wwPDB NMR Structure Validation Summary Report (i)

Jun 24, 2024 – 11:20 AM EDT

PDB ID	:	6W4E
BMRB ID	:	30734
Title	:	NMR-driven structure of KRAS4B-GTP 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

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

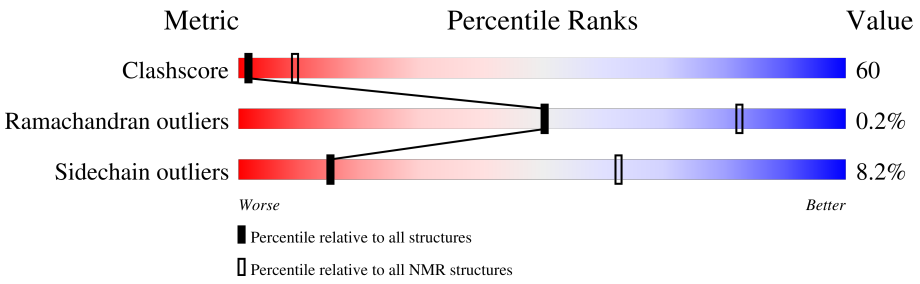
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	200	86% 12% ••
1	D	200	87% 12% •
2	B	185	78% 11% 10% •
2	C	185	74% 16% 9% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:202-A:398, D:399-D:596 (395)	0.33	15
2	B:1-B:165, C:1-C:167 (332)	0.69	16

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

3 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12112 atoms, of which 1536 are hydrogens and 0 are deuteriums.

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called GTPase KRas.

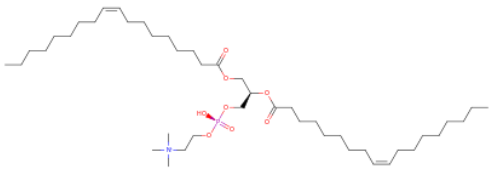
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	184	1830	920	358	256	289	7	0
2	C	184	1830	920	358	256	289	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP P01116
B	12	ASP	GLY	conflict	UNP P01116
C	1	SER	-	expression tag	UNP P01116
C	12	ASP	GLY	conflict	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

PCW



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

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

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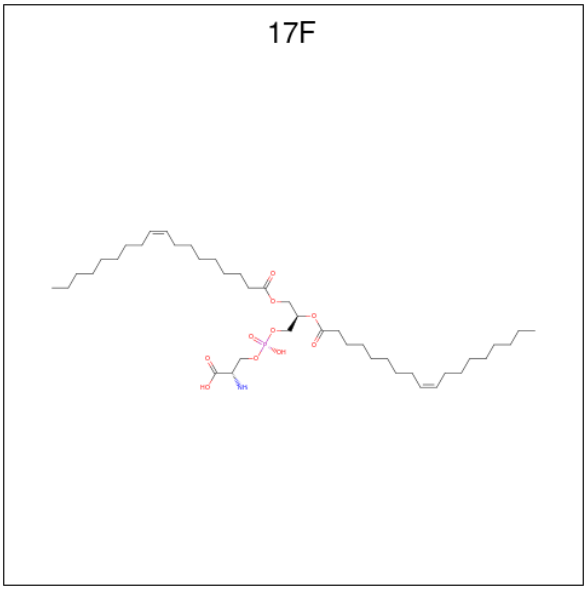
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	1	8	1
			Total	C	N	O	P
3	C	1	54	44	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: $C_{42}H_{78}NO_{10}P$).



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

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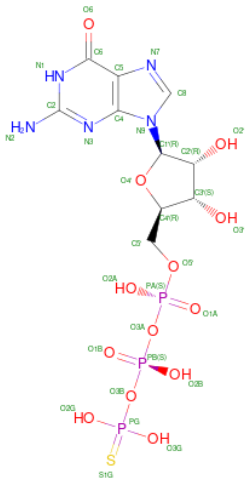
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	D	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	B	1	57	42	3	1	10	1
			Total	C	H	N	O	P
4	B	1	57	42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

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).

GSP



Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
5	B	1	38	10	6	5	13	3	1
5	C	1	38	10	6	5	13	3	1

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

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

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Apolipoprotein A-I

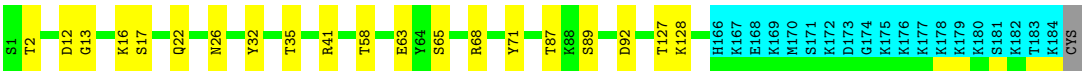
Chain A:

• Molecule 1: Apolipoprotein A-I

Chain D:

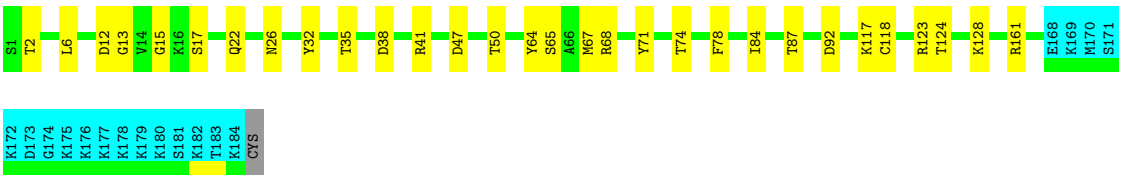
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

Chain C:

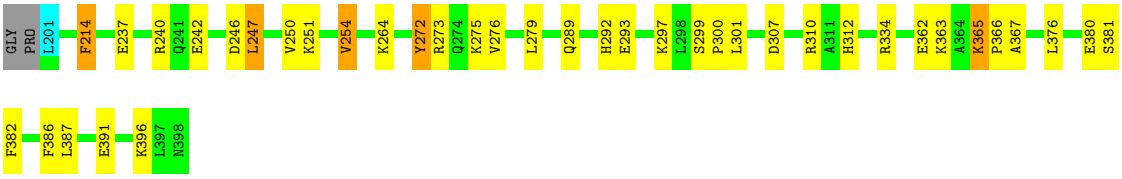


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 15. Colouring as in section 4.1 above.

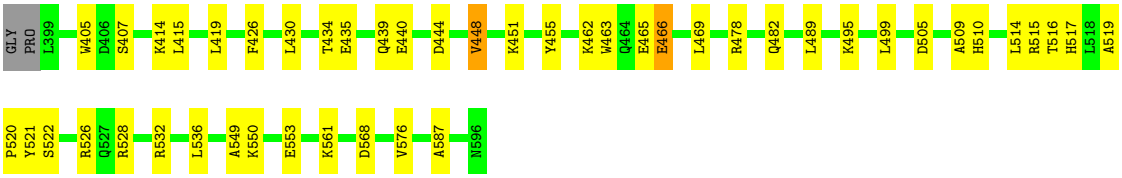
• Molecule 1: Apolipoprotein A-I

Chain A:



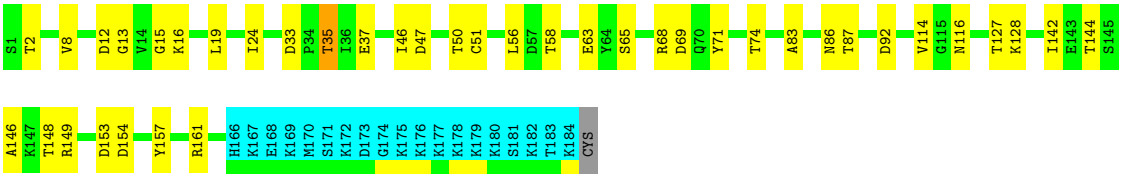
• Molecule 1: Apolipoprotein A-I

Chain D:



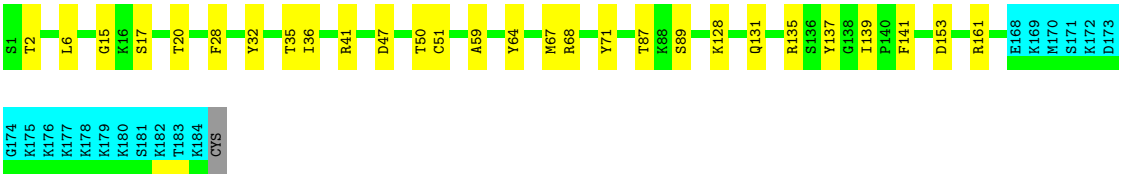
• Molecule 2: GTPase KRas

Chain B:



• Molecule 2: GTPase KRas

Chain C:



5 Refinement protocol and experimental data overview (i)

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

Of the 3000 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	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality (i)

6.1 Standard geometry (i)

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

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1615	380	1616	24±4
1	D	1623	379	1626	21±4
2	B	1315	302	1290	18±4
2	C	1334	308	1310	20±3
3	A	1026	0	1520	362±21
3	B	324	0	480	159±15
3	C	648	0	960	324±22
3	D	1458	0	2160	557±21
4	A	162	9	228	62±11
4	B	162	9	228	69±10
4	C	270	15	380	109±13
4	D	270	15	380	106±15
5	B	32	6	12	9±3
5	C	32	6	12	9±2
6	B	1	0	0	1±0
6	C	1	0	0	1±0
All	All	205460	28580	244046	27079

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

5 of 9358 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:626:PCW:C20	3:D:626:PCW:H251	1.20	1.67	15	1
3:A:414:PCW:H472	3:A:414:PCW:H432	1.16	1.18	16	20
3:A:409:PCW:C19	3:A:409:PCW:H142	1.15	1.72	14	20
3:A:420:PCW:H372	3:D:618:PCW:H431	1.15	1.16	18	18
3:D:624:PCW:H20	3:D:624:PCW:H241	1.15	1.17	10	20

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/200 (98%)	191±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	32	76
1	D	196/200 (98%)	190±1 (97±1%)	5±1 (3±1%)	0±0 (0±0%)	54	85
2	B	164/185 (89%)	154±2 (94±1%)	10±2 (6±1%)	0±1 (0±0%)	50	82
2	C	166/185 (90%)	158±2 (95±1%)	8±2 (5±1%)	0±0 (0±0%)	54	85
All	All	14440/15400 (94%)	13864 (96%)	542 (4%)	34 (0%)	50	82

5 of 9 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	B	37	GLU	3
1	D	420	GLY	3
2	C	37	GLU	2
1	D	498	PRO	2

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	173/175 (99%)	162±2 (93±1%)	12±2 (7±1%)	20	69
1	D	174/175 (99%)	161±2 (93±1%)	13±2 (7±1%)	18	66
2	B	146/165 (88%)	131±3 (90±2%)	15±3 (10±2%)	11	56
2	C	148/165 (90%)	135±3 (91±2%)	13±3 (9±2%)	13	59
All	All	12820/13600 (94%)	11771 (92%)	1049 (8%)	15	62

5 of 232 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	550	LYS	18
1	A	272	TYR	17
2	B	2	THR	16
2	B	87	THR	16
1	D	516	THR	15

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	C	216	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	612	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	602	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	214	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	605	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	207	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	210	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	611	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	205	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	401	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	629	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	C	211	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	632	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	B	210	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	C	213	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	610	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	609	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	208	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	219	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	420	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	B	211	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	627	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	601	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	607	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	205	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	B	209	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	619	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	416	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	608	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	617	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	413	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	206	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	407	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	421	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	616	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	603	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	415	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	A	402	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	623	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	626	-	53,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	C	209	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	408	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	412	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	405	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	620	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	422	-	52,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	614	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	217	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	404	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	613	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	604	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	625	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	414	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	418	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	419	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	403	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	206	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	624	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	606	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	630	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	C	208	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	628	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	C	218	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	622	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	411	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	410	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	621	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	618	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	215	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	615	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	212	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	417	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	GSP	C	201	6	29,34,34	1.41±0.02	2±1 (8±2%)
4	17F	D	631	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	GSP	B	201	-	29,34,34	1.41±0.02	2±1 (8±2%)
3	PCW	C	207	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	409	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	406	-	53,53,53	0.82±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types,

if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	C	216	-	59,61,61	2.67±0.00	10±0 (17±0%)
3	PCW	D	612	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	D	602	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	17F	C	214	-	54,60,60	1.12±0.03	4±0 (7±0%)
3	PCW	D	605	-	59,61,61	2.63±0.01	7±0 (12±0%)
3	PCW	B	207	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	C	210	-	59,61,61	2.60±0.01	7±0 (11±0%)
3	PCW	D	611	-	59,61,61	2.61±0.01	7±1 (11±0%)
3	PCW	B	203	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	B	205	-	59,61,61	2.68±0.01	10±1 (17±0%)
3	PCW	A	401	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	17F	D	629	-	54,60,60	1.12±0.02	4±0 (6±0%)
3	PCW	C	211	-	59,61,61	2.60±0.02	6±0 (10±0%)
4	17F	D	632	-	54,60,60	1.09±0.05	4±0 (8±0%)
4	17F	B	210	-	54,60,60	1.13±0.02	4±1 (8±1%)
4	17F	C	213	-	54,60,60	1.10±0.03	4±0 (7±0%)
3	PCW	D	610	-	59,61,61	2.59±0.01	6±1 (10±0%)
3	PCW	D	609	-	59,61,61	2.59±0.00	7±1 (11±0%)
3	PCW	B	208	-	59,61,61	2.58±0.01	6±1 (10±1%)
4	17F	C	219	-	54,60,60	1.09±0.04	4±0 (8±0%)
3	PCW	A	420	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	B	204	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	B	211	-	54,60,60	1.16±0.03	4±0 (7±0%)
3	PCW	D	627	-	59,61,61	2.60±0.02	7±1 (12±1%)
3	PCW	D	601	-	59,61,61	2.60±0.01	7±1 (11±1%)
3	PCW	D	607	-	59,61,61	2.59±0.01	7±0 (11±0%)
3	PCW	C	205	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	C	204	-	59,61,61	2.60±0.01	6±1 (10±0%)
4	17F	B	209	-	54,60,60	1.12±0.03	5±0 (9±0%)
3	PCW	D	619	-	59,61,61	2.61±0.01	7±0 (12±0%)
4	17F	A	416	-	54,60,60	1.13±0.04	4±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	D	608	-	59,61,61	2.60±0.01	7±1 (11±1%)
3	PCW	D	617	-	59,61,61	2.58±0.01	6±0 (10±0%)
3	PCW	A	413	-	59,61,61	2.59±0.00	6±0 (10±0%)
3	PCW	C	206	-	59,61,61	2.60±0.01	7±0 (11±0%)
3	PCW	A	407	-	59,61,61	2.59±0.02	6±1 (10±0%)
3	PCW	A	421	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	D	616	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	D	603	-	59,61,61	2.61±0.02	7±1 (11±1%)
4	17F	A	415	-	54,60,60	1.34±0.04	8±0 (15±0%)
3	PCW	A	402	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	623	-	59,61,61	2.58±0.02	6±0 (10±0%)
3	PCW	D	626	-	59,61,61	2.62±0.01	7±1 (11±0%)
3	PCW	C	209	-	59,61,61	2.58±0.01	6±0 (10±0%)
3	PCW	A	408	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	A	412	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	A	405	-	59,61,61	2.60±0.01	6±1 (10±0%)
3	PCW	D	620	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	17F	A	422	-	54,60,60	1.12±0.03	4±0 (7±0%)
3	PCW	D	614	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	C	217	-	59,61,61	2.61±0.01	8±0 (12±0%)
3	PCW	A	404	-	59,61,61	2.58±0.02	7±1 (11±1%)
3	PCW	D	613	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	D	604	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	625	-	59,61,61	2.57±0.01	6±1 (10±1%)
3	PCW	A	414	-	59,61,61	2.62±0.02	7±1 (11±0%)
3	PCW	A	418	-	59,61,61	2.61±0.02	7±1 (11±0%)
3	PCW	A	419	-	59,61,61	2.60±0.01	7±0 (12±0%)
3	PCW	A	403	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	B	206	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	C	203	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	D	624	-	59,61,61	2.58±0.02	6±0 (10±0%)
3	PCW	D	606	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	D	630	-	54,60,60	1.33±0.03	8±0 (15±0%)
3	PCW	C	208	-	59,61,61	2.60±0.01	7±1 (11±0%)
4	17F	D	628	-	54,60,60	1.10±0.02	4±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	17F	C	218	-	54,60,60	1.12±0.02	5±1 (9±1%)
3	PCW	D	622	-	59,61,61	2.57±0.01	6±0 (10±0%)
3	PCW	A	411	-	59,61,61	2.62±0.01	6±0 (10±0%)
3	PCW	A	410	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	621	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	D	618	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	17F	C	215	-	54,60,60	1.23±0.03	4±0 (7±0%)
3	PCW	D	615	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	C	212	-	59,61,61	2.60±0.01	7±0 (11±0%)
3	PCW	A	417	-	59,61,61	2.59±0.02	6±1 (11±1%)
5	GSP	C	201	6	32,54,54	1.58±0.04	6±0 (18±0%)
4	17F	D	631	-	54,60,60	1.15±0.03	4±0 (7±0%)
5	GSP	B	201	-	32,54,54	1.67±0.24	6±0 (18±0%)
3	PCW	C	207	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	A	409	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	A	406	-	59,61,61	2.60±0.01	6±0 (10±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	608	-	-	0±0,57,57,57	-
3	PCW	C	216	-	-	0±0,57,57,57	-
4	17F	B	211	-	-	0±0,59,59,59	-
3	PCW	D	613	-	-	0±0,57,57,57	-
3	PCW	D	605	-	-	0±0,57,57,57	-
3	PCW	B	206	-	-	0±0,57,57,57	-
3	PCW	D	617	-	-	0±0,57,57,57	-
3	PCW	D	603	-	-	0±0,57,57,57	-
3	PCW	D	614	-	-	0±0,57,57,57	-
4	17F	B	210	-	-	1±0,59,59,59	-
3	PCW	D	625	-	-	0±0,57,57,57	-
3	PCW	A	411	-	-	0±0,57,57,57	-
3	PCW	D	601	-	-	0±0,57,57,57	-
4	17F	C	215	-	-	1±0,59,59,59	-
3	PCW	D	622	-	-	0±0,57,57,57	-
3	PCW	C	203	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	D	610	-	-	0±0,57,57,57	-
3	PCW	C	217	-	-	0±0,57,57,57	-
3	PCW	D	606	-	-	0±0,57,57,57	-
3	PCW	D	615	-	-	0±0,57,57,57	-
3	PCW	A	404	-	-	0±0,57,57,57	-
3	PCW	B	208	-	-	0±0,57,57,57	-
3	PCW	B	205	-	-	0±0,57,57,57	-
3	PCW	D	621	-	-	0±0,57,57,57	-
3	PCW	C	208	-	-	0±0,57,57,57	-
3	PCW	C	212	-	-	0±0,57,57,57	-
4	17F	D	629	-	-	0±0,59,59,59	-
3	PCW	C	209	-	-	0±0,57,57,57	-
3	PCW	A	421	-	-	0±0,57,57,57	-
3	PCW	C	204	-	-	0±0,57,57,57	-
3	PCW	D	619	-	-	0±0,57,57,57	-
3	PCW	D	604	-	-	0±0,57,57,57	-
3	PCW	A	418	-	-	0±0,57,57,57	-
3	PCW	D	624	-	-	0±0,57,57,57	-
3	PCW	A	402	-	-	0±0,57,57,57	-
4	17F	C	213	-	-	0±0,59,59,59	-
3	PCW	A	420	-	-	0±0,57,57,57	-
3	PCW	A	403	-	-	0±0,57,57,57	-
3	PCW	A	419	-	-	0±0,57,57,57	-
3	PCW	B	203	-	-	0±0,57,57,57	-
5	GSP	B	201	-	-	0±0,17,38,38	0±0,3,3,3
4	17F	D	632	-	-	0±0,59,59,59	-
3	PCW	A	409	-	-	0±0,57,57,57	-
3	PCW	A	417	-	-	0±0,57,57,57	-
4	17F	C	214	-	-	0±0,59,59,59	-
4	17F	A	422	-	-	0±0,59,59,59	-
3	PCW	A	413	-	-	0±0,57,57,57	-
3	PCW	D	609	-	-	0±0,57,57,57	-
3	PCW	C	207	-	-	0±0,57,57,57	-
3	PCW	A	412	-	-	0±0,57,57,57	-
3	PCW	D	626	-	-	0±0,57,57,57	-
3	PCW	C	211	-	-	0±0,57,57,57	-
3	PCW	A	405	-	-	0±0,57,57,57	-
3	PCW	D	602	-	-	0±0,57,57,57	-
4	17F	B	209	-	-	0±0,59,59,59	-
3	PCW	D	623	-	-	0±0,57,57,57	-
4	17F	D	628	-	-	0±0,59,59,59	-
3	PCW	D	627	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GSP	C	201	6	-	0±0,17,38,38	0±0,3,3,3
3	PCW	A	407	-	-	0±0,57,57,57	-
3	PCW	D	618	-	-	0±0,57,57,57	-
3	PCW	D	616	-	-	0±0,57,57,57	-
3	PCW	D	612	-	-	0±0,57,57,57	-
3	PCW	B	204	-	-	0±0,57,57,57	-
3	PCW	C	205	-	-	0±0,57,57,57	-
4	17F	A	415	-	-	0±0,59,59,59	-
4	17F	C	219	-	-	0±0,59,59,59	-
3	PCW	D	620	-	-	0±0,57,57,57	-
3	PCW	B	207	-	-	0±0,57,57,57	-
3	PCW	A	414	-	-	0±0,57,57,57	-
3	PCW	C	206	-	-	0±0,57,57,57	-
3	PCW	A	410	-	-	0±0,57,57,57	-
4	17F	A	416	-	-	0±0,59,59,59	-
3	PCW	A	401	-	-	0±0,57,57,57	-
3	PCW	C	210	-	-	0±0,57,57,57	-
3	PCW	D	607	-	-	0±0,57,57,57	-
4	17F	D	631	-	-	0±0,59,59,59	-
3	PCW	D	611	-	-	0±0,57,57,57	-
4	17F	D	630	-	-	0±0,59,59,59	-
3	PCW	A	408	-	-	0±0,57,57,57	-
4	17F	C	218	-	-	1±0,59,59,59	-
3	PCW	A	406	-	-	0±0,57,57,57	-

5 of 10 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	C	201	GSP	C5-C6	4.25	1.39	1.47	14	20
5	B	201	GSP	C5-C6	4.25	1.39	1.47	19	20
5	C	201	GSP	O4'-C1'	2.71	1.44	1.40	10	20
5	B	201	GSP	O4'-C1'	2.64	1.44	1.40	17	20
5	C	201	GSP	PA-O3A	2.17	1.61	1.59	18	2

5 of 611 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	D	621	PCW	C8-N-C7	17.71	62.46	108.98	15	20
3	D	616	PCW	C8-N-C7	17.70	62.48	108.98	19	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	212	PCW	C8-N-C7	17.69	62.50	108.98	10	20
3	D	615	PCW	C8-N-C7	17.69	62.51	108.98	18	20
3	D	622	PCW	C8-N-C7	17.69	62.51	108.98	11	20

There are no chirality outliers.

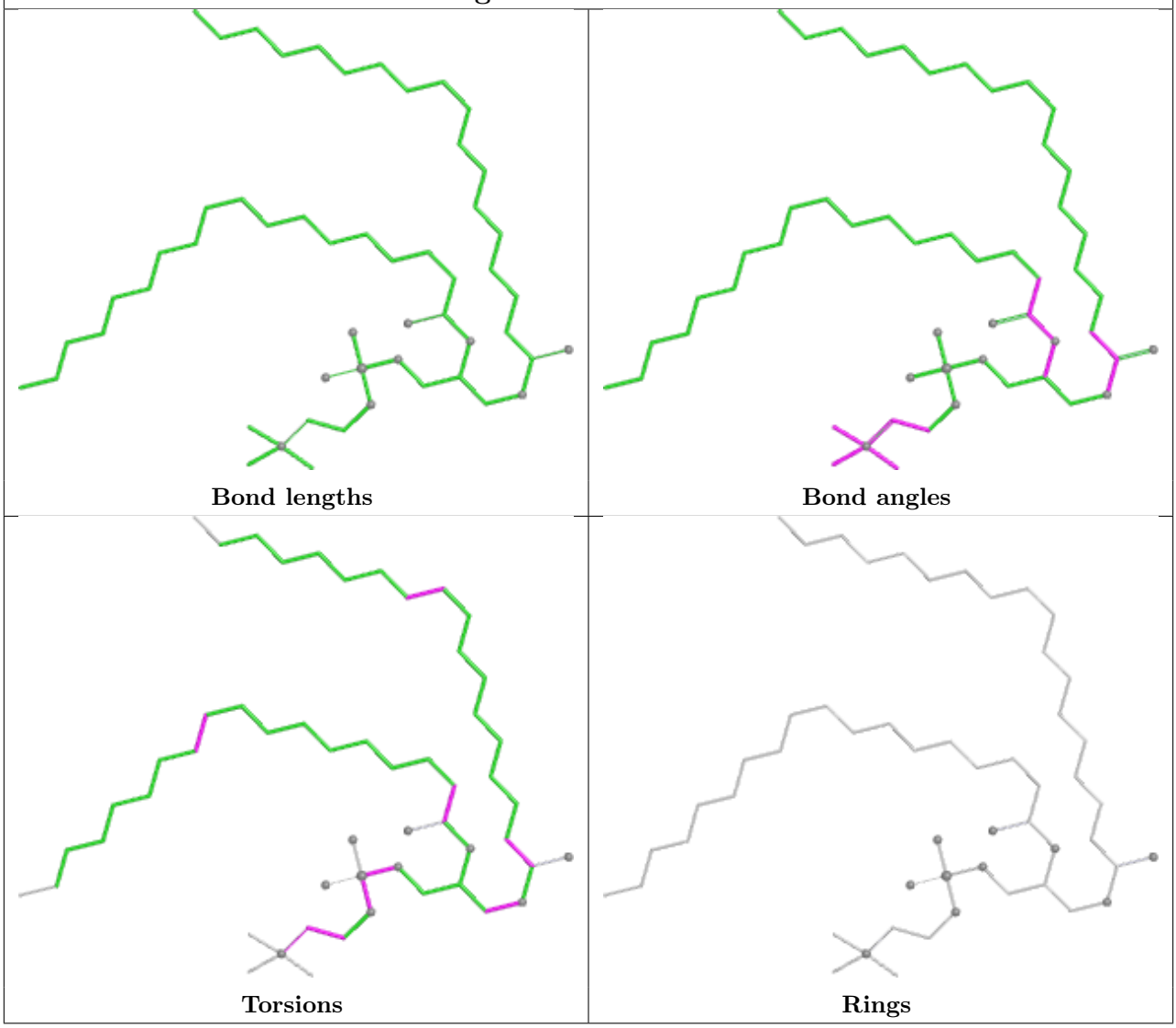
5 of 6 unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
4	B	210	17F	O10-C17-O9-C5	20
4	C	215	17F	O10-C17-O9-C5	20
4	C	218	17F	O10-C17-O9-C5	20
4	C	218	17F	C18-C17-O9-C5	8
4	C	215	17F	C18-C17-O9-C5	3

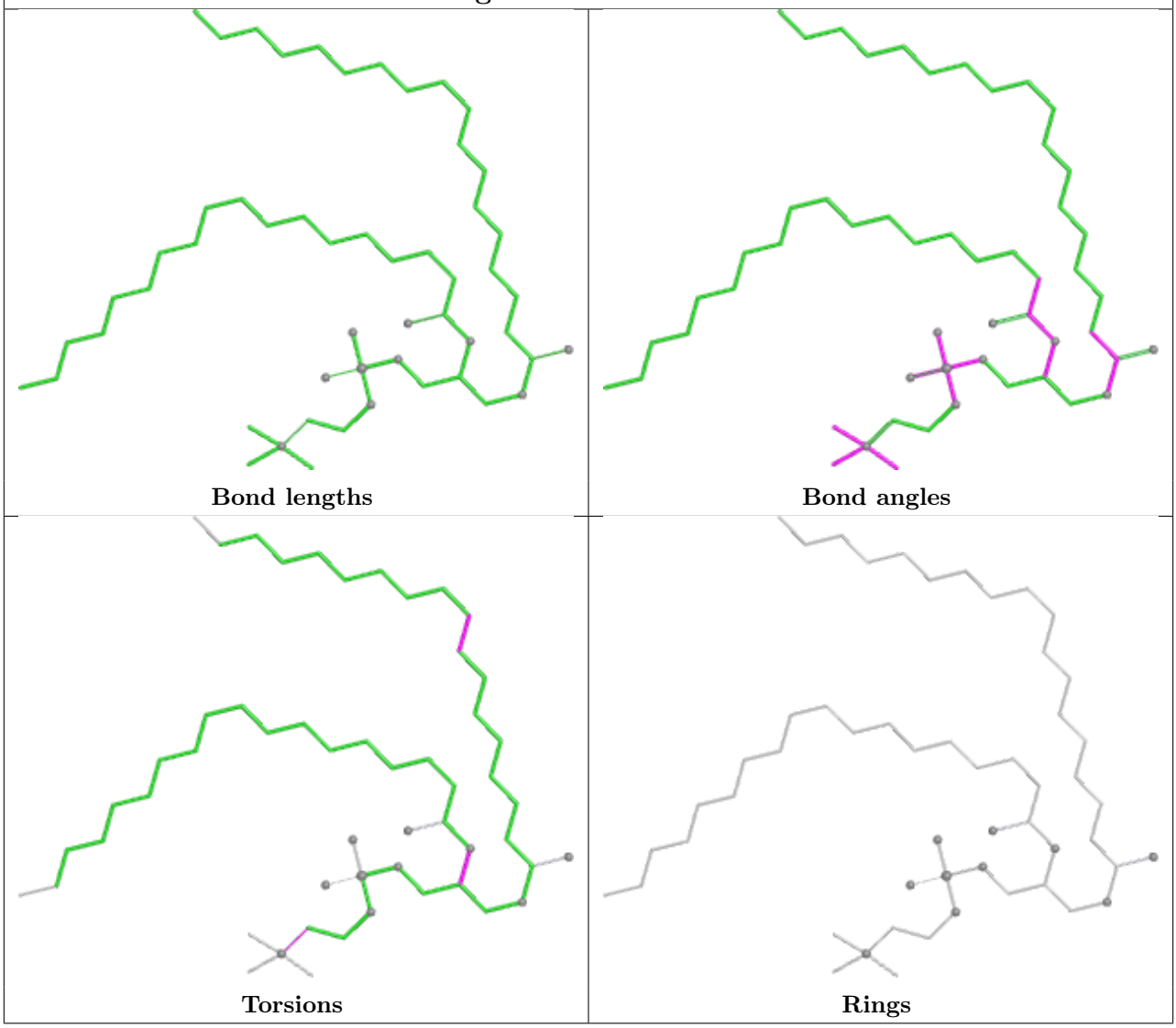
There are no ring outliers.

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 then 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.

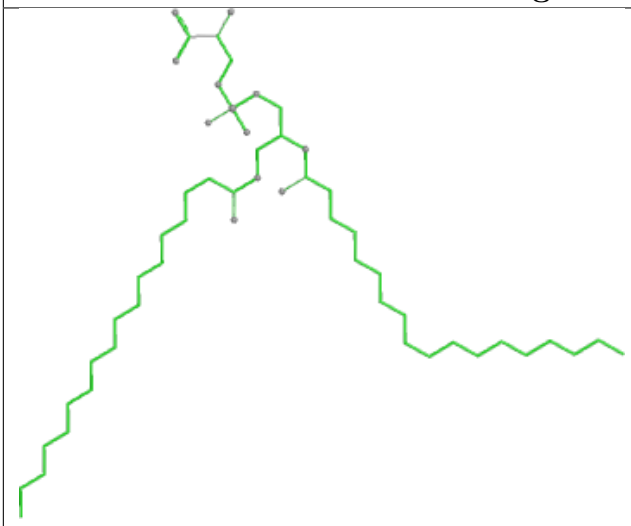
Ligand PCW D 608



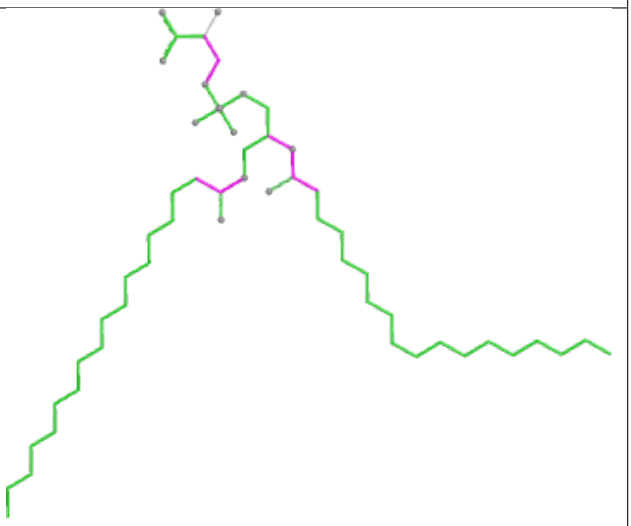
Ligand PCW C 216



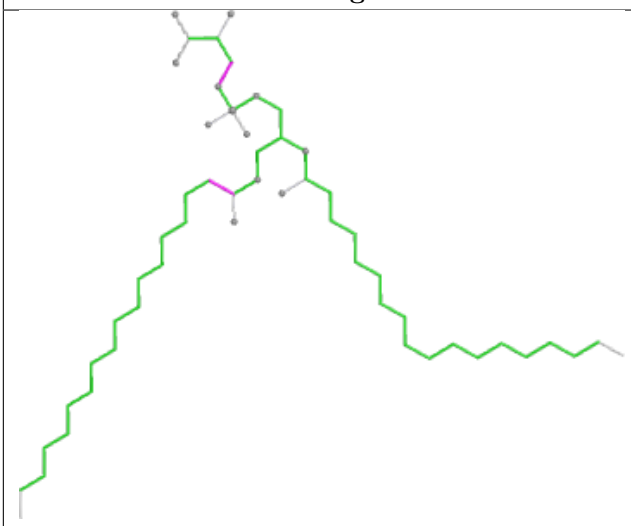
Ligand 17F B 211



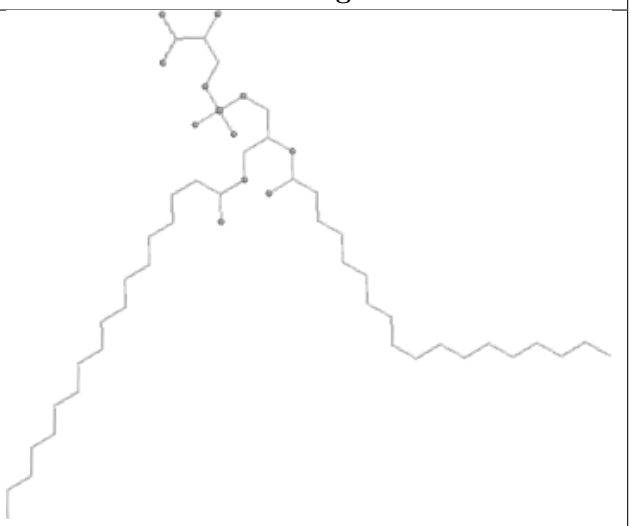
Bond lengths



Bond angles

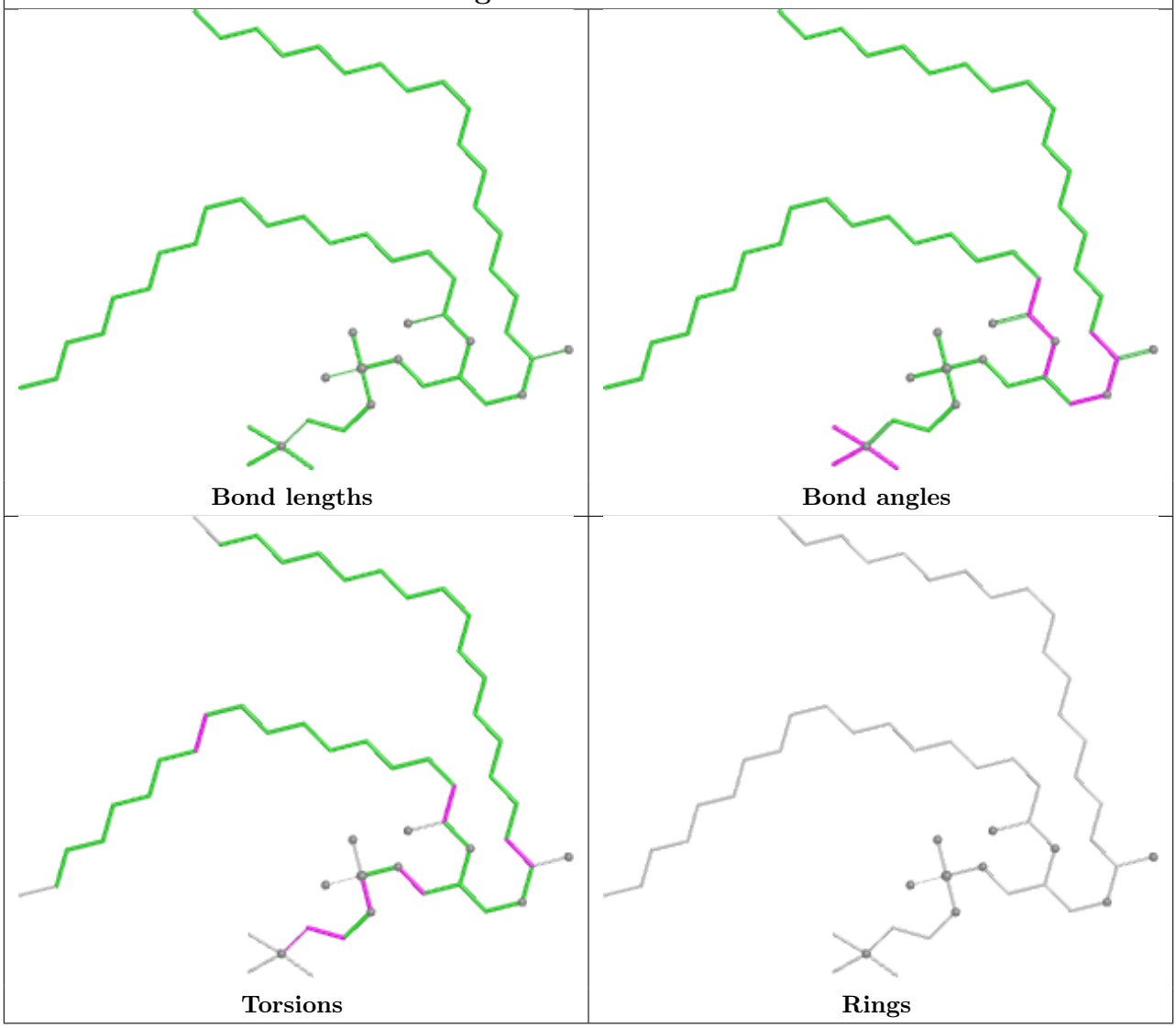


Torsions

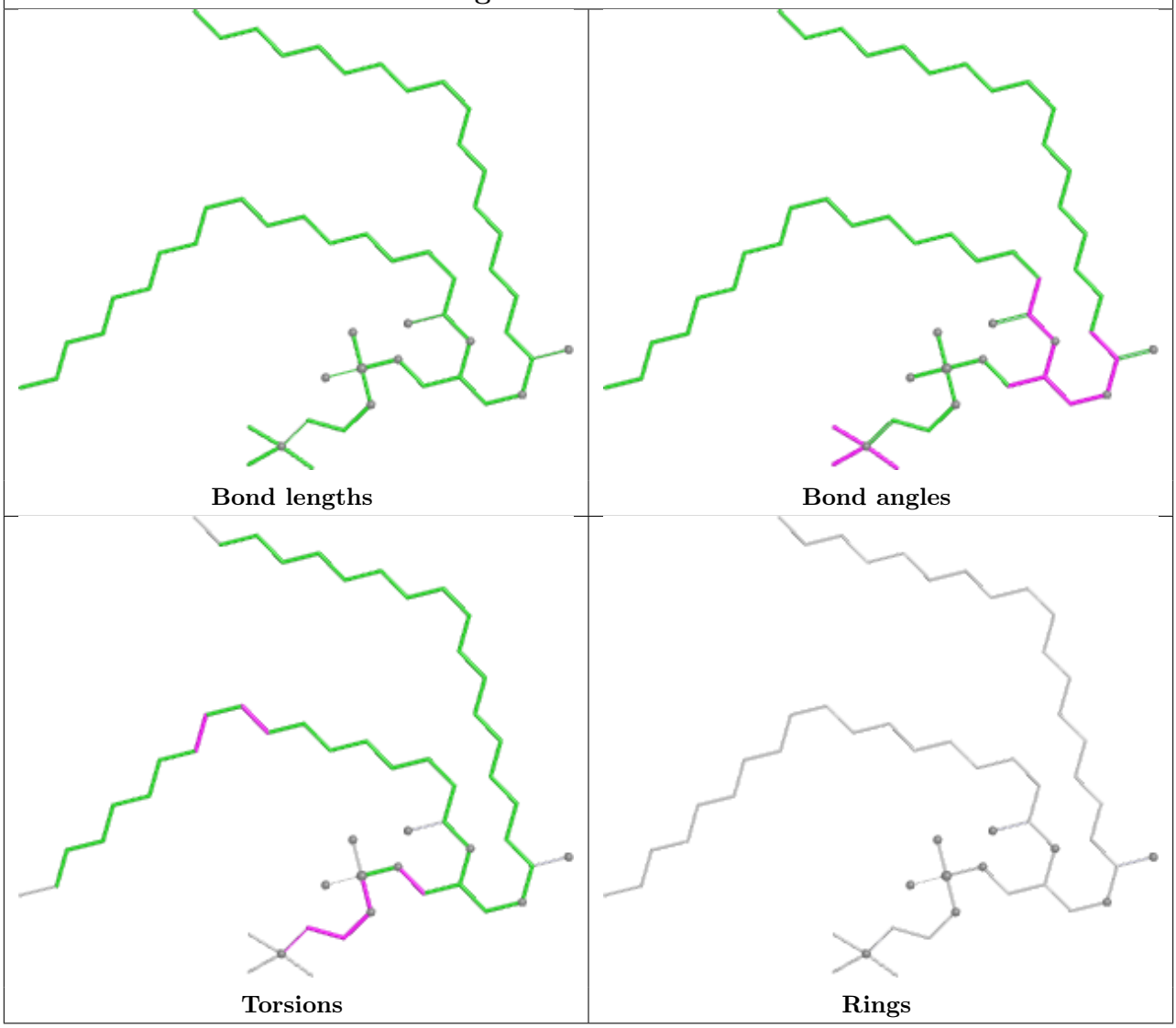


Rings

Ligand PCW D 613



Ligand PCW D 605



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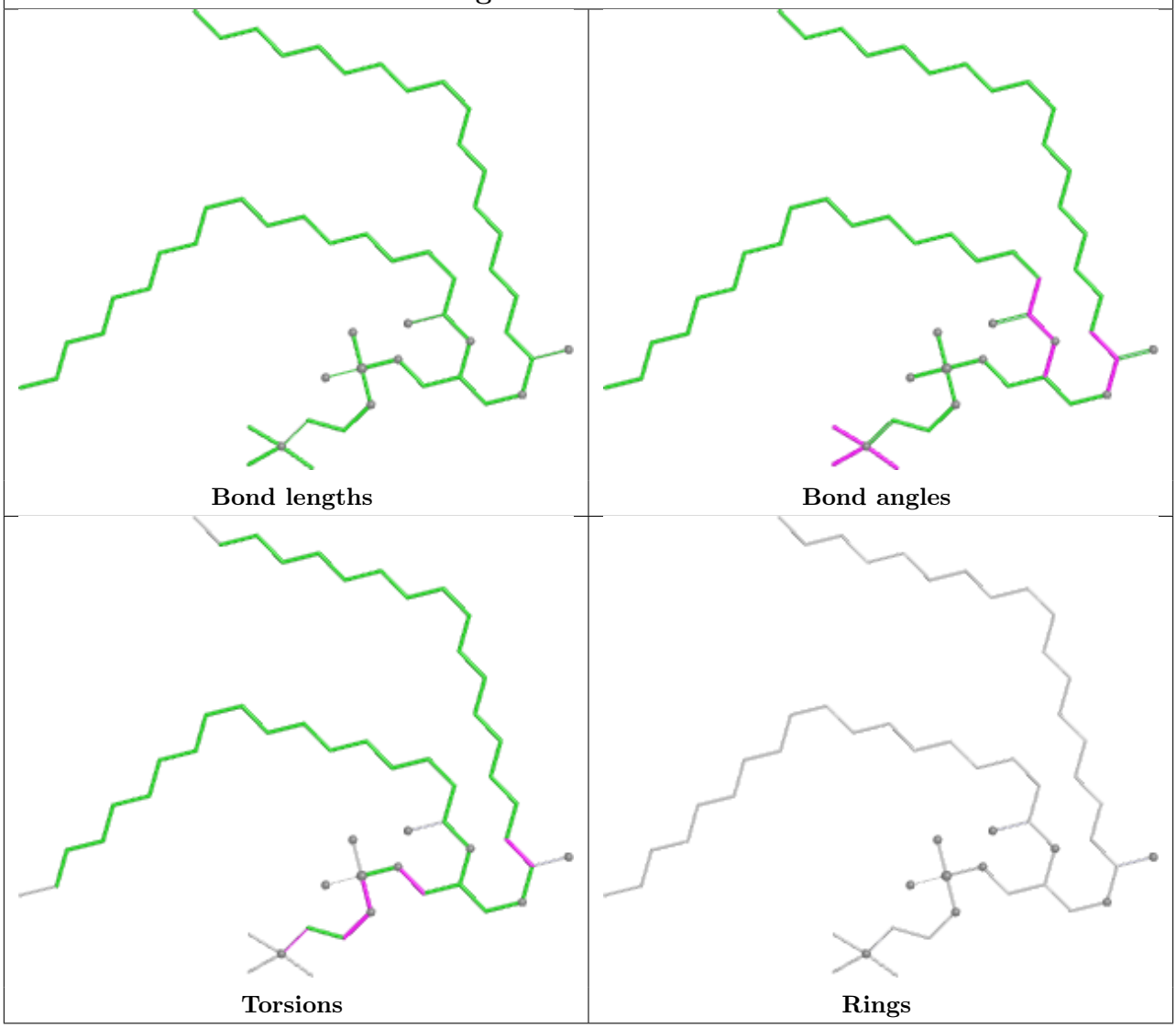

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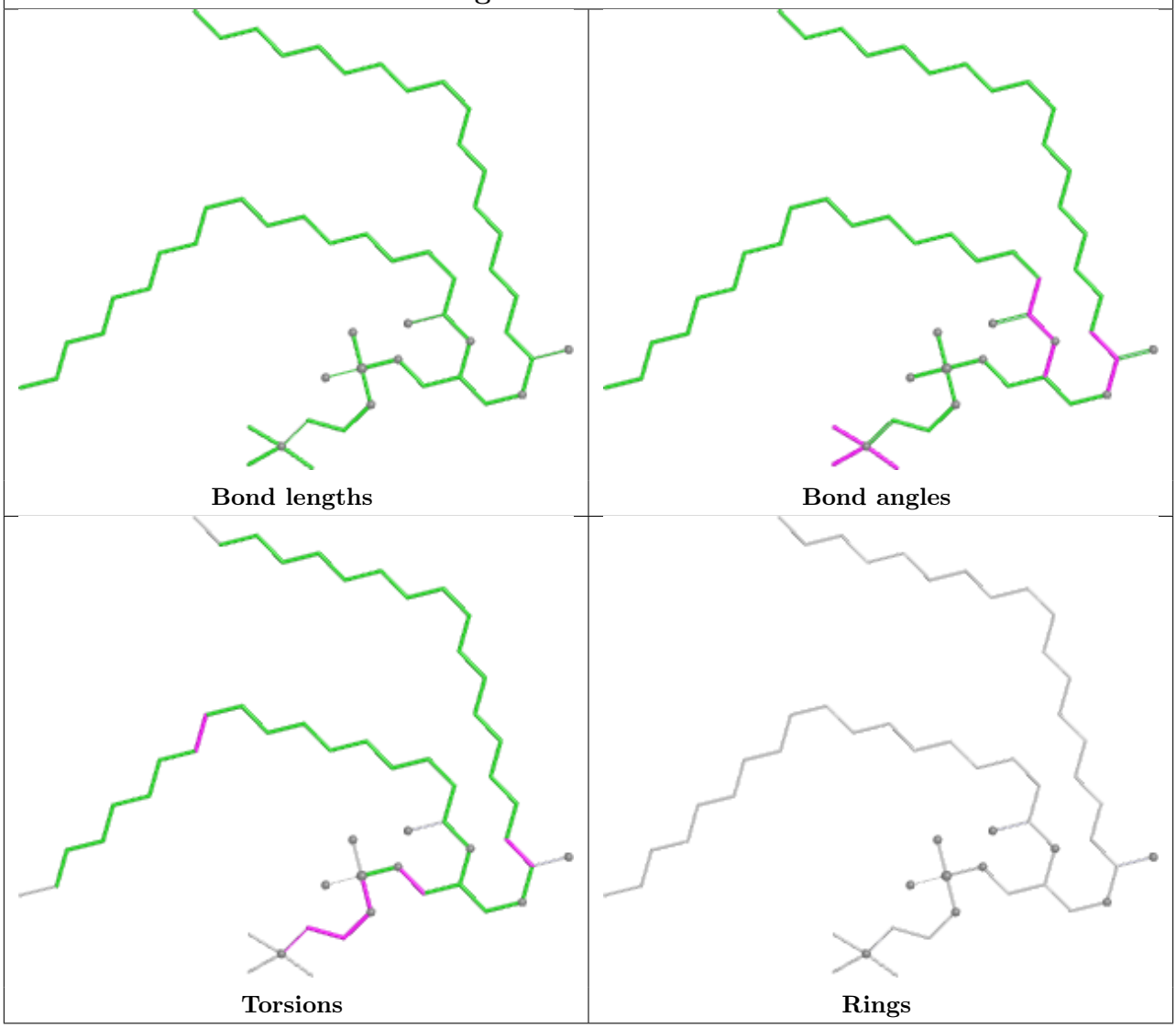

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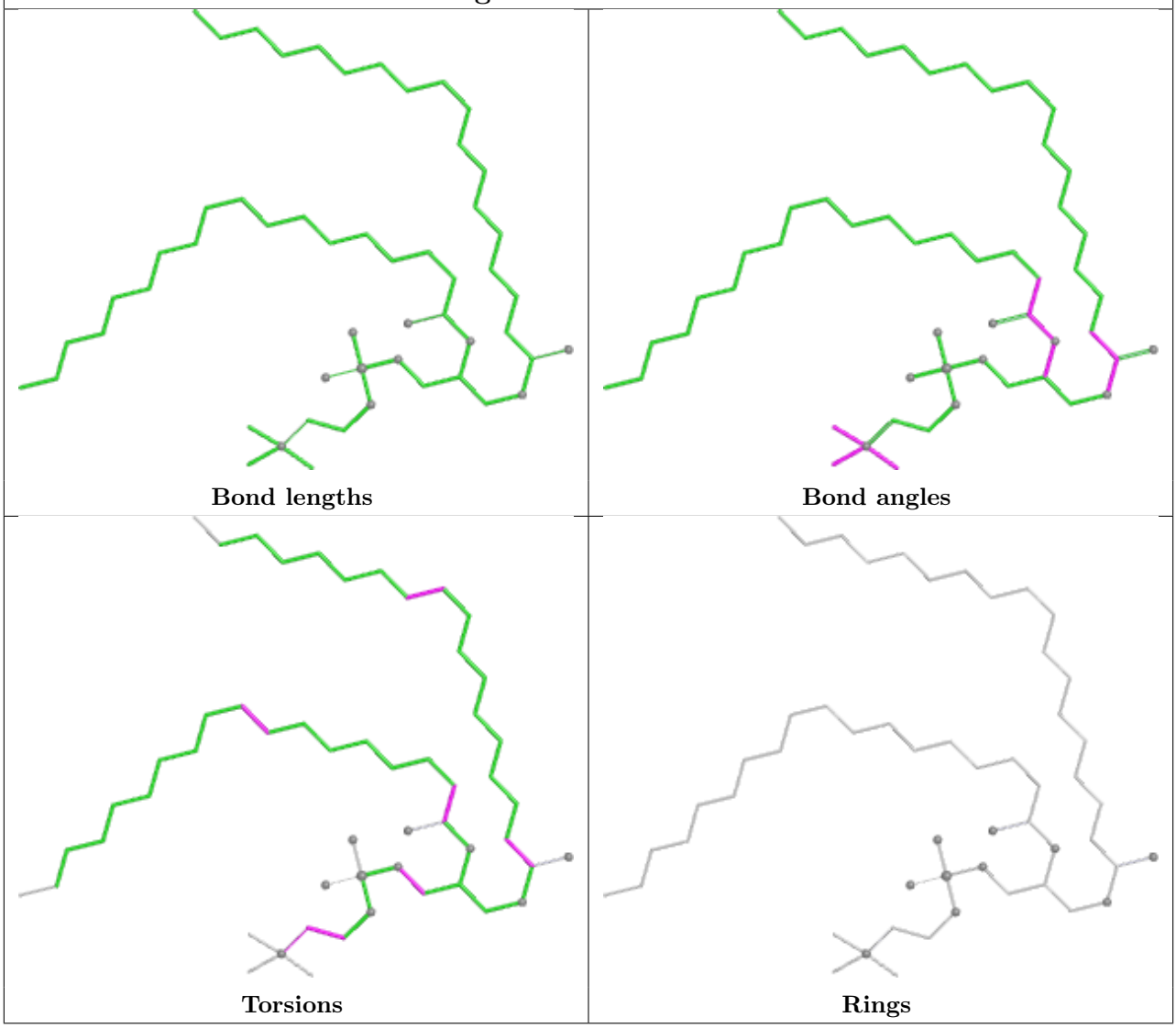

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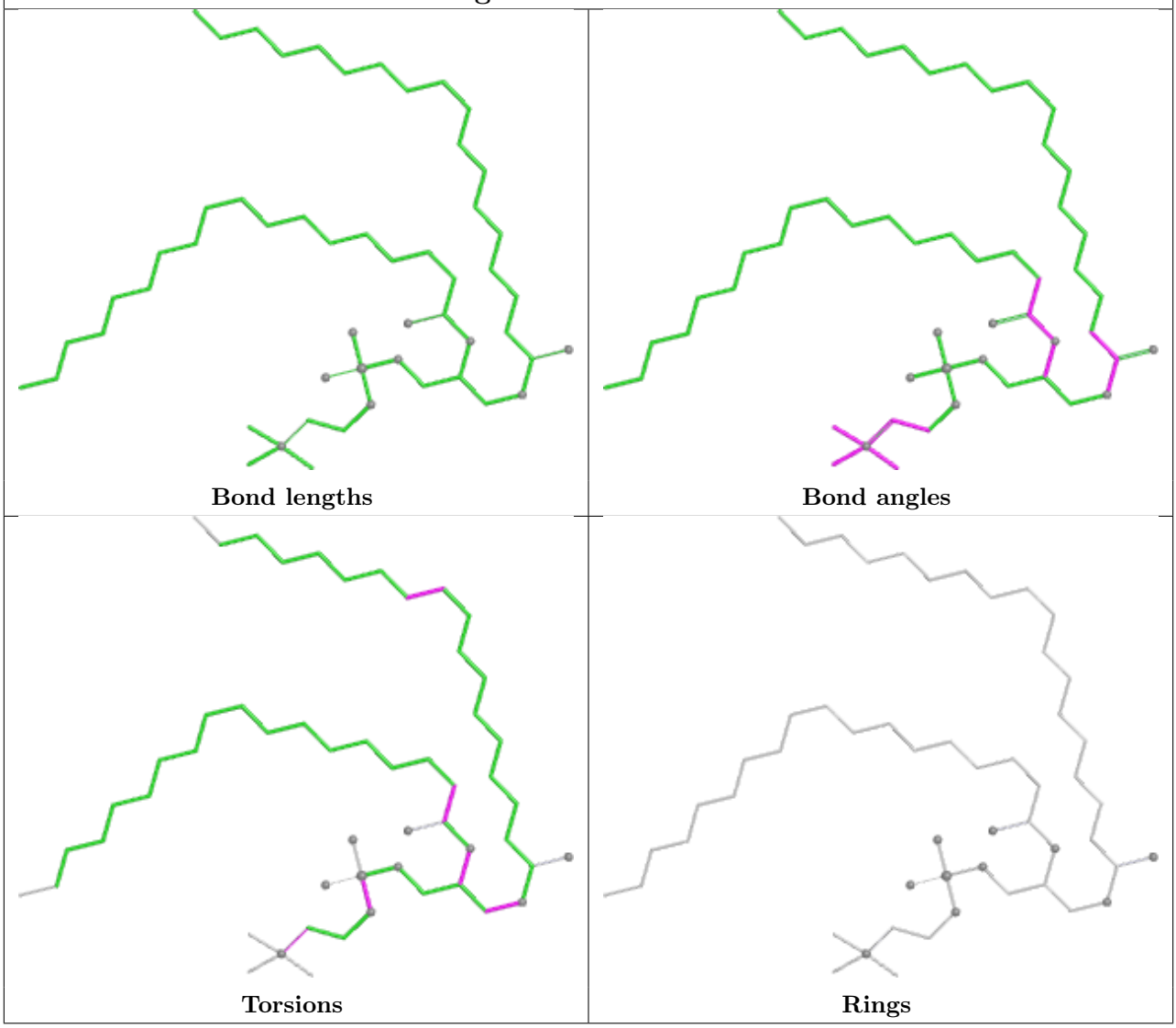
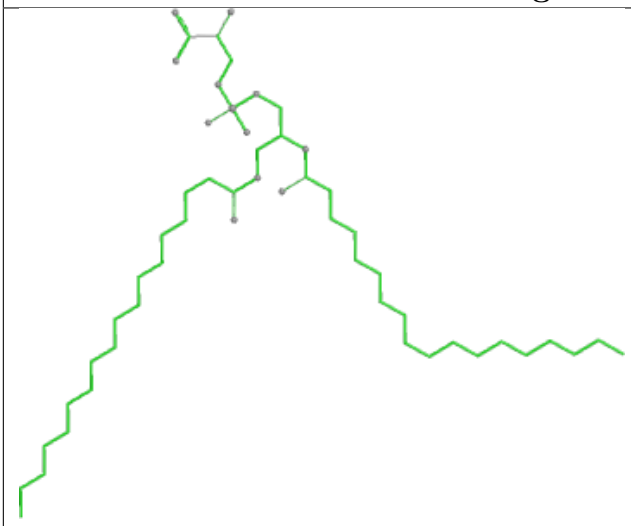
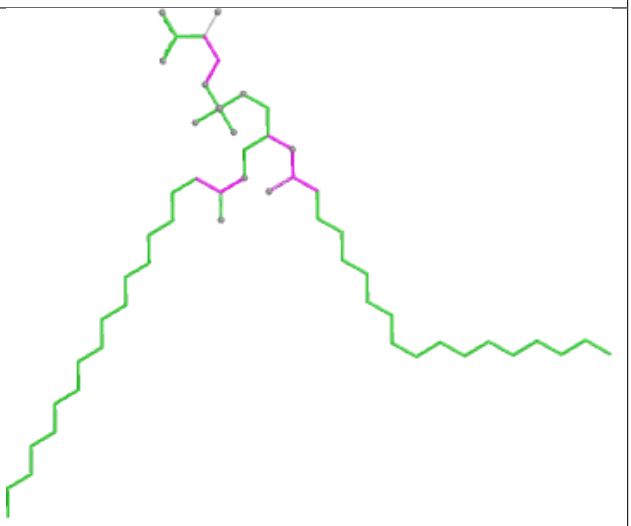


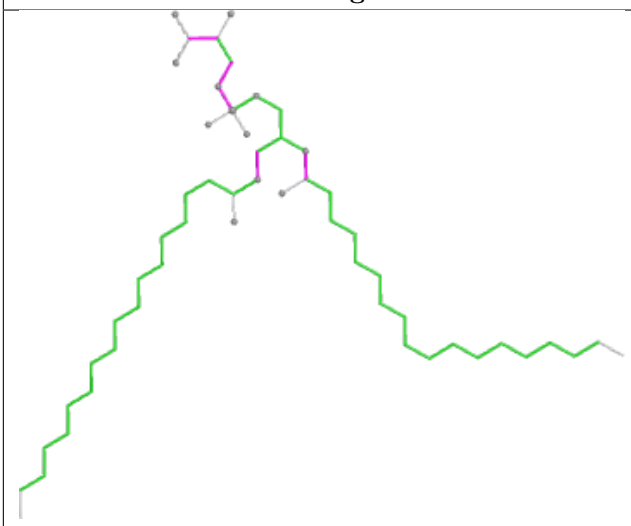
Ligand 17F B 210



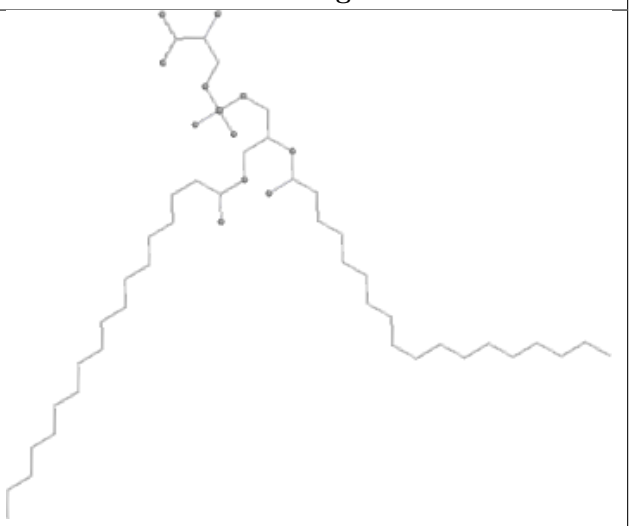
Bond lengths



Bond angles

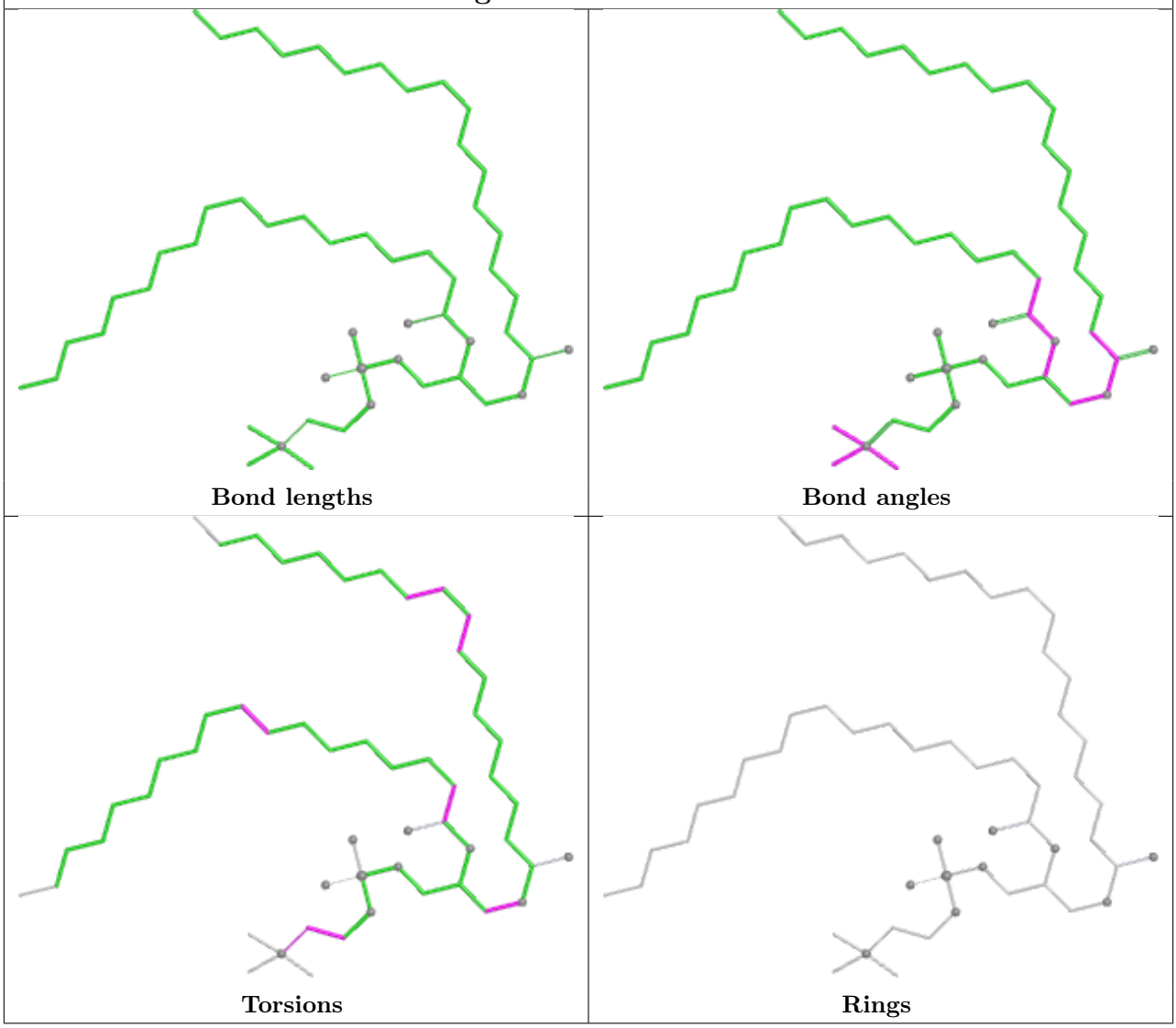


Torsions

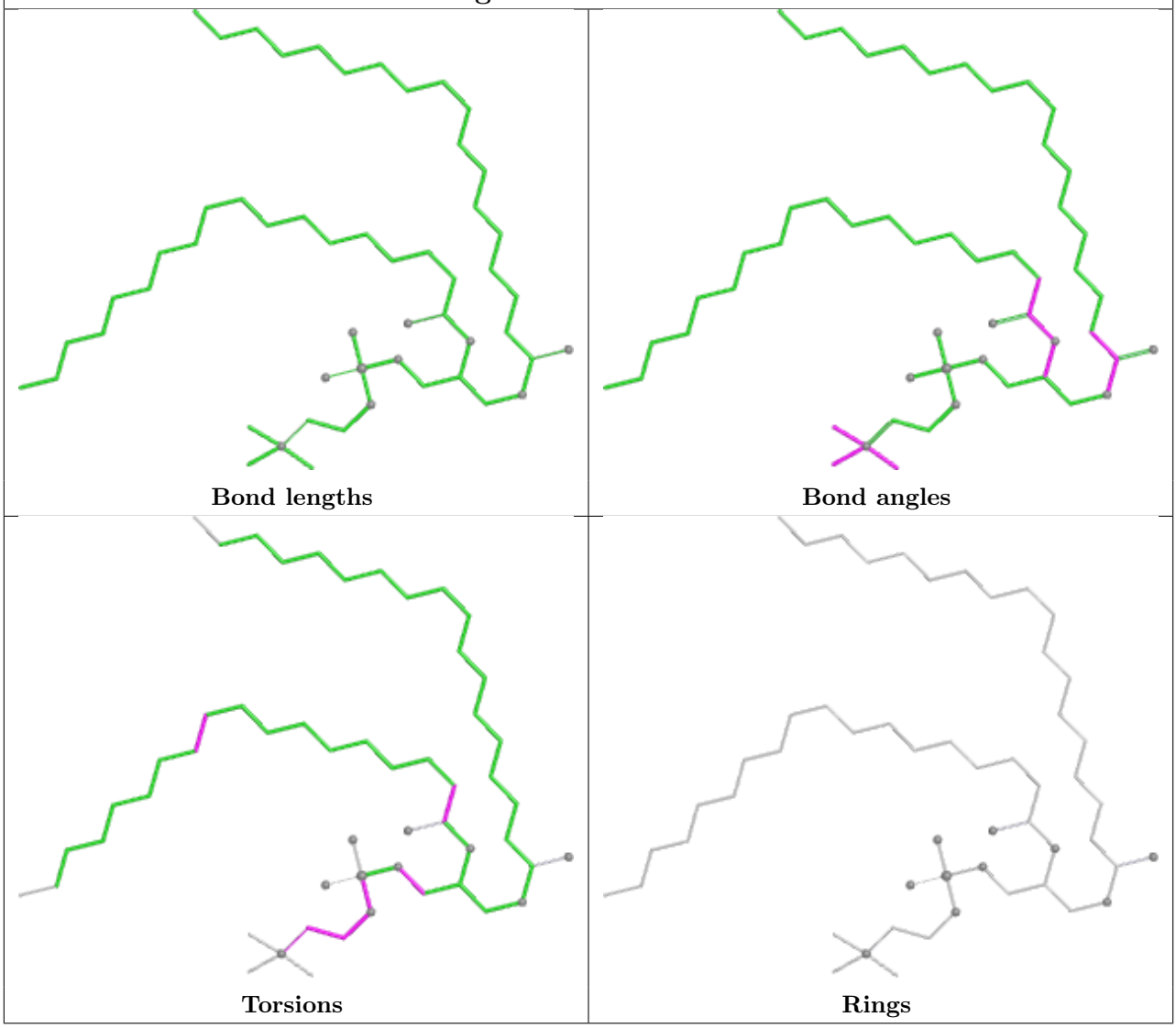


Rings

Ligand PCW D 625



Ligand PCW A 411



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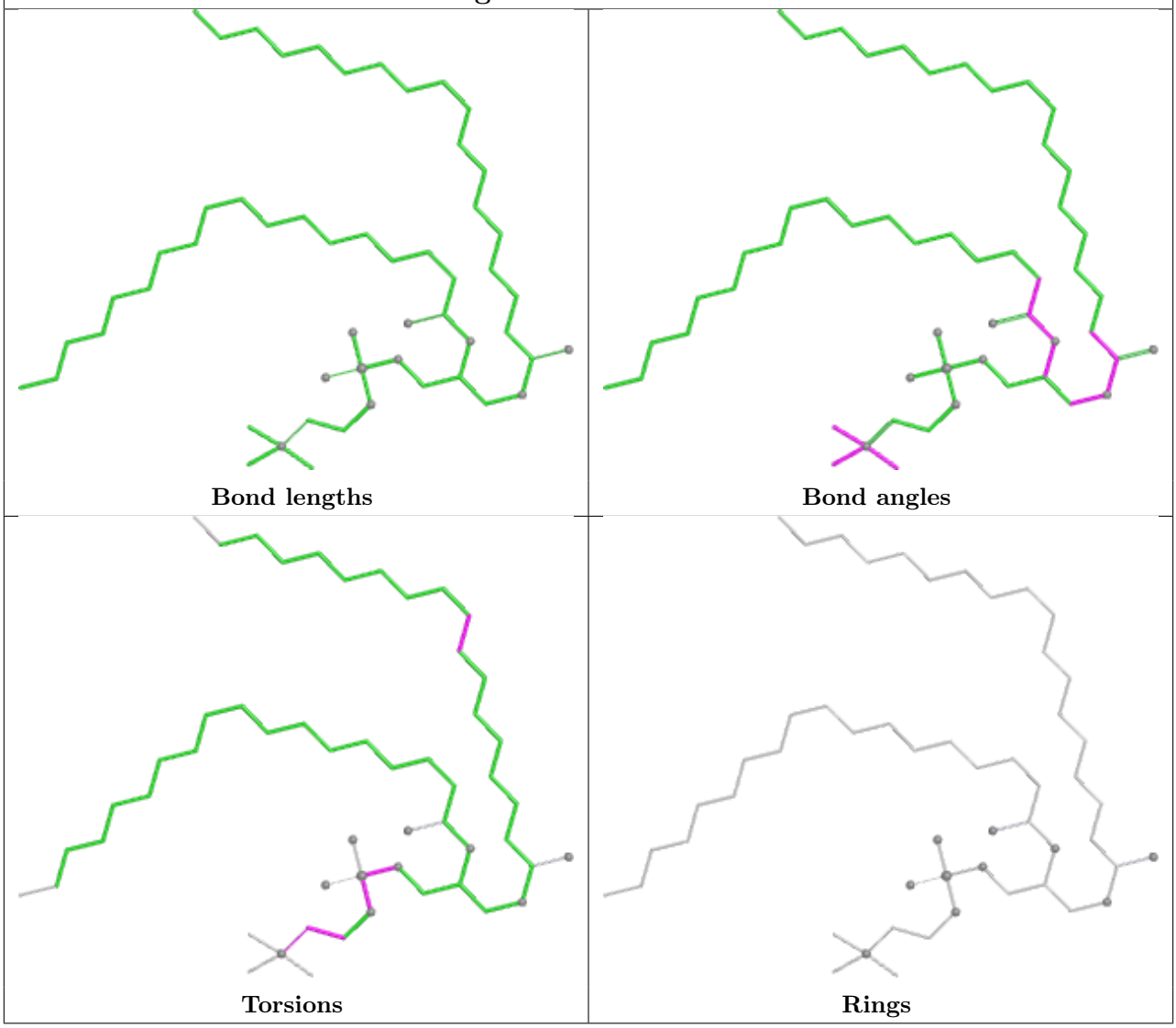
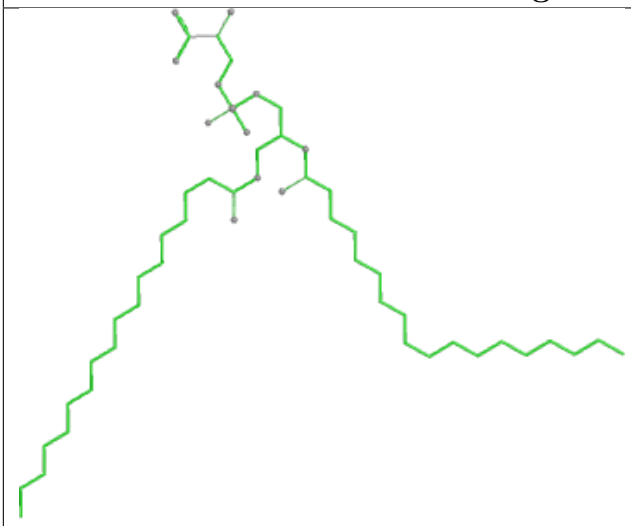
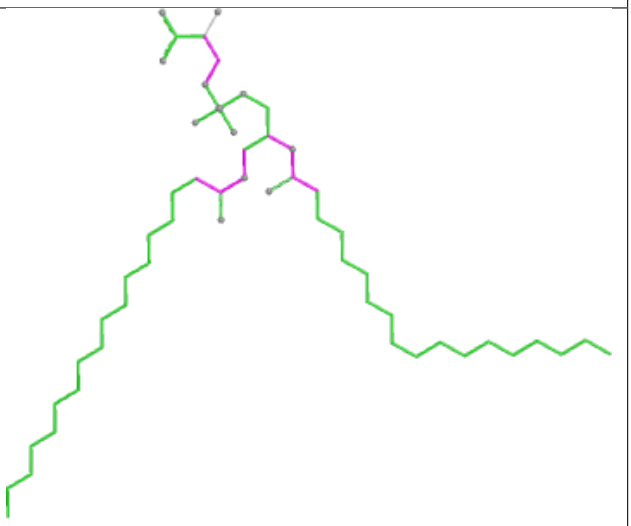


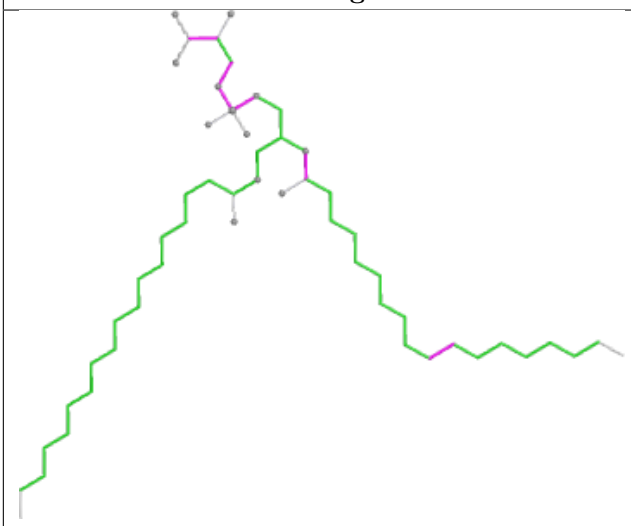
Ligand 17F C 215



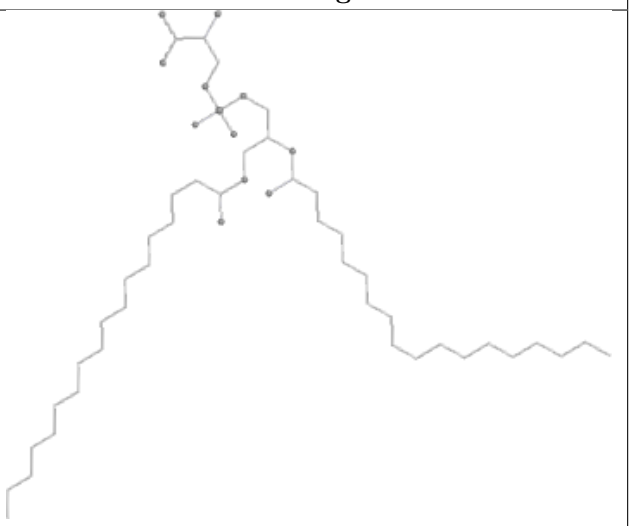
Bond lengths



Bond angles

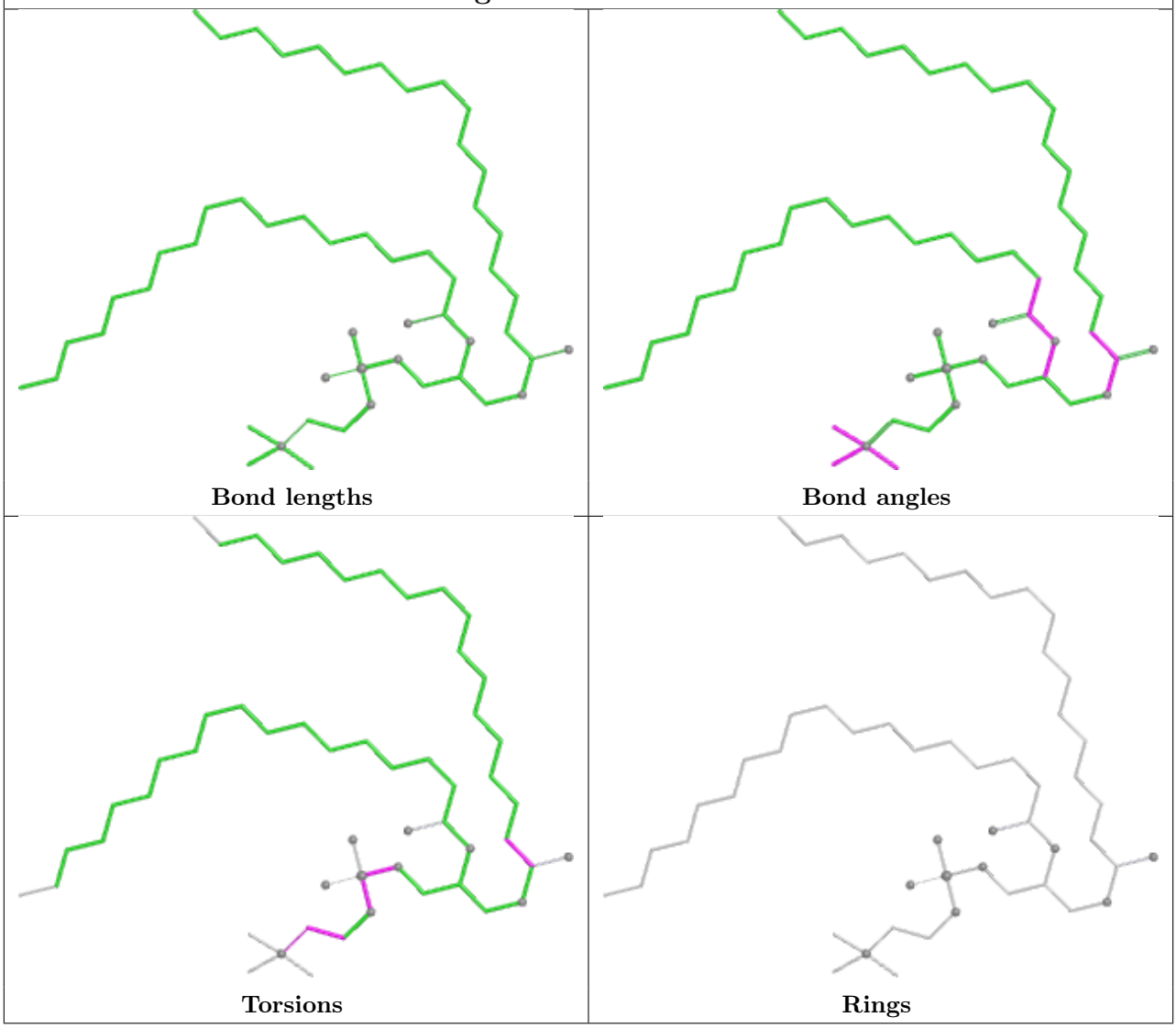


Torsions

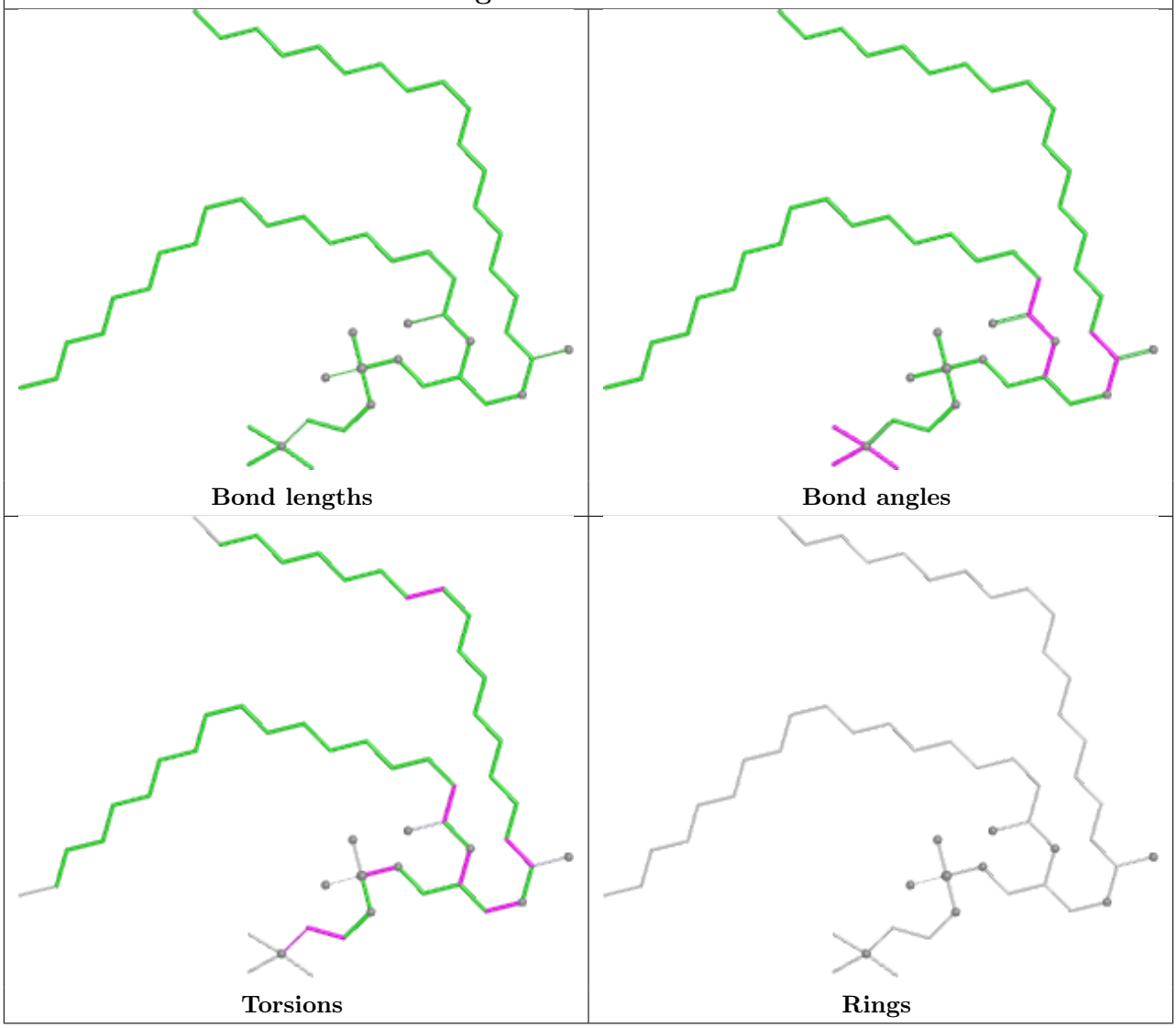


Rings

Ligand PCW D 622



Ligand PCW C 203



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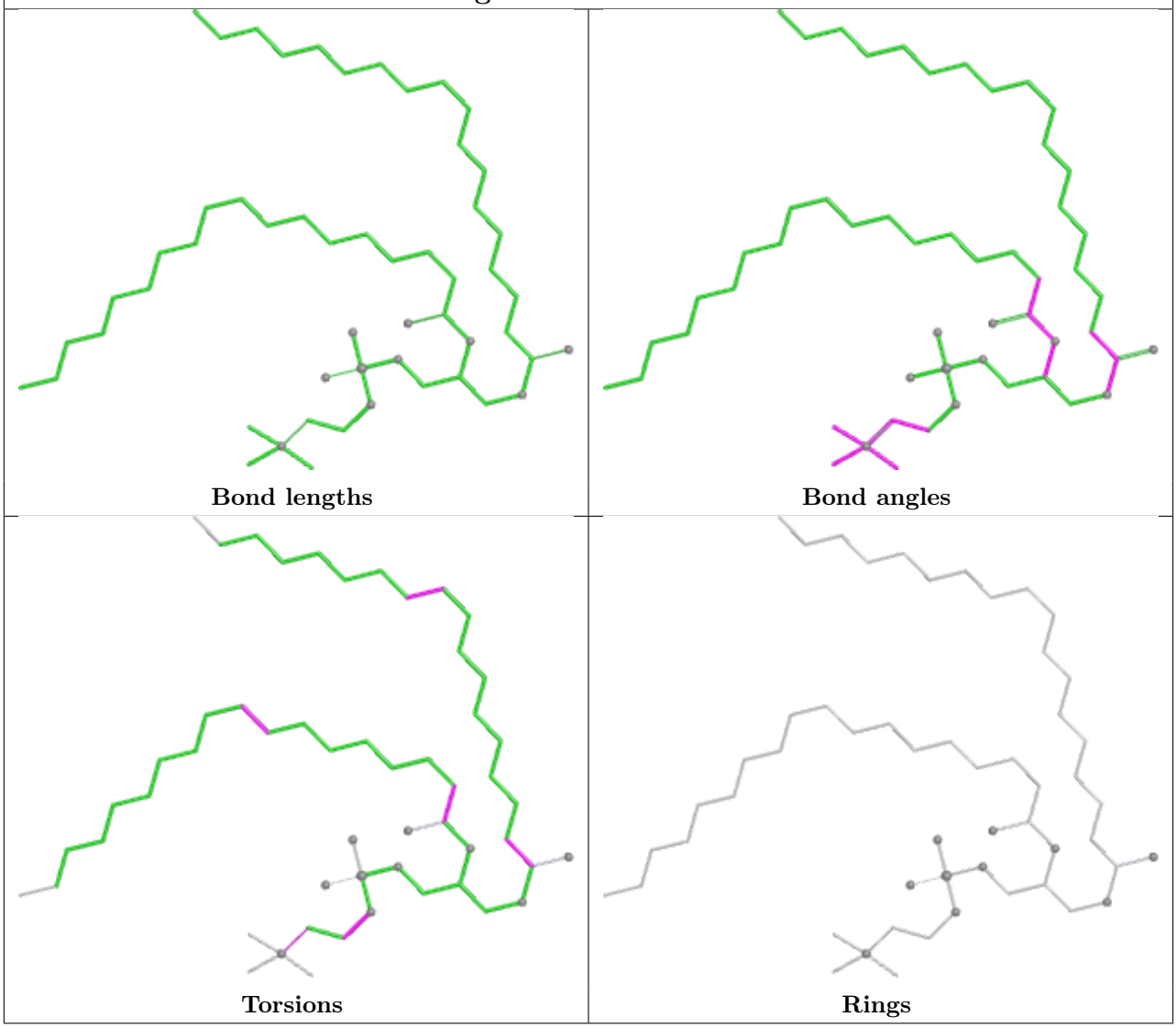

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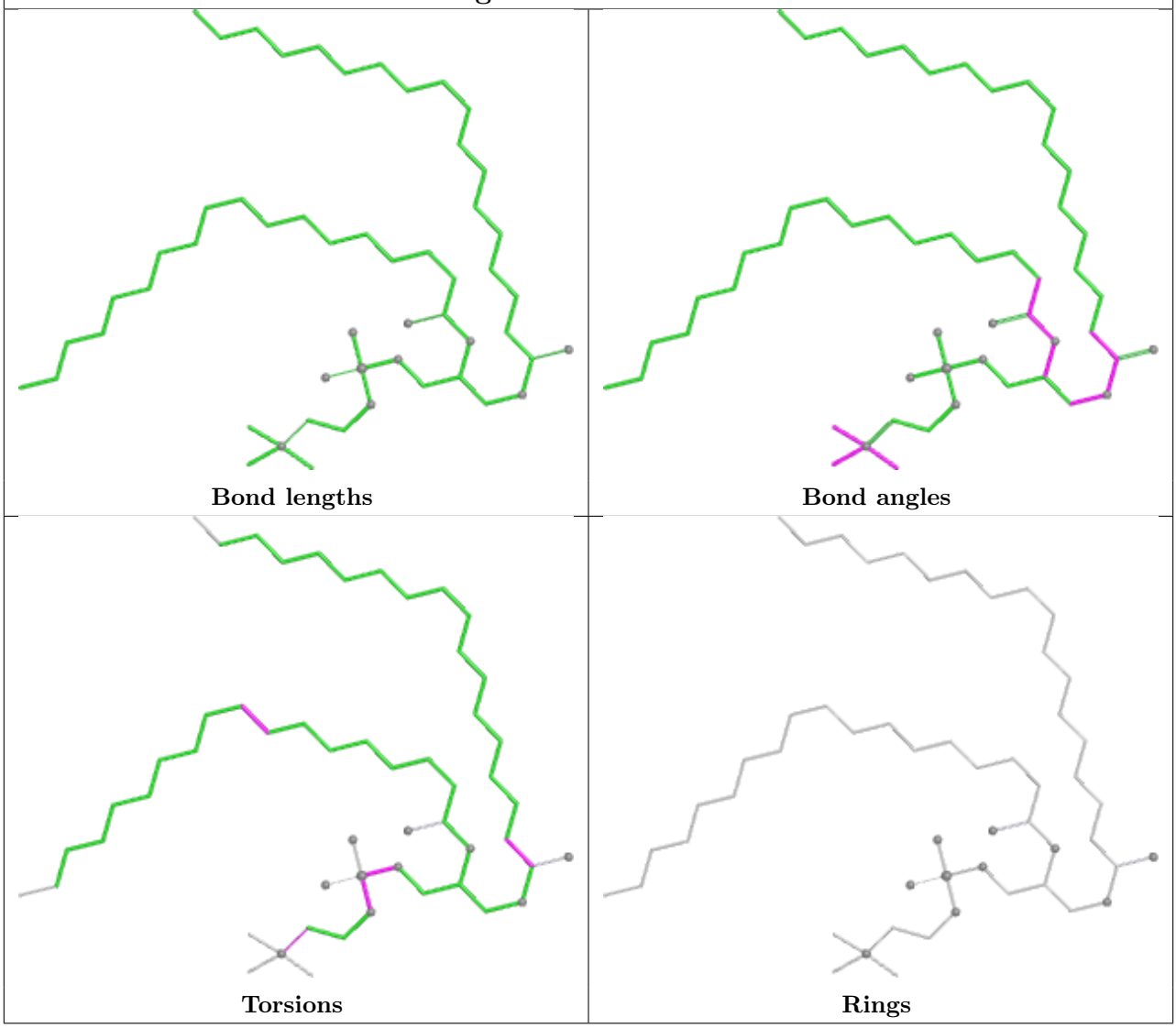

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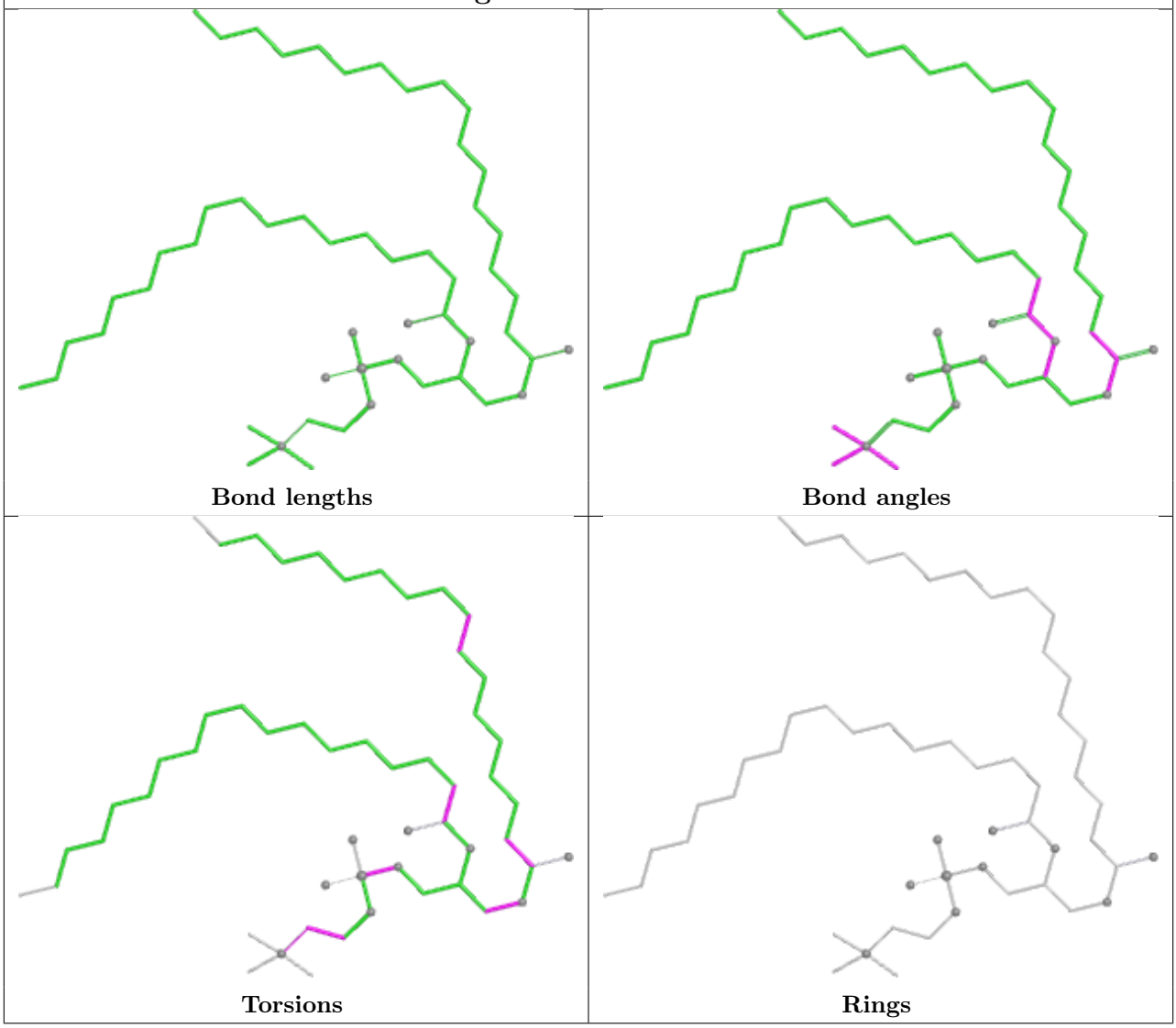

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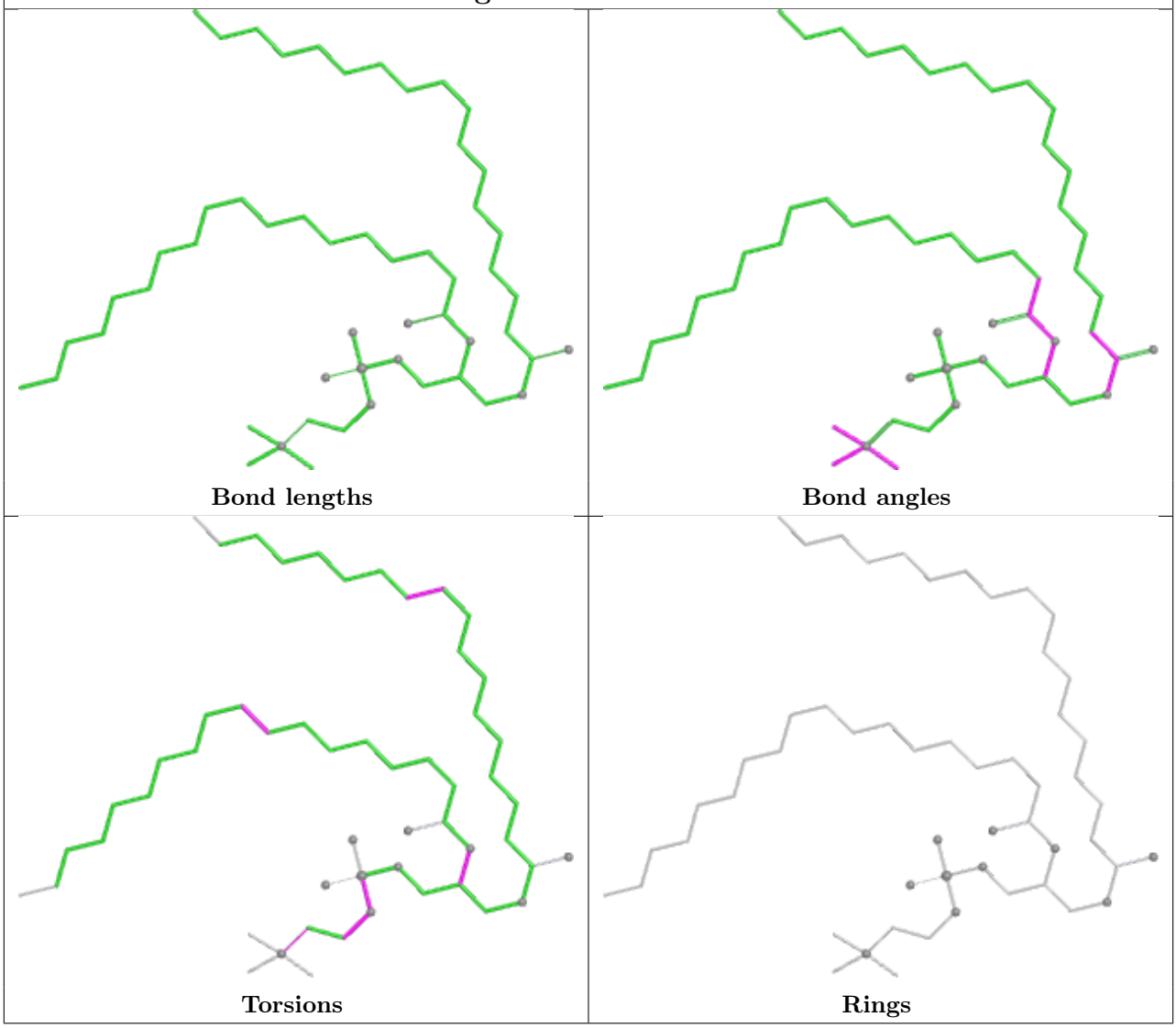
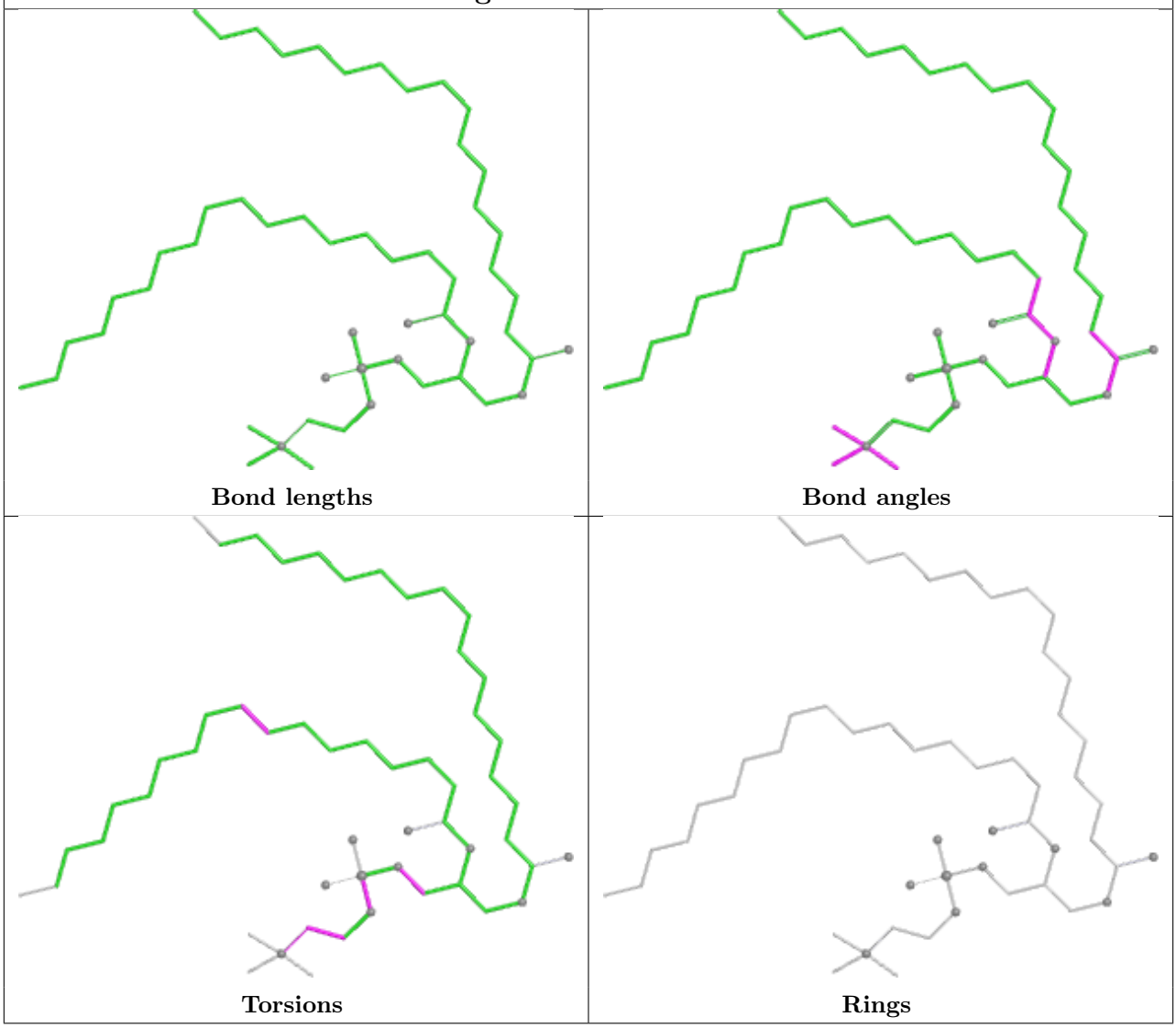
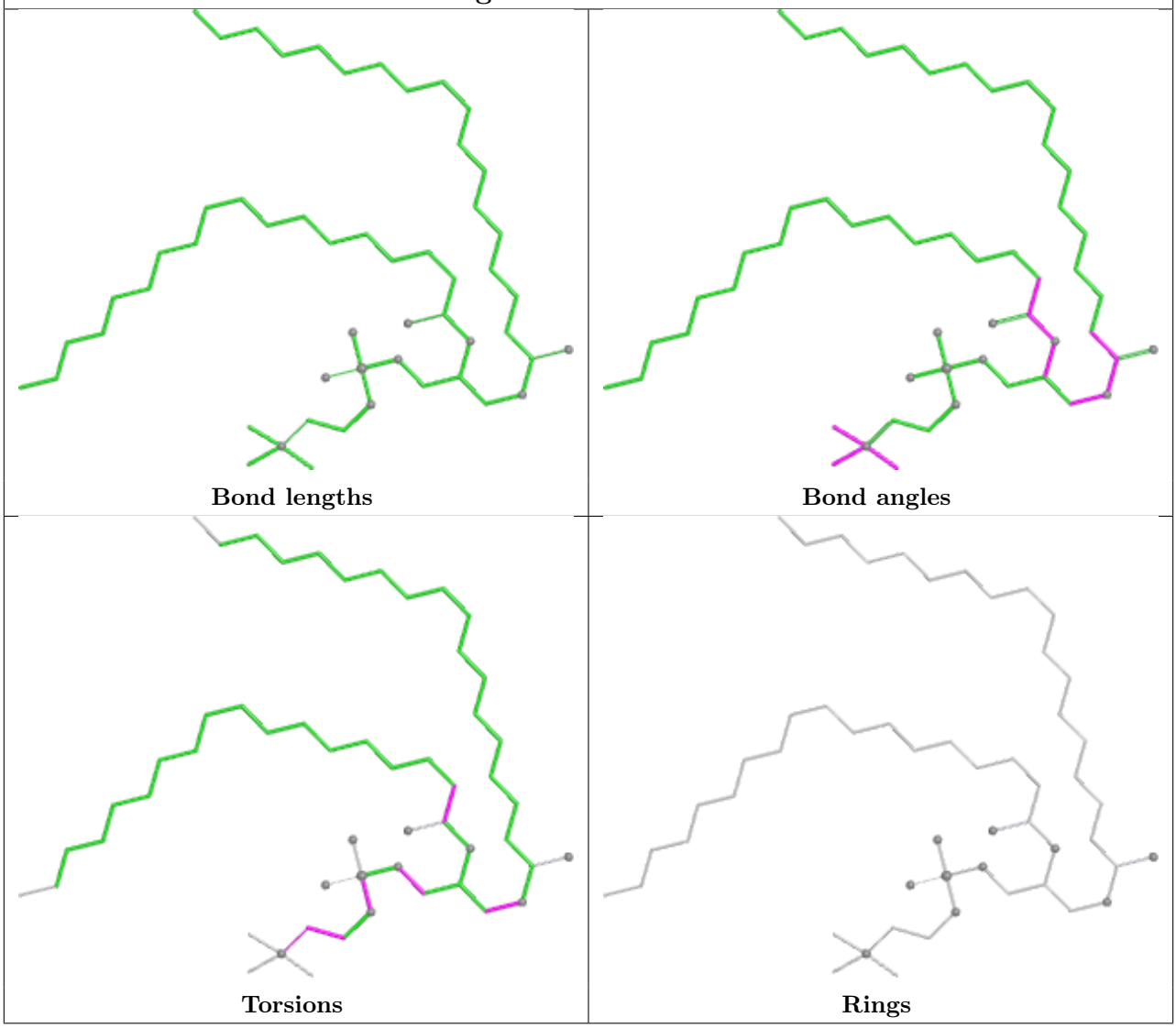


Ligand PCW A 404



Ligand PCW B 208



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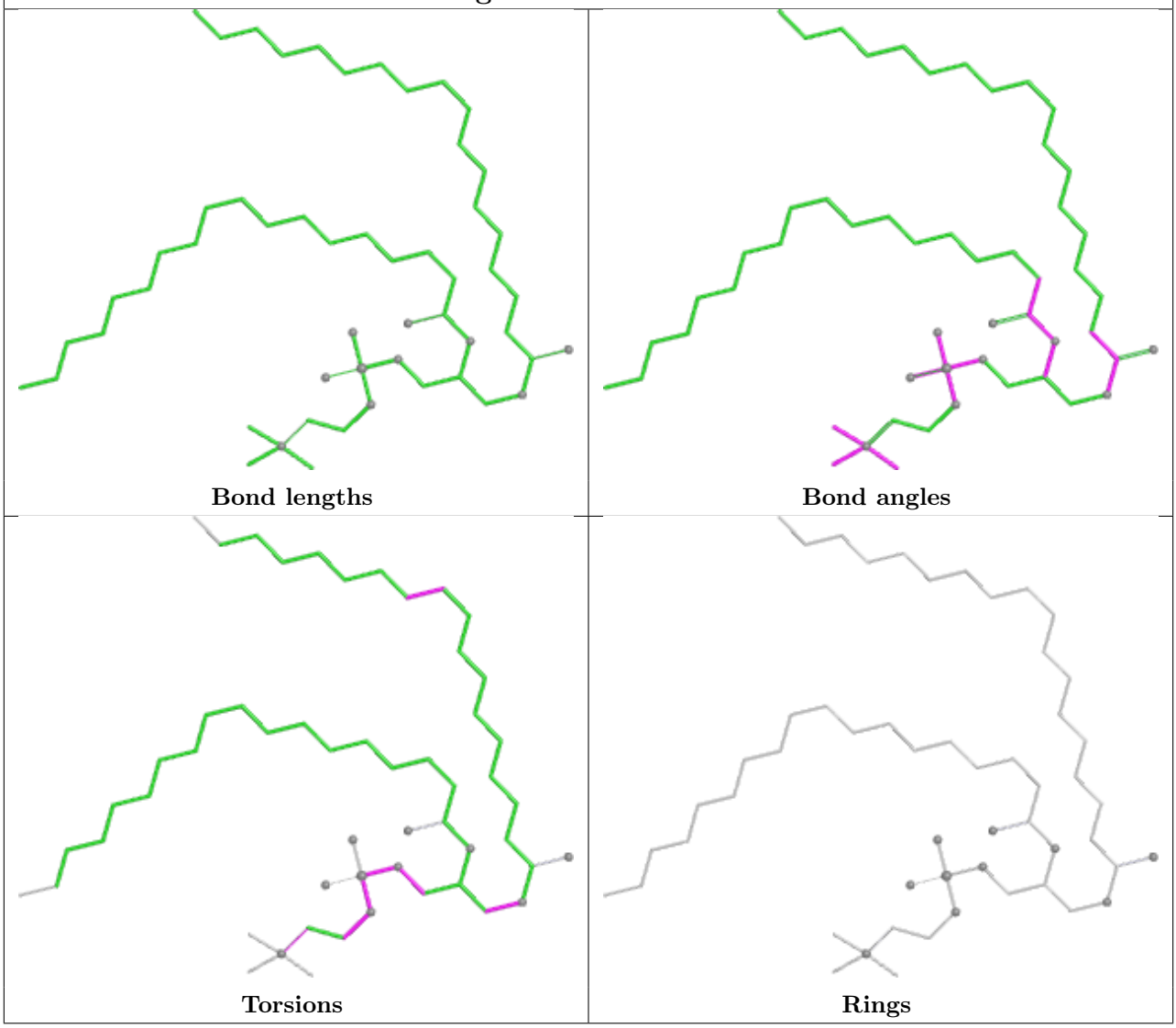

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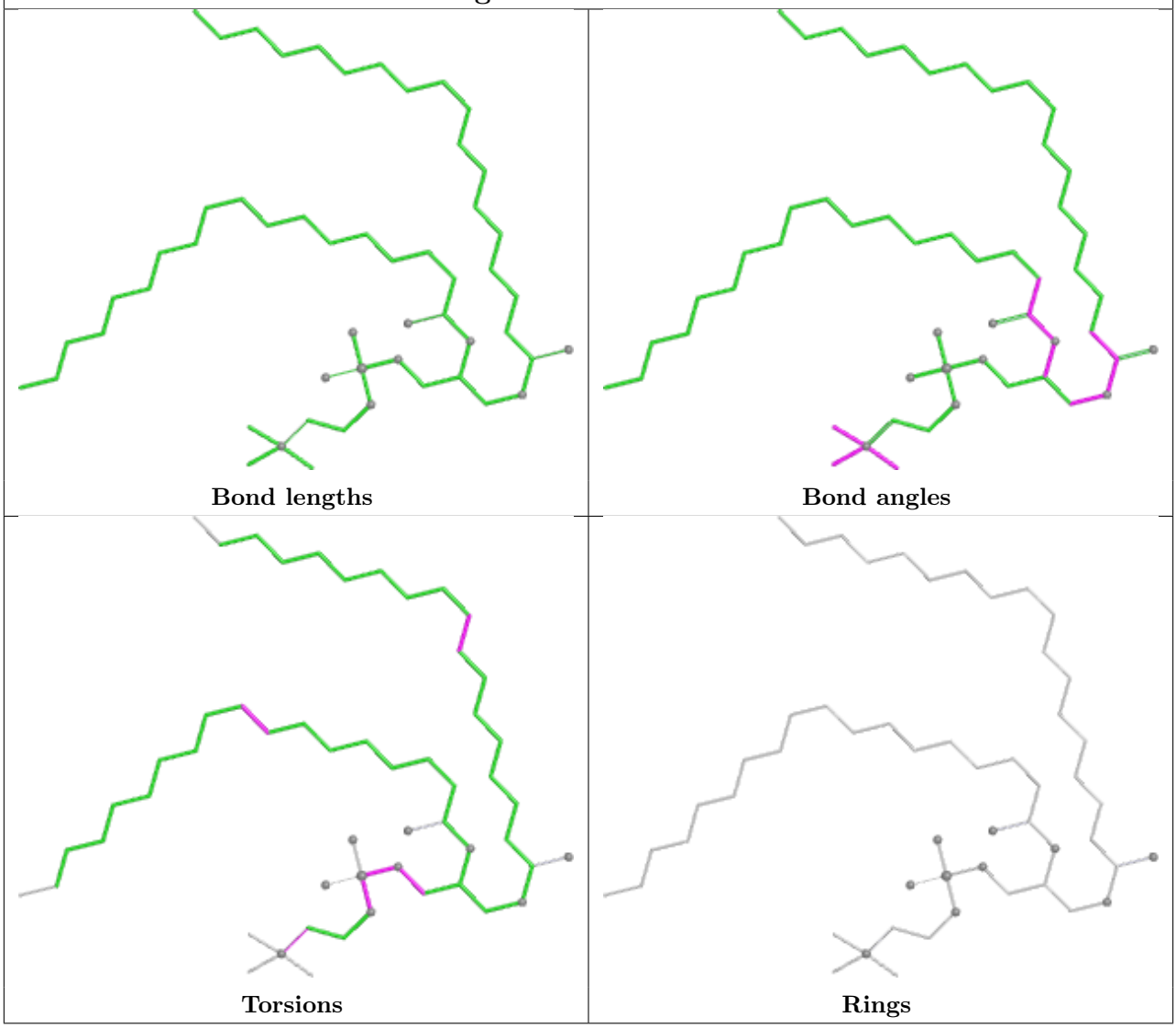

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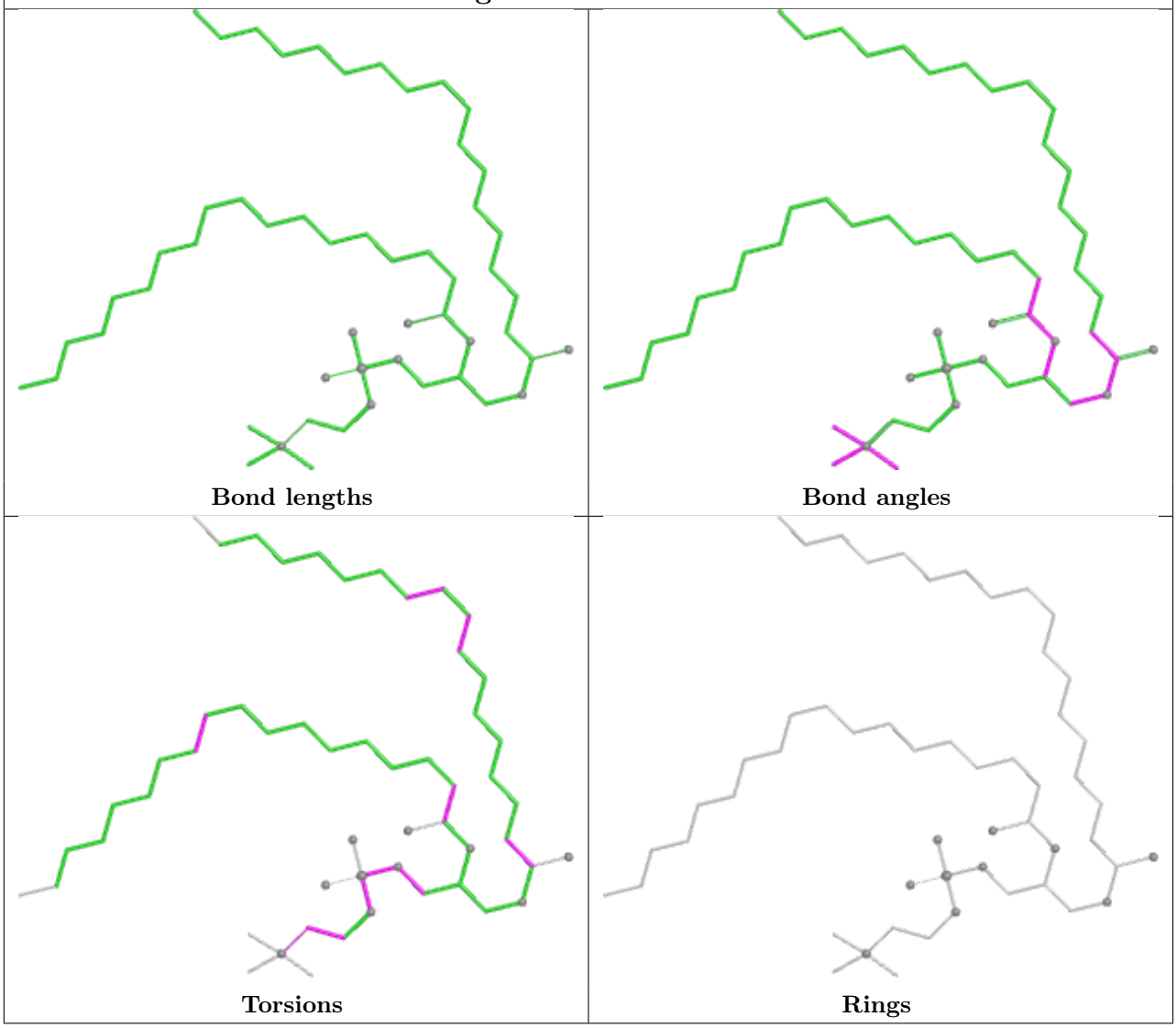

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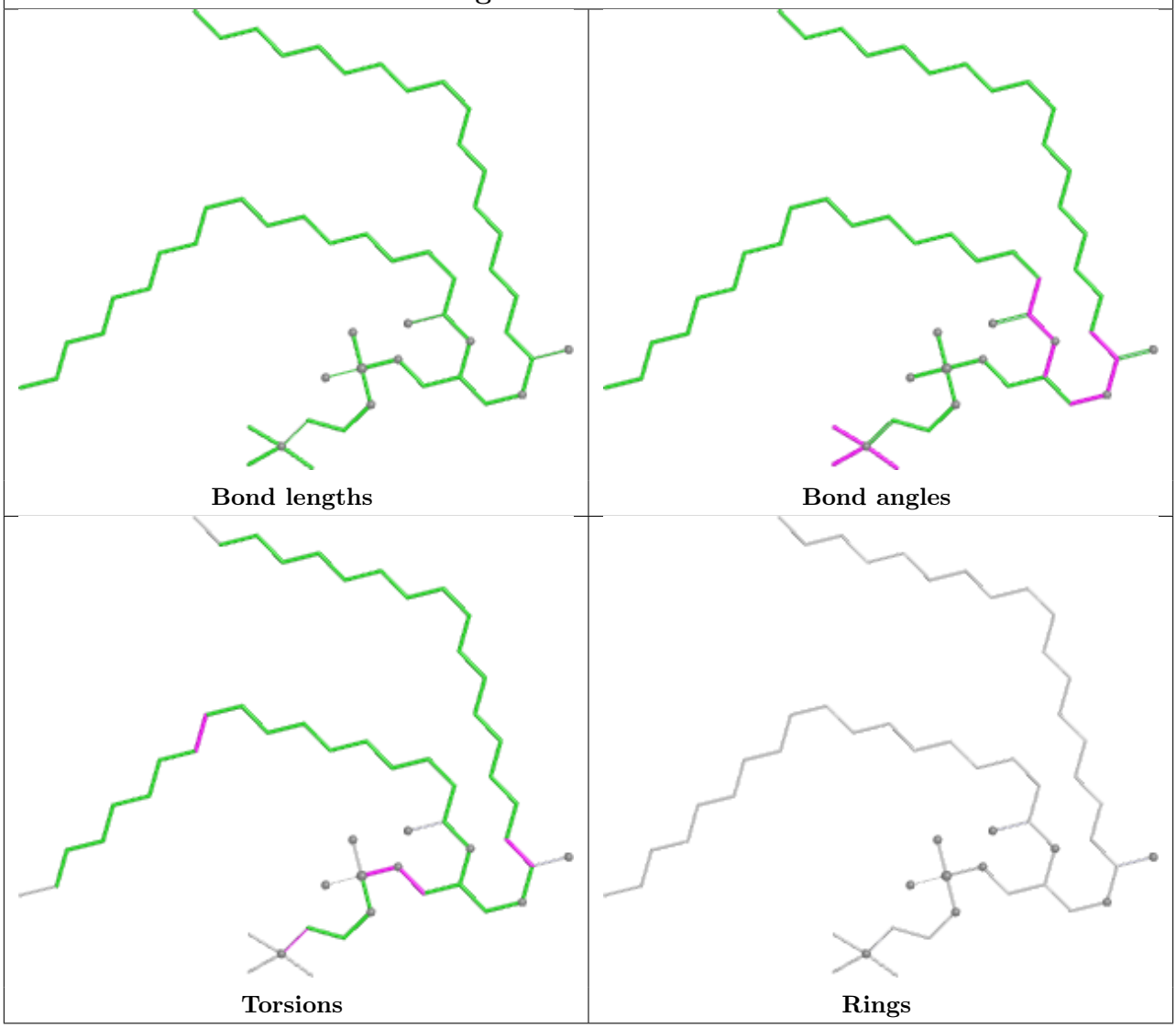
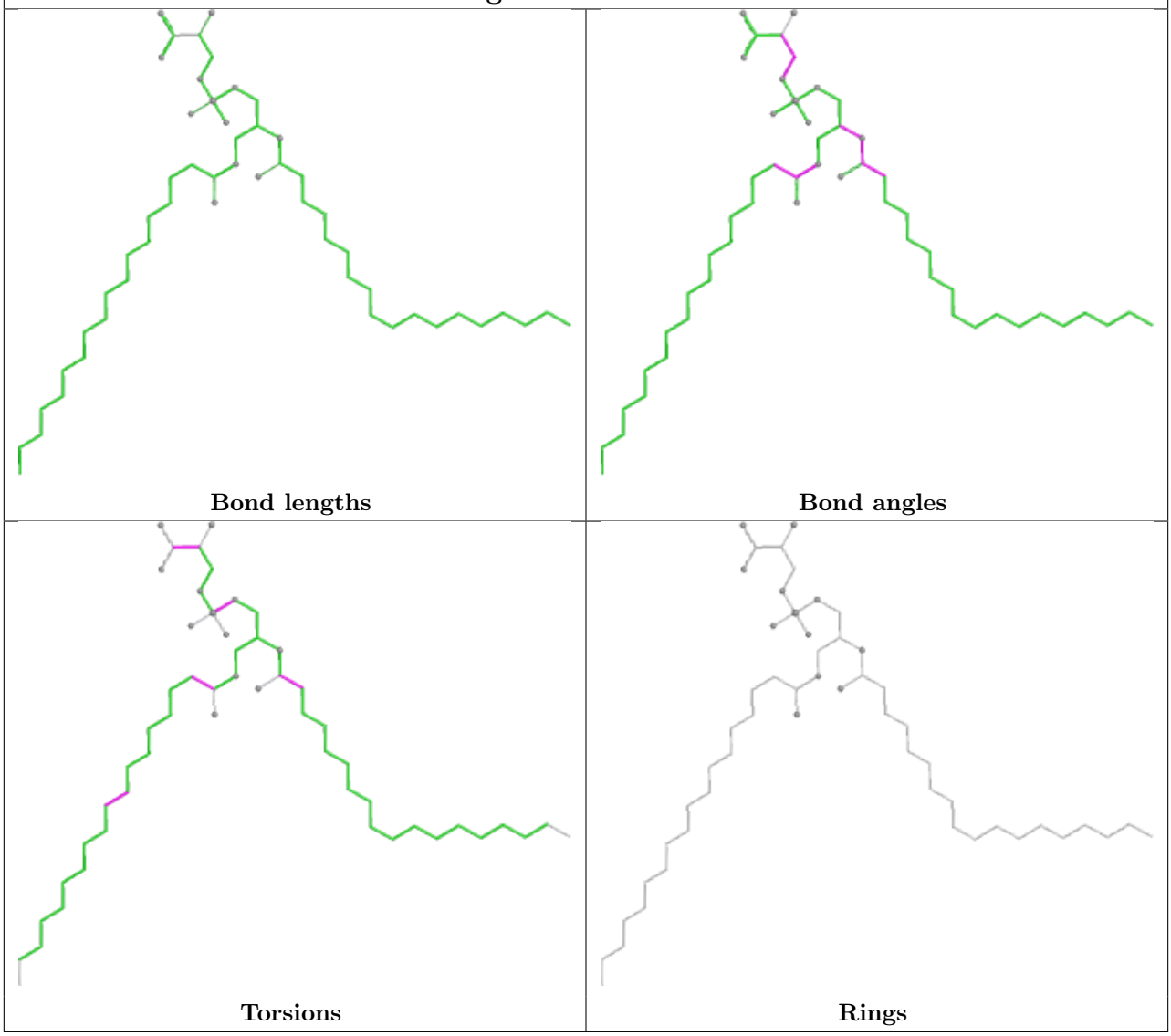


Ligand 17F D 629



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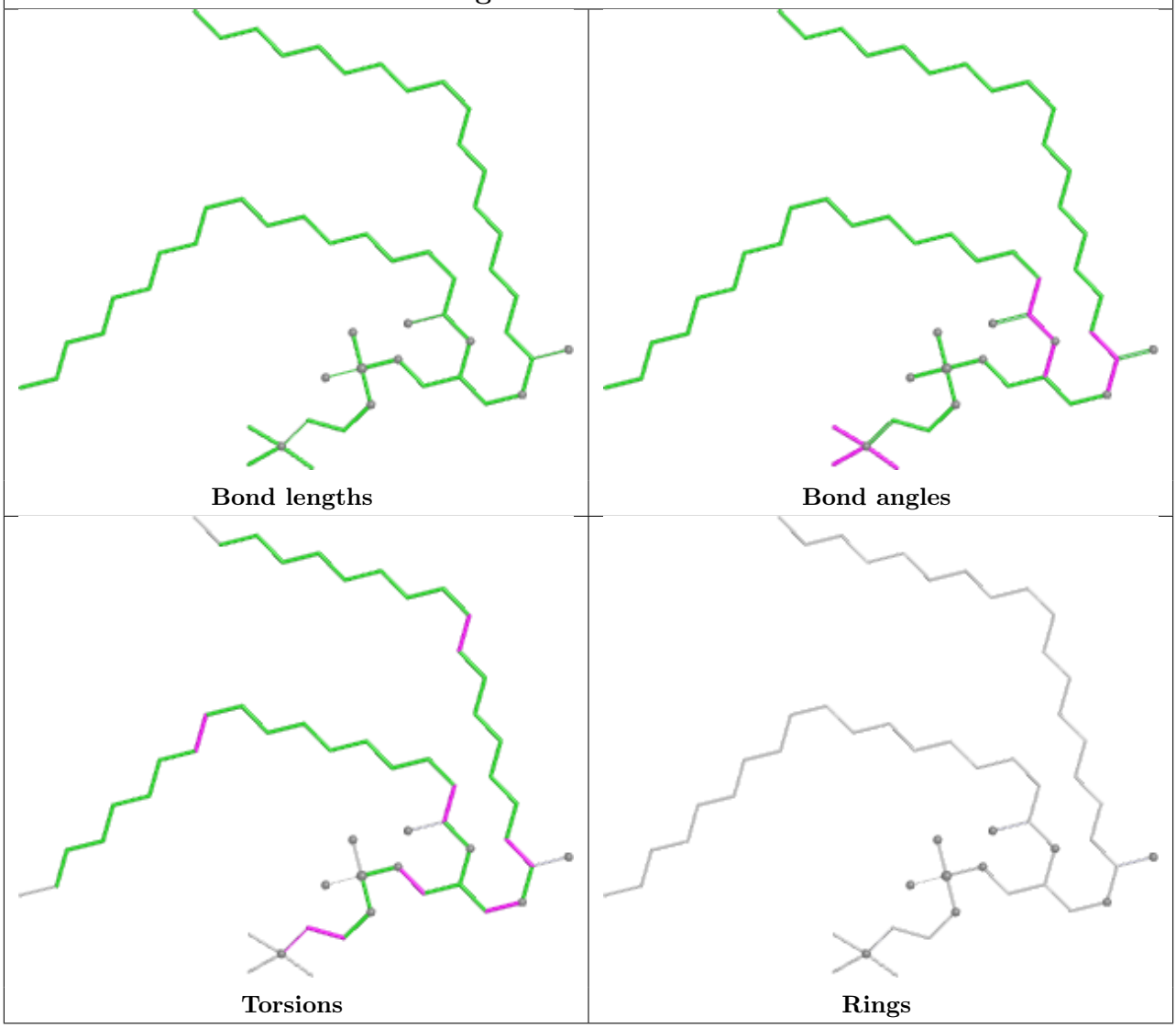

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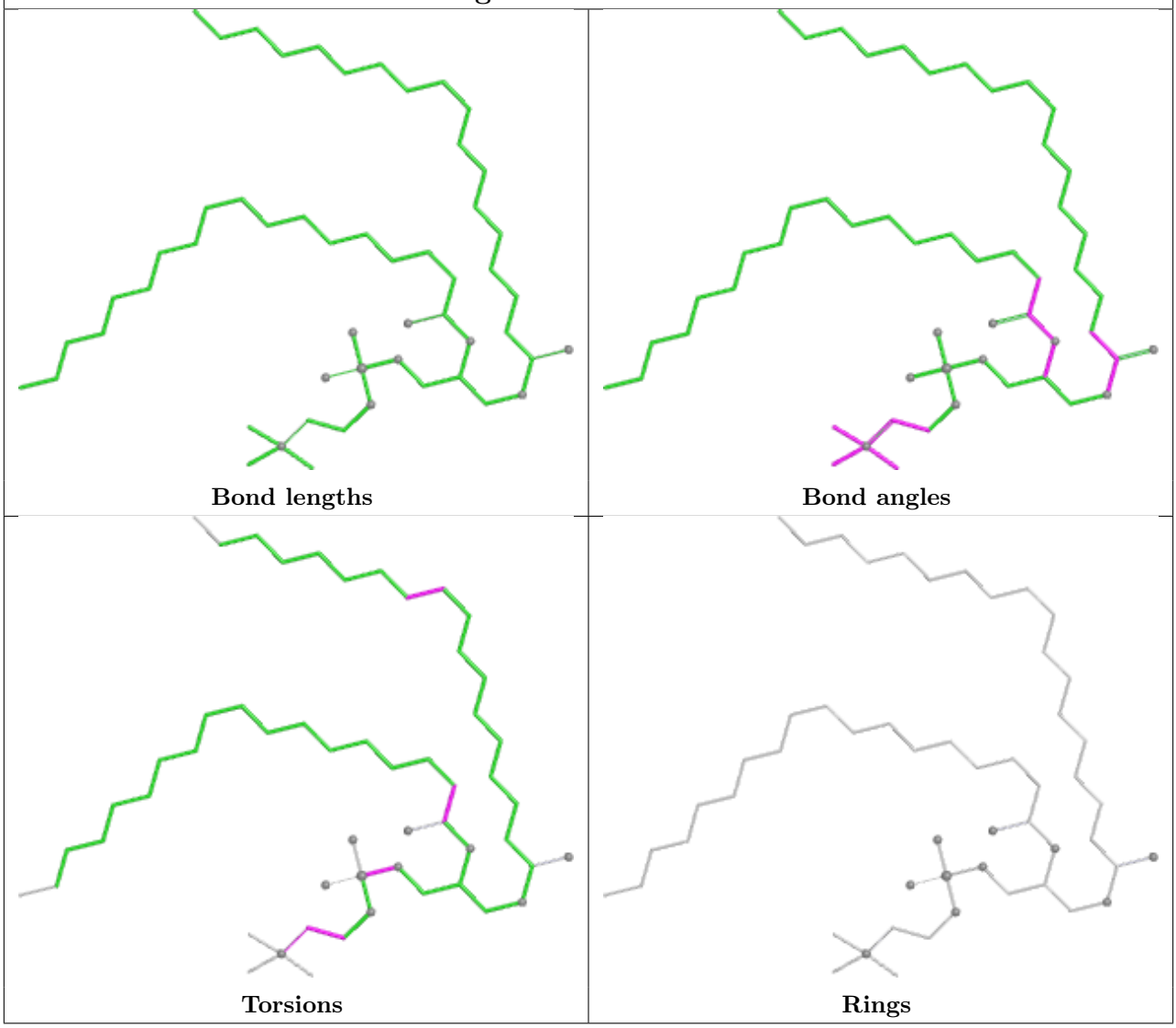

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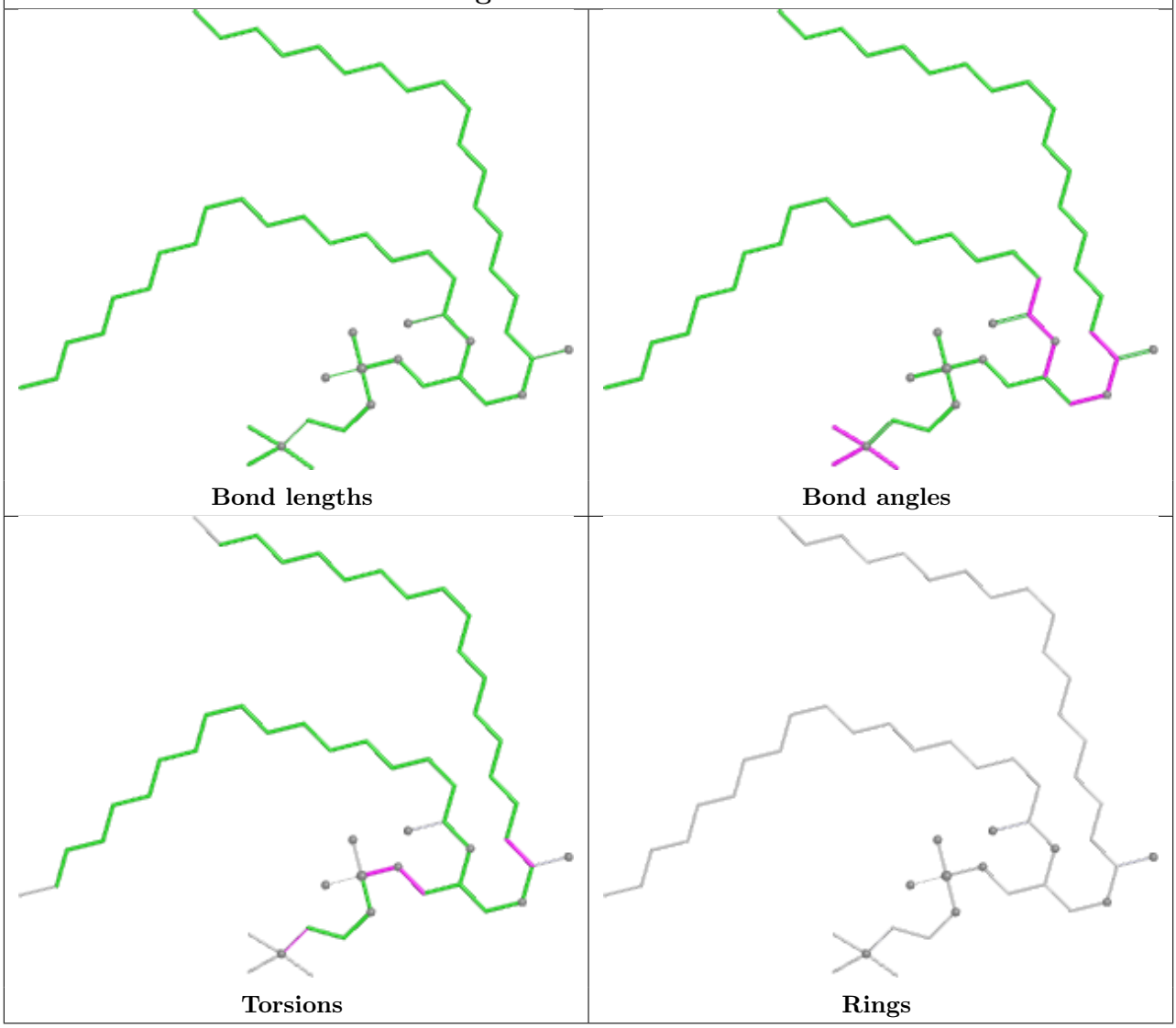

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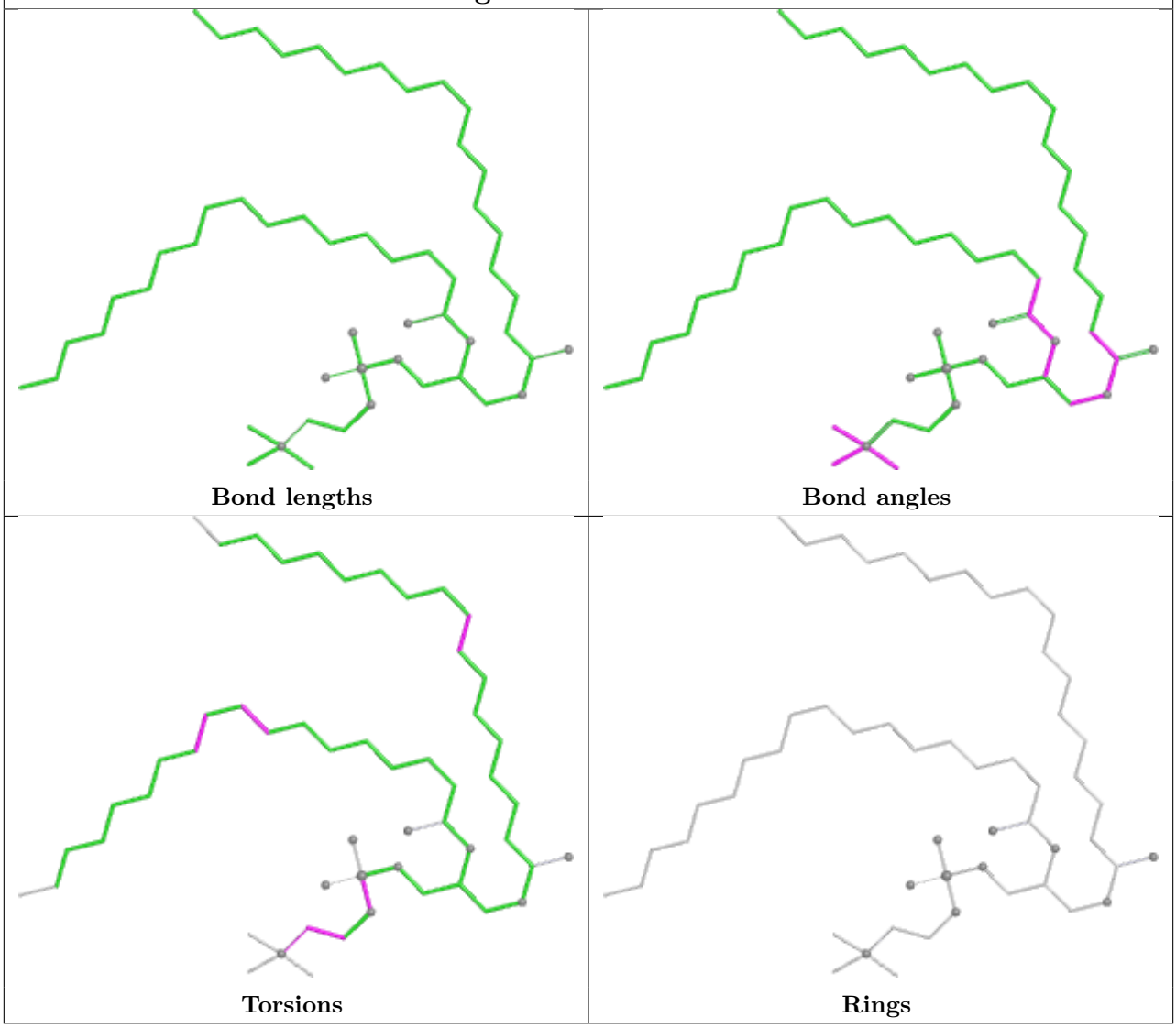

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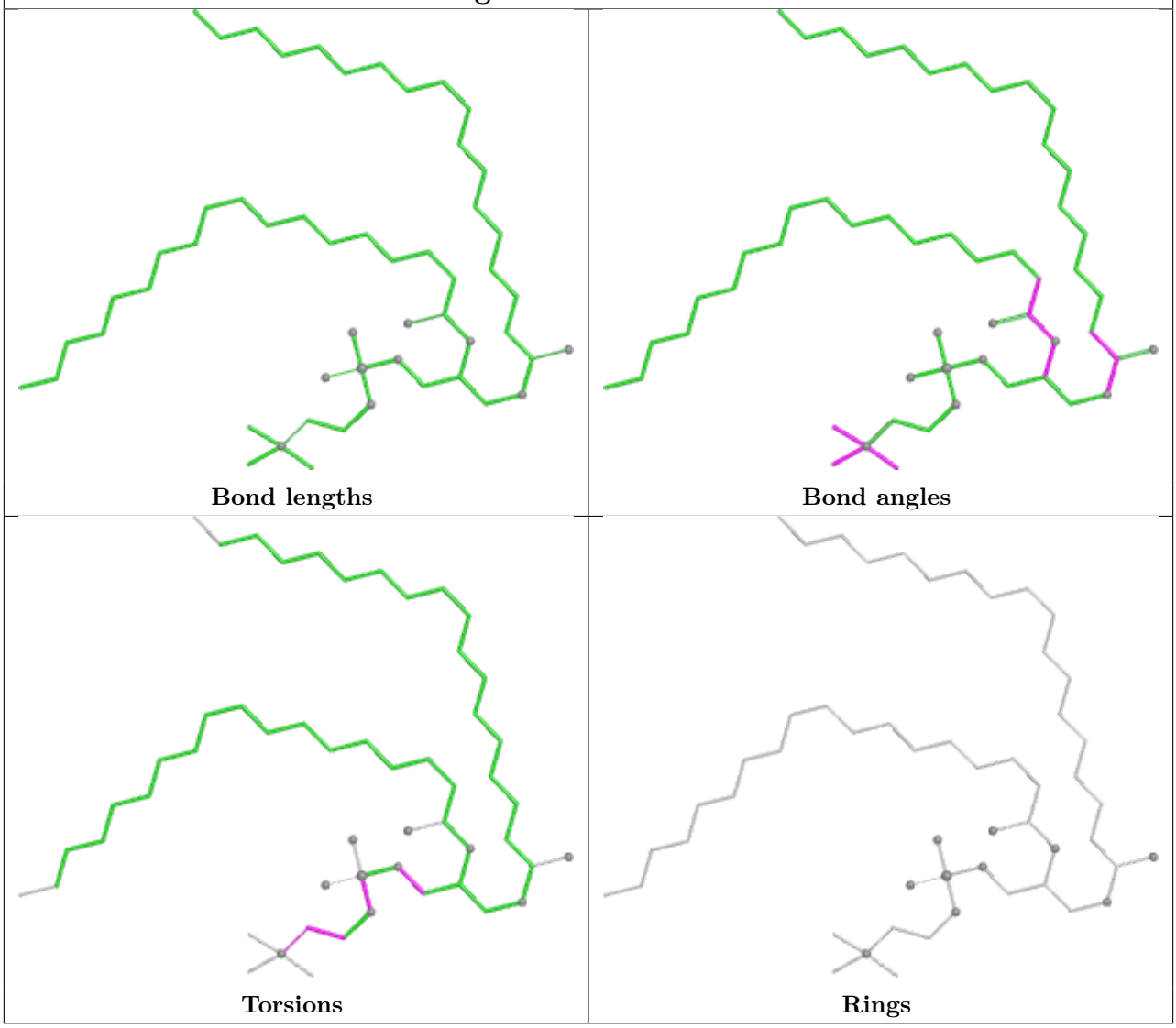

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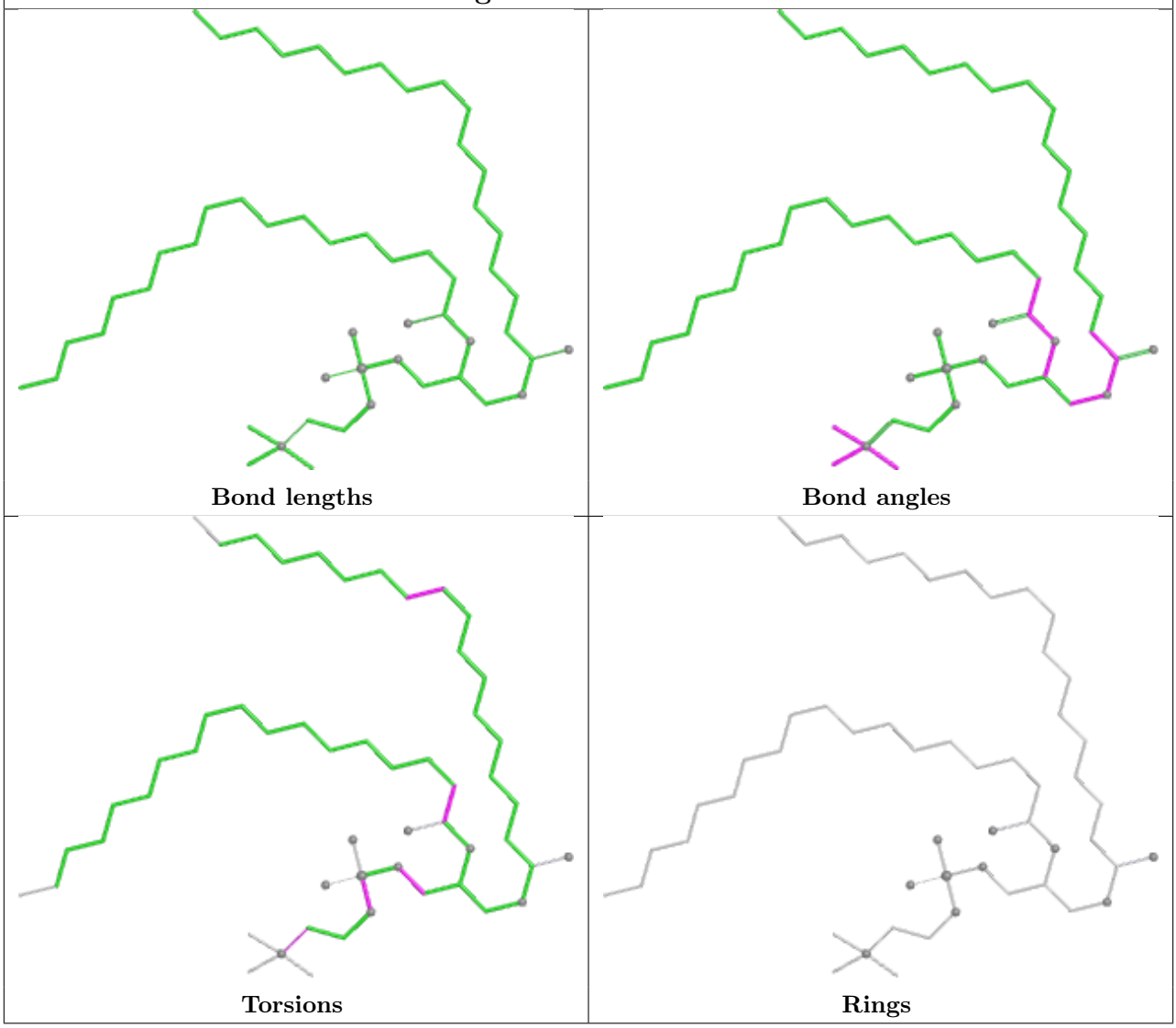

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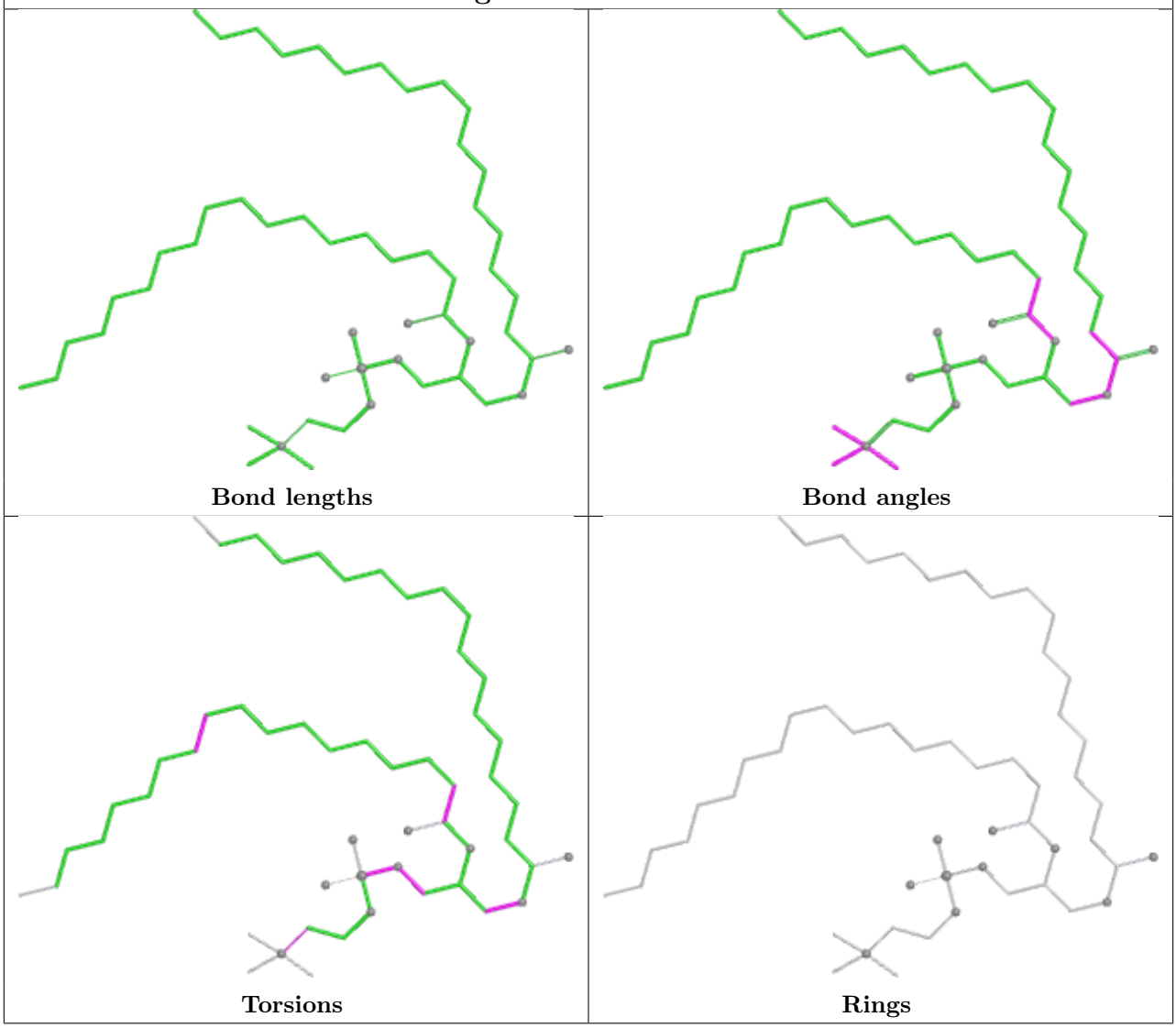

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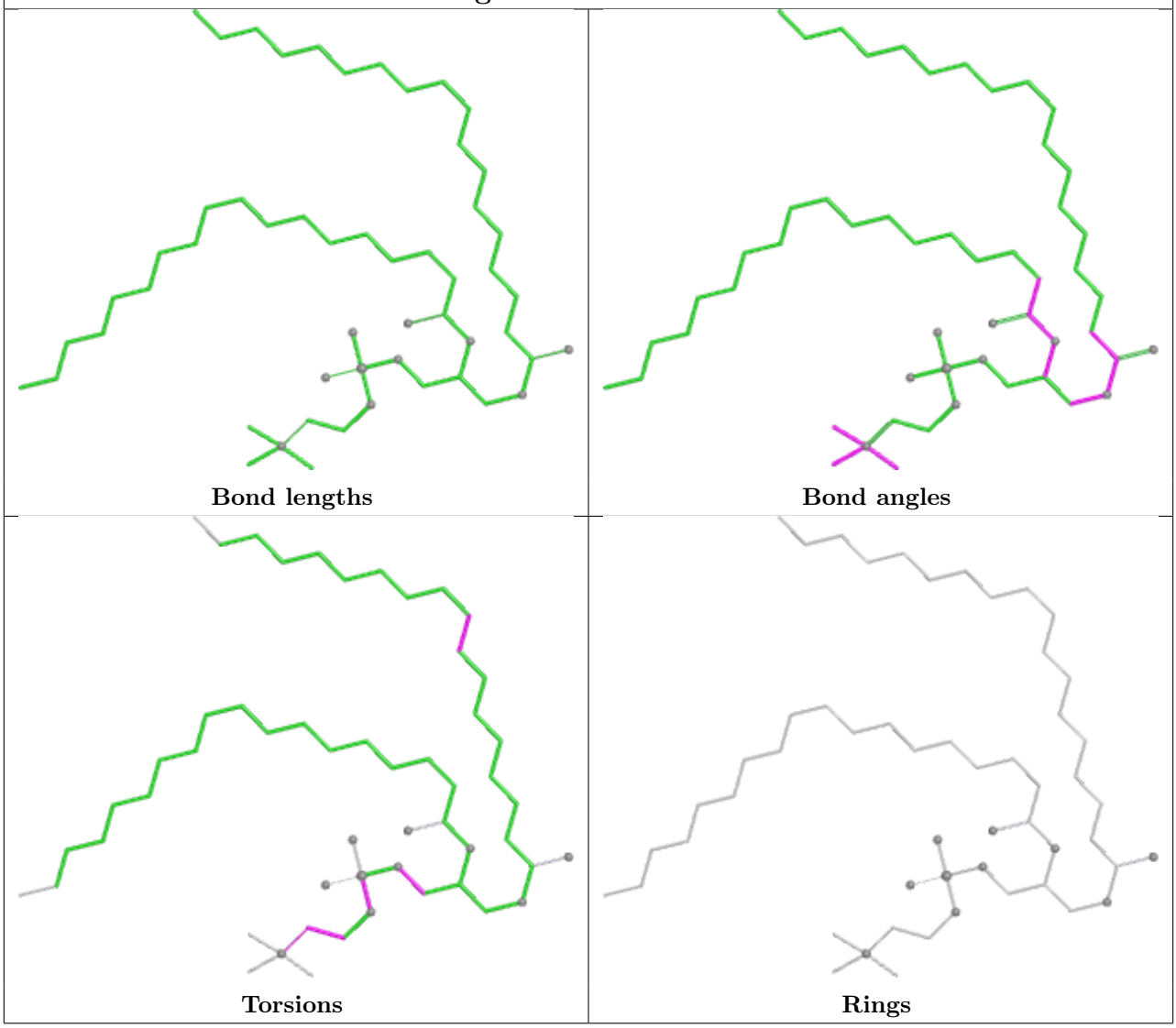
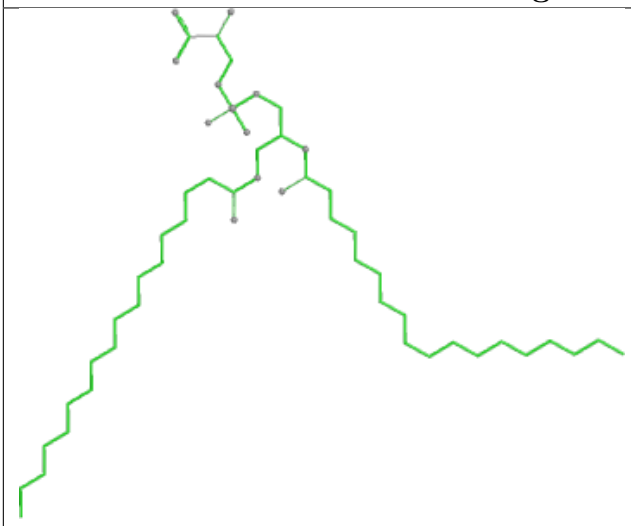
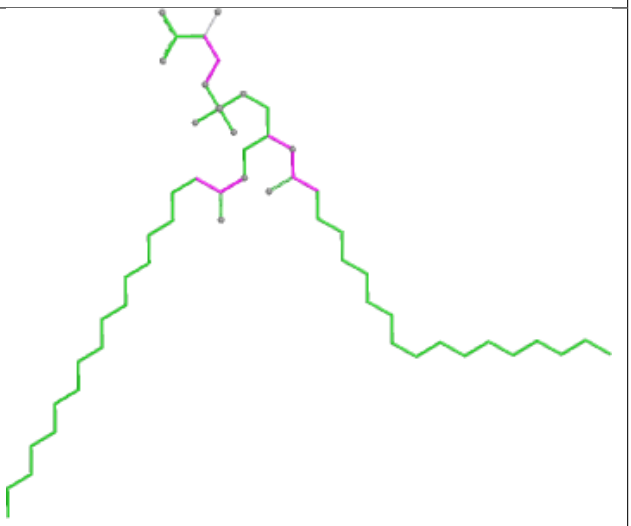


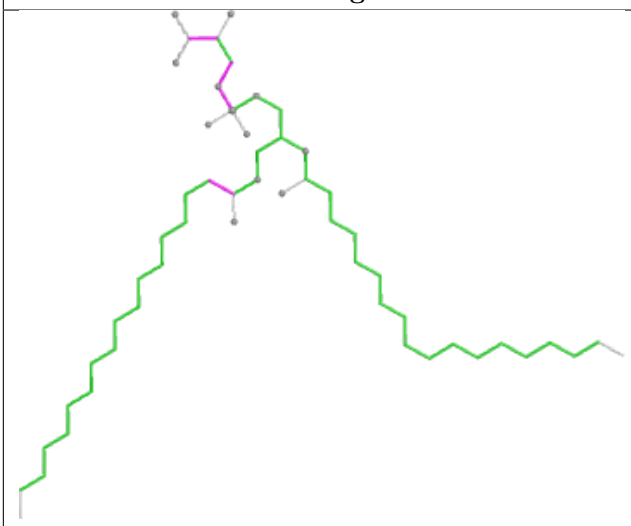
Ligand 17F C 213



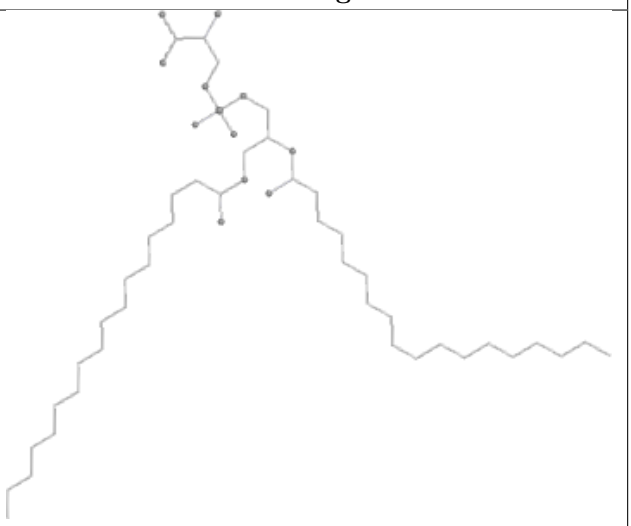
Bond lengths



Bond angles

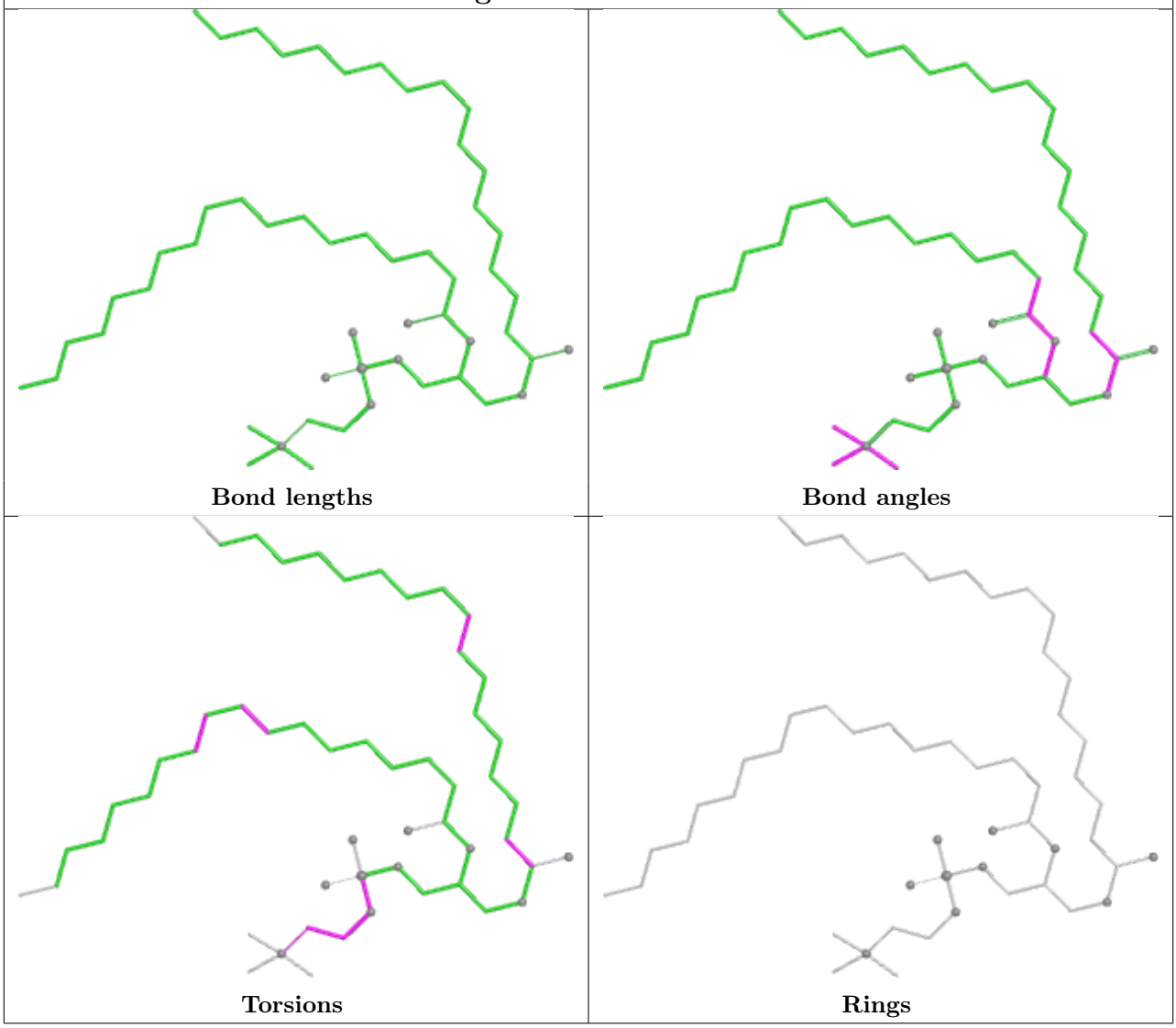


Torsions

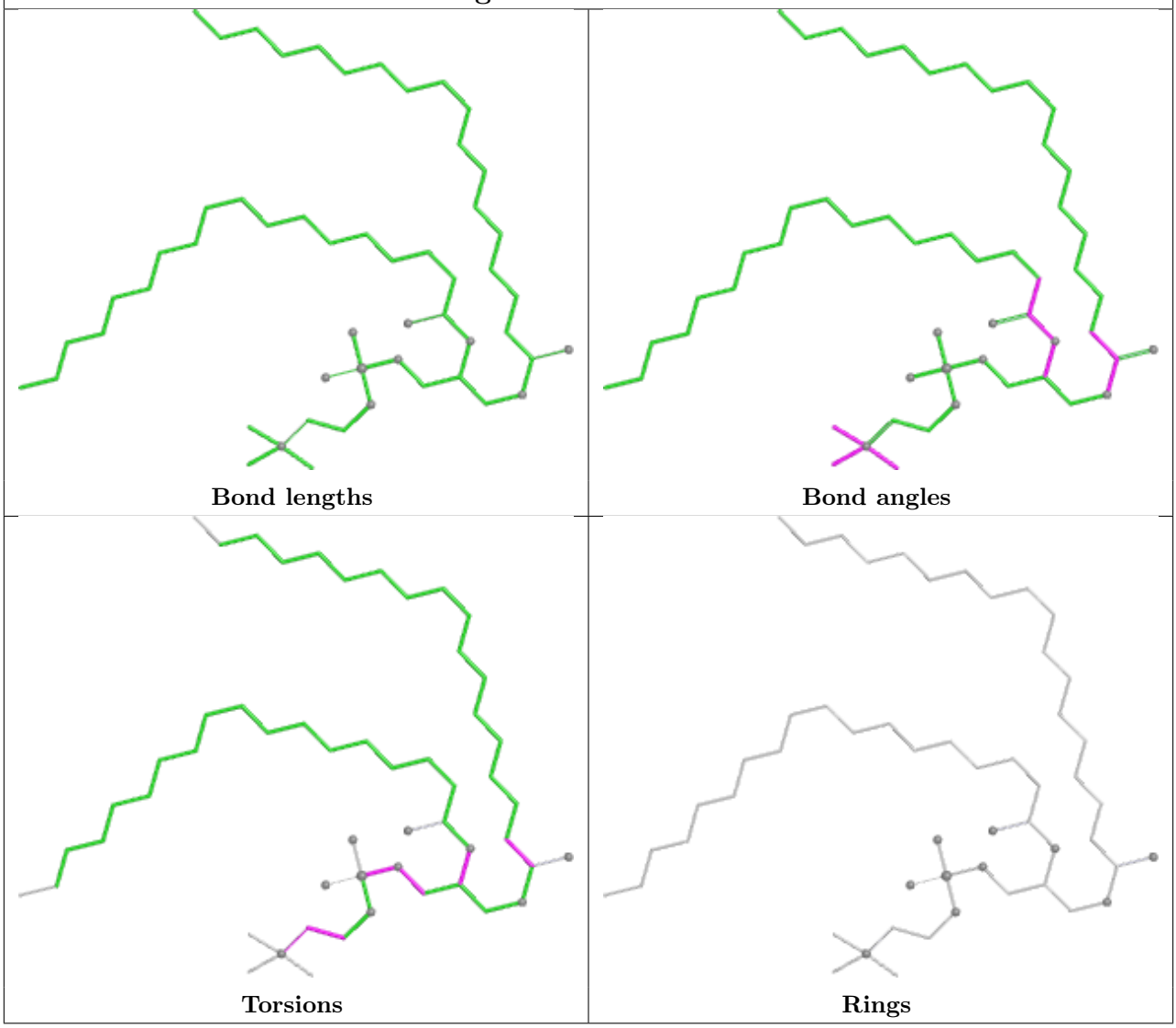


Rings

Ligand PCW A 420



Ligand PCW A 403



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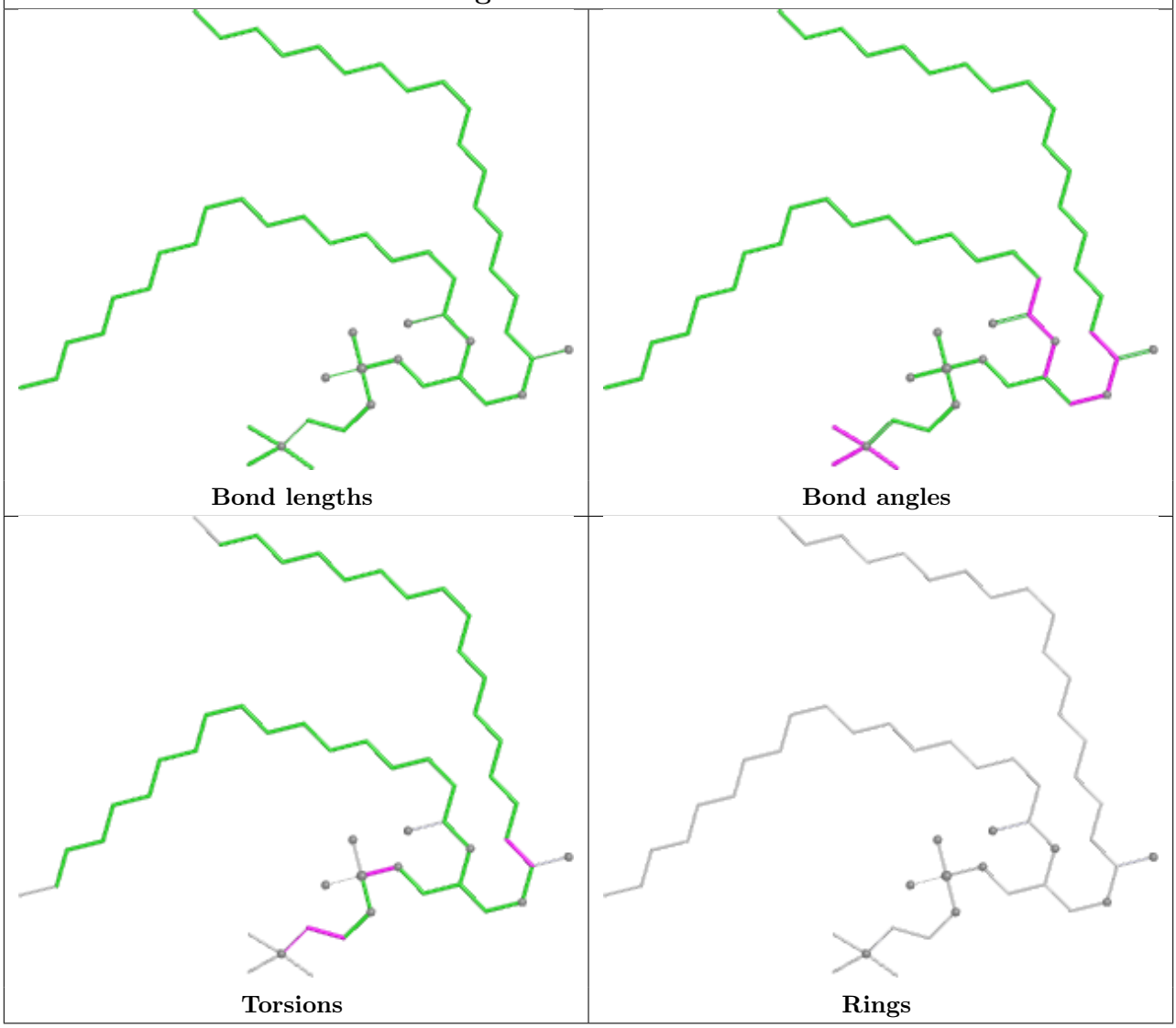
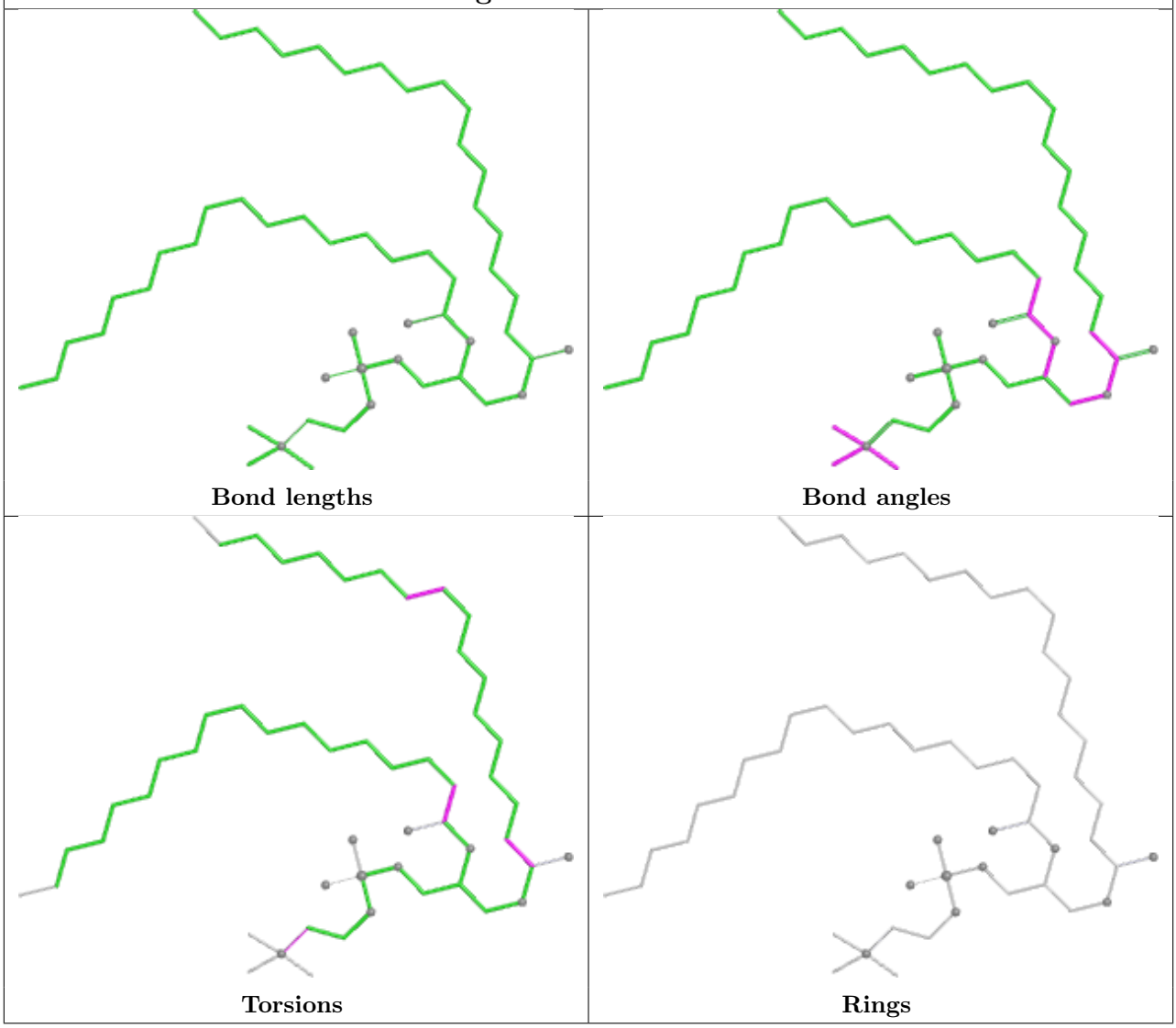
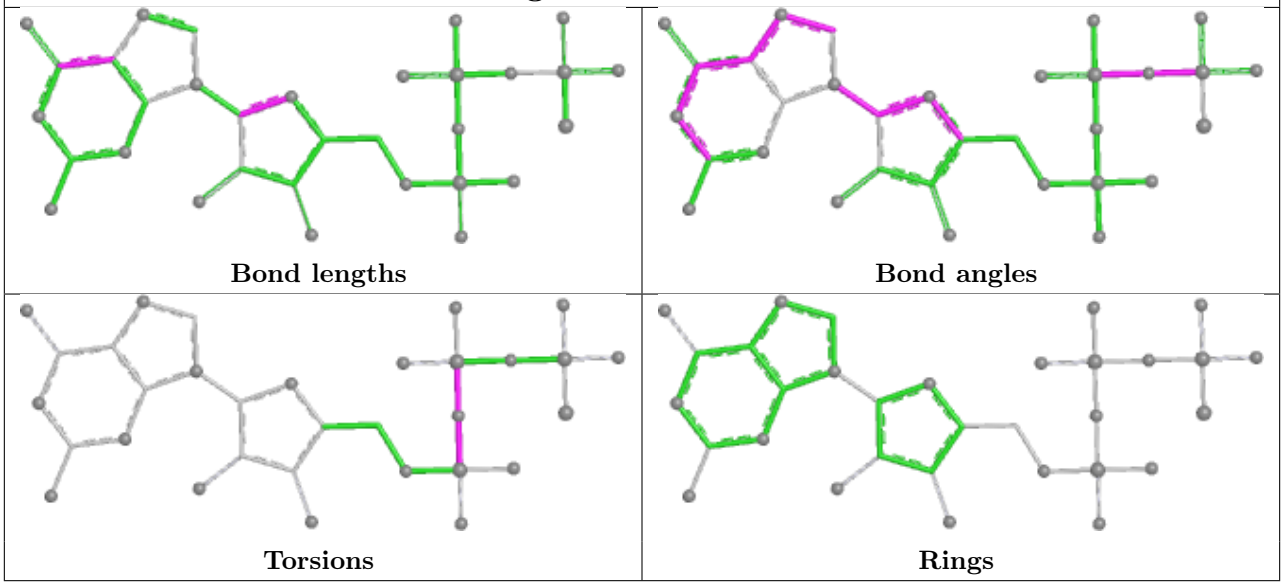


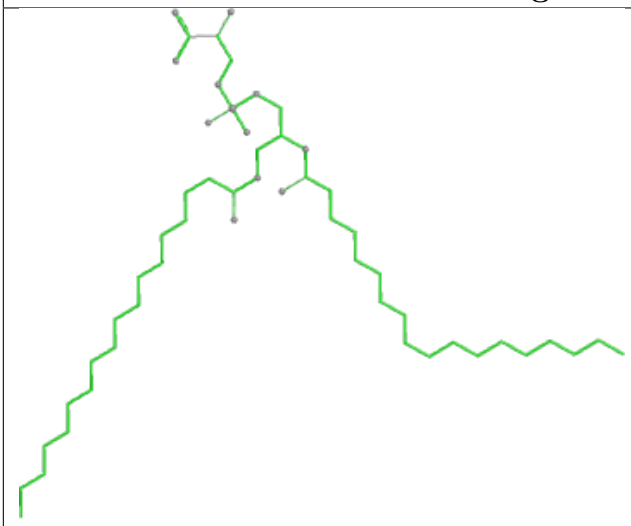
Ligand PCW B 203



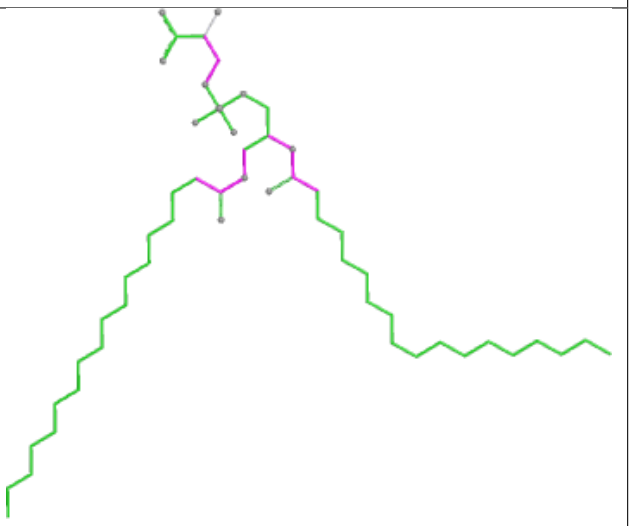
Ligand GSP B 201



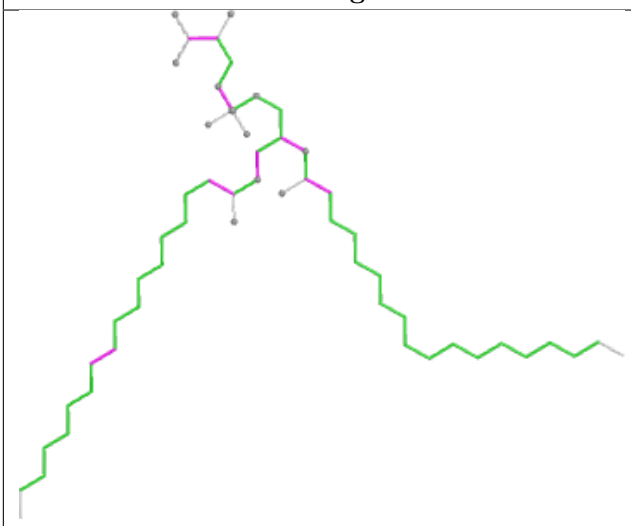
Ligand 17F D 632



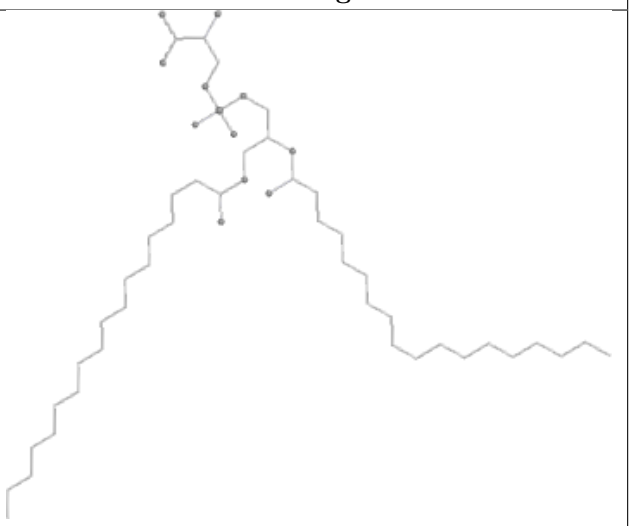
Bond lengths



Bond angles

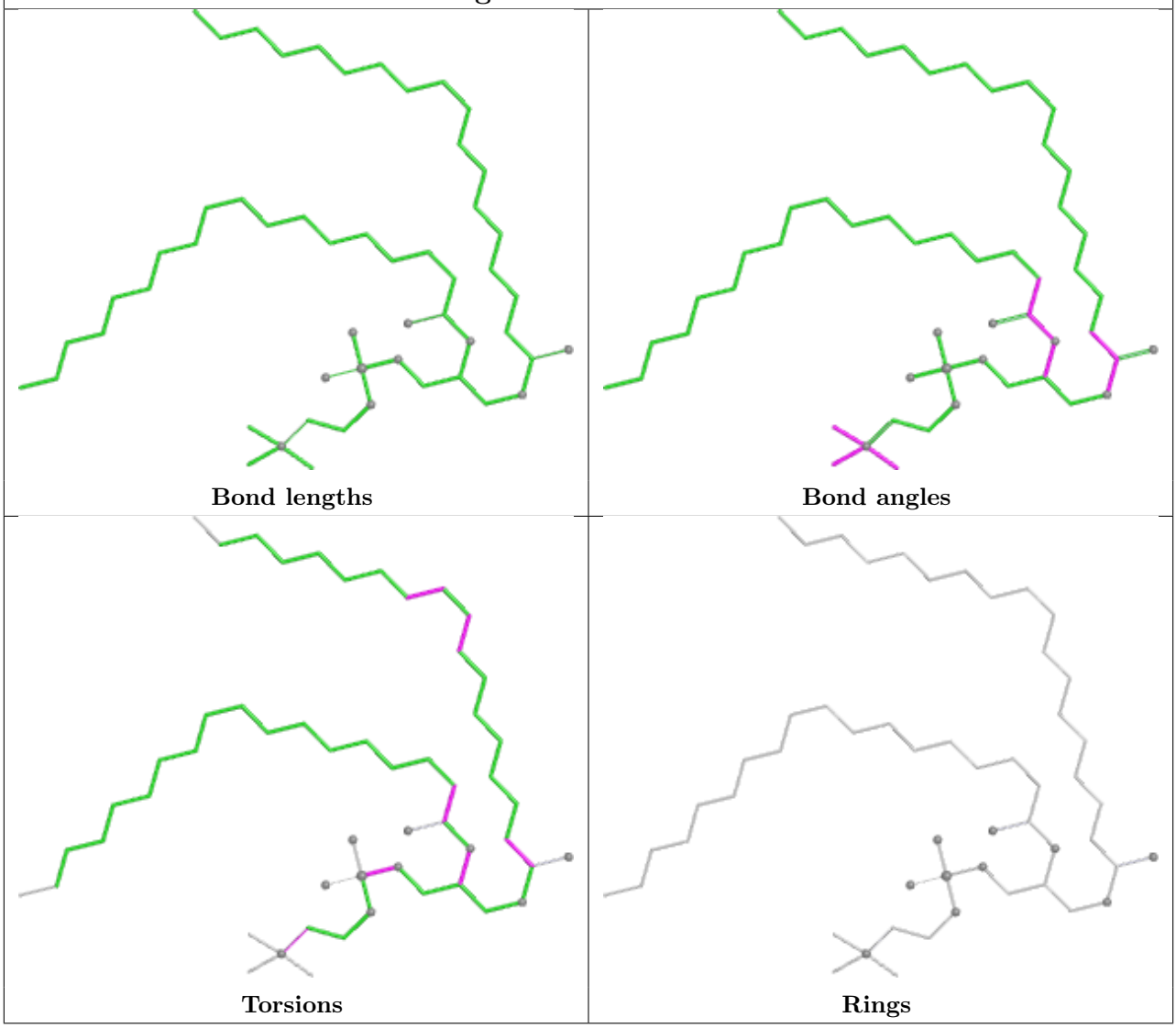


Torsions

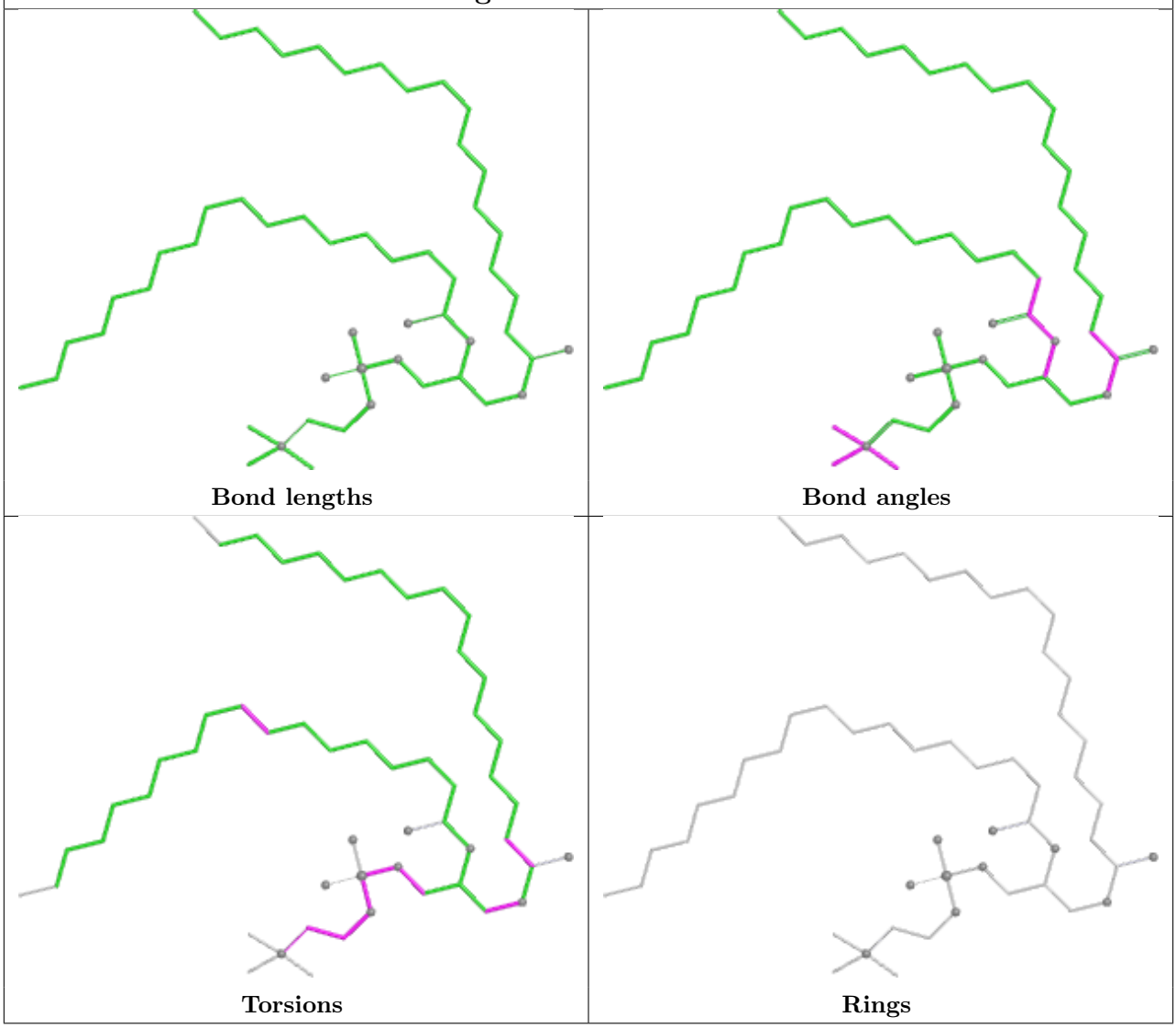


Rings

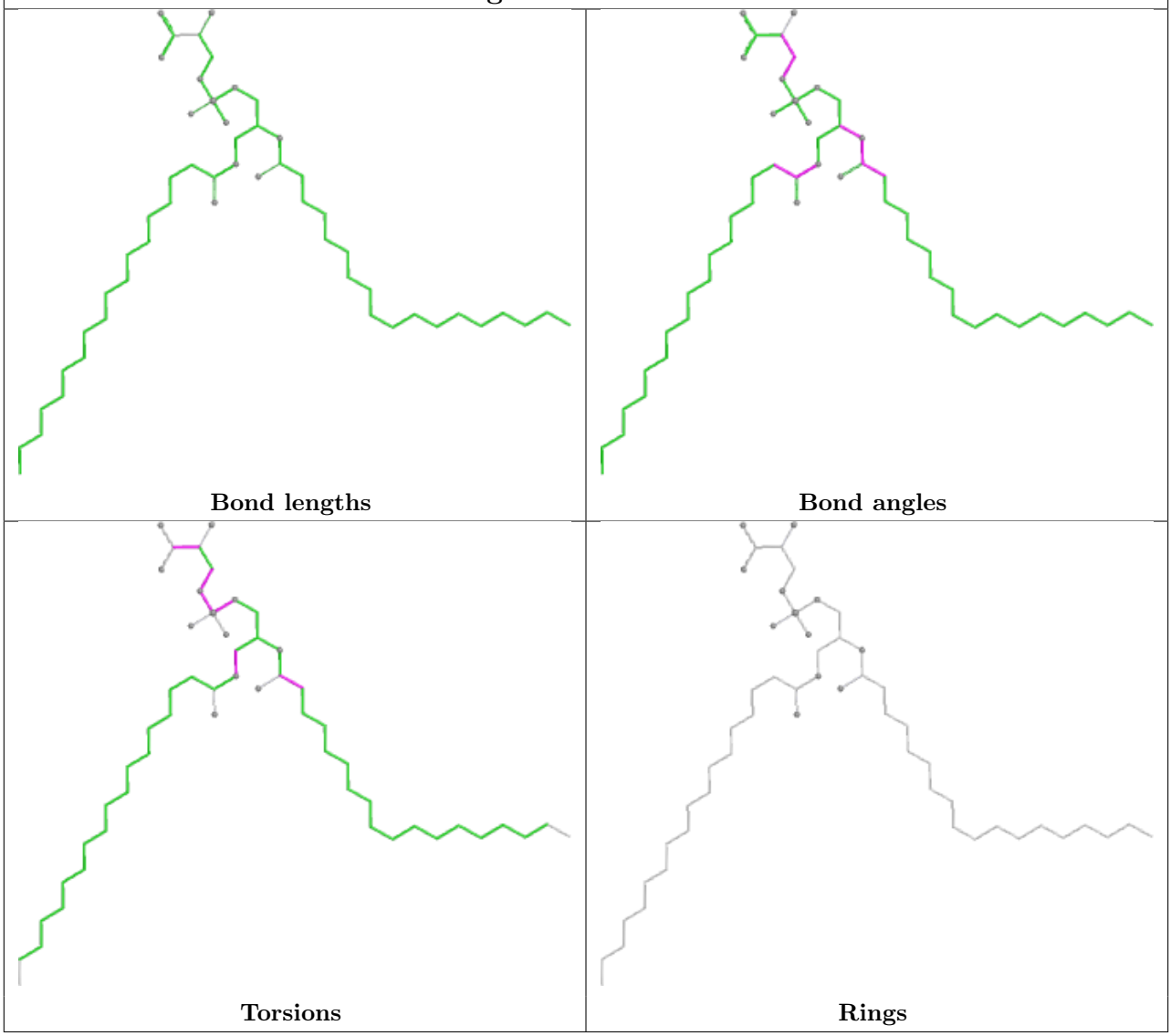
Ligand PCW A 409



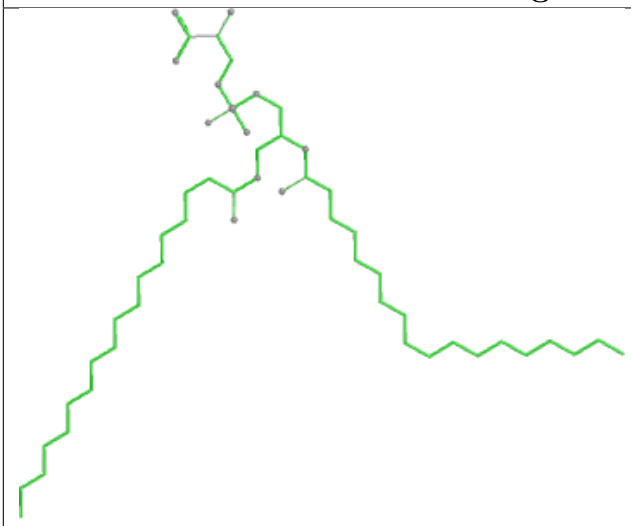
Ligand PCW A 417



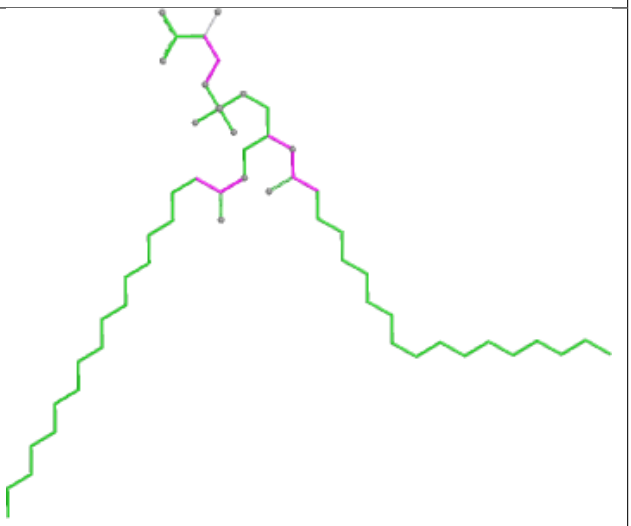
Ligand 17F C 214



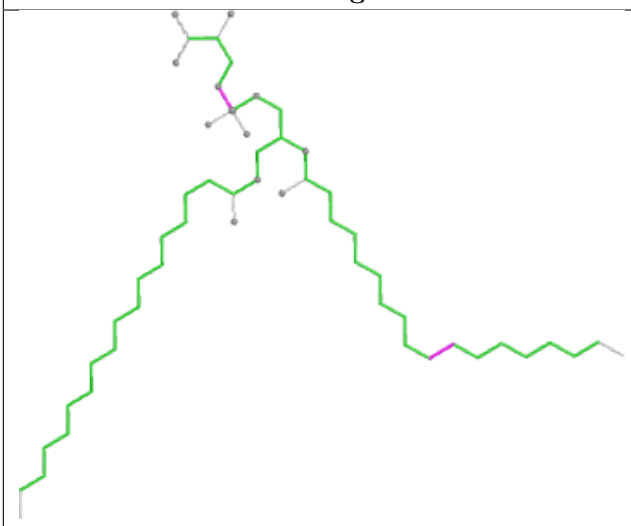
Ligand 17F A 422



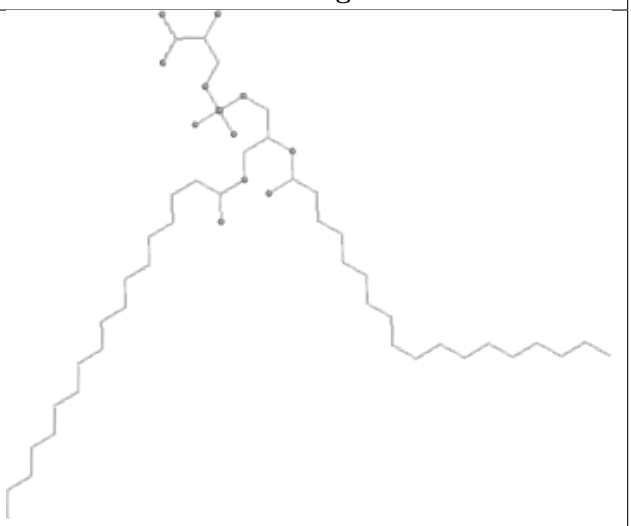
Bond lengths



Bond angles

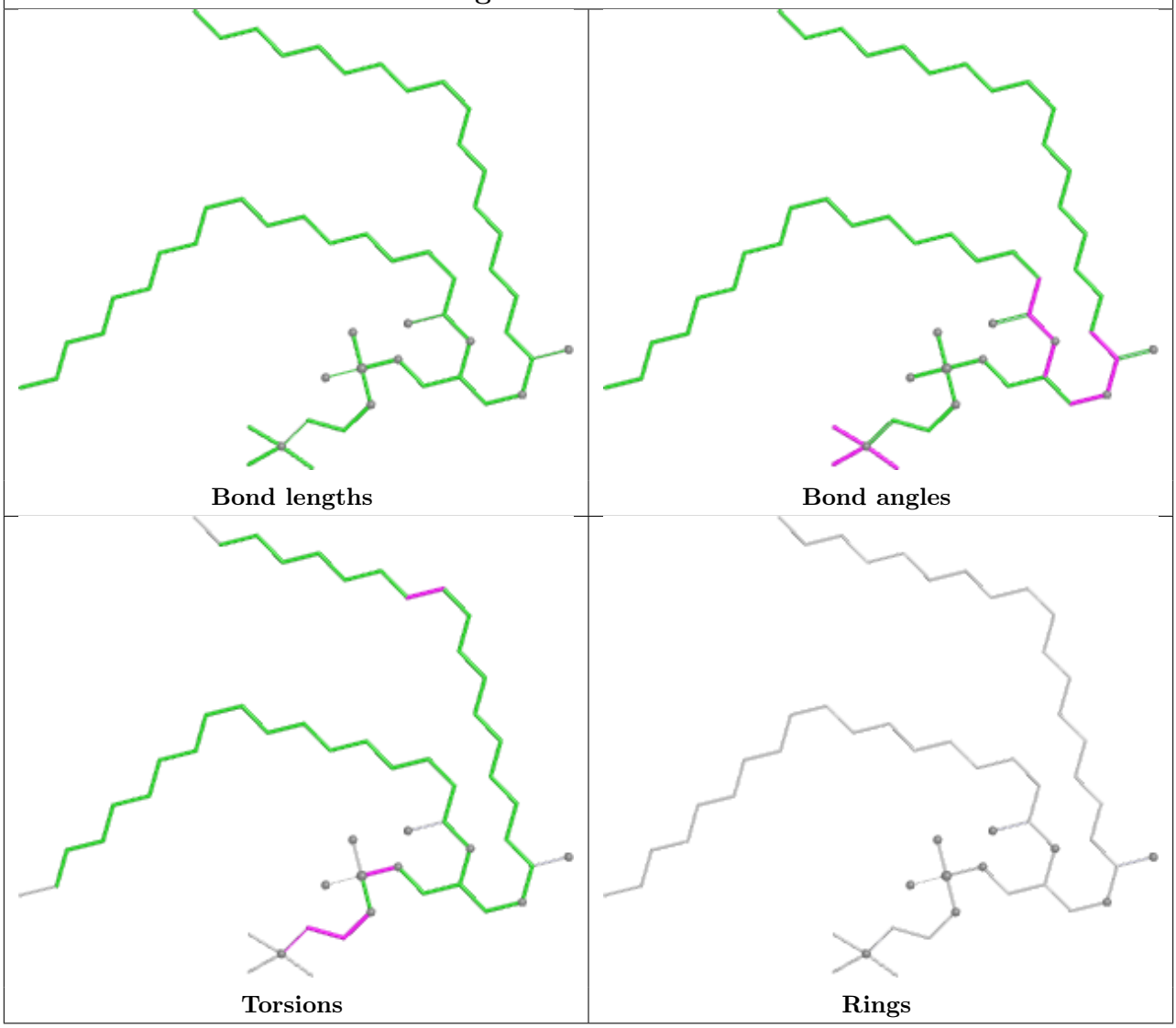


Torsions

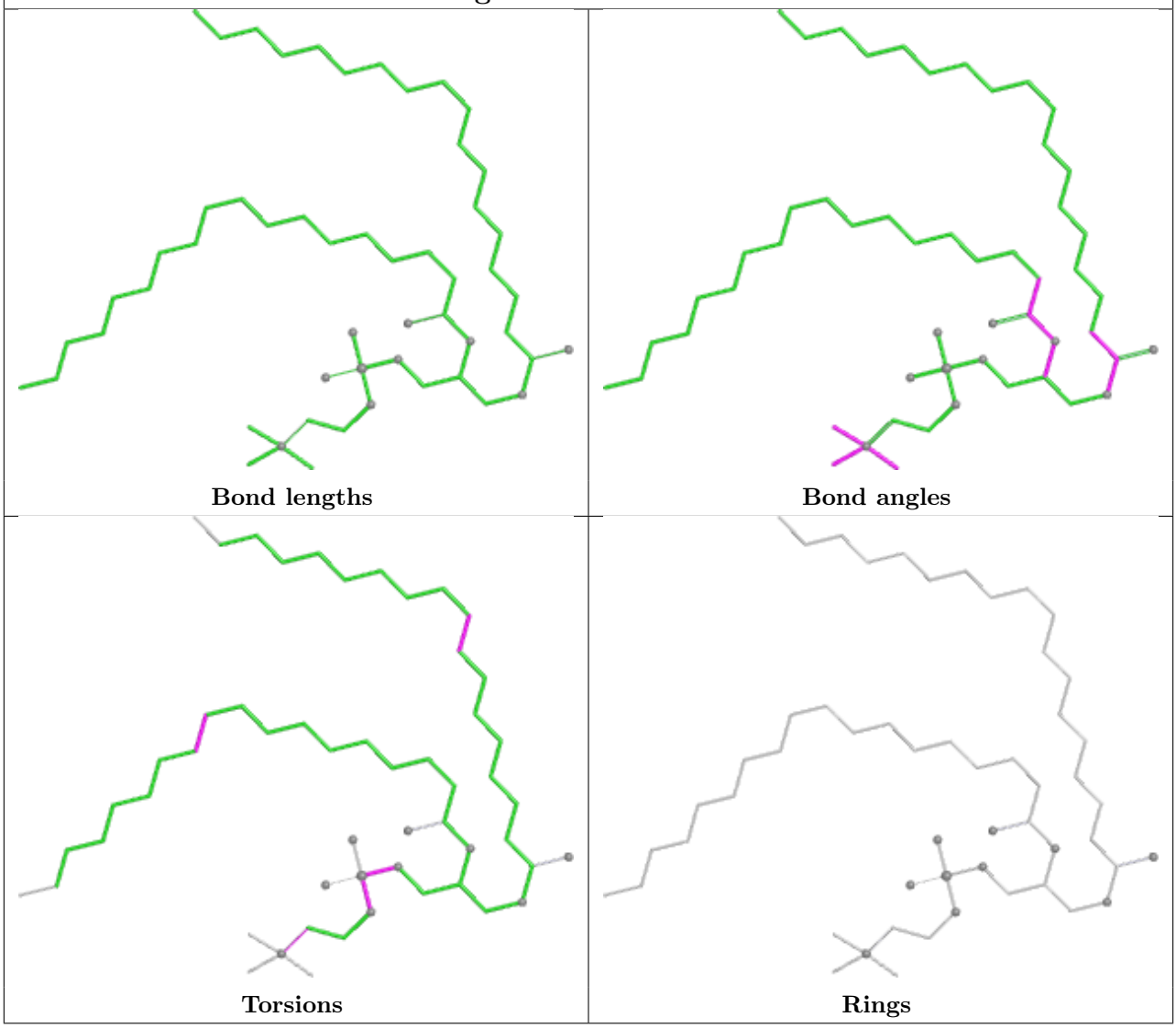


Rings

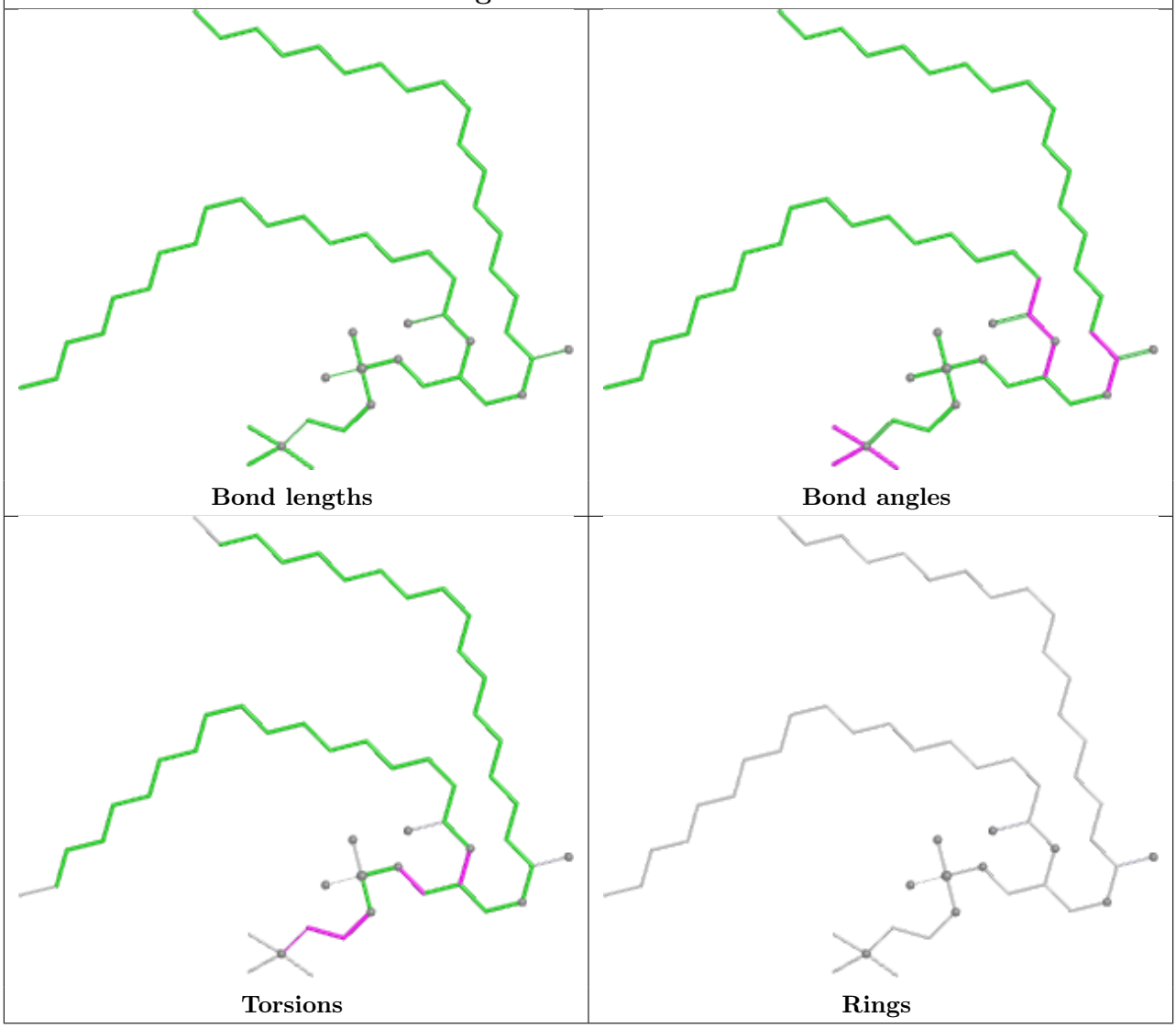
Ligand PCW A 413



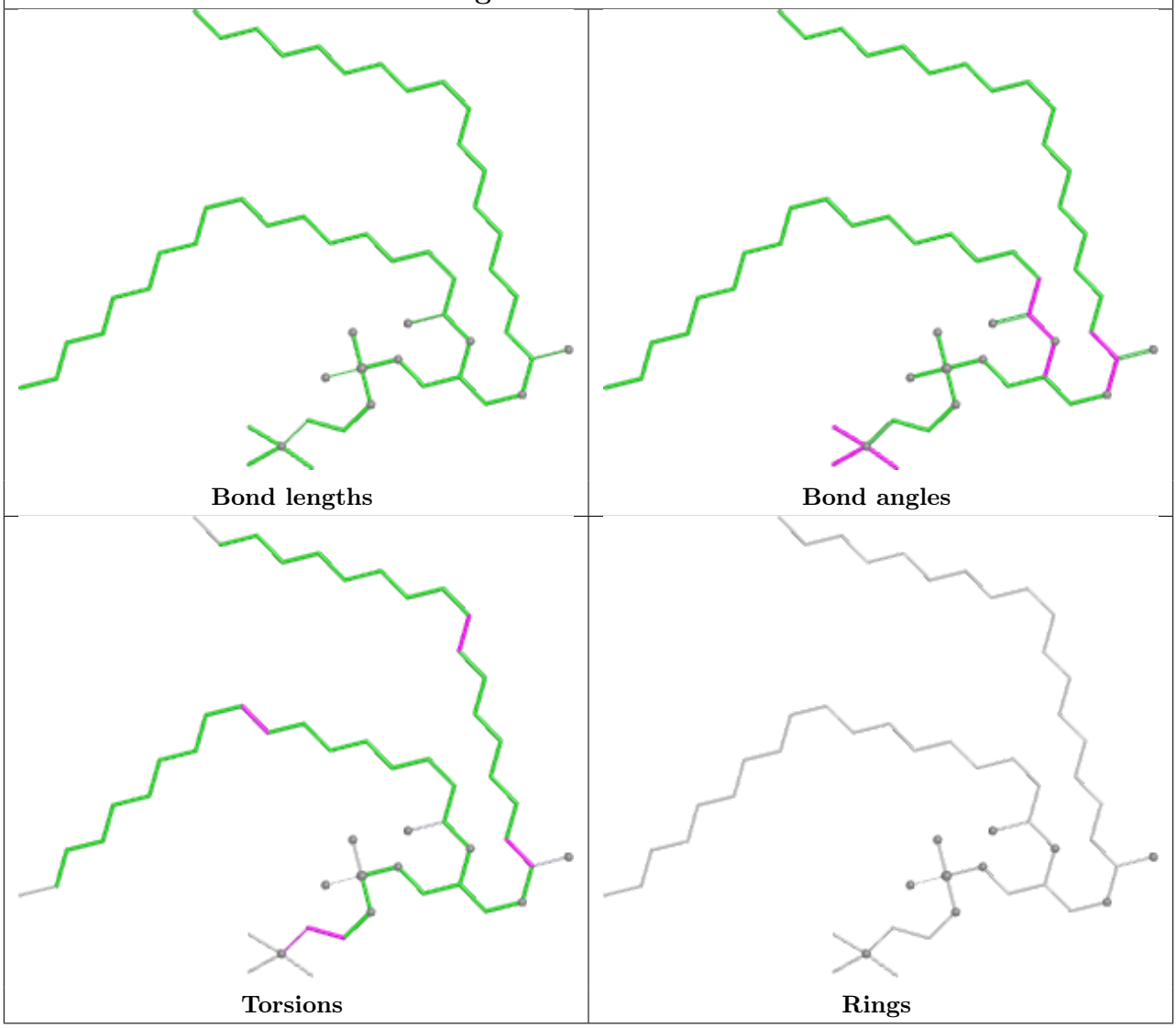
Ligand PCW D 609



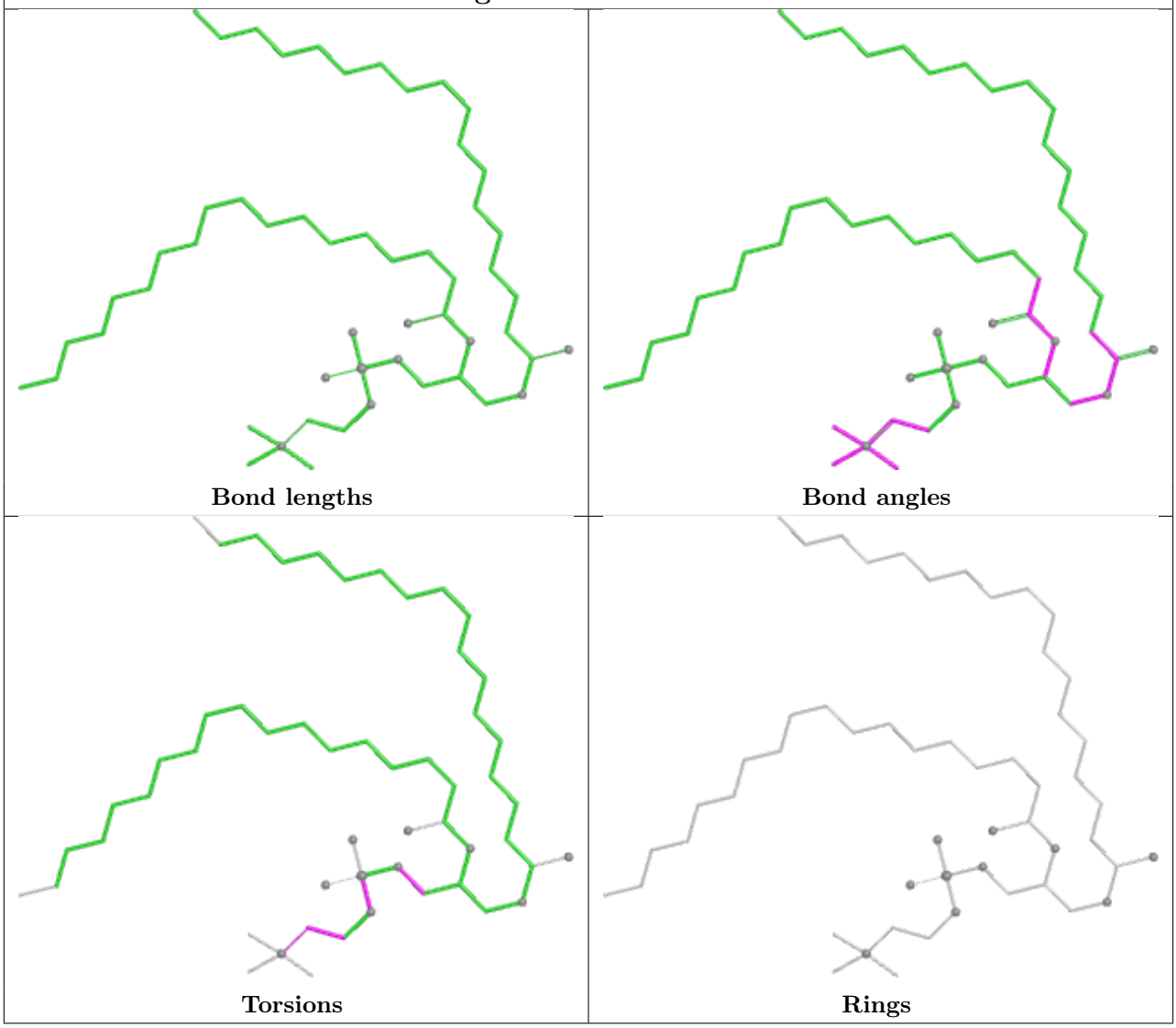
Ligand PCW C 207



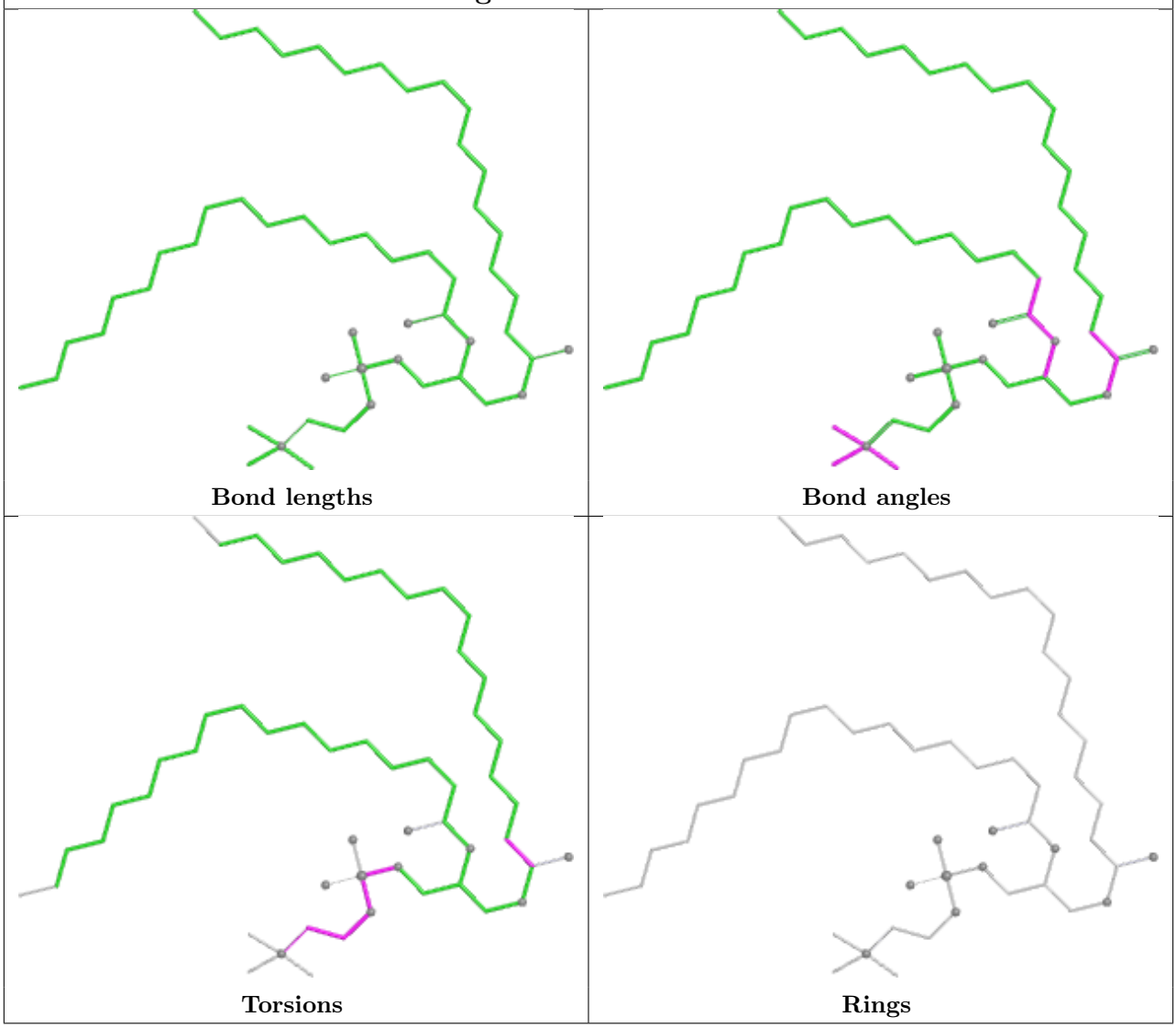
Ligand PCW A 412



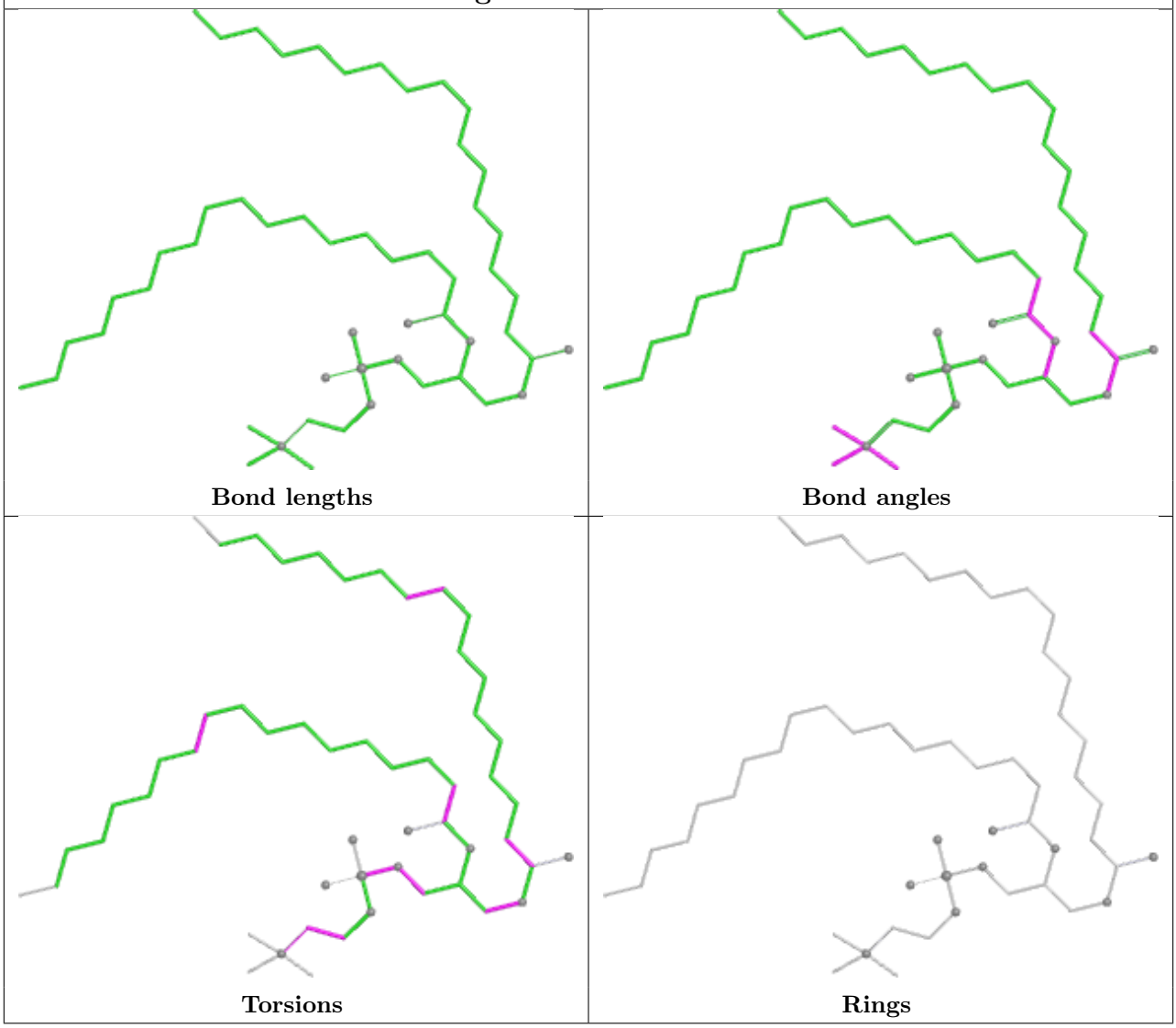
Ligand PCW D 626



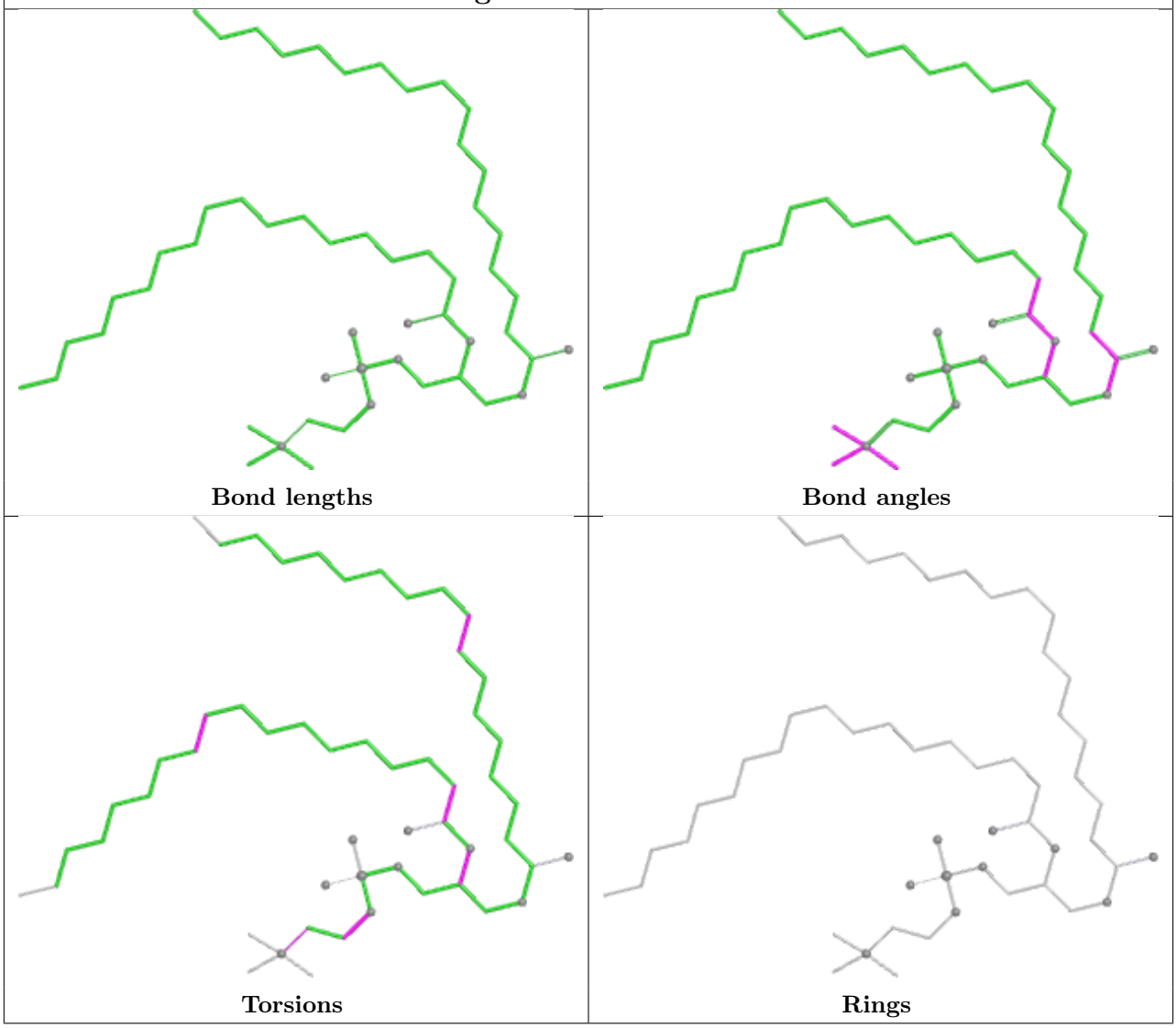
Ligand PCW C 211



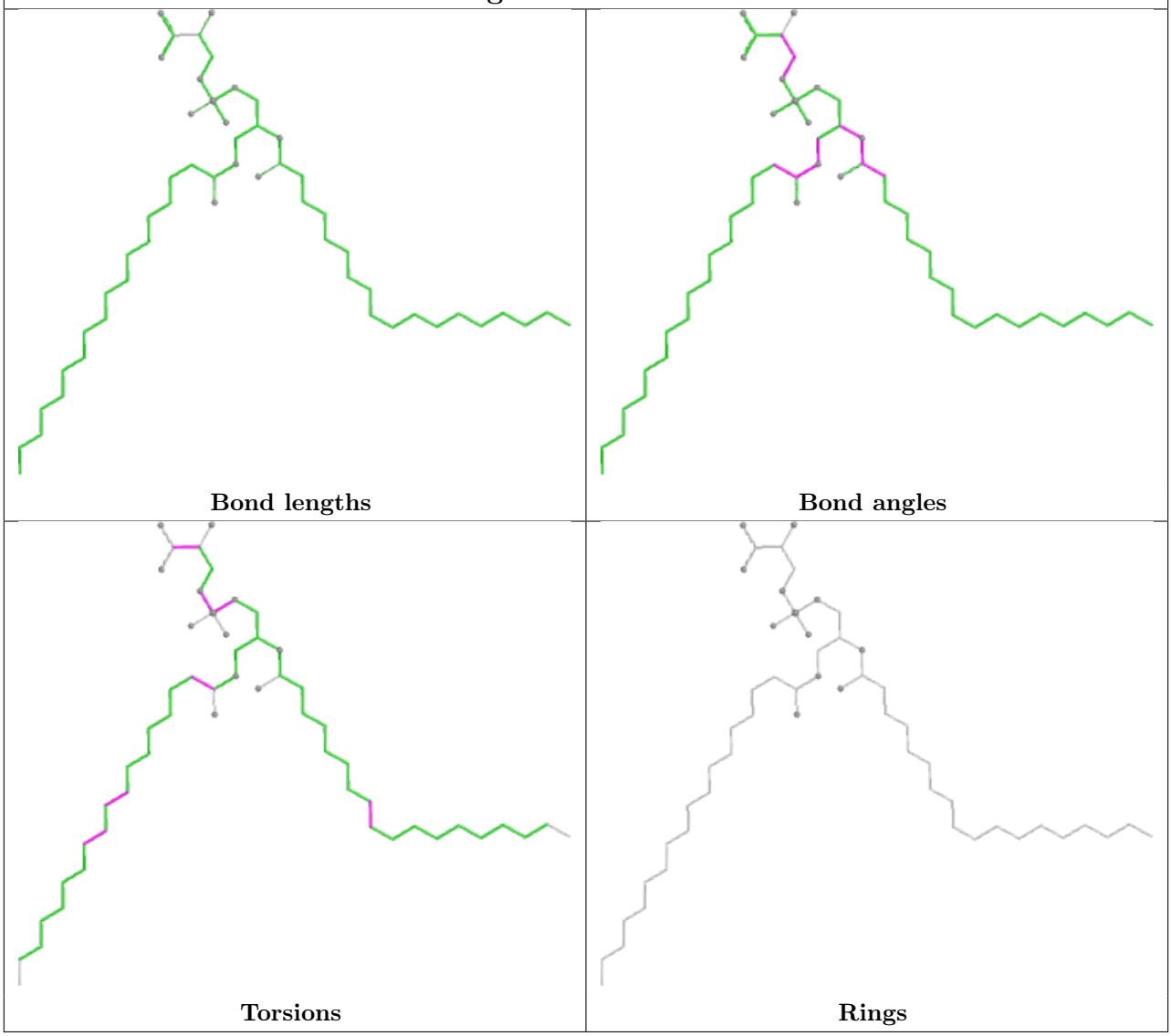
Ligand PCW A 405



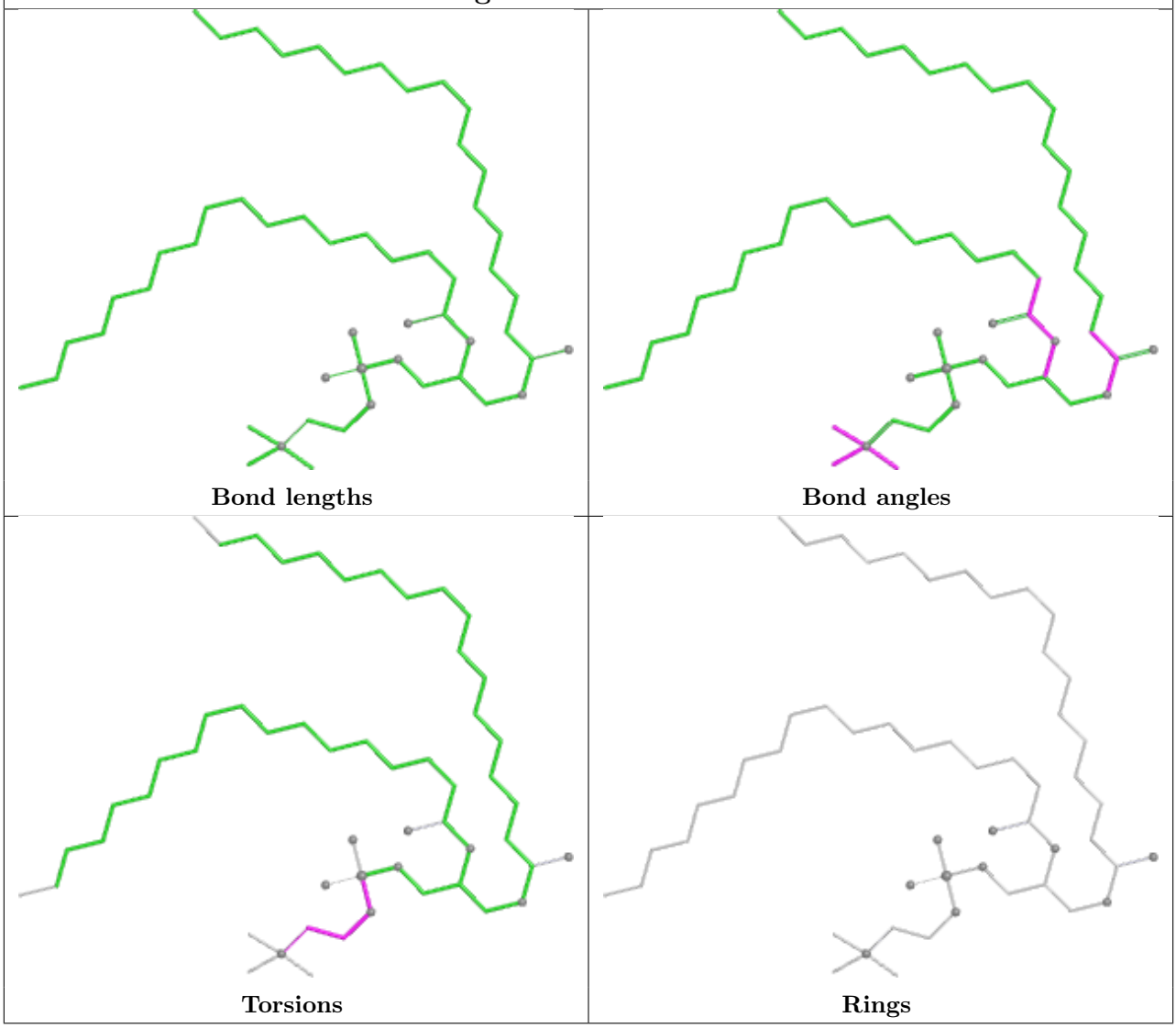
Ligand PCW D 602



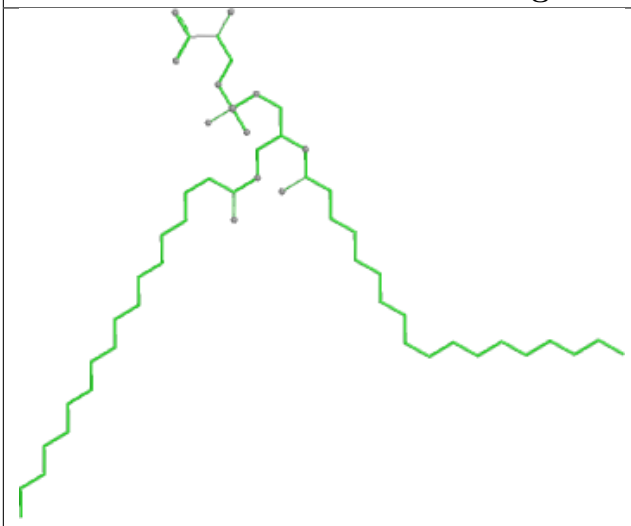
Ligand 17F B 209



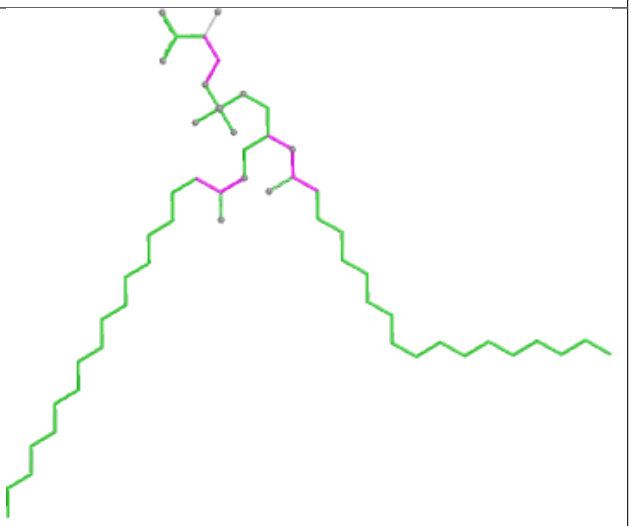
Ligand PCW D 623



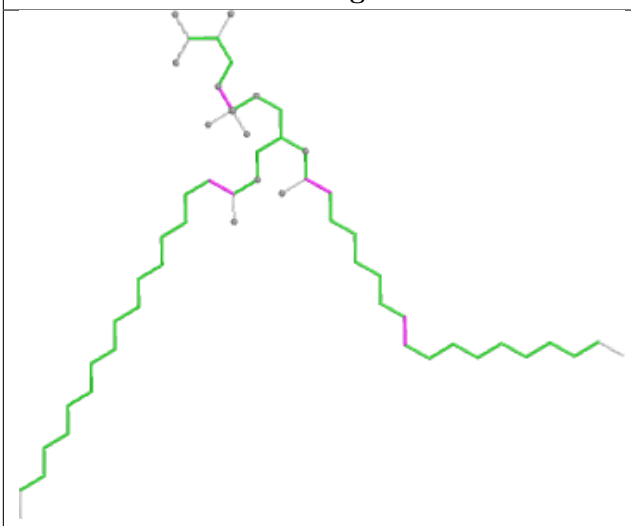
Ligand 17F D 628



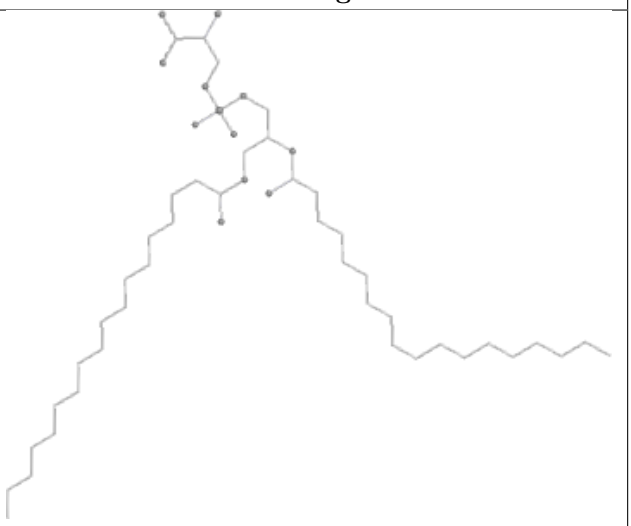
Bond lengths



Bond angles

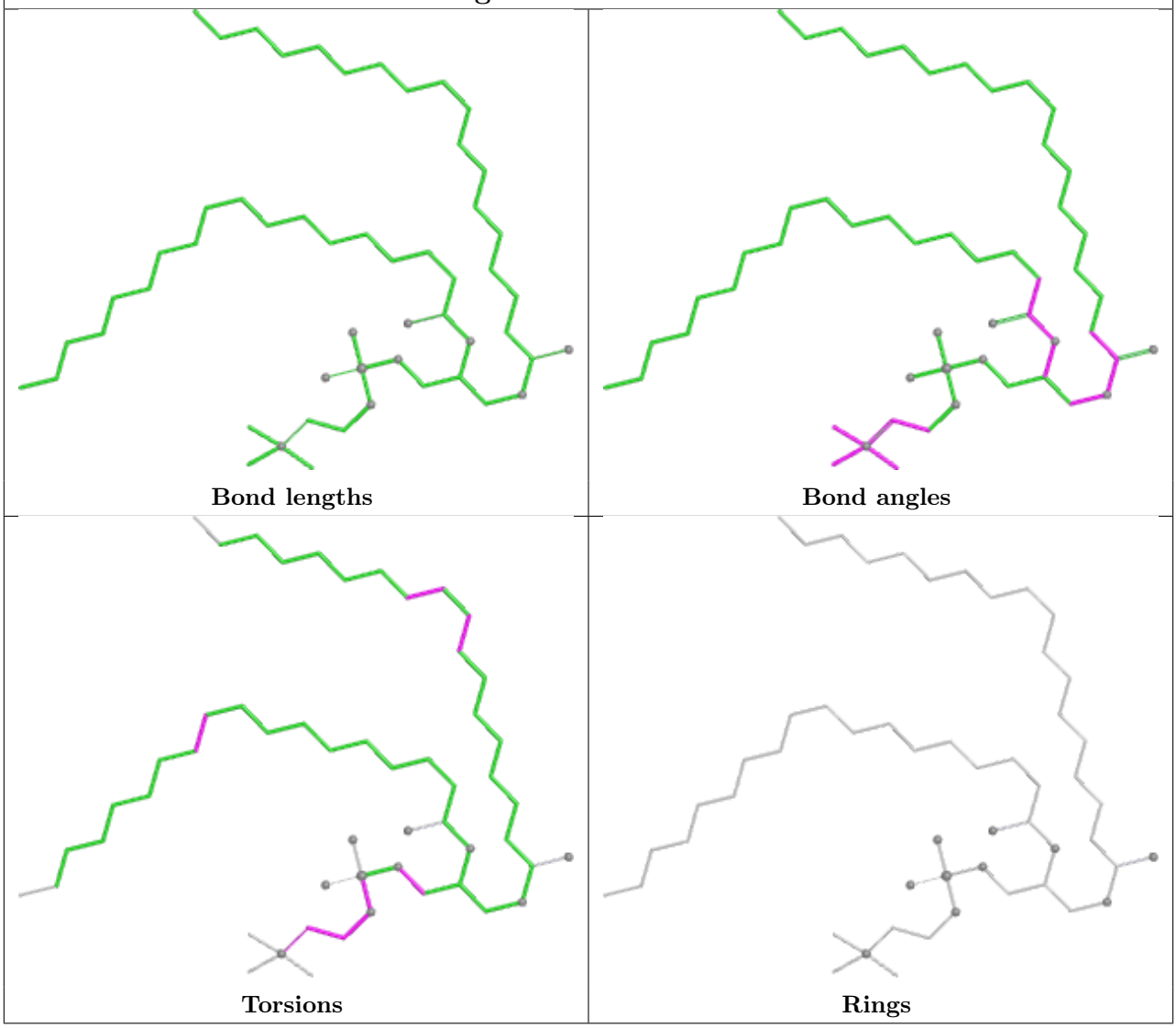


Torsions

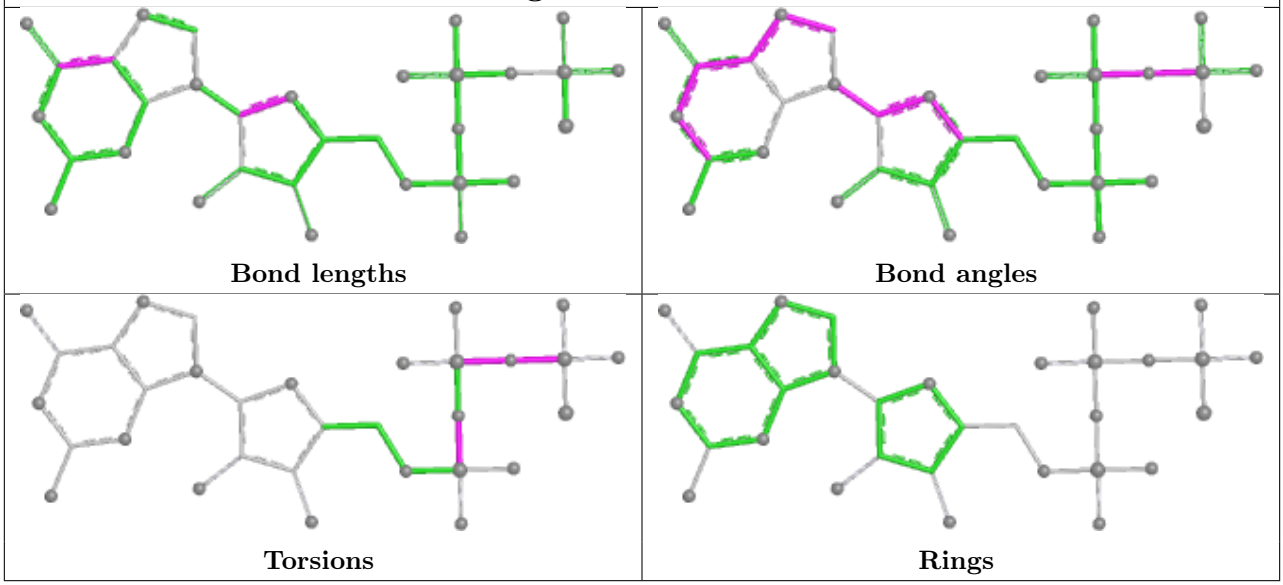


Rings

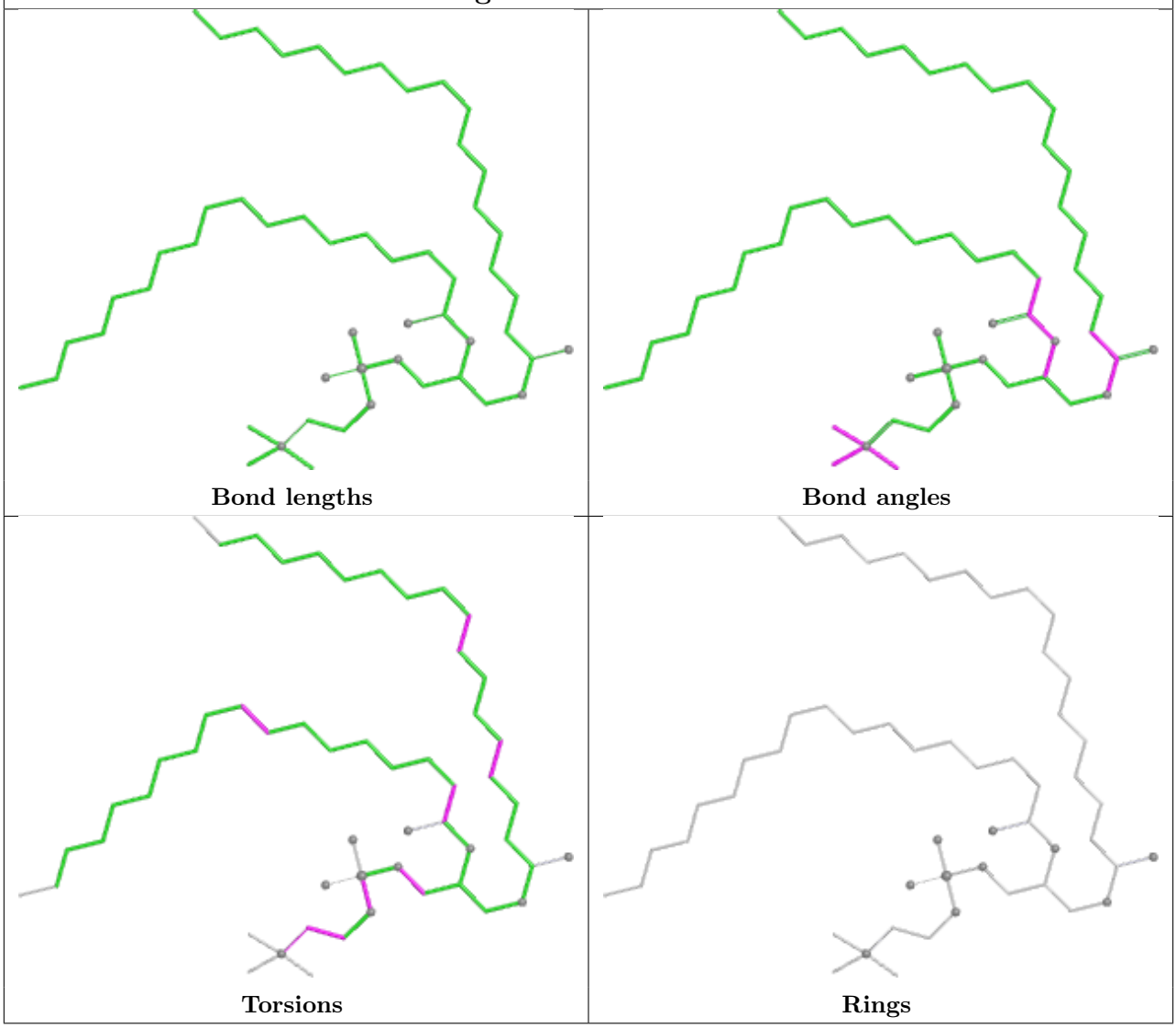
Ligand PCW D 627



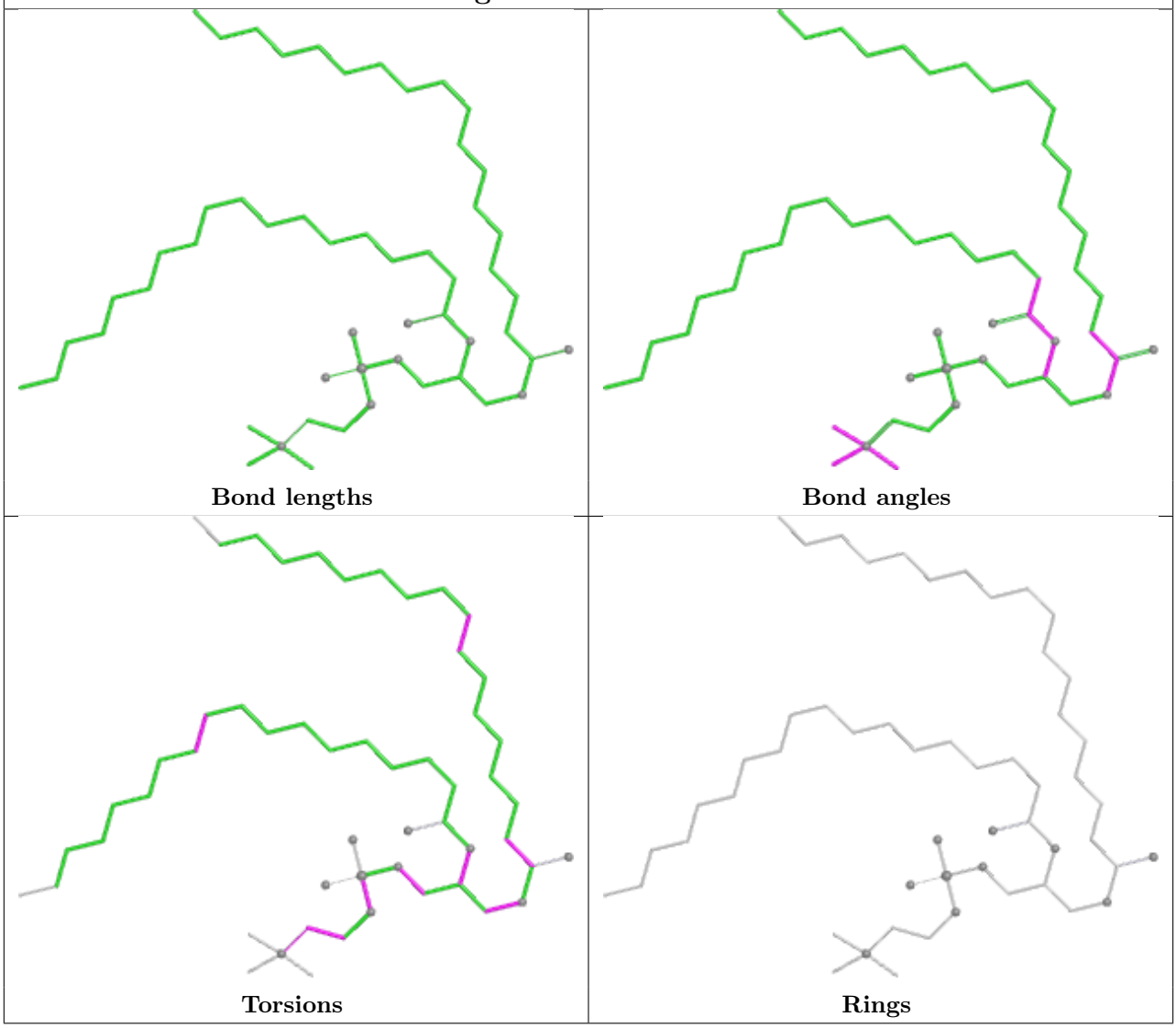
Ligand GSP C 201



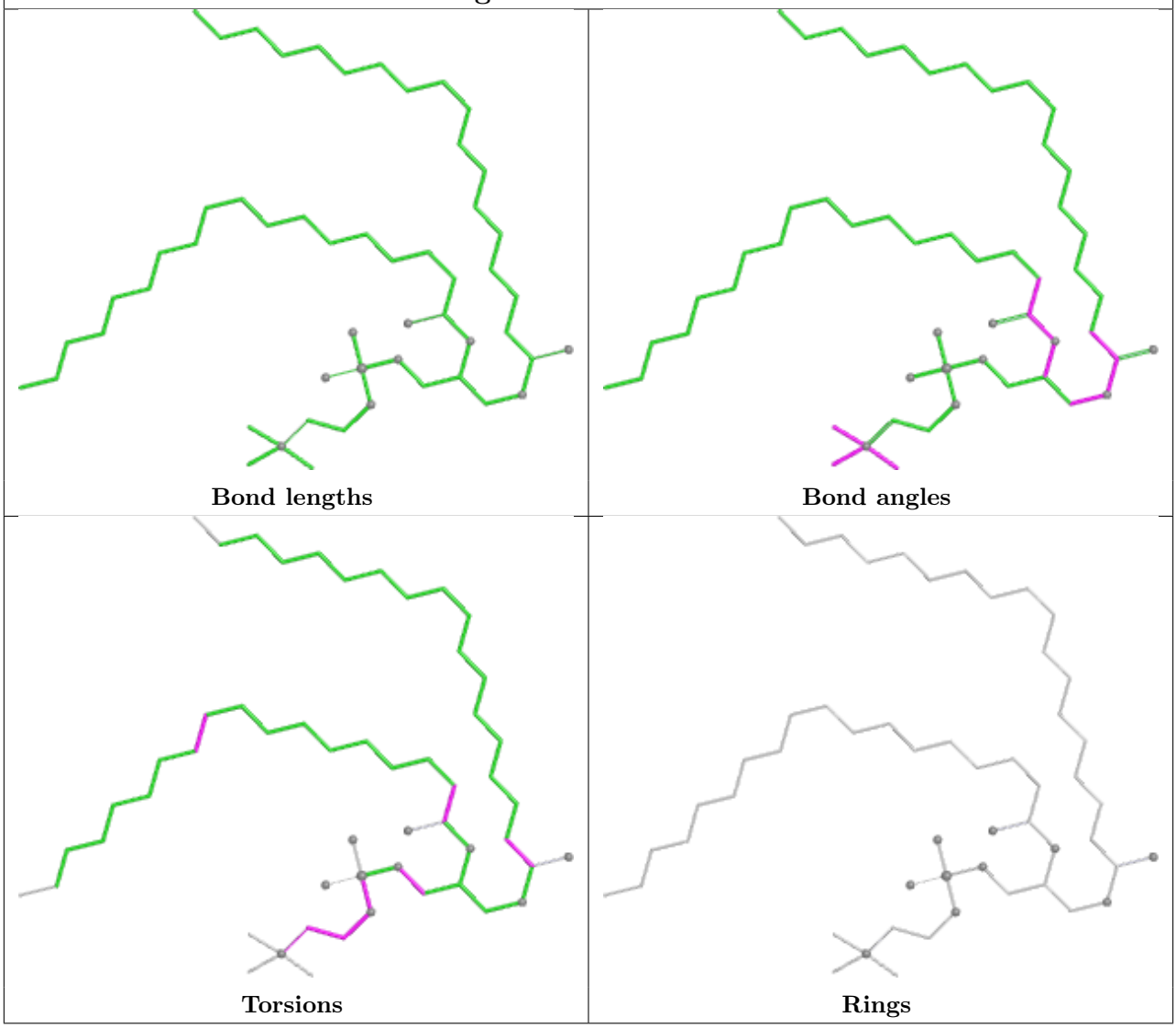
Ligand PCW A 407



Ligand PCW D 618



Ligand PCW D 616



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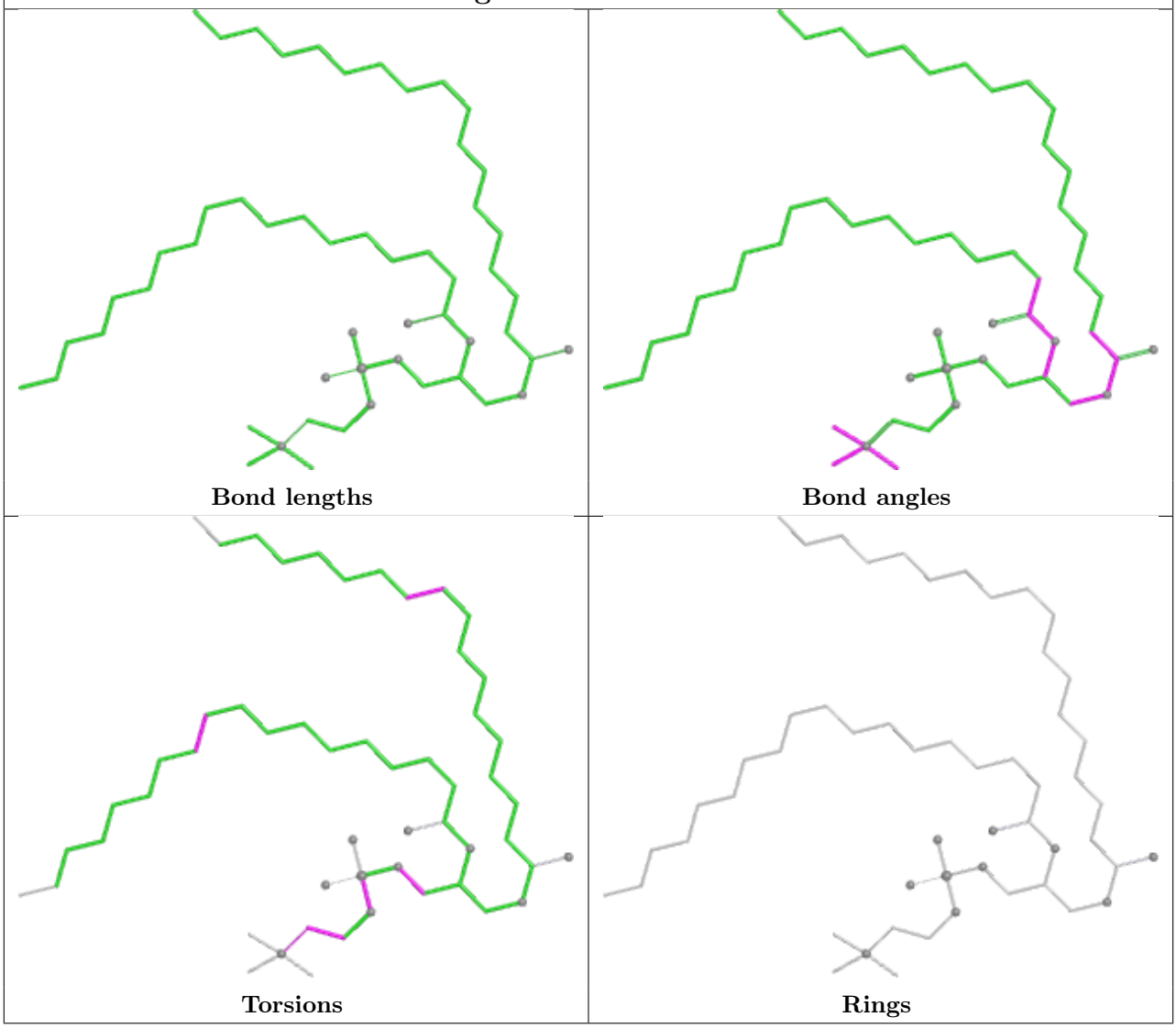
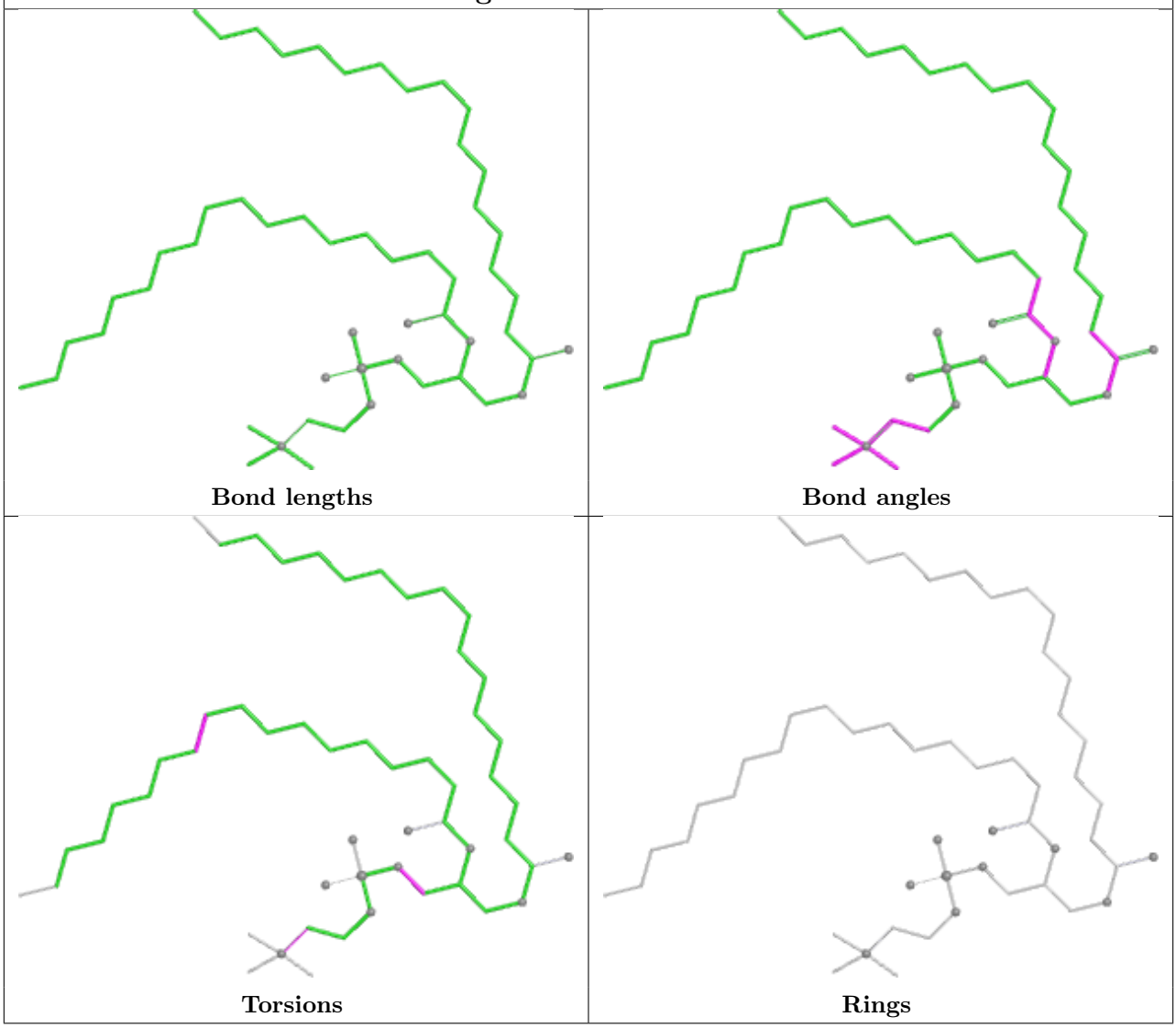
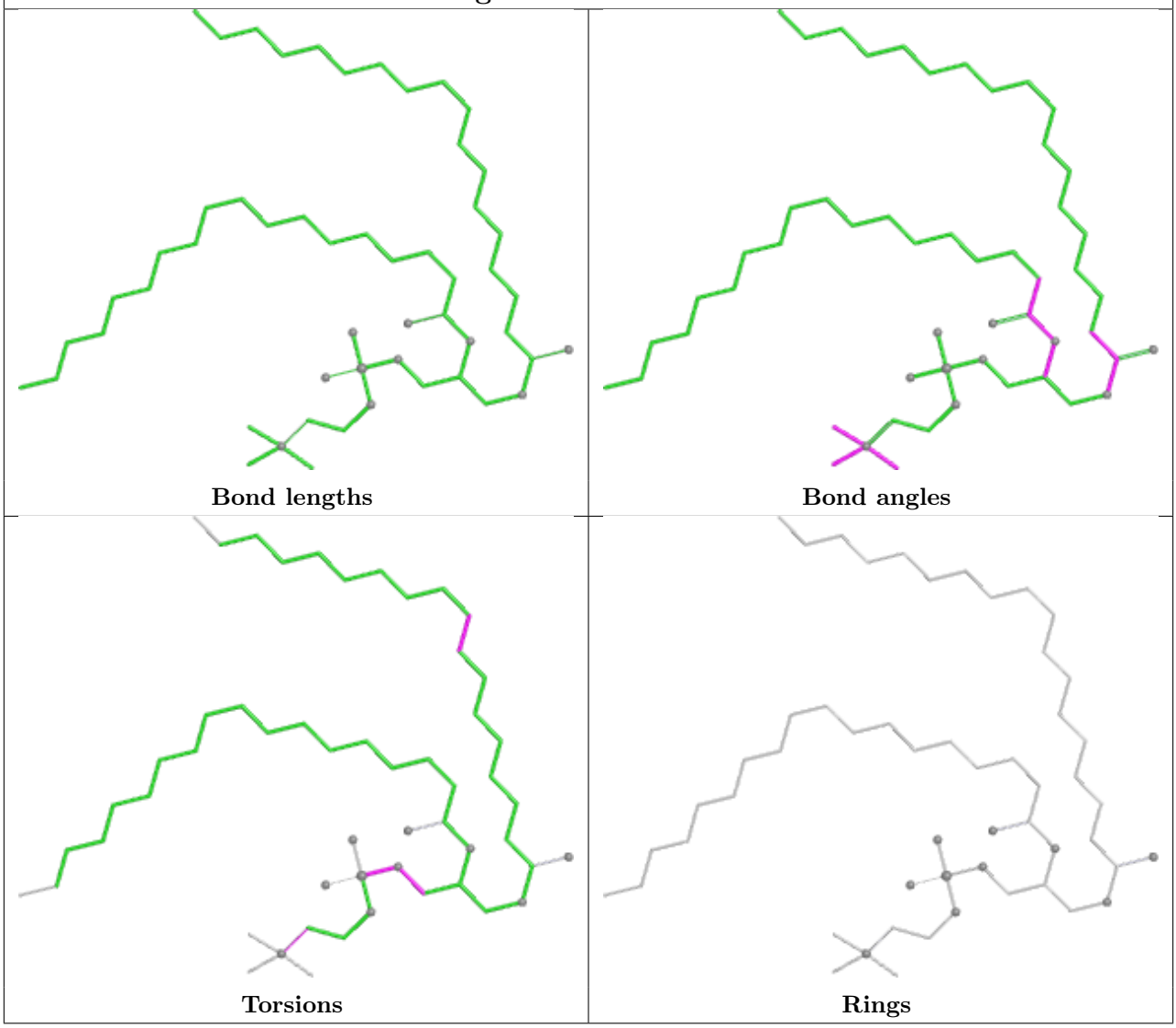


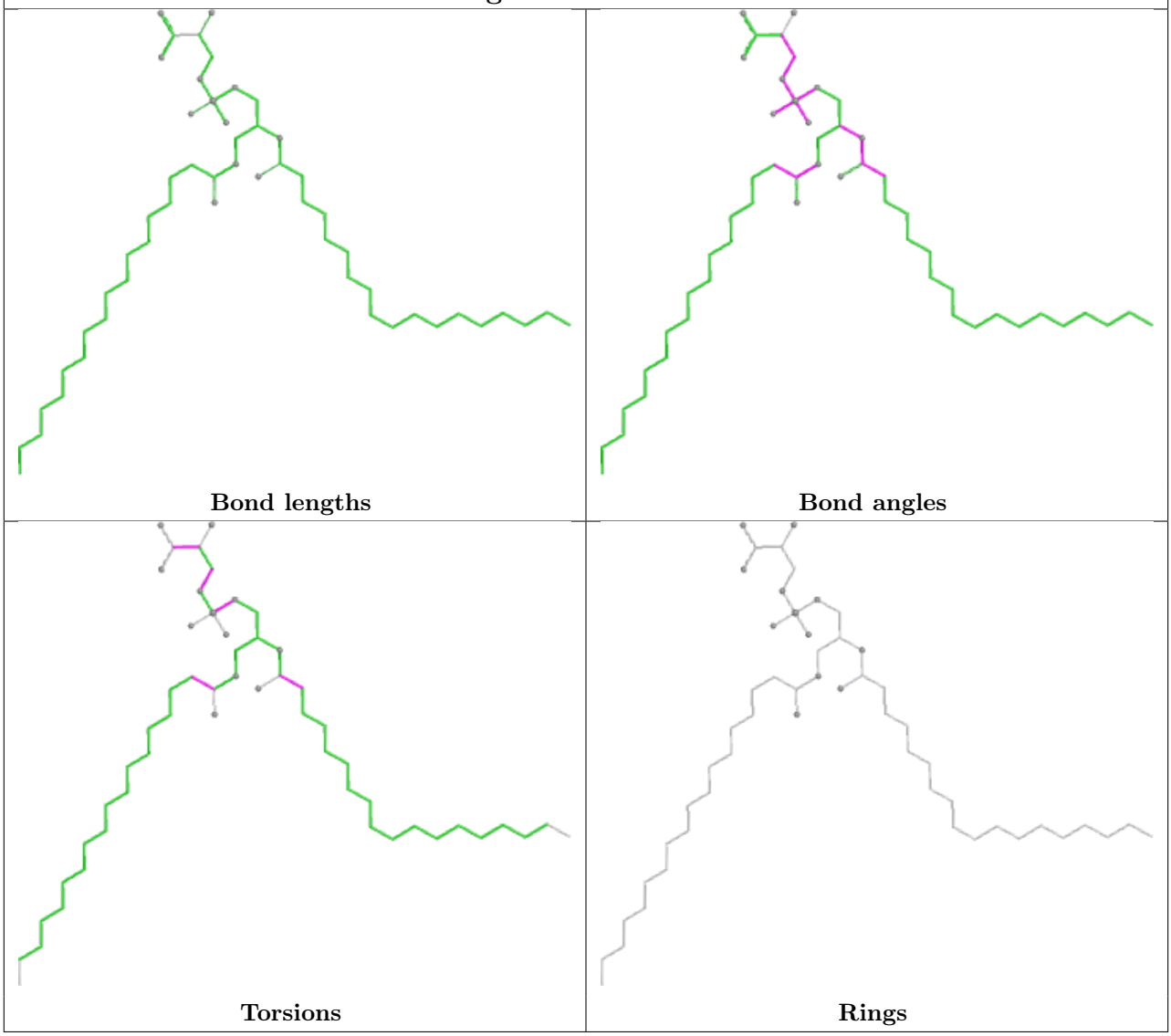
Ligand PCW B 204



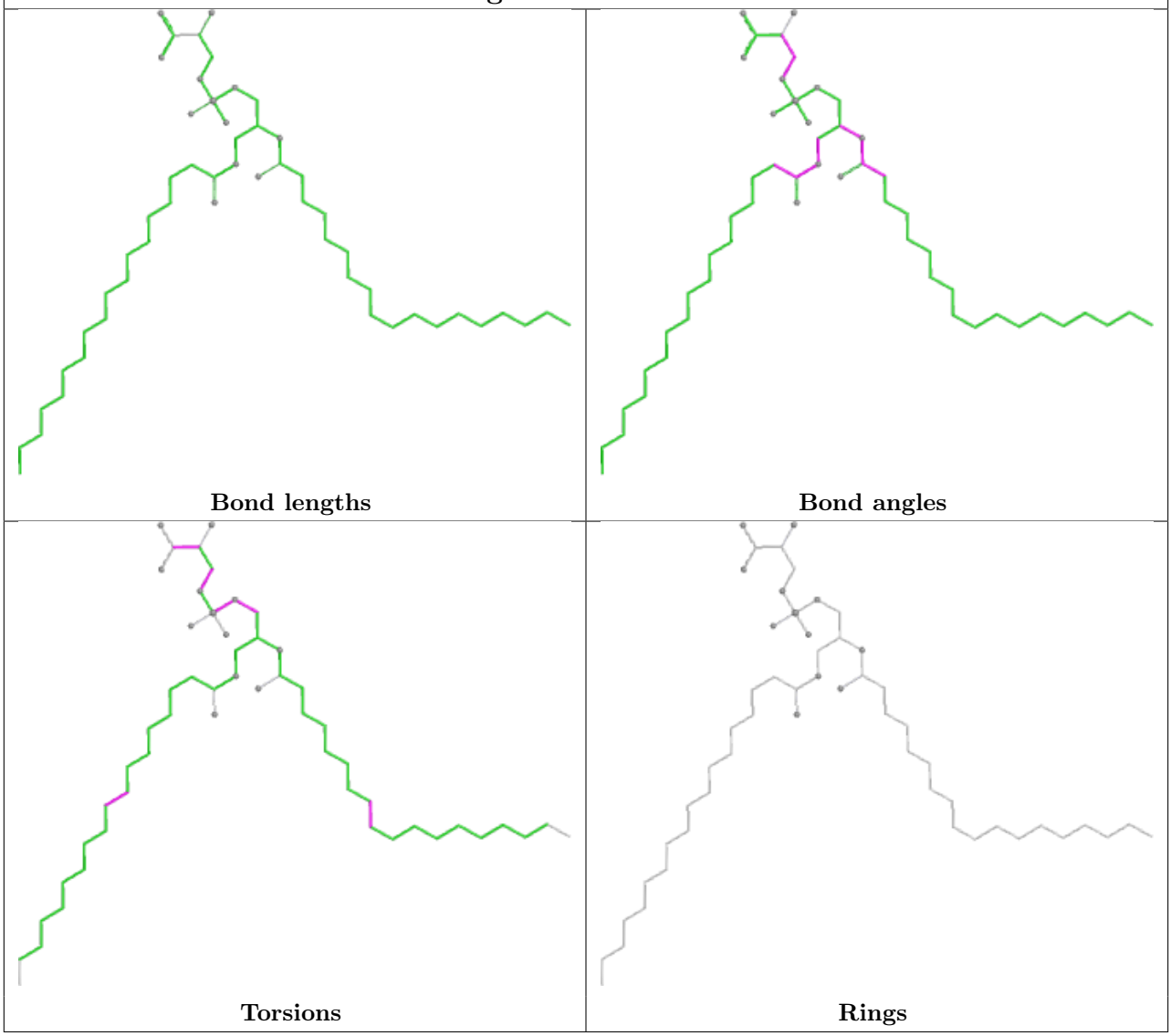
Ligand PCW C 205



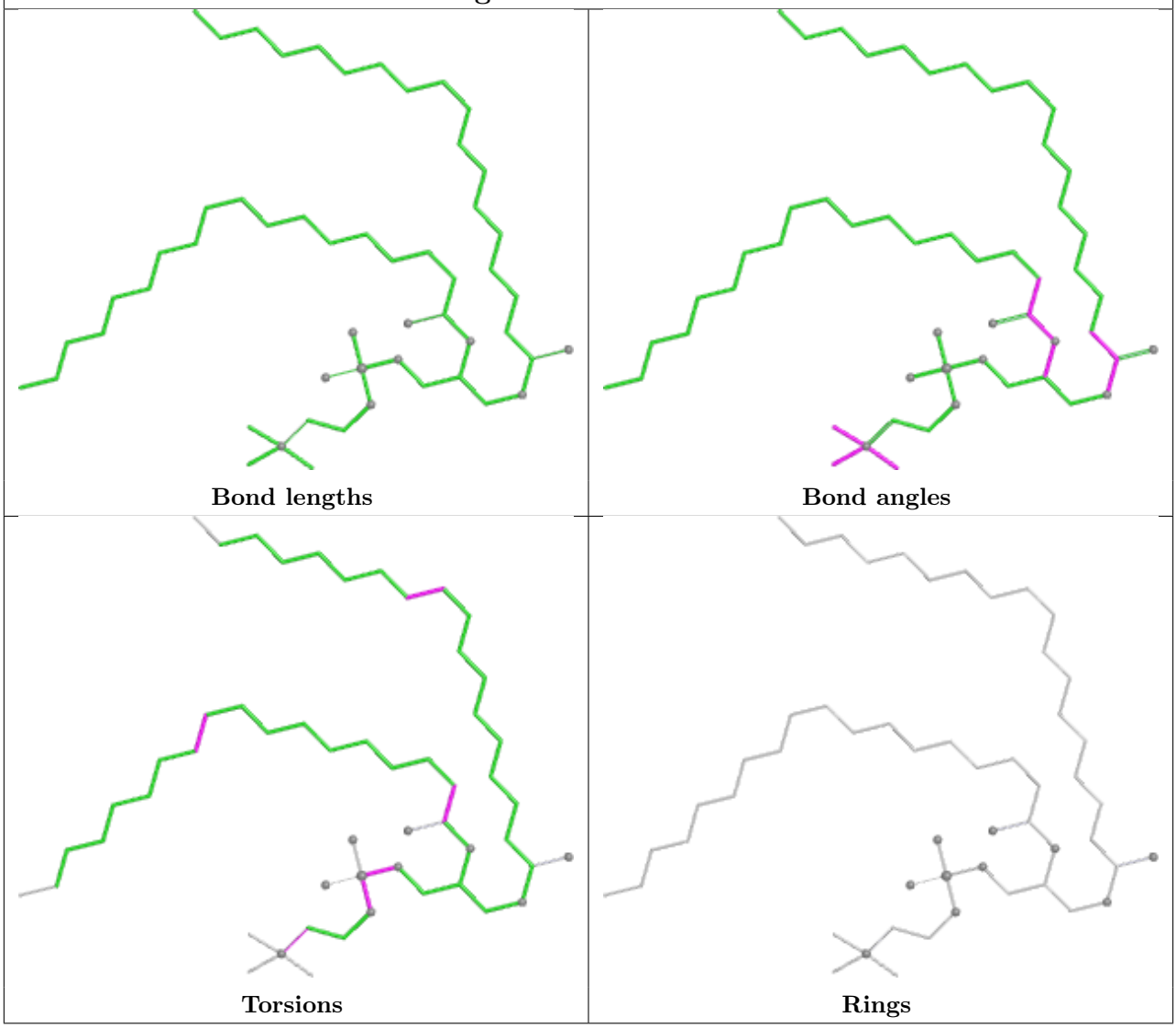
Ligand 17F A 415



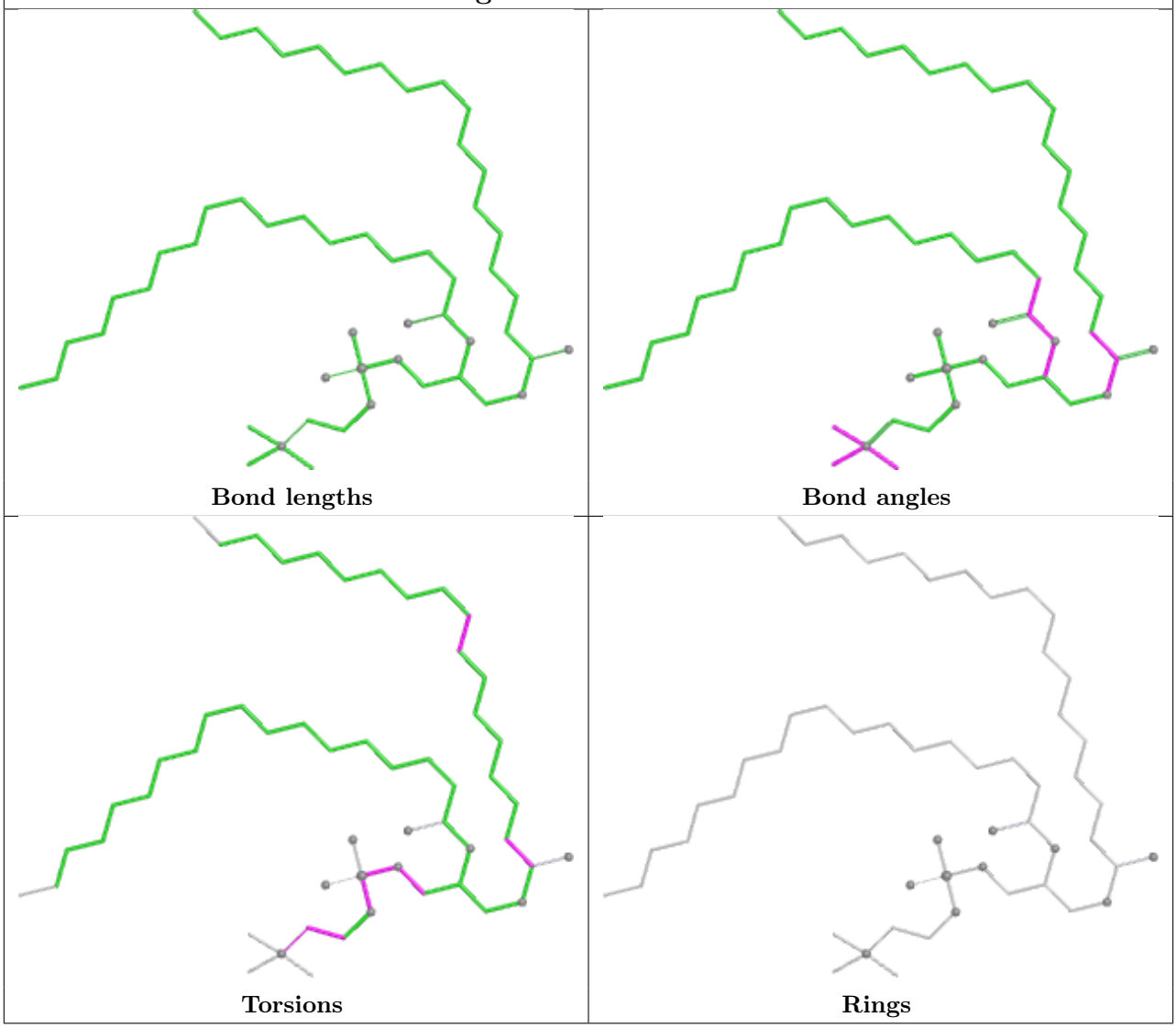
Ligand 17F C 219



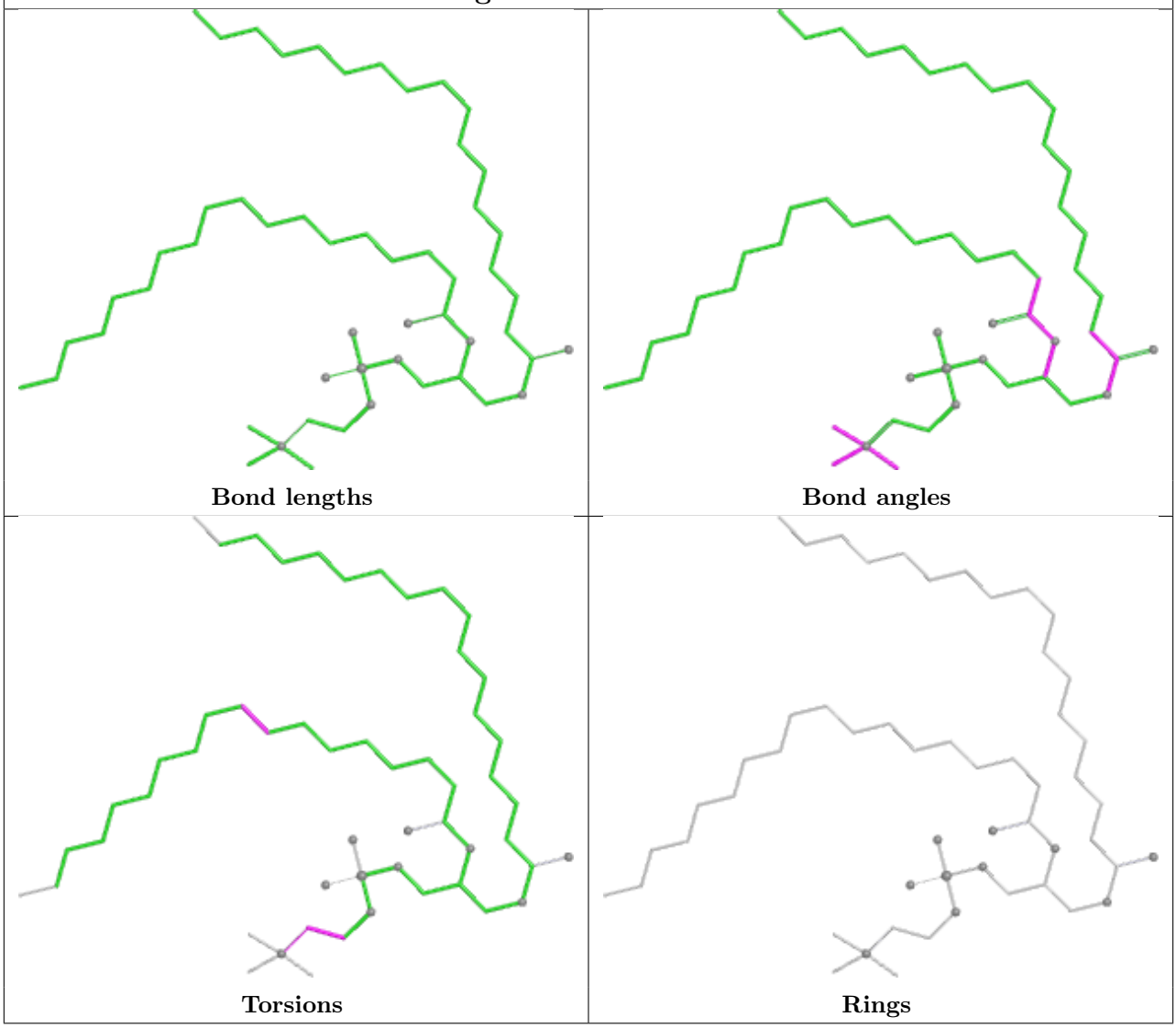
Ligand PCW D 620



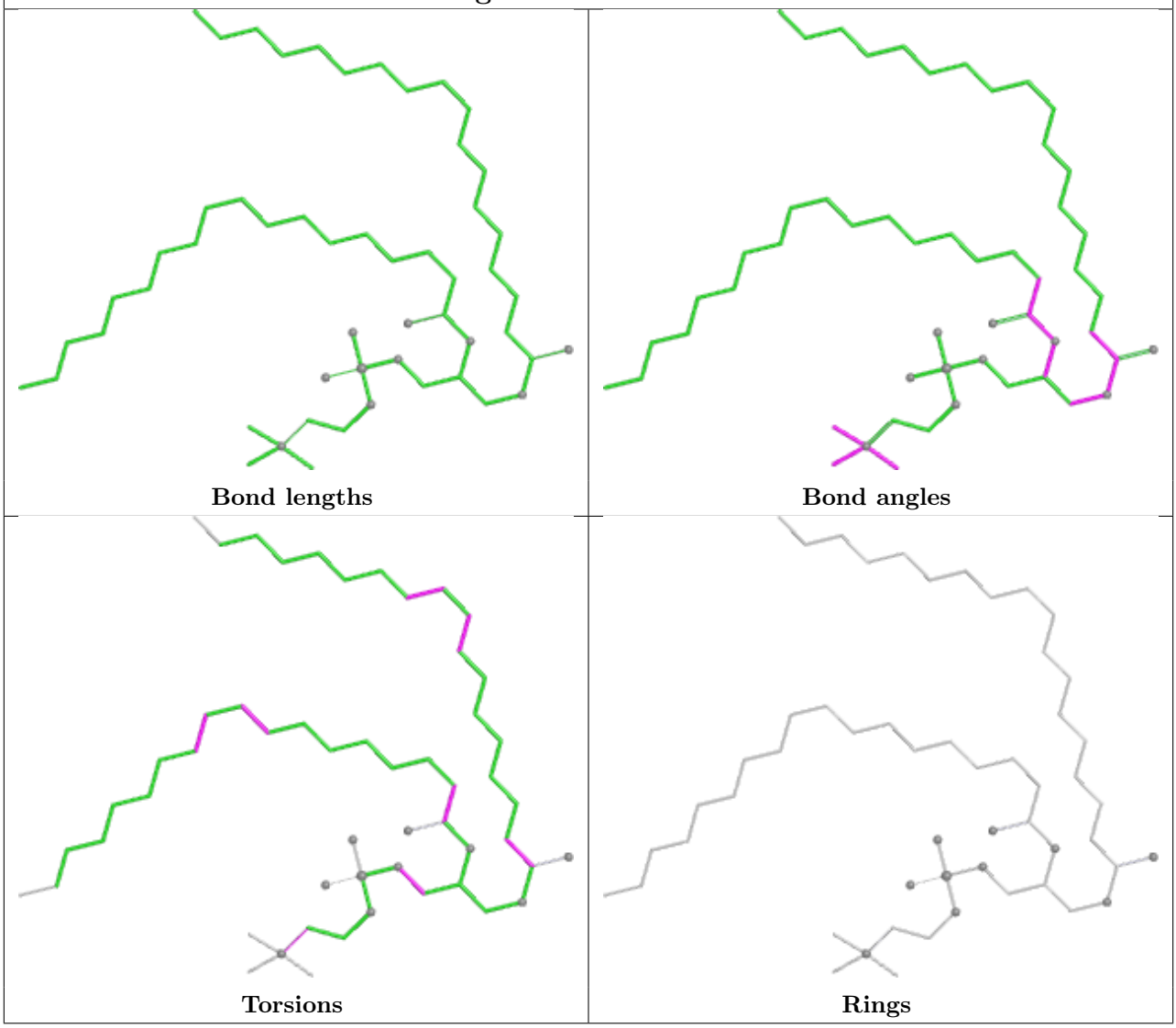
Ligand PCW B 207



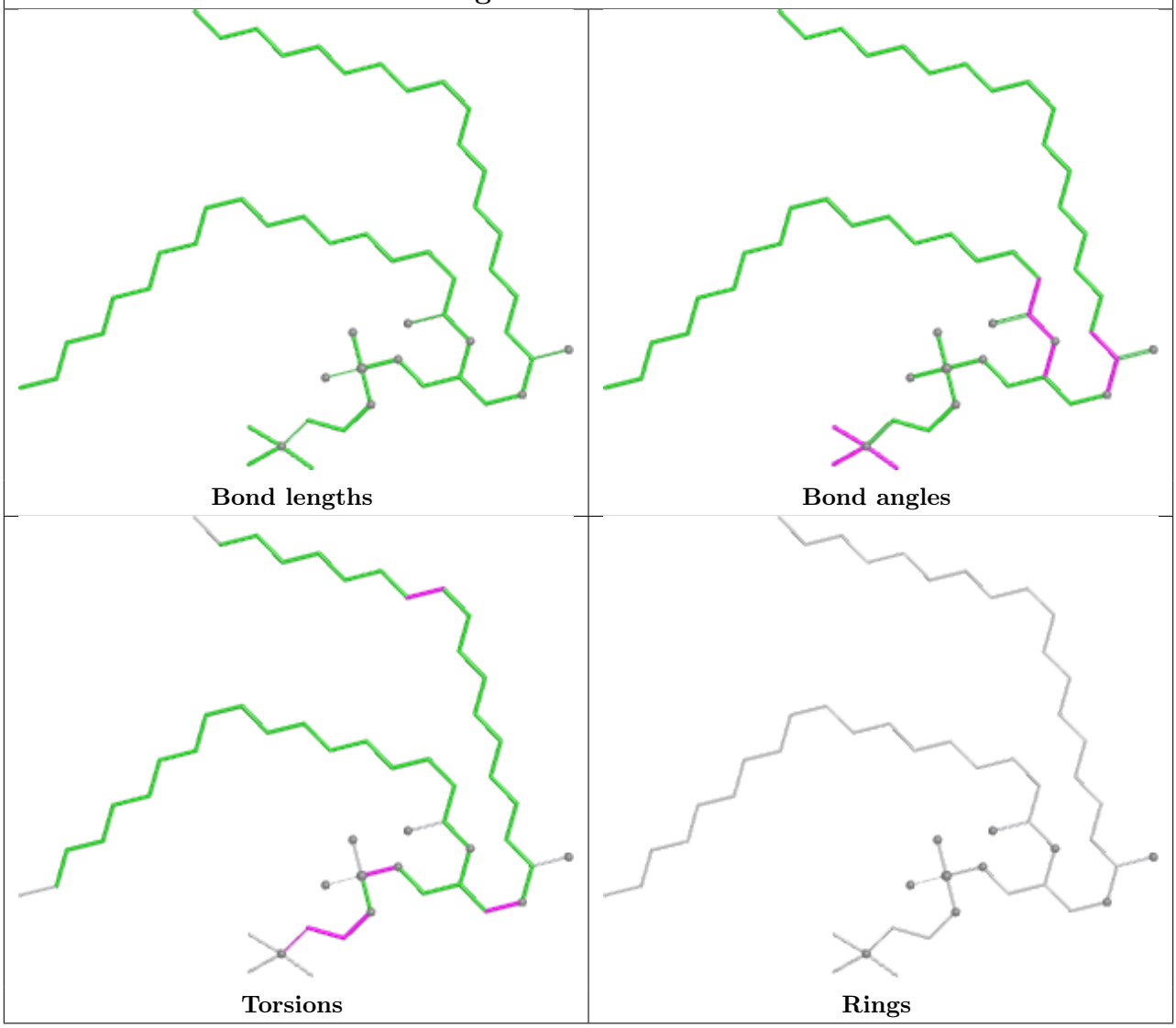
Ligand PCW A 414



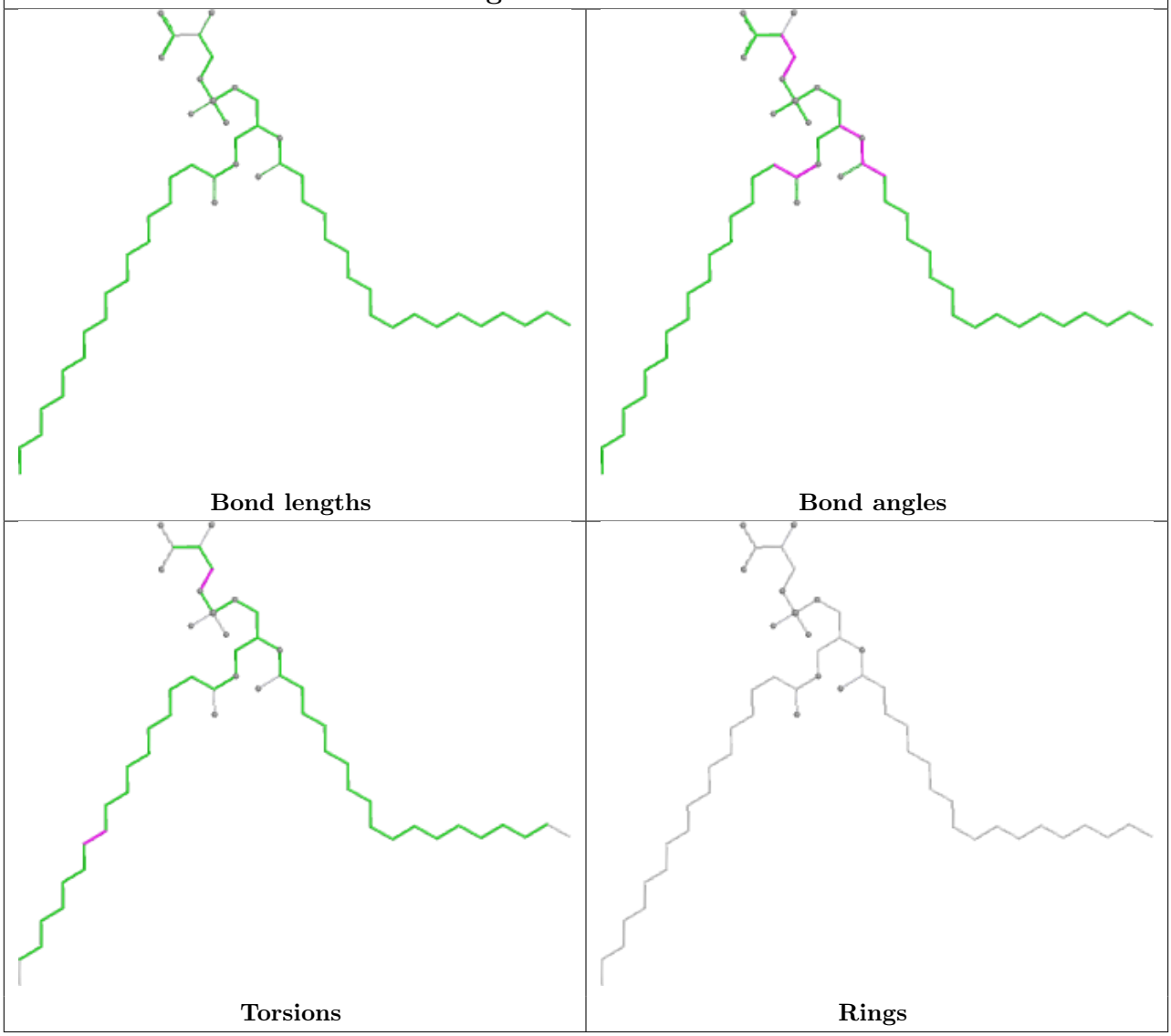
Ligand PCW C 206



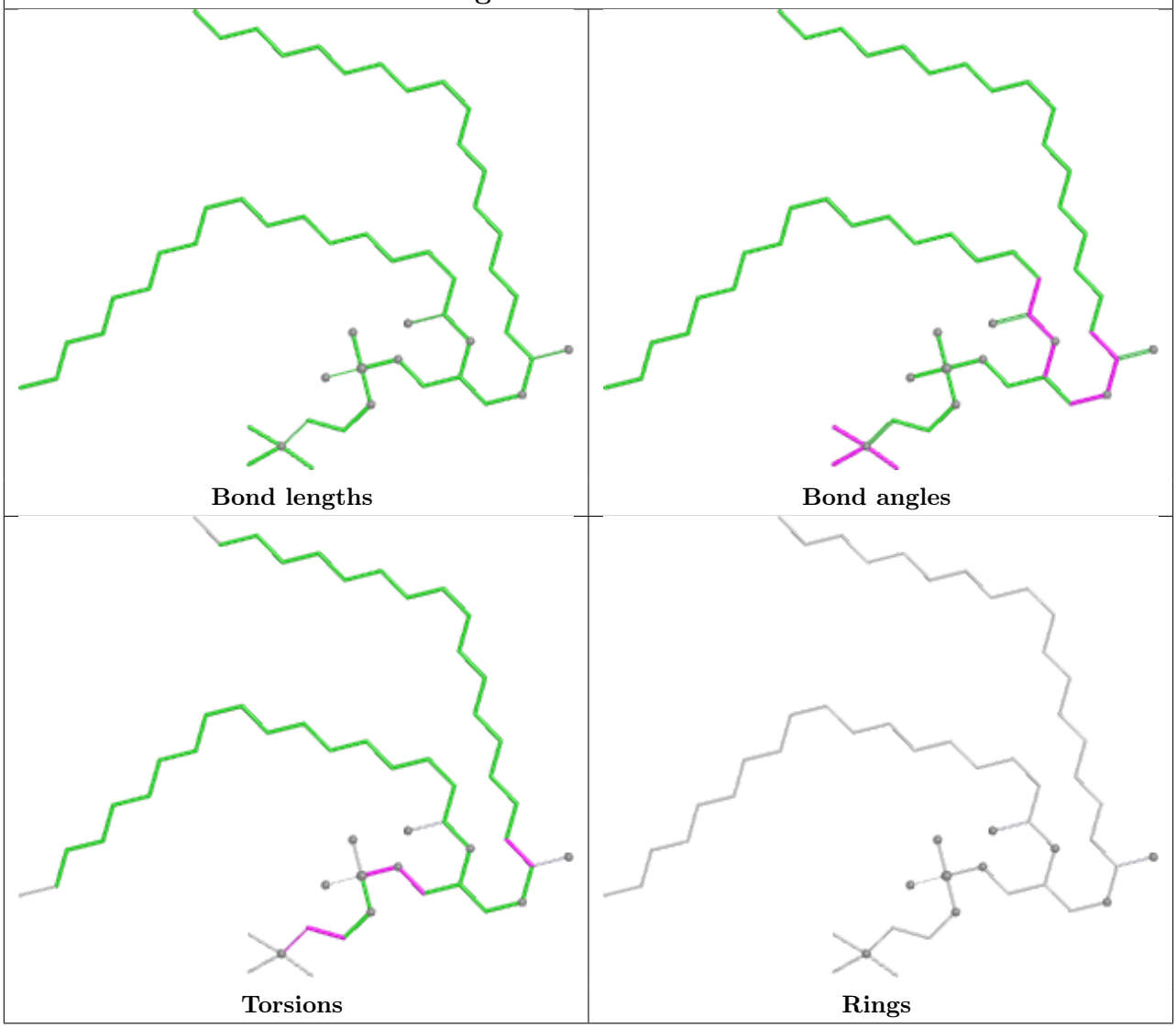
Ligand PCW A 410



Ligand 17F A 416



Ligand PCW A 401



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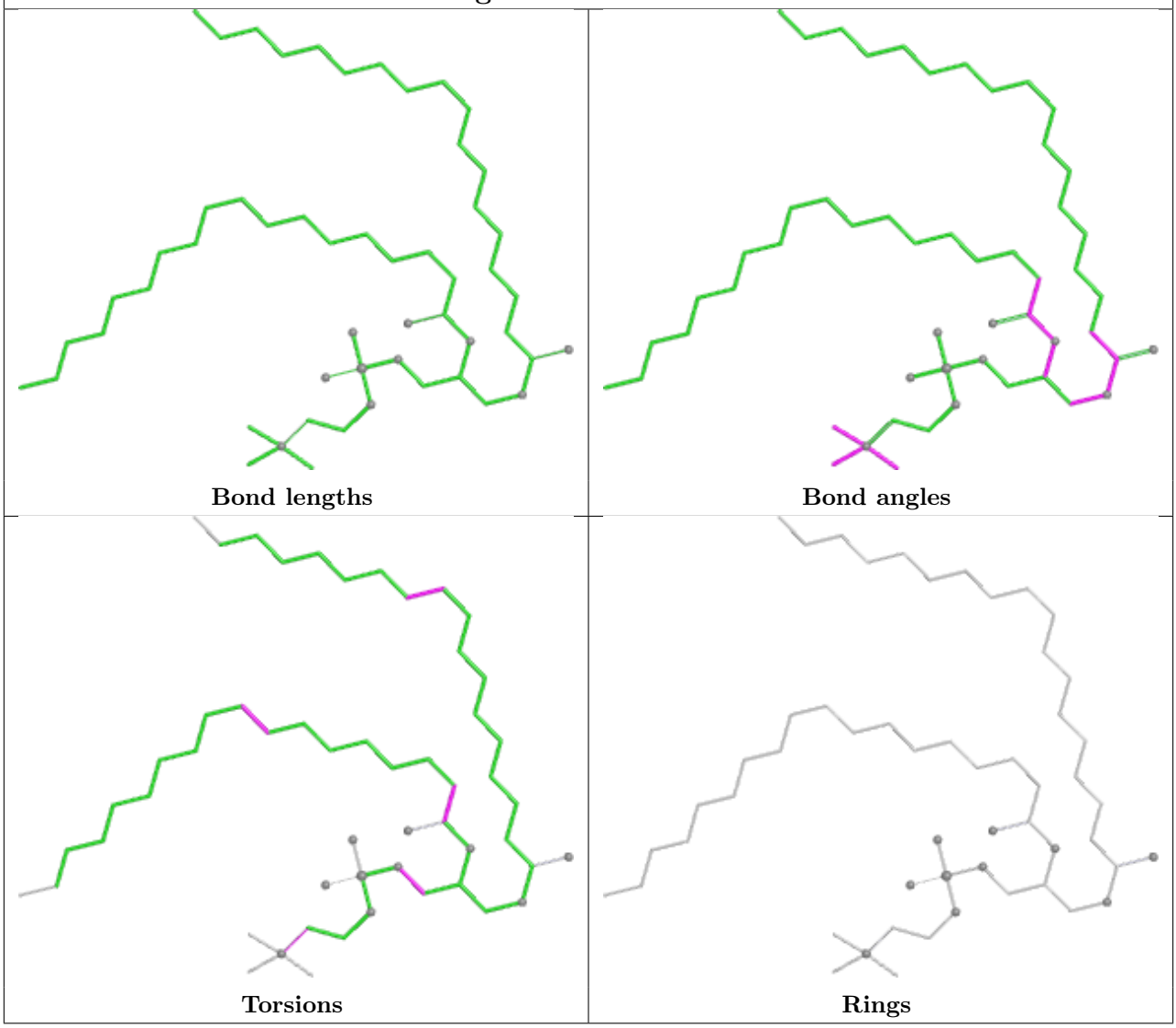
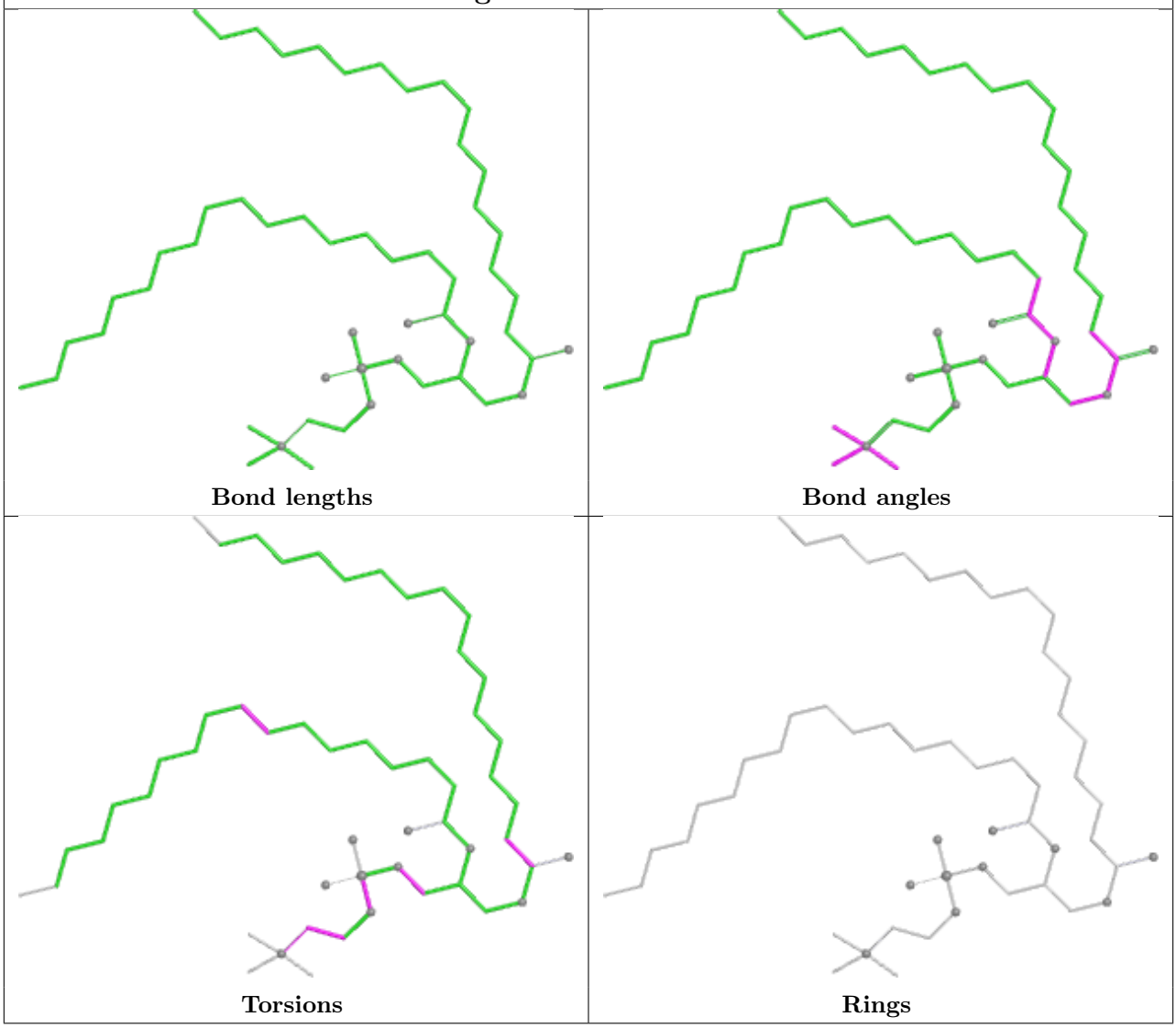
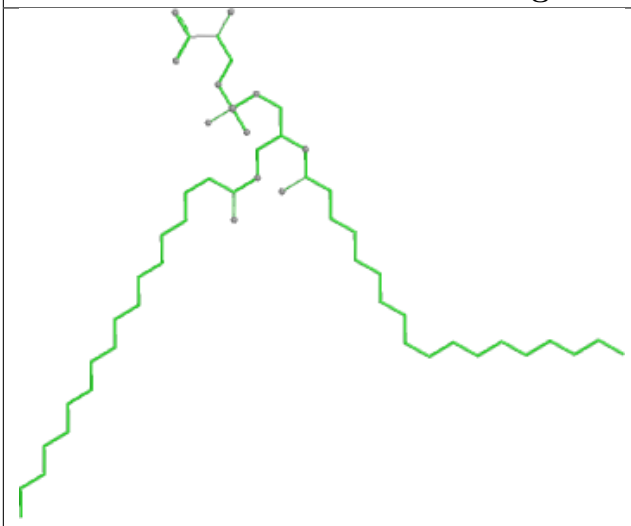


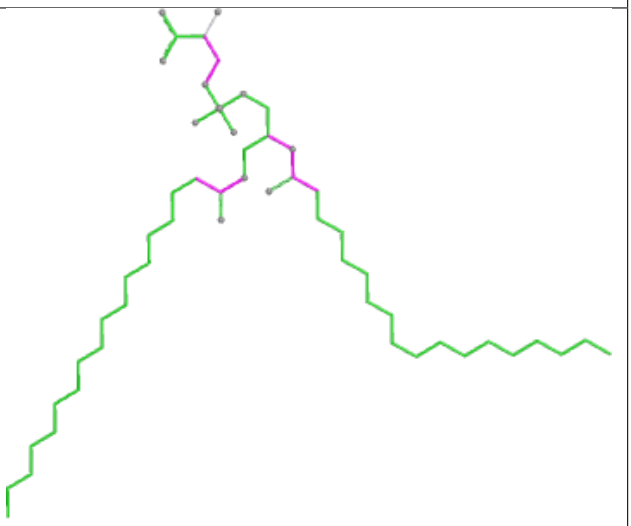
Ligand PCW D 607



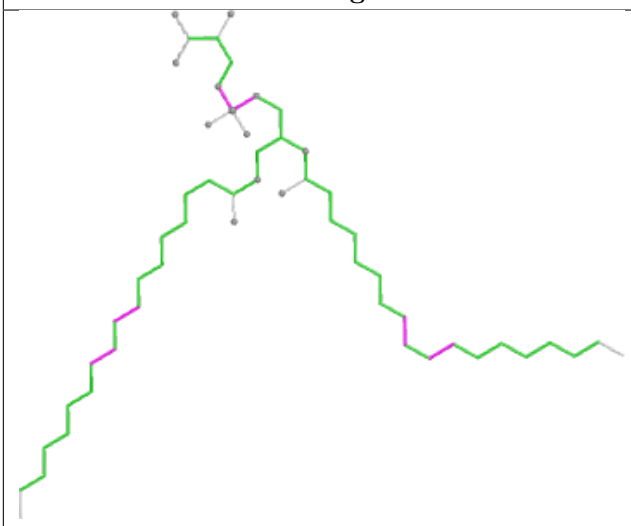
Ligand 17F D 631



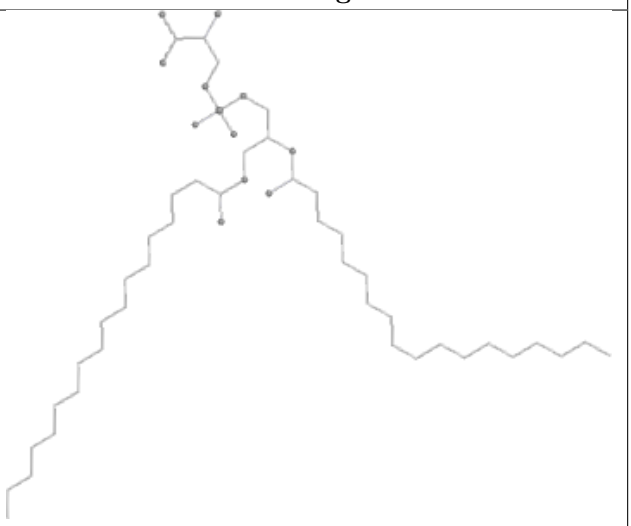
Bond lengths



Bond angles

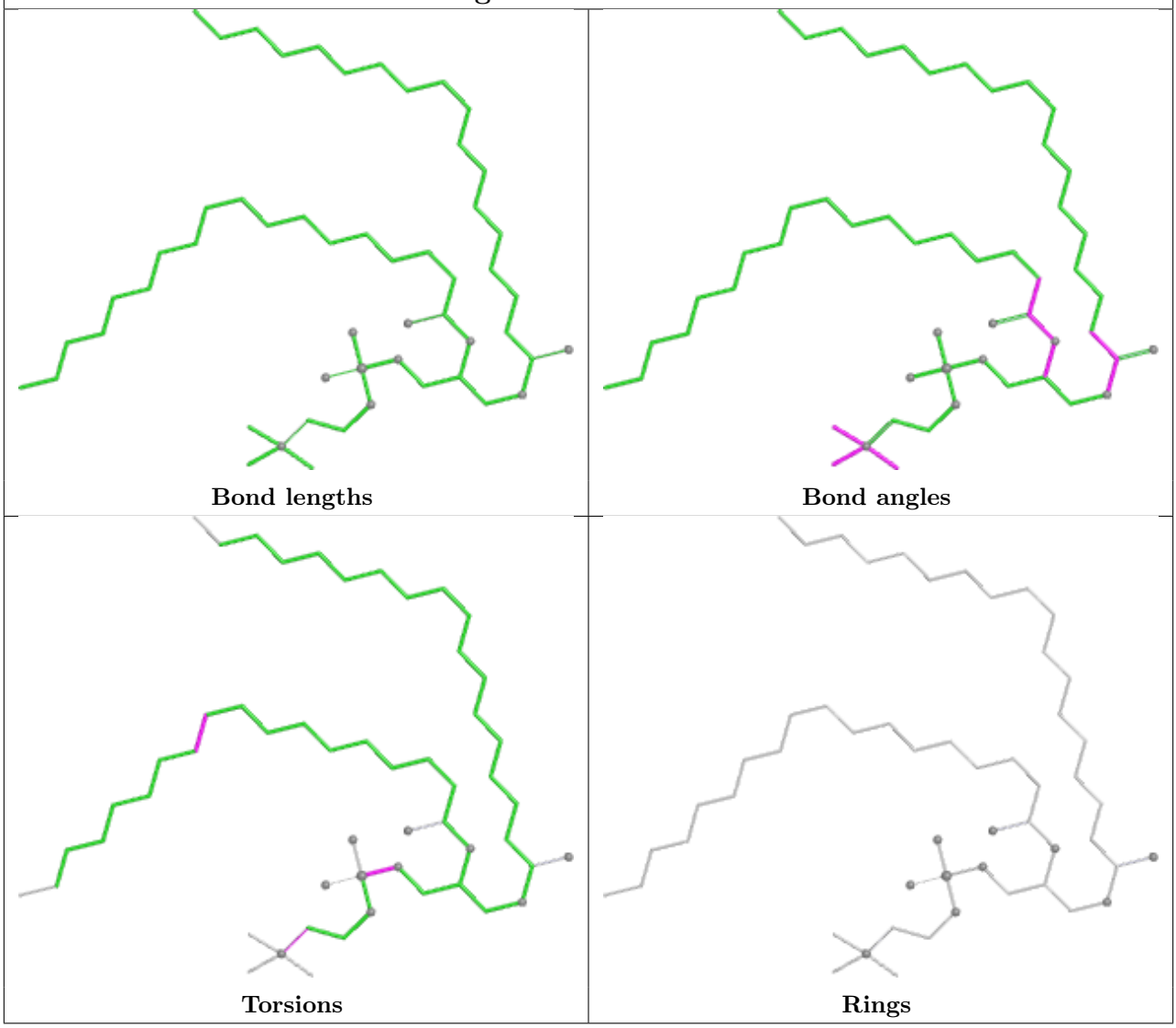


Torsions

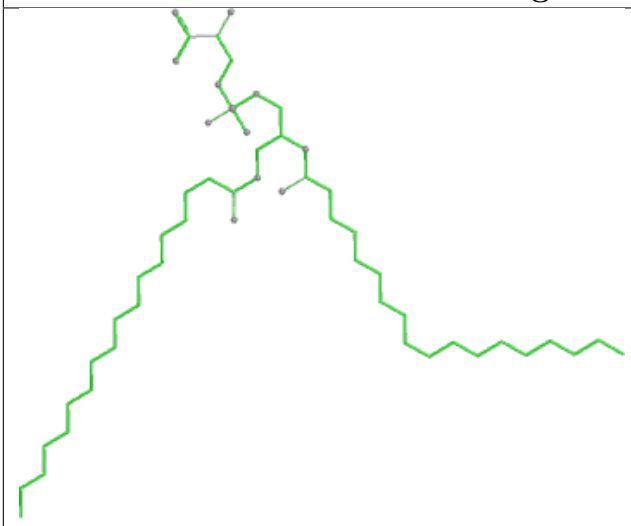


Rings

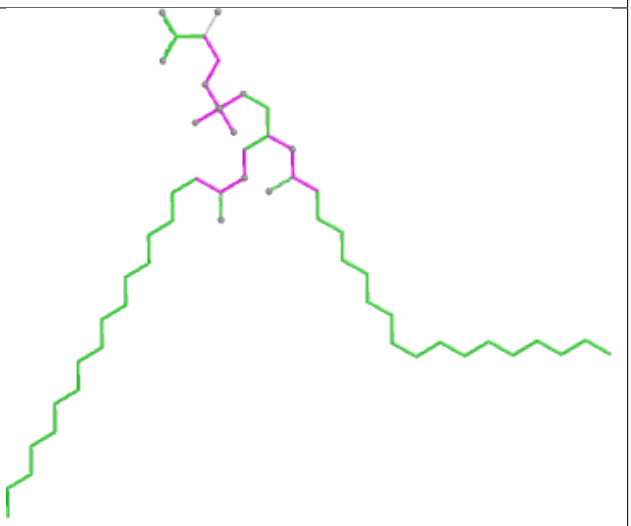
Ligand PCW D 611



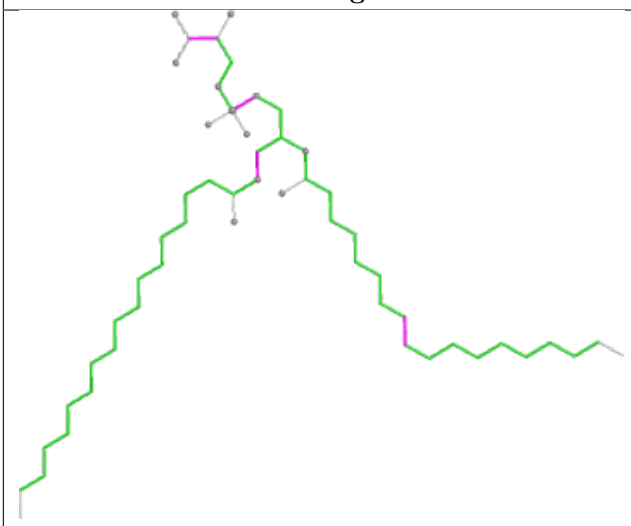
Ligand 17F D 630



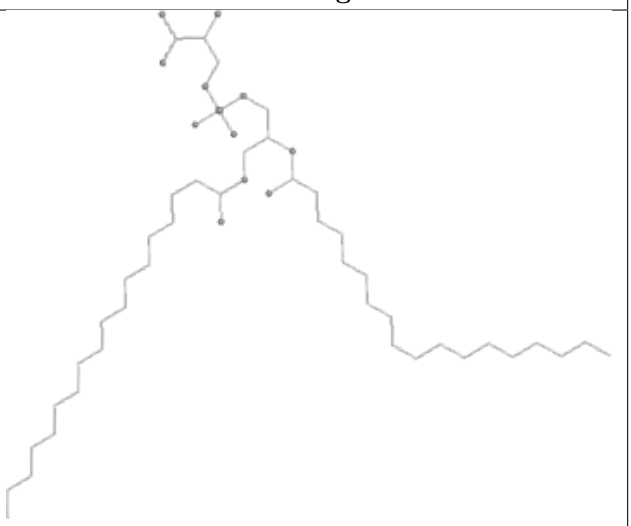
Bond lengths



Bond angles

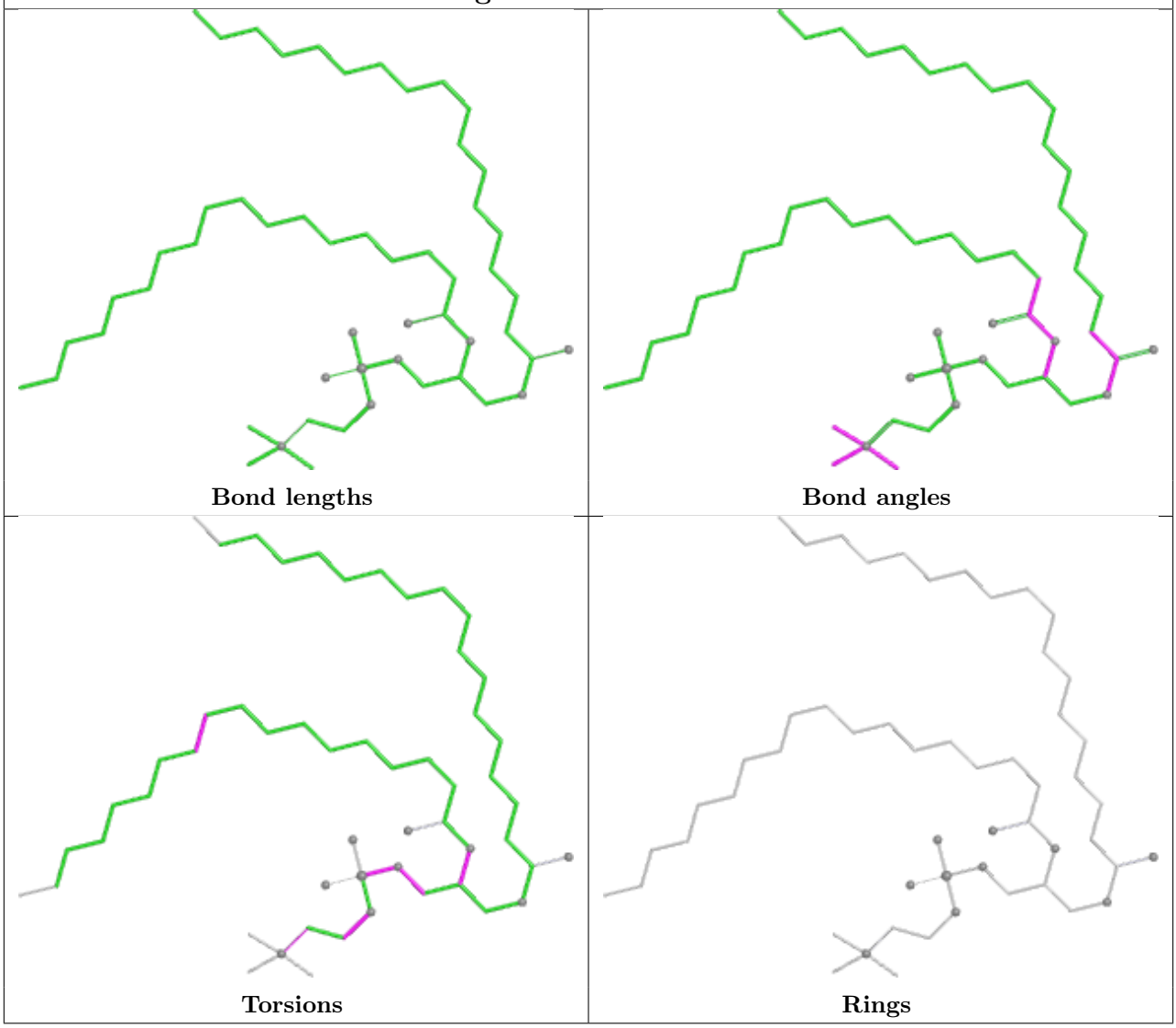


Torsions

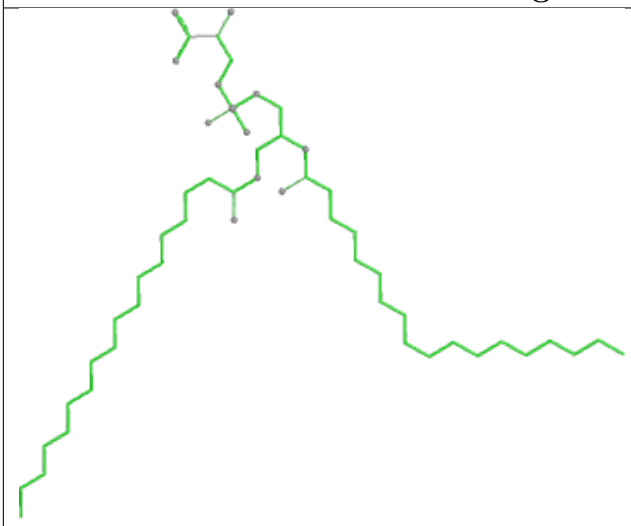


Rings

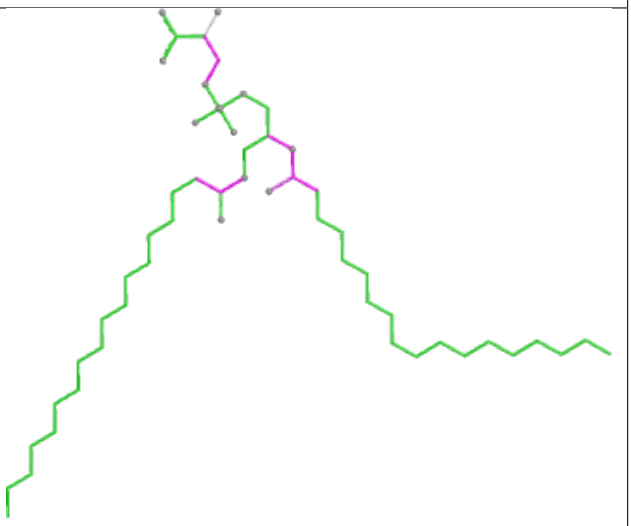
Ligand PCW A 408



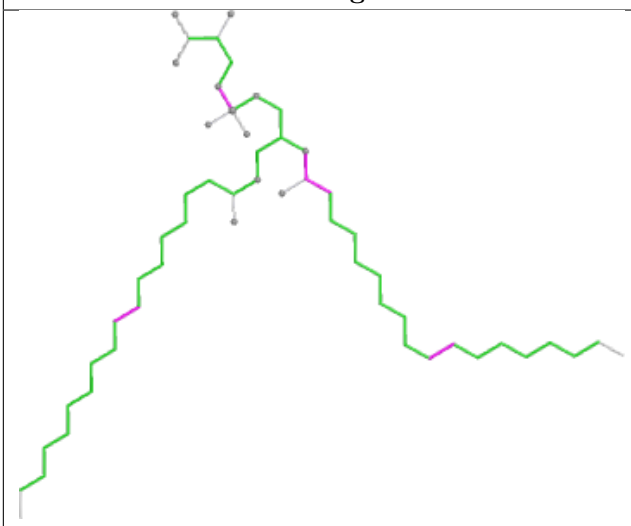
Ligand 17F C 218



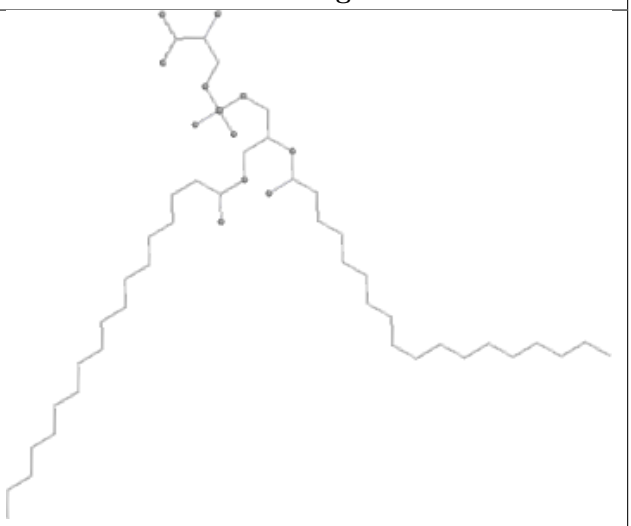
Bond lengths



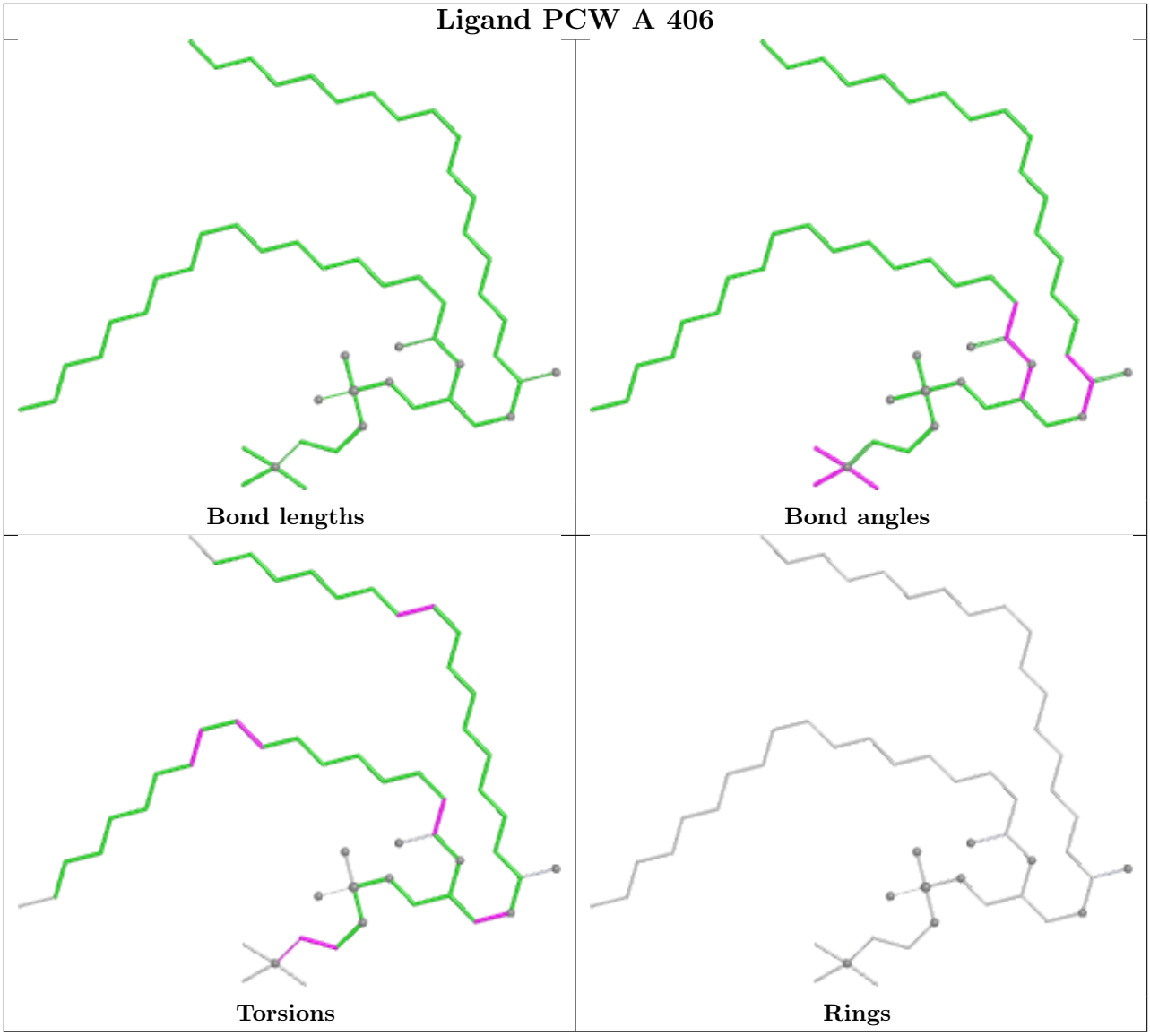
Bond angles



Torsions



Rings



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	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 93) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	6	LEU	HD11	0.763	.	2
1	B	6	LEU	HD12	0.763	.	2
1	B	6	LEU	HD13	0.763	.	2
1	B	8	VAL	HG21	0.7528	.	2
1	B	8	VAL	HG22	0.7528	.	2
1	B	8	VAL	HG23	0.7528	.	2
1	B	14	VAL	HG21	0.9725	.	2
1	B	14	VAL	HG22	0.9725	.	2
1	B	14	VAL	HG23	0.9725	.	2
1	B	19	LEU	HD11	0.4104	.	2
1	B	19	LEU	HD12	0.4104	.	2
1	B	19	LEU	HD13	0.4104	.	2
1	B	19	LEU	HD21	0.5804	.	2
1	B	19	LEU	HD22	0.5804	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	19	LEU	HD23	0.5804	.	2
1	B	21	ILE	HD11	0.4182	.	1
1	B	21	ILE	HD12	0.4182	.	1
1	B	21	ILE	HD13	0.4182	.	1
1	B	23	LEU	HD11	-0.477	.	2
1	B	23	LEU	HD12	-0.477	.	2
1	B	23	LEU	HD13	-0.477	.	2
1	B	24	ILE	HD11	0.2691	.	1
1	B	24	ILE	HD12	0.2691	.	1
1	B	24	ILE	HD13	0.2691	.	1
1	B	36	ILE	HD11	0.5397	.	1
1	B	36	ILE	HD12	0.5397	.	1
1	B	36	ILE	HD13	0.5397	.	1
1	B	44	VAL	HG11	0.5353	.	2
1	B	44	VAL	HG12	0.5353	.	2
1	B	44	VAL	HG13	0.5353	.	2
1	B	45	VAL	HG11	0.4379	.	2
1	B	45	VAL	HG12	0.4379	.	2
1	B	45	VAL	HG13	0.4379	.	2
1	B	46	ILE	HD11	0.2525	.	1
1	B	46	ILE	HD12	0.2525	.	1
1	B	46	ILE	HD13	0.2525	.	1
1	B	55	ILE	HD11	0.3369	.	1
1	B	55	ILE	HD12	0.3369	.	1
1	B	55	ILE	HD13	0.3369	.	1
1	B	56	LEU	HD11	0.5372	.	2
1	B	56	LEU	HD12	0.5372	.	2
1	B	56	LEU	HD13	0.5372	.	2
1	B	79	LEU	HD11	-0.1312	.	2
1	B	79	LEU	HD12	-0.1312	.	2
1	B	79	LEU	HD13	-0.1312	.	2
1	B	79	LEU	HD21	-0.015	.	2
1	B	79	LEU	HD22	-0.015	.	2
1	B	79	LEU	HD23	-0.015	.	2
1	B	81	VAL	HG21	0.4663	.	2
1	B	81	VAL	HG22	0.4663	.	2
1	B	81	VAL	HG23	0.4663	.	2
1	B	84	ILE	HD11	0.5865	.	1
1	B	84	ILE	HD12	0.5865	.	1
1	B	84	ILE	HD13	0.5865	.	1
1	B	93	ILE	HD11	0.6063	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	93	ILE	HD12	0.6063	.	1
1	B	93	ILE	HD13	0.6063	.	1
1	B	100	ILE	HD11	0.0964	.	1
1	B	100	ILE	HD12	0.0964	.	1
1	B	100	ILE	HD13	0.0964	.	1
1	B	103	VAL	HG11	0.8243	.	2
1	B	103	VAL	HG12	0.8243	.	2
1	B	103	VAL	HG13	0.8243	.	2
1	B	112	VAL	HG11	0.5953	.	2
1	B	112	VAL	HG12	0.5953	.	2
1	B	112	VAL	HG13	0.5953	.	2
1	B	113	LEU	HD11	0.8748	.	2
1	B	113	LEU	HD12	0.8748	.	2
1	B	113	LEU	HD13	0.8748	.	2
1	B	120	LEU	HD11	0.6958	.	2
1	B	120	LEU	HD12	0.6958	.	2
1	B	120	LEU	HD13	0.6958	.	2
1	B	125	VAL	HG11	-0.3248	.	2
1	B	125	VAL	HG12	-0.3248	.	2
1	B	125	VAL	HG13	-0.3248	.	2
1	B	133	LEU	HD11	0.2014	.	2
1	B	133	LEU	HD12	0.2014	.	2
1	B	133	LEU	HD13	0.2014	.	2
1	B	139	ILE	HD11	0.7118	.	1
1	B	139	ILE	HD12	0.7118	.	1
1	B	139	ILE	HD13	0.7118	.	1
1	B	142	ILE	HD11	0.5035	.	1
1	B	142	ILE	HD12	0.5035	.	1
1	B	142	ILE	HD13	0.5035	.	1
1	B	159	LEU	HD11	0.51	.	2
1	B	159	LEU	HD12	0.51	.	2
1	B	159	LEU	HD13	0.51	.	2
1	B	160	VAL	HG11	-0.2062	.	2
1	B	160	VAL	HG12	-0.2062	.	2
1	B	160	VAL	HG13	-0.2062	.	2
1	B	163	ILE	HD11	0.5261	.	1
1	B	163	ILE	HD12	0.5261	.	1
1	B	163	ILE	HD13	0.5261	.	1

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)

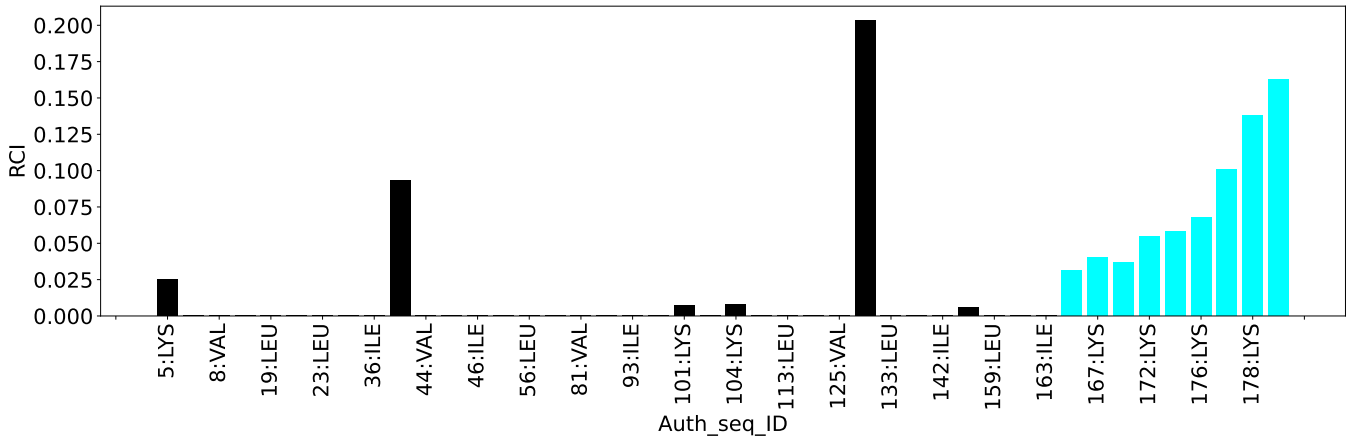
The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 138 atoms were assigned a chemical shift out of a possible 10171. 0 out of 133 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	14/3625 (0%)	7/1466 (0%)	0/1454 (0%)	7/705 (1%)
Sidechain	124/5899 (2%)	93/3793 (2%)	31/1847 (2%)	0/259 (0%)
Aromatic	0/647 (0%)	0/318 (0%)	0/304 (0%)	0/25 (0%)
Overall	138/10171 (1%)	100/5577 (2%)	31/3605 (1%)	7/989 (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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B: