



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 23, 2026 – 06:31 AM UTC

PDB ID : 6CC9 / pdb_00006cc9
BMRB ID : 30400
Title : NMR data-driven model of GTPase KRas-GMPPNP:Cmpd2 complex tethered to a nanodisc
Authors : Fang, Z.; Marshall, C.B.; Nishikawa, T.; Gossert, A.D.; Jansen, J.M.; Jahnke, W.; Ikura, M.
Deposited on : 2018-02-06

This is a wwPDB NMR Structure 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/NMRValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

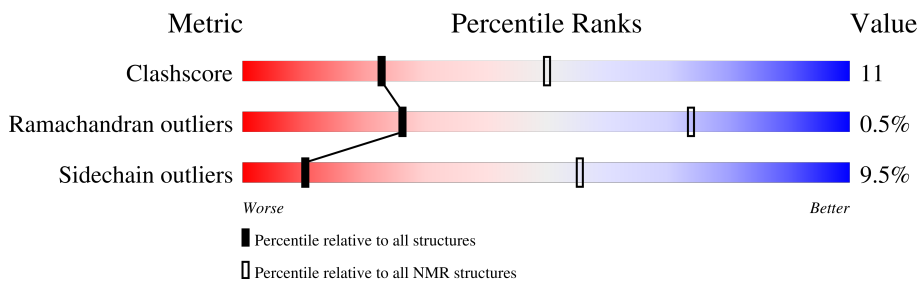
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	200	
1	C	200	
2	B	187	

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:239-A:395, C:401-C:596 (353)	0.44	8
2	B:2-B:172 (171)	0.88	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 3, 6, 7, 8, 9
2	4, 10
Single-model clusters	1; 5

3 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9535 atoms, of which 429 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	198	1645	1019	22	287	314	3	0
1	C	198	1646	1019	22	287	315	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P02647
A	200	PRO	-	expression tag	UNP P02647
C	397	GLY	-	expression tag	UNP P02647
C	398	PRO	-	expression tag	UNP P02647

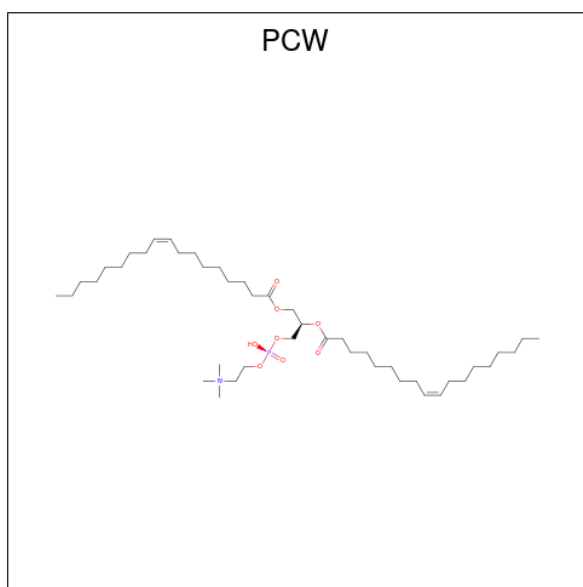
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	185	1842	926	363	257	287	9	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116
B	12	VAL	GLY	engineered mutation	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



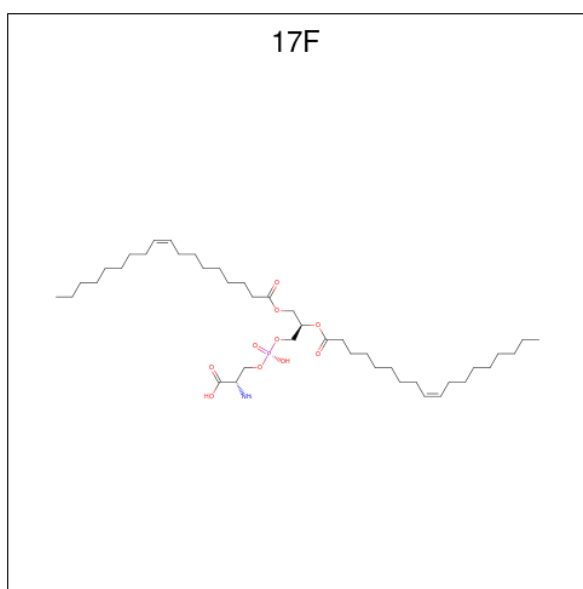
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	A	1	54	44	1	8	1
3	B	1	54	44	1	8	1
3	B	1	54	44	1	8	1
3	B	1	54	44	1	8	1
3	B	1	54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P).



Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1

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Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
4	B	1	Total 54	42	1	10	1
4	B	1	Total 54	42	1	10	1
4	B	1	Total 54	42	1	10	1
4	B	1	Total 54	42	1	10	1
4	B	1	Total 54	42	1	10	1
4	B	1	Total 54	42	1	10	1
4	C	1	Total 54	42	1	10	1
4	C	1	Total 54	42	1	10	1
4	C	1	Total 54	42	1	10	1
4	C	1	Total 54	42	1	10	1
4	C	1	Total 54	42	1	10	1
4	C	1	Total 54	42	1	10	1
4	C	1	Total 54	42	1	10	1

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

Mol	Chain	Residues	Atoms						
			Total	Br	C	Cl	H	N	O
7	B	1	49	1	21	1	22	3	1



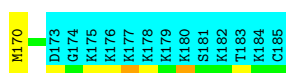
- Molecule 1: Apolipoprotein A-I

Chain C: 80% 18%



- Molecule 2: GTPase KRas

Chain B: 74% 18% 7%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 3000 calculated structures, 10 were deposited, based on the following criterion: *10 structures for lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
HADDOCK	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	268
Number of shifts mapped to atoms	193
Number of unparsed shifts	0
Number of shifts with mapping errors	75
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 17F, EWS, MG, PCW, GNP

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 (average) 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	A	0.41±0.01	0±0/1305 (0.0± 0.0%)	0.78±0.01	0±0/1752 (0.0± 0.0%)
1	C	0.40±0.01	0±0/1634 (0.0± 0.0%)	0.80±0.01	0±0/2196 (0.0± 0.0%)
2	B	0.33±0.00	0±0/1390 (0.0± 0.0%)	0.67±0.03	0±0/1875 (0.0± 0.0%)
All	All	0.38	0/43290 (0.0%)	0.75	2/58230 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	5	LYS	CD-CE-NZ	13.26	154.32	111.90	6	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1284	18	1297	28±5
1	C	1607	22	1603	35±8
2	B	1368	322	1356	17±5
3	A	540	0	840	32±9
3	B	1512	0	2351	78±17
3	C	1404	0	2182	63±16

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
4	A	54	0	76	5±2
4	B	432	0	608	37±5
4	C	378	0	532	26±7
5	B	32	0	13	1±1
7	B	27	22	0	9±4
All	All	86390	3840	108600	2184

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 11.

5 of 1707 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:72:MET:HA	7:B:239:EWS:BRA	1.57	1.53	3	5
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.48	1.34	10	1
1:A:393:TYR:CE1	3:A:406:PCW:H271	1.45	1.46	8	1
1:A:393:TYR:CD1	3:A:406:PCW:C27	1.43	2.01	8	2
1:A:393:TYR:CD1	3:A:406:PCW:H271	1.37	1.51	8	1

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	A	157/200 (78%)	153±1 (98±1%)	3±1 (2±1%)	1±0 (1±0%)	23	72
1	C	195/200 (98%)	190±1 (98±1%)	4±2 (2±1%)	1±0 (1±0%)	26	74
2	B	171/187 (91%)	160±4 (94±2%)	10±4 (6±3%)	0±0 (0±0%)	37	78
All	All	5230/5870 (89%)	5036 (96%)	169 (3%)	25 (0%)	26	74

5 of 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	10
1	C	563	LYS	9

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Mol	Chain	Res	Type	Models (Total)
2	B	60	GLY	1
2	B	119	ASP	1
2	B	14	VAL	1

6.3.2 Protein sidechains [i](#)

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 NMR 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	A	135/175 (77%)	122±3 (91±2%)	13±3 (9±2%)	10	55
1	C	172/175 (98%)	157±2 (91±1%)	15±2 (9±1%)	11	57
2	B	152/166 (92%)	137±1 (90±1%)	15±1 (10±1%)	9	54
All	All	4590/5160 (89%)	4155 (91%)	435 (9%)	10	55

5 of 177 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	254	VAL	10
2	B	35	THR	9
2	B	74	THR	9
2	B	124	THR	9
2	B	127	THR	9

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 83 ligands modelled in this entry, 1 is monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	B	218	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	B	225	-	53,53,53	1.05±0.01	4±1 (7±1%)
3	PCW	B	233	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	B	209	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	C	609	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	603	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	408	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	B	204	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	402	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	C	601	-	53,53,53	1.04±0.01	5±0 (8±0%)
4	17F	B	229	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	605	-	53,53,53	1.06±0.01	5±0 (8±0%)
3	PCW	A	410	-	53,53,53	1.07±0.01	4±0 (7±0%)
4	17F	C	627	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	205	-	53,53,53	1.04±0.01	4±1 (8±1%)
3	PCW	B	216	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	17F	C	629	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	214	-	53,53,53	1.05±0.02	4±0 (7±0%)
3	PCW	B	210	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	618	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	235	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	611	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	B	232	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	202	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	407	-	52,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	C	614	-	53,53,53	1.04±0.01	4±0 (6±0%)

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
3	PCW	B	212	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	B	236	-	52,53,53	0.92±0.01	1±0 (1±0%)
4	17F	B	231	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	224	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	B	234	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	615	-	53,53,53	1.05±0.01	4±0 (6±0%)
7	EWS	B	239	-	30,30,30	2.27±0.00	10±0 (33±0%)
3	PCW	B	208	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	B	223	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	633	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	623	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	607	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	610	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	625	-	53,53,53	1.04±0.01	4±1 (7±1%)
5	GNP	B	237	-	34,34,34	1.42±0.02	5±0 (14±0%)
3	PCW	B	219	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	608	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	17F	B	226	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	604	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	606	-	53,53,53	1.04±0.01	4±0 (8±0%)
3	PCW	B	222	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	A	403	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	B	217	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	602	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	411	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	C	632	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	616	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	201	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	628	-	52,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	B	220	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	626	-	53,53,53	1.04±0.01	5±0 (8±0%)
3	PCW	B	215	-	53,53,53	1.05±0.01	5±0 (9±0%)
4	17F	B	227	-	52,53,53	0.93±0.01	1±0 (1±0%)
3	PCW	B	203	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	631	-	52,53,53	0.92±0.01	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
4	17F	B	228	-	52,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	B	213	-	53,53,53	1.05±0.01	3±0 (6±0%)
3	PCW	C	617	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	404	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	B	206	-	53,53,53	1.05±0.01	4±0 (8±0%)
3	PCW	C	613	-	53,53,53	1.08±0.01	6±0 (10±0%)
3	PCW	C	621	-	53,53,53	1.05±0.01	4±0 (8±0%)
3	PCW	B	207	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	630	-	52,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	401	-	53,53,53	1.04±0.02	4±0 (7±0%)
3	PCW	A	405	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	624	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	221	-	53,53,53	1.07±0.01	5±0 (9±0%)
3	PCW	B	211	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	406	-	53,53,53	1.06±0.01	5±0 (9±0%)
3	PCW	C	622	-	53,53,53	1.06±0.01	4±0 (7±0%)
4	17F	B	230	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	612	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	619	-	53,53,53	1.04±0.01	3±0 (6±0%)
3	PCW	A	409	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	620	-	53,53,53	1.04±0.01	5±0 (8±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	B	218	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	225	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	233	-	59,61,61	2.31±0.01	5±0 (8±0%)
3	PCW	B	209	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	C	609	-	59,61,61	2.32±0.01	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	C	603	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	408	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	204	-	59,61,61	2.77±0.01	9±0 (15±0%)
3	PCW	A	402	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	601	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	B	229	-	54,60,60	1.07±0.04	5±0 (9±0%)
3	PCW	C	605	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	410	-	59,61,61	2.33±0.01	5±0 (8±0%)
4	17F	C	627	-	54,60,60	1.06±0.01	5±0 (9±0%)
3	PCW	B	205	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	216	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	629	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	B	214	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	210	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	618	-	59,61,61	2.33±0.01	5±0 (8±0%)
3	PCW	B	235	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	611	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	B	232	-	54,60,60	1.05±0.03	5±0 (9±0%)
3	PCW	B	202	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	407	-	54,60,60	1.77±0.03	10±1 (17±1%)
3	PCW	C	614	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	212	-	59,61,61	0.84±0.00	1±0 (1±0%)
4	17F	B	236	-	54,60,60	1.05±0.03	5±0 (9±0%)
4	17F	B	231	-	54,60,60	1.06±0.03	5±0 (9±0%)
3	PCW	B	224	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	234	-	59,61,61	2.77±0.01	9±0 (15±0%)
3	PCW	C	615	-	59,61,61	2.32±0.01	5±0 (8±0%)
7	EWS	B	239	-	37,42,42	1.39±0.01	2±0 (5±0%)
3	PCW	B	208	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	223	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	C	633	-	54,60,60	1.04±0.02	4±0 (7±0%)
3	PCW	C	623	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	607	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	610	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	625	-	59,61,61	2.32±0.01	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
5	GNP	B	237	-	47,54,54	0.96±0.01	2±0 (4±0%)
3	PCW	B	219	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	C	608	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	B	226	-	54,60,60	1.07±0.02	5±0 (9±0%)
3	PCW	C	604	-	59,61,61	2.33±0.00	5±0 (8±0%)
3	PCW	C	606	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	222	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	403	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	217	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	602	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	411	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	632	-	54,60,60	1.05±0.03	5±0 (9±0%)
3	PCW	C	616	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	201	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	628	-	54,60,60	1.12±0.03	6±0 (10±0%)
3	PCW	B	220	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	626	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	215	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	B	227	-	54,60,60	1.05±0.02	5±0 (8±0%)
3	PCW	B	203	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	631	-	54,60,60	1.05±0.03	5±0 (9±0%)
4	17F	B	228	-	54,60,60	1.08±0.03	5±1 (9±1%)
3	PCW	B	213	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	617	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	404	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	206	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	C	613	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	C	621	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	207	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	C	630	-	54,60,60	1.80±0.03	10±0 (17±0%)
3	PCW	A	401	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	405	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	624	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	221	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	B	211	-	59,61,61	2.32±0.01	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	406	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	C	622	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	B	230	-	54,60,60	1.10±0.05	5±0 (9±0%)
3	PCW	C	612	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	619	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	409	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	620	-	59,61,61	0.85±0.01	1±0 (1±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	B	218	-	-	0±0,57,57,57	-
3	PCW	C	618	-	-	0±0,57,57,57	-
3	PCW	C	611	-	-	0±0,57,57,57	-
3	PCW	C	614	-	-	0±0,57,57,57	-
3	PCW	B	223	-	-	0±0,57,57,57	-
3	PCW	C	610	-	-	0±0,57,57,57	-
3	PCW	C	606	-	-	0±0,57,57,57	-
3	PCW	B	233	-	-	0±0,57,57,57	-
3	PCW	B	209	-	-	0±0,57,57,57	-
4	17F	B	236	-	-	0±0,59,59,59	-
4	17F	C	631	-	-	0±0,59,59,59	-
4	17F	C	627	-	-	0±0,59,59,59	-
4	17F	C	629	-	-	0±0,59,59,59	-
3	PCW	A	404	-	-	0±0,57,57,57	-
3	PCW	C	623	-	-	0±0,57,57,57	-
4	17F	C	630	-	-	0±0,59,59,59	-
3	PCW	B	208	-	-	0±0,57,57,57	-
4	17F	B	226	-	-	0±0,59,59,59	-
3	PCW	B	205	-	-	0±0,57,57,57	-
7	EWS	B	239	-	-	0±0,12,22,22	1±0,4,4,4
3	PCW	C	613	-	-	0±0,57,57,57	-
3	PCW	C	619	-	-	0±0,57,57,57	-
3	PCW	B	203	-	-	0±0,57,57,57	-
4	17F	B	230	-	-	0±0,59,59,59	-
3	PCW	B	204	-	-	0±0,57,57,57	-
3	PCW	B	213	-	-	0±0,57,57,57	-
3	PCW	C	626	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	409	-	-	0±0,57,57,57	-
3	PCW	B	206	-	-	0±0,57,57,57	-
3	PCW	C	602	-	-	0±0,57,57,57	-
3	PCW	C	608	-	-	0±0,57,57,57	-
3	PCW	C	622	-	-	0±0,57,57,57	-
3	PCW	A	408	-	-	0±0,57,57,57	-
3	PCW	C	617	-	-	0±0,57,57,57	-
3	PCW	B	221	-	-	0±0,57,57,57	-
3	PCW	C	612	-	-	0±0,57,57,57	-
3	PCW	B	212	-	-	0±0,57,57,57	-
3	PCW	C	625	-	-	0±0,57,57,57	-
3	PCW	C	601	-	-	0±0,57,57,57	-
4	17F	B	227	-	-	0±0,59,59,59	-
3	PCW	B	235	-	-	0±0,57,57,57	-
4	17F	C	632	-	-	0±0,59,59,59	-
4	17F	A	407	-	-	0±0,59,59,59	-
3	PCW	A	406	-	-	0±0,57,57,57	-
3	PCW	C	620	-	-	0±0,57,57,57	-
5	GNP	B	237	-	-	0±0,18,38,38	0±0,3,3,3
3	PCW	B	211	-	-	0±0,57,57,57	-
3	PCW	C	621	-	-	0±0,57,57,57	-
3	PCW	C	605	-	-	0±0,57,57,57	-
4	17F	B	228	-	-	0±0,59,59,59	-
3	PCW	C	603	-	-	0±0,57,57,57	-
3	PCW	B	207	-	-	0±0,57,57,57	-
3	PCW	B	219	-	-	0±0,57,57,57	-
3	PCW	B	225	-	-	0±0,57,57,57	-
3	PCW	C	609	-	-	0±0,57,57,57	-
3	PCW	B	224	-	-	0±0,57,57,57	-
3	PCW	A	410	-	-	0±0,57,57,57	-
3	PCW	B	215	-	-	0±0,57,57,57	-
3	PCW	B	222	-	-	0±0,57,57,57	-
3	PCW	B	220	-	-	0±0,57,57,57	-
3	PCW	C	616	-	-	0±0,57,57,57	-
4	17F	C	628	-	-	0±0,59,59,59	-
3	PCW	B	202	-	-	0±0,57,57,57	-
3	PCW	A	405	-	-	0±0,57,57,57	-
3	PCW	C	604	-	-	0±0,57,57,57	-
3	PCW	C	615	-	-	0±0,57,57,57	-
4	17F	B	231	-	-	0±0,59,59,59	-
3	PCW	B	201	-	-	0±0,57,57,57	-
3	PCW	B	214	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	B	210	-	-	0±0,57,57,57	-
3	PCW	C	624	-	-	0±0,57,57,57	-
3	PCW	B	216	-	-	0±0,57,57,57	-
3	PCW	B	217	-	-	0±0,57,57,57	-
4	17F	B	229	-	-	0±0,59,59,59	-
3	PCW	A	411	-	-	0±0,57,57,57	-
3	PCW	A	401	-	-	0±0,57,57,57	-
4	17F	B	232	-	-	0±0,59,59,59	-
3	PCW	B	234	-	-	0±0,57,57,57	-
4	17F	C	633	-	-	0±0,59,59,59	-
3	PCW	C	607	-	-	0±0,57,57,57	-
3	PCW	A	403	-	-	0±0,57,57,57	-
3	PCW	A	402	-	-	0±0,57,57,57	-

5 of 312 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
7	B	239	EWS	CAV-CBA	6.58	1.34	1.45	8	10
7	B	239	EWS	CAI-CAJ	5.02	1.39	1.51	8	10
5	B	237	GNP	PG-O1G	4.61	1.53	1.46	4	10
7	B	239	EWS	CAV-CAU	3.94	1.36	1.41	2	10
5	B	237	GNP	PG-O3G	3.36	1.47	1.56	4	10

5 of 371 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	210	PCW	C8-N-C7	12.13	77.11	108.98	10	10
3	A	409	PCW	C8-N-C7	12.06	77.30	108.98	6	10
3	C	604	PCW	C8-N-C7	12.02	77.40	108.98	7	10
3	C	612	PCW	C8-N-C7	12.02	77.41	108.98	7	10
3	A	408	PCW	C8-N-C7	12.01	77.42	108.98	1	10

There are no chirality outliers.

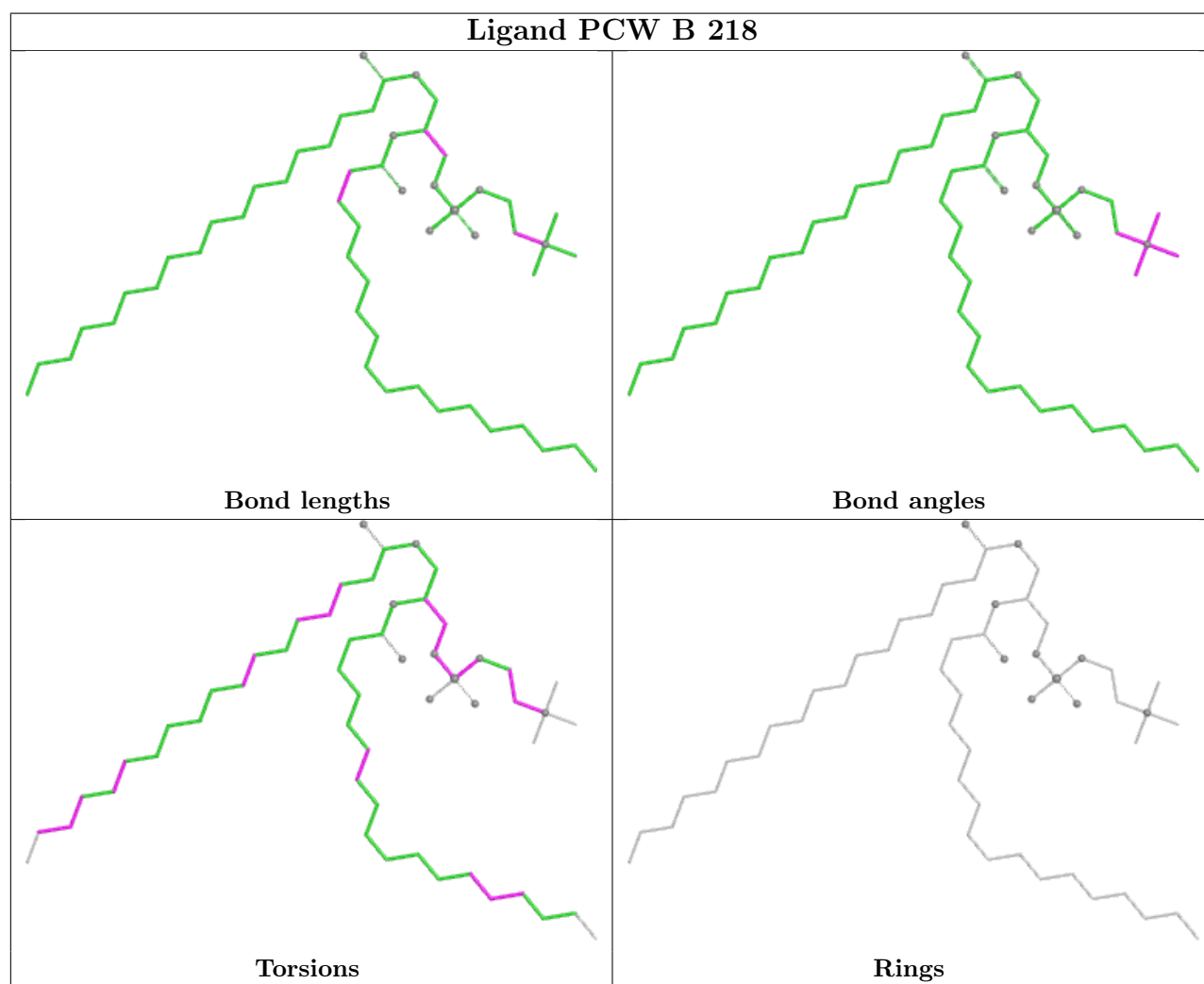
All unique torsion outliers are listed below.

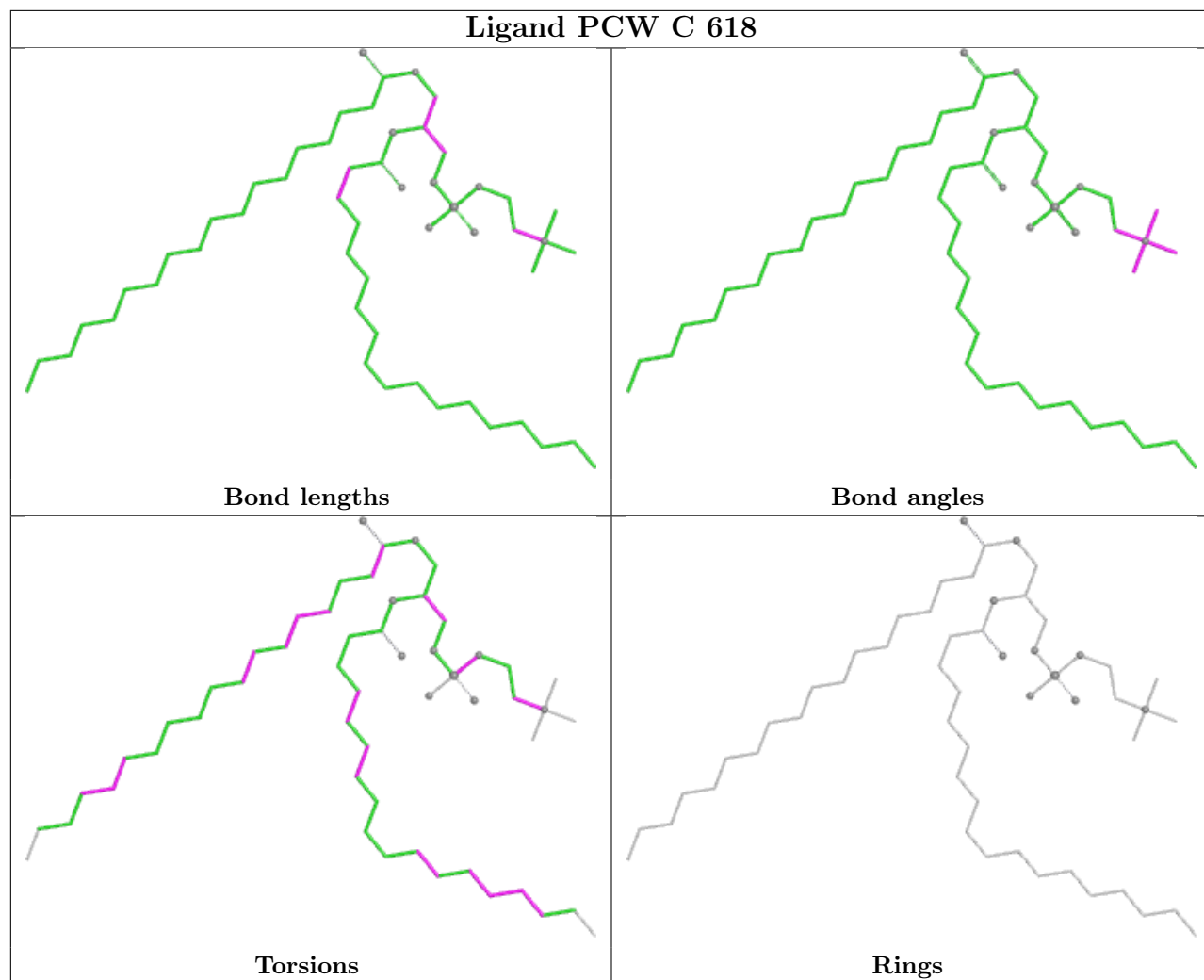
Mol	Chain	Res	Type	Atoms	Models (Total)
5	B	237	GNP	PG-N3B-PB-O1B	1

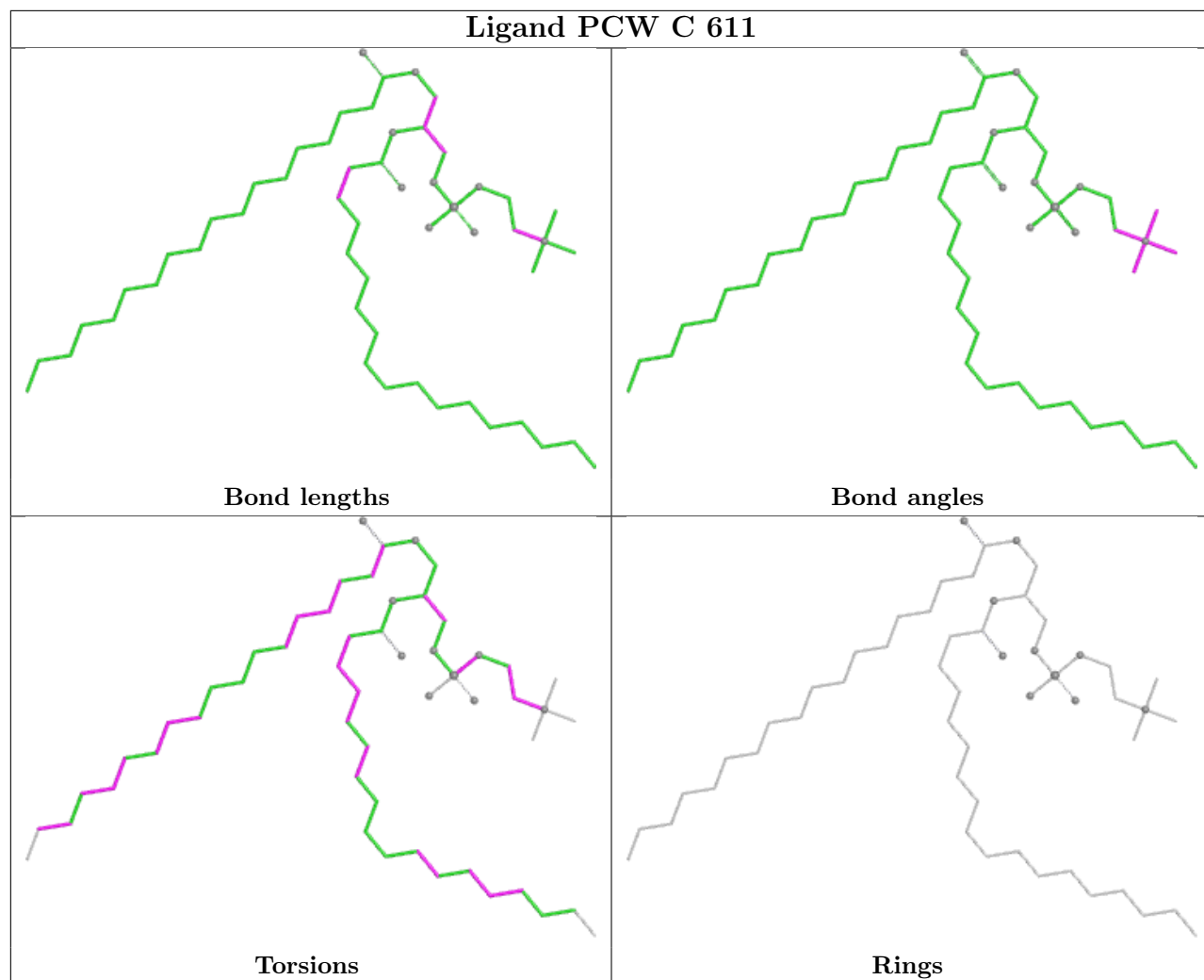
All unique ring outliers are listed below.

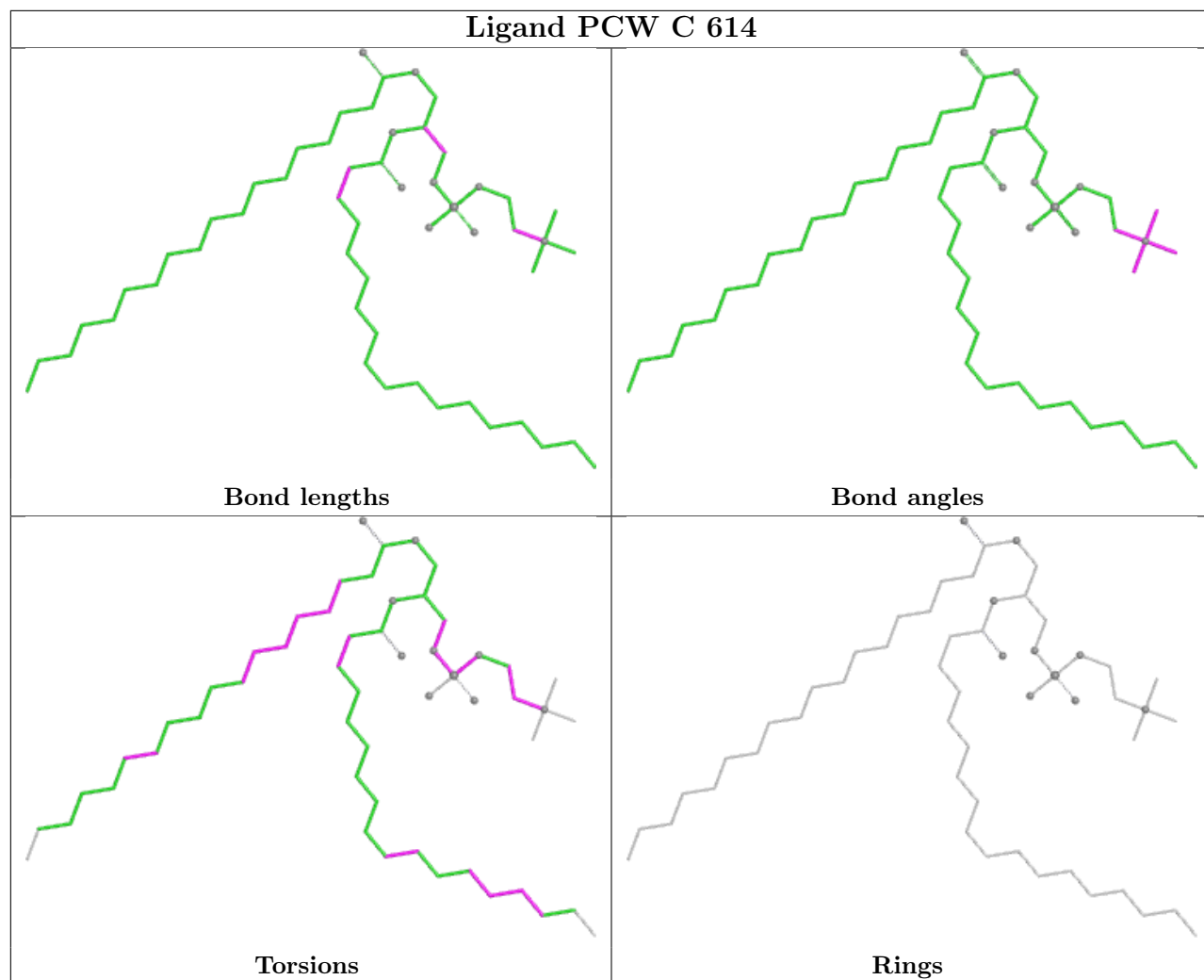
Mol	Chain	Res	Type	Atoms	Models (Total)
7	B	239	EWS	CAC-CAD-CAE-CAF-CAH-NAG	10

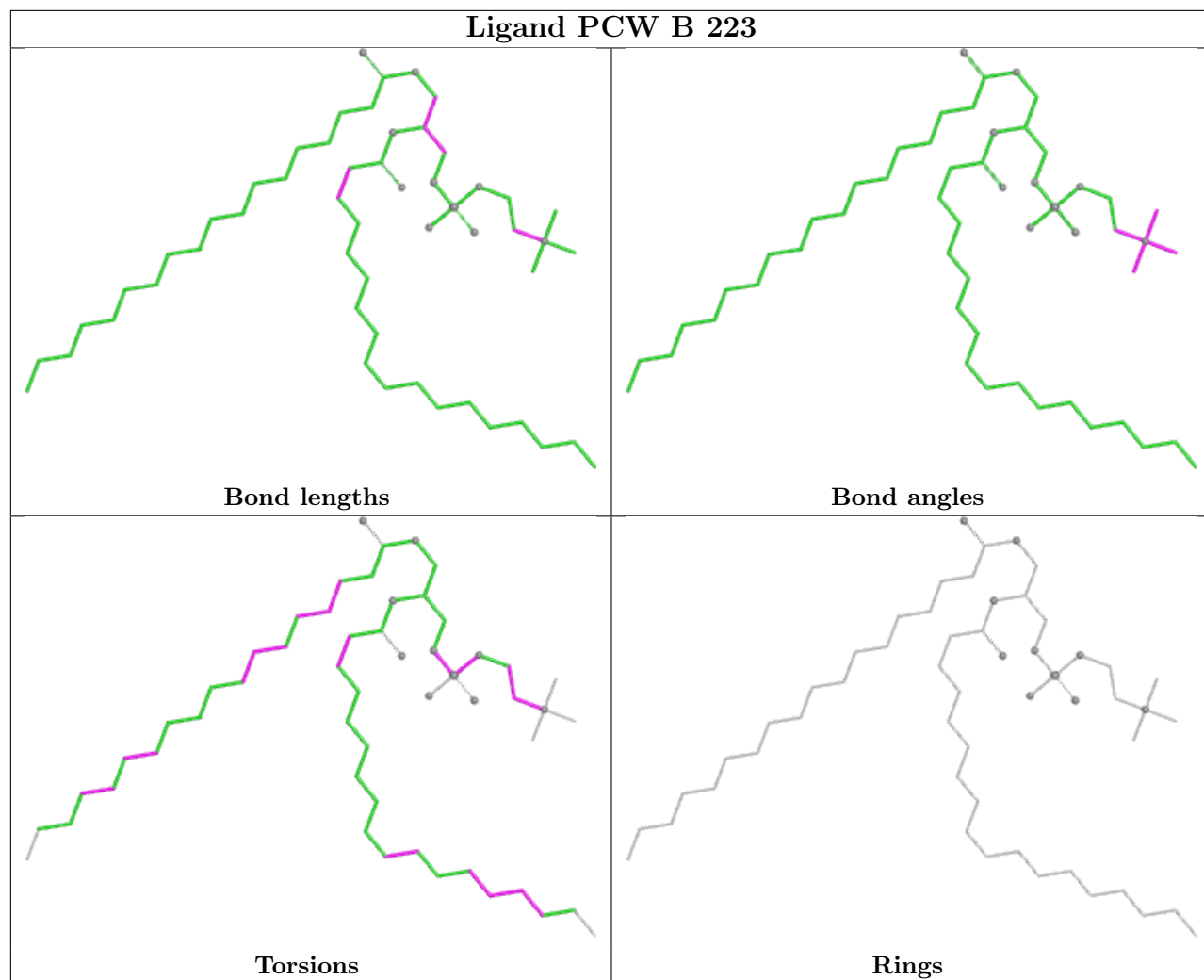
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

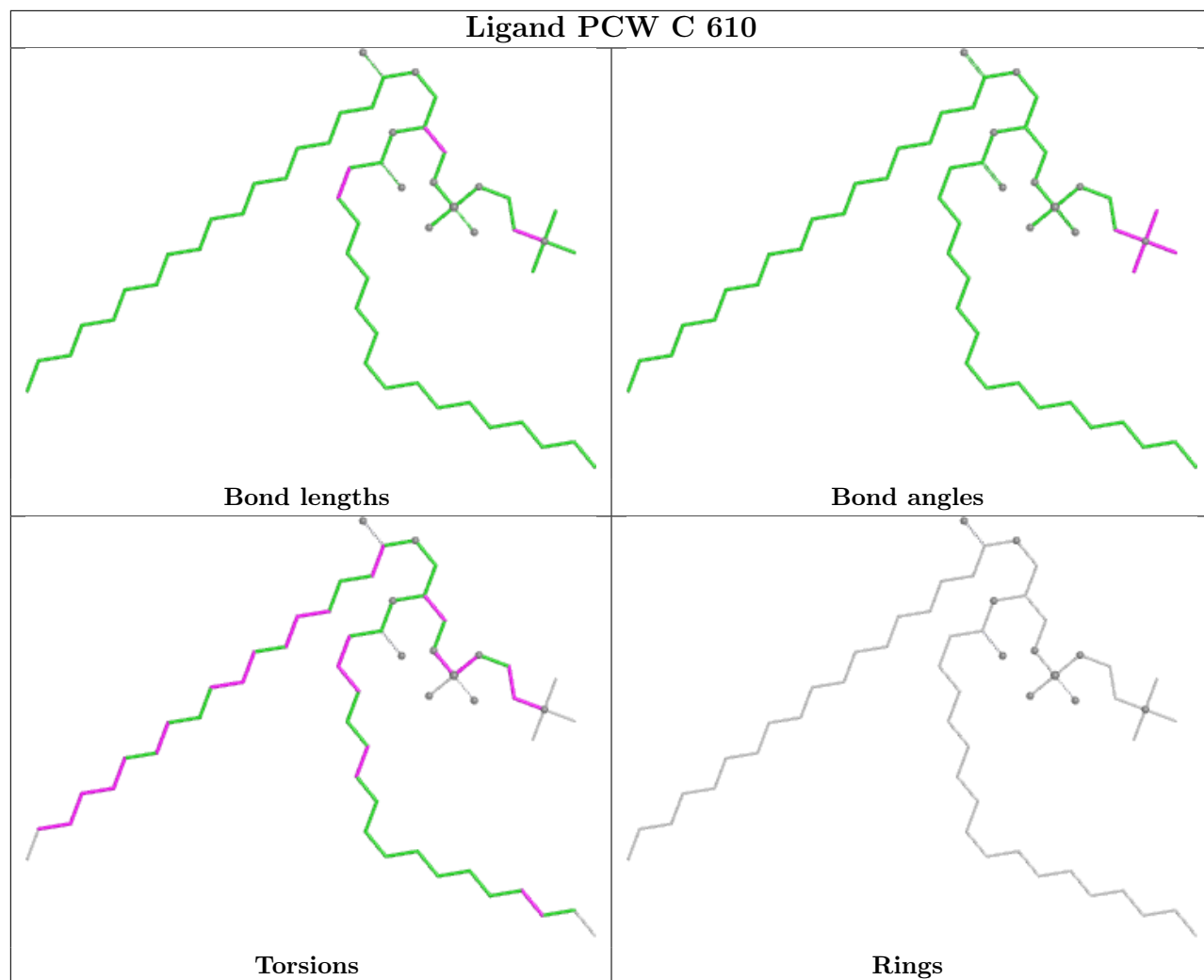


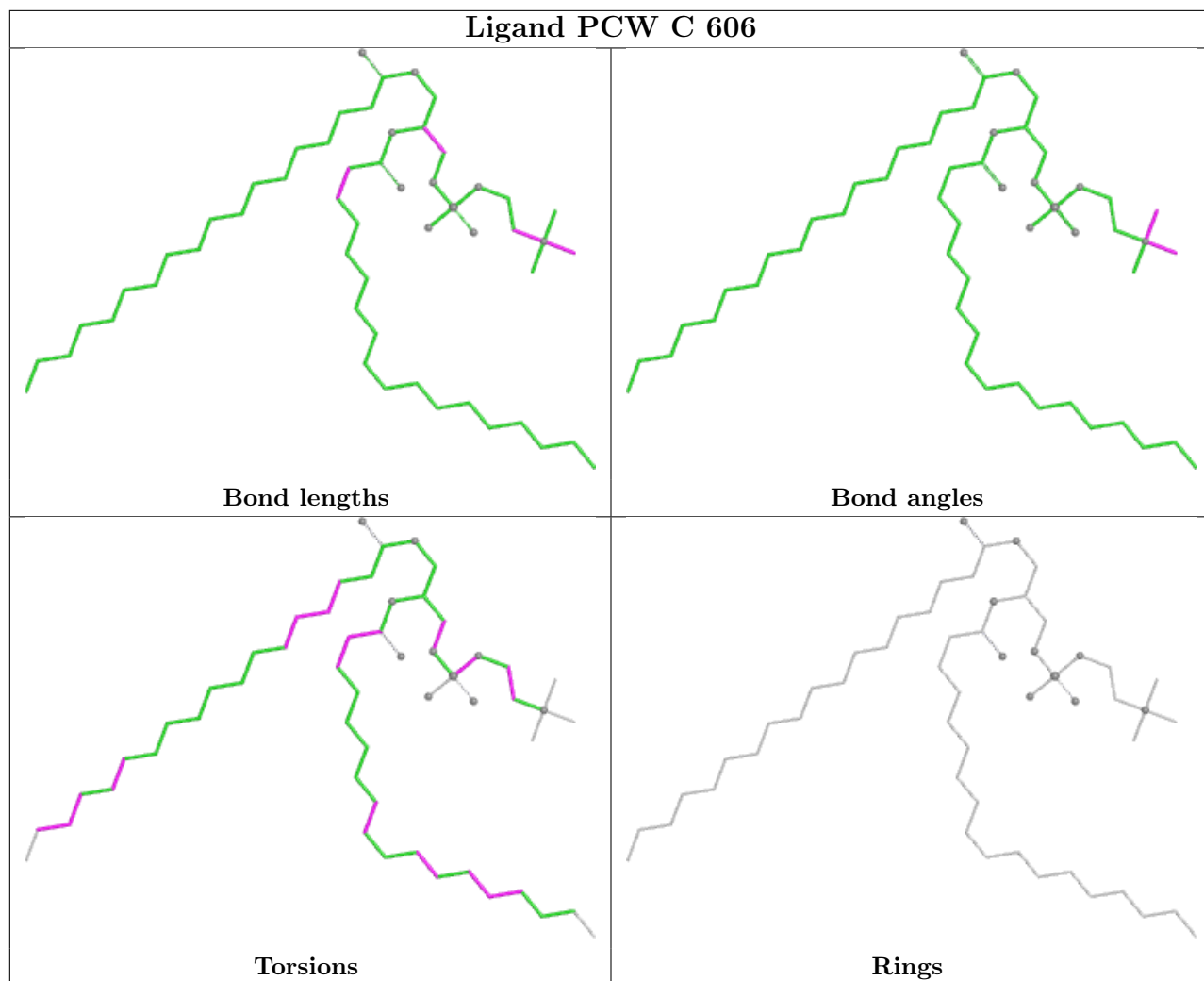


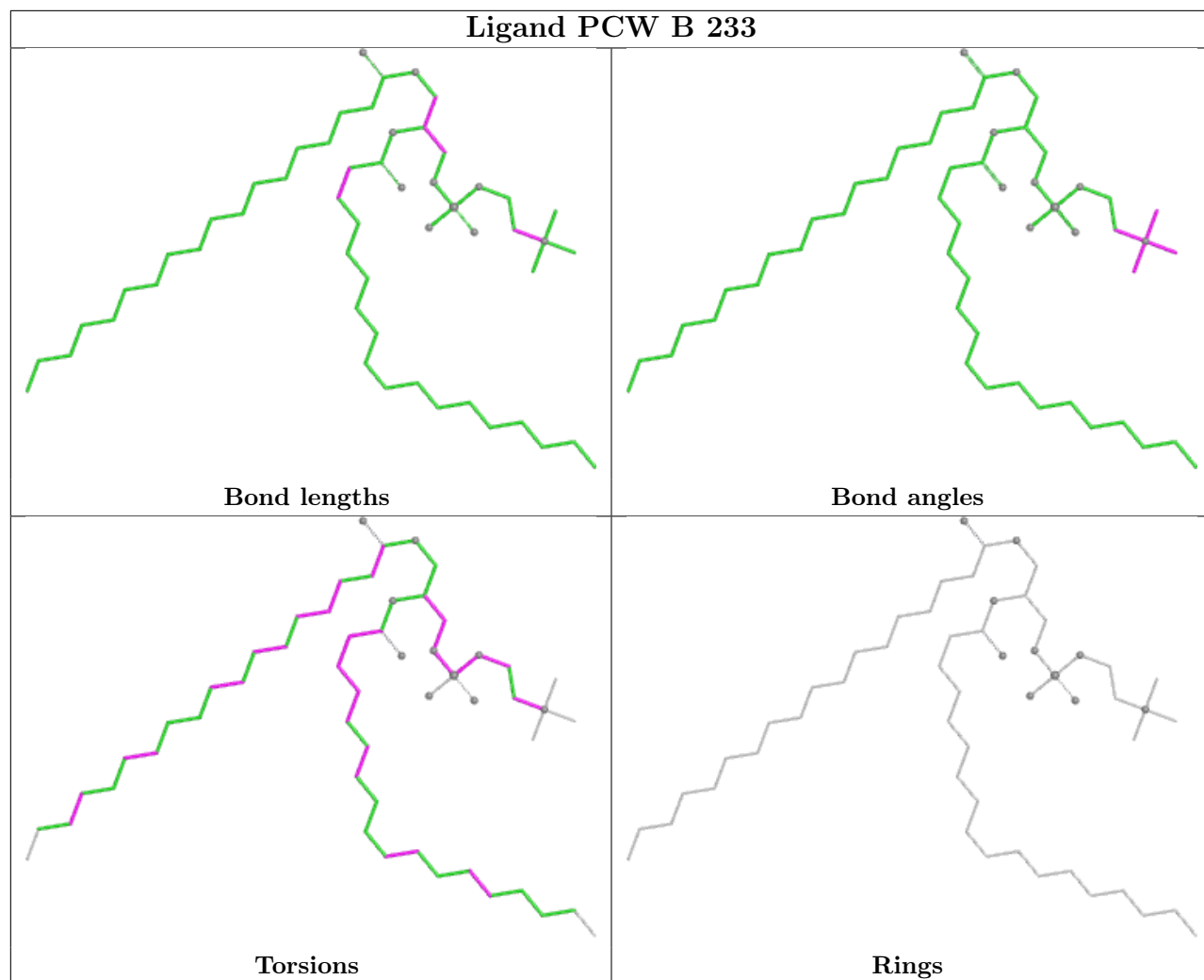


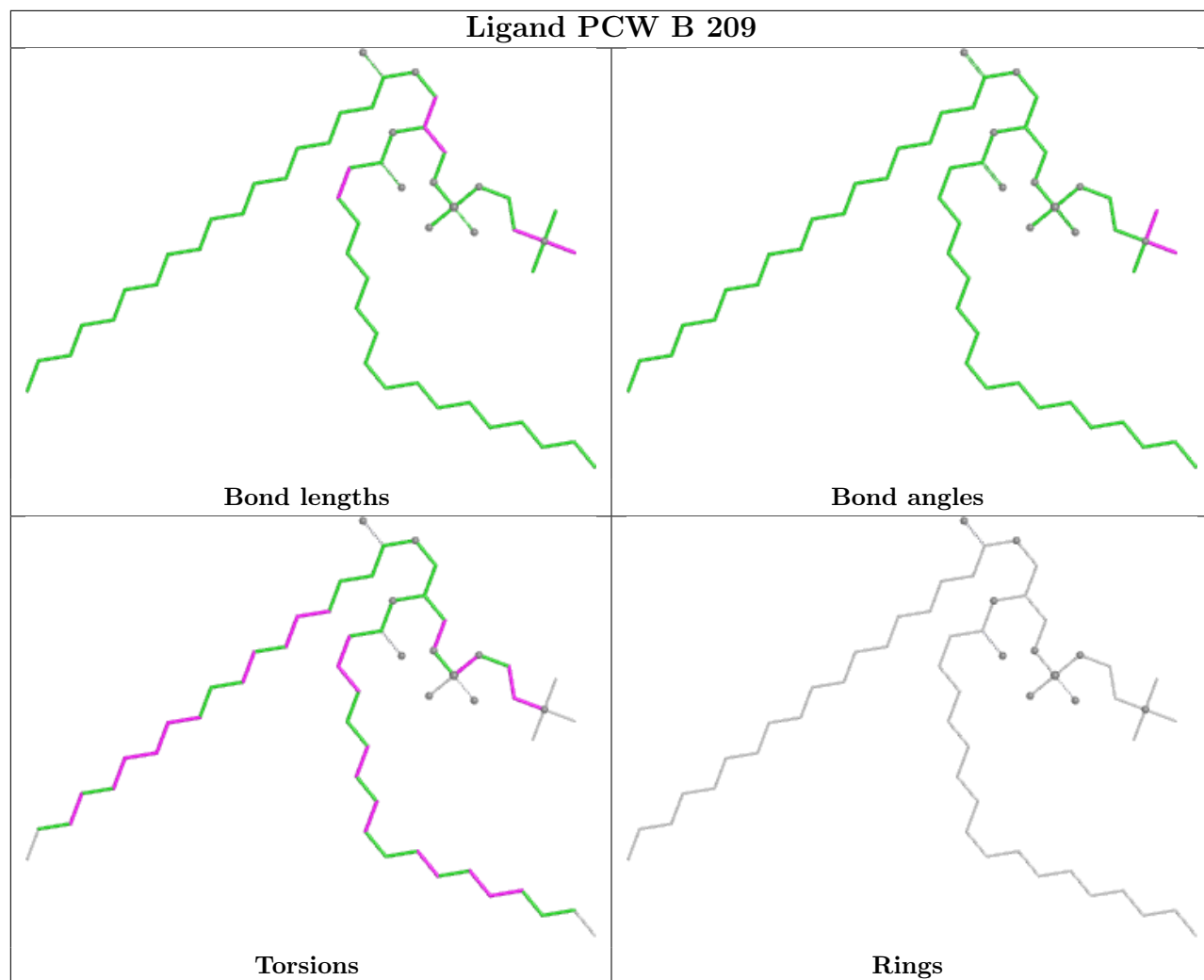


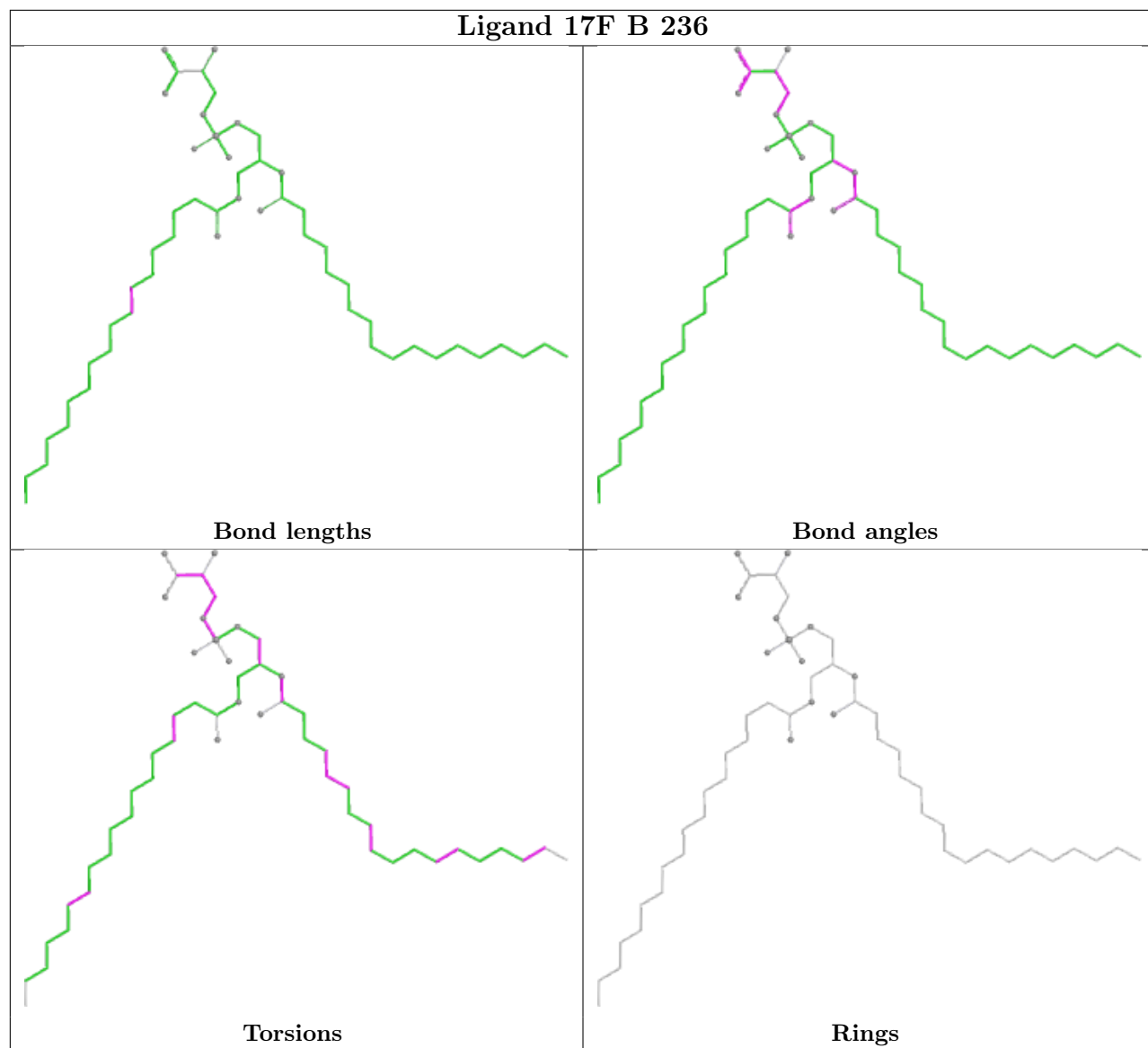


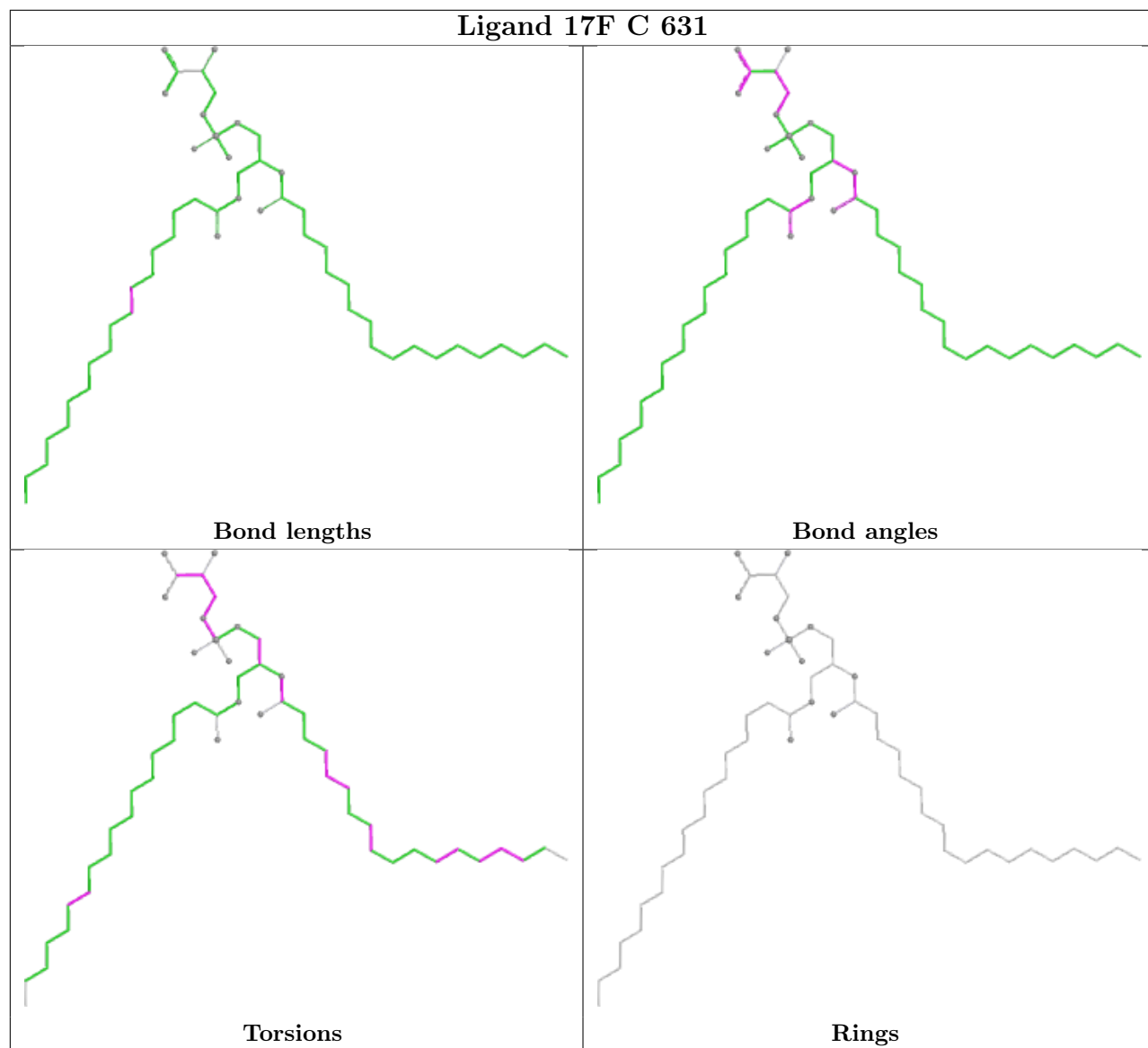


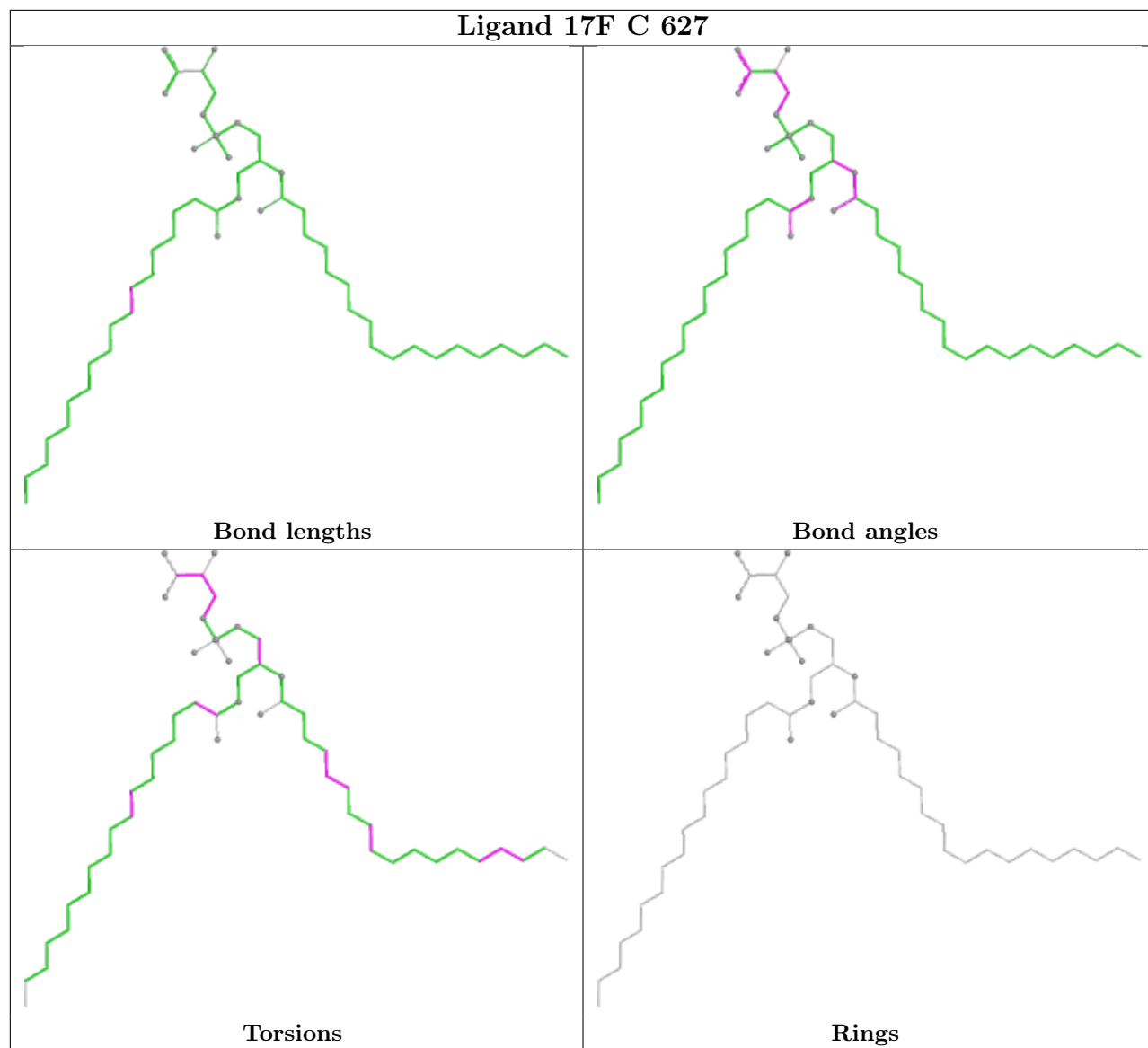


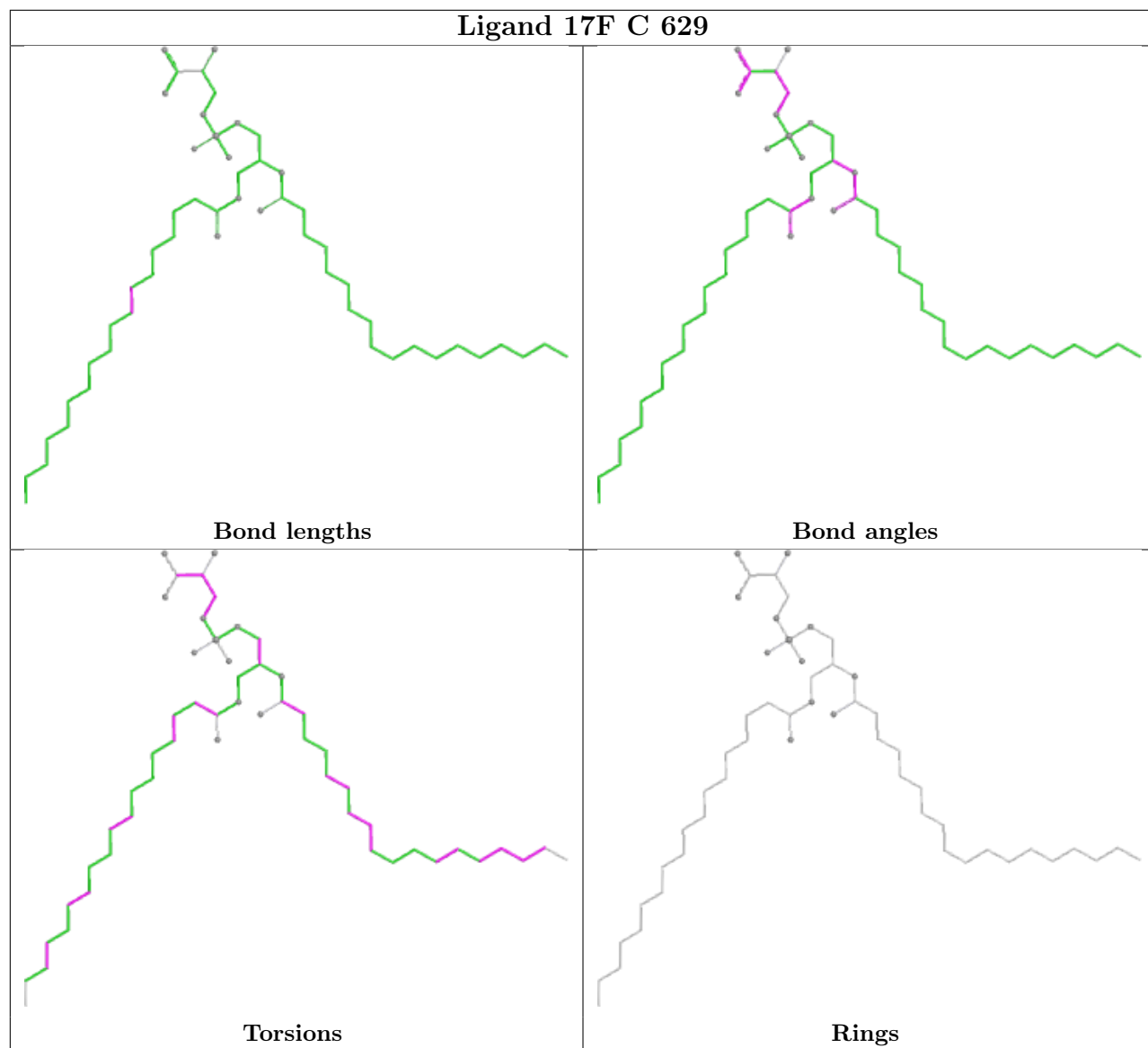


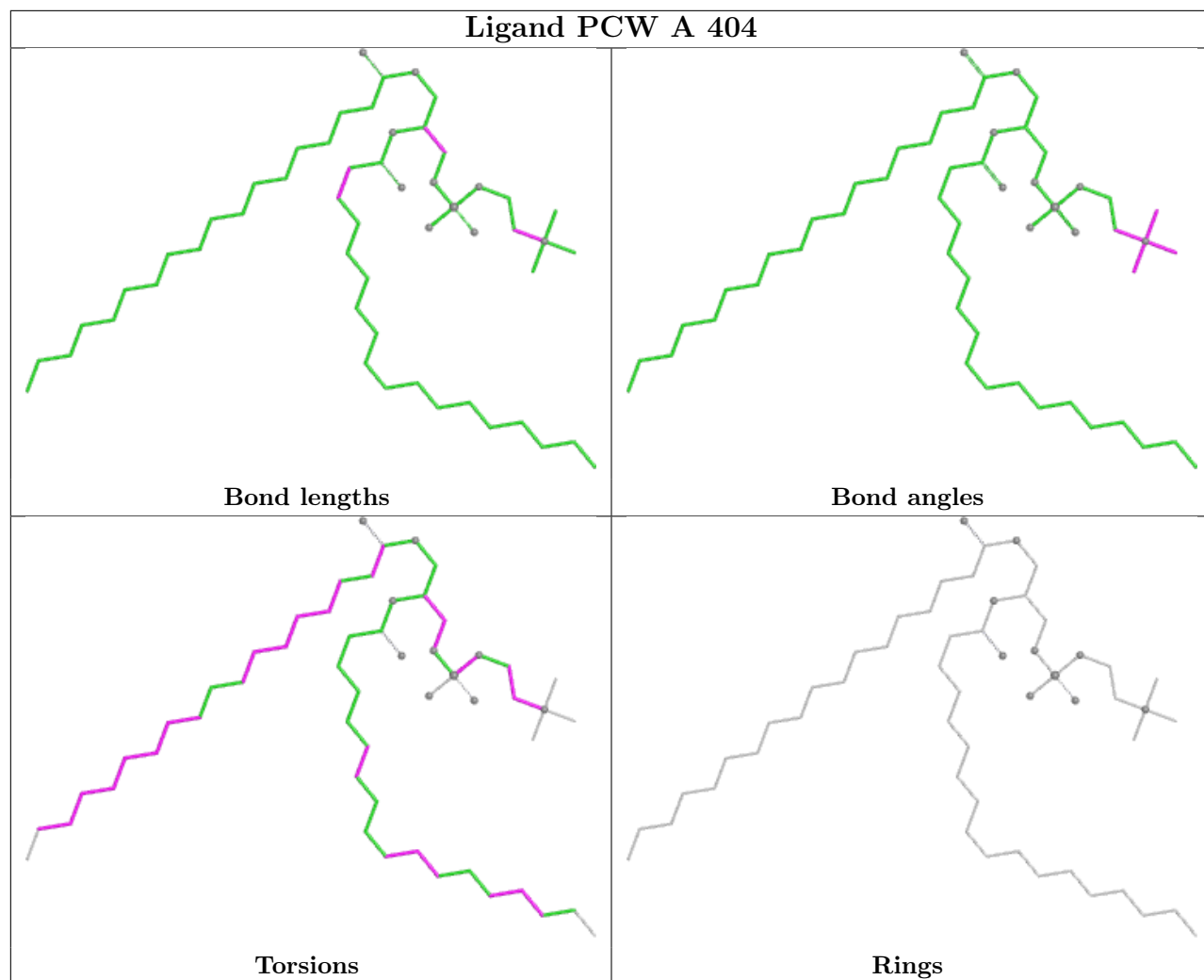


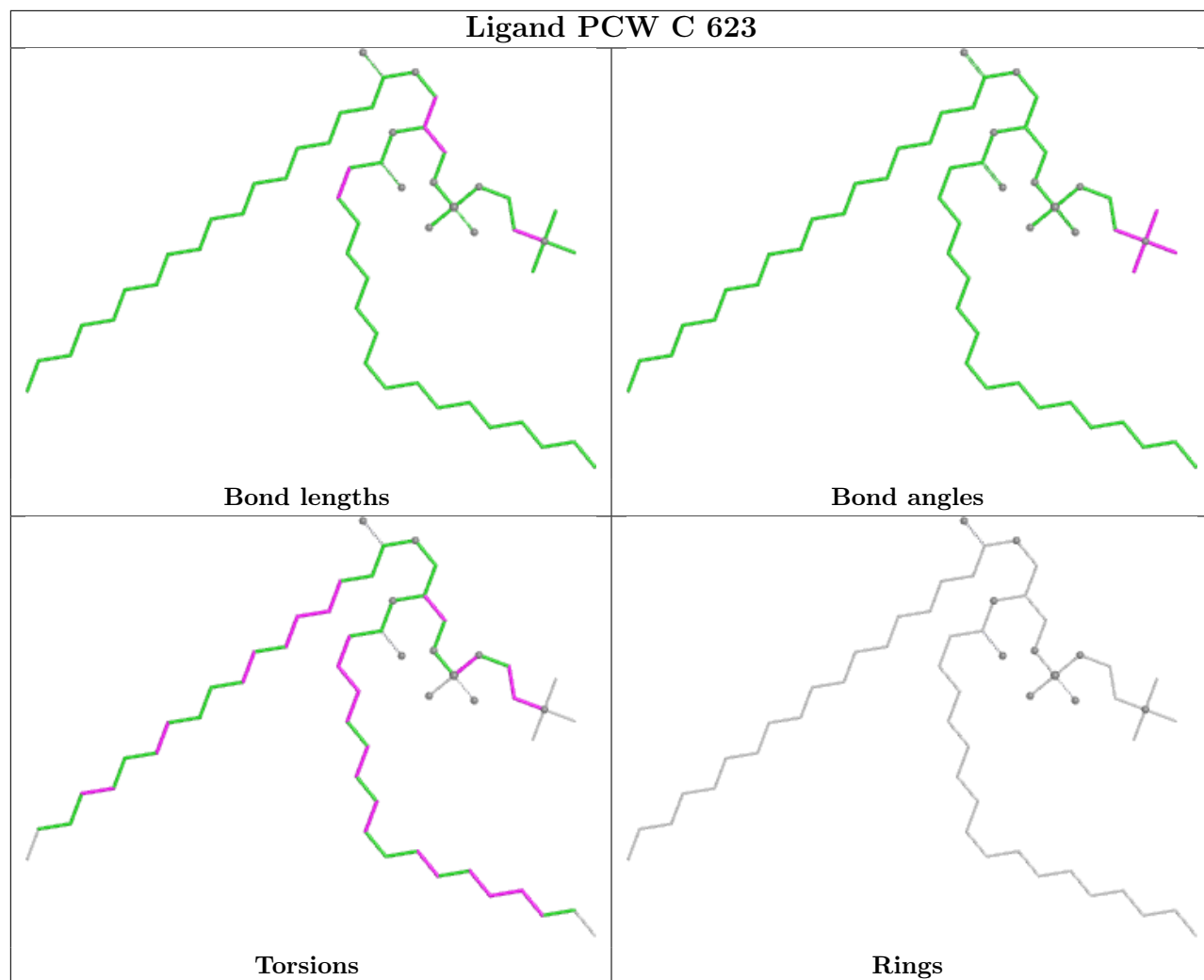


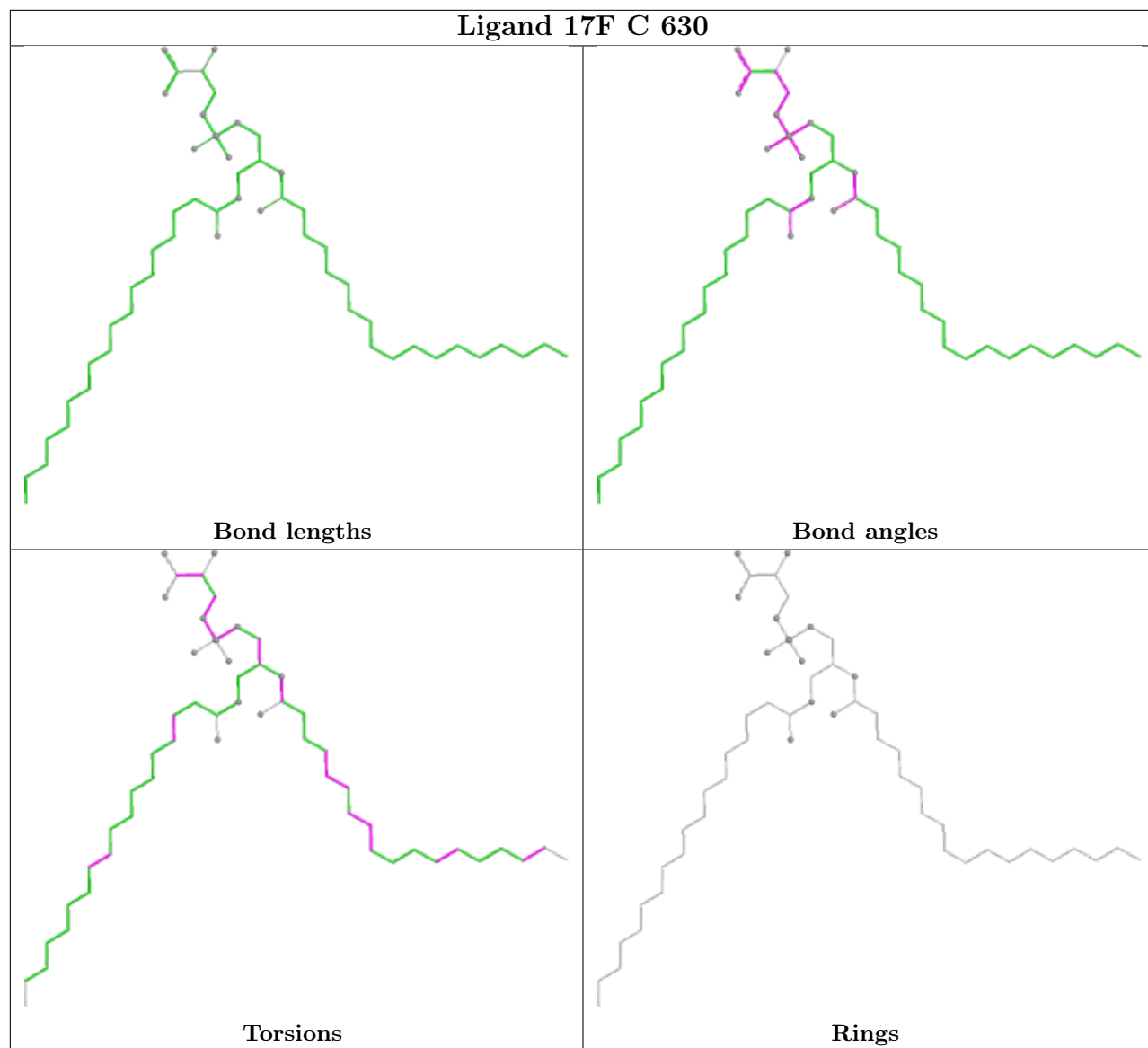


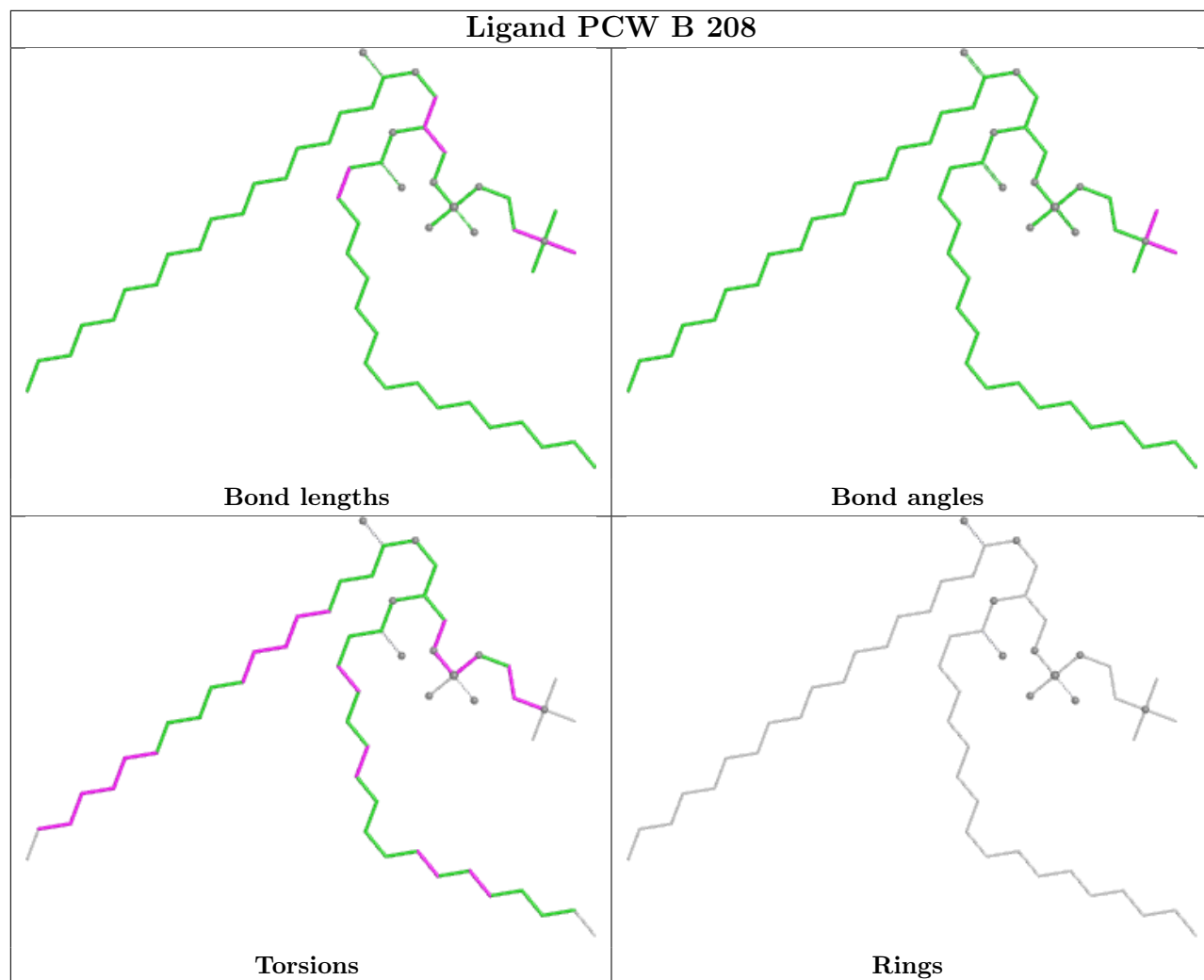


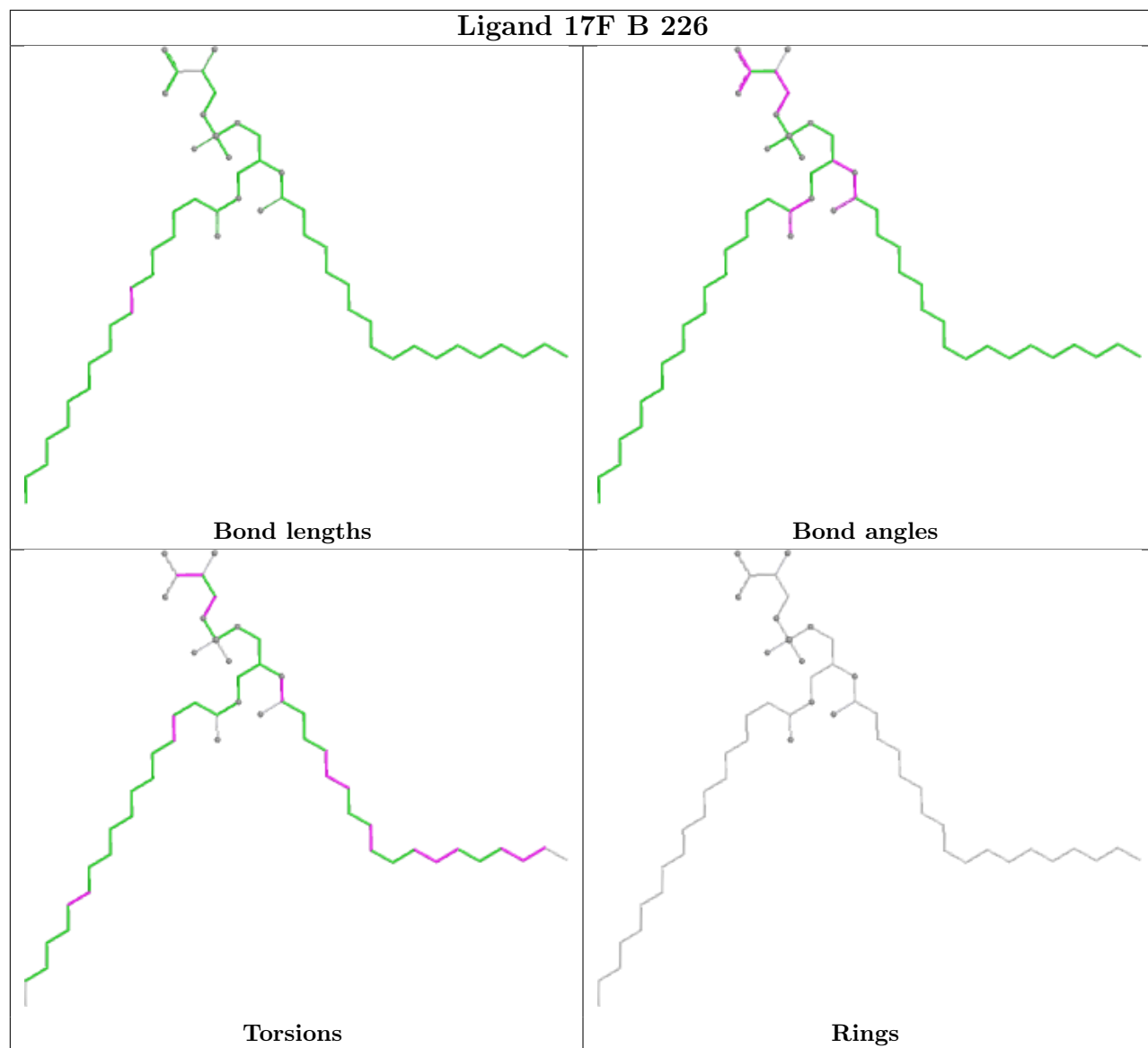


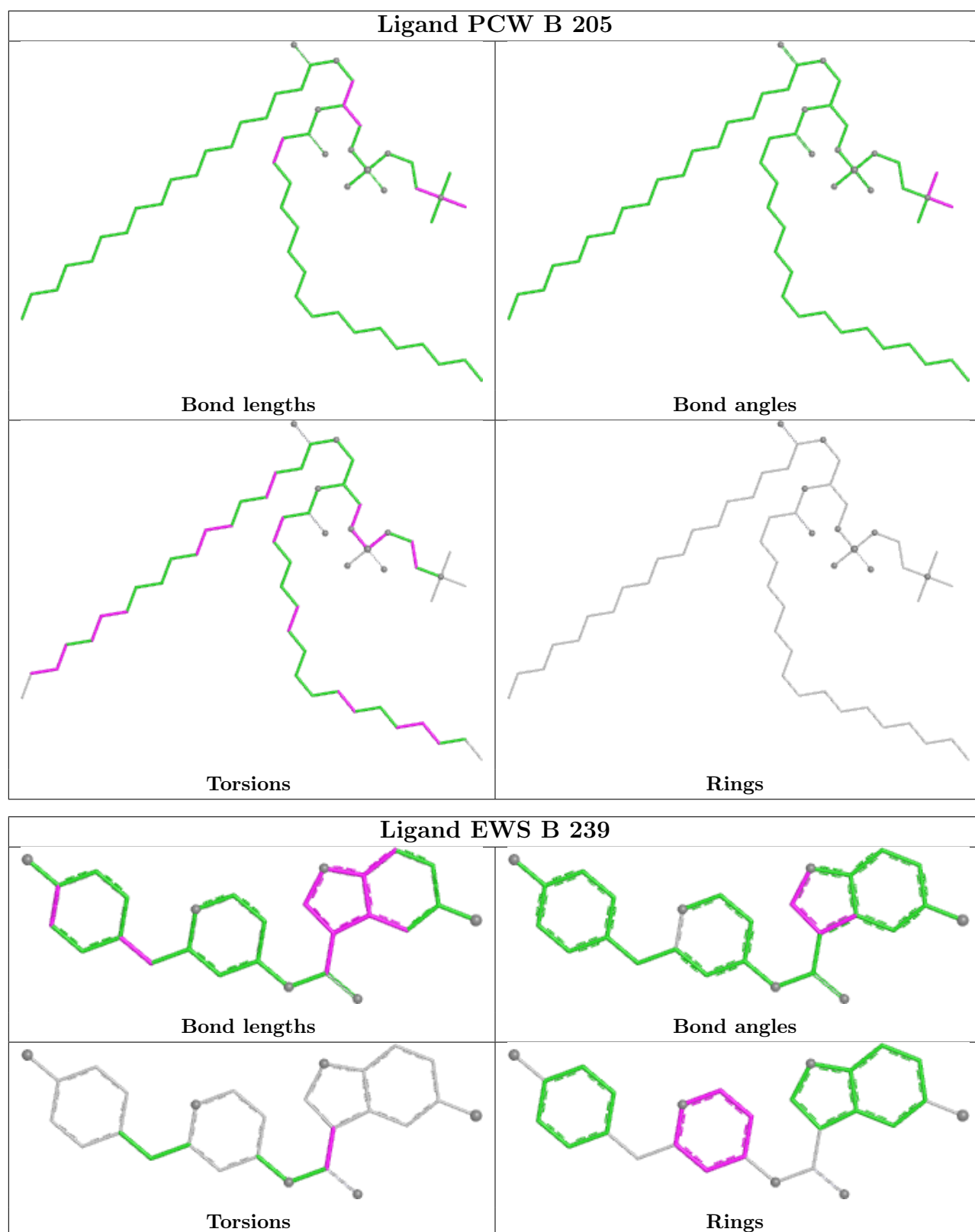


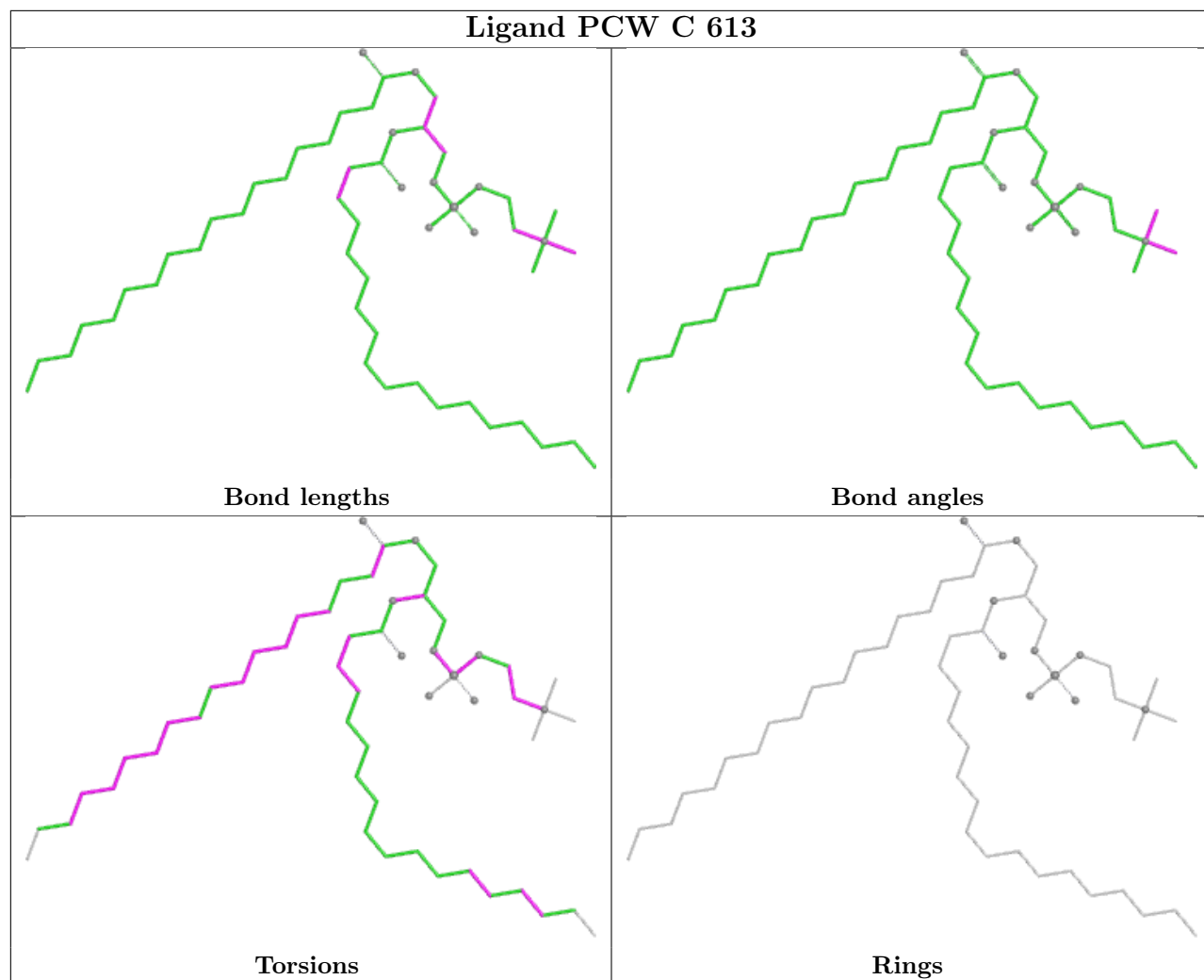


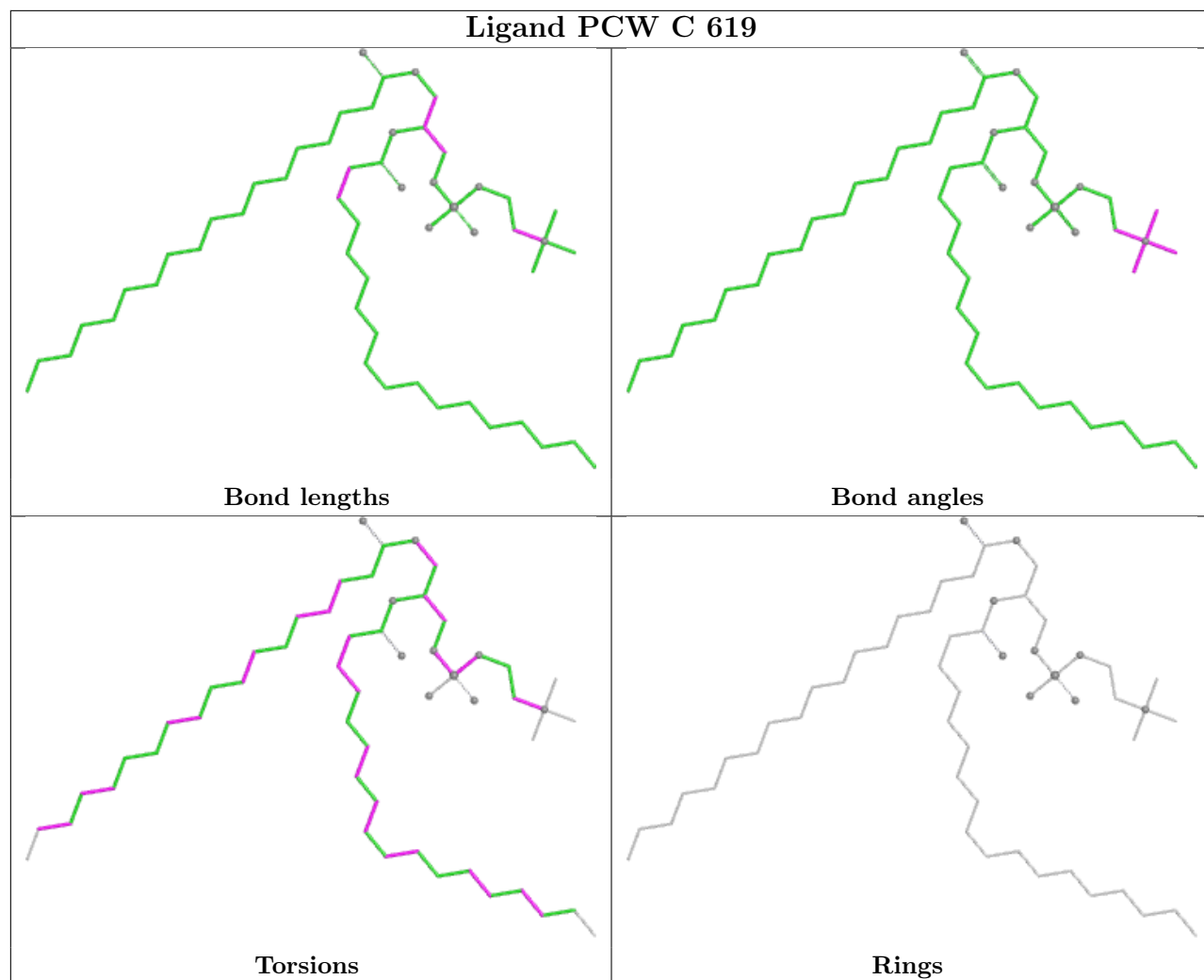


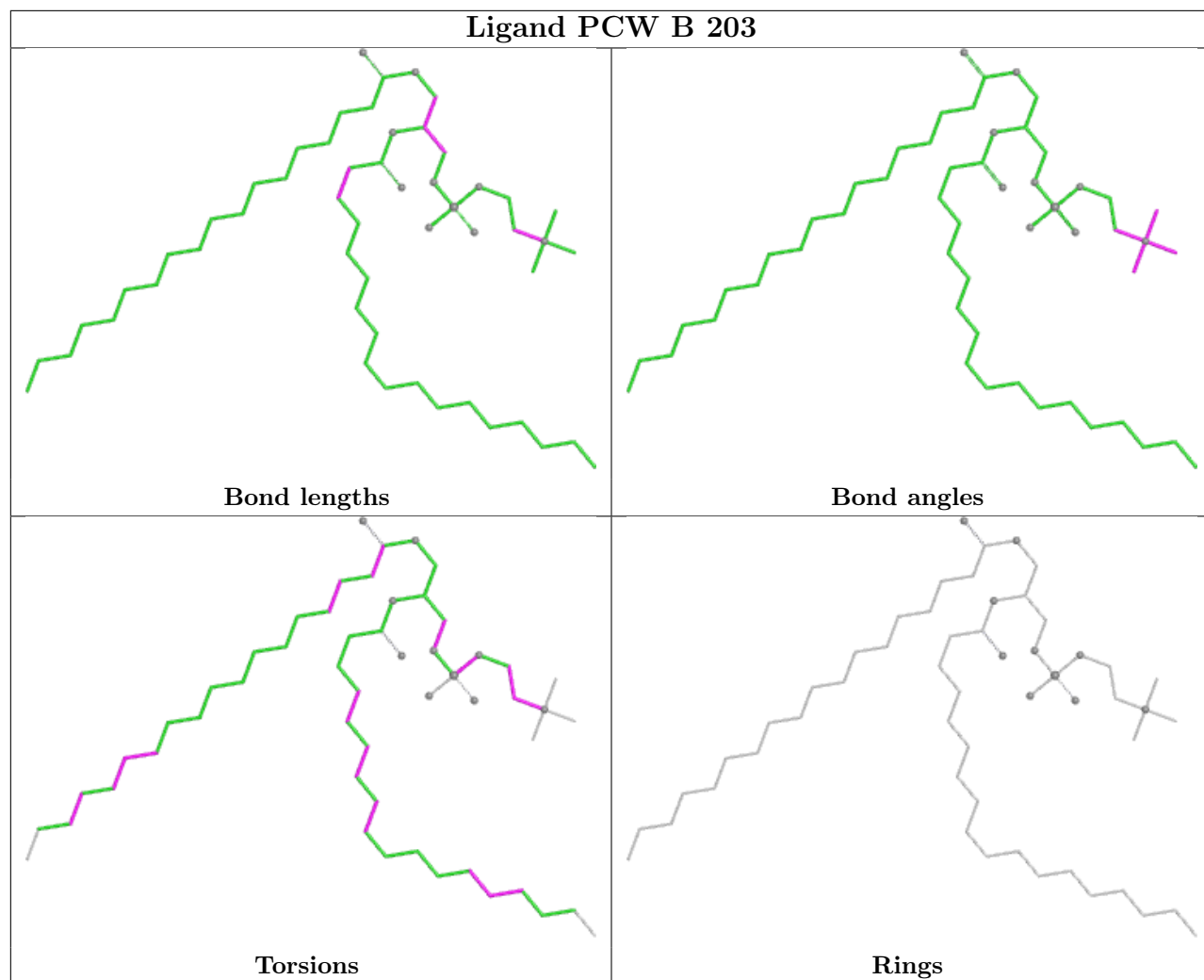


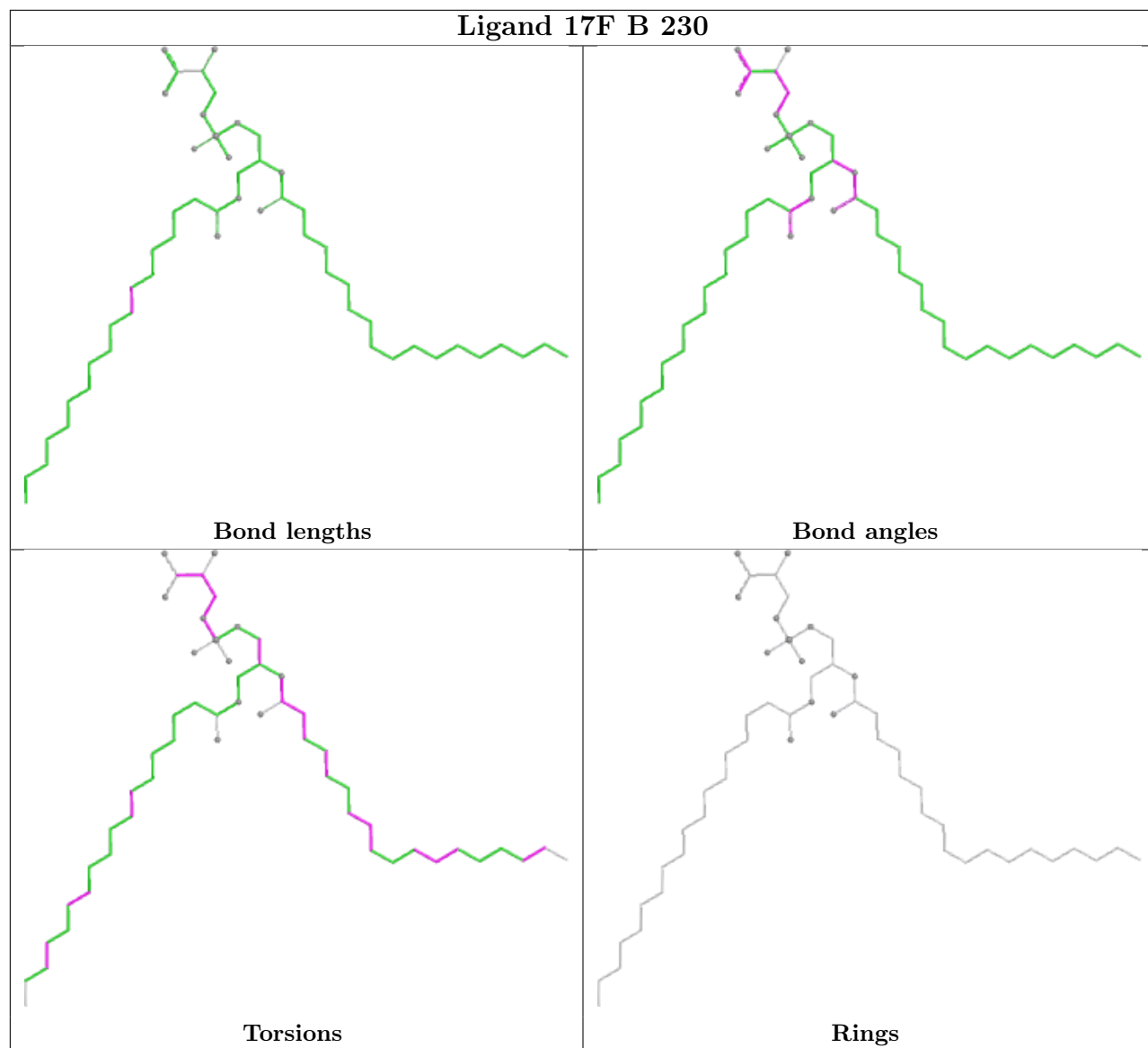


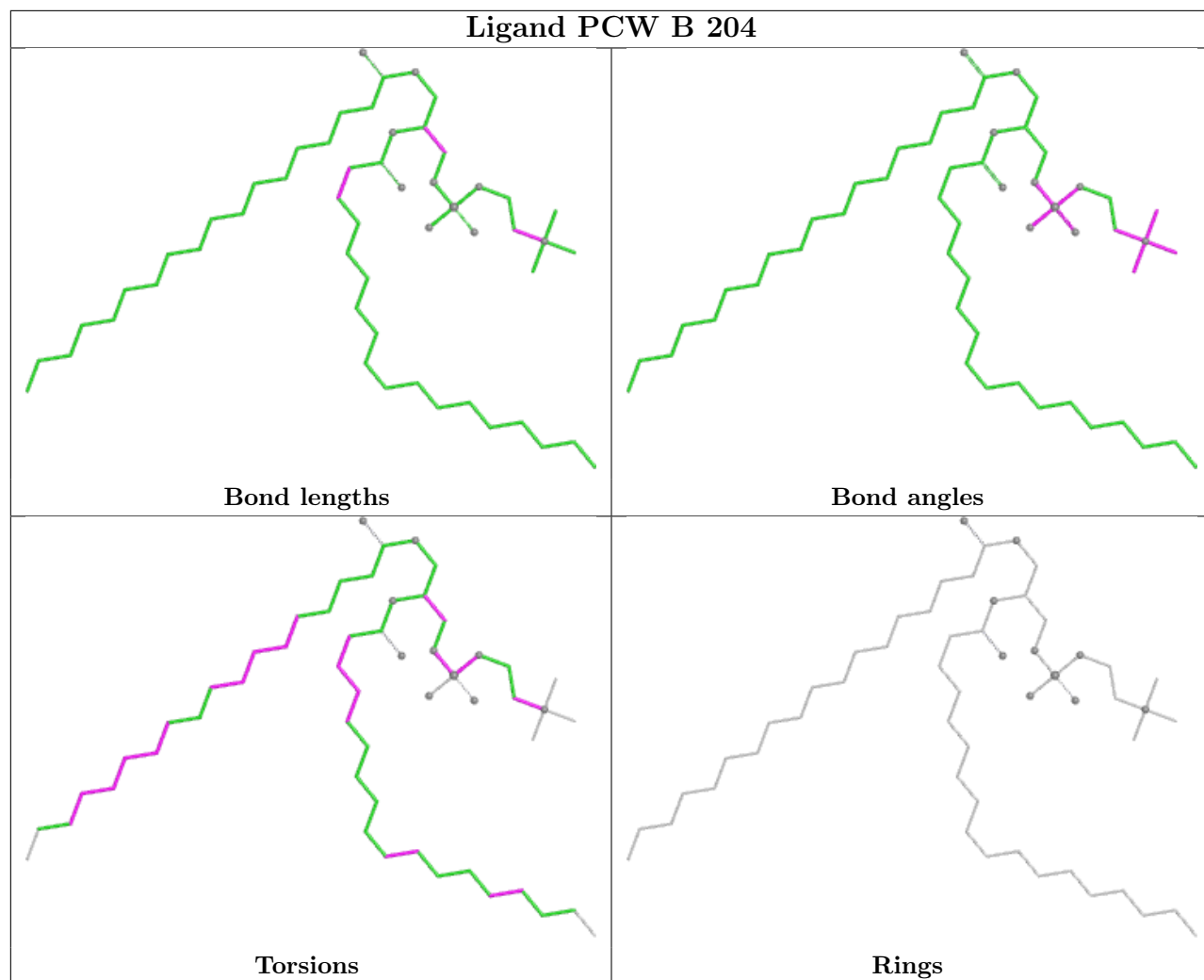


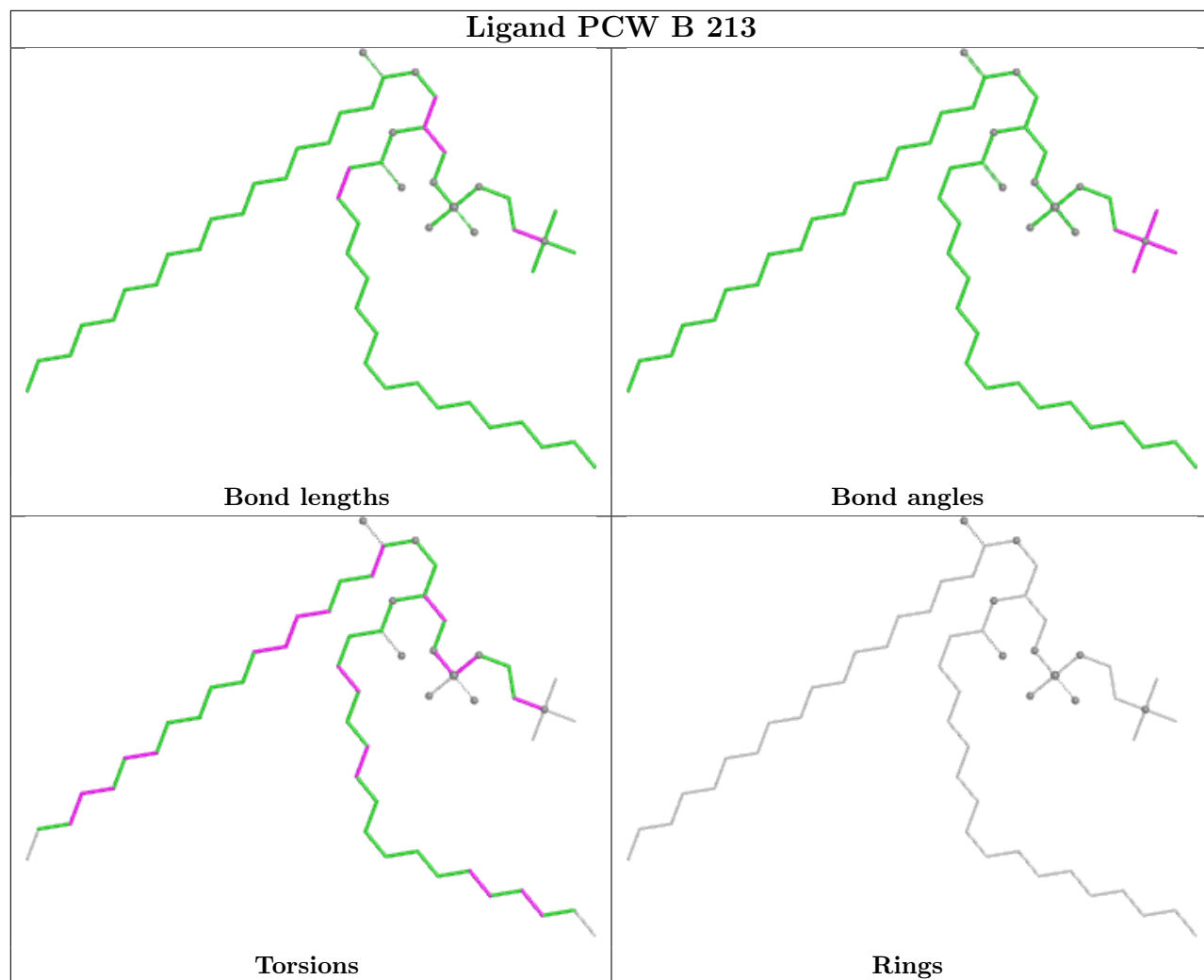


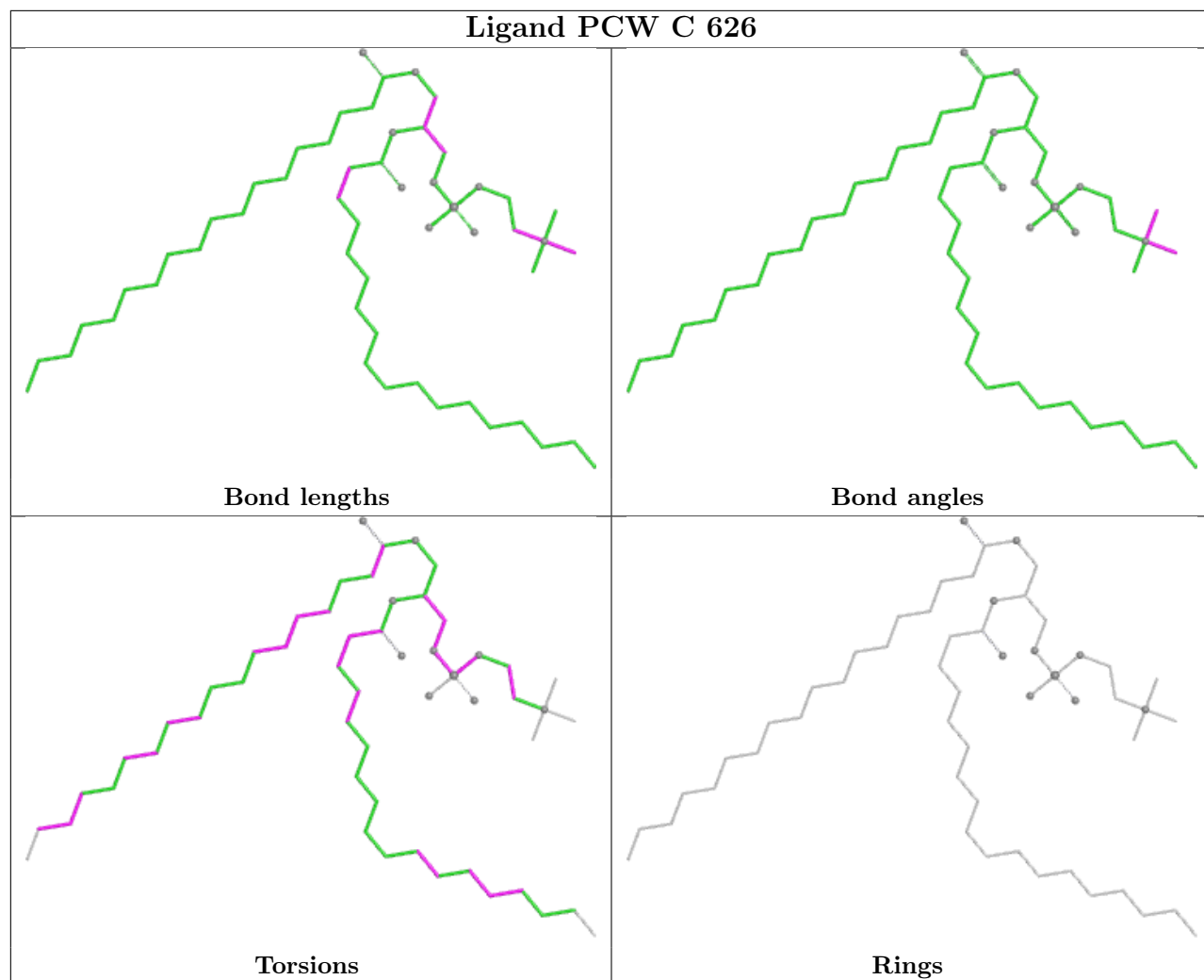


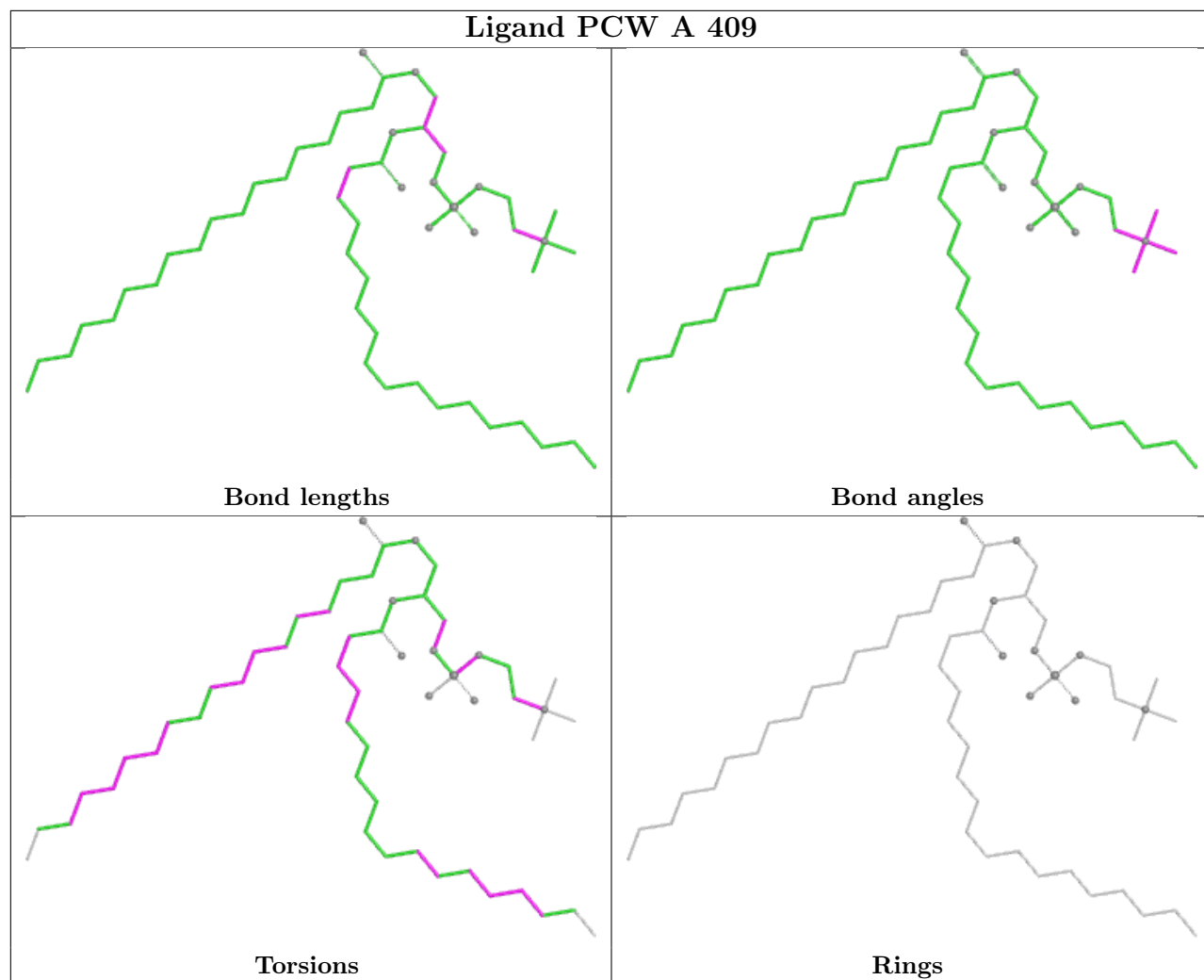


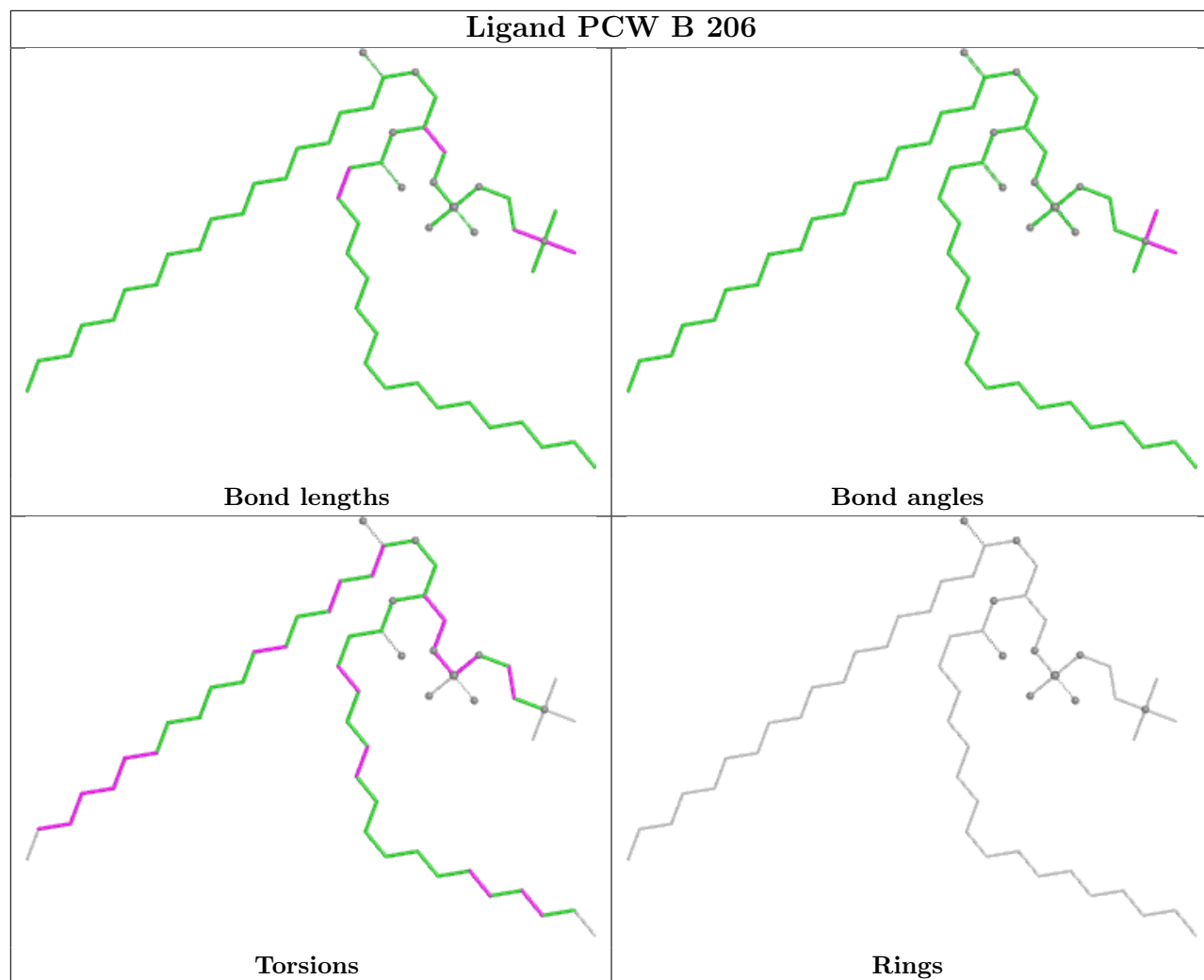


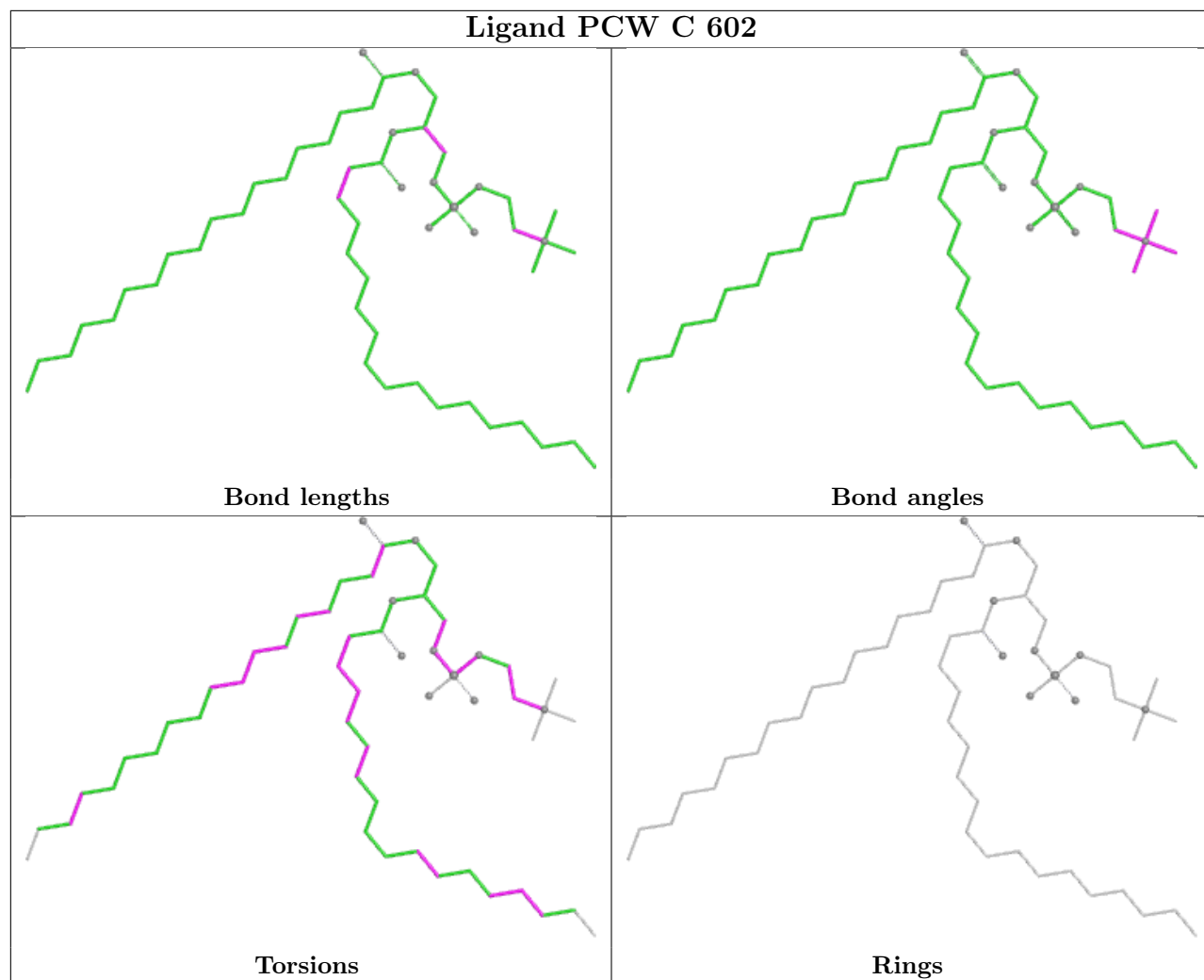


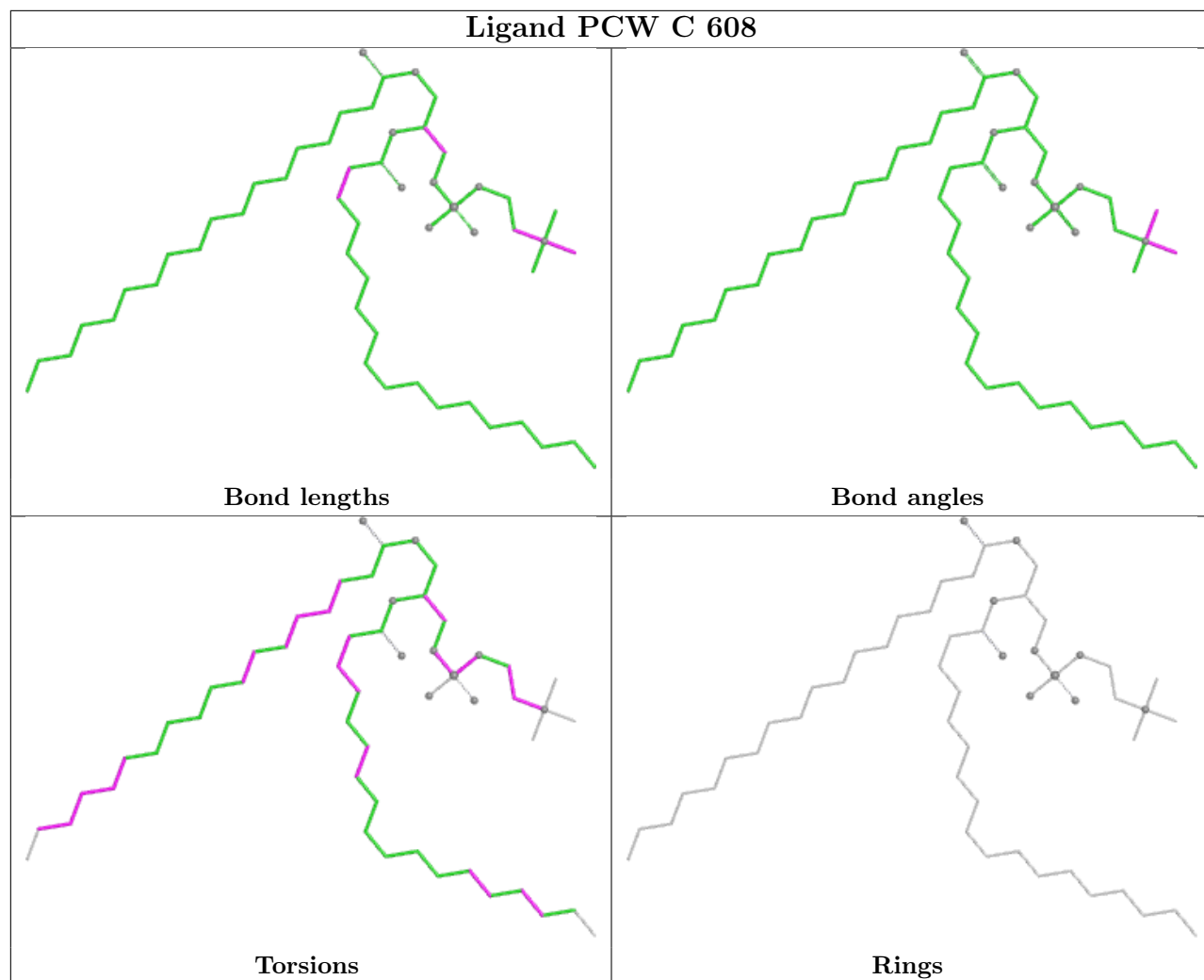


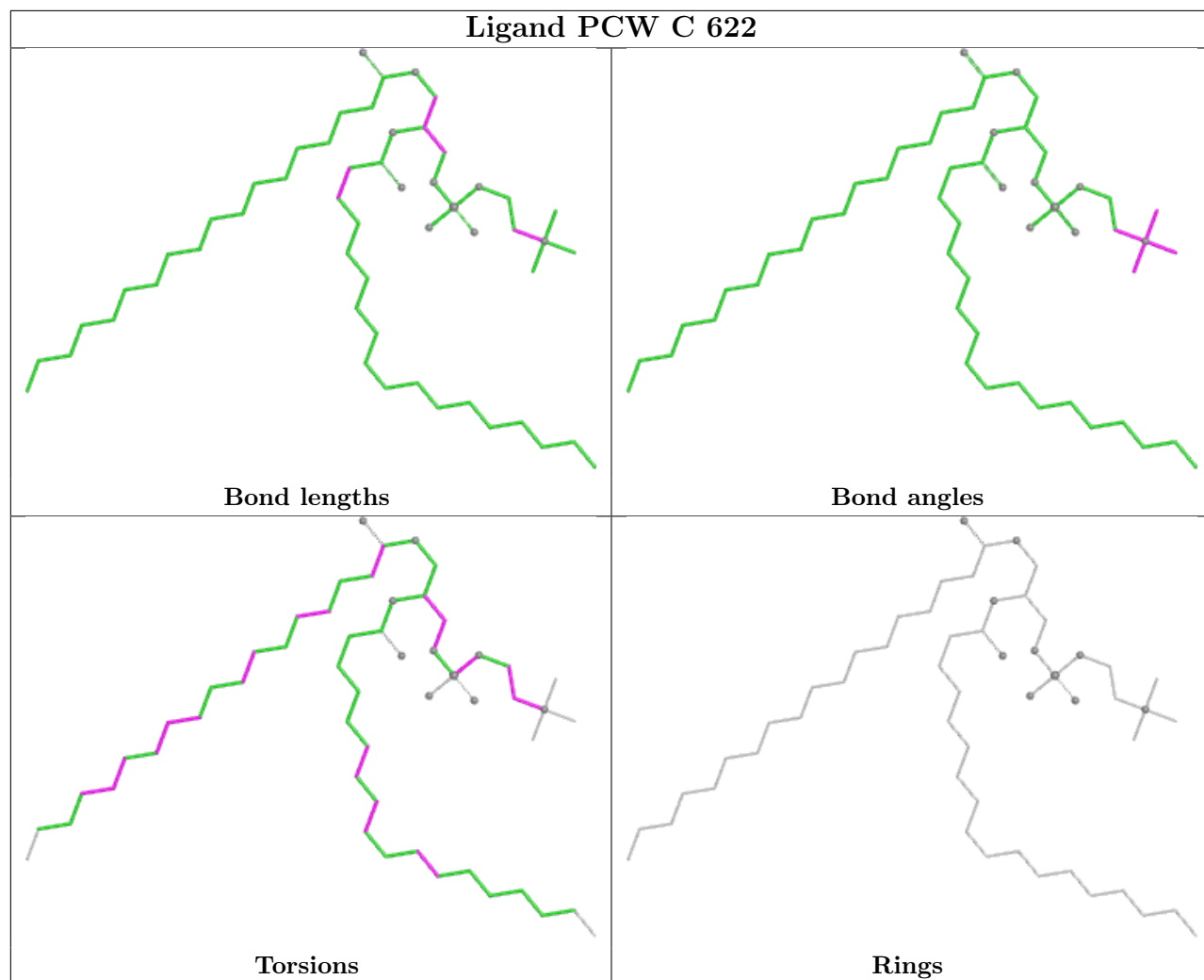


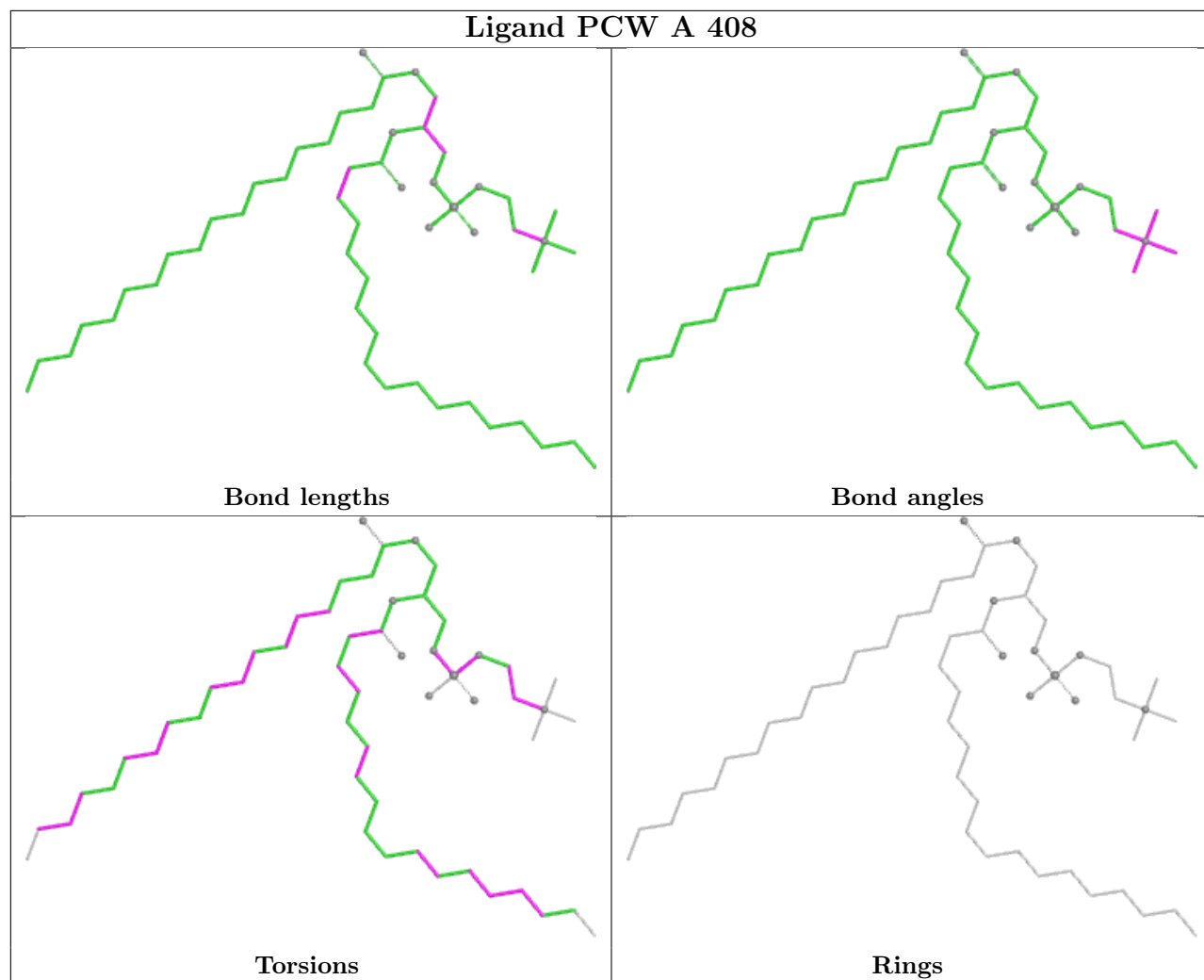


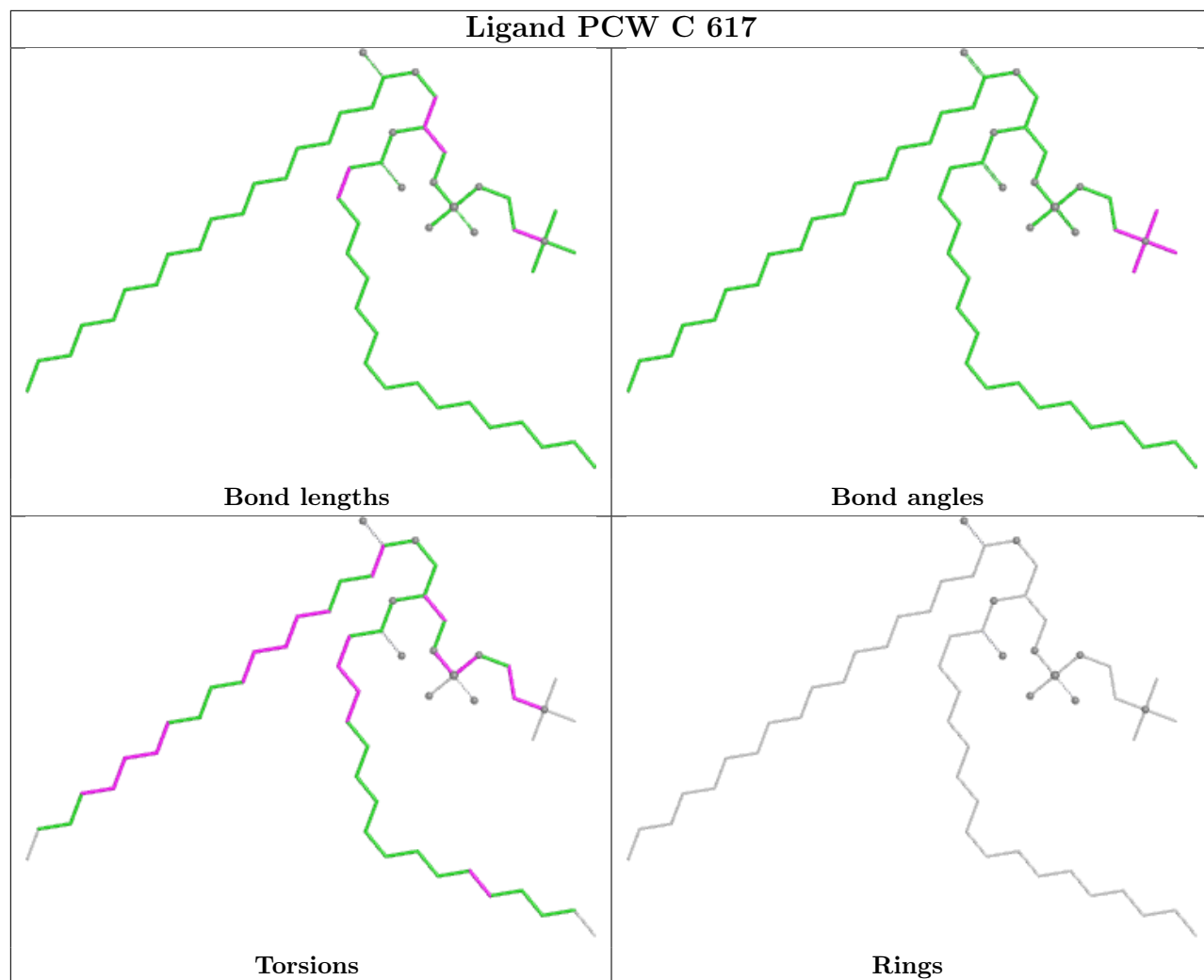


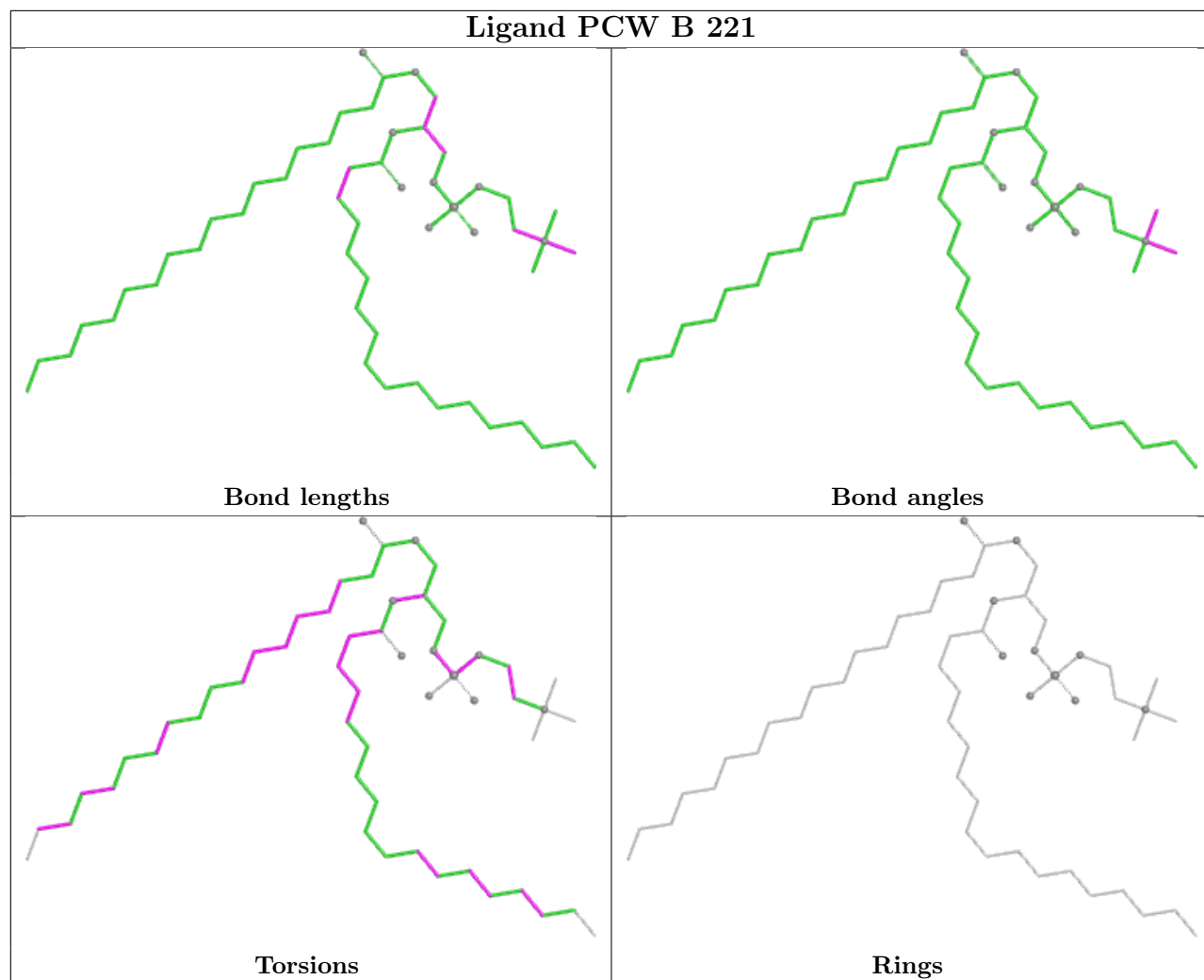


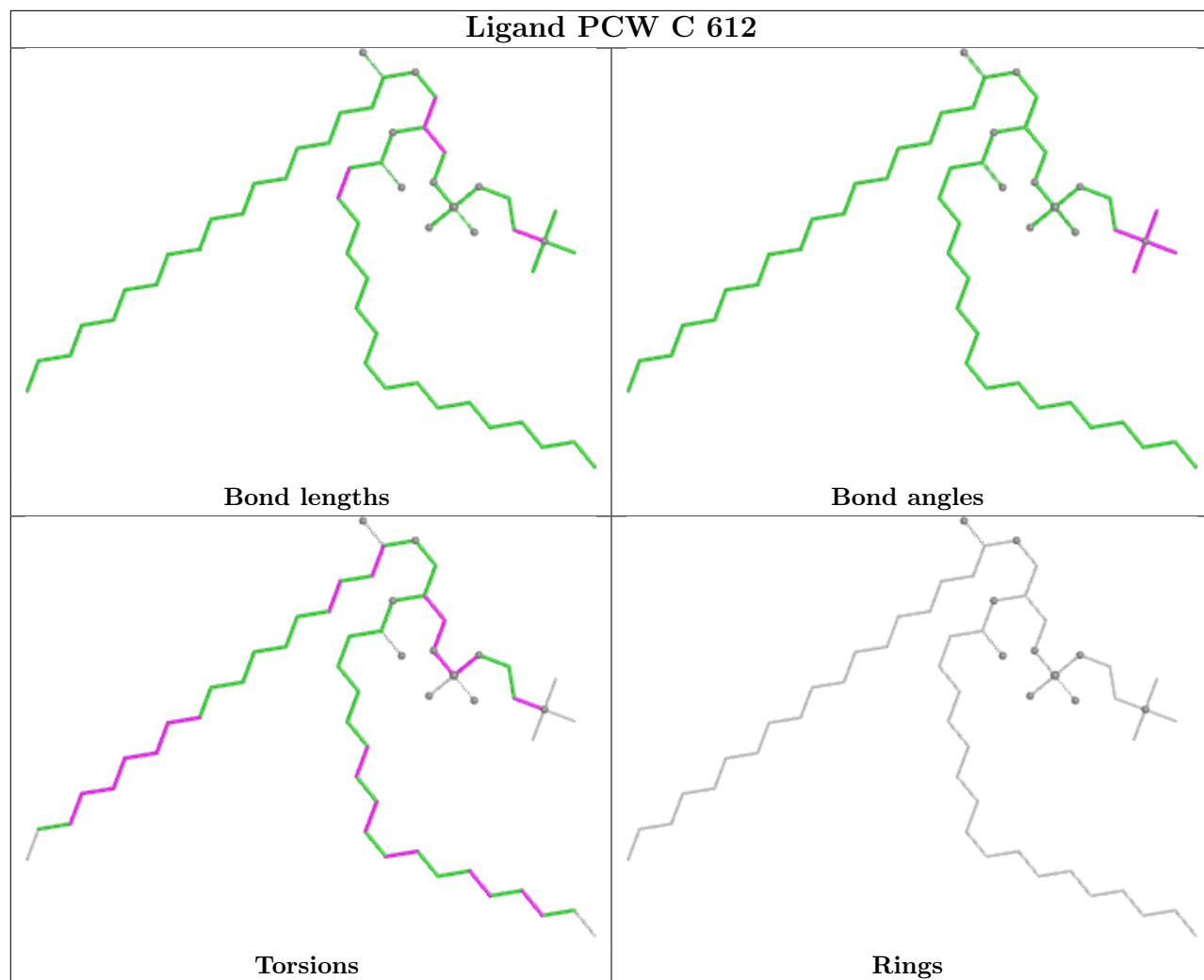


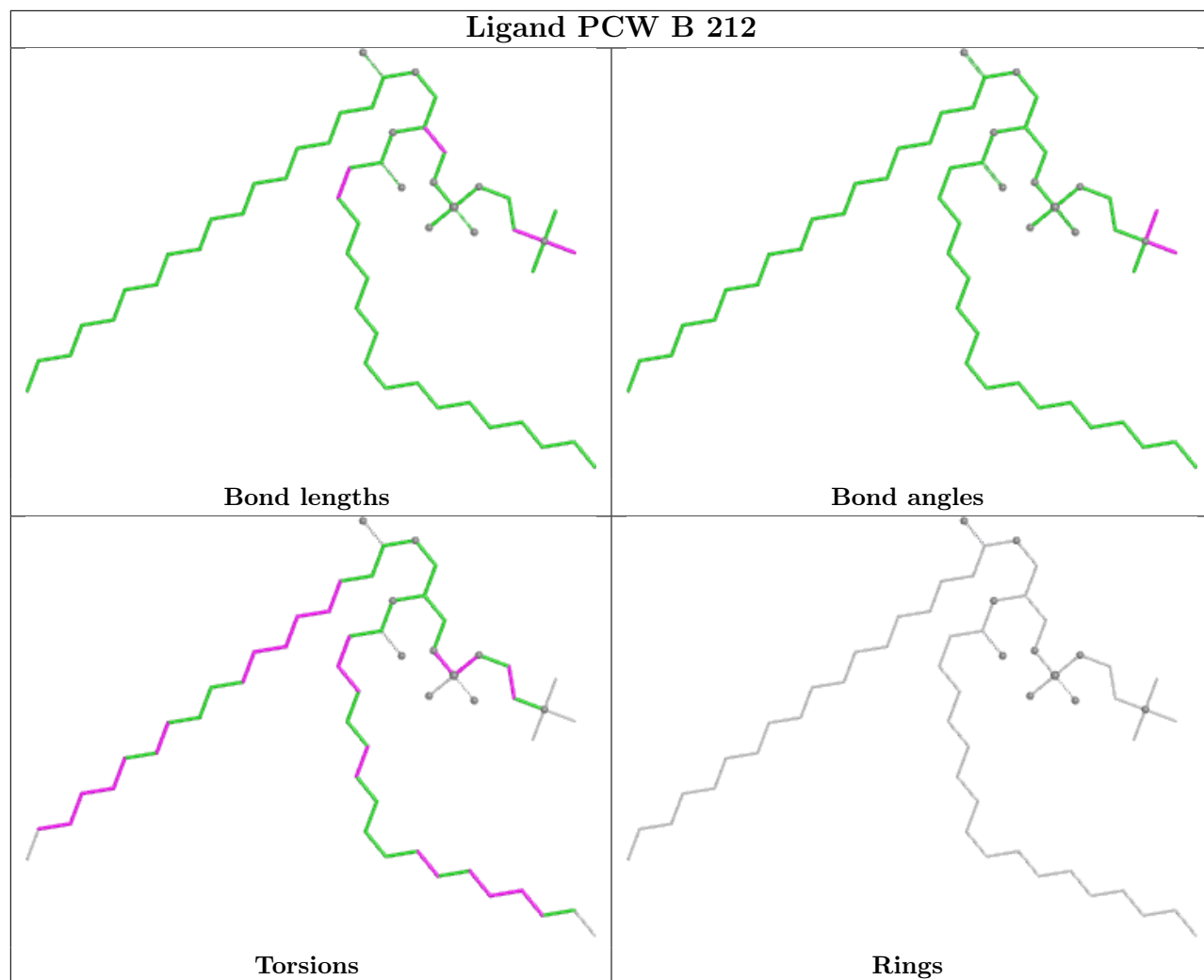


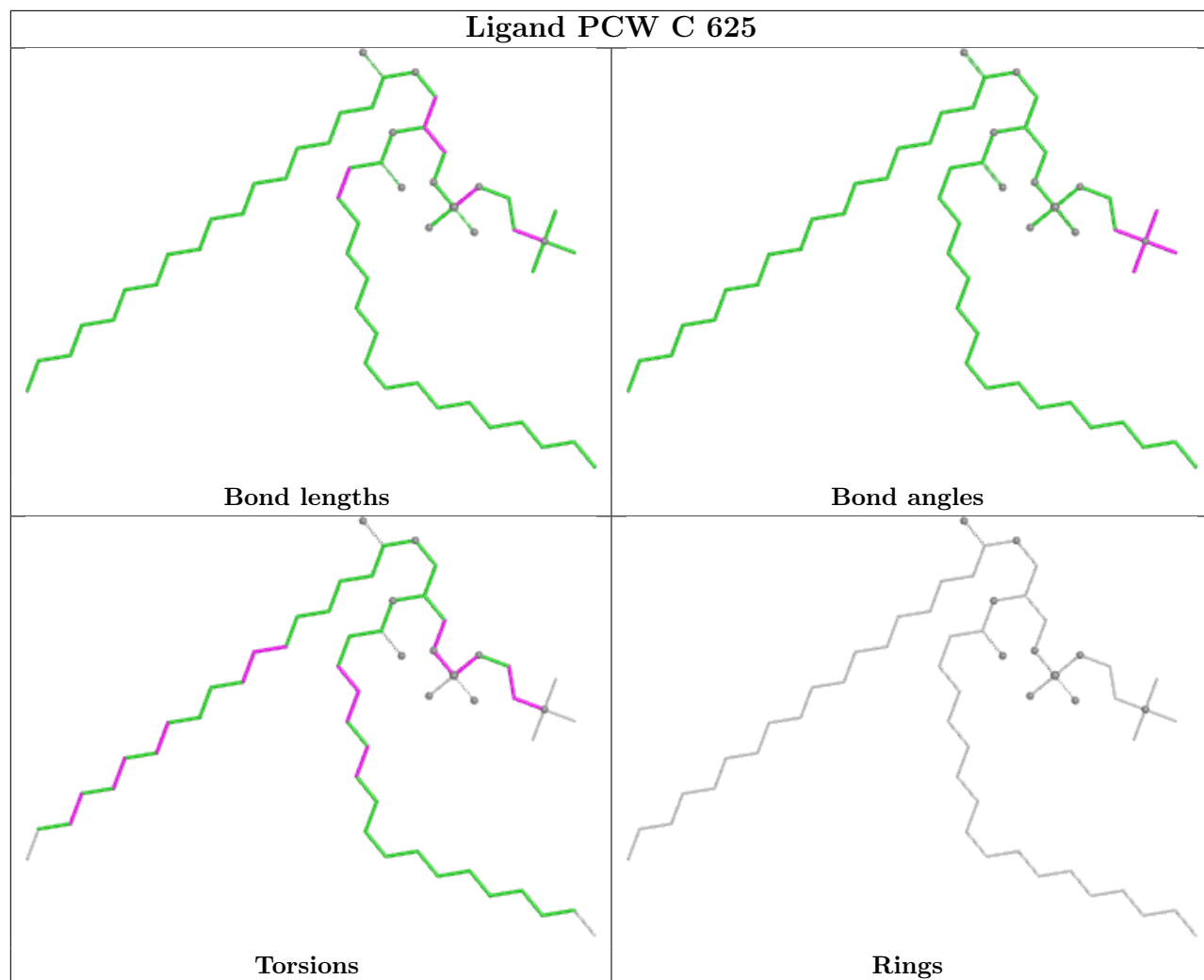


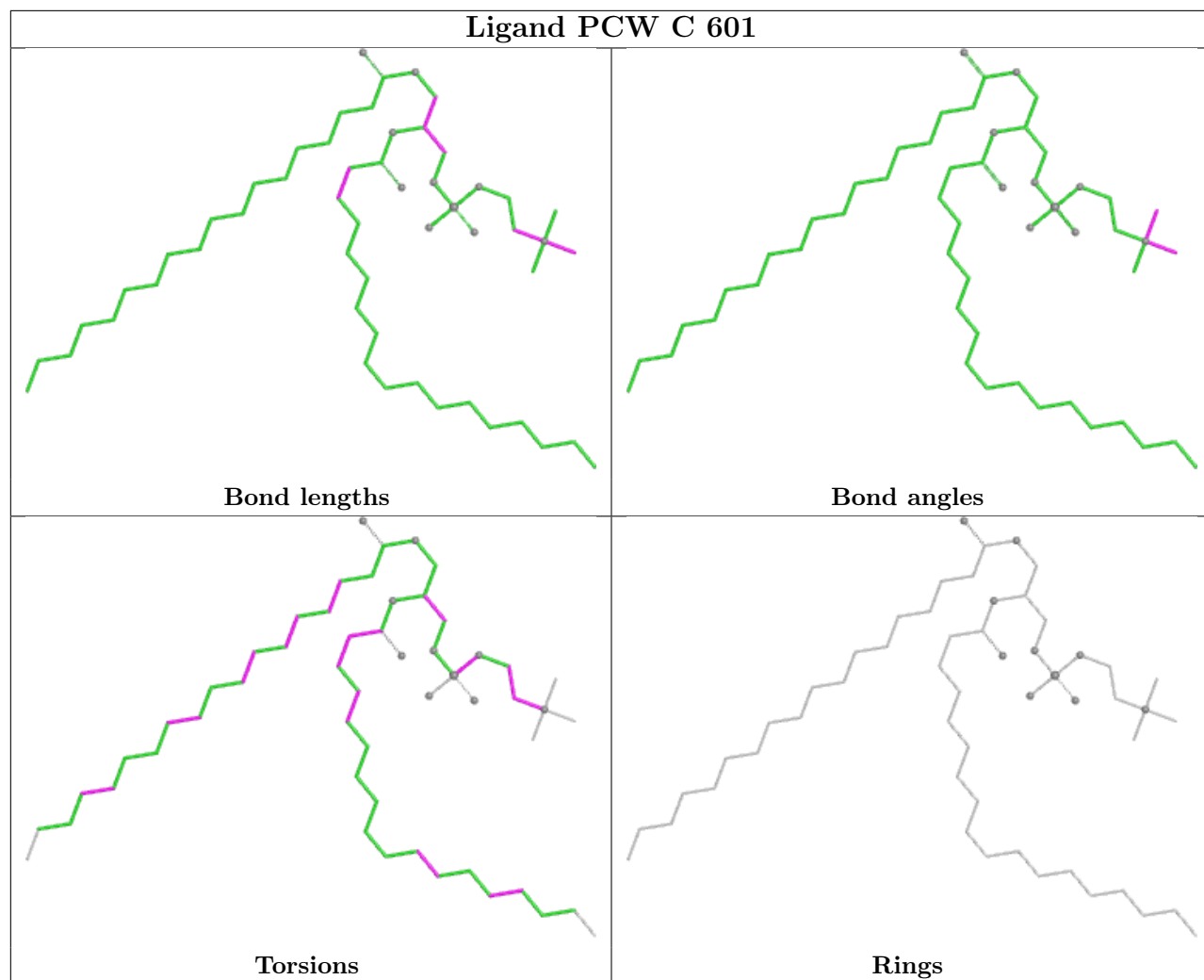


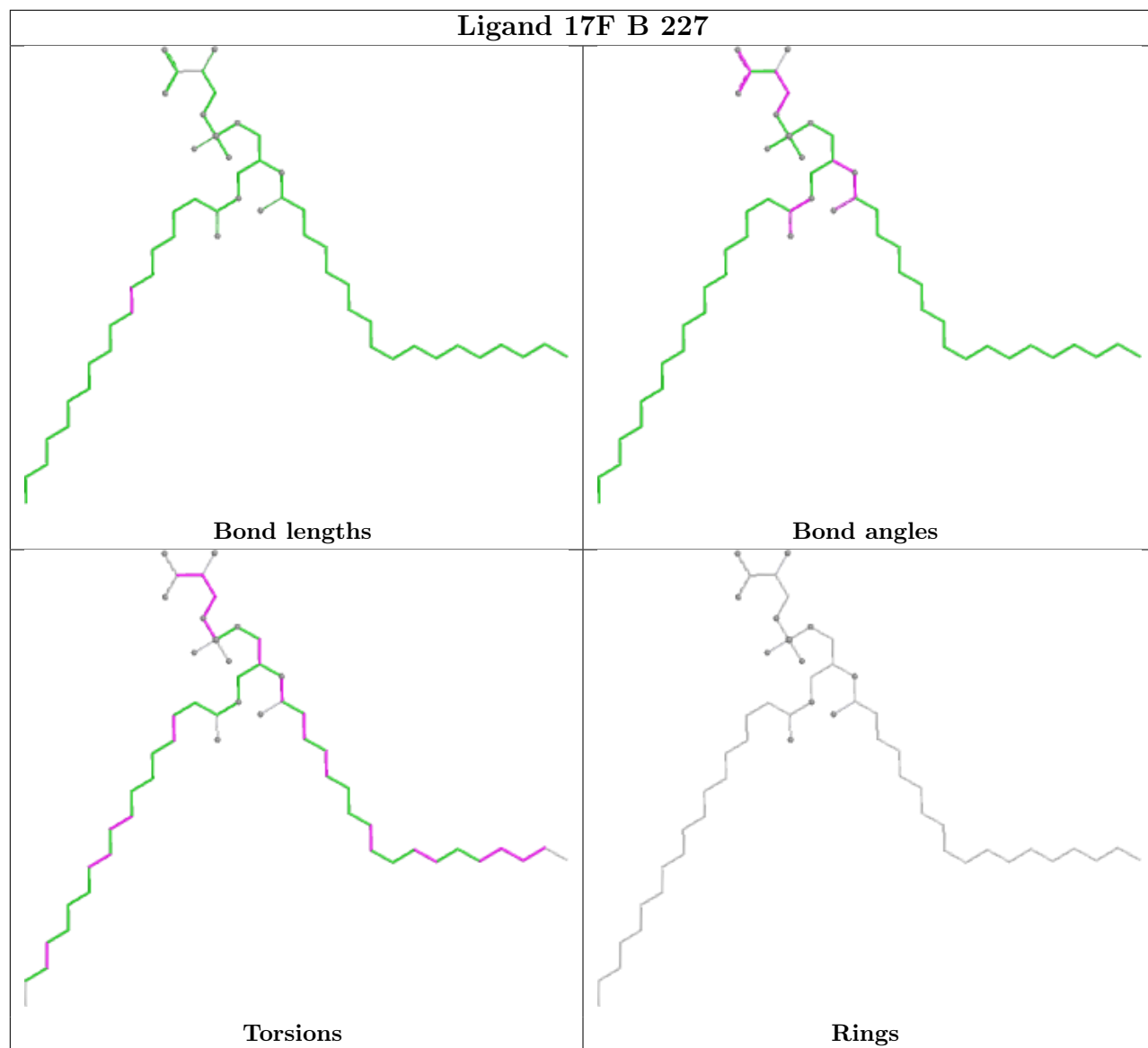


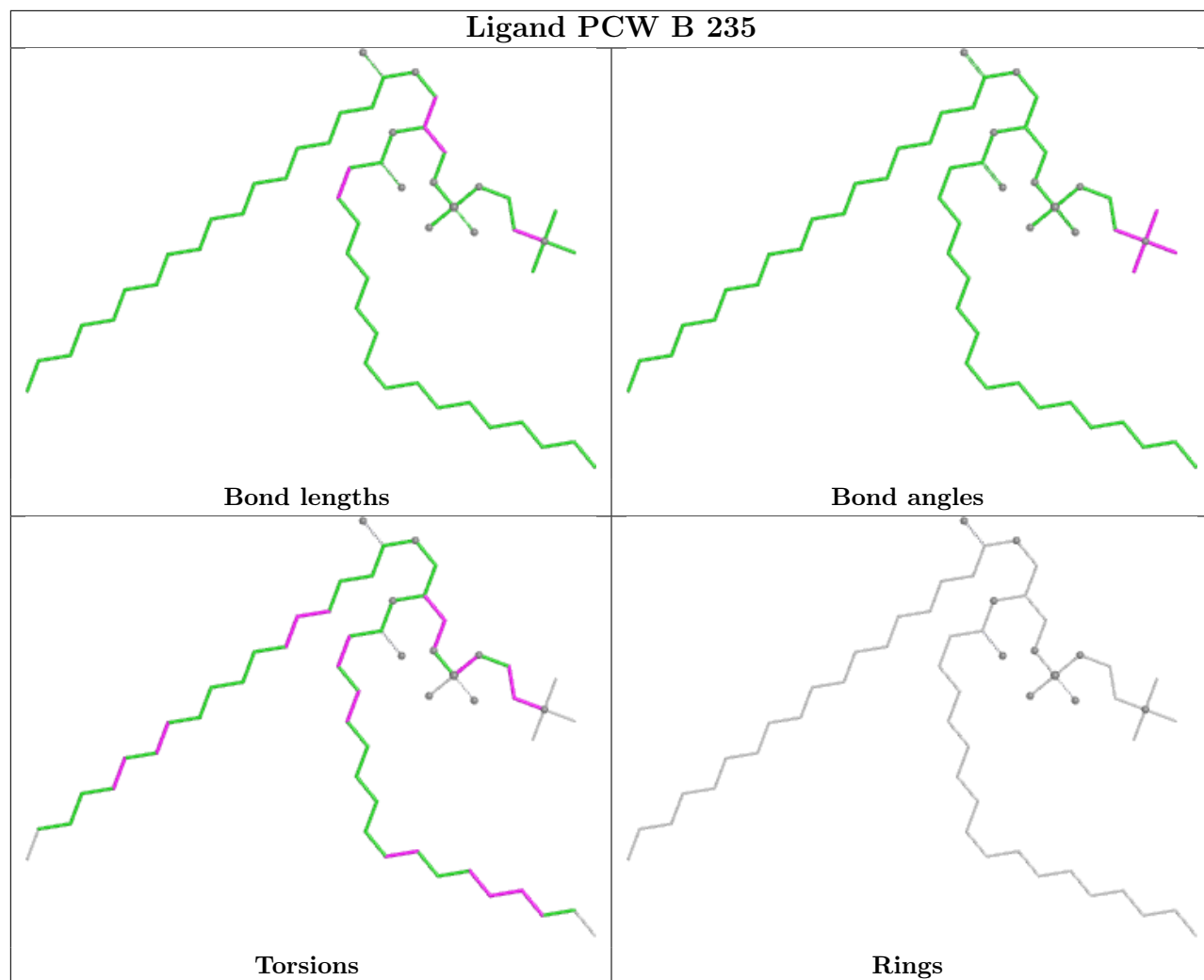


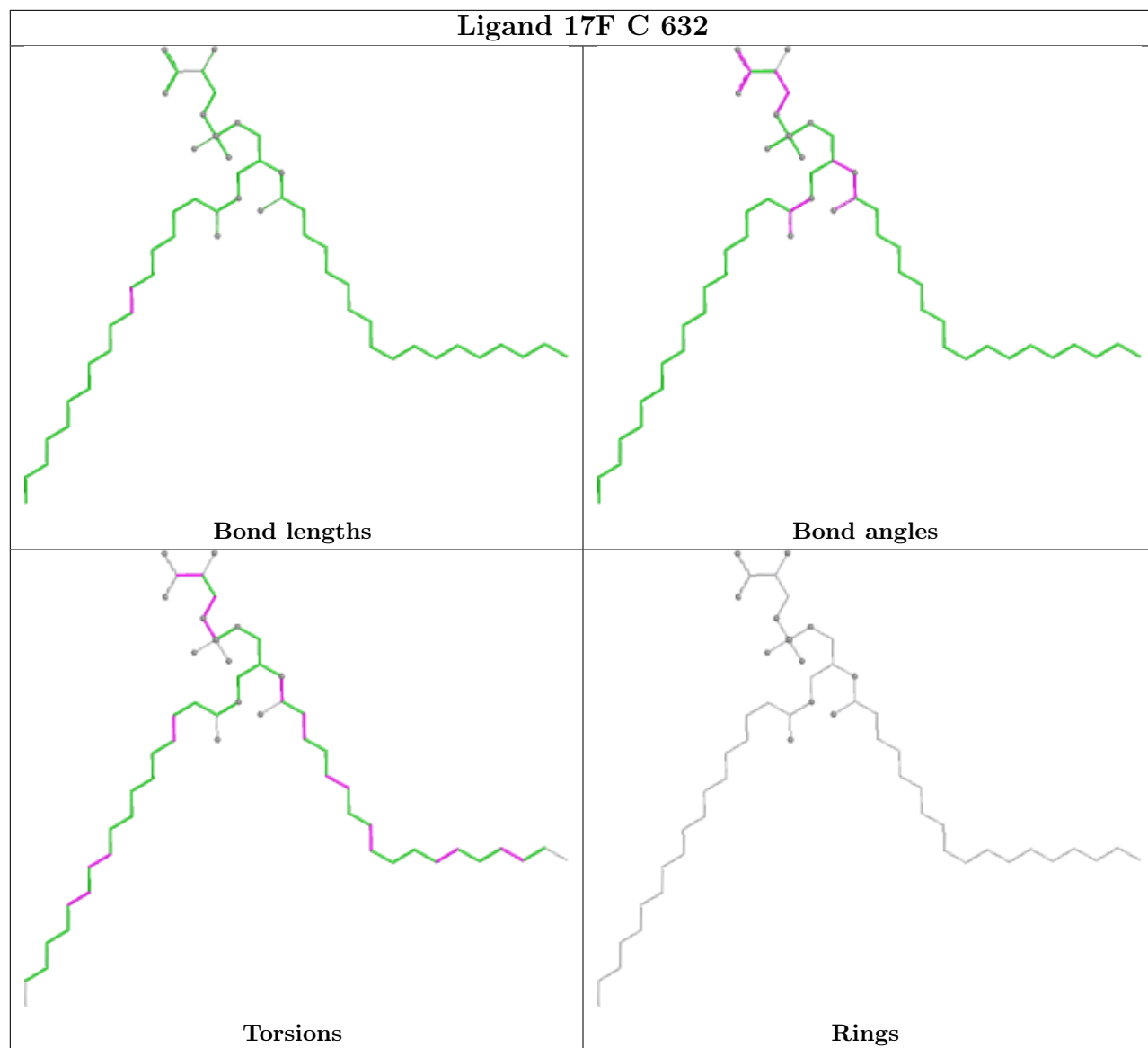


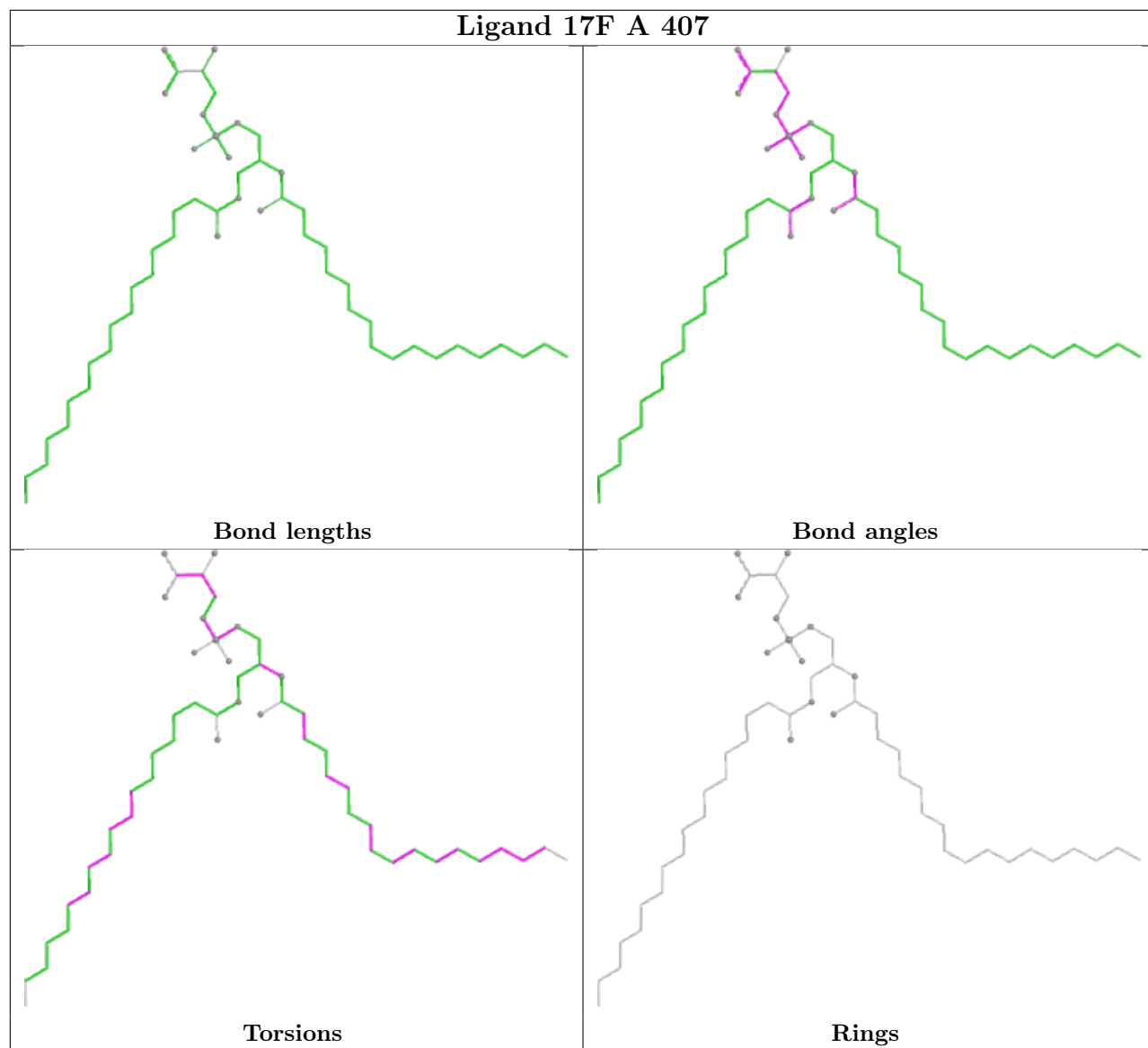


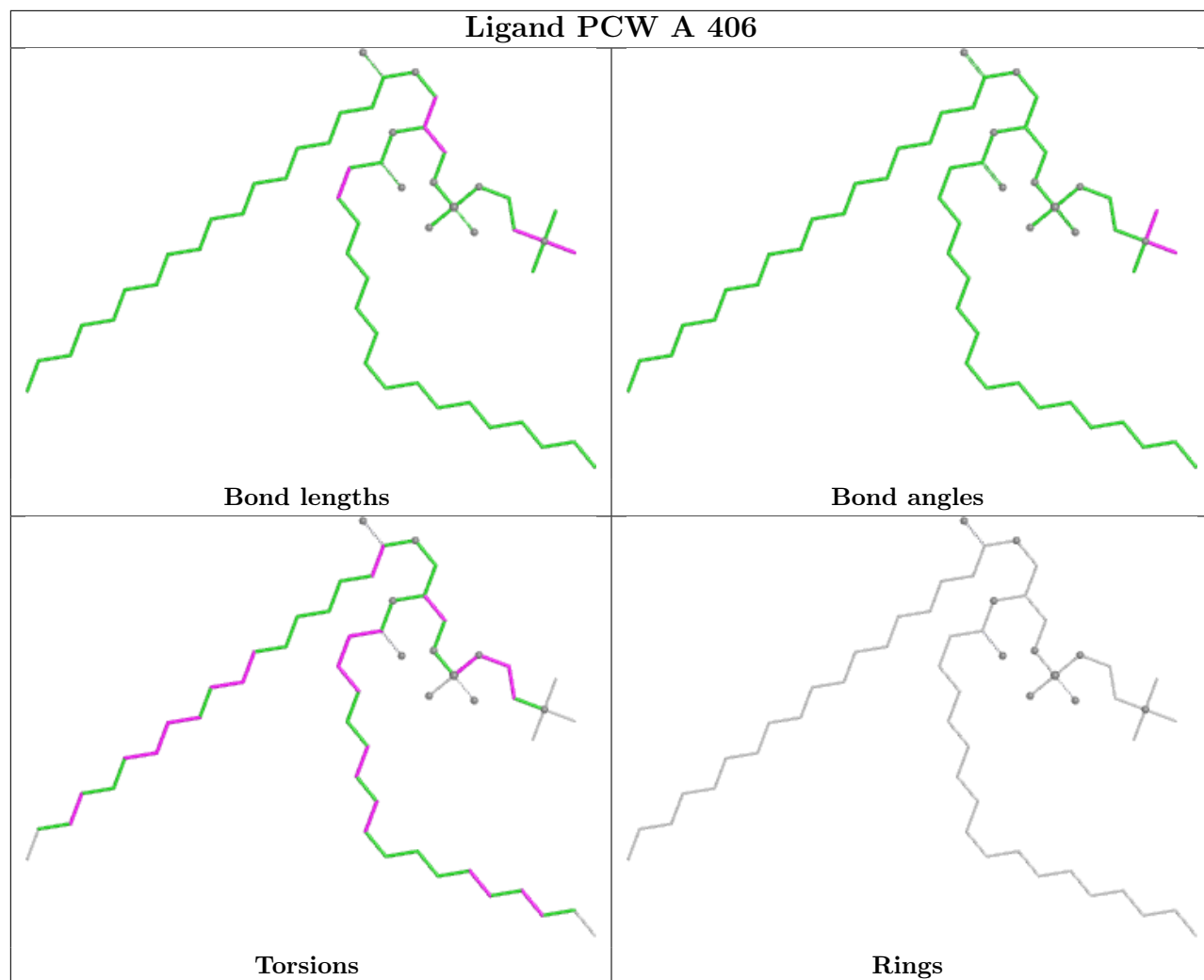


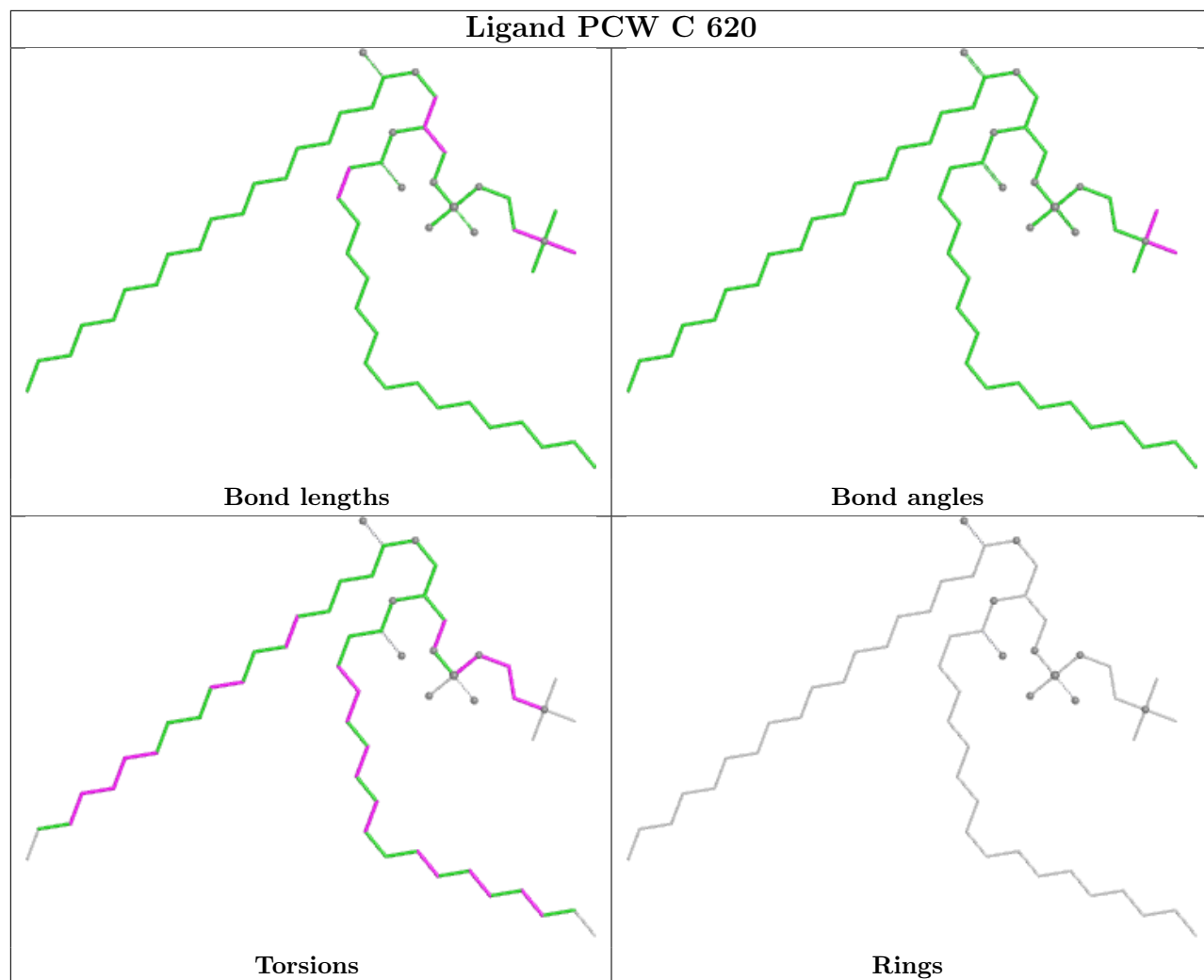


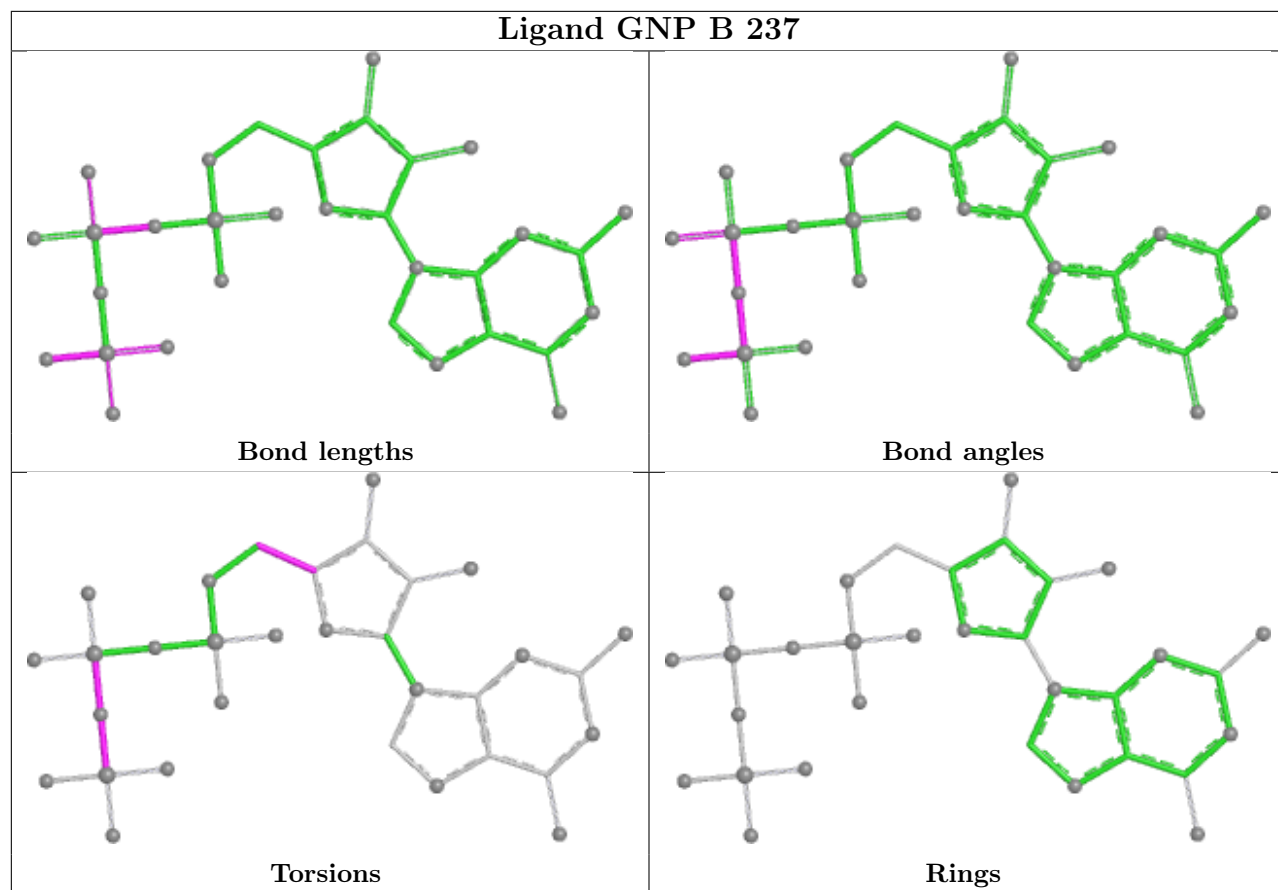


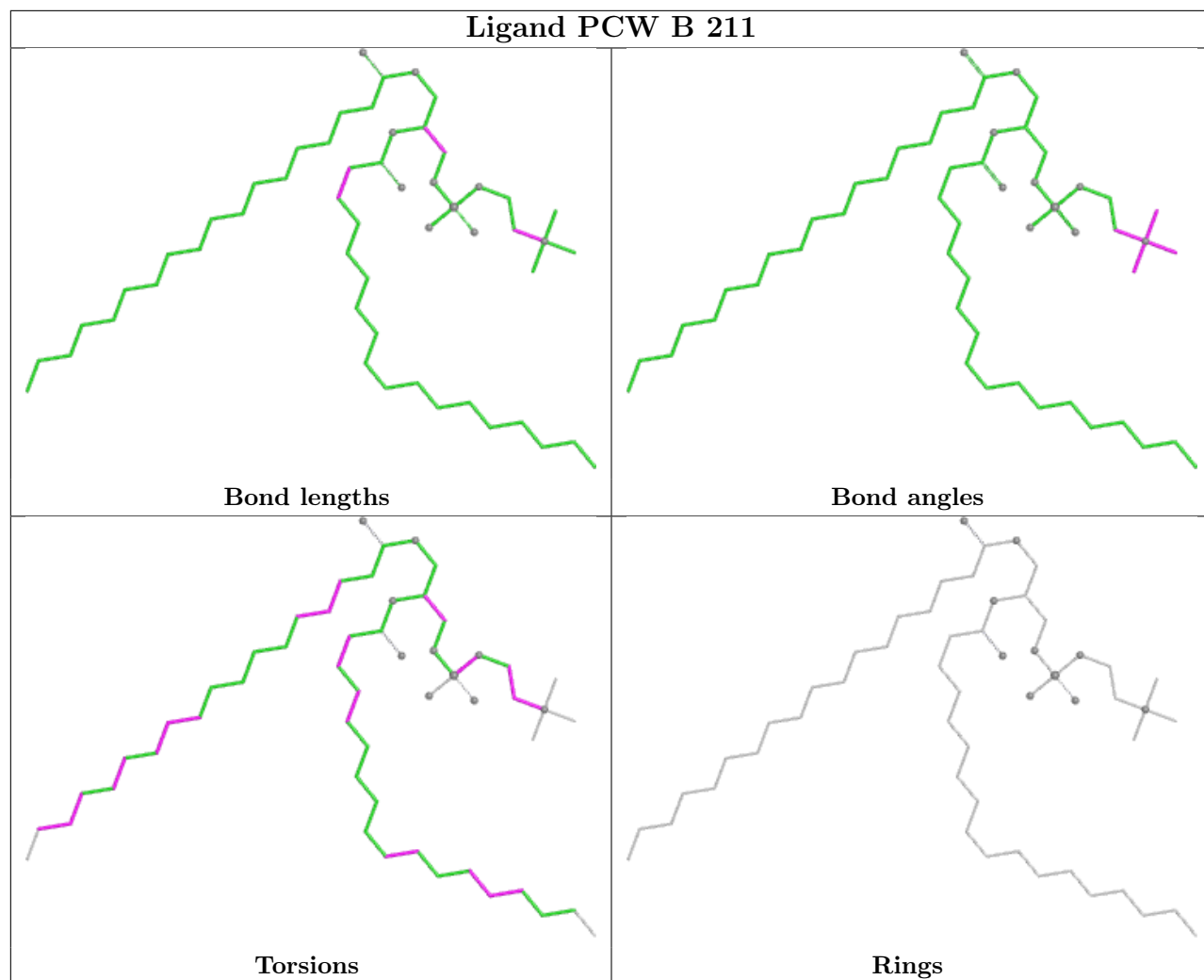


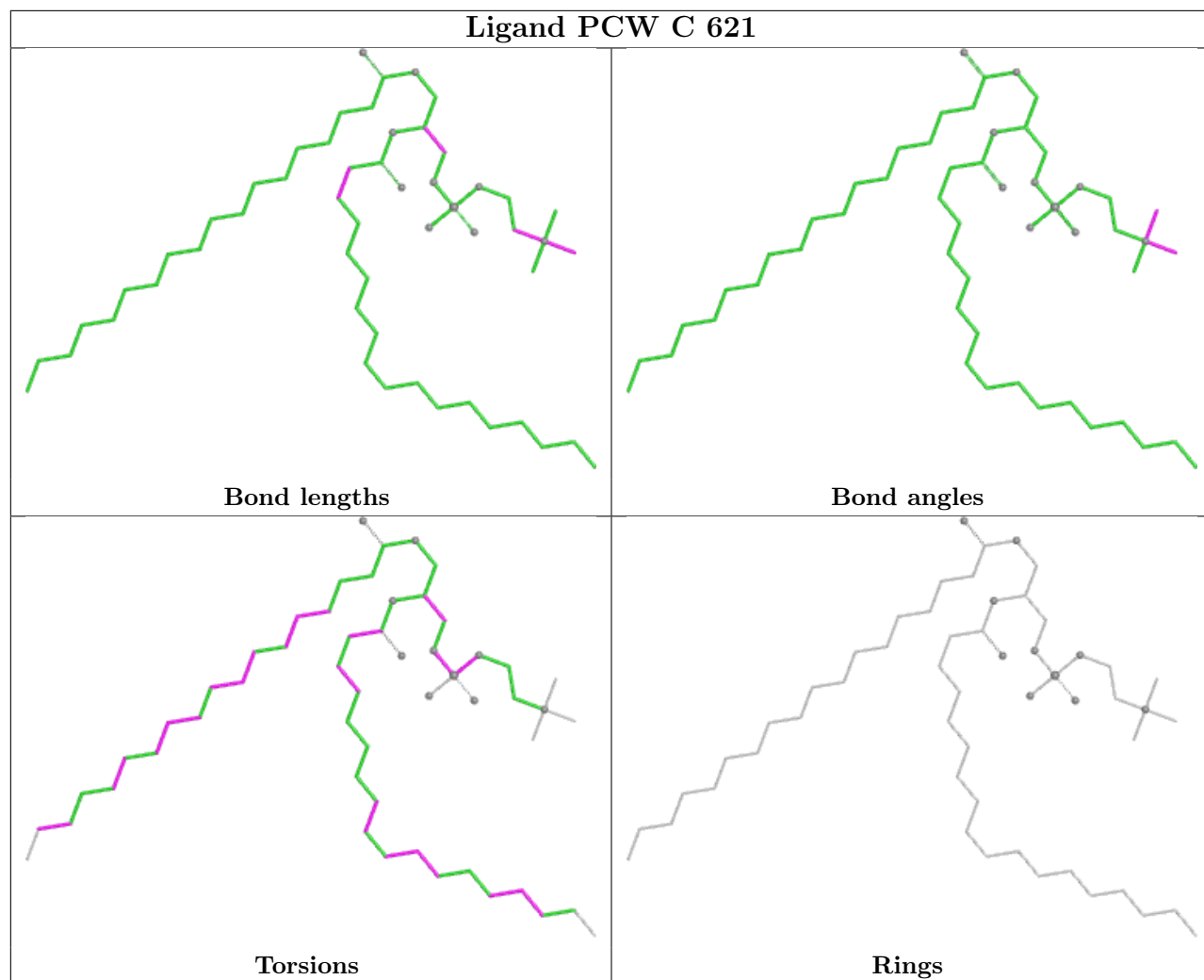


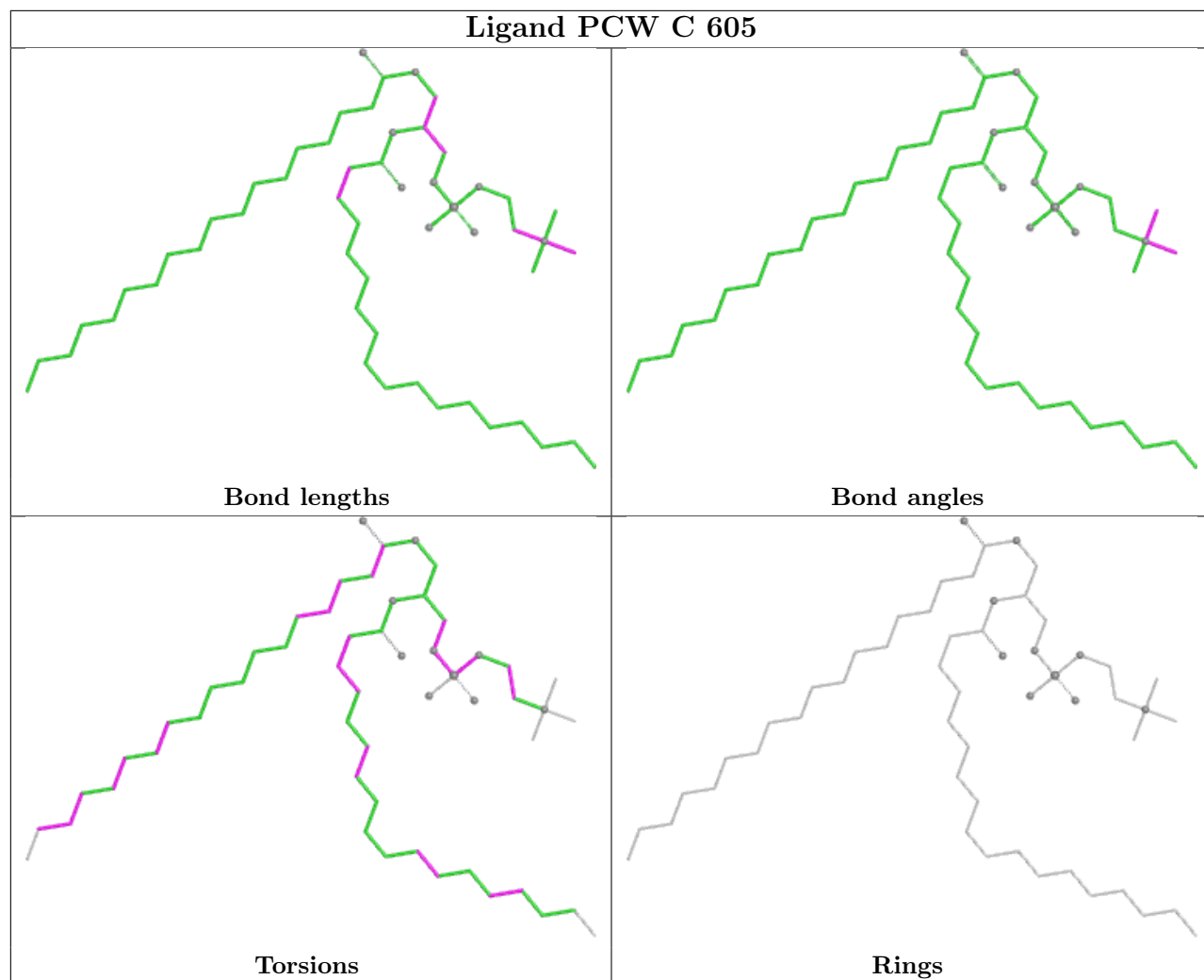


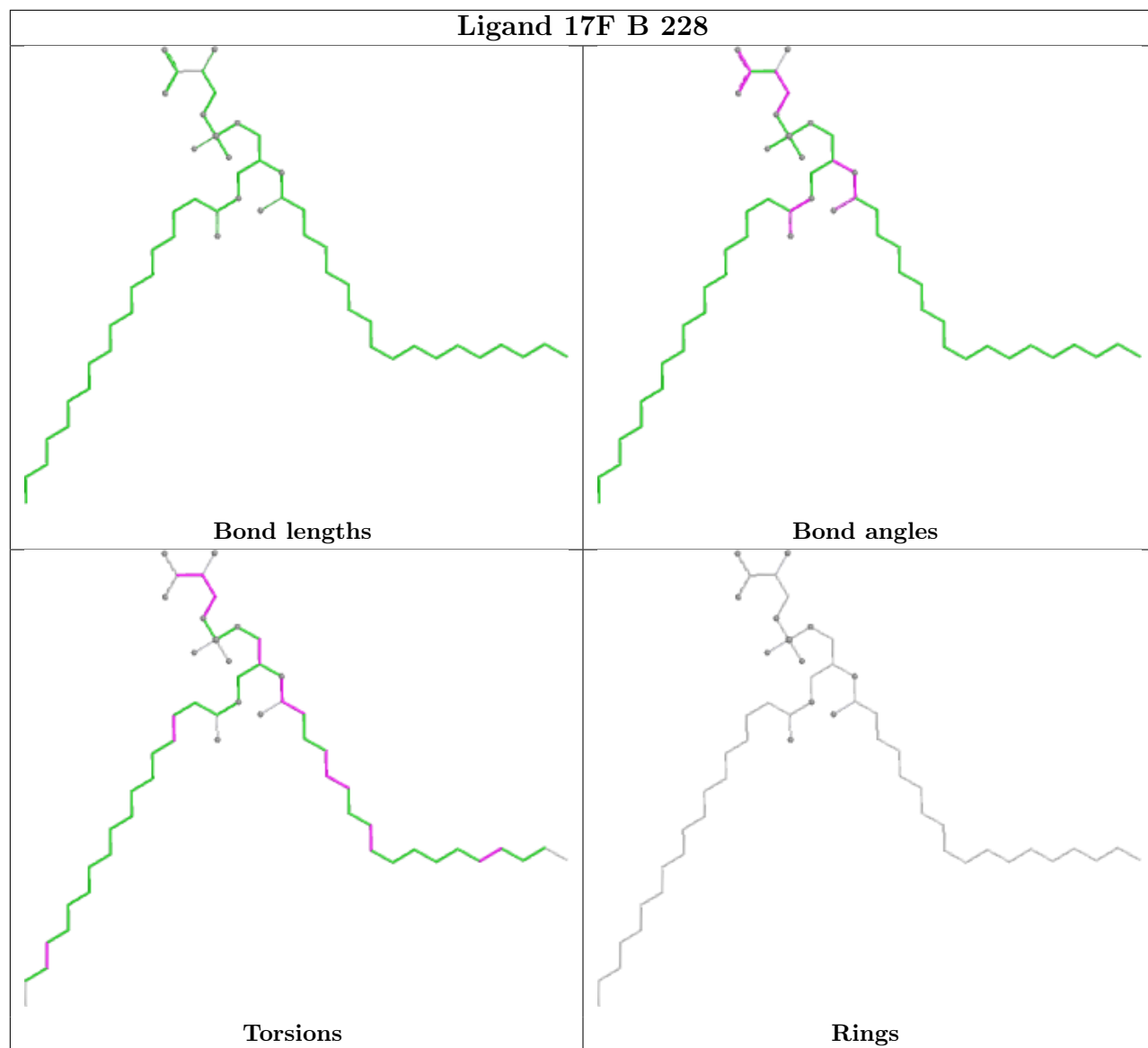


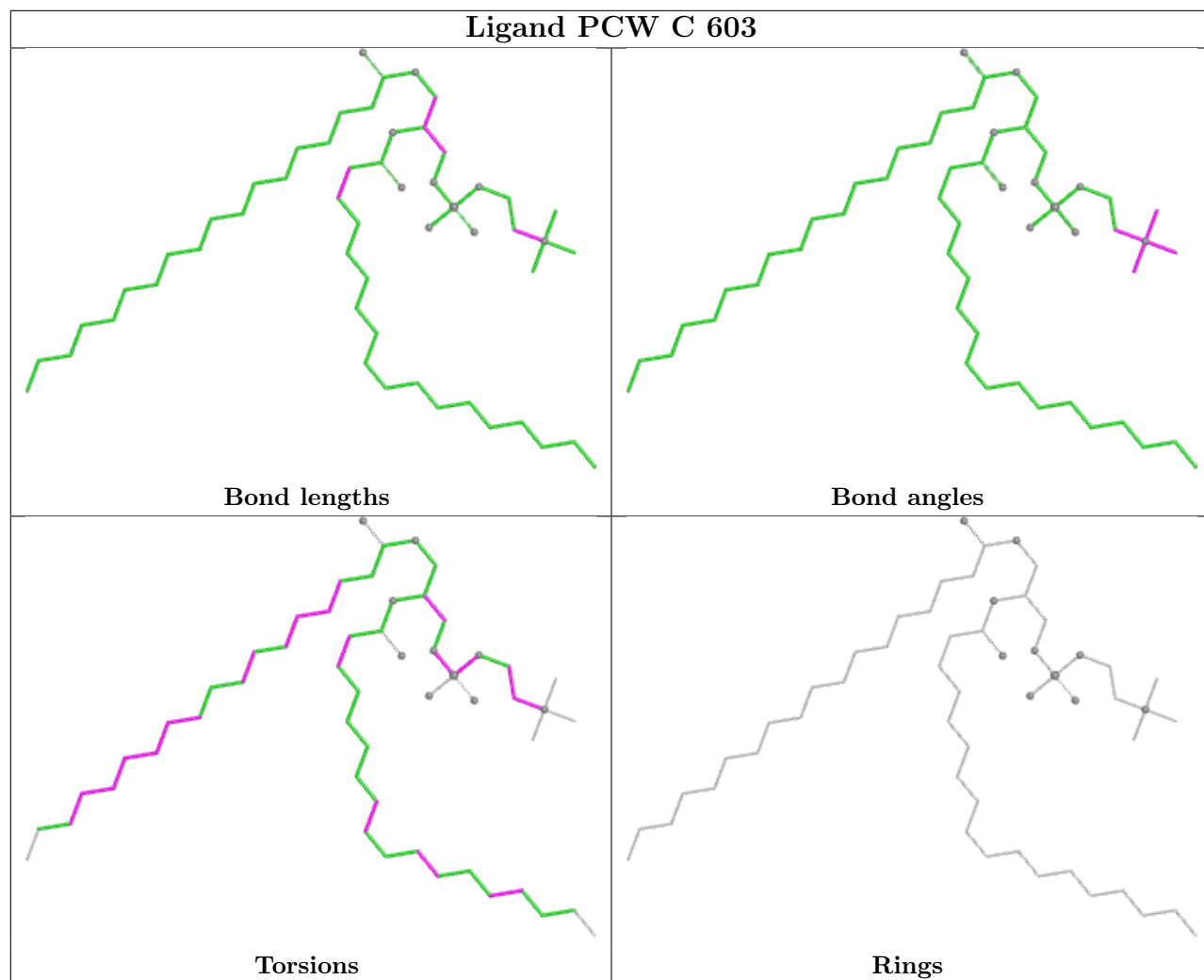


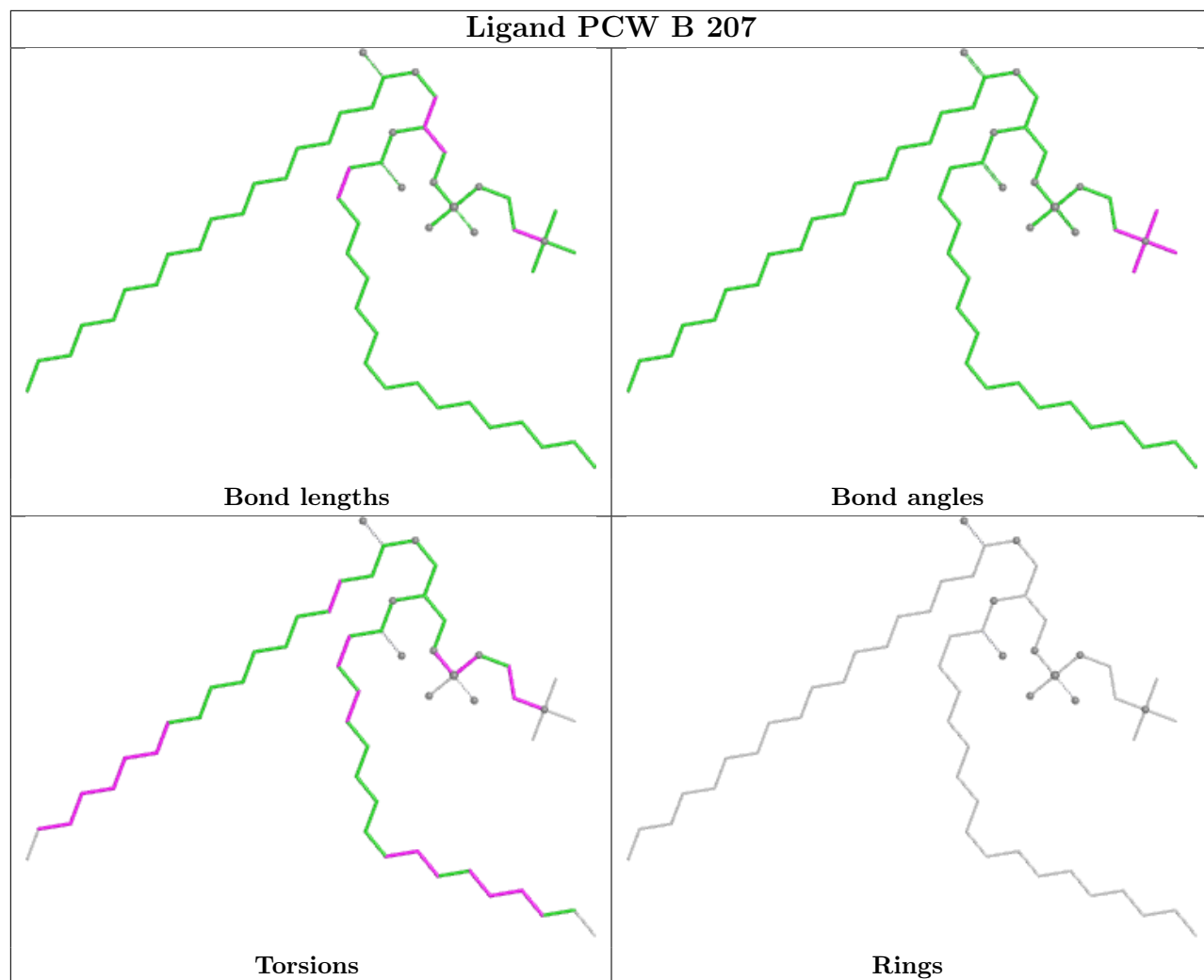


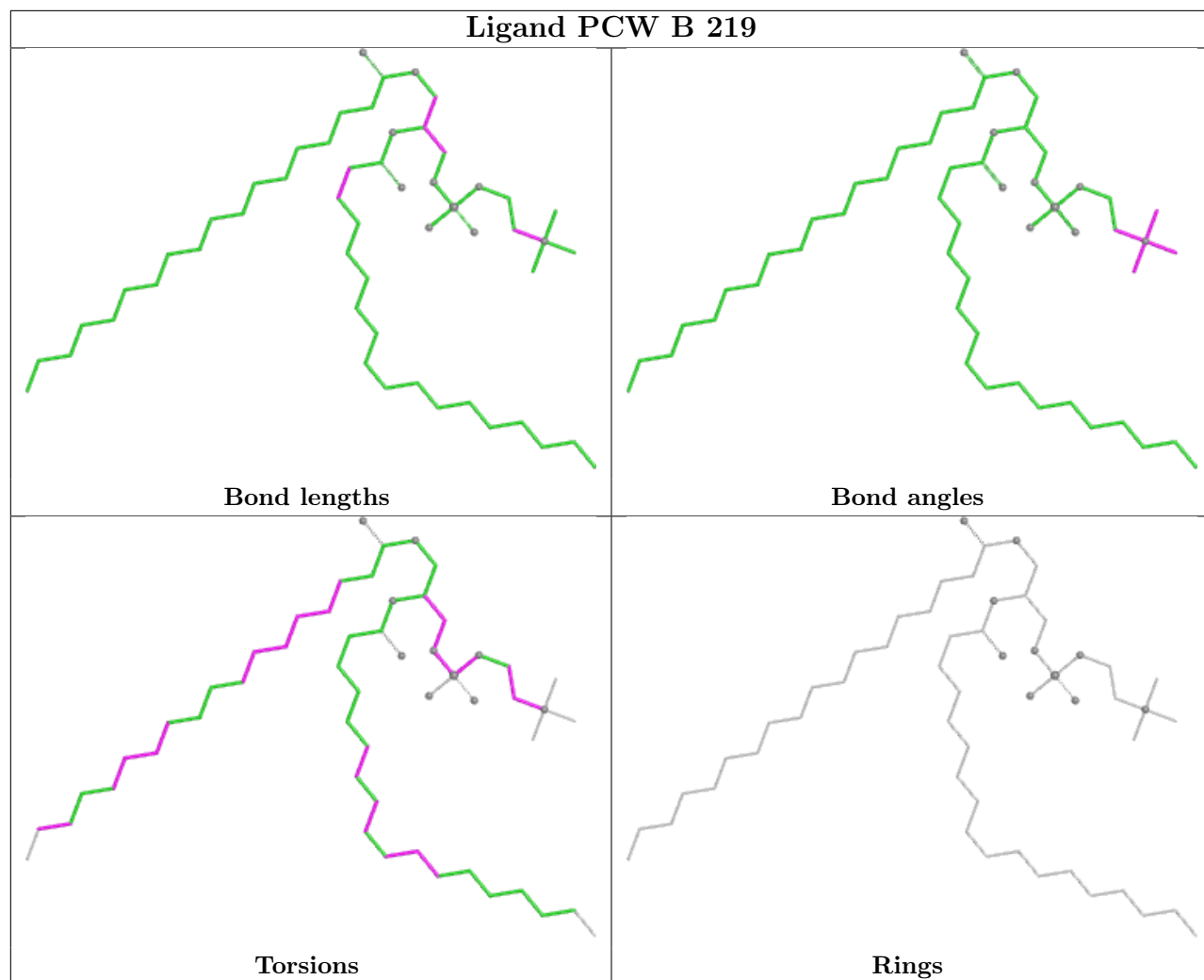


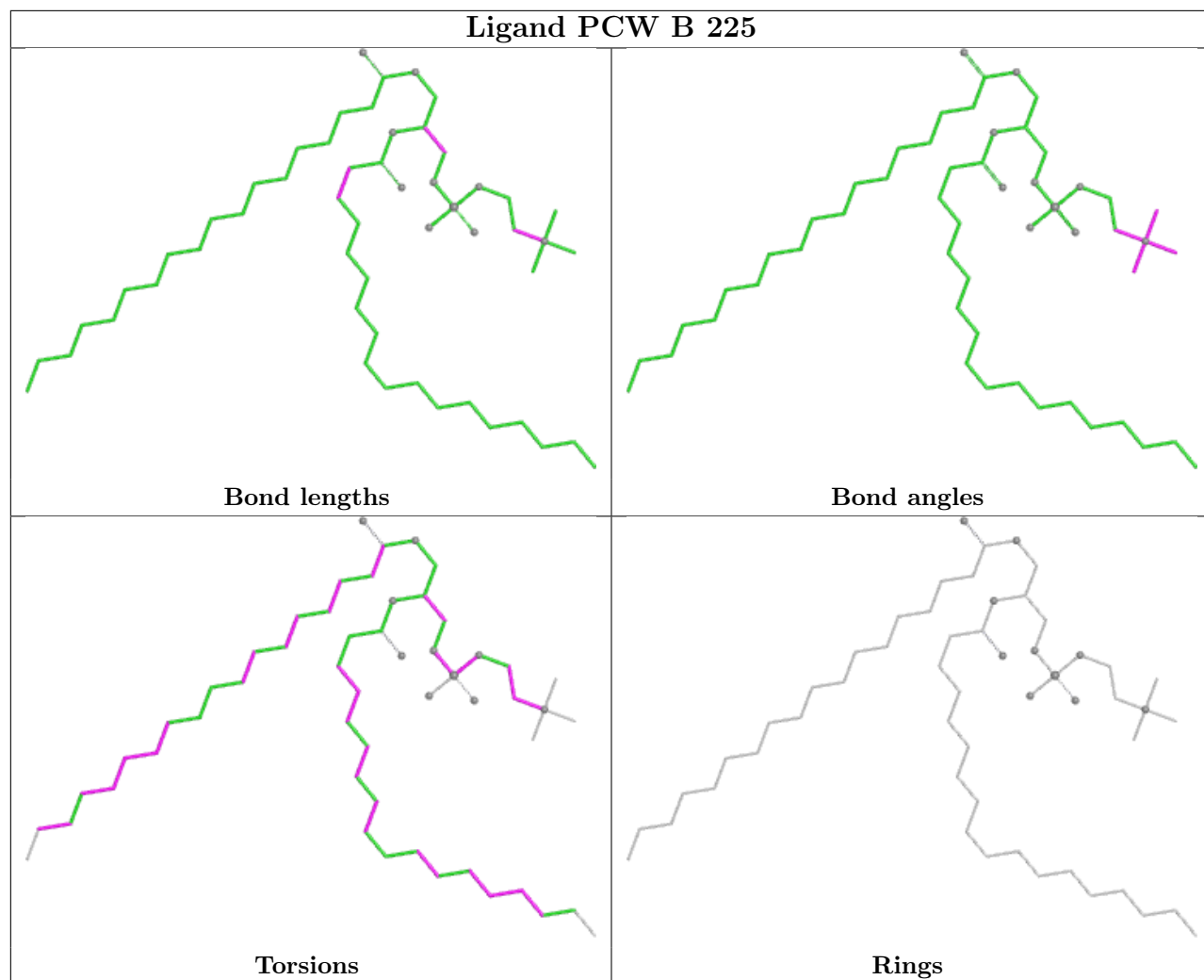


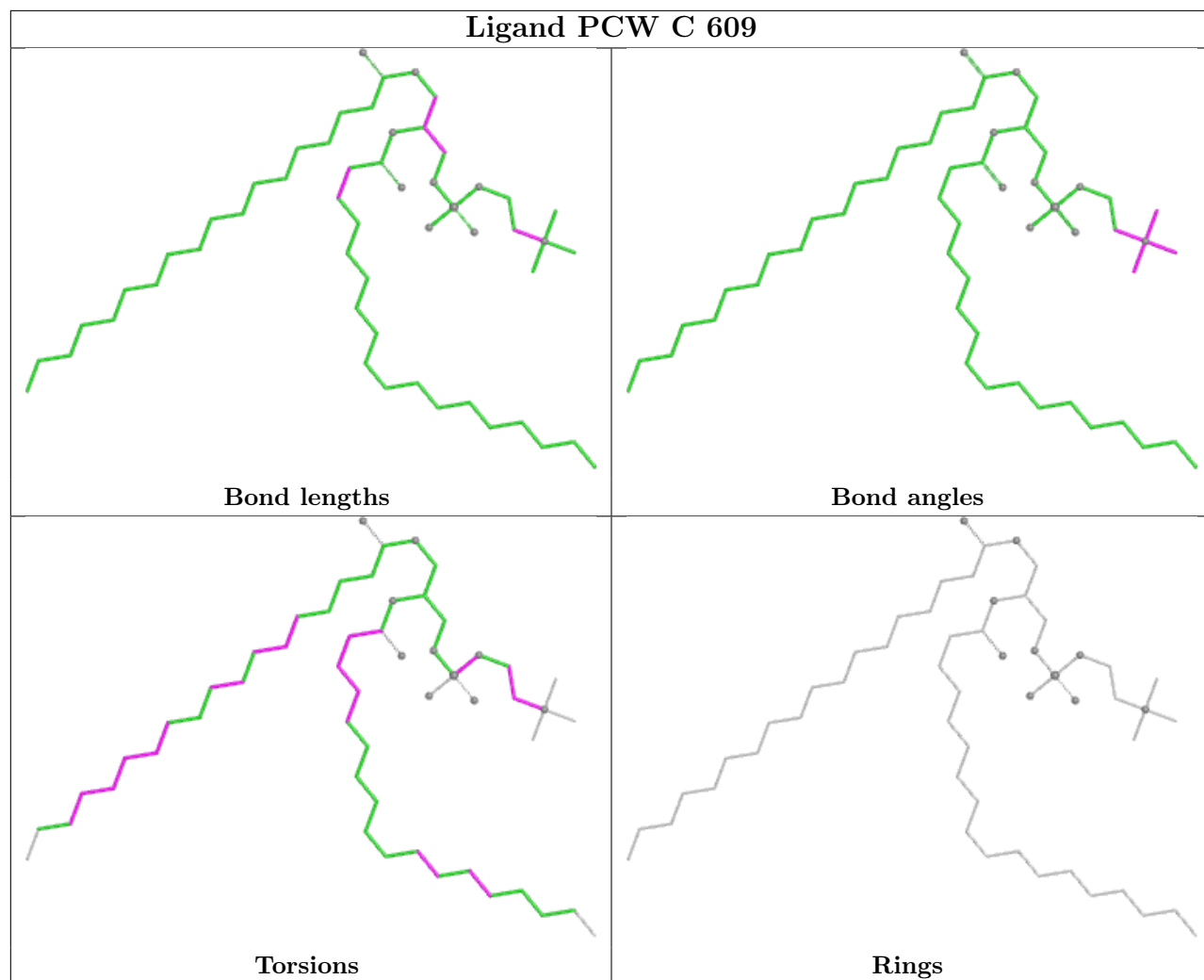


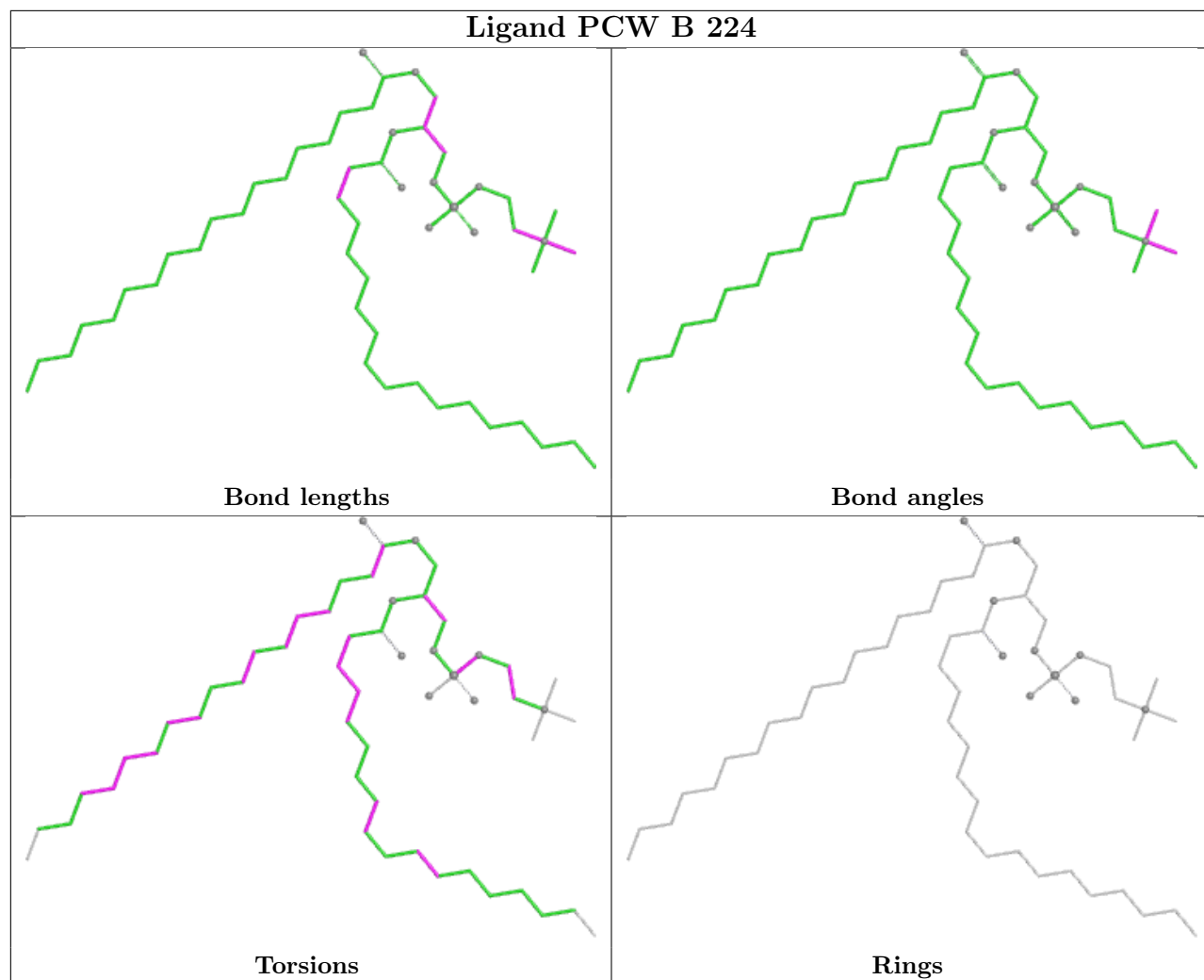


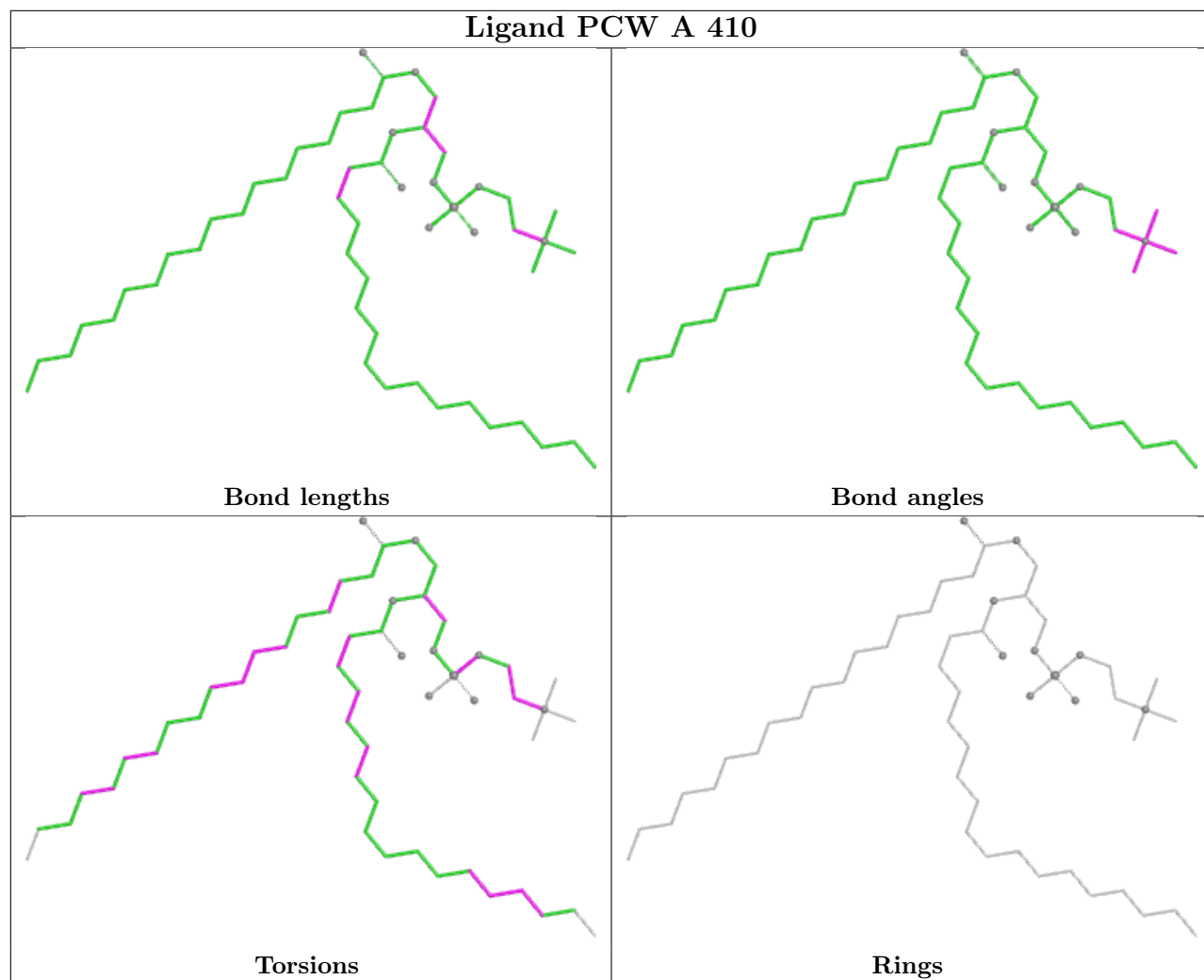


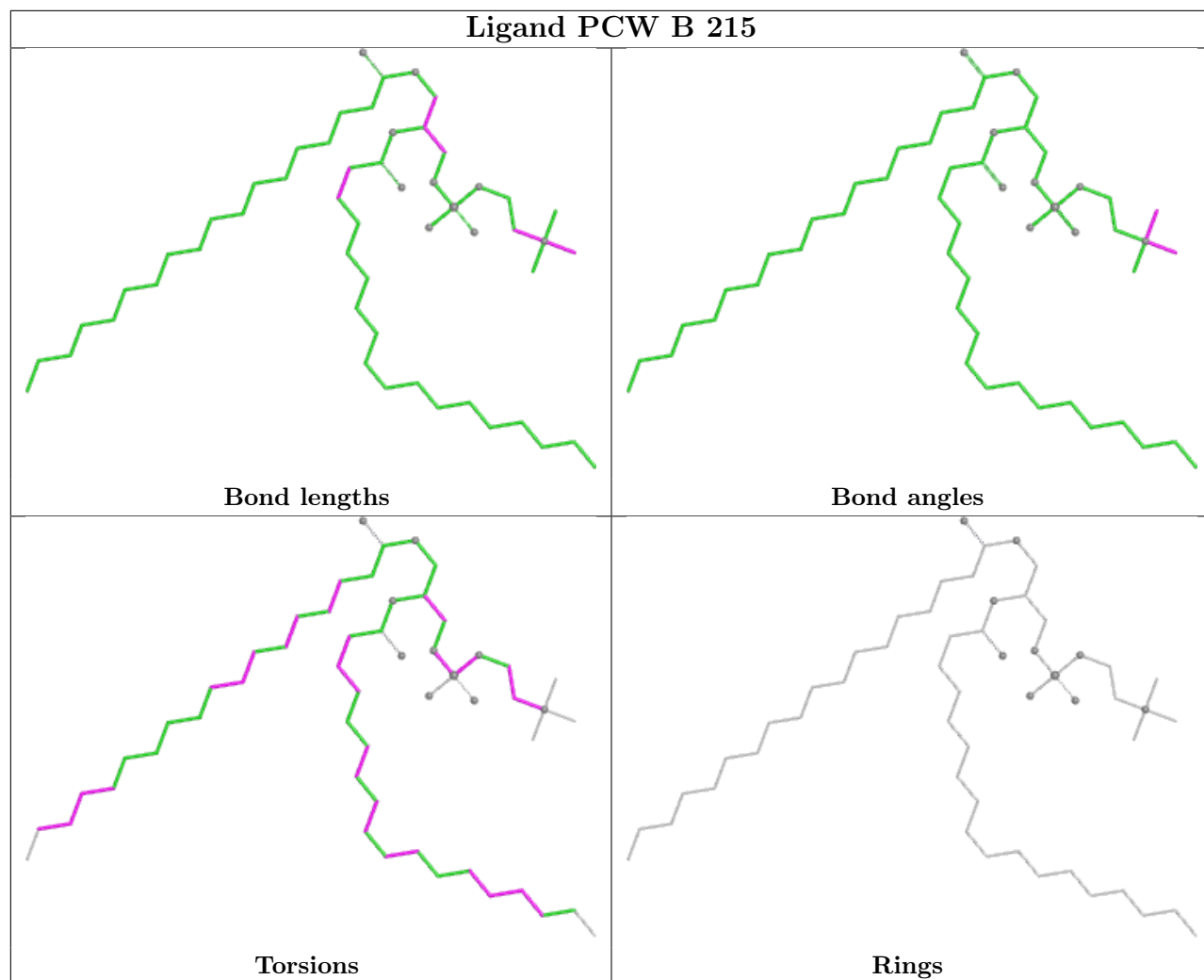


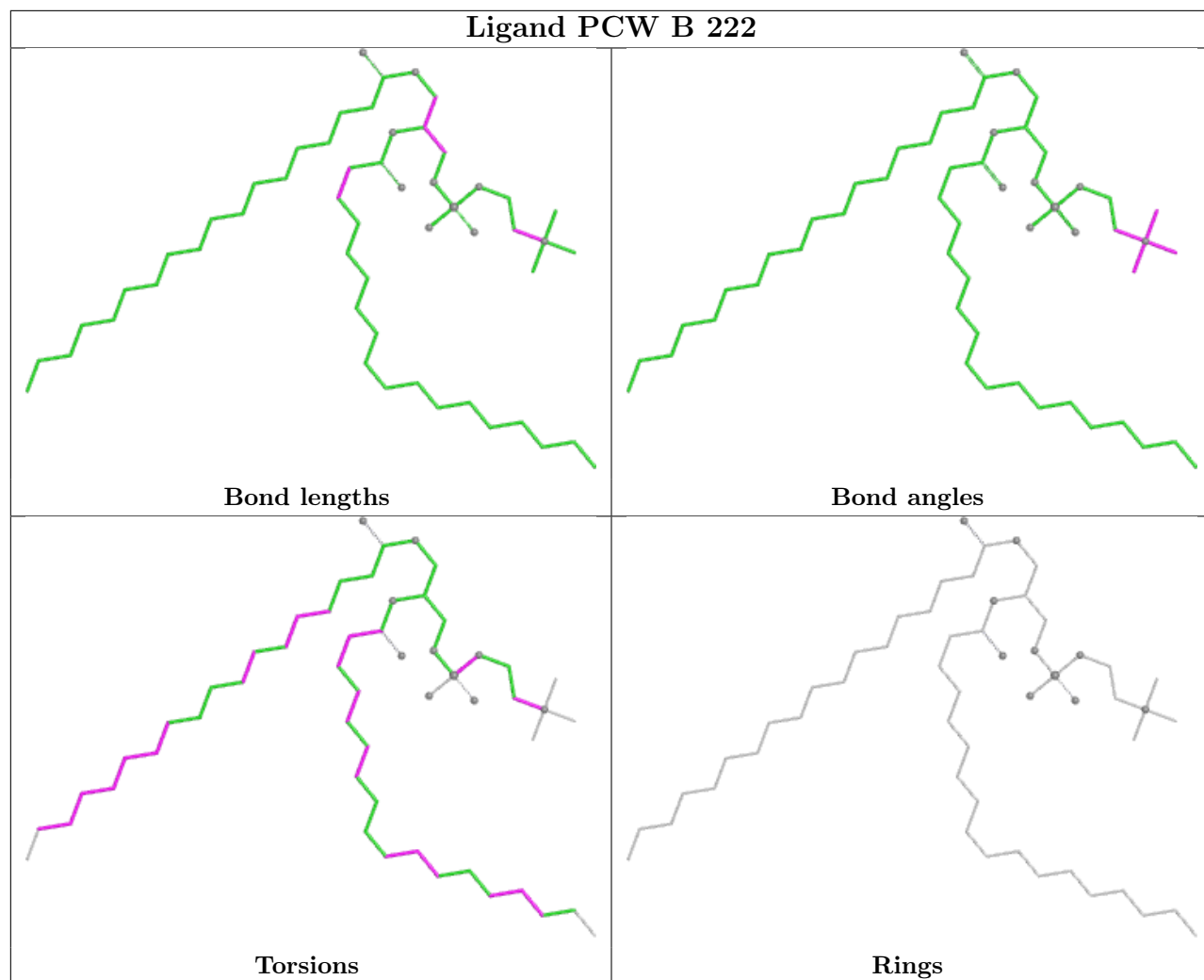


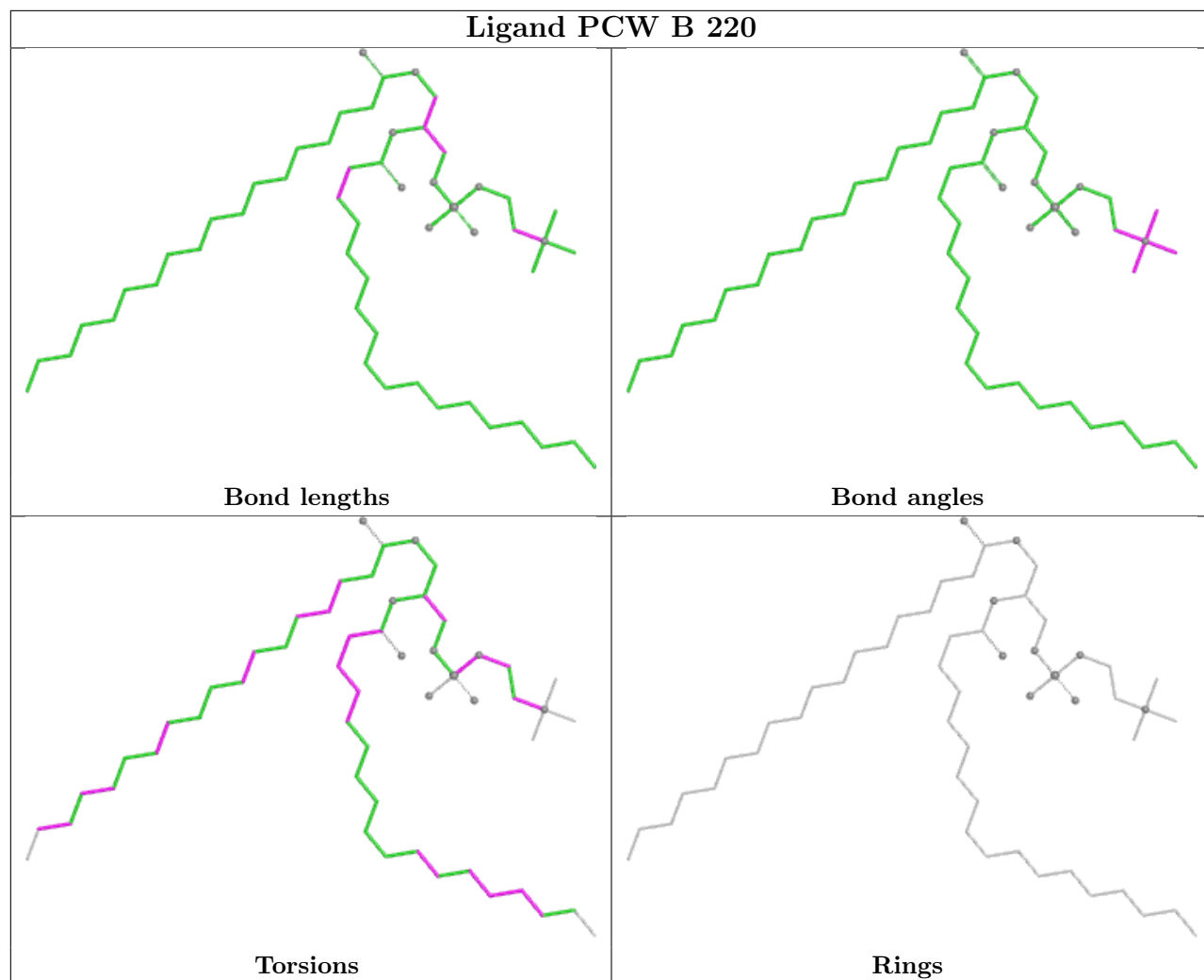


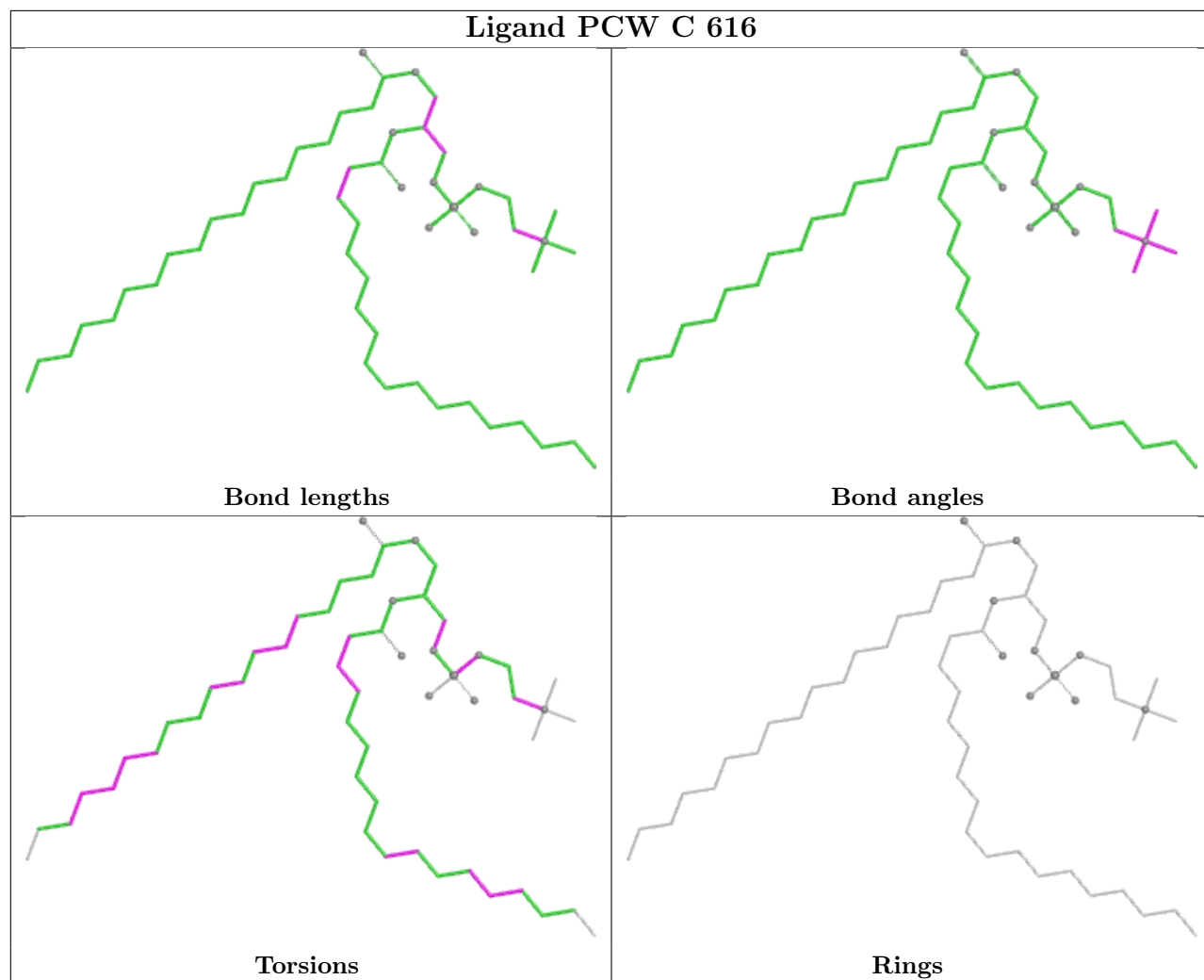


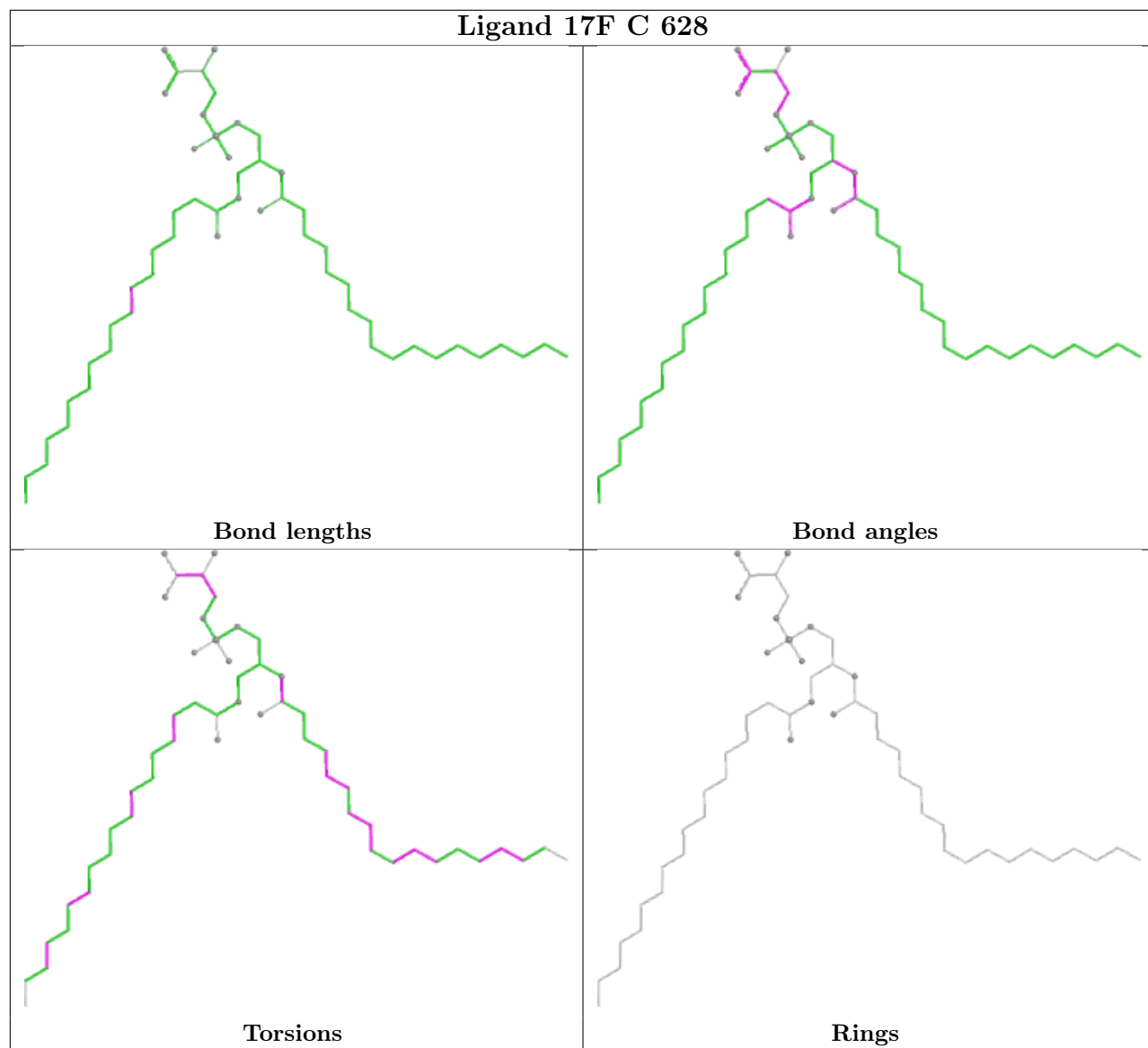


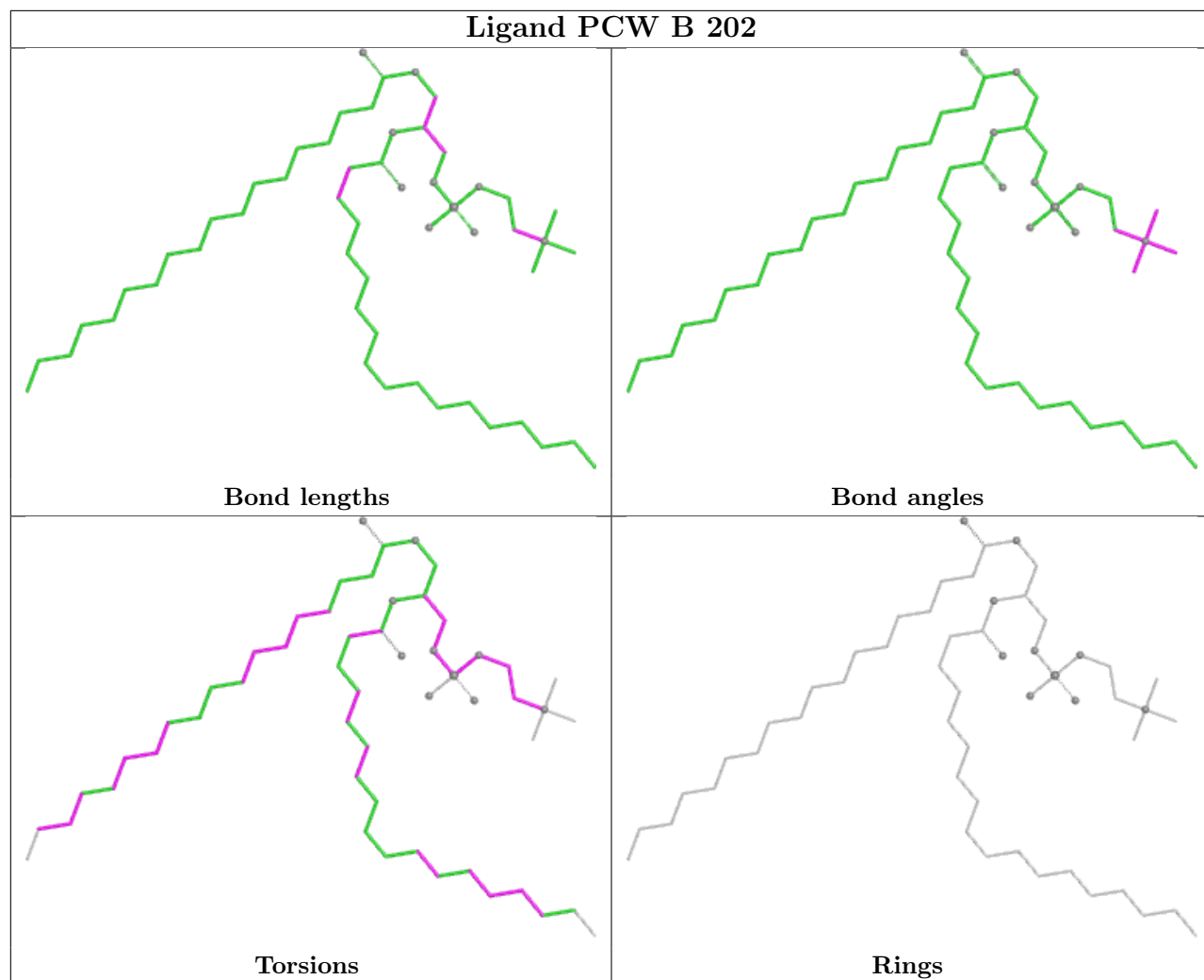


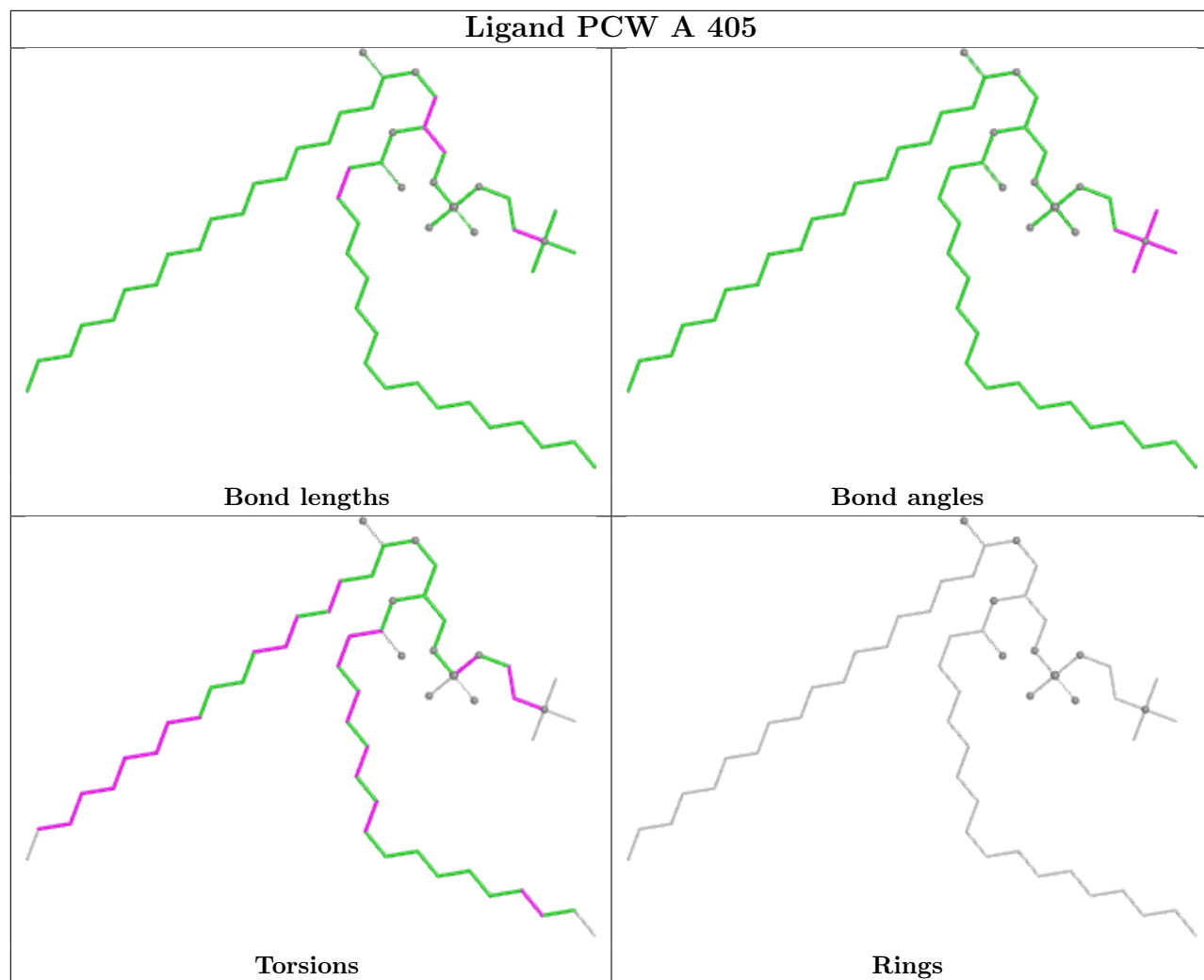


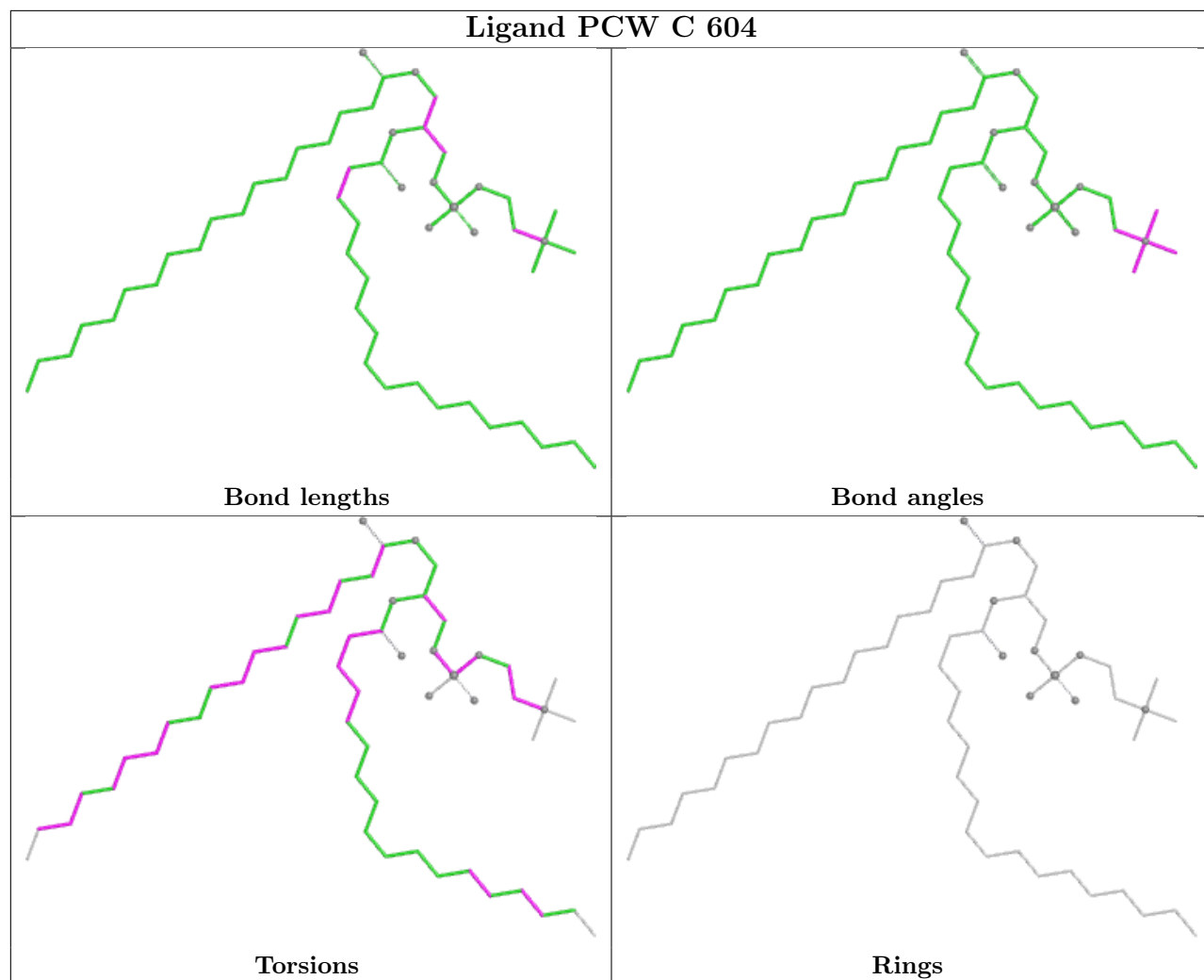


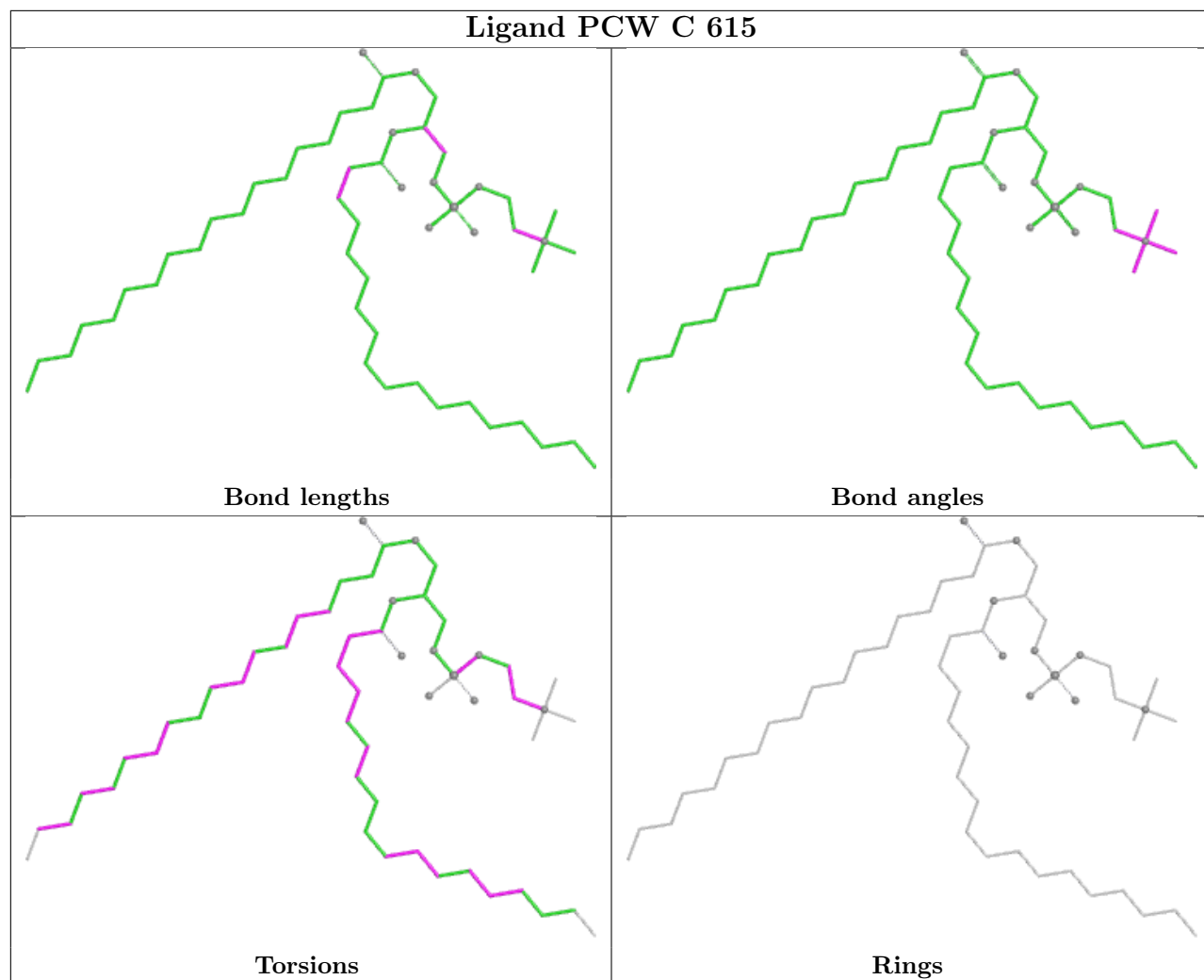


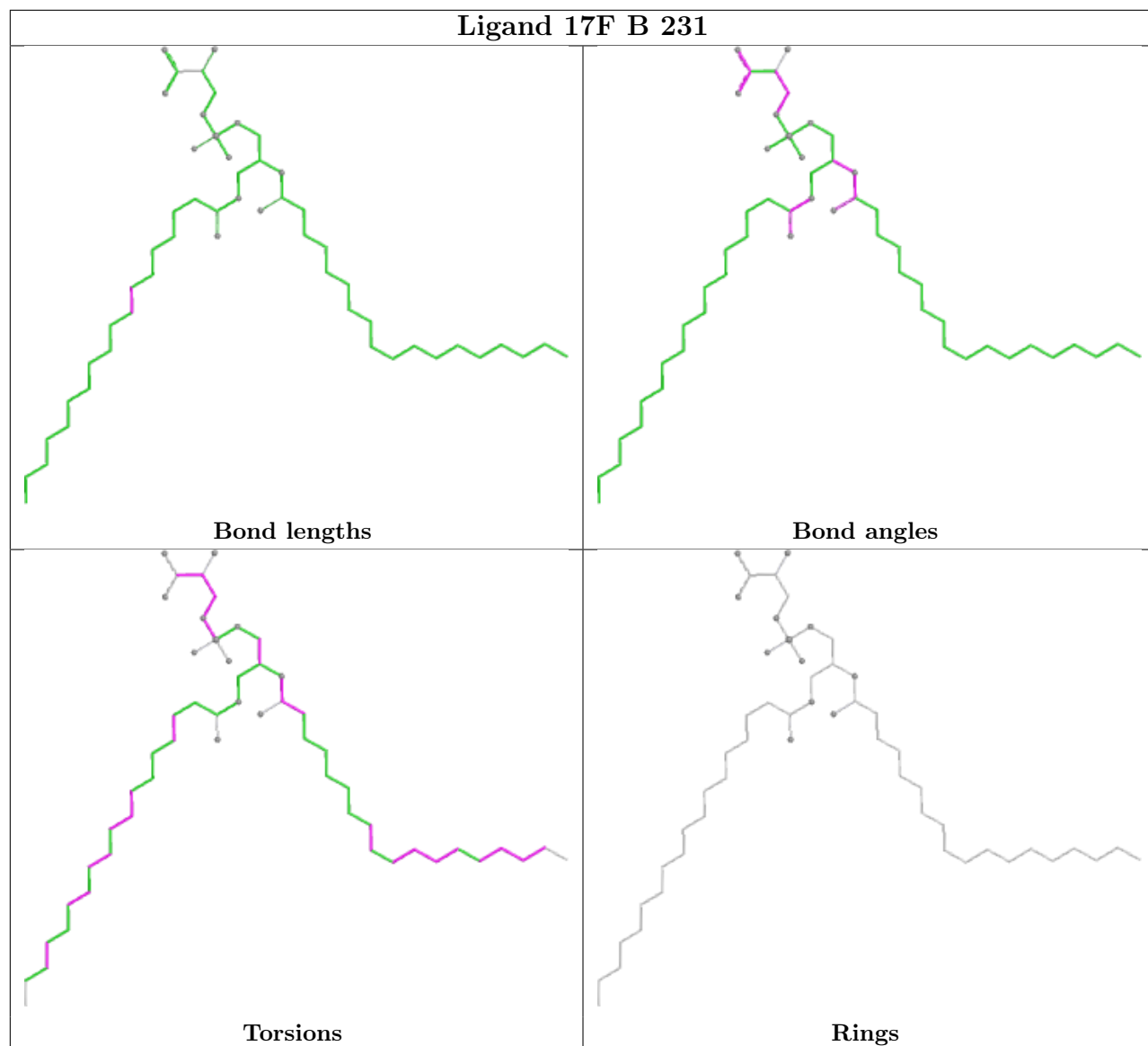


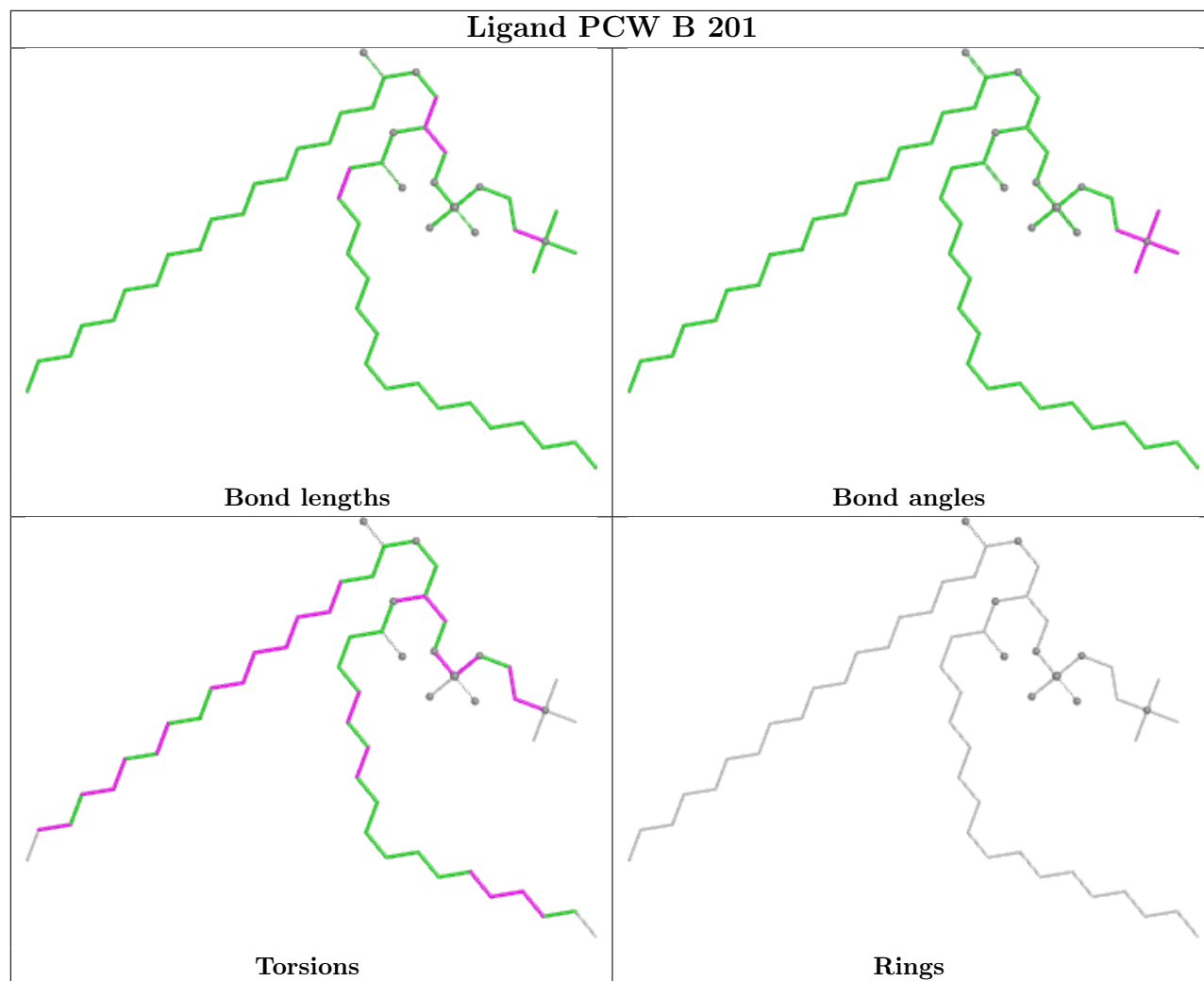


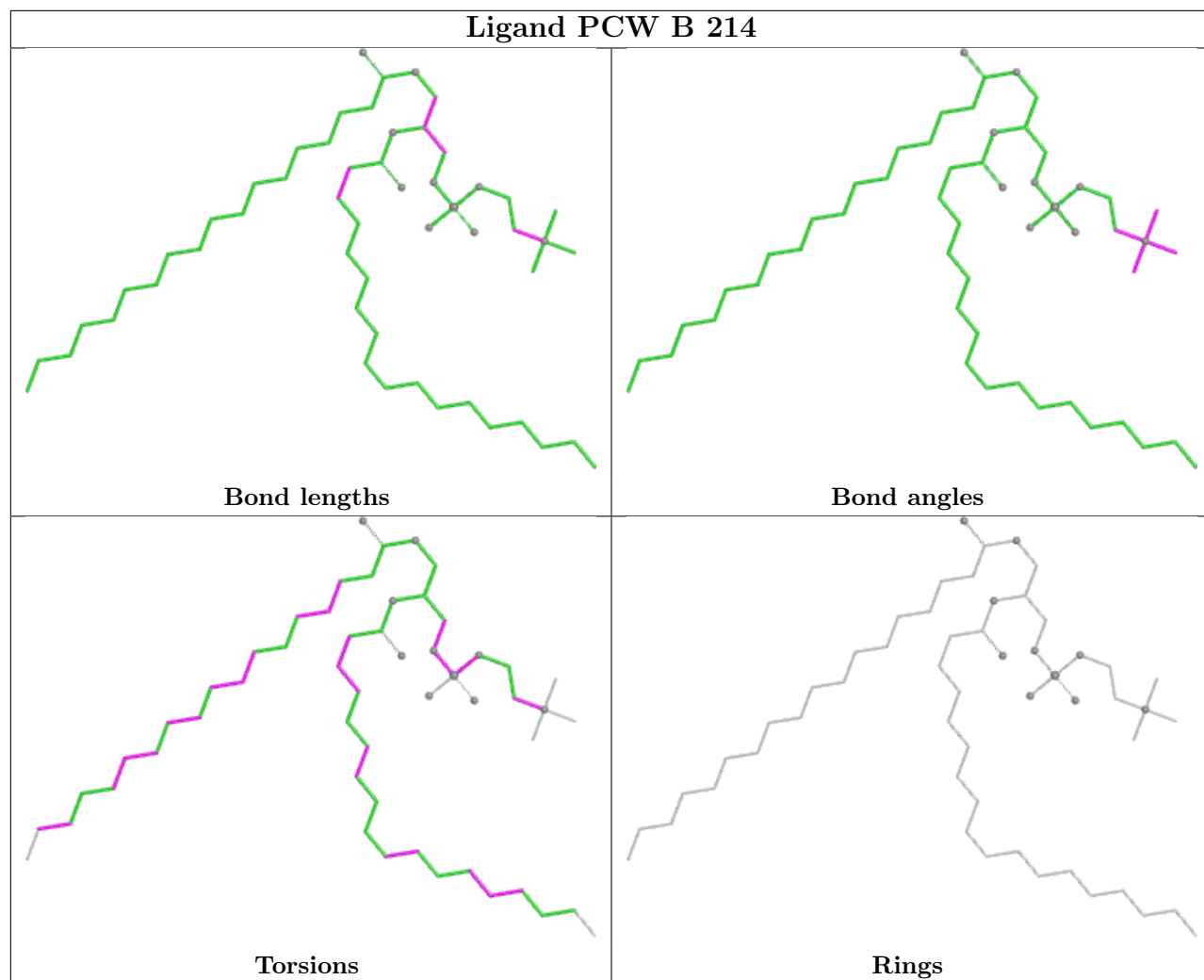


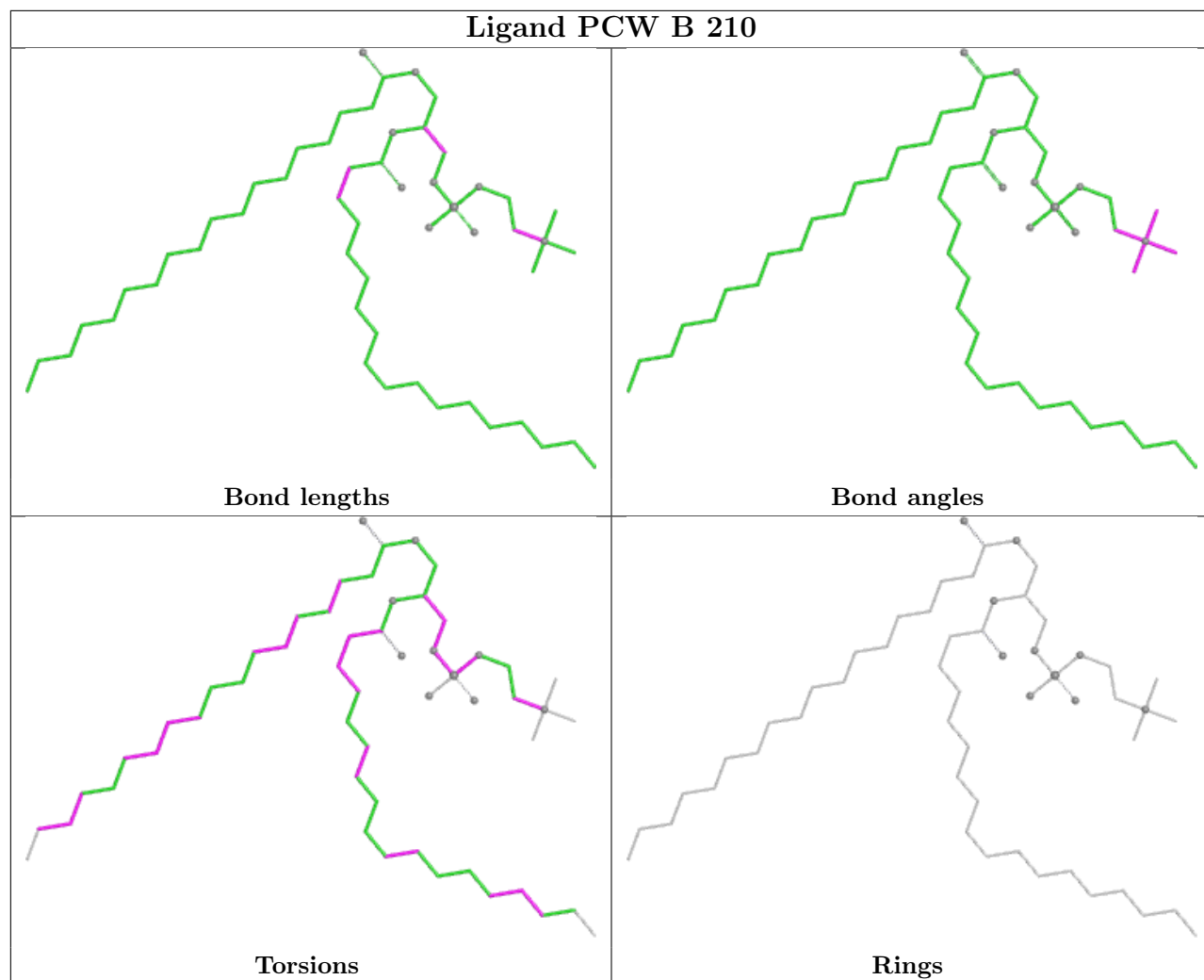


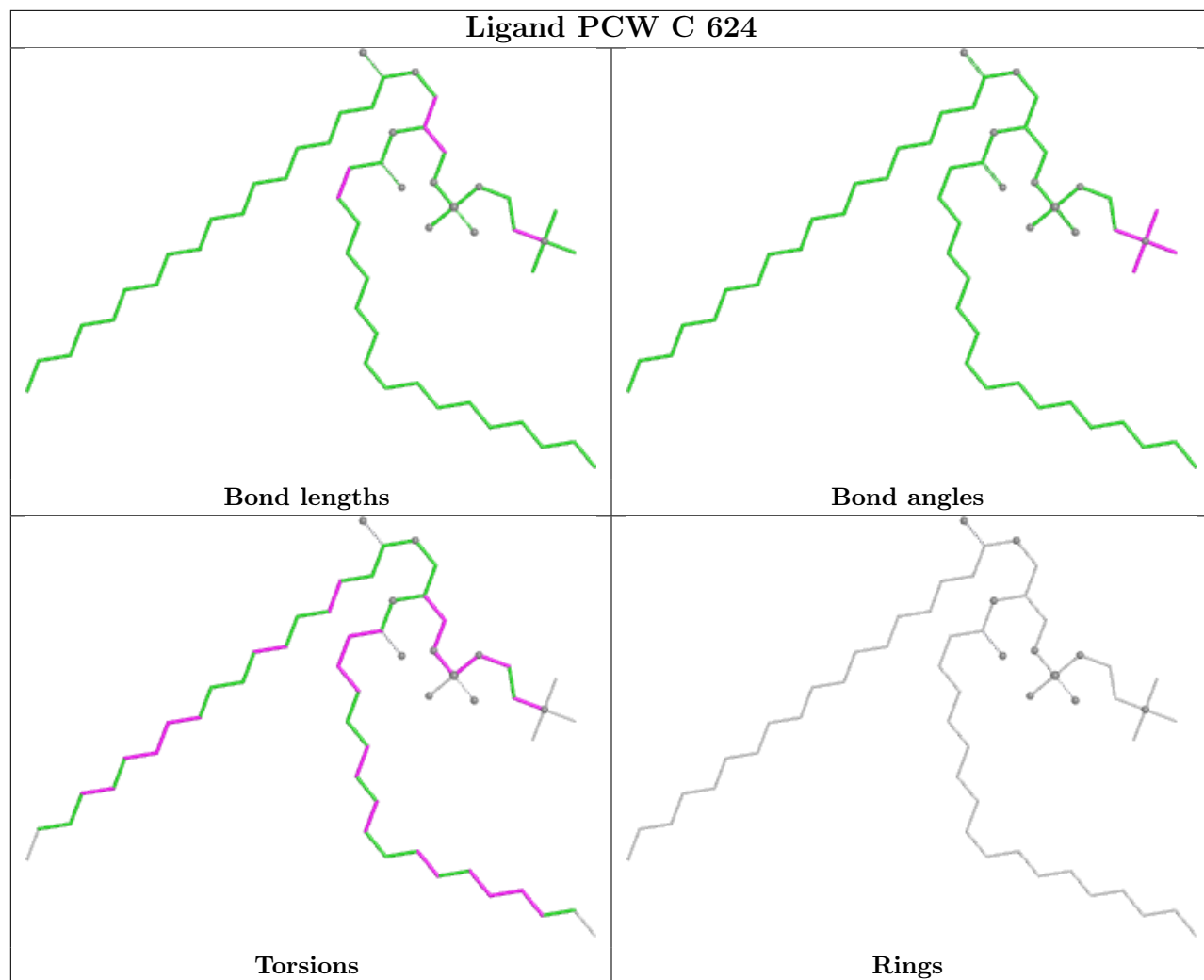


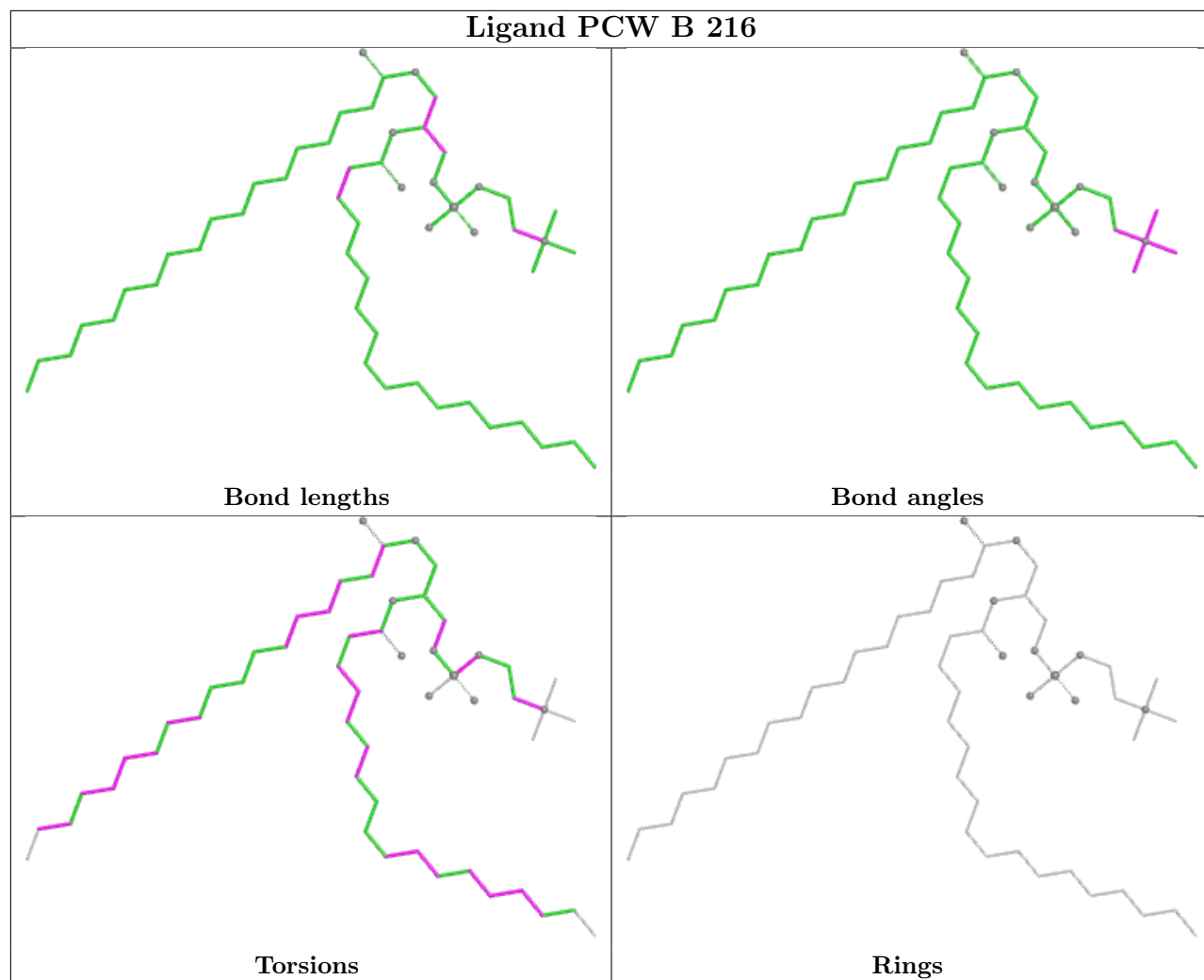


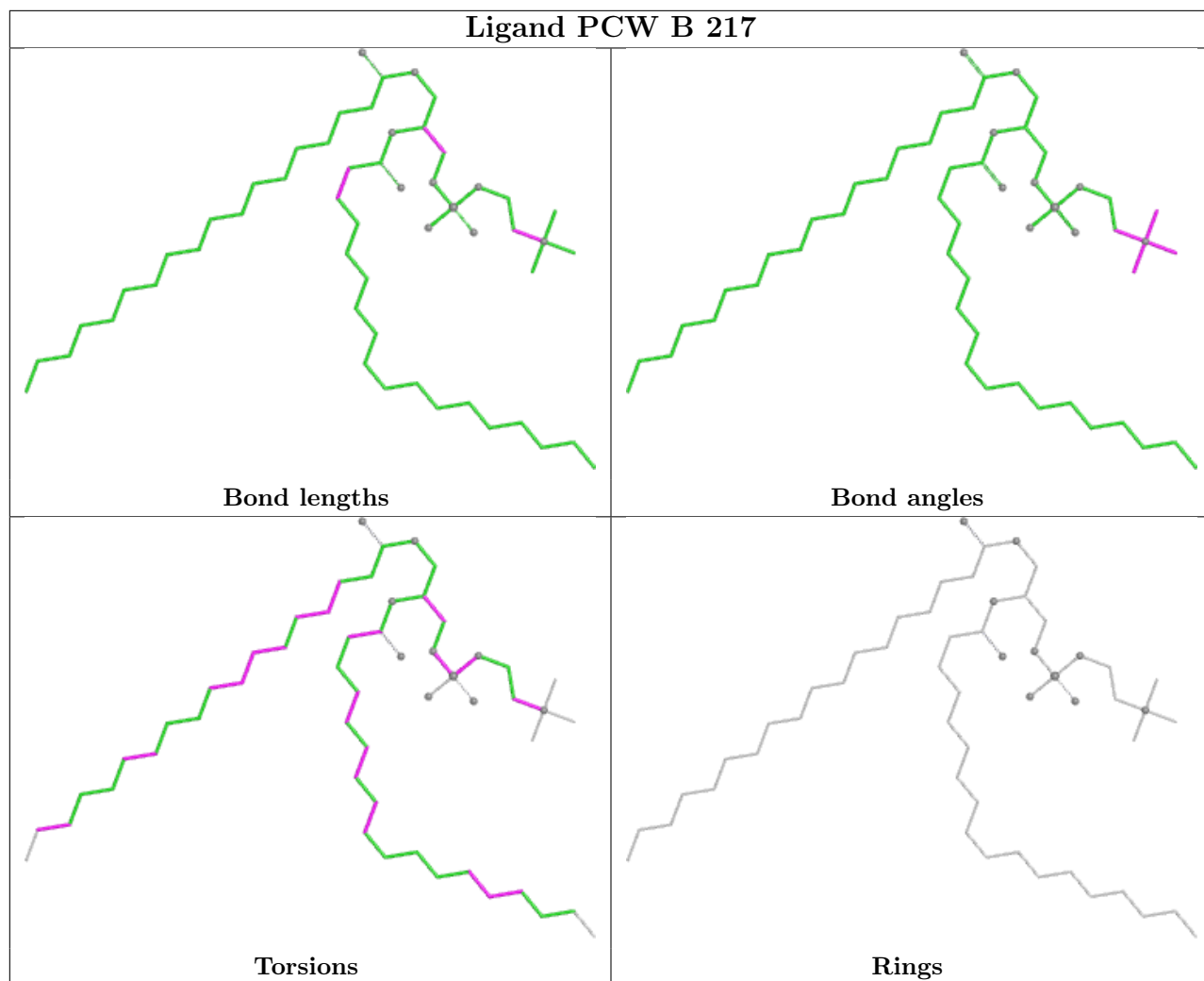


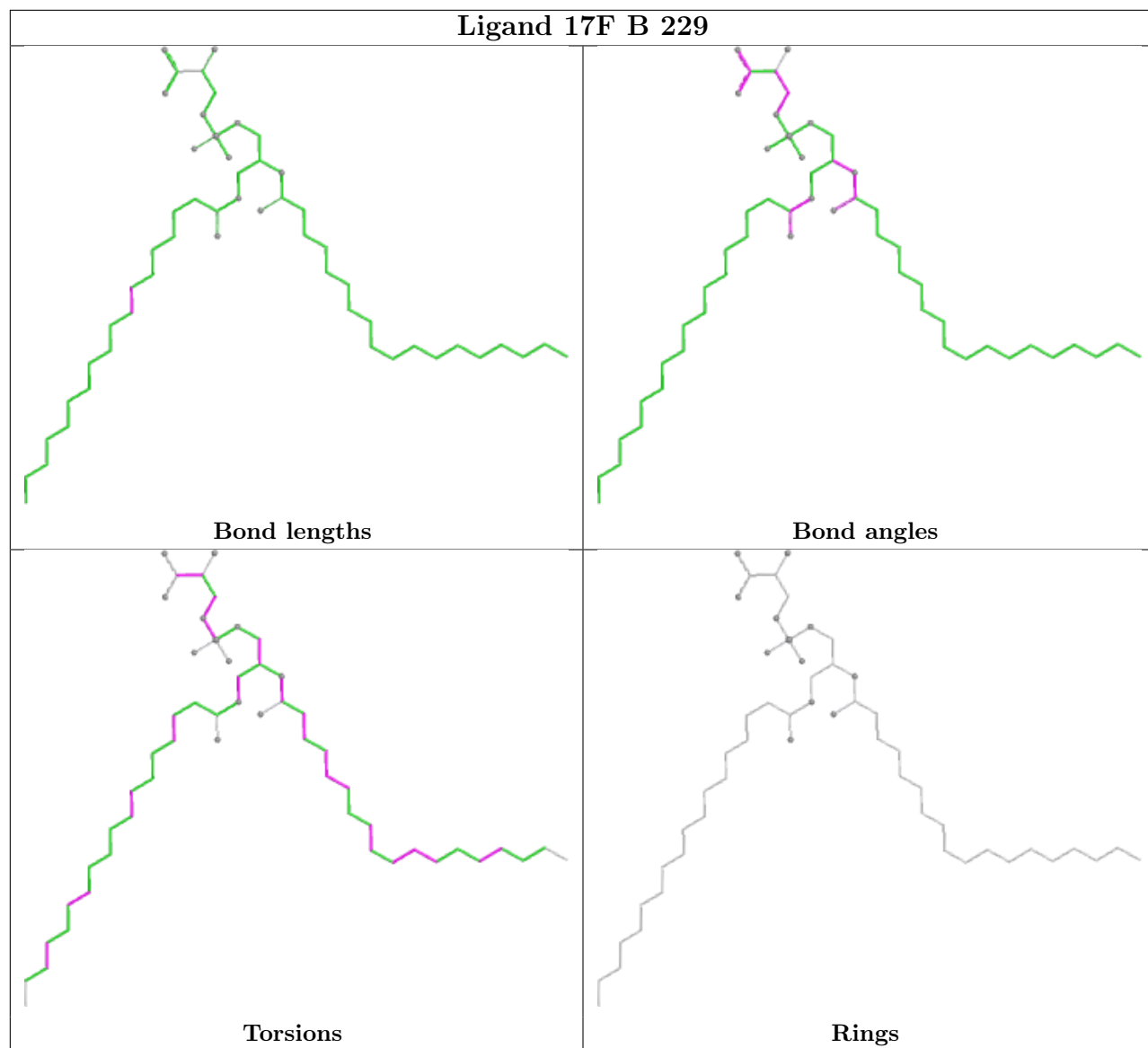


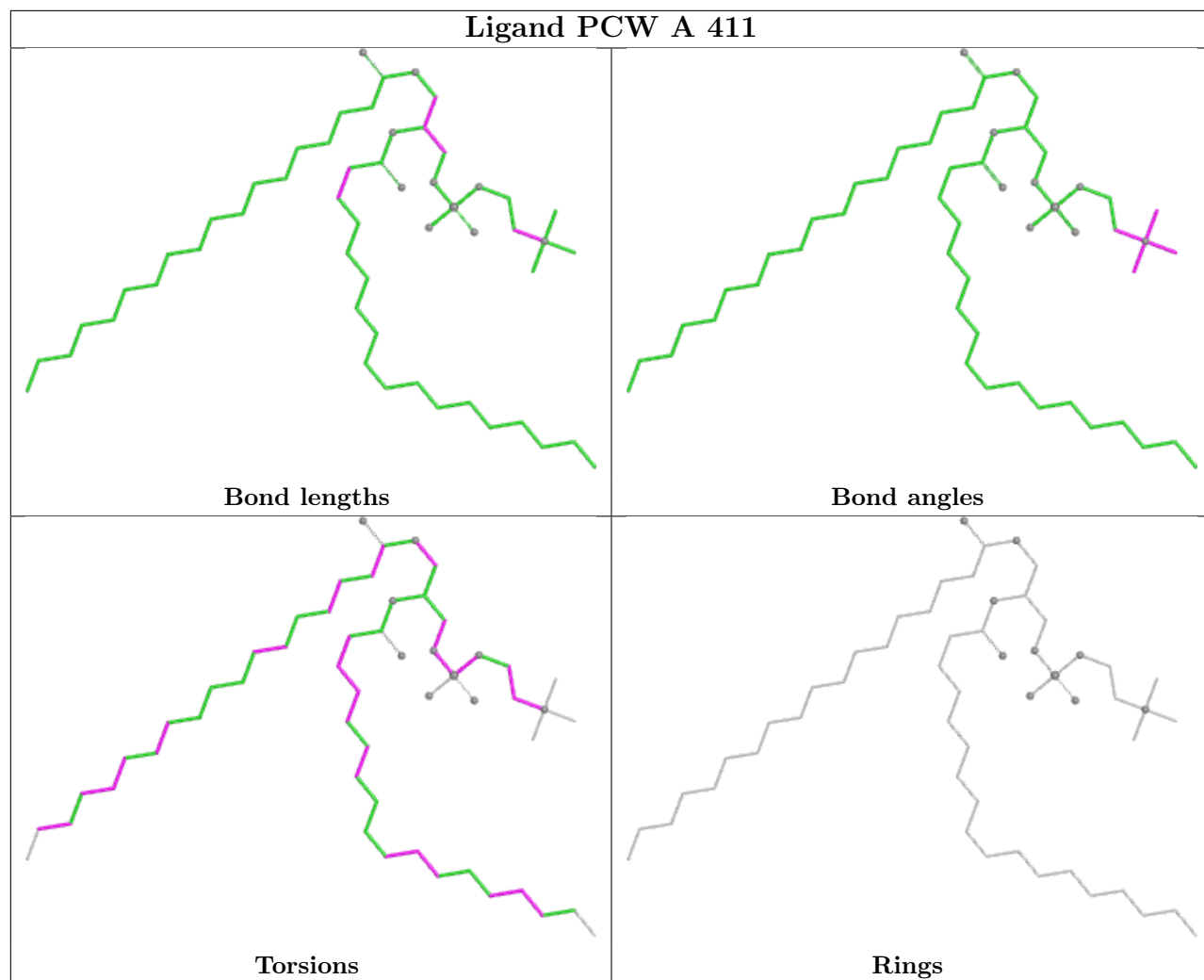


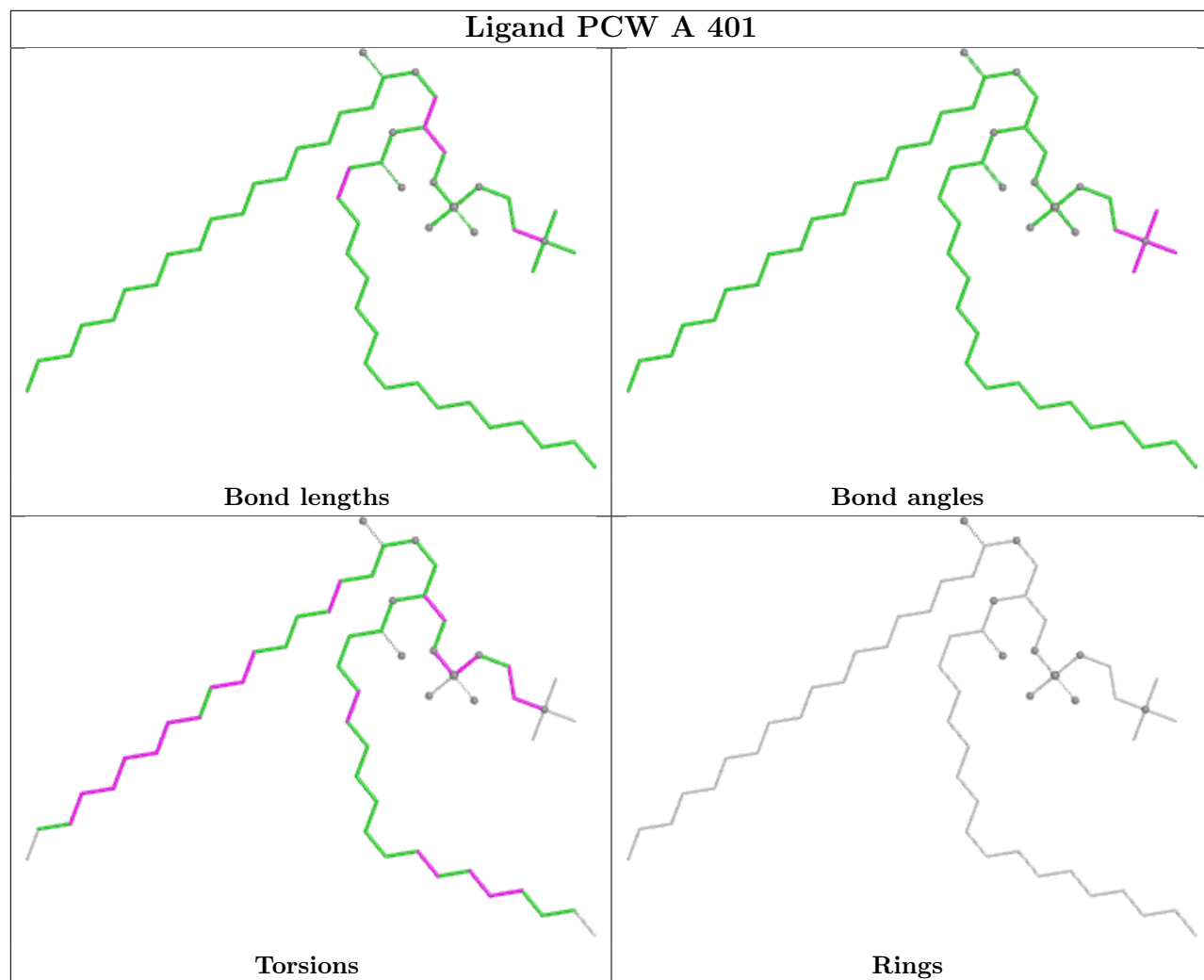


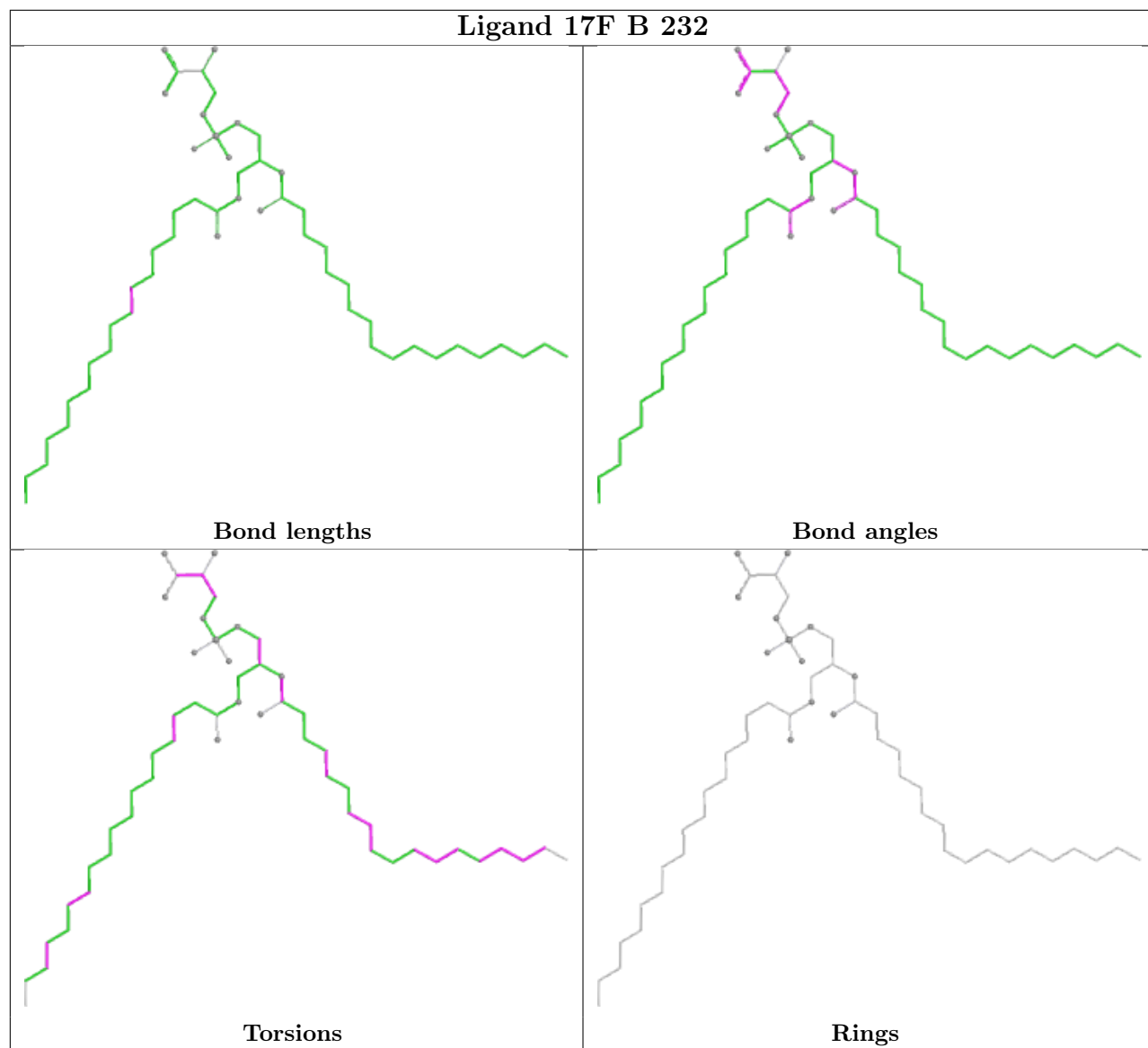


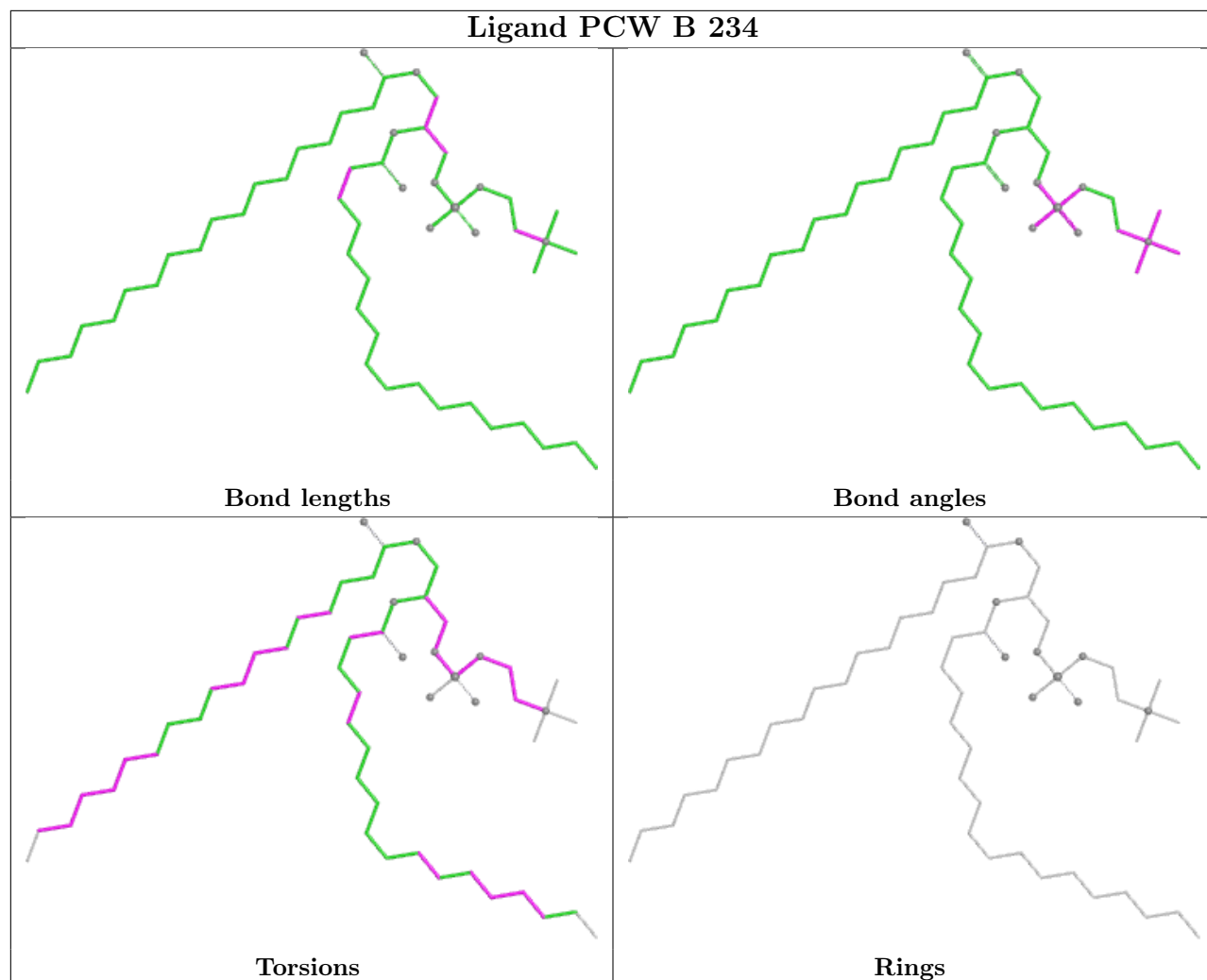


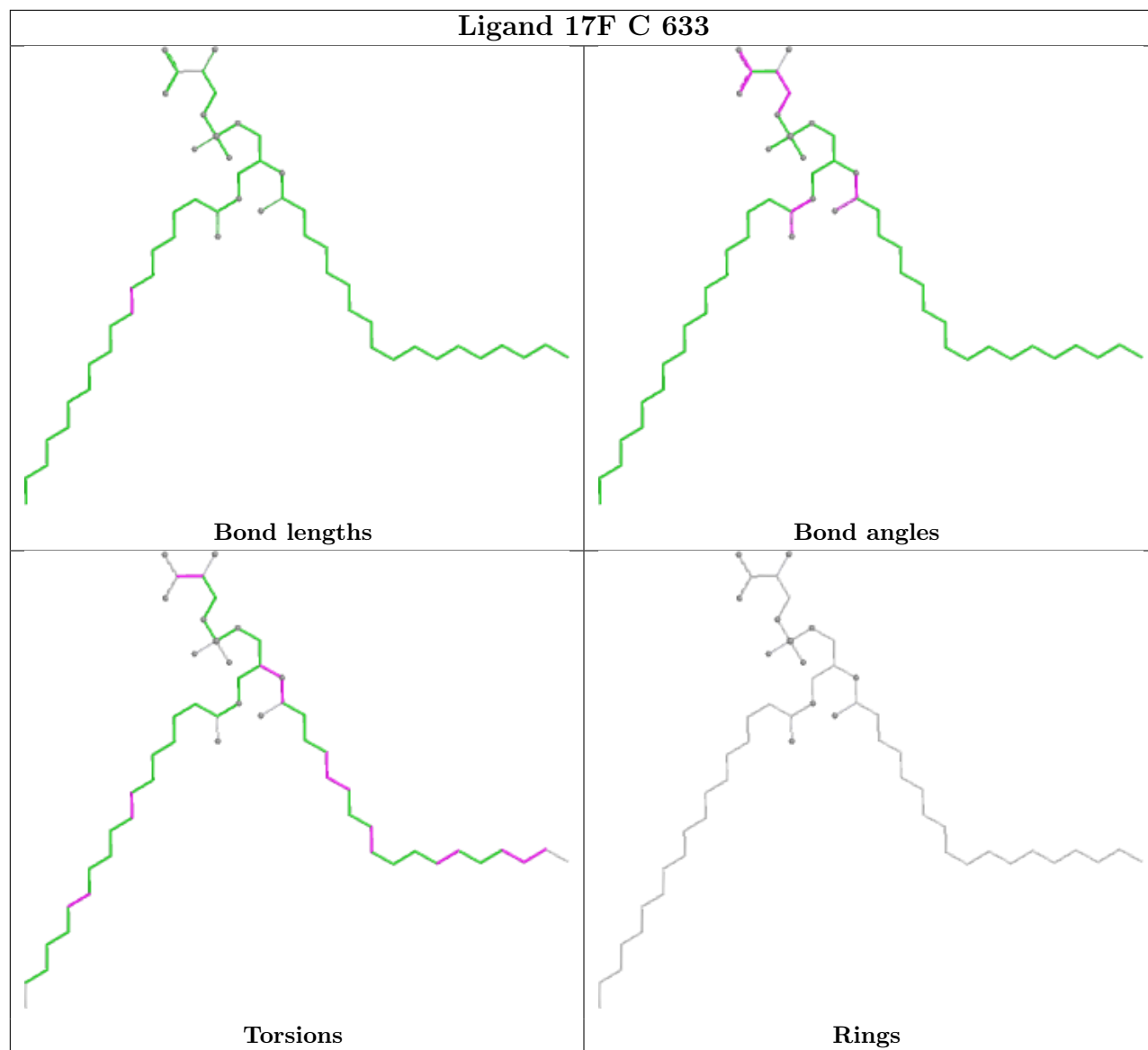


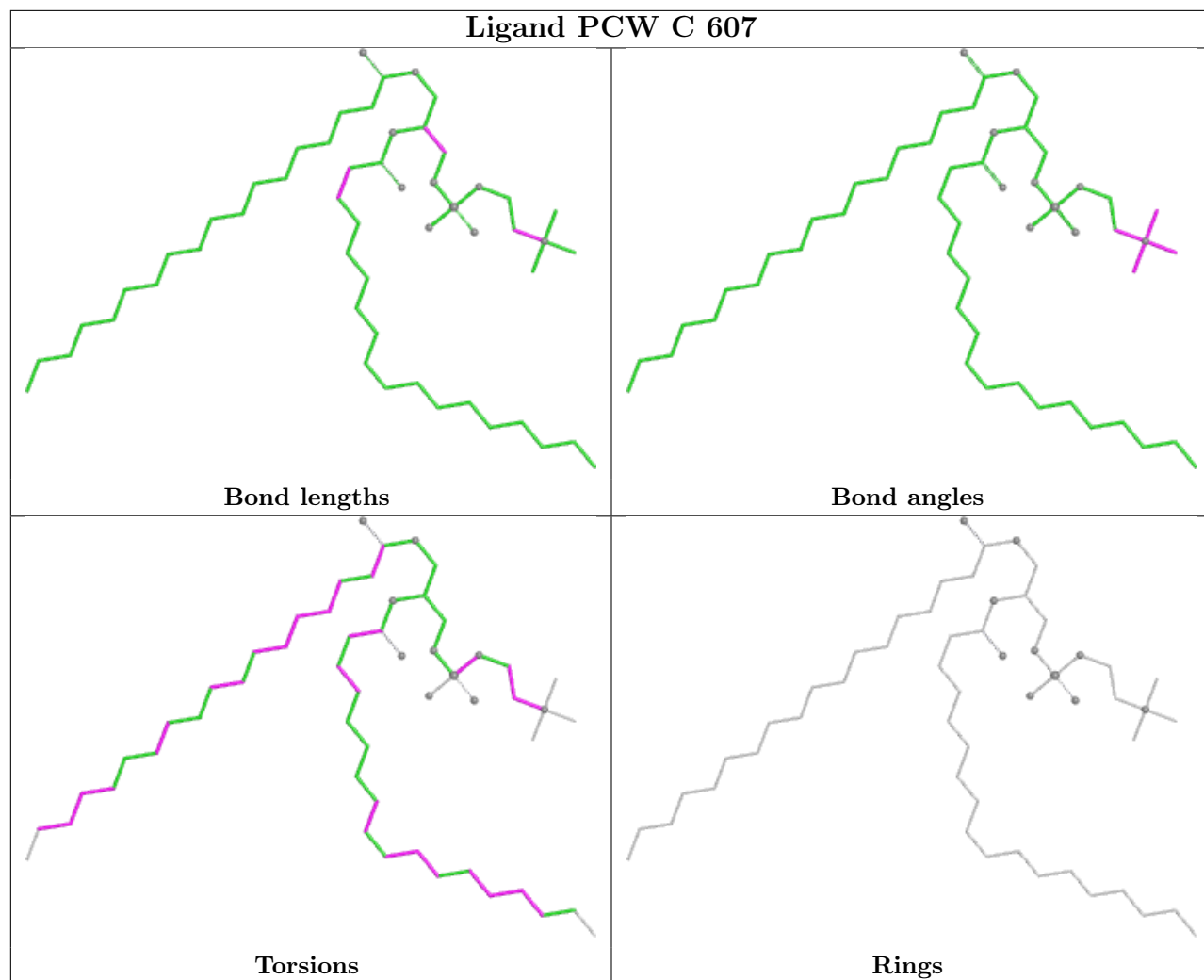


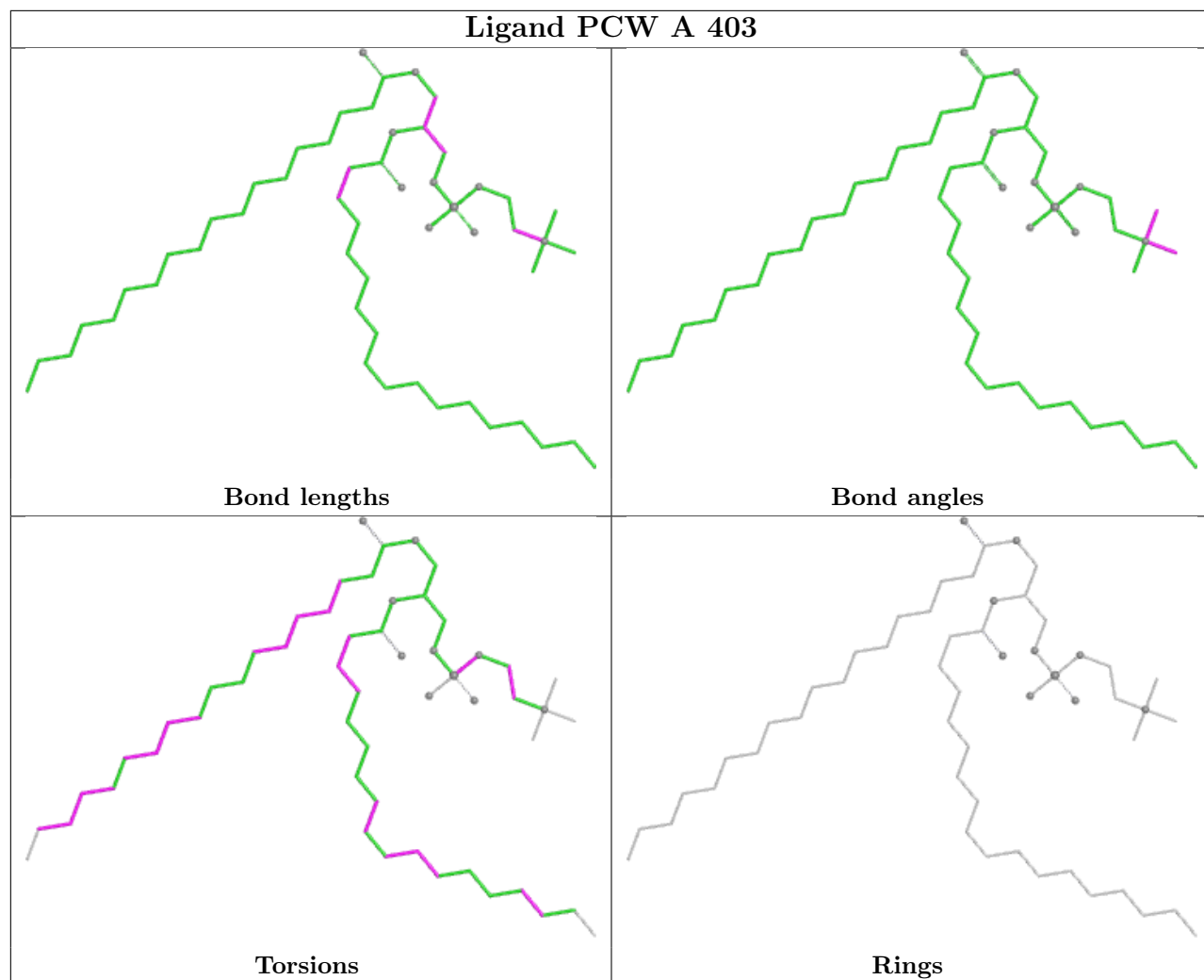


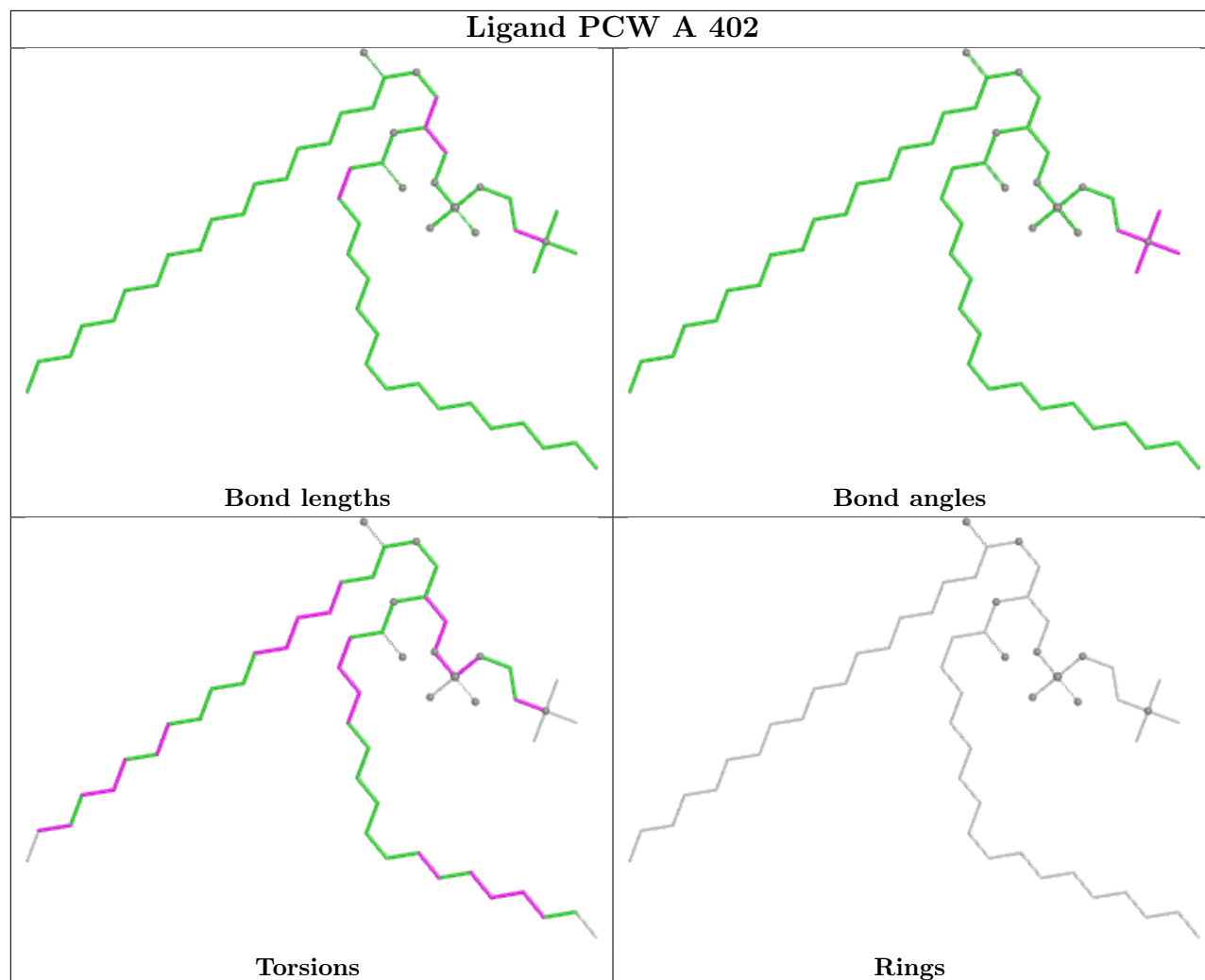












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *resonance_list_nmrstar_50_51.txt*

7.1.1 Bookkeeping i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	268
Number of shifts mapped to atoms	193
Number of unparsed shifts	0
Number of shifts with mapping errors	75
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 75) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	6	LEU	HD21	0.865	?	.
1	B	6	LEU	HD22	0.865	?	.
1	B	6	LEU	HD23	0.865	?	.
1	B	14	VAL	HG11	0.892	?	.
1	B	14	VAL	HG12	0.892	?	.
1	B	14	VAL	HG13	0.892	?	.
1	B	19	LEU	HD11	0.547	?	.
1	B	19	LEU	HD12	0.547	?	.
1	B	19	LEU	HD13	0.547	?	.
1	B	21	ILE	HD11	0.513	?	1
1	B	21	ILE	HD12	0.513	?	1
1	B	21	ILE	HD13	0.513	?	1
1	B	23	LEU	HD11	-0.325	?	.
1	B	23	LEU	HD12	-0.325	?	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	23	LEU	HD13	-0.325	?	.
1	B	24	ILE	HD11	0.389	?	1
1	B	24	ILE	HD12	0.389	?	1
1	B	24	ILE	HD13	0.389	?	1
1	B	36	ILE	HD11	0.714	?	1
1	B	36	ILE	HD12	0.714	?	1
1	B	36	ILE	HD13	0.714	?	1
1	B	46	ILE	HD11	0.361	?	1
1	B	46	ILE	HD12	0.361	?	1
1	B	46	ILE	HD13	0.361	?	1
1	B	55	ILE	HD11	0.451	?	1
1	B	55	ILE	HD12	0.451	?	1
1	B	55	ILE	HD13	0.451	?	1
1	B	79	LEU	HD11	0.023	?	.
1	B	79	LEU	HD12	0.023	?	.
1	B	79	LEU	HD13	0.023	?	.
1	B	79	LEU	HD21	0.081	?	.
1	B	79	LEU	HD22	0.081	?	.
1	B	79	LEU	HD23	0.081	?	.
1	B	84	ILE	HD11	0.7	?	1
1	B	84	ILE	HD12	0.7	?	1
1	B	84	ILE	HD13	0.7	?	1
1	B	93	ILE	HD11	0.724	?	1
1	B	93	ILE	HD12	0.724	?	1
1	B	93	ILE	HD13	0.724	?	1
1	B	100	ILE	HD11	0.234	?	1
1	B	100	ILE	HD12	0.234	?	1
1	B	100	ILE	HD13	0.234	?	1
1	B	113	LEU	HD11	0.989	?	.
1	B	113	LEU	HD12	0.989	?	.
1	B	113	LEU	HD13	0.989	?	.
1	B	113	LEU	HD21	1.261	?	.
1	B	113	LEU	HD22	1.261	?	.
1	B	113	LEU	HD23	1.261	?	.
1	B	120	LEU	HD21	0.8	?	.
1	B	120	LEU	HD22	0.8	?	.
1	B	120	LEU	HD23	0.8	?	.
1	B	125	VAL	HG11	-0.21	?	.
1	B	125	VAL	HG12	-0.21	?	.
1	B	125	VAL	HG13	-0.21	?	.
1	B	133	LEU	HD11	0.344	?	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	133	LEU	HD12	0.344	?	.
1	B	133	LEU	HD13	0.344	?	.
1	B	133	LEU	HD21	0.39	?	.
1	B	133	LEU	HD22	0.39	?	.
1	B	133	LEU	HD23	0.39	?	.
1	B	139	ILE	HD11	0.809	?	1
1	B	139	ILE	HD12	0.809	?	1
1	B	139	ILE	HD13	0.809	?	1
1	B	142	ILE	HD11	0.618	?	1
1	B	142	ILE	HD12	0.618	?	1
1	B	142	ILE	HD13	0.618	?	1
1	B	159	LEU	HD11	0.613	?	.
1	B	159	LEU	HD12	0.613	?	.
1	B	159	LEU	HD13	0.613	?	.
1	B	160	VAL	HG11	-0.056	?	.
1	B	160	VAL	HG12	-0.056	?	.
1	B	160	VAL	HG13	-0.056	?	.
1	B	163	ILE	HD11	0.612	?	1
1	B	163	ILE	HD12	0.612	?	1
1	B	163	ILE	HD13	0.612	?	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	84	-0.47 ± 0.76	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 254 atoms were assigned a chemical shift out of a possible 7385. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	154/2608 (6%)	77/1053 (7%)	0/1048 (0%)	77/507 (15%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	100/4339 (2%)	75/2790 (3%)	25/1354 (2%)	0/195 (0%)
Aromatic	0/438 (0%)	0/222 (0%)	0/208 (0%)	0/8 (0%)
Overall	254/7385 (3%)	152/4065 (4%)	25/2610 (1%)	77/710 (11%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:

