



wwPDB NMR Structure Validation Summary Report ⓘ

Aug 6, 2020 – 03:42 PM BST

PDB ID : 6PTS
Title : NMR data-driven model of KRas-GMPPNP:RBD-CRD complex tethered to a nanodisc (state A)
Authors : Fang, Z.; Lee, K.; Gasmi-Seabrook, G.; Ikura, M.; Marshall, C.B.
Deposited on : 2019-07-16

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.13.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

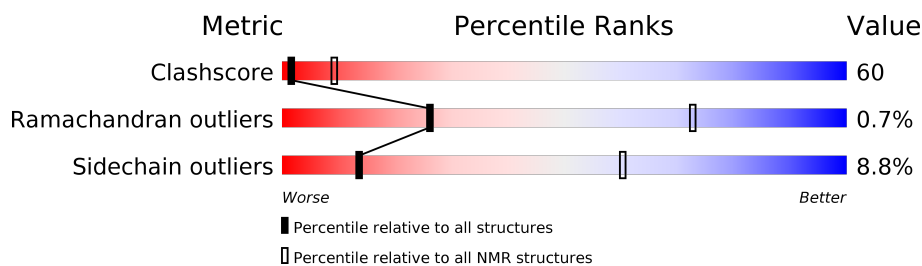
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 5%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	198	83% 16% .
1	C	198	78% 22%
2	B	185	73% 20% 7%
3	D	132	77% 23% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:201-A:398, C:399-C:596 (396)	0.29	5
2	B:1-B:172, D:356-D:487 (304)	1.04	3

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	2, 3, 4, 6, 7, 8
2	1, 9, 10
Single-model clusters	5

3 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11566 atoms, of which 1424 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	198	Total	C	H	N	O	S	0
			2004	1019	381	287	314	3	
1	C	198	Total	C	H	N	O	S	0
			2002	1019	379	287	314	3	

- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1835	923	359	257	287	9	

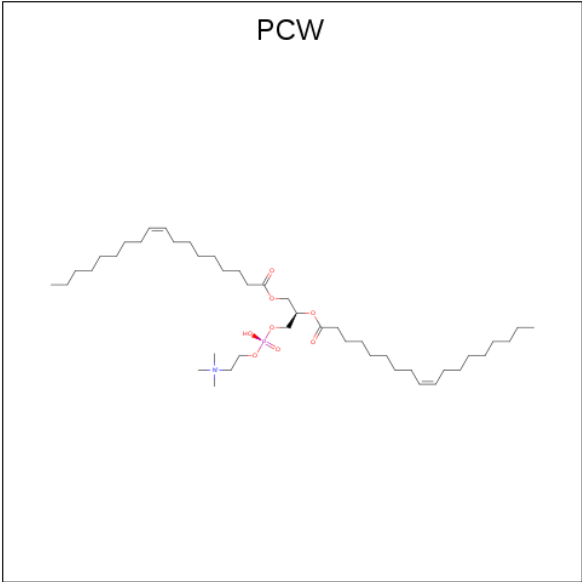
- Molecule 3 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms						Trace
3	D	132	Total	C	H	N	O	S	0
			1316	677	251	194	182	12	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	403	GLN	HIS	conflict	UNP P04049

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



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

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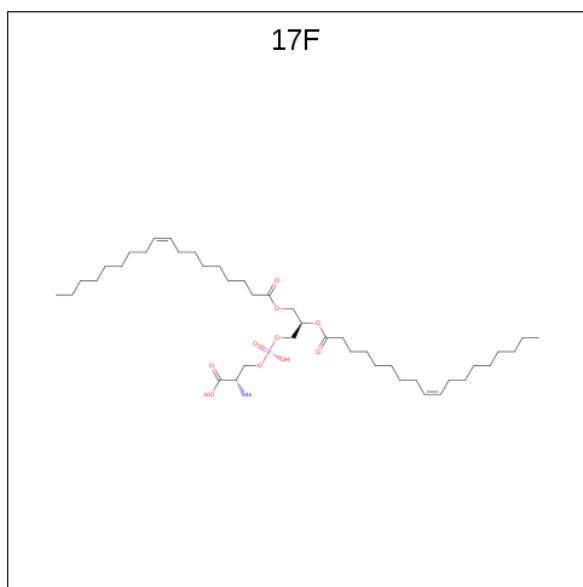
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
4	C	1	Total 54	44	1	8	1
4	C	1	Total 54	44	1	8	1
4	C	1	Total 54	44	1	8	1
4	C	1	Total 54	44	1	8	1
4	C	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	B	1	Total 54	44	1	8	1
4	D	1	Total 54	44	1	8	1
4	D	1	Total 54	44	1	8	1
4	D	1	Total 54	44	1	8	1
4	D	1	Total 54	44	1	8	1

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

- Molecule 5 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: C₄₂H₇₈NO₁₀P).



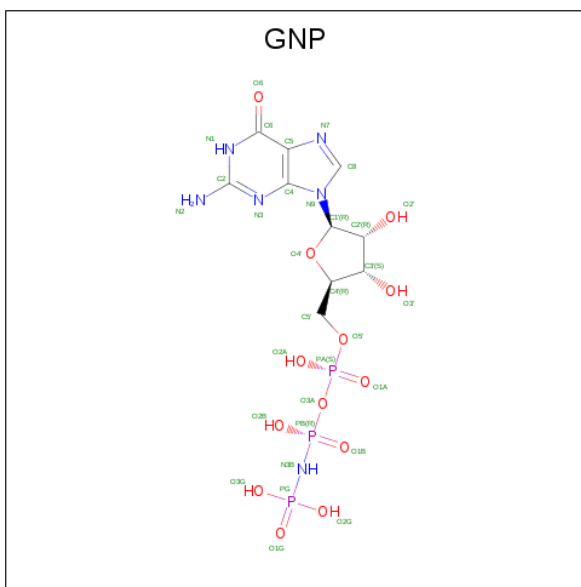
Mol	Chain	Residues	Atoms					
5	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1

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Mol	Chain	Residues	Atoms					
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					
6	B	1	Total	C	H	N	O	P
			38	10	6	6	13	3

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
7	B	1	Total	Mg
			1	1

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

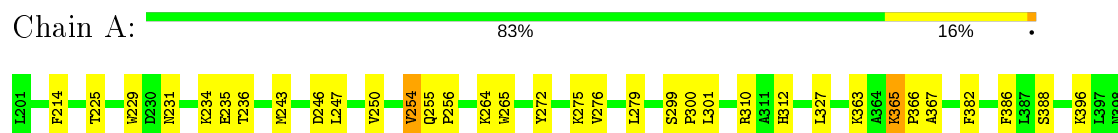
Mol	Chain	Residues	Atoms	
8	D	2	Total	Zn
			2	2

4 Residue-property plots

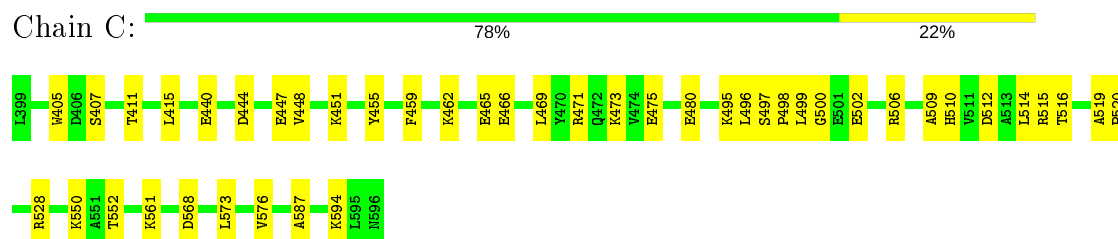
4.1 Average score per residue in the NMR ensemble

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.

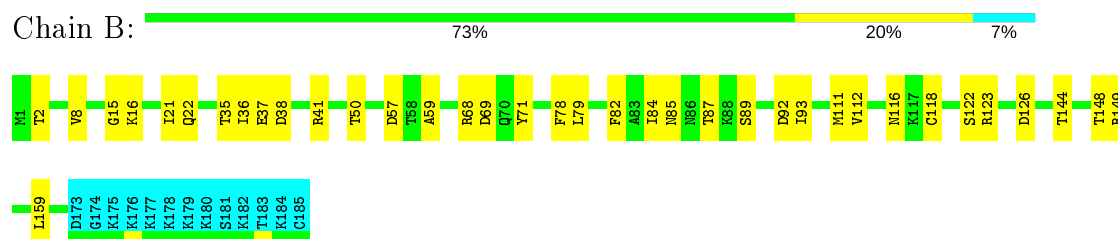
- Molecule 1: Apolipoprotein A-I



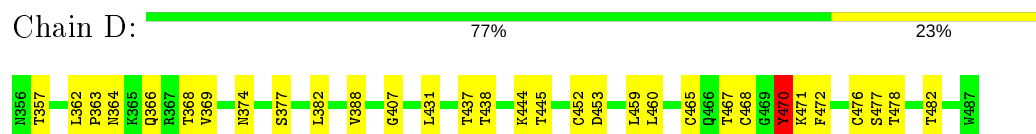
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



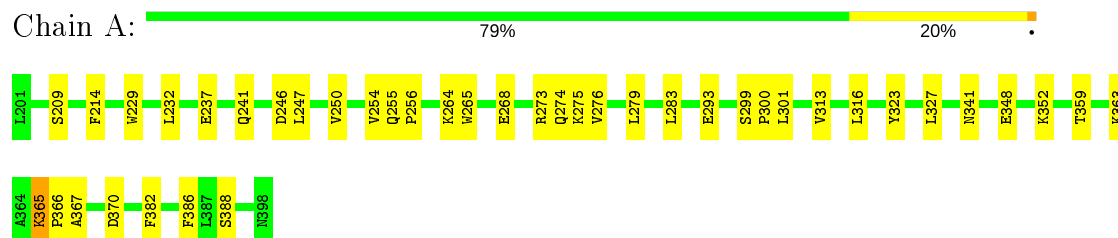
- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase



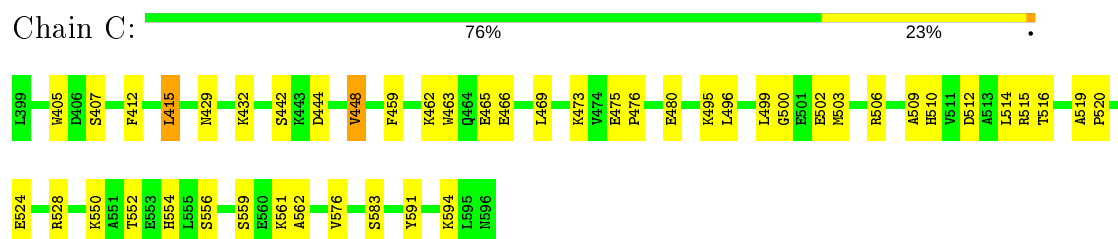
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

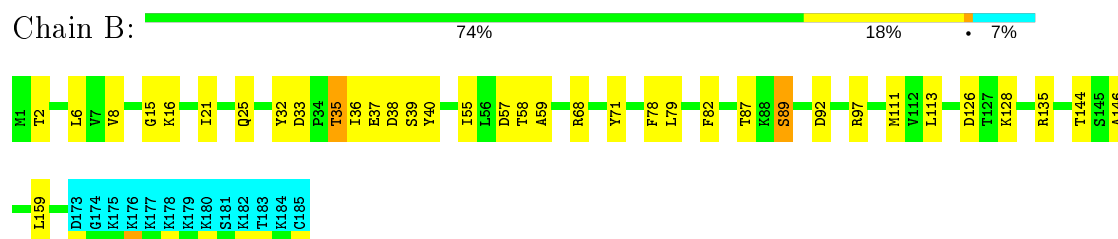
- Molecule 1: Apolipoprotein A-I



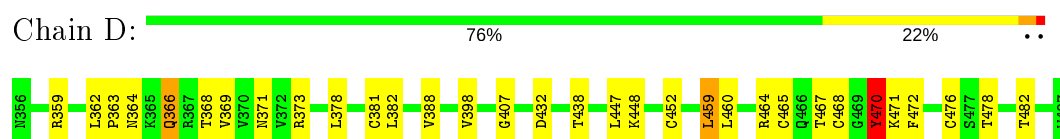
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase



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: *structures with the 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	557
Number of shifts mapped to atoms	557
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	5%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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: ZN, 17F, MG, GNP, 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	0.25±0.00	0±0/1650 (0.0± 0.0%)	0.39±0.00	0±0/2218 (0.0± 0.0%)
1	C	0.25±0.00	0±0/1650 (0.0± 0.0%)	0.40±0.00	0±0/2218 (0.0± 0.0%)
2	B	0.27±0.00	0±0/1395 (0.0± 0.0%)	0.39±0.01	0±0/1880 (0.0± 0.0%)
3	D	0.51±0.00	2±0/1088 (0.2± 0.0%)	3.77±0.00	9±0/1466 (0.6± 0.0%)
All	All	0.32	21/57830 (0.0%)	1.68	90/77820 (0.1%)

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

Mol	Chain	Chirality	Planarity
3	D	0.0±0.0	1.0±0.0
All	All	0	10

All 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
3	D	470	TYR	CB-CG	10.12	1.66	1.51	3	10
3	D	470	TYR	CZ-OH	7.26	1.50	1.37	9	10
3	D	470	TYR	CG-CD2	5.05	1.45	1.39	5	1

5 of 9 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	D	470	TYR	CG-CD1-CE1	-69.49	65.71	121.30	9	10
3	D	470	TYR	CZ-CE2-CD2	-61.73	64.24	119.80	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	470	TYR	CG-CD2-CE2	-61.26	72.30	121.30	6	10
3	D	470	TYR	CD1-CG-CD2	-56.63	55.61	117.90	1	10
3	D	470	TYR	CD1-CE1-CZ	-55.41	69.93	119.80	9	10

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
3	D	470	TYR	Sidechain	10

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	1623	381	1626	23±6
1	C	1623	379	1626	24±4
2	B	1373	319	1359	23±5
3	D	1065	251	1070	13±2
4	A	810	0	1200	302±24
4	B	648	0	960	281±37
4	C	1350	0	2000	542±22
4	D	648	0	960	282±17
5	A	108	6	152	34±8
5	B	162	9	228	69±11
5	C	378	21	532	149±9
5	D	216	12	304	98±23
6	B	32	6	13	3±2
7	B	1	0	0	0±0
All	All	100390	13840	120300	13335

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 60.

5 of 7265 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:207:PCW:H251	4:B:207:PCW:C20	1.19	1.67	10	1
4:D:508:PCW:H222	4:D:508:PCW:C27	1.17	1.68	9	3
4:A:405:PCW:C19	4:A:405:PCW:H142	1.17	1.70	7	5
4:A:405:PCW:H142	4:A:405:PCW:C19	1.16	1.71	8	5
4:B:202:PCW:H362	4:B:202:PCW:C31	1.16	1.70	6	2

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	196/198 (99%)	190±1 (97±1%)	5±1 (2±1%)	1±0 (1±0%)	29	74
1	C	196/198 (99%)	191±1 (97±1%)	6±1 (3±1%)	0±0 (0±0%)	100	100
2	B	171/185 (92%)	162±2 (95±1%)	9±2 (5±1%)	0±0 (0±0%)	50	82
3	D	130/132 (98%)	112±2 (86±2%)	15±3 (12±2%)	3±1 (2±1%)	9	46
All	All	6930/7130 (97%)	6543 (94%)	341 (5%)	46 (1%)	26	73

5 of 15 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
3	D	364	ASN	10
3	D	407	GLY	10
3	D	374	ASN	5
3	D	375	GLY	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	174/174 (100%)	162±4 (93±2%)	12±4 (7±2%)	19	67
1	C	174/174 (100%)	159±2 (91±1%)	15±2 (9±1%)	14	61
2	B	152/164 (93%)	139±3 (92±2%)	13±3 (8±2%)	14	61
3	D	119/119 (100%)	105±3 (88±3%)	15±3 (12±3%)	8	50
All	All	6190/6310 (98%)	5648 (91%)	542 (9%)	13	60

5 of 180 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	C	550	LYS	10
3	D	460	LEU	10
1	C	516	THR	10
3	D	468	CYS	10
2	B	87	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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 3 are 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
4	PCW	C	621	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	D	507	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	B	207	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	D	502	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	617	-	53,53,53	0.81±0.00	0±0 (0±0%)
5	17F	A	410	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	D	508	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	B	203	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	B	202	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	A	412	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	A	414	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	B	204	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	A	405	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	B	210	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	C	626	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	D	504	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	608	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	610	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	D	505	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	B	206	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	A	413	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	B	209	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	C	603	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	602	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	B	201	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	B	214	-	50,53,53	0.78±0.00	0±0 (0±0%)
5	17F	C	627	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	A	407	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	D	515	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	A	417	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	A	416	-	53,53,53	0.81±0.00	0±0 (0±0%)
5	17F	D	513	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	C	604	-	53,53,53	0.81±0.00	0±0 (0±0%)
5	17F	C	628	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	C	623	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	612	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	605	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	613	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	D	512	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	C	601	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	C	630	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	C	625	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	D	509	-	53,53,53	0.80±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	C	618	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	D	510	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	624	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	A	408	-	53,53,53	0.81±0.00	0±0 (0±0%)
5	17F	A	409	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	A	406	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	D	511	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	C	609	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	614	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	C	616	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	D	516	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	D	501	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	C	606	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	B	212	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	C	619	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	A	411	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	D	506	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	D	503	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	C	629	-	50,53,53	0.78±0.00	0±0 (0±0%)
5	17F	D	514	-	50,53,53	0.78±0.00	0±0 (0±0%)
6	GNP	B	216	-	28,34,34	2.92±0.00	2±0 (7±0%)
4	PCW	B	208	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	B	211	-	53,53,53	0.81±0.00	0±0 (0±0%)
5	17F	C	631	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	A	415	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	A	404	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	620	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	A	403	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	622	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	A	402	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	C	632	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	B	205	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	PCW	C	607	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	B	215	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	A	401	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	PCW	C	611	-	53,53,53	0.80±0.00	0±0 (0±0%)
5	17F	B	213	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	PCW	C	615	-	53,53,53	0.81±0.00	0±0 (0±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
4	PCW	C	621	-	59,61,61	2.65±0.00	1±0 (1±0%)
4	PCW	D	507	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	B	207	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	D	502	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	617	-	59,61,61	2.65±0.00	1±0 (1±0%)
5	17F	A	410	-	52,60,60	1.15±0.00	0±0 (0±0%)
4	PCW	D	508	-	59,61,61	2.62±0.00	1±0 (1±0%)
4	PCW	B	203	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	B	202	-	59,61,61	2.62±0.00	1±0 (1±0%)
4	PCW	A	412	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	A	414	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	B	204	-	59,61,61	2.61±0.00	1±0 (1±0%)
4	PCW	A	405	-	59,61,61	2.61±0.00	1±0 (1±0%)
4	PCW	B	210	-	59,61,61	2.65±0.00	1±0 (1±0%)
5	17F	C	626	-	52,60,60	1.11±0.00	0±0 (0±0%)
4	PCW	D	504	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	C	608	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	610	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	D	505	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	B	206	-	59,61,61	2.62±0.00	1±0 (1±0%)
4	PCW	A	413	-	59,61,61	2.65±0.00	1±0 (1±0%)
4	PCW	B	209	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	603	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	C	602	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	B	201	-	59,61,61	2.63±0.00	1±0 (1±0%)
5	17F	B	214	-	52,60,60	1.08±0.00	0±0 (0±0%)
5	17F	C	627	-	52,60,60	1.13±0.00	0±0 (0±0%)
4	PCW	A	407	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	D	515	-	59,61,61	2.65±0.00	1±0 (1±0%)
4	PCW	A	417	-	59,61,61	2.62±0.00	1±0 (1±0%)
4	PCW	A	416	-	59,61,61	2.62±0.00	1±0 (1±0%)
5	17F	D	513	-	52,60,60	1.14±0.00	0±0 (0±0%)
4	PCW	C	604	-	59,61,61	2.64±0.00	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
5	17F	C	628	-	52,60,60	1.13±0.00	0±0 (0±0%)
4	PCW	C	623	-	59,61,61	2.61±0.00	1±0 (1±0%)
4	PCW	C	612	-	59,61,61	2.65±0.00	1±0 (1±0%)
4	PCW	C	605	-	59,61,61	2.68±0.00	1±0 (1±0%)
4	PCW	C	613	-	59,61,61	2.63±0.00	1±0 (1±0%)
5	17F	D	512	-	52,60,60	1.11±0.00	0±0 (0±0%)
4	PCW	C	601	-	59,61,61	2.64±0.00	1±0 (1±0%)
5	17F	C	630	-	52,60,60	1.32±0.00	0±0 (0±0%)
4	PCW	C	625	-	59,61,61	2.62±0.00	1±0 (1±0%)
4	PCW	D	509	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	618	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	D	510	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	C	624	-	59,61,61	2.67±0.00	1±0 (1±0%)
4	PCW	A	408	-	59,61,61	2.66±0.00	1±0 (1±0%)
5	17F	A	409	-	52,60,60	1.39±0.00	0±0 (0±0%)
4	PCW	A	406	-	59,61,61	2.64±0.00	1±0 (1±0%)
5	17F	D	511	-	52,60,60	1.14±0.00	0±0 (0±0%)
4	PCW	C	609	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	614	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	C	616	-	59,61,61	2.65±0.00	1±0 (1±0%)
4	PCW	D	516	-	59,61,61	2.72±0.00	1±0 (1±0%)
4	PCW	D	501	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	C	606	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	B	212	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	619	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	A	411	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	D	506	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	D	503	-	59,61,61	2.73±0.00	1±0 (1±0%)
5	17F	C	629	-	52,60,60	1.10±0.00	0±0 (0±0%)
5	17F	D	514	-	52,60,60	1.24±0.00	1±0 (1±0%)
6	GNP	B	216	-	30,54,54	1.58±0.00	0±0 (0±0%)
4	PCW	B	208	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	B	211	-	59,61,61	2.63±0.00	1±0 (1±0%)
5	17F	C	631	-	52,60,60	1.18±0.00	0±0 (0±0%)
4	PCW	A	415	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	A	404	-	59,61,61	2.62±0.00	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	PCW	C	620	-	59,61,61	2.61±0.00	1±0 (1±0%)
4	PCW	A	403	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	PCW	C	622	-	59,61,61	2.61±0.00	1±0 (1±0%)
4	PCW	A	402	-	59,61,61	2.65±0.00	1±0 (1±0%)
5	17F	C	632	-	52,60,60	1.14±0.00	0±0 (0±0%)
4	PCW	B	205	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	607	-	59,61,61	2.64±0.00	1±0 (1±0%)
5	17F	B	215	-	52,60,60	1.15±0.00	0±0 (0±0%)
4	PCW	A	401	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	PCW	C	611	-	59,61,61	2.65±0.00	1±0 (1±0%)
5	17F	B	213	-	52,60,60	1.12±0.00	0±0 (0±0%)
4	PCW	C	615	-	59,61,61	2.62±0.00	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
4	PCW	A	414	-	-	0±0,57,57,57	-
5	17F	C	627	-	-	1±0,55,59,59	-
5	17F	C	628	-	-	0±0,55,59,59	-
4	PCW	C	623	-	-	0±0,57,57,57	-
4	PCW	C	618	-	-	0±0,57,57,57	-
4	PCW	A	412	-	-	0±0,57,57,57	-
4	PCW	D	502	-	-	0±0,57,57,57	-
4	PCW	A	408	-	-	0±0,57,57,57	-
4	PCW	D	510	-	-	0±0,57,57,57	-
4	PCW	A	411	-	-	0±0,57,57,57	-
4	PCW	A	406	-	-	0±0,57,57,57	-
4	PCW	B	202	-	-	0±0,57,57,57	-
4	PCW	C	614	-	-	0±0,57,57,57	-
4	PCW	C	601	-	-	0±0,57,57,57	-
4	PCW	D	515	-	-	0±0,57,57,57	-
5	17F	C	629	-	-	0±0,55,59,59	-
4	PCW	C	602	-	-	0±0,57,57,57	-
5	17F	D	511	-	-	0±0,55,59,59	-
4	PCW	D	506	-	-	0±0,57,57,57	-
4	PCW	B	205	-	-	0±0,57,57,57	-
4	PCW	D	503	-	-	0±0,57,57,57	-
4	PCW	C	622	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	D	501	-	-	0±0,57,57,57	-
4	PCW	B	211	-	-	0±0,57,57,57	-
4	PCW	C	609	-	-	0±0,57,57,57	-
4	PCW	C	603	-	-	0±0,57,57,57	-
4	PCW	B	206	-	-	0±0,57,57,57	-
5	17F	C	630	-	-	0±0,55,59,59	-
4	PCW	A	402	-	-	0±0,57,57,57	-
5	17F	B	213	-	-	0±0,55,59,59	-
4	PCW	D	505	-	-	0±0,57,57,57	-
4	PCW	D	504	-	-	0±0,57,57,57	-
5	17F	C	631	-	-	0±0,55,59,59	-
4	PCW	A	416	-	-	0±0,57,57,57	-
4	PCW	D	508	-	-	0±0,57,57,57	-
4	PCW	B	209	-	-	0±0,57,57,57	-
5	17F	C	626	-	-	0±0,55,59,59	-
6	GNP	B	216	-	-	0±0,17,38,38	0±0,3,3,3
4	PCW	C	608	-	-	0±0,57,57,57	-
5	17F	D	513	-	-	0±0,55,59,59	-
4	PCW	B	210	-	-	0±0,57,57,57	-
4	PCW	A	404	-	-	0±0,57,57,57	-
4	PCW	C	611	-	-	0±0,57,57,57	-
4	PCW	C	615	-	-	0±0,57,57,57	-
4	PCW	A	413	-	-	0±0,57,57,57	-
4	PCW	D	516	-	-	0±0,57,57,57	-
4	PCW	C	619	-	-	0±0,57,57,57	-
4	PCW	C	613	-	-	0±0,57,57,57	-
4	PCW	C	604	-	-	0±0,57,57,57	-
4	PCW	A	417	-	-	0±0,57,57,57	-
4	PCW	C	607	-	-	0±0,57,57,57	-
5	17F	A	409	-	-	0±0,55,59,59	-
4	PCW	C	625	-	-	0±0,57,57,57	-
5	17F	C	632	-	-	0±0,55,59,59	-
4	PCW	C	616	-	-	0±0,57,57,57	-
5	17F	D	514	-	-	1±0,55,59,59	-
4	PCW	A	405	-	-	0±0,57,57,57	-
4	PCW	C	606	-	-	0±0,57,57,57	-
4	PCW	C	612	-	-	0±0,57,57,57	-
4	PCW	C	624	-	-	0±0,57,57,57	-
5	17F	B	214	-	-	0±0,55,59,59	-
4	PCW	D	509	-	-	0±0,57,57,57	-
4	PCW	B	204	-	-	0±0,57,57,57	-
4	PCW	C	621	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	D	507	-	-	0±0,57,57,57	-
4	PCW	A	407	-	-	0±0,57,57,57	-
4	PCW	C	610	-	-	0±0,57,57,57	-
5	17F	B	215	-	-	0±0,55,59,59	-
4	PCW	C	617	-	-	0±0,57,57,57	-
4	PCW	B	208	-	-	0±0,57,57,57	-
4	PCW	B	212	-	-	0±0,57,57,57	-
4	PCW	B	207	-	-	0±0,57,57,57	-
4	PCW	C	620	-	-	0±0,57,57,57	-
5	17F	D	512	-	-	1±0,55,59,59	-
5	17F	A	410	-	-	0±0,55,59,59	-
4	PCW	A	403	-	-	0±0,57,57,57	-
4	PCW	A	415	-	-	0±0,57,57,57	-
4	PCW	B	201	-	-	0±0,57,57,57	-
4	PCW	A	401	-	-	0±0,57,57,57	-
4	PCW	C	605	-	-	0±0,57,57,57	-
4	PCW	B	203	-	-	0±0,57,57,57	-

All 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
6	B	216	GNP	C4-N9	10.56	1.33	1.47	6	10
6	B	216	GNP	C5-C6	7.97	1.39	1.52	6	10

5 of 65 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
4	C	610	PCW	C8-N-C7	18.05	62.55	108.97	8	10
4	A	417	PCW	C8-N-C7	18.05	62.55	108.97	9	10
4	D	516	PCW	C8-N-C7	18.05	62.56	108.97	6	10
4	A	402	PCW	C8-N-C7	18.05	62.56	108.97	3	10
4	B	210	PCW	C8-N-C7	18.05	62.57	108.97	8	10

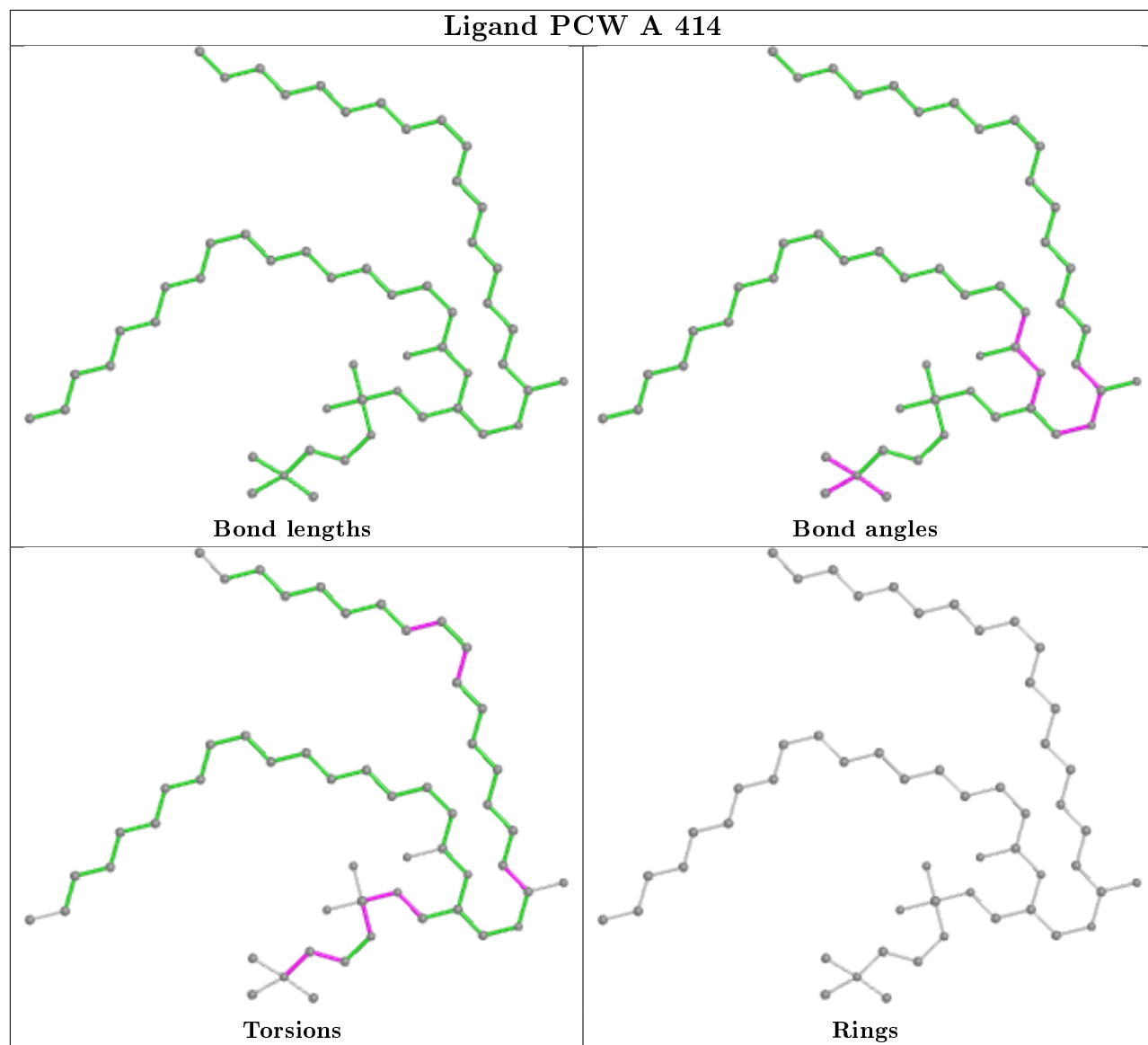
There are no chirality outliers.

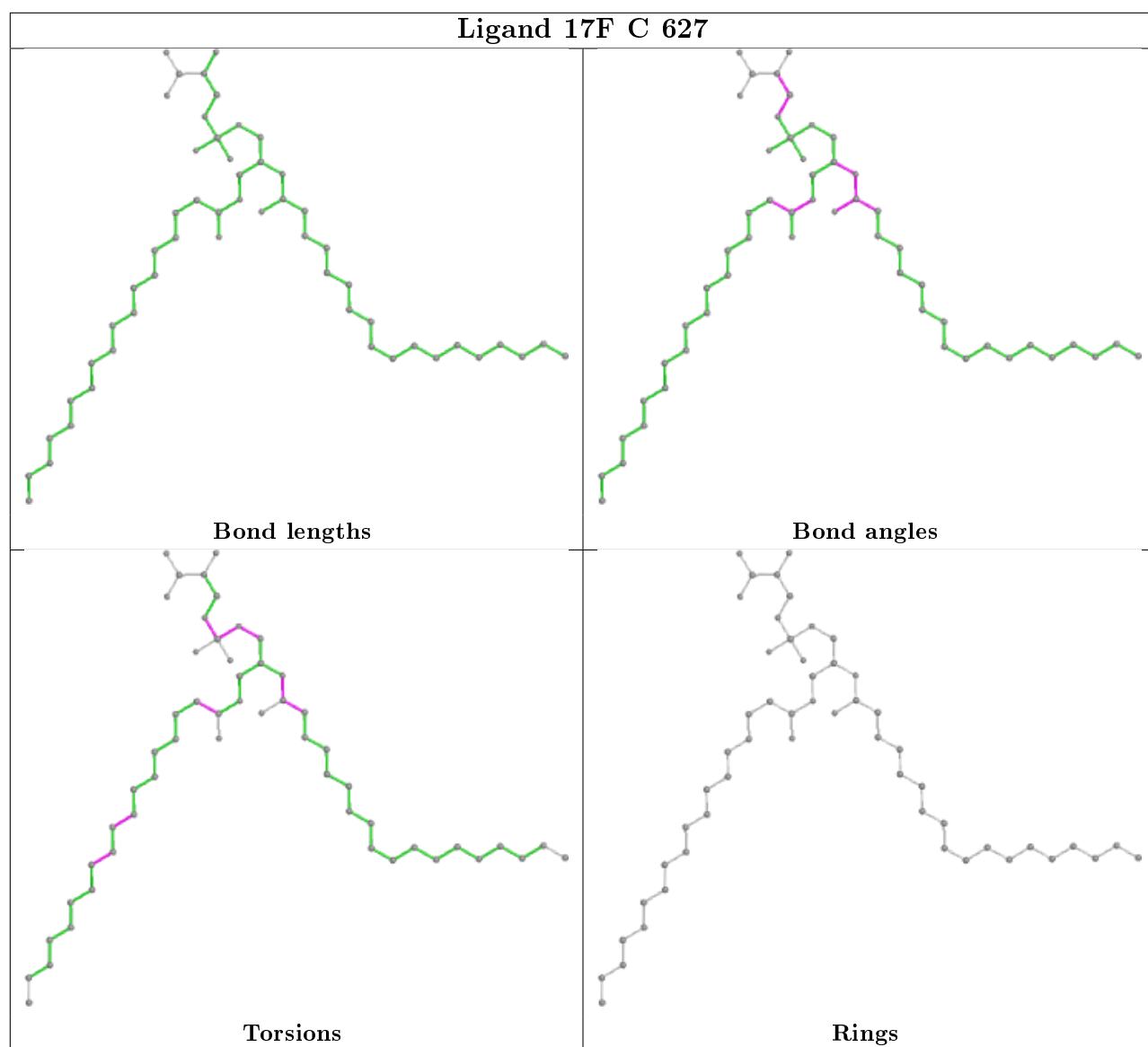
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

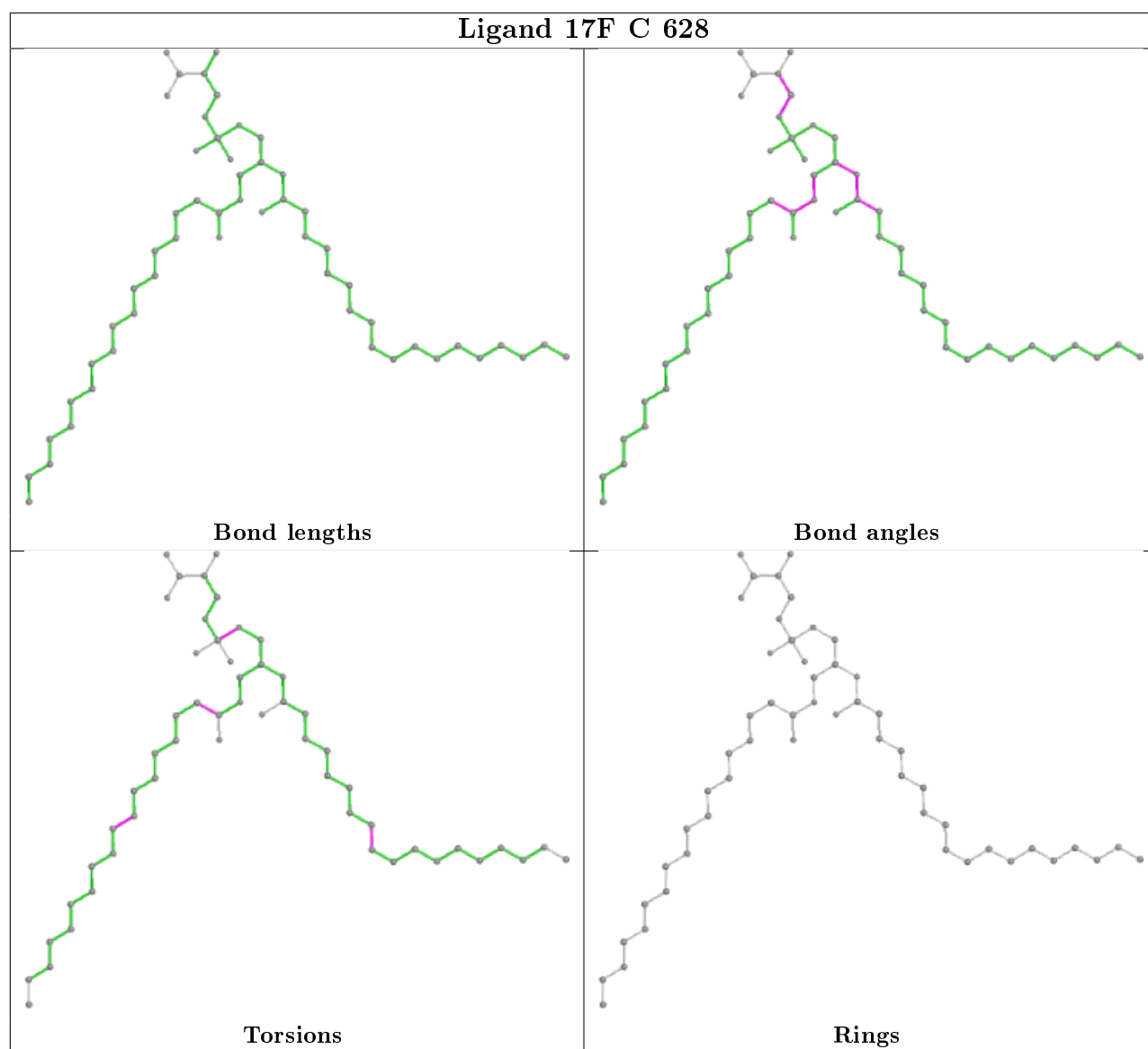
Mol	Chain	Res	Type	Atoms	Models (Total)
5	C	627	17F	O10-C17-O9-C5	10
5	D	514	17F	O10-C17-O9-C5	10
5	D	512	17F	O10-C17-O9-C5	10

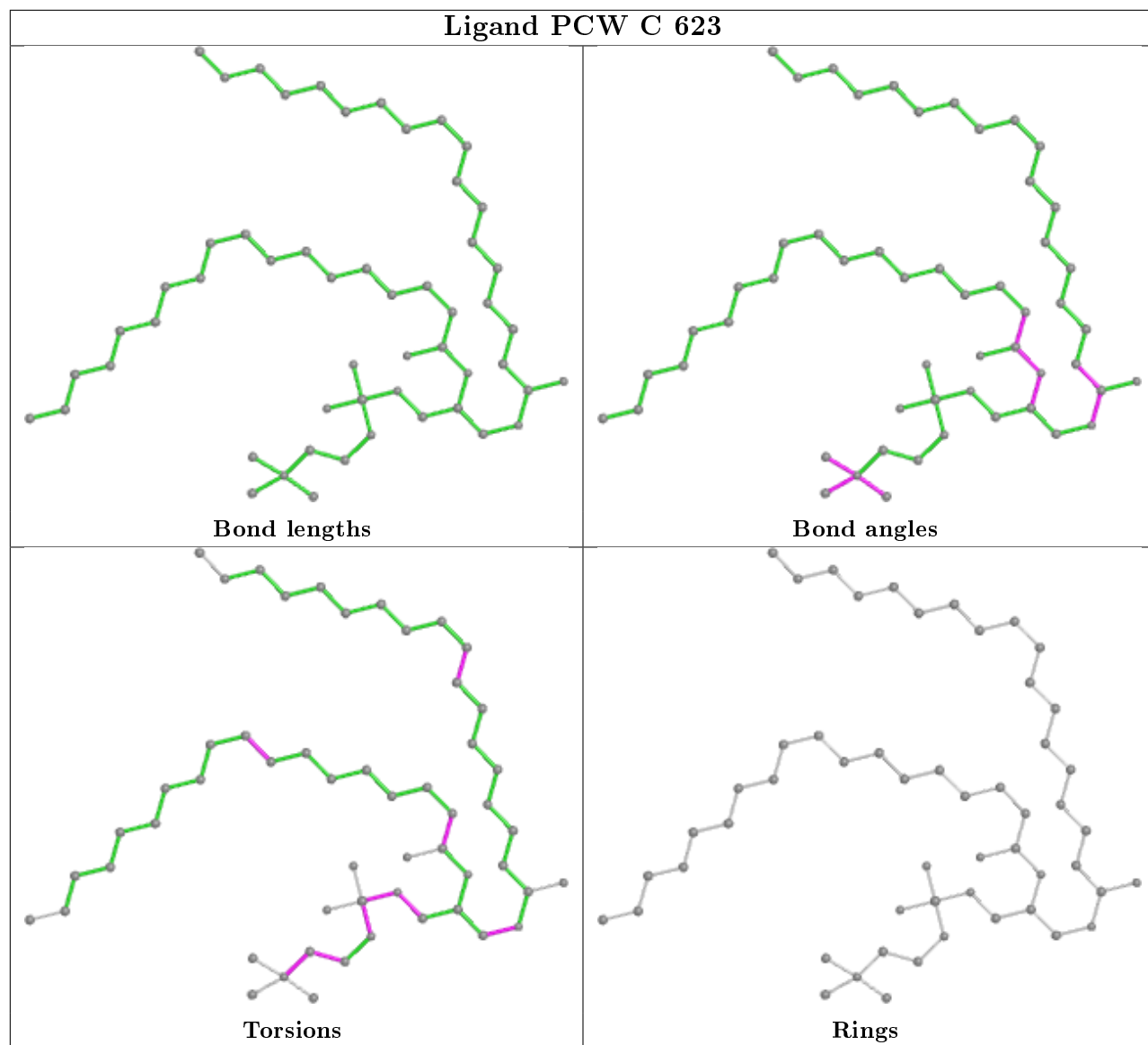
There are no ring outliers.

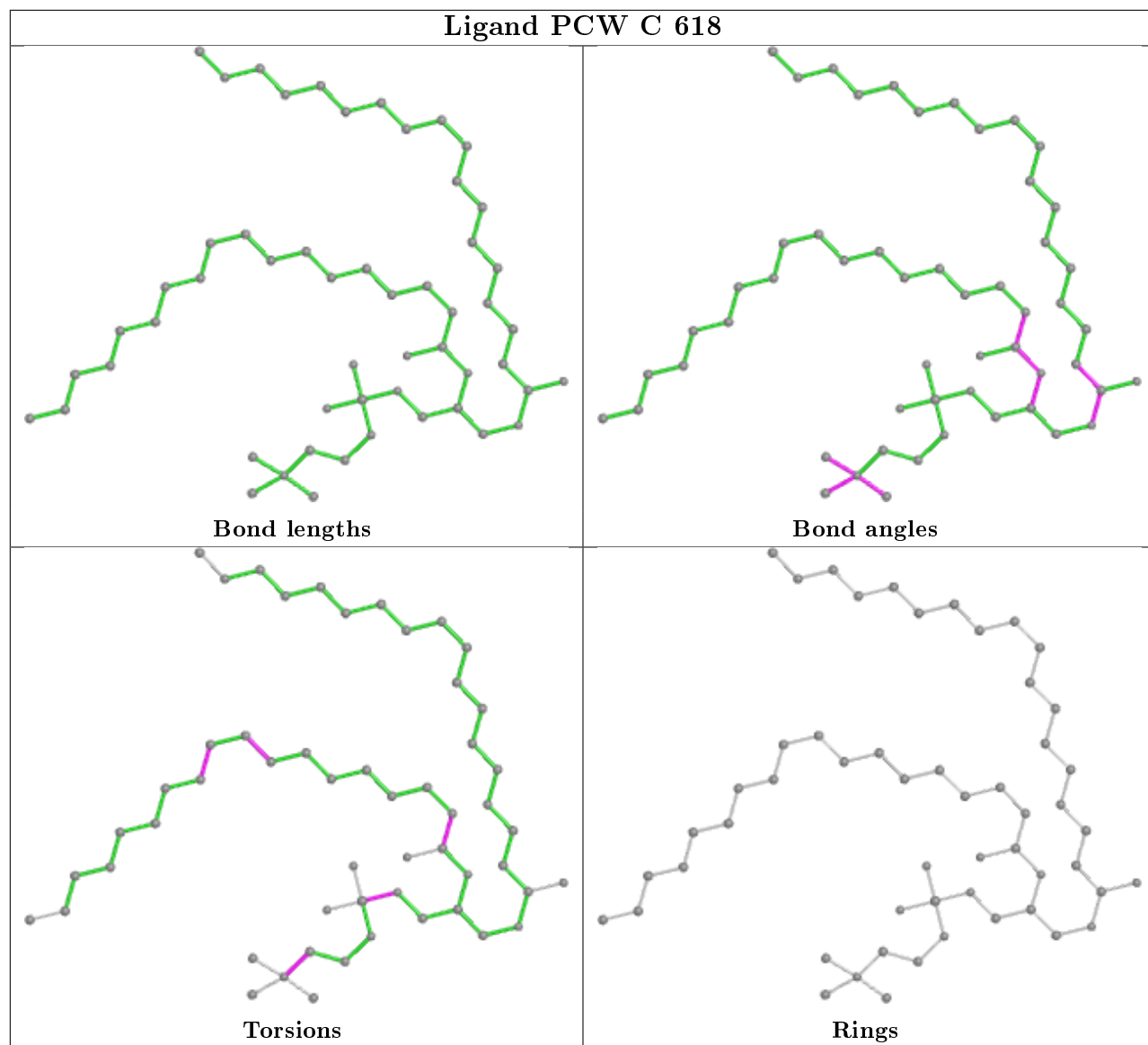
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

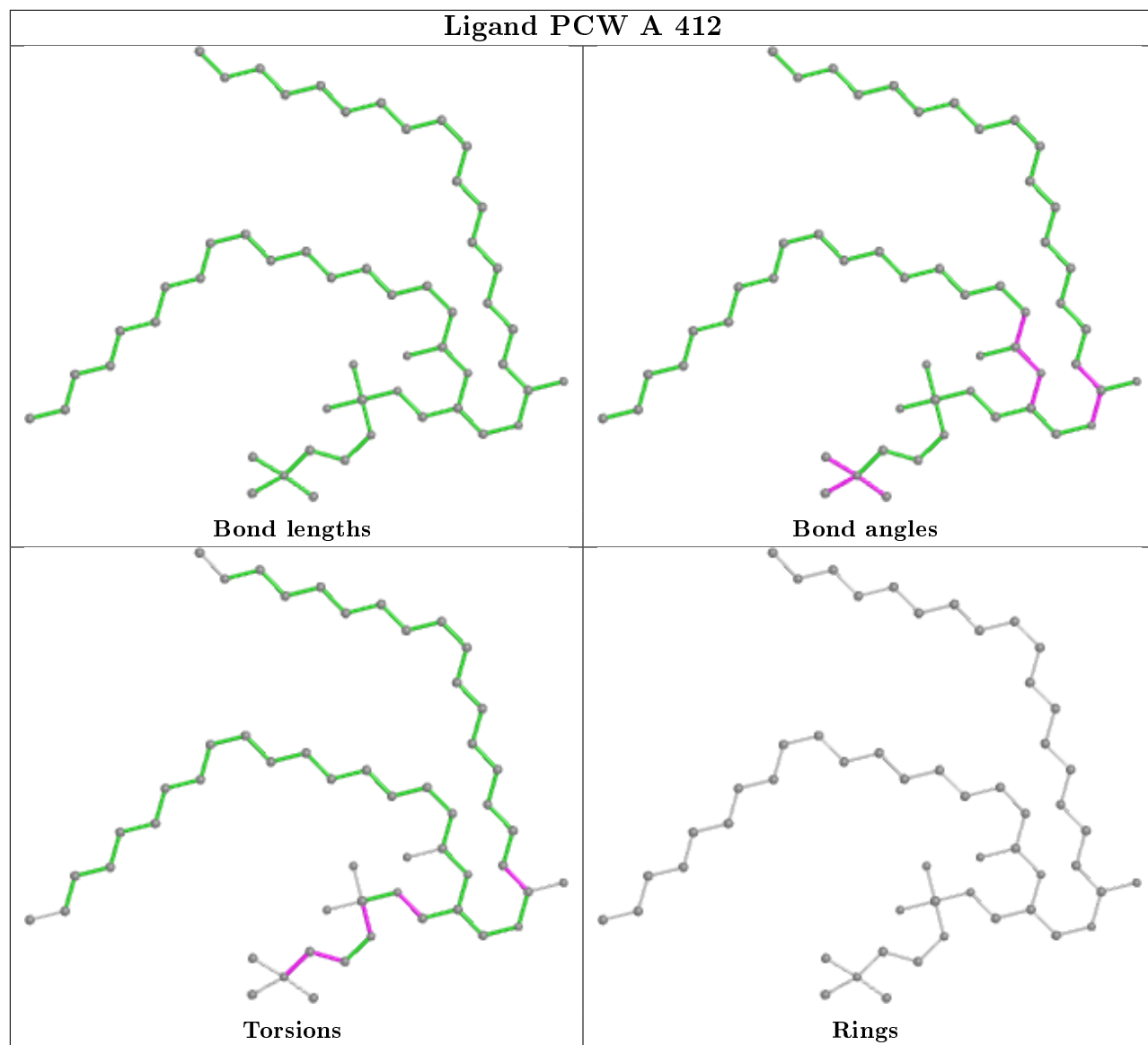


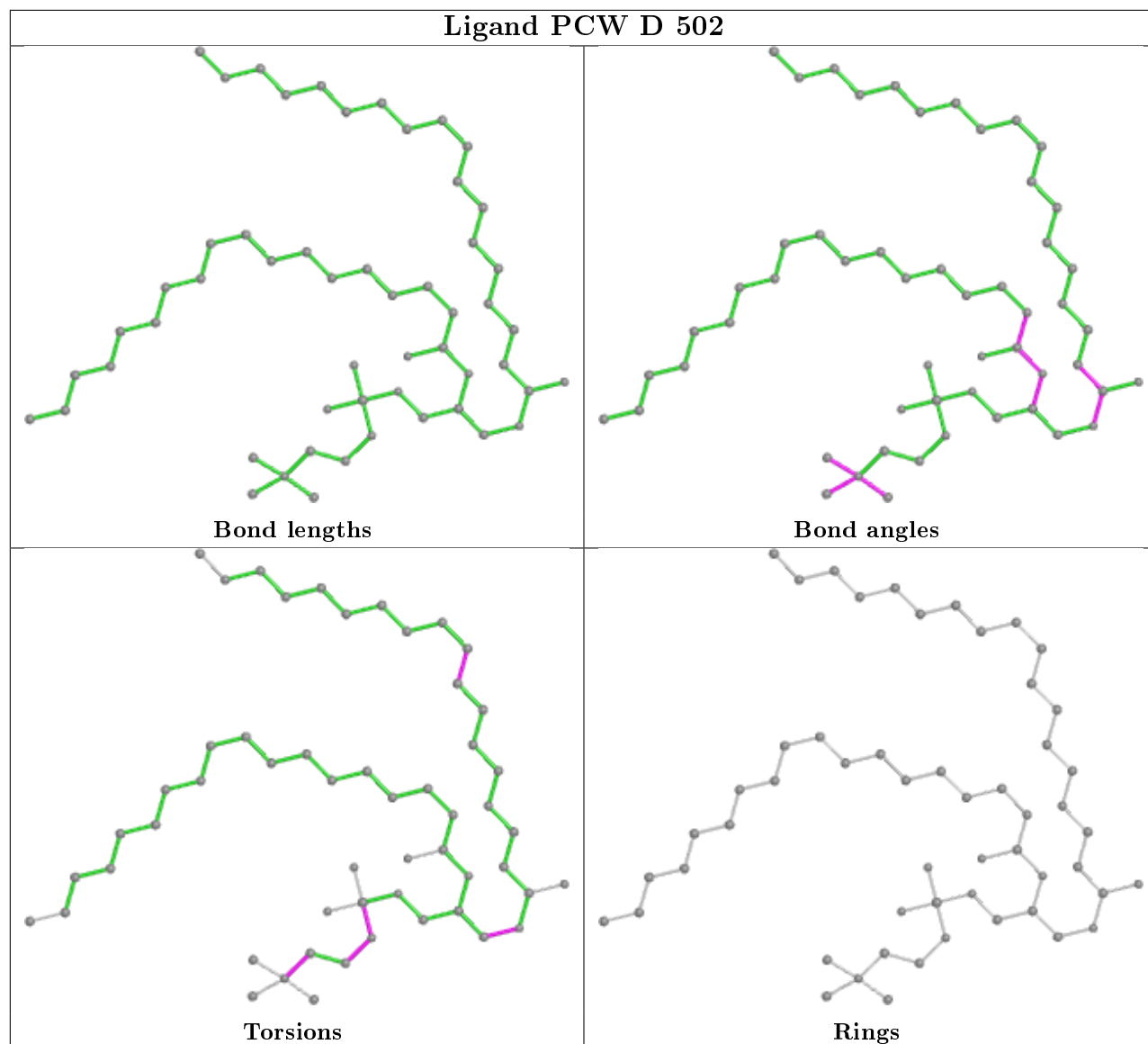


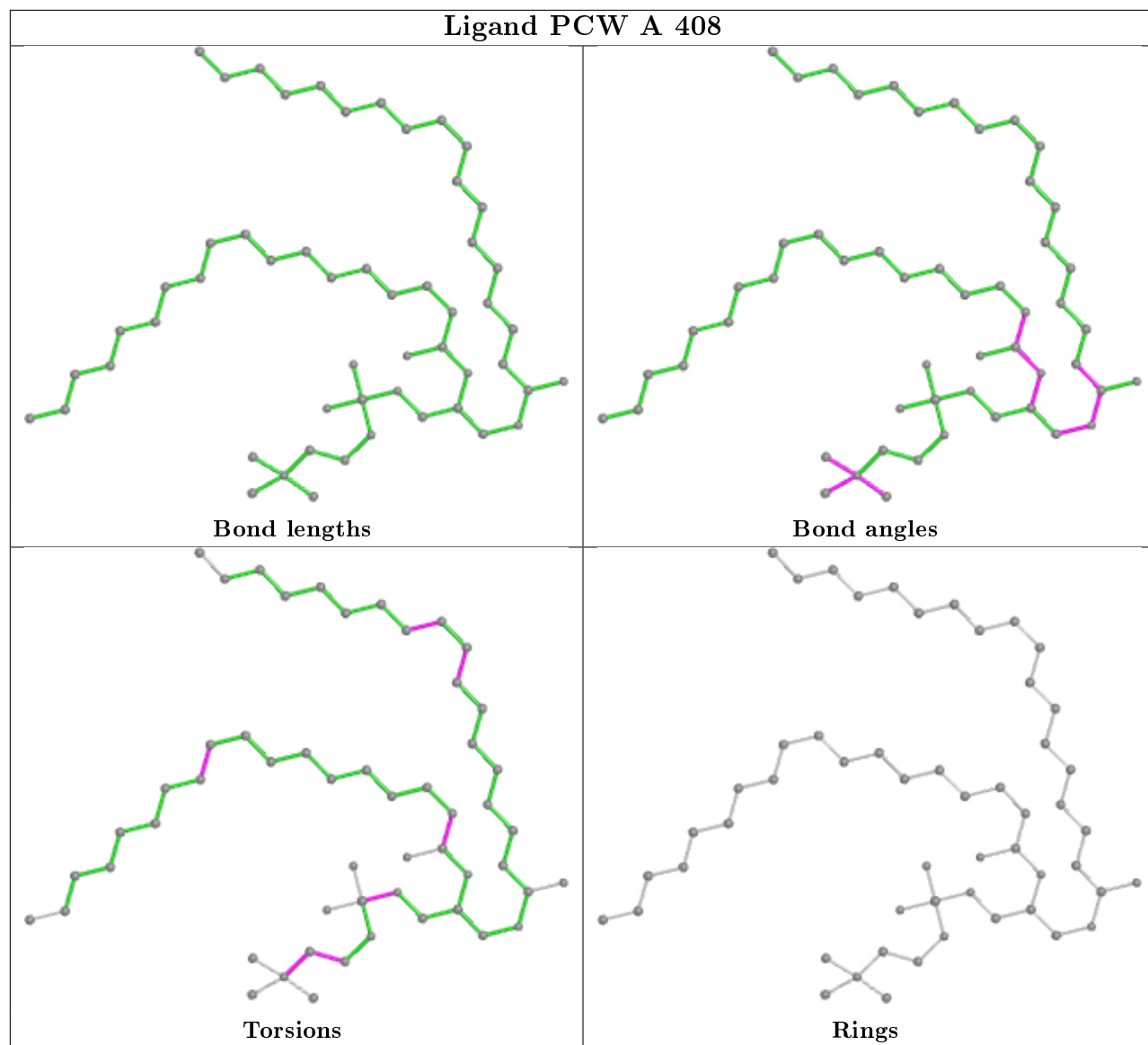


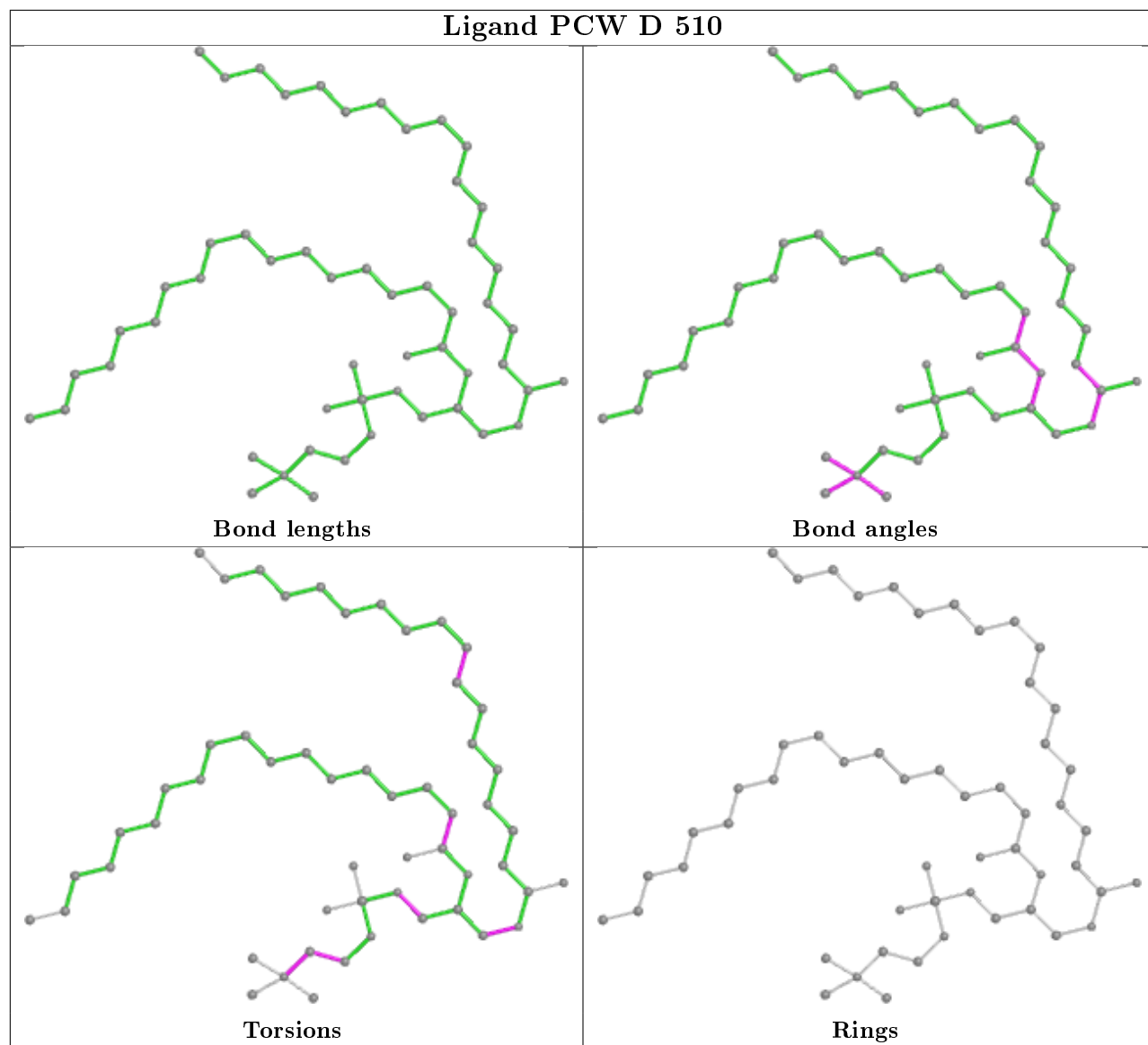


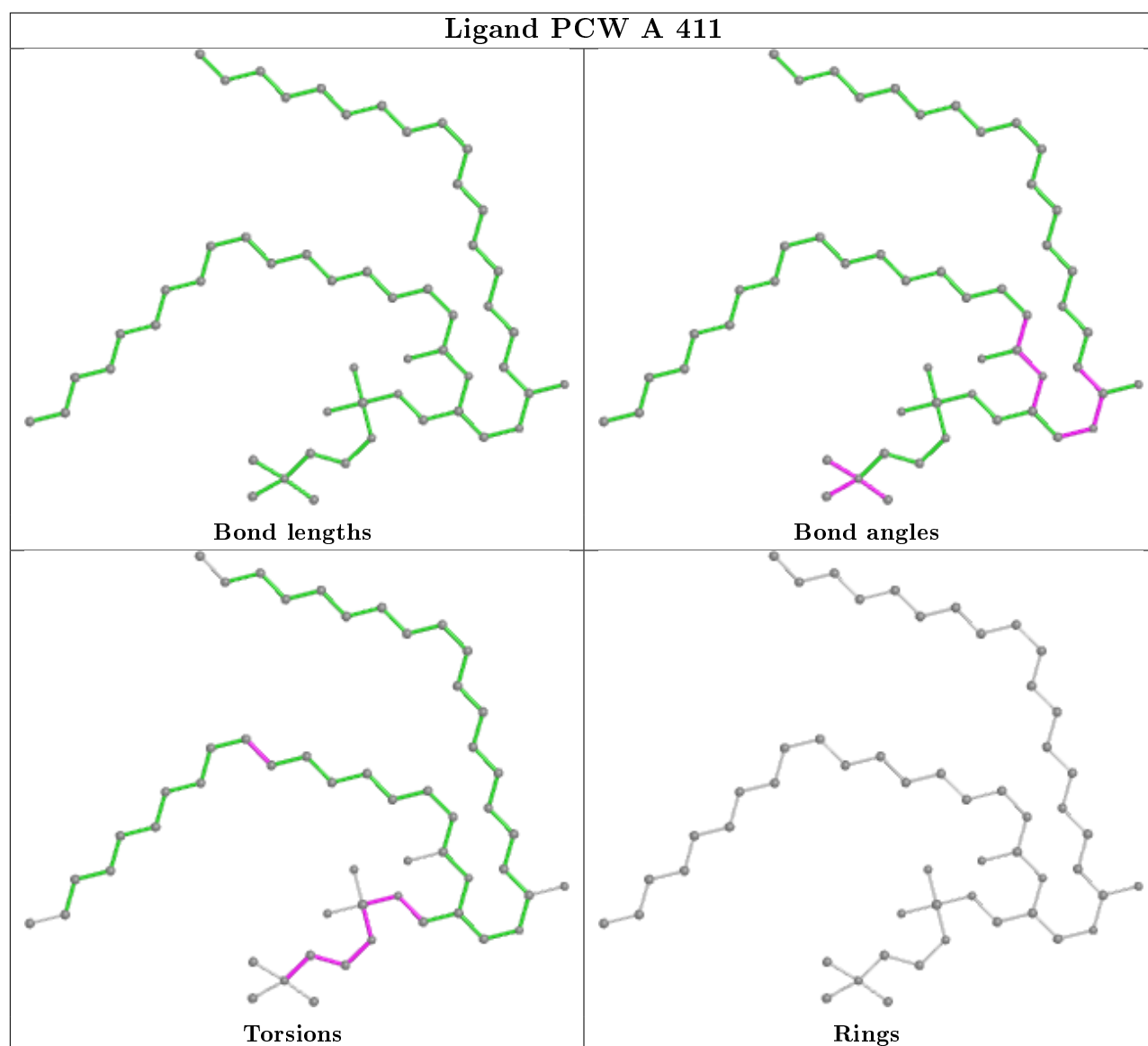


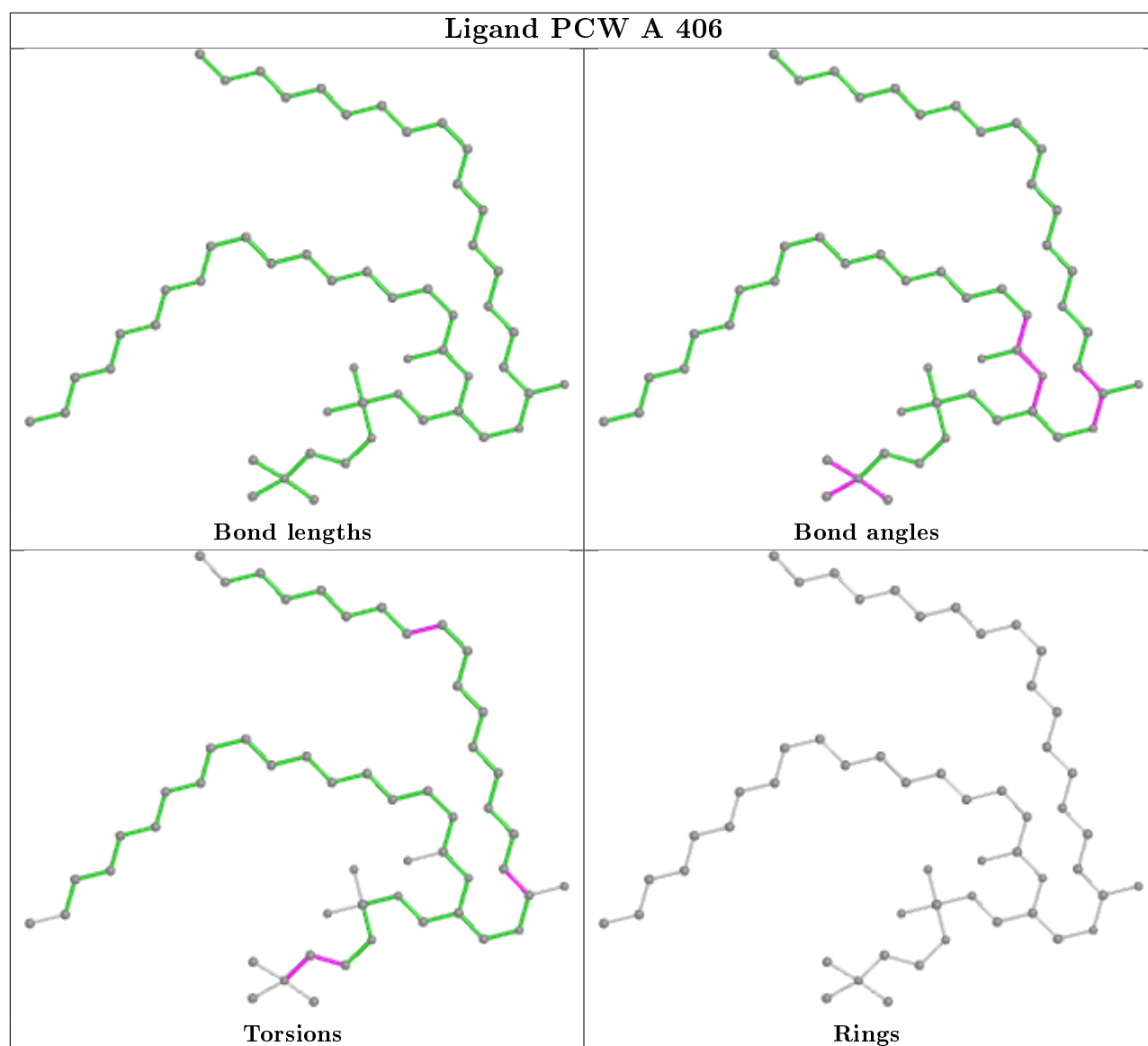


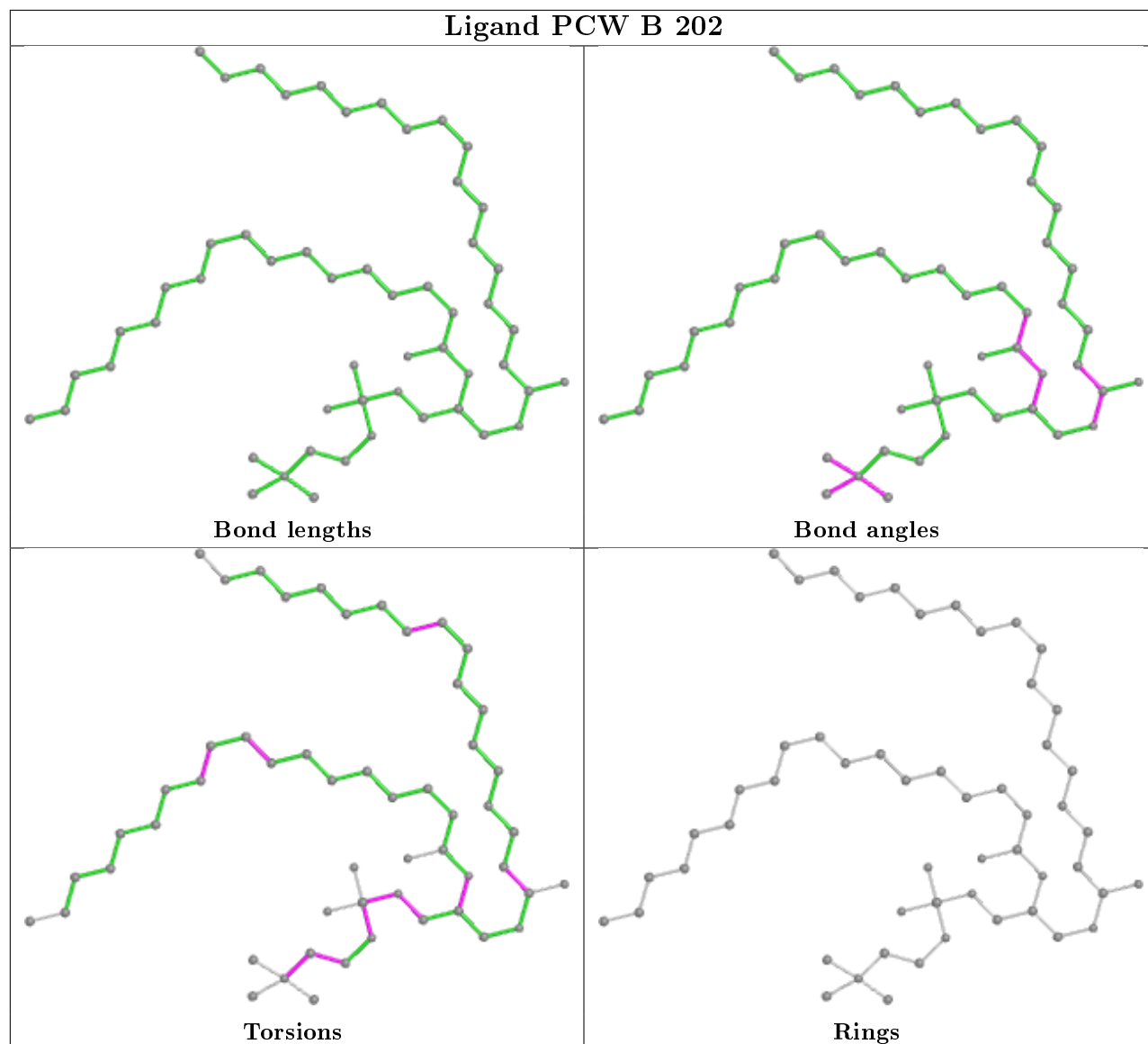


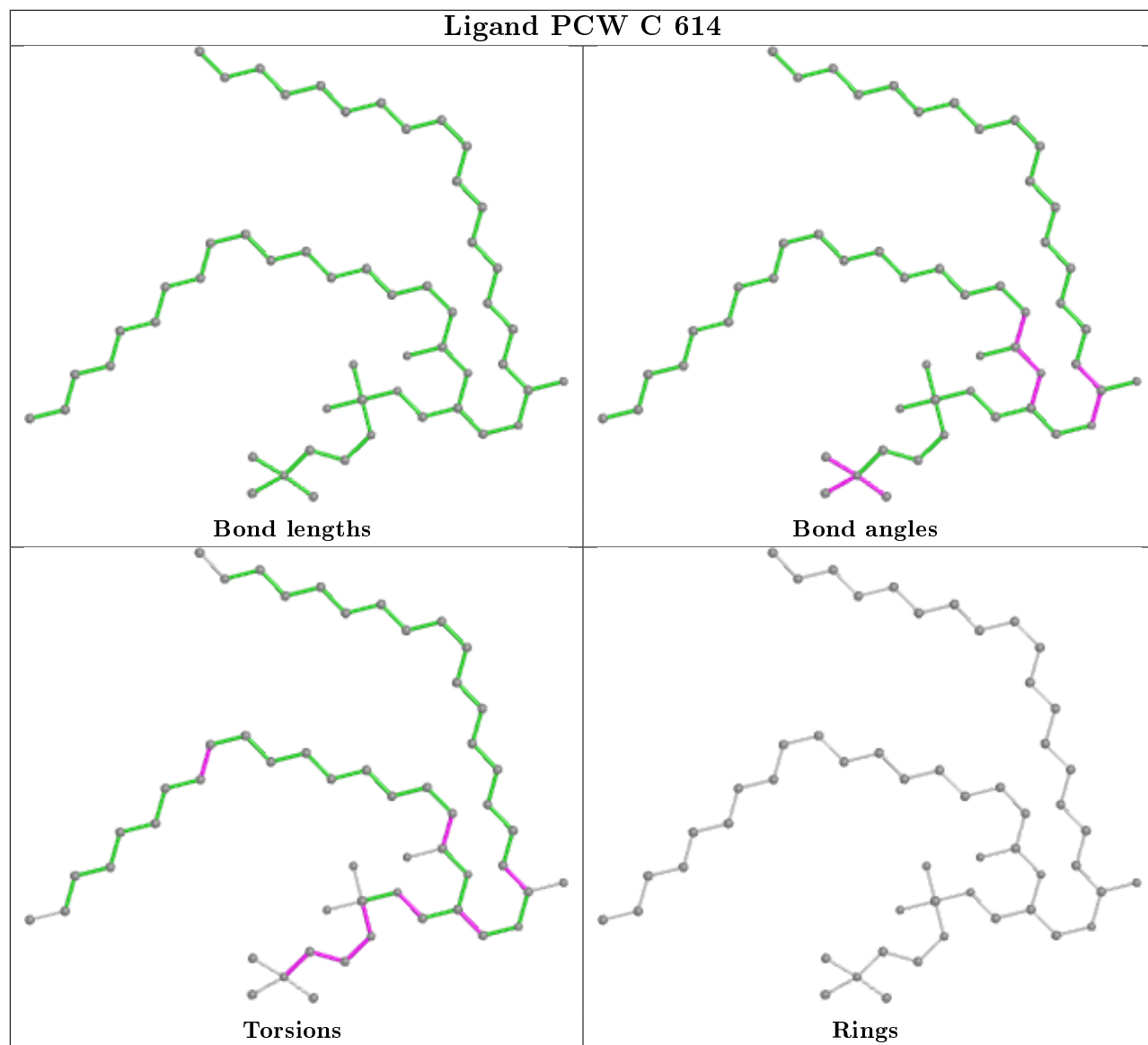


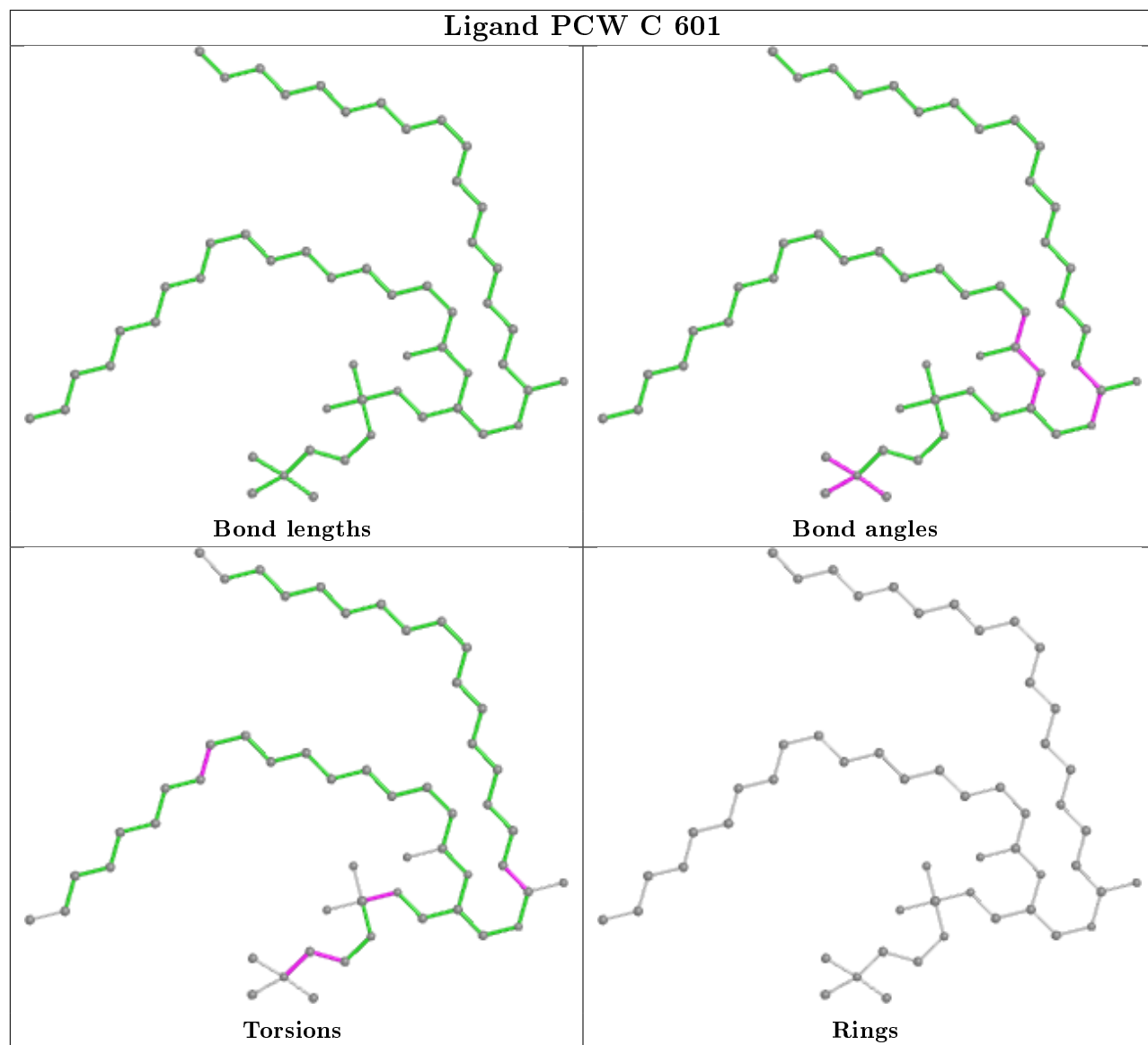


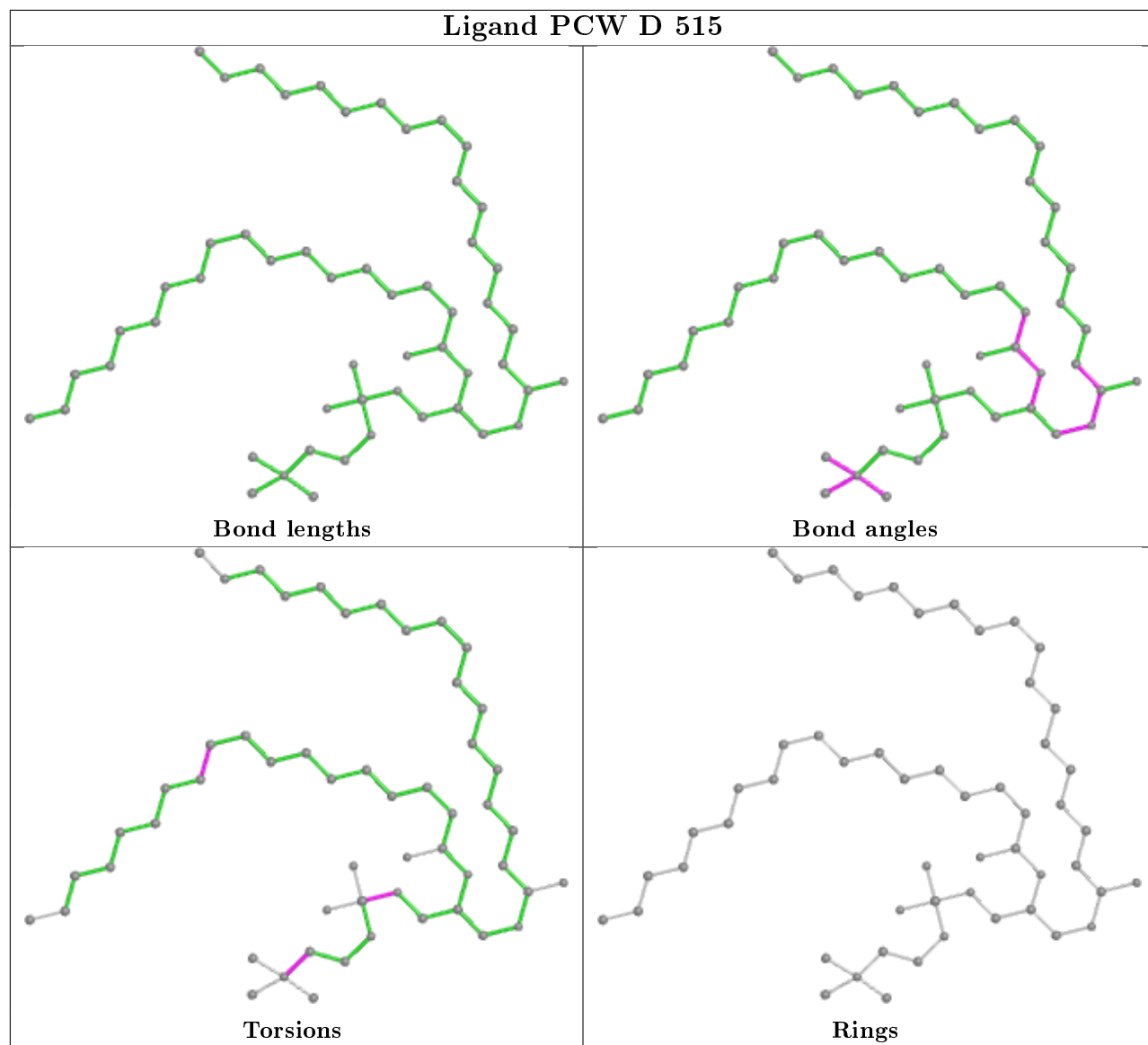


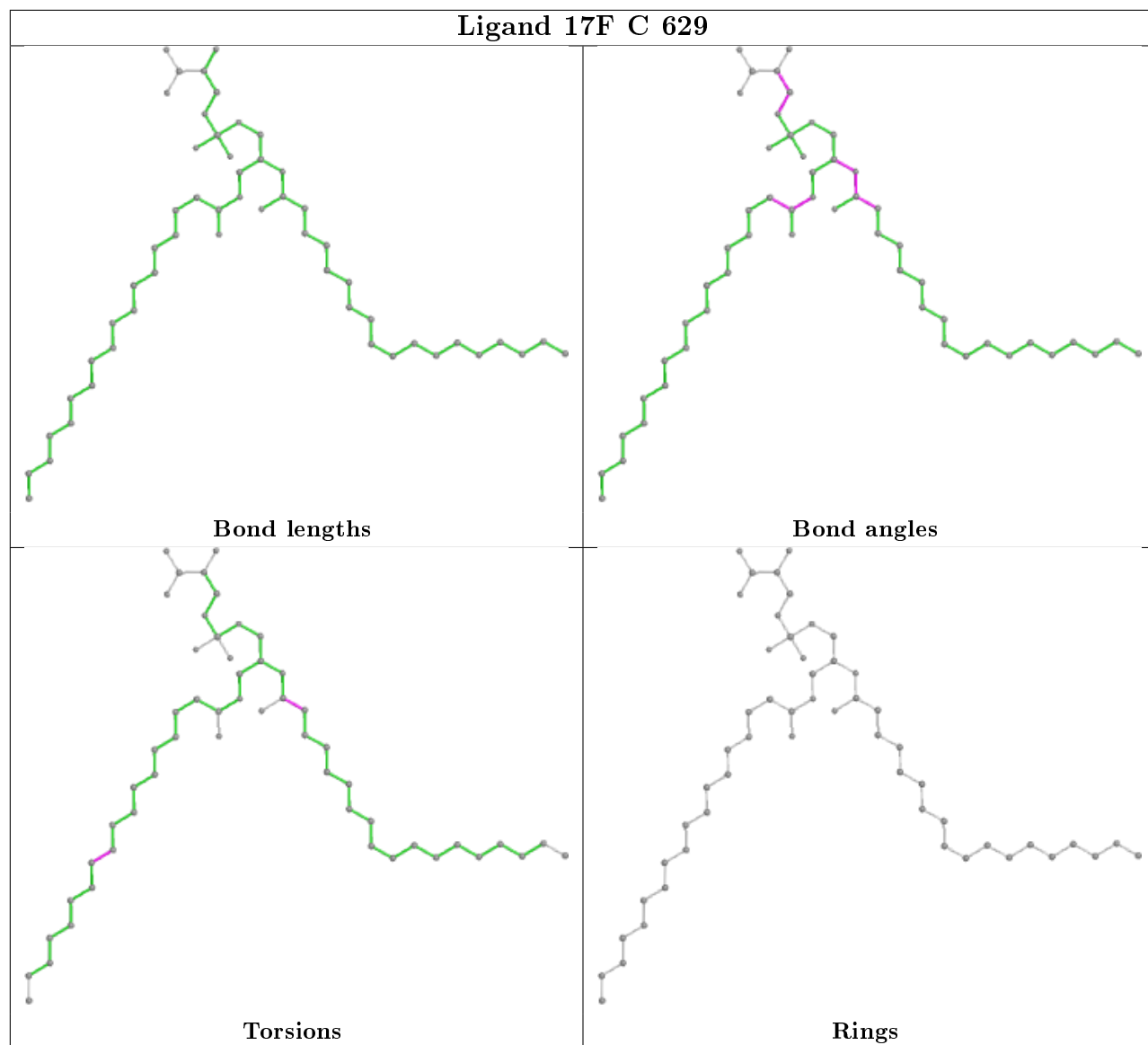


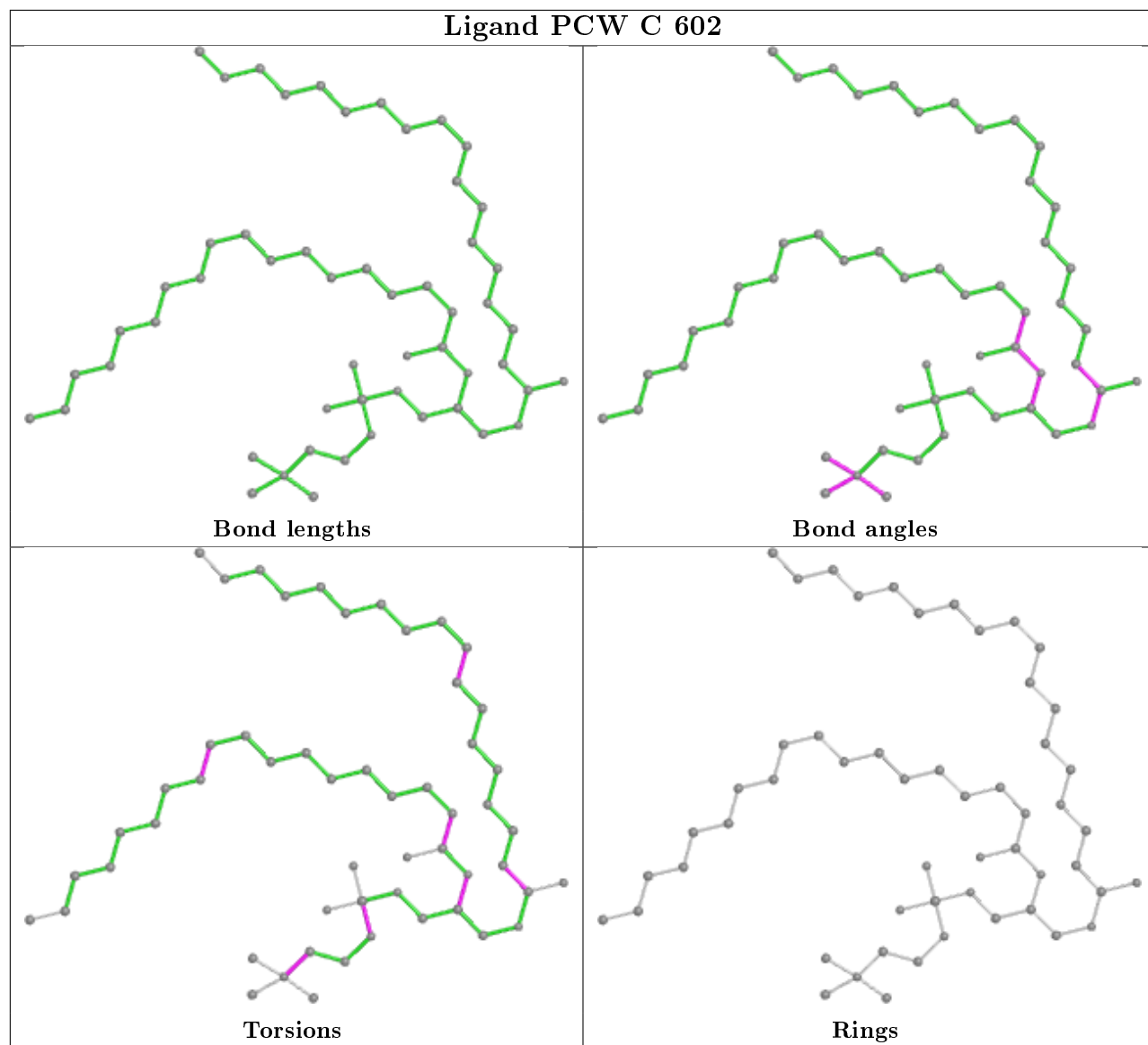


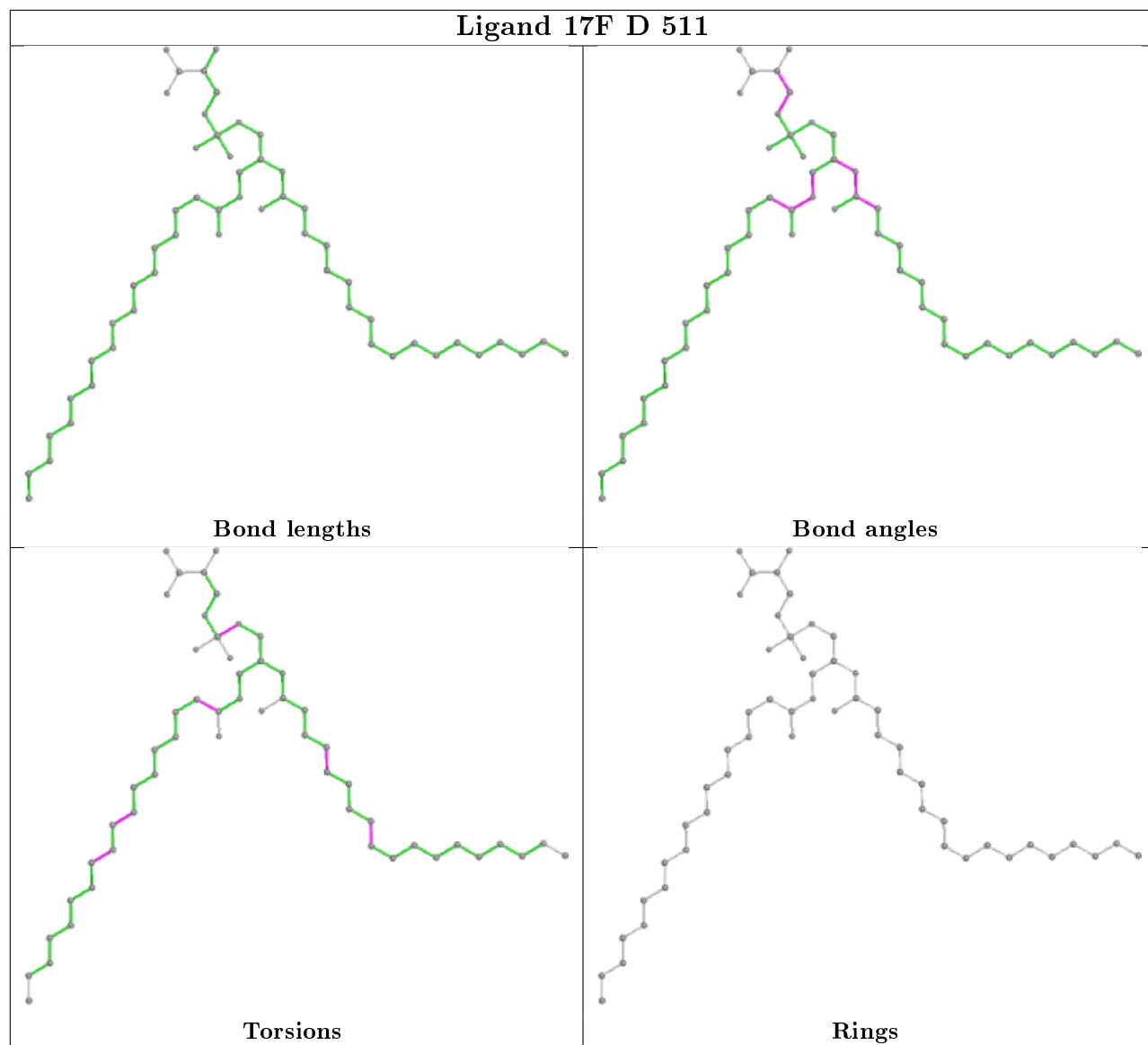


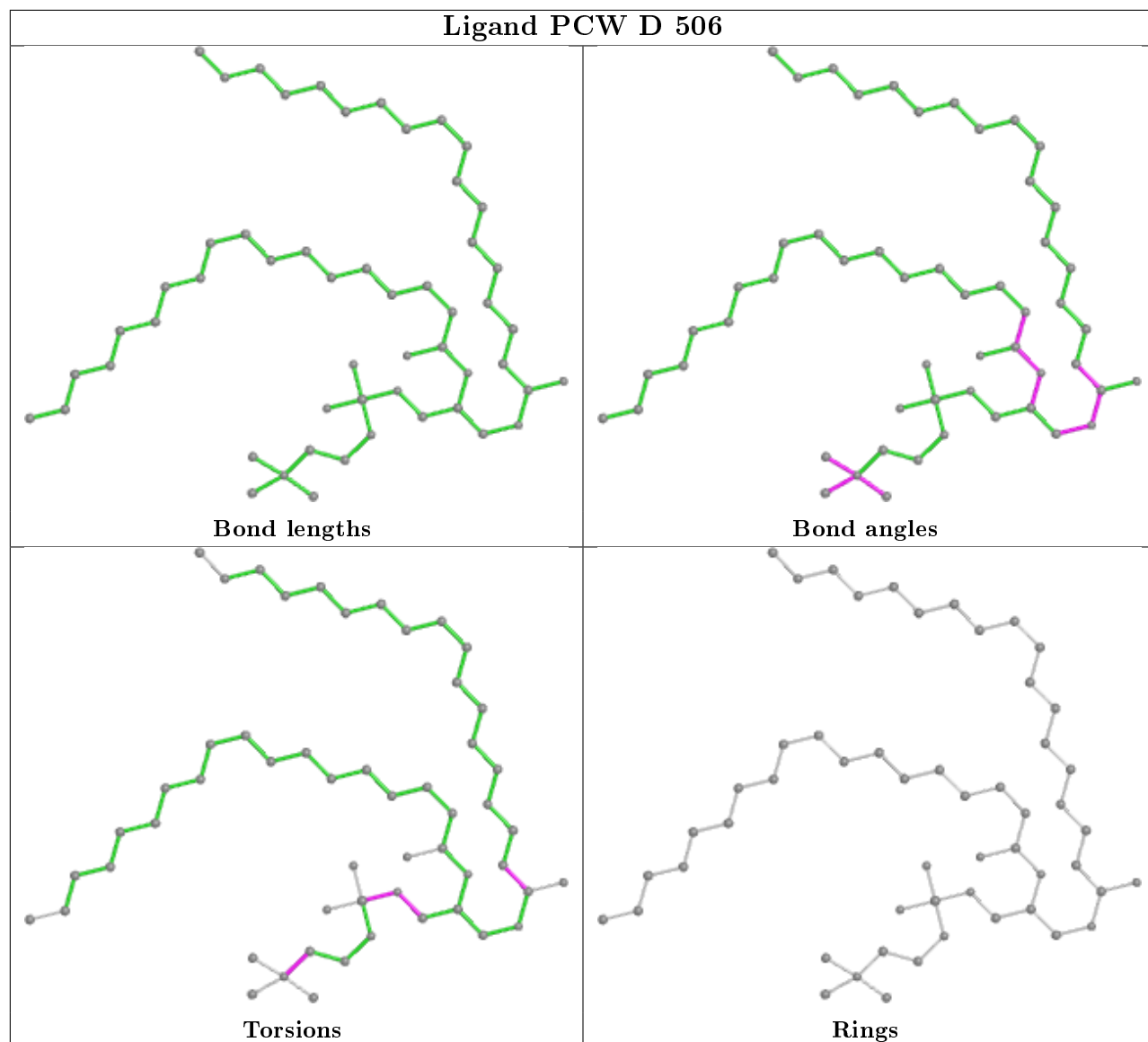


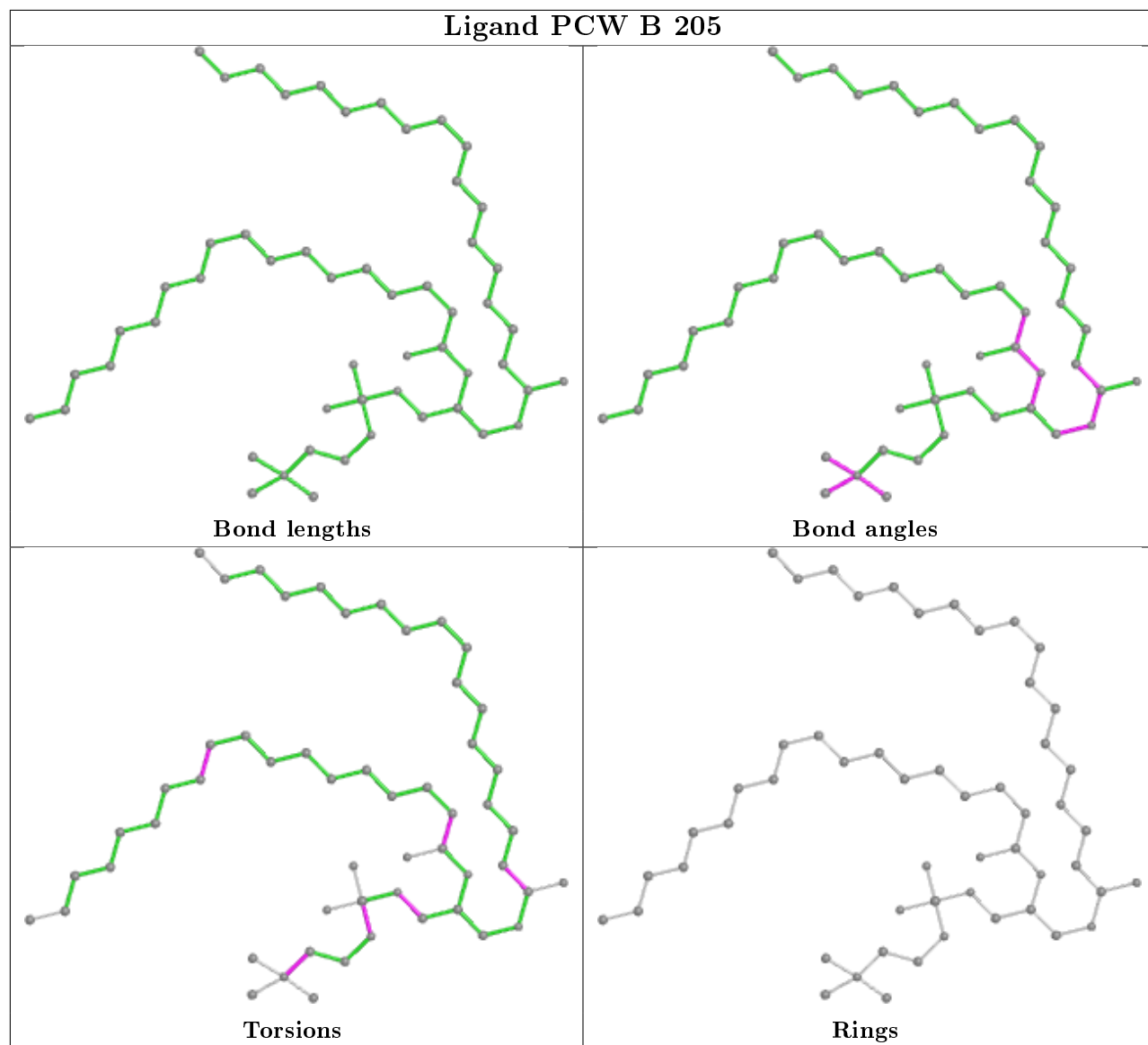


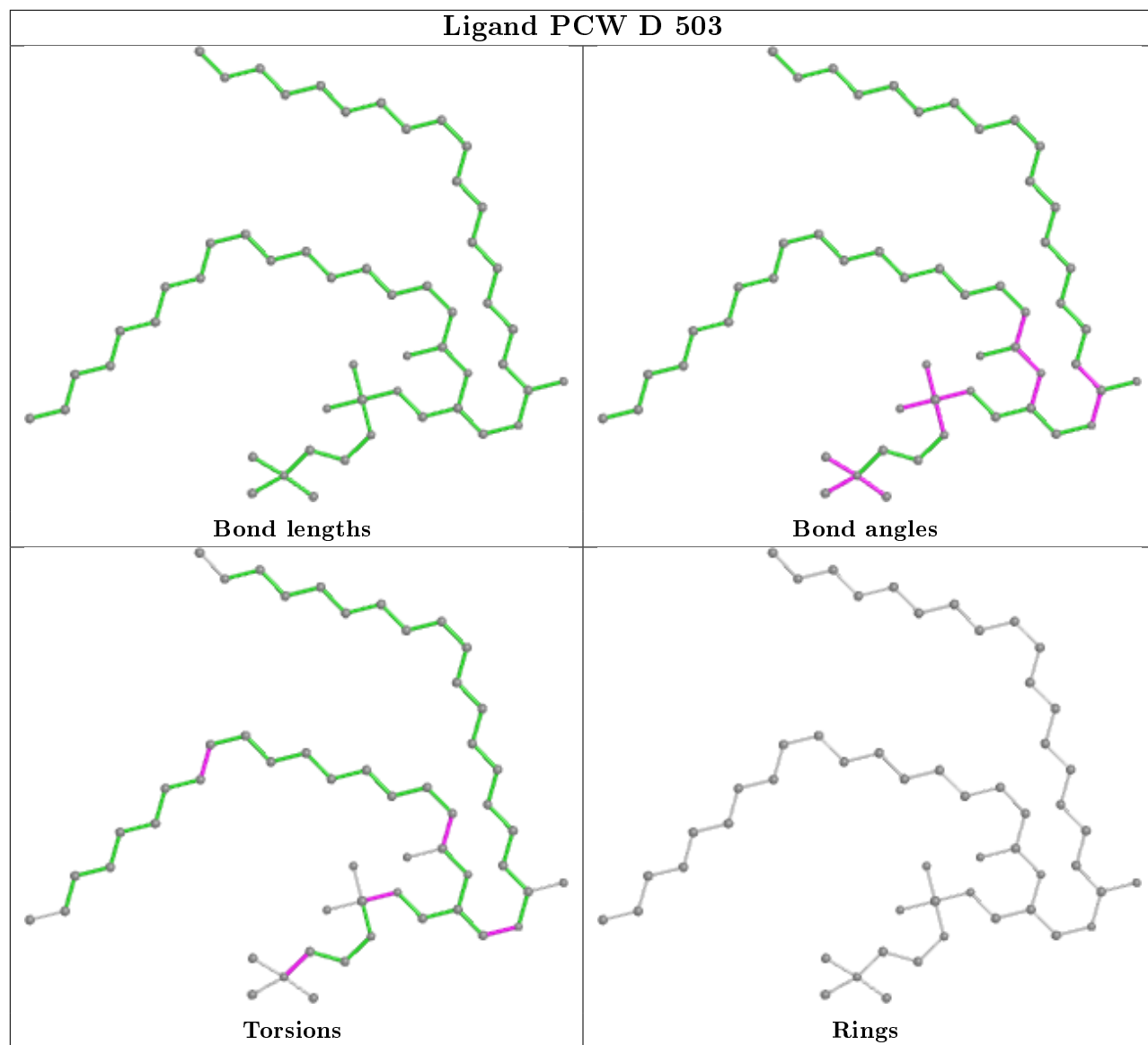


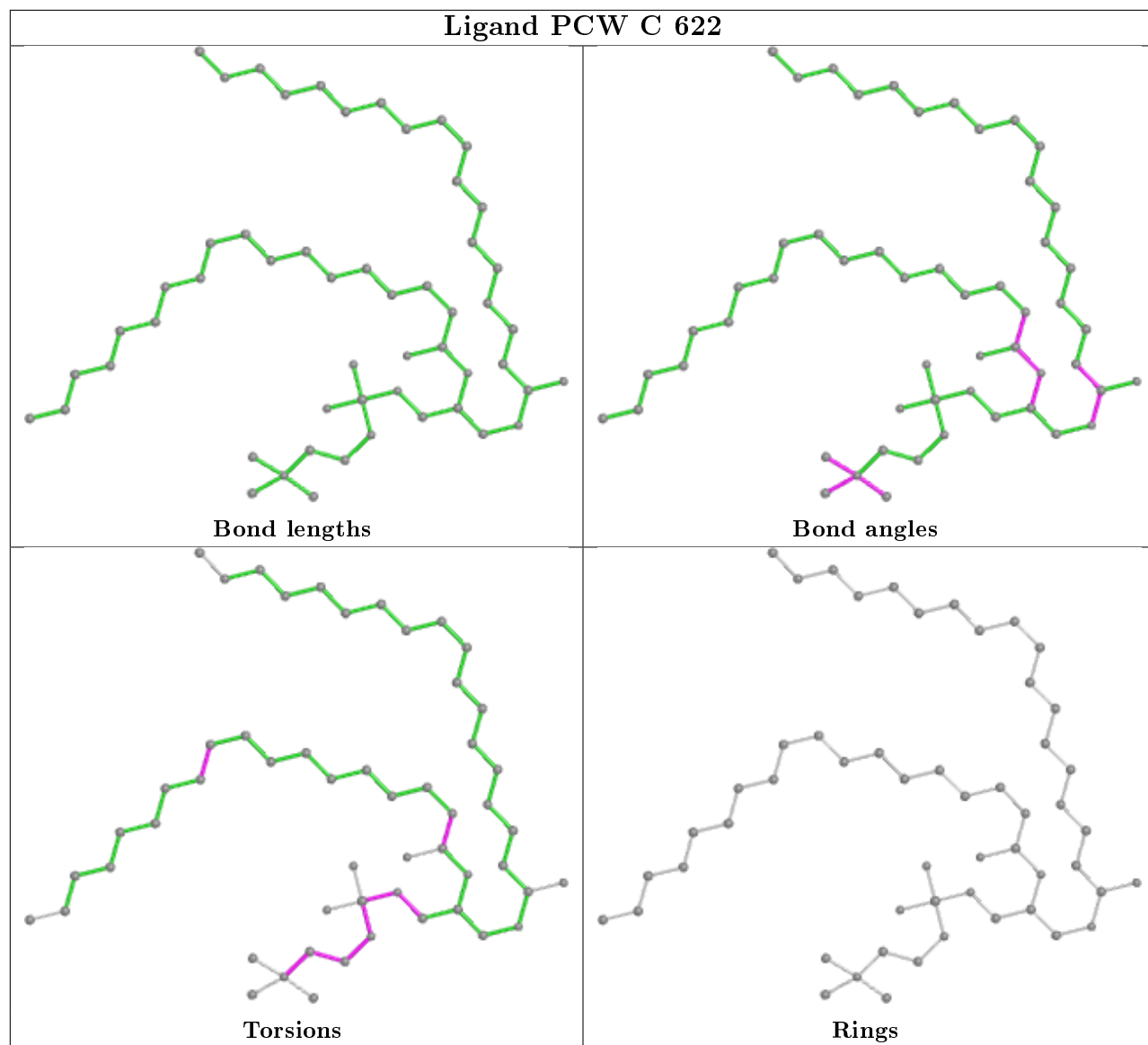


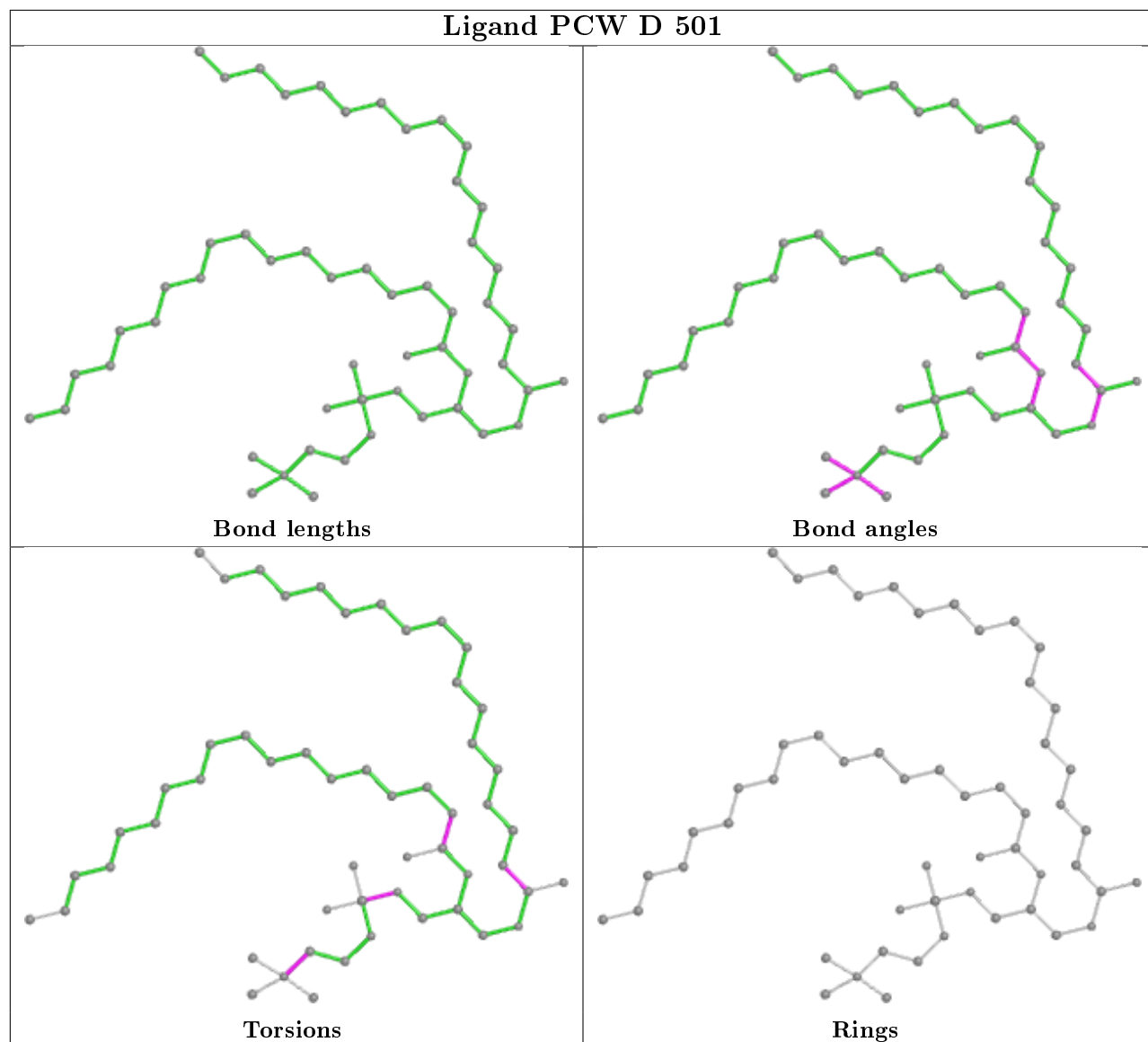


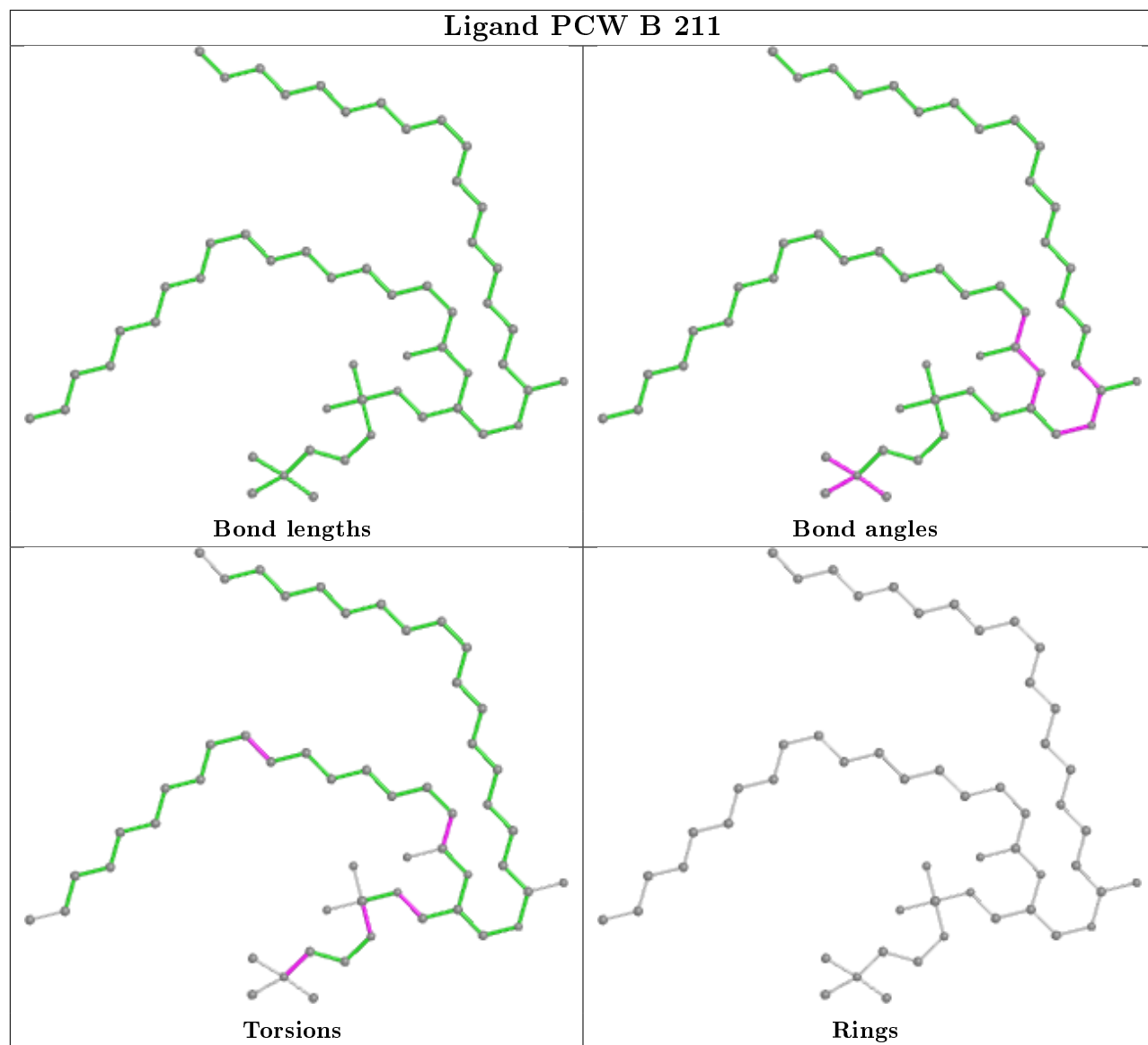


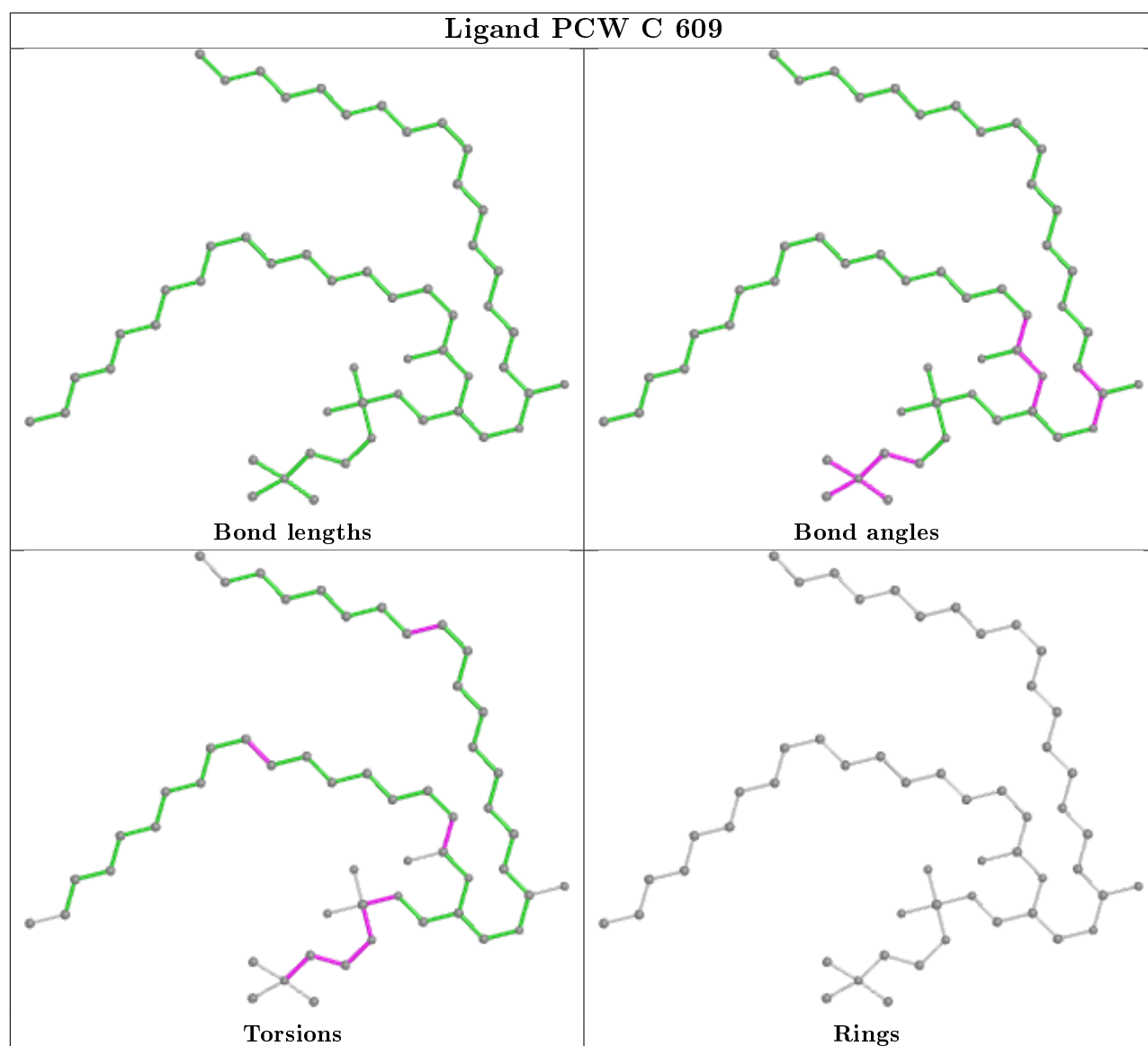


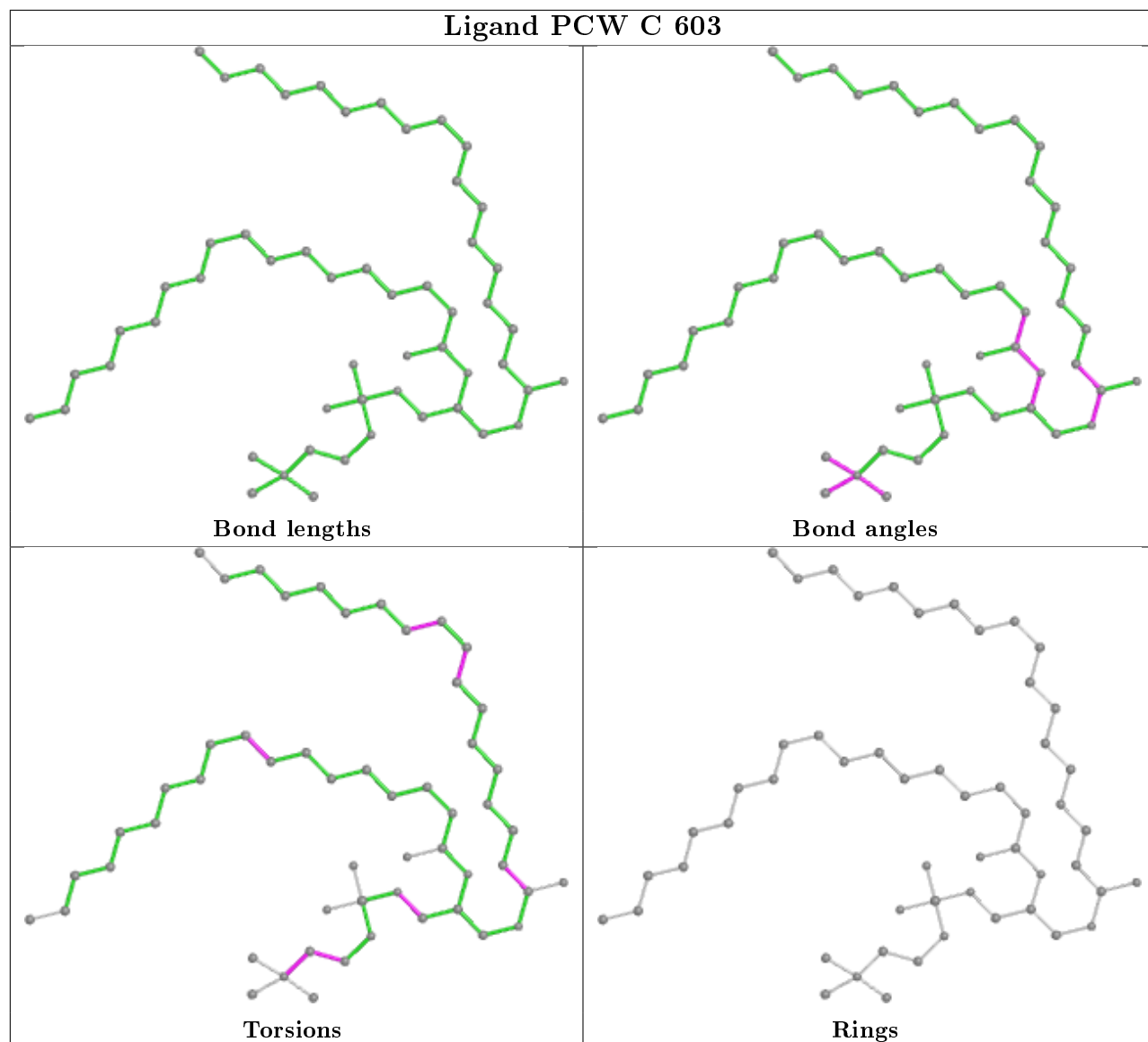


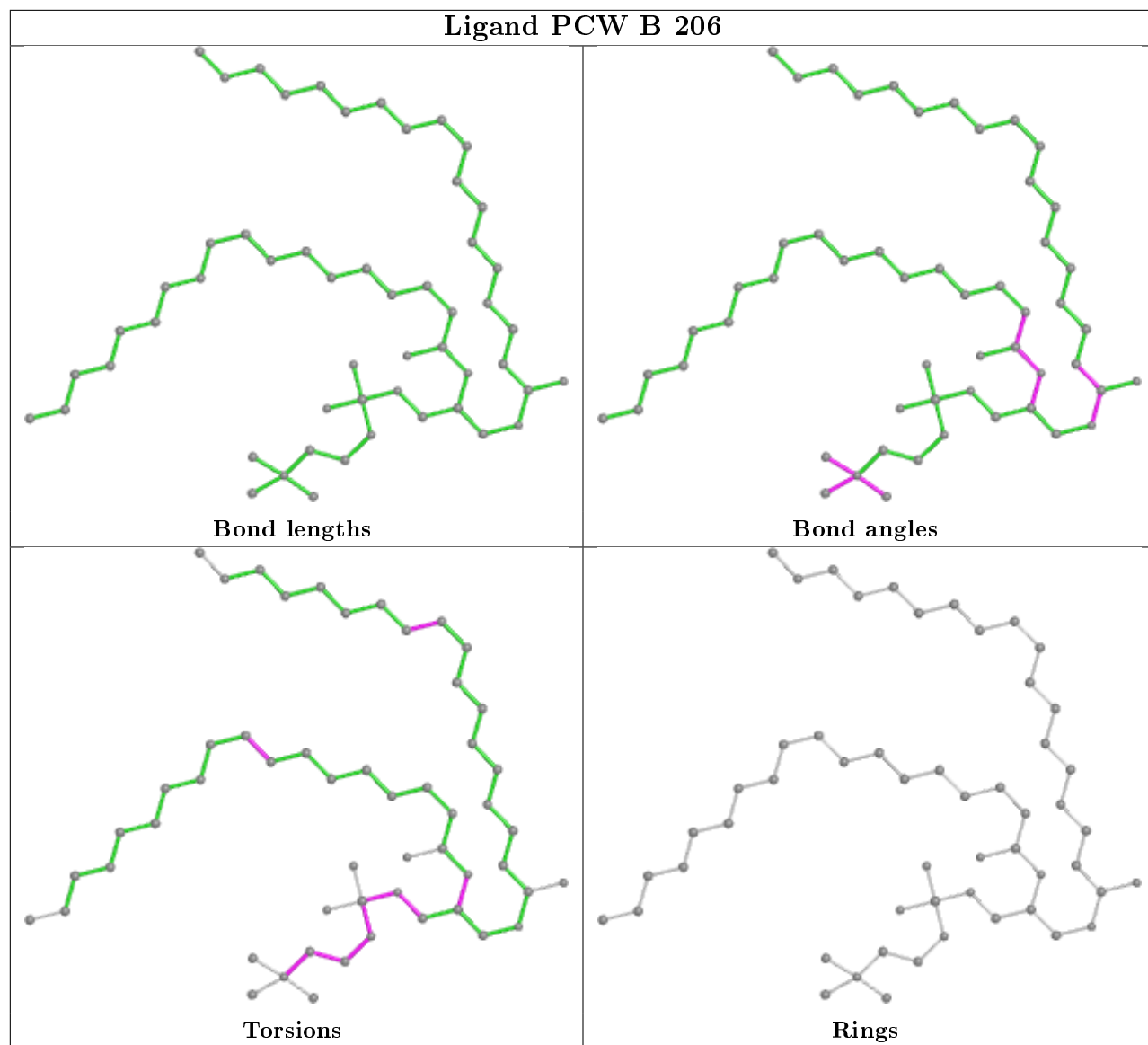


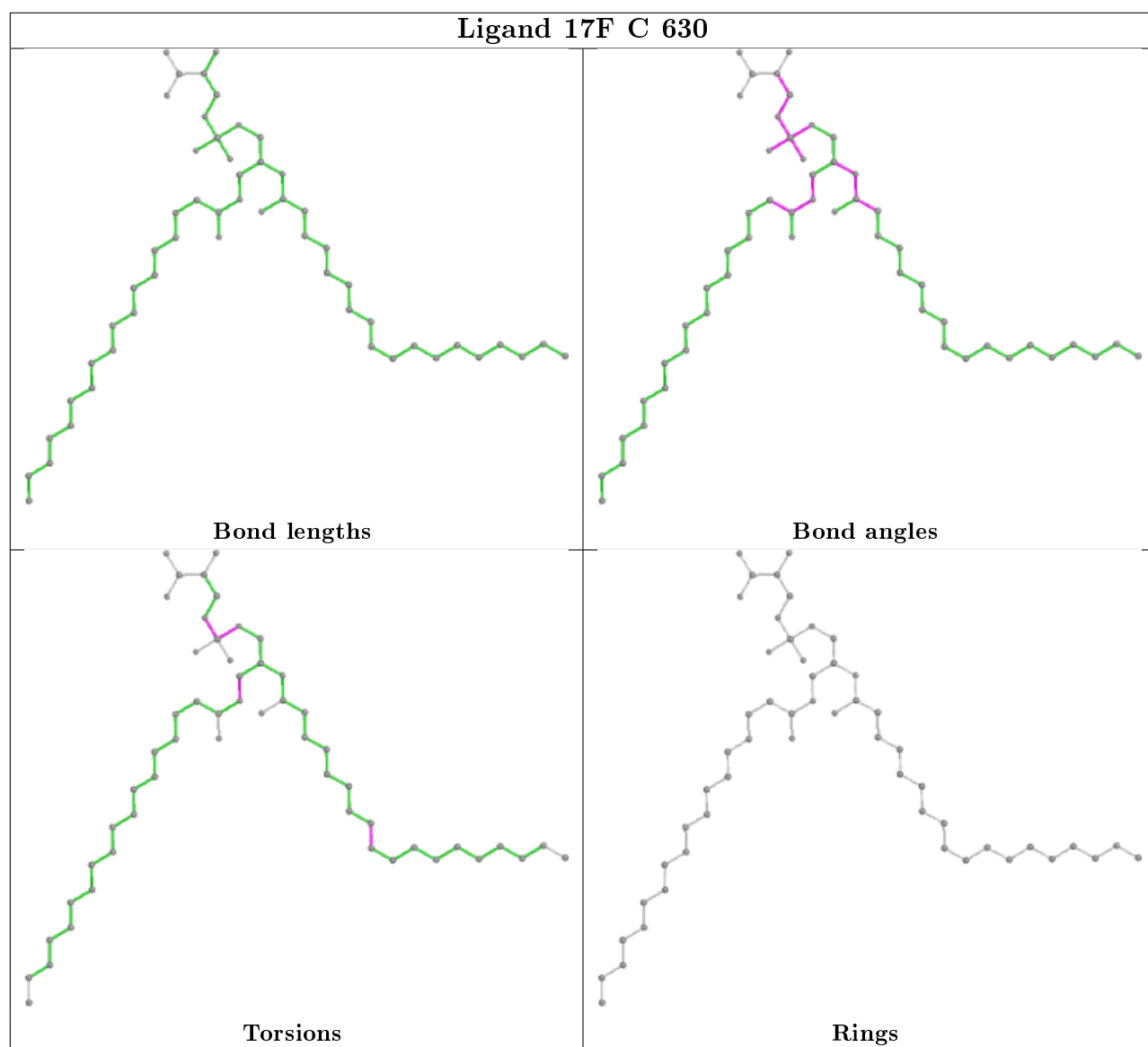


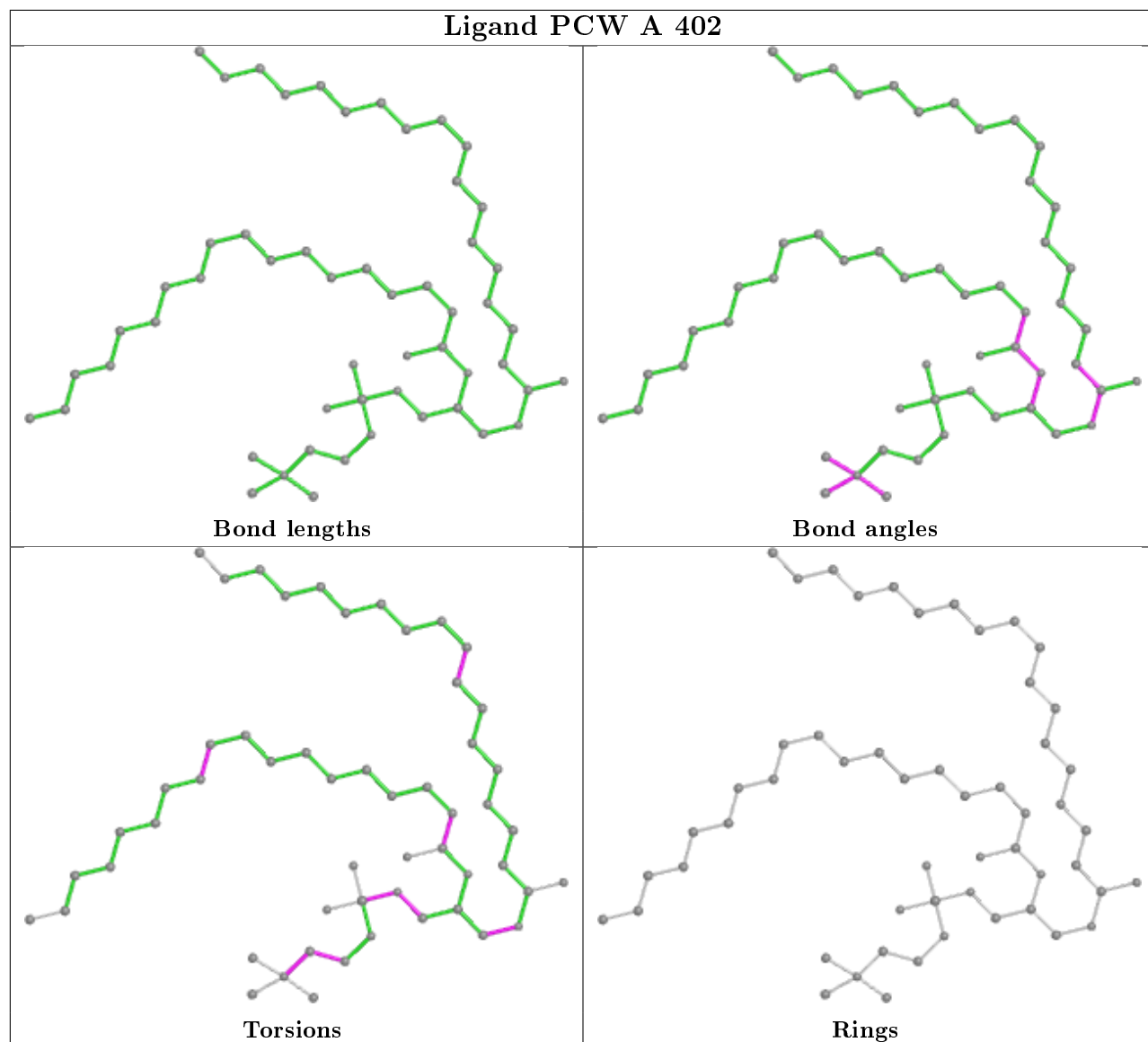


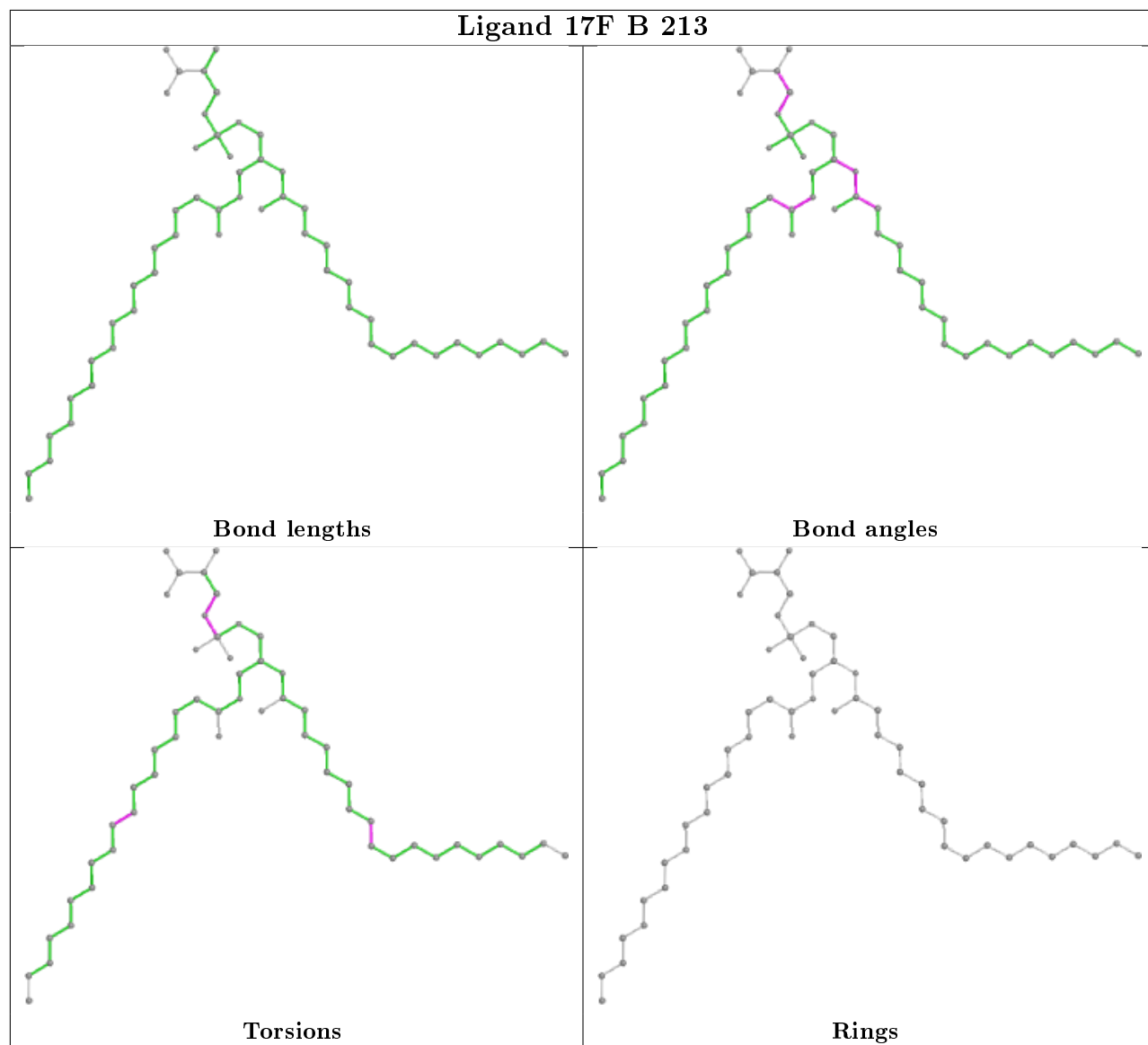


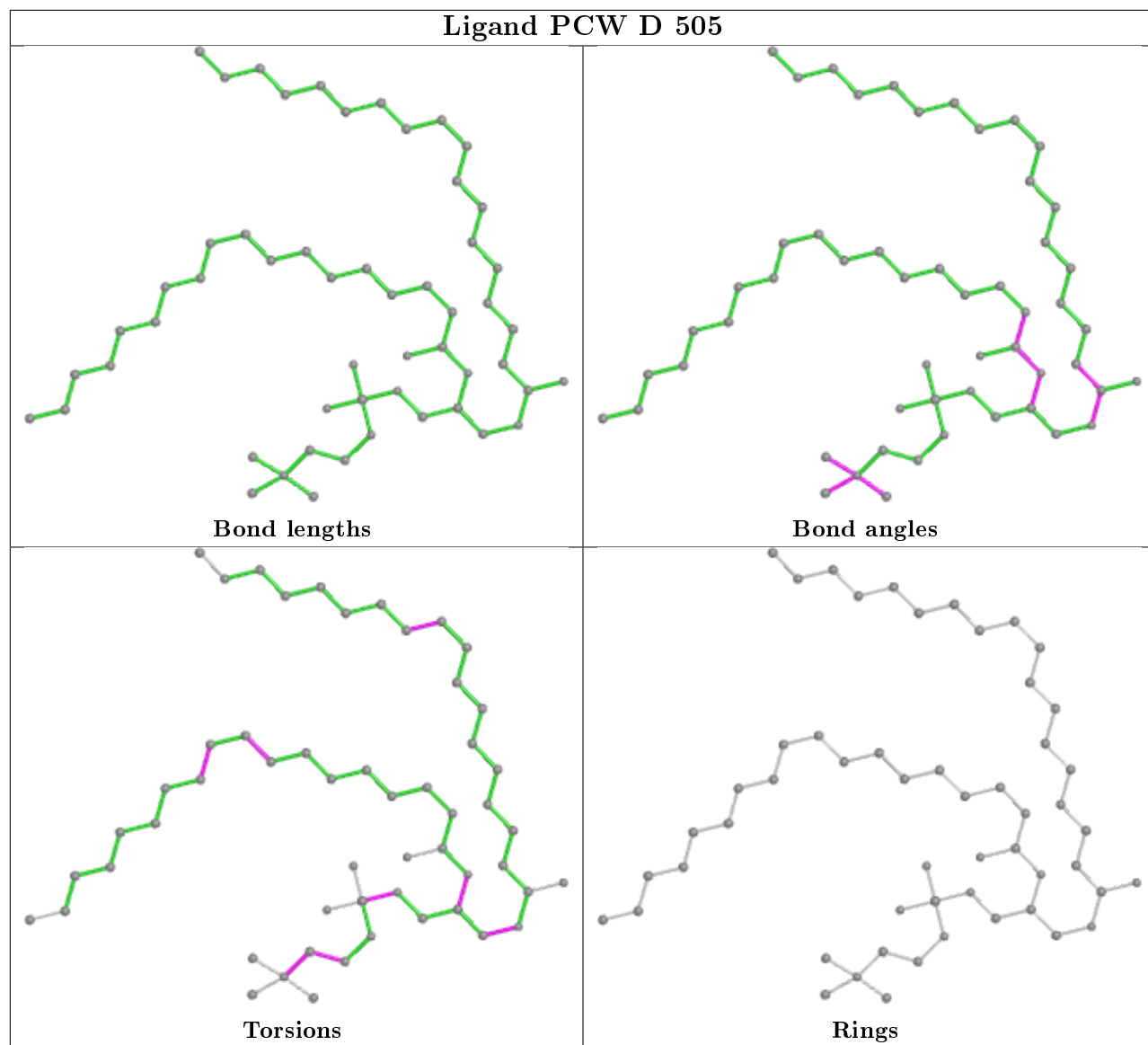


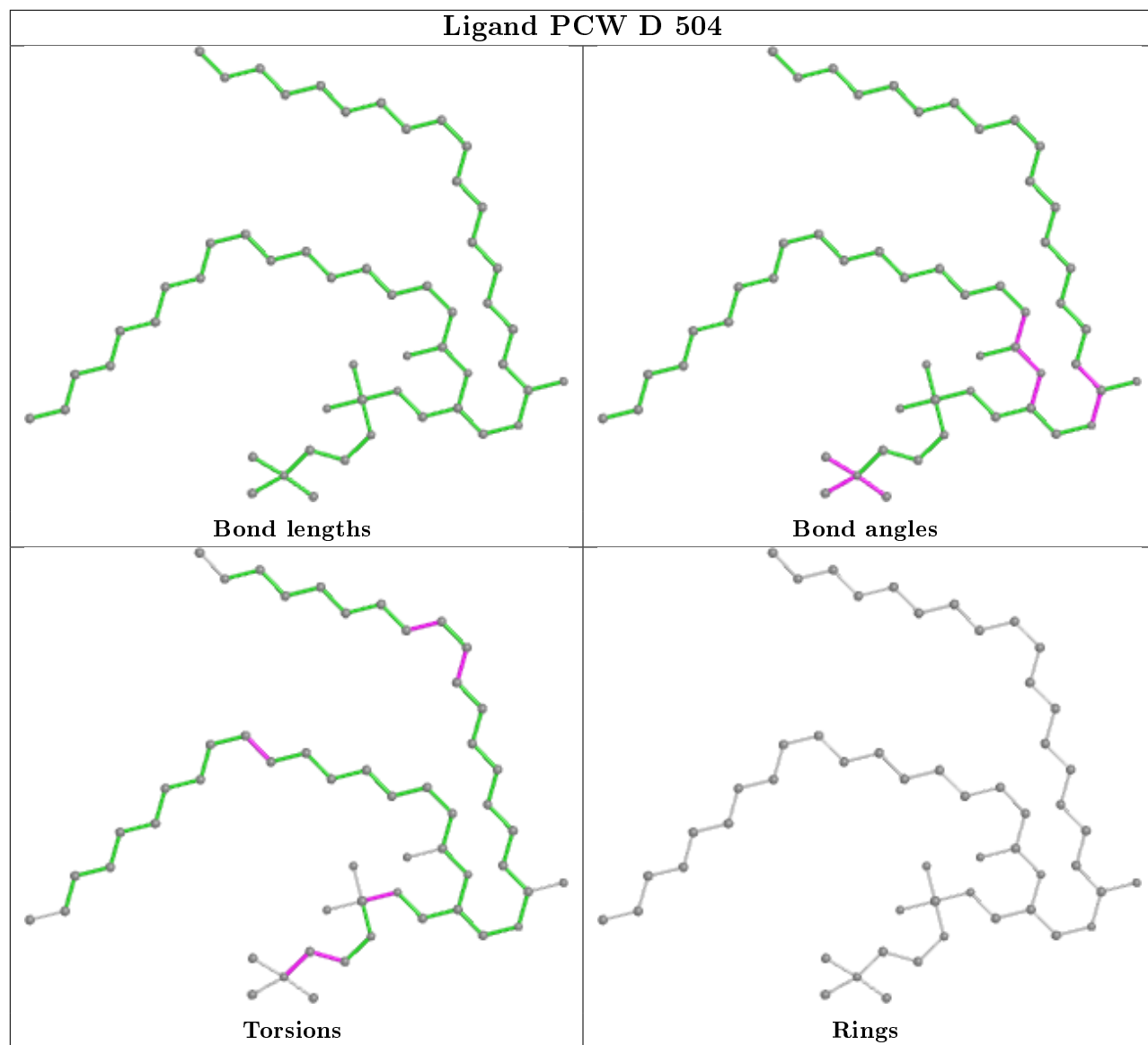


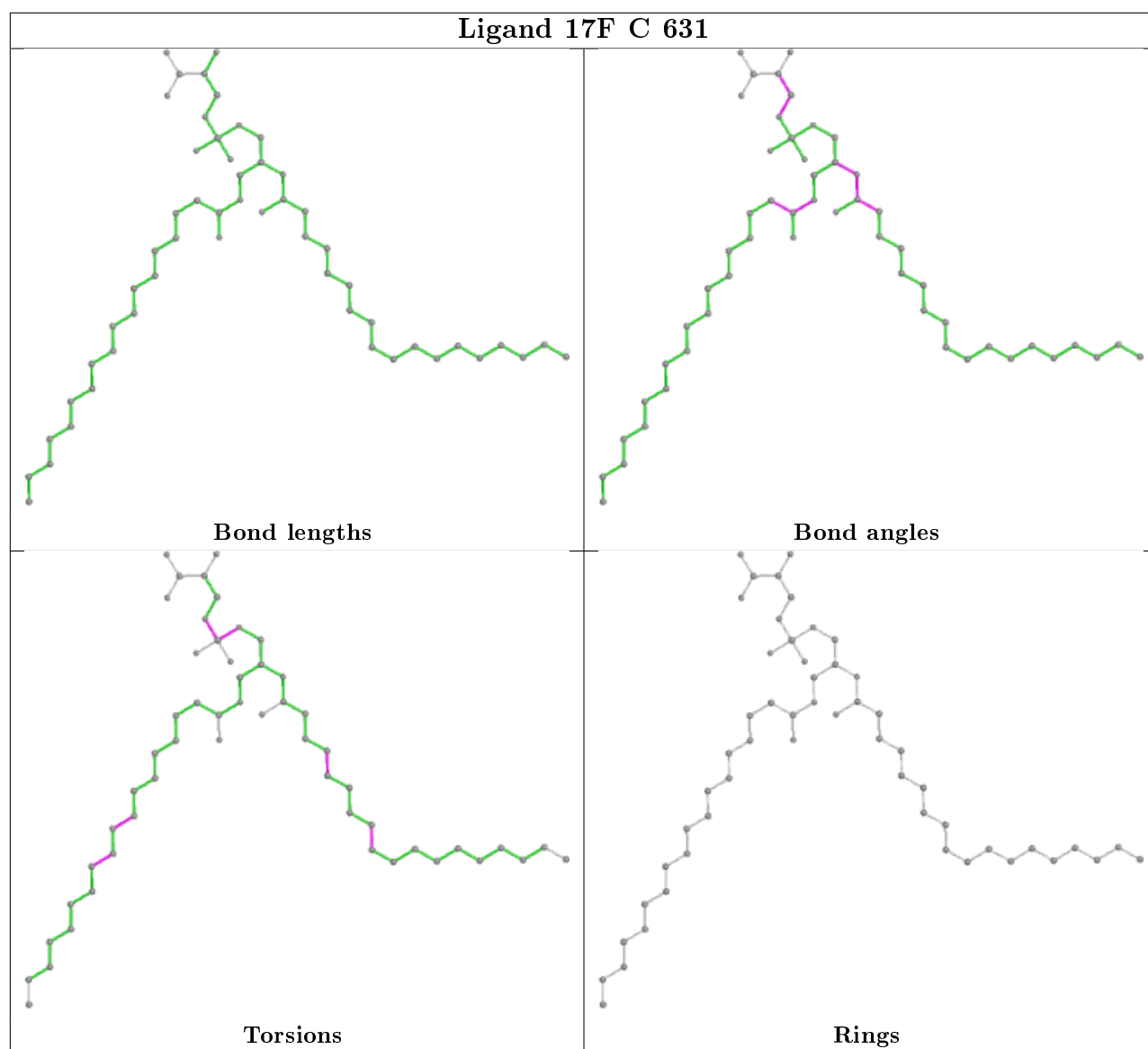


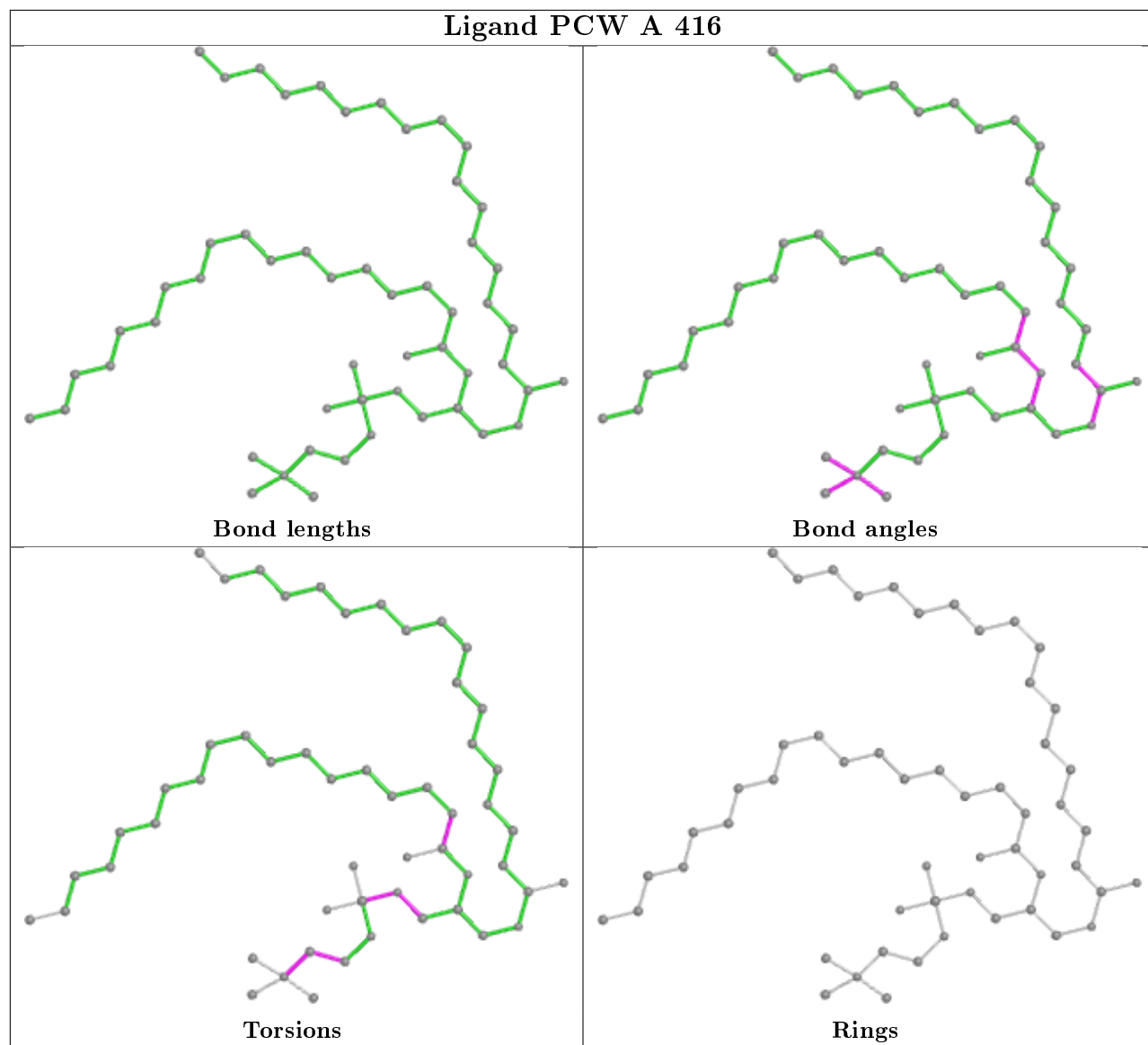


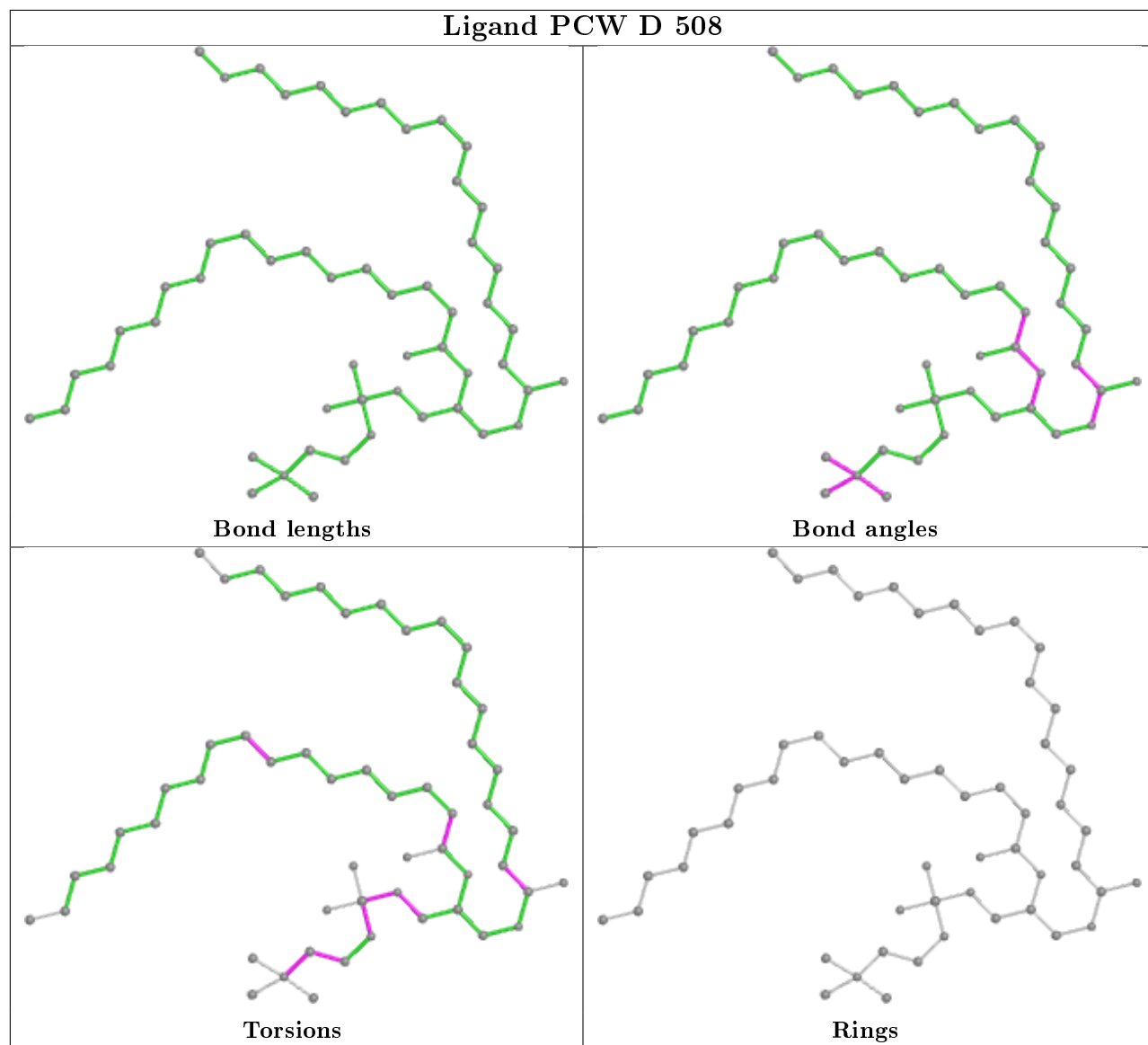


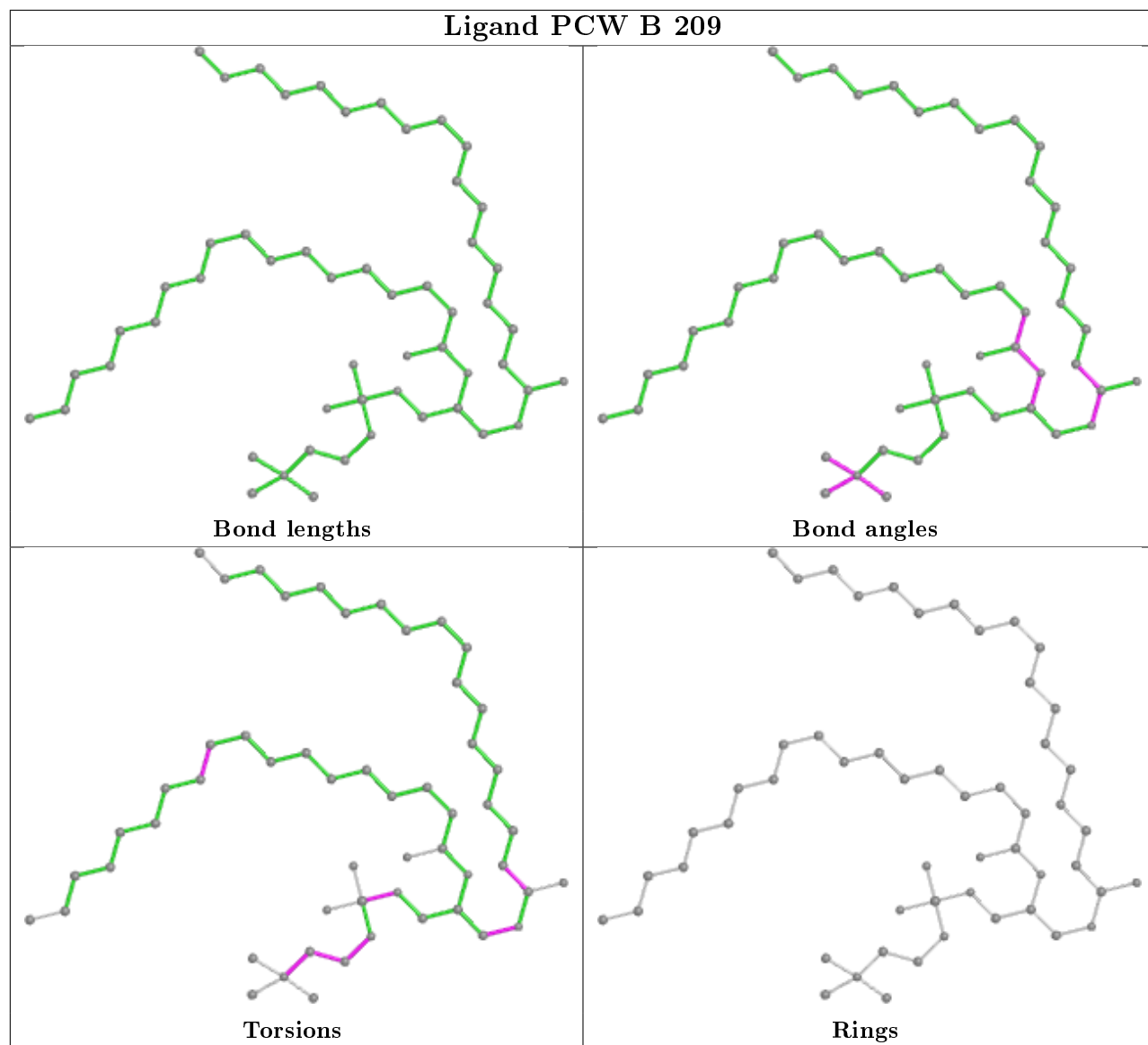


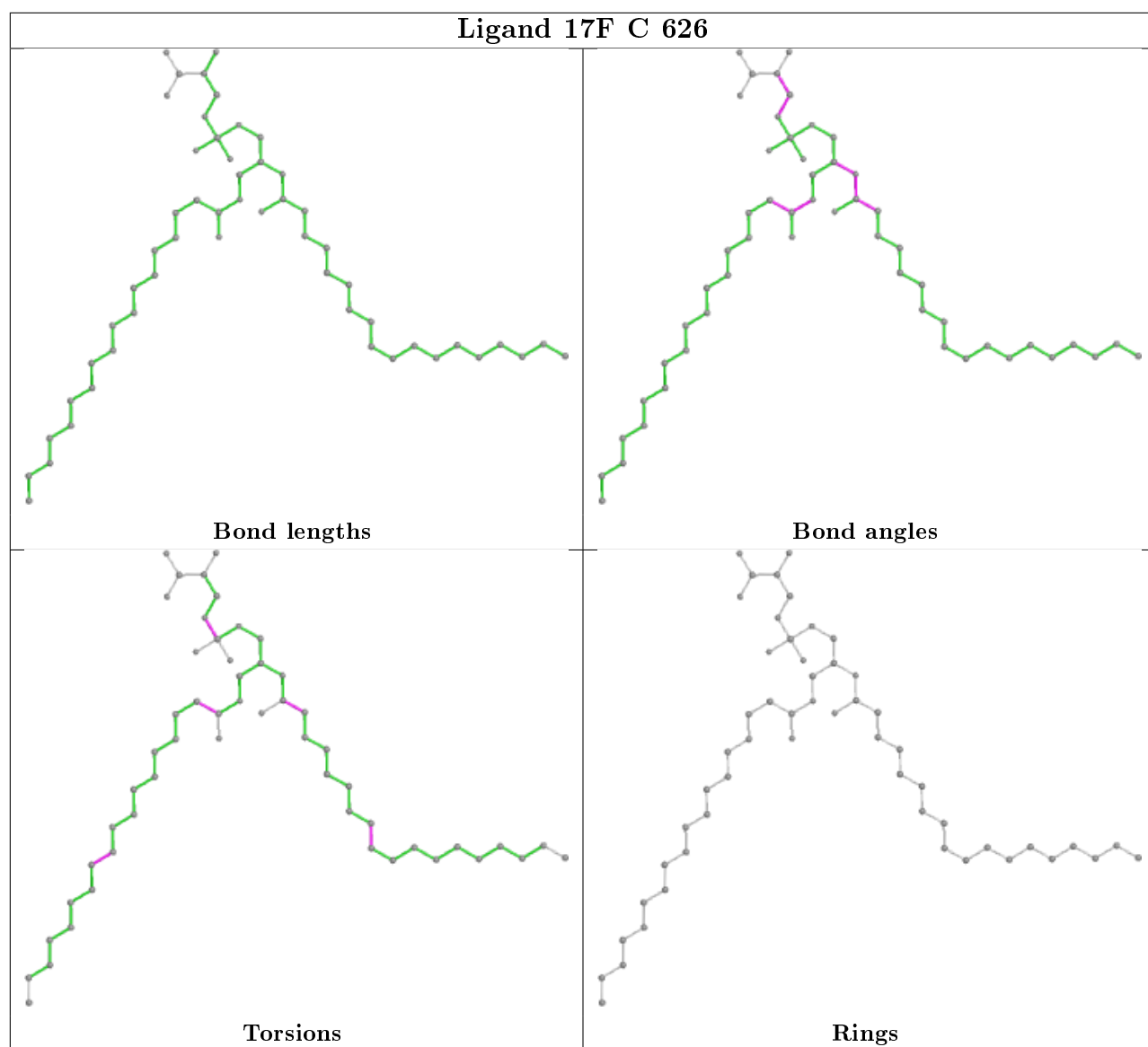


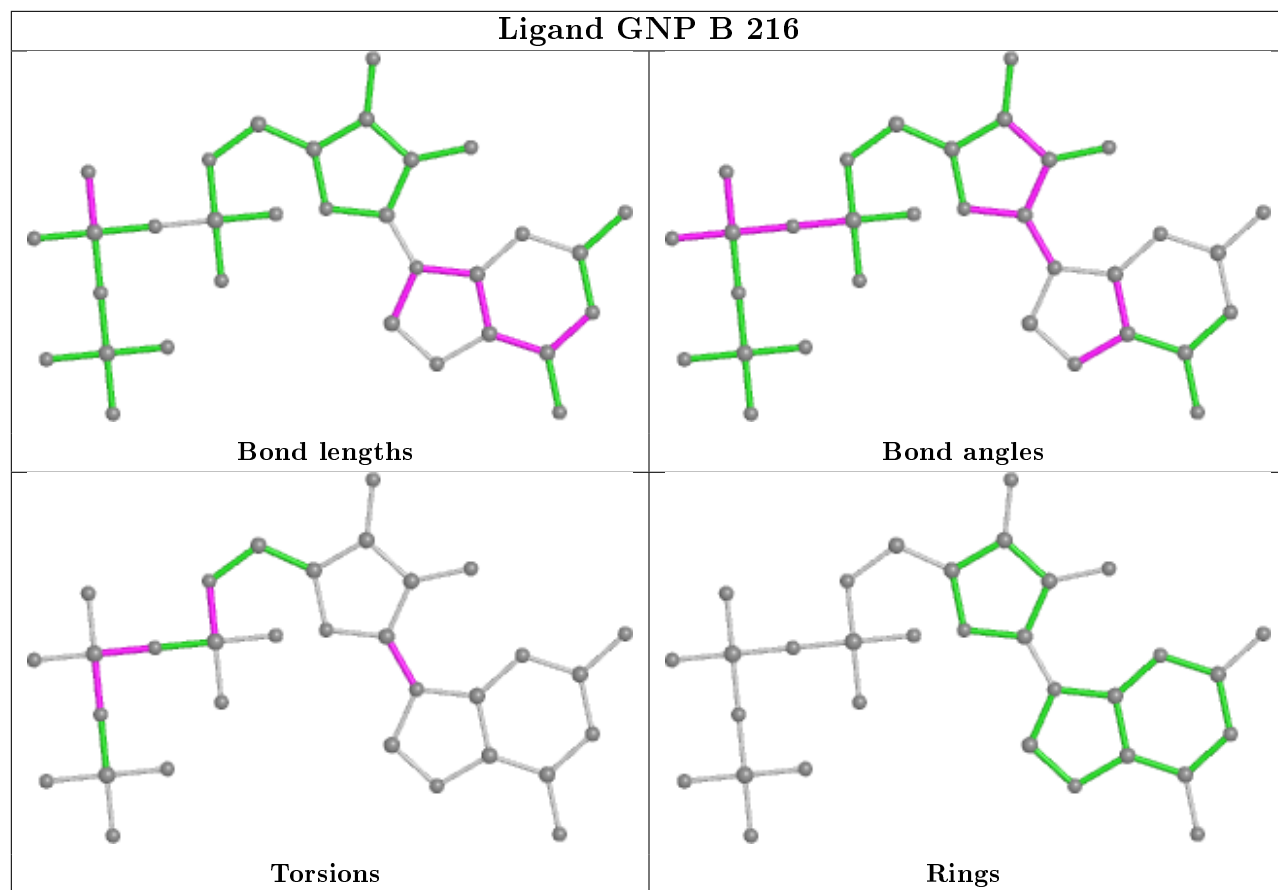


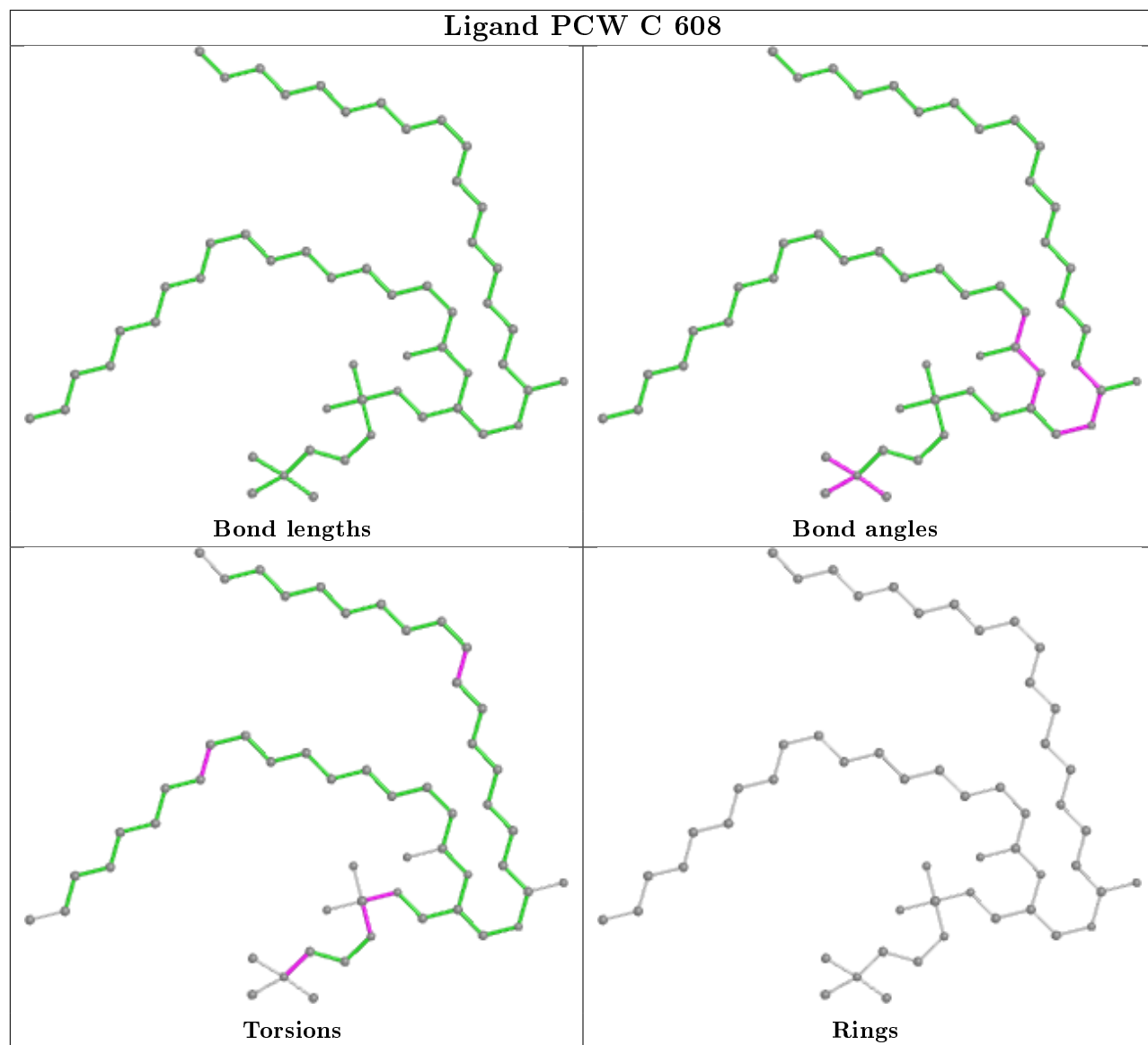


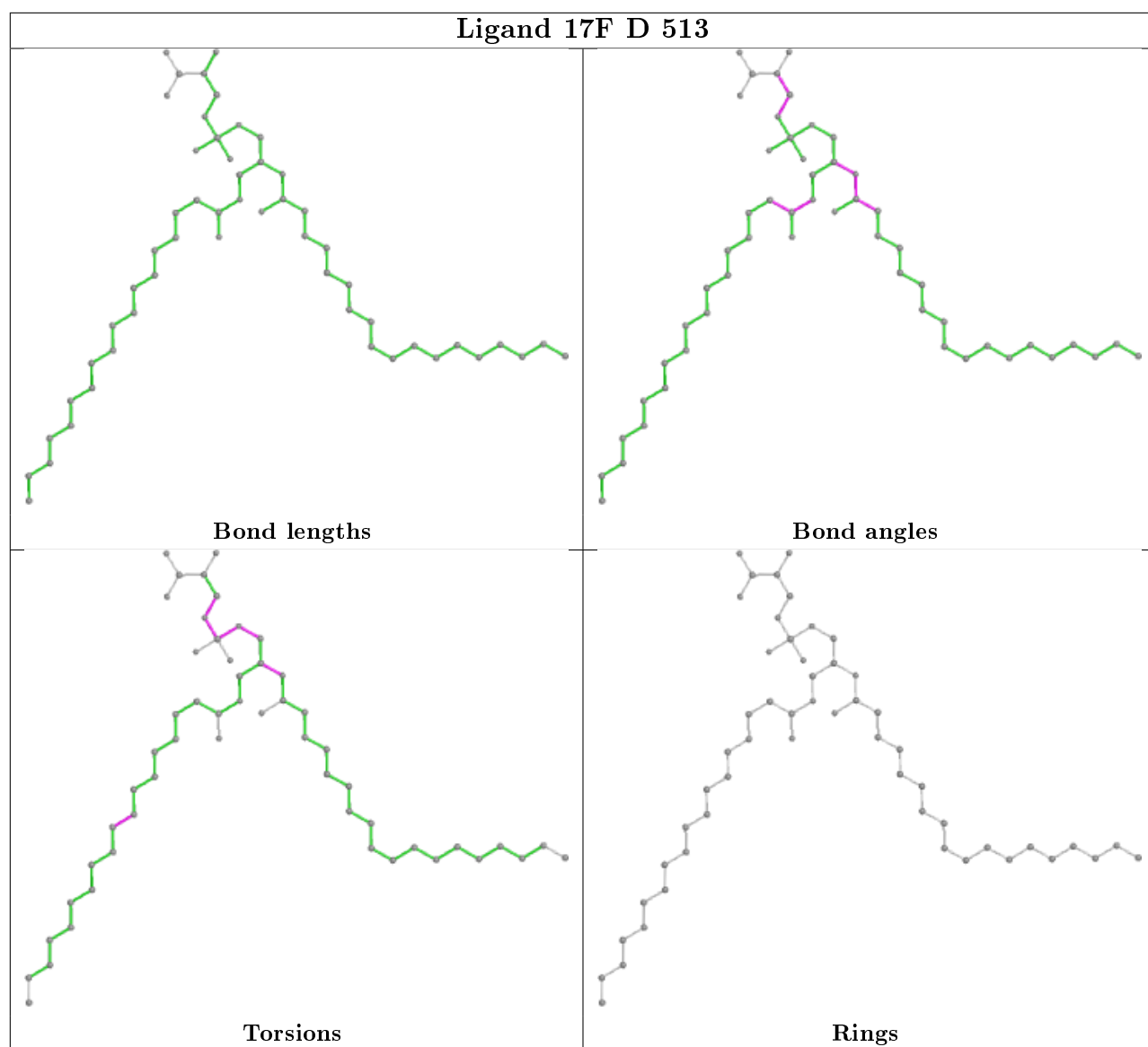


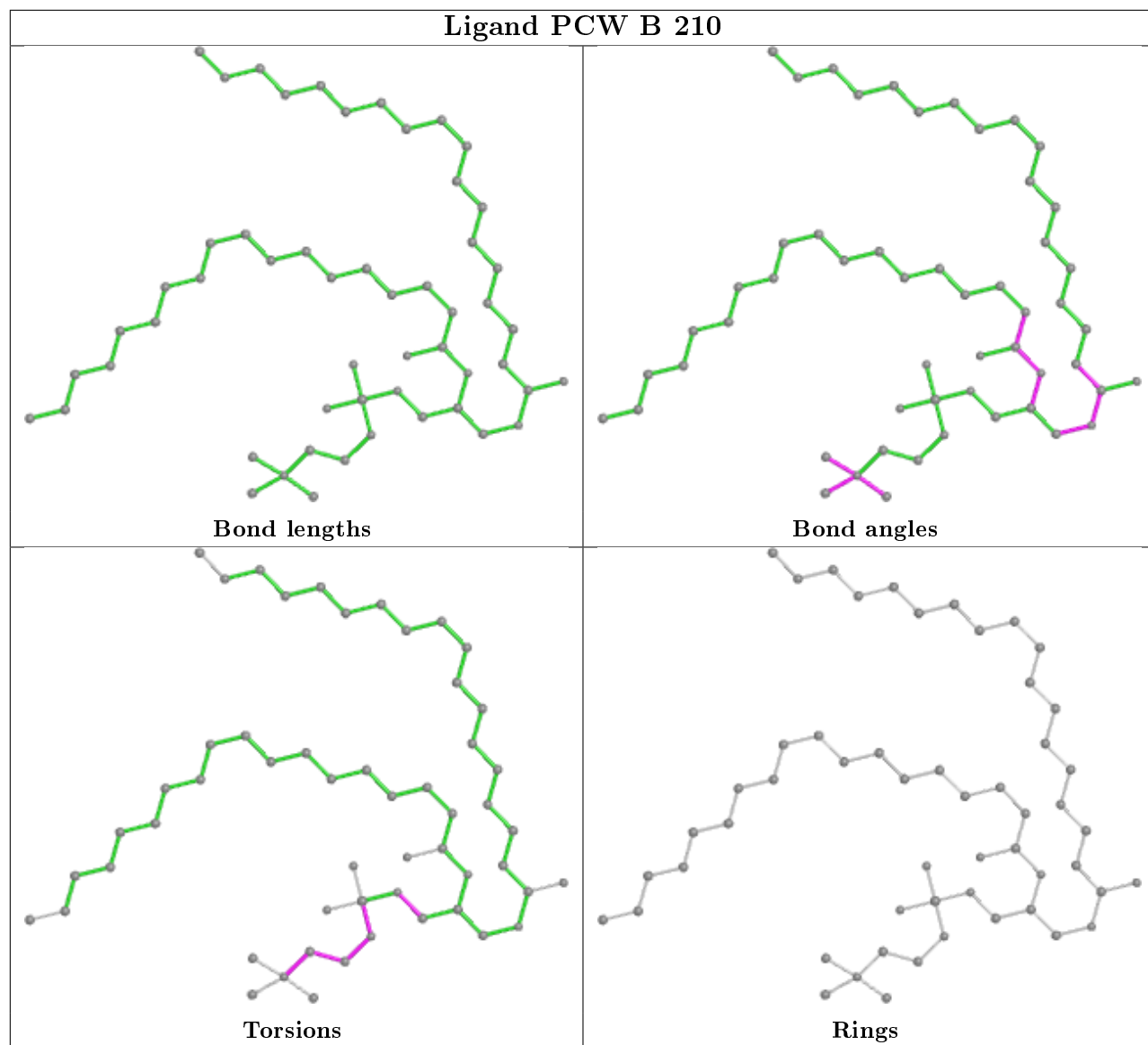


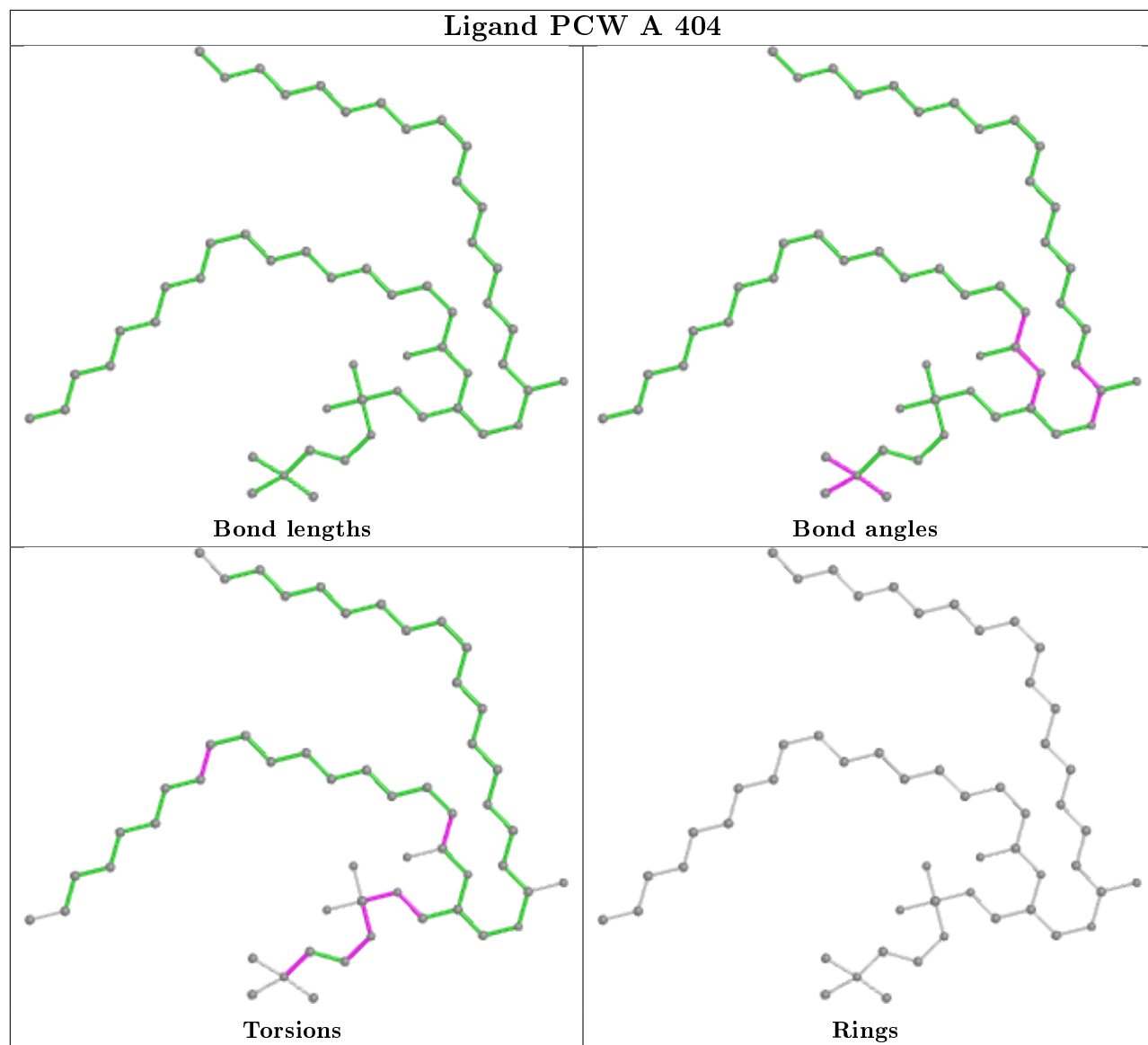


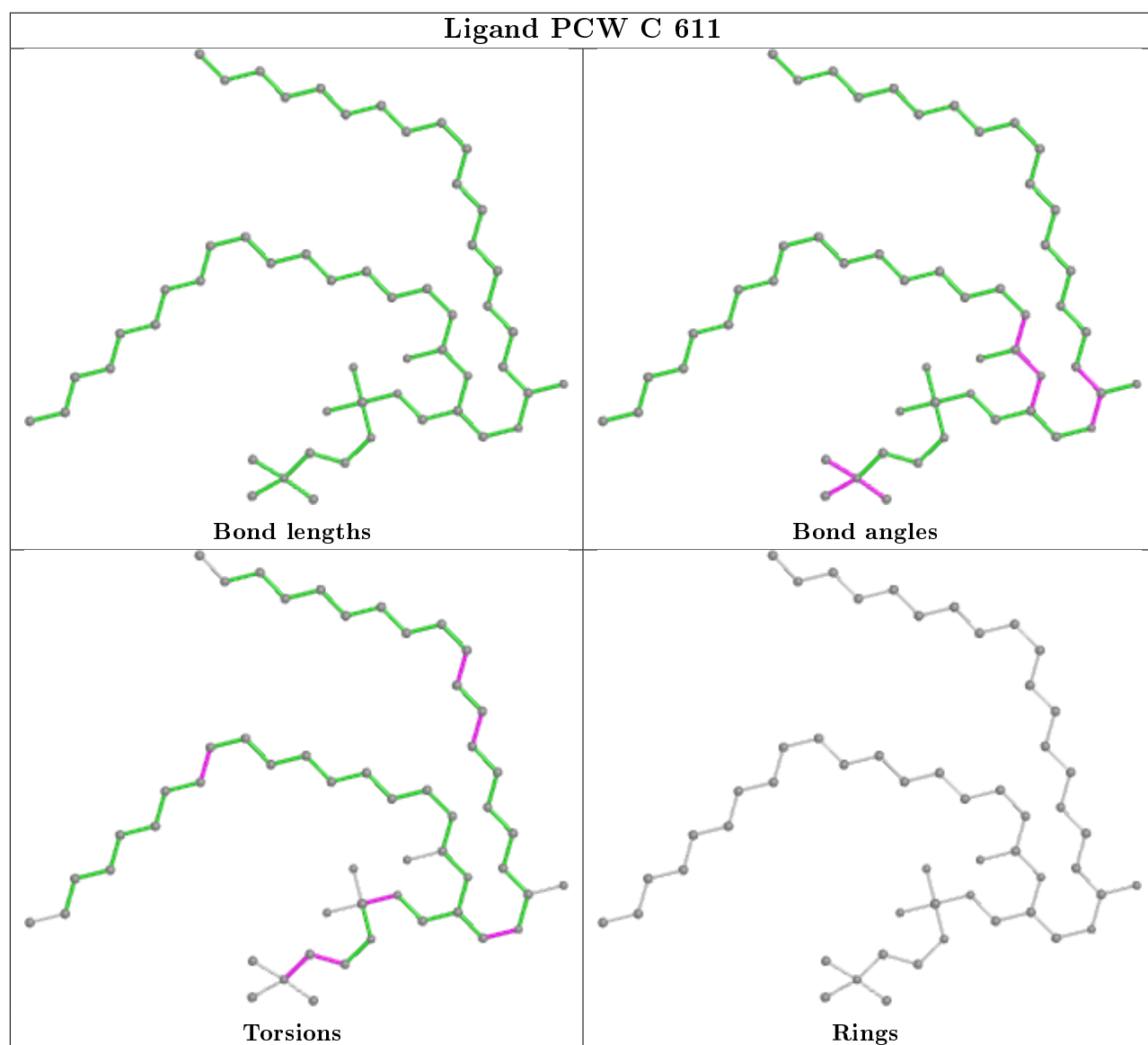


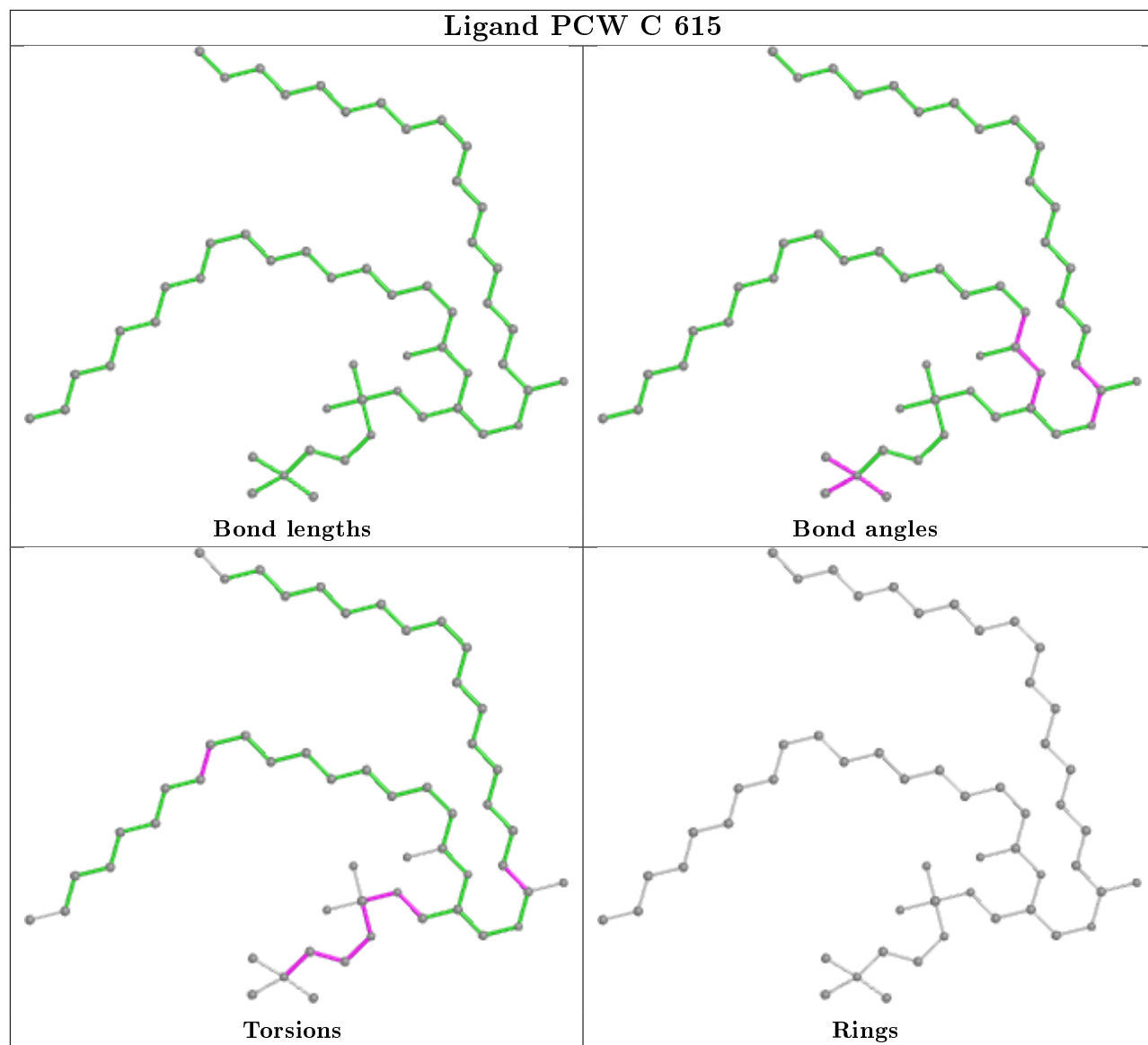


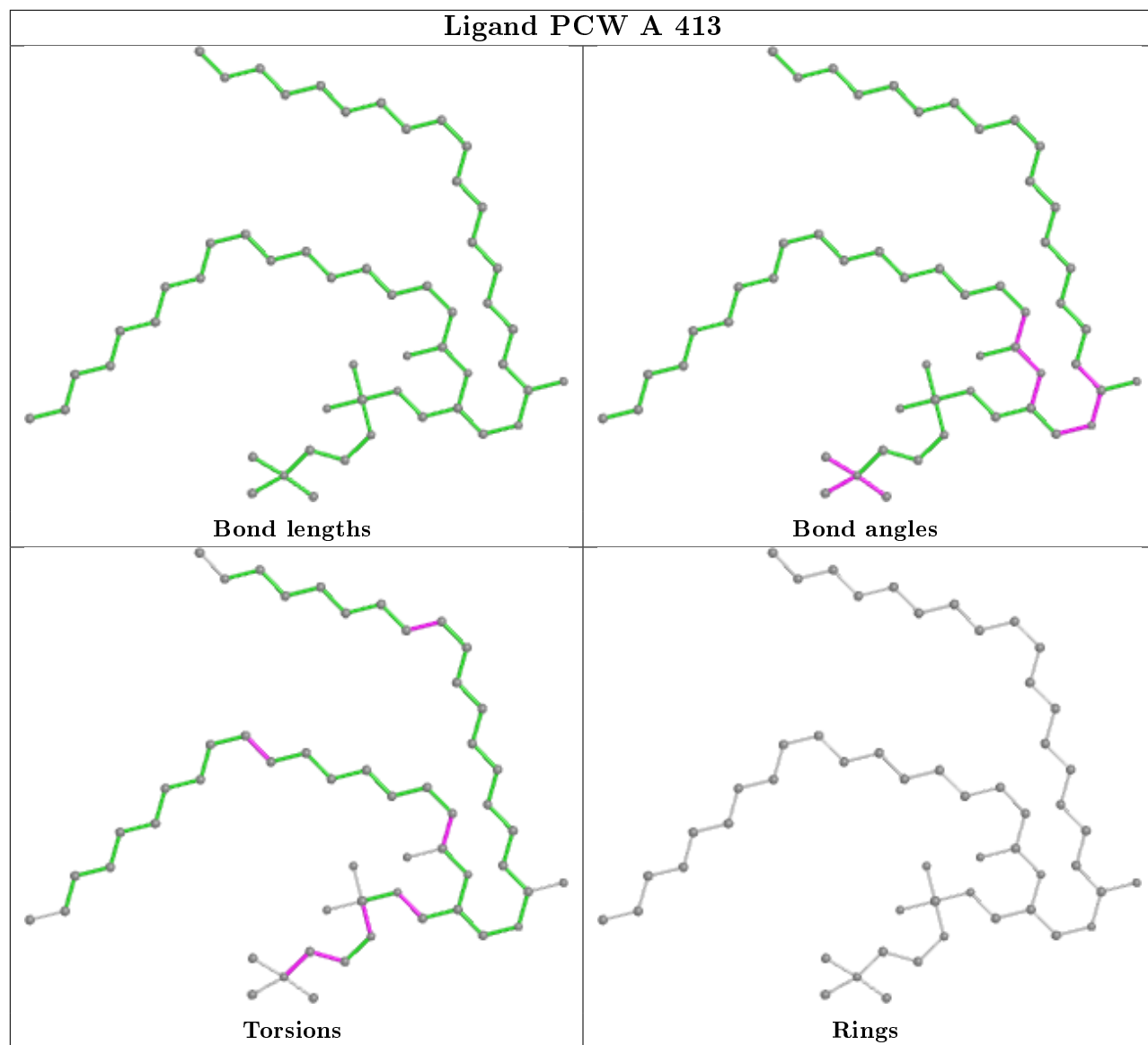


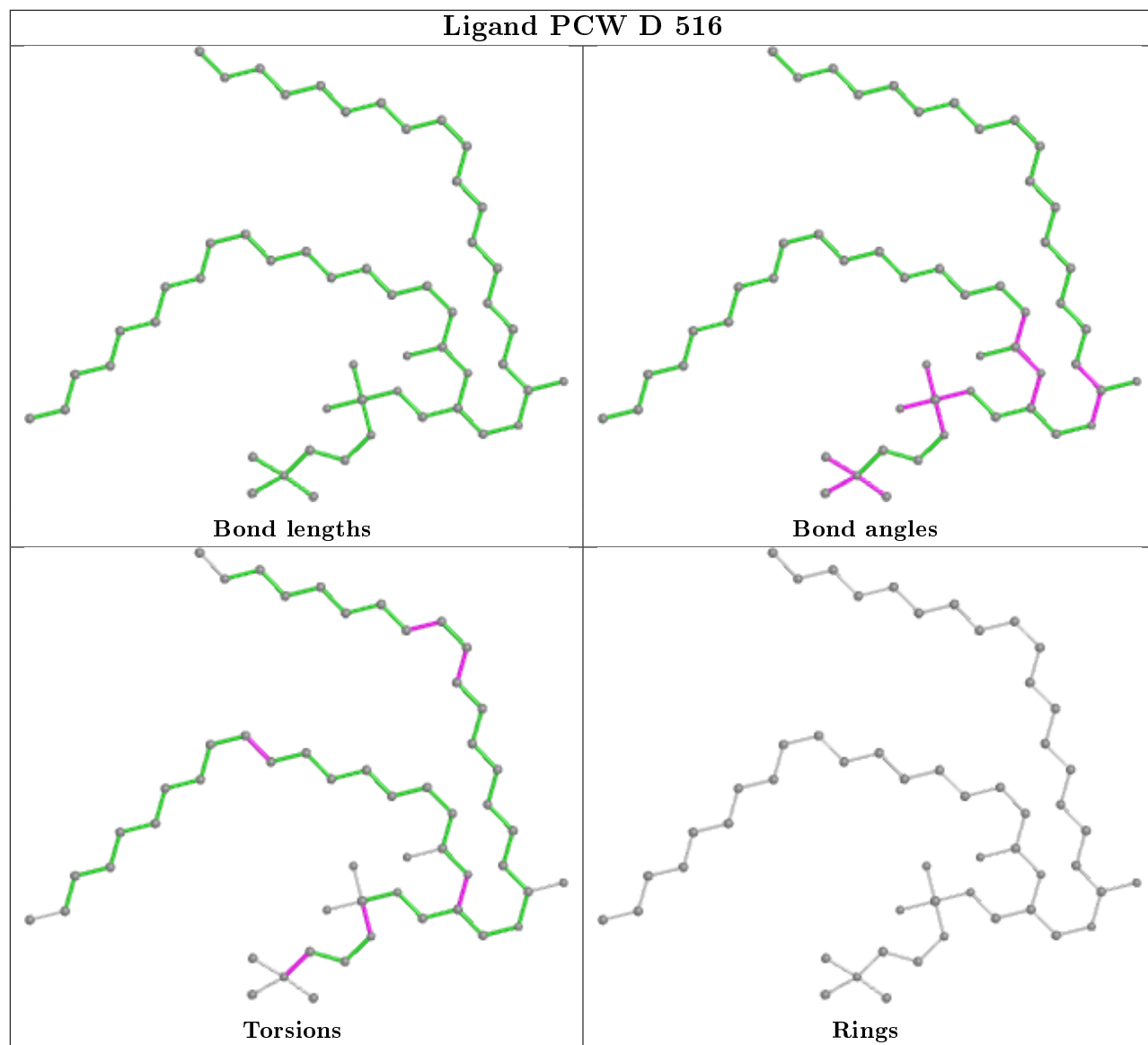


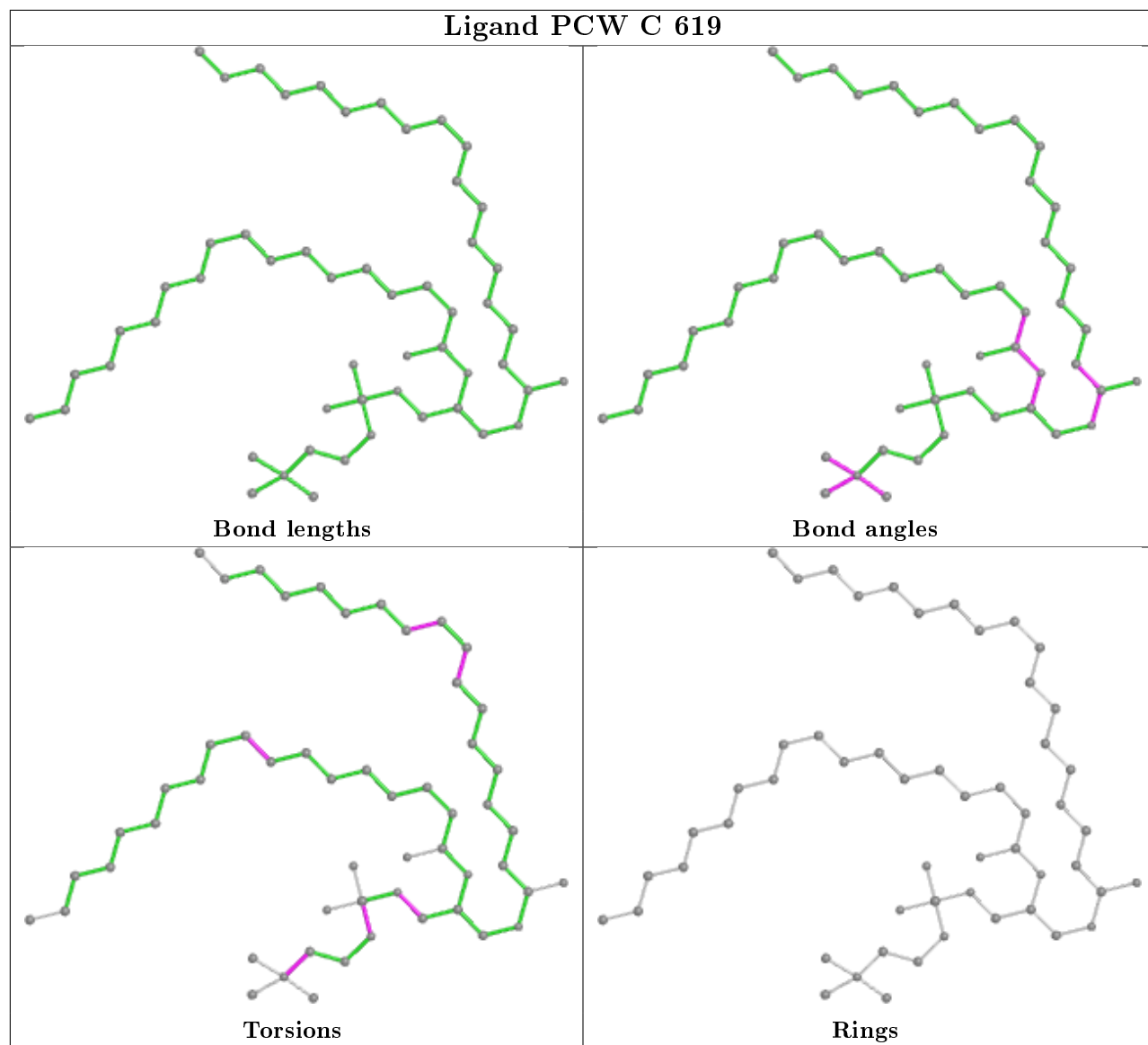


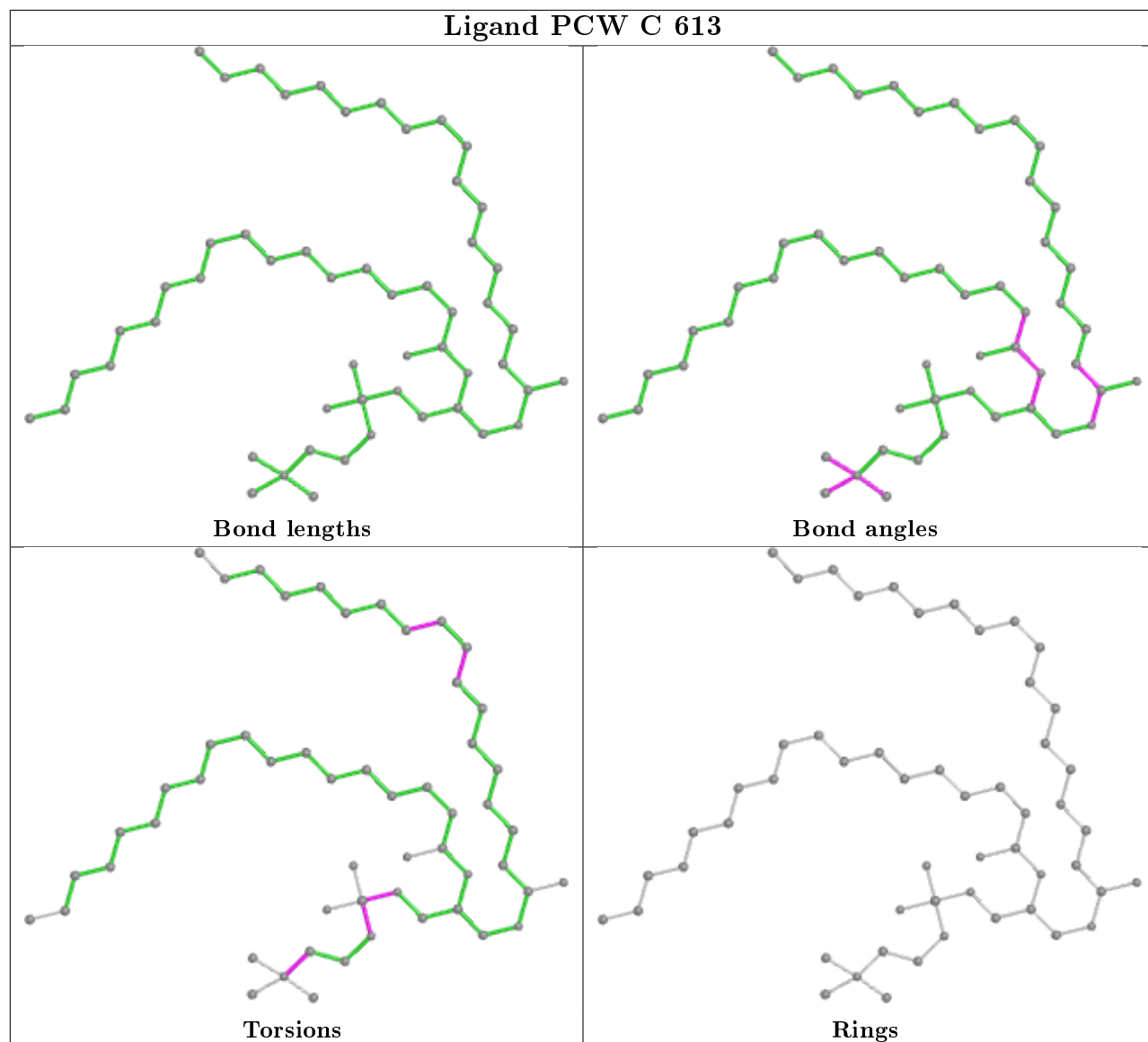


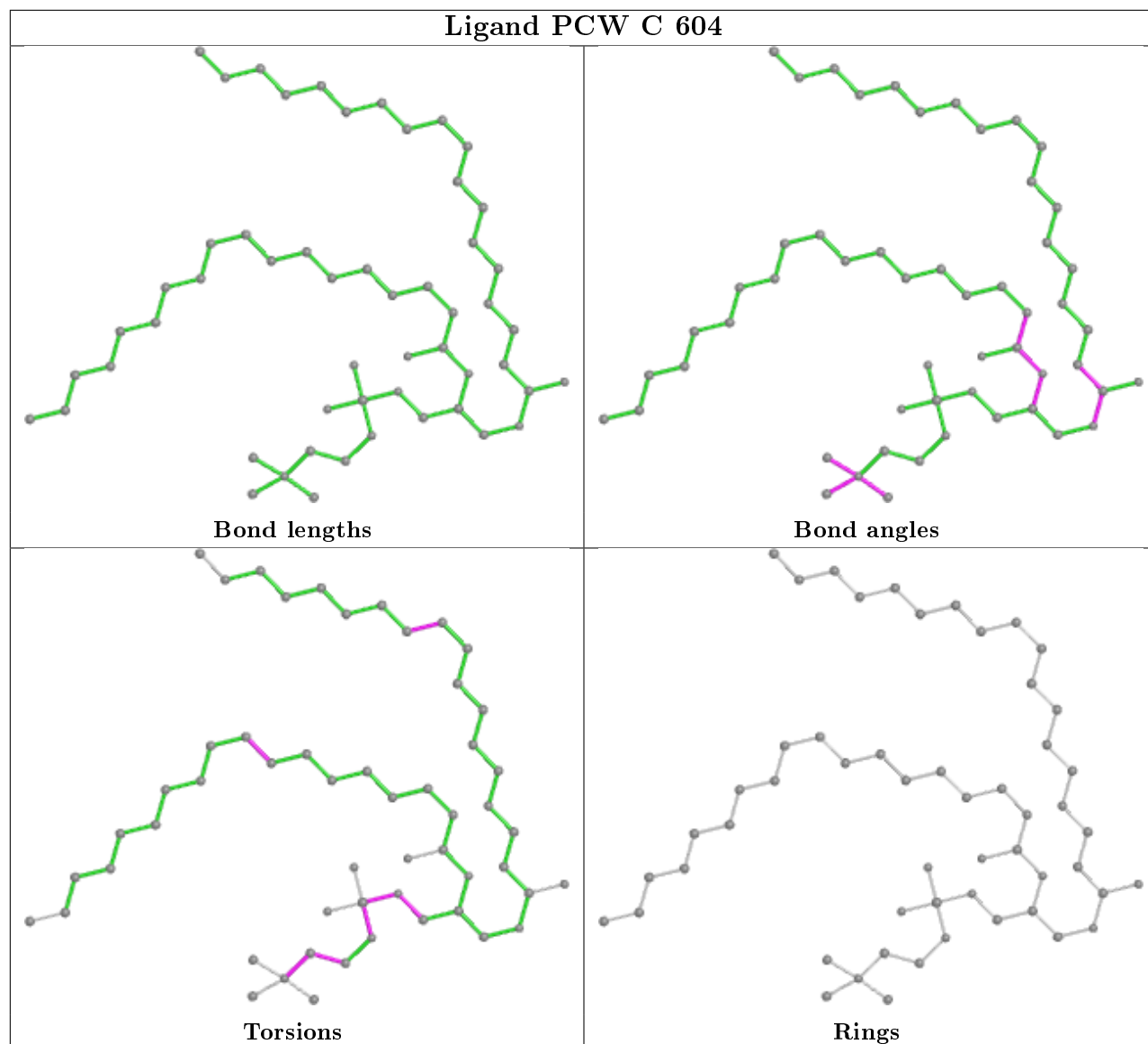


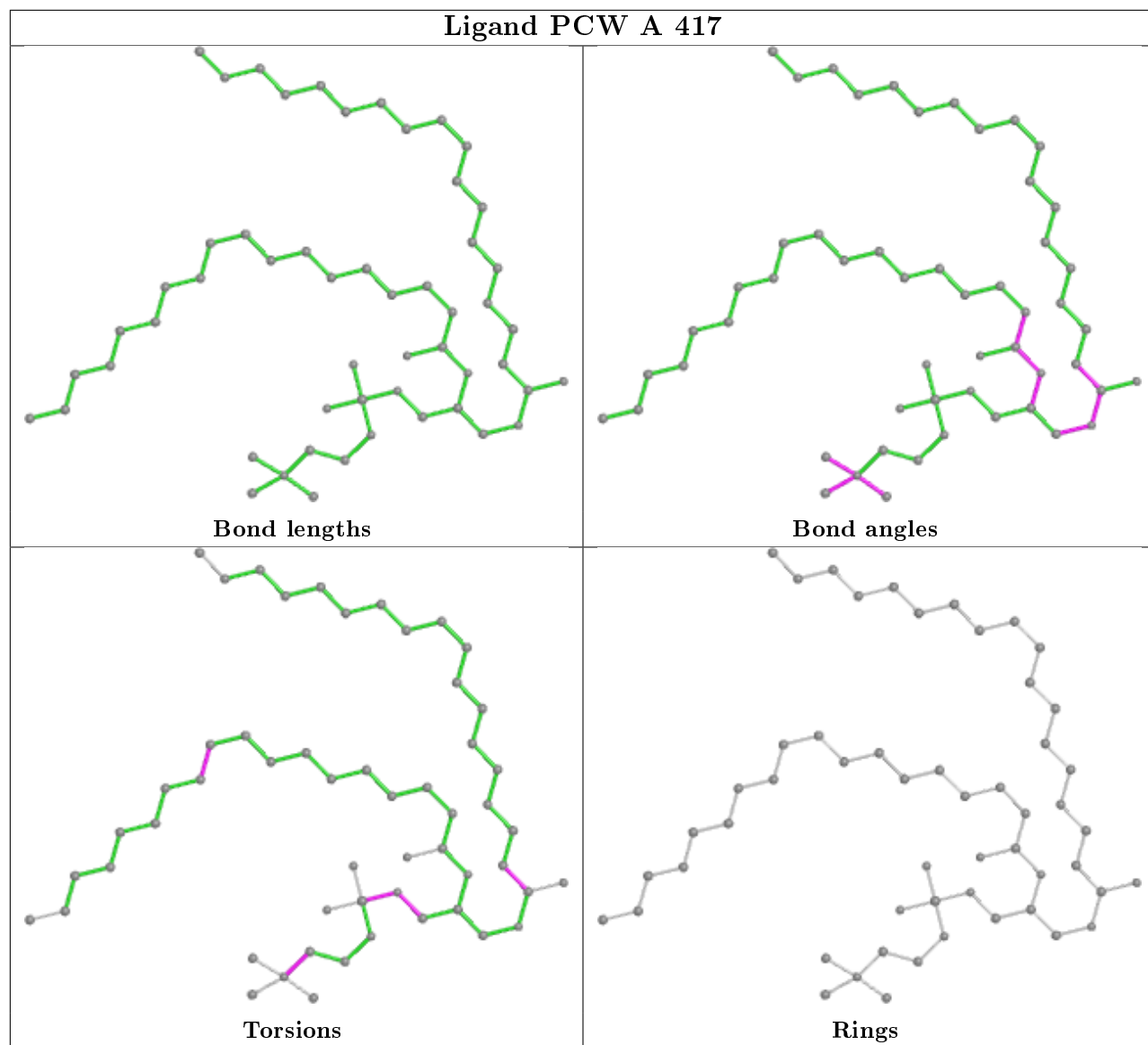


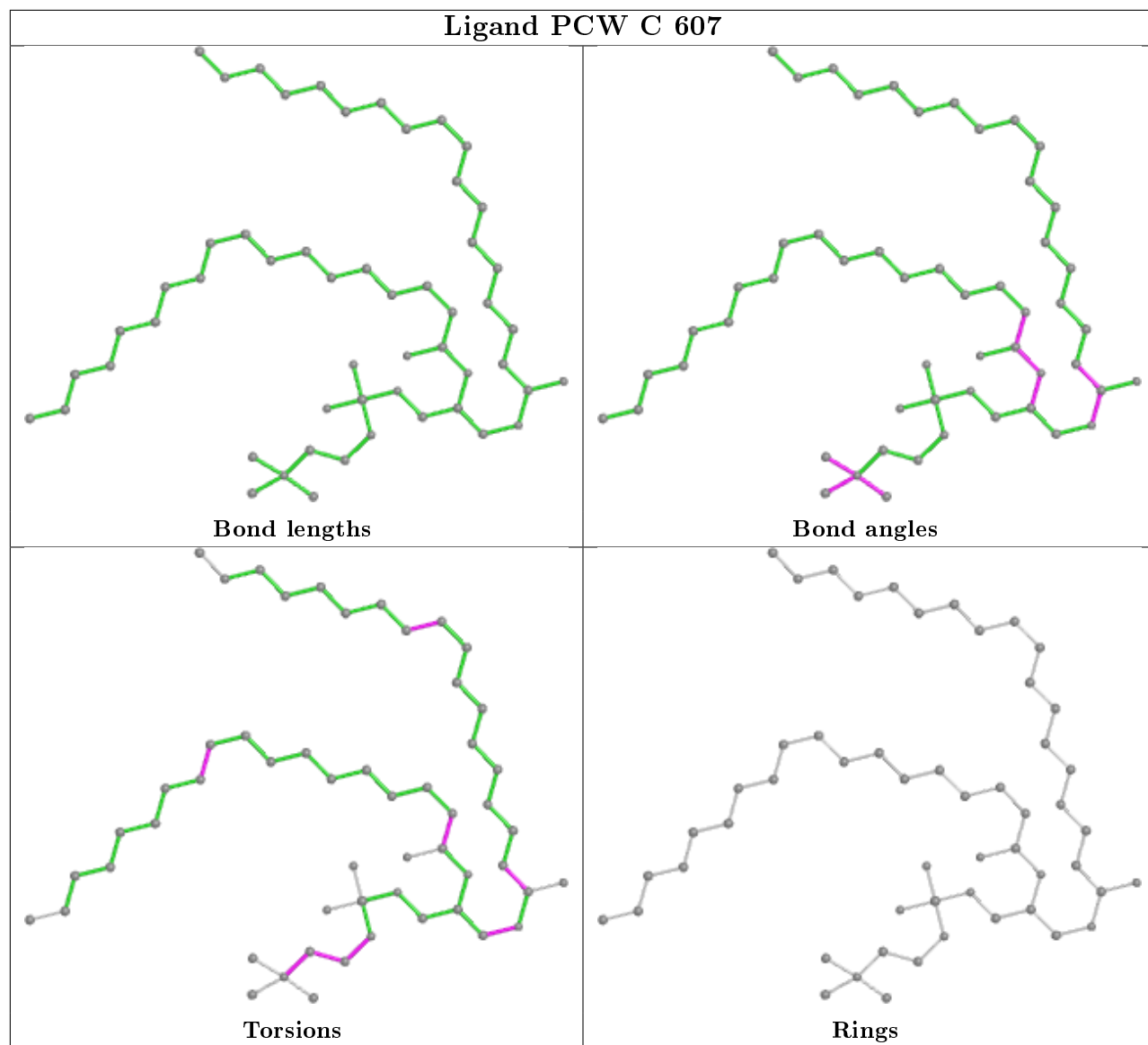


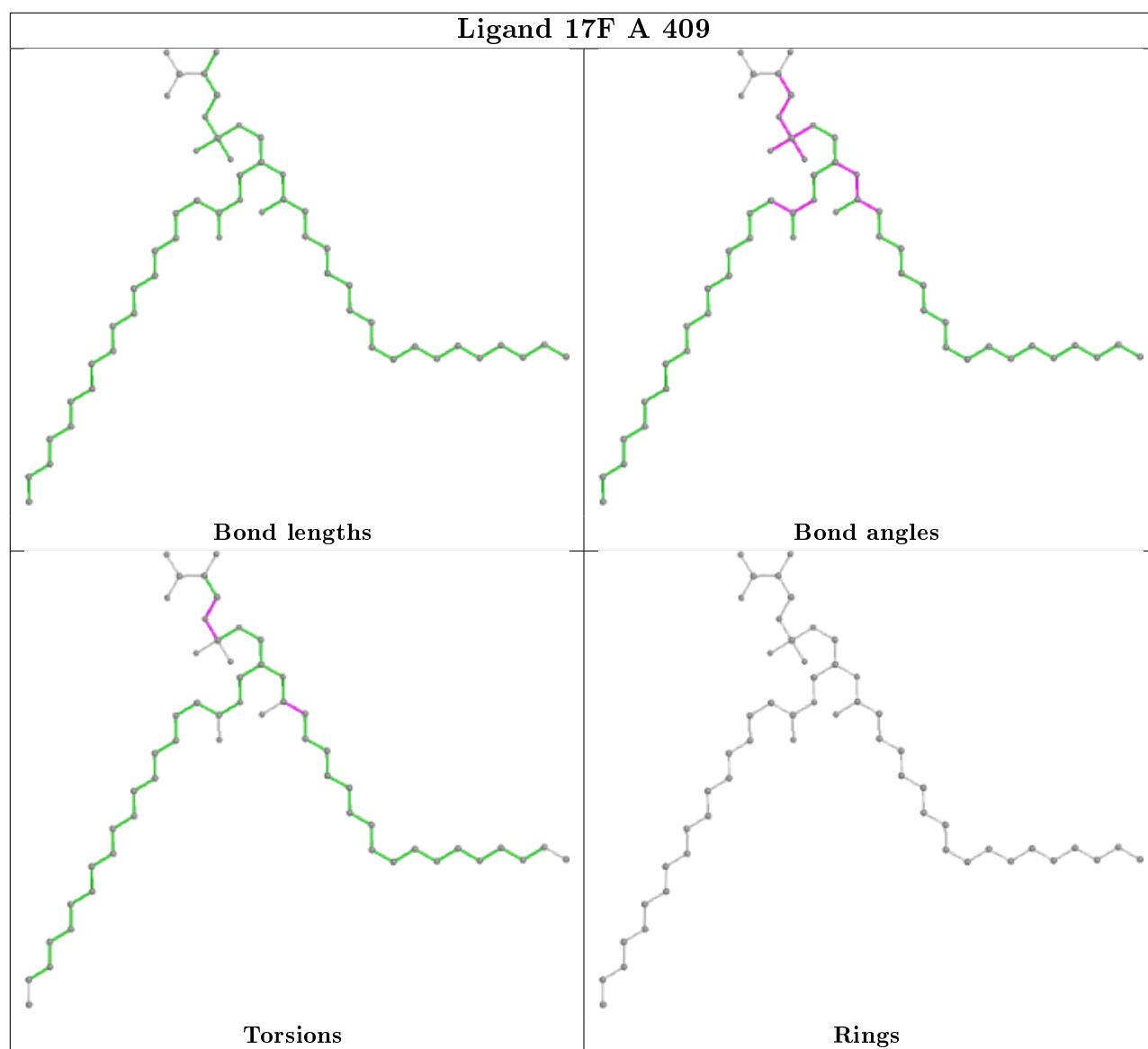


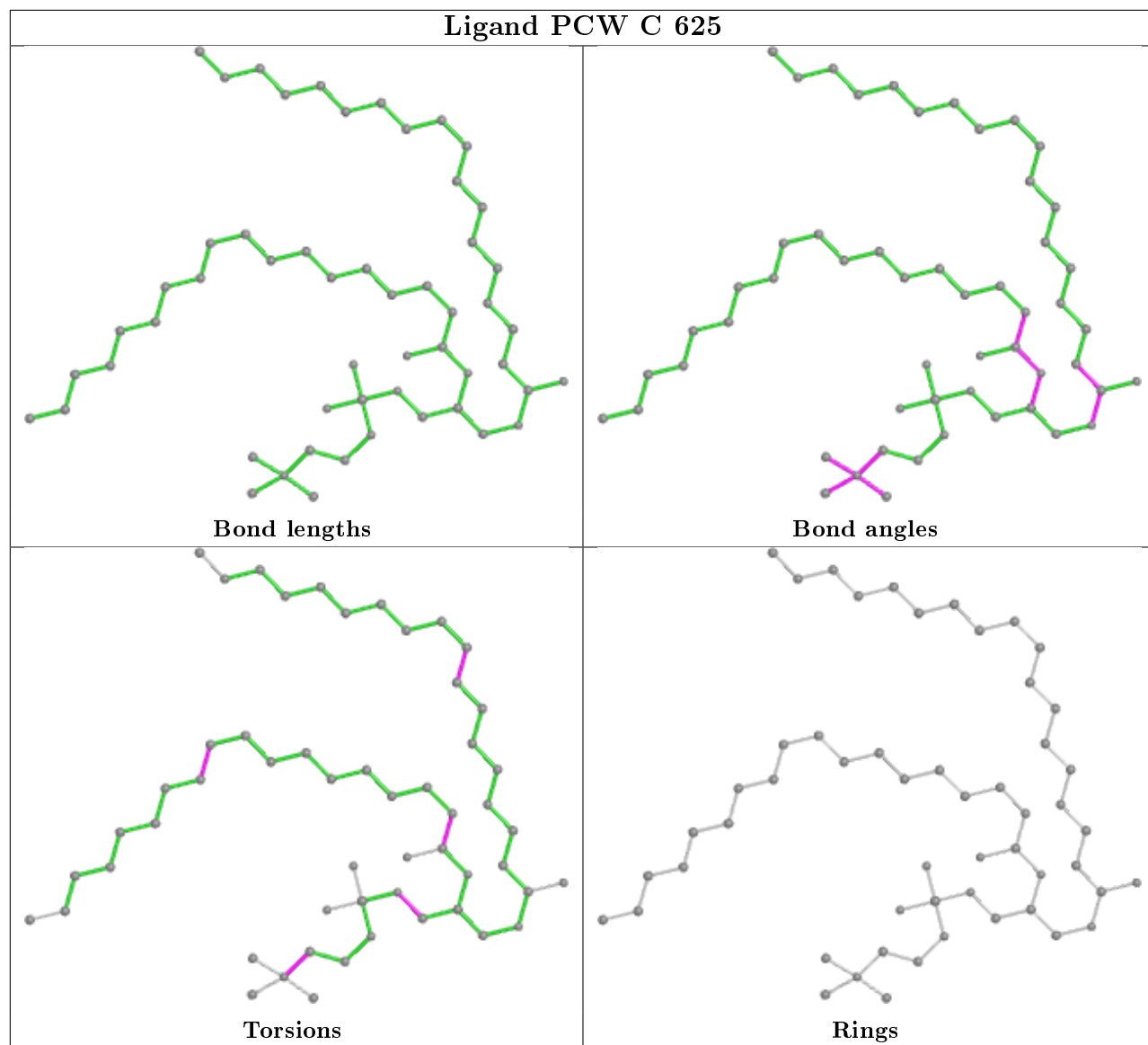


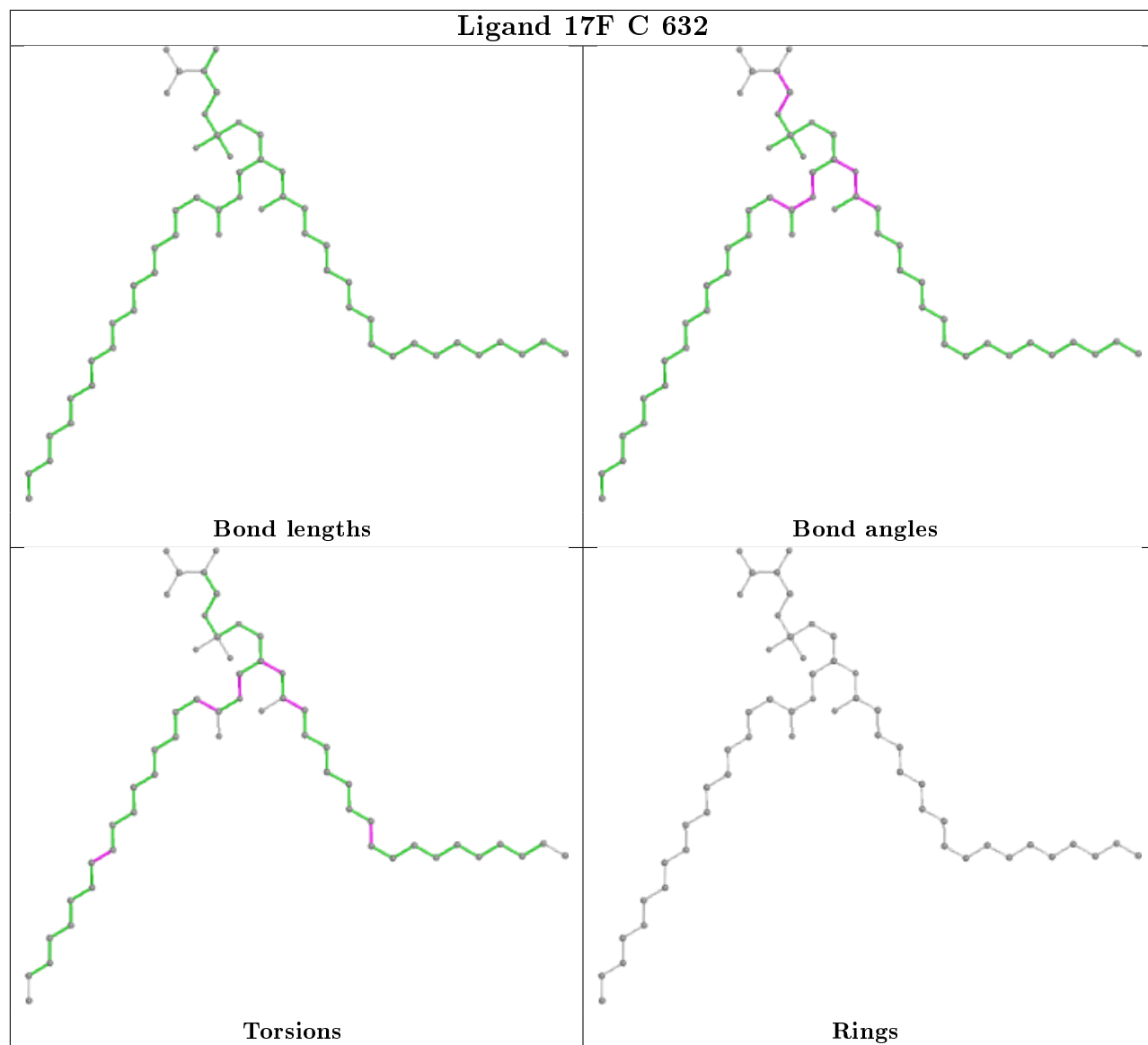


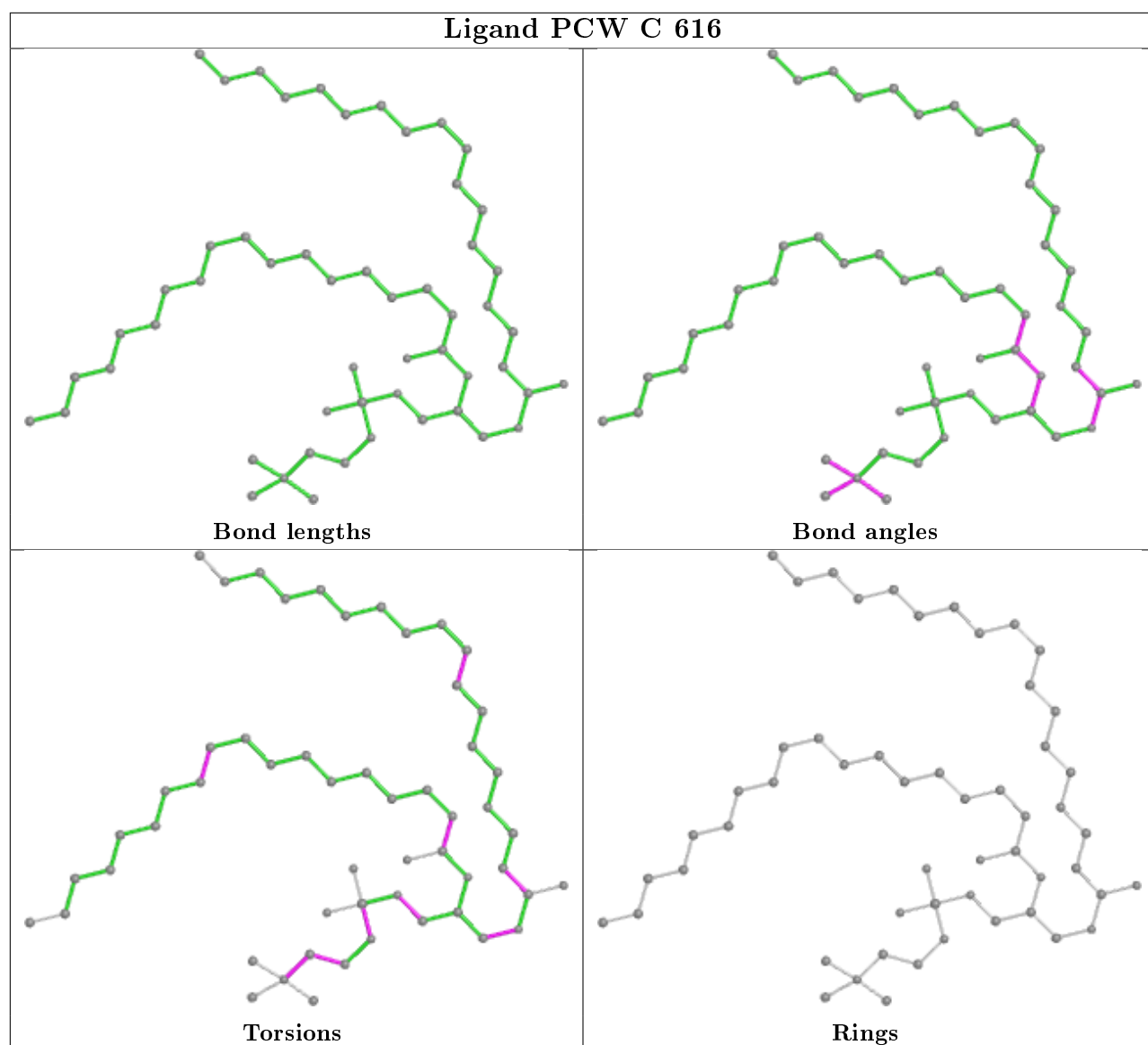


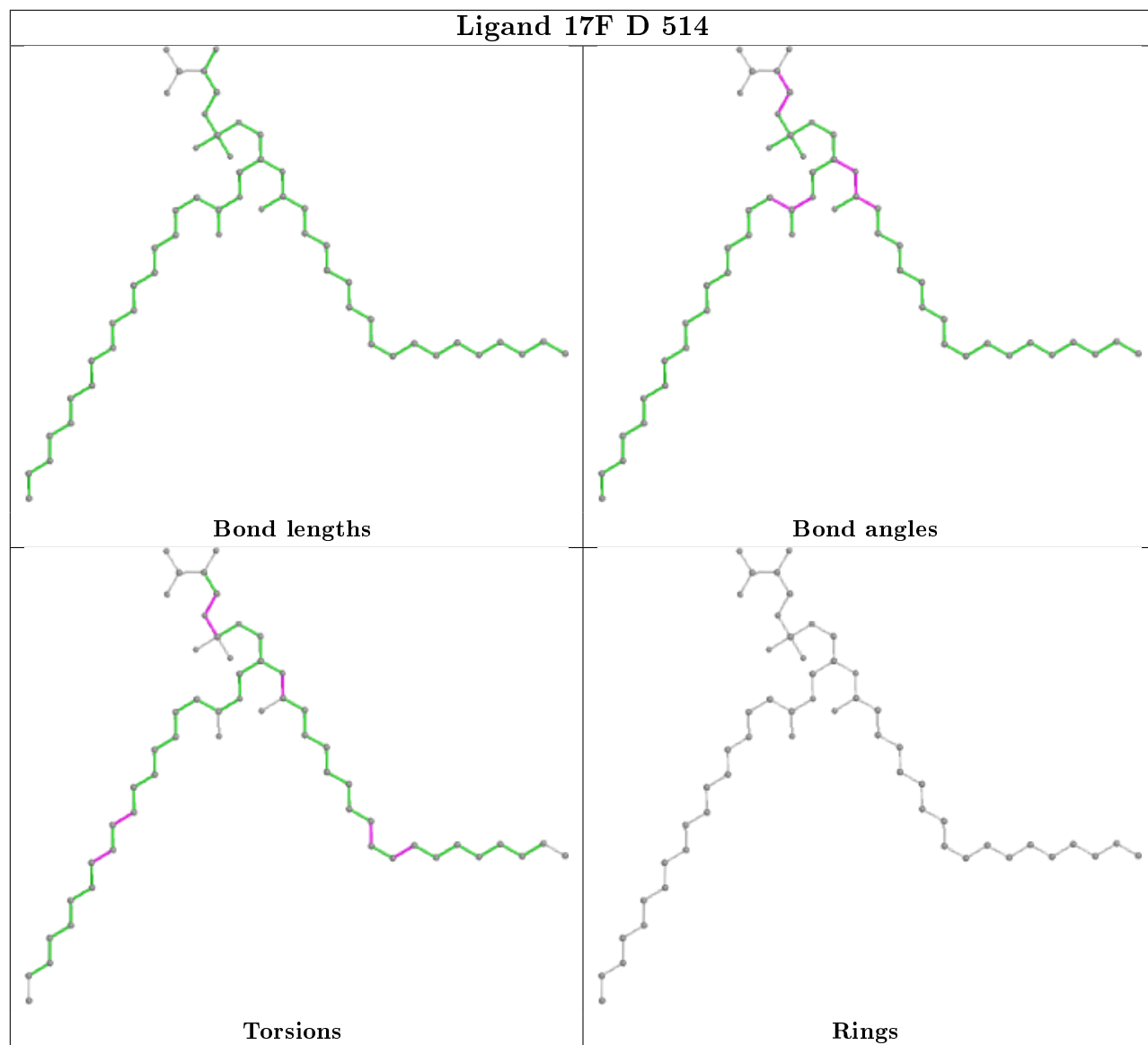


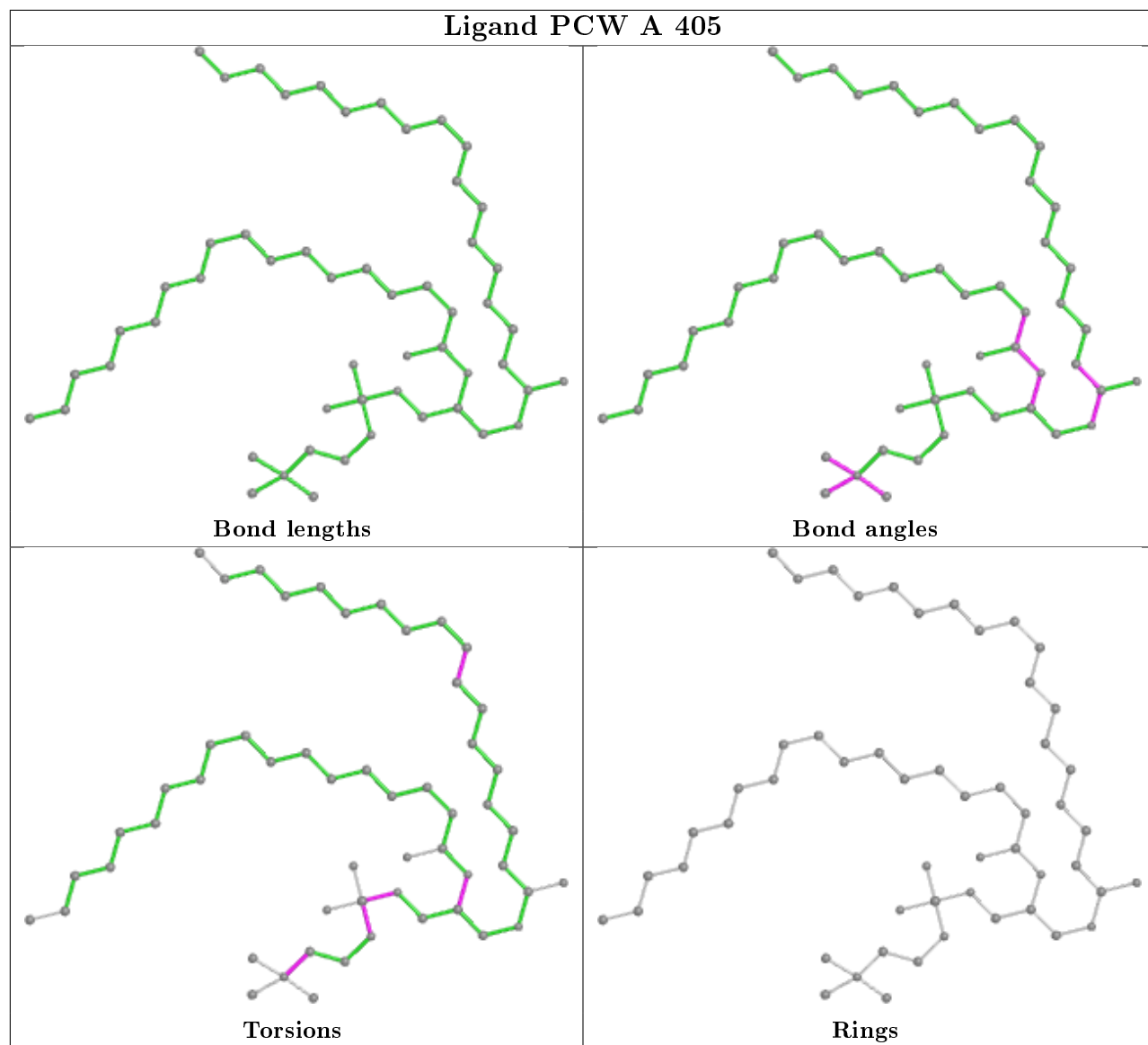


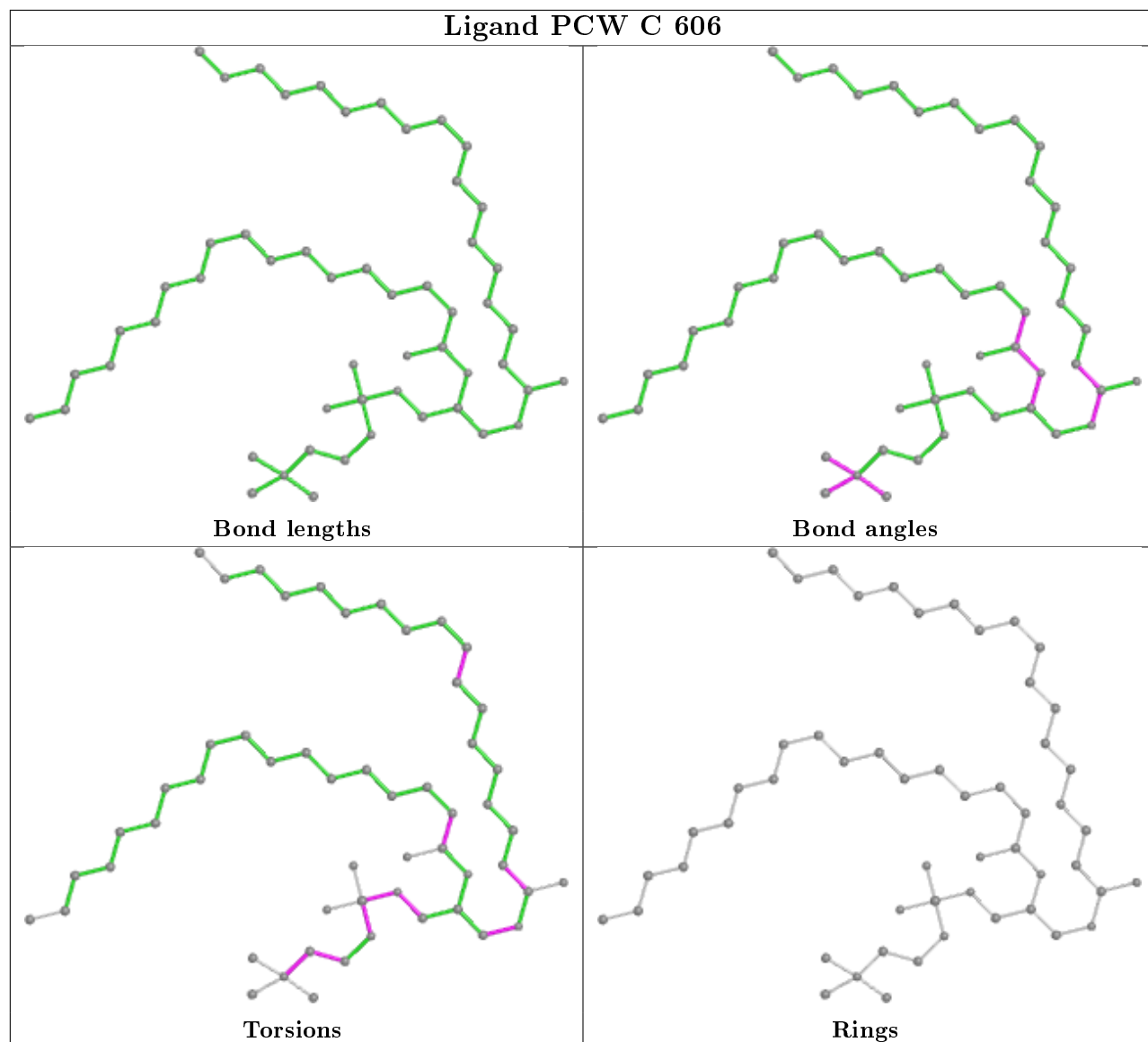


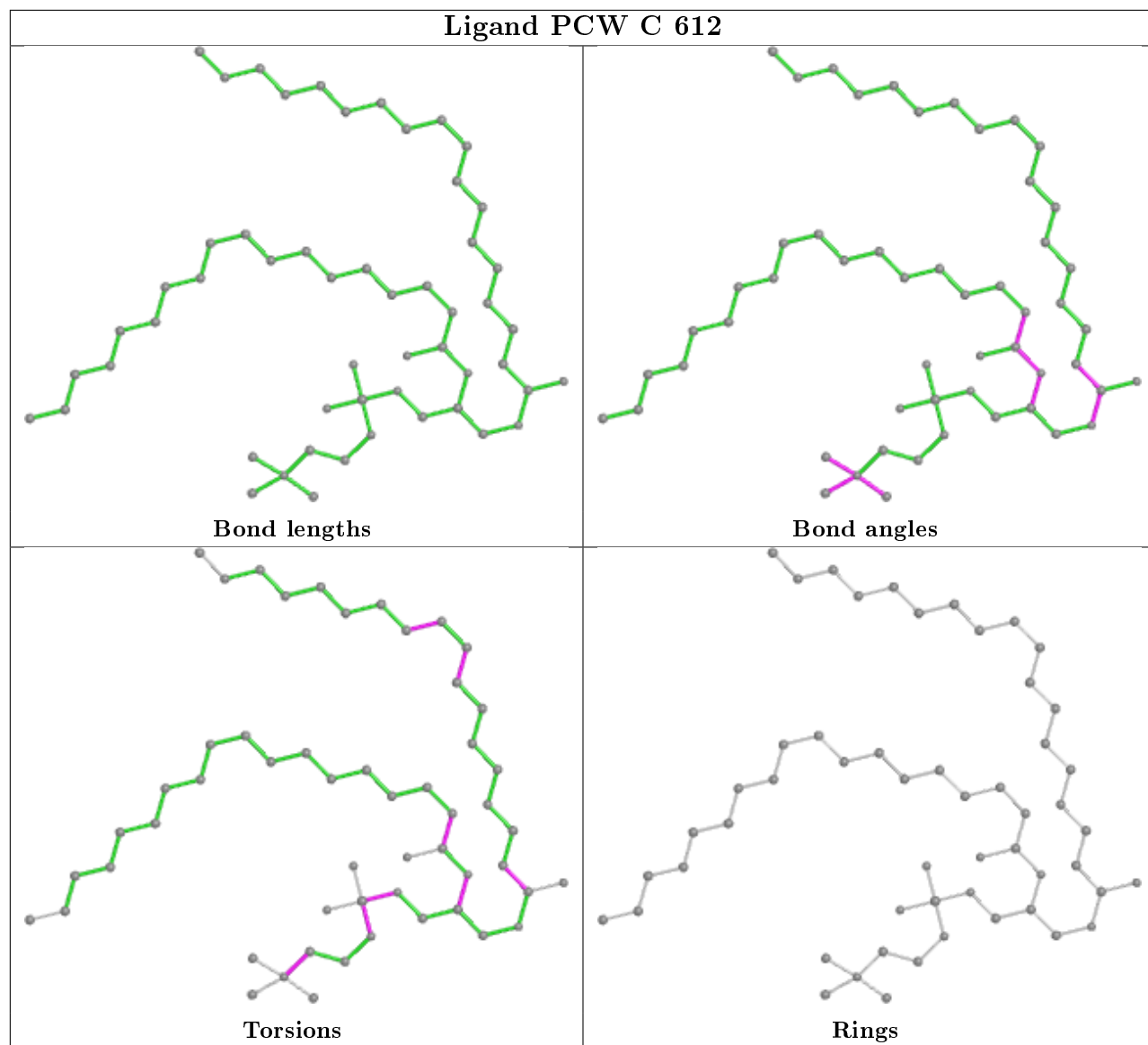


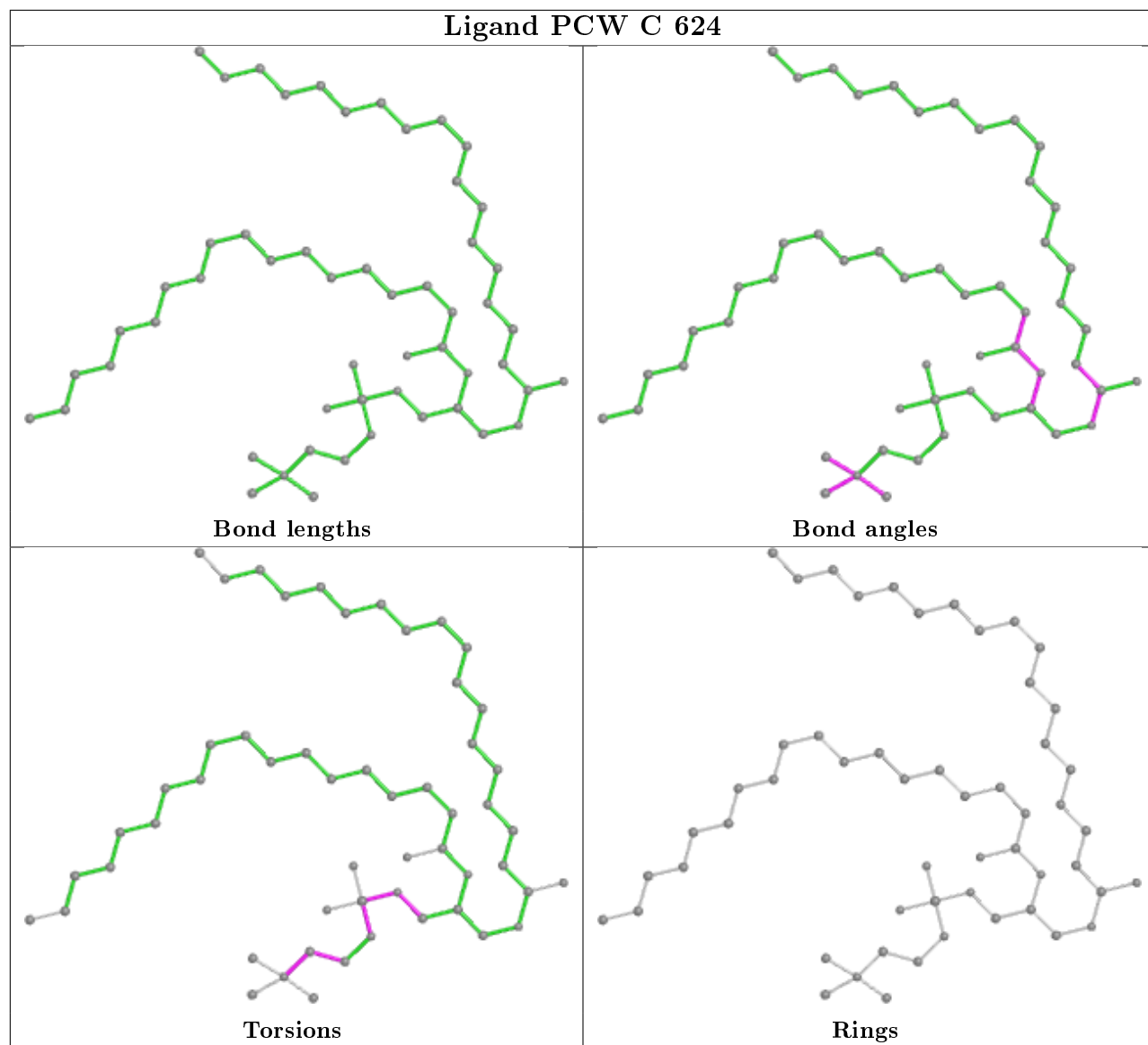


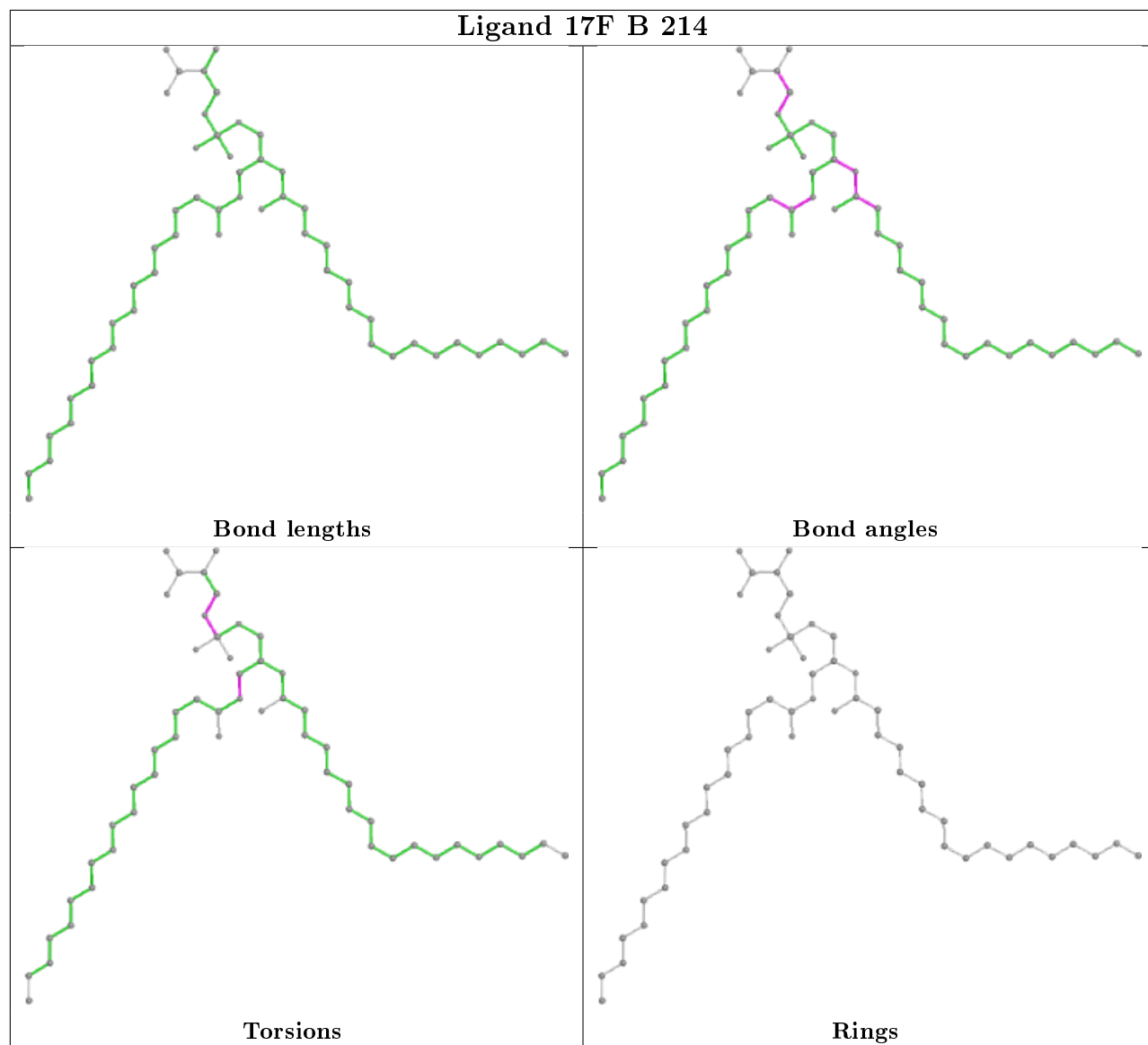


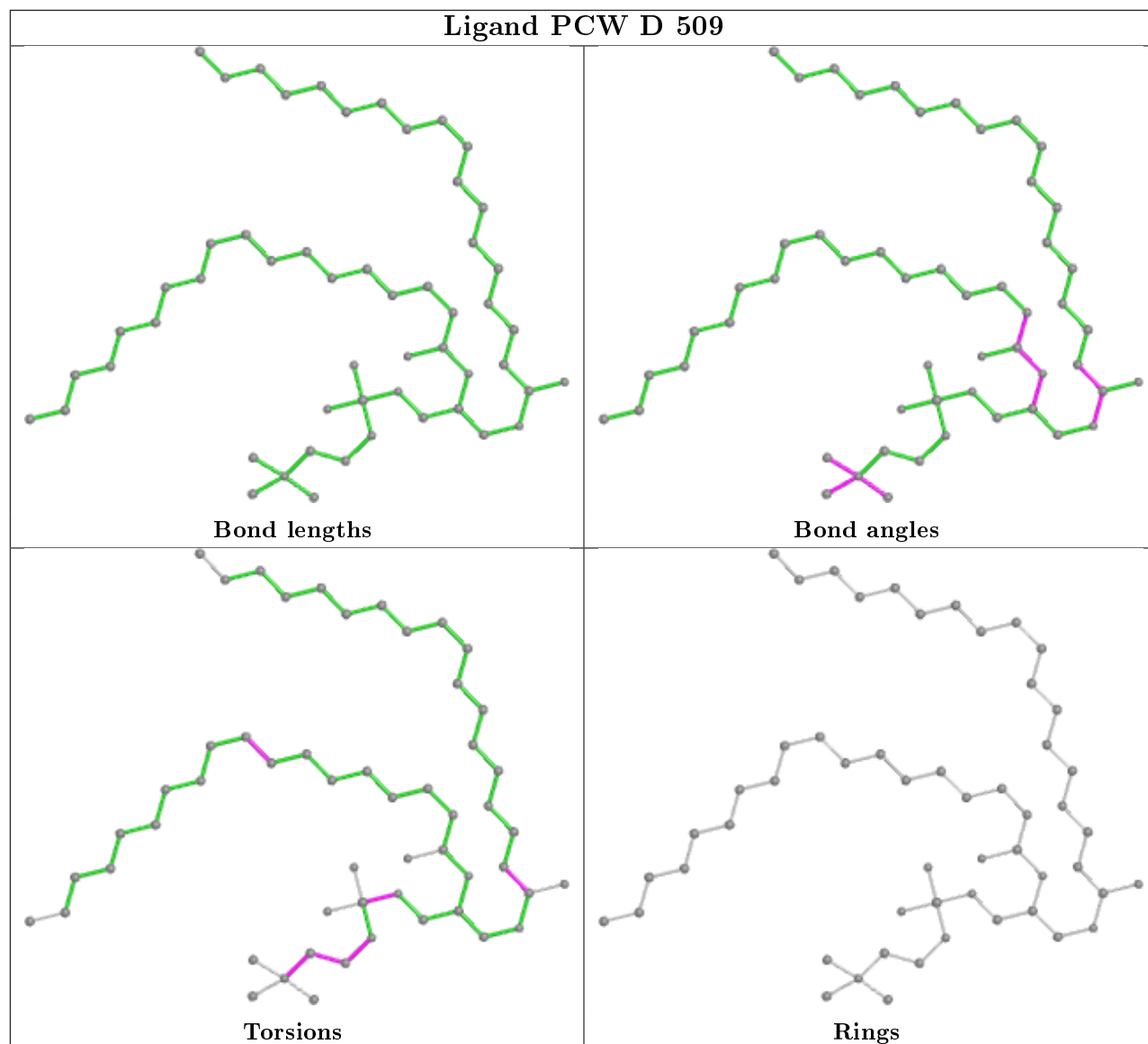


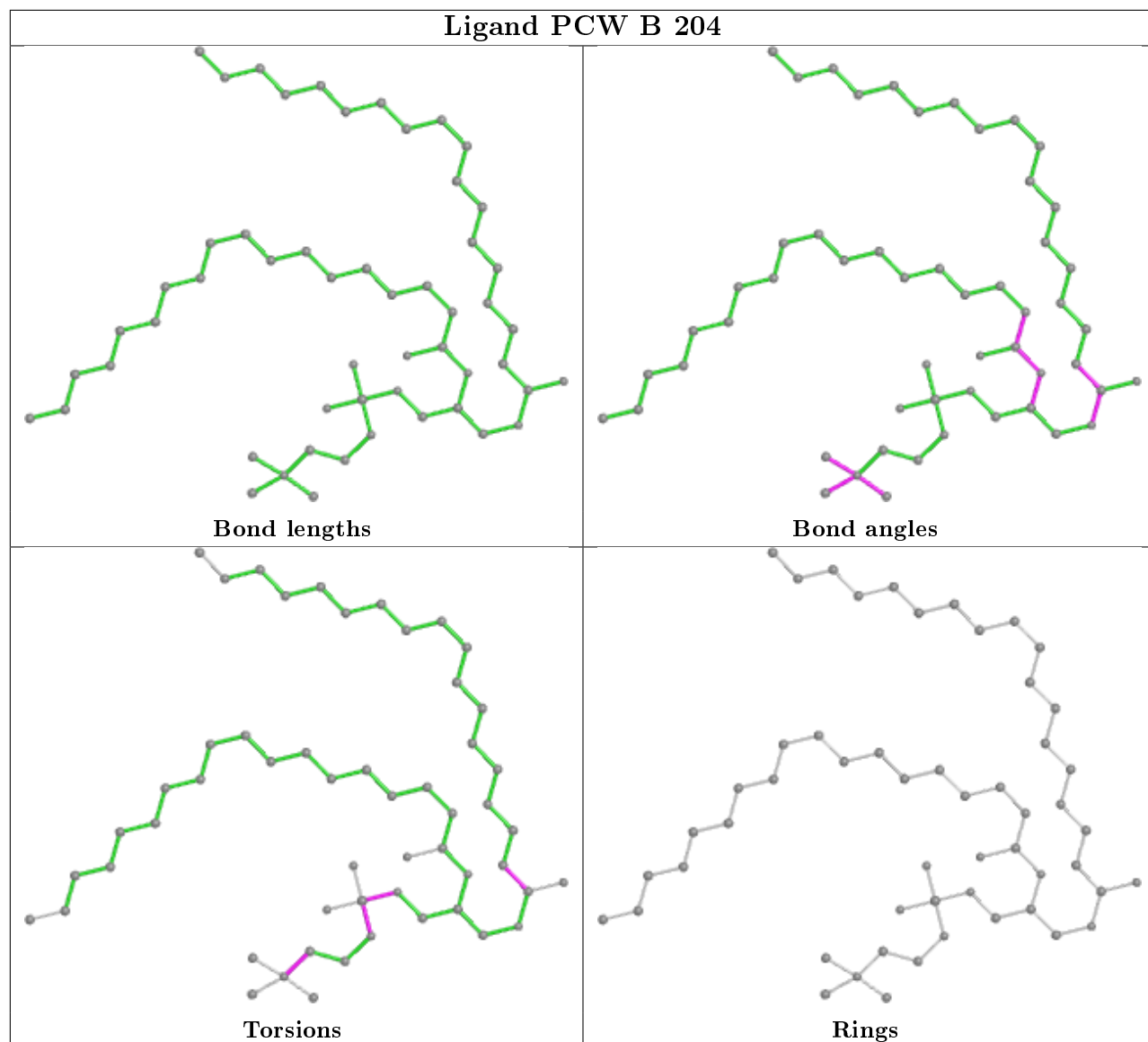


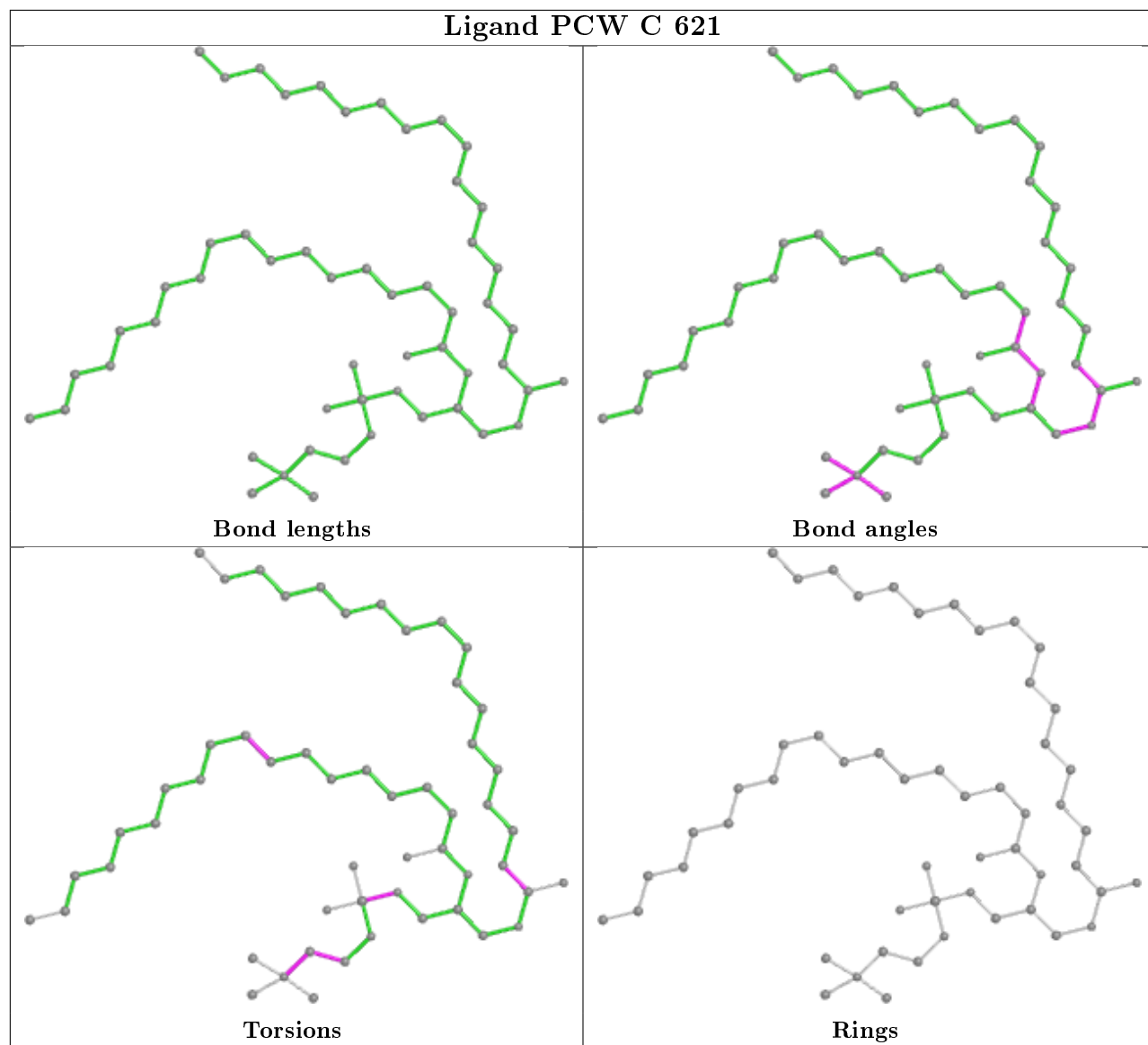


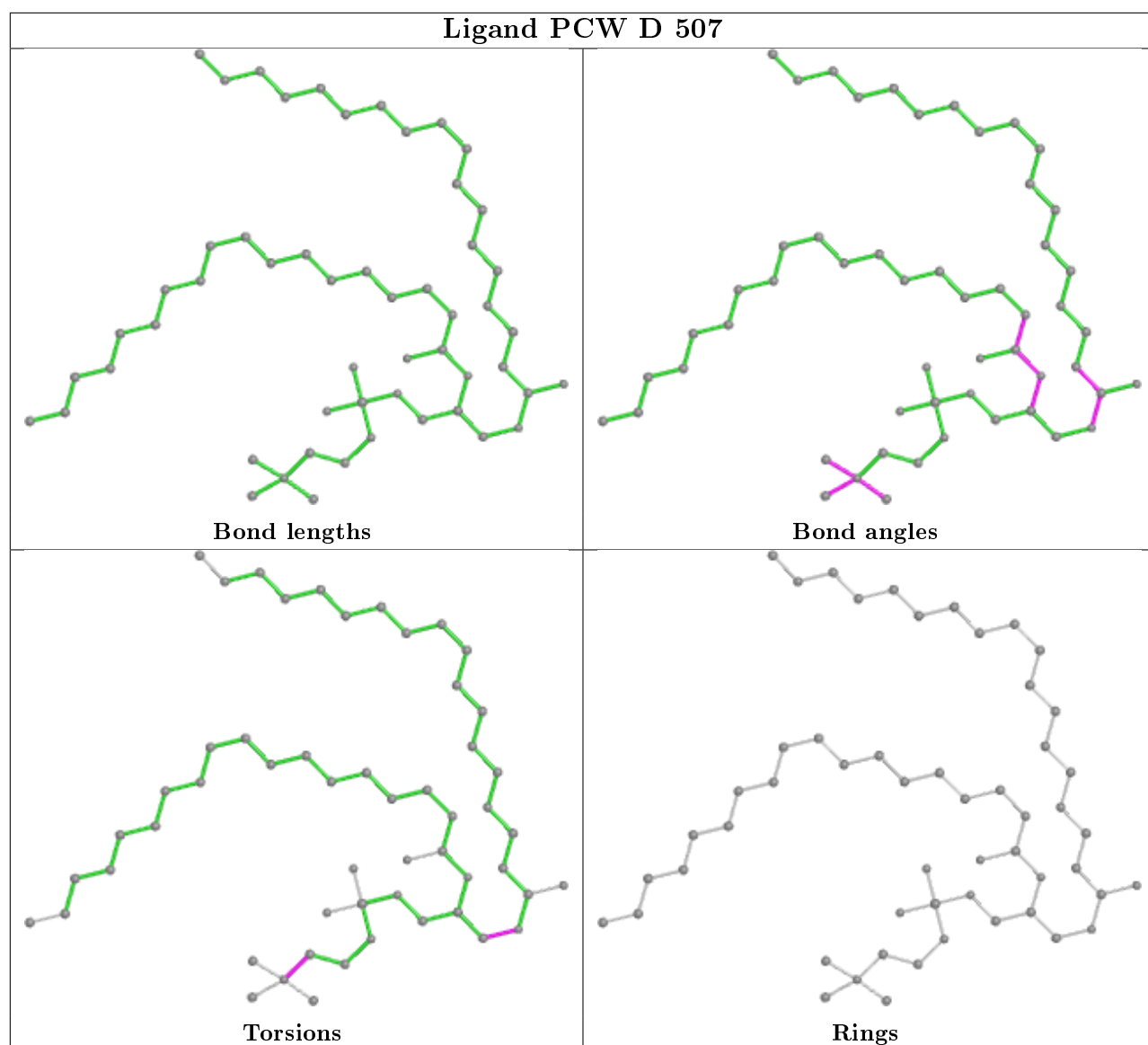


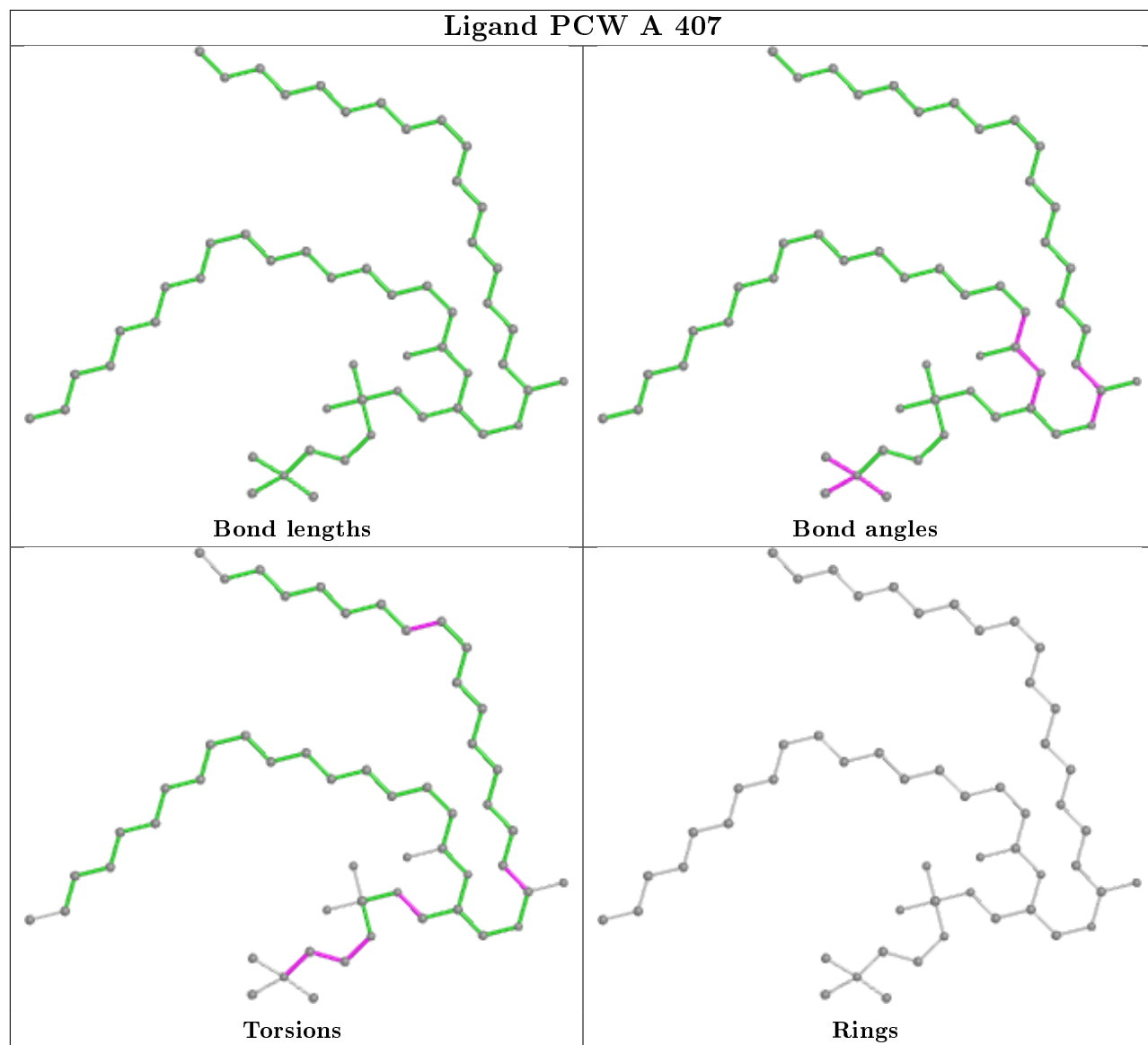


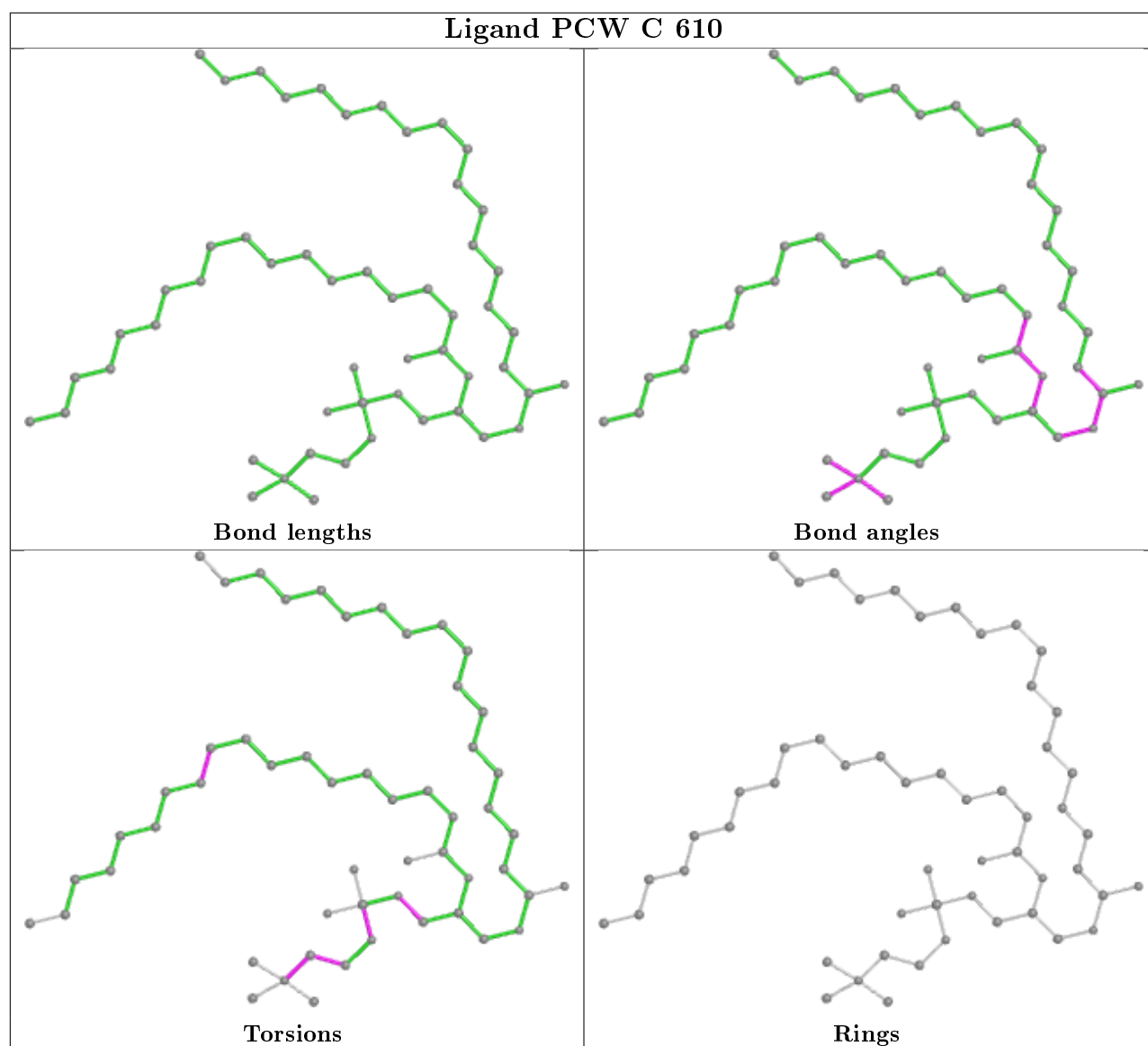


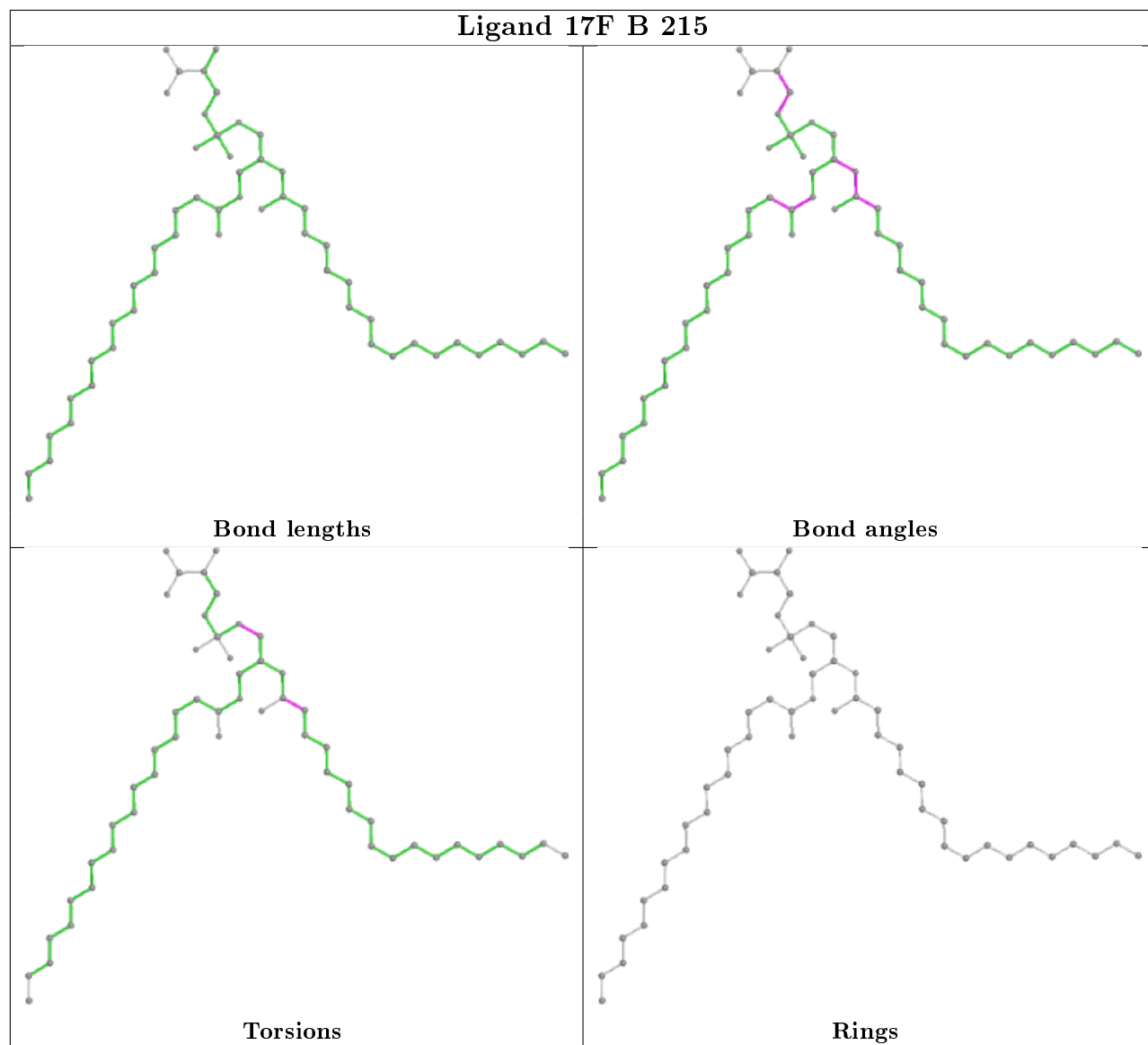


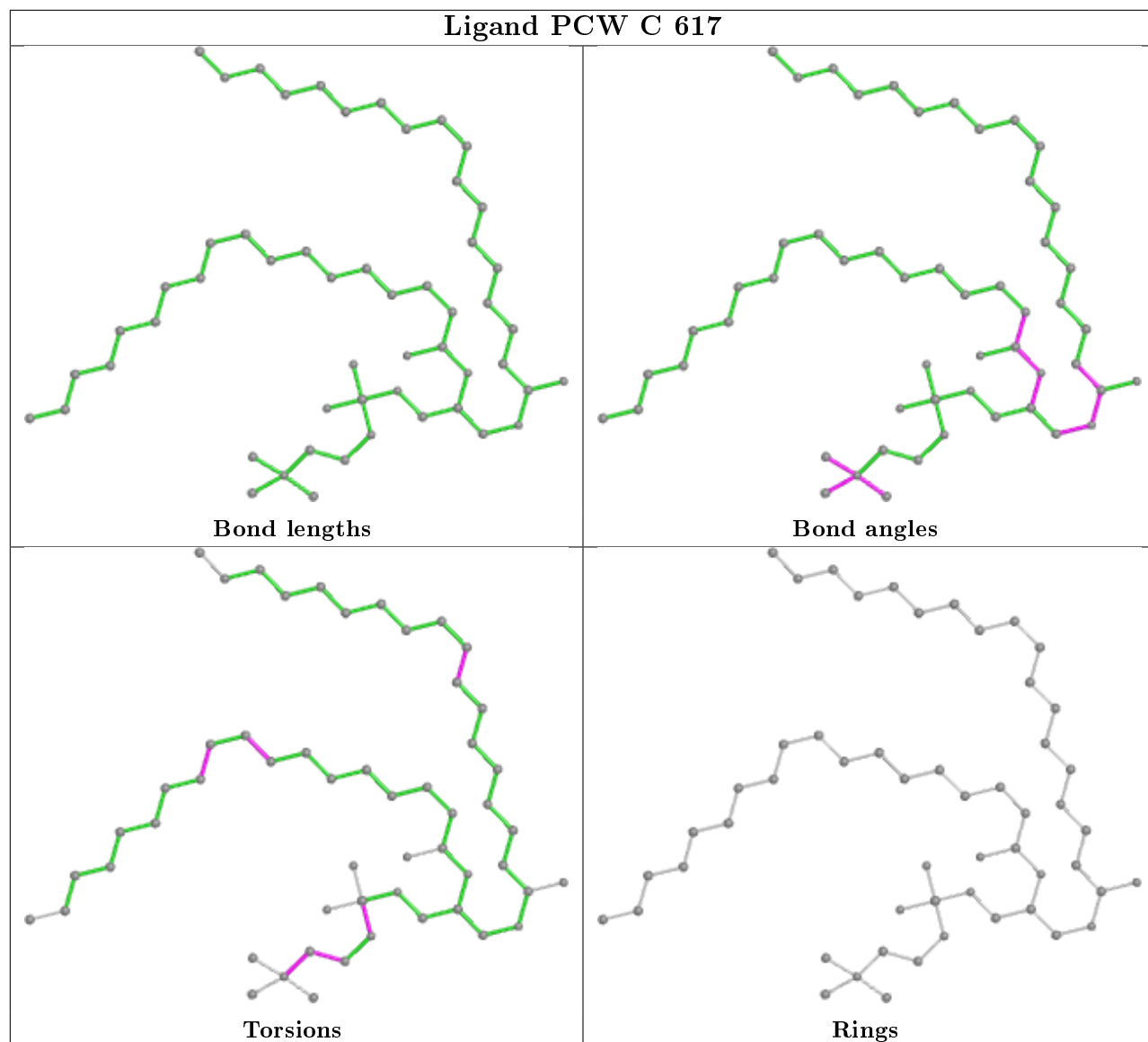


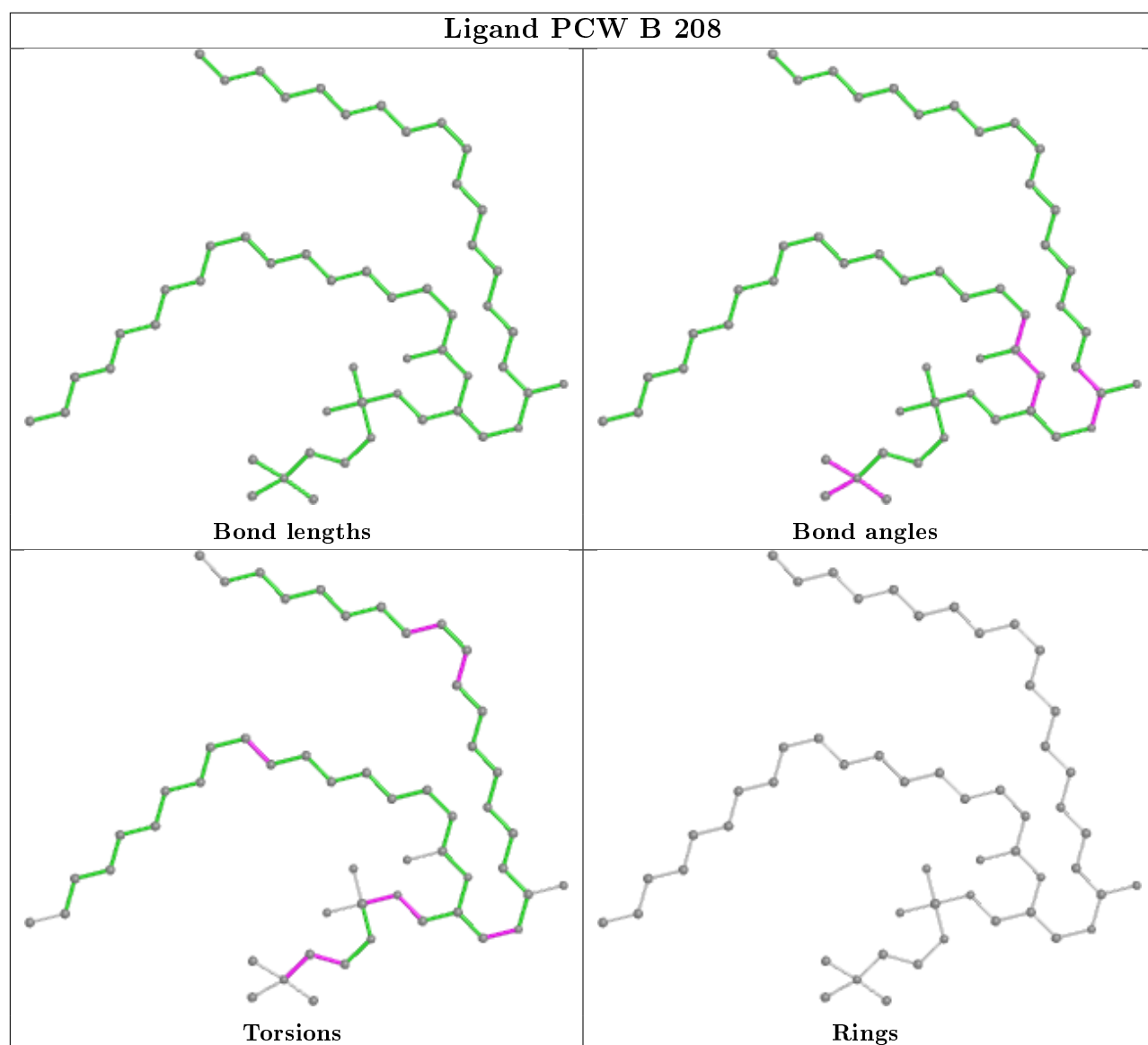


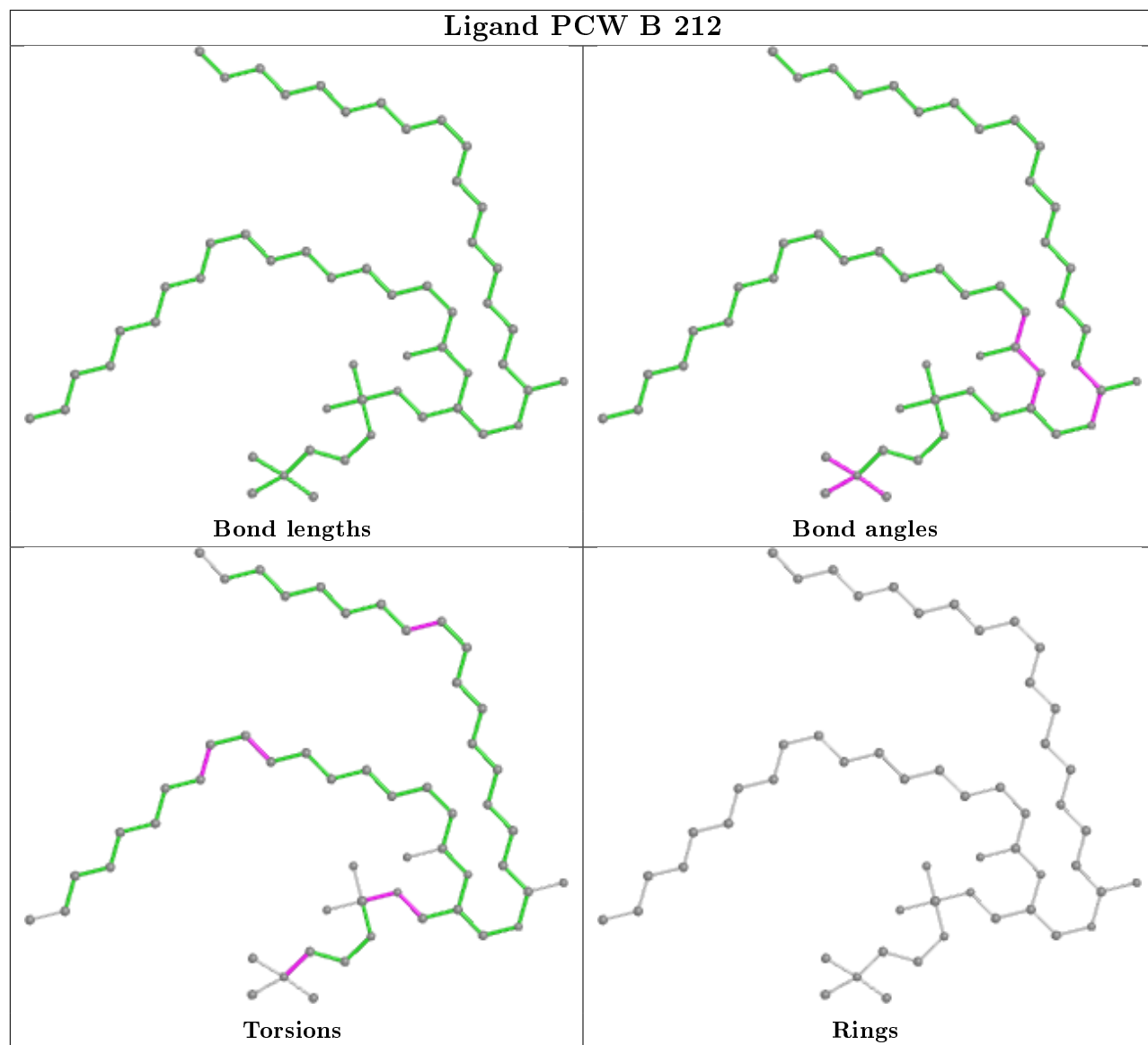


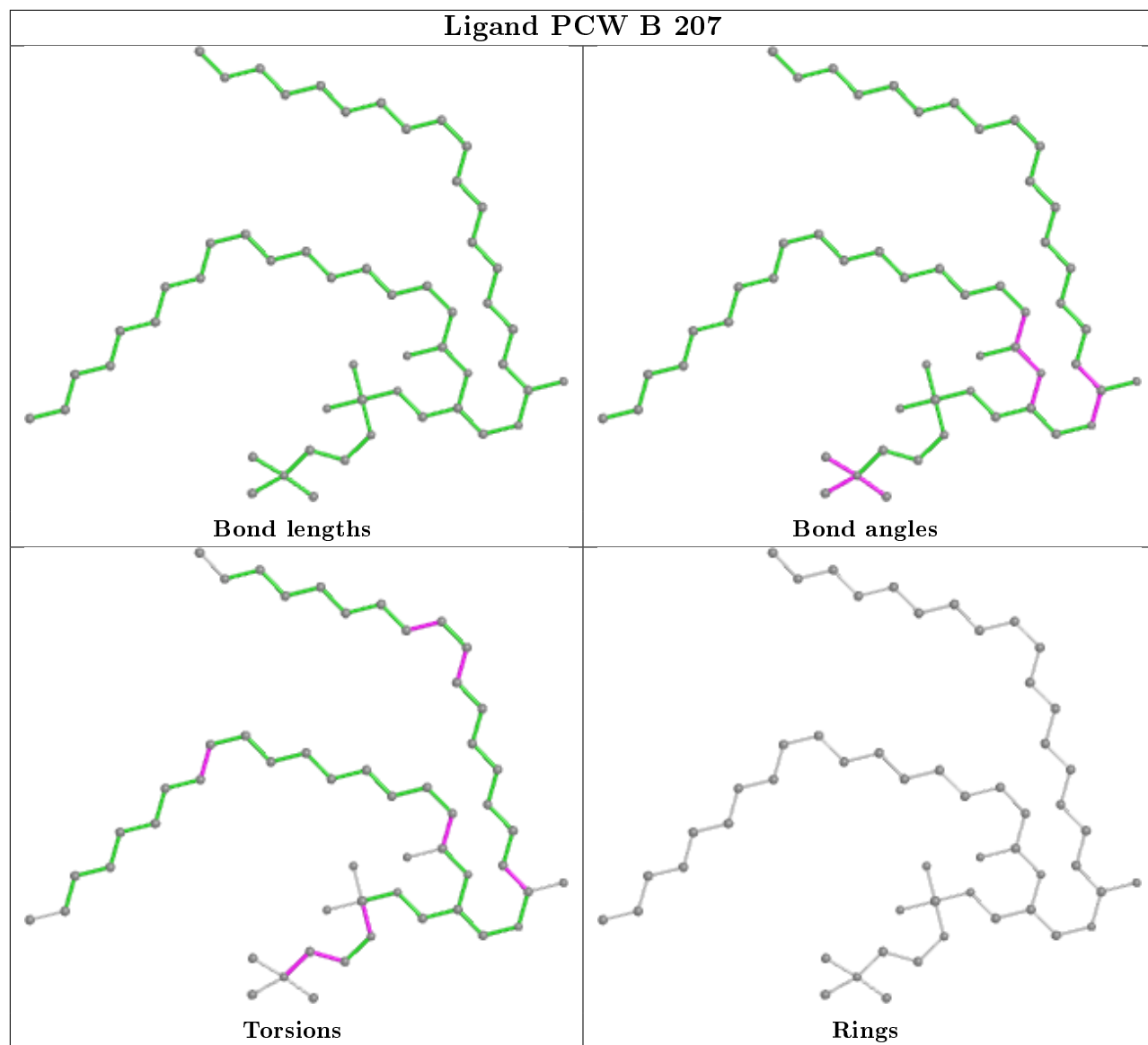


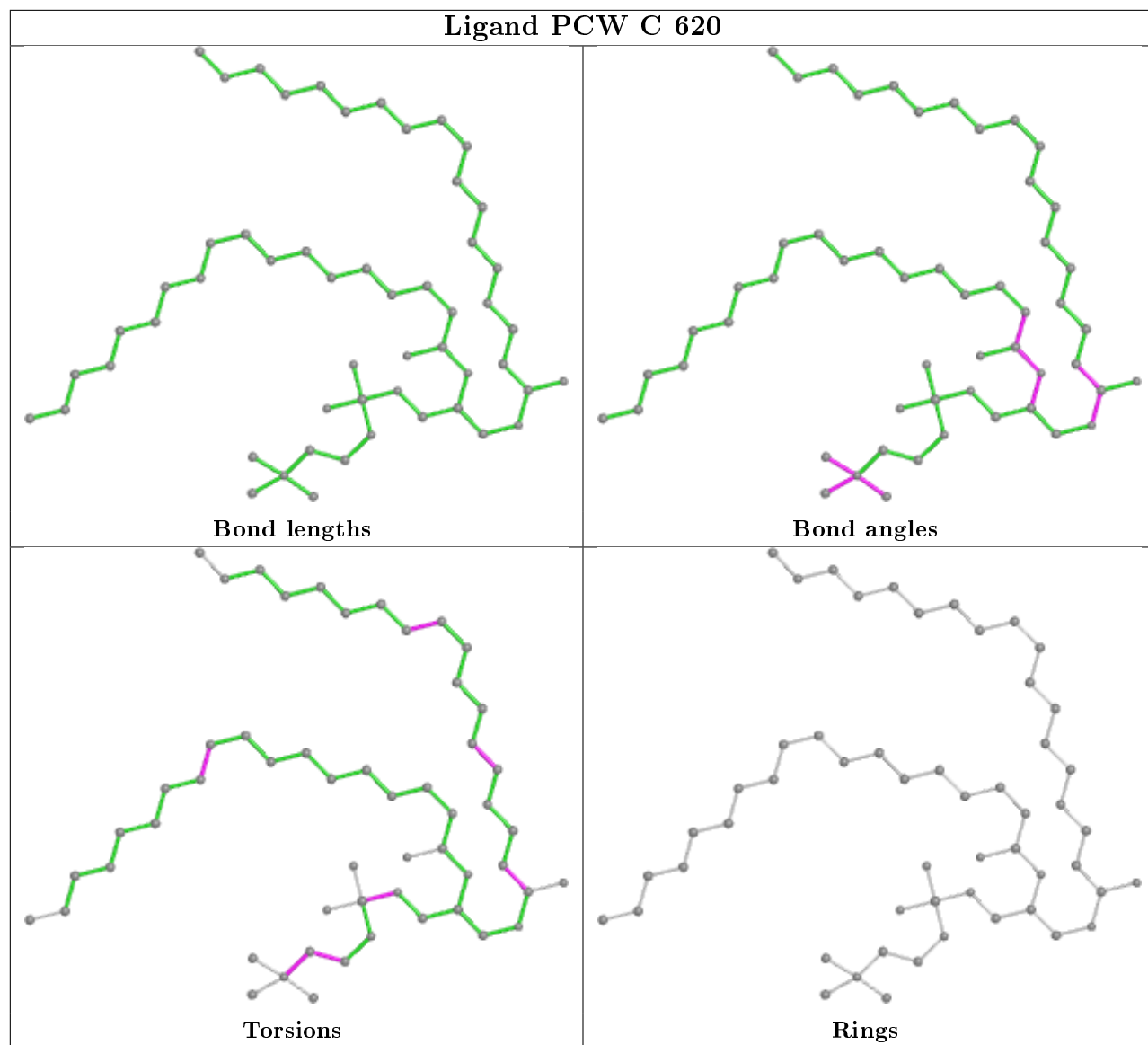


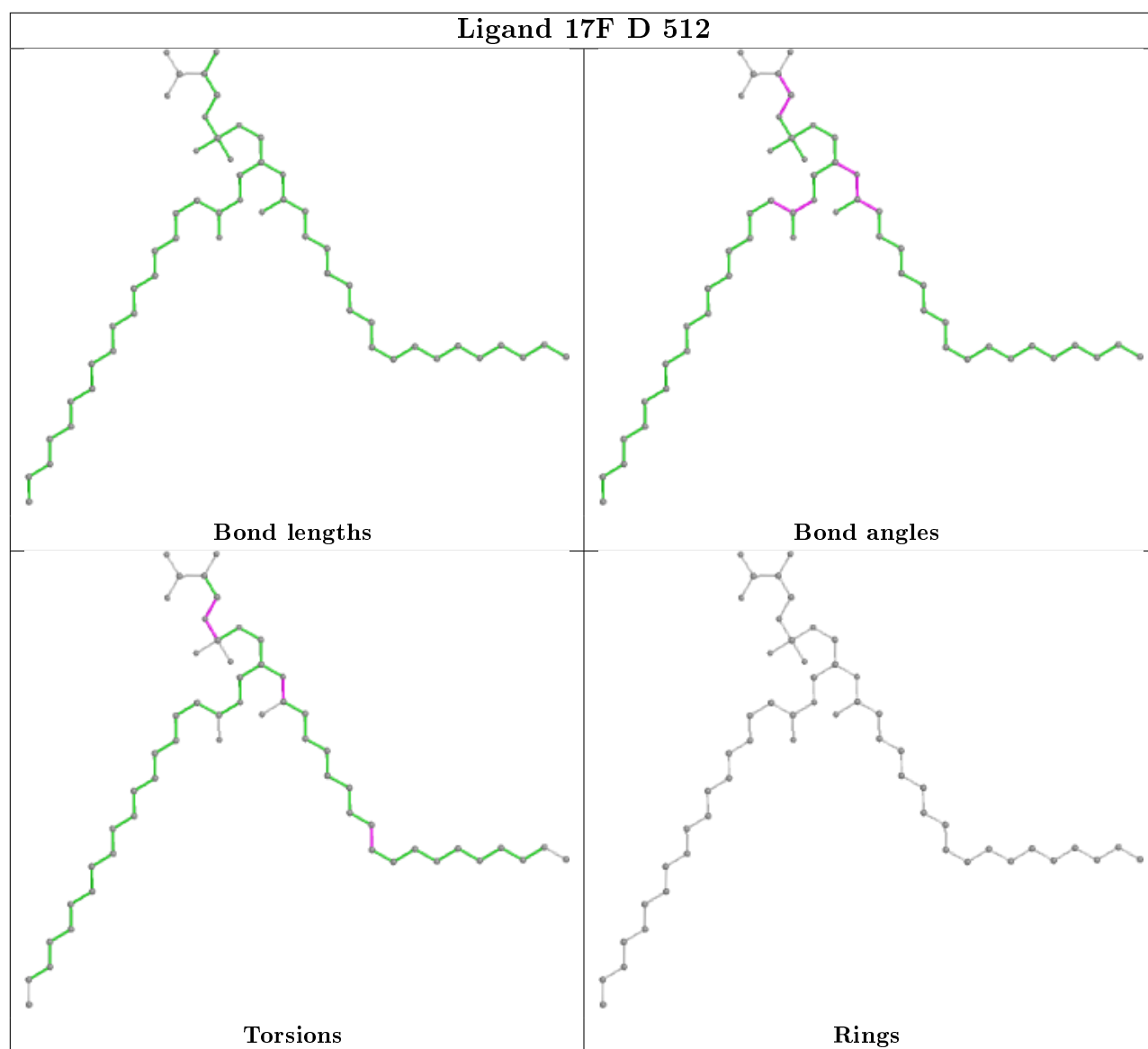


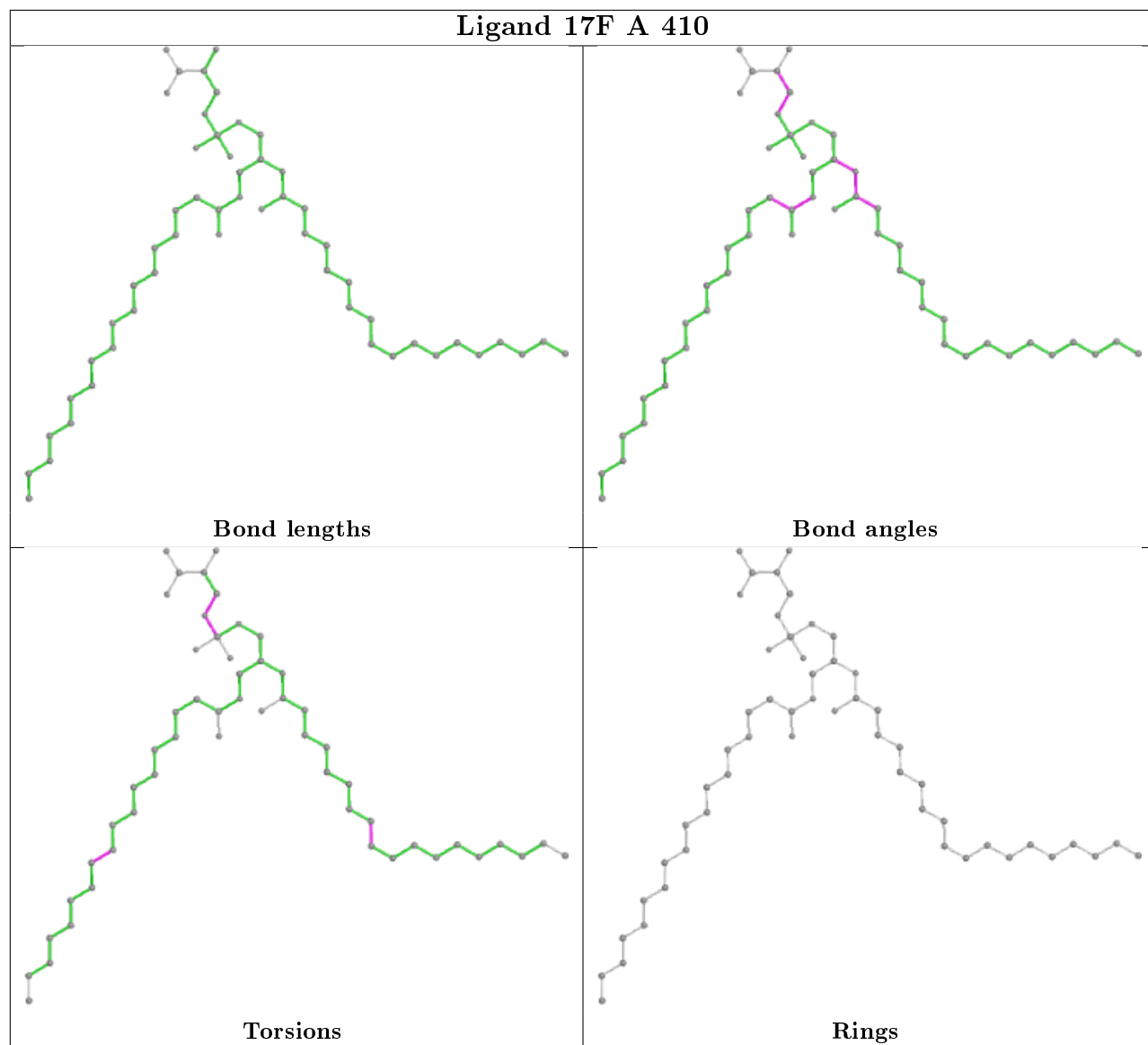


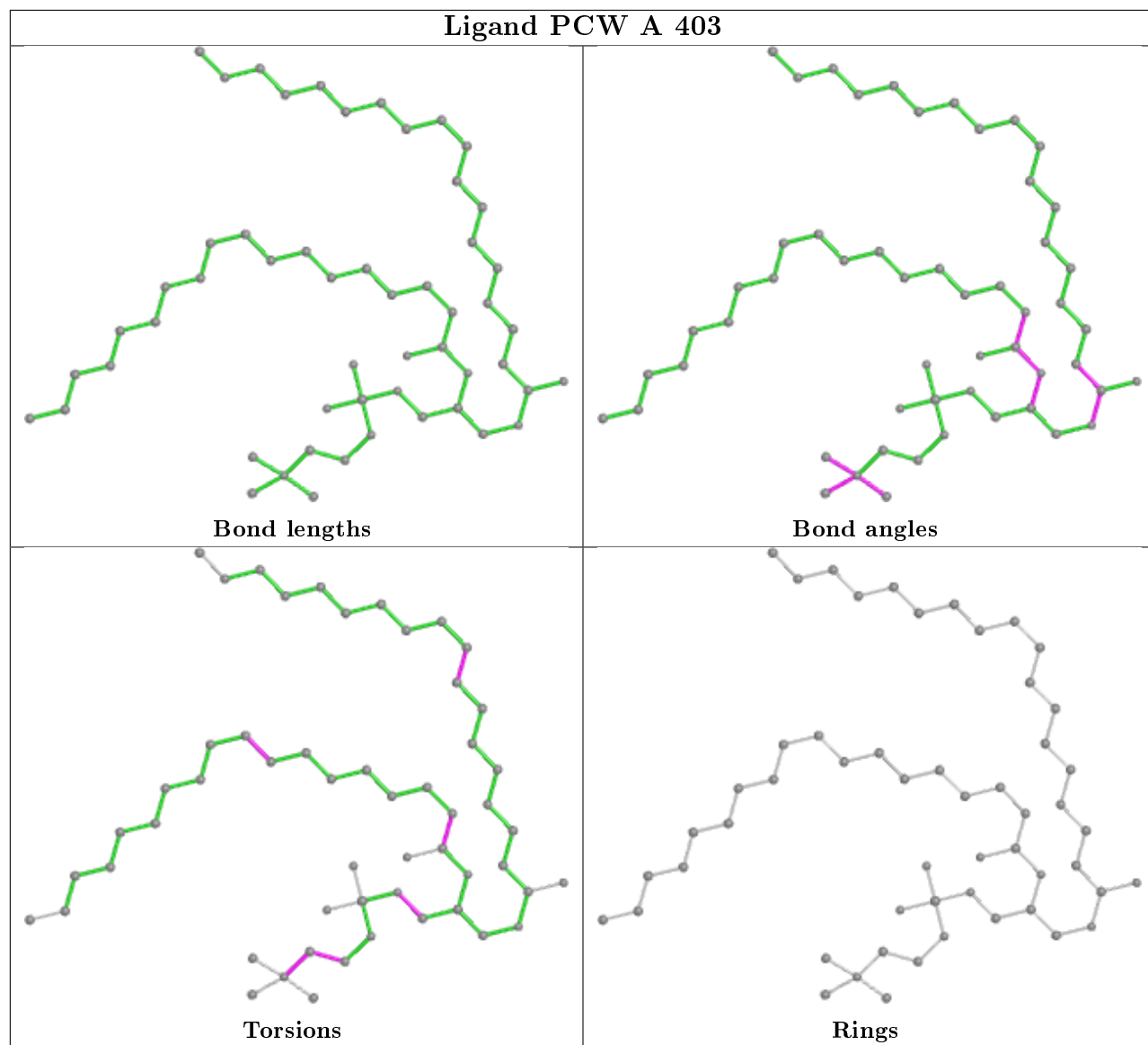


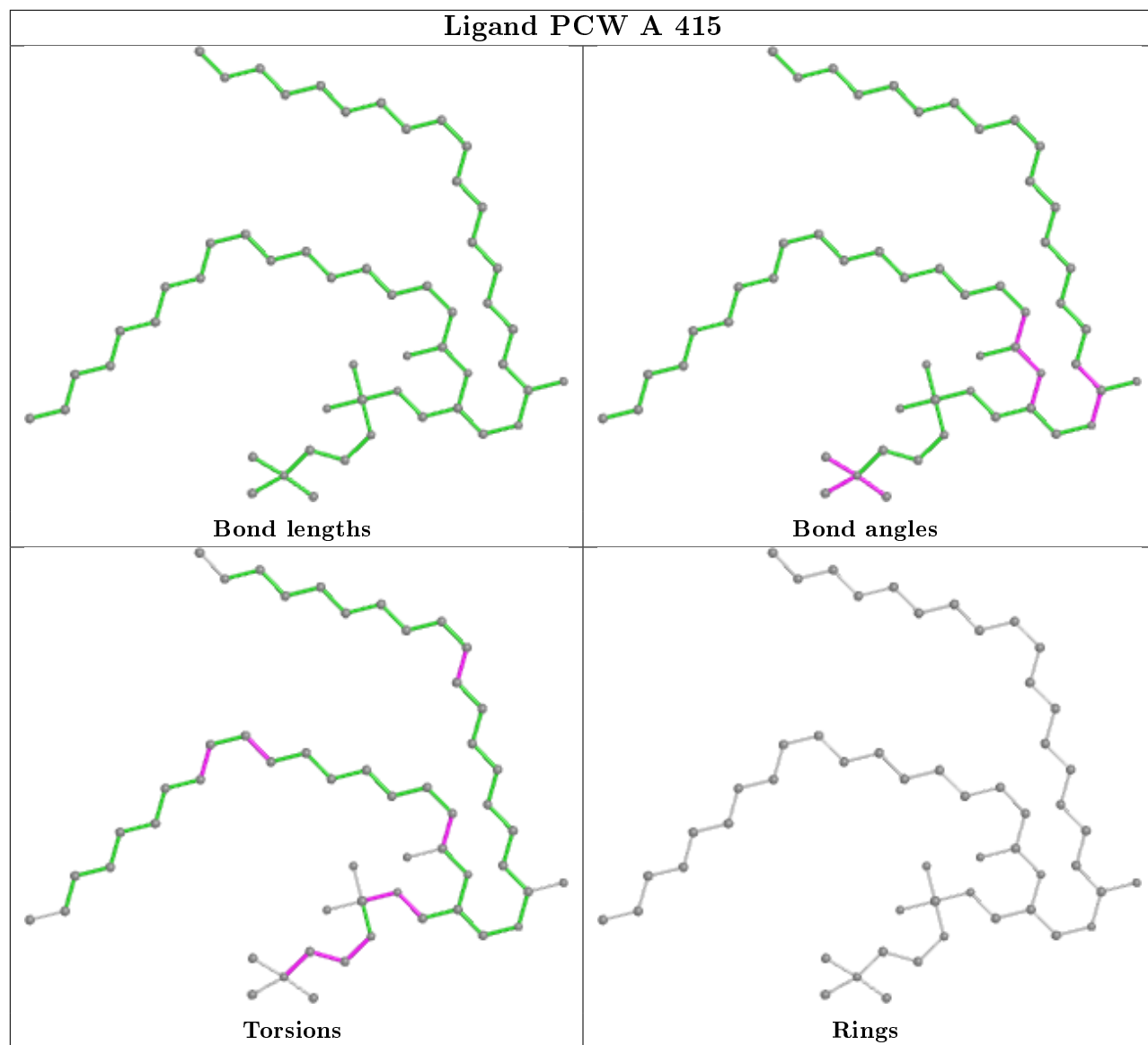


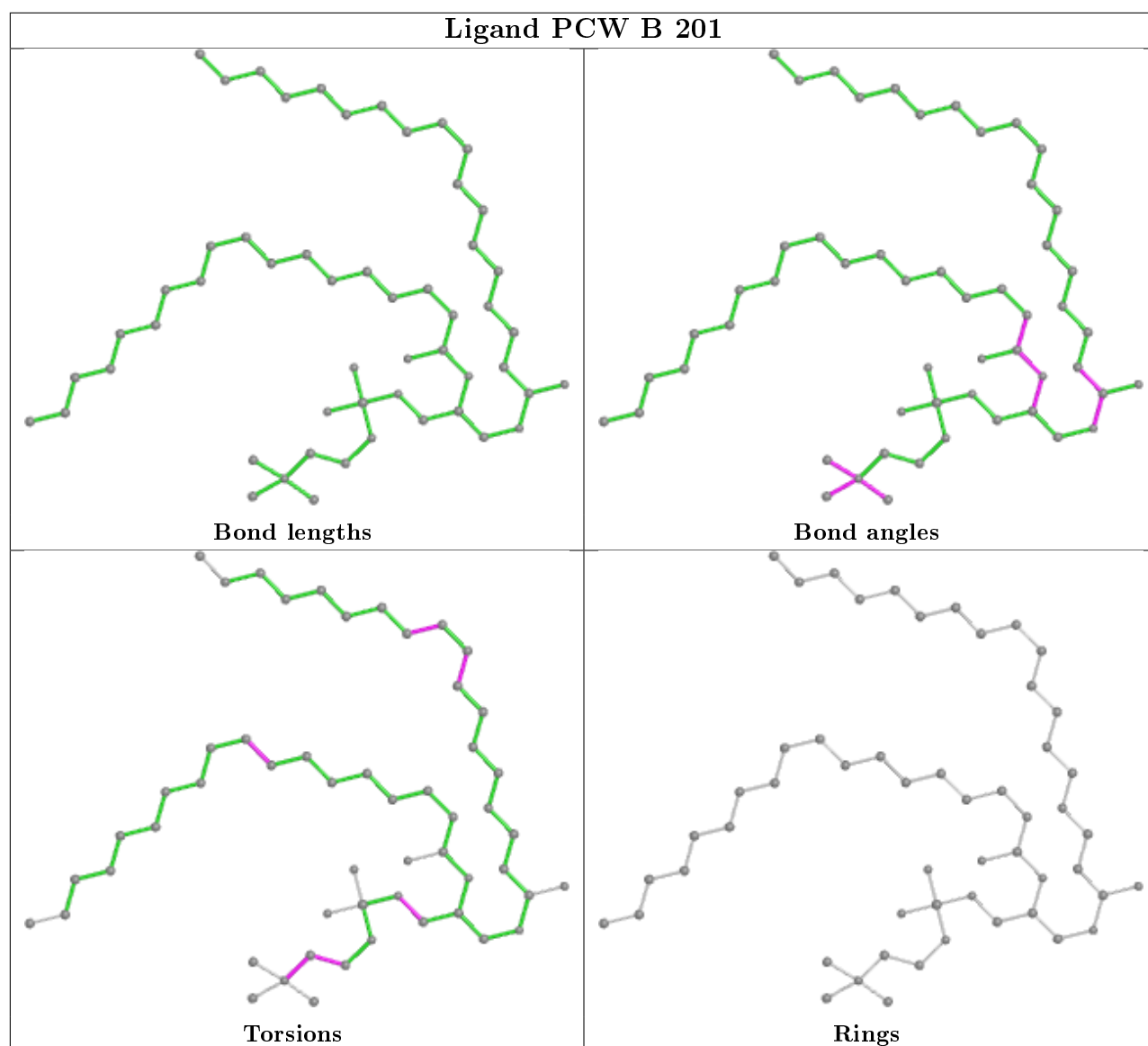


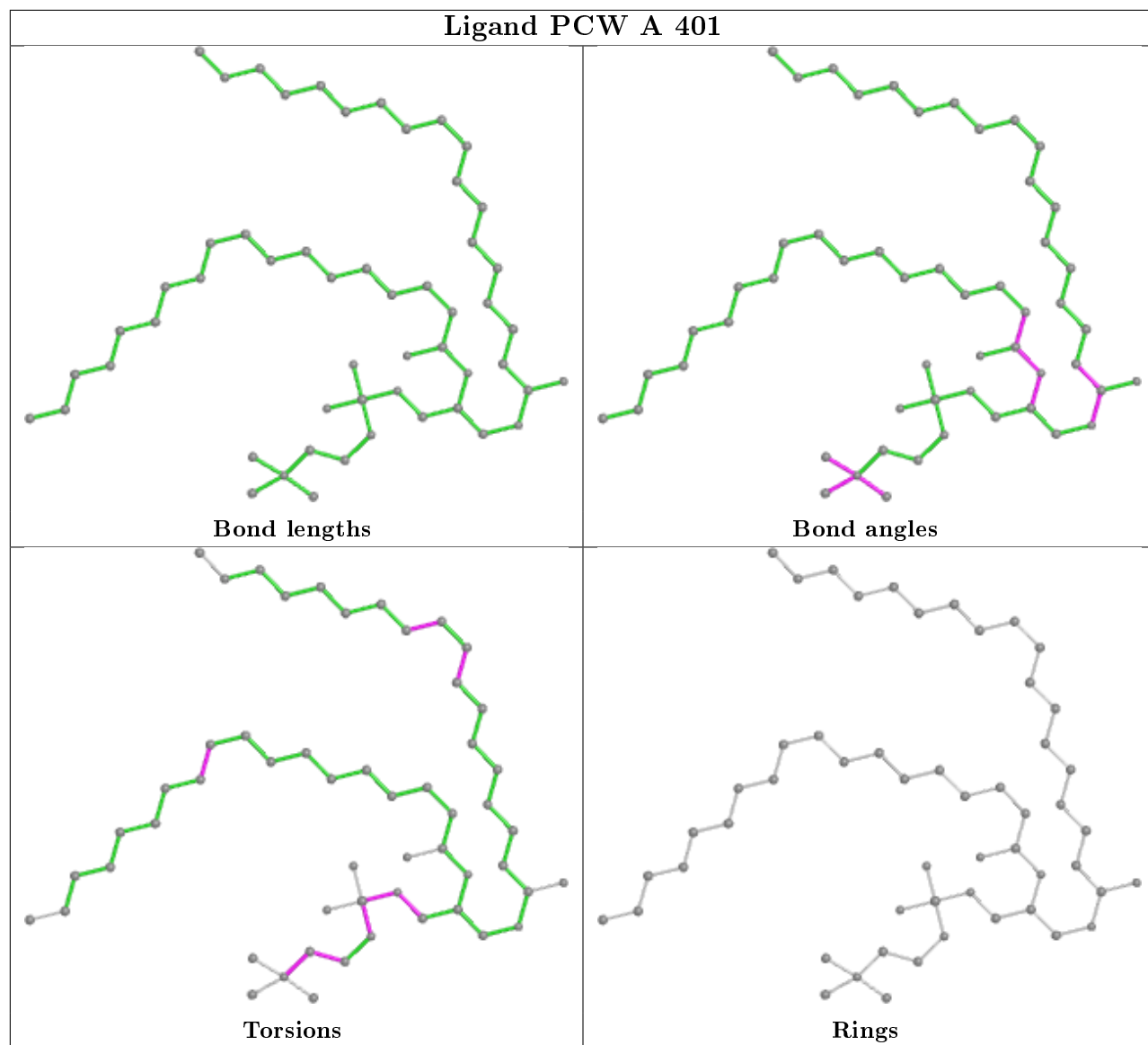


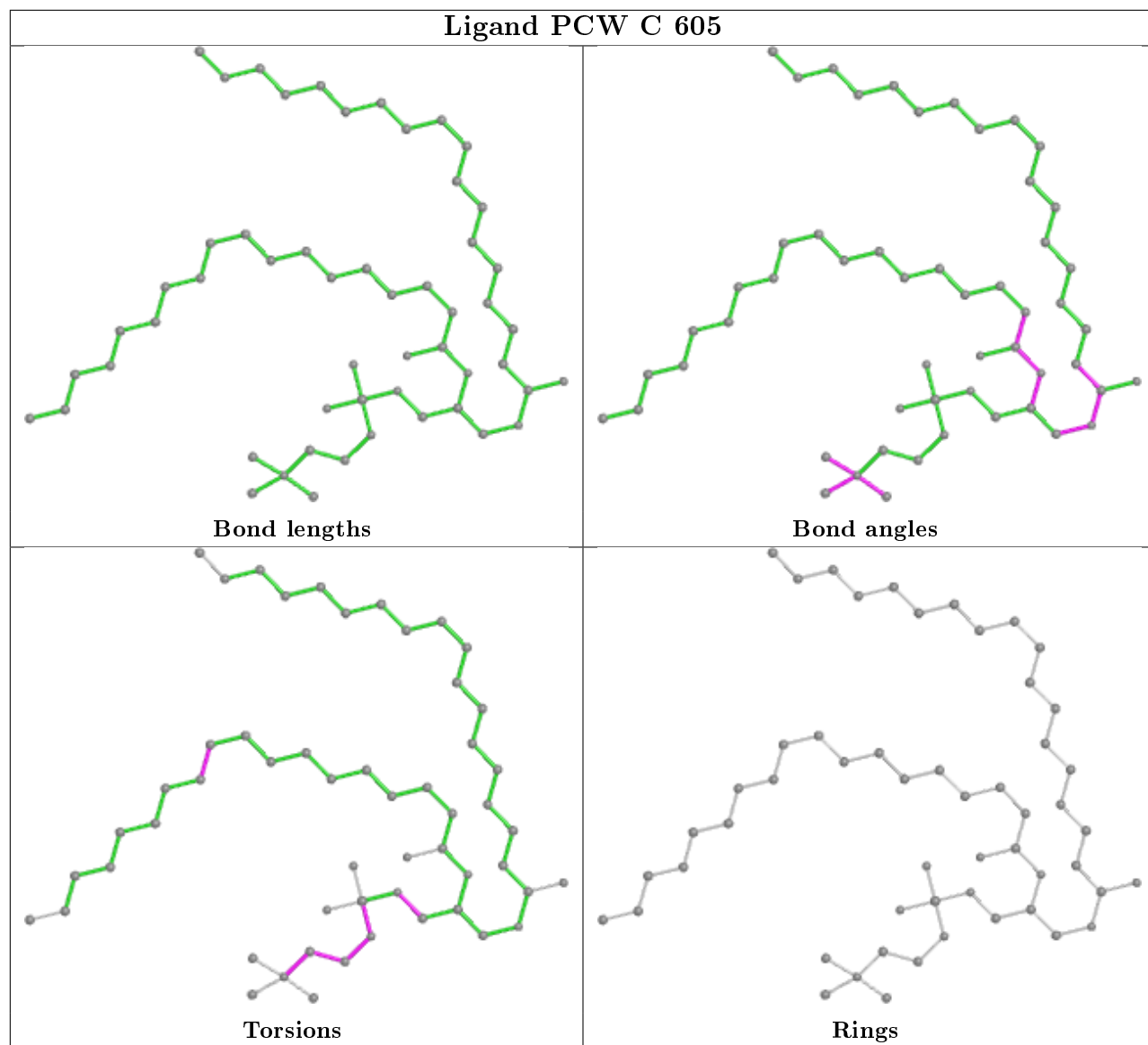


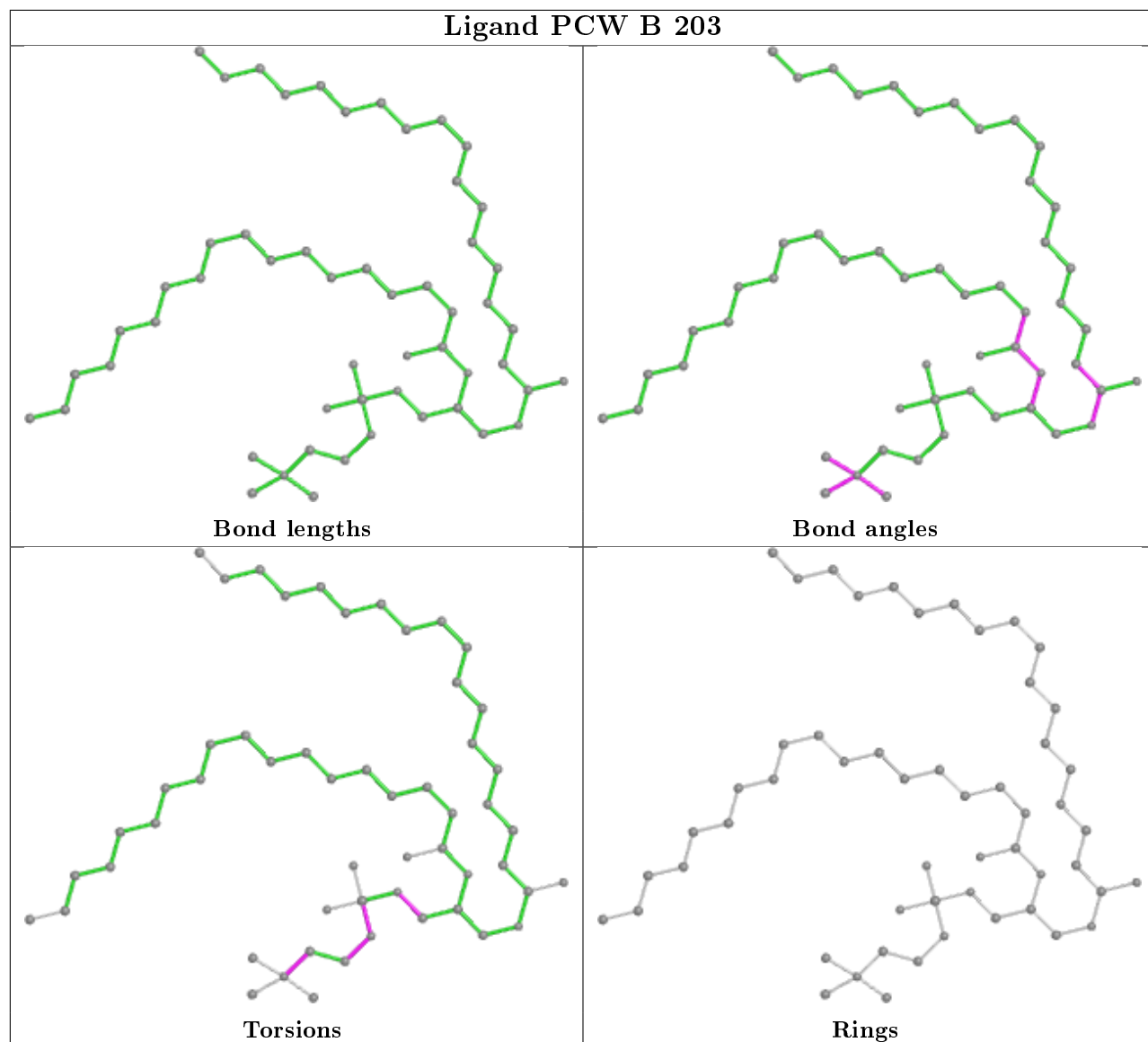












6.7 Other polymers [i](#)

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

The completeness of assignment taking into account all chemical shift lists is 5% for the well-defined parts and 5% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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	557
Number of shifts mapped to atoms	557
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

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	198	-0.54 ± 0.37	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 5%, i.e. 475 atoms were assigned a chemical shift out of a possible 9009. 4 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	394/3456 (11%)	197/1378 (14%)	0/1400 (0%)	197/678 (29%)
Sidechain	81/4938 (2%)	40/2896 (1%)	41/1786 (2%)	0/256 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/615 (0%)	0/329 (0%)	0/256 (0%)	0/30 (0%)
Overall	475/9009 (5%)	237/4603 (5%)	41/3442 (1%)	197/964 (20%)

7.1.4 Statistically unusual chemical shifts [i](#)

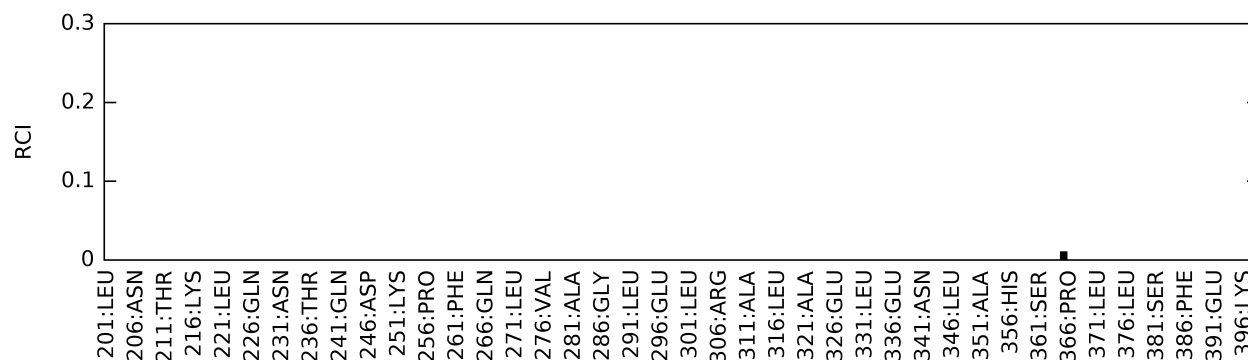
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	48	GLY	N	140.27	129.07 – 90.27	7.9

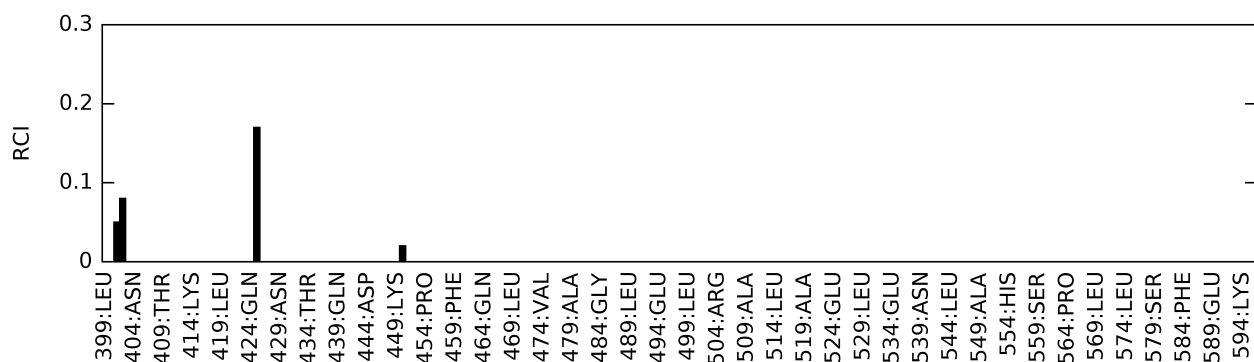
7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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.

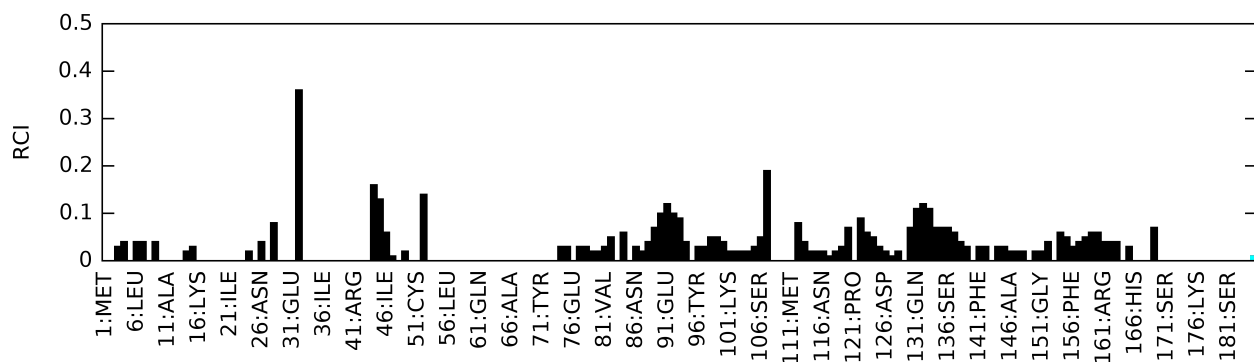
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain D:

