



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 27, 2026 – 08:26 AM UTC

PDB ID : 6PTW / pdb_00006ptw
BMRB ID : 30640
Title : NMR data-driven model of KRas-GMPPNP:RBD-CRD complex tethered to a nanodisc (state B)
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

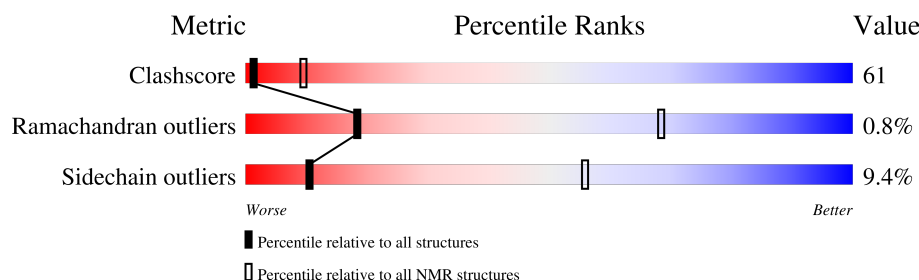
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 6%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	198	80% 12% 8%
1	C	198	83% 16% .
2	B	185	78% 16% 5%
3	D	132	79% 18% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 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:205-A:387, C:400-C:596 (380)	0.35	2
2	B:1-B:175, D:356-D:487 (307)	1.90	8

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

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	

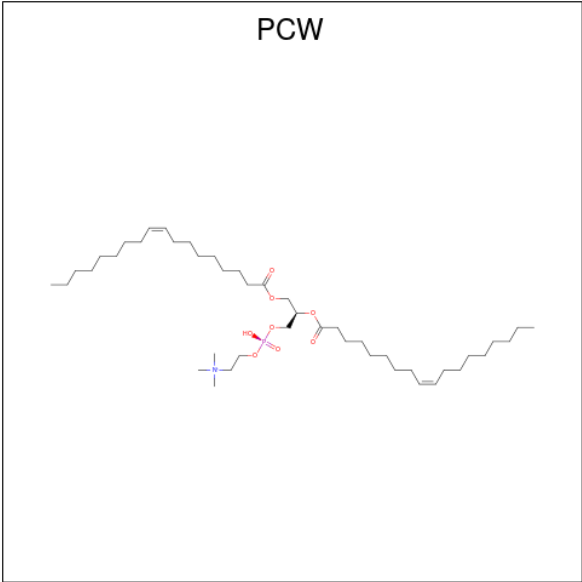
- Molecule 3 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

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 (CCD ID: 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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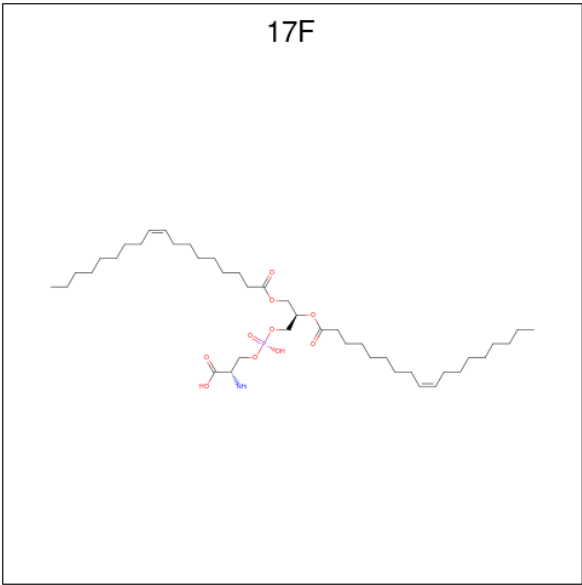
Mol	Chain	Residues	Atoms				
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	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
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

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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
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 (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P).



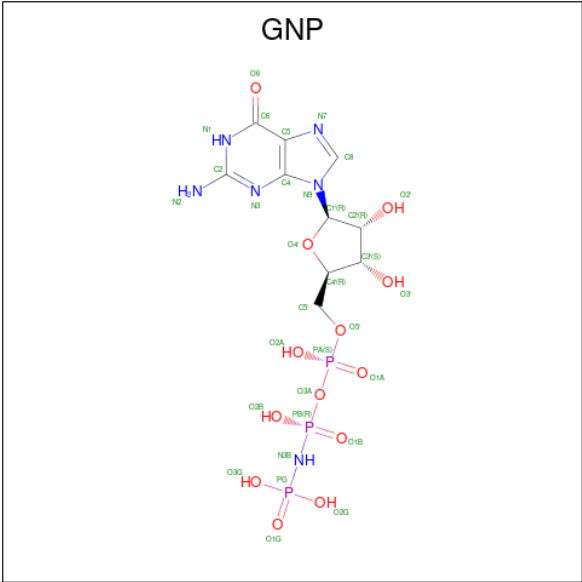
Mol	Chain	Residues	Atoms					
5	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1

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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	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
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 (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
7	B	1	1	1

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

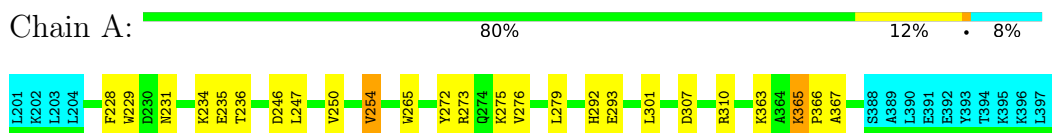
Mol	Chain	Residues	Atoms	
			Total	Zn
8	D	2	2	2

4 Residue-property plots

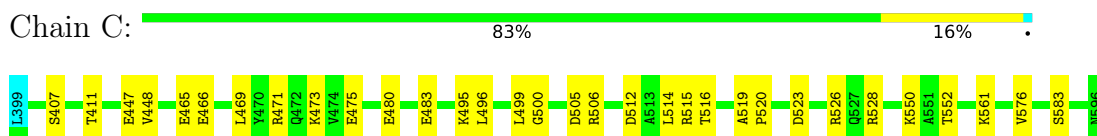
4.1 Average score per residue in the NMR ensemble

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.

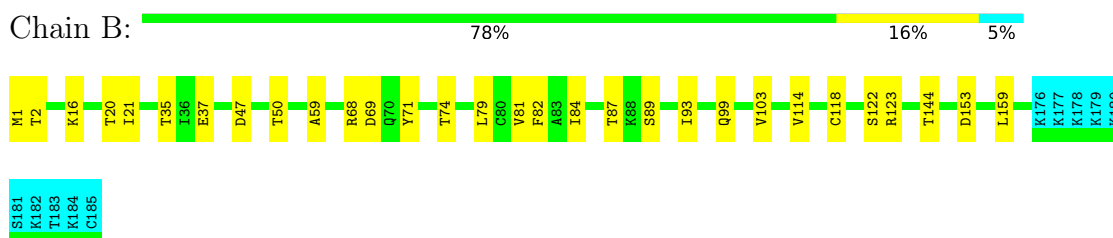
- Molecule 1: Apolipoprotein A-I



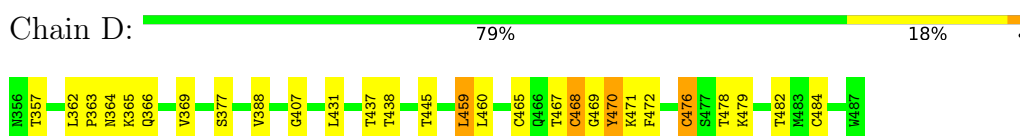
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



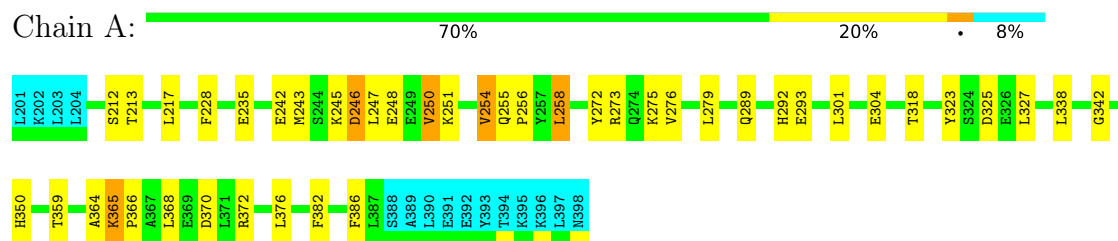
- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase



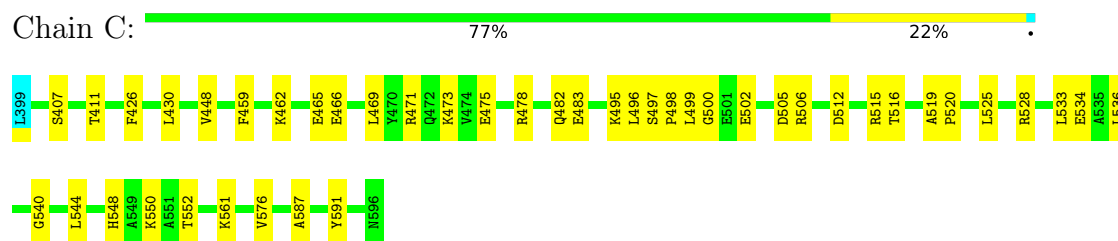
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

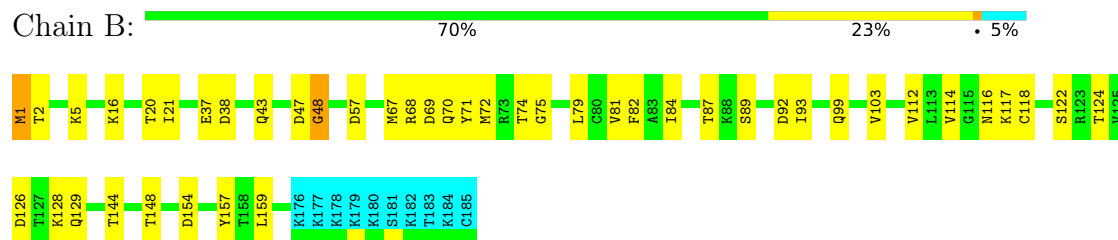
- Molecule 1: Apolipoprotein A-I



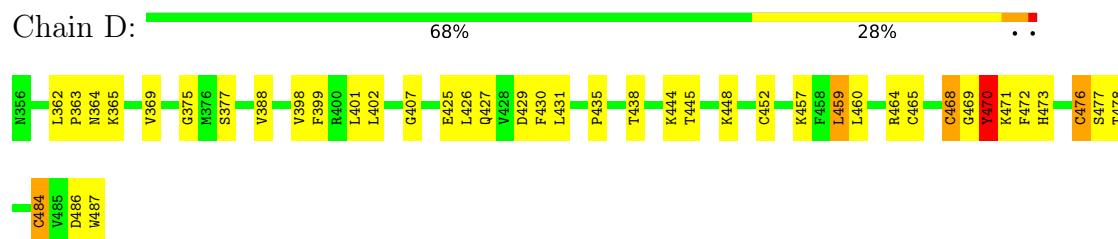
- Molecule 1: Apolipoprotein A-I



- 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	437
Number of unparsed shifts	0
Number of shifts with mapping errors	120
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	6%

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: MG, GNP, ZN, 17F, 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	0.39±0.01	0±0/1527 (0.0± 0.0%)	0.78±0.01	0±0/2055 (0.0± 0.0%)
1	C	0.39±0.00	0±0/1642 (0.0± 0.0%)	0.82±0.00	0±0/2207 (0.0± 0.0%)
2	B	0.35±0.01	0±0/1416 (0.0± 0.0%)	0.70±0.01	0±0/1907 (0.0± 0.0%)
3	D	0.46±0.01	2±0/1088 (0.2± 0.0%)	2.30±0.01	7±0/1466 (0.5± 0.0%)
All	All	0.39	20/56730 (0.0%)	1.22	70/76350 (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	6.78	1.66	1.51	7	10
3	D	470	TYR	CZ-OH	5.85	1.50	1.38	8	10

5 of 7 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	CD1-CG-CD2	-41.83	55.36	118.10	8	10
3	D	470	TYR	CG-CD1-CE1	-36.94	65.79	121.20	4	10
3	D	470	TYR	CG-CD2-CE2	-32.67	72.19	121.20	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	470	TYR	CE1-CZ-CE2	-31.53	57.24	120.30	10	10
3	D	470	TYR	CZ-CE2-CD2	-30.80	64.17	119.60	2	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	1500	352	1489	22±6
1	C	1615	378	1616	20±5
2	B	1394	325	1379	24±2
3	D	1065	251	1070	21±5
4	A	756	0	1120	267±30
4	B	216	0	320	103±9
4	C	1350	0	2000	520±18
4	D	1134	0	1680	494±41
5	A	54	3	76	11±3
5	C	324	18	456	132±12
5	D	486	27	684	202±17
6	B	32	6	13	5±2
7	B	1	0	0	1±0
All	All	99290	13600	119030	13215

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 61.

5 of 6611 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:511:PCW:H222	4:D:511:PCW:C27	1.20	1.65	2	5
4:D:509:PCW:H231	4:D:509:PCW:C28	1.17	1.69	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:H283	4:D:509:PCW:C23	1.16	1.70	1	1
4:A:413:PCW:H11	4:C:617:PCW:H411	1.14	1.17	5	10
4:B:203:PCW:H121	4:B:203:PCW:H371	1.14	1.19	1	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	183/198 (92%)	178±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	26	74
1	C	196/198 (99%)	191±1 (97±1%)	5±1 (3±0%)	0±0 (0±0%)	49	83
2	B	174/185 (94%)	165±3 (95±1%)	9±3 (5±1%)	1±0 (0±0%)	37	78
3	D	130/132 (98%)	112±2 (86±2%)	14±2 (11±2%)	4±1 (3±1%)	6	41
All	All	6830/7130 (96%)	6449 (94%)	329 (5%)	52 (1%)	18	68

5 of 17 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	8
3	D	407	GLY	8
3	D	374	ASN	4
3	D	375	GLY	3

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	160/174 (92%)	147±3 (92±2%)	13±3 (8±2%)	13	60
1	C	173/174 (99%)	160±2 (92±1%)	13±2 (8±1%)	14	62
2	B	154/164 (94%)	140±2 (91±2%)	14±2 (9±2%)	11	56
3	D	119/119 (100%)	102±2 (86±2%)	17±2 (14±2%)	5	45
All	All	6060/6310 (96%)	5492 (91%)	568 (9%)	10	56

5 of 172 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
2	B	20	THR	10
2	B	87	THR	10
3	D	445	THR	10
3	D	459	LEU	10

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 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	618	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	524	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	605	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	410	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	601	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	412	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	521	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	D	529	-	52,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	506	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	413	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	623	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	403	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	625	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	511	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	508	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	523	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	A	404	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	518	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	522	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	A	401	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	411	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	615	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	631	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	D	520	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	613	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	405	-	53,53,53	0.82±0.00	0±0 (0±0%)
6	GNP	B	205	-	34,34,34	1.22±0.01	2±0 (6±1%)
4	PCW	C	604	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	501	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	502	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	513	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	606	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	526	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	510	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	516	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	603	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	621	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	402	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	A	409	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	A	407	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	408	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	505	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	619	-	53,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	B	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	503	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	519	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	D	515	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	612	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	509	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	528	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	512	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	620	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	609	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	624	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	610	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	629	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	614	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	611	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	201	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	514	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	607	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	406	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	414	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	507	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	415	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	626	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	C	630	-	52,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	608	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	530	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	C	627	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	D	504	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	616	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	202	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	527	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	517	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	617	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	525	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	622	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	602	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	628	-	52,53,53	0.83±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
4	PCW	C	618	-	59,61,61	2.62±0.01	7±0 (12±0%)
5	17F	D	524	-	54,60,60	1.15±0.03	4±0 (7±0%)
4	PCW	C	605	-	59,61,61	2.63±0.01	7±0 (11±0%)
4	PCW	A	410	-	59,61,61	2.59±0.02	7±1 (11±1%)
4	PCW	C	601	-	59,61,61	2.60±0.01	7±0 (11±0%)
4	PCW	A	412	-	59,61,61	2.60±0.02	7±0 (11±0%)
5	17F	D	521	-	54,60,60	1.11±0.03	5±0 (9±0%)
5	17F	D	529	-	54,60,60	1.13±0.02	5±1 (9±0%)
4	PCW	D	506	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	A	413	-	59,61,61	2.61±0.00	6±0 (10±0%)
4	PCW	C	623	-	59,61,61	2.57±0.01	6±0 (10±0%)
4	PCW	A	403	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	625	-	59,61,61	2.59±0.02	7±1 (11±1%)
4	PCW	D	511	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	D	508	-	59,61,61	2.61±0.01	7±0 (11±0%)
5	17F	D	523	-	54,60,60	1.12±0.03	4±0 (7±0%)
4	PCW	A	404	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	518	-	59,61,61	2.62±0.01	7±0 (11±0%)
5	17F	D	522	-	54,60,60	1.15±0.02	5±1 (8±1%)
4	PCW	A	401	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	A	411	-	59,61,61	2.61±0.02	7±0 (11±0%)
4	PCW	C	615	-	59,61,61	2.61±0.02	6±0 (10±0%)
5	17F	C	631	-	54,60,60	1.09±0.04	4±0 (7±0%)
5	17F	D	520	-	54,60,60	1.12±0.03	4±0 (8±0%)
4	PCW	C	613	-	59,61,61	2.60±0.01	6±1 (10±1%)
4	PCW	A	405	-	59,61,61	2.59±0.01	6±0 (10±0%)
6	GNP	B	205	-	47,54,54	1.81±0.02	11±1 (23±2%)
4	PCW	C	604	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	D	501	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	D	502	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	513	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	C	606	-	59,61,61	2.59±0.01	6±0 (10±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	PCW	D	526	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	PCW	D	510	-	59,61,61	2.60±0.01	6±1 (10±1%)
4	PCW	D	516	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	C	603	-	59,61,61	2.60±0.01	7±1 (11±1%)
4	PCW	C	621	-	59,61,61	2.57±0.01	6±0 (10±0%)
4	PCW	A	402	-	59,61,61	2.60±0.01	6±0 (10±0%)
5	17F	A	409	-	54,60,60	1.12±0.02	4±0 (7±0%)
4	PCW	A	407	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	A	408	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	505	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	619	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	B	203	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	D	503	-	59,61,61	2.60±0.01	6±0 (11±0%)
5	17F	D	519	-	54,60,60	1.35±0.03	8±0 (15±0%)
4	PCW	D	515	-	59,61,61	2.60±0.02	6±1 (11±1%)
4	PCW	C	612	-	59,61,61	2.61±0.01	6±1 (10±1%)
4	PCW	D	509	-	59,61,61	2.58±0.00	6±0 (10±0%)
4	PCW	D	528	-	59,61,61	2.61±0.01	8±1 (12±1%)
4	PCW	D	512	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	C	620	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	C	609	-	59,61,61	2.59±0.00	7±1 (11±1%)
4	PCW	C	624	-	59,61,61	2.62±0.01	7±0 (11±0%)
4	PCW	C	610	-	59,61,61	2.59±0.00	7±1 (11±1%)
5	17F	C	629	-	54,60,60	1.13±0.05	4±0 (7±0%)
4	PCW	C	614	-	59,61,61	2.61±0.01	6±1 (11±1%)
4	PCW	C	611	-	59,61,61	2.59±0.01	6±0 (11±0%)
4	PCW	B	201	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	B	204	-	59,61,61	2.59±0.00	6±0 (10±0%)
4	PCW	D	514	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	607	-	59,61,61	2.58±0.01	6±0 (11±0%)
4	PCW	A	406	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	A	414	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	D	507	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	A	415	-	59,61,61	2.57±0.01	6±0 (11±0%)
5	17F	C	626	-	54,60,60	1.10±0.02	4±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	17F	C	630	-	54,60,60	1.12±0.03	4±0 (7±0%)
4	PCW	C	608	-	59,61,61	2.60±0.01	7±1 (11±1%)
5	17F	D	530	-	54,60,60	1.09±0.05	4±0 (8±0%)
5	17F	C	627	-	54,60,60	1.12±0.03	4±0 (7±0%)
4	PCW	D	504	-	59,61,61	2.69±0.01	10±0 (17±0%)
4	PCW	C	616	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	B	202	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	PCW	D	527	-	59,61,61	2.67±0.01	10±0 (16±0%)
4	PCW	D	517	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	C	617	-	59,61,61	2.61±0.01	7±0 (11±0%)
5	17F	D	525	-	54,60,60	1.24±0.03	4±0 (8±0%)
4	PCW	C	622	-	59,61,61	2.58±0.02	6±0 (10±0%)
4	PCW	C	602	-	59,61,61	2.58±0.01	6±0 (10±0%)
5	17F	C	628	-	54,60,60	1.35±0.03	9±0 (16±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
5	17F	D	529	-	-	1±0,59,59,59	-
4	PCW	A	403	-	-	0±0,57,57,57	-
4	PCW	A	404	-	-	0±0,57,57,57	-
4	PCW	D	518	-	-	0±0,57,57,57	-
4	PCW	C	613	-	-	0±0,57,57,57	-
4	PCW	A	413	-	-	0±0,57,57,57	-
4	PCW	C	606	-	-	0±0,57,57,57	-
5	17F	D	523	-	-	0±0,59,59,59	-
5	17F	D	522	-	-	1±0,59,59,59	-
4	PCW	D	503	-	-	0±0,57,57,57	-
4	PCW	C	610	-	-	0±0,57,57,57	-
4	PCW	D	513	-	-	0±0,57,57,57	-
4	PCW	B	204	-	-	0±0,57,57,57	-
4	PCW	D	514	-	-	0±0,57,57,57	-
5	17F	C	629	-	-	0±0,59,59,59	-
4	PCW	C	615	-	-	0±0,57,57,57	-
4	PCW	A	415	-	-	0±0,57,57,57	-
5	17F	C	626	-	-	0±0,59,59,59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	17F	D	520	-	-	0±0,59,59,59	-
5	17F	C	627	-	-	0±0,59,59,59	-
4	PCW	D	505	-	-	0±0,57,57,57	-
4	PCW	D	507	-	-	0±0,57,57,57	-
4	PCW	C	612	-	-	0±0,57,57,57	-
5	17F	D	521	-	-	0±0,59,59,59	-
4	PCW	A	401	-	-	0±0,57,57,57	-
4	PCW	A	405	-	-	0±0,57,57,57	-
4	PCW	D	528	-	-	0±0,57,57,57	-
4	PCW	D	512	-	-	0±0,57,57,57	-
5	17F	D	525	-	-	1±0,59,59,59	-
4	PCW	D	508	-	-	0±0,57,57,57	-
4	PCW	C	607	-	-	0±0,57,57,57	-
4	PCW	C	611	-	-	0±0,57,57,57	-
4	PCW	C	614	-	-	0±0,57,57,57	-
4	PCW	A	407	-	-	0±0,57,57,57	-
4	PCW	C	621	-	-	0±0,57,57,57	-
4	PCW	D	527	-	-	0±0,57,57,57	-
4	PCW	A	411	-	-	0±0,57,57,57	-
4	PCW	C	604	-	-	0±0,57,57,57	-
4	PCW	A	402	-	-	0±0,57,57,57	-
5	17F	C	631	-	-	0±0,59,59,59	-
4	PCW	C	623	-	-	0±0,57,57,57	-
4	PCW	C	609	-	-	0±0,57,57,57	-
4	PCW	D	504	-	-	0±0,57,57,57	-
4	PCW	C	616	-	-	0±0,57,57,57	-
4	PCW	C	620	-	-	0±0,57,57,57	-
4	PCW	C	601	-	-	0±0,57,57,57	-
4	PCW	D	517	-	-	0±0,57,57,57	-
4	PCW	A	408	-	-	0±0,57,57,57	-
4	PCW	D	502	-	-	0±0,57,57,57	-
4	PCW	D	526	-	-	0±0,57,57,57	-
4	PCW	D	516	-	-	0±0,57,57,57	-
4	PCW	A	412	-	-	0±0,57,57,57	-
4	PCW	B	202	-	-	0±0,57,57,57	-
4	PCW	C	622	-	-	0±0,57,57,57	-
5	17F	C	628	-	-	0±0,59,59,59	-
4	PCW	D	515	-	-	0±0,57,57,57	-
5	17F	D	519	-	-	0±0,59,59,59	-
4	PCW	D	510	-	-	0±0,57,57,57	-
4	PCW	C	624	-	-	0±0,57,57,57	-
4	PCW	C	608	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	D	506	-	-	0±0,57,57,57	-
5	17F	D	530	-	-	0±0,59,59,59	-
4	PCW	C	618	-	-	0±0,57,57,57	-
4	PCW	B	203	-	-	0±0,57,57,57	-
5	17F	A	409	-	-	0±0,59,59,59	-
4	PCW	C	625	-	-	0±0,57,57,57	-
4	PCW	C	603	-	-	0±0,57,57,57	-
4	PCW	B	201	-	-	0±0,57,57,57	-
4	PCW	C	617	-	-	0±0,57,57,57	-
4	PCW	C	602	-	-	0±0,57,57,57	-
4	PCW	D	501	-	-	0±0,57,57,57	-
5	17F	D	524	-	-	0±0,59,59,59	-
4	PCW	A	410	-	-	0±0,57,57,57	-
5	17F	C	630	-	-	0±0,59,59,59	-
4	PCW	C	619	-	-	0±0,57,57,57	-
4	PCW	C	605	-	-	0±0,57,57,57	-
4	PCW	D	509	-	-	0±0,57,57,57	-
6	GNP	B	205	-	-	0±0,18,38,38	0±0,3,3,3
4	PCW	D	511	-	-	0±0,57,57,57	-
4	PCW	A	406	-	-	0±0,57,57,57	-
4	PCW	A	414	-	-	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	205	GNP	PB-O2B	3.19	1.48	1.56	5	10
6	B	205	GNP	C5-N7	2.96	1.33	1.39	2	10
6	B	205	GNP	PB-O3A	2.24	1.61	1.59	2	2

5 of 586 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	17.69	62.50	108.98	10	10
4	C	625	PCW	C8-N-C7	17.69	62.51	108.98	7	10
4	C	613	PCW	C8-N-C7	17.69	62.52	108.98	1	10
4	D	501	PCW	C8-N-C7	17.69	62.52	108.98	7	10
4	C	621	PCW	C8-N-C7	17.69	62.52	108.98	3	10

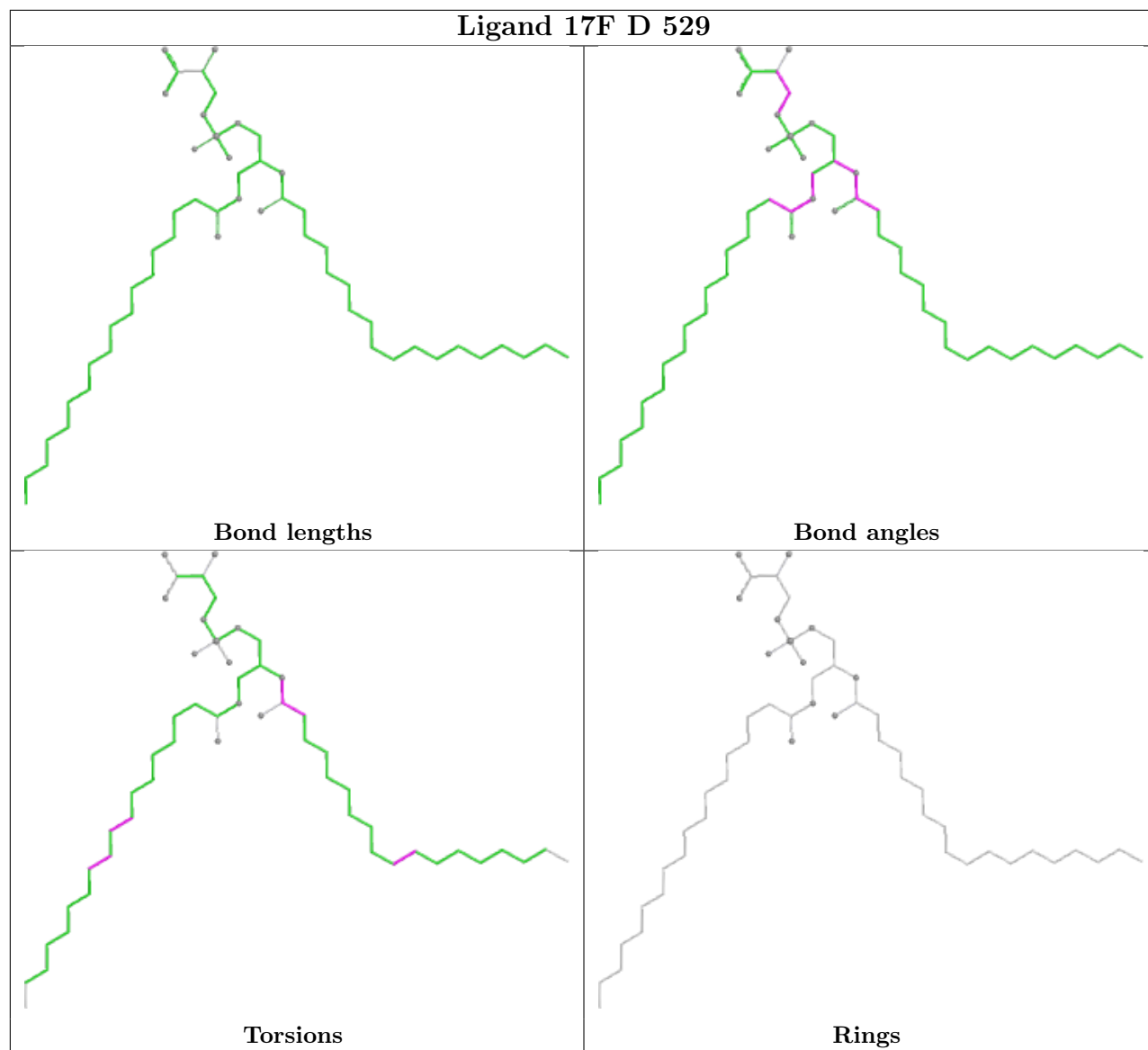
There are no chirality outliers.

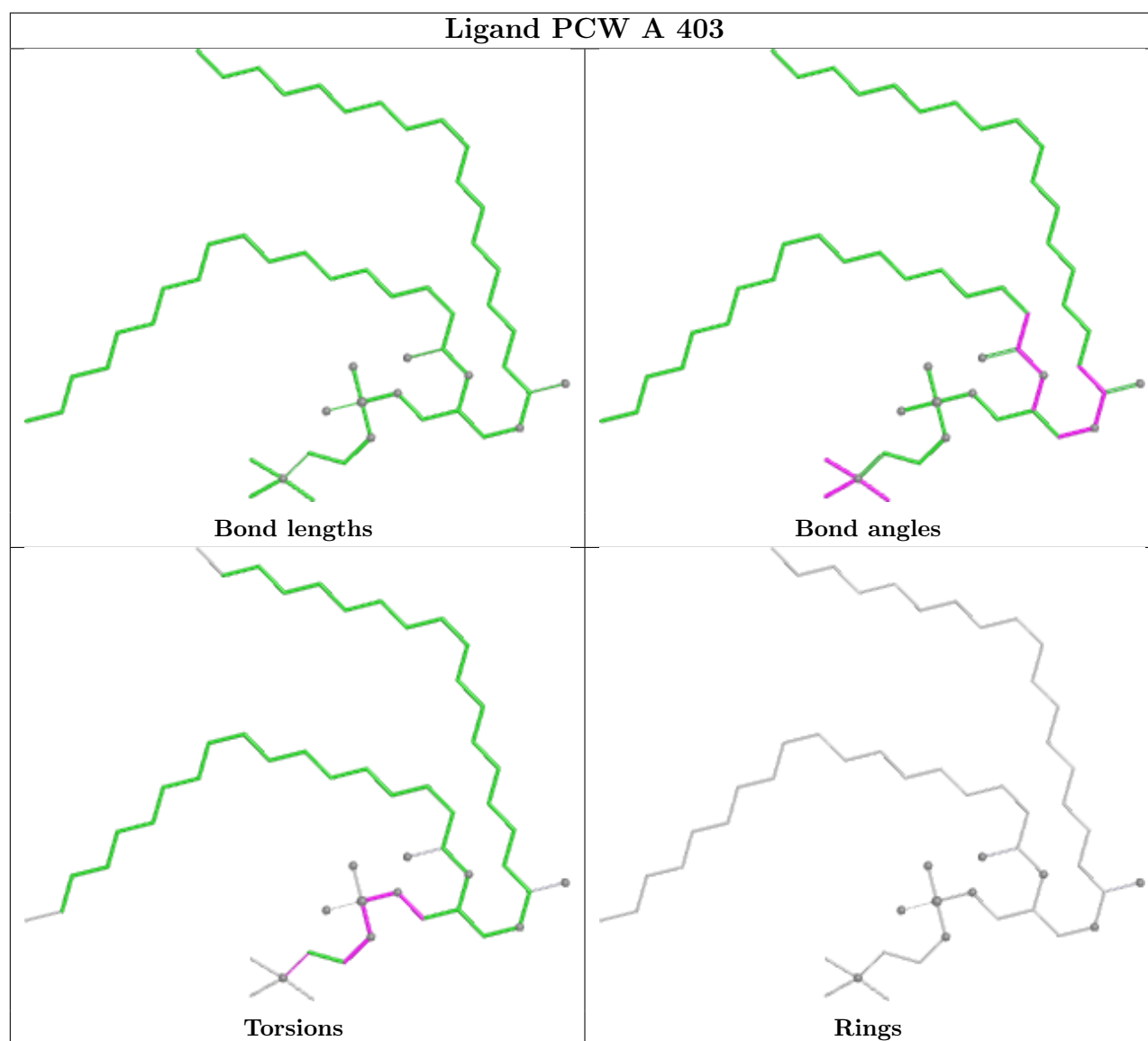
5 of 6 unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

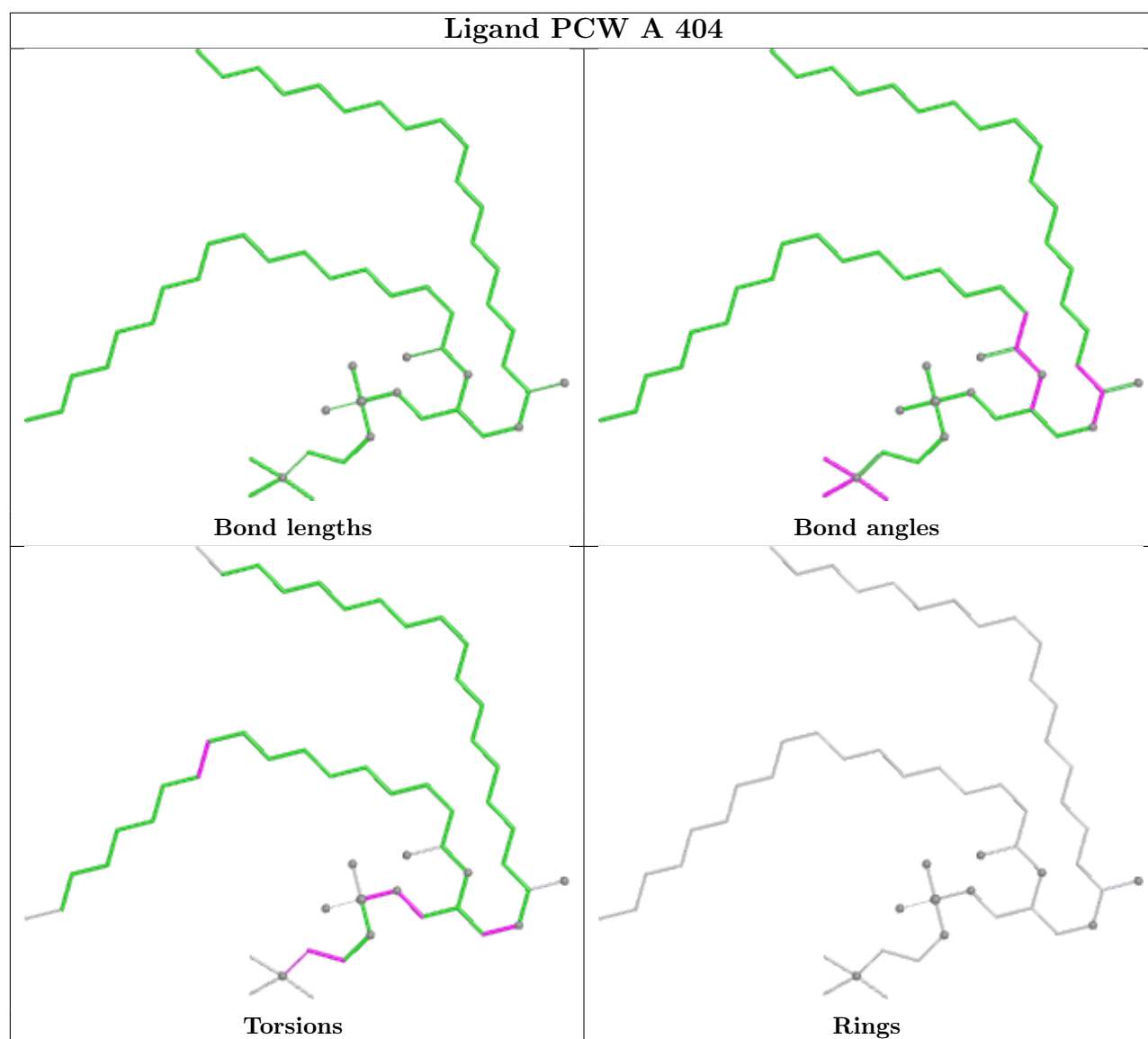
Mol	Chain	Res	Type	Atoms	Models (Total)
5	D	522	17F	O10-C17-O9-C5	10
5	D	525	17F	O10-C17-O9-C5	10
5	D	529	17F	O10-C17-O9-C5	10
5	D	522	17F	C18-C17-O9-C5	2
5	D	525	17F	C18-C17-O9-C5	1

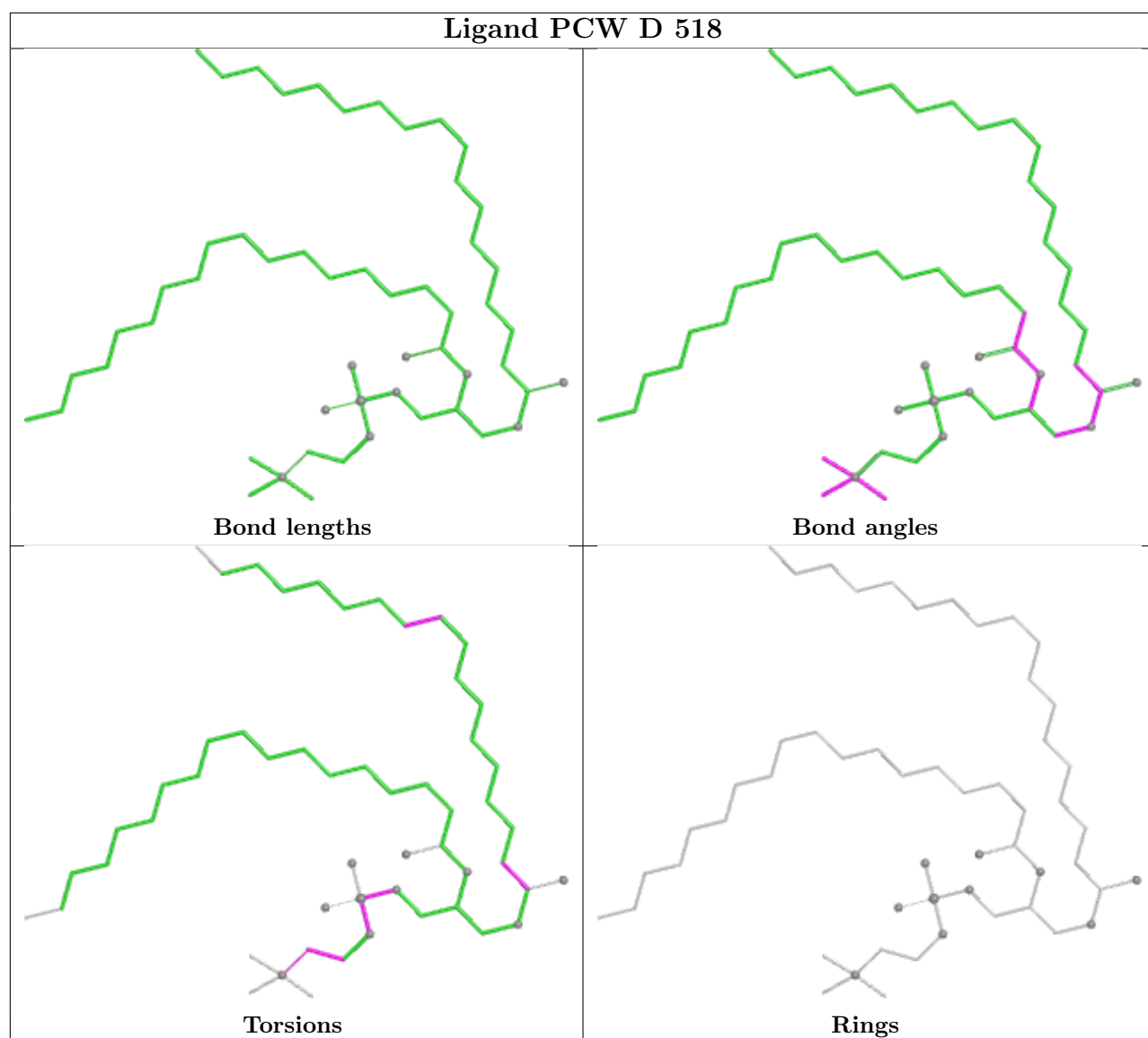
There are no ring outliers.

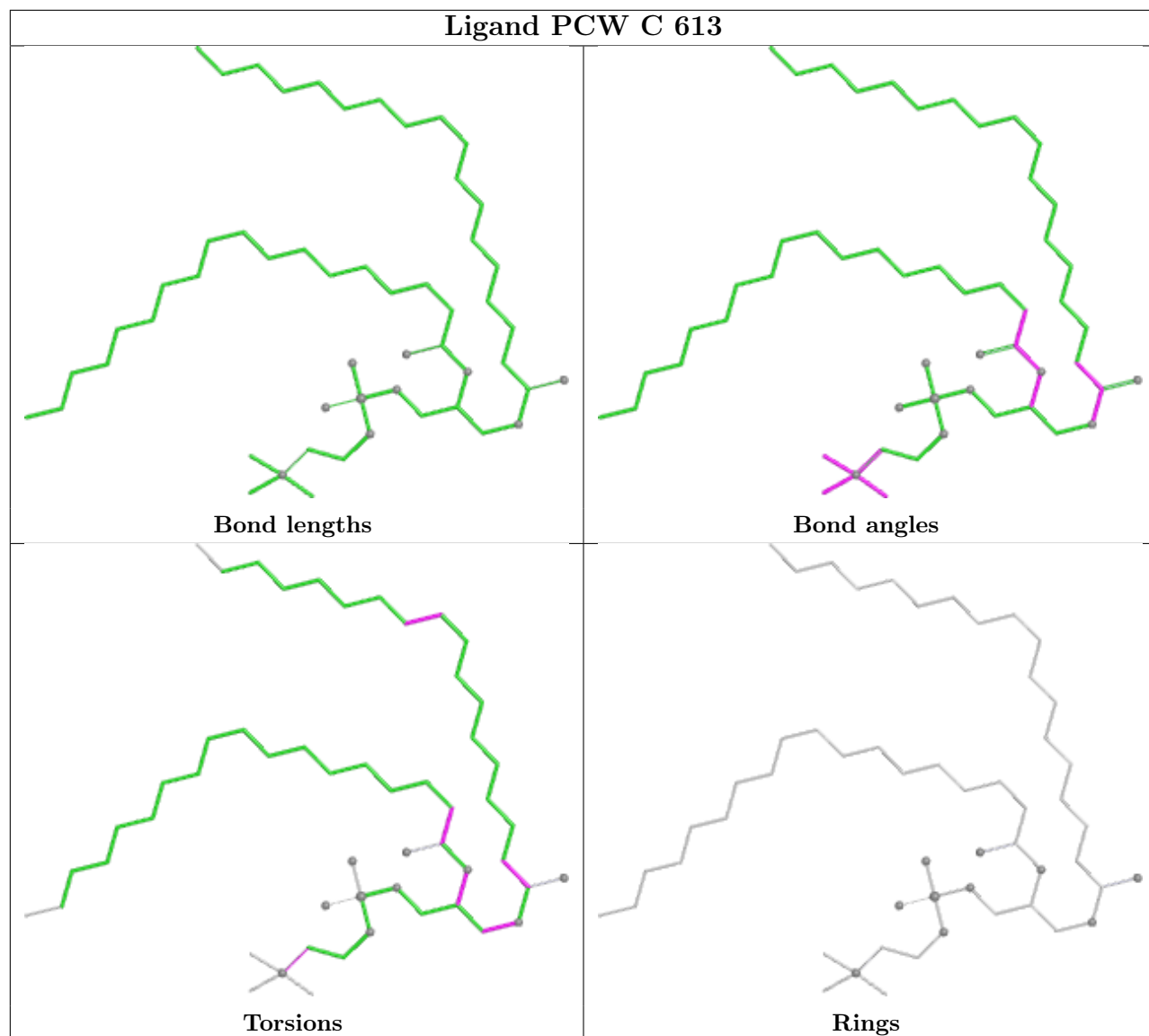
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

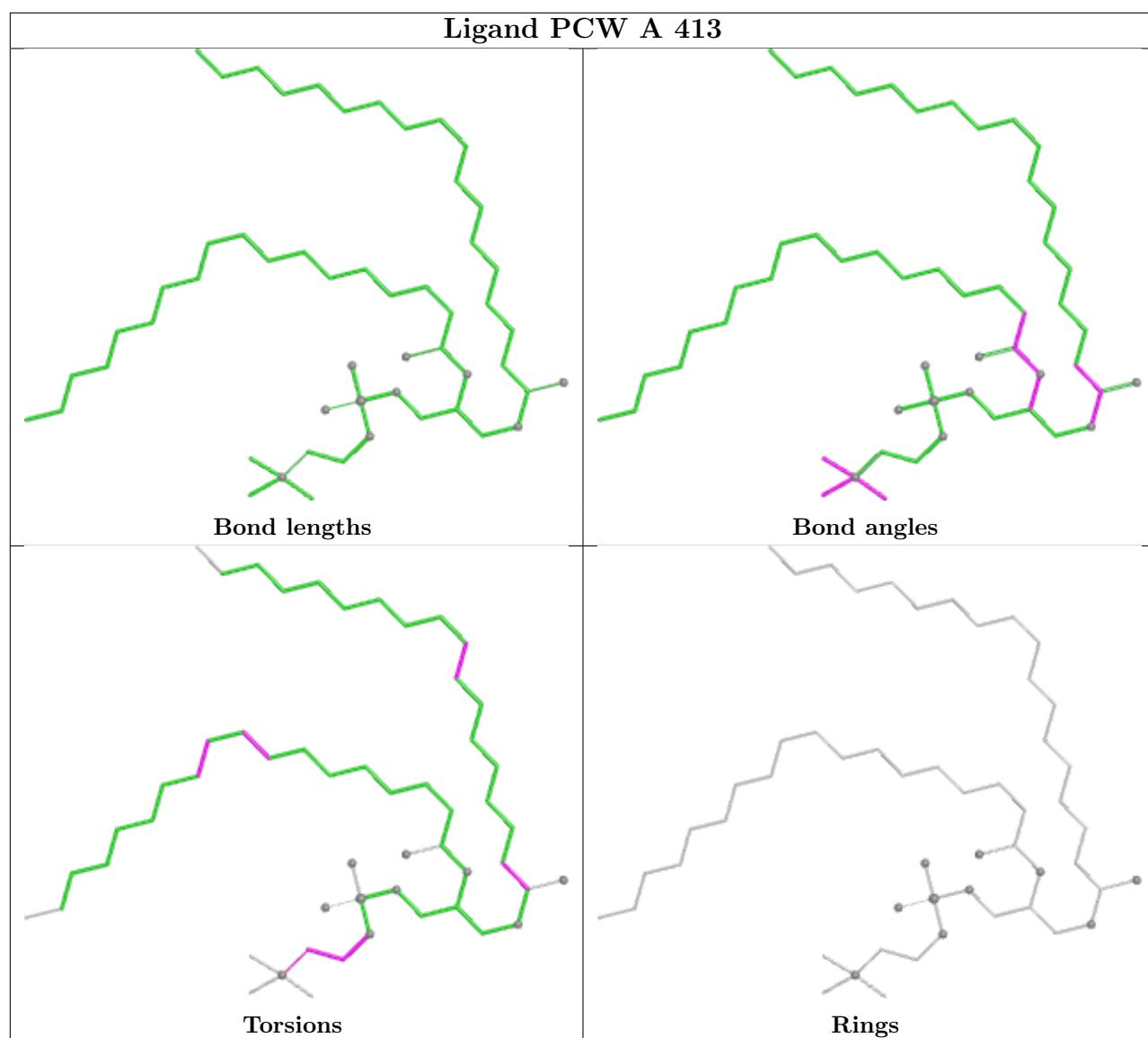


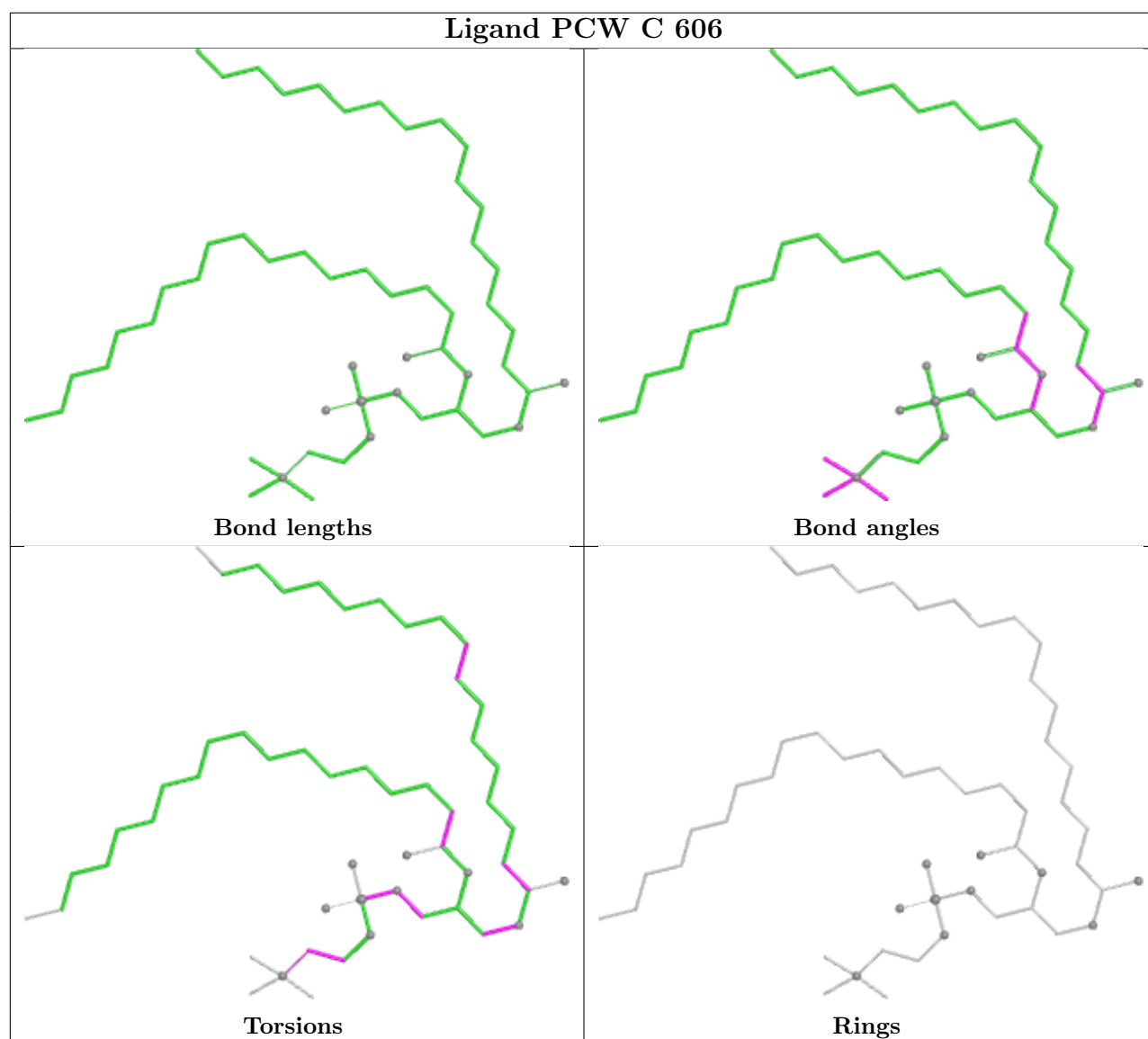


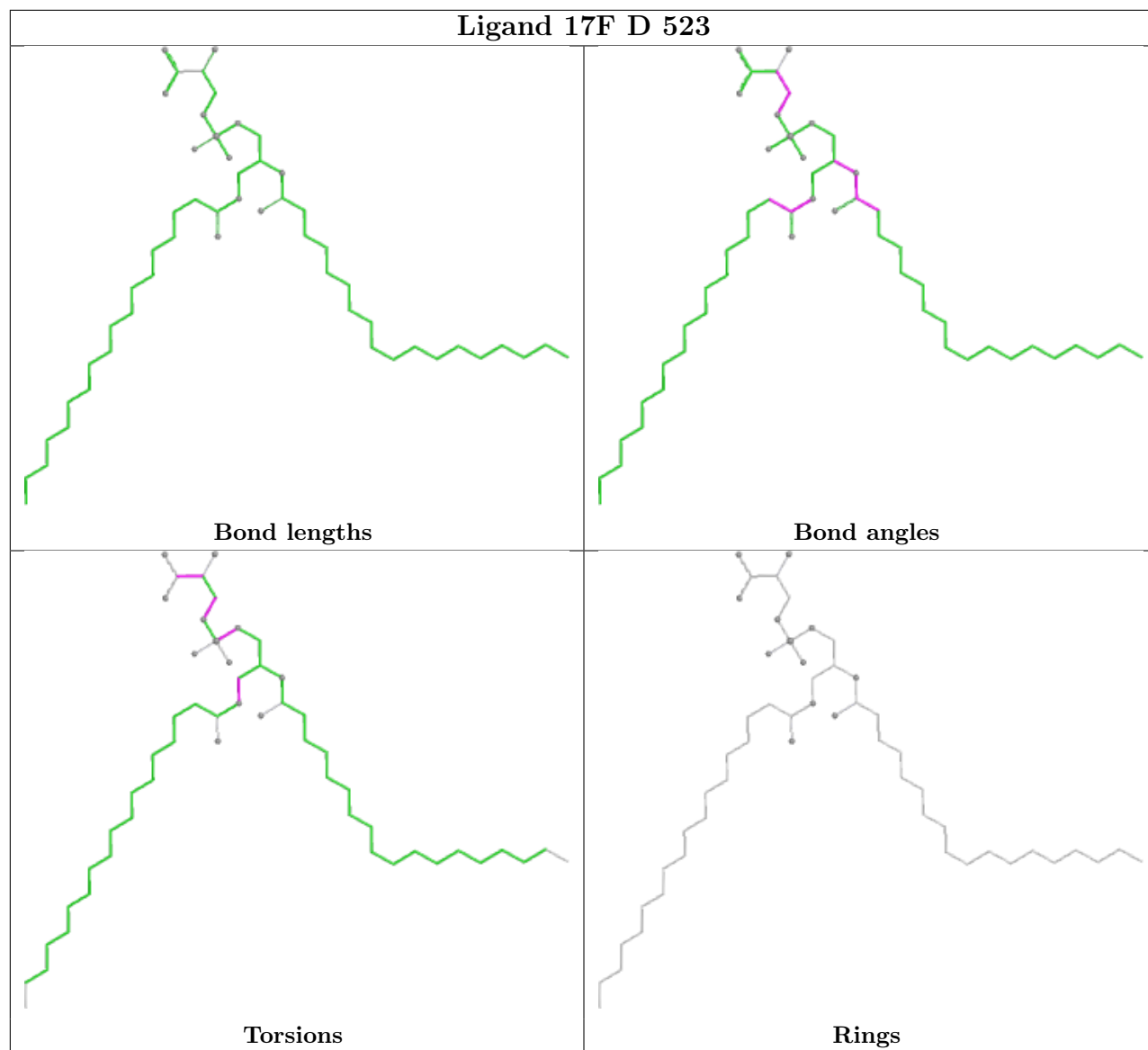


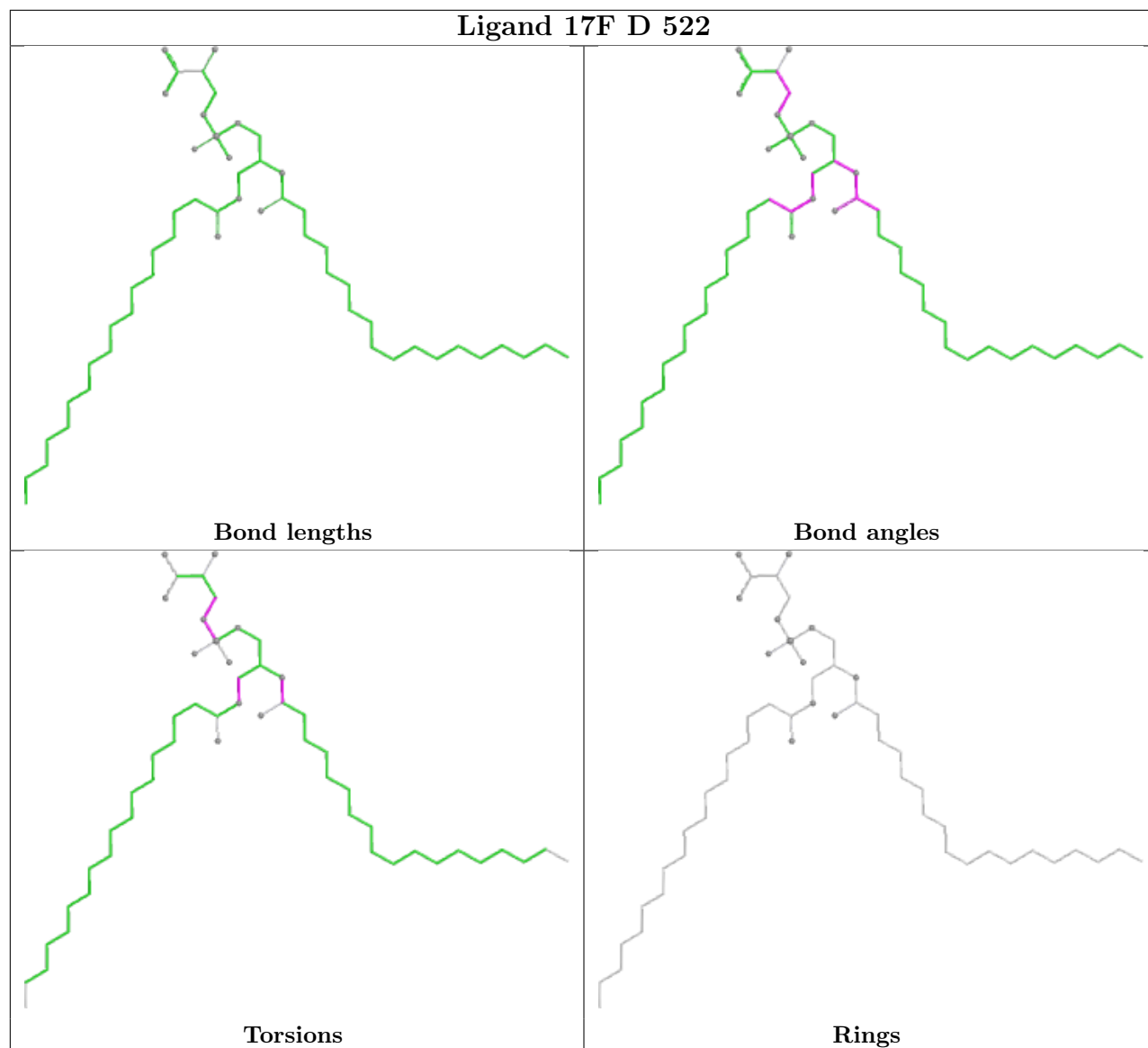


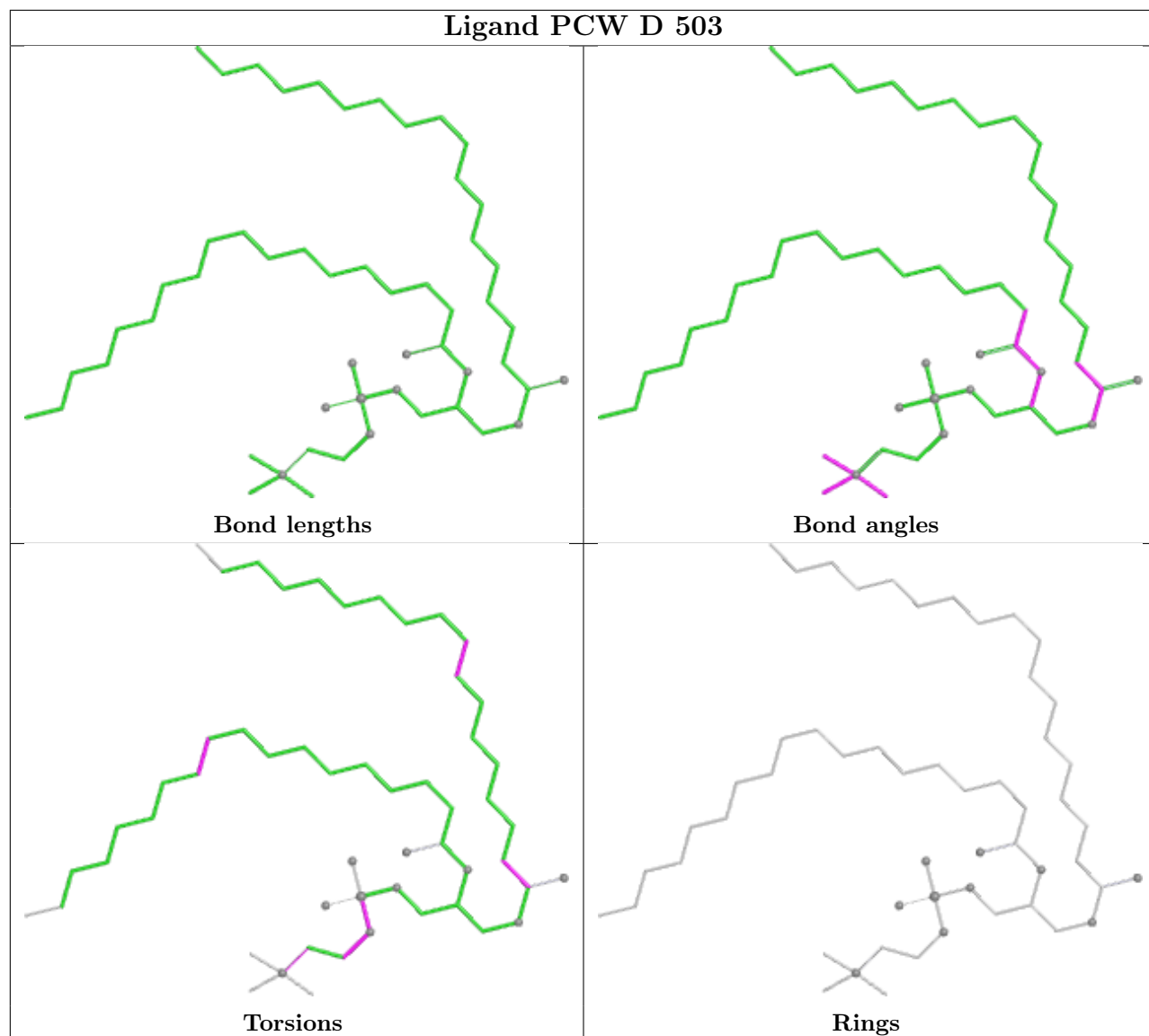


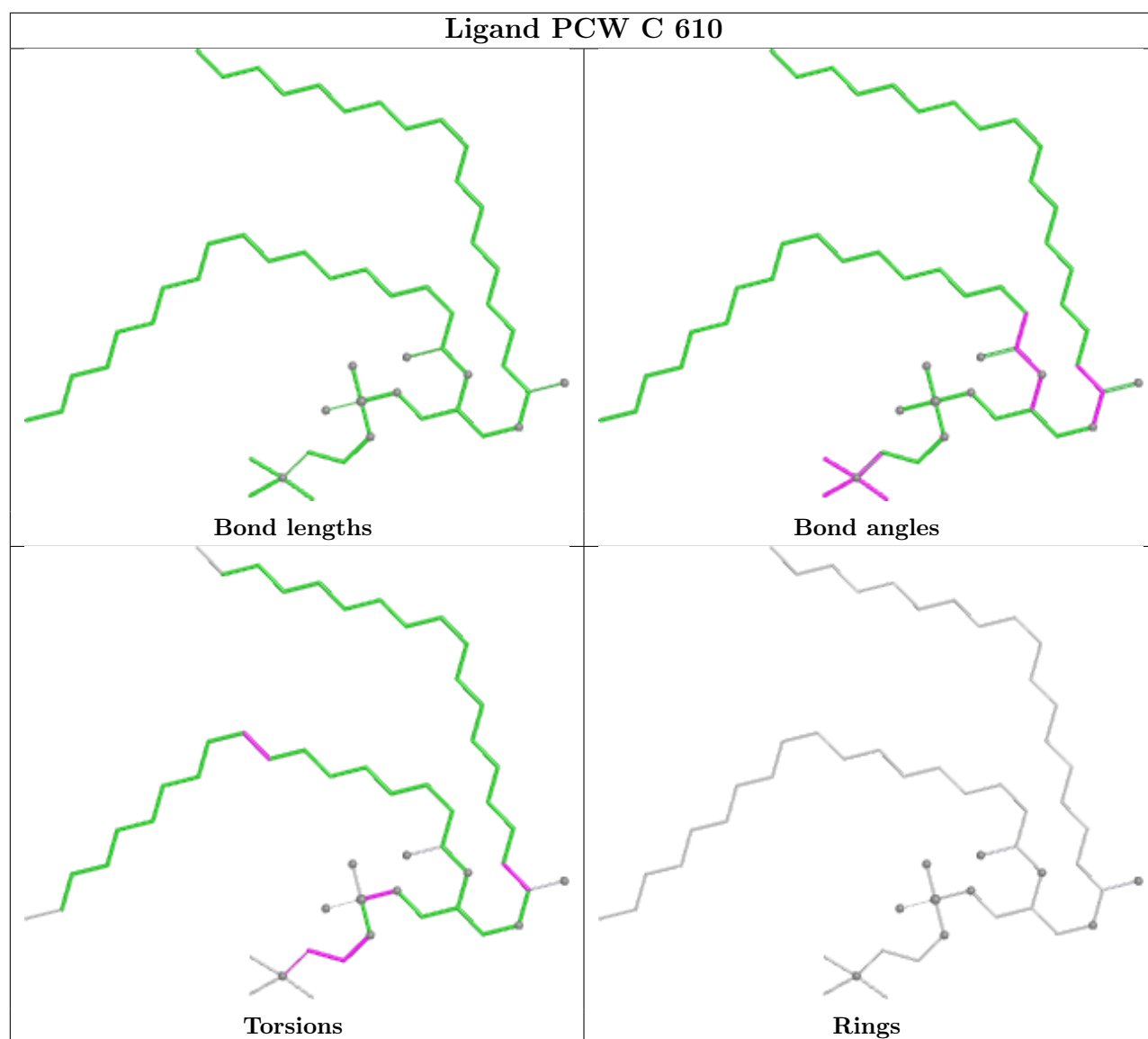


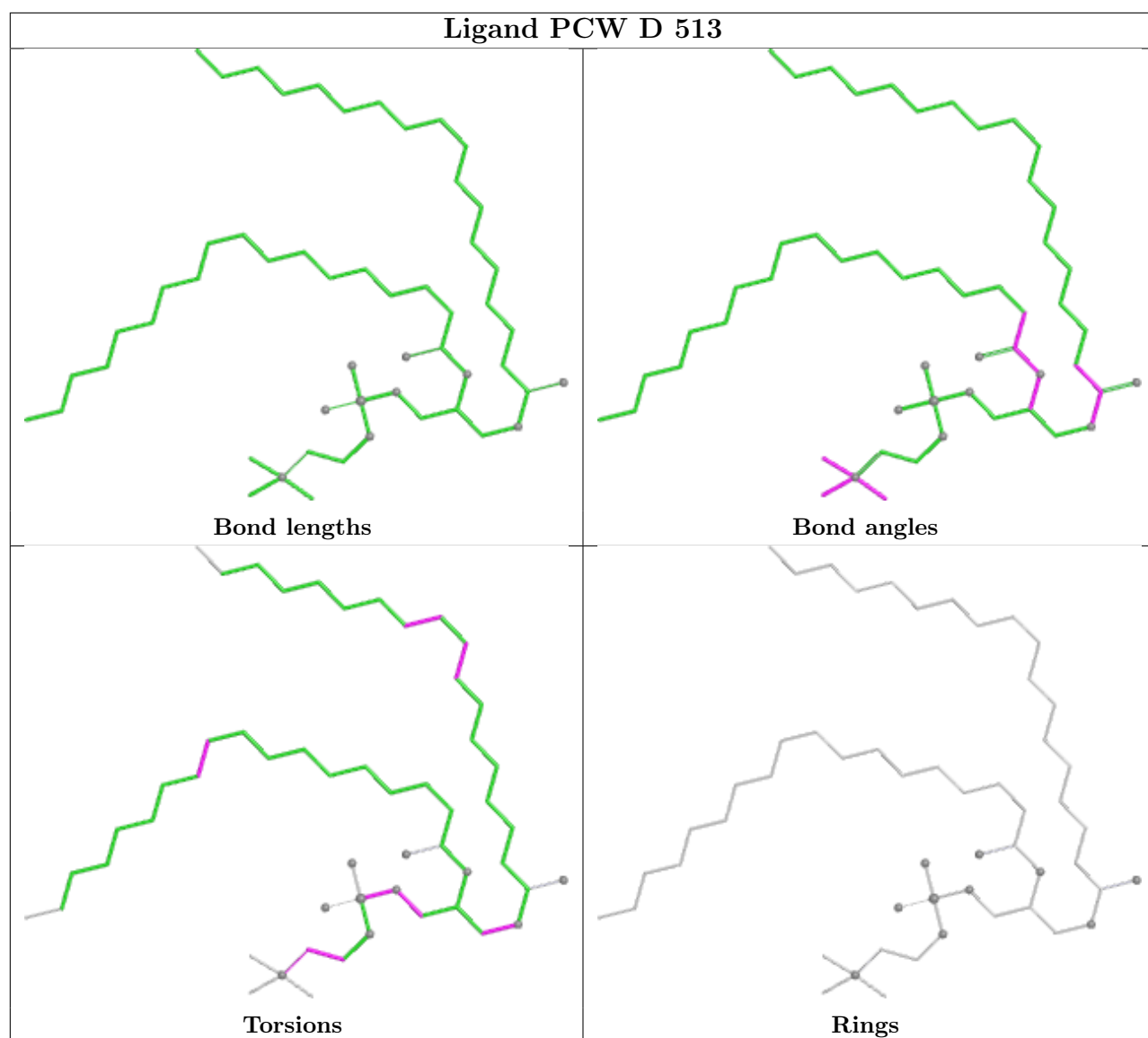


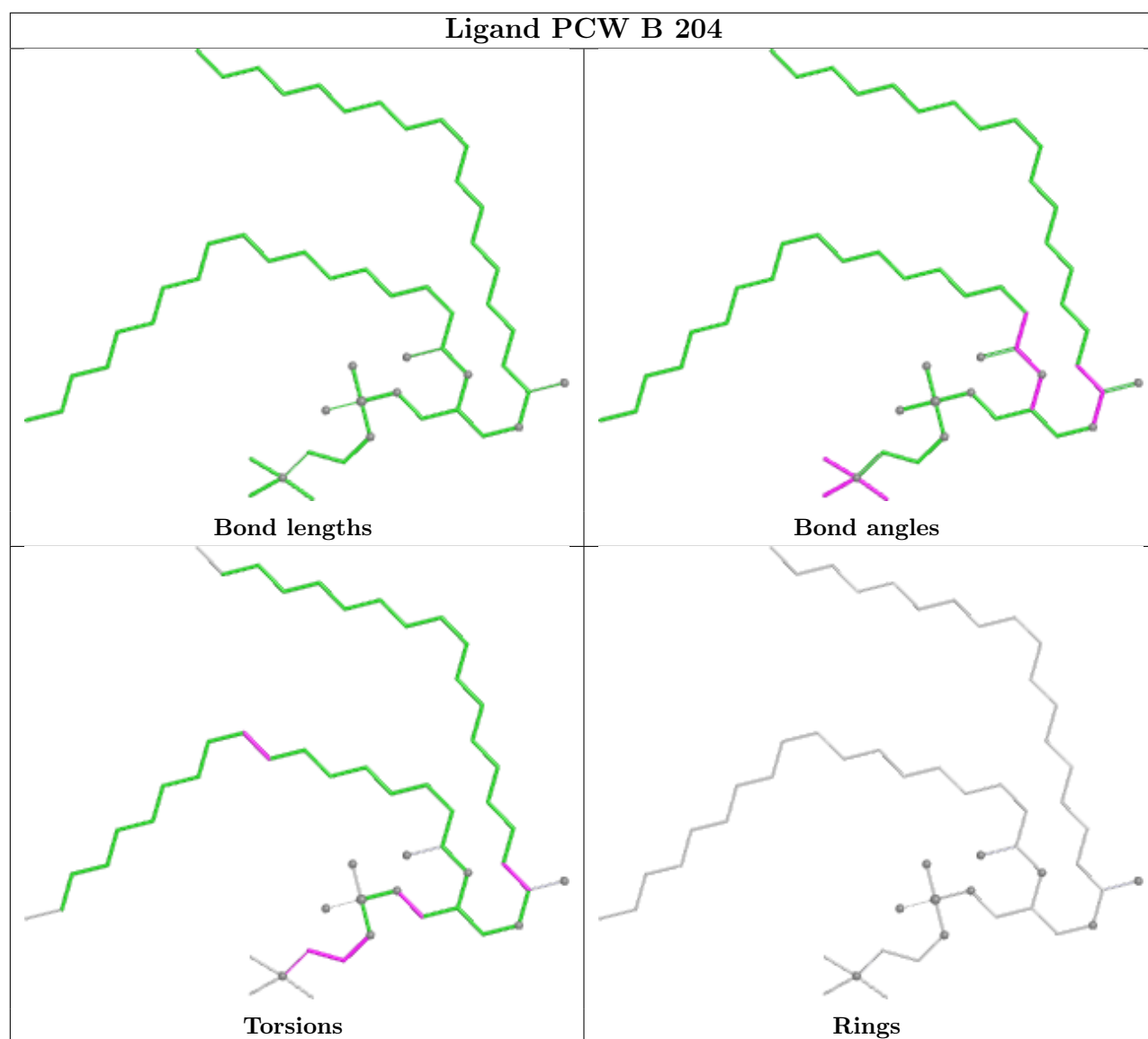


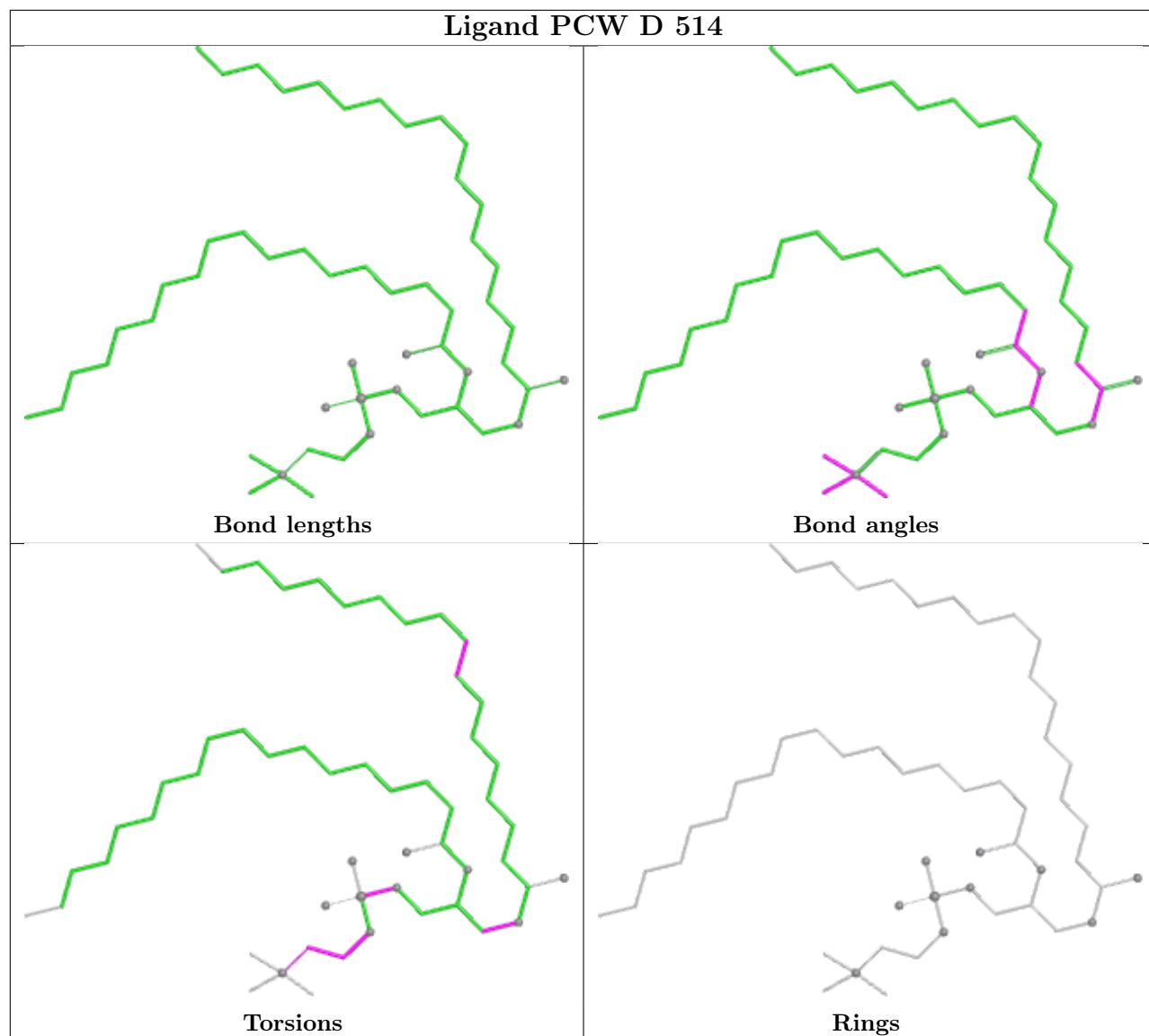


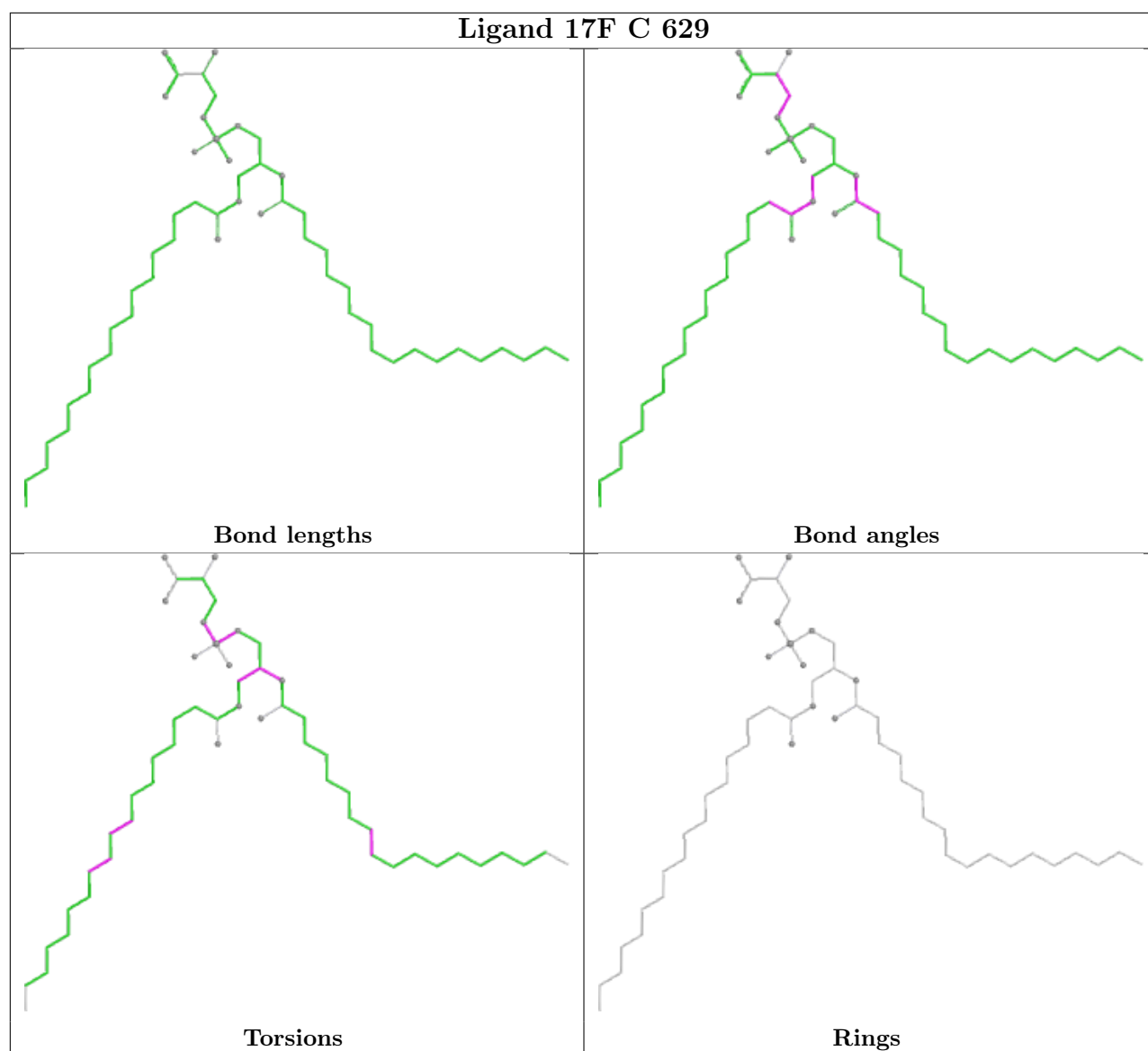


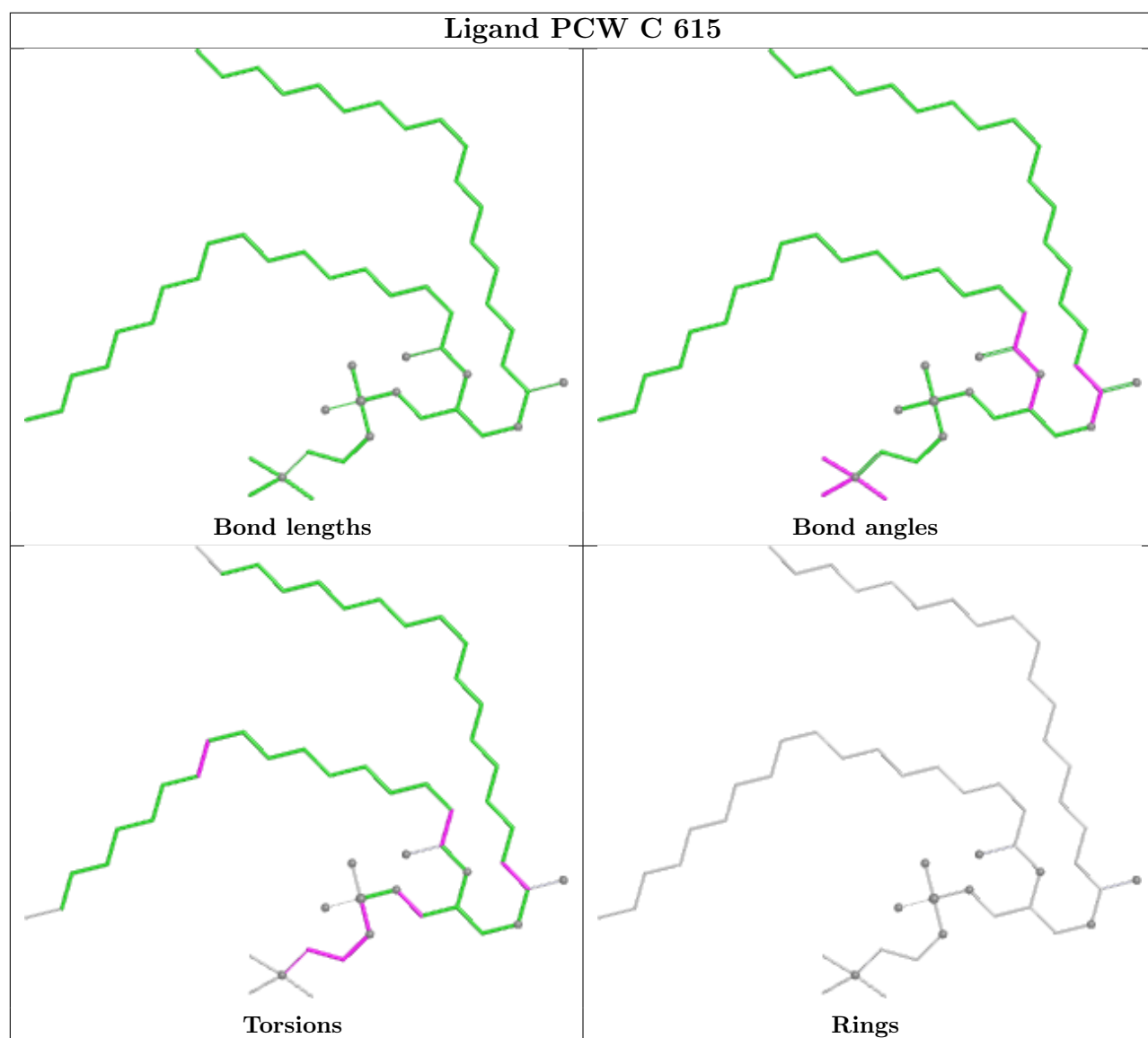


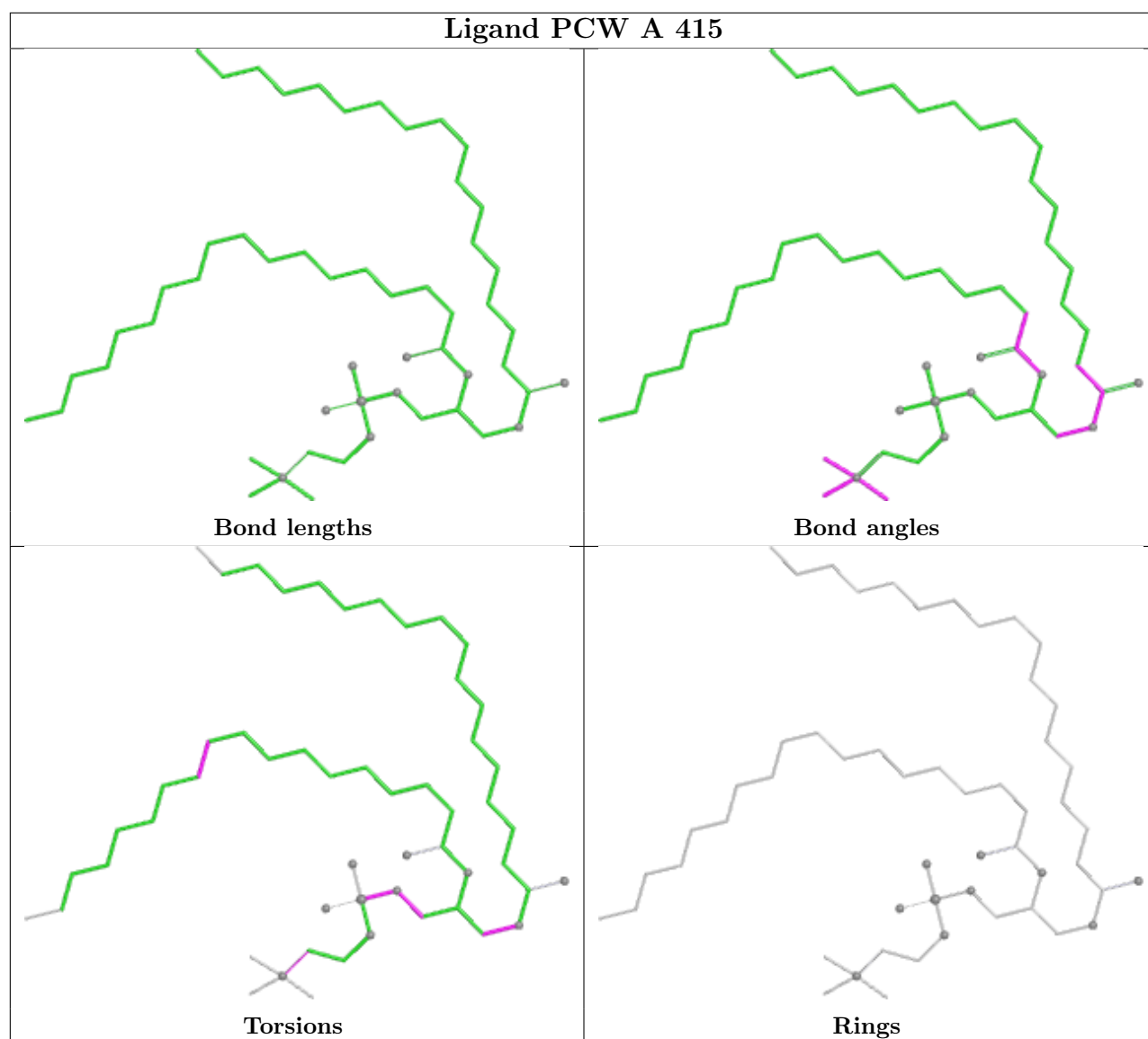


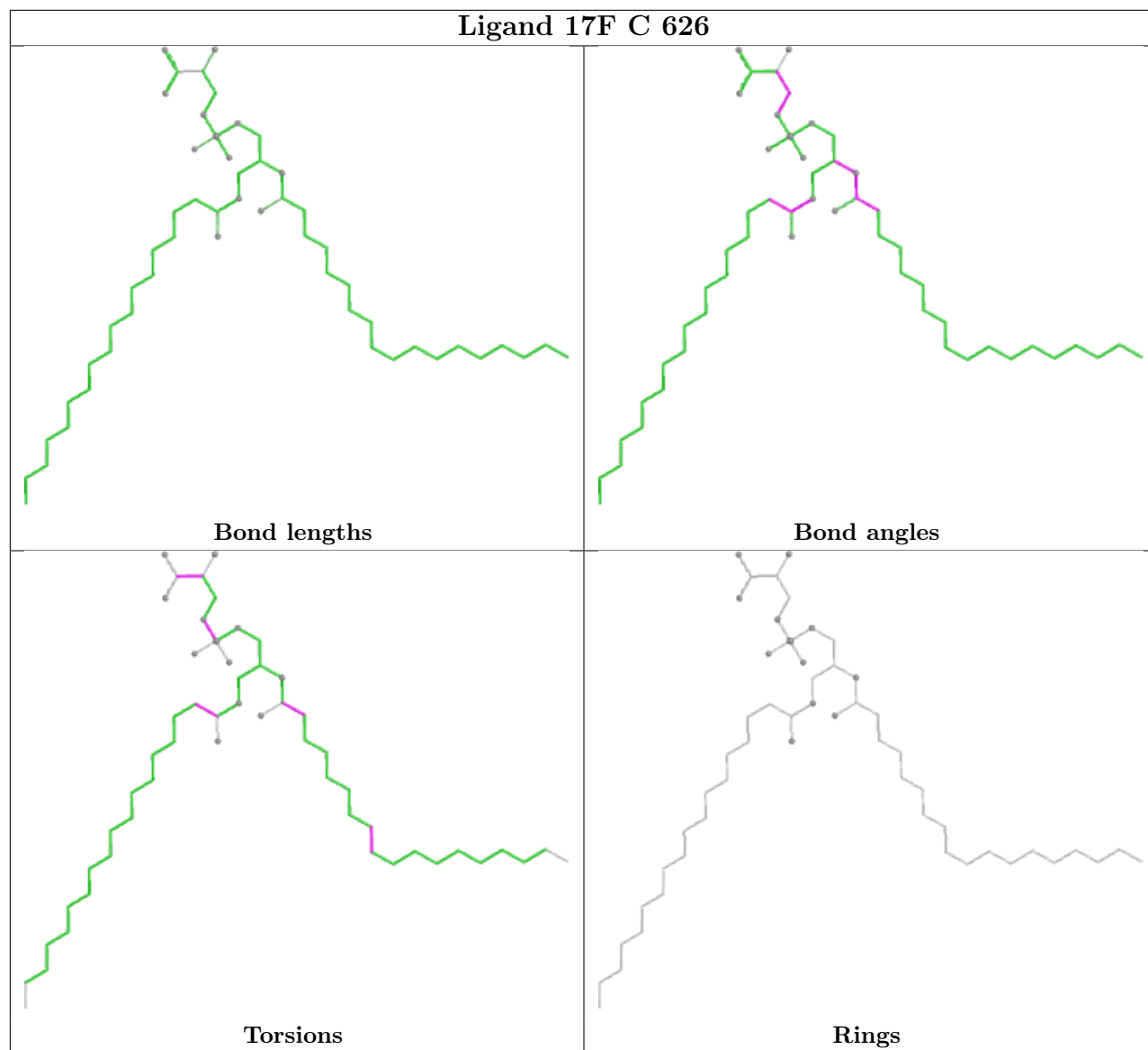


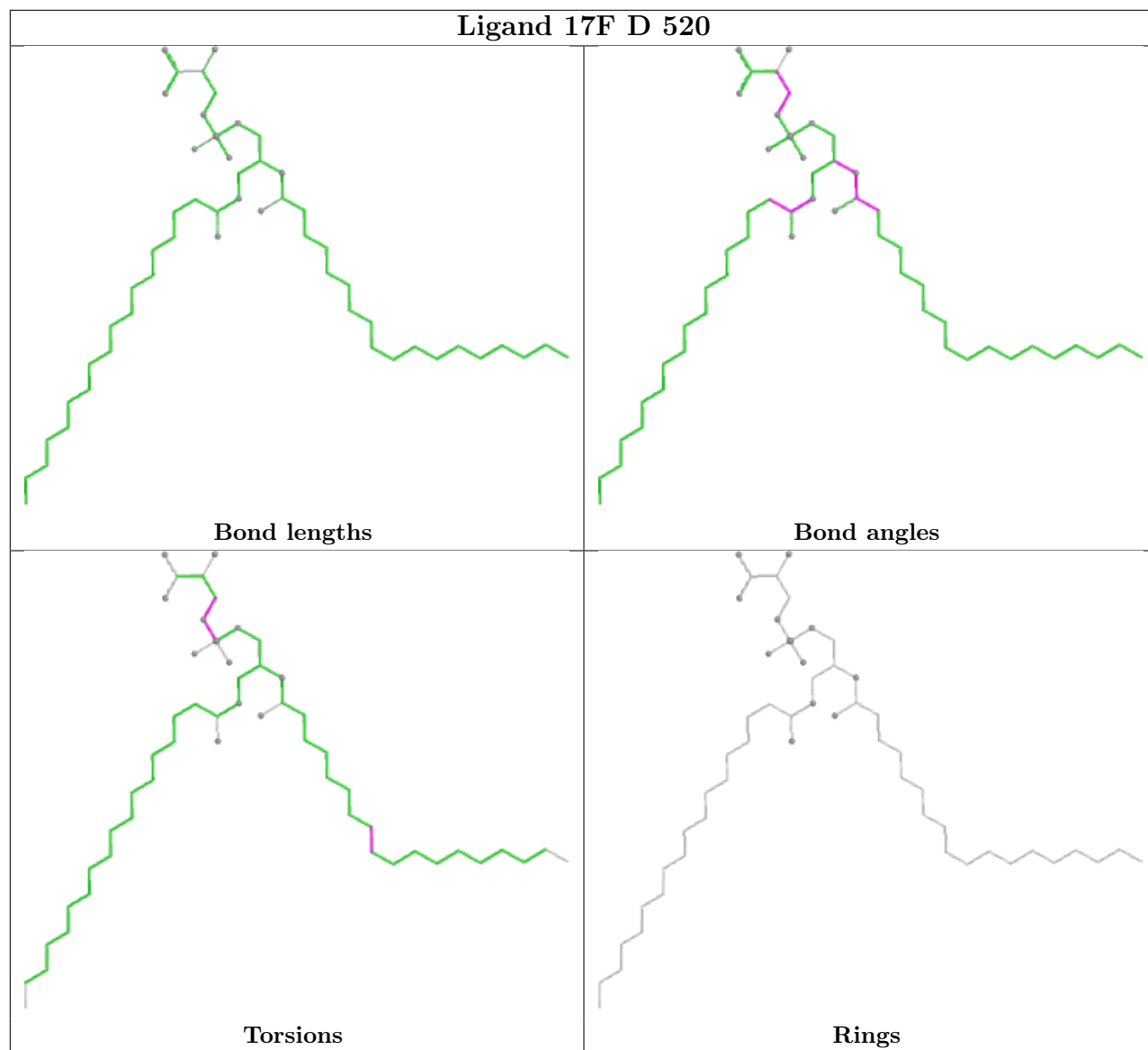


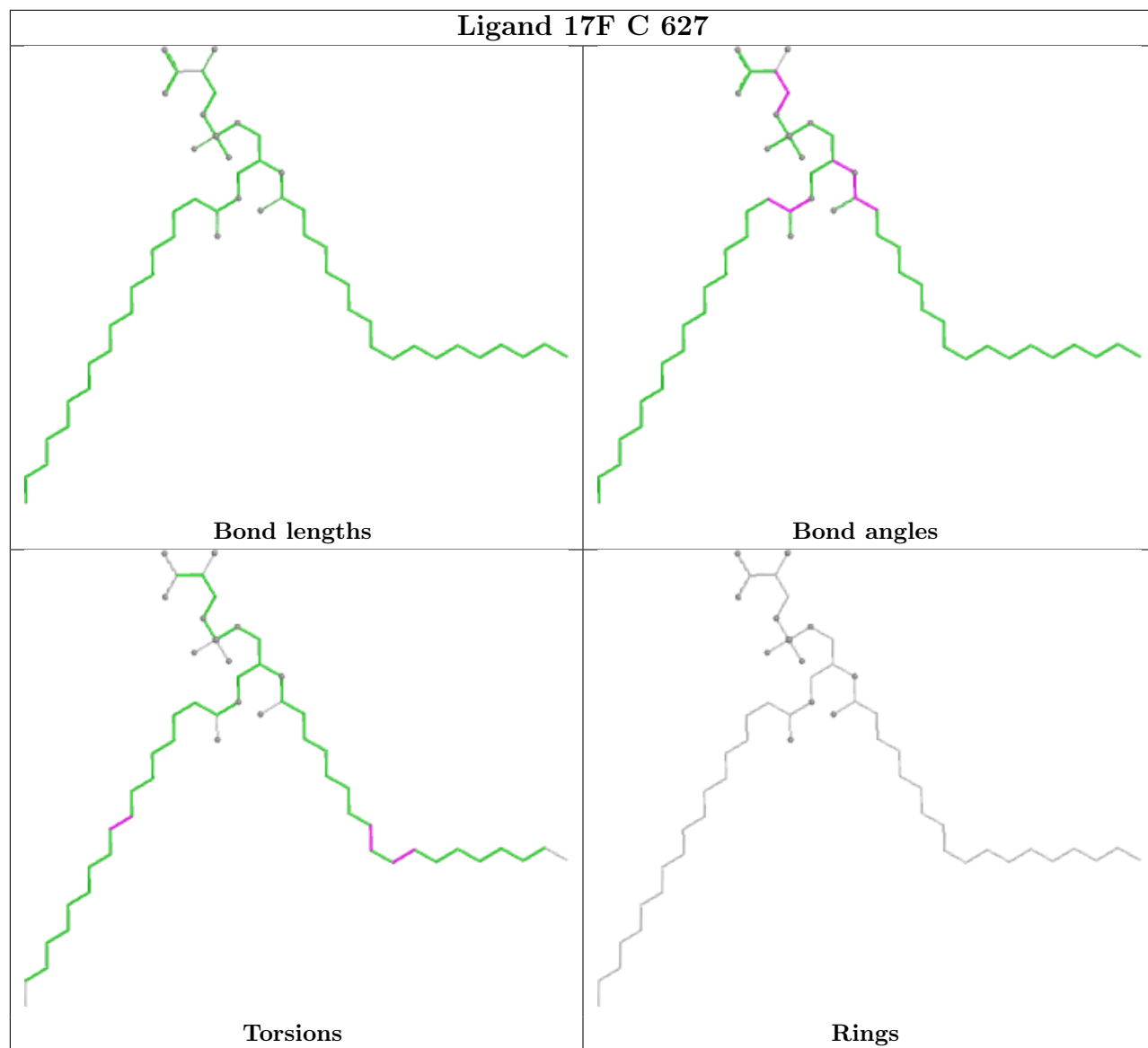


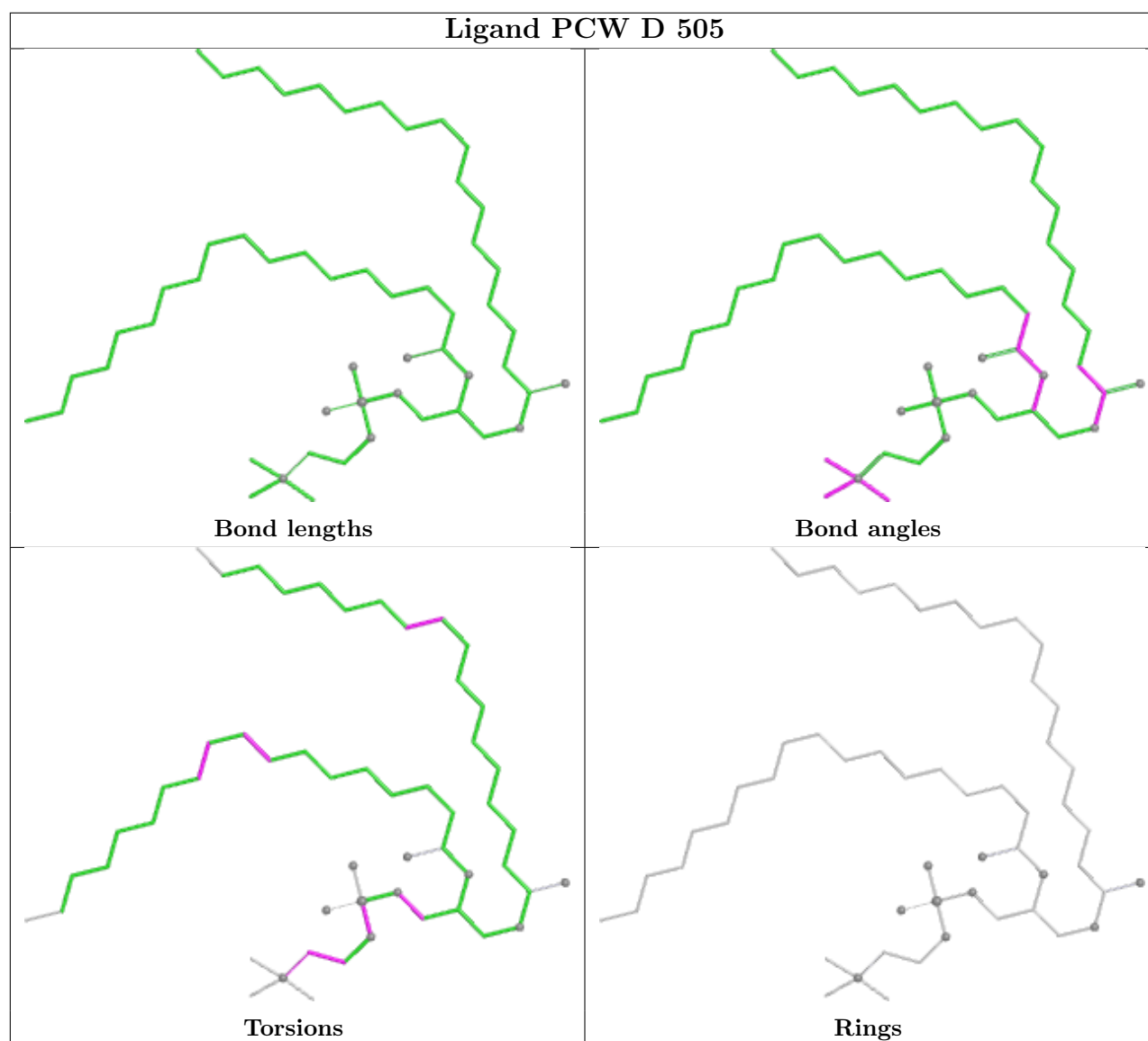


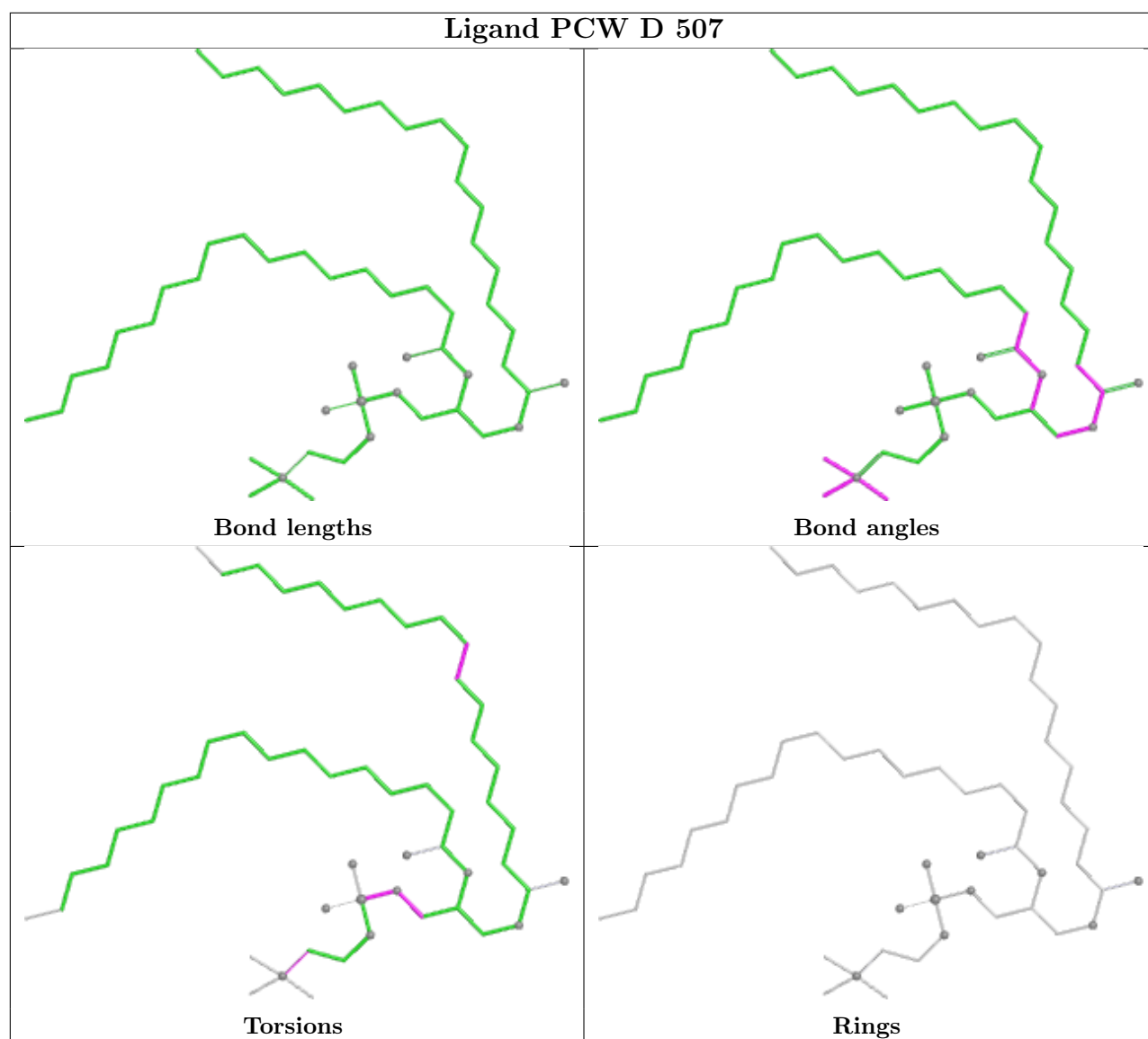


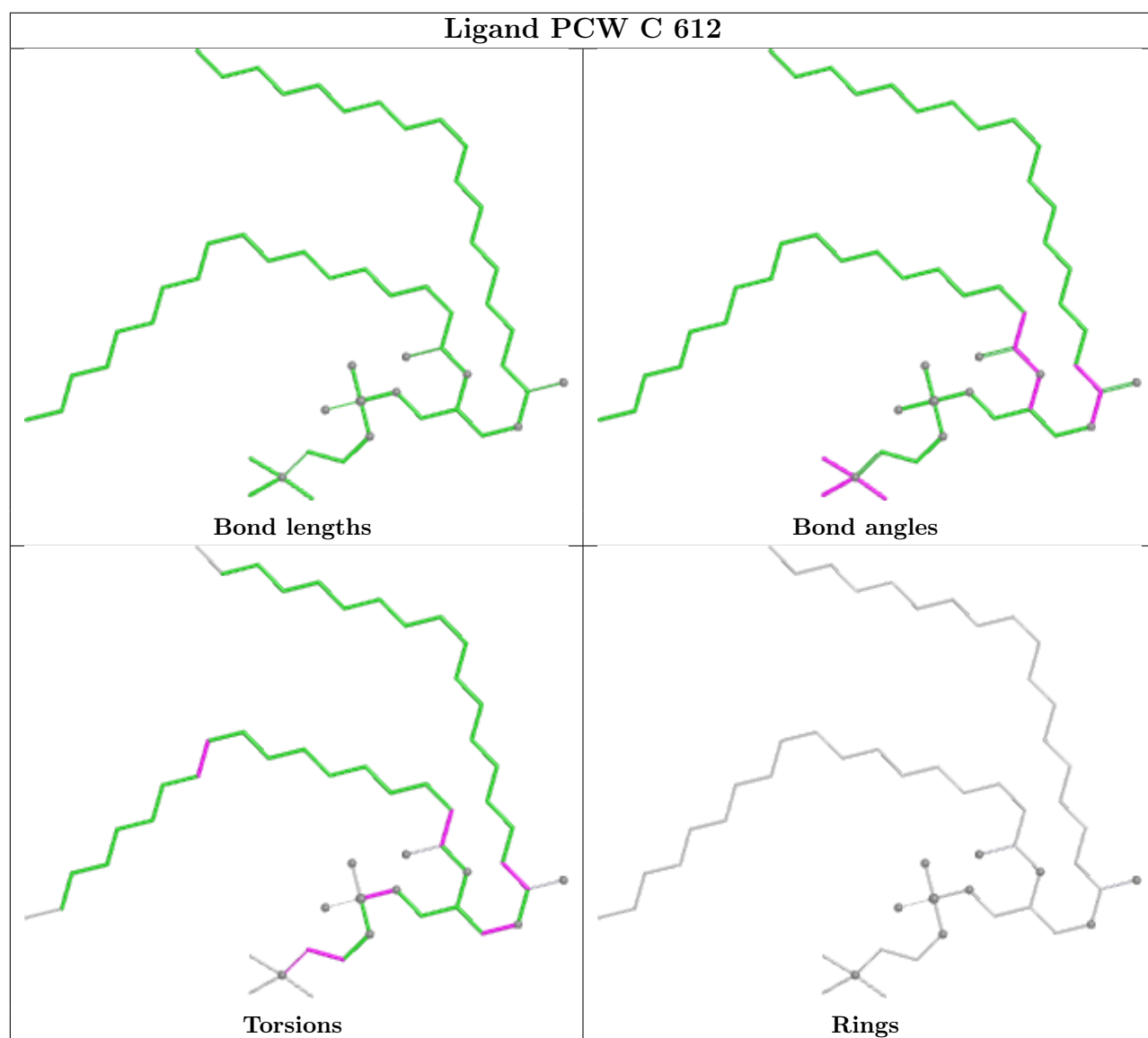


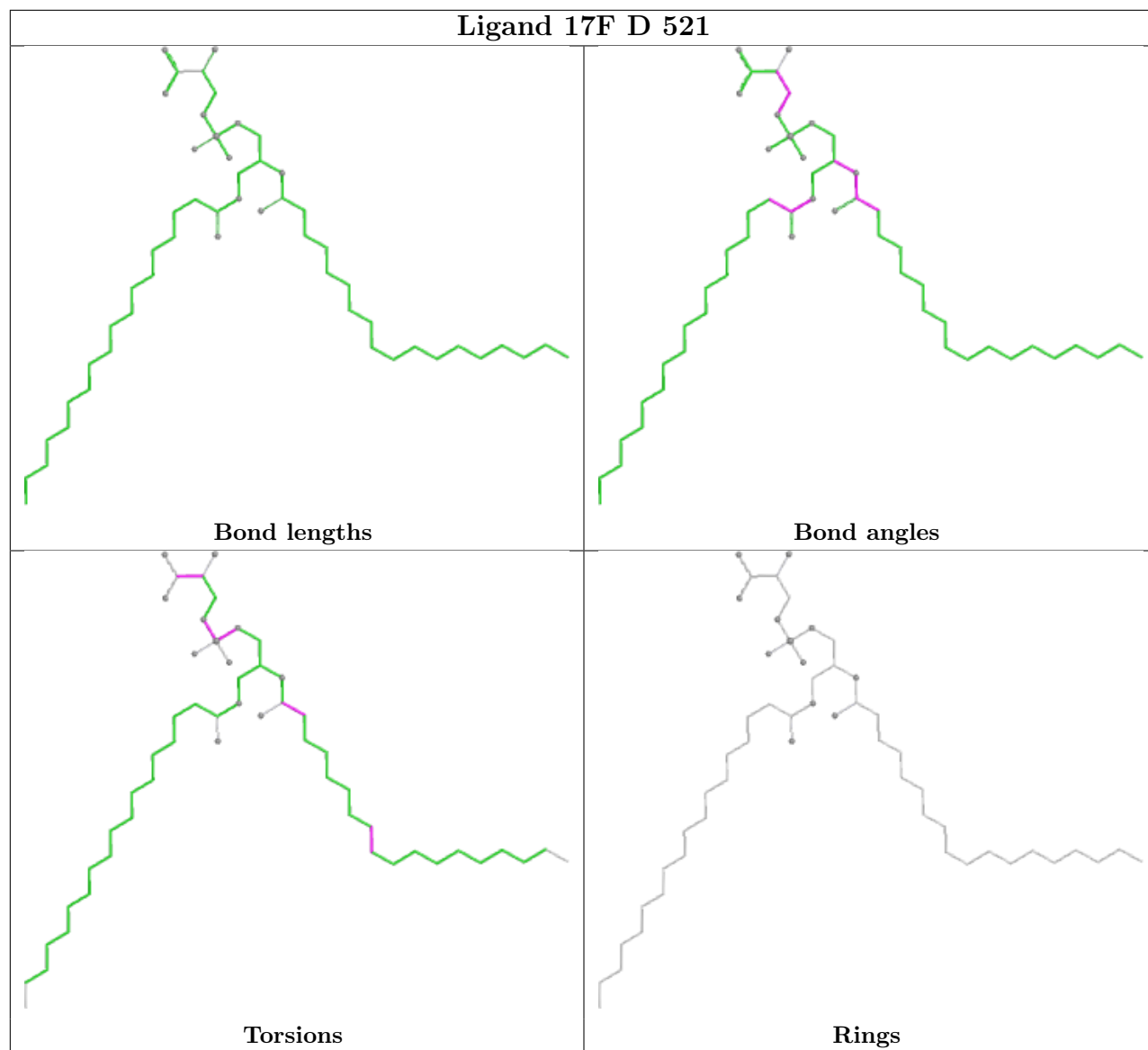


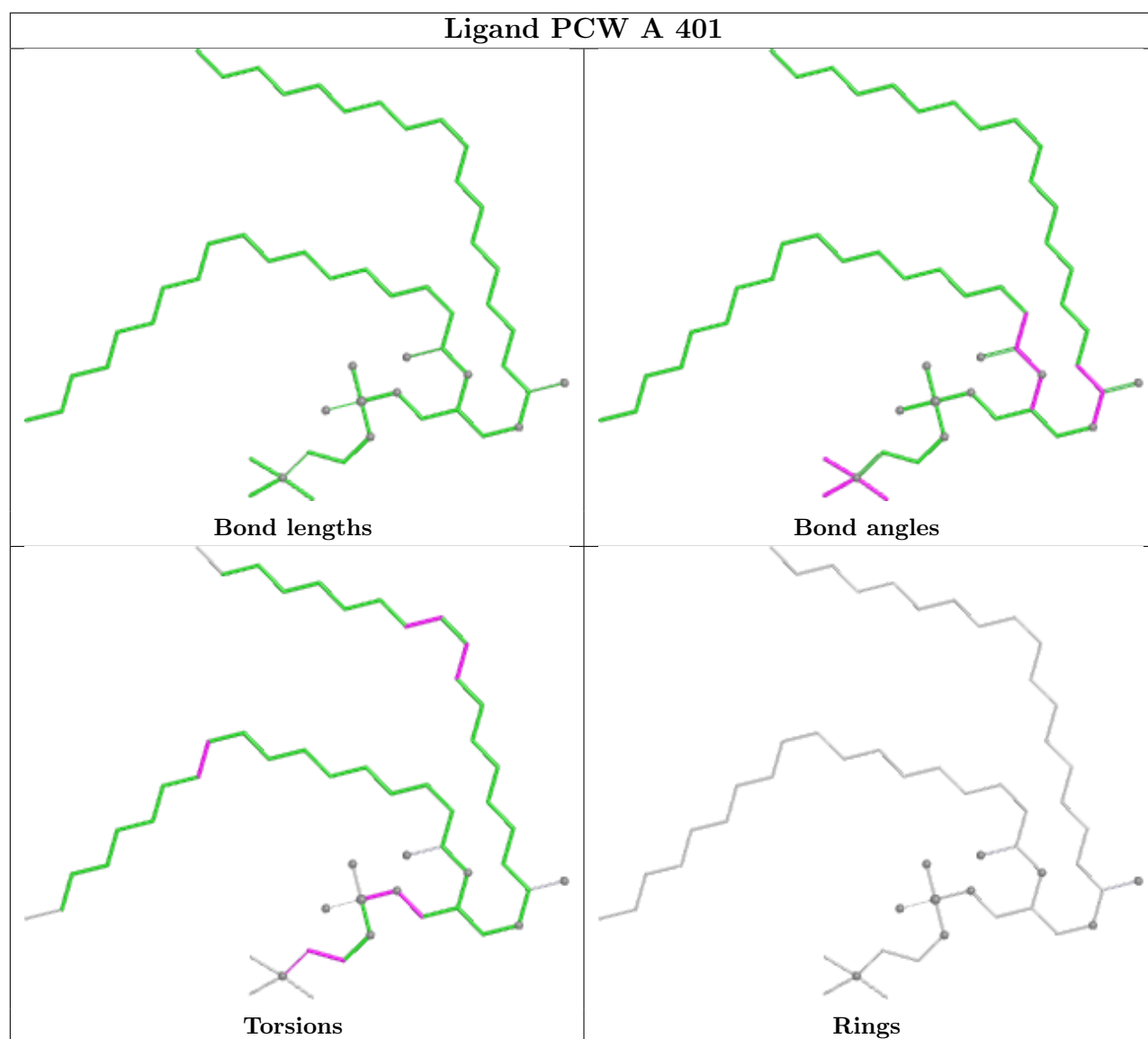


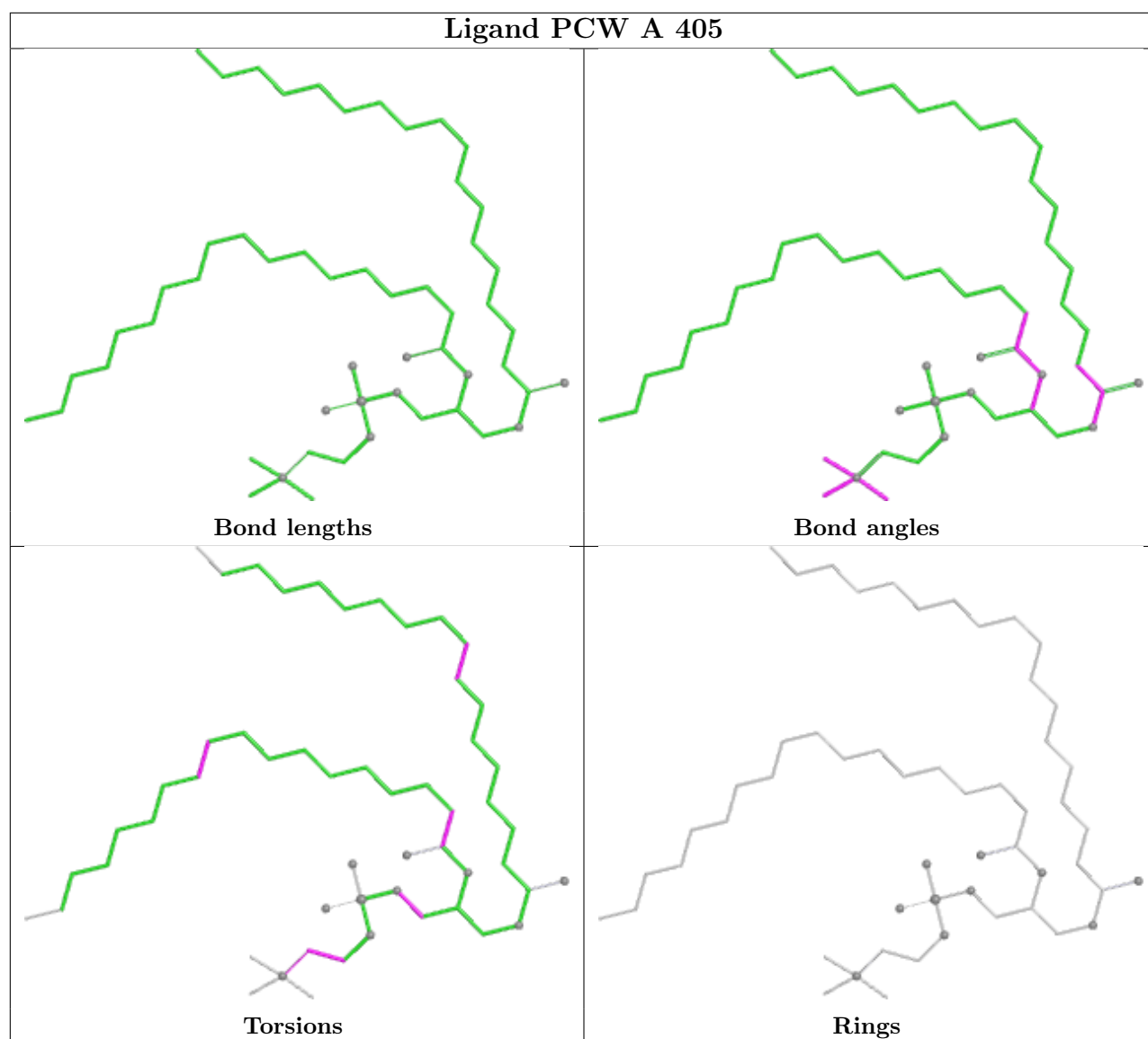


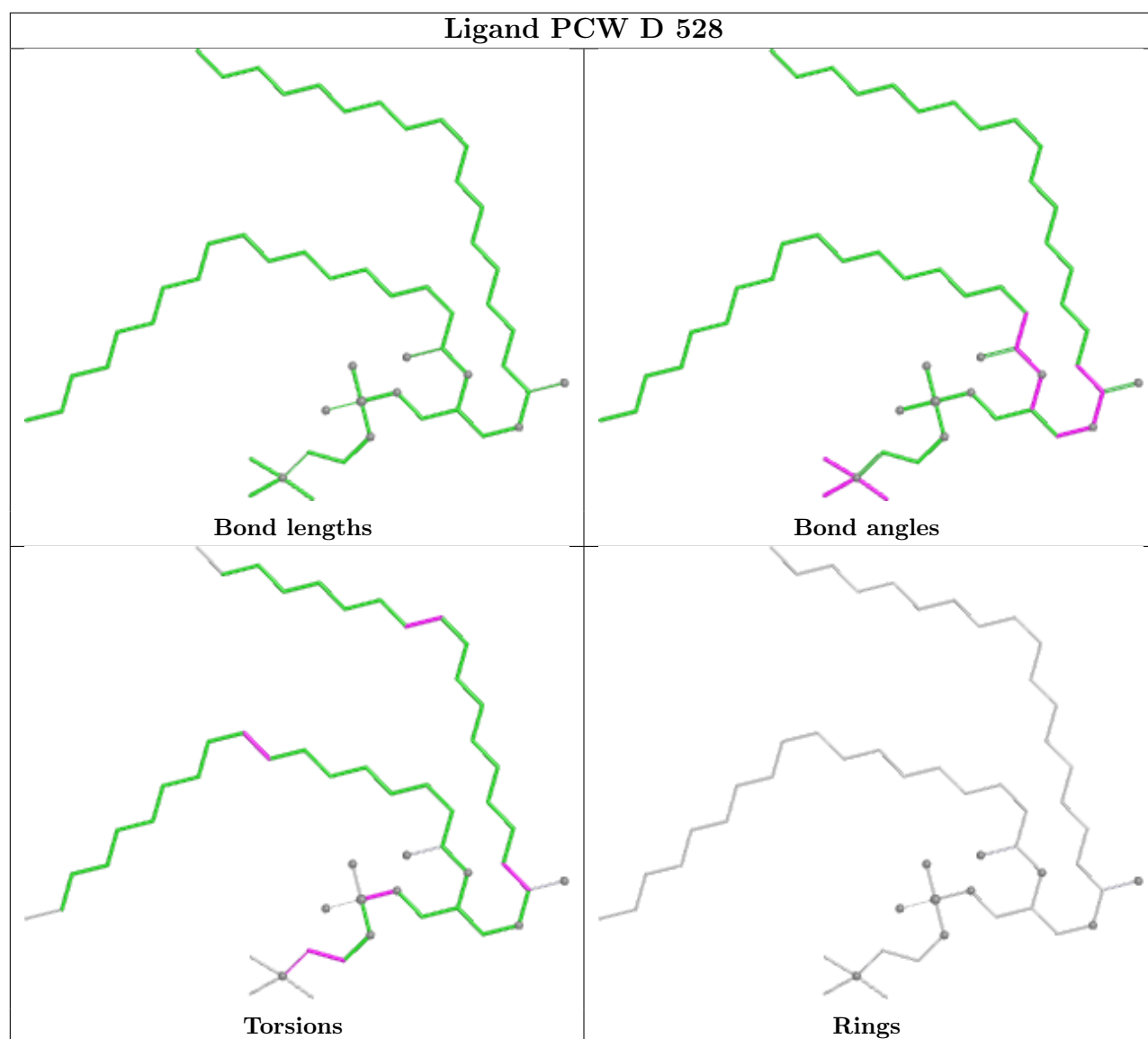


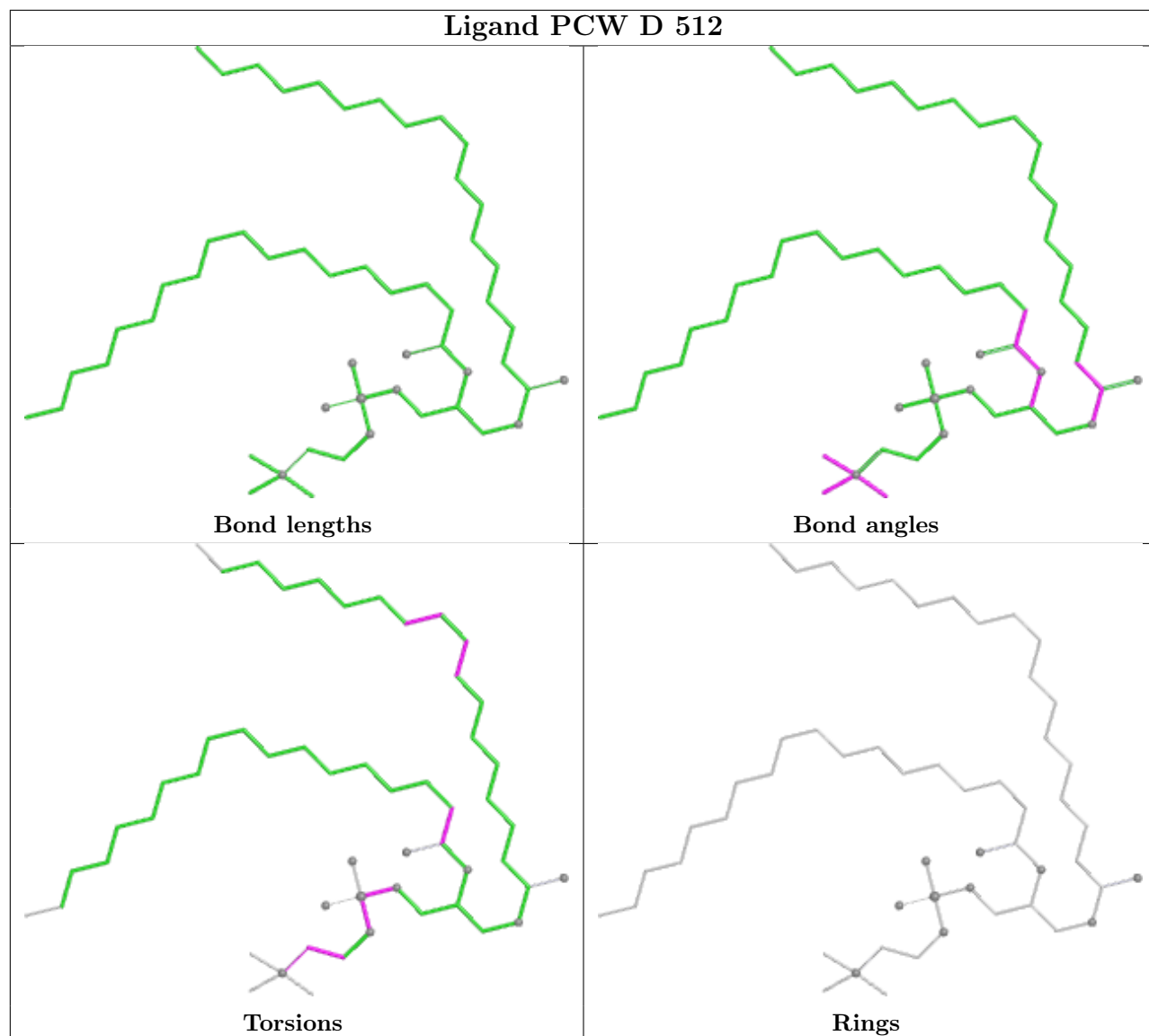


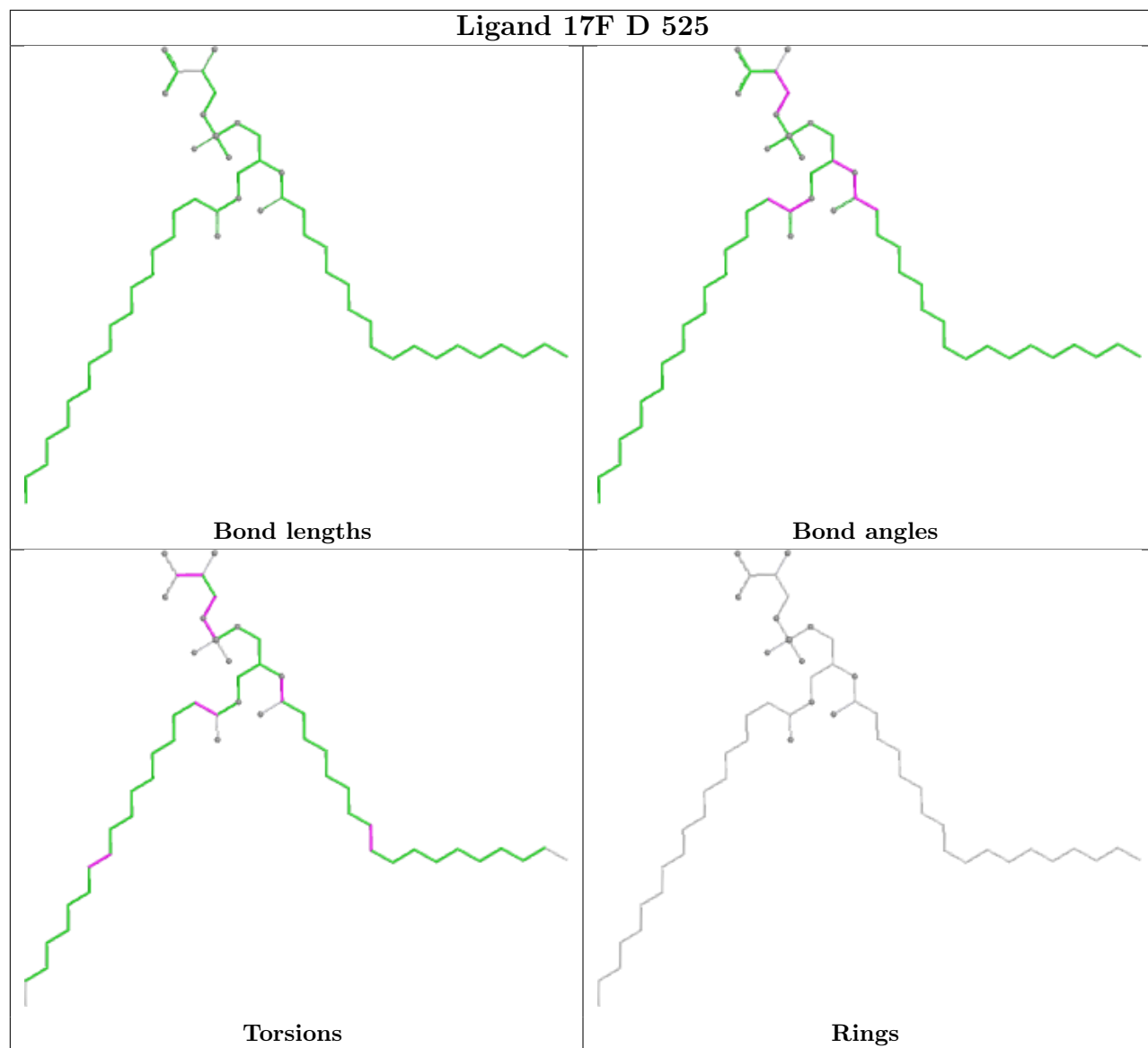


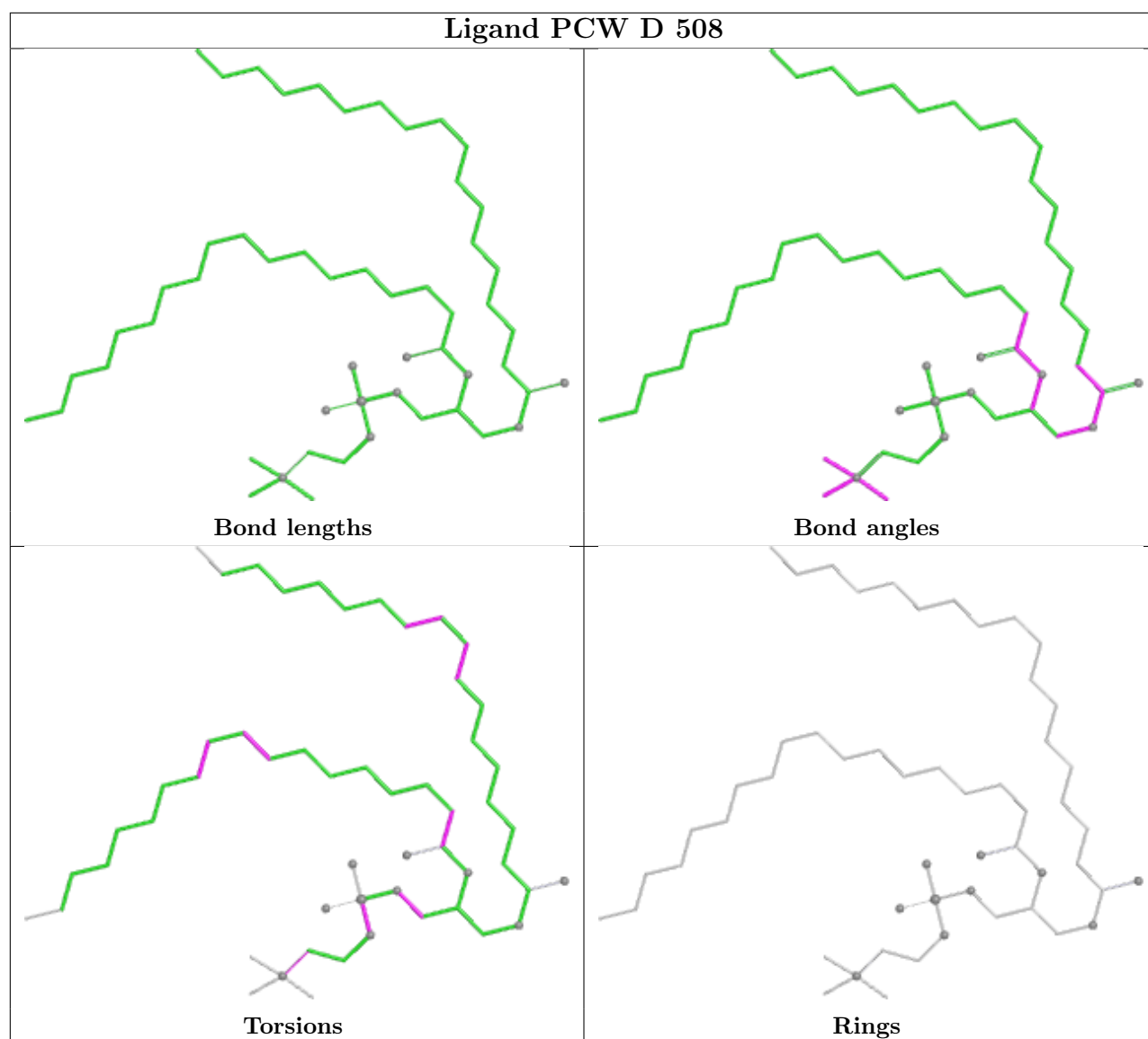


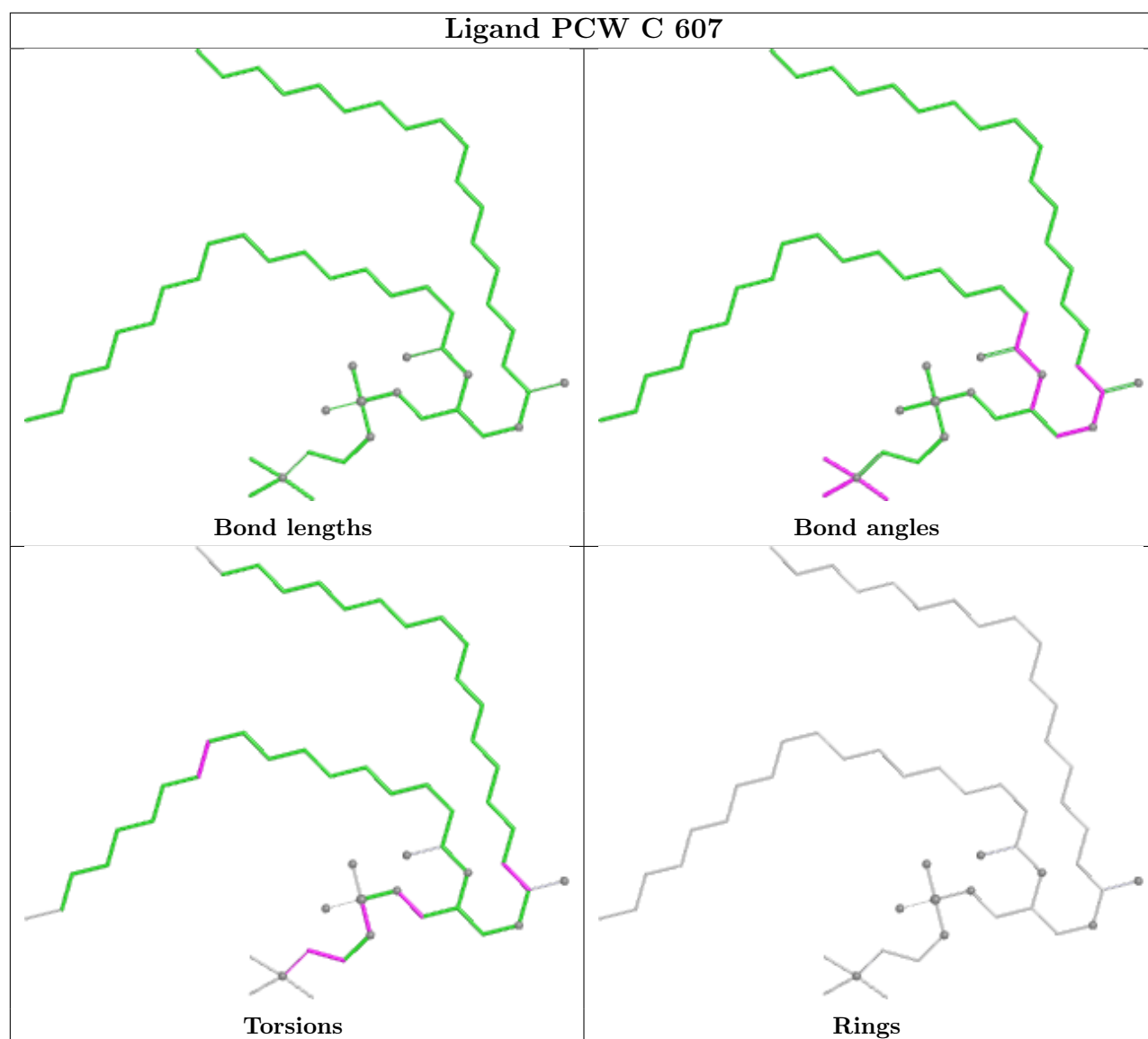


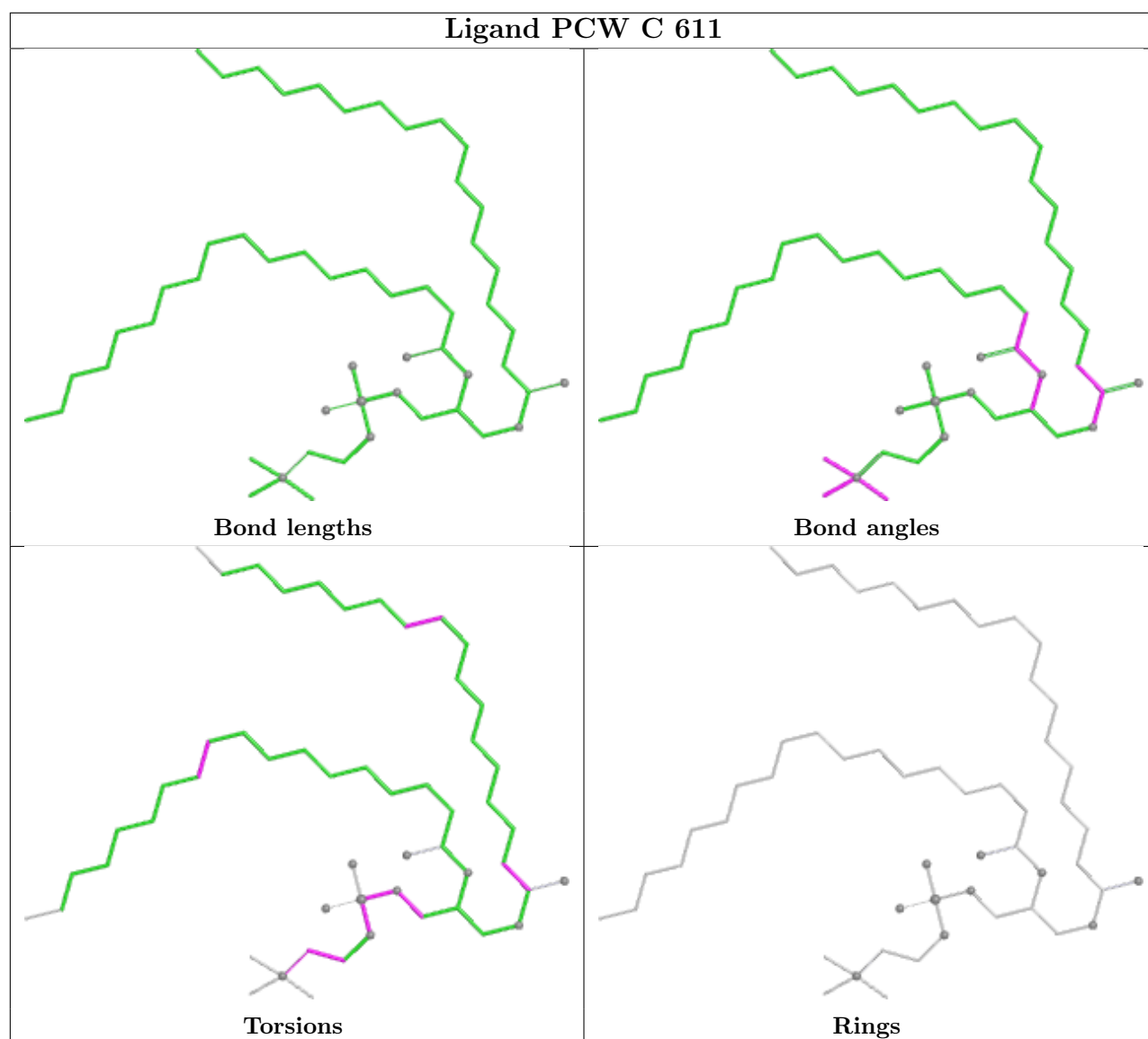


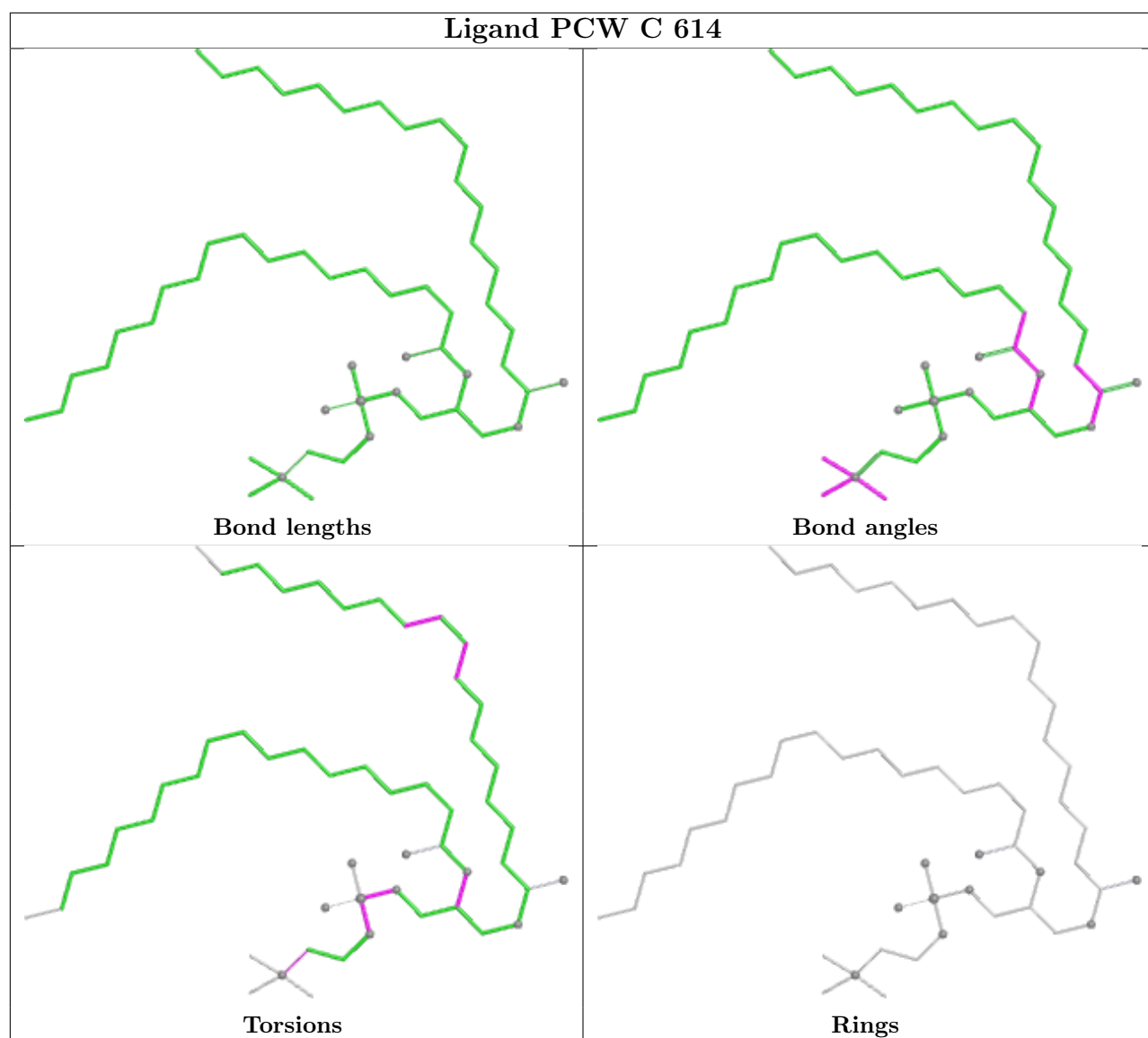


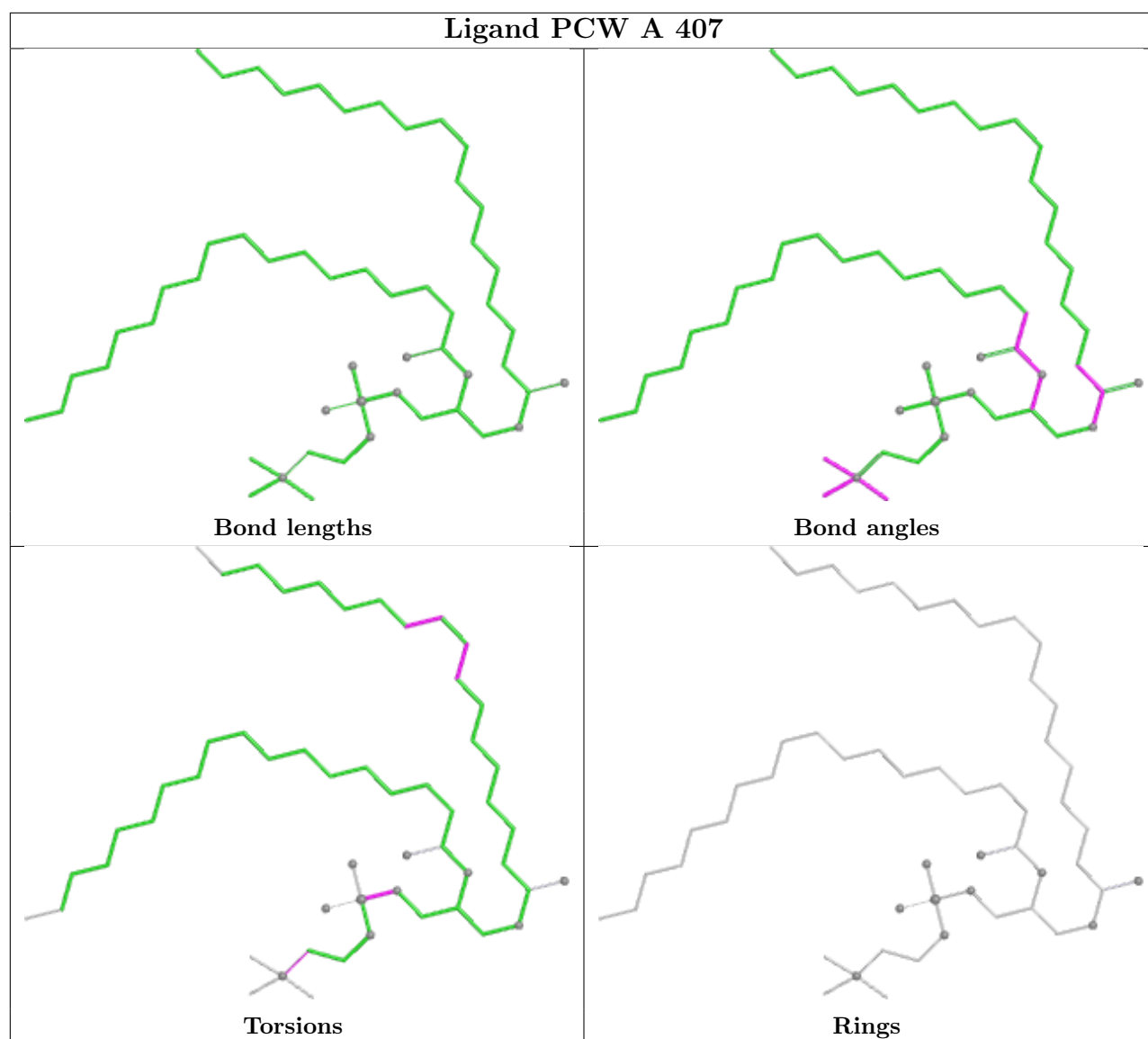


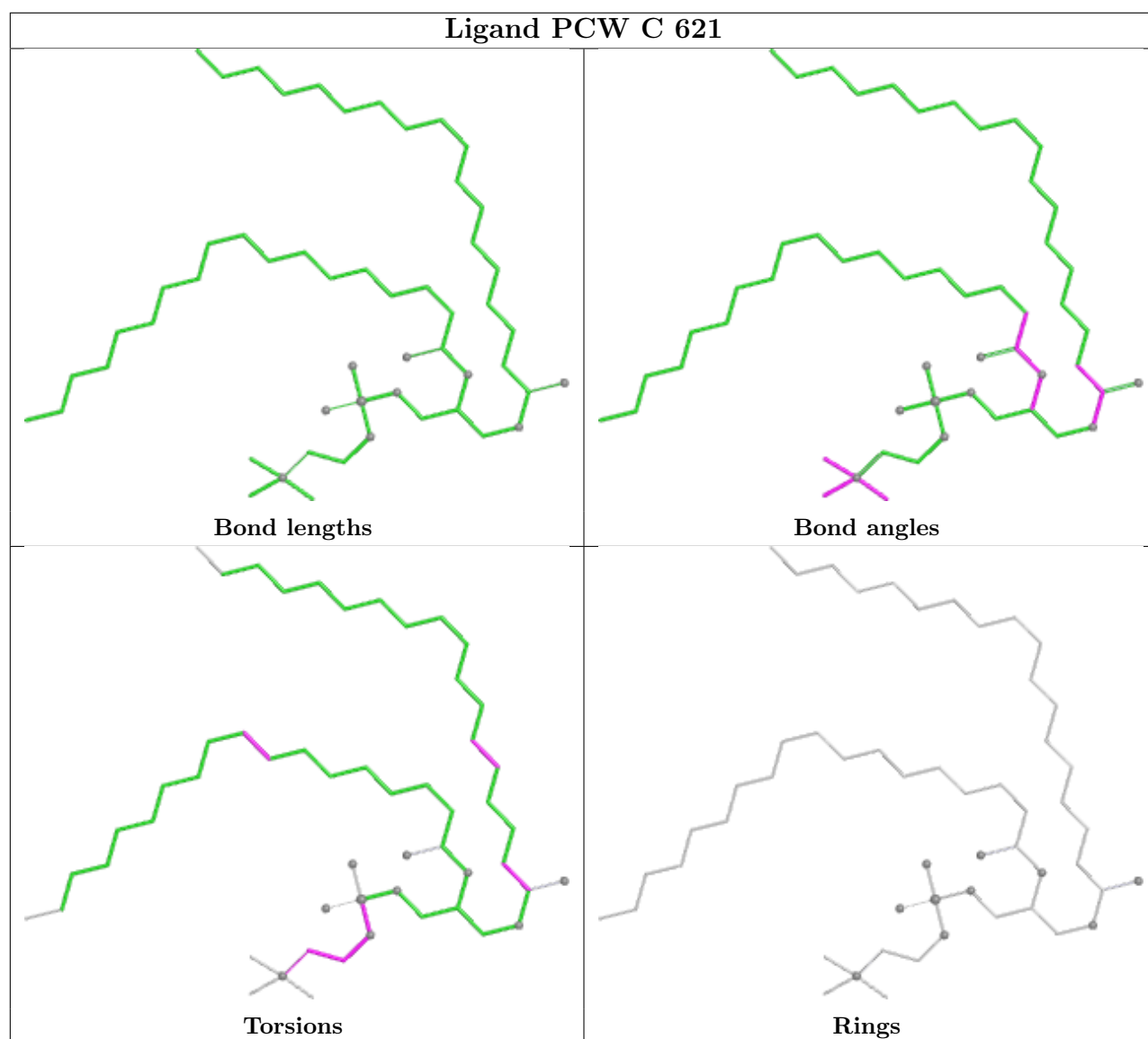


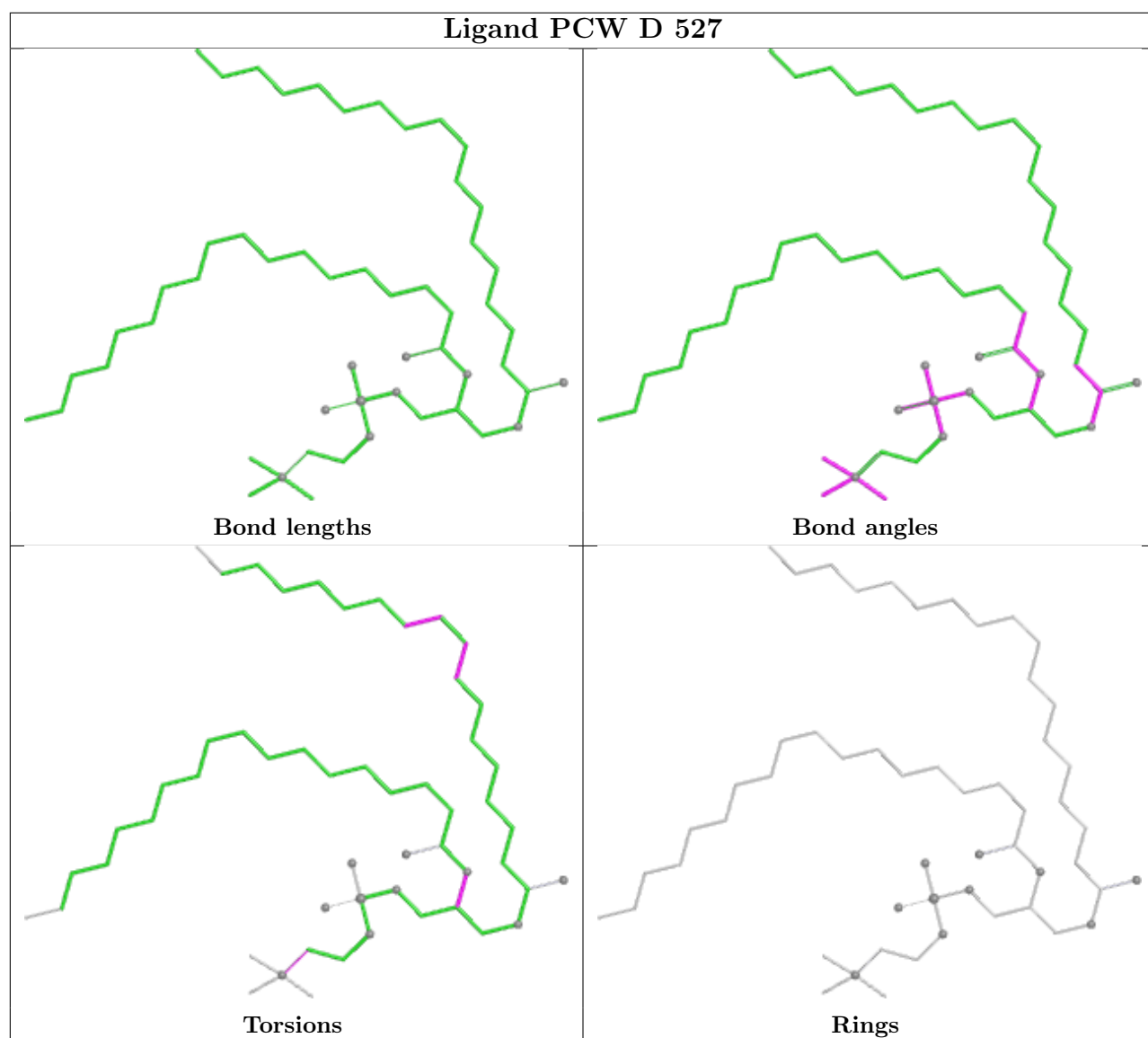


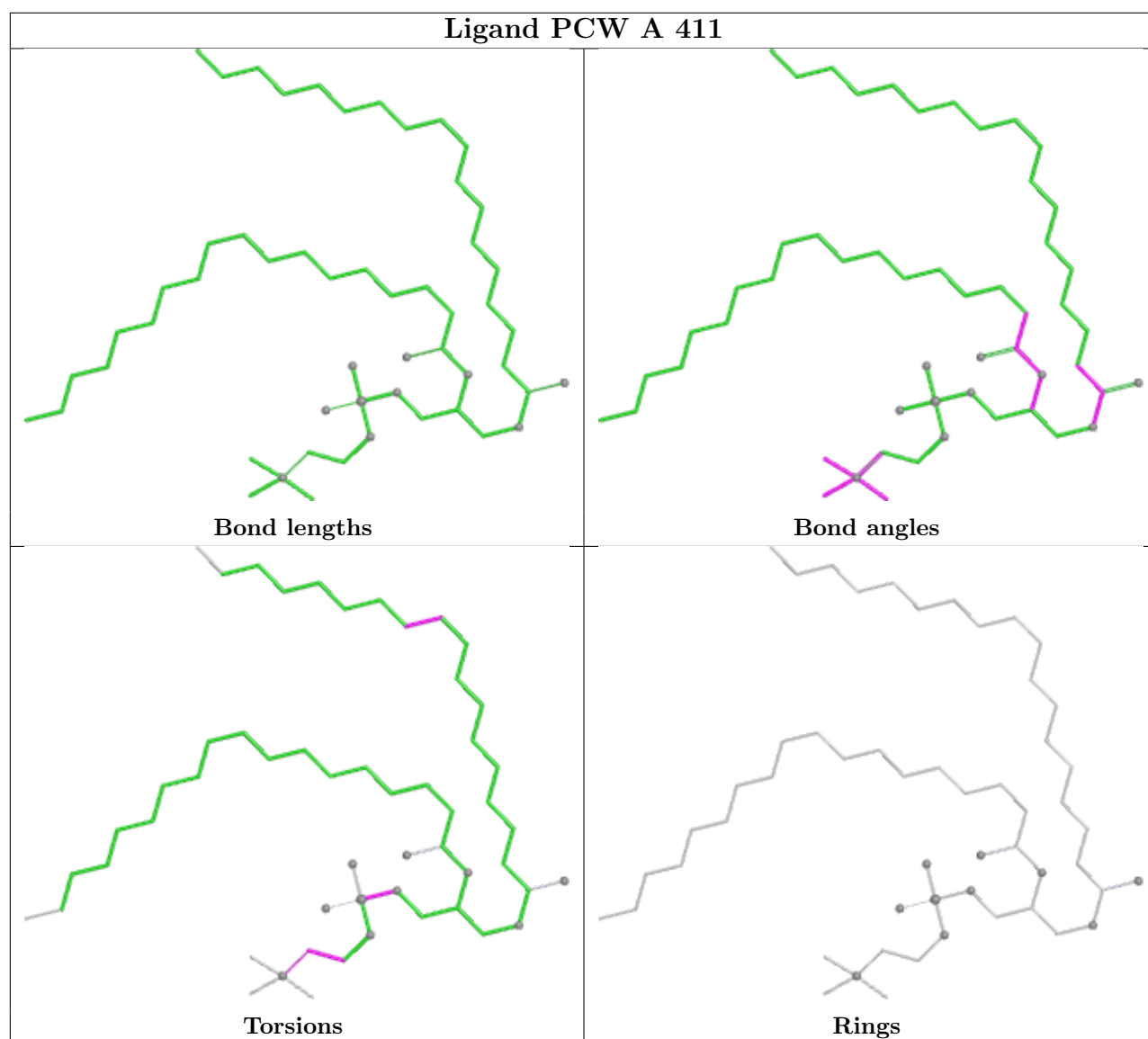


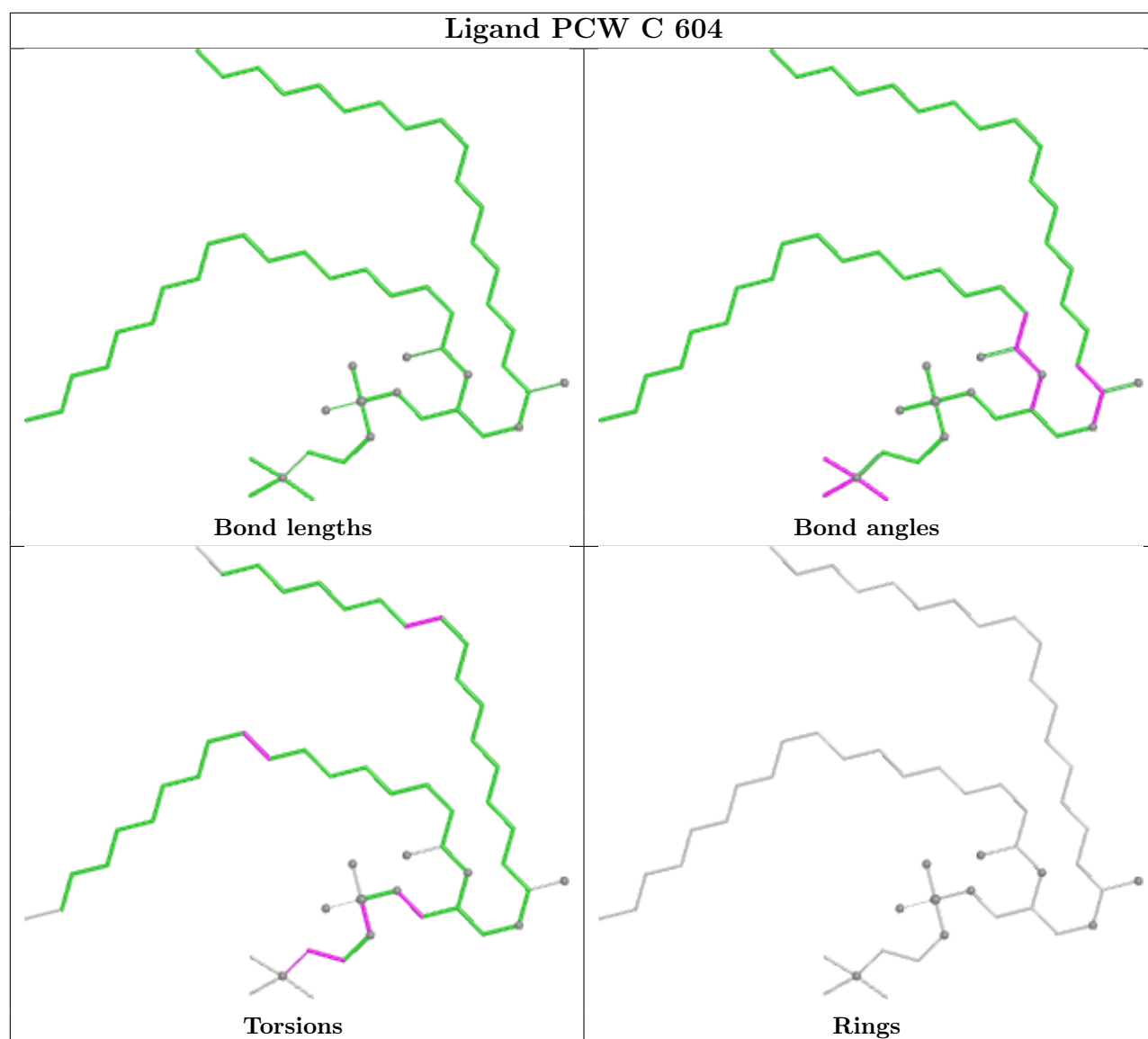


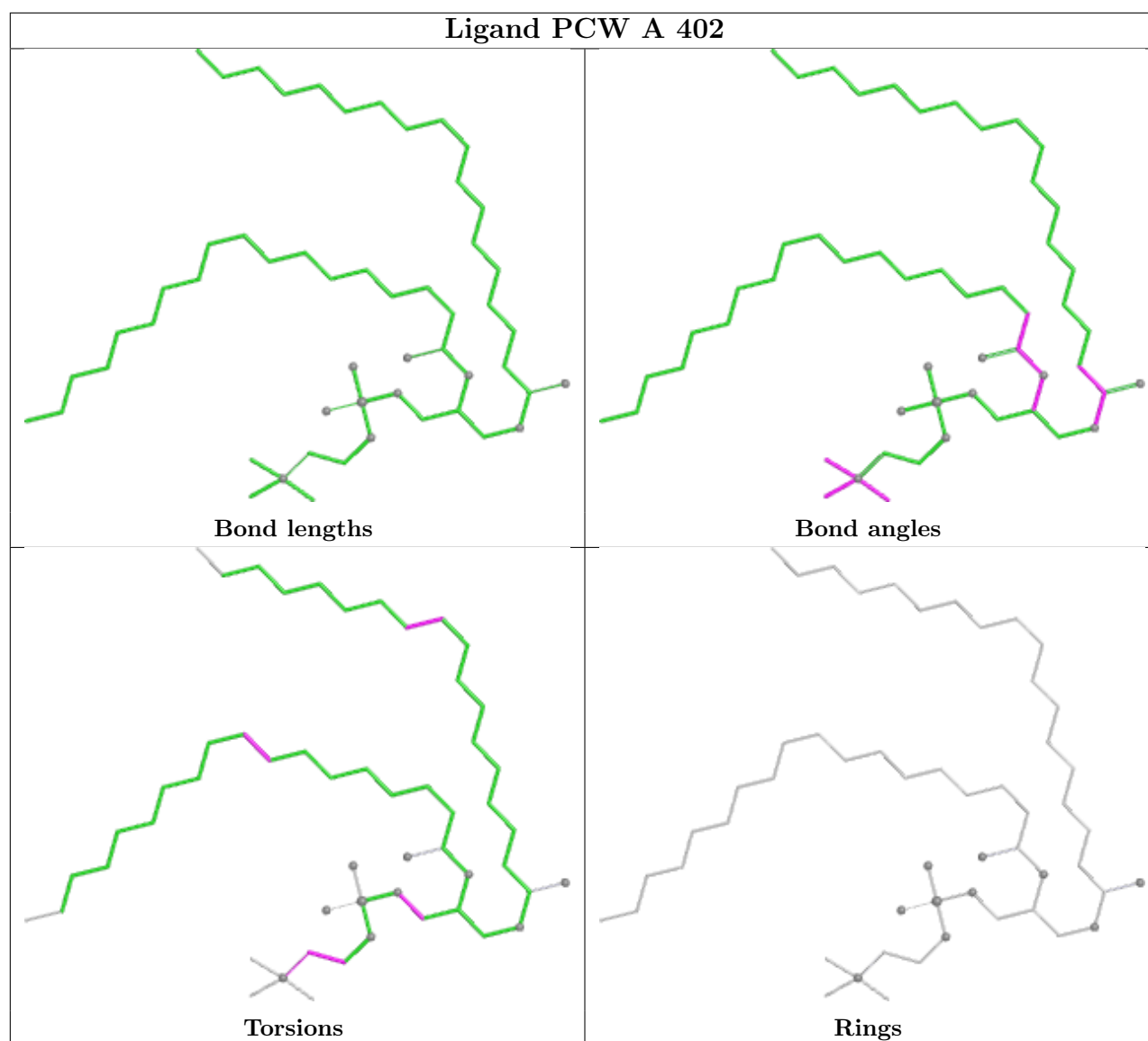


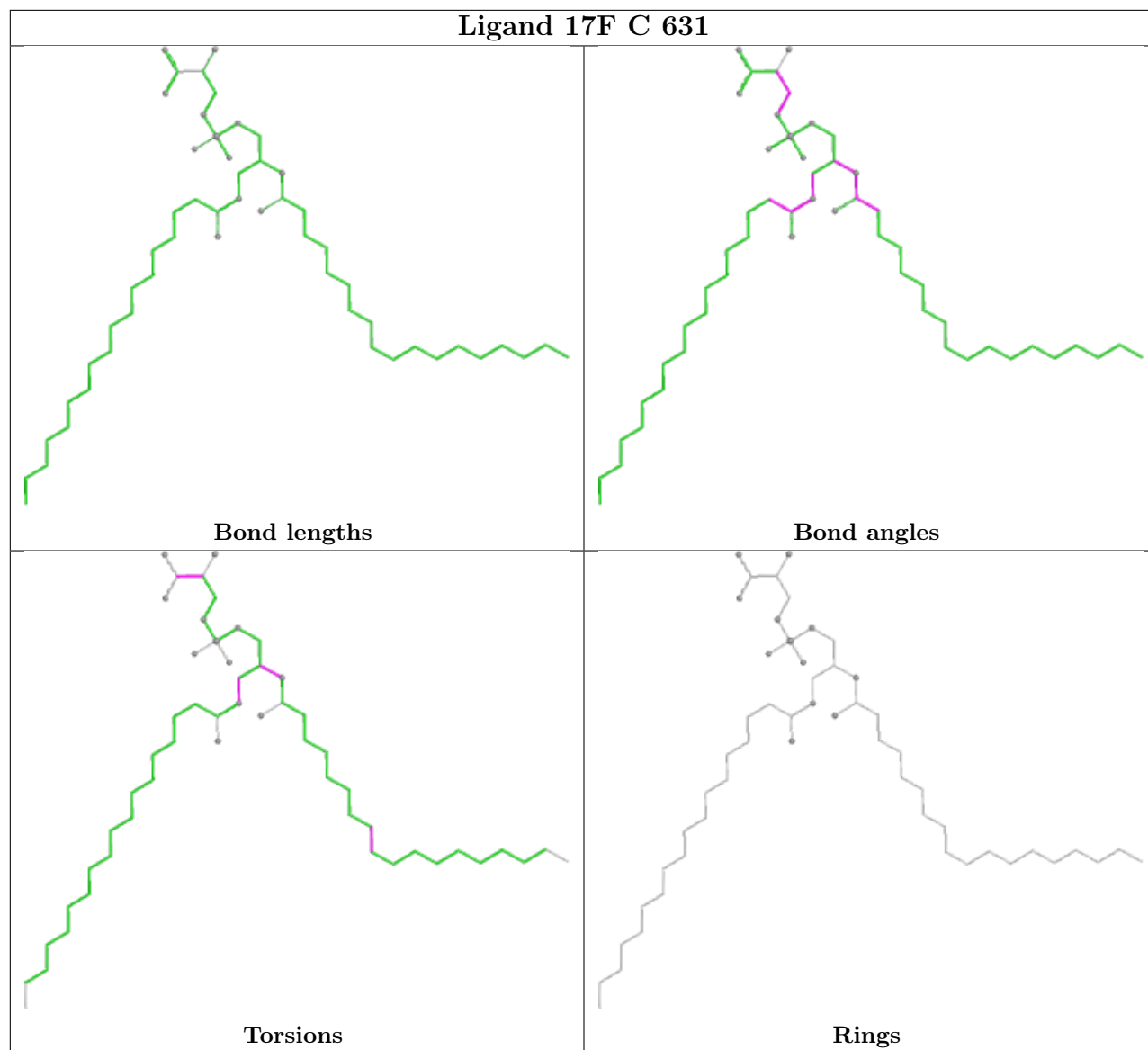


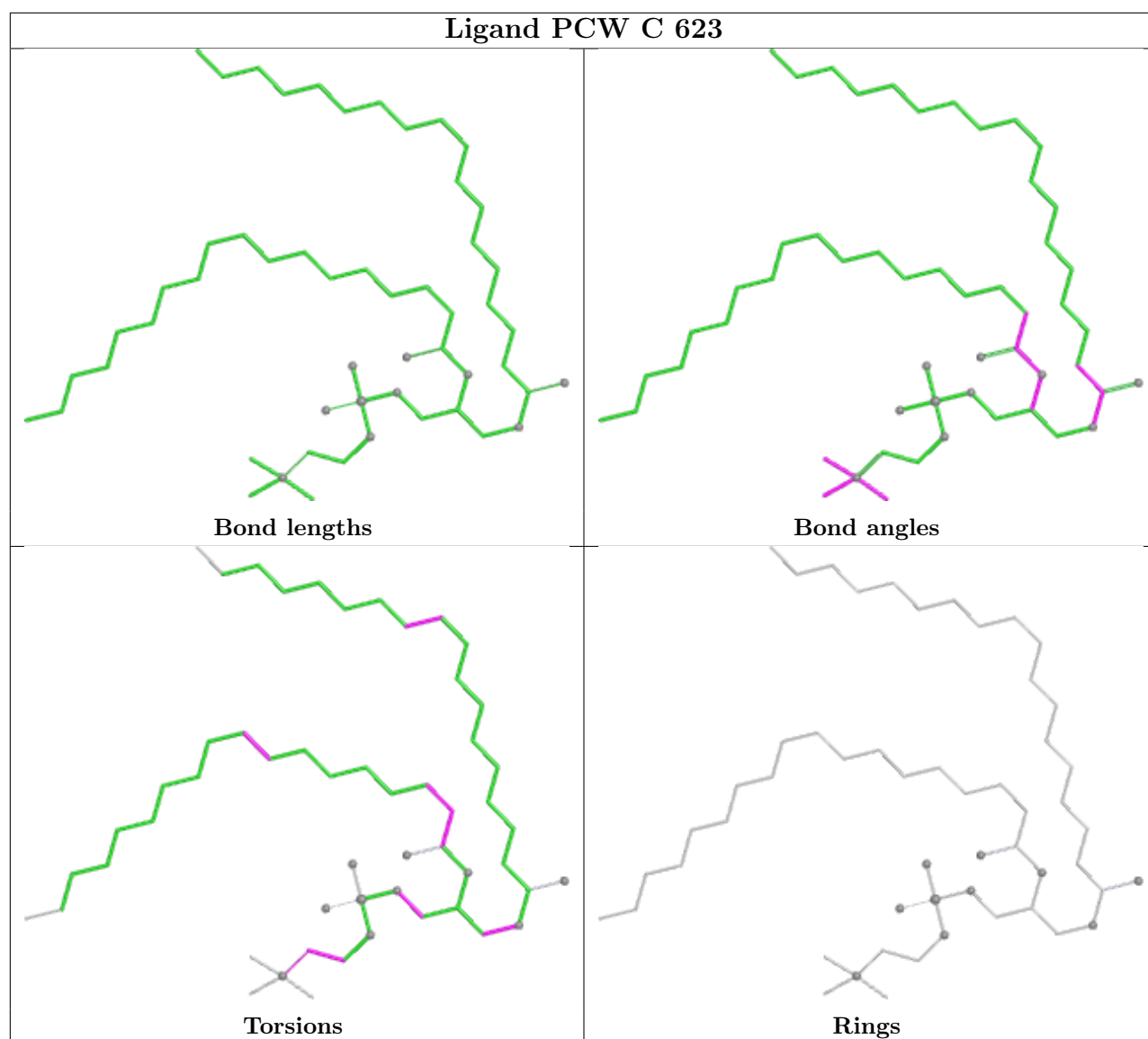


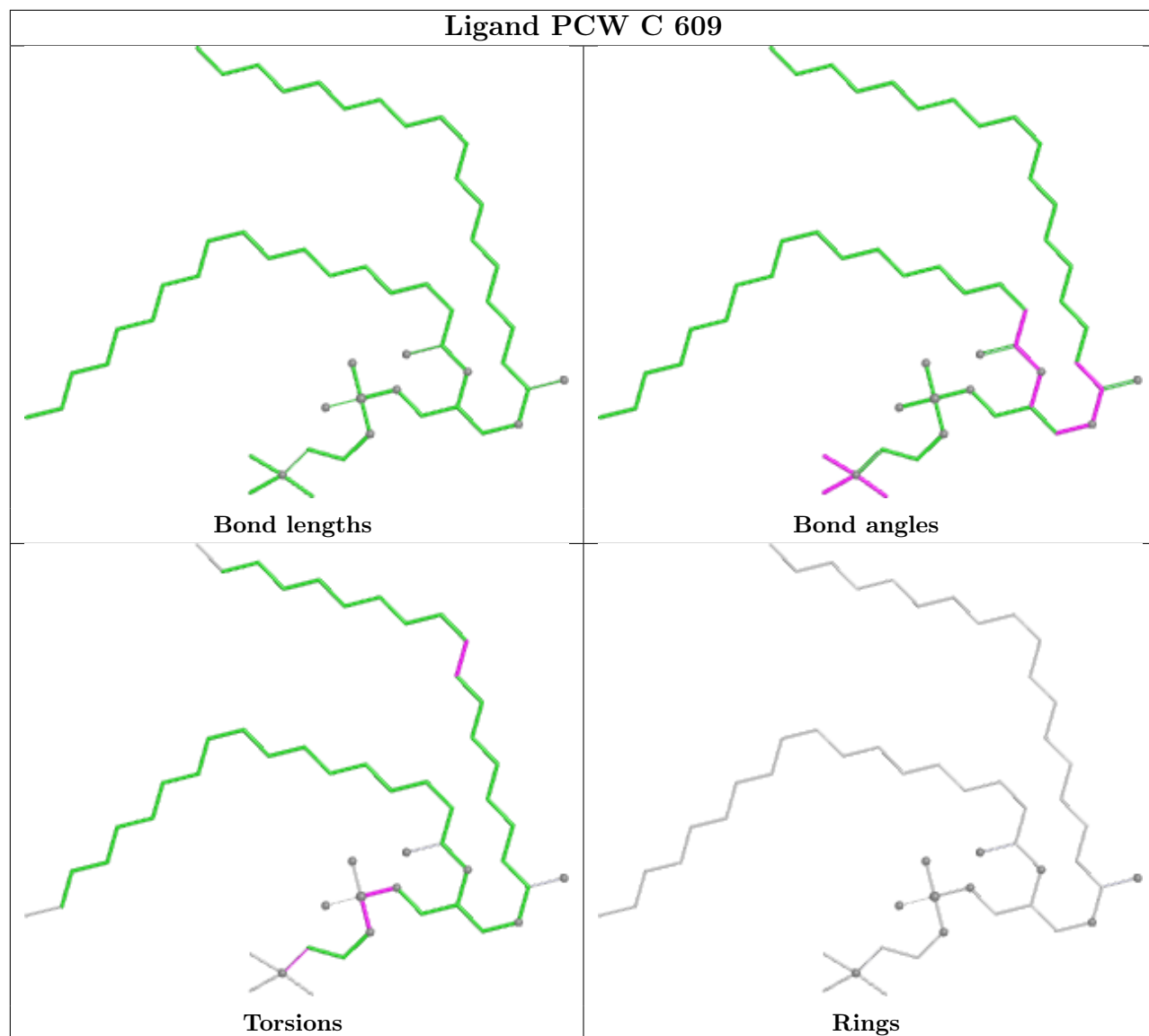


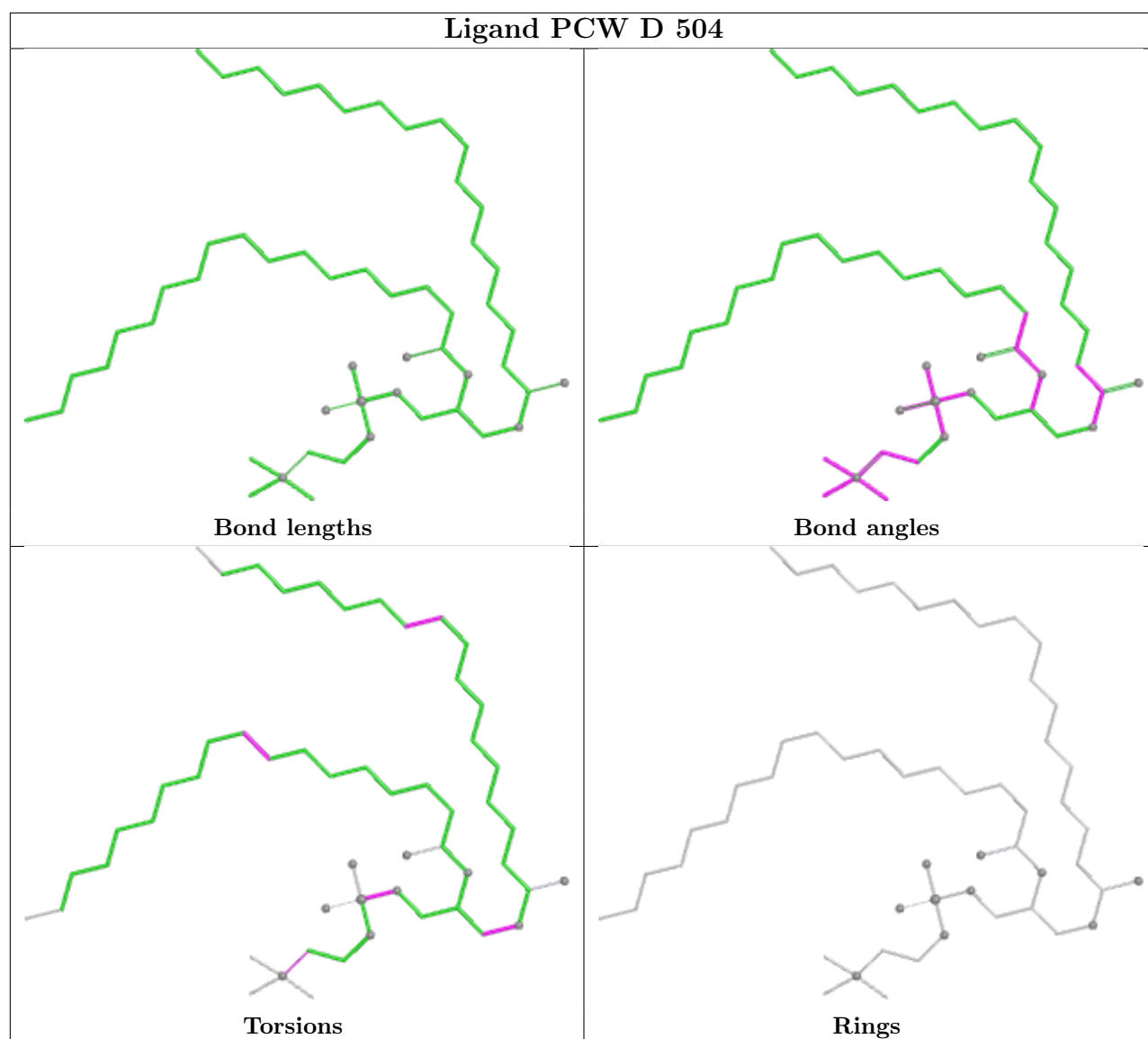


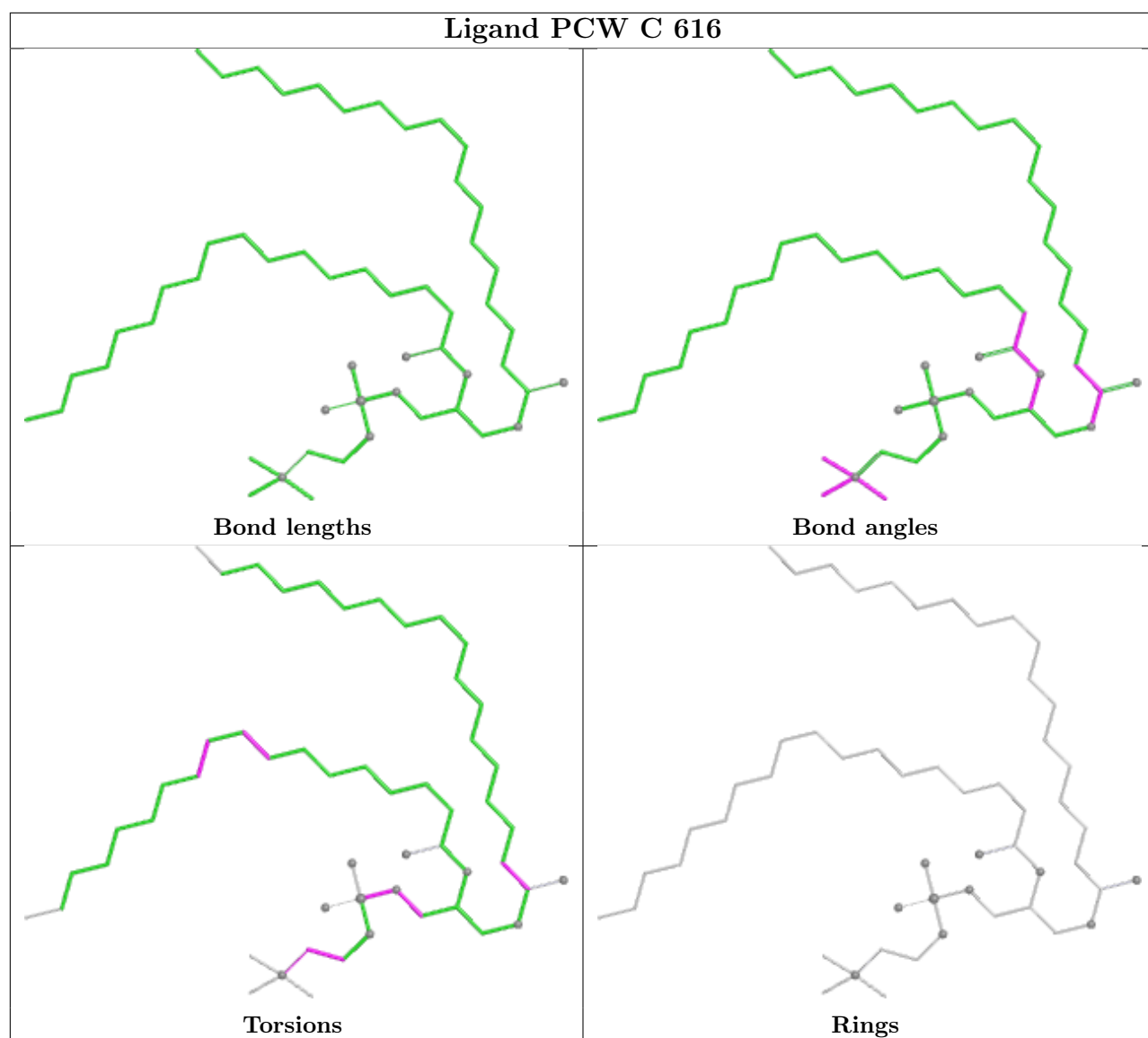


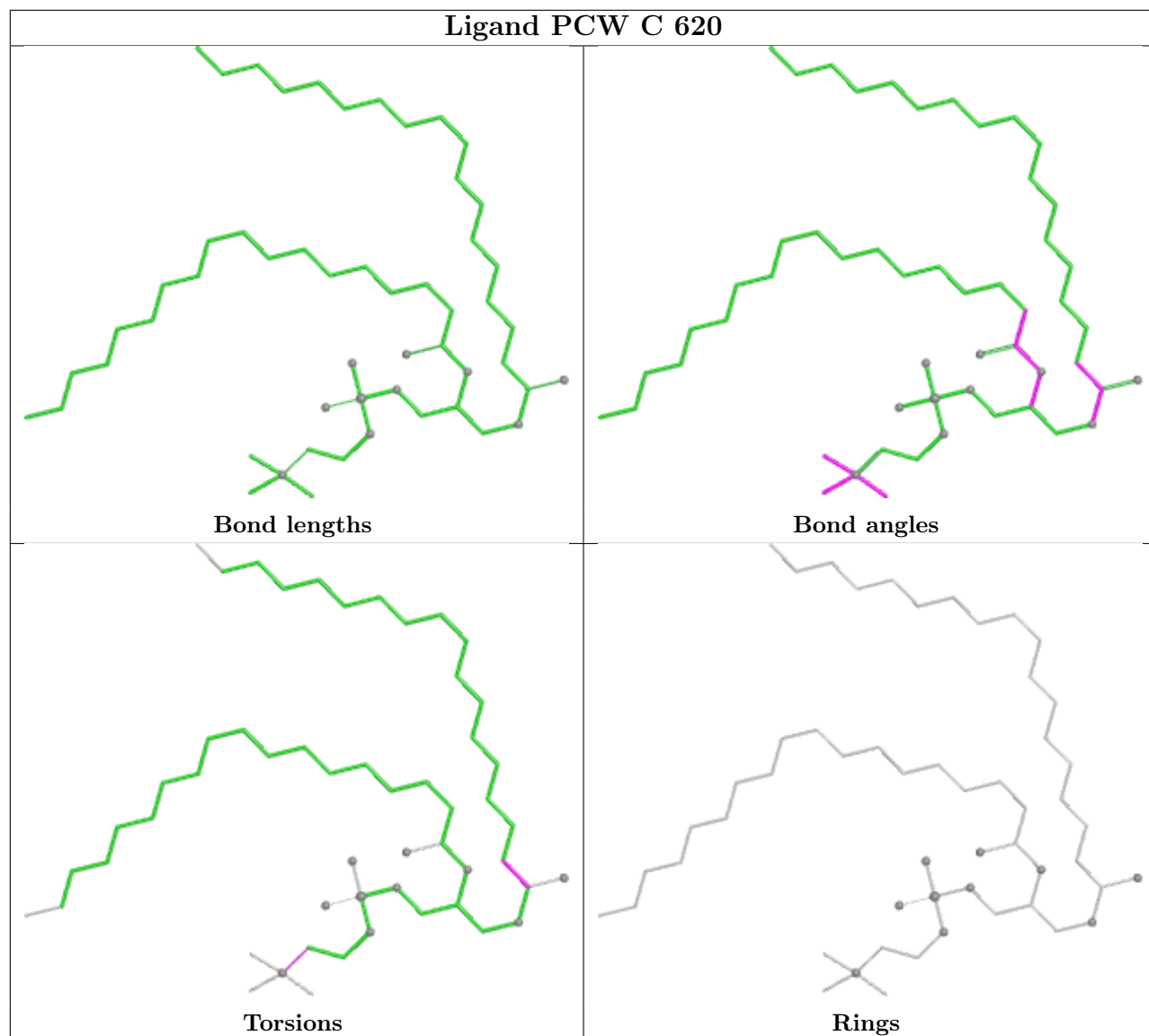


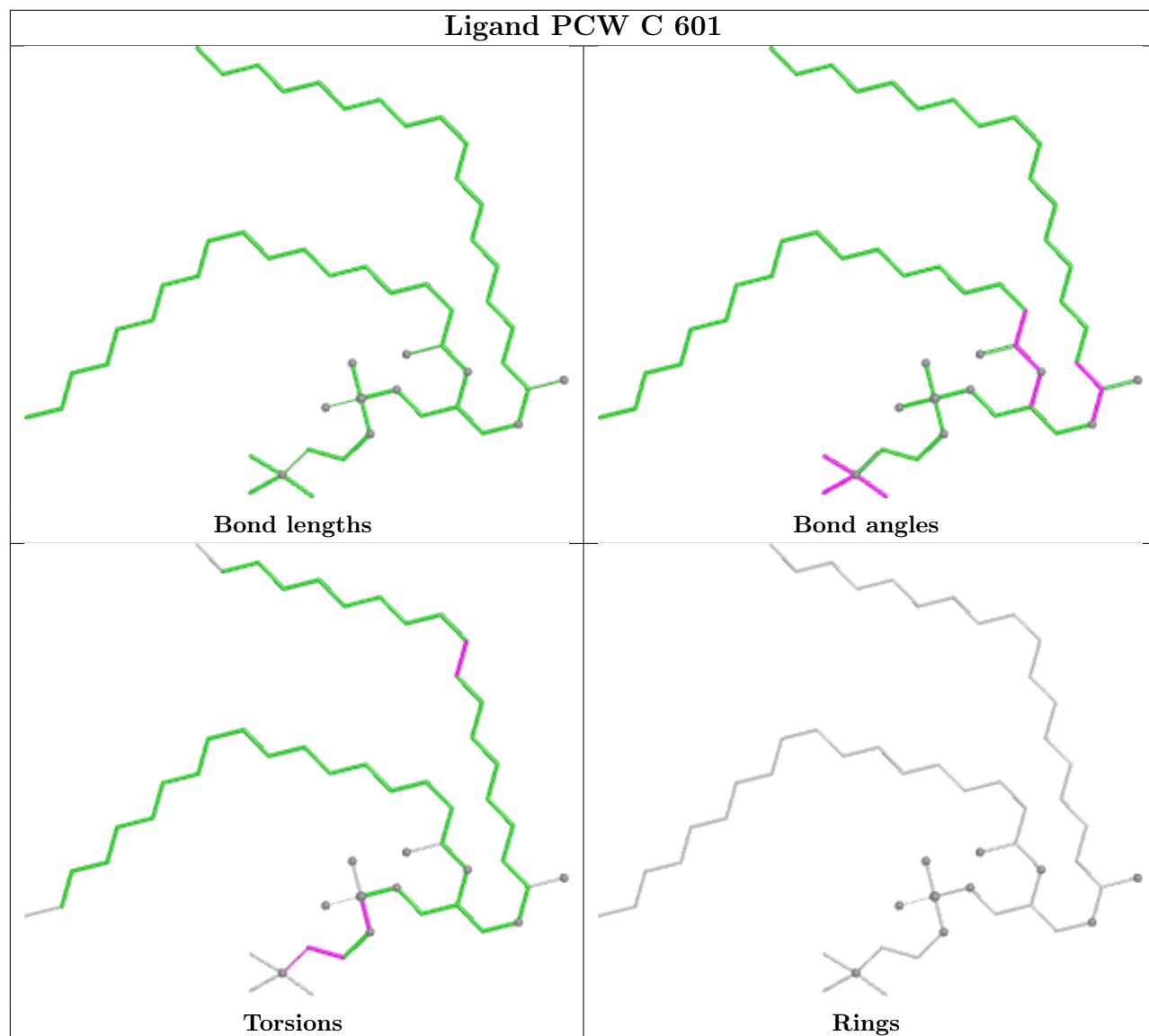


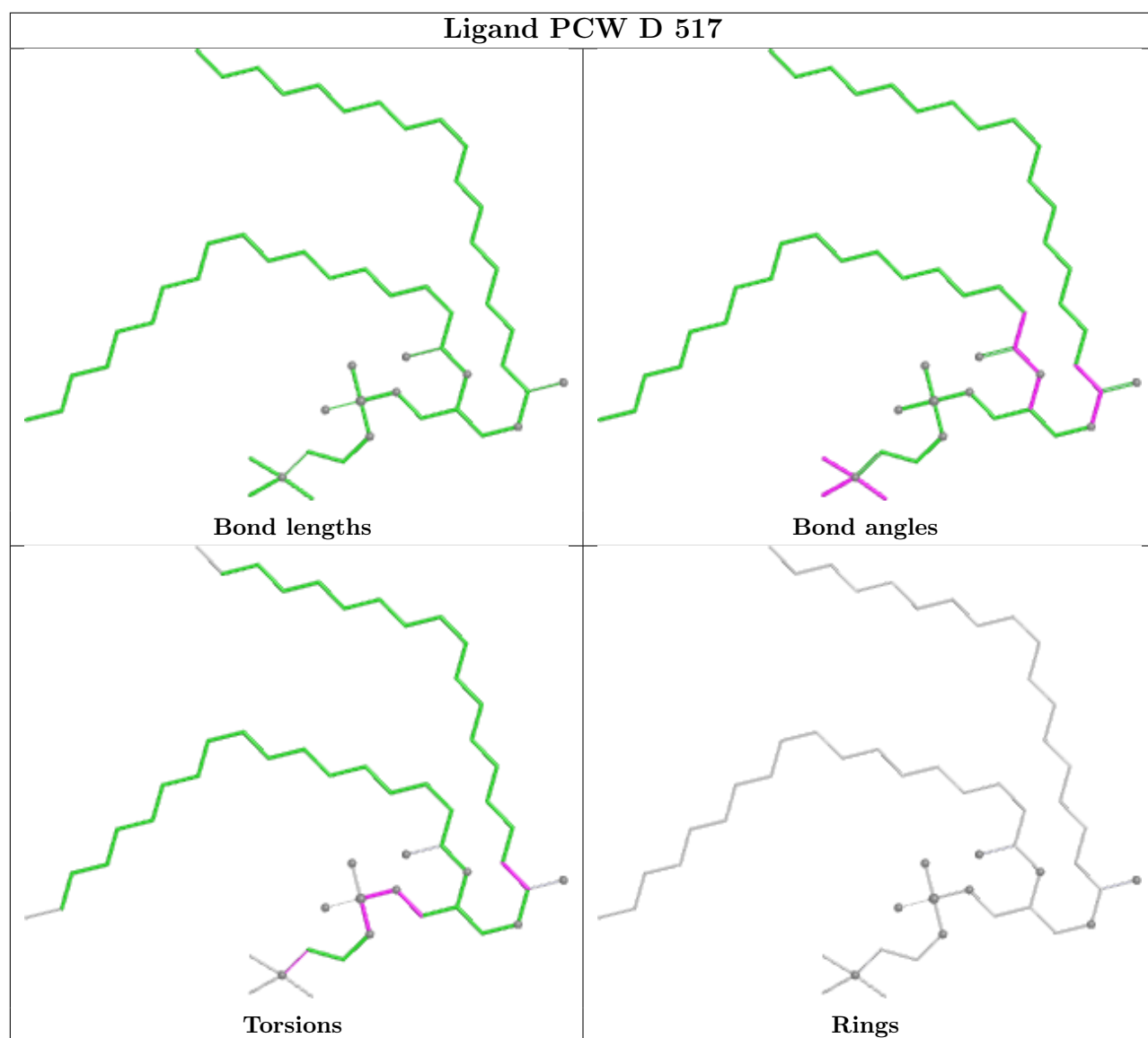


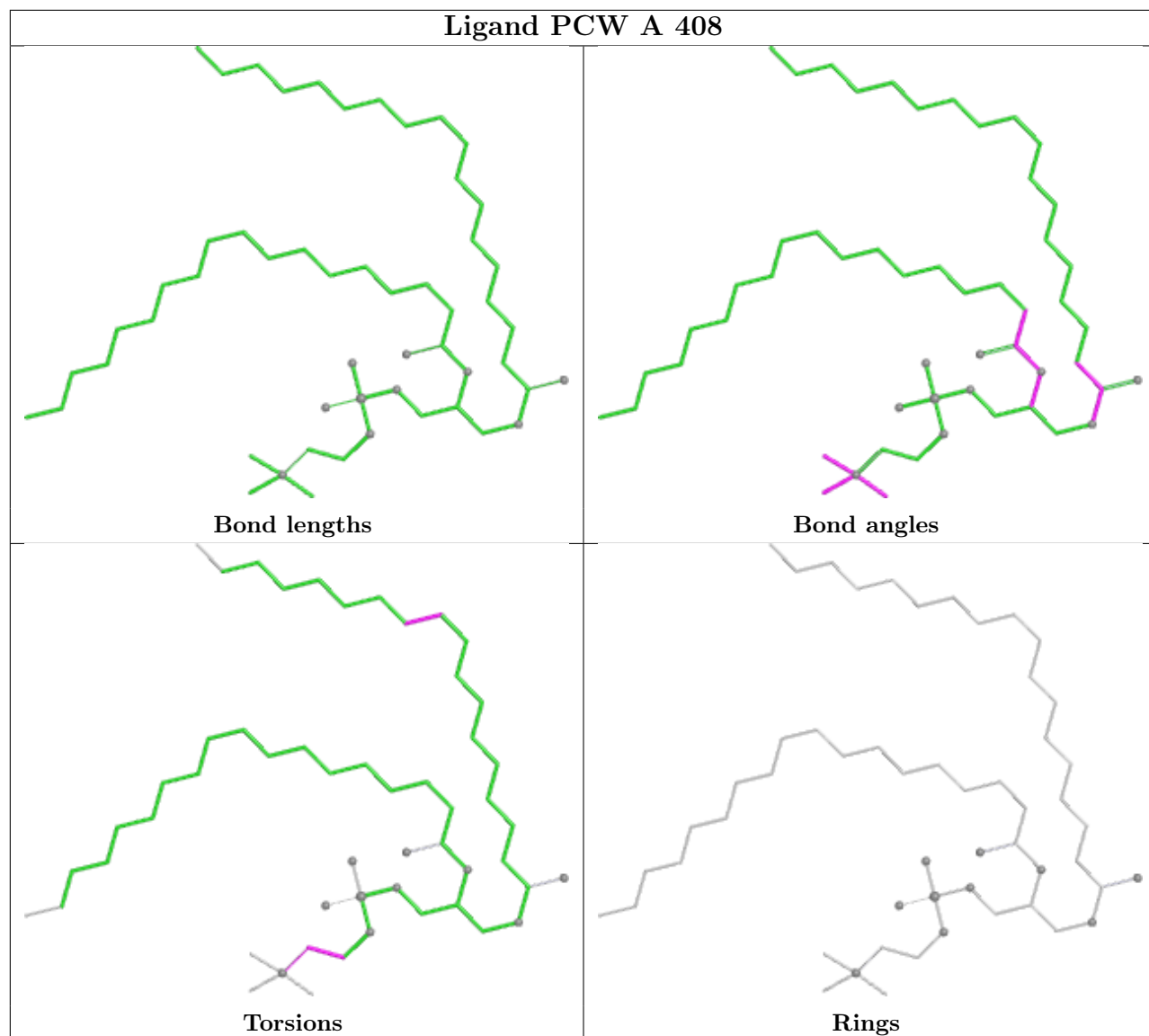


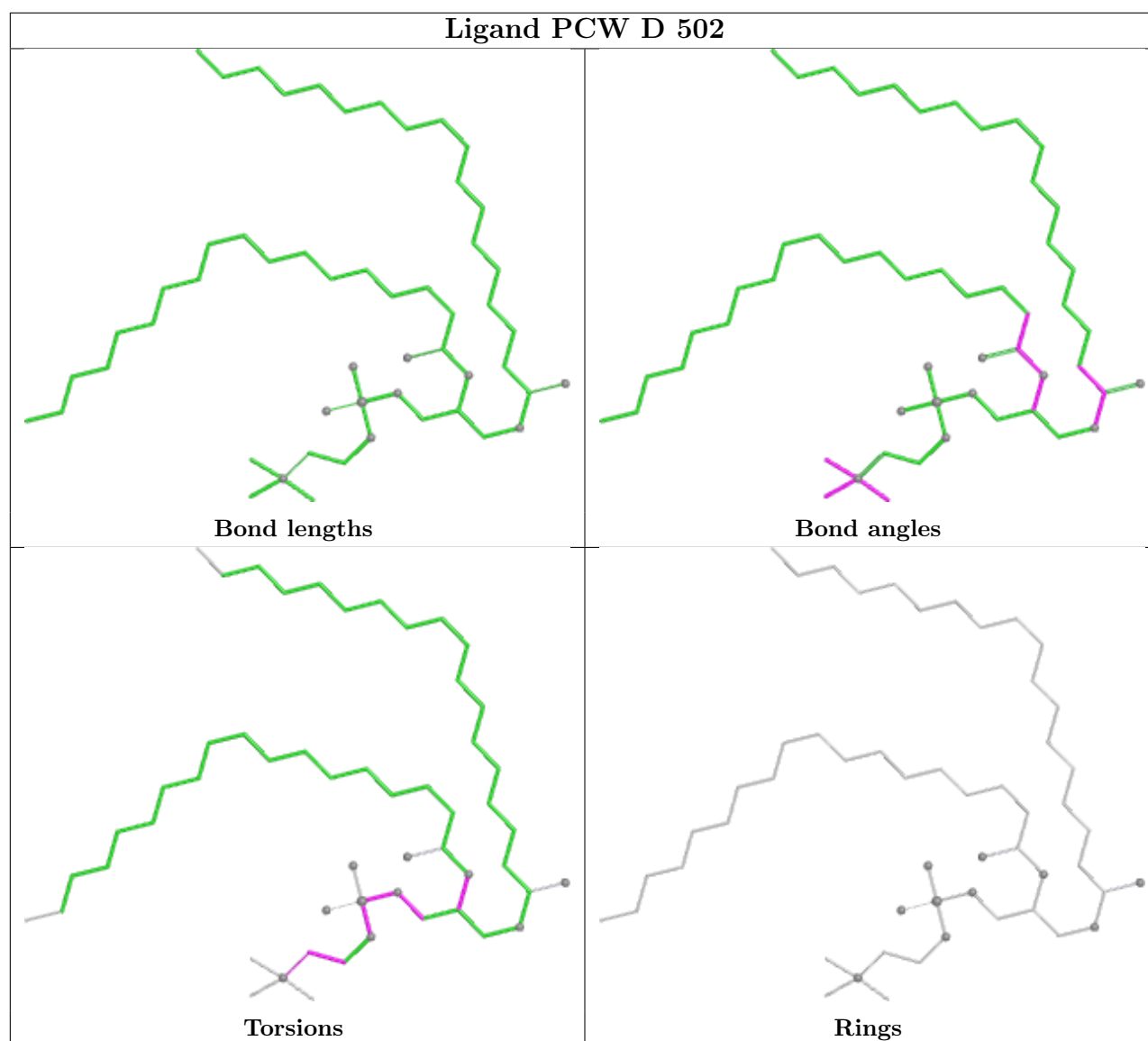


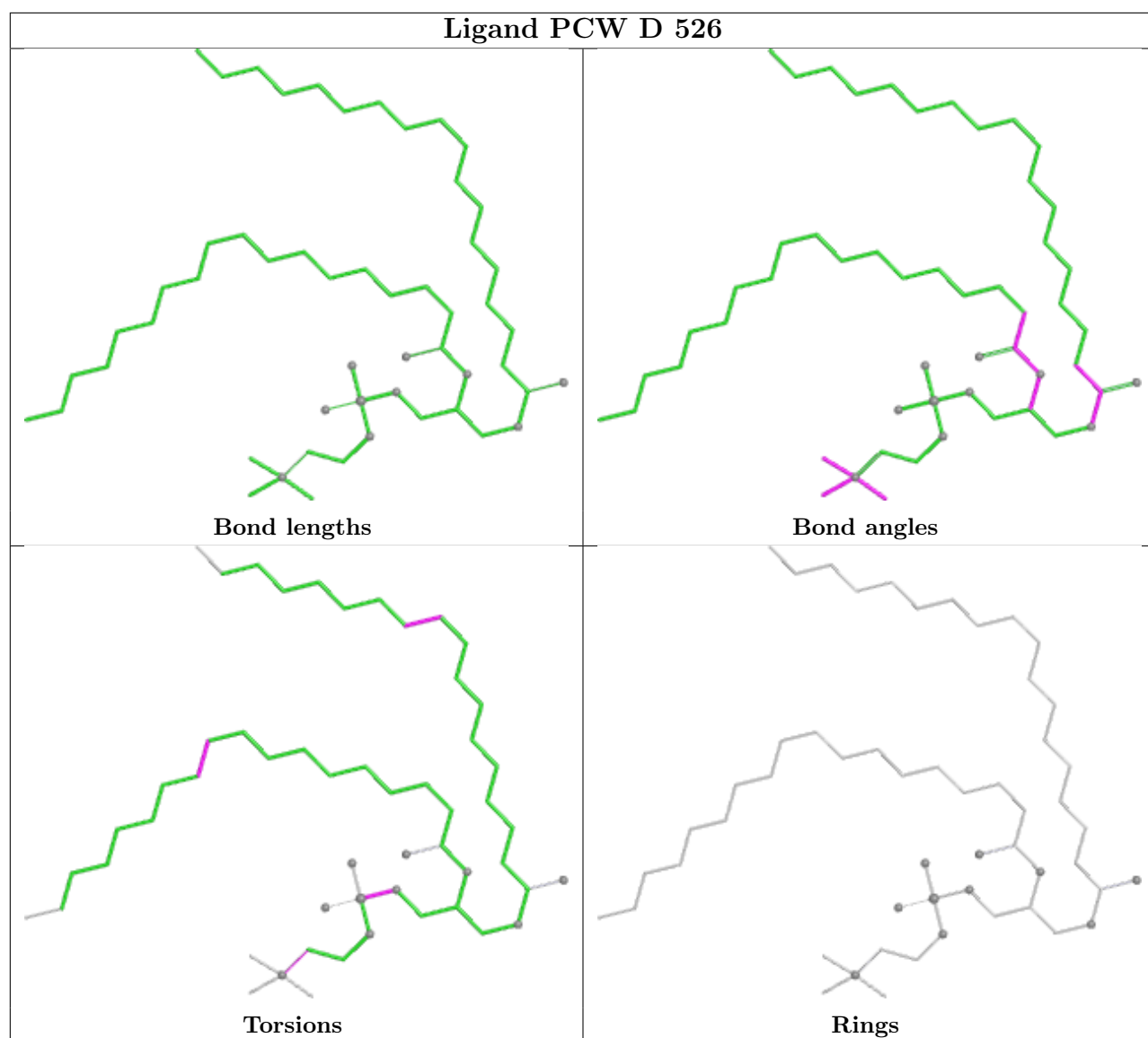


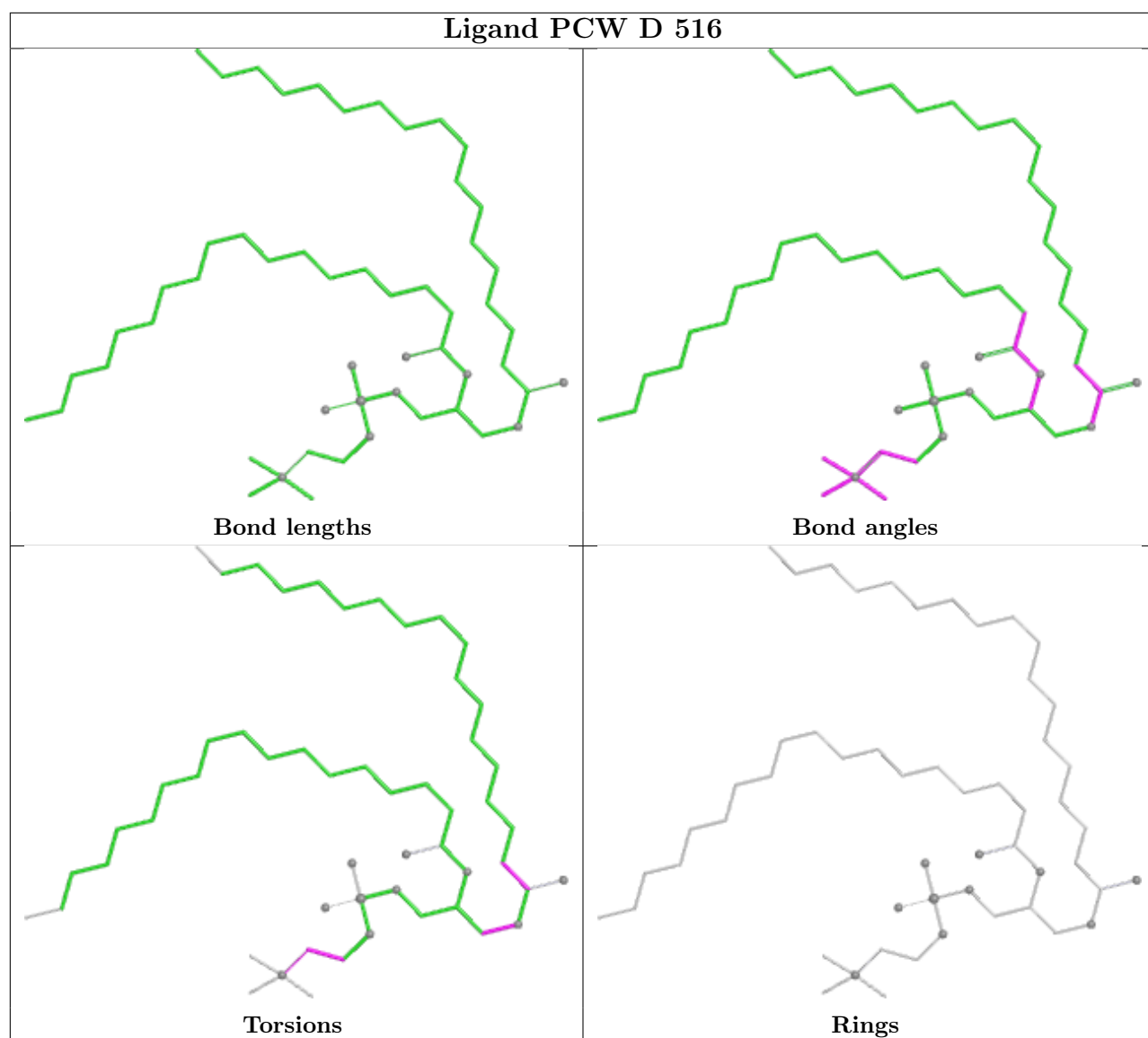


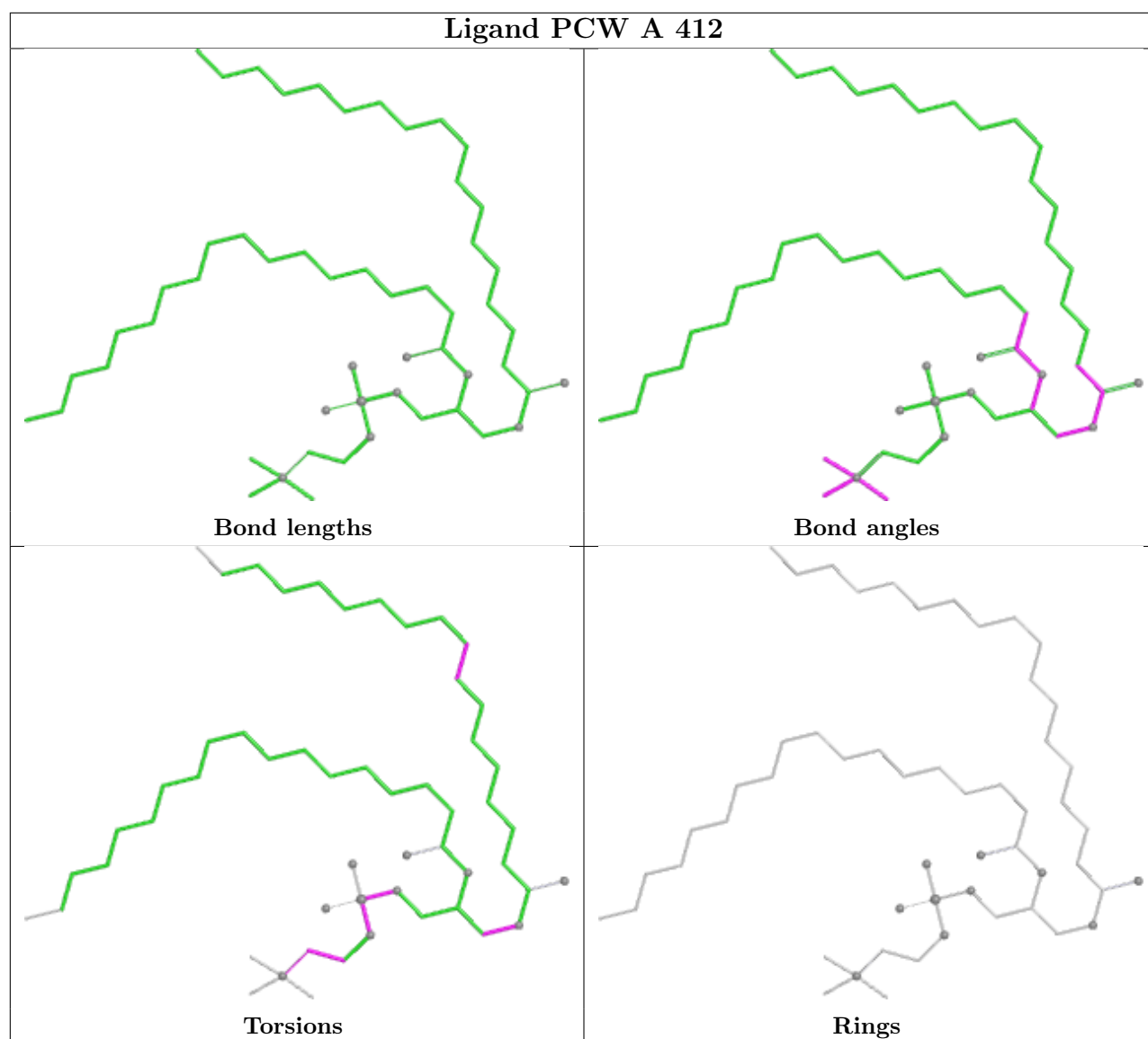


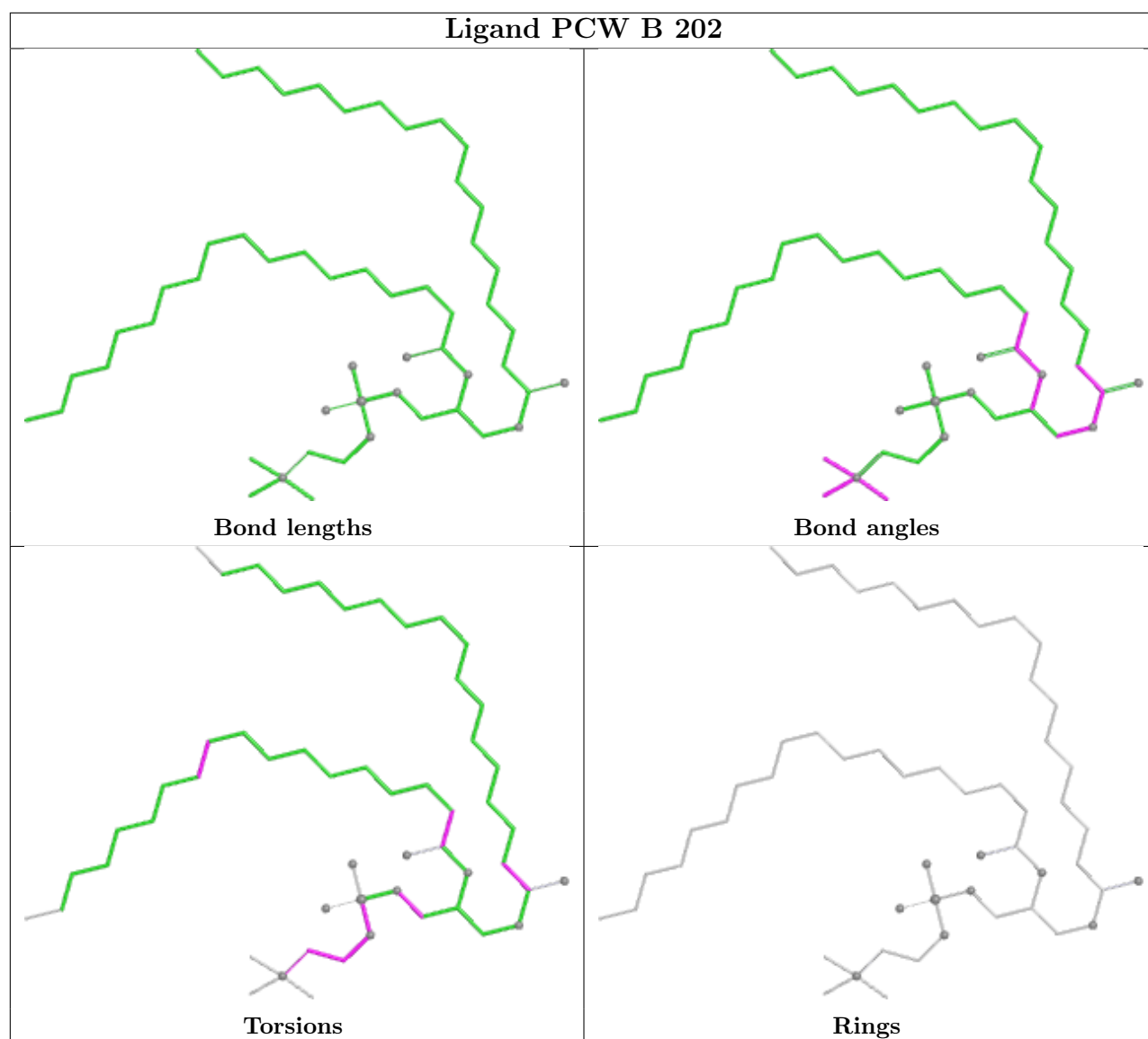


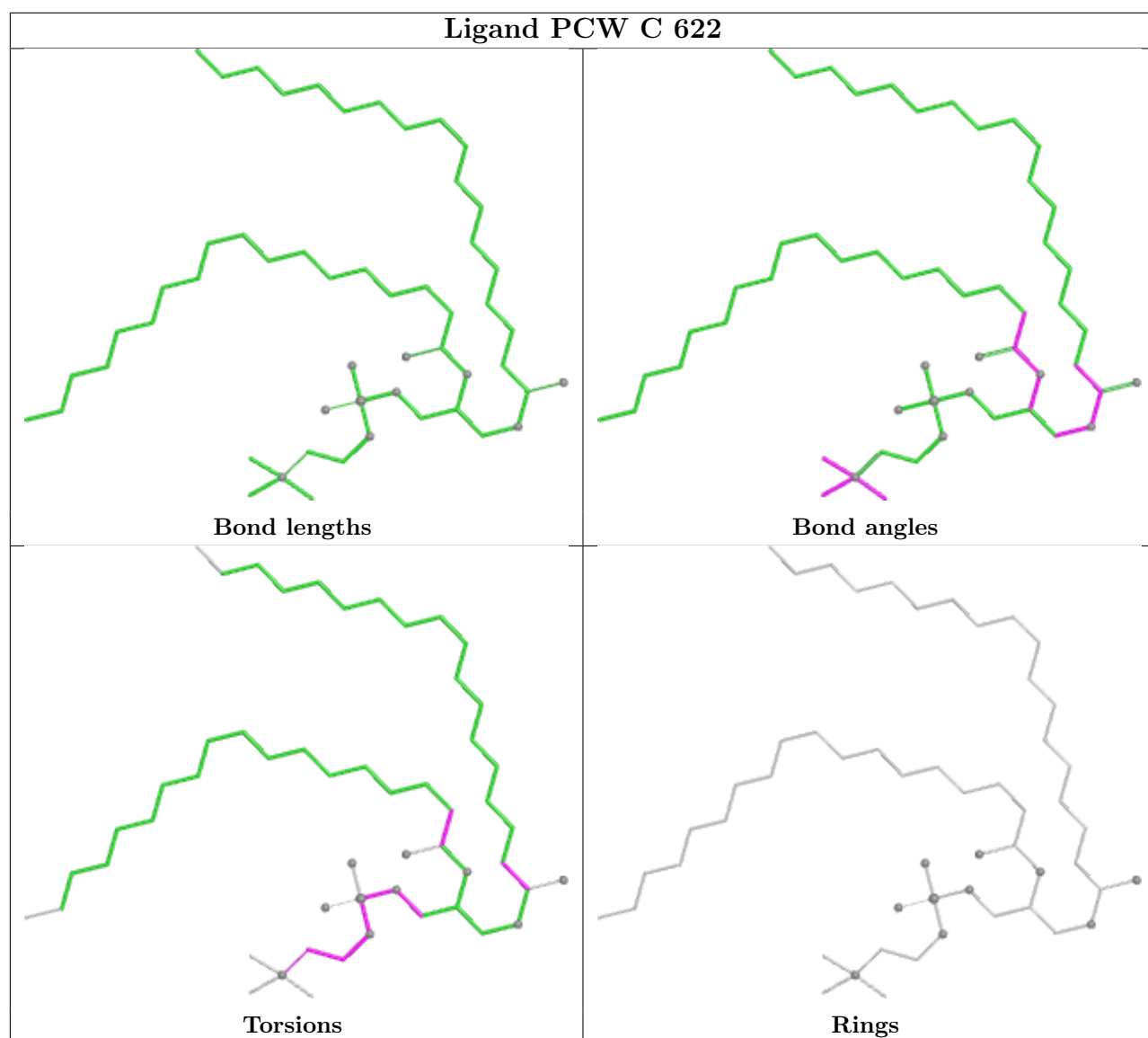


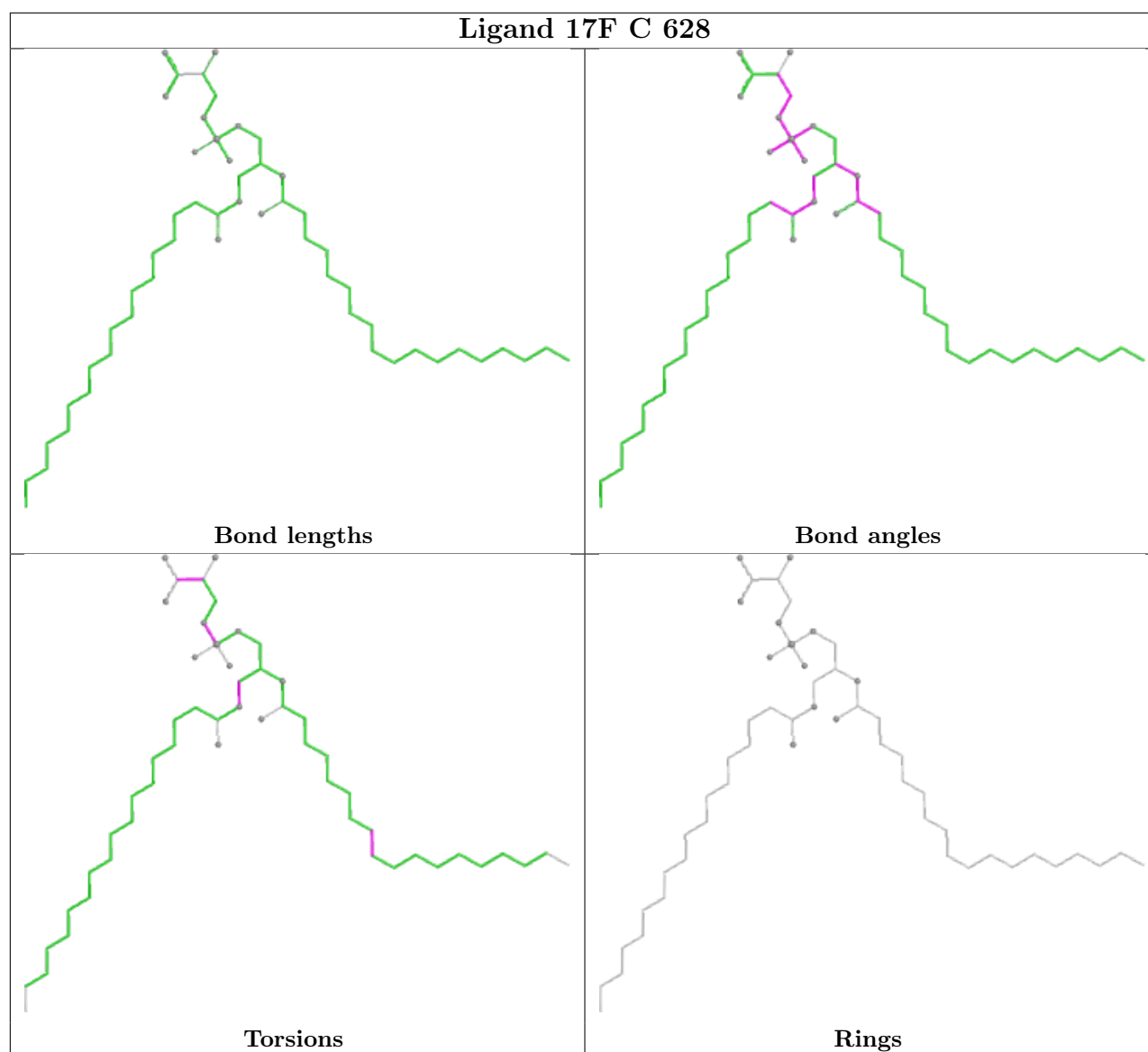


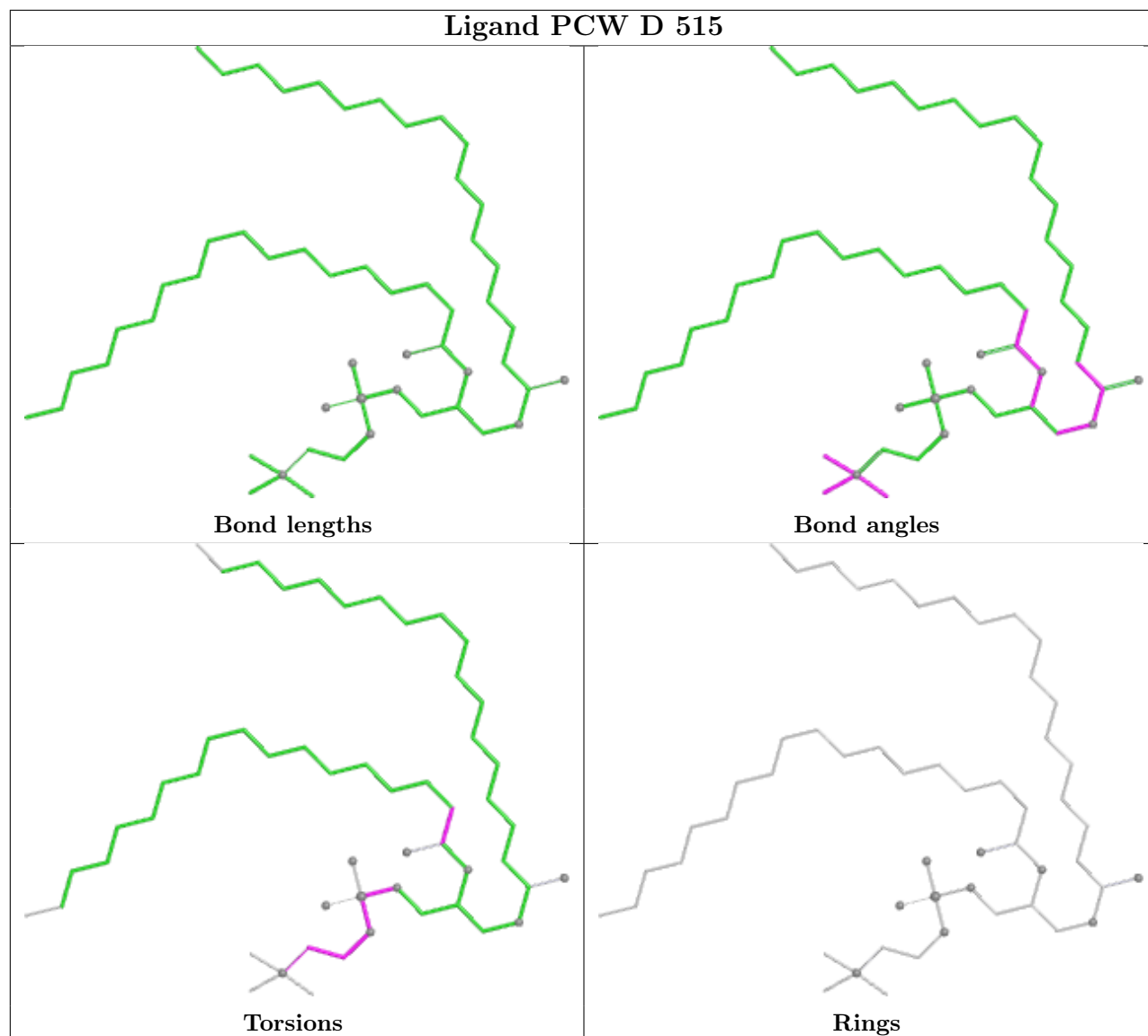


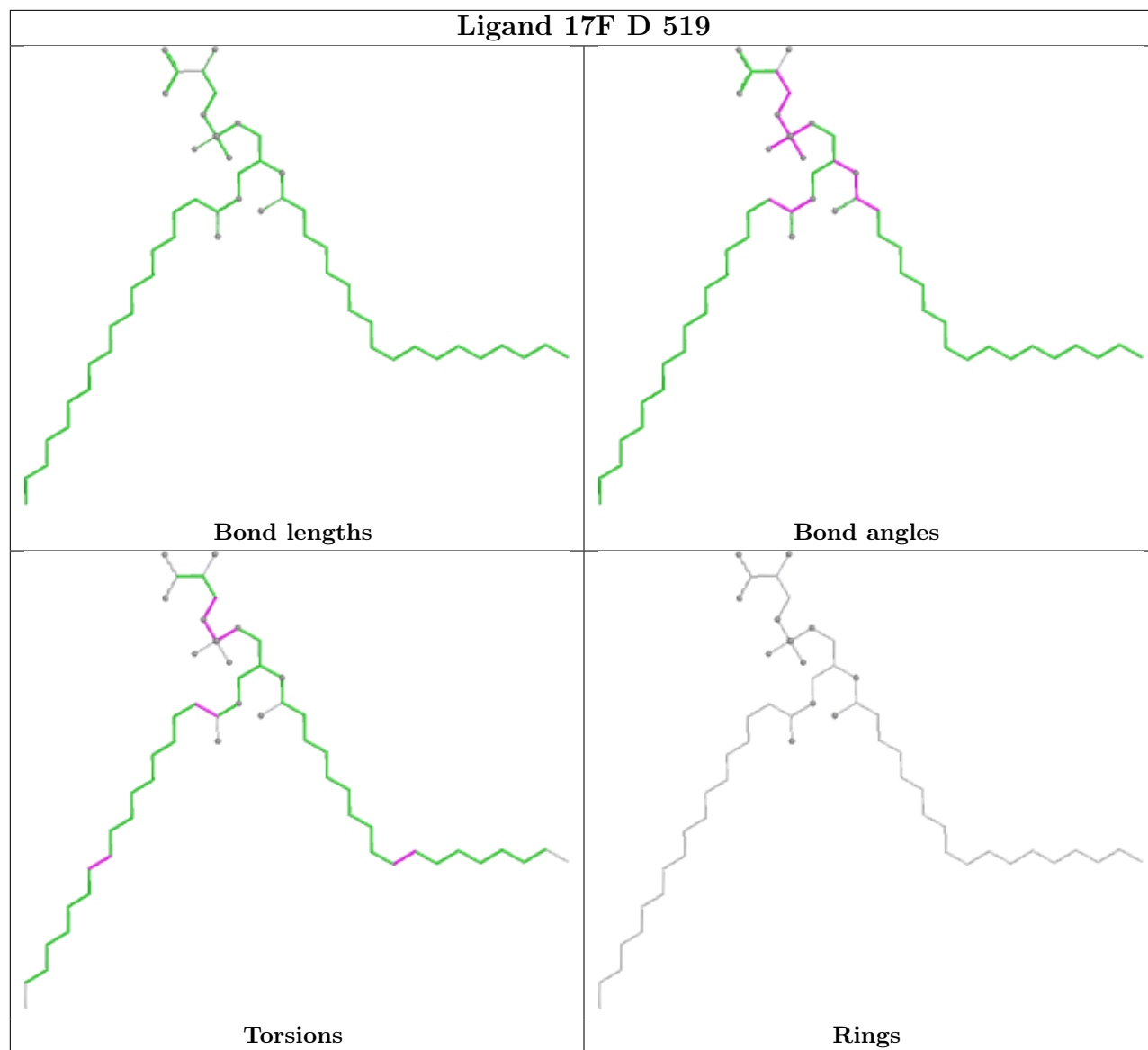


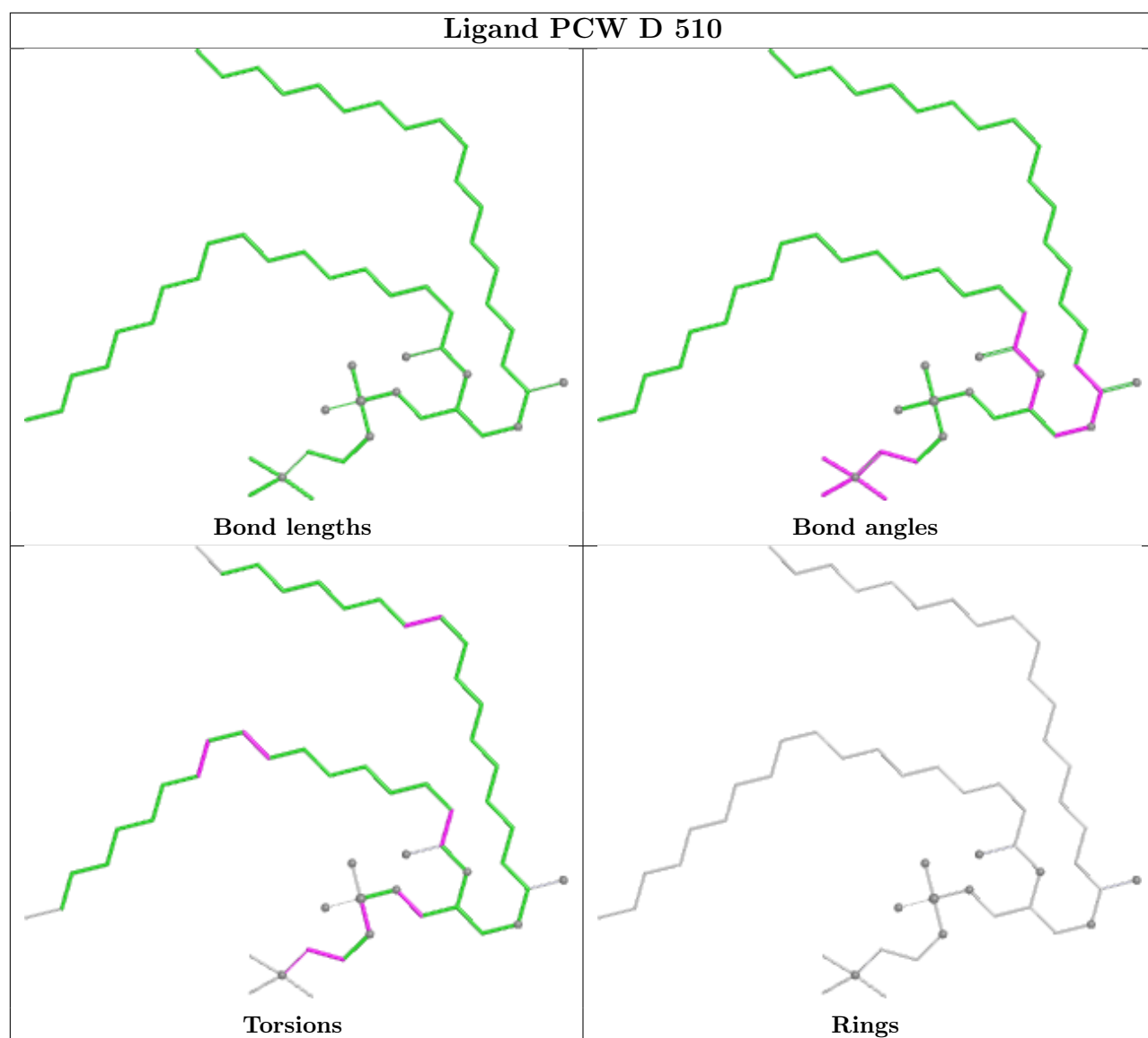


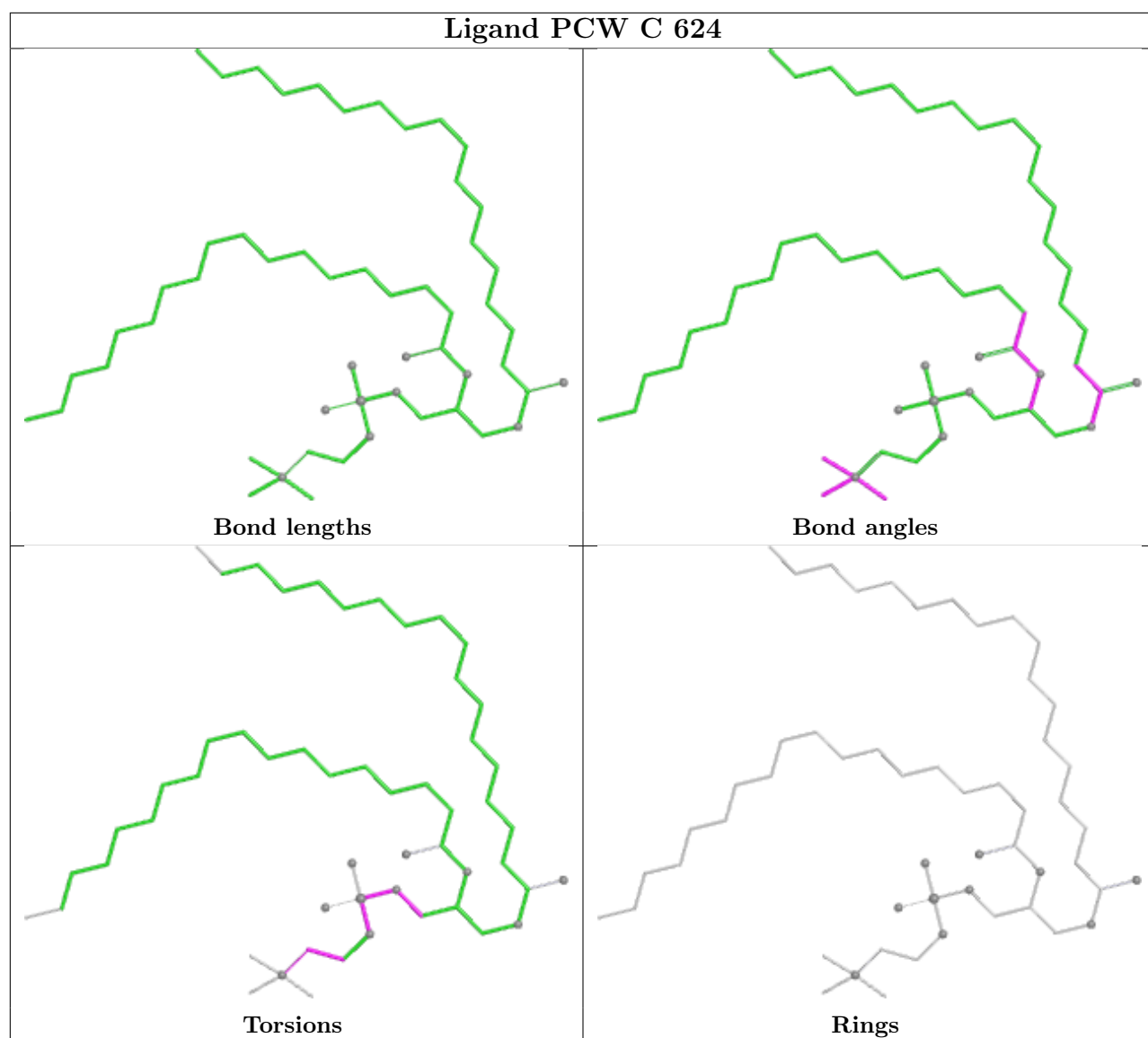


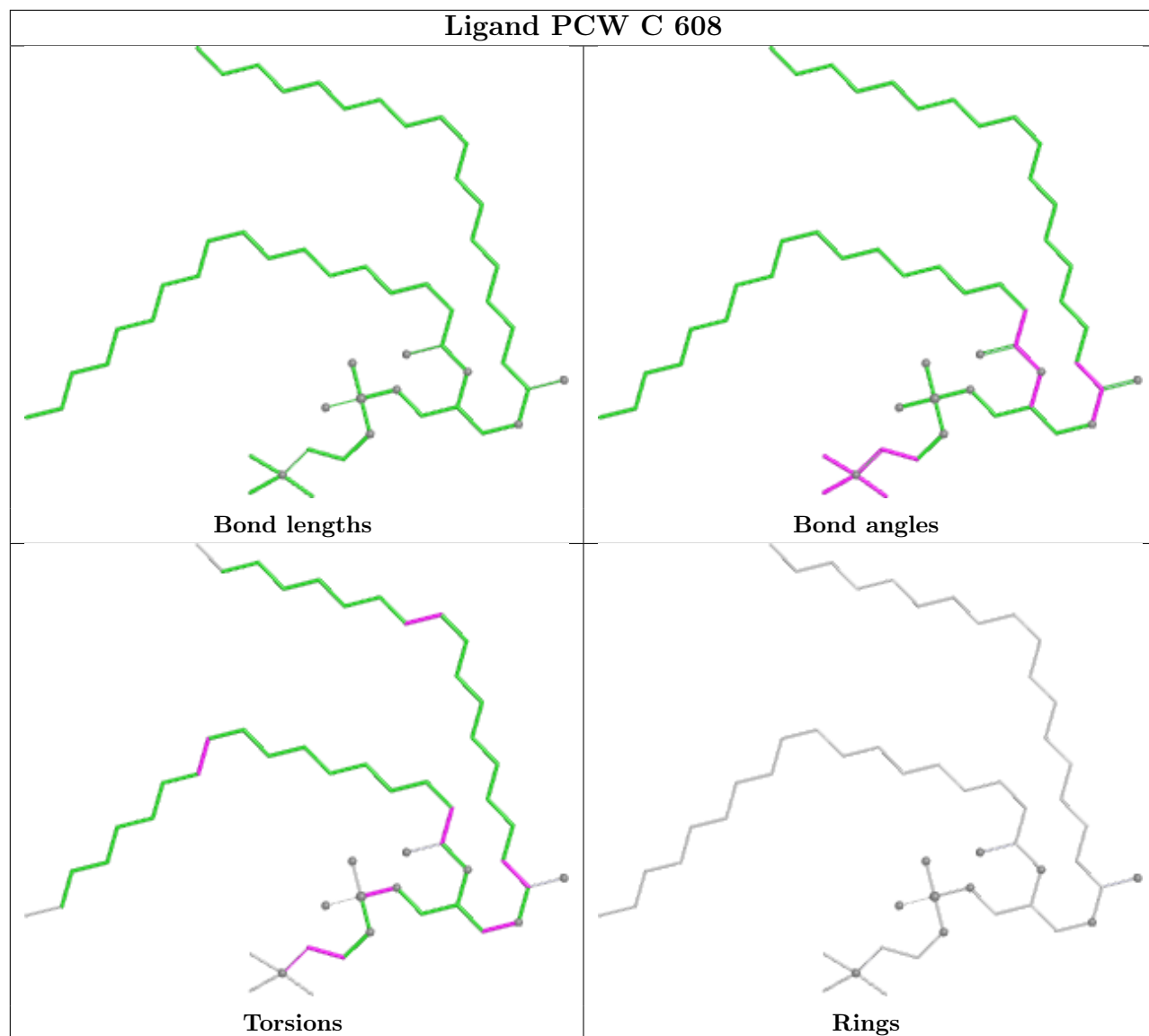


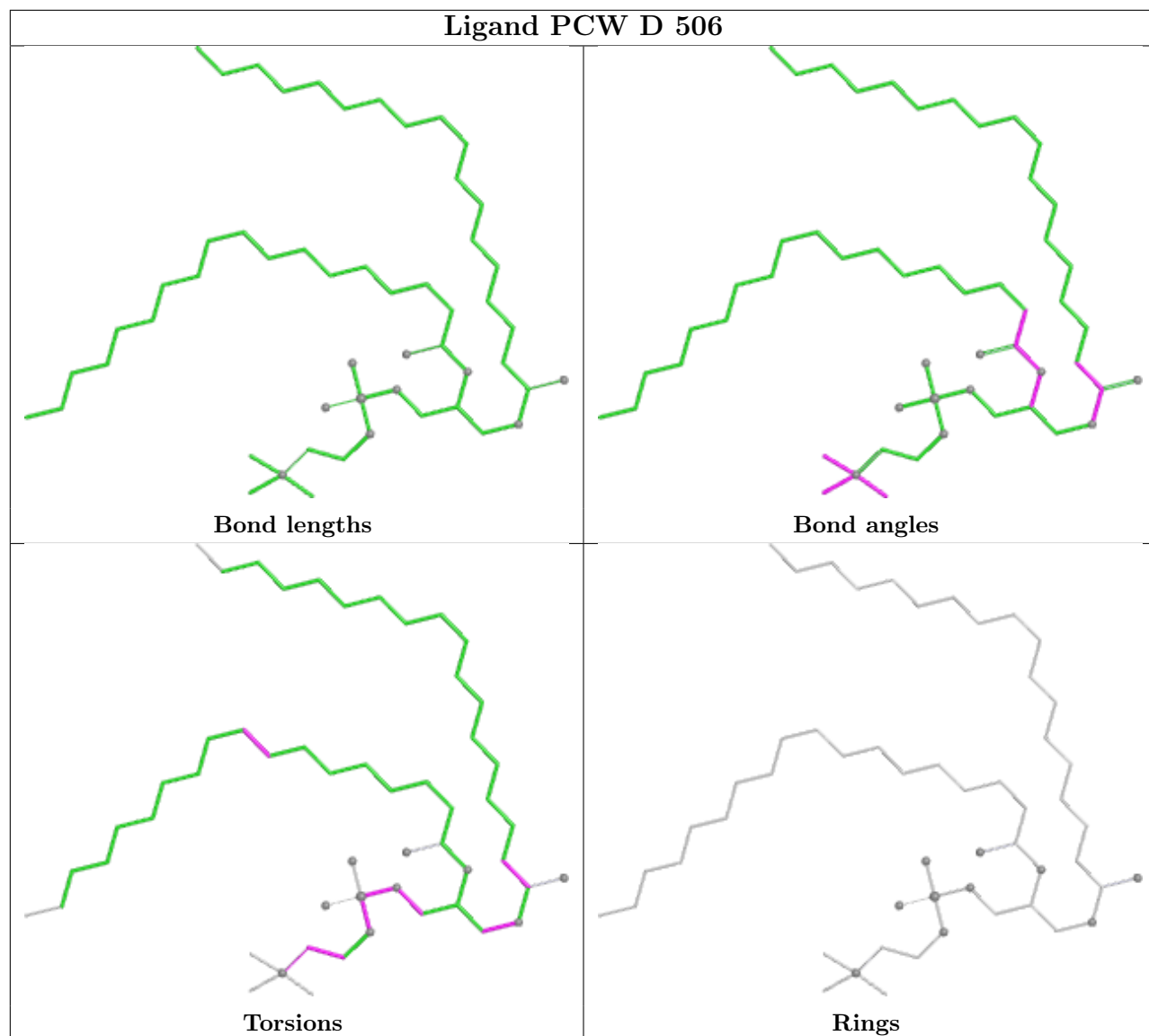


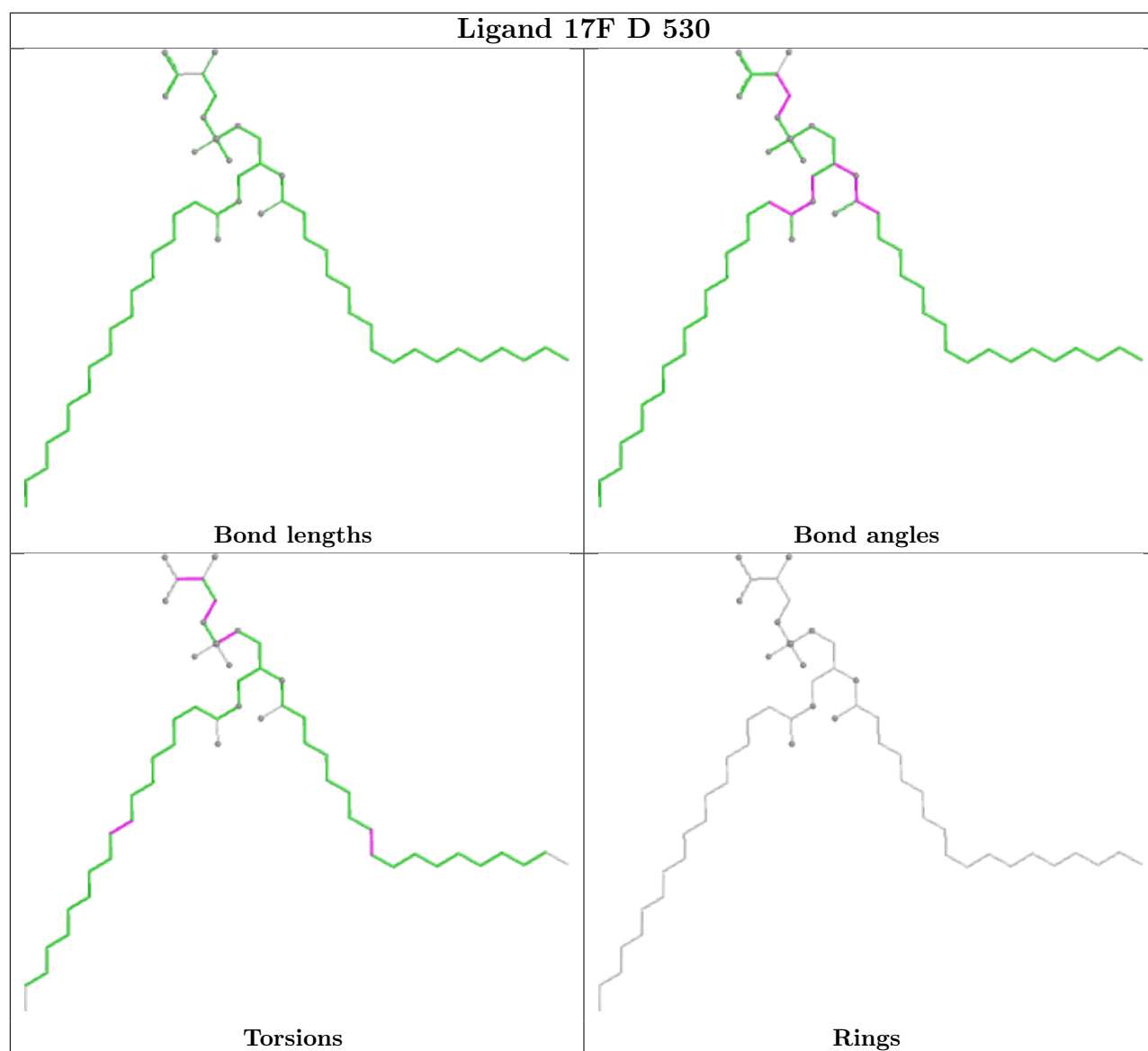


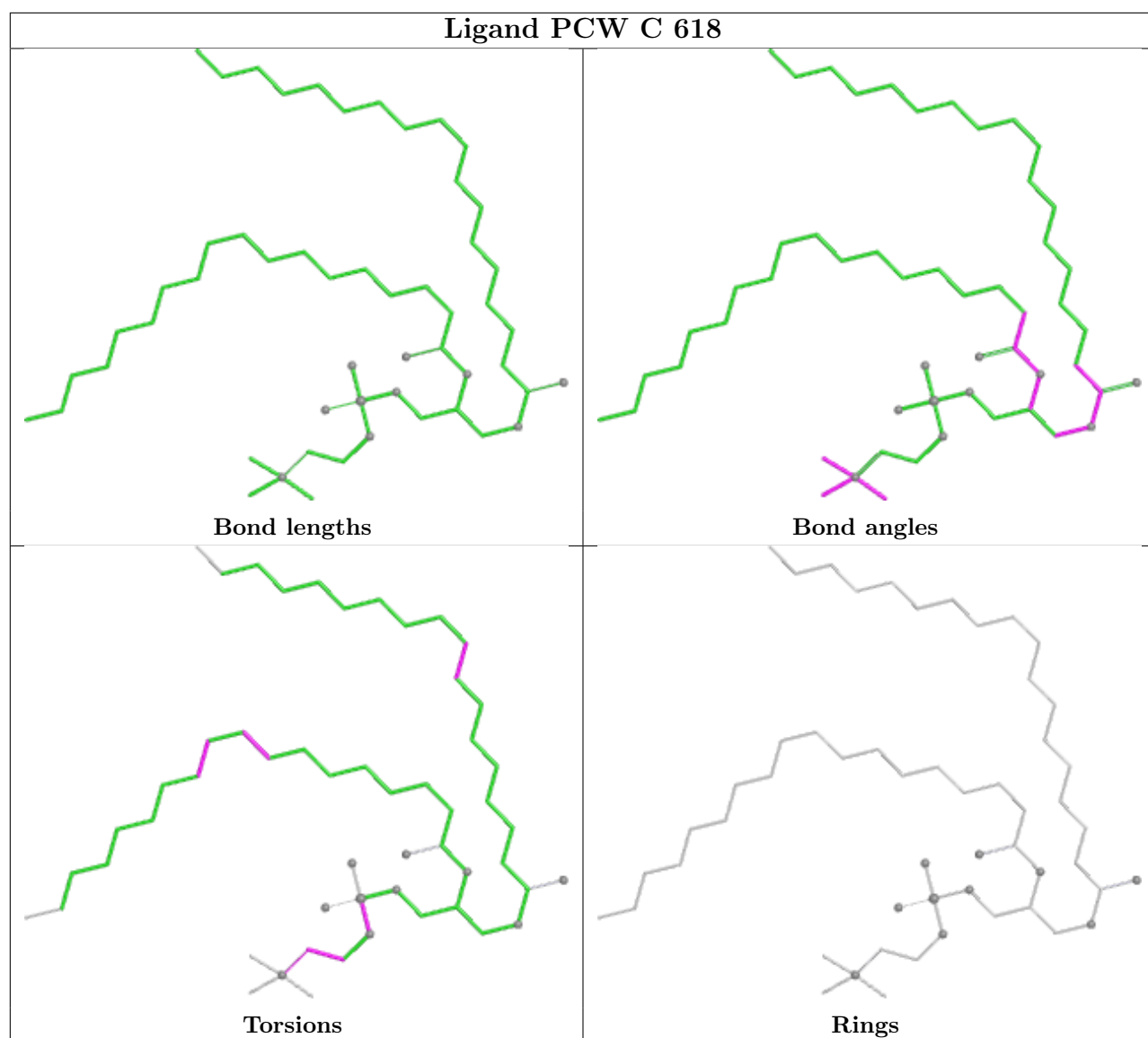


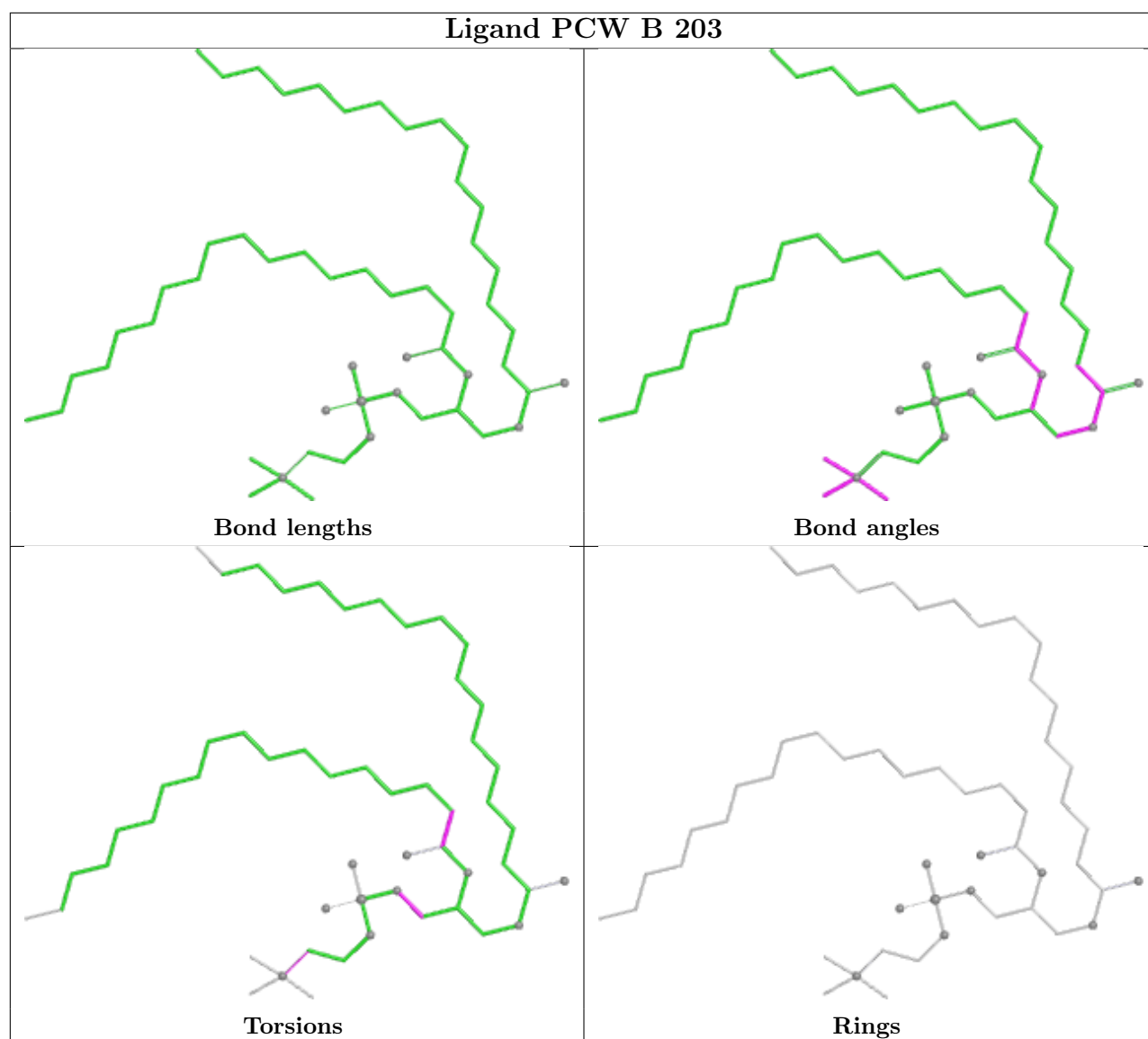


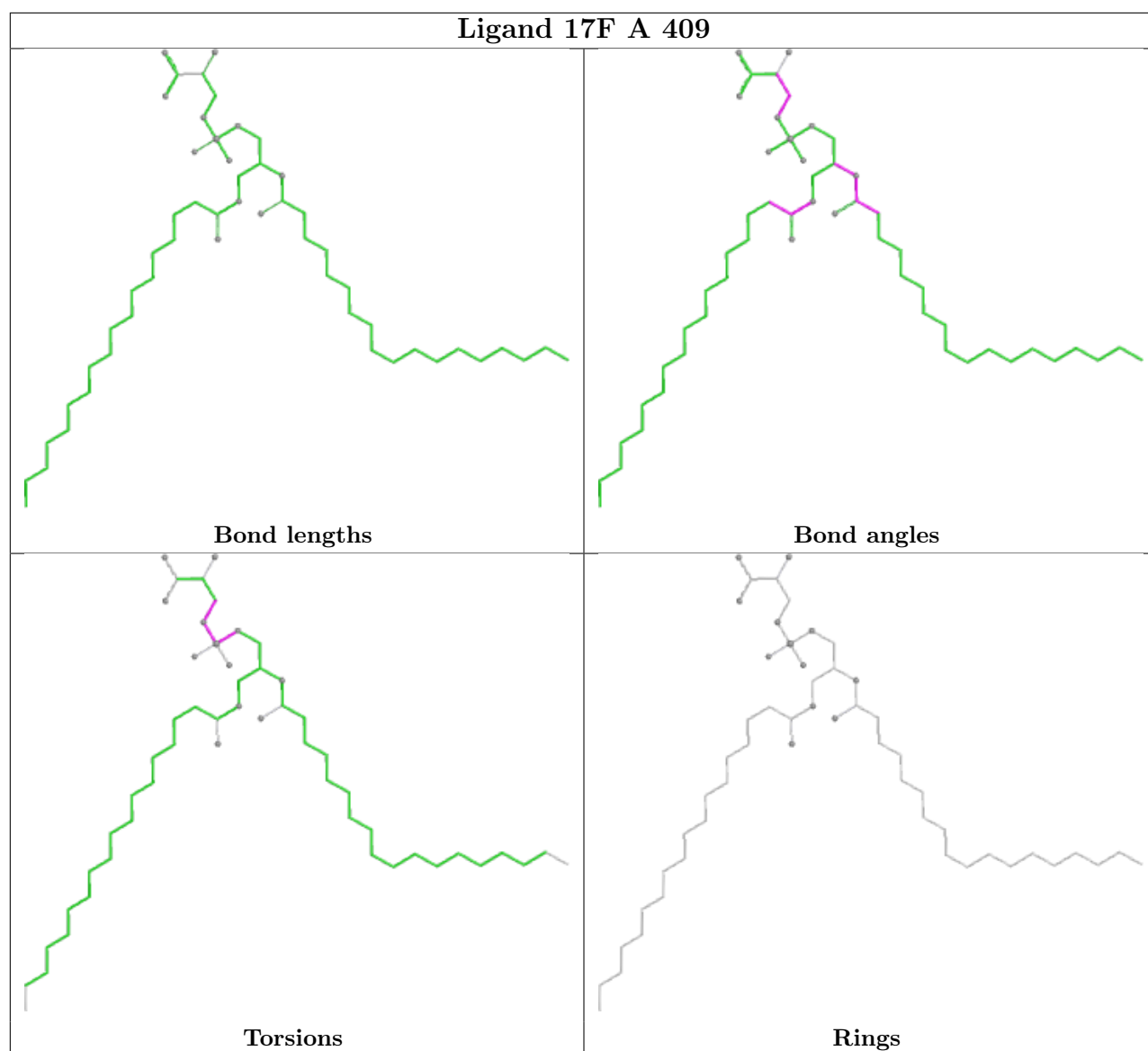


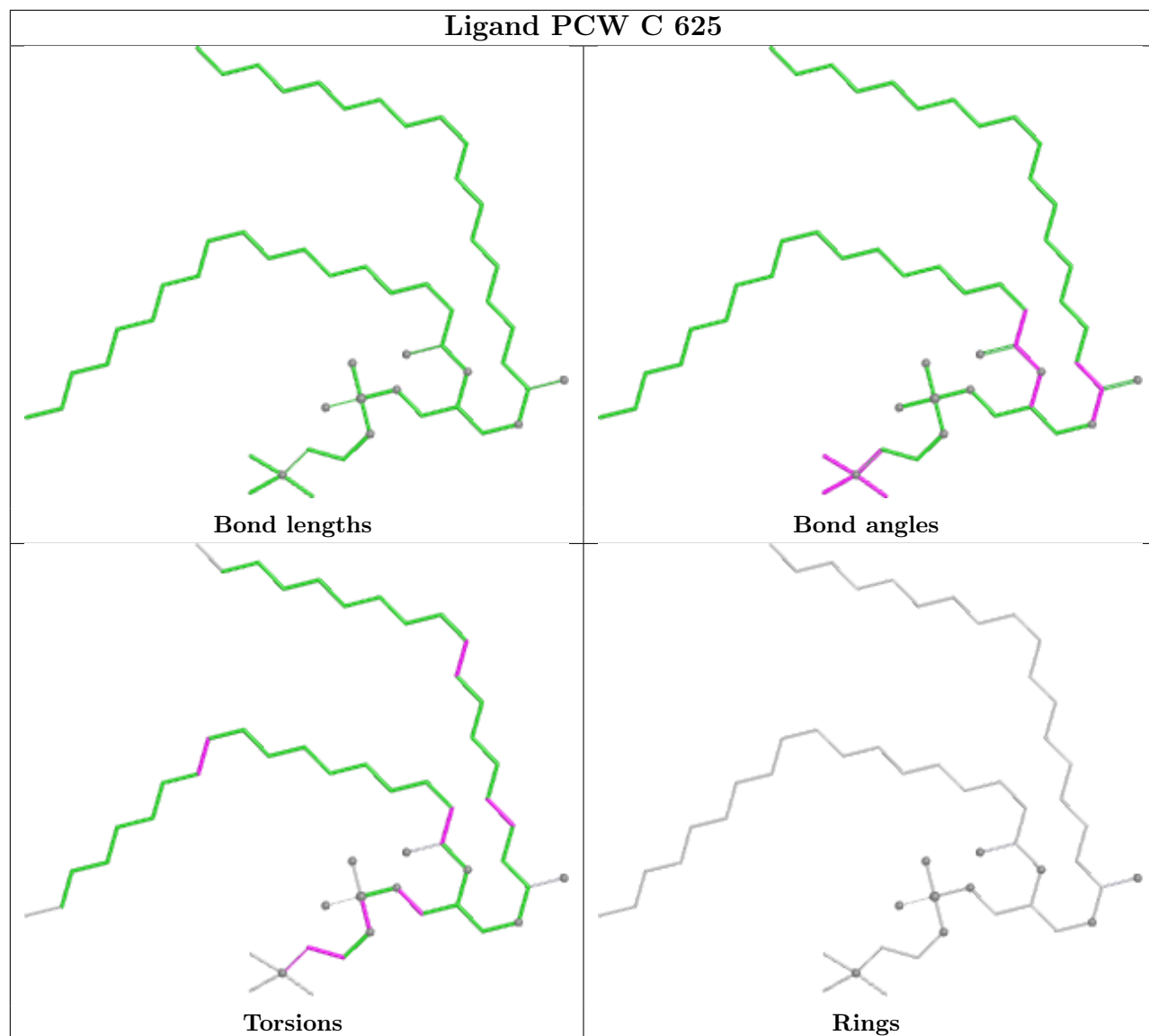


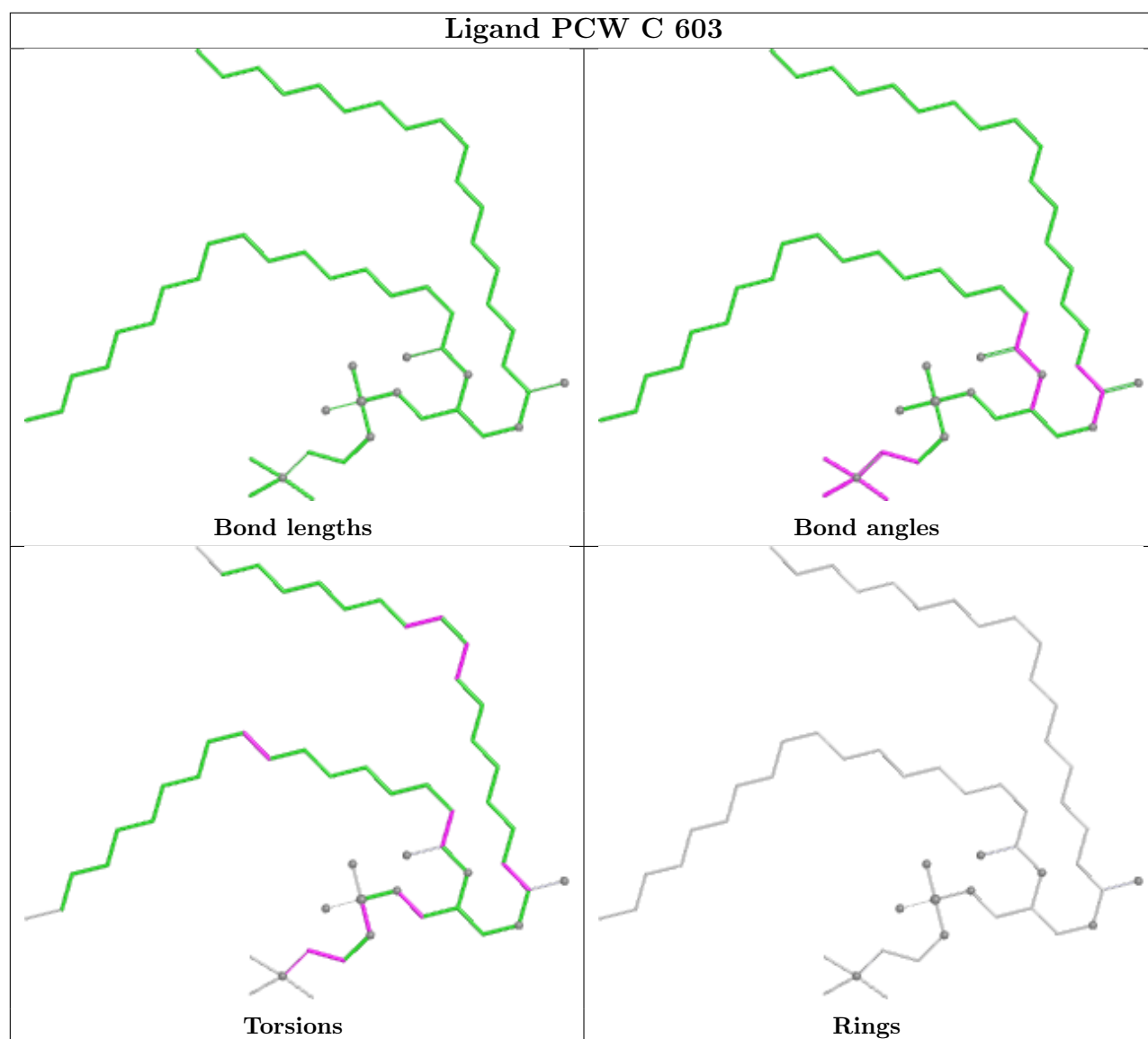


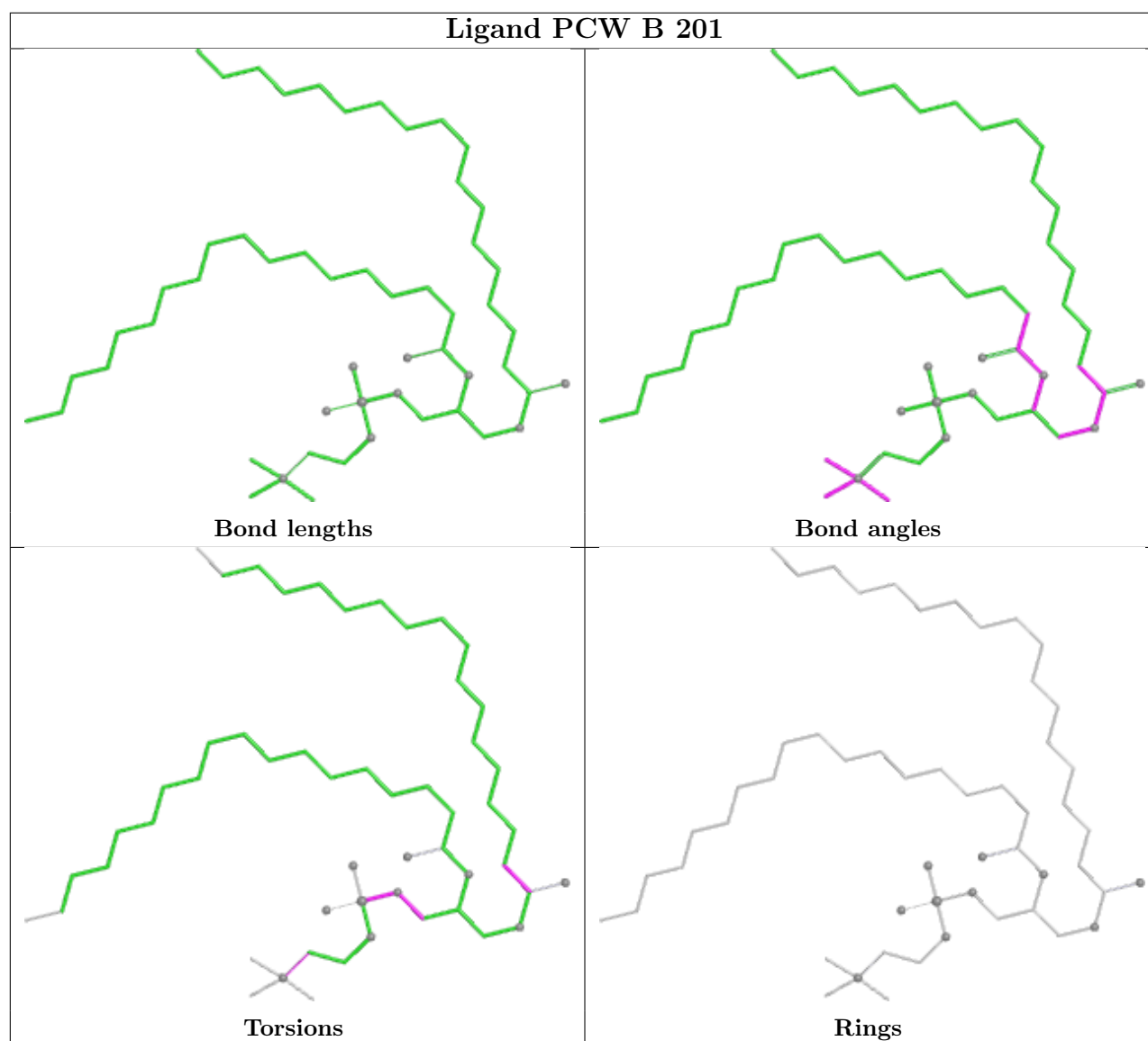


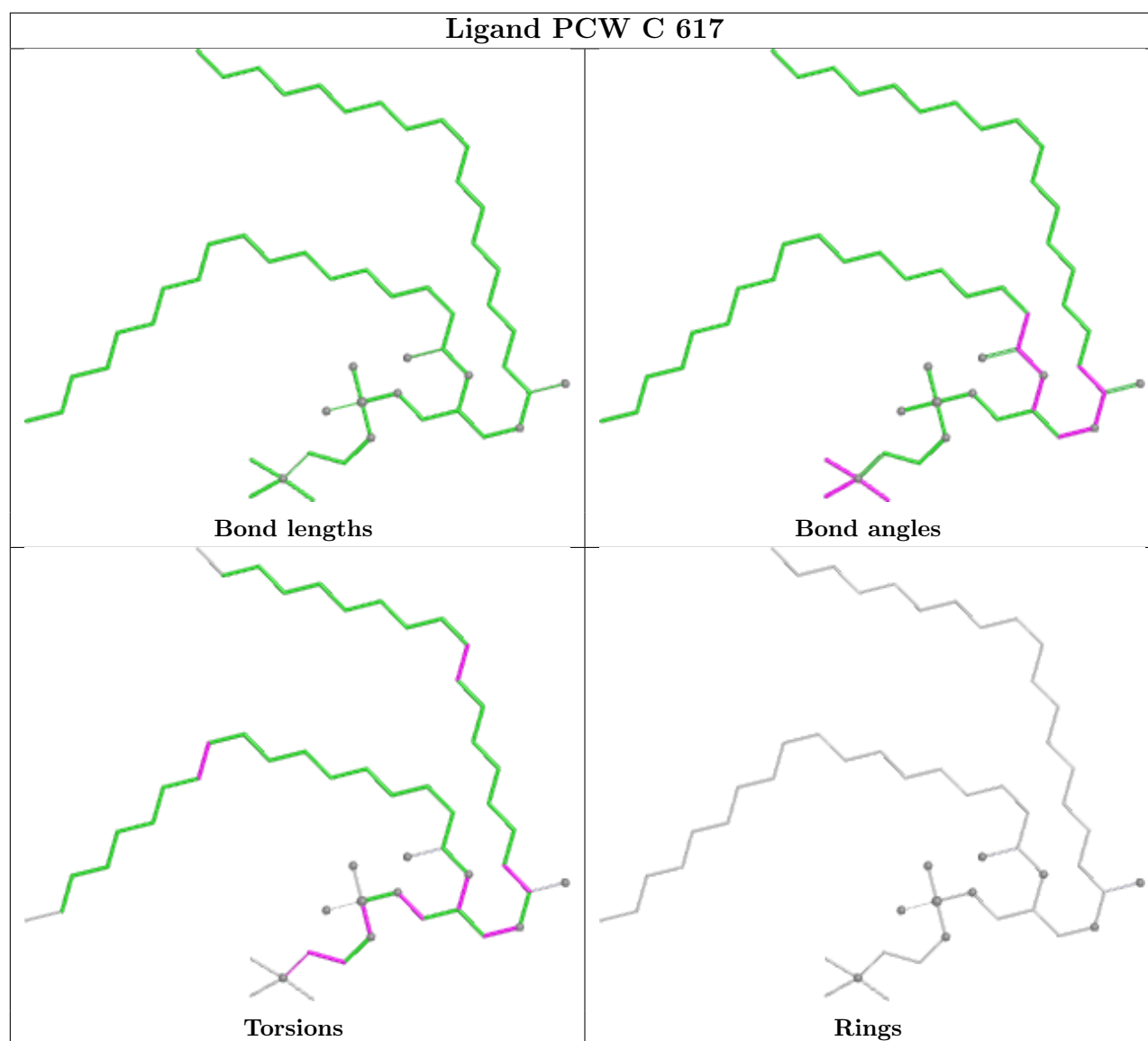


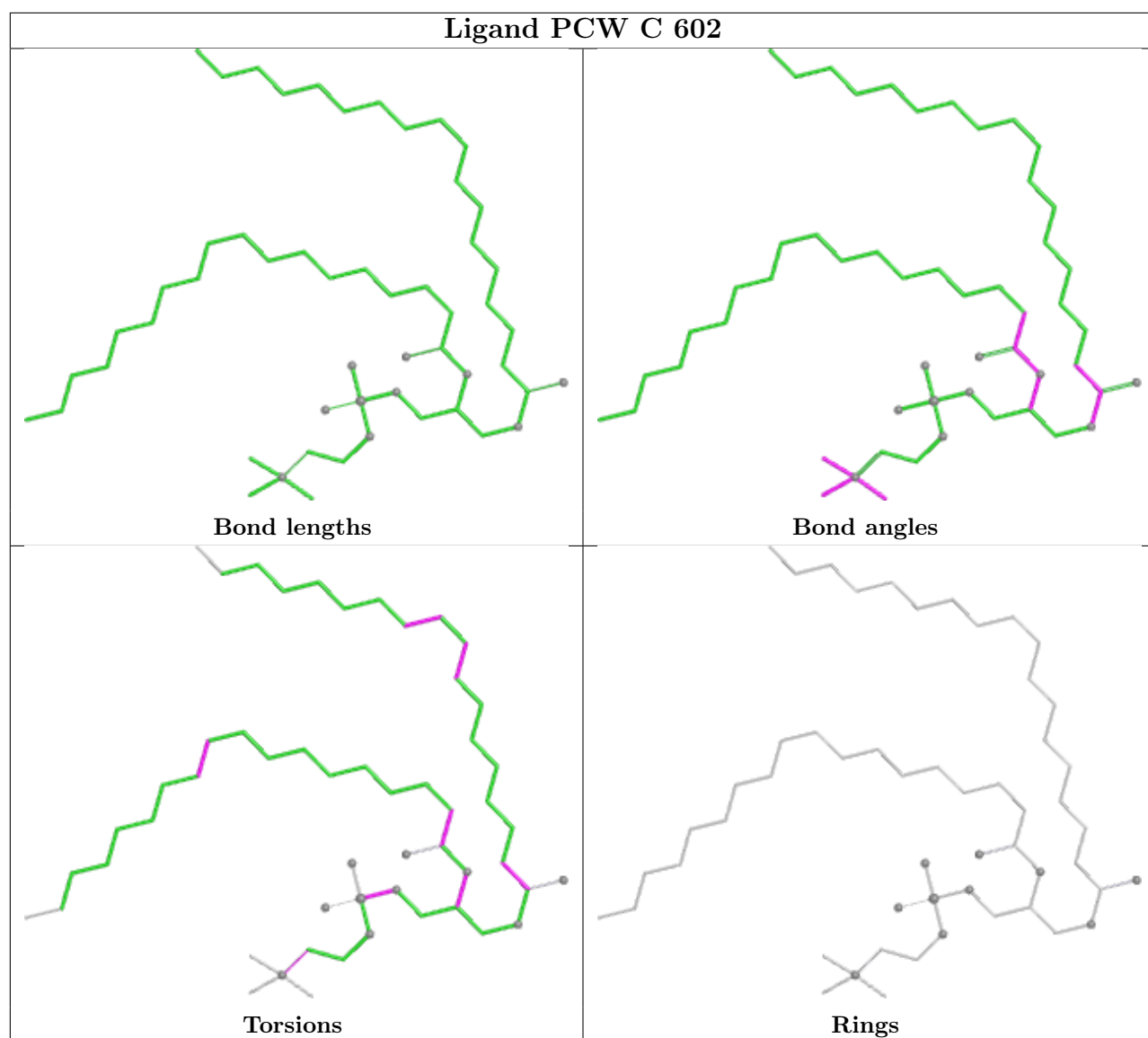


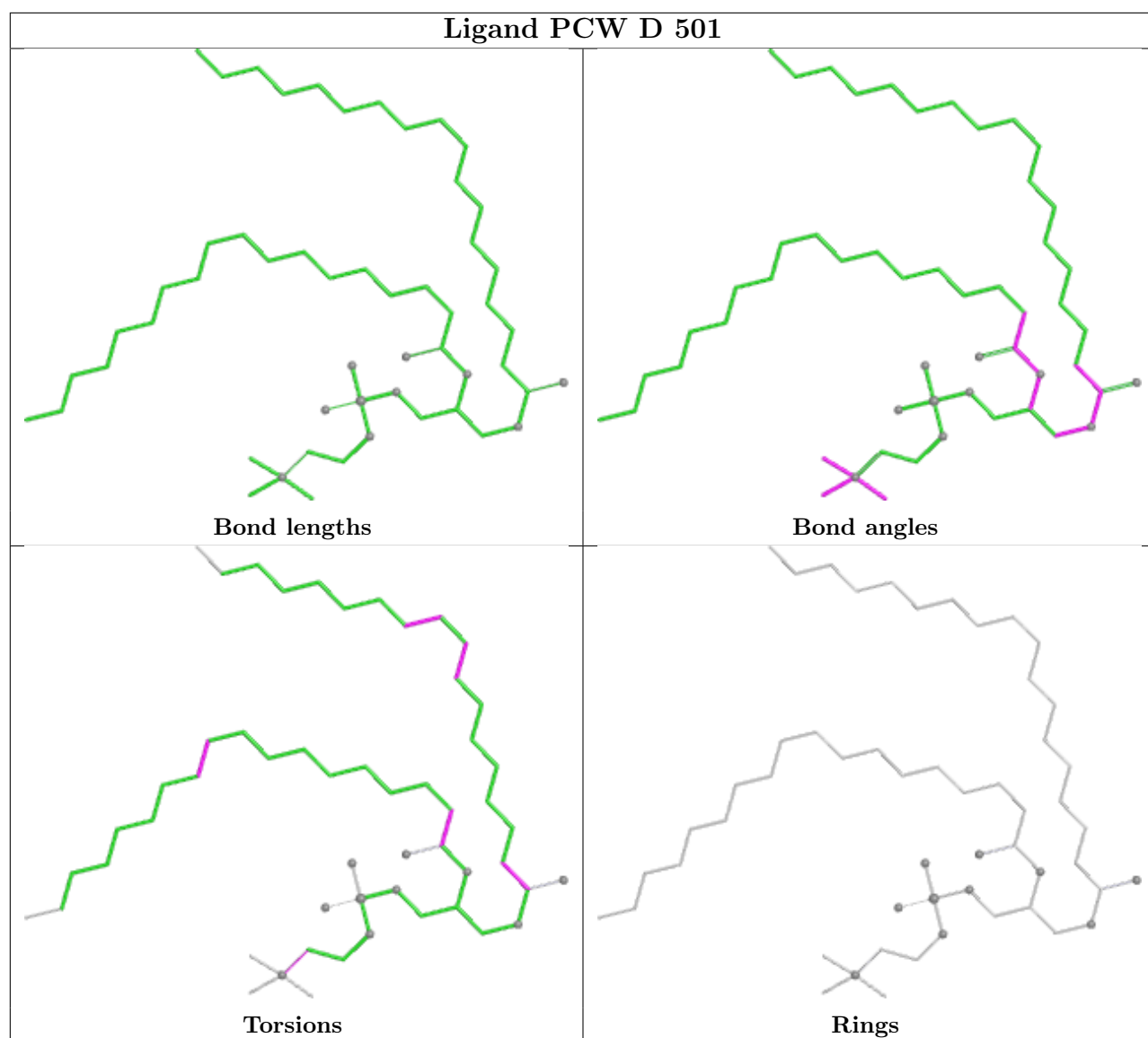


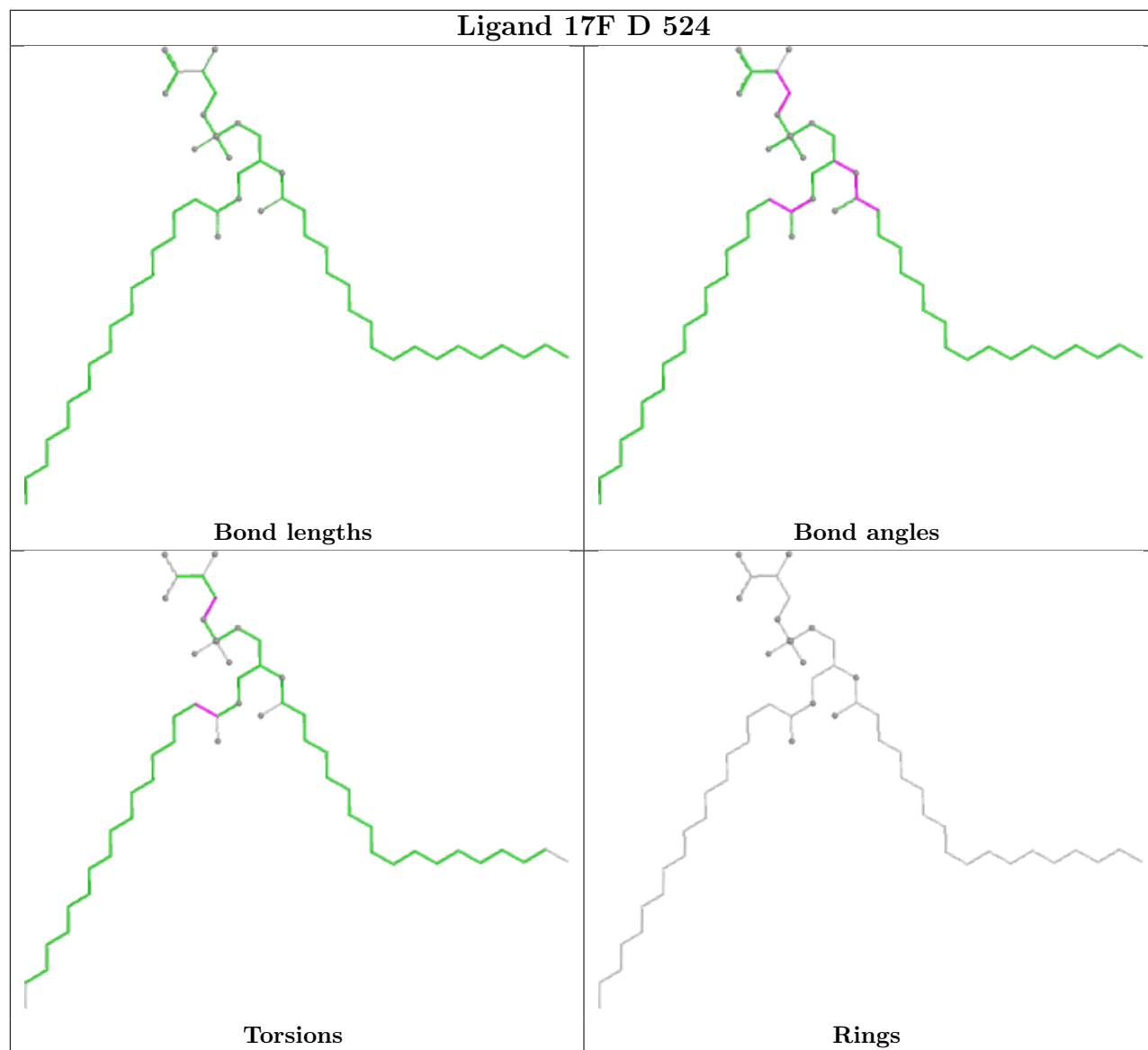


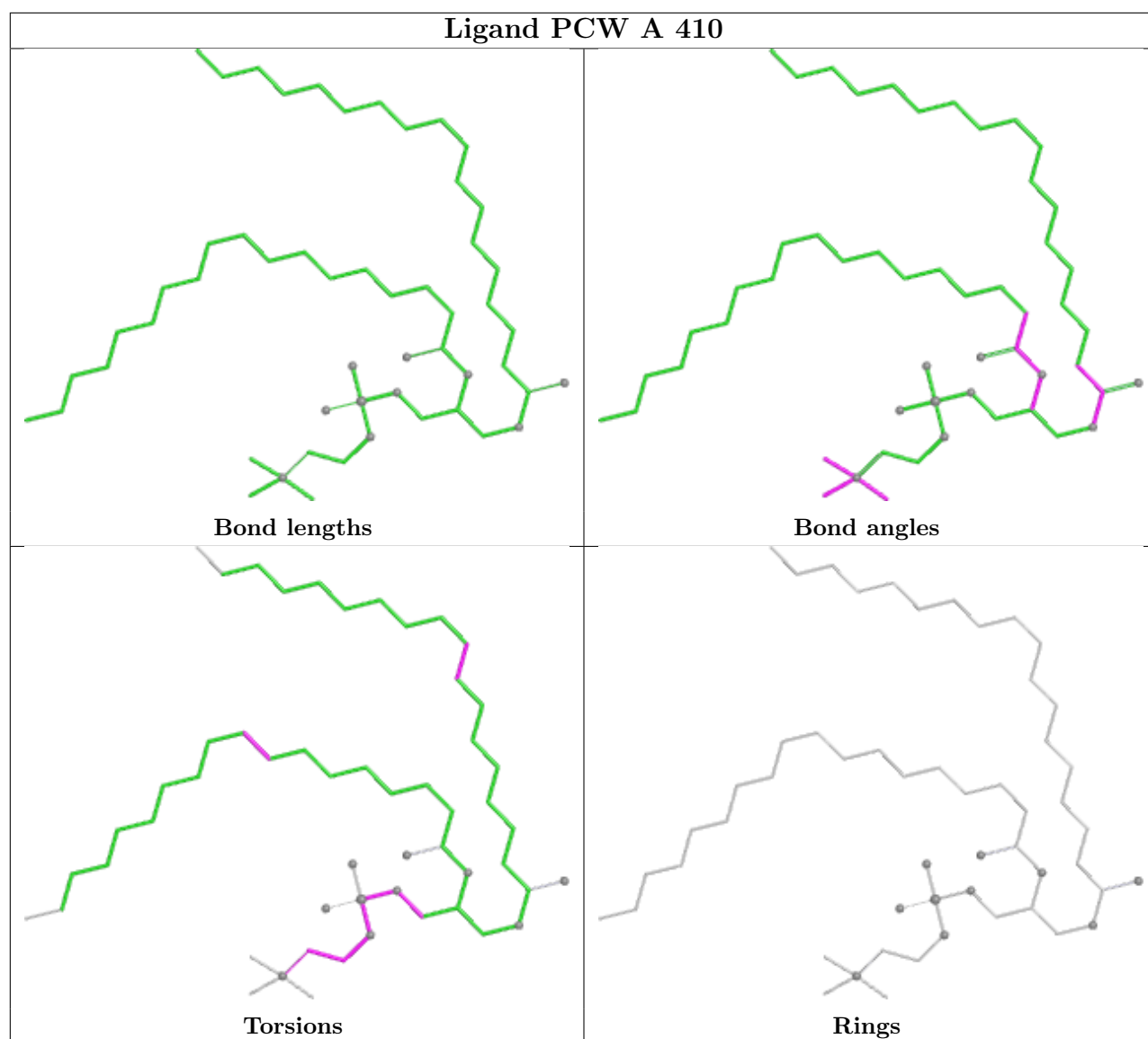


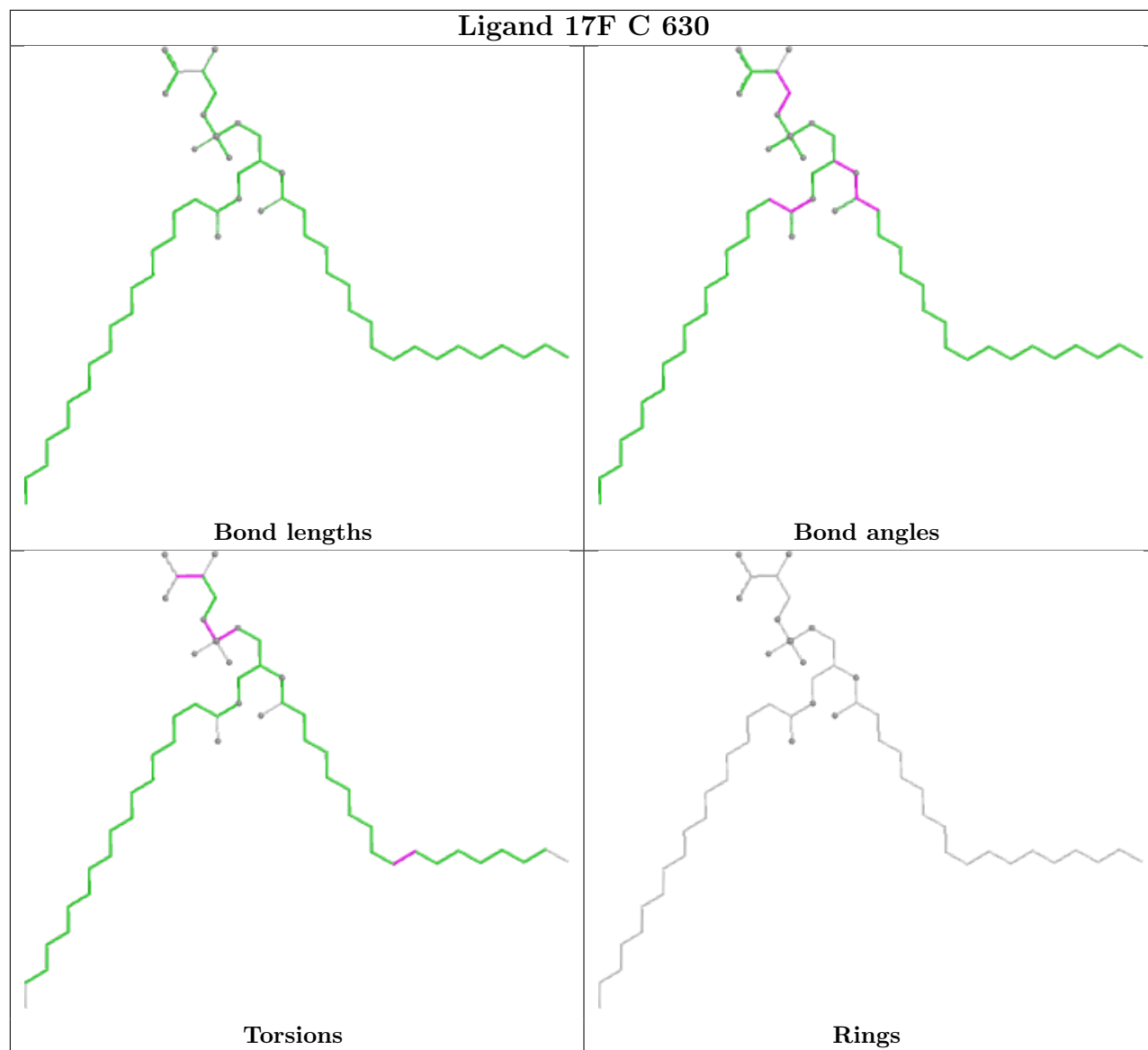


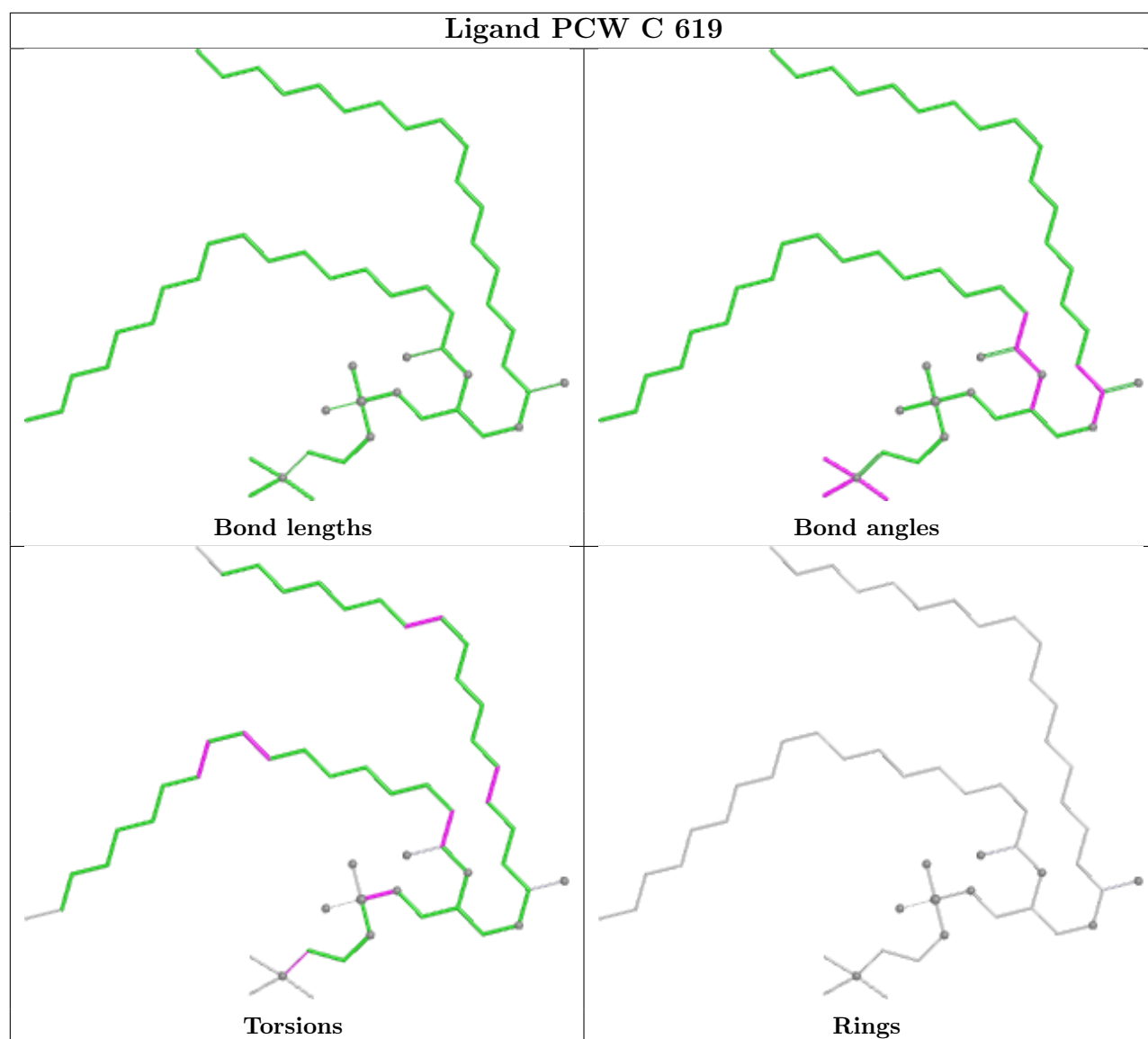


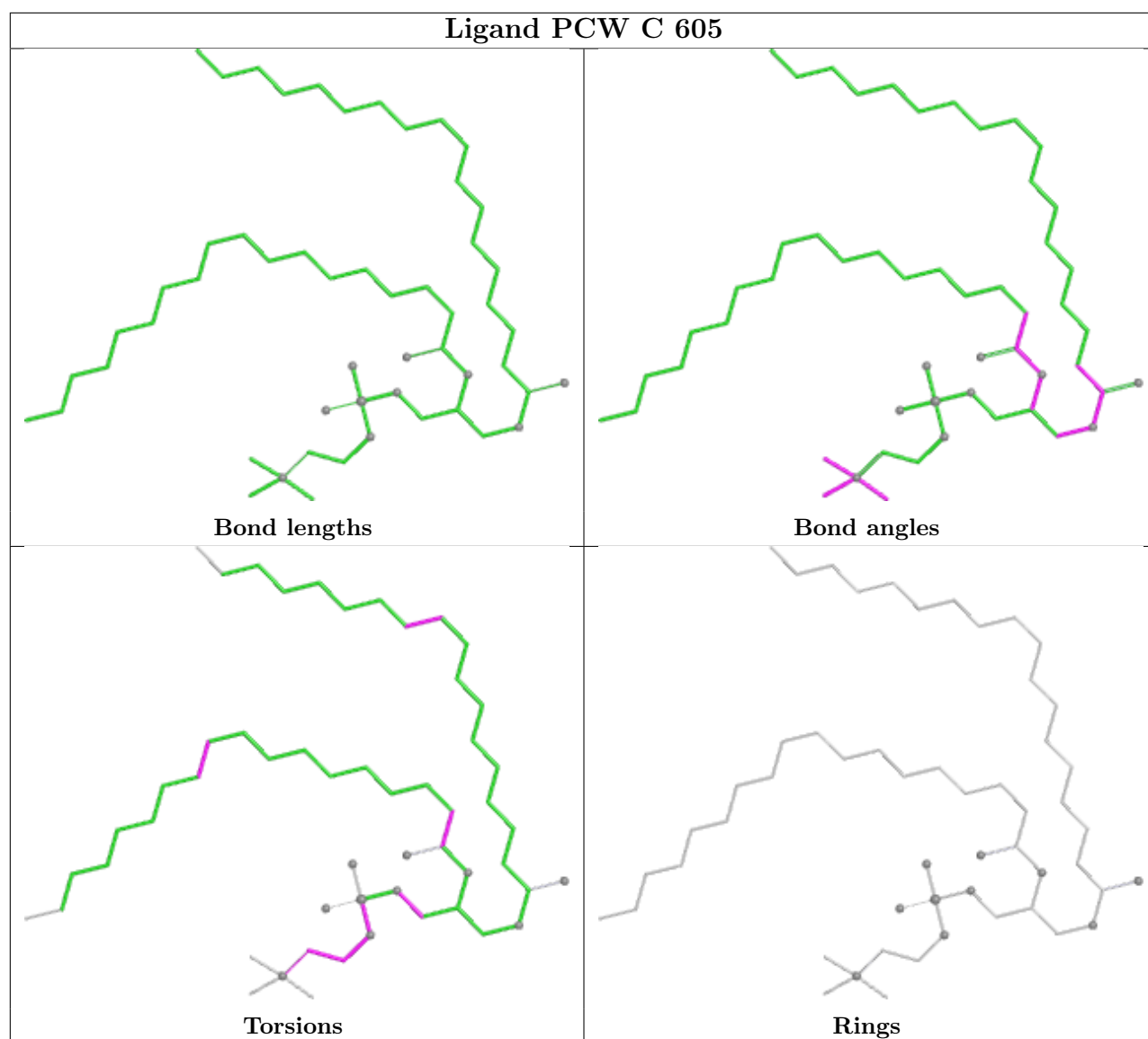


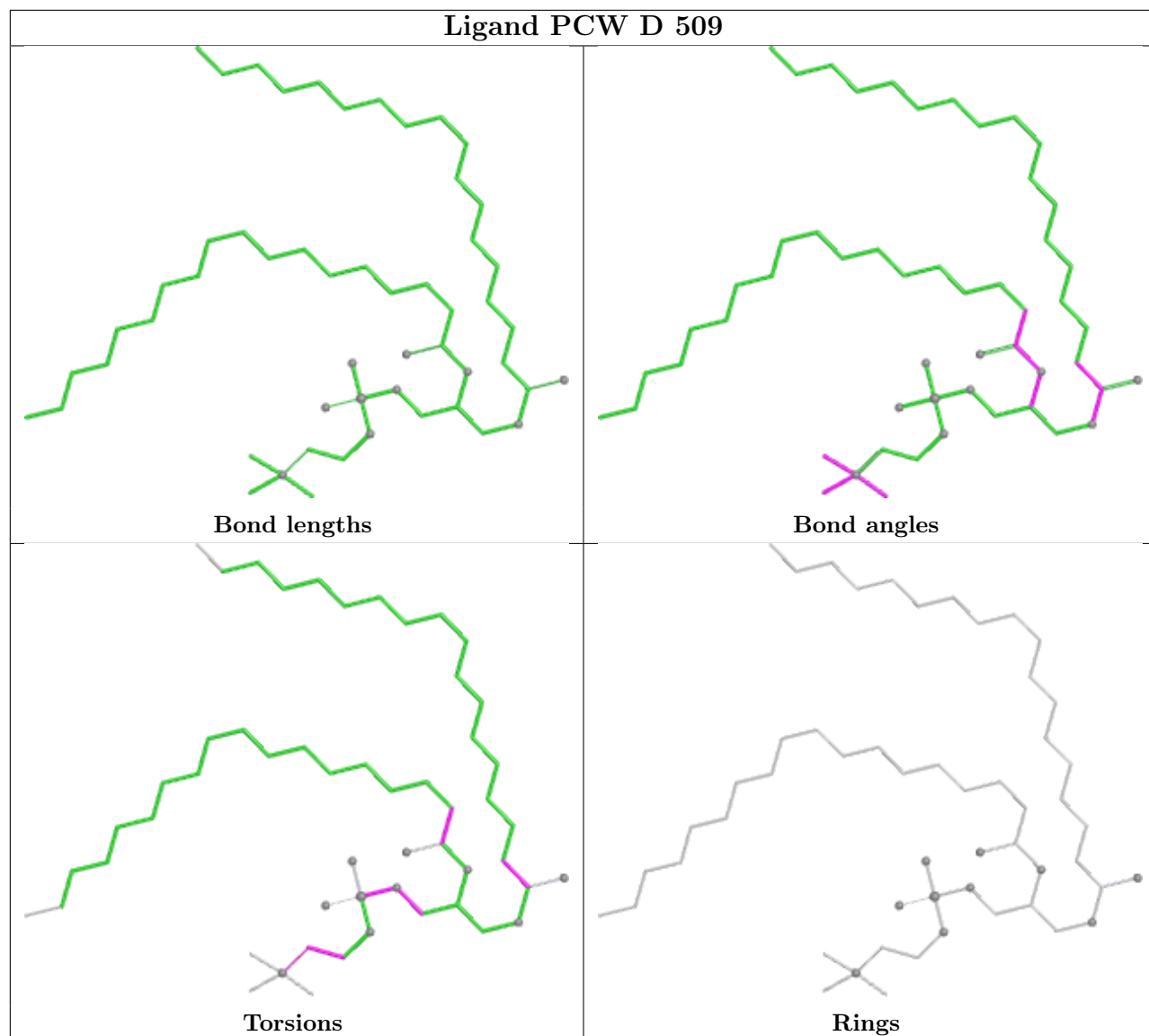


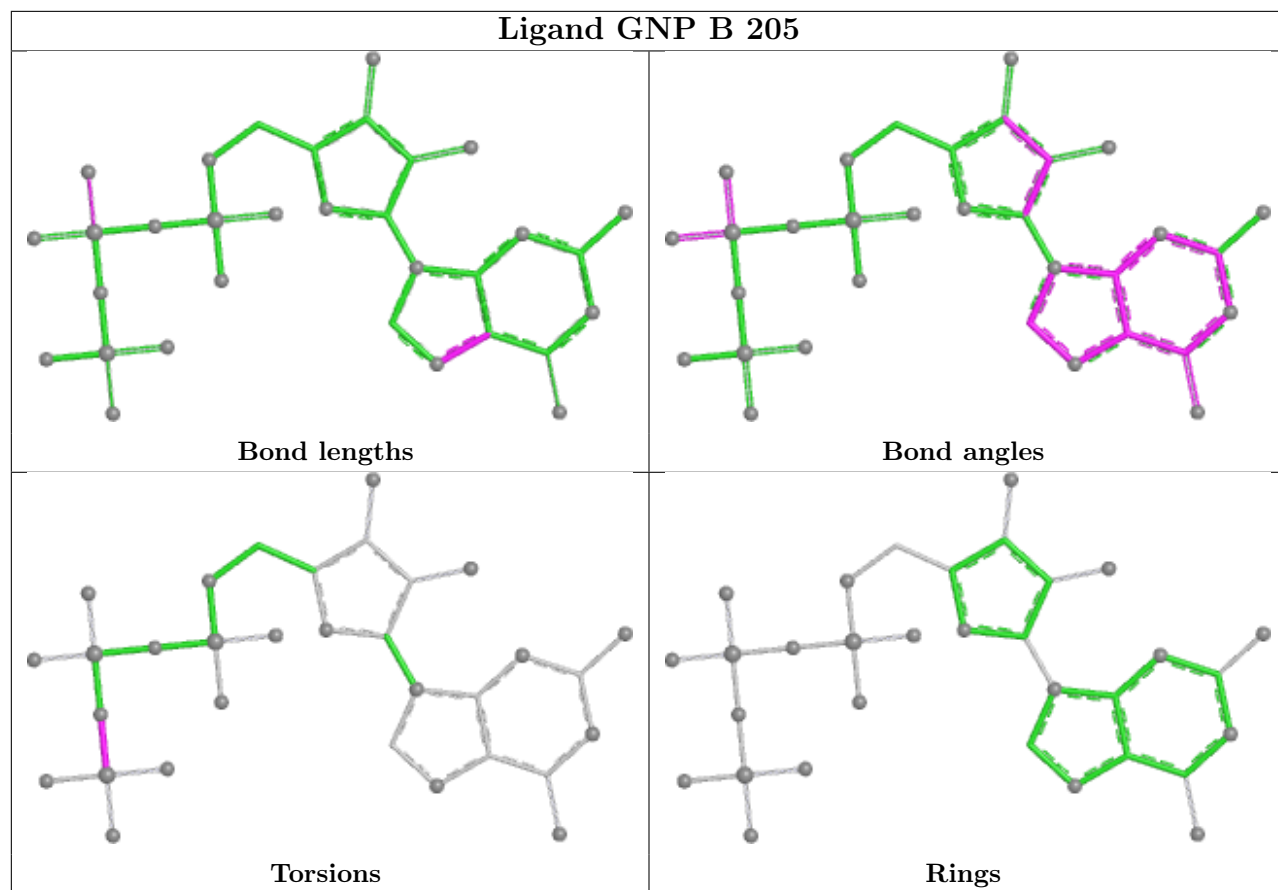


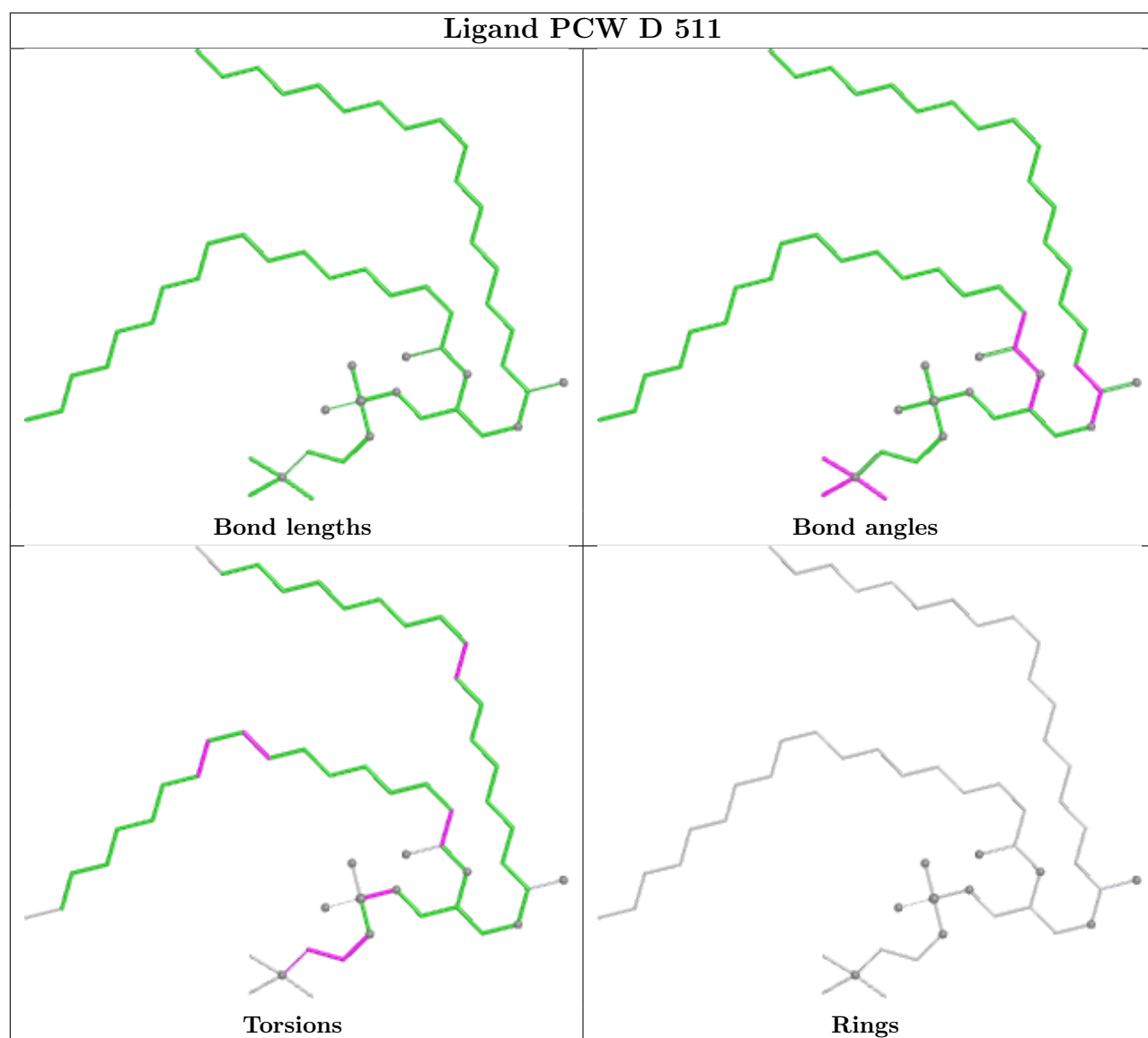


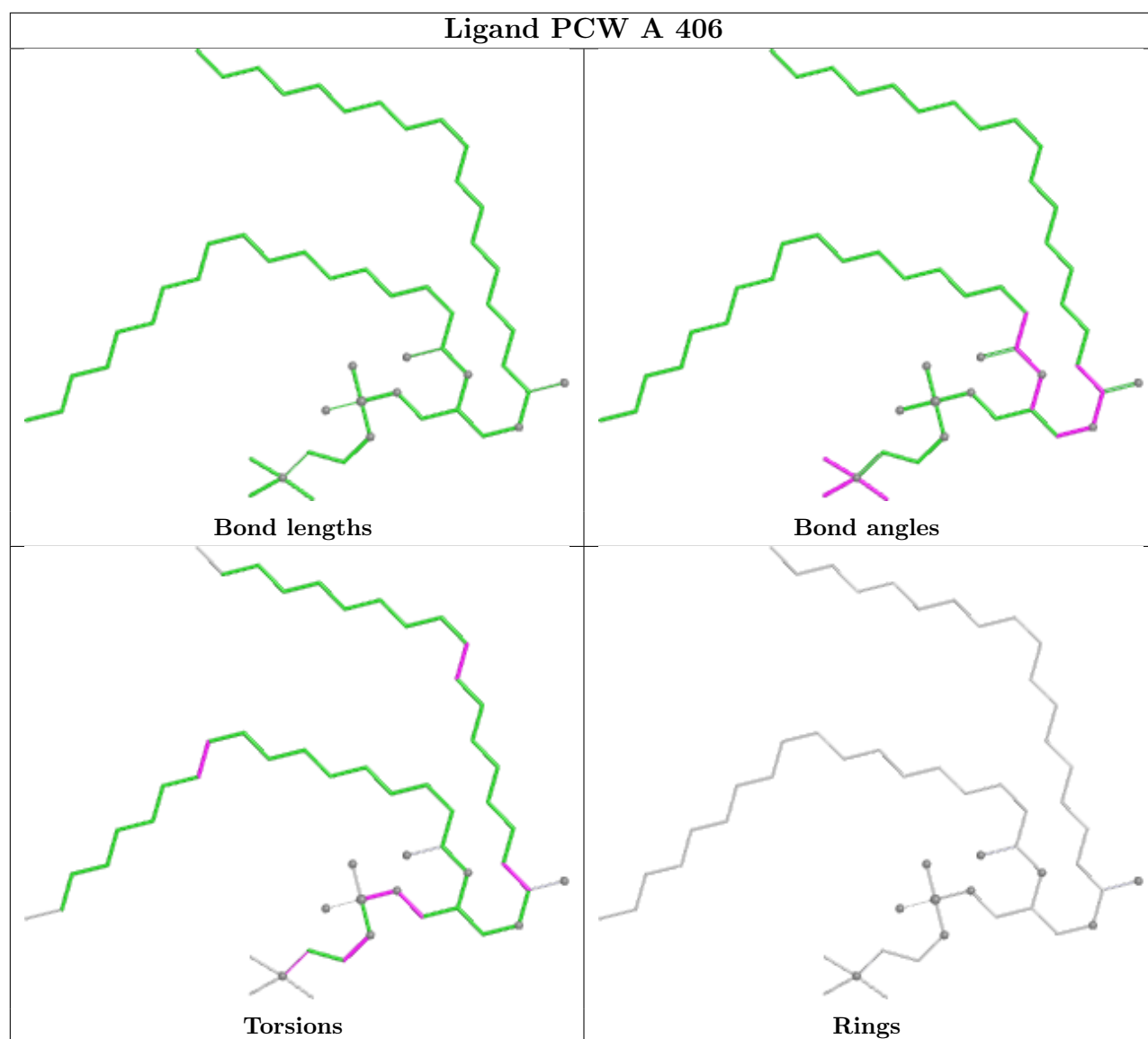


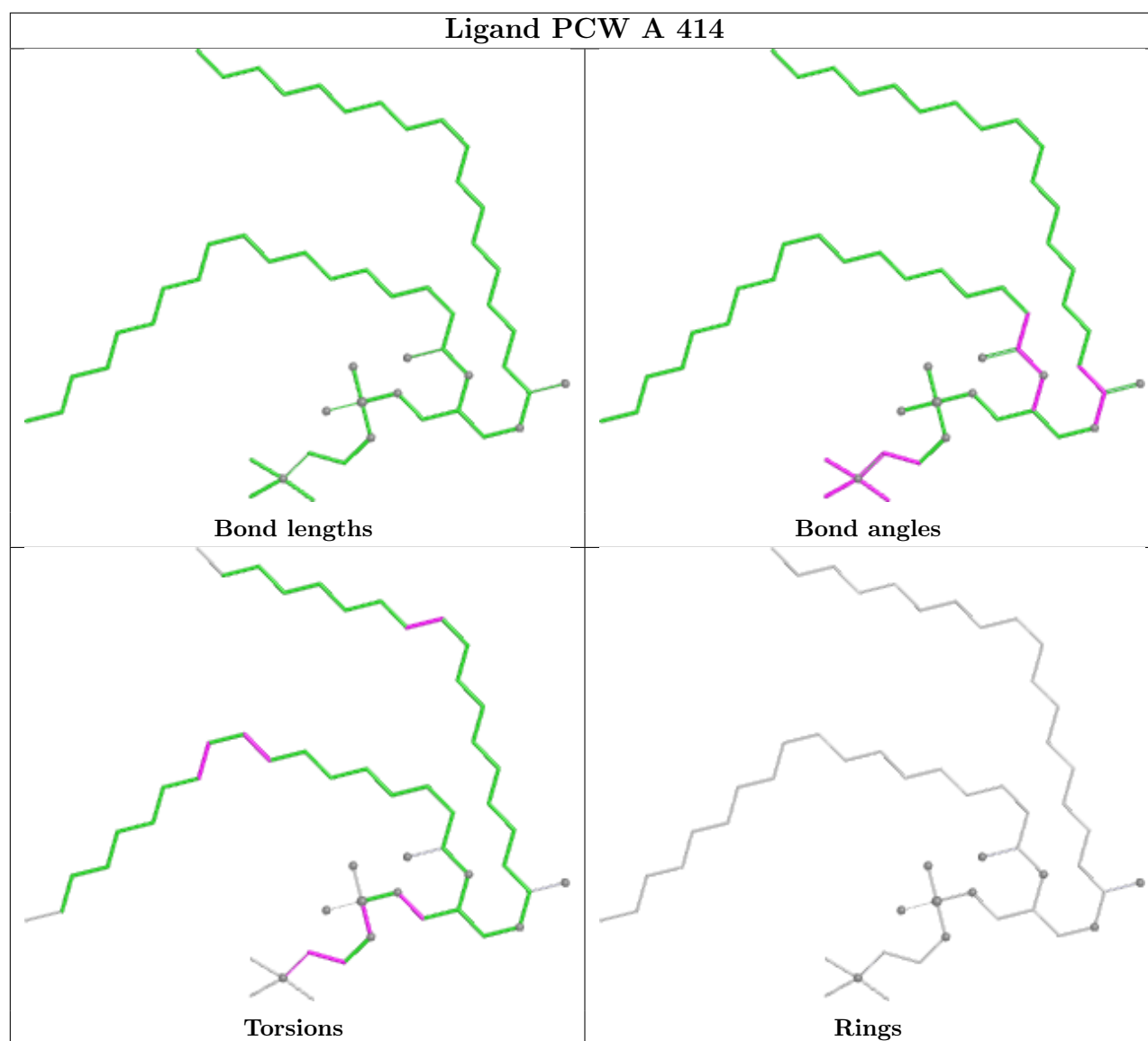












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 6% 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	437
Number of unparsed shifts	0
Number of shifts with mapping errors	120
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 120) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	401	LEU	HD21	0.714	.	.
1	C	401	LEU	HD22	0.714	.	.
1	C	401	LEU	HD23	0.714	.	.
1	B	6	LEU	HD21	0.982	.	.
1	B	6	LEU	HD22	0.982	.	.
1	B	6	LEU	HD23	0.982	.	.
1	B	19	LEU	HD11	0.65	.	.
1	B	19	LEU	HD12	0.65	.	.
1	B	19	LEU	HD13	0.65	.	.
1	B	21	ILE	HD11	0.649	.	1
1	B	21	ILE	HD12	0.649	.	1
1	B	21	ILE	HD13	0.649	.	1
1	B	23	LEU	HD11	-0.175	.	.
1	B	23	LEU	HD12	-0.175	.	.

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Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	23	LEU	HD13	-0.175	.	.
1	B	24	ILE	HD11	0.486	.	1
1	B	24	ILE	HD12	0.486	.	1
1	B	24	ILE	HD13	0.486	.	1
1	B	36	ILE	HD11	0.691	.	1
1	B	36	ILE	HD12	0.691	.	1
1	B	36	ILE	HD13	0.691	.	1
1	B	46	ILE	HD11	0.466	.	1
1	B	46	ILE	HD12	0.466	.	1
1	B	46	ILE	HD13	0.466	.	1
1	B	55	ILE	HD11	0.567	.	1
1	B	55	ILE	HD12	0.567	.	1
1	B	55	ILE	HD13	0.567	.	1
1	B	79	LEU	HD11	0.154	.	.
1	B	79	LEU	HD12	0.154	.	.
1	B	79	LEU	HD13	0.154	.	.
1	B	79	LEU	HD21	0.208	.	.
1	B	79	LEU	HD22	0.208	.	.
1	B	79	LEU	HD23	0.208	.	.
1	B	84	ILE	HD11	0.802	.	1
1	B	84	ILE	HD12	0.802	.	1
1	B	84	ILE	HD13	0.802	.	1
1	B	93	ILE	HD11	0.833	.	1
1	B	93	ILE	HD12	0.833	.	1
1	B	93	ILE	HD13	0.833	.	1
1	B	100	ILE	HD11	0.34	.	1
1	B	100	ILE	HD12	0.34	.	1
1	B	100	ILE	HD13	0.34	.	1
1	B	113	LEU	HD11	1.088	.	.
1	B	113	LEU	HD12	1.088	.	.
1	B	113	LEU	HD13	1.088	.	.
1	B	113	LEU	HD21	1.352	.	.
1	B	113	LEU	HD22	1.352	.	.
1	B	113	LEU	HD23	1.352	.	.
1	B	120	LEU	HD21	0.91	.	.
1	B	120	LEU	HD22	0.91	.	.
1	B	120	LEU	HD23	0.91	.	.
1	B	125	VAL	HG11	-0.082	.	.
1	B	125	VAL	HG12	-0.082	.	.
1	B	125	VAL	HG13	-0.082	.	.
1	B	133	LEU	HD11	0.413	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	133	LEU	HD12	0.413	.	.
1	B	133	LEU	HD13	0.413	.	.
1	B	133	LEU	HD21	0.476	.	.
1	B	133	LEU	HD22	0.476	.	.
1	B	133	LEU	HD23	0.476	.	.
1	B	139	ILE	HD11	0.922	.	1
1	B	139	ILE	HD12	0.922	.	1
1	B	139	ILE	HD13	0.922	.	1
1	B	142	ILE	HD11	0.715	.	1
1	B	142	ILE	HD12	0.715	.	1
1	B	142	ILE	HD13	0.715	.	1
1	B	159	LEU	HD11	0.729	.	.
1	B	159	LEU	HD12	0.729	.	.
1	B	159	LEU	HD13	0.729	.	.
1	B	160	VAL	HG11	0.038	.	.
1	B	160	VAL	HG12	0.038	.	.
1	B	160	VAL	HG13	0.038	.	.
1	B	163	ILE	HD11	0.737	.	1
1	B	163	ILE	HD12	0.737	.	1
1	B	163	ILE	HD13	0.737	.	1
1	D	358	ILE	HD11	0.625	.	1
1	D	358	ILE	HD12	0.625	.	1
1	D	358	ILE	HD13	0.625	.	1
1	D	370	VAL	HG11	0.794	.	.
1	D	370	VAL	HG12	0.794	.	.
1	D	370	VAL	HG13	0.794	.	.
1	D	378	LEU	HD11	0.581	.	.
1	D	378	LEU	HD12	0.581	.	.
1	D	378	LEU	HD13	0.581	.	.
1	D	386	LEU	HD21	0.698	.	.
1	D	386	LEU	HD22	0.698	.	.
1	D	386	LEU	HD23	0.698	.	.
1	D	388	VAL	HG11	1.126	.	.
1	D	388	VAL	HG12	1.126	.	.
1	D	388	VAL	HG13	1.126	.	.
1	D	388	VAL	HG21	1.087	.	.
1	D	388	VAL	HG22	1.087	.	.
1	D	388	VAL	HG23	1.087	.	.
1	D	398	VAL	HG21	0.273	.	.
1	D	398	VAL	HG22	0.273	.	.
1	D	398	VAL	HG23	0.273	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	D	412	LEU	HD11	0.652	.	.
1	D	412	LEU	HD12	0.652	.	.
1	D	412	LEU	HD13	0.652	.	.
1	D	421	LEU	HD11	0.839	.	.
1	D	421	LEU	HD12	0.839	.	.
1	D	421	LEU	HD13	0.839	.	.
1	D	422	ILE	HD11	0.954	.	1
1	D	422	ILE	HD12	0.954	.	1
1	D	422	ILE	HD13	0.954	.	1
1	D	436	LEU	HD21	0.712	.	.
1	D	436	LEU	HD22	0.712	.	.
1	D	436	LEU	HD23	0.712	.	.
1	D	454	ILE	HD11	0.674	.	1
1	D	454	ILE	HD12	0.674	.	1
1	D	454	ILE	HD13	0.674	.	1
1	D	459	LEU	HD11	-0.052	.	.
1	D	459	LEU	HD12	-0.052	.	.
1	D	459	LEU	HD13	-0.052	.	.
1	D	480	VAL	HG11	0.57	.	.
1	D	480	VAL	HG12	0.57	.	.
1	D	480	VAL	HG13	0.57	.	.
1	D	485	VAL	HG11	0.712	.	.
1	D	485	VAL	HG12	0.712	.	.
1	D	485	VAL	HG13	0.712	.	.

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	-0.53 ± 0.24	Should be applied

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 6%, i.e. 555 atoms were assigned a chemical shift out of a possible 9668. 0 out of 128 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	394/3423 (12%)	197/1384 (14%)	0/1374 (0%)	197/665 (30%)
Sidechain	161/5595 (3%)	120/3599 (3%)	41/1743 (2%)	0/253 (0%)
Aromatic	0/650 (0%)	0/325 (0%)	0/295 (0%)	0/30 (0%)
Overall	555/9668 (6%)	317/5308 (6%)	41/3412 (1%)	197/948 (21%)

7.1.4 Statistically unusual chemical shifts [i](#)

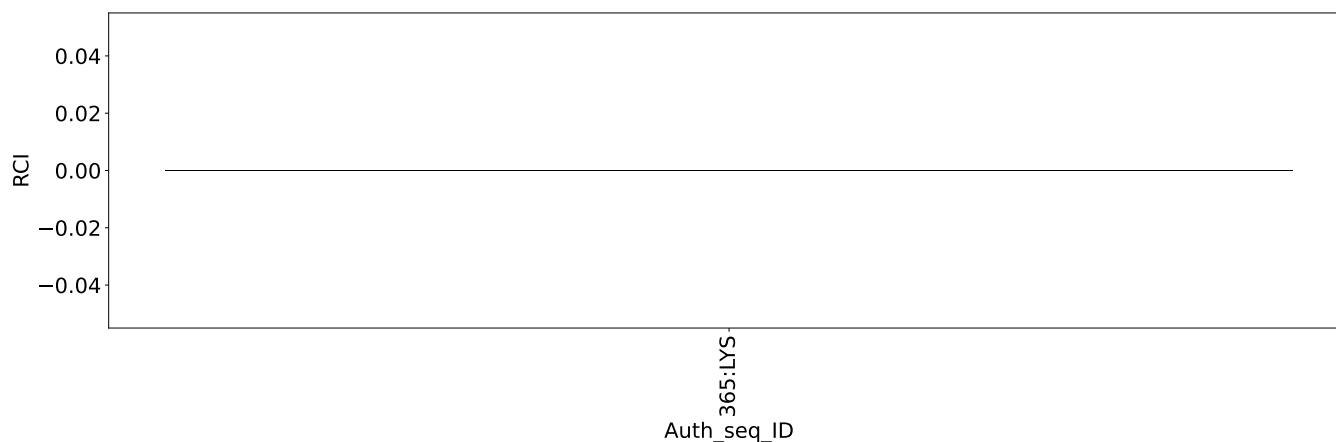
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	48	GLY	N	140.27	91.59 – 127.52	8.6

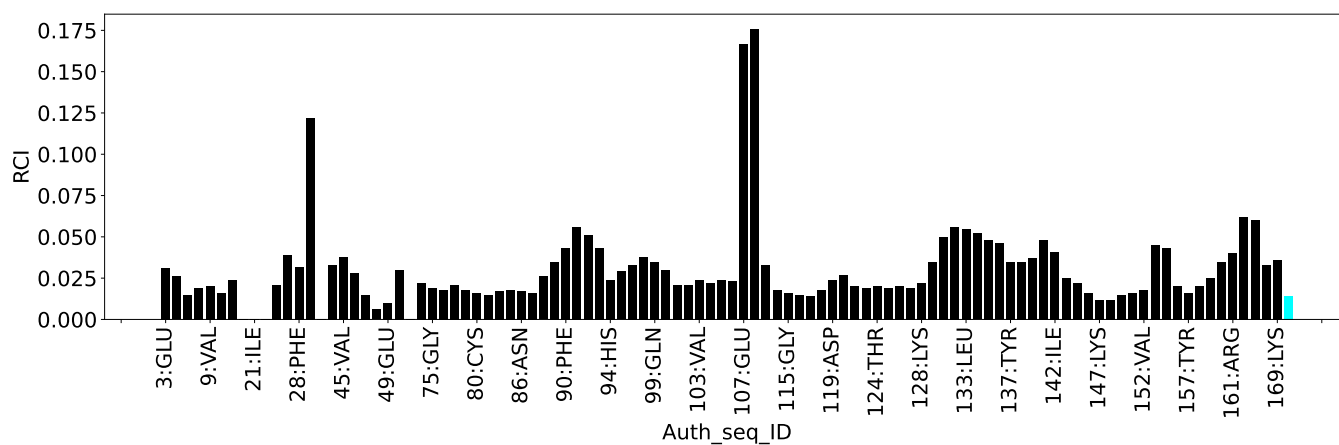
7.1.5 Random Coil Index (RCI) plots [i](#)

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

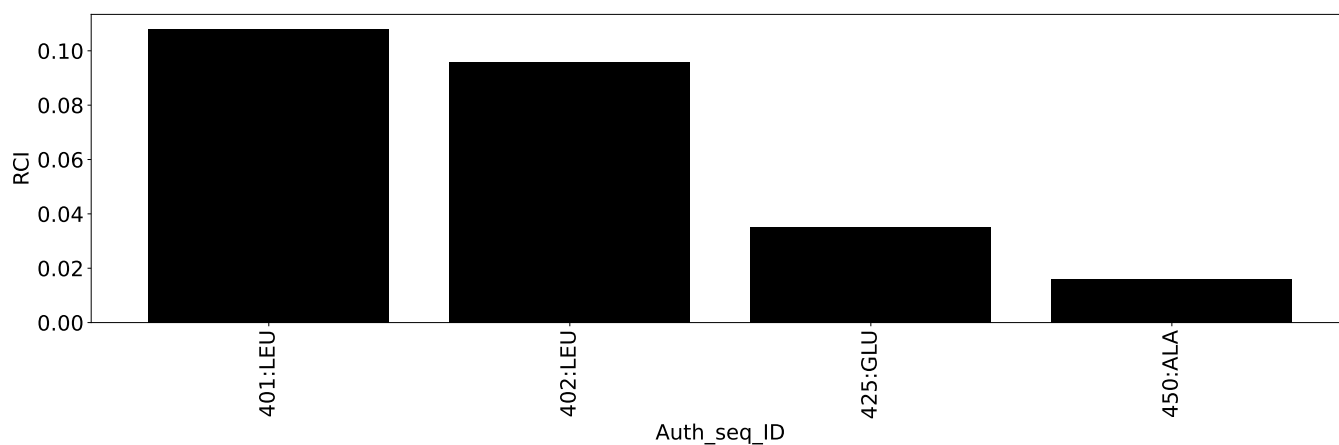
Random coil index (RCI) for chain A:



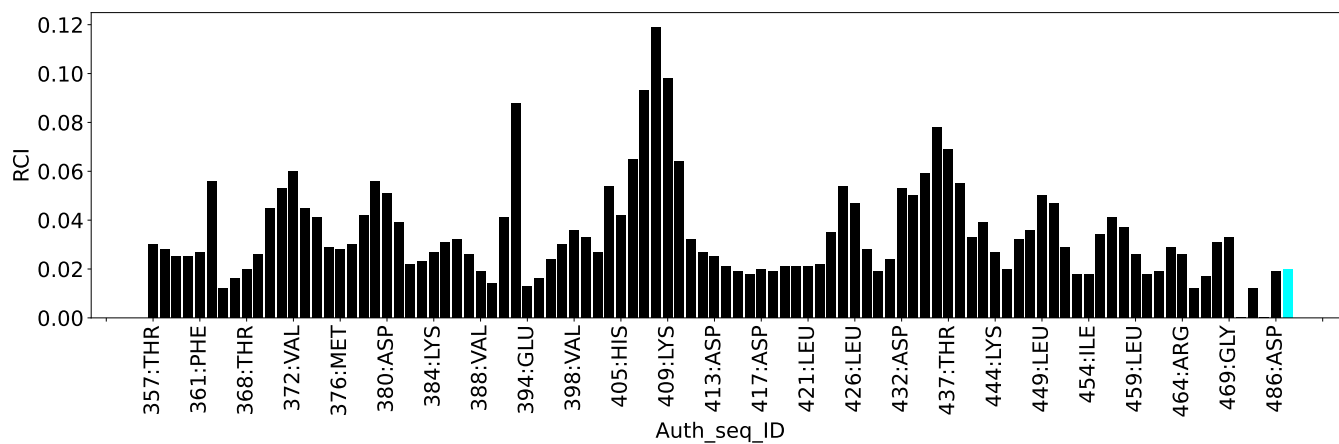
Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	51
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	2
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	49
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	None	None
0.2-0.5 (Medium)	0.1	0.28
>0.5 (Large)	48.5	33.47

8.2.2 Average number of dihedral-angle violations per model [i](#)

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

9 Distance violation analysis ⓘ

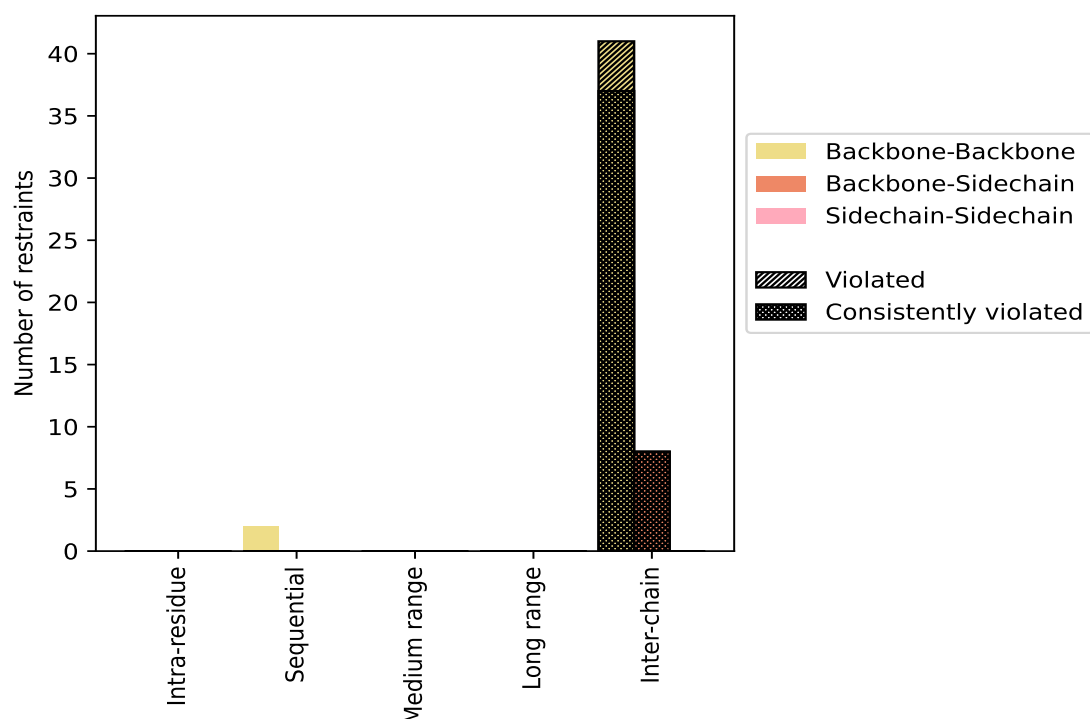
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	2	3.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	3.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	49	96.1	49	100.0	96.1	45	91.8	88.2
Backbone-Backbone	41	80.4	41	100.0	80.4	37	90.2	72.5
Backbone-Sidechain	8	15.7	8	100.0	15.7	8	100.0	15.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	51	100.0	49	96.1	96.1	45	88.2	88.2
Backbone-Backbone	43	84.3	41	95.3	80.4	37	86.0	72.5
Backbone-Sidechain	8	15.7	8	100.0	15.7	8	100.0	15.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

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

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



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

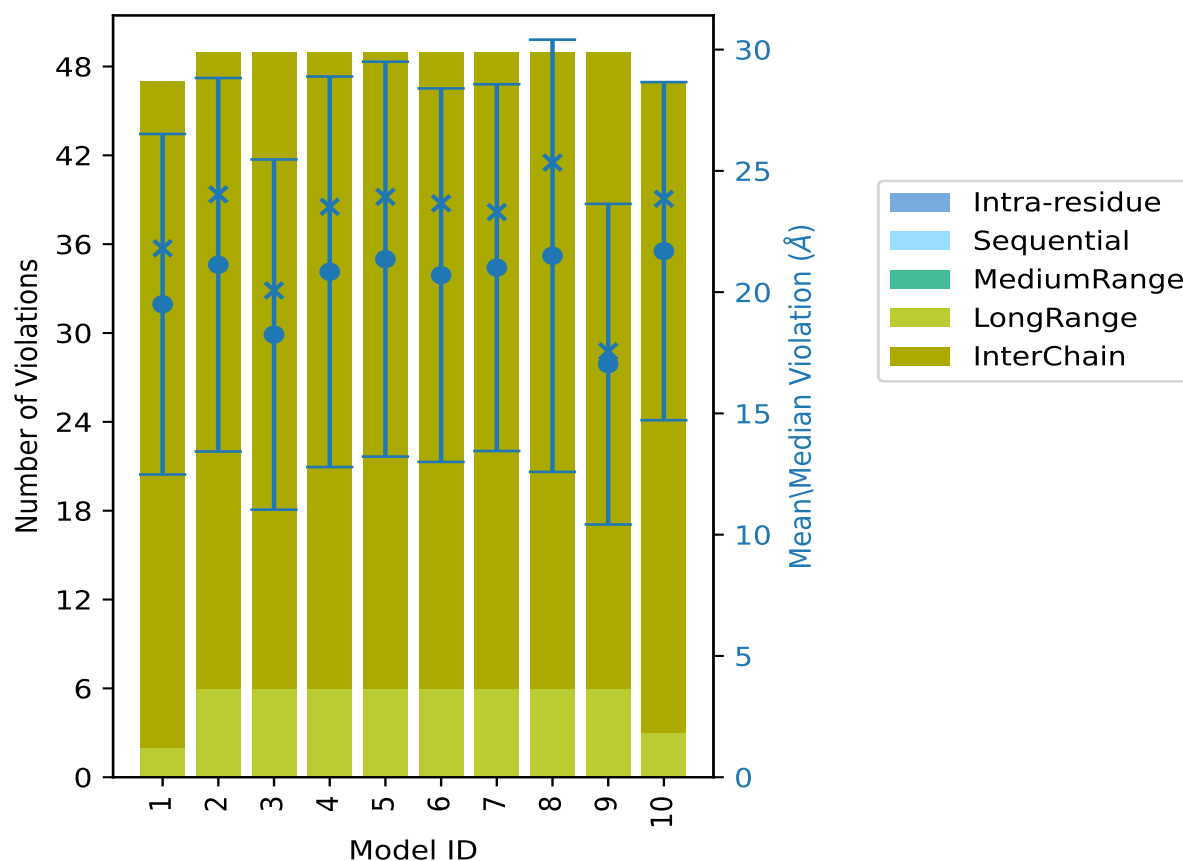
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	2	45	47	19.5	29.19	7.02	21.81
2	0	0	0	6	43	49	21.13	30.89	7.7	24.03
3	0	0	0	6	43	49	18.25	26.66	7.22	20.07
4	0	0	0	6	43	49	20.84	32.18	8.05	23.52
5	0	0	0	6	43	49	21.36	32.99	8.14	23.93
6	0	0	0	6	43	49	20.7	30.52	7.7	23.66
7	0	0	0	6	43	49	21.01	30.05	7.56	23.3
8	0	0	0	6	43	49	21.5	33.47	8.91	25.34
9	0	0	0	6	43	49	17.03	26.91	6.61	17.56
10	0	0	0	3	44	47	21.69	29.56	6.97	23.85

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2(IR:0, SQ:2, MR:0, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0

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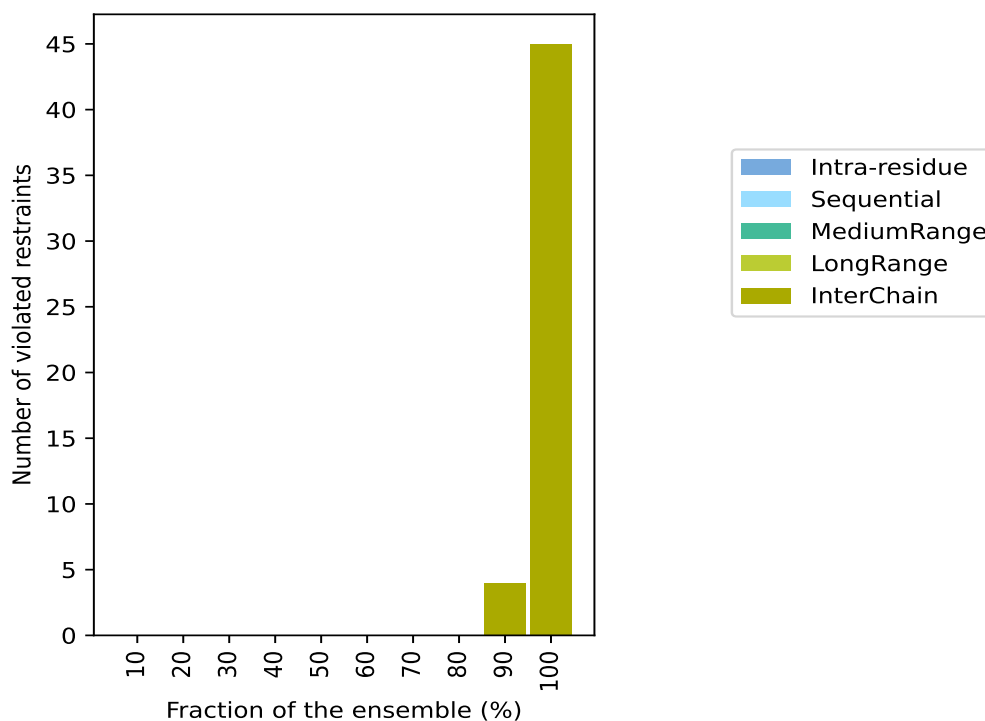
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	4	4	9	90.0
0	0	0	0	45	45	10	100.0

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

⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

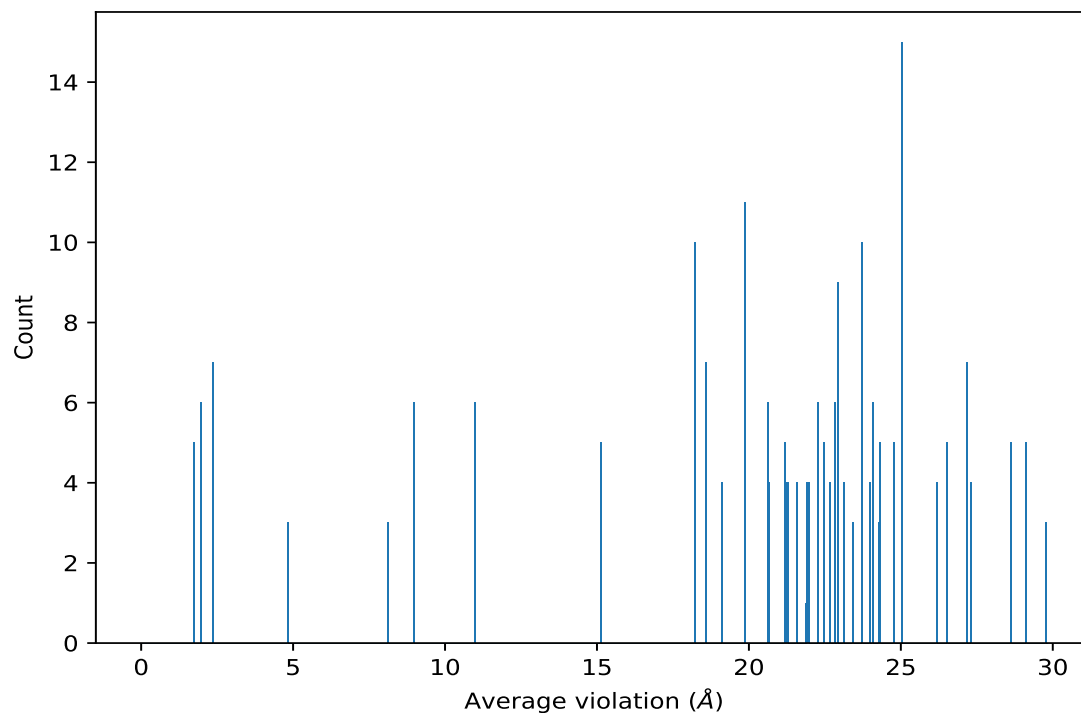


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C6	10	29.79	2.64	30.04
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	10	29.79	2.64	30.04
(1,1)	1:201:A:LEU:N	2:78:B:PHE:CE2	10	29.79	2.64	30.04
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C6	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	2:161:B:ARG:O	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	2:78:B:PHE:CE2	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	2:185:B:CYS:N	10	29.14	1.72	29.44
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C6	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C4	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	4:202:B:PCW:O3	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C2	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	2:185:B:CYS:N	10	28.64	1.43	28.82
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C6	10	27.3	1.66	27.58
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	10	27.3	1.66	27.58

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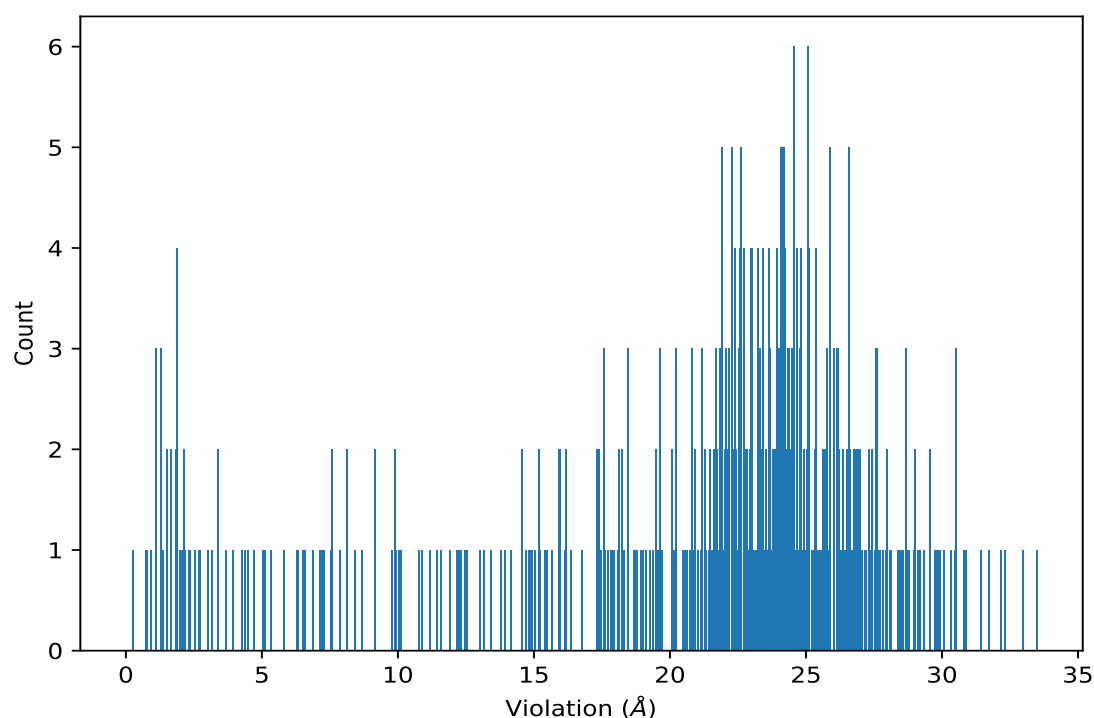
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:204:A:LEU:N	2:161:B:ARG:O	10	27.3	1.66	27.58
(1,4)	1:204:A:LEU:N	2:78:B:PHE:CE2	10	27.3	1.66	27.58
(1,9)	1:209:A:SER:N	4:202:B:PCW:C6	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:O2	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	2:185:B:CYS:H	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:C4	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:O3	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:C2	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	2:185:B:CYS:N	10	27.2	1.97	27.53
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C6	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C4	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	2:185:B:CYS:H	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	4:202:B:PCW:O3	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	2:185:B:CYS:N	10	26.54	1.86	26.95
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C6	10	26.16	1.48	26.35
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	10	26.16	1.48	26.35
(1,7)	1:207:A:TRP:N	4:202:B:PCW:O3	10	26.16	1.48	26.35
(1,7)	1:207:A:TRP:N	2:185:B:CYS:N	10	26.16	1.48	26.35
(1,34)	1:234:A:LYS:O	4:203:B:PCW:C3	10	25.04	1.54	25.54
(1,34)	1:234:A:LYS:O	4:203:B:PCW:O3	10	25.04	1.54	25.54
(1,34)	1:234:A:LYS:O	4:202:B:PCW:O3	10	25.04	1.54	25.54
(1,34)	1:234:A:LYS:O	2:185:B:CYS:HG	10	25.04	1.54	25.54
(1,37)	1:237:A:GLU:O	4:203:B:PCW:C3	10	25.03	1.47	25.27
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	10	25.03	1.47	25.27
(1,37)	1:237:A:GLU:O	2:185:B:CYS:HG	10	25.03	1.47	25.27
(1,37)	1:237:A:GLU:O	4:202:B:PCW:O3	10	25.03	1.47	25.27
(1,12)	1:212:A:SER:N	4:202:B:PCW:C6	10	25.0	2.83	25.7

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	8	33.47
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	5	32.99
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	8	32.34
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	4	32.18
(1,2)	1:202:A:LYS:N	4:202:B:PCW:C4	4	31.71
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C2	8	31.43
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	2	30.89
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	5	30.8
(1,9)	1:209:A:SER:N	4:202:B:PCW:C2	8	30.54
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	8	30.54

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found