



# wwPDB NMR Structure Validation Summary Report ⓘ

Aug 9, 2020 – 06:01 PM BST

PDB ID : 6W4F  
Title : NMR-driven structure of KRAS4B-GDP homodimer on a lipid bilayer nanodisc  
Authors : Lee, K.; Fang, Z.; Enomoto, M.; Gasmi-Seabrook, G.M.; Zheng, L.; Marshall, C.B.; Ikura, M.  
Deposited on : 2020-03-10

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

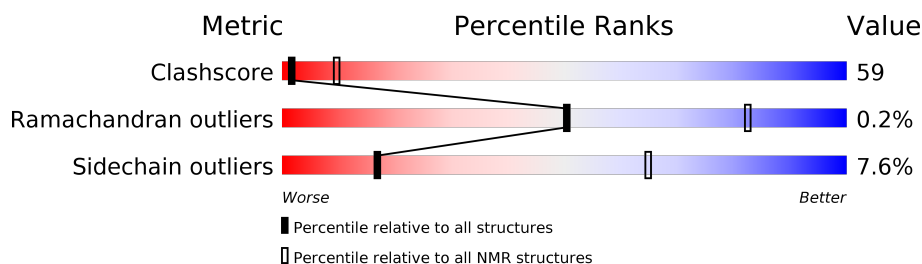
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 1%.

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  $\geq 3$ , 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	79% 13% 7% .
1	D	200	85% 14% ..
2	B	184	81% 7% 10% .
2	C	184	83% 8% 8% .

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:214-A:398, D:399-D:595 (382)	0.20	7
2	B:2-B:61, B:65-B:166, C:2-C:61, C:65-C:170 (328)	0.60	15

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 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 5, 6, 11, 13, 14, 17
2	7, 16, 18, 20
3	1, 2, 9, 10
4	4, 12, 15, 19
Single-model clusters	8

### 3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12018 atoms, of which 1522 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	D	198	Total	C	H	N	O	S	0
			2002	1019	379	287	314	3	

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
D	397	GLY	-	expression tag	UNP P02647
D	398	PRO	-	expression tag	UNP P02647

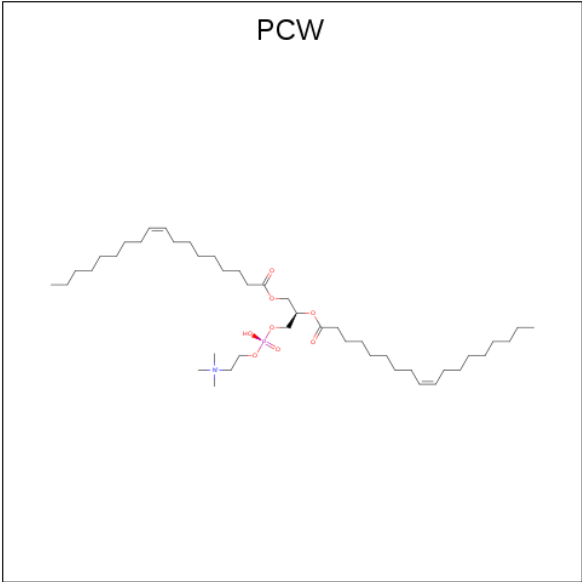
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	180	Total	C	H	N	O	S	0
			1788	898	352	252	279	7	
2	C	180	Total	C	H	N	O	S	0
			1788	898	352	252	279	7	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ASP	GLY	conflict	UNP P01116
C	12	ASP	GLY	conflict	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



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
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				
			Total	C	N	O	P
3	A	1	Total 54	44	1	8	1
3	A	1	Total 54	44	1	8	1
3	A	1	Total 54	44	1	8	1
3	A	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1

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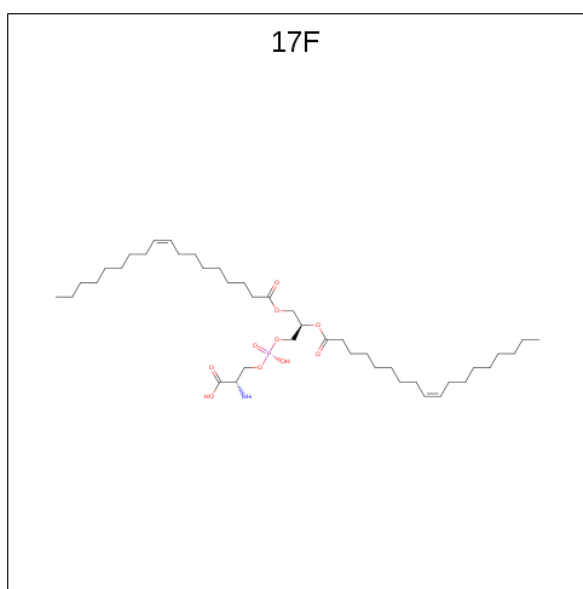
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54	44	1	8	1
3	D	1	Total 54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

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

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: C<sub>42</sub>H<sub>78</sub>NO<sub>10</sub>P).



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

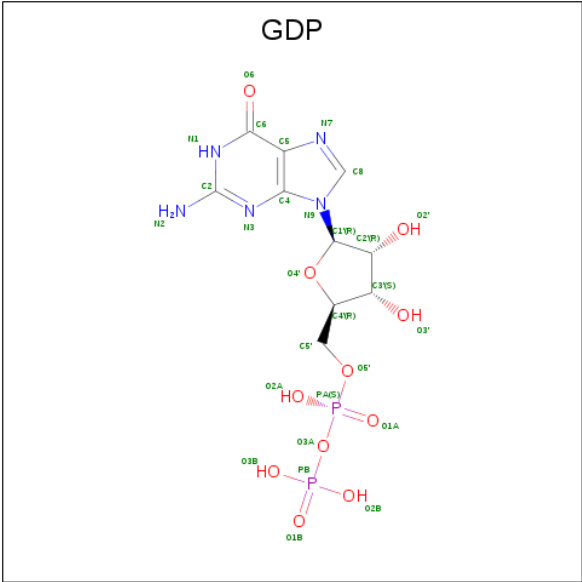
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Mol	Chain	Residues	Atoms					
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					
5	B	1	Total	C	H	N	O	P
			33	10	5	5	11	2
5	C	1	Total	C	H	N	O	P
			33	10	5	5	11	2

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

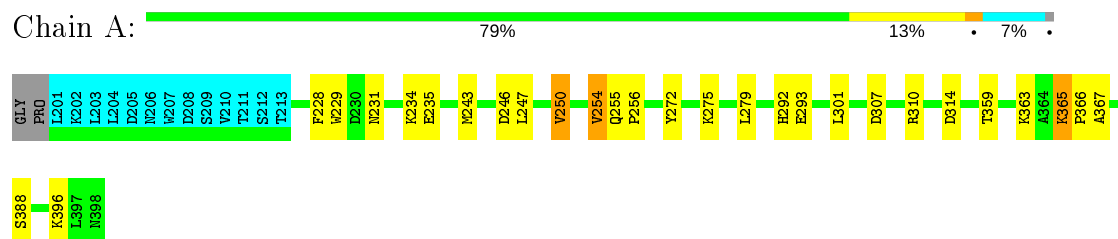
Mol	Chain	Residues	Atoms	
6	B	1	Total	Mg
			1	1
6	C	1	Total	Mg
			1	1

## 4 Residue-property plots [i](#)

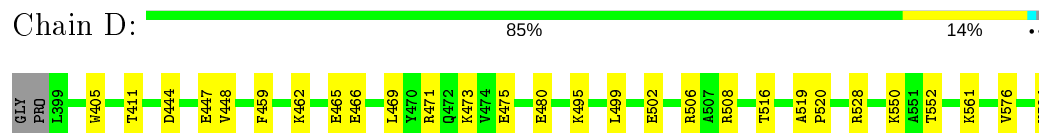
### 4.1 Average score per residue in the NMR ensemble

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.

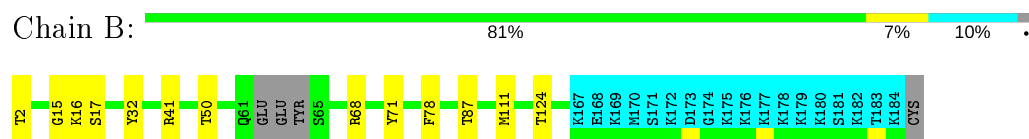
- Molecule 1: Apolipoprotein A-I



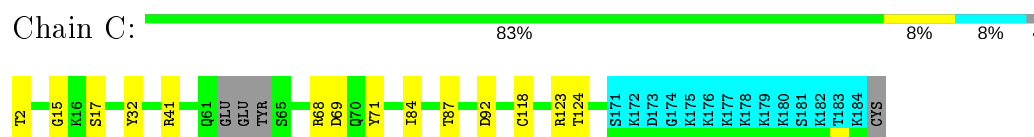
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



- Molecule 2: GTPase KRas



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

The representative model is number 7. Colouring as in section 4.1 above.



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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	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	190
Number of shifts mapped to atoms	190
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1519	358	1524	23±4
1	D	1615	376	1620	20±4
2	B	1289	298	1268	13±4
2	C	1324	308	1309	14±5
3	A	972	0	1440	360±23
3	B	594	0	880	276±18
3	C	432	0	640	202±22
3	D	1458	0	2160	555±25
4	A	108	6	152	33±8
4	B	216	12	304	85±11
4	C	108	6	152	49±8
4	D	432	24	608	164±12
5	B	28	5	12	7±2
5	C	28	5	12	6±3
6	B	1	0	0	1±0
6	C	1	0	0	1±0
All	All	202500	27960	241622	26238

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 59.

5 of 10242 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:H142	3:A:411:PCW:C19	1.18	1.69	6	11
3:B:209:PCW:C27	3:B:209:PCW:H222	1.17	1.70	7	2
3:A:401:PCW:H62	3:B:209:PCW:H131	1.16	1.17	19	1
3:B:209:PCW:H222	3:B:209:PCW:C27	1.16	1.70	4	1
3:A:411:PCW:C19	3:A:411:PCW:H142	1.15	1.70	19	9

## 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	184/200 (92%)	179±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	32	76
1	D	196/200 (98%)	190±2 (97±1%)	6±2 (3±1%)	0±0 (0±0%)	100	100
2	B	159/184 (86%)	154±2 (97±1%)	5±2 (3±1%)	0±0 (0±0%)	50	82
2	C	163/184 (89%)	157±2 (96±1%)	6±2 (3±1%)	0±0 (0±0%)	54	85
All	All	14040/15360 (91%)	13600 (97%)	411 (3%)	29 (0%)	50	82

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

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	20
2	C	110	PRO	2
2	B	34	PRO	2
2	B	122	SER	1
2	B	48	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	161/175 (92%)	150±3 (93±2%)	11±3 (7±2%)	19	68
1	D	173/175 (99%)	160±2 (92±1%)	13±2 (8±1%)	16	64
2	B	143/164 (87%)	132±3 (92±2%)	11±3 (8±2%)	16	64
2	C	147/164 (90%)	135±3 (92±2%)	12±3 (8±2%)	15	63
All	All	12480/13560 (92%)	11533 (92%)	947 (8%)	17	65

5 of 224 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	D	516	THR	18
1	D	561	LYS	17
2	B	87	THR	17
1	A	254	VAL	17
1	D	550	LYS	17

### 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, 2 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.



Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	D	613	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	A	417	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	B	212	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	419	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	D	618	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	C	205	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	D	631	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	C	212	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	17F	D	629	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	A	406	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	B	210	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	603	-	53,53,53	0.81±0.00	0±0 (0±0%)
5	GDP	C	201	-	24,30,30	1.53±0.00	0±0 (0±0%)
4	17F	D	630	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	A	405	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	B	208	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	413	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	B	217	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	17F	A	414	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	D	601	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	17F	D	635	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	B	205	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	B	206	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	D	609	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	17F	D	633	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	D	615	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	A	403	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	407	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	C	207	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	A	401	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	C	209	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	402	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	B	211	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	420	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	620	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	D	628	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	A	410	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	C	206	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	C	211	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	B	207	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	627	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	D	623	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	B	213	-	53,53,53	0.81±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	D	610	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	C	204	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	625	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	D	621	-	53,53,53	0.81±0.00	0±0 (0±0%)
4	17F	B	215	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	17F	A	415	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	B	204	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	D	605	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	612	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	626	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	409	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	B	209	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	416	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	608	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	624	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	C	208	-	53,53,53	0.81±0.00	0±0 (0±0%)
5	GDP	B	201	-	24,30,30	1.35±0.00	0±0 (0±0%)
3	PCW	D	602	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	A	411	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	604	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	614	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	C	203	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	D	632	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	B	203	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	607	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	D	617	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	412	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	D	622	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	408	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	B	216	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	D	611	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	A	418	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	616	-	53,53,53	0.81±0.00	0±0 (0±0%)
3	PCW	A	404	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	C	210	-	50,53,53	0.78±0.00	0±0 (0±0%)
4	17F	B	214	-	50,53,53	0.78±0.00	0±0 (0±0%)
3	PCW	D	619	-	53,53,53	0.80±0.00	0±0 (0±0%)
3	PCW	D	606	-	53,53,53	0.80±0.00	0±0 (0±0%)
4	17F	D	634	-	50,53,53	0.78±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	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	D	613	-	59,61,61	2.62±0.00	1±0 (1±0%)
3	PCW	A	417	-	59,61,61	2.68±0.00	1±0 (1±0%)
3	PCW	B	212	-	59,61,61	2.61±0.00	1±0 (1±0%)
3	PCW	A	419	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	D	618	-	59,61,61	2.67±0.00	1±0 (1±0%)
3	PCW	C	205	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	17F	D	631	-	52,60,60	1.14±0.00	0±0 (0±0%)
3	PCW	C	212	-	59,61,61	2.71±0.00	1±0 (1±0%)
4	17F	D	629	-	52,60,60	1.11±0.00	0±0 (0±0%)
3	PCW	A	406	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	B	210	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	D	603	-	59,61,61	2.63±0.00	1±0 (1±0%)
5	GDP	C	201	-	31,47,47	2.04±0.00	2±0 (6±0%)
4	17F	D	630	-	52,60,60	1.07±0.00	0±0 (0±0%)
3	PCW	A	405	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	B	208	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	A	413	-	59,61,61	2.68±0.00	1±0 (1±0%)
4	17F	B	217	-	52,60,60	1.28±0.00	1±0 (1±0%)
4	17F	A	414	-	52,60,60	1.34±0.00	0±0 (0±0%)
3	PCW	D	601	-	59,61,61	2.62±0.00	1±0 (1±0%)
4	17F	D	635	-	52,60,60	1.03±0.00	0±0 (0±0%)
3	PCW	B	205	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	B	206	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	D	609	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	17F	D	633	-	52,60,60	1.16±0.00	0±0 (0±0%)
3	PCW	D	615	-	59,61,61	2.66±0.00	1±0 (1±0%)
3	PCW	A	403	-	59,61,61	2.62±0.00	1±0 (1±0%)
3	PCW	A	407	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	C	207	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	A	401	-	59,61,61	2.61±0.00	1±0 (1±0%)
3	PCW	C	209	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	A	402	-	59,61,61	2.65±0.00	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	B	211	-	59,61,61	2.62±0.00	1±0 (1±0%)
3	PCW	A	420	-	59,61,61	2.62±0.00	1±0 (1±0%)
3	PCW	D	620	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	17F	D	628	-	52,60,60	1.11±0.00	0±0 (0±0%)
3	PCW	A	410	-	59,61,61	2.61±0.00	1±0 (1±0%)
3	PCW	C	206	-	59,61,61	2.64±0.00	1±0 (1±0%)
4	17F	C	211	-	52,60,60	1.15±0.00	0±0 (0±0%)
3	PCW	B	207	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	D	627	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	D	623	-	59,61,61	2.61±0.00	1±0 (1±0%)
3	PCW	B	213	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	D	610	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	C	204	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	D	625	-	59,61,61	2.62±0.00	1±0 (1±0%)
3	PCW	D	621	-	59,61,61	2.60±0.00	1±0 (1±0%)
4	17F	B	215	-	52,60,60	1.13±0.00	0±0 (0±0%)
4	17F	A	415	-	52,60,60	1.13±0.00	0±0 (0±0%)
3	PCW	B	204	-	59,61,61	2.72±0.00	1±0 (1±0%)
3	PCW	D	605	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	D	612	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	D	626	-	59,61,61	2.66±0.00	1±0 (1±0%)
3	PCW	A	409	-	59,61,61	2.61±0.00	1±0 (1±0%)
3	PCW	B	209	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	A	416	-	59,61,61	2.62±0.00	1±0 (1±0%)
3	PCW	D	608	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	D	624	-	59,61,61	2.61±0.00	1±0 (1±0%)
3	PCW	C	208	-	59,61,61	2.64±0.00	1±0 (1±0%)
5	GDP	B	201	-	31,47,47	1.89±0.00	2±0 (6±0%)
3	PCW	D	602	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	A	411	-	59,61,61	2.61±0.00	1±0 (1±0%)
3	PCW	D	604	-	59,61,61	2.68±0.00	1±0 (1±0%)
3	PCW	D	614	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	C	203	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	17F	D	632	-	52,60,60	1.37±0.00	0±0 (0±0%)
3	PCW	B	203	-	59,61,61	2.64±0.00	1±0 (1±0%)
3	PCW	D	607	-	59,61,61	2.63±0.00	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	D	617	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	A	412	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	D	622	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	A	408	-	59,61,61	2.65±0.00	1±0 (1±0%)
4	17F	B	216	-	52,60,60	1.12±0.00	0±0 (0±0%)
3	PCW	D	611	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	A	418	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	D	616	-	59,61,61	2.65±0.00	1±0 (1±0%)
3	PCW	A	404	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	17F	C	210	-	52,60,60	1.15±0.00	0±0 (0±0%)
4	17F	B	214	-	52,60,60	1.13±0.00	0±0 (0±0%)
3	PCW	D	619	-	59,61,61	2.63±0.00	1±0 (1±0%)
3	PCW	D	606	-	59,61,61	2.63±0.00	1±0 (1±0%)
4	17F	D	634	-	52,60,60	1.12±0.00	0±0 (0±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	D	601	-	-	0±0,57,57,57	-
3	PCW	A	419	-	-	0±0,57,57,57	-
3	PCW	A	420	-	-	0±0,57,57,57	-
4	17F	D	635	-	-	0±0,55,59,59	-
3	PCW	D	627	-	-	0±0,57,57,57	-
4	17F	B	215	-	-	1±0,55,59,59	-
3	PCW	C	209	-	-	0±0,57,57,57	-
3	PCW	B	204	-	-	0±0,57,57,57	-
3	PCW	D	615	-	-	0±0,57,57,57	-
3	PCW	D	612	-	-	0±0,57,57,57	-
3	PCW	A	407	-	-	0±0,57,57,57	-
3	PCW	C	208	-	-	0±0,57,57,57	-
4	17F	A	415	-	-	0±0,55,59,59	-
3	PCW	A	412	-	-	0±0,57,57,57	-
3	PCW	A	416	-	-	0±0,57,57,57	-
3	PCW	D	623	-	-	0±0,57,57,57	-
3	PCW	C	204	-	-	0±0,57,57,57	-
3	PCW	B	206	-	-	0±0,57,57,57	-
4	17F	B	214	-	-	0±0,55,59,59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	D	614	-	-	0±0,57,57,57	-
3	PCW	D	604	-	-	0±0,57,57,57	-
4	17F	D	633	-	-	0±0,55,59,59	-
3	PCW	D	607	-	-	0±0,57,57,57	-
4	17F	B	216	-	-	0±0,55,59,59	-
3	PCW	B	211	-	-	0±0,57,57,57	-
3	PCW	D	613	-	-	0±0,57,57,57	-
4	17F	C	210	-	-	0±0,55,59,59	-
3	PCW	A	406	-	-	0±0,57,57,57	-
3	PCW	A	404	-	-	0±0,57,57,57	-
3	PCW	A	413	-	-	0±0,57,57,57	-
3	PCW	A	409	-	-	0±0,57,57,57	-
3	PCW	A	405	-	-	0±0,57,57,57	-
3	PCW	D	610	-	-	0±0,57,57,57	-
4	17F	D	634	-	-	0±0,55,59,59	-
3	PCW	B	209	-	-	0±0,57,57,57	-
4	17F	A	414	-	-	0±0,55,59,59	-
3	PCW	B	205	-	-	0±0,57,57,57	-
3	PCW	D	603	-	-	0±0,57,57,57	-
3	PCW	D	609	-	-	0±0,57,57,57	-
4	17F	D	628	-	-	0±0,55,59,59	-
3	PCW	C	203	-	-	0±0,57,57,57	-
4	17F	D	630	-	-	0±0,55,59,59	-
3	PCW	D	605	-	-	0±0,57,57,57	-
3	PCW	B	203	-	-	0±0,57,57,57	-
5	GDP	B	201	-	-	0±0,12,32,32	0±0,3,3,3
3	PCW	D	611	-	-	0±0,57,57,57	-
3	PCW	A	402	-	-	0±0,57,57,57	-
3	PCW	C	206	-	-	0±0,57,57,57	-
3	PCW	D	625	-	-	0±0,57,57,57	-
3	PCW	D	606	-	-	0±0,57,57,57	-
3	PCW	D	620	-	-	0±0,57,57,57	-
4	17F	D	629	-	-	2±0,55,59,59	-
4	17F	D	631	-	-	0±0,55,59,59	-
3	PCW	D	616	-	-	0±0,57,57,57	-
3	PCW	D	608	-	-	0±0,57,57,57	-
3	PCW	D	624	-	-	0±0,57,57,57	-
4	17F	B	217	-	-	1±0,55,59,59	-
3	PCW	A	401	-	-	0±0,57,57,57	-
3	PCW	A	418	-	-	0±0,57,57,57	-
3	PCW	A	410	-	-	0±0,57,57,57	-
3	PCW	C	205	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	D	621	-	-	0±0,57,57,57	-
3	PCW	A	411	-	-	0±0,57,57,57	-
3	PCW	D	618	-	-	0±0,57,57,57	-
3	PCW	C	212	-	-	0±0,57,57,57	-
3	PCW	A	417	-	-	0±0,57,57,57	-
3	PCW	B	208	-	-	0±0,57,57,57	-
3	PCW	C	207	-	-	0±0,57,57,57	-
3	PCW	B	207	-	-	0±0,57,57,57	-
5	GDP	C	201	-	-	0±0,12,32,32	0±0,3,3,3
3	PCW	A	403	-	-	0±0,57,57,57	-
3	PCW	D	619	-	-	0±0,57,57,57	-
3	PCW	D	617	-	-	0±0,57,57,57	-
3	PCW	D	622	-	-	0±0,57,57,57	-
3	PCW	B	212	-	-	0±0,57,57,57	-
4	17F	D	632	-	-	0±0,55,59,59	-
3	PCW	A	408	-	-	0±0,57,57,57	-
3	PCW	D	602	-	-	0±0,57,57,57	-
3	PCW	B	210	-	-	0±0,57,57,57	-
3	PCW	D	626	-	-	0±0,57,57,57	-
3	PCW	B	213	-	-	0±0,57,57,57	-
4	17F	C	211	-	-	0±0,55,59,59	-

There are no bond-length outliers.

5 of 69 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	407	PCW	C8-N-C7	18.05	62.56	108.97	7	20
3	D	614	PCW	C8-N-C7	18.05	62.56	108.97	18	20
3	A	405	PCW	C8-N-C7	18.05	62.58	108.97	19	20
3	C	207	PCW	C8-N-C7	18.04	62.58	108.97	12	20
3	C	204	PCW	C8-N-C7	18.05	62.58	108.97	13	20

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)
4	D	629	17F	O10-C17-O9-C5	20
4	D	629	17F	C18-C17-O9-C5	20
4	B	217	17F	O10-C17-O9-C5	20

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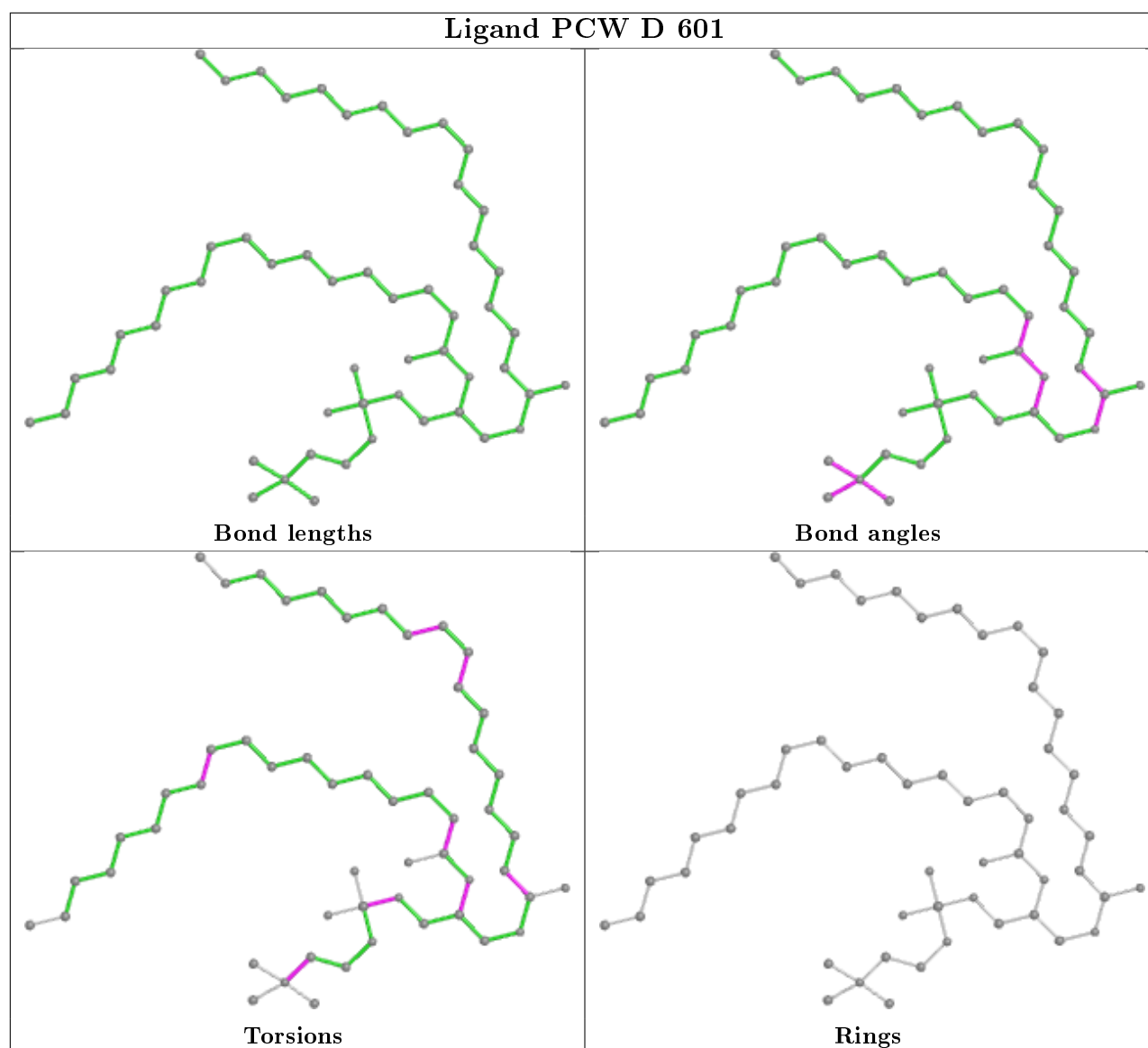
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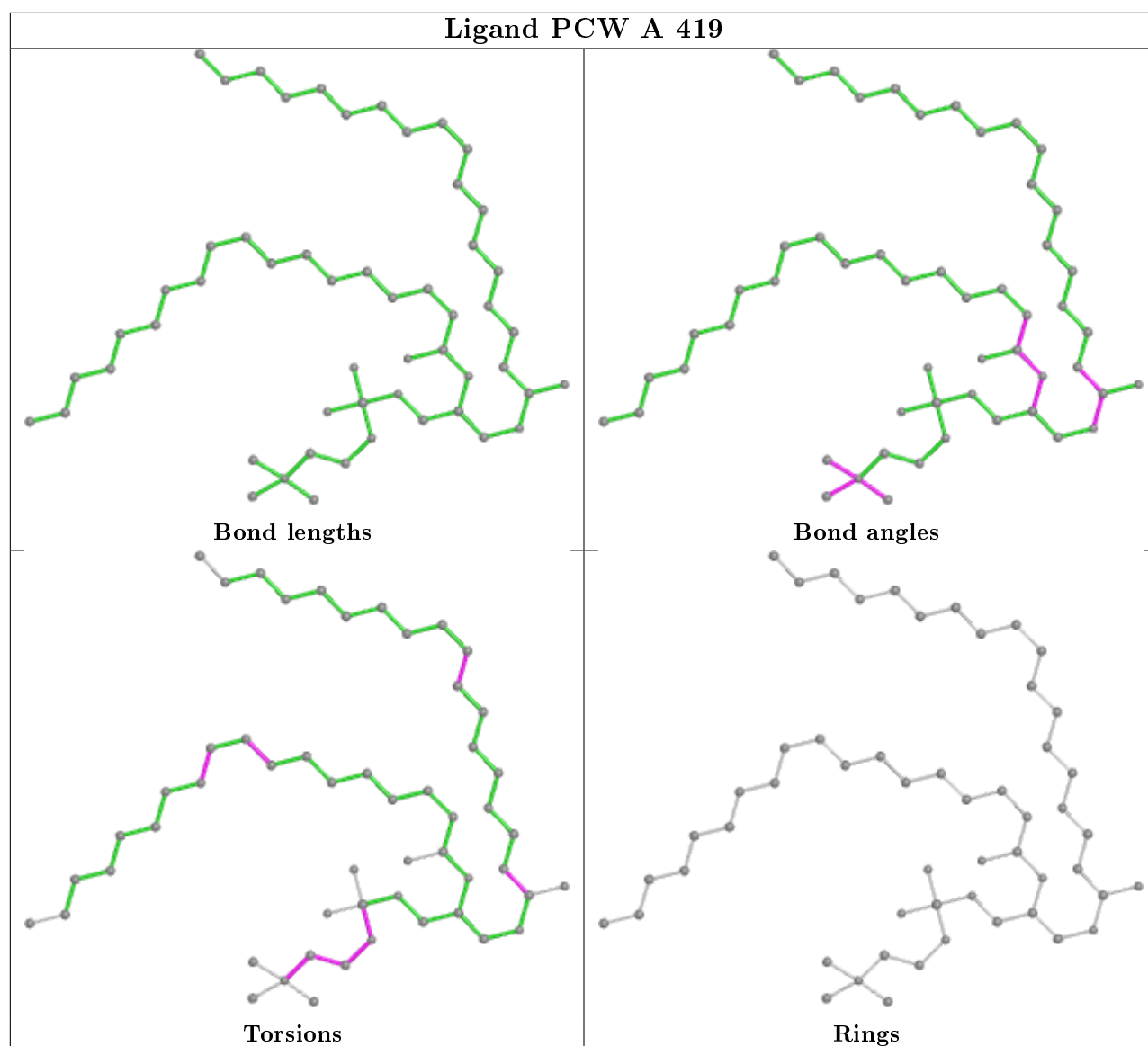
Mol	Chain	Res	Type	Atoms	Models (Total)
4	B	215	17F	O10-C17-O9-C5	20

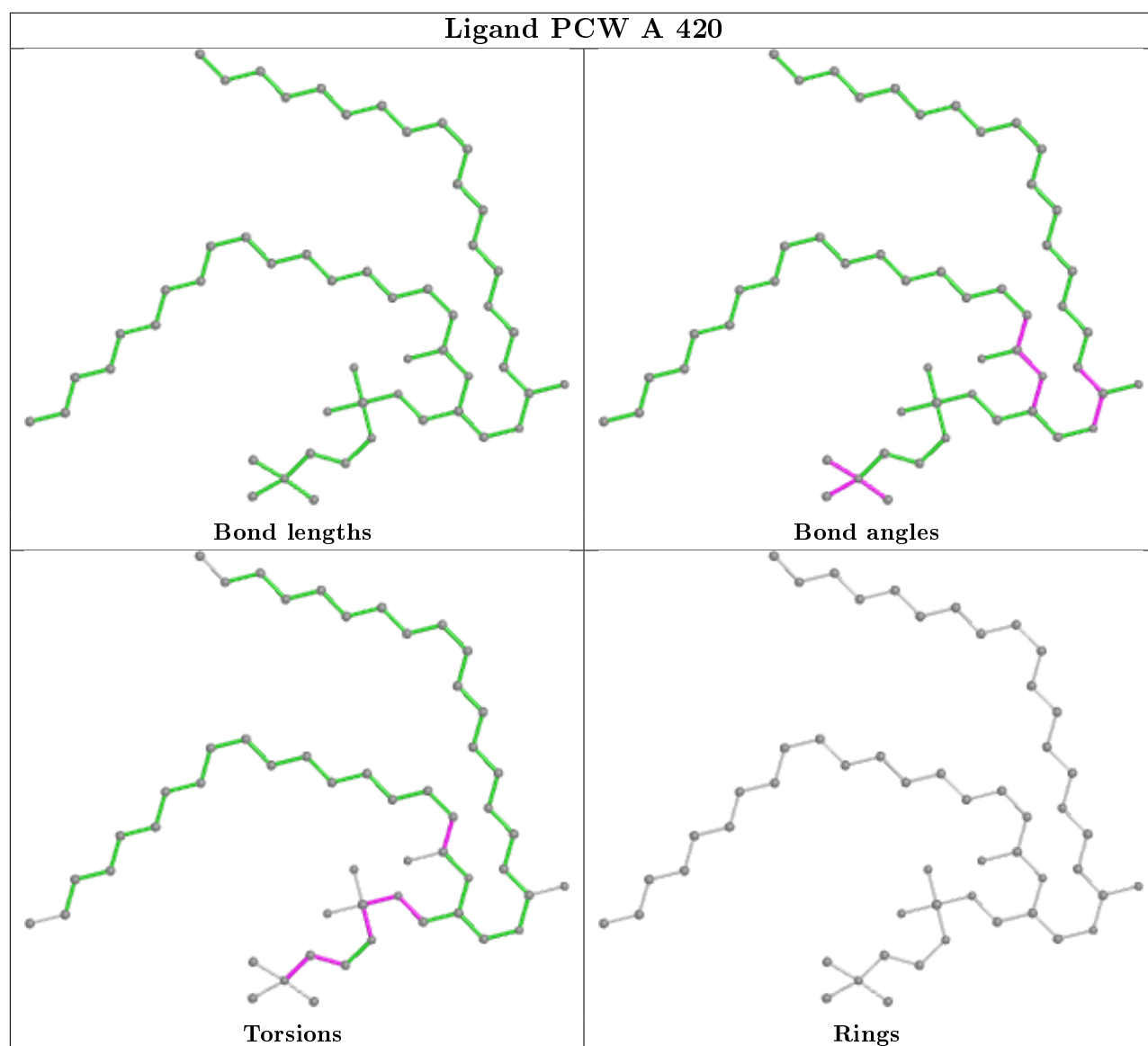
There are no ring outliers.

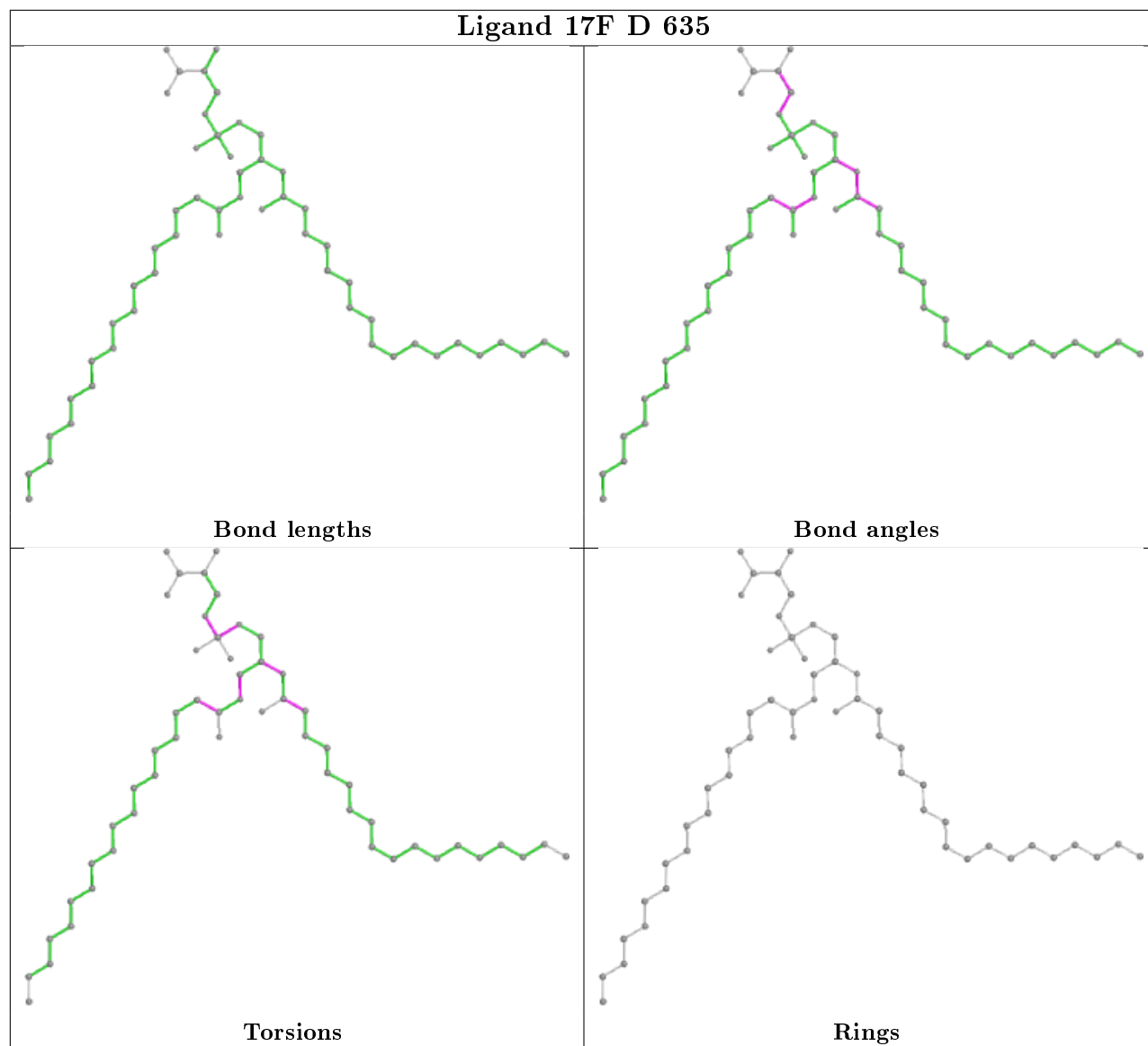
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

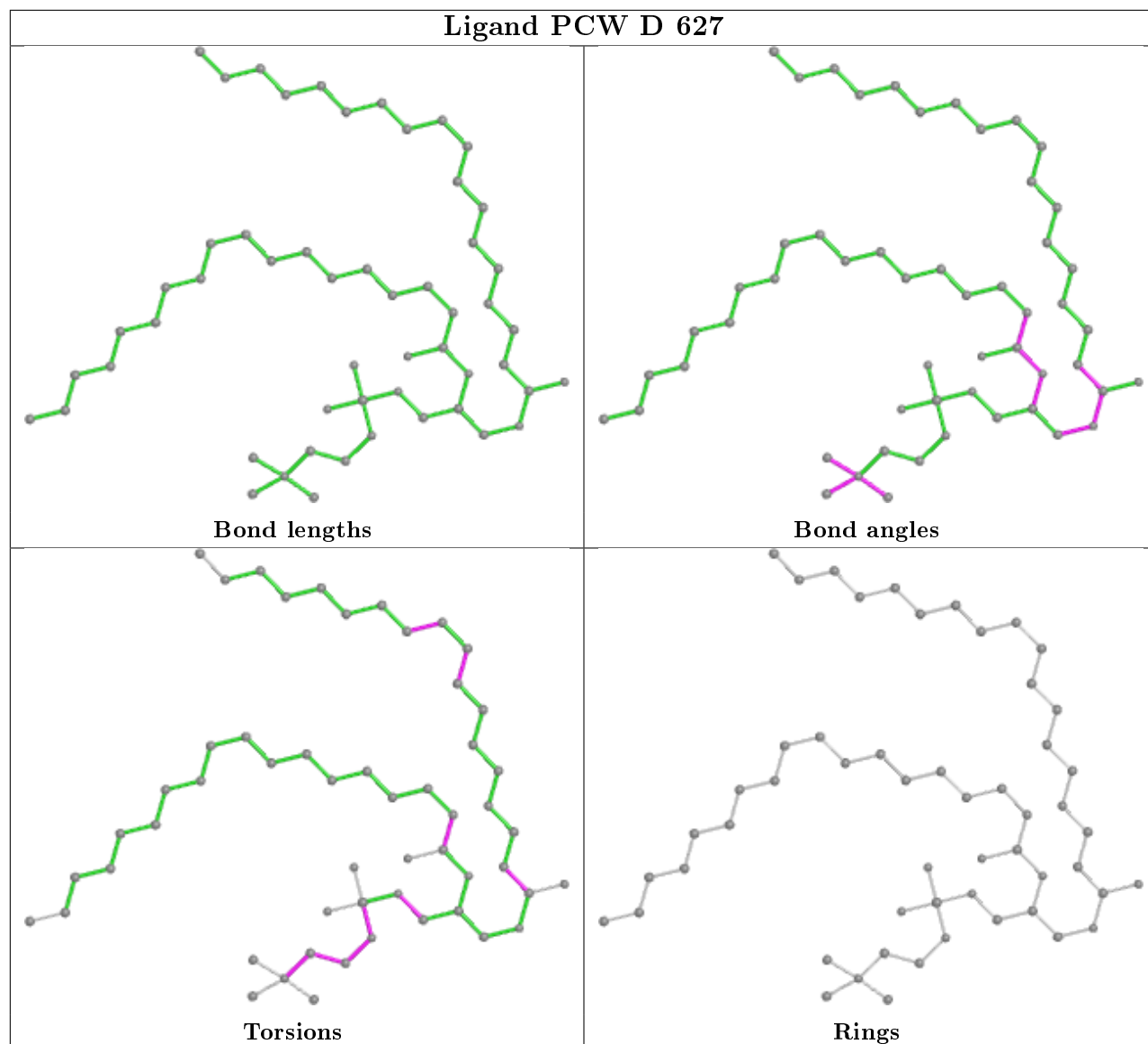


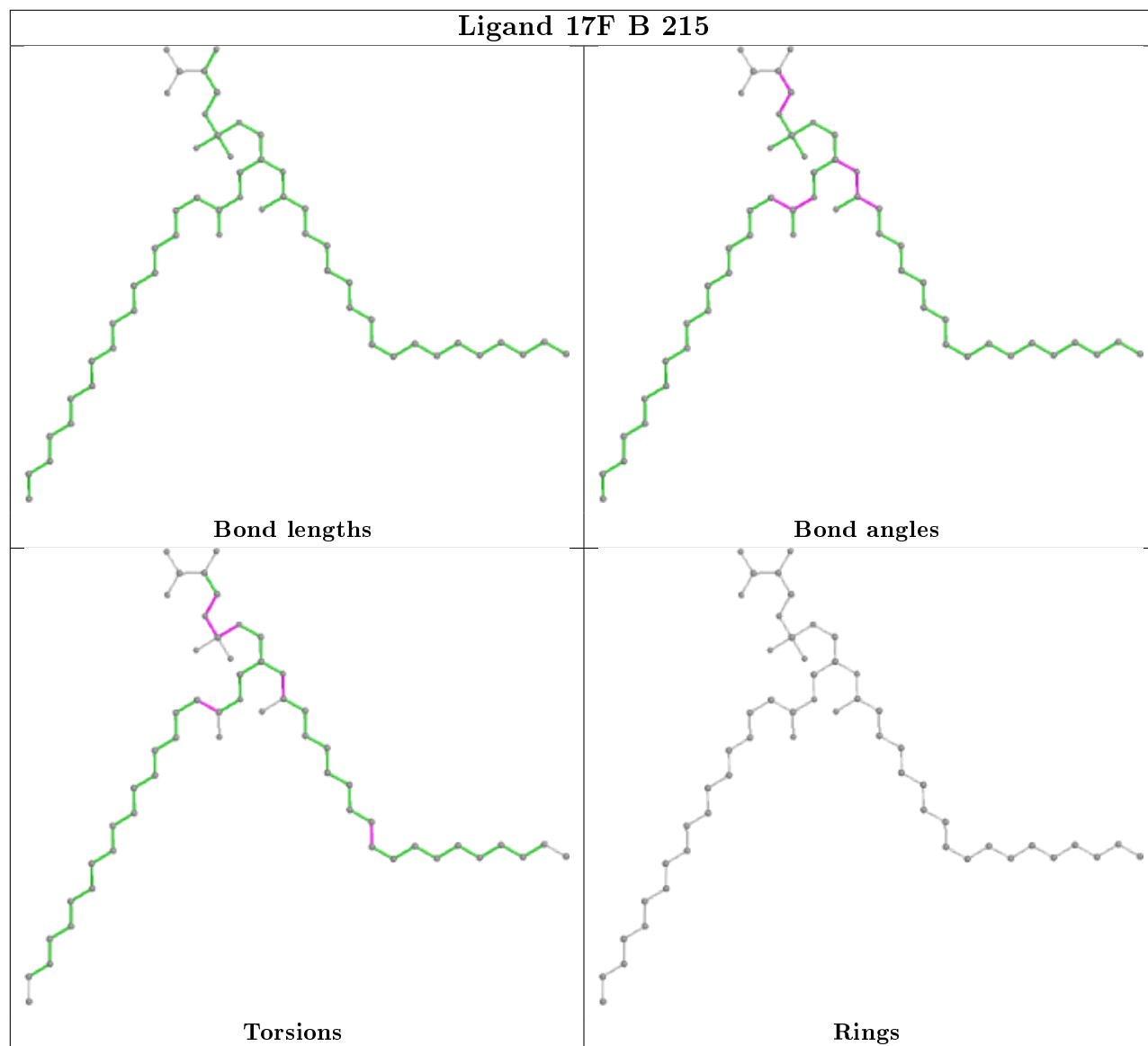


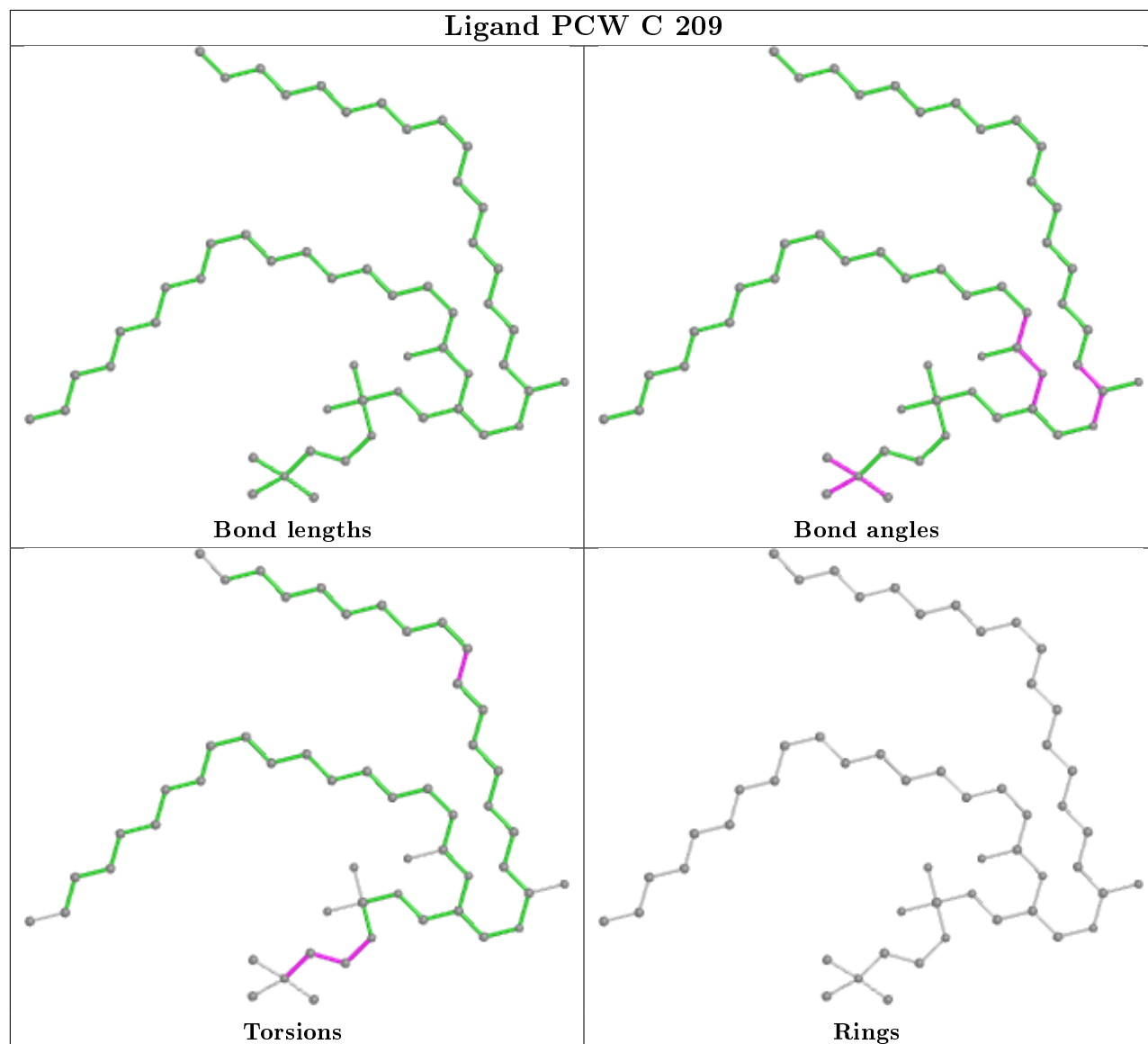


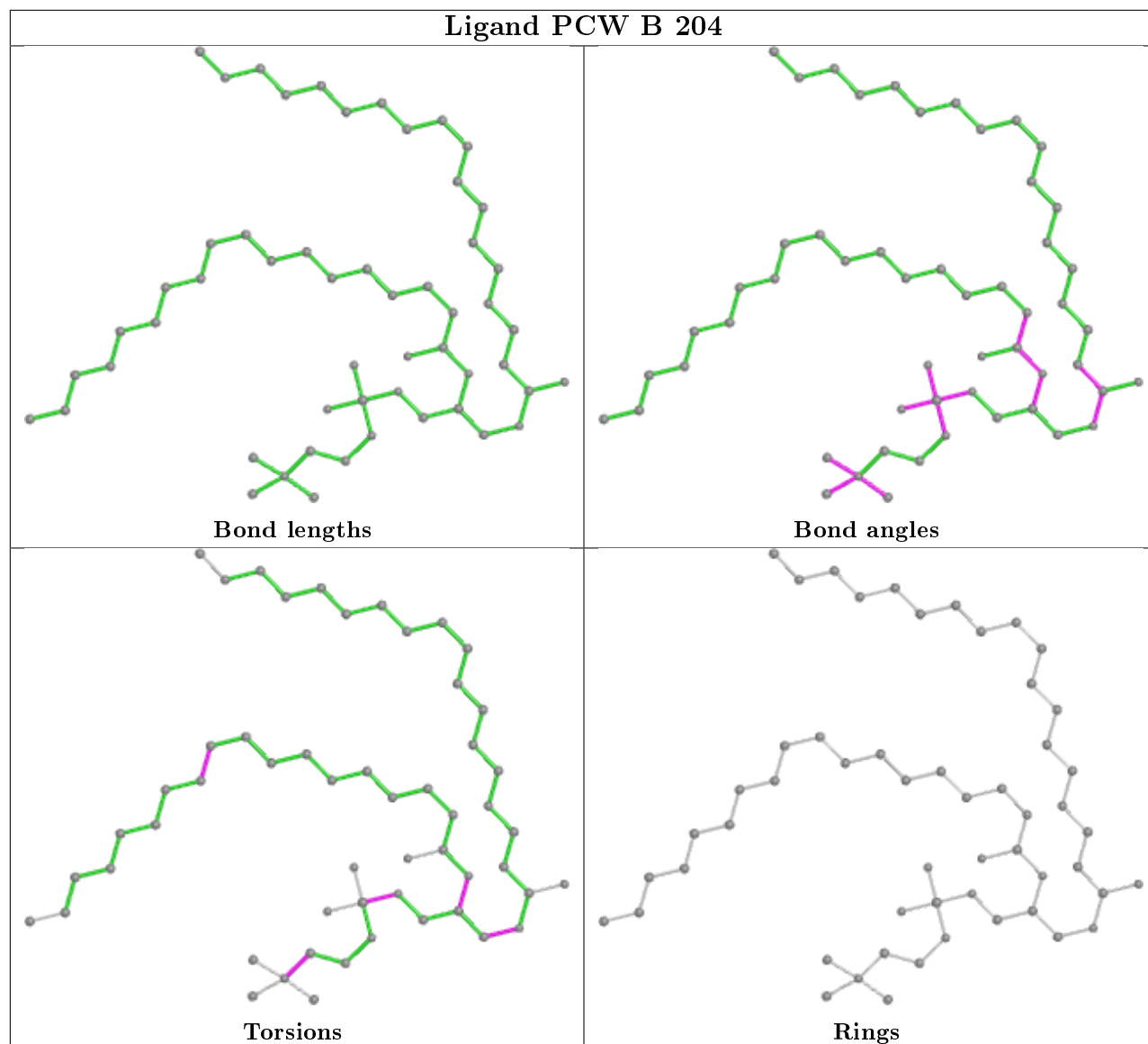




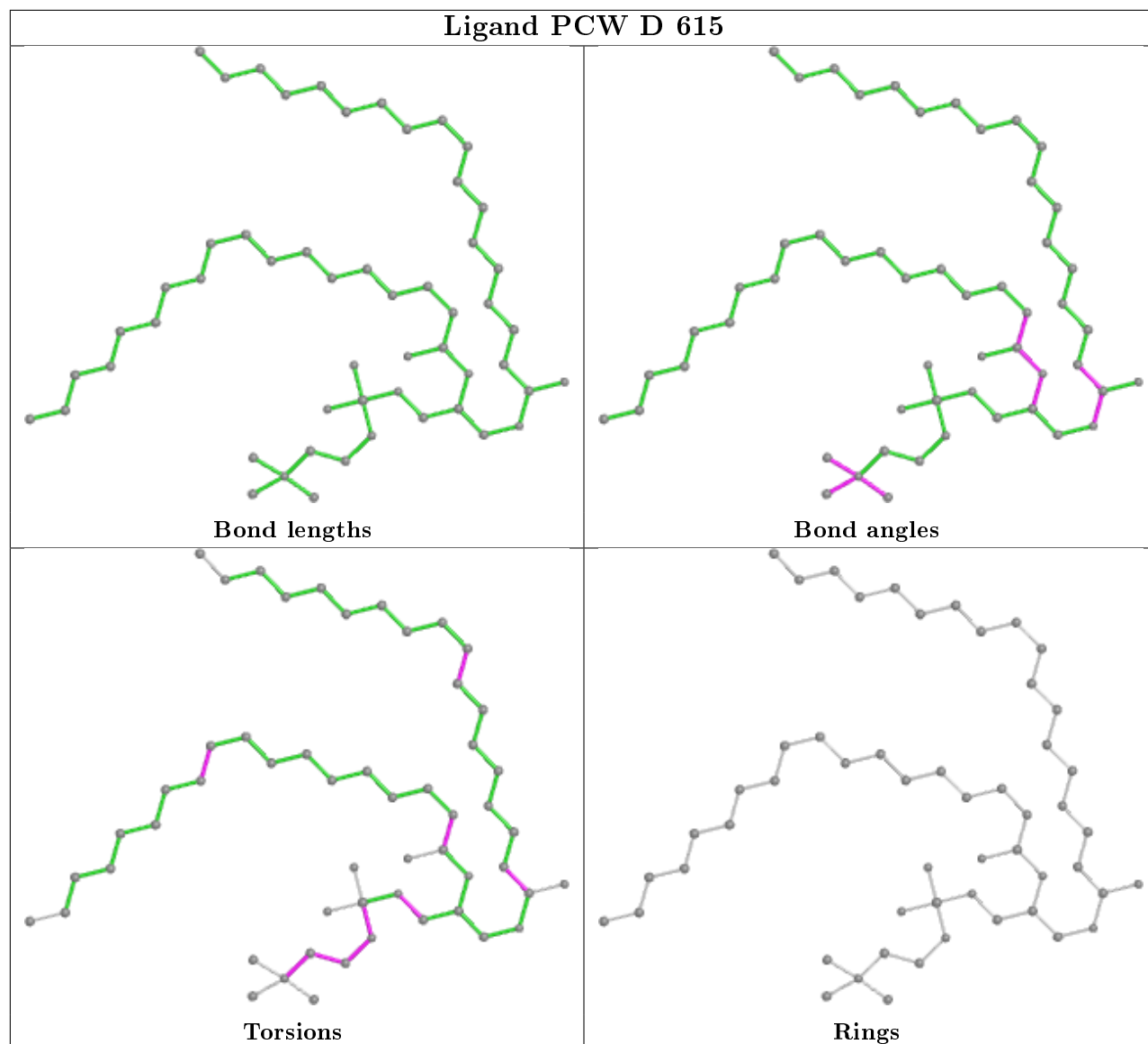


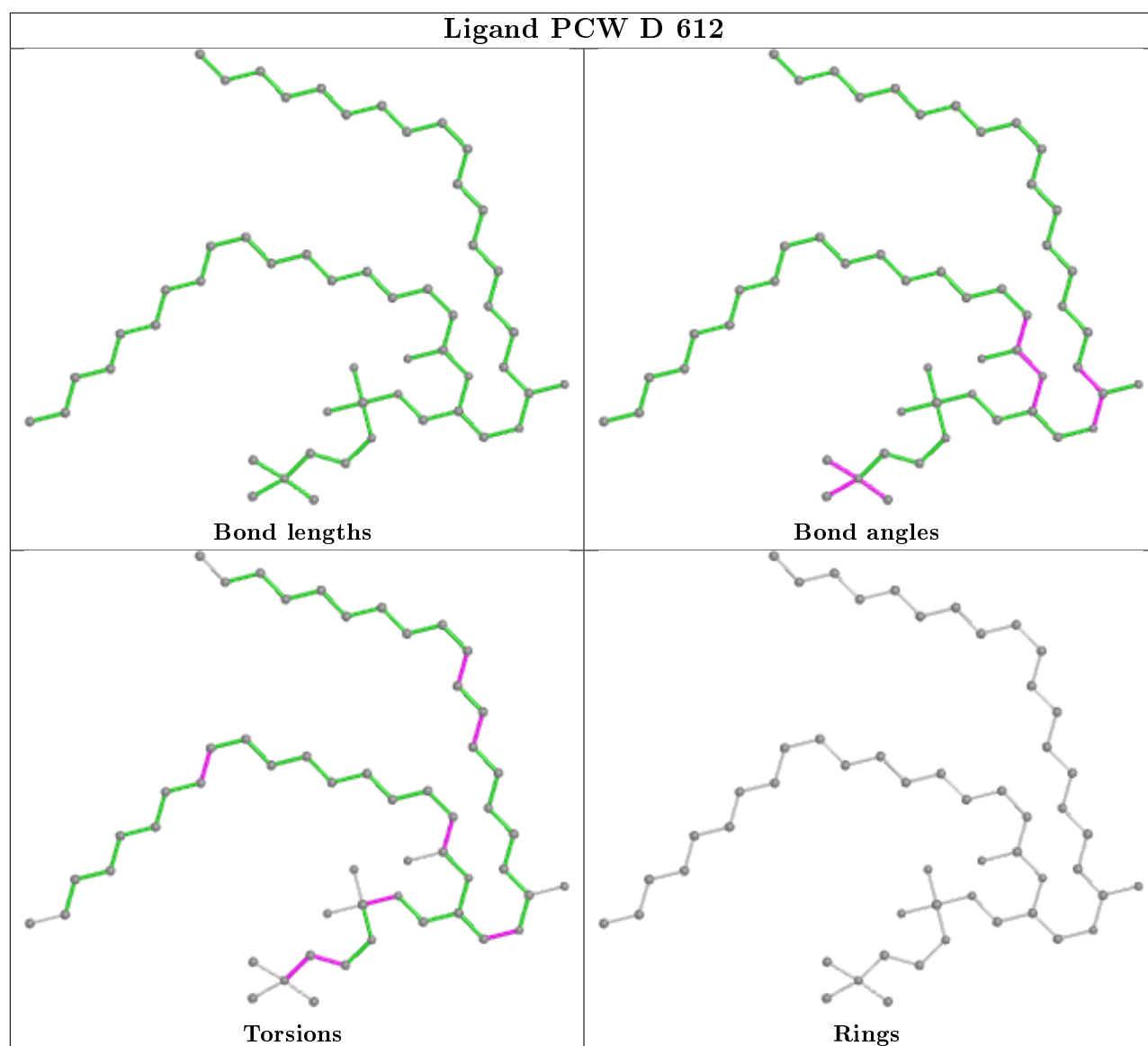


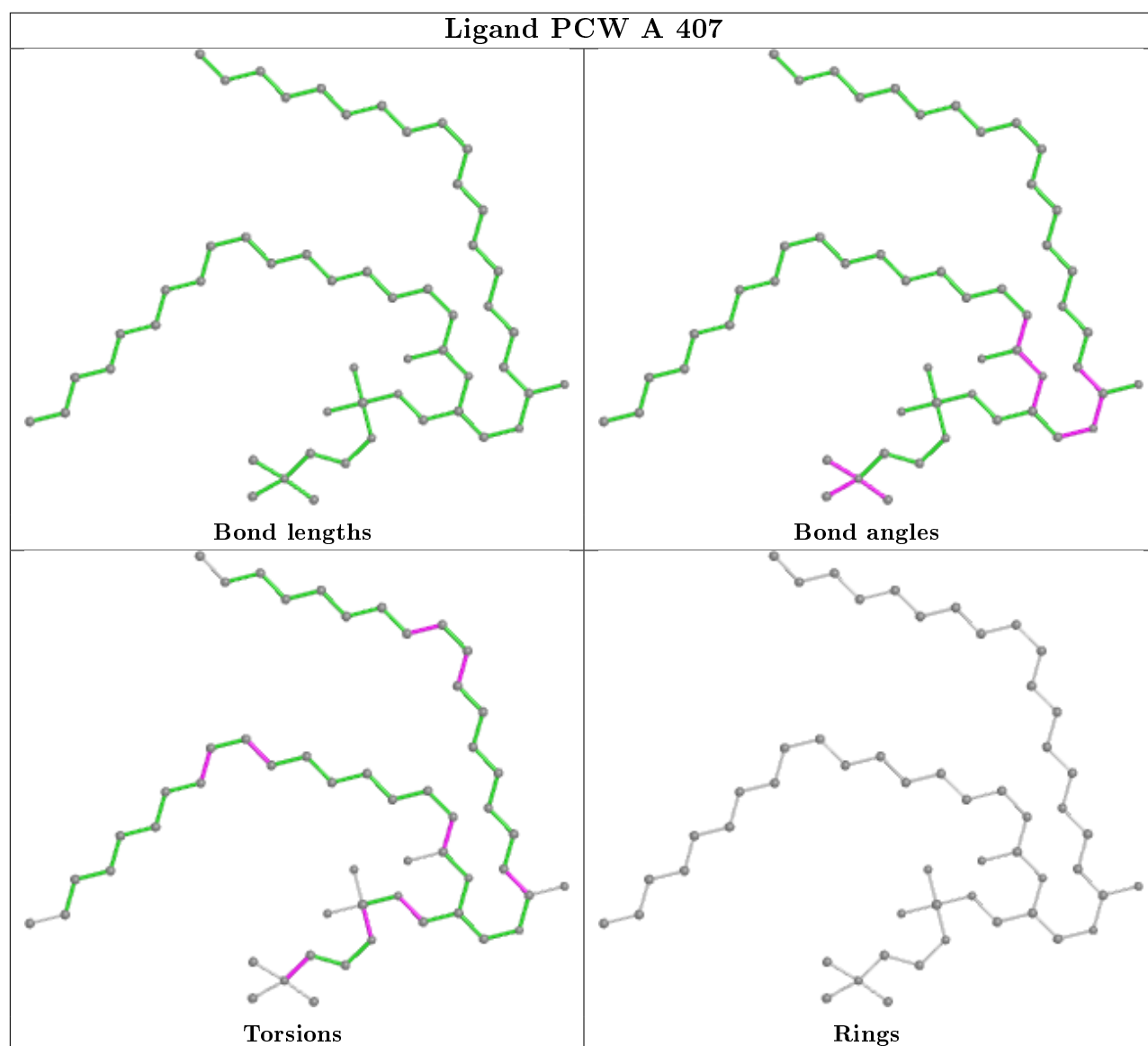


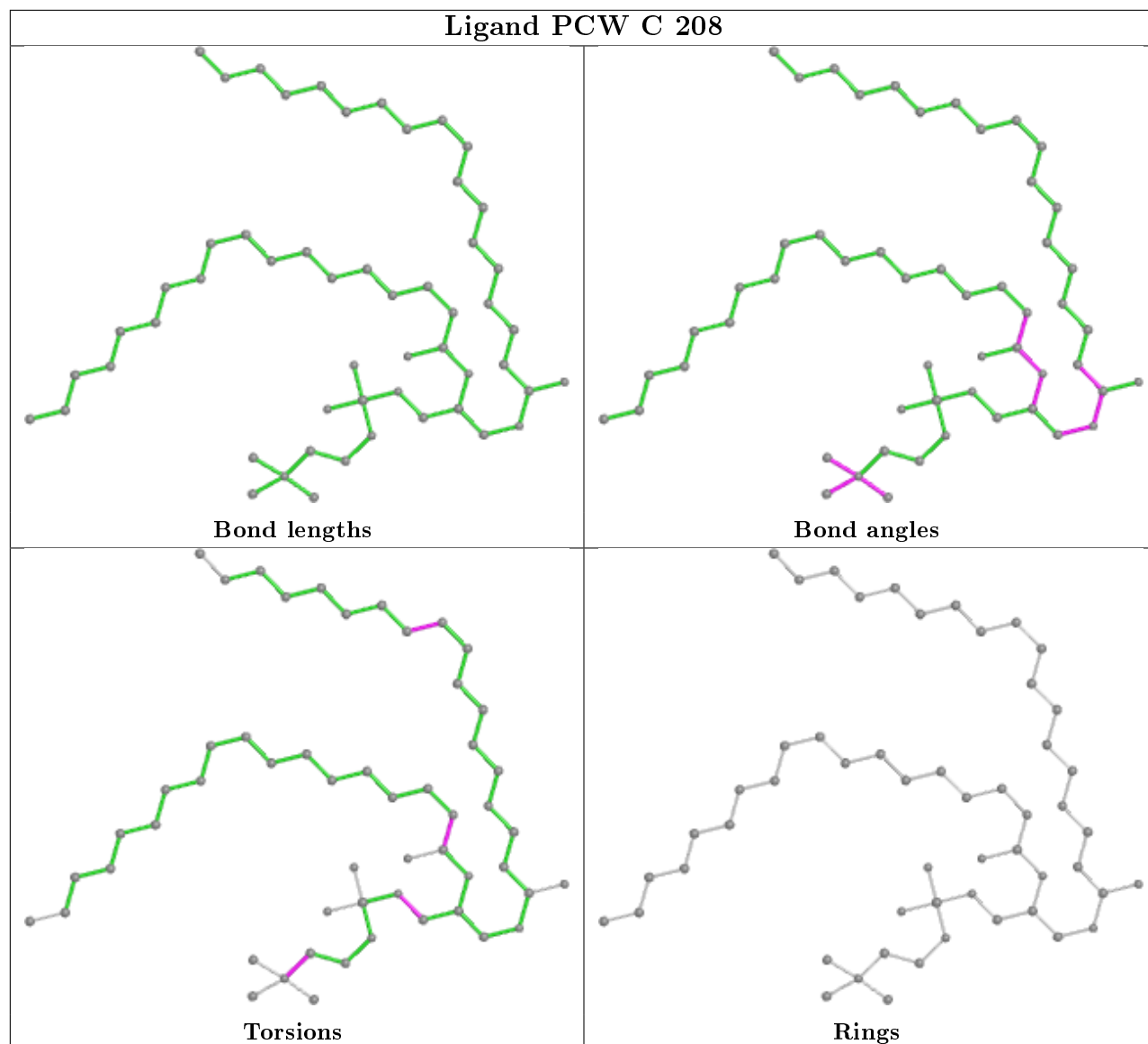


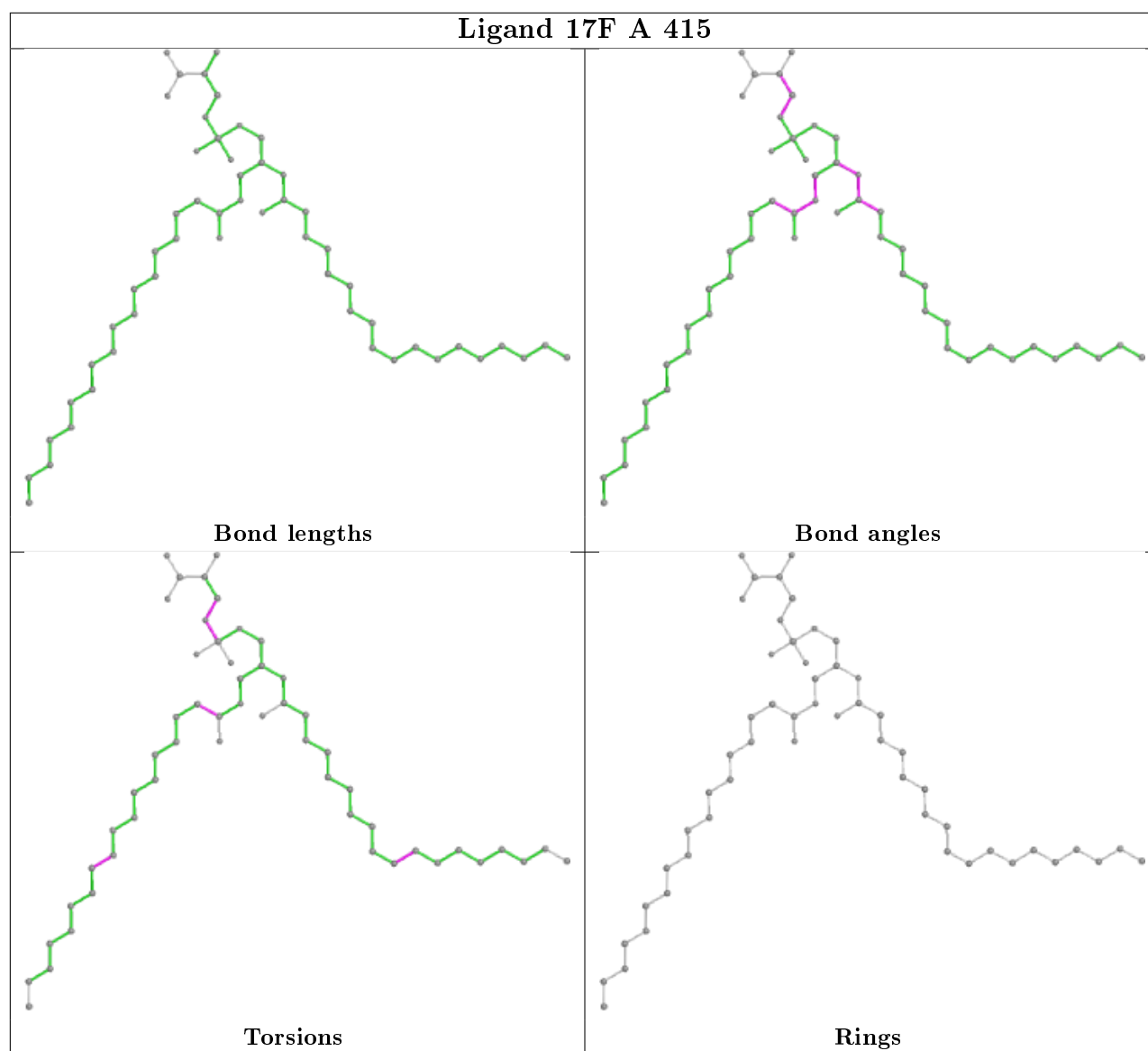


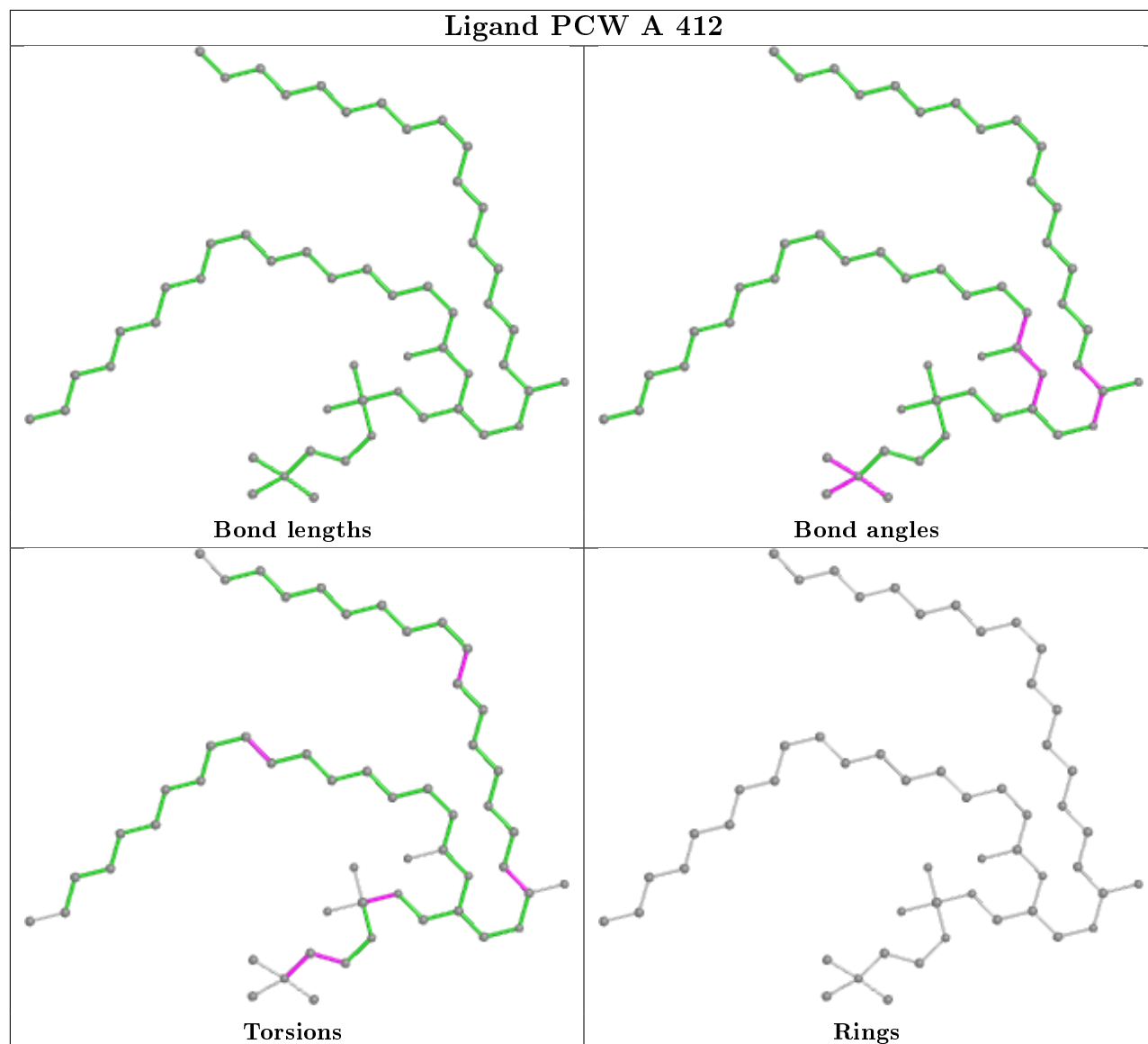


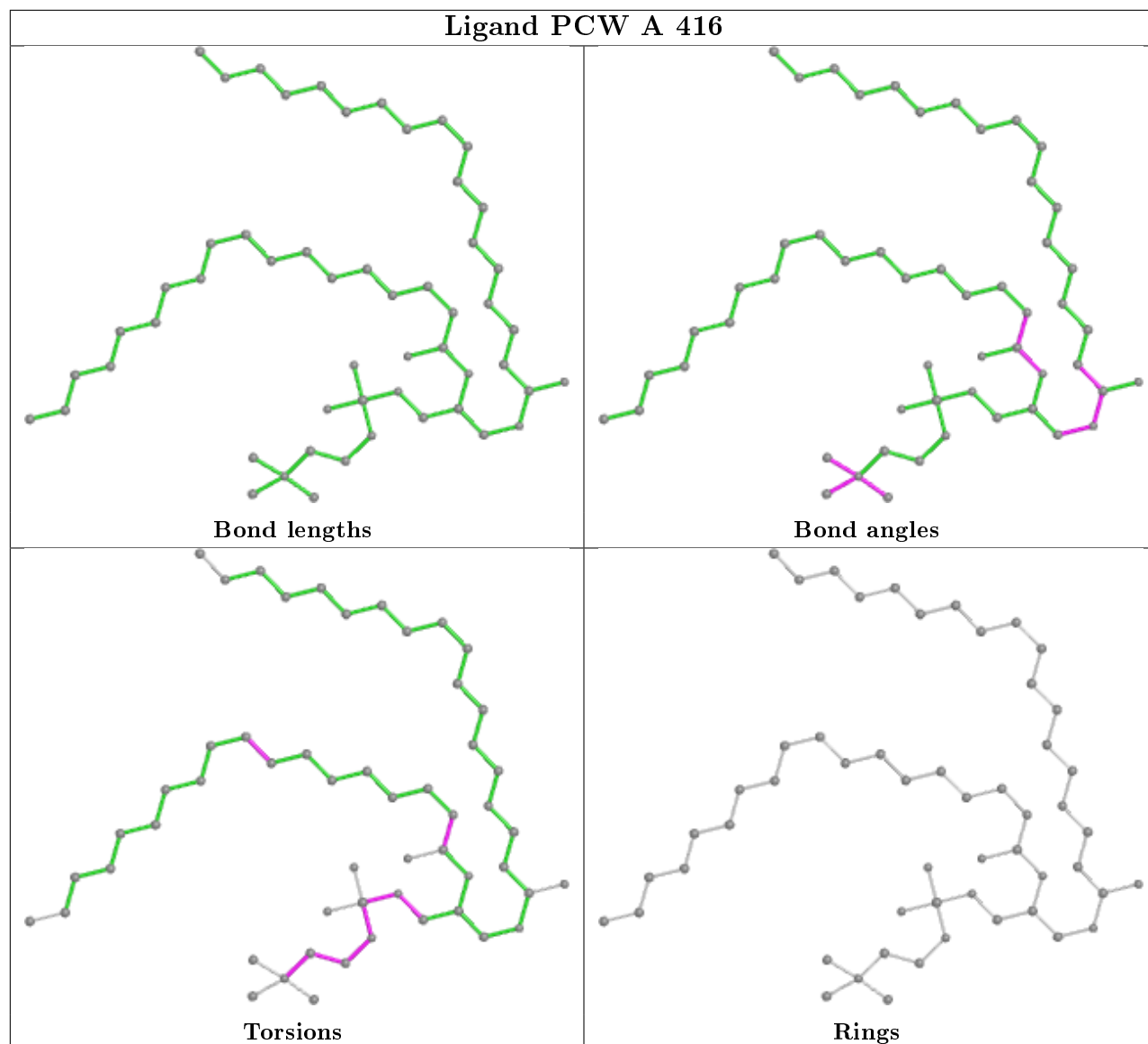


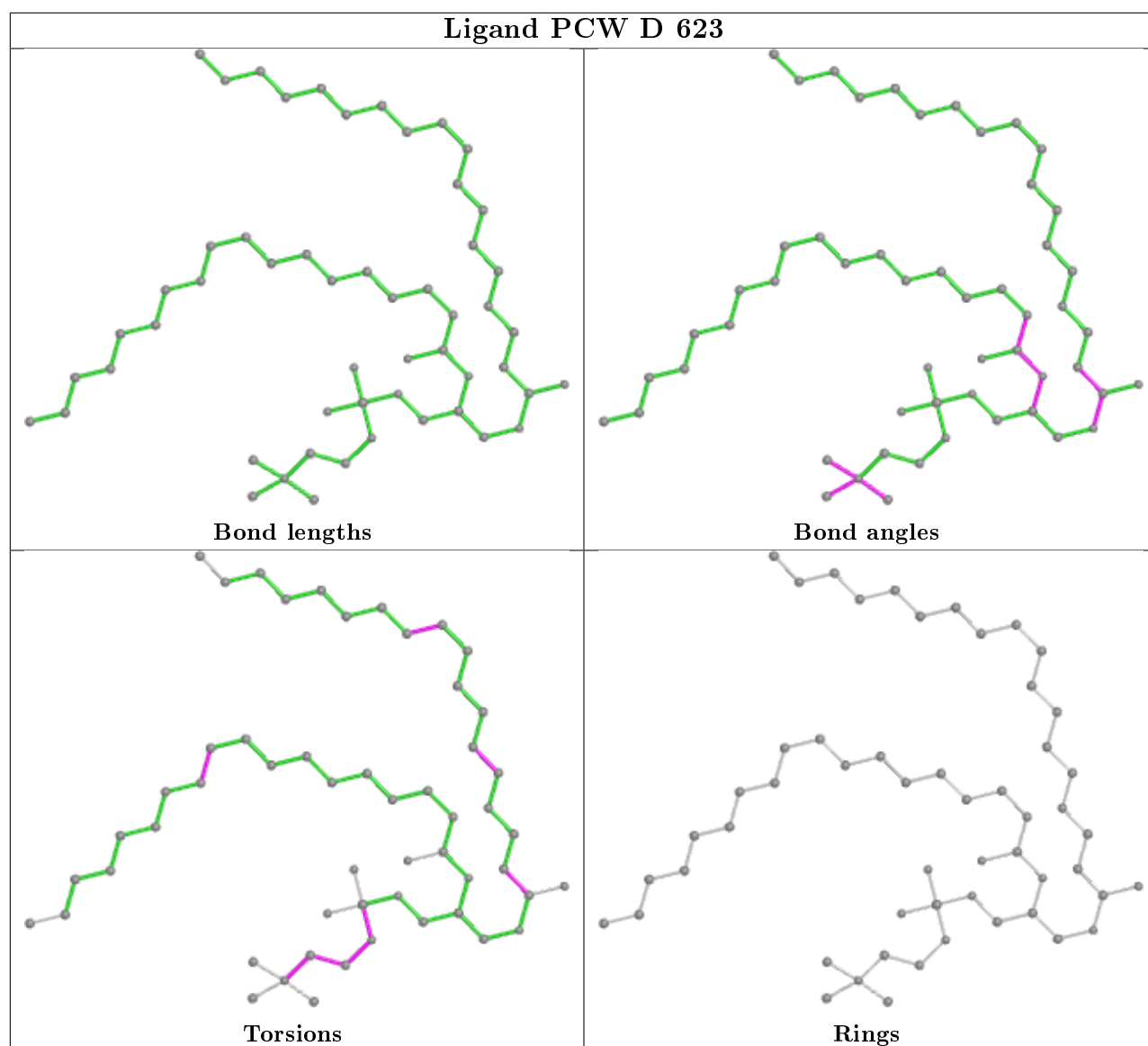




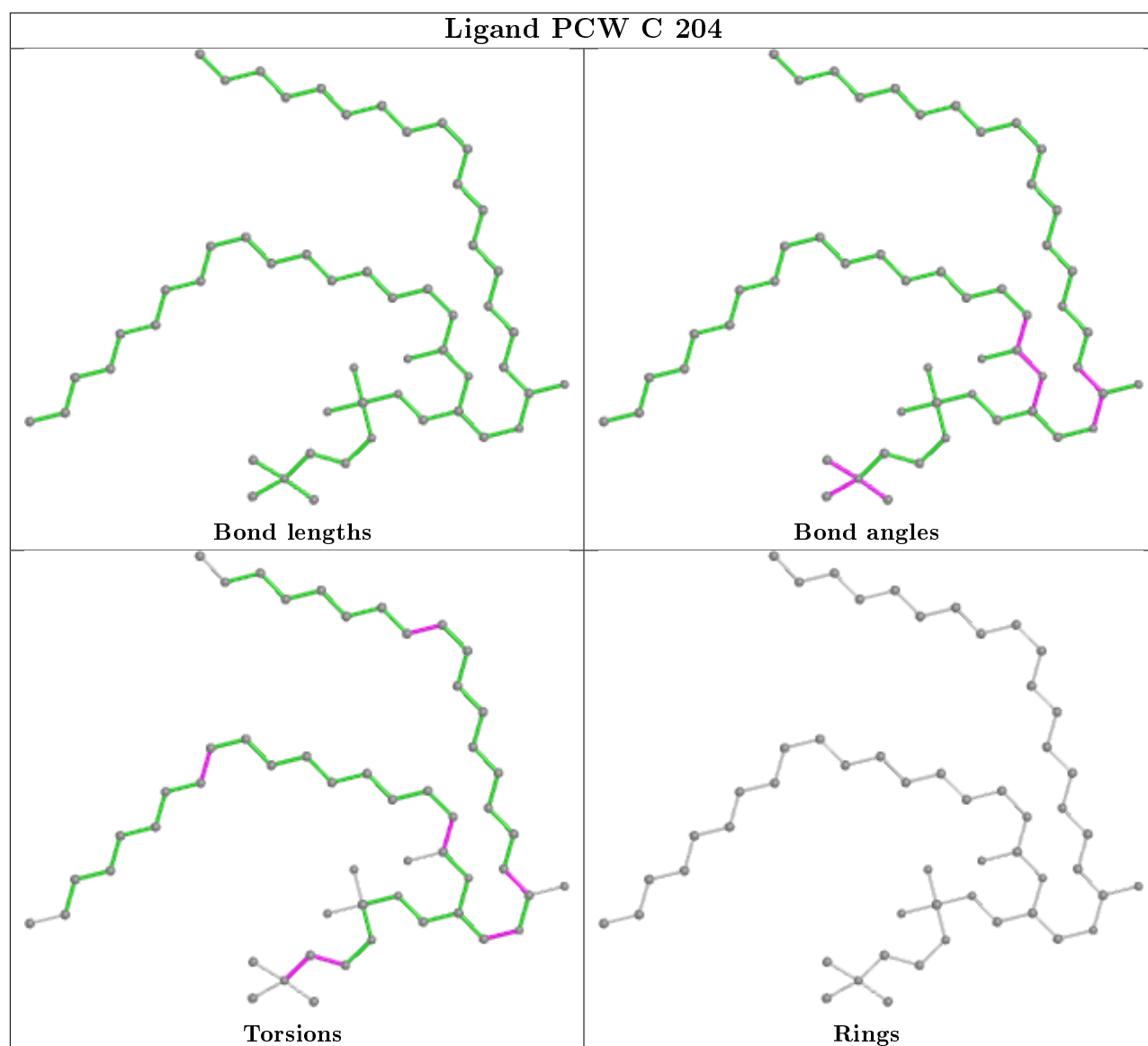


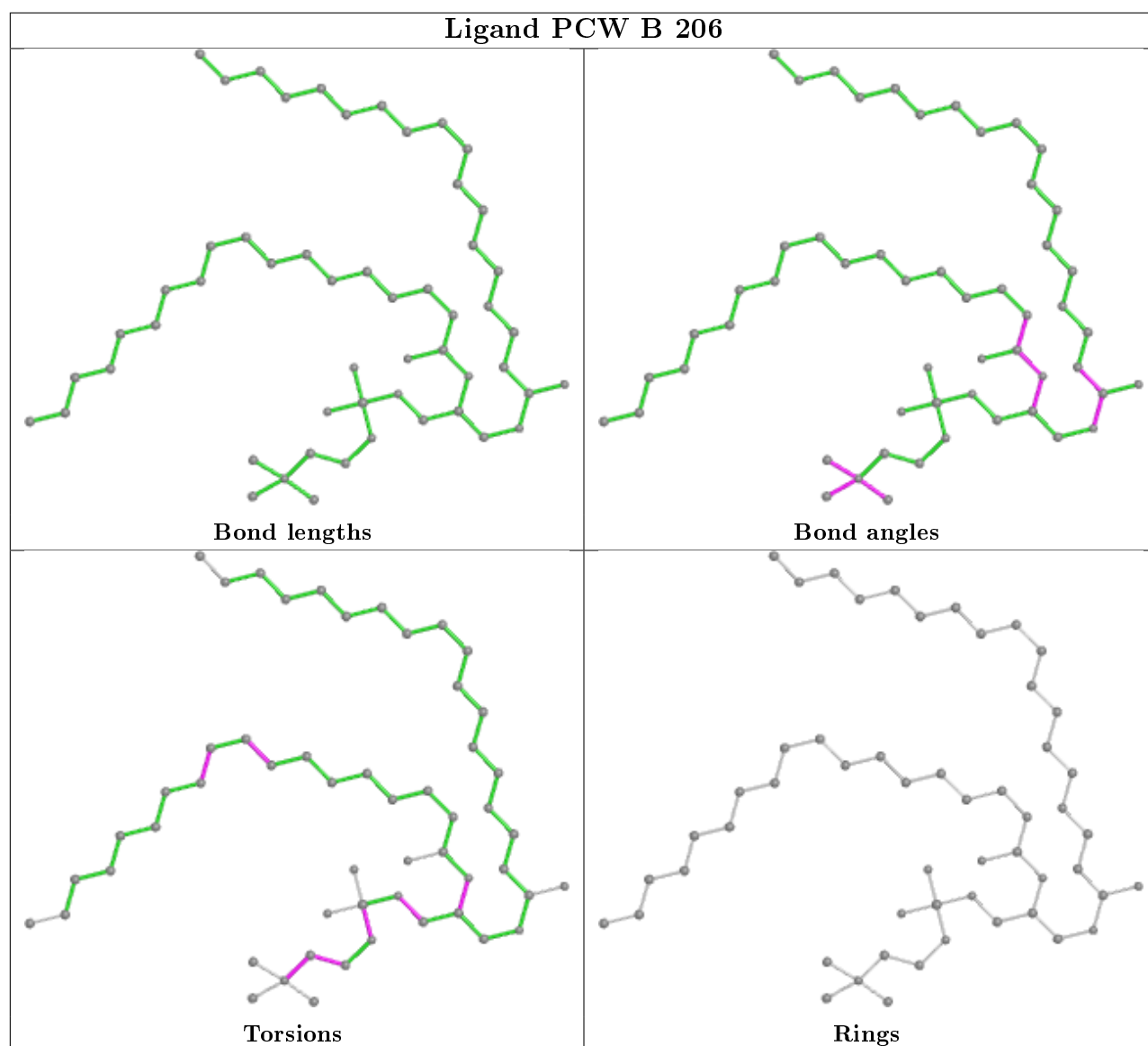


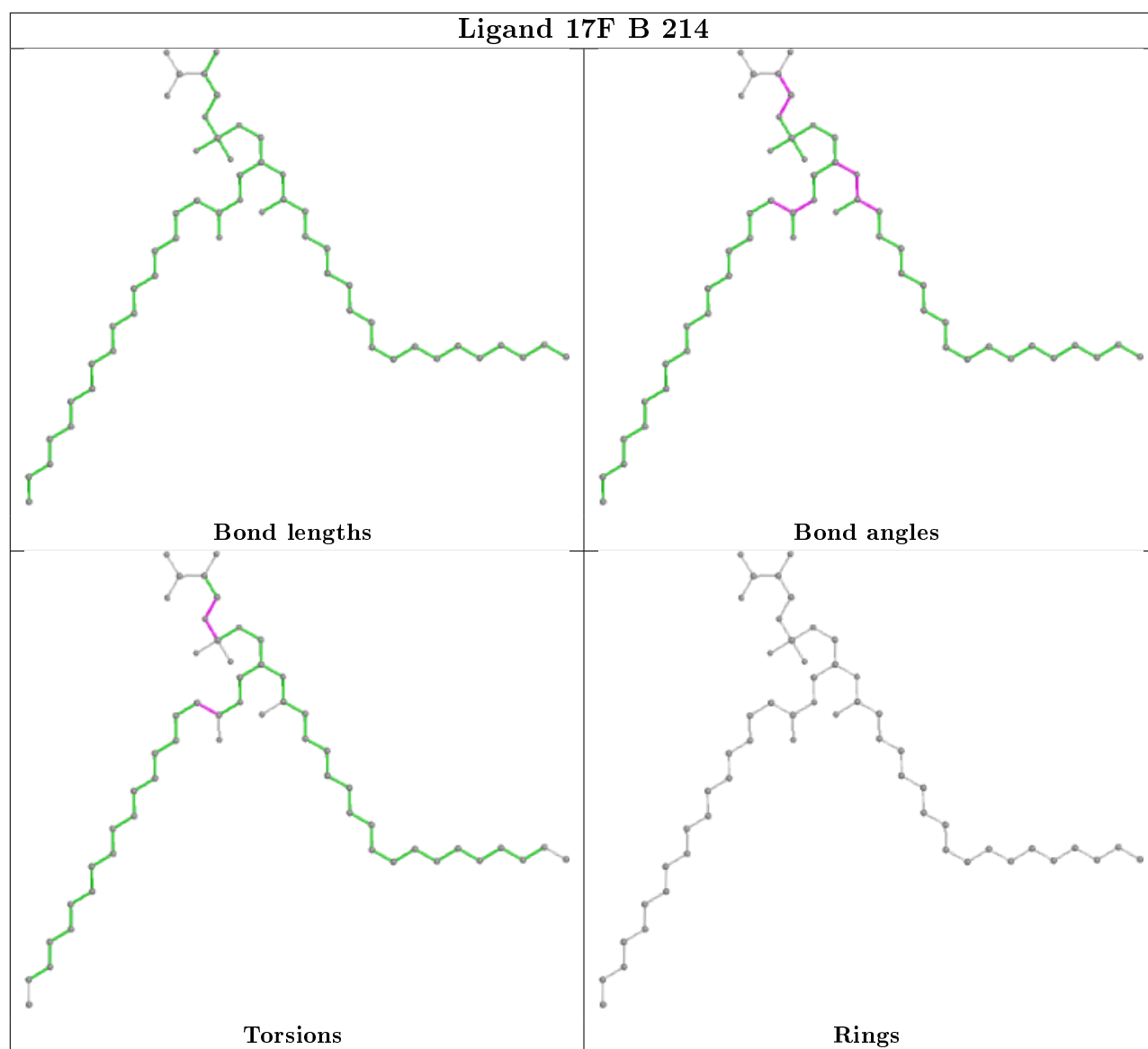


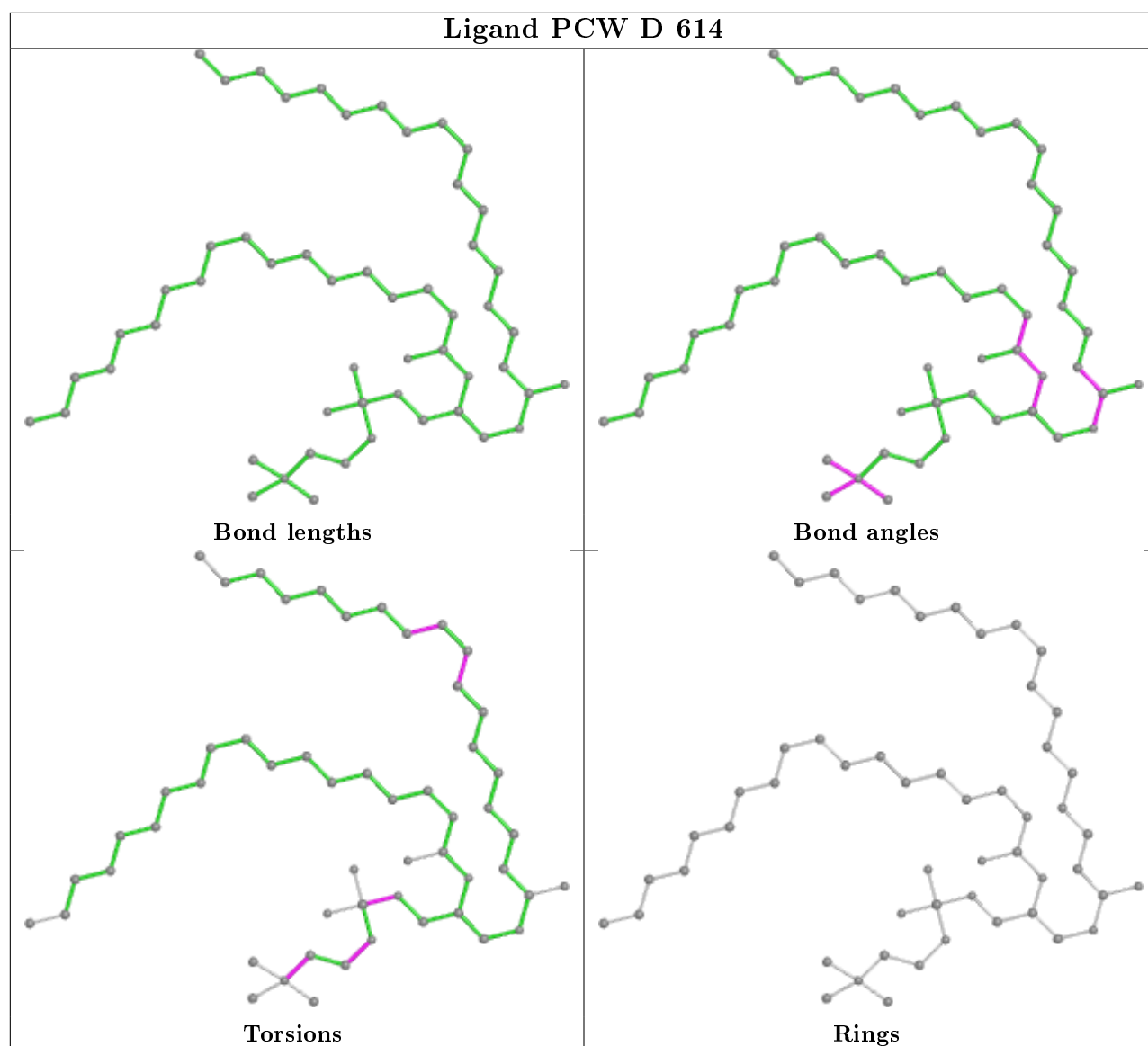


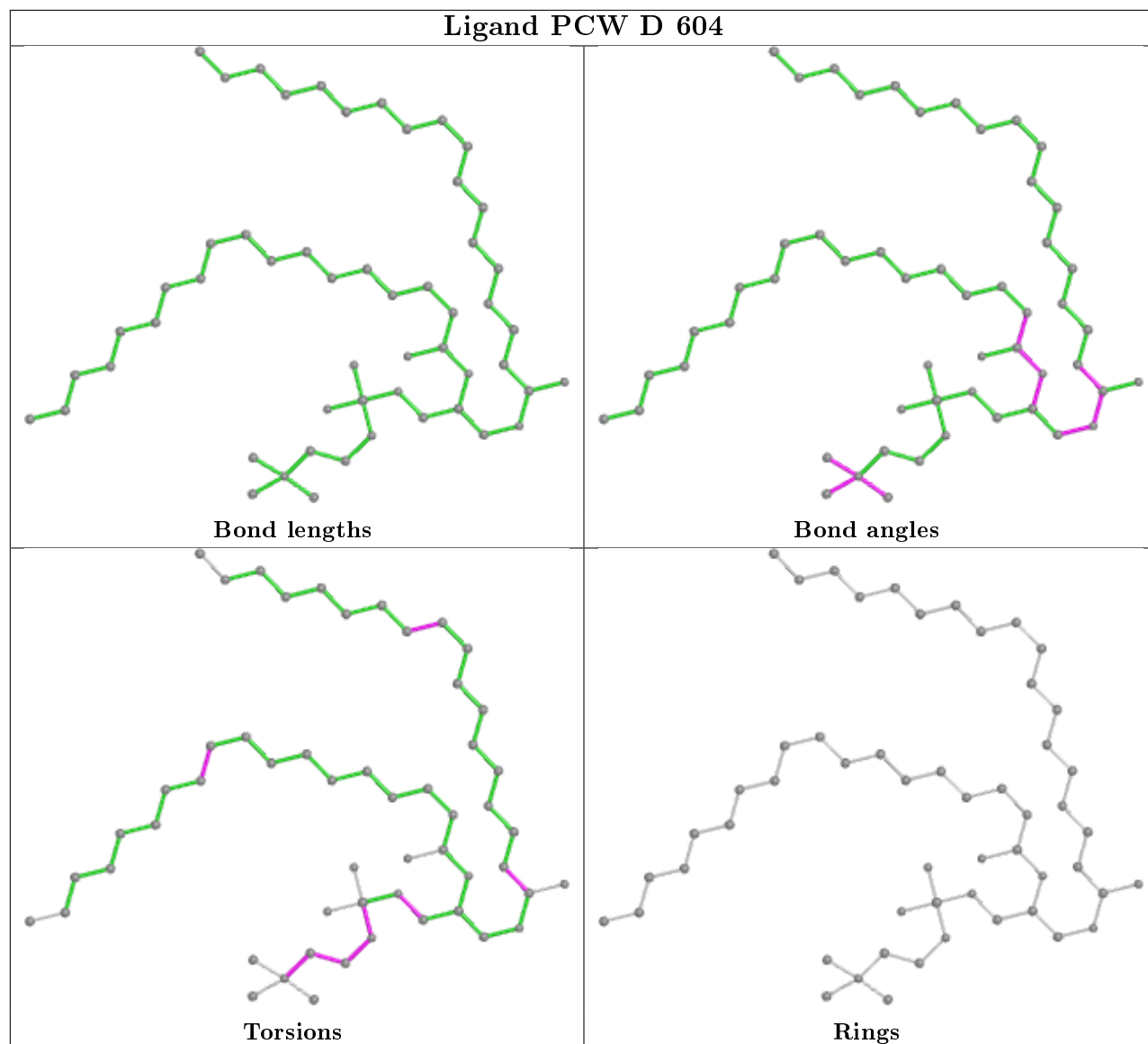


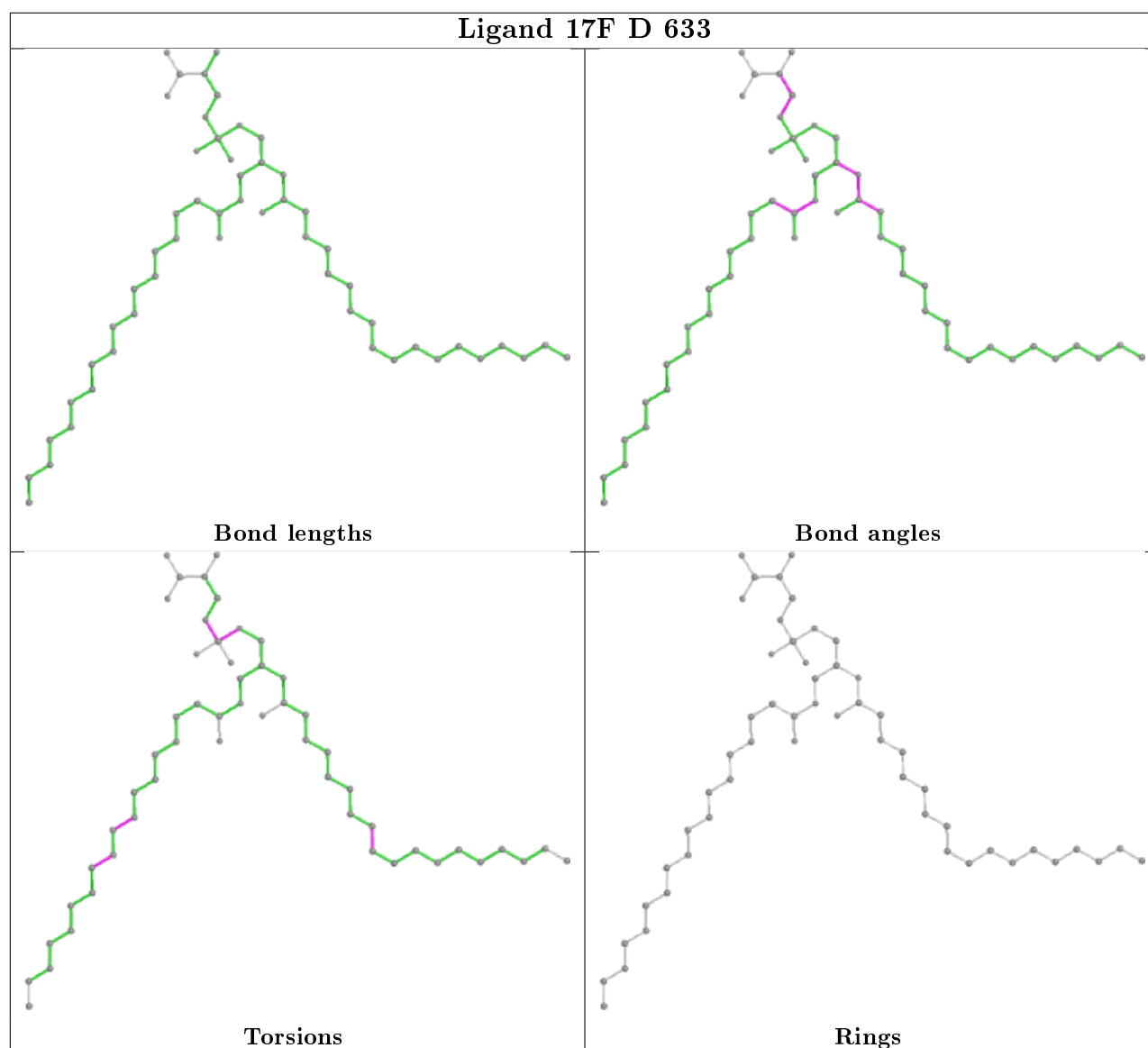


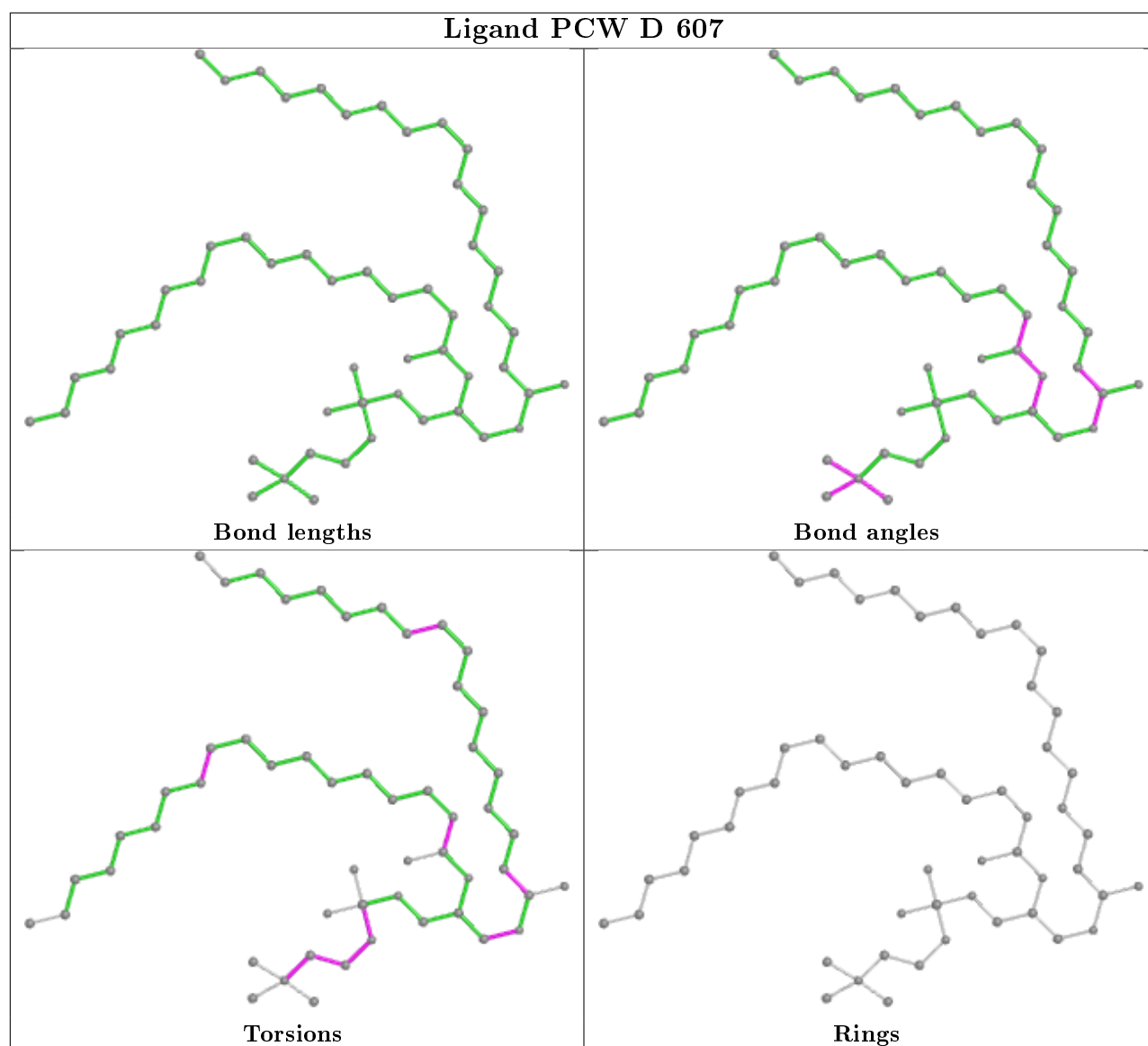


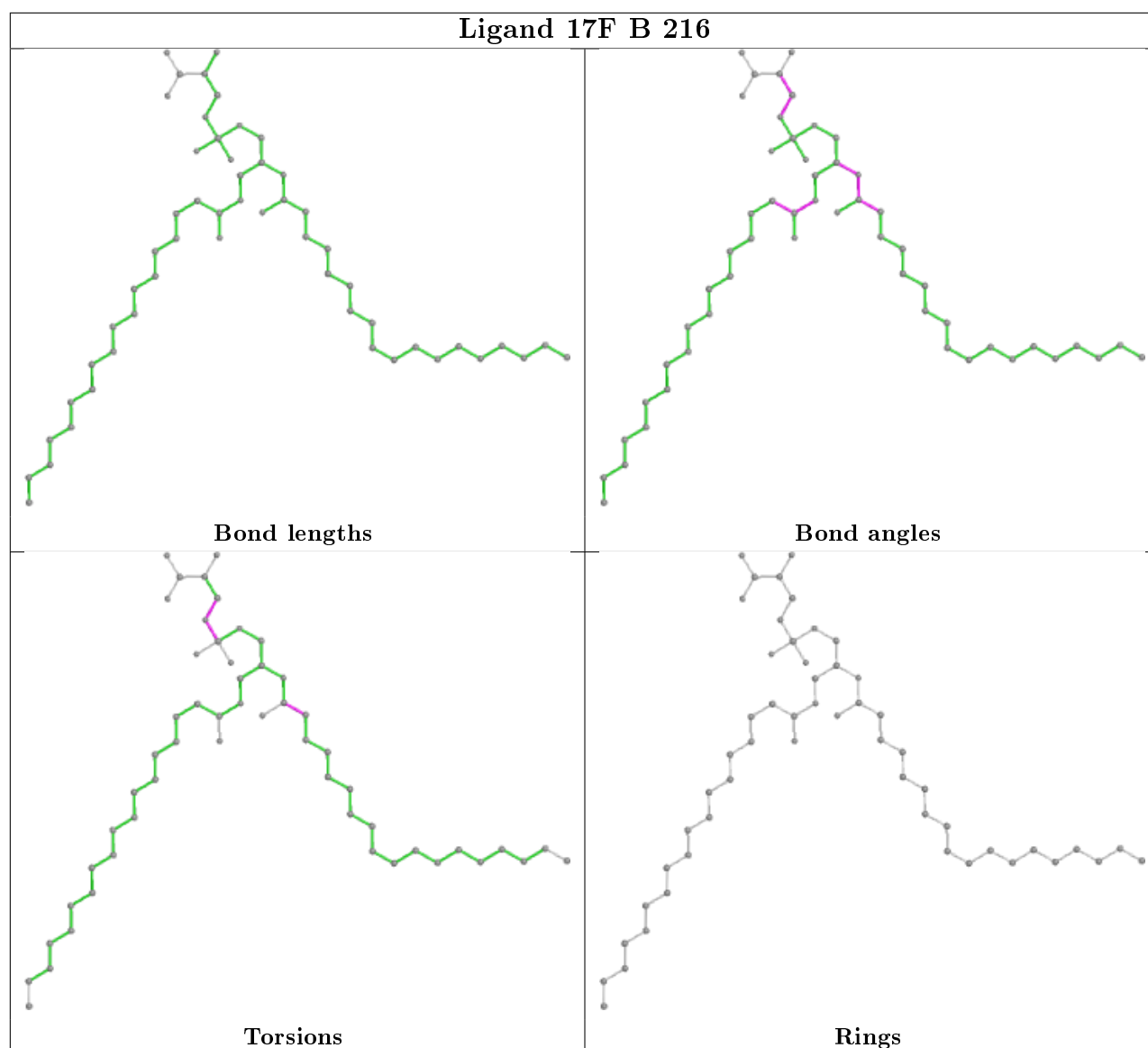




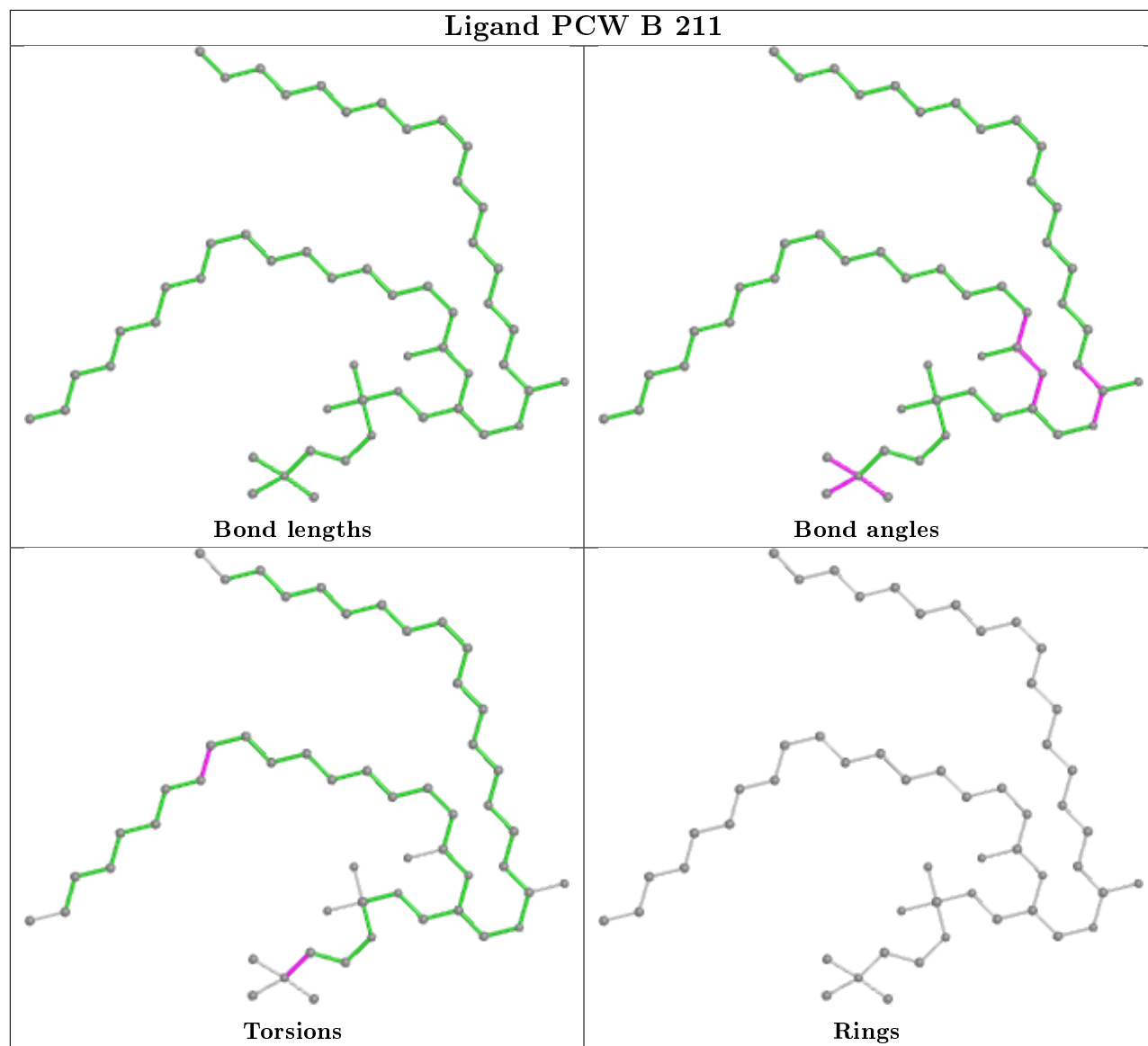


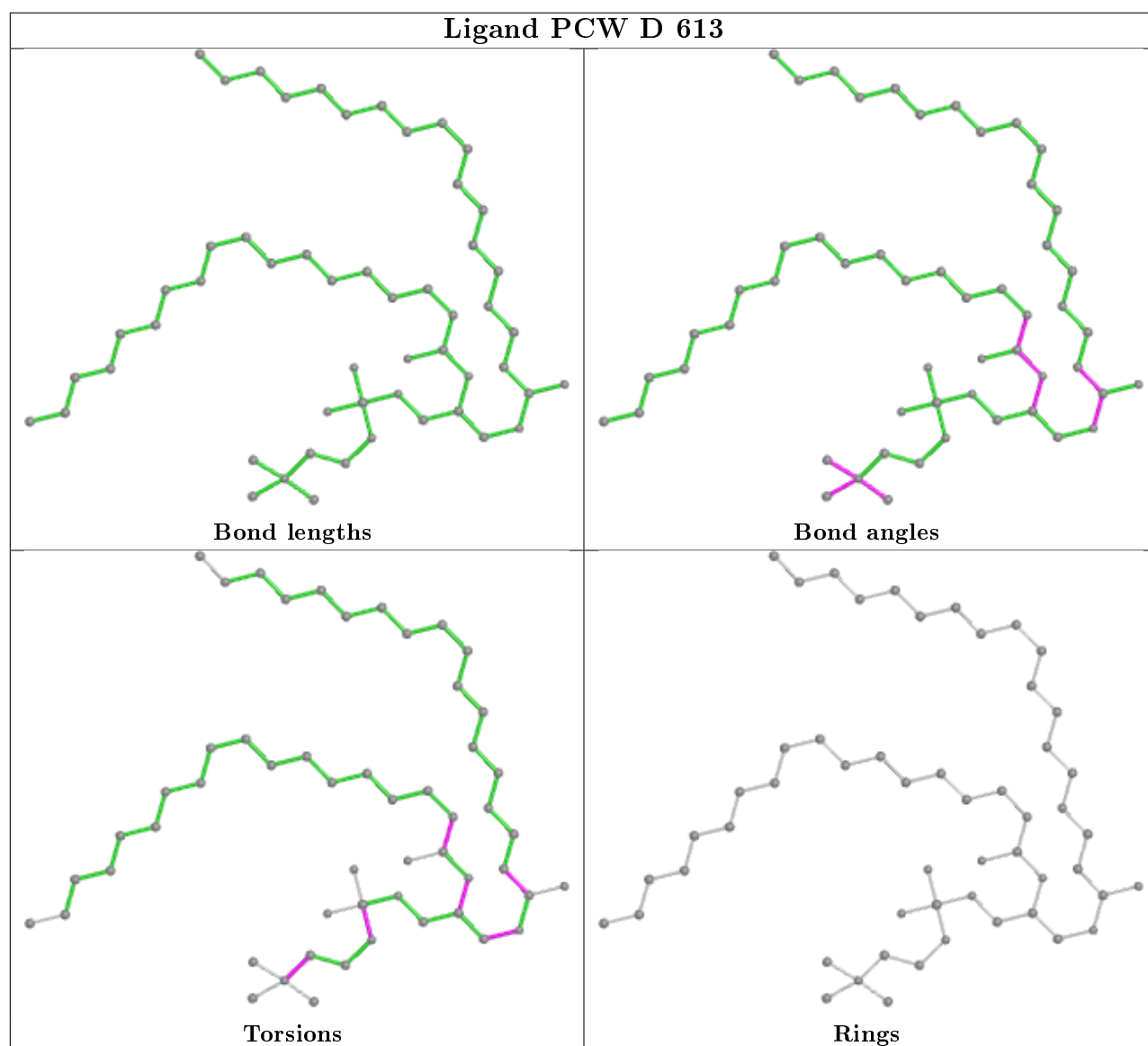


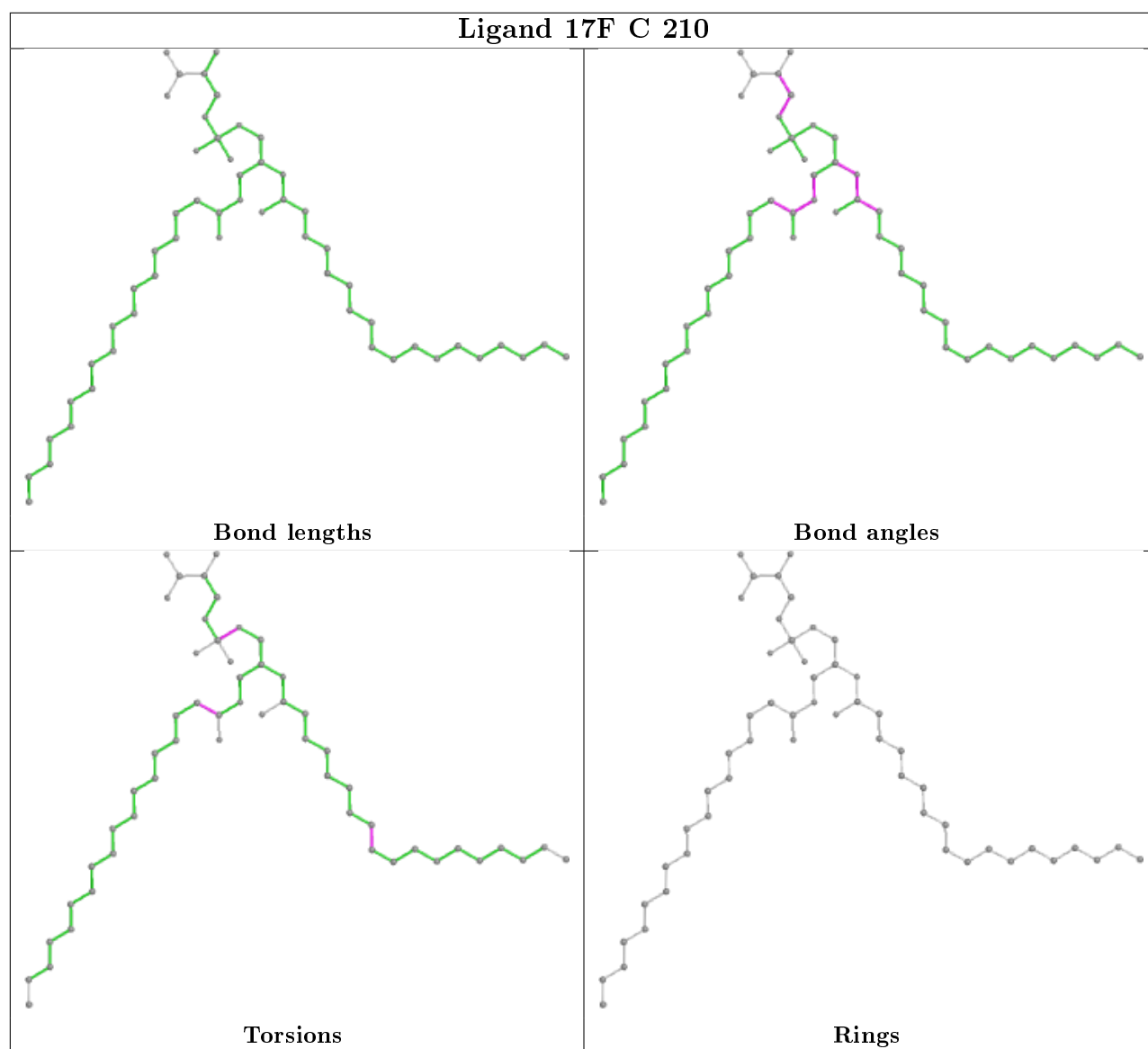


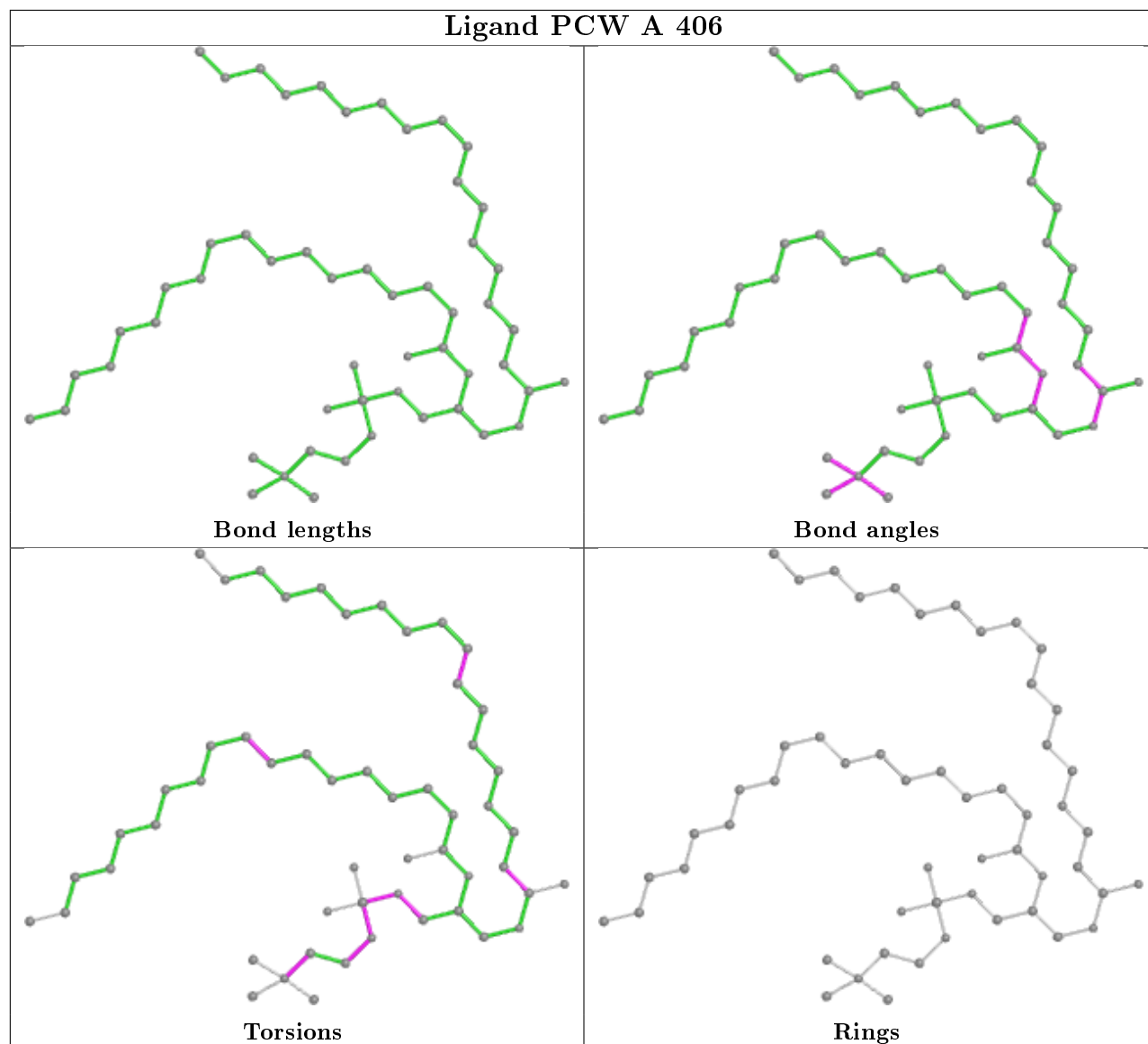


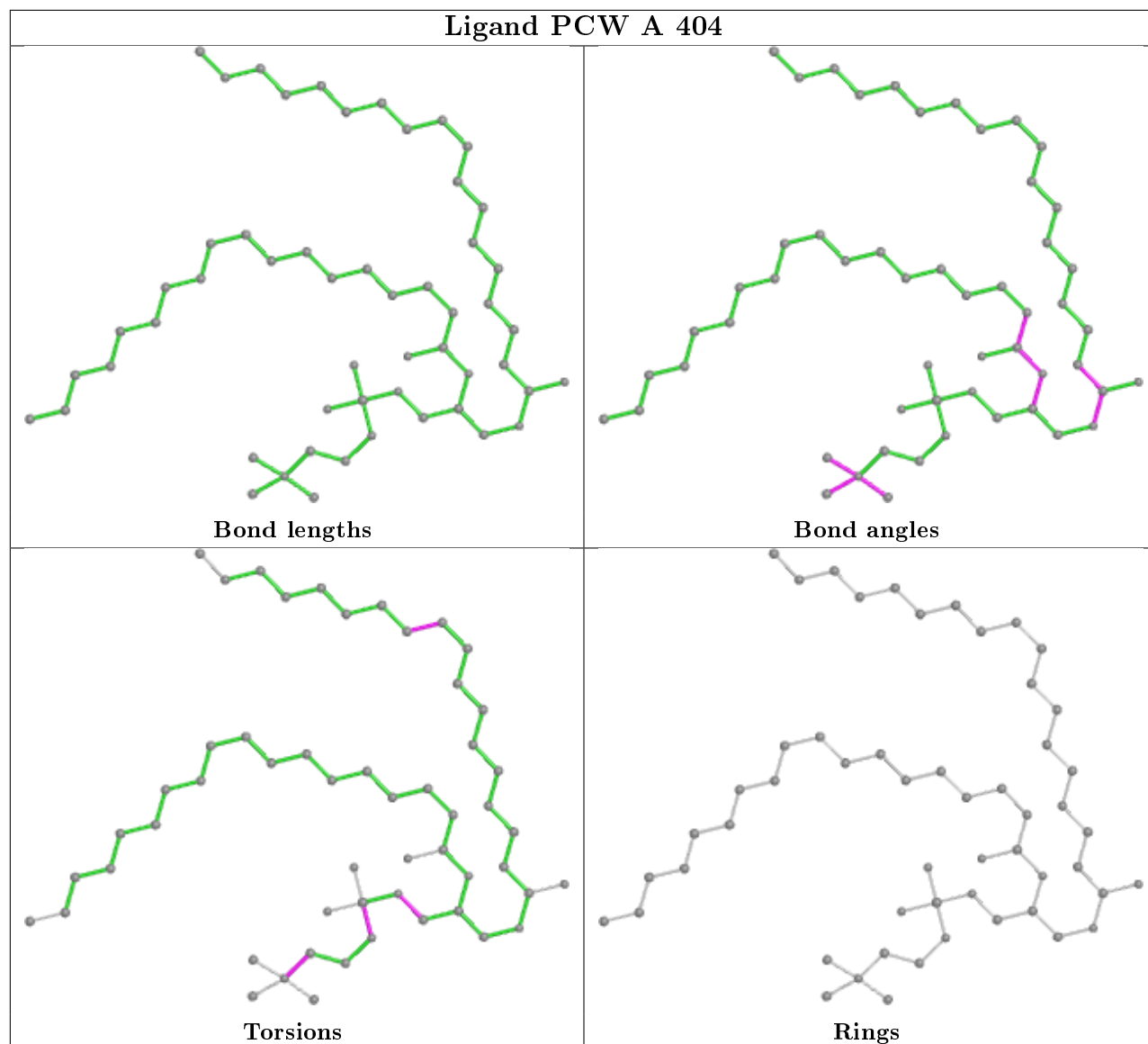


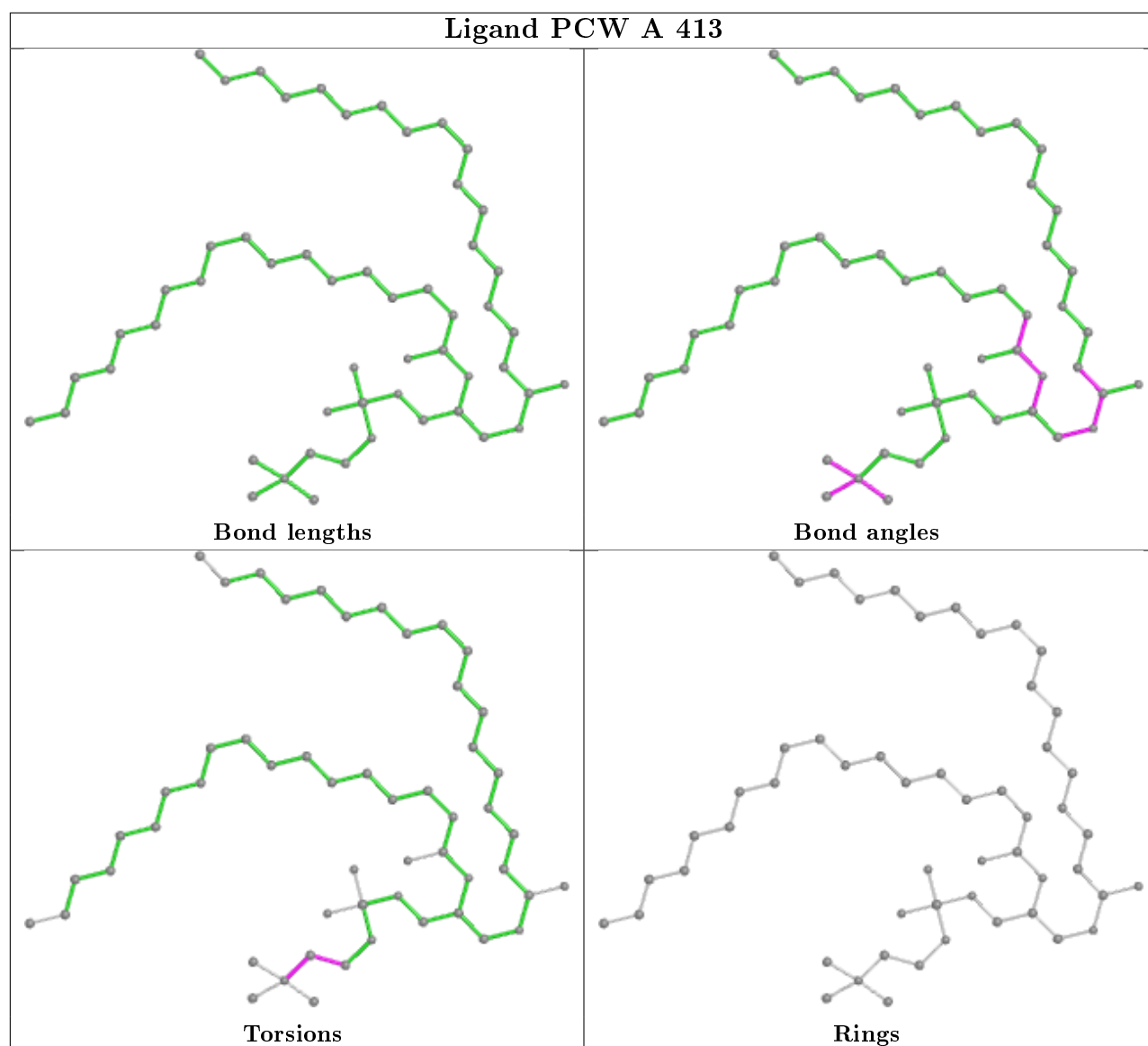


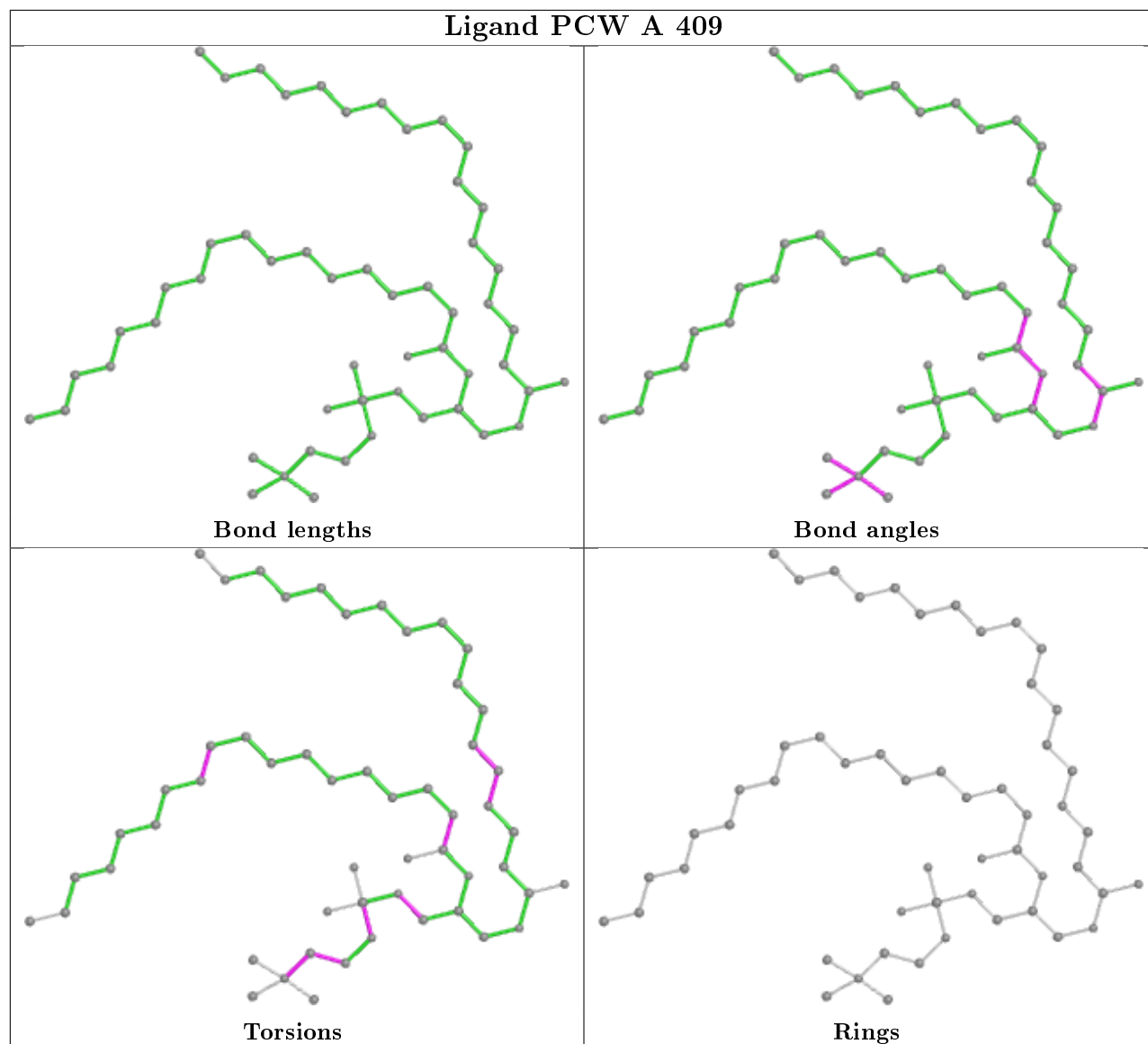


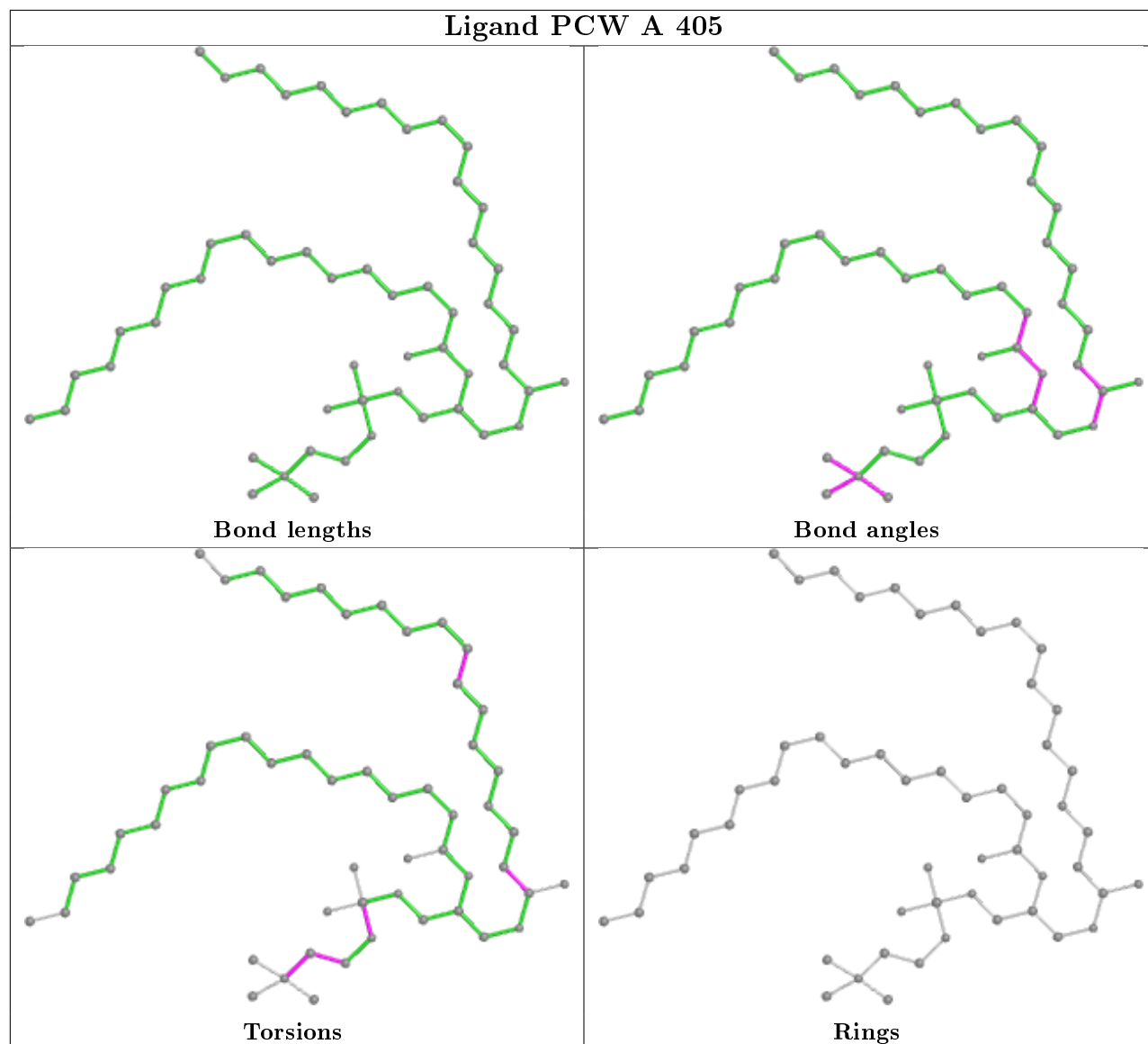




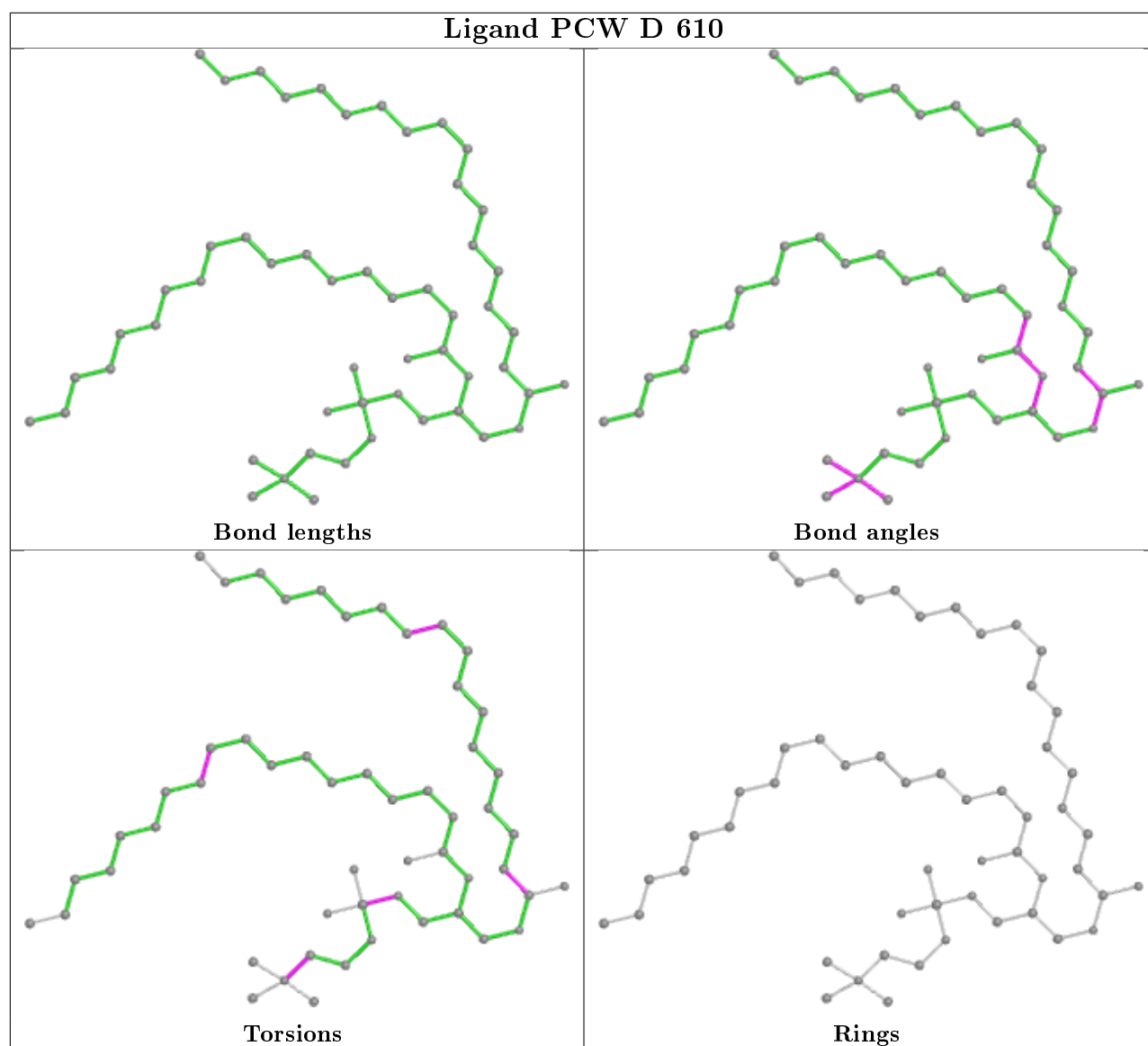


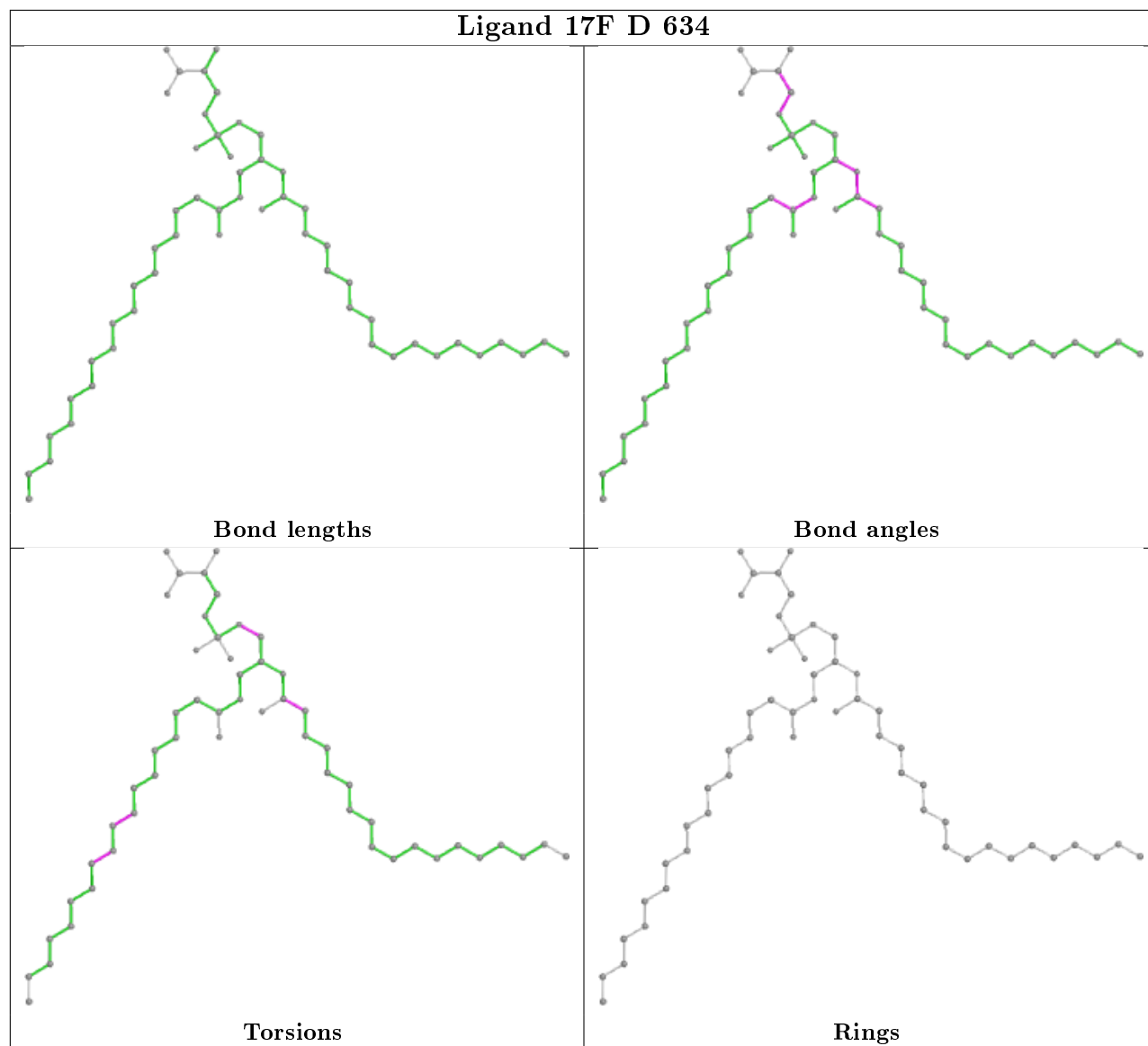


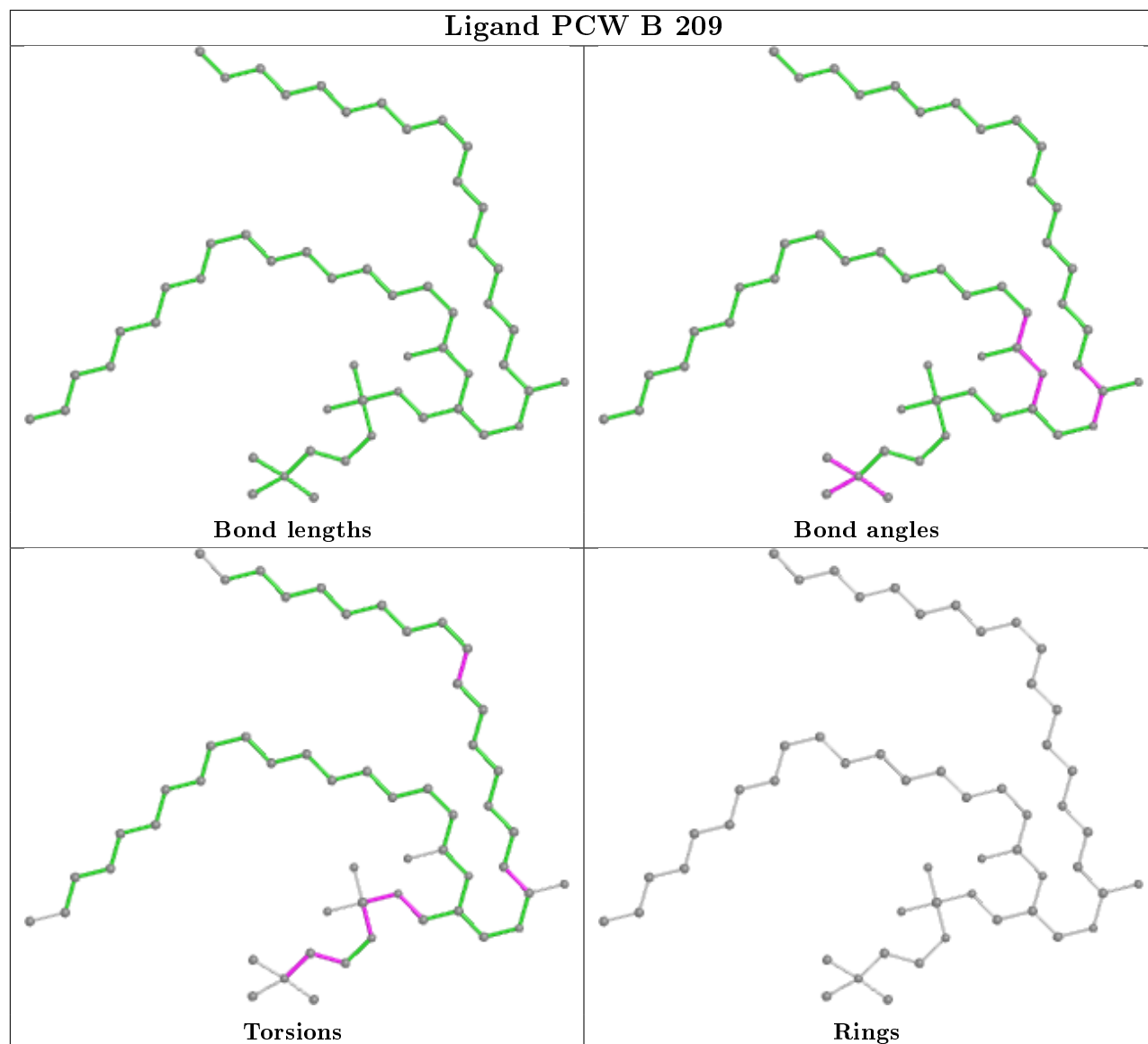


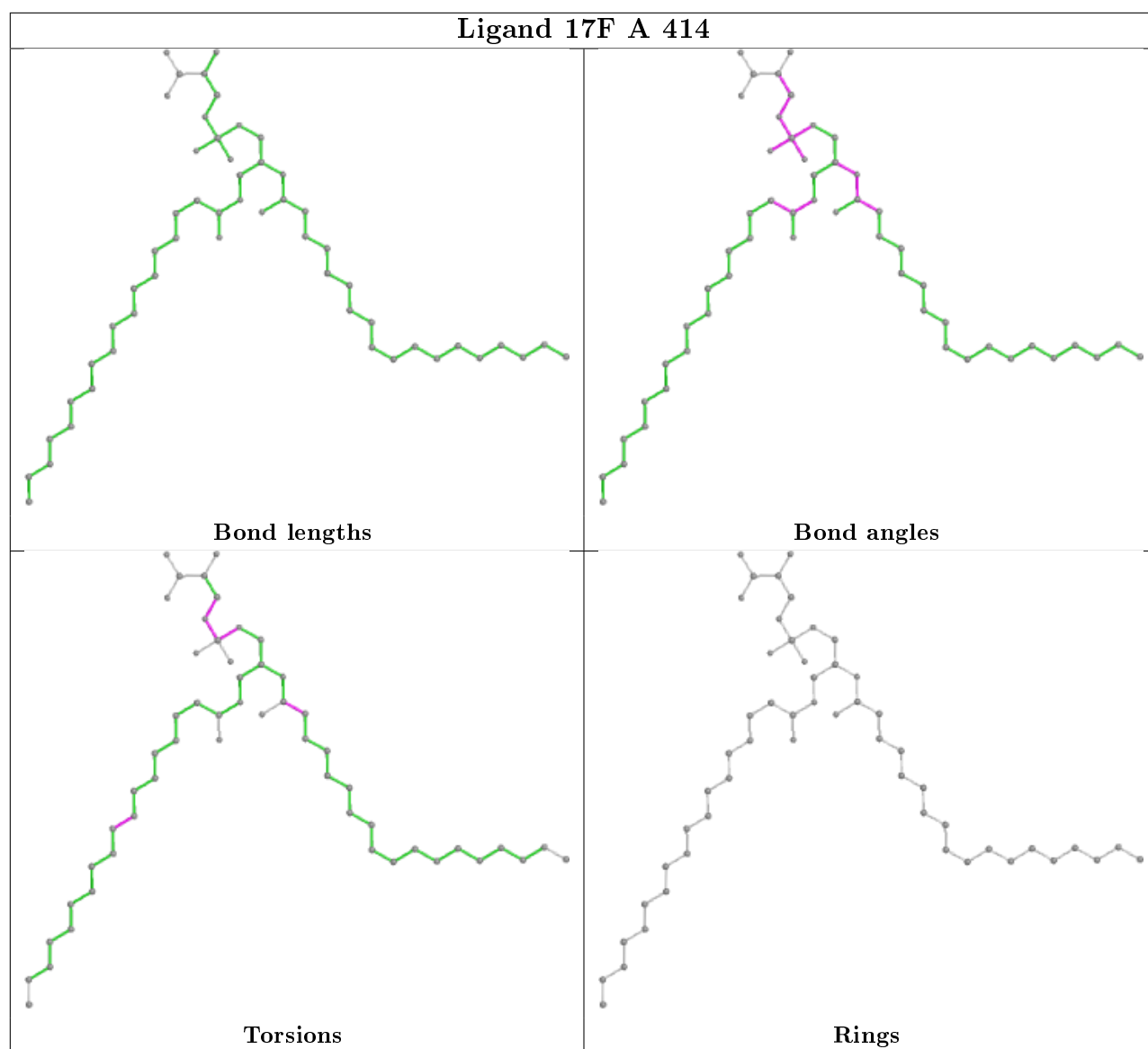


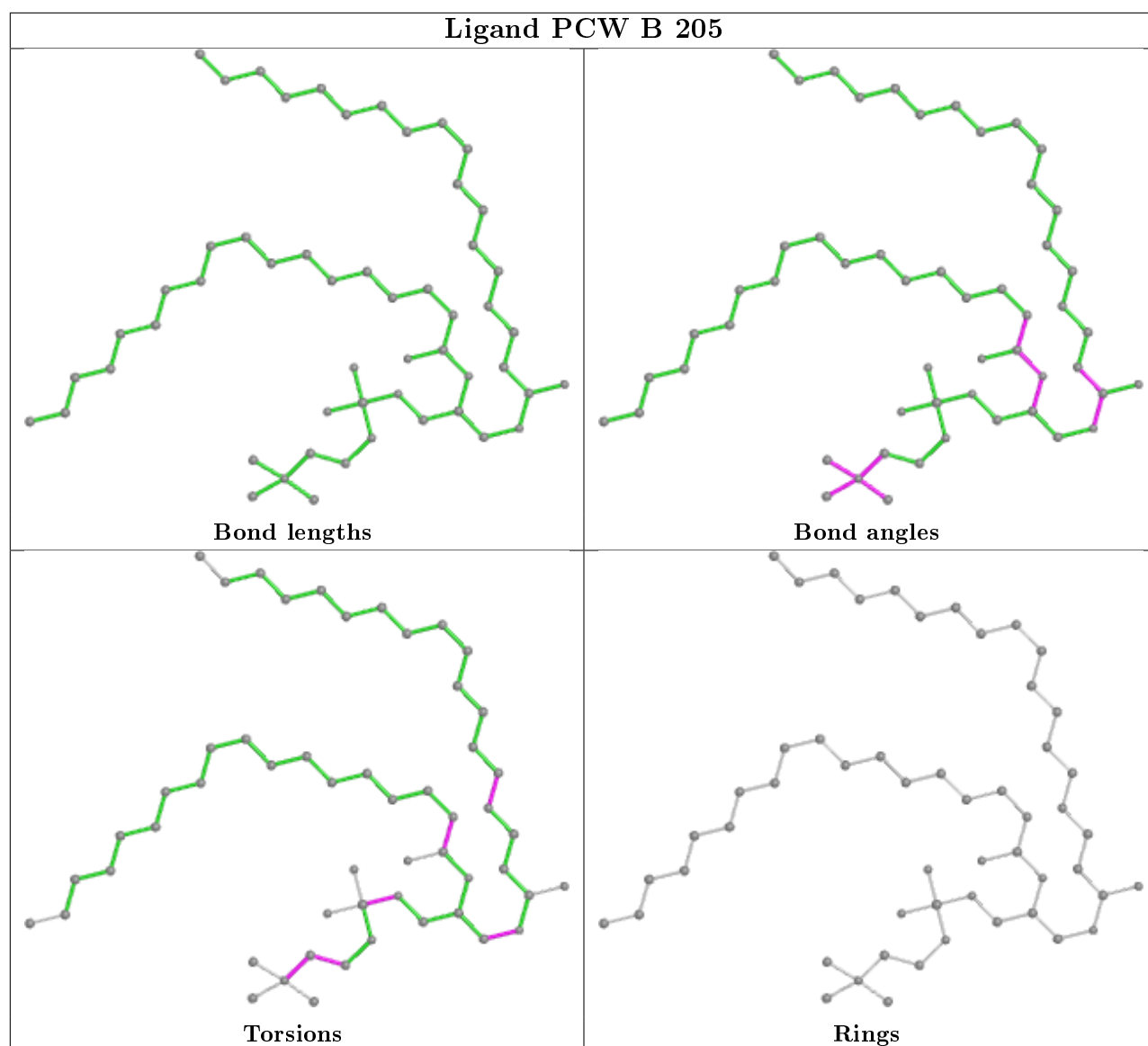


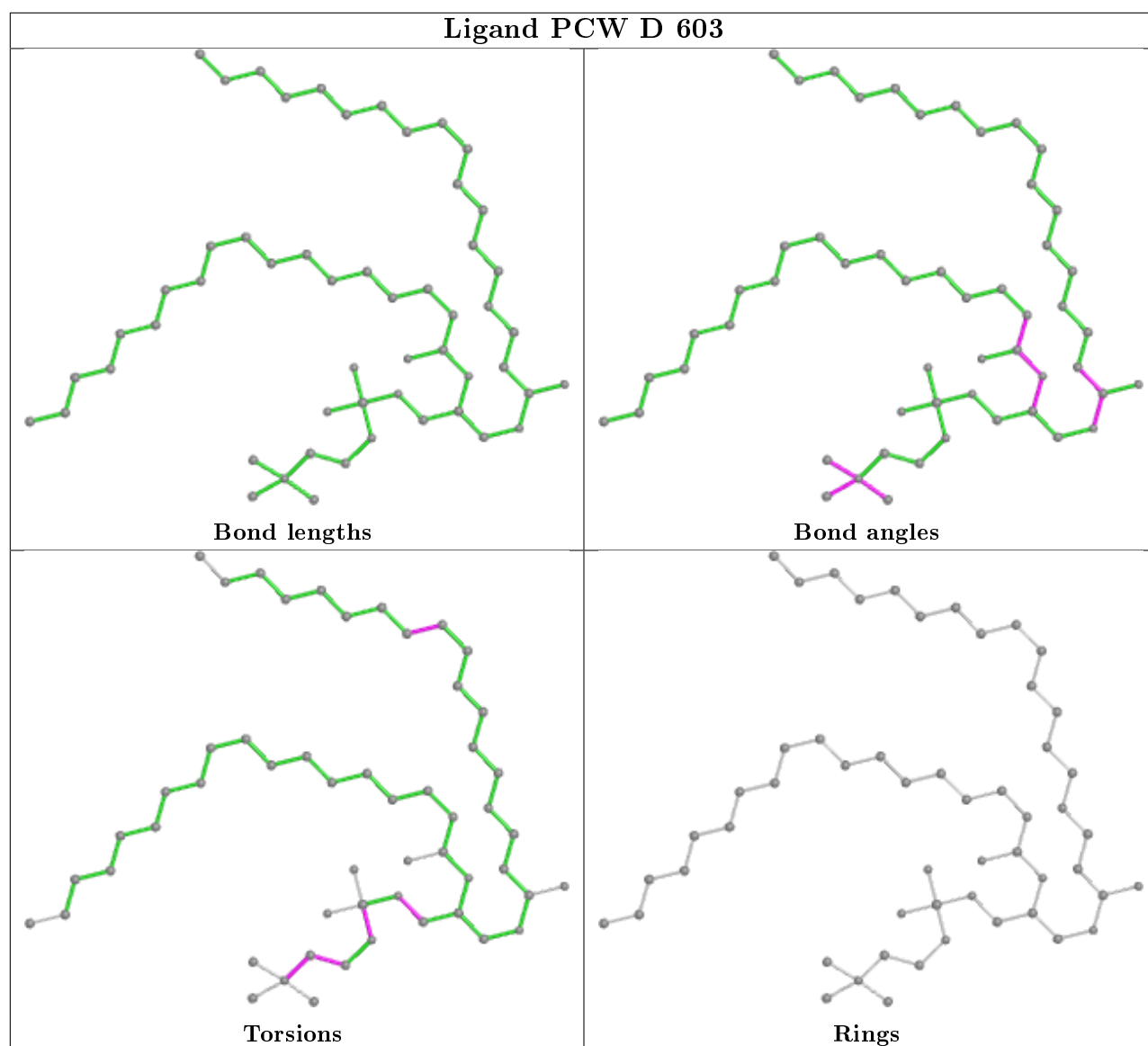


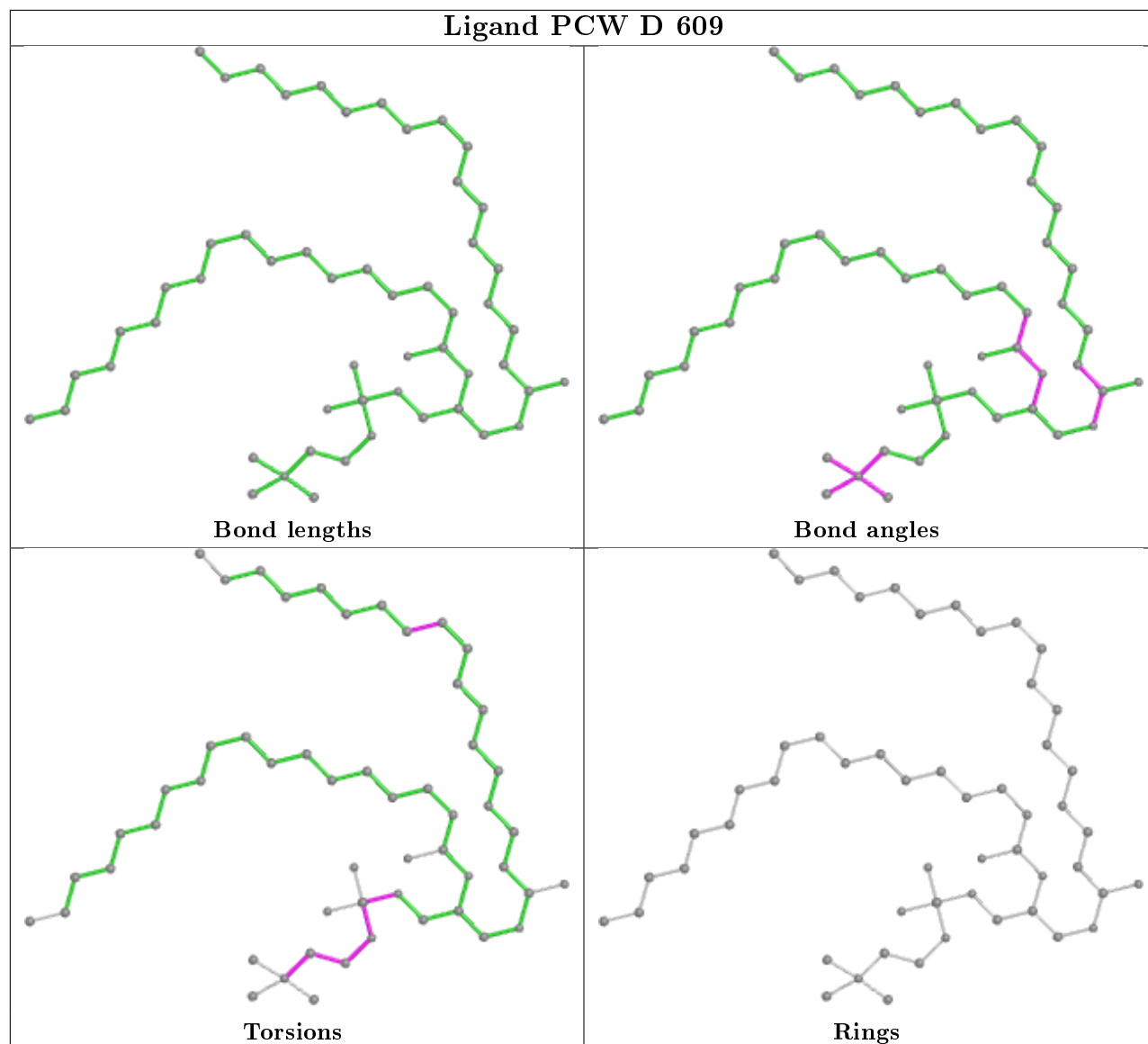


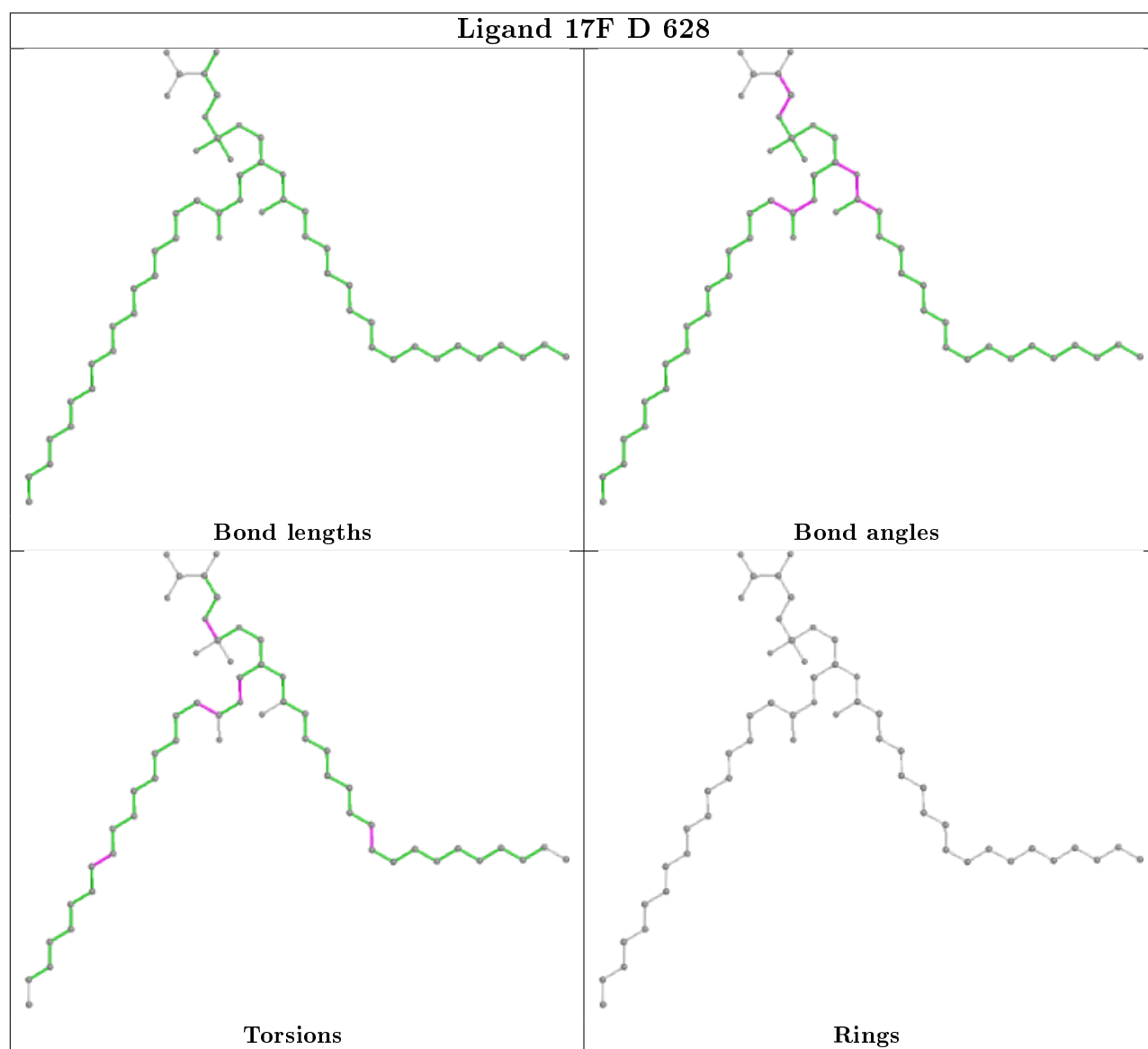




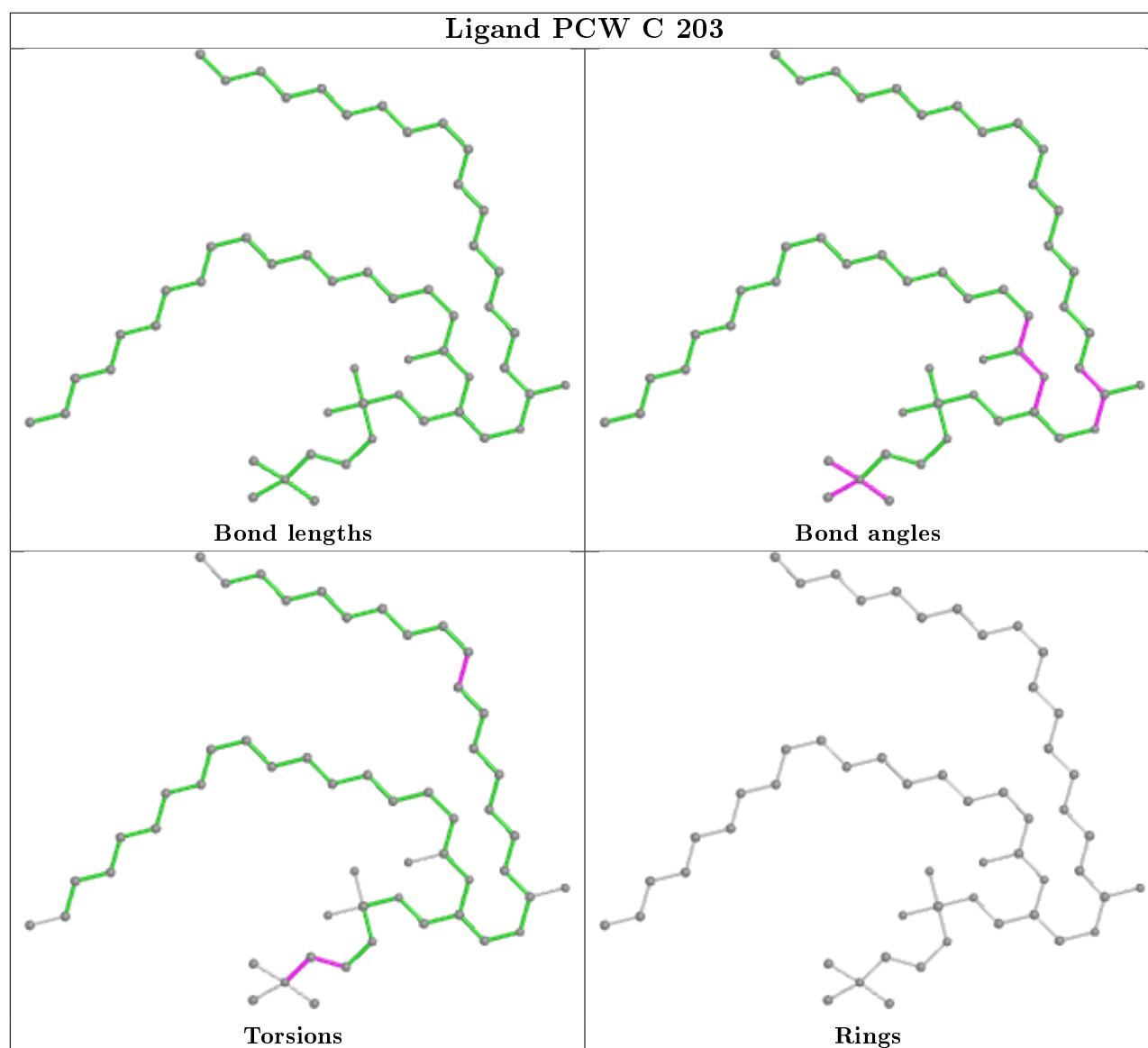


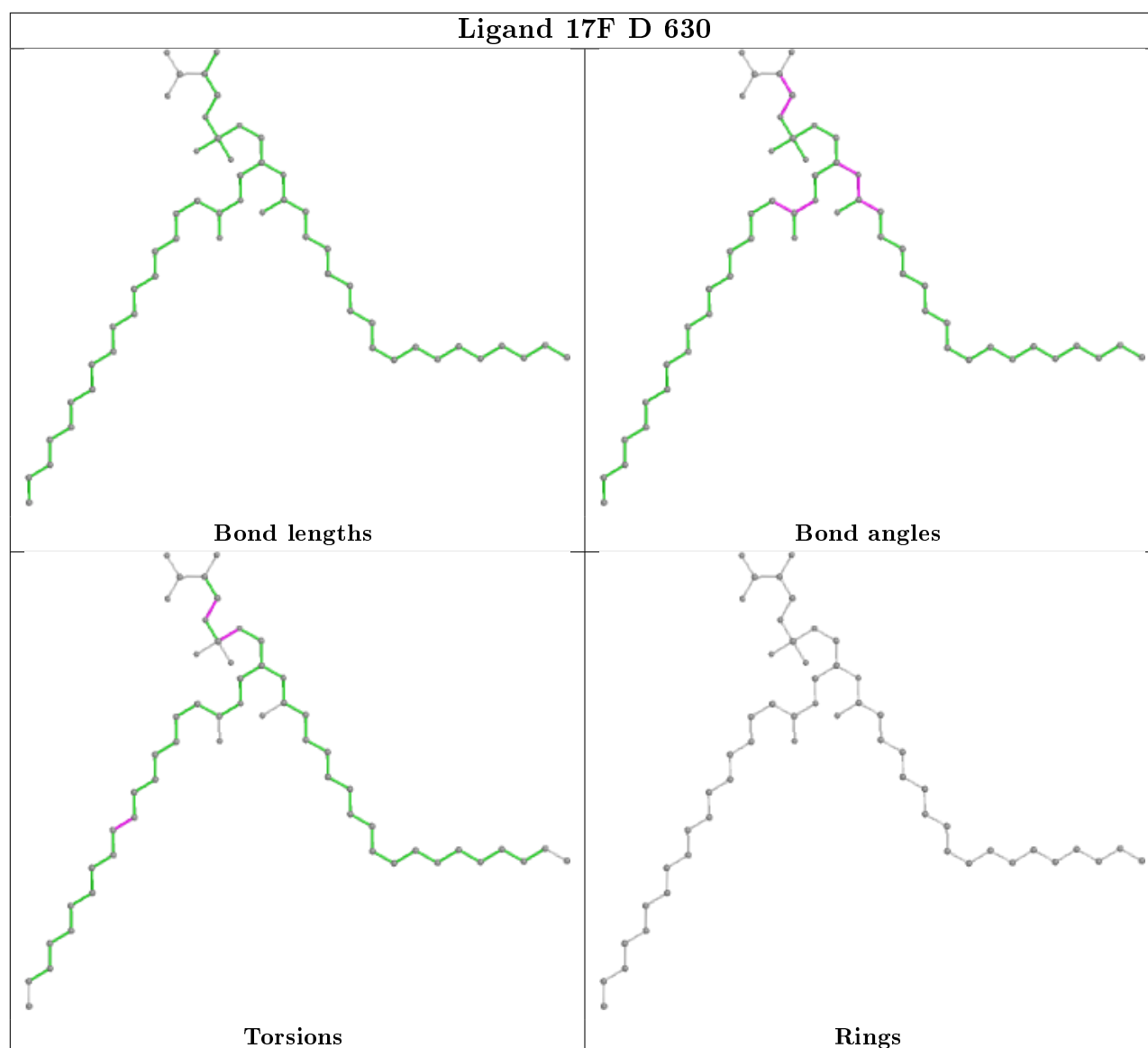


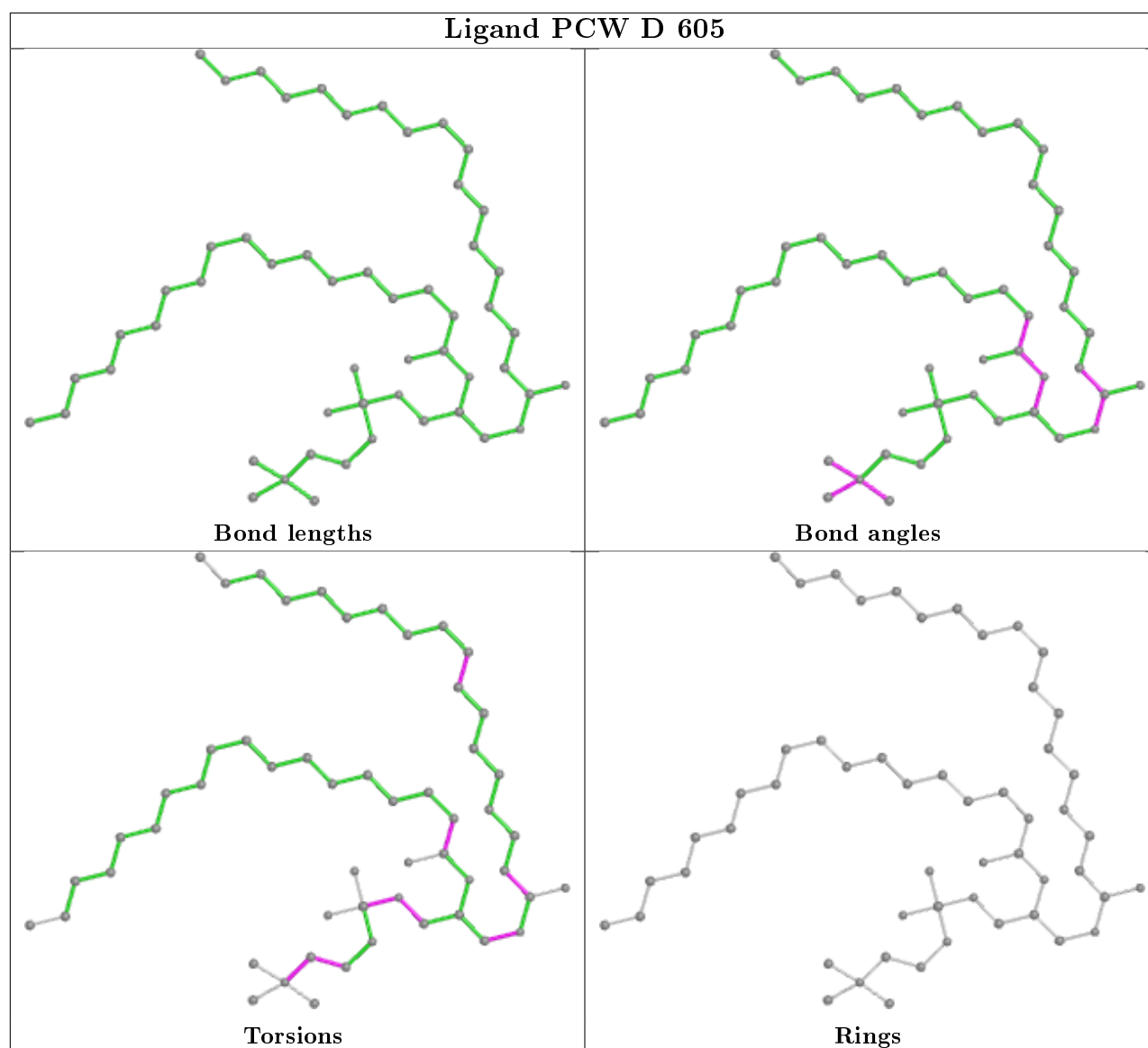


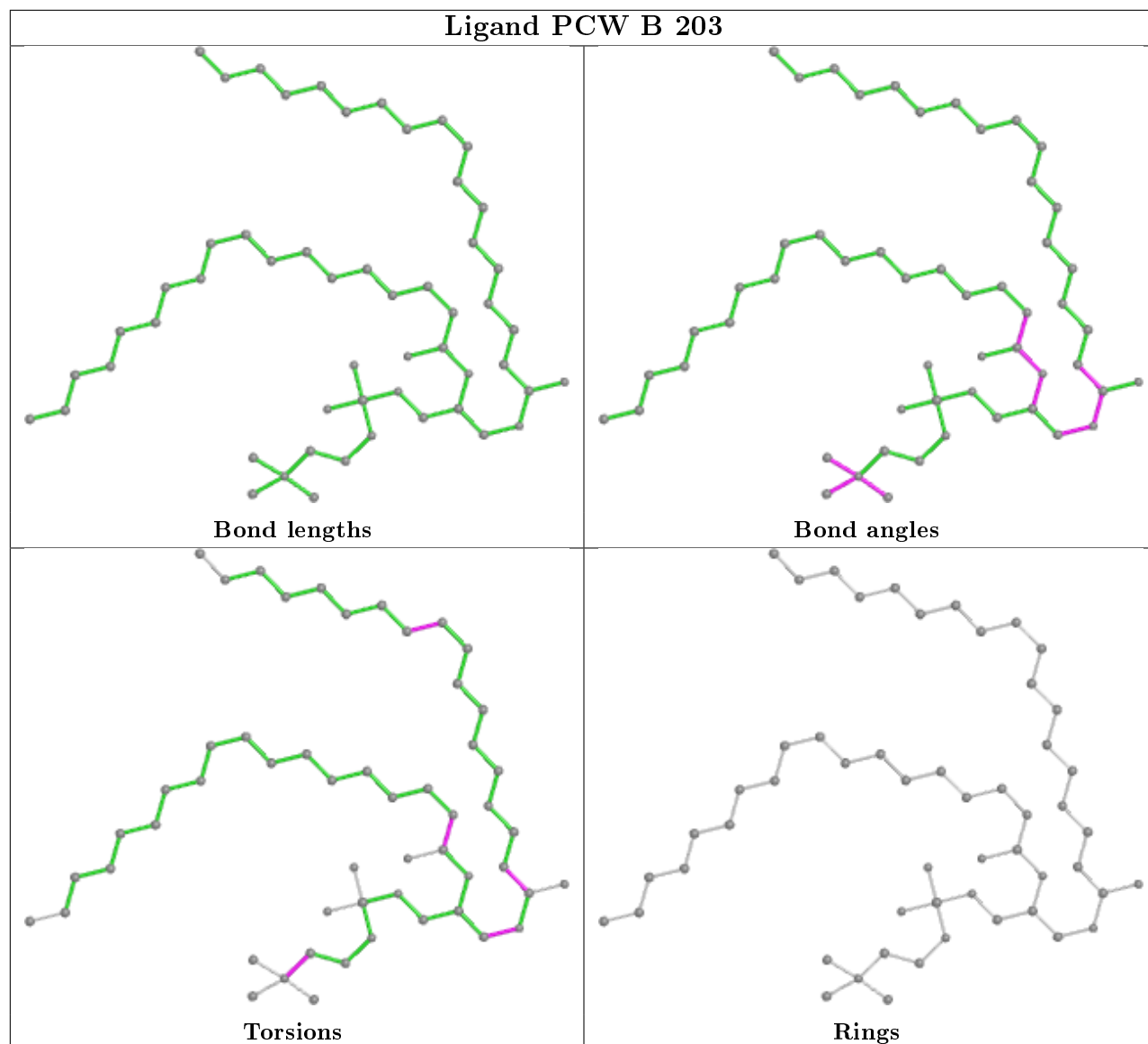


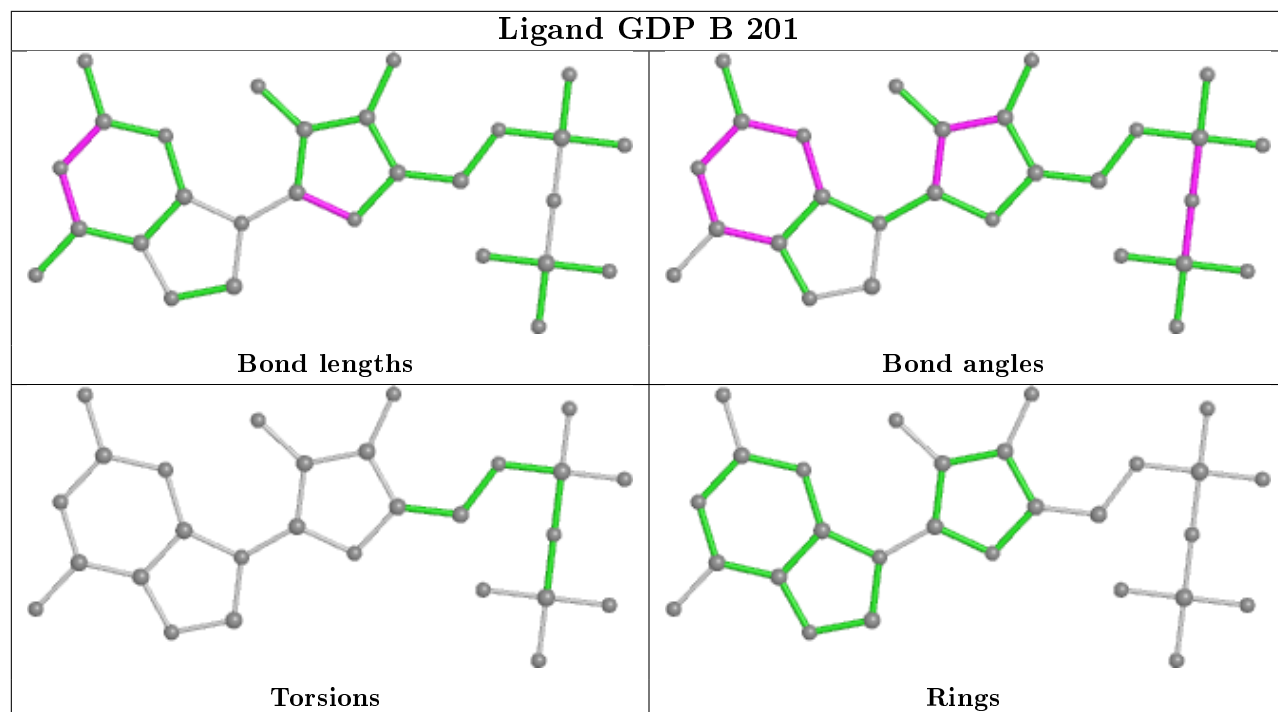


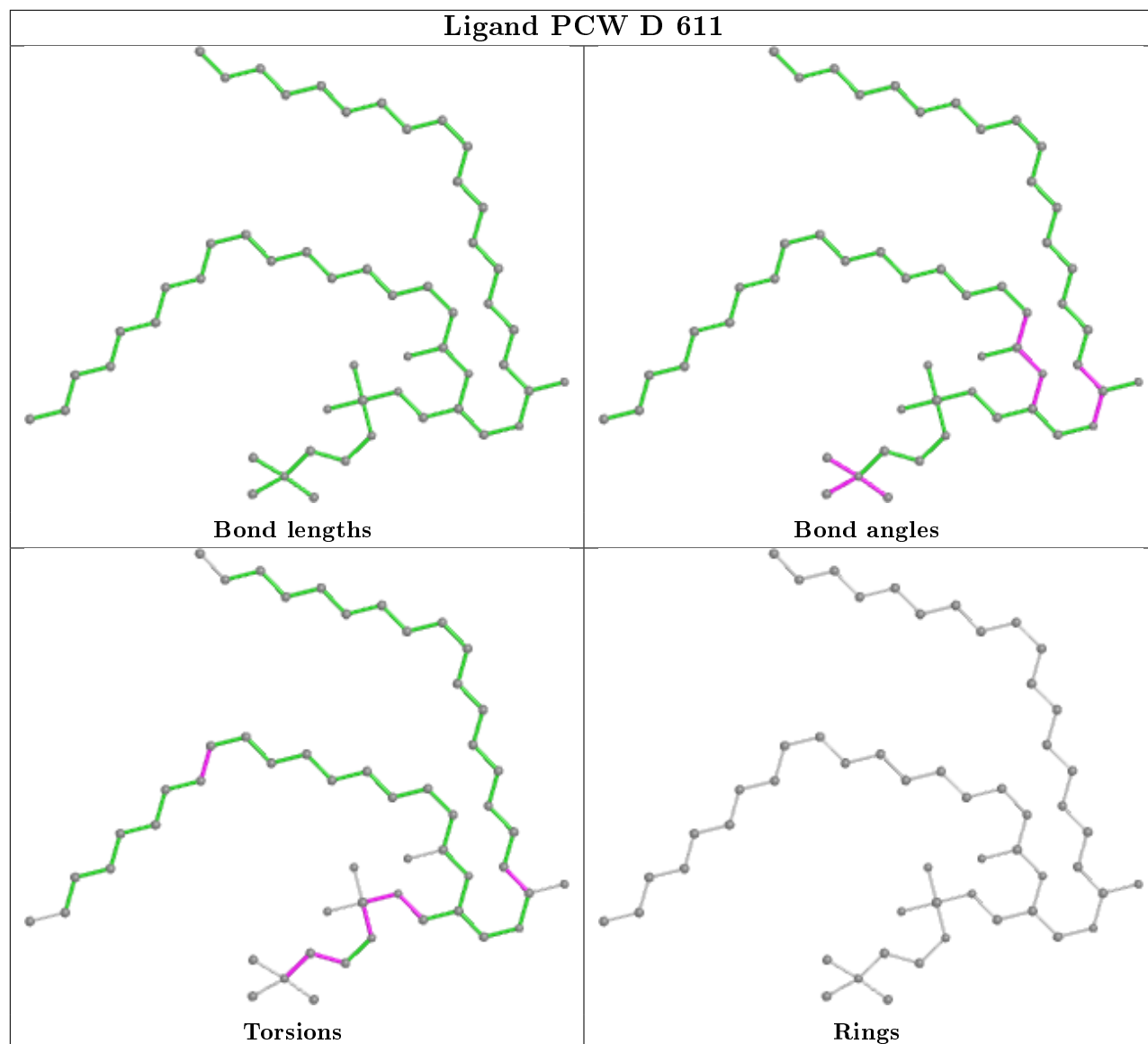


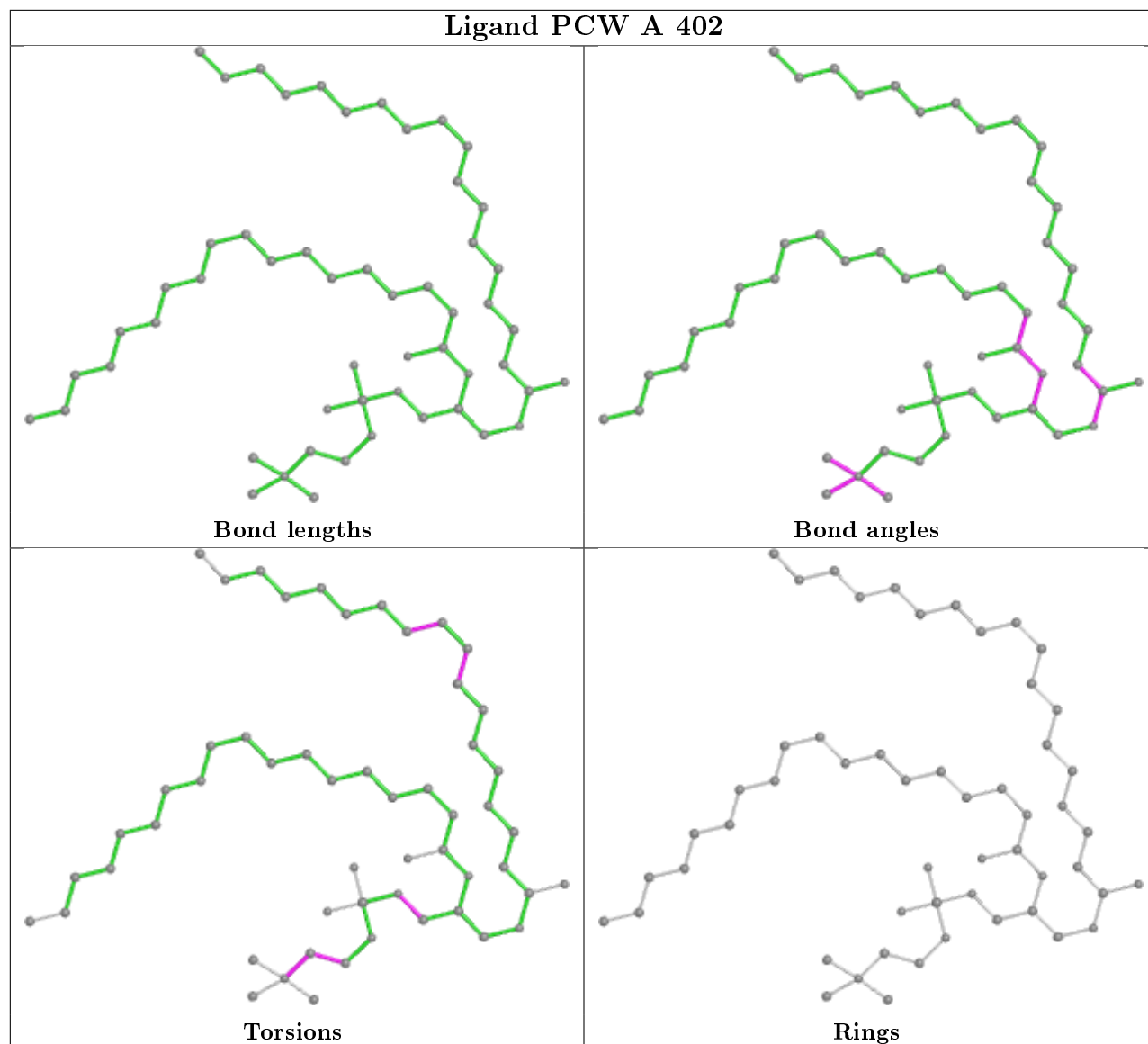


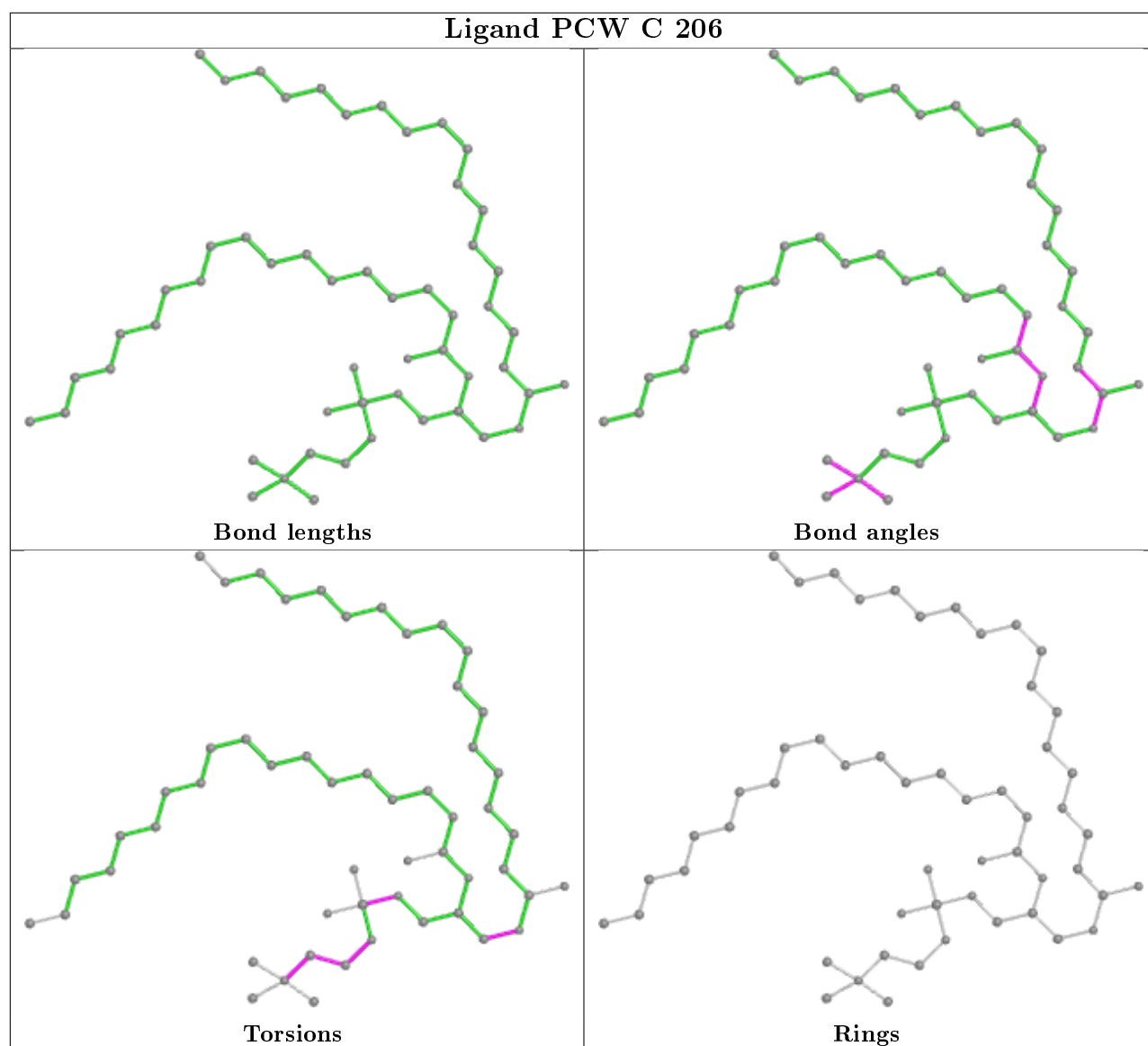




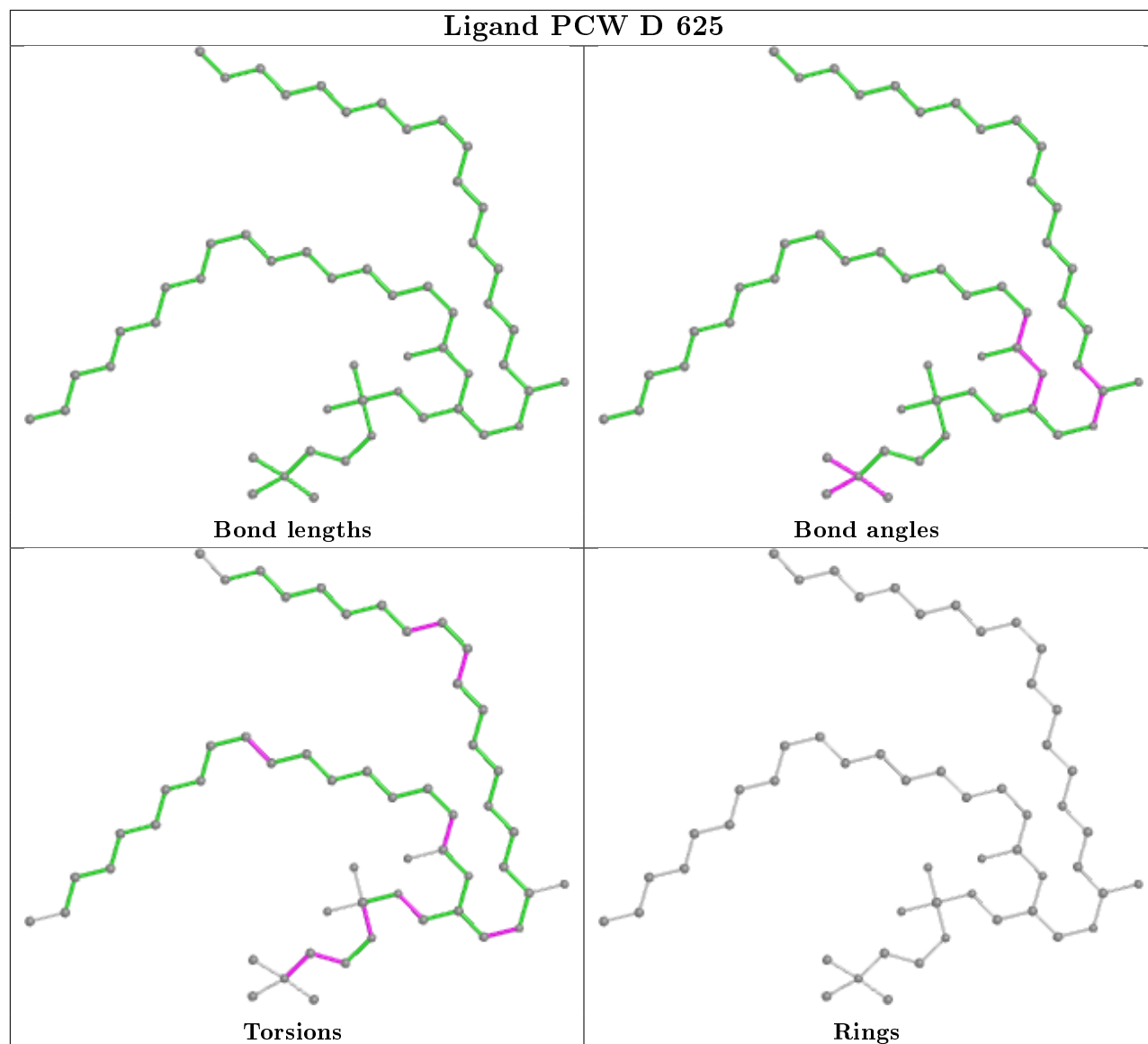


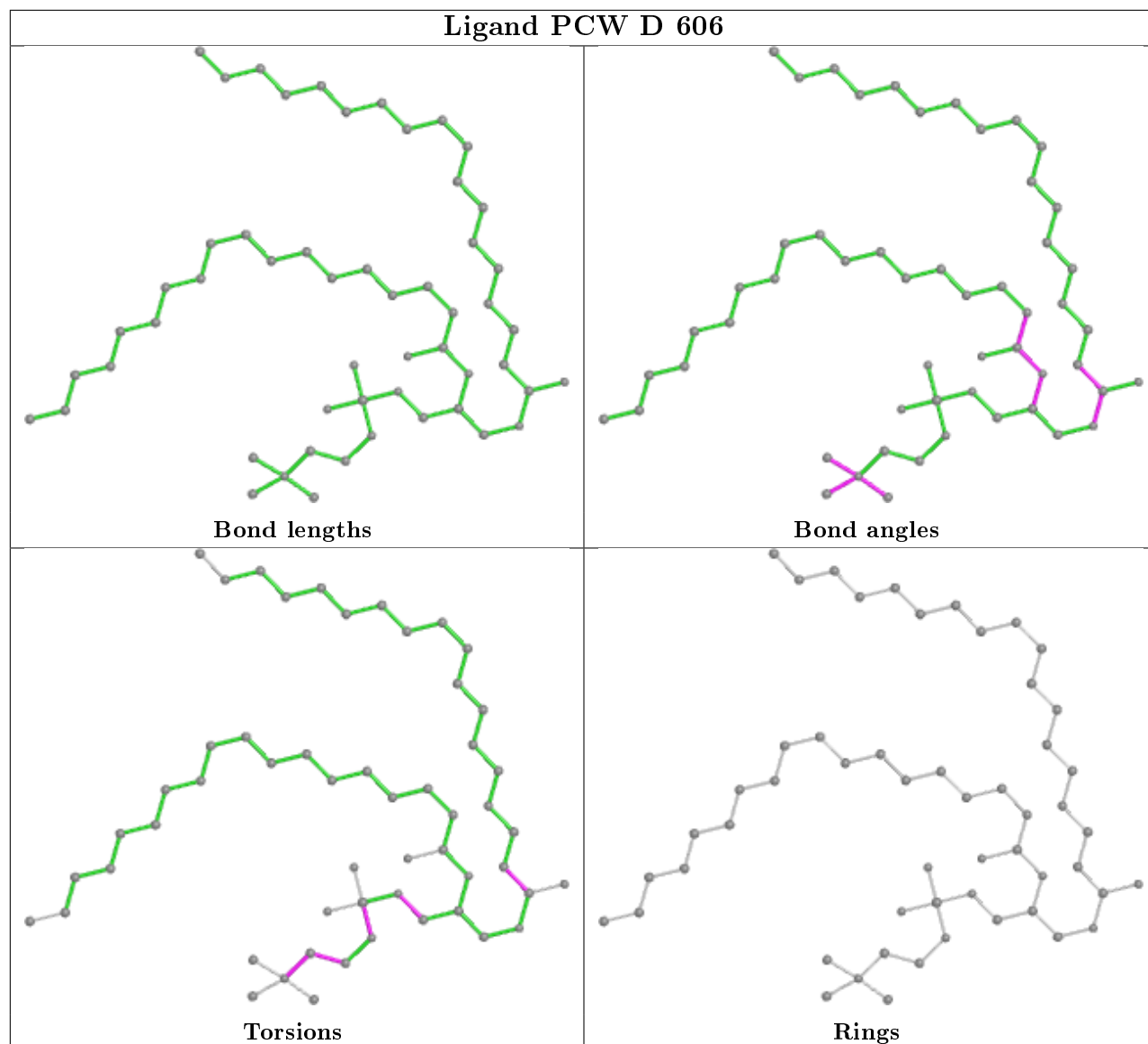


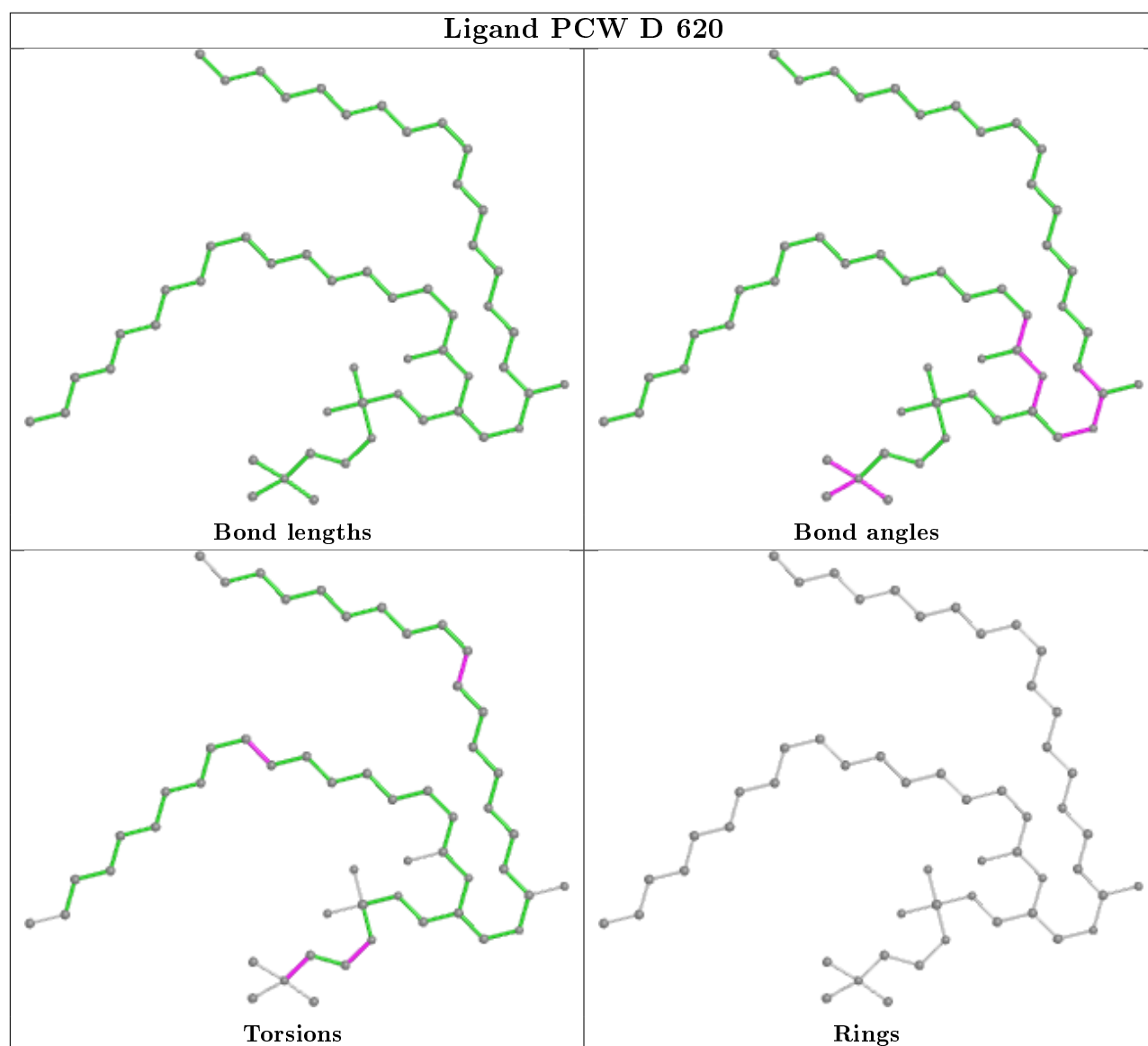


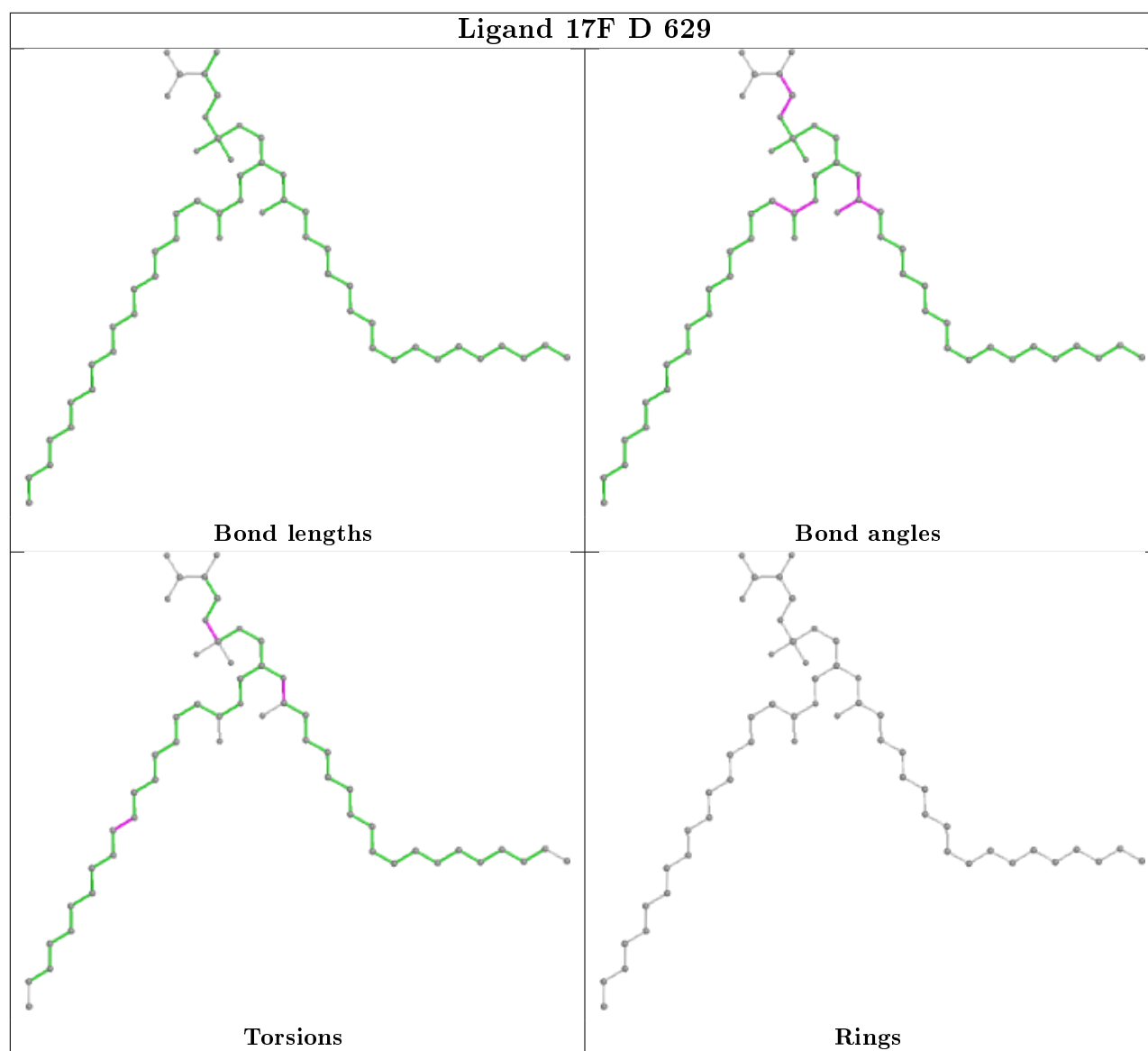


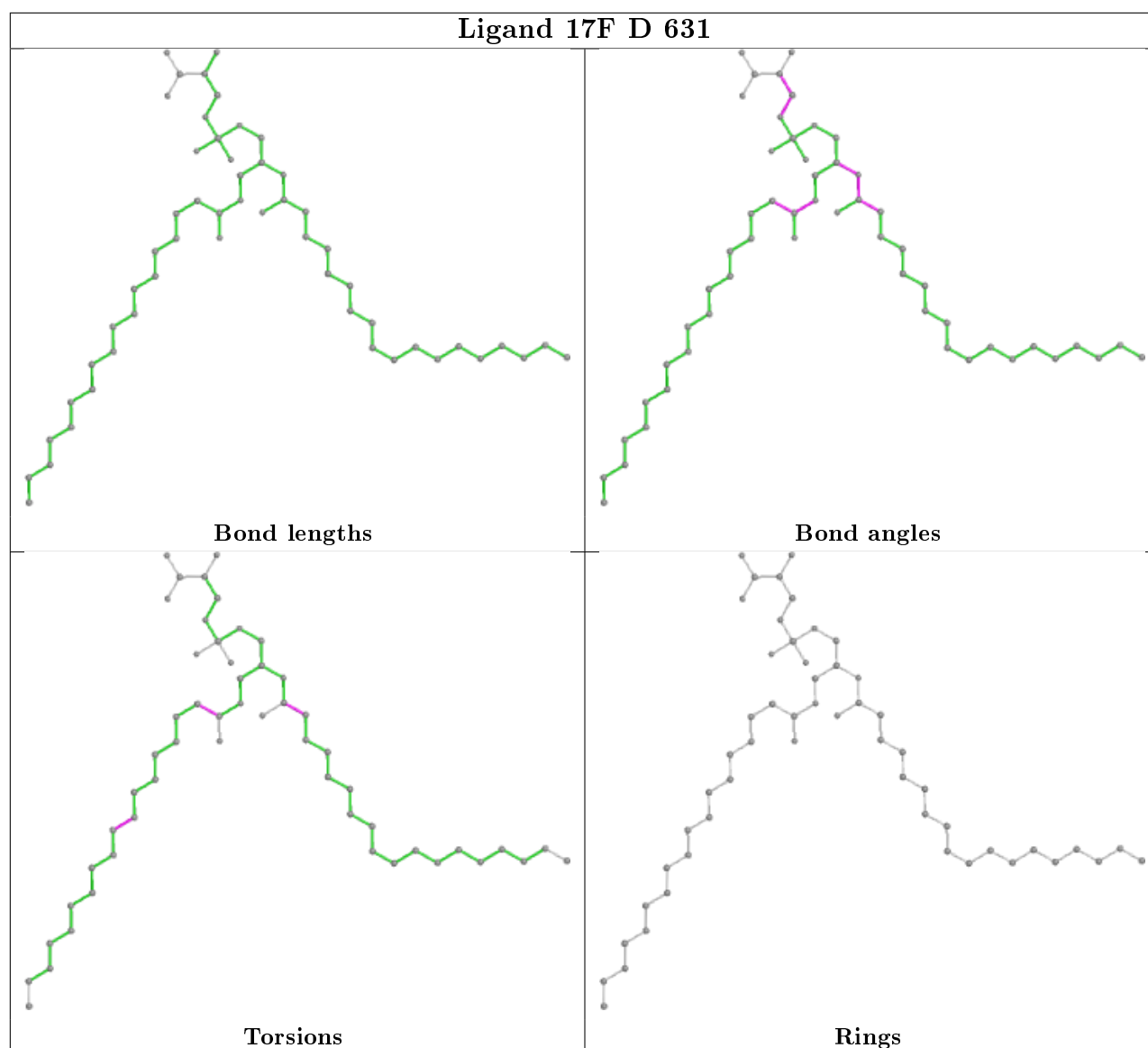


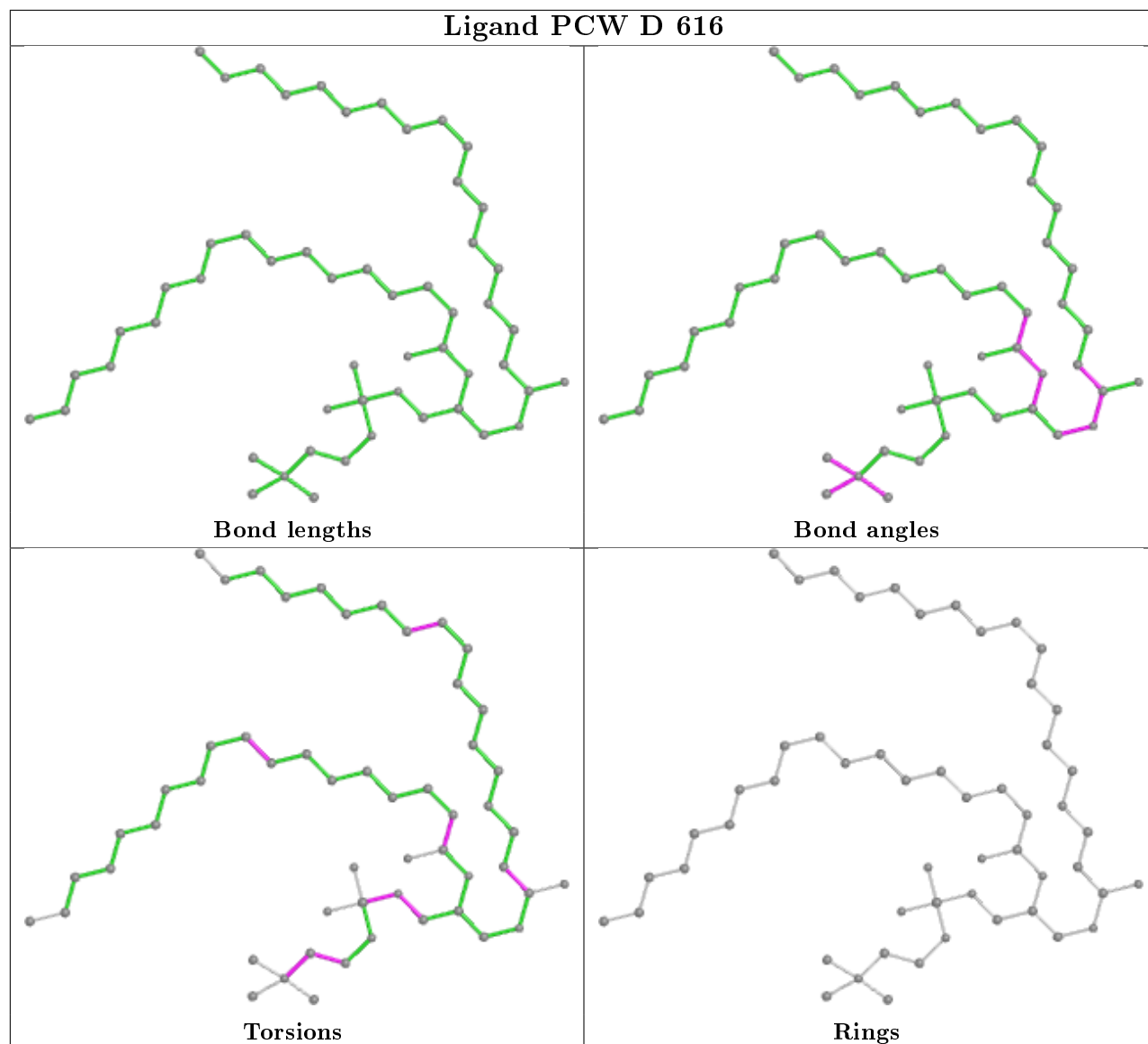


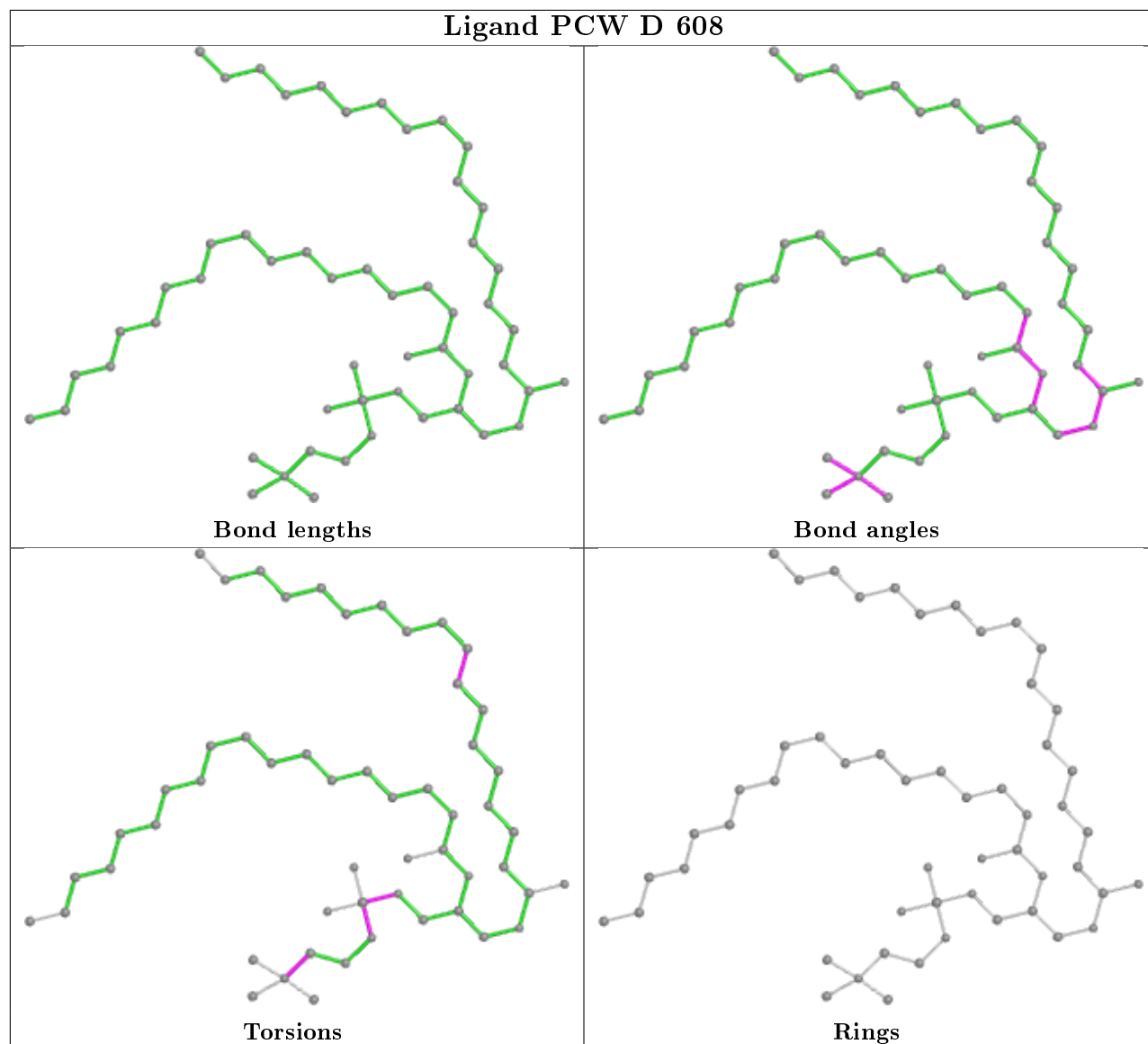


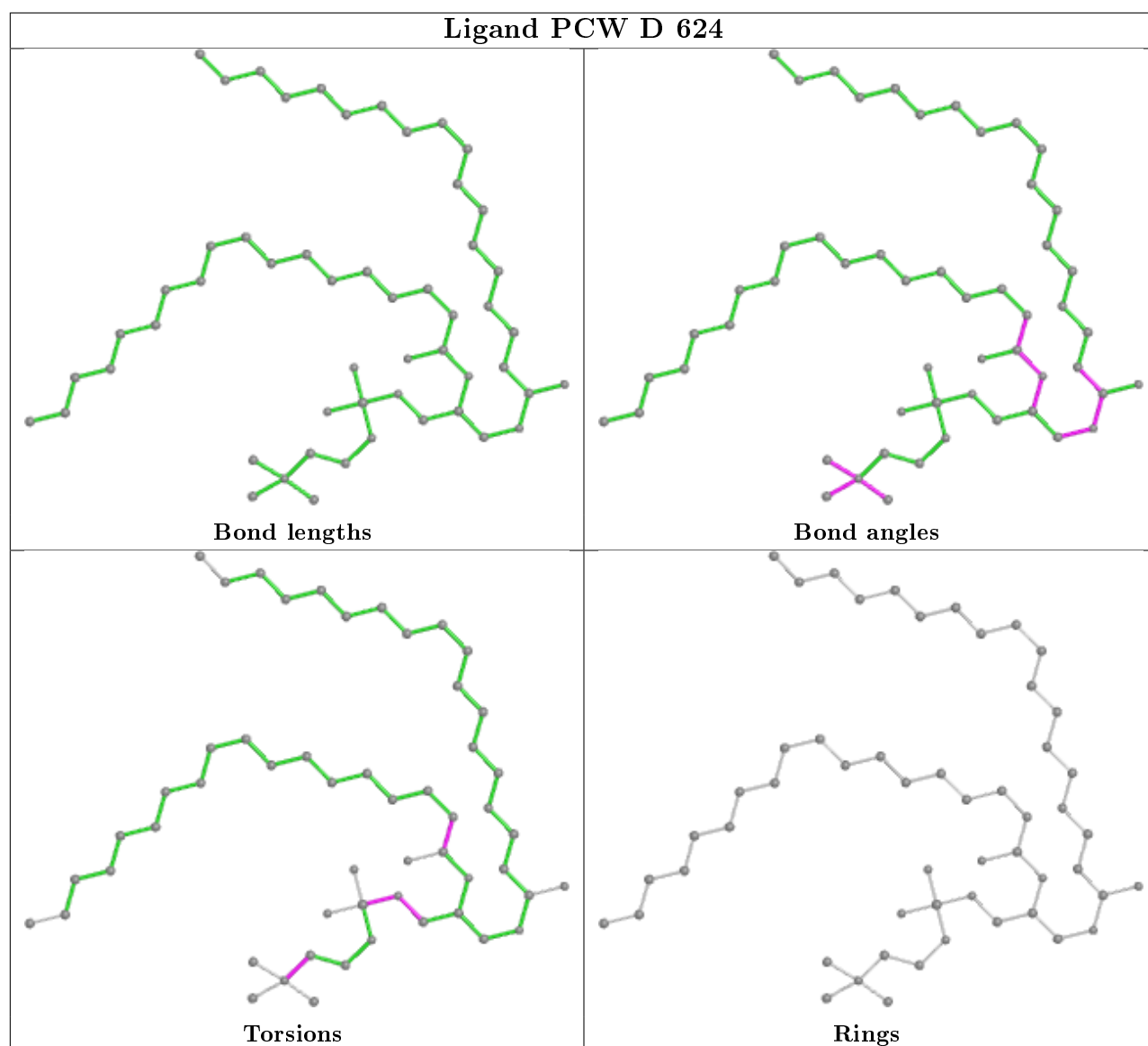




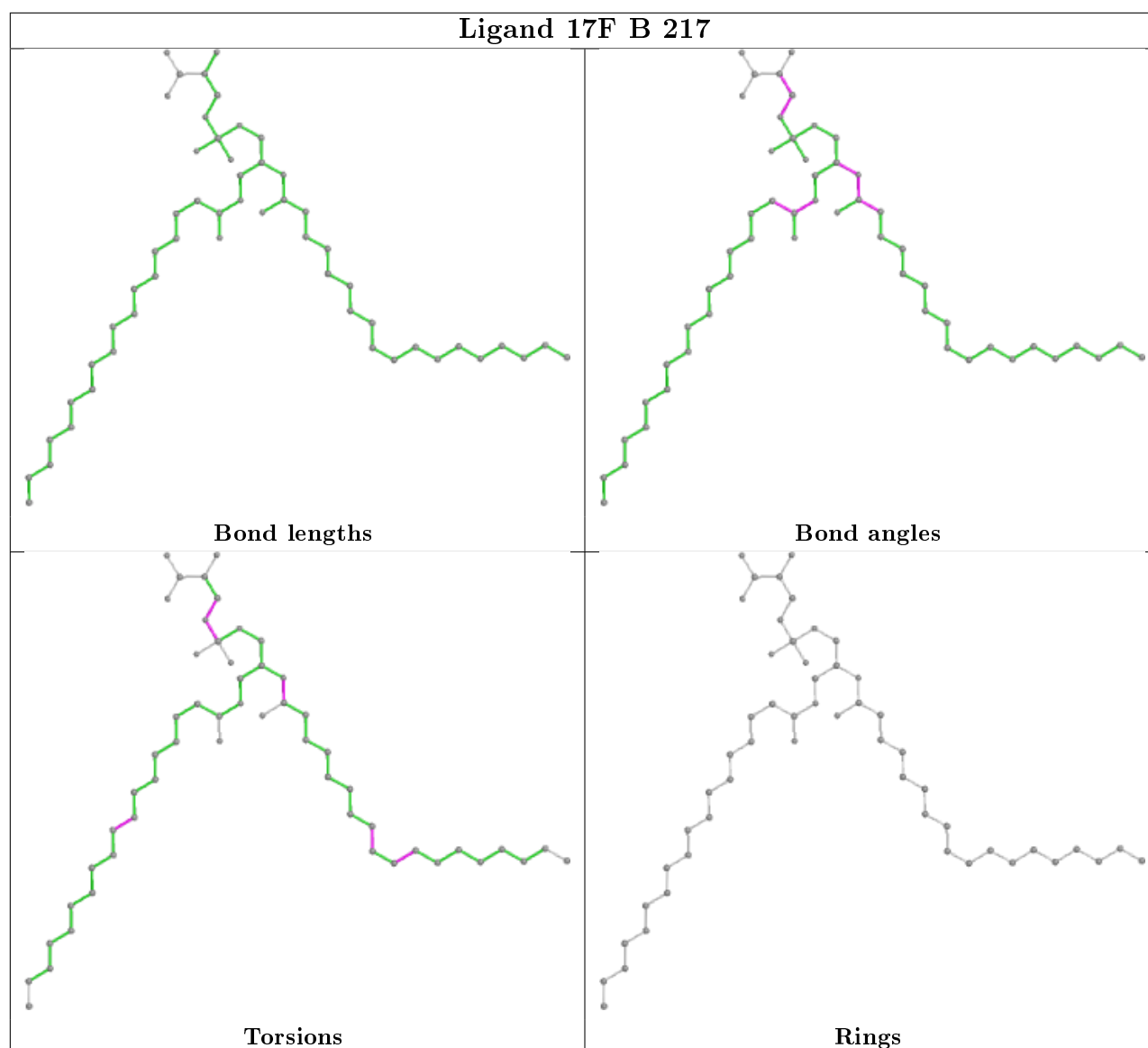


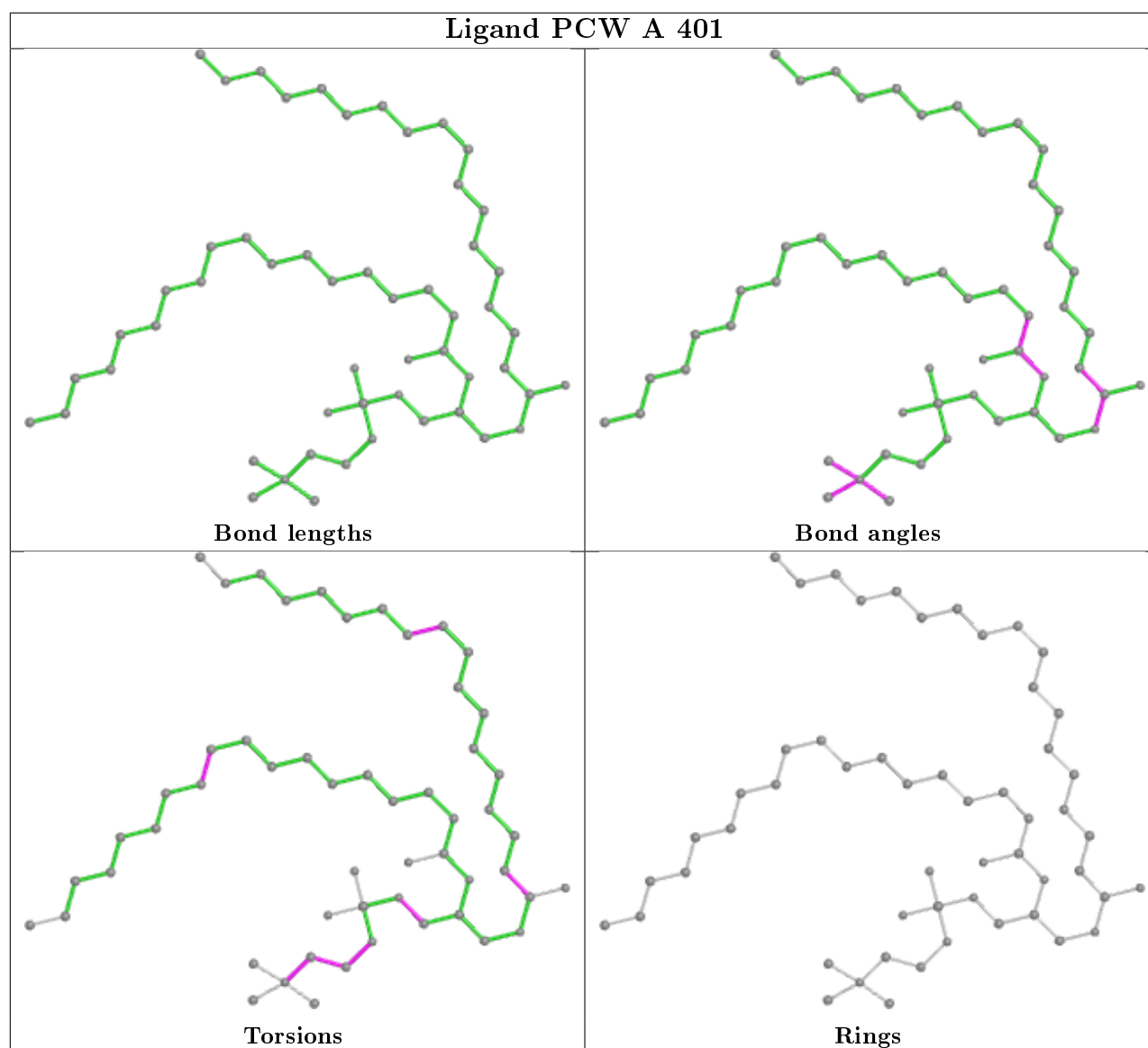


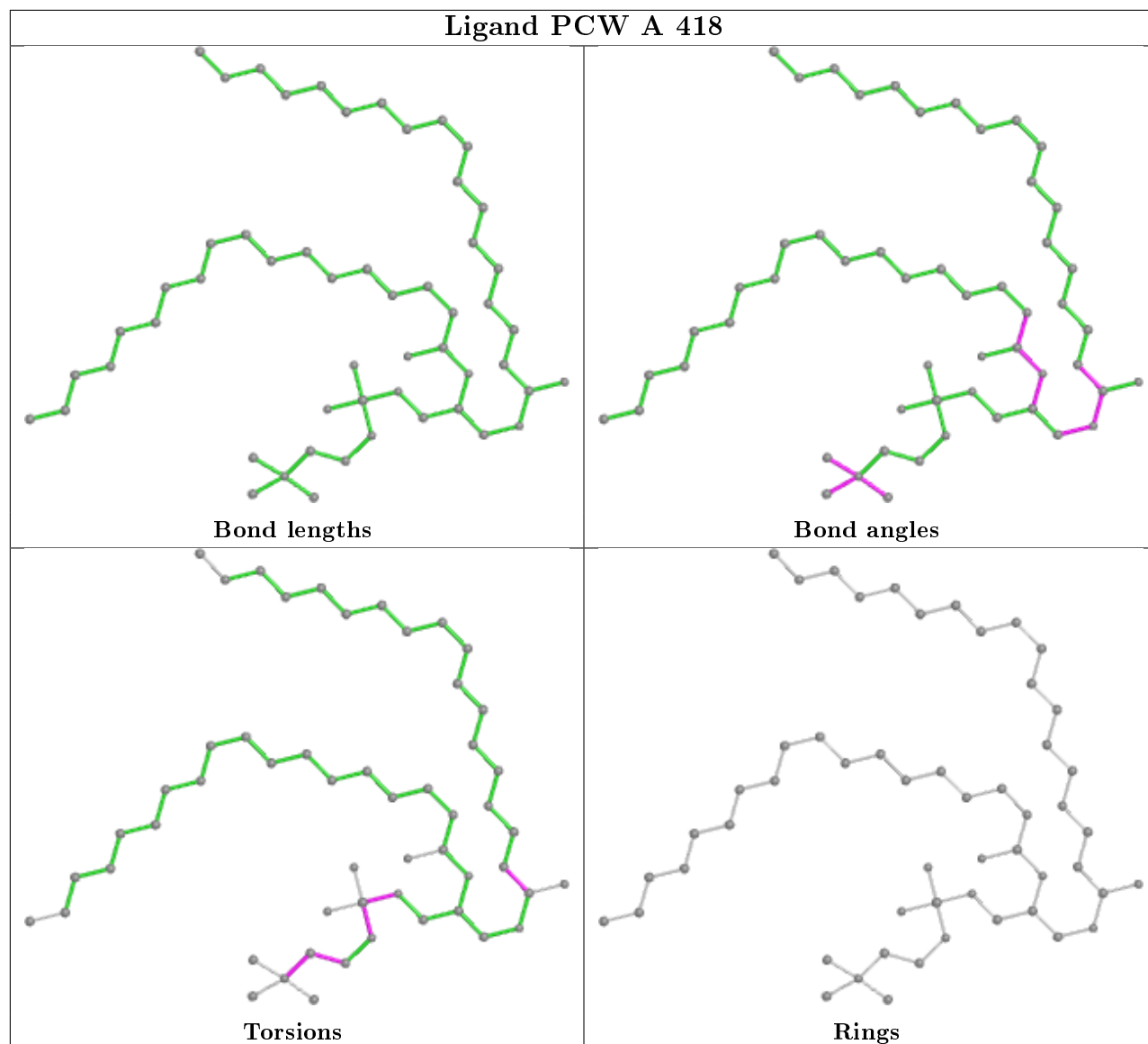


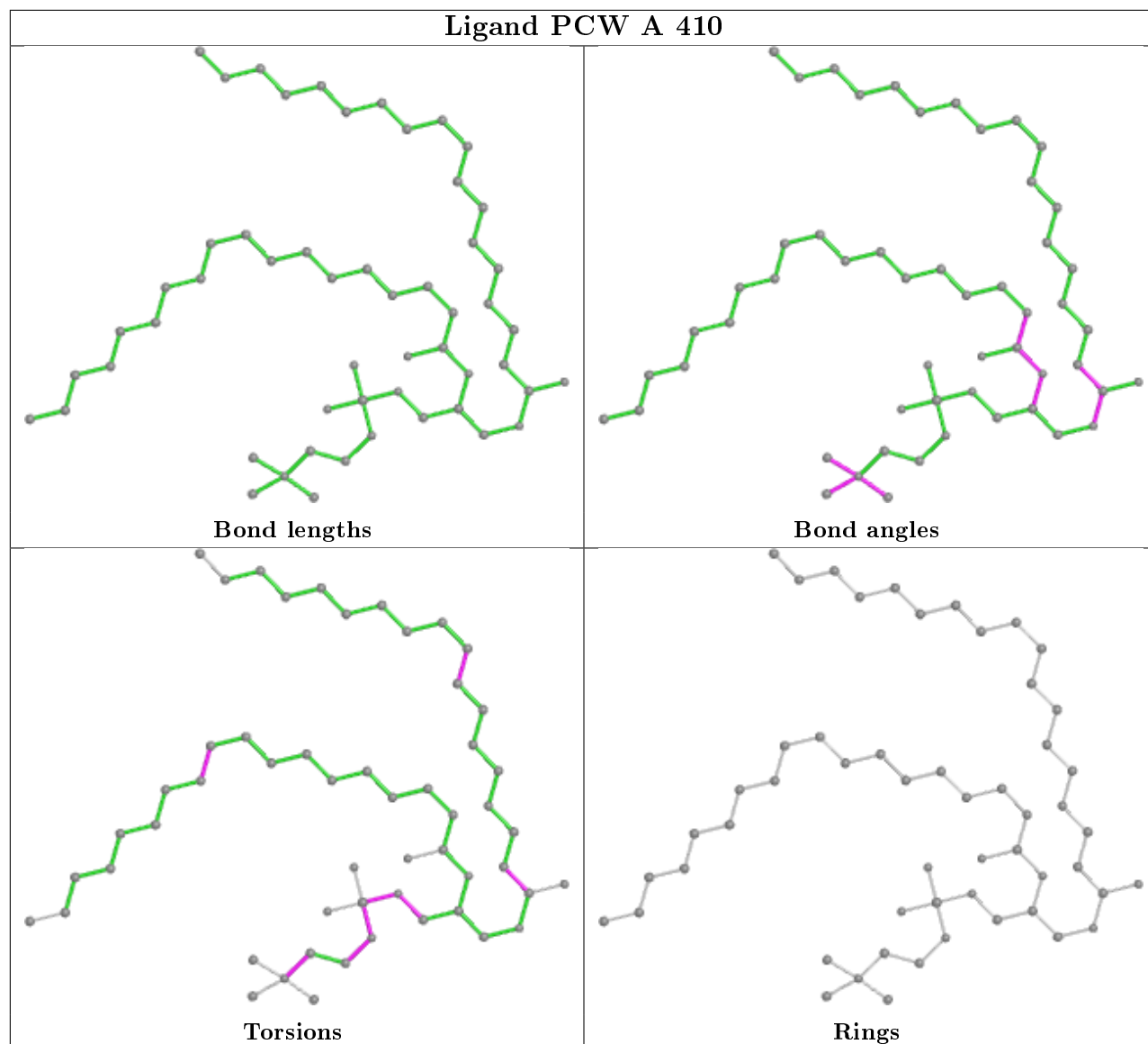


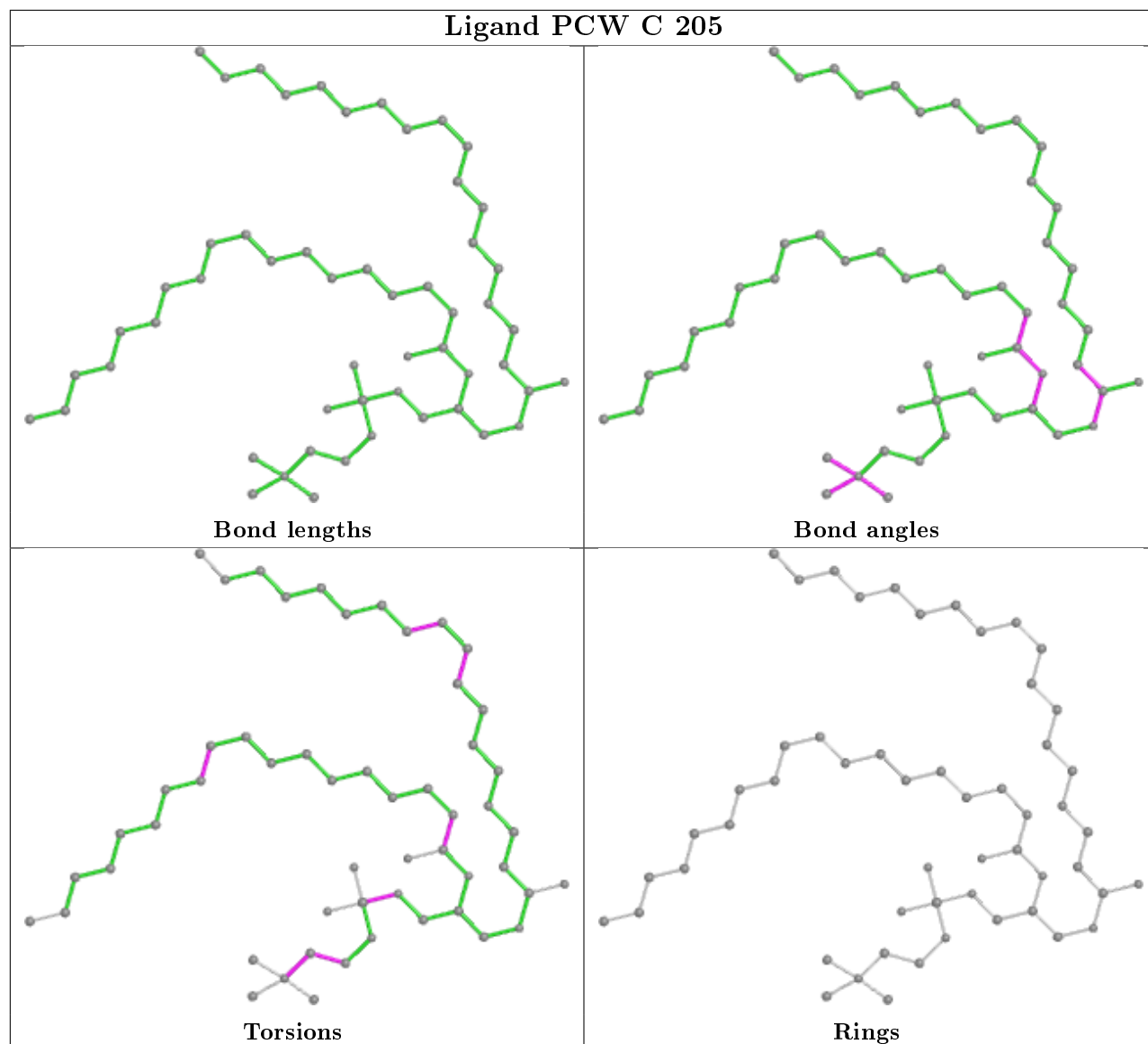


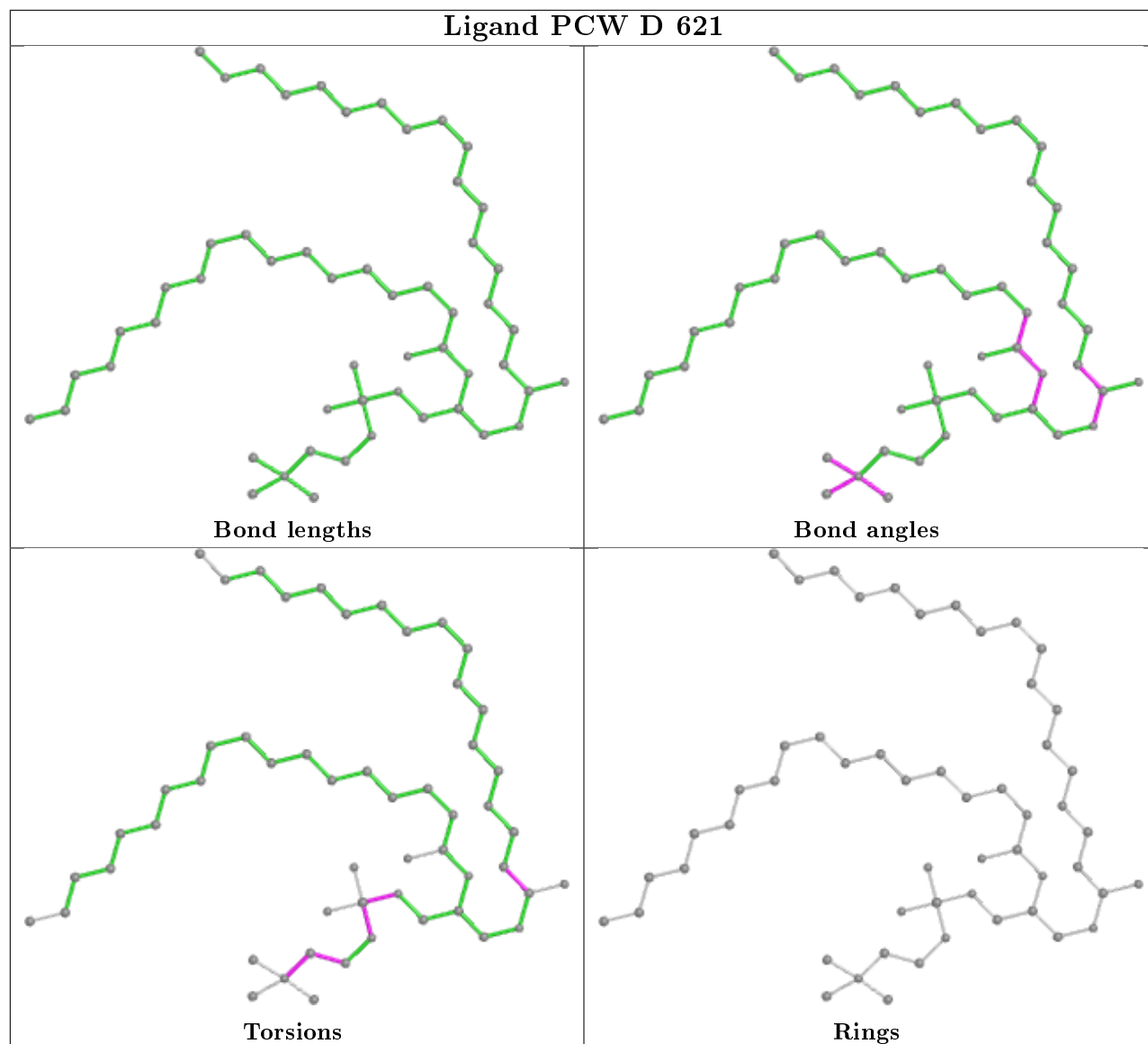


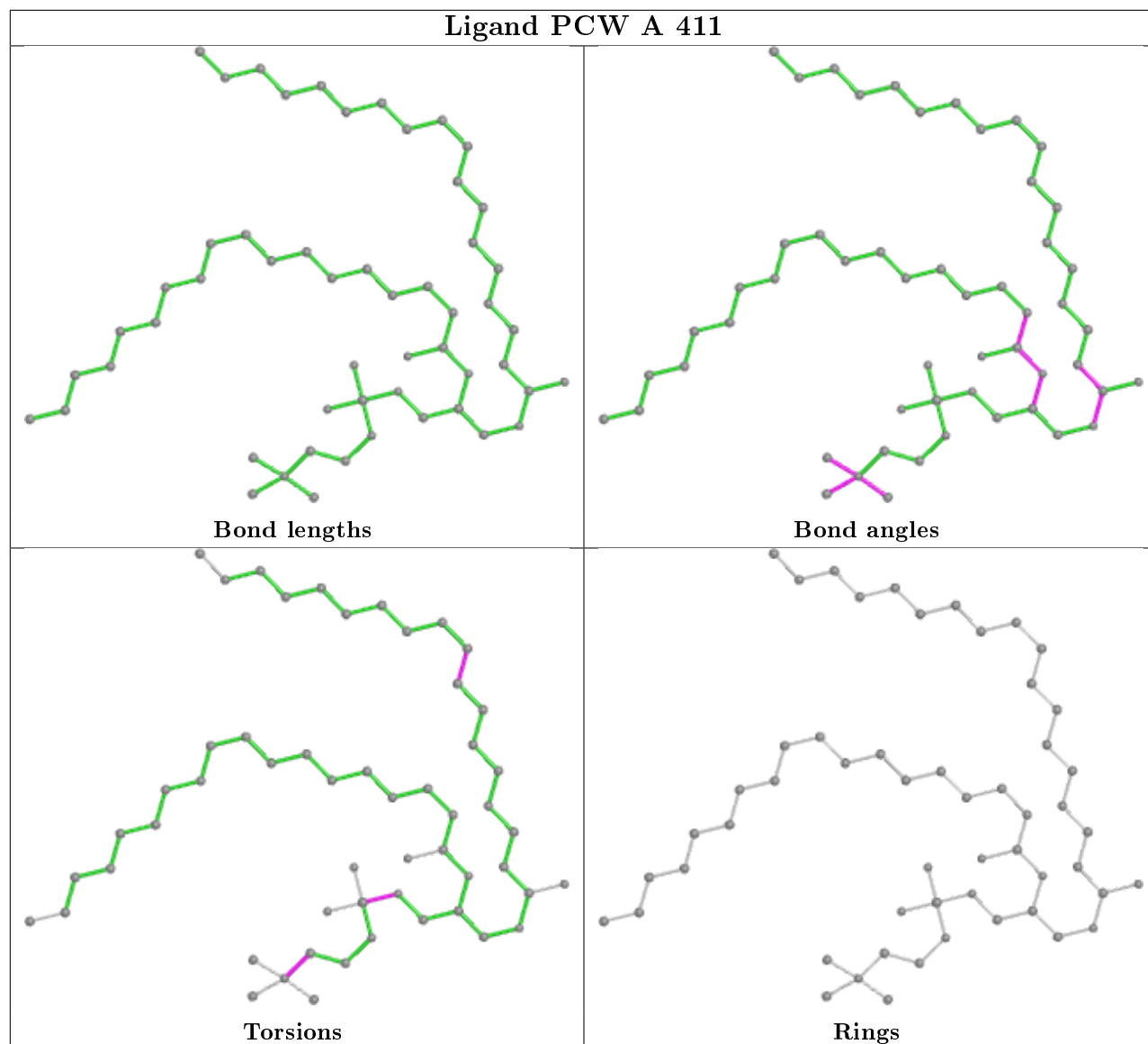


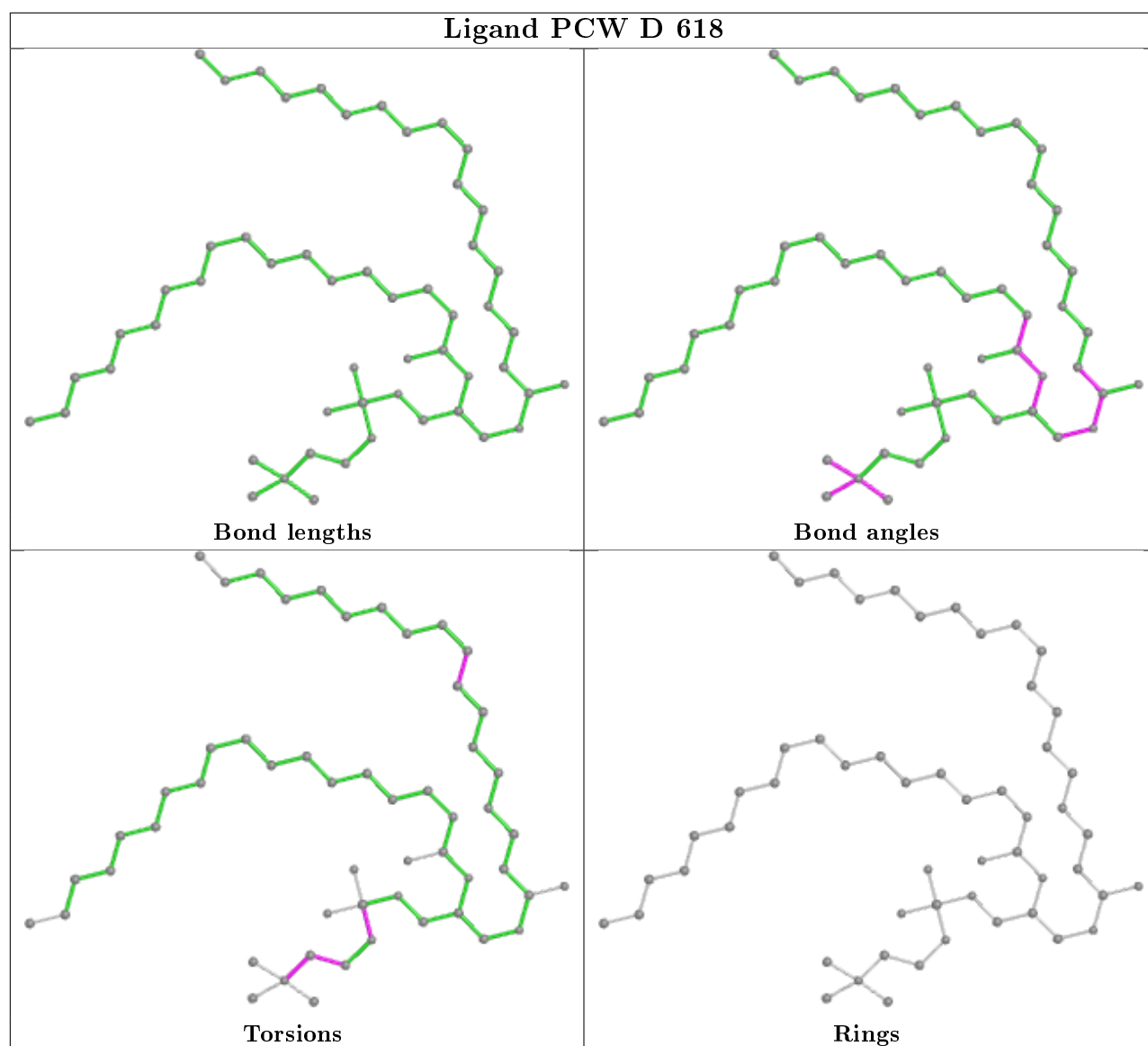




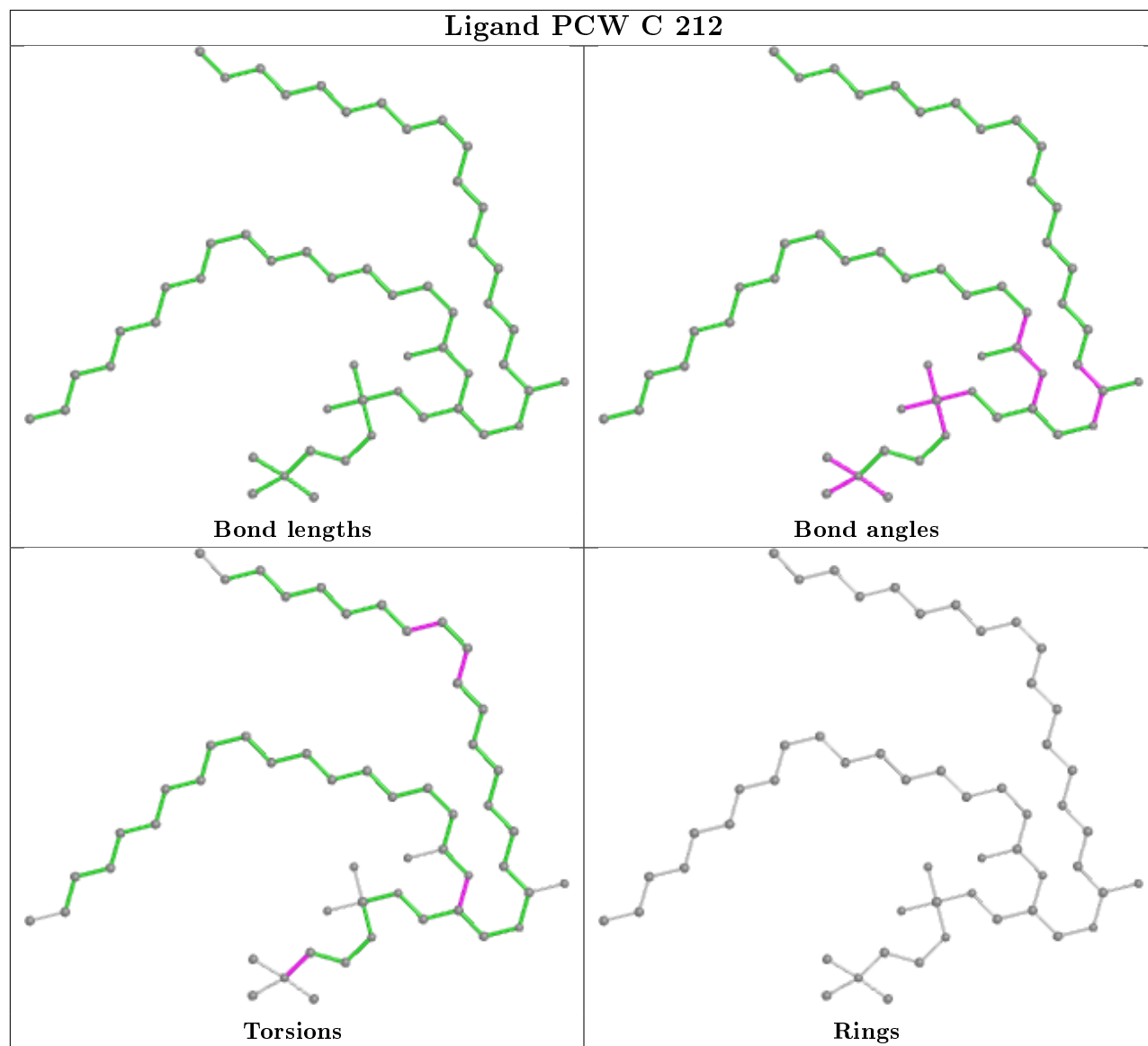


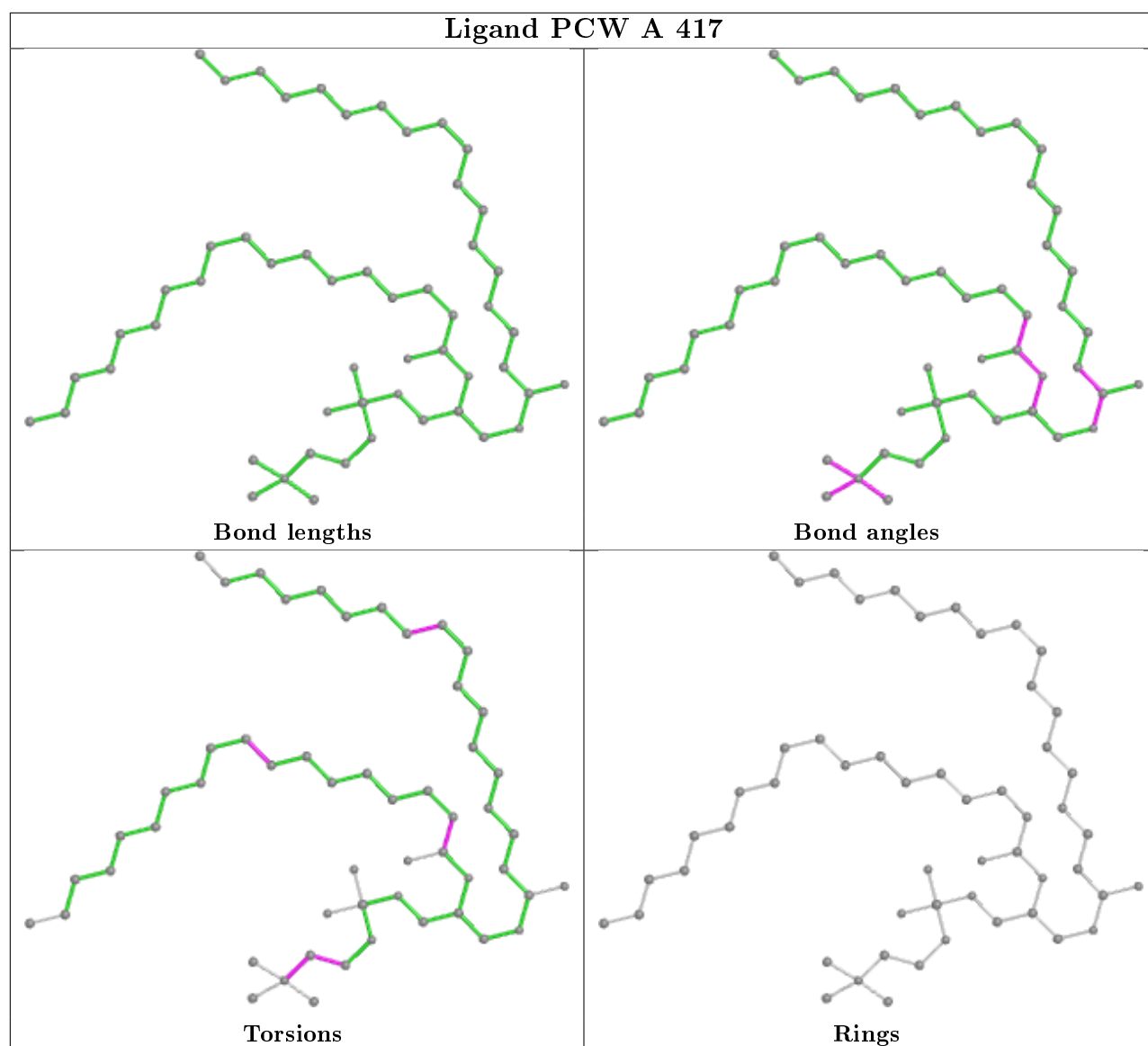


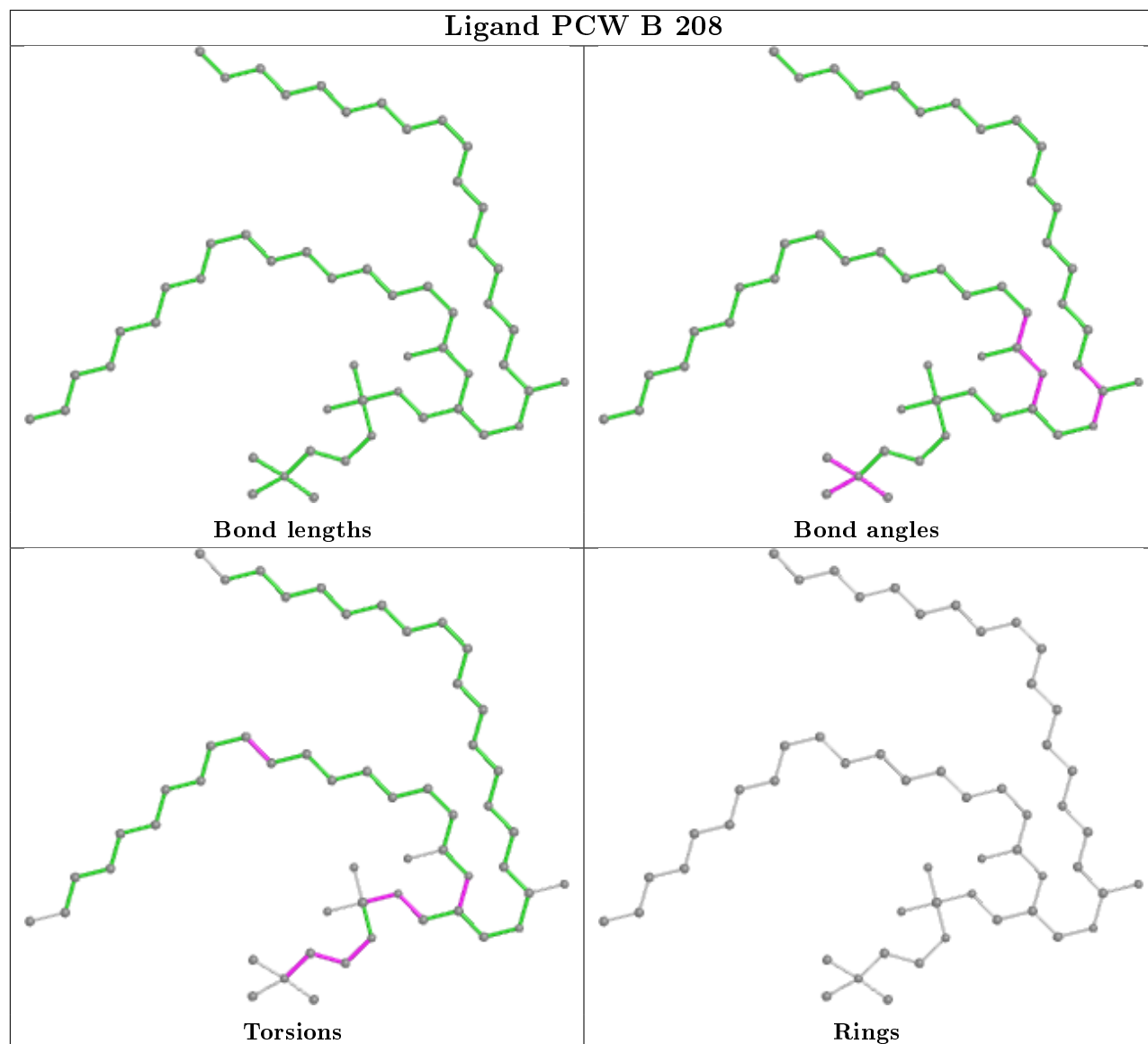


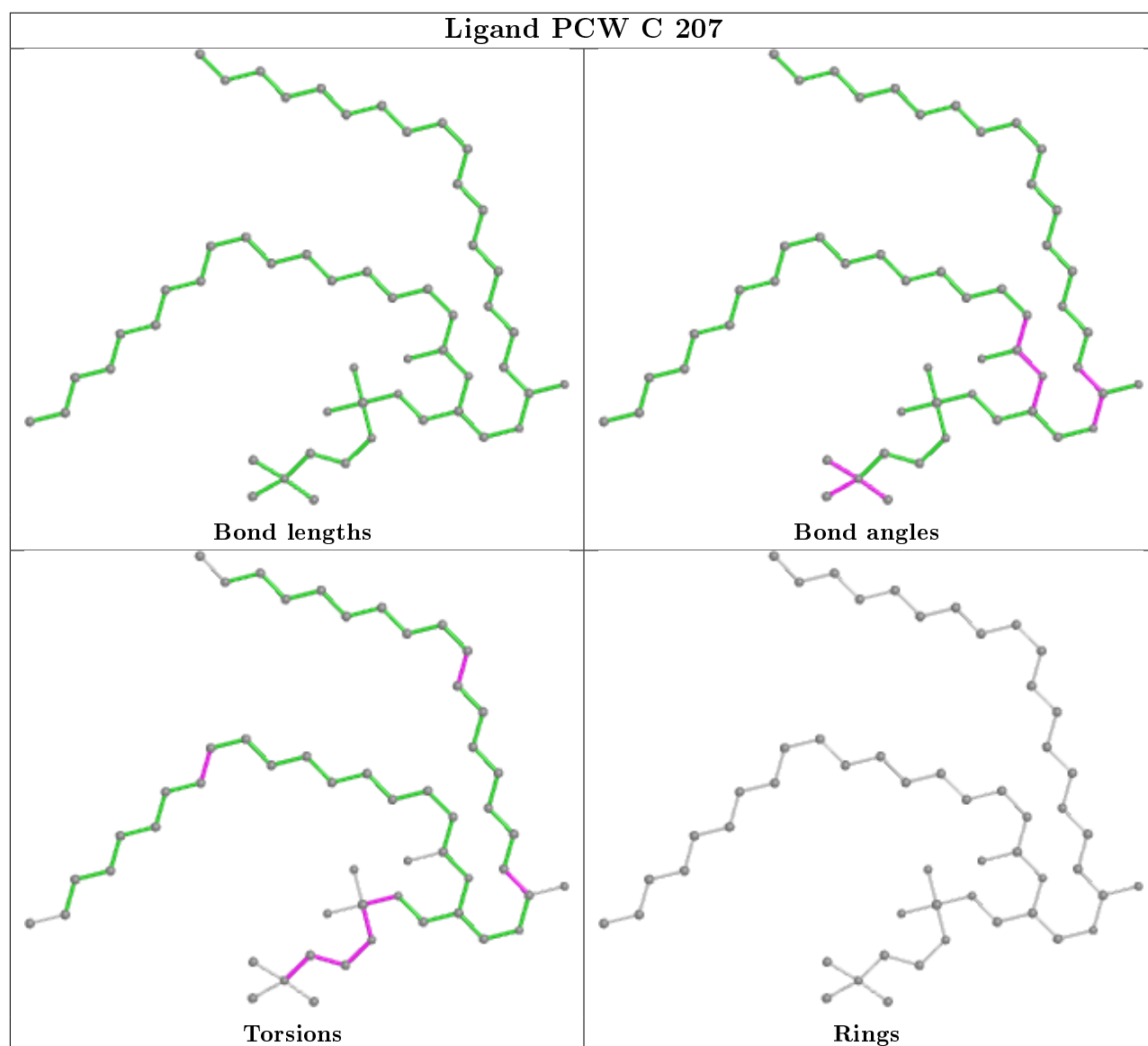


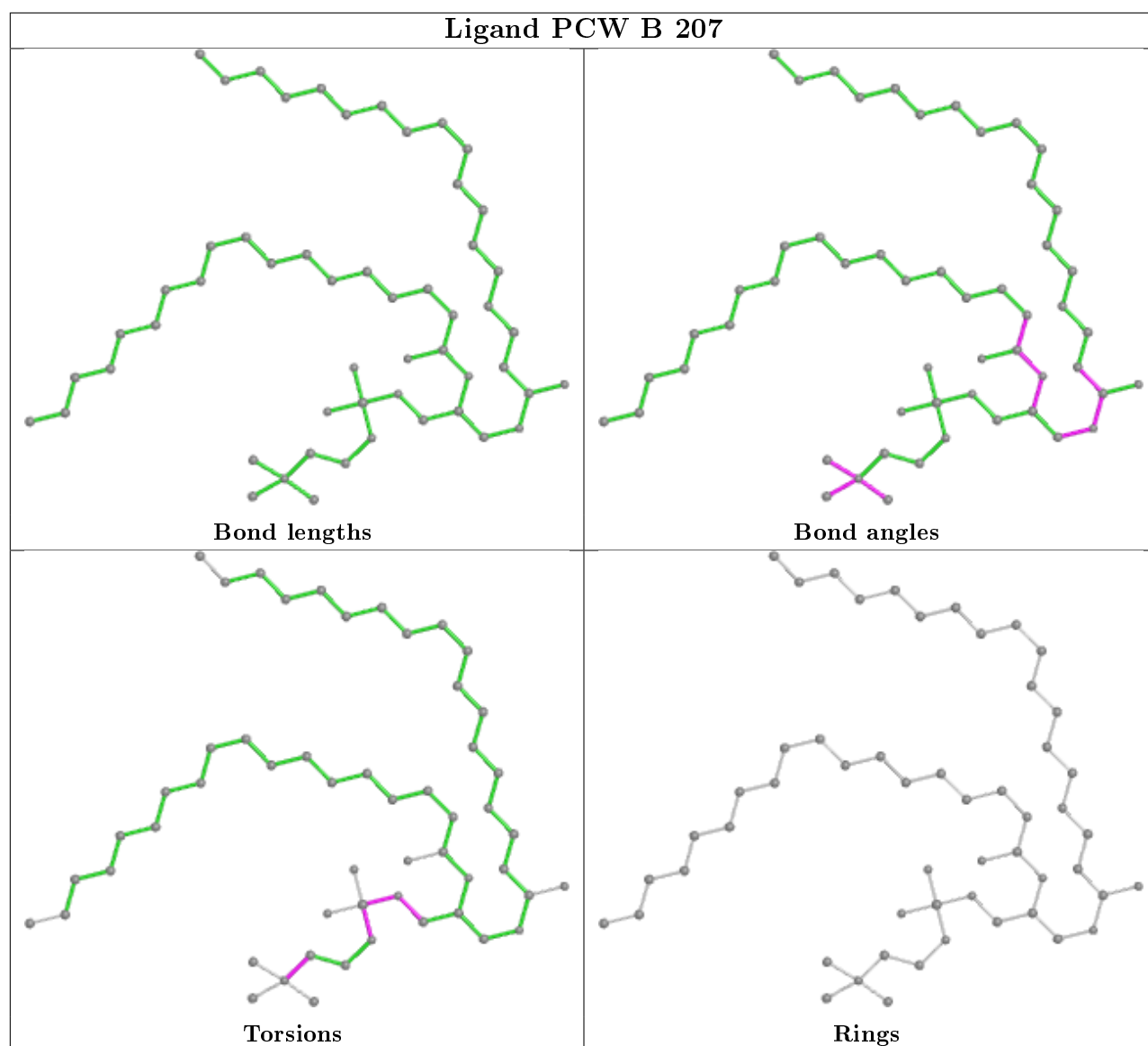


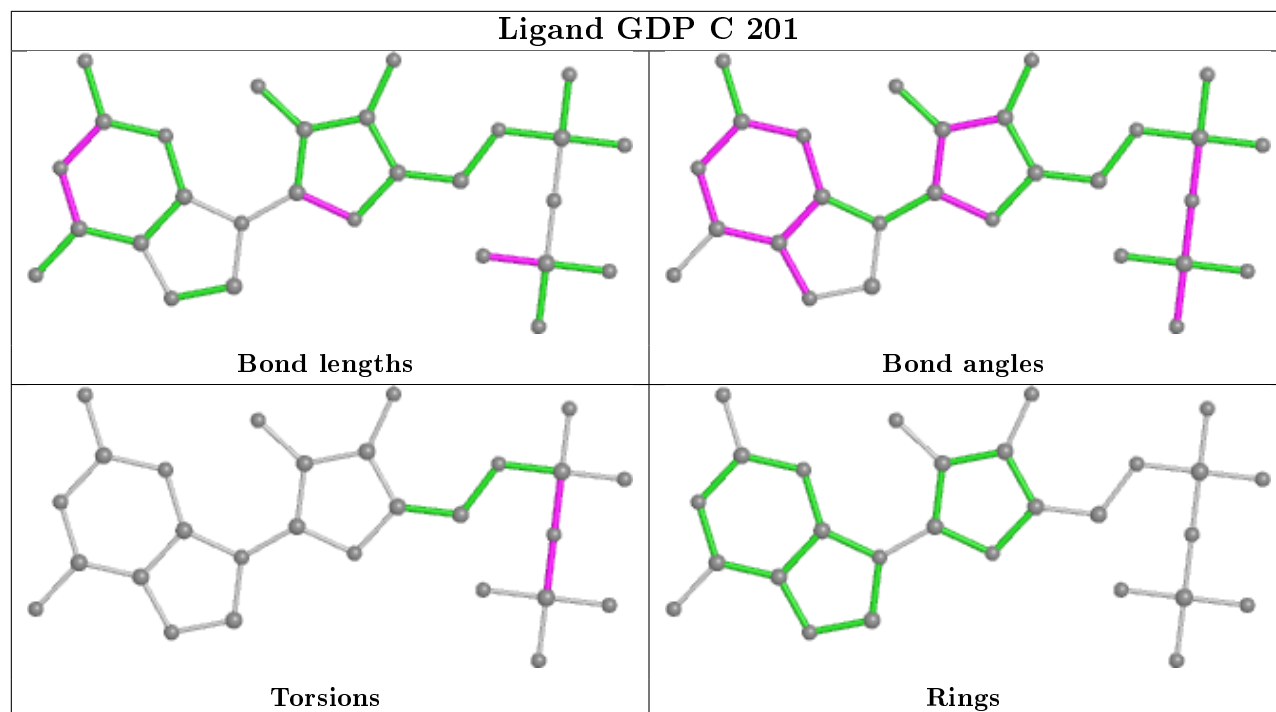


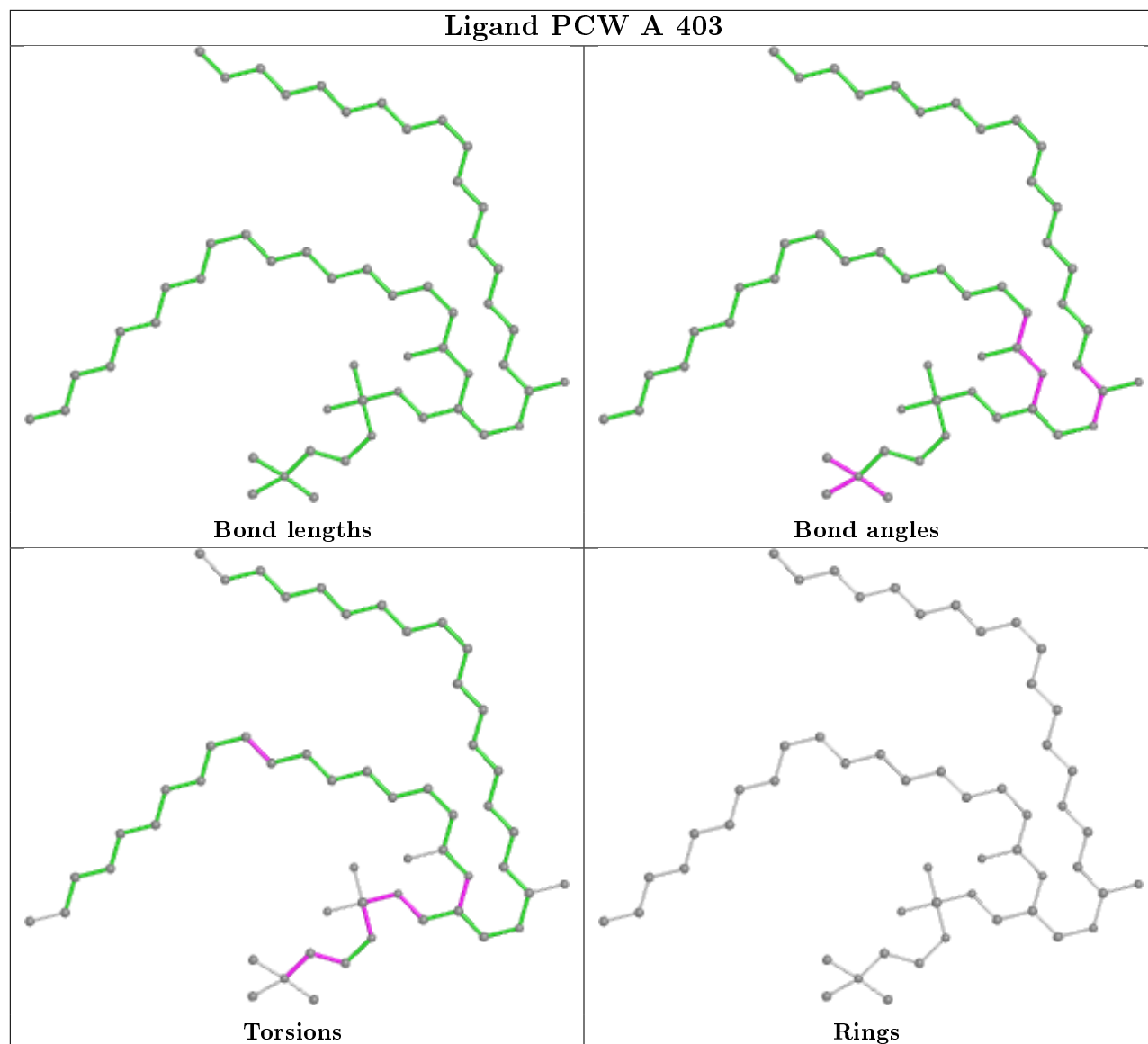


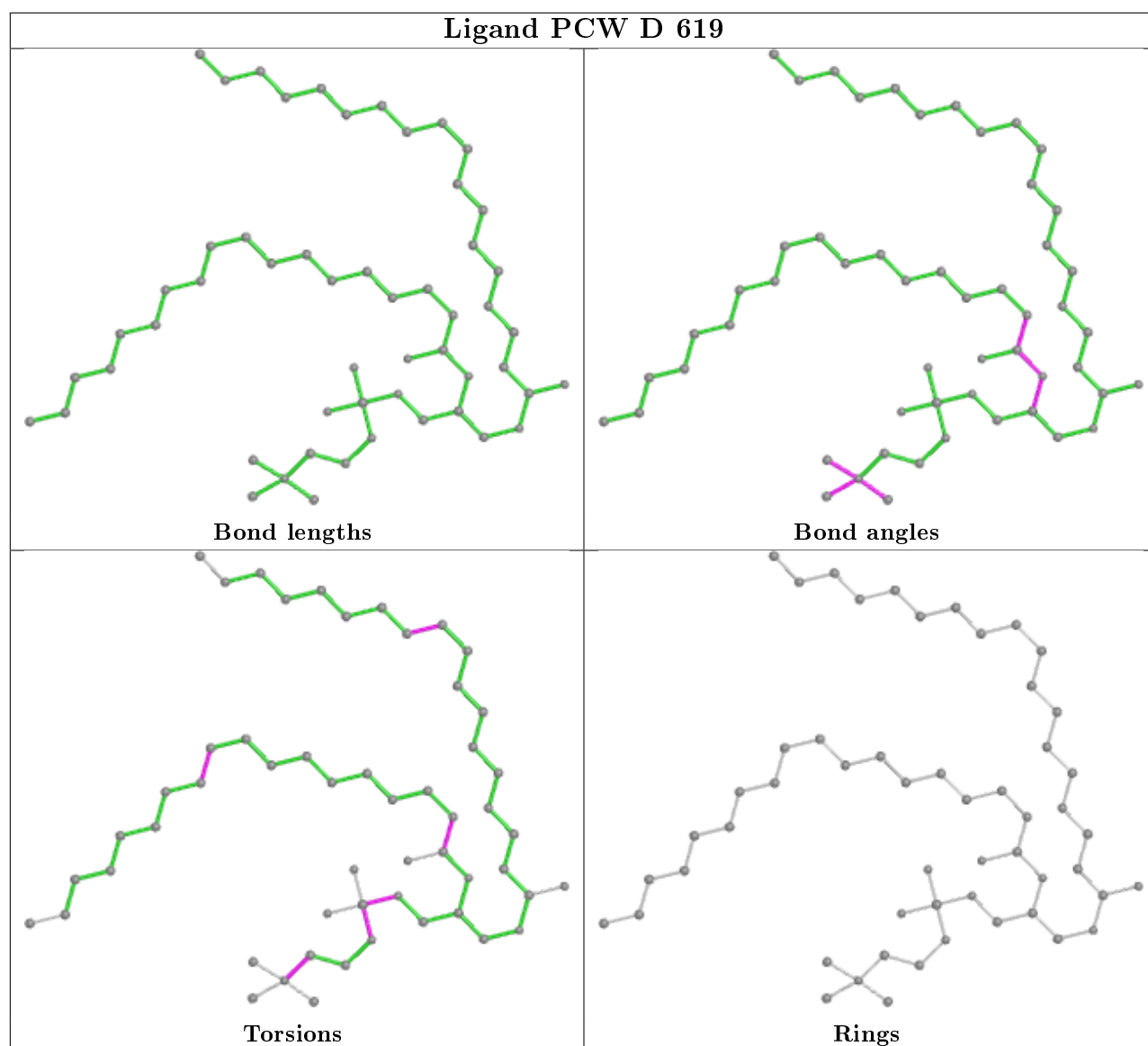




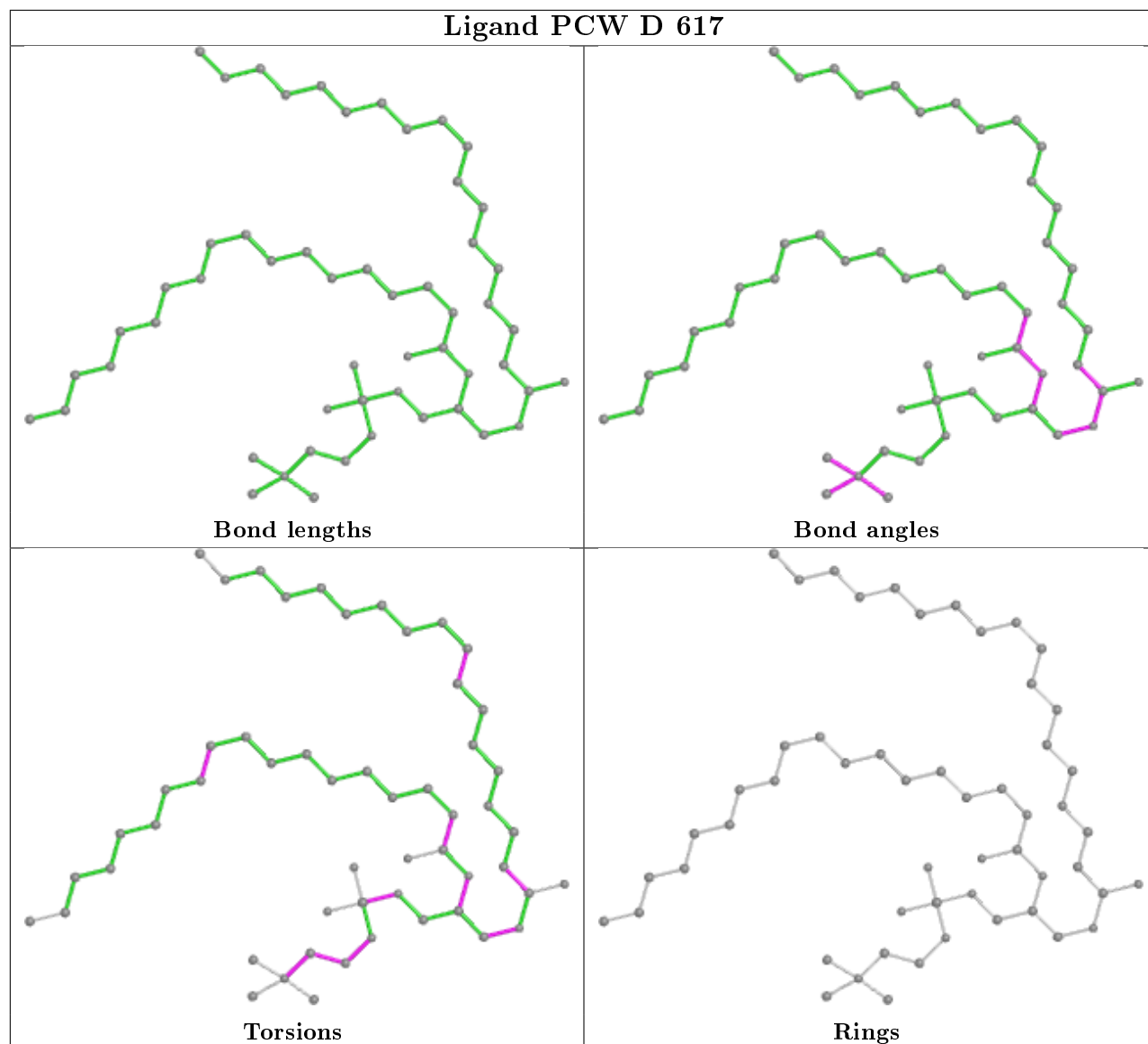


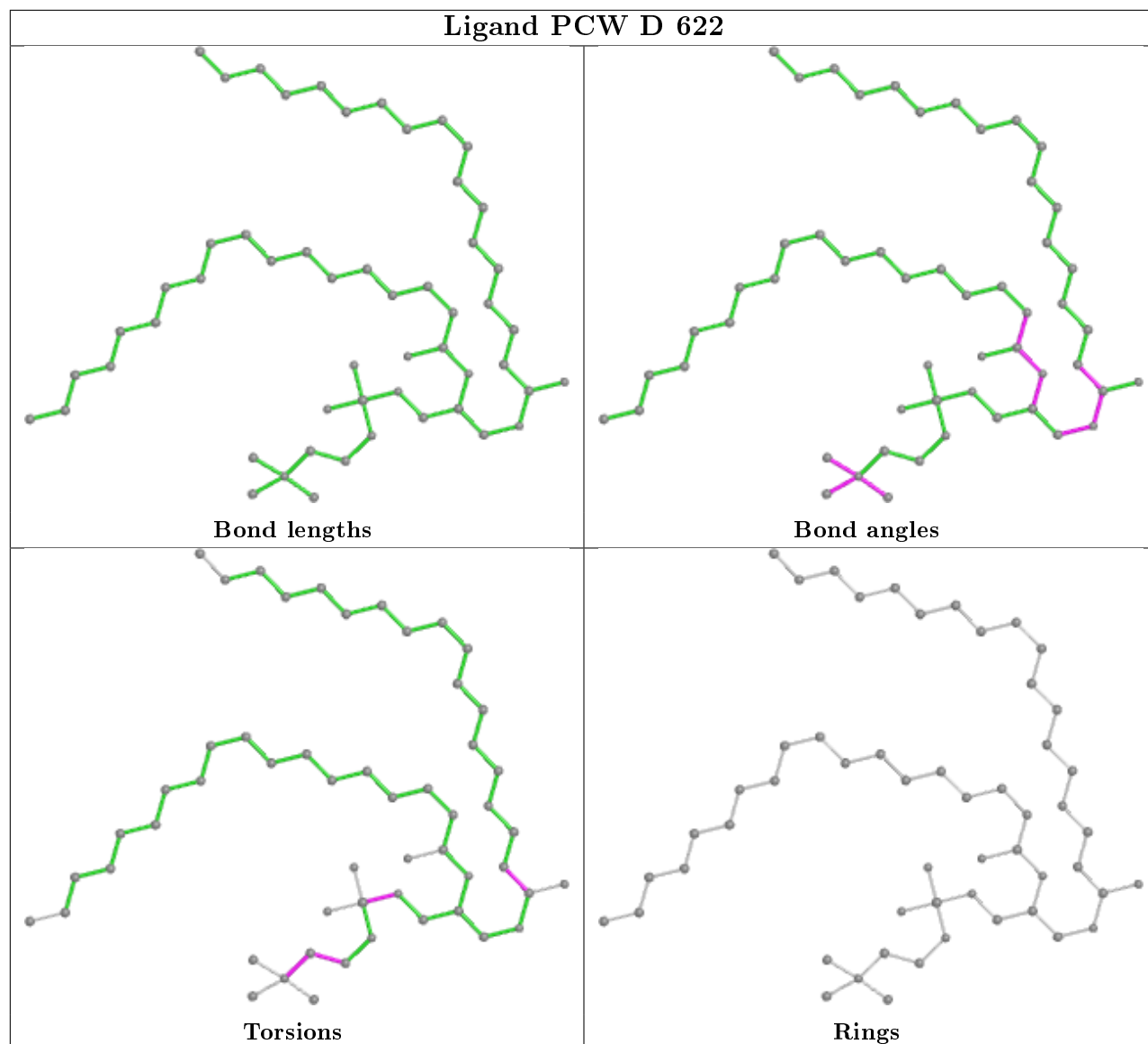


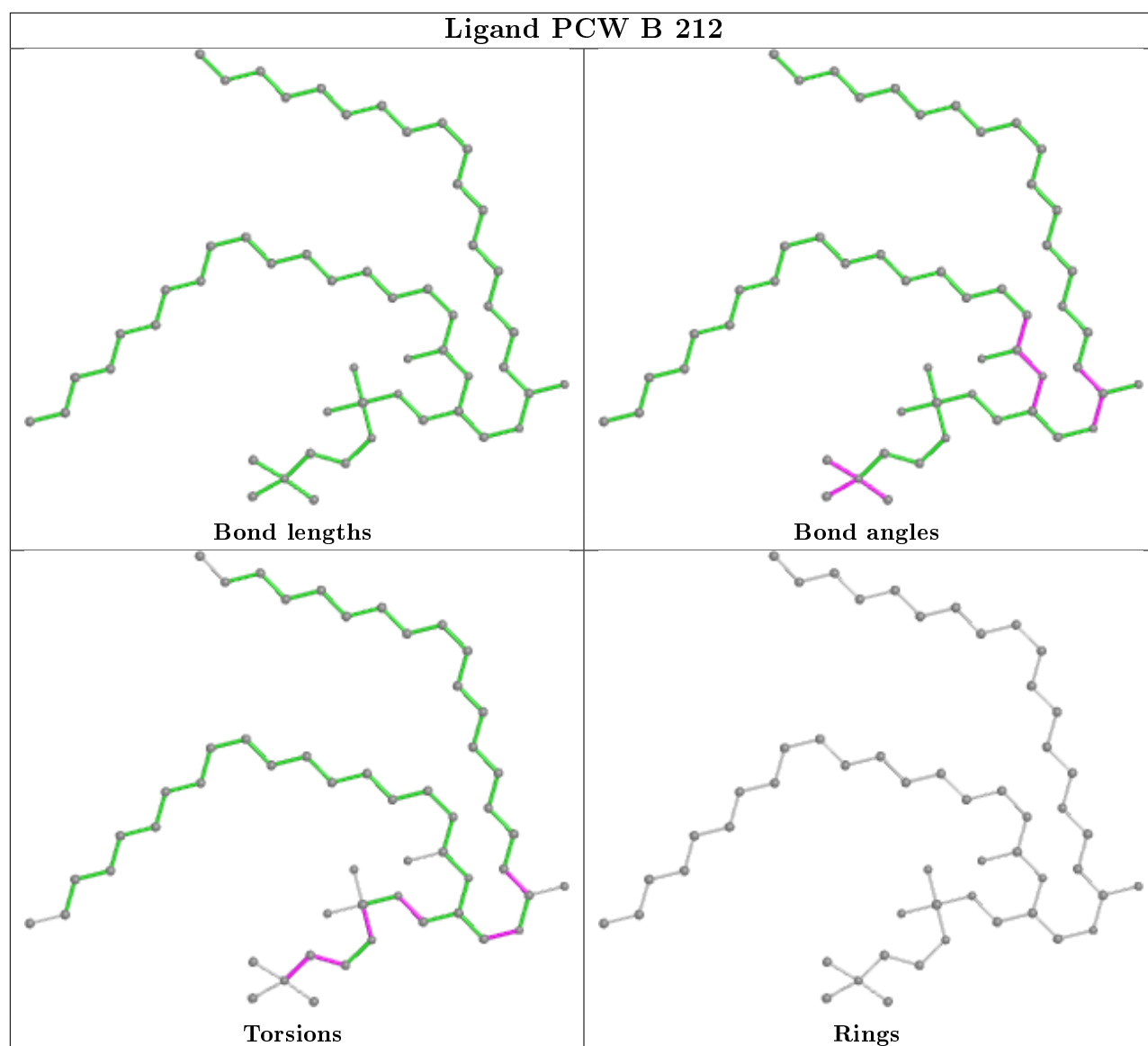


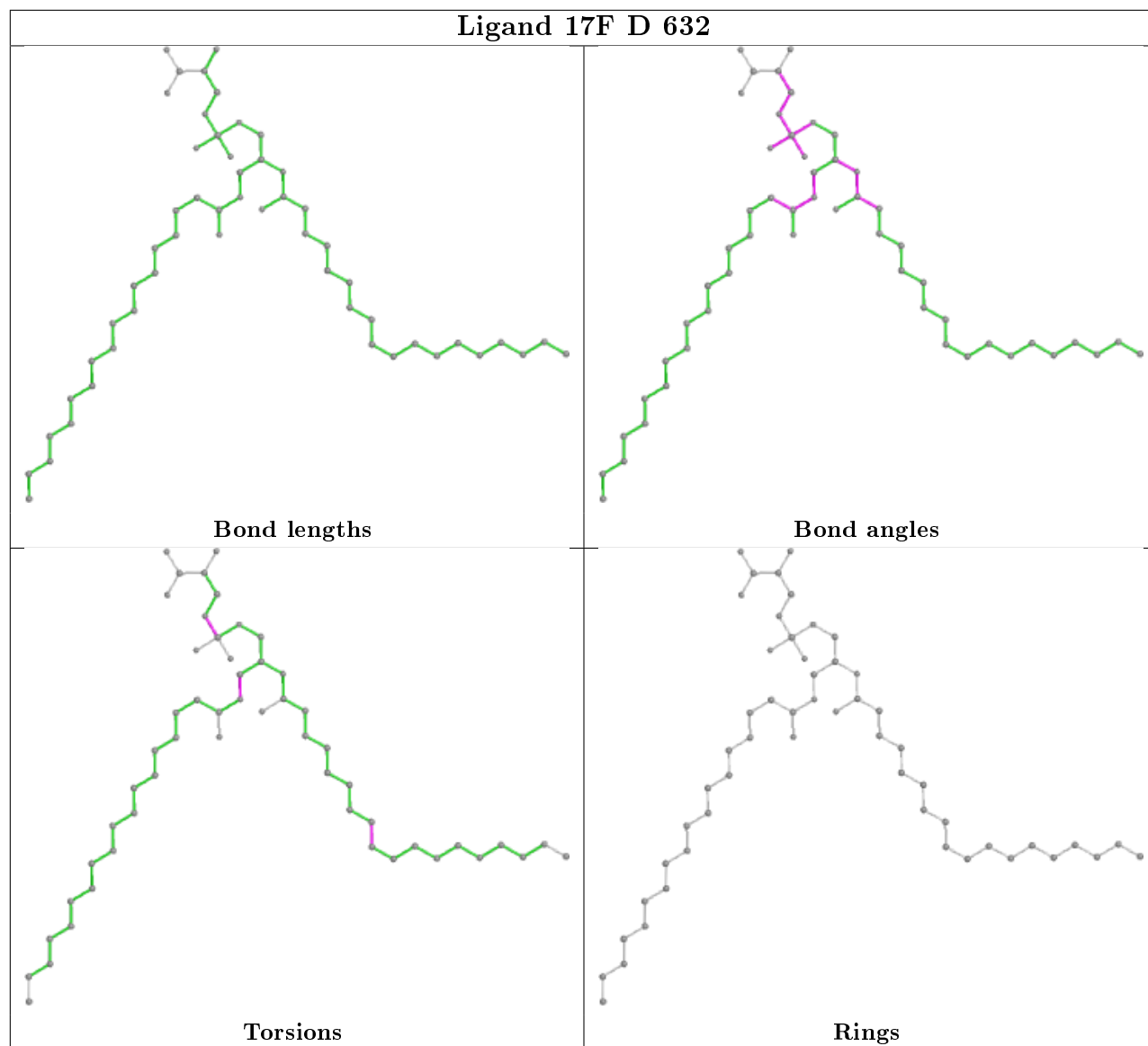


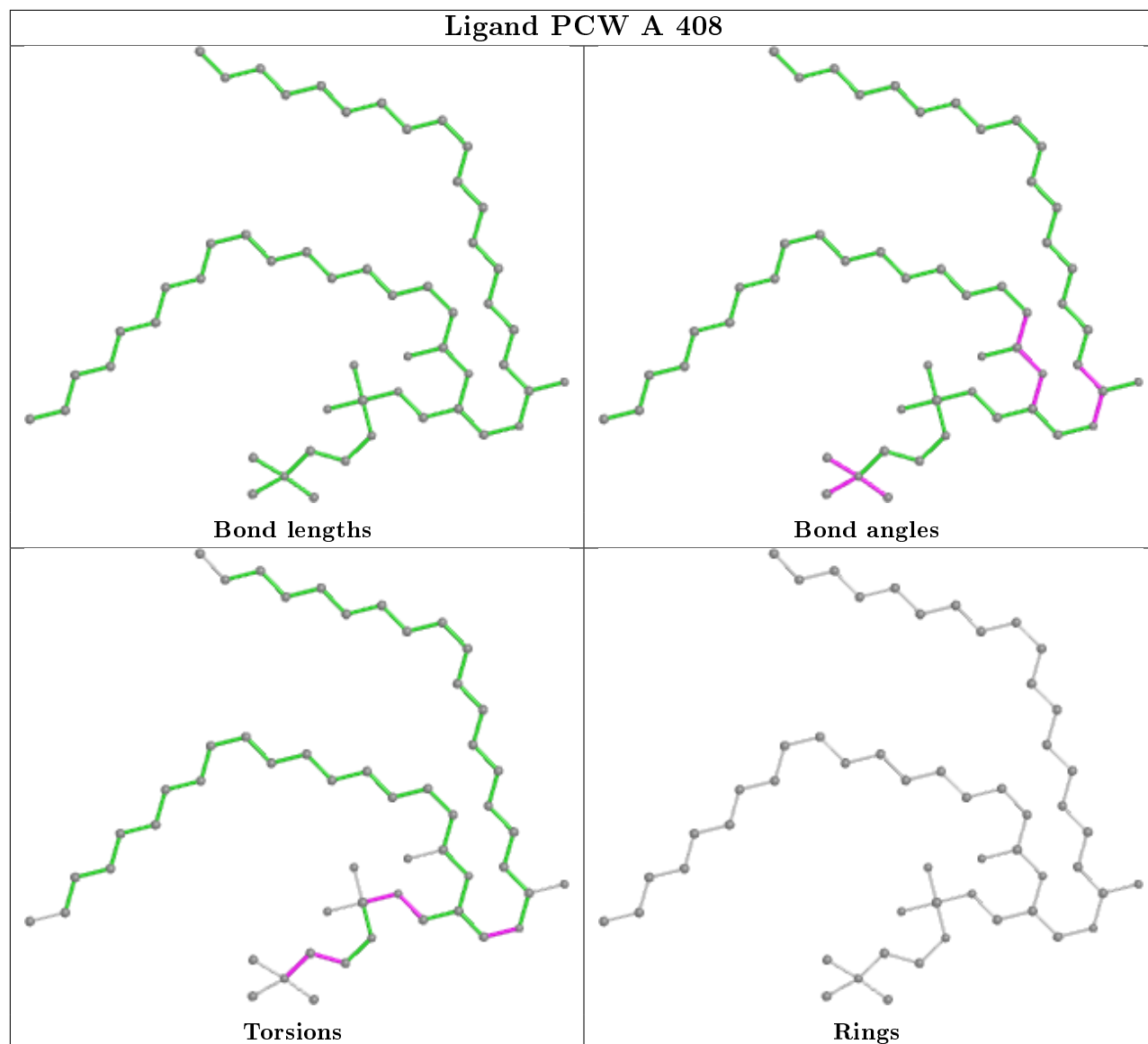


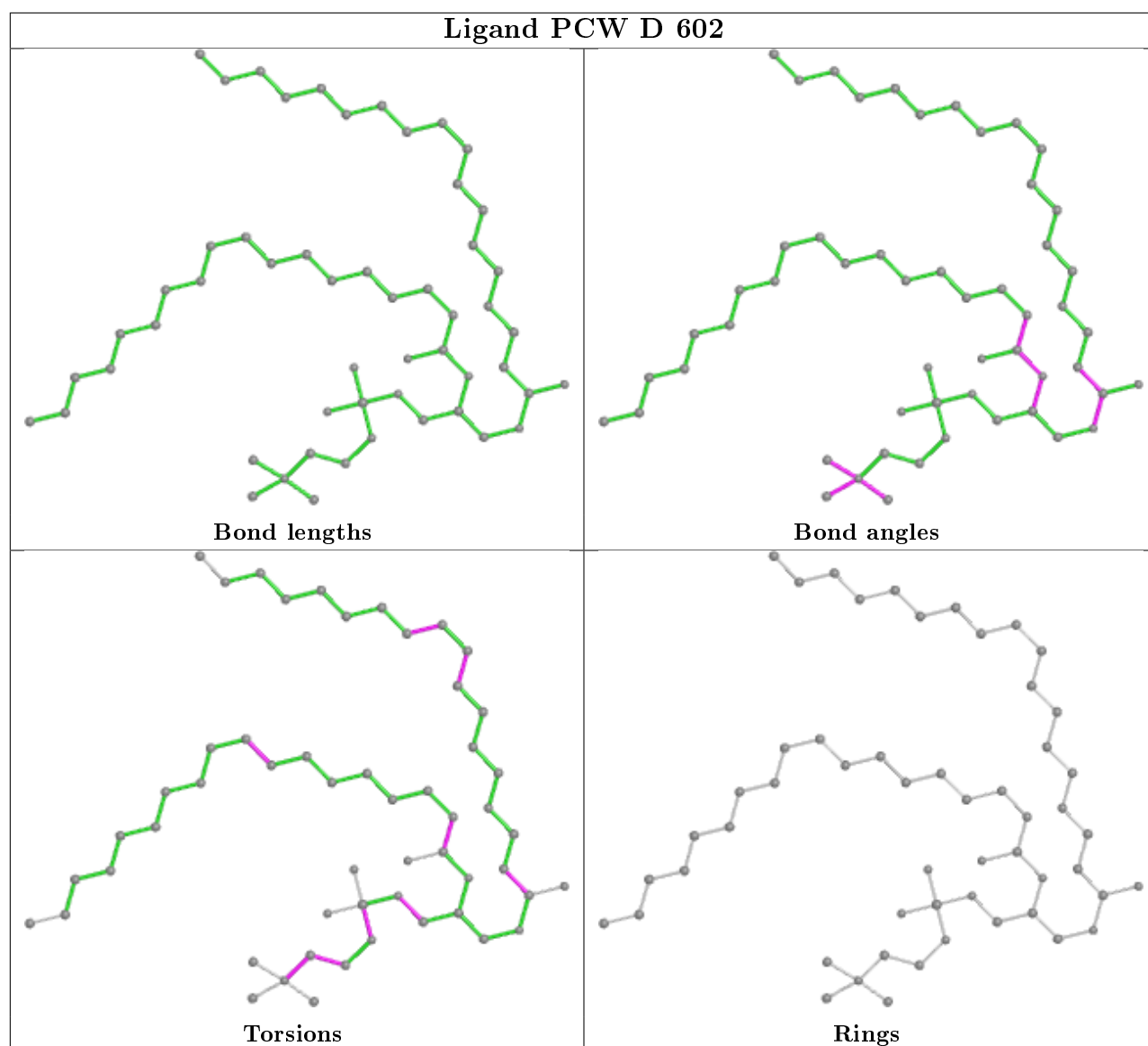


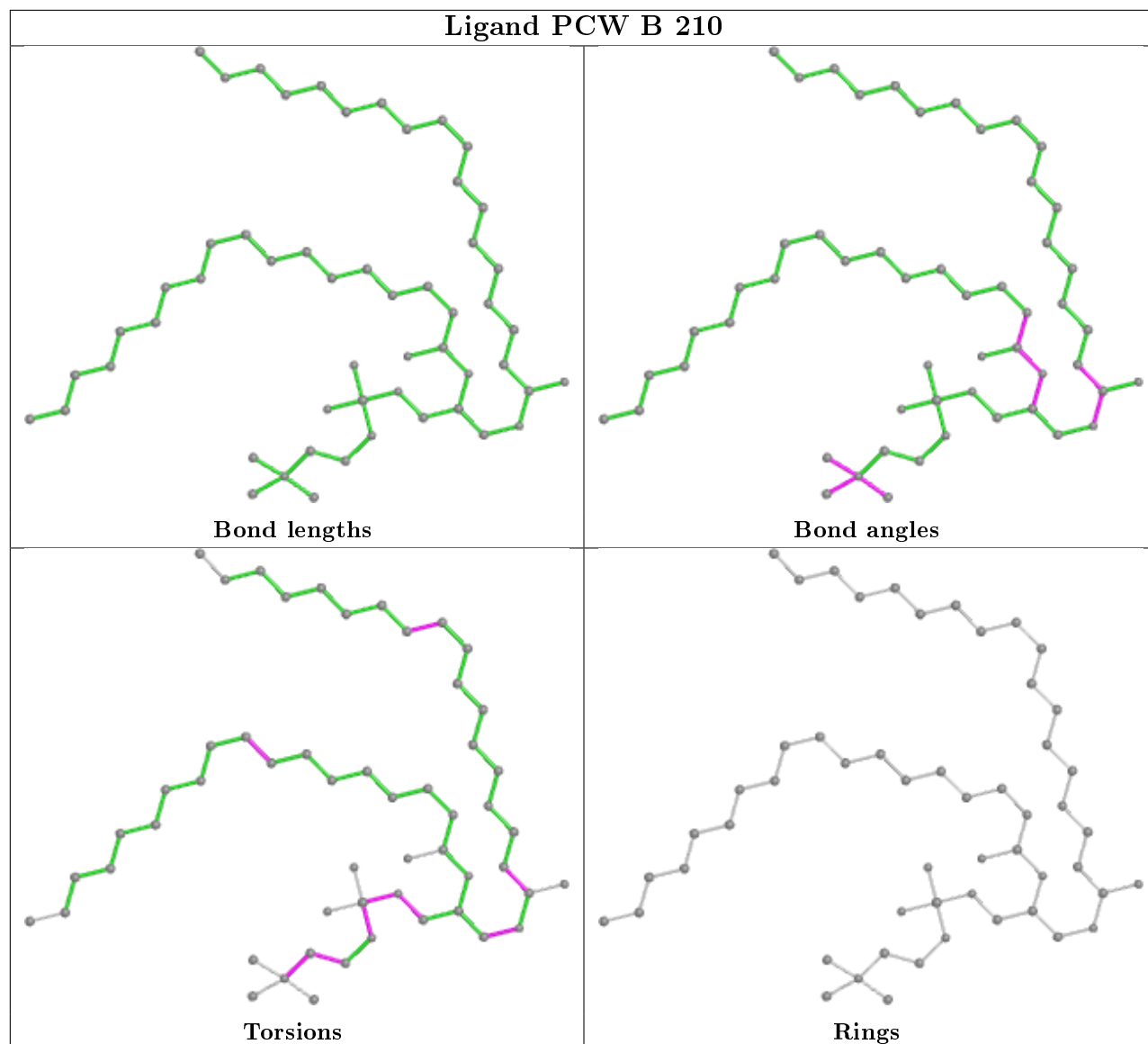


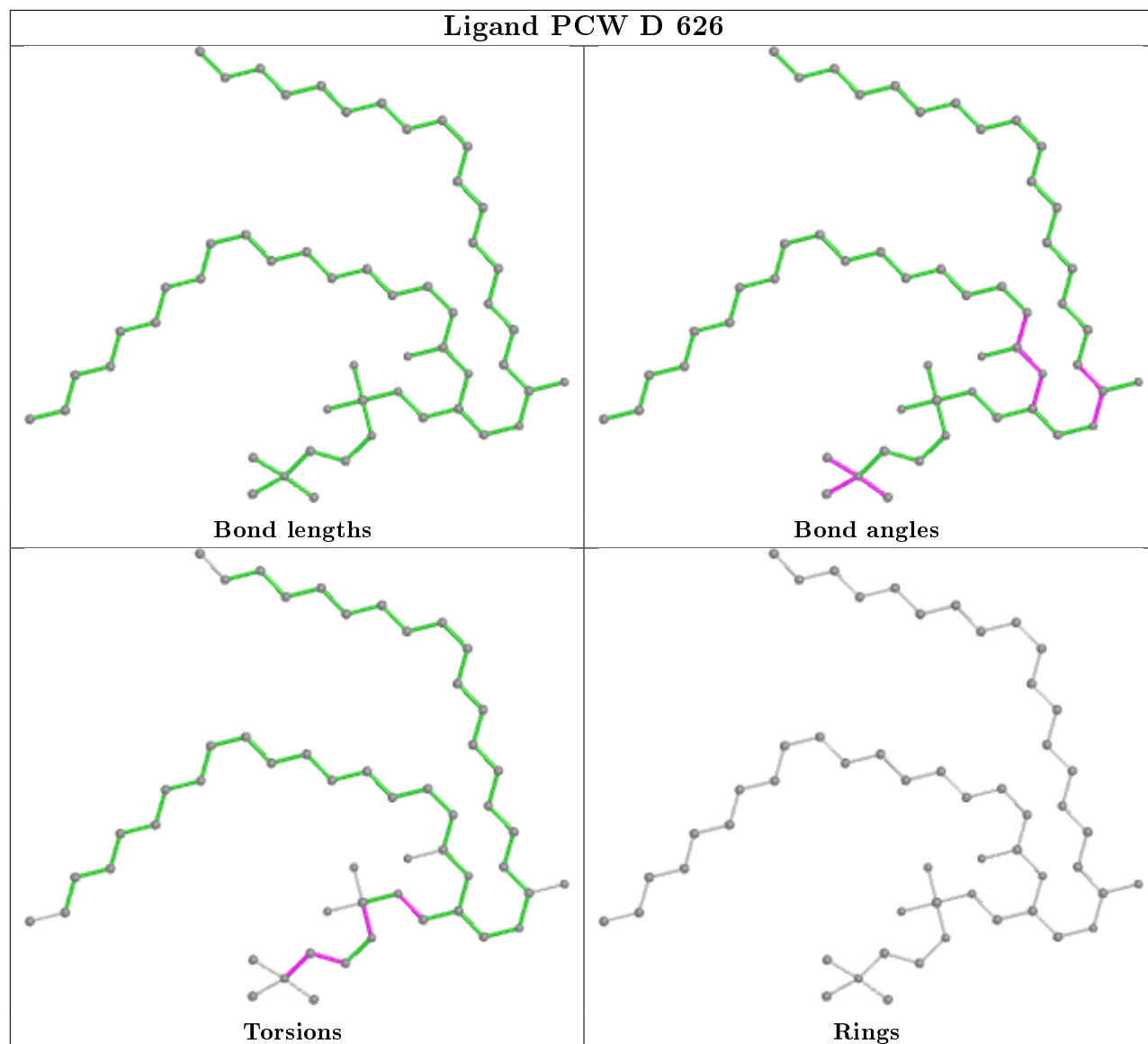




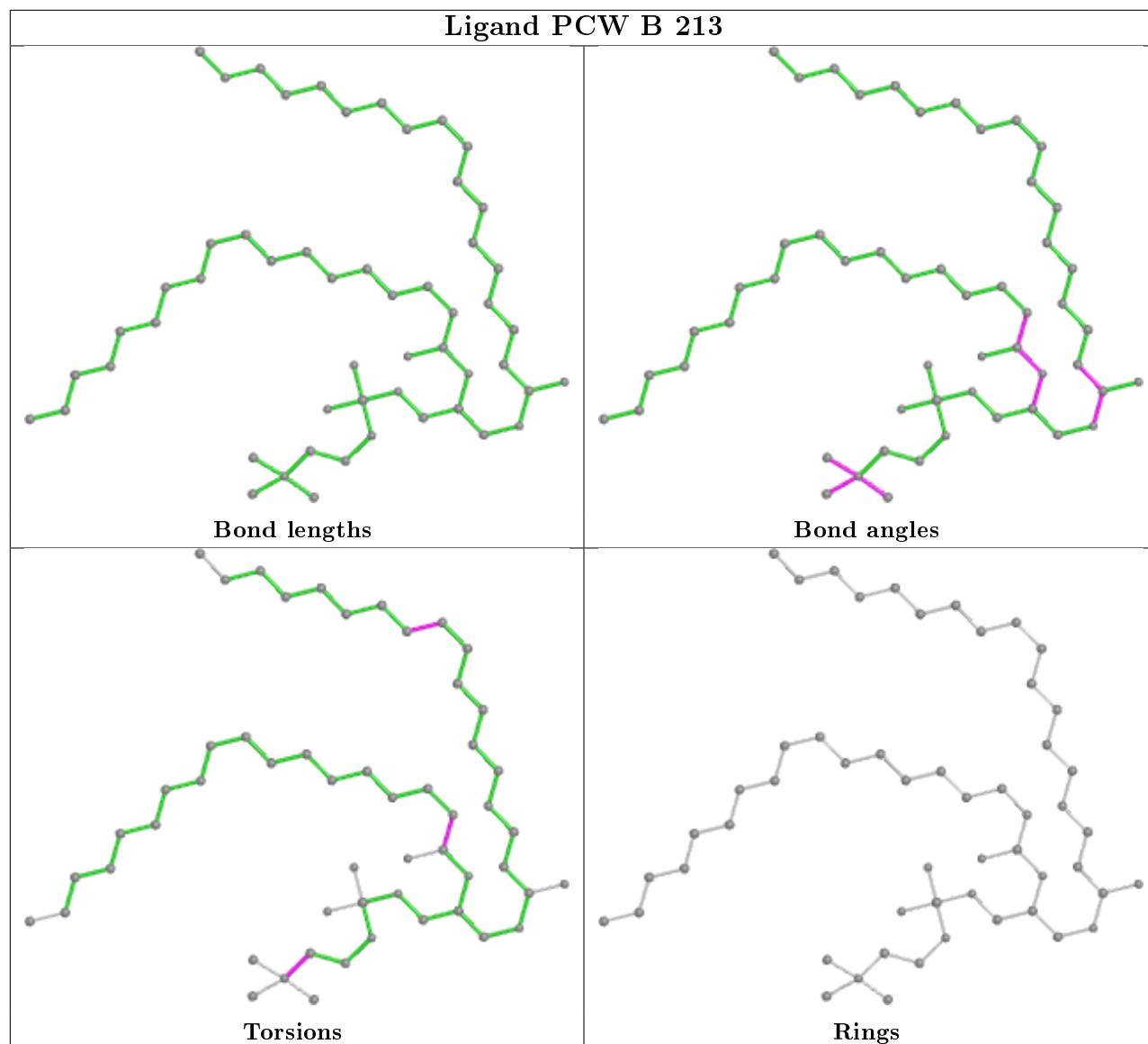


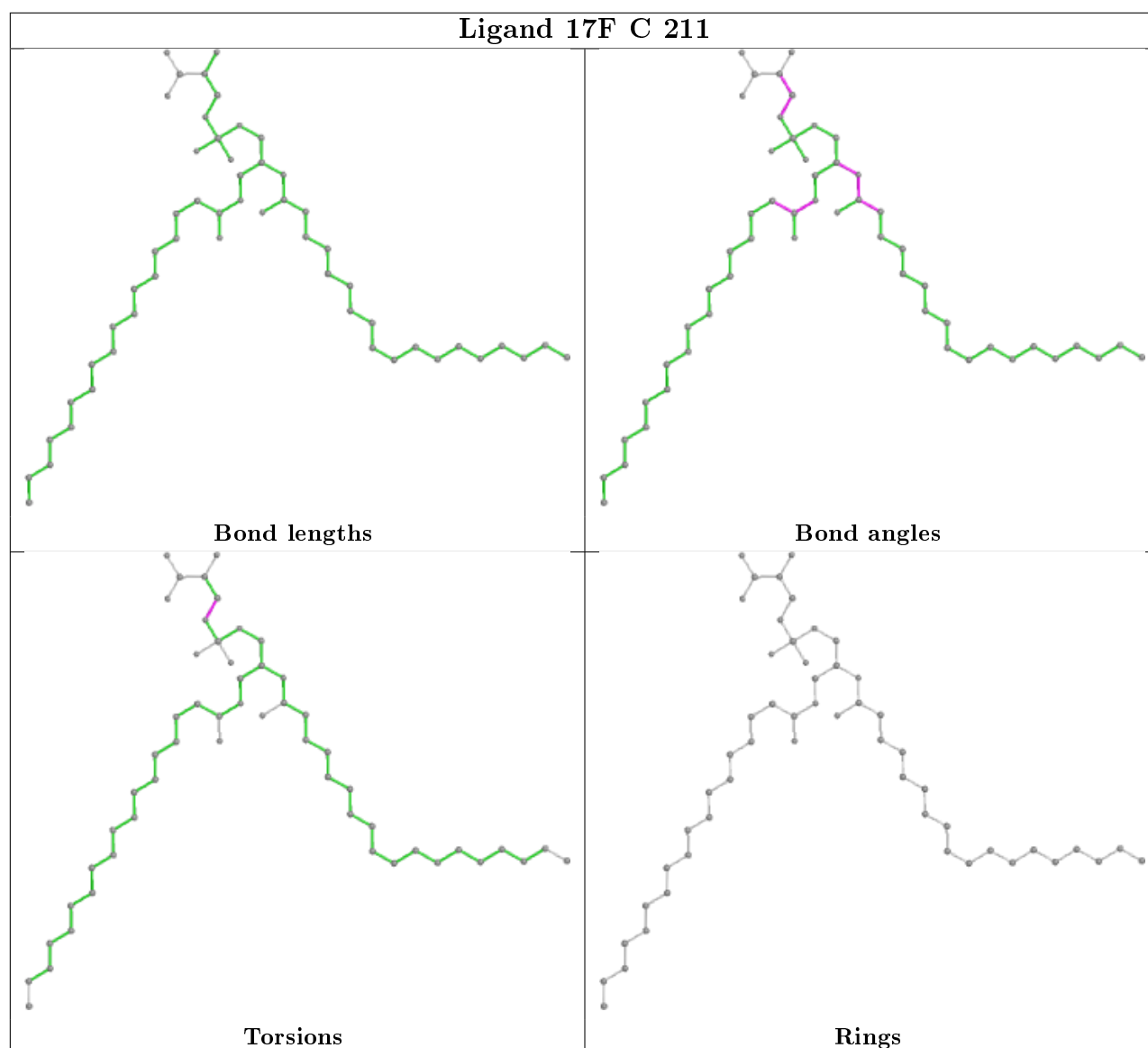












## 6.7 Other polymers [i](#)

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 1% for the well-defined parts and 1% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_0*

#### 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	190
Number of shifts mapped to atoms	190
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

#### 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 1%, i.e. 107 atoms were assigned a chemical shift out of a possible 9070. 0 out of 130 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	14/3506 (0%)	7/1398 (1%)	0/1420 (0%)	7/688 (1%)
Sidechain	93/4986 (2%)	40/2917 (1%)	53/1812 (3%)	0/257 (0%)
Aromatic	0/578 (0%)	0/308 (0%)	0/245 (0%)	0/25 (0%)
Overall	107/9070 (1%)	47/4623 (1%)	53/3477 (2%)	7/970 (1%)

#### 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.

Random coil index (RCI) for chain B:

