



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:43 PM UTC

PDB ID : 6CCH / pdb_00006cch
BMRB ID : 30401
Title : NMR data-driven model of GTPase KRas-GMPPNP tethered to a nanodisc (E3 state)
Authors : Fang, Z.; Marshall, C.B.; Nishikawa, T.; Gossert, A.D.; Jansen, J.M.; Jahnke, W.; Ikura, M.
Deposited on : 2018-02-07

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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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

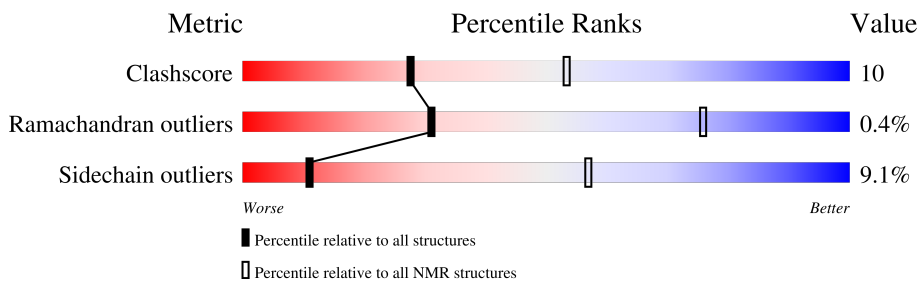
1 Overall quality at a glance

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	68% 14% 16% .
1	C	200	82% 15% ..
2	B	187	81% 11% 7% .

2 Ensemble composition and analysis i

This entry contains 7 models. Model 3 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:231-A:395, C:401-C:596 (361)	0.43	3
2	B:1-B:172 (172)	0.73	1

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4
2	3, 5, 7
Single-model clusters	6

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9487 atoms, of which 407 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

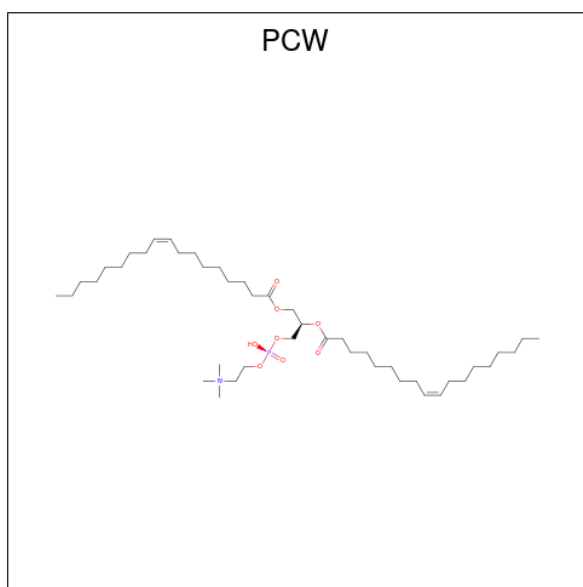
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	185	1843	926	363	257	288	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).



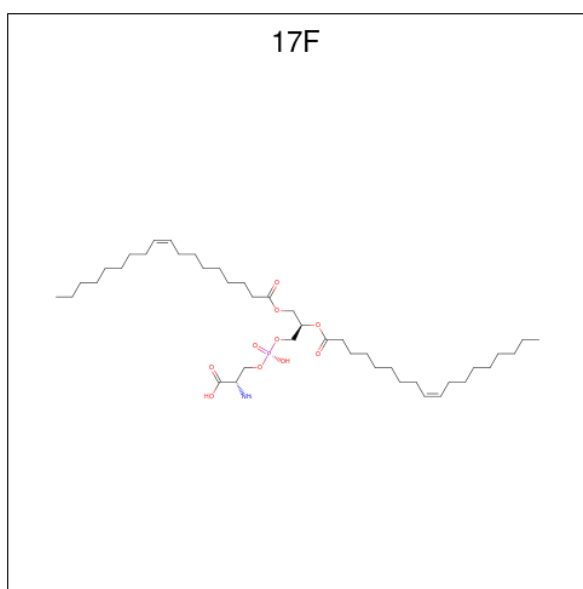
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total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

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



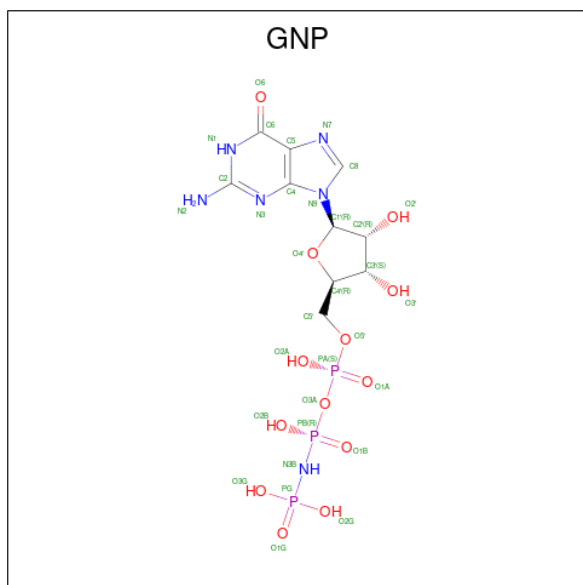
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1

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

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



Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	B	1	32	10	6	13	3

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

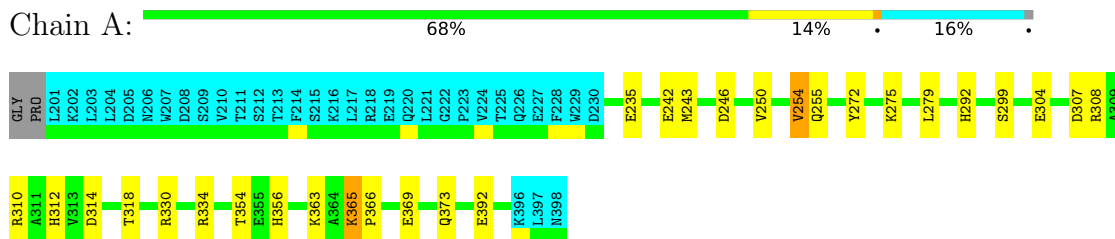
Mol	Chain	Residues	Atoms	
			Total	Mg
6	B	1	1	1

4 Residue-property plots [i](#)

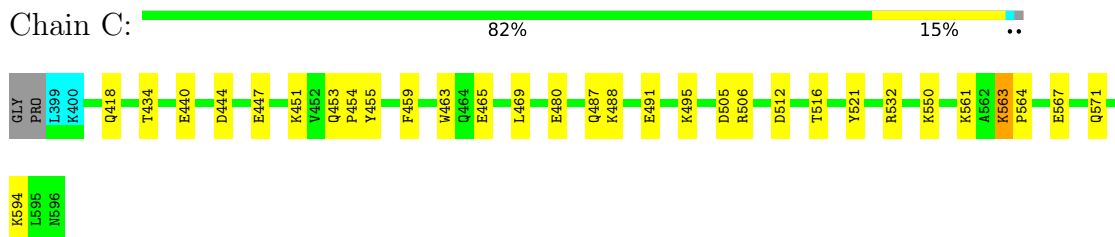
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

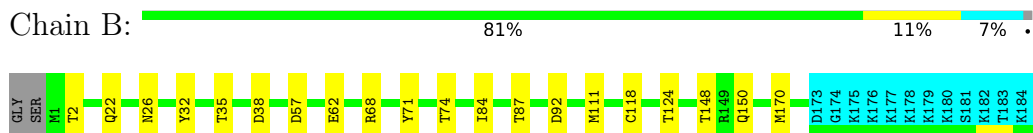
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

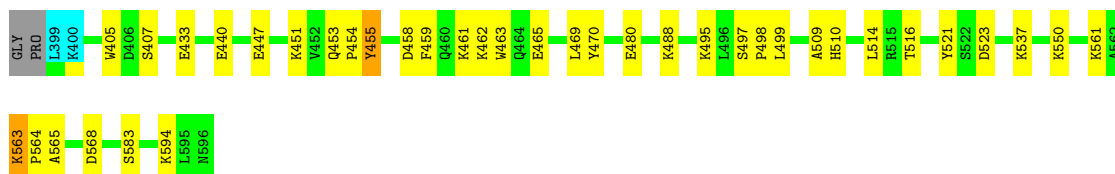
- Molecule 1: Apolipoprotein A-I





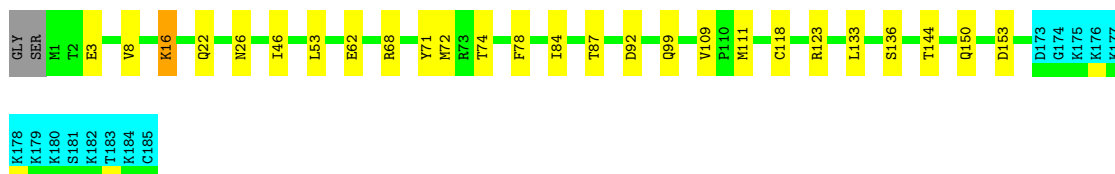
- Molecule 1: Apolipoprotein A-I

Chain C: 79% 18% ...



- Molecule 2: GTPase KRas

Chain B: 78% 13% 7%



5 Refinement protocol and experimental data overview

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

Of the 3000 calculated structures, 7 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	structure calculation	
CNS	refinement	

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, GNP, MG, PCW

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±0/1368 (0.0± 0.0%)	0.79±0.01	0±0/1836 (0.0± 0.0%)
1	C	0.40±0.00	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±0/1398 (0.0± 0.0%)	0.68±0.01	0±0/1885 (0.0± 0.0%)
All	All	0.38	0/30800 (0.0%)	0.76	1/41419 (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	36	ILE	N-CA-C	-5.13	107.40	111.81	7	1

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	1347	18	1355	30±7
1	C	1607	22	1601	42±16
2	B	1376	323	1366	13±3
3	A	3456	0	5374	126±20
4	A	864	0	1216	47±4
5	B	32	0	13	1±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	60781	2541	76490	1325

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 10.

5 of 1082 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:8:PCW:H272	1:C:459:PHE:CZ	1.65	1.18	6	1
3:A:15:PCW:H281	1:C:554:HIS:CE1	1.64	1.26	6	1
3:A:15:PCW:C28	1:C:554:HIS:CE1	1.55	1.85	6	1
3:A:65:PCW:H281	1:C:488:LYS:CE	1.54	1.23	6	2
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.51	1.34	1	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	165/200 (82%)	161±1 (98±1%)	3±1 (2±1%)	1±0 (1±0%)	23	72
1	C	195/200 (98%)	190±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	23	72
2	B	171/187 (91%)	164±3 (96±2%)	7±3 (4±2%)	0±0 (0±0%)	49	83
All	All	3717/4109 (90%)	3605 (97%)	96 (3%)	16 (0%)	31	76

All 4 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	7
1	C	563	LYS	7
1	C	420	GLY	1
2	B	36	ILE	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	142/175 (81%)	129±3 (91±2%)	13±3 (9±2%)	10	55
1	C	172/175 (98%)	156±2 (91±1%)	16±2 (9±1%)	10	55
2	B	153/166 (92%)	140±3 (92±2%)	13±3 (8±2%)	12	59
All	All	3269/3612 (91%)	2970 (91%)	299 (9%)	11	57

5 of 154 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	7
2	B	74	THR	7
1	A	312	HIS	6
2	B	92	ASP	6
1	C	550	LYS	6

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 [i](#)

Of 82 ligands modelled in this entry, 1 is monoatomic - leaving 81 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	A	46	-	53,53,53	1.04±0.00	4±0 (6±0%)
3	PCW	A	8	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	30	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	2	-	53,53,53	1.04±0.00	4±0 (7±0%)
4	17F	A	40	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	5	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	43	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	42	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	50	-	53,53,53	1.04±0.01	5±0 (9±0%)
4	17F	A	37	-	52,53,53	0.92±0.00	1±0 (1±0%)
3	PCW	A	17	-	53,53,53	1.04±0.01	3±0 (6±0%)
3	PCW	A	62	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	17F	A	75	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	4	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	6	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	A	25	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	69	-	53,53,53	1.05±0.01	4±1 (7±1%)
3	PCW	A	3	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	9	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	A	71	-	53,53,53	1.04±0.01	3±0 (6±0%)
3	PCW	A	64	-	53,53,53	1.05±0.01	3±0 (6±0%)
3	PCW	A	13	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	11	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	27	-	53,53,53	1.07±0.01	5±0 (9±0%)
4	17F	A	39	-	52,53,53	0.92±0.00	1±0 (1±0%)
3	PCW	A	63	-	53,53,53	1.04±0.01	3±0 (6±0%)
4	17F	A	34	-	52,53,53	0.92±0.01	1±0 (1±0%)
4	17F	A	77	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	60	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	61	-	53,53,53	1.05±0.01	4±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	A	36	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	57	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	67	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	A	41	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	65	-	53,53,53	1.04±0.00	5±1 (9±1%)
3	PCW	A	31	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	72	-	53,53,53	1.05±0.01	5±0 (8±0%)
4	17F	A	35	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	44	-	53,53,53	1.05±0.01	3±0 (6±0%)
3	PCW	A	45	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	22	-	53,53,53	1.04±0.00	4±0 (7±0%)
5	GNP	B	201	-	34,34,34	1.51±0.02	5±0 (14±0%)
3	PCW	A	18	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	32	-	53,53,53	1.06±0.01	5±0 (8±0%)
4	17F	A	73	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	23	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	16	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	A	20	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	80	-	52,53,53	0.91±0.01	1±0 (1±0%)
3	PCW	A	15	-	53,53,53	1.04±0.01	5±0 (8±0%)
3	PCW	A	48	-	53,53,53	1.04±0.01	5±0 (8±0%)
3	PCW	A	49	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	55	-	53,53,53	1.07±0.01	5±0 (9±0%)
4	17F	A	38	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	51	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	21	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	54	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	56	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	1	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	A	79	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	66	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	A	68	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	19	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	A	28	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	47	-	53,53,53	1.05±0.01	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	7	-	53,53,53	1.05±0.00	5±0 (9±0%)
4	17F	A	74	-	52,53,53	0.91±0.00	0±0 (0±0%)
3	PCW	A	26	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	52	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	70	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	14	-	53,53,53	1.05±0.00	4±0 (7±0%)
3	PCW	A	24	-	53,53,53	1.04±0.01	3±0 (6±0%)
4	17F	A	78	-	52,53,53	0.92±0.00	1±0 (1±0%)
3	PCW	A	10	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	A	29	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	A	53	-	53,53,53	1.04±0.01	4±0 (7±0%)
4	17F	A	76	-	52,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	59	-	53,53,53	1.06±0.01	4±0 (7±0%)
4	17F	A	33	-	52,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	12	-	53,53,53	1.05±0.00	5±0 (9±0%)
3	PCW	A	58	-	53,53,53	1.04±0.01	4±0 (7±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	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	A	46	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	8	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	30	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	A	2	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	A	40	-	54,60,60	1.04±0.01	5±0 (9±0%)
3	PCW	A	5	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	43	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	42	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	50	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	37	-	54,60,60	1.05±0.01	5±0 (9±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	17	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	62	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	75	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	4	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	6	-	59,61,61	2.76±0.01	9±0 (15±0%)
3	PCW	A	25	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	69	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	3	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	9	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	71	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	64	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	13	-	59,61,61	2.33±0.00	5±0 (8±0%)
3	PCW	A	11	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	27	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	39	-	54,60,60	1.07±0.02	5±0 (9±0%)
3	PCW	A	63	-	59,61,61	2.77±0.01	9±0 (15±0%)
4	17F	A	34	-	54,60,60	1.05±0.02	5±0 (9±0%)
4	17F	A	77	-	54,60,60	1.79±0.02	10±0 (18±0%)
3	PCW	A	60	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	61	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	A	36	-	54,60,60	1.07±0.03	5±0 (9±0%)
3	PCW	A	57	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	67	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	41	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	65	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	31	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	72	-	59,61,61	0.83±0.01	1±0 (1±0%)
4	17F	A	35	-	54,60,60	1.04±0.01	5±0 (9±0%)
3	PCW	A	44	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	45	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	22	-	59,61,61	2.32±0.01	5±0 (8±0%)
5	GNP	B	201	-	47,54,54	0.83±0.01	1±0 (2±0%)
3	PCW	A	18	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	32	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	73	-	54,60,60	1.06±0.02	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	23	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	16	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	20	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	80	-	54,60,60	1.04±0.02	4±0 (7±0%)
3	PCW	A	15	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	48	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	49	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	55	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	A	38	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	A	51	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	21	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	54	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	56	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	1	-	59,61,61	2.33±0.01	5±0 (8±0%)
4	17F	A	79	-	54,60,60	1.05±0.01	5±0 (8±0%)
3	PCW	A	66	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	68	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	19	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	28	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	47	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	A	7	-	59,61,61	0.85±0.01	1±0 (1±0%)
4	17F	A	74	-	54,60,60	1.09±0.02	5±0 (9±0%)
3	PCW	A	26	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	52	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	70	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	14	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	24	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	78	-	54,60,60	1.06±0.02	5±0 (9±0%)
3	PCW	A	10	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	29	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	53	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	A	76	-	54,60,60	1.04±0.02	5±0 (9±0%)
3	PCW	A	59	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	A	33	-	54,60,60	1.77±0.01	9±0 (16±0%)
3	PCW	A	12	-	59,61,61	0.84±0.01	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	58	-	59,61,61	2.32±0.01	5±0 (8±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	A	30	-	-	0±0,57,57,57	-
4	17F	A	37	-	-	0±0,59,59,59	-
3	PCW	A	11	-	-	0±0,57,57,57	-
3	PCW	A	50	-	-	0±0,57,57,57	-
3	PCW	A	46	-	-	0±0,57,57,57	-
3	PCW	A	57	-	-	0±0,57,57,57	-
4	17F	A	35	-	-	0±0,59,59,59	-
3	PCW	A	44	-	-	0±0,57,57,57	-
3	PCW	A	27	-	-	0±0,57,57,57	-
3	PCW	A	13	-	-	0±0,57,57,57	-
3	PCW	A	18	-	-	0±0,57,57,57	-
3	PCW	A	31	-	-	0±0,57,57,57	-
3	PCW	A	8	-	-	0±0,57,57,57	-
3	PCW	A	67	-	-	0±0,57,57,57	-
3	PCW	A	19	-	-	0±0,57,57,57	-
3	PCW	A	45	-	-	0±0,57,57,57	-
3	PCW	A	55	-	-	0±0,57,57,57	-
3	PCW	A	26	-	-	0±0,57,57,57	-
3	PCW	A	65	-	-	0±0,57,57,57	-
3	PCW	A	14	-	-	0±0,57,57,57	-
3	PCW	A	22	-	-	0±0,57,57,57	-
5	GNP	B	201	-	-	0±0,18,38,38	0±0,3,3,3
3	PCW	A	47	-	-	0±0,57,57,57	-
3	PCW	A	48	-	-	0±0,57,57,57	-
4	17F	A	79	-	-	0±0,59,59,59	-
3	PCW	A	51	-	-	0±0,57,57,57	-
3	PCW	A	25	-	-	0±0,57,57,57	-
3	PCW	A	66	-	-	0±0,57,57,57	-
3	PCW	A	20	-	-	0±0,57,57,57	-
3	PCW	A	70	-	-	0±0,57,57,57	-
3	PCW	A	28	-	-	0±0,57,57,57	-
4	17F	A	38	-	-	0±0,59,59,59	-
3	PCW	A	7	-	-	0±0,57,57,57	-
3	PCW	A	24	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	54	-	-	0±0,57,57,57	-
4	17F	A	74	-	-	0±0,59,59,59	-
3	PCW	A	29	-	-	0±0,57,57,57	-
3	PCW	A	6	-	-	0±0,57,57,57	-
4	17F	A	40	-	-	0±0,59,59,59	-
3	PCW	A	64	-	-	0±0,57,57,57	-
4	17F	A	76	-	-	0±0,59,59,59	-
3	PCW	A	4	-	-	0±0,57,57,57	-
3	PCW	A	2	-	-	0±0,57,57,57	-
3	PCW	A	21	-	-	0±0,57,57,57	-
3	PCW	A	9	-	-	0±0,57,57,57	-
4	17F	A	78	-	-	0±0,59,59,59	-
3	PCW	A	71	-	-	0±0,57,57,57	-
3	PCW	A	68	-	-	0±0,57,57,57	-
4	17F	A	77	-	-	0±0,59,59,59	-
4	17F	A	73	-	-	0±0,59,59,59	-
3	PCW	A	15	-	-	0±0,57,57,57	-
3	PCW	A	59	-	-	0±0,57,57,57	-
3	PCW	A	1	-	-	0±0,57,57,57	-
3	PCW	A	12	-	-	0±0,57,57,57	-
3	PCW	A	52	-	-	0±0,57,57,57	-
4	17F	A	80	-	-	0±0,59,59,59	-
3	PCW	A	72	-	-	0±0,57,57,57	-
3	PCW	A	58	-	-	0±0,57,57,57	-
3	PCW	A	69	-	-	0±0,57,57,57	-
3	PCW	A	16	-	-	0±0,57,57,57	-
4	17F	A	39	-	-	0±0,59,59,59	-
3	PCW	A	43	-	-	0±0,57,57,57	-
3	PCW	A	42	-	-	0±0,57,57,57	-
4	17F	A	34	-	-	0±0,59,59,59	-
3	PCW	A	10	-	-	0±0,57,57,57	-
3	PCW	A	3	-	-	0±0,57,57,57	-
3	PCW	A	53	-	-	0±0,57,57,57	-
3	PCW	A	17	-	-	0±0,57,57,57	-
4	17F	A	33	-	-	0±0,59,59,59	-
3	PCW	A	63	-	-	0±0,57,57,57	-
3	PCW	A	5	-	-	0±0,57,57,57	-
4	17F	A	36	-	-	0±0,59,59,59	-
4	17F	A	75	-	-	0±0,59,59,59	-
3	PCW	A	60	-	-	0±0,57,57,57	-
3	PCW	A	61	-	-	0±0,57,57,57	-
3	PCW	A	62	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	23	-	-	0±0,57,57,57	-
3	PCW	A	32	-	-	0±0,57,57,57	-
3	PCW	A	56	-	-	0±0,57,57,57	-
3	PCW	A	49	-	-	0±0,57,57,57	-
3	PCW	A	41	-	-	0±0,57,57,57	-

5 of 298 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
5	B	201	GNP	PG-O1G	4.65	1.53	1.46	5	7
5	B	201	GNP	PB-O2B	3.96	1.46	1.56	6	7
5	B	201	GNP	PG-O3G	3.51	1.47	1.56	7	7
5	B	201	GNP	PB-O3A	2.96	1.55	1.59	7	7
5	B	201	GNP	PG-O2G	2.89	1.49	1.56	7	7

5 of 357 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	A	43	PCW	C8-N-C7	12.05	77.31	108.98	5	7
3	A	53	PCW	C8-N-C7	11.99	77.49	108.98	6	7
3	A	41	PCW	C8-N-C7	11.98	77.50	108.98	3	7
3	A	45	PCW	C8-N-C7	11.98	77.50	108.98	5	7
3	A	59	PCW	C8-N-C7	11.98	77.50	108.98	5	7

There are no chirality outliers.

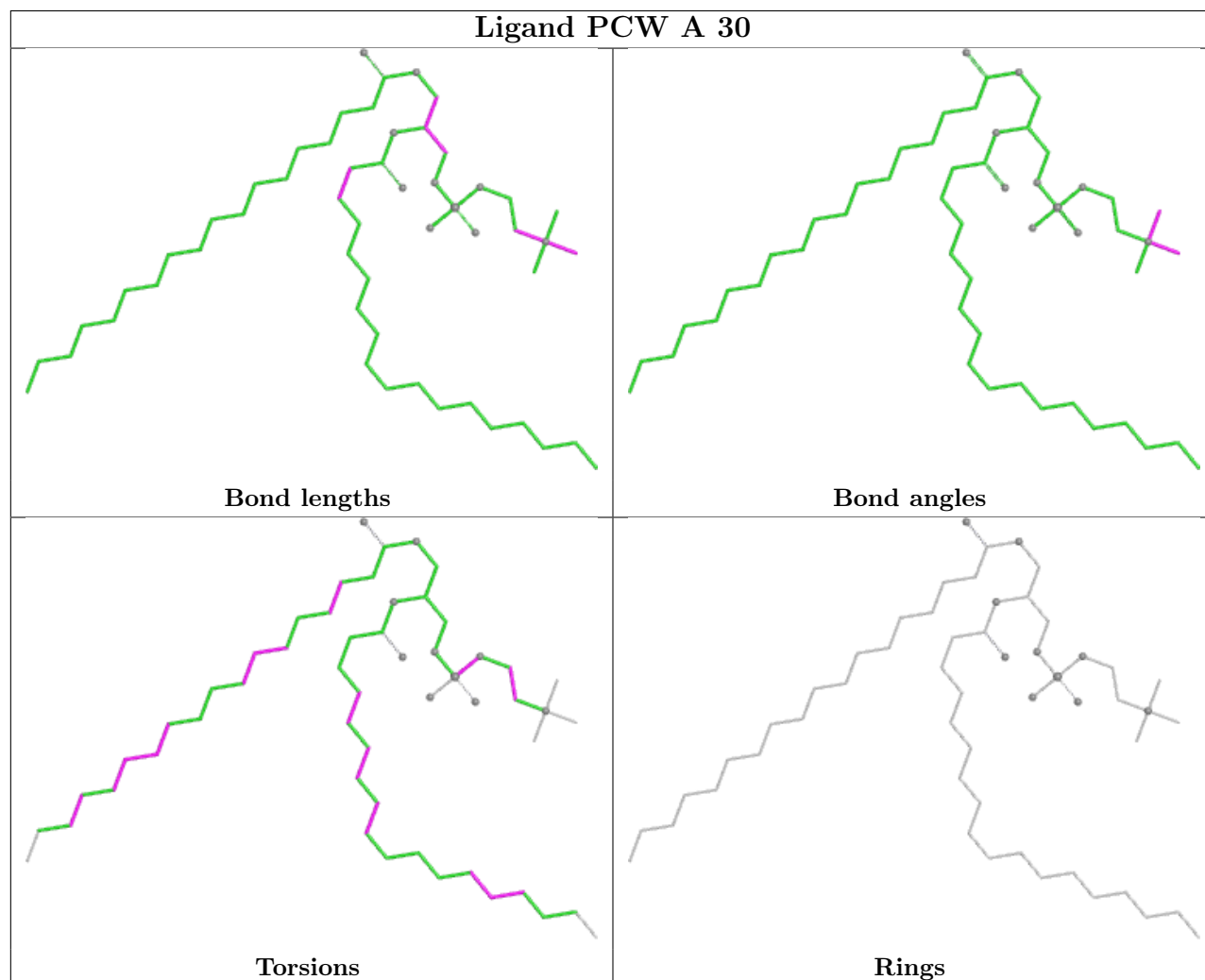
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

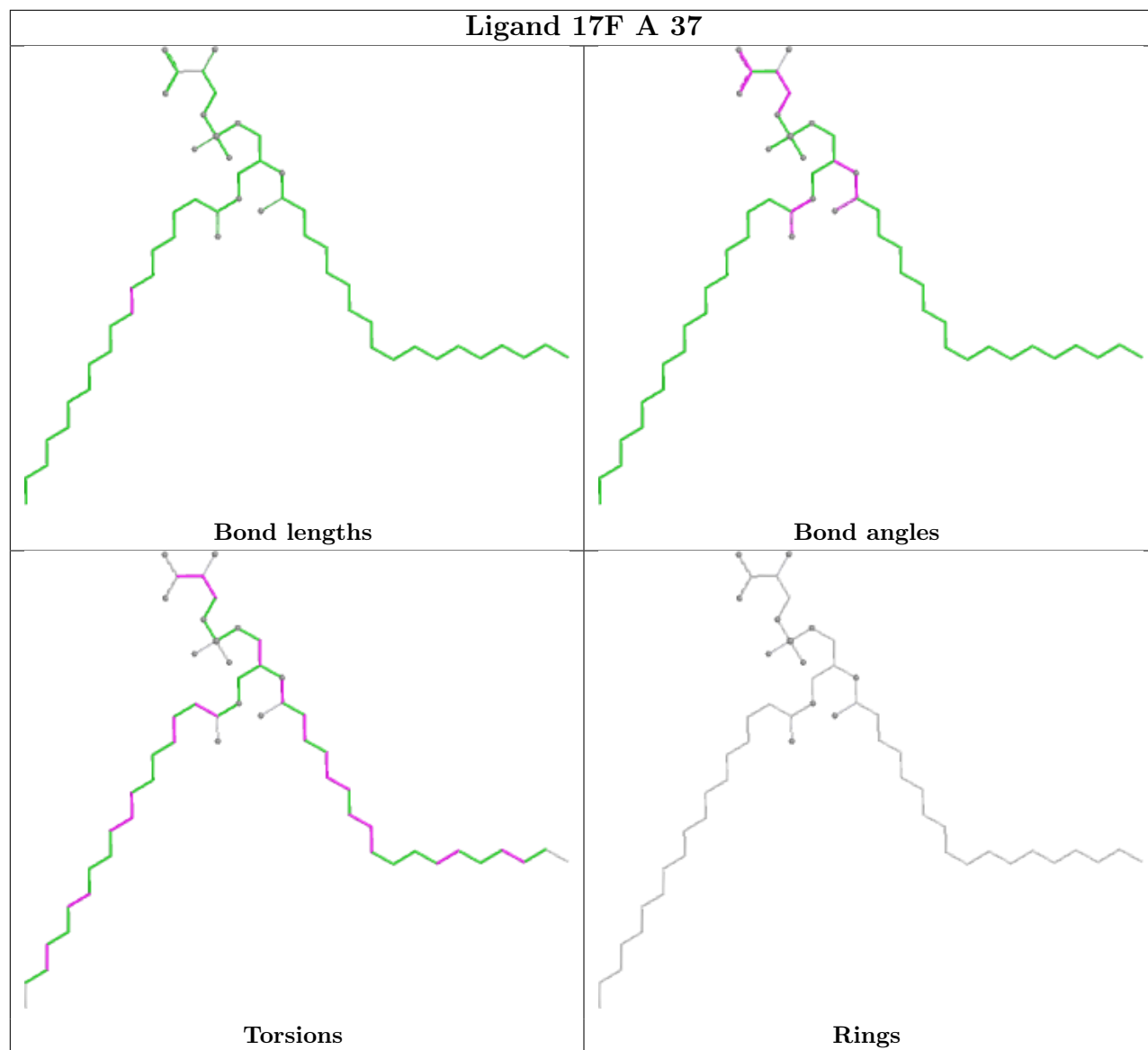
Mol	Chain	Res	Type	Atoms	Models (Total)
5	B	201	GNP	PB-N3B-PG-O1G	3
5	B	201	GNP	PG-N3B-PB-O1B	1

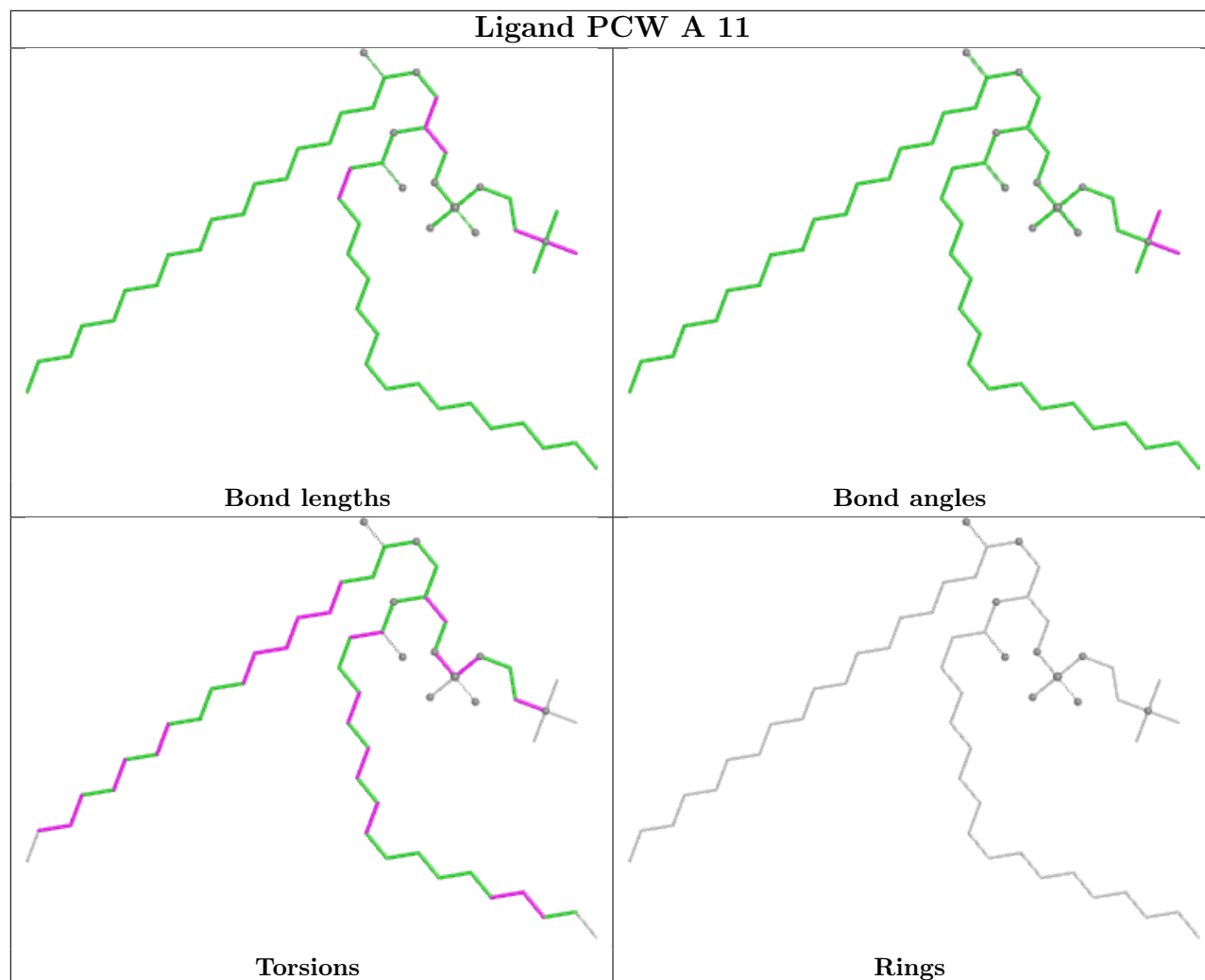
There are no ring outliers.

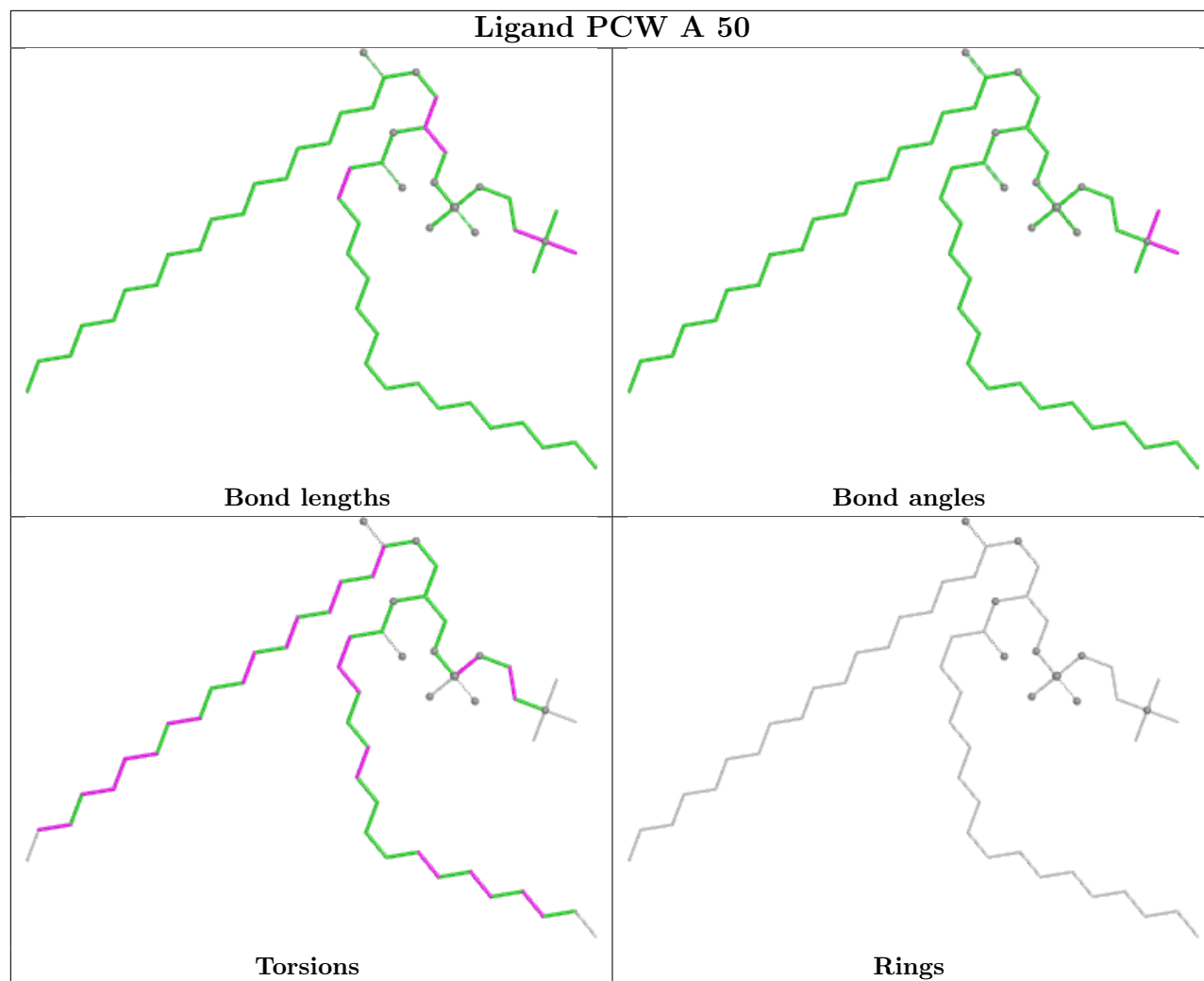
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

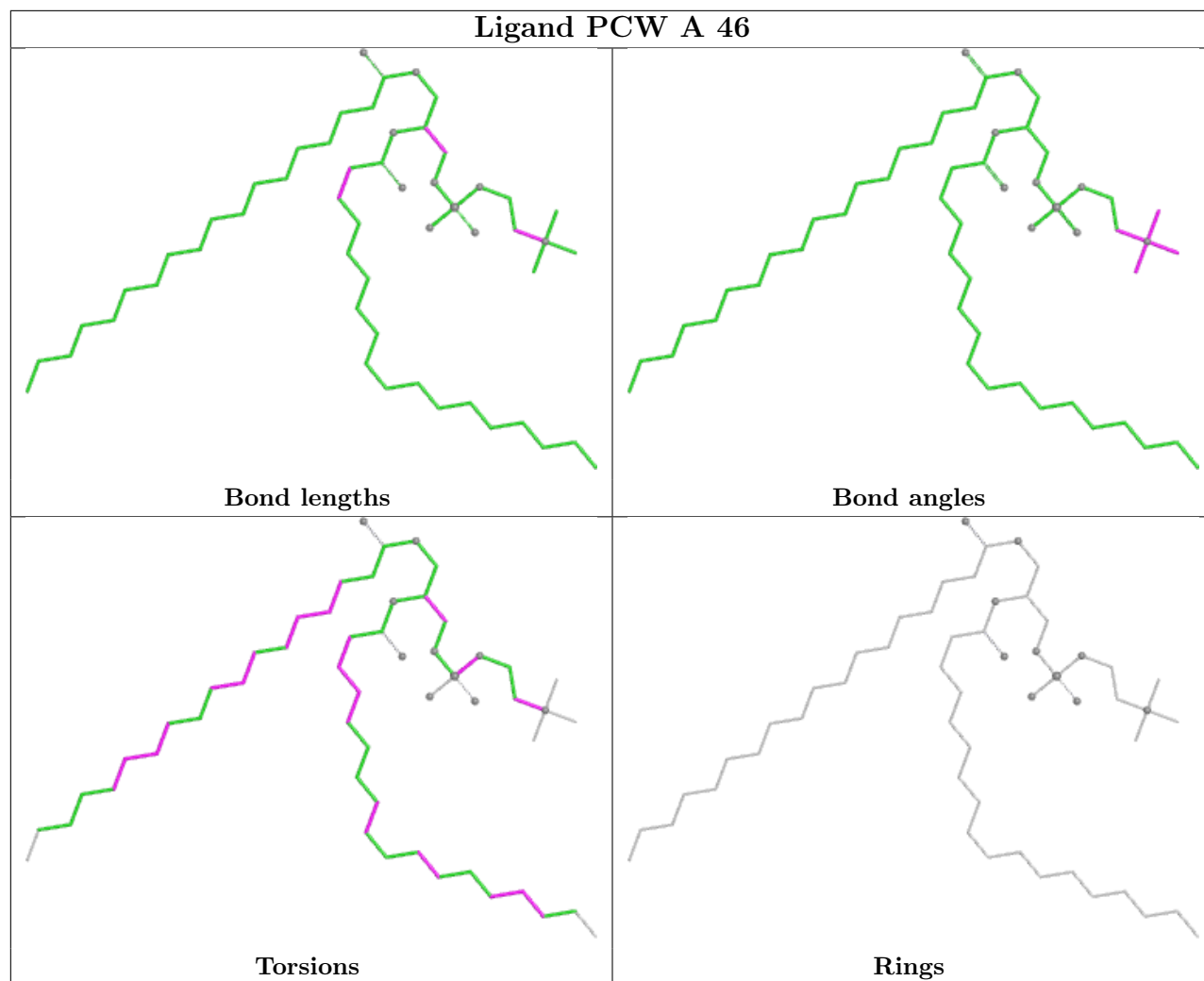
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

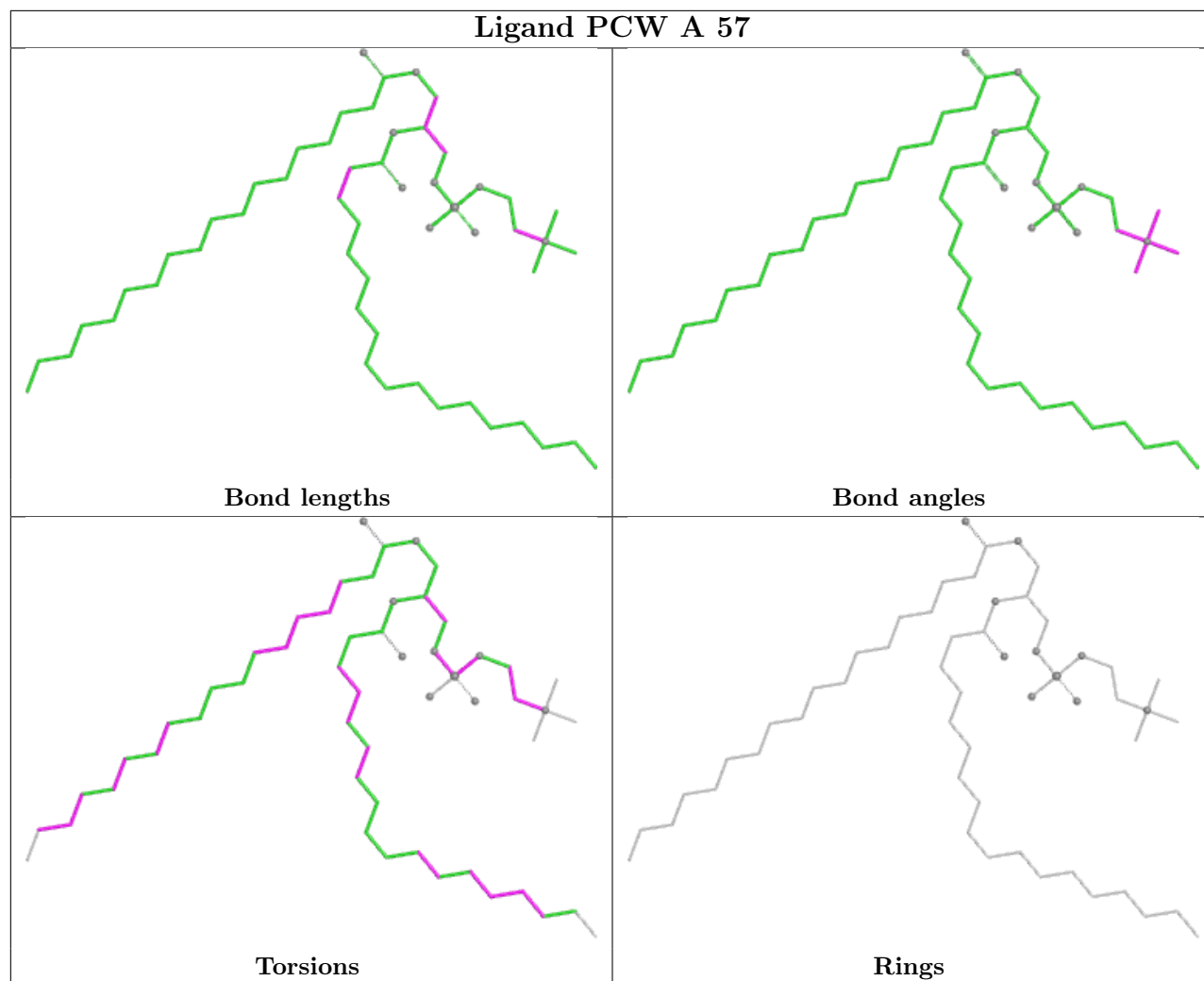


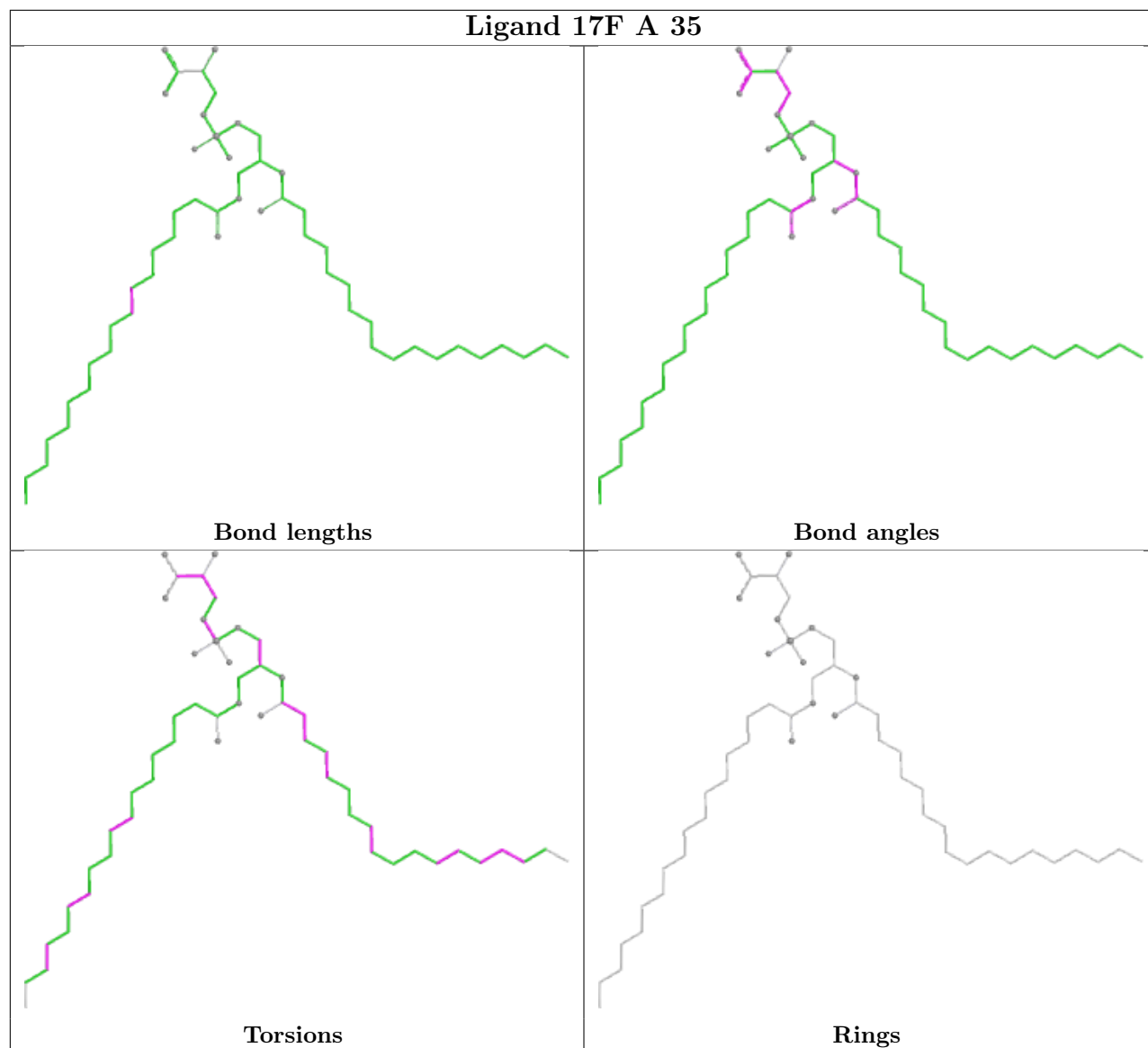


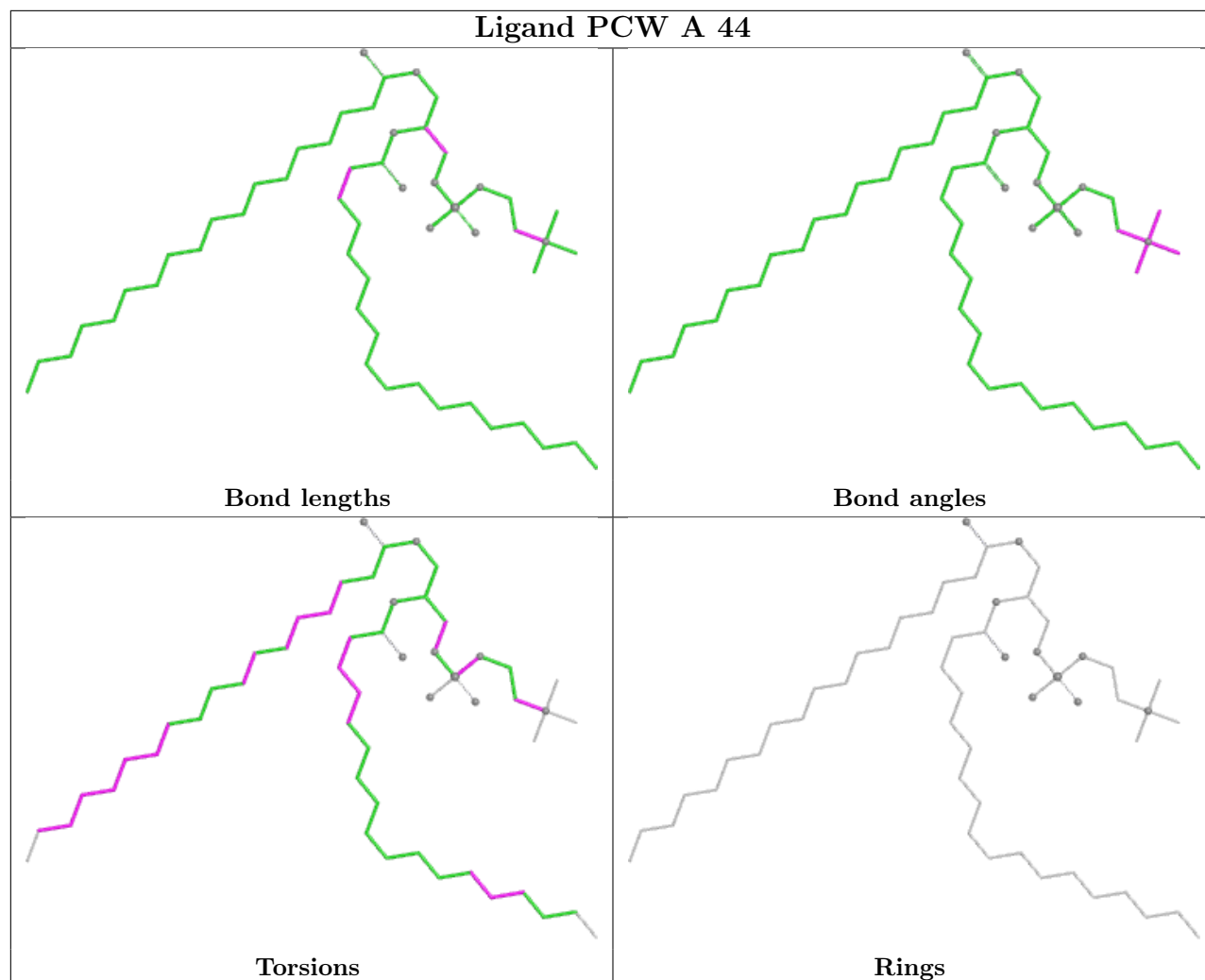


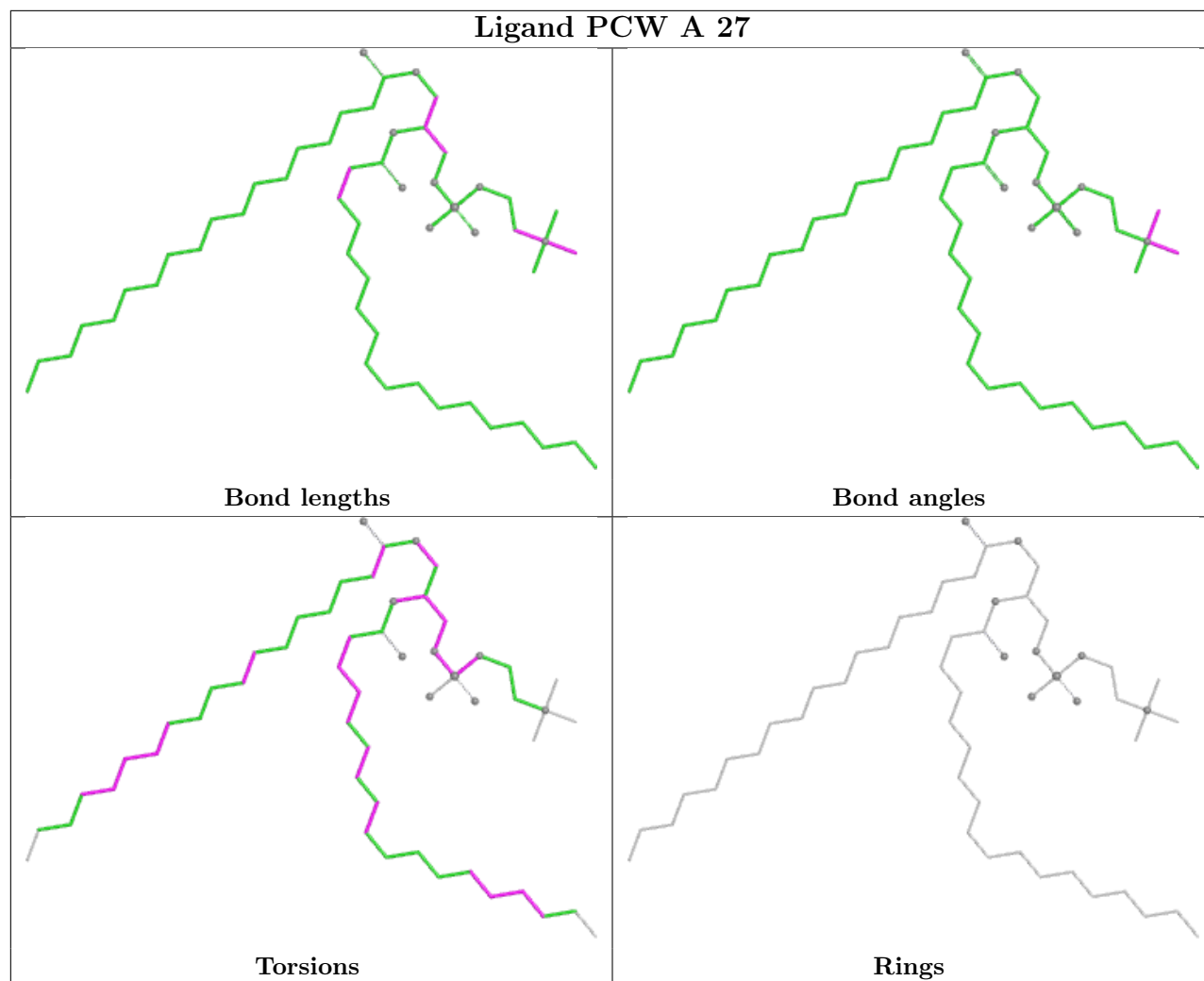


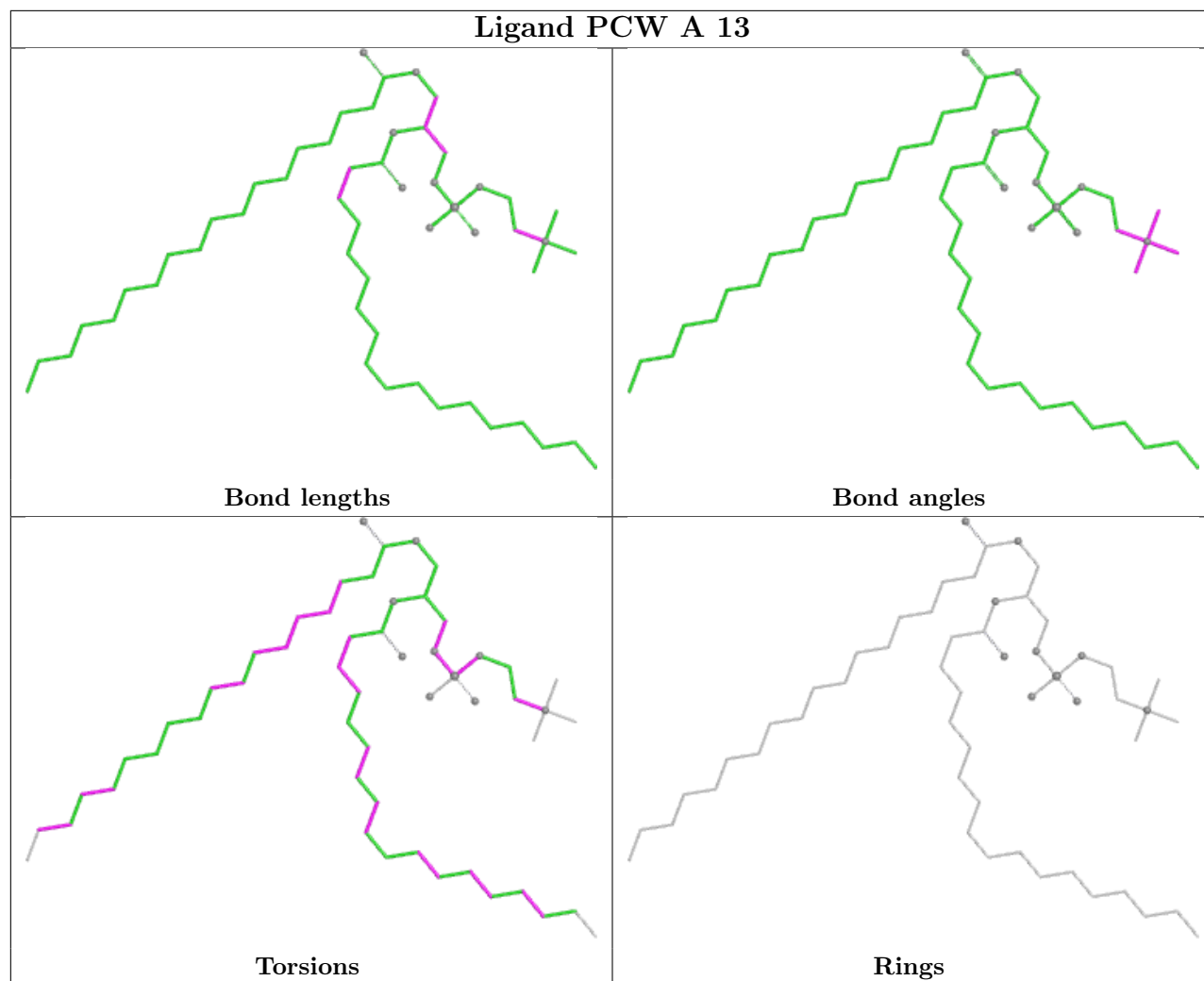


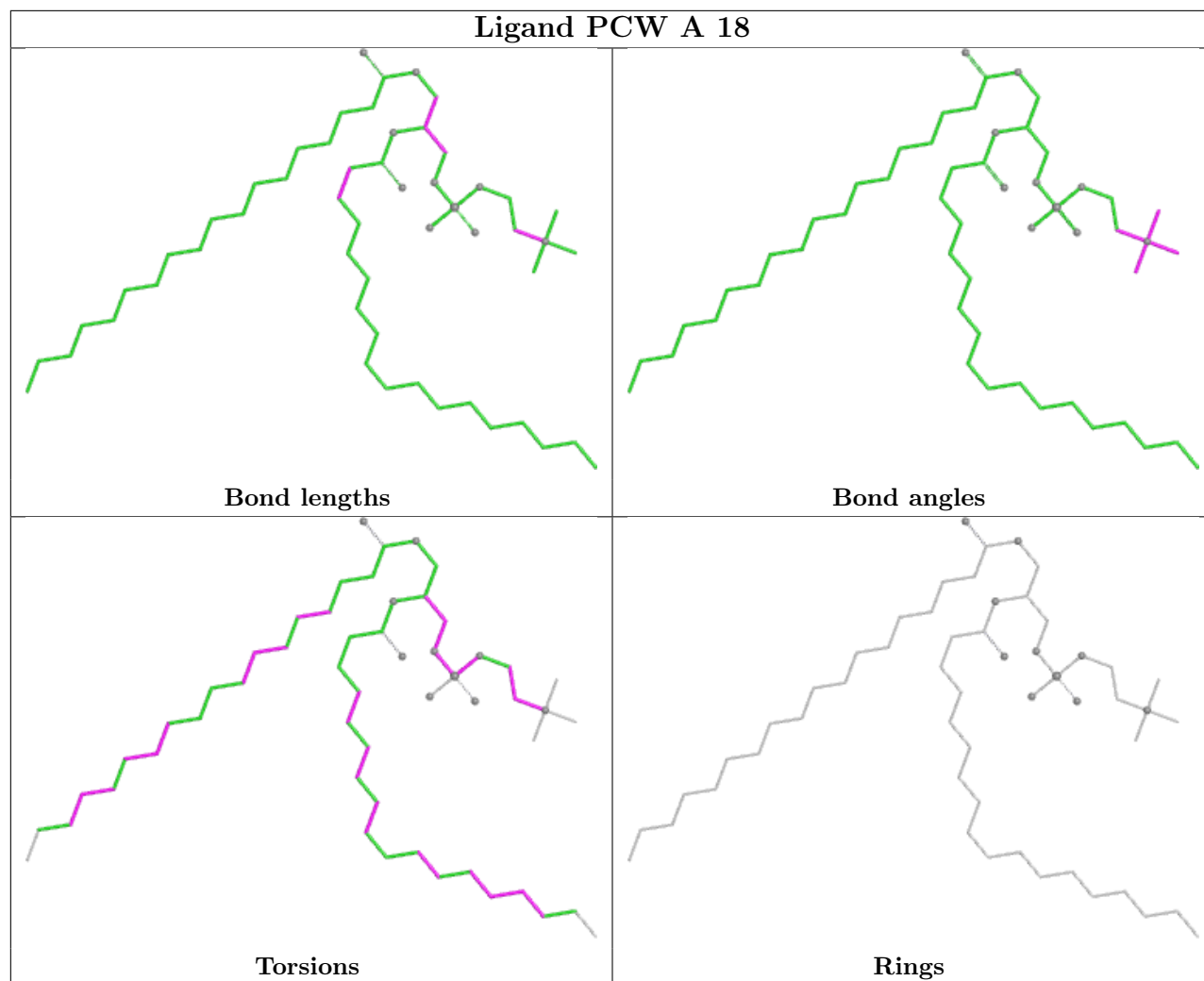


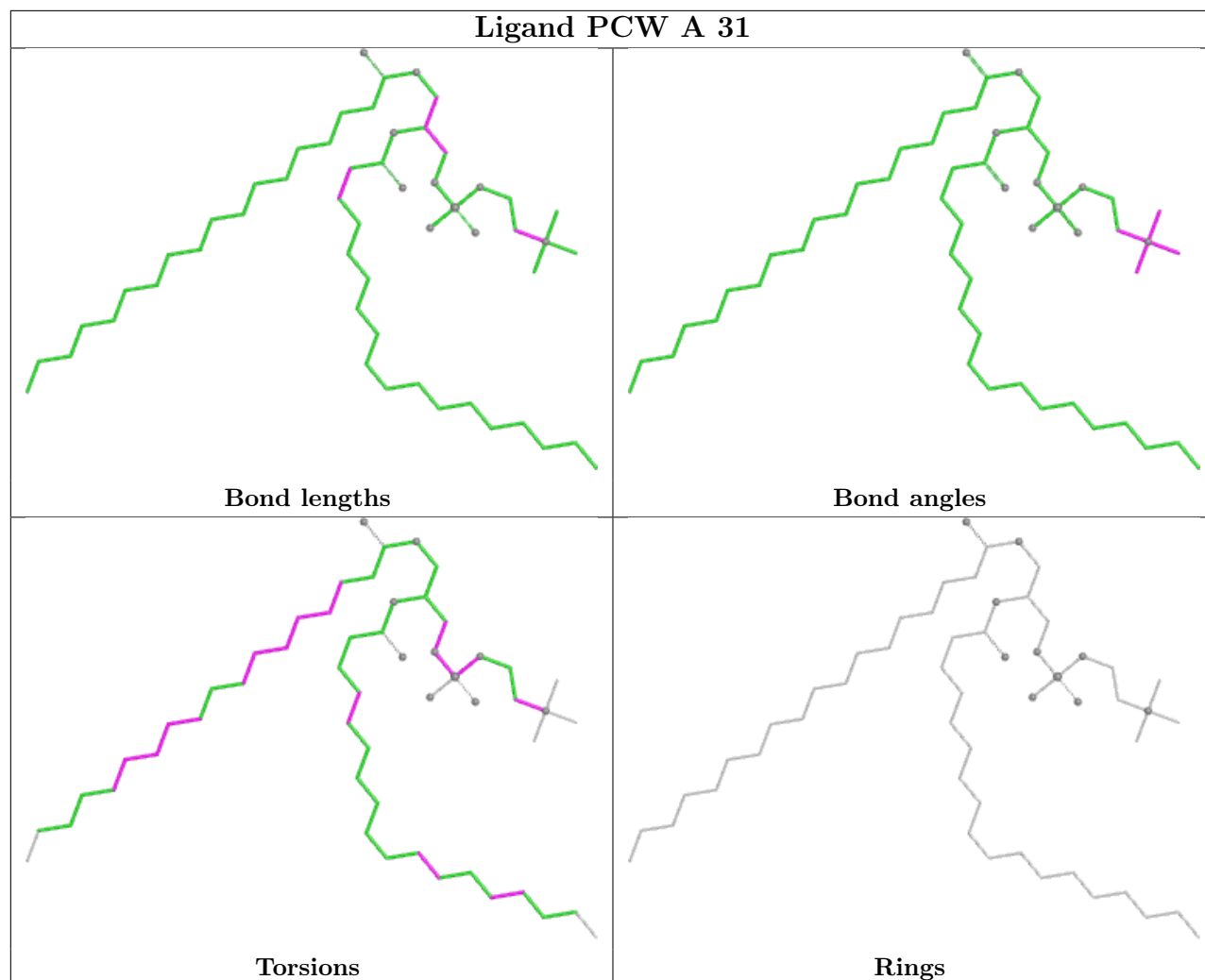


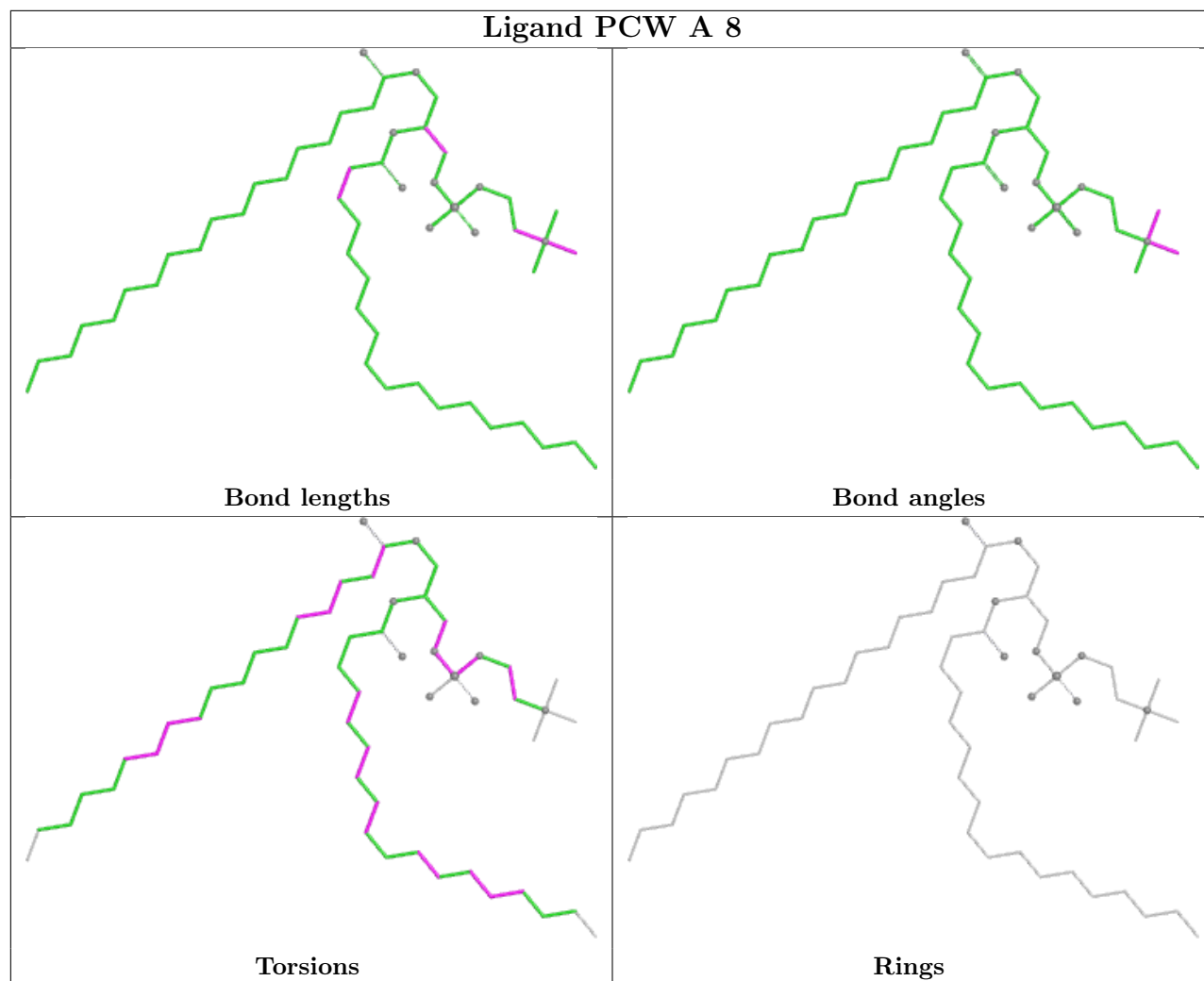


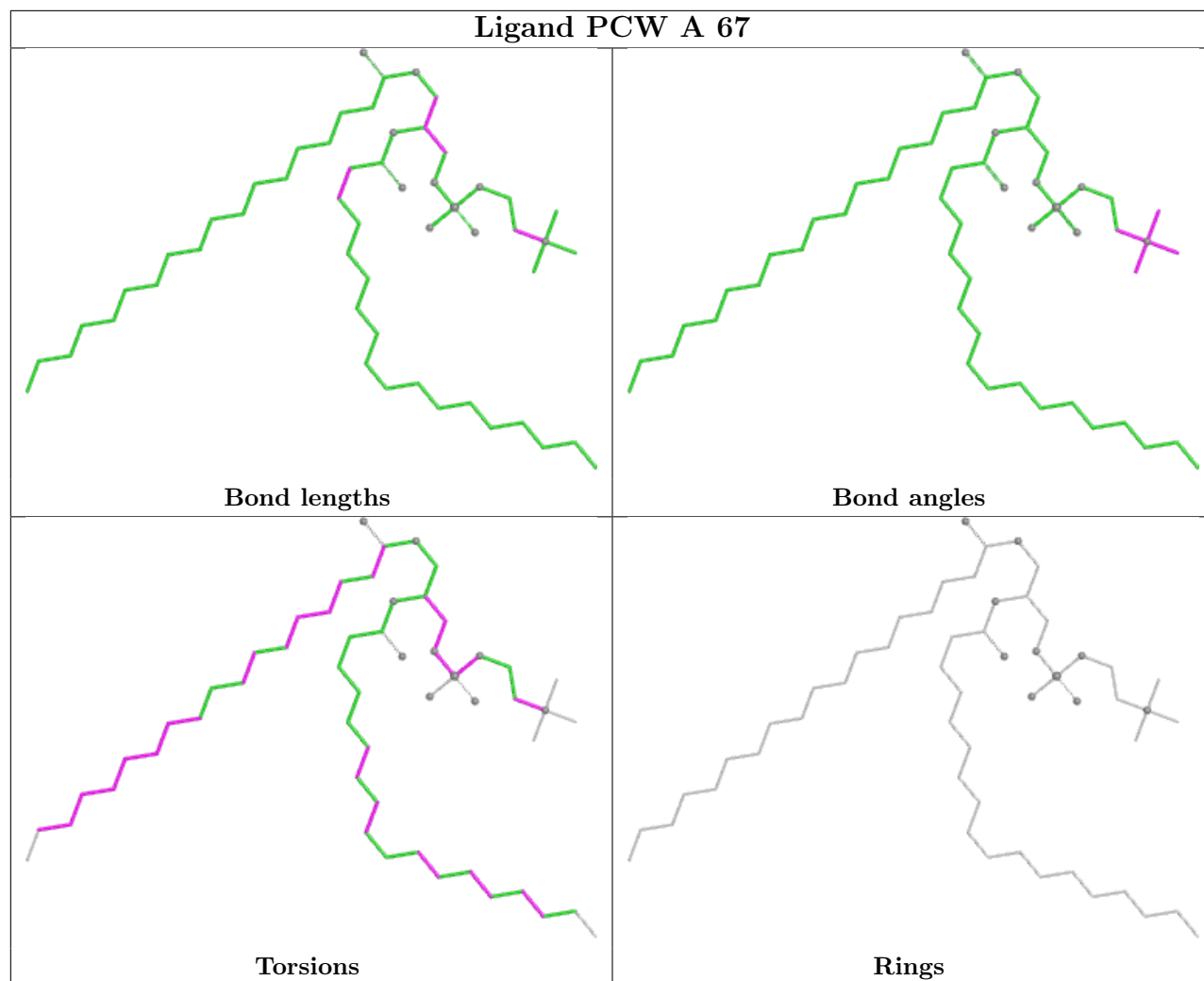


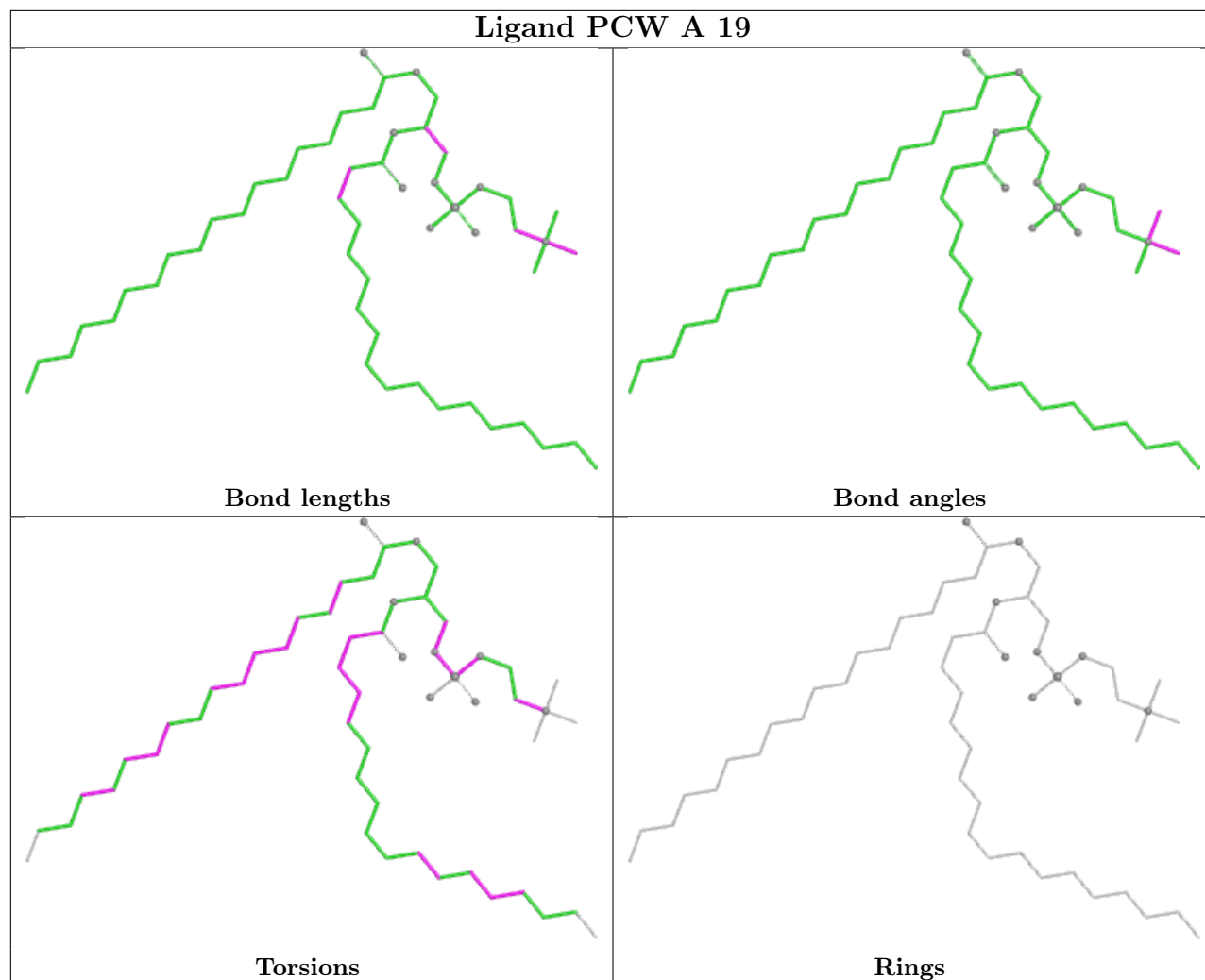


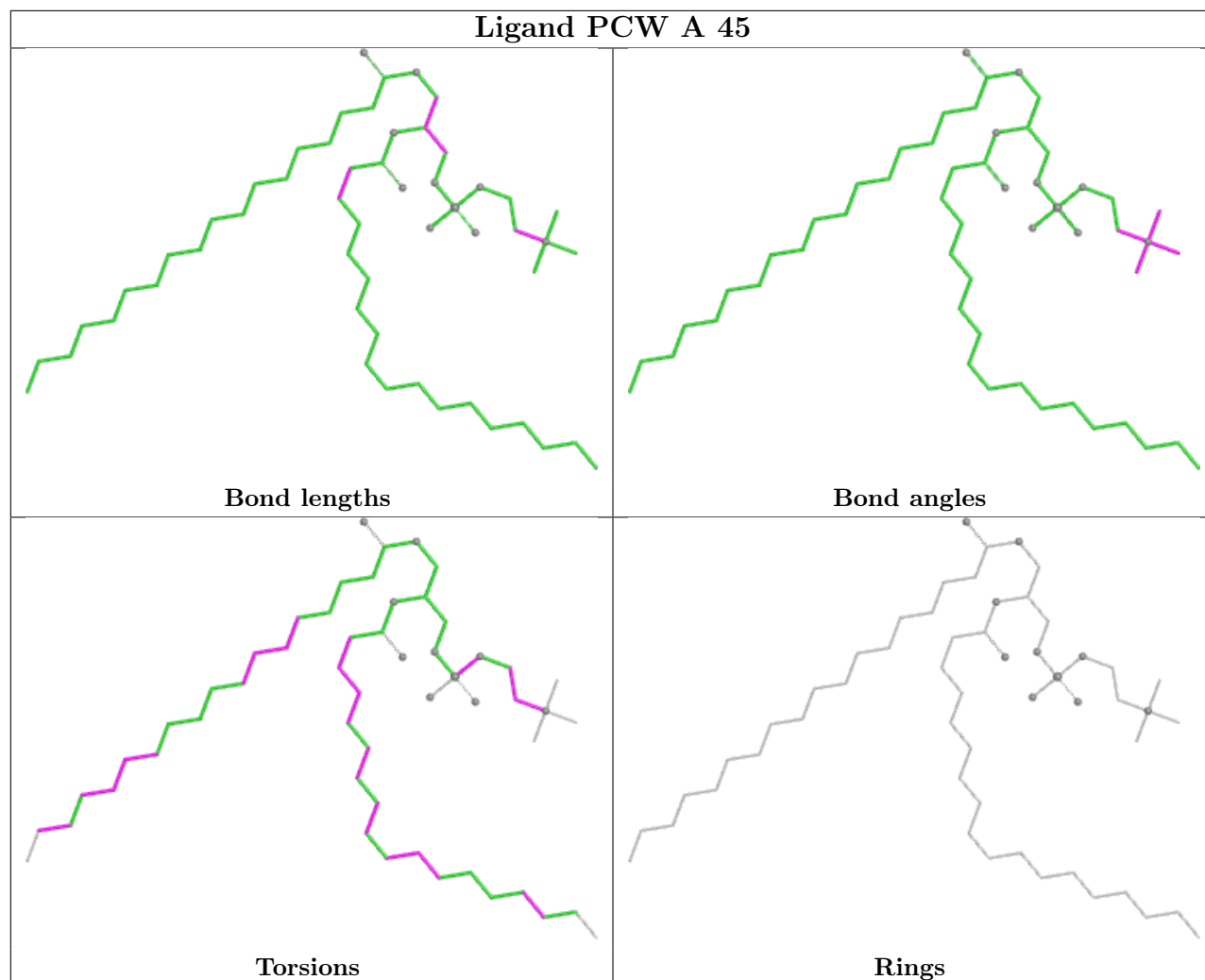


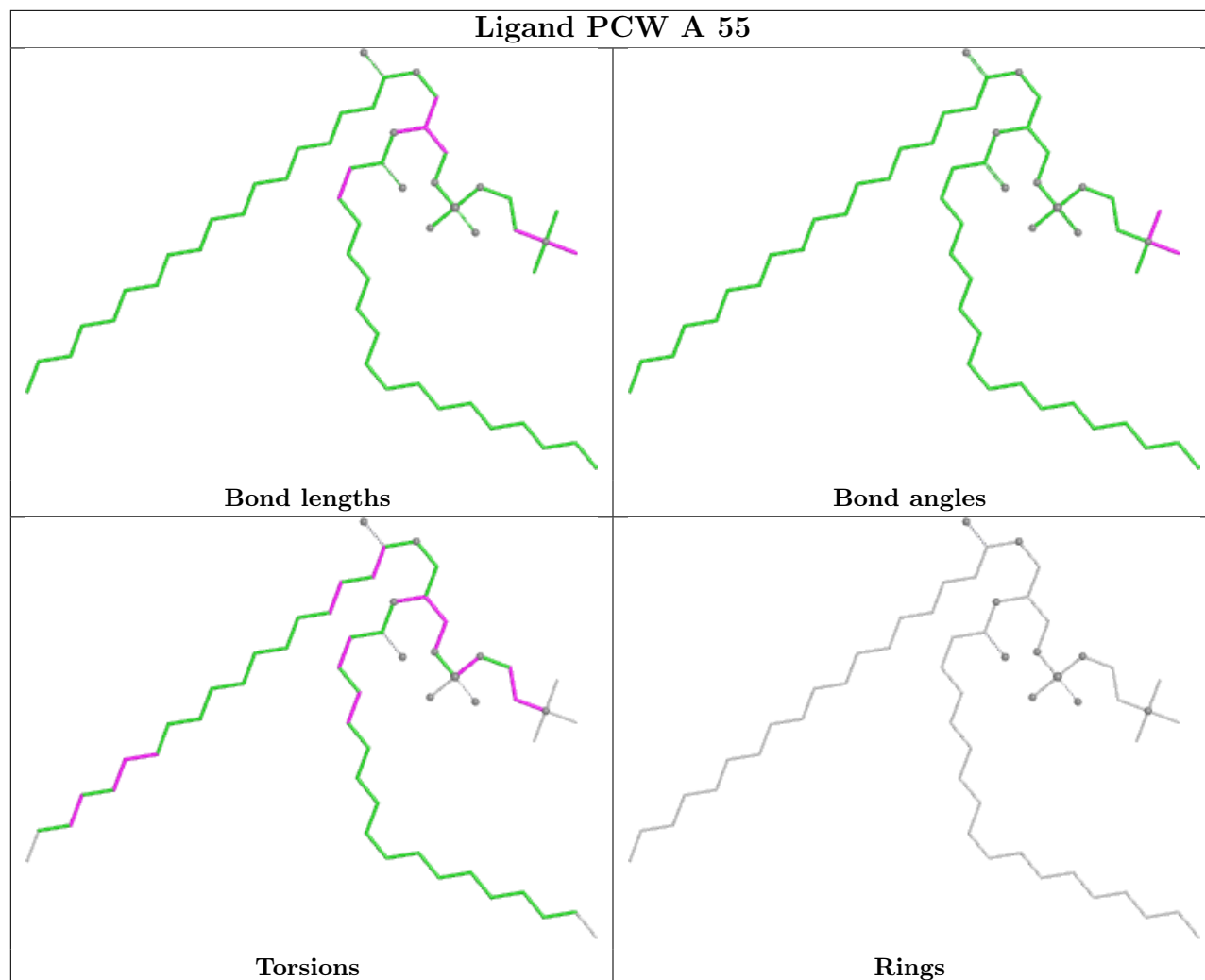


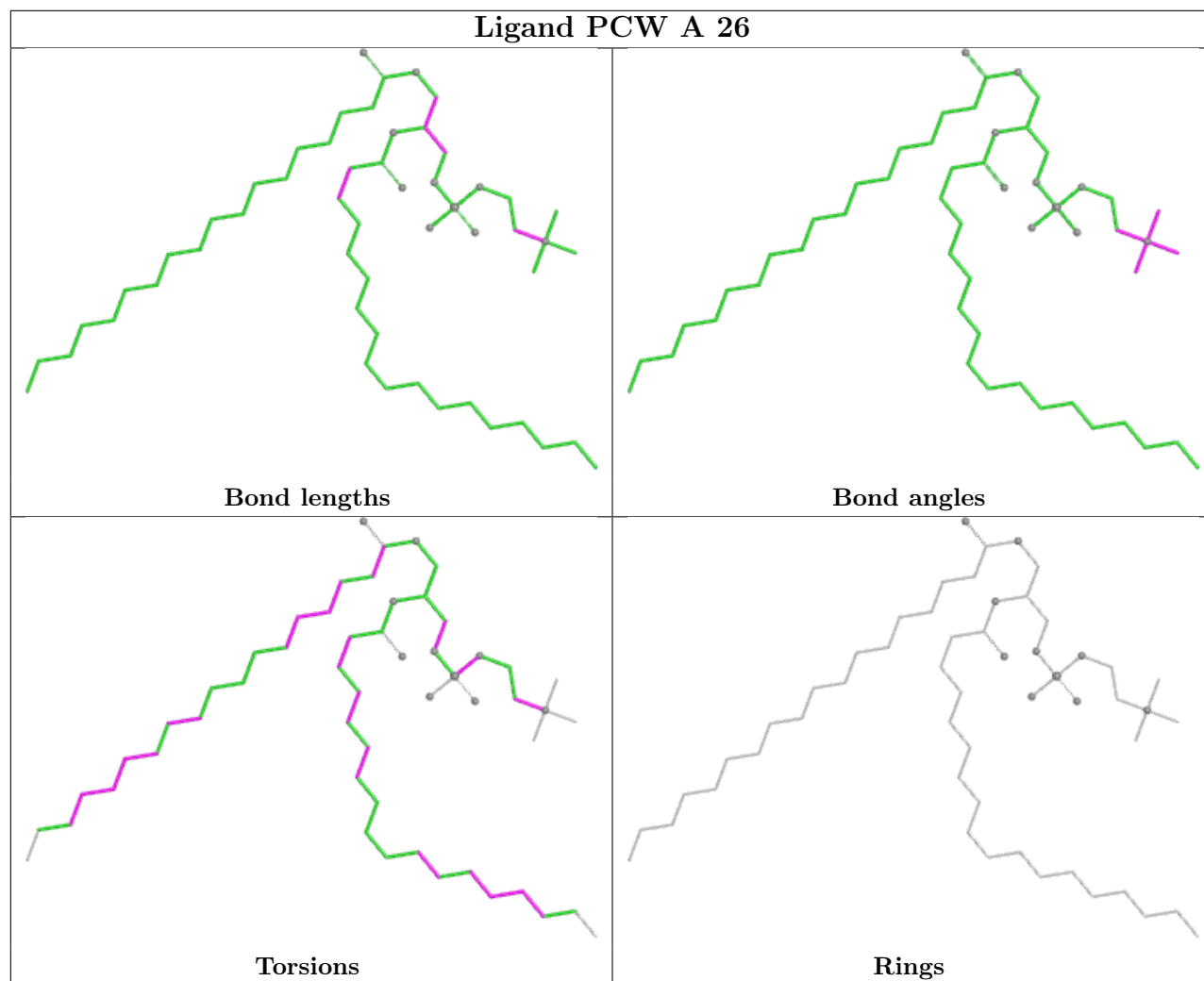


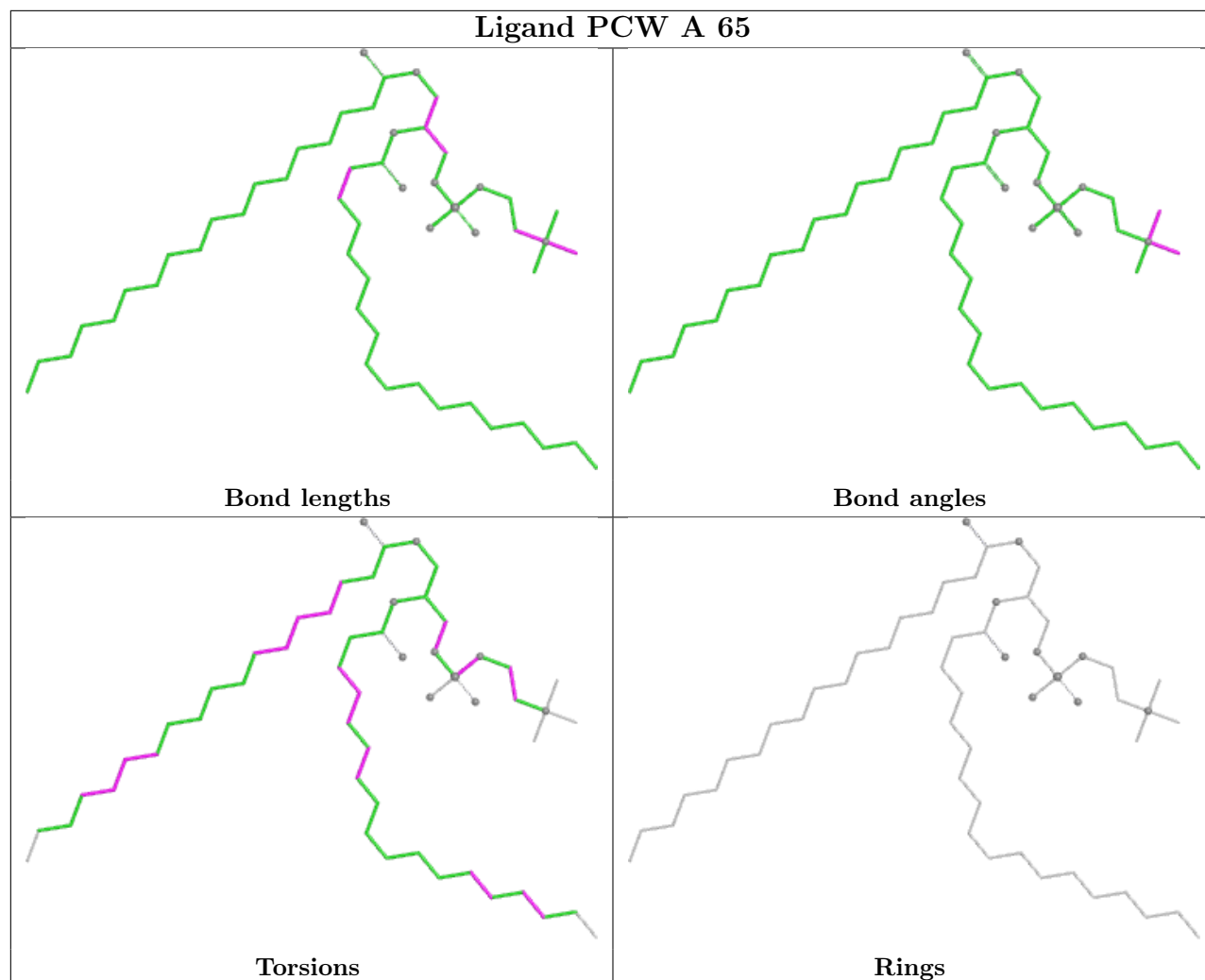


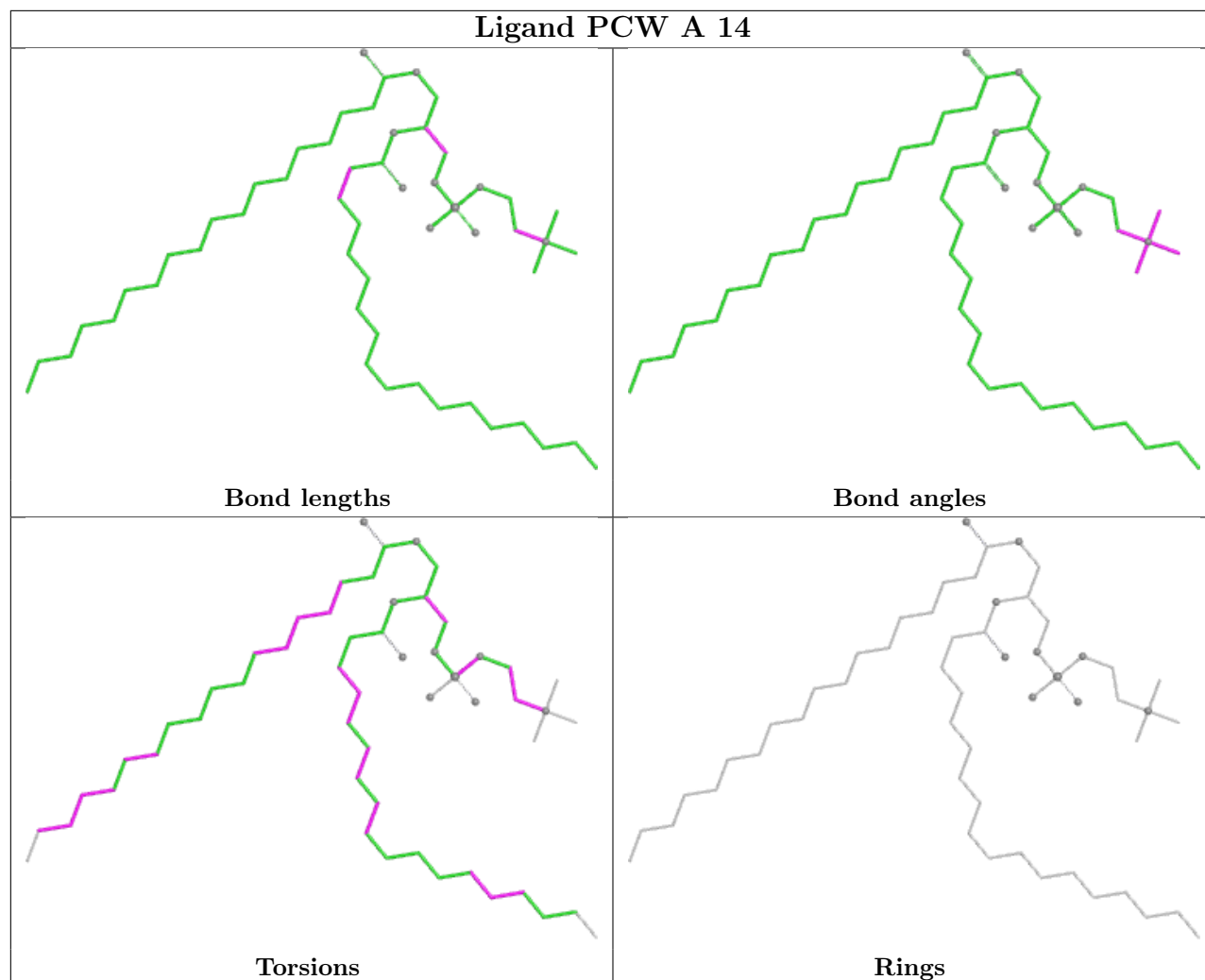


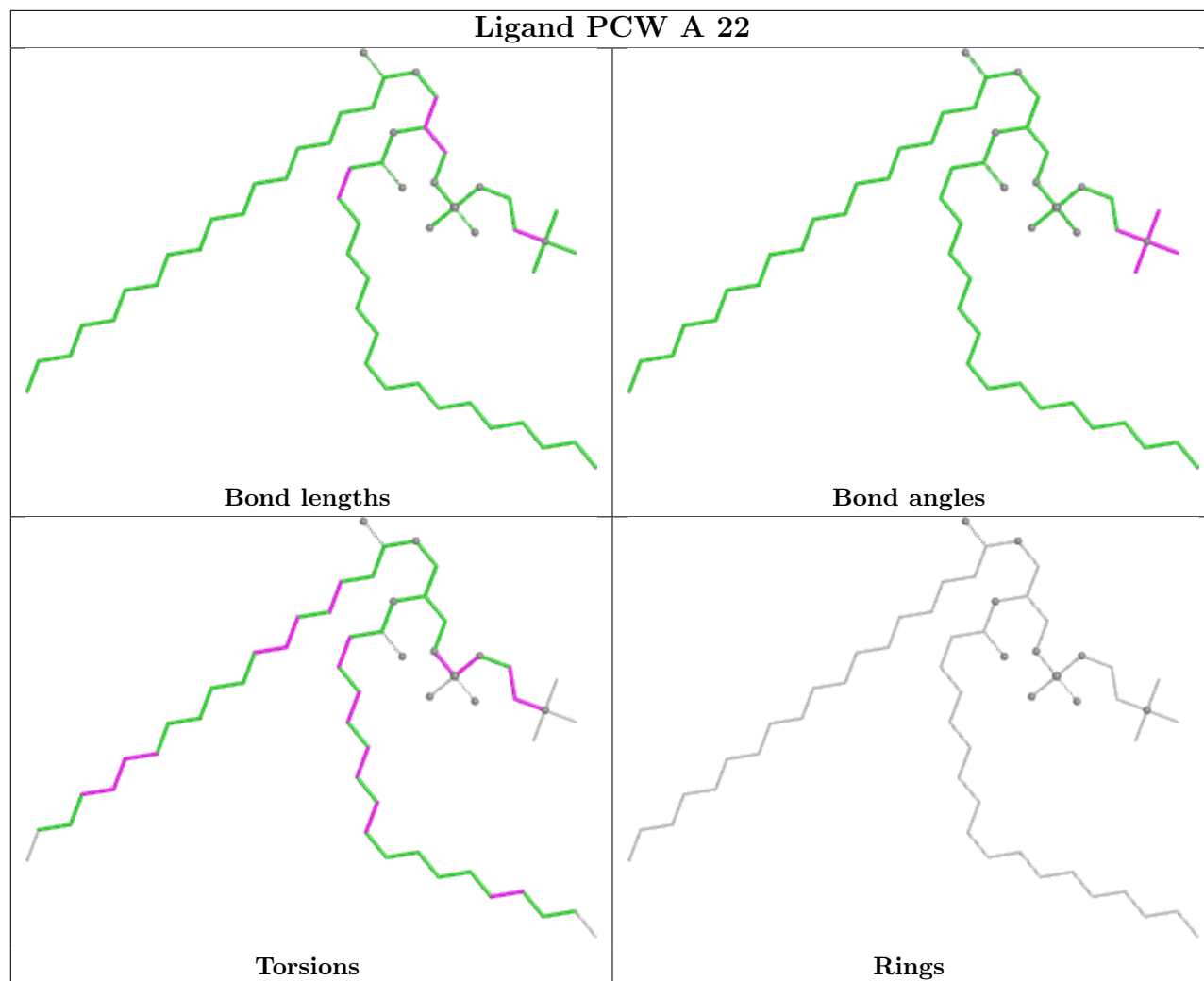


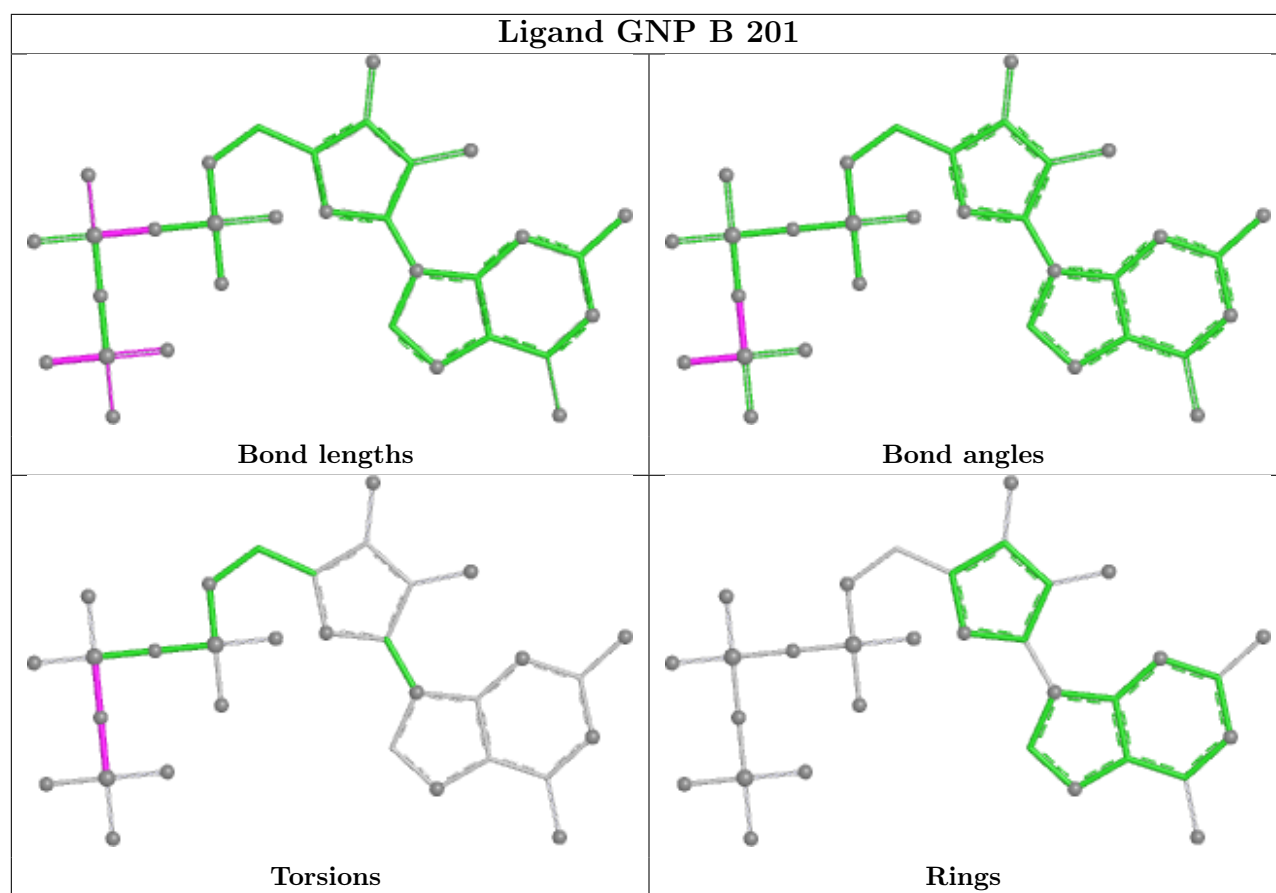


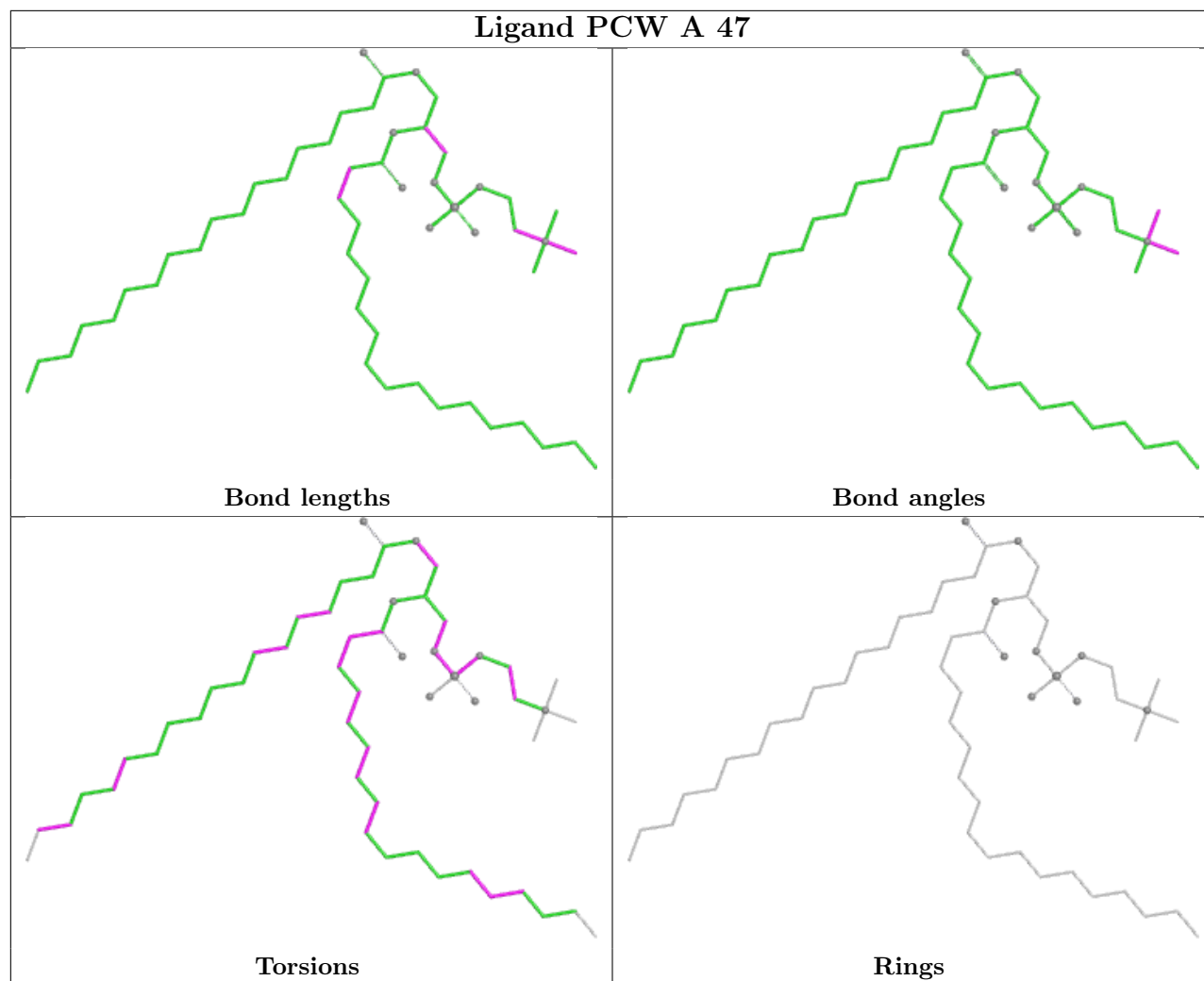


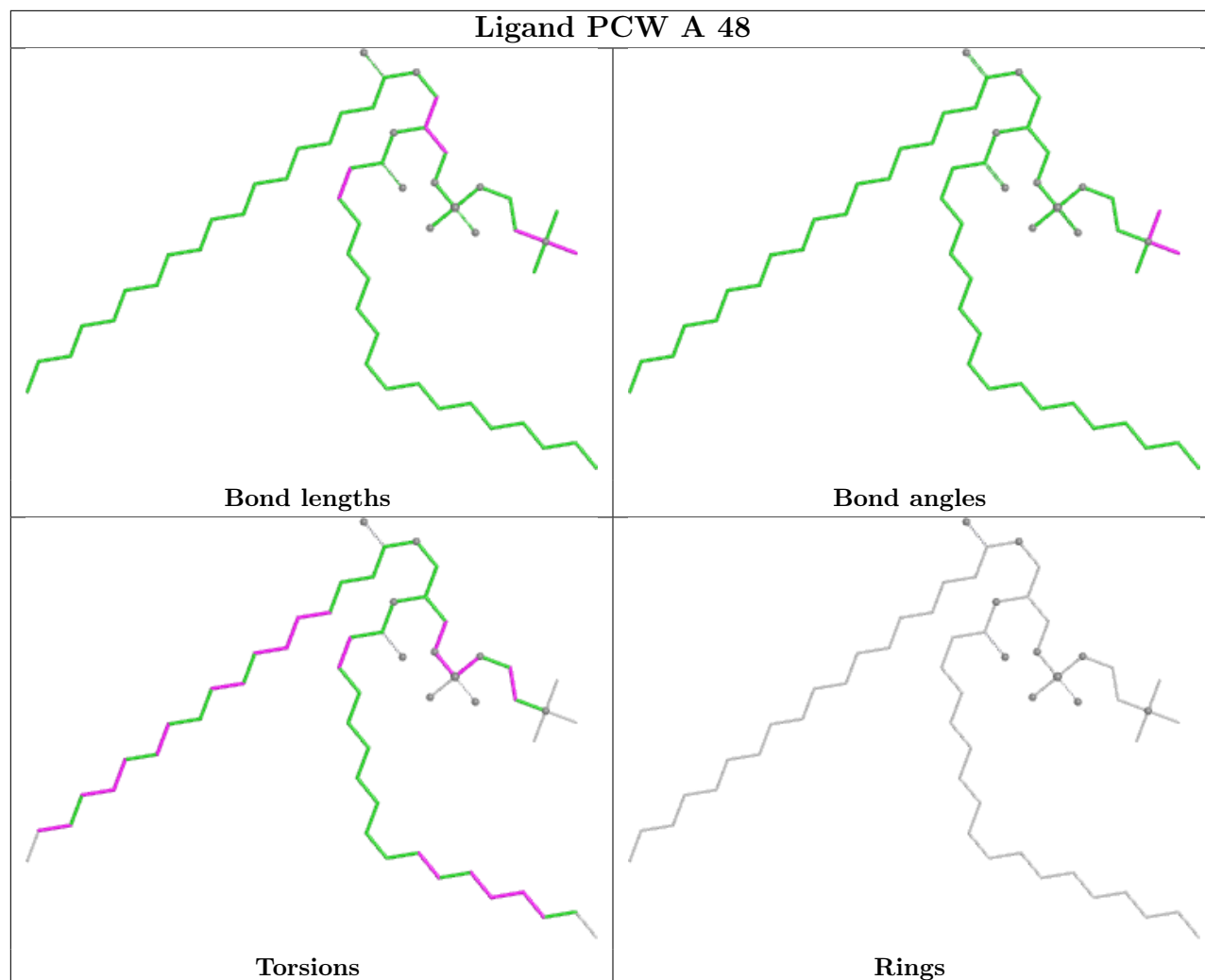


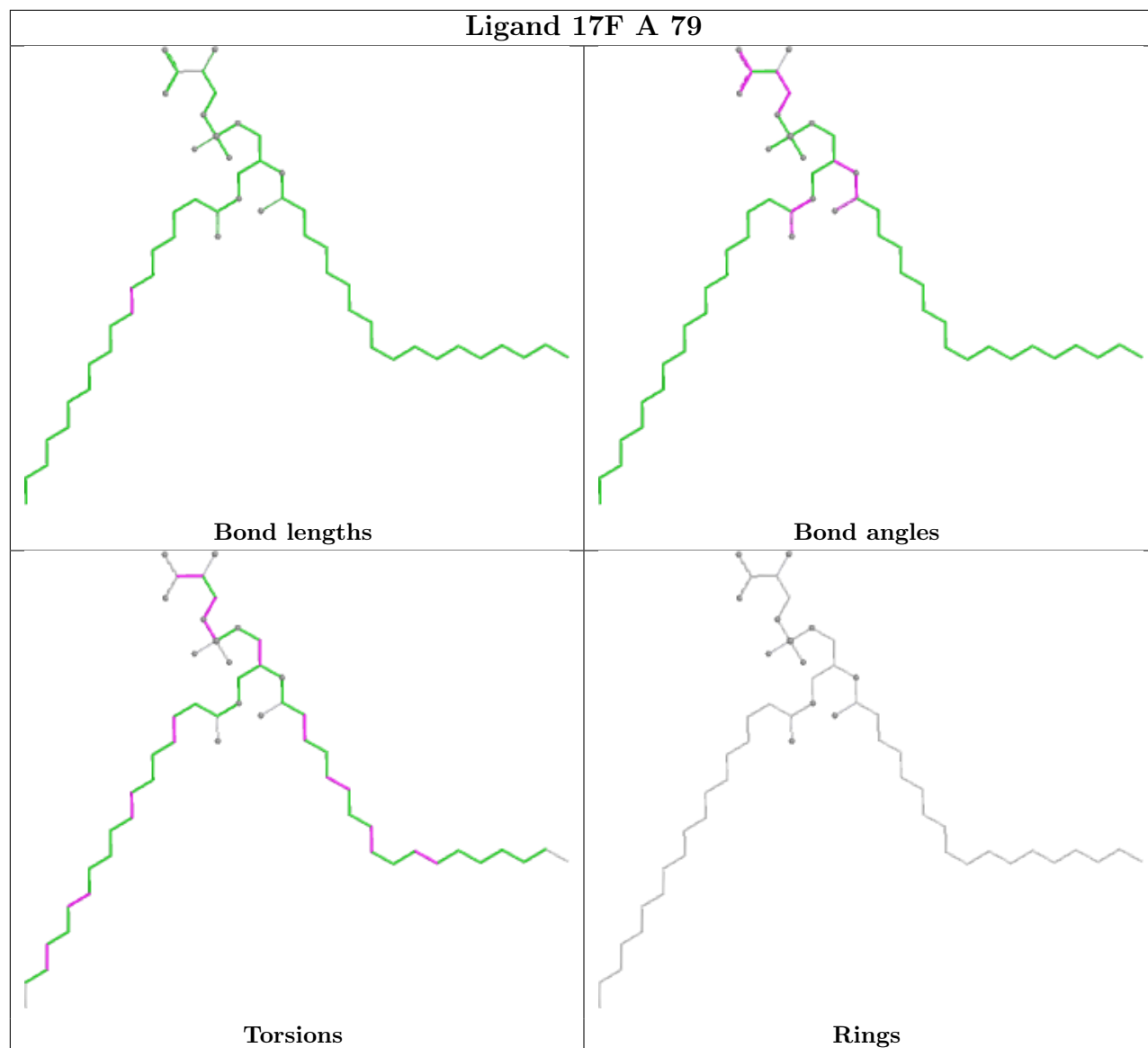


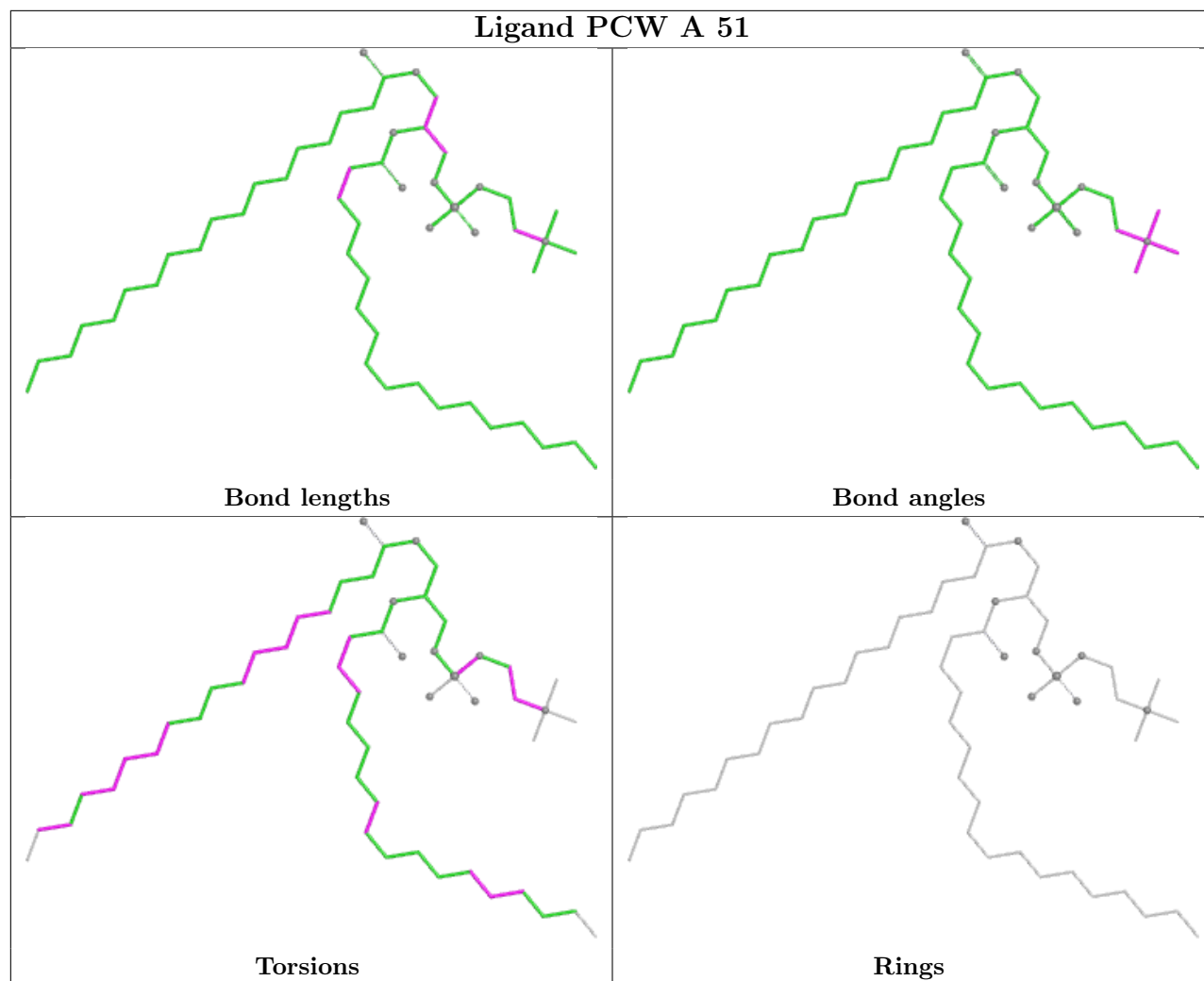


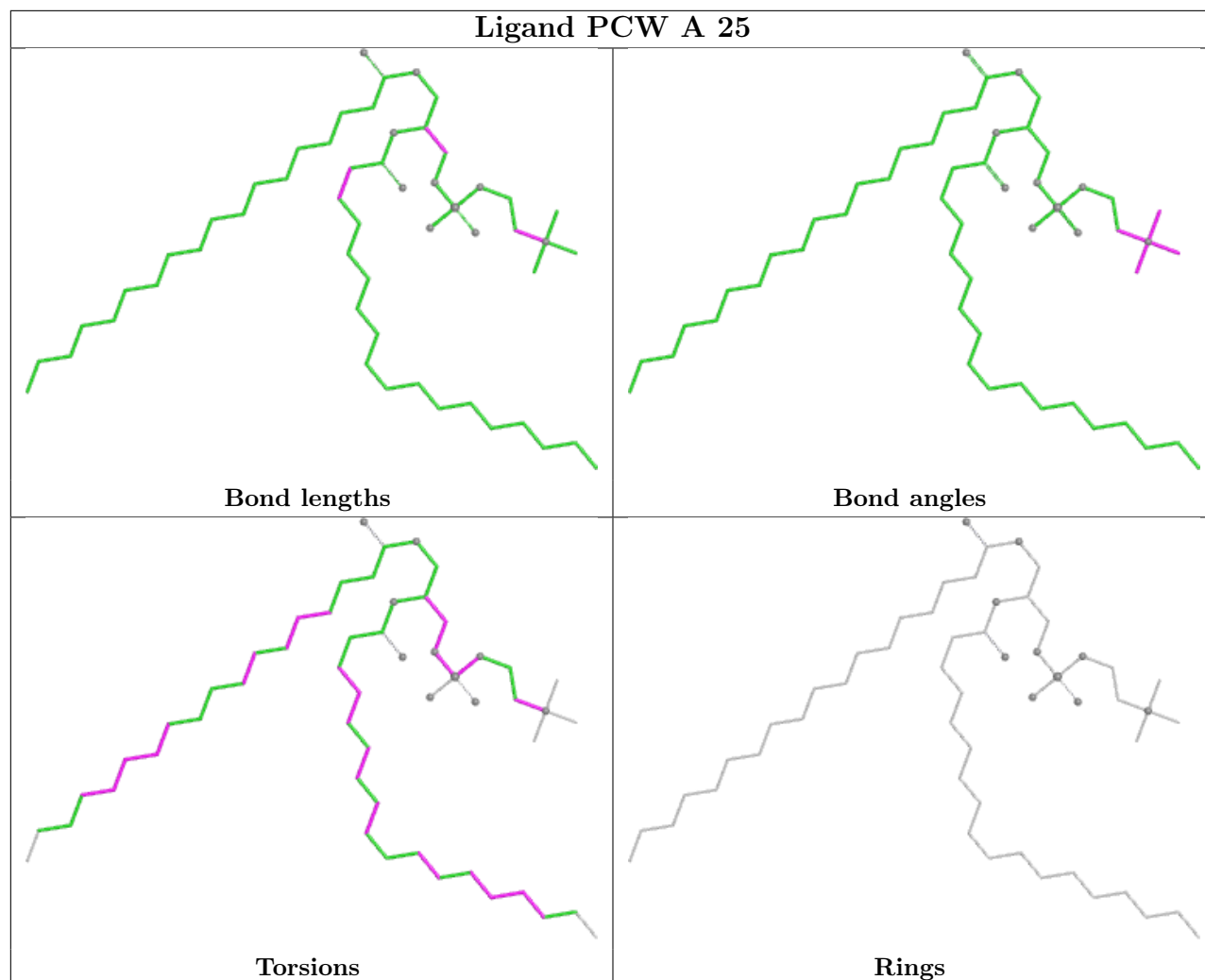


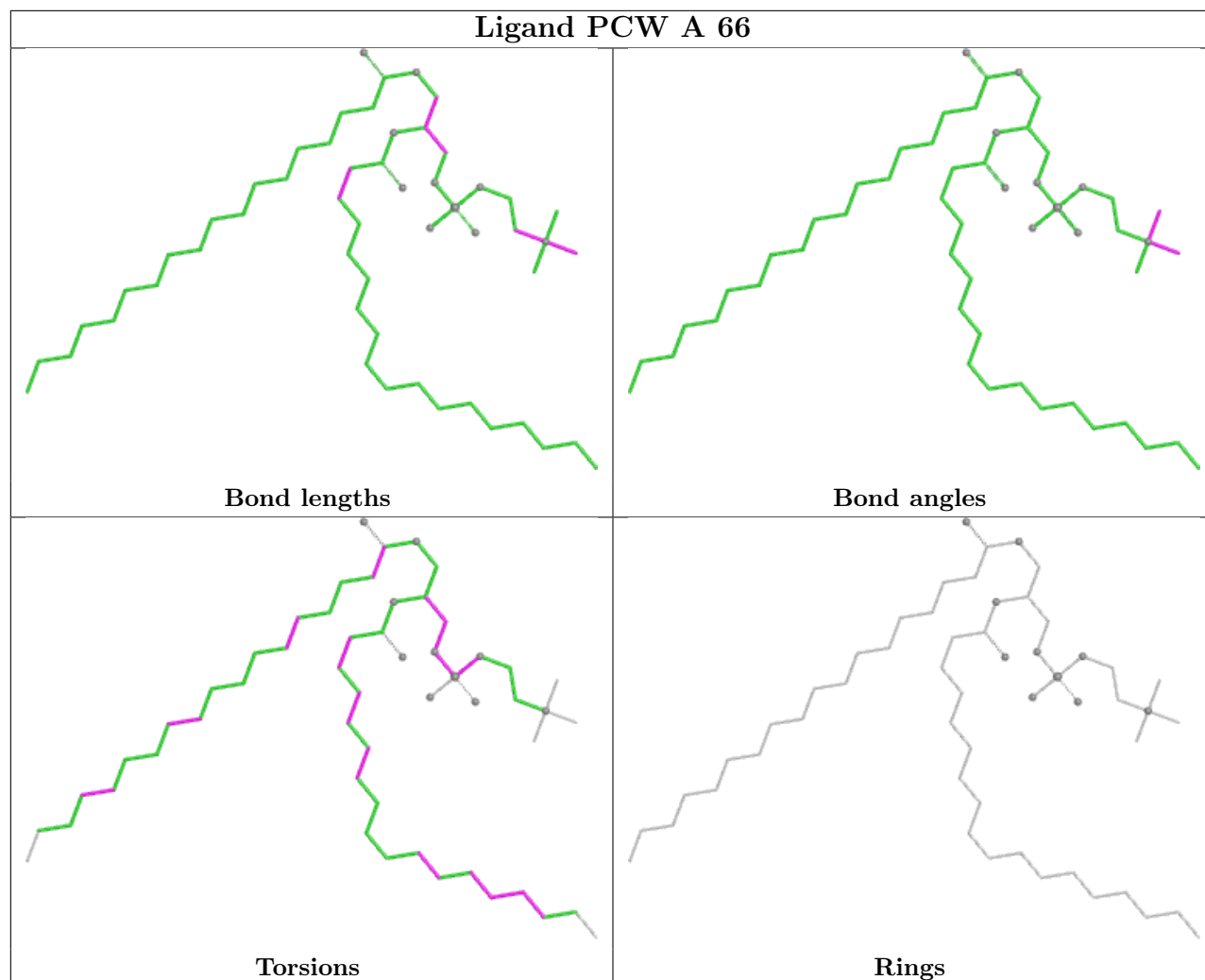


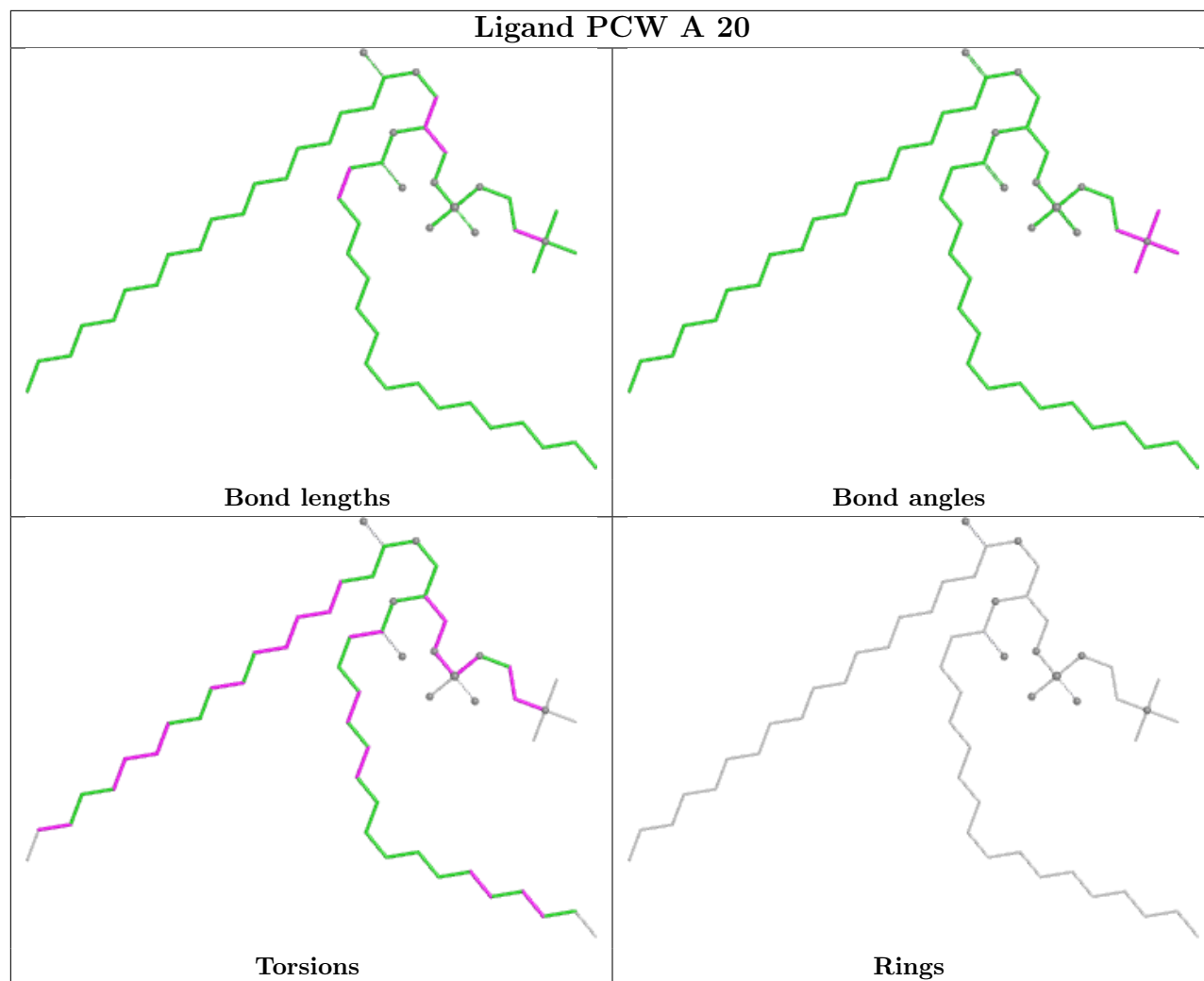


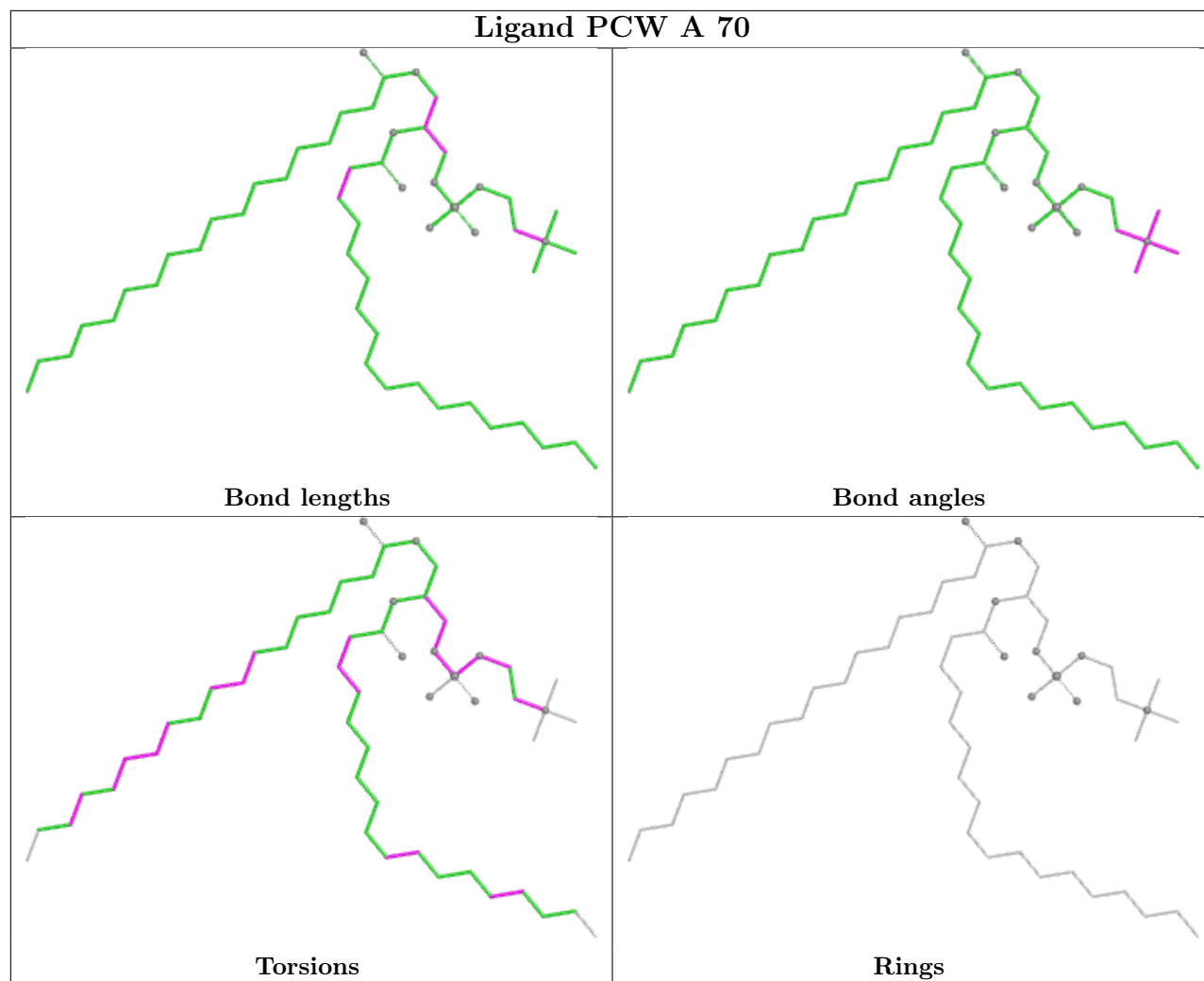


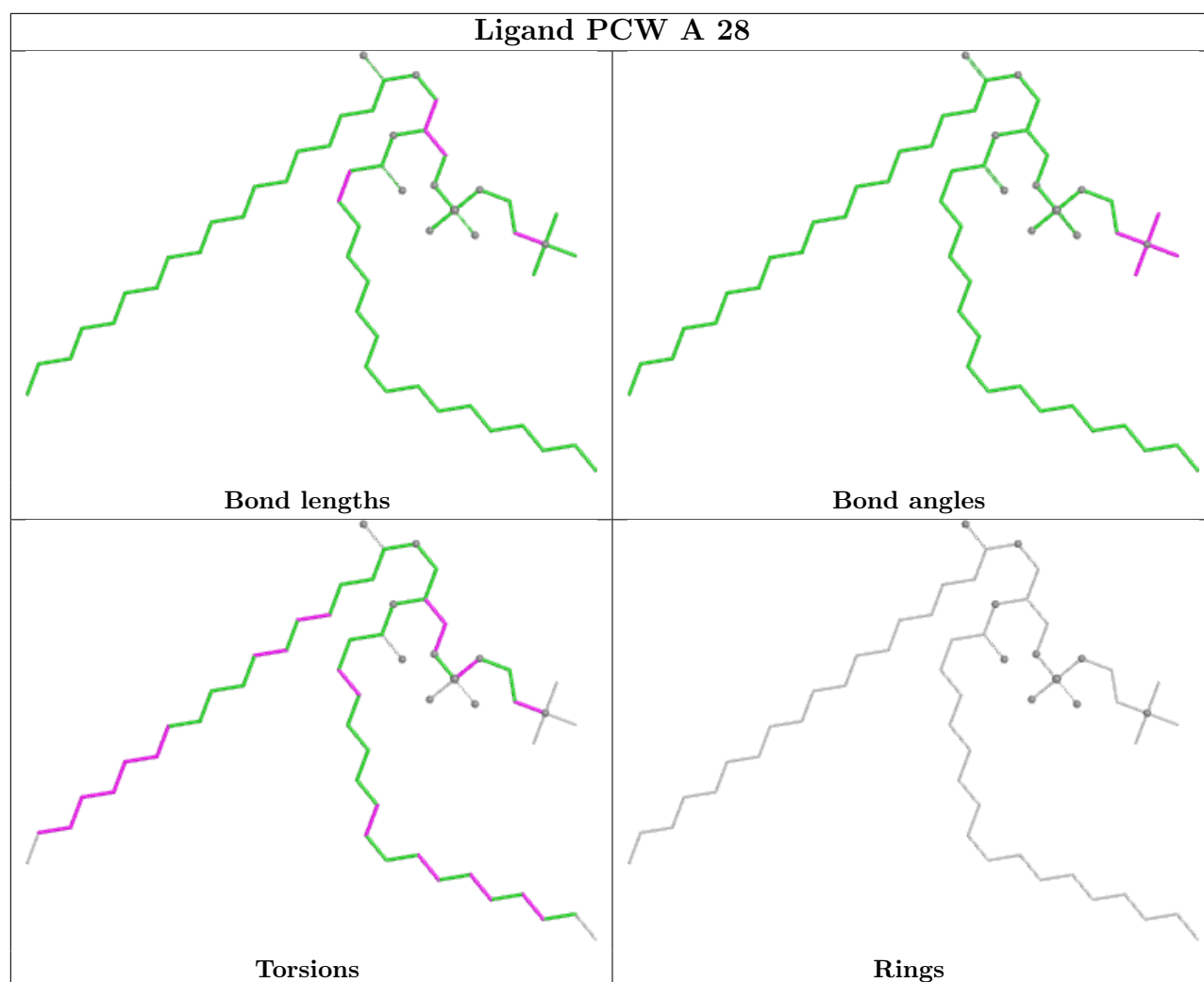


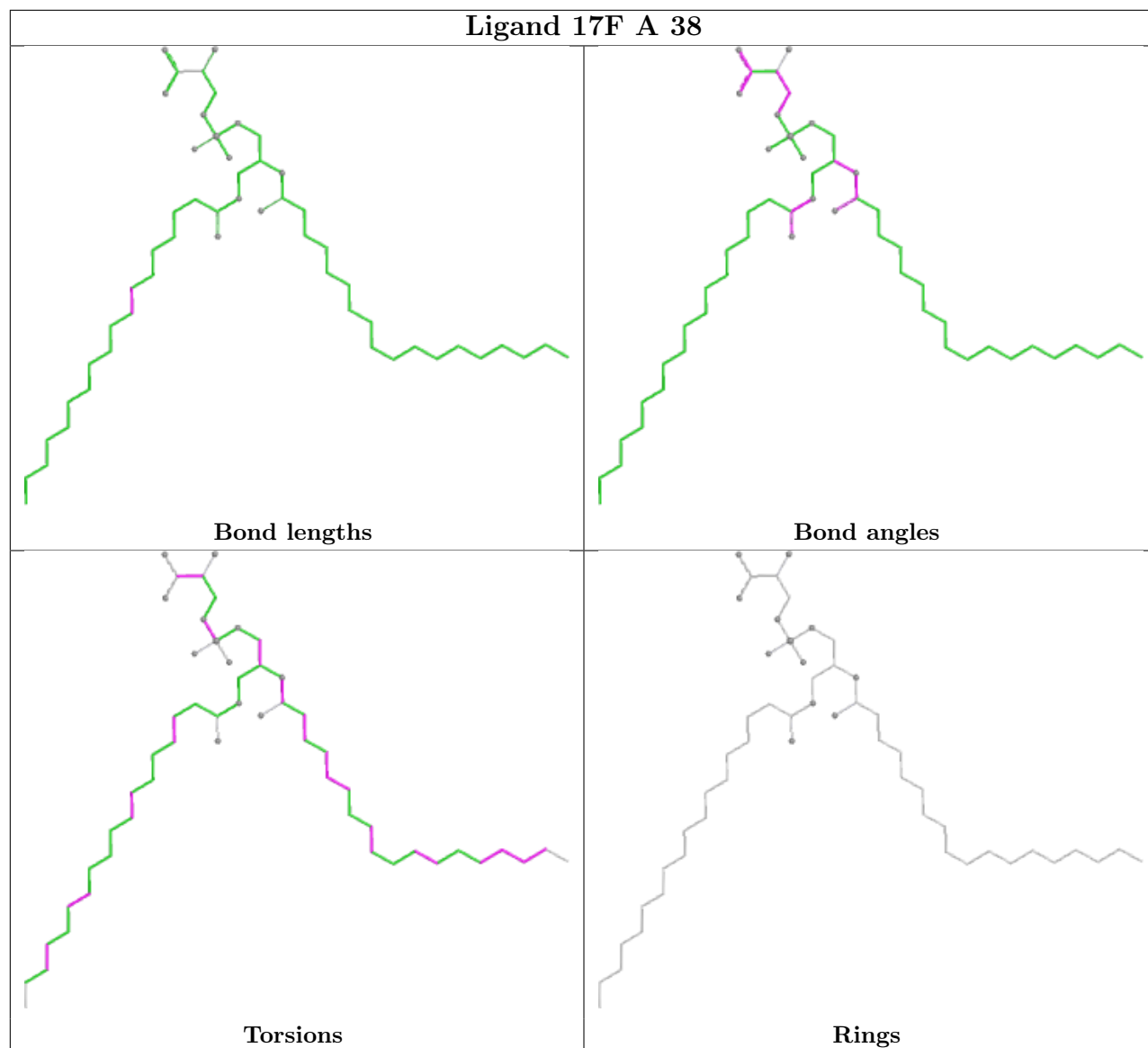


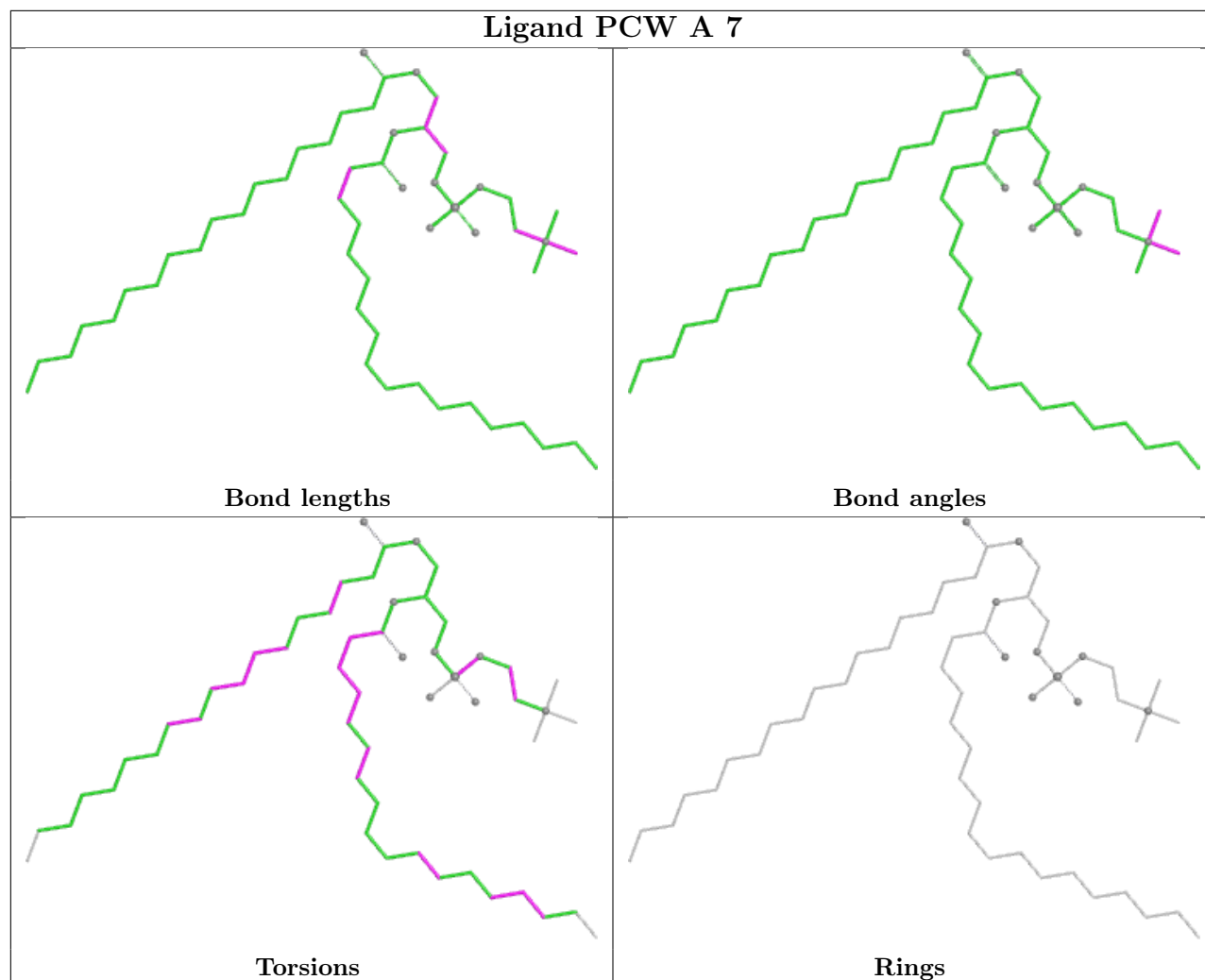


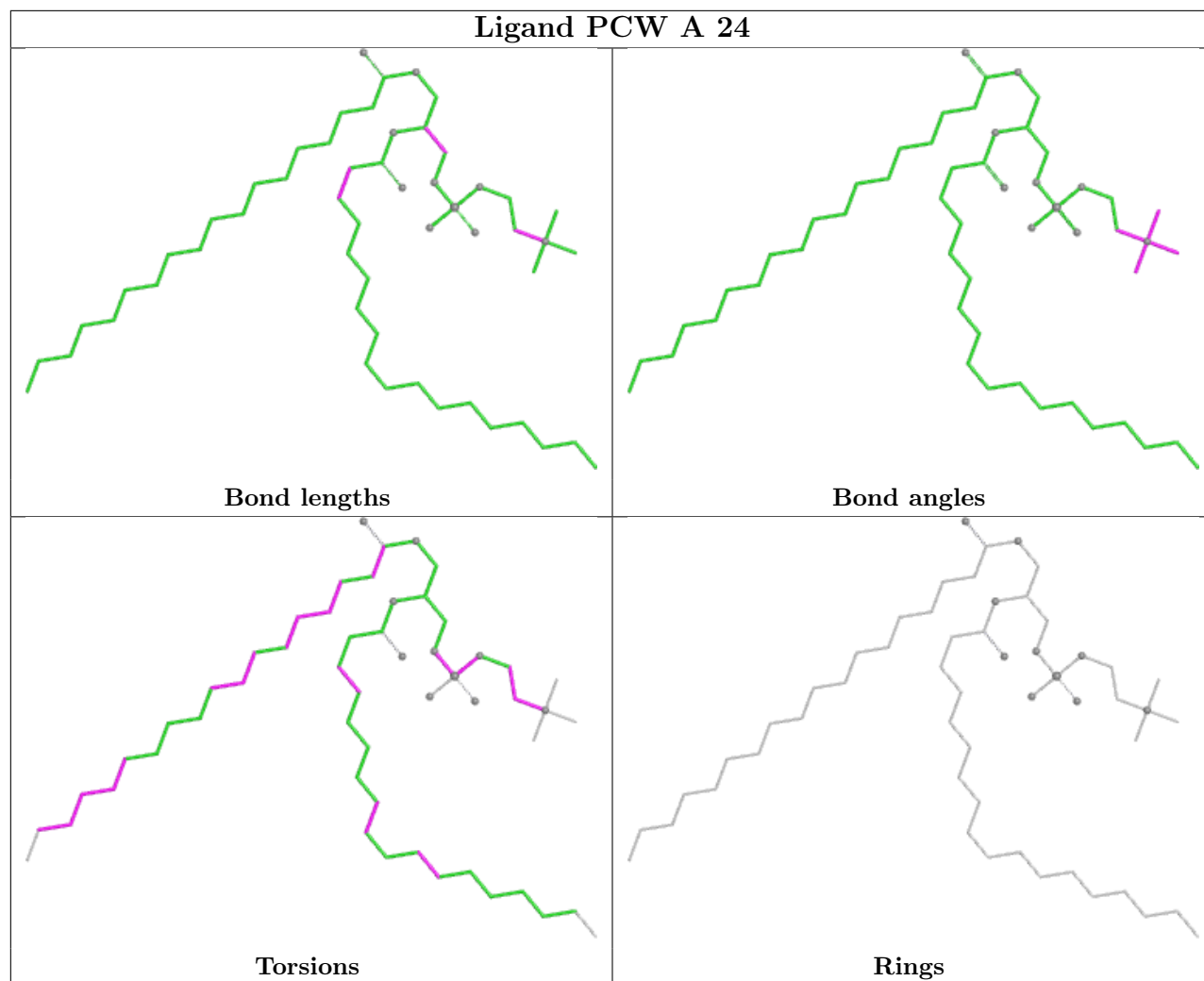


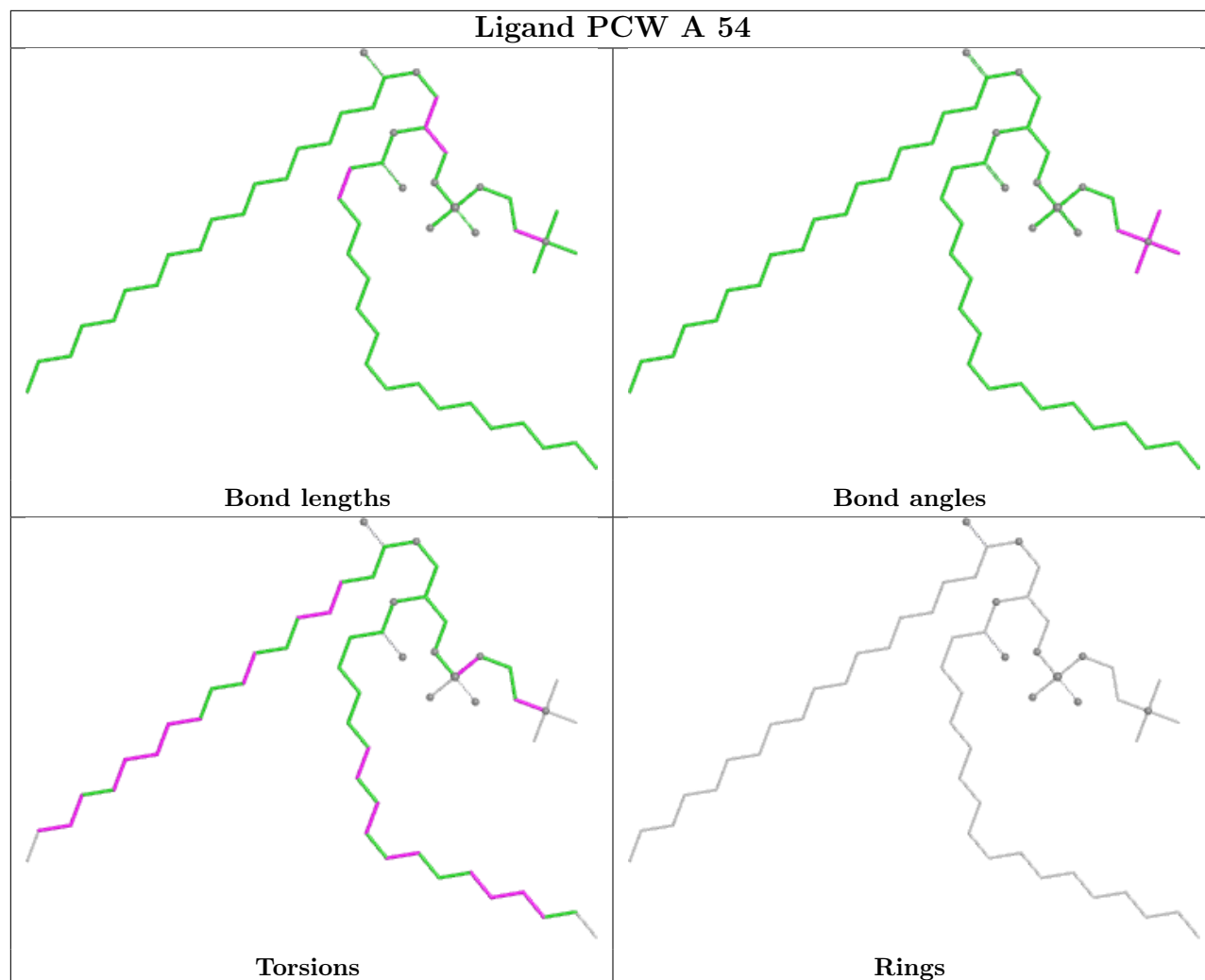


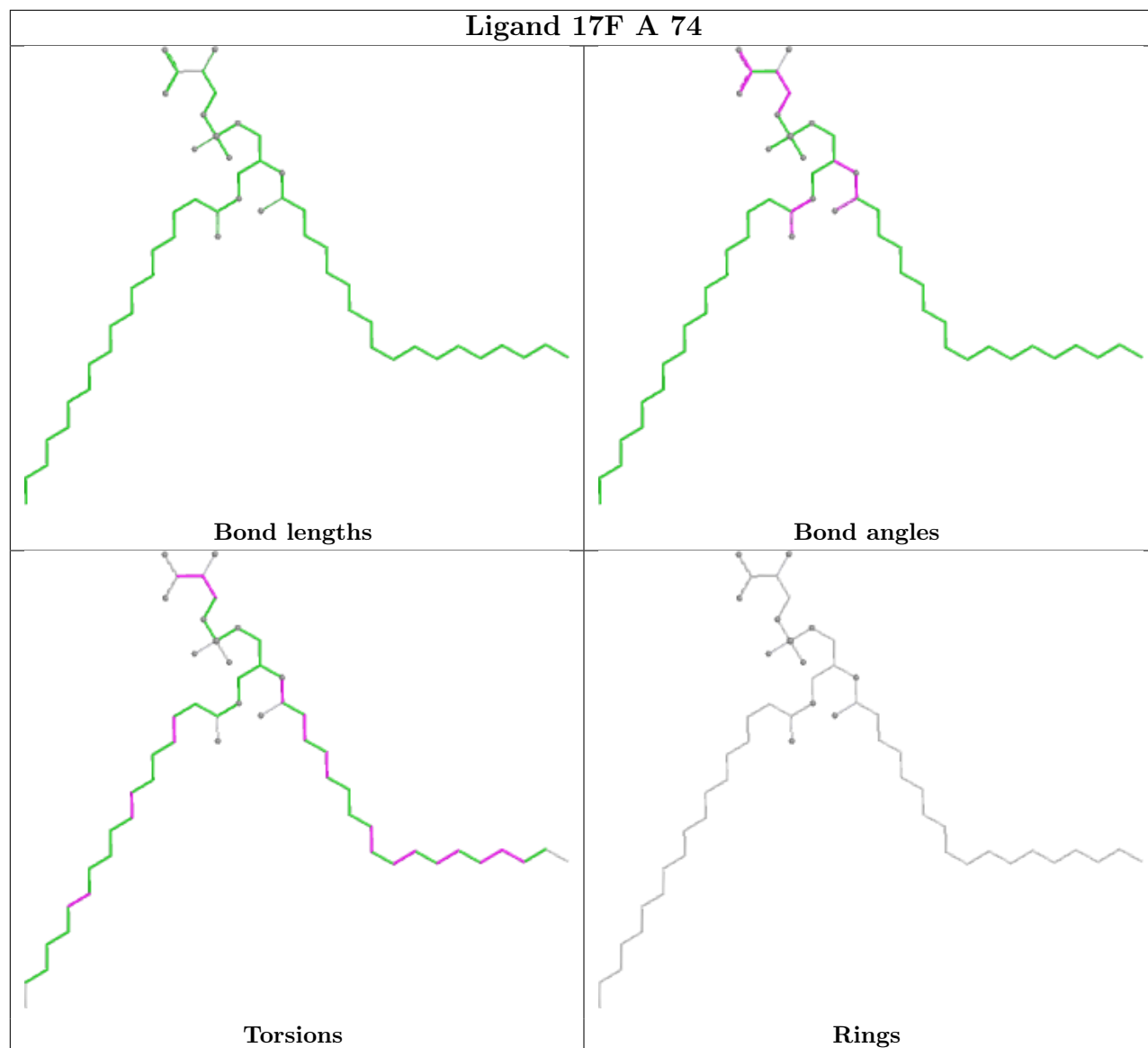


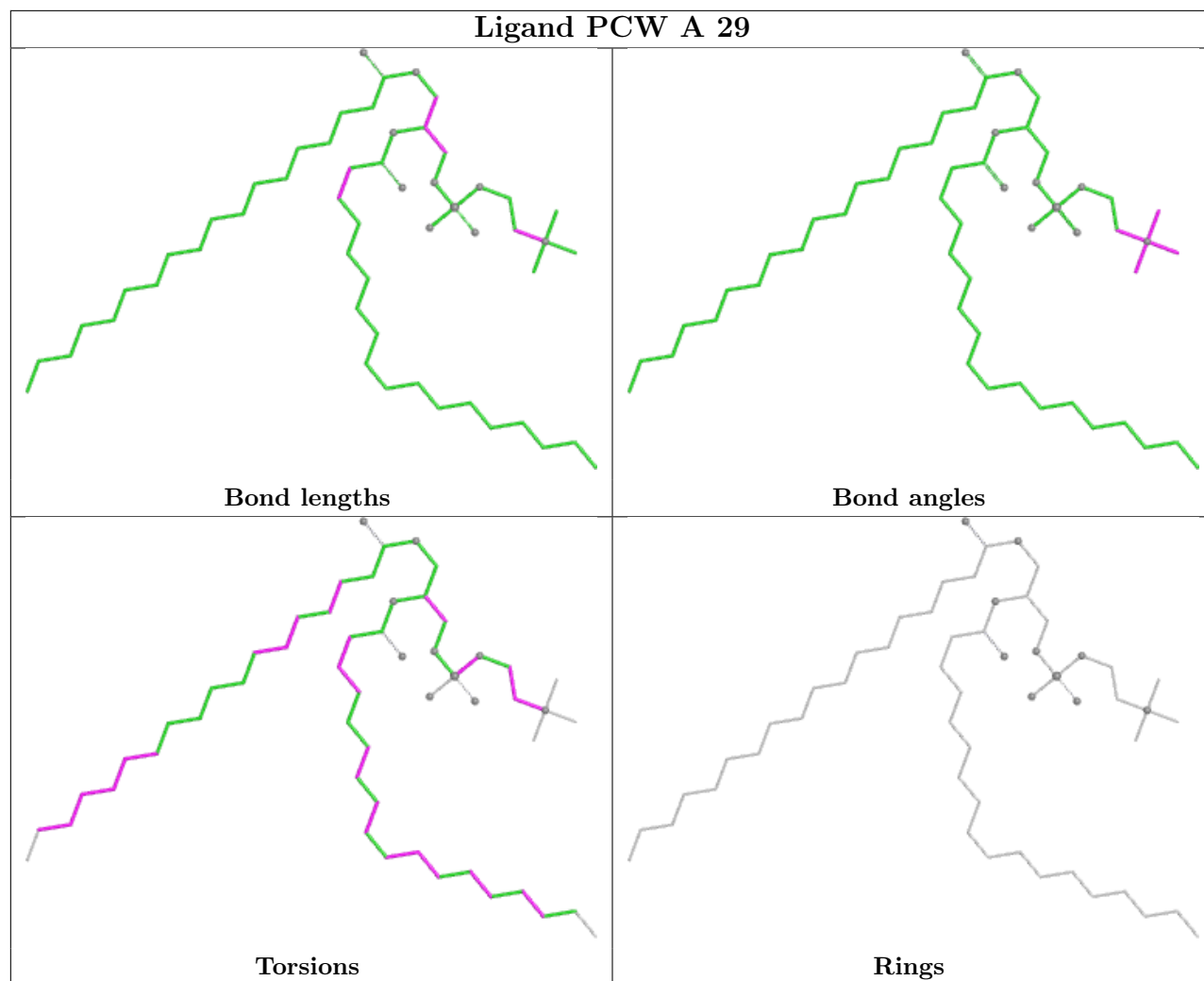


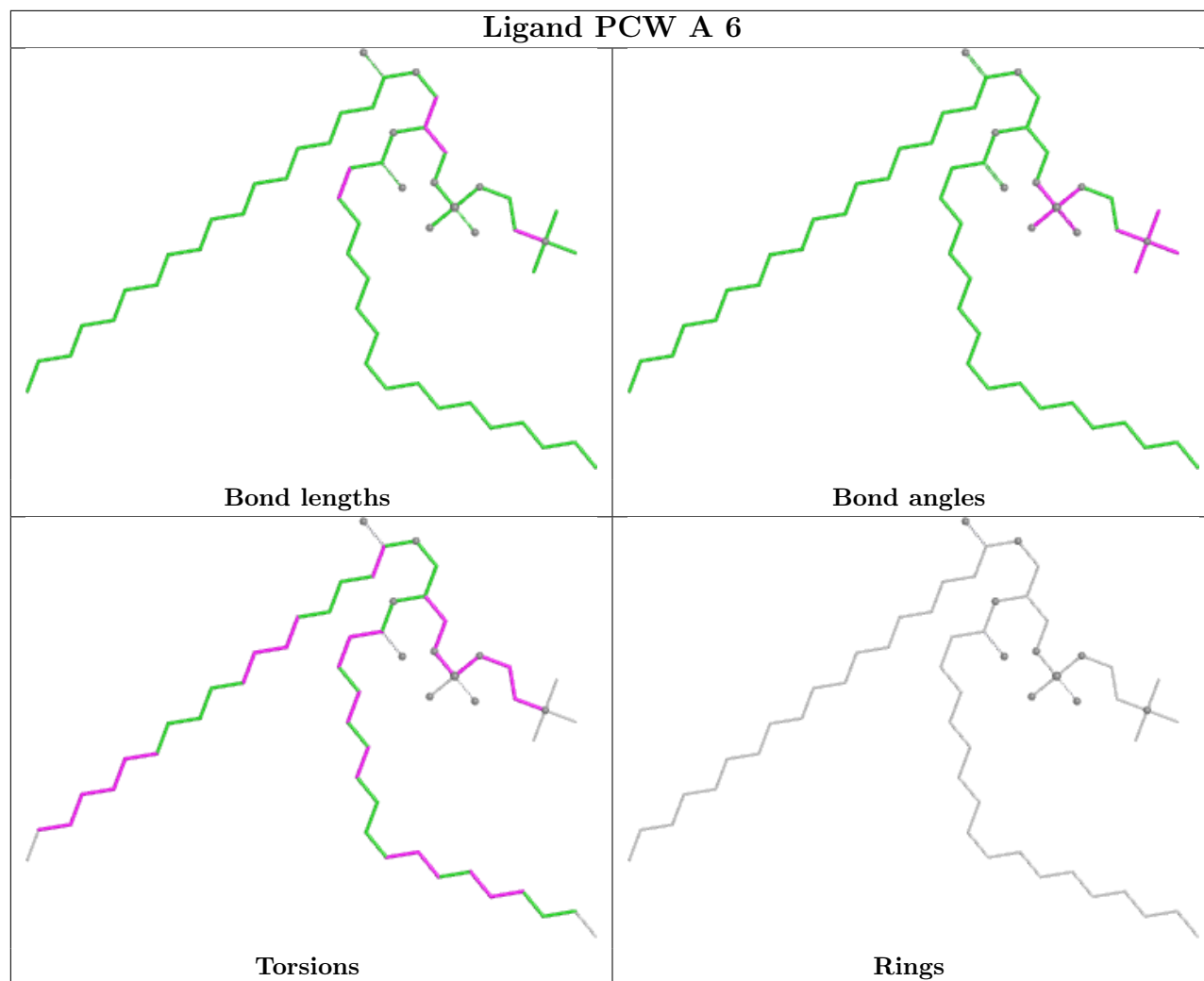


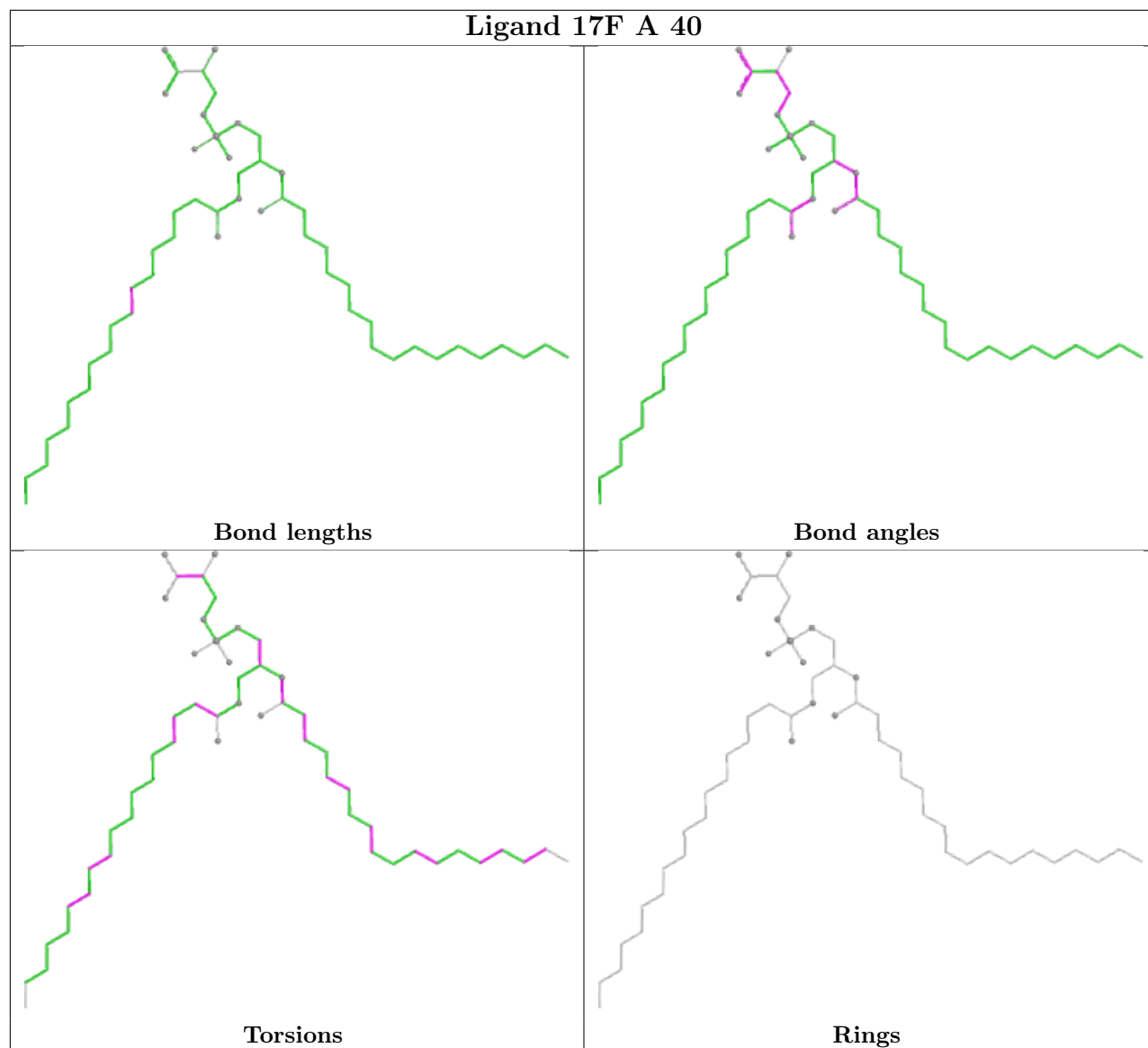


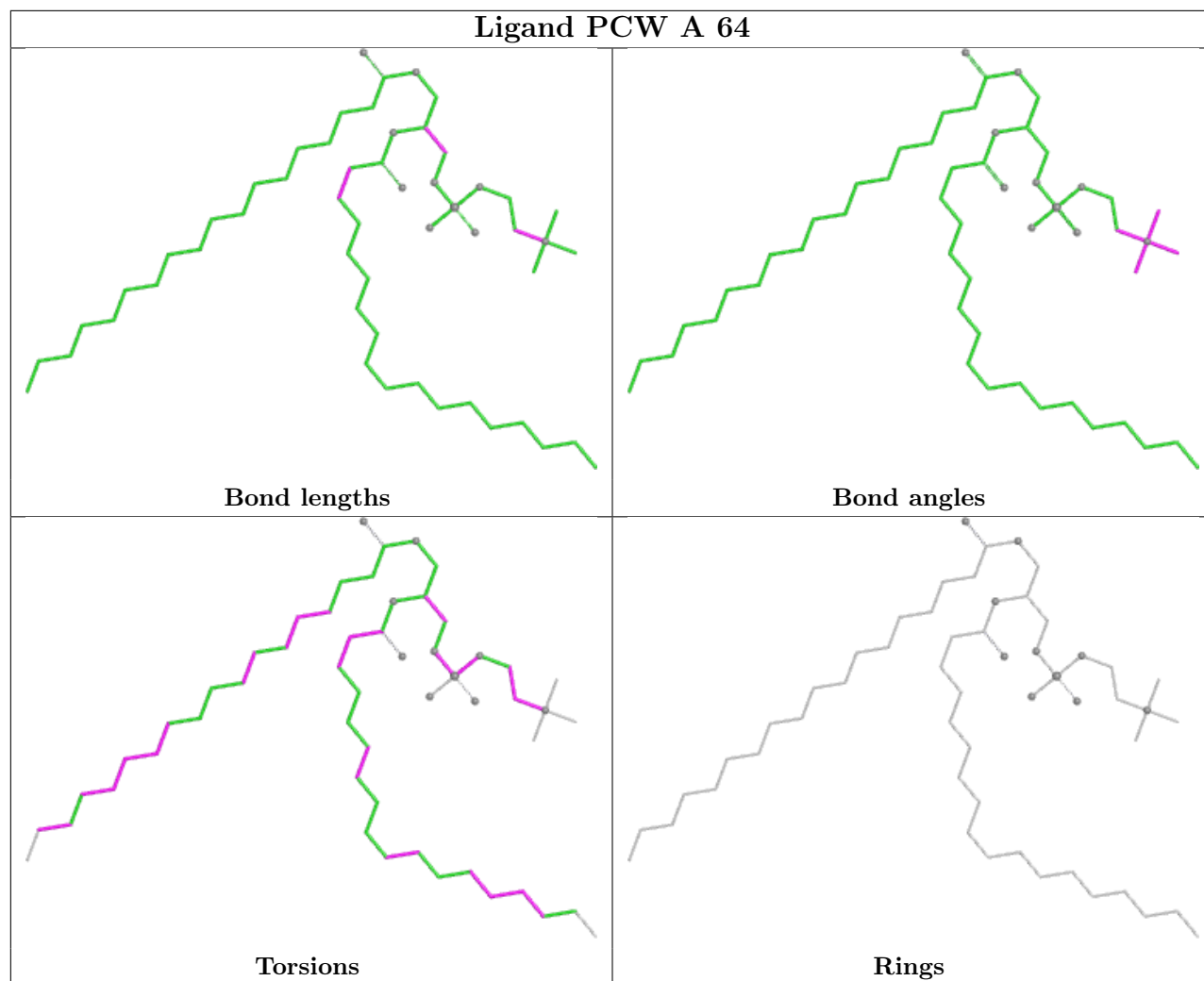


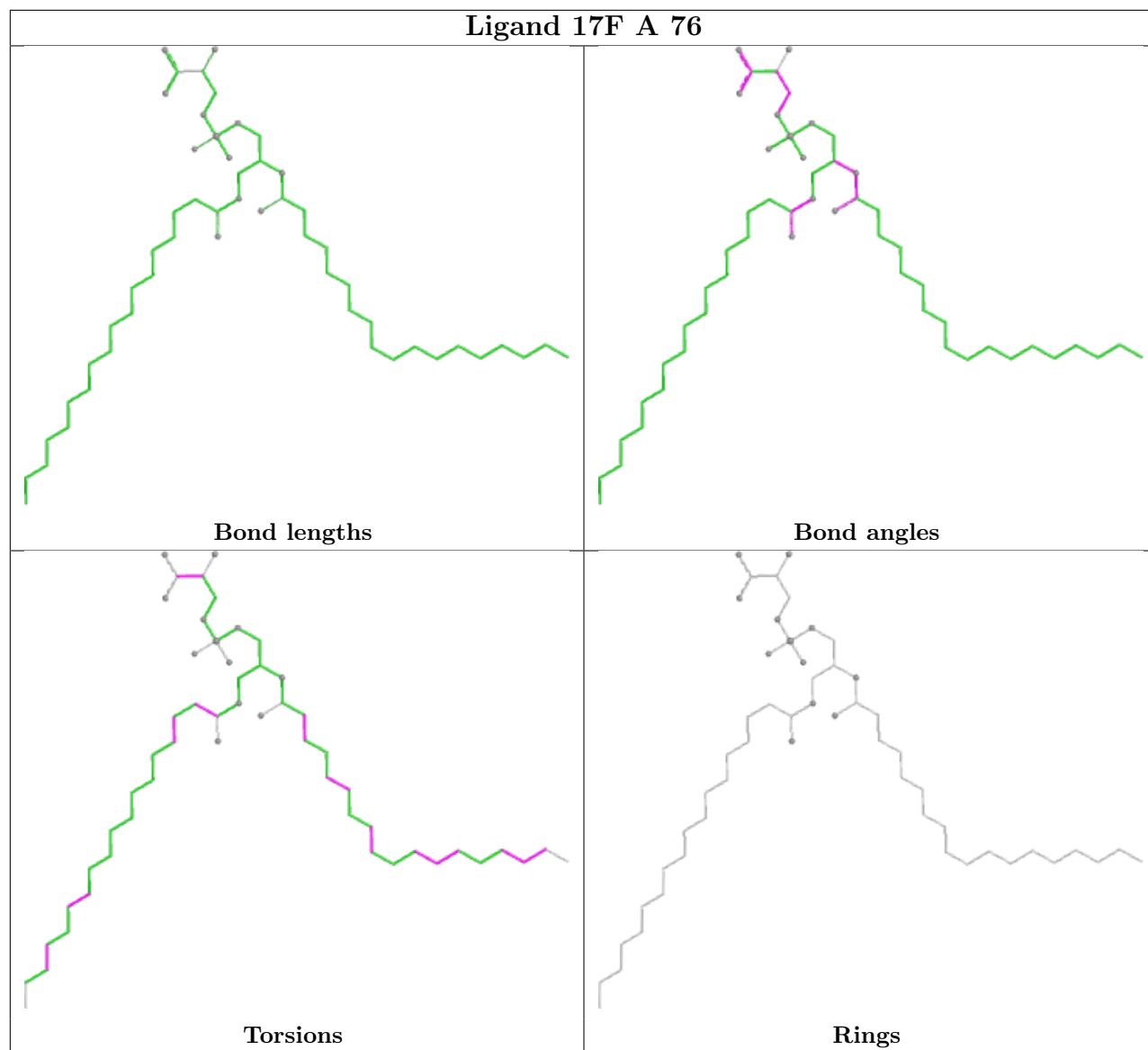


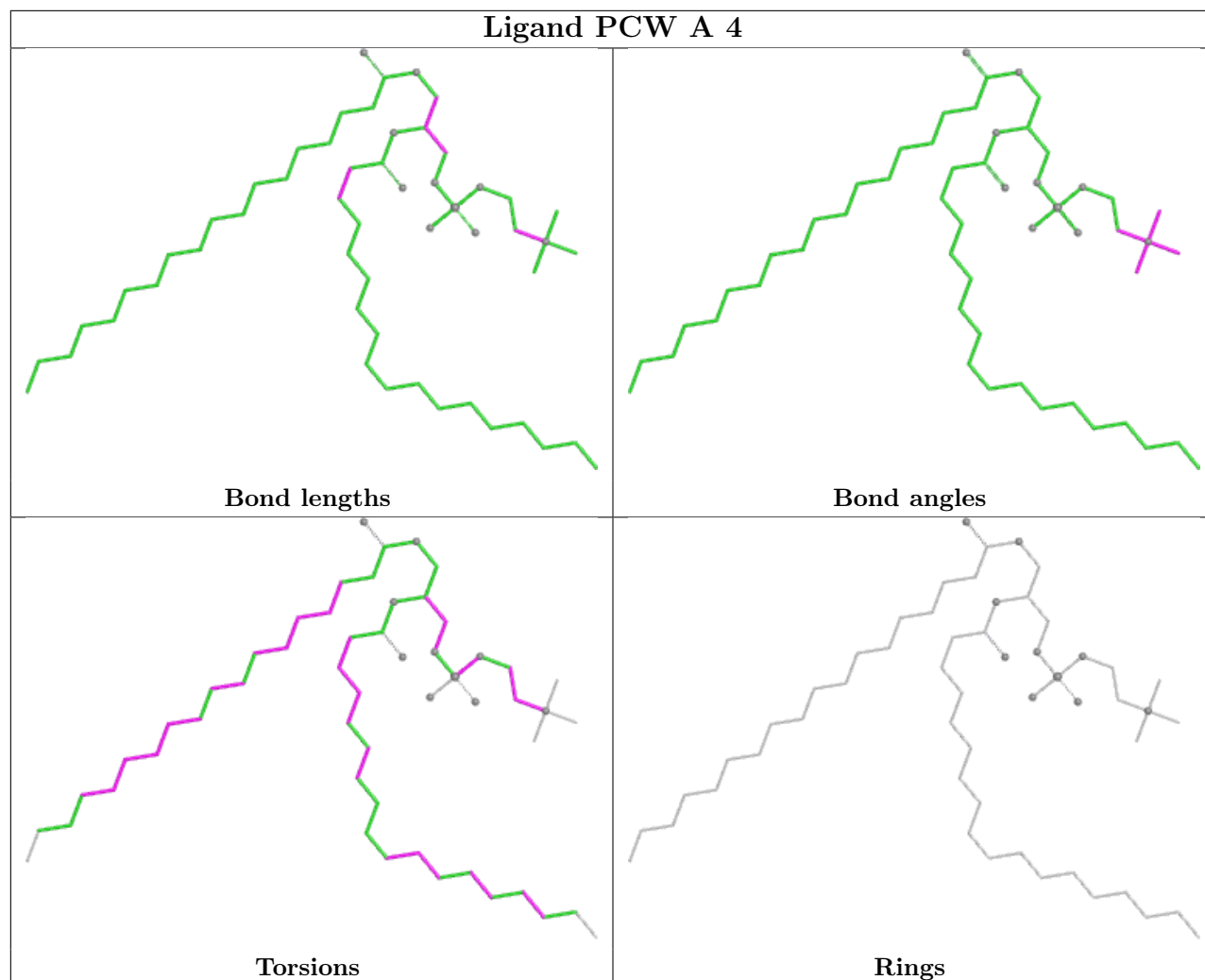


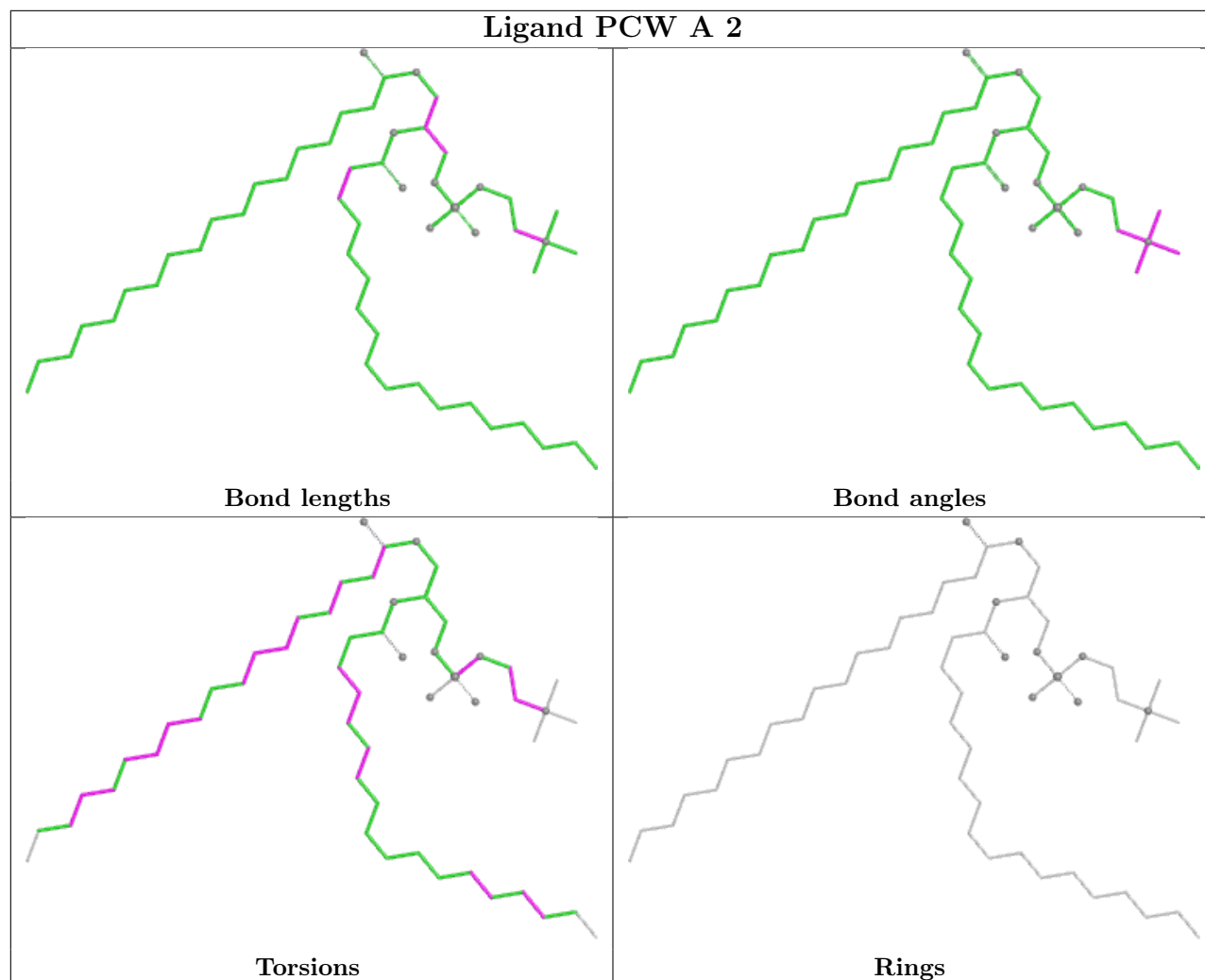


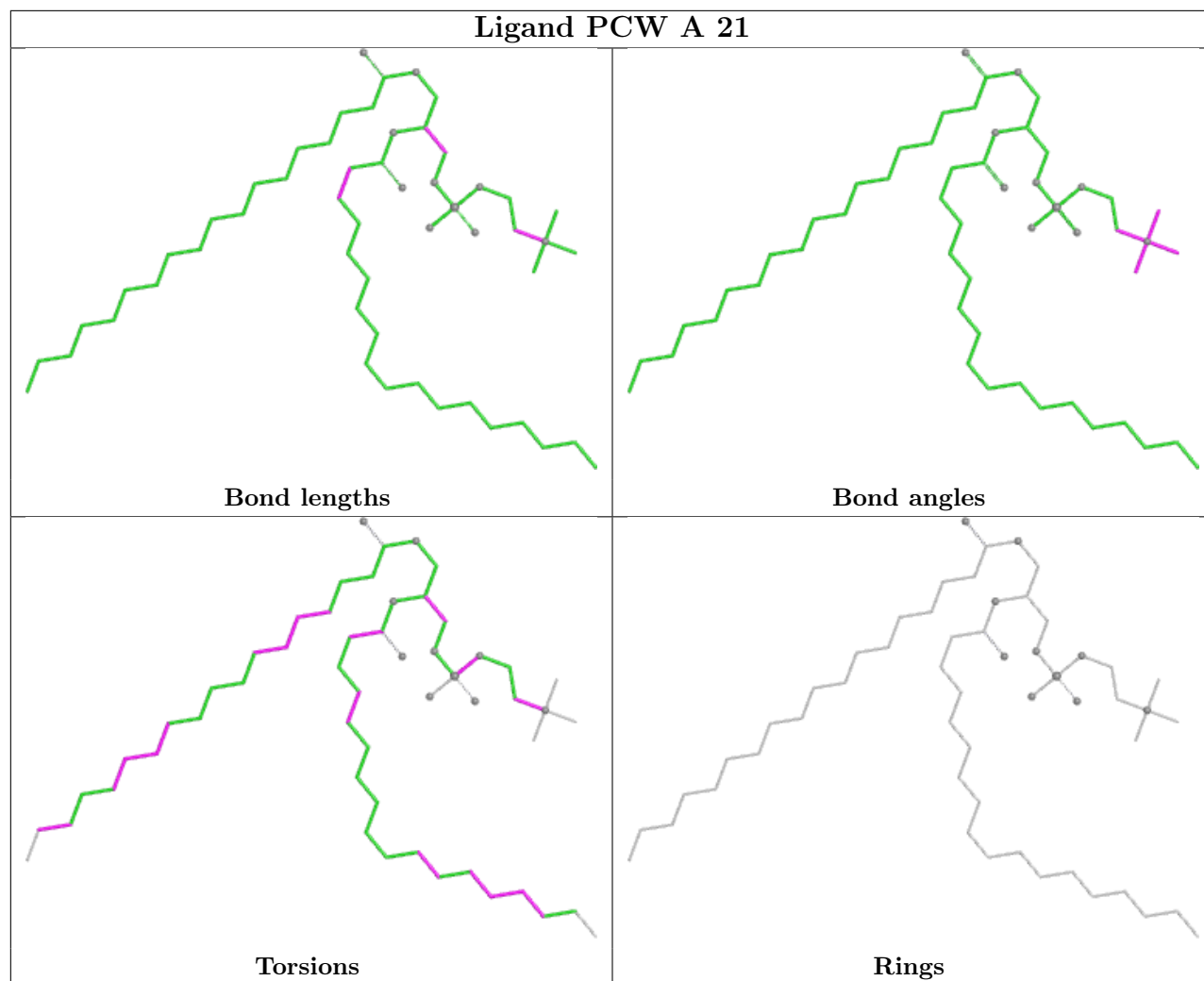


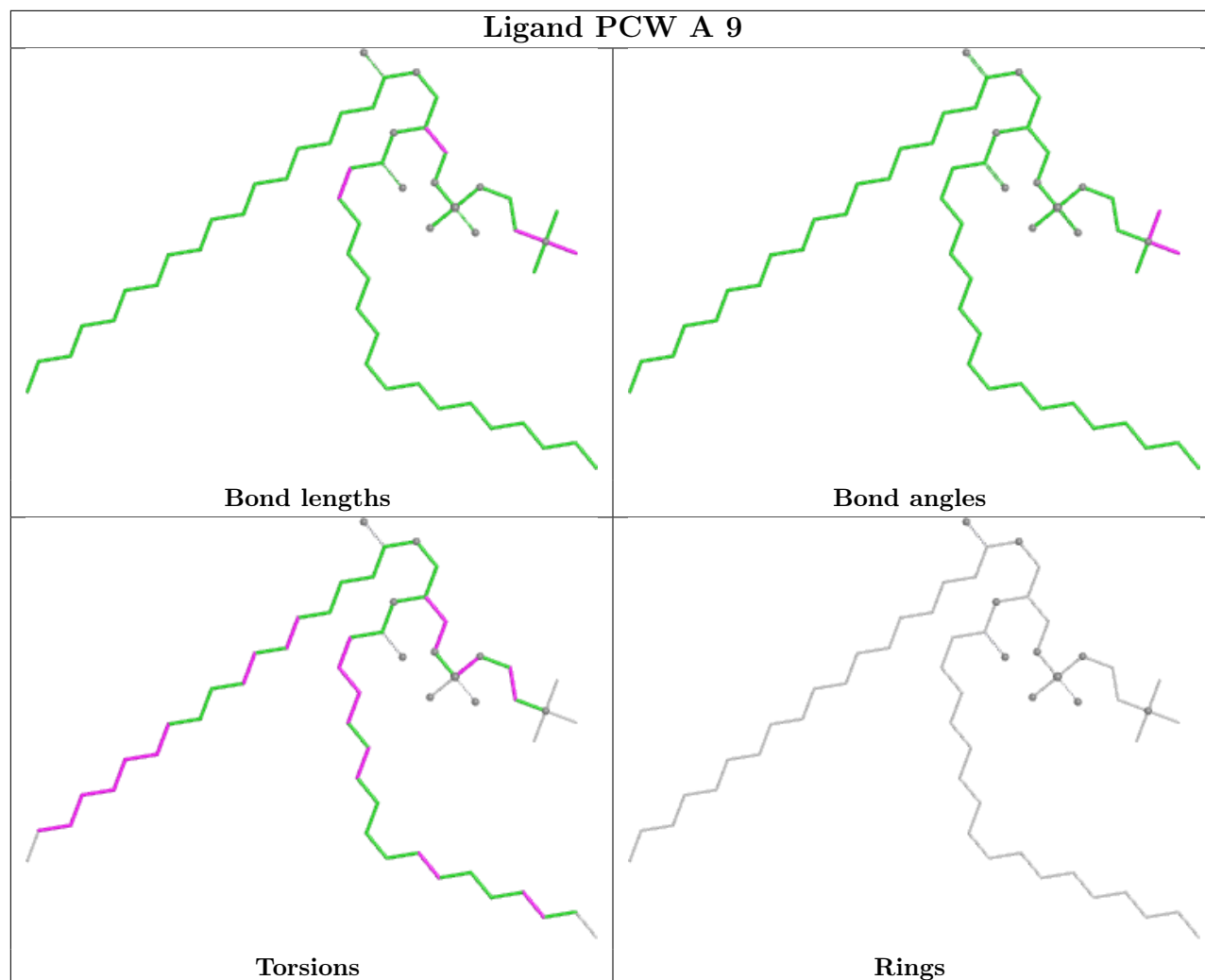


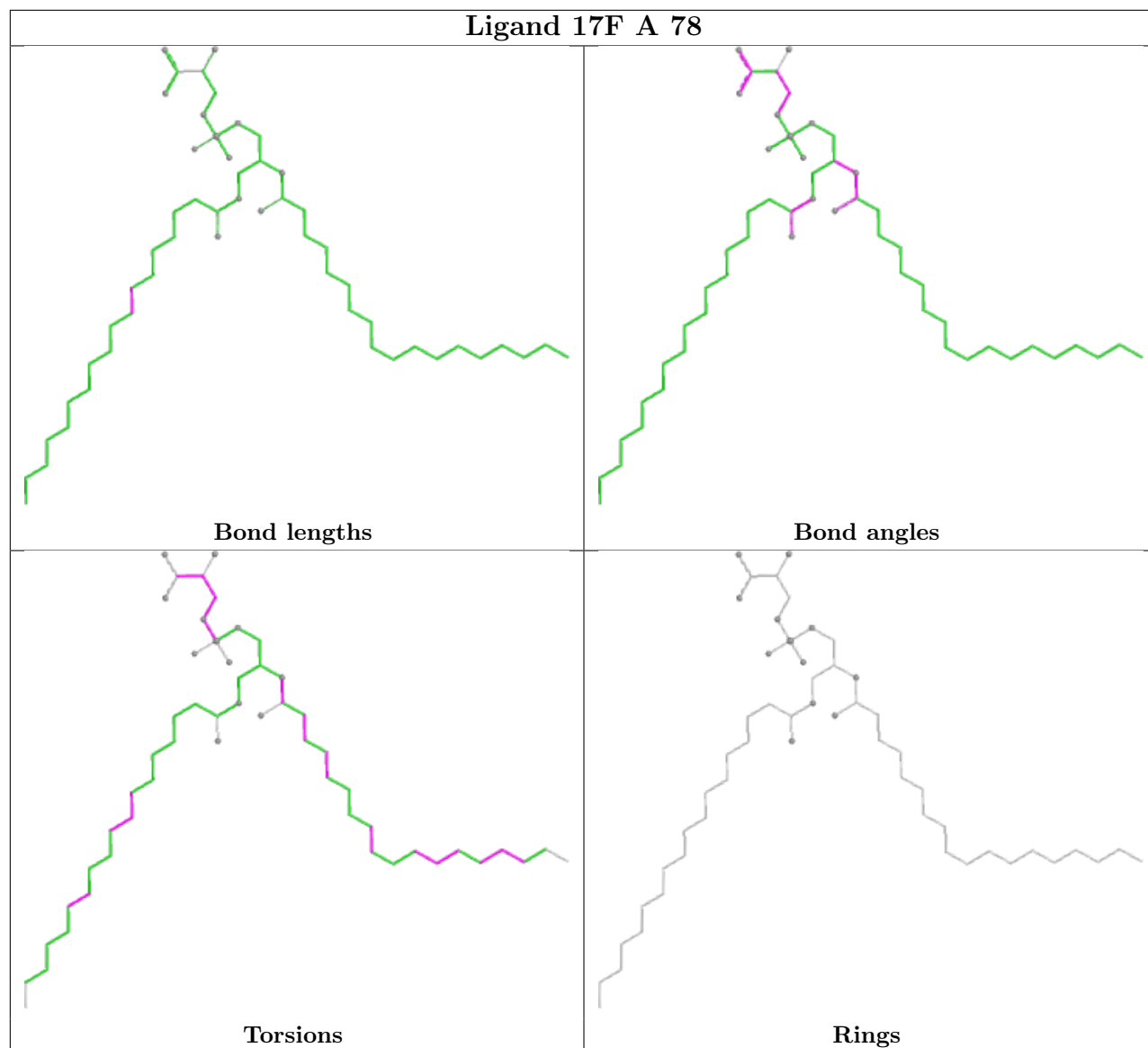


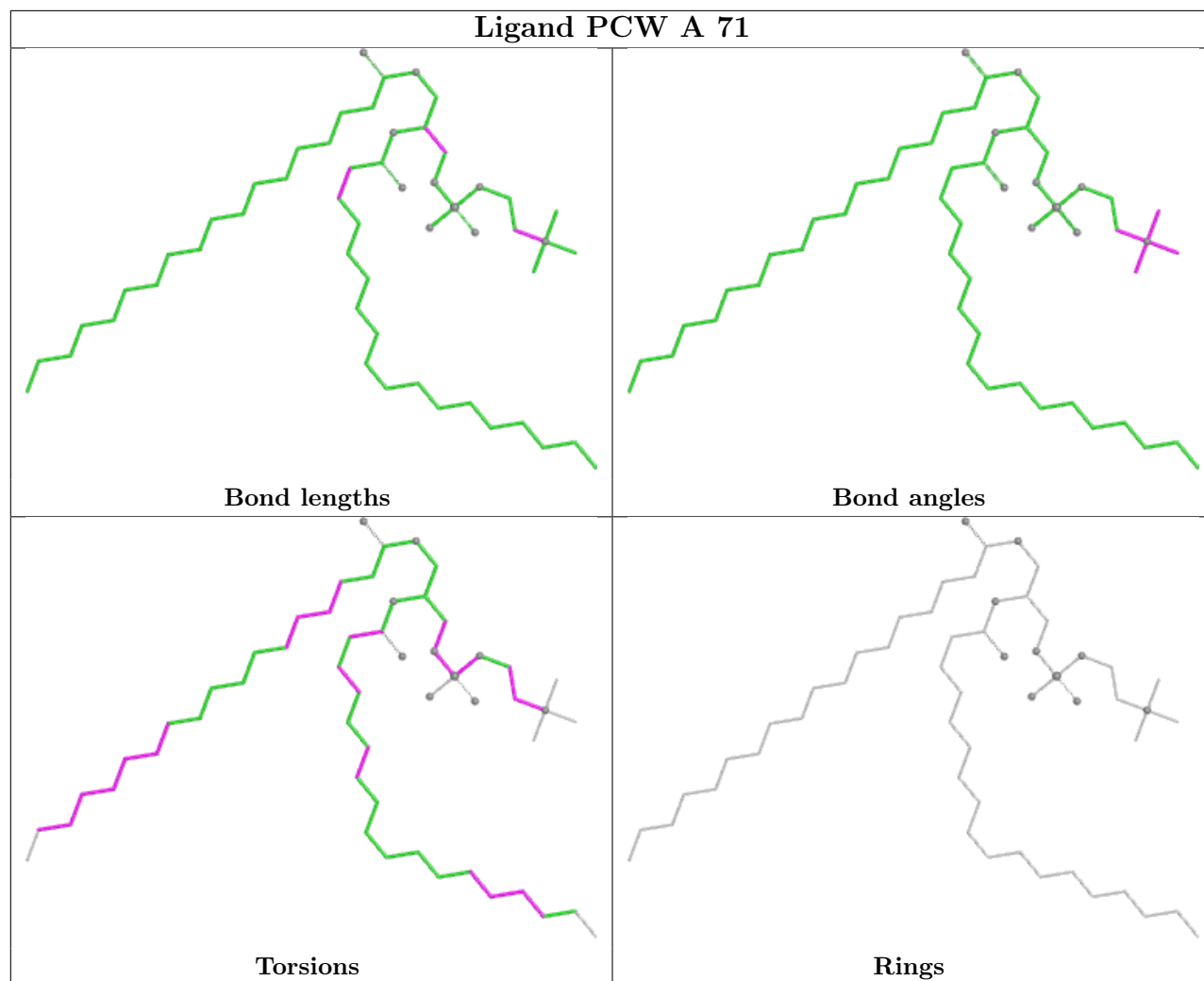


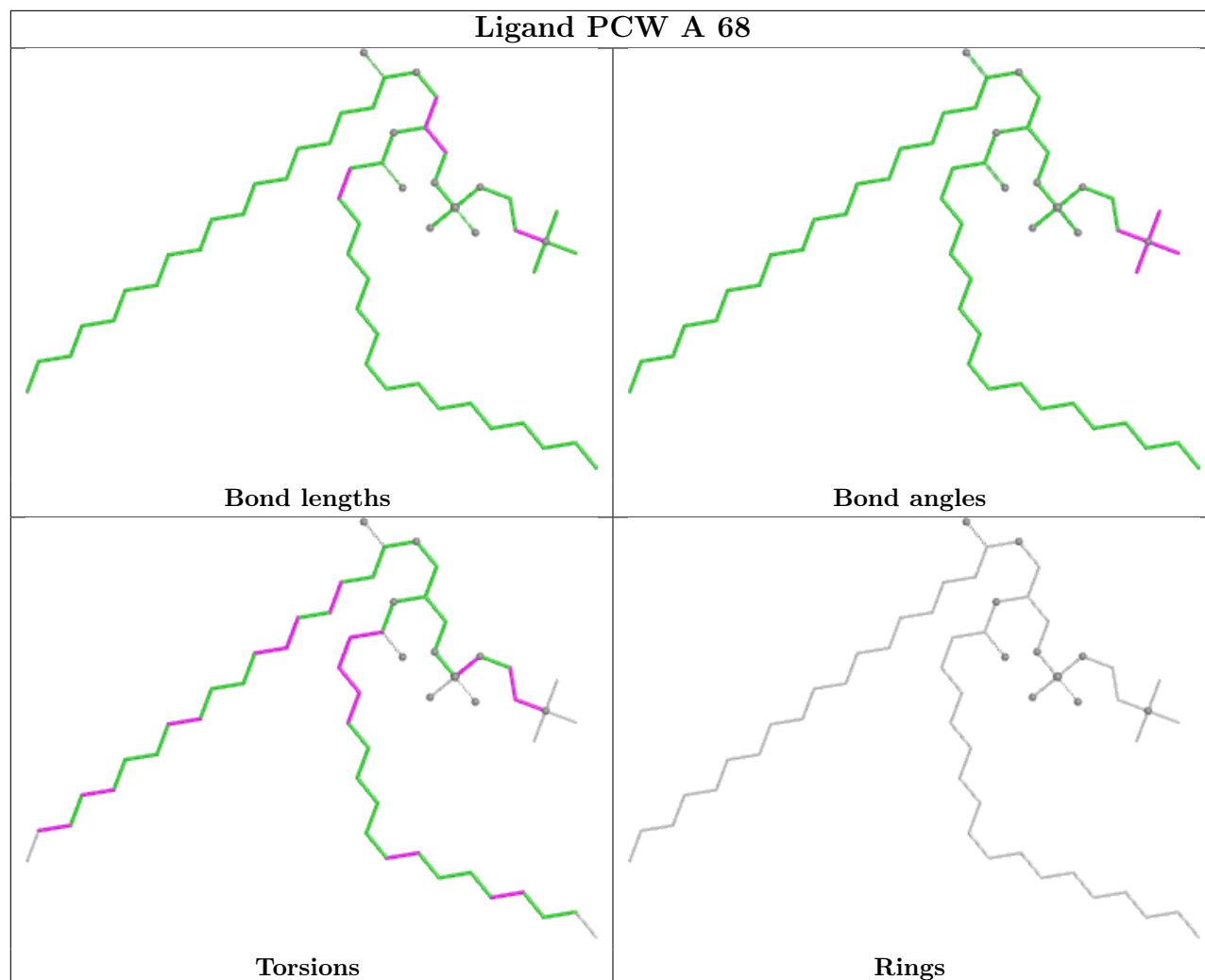


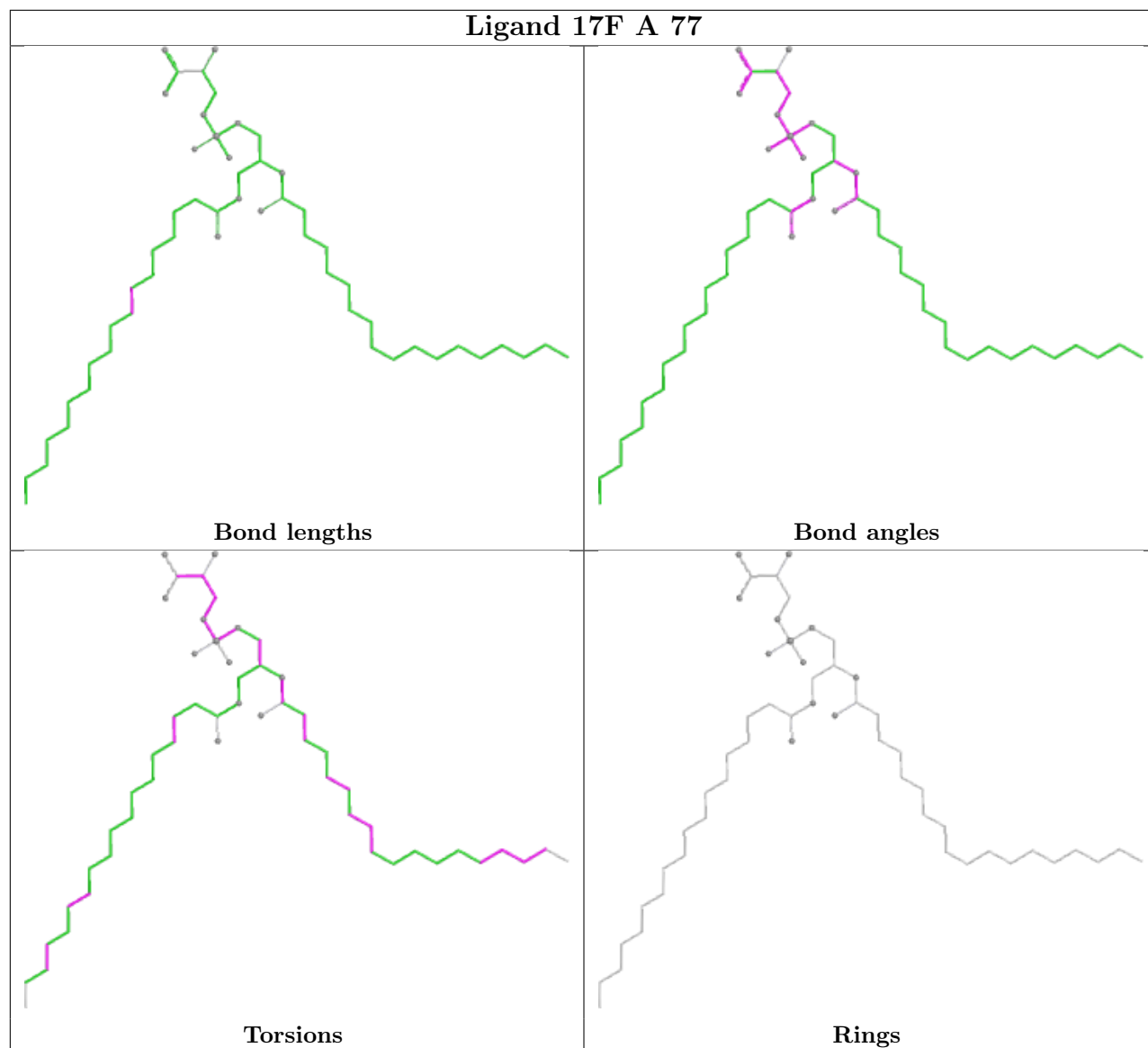


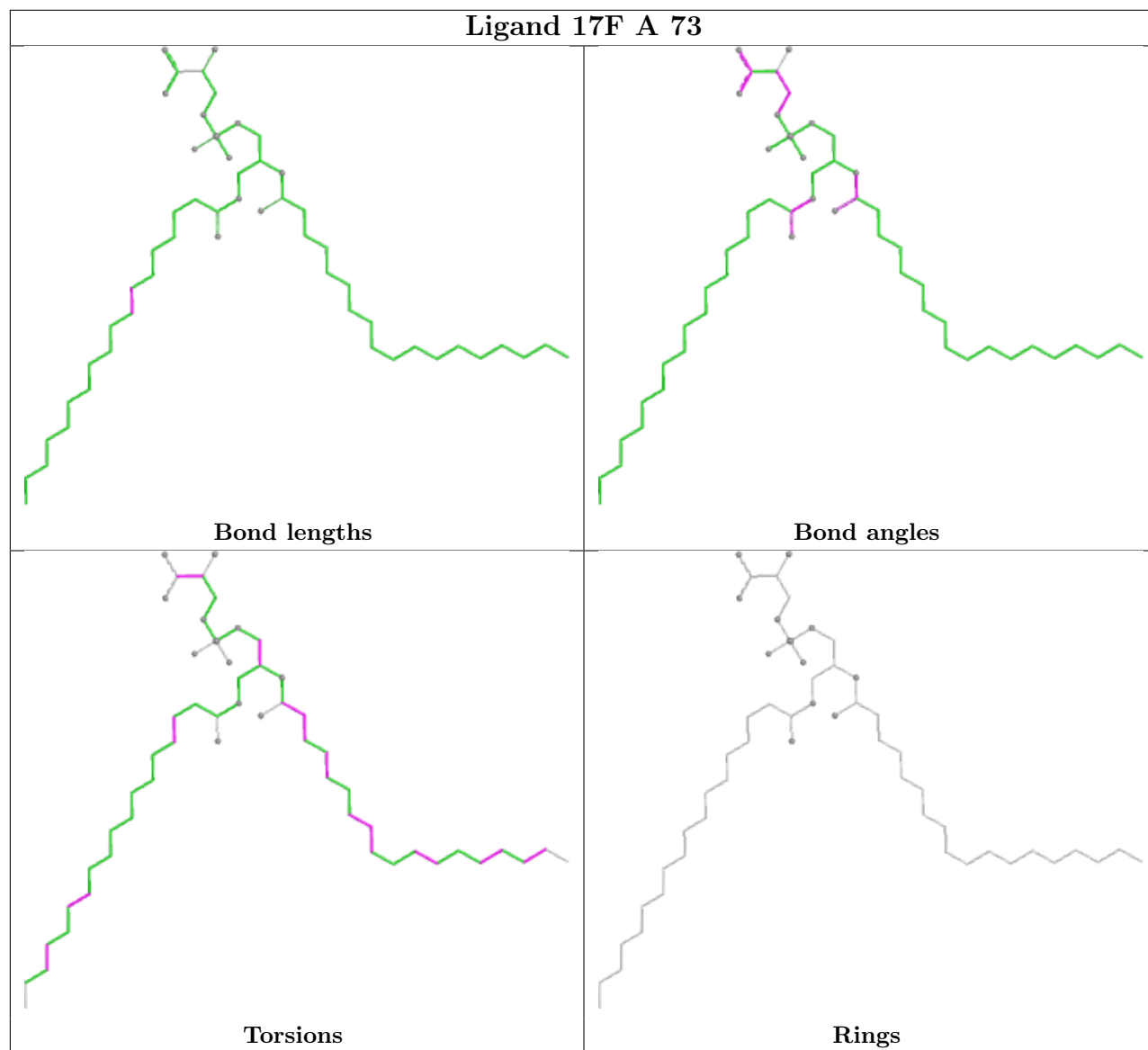


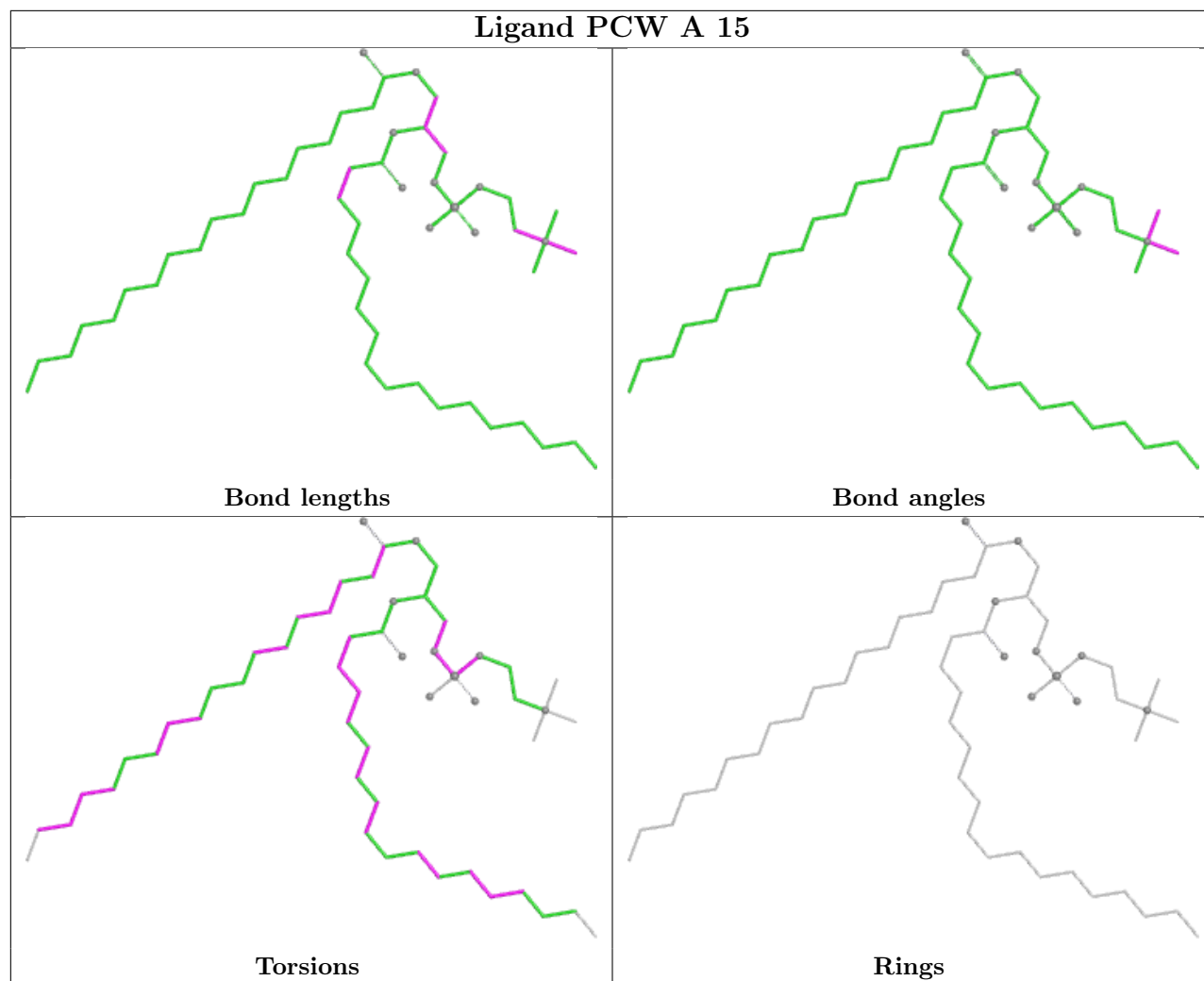


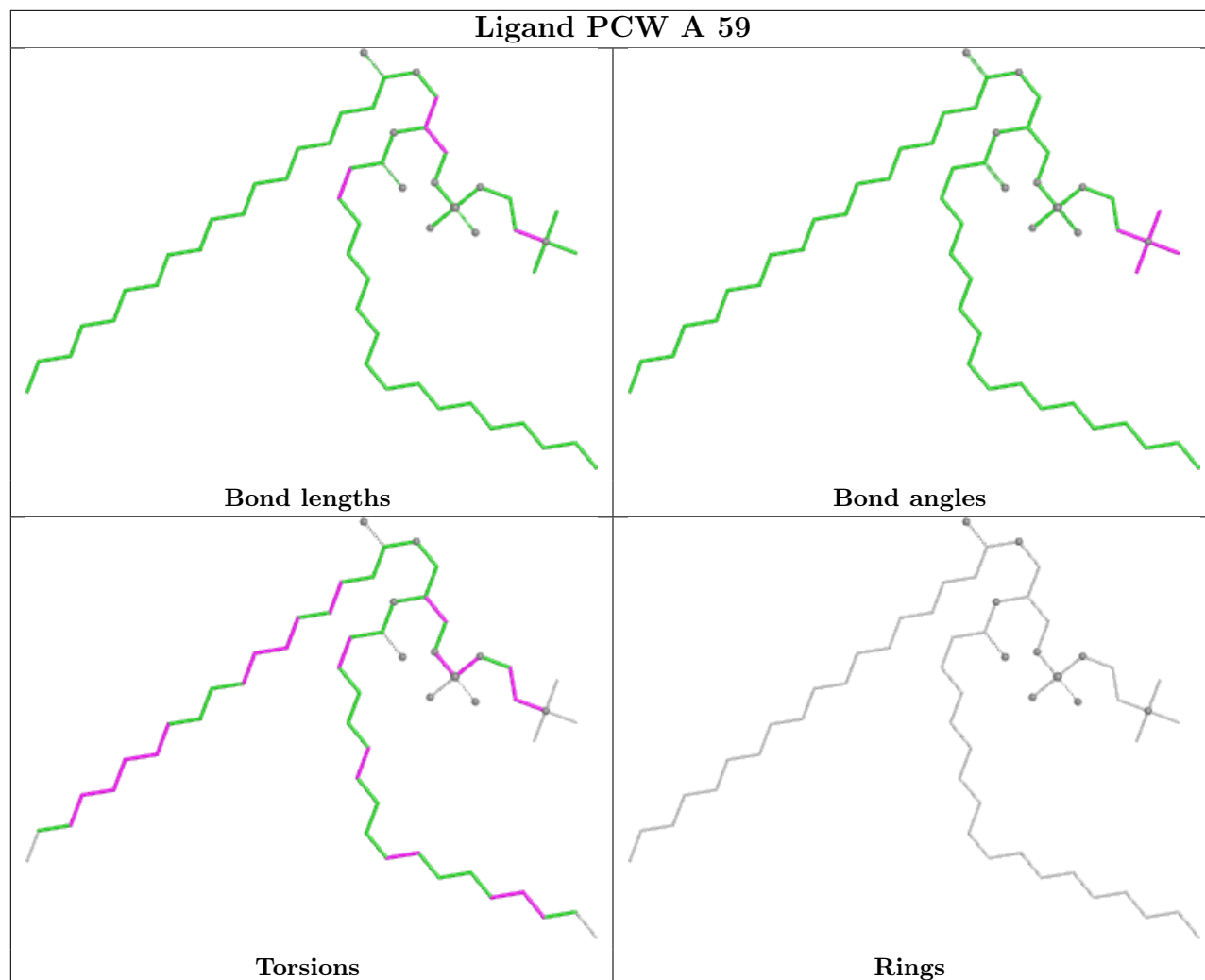


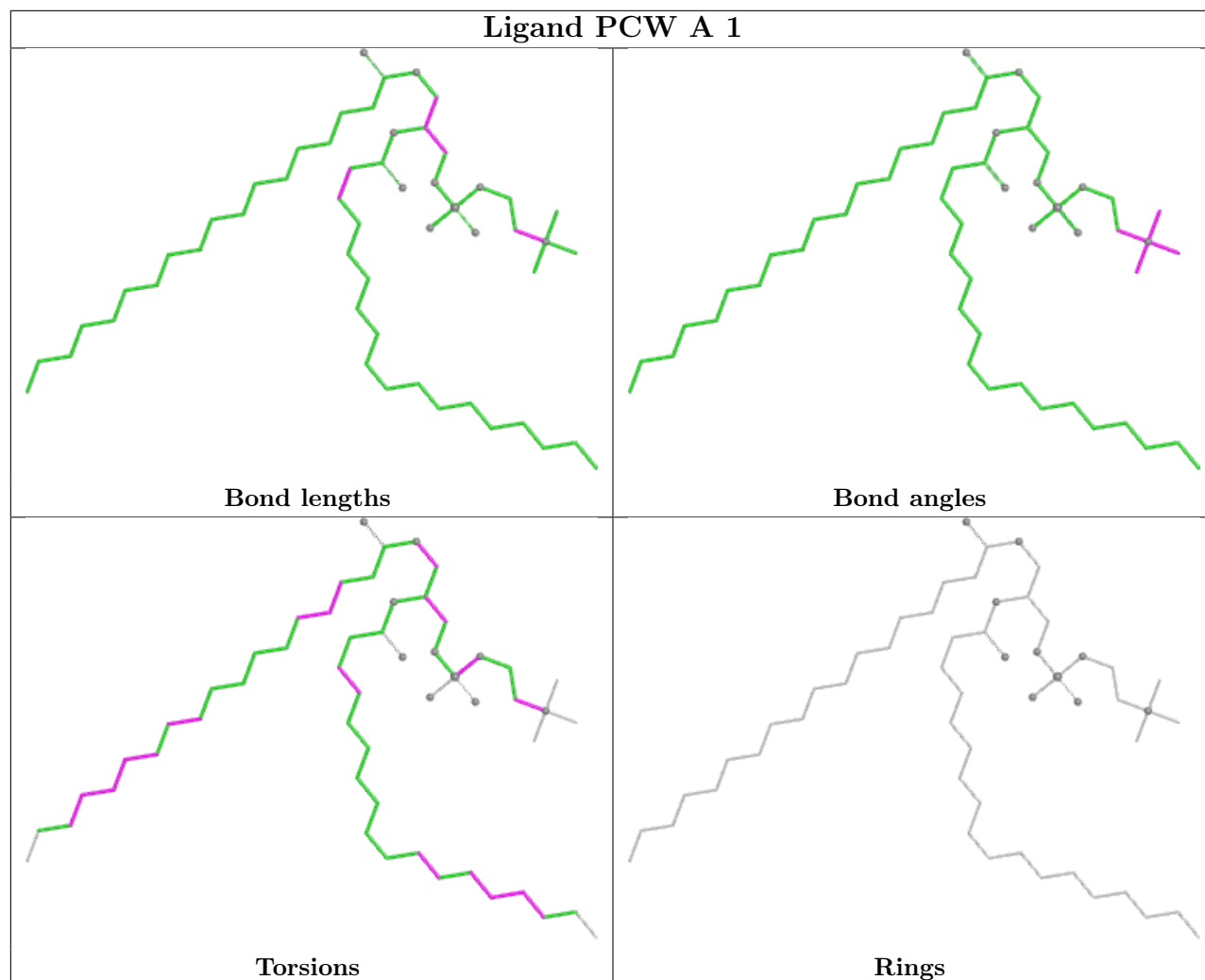


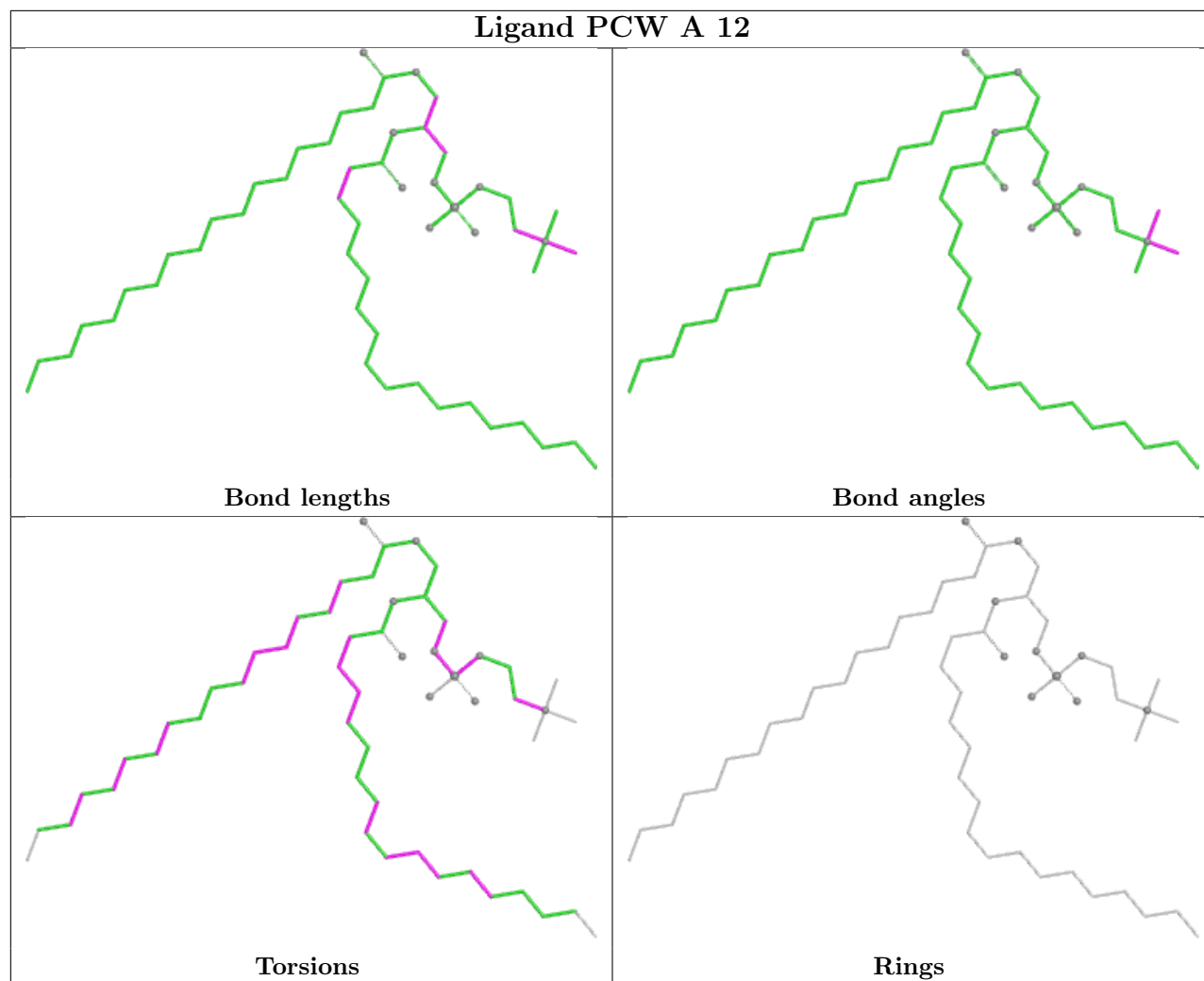


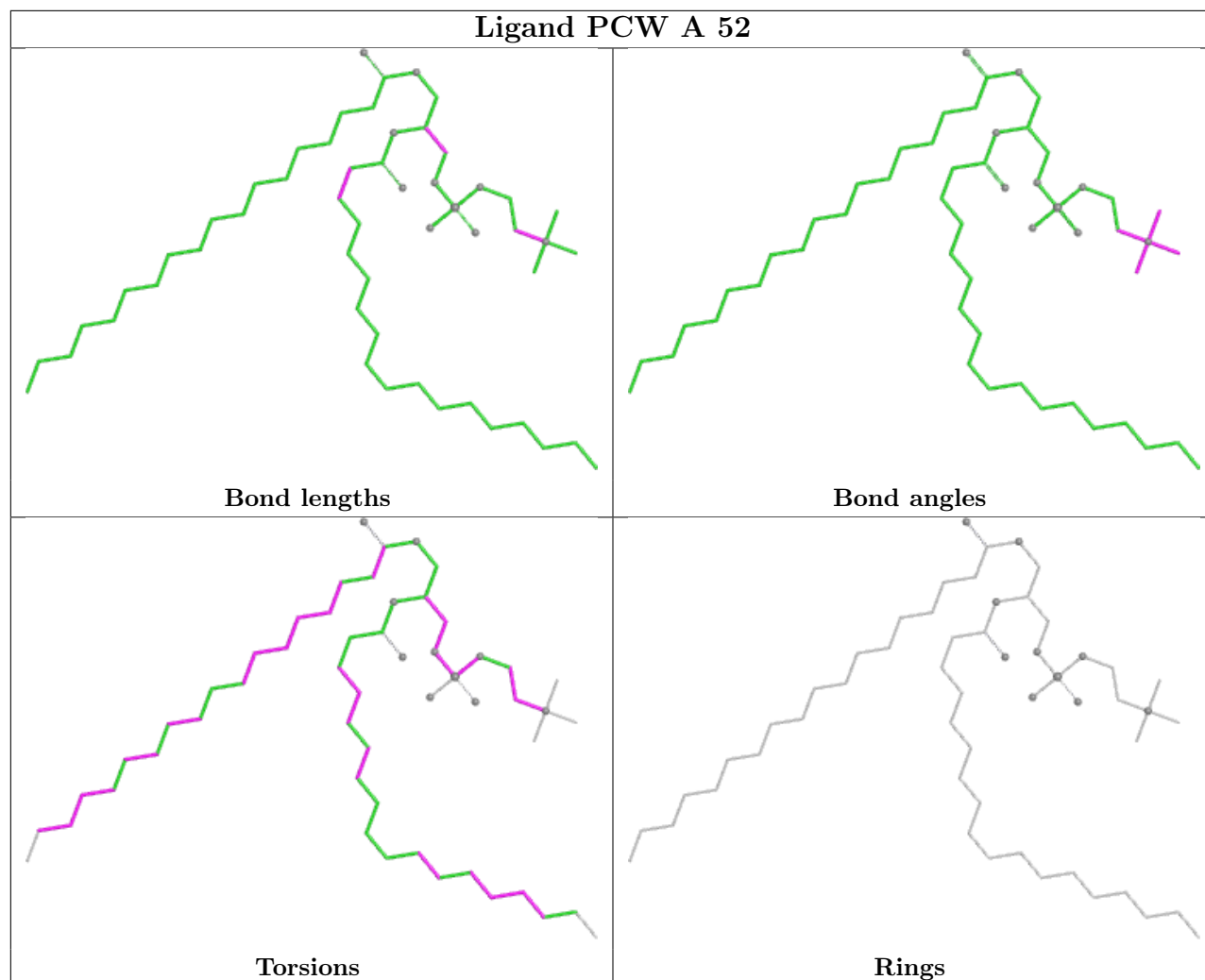


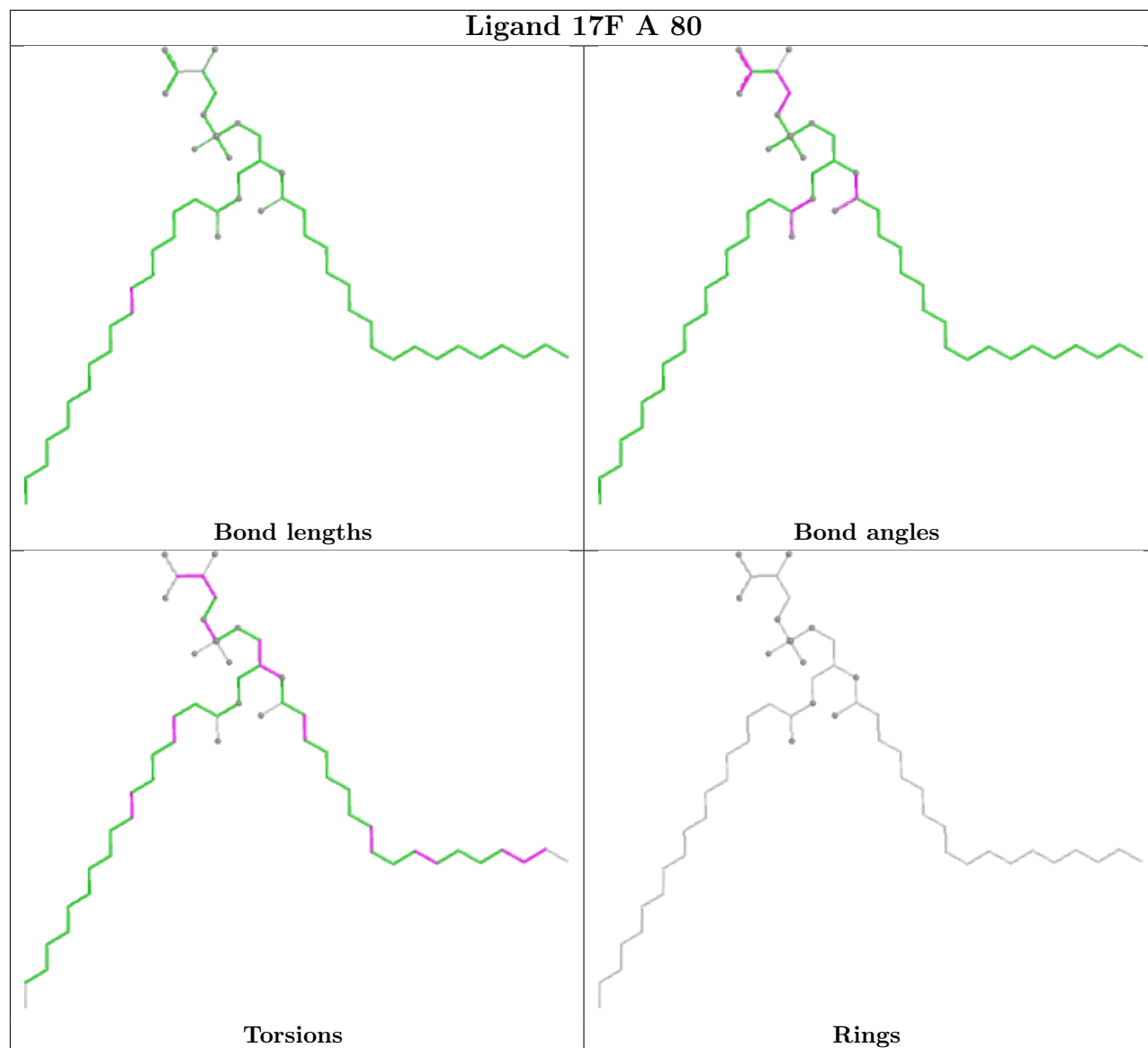


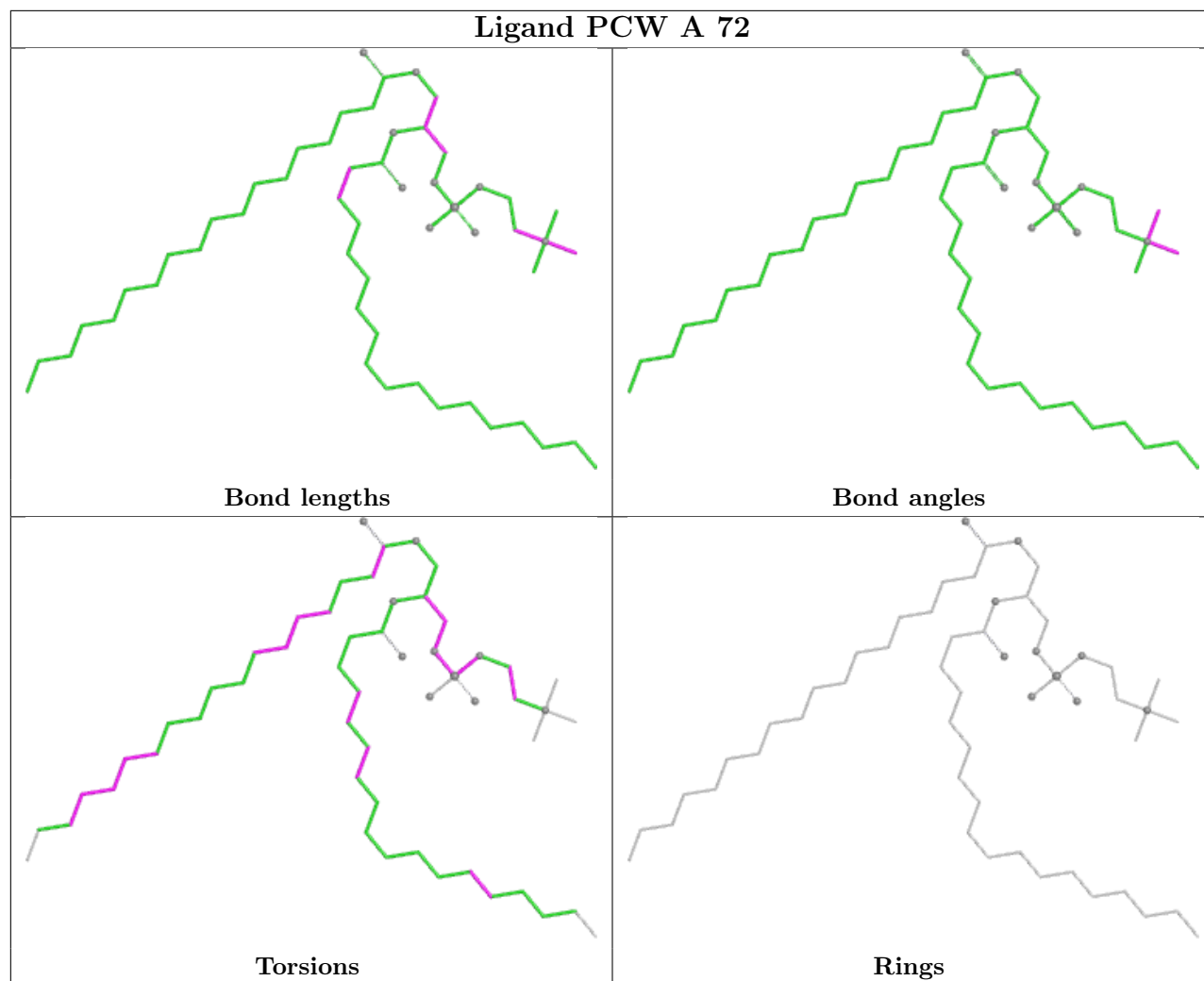


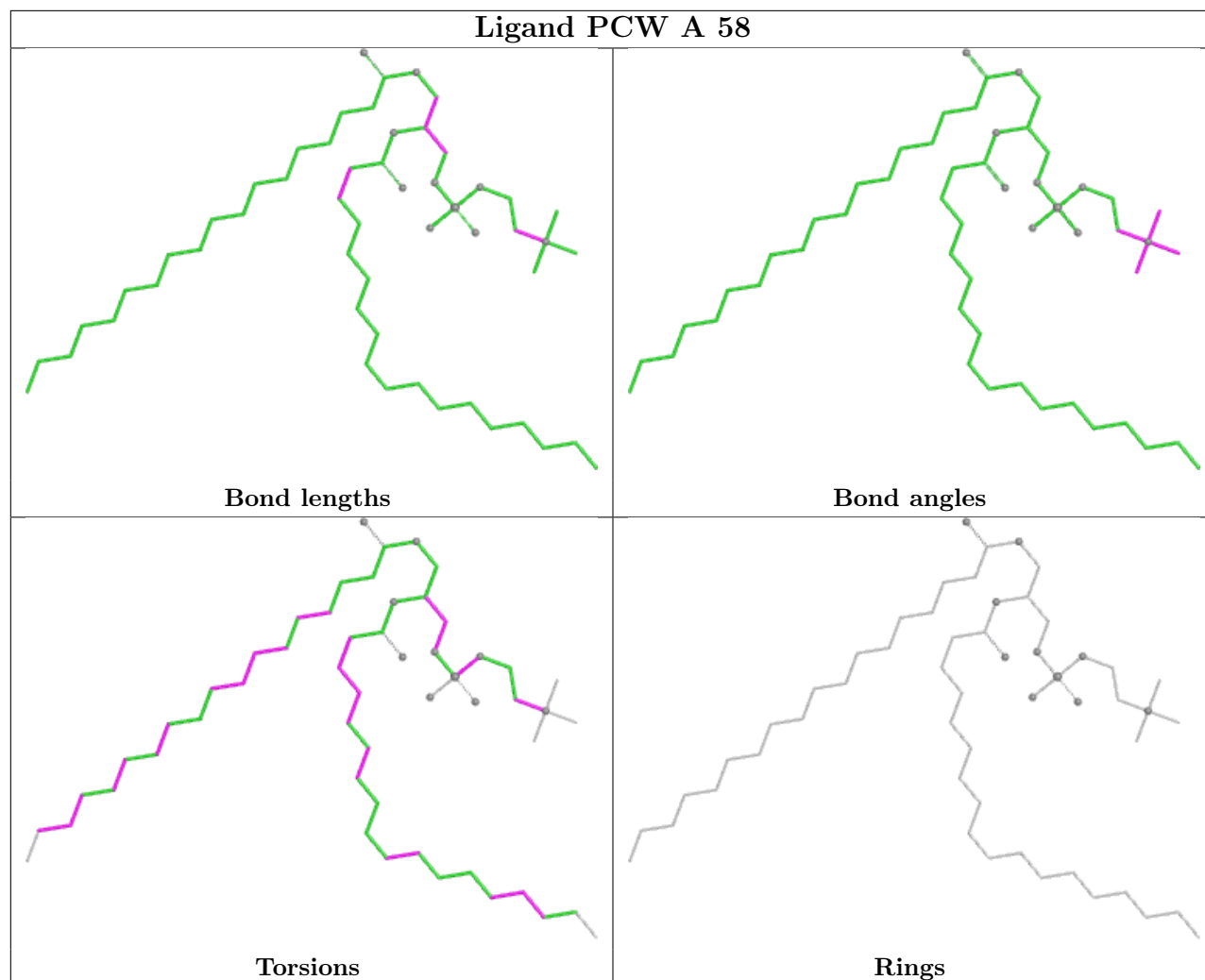


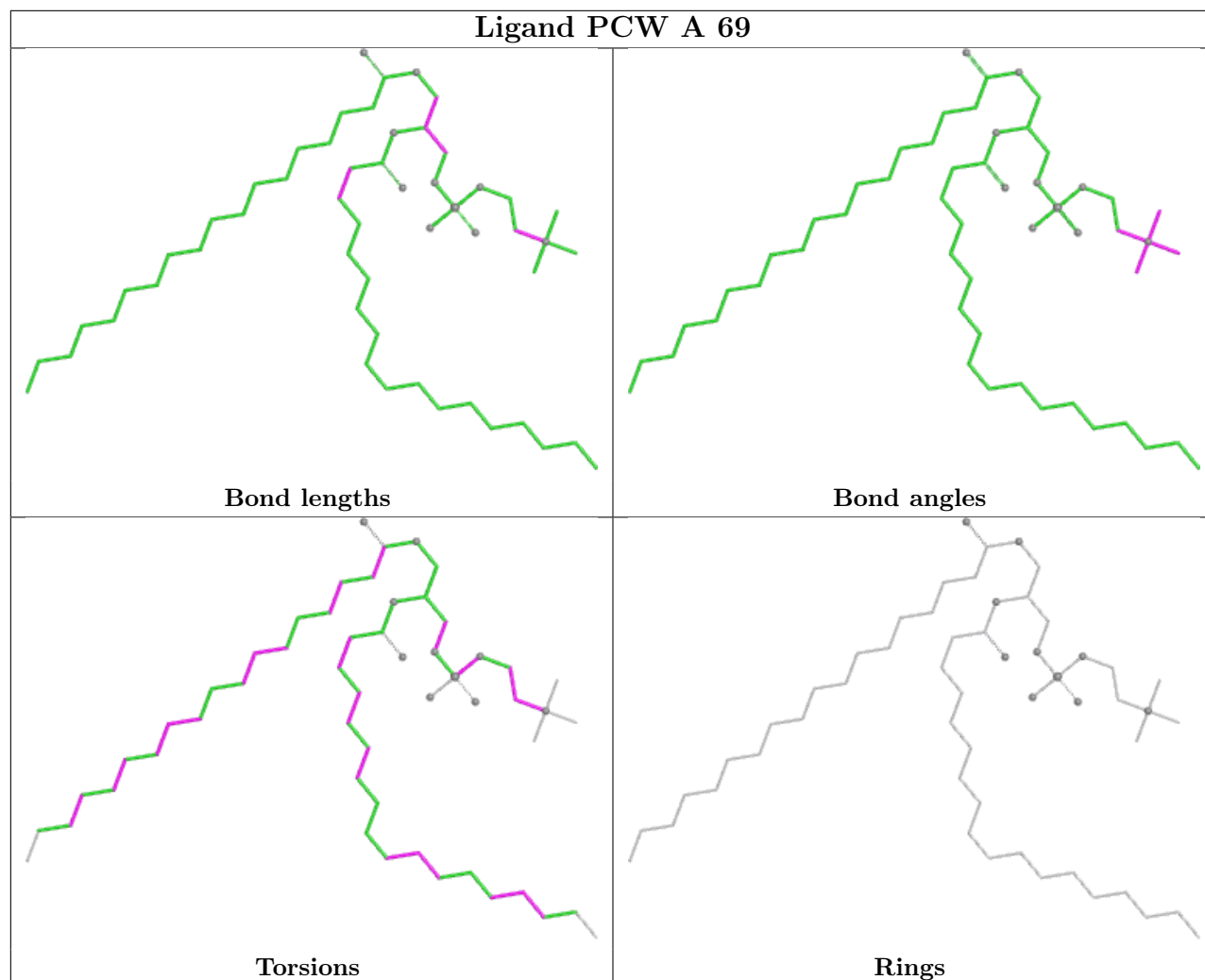


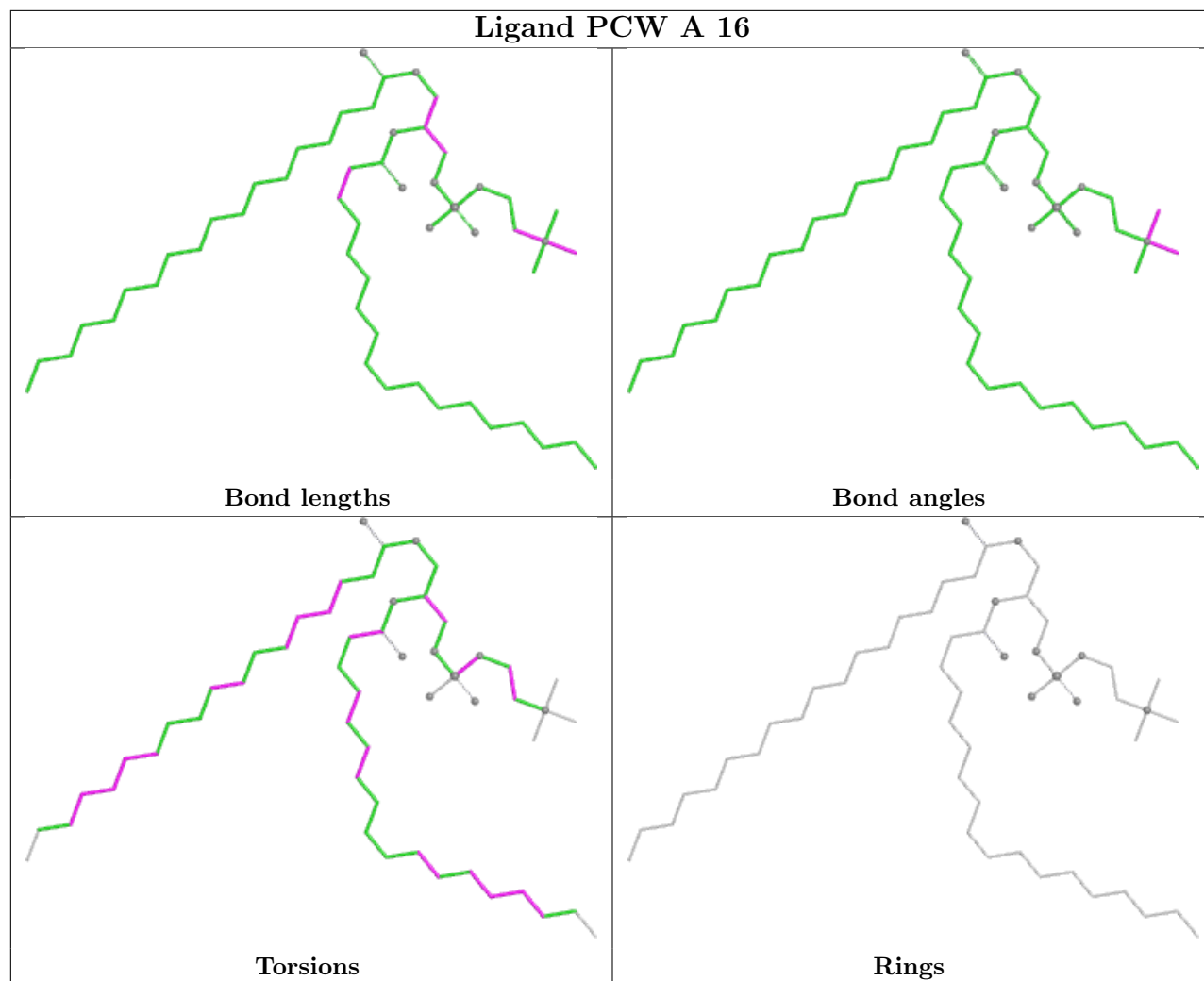


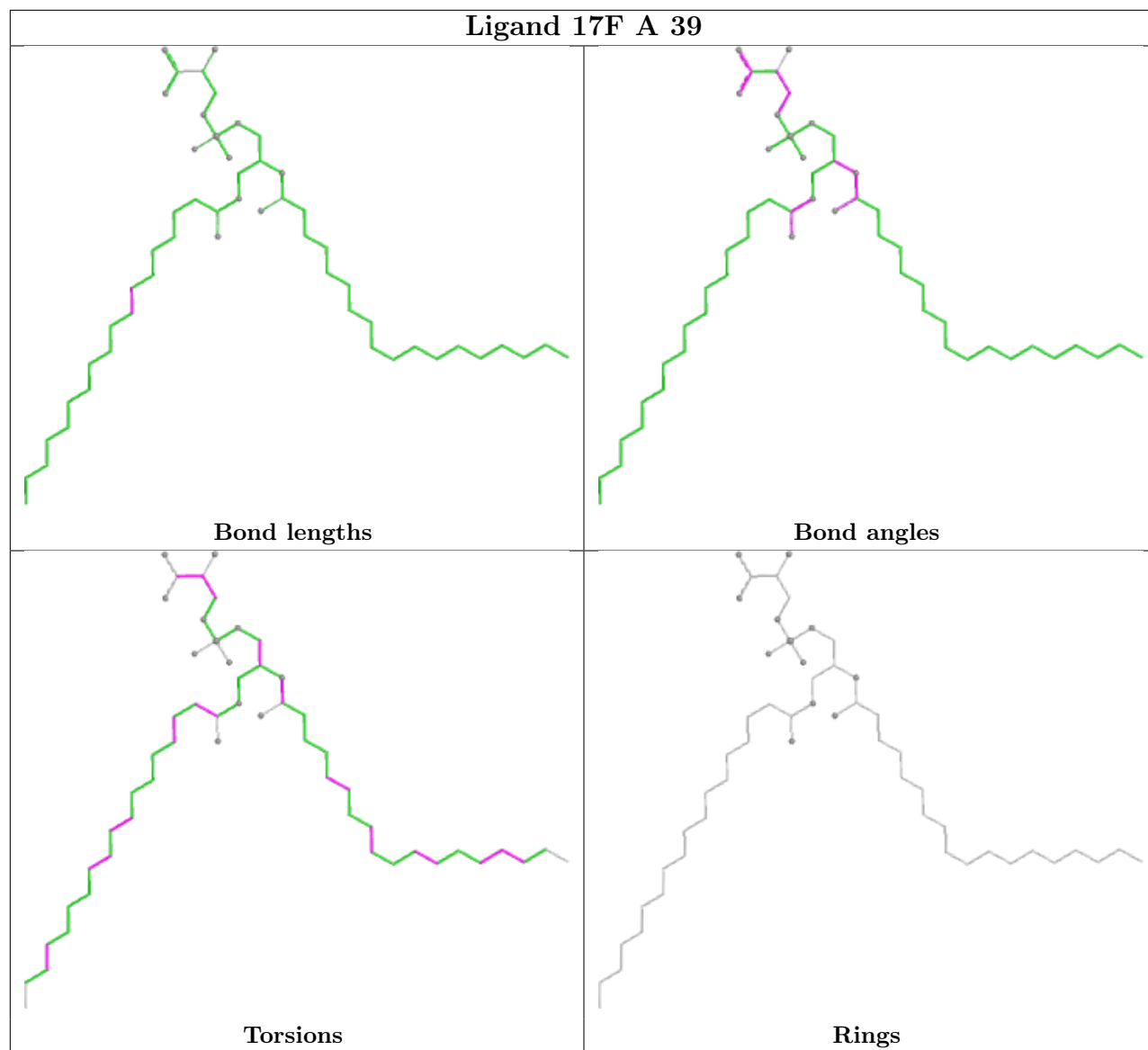


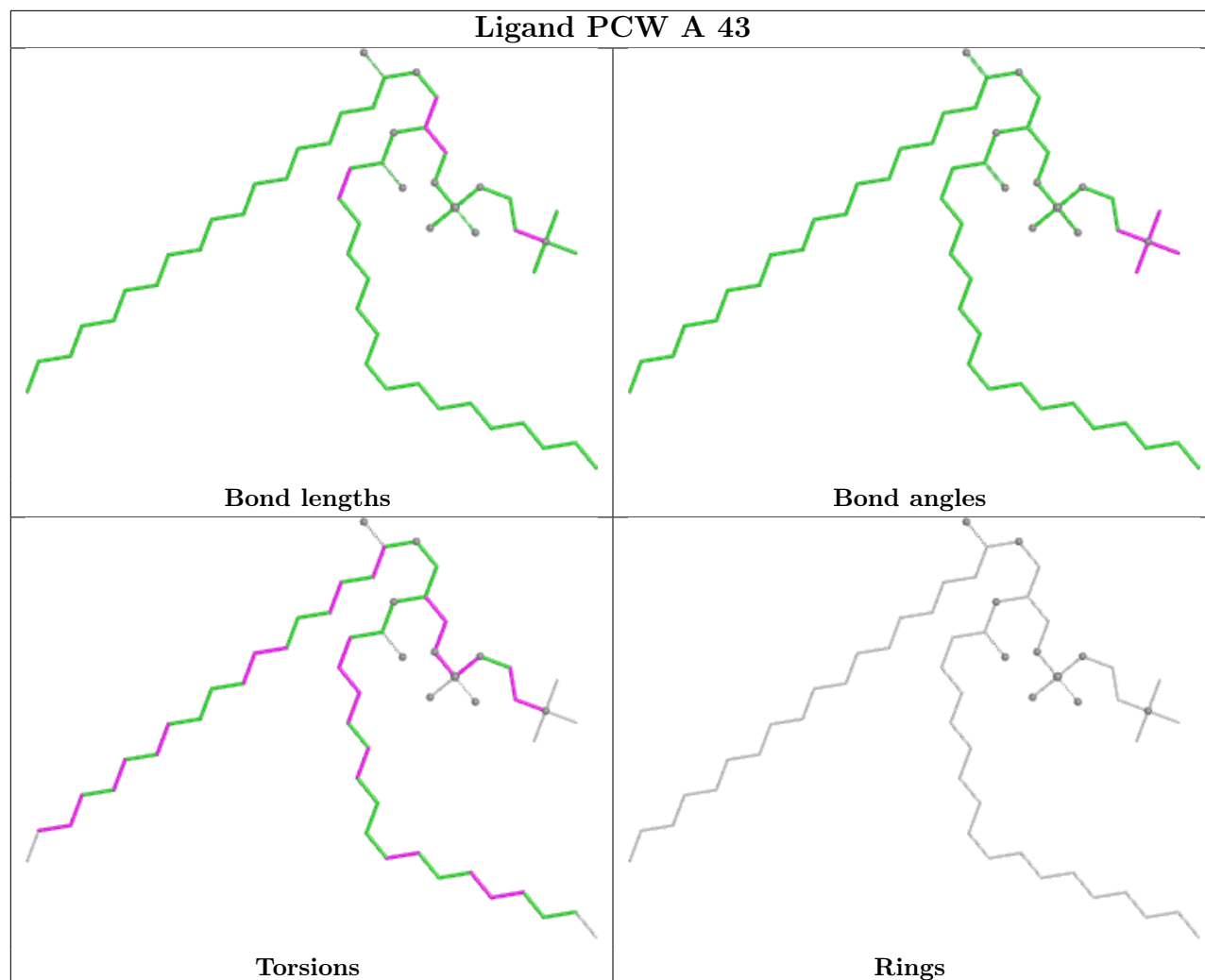


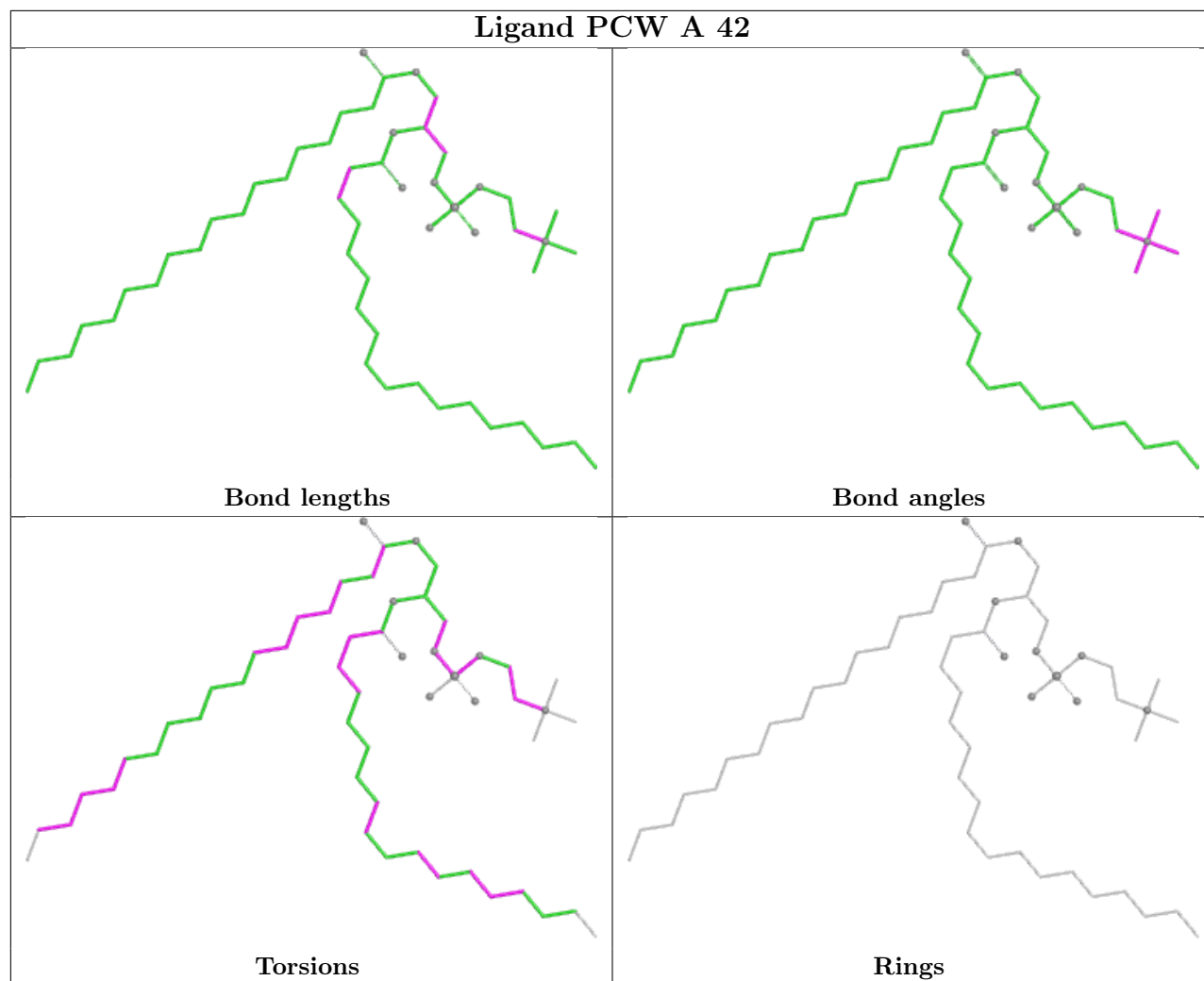


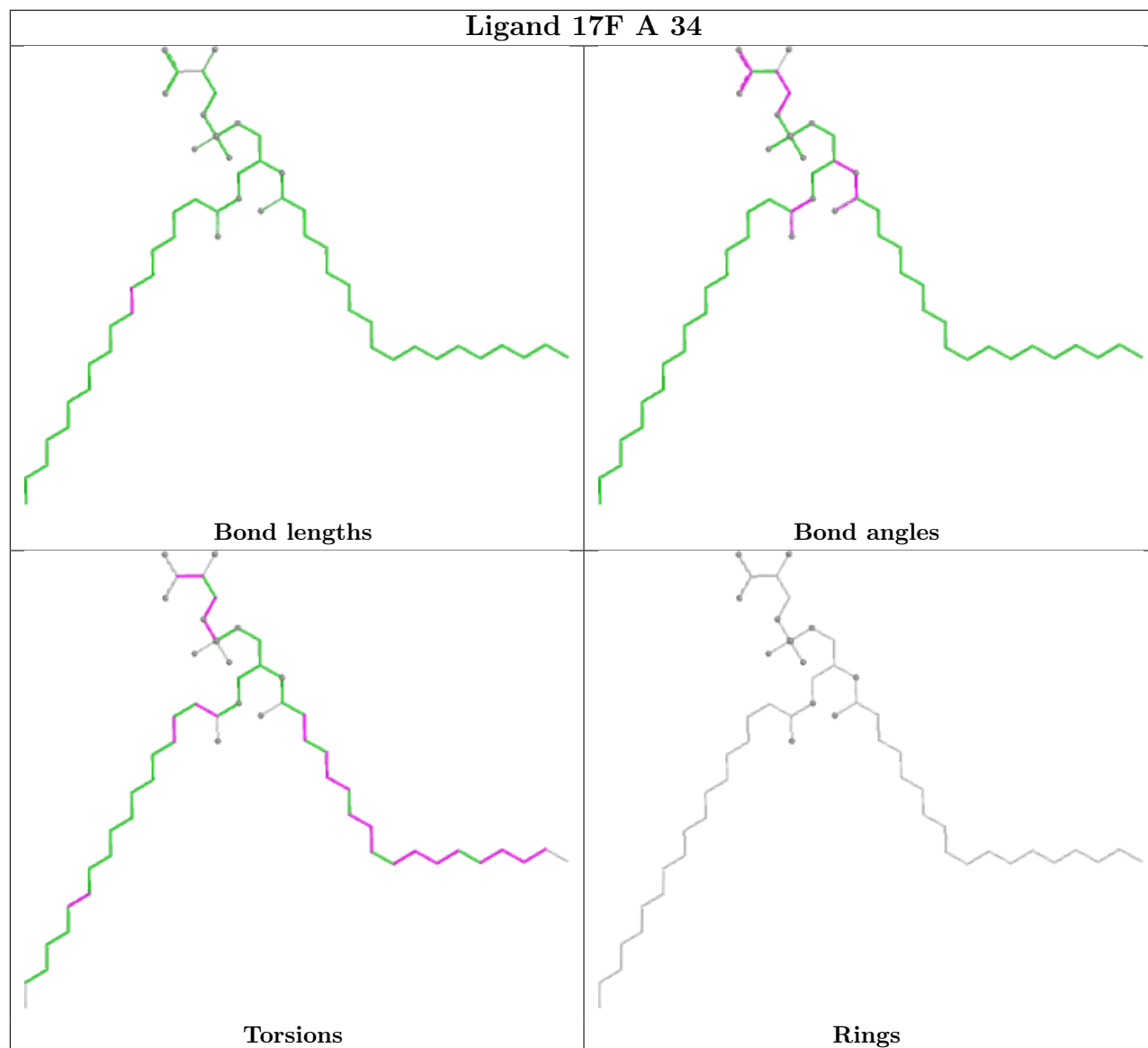


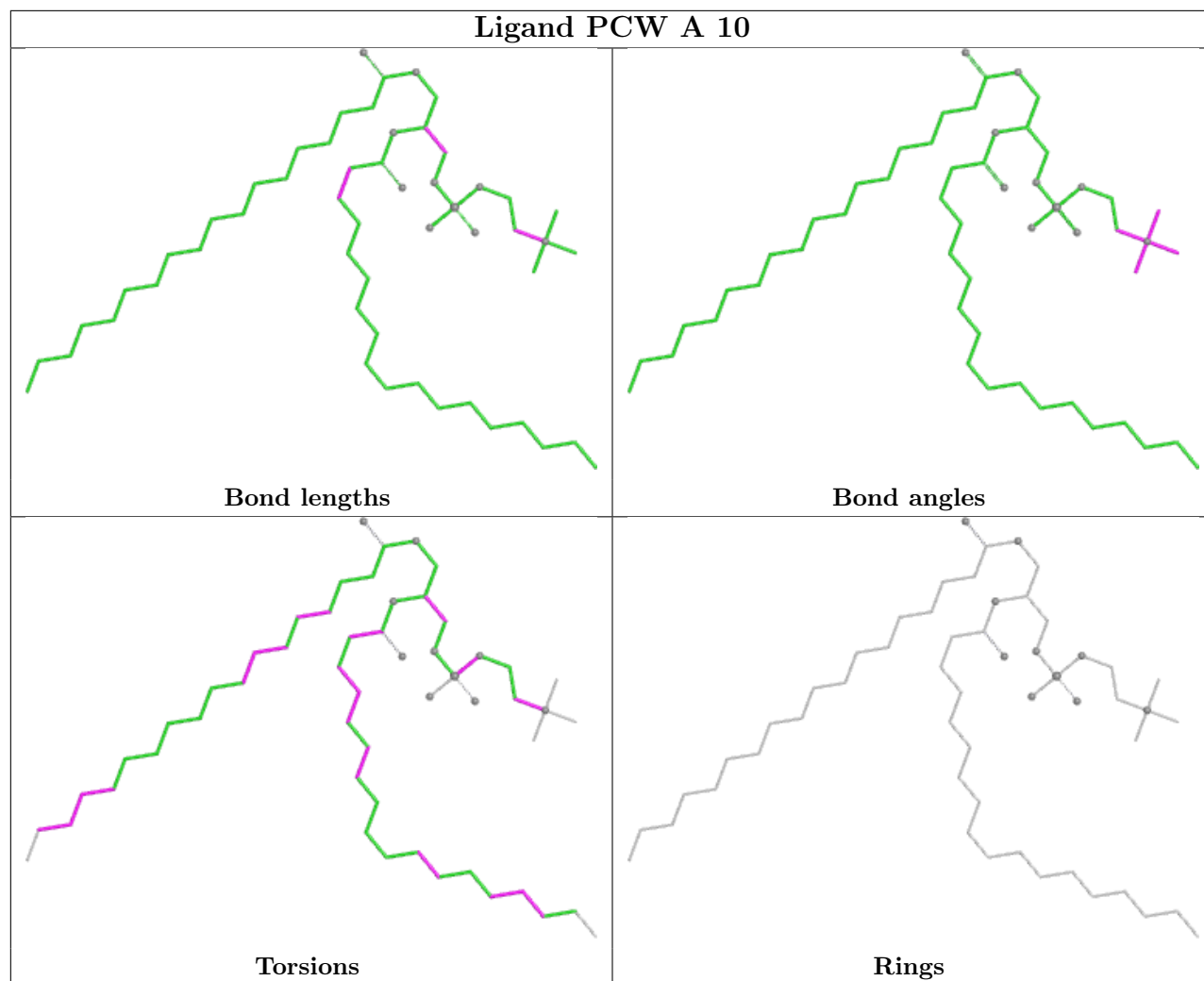


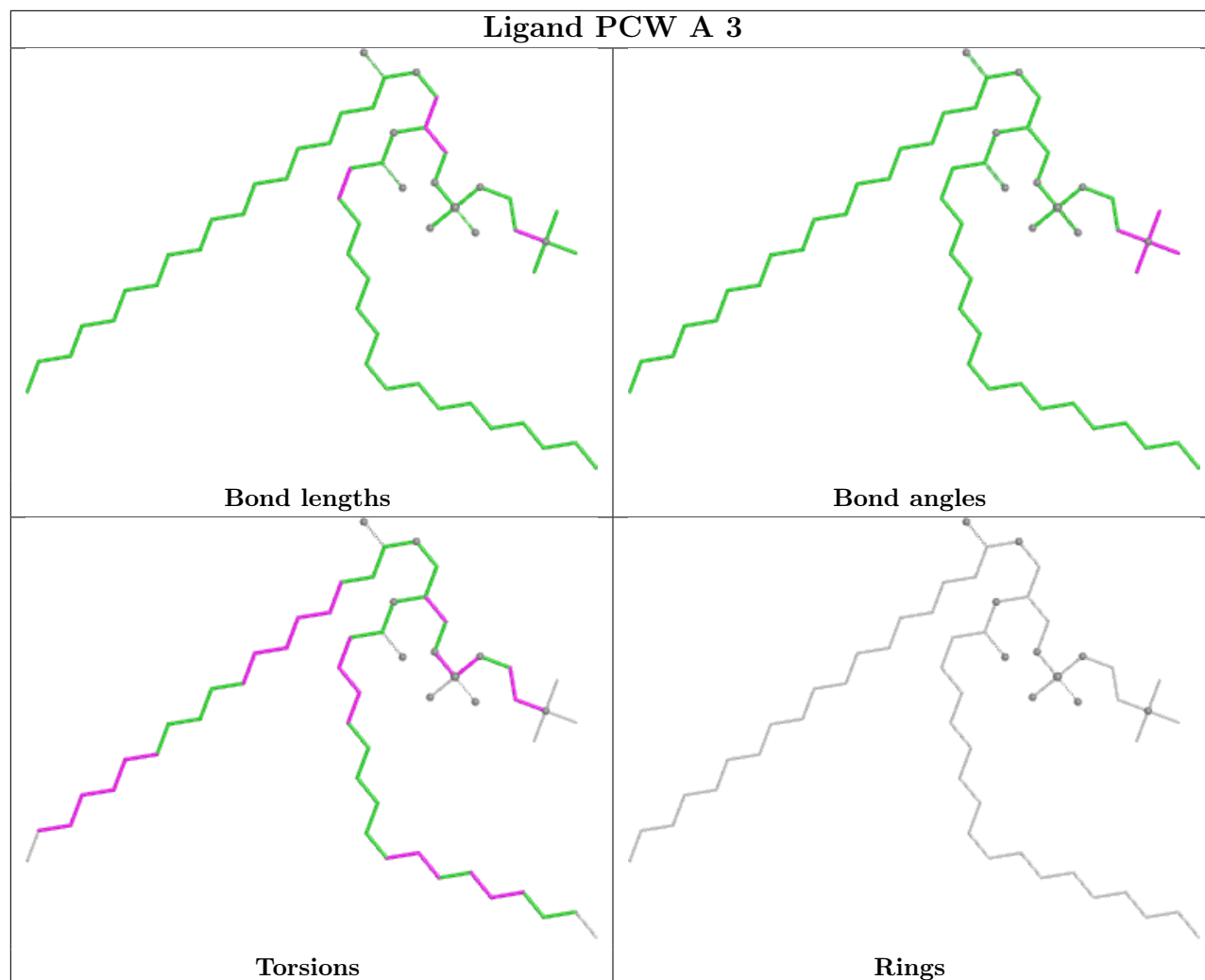


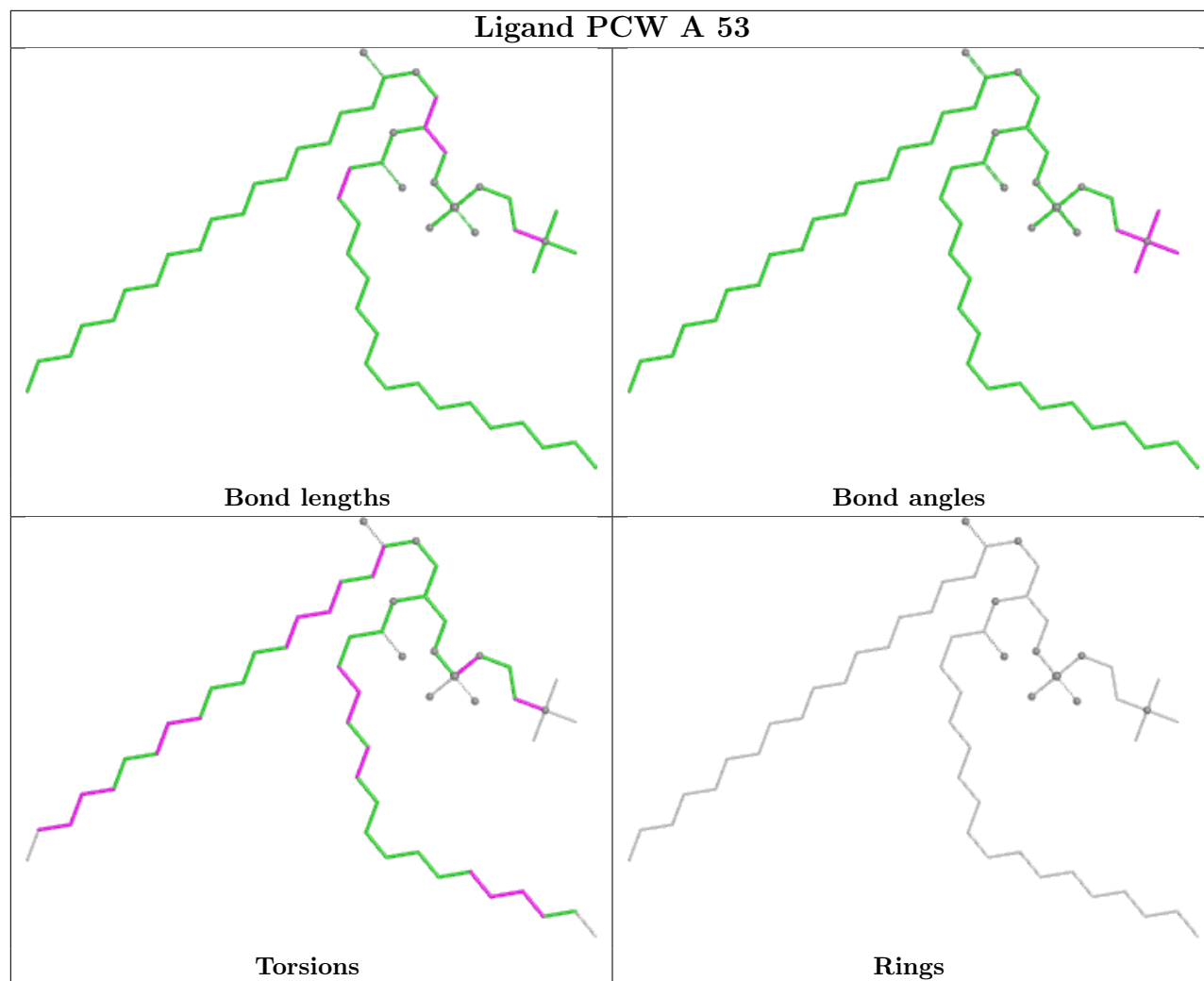


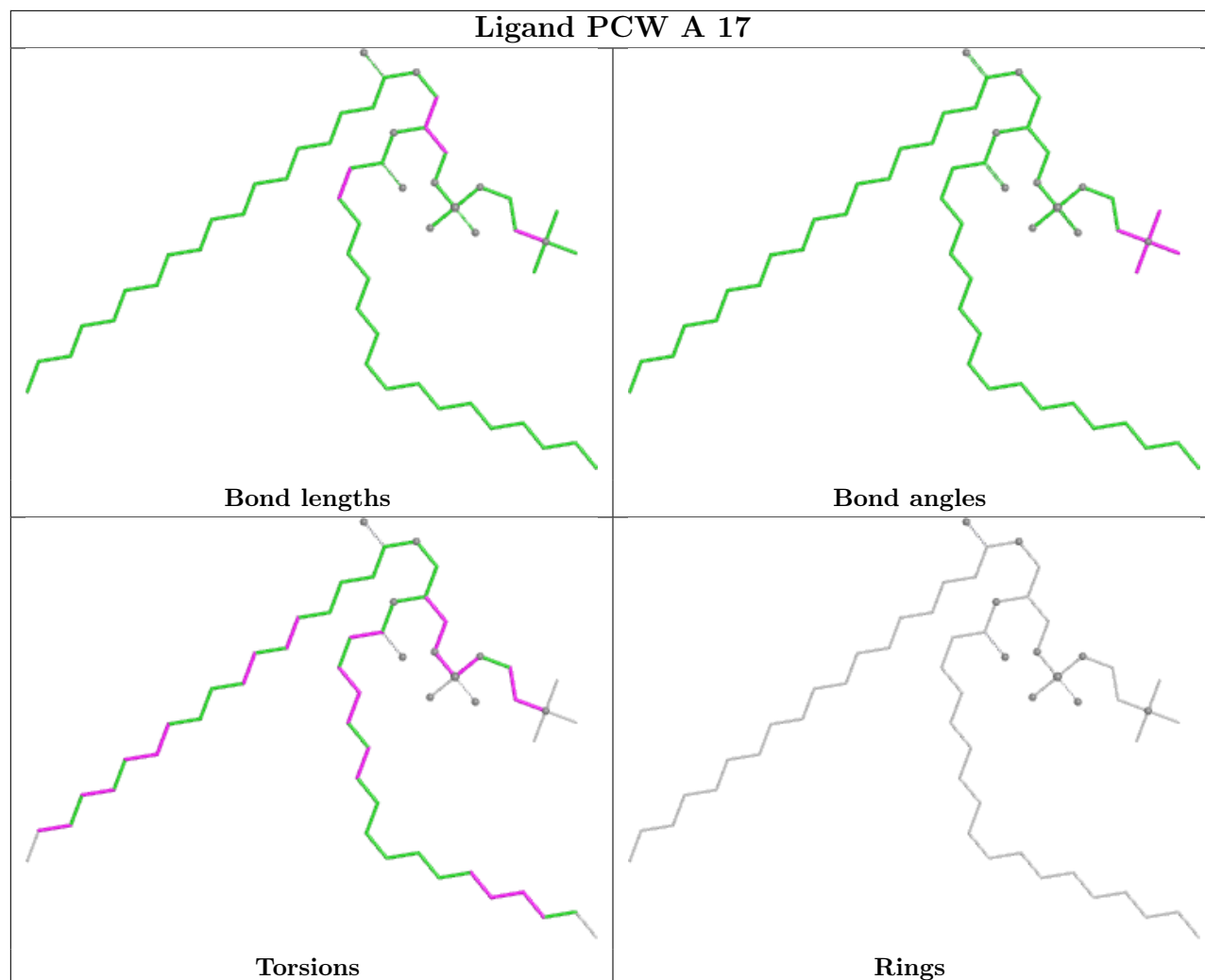


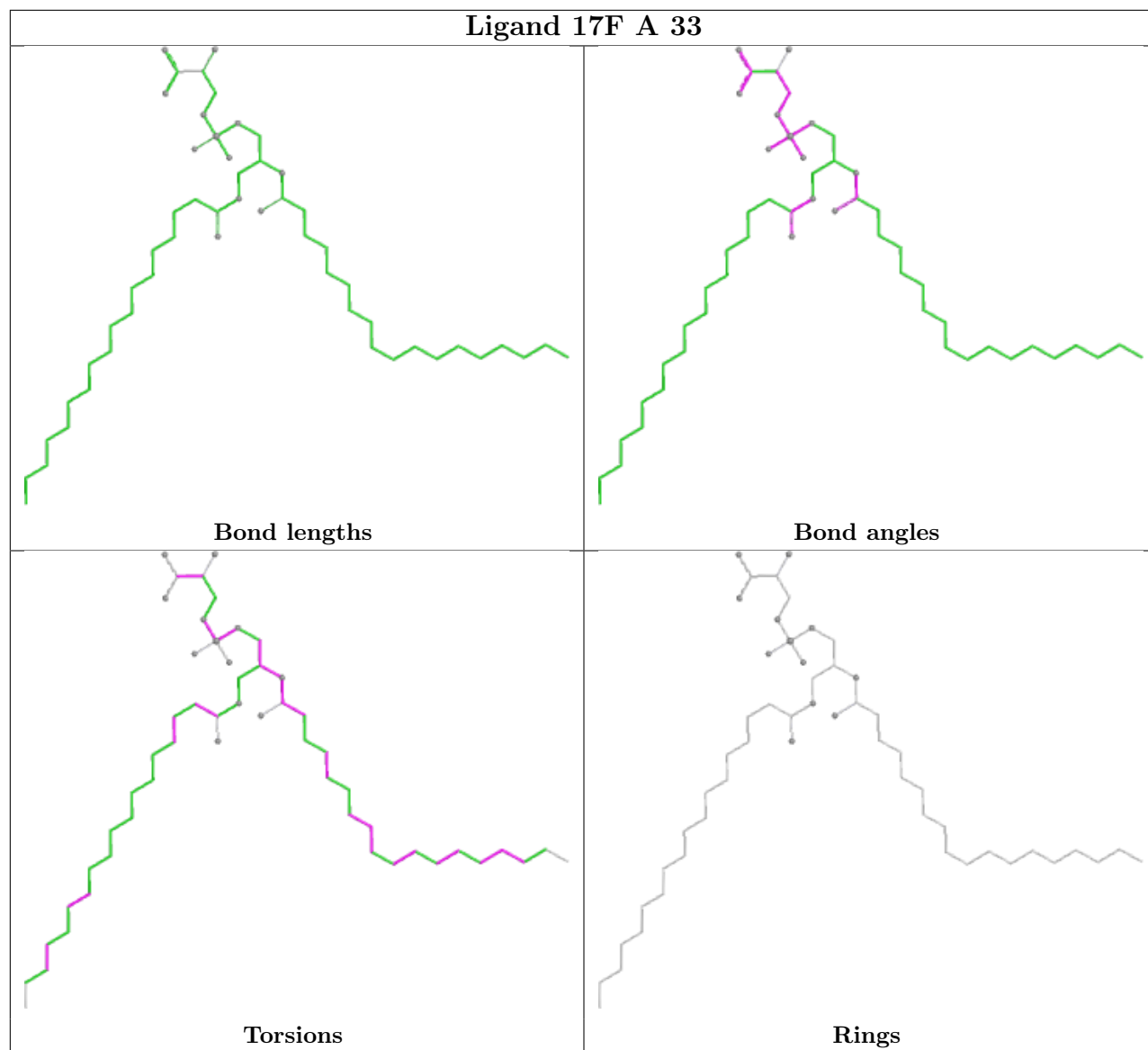


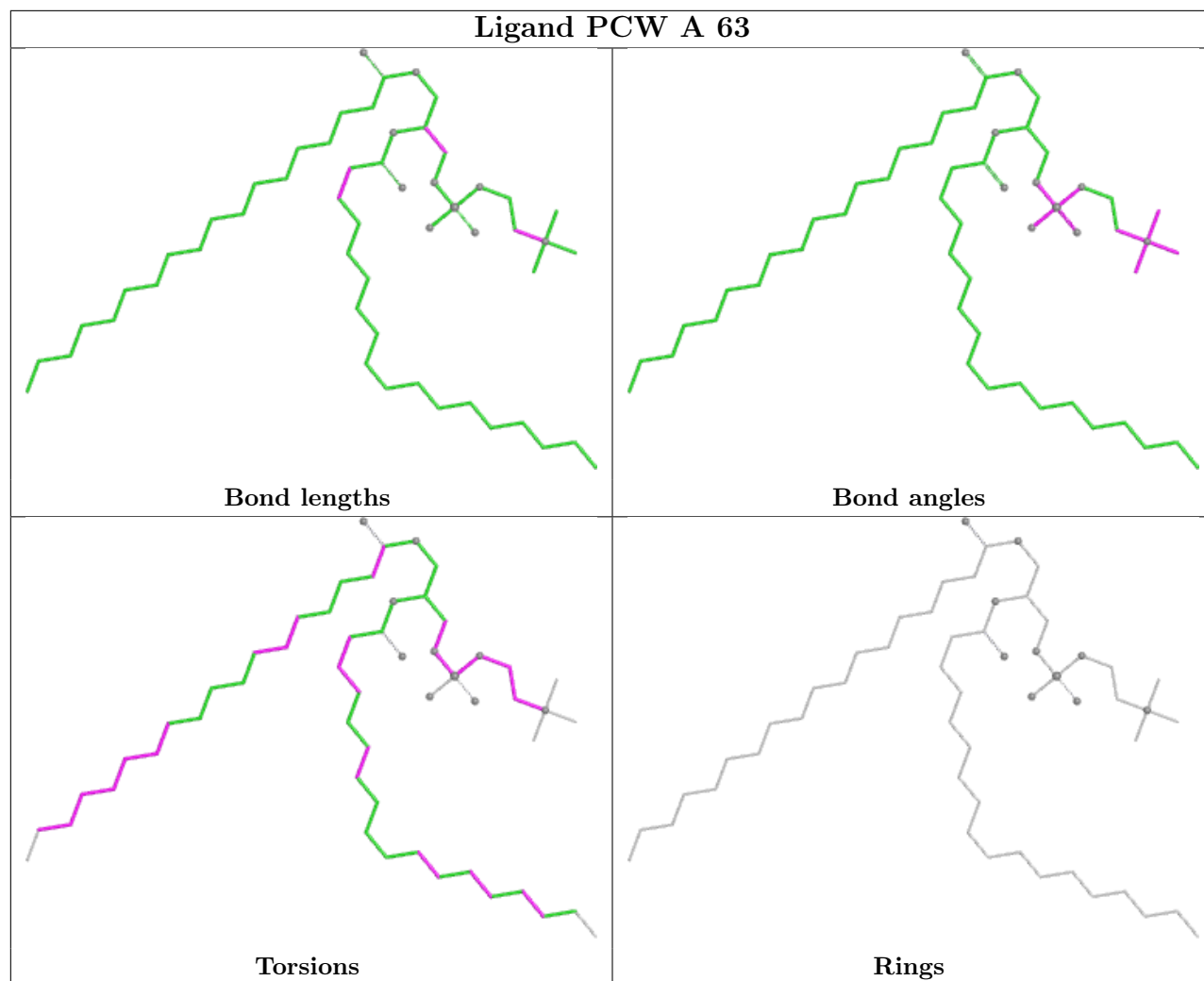


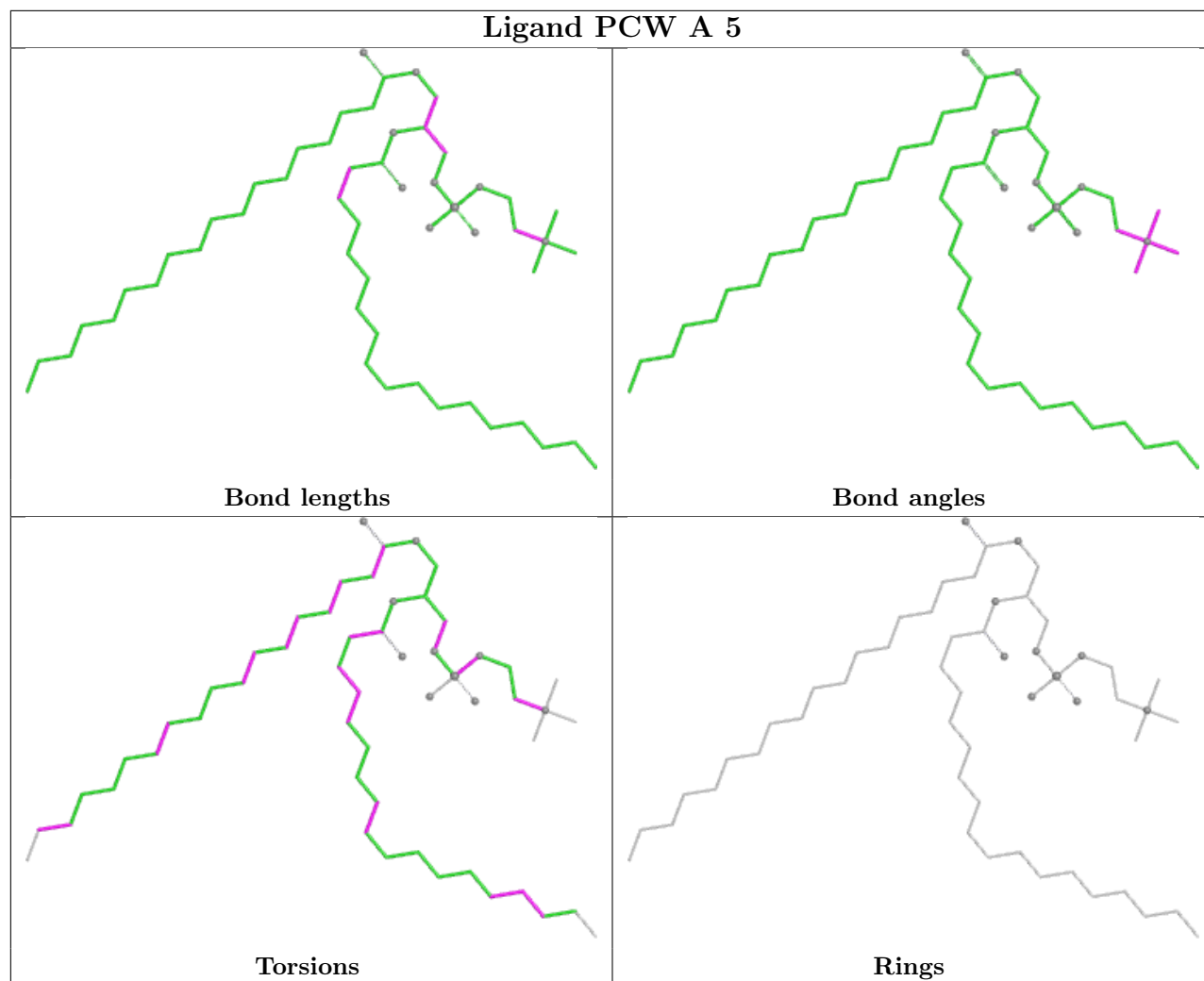


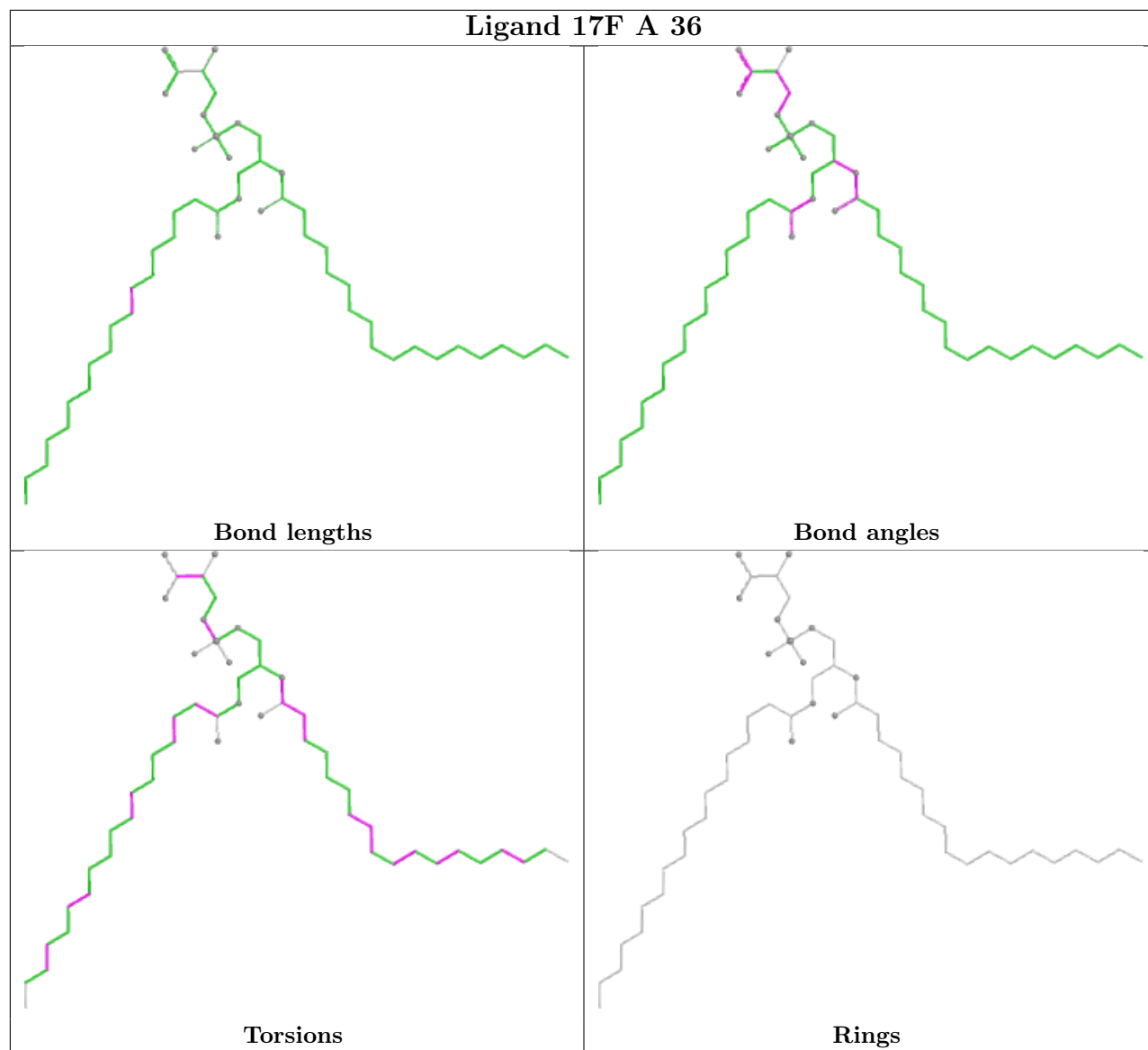


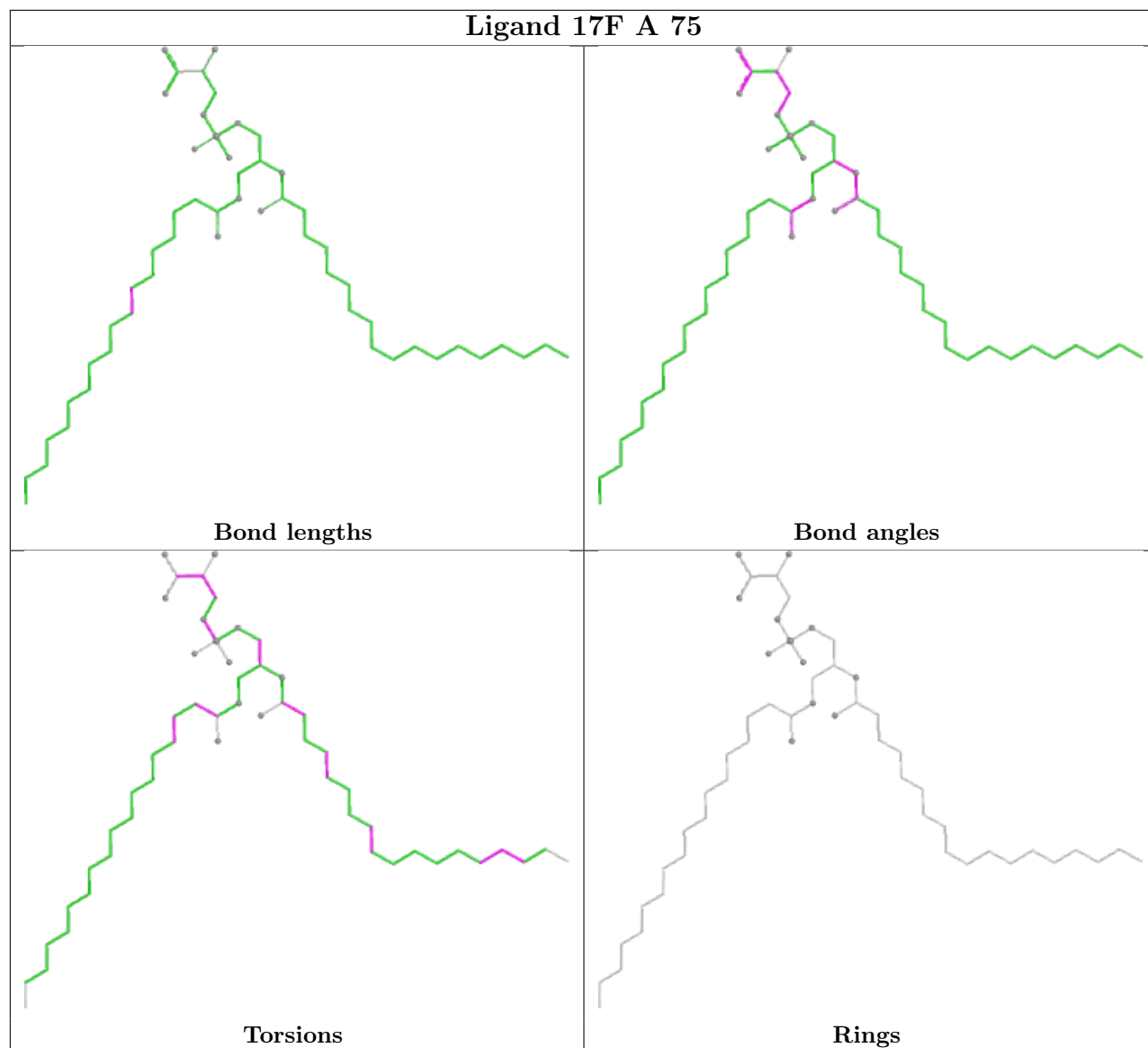


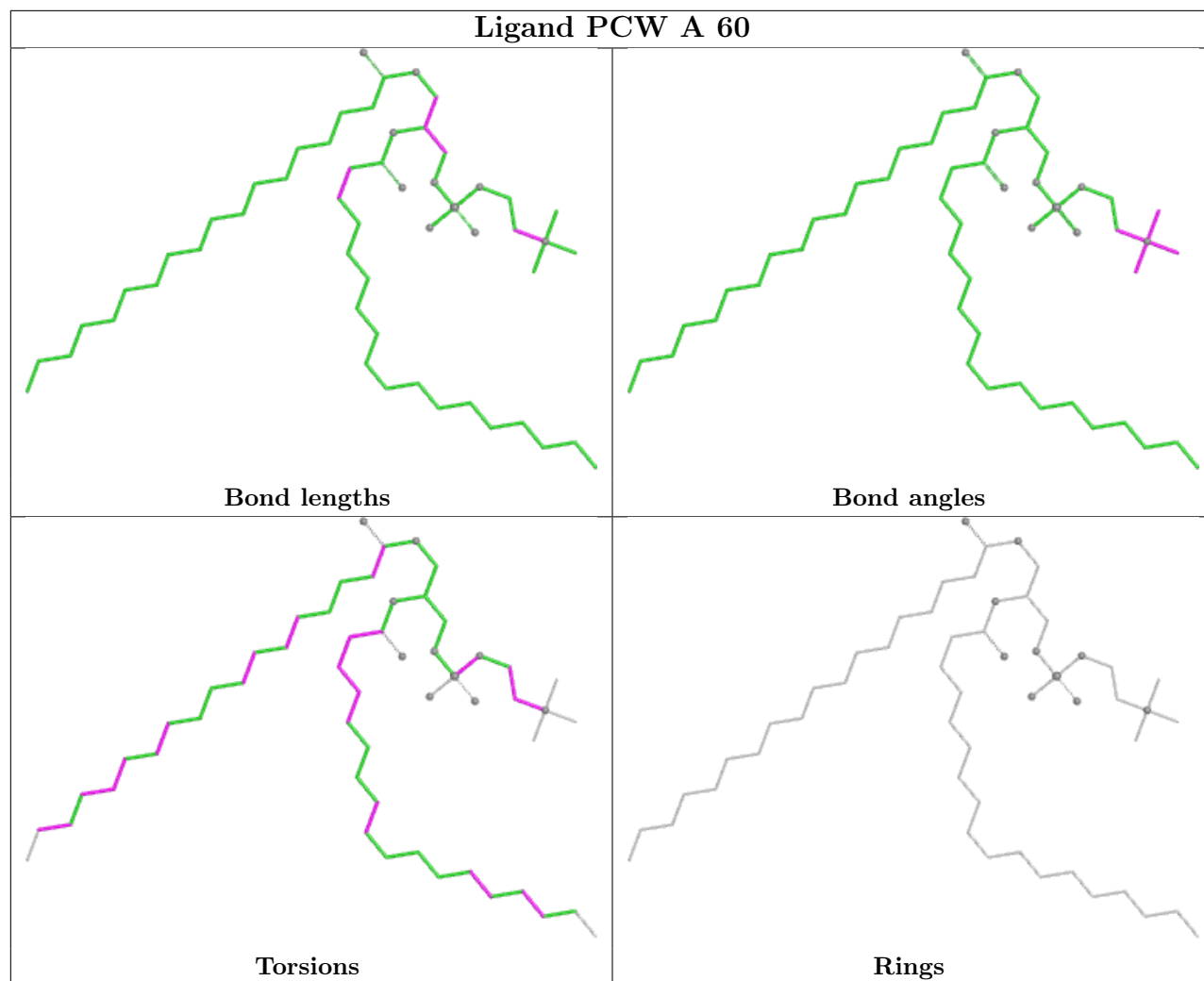


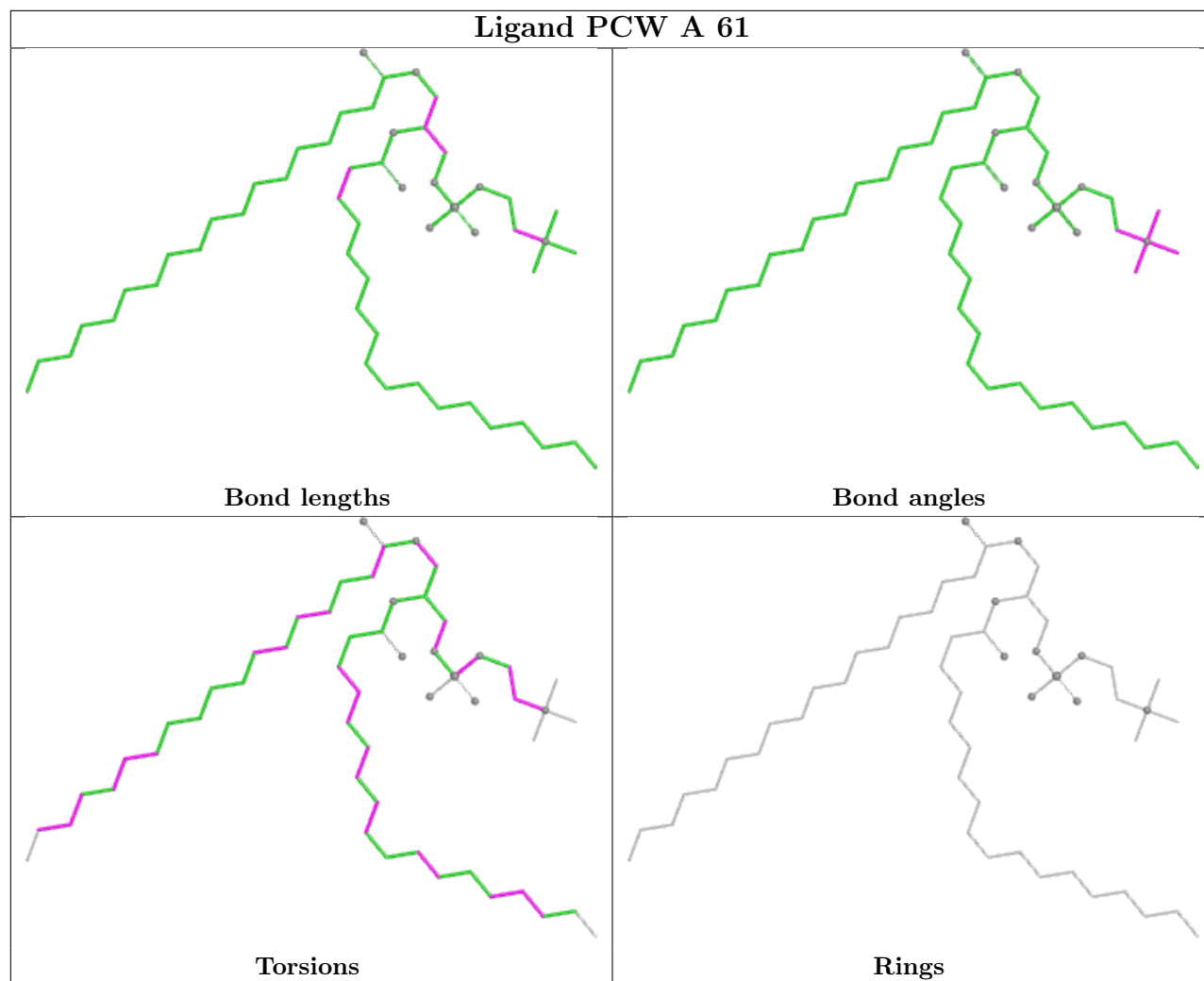


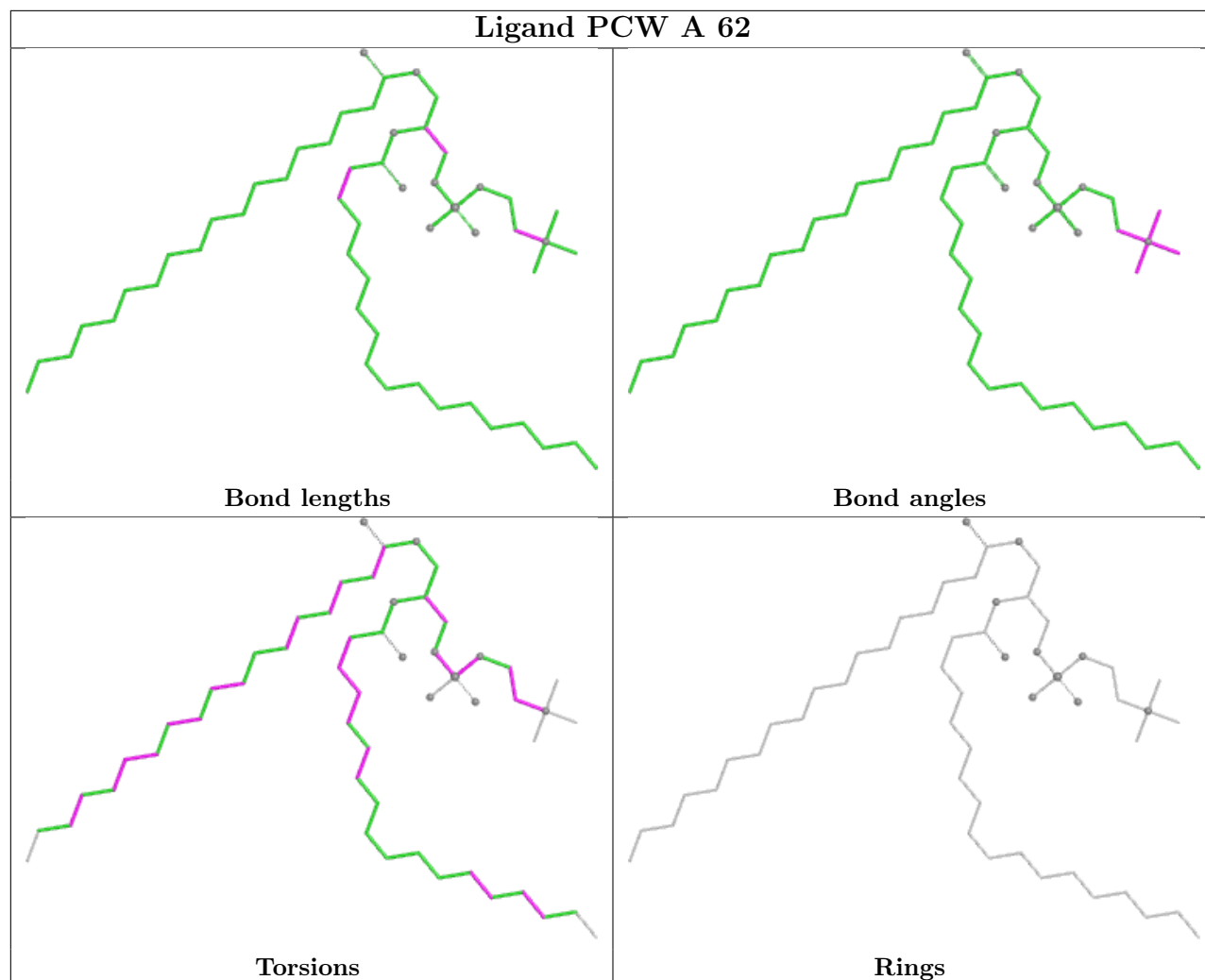


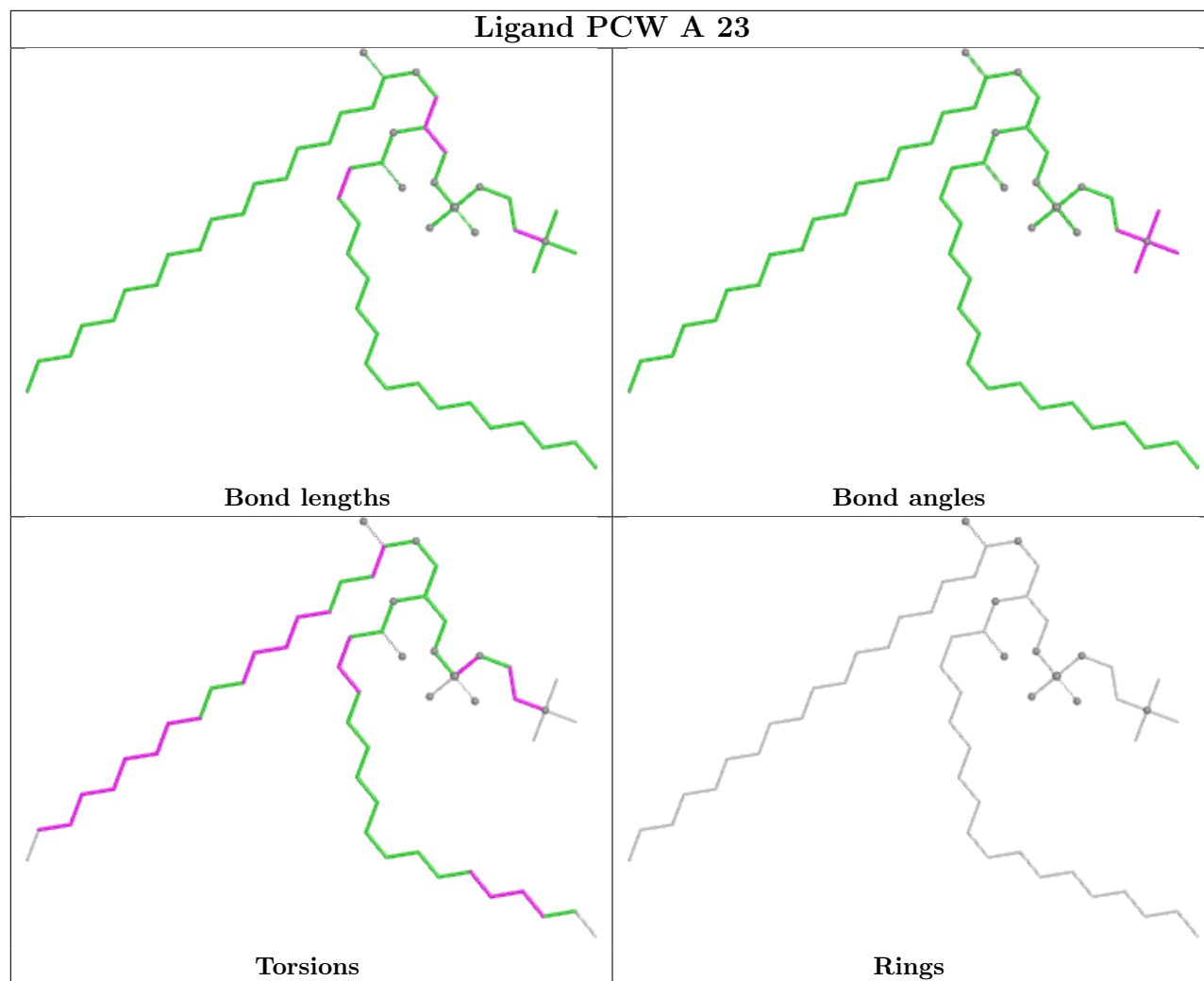


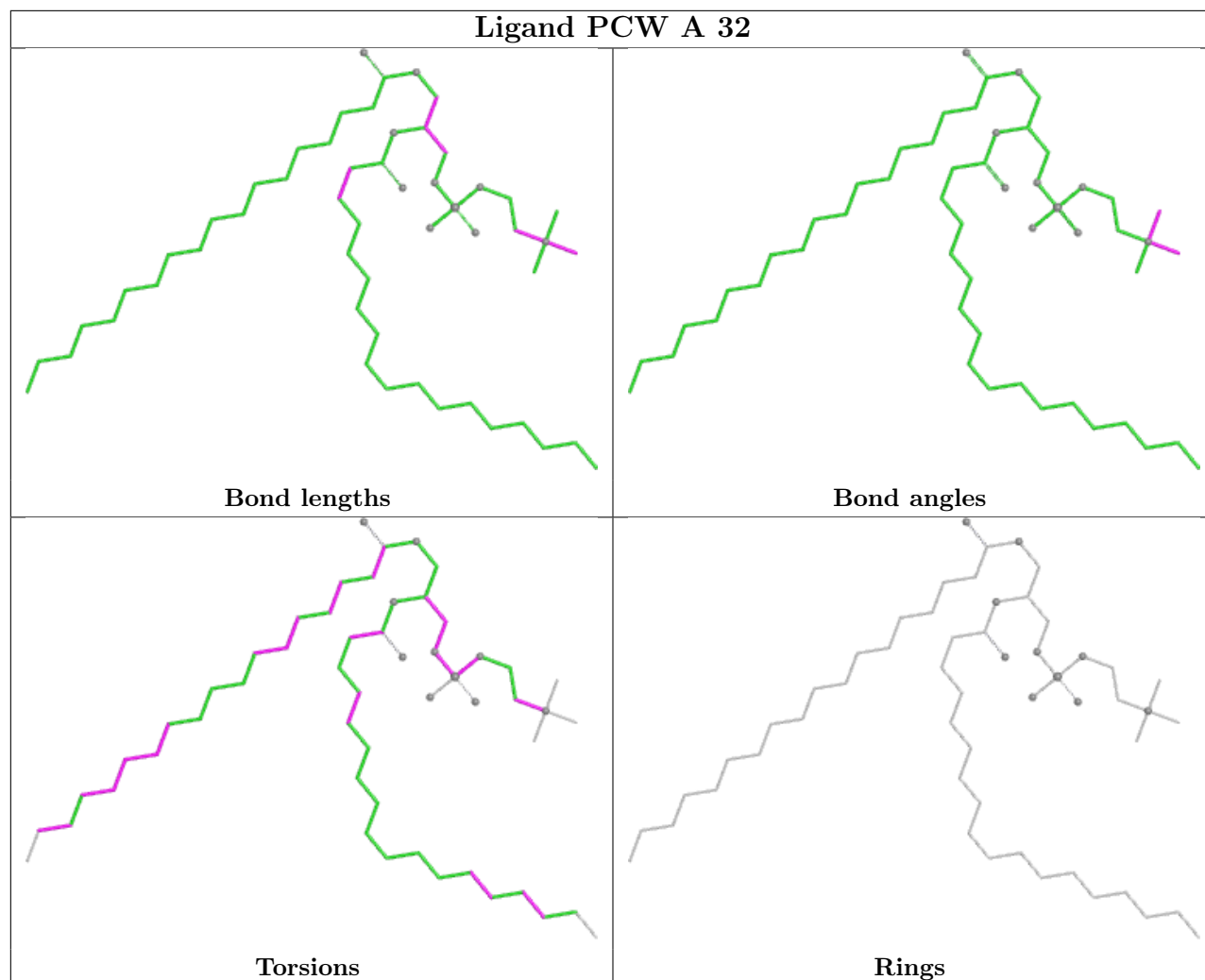


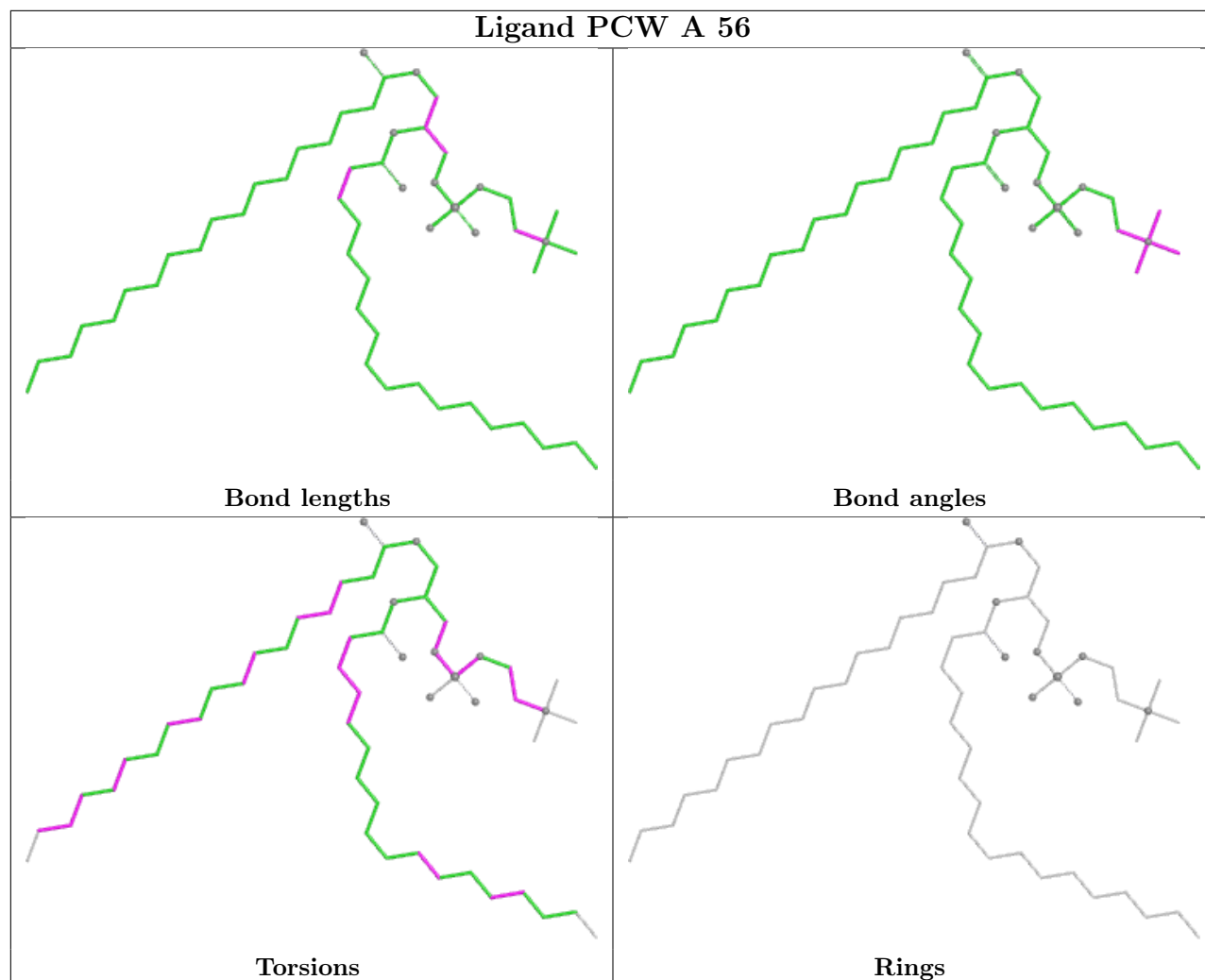


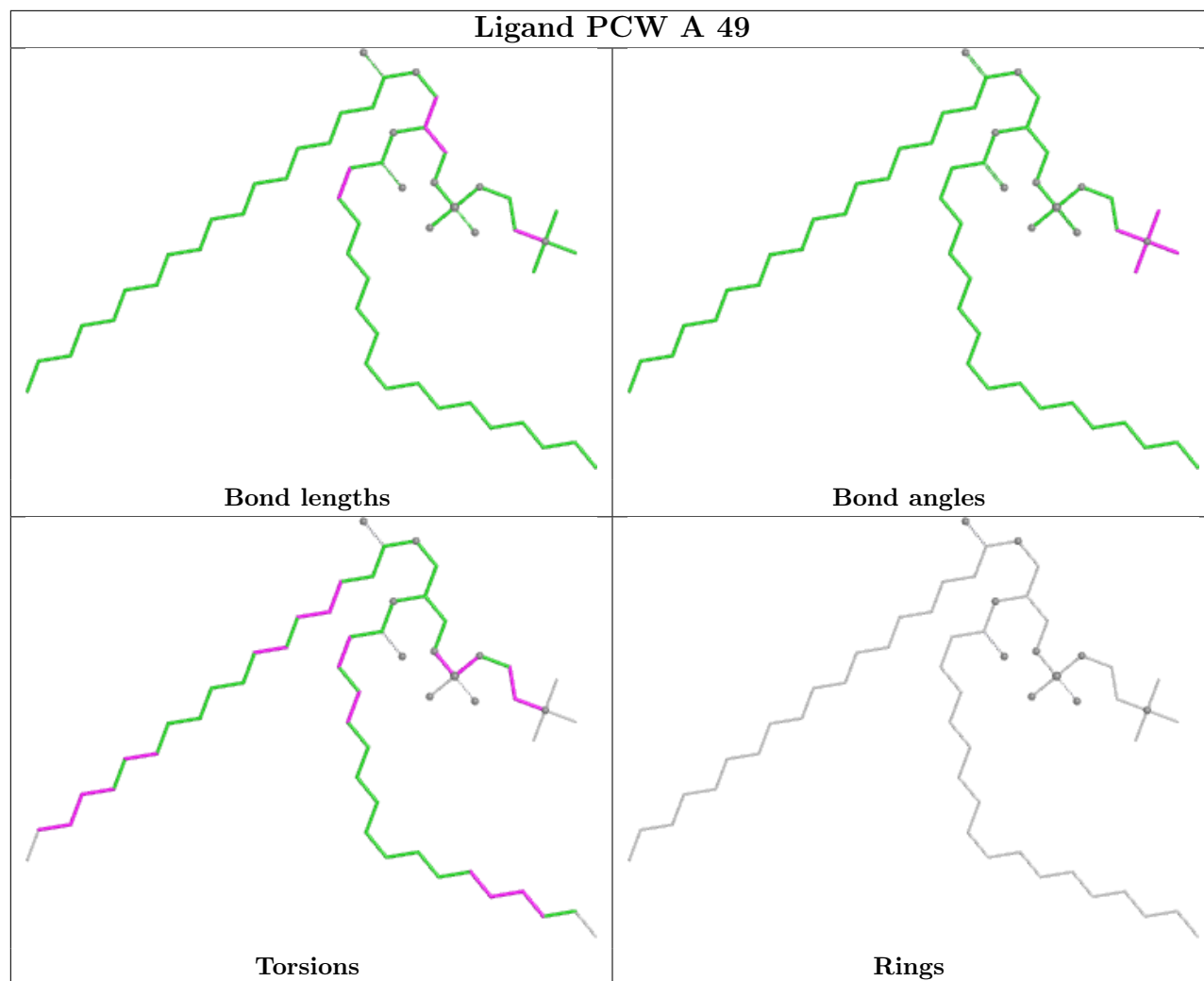


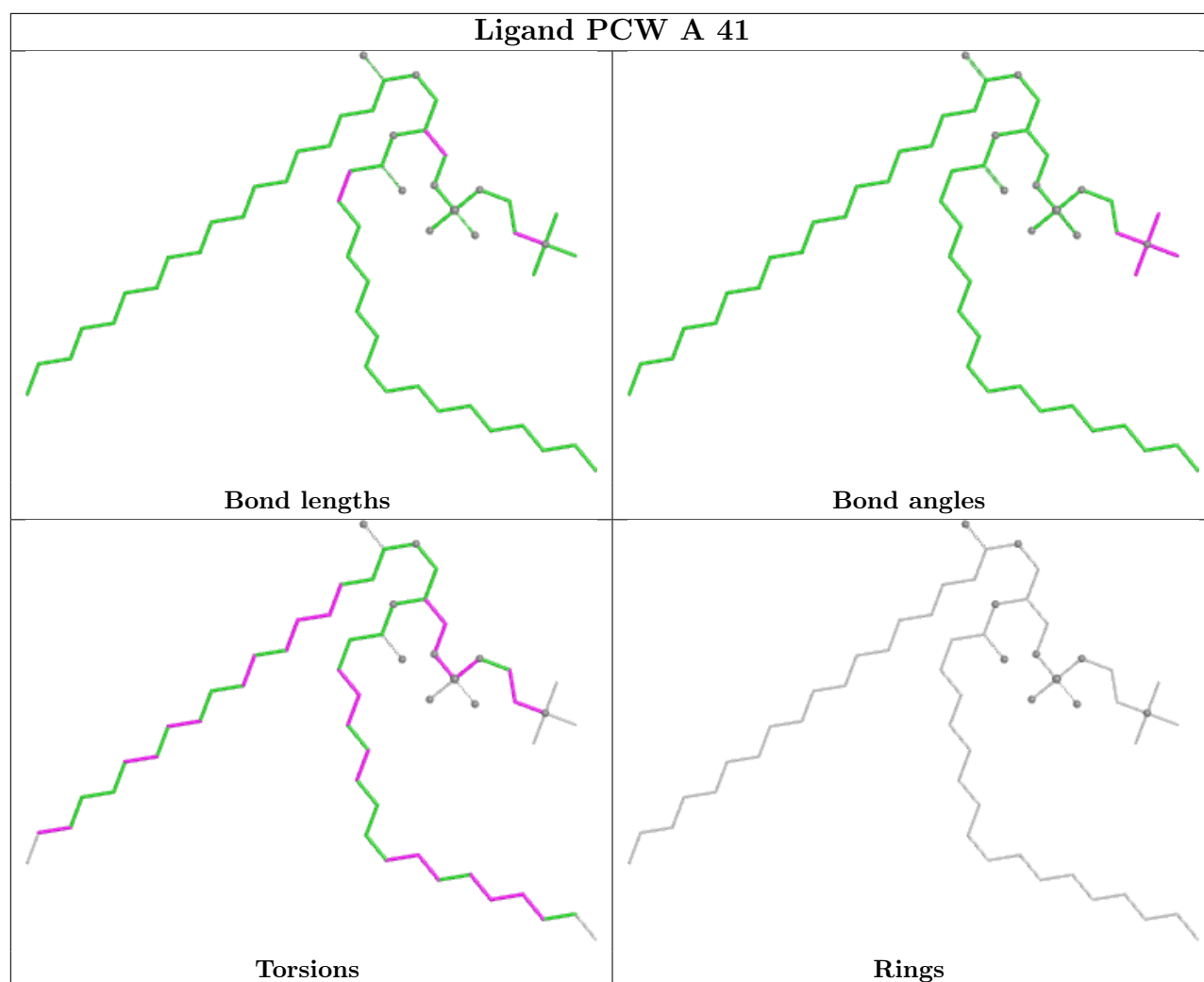












6.7 Other polymers [i](#)

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. 256 atoms were assigned a chemical shift out of a possible 7501. 0 out of 100 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	156/2654 (6%)	78/1072 (7%)	0/1066 (0%)	78/516 (15%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	100/4409 (2%)	75/2834 (3%)	25/1378 (2%)	0/197 (0%)
Aromatic	0/438 (0%)	0/222 (0%)	0/208 (0%)	0/8 (0%)
Overall	256/7501 (3%)	153/4128 (4%)	25/2652 (1%)	78/721 (11%)

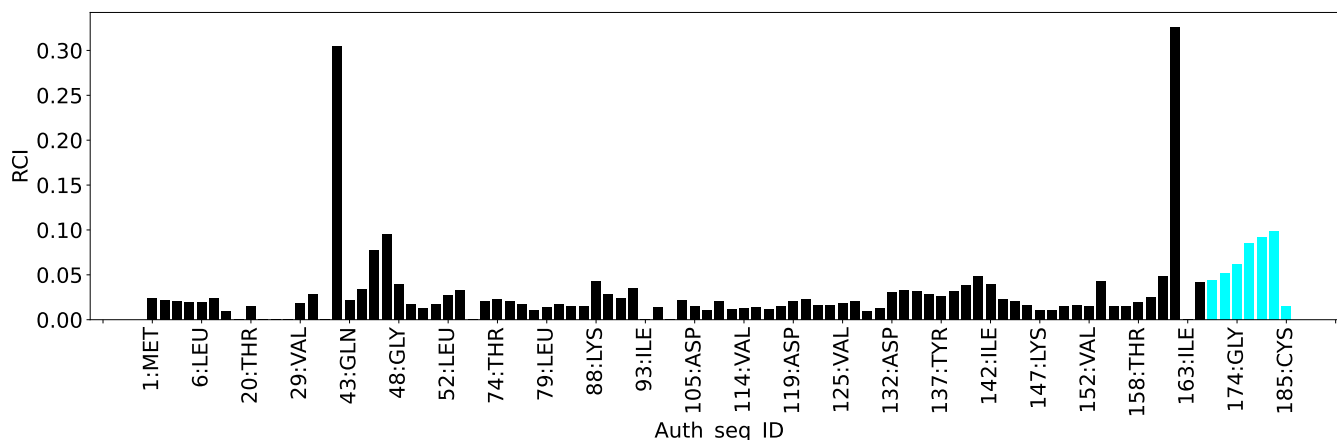
7.1.4 Statistically unusual chemical shifts [i](#)

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:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	57
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	57
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.4	0.2
0.2-0.5 (Medium)	1.4	0.44
>0.5 (Large)	39.3	22.62

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

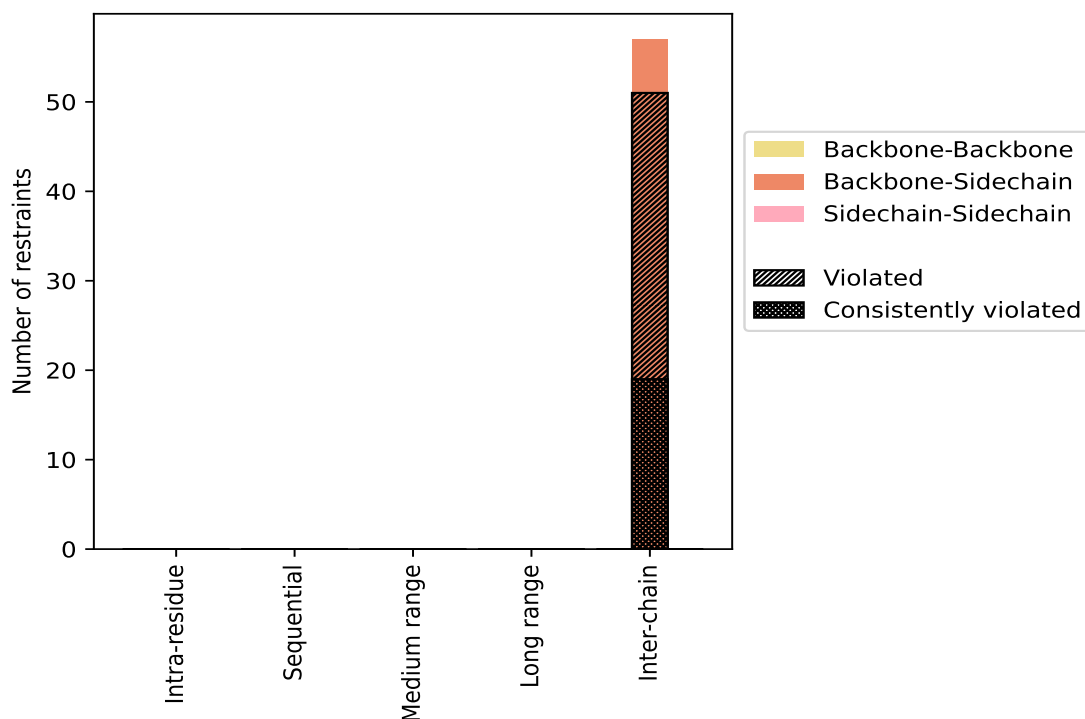
9.1 Summary of distance violations

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	57	100.0	51	89.5	89.5	19	33.3	33.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	57	100.0	51	89.5	89.5	19	33.3	33.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	57	100.0	51	89.5	89.5	19	33.3	33.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	57	100.0	51	89.5	89.5	19	33.3	33.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

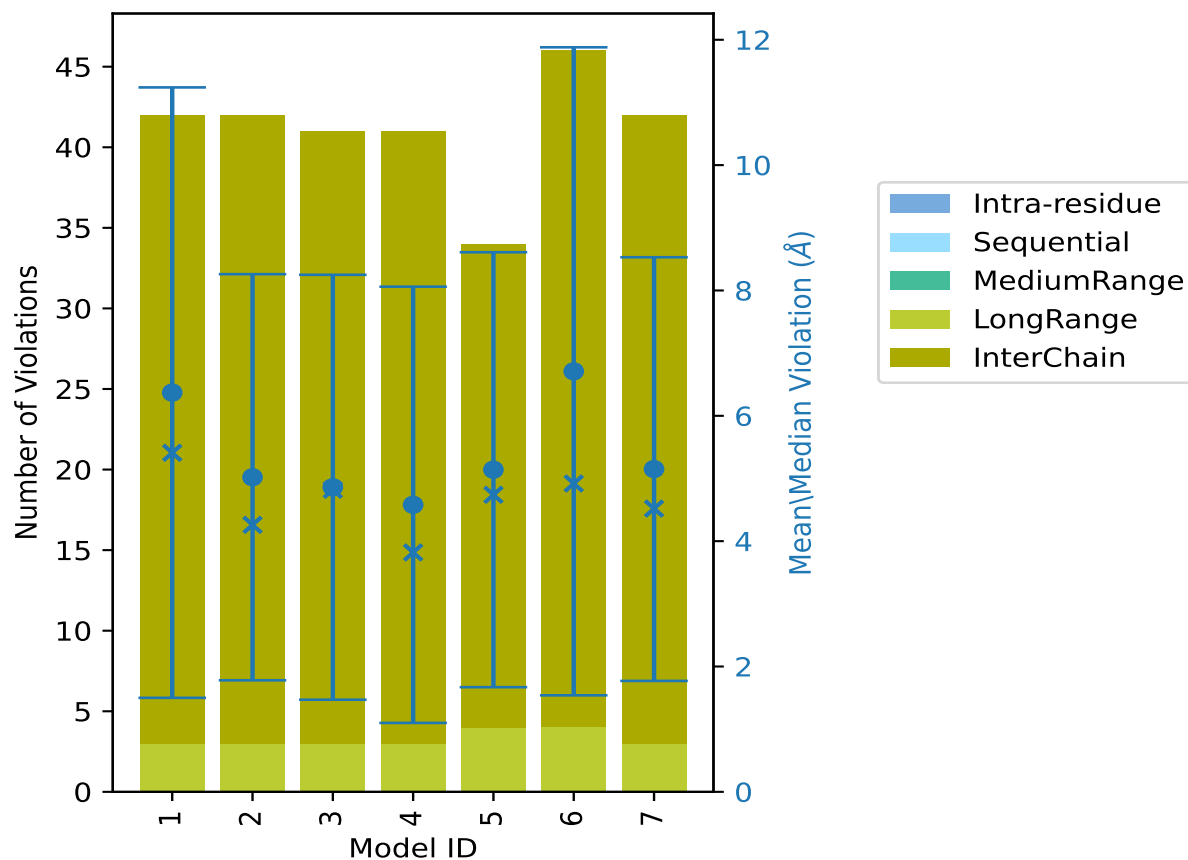
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	3	39	42	6.37	22.62	4.87	5.41
2	0	0	0	3	39	42	5.02	13.14	3.24	4.26
3	0	0	0	3	38	41	4.86	11.32	3.39	4.82
4	0	0	0	3	38	41	4.58	13.22	3.48	3.82
5	0	0	0	4	30	34	5.14	14.32	3.47	4.74
6	0	0	0	4	42	46	6.71	19.56	5.17	4.92
7	0	0	0	3	39	42	5.15	14.17	3.38	4.52

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

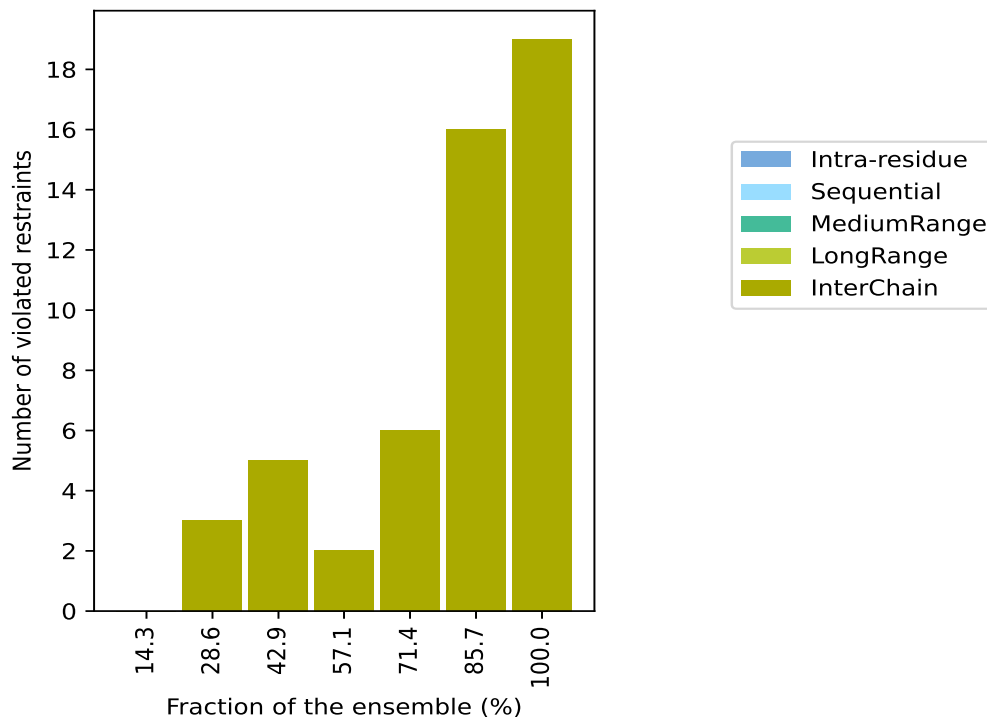
9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6(IR:0, SQ:0, MR:0, LR:0, IC:6) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	14.3
0	0	0	0	3	3	2	28.6
0	0	0	0	5	5	3	42.9
0	0	0	0	2	2	4	57.1
0	0	0	0	6	6	5	71.4
0	0	0	0	16	16	6	85.7
0	0	0	0	19	19	7	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

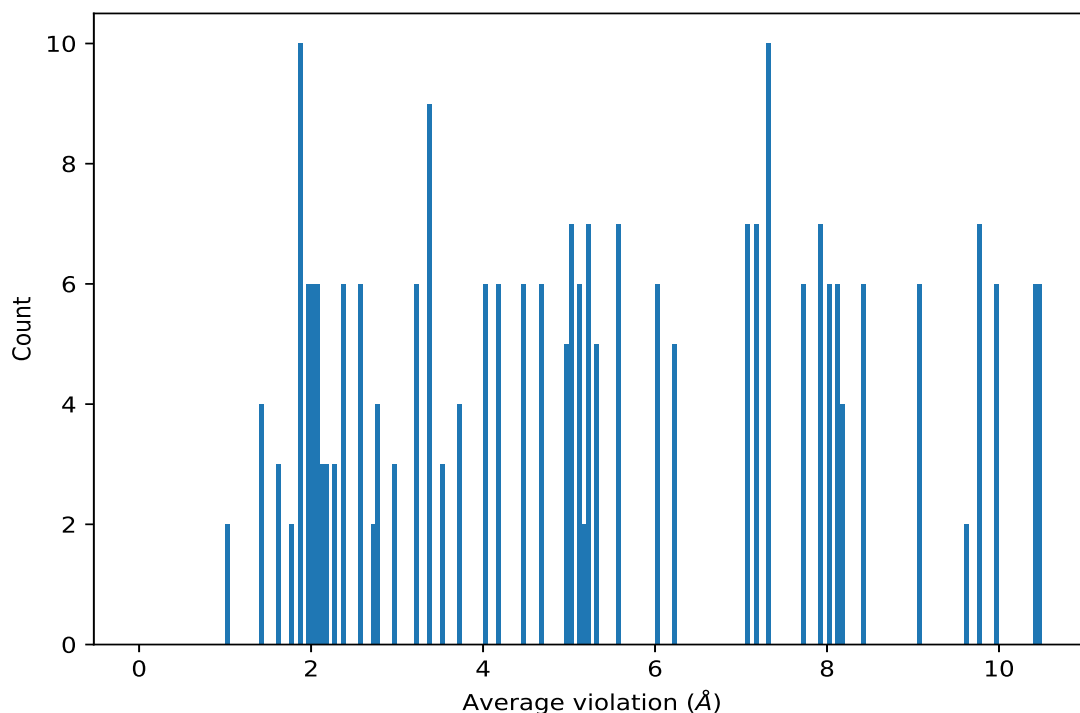
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,51)	2:142:B:ILE:H	3:3:A:PCW:N	7	10.46	1.11	10.19
(1,51)	2:142:B:ILE:H	3:23:A:PCW:N	7	10.46	1.11	10.19
(1,51)	2:142:B:ILE:N	4:39:A:17F:N1	7	10.46	1.11	10.19
(1,51)	2:142:B:ILE:H	4:34:A:17F:O4	7	10.46	1.11	10.19
(1,51)	2:142:B:ILE:H	4:39:A:17F:O4	7	10.46	1.11	10.19
(1,51)	2:142:B:ILE:H	4:38:A:17F:O5	7	10.46	1.11	10.19
(1,8)	3:8:A:PCW:N	2:172:B:LYS:HZ2	7	10.44	4.86	9.33
(1,8)	3:8:A:PCW:N	2:185:B:CYS:SG	7	10.44	4.86	9.33
(1,8)	3:8:A:PCW:P	2:184:B:LYS:HZ2	7	10.44	4.86	9.33
(1,8)	3:8:A:PCW:N	2:178:B:LYS:HZ1	7	10.44	4.86	9.33
(1,8)	3:8:A:PCW:N	2:184:B:LYS:CB	7	10.44	4.86	9.33
(1,8)	3:8:A:PCW:N	2:105:B:ASP:OD1	7	10.44	4.86	9.33
(1,29)	3:29:A:PCW:N	2:137:B:TYR:HH	7	9.98	3.87	10.1
(1,29)	3:29:A:PCW:N	2:133:B:LEU:CD1	7	9.98	3.87	10.1
(1,29)	3:29:A:PCW:P	2:172:B:LYS:HZ3	7	9.98	3.87	10.1
(1,29)	3:29:A:PCW:N	2:178:B:LYS:HZ1	7	9.98	3.87	10.1

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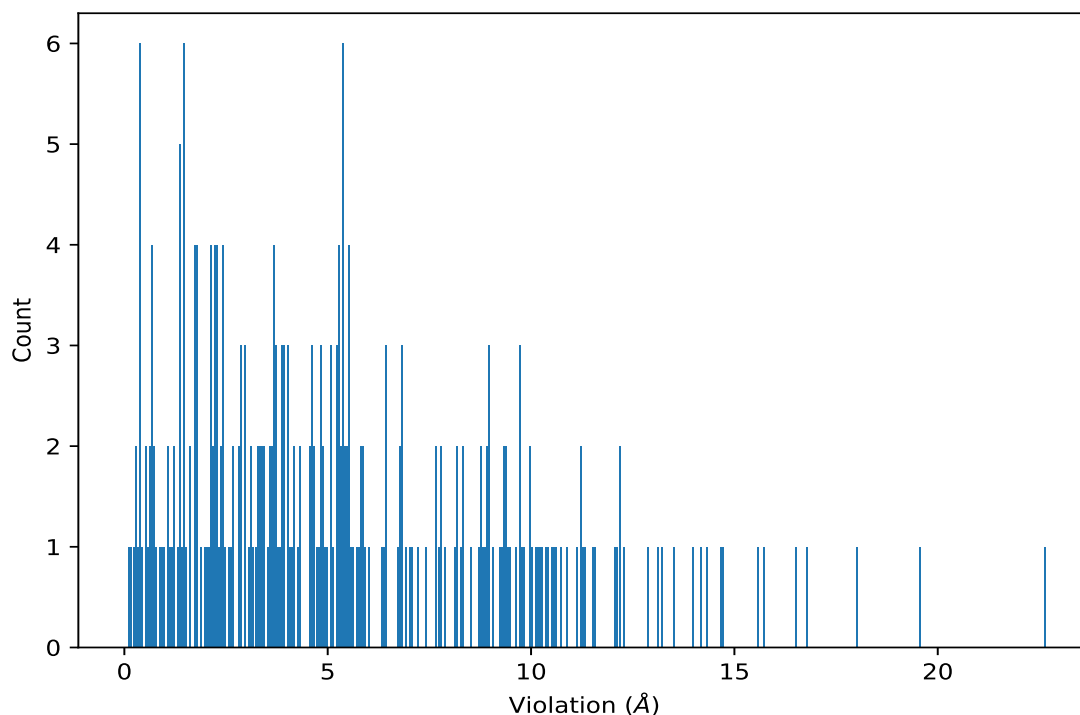
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,29)	3:29:A:PCW:O2	2:178:B:LYS:HZ1	7	9.98	3.87	10.1
(1,29)	3:29:A:PCW:O2	2:132:B:ASP:OD2	7	9.98	3.87	10.1
(1,21)	3:21:A:PCW:N	2:172:B:LYS:HZ2	7	9.78	3.82	10.42
(1,21)	3:21:A:PCW:N	2:184:B:LYS:HZ3	7	9.78	3.82	10.42
(1,21)	3:21:A:PCW:O31	2:177:B:LYS:HZ1	7	9.78	3.82	10.42
(1,21)	3:21:A:PCW:N	2:184:B:LYS:HZ2	7	9.78	3.82	10.42
(1,21)	3:21:A:PCW:O31	2:176:B:LYS:HZ2	7	9.78	3.82	10.42
(1,21)	3:21:A:PCW:O31	2:137:B:TYR:OH	7	9.78	3.82	10.42
(1,21)	3:21:A:PCW:P	2:176:B:LYS:CE	7	9.78	3.82	10.42
(1,52)	2:159:B:LEU:O	2:2:B:THR:N	7	9.62	0.42	9.7
(1,52)	2:159:B:LEU:C	2:2:B:THR:N	7	9.62	0.42	9.7
(1,5)	3:5:A:PCW:P	2:174:B:GLY:O	7	8.43	3.08	8.1
(1,5)	3:5:A:PCW:O31	2:175:B:LYS:HZ2	7	8.43	3.08	8.1
(1,5)	3:5:A:PCW:O31	2:105:B:ASP:OD2	7	8.43	3.08	8.1
(1,5)	3:5:A:PCW:P	2:184:B:LYS:HZ1	7	8.43	3.08	8.1
(1,5)	3:5:A:PCW:P	2:137:B:TYR:HH	7	8.43	3.08	8.1
(1,5)	3:5:A:PCW:P	2:176:B:LYS:HZ1	7	8.43	3.08	8.1
(1,57)	2:185:B:CYS:H	3:32:A:PCW:N	7	7.94	8.69	1.78
(1,57)	2:185:B:CYS:HG	3:12:A:PCW:N	7	7.94	8.69	1.78
(1,57)	2:185:B:CYS:H	3:27:A:PCW:P	7	7.94	8.69	1.78
(1,57)	2:185:B:CYS:O	4:40:A:17F:O5	7	7.94	8.69	1.78
(1,57)	2:185:B:CYS:O	3:27:A:PCW:N	7	7.94	8.69	1.78
(1,57)	2:185:B:CYS:H	4:39:A:17F:O4	7	7.94	8.69	1.78
(1,57)	2:185:B:CYS:HG	3:18:A:PCW:N	7	7.94	8.69	1.78
(1,32)	3:32:A:PCW:N	2:177:B:LYS:HZ2	7	7.73	2.53	8.16
(1,32)	3:32:A:PCW:N	2:173:B:ASP:OD1	7	7.73	2.53	8.16
(1,32)	3:32:A:PCW:N	2:105:B:ASP:OD2	7	7.73	2.53	8.16
(1,32)	3:32:A:PCW:N	2:173:B:ASP:OD2	7	7.73	2.53	8.16
(1,32)	3:32:A:PCW:P	2:105:B:ASP:OD2	7	7.73	2.53	8.16
(1,32)	3:32:A:PCW:N	2:132:B:ASP:OD2	7	7.73	2.53	8.16
(1,53)	2:171:B:SER:O	4:40:A:17F:O5	7	7.31	3.14	5.73
(1,53)	2:171:B:SER:O	3:1:A:PCW:N	7	7.31	3.14	5.73
(1,53)	2:171:B:SER:C	3:9:A:PCW:N	7	7.31	3.14	5.73
(1,53)	2:171:B:SER:OG	2:2:B:THR:N	7	7.31	3.14	5.73
(1,53)	2:171:B:SER:HG	2:2:B:THR:N	7	7.31	3.14	5.73
(1,10)	3:10:A:PCW:N	2:172:B:LYS:HZ2	7	7.19	3.32	4.93

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	2:185:B:CYS:H	3:32:A:PCW:N	1	22.62
(1,57)	2:185:B:CYS:H	4:39:A:17F:O4	6	19.56
(1,8)	3:8:A:PCW:N	2:172:B:LYS:HZ2	1	18.04
(1,21)	3:21:A:PCW:O31	2:137:B:TYR:OH	6	16.78
(1,3)	3:3:A:PCW:N	2:105:B:ASP:OD2	6	16.54
(1,18)	3:18:A:PCW:N	2:105:B:ASP:OD1	6	15.73
(1,15)	3:15:A:PCW:N	2:105:B:ASP:OD1	1	15.57
(1,27)	3:27:A:PCW:N	2:105:B:ASP:OD1	6	14.7
(1,8)	3:8:A:PCW:N	2:105:B:ASP:OD1	6	14.66
(1,29)	3:29:A:PCW:N	2:178:B:LYS:HZ1	5	14.32

10 Dihedral-angle violation analysis

No dihedral-angle restraints found