten, M.; Jakobi, A.; Bina, D.; Mujakic, I.; Gardian, Z.; Kaftan, D.; Castro-Hartmann, P.
Deposited on : 2024-10-09
Resolution : 2.30 Å (reported)
Based on initial model : .

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:

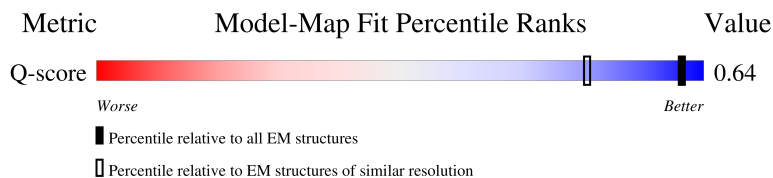
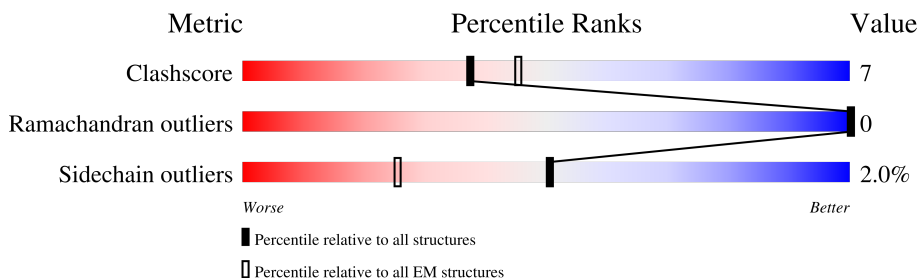
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up 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) : 2.46

1 Overall quality at a glance

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

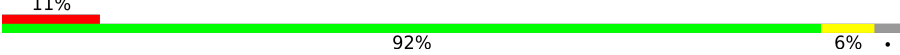

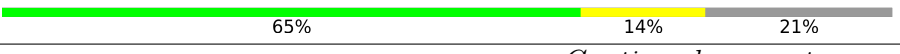
The reported resolution of this entry is 2.30 Å.

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.









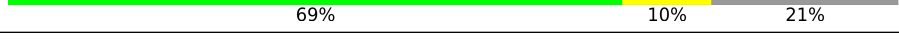
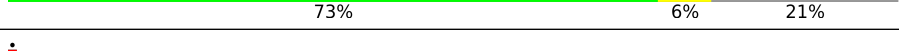
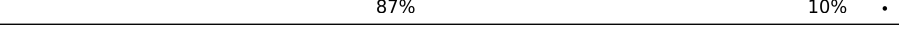
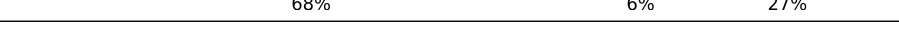
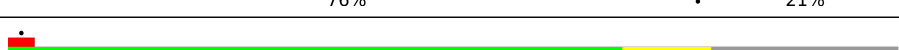

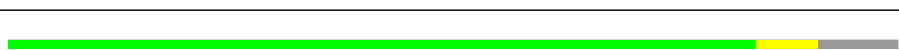

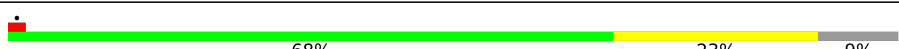





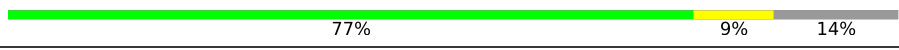
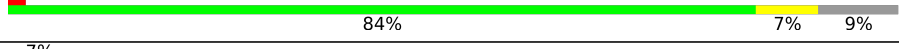



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	71	
1	Ab	71	
1	Ac	71	

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Mol	Chain	Length	Quality of chain
1	Ad	71	
1	Ae	71	
1	Af	71	
1	Ag	71	
1	Ah	71	
1	Ai	71	
1	Aj	71	
1	Ak	71	
1	Al	71	
1	Am	71	
1	An	71	
1	Ao	71	
1	Ap	71	
2	BA	44	
2	BB	44	
2	BC	44	
2	BD	44	
2	BE	44	
2	BF	44	
2	BG	44	
2	BH	44	
2	BI	44	
2	BJ	44	
2	BK	44	
2	BL	44	




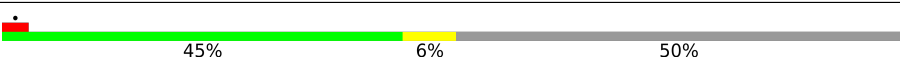
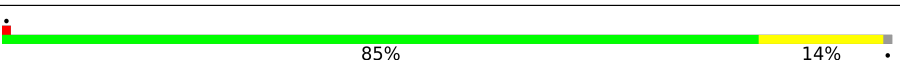

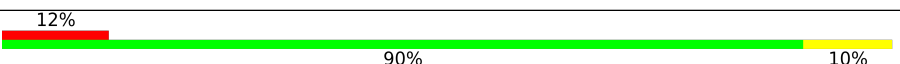
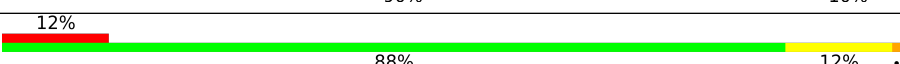
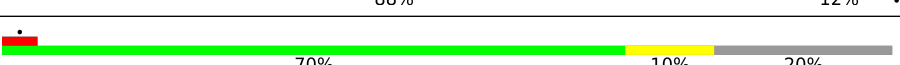
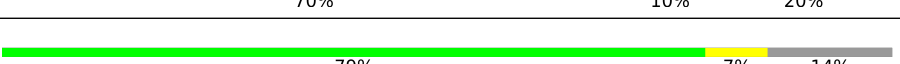
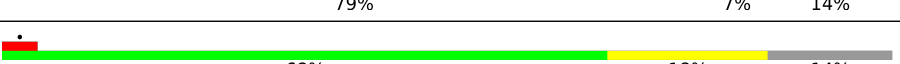
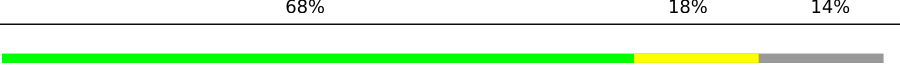

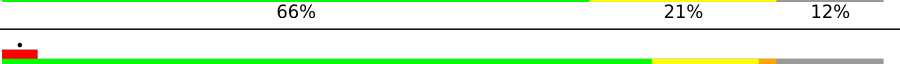



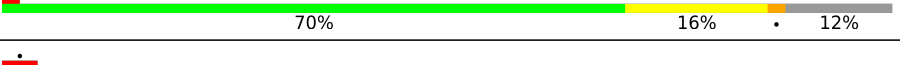

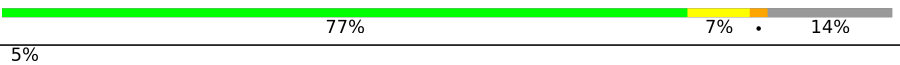
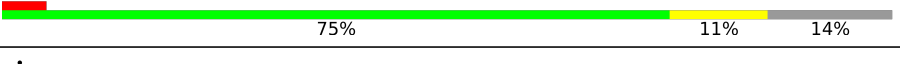


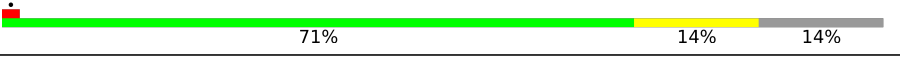

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Mol	Chain	Length	Quality of chain
2	BM	44	
2	BN	44	
2	BO	44	
2	BP	44	
2	BQ	44	
2	BR	44	
2	BS	44	
2	BT	44	
2	BU	44	
2	BV	44	
2	BW	44	
2	BX	44	
2	Ba	44	
2	Bb	44	
2	Bc	44	
2	Bd	44	
2	Be	44	
2	Bf	44	
2	Bg	44	
2	Bh	44	
2	Bi	44	
2	Bj	44	
2	Bk	44	
2	Bl	44	
2	Bm	44	

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Mol	Chain	Length	Quality of chain
2	Bn	44	
2	Bo	44	
2	Bp	44	
3	S	204	
4	L	274	
5	M	392	
6	H	60	
7	K	179	
8	C	373	
9	AA	56	
9	AB	56	
9	AC	56	
9	AD	56	
9	AE	56	
9	AF	56	
9	AG	56	
9	AH	56	
9	AI	56	
9	AJ	56	
9	AK	56	
9	AL	56	
9	AM	56	
9	AN	56	
9	AO	56	
9	AP	56	

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Mol	Chain	Length	Quality of chain
9	AQ	56	
9	AR	56	
9	AS	56	
9	AT	56	
9	AU	56	
9	AV	56	
9	AW	56	
9	AX	56	

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
11	BCL	Ao	101	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49808 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 Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	69	Total	C	N	O	S	0	0
			520	340	90	86	4		
1	Ab	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
1	Ac	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Ad	54	Total	C	N	O	S	0	0
			426	281	75	67	3		
1	Ae	59	Total	C	N	O	S	0	0
			454	298	80	73	3		
1	Af	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Ag	57	Total	C	N	O	S	0	0
			445	292	78	71	4		
1	Ah	53	Total	C	N	O	S	0	0
			411	272	69	67	3		
1	Ai	57	Total	C	N	O	S	0	0
			445	292	78	71	4		
1	Aj	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
1	Ak	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Al	69	Total	C	N	O	S	0	0
			520	340	90	86	4		
1	Am	52	Total	C	N	O	S	0	0
			417	276	73	65	3		
1	An	56	Total	C	N	O	S	0	0
			440	289	77	70	4		
1	Ao	56	Total	C	N	O	S	0	0
			437	287	77	70	3		
1	Ap	55	Total	C	N	O	S	0	0
			432	284	76	69	3		

- Molecule 2 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ba	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bb	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bc	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bd	37	Total	C	N	O		0	0
			316	213	54	49			
2	Be	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bf	34	Total	C	N	O		0	0
			292	200	51	41			
2	Bg	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bh	36	Total	C	N	O		0	0
			309	209	53	47			
2	Bi	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bj	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bk	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bl	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bm	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bn	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bo	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	Bp	35	Total	C	N	O		0	0
			300	204	52	44			
2	BA	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BB	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BC	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BD	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BE	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	BF	39	Total	C	N	O	S	0	0
			328	220	56	51	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BG	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BH	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BI	38	Total	C	N	O	S	0	0
			324	218	55	50	1		
2	BJ	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BK	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BL	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BM	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BN	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BO	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BP	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BQ	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BR	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BS	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BT	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BU	39	Total	C	N	O	S	0	0
			328	220	56	51	1		
2	BV	41	Total	C	N	O	S	0	0
			341	228	59	53	1		
2	BW	40	Total	C	N	O	S	0	0
			332	222	57	52	1		
2	BX	40	Total	C	N	O	S	0	0
			332	222	57	52	1		

- Molecule 3 is a protein called reaction centre S sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	103	Total	C	N	O	S	0	0
			800	498	150	148	4		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	271	Total	C	N	O	S	0	0
			2134	1435	346	342	11		

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	335	Total	C	N	O	S	0	0
			2697	1789	441	457	10		

- Molecule 6 is a protein called reaction centre Ht sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	60	Total	C	N	O	S	0	0
			510	338	85	85	2		

- Molecule 7 is a protein called reaction centre Hc sub unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	179	Total	C	N	O	S	0	0
			1373	873	231	262	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	298	Total	C	N	O	S	0	0
			2330	1463	421	429	17		

- Molecule 9 is a protein called Light-harvesting protein.

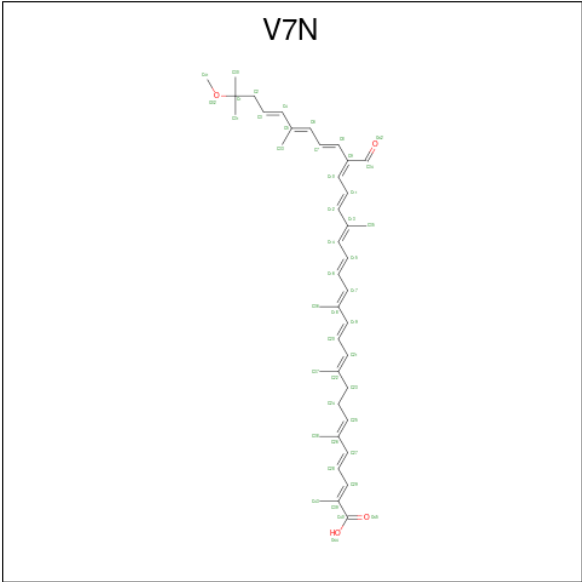
Mol	Chain	Residues	Atoms					AltConf	Trace
9	AA	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AB	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AC	48	Total	C	N	O	S	0	0
			391	262	65	60	4		
9	AD	49	Total	C	N	O	S	0	0
			400	267	67	62	4		
9	AE	49	Total	C	N	O	S	0	0
			400	267	67	62	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AG	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AH	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AI	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AJ	48	Total 391	C 262	N 65	O 60	S 4	0	0
9	AK	48	Total 392	C 262	N 66	O 61	S 3	0	0
9	AL	48	Total 391	C 262	N 65	O 60	S 4	0	0
9	AM	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AN	48	Total 392	C 262	N 66	O 61	S 3	0	0
9	AO	48	Total 391	C 262	N 65	O 60	S 4	0	0
9	AP	48	Total 391	C 262	N 65	O 60	S 4	0	0
9	AQ	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AR	48	Total 391	C 262	N 65	O 60	S 4	0	0
9	AS	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AT	48	Total 392	C 262	N 66	O 61	S 3	0	0
9	AU	48	Total 392	C 262	N 66	O 61	S 3	0	0
9	AV	48	Total 391	C 262	N 65	O 60	S 4	0	0
9	AW	49	Total 400	C 267	N 67	O 62	S 4	0	0
9	AX	48	Total 391	C 262	N 65	O 60	S 4	0	0

- Molecule 10 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
10	Aa	1	Total	C	O	0
			45	41	4	
10	Bb	1	Total	C	O	0
			45	41	4	
10	Bc	1	Total	C	O	0
			45	41	4	
10	Bd	1	Total	C	O	0
			45	41	4	
10	Be	1	Total	C	O	0
			45	41	4	
10	Bf	1	Total	C	O	0
			45	41	4	
10	Bg	1	Total	C	O	0
			45	41	4	
10	Bh	1	Total	C	O	0
			45	41	4	
10	Bi	1	Total	C	O	0
			45	41	4	
10	Bj	1	Total	C	O	0
			45	41	4	
10	Bk	1	Total	C	O	0
			45	41	4	
10	Bl	1	Total	C	O	0
			45	41	4	
10	Bm	1	Total	C	O	0
			45	41	4	
10	An	1	Total	C	O	0
			45	41	4	

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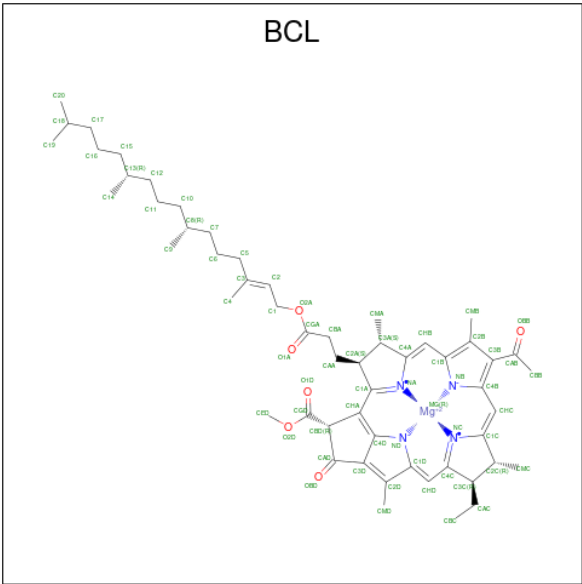
Mol	Chain	Residues	Atoms			AltConf
10	Bn	1	Total	C	O	0
			45	41	4	
10	Bp	1	Total	C	O	0
			45	41	4	
10	BA	1	Total	C	O	0
			45	41	4	
10	BB	1	Total	C	O	0
			45	41	4	
10	BC	1	Total	C	O	0
			45	41	4	
10	BD	1	Total	C	O	0
			45	41	4	
10	BF	1	Total	C	O	0
			45	41	4	
10	AF	1	Total	C	O	0
			45	41	4	
10	BG	1	Total	C	O	0
			45	41	4	
10	BH	1	Total	C	O	0
			45	41	4	
10	BI	1	Total	C	O	0
			45	41	4	
10	BJ	1	Total	C	O	0
			45	41	4	
10	BK	1	Total	C	O	0
			45	41	4	
10	AL	1	Total	C	O	0
			45	41	4	
10	BL	1	Total	C	O	0
			45	41	4	
10	BN	1	Total	C	O	0
			45	41	4	
10	BO	1	Total	C	O	0
			45	41	4	
10	BP	1	Total	C	O	0
			45	41	4	
10	BQ	1	Total	C	O	0
			45	41	4	
10	BR	1	Total	C	O	0
			45	41	4	
10	BS	1	Total	C	O	0
			45	41	4	

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Mol	Chain	Residues	Atoms			AltConf
10	BT	1	Total	C	O	0
			45	41	4	
10	BU	1	Total	C	O	0
			45	41	4	
10	BV	1	Total	C	O	0
			45	41	4	
10	BW	1	Total	C	O	0
			45	41	4	
10	BX	1	Total	C	O	0
			45	41	4	

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



Mol	Chain	Residues	Atoms					AltConf
11	Aa	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ba	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bb	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bc	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	Ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bd	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Be	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Af	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bf	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bg	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bh	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ai	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bi	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Aj	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bj	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ak	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bk	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Al	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bl	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Am	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bm	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bn	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Ao	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	Bo	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bp	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	Bp	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BH	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BO	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BP	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	BR	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BS	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BU	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BV	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0
11	BX	1	Total 66	C 55	Mg 1	N 4	O 6	0

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



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Mol	Chain	Residues	Atoms			AltConf
12	Bl	1	Total	C	O	0
			35	24	11	
12	Bo	1	Total	C	O	0
			35	24	11	
12	Bp	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			35	24	11	
12	M	1	Total	C	O	0
			35	24	11	
12	K	1	Total	C	O	0
			35	24	11	
12	C	1	Total	C	O	0
			35	24	11	
12	BA	1	Total	C	O	0
			35	24	11	
12	BA	1	Total	C	O	0
			35	24	11	
12	BB	1	Total	C	O	0
			35	24	11	
12	BC	1	Total	C	O	0
			35	24	11	
12	BD	1	Total	C	O	0
			35	24	11	
12	BE	1	Total	C	O	0
			35	24	11	
12	BF	1	Total	C	O	0
			35	24	11	
12	BG	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BH	1	Total	C	O	0
			35	24	11	
12	BI	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BK	1	Total	C	O	0
			35	24	11	
12	BL	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
12	BM	1	Total	C	O	0
			35	24	11	
12	BO	1	Total	C	O	0
			35	24	11	
12	BO	1	Total	C	O	0
			35	24	11	
12	BQ	1	Total	C	O	0
			35	24	11	
12	BQ	1	Total	C	O	0
			35	24	11	
12	BR	1	Total	C	O	0
			35	24	11	
12	BS	1	Total	C	O	0
			35	24	11	
12	BU	1	Total	C	O	0
			35	24	11	
12	BU	1	Total	C	O	0
			35	24	11	
12	AW	1	Total	C	O	0
			35	24	11	
12	BW	1	Total	C	O	0
			35	24	11	
12	BW	1	Total	C	O	0
			35	24	11	
12	AX	1	Total	C	O	0
			35	24	11	

- Molecule 13 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (CCD ID: PEX) (formula: C₂₅H₄₉NO₈P).

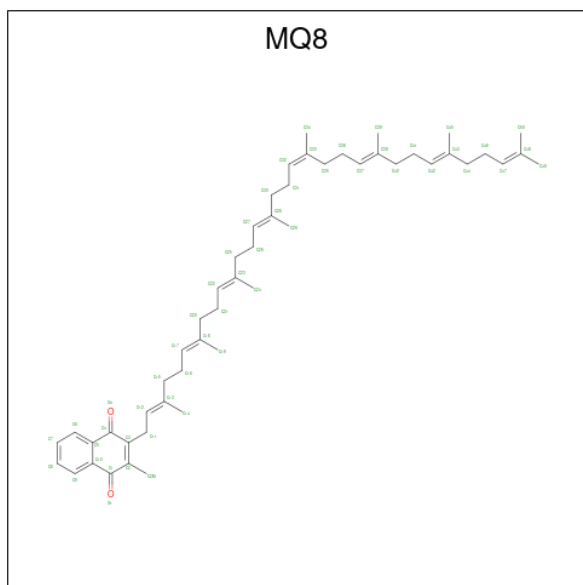


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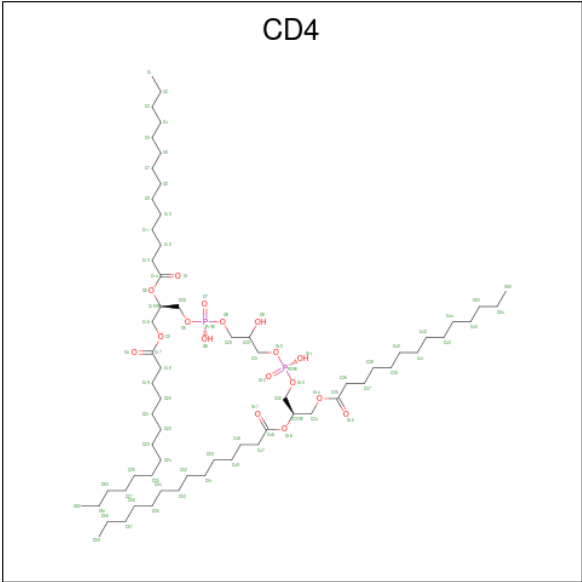
Mol	Chain	Residues	Atoms					AltConf
13	AP	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AS	1	Total	C	N	O	P	0
			35	25	1	8	1	
13	AT	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 14 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



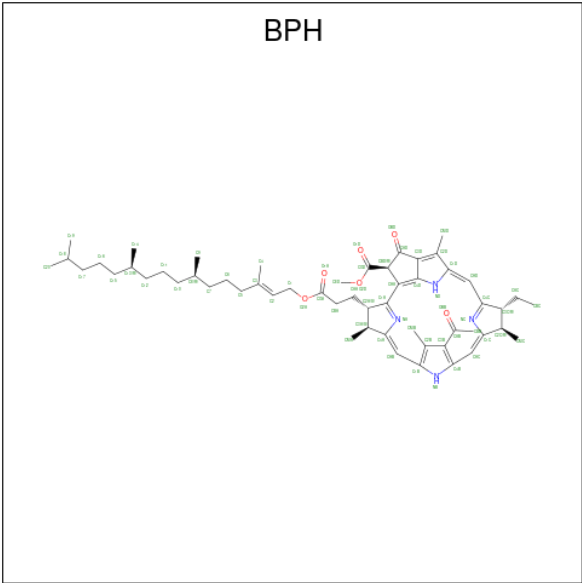
Mol	Chain	Residues	Atoms			AltConf
14	Ad	1	Total	C	O	0
			53	51	2	
14	L	1	Total	C	O	0
			53	51	2	
14	M	1	Total	C	O	0
			53	51	2	

- Molecule 15 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: $C_{65}H_{126}O_{17}P_2$).



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

- Molecule 16 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).

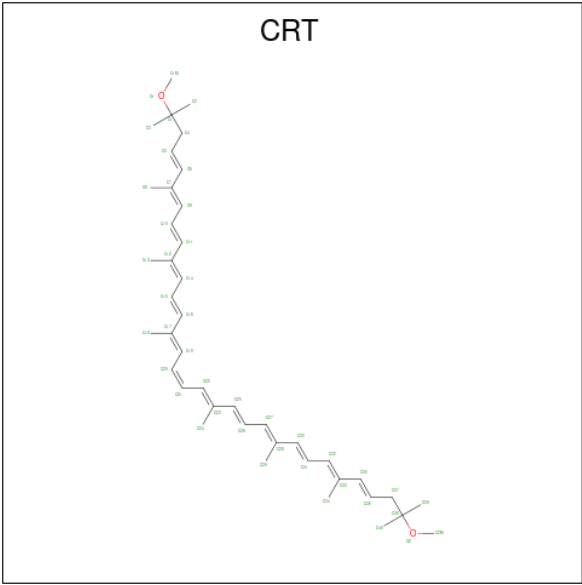


Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	N	O	0
			65	55	4	6	
16	M	1	Total	C	N	O	0
			65	55	4	6	

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

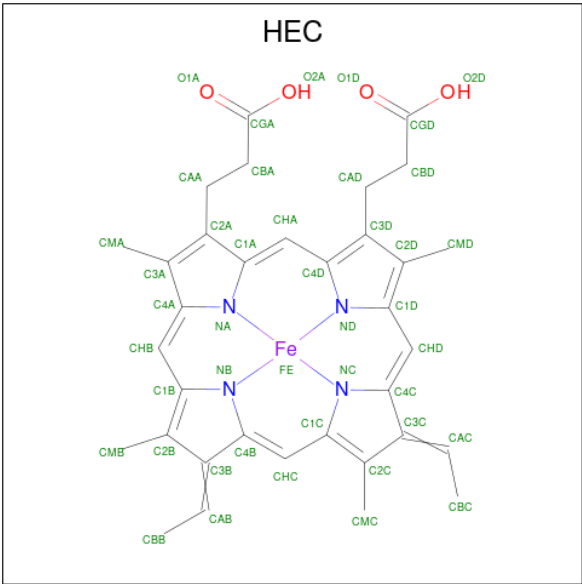
Mol	Chain	Residues	Atoms		AltConf
17	M	1	Total	Fe	0
			1	1	

- Molecule 18 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



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

- Molecule 19 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

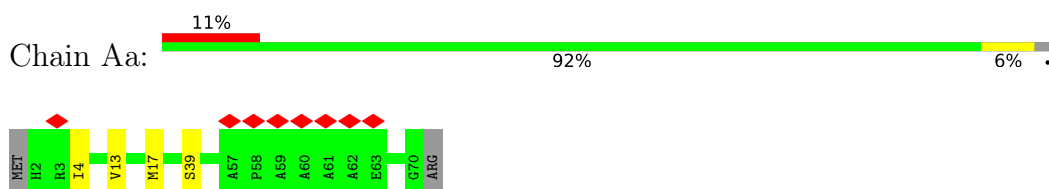
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		AltConf
20	Aa	2	Total 2	O 2	0
20	Ac	1	Total 1	O 1	0
20	Ae	1	Total 1	O 1	0
20	Ag	1	Total 1	O 1	0
20	Bj	1	Total 1	O 1	0
20	Ak	1	Total 1	O 1	0
20	Al	2	Total 2	O 2	0
20	Am	3	Total 3	O 3	0
20	An	1	Total 1	O 1	0
20	S	2	Total 2	O 2	0
20	L	10	Total 10	O 10	0
20	M	8	Total 8	O 8	0
20	C	3	Total 3	O 3	0
20	AC	1	Total 1	O 1	0
20	BO	1	Total 1	O 1	0

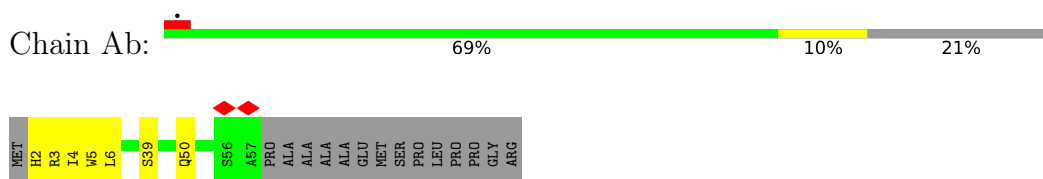
3 Residue-property plots [i](#)

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

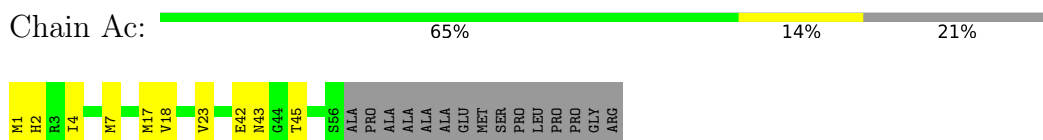
- Molecule 1: Light-harvesting protein



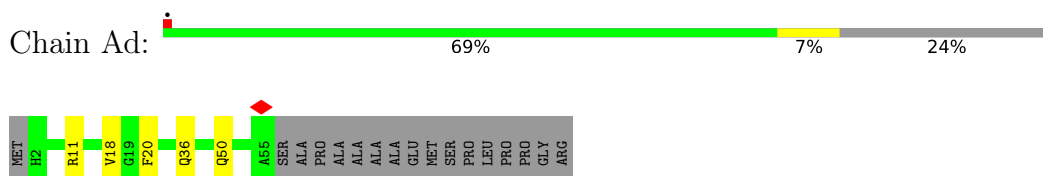
- Molecule 1: Light-harvesting protein



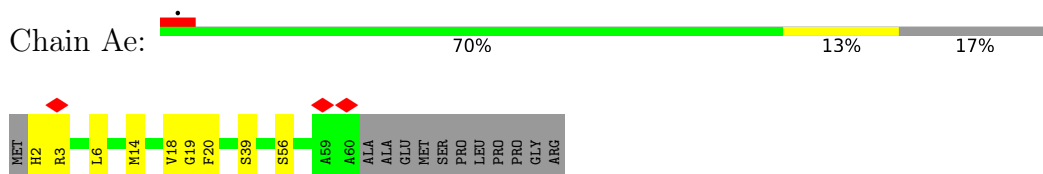
- Molecule 1: Light-harvesting protein



- Molecule 1: Light-harvesting protein



- Molecule 1: Light-harvesting protein



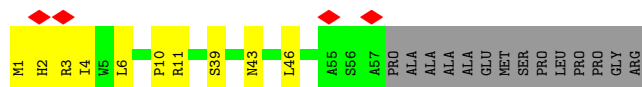
- Molecule 1: Light-harvesting protein

Chain Af:  65% 14% 21%



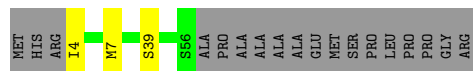
- Molecule 1: Light-harvesting protein

Chain Ag:  6% 66% 14% 20%



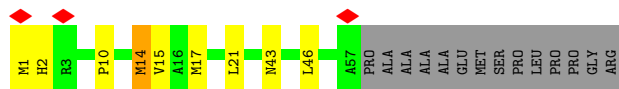
- Molecule 1: Light-harvesting protein

Chain Ah:  70% . 25%



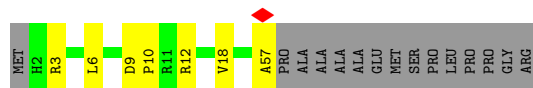
- Molecule 1: Light-harvesting protein

Chain Ai:  68% 11% . 20%




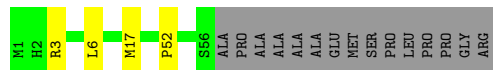
- Molecule 1: Light-harvesting protein

Chain Aj:  69% 10% 21%



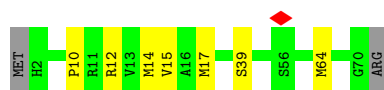
- Molecule 1: Light-harvesting protein

Chain Ak:  73% 6% 21%

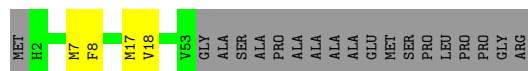


- Molecule 1: Light-harvesting protein

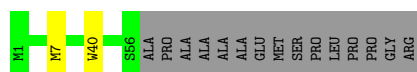
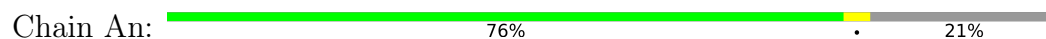
Chain Al:  87% 10% .



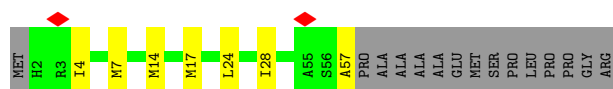
- Molecule 1: Light-harvesting protein



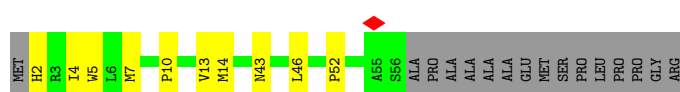
- Molecule 1: Light-harvesting protein



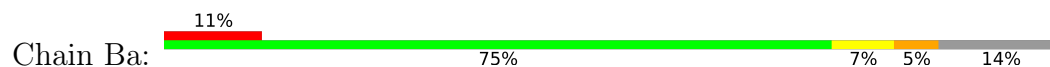
- Molecule 1: Light-harvesting protein



- Molecule 1: Light-harvesting protein




- Molecule 2: Light-harvesting protein



- Molecule 2: Light-harvesting protein




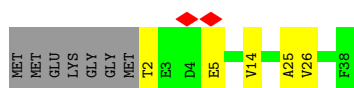
- Molecule 2: Light-harvesting protein

Chain Bc:  66% 20% 14%



- Molecule 2: Light-harvesting protein

Chain Bd:  5% 73% 11% 16%



- Molecule 2: Light-harvesting protein

Chain Be:  5% 68% 18% 14%




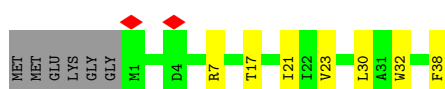
- Molecule 2: Light-harvesting protein

Chain Bf:  68% 9% 23%



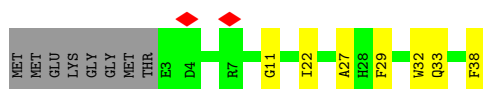
- Molecule 2: Light-harvesting protein

Chain Bg:  5% 70% 16% 14%



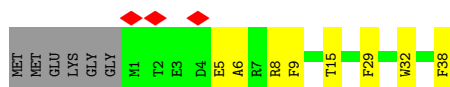
- Molecule 2: Light-harvesting protein

Chain Bh:  5% 66% 16% 18%

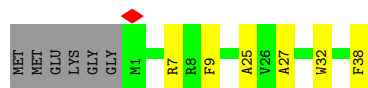
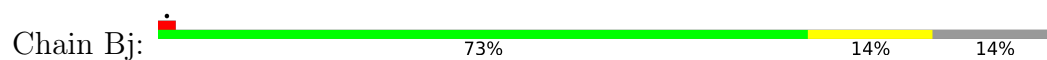


- Molecule 2: Light-harvesting protein

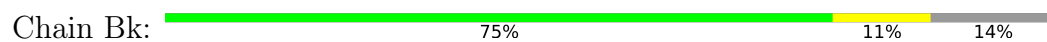
Chain Bi:  7% 68% 18% 14%



- Molecule 2: Light-harvesting protein



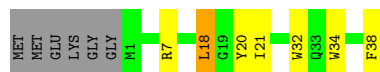
- Molecule 2: Light-harvesting protein



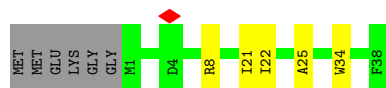
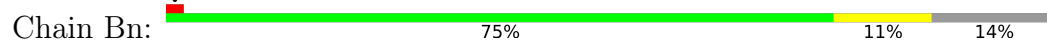
- Molecule 2: Light-harvesting protein



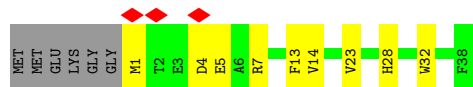
- Molecule 2: Light-harvesting protein



- Molecule 2: Light-harvesting protein

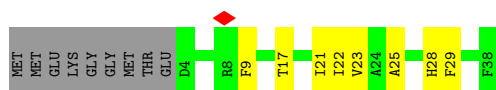


- Molecule 2: Light-harvesting protein



- Molecule 2: Light-harvesting protein





- Molecule 2: Light-harvesting protein

Chain BA: 84% 7% 9%



- Molecule 2: Light-harvesting protein

Chain BB: 5% 59% 23% 7% 11%



- Molecule 2: Light-harvesting protein

Chain BC: 68% 23% 9%



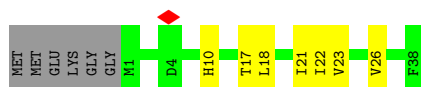
- Molecule 2: Light-harvesting protein

Chain BD: 80% 11% 9%



- Molecule 2: Light-harvesting protein

Chain BE: 70% 16% 14%



- Molecule 2: Light-harvesting protein

Chain BF: 59% 30% 11%




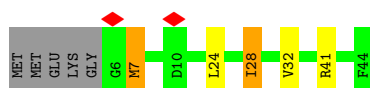
- Molecule 2: Light-harvesting protein

Chain BG:  68% 20% 11%




- Molecule 2: Light-harvesting protein

Chain BH:  5% 77% 7% 5% 11%




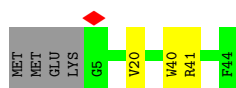
- Molecule 2: Light-harvesting protein

Chain BI:  77% 9% 14%



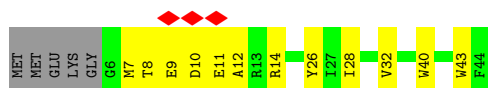
- Molecule 2: Light-harvesting protein

Chain BJ:  84% 7% 9%



- Molecule 2: Light-harvesting protein

Chain BK:  7% 61% 27% 11%




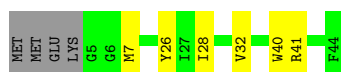
- Molecule 2: Light-harvesting protein

Chain BL:  66% 23% 11%




- Molecule 2: Light-harvesting protein

Chain BM:  77% 14% 9%



- Molecule 2: Light-harvesting protein

Chain BN:  66% 23% 11%



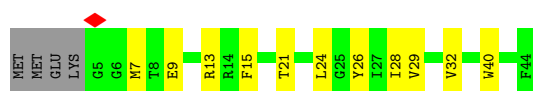
- Molecule 2: Light-harvesting protein

Chain BO:  70% 18% 11%




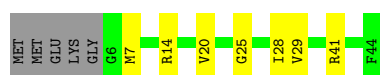
- Molecule 2: Light-harvesting protein

Chain BP:  66% 25% 9%



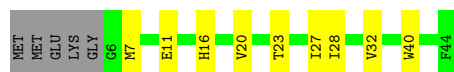
- Molecule 2: Light-harvesting protein

Chain BQ:  73% 16% 11%



- Molecule 2: Light-harvesting protein

Chain BR:  68% 20% 11%




- Molecule 2: Light-harvesting protein

Chain BS:  64% 25% 11%

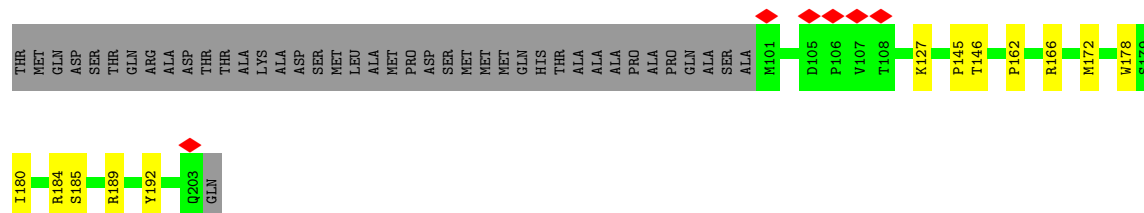
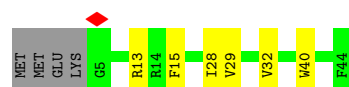
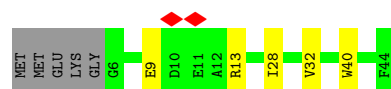



- Molecule 2: Light-harvesting protein

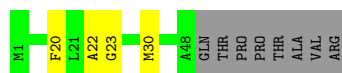
Chain BT:  70% 18% 11%



- Molecule 2: Light-harvesting protein



Chain AA:  79% 7% 14%



- Molecule 9: Light-harvesting protein

Chain AB:  68% 18% 14%



- Molecule 9: Light-harvesting protein

Chain AC:  71% 14% 14%




- Molecule 9: Light-harvesting protein

Chain AD:  66% 21% 12%



- Molecule 9: Light-harvesting protein

Chain AE:  73% 12% 12%



- Molecule 9: Light-harvesting protein

Chain AF:  71% 16% 12%



- Molecule 9: Light-harvesting protein

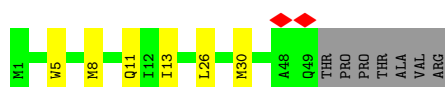
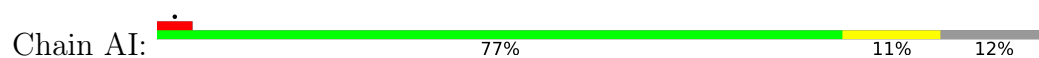
Chain AG:  5% 62% 25% 12%



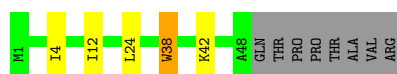
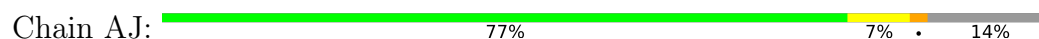
• Molecule 9: Light-harvesting protein



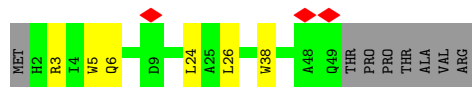
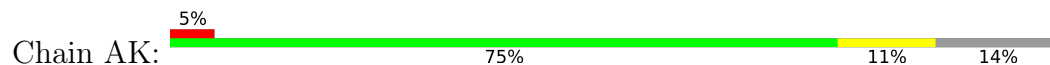
• Molecule 9: Light-harvesting protein



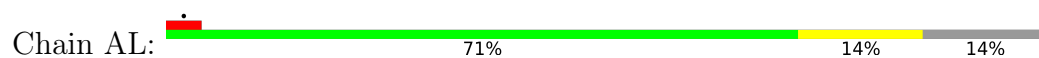
• Molecule 9: Light-harvesting protein



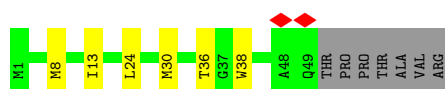
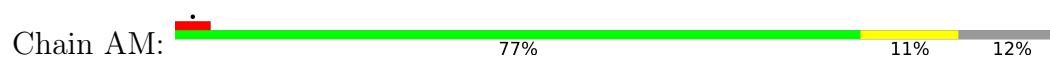
• Molecule 9: Light-harvesting protein



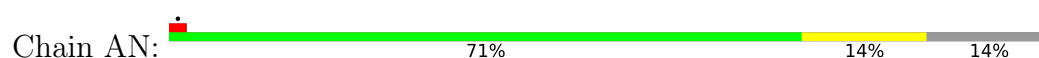
• Molecule 9: Light-harvesting protein



• Molecule 9: Light-harvesting protein

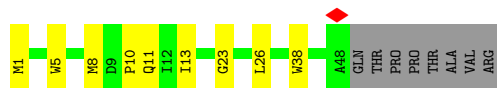


• Molecule 9: Light-harvesting protein





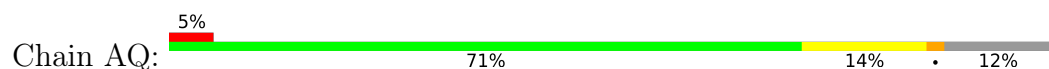
- Molecule 9: Light-harvesting protein



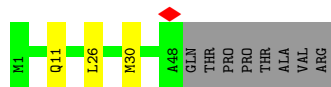
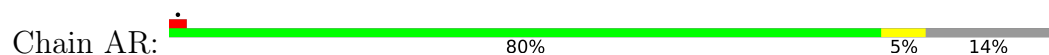
- Molecule 9: Light-harvesting protein



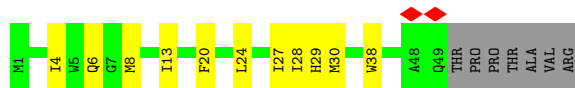
- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



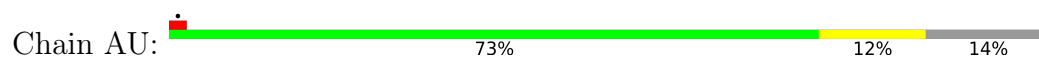
- Molecule 9: Light-harvesting protein



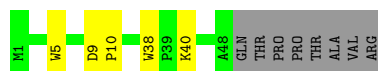
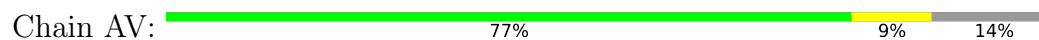
- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



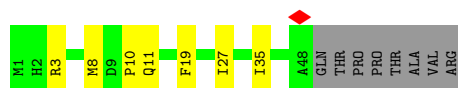
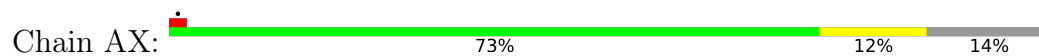
- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



- Molecule 9: Light-harvesting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129052	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF was performed within cryosparc	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.548	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0687	Depositor
Map size (\AA)	439.19998, 439.19998, 439.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.732, 0.732, 0.732	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V7N, LMT, MQ8, FE, BPH, PEX, CD4, HEC, CRT, BCL

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	0.15	0/535	0.33	0/731
1	Ab	0.15	0/448	0.23	0/609
1	Ac	0.16	0/451	0.30	0/612
1	Ad	0.16	0/437	0.28	0/594
1	Ae	0.15	0/466	0.24	0/635
1	Af	0.16	0/451	0.28	0/612
1	Ag	0.16	0/456	0.26	0/619
1	Ah	0.16	0/421	0.27	0/573
1	Ai	0.15	0/456	0.27	0/619
1	Aj	0.15	0/448	0.24	0/609
1	Ak	0.15	0/451	0.22	0/612
1	Al	0.18	0/535	0.34	0/731
1	Am	0.17	0/428	0.24	0/582
1	An	0.17	0/451	0.27	0/612
1	Ao	0.15	0/448	0.27	0/609
1	Ap	0.14	0/443	0.26	0/602
2	BA	0.13	0/346	0.24	0/471
2	BB	0.14	0/342	0.28	0/466
2	BC	0.13	0/346	0.24	0/471
2	BD	0.14	0/346	0.24	0/471
2	BE	0.15	0/338	0.26	0/461
2	BF	0.13	0/342	0.23	0/466
2	BG	0.17	0/342	0.38	0/466
2	BH	0.13	0/342	0.25	0/466
2	BI	0.15	0/338	0.32	0/461
2	BJ	0.13	0/346	0.22	0/471
2	BK	0.14	0/342	0.27	0/466
2	BL	0.14	0/342	0.21	0/466
2	BM	0.13	0/346	0.22	0/471
2	BN	0.20	0/342	0.36	0/466
2	BO	0.14	0/342	0.29	0/466
2	BP	0.15	0/346	0.30	0/471

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BQ	0.21	0/342	0.36	0/466
2	BR	0.14	0/342	0.24	0/466
2	BS	0.13	0/342	0.24	0/466
2	BT	0.16	0/342	0.30	0/466
2	BU	0.13	0/342	0.27	0/466
2	BV	0.15	0/355	0.34	0/482
2	BW	0.15	0/346	0.31	0/471
2	BX	0.14	0/346	0.30	0/471
2	Ba	0.15	0/338	0.23	0/461
2	Bb	0.20	0/338	0.35	0/461
2	Bc	0.18	0/338	0.29	0/461
2	Bd	0.16	0/330	0.22	0/451
2	Be	0.18	0/338	0.29	0/461
2	Bf	0.16	0/306	0.21	0/418
2	Bg	0.16	0/338	0.22	0/461
2	Bh	0.15	0/323	0.19	0/441
2	Bi	0.15	0/338	0.21	0/461
2	Bj	0.16	0/338	0.20	0/461
2	Bk	0.16	0/338	0.22	0/461
2	Bl	0.17	0/338	0.23	0/461
2	Bm	0.17	0/338	0.24	0/461
2	Bn	0.15	0/338	0.21	0/461
2	Bo	0.15	0/338	0.22	0/461
2	Bp	0.15	0/314	0.20	0/429
3	S	0.12	0/819	0.28	0/1112
4	L	0.15	0/2217	0.30	0/3031
5	M	0.18	0/2796	0.34	0/3821
6	H	0.14	0/529	0.27	0/716
7	K	0.14	0/1408	0.33	0/1925
8	C	0.18	0/2395	0.35	0/3268
9	AA	0.15	0/405	0.29	0/547
9	AB	0.17	0/405	0.36	0/547
9	AC	0.16	0/405	0.31	0/547
9	AD	0.16	0/414	0.33	0/559
9	AE	0.15	0/414	0.33	0/559
9	AF	0.16	0/414	0.30	0/559
9	AG	0.15	0/414	0.29	0/559
9	AH	0.16	0/414	0.36	0/559
9	AI	0.15	0/414	0.31	0/559
9	AJ	0.17	0/405	0.33	0/547
9	AK	0.16	0/406	0.32	0/549
9	AL	0.16	0/405	0.31	0/547
9	AM	0.15	0/414	0.29	0/559

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	AN	0.15	0/406	0.29	0/549
9	AO	0.14	0/405	0.30	0/547
9	AP	0.14	0/405	0.29	0/547
9	AQ	0.14	0/414	0.31	0/559
9	AR	0.14	0/405	0.28	0/547
9	AS	0.14	0/414	0.31	0/559
9	AT	0.14	0/406	0.31	0/549
9	AU	0.15	0/406	0.33	0/549
9	AV	0.15	0/405	0.30	0/547
9	AW	0.15	0/414	0.32	0/559
9	AX	0.17	0/405	0.38	0/547
All	All	0.16	0/40877	0.29	0/55591

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	520	0	532	3	0
1	Ab	437	0	450	5	0
1	Ac	440	0	457	7	0
1	Ad	426	0	440	2	0
1	Ae	454	0	467	5	0
1	Af	440	0	457	13	0
1	Ag	445	0	462	8	0
1	Ah	411	0	425	0	0
1	Ai	445	0	462	5	0
1	Aj	437	0	450	5	0
1	Ak	440	0	457	4	0
1	Al	520	0	532	6	0
1	Am	417	0	432	3	0
1	An	440	0	457	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ao	437	0	450	8	0
1	Ap	432	0	445	9	0
2	BA	332	0	308	3	0
2	BB	328	0	305	12	0
2	BC	332	0	308	6	0
2	BD	332	0	308	7	0
2	BE	324	0	305	5	0
2	BF	328	0	305	12	0
2	BG	328	0	305	10	0
2	BH	328	0	305	4	0
2	BI	324	0	305	3	0
2	BJ	332	0	308	3	0
2	BK	328	0	305	10	0
2	BL	328	0	305	8	0
2	BM	332	0	308	6	0
2	BN	328	0	305	9	0
2	BO	328	0	305	6	0
2	BP	332	0	308	12	0
2	BQ	328	0	305	7	0
2	BR	328	0	305	5	0
2	BS	328	0	305	8	0
2	BT	328	0	305	10	0
2	BU	328	0	305	4	0
2	BV	341	0	321	8	0
2	BW	332	0	308	6	0
2	BX	332	0	308	7	0
2	Ba	324	0	305	3	0
2	Bb	324	0	305	9	0
2	Bc	324	0	305	7	0
2	Bd	316	0	293	3	0
2	Be	324	0	305	9	0
2	Bf	292	0	276	4	0
2	Bg	324	0	305	8	0
2	Bh	309	0	286	5	0
2	Bi	324	0	305	5	0
2	Bj	324	0	305	5	0
2	Bk	324	0	305	5	0
2	Bl	324	0	305	6	0
2	Bm	324	0	305	8	0
2	Bn	324	0	305	5	0
2	Bo	324	0	305	13	0
2	Bp	300	0	278	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	800	0	793	9	0
4	L	2134	0	2107	26	0
5	M	2697	0	2621	34	0
6	H	510	0	500	4	0
7	K	1373	0	1347	12	0
8	C	2330	0	2254	28	0
9	AA	391	0	394	5	0
9	AB	391	0	394	11	0
9	AC	391	0	394	9	0
9	AD	400	0	402	12	0
9	AE	400	0	402	6	0
9	AF	400	0	402	7	0
9	AG	400	0	402	11	0
9	AH	400	0	402	10	0
9	AI	400	0	402	7	0
9	AJ	391	0	394	5	0
9	AK	392	0	390	8	0
9	AL	391	0	394	7	0
9	AM	400	0	402	7	0
9	AN	392	0	390	8	0
9	AO	391	0	394	8	0
9	AP	391	0	394	10	0
9	AQ	400	0	402	7	0
9	AR	391	0	394	2	0
9	AS	400	0	402	10	0
9	AT	392	0	389	11	0
9	AU	392	0	390	7	0
9	AV	391	0	394	6	0
9	AW	400	0	402	14	0
9	AX	391	0	393	7	0
10	AF	45	0	0	0	0
10	AL	45	0	0	0	0
10	Aa	45	0	0	0	0
10	An	45	0	0	0	0
10	BA	45	0	0	0	0
10	BB	45	0	0	0	0
10	BC	45	0	0	0	0
10	BD	45	0	0	0	0
10	BF	45	0	0	0	0
10	BG	45	0	0	0	0
10	BH	45	0	0	0	0
10	BI	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BJ	45	0	0	0	0
10	BK	45	0	0	0	0
10	BL	45	0	0	0	0
10	BN	45	0	0	0	0
10	BO	45	0	0	0	0
10	BP	45	0	0	0	0
10	BQ	45	0	0	0	0
10	BR	45	0	0	0	0
10	BS	45	0	0	1	0
10	BT	45	0	0	1	0
10	BU	45	0	0	0	0
10	BV	45	0	0	1	0
10	BW	45	0	0	0	0
10	BX	45	0	0	0	0
10	Bb	45	0	0	0	0
10	Bc	45	0	0	0	0
10	Bd	45	0	0	0	0
10	Be	45	0	0	0	0
10	Bf	45	0	0	0	0
10	Bg	45	0	0	0	0
10	Bh	45	0	0	0	0
10	Bi	45	0	0	0	0
10	Bj	45	0	0	0	0
10	Bk	45	0	0	0	0
10	Bl	45	0	0	0	0
10	Bm	45	0	0	0	0
10	Bn	45	0	0	0	0
10	Bp	45	0	0	0	0
11	AB	66	0	74	3	0
11	AC	66	0	74	2	0
11	AD	66	0	74	3	0
11	AE	66	0	74	4	0
11	AF	66	0	74	2	0
11	AG	66	0	74	1	0
11	AH	66	0	74	2	0
11	AI	132	0	142	5	0
11	AJ	132	0	146	3	0
11	AK	66	0	74	5	0
11	AL	66	0	74	3	0
11	AM	132	0	146	4	0
11	AN	66	0	74	3	0
11	AO	66	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AP	66	0	74	2	0
11	AQ	132	0	145	4	0
11	AR	66	0	74	6	0
11	AS	66	0	74	3	0
11	AT	132	0	147	10	0
11	AU	66	0	73	2	0
11	AV	66	0	74	5	0
11	AW	198	0	216	7	0
11	AX	66	0	74	4	0
11	Aa	66	0	74	0	0
11	Ab	66	0	74	2	0
11	Ac	66	0	74	2	0
11	Ad	66	0	74	1	0
11	Ae	66	0	74	4	0
11	Af	66	0	74	2	0
11	Ah	66	0	74	1	0
11	Ai	66	0	72	0	0
11	Aj	66	0	74	2	0
11	Ak	66	0	74	2	0
11	Al	66	0	74	9	0
11	Am	66	0	74	9	0
11	Ao	66	0	74	26	0
11	BA	132	0	147	6	0
11	BB	66	0	74	3	0
11	BC	66	0	74	2	0
11	BD	66	0	74	4	0
11	BE	66	0	74	1	0
11	BF	66	0	74	3	0
11	BG	66	0	74	2	0
11	BH	66	0	71	1	0
11	BI	66	0	74	5	0
11	BK	66	0	74	1	0
11	BL	66	0	74	1	0
11	BN	66	0	74	3	0
11	BO	66	0	74	1	0
11	BP	66	0	74	2	0
11	BR	66	0	74	0	0
11	BS	66	0	74	1	0
11	BU	66	0	74	1	0
11	BV	66	0	74	0	0
11	BX	66	0	74	4	0
11	Ba	66	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Bb	66	0	74	2	0
11	Bc	66	0	74	0	0
11	Bd	66	0	74	1	0
11	Be	66	0	74	3	0
11	Bf	66	0	74	1	0
11	Bg	66	0	74	1	0
11	Bh	66	0	74	1	0
11	Bi	66	0	74	1	0
11	Bj	66	0	74	3	0
11	Bk	66	0	74	1	0
11	Bl	66	0	74	4	0
11	Bm	66	0	74	3	0
11	Bn	66	0	74	2	0
11	Bo	66	0	74	3	0
11	Bp	132	0	148	12	0
11	L	132	0	148	3	0
11	M	132	0	147	3	0
12	AW	35	0	45	1	0
12	AX	35	0	42	2	0
12	Aa	35	0	46	0	0
12	Ad	35	0	45	2	0
12	Aj	35	0	46	0	0
12	BA	70	0	88	5	0
12	BB	35	0	45	2	0
12	BC	35	0	44	2	0
12	BD	35	0	45	1	0
12	BE	35	0	45	1	0
12	BF	35	0	45	2	0
12	BG	35	0	45	1	0
12	BH	70	0	87	3	0
12	BI	35	0	45	2	0
12	BK	70	0	90	1	0
12	BL	35	0	45	0	0
12	BM	35	0	45	2	0
12	BO	70	0	88	3	0
12	BQ	70	0	90	1	0
12	BR	35	0	45	1	0
12	BS	35	0	45	4	0
12	BU	70	0	90	0	0
12	BW	70	0	91	4	0
12	Ba	35	0	45	0	0
12	Bb	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Bc	35	0	44	1	0
12	Bd	35	0	45	1	0
12	Be	35	0	45	1	0
12	Bf	70	0	86	3	0
12	Bh	70	0	89	2	0
12	Bj	70	0	88	2	0
12	Bl	35	0	44	0	0
12	Bo	35	0	44	3	0
12	Bp	35	0	44	1	0
12	C	35	0	45	0	0
12	K	35	0	46	1	0
12	L	35	0	46	0	0
12	M	35	0	46	2	0
13	AA	35	0	49	4	0
13	AD	35	0	49	3	0
13	AE	35	0	49	2	0
13	AJ	35	0	48	1	0
13	AP	35	0	49	2	0
13	AS	35	0	49	2	0
13	AT	35	0	45	2	0
13	Aj	35	0	49	2	0
13	Ba	35	0	49	1	0
13	Bc	35	0	49	4	0
13	Be	70	0	98	6	0
13	Bg	35	0	49	1	0
13	Bh	35	0	49	1	0
13	Bk	35	0	49	1	0
13	Bm	35	0	49	2	0
13	Bn	35	0	46	3	0
14	Ad	53	0	72	9	0
14	L	53	0	72	6	0
14	M	53	0	70	4	0
15	Af	84	0	124	9	0
15	M	84	0	124	1	0
16	L	65	0	76	6	0
16	M	65	0	76	4	0
17	M	1	0	0	0	0
18	M	44	0	60	0	0
19	C	172	0	122	6	0
20	AC	1	0	0	0	0
20	Aa	2	0	0	0	0
20	Ac	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	Ae	1	0	0	0	0
20	Ag	1	0	0	0	0
20	Ak	1	0	0	0	0
20	Al	2	0	0	0	0
20	Am	3	0	0	0	0
20	An	1	0	0	0	0
20	BO	1	0	0	0	0
20	Bj	1	0	0	0	0
20	C	3	0	0	0	0
20	L	10	0	0	0	0
20	M	8	0	0	0	0
20	S	2	0	0	0	0
All	All	49808	0	48618	719	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 7.

The worst 5 of 719 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)
11:Ao:101:BCL:CED	2:Bo:23:VAL:HG12	1.84	1.08
11:Ao:101:BCL:HED3	2:Bo:23:VAL:HG12	1.46	0.97
11:Ao:101:BCL:H122	11:Ao:101:BCL:H91	1.56	0.86
11:Ao:101:BCL:HED1	2:Bo:23:VAL:HG12	1.56	0.86
11:Ao:101:BCL:H91	11:Ao:101:BCL:C14	2.09	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	67/71 (94%)	64 (96%)	3 (4%)	0	100	100
1	Ab	54/71 (76%)	54 (100%)	0	0	100	100
1	Ac	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
1	Ad	52/71 (73%)	52 (100%)	0	0	100	100
1	Ae	57/71 (80%)	57 (100%)	0	0	100	100
1	Af	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
1	Ag	55/71 (78%)	55 (100%)	0	0	100	100
1	Ah	51/71 (72%)	49 (96%)	2 (4%)	0	100	100
1	Ai	55/71 (78%)	55 (100%)	0	0	100	100
1	Aj	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
1	Ak	54/71 (76%)	54 (100%)	0	0	100	100
1	Al	67/71 (94%)	62 (92%)	5 (8%)	0	100	100
1	Am	50/71 (70%)	50 (100%)	0	0	100	100
1	An	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
1	Ao	54/71 (76%)	54 (100%)	0	0	100	100
1	Ap	53/71 (75%)	53 (100%)	0	0	100	100
2	BA	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	BB	37/44 (84%)	37 (100%)	0	0	100	100
2	BC	38/44 (86%)	38 (100%)	0	0	100	100
2	BD	38/44 (86%)	35 (92%)	3 (8%)	0	100	100
2	BE	36/44 (82%)	36 (100%)	0	0	100	100
2	BF	37/44 (84%)	37 (100%)	0	0	100	100
2	BG	37/44 (84%)	37 (100%)	0	0	100	100
2	BH	37/44 (84%)	37 (100%)	0	0	100	100
2	BI	36/44 (82%)	36 (100%)	0	0	100	100
2	BJ	38/44 (86%)	35 (92%)	3 (8%)	0	100	100
2	BK	37/44 (84%)	37 (100%)	0	0	100	100
2	BL	37/44 (84%)	37 (100%)	0	0	100	100
2	BM	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	BN	37/44 (84%)	36 (97%)	1 (3%)	0	100	100
2	BO	37/44 (84%)	37 (100%)	0	0	100	100
2	BP	38/44 (86%)	38 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BQ	37/44 (84%)	37 (100%)	0	0	100	100
2	BR	37/44 (84%)	37 (100%)	0	0	100	100
2	BS	37/44 (84%)	37 (100%)	0	0	100	100
2	BT	37/44 (84%)	35 (95%)	2 (5%)	0	100	100
2	BU	37/44 (84%)	37 (100%)	0	0	100	100
2	BV	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
2	BW	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	BX	38/44 (86%)	36 (95%)	2 (5%)	0	100	100
2	Ba	36/44 (82%)	36 (100%)	0	0	100	100
2	Bb	36/44 (82%)	35 (97%)	1 (3%)	0	100	100
2	Bc	36/44 (82%)	36 (100%)	0	0	100	100
2	Bd	35/44 (80%)	35 (100%)	0	0	100	100
2	Be	36/44 (82%)	36 (100%)	0	0	100	100
2	Bf	32/44 (73%)	32 (100%)	0	0	100	100
2	Bg	36/44 (82%)	36 (100%)	0	0	100	100
2	Bh	34/44 (77%)	34 (100%)	0	0	100	100
2	Bi	36/44 (82%)	36 (100%)	0	0	100	100
2	Bj	36/44 (82%)	36 (100%)	0	0	100	100
2	Bk	36/44 (82%)	36 (100%)	0	0	100	100
2	Bl	36/44 (82%)	36 (100%)	0	0	100	100
2	Bm	36/44 (82%)	36 (100%)	0	0	100	100
2	Bn	36/44 (82%)	36 (100%)	0	0	100	100
2	Bo	36/44 (82%)	36 (100%)	0	0	100	100
2	Bp	33/44 (75%)	33 (100%)	0	0	100	100
3	S	101/204 (50%)	99 (98%)	2 (2%)	0	100	100
4	L	269/274 (98%)	262 (97%)	7 (3%)	0	100	100
5	M	333/392 (85%)	327 (98%)	6 (2%)	0	100	100
6	H	58/60 (97%)	58 (100%)	0	0	100	100
7	K	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
8	C	296/373 (79%)	287 (97%)	9 (3%)	0	100	100
9	AA	46/56 (82%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AB	46/56 (82%)	46 (100%)	0	0	100	100
9	AC	46/56 (82%)	46 (100%)	0	0	100	100
9	AD	47/56 (84%)	47 (100%)	0	0	100	100
9	AE	47/56 (84%)	47 (100%)	0	0	100	100
9	AF	47/56 (84%)	47 (100%)	0	0	100	100
9	AG	47/56 (84%)	47 (100%)	0	0	100	100
9	AH	47/56 (84%)	47 (100%)	0	0	100	100
9	AI	47/56 (84%)	47 (100%)	0	0	100	100
9	AJ	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
9	AK	46/56 (82%)	46 (100%)	0	0	100	100
9	AL	46/56 (82%)	46 (100%)	0	0	100	100
9	AM	47/56 (84%)	47 (100%)	0	0	100	100
9	AN	46/56 (82%)	46 (100%)	0	0	100	100
9	AO	46/56 (82%)	46 (100%)	0	0	100	100
9	AP	46/56 (82%)	46 (100%)	0	0	100	100
9	AQ	47/56 (84%)	47 (100%)	0	0	100	100
9	AR	46/56 (82%)	46 (100%)	0	0	100	100
9	AS	47/56 (84%)	47 (100%)	0	0	100	100
9	AT	46/56 (82%)	46 (100%)	0	0	100	100
9	AU	46/56 (82%)	46 (100%)	0	0	100	100
9	AV	46/56 (82%)	46 (100%)	0	0	100	100
9	AW	47/56 (84%)	47 (100%)	0	0	100	100
9	AX	46/56 (82%)	45 (98%)	1 (2%)	0	100	100
All	All	4695/5722 (82%)	4623 (98%)	72 (2%)	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	53/55 (96%)	52 (98%)	1 (2%)	52	69
1	Ab	45/55 (82%)	43 (96%)	2 (4%)	24	35
1	Ac	46/55 (84%)	45 (98%)	1 (2%)	47	65
1	Ad	44/55 (80%)	41 (93%)	3 (7%)	13	18
1	Ae	46/55 (84%)	43 (94%)	3 (6%)	14	20
1	Af	46/55 (84%)	46 (100%)	0	100	100
1	Ag	46/55 (84%)	45 (98%)	1 (2%)	47	65
1	Ah	43/55 (78%)	40 (93%)	3 (7%)	12	17
1	Ai	46/55 (84%)	43 (94%)	3 (6%)	14	20
1	Aj	45/55 (82%)	44 (98%)	1 (2%)	47	65
1	Ak	46/55 (84%)	46 (100%)	0	100	100
1	Al	53/55 (96%)	52 (98%)	1 (2%)	52	69
1	Am	44/55 (80%)	43 (98%)	1 (2%)	45	63
1	An	46/55 (84%)	45 (98%)	1 (2%)	47	65
1	Ao	45/55 (82%)	45 (100%)	0	100	100
1	Ap	45/55 (82%)	44 (98%)	1 (2%)	47	65
2	BA	30/34 (88%)	30 (100%)	0	100	100
2	BB	30/34 (88%)	27 (90%)	3 (10%)	6	8
2	BC	30/34 (88%)	28 (93%)	2 (7%)	13	19
2	BD	30/34 (88%)	30 (100%)	0	100	100
2	BE	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	BF	30/34 (88%)	30 (100%)	0	100	100
2	BG	30/34 (88%)	30 (100%)	0	100	100
2	BH	30/34 (88%)	28 (93%)	2 (7%)	13	19
2	BI	30/34 (88%)	30 (100%)	0	100	100
2	BJ	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	BK	30/34 (88%)	30 (100%)	0	100	100
2	BL	30/34 (88%)	30 (100%)	0	100	100
2	BM	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	BN	30/34 (88%)	30 (100%)	0	100	100
2	BO	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	BP	30/34 (88%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BQ	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	BR	30/34 (88%)	30 (100%)	0	100	100
2	BS	30/34 (88%)	28 (93%)	2 (7%)	13	19
2	BT	30/34 (88%)	30 (100%)	0	100	100
2	BU	30/34 (88%)	30 (100%)	0	100	100
2	BV	31/34 (91%)	31 (100%)	0	100	100
2	BW	30/34 (88%)	30 (100%)	0	100	100
2	BX	30/34 (88%)	30 (100%)	0	100	100
2	Ba	30/34 (88%)	28 (93%)	2 (7%)	13	19
2	Bb	30/34 (88%)	30 (100%)	0	100	100
2	Bc	30/34 (88%)	30 (100%)	0	100	100
2	Bd	29/34 (85%)	28 (97%)	1 (3%)	32	47
2	Be	30/34 (88%)	30 (100%)	0	100	100
2	Bf	26/34 (76%)	26 (100%)	0	100	100
2	Bg	30/34 (88%)	30 (100%)	0	100	100
2	Bh	28/34 (82%)	28 (100%)	0	100	100
2	Bi	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	Bj	30/34 (88%)	30 (100%)	0	100	100
2	Bk	30/34 (88%)	30 (100%)	0	100	100
2	Bl	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	Bm	30/34 (88%)	29 (97%)	1 (3%)	33	48
2	Bn	30/34 (88%)	30 (100%)	0	100	100
2	Bo	30/34 (88%)	30 (100%)	0	100	100
2	Bp	27/34 (79%)	27 (100%)	0	100	100
3	S	84/158 (53%)	84 (100%)	0	100	100
4	L	213/216 (99%)	210 (99%)	3 (1%)	62	77
5	M	272/311 (88%)	266 (98%)	6 (2%)	47	65
6	H	51/51 (100%)	50 (98%)	1 (2%)	50	68
7	K	146/146 (100%)	139 (95%)	7 (5%)	21	32
8	C	251/302 (83%)	247 (98%)	4 (2%)	58	74
9	AA	38/45 (84%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AB	38/45 (84%)	38 (100%)	0	100	100
9	AC	38/45 (84%)	38 (100%)	0	100	100
9	AD	39/45 (87%)	39 (100%)	0	100	100
9	AE	39/45 (87%)	34 (87%)	5 (13%)	3	4
9	AF	39/45 (87%)	37 (95%)	2 (5%)	20	29
9	AG	39/45 (87%)	39 (100%)	0	100	100
9	AH	39/45 (87%)	38 (97%)	1 (3%)	41	58
9	AI	39/45 (87%)	39 (100%)	0	100	100
9	AJ	38/45 (84%)	37 (97%)	1 (3%)	41	58
9	AK	38/45 (84%)	38 (100%)	0	100	100
9	AL	38/45 (84%)	37 (97%)	1 (3%)	41	58
9	AM	39/45 (87%)	39 (100%)	0	100	100
9	AN	38/45 (84%)	38 (100%)	0	100	100
9	AO	38/45 (84%)	37 (97%)	1 (3%)	41	58
9	AP	38/45 (84%)	37 (97%)	1 (3%)	41	58
9	AQ	39/45 (87%)	38 (97%)	1 (3%)	41	58
9	AR	38/45 (84%)	38 (100%)	0	100	100
9	AS	39/45 (87%)	38 (97%)	1 (3%)	41	58
9	AT	38/45 (84%)	37 (97%)	1 (3%)	41	58
9	AU	38/45 (84%)	38 (100%)	0	100	100
9	AV	38/45 (84%)	38 (100%)	0	100	100
9	AW	39/45 (87%)	39 (100%)	0	100	100
9	AX	38/45 (84%)	37 (97%)	1 (3%)	41	58
All	All	3869/4504 (86%)	3790 (98%)	79 (2%)	50	68

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	AE	30	MET
9	AP	4	ILE
2	BE	26	VAL
9	AJ	38	TRP
2	BS	32	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
8	C	260	GLN
9	AU	49	GLN
9	AD	49	GLN
9	AO	45	GLN
9	AC	2	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 202 ligands modelled in this entry, 1 is monoatomic - leaving 201 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	$\# Z > 2$
10	V7N	BG	101	-	43,44,44	1.99	10 (23%)	44,54,54	1.63	9 (20%)
14	MQ8	Ad	103	-	54,54,54	0.30	0	66,69,69	0.56	1 (1%)
10	V7N	Bf	1202	-	43,44,44	1.97	9 (20%)	44,54,54	1.69	10 (22%)
10	V7N	BO	102	-	43,44,44	2.00	10 (23%)	44,54,54	1.62	10 (22%)
11	BCL	AN	101	-	64,74,74	1.25	5 (7%)	78,115,115	1.50	10 (12%)
12	LMT	BO	101	-	36,36,36	1.19	6 (16%)	47,47,47	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AJ	1102	-	64,74,74	1.25	4 (6%)	78,115,115	1.50	9 (11%)
18	CRT	M	407	-	41,43,43	0.39	0	50,54,54	0.81	1 (2%)
11	BCL	AU	1001	13	64,74,74	1.26	5 (7%)	78,115,115	1.52	11 (14%)
12	LMT	Be	1102	-	36,36,36	1.17	5 (13%)	47,47,47	1.08	3 (6%)
13	PEX	Ba	1101	-	34,34,34	0.55	0	37,39,39	0.51	0
10	V7N	BS	103	-	43,44,44	2.04	9 (20%)	44,54,54	1.66	8 (18%)
10	V7N	BN	102	-	43,44,44	1.98	10 (23%)	44,54,54	1.58	9 (20%)
10	V7N	BU	104	-	43,44,44	1.96	10 (23%)	44,54,54	1.56	8 (18%)
11	BCL	AE	1102	-	64,74,74	1.25	5 (7%)	78,115,115	1.51	12 (15%)
11	BCL	AJ	1103	-	64,74,74	1.27	5 (7%)	78,115,115	1.58	12 (15%)
11	BCL	AT	1103	-	64,74,74	1.26	5 (7%)	78,115,115	1.48	10 (12%)
11	BCL	AO	101	12	64,74,74	1.24	5 (7%)	78,115,115	1.50	12 (15%)
12	LMT	BD	102	-	36,36,36	1.17	5 (13%)	47,47,47	1.07	2 (4%)
13	PEX	Bm	102	-	34,34,34	0.55	0	37,39,39	0.50	0
12	LMT	Bf	1203	-	36,36,36	1.19	5 (13%)	47,47,47	1.00	3 (6%)
10	V7N	BX	101	-	43,44,44	2.03	10 (23%)	44,54,54	1.55	9 (20%)
10	V7N	BF	103	-	43,44,44	2.00	10 (23%)	44,54,54	1.61	9 (20%)
19	HEC	C	402	8	32,50,50	2.21	4 (12%)	24,82,82	1.49	3 (12%)
11	BCL	Aj	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.58	11 (14%)
11	BCL	AK	101	-	64,74,74	1.28	5 (7%)	78,115,115	1.57	12 (15%)
12	LMT	BA	105	-	36,36,36	1.19	6 (16%)	47,47,47	1.08	2 (4%)
10	V7N	Bj	1202	-	43,44,44	2.00	10 (23%)	44,54,54	1.52	9 (20%)
13	PEX	Bh	1203	-	34,34,34	0.54	0	37,39,39	0.60	1 (2%)
11	BCL	Ae	101	-	64,74,74	1.28	7 (10%)	78,115,115	1.61	13 (16%)
10	V7N	BB	102	-	43,44,44	2.00	10 (23%)	44,54,54	1.56	9 (20%)
12	LMT	BK	101	-	36,36,36	1.16	5 (13%)	47,47,47	1.08	2 (4%)
13	PEX	Bk	102	-	34,34,34	0.56	0	37,39,39	0.50	0
12	LMT	BH	101	11	36,36,36	1.17	5 (13%)	47,47,47	1.02	3 (6%)
13	PEX	Be	1101	-	34,34,34	0.54	0	37,39,39	0.51	0
11	BCL	BU	102	-	64,74,74	1.25	4 (6%)	78,115,115	1.52	11 (14%)
11	BCL	BX	102	-	64,74,74	1.24	4 (6%)	78,115,115	1.64	14 (17%)
10	V7N	Bg	101	-	43,44,44	2.00	10 (23%)	44,54,54	1.65	9 (20%)
11	BCL	Ak	101	-	64,74,74	1.28	5 (7%)	78,115,115	1.50	9 (11%)
12	LMT	Ad	102	-	36,36,36	1.17	6 (16%)	47,47,47	1.03	2 (4%)
11	BCL	BL	102	-	64,74,74	1.25	6 (9%)	78,115,115	1.47	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	BR	101	-	64,74,74	1.23	4 (6%)	78,115,115	1.58	10 (12%)
12	LMT	BH	103	-	36,36,36	1.18	5 (13%)	47,47,47	0.94	1 (2%)
11	BCL	Ab	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.51	11 (14%)
11	BCL	AC	101	-	64,74,74	1.25	6 (9%)	78,115,115	1.52	9 (11%)
12	LMT	AW	1201	-	36,36,36	1.15	6 (16%)	47,47,47	1.08	4 (8%)
11	BCL	Bd	1203	-	64,74,74	1.26	4 (6%)	78,115,115	1.60	15 (19%)
11	BCL	AG	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.44	9 (11%)
10	V7N	Bc	1202	-	43,44,44	1.99	10 (23%)	44,54,54	1.67	10 (22%)
11	BCL	AW	1202	-	64,74,74	1.28	6 (9%)	78,115,115	1.61	13 (16%)
11	BCL	BP	101	-	64,74,74	1.25	4 (6%)	78,115,115	1.58	11 (14%)
12	LMT	BA	104	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	2 (4%)
12	LMT	BC	102	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	1 (2%)
12	LMT	Bf	1201	-	36,36,36	1.21	6 (16%)	47,47,47	0.93	1 (2%)
11	BCL	Bn	103	-	64,74,74	1.27	4 (6%)	78,115,115	1.55	13 (16%)
10	V7N	BW	102	-	43,44,44	2.01	10 (23%)	44,54,54	1.58	9 (20%)
10	V7N	Bn	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.53	8 (18%)
11	BCL	Ah	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.50	10 (12%)
10	V7N	Aa	101	-	43,44,44	2.01	10 (23%)	44,54,54	1.60	11 (25%)
12	LMT	Aj	102	-	36,36,36	1.13	5 (13%)	47,47,47	1.09	2 (4%)
10	V7N	Bd	1202	-	43,44,44	1.97	9 (20%)	44,54,54	1.59	9 (20%)
10	V7N	BT	101	-	43,44,44	2.00	10 (23%)	44,54,54	1.54	8 (18%)
11	BCL	Am	101	-	64,74,74	1.65	12 (18%)	78,115,115	2.35	21 (26%)
11	BCL	Bh	1205	-	64,74,74	1.27	5 (7%)	78,115,115	1.57	13 (16%)
12	LMT	BG	103	-	36,36,36	1.18	6 (16%)	47,47,47	0.93	2 (4%)
11	BCL	Af	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.52	11 (14%)
11	BCL	BK	102	-	64,74,74	1.26	4 (6%)	78,115,115	1.60	13 (16%)
11	BCL	BD	101	-	64,74,74	1.27	4 (6%)	78,115,115	1.55	13 (16%)
12	LMT	BQ	102	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	2 (4%)
12	LMT	Bb	1201	-	36,36,36	1.17	5 (13%)	47,47,47	1.01	1 (2%)
11	BCL	Bl	1203	-	64,74,74	1.25	6 (9%)	78,115,115	1.55	13 (16%)
19	HEC	C	404	8	32,50,50	2.11	3 (9%)	24,82,82	1.77	6 (25%)
10	V7N	An	101	-	43,44,44	2.02	9 (20%)	44,54,54	1.56	10 (22%)
13	PEX	AA	1101	-	34,34,34	0.54	0	37,39,39	0.53	0
11	BCL	BG	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.52	13 (16%)
11	BCL	Al	101	-	64,74,74	1.63	14 (21%)	78,115,115	2.41	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AT	1102	-	64,74,74	1.25	7 (10%)	78,115,115	1.52	14 (17%)
19	HEC	C	405	8	32,50,50	2.11	3 (9%)	24,82,82	1.43	2 (8%)
12	LMT	BE	102	-	36,36,36	1.17	5 (13%)	47,47,47	0.94	0
11	BCL	L	301	-	64,74,74	1.22	6 (9%)	78,115,115	1.51	11 (14%)
11	BCL	L	302	-	64,74,74	1.25	6 (9%)	78,115,115	1.49	9 (11%)
11	BCL	AD	1102	-	64,74,74	1.26	4 (6%)	78,115,115	1.47	9 (11%)
12	LMT	BW	101	-	36,36,36	1.21	6 (16%)	47,47,47	1.09	1 (2%)
10	V7N	BC	103	-	43,44,44	1.97	9 (20%)	44,54,54	1.61	10 (22%)
11	BCL	Bb	1203	-	64,74,74	1.26	6 (9%)	78,115,115	1.43	9 (11%)
12	LMT	Bh	1201	-	36,36,36	1.19	6 (16%)	47,47,47	1.01	2 (4%)
13	PEX	AS	1101	-	34,34,34	0.55	0	37,39,39	0.47	0
11	BCL	AH	101	-	64,74,74	1.28	5 (7%)	78,115,115	1.49	10 (12%)
11	BCL	Bg	103	-	64,74,74	1.27	5 (7%)	78,115,115	1.54	10 (12%)
12	LMT	C	401	-	36,36,36	1.16	5 (13%)	47,47,47	1.01	2 (4%)
11	BCL	AV	1001	-	64,74,74	1.25	6 (9%)	78,115,115	1.53	11 (14%)
11	BCL	BS	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.48	12 (15%)
10	V7N	Bp	1202	-	43,44,44	1.99	9 (20%)	44,54,54	1.59	8 (18%)
11	BCL	BC	101	-	64,74,74	1.26	5 (7%)	78,115,115	1.62	12 (15%)
10	V7N	BH	102	-	43,44,44	1.96	9 (20%)	44,54,54	1.59	8 (18%)
10	V7N	BD	103	-	43,44,44	1.98	9 (20%)	44,54,54	1.56	8 (18%)
11	BCL	M	405	-	64,74,74	1.23	6 (9%)	78,115,115	1.53	10 (12%)
12	LMT	BO	104	11	36,36,36	1.14	6 (16%)	47,47,47	0.87	0
14	MQ8	L	305	-	54,54,54	0.38	1 (1%)	66,69,69	0.57	1 (1%)
15	CD4	Af	102	-	83,83,83	0.41	1 (1%)	89,95,95	0.39	0
11	BCL	Ai	101	-	64,74,74	1.28	5 (7%)	78,115,115	1.50	11 (14%)
11	BCL	AS	1102	-	64,74,74	1.25	6 (9%)	78,115,115	1.65	15 (19%)
12	LMT	Bh	1204	-	36,36,36	1.16	5 (13%)	47,47,47	0.98	2 (4%)
10	V7N	BQ	103	-	43,44,44	2.00	10 (23%)	44,54,54	1.59	8 (18%)
11	BCL	BB	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.67	15 (19%)
13	PEX	Aj	103	-	34,34,34	0.55	0	37,39,39	0.54	0
10	V7N	Bh	1202	-	43,44,44	1.96	10 (23%)	44,54,54	1.61	8 (18%)
12	LMT	BI	103	-	36,36,36	1.18	6 (16%)	47,47,47	0.98	2 (4%)
10	V7N	BL	101	-	43,44,44	2.00	10 (23%)	44,54,54	1.58	9 (20%)
11	BCL	AF	102	-	64,74,74	1.23	5 (7%)	78,115,115	1.52	10 (12%)
12	LMT	Bp	1201	-	36,36,36	1.19	6 (16%)	47,47,47	0.99	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AI	102	13	64,74,74	1.25	5 (7%)	78,115,115	1.49	9 (11%)
11	BCL	Ao	101	-	64,74,74	1.64	13 (20%)	78,115,115	2.24	19 (24%)
11	BCL	BF	101	-	64,74,74	1.26	4 (6%)	78,115,115	1.57	13 (16%)
11	BCL	AW	1203	-	64,74,74	1.28	5 (7%)	78,115,115	1.52	10 (12%)
13	PEX	AJ	1101	11	34,34,34	0.54	0	37,39,39	0.56	0
12	LMT	BL	103	-	36,36,36	1.18	5 (13%)	47,47,47	1.01	1 (2%)
11	BCL	BO	103	-	64,74,74	1.25	5 (7%)	78,115,115	1.57	11 (14%)
16	BPH	L	303	-	51,70,70	0.88	1 (1%)	52,101,101	0.95	4 (7%)
11	BCL	BH	104	12	64,74,74	1.23	4 (6%)	78,115,115	1.62	13 (16%)
12	LMT	Bj	1203	-	36,36,36	1.18	5 (13%)	47,47,47	0.98	2 (4%)
13	PEX	Bn	102	11	34,34,34	0.55	0	37,39,39	0.48	0
12	LMT	BU	101	-	36,36,36	1.19	5 (13%)	47,47,47	1.04	1 (2%)
12	LMT	Bd	1201	-	36,36,36	1.18	5 (13%)	47,47,47	0.88	0
12	LMT	BQ	101	-	36,36,36	1.16	5 (13%)	47,47,47	1.01	2 (4%)
11	BCL	AB	101	-	64,74,74	1.29	5 (7%)	78,115,115	1.50	11 (14%)
11	BCL	BA	101	-	64,74,74	1.28	6 (9%)	78,115,115	4.91	15 (19%)
10	V7N	AL	102	-	43,44,44	1.96	9 (20%)	44,54,54	1.58	8 (18%)
11	BCL	BI	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.58	13 (16%)
11	BCL	Aa	102	-	64,74,74	1.28	6 (9%)	78,115,115	1.54	10 (12%)
13	PEX	AP	1101	-	34,34,34	0.53	0	37,39,39	0.53	0
11	BCL	Bm	103	-	64,74,74	1.28	5 (7%)	78,115,115	1.59	13 (16%)
10	V7N	Bm	101	-	43,44,44	2.01	9 (20%)	44,54,54	1.57	11 (25%)
11	BCL	BN	101	-	64,74,74	1.27	4 (6%)	78,115,115	1.52	11 (14%)
10	V7N	Bb	1202	-	43,44,44	1.97	10 (23%)	44,54,54	1.59	9 (20%)
10	V7N	Be	1103	-	43,44,44	2.02	9 (20%)	44,54,54	1.62	10 (22%)
12	LMT	Aa	103	-	36,36,36	1.15	5 (13%)	47,47,47	0.91	1 (2%)
12	LMT	L	304	-	36,36,36	1.13	5 (13%)	47,47,47	1.05	2 (4%)
11	BCL	AM	102	-	64,74,74	1.26	6 (9%)	78,115,115	1.54	13 (16%)
12	LMT	Bl	1201	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
10	V7N	BV	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.66	10 (22%)
11	BCL	M	404	-	64,74,74	1.25	6 (9%)	78,115,115	1.53	9 (11%)
11	BCL	Bj	1204	-	64,74,74	1.24	6 (9%)	78,115,115	1.58	12 (15%)
11	BCL	Ad	101	-	64,74,74	1.28	6 (9%)	78,115,115	1.50	10 (12%)
11	BCL	AR	101	-	64,74,74	1.24	5 (7%)	78,115,115	1.54	10 (12%)
11	BCL	BV	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.49	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AM	101	-	64,74,74	1.28	5 (7%)	78,115,115	1.45	10 (12%)
10	V7N	AF	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.64	11 (25%)
11	BCL	AQ	102	-	64,74,74	1.28	7 (10%)	78,115,115	1.47	12 (15%)
11	BCL	AX	1202	-	64,74,74	1.24	5 (7%)	78,115,115	1.58	11 (14%)
11	BCL	Bi	102	-	64,74,74	1.25	5 (7%)	78,115,115	1.46	10 (12%)
11	BCL	Bk	103	-	64,74,74	1.26	5 (7%)	78,115,115	3.75	14 (17%)
10	V7N	Bk	101	-	43,44,44	1.97	10 (23%)	44,54,54	1.57	8 (18%)
11	BCL	AQ	101	-	64,74,74	1.28	6 (9%)	78,115,115	1.53	10 (12%)
12	LMT	BK	103	-	36,36,36	1.20	6 (16%)	47,47,47	1.13	3 (6%)
12	LMT	AX	1201	-	36,36,36	1.14	5 (13%)	47,47,47	1.22	4 (8%)
12	LMT	BR	102	-	36,36,36	1.18	5 (13%)	47,47,47	0.96	2 (4%)
12	LMT	BW	103	-	36,36,36	1.16	6 (16%)	47,47,47	1.03	3 (6%)
15	CD4	M	403	-	83,83,83	0.37	0	89,95,95	0.36	0
11	BCL	Bf	1204	-	64,74,74	1.25	5 (7%)	78,115,115	1.47	10 (12%)
13	PEX	Bg	102	-	34,34,34	0.54	0	37,39,39	0.51	0
11	BCL	Bc	1204	-	64,74,74	1.27	5 (7%)	78,115,115	1.60	12 (15%)
11	BCL	AI	101	-	64,74,74	1.25	5 (7%)	78,115,115	1.52	11 (14%)
12	LMT	BU	103	-	36,36,36	1.16	5 (13%)	47,47,47	1.05	2 (4%)
10	V7N	BI	101	-	43,44,44	1.99	10 (23%)	44,54,54	1.63	9 (20%)
10	V7N	BJ	101	-	43,44,44	1.95	9 (20%)	44,54,54	1.65	11 (25%)
13	PEX	AE	1101	-	34,34,34	0.54	0	37,39,39	0.57	0
10	V7N	Bi	101	-	43,44,44	2.02	9 (20%)	44,54,54	1.61	9 (20%)
13	PEX	AT	1101	-	34,34,34	0.55	0	37,39,39	0.51	0
12	LMT	BB	103	-	36,36,36	1.17	6 (16%)	47,47,47	1.07	2 (4%)
10	V7N	BK	104	-	43,44,44	1.99	10 (23%)	44,54,54	1.60	8 (18%)
11	BCL	Bo	1202	-	64,74,74	1.26	5 (7%)	78,115,115	1.49	9 (11%)
12	LMT	BS	102	-	36,36,36	1.17	6 (16%)	47,47,47	0.95	2 (4%)
10	V7N	BR	103	-	43,44,44	2.00	10 (23%)	44,54,54	1.63	10 (22%)
11	BCL	Bp	1203	-	64,74,74	1.65	12 (18%)	78,115,115	2.28	19 (24%)
13	PEX	Bc	1203	-	34,34,34	0.55	0	37,39,39	0.53	0
13	PEX	Be	1104	-	34,34,34	0.56	0	37,39,39	0.54	0
12	LMT	M	401	-	36,36,36	1.17	5 (13%)	47,47,47	1.00	2 (4%)
11	BCL	Be	1105	-	64,74,74	1.26	4 (6%)	78,115,115	1.46	10 (12%)
12	LMT	Bj	1201	-	36,36,36	1.16	5 (13%)	47,47,47	0.96	2 (4%)
10	V7N	BA	102	-	43,44,44	1.98	10 (23%)	44,54,54	1.55	8 (18%)
11	BCL	BE	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.50	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BCL	AL	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.53	11 (14%)
12	LMT	Bc	1201	-	36,36,36	1.19	6 (16%)	47,47,47	1.02	2 (4%)
11	BCL	Ac	101	-	64,74,74	1.28	5 (7%)	78,115,115	1.57	11 (14%)
11	BCL	Ba	1102	-	64,74,74	1.26	5 (7%)	78,115,115	1.51	11 (14%)
12	LMT	BM	1001	-	36,36,36	1.17	6 (16%)	47,47,47	1.00	1 (2%)
12	LMT	Bo	1201	-	36,36,36	1.19	5 (13%)	47,47,47	0.94	2 (4%)
19	HEC	C	403	8	32,50,50	2.15	3 (9%)	24,82,82	1.52	4 (16%)
11	BCL	BA	103	-	64,74,74	1.24	6 (9%)	78,115,115	1.60	13 (16%)
11	BCL	Bp	1204	-	64,74,74	1.26	4 (6%)	78,115,115	1.52	10 (12%)
12	LMT	Ba	1103	-	36,36,36	1.16	5 (13%)	47,47,47	0.98	2 (4%)
12	LMT	K	201	-	36,36,36	1.15	5 (13%)	47,47,47	1.03	2 (4%)
12	LMT	BF	102	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	2 (4%)
10	V7N	Bl	1202	-	43,44,44	2.02	10 (23%)	44,54,54	1.48	9 (20%)
11	BCL	AW	1204	-	64,74,74	1.21	5 (7%)	78,115,115	1.44	11 (14%)
13	PEX	AD	1101	-	34,34,34	0.55	0	37,39,39	0.54	0
14	MQ8	M	408	-	54,54,54	0.46	1 (1%)	66,69,69	0.60	2 (3%)
10	V7N	BP	102	-	43,44,44	1.97	10 (23%)	44,54,54	1.59	11 (25%)
16	BPH	M	406	-	51,70,70	0.89	1 (1%)	52,101,101	0.98	2 (3%)
11	BCL	AP	1102	-	64,74,74	1.24	5 (7%)	78,115,115	1.51	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	V7N	BG	101	-	-	5/53/53/53	-
14	MQ8	Ad	103	-	-	32/47/67/67	0/2/2/2
10	V7N	Bf	1202	-	-	13/53/53/53	-
10	V7N	BO	102	-	-	11/53/53/53	-
11	BCL	AN	101	-	-	6/37/137/137	-
12	LMT	BO	101	-	-	8/21/61/61	0/2/2/2
11	BCL	AJ	1102	-	-	7/37/137/137	-
18	CRT	M	407	-	-	3/51/51/51	-
11	BCL	AU	1001	13	-	4/37/137/137	-
12	LMT	Be	1102	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PEX	Ba	1101	-	-	14/38/38/38	-
10	V7N	BS	103	-	-	14/53/53/53	-
10	V7N	BN	102	-	-	5/53/53/53	-
10	V7N	BU	104	-	-	4/53/53/53	-
11	BCL	AE	1102	-	-	10/37/137/137	-
11	BCL	AJ	1103	-	-	6/37/137/137	-
11	BCL	AT	1103	-	-	9/37/137/137	-
11	BCL	AO	101	12	-	13/37/137/137	-
12	LMT	BD	102	-	-	10/21/61/61	0/2/2/2
13	PEX	Bm	102	-	-	9/38/38/38	-
12	LMT	Bf	1203	-	-	8/21/61/61	0/2/2/2
10	V7N	BX	101	-	-	11/53/53/53	-
10	V7N	BF	103	-	-	11/53/53/53	-
19	HEC	C	402	8	-	3/10/54/54	-
11	BCL	Aj	101	-	-	4/37/137/137	-
11	BCL	AK	101	-	-	11/37/137/137	-
12	LMT	BA	105	-	-	7/21/61/61	0/2/2/2
10	V7N	Bj	1202	-	-	14/53/53/53	-
13	PEX	Bh	1203	-	-	15/38/38/38	-
11	BCL	Ae	101	-	-	7/37/137/137	-
10	V7N	BB	102	-	-	11/53/53/53	-
12	LMT	BK	101	-	-	6/21/61/61	0/2/2/2
13	PEX	Bk	102	-	-	19/38/38/38	-
12	LMT	BH	101	11	-	6/21/61/61	0/2/2/2
13	PEX	Be	1101	-	-	12/38/38/38	-
11	BCL	BU	102	-	-	9/37/137/137	-
11	BCL	BX	102	-	-	9/37/137/137	-
10	V7N	Bg	101	-	-	12/53/53/53	-
11	BCL	Ak	101	-	-	8/37/137/137	-
12	LMT	Ad	102	-	-	13/21/61/61	0/2/2/2
11	BCL	BL	102	-	-	3/37/137/137	-
11	BCL	BR	101	-	-	9/37/137/137	-
12	LMT	BH	103	-	-	9/21/61/61	0/2/2/2
11	BCL	Ab	101	-	-	11/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	AC	101	-	-	4/37/137/137	-
12	LMT	AW	1201	-	-	10/21/61/61	0/2/2/2
11	BCL	Bd	1203	-	-	7/37/137/137	-
11	BCL	AG	101	-	-	7/37/137/137	-
10	V7N	Bc	1202	-	-	14/53/53/53	-
11	BCL	AW	1202	-	-	2/37/137/137	-
11	BCL	BP	101	-	-	8/37/137/137	-
12	LMT	BA	104	-	-	8/21/61/61	0/2/2/2
12	LMT	BC	102	-	-	10/21/61/61	0/2/2/2
12	LMT	Bf	1201	-	-	8/21/61/61	0/2/2/2
11	BCL	Bn	103	-	-	11/37/137/137	-
10	V7N	BW	102	-	-	9/53/53/53	-
10	V7N	Bn	101	-	-	14/53/53/53	-
11	BCL	Ah	101	-	-	3/37/137/137	-
10	V7N	Aa	101	-	-	16/53/53/53	-
12	LMT	Aj	102	-	-	10/21/61/61	0/2/2/2
10	V7N	Bd	1202	-	-	10/53/53/53	-
10	V7N	BT	101	-	-	7/53/53/53	-
11	BCL	Am	101	-	-	11/37/137/137	-
11	BCL	Bh	1205	-	-	5/37/137/137	-
12	LMT	BG	103	-	-	6/21/61/61	0/2/2/2
11	BCL	Af	101	-	-	4/37/137/137	-
11	BCL	BK	102	-	-	15/37/137/137	-
11	BCL	BD	101	-	-	6/37/137/137	-
12	LMT	BQ	102	-	-	6/21/61/61	0/2/2/2
12	LMT	Bb	1201	-	-	10/21/61/61	0/2/2/2
11	BCL	Bl	1203	-	-	8/37/137/137	-
19	HEC	C	404	8	-	2/10/54/54	-
10	V7N	An	101	-	-	12/53/53/53	-
13	PEX	AA	1101	-	-	15/38/38/38	-
11	BCL	BG	102	-	-	9/37/137/137	-
11	BCL	Al	101	-	-	22/37/137/137	-
11	BCL	AT	1102	-	-	10/37/137/137	-
19	HEC	C	405	8	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	BE	102	-	-	11/21/61/61	0/2/2/2
11	BCL	L	301	-	-	2/37/137/137	-
11	BCL	L	302	-	-	2/37/137/137	-
11	BCL	AD	1102	-	-	4/37/137/137	-
12	LMT	BW	101	-	-	6/21/61/61	0/2/2/2
10	V7N	BC	103	-	-	5/53/53/53	-
11	BCL	Bb	1203	-	-	7/37/137/137	-
12	LMT	Bh	1201	-	-	6/21/61/61	0/2/2/2
13	PEX	AS	1101	-	-	16/38/38/38	-
11	BCL	AH	101	-	-	9/37/137/137	-
11	BCL	Bg	103	-	-	11/37/137/137	-
12	LMT	C	401	-	-	6/21/61/61	0/2/2/2
11	BCL	AV	1001	-	-	6/37/137/137	-
11	BCL	BS	101	-	-	9/37/137/137	-
10	V7N	Bp	1202	-	-	10/53/53/53	-
11	BCL	BC	101	-	-	10/37/137/137	-
10	V7N	BH	102	-	-	2/53/53/53	-
10	V7N	BD	103	-	-	5/53/53/53	-
11	BCL	M	405	-	-	5/37/137/137	-
12	LMT	BO	104	11	-	8/21/61/61	0/2/2/2
14	MQ8	L	305	-	-	27/47/67/67	0/2/2/2
15	CD4	Af	102	-	-	22/94/94/94	-
11	BCL	Ai	101	-	-	11/37/137/137	-
11	BCL	AS	1102	-	-	7/37/137/137	-
12	LMT	Bh	1204	-	-	5/21/61/61	0/2/2/2
10	V7N	BQ	103	-	-	4/53/53/53	-
11	BCL	BB	101	-	-	8/37/137/137	-
13	PEX	Aj	103	-	-	10/38/38/38	-
10	V7N	Bh	1202	-	-	9/53/53/53	-
12	LMT	BI	103	-	-	7/21/61/61	0/2/2/2
10	V7N	BL	101	-	-	6/53/53/53	-
11	BCL	AF	102	-	-	10/37/137/137	-
12	LMT	Bp	1201	-	-	6/21/61/61	0/2/2/2
11	BCL	AI	102	13	-	7/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	Ao	101	-	-	21/37/137/137	-
11	BCL	BF	101	-	-	12/37/137/137	-
11	BCL	AW	1203	-	-	7/37/137/137	-
13	PEX	AJ	1101	11	-	18/38/38/38	-
12	LMT	BL	103	-	-	8/21/61/61	0/2/2/2
11	BCL	BO	103	-	-	8/37/137/137	-
16	BPH	L	303	-	-	8/37/105/105	0/5/6/6
11	BCL	BH	104	12	-	6/37/137/137	-
12	LMT	Bj	1203	-	-	6/21/61/61	0/2/2/2
13	PEX	Bn	102	11	-	15/38/38/38	-
12	LMT	BU	101	-	-	9/21/61/61	0/2/2/2
12	LMT	Bd	1201	-	-	9/21/61/61	0/2/2/2
12	LMT	BQ	101	-	-	3/21/61/61	0/2/2/2
11	BCL	AB	101	-	-	6/37/137/137	-
11	BCL	BA	101	-	-	6/37/137/137	-
10	V7N	AL	102	-	-	6/53/53/53	-
11	BCL	BI	102	-	-	8/37/137/137	-
11	BCL	Aa	102	-	-	5/37/137/137	-
13	PEX	AP	1101	-	-	18/38/38/38	-
11	BCL	Bm	103	-	-	2/37/137/137	-
10	V7N	Bm	101	-	-	17/53/53/53	-
11	BCL	BN	101	-	-	6/37/137/137	-
10	V7N	Bb	1202	-	-	15/53/53/53	-
10	V7N	Be	1103	-	-	12/53/53/53	-
12	LMT	Aa	103	-	-	5/21/61/61	0/2/2/2
12	LMT	L	304	-	-	10/21/61/61	0/2/2/2
11	BCL	AM	102	-	-	11/37/137/137	-
12	LMT	Bl	1201	-	-	7/21/61/61	0/2/2/2
10	V7N	BV	101	-	-	12/53/53/53	-
11	BCL	M	404	-	-	3/37/137/137	-
11	BCL	Bj	1204	-	-	8/37/137/137	-
11	BCL	Ad	101	-	-	5/37/137/137	-
11	BCL	AR	101	-	-	8/37/137/137	-
11	BCL	BV	102	-	-	10/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	AM	101	-	-	5/37/137/137	-
10	V7N	AF	101	-	-	17/53/53/53	-
11	BCL	AQ	102	-	-	9/37/137/137	-
11	BCL	AX	1202	-	-	5/37/137/137	-
11	BCL	Bi	102	-	-	4/37/137/137	-
11	BCL	Bk	103	-	-	2/37/137/137	-
10	V7N	Bk	101	-	-	11/53/53/53	-
11	BCL	AQ	101	-	-	10/37/137/137	-
12	LMT	BK	103	-	-	7/21/61/61	0/2/2/2
12	LMT	AX	1201	-	-	9/21/61/61	0/2/2/2
12	LMT	BR	102	-	-	7/21/61/61	0/2/2/2
12	LMT	BW	103	-	-	6/21/61/61	0/2/2/2
15	CD4	M	403	-	-	18/94/94/94	-
11	BCL	Bf	1204	-	-	13/37/137/137	-
13	PEX	Bg	102	-	-	21/38/38/38	-
11	BCL	Bc	1204	-	-	8/37/137/137	-
11	BCL	AI	101	-	-	5/37/137/137	-
12	LMT	BU	103	-	-	5/21/61/61	0/2/2/2
10	V7N	BI	101	-	-	6/53/53/53	-
10	V7N	BJ	101	-	-	15/53/53/53	-
13	PEX	AE	1101	-	-	18/38/38/38	-
10	V7N	Bi	101	-	-	9/53/53/53	-
13	PEX	AT	1101	-	-	13/38/38/38	-
12	LMT	BB	103	-	-	14/21/61/61	0/2/2/2
10	V7N	BK	104	-	-	7/53/53/53	-
11	BCL	Bo	1202	-	-	16/37/137/137	-
12	LMT	BS	102	-	-	13/21/61/61	0/2/2/2
10	V7N	BR	103	-	-	10/53/53/53	-
11	BCL	Bp	1203	-	-	19/37/137/137	-
13	PEX	Bc	1203	-	-	21/38/38/38	-
13	PEX	Be	1104	-	-	19/38/38/38	-
12	LMT	M	401	-	-	10/21/61/61	0/2/2/2
11	BCL	Be	1105	-	-	4/37/137/137	-
12	LMT	Bj	1201	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	V7N	BA	102	-	-	6/53/53/53	-
11	BCL	BE	101	-	-	8/37/137/137	-
11	BCL	AL	101	-	-	4/37/137/137	-
12	LMT	Bc	1201	-	-	7/21/61/61	0/2/2/2
11	BCL	Ac	101	-	-	7/37/137/137	-
11	BCL	Ba	1102	-	-	4/37/137/137	-
12	LMT	BM	1001	-	-	7/21/61/61	0/2/2/2
12	LMT	Bo	1201	-	-	5/21/61/61	0/2/2/2
19	HEC	C	403	8	-	2/10/54/54	-
11	BCL	BA	103	-	-	4/37/137/137	-
11	BCL	Bp	1204	-	-	9/37/137/137	-
12	LMT	Ba	1103	-	-	5/21/61/61	0/2/2/2
12	LMT	K	201	-	-	9/21/61/61	0/2/2/2
12	LMT	BF	102	-	-	8/21/61/61	0/2/2/2
10	V7N	Bl	1202	-	-	8/53/53/53	-
11	BCL	AW	1204	-	-	6/37/137/137	-
13	PEX	AD	1101	-	-	19/38/38/38	-
14	MQ8	M	408	-	-	20/47/67/67	0/2/2/2
10	V7N	BP	102	-	-	13/53/53/53	-
16	BPH	M	406	-	-	6/37/105/105	0/5/6/6
11	BCL	AP	1102	-	-	5/37/137/137	-

The worst 5 of 1128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	402	HEC	C2B-C3B	-7.21	1.33	1.40
10	BX	101	V7N	C28-C27	7.00	1.52	1.34
10	Be	1103	V7N	C28-C27	6.95	1.52	1.34
10	Bl	1202	V7N	C28-C27	6.94	1.52	1.34
10	Bc	1202	V7N	C28-C27	6.88	1.52	1.34

The worst 5 of 1466 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BA	101	BCL	O1D-CGD-CBD	-26.04	71.21	124.48
11	Bk	103	BCL	O2A-CGA-O1A	-25.35	59.61	123.59
11	BA	101	BCL	O2D-CGD-O1D	-24.00	76.91	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BA	101	BCL	O2D-CGD-CBD	20.74	148.12	111.27
11	Bk	103	BCL	O2A-CGA-CBA	15.74	161.30	111.91

There are no chirality outliers.

5 of 1833 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Aa	101	V7N	C30-C1-C2-C3
10	Aa	101	V7N	C31-C1-C2-C3
10	Aa	101	V7N	O42-C34-C9-C10
10	Aa	101	V7N	O42-C34-C9-C8
10	Bb	1202	V7N	C31-C1-C2-C3

There are no ring outliers.

139 monomers are involved in 333 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Ad	103	MQ8	9	0
11	AN	101	BCL	3	0
11	AJ	1102	BCL	1	0
11	AU	1001	BCL	2	0
12	Be	1102	LMT	1	0
13	Ba	1101	PEX	1	0
10	BS	103	V7N	1	0
11	AE	1102	BCL	4	0
11	AJ	1103	BCL	2	0
11	AT	1103	BCL	5	0
11	AO	101	BCL	5	0
12	BD	102	LMT	1	0
13	Bm	102	PEX	2	0
12	Bf	1203	LMT	2	0
19	C	402	HEC	1	0
11	Aj	101	BCL	2	0
11	AK	101	BCL	5	0
13	Bh	1203	PEX	1	0
11	Ae	101	BCL	4	0
12	BK	101	LMT	1	0
13	Bk	102	PEX	1	0
13	Be	1101	PEX	1	0
11	BU	102	BCL	1	0
11	BX	102	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Ak	101	BCL	2	0
12	Ad	102	LMT	2	0
11	BL	102	BCL	1	0
12	BH	103	LMT	3	0
11	Ab	101	BCL	2	0
11	AC	101	BCL	2	0
12	AW	1201	LMT	1	0
11	Bd	1203	BCL	1	0
11	AG	101	BCL	1	0
11	AW	1202	BCL	2	0
11	BP	101	BCL	2	0
12	BA	104	LMT	5	0
12	BC	102	LMT	2	0
12	Bf	1201	LMT	1	0
11	Bn	103	BCL	2	0
11	Ah	101	BCL	1	0
10	BT	101	V7N	1	0
11	Am	101	BCL	9	0
11	Bh	1205	BCL	1	0
12	BG	103	LMT	1	0
11	Af	101	BCL	2	0
11	BK	102	BCL	1	0
11	BD	101	BCL	4	0
12	Bb	1201	LMT	2	0
11	Bl	1203	BCL	4	0
19	C	404	HEC	2	0
13	AA	1101	PEX	4	0
11	BG	102	BCL	2	0
11	Al	101	BCL	9	0
11	AT	1102	BCL	5	0
19	C	405	HEC	2	0
12	BE	102	LMT	1	0
11	L	302	BCL	3	0
11	AD	1102	BCL	3	0
12	BW	101	LMT	1	0
11	Bb	1203	BCL	2	0
12	Bh	1201	LMT	2	0
13	AS	1101	PEX	2	0
11	AH	101	BCL	2	0
11	Bg	103	BCL	1	0
11	AV	1001	BCL	5	0
11	BS	101	BCL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	BC	101	BCL	2	0
11	M	405	BCL	1	0
12	BO	104	LMT	3	0
14	L	305	MQ8	6	0
15	Af	102	CD4	9	0
11	AS	1102	BCL	3	0
11	BB	101	BCL	3	0
13	Aj	103	PEX	2	0
12	BI	103	LMT	2	0
11	AF	102	BCL	2	0
12	Bp	1201	LMT	1	0
11	AI	102	BCL	4	0
11	Ao	101	BCL	26	0
11	BF	101	BCL	3	0
11	AW	1203	BCL	4	0
13	AJ	1101	PEX	1	0
11	BO	103	BCL	1	0
16	L	303	BPH	6	0
11	BH	104	BCL	1	0
13	Bn	102	PEX	3	0
12	Bd	1201	LMT	1	0
12	BQ	101	LMT	1	0
11	AB	101	BCL	3	0
11	BA	101	BCL	6	0
11	BI	102	BCL	5	0
13	AP	1101	PEX	2	0
11	Bm	103	BCL	3	0
11	BN	101	BCL	3	0
11	AM	102	BCL	2	0
10	BV	101	V7N	1	0
11	M	404	BCL	2	0
11	Bj	1204	BCL	3	0
11	Ad	101	BCL	1	0
11	AR	101	BCL	6	0
11	AM	101	BCL	2	0
11	AX	1202	BCL	4	0
11	Bi	102	BCL	1	0
11	Bk	103	BCL	1	0
11	AQ	101	BCL	4	0
12	AX	1201	LMT	2	0
12	BR	102	LMT	1	0
12	BW	103	LMT	3	0

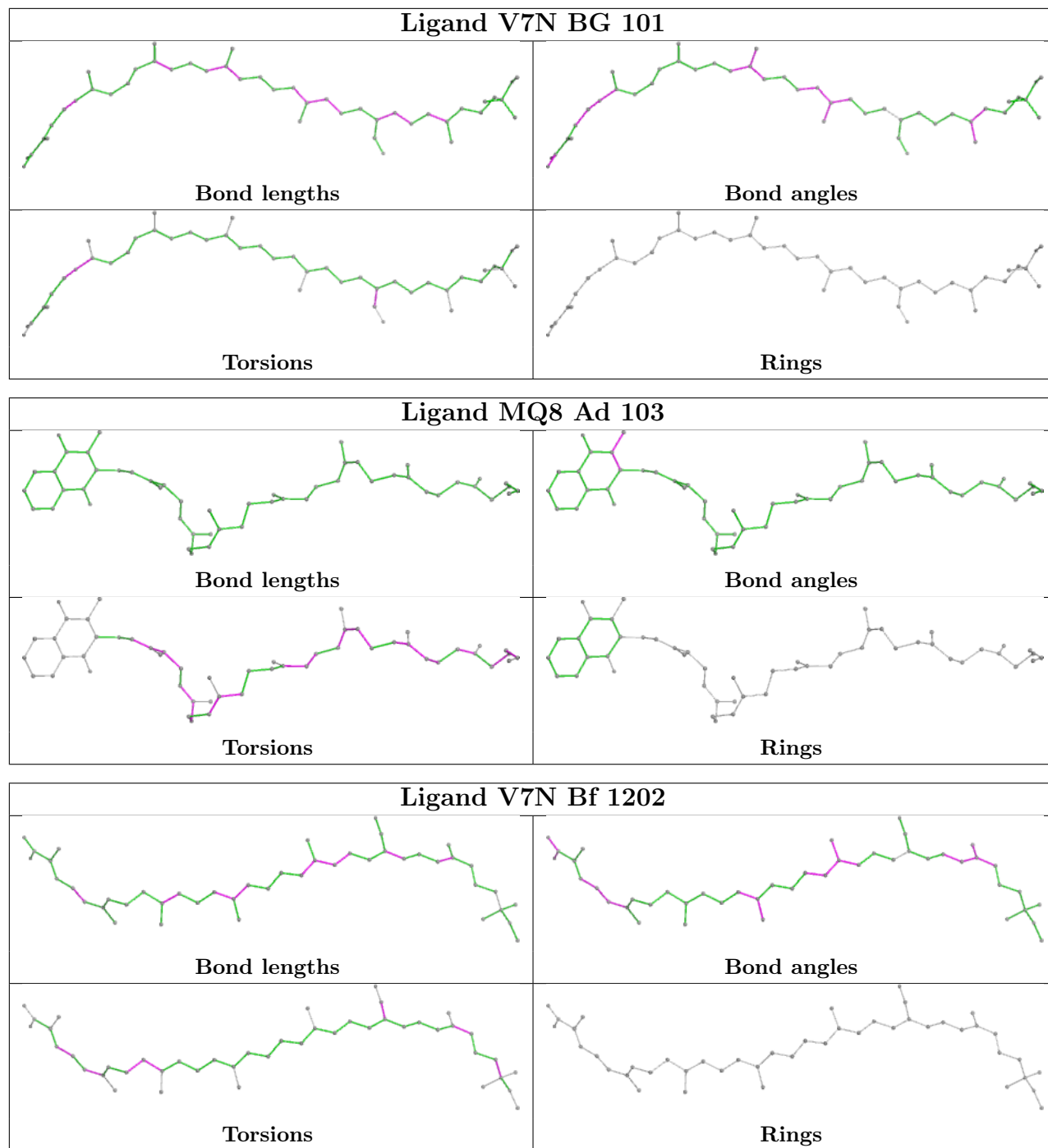
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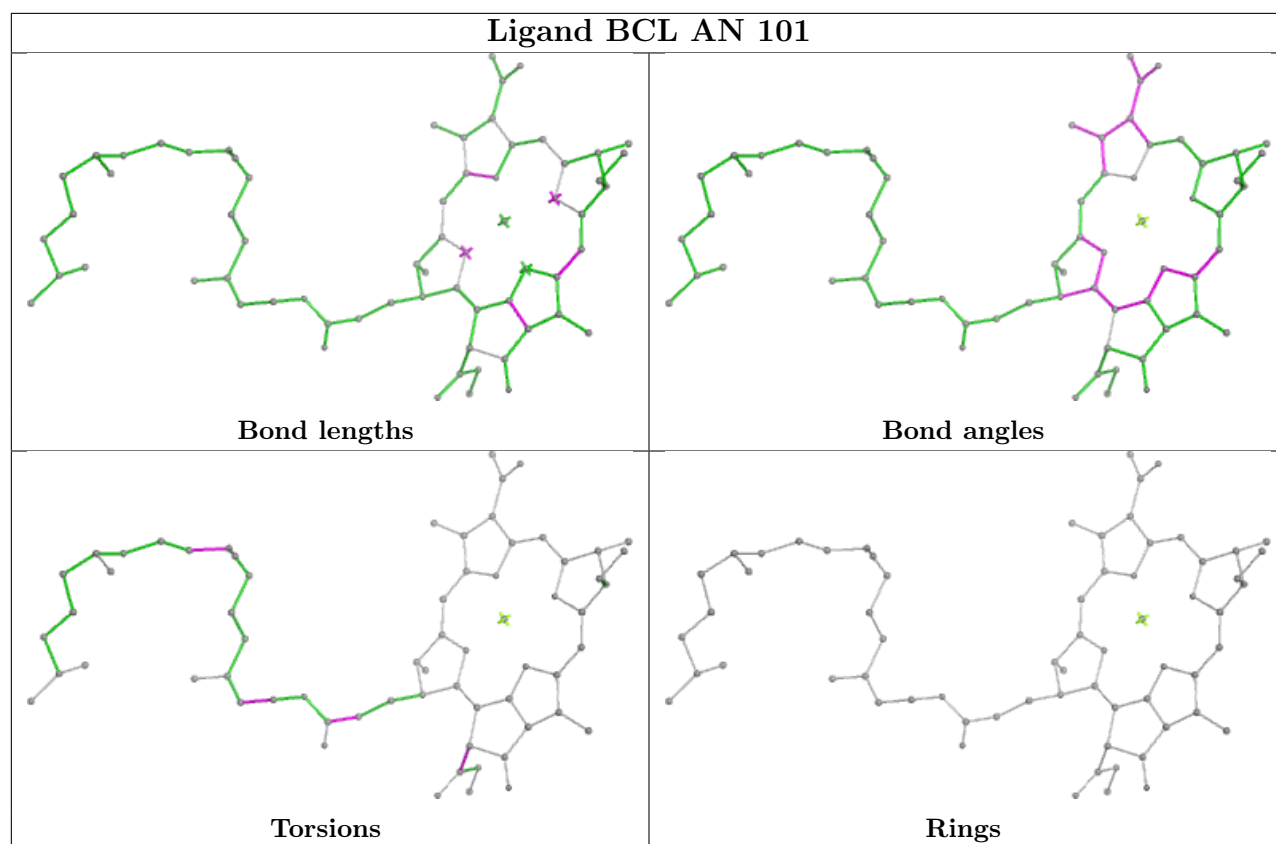
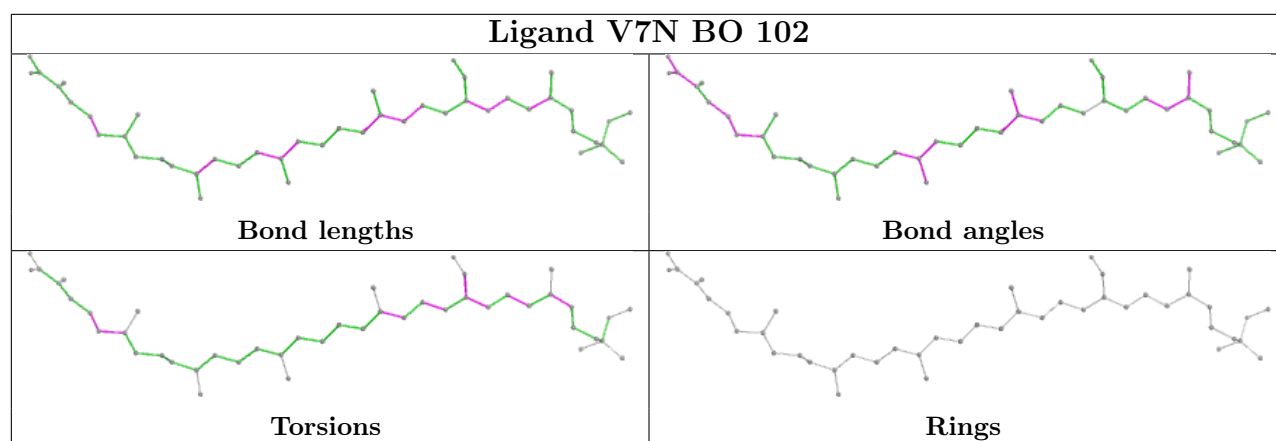
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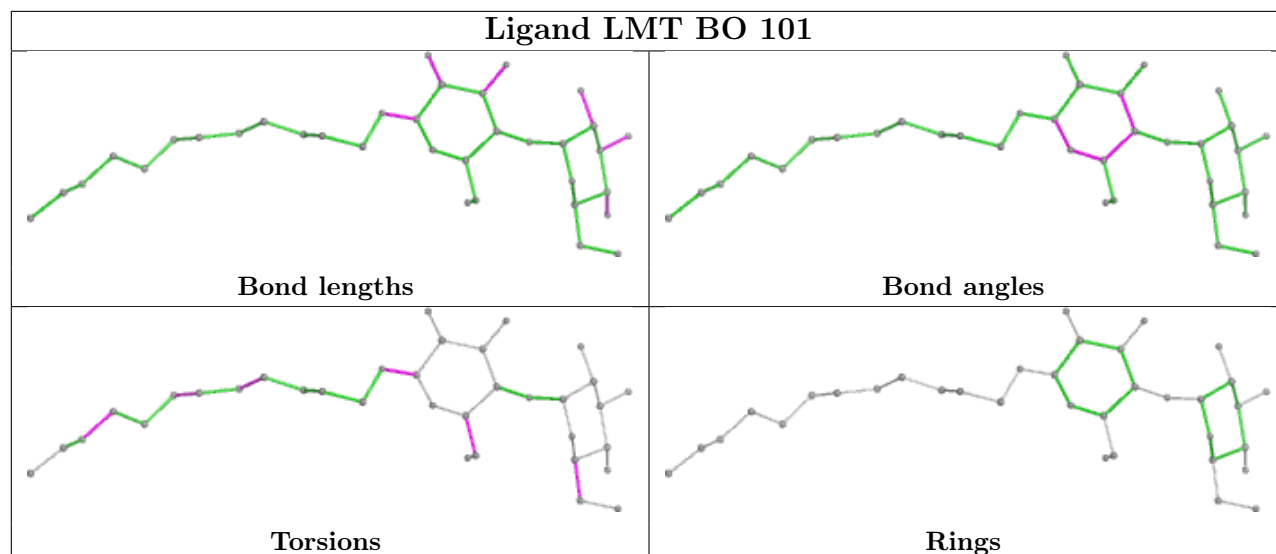
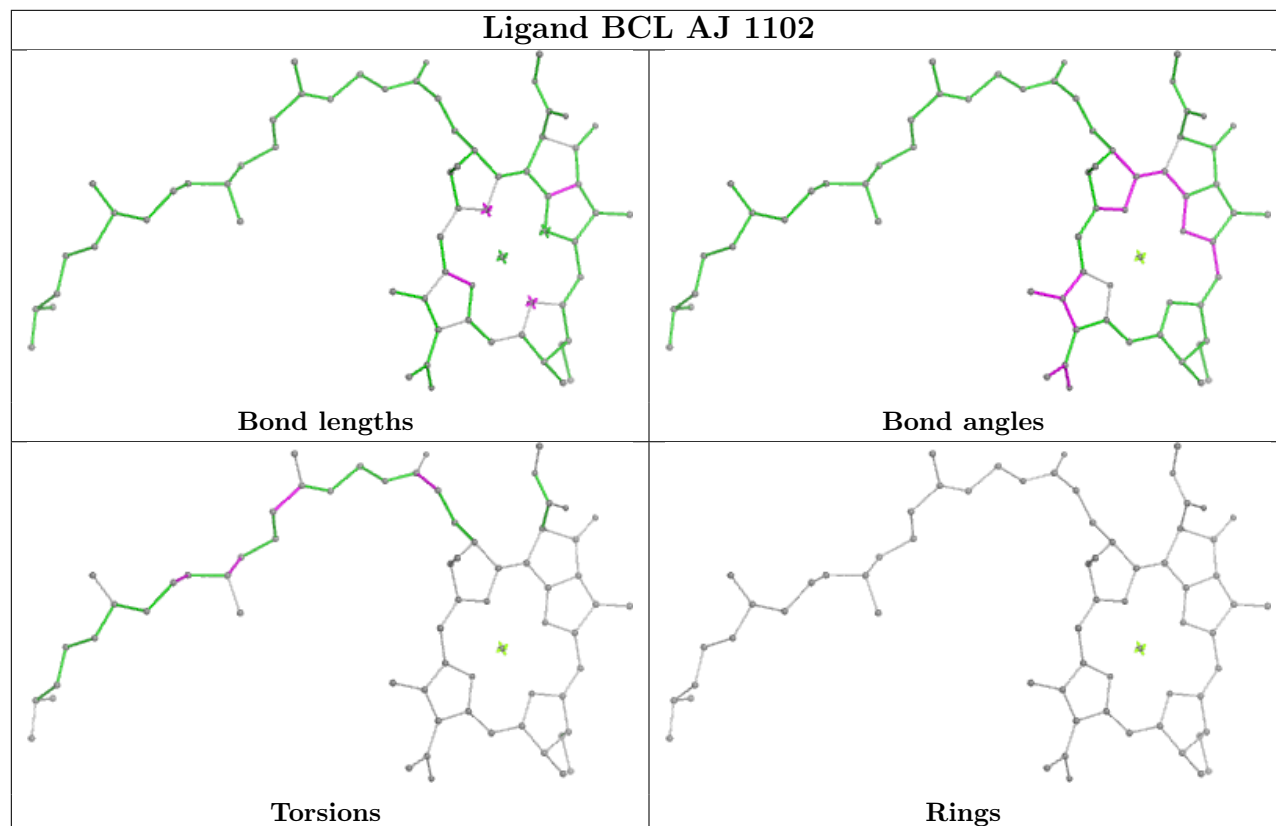
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	M	403	CD4	1	0
11	Bf	1204	BCL	1	0
13	Bg	102	PEX	1	0
11	AI	101	BCL	1	0
13	AE	1101	PEX	2	0
13	AT	1101	PEX	2	0
12	BB	103	LMT	2	0
11	Bo	1202	BCL	3	0
12	BS	102	LMT	4	0
11	Bp	1203	BCL	11	0
13	Bc	1203	PEX	4	0
13	Be	1104	PEX	5	0
12	M	401	LMT	2	0
11	Be	1105	BCL	3	0
12	Bj	1201	LMT	2	0
11	BE	101	BCL	1	0
11	AL	101	BCL	3	0
12	Bc	1201	LMT	1	0
11	Ac	101	BCL	2	0
11	Ba	1102	BCL	1	0
12	BM	1001	LMT	2	0
12	Bo	1201	LMT	3	0
19	C	403	HEC	1	0
11	Bp	1204	BCL	1	0
12	K	201	LMT	1	0
12	BF	102	LMT	2	0
11	AW	1204	BCL	1	0
13	AD	1101	PEX	3	0
14	M	408	MQ8	4	0
16	M	406	BPH	4	0
11	AP	1102	BCL	2	0

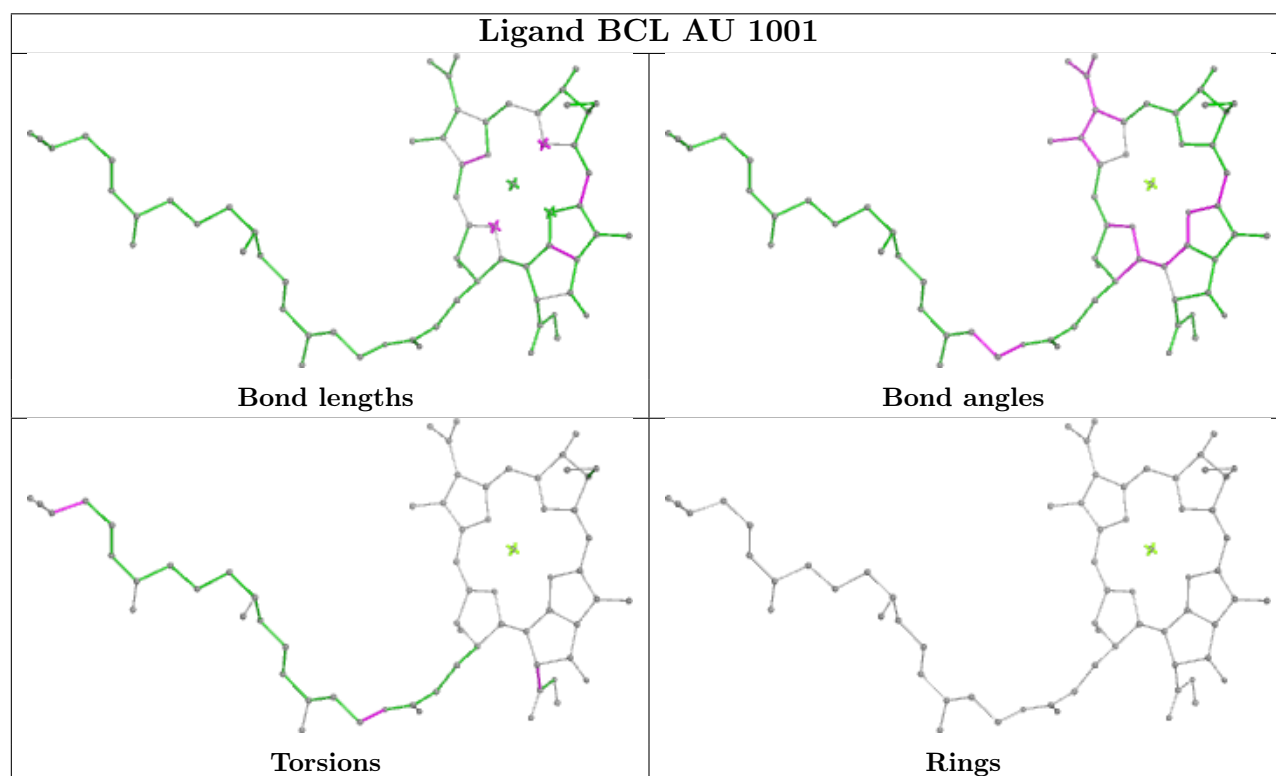
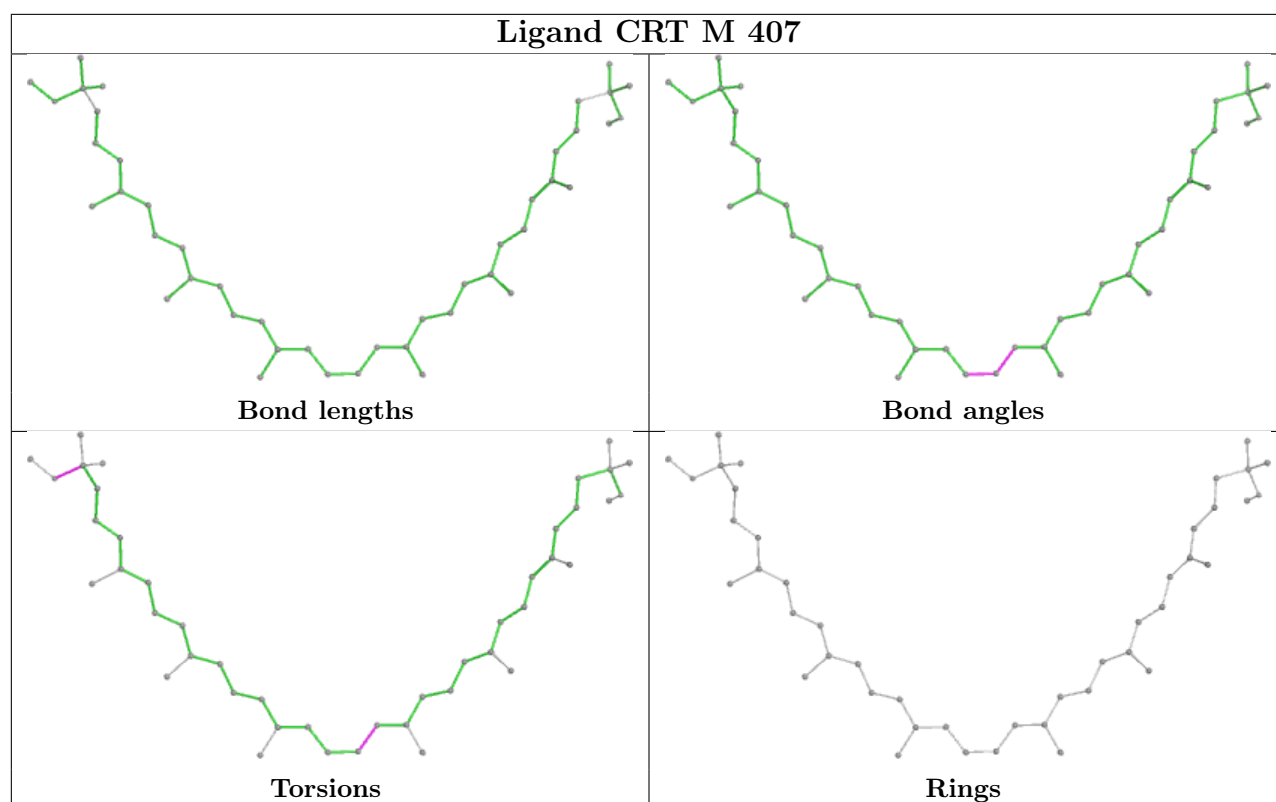
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

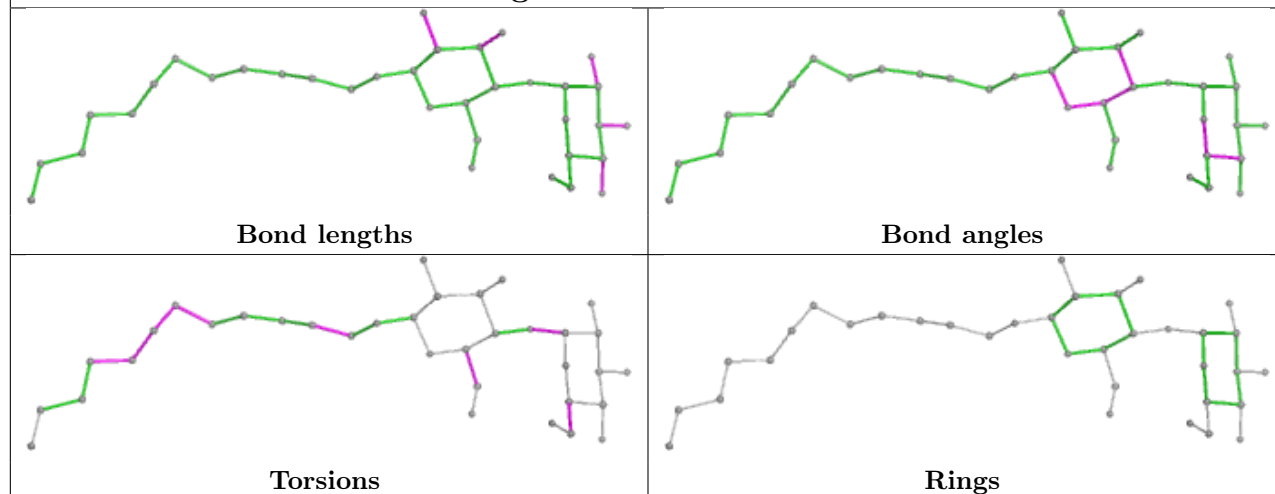
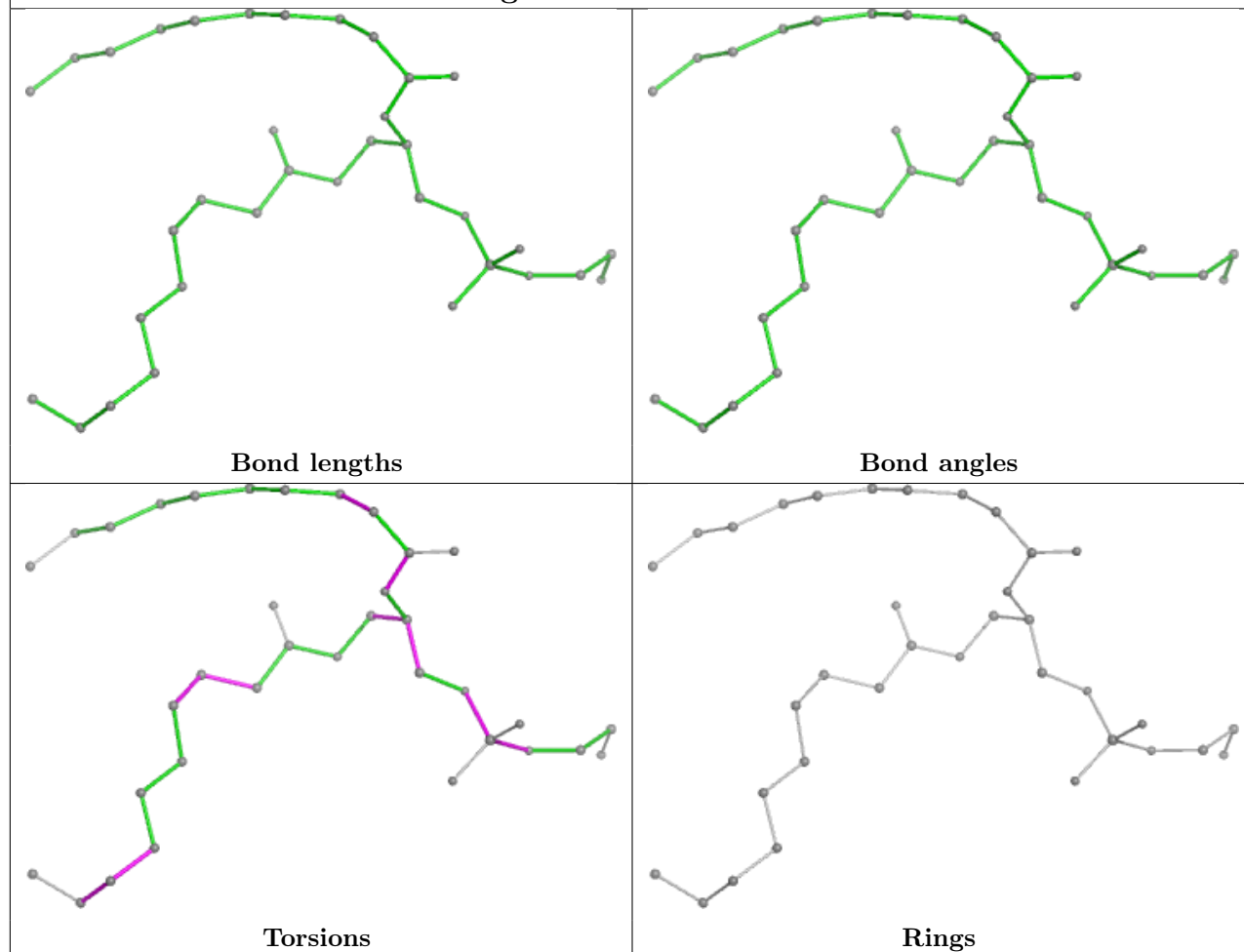
equivalents in the CSD to analyse the geometry.

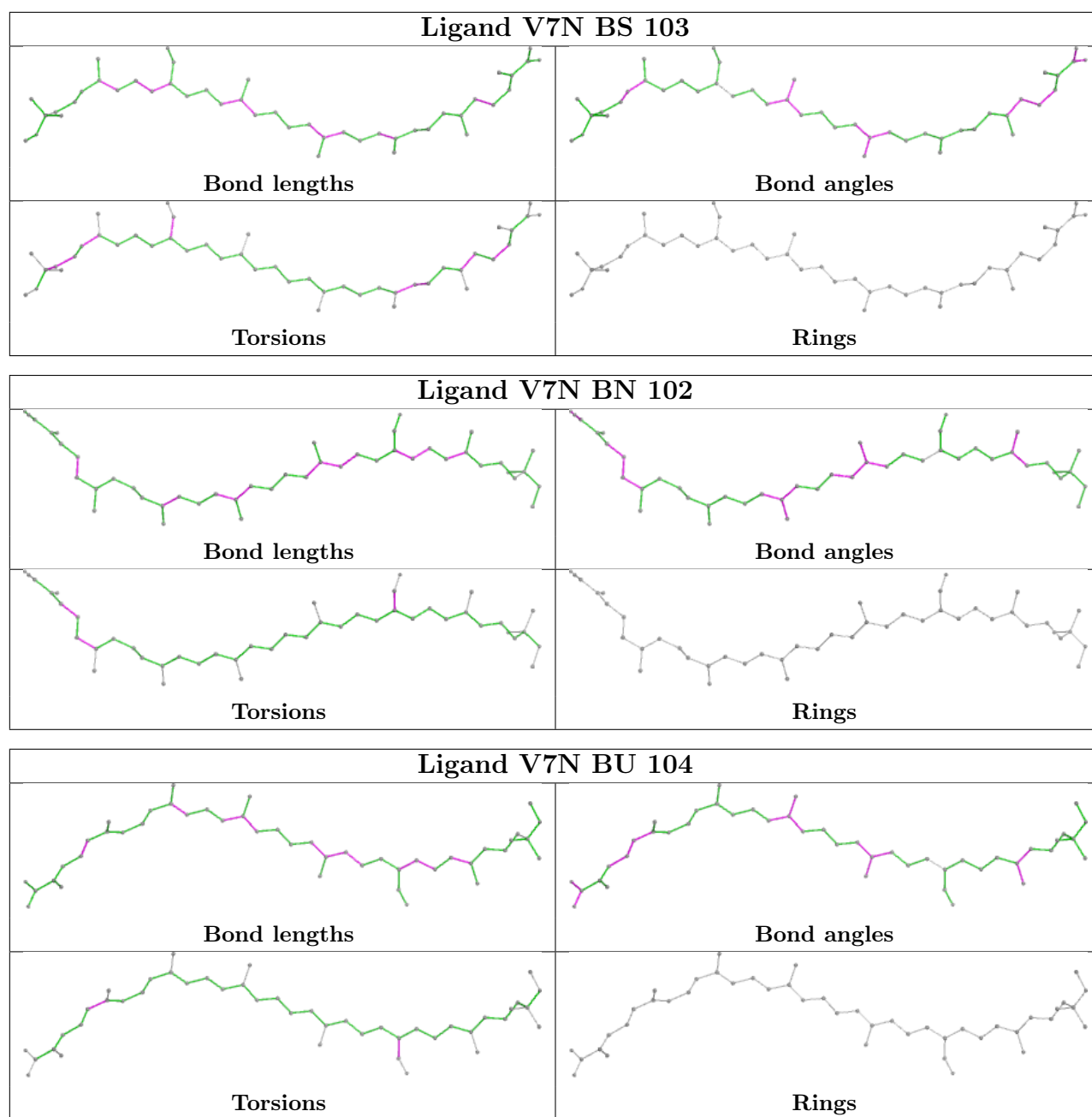


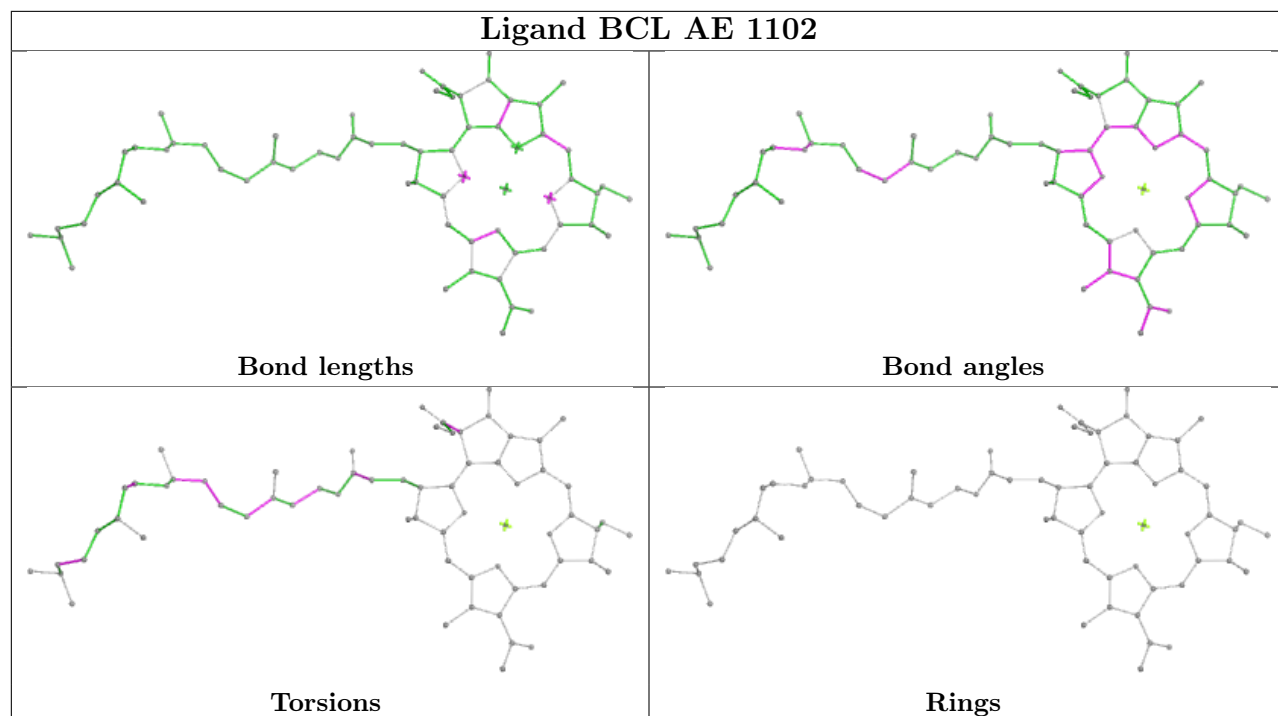


Ligand LMT BO 101**Ligand BCL AJ 1102**

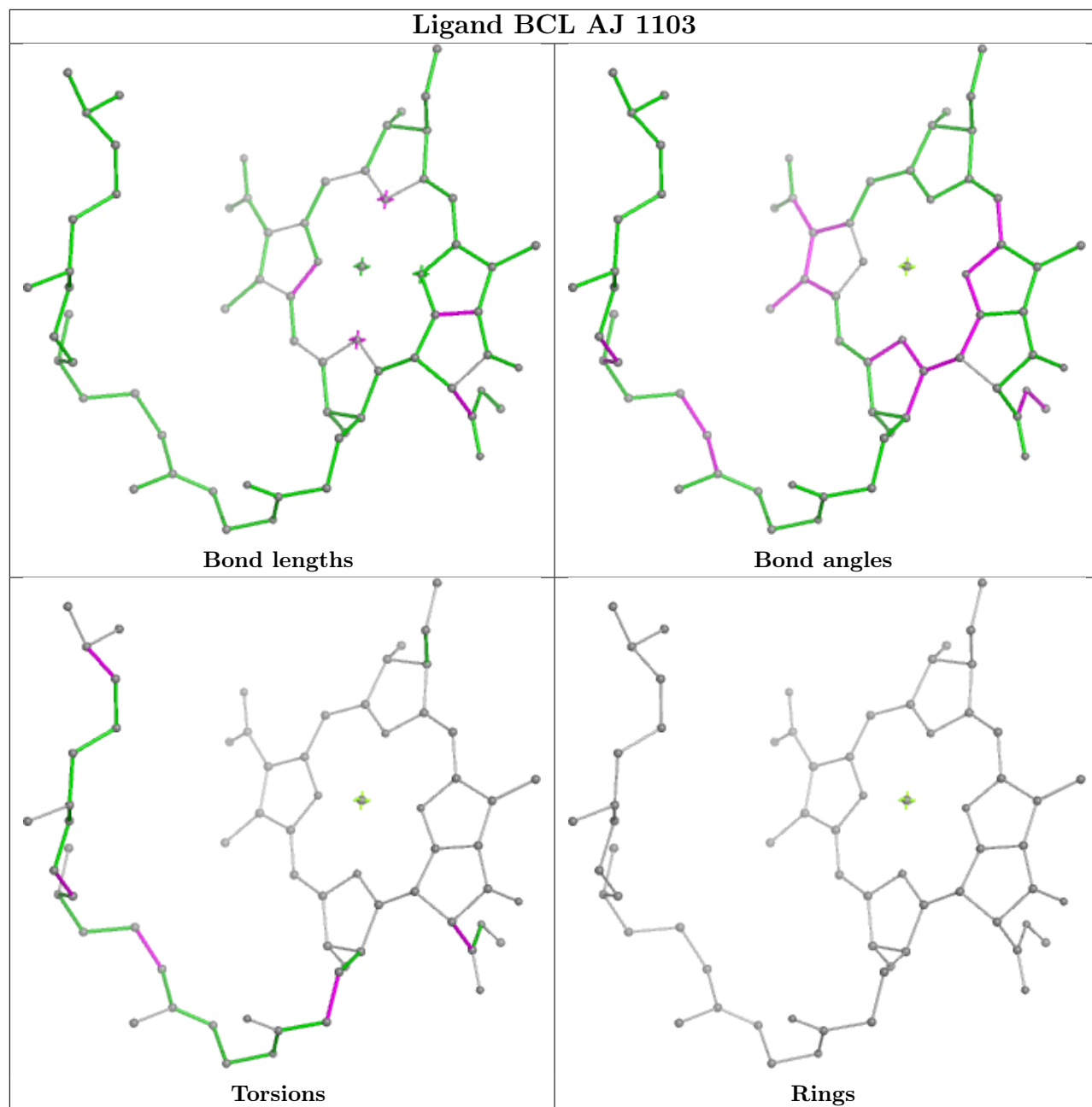


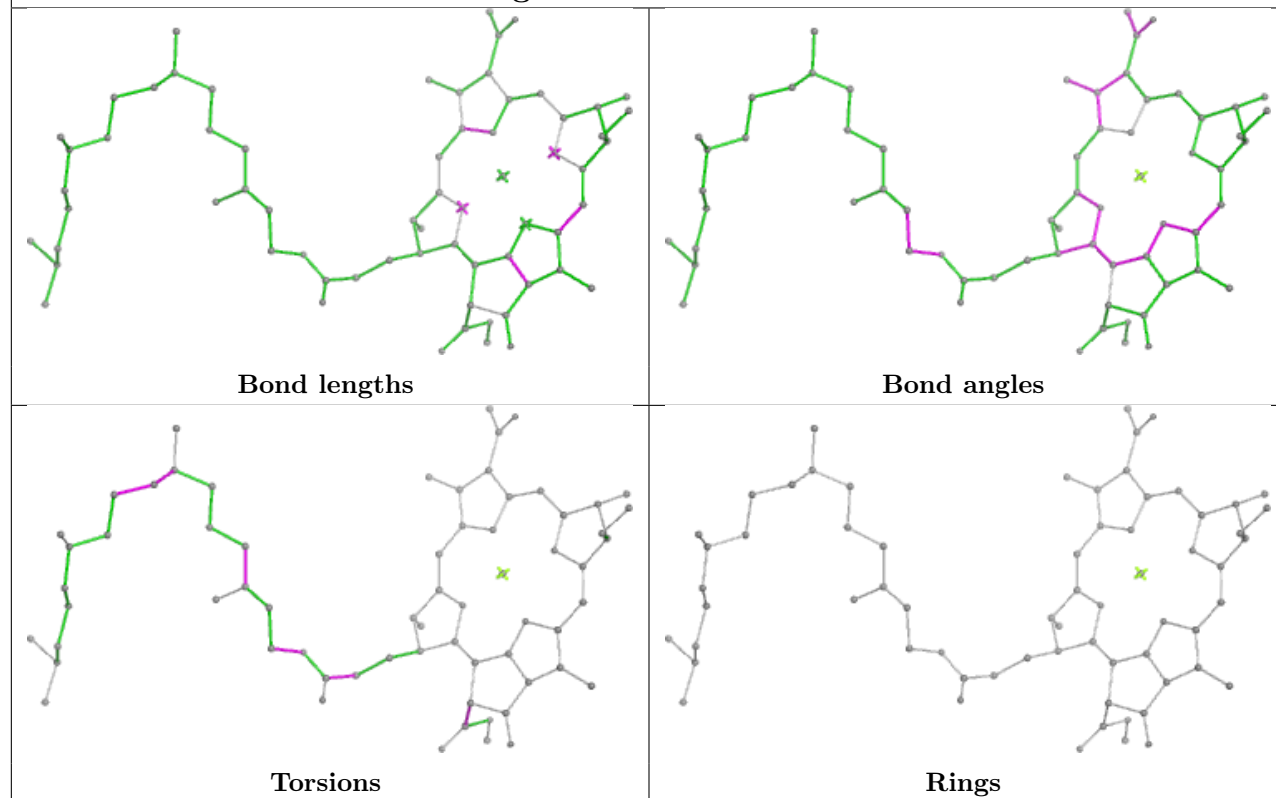
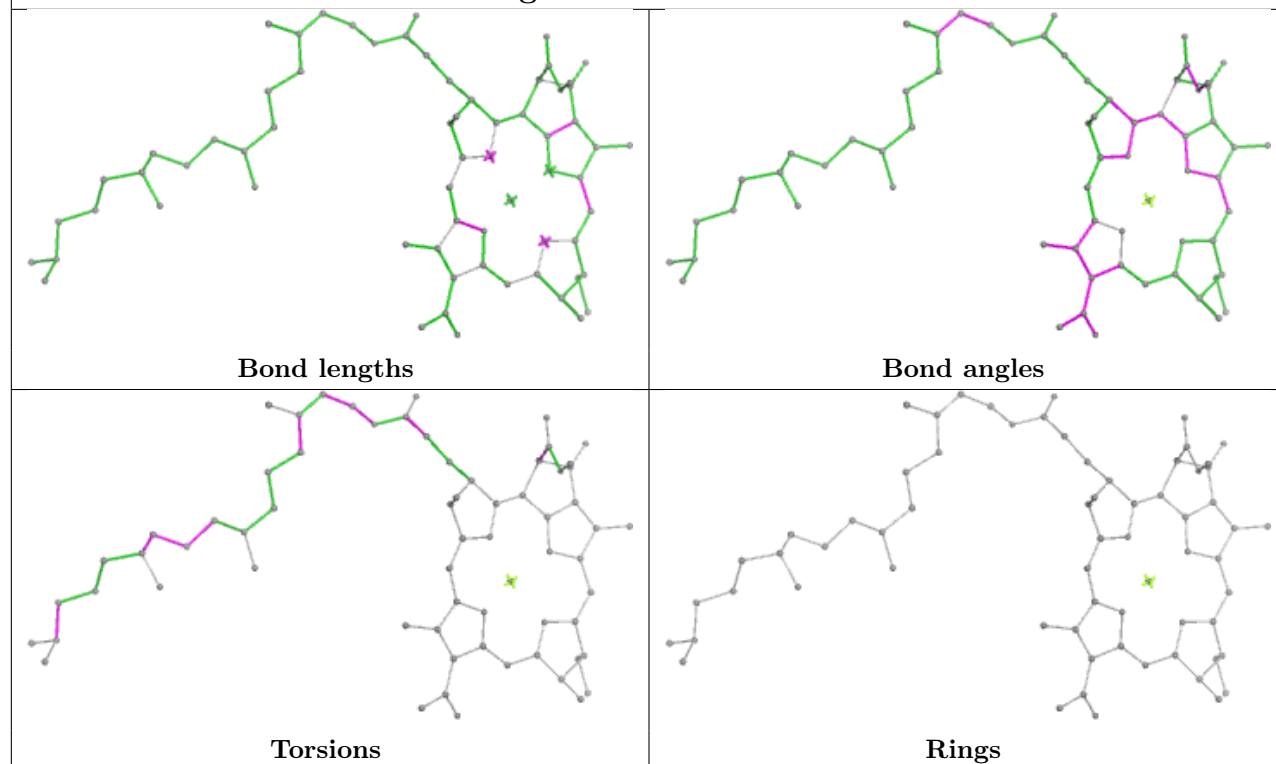
Ligand LMT Be 1102**Ligand PEX Ba 1101**

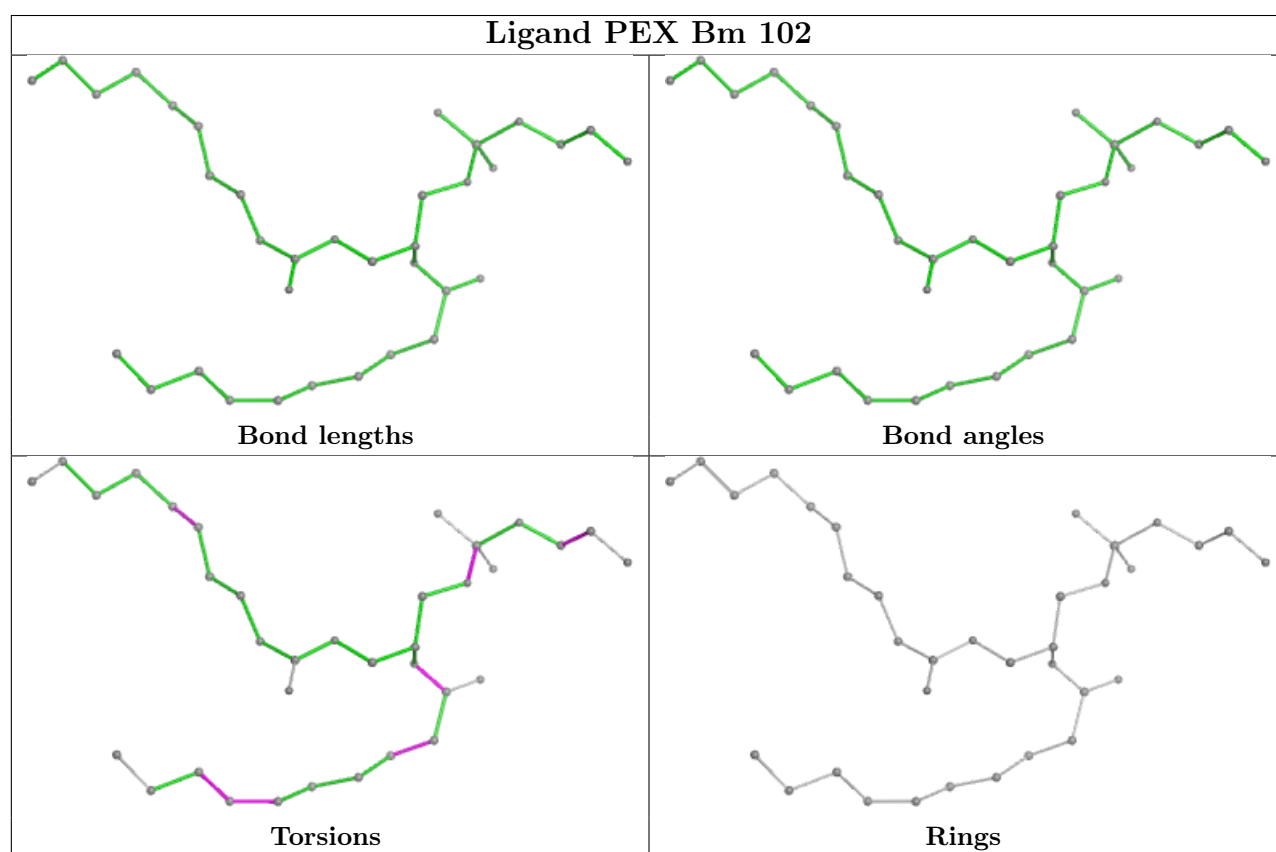
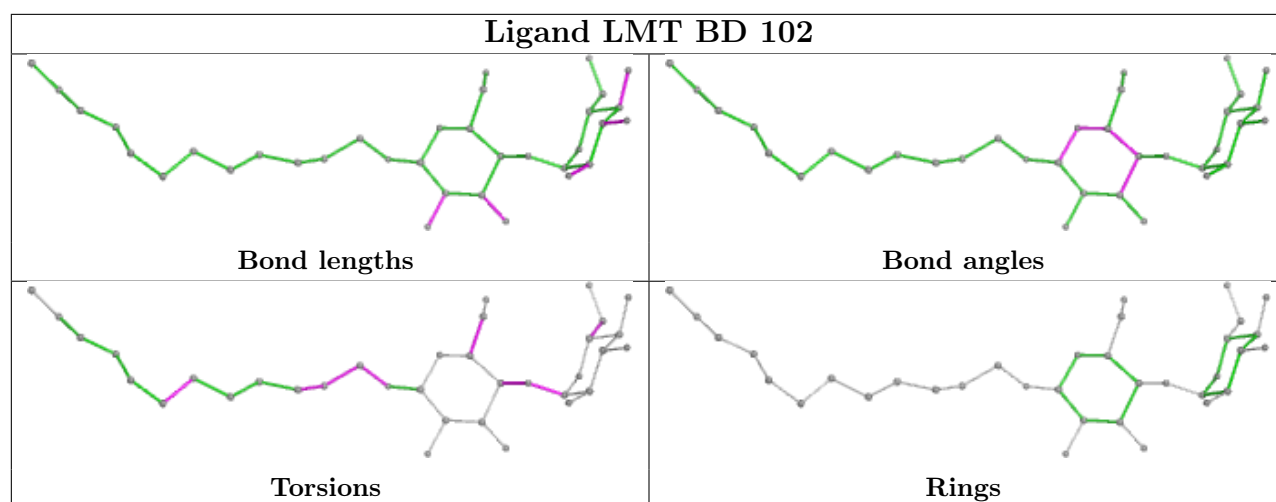


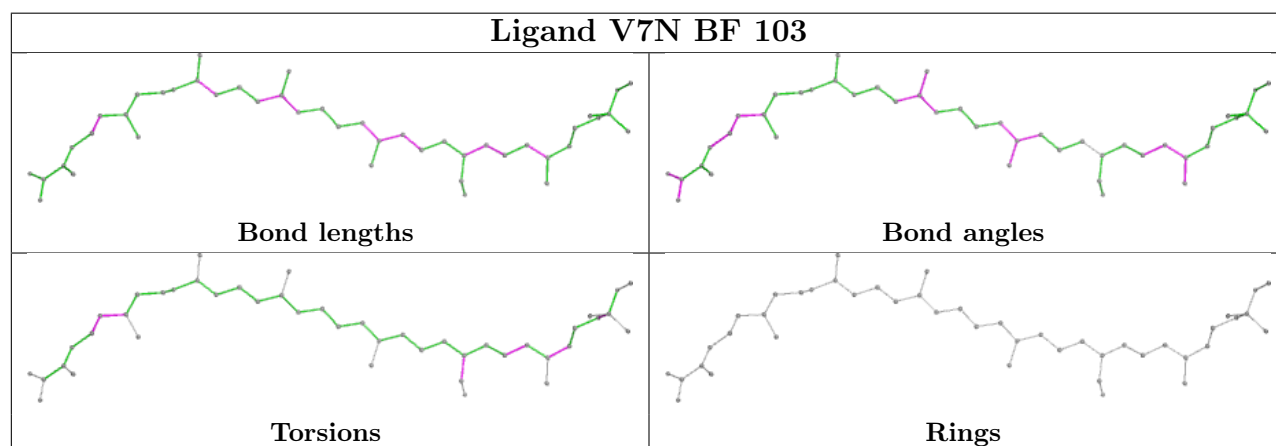
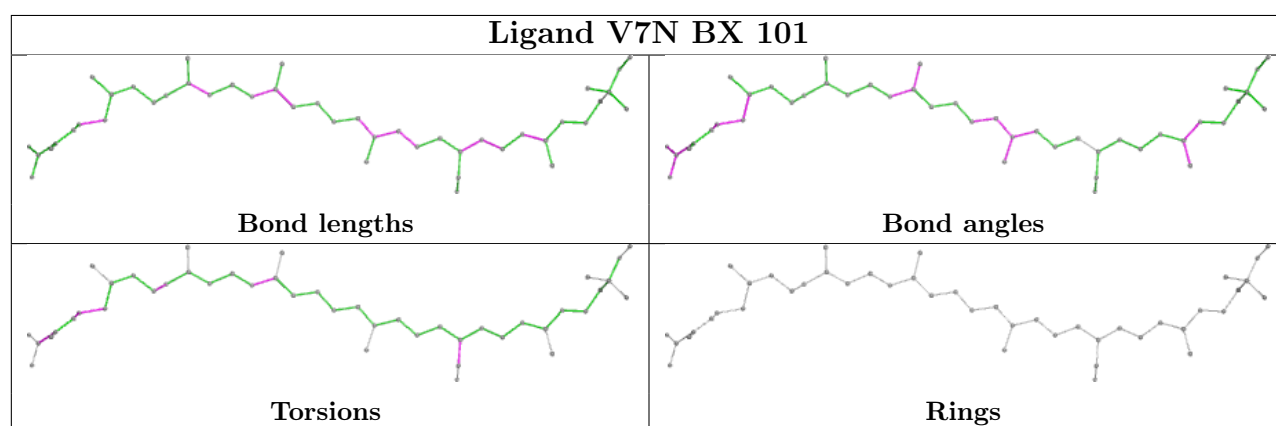
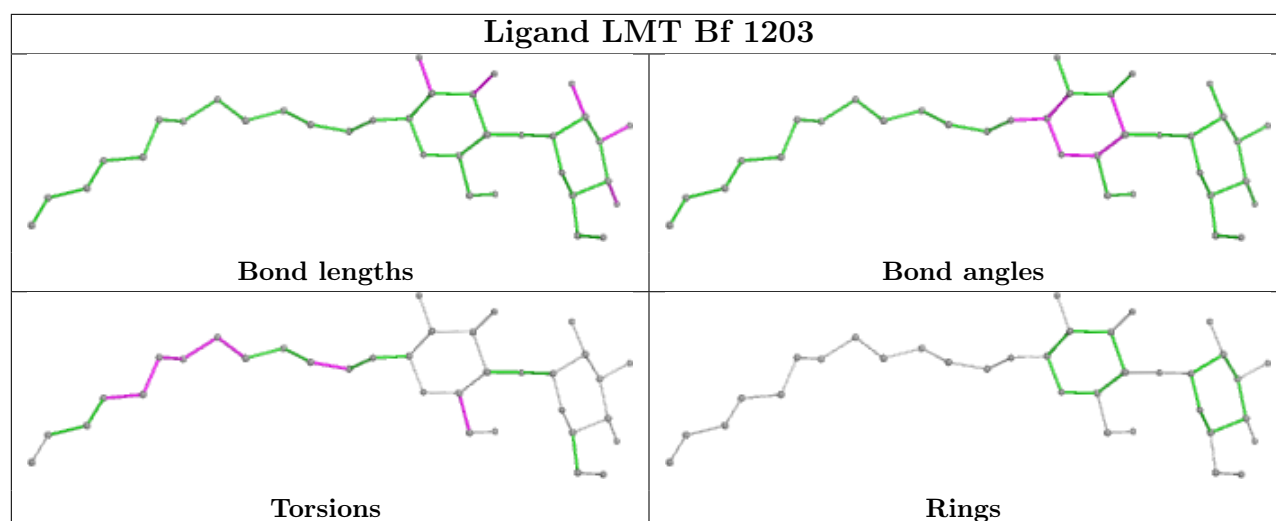


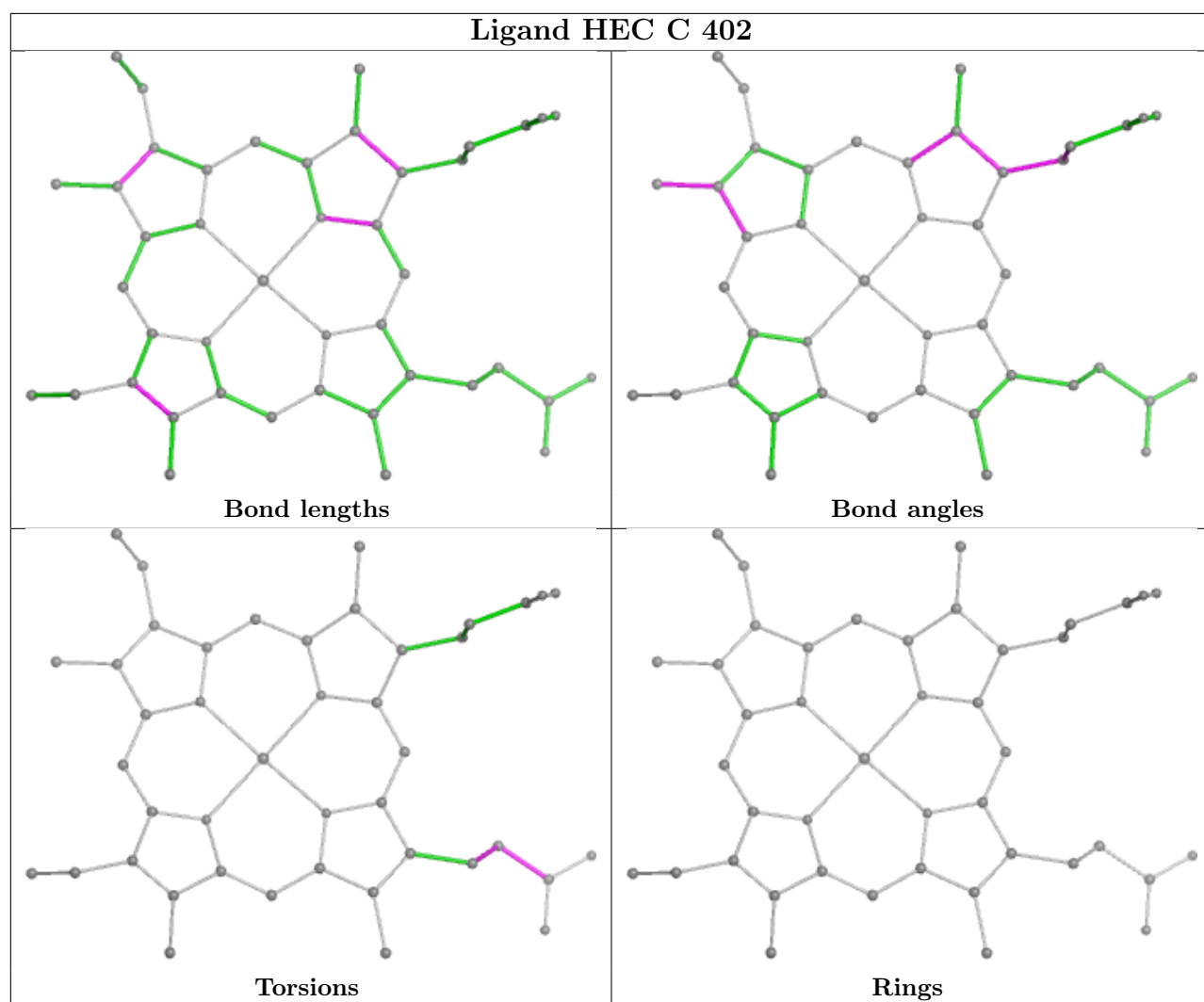
Ligand BCL AJ 1103

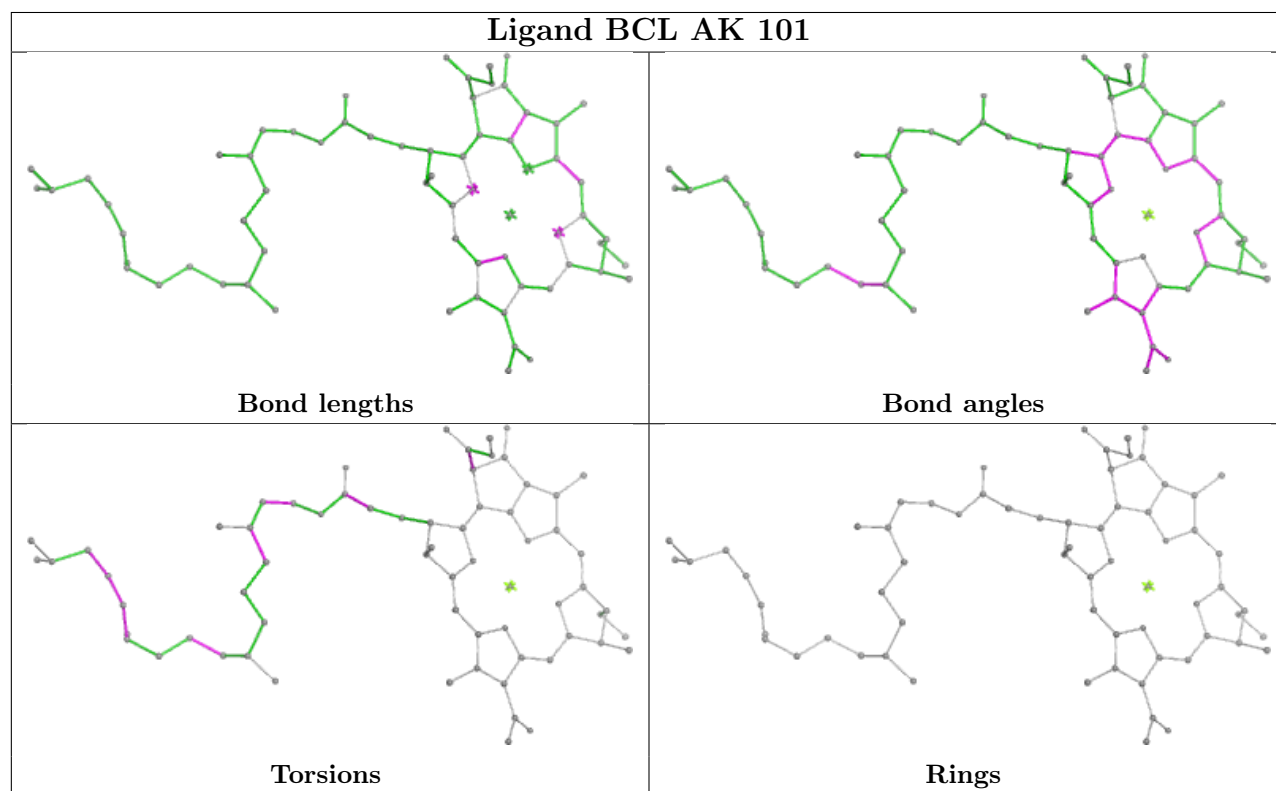
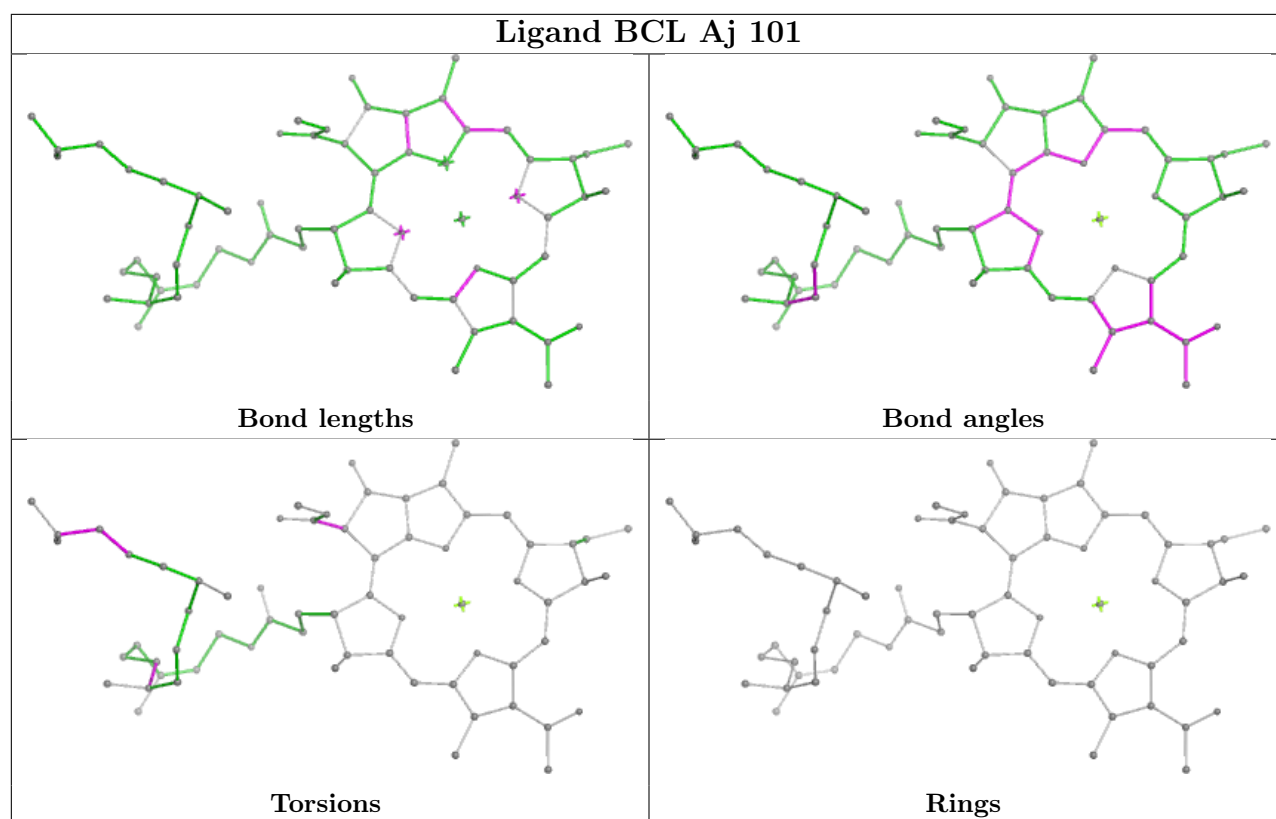


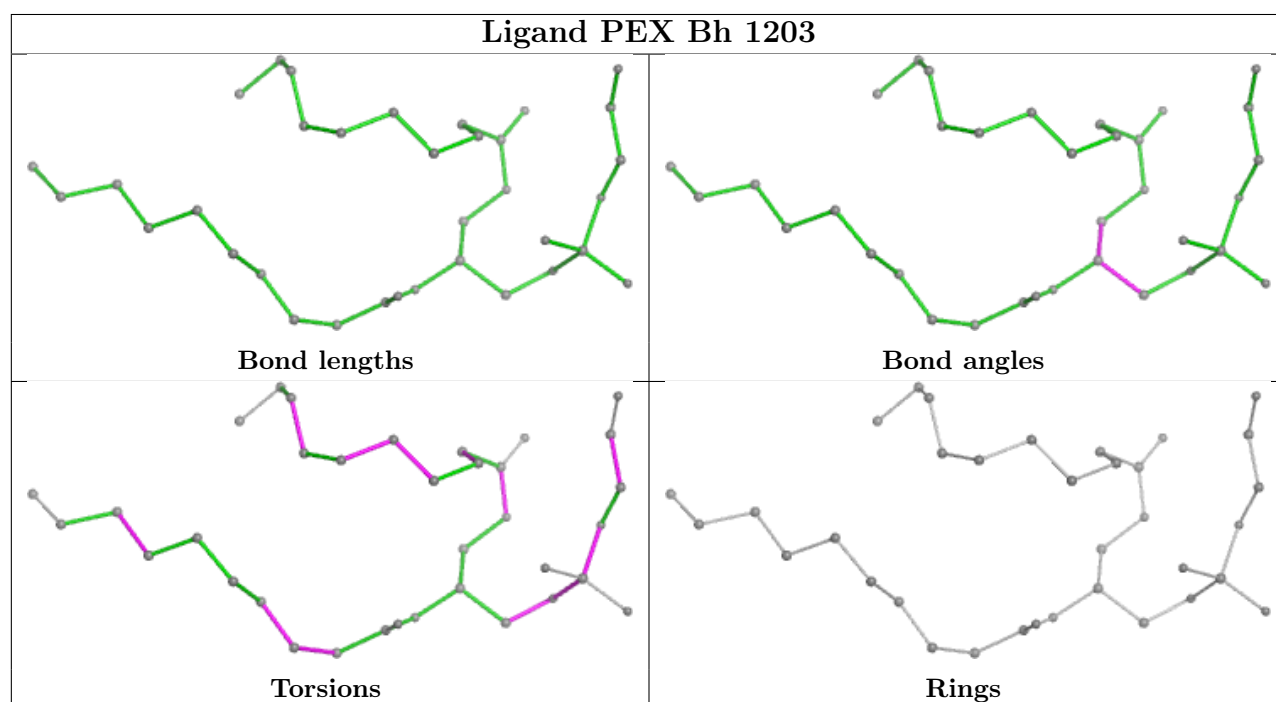
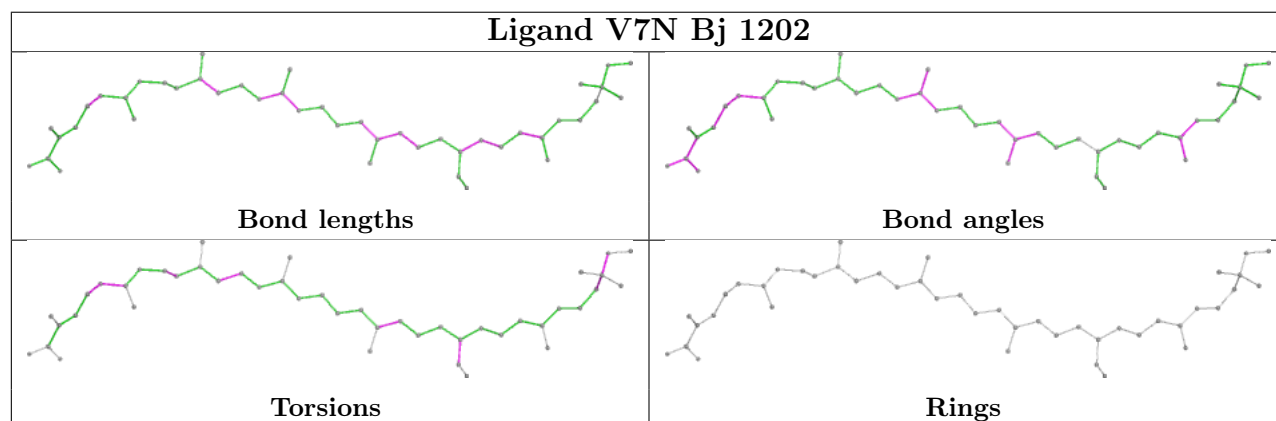
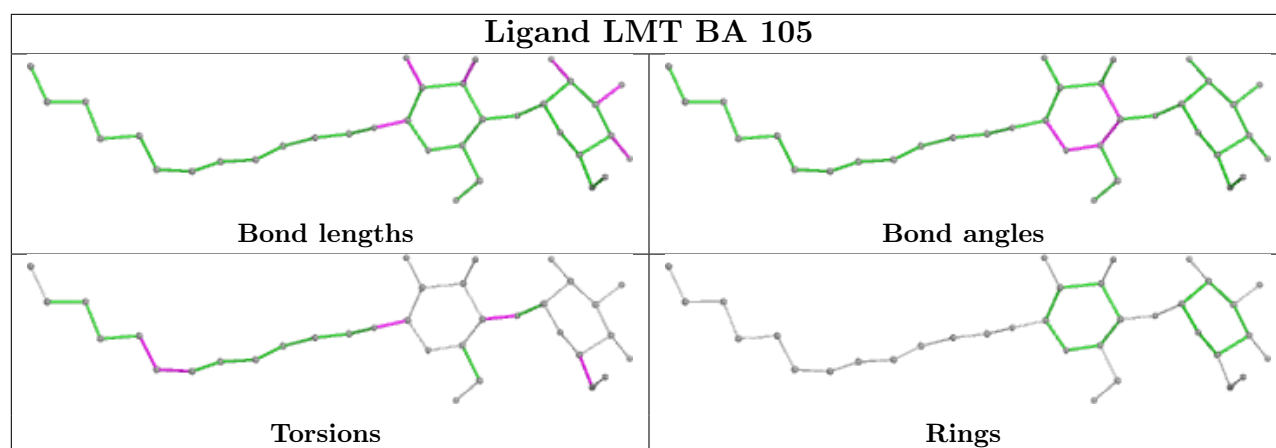
Ligand BCL AT 1103**Ligand BCL AO 101**

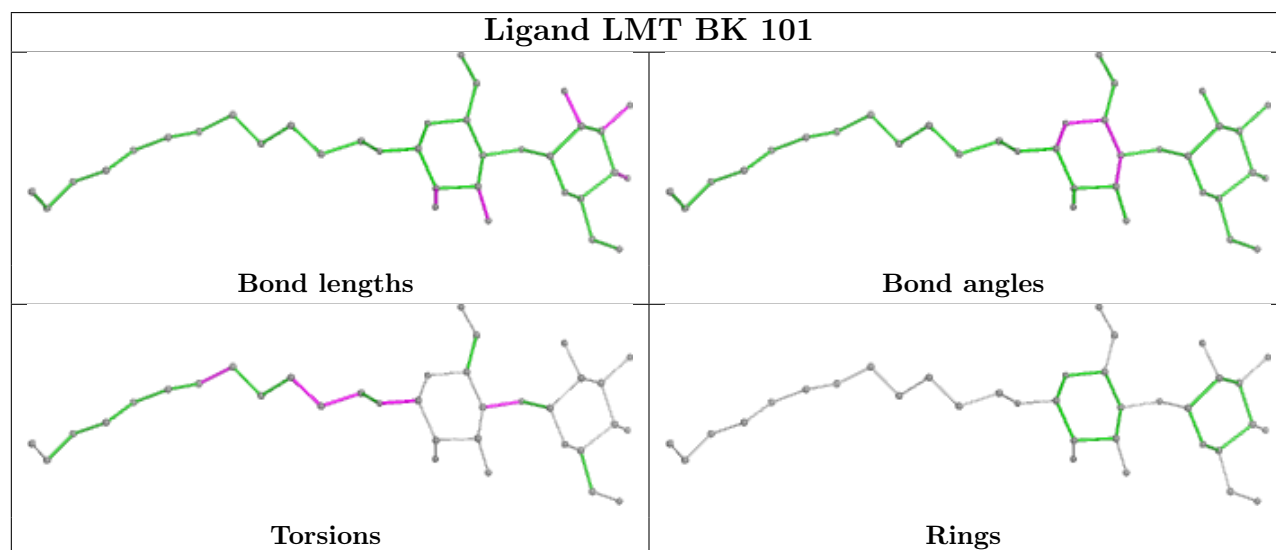
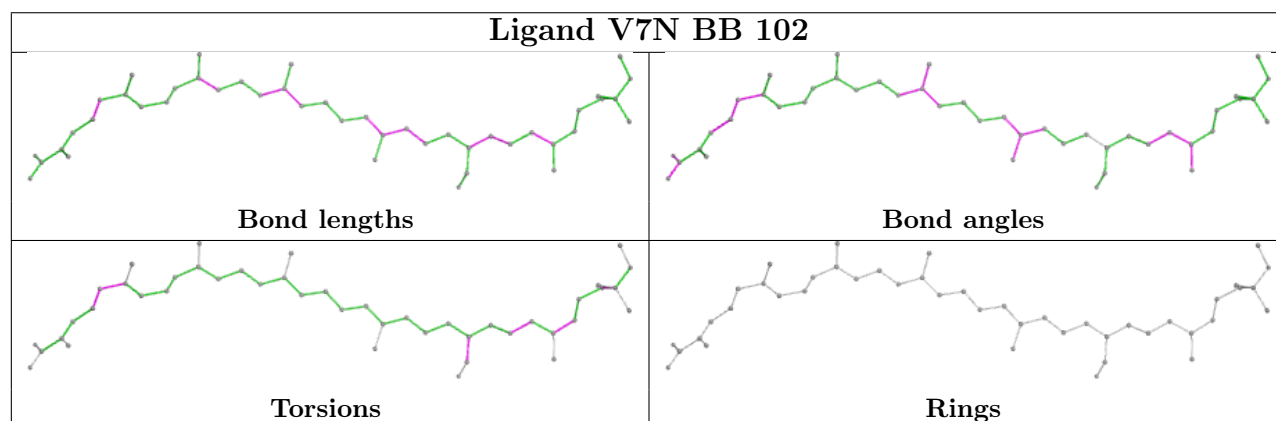
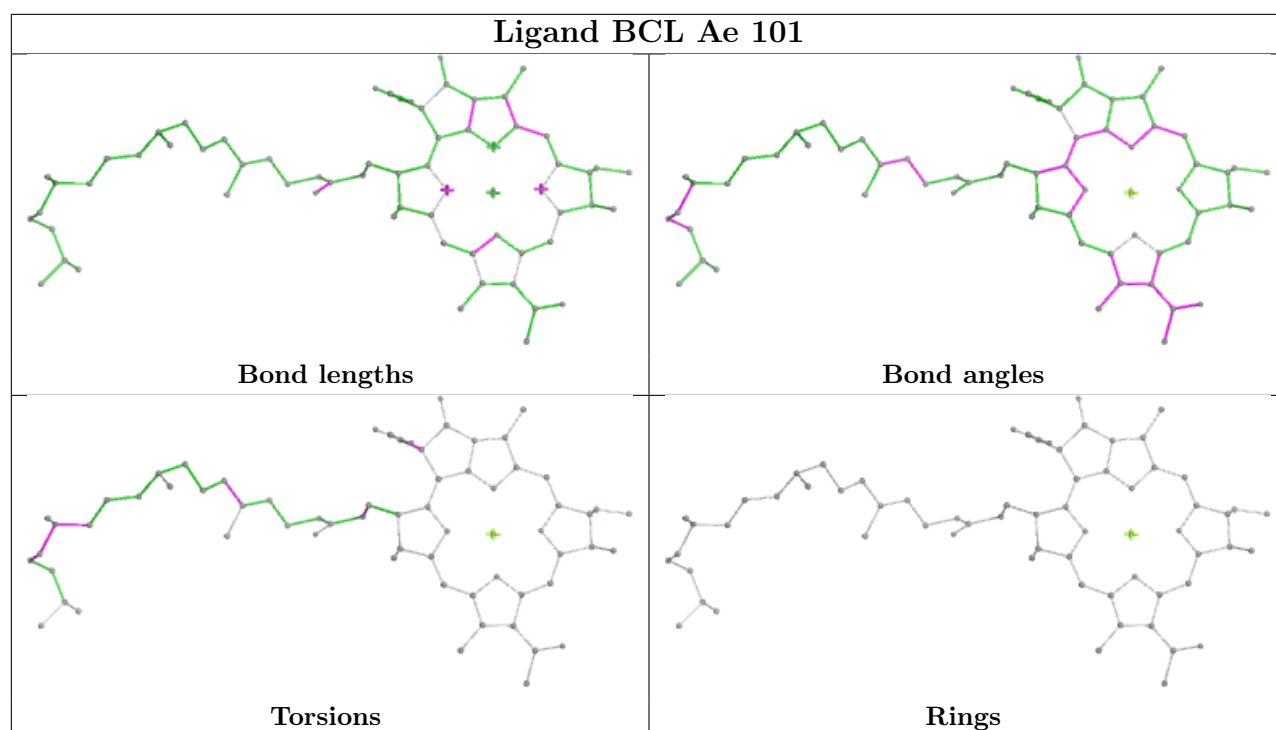


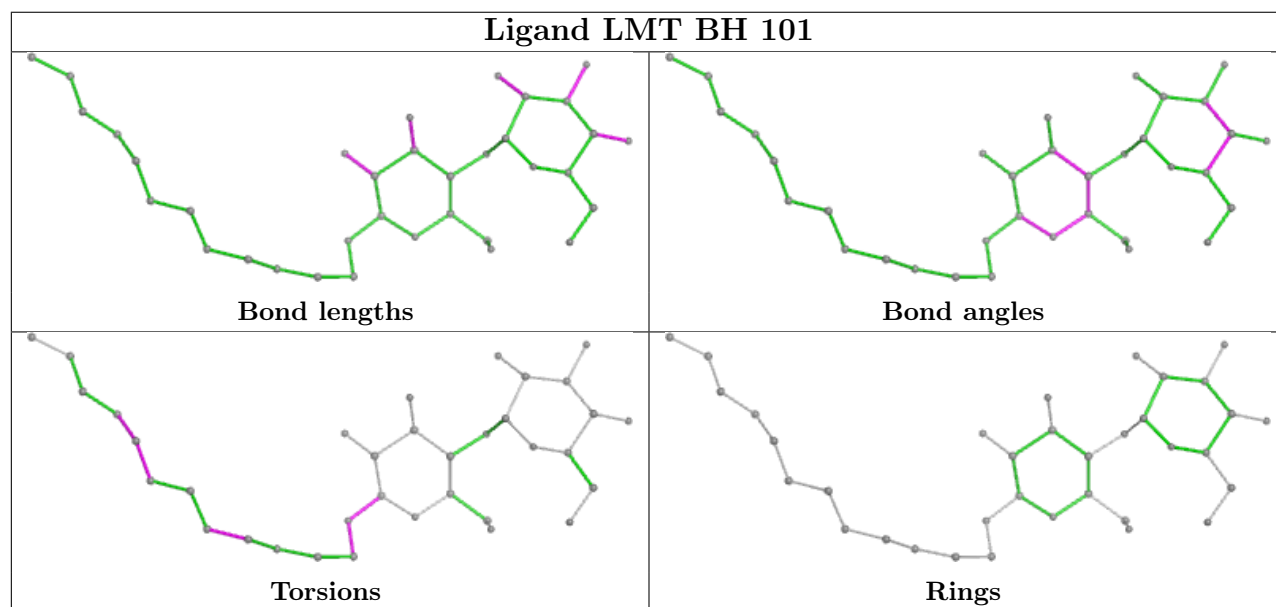
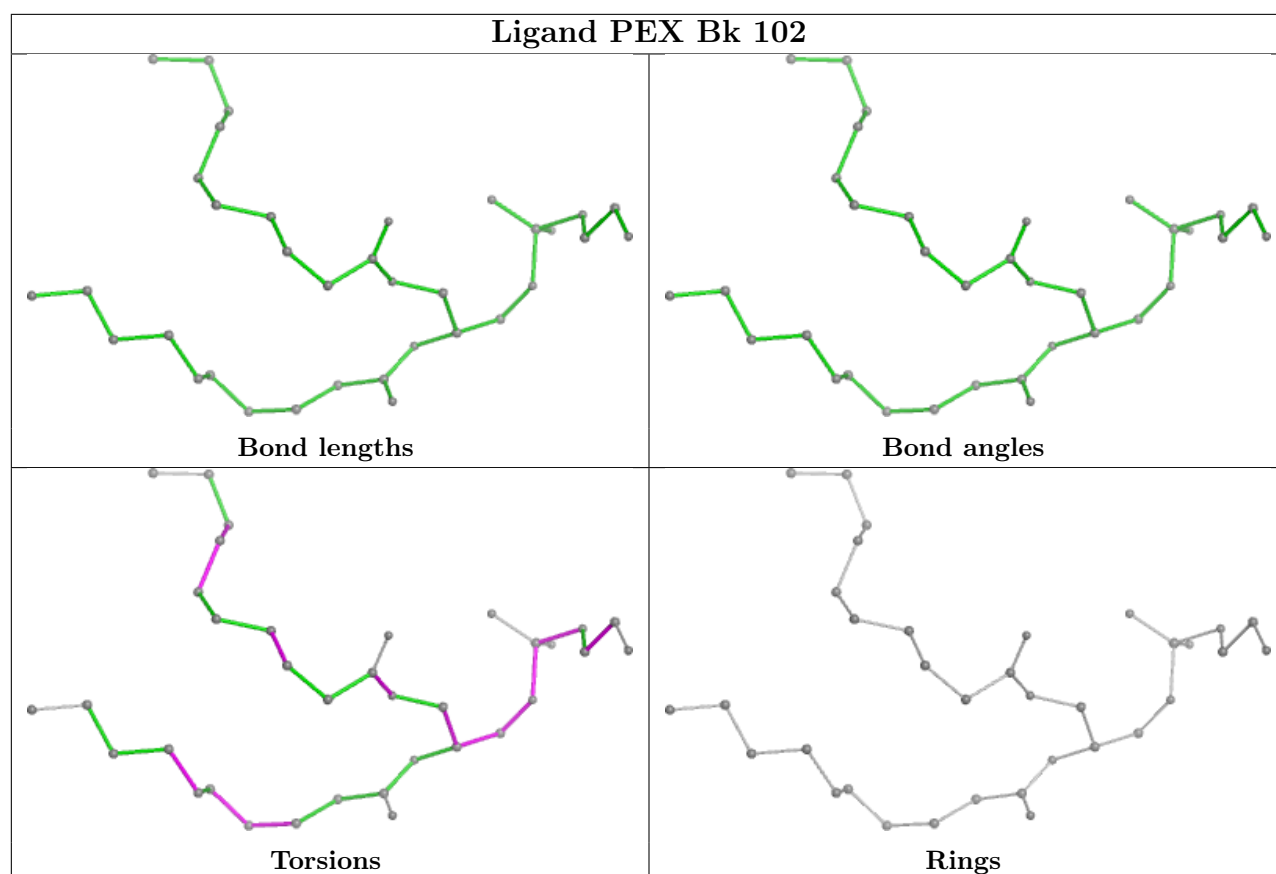


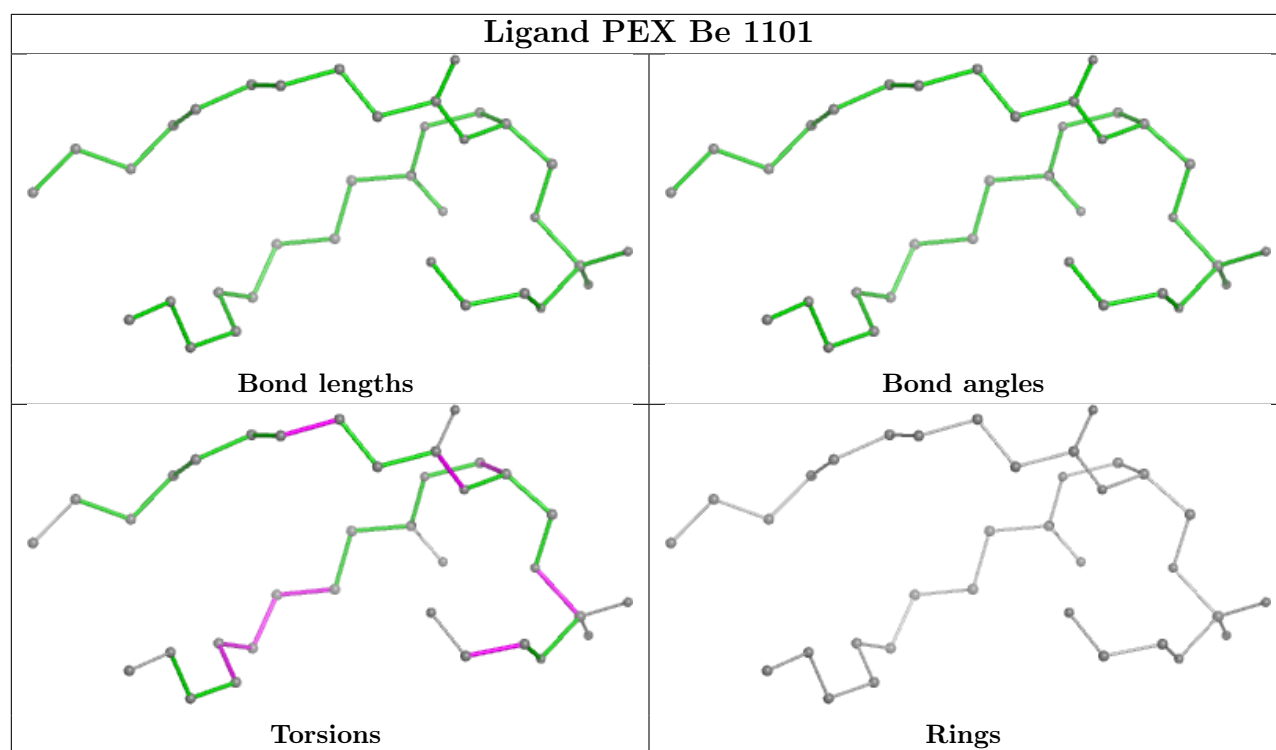


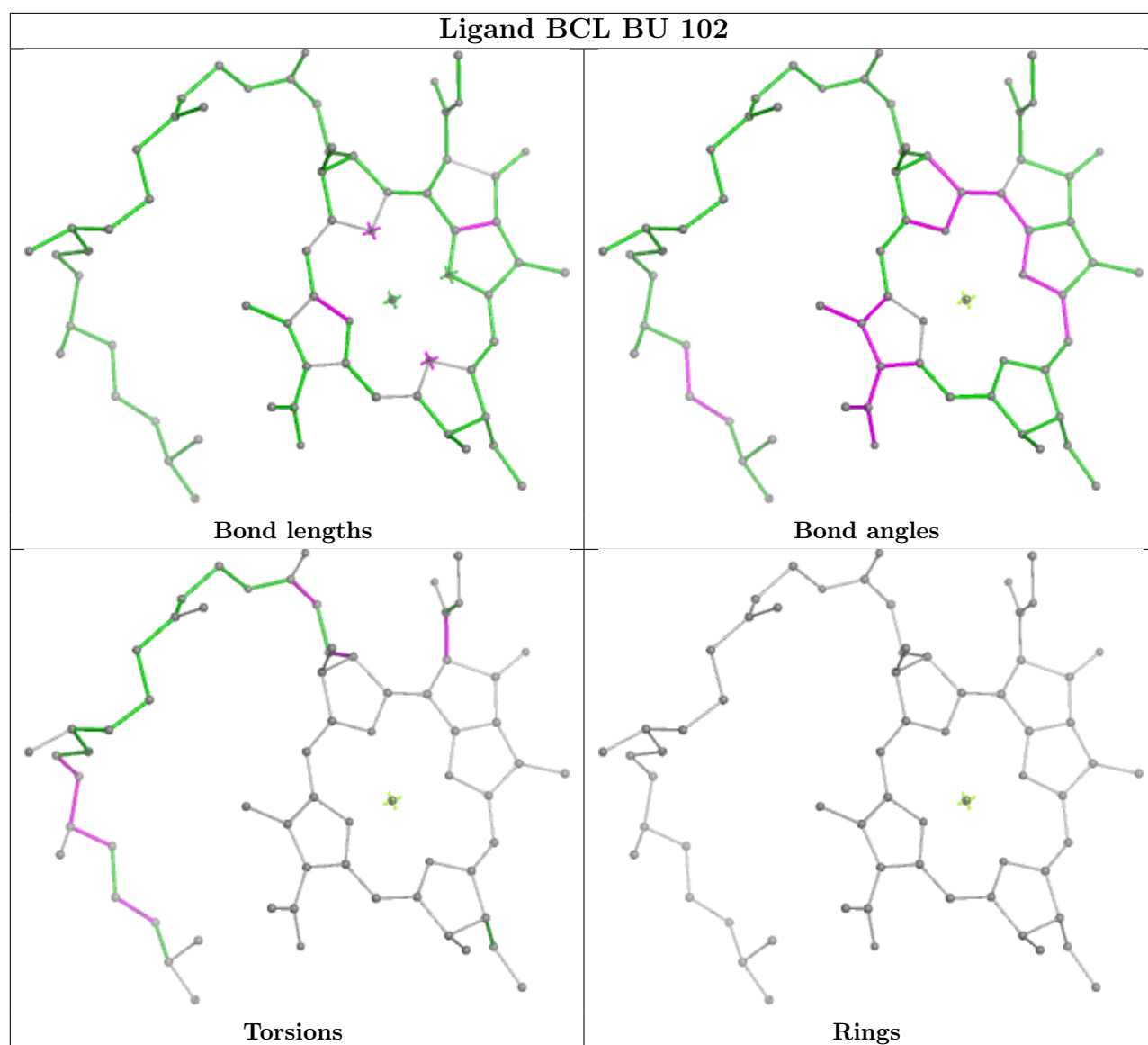


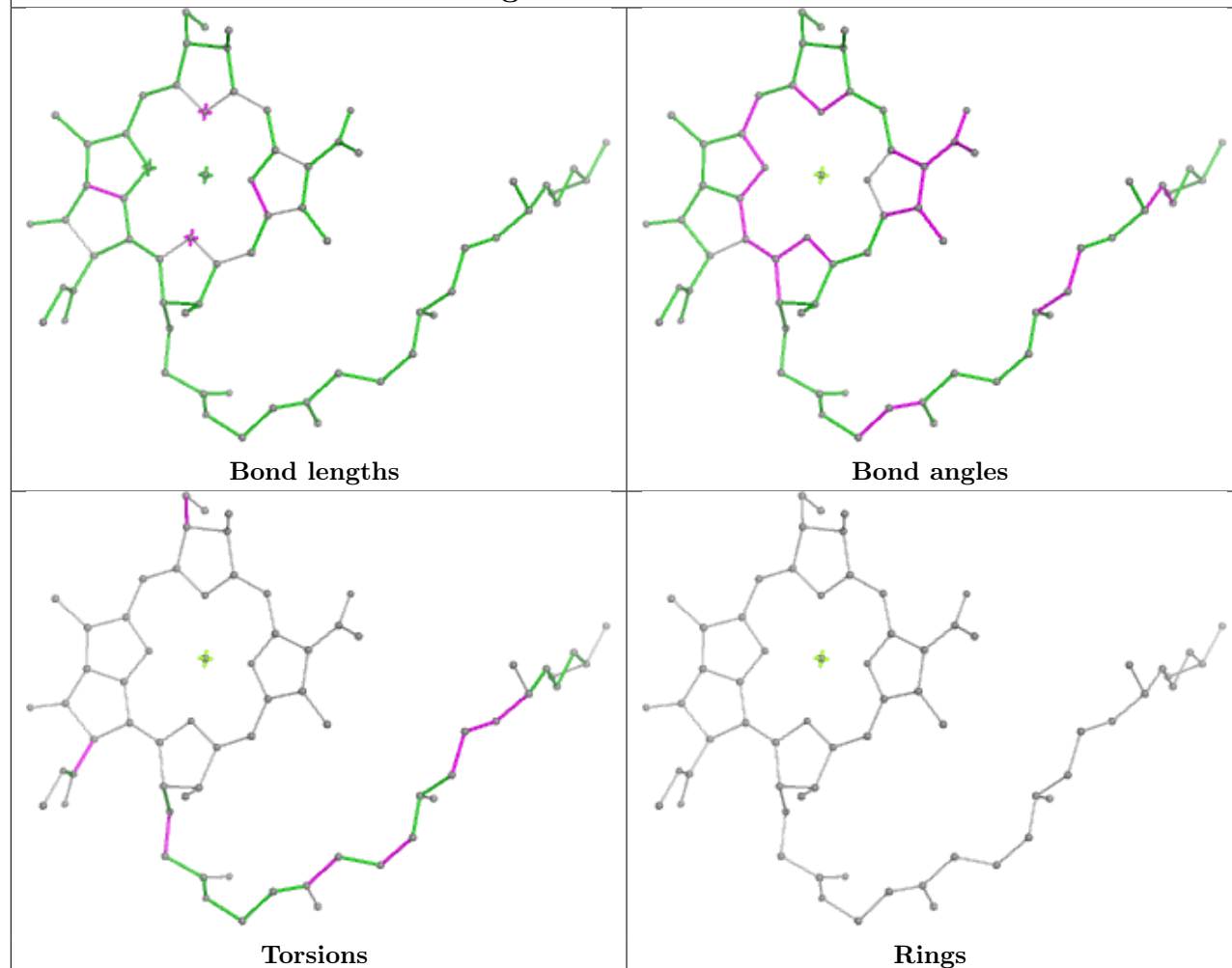
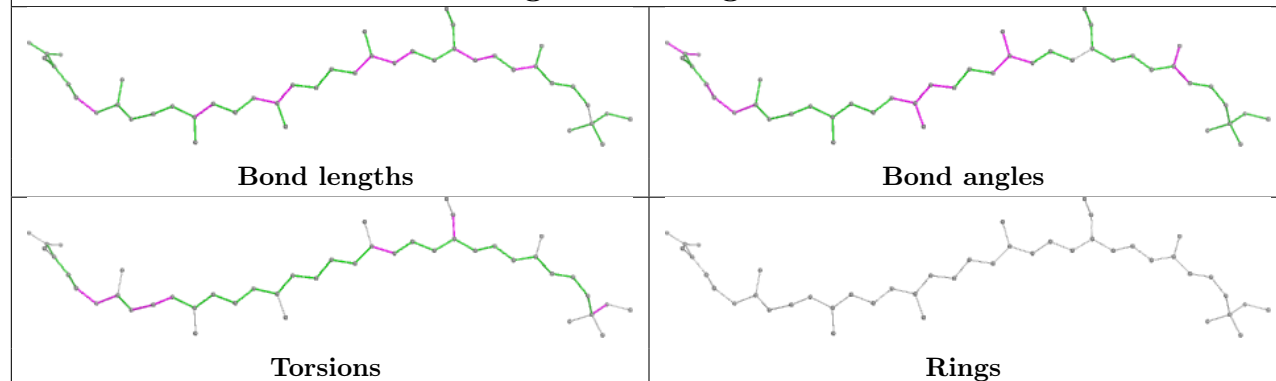


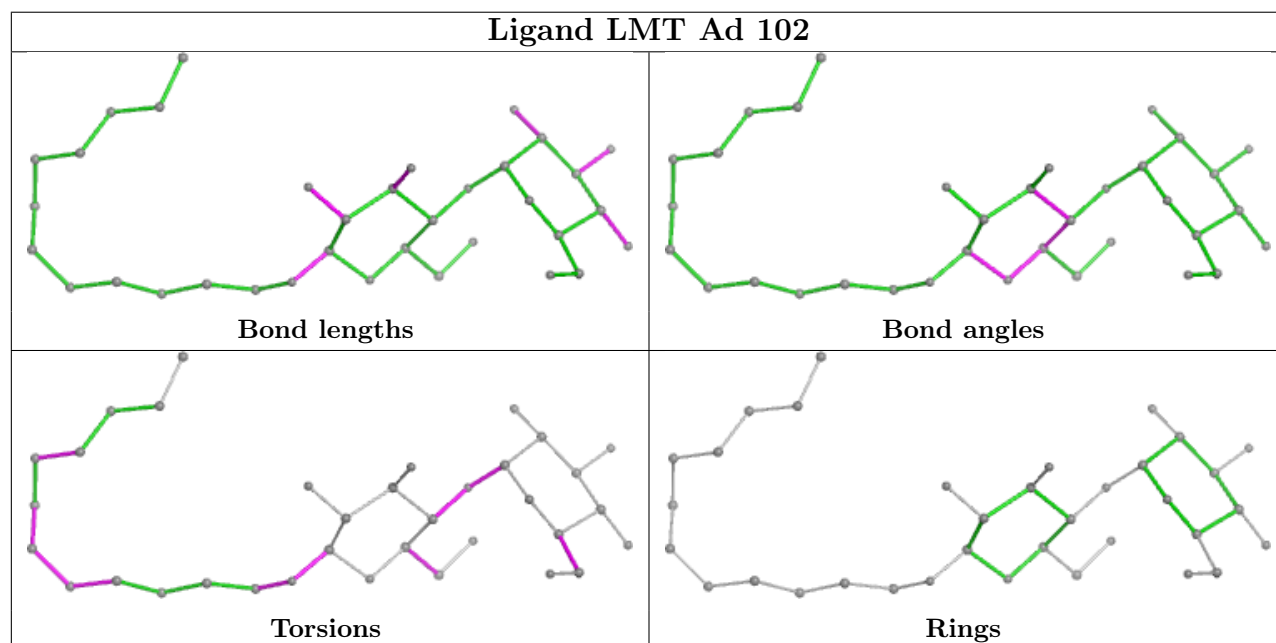
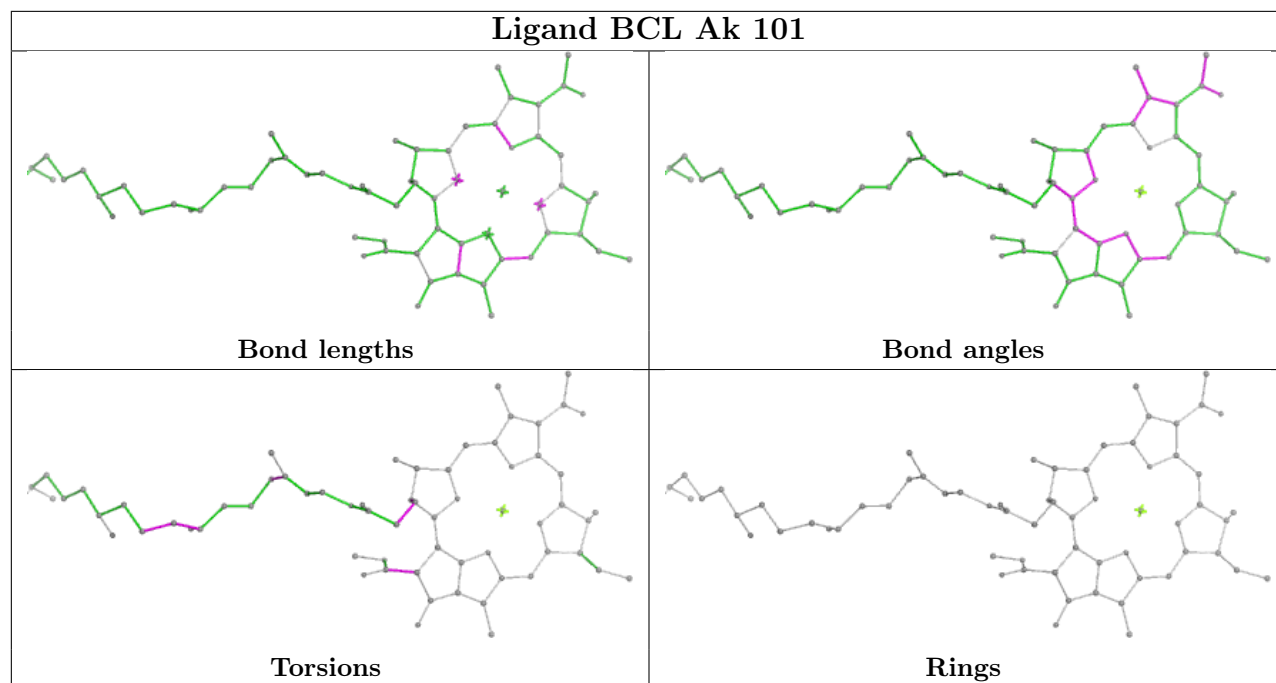


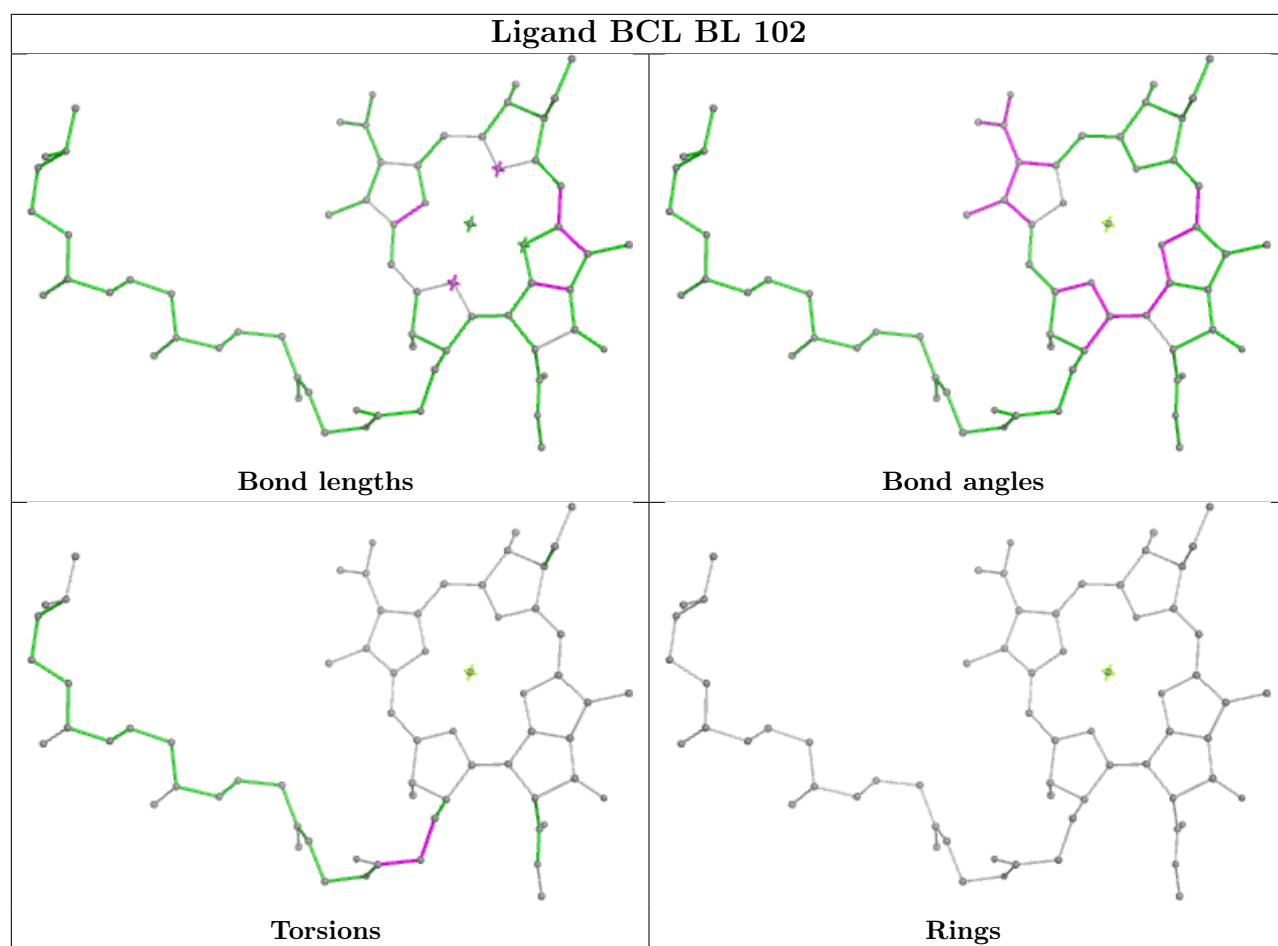




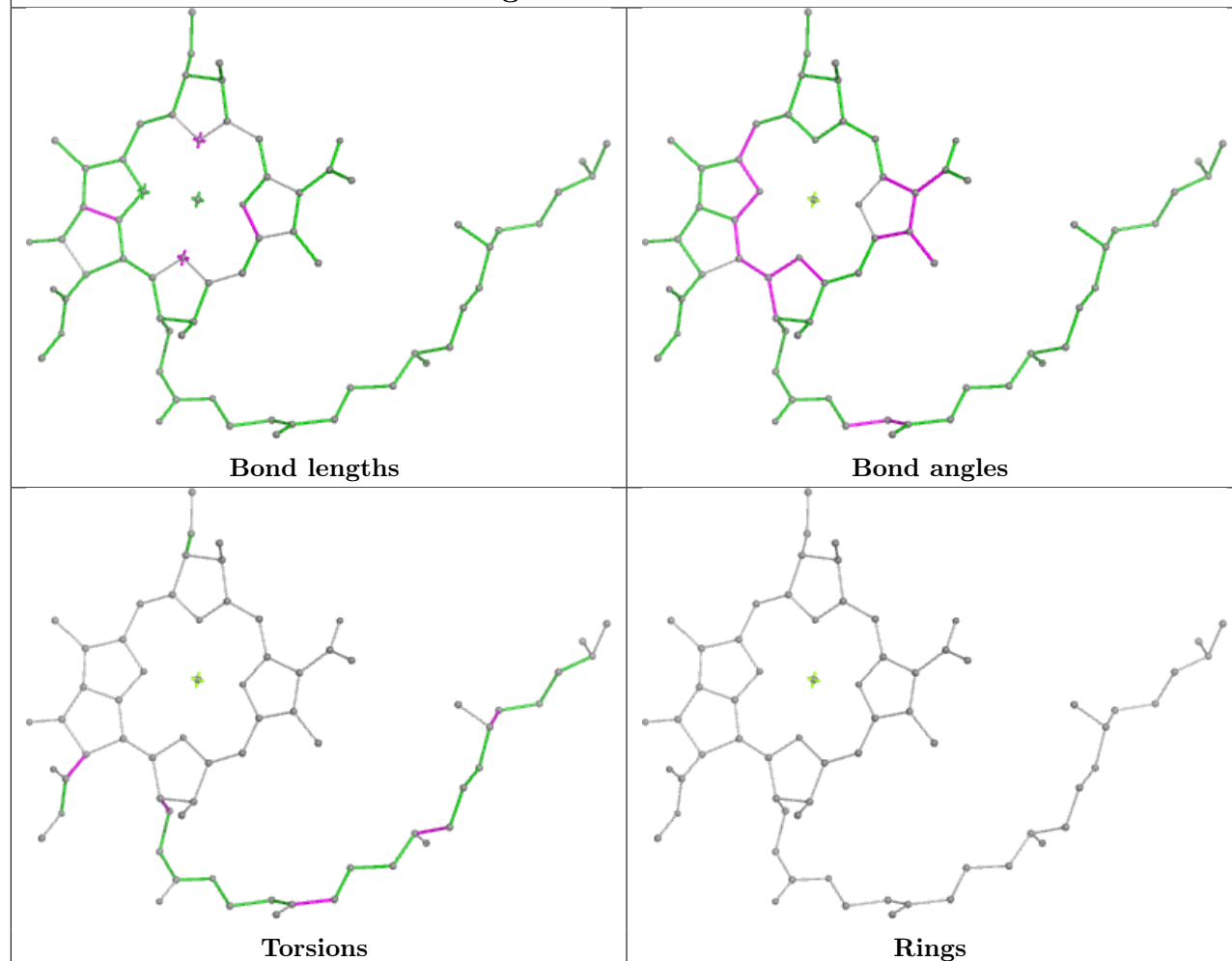


Ligand BCL BX 102**Ligand V7N Bg 101**

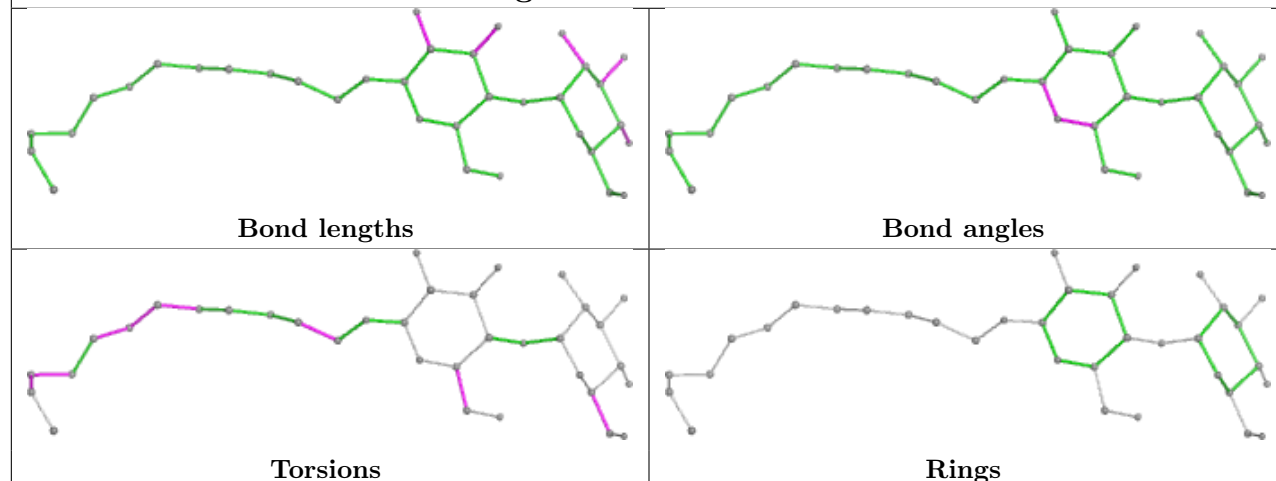




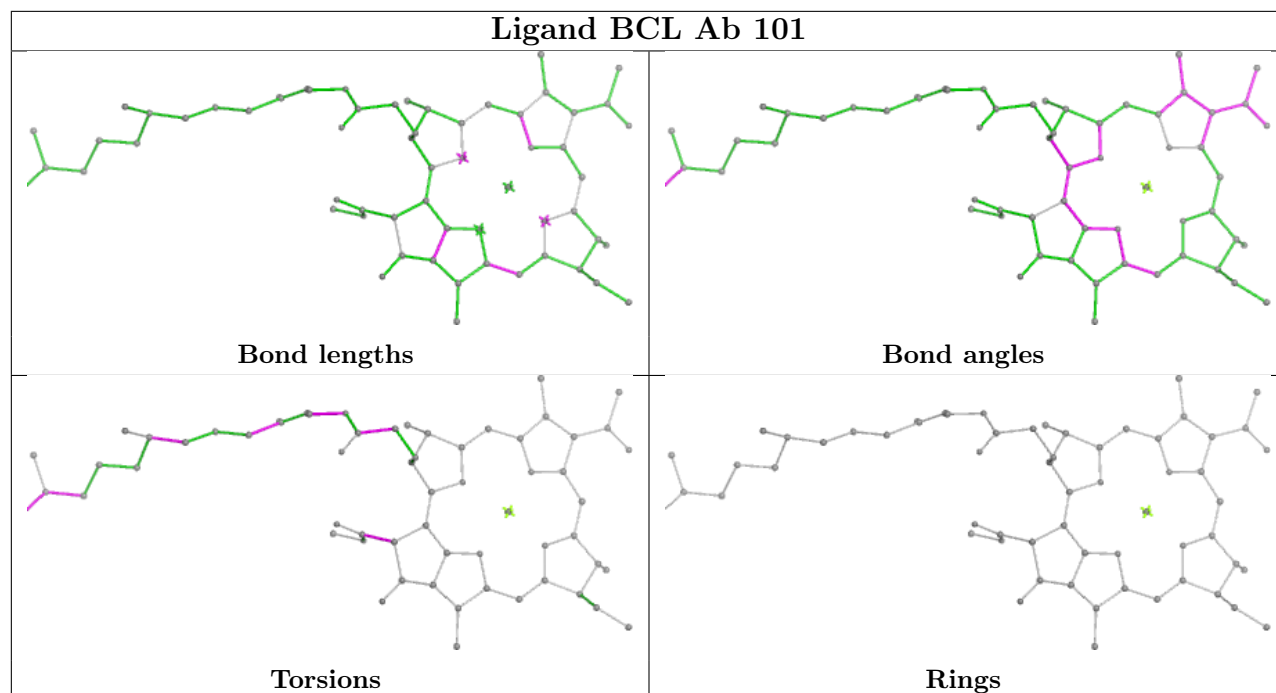
Ligand BCL BR 101



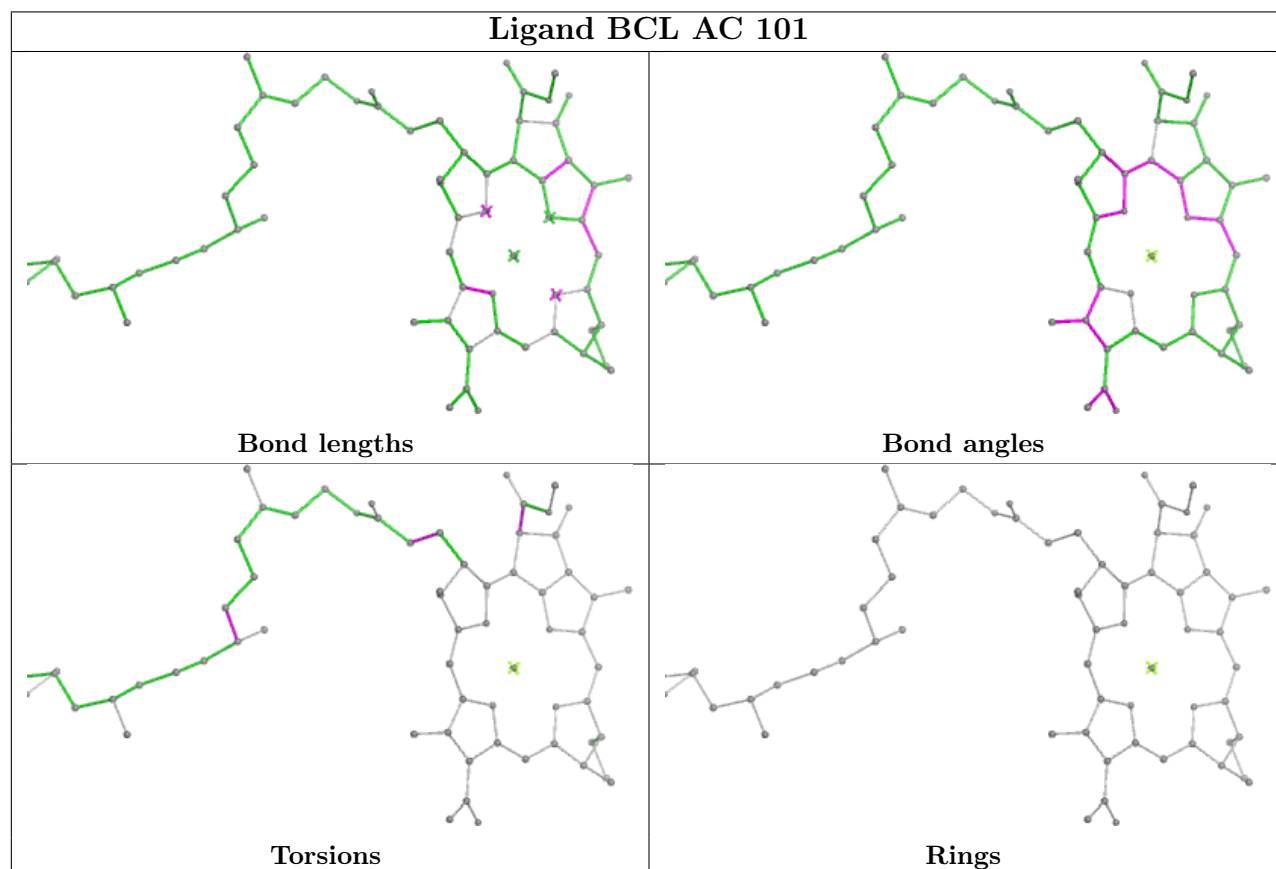
Ligand LMT BH 103

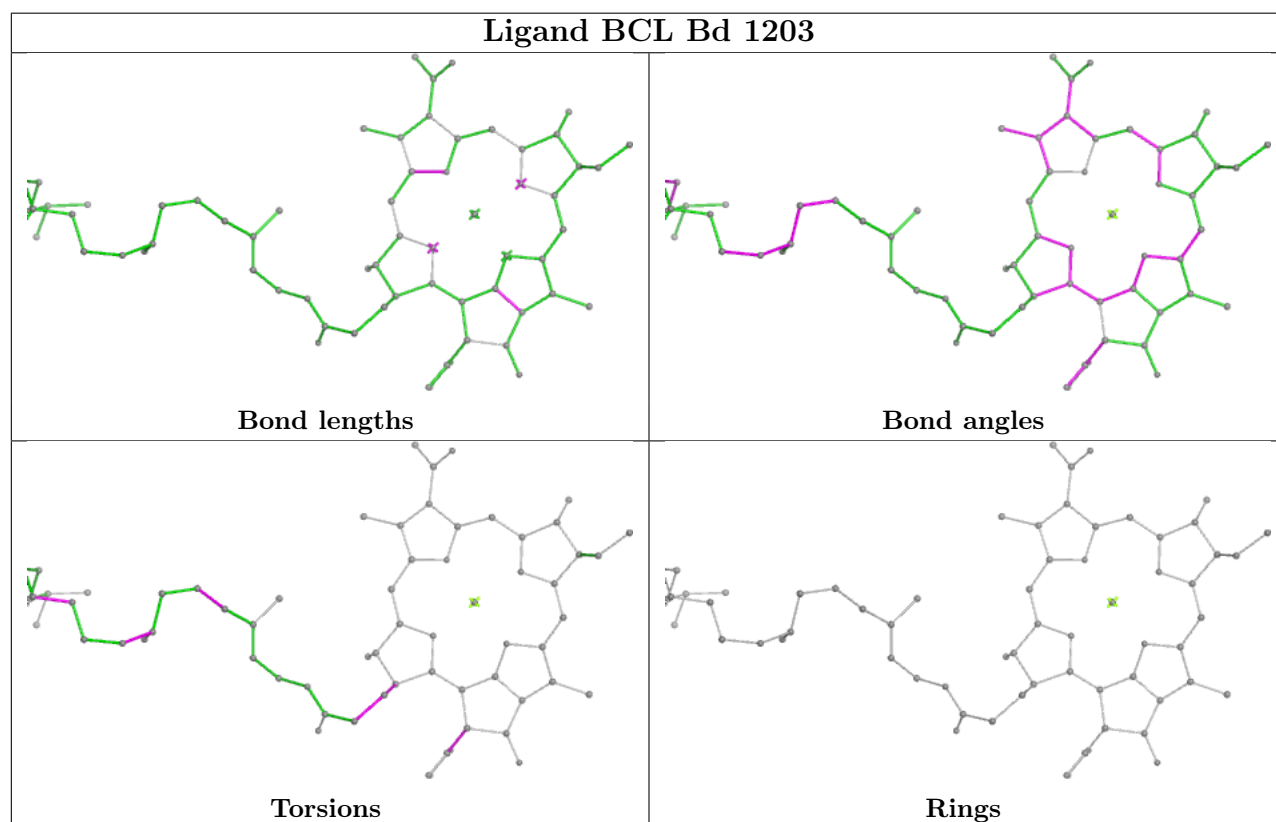
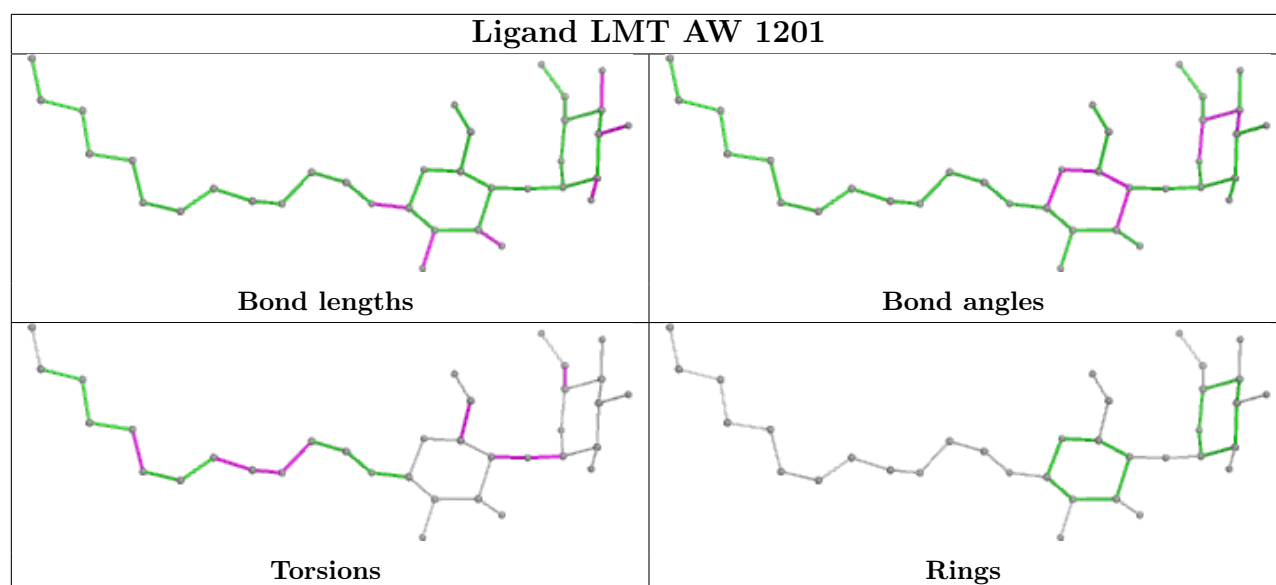


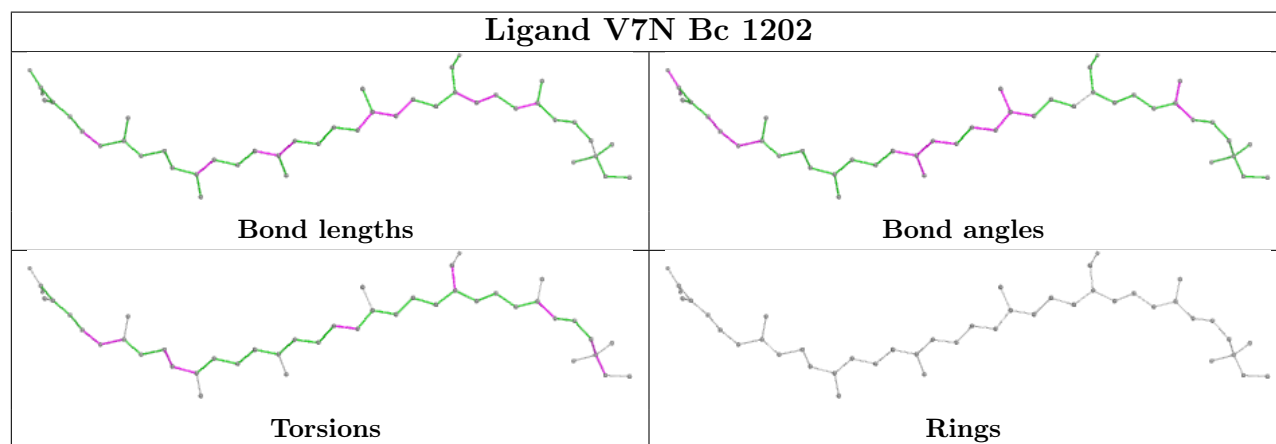
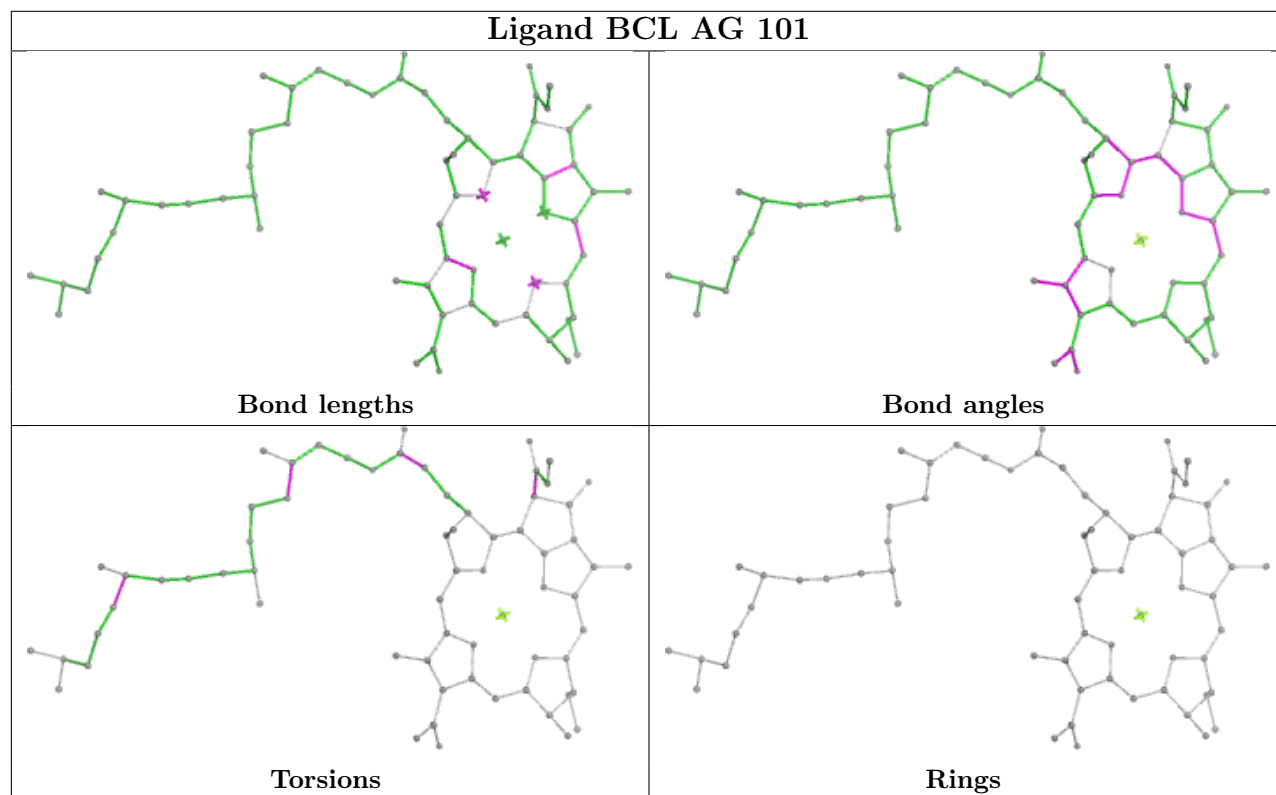
Ligand BCL Ab 101

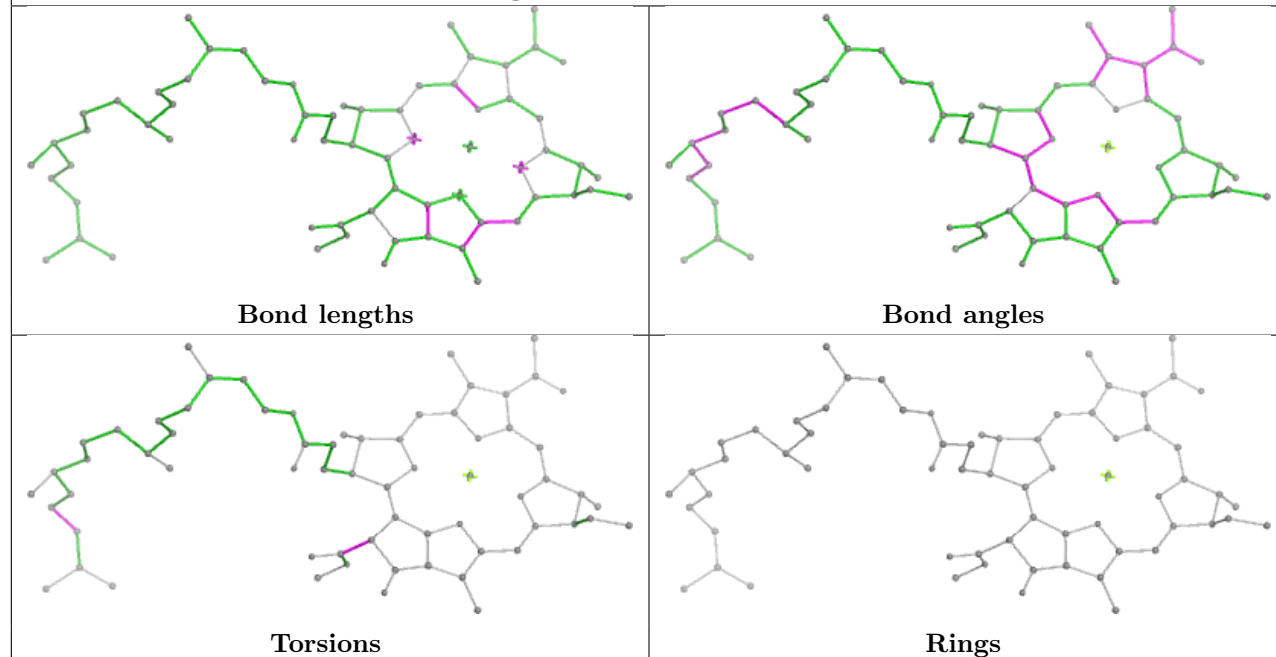
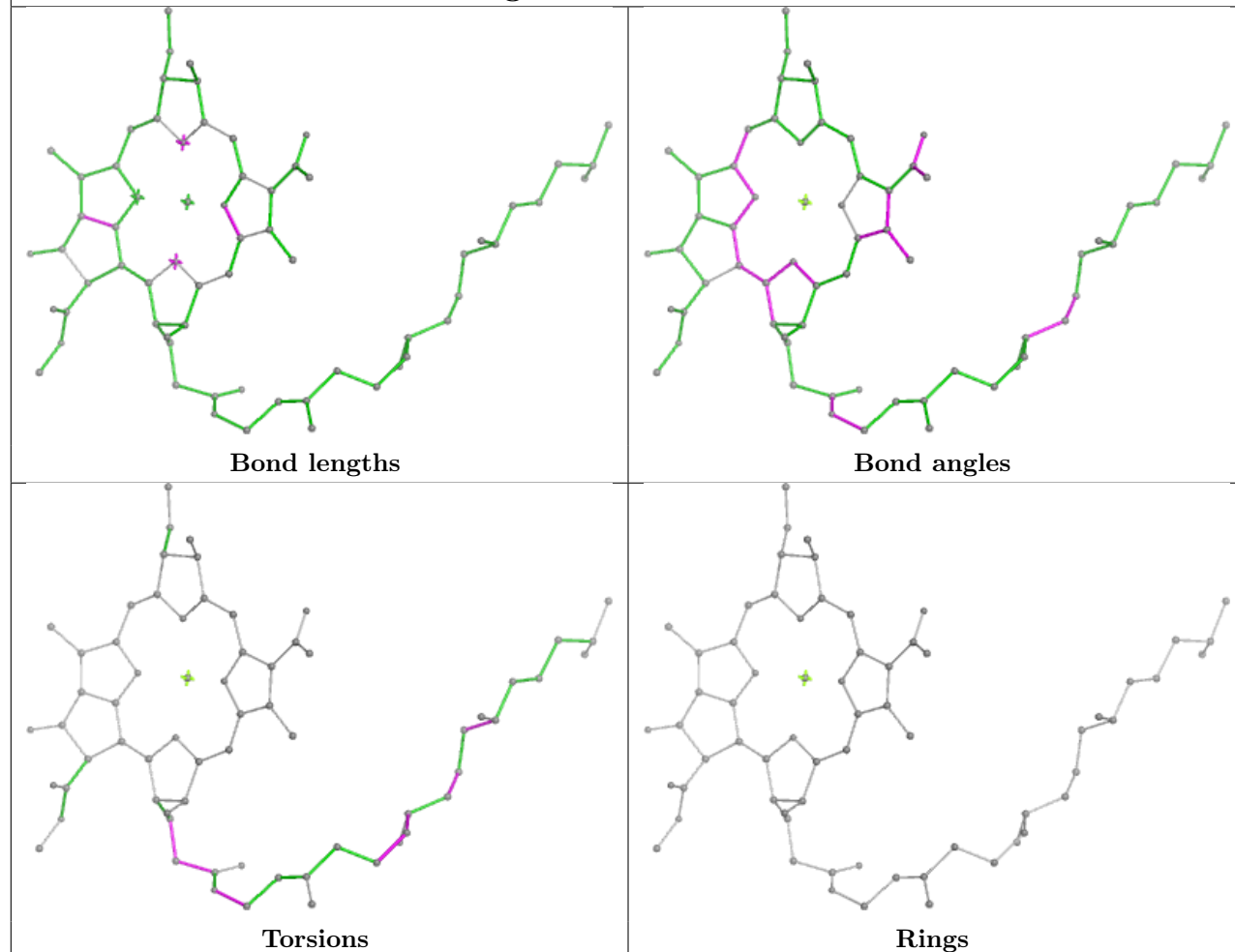


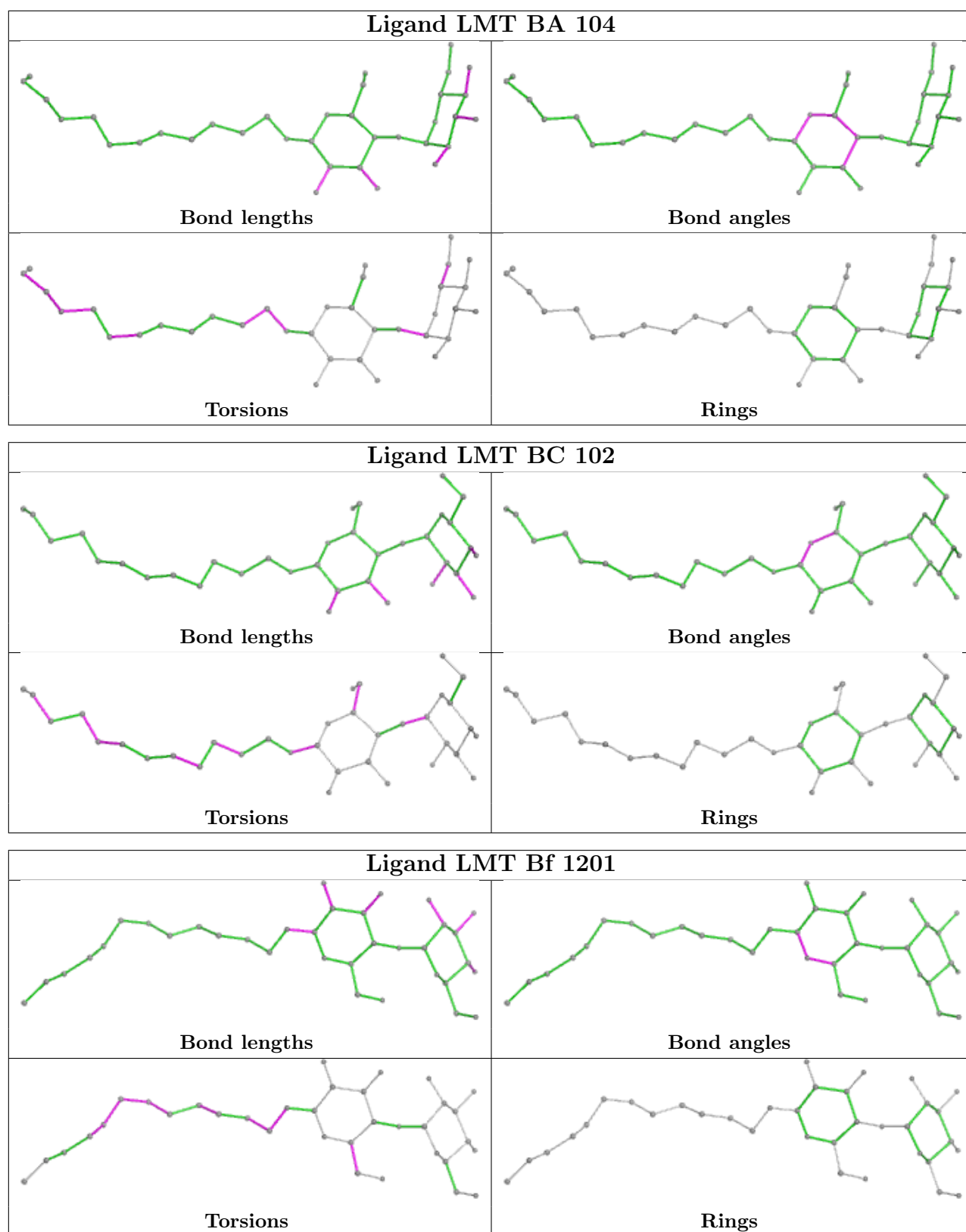
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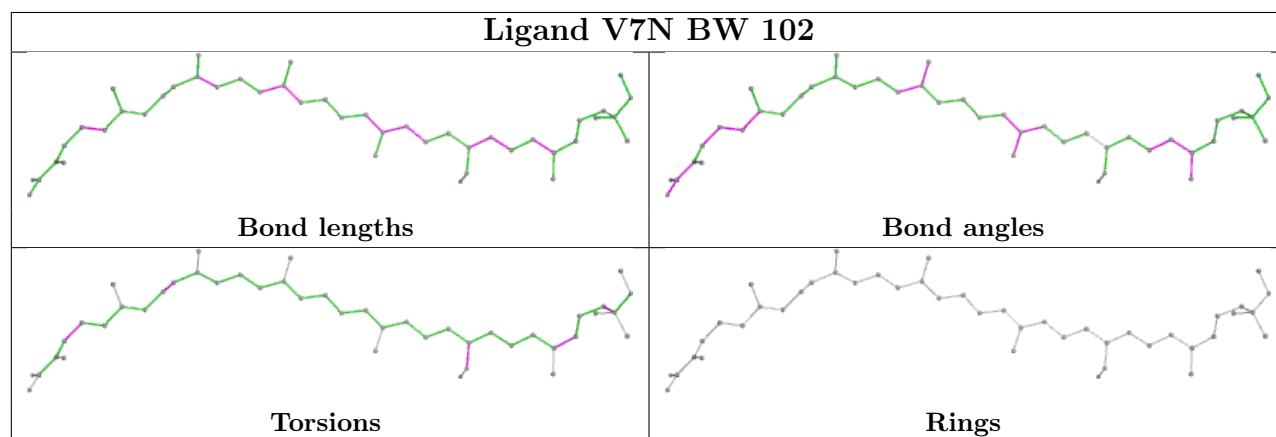
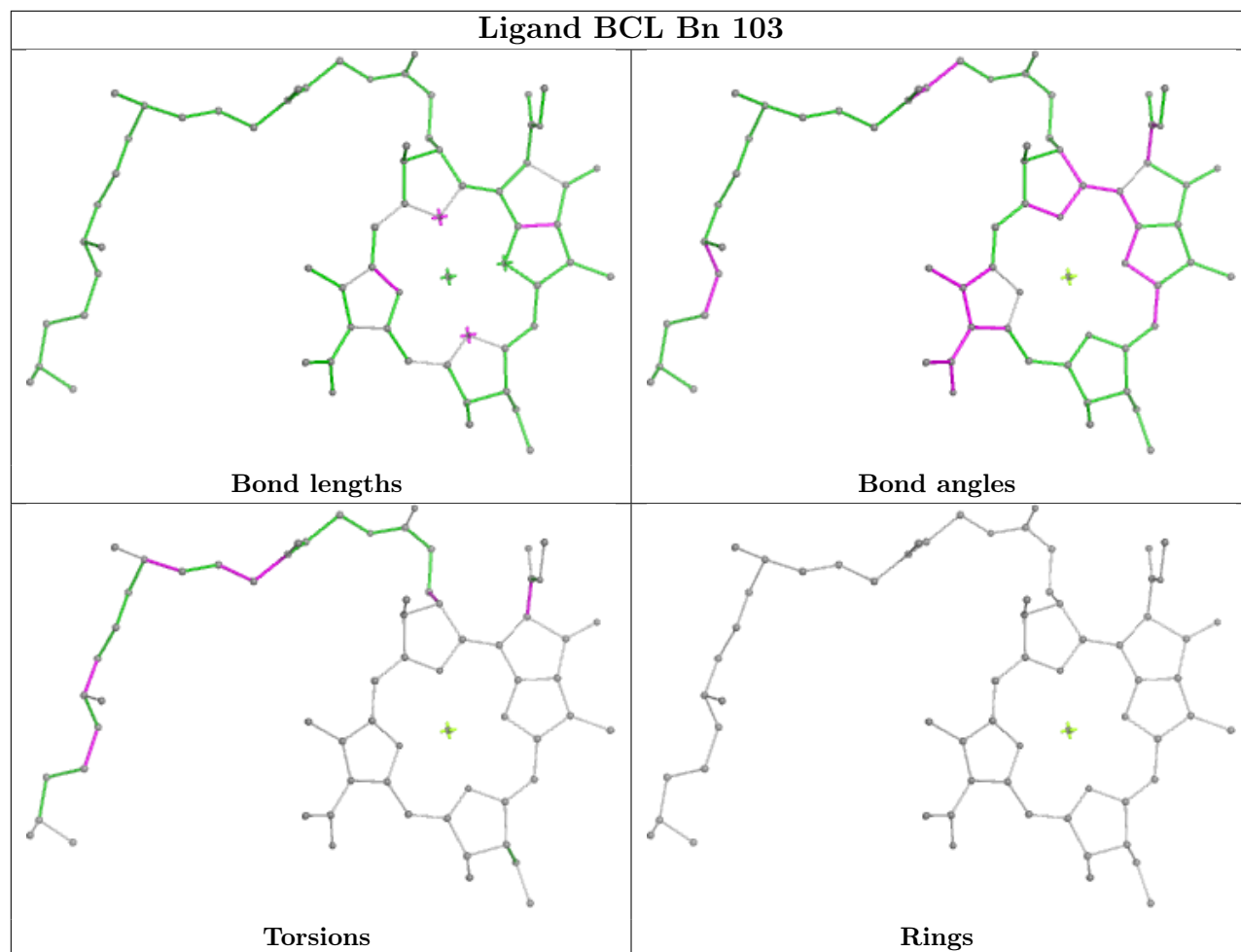


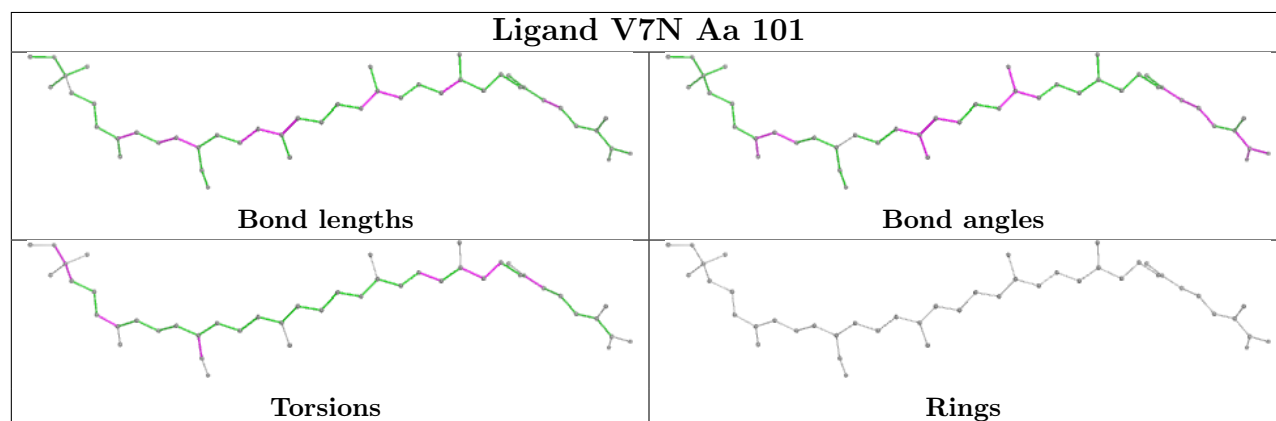
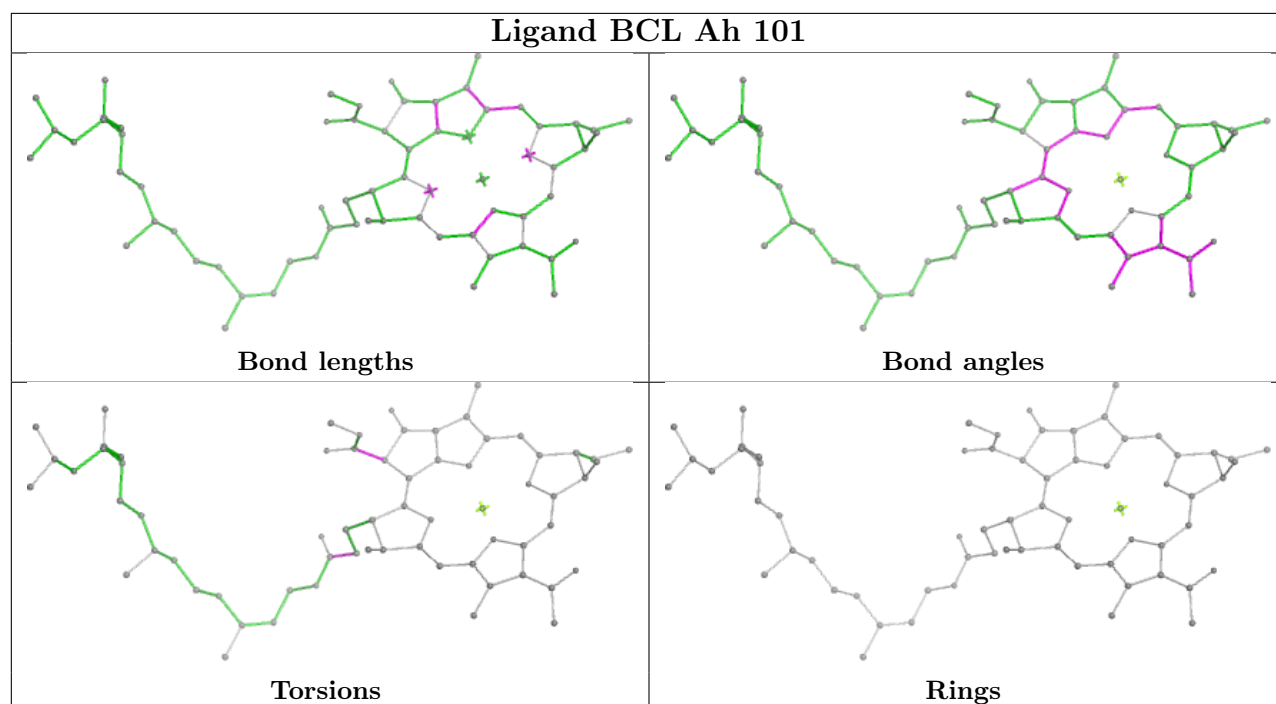
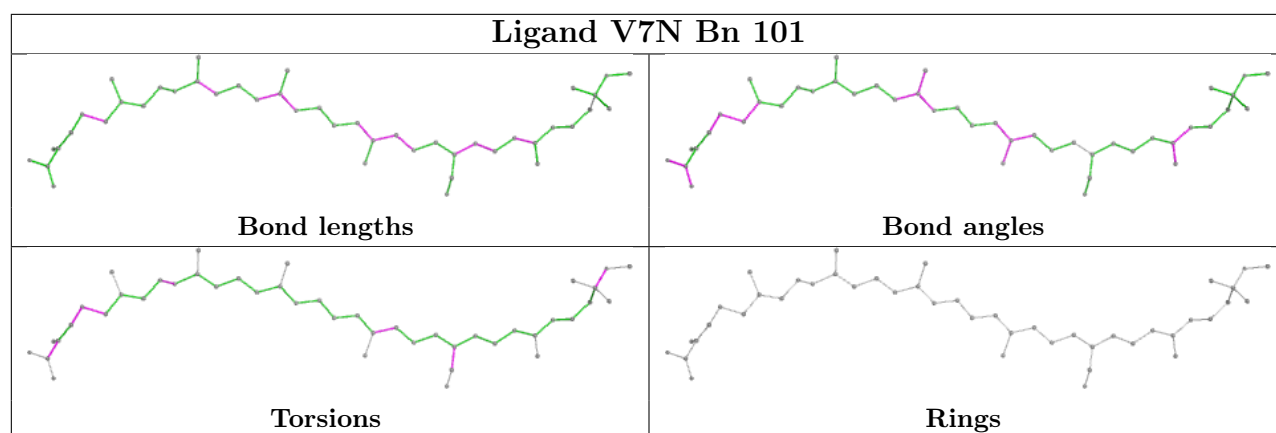


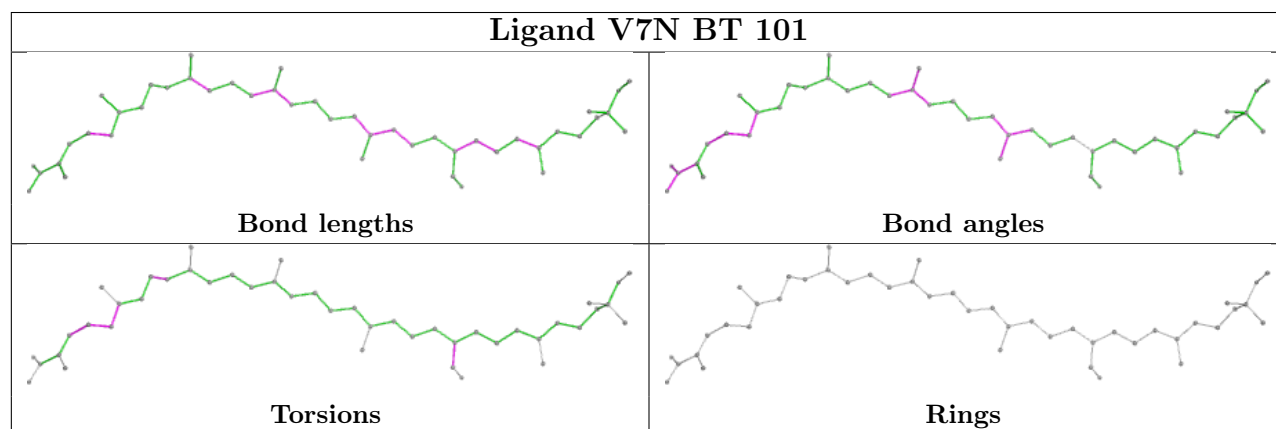
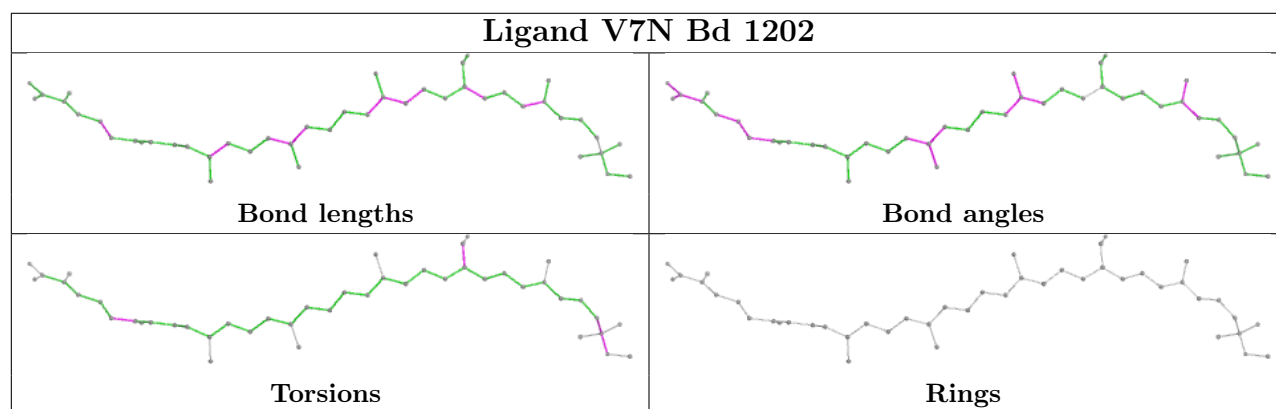
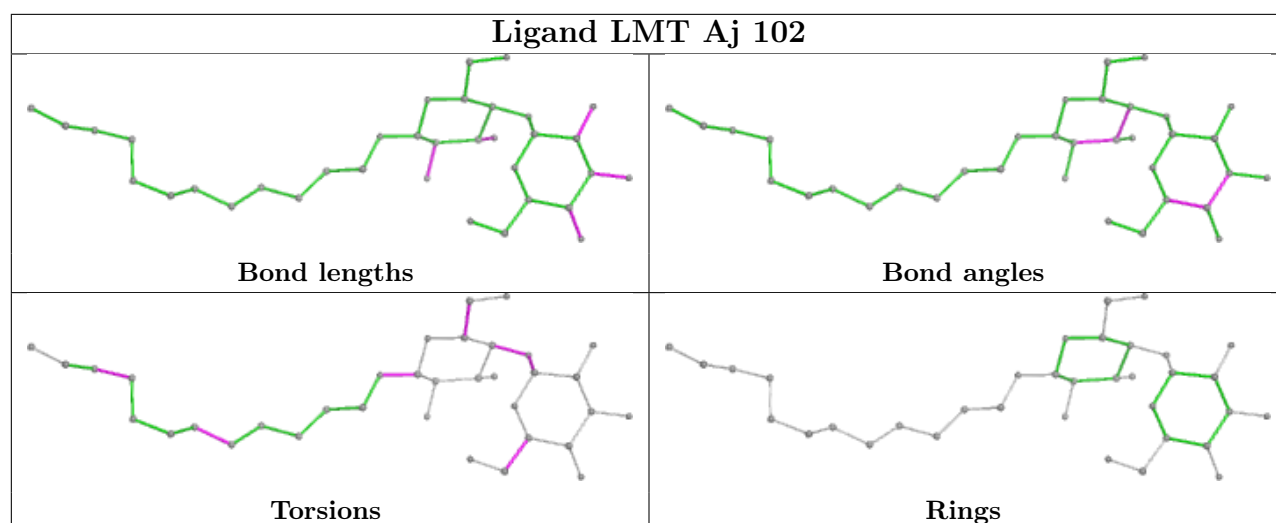


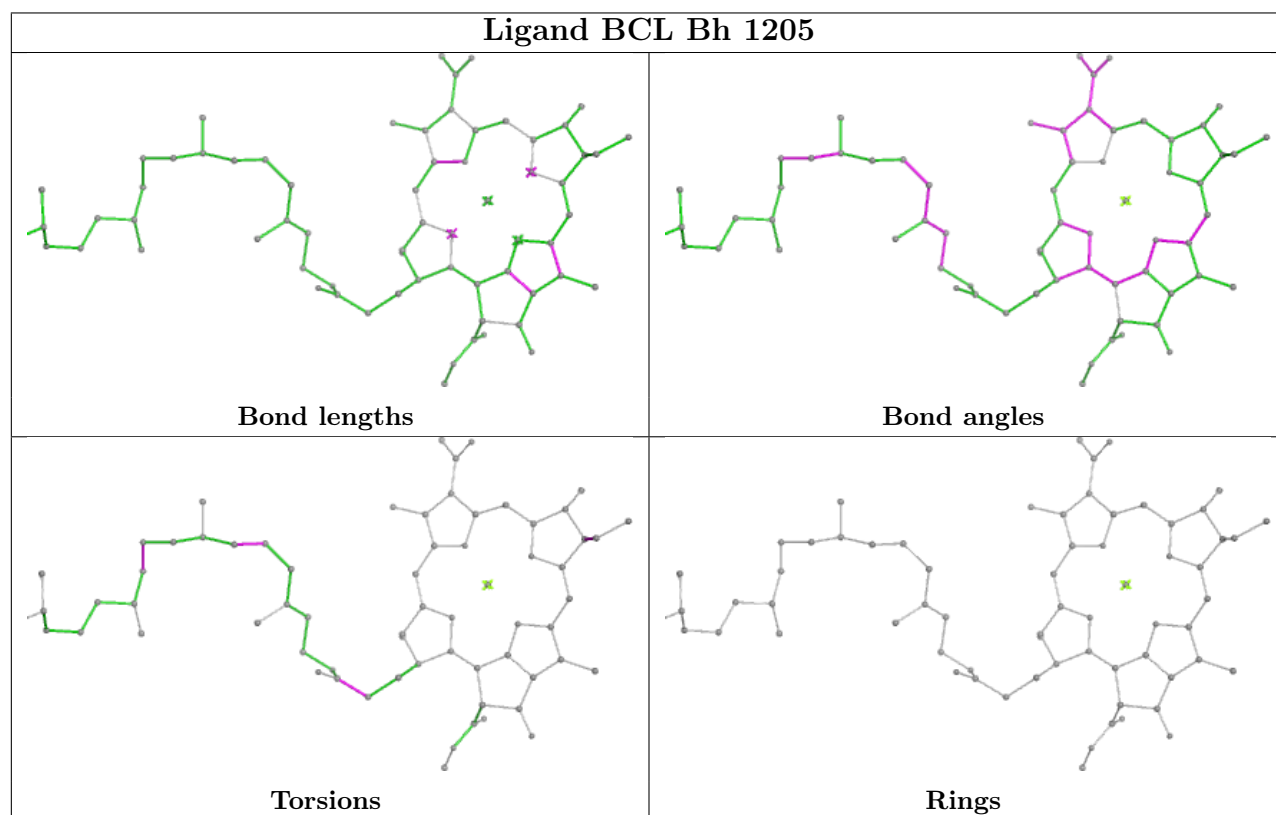
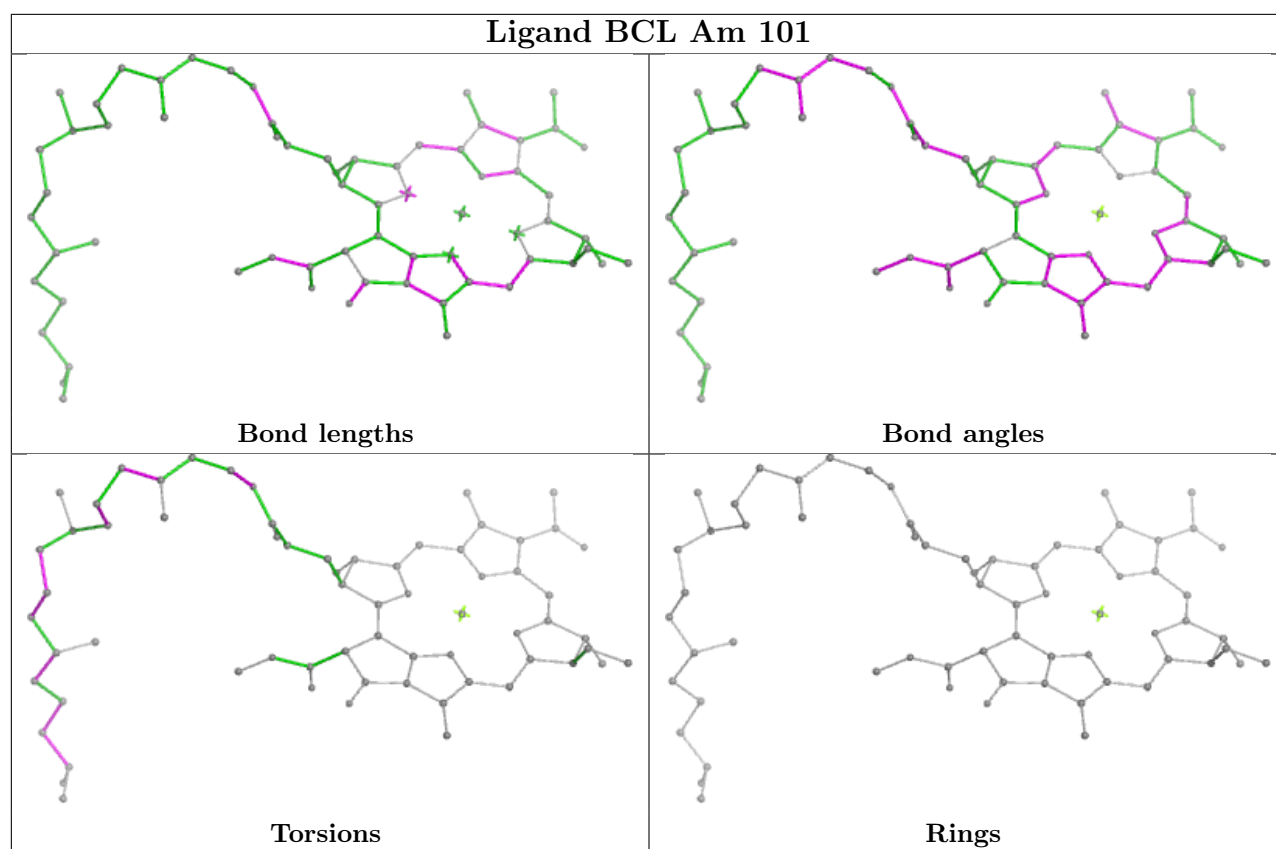
Ligand BCL AW 1202**Ligand BCL BP 101**

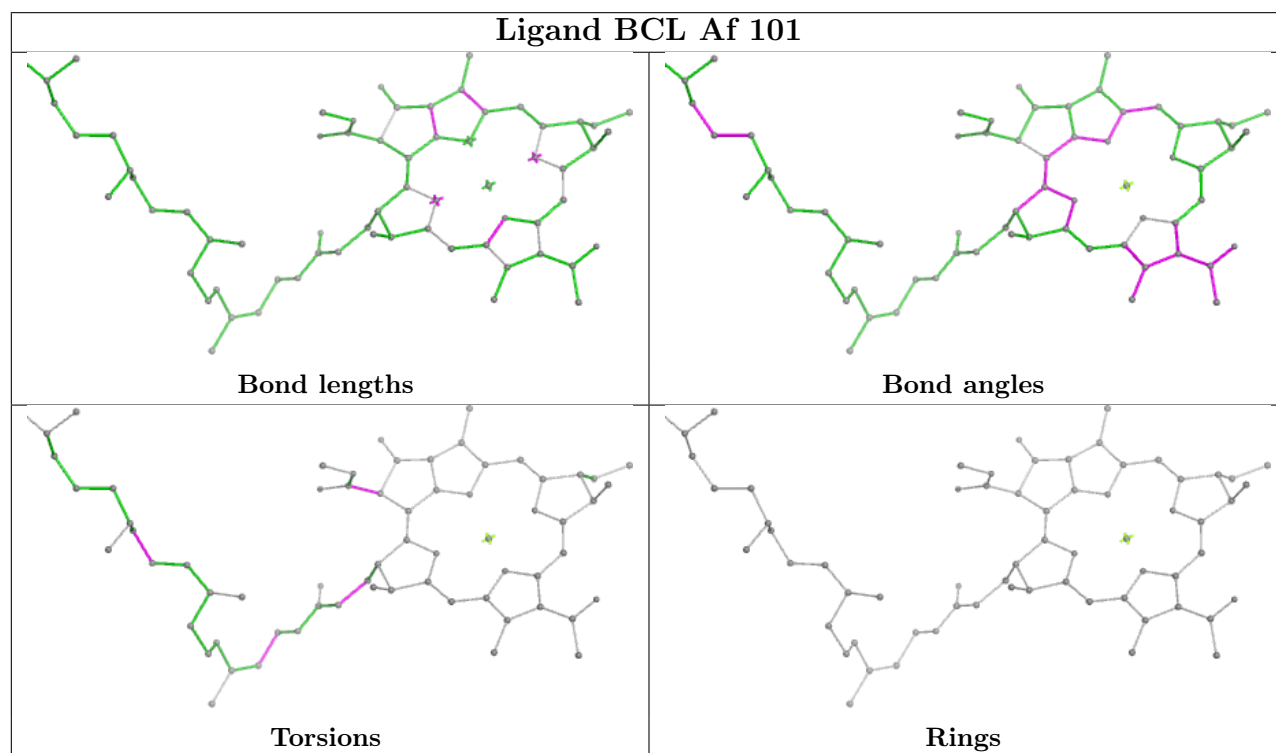
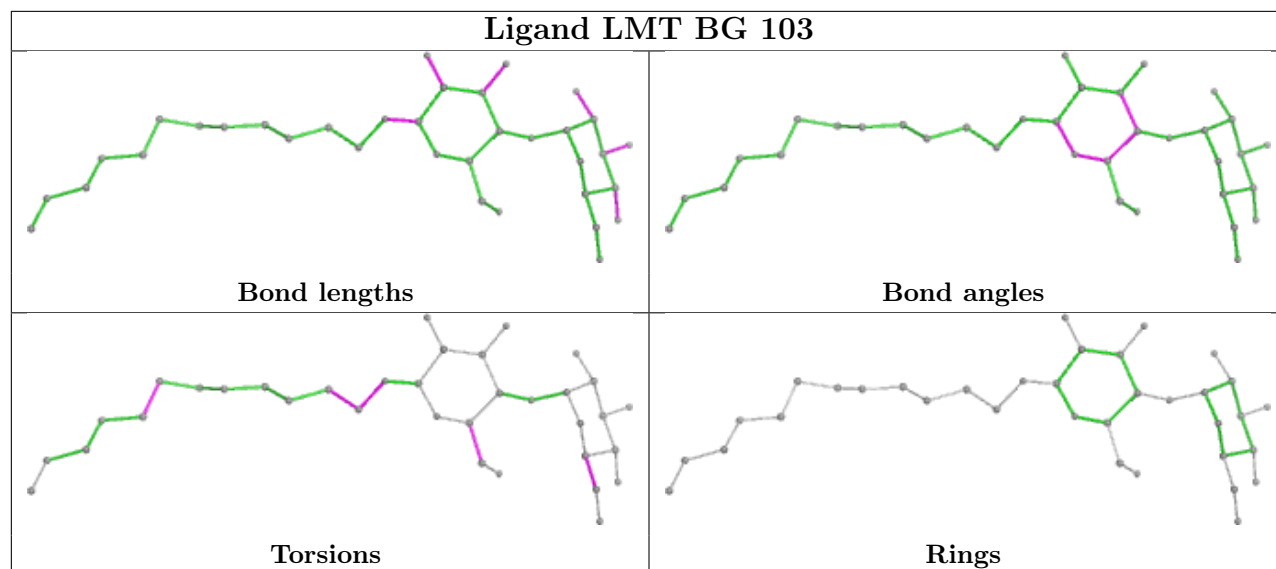




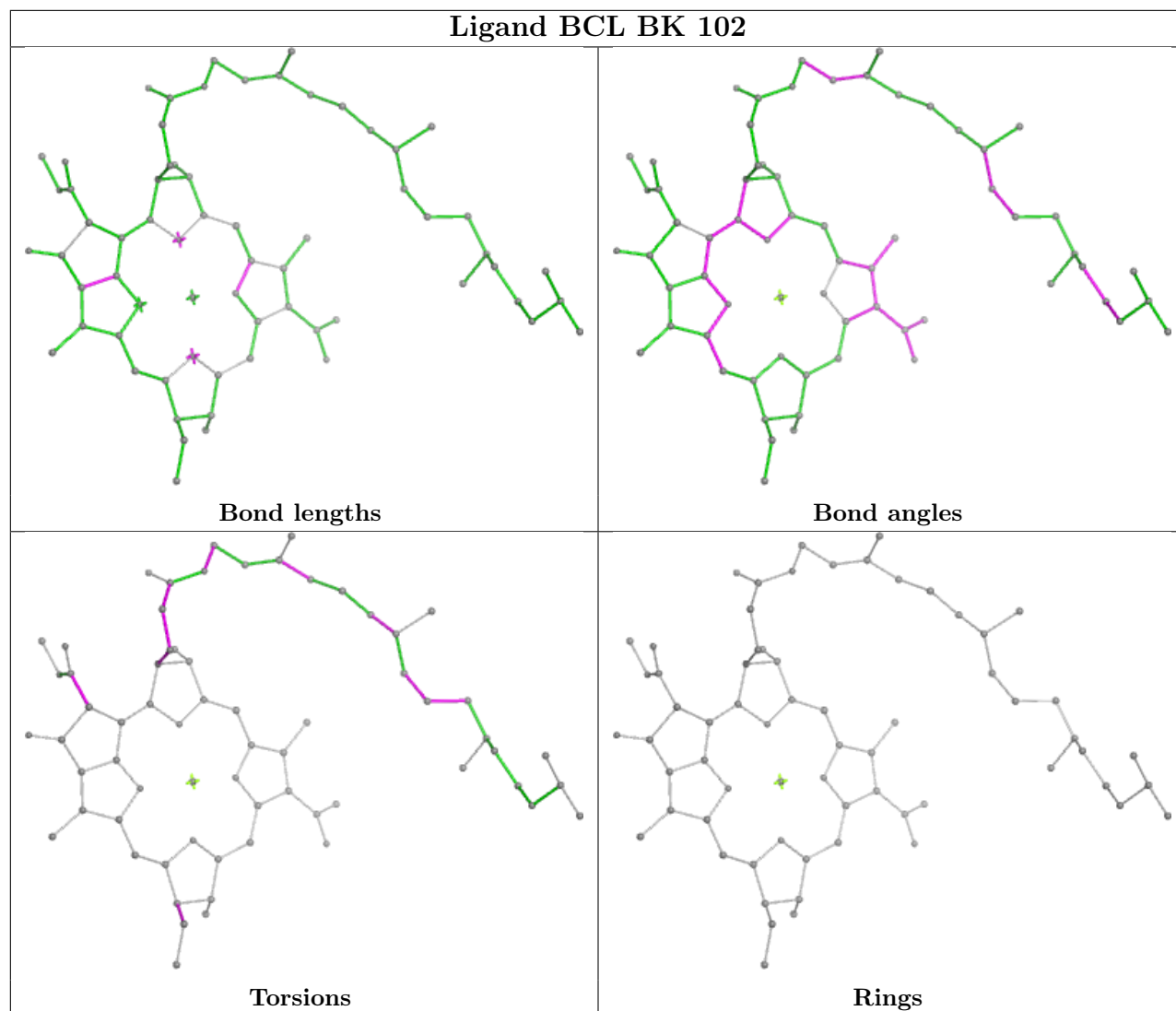




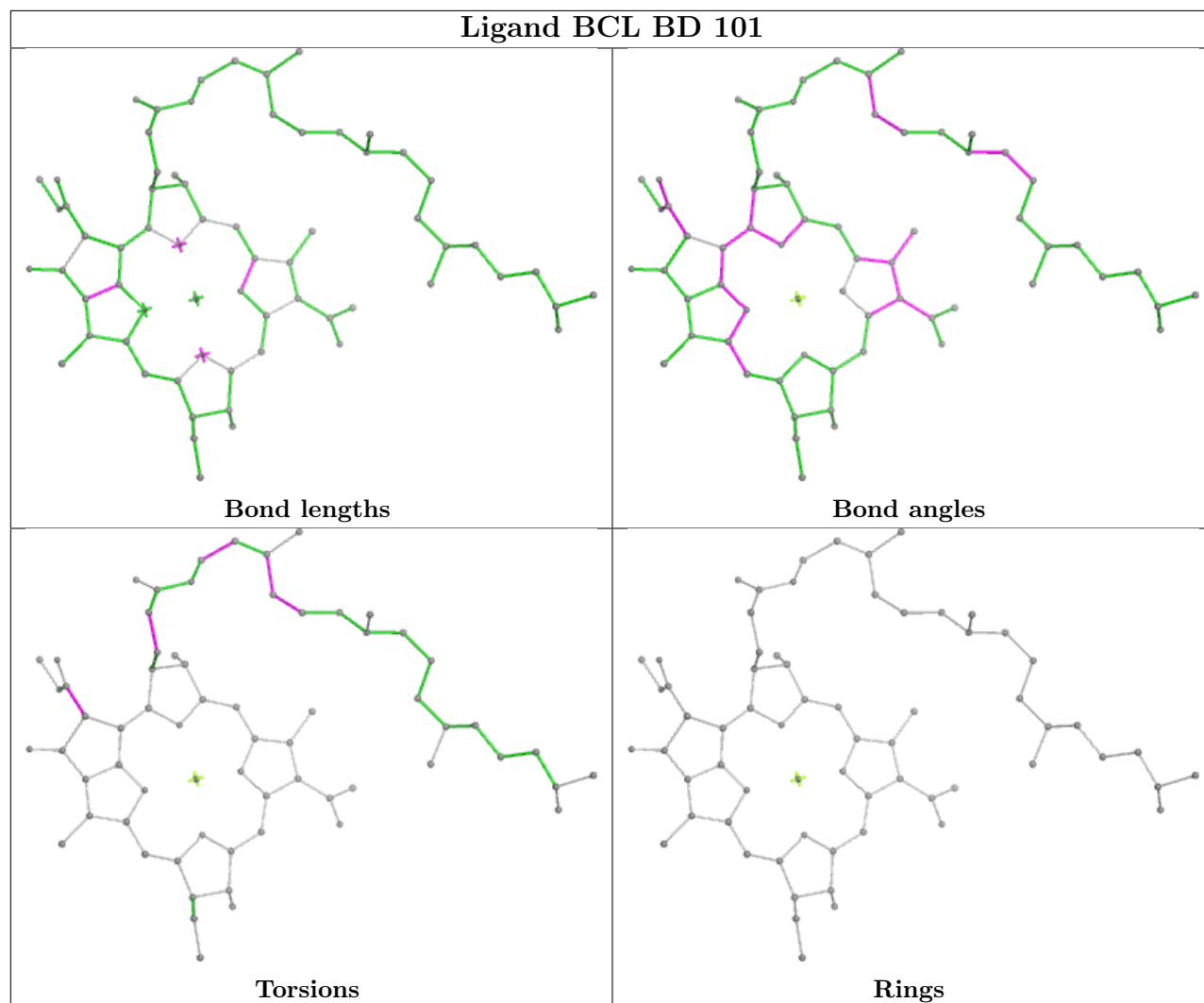




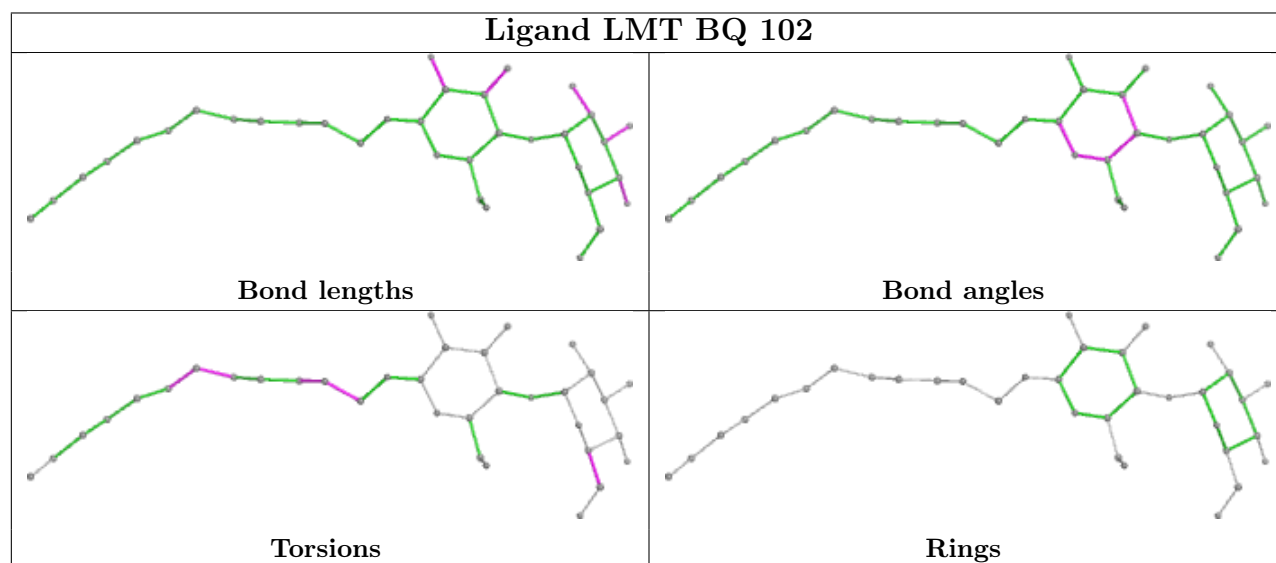
Ligand BCL BK 102

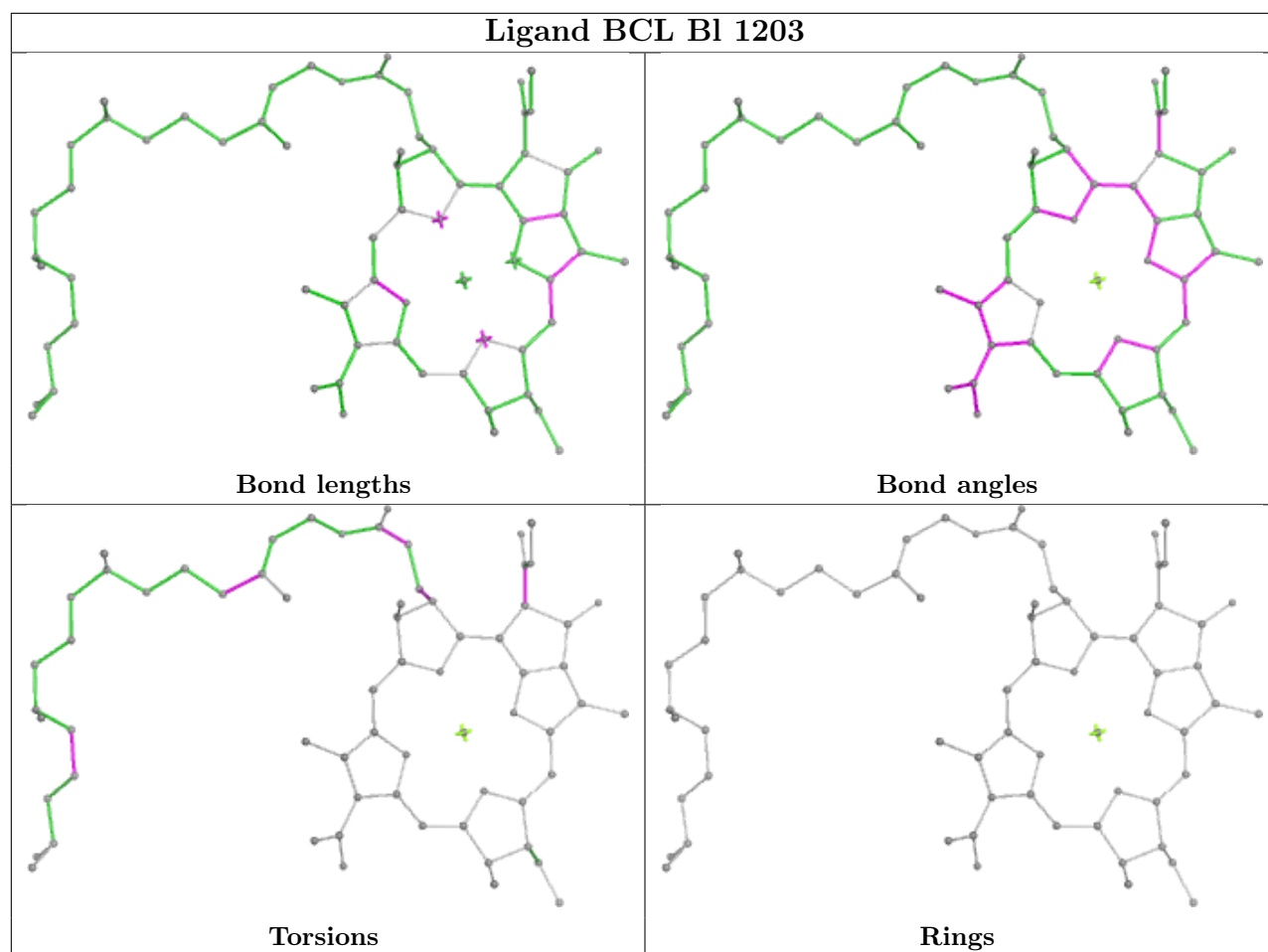
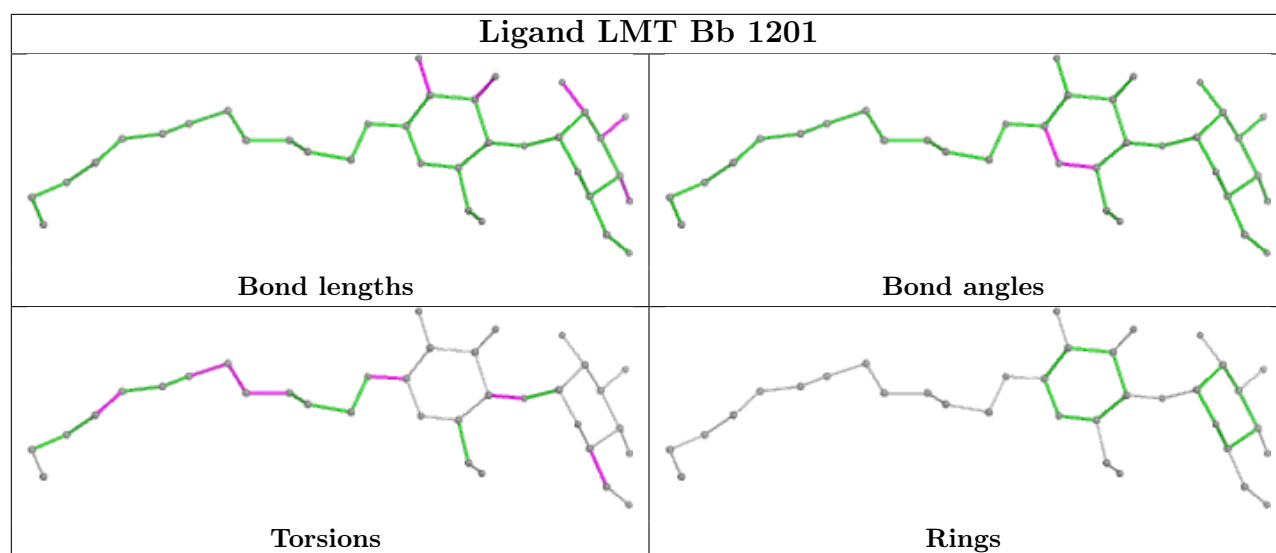


Ligand BCL BD 101

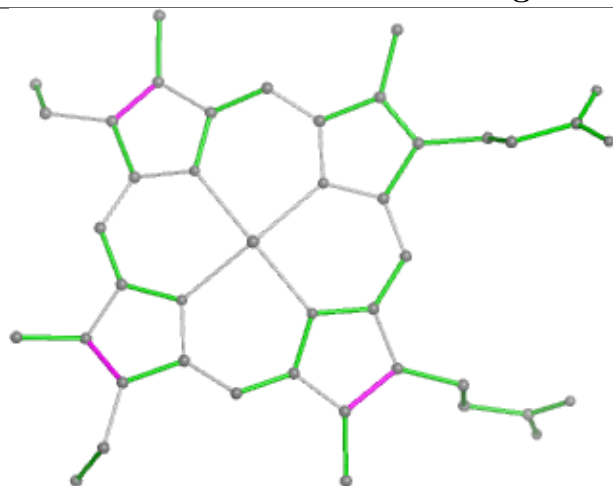


Ligand LMT BQ 102

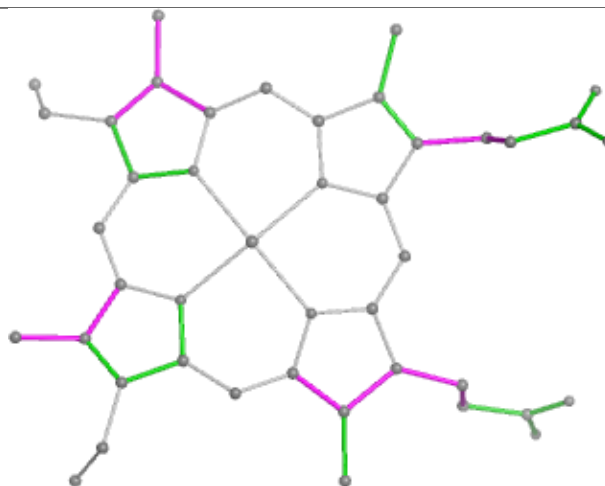




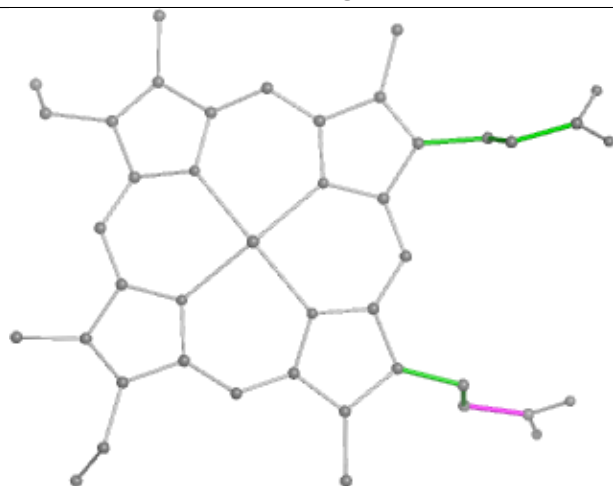
Ligand HEC C 404



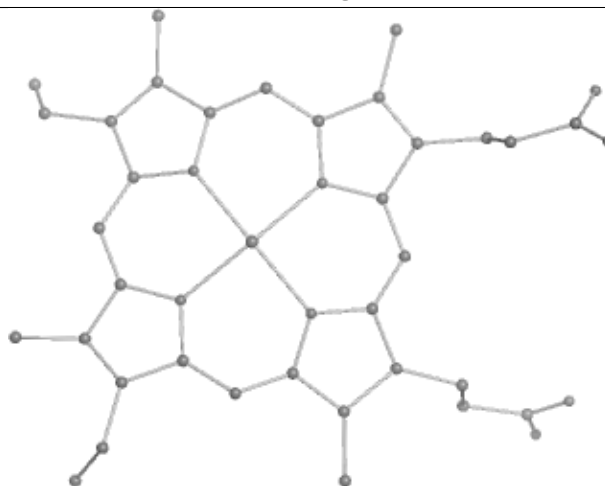
Bond lengths



Bond angles

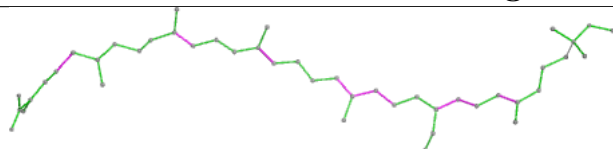


Torsions

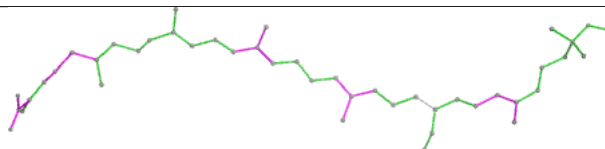


Rings

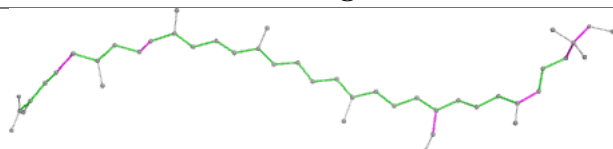
Ligand V7N An 101



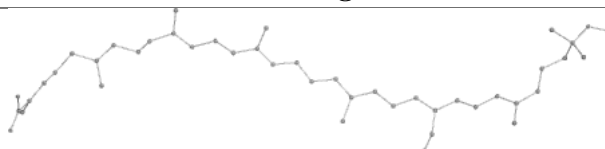
Bond lengths



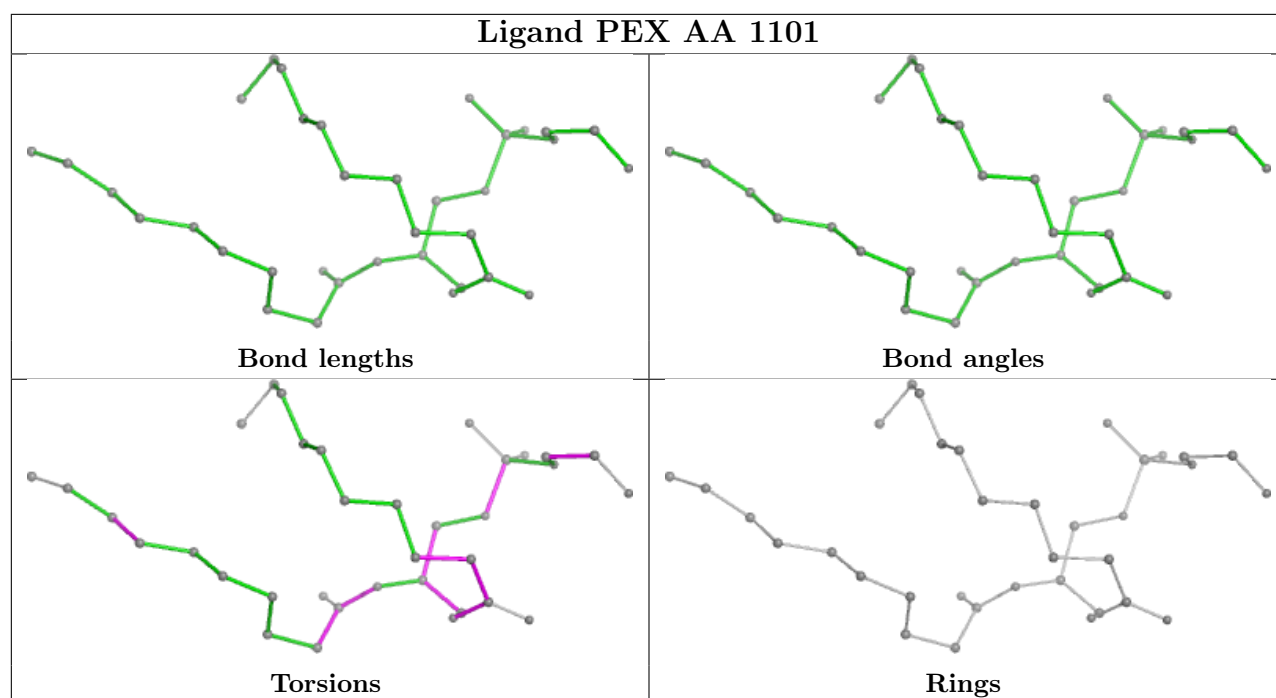
Bond angles



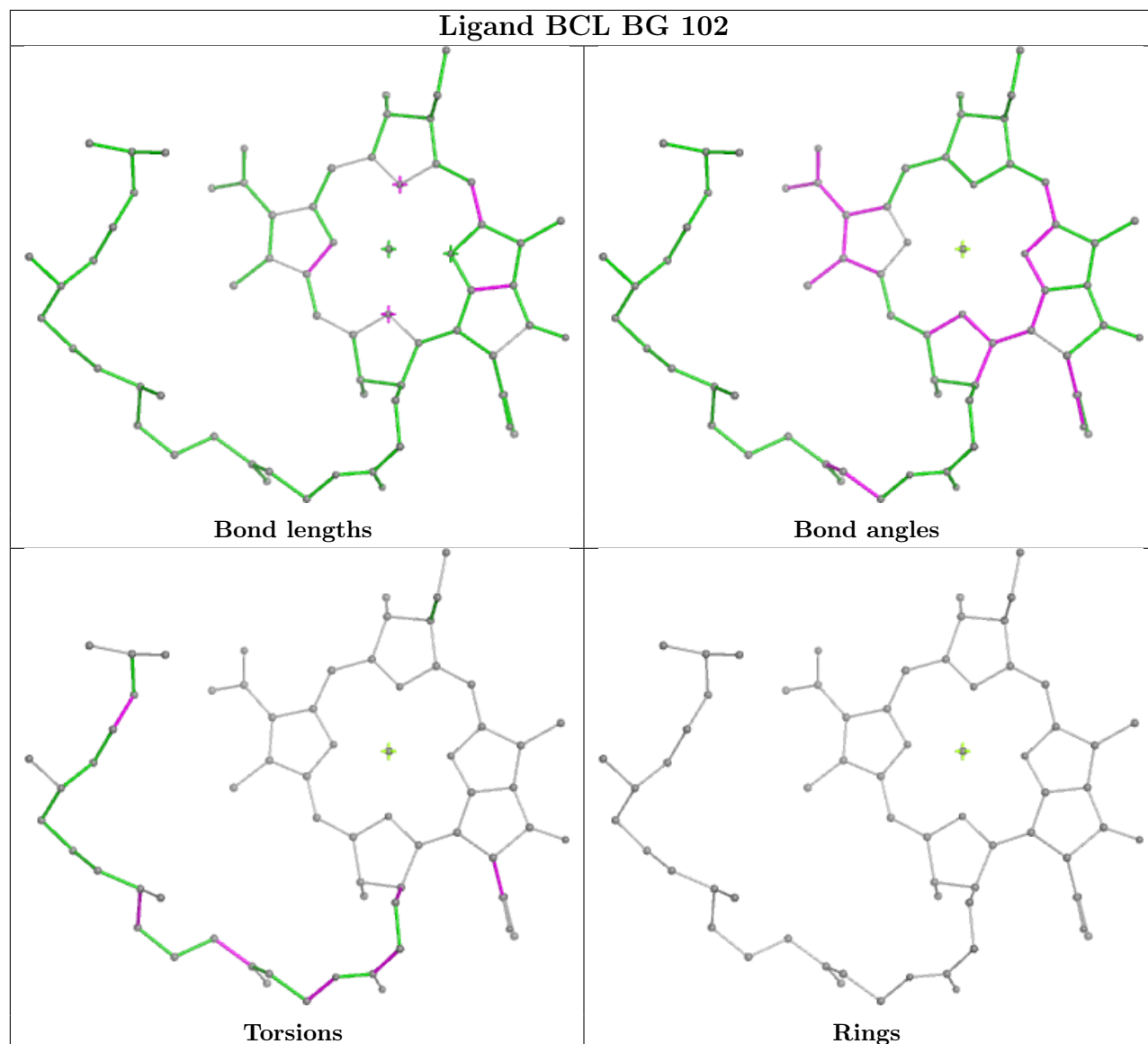
Torsions

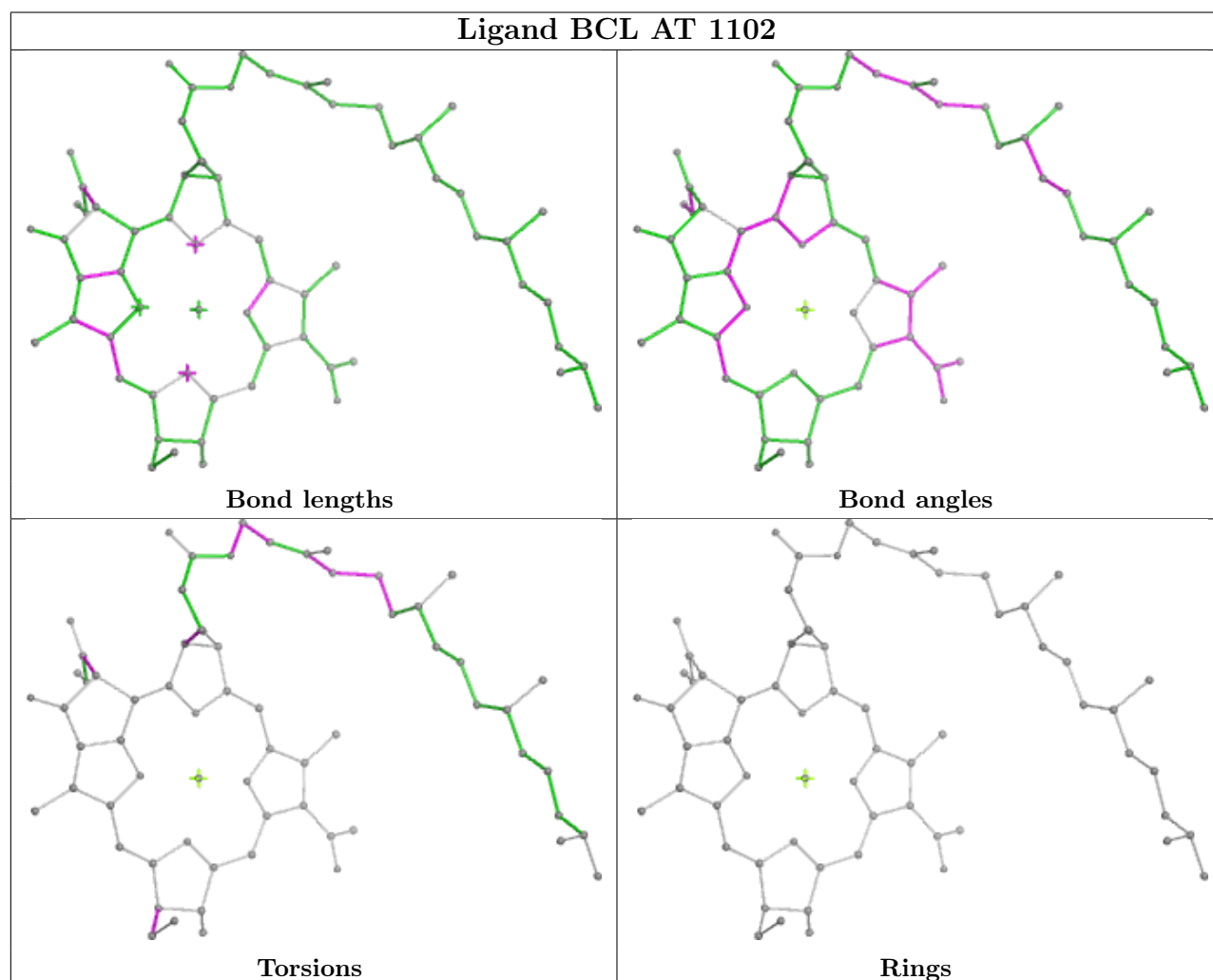
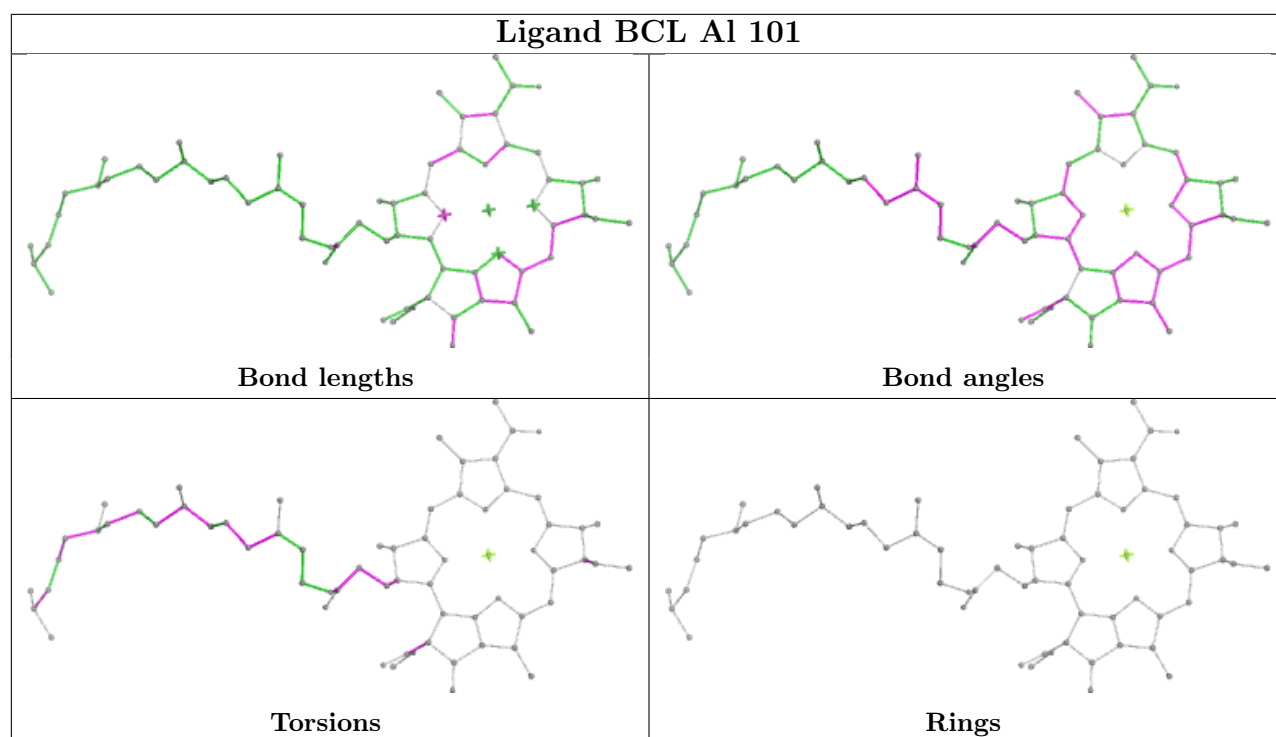


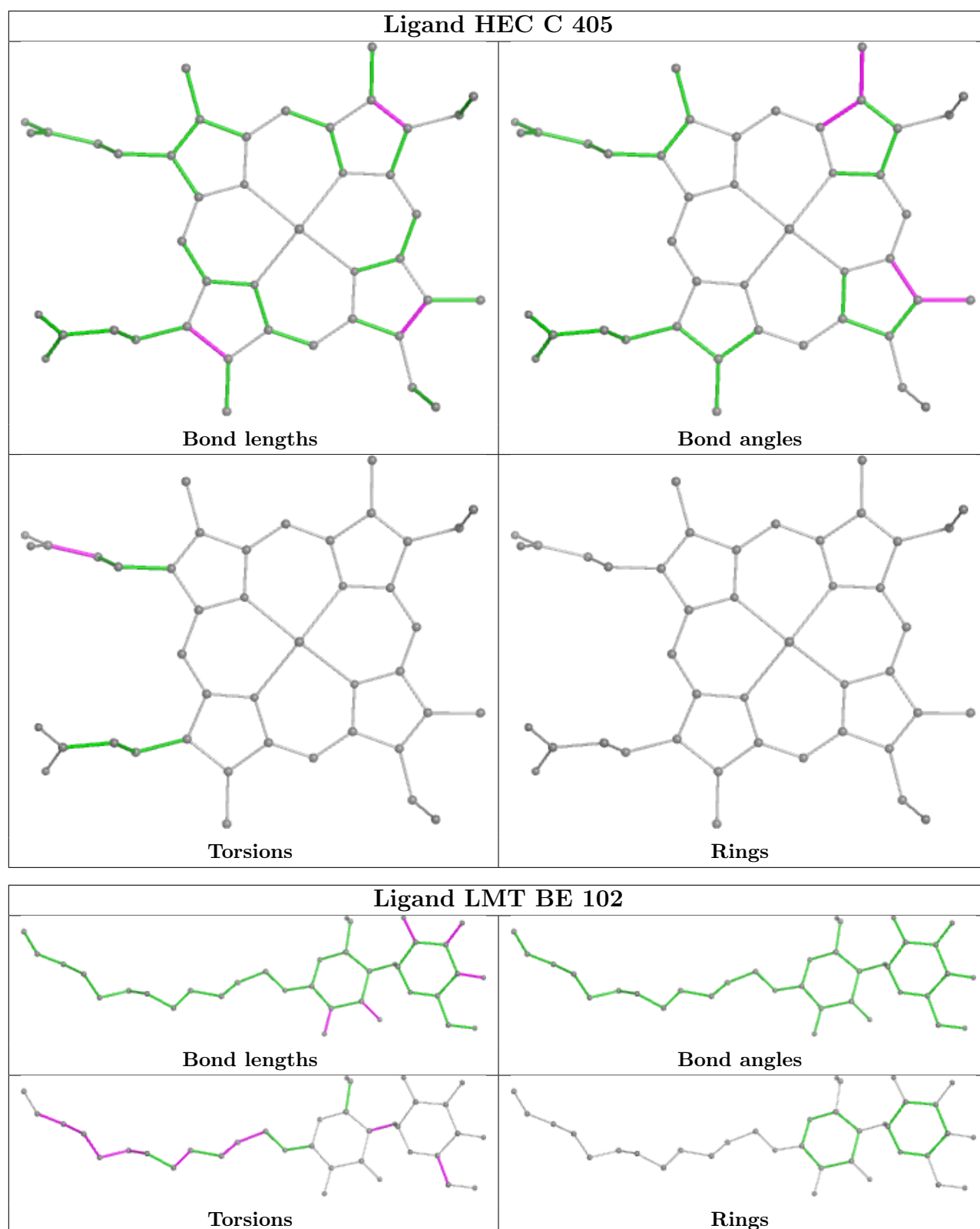
Rings



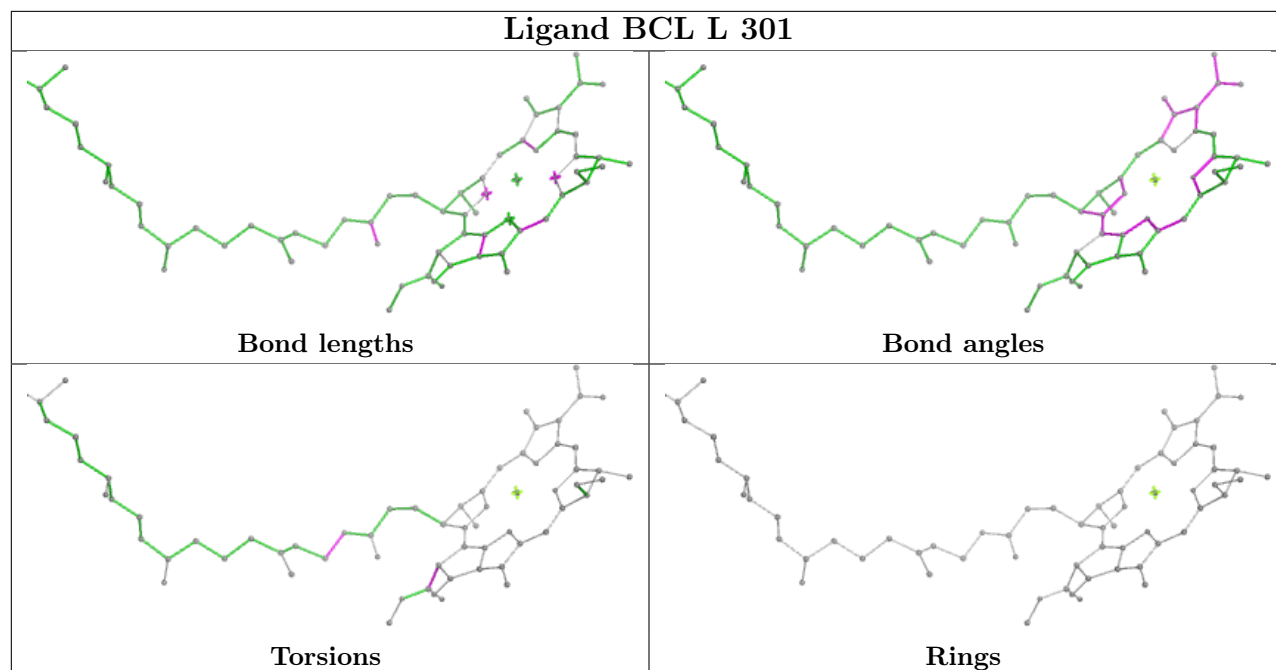
Ligand BCL BG 102



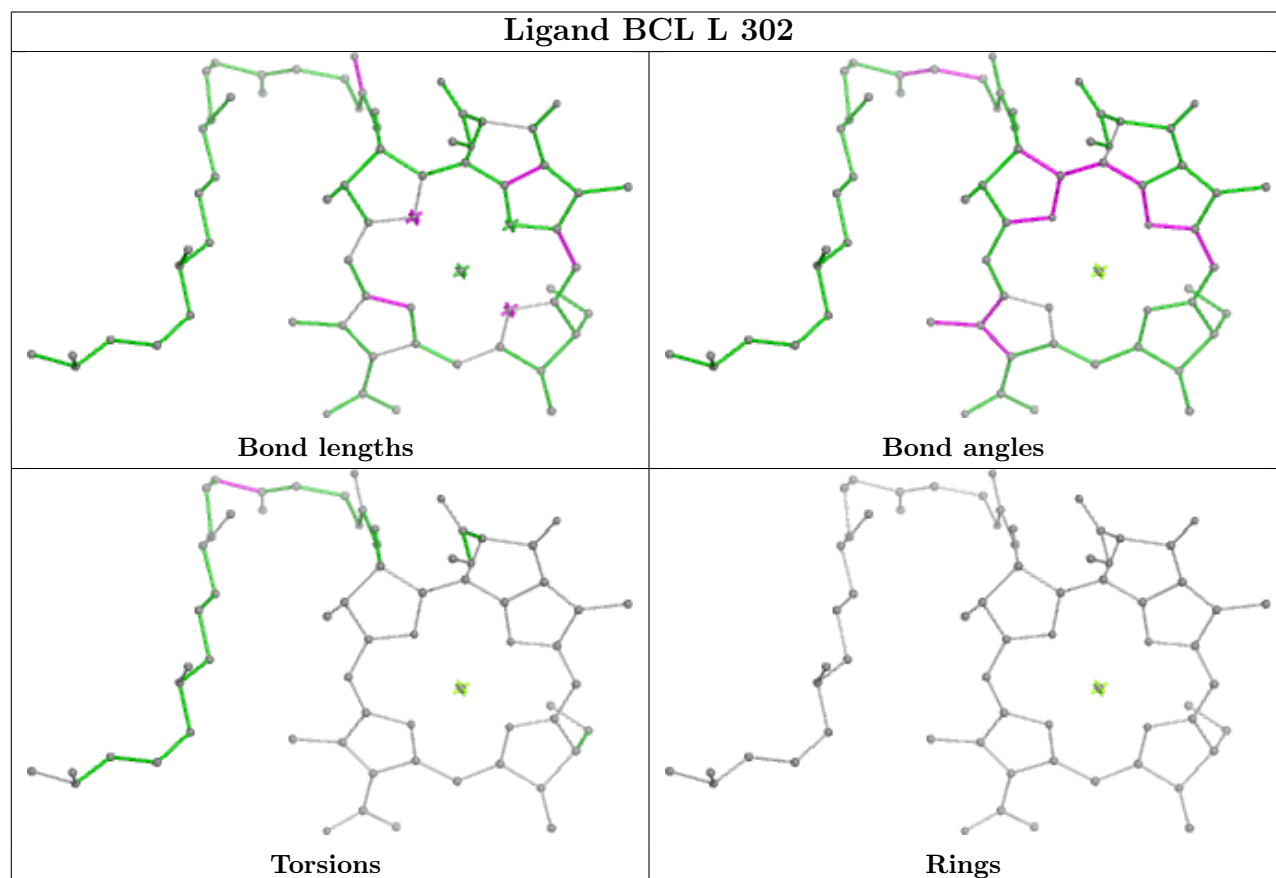


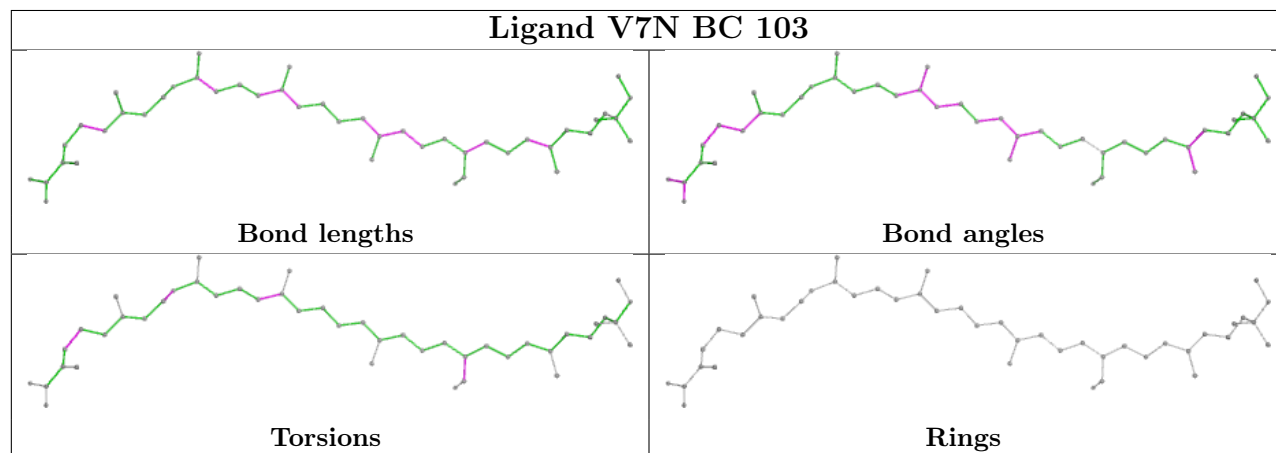
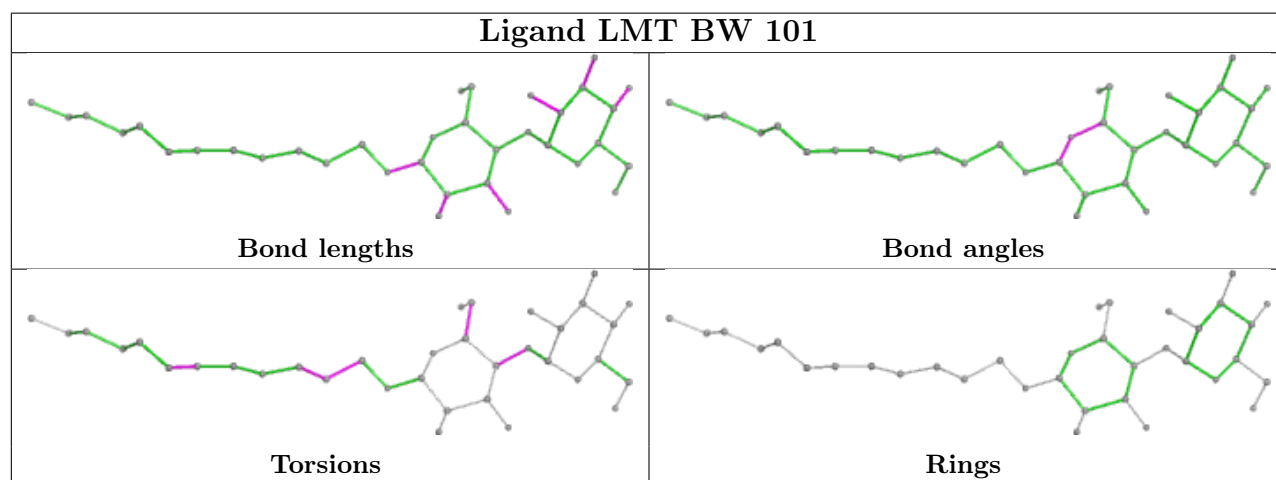
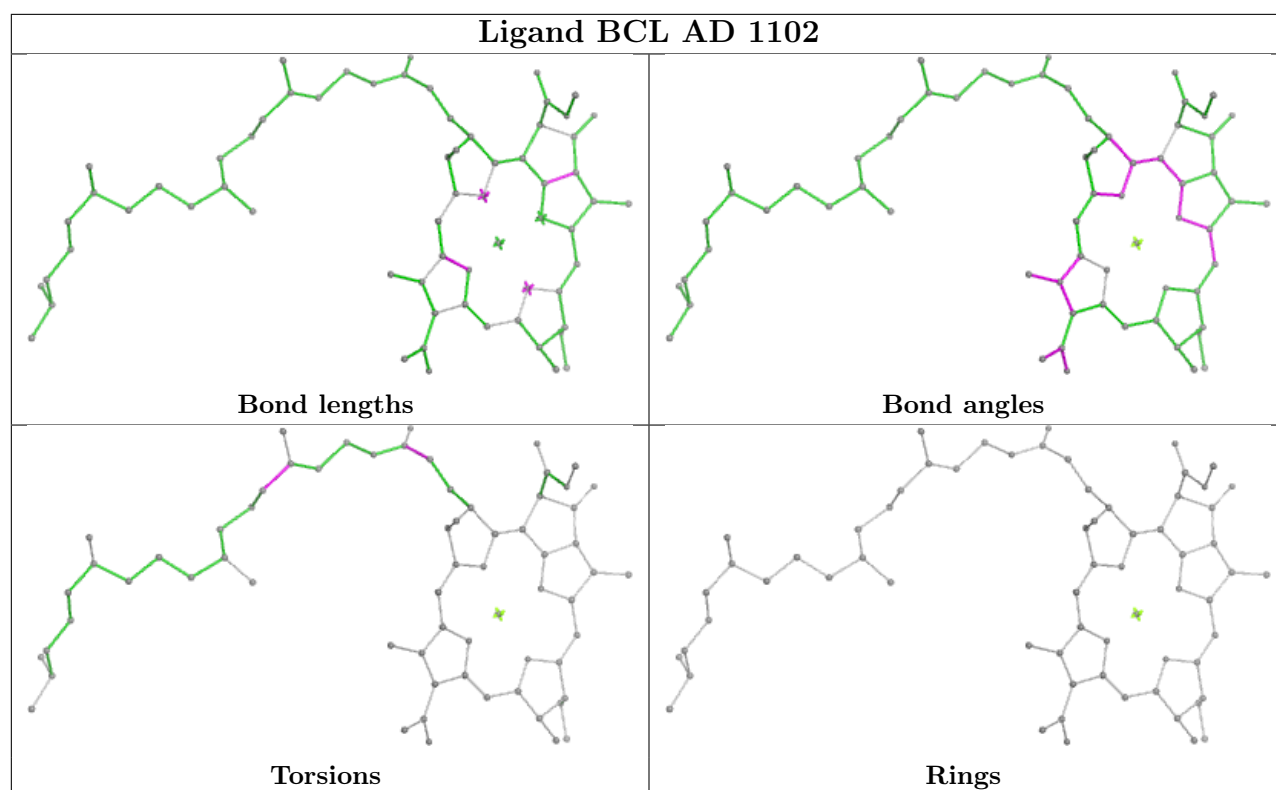


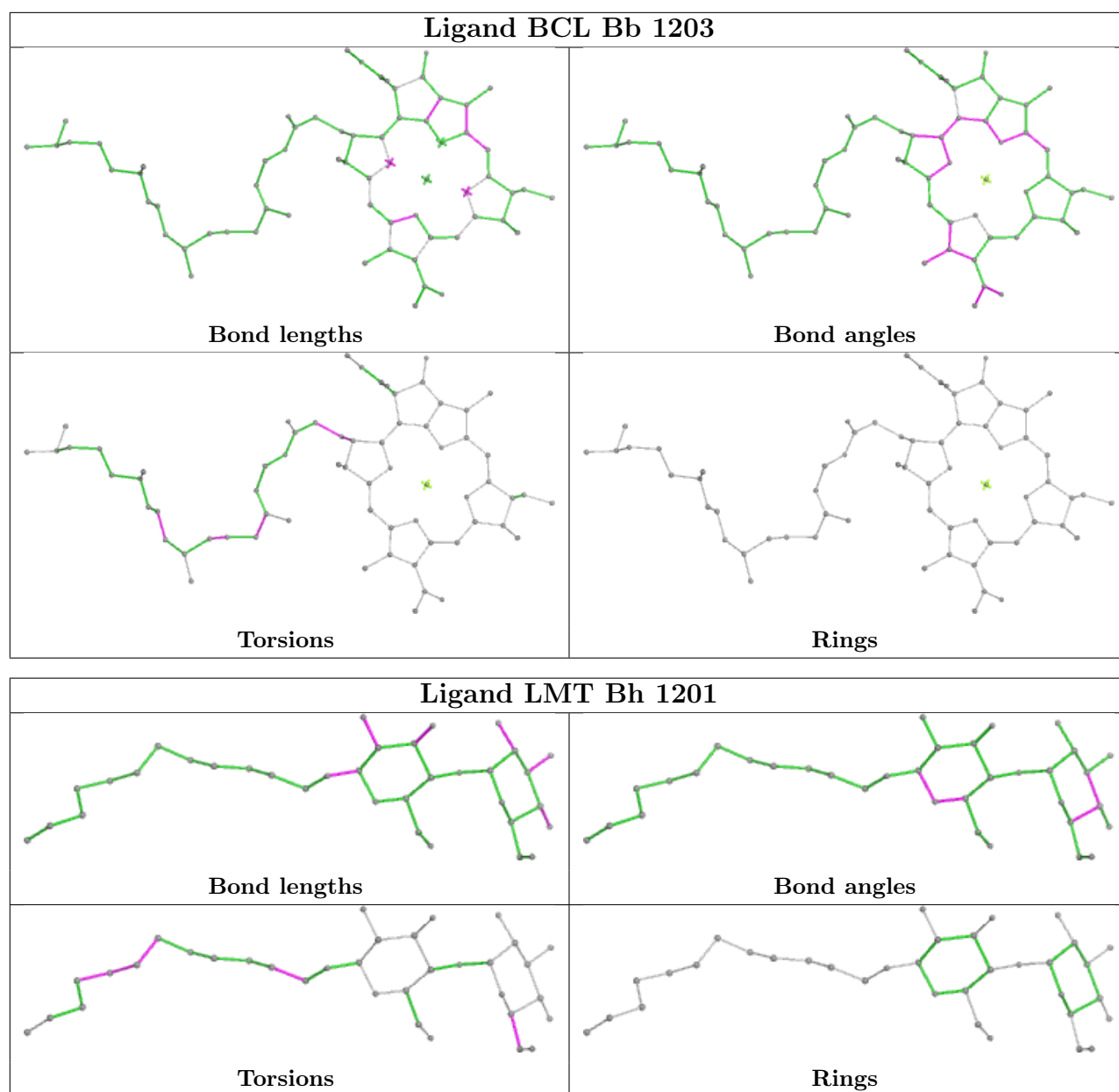
Ligand BCL L 301



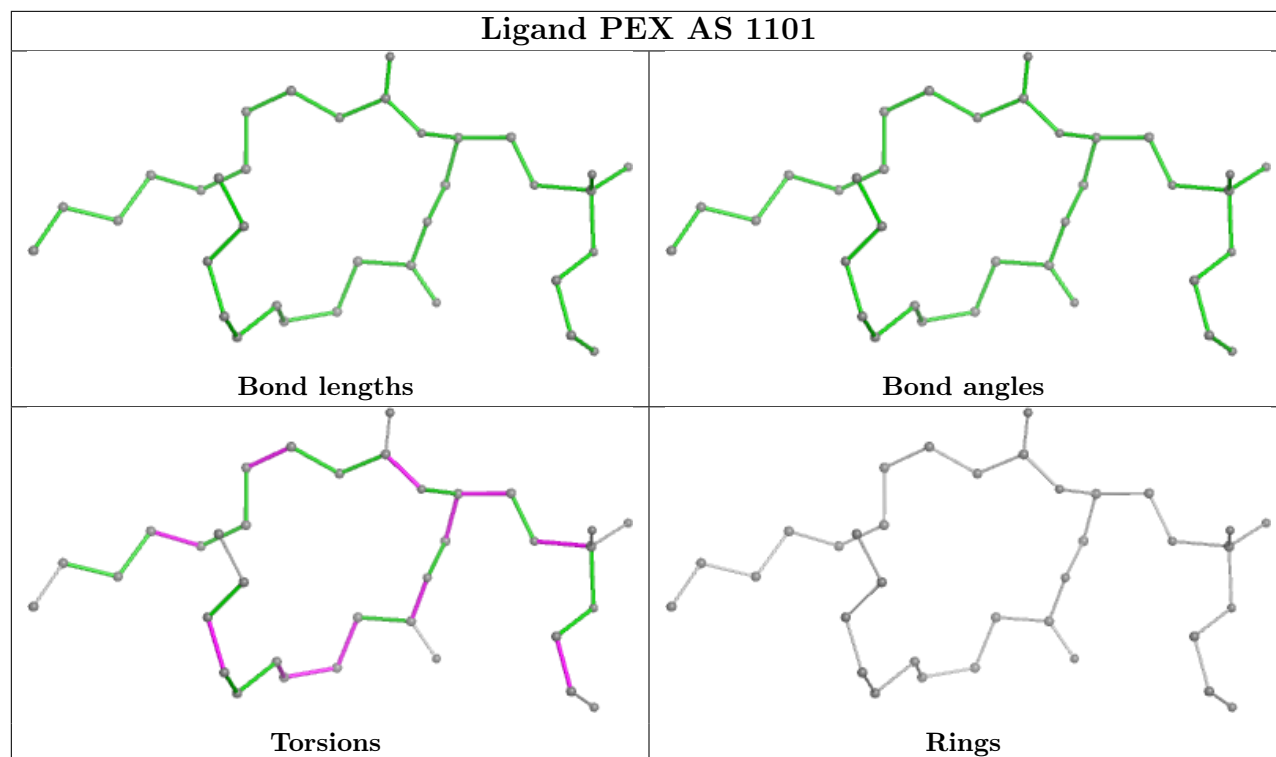
Ligand BCL L 302



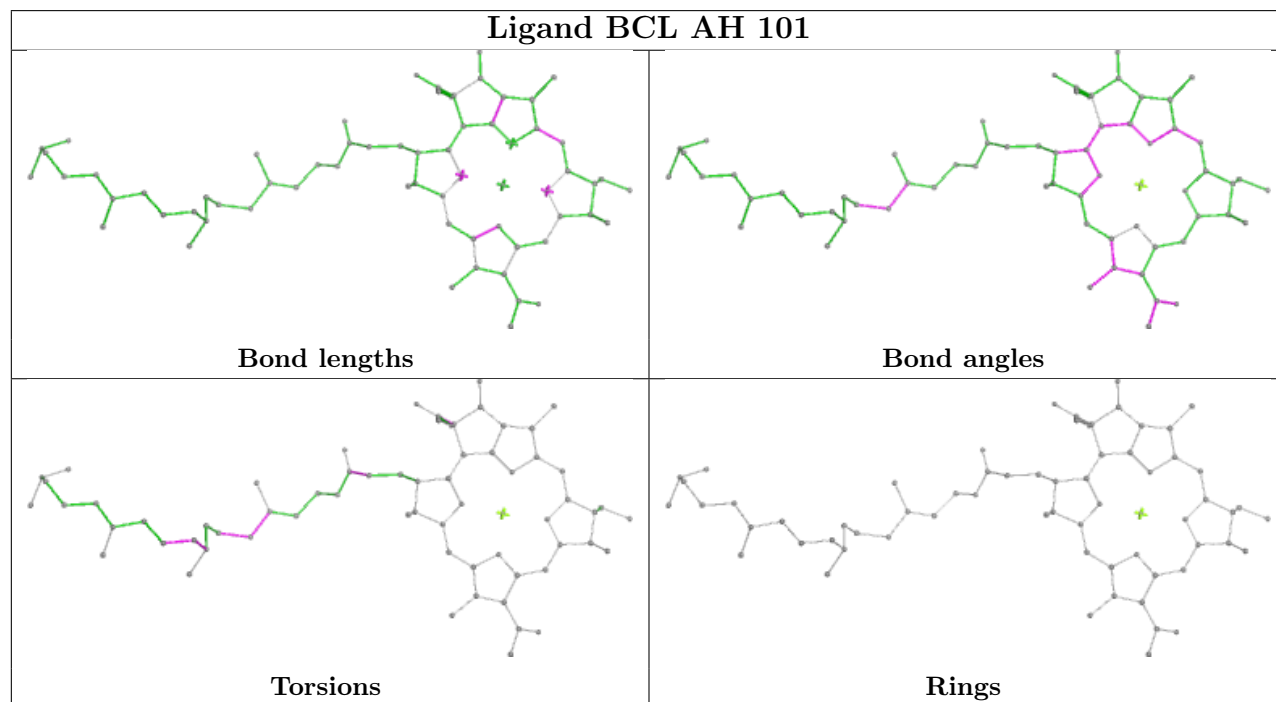


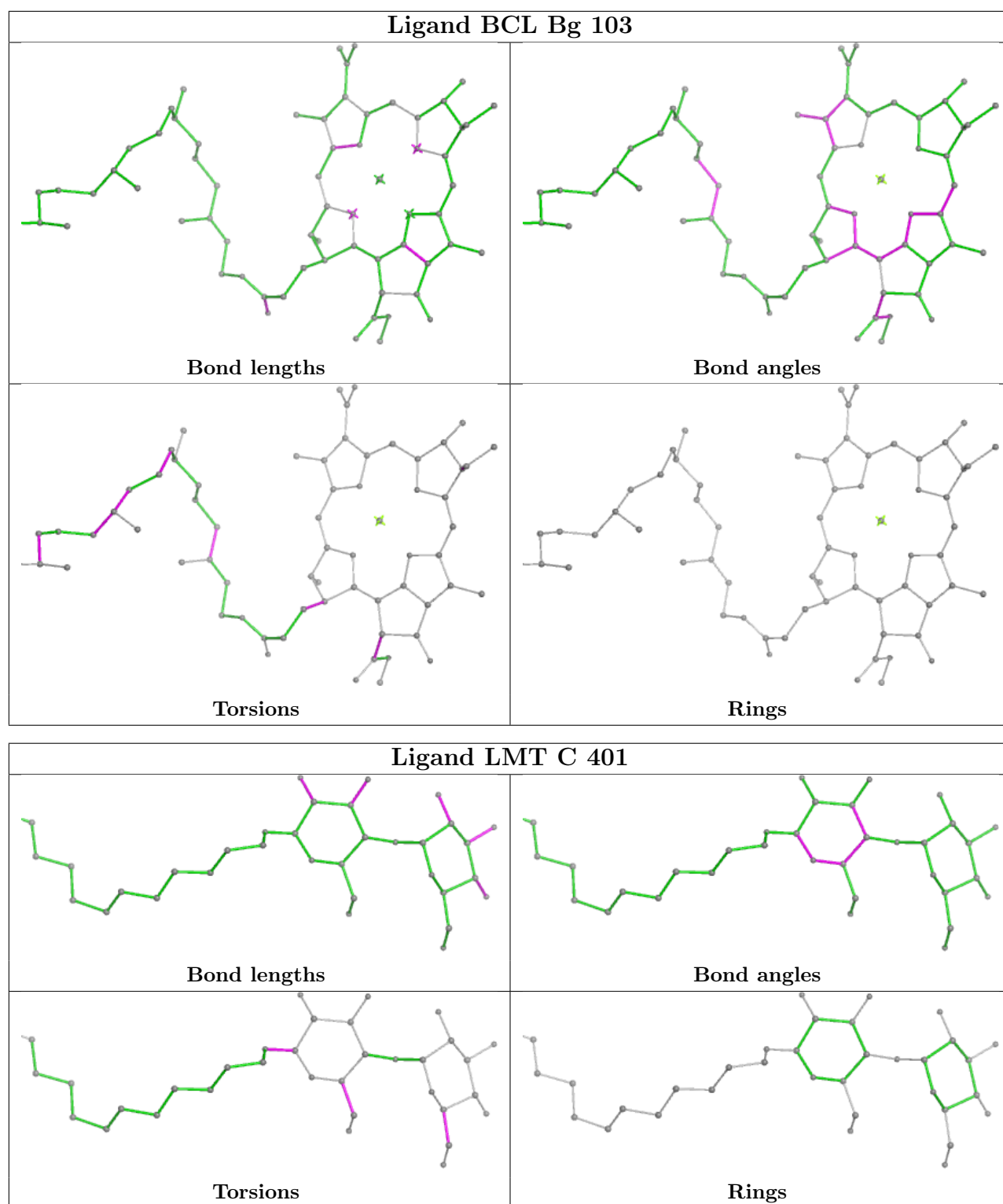


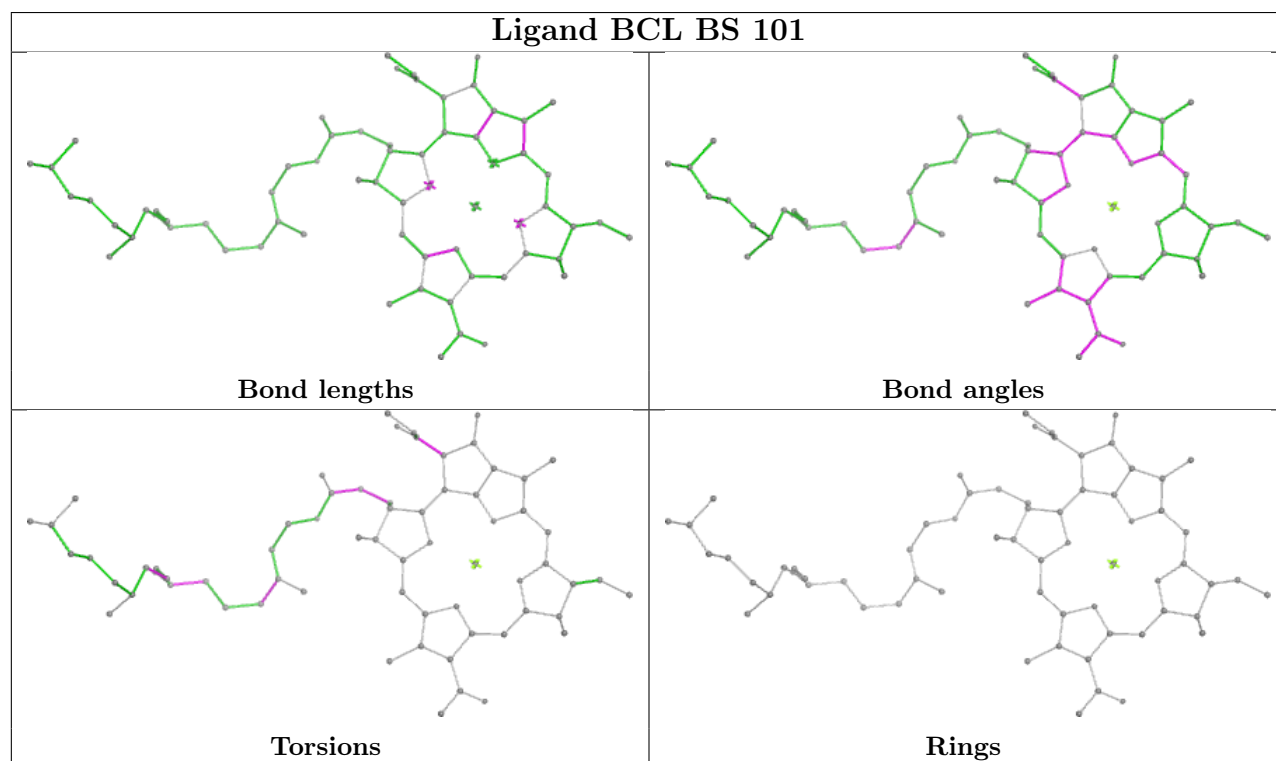
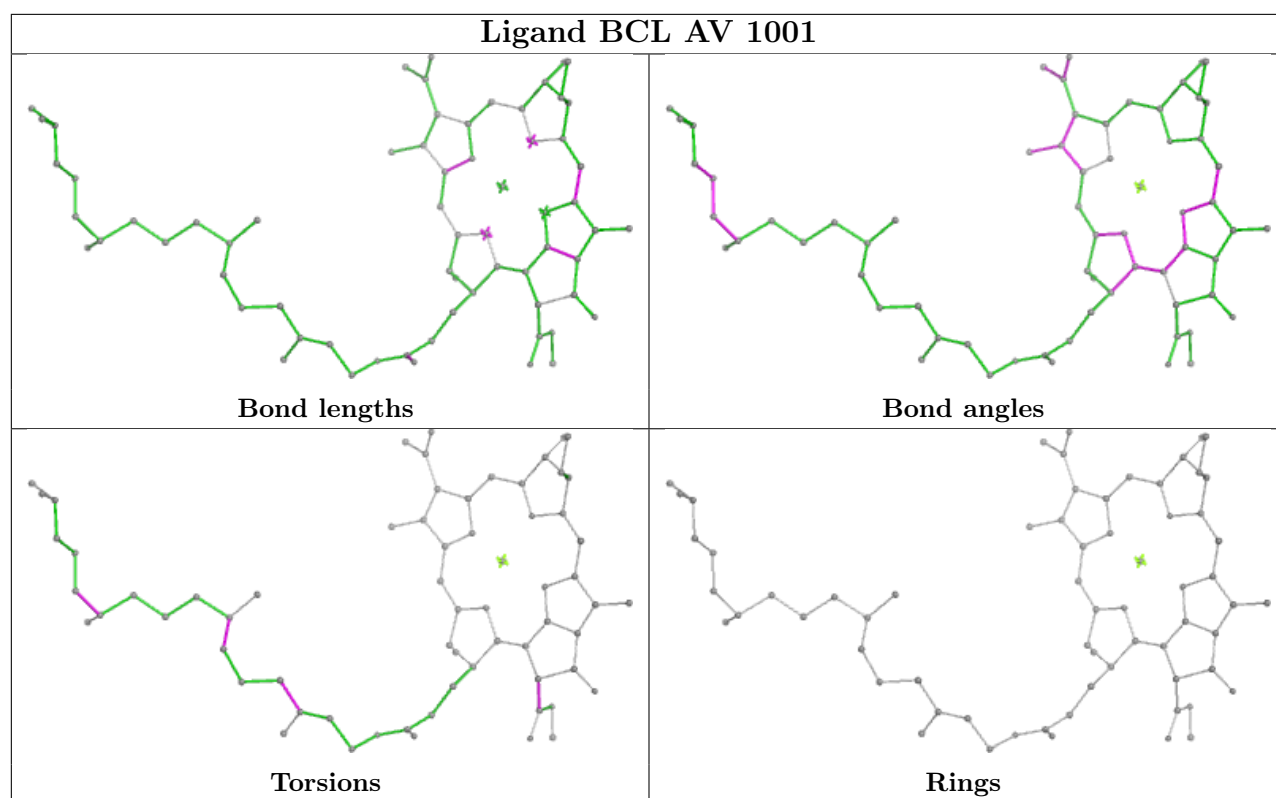
Ligand PEX AS 1101

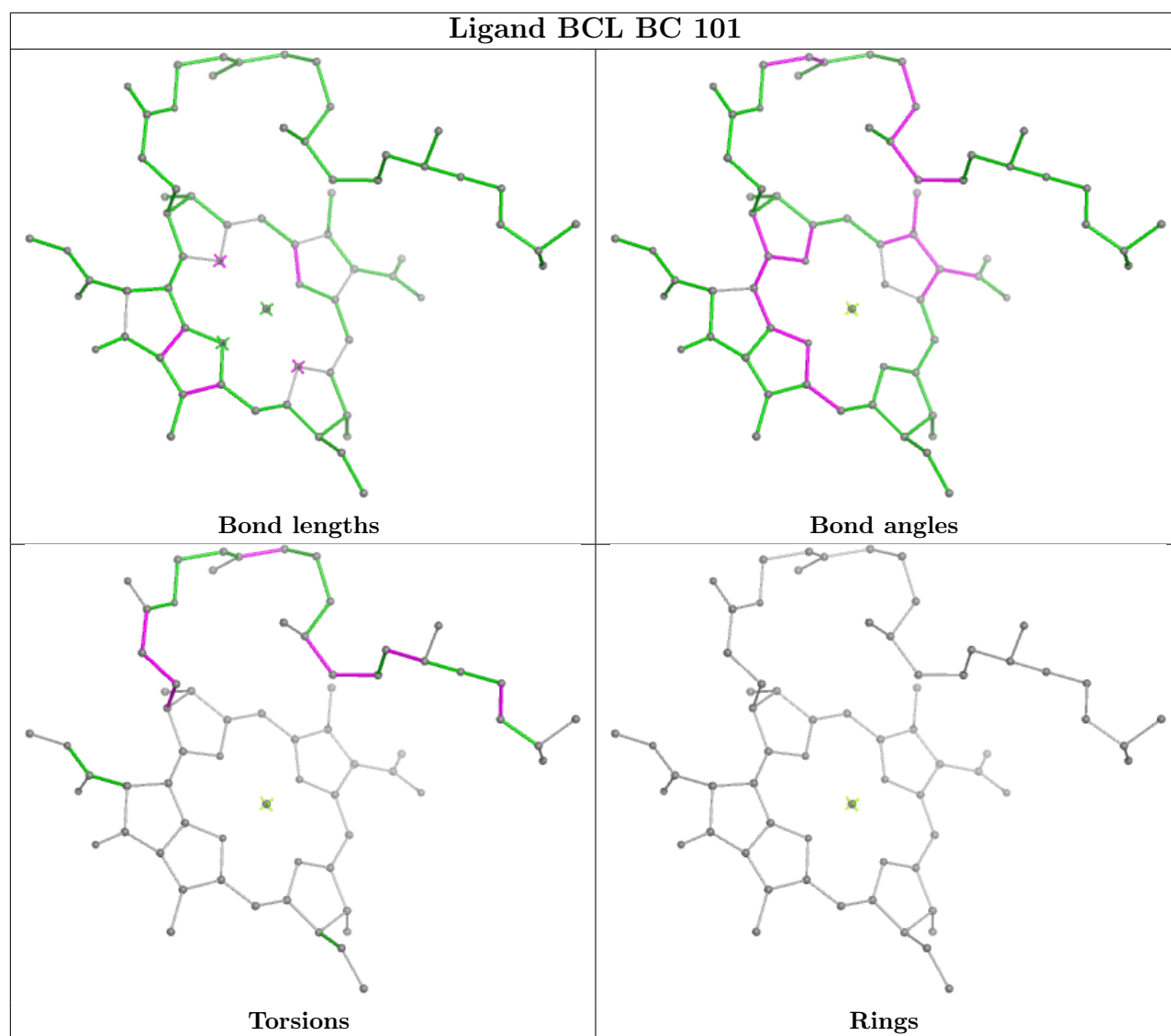
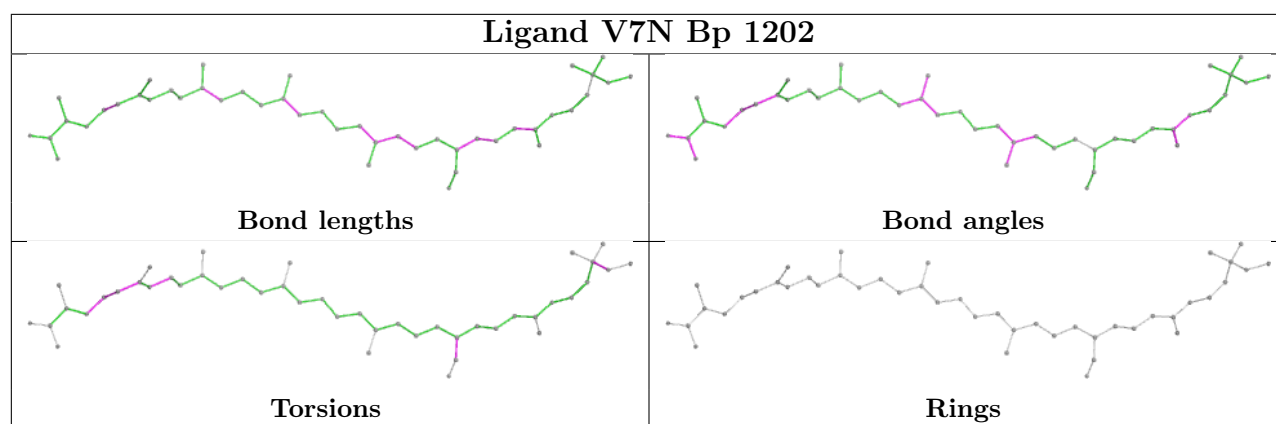


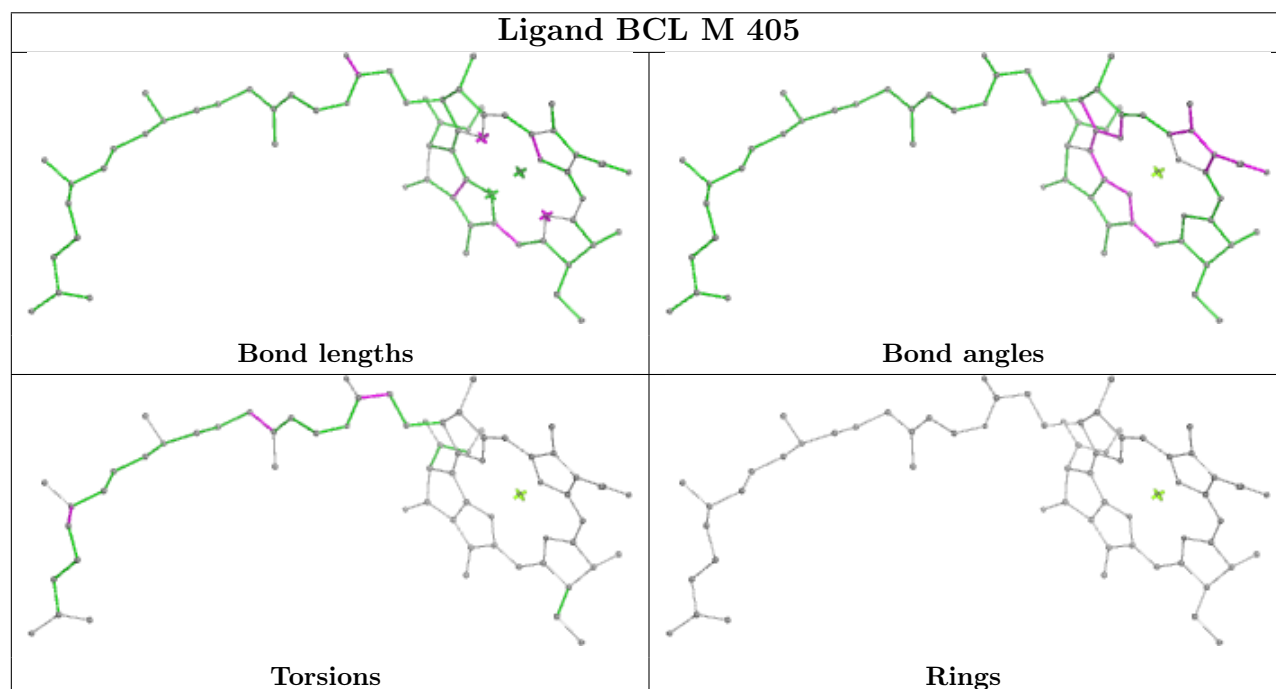
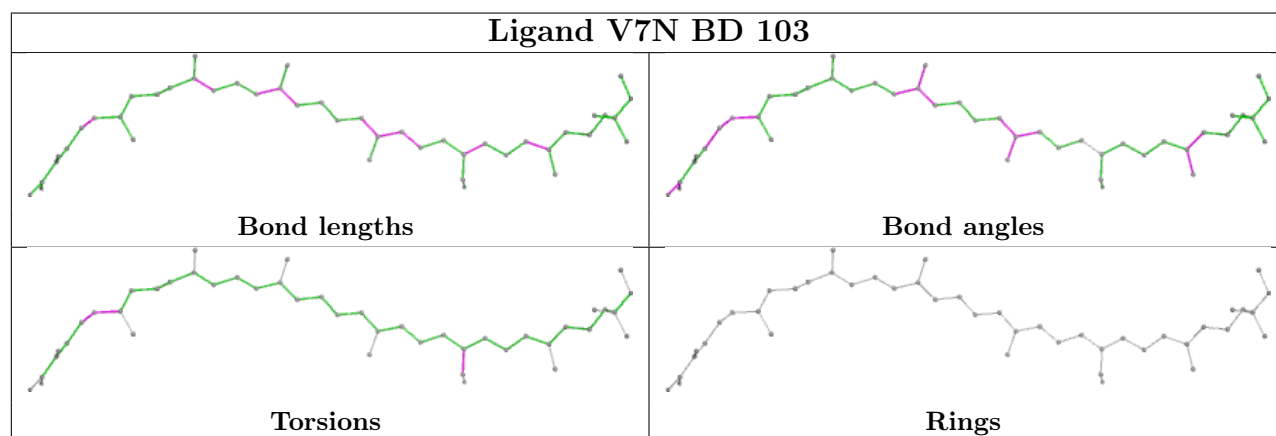
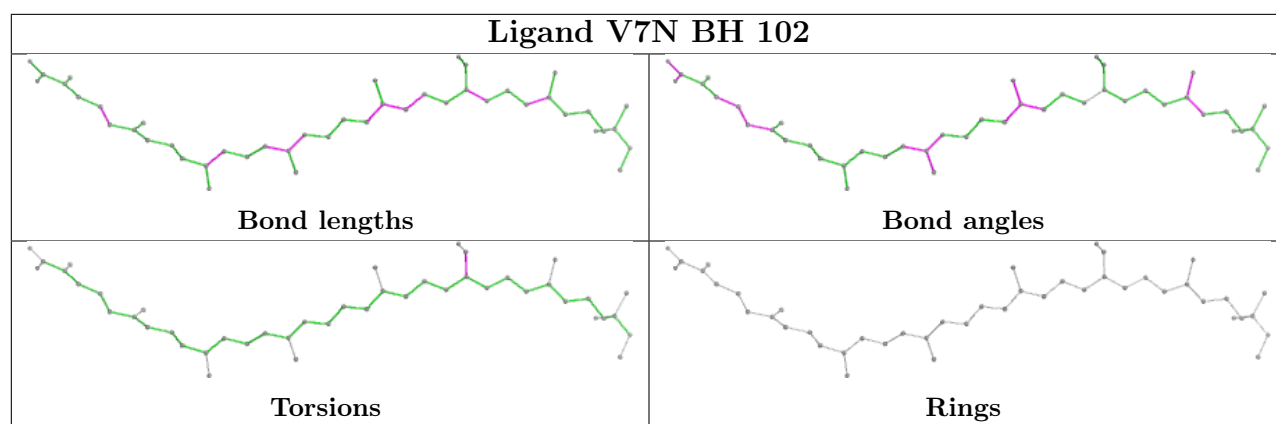
Ligand BCL AH 101

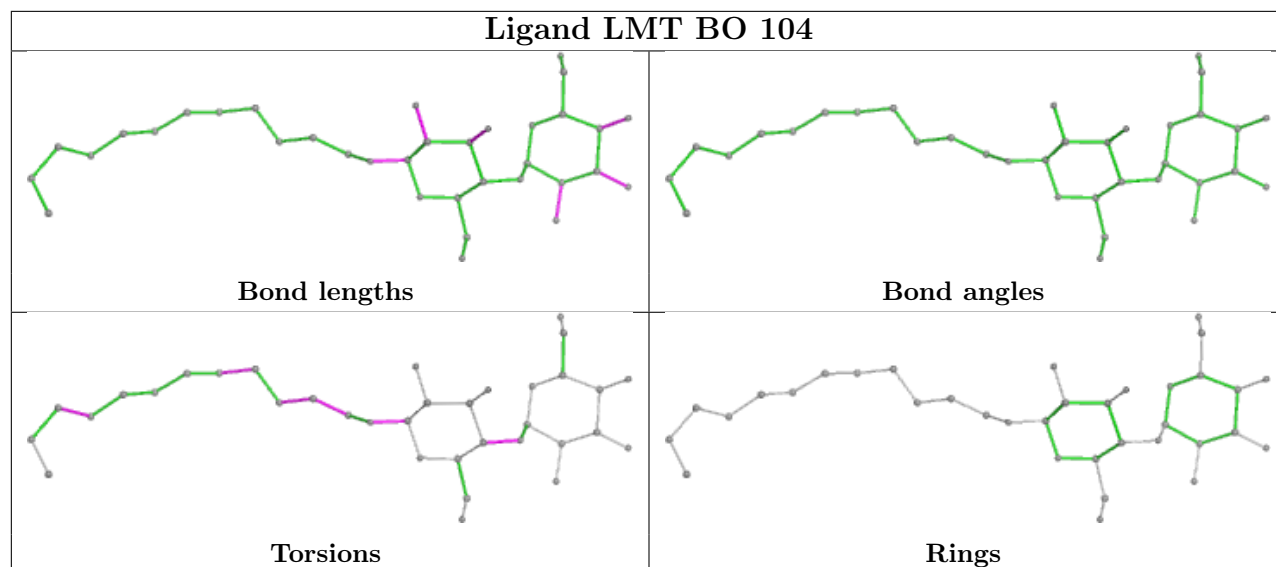
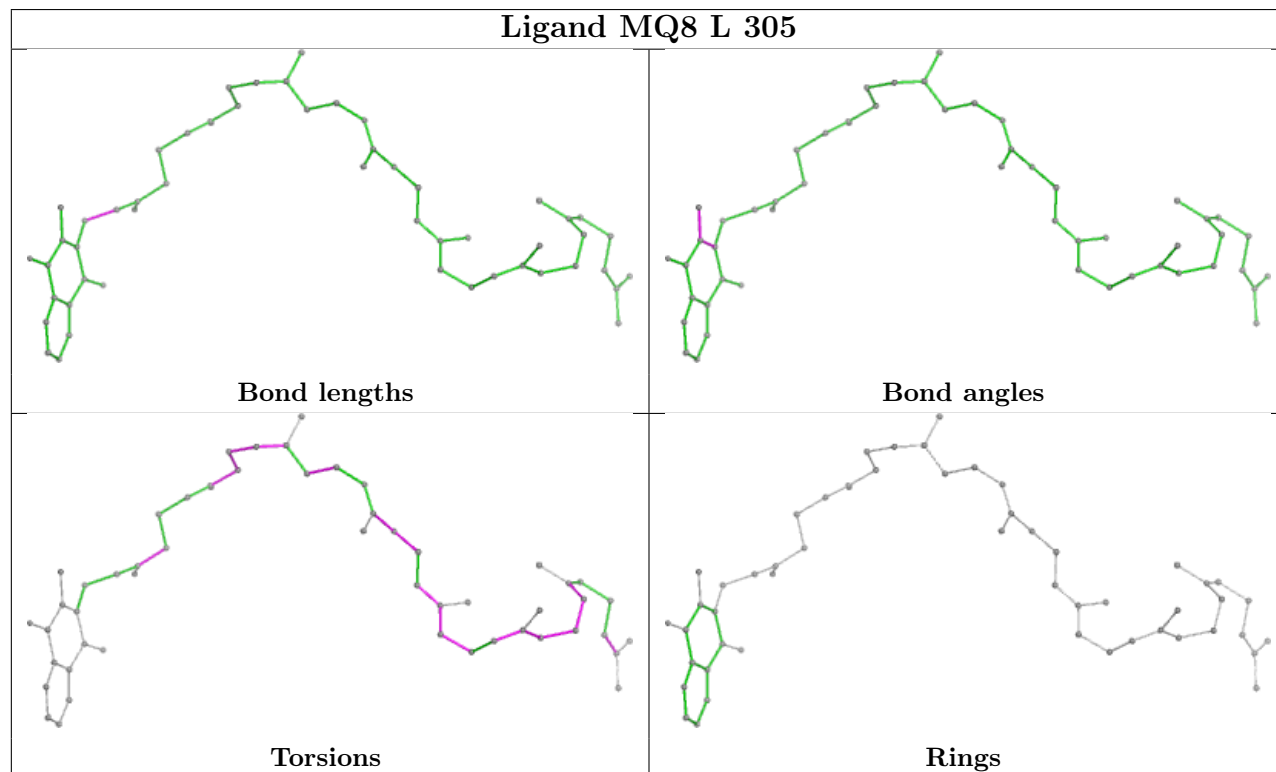


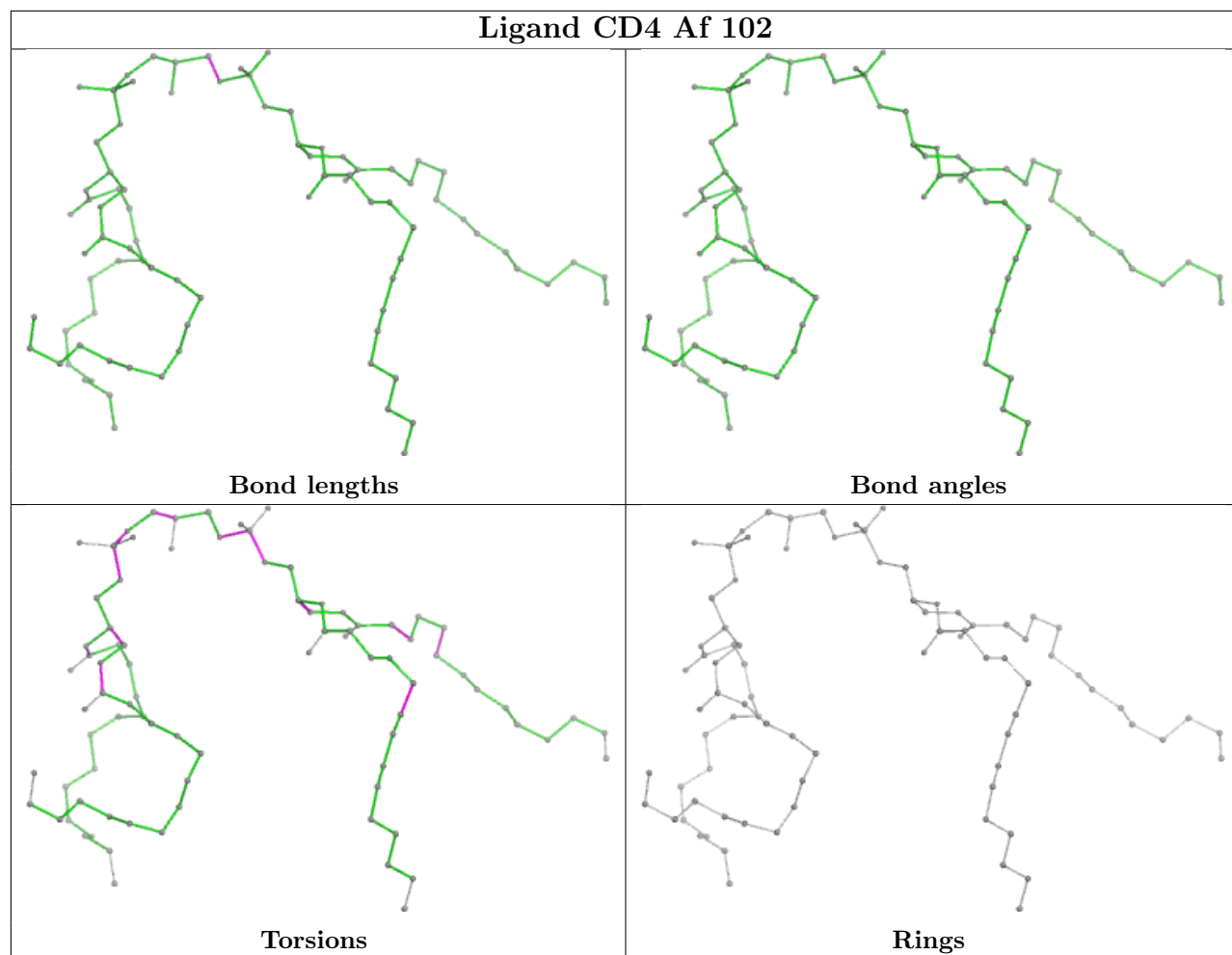


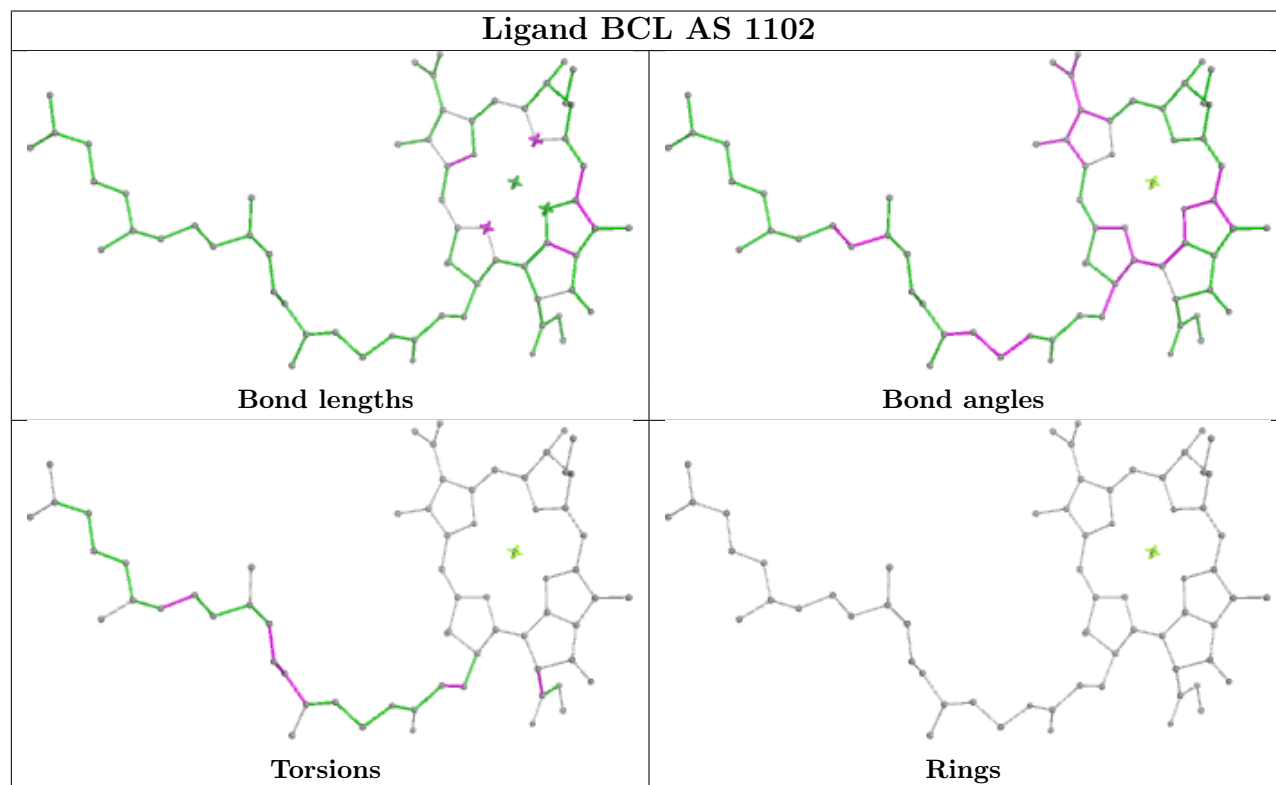
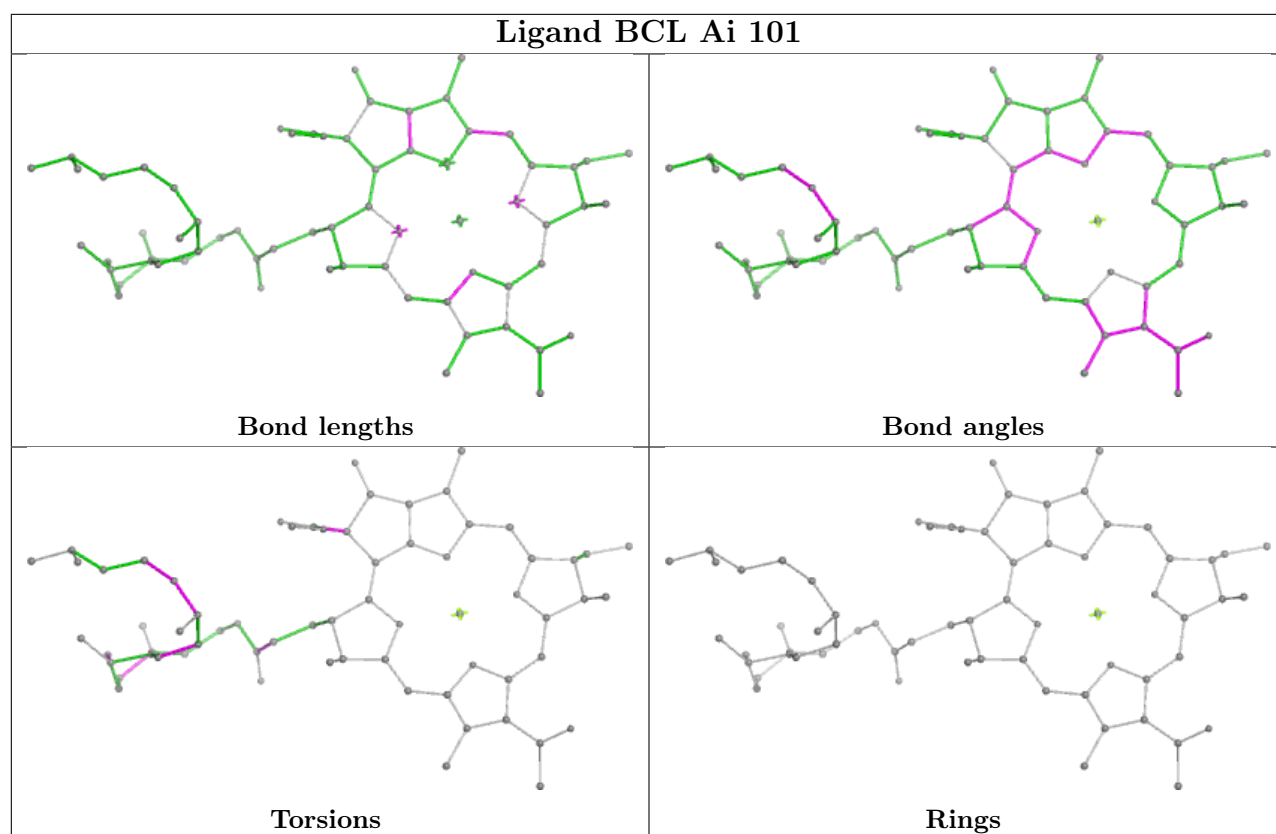


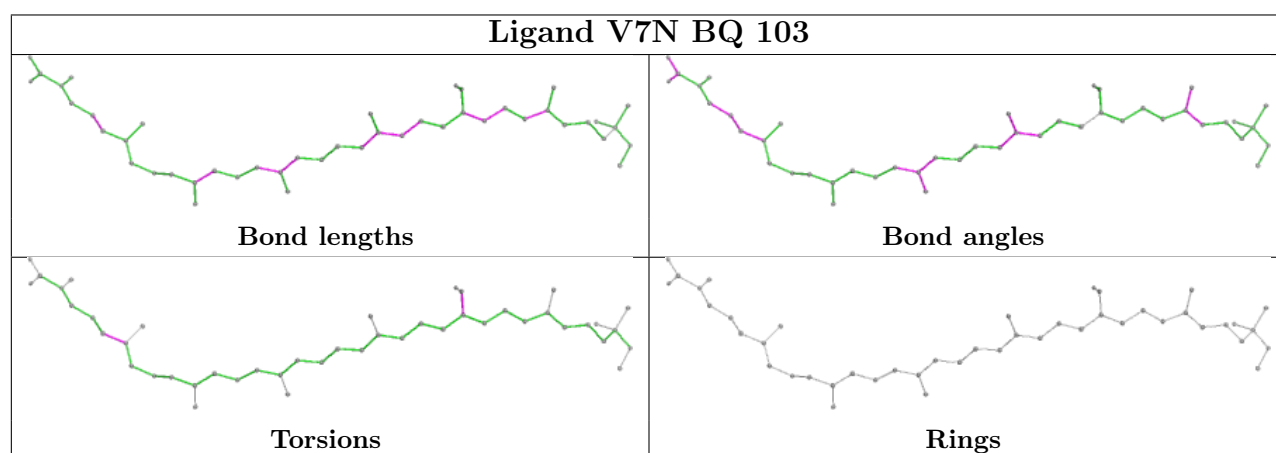
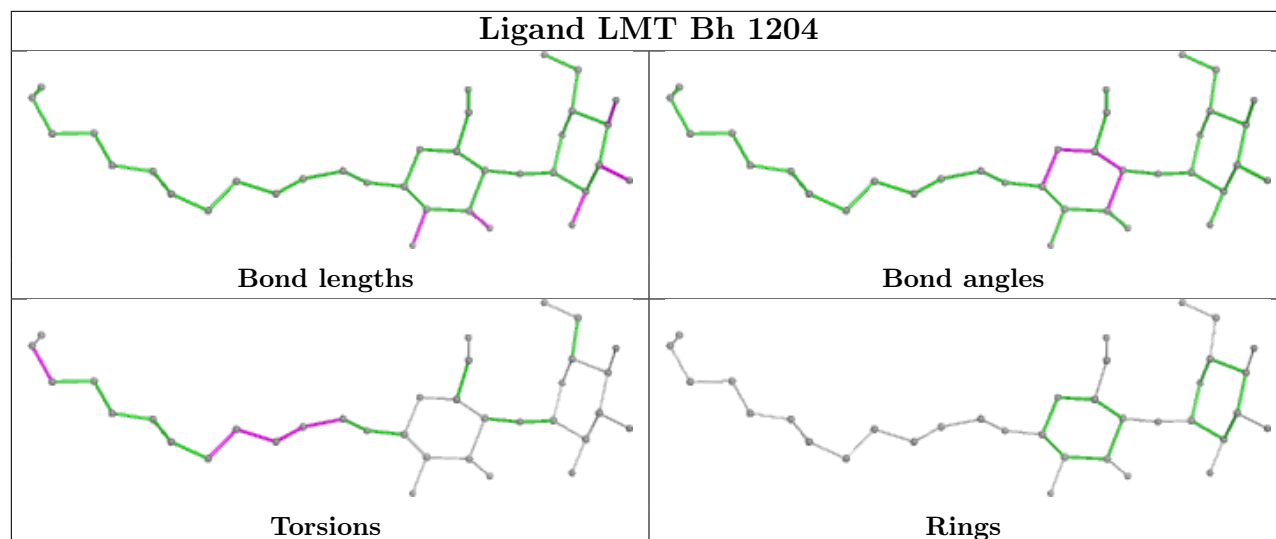




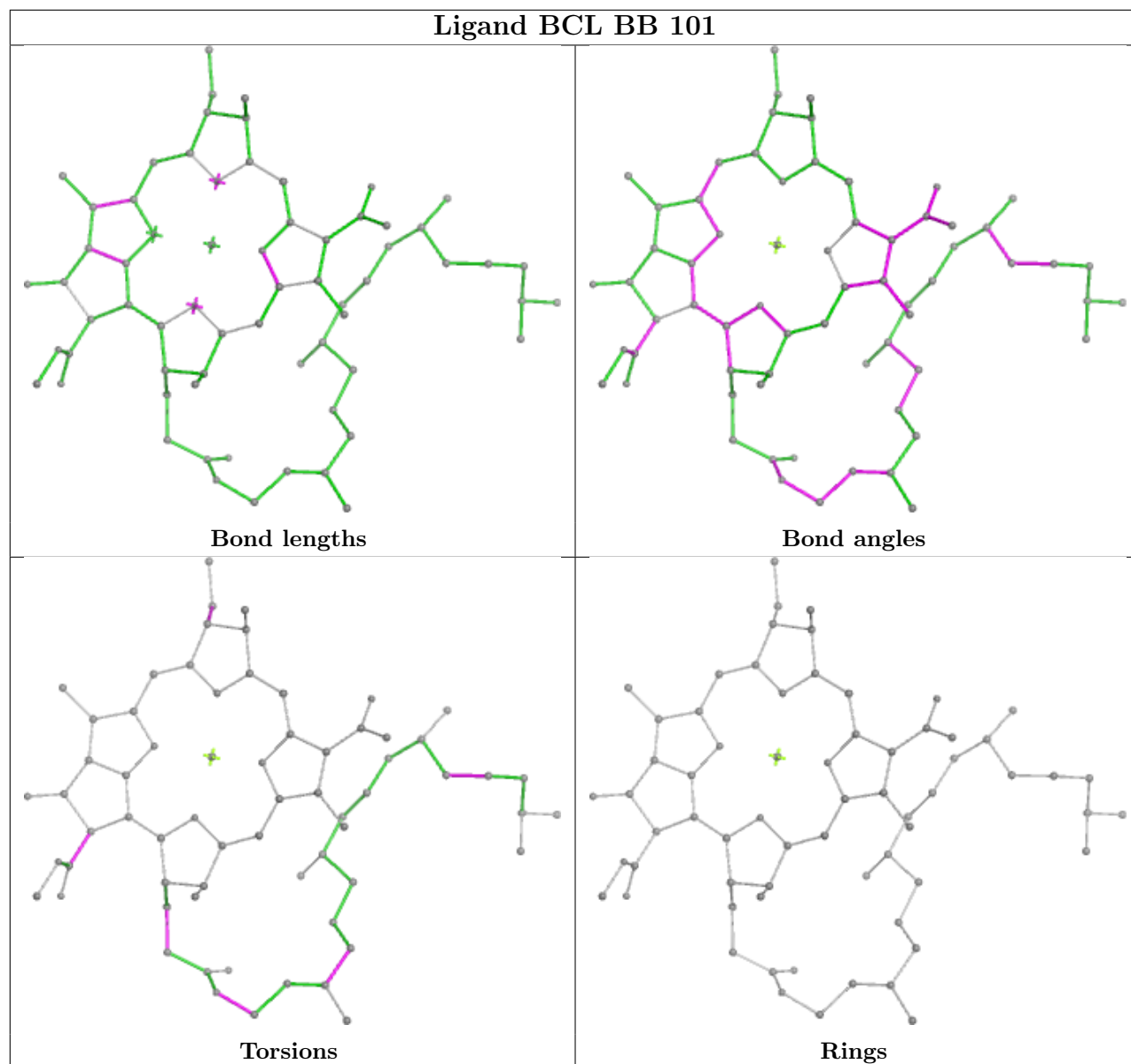
Ligand LMT BO 104**Ligand MQ8 L 305**

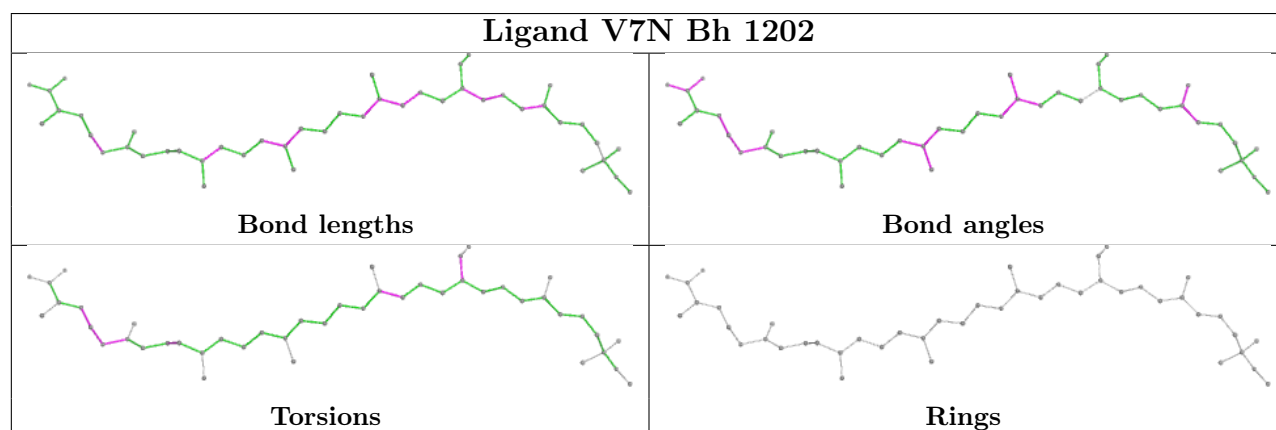
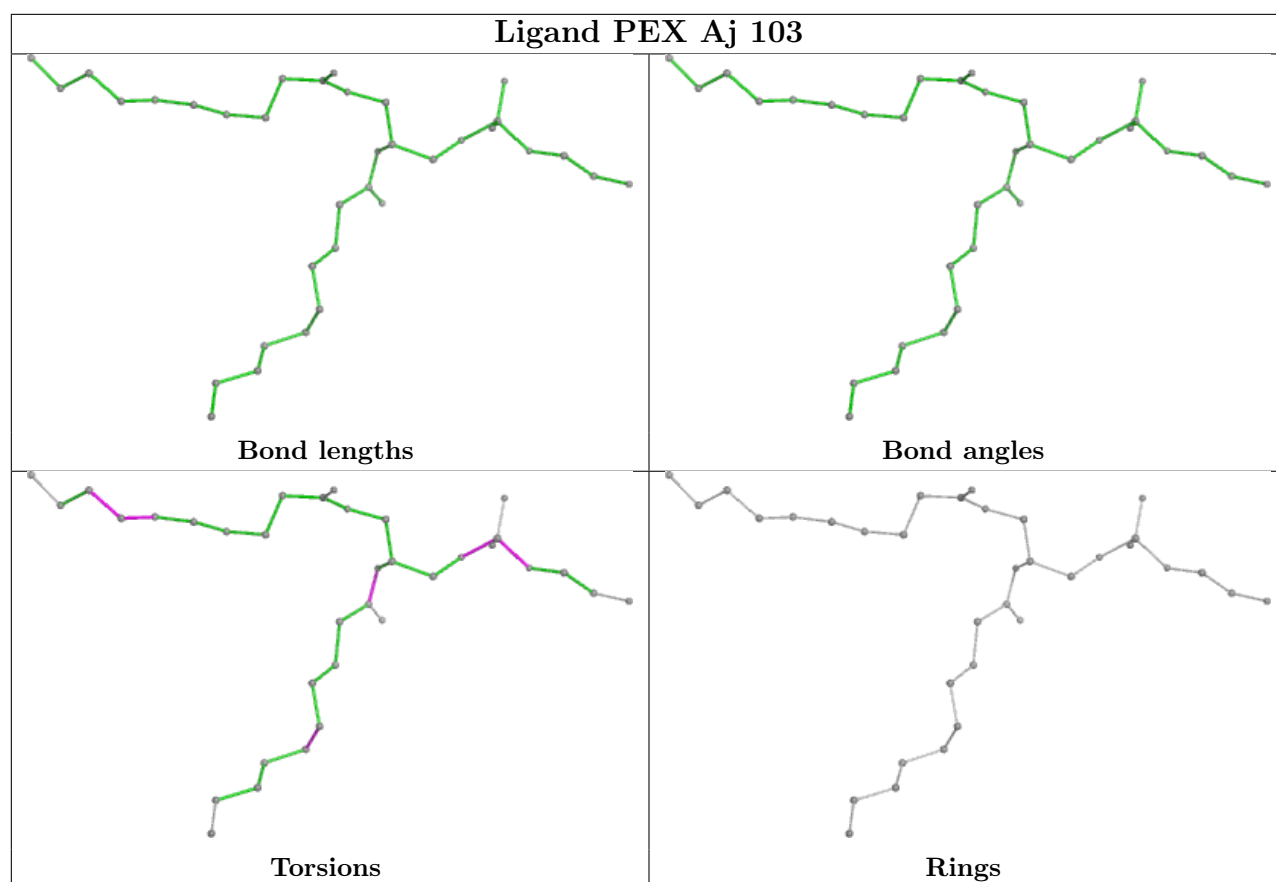


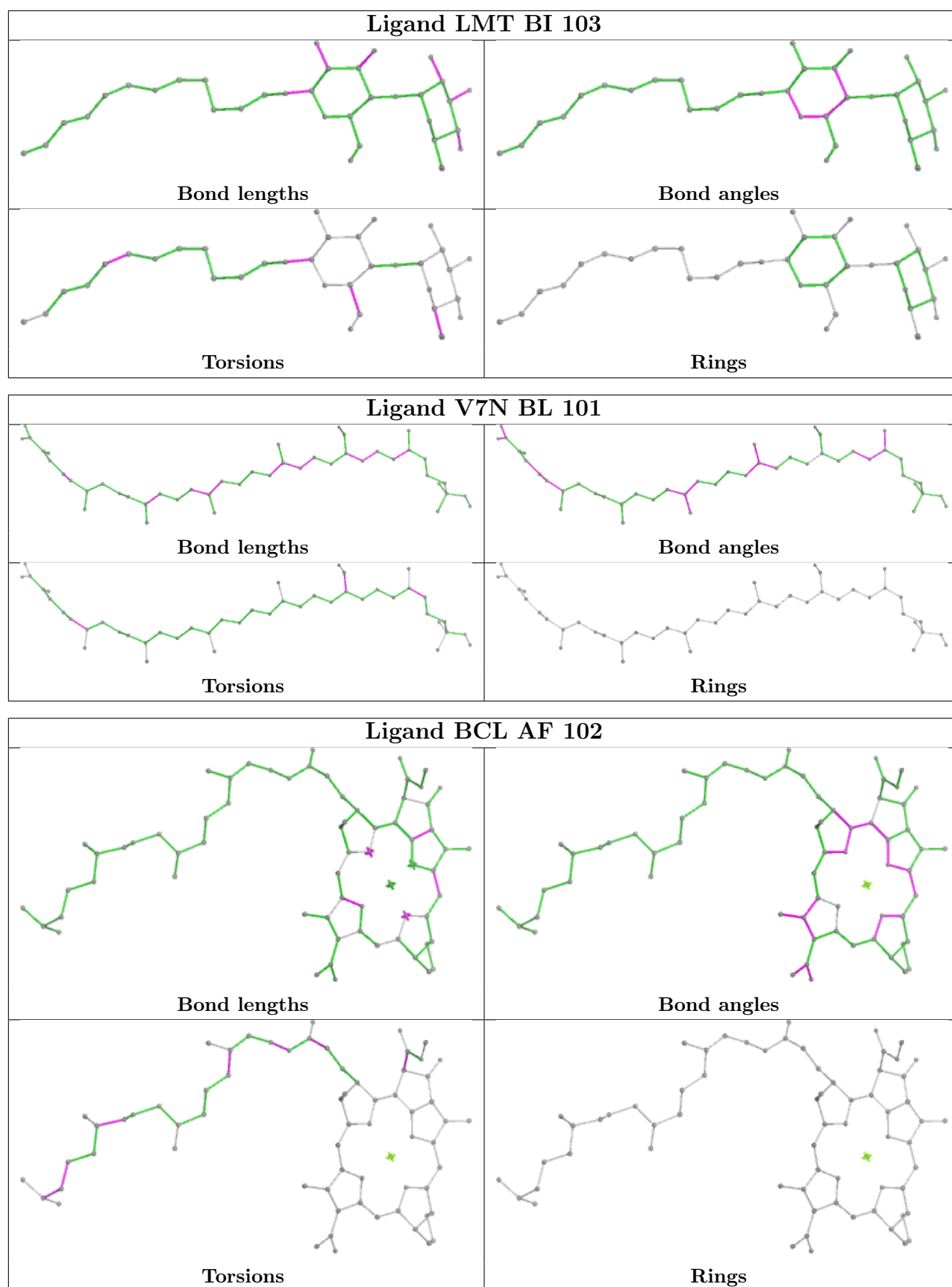


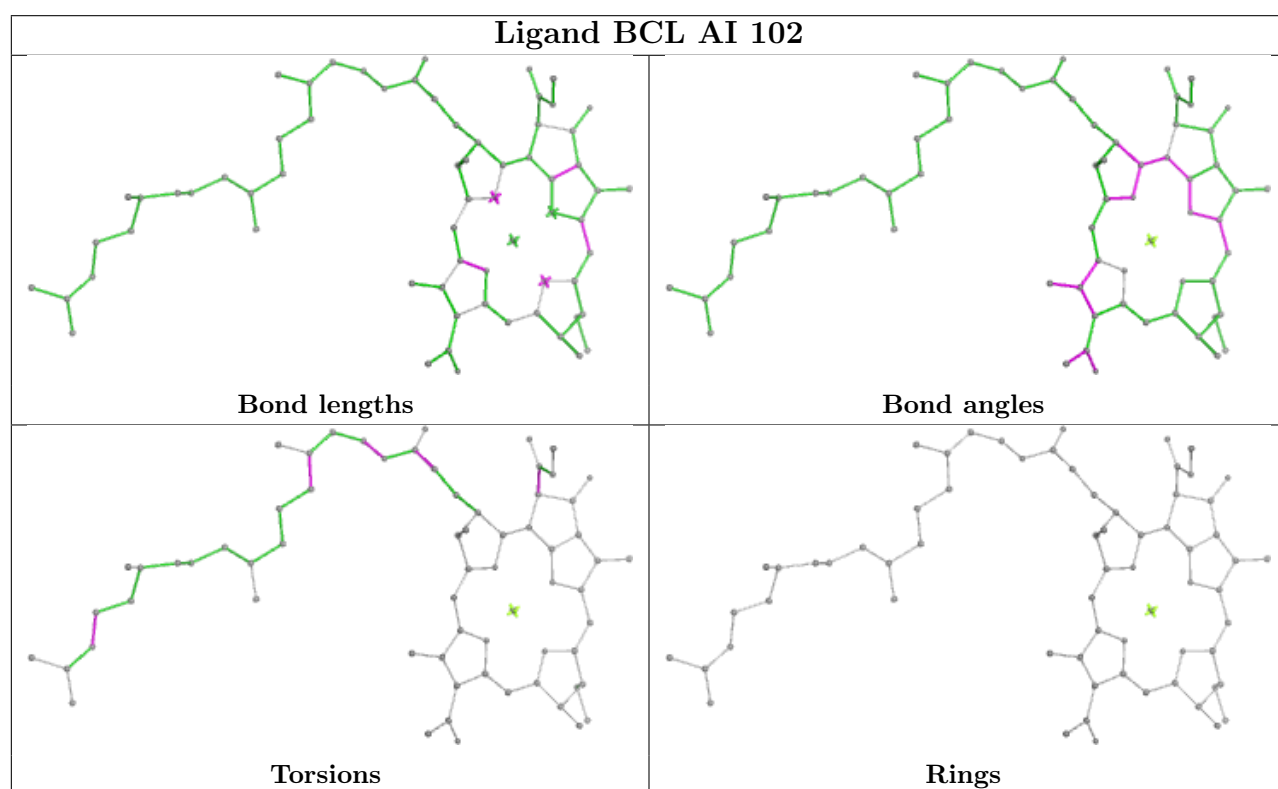
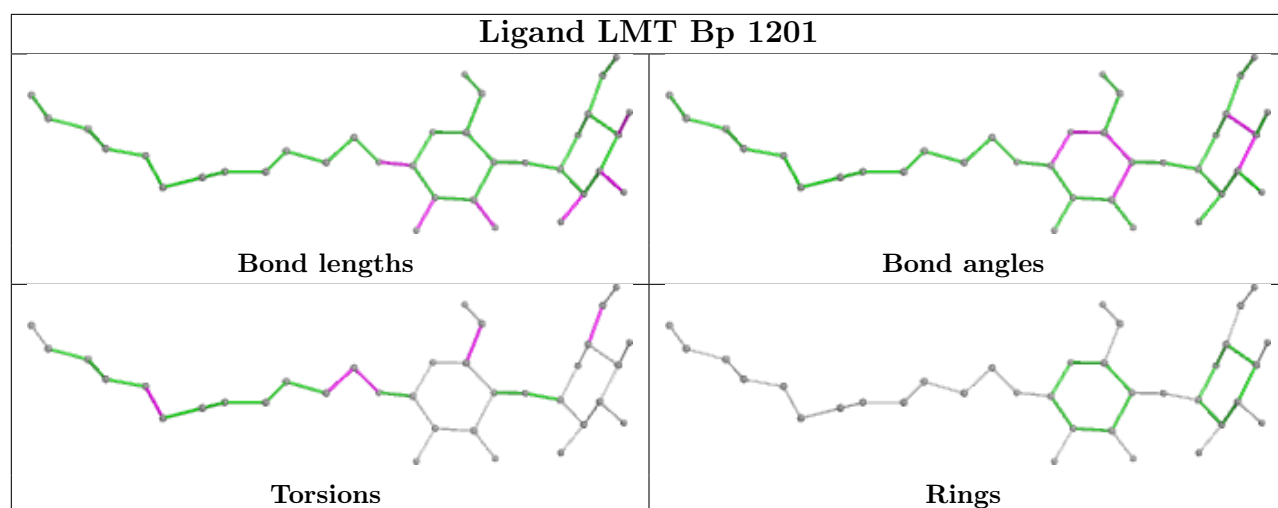


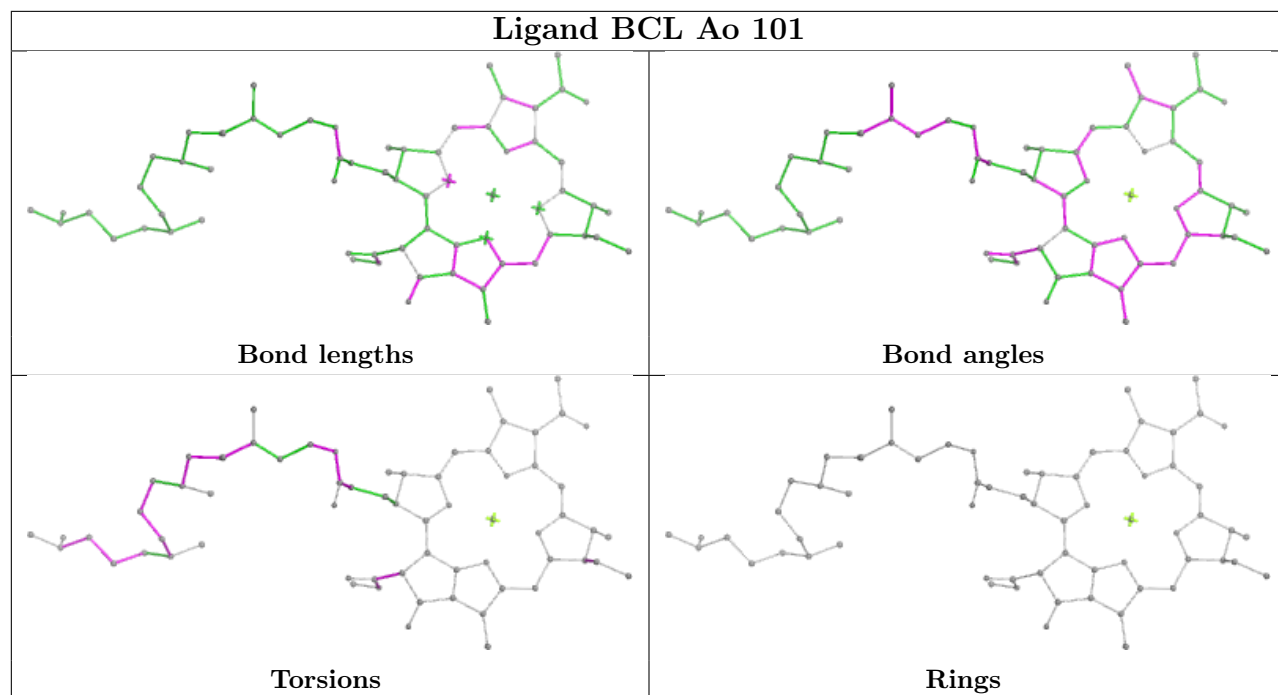
Ligand BCL BB 101

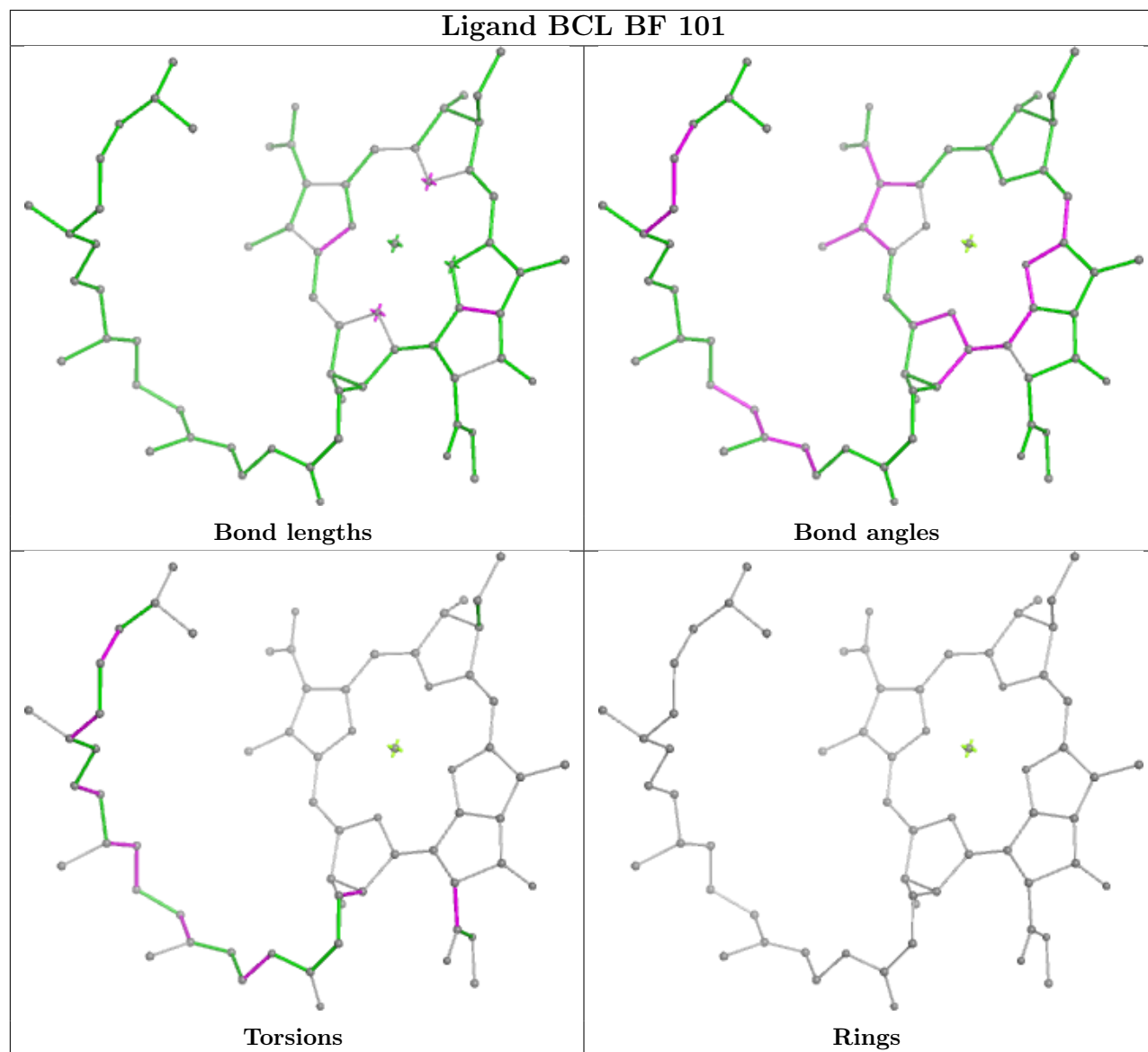


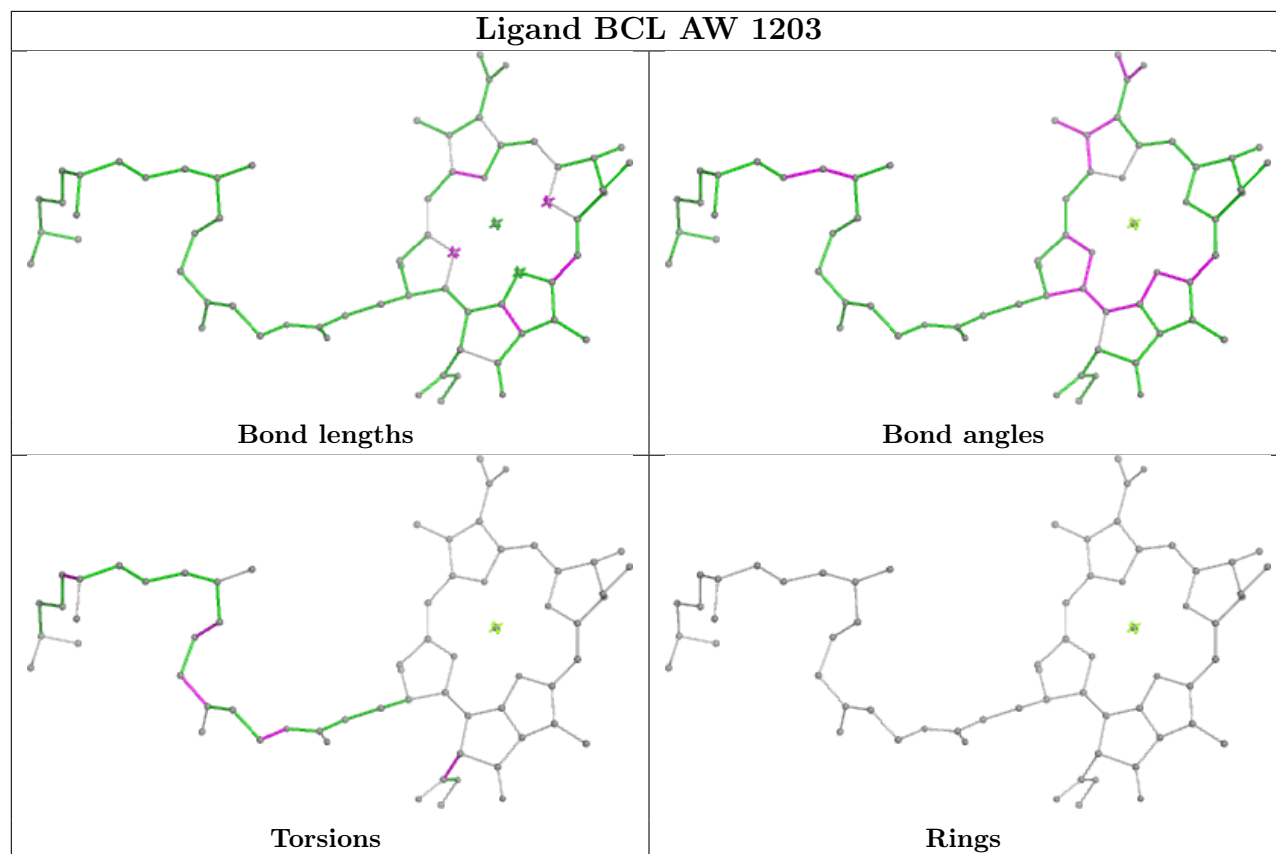
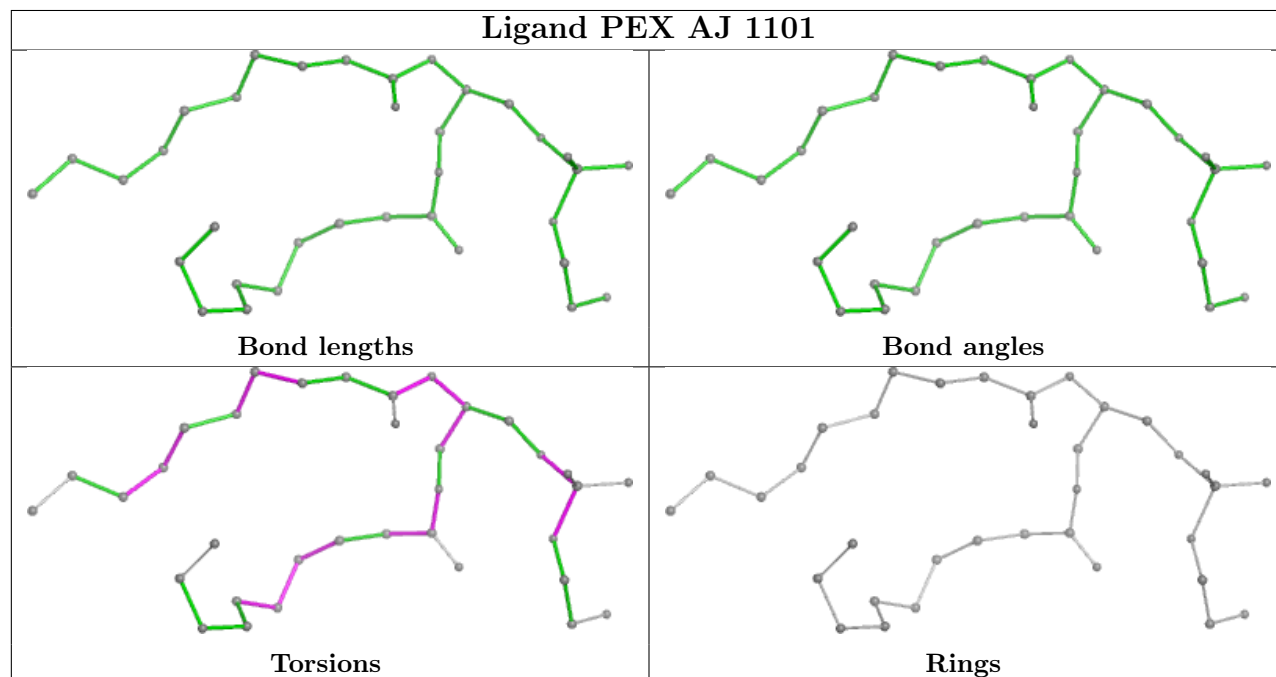


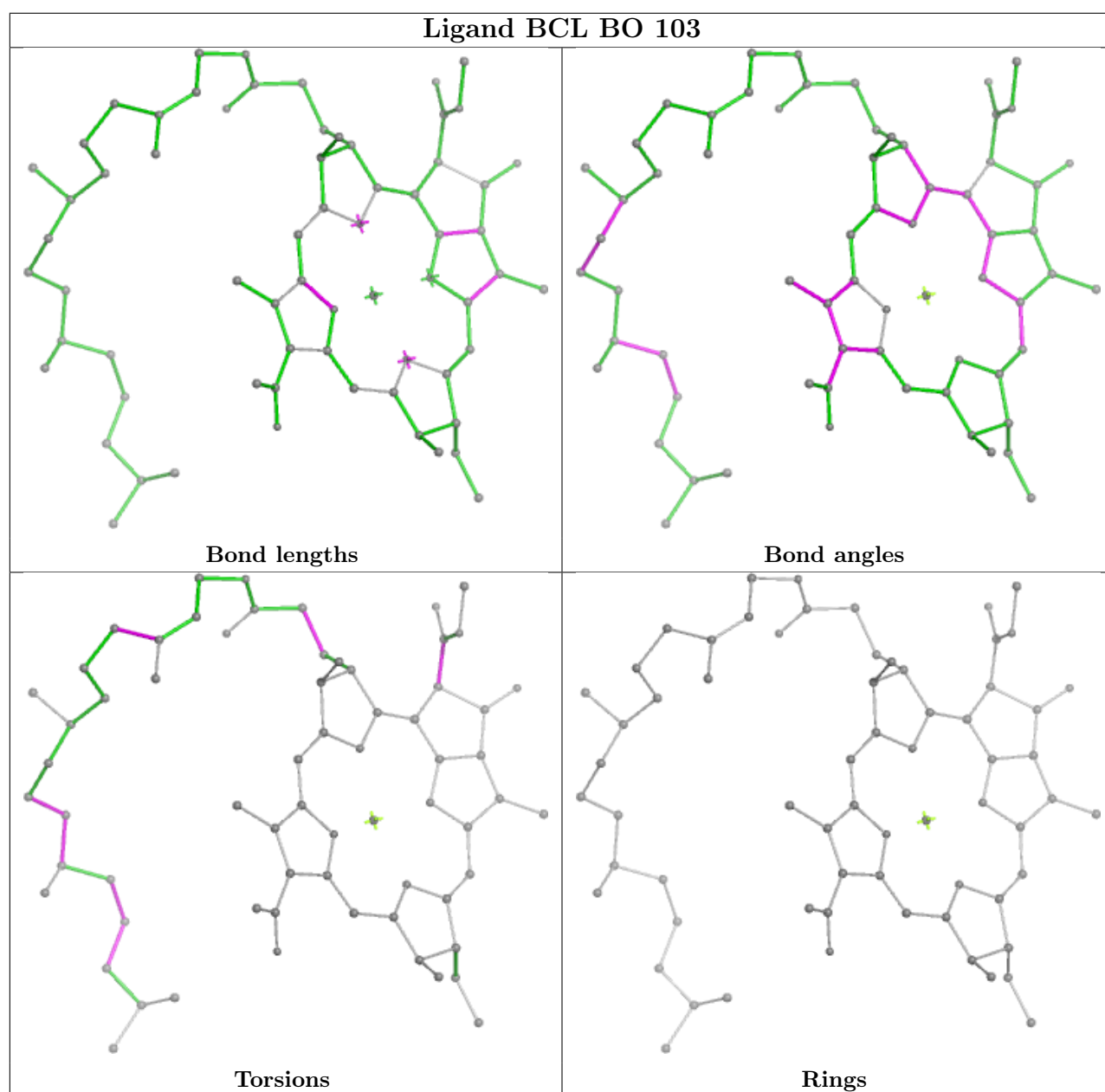
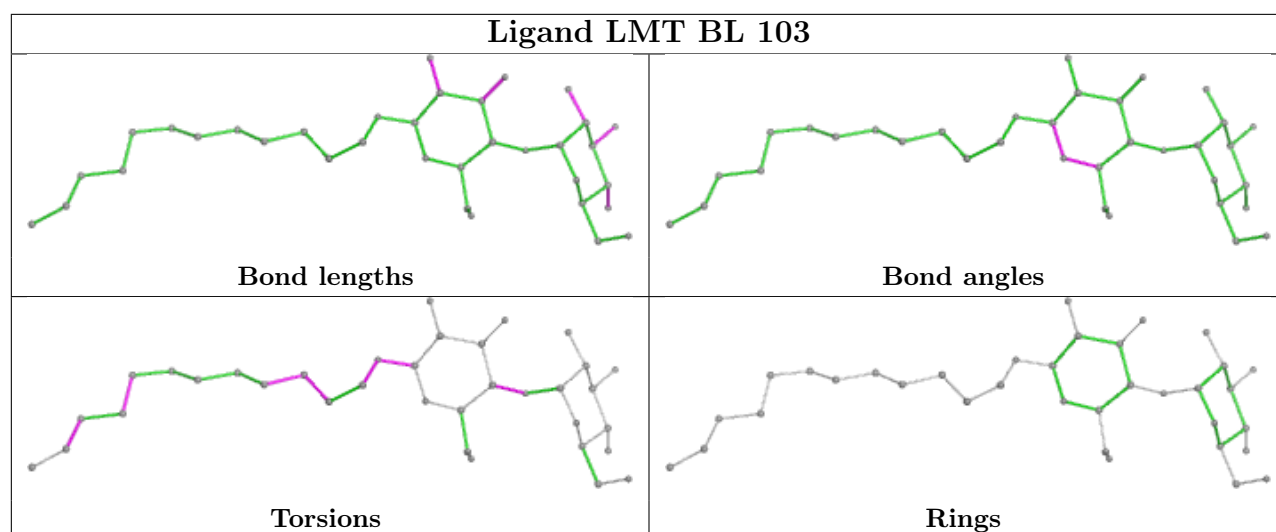


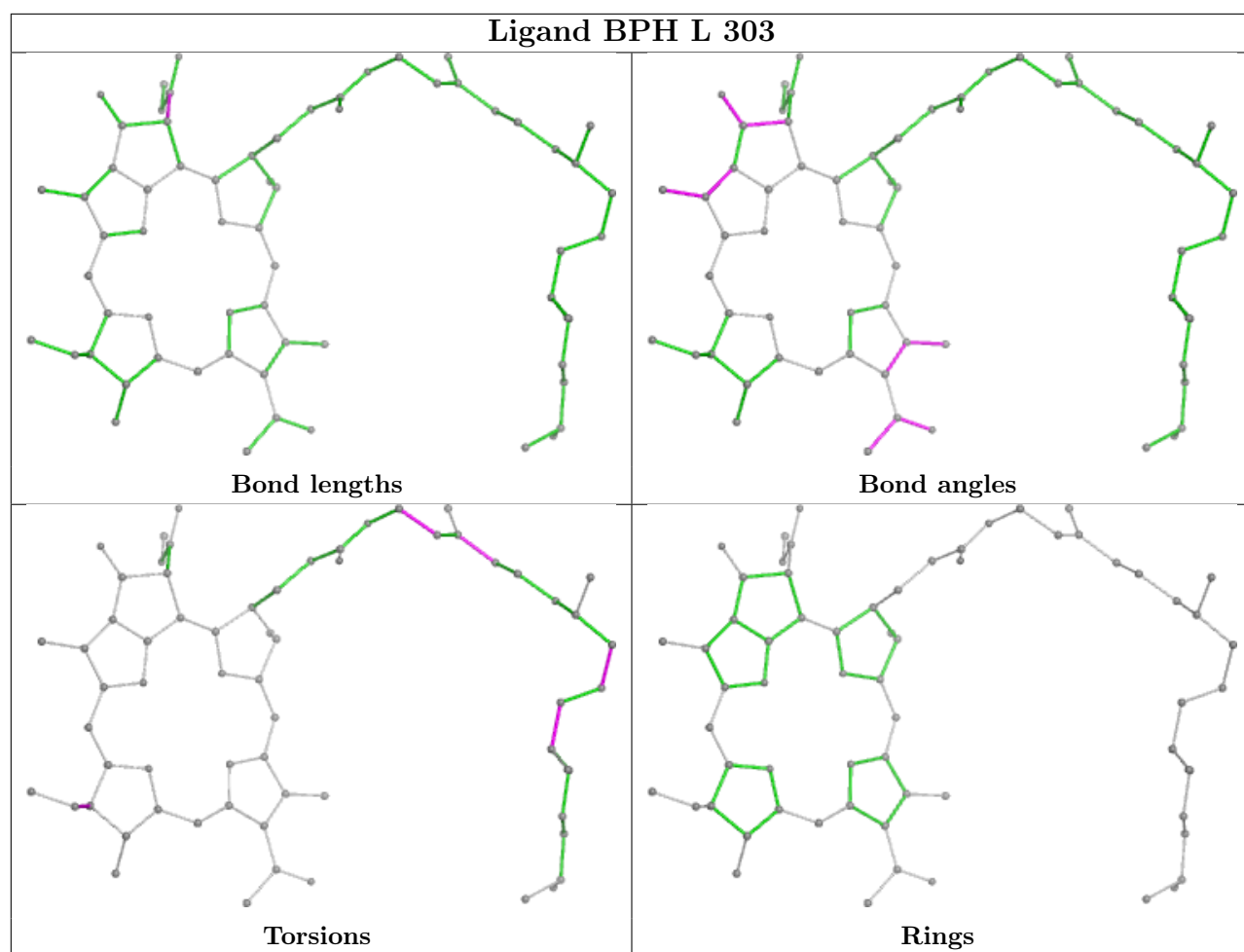




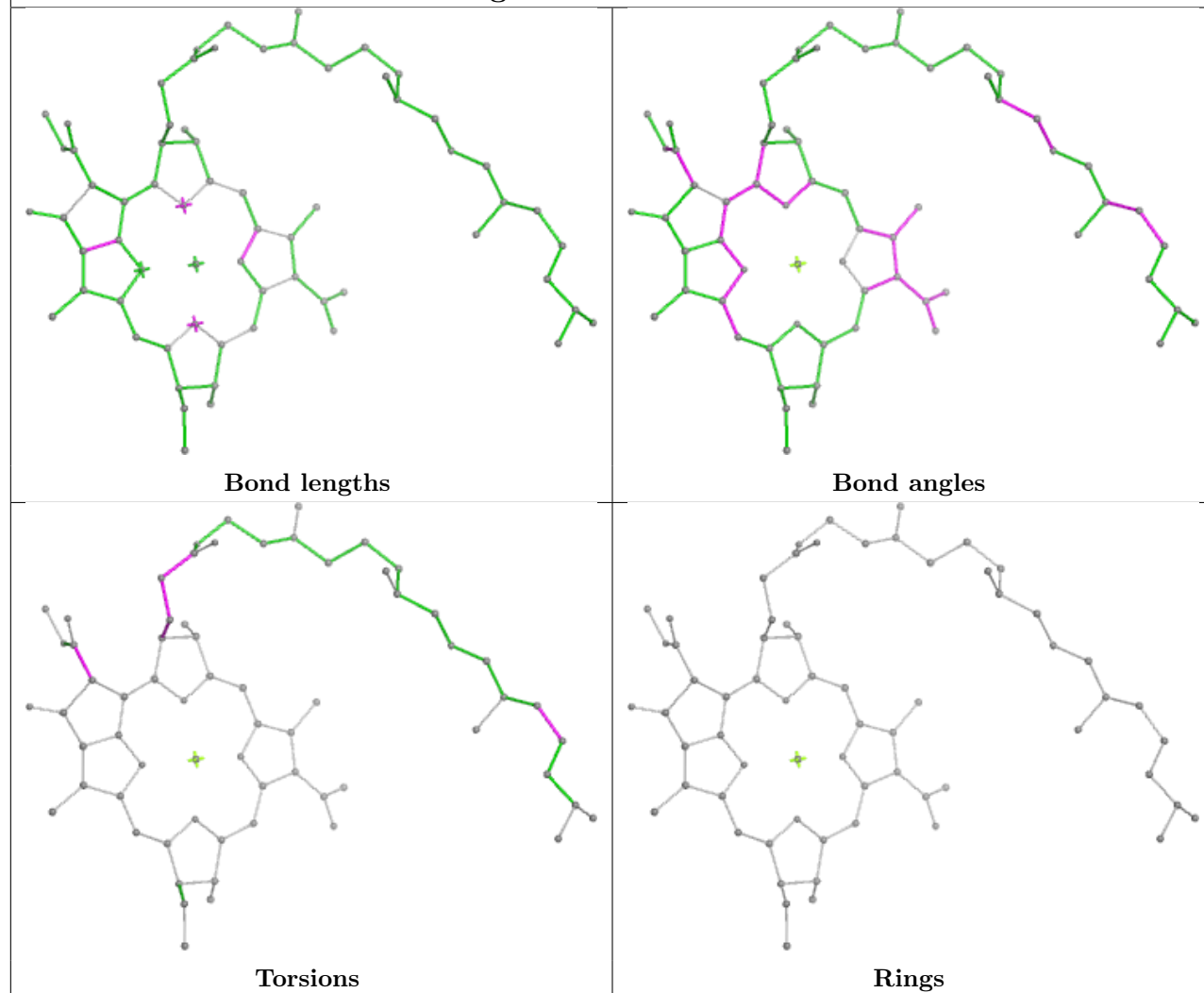


Ligand BCL AW 1203**Ligand PEX AJ 1101**

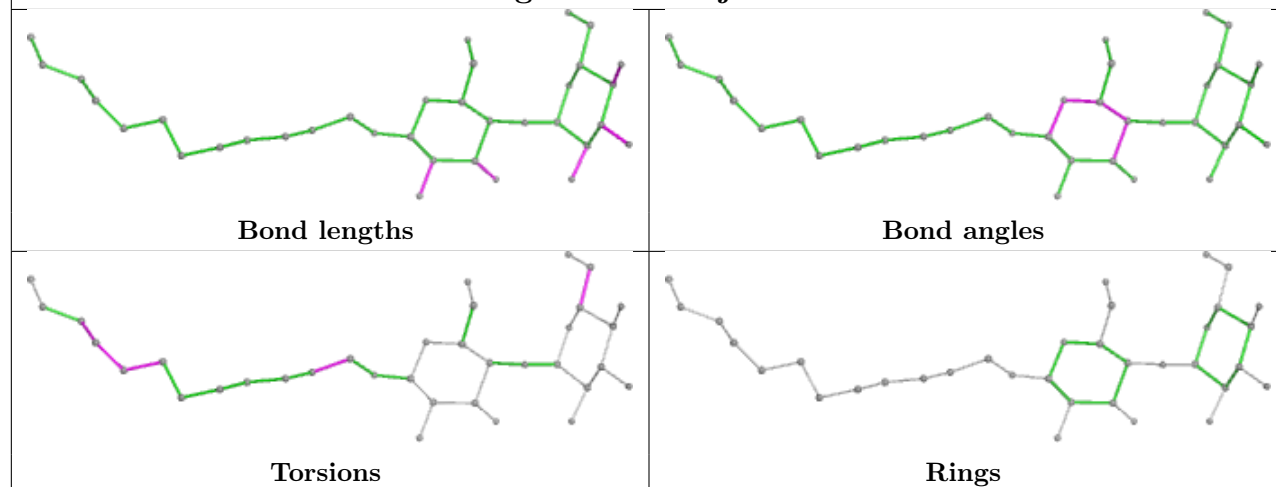


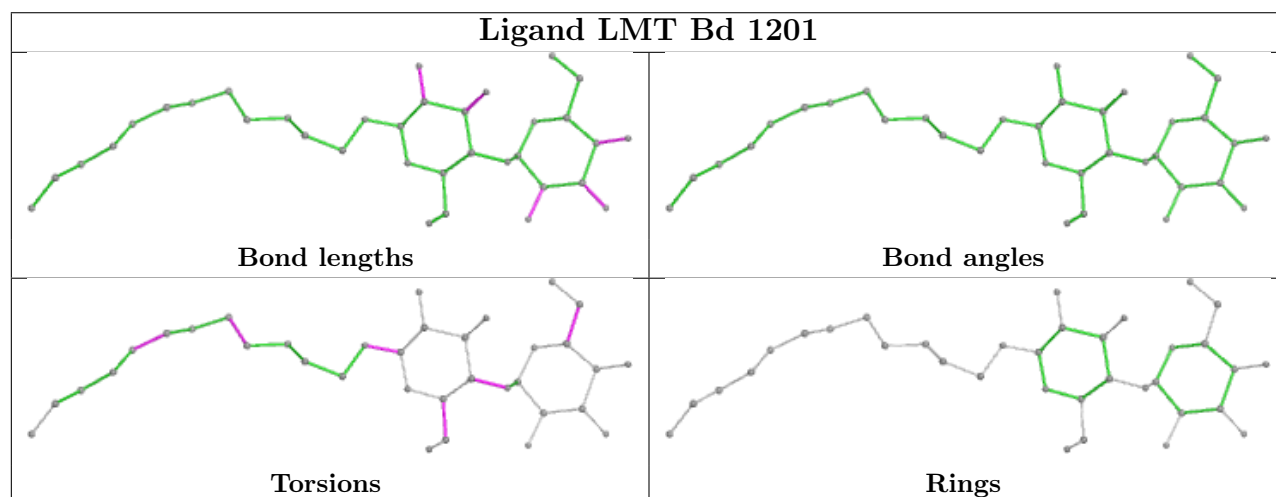
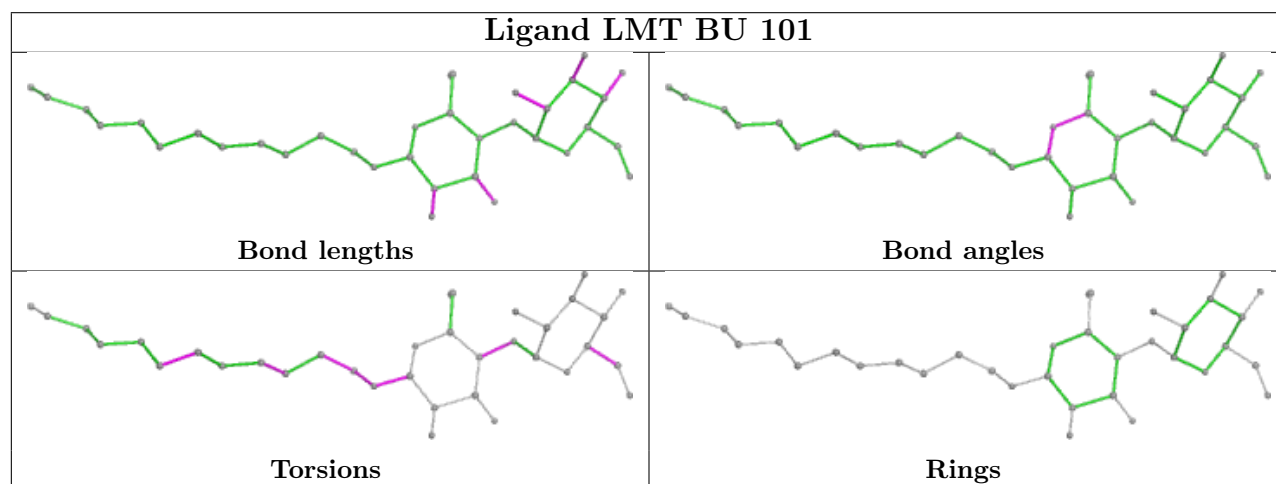
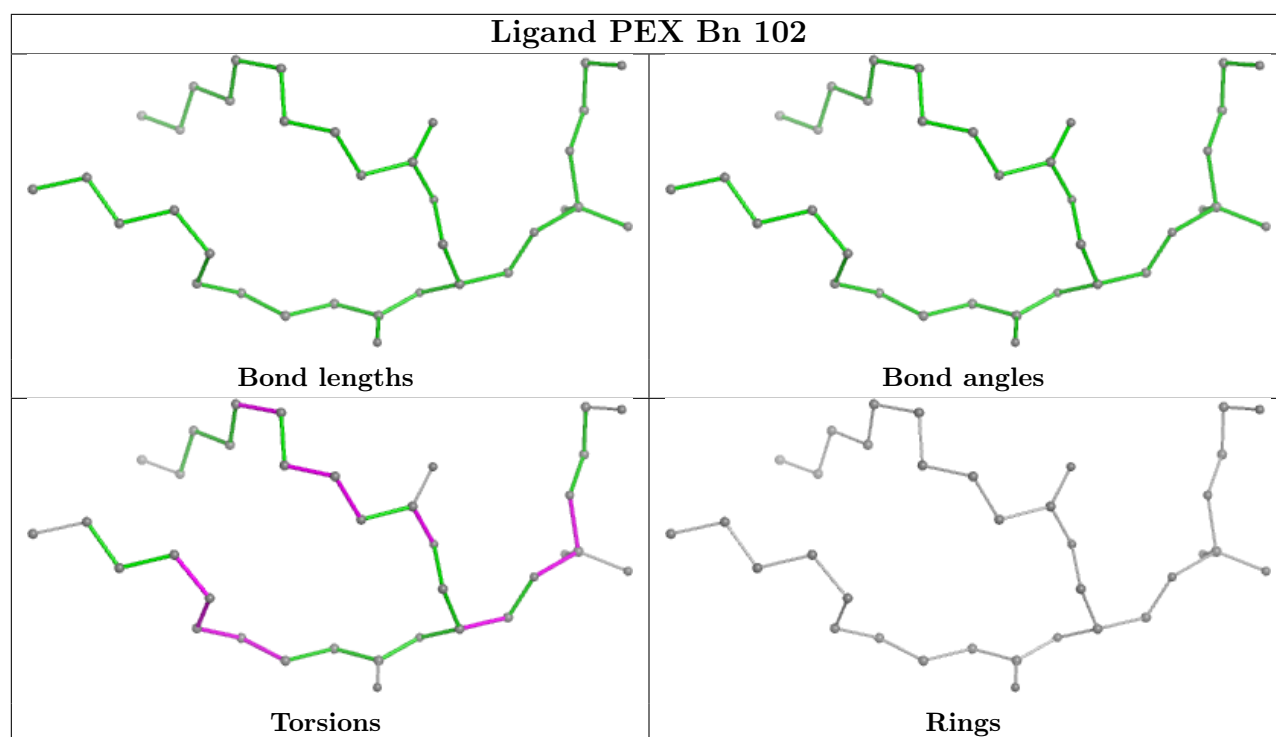


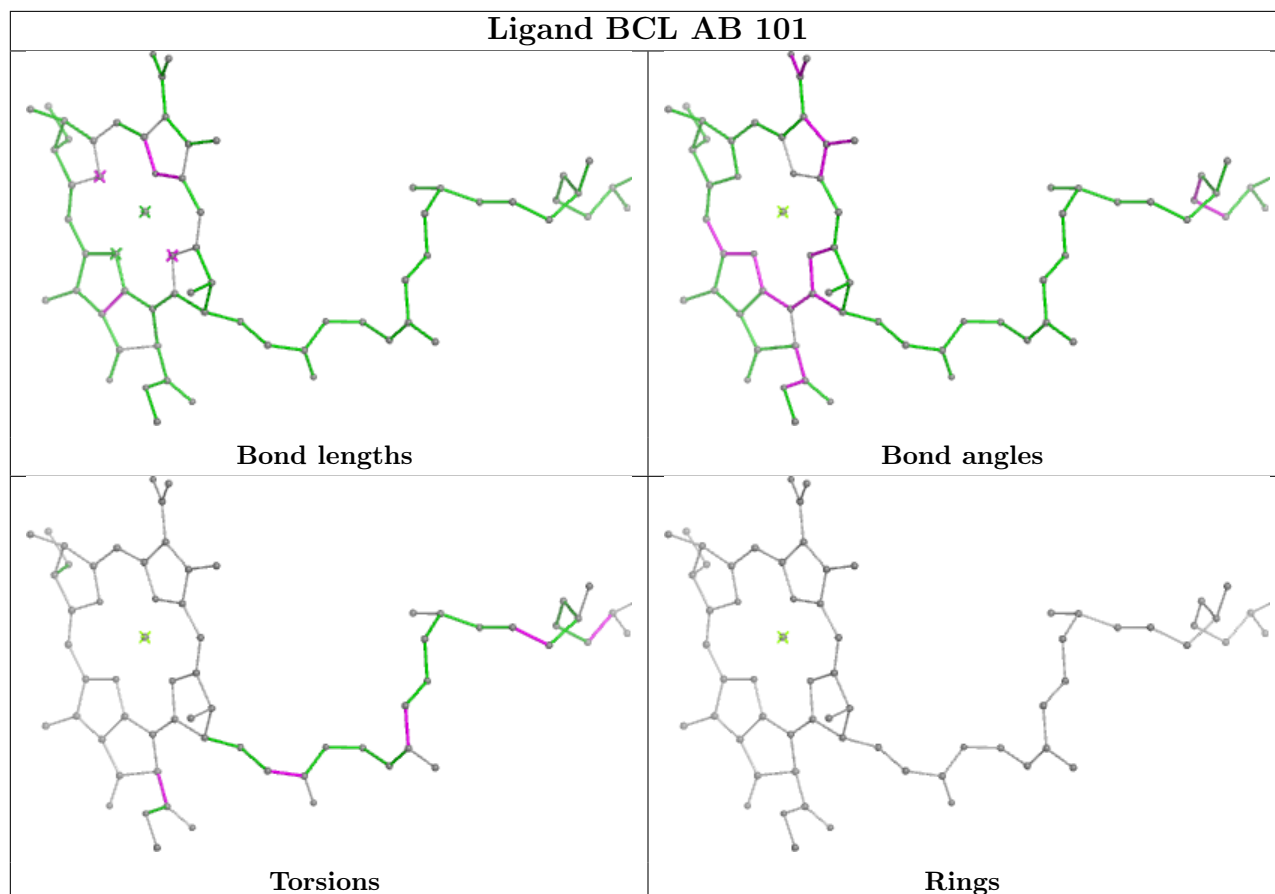
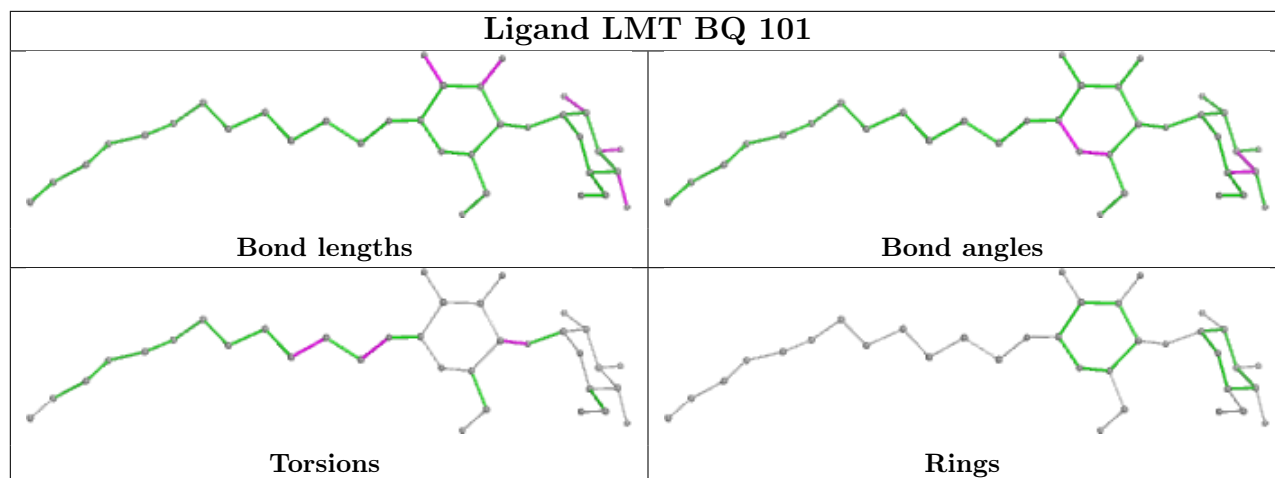
Ligand BCL BH 104

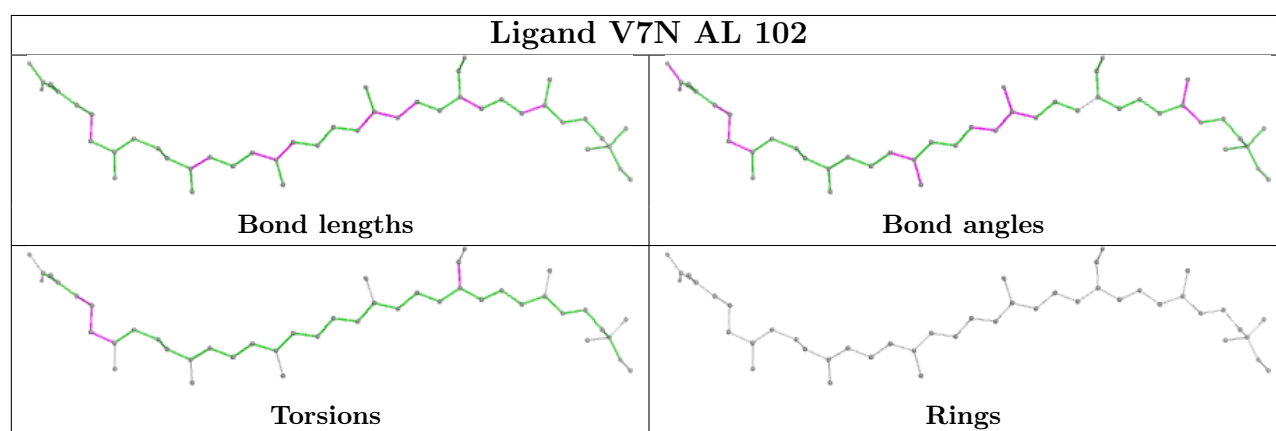
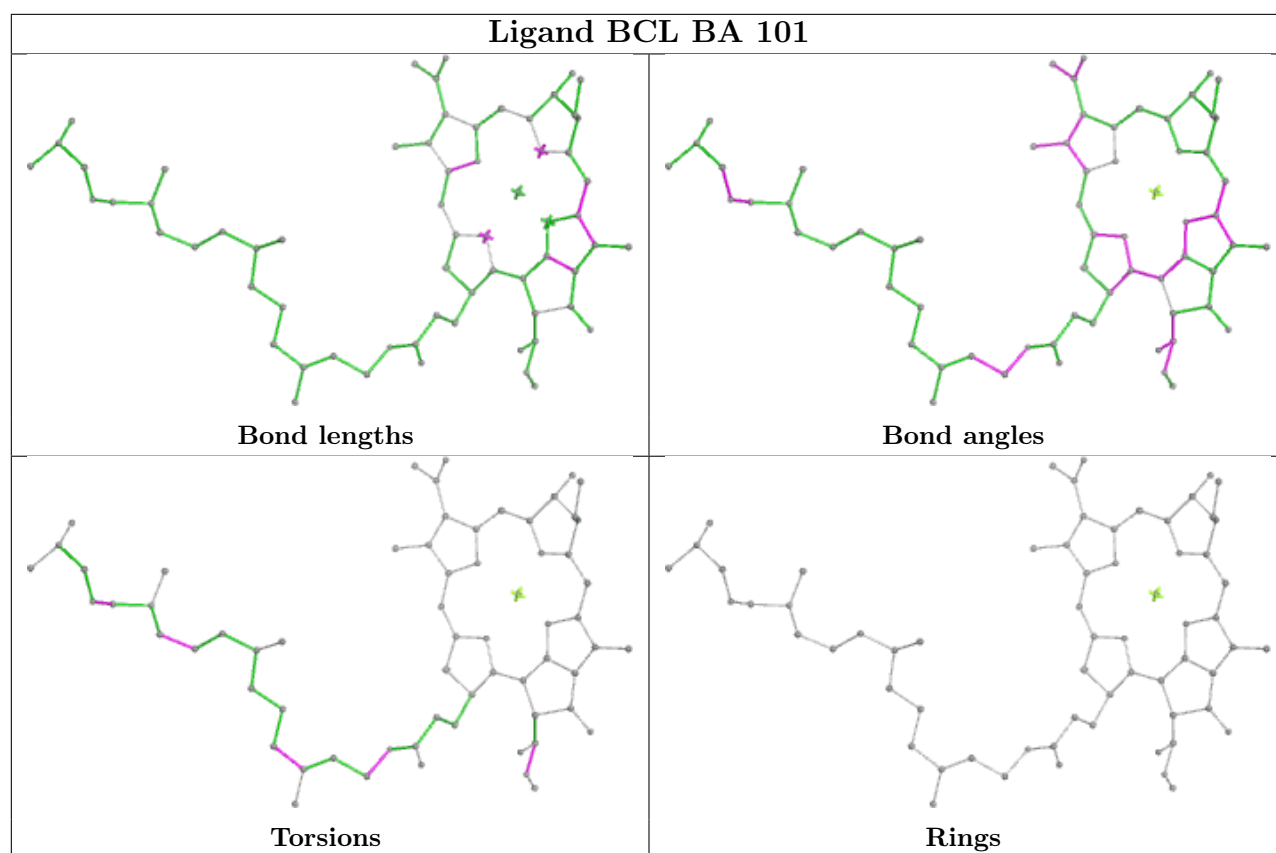


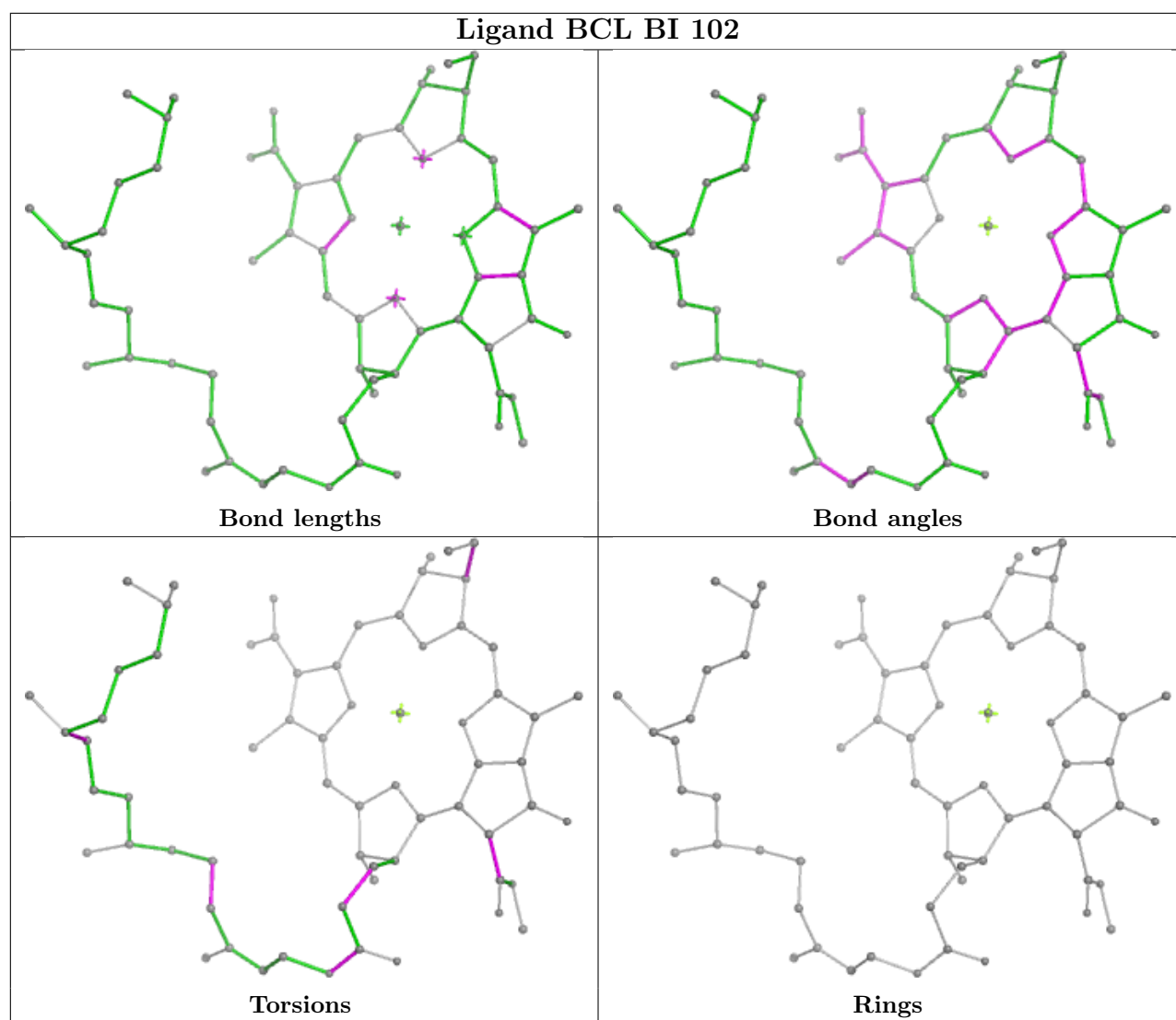
Ligand LMT Bj 1203

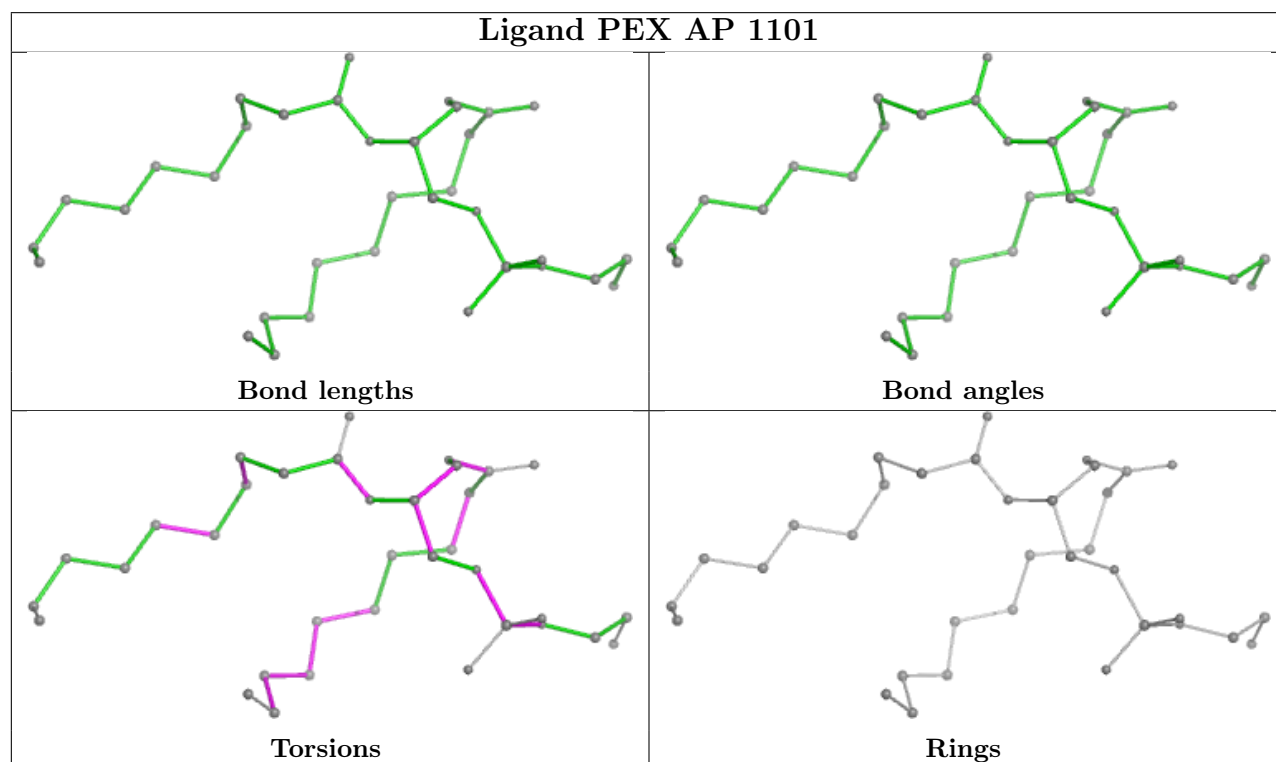
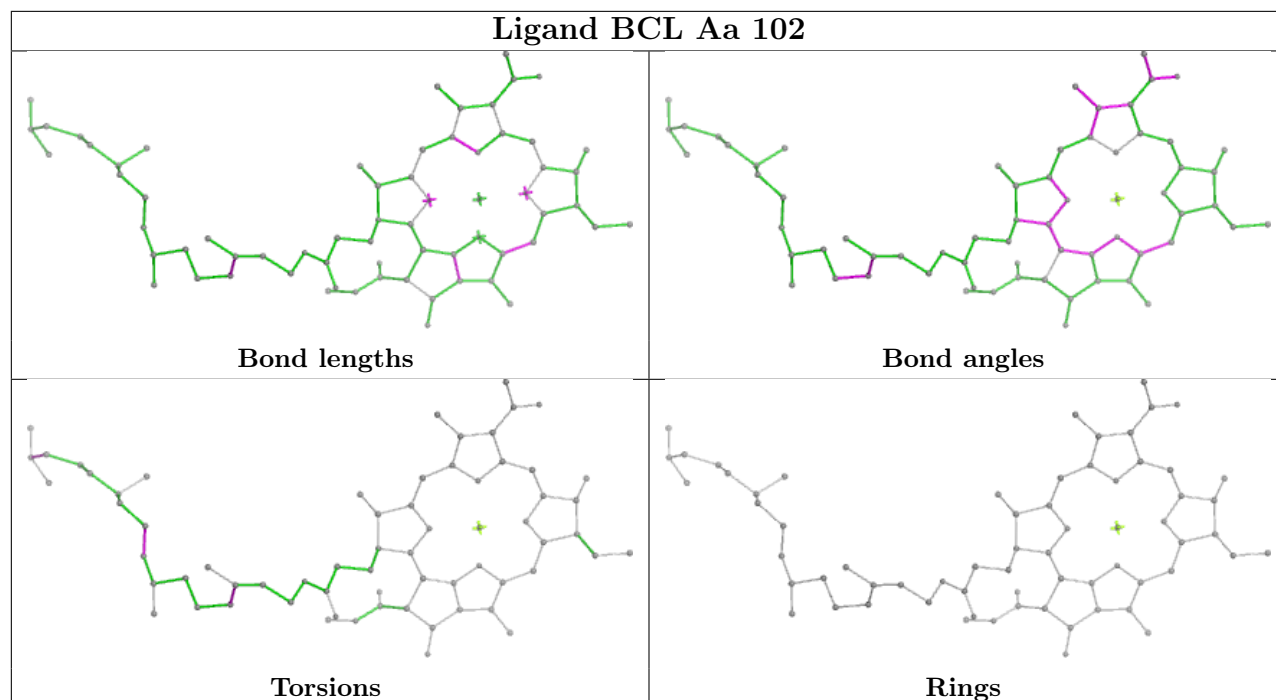


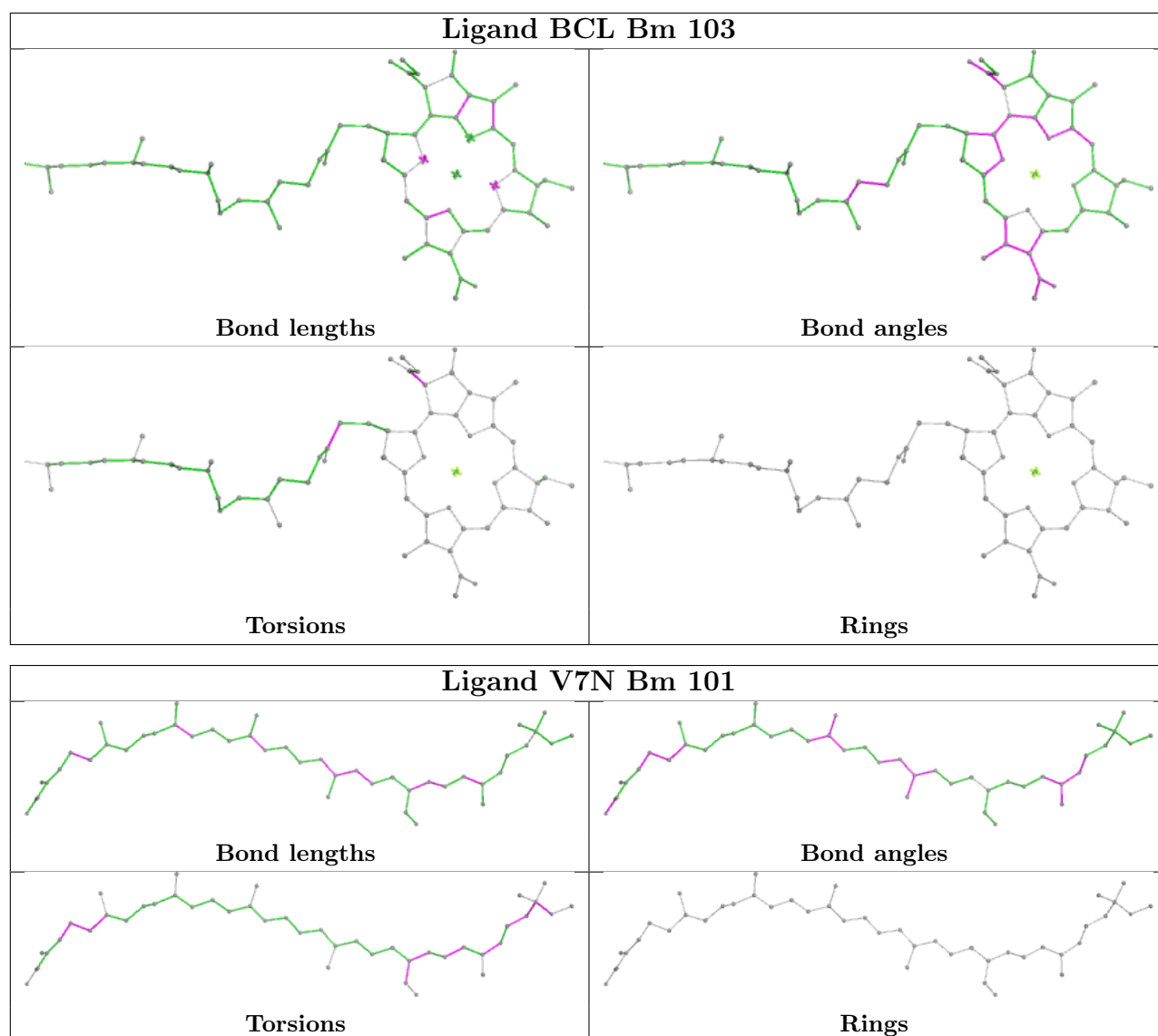


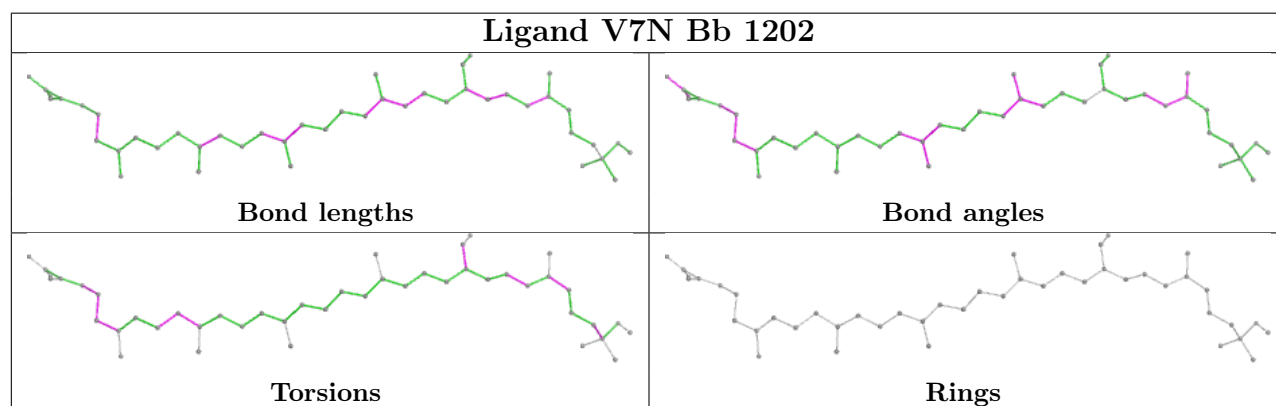
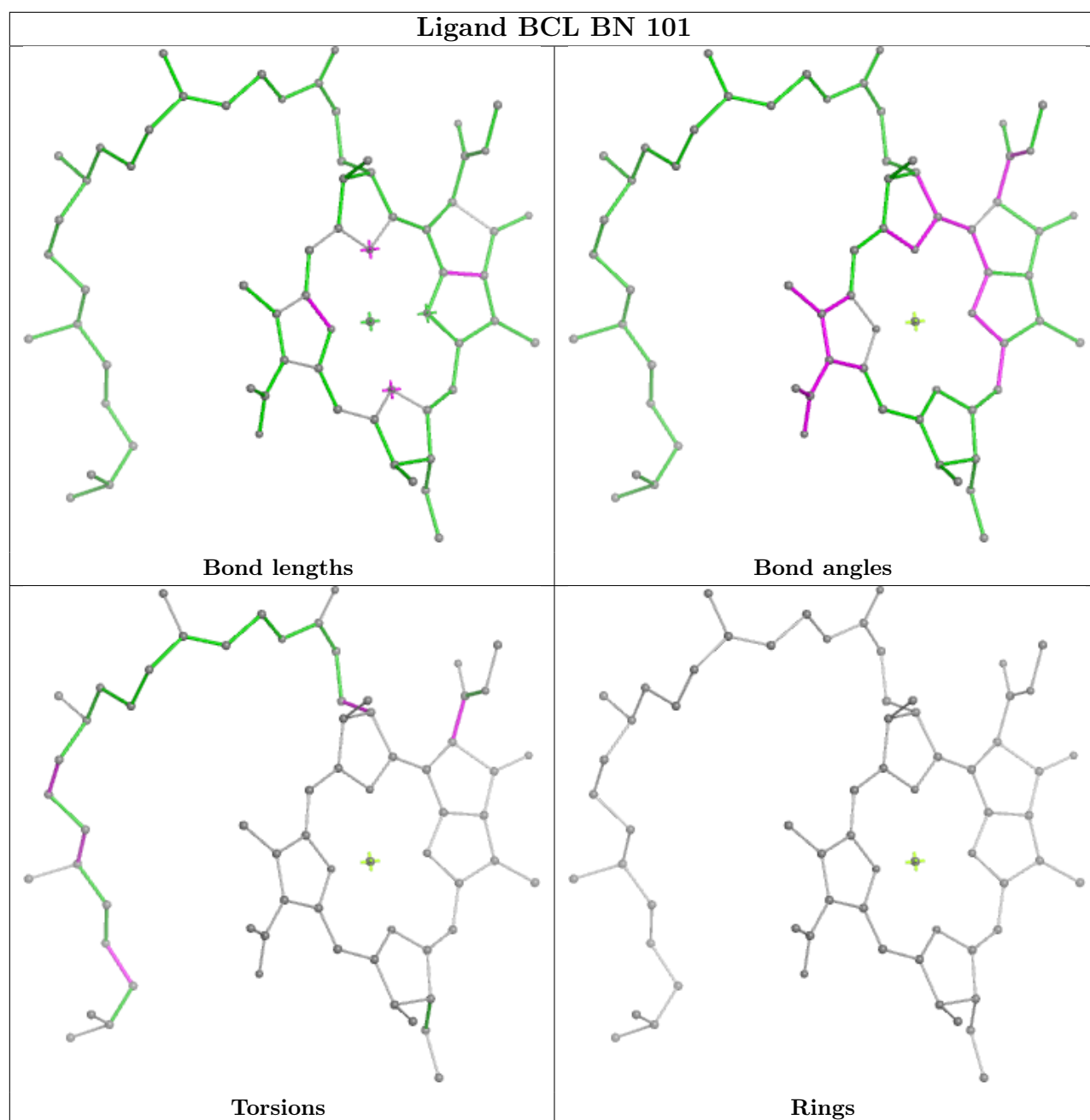


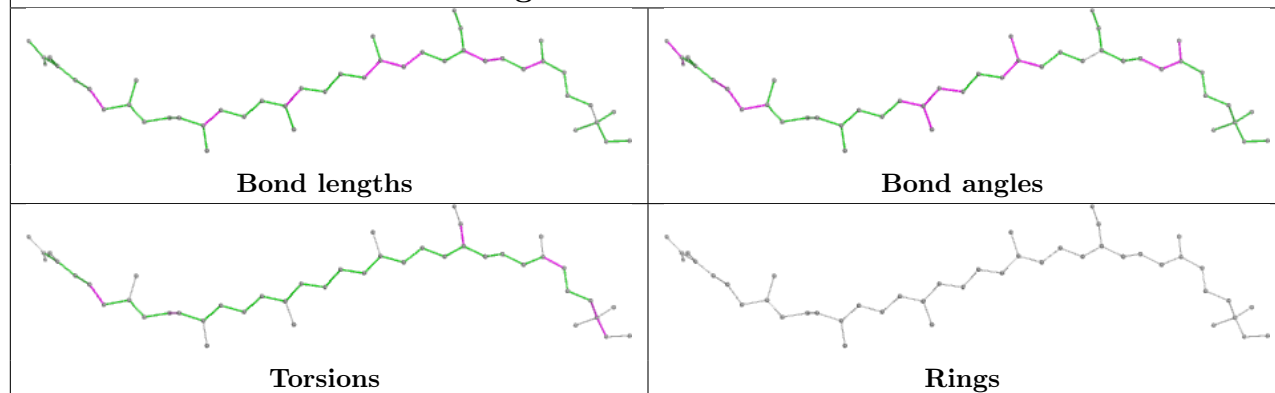
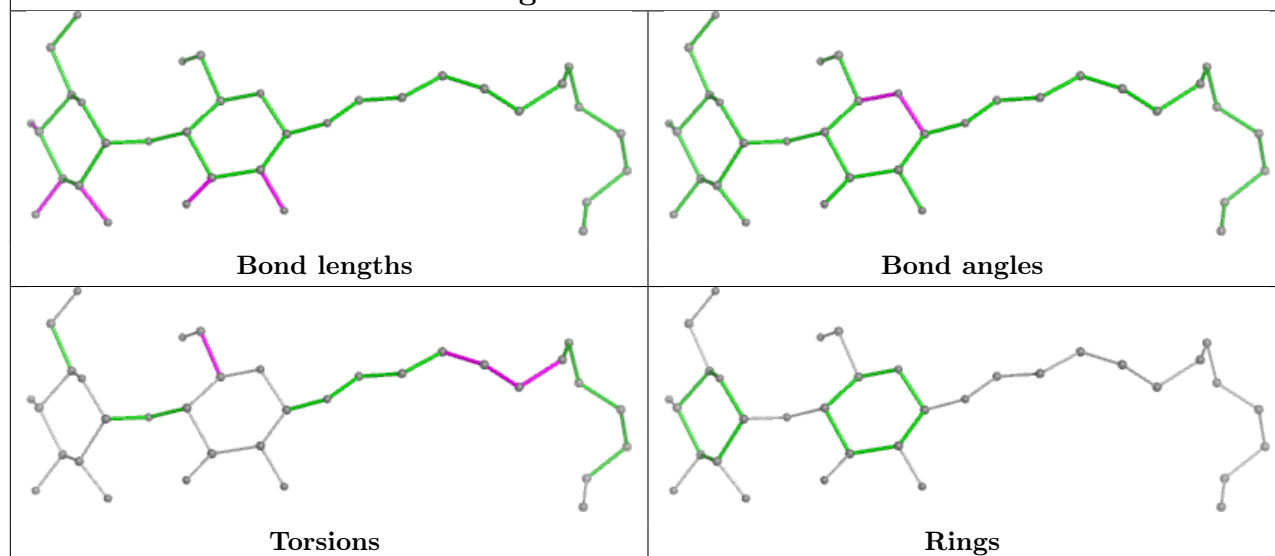
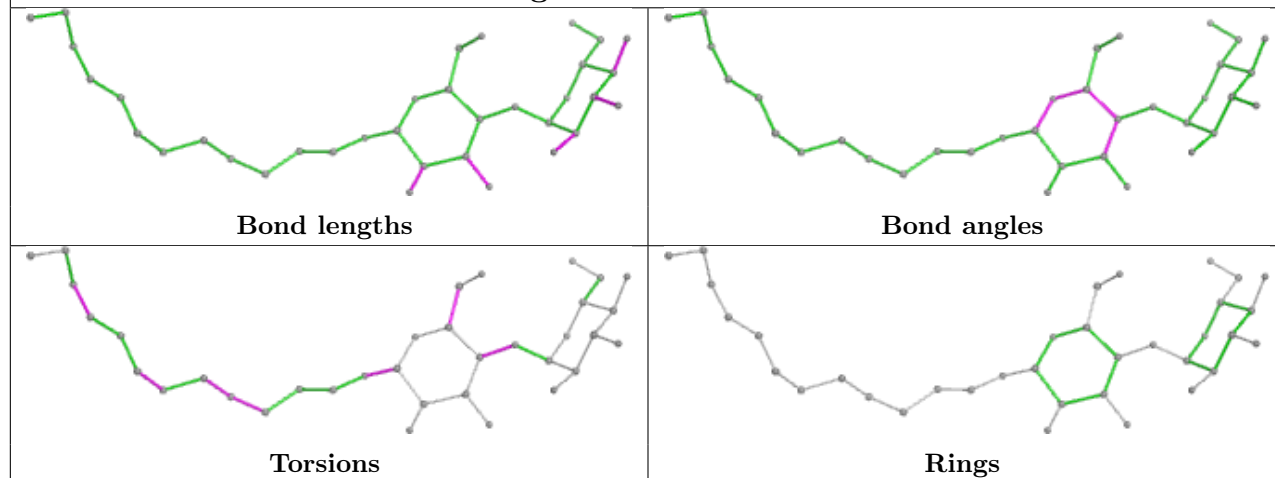




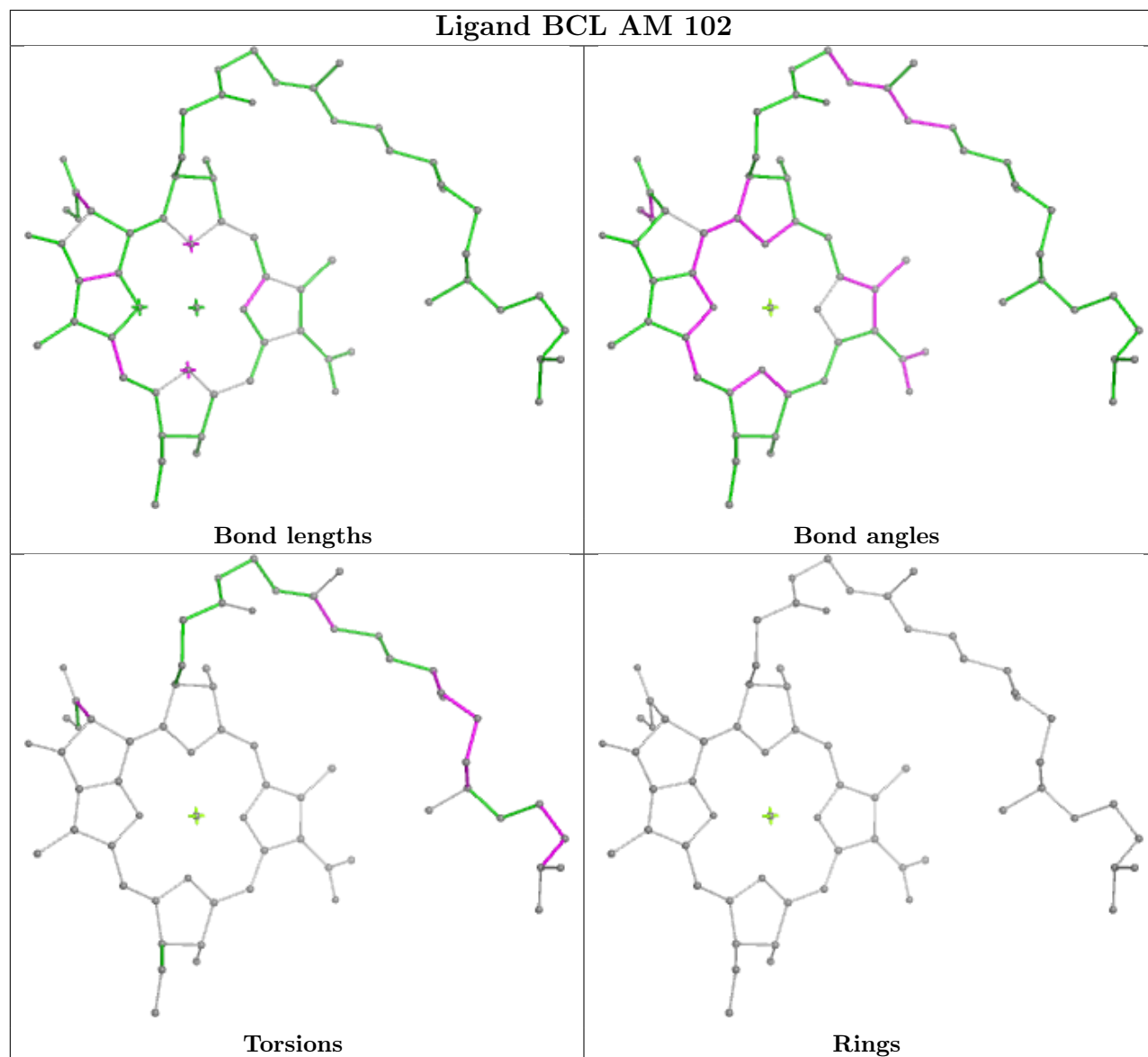




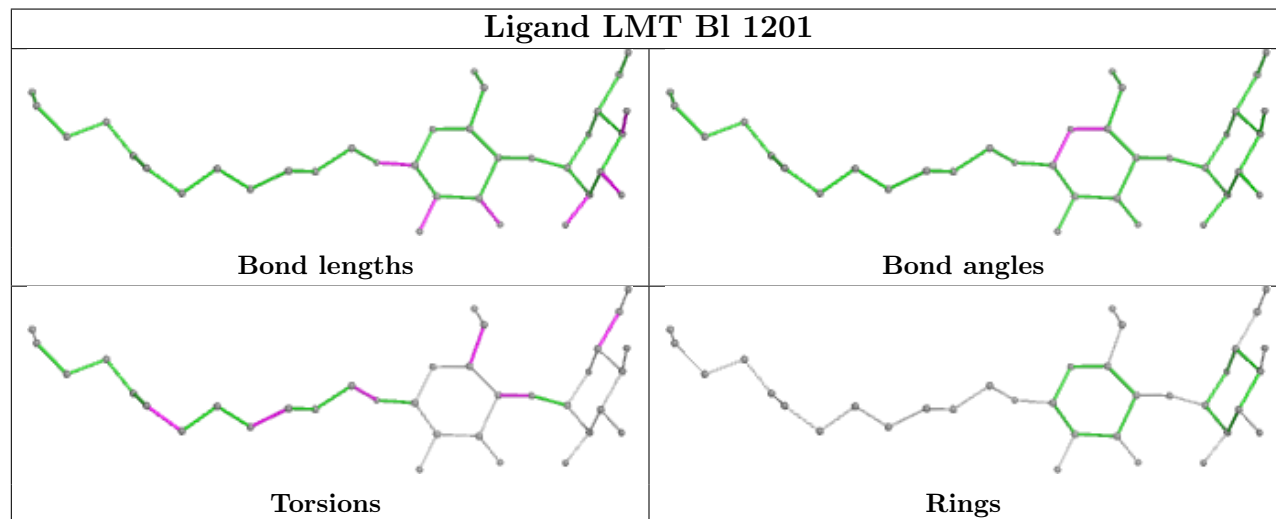


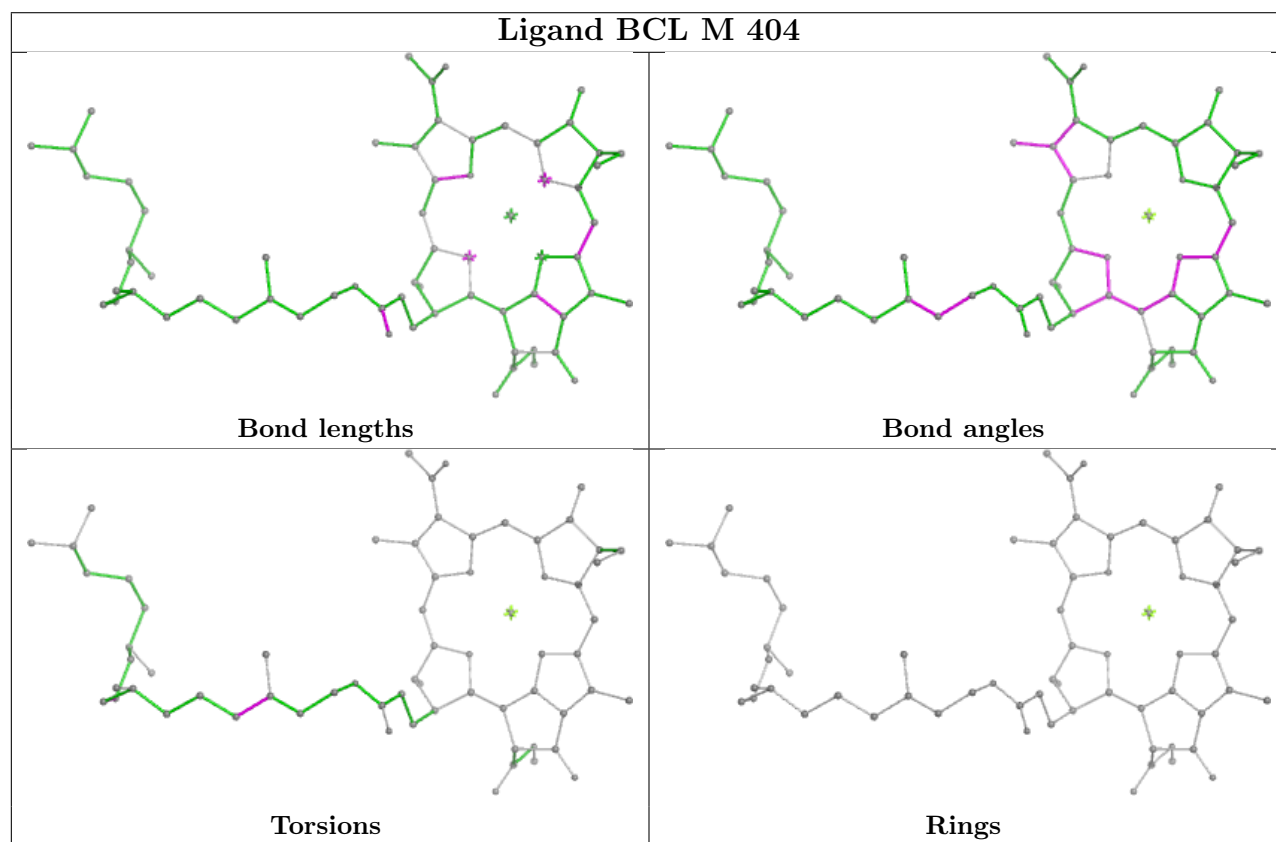
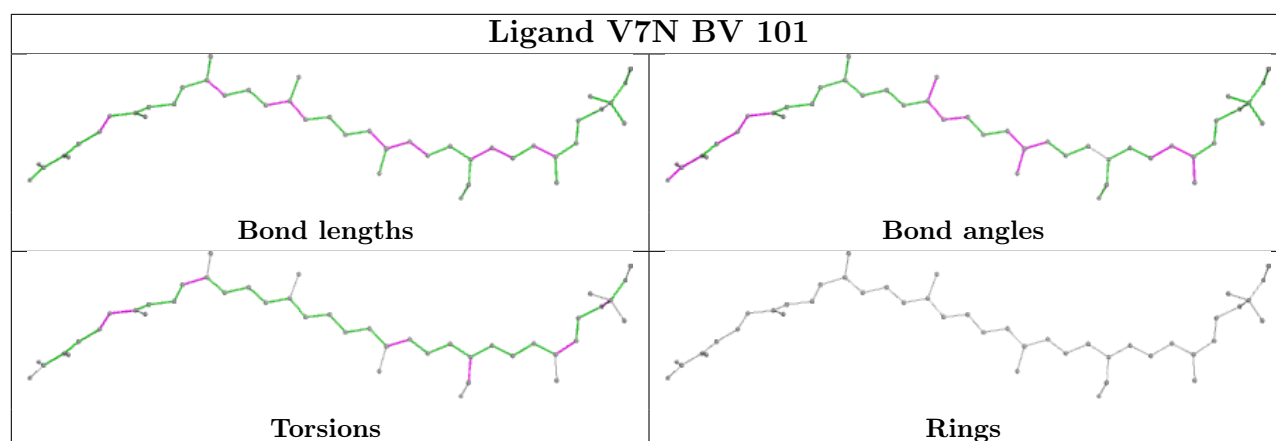
Ligand V7N Be 1103**Ligand LMT Aa 103****Ligand LMT L 304**

Ligand BCL AM 102

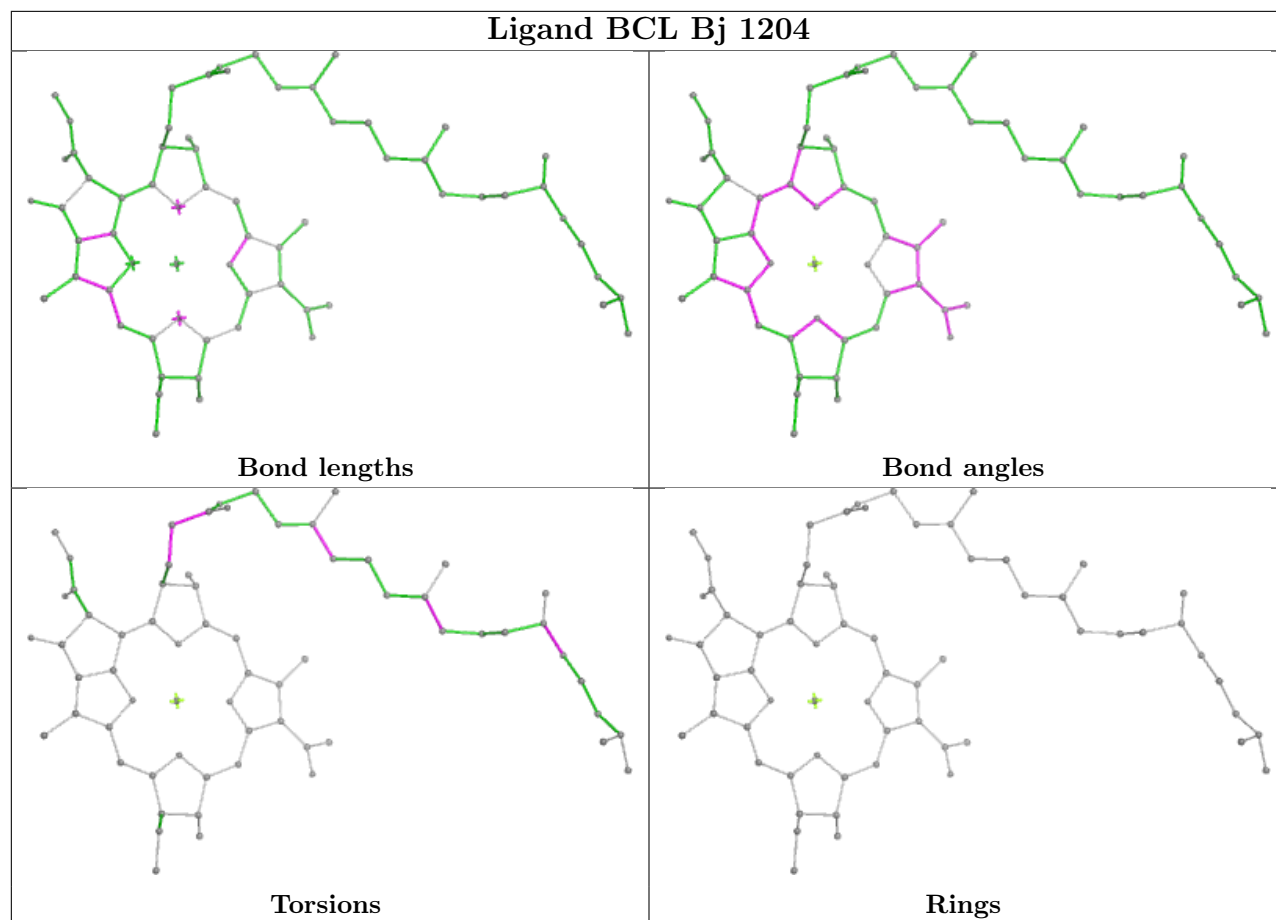


Ligand LMT BI 1201

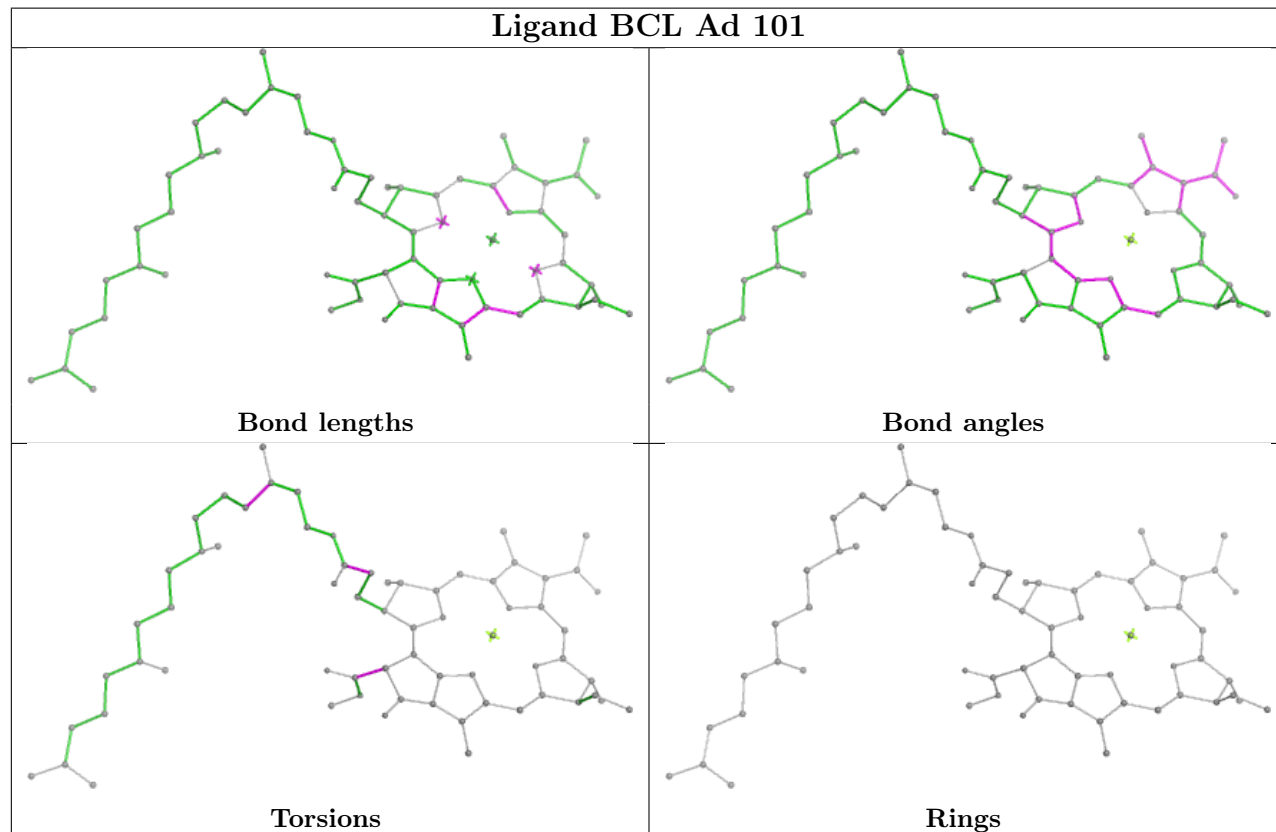


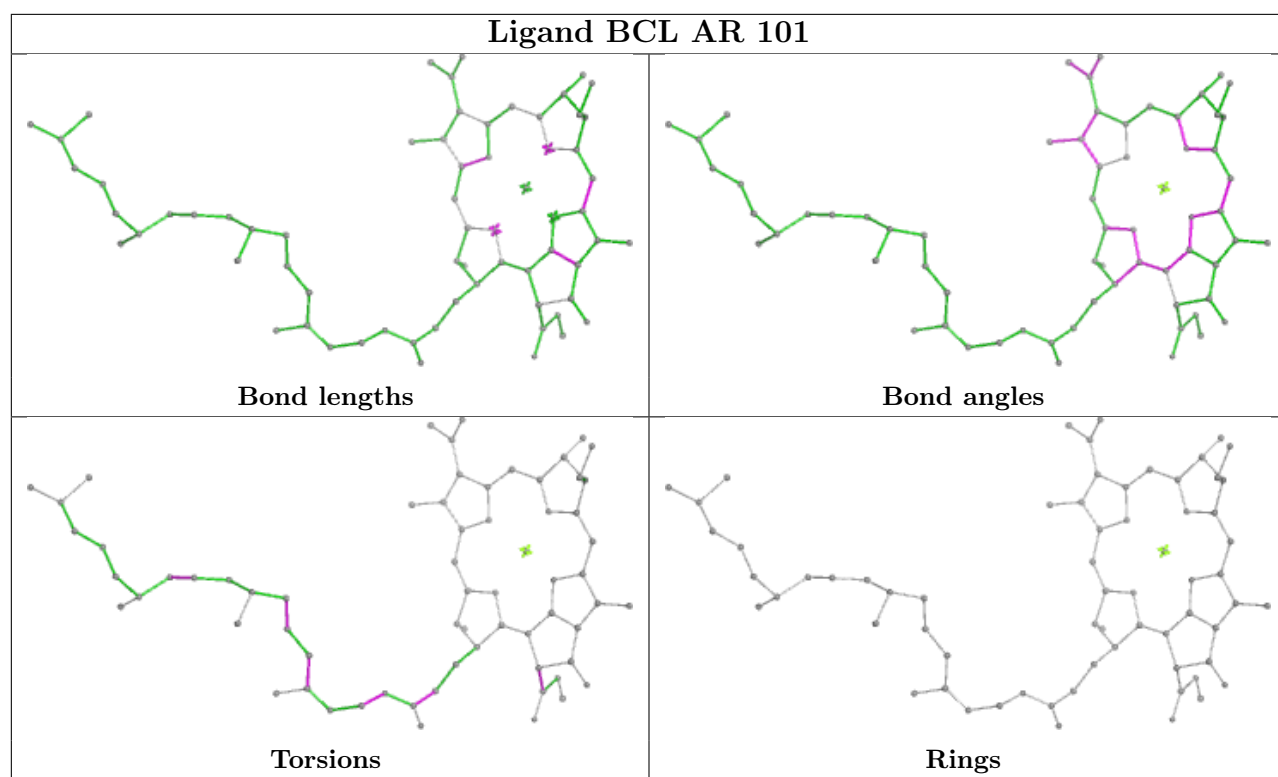


Ligand BCL Bj 1204

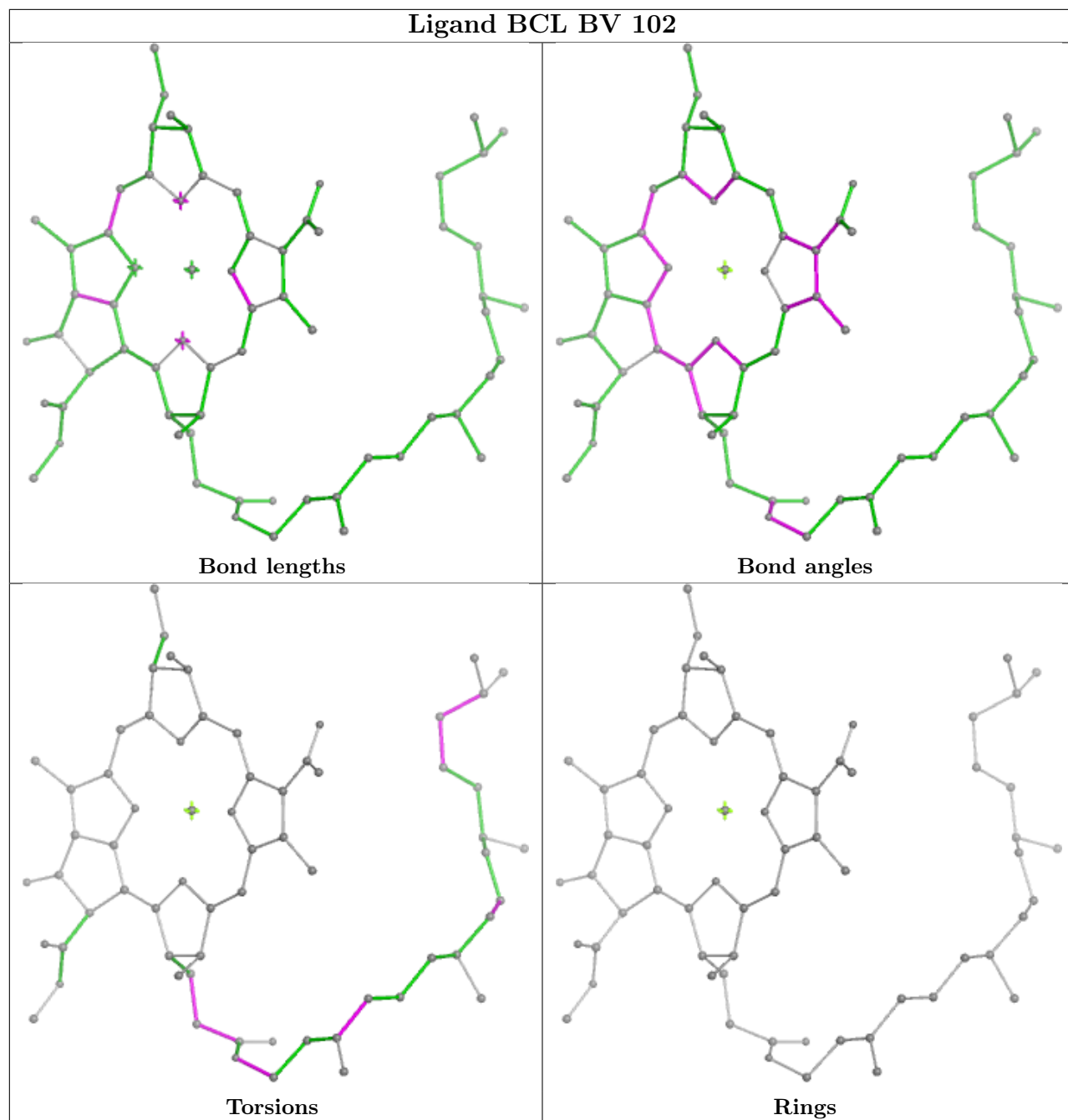


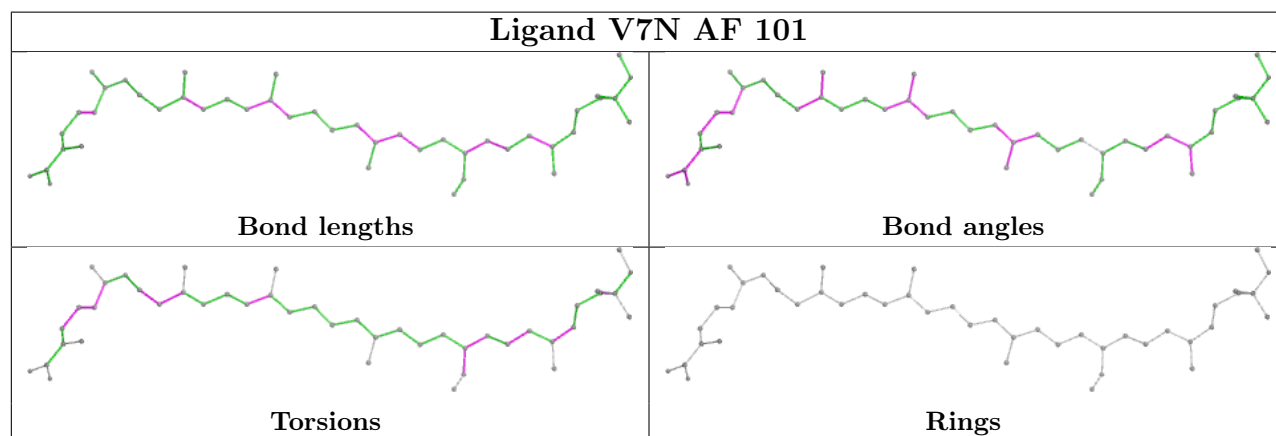
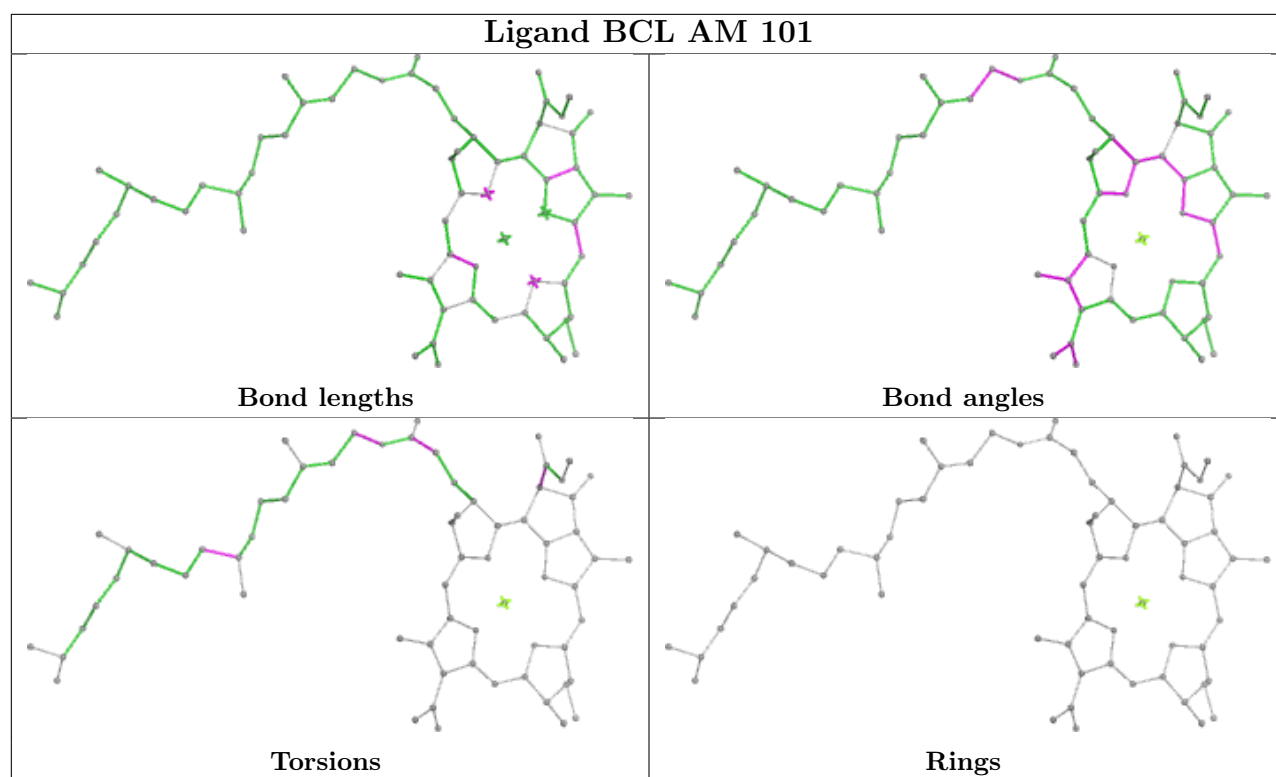
Ligand BCL Ad 101



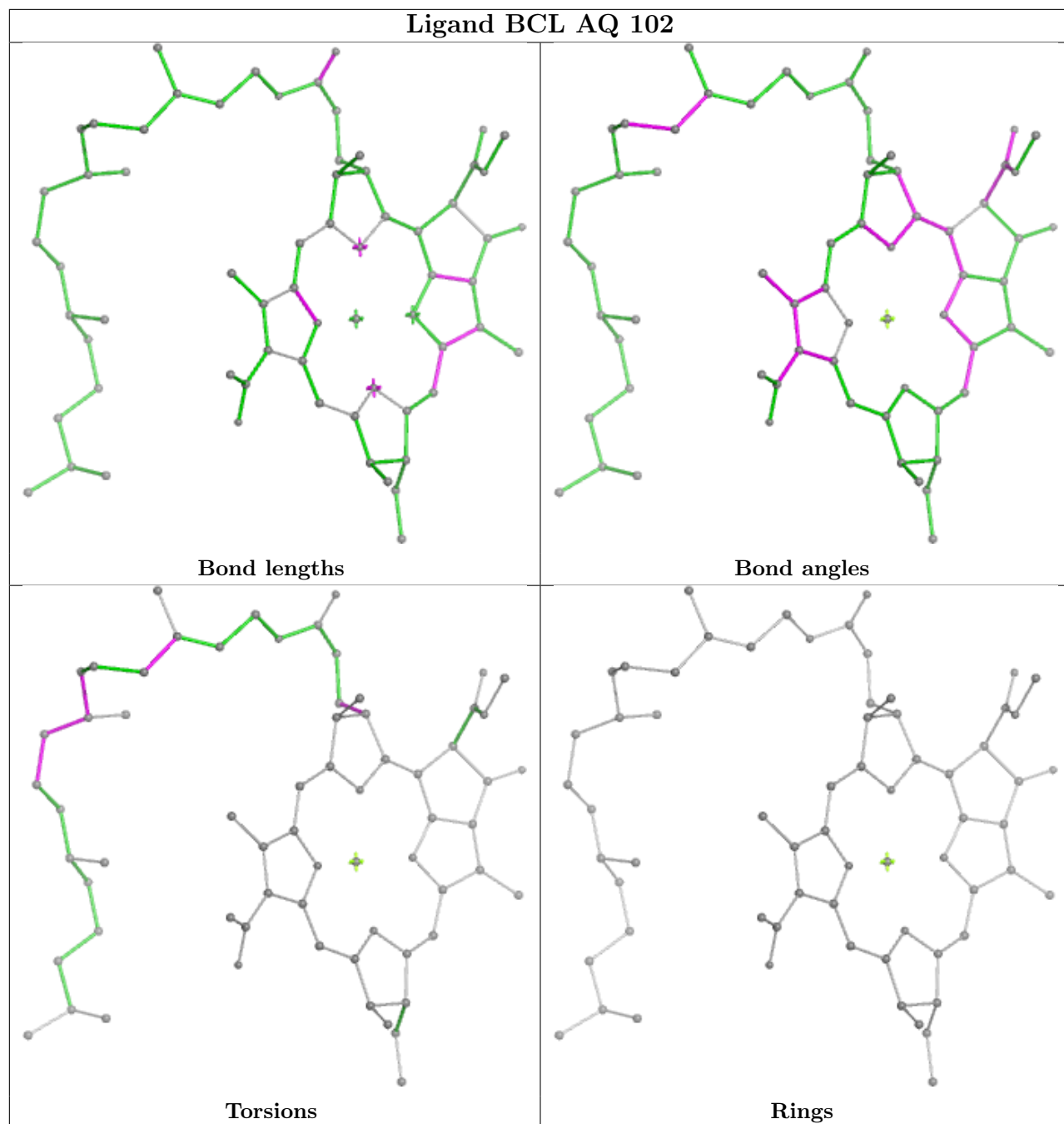


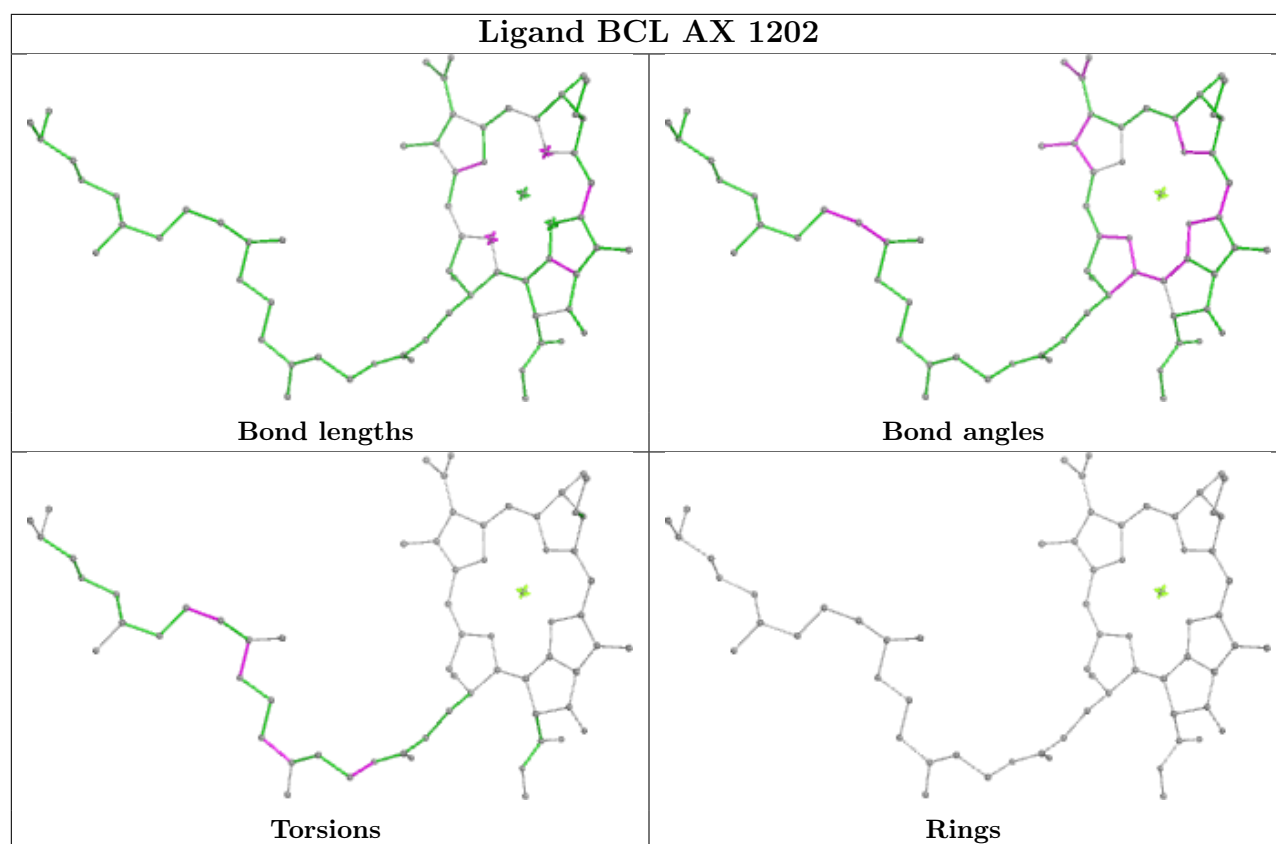
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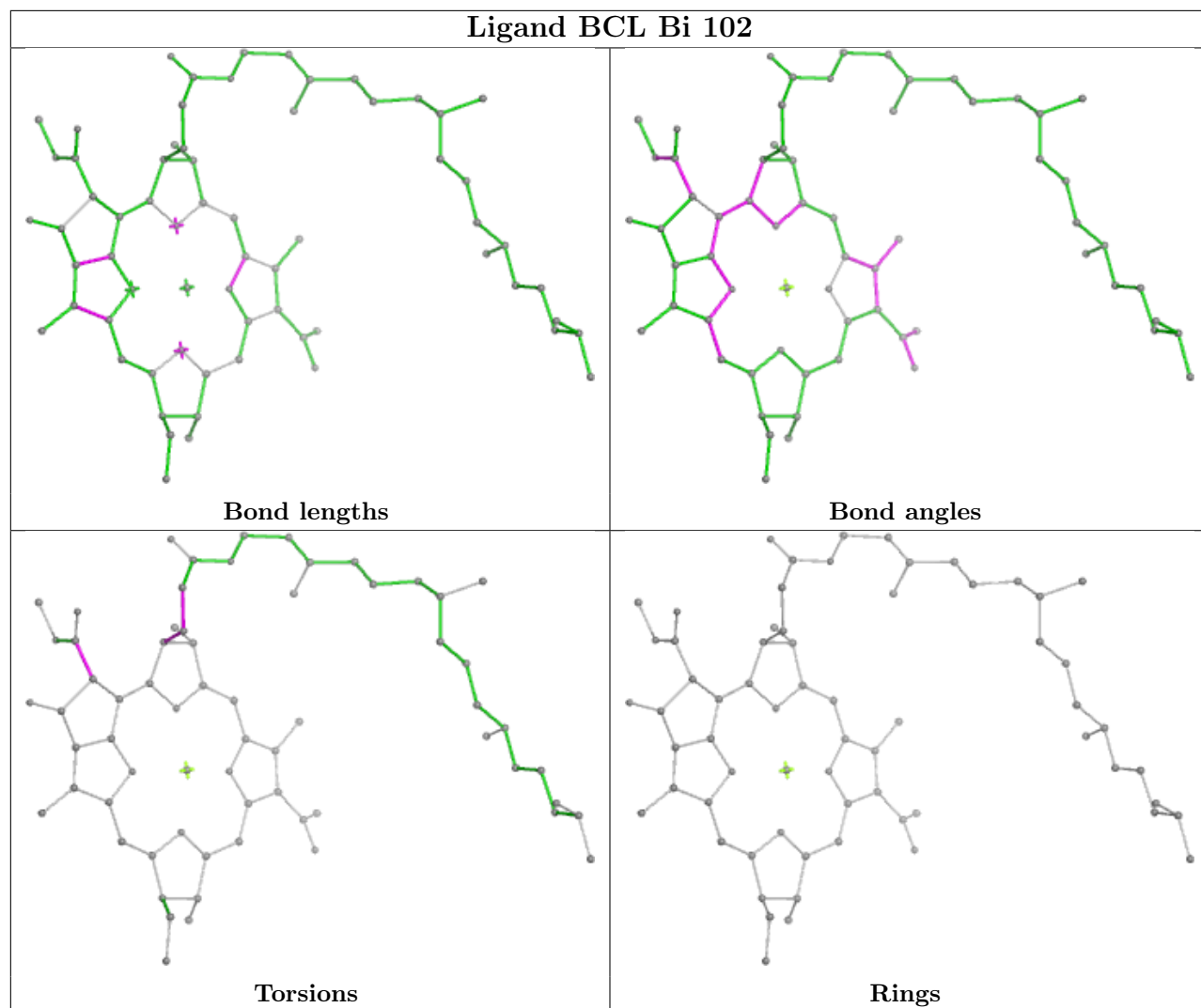


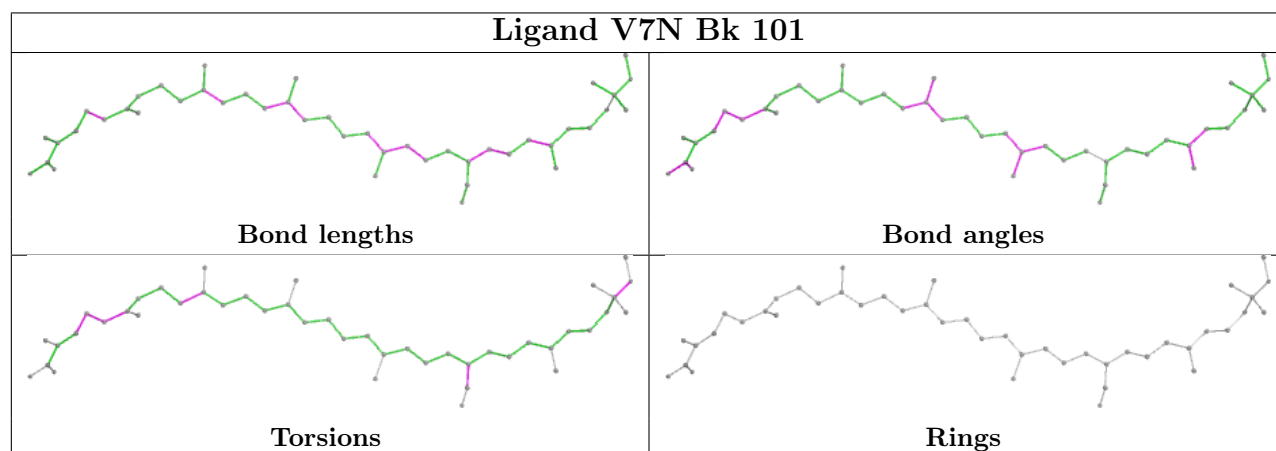
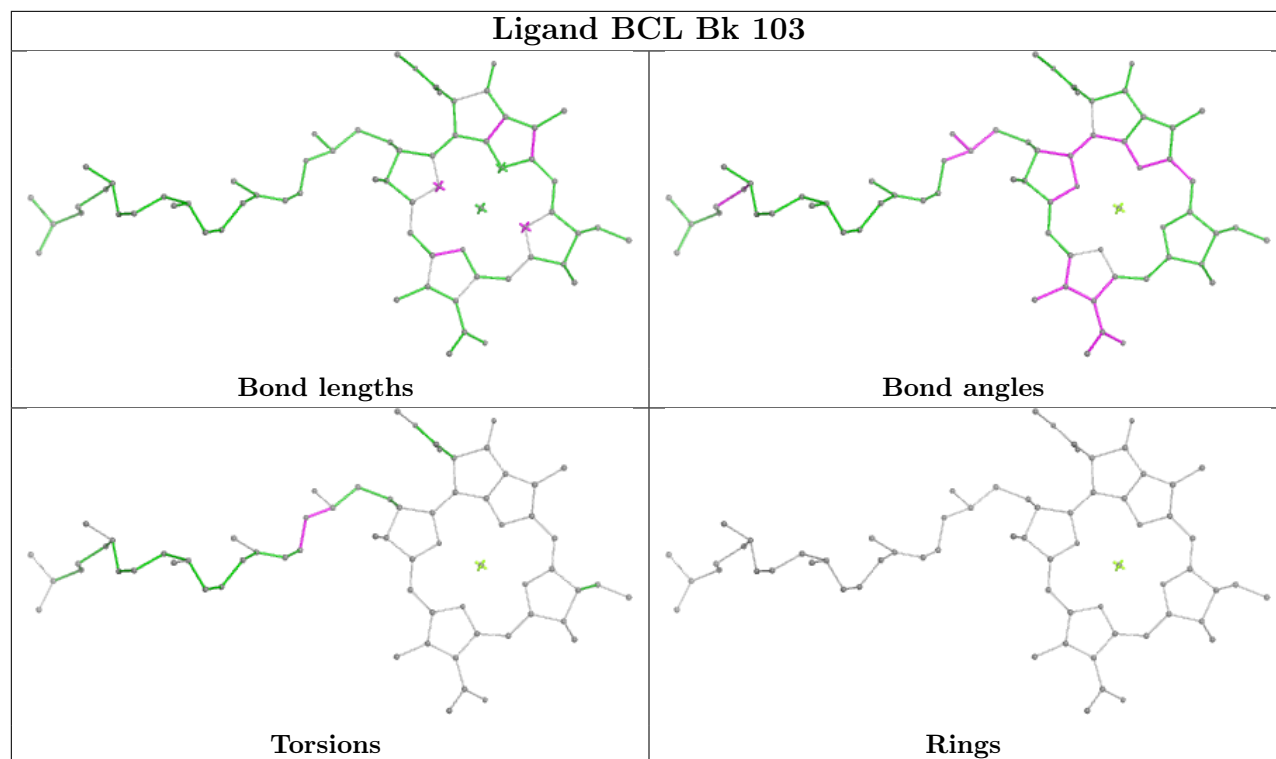


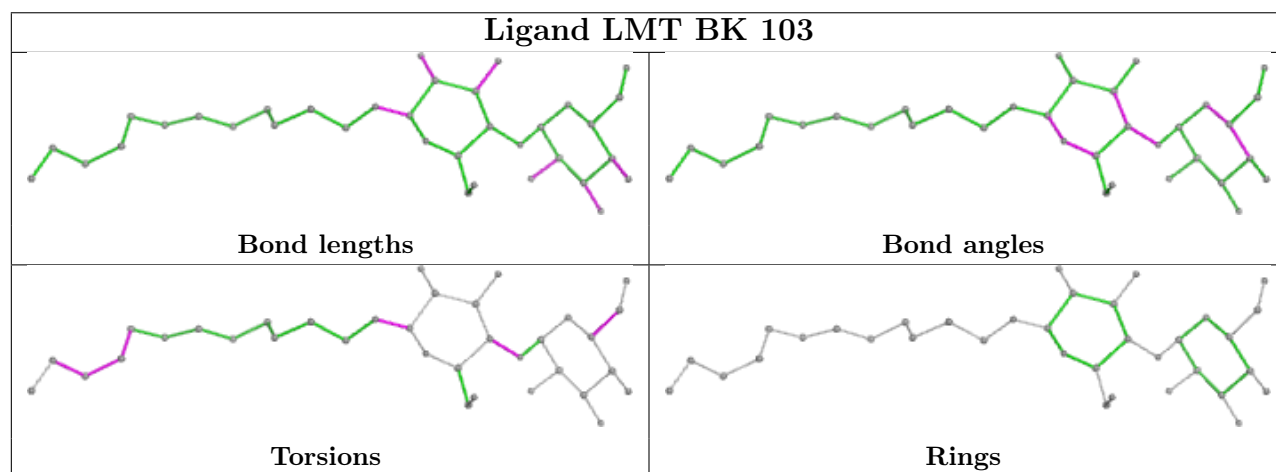
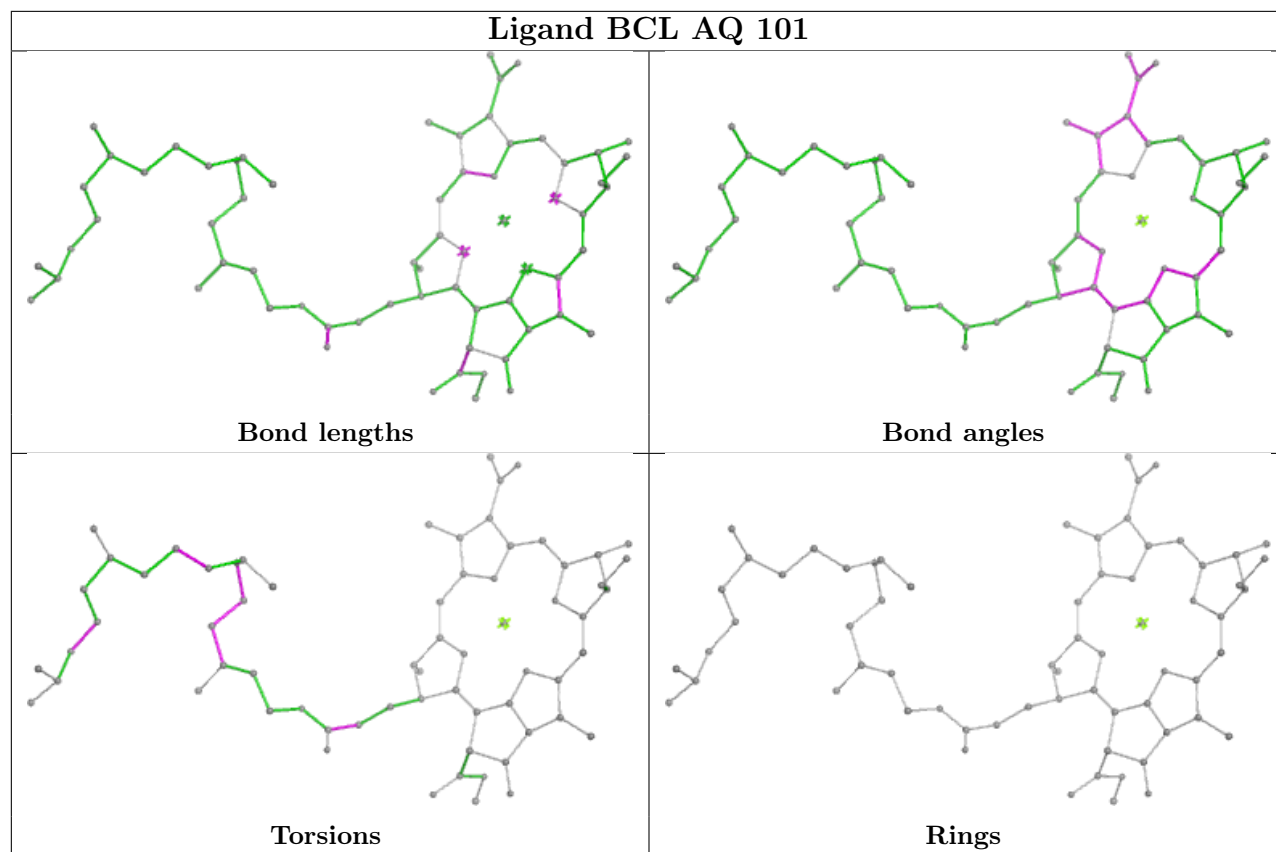
Ligand BCL AQ 102

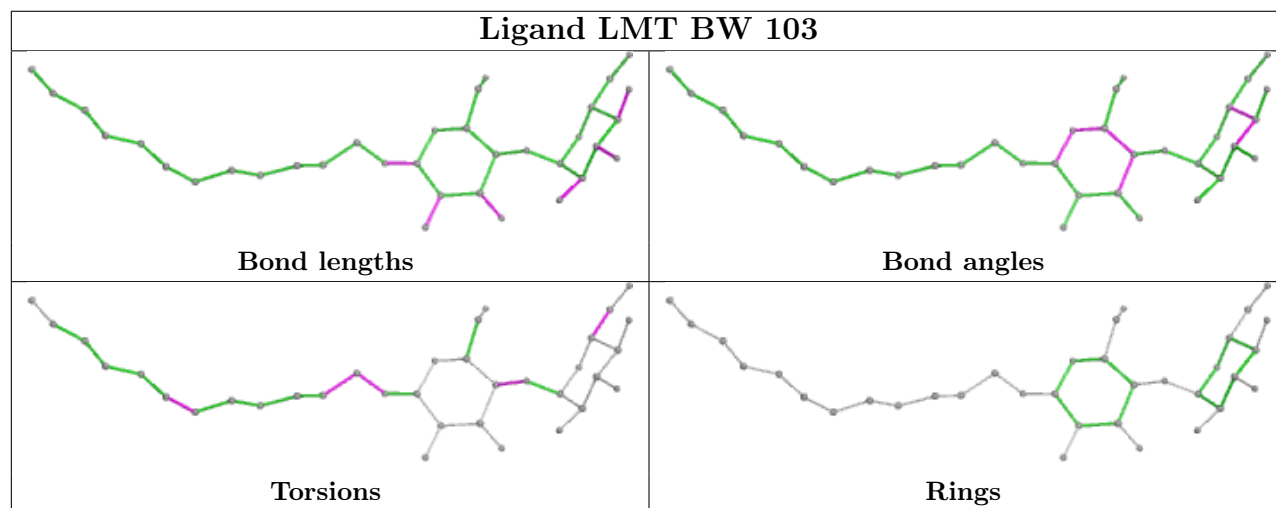
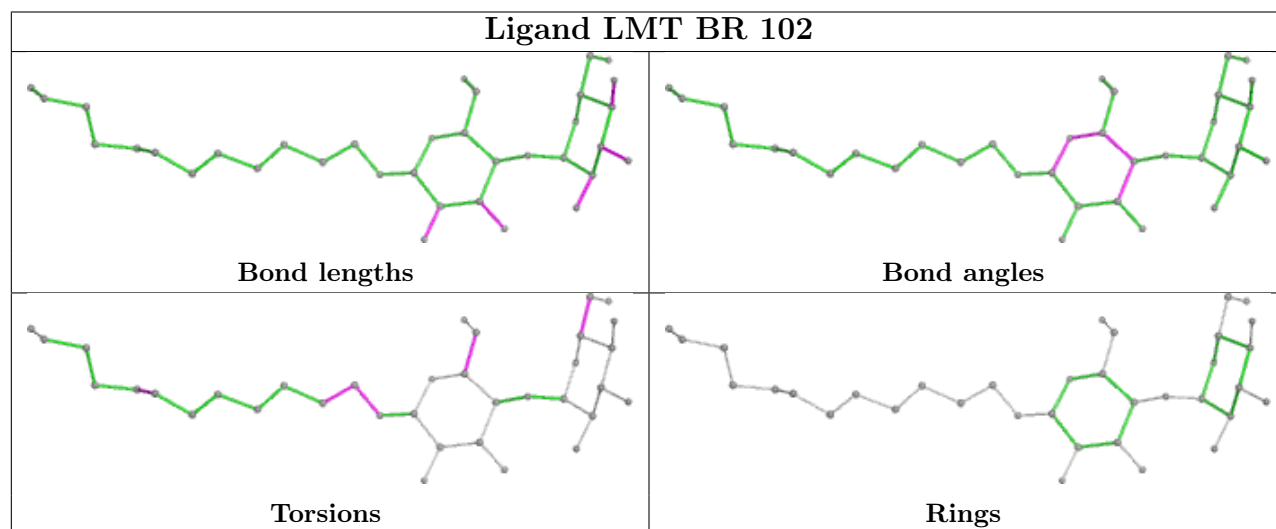
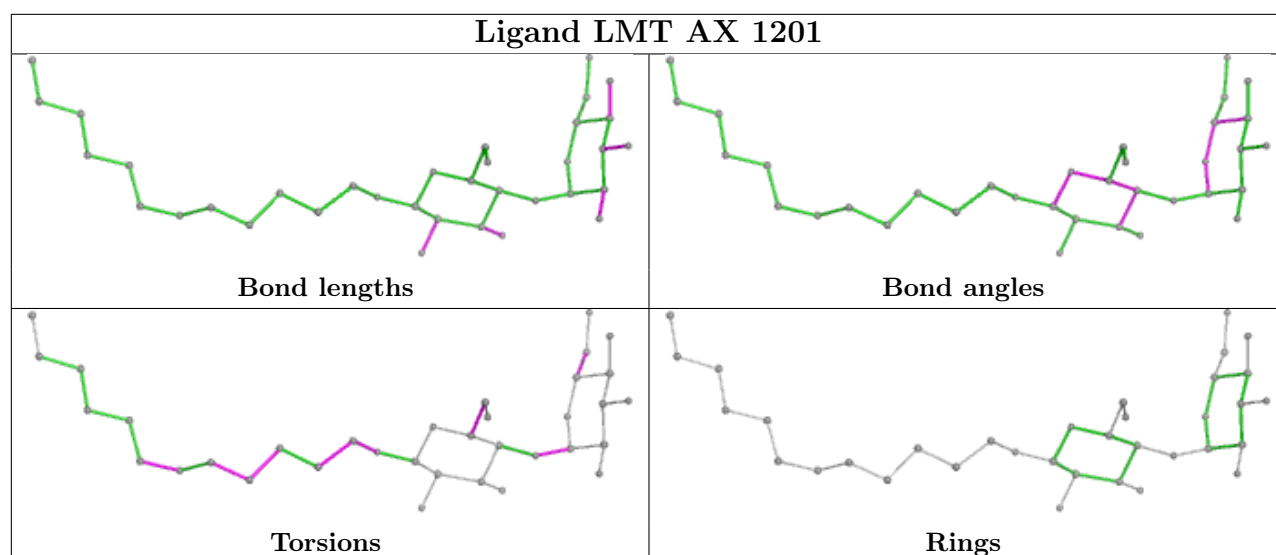


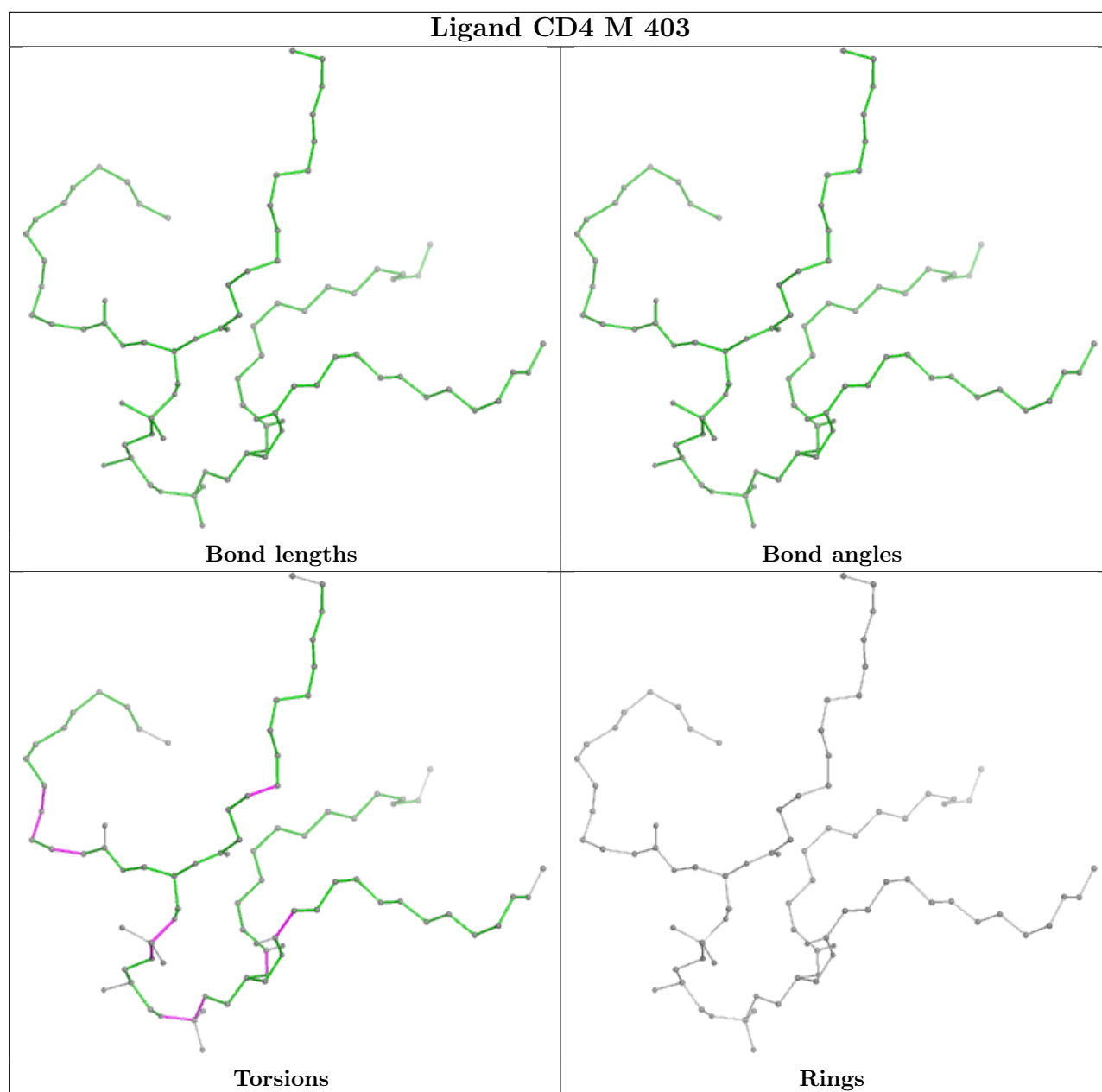


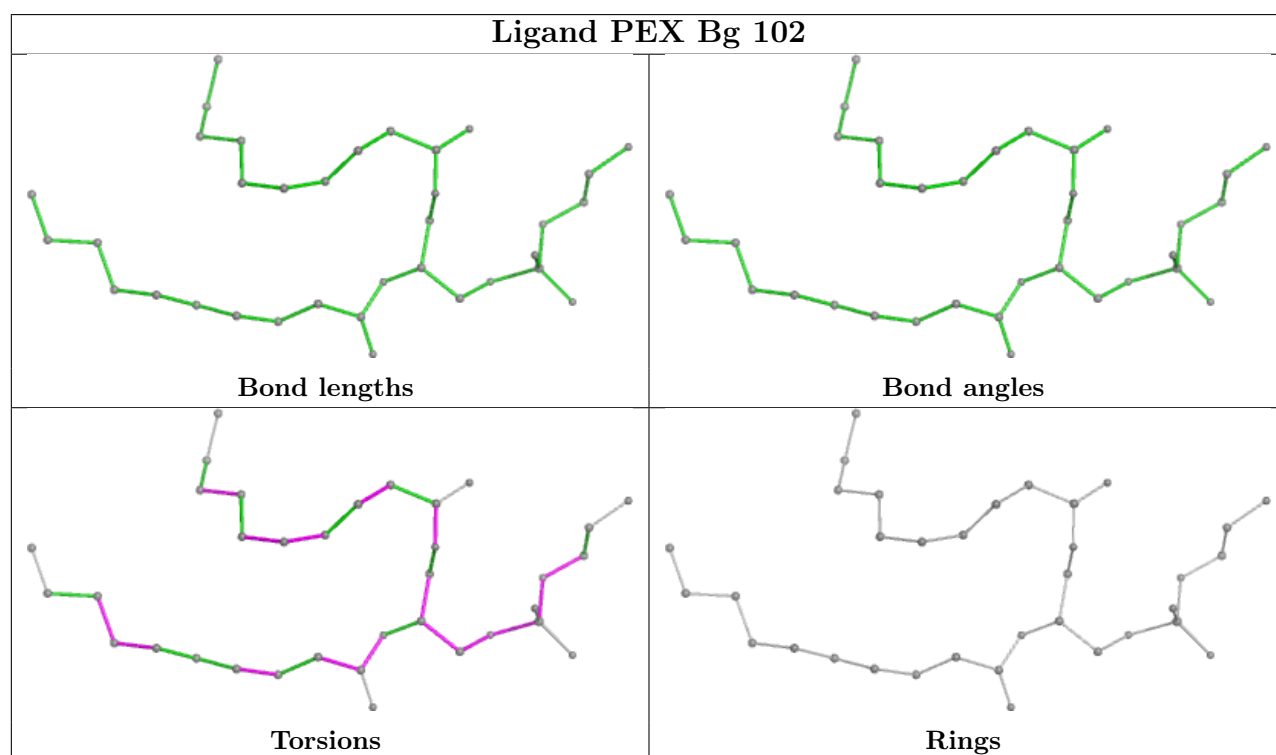
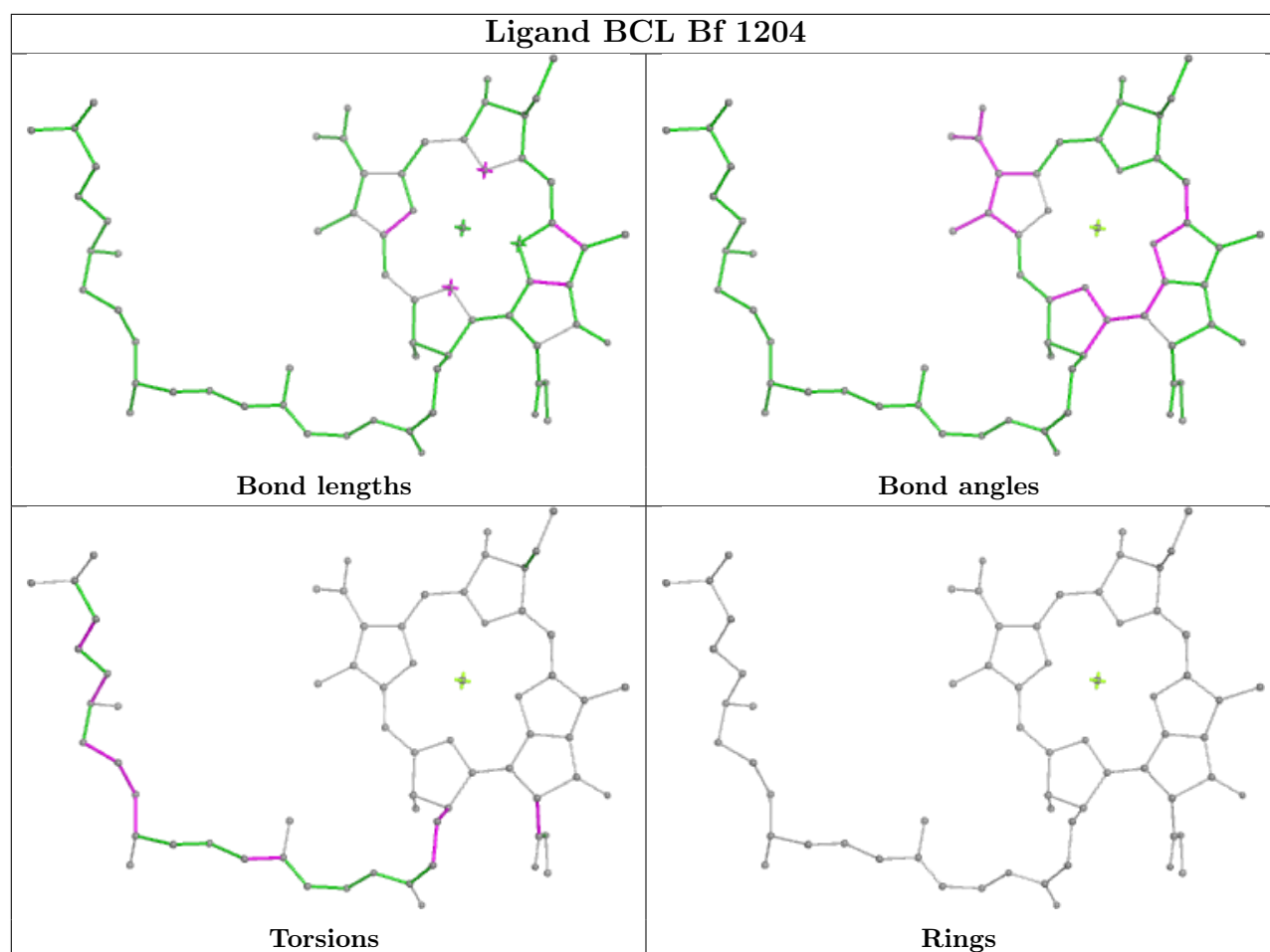


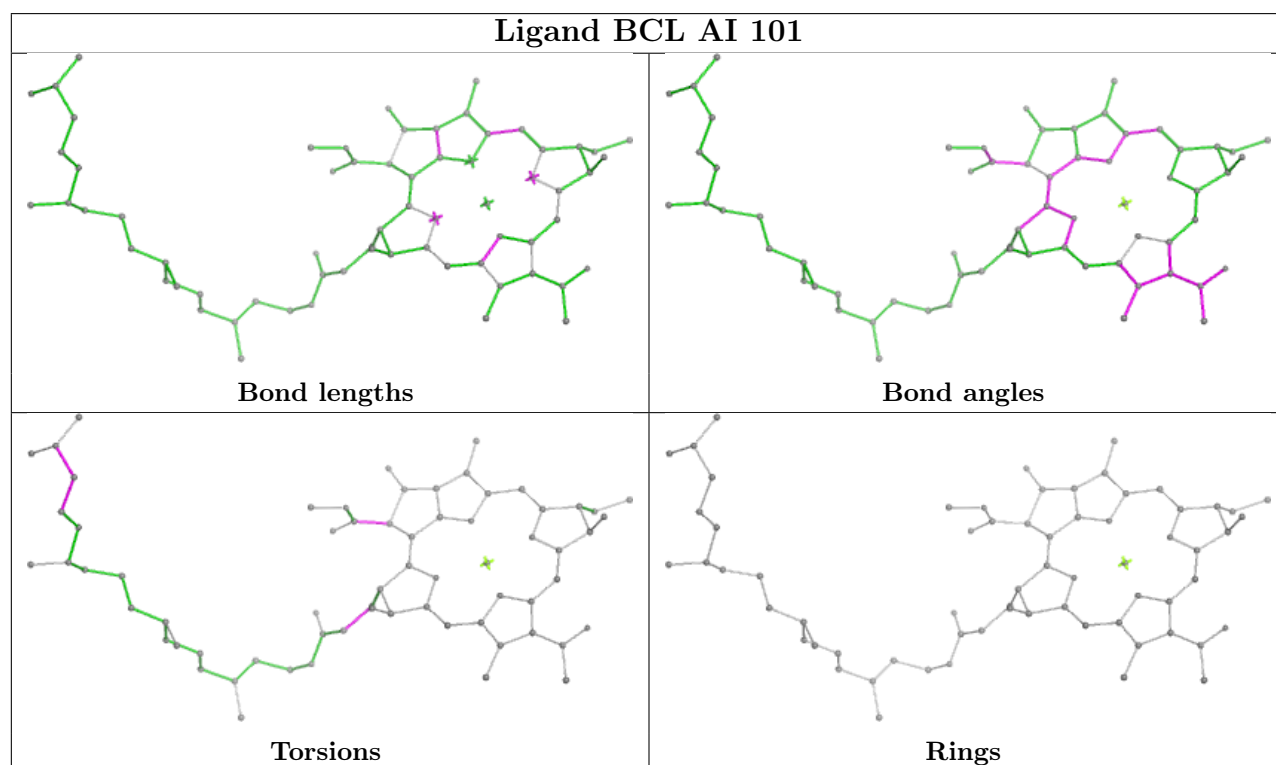
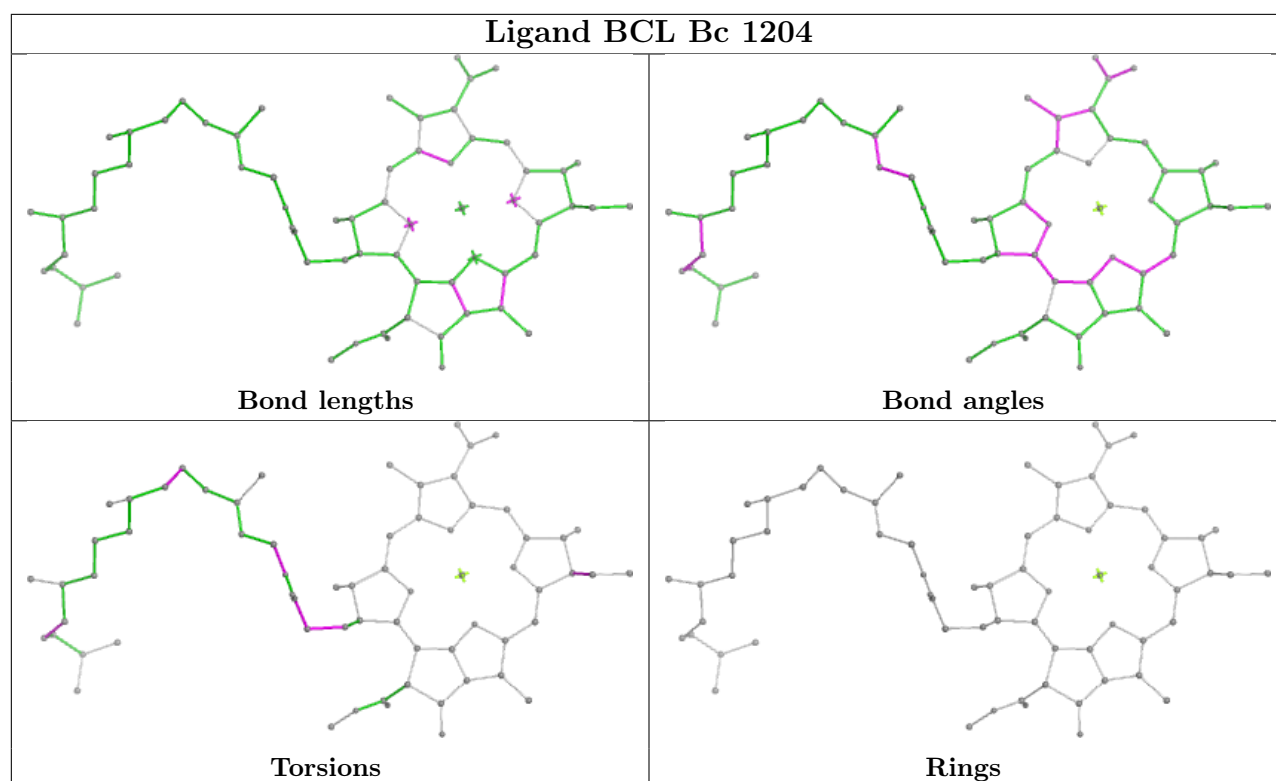


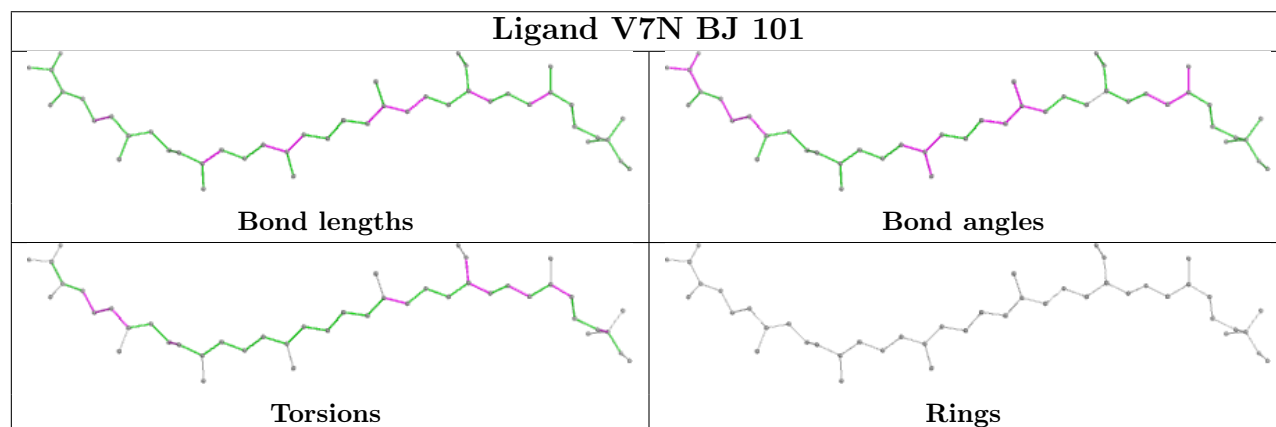
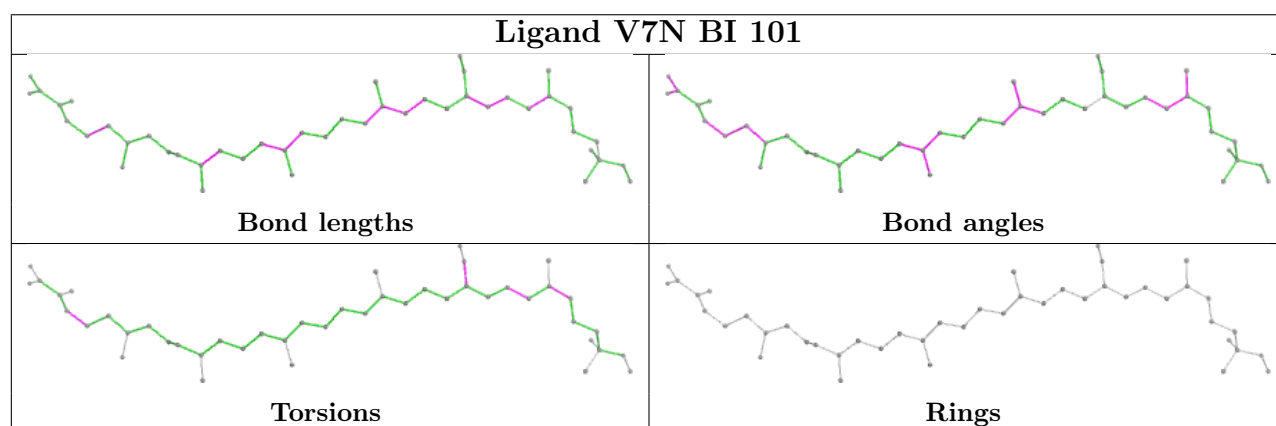
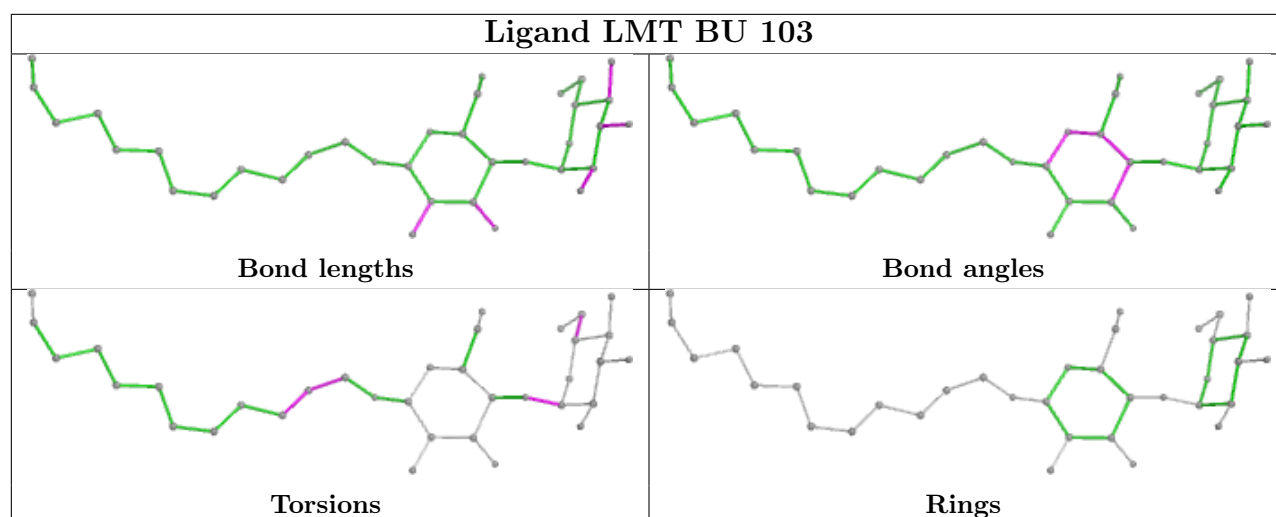


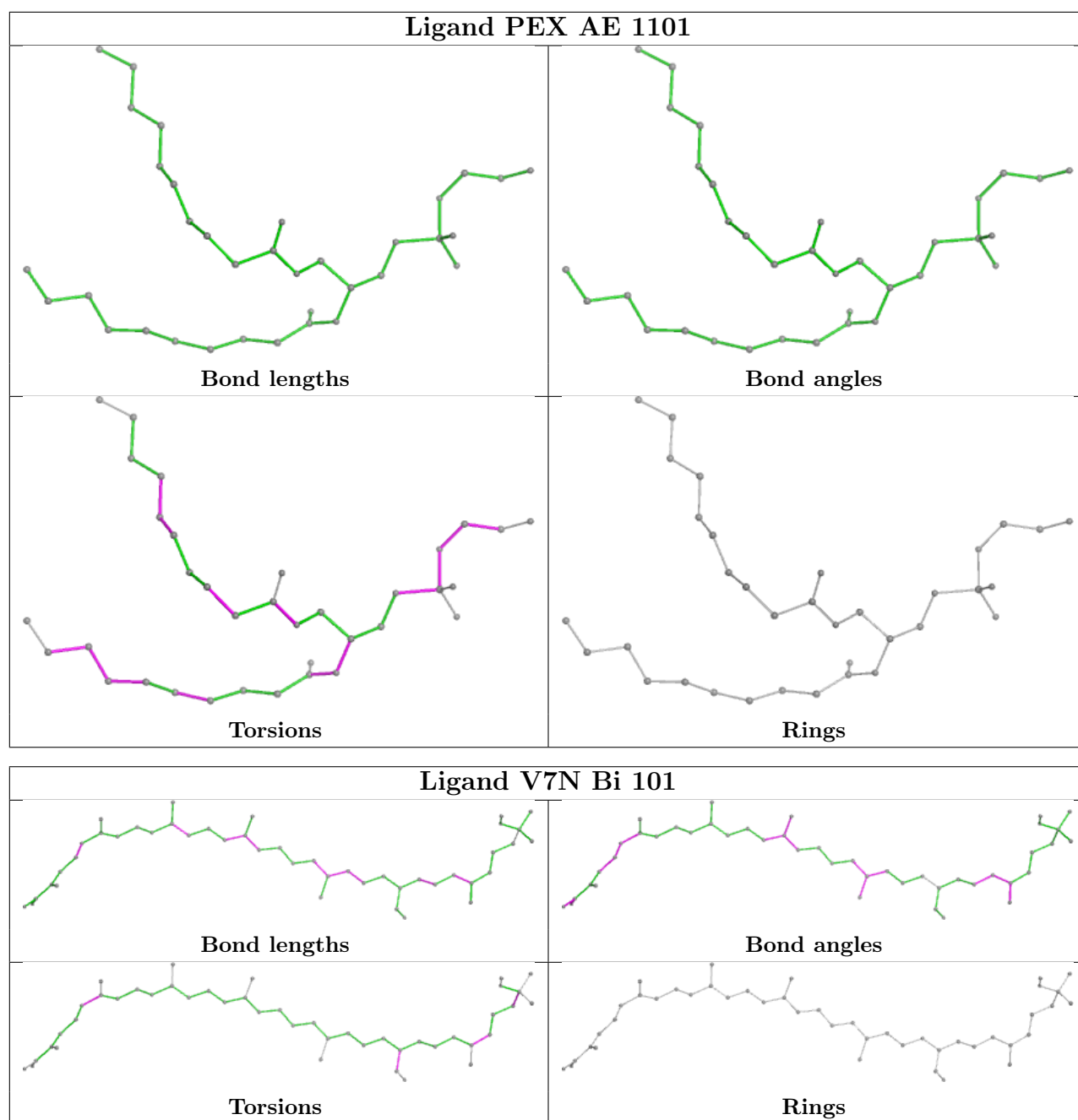


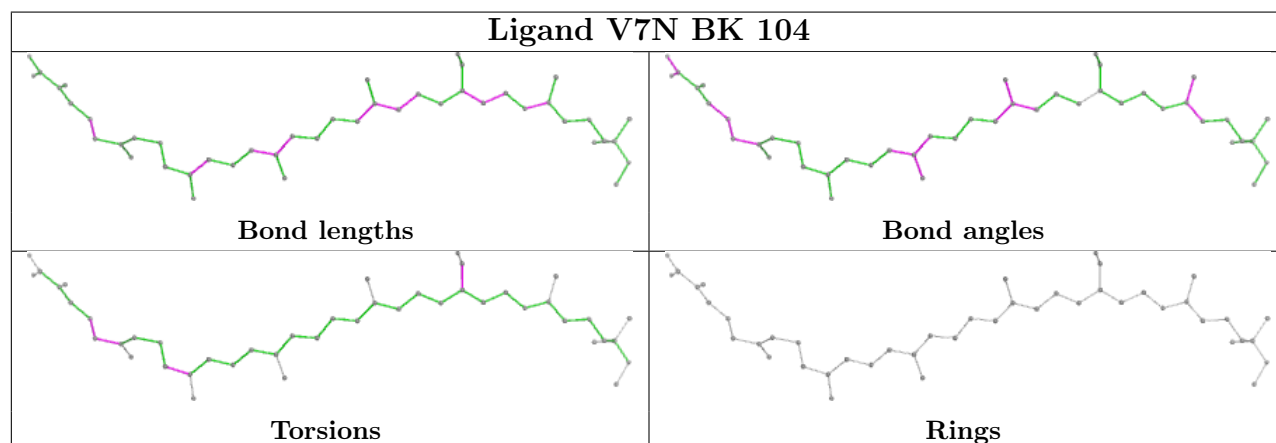
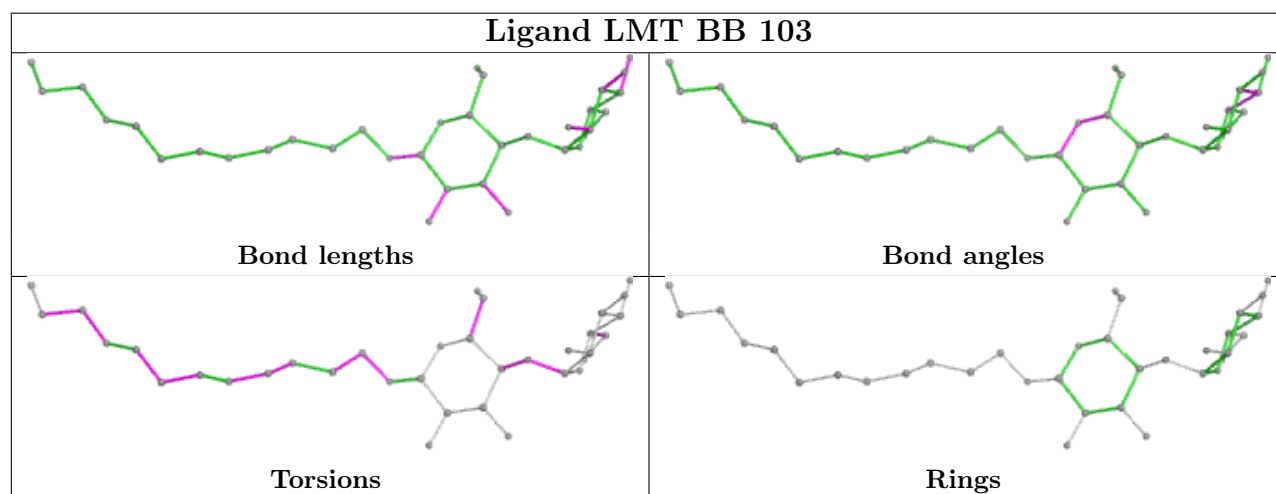
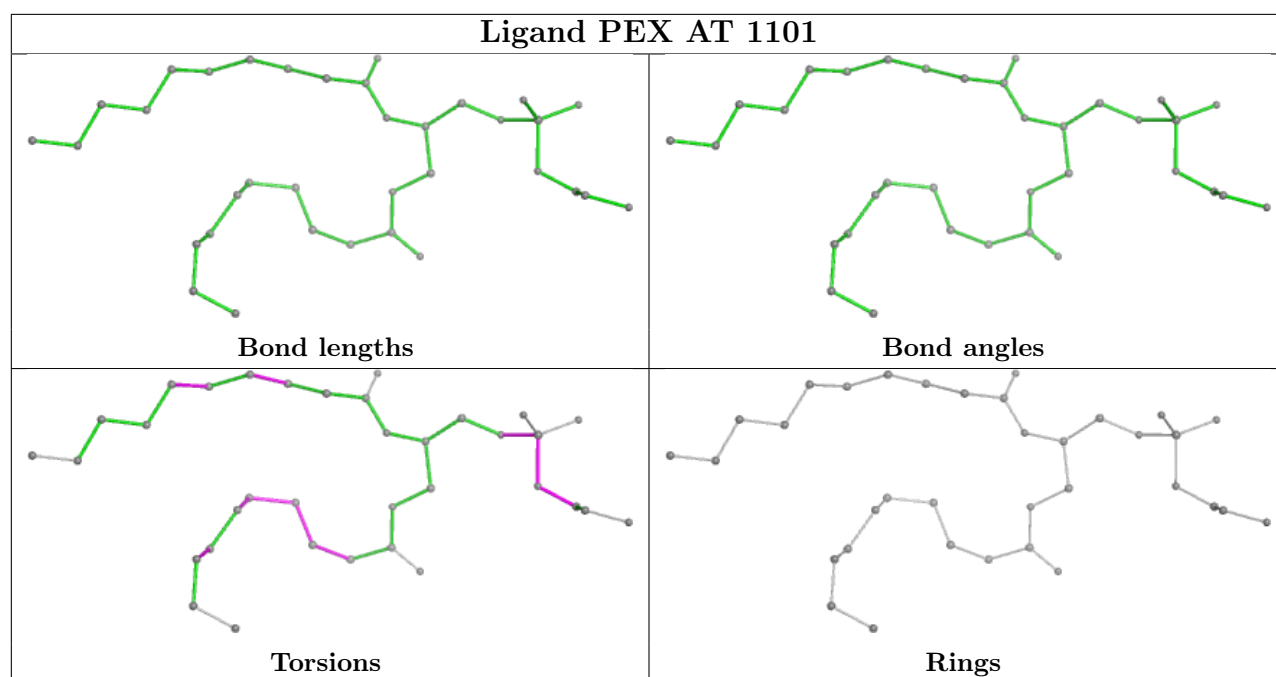


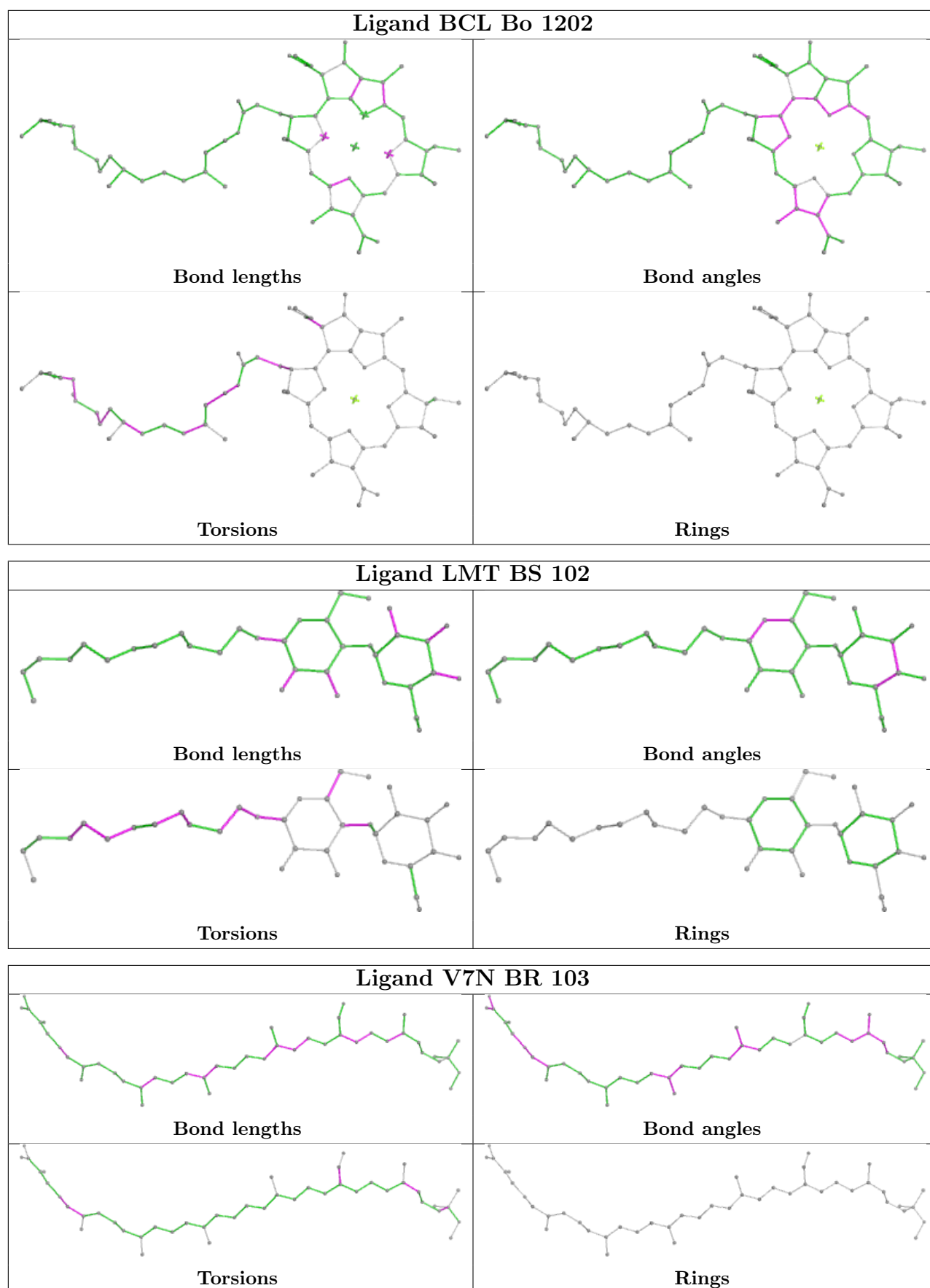


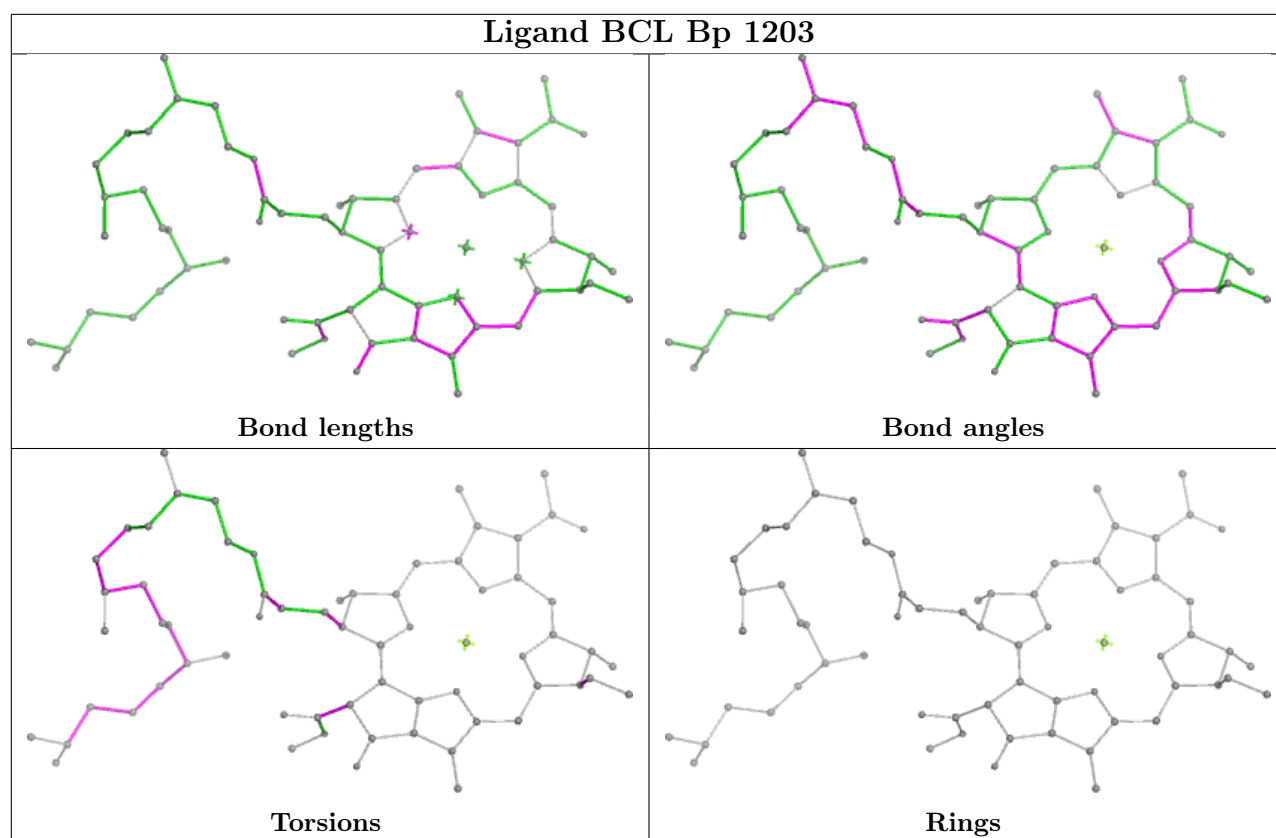


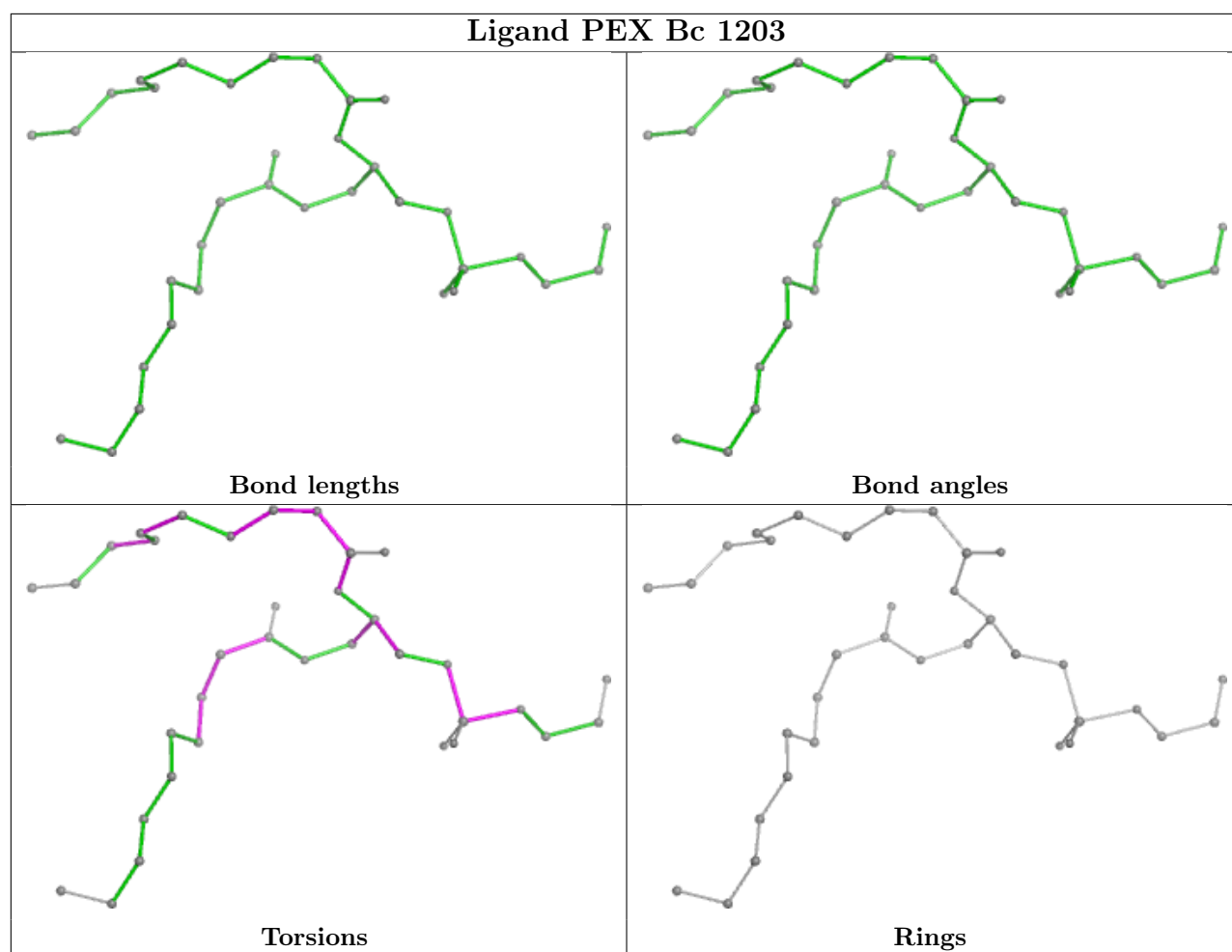




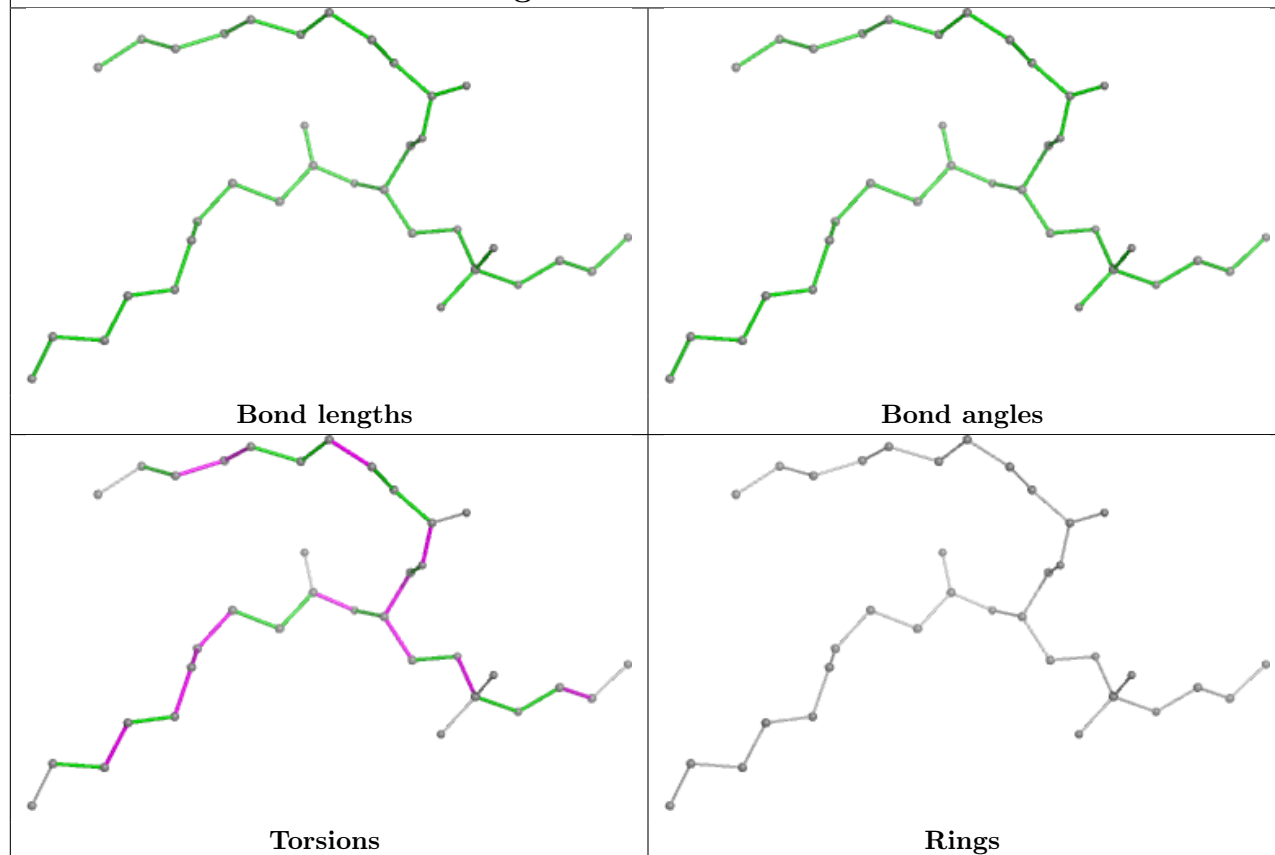




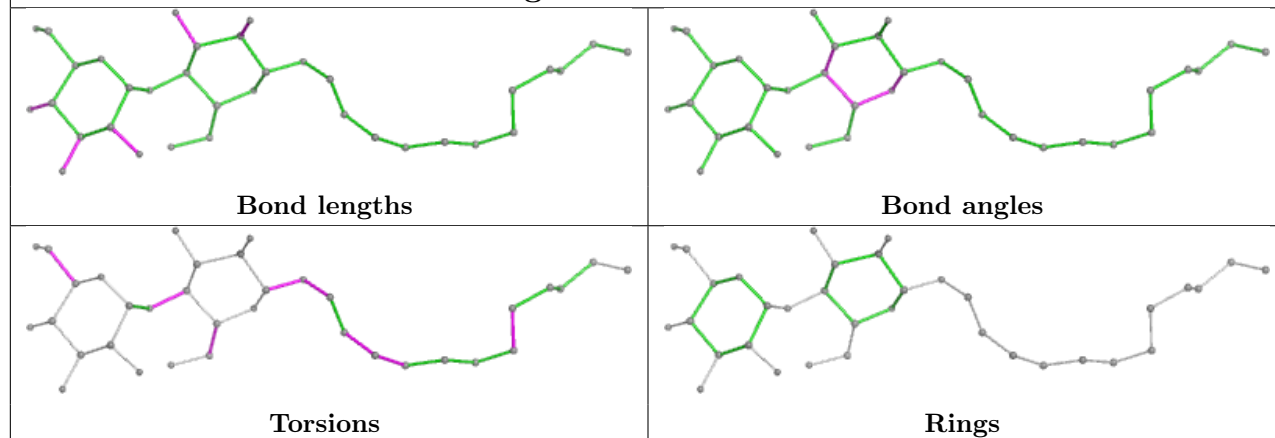




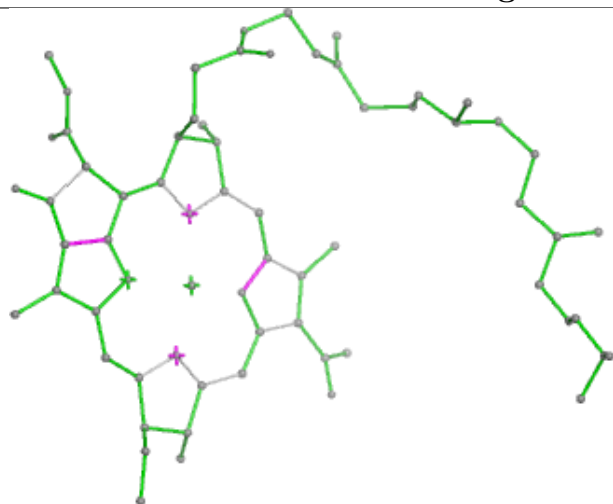
Ligand PEX Be 1104



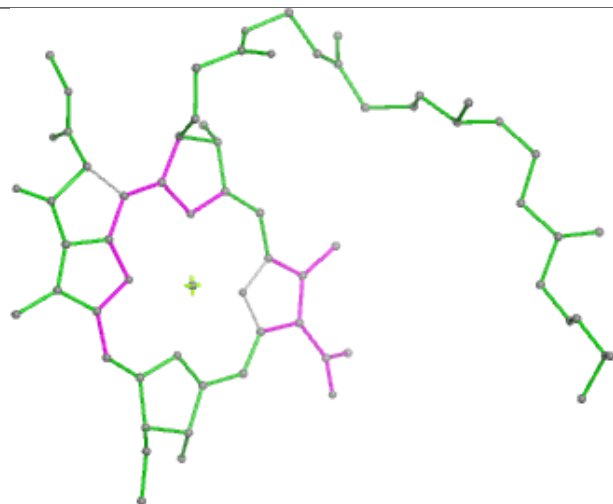
Ligand LMT M 401



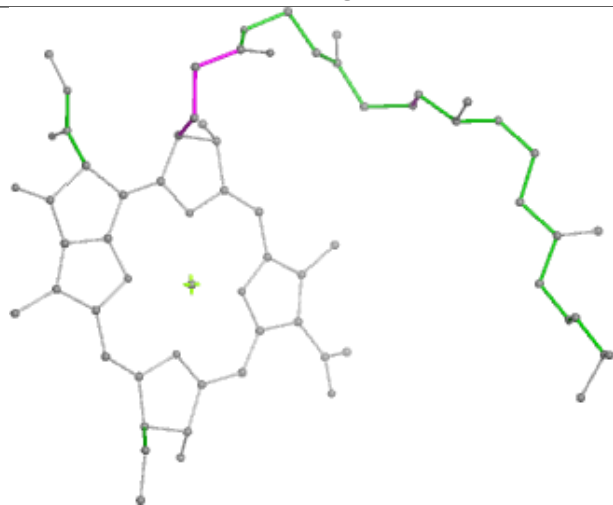
Ligand BCL Be 1105



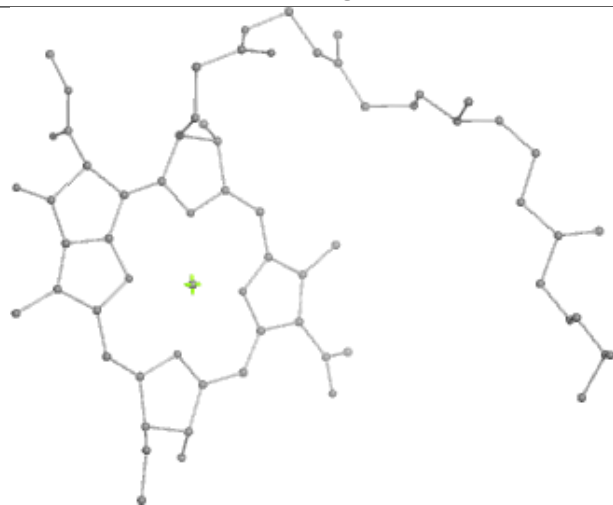
Bond lengths



Bond angles

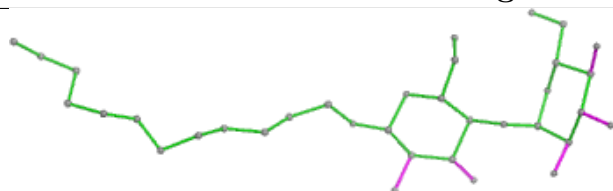


Torsions

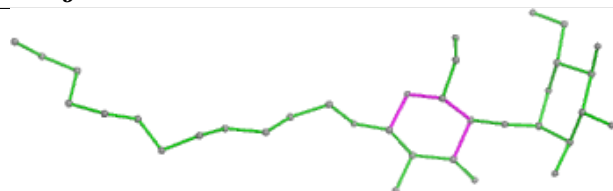


Rings

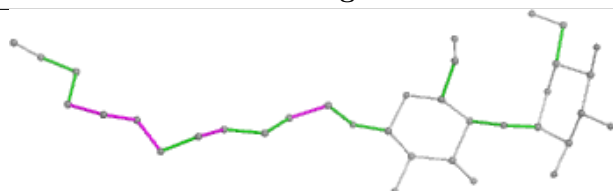
Ligand LMT Bj 1201



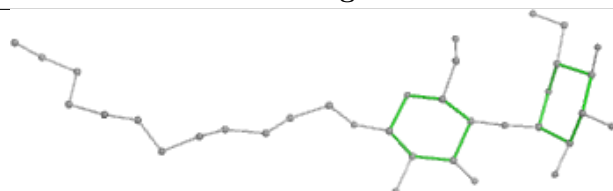
Bond lengths



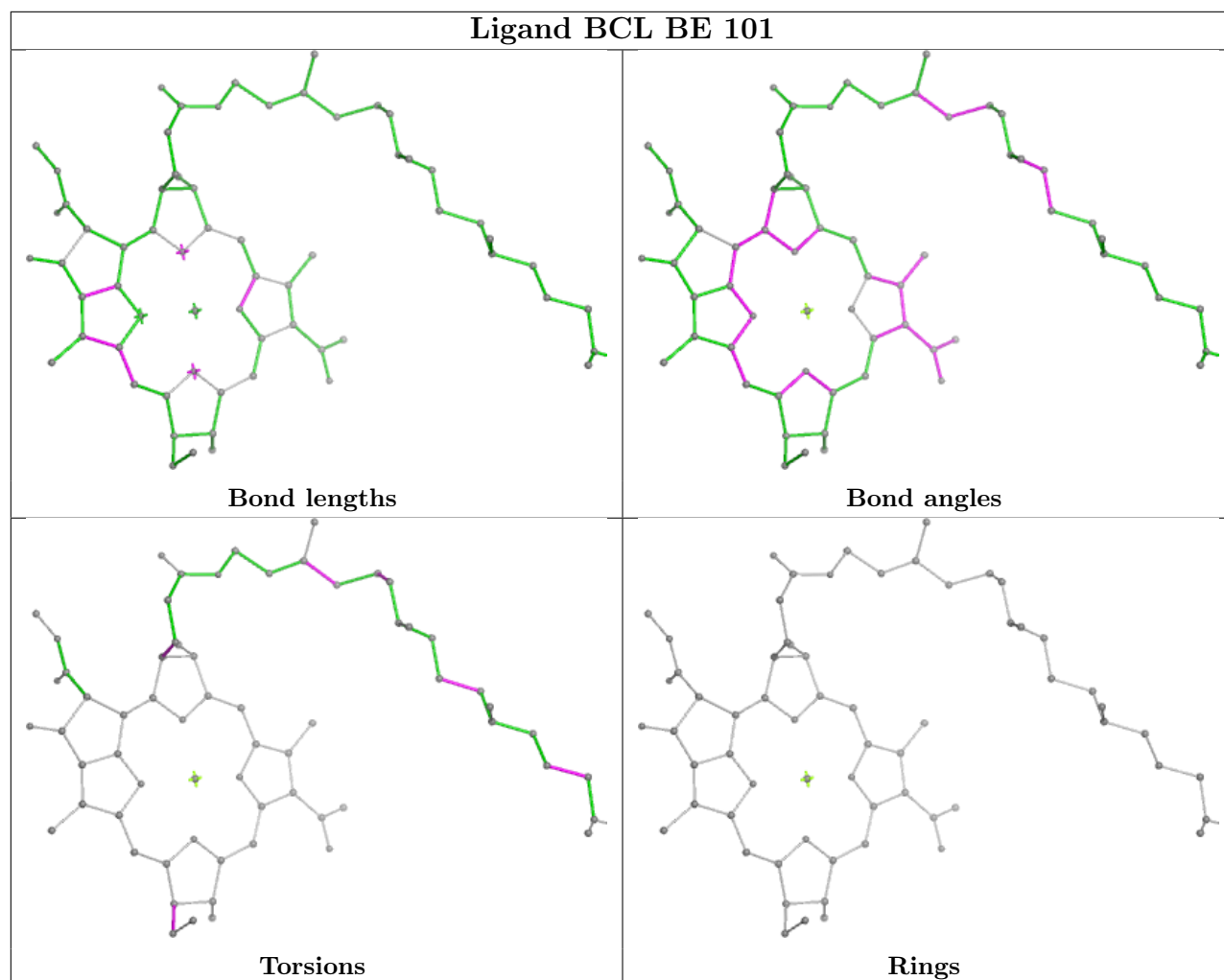
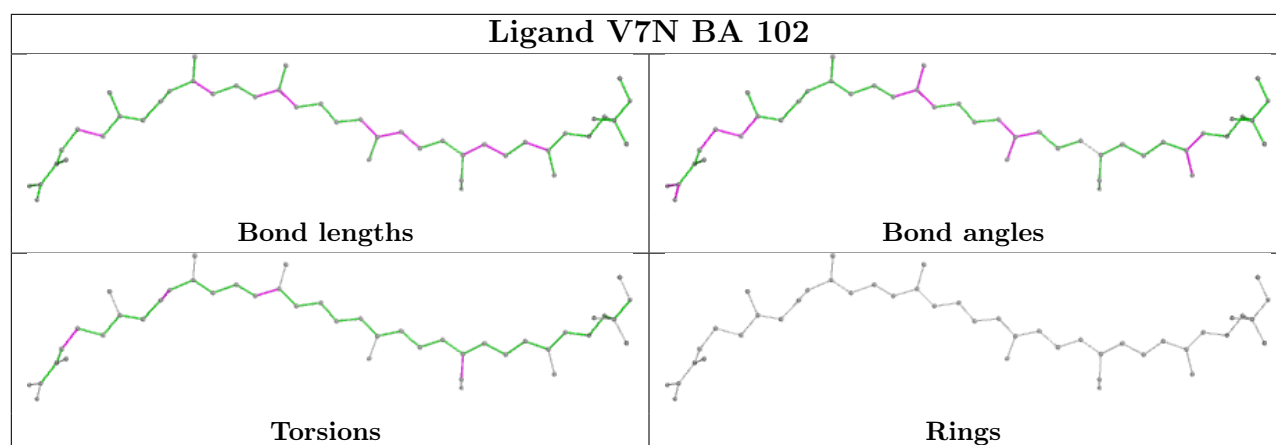
Bond angles

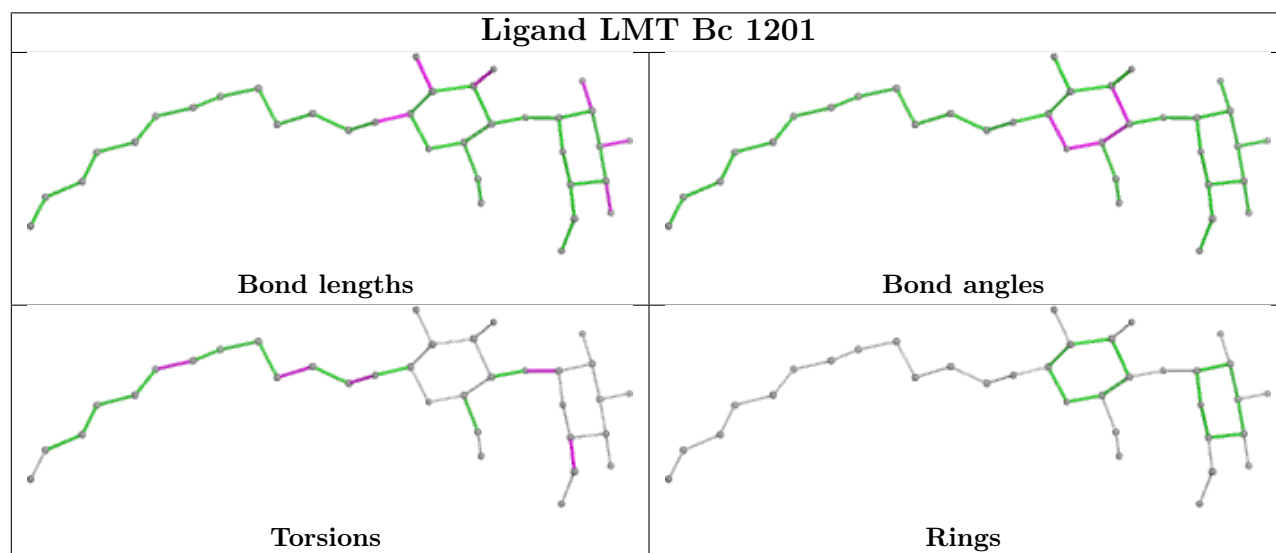
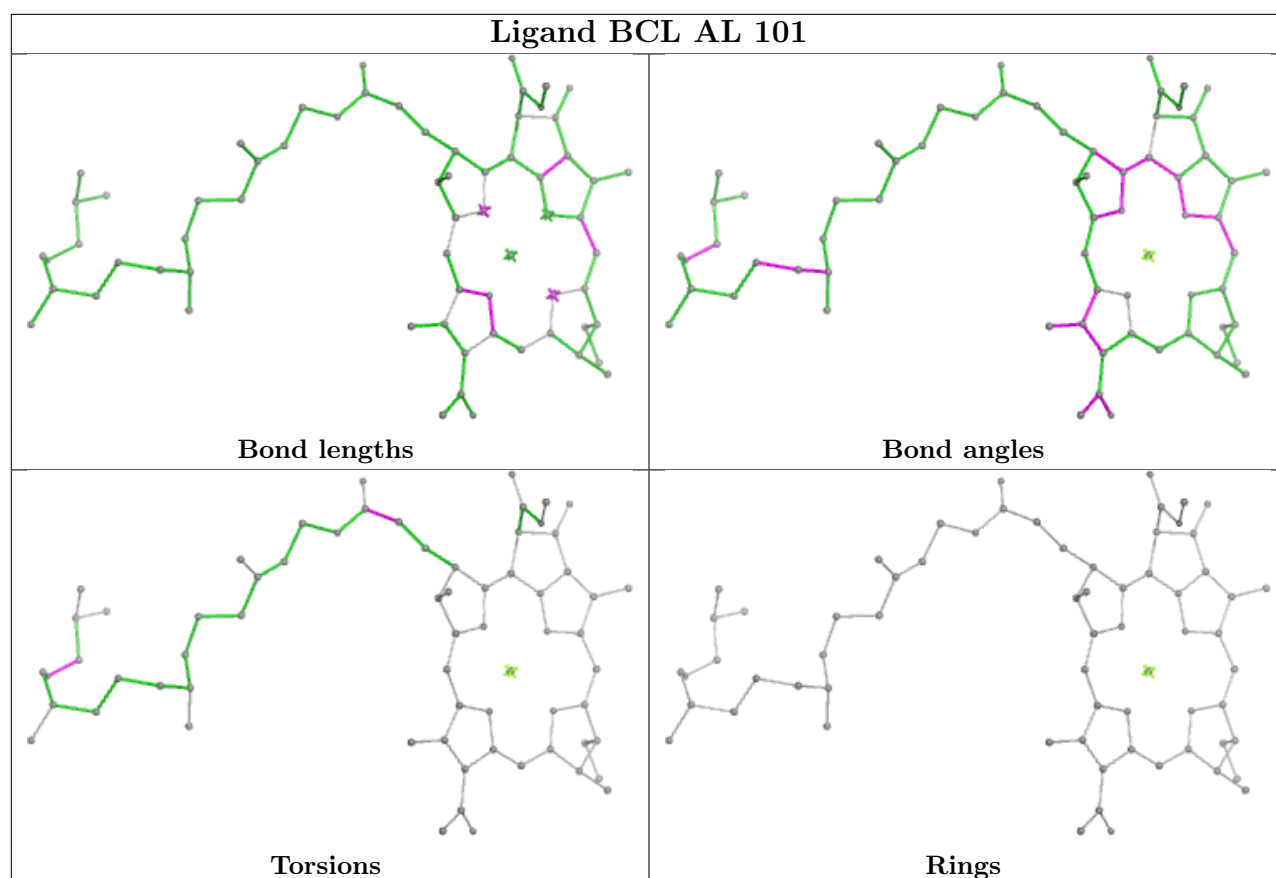


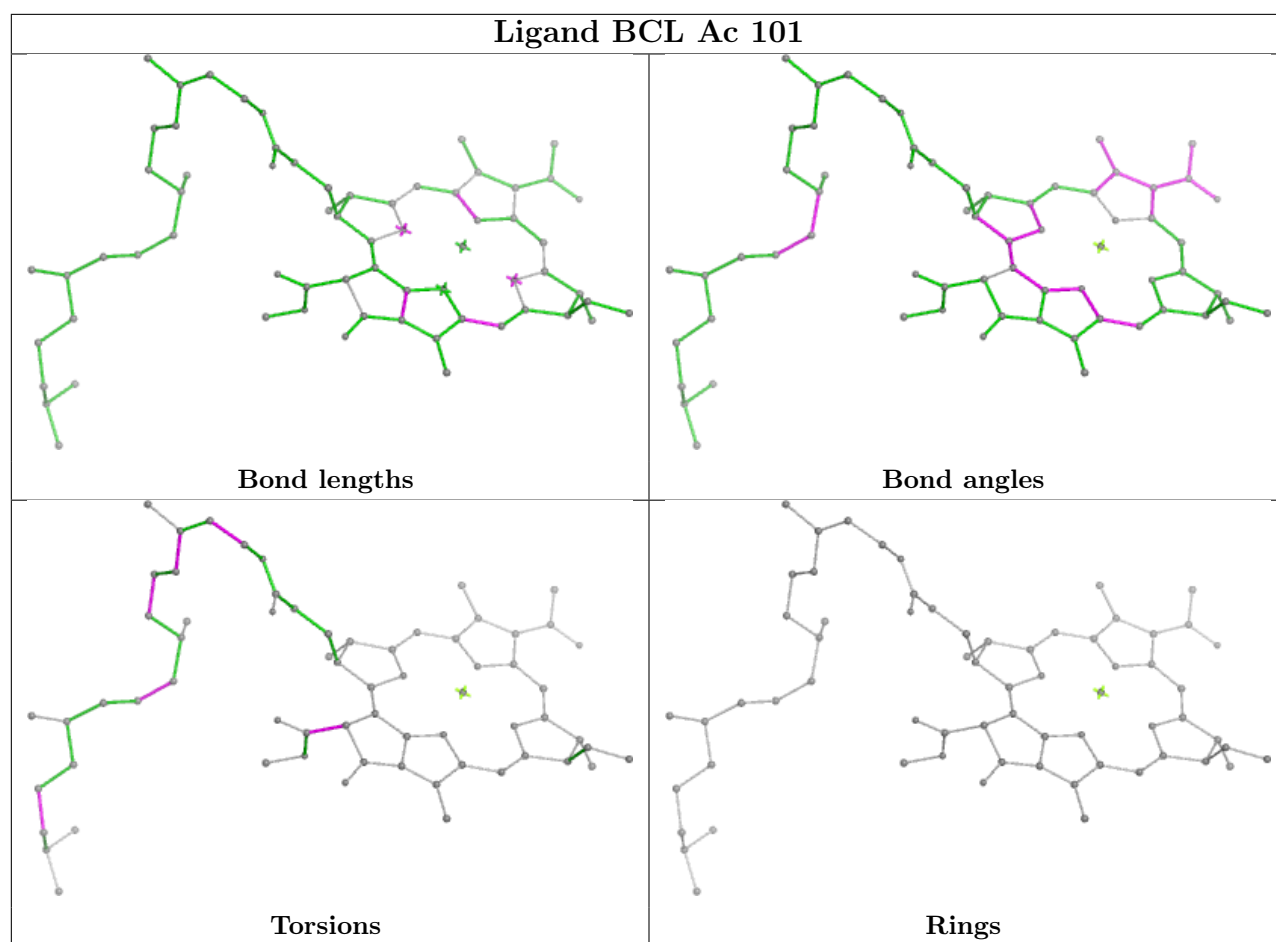
Torsions



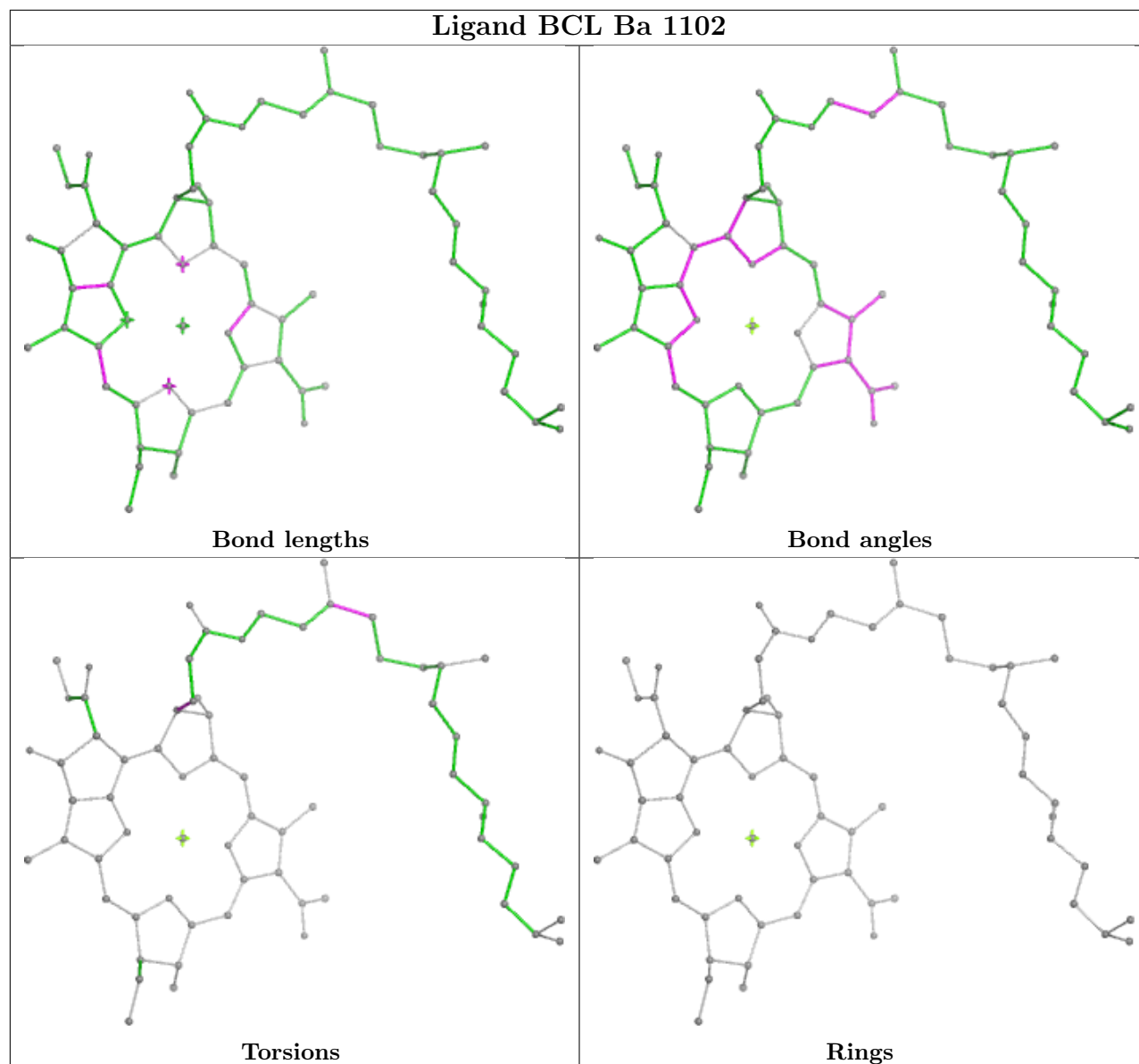
Rings



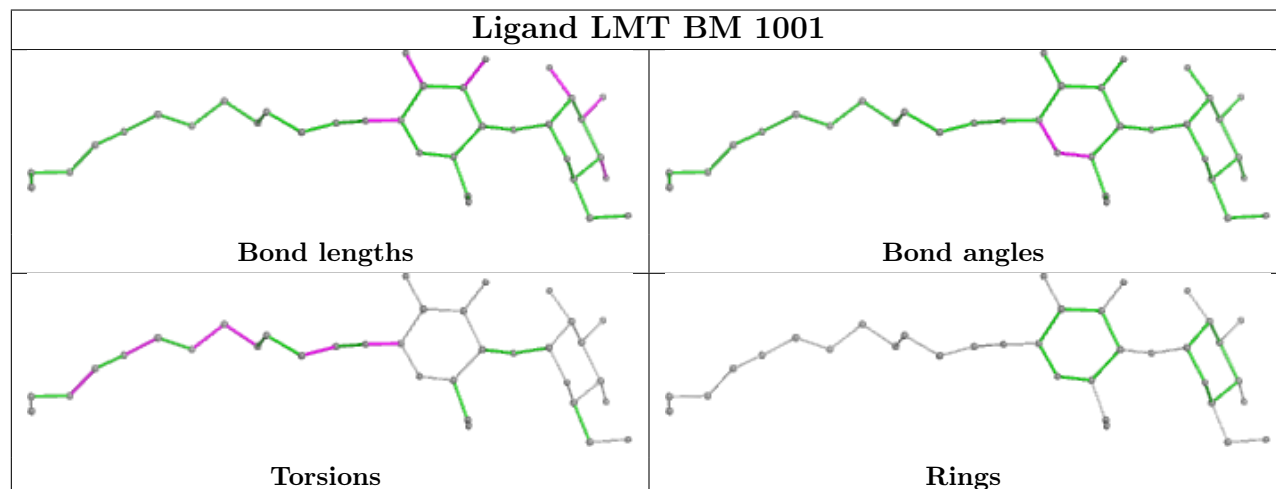




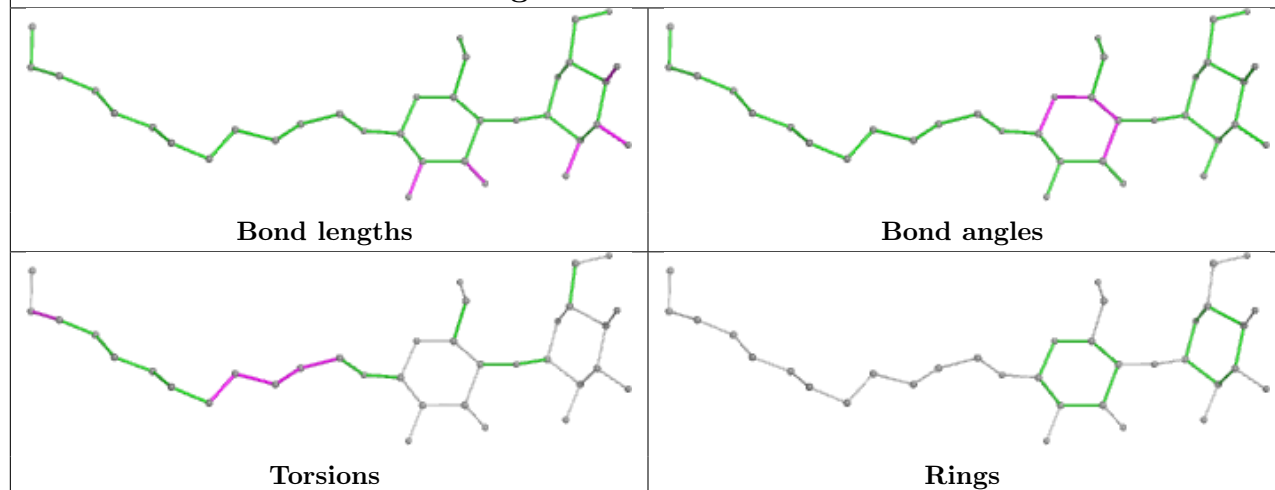
Ligand BCL Ba 1102



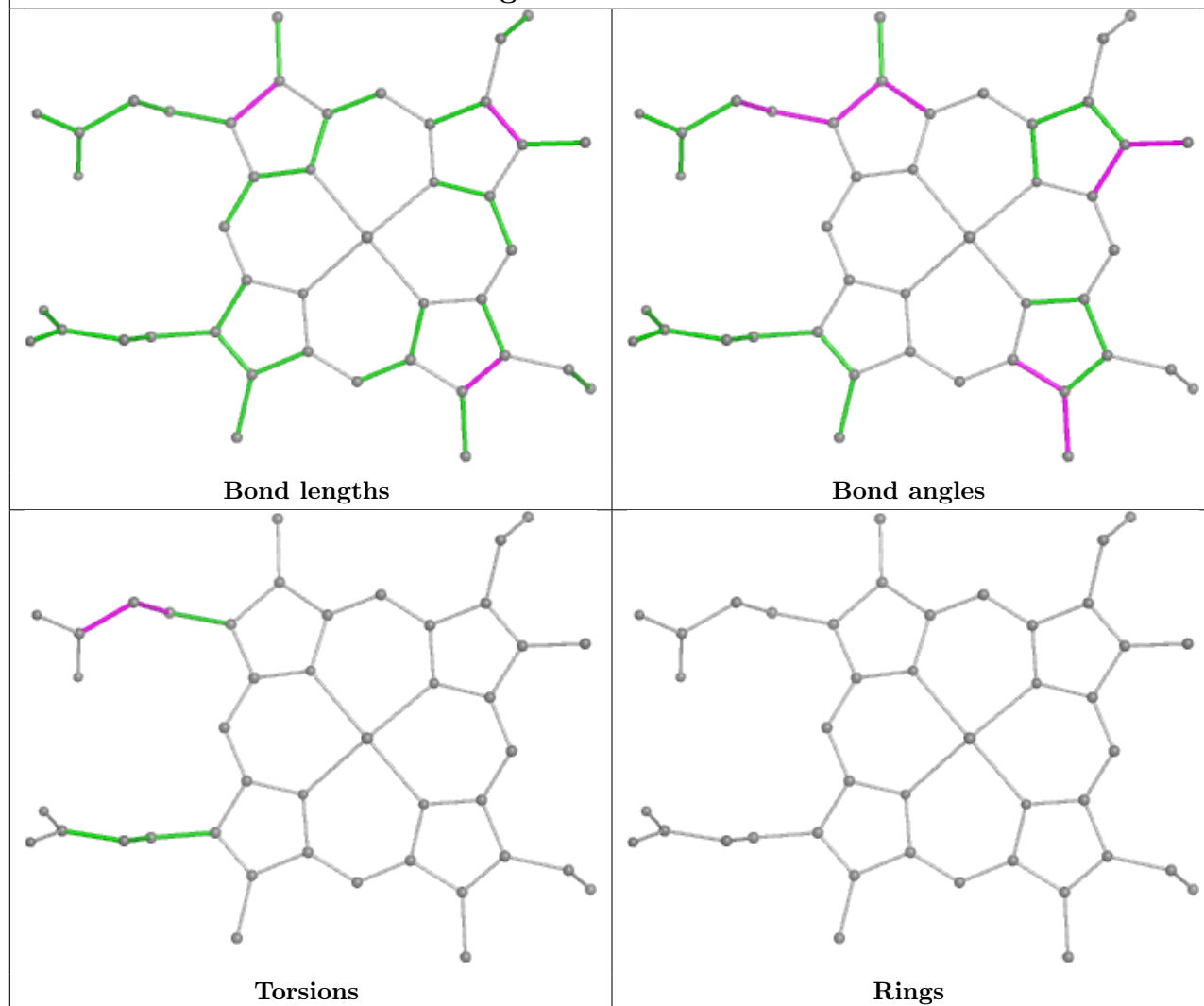
Ligand LMT BM 1001



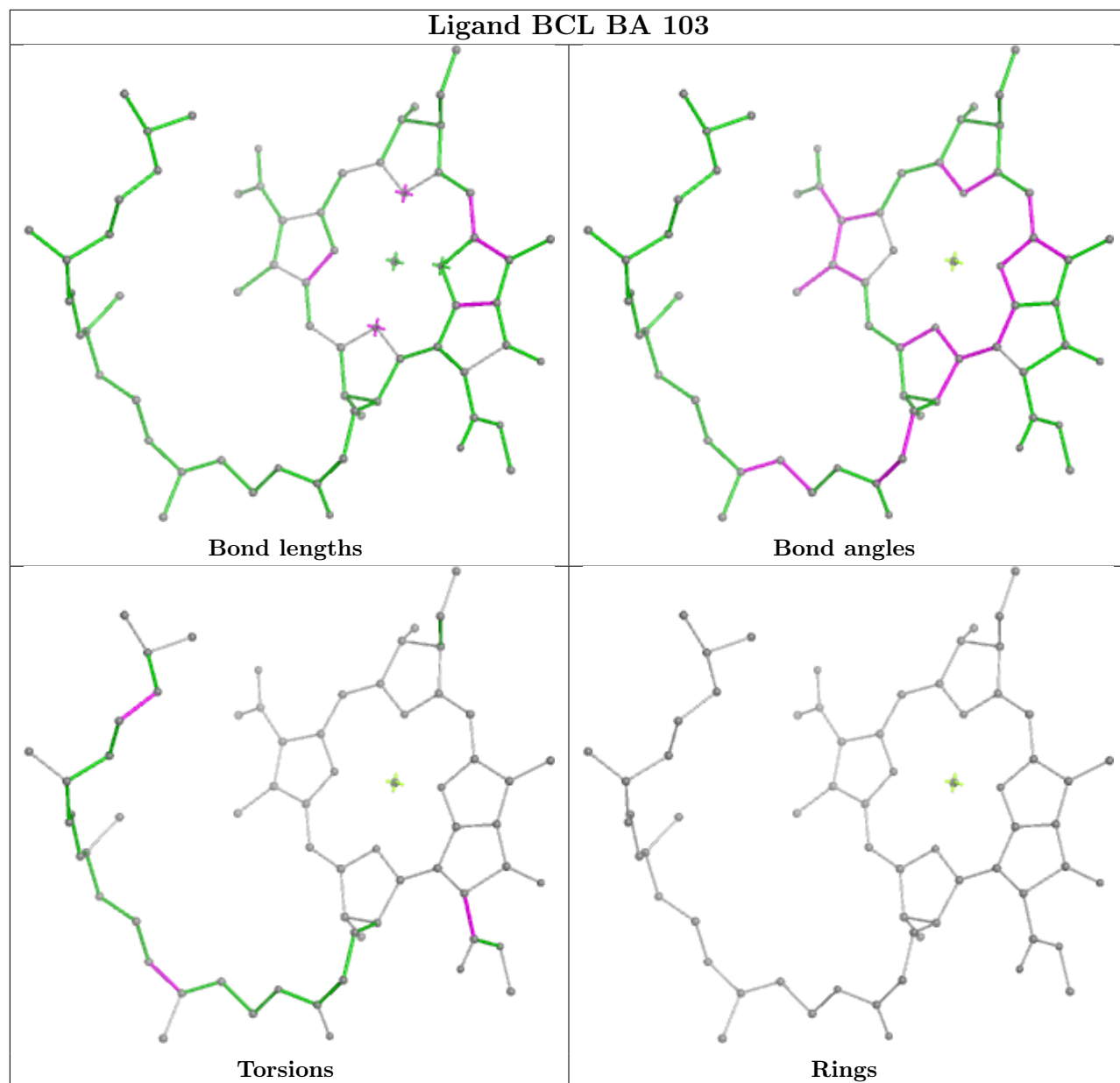
Ligand LMT Bo 1201

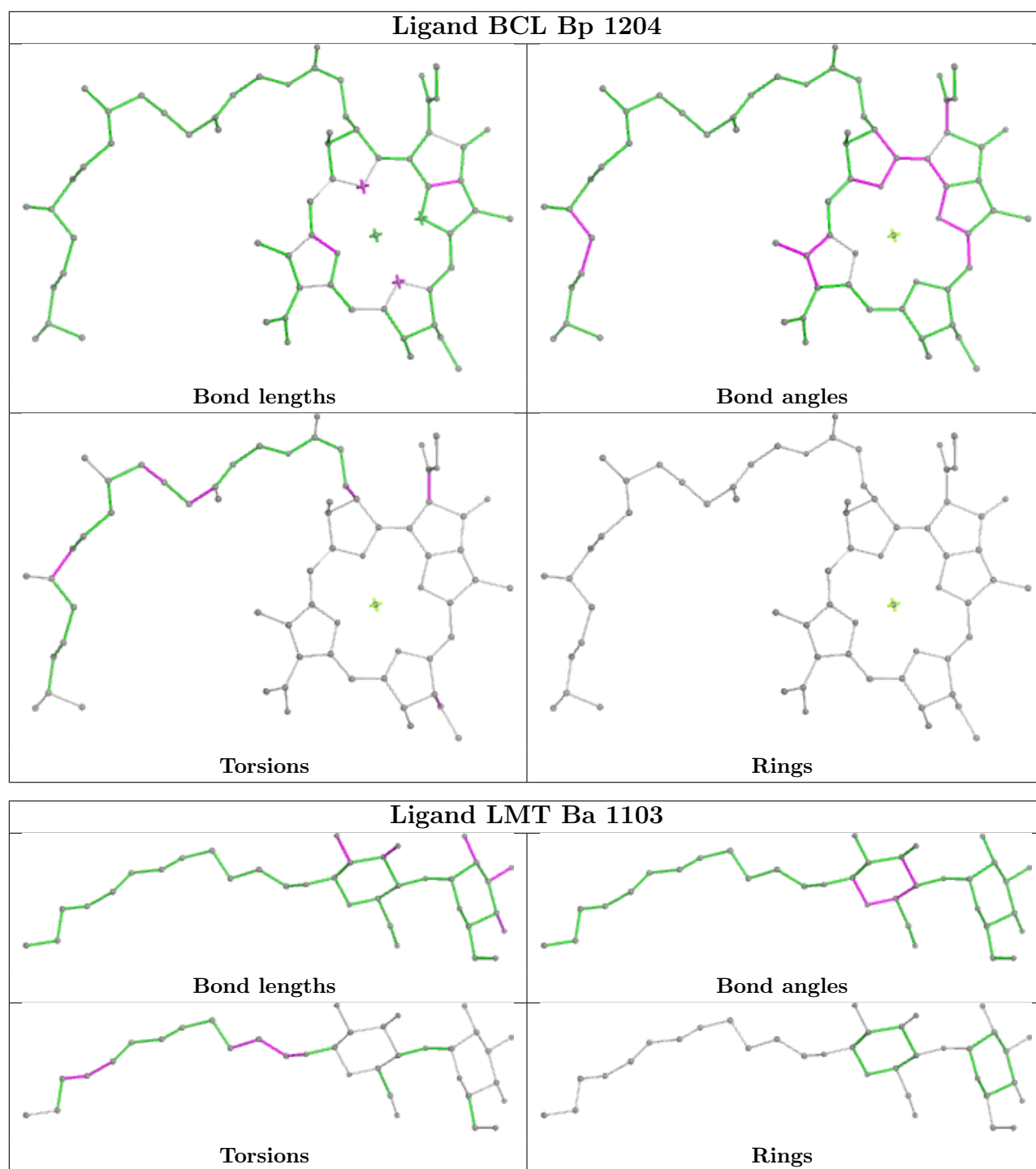


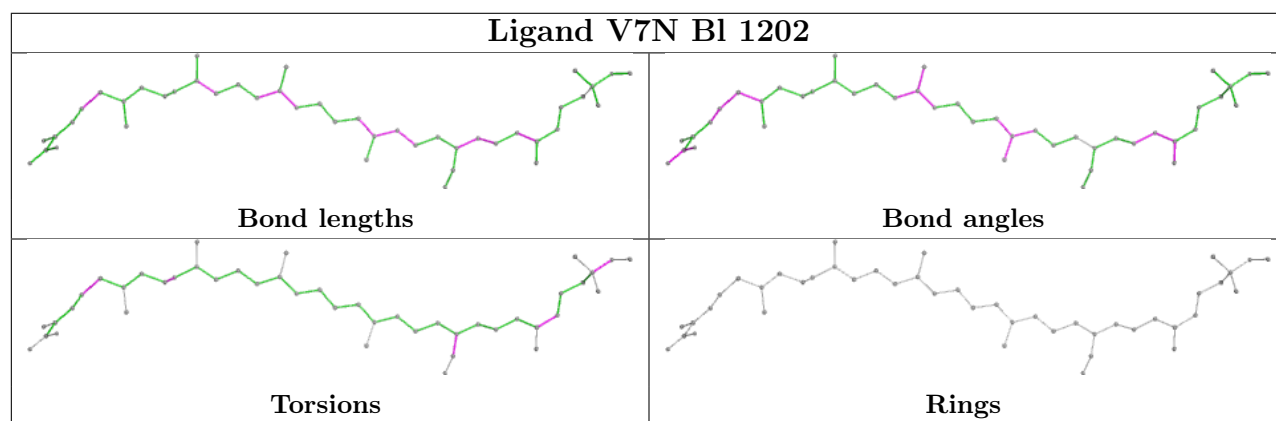
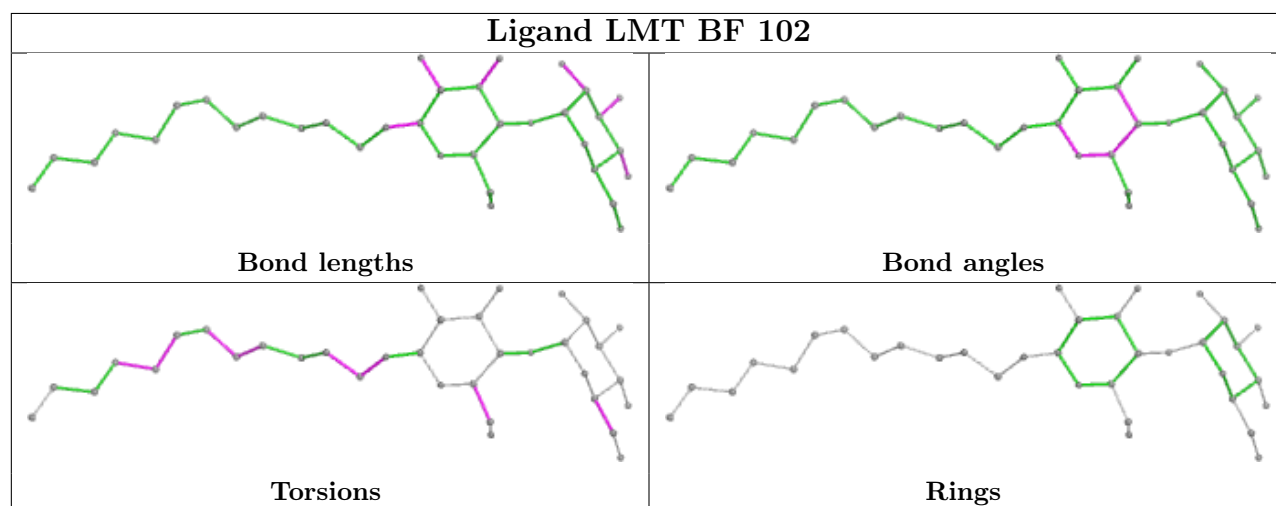
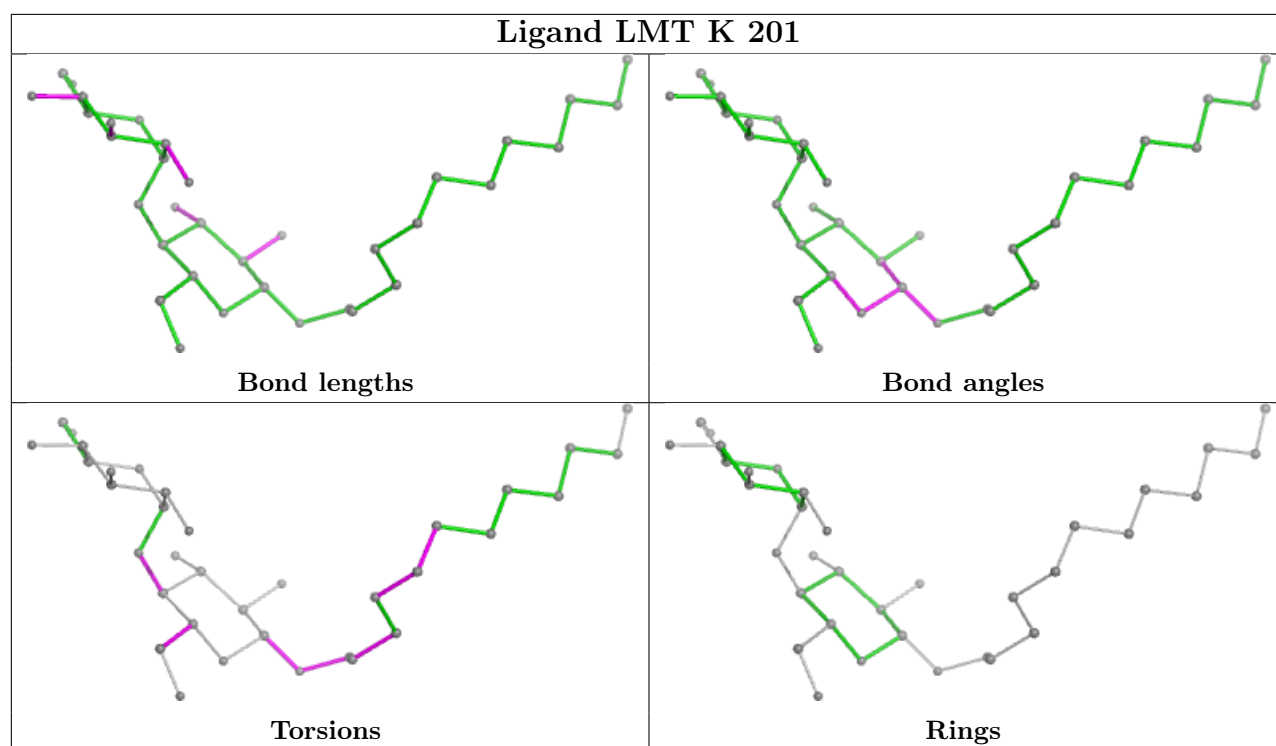
Ligand HEC C 403



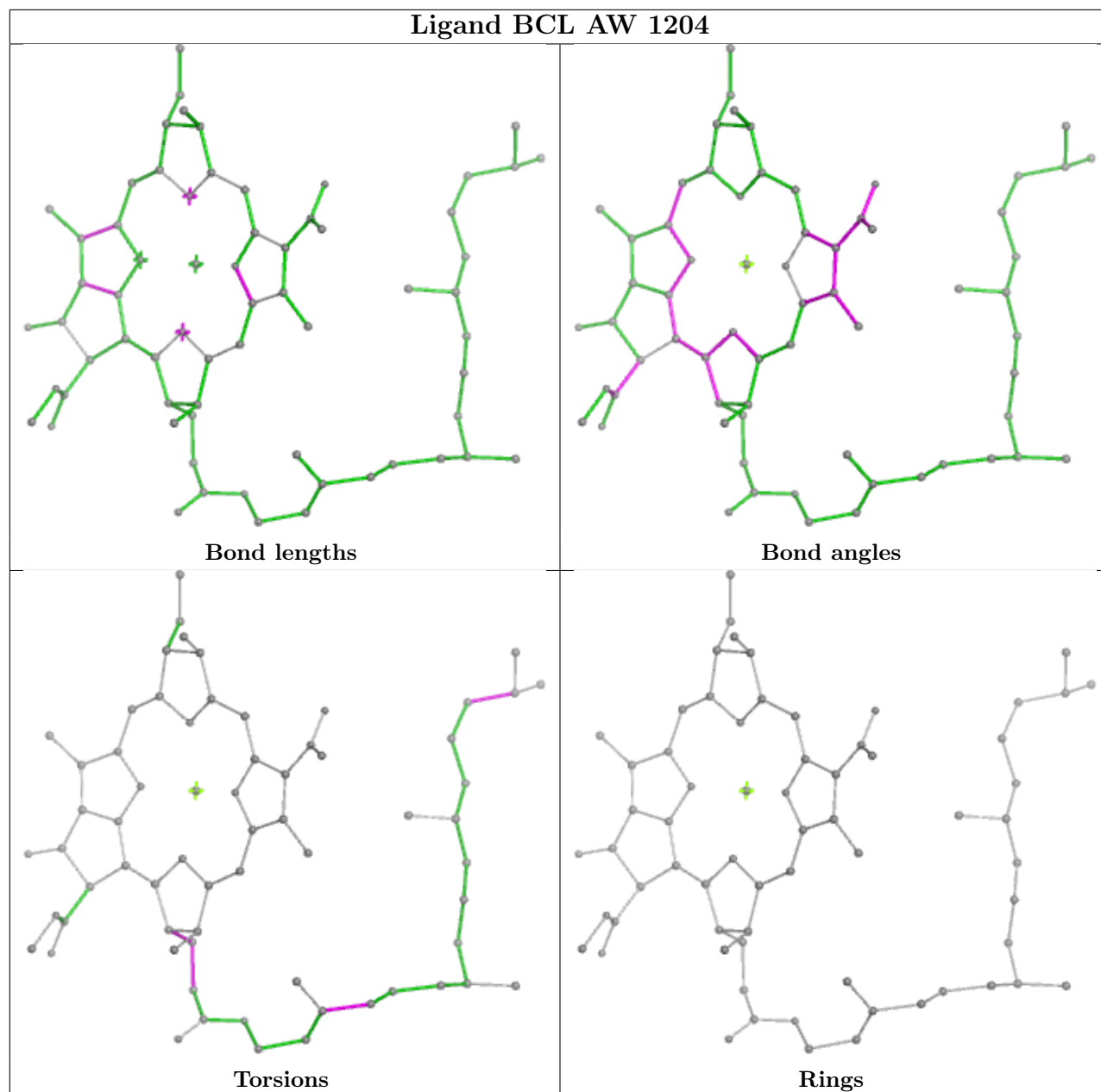
Ligand BCL BA 103

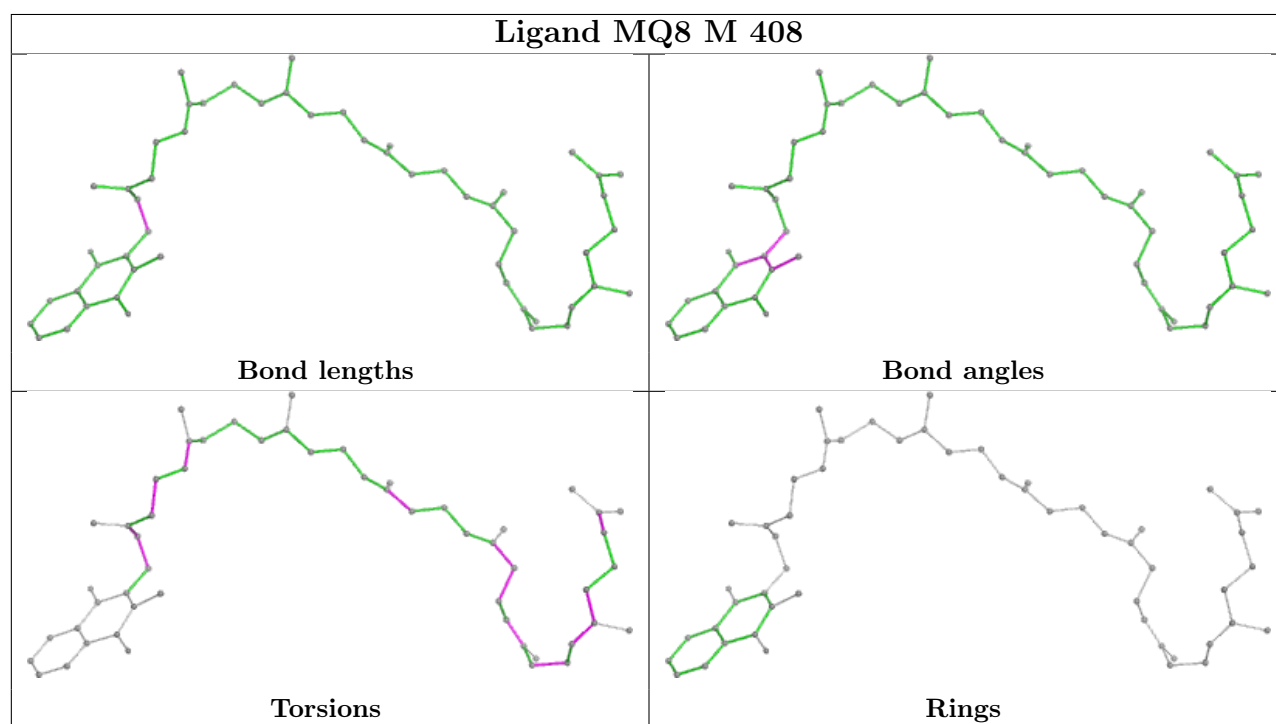
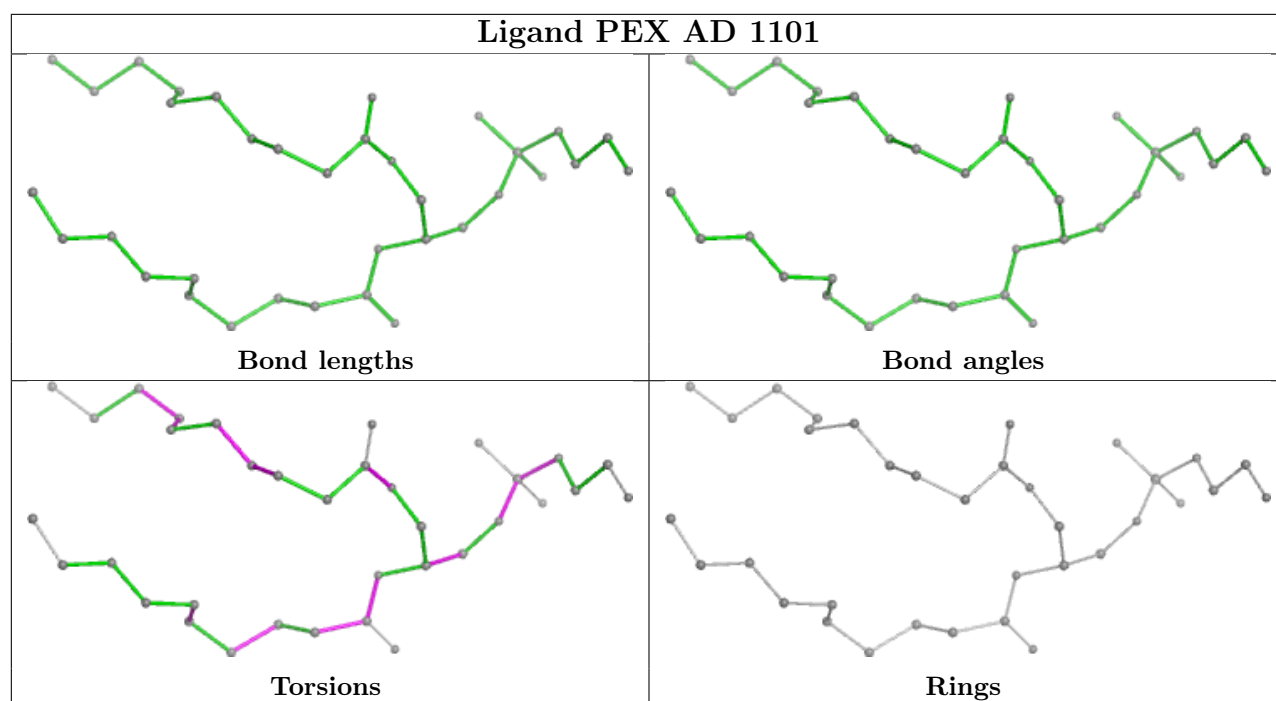


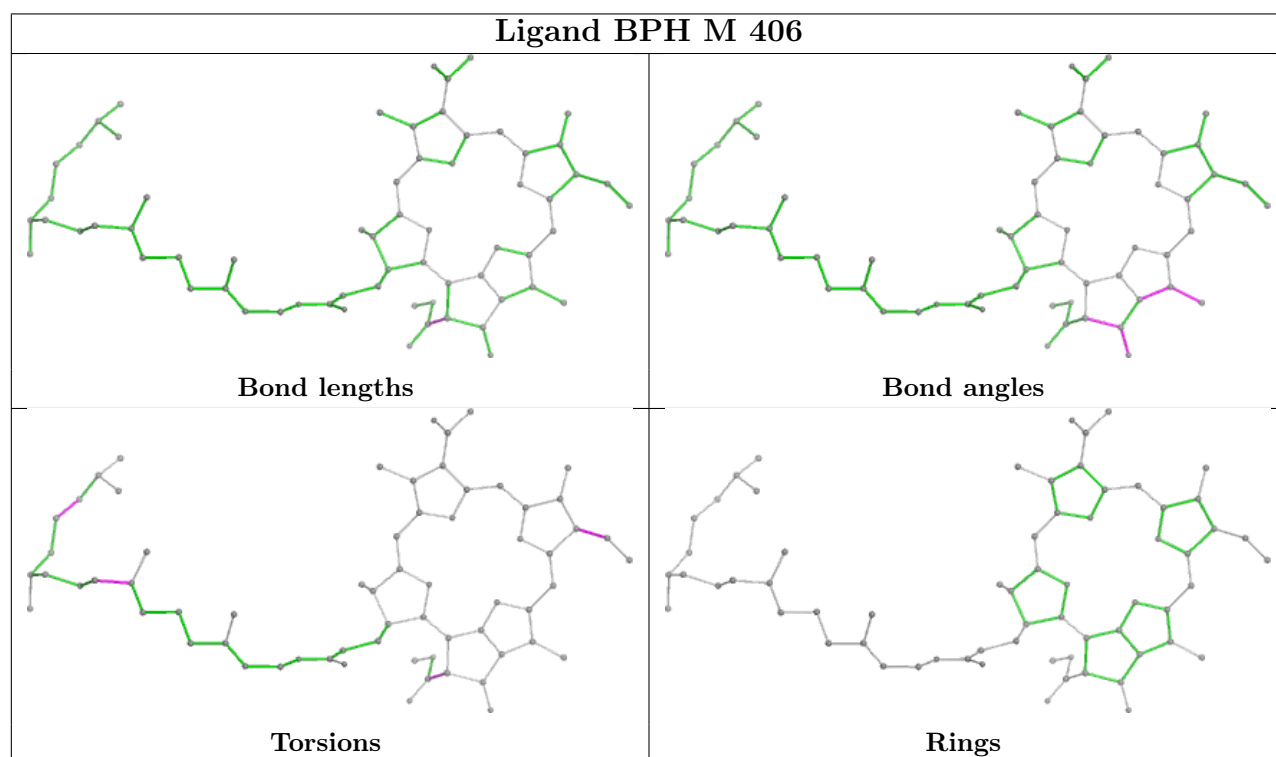
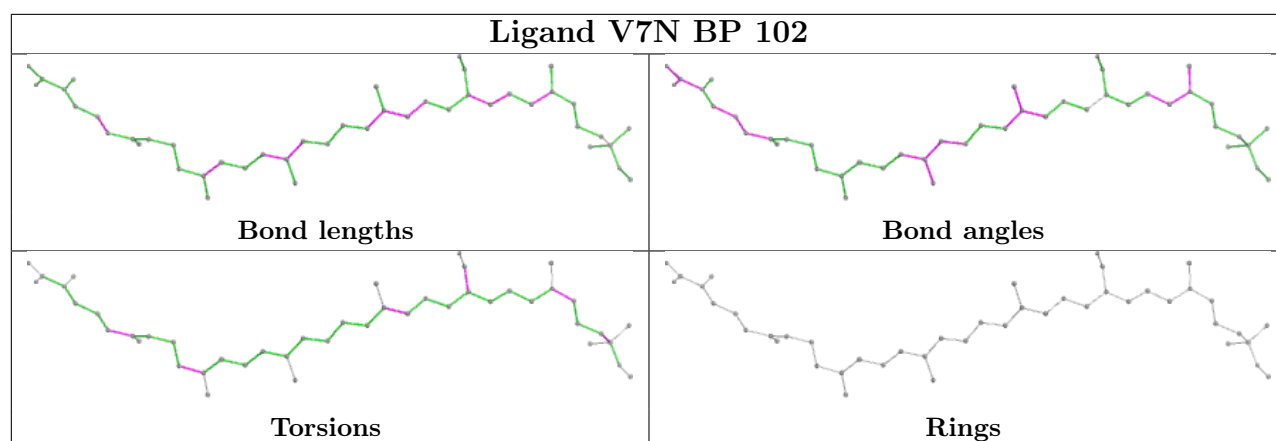


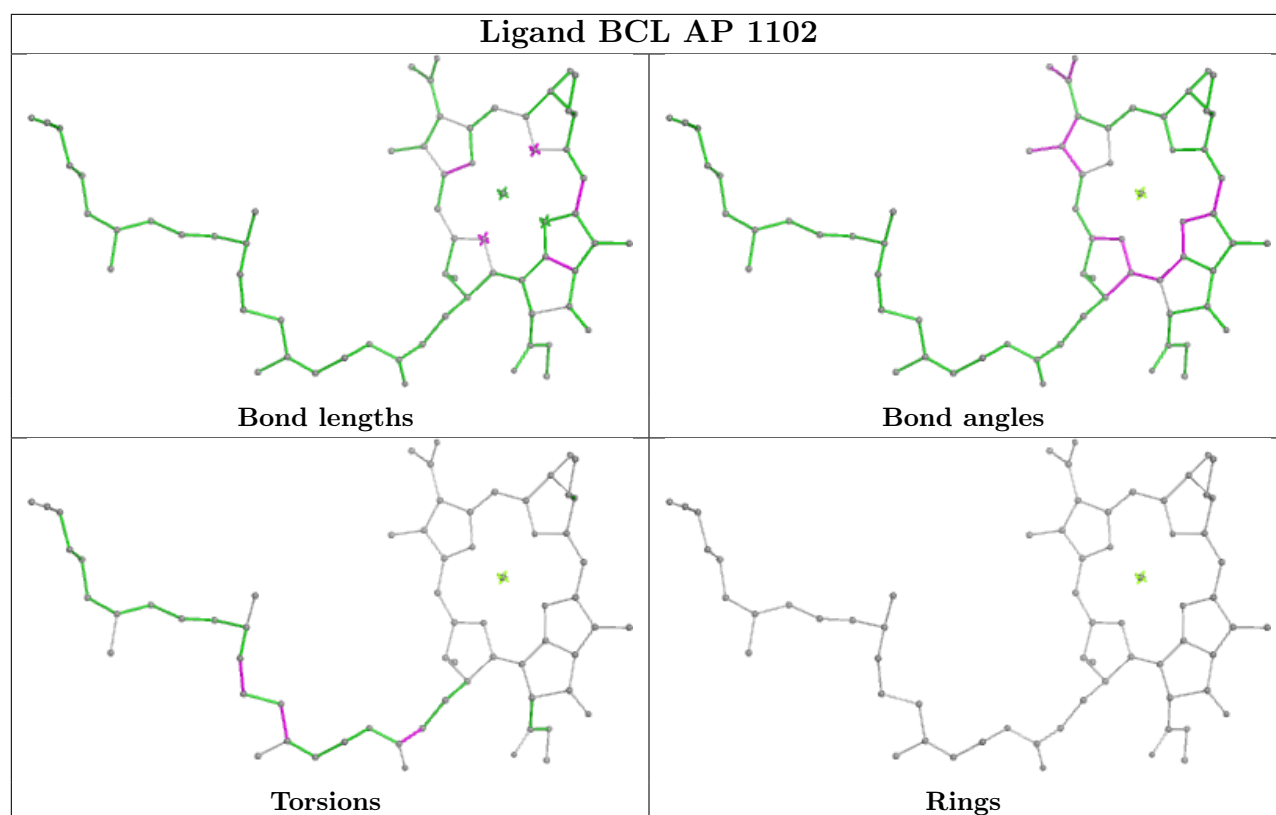


Ligand BCL AW 1204









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.

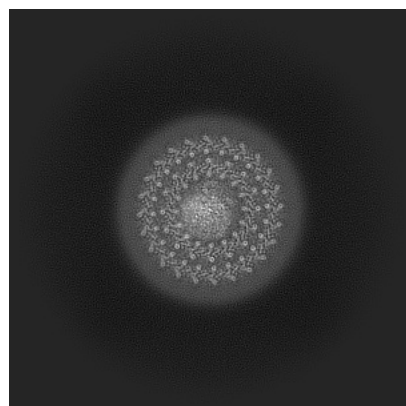
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51760. These allow visual inspection of the internal detail of the map and identification of artifacts.

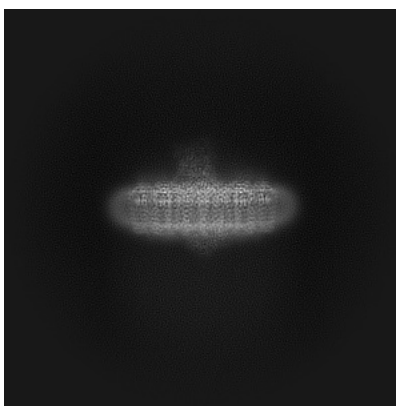
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

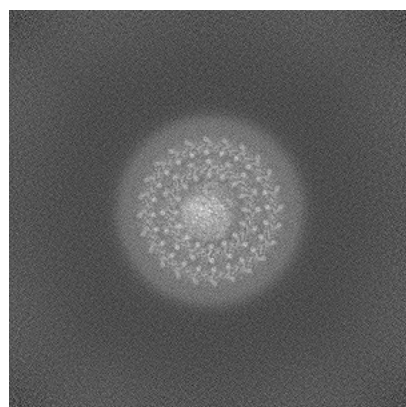


Y

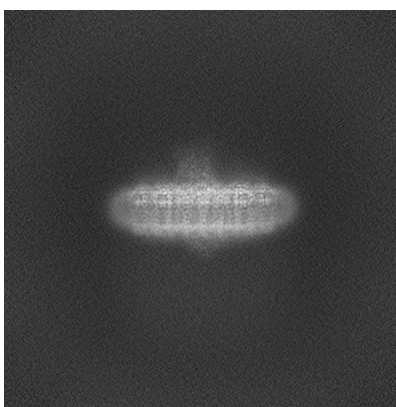


Z

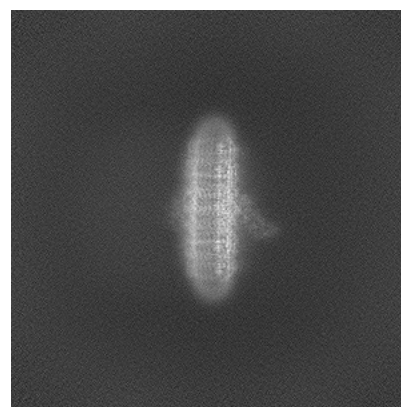
6.1.2 Raw map



X



Y

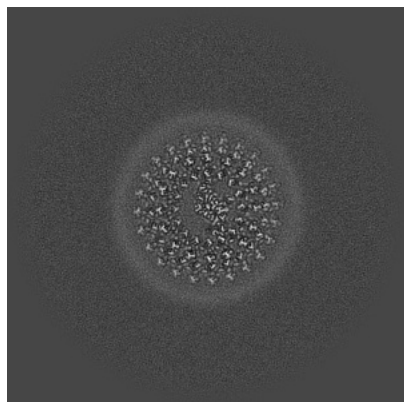


Z

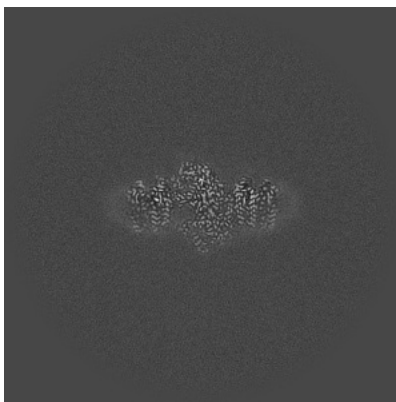
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

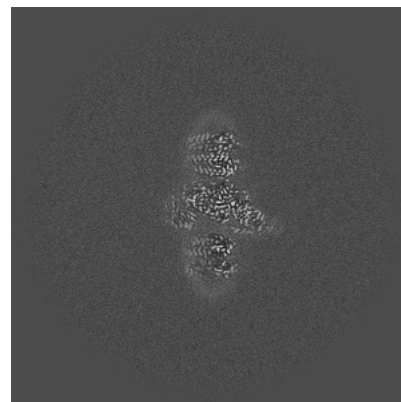
6.2.1 Primary map



X Index: 300

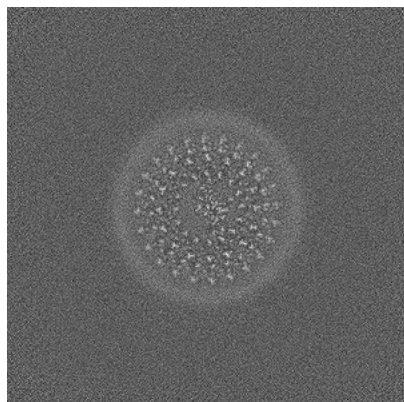


Y Index: 300

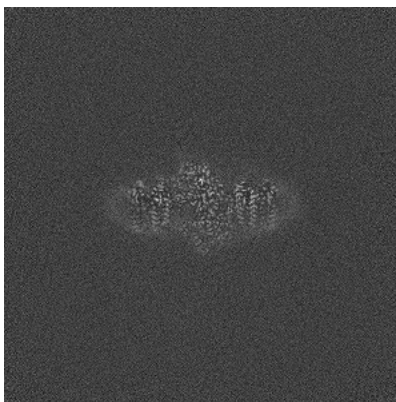


Z Index: 300

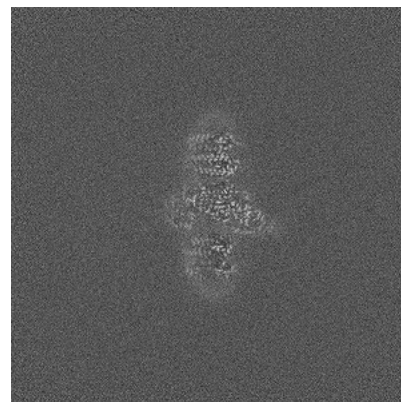
6.2.2 Raw map



X Index: 300



Y Index: 300

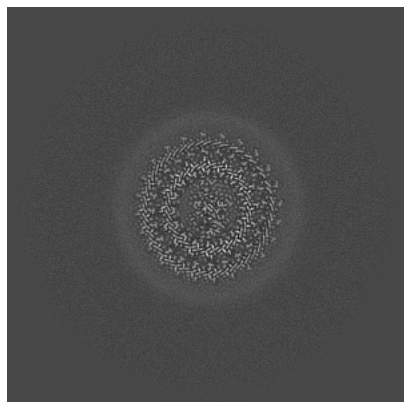


Z Index: 300

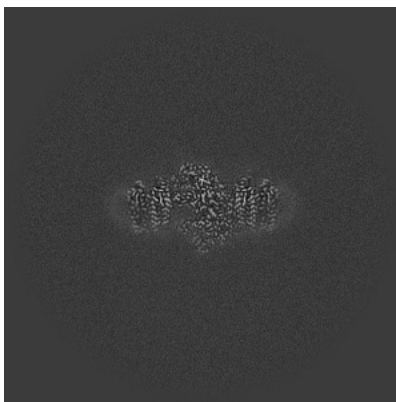
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

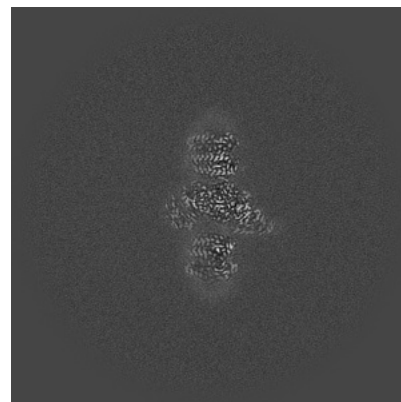
6.3.1 Primary map



X Index: 311

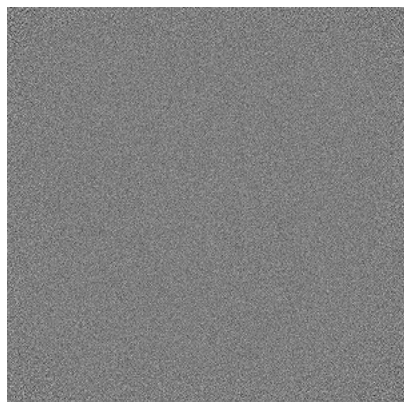


Y Index: 301

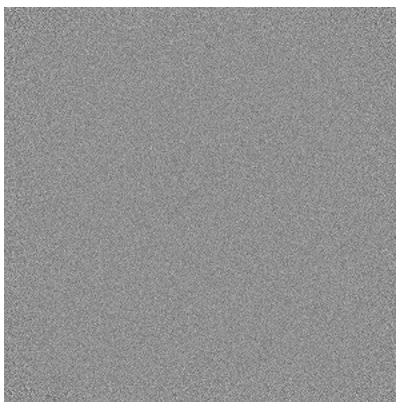


Z Index: 299

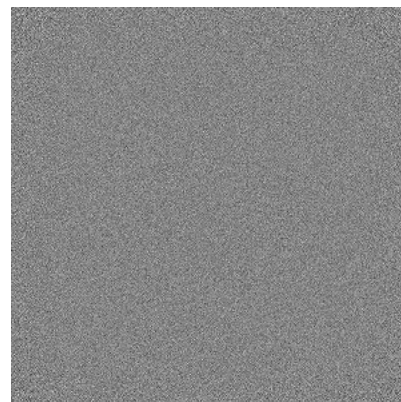
6.3.2 Raw map



X Index: 0



Y Index: 0

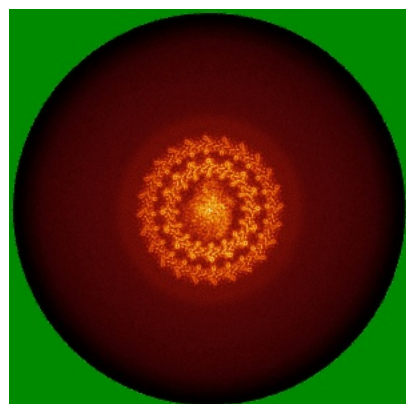


Z Index: 599

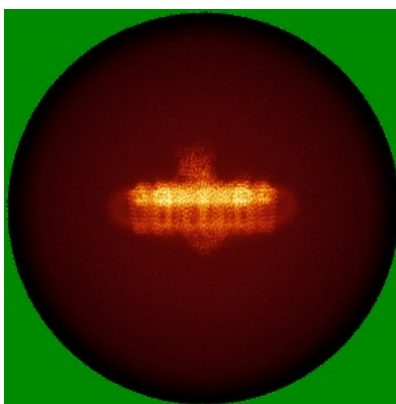
The images above show the largest variance slices of the map in three orthogonal directions.

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

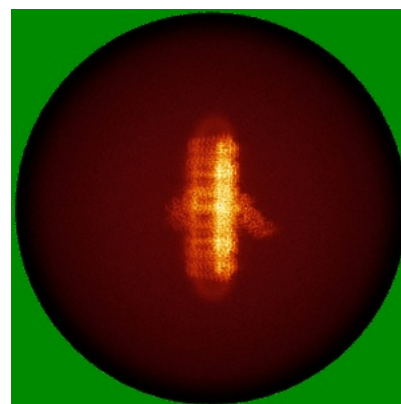
6.4.1 Primary map



X

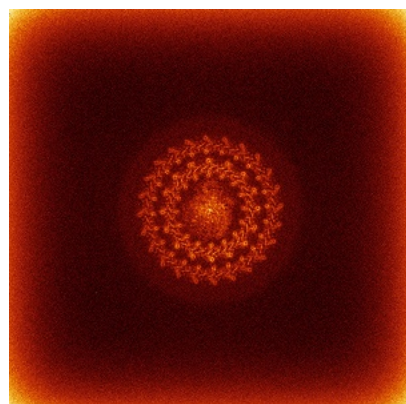


Y

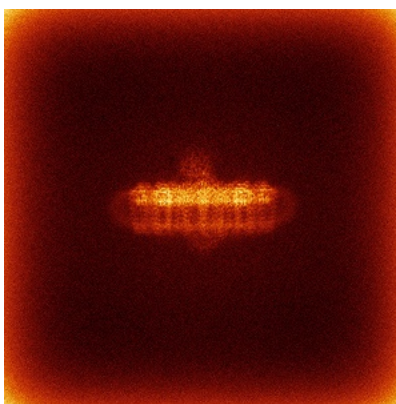


Z

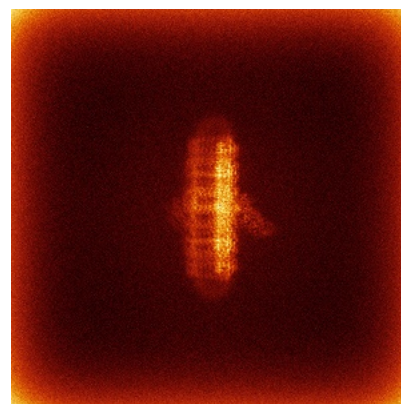
6.4.2 Raw map



X



Y

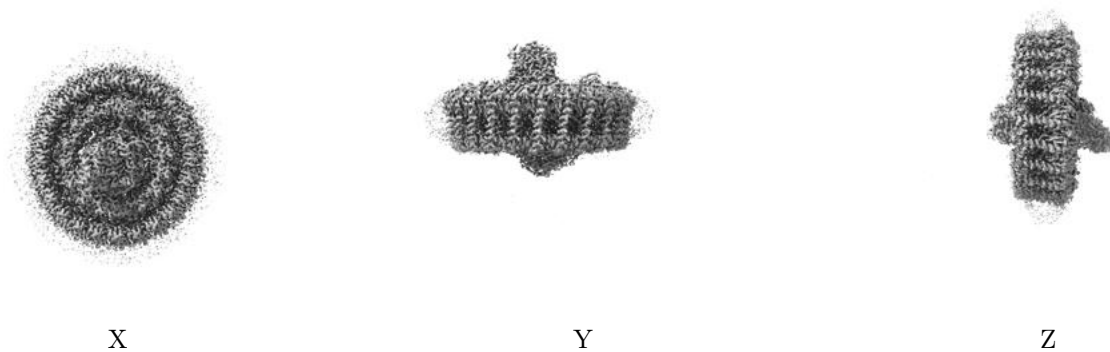


Z

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.

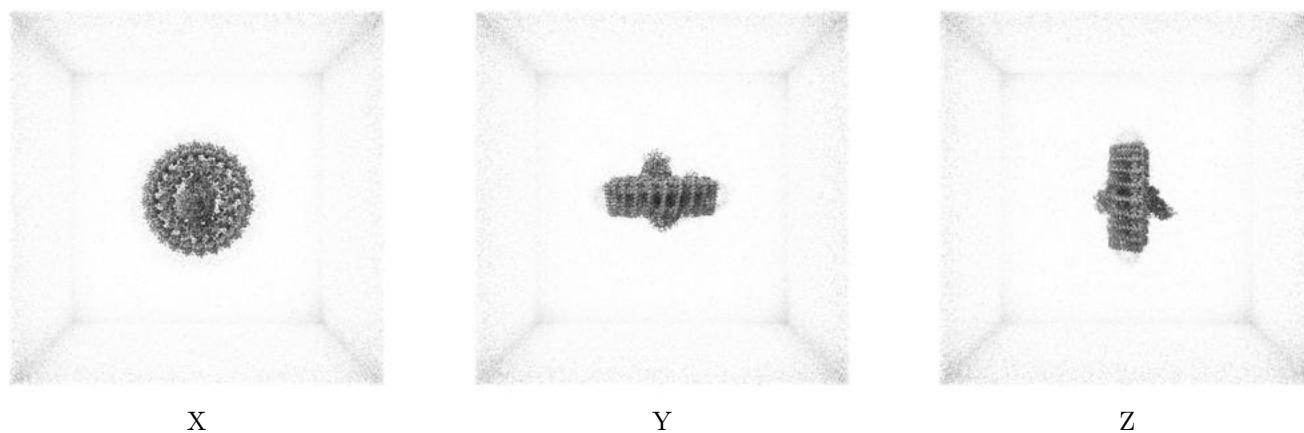
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0687. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

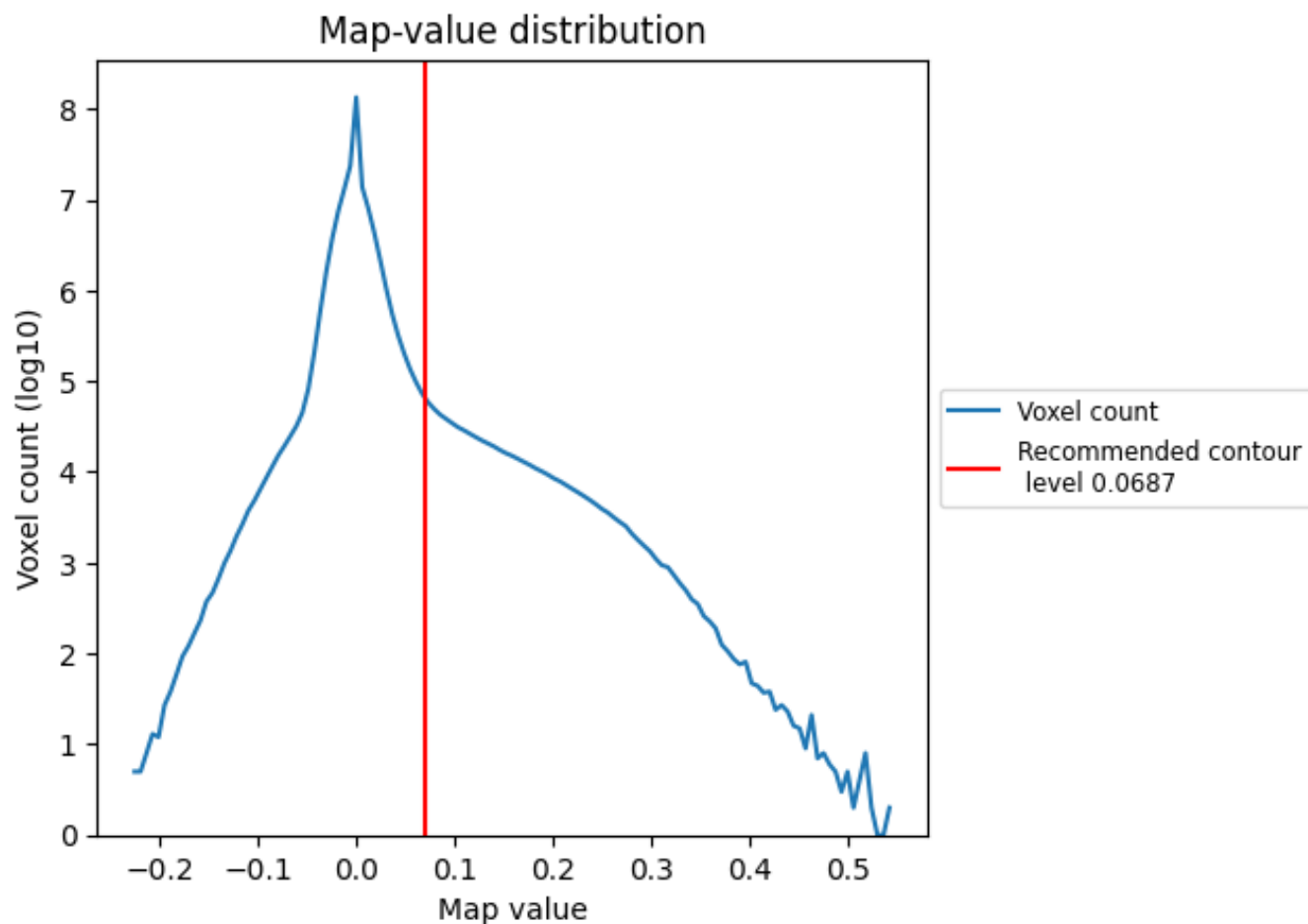
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

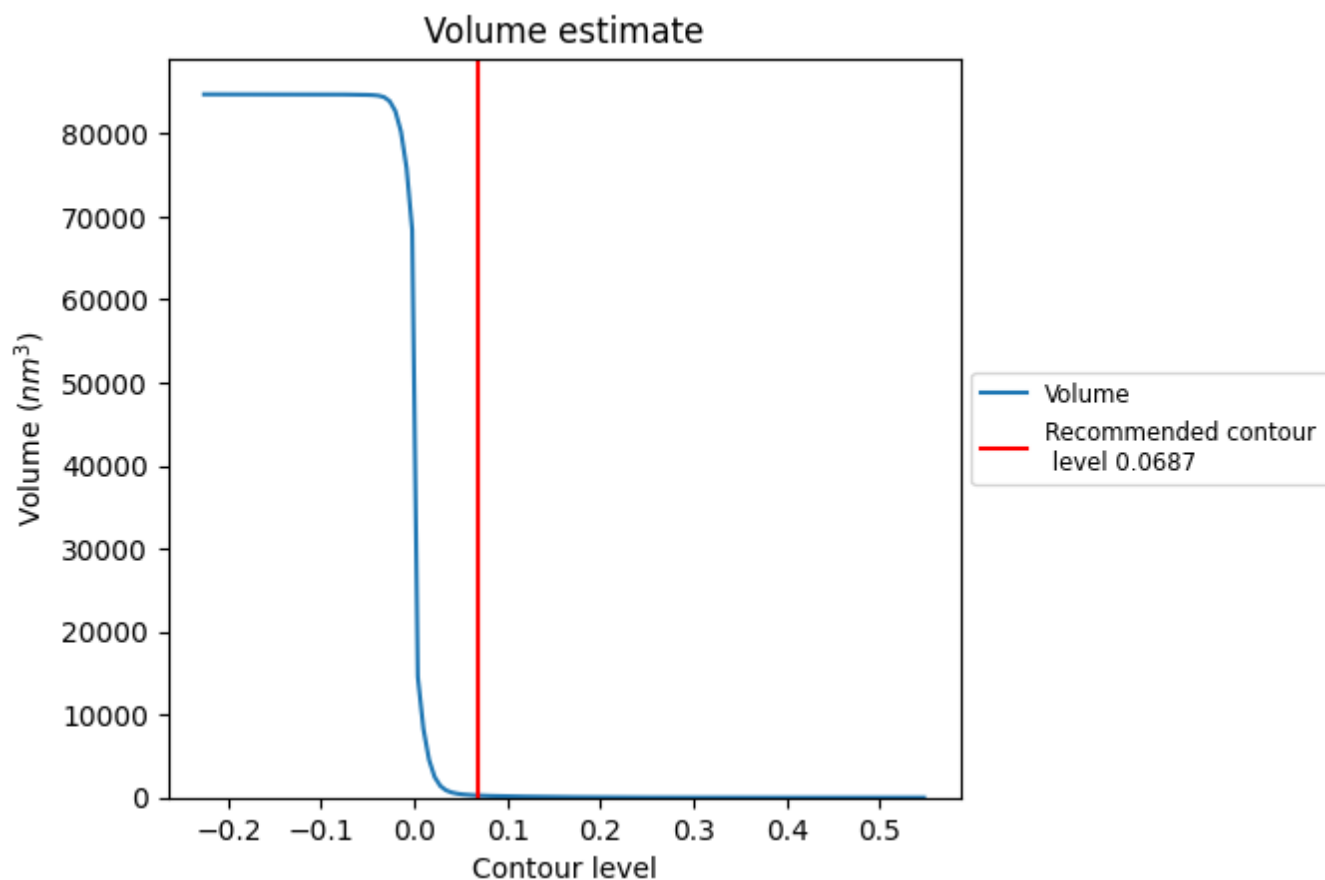
This section contains the results of statistical analysis of the map.

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.

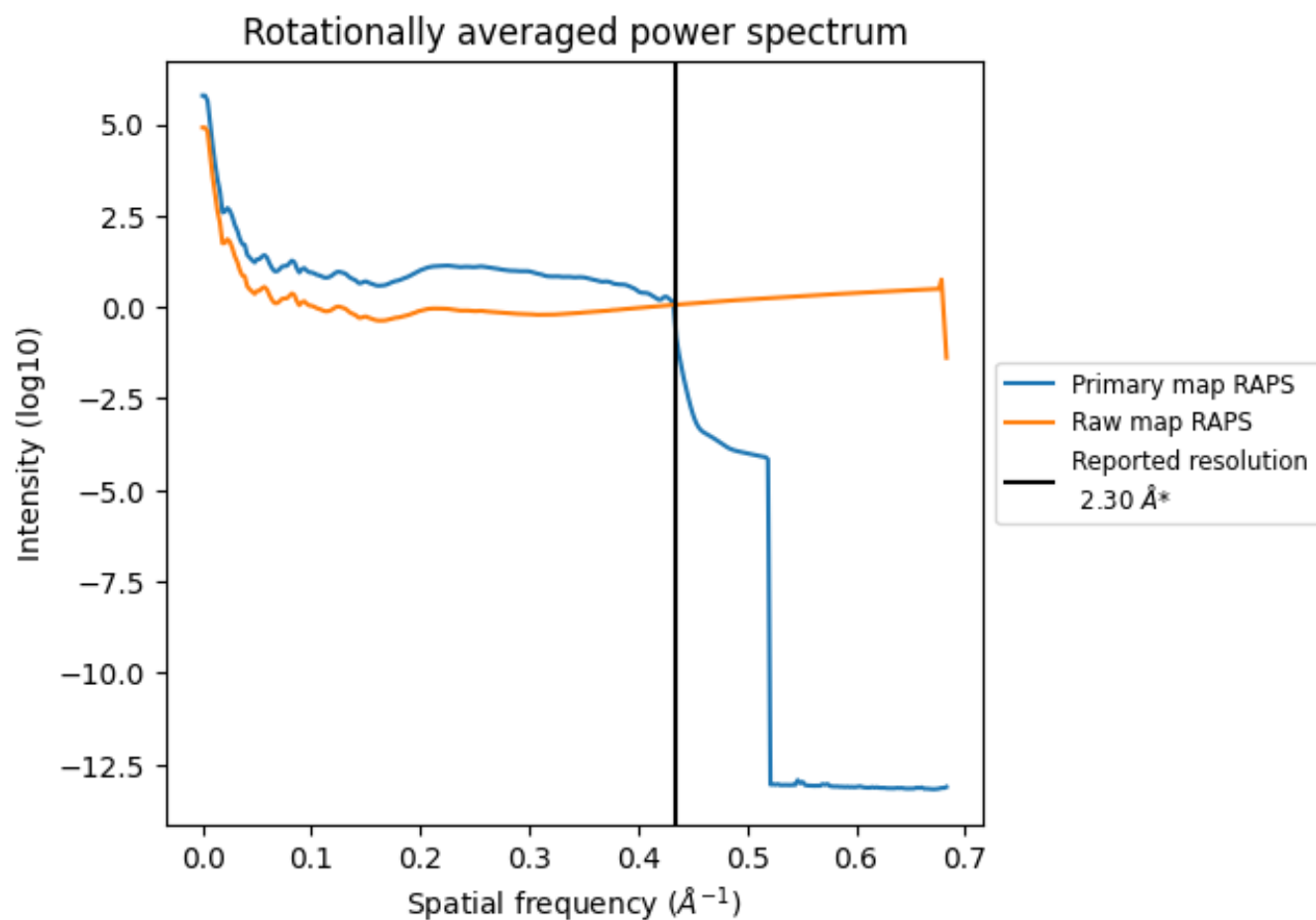
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm³; this corresponds to an approximate mass of 227 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 ⓘ

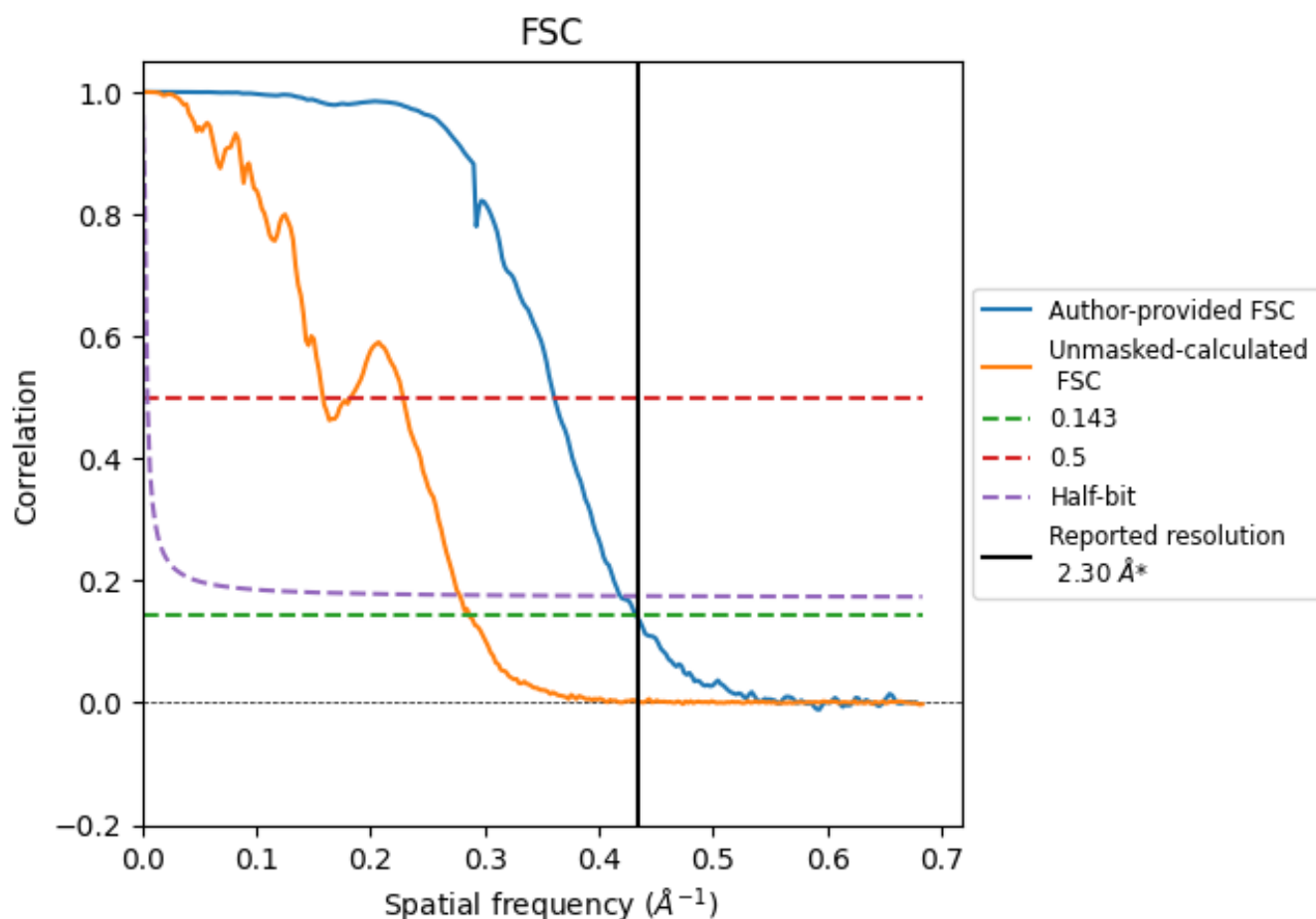


*Reported resolution corresponds to spatial frequency of 0.435 \AA^{-1}

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 0.435 \AA^{-1}

8.2 Resolution estimates [i](#)

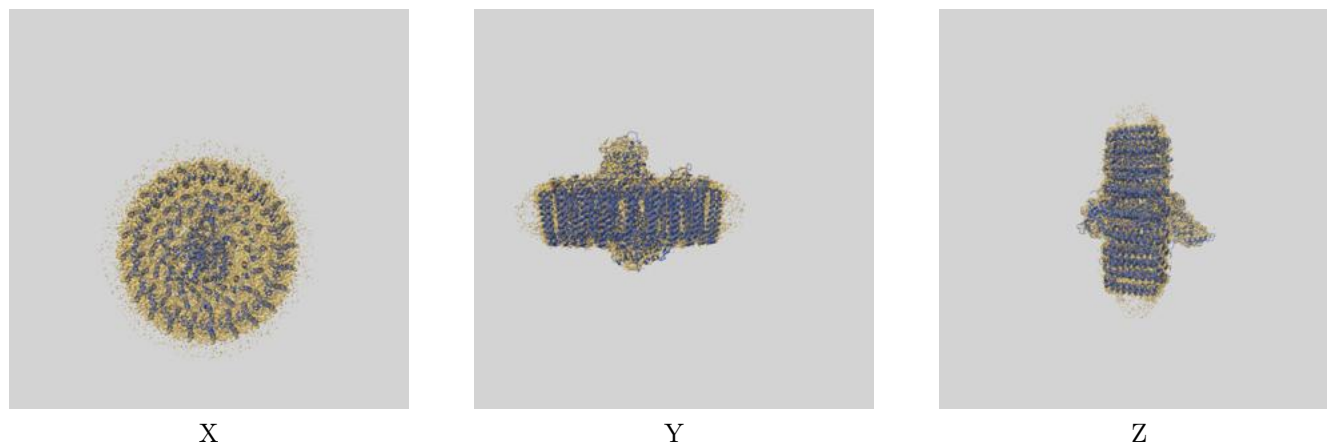
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.31	2.77	2.39
Unmasked-calculated*	3.49	6.32	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

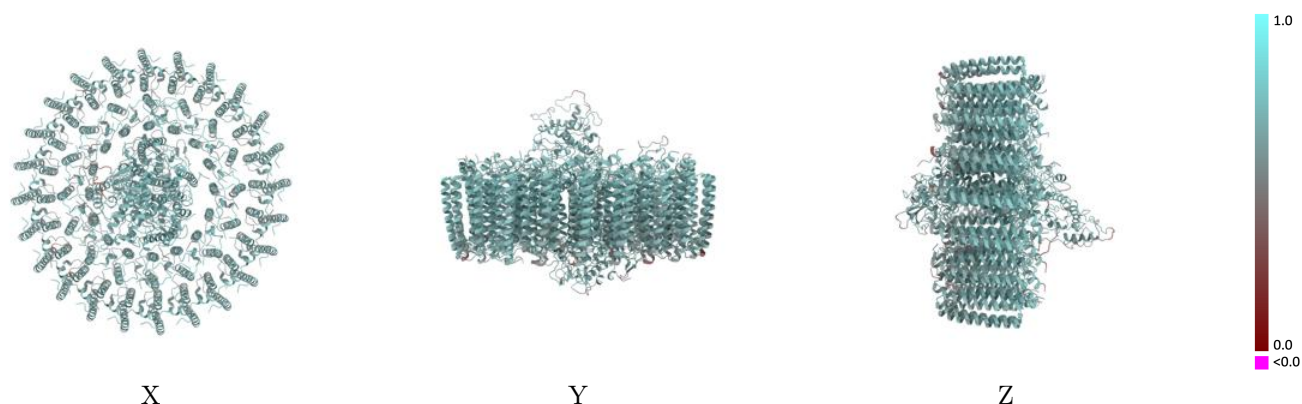
This section contains information regarding the fit between EMDB map EMD-51760 and PDB model 9H19. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



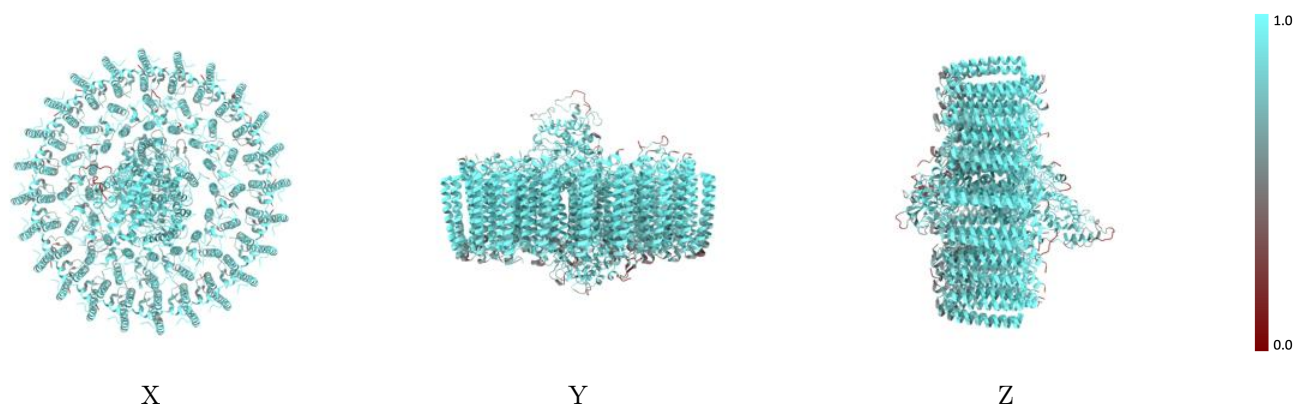
The images above show the 3D surface view of the map at the recommended contour level 0.0687 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



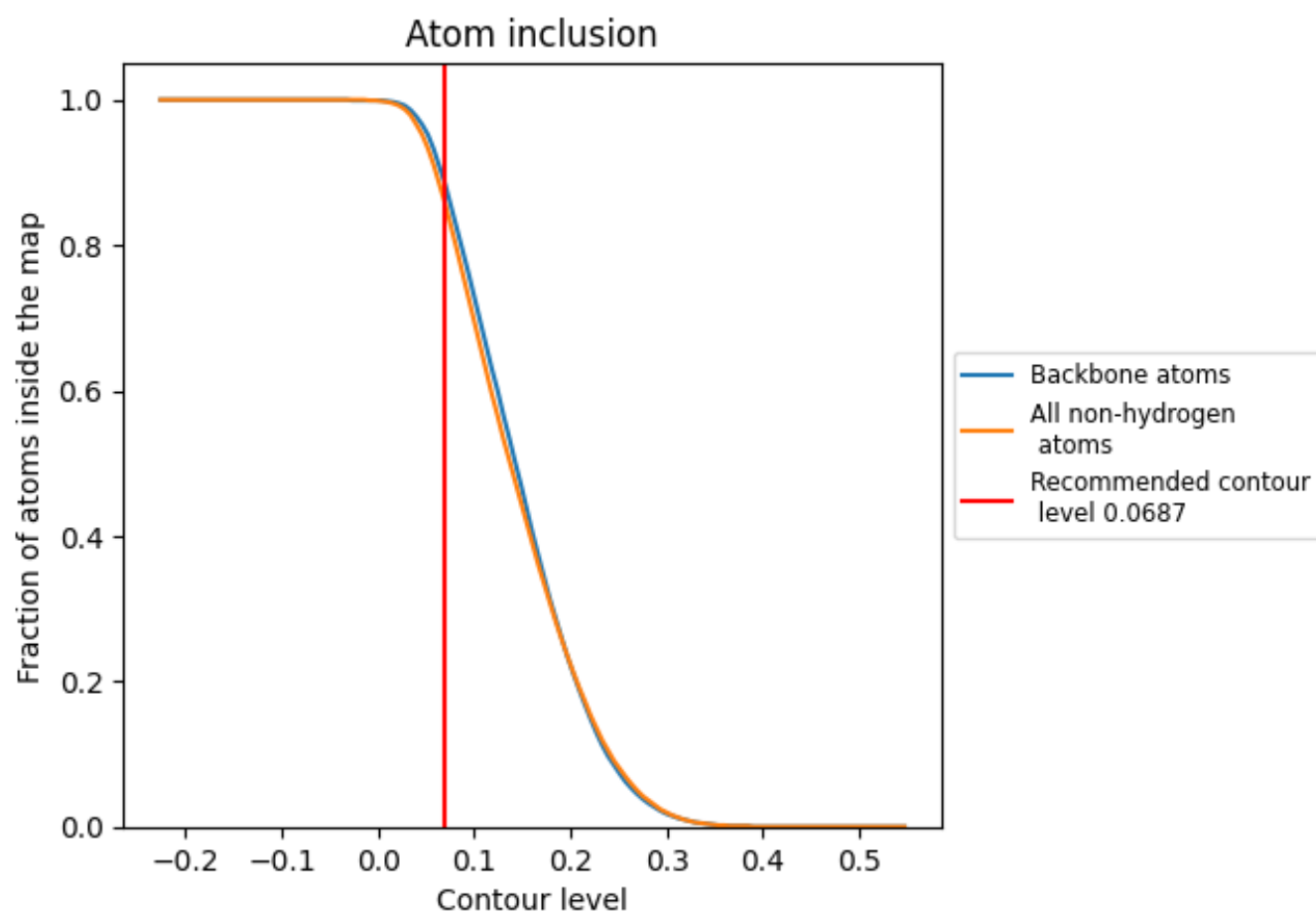
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0687).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0687) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.6400
AA	 0.9230	 0.6540
AB	 0.8400	 0.6280
AC	 0.9150	 0.6520
AD	 0.9100	 0.6460
AE	 0.8320	 0.6320
AF	 0.8840	 0.6390
AG	 0.8880	 0.6450
AH	 0.8370	 0.6310
AI	 0.8410	 0.6360
AJ	 0.8870	 0.6450
AK	 0.8210	 0.6220
AL	 0.8860	 0.6360
AM	 0.8680	 0.6290
AN	 0.8430	 0.6310
AO	 0.8850	 0.6440
AP	 0.8960	 0.6410
AQ	 0.8240	 0.6230
AR	 0.8650	 0.6390
AS	 0.8590	 0.6270
AT	 0.7960	 0.6160
AU	 0.8630	 0.6340
AV	 0.9210	 0.6460
AW	 0.8110	 0.6230
AX	 0.9080	 0.6480
Aa	 0.7400	 0.5820
Ab	 0.8950	 0.6480
Ac	 0.9160	 0.6550
Ad	 0.8350	 0.6300
Ae	 0.8930	 0.6580
Af	 0.8440	 0.6320
Ag	 0.9050	 0.6450
Ah	 0.9180	 0.6580
Ai	 0.8550	 0.6320
Aj	 0.8510	 0.6370























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Chain	Atom inclusion	Q-score
Ak	 0.9510	 0.6740
Al	 0.9370	 0.6650
Am	 0.9420	 0.6700
An	 0.9370	 0.6630
Ao	 0.8830	 0.6450
Ap	 0.8980	 0.6350
BA	 0.8520	 0.6330
BB	 0.8130	 0.6180
BC	 0.8810	 0.6380
BD	 0.8830	 0.6490
BE	 0.8120	 0.6020
BF	 0.8580	 0.6280
BG	 0.8540	 0.6270
BH	 0.8000	 0.5960
BI	 0.8620	 0.6290
BJ	 0.8930	 0.6440
BK	 0.7670	 0.6010
BL	 0.8560	 0.6320
BM	 0.8740	 0.6290
BN	 0.8610	 0.6280
BO	 0.8340	 0.6240
BP	 0.8510	 0.6350
BQ	 0.8010	 0.6050
BR	 0.8480	 0.6300
BS	 0.8410	 0.6030
BT	 0.7680	 0.5560
BU	 0.8060	 0.5860
BV	 0.8350	 0.6220
BW	 0.8190	 0.6160
BX	 0.8670	 0.6400
Ba	 0.7980	 0.6120
Bb	 0.8480	 0.6360
Bc	 0.8570	 0.6410
Bd	 0.8810	 0.6520
Be	 0.8650	 0.6430
Bf	 0.8750	 0.6510
Bg	 0.8590	 0.6410
Bh	 0.8450	 0.6360
Bi	 0.7950	 0.6150
Bj	 0.8450	 0.6470
Bk	 0.8860	 0.6590
Bl	 0.8970	 0.6660

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Chain	Atom inclusion	Q-score
Bm	 0.8810	 0.6500
Bn	 0.8790	 0.6500
Bo	 0.8420	 0.6360
Bp	 0.8480	 0.6400
C	 0.8740	 0.6460
H	 0.7870	 0.6460
K	 0.7460	 0.6060
L	 0.9510	 0.6890
M	 0.9380	 0.6800
S	 0.8520	 0.6610