



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:31 PM UTC

PDB ID : 9YH1 / pdb_00009yh1
EMDB ID : EMD-72948
Title : Structure of flagellin FlaB filament in *H. pylori*
Authors : Kumar, R.; Yu, H.; Tachiyama, S.; Liu, J.
Deposited on : 2025-09-29
Resolution : 3.22 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

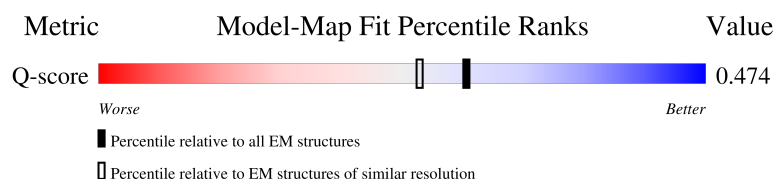
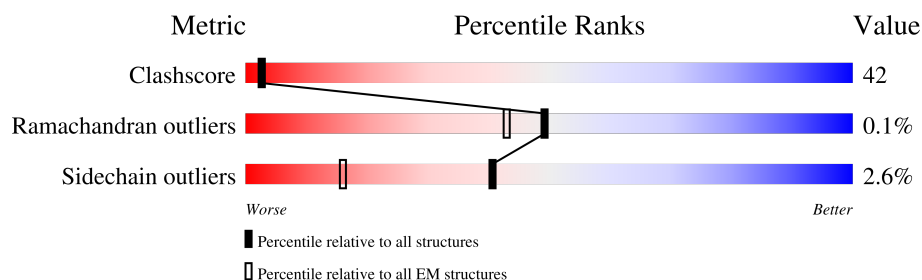
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 Å.

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.





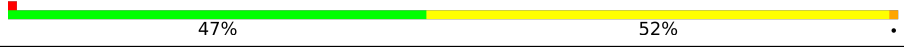
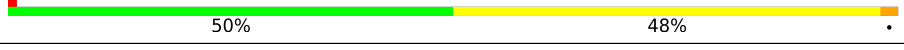



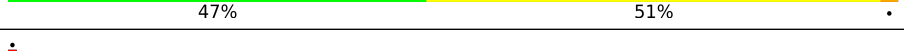
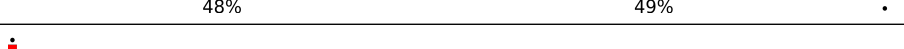
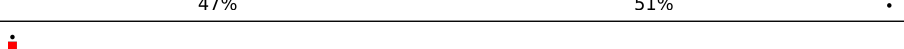
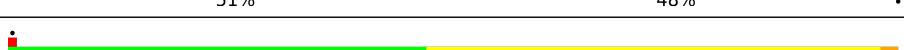
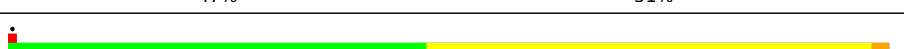

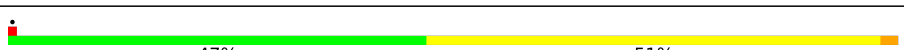
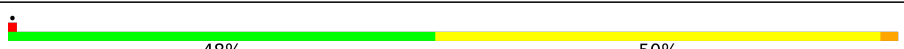










Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.72 - 3.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	513	
1	A2	513	
1	A3	513	
1	A4	513	




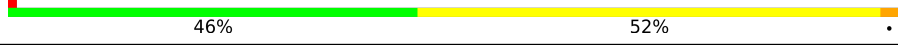
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Mol	Chain	Length	Quality of chain
1	A5	513	
1	A6	513	
1	A7	513	
1	A8	513	
1	A9	513	
1	AA	513	
1	AB	513	
1	AC	513	
1	AD	513	
1	AE	513	
1	AF	513	
1	AG	513	
1	AH	513	
1	AI	513	
1	AJ	513	
1	AK	513	
1	AL	513	
1	AM	513	
1	AN	513	
1	AO	513	
1	AP	513	
1	AQ	513	
1	AR	513	
1	AS	513	
1	AT	513	

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Mol	Chain	Length	Quality of chain
1	AU	513	
1	AV	513	
1	AW	513	
1	AX	513	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P8E	A1	604	X	-	-	-
2	P8E	A2	604	X	-	-	-
2	P8E	A3	604	X	-	-	-
2	P8E	A4	604	X	-	-	-
2	P8E	A5	604	X	-	-	-
2	P8E	A6	604	X	-	-	-
2	P8E	A7	604	X	-	-	-
2	P8E	A8	604	X	-	-	-
2	P8E	A9	604	X	-	-	-
2	P8E	AA	604	X	-	-	-
2	P8E	AB	604	X	-	-	-
2	P8E	AC	604	X	-	-	-
2	P8E	AD	604	X	-	-	-
2	P8E	AE	604	X	-	-	-
2	P8E	AF	604	X	-	-	-
2	P8E	AG	604	X	-	-	-
2	P8E	AH	604	X	-	-	-
2	P8E	AI	604	X	-	-	-
2	P8E	AJ	604	X	-	-	-
2	P8E	AK	604	X	-	-	-
2	P8E	AL	604	X	-	-	-
2	P8E	AM	604	X	-	-	-
2	P8E	AN	604	X	-	-	-
2	P8E	AO	604	X	-	-	-
2	P8E	AP	604	X	-	-	-
2	P8E	AQ	604	X	-	-	-
2	P8E	AR	604	X	-	-	-
2	P8E	AS	604	X	-	-	-
2	P8E	AT	604	X	-	-	-
2	P8E	AU	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P8E	AV	604	X	-	-	-
2	P8E	AW	604	X	-	-	-
2	P8E	AX	604	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 133980 atoms, of which 4752 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellin.

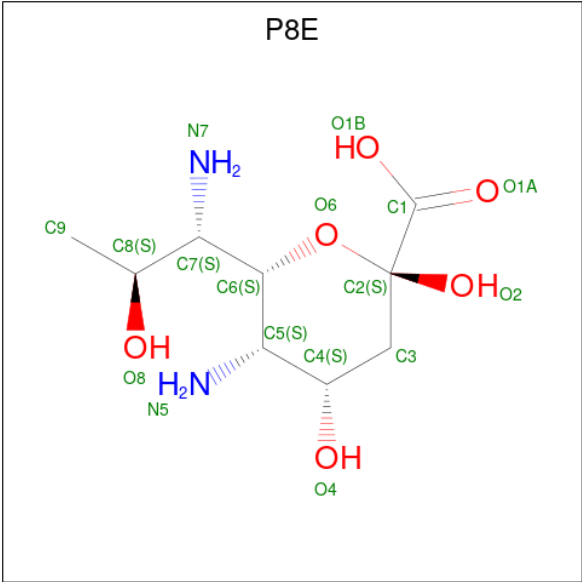
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A2	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A3	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A4	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A5	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A6	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A7	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A8	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	A9	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AA	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AB	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AC	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AD	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AE	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AF	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AG	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		
1	AH	513	Total	C	N	O	S	0	0
			3772	2289	695	775	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AI	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AJ	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AK	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AL	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AM	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AN	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AO	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AP	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AQ	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AR	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AS	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AT	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AU	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AV	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AW	513	Total 3772	C 2289	N 695	O 775	S 13	0	0
1	AX	513	Total 3772	C 2289	N 695	O 775	S 13	0	0

- Molecule 2 is 5,7-diamino-3,5,7,9-tetradexoxy-L-glycero-alpha-L-manno-non-2-ulopyranosonic acid (CCD ID: P8E) (formula: C₉H₁₈N₂O₆).



Mol	Chain	Residues	Atoms					AltConf
2	A1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A4	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	A4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	AB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AE	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	AE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	AI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AL	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	AL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AN	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	AN	1	Total	C	H	N	O	0
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2	AN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AO	1	Total	C	H	N	O	0
			32	9	16	2	5	
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			32	9	16	2	5	
2	AO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AO	1	Total	C	H	N	O	0
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2	AO	1	Total	C	H	N	O	0
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			32	9	16	2	5	
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			32	9	16	2	5	
2	AP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AP	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
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2	AQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AS	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
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			32	9	16	2	5	
2	AS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AS	1	Total	C	H	N	O	0
			32	9	16	2	5	
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2	AT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AU	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
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			32	9	16	2	5	
2	AU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AW	1	Total	C	H	N	O	0
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2	AW	1	Total	C	H	N	O	0
			32	9	16	2	5	

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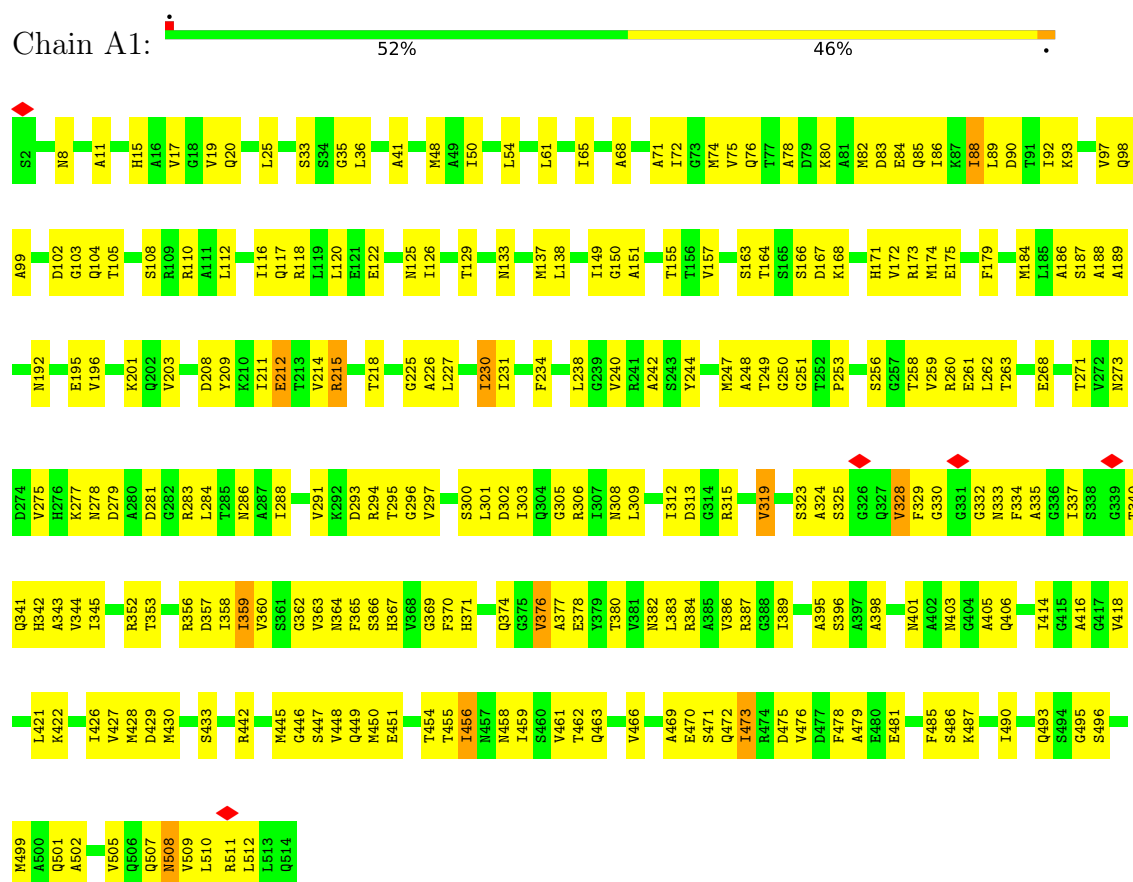
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Mol	Chain	Residues	Atoms					AltConf
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2	AX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	AX	1	Total	C	H	N	O	0
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2	AX	1	Total	C	H	N	O	0
			32	9	16	2	5	

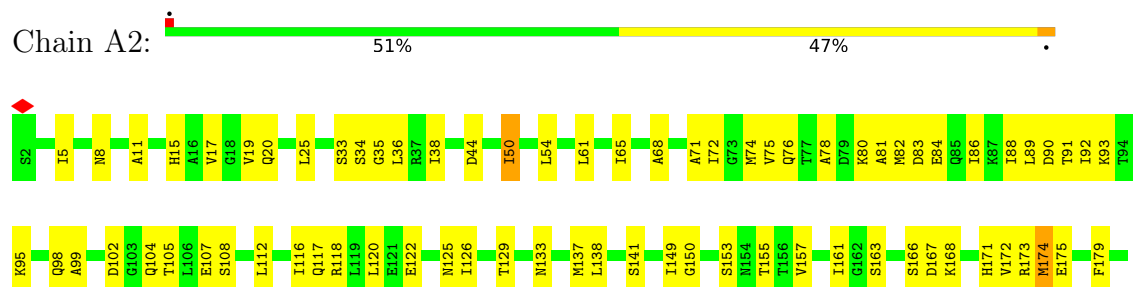
3 Residue-property plots

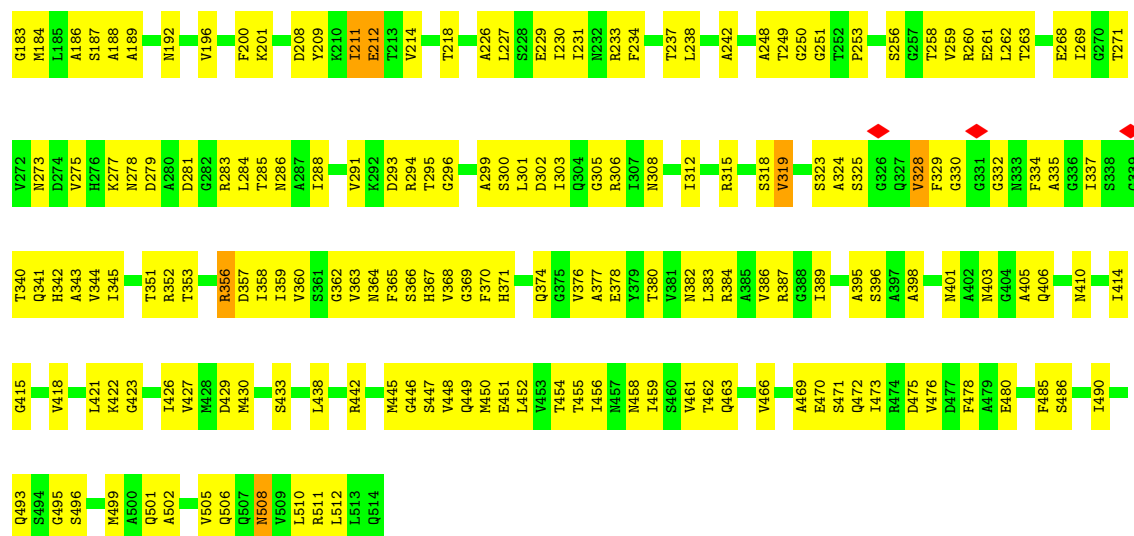
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flagellin

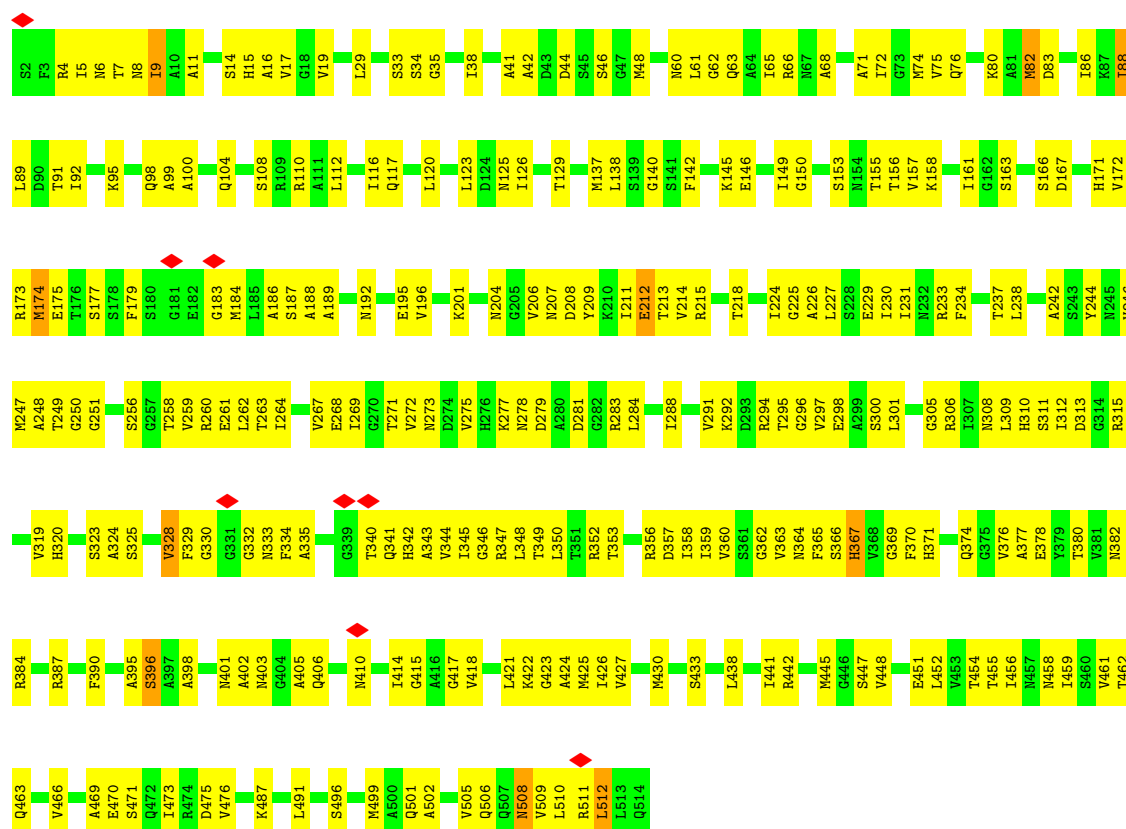


• Molecule 1: Flagellin



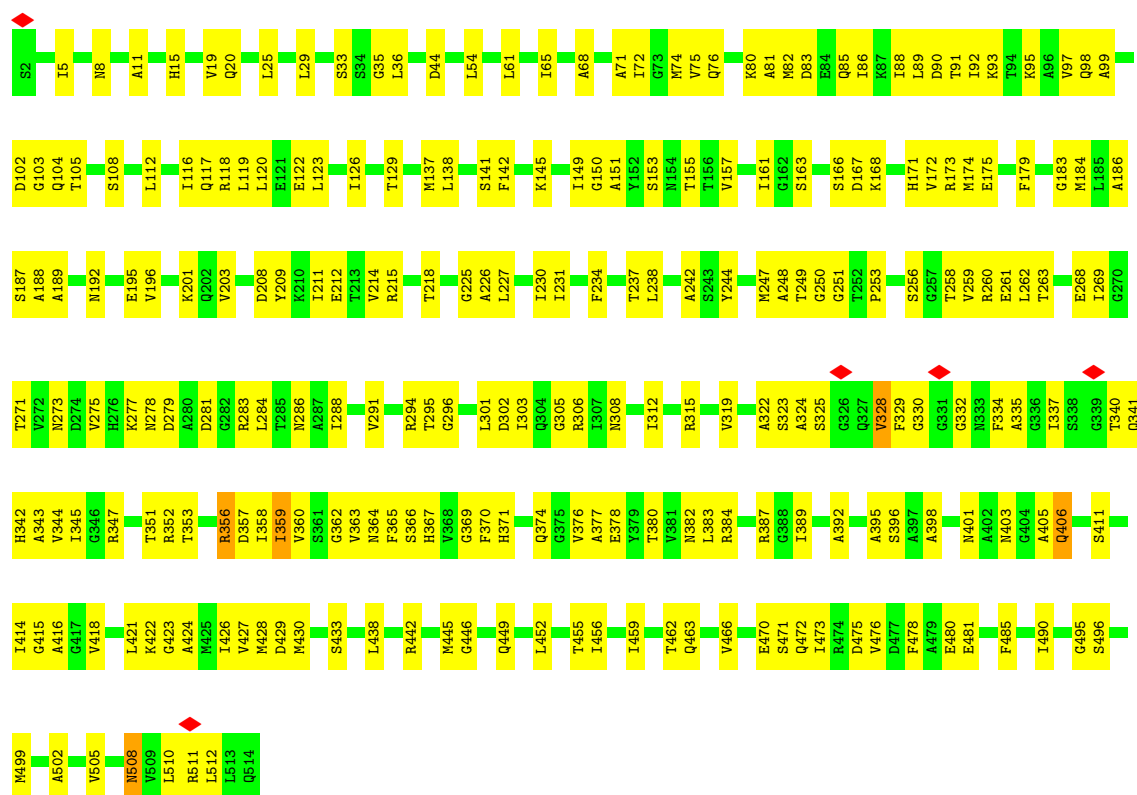


• Molecule 1: Flagellin

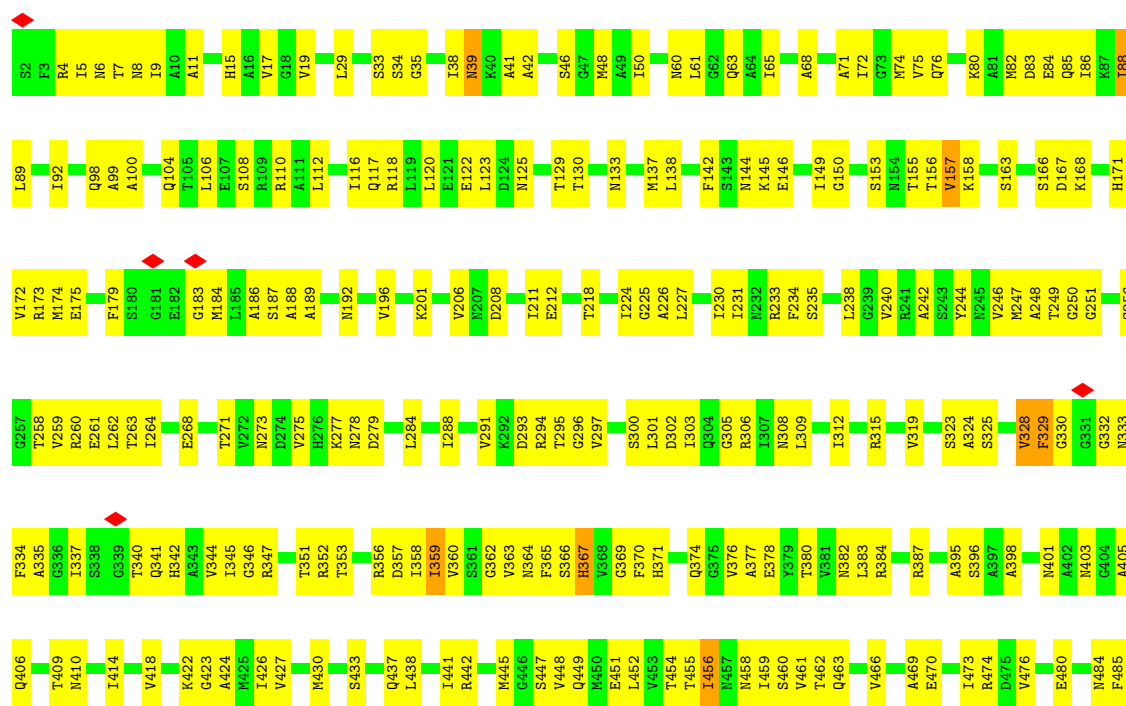


• Molecule 1: Flagellin



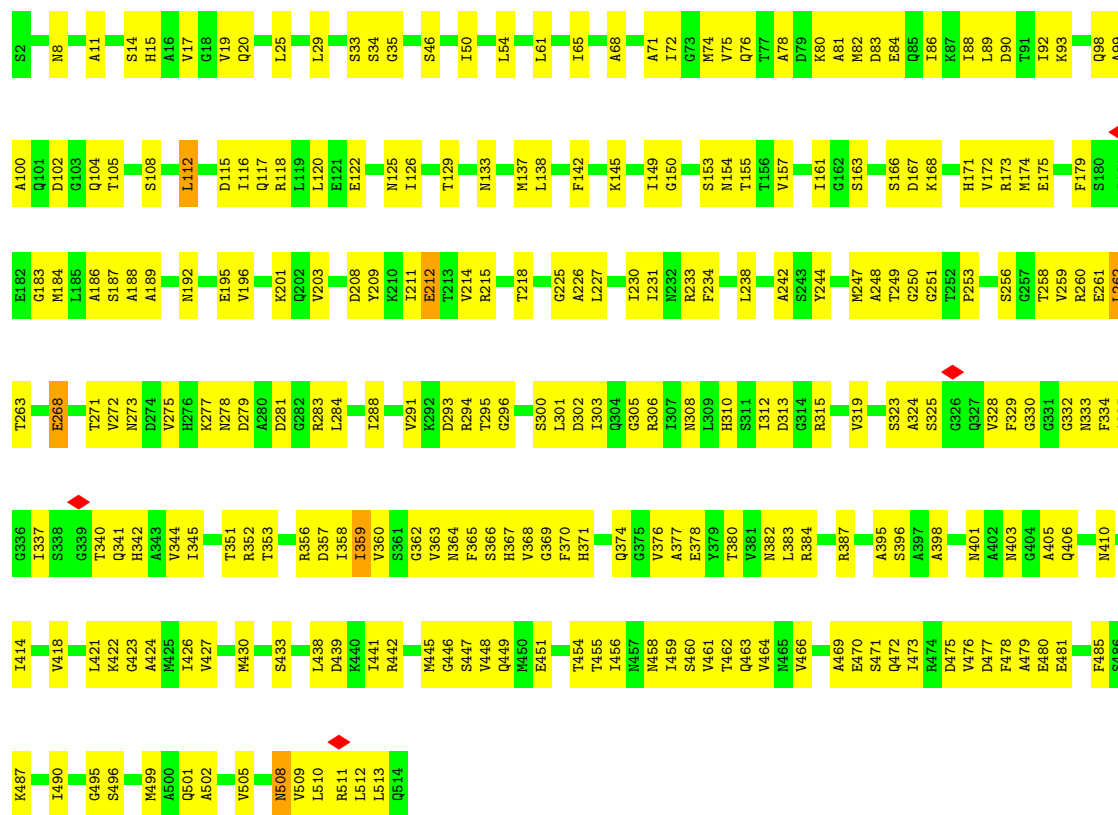


• Molecule 1: Flagellin

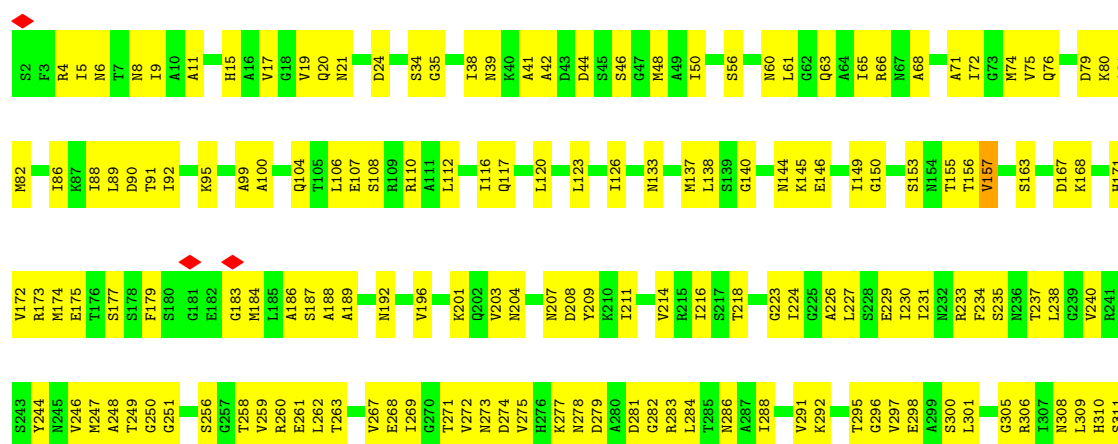


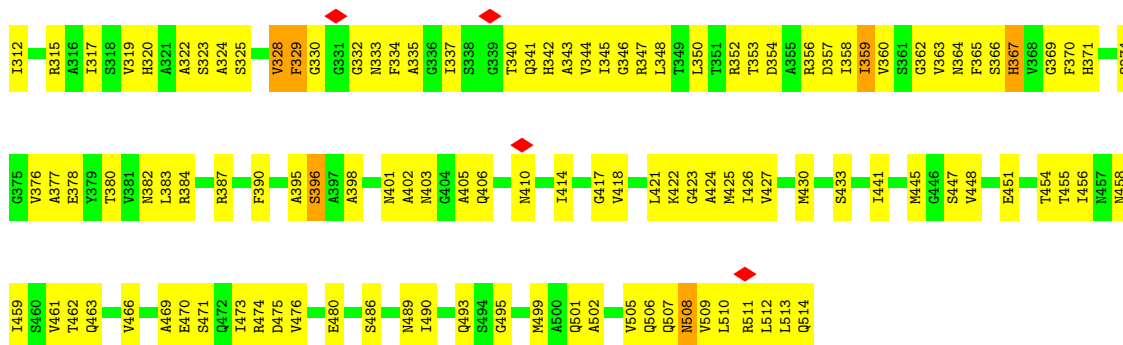


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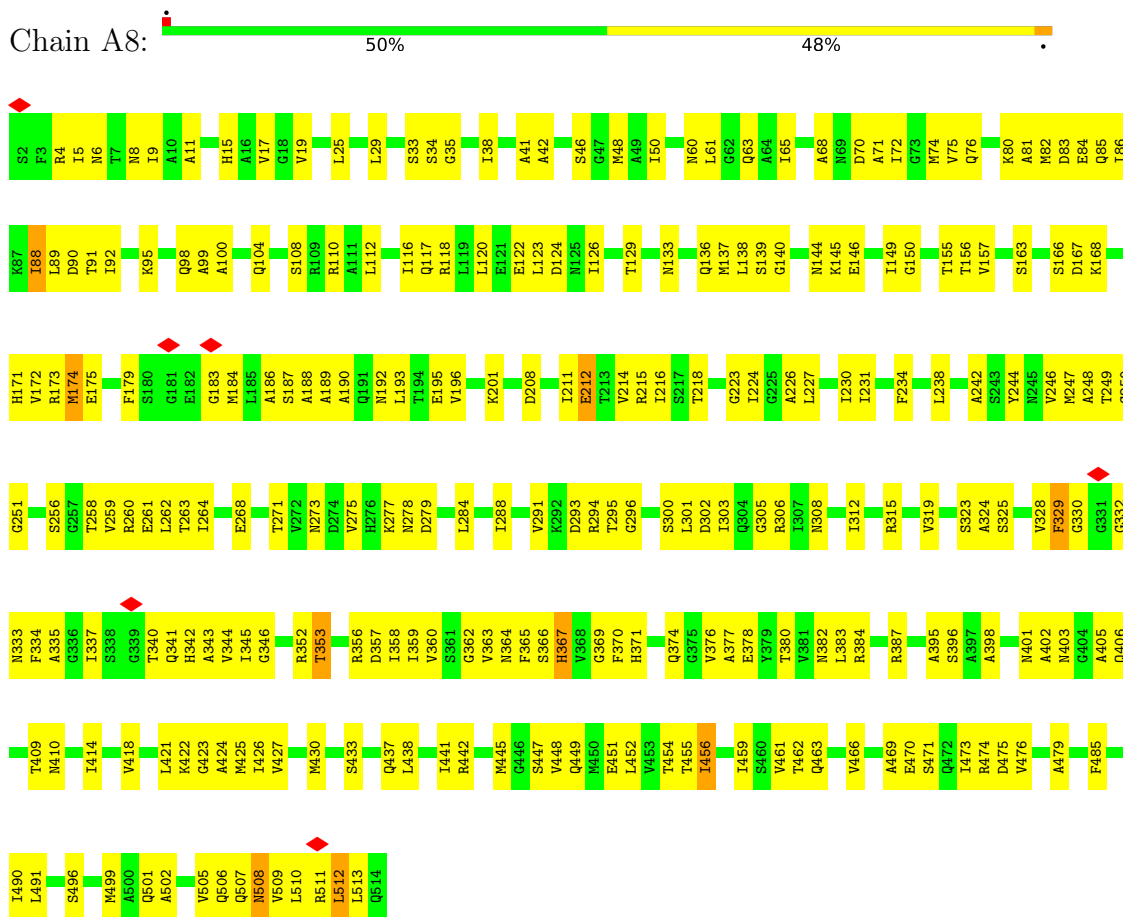


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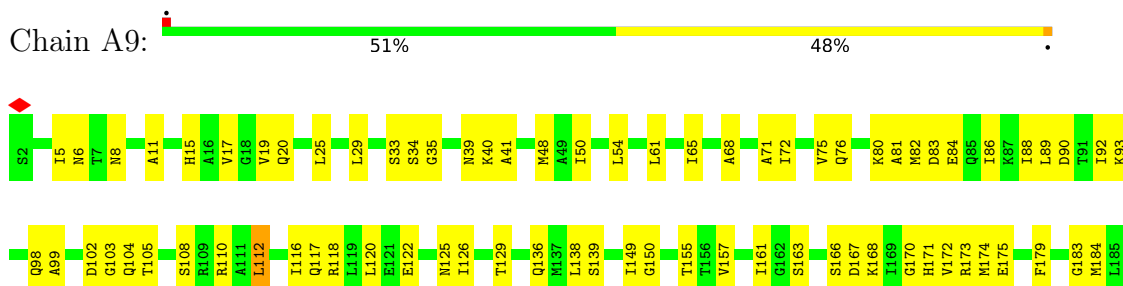


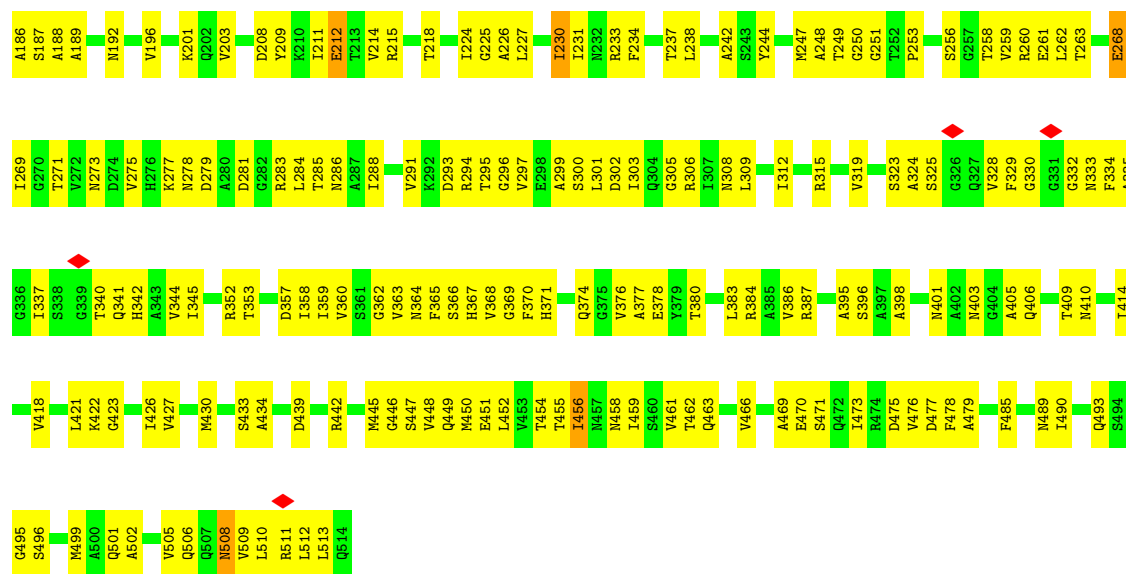


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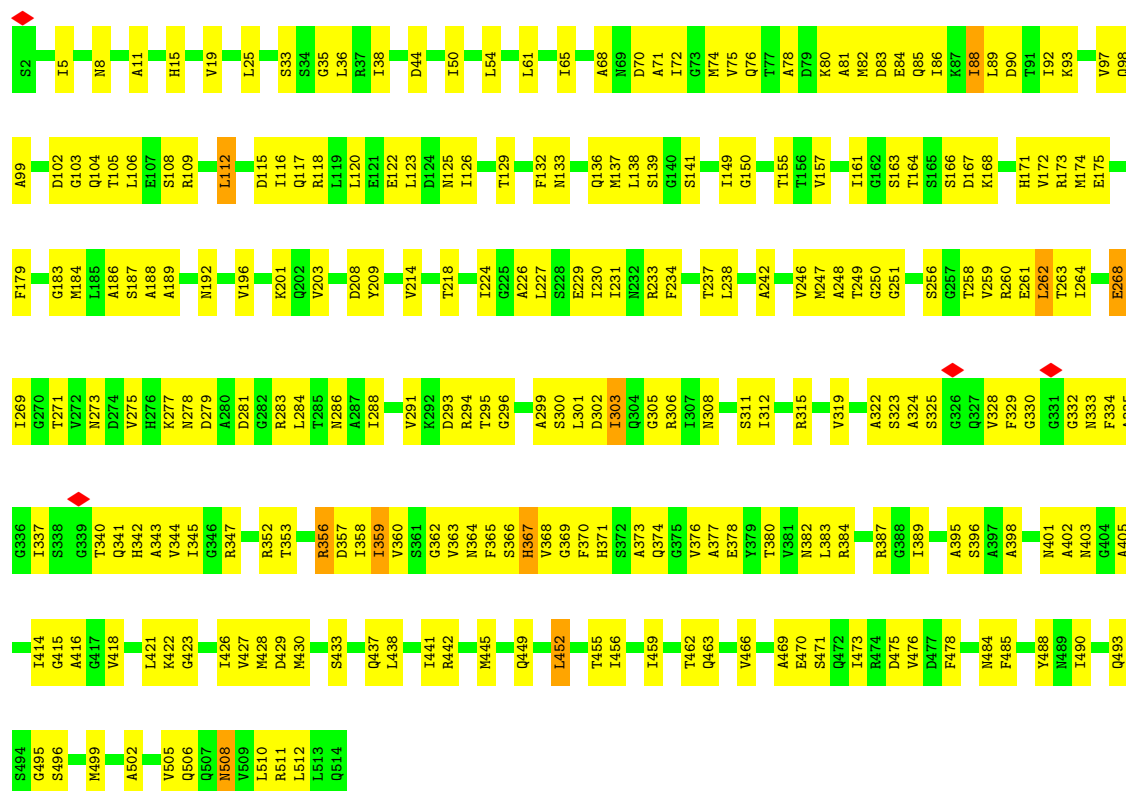


• Molecule 1: Flagellin



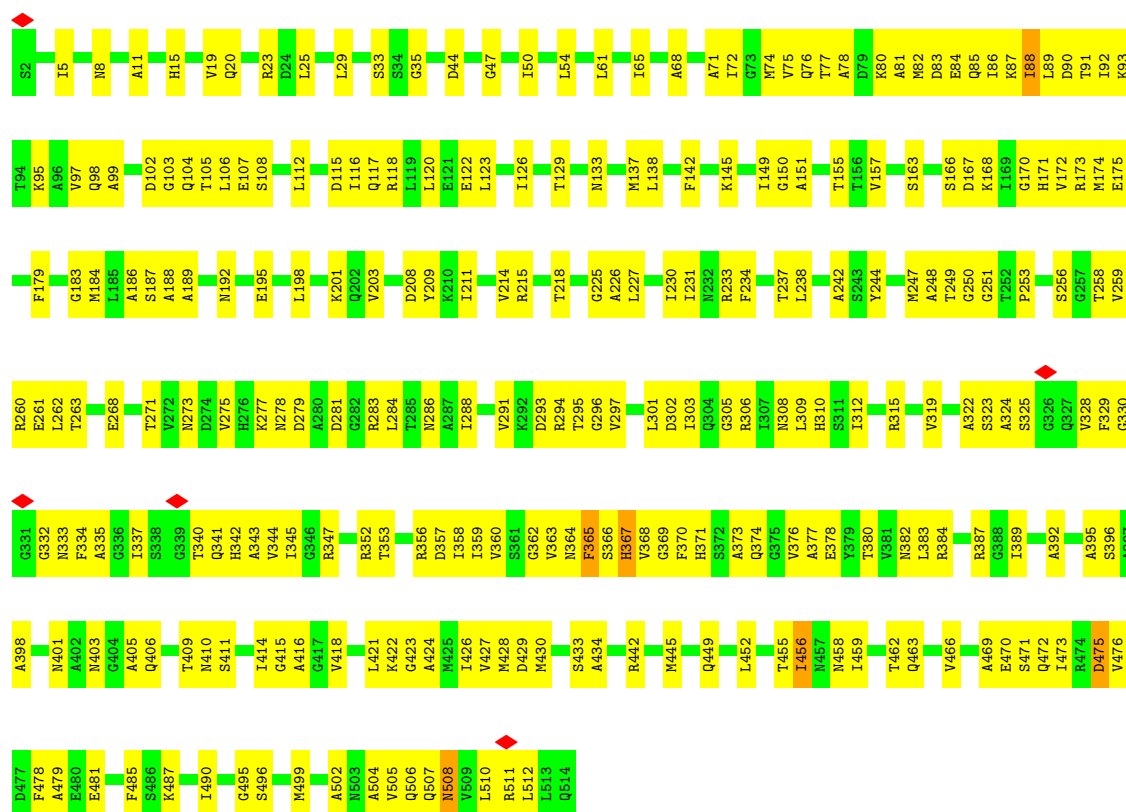


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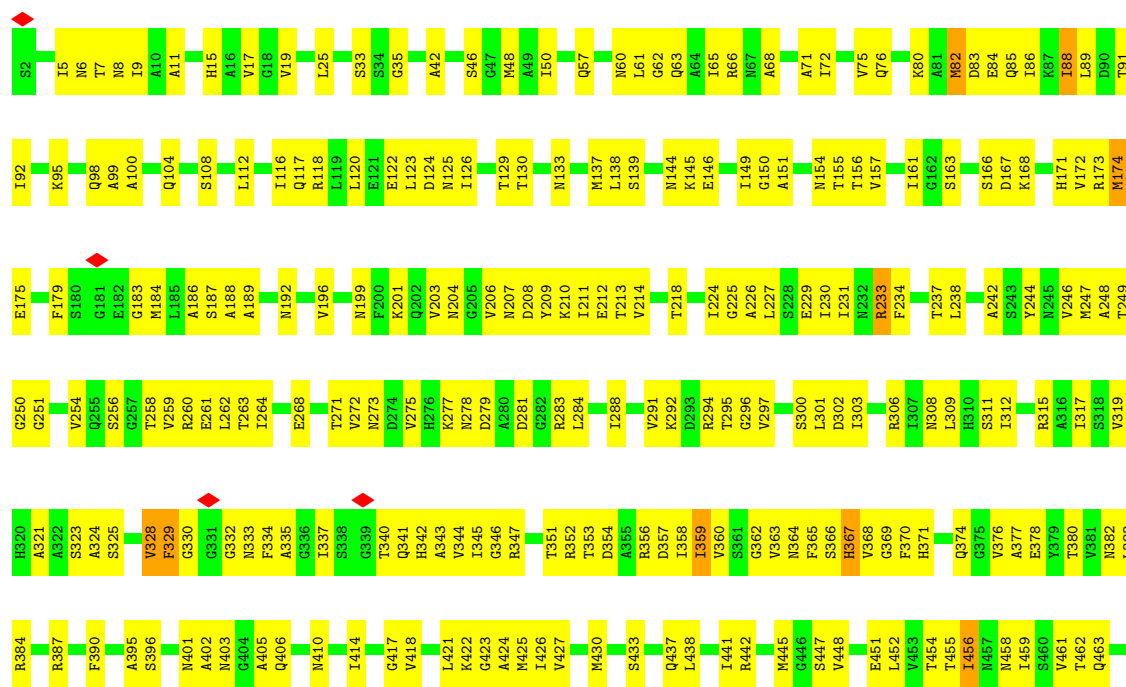


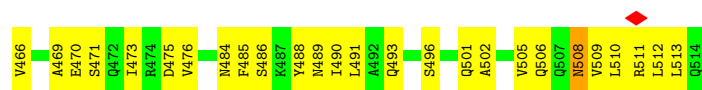
• Molecule 1: Flagellin



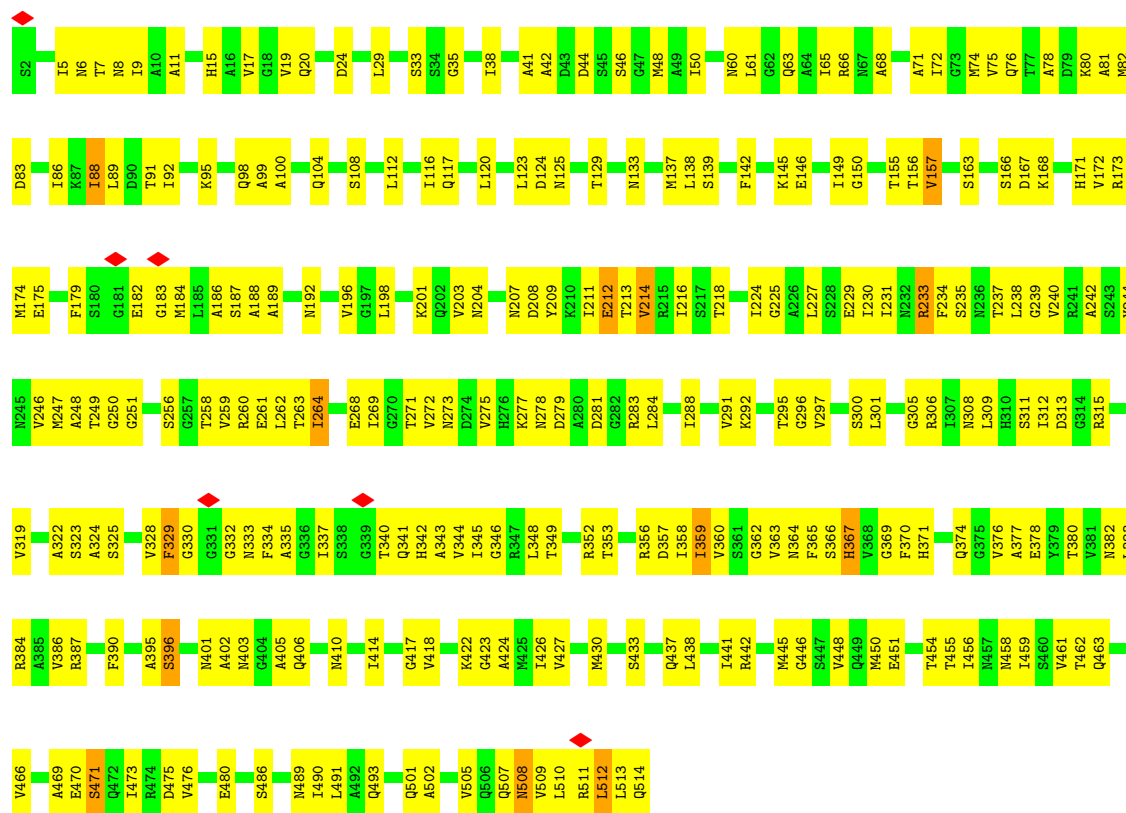


• Molecule 1: Flagellin

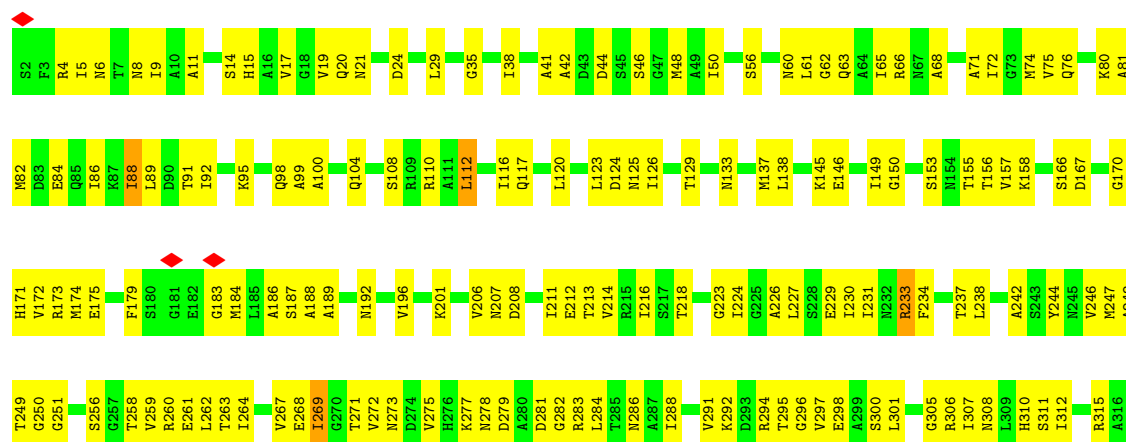




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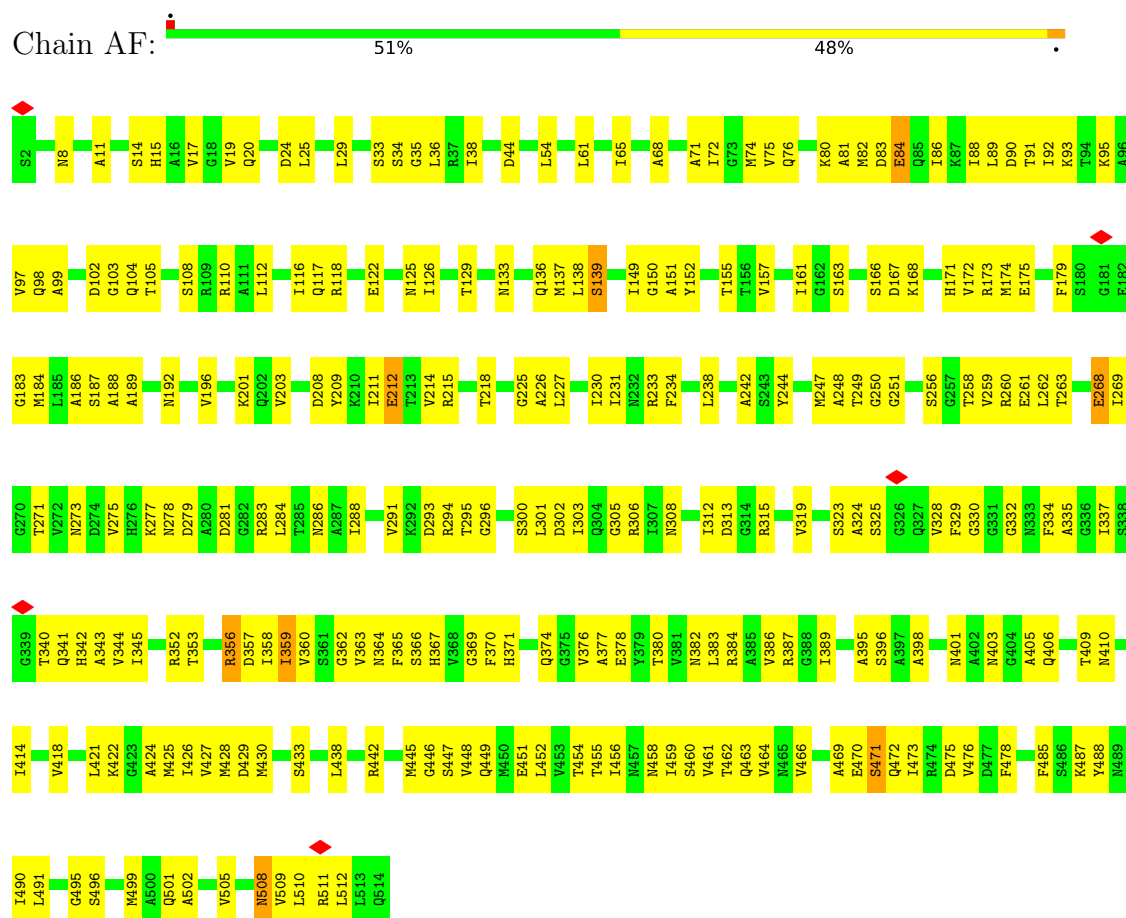


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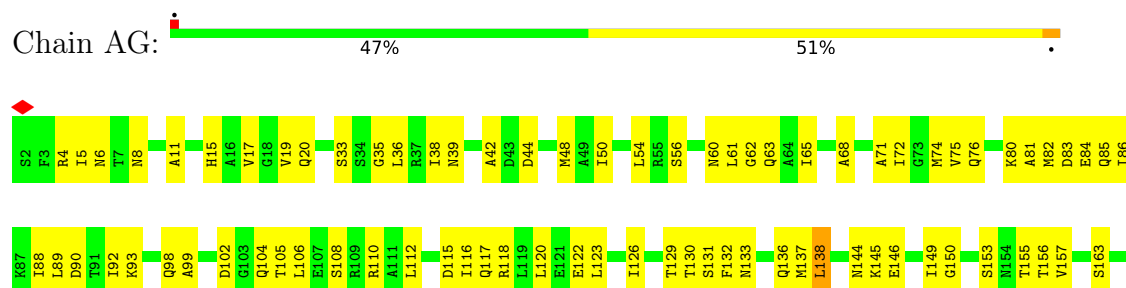


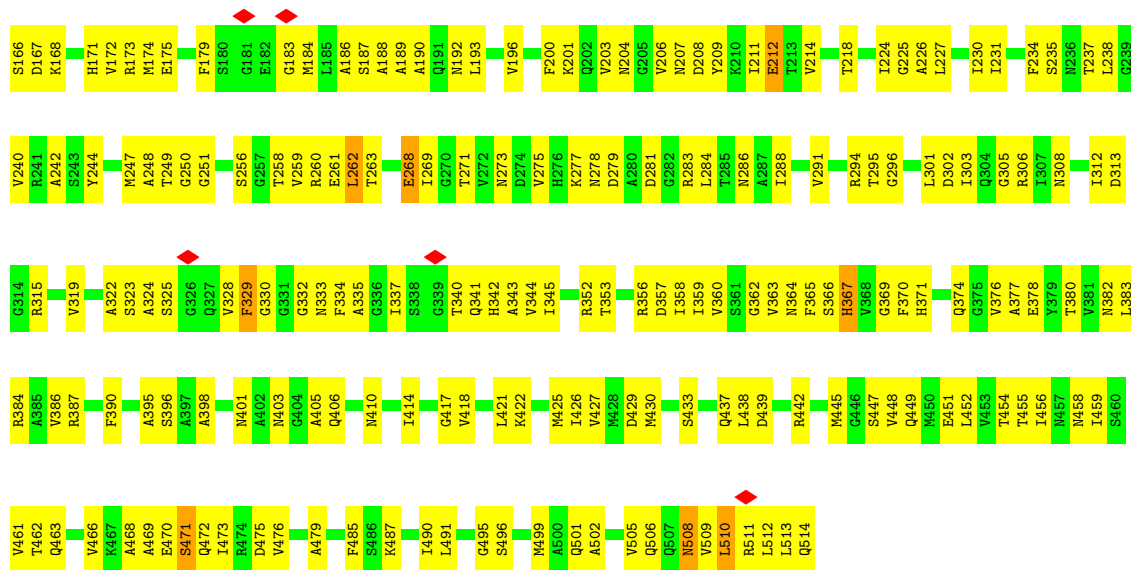


• Molecule 1: Flagellin

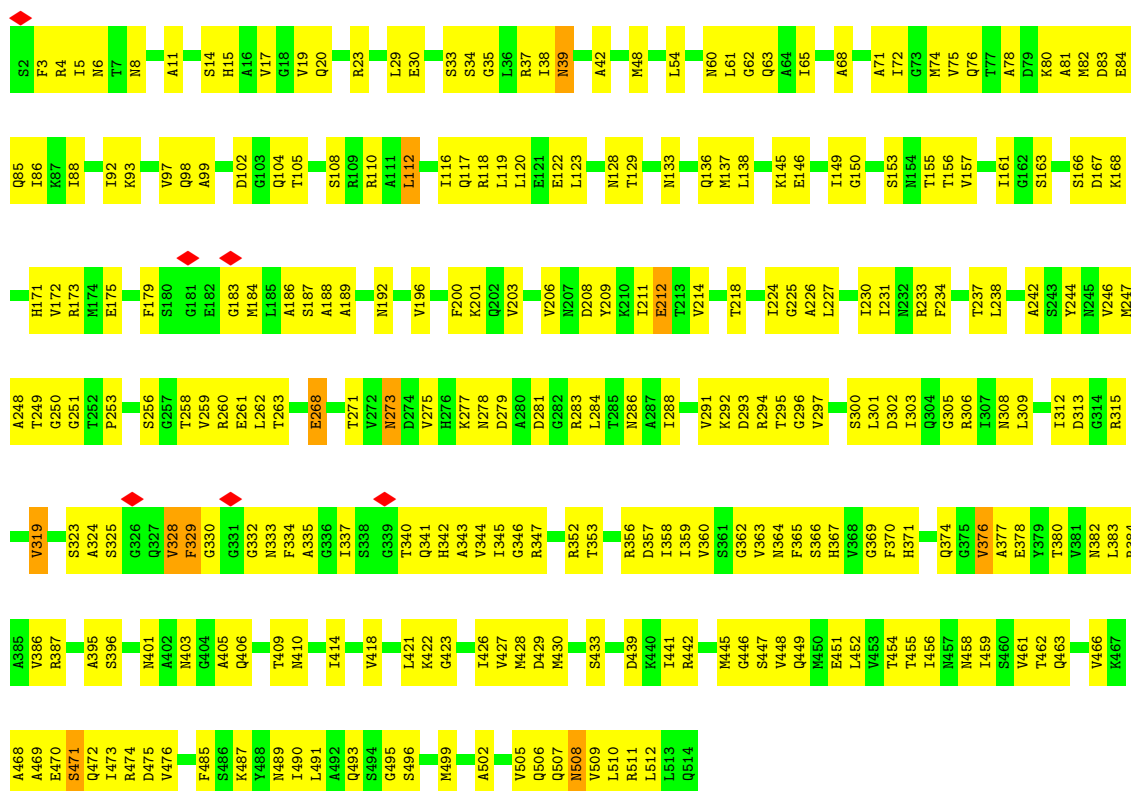


• Molecule 1: Flagellin



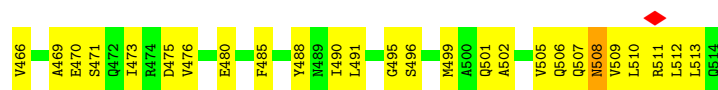


• Molecule 1: Flagellin



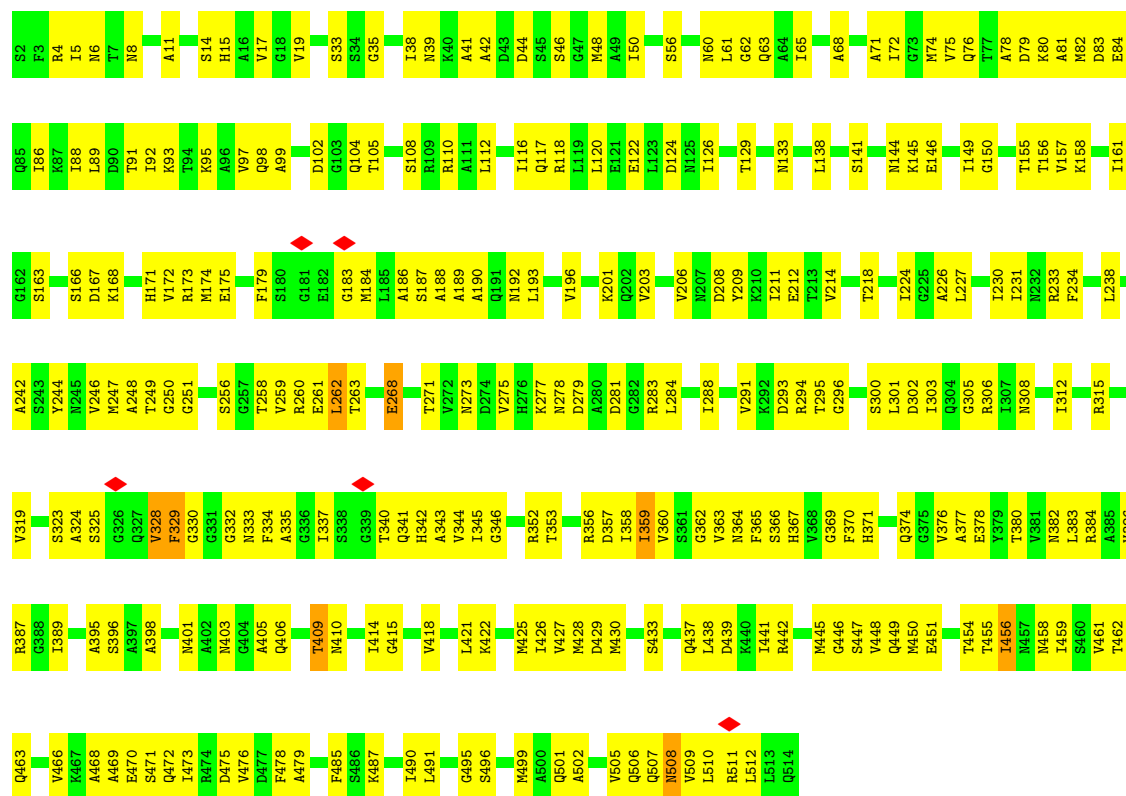
• Molecule 1: Flagellin





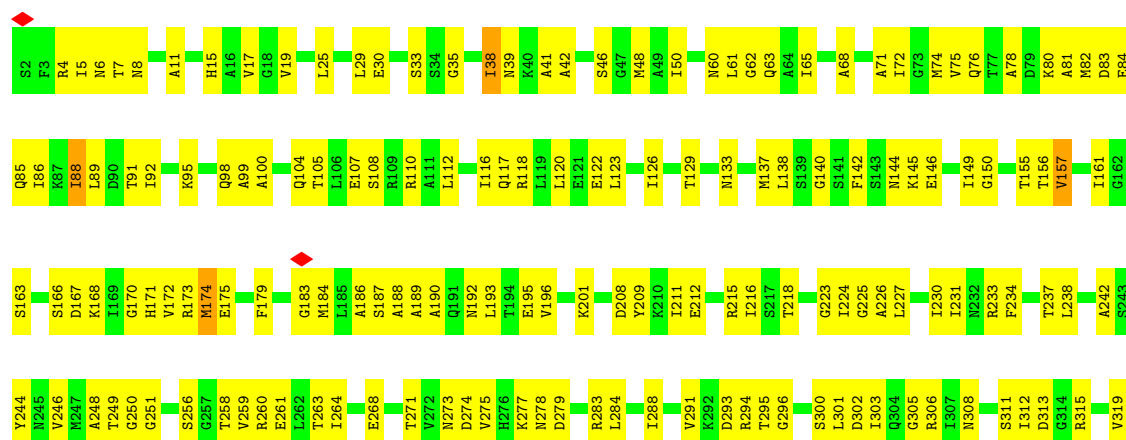
• Molecule 1: Flagellin

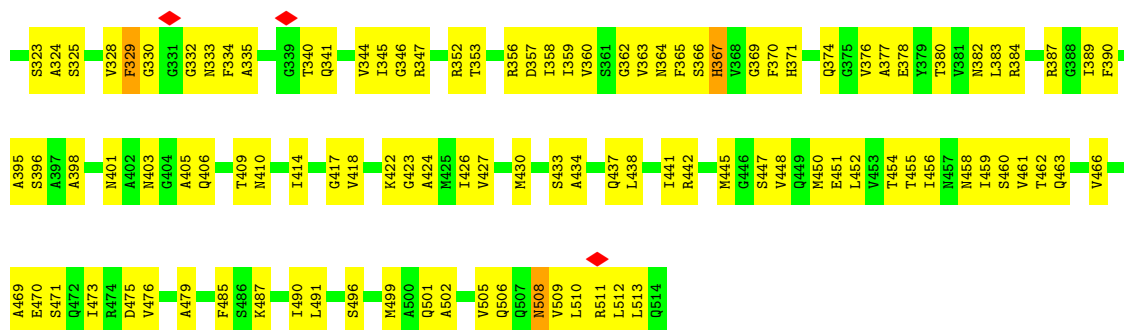
Chain AK: 48% 50%



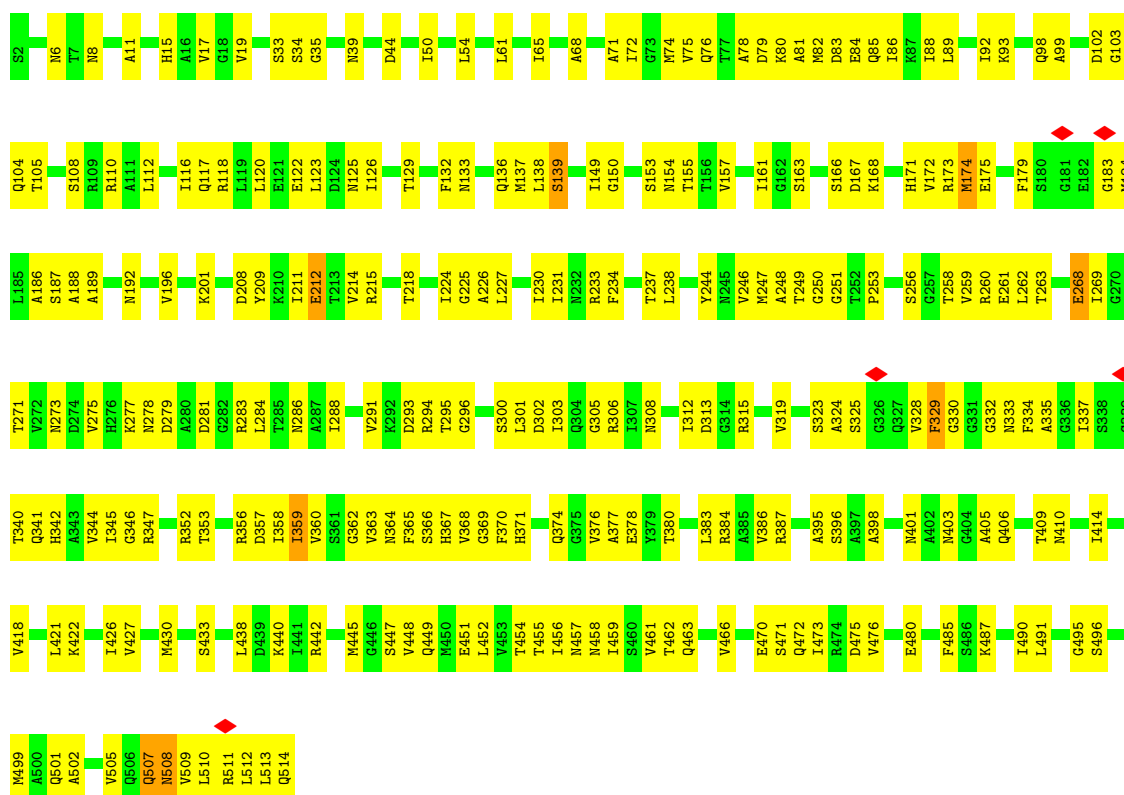
• Molecule 1: Flagellin

Chain AL: 48% 50%

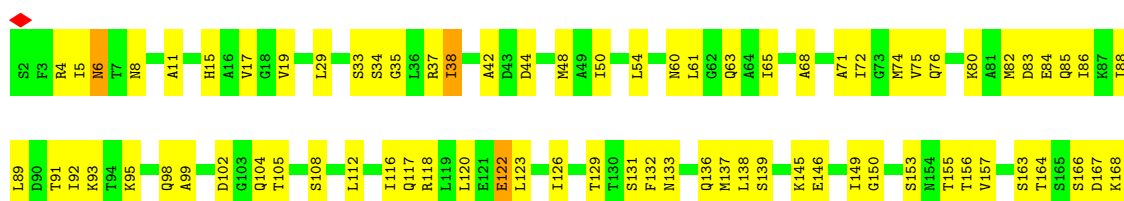


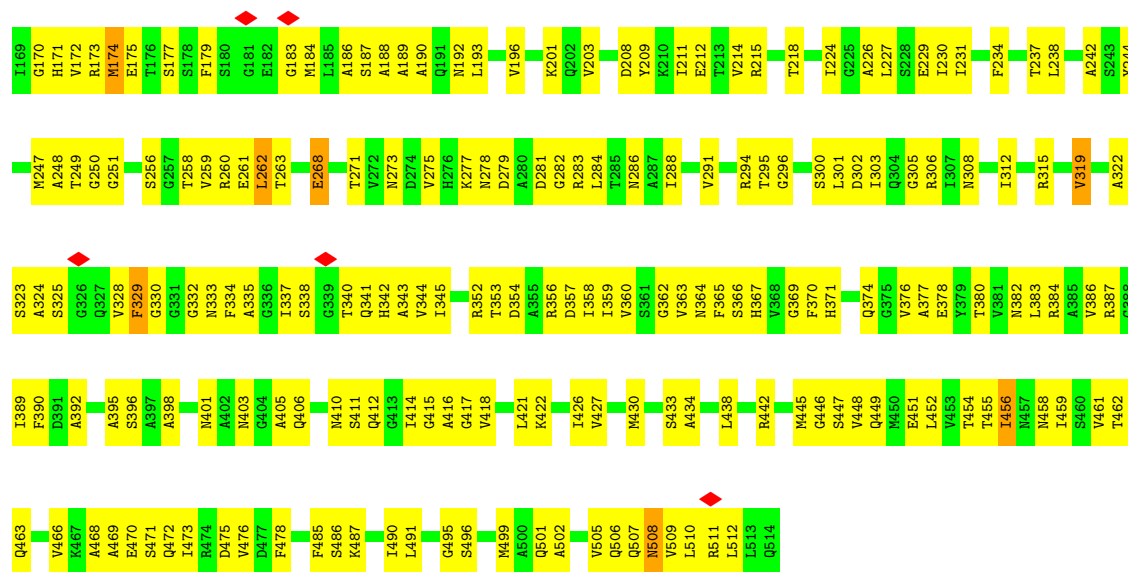


• Molecule 1: Flagellin

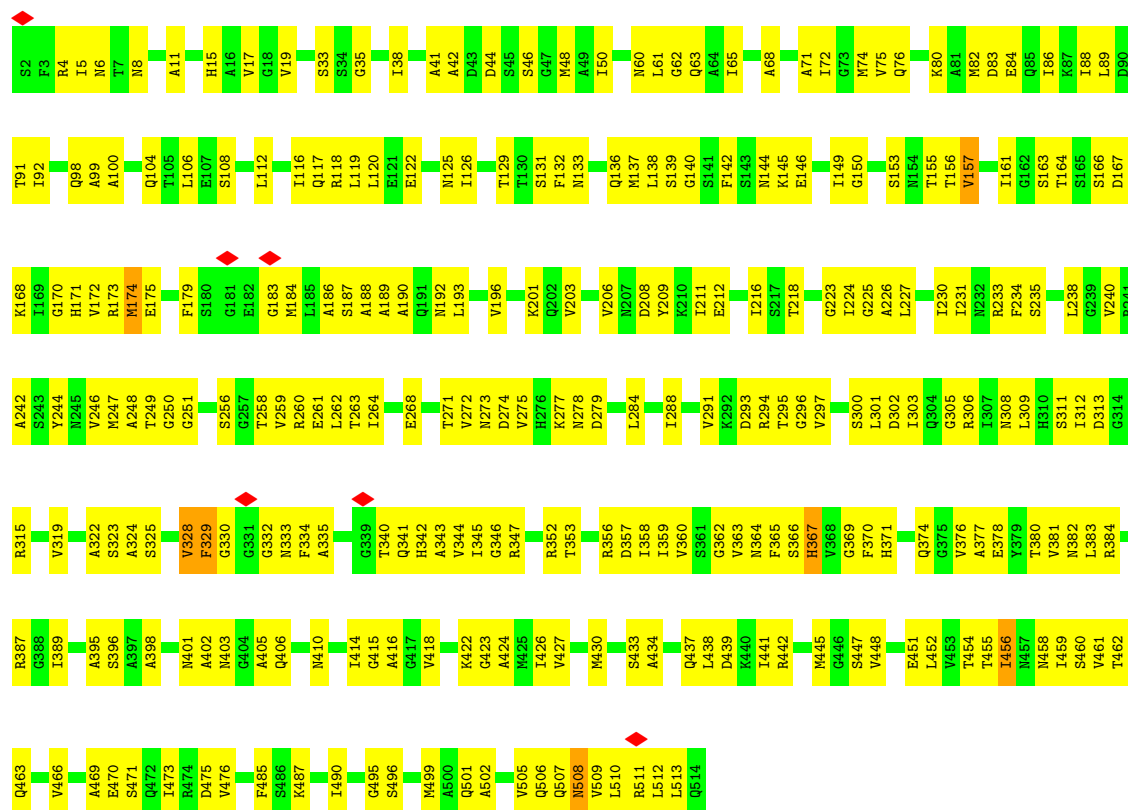


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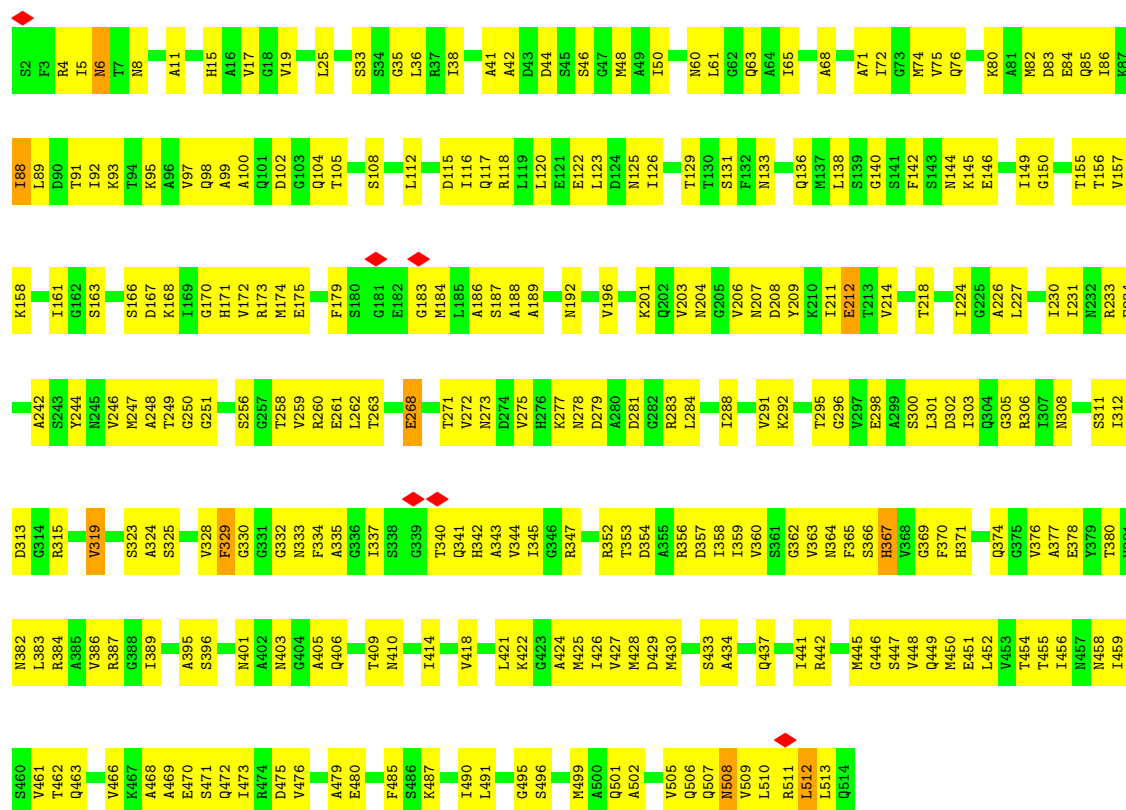


• Molecule 1: Flagellin

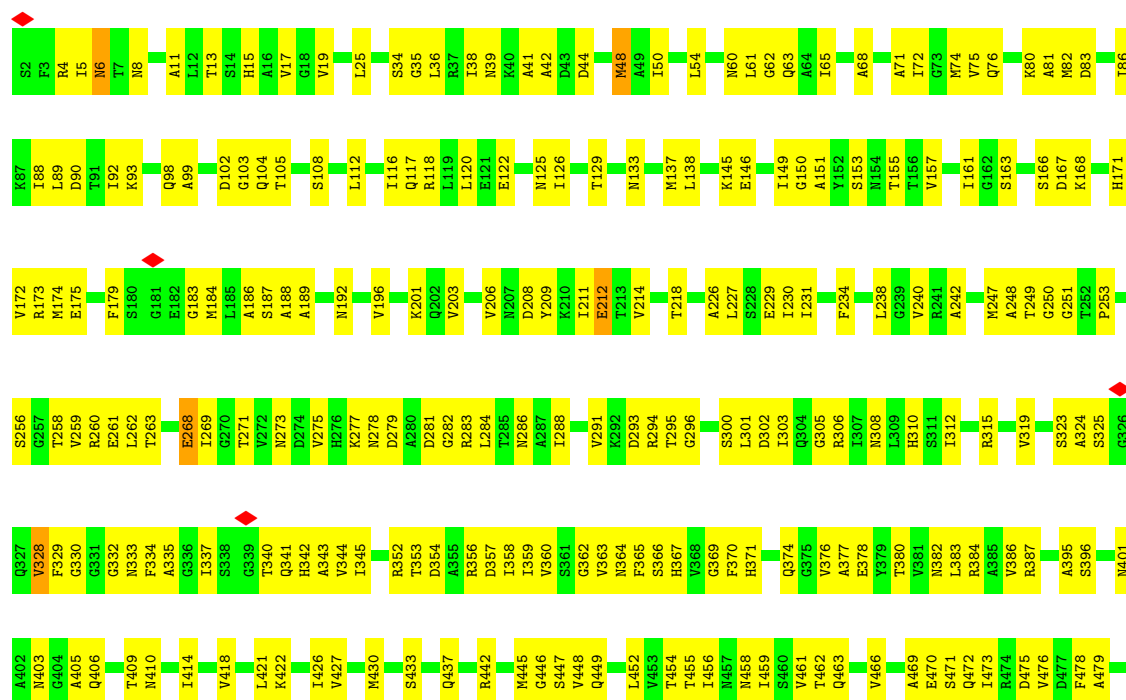


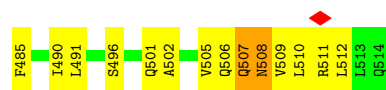
• Molecule 1: Flagellin



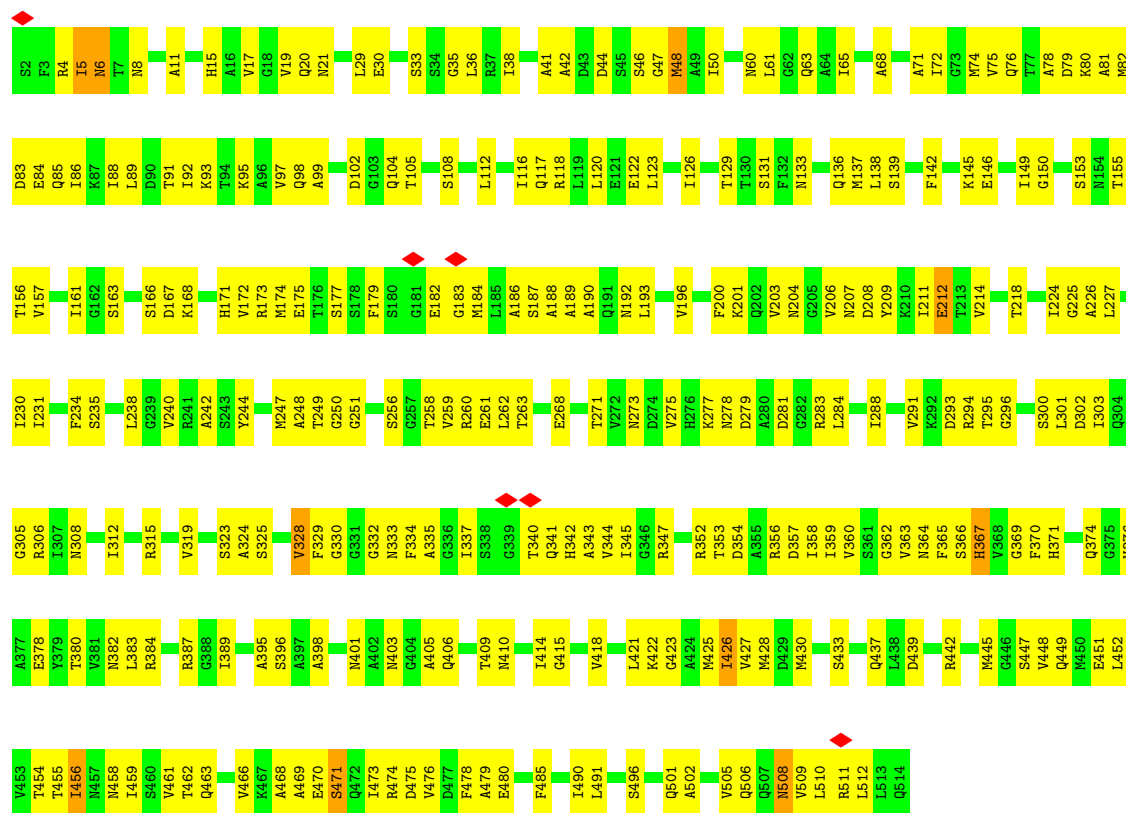


• Molecule 1: Flagellin

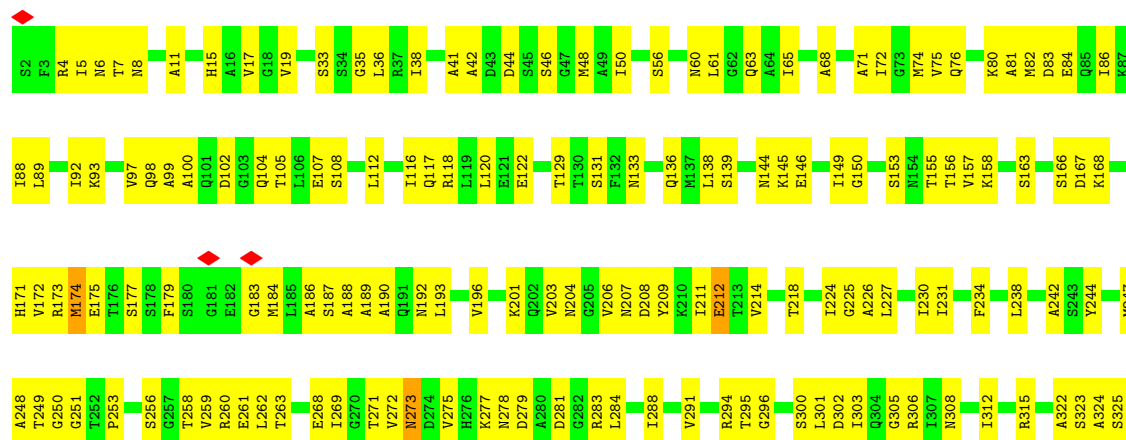


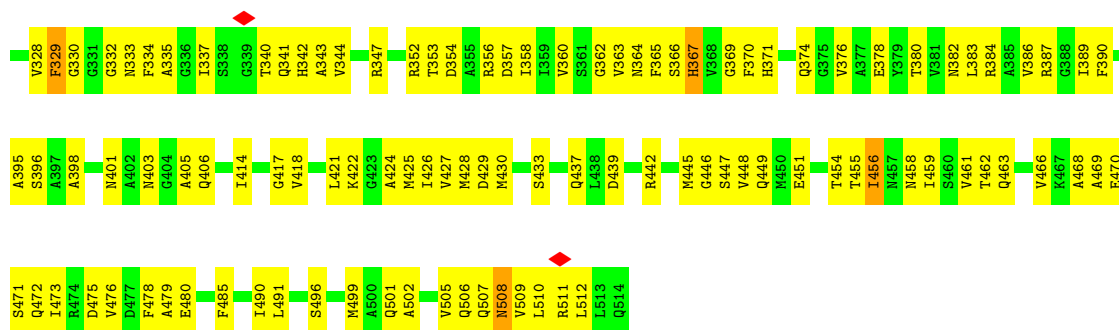


• Molecule 1: Flagellin

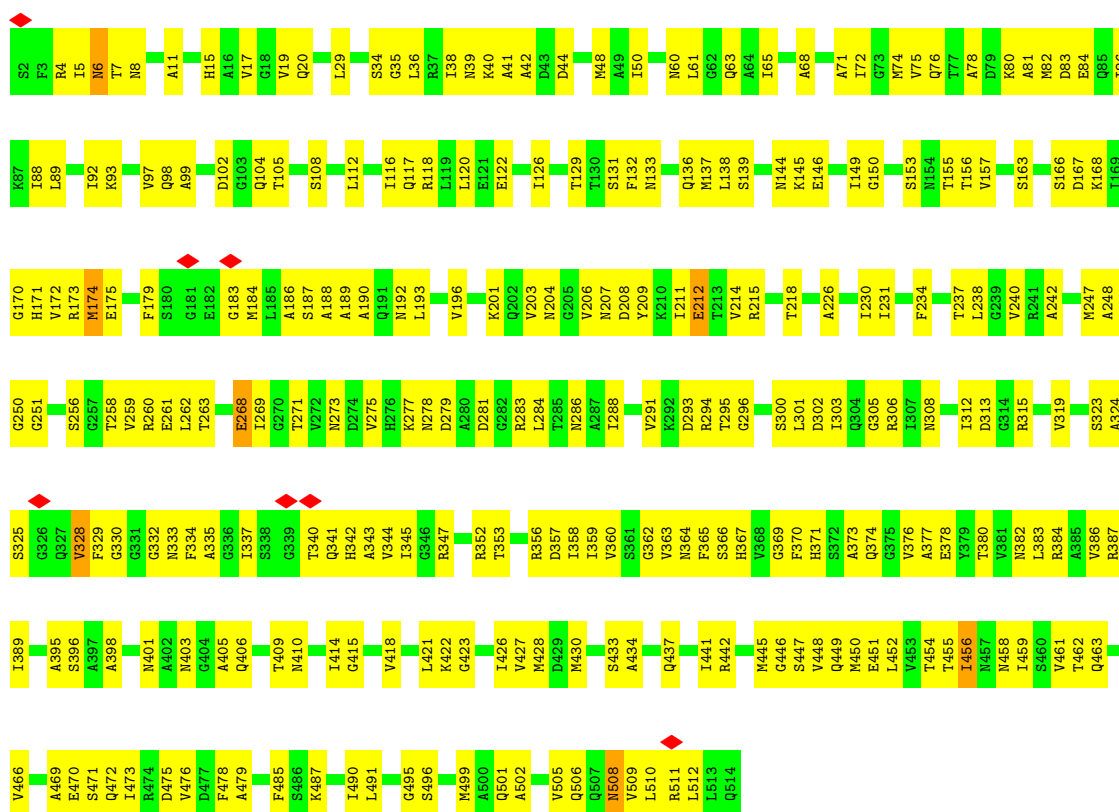


• Molecule 1: Flagellin

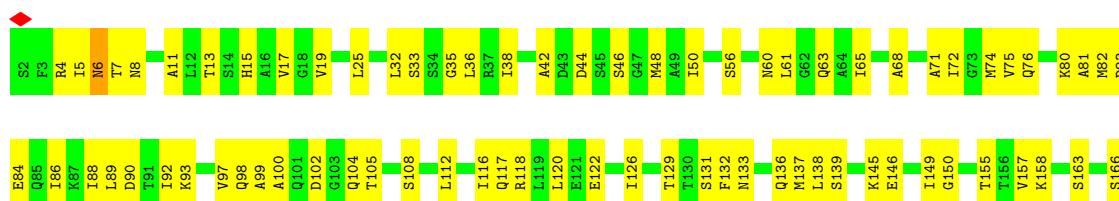




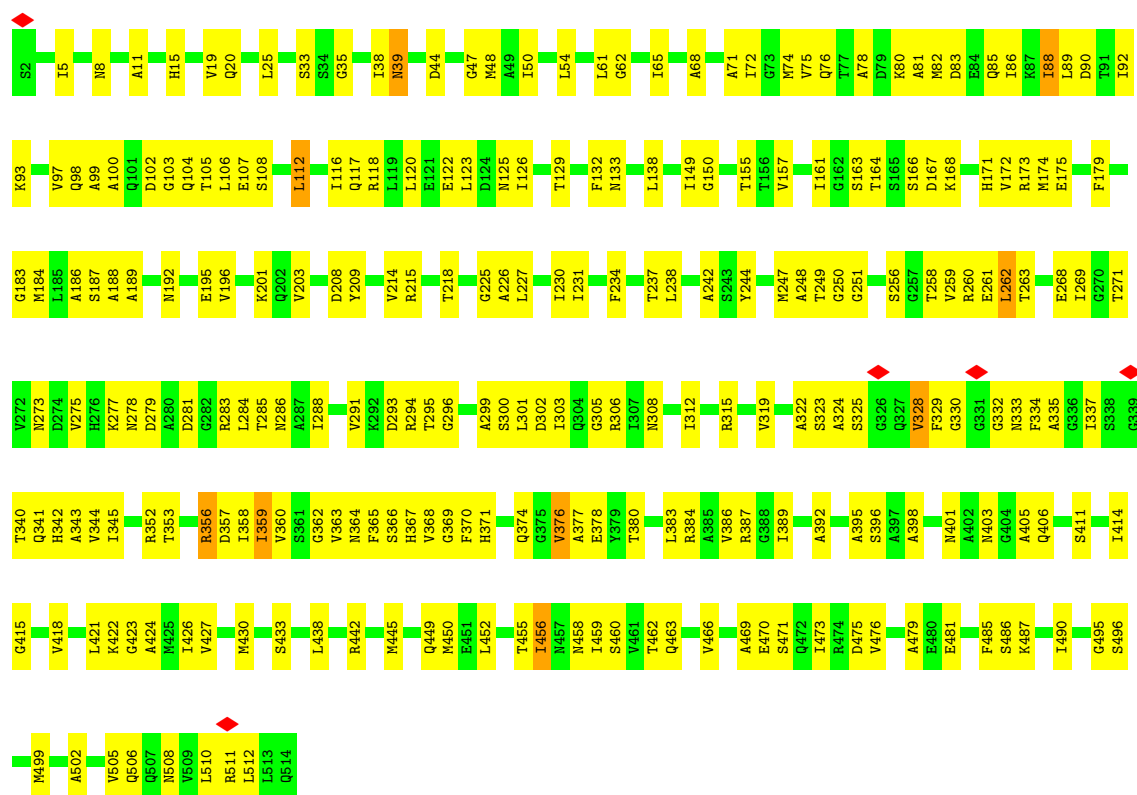
• Molecule 1: Flagellin



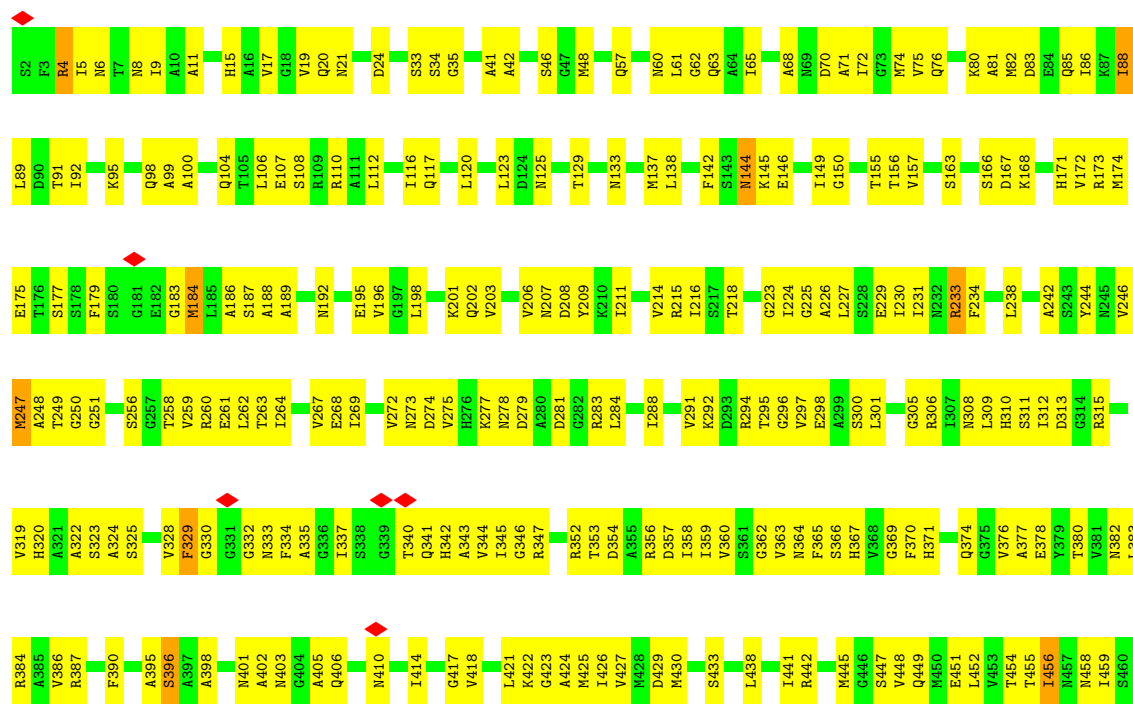
• Molecule 1: Flagellin







• Molecule 1: Flagellin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60029	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.052	Depositor
Map size (\AA)	478.464, 478.464, 478.464	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P8E

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 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	A1	0.14	0/3800	0.29	0/5130
1	A2	0.14	0/3800	0.26	0/5130
1	A3	0.14	0/3800	0.28	0/5130
1	A4	0.14	0/3800	0.28	0/5130
1	A5	0.14	0/3800	0.29	0/5130
1	A6	0.14	0/3800	0.28	0/5130
1	A7	0.13	0/3800	0.28	0/5130
1	A8	0.14	0/3800	0.29	0/5130
1	A9	0.14	0/3800	0.28	0/5130
1	AA	0.13	0/3800	0.26	0/5130
1	AB	0.13	0/3800	0.27	0/5130
1	AC	0.14	0/3800	0.29	0/5130
1	AD	0.13	0/3800	0.28	0/5130
1	AE	0.14	0/3800	0.27	0/5130
1	AF	0.14	0/3800	0.28	0/5130
1	AG	0.14	0/3800	0.28	0/5130
1	AH	0.15	0/3800	0.29	0/5130
1	AI	0.14	0/3800	0.30	0/5130
1	AJ	0.14	0/3800	0.29	0/5130
1	AK	0.14	0/3800	0.28	0/5130
1	AL	0.14	0/3800	0.29	0/5130
1	AM	0.14	0/3800	0.28	0/5130
1	AN	0.15	0/3800	0.29	0/5130
1	AO	0.14	0/3800	0.29	0/5130
1	AP	0.15	0/3800	0.28	0/5130
1	AQ	0.14	0/3800	0.29	0/5130
1	AR	0.14	0/3800	0.29	0/5130
1	AS	0.15	0/3800	0.29	0/5130
1	AT	0.15	0/3800	0.30	0/5130
1	AU	0.14	0/3800	0.28	0/5130
1	AV	0.14	0/3800	0.28	0/5130
1	AW	0.14	0/3800	0.28	0/5130

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AX	0.13	0/3800	0.28	0/5130
All	All	0.14	0/125400	0.28	0/169290

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	3772	0	3733	381	0
1	A2	3772	0	3733	341	0
1	A3	3772	0	3733	345	0
1	A4	3772	0	3733	312	0
1	A5	3772	0	3733	360	0
1	A6	3772	0	3733	367	0
1	A7	3772	0	3733	381	0
1	A8	3772	0	3733	373	0
1	A9	3772	0	3733	365	0
1	AA	3772	0	3733	333	0
1	AB	3772	0	3733	323	0
1	AC	3772	0	3733	379	0
1	AD	3772	0	3733	361	0
1	AE	3772	0	3733	373	0
1	AF	3772	0	3733	369	0
1	AG	3772	0	3733	394	0
1	AH	3772	0	3733	401	0
1	AI	3772	0	3733	396	0
1	AJ	3772	0	3733	404	0
1	AK	3772	0	3733	405	0
1	AL	3772	0	3733	375	0
1	AM	3772	0	3733	370	0
1	AN	3772	0	3733	386	0
1	AO	3772	0	3733	387	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AP	3772	0	3733	391	0
1	AQ	3772	0	3733	394	0
1	AR	3772	0	3733	408	0
1	AS	3772	0	3733	389	0
1	AT	3772	0	3733	412	0
1	AU	3772	0	3733	388	0
1	AV	3772	0	3733	326	0
1	AW	3772	0	3733	320	0
1	AX	3772	0	3733	367	0
2	A1	144	144	0	3	0
2	A2	144	144	0	3	0
2	A3	144	144	0	4	0
2	A4	144	144	0	4	0
2	A5	144	144	0	3	0
2	A6	144	144	0	3	0
2	A7	144	144	0	4	0
2	A8	144	144	0	3	0
2	A9	144	144	0	3	0
2	AA	144	144	0	3	0
2	AB	144	144	0	3	0
2	AC	144	144	0	4	0
2	AD	144	144	0	4	0
2	AE	144	144	0	4	0
2	AF	144	144	0	2	0
2	AG	144	144	0	2	0
2	AH	144	144	0	2	0
2	AI	144	144	0	2	0
2	AJ	144	144	0	4	0
2	AK	144	144	0	2	0
2	AL	144	144	0	4	0
2	AM	144	144	0	3	0
2	AN	144	144	0	3	0
2	AO	144	144	0	2	0
2	AP	144	144	0	3	0
2	AQ	144	144	0	3	0
2	AR	144	144	0	2	0
2	AS	144	144	0	2	0
2	AT	144	144	0	2	0
2	AU	144	144	0	3	0
2	AV	144	144	0	3	0
2	AW	144	144	0	3	0
2	AX	144	144	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	129228	4752	123189	10561	0

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 42.

The worst 5 of 10561 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:264:ILE:HG22	1:A3:319:VAL:HG23	1.22	1.17
1:AG:99:ALA:HB2	1:AG:112:LEU:HD22	1.27	1.16
1:AJ:68:ALA:HB3	1:AJ:456:ILE:HD11	1.25	1.15
1:AM:99:ALA:HB2	1:AM:112:LEU:HD22	1.28	1.15
1:AT:99:ALA:HB2	1:AT:112:LEU:HD23	1.23	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 EM 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	A1	511/513 (100%)	476 (93%)	35 (7%)	0	100	100
1	A2	511/513 (100%)	478 (94%)	33 (6%)	0	100	100
1	A3	511/513 (100%)	478 (94%)	33 (6%)	0	100	100
1	A4	511/513 (100%)	478 (94%)	33 (6%)	0	100	100
1	A5	511/513 (100%)	478 (94%)	32 (6%)	1 (0%)	43	73
1	A6	511/513 (100%)	479 (94%)	32 (6%)	0	100	100
1	A7	511/513 (100%)	480 (94%)	30 (6%)	1 (0%)	43	73
1	A8	511/513 (100%)	482 (94%)	28 (6%)	1 (0%)	43	73
1	A9	511/513 (100%)	476 (93%)	35 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	511/513 (100%)	477 (93%)	34 (7%)	0	100	100
1	AB	511/513 (100%)	483 (94%)	28 (6%)	0	100	100
1	AC	511/513 (100%)	480 (94%)	30 (6%)	1 (0%)	43	73
1	AD	511/513 (100%)	482 (94%)	28 (6%)	1 (0%)	43	73
1	AE	511/513 (100%)	479 (94%)	32 (6%)	0	100	100
1	AF	511/513 (100%)	479 (94%)	32 (6%)	0	100	100
1	AG	511/513 (100%)	481 (94%)	29 (6%)	1 (0%)	43	73
1	AH	511/513 (100%)	477 (93%)	33 (6%)	1 (0%)	43	73
1	AI	511/513 (100%)	478 (94%)	32 (6%)	1 (0%)	43	73
1	AJ	511/513 (100%)	480 (94%)	30 (6%)	1 (0%)	43	73
1	AK	511/513 (100%)	476 (93%)	34 (7%)	1 (0%)	43	73
1	AL	511/513 (100%)	479 (94%)	31 (6%)	1 (0%)	43	73
1	AM	511/513 (100%)	479 (94%)	31 (6%)	1 (0%)	43	73
1	AN	511/513 (100%)	479 (94%)	31 (6%)	1 (0%)	43	73
1	AO	511/513 (100%)	479 (94%)	31 (6%)	1 (0%)	43	73
1	AP	511/513 (100%)	477 (93%)	33 (6%)	1 (0%)	43	73
1	AQ	511/513 (100%)	476 (93%)	35 (7%)	0	100	100
1	AR	511/513 (100%)	477 (93%)	34 (7%)	0	100	100
1	AS	511/513 (100%)	479 (94%)	31 (6%)	1 (0%)	43	73
1	AT	511/513 (100%)	478 (94%)	33 (6%)	0	100	100
1	AU	511/513 (100%)	478 (94%)	32 (6%)	1 (0%)	43	73
1	AV	511/513 (100%)	477 (93%)	33 (6%)	1 (0%)	43	73
1	AW	511/513 (100%)	476 (93%)	35 (7%)	0	100	100
1	AX	511/513 (100%)	480 (94%)	30 (6%)	1 (0%)	43	73
All	All	16863/16929 (100%)	15791 (94%)	1053 (6%)	19 (0%)	49	78

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AG	329	PHE
1	AP	329	PHE
1	AV	329	PHE
1	AC	329	PHE
1	AD	329	PHE

5.3.2 Protein sidechains ⓘ

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 EM 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	A1	404/404 (100%)	392 (97%)	12 (3%)	36	64
1	A2	404/404 (100%)	389 (96%)	15 (4%)	30	60
1	A3	404/404 (100%)	389 (96%)	15 (4%)	30	60
1	A4	404/404 (100%)	395 (98%)	9 (2%)	45	69
1	A5	404/404 (100%)	392 (97%)	12 (3%)	36	64
1	A6	404/404 (100%)	395 (98%)	9 (2%)	45	69
1	A7	404/404 (100%)	393 (97%)	11 (3%)	39	66
1	A8	404/404 (100%)	392 (97%)	12 (3%)	36	64
1	A9	404/404 (100%)	395 (98%)	9 (2%)	45	69
1	AA	404/404 (100%)	391 (97%)	13 (3%)	34	63
1	AB	404/404 (100%)	396 (98%)	8 (2%)	48	70
1	AC	404/404 (100%)	393 (97%)	11 (3%)	39	66
1	AD	404/404 (100%)	389 (96%)	15 (4%)	30	60
1	AE	404/404 (100%)	390 (96%)	14 (4%)	32	61
1	AF	404/404 (100%)	395 (98%)	9 (2%)	45	69
1	AG	404/404 (100%)	393 (97%)	11 (3%)	39	66
1	AH	404/404 (100%)	393 (97%)	11 (3%)	39	66
1	AI	404/404 (100%)	394 (98%)	10 (2%)	42	67
1	AJ	404/404 (100%)	394 (98%)	10 (2%)	42	67
1	AK	404/404 (100%)	395 (98%)	9 (2%)	45	69
1	AL	404/404 (100%)	395 (98%)	9 (2%)	45	69
1	AM	404/404 (100%)	395 (98%)	9 (2%)	45	69
1	AN	404/404 (100%)	392 (97%)	12 (3%)	36	64
1	AO	404/404 (100%)	397 (98%)	7 (2%)	53	72
1	AP	404/404 (100%)	396 (98%)	8 (2%)	48	70
1	AQ	404/404 (100%)	394 (98%)	10 (2%)	42	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AR	404/404 (100%)	392 (97%)	12 (3%)	36	64
1	AS	404/404 (100%)	397 (98%)	7 (2%)	53	72
1	AT	404/404 (100%)	396 (98%)	8 (2%)	48	70
1	AU	404/404 (100%)	396 (98%)	8 (2%)	48	70
1	AV	404/404 (100%)	394 (98%)	10 (2%)	42	67
1	AW	404/404 (100%)	392 (97%)	12 (3%)	36	64
1	AX	404/404 (100%)	389 (96%)	15 (4%)	30	60
All	All	13332/13332 (100%)	12980 (97%)	352 (3%)	41	66

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AL	367	HIS
1	AR	367	HIS
1	AM	268	GLU
1	AO	456	ILE
1	AT	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 387 such sidechains are listed below:

Mol	Chain	Res	Type
1	AK	286	ASN
1	AO	401	ASN
1	AL	6	ASN
1	AM	410	ASN
1	AP	410	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

297 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	AD	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AN	608	-	15,16,17	1.09	1 (6%)	17,23,26	2.01	3 (17%)
2	P8E	AC	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AP	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AL	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.23	4 (23%)
2	P8E	AA	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AK	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	A7	609	-	15,16,17	1.07	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AD	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	A6	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.01	3 (17%)
2	P8E	AE	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.09	3 (17%)
2	P8E	AI	606	-	15,16,17	1.10	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AT	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AQ	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AA	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AM	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	AX	606	-	15,16,17	1.08	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AJ	607	-	15,16,17	1.04	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AW	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.27	3 (17%)
2	P8E	AN	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AL	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A9	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	AU	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.01	3 (17%)
2	P8E	AD	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.30	4 (23%)
2	P8E	AW	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	A2	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.20	4 (23%)
2	P8E	AA	607	-	15,16,17	1.07	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AF	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.28	3 (17%)
2	P8E	AO	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	A9	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	AS	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AL	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.30	4 (23%)
2	P8E	A2	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A8	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AE	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	AT	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	A5	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AT	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AG	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.01	2 (11%)
2	P8E	A6	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	A6	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	A9	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AE	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.05	2 (11%)
2	P8E	AJ	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A8	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AM	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	A1	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AI	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AT	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.26	3 (17%)
2	P8E	A4	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	2 (11%)
2	P8E	AU	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A6	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	AD	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AO	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	A3	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.32	4 (23%)
2	P8E	AJ	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.31	4 (23%)
2	P8E	A6	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	A1	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	A5	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AE	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.06	3 (17%)
2	P8E	AS	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AB	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AO	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.02	2 (11%)
2	P8E	AH	607	-	15,16,17	1.06	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AE	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AQ	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	A9	607	-	15,16,17	1.06	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AM	609	-	15,16,17	1.09	1 (6%)	17,23,26	2.08	3 (17%)
2	P8E	A4	607	-	15,16,17	1.07	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AF	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	A5	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	A4	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AN	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AG	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AW	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A5	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AF	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.01	3 (17%)
2	P8E	AC	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	A6	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.26	3 (17%)
2	P8E	AS	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.03	2 (11%)
2	P8E	AC	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AU	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AB	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AV	604	-	15,16,17	1.16	1 (6%)	17,23,26	2.21	3 (17%)
2	P8E	A5	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.30	4 (23%)
2	P8E	AB	607	-	15,16,17	1.07	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A7	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	A8	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	A4	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.01	3 (17%)
2	P8E	AE	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AU	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	AG	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.93	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	A3	601	-	15,16,17	1.07	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	A4	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	AS	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A7	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AQ	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	2 (11%)
2	P8E	A7	601	-	15,16,17	1.07	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A2	607	-	15,16,17	1.07	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A3	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	A8	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AH	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	2 (11%)
2	P8E	AC	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	AA	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	AP	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AQ	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AR	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.23	4 (23%)
2	P8E	A4	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	A6	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	AA	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	2 (11%)
2	P8E	A6	607	-	15,16,17	1.06	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AH	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AJ	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AW	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	AG	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AC	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AP	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AR	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AK	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A1	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.01	3 (17%)
2	P8E	A3	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AN	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.02	2 (11%)
2	P8E	AB	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	A2	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AT	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AC	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AB	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	AK	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	2 (11%)
2	P8E	AB	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AF	607	-	15,16,17	1.06	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AU	606	-	15,16,17	1.11	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AL	609	-	15,16,17	1.07	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AV	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	A2	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.26	3 (17%)
2	P8E	A2	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	2 (11%)
2	P8E	AW	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	2 (11%)
2	P8E	AX	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AH	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AX	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AM	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.19	4 (23%)
2	P8E	A1	607	-	15,16,17	1.06	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AC	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.31	4 (23%)
2	P8E	AK	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	A9	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	AG	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	AG	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.06	3 (17%)
2	P8E	A2	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	A5	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AK	606	-	15,16,17	1.10	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AH	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	AQ	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.92	3 (17%)
2	P8E	AT	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A9	609	-	15,16,17	1.09	1 (6%)	17,23,26	2.09	3 (17%)
2	P8E	A4	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	AM	607	-	15,16,17	1.06	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AJ	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AV	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.89	3 (17%)
2	P8E	AI	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AP	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	A7	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	AU	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AQ	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.26	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	AD	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.09	3 (17%)
2	P8E	A1	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AP	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	2 (11%)
2	P8E	AX	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	A3	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	A5	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.02	2 (11%)
2	P8E	AP	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.28	3 (17%)
2	P8E	AT	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	2 (11%)
2	P8E	AP	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AM	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	2 (11%)
2	P8E	AQ	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AA	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A1	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.25	3 (17%)
2	P8E	A1	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	A3	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	A2	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	A5	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	A8	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.30	4 (23%)
2	P8E	AB	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.88	3 (17%)
2	P8E	AV	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.01	3 (17%)
2	P8E	AW	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.06	3 (17%)
2	P8E	AD	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AI	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AA	609	-	15,16,17	1.09	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A1	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AB	604	-	15,16,17	1.12	1 (6%)	17,23,26	2.25	3 (17%)
2	P8E	AB	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	2 (11%)
2	P8E	AS	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.28	3 (17%)
2	P8E	AG	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.27	3 (17%)
2	P8E	A9	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AK	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.28	3 (17%)
2	P8E	AL	607	-	15,16,17	1.04	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	AC	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	AJ	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	AS	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	AM	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.27	3 (17%)
2	P8E	AO	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AR	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A7	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AO	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AV	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.23	4 (23%)
2	P8E	A9	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.26	3 (17%)
2	P8E	A5	607	-	15,16,17	1.04	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AF	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	AK	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AO	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AG	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AN	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	A9	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AS	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AR	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.28	3 (17%)
2	P8E	AT	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AU	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	AX	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AH	609	-	15,16,17	1.09	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AV	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AN	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.25	3 (17%)
2	P8E	AA	604	-	15,16,17	1.12	1 (6%)	17,23,26	2.25	3 (17%)
2	P8E	AR	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	A3	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AS	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	A4	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.26	3 (17%)
2	P8E	A2	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AR	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AI	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	AK	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AN	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AJ	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AL	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.03	2 (11%)
2	P8E	AR	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.06	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	AV	608	-	15,16,17	1.07	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	AF	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	AQ	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AO	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	A8	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AA	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AF	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.95	3 (17%)
2	P8E	AI	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.27	3 (17%)
2	P8E	AL	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	A3	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.15	3 (17%)
2	P8E	AK	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.23	4 (23%)
2	P8E	AS	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	AQ	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.20	4 (23%)
2	P8E	AE	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AX	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.22	4 (23%)
2	P8E	A8	609	-	15,16,17	1.07	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AF	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.20	4 (23%)
2	P8E	AJ	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.06	2 (11%)
2	P8E	AM	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	A8	607	-	15,16,17	1.04	1 (6%)	17,23,26	2.13	3 (17%)
2	P8E	A7	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.31	4 (23%)
2	P8E	AM	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AO	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.30	4 (23%)
2	P8E	AU	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	AW	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AC	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AI	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AE	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AF	609	-	15,16,17	1.09	1 (6%)	17,23,26	2.08	3 (17%)
2	P8E	AI	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	AO	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AU	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.30	3 (17%)
2	P8E	AD	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	A6	609	-	15,16,17	1.09	1 (6%)	17,23,26	2.09	3 (17%)
2	P8E	AI	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.02	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P8E	AN	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	AP	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AW	603	-	15,16,17	1.08	1 (6%)	17,23,26	2.00	3 (17%)
2	P8E	AX	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AD	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AH	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.94	3 (17%)
2	P8E	AL	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AV	607	-	15,16,17	1.07	1 (6%)	17,23,26	2.10	3 (17%)
2	P8E	AH	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.92	3 (17%)
2	P8E	AE	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.32	4 (23%)
2	P8E	A4	609	-	15,16,17	1.08	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AN	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.21	4 (23%)
2	P8E	AG	601	-	15,16,17	1.06	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	AV	605	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	2 (11%)
2	P8E	AX	604	-	15,16,17	1.10	1 (6%)	17,23,26	2.31	4 (23%)
2	P8E	AH	604	-	15,16,17	1.11	1 (6%)	17,23,26	2.25	3 (17%)
2	P8E	AW	607	-	15,16,17	1.07	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AR	606	-	15,16,17	1.10	1 (6%)	17,23,26	1.93	3 (17%)
2	P8E	A7	606	-	15,16,17	1.08	1 (6%)	17,23,26	1.90	3 (17%)
2	P8E	AJ	603	-	15,16,17	1.07	1 (6%)	17,23,26	2.02	3 (17%)
2	P8E	AT	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.05	3 (17%)
2	P8E	A3	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.04	3 (17%)
2	P8E	AL	606	-	15,16,17	1.09	1 (6%)	17,23,26	1.91	3 (17%)
2	P8E	AR	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.12	3 (17%)
2	P8E	A8	605	-	15,16,17	1.11	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	AX	609	-	15,16,17	1.07	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	AP	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.23	4 (23%)
2	P8E	A1	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.20	4 (23%)
2	P8E	A7	608	-	15,16,17	1.08	1 (6%)	17,23,26	2.03	3 (17%)
2	P8E	AD	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.20	4 (23%)

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
2	P8E	AD	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AN	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AC	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AP	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AL	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AA	603	-	-	3/11/28/32	0/1/1/1
2	P8E	AK	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A7	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AD	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A6	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AE	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AI	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AT	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AQ	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AA	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AM	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AX	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AJ	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AW	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AN	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AL	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A9	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AU	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AD	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AW	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A2	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AA	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AF	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AO	606	-	-	2/11/28/32	0/1/1/1
2	P8E	A9	603	-	-	3/11/28/32	0/1/1/1
2	P8E	AS	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AL	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A2	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A8	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AE	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AT	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A5	606	-	-	2/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AT	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AG	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A6	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A6	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A9	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AE	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AJ	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A8	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AM	606	-	-	2/11/28/32	0/1/1/1
2	P8E	A1	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AT	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AI	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A4	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AU	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A6	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AD	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AO	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A3	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AJ	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A6	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A1	608	-	-	2/11/28/32	0/1/1/1
2	P8E	A5	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AE	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AS	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AB	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AO	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AH	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AE	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AQ	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A9	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AM	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A4	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AF	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A5	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A4	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AN	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AG	609	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AW	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A5	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AF	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AC	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AS	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AV	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AC	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AB	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AU	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A5	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AB	607	-	-	6/11/28/32	0/1/1/1
2	P8E	A7	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A8	606	-	-	2/11/28/32	0/1/1/1
2	P8E	A4	603	-	-	3/11/28/32	0/1/1/1
2	P8E	AE	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AU	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AG	606	-	-	2/11/28/32	0/1/1/1
2	P8E	A3	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A4	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AS	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A7	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AQ	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A7	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A2	607	-	-	6/11/28/32	0/1/1/1
2	P8E	A3	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A8	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AH	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AC	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AA	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AP	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AQ	603	-	-	3/11/28/32	0/1/1/1
2	P8E	AR	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A4	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A6	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AA	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A6	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AH	602	-	-	0/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AJ	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AW	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AG	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AC	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AP	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AR	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AK	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A1	603	-	-	3/11/28/32	0/1/1/1
2	P8E	A3	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AN	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AB	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A2	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AT	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AC	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AB	603	-	-	3/11/28/32	0/1/1/1
2	P8E	AK	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AB	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AF	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AU	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AL	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AV	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A2	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A2	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AW	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AX	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AH	608	-	-	0/11/28/32	0/1/1/1
2	P8E	AX	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AM	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AC	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A1	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AK	603	-	-	2/11/28/32	0/1/1/1
2	P8E	A9	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AG	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AG	608	-	-	0/11/28/32	0/1/1/1
2	P8E	A2	603	-	-	2/11/28/32	0/1/1/1
2	P8E	A5	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AK	606	-	-	2/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AH	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AQ	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AT	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A9	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A4	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AM	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AJ	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AV	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AI	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AP	606	-	-	2/11/28/32	0/1/1/1
2	P8E	A7	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AU	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AQ	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AD	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A1	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AP	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AX	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A3	608	-	-	0/11/28/32	0/1/1/1
2	P8E	AP	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A5	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A7	608	-	-	0/11/28/32	0/1/1/1
2	P8E	AT	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AP	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AM	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AQ	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AA	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A1	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	A1	605	-	-	3/11/28/32	0/1/1/1
2	P8E	A3	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A2	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A5	603	-	-	3/11/28/32	0/1/1/1
2	P8E	A8	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AB	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AV	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AW	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AD	606	-	-	2/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AI	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AA	609	-	-	3/11/28/32	0/1/1/1
2	P8E	A1	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AB	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AB	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AS	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AG	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AK	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A9	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AL	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AC	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AJ	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AS	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AM	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AO	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AR	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A7	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AO	603	-	-	3/11/28/32	0/1/1/1
2	P8E	AV	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A9	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	A5	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AF	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AK	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AO	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AG	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AN	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A9	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AS	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AR	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AT	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AU	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AX	608	-	-	0/11/28/32	0/1/1/1
2	P8E	AH	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AV	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AN	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AA	604	-	1/1/7/7	9/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AR	603	-	-	2/11/28/32	0/1/1/1
2	P8E	A3	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AS	603	-	-	2/11/28/32	0/1/1/1
2	P8E	A4	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A2	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AR	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AI	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AK	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AN	603	-	-	3/11/28/32	0/1/1/1
2	P8E	AJ	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AL	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AR	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AV	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AF	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AQ	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AO	607	-	-	6/11/28/32	0/1/1/1
2	P8E	A8	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AA	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AF	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AI	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AL	603	-	-	2/11/28/32	0/1/1/1
2	P8E	A3	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AK	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AS	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AQ	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AE	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AX	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A8	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AF	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AJ	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AM	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A8	607	-	-	6/11/28/32	0/1/1/1
2	P8E	A7	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AM	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AO	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AU	605	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AW	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AC	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AU	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AE	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AF	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AI	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AI	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AO	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AD	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A6	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AI	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AN	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AP	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AW	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AX	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AD	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AH	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AL	608	-	-	1/11/28/32	0/1/1/1
2	P8E	AV	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AH	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AE	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	A4	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AN	602	-	-	0/11/28/32	0/1/1/1
2	P8E	AG	601	-	-	0/11/28/32	0/1/1/1
2	P8E	AX	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AV	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AH	604	-	1/1/7/7	9/11/28/32	0/1/1/1
2	P8E	AW	607	-	-	6/11/28/32	0/1/1/1
2	P8E	AR	606	-	-	2/11/28/32	0/1/1/1
2	P8E	A7	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AJ	603	-	-	2/11/28/32	0/1/1/1
2	P8E	AT	608	-	-	1/11/28/32	0/1/1/1
2	P8E	A3	605	-	-	3/11/28/32	0/1/1/1
2	P8E	AL	606	-	-	2/11/28/32	0/1/1/1
2	P8E	AR	607	-	-	6/11/28/32	0/1/1/1
2	P8E	A8	605	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	AX	609	-	-	3/11/28/32	0/1/1/1
2	P8E	AP	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A1	602	-	-	0/11/28/32	0/1/1/1
2	P8E	A6	604	-	1/1/7/7	8/11/28/32	0/1/1/1
2	P8E	AD	602	-	-	0/11/28/32	0/1/1/1

The worst 5 of 297 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AV	604	P8E	O6-C6	-2.59	1.40	1.44
2	AK	605	P8E	O6-C6	-2.48	1.40	1.44
2	AF	605	P8E	O6-C6	-2.48	1.40	1.44
2	AR	605	P8E	O6-C6	-2.47	1.40	1.44
2	AI	605	P8E	O6-C6	-2.47	1.40	1.44

The worst 5 of 914 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AE	604	P8E	O6-C2-C1	8.22	123.23	107.72
2	A3	604	P8E	O6-C2-C1	8.22	123.23	107.72
2	AJ	604	P8E	O6-C2-C1	8.21	123.22	107.72
2	AC	604	P8E	O6-C2-C1	8.20	123.21	107.72
2	AU	604	P8E	O6-C2-C1	8.20	123.21	107.72

5 of 33 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A1	604	P8E	C2
2	A2	604	P8E	C2
2	A3	604	P8E	C2
2	A4	604	P8E	C2
2	A5	604	P8E	C2

5 of 853 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A1	604	P8E	N7-C7-C8-C9
2	A1	604	P8E	C6-C7-C8-O8
2	A1	604	P8E	O6-C6-C7-N7
2	A1	604	P8E	O1A-C1-C2-C3
2	A1	604	P8E	O1B-C1-C2-C3

There are no ring outliers.

80 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AN	608	P8E	1	0
2	AL	602	P8E	1	0
2	A7	609	P8E	1	0
2	AE	609	P8E	1	0
2	AX	606	P8E	2	0
2	AN	609	P8E	1	0
2	A2	609	P8E	1	0
2	AT	602	P8E	1	0
2	A5	606	P8E	1	0
2	A8	602	P8E	1	0
2	AM	606	P8E	2	0
2	A1	606	P8E	2	0
2	AO	602	P8E	1	0
2	A5	602	P8E	1	0
2	AB	609	P8E	1	0
2	AM	609	P8E	1	0
2	A5	609	P8E	1	0
2	AG	609	P8E	1	0
2	AW	609	P8E	1	0
2	AC	609	P8E	1	0
2	AU	608	P8E	1	0
2	A7	602	P8E	1	0
2	A8	606	P8E	1	0
2	AE	602	P8E	1	0
2	AU	602	P8E	1	0
2	A4	606	P8E	2	0
2	AS	609	P8E	1	0
2	A3	609	P8E	1	0
2	AP	609	P8E	1	0
2	AR	602	P8E	1	0
2	A6	606	P8E	2	0
2	AH	602	P8E	1	0
2	AJ	602	P8E	1	0
2	AW	606	P8E	2	0
2	AC	602	P8E	1	0
2	A3	606	P8E	2	0
2	AL	609	P8E	1	0
2	AV	609	P8E	1	0
2	AG	602	P8E	1	0
2	AQ	606	P8E	2	0

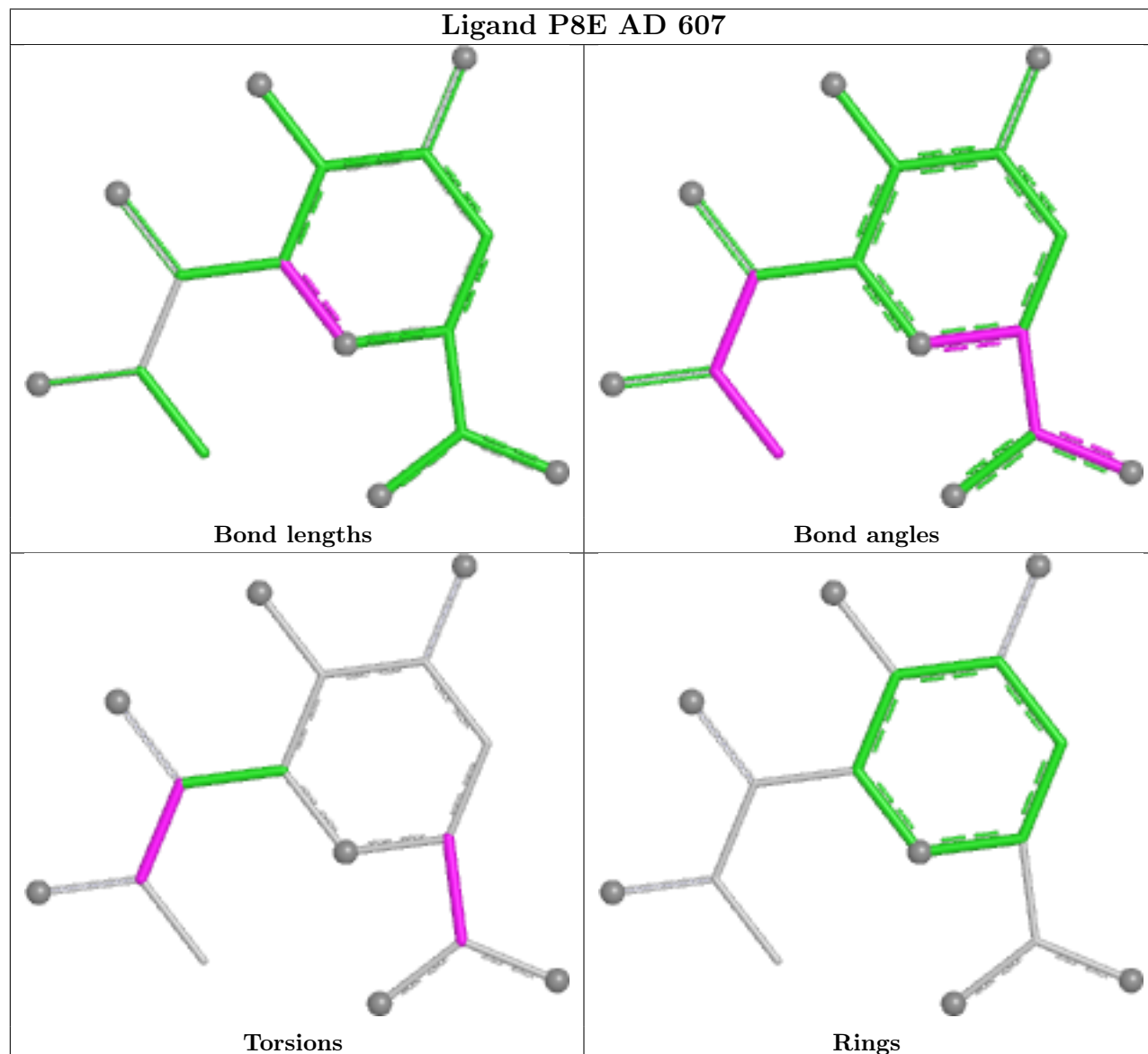
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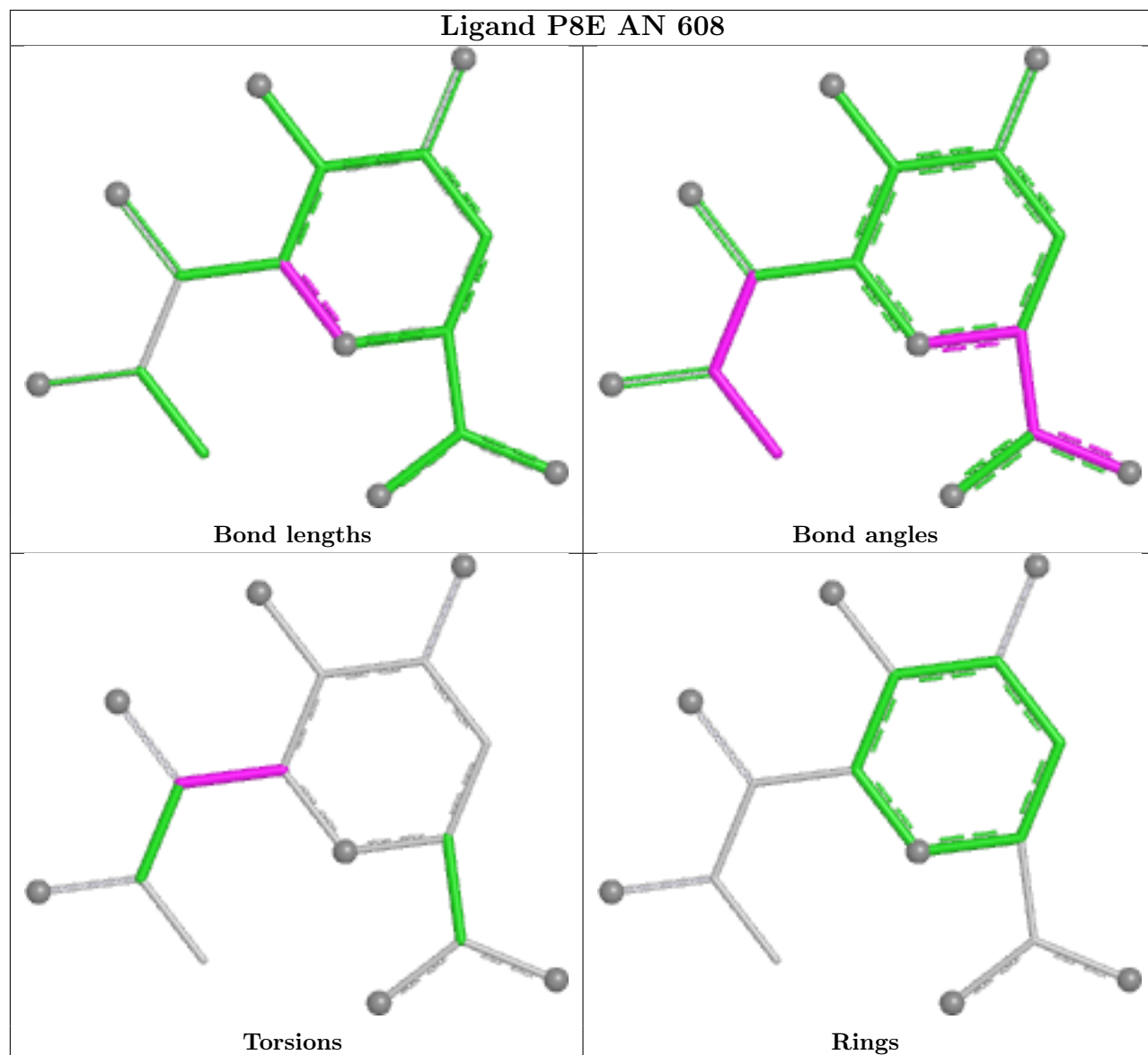
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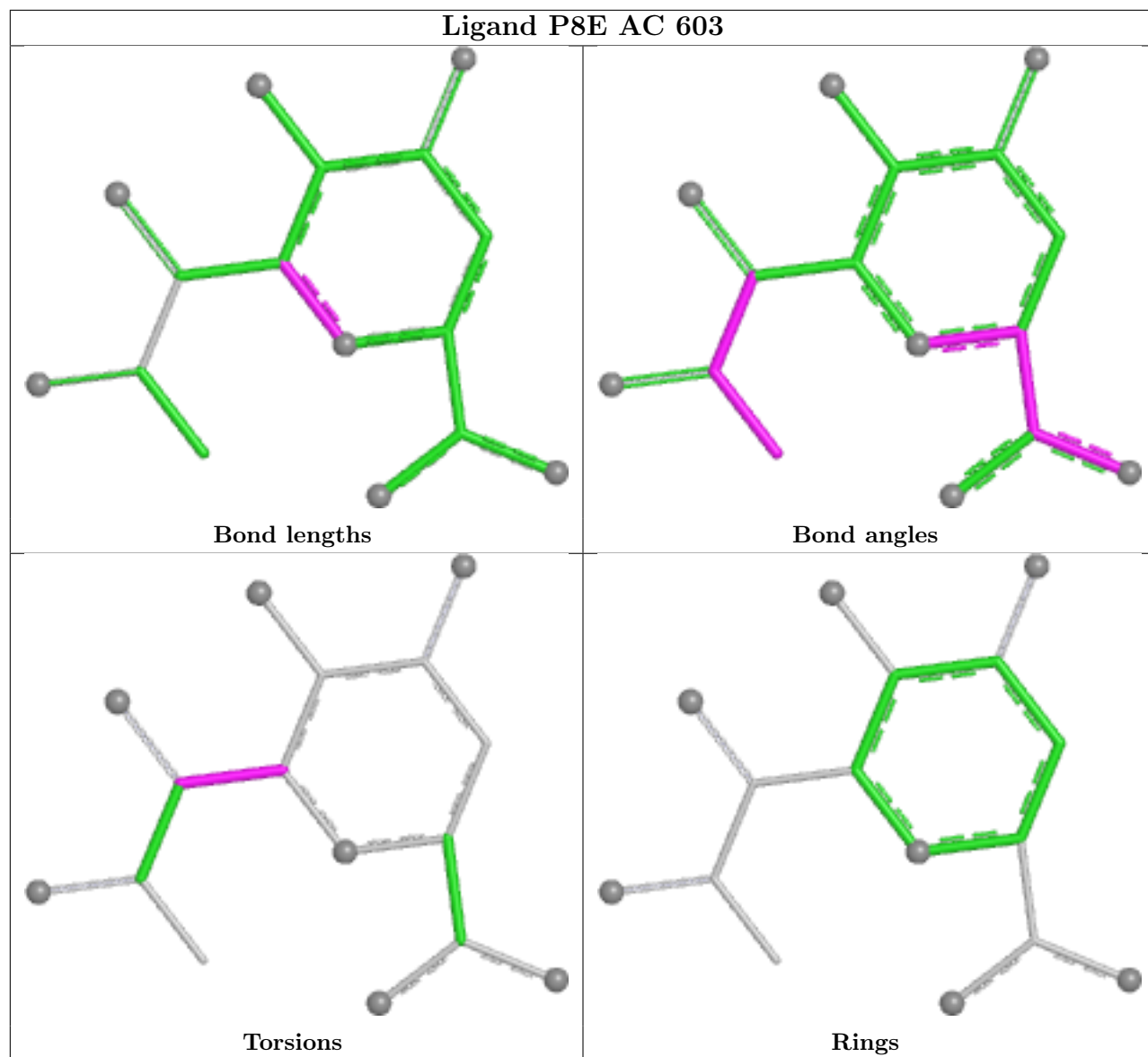
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AT	609	P8E	1	0
2	A9	609	P8E	1	0
2	A4	602	P8E	1	0
2	AJ	609	P8E	1	0
2	AV	606	P8E	2	0
2	AI	609	P8E	1	0
2	AP	606	P8E	1	0
2	AU	609	P8E	1	0
2	AD	609	P8E	1	0
2	AQ	609	P8E	1	0
2	A3	602	P8E	1	0
2	AB	606	P8E	2	0
2	AD	606	P8E	2	0
2	AA	609	P8E	1	0
2	A1	609	P8E	1	0
2	A9	606	P8E	2	0
2	AC	606	P8E	2	0
2	AJ	606	P8E	2	0
2	AK	609	P8E	1	0
2	AO	609	P8E	1	0
2	AH	609	P8E	1	0
2	A2	606	P8E	2	0
2	AR	609	P8E	1	0
2	AI	602	P8E	1	0
2	AF	606	P8E	1	0
2	AA	606	P8E	2	0
2	AK	602	P8E	1	0
2	AS	602	P8E	1	0
2	AE	606	P8E	2	0
2	AX	602	P8E	1	0
2	A8	609	P8E	1	0
2	AF	609	P8E	1	0
2	A6	609	P8E	1	0
2	A4	609	P8E	1	0
2	AN	602	P8E	1	0
2	A7	606	P8E	2	0
2	AL	606	P8E	2	0
2	AX	609	P8E	1	0
2	AP	602	P8E	1	0
2	AD	602	P8E	1	0

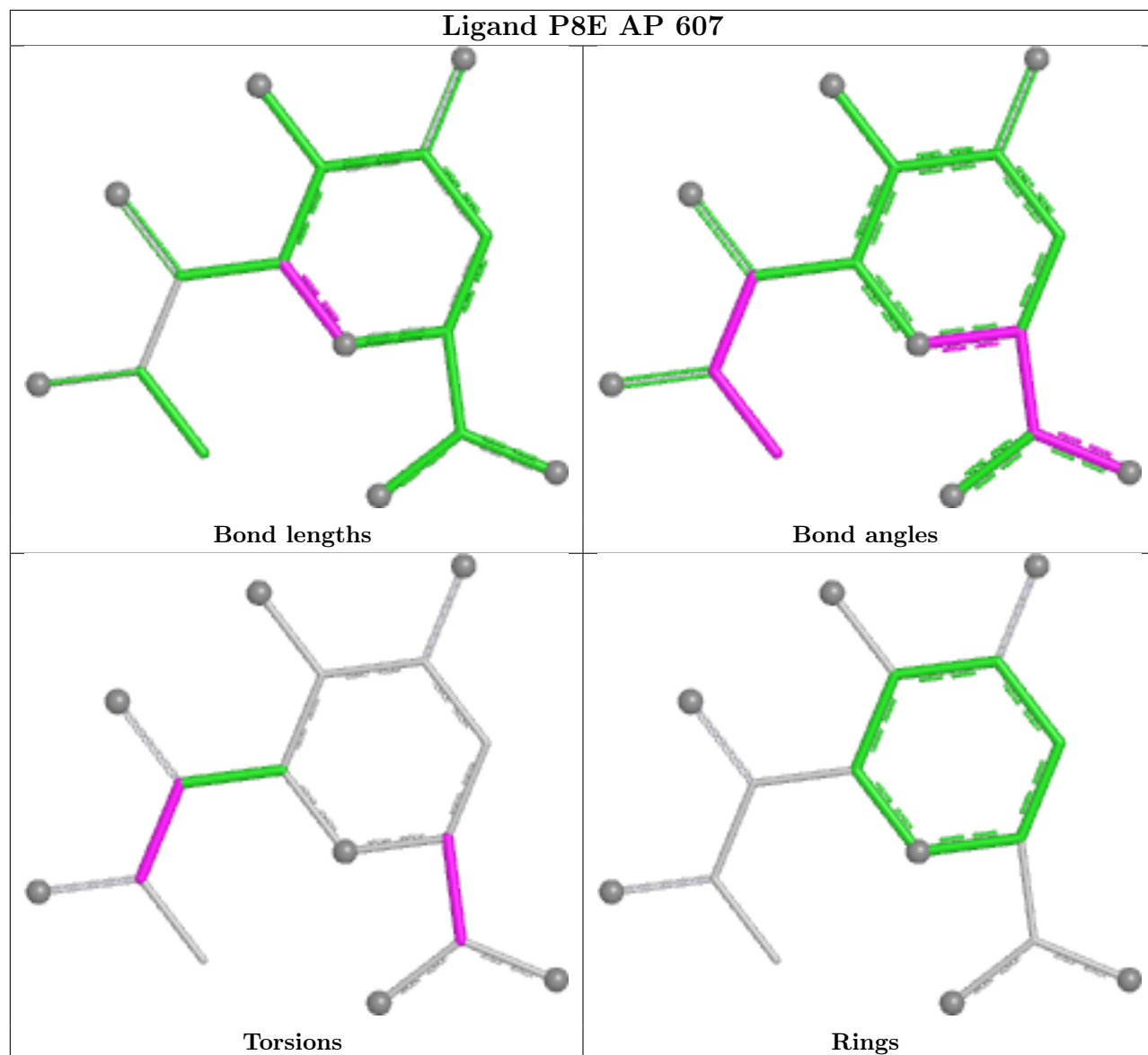
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

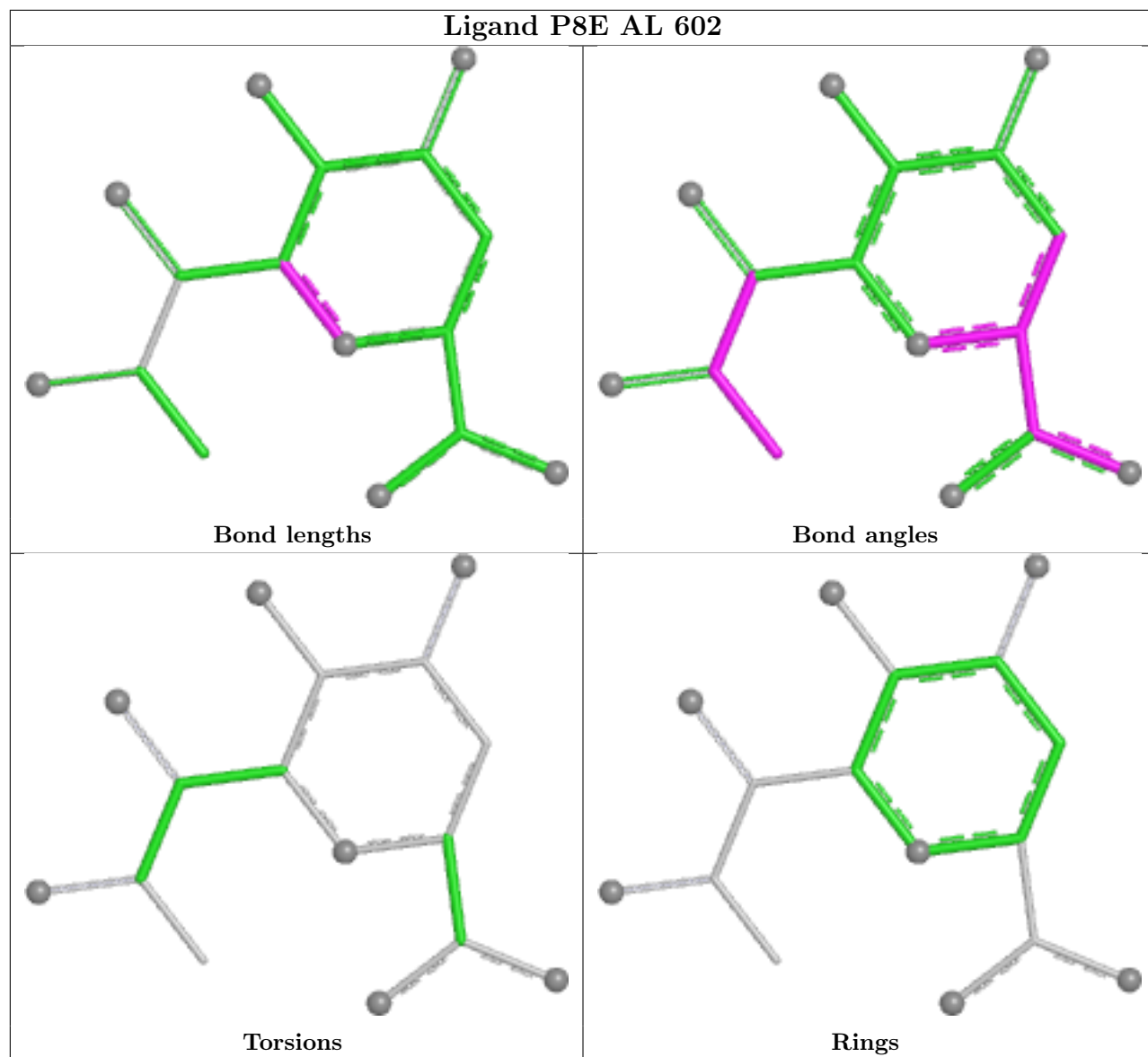
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

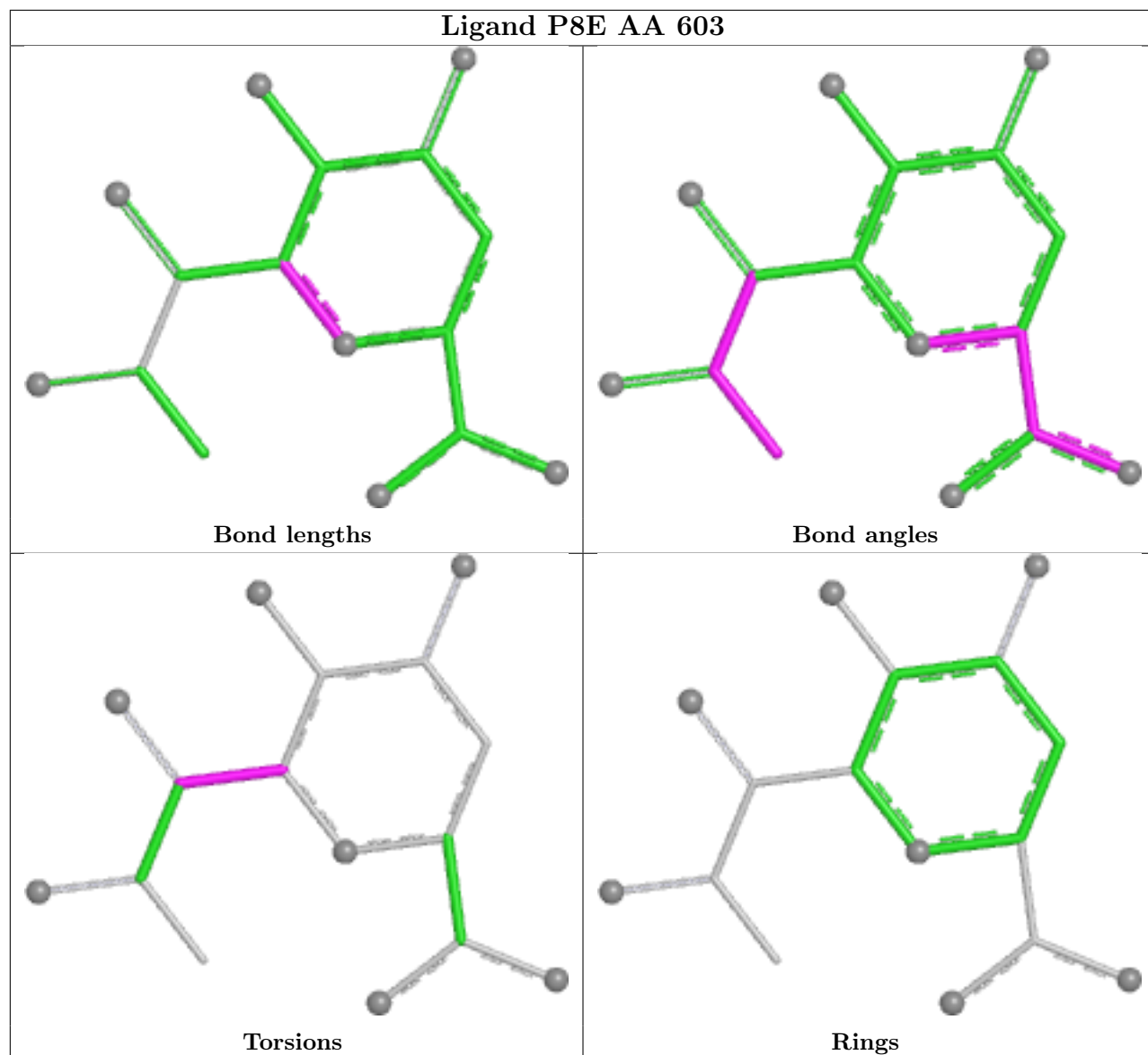


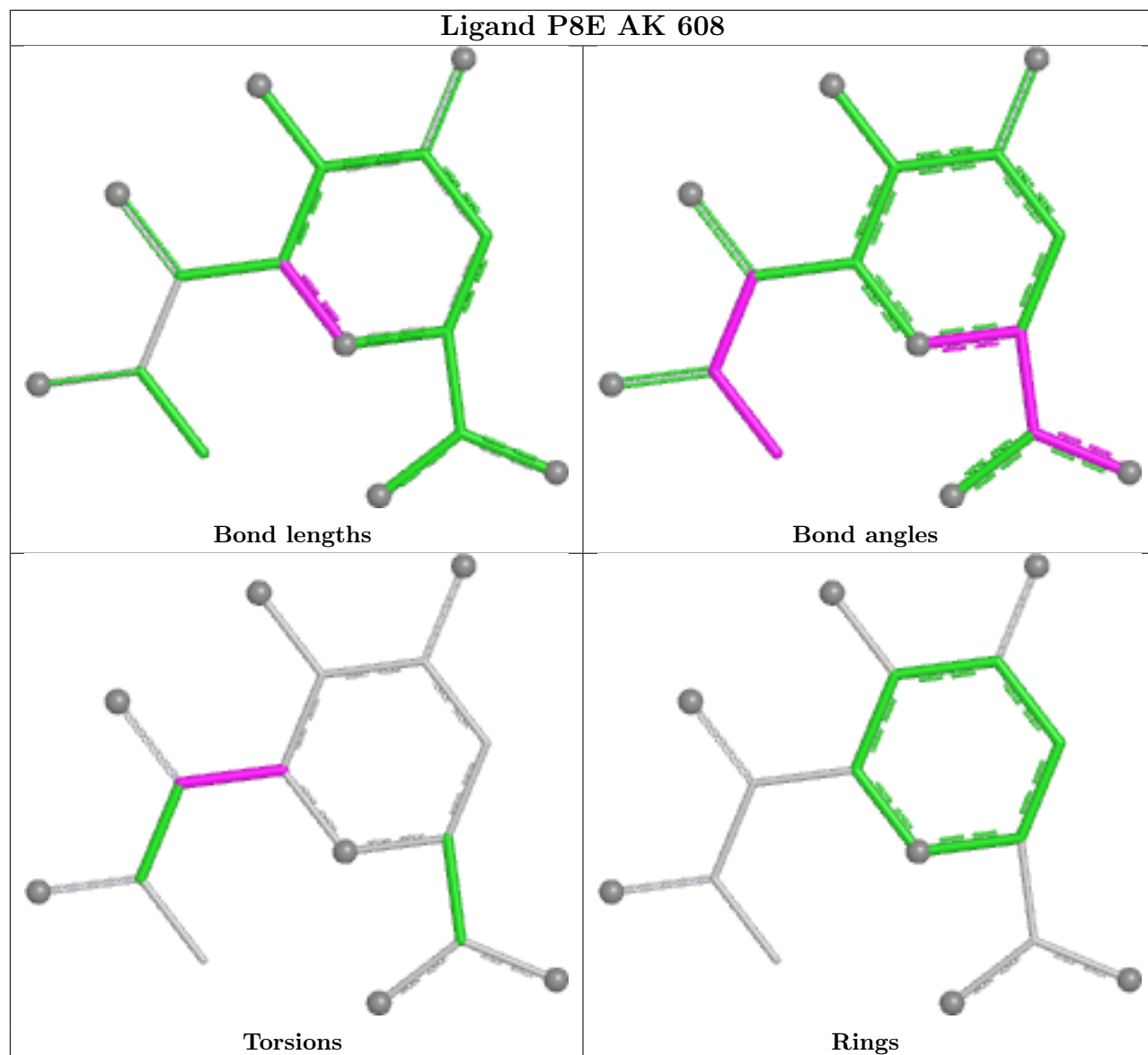


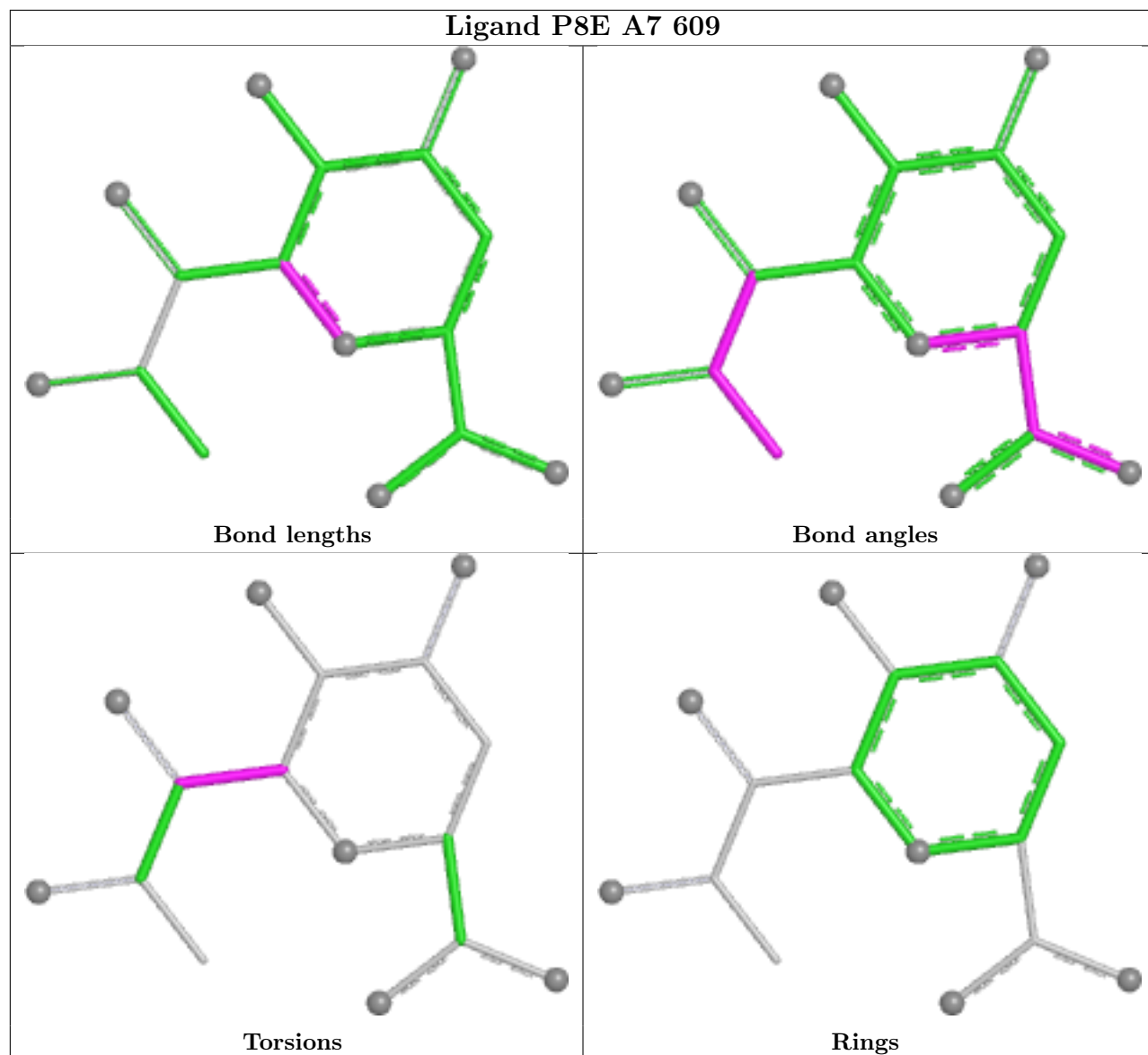


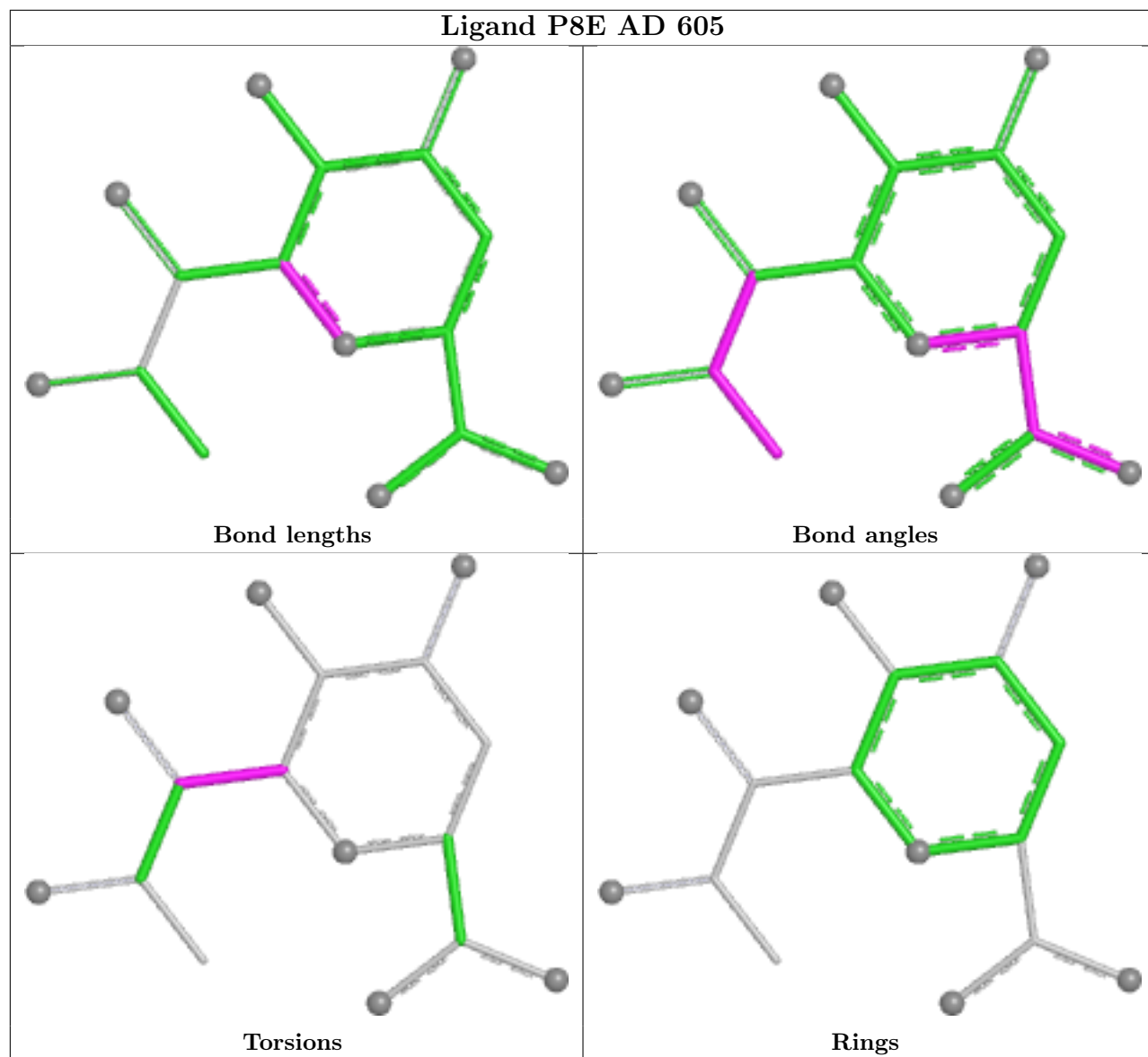


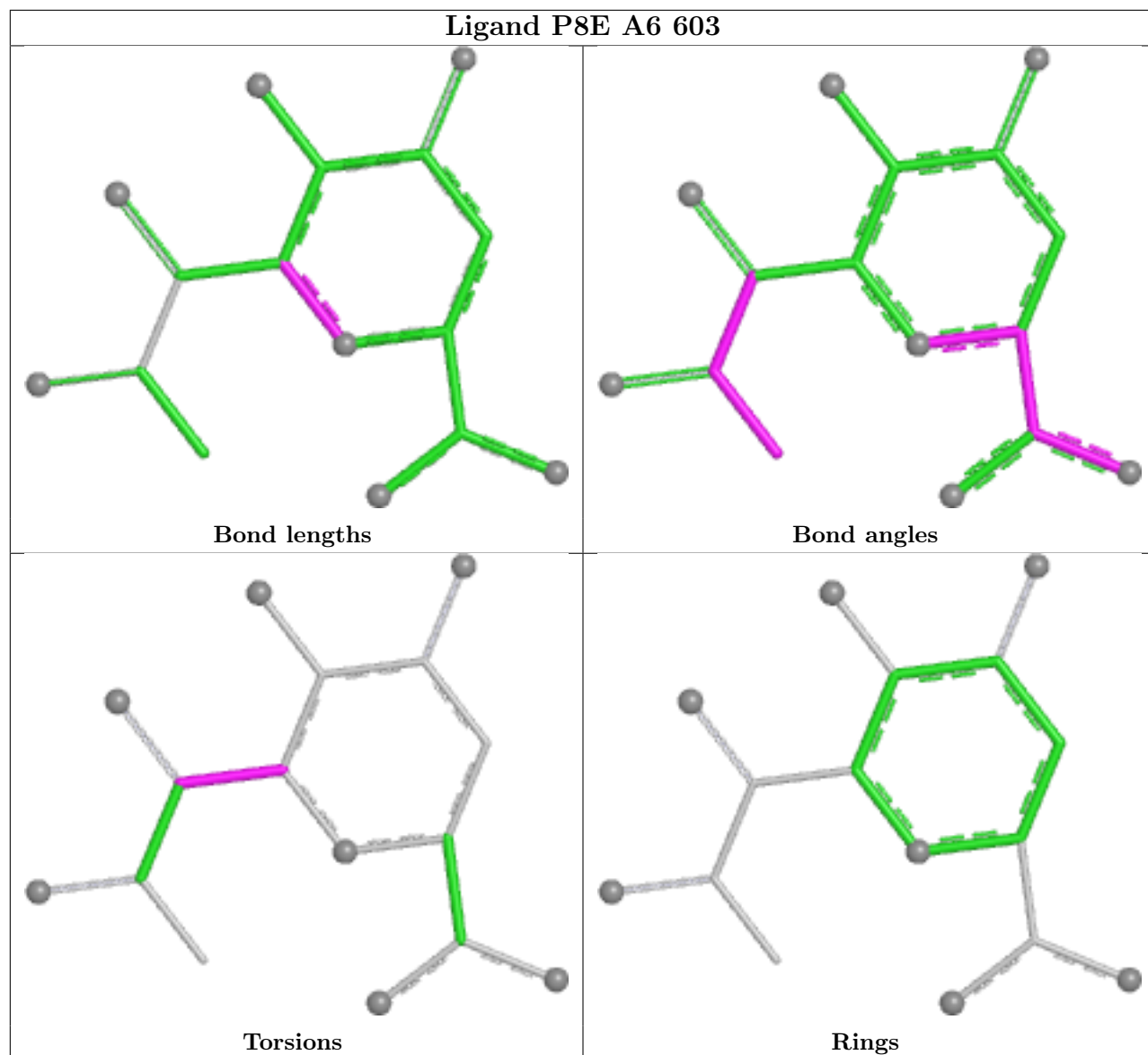


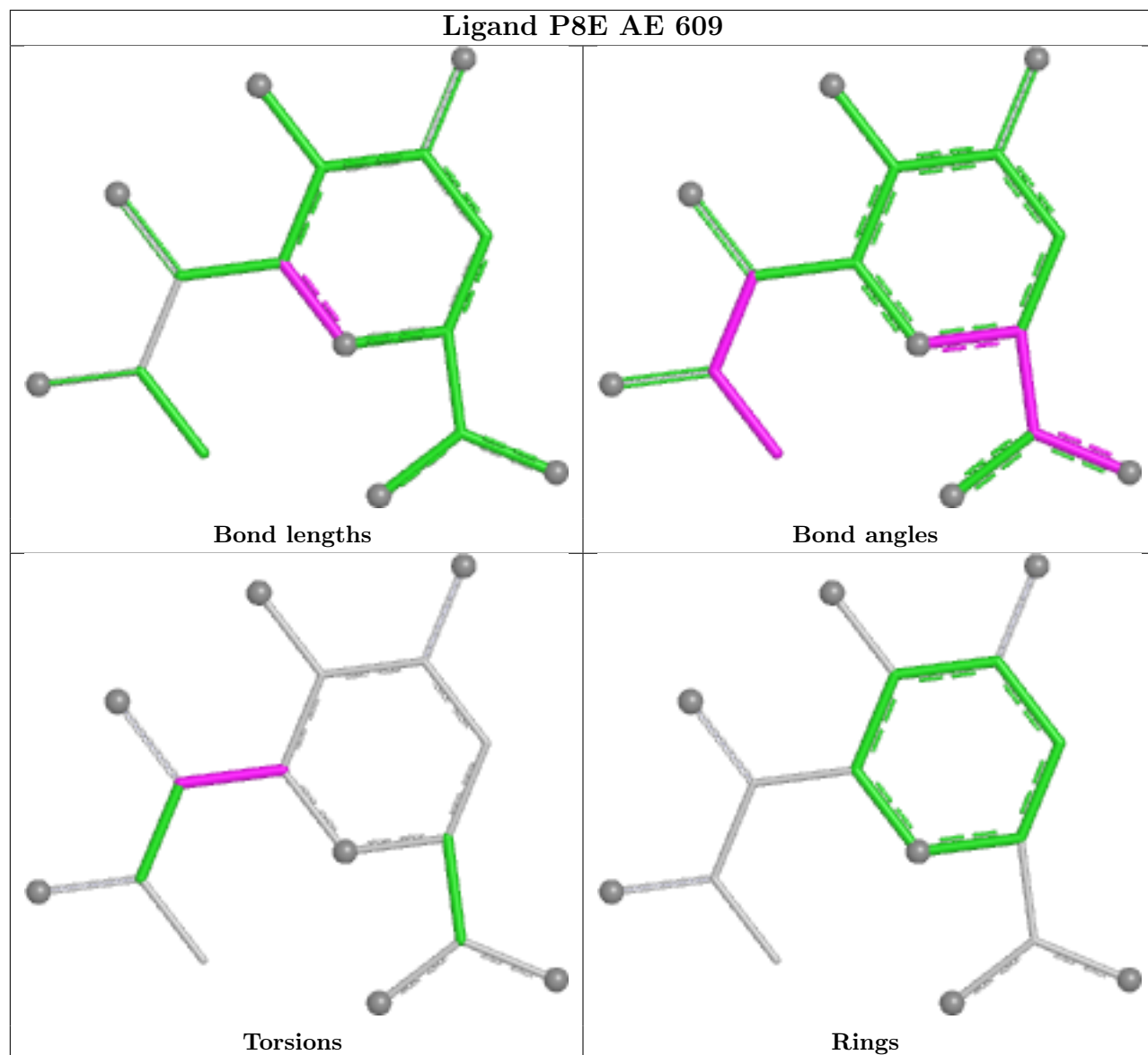


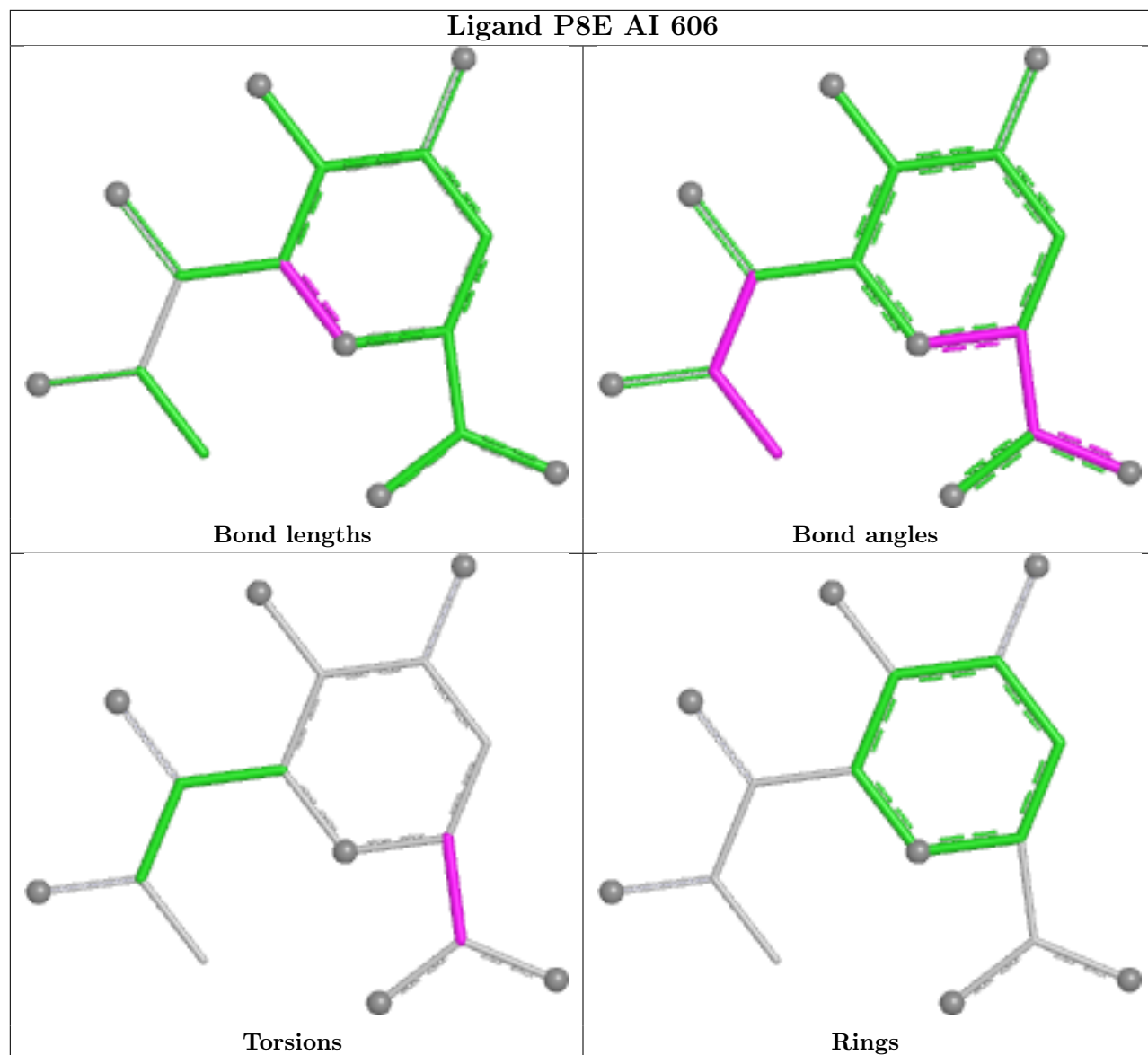


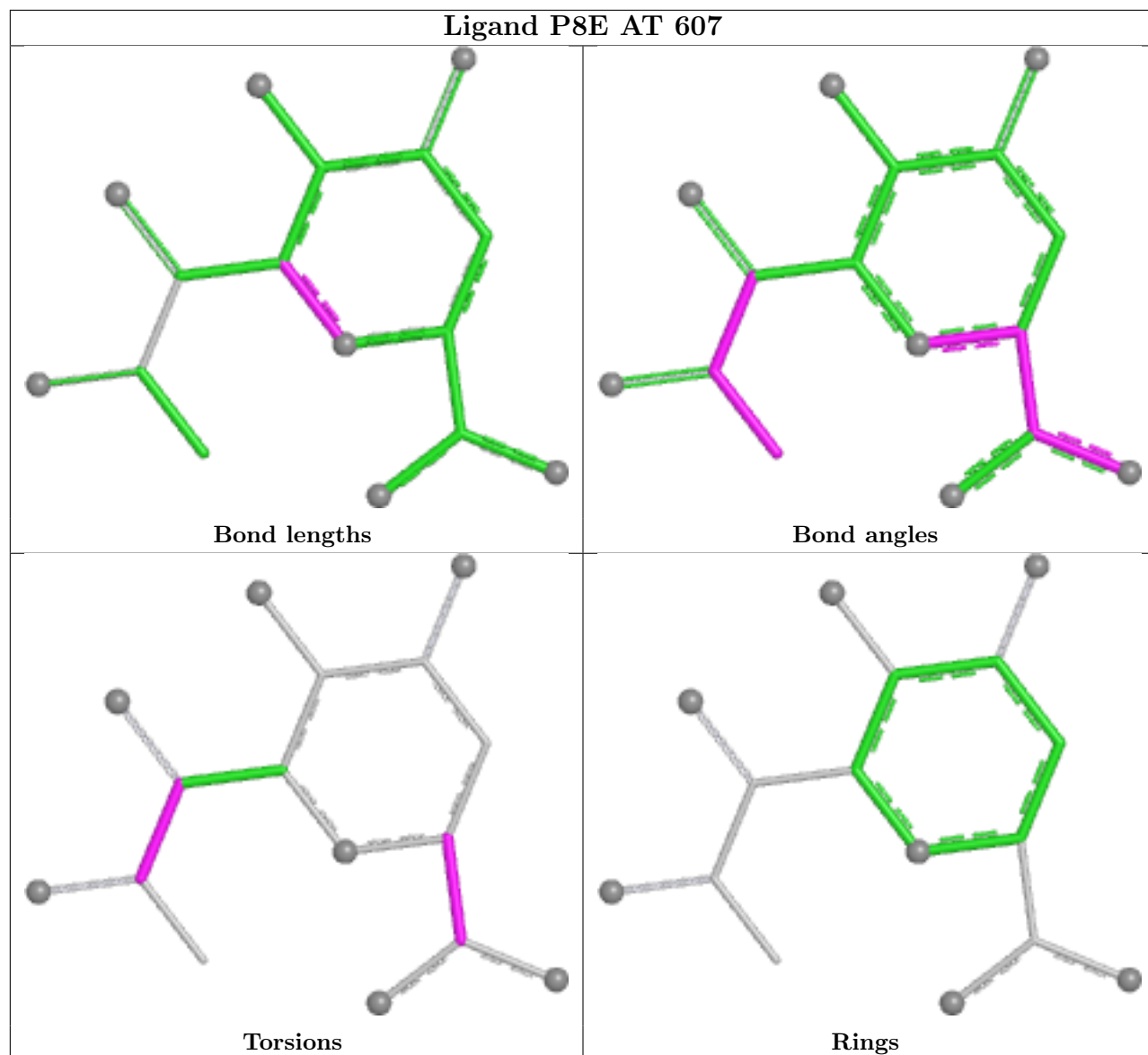


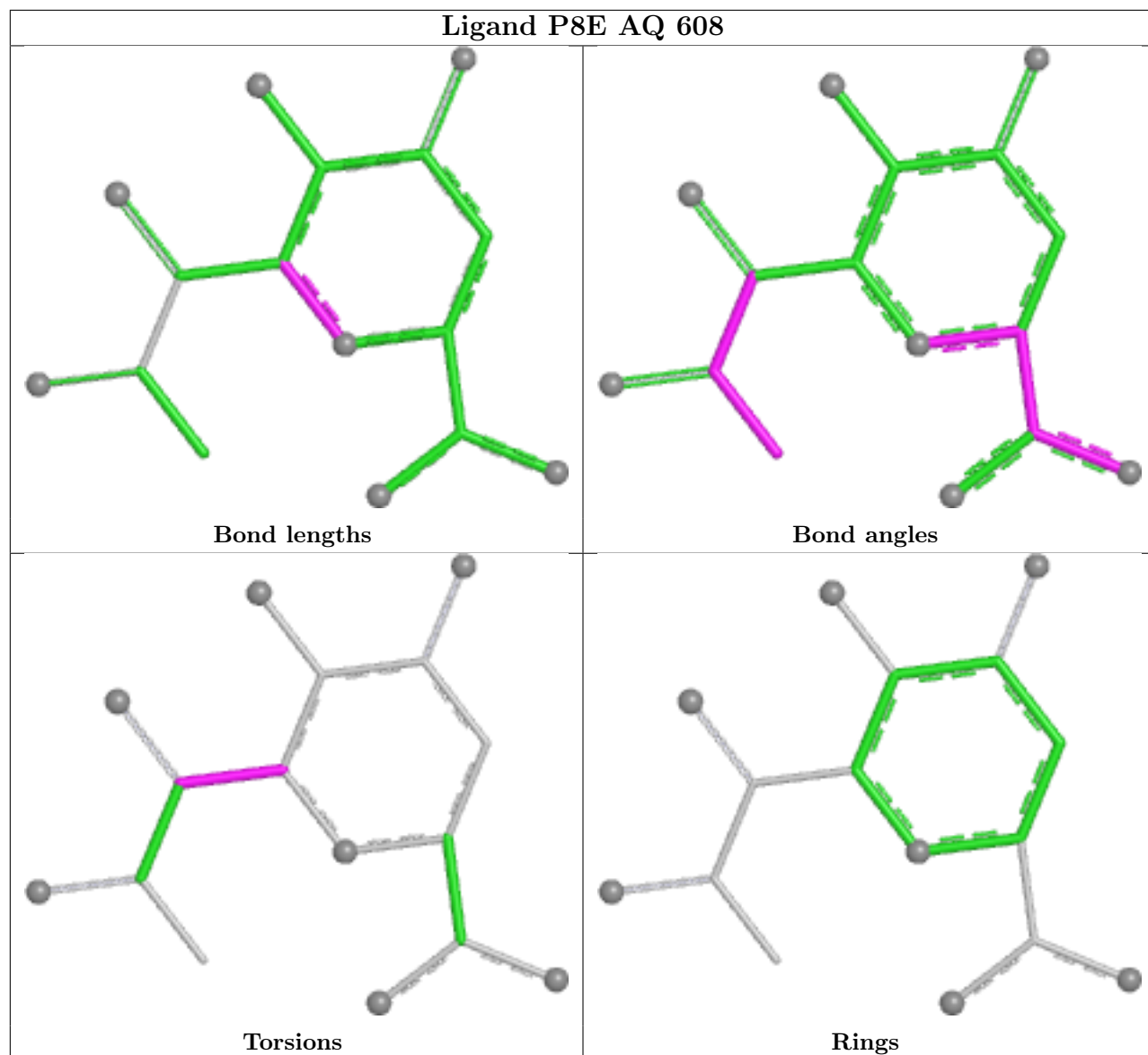


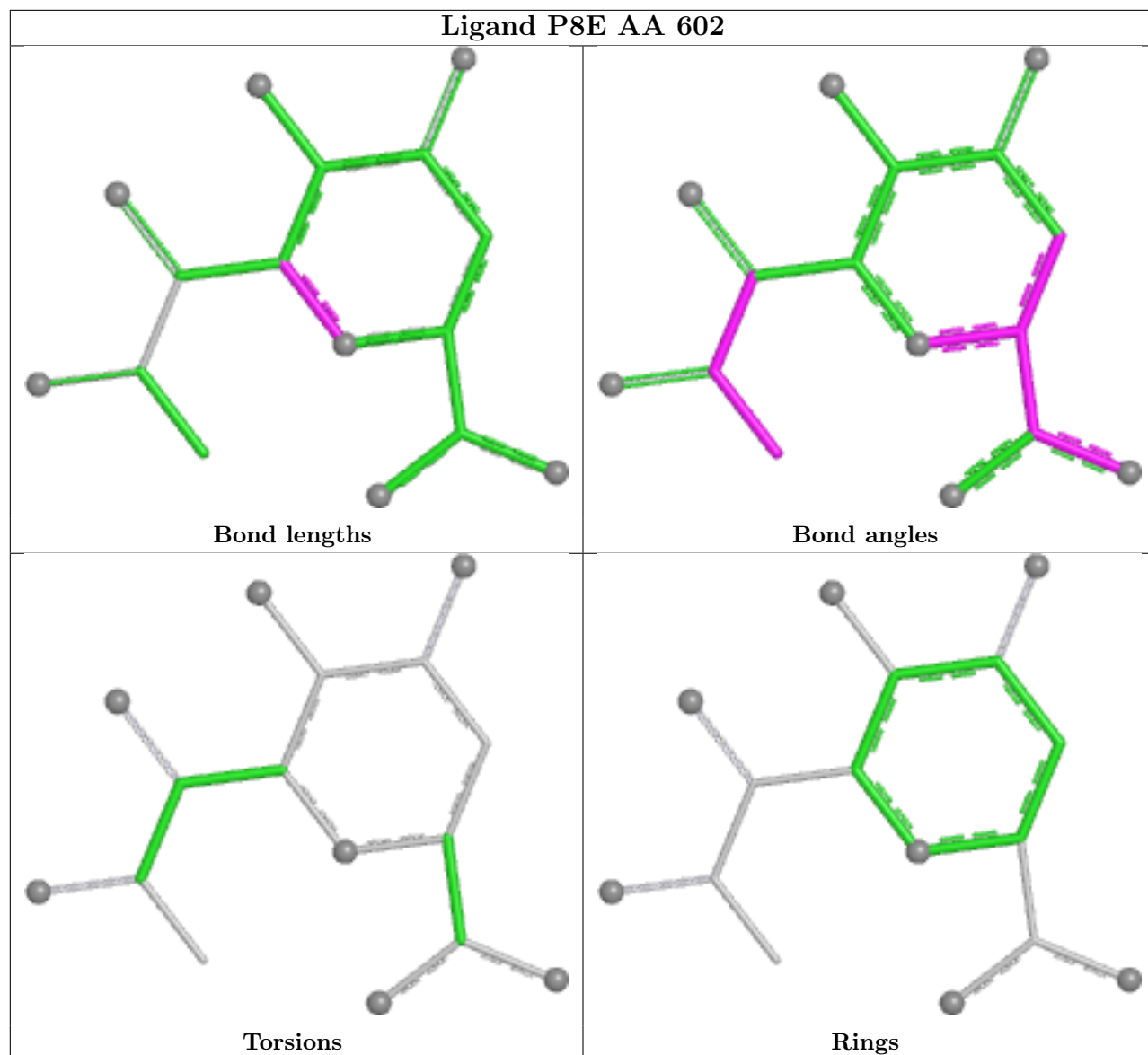


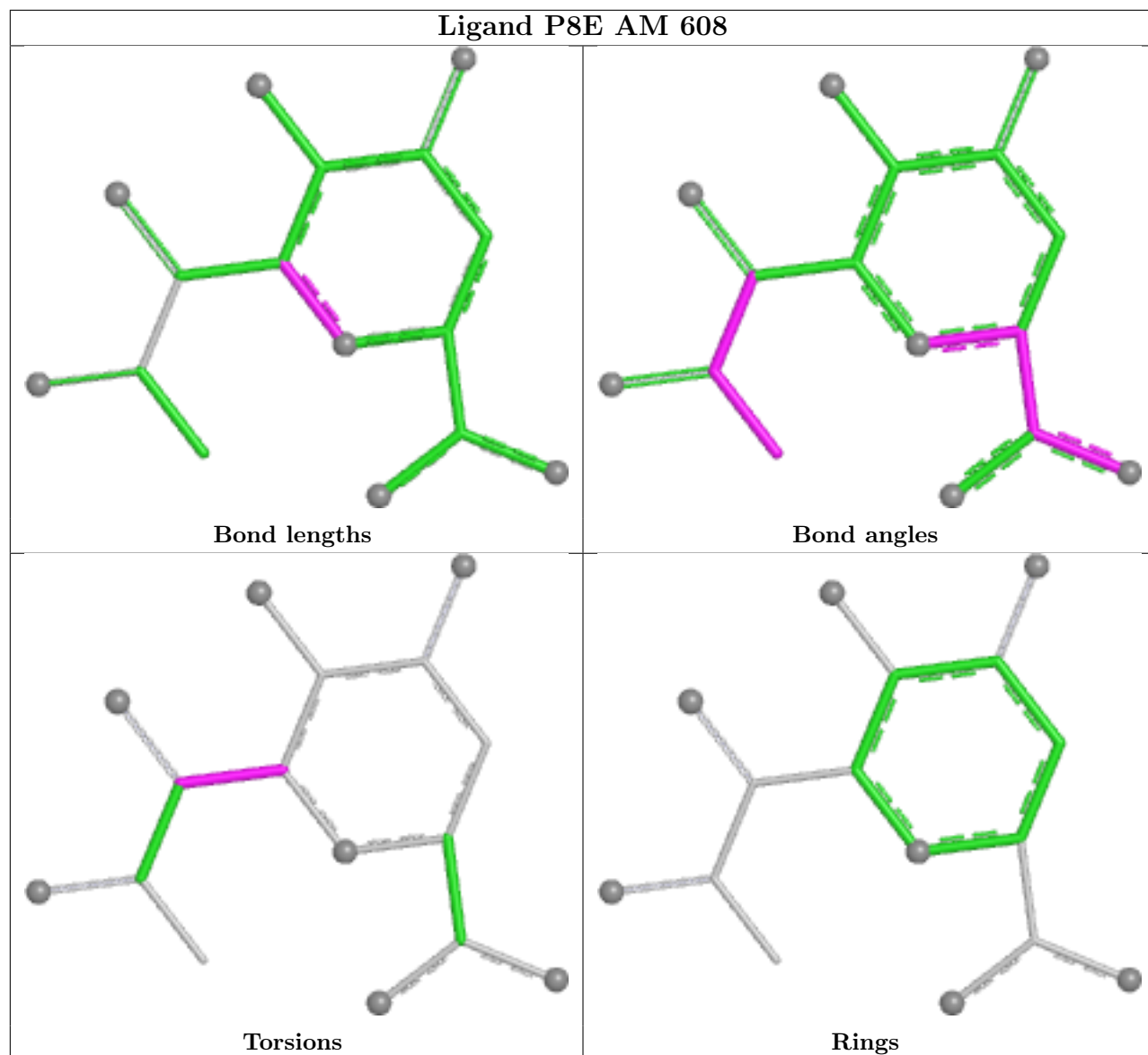


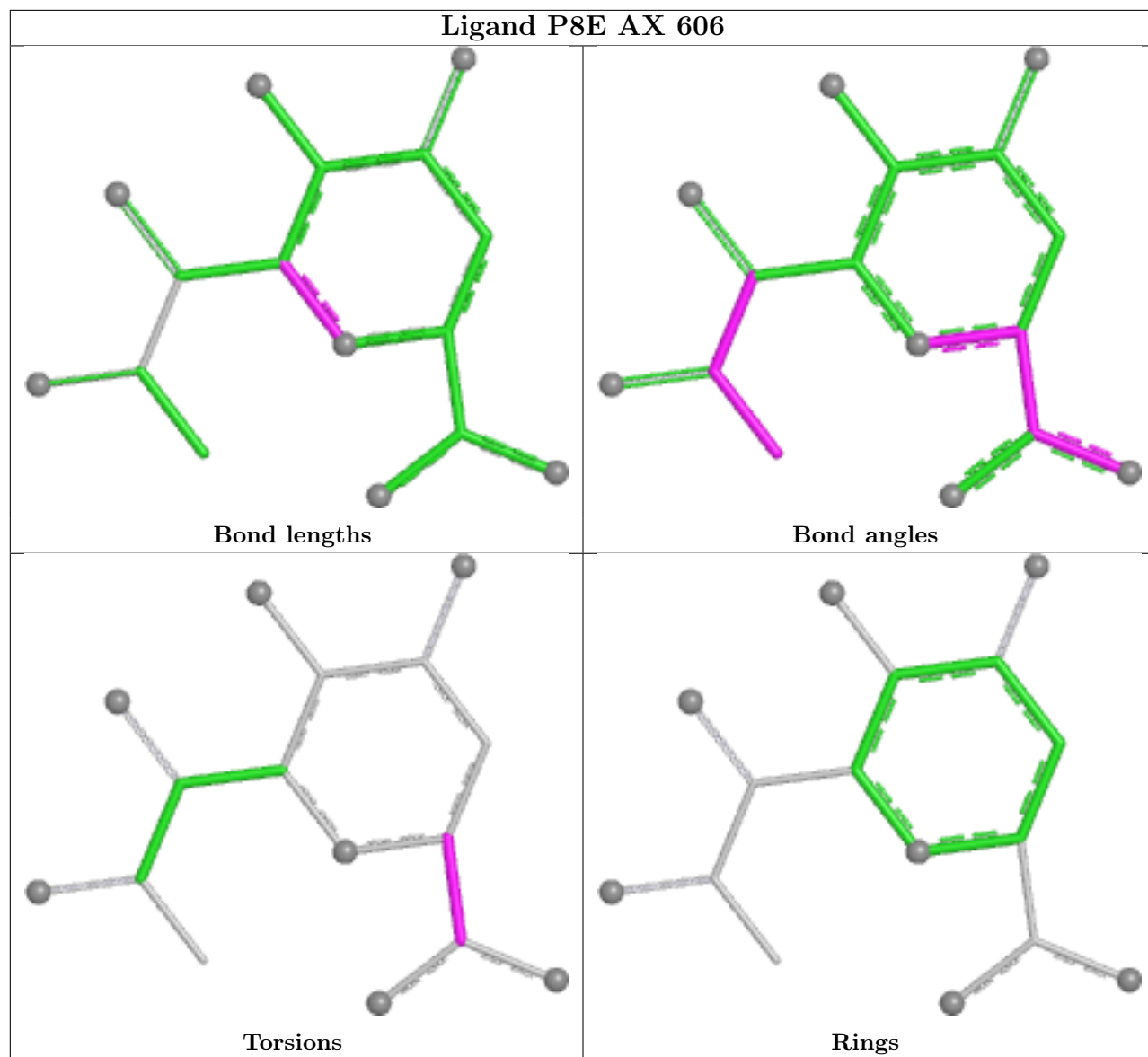


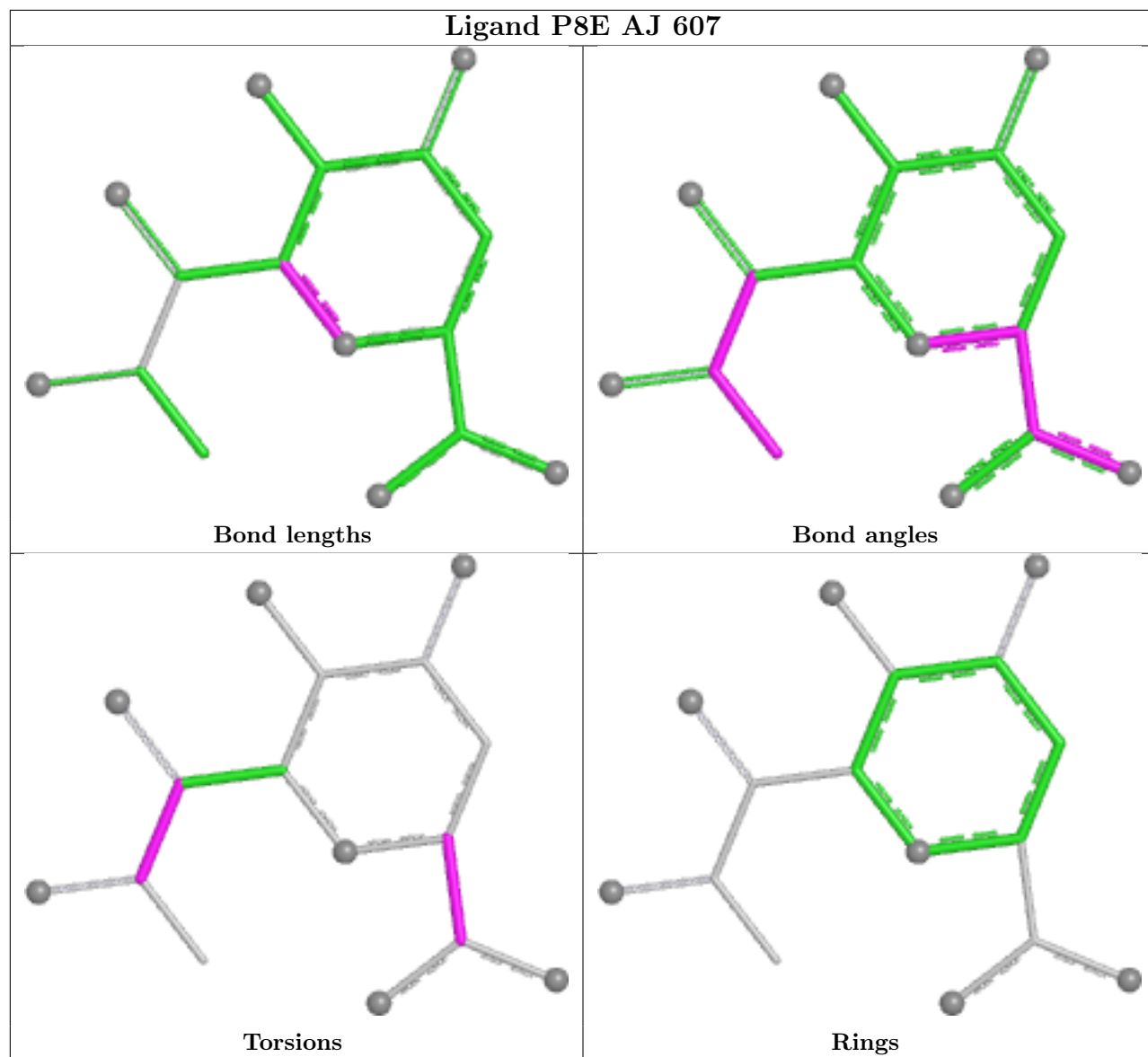


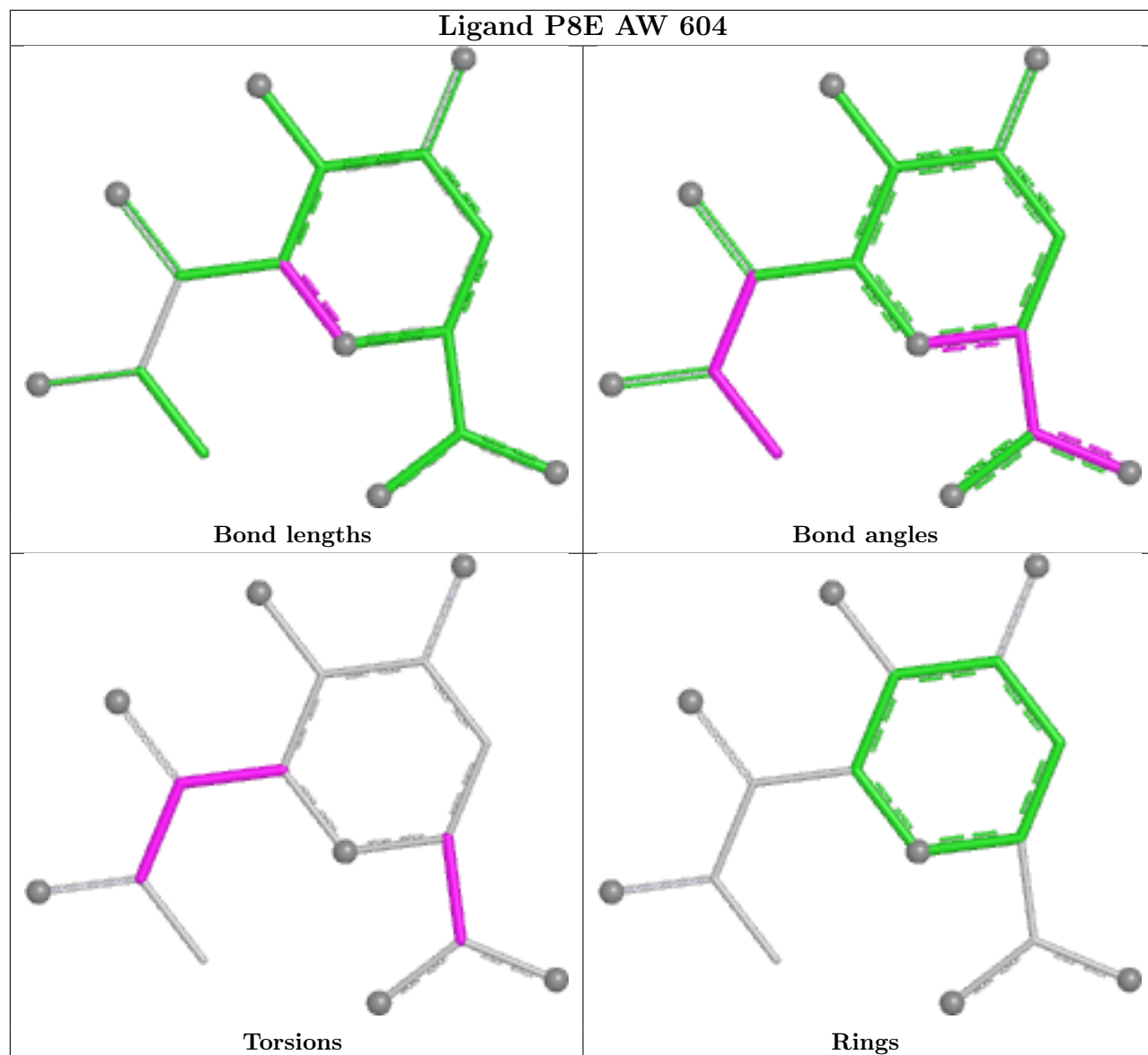


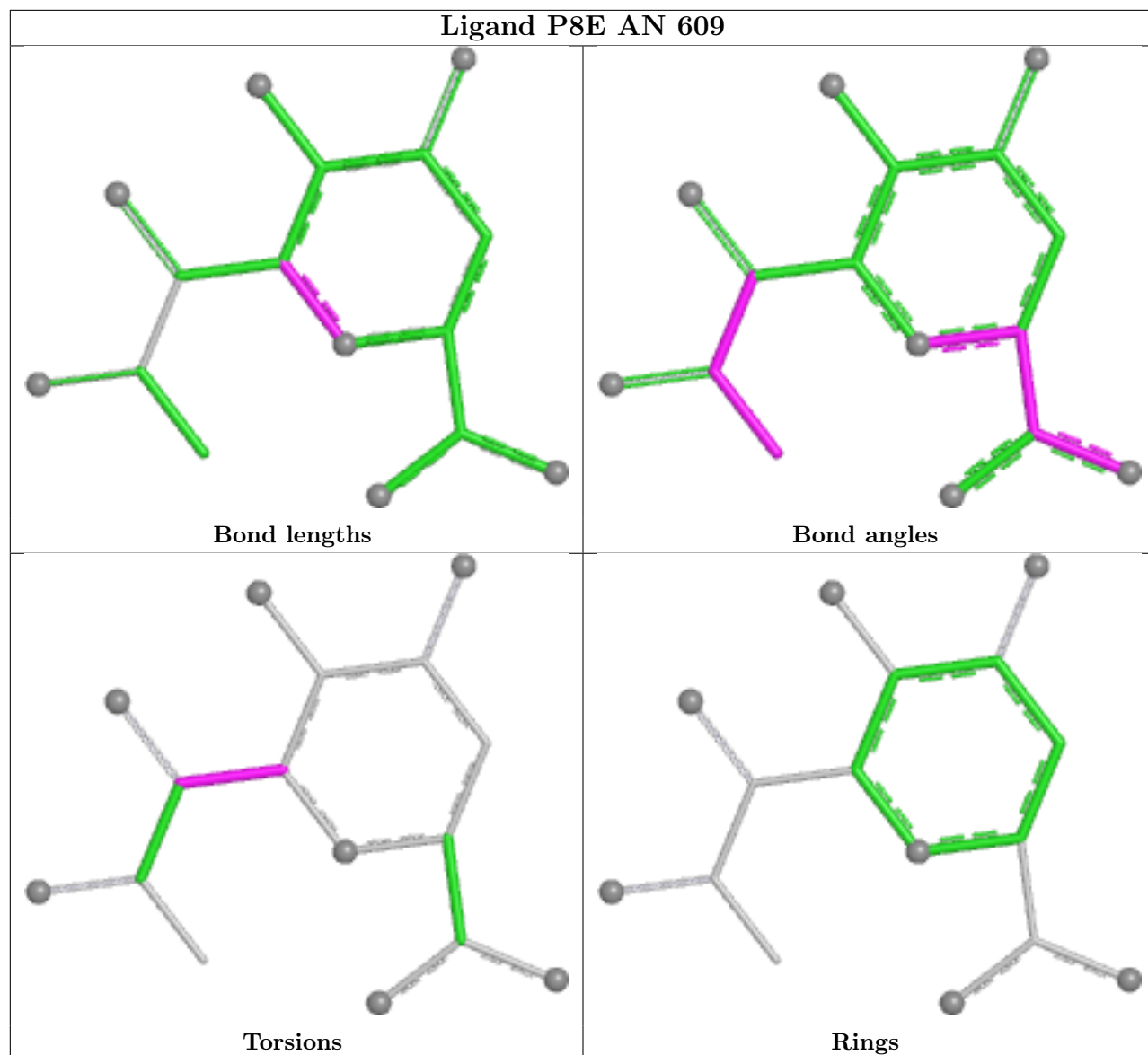


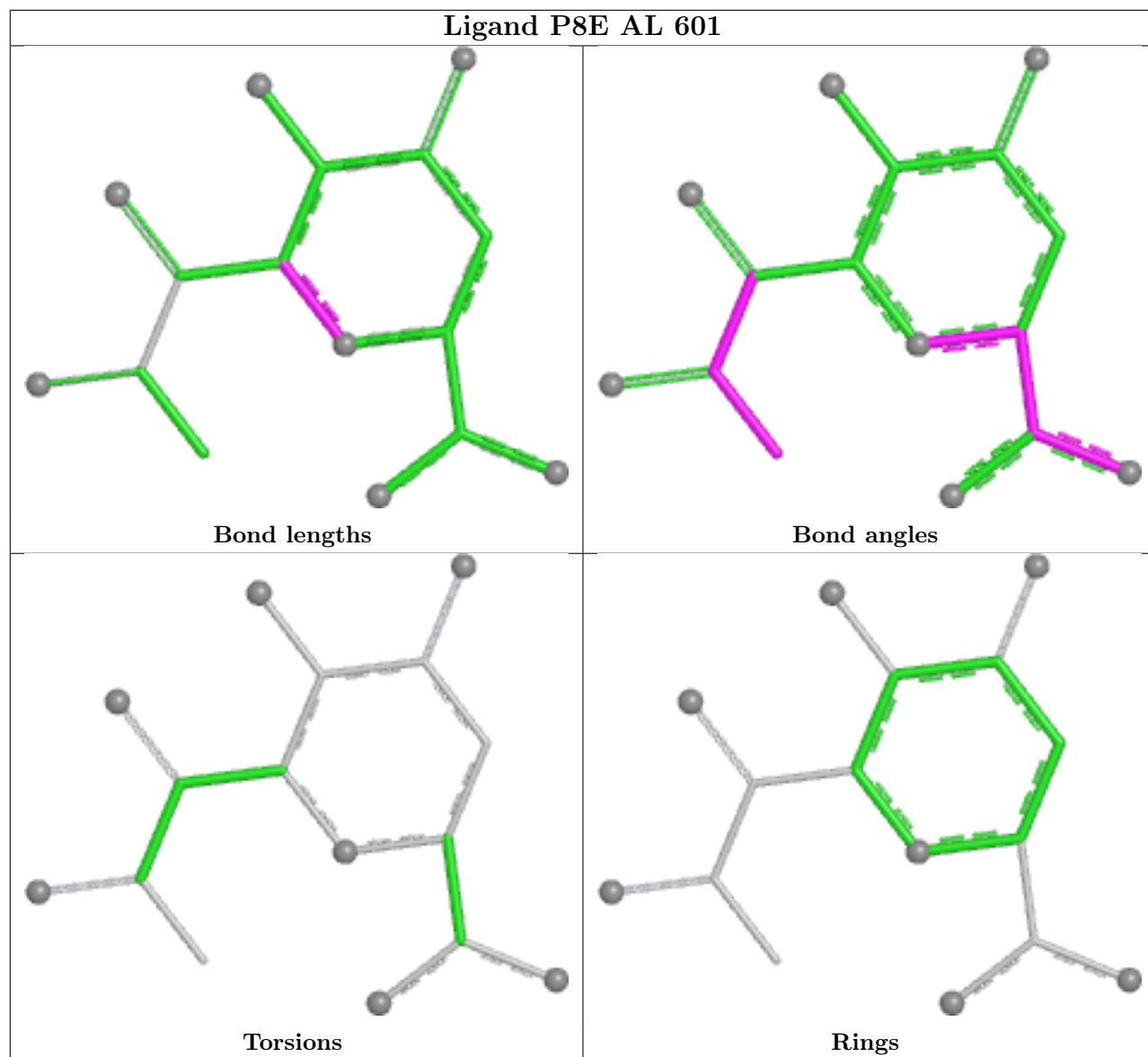


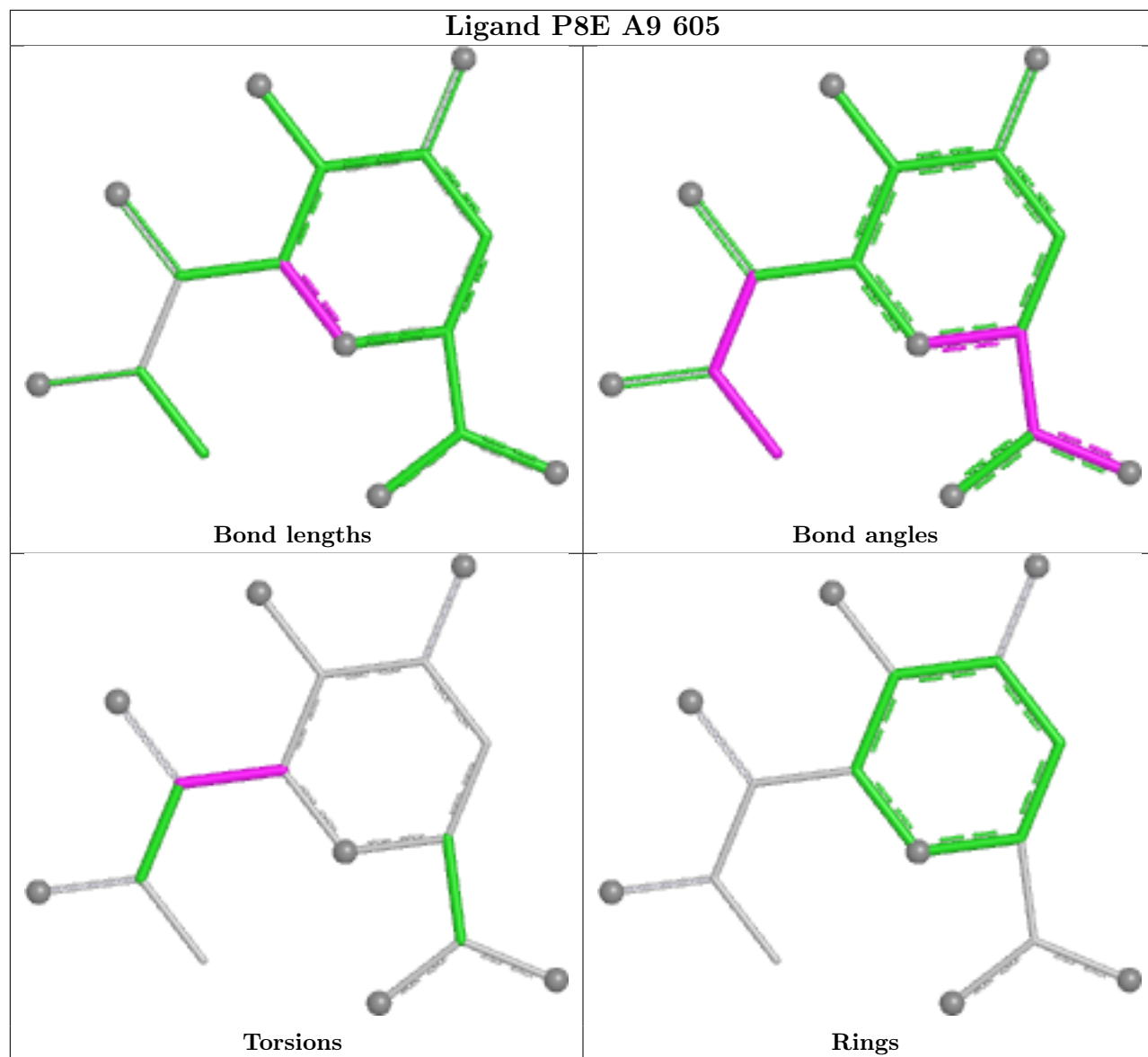


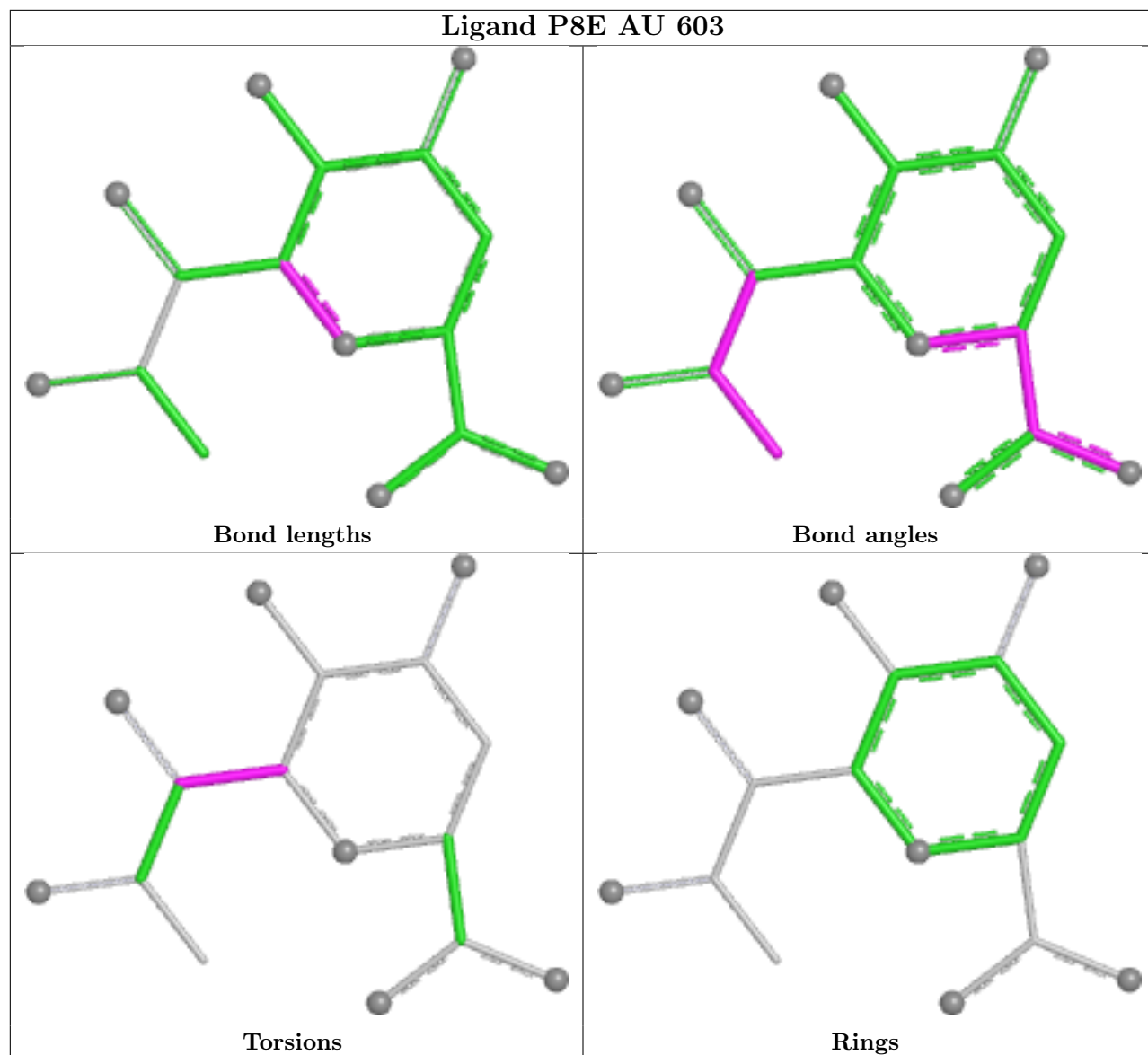


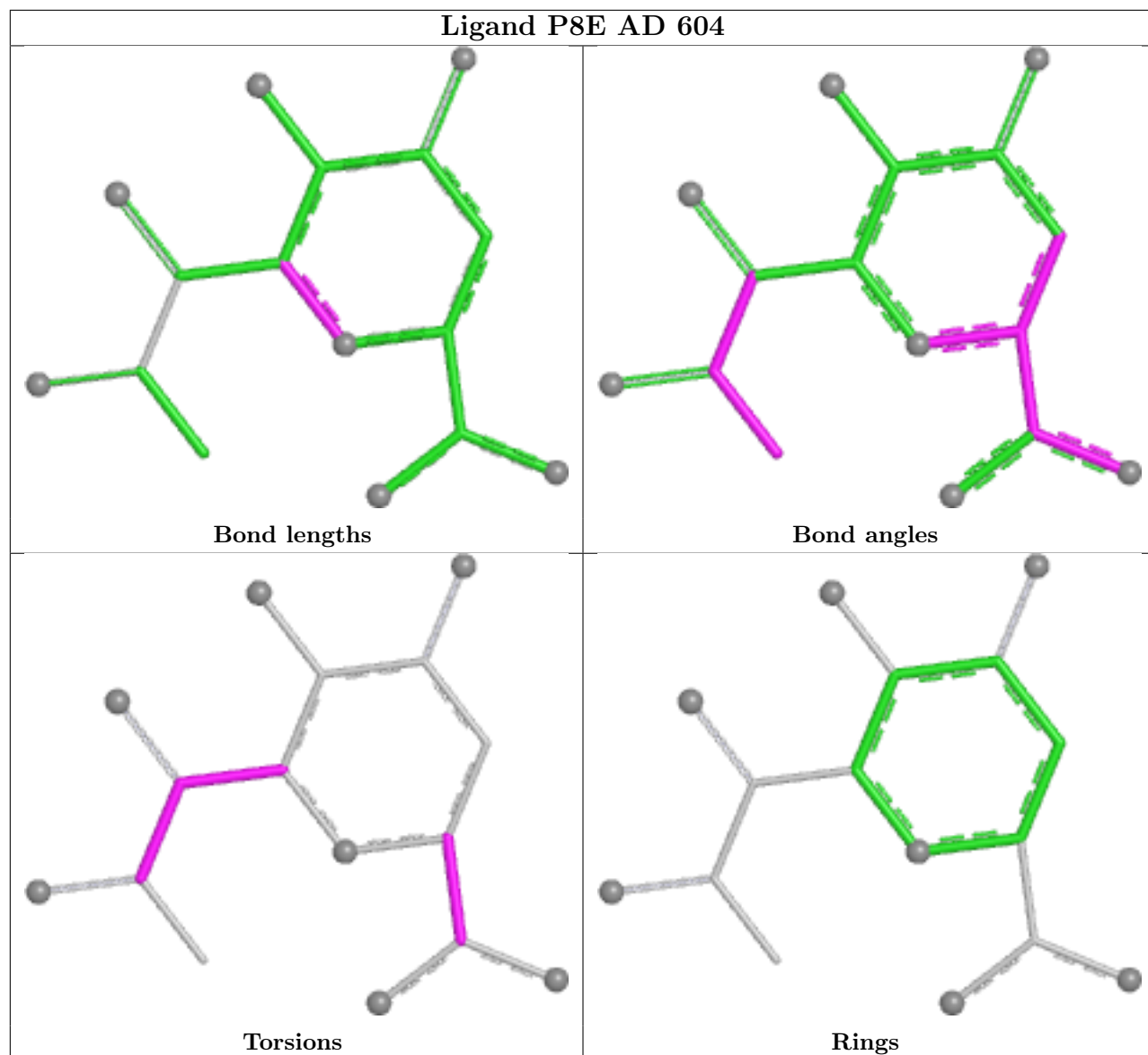


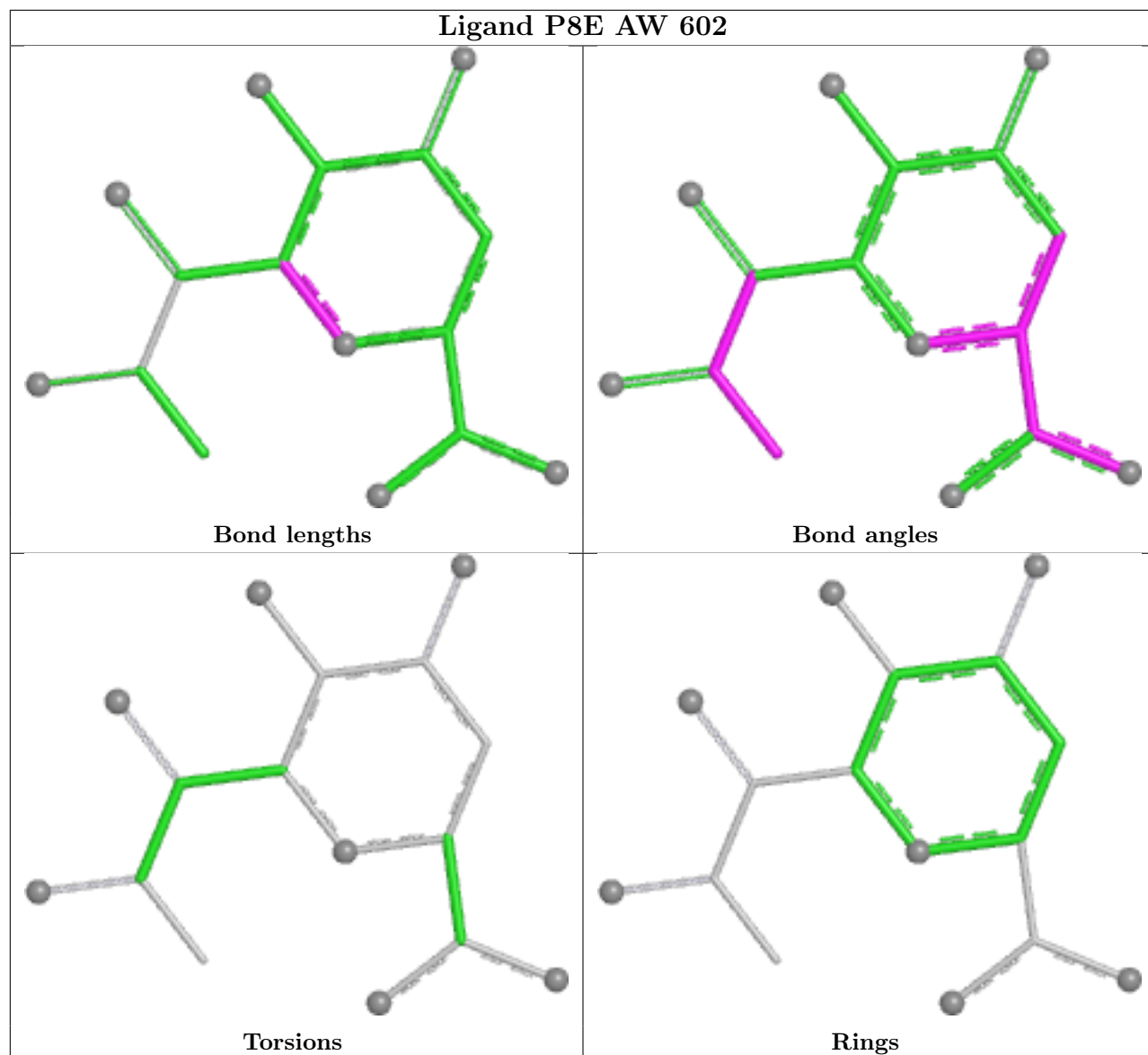


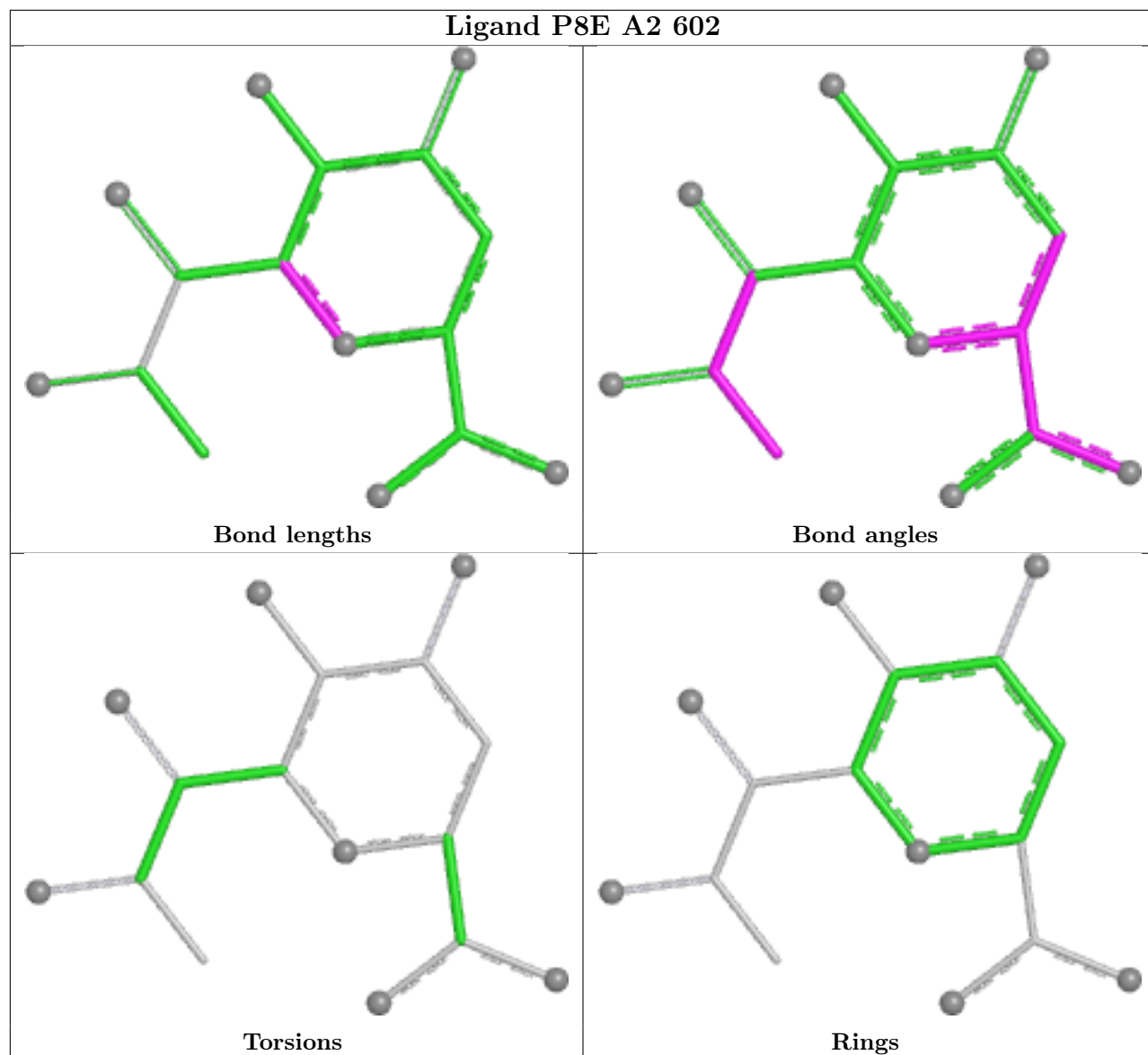


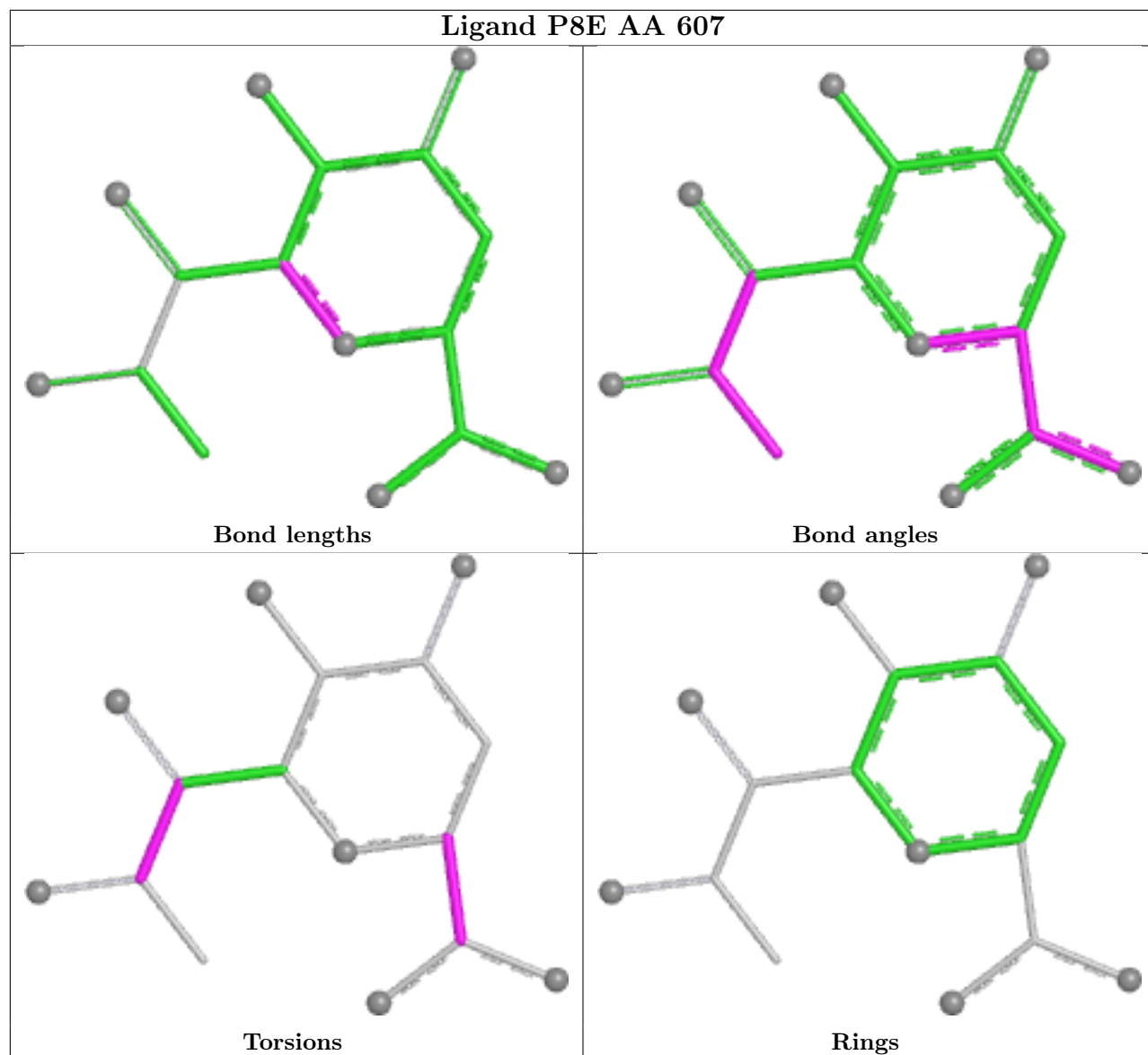


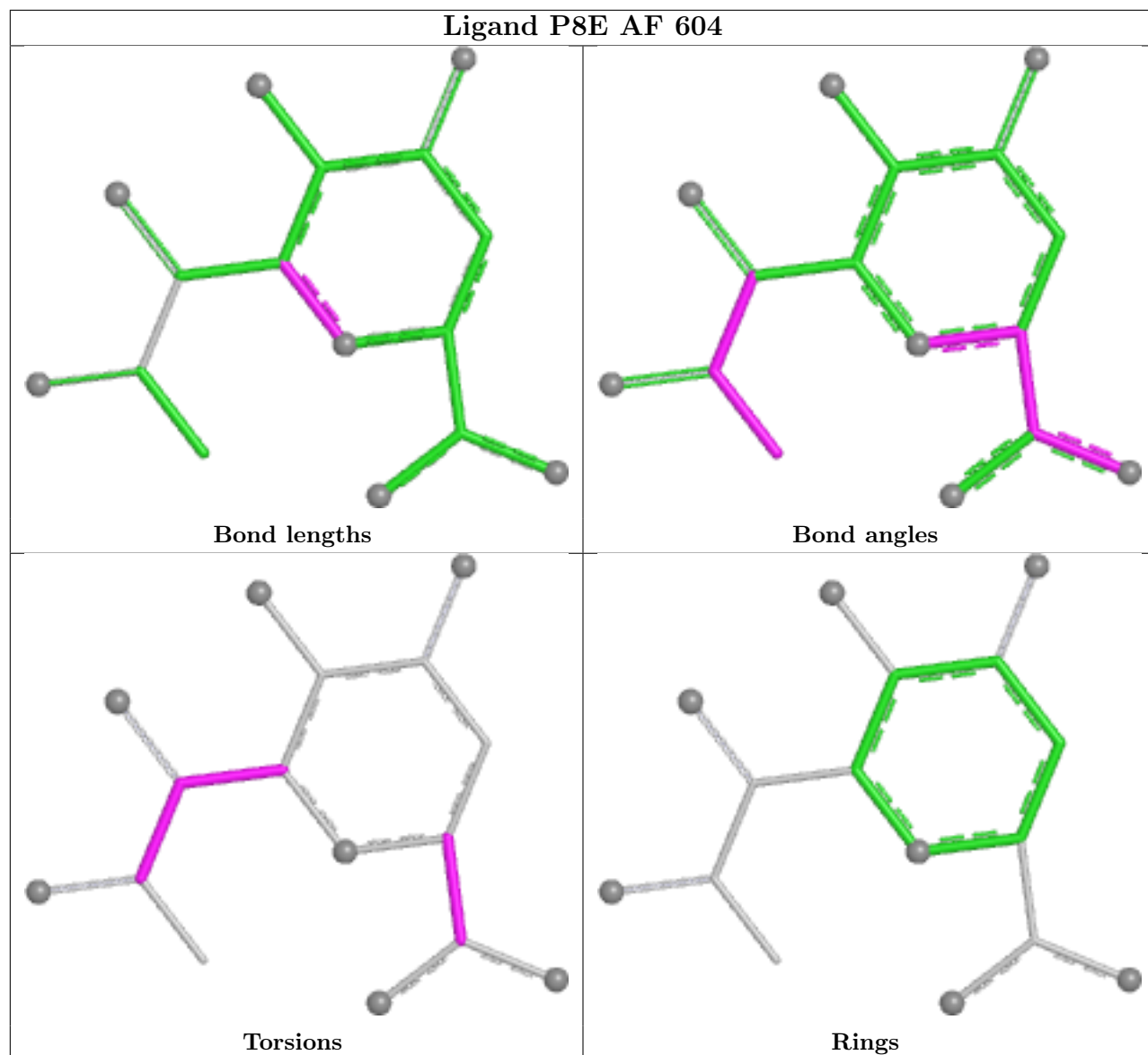


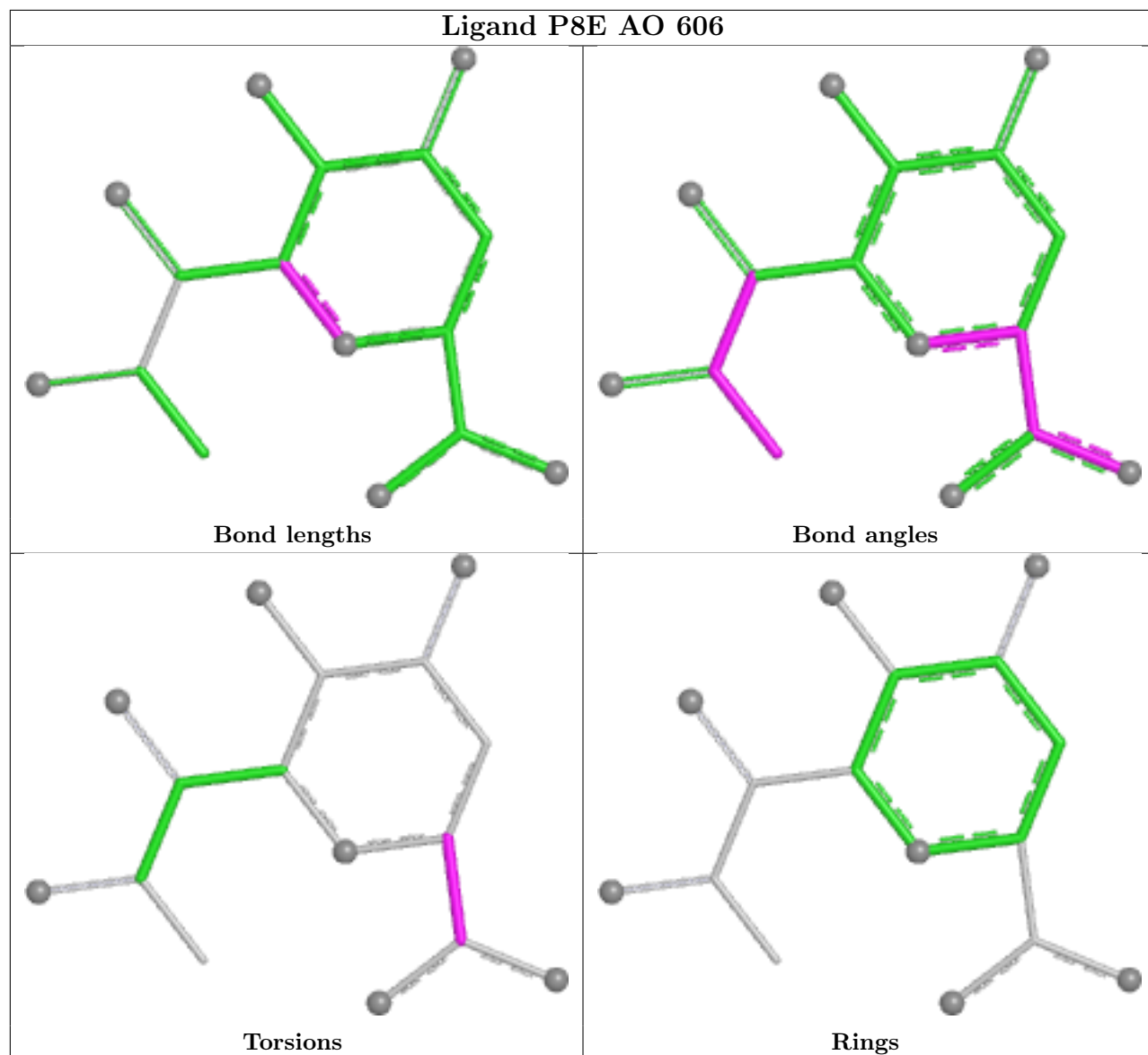


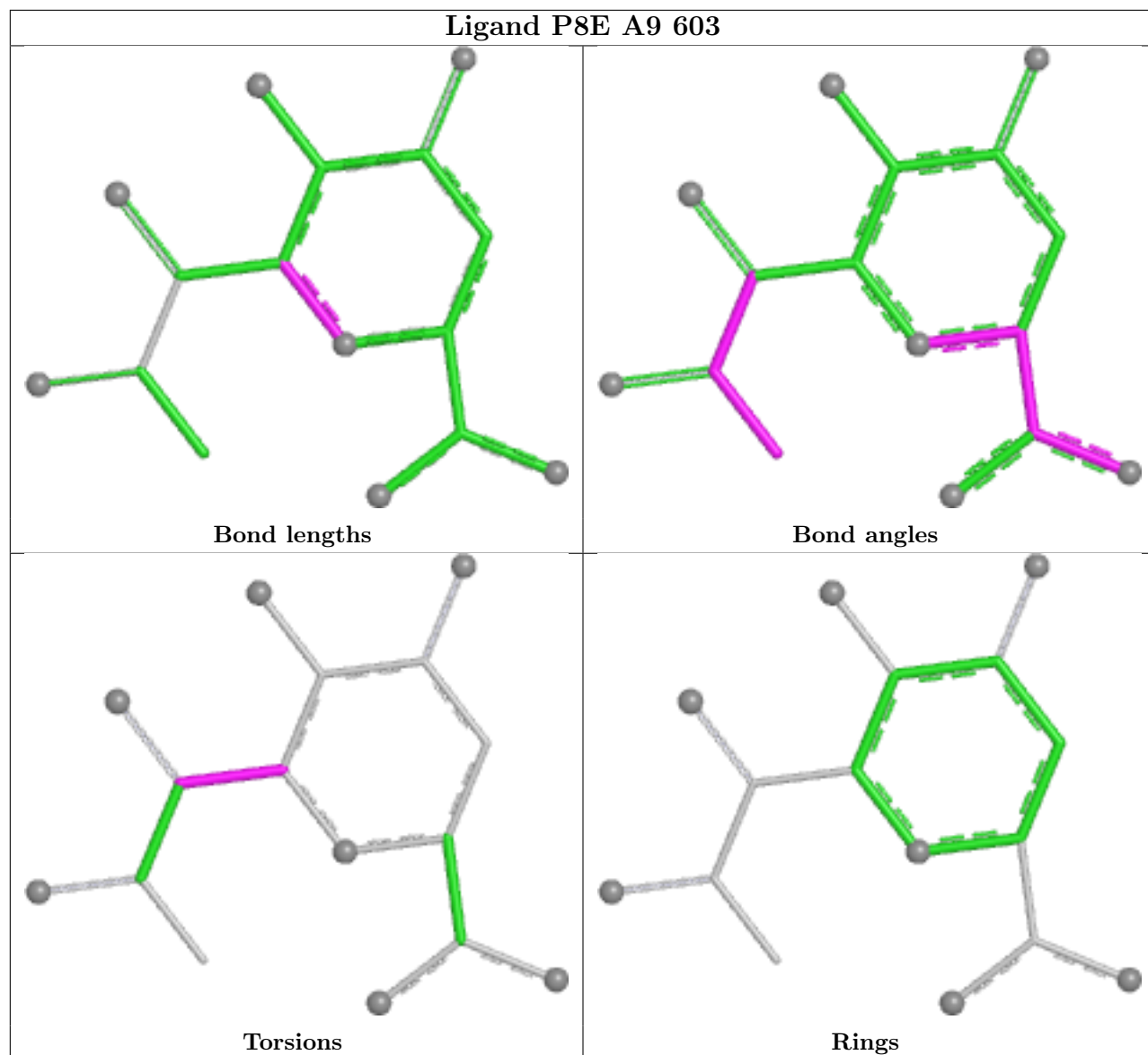


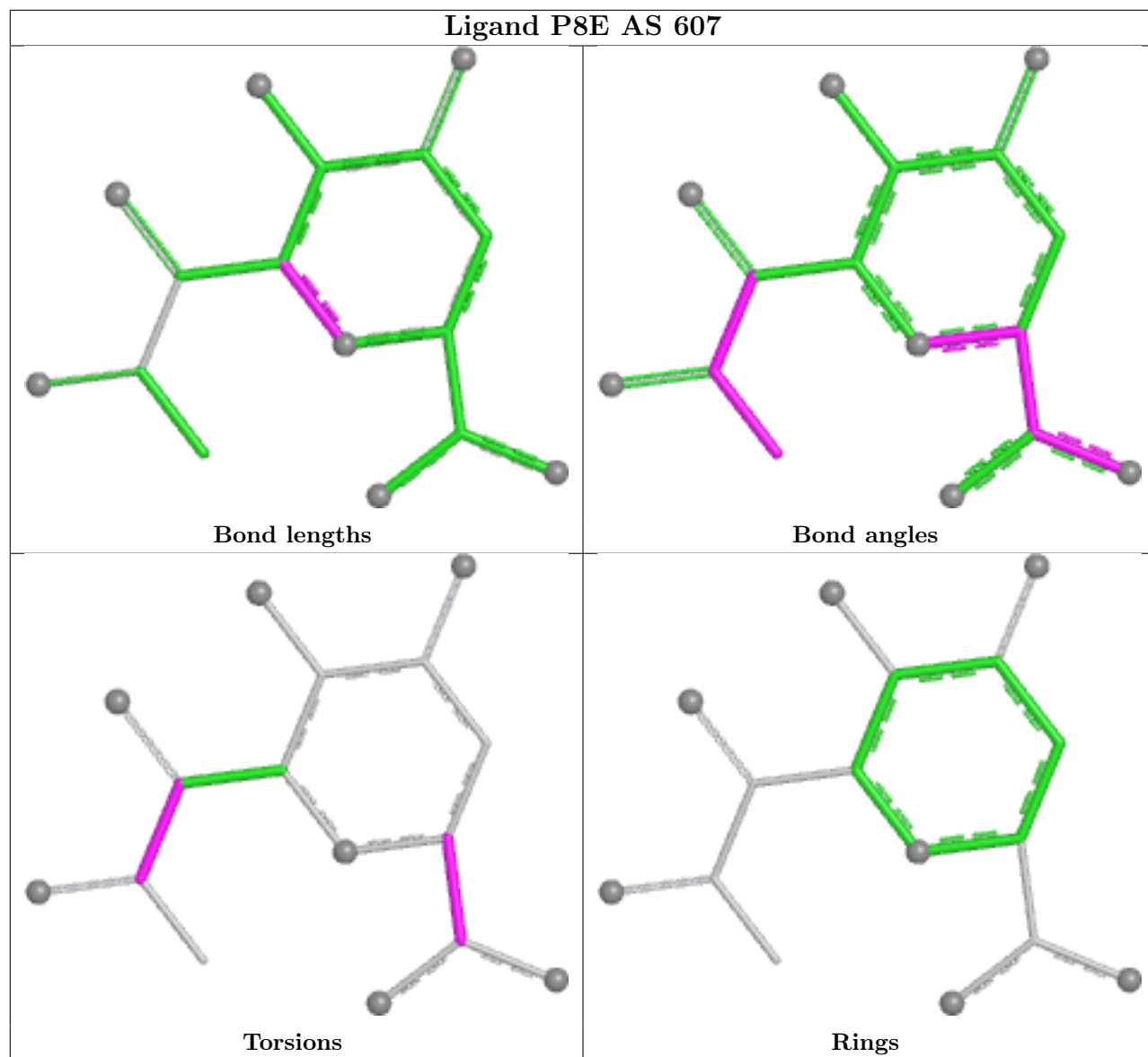


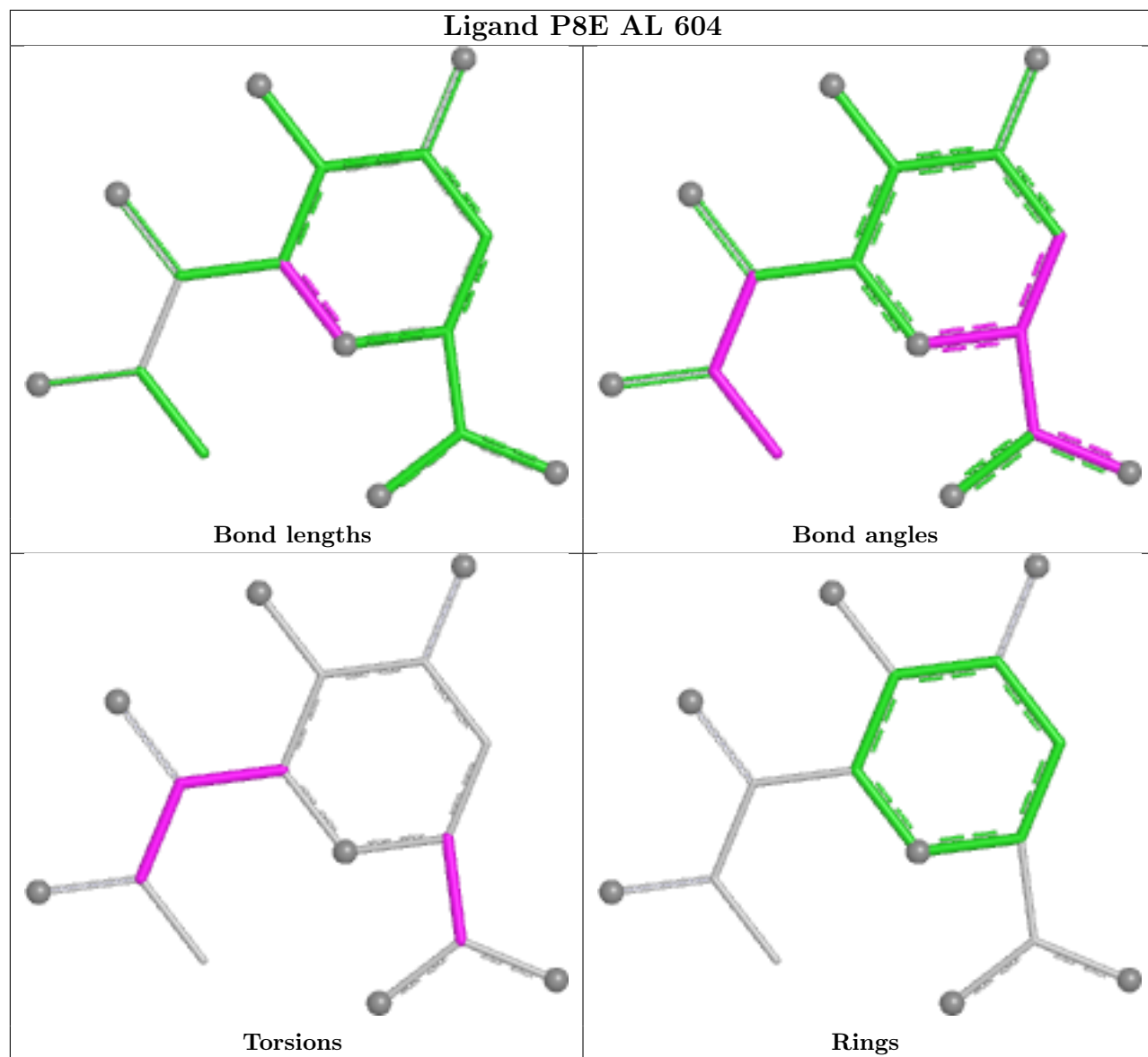


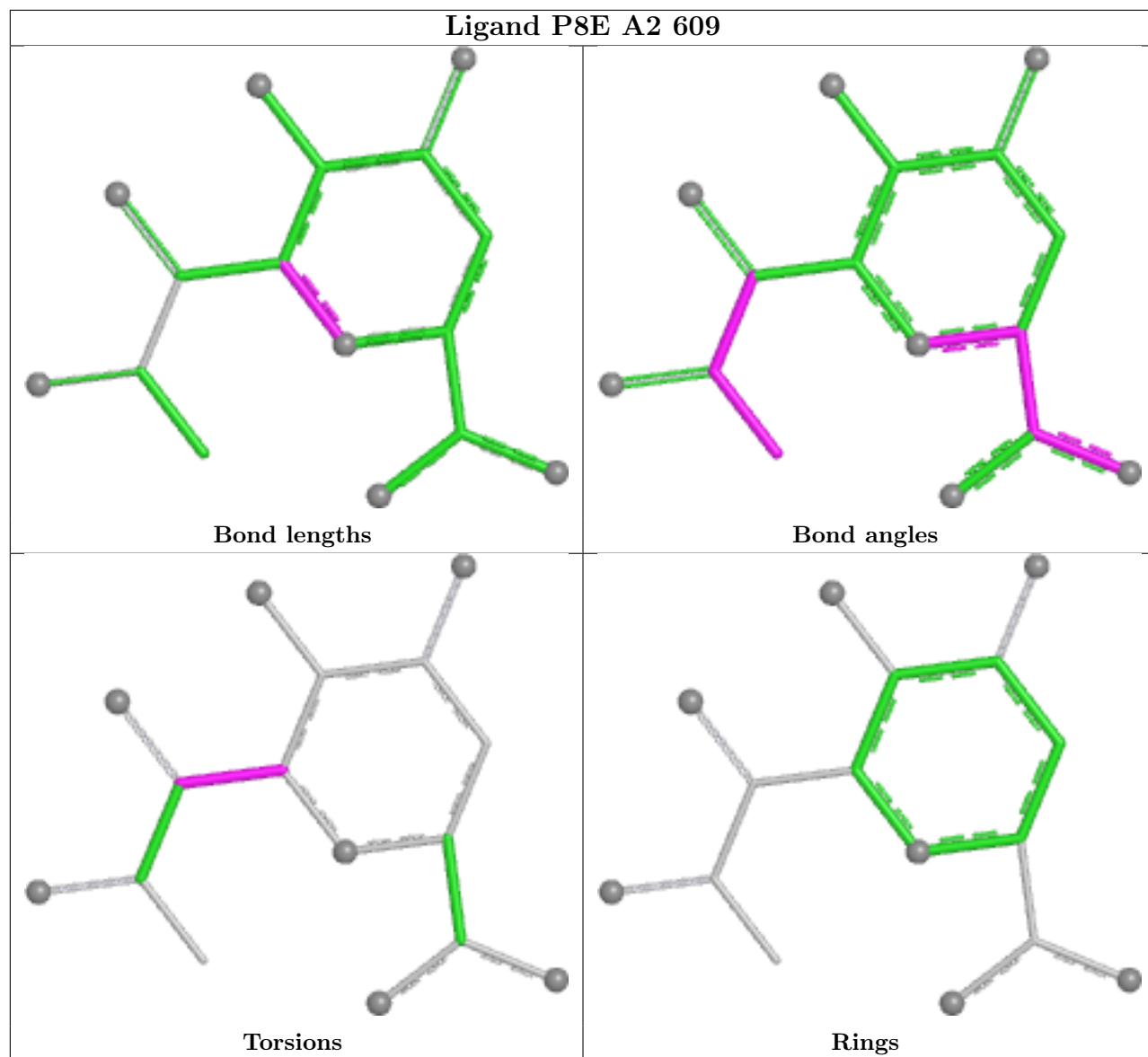


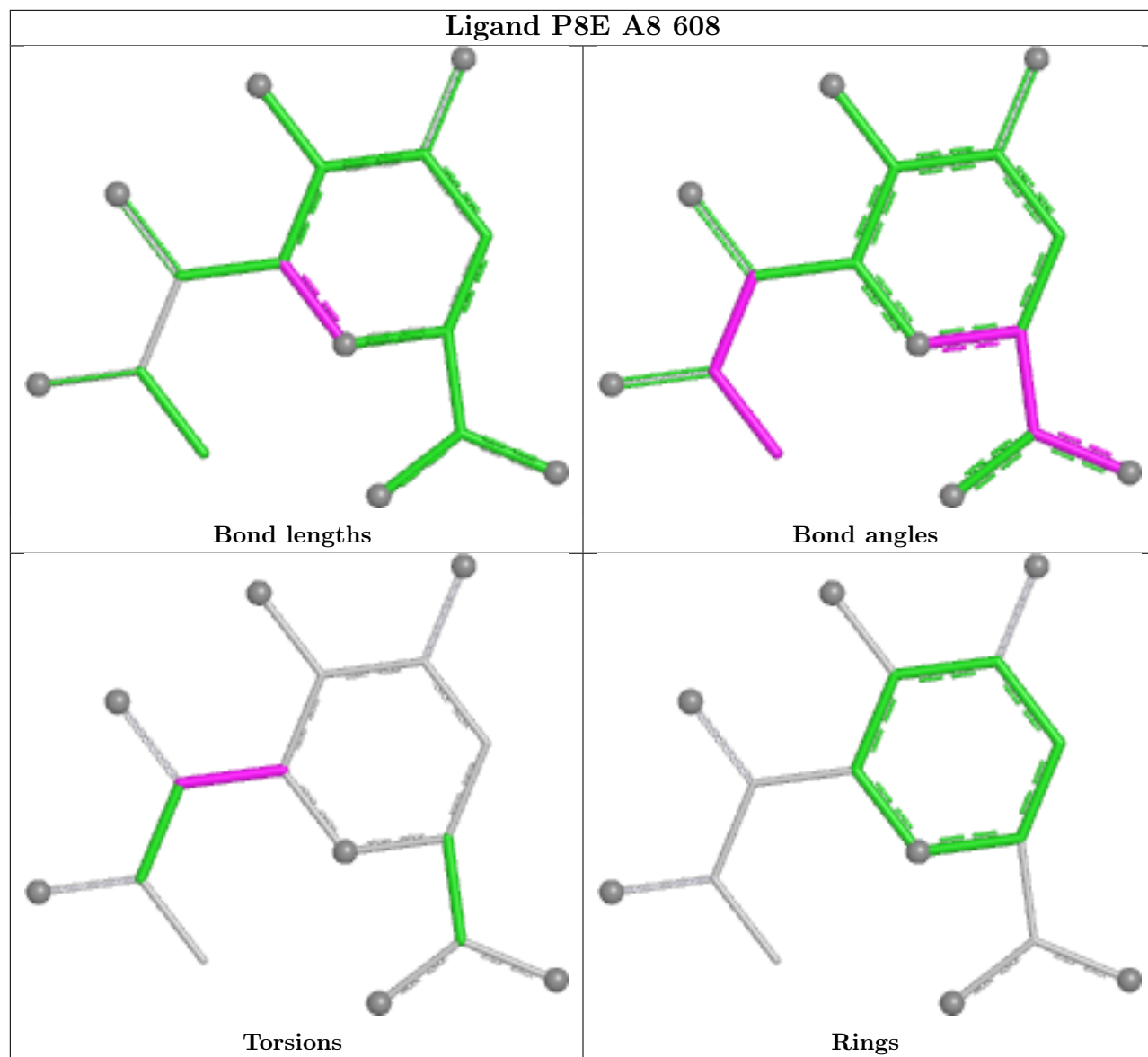


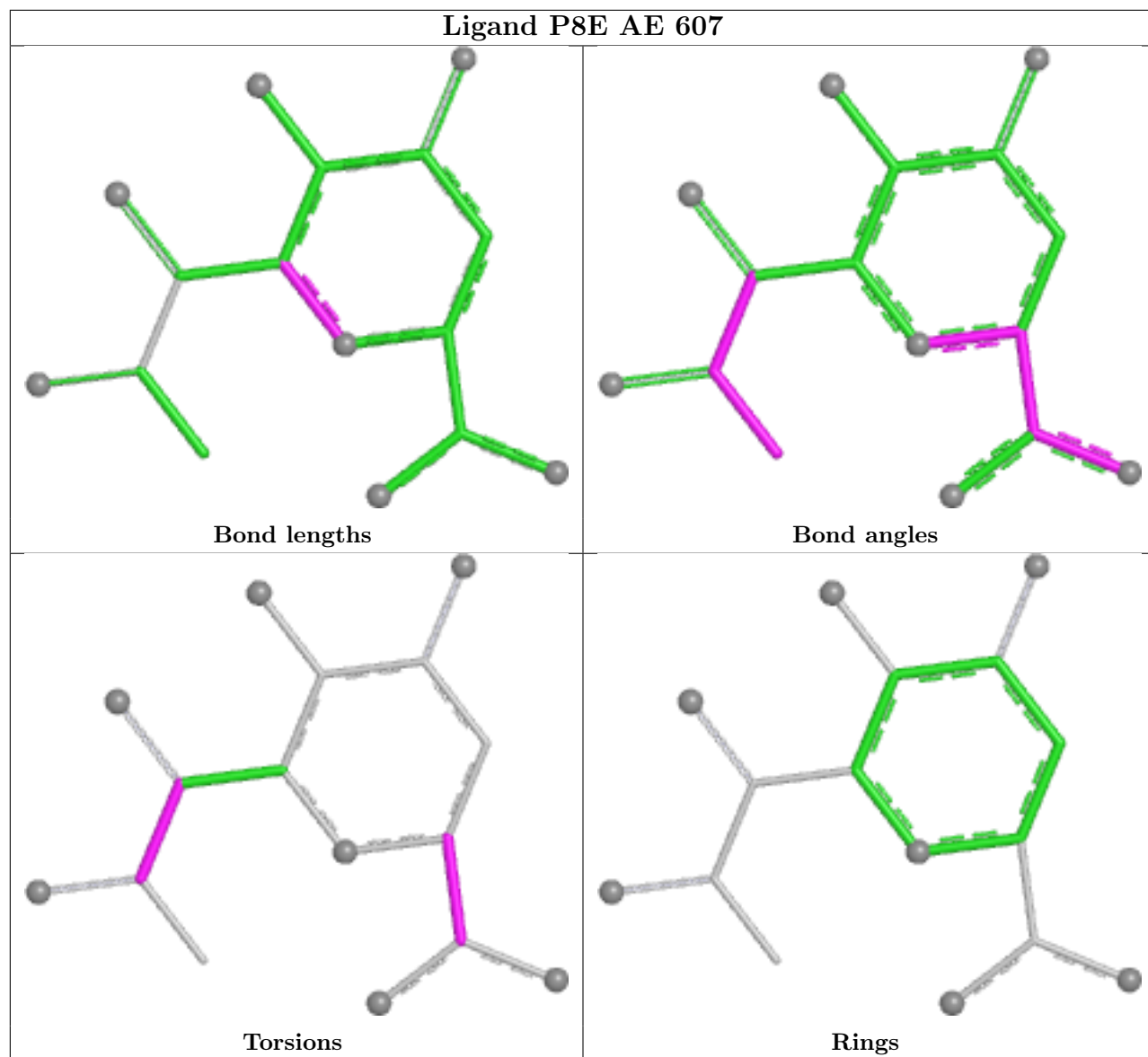


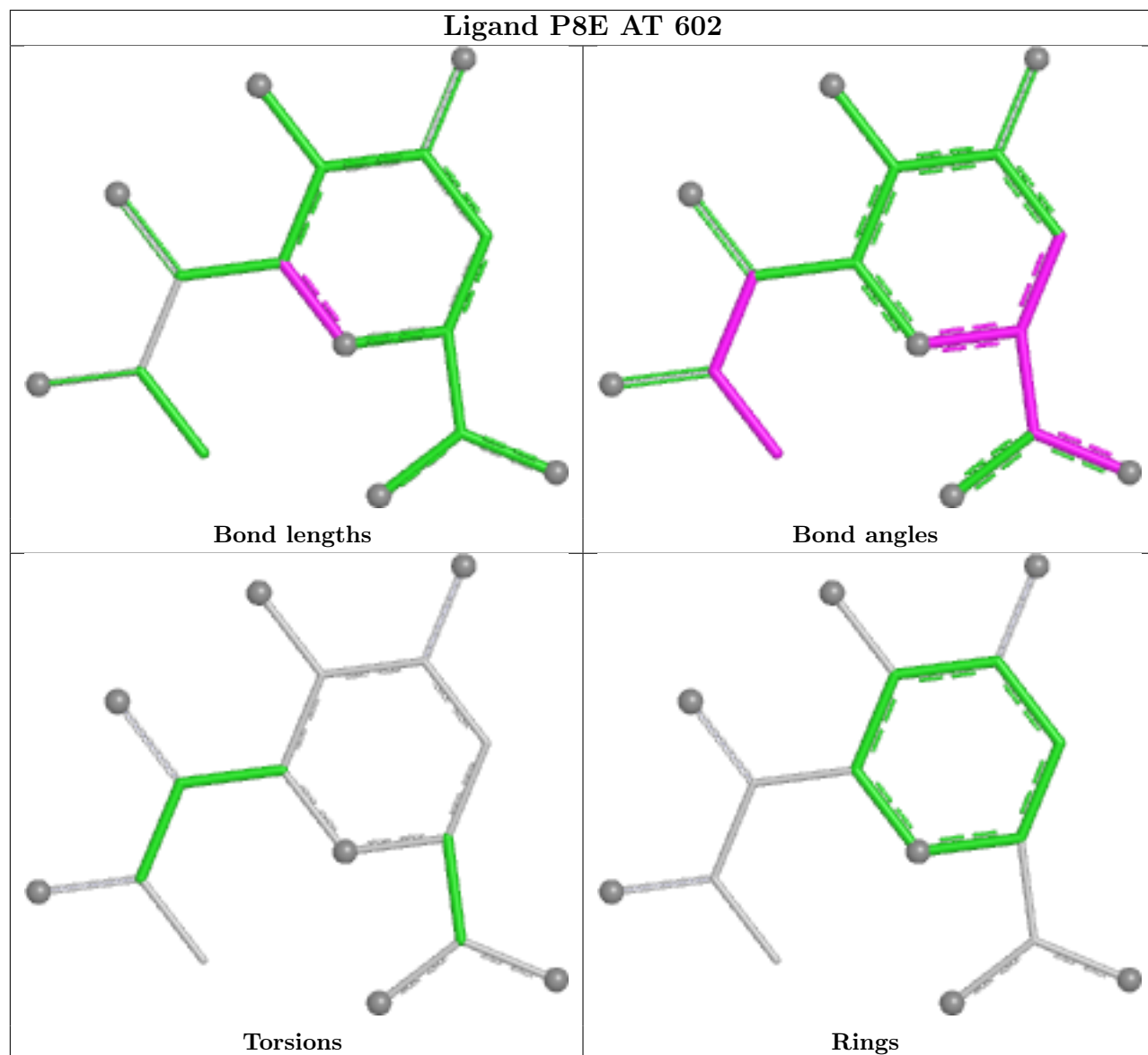


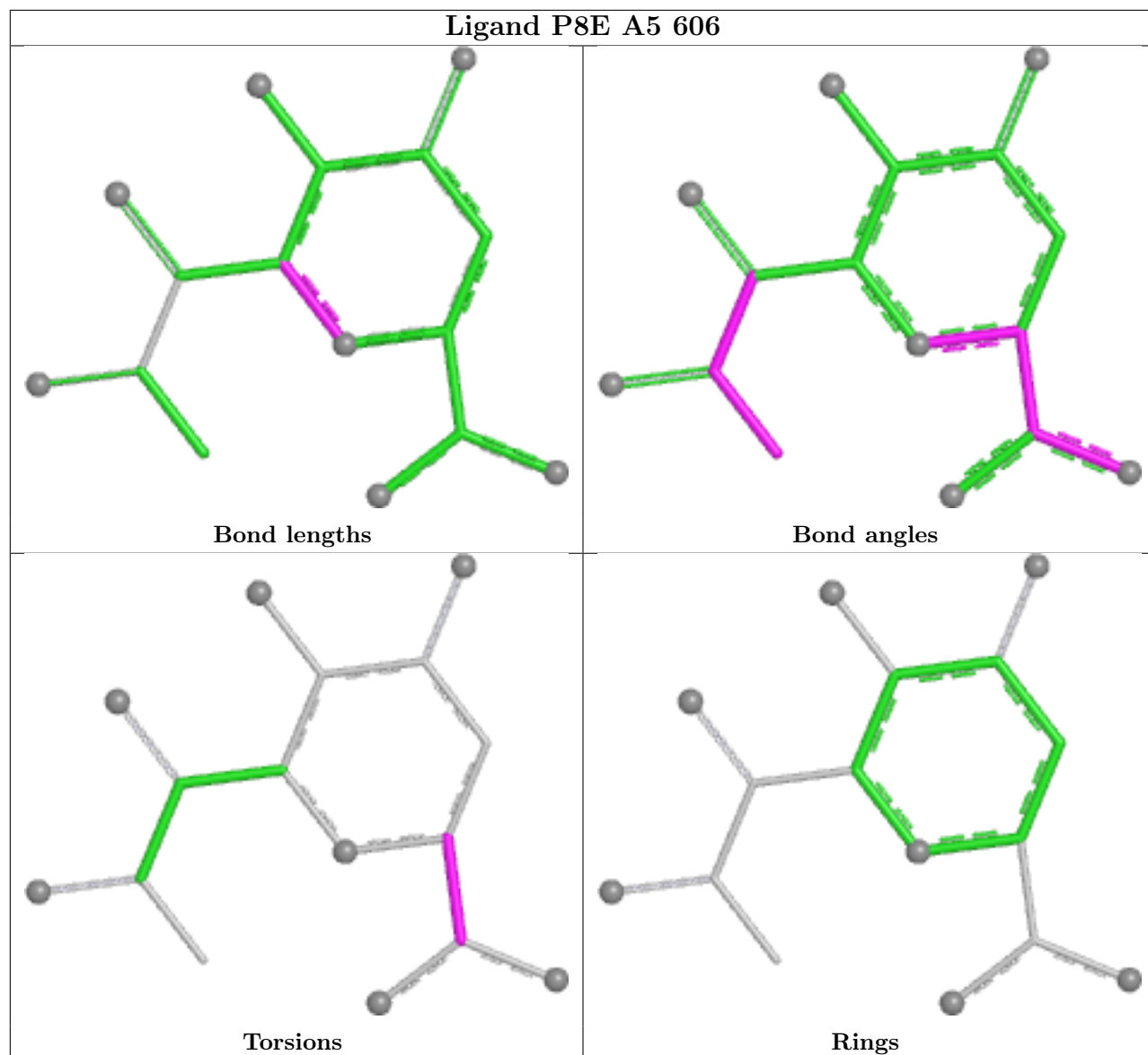


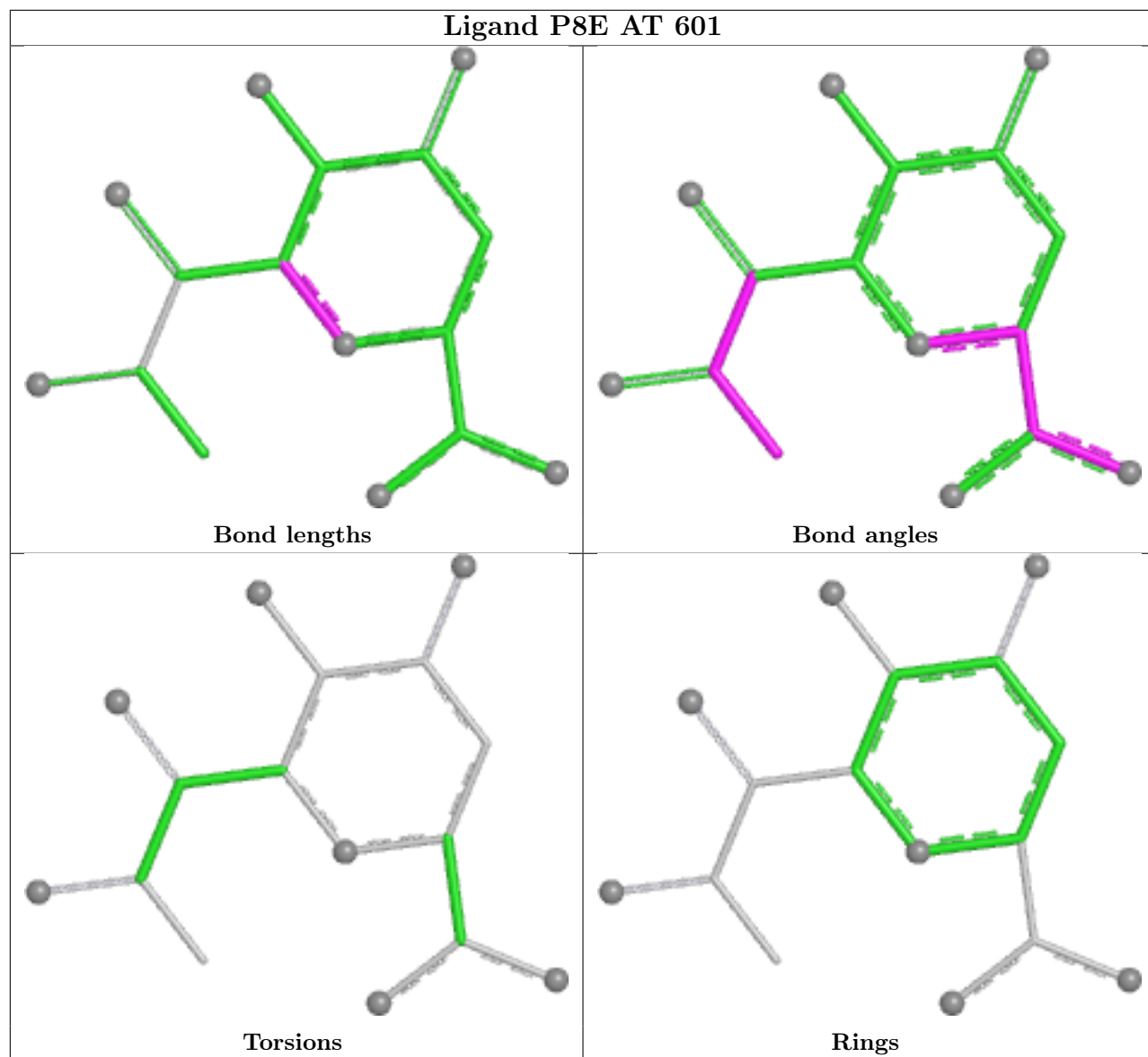


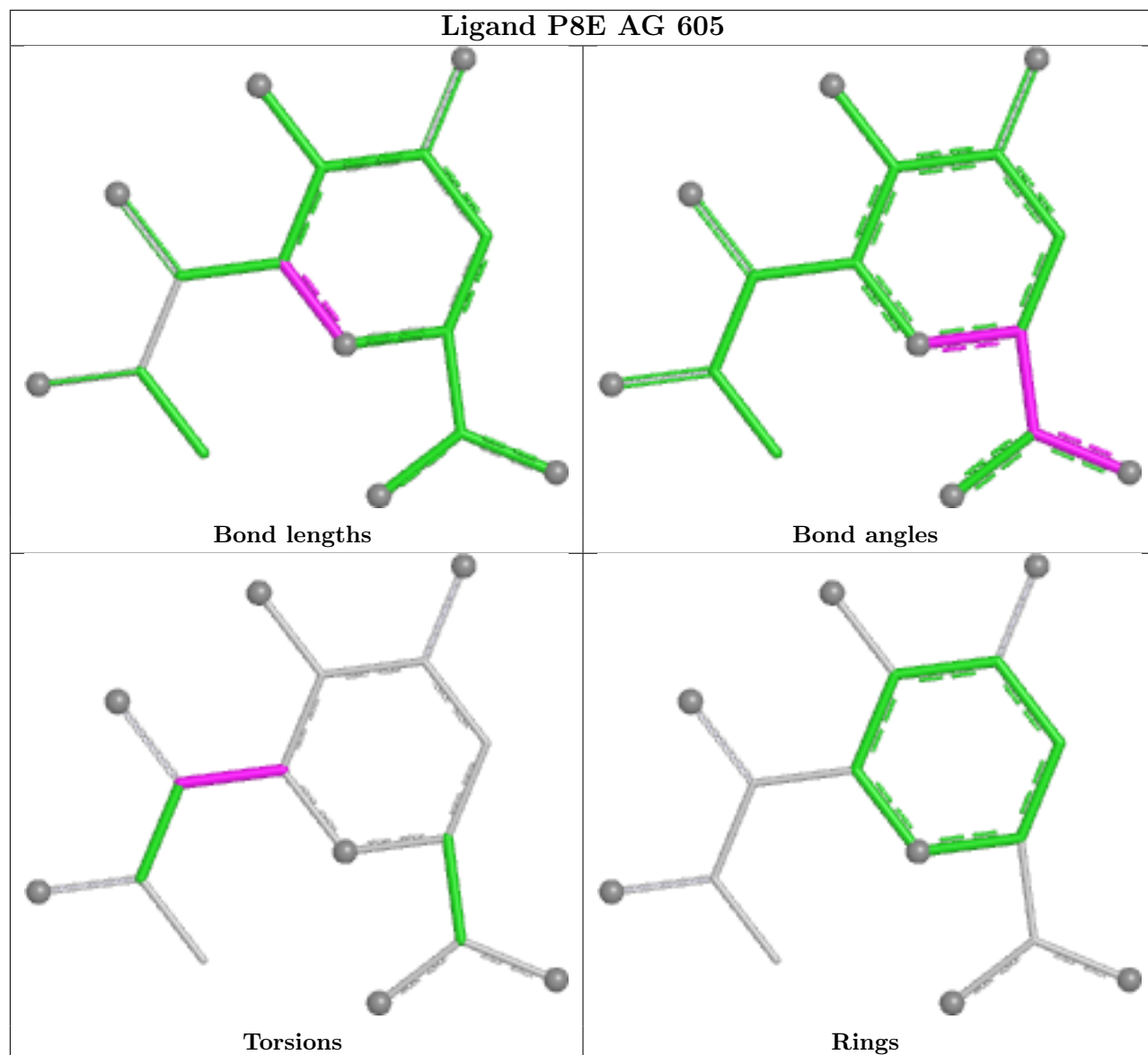


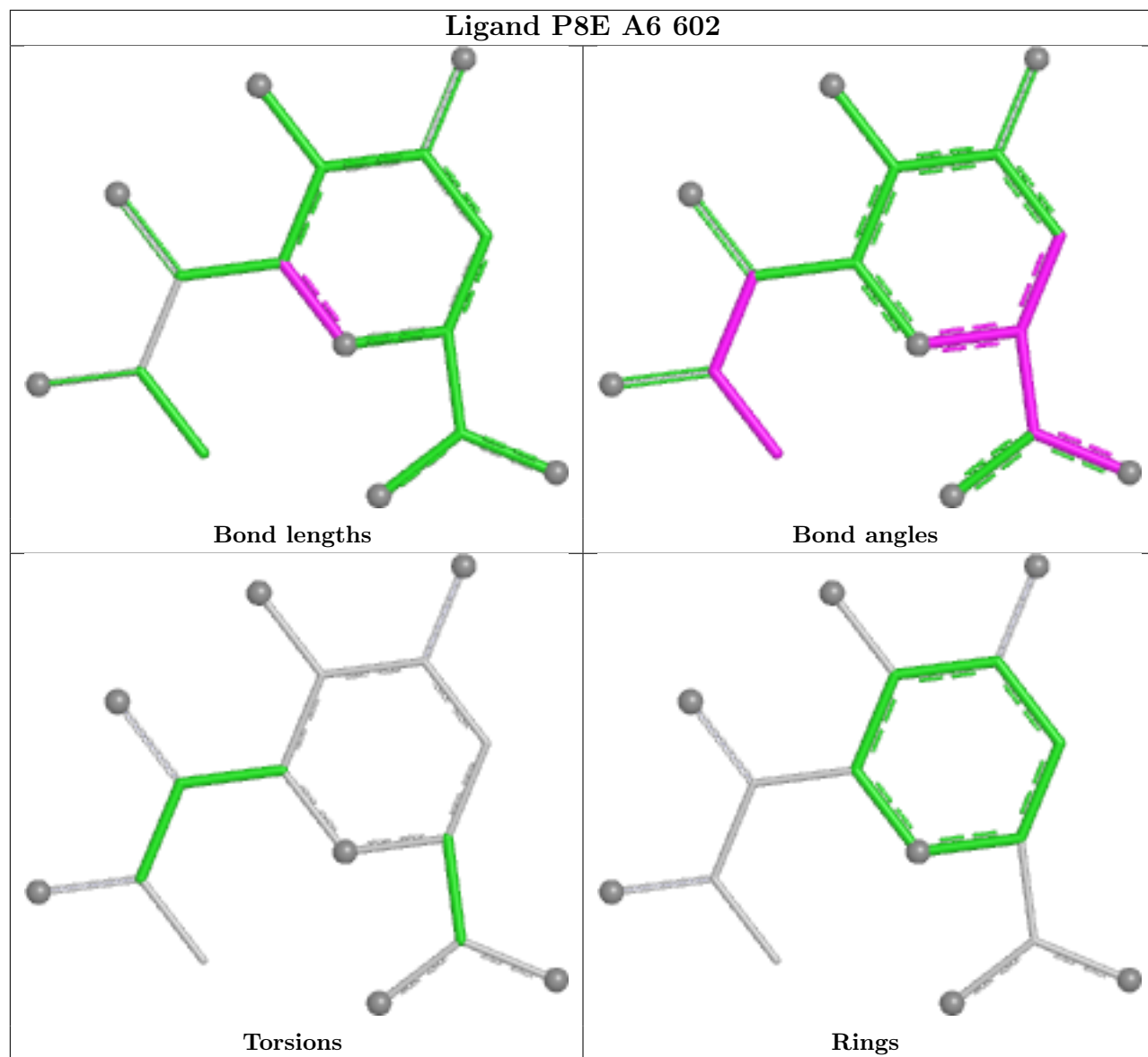


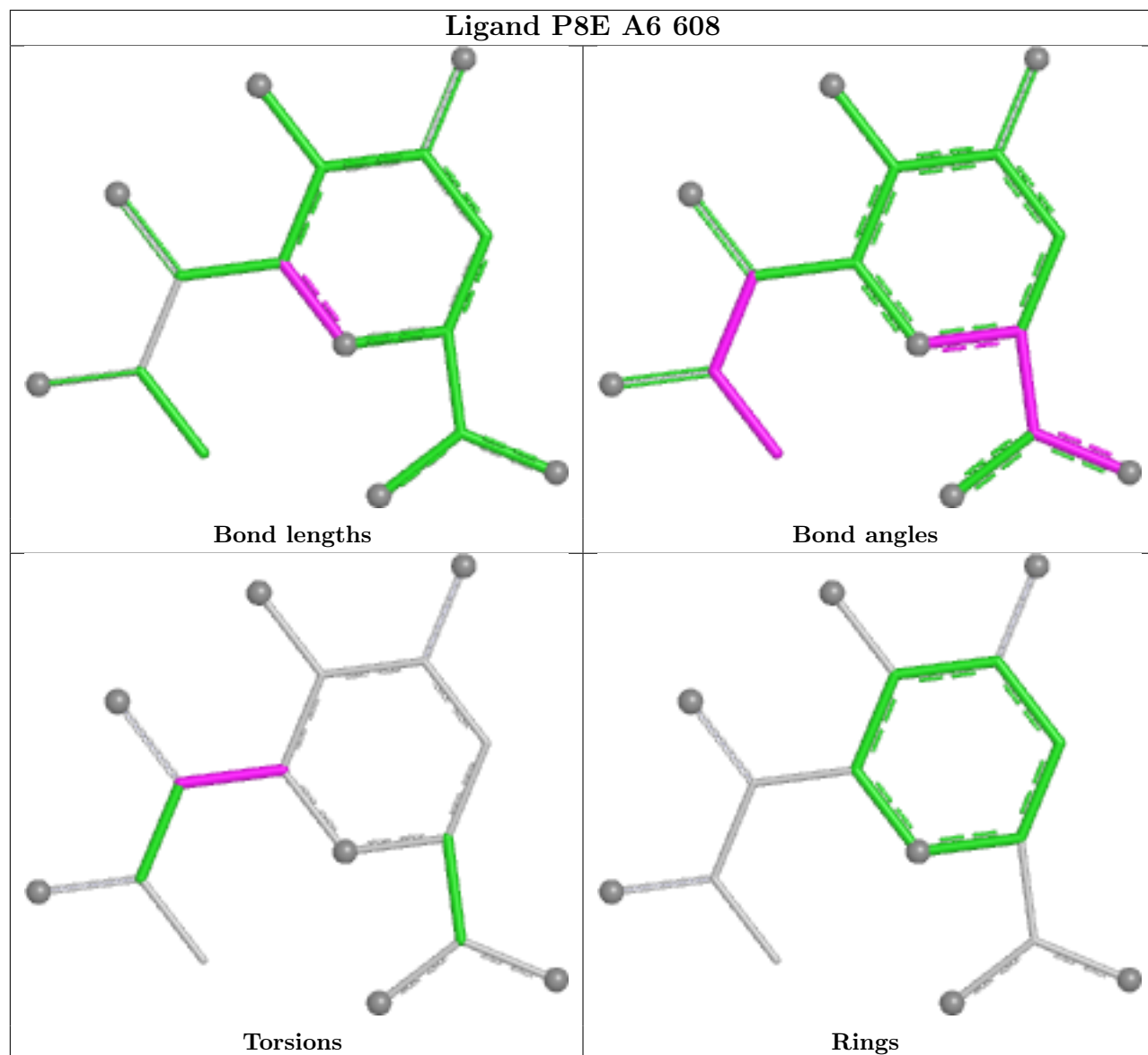


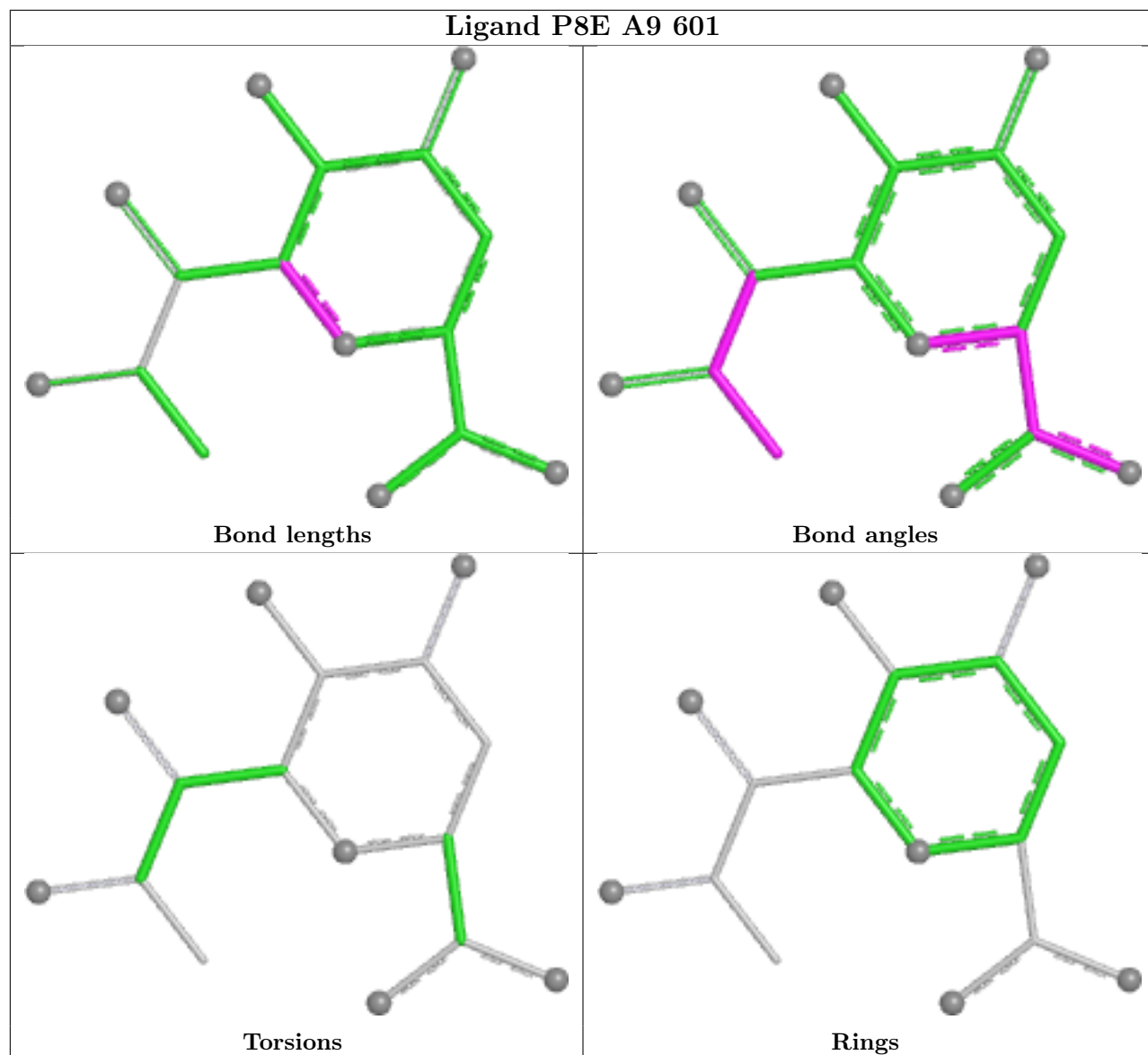


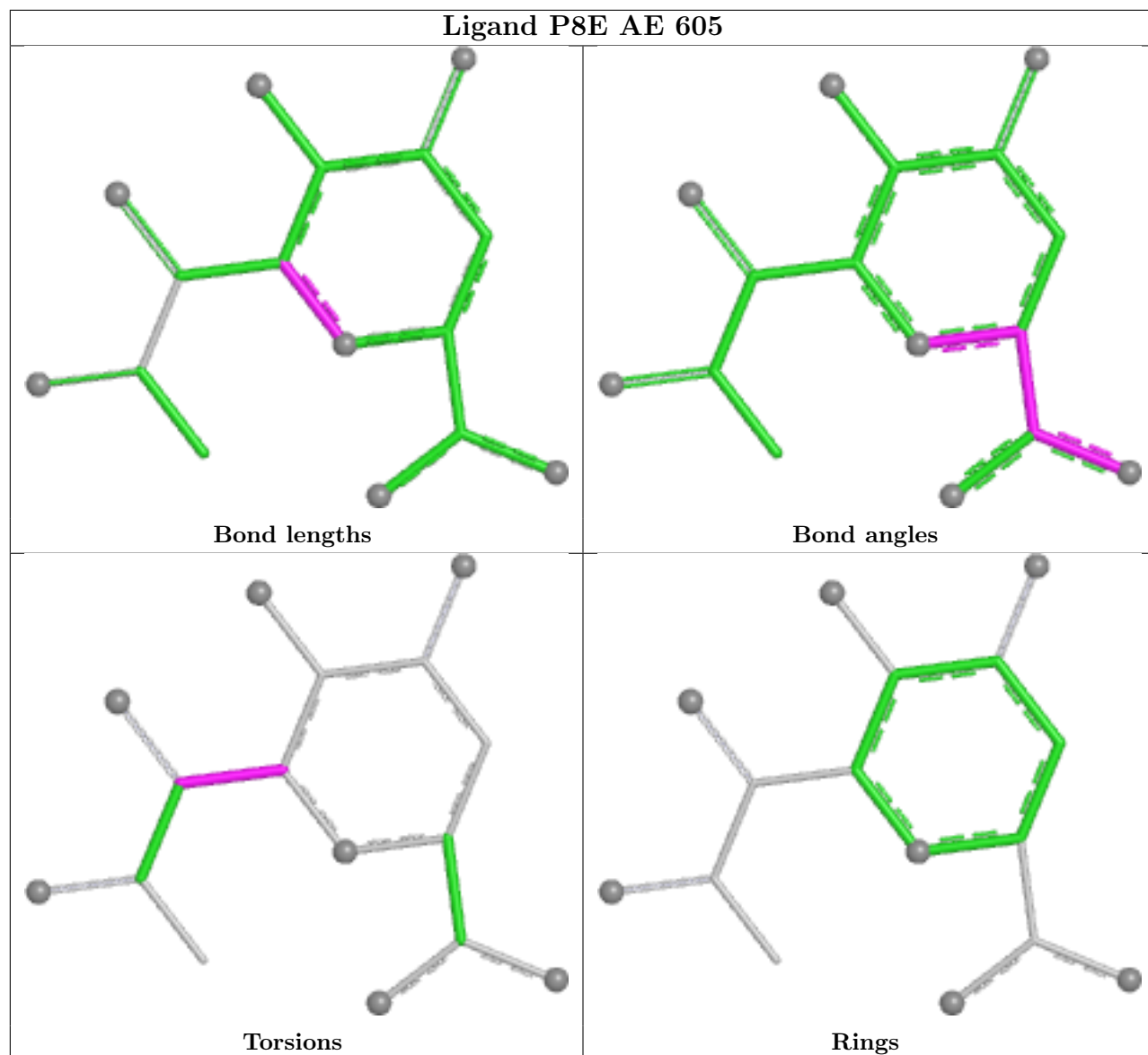


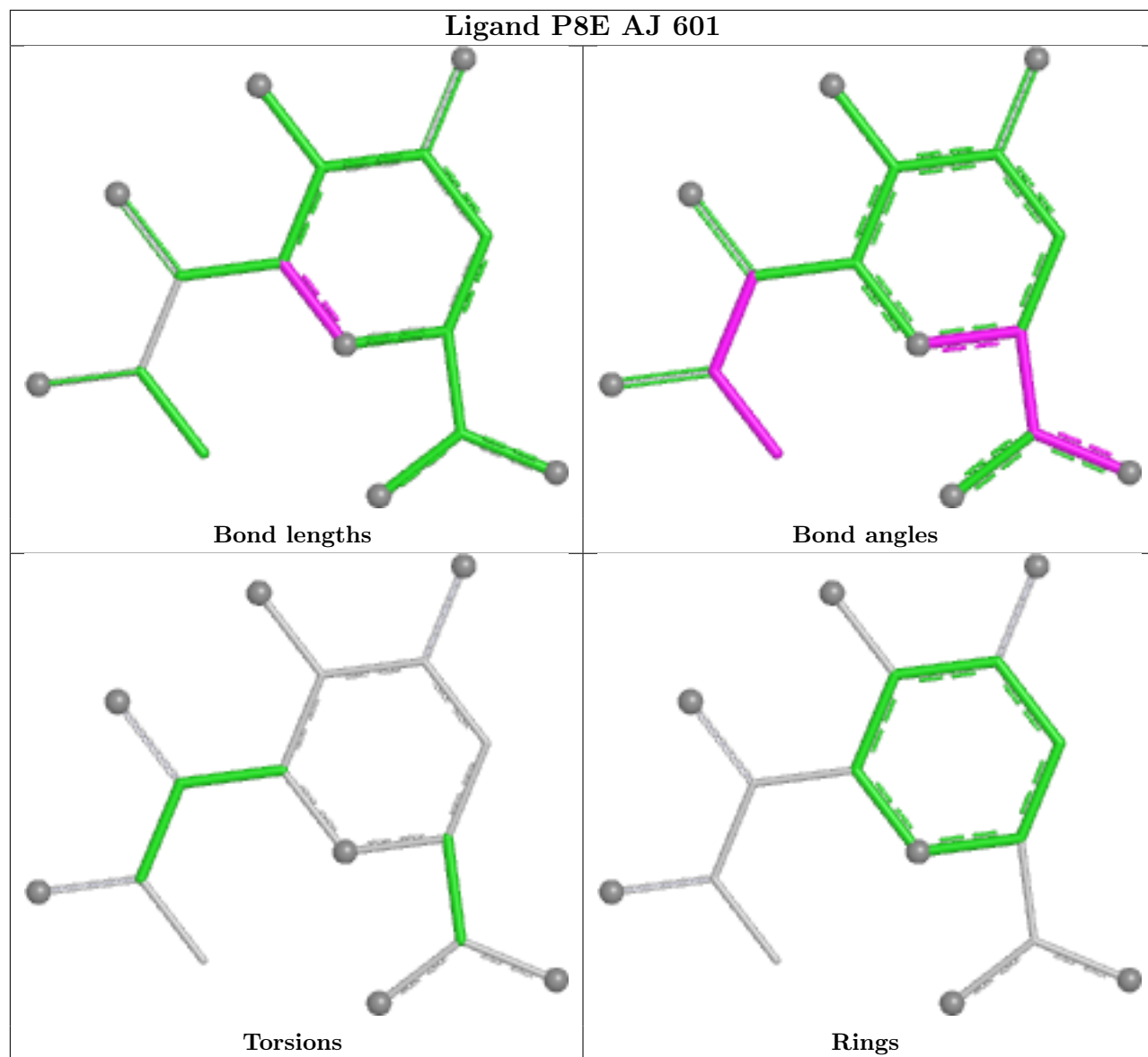


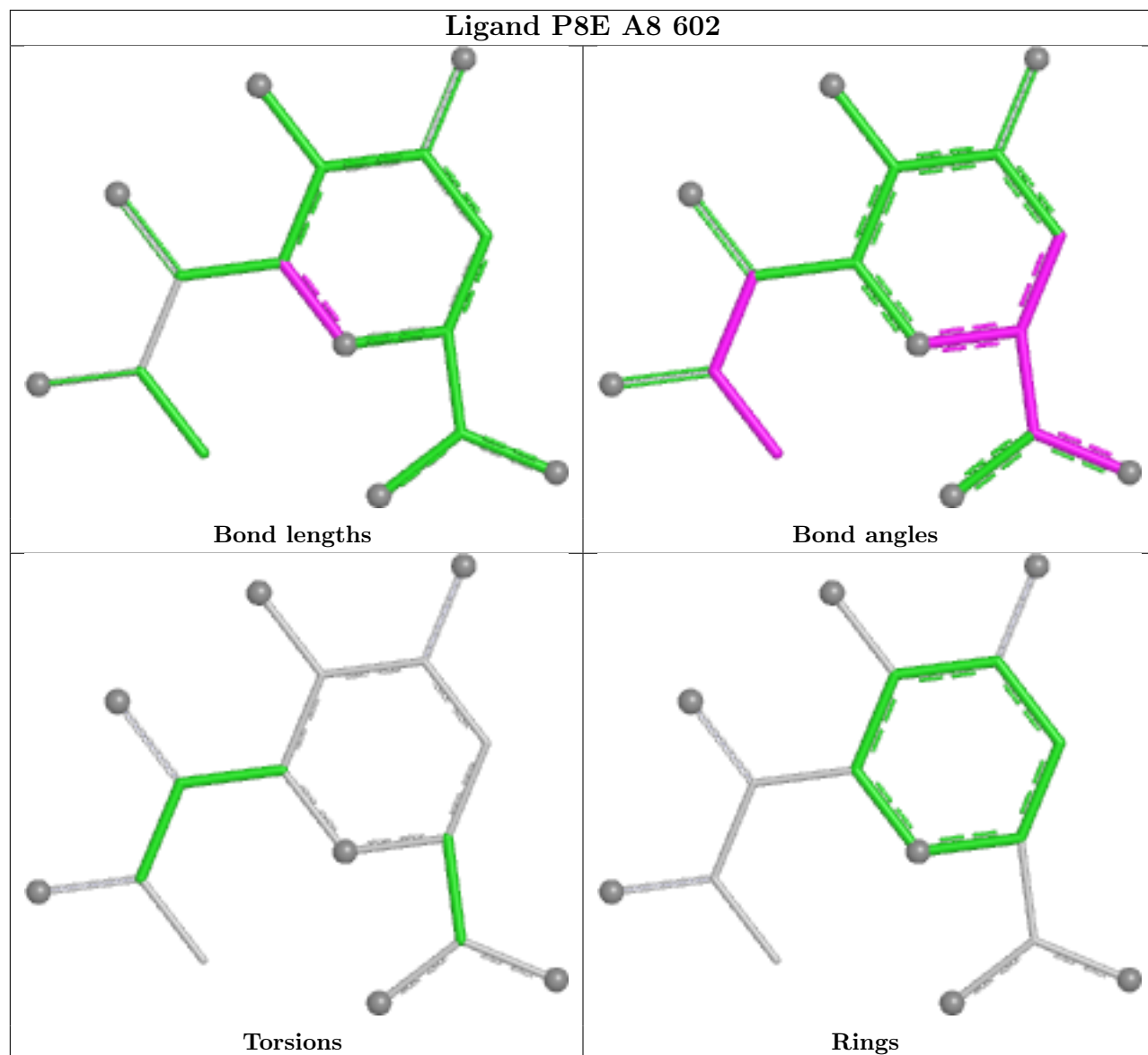


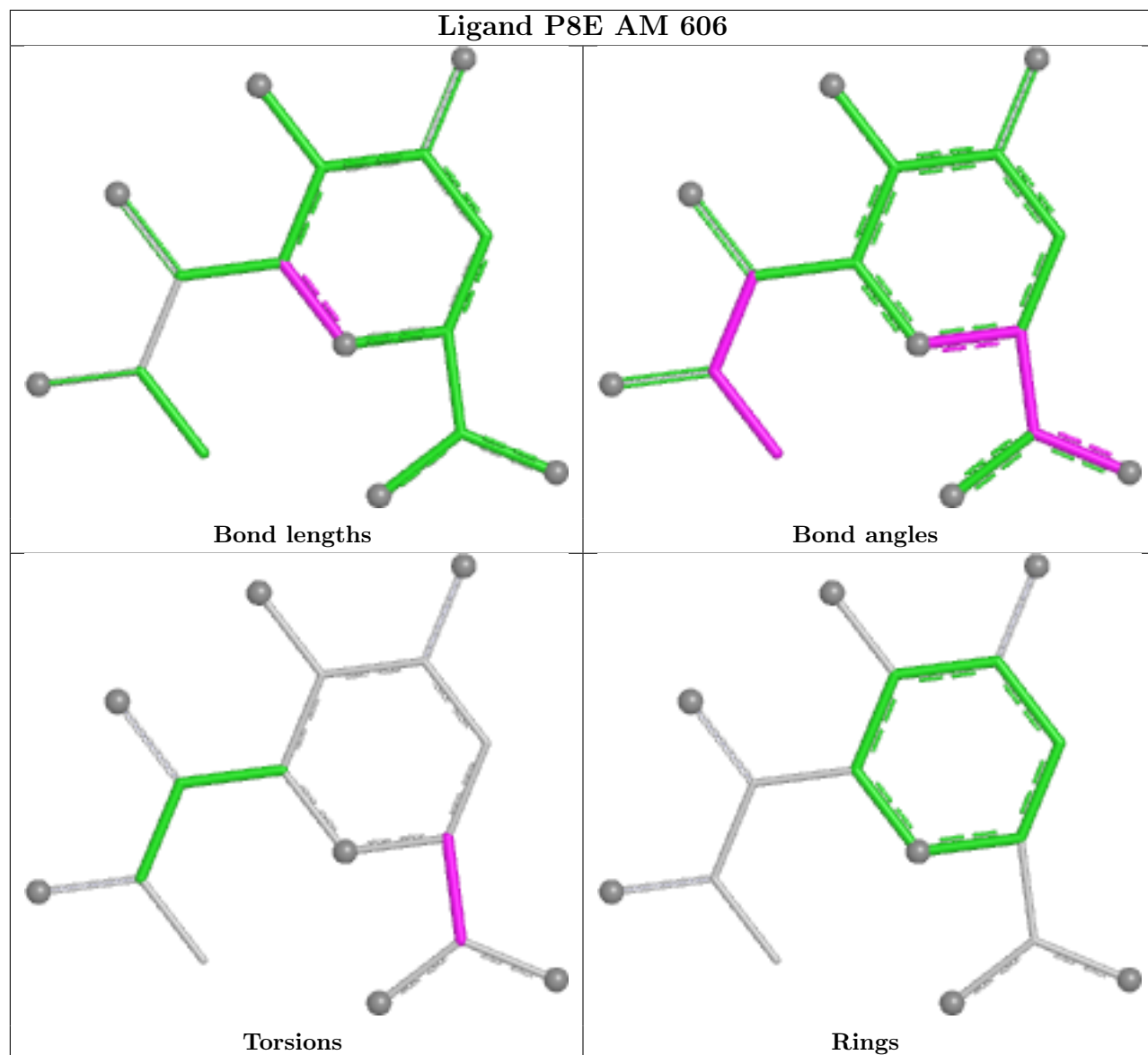


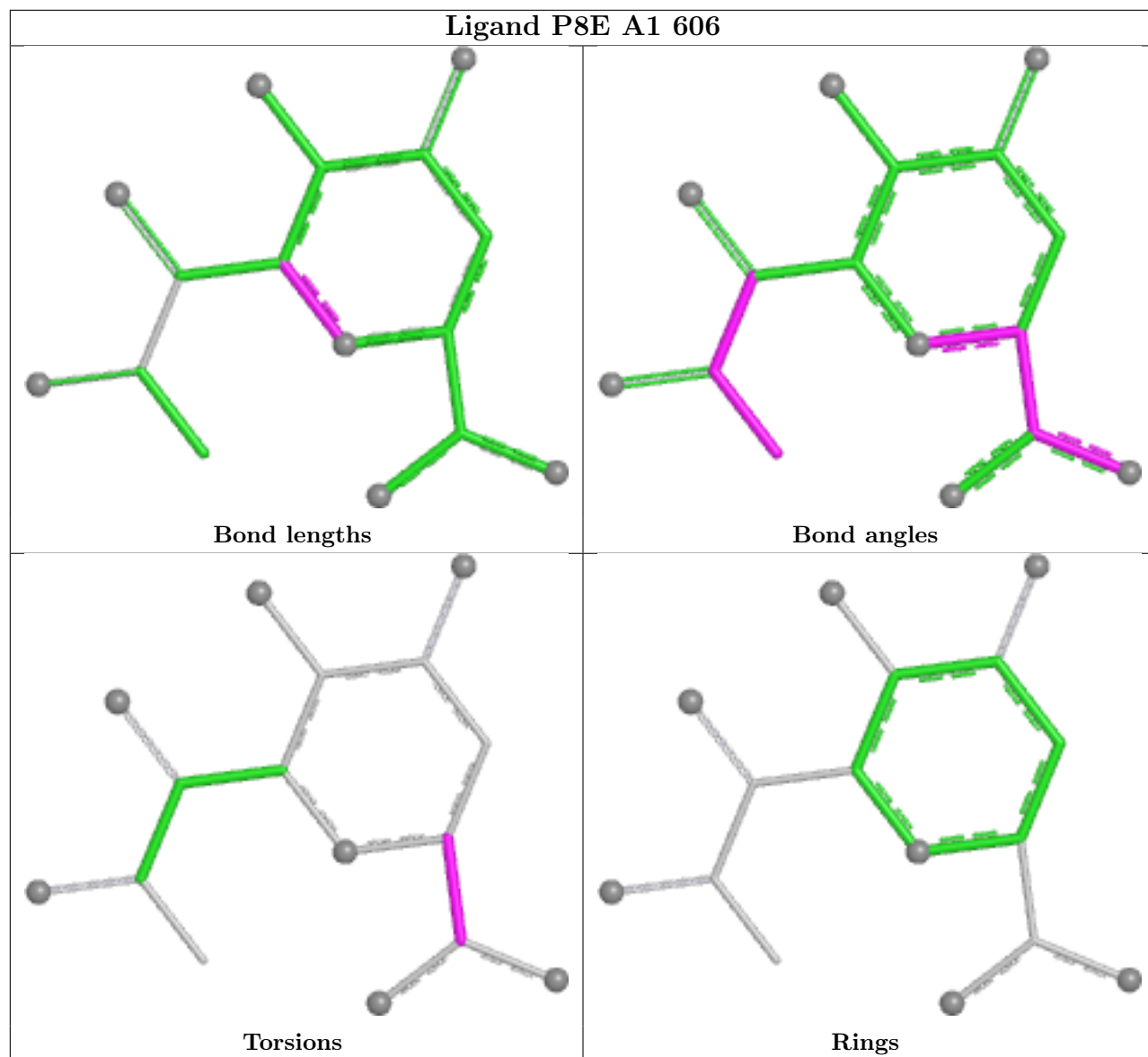


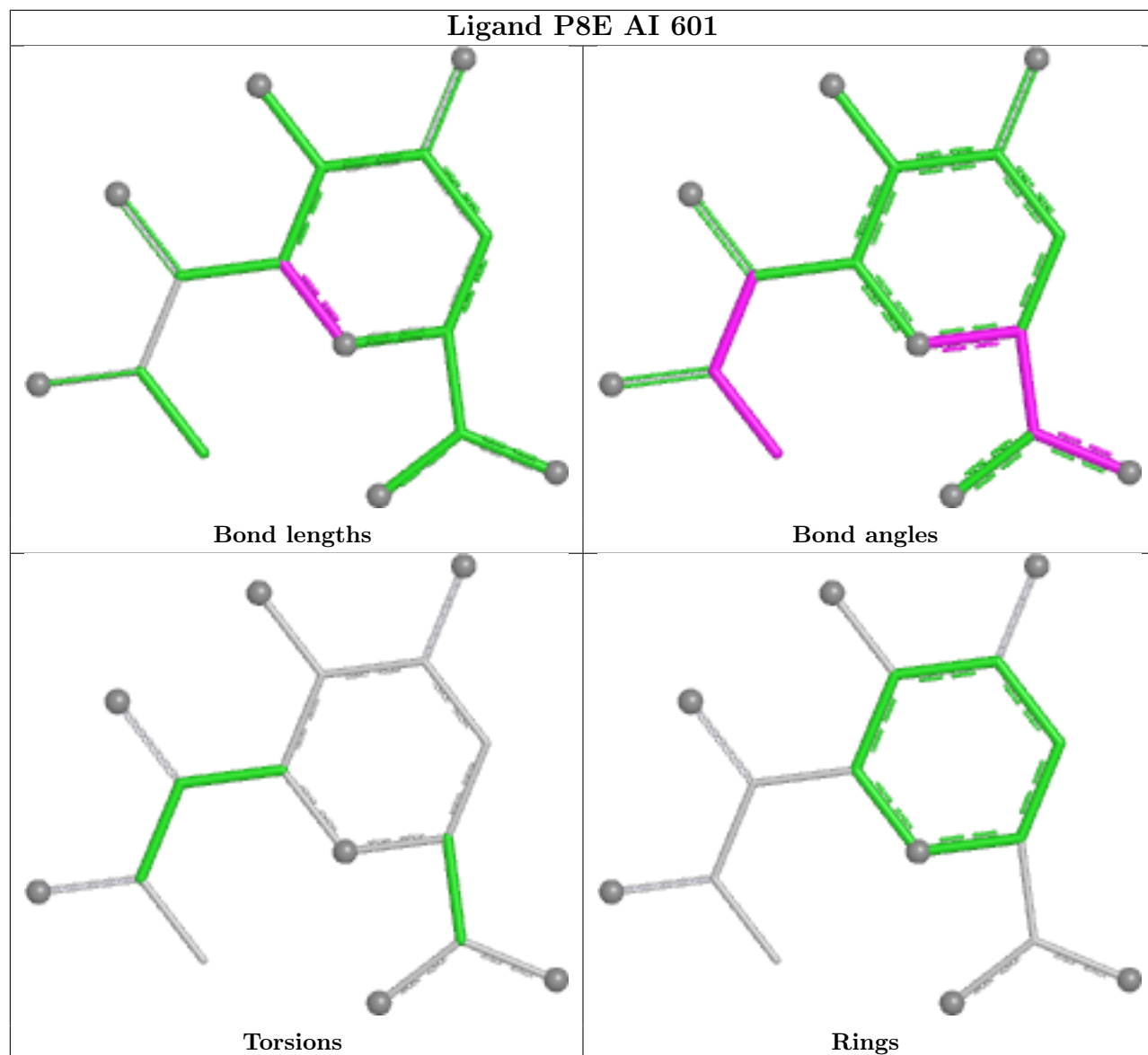


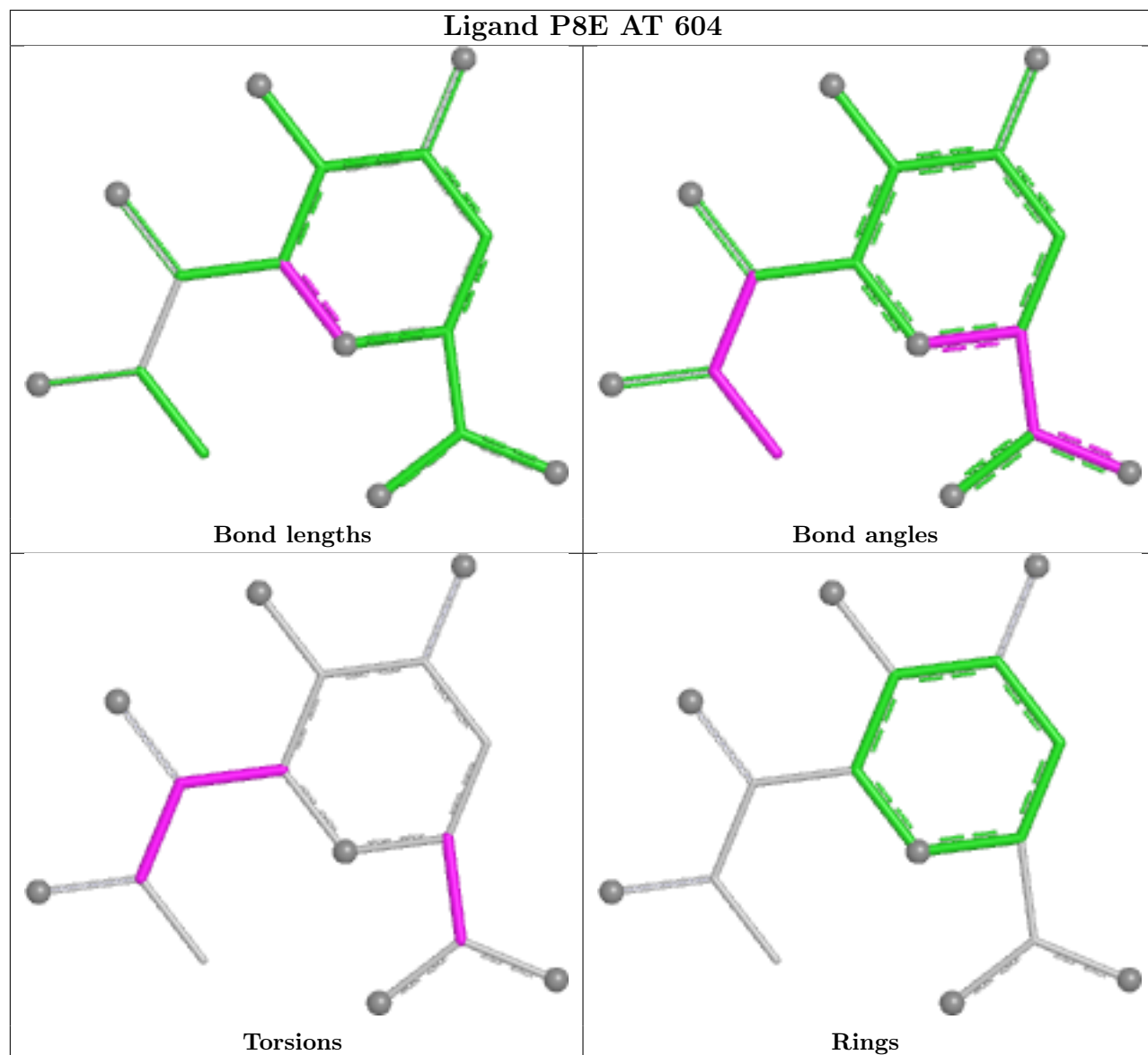


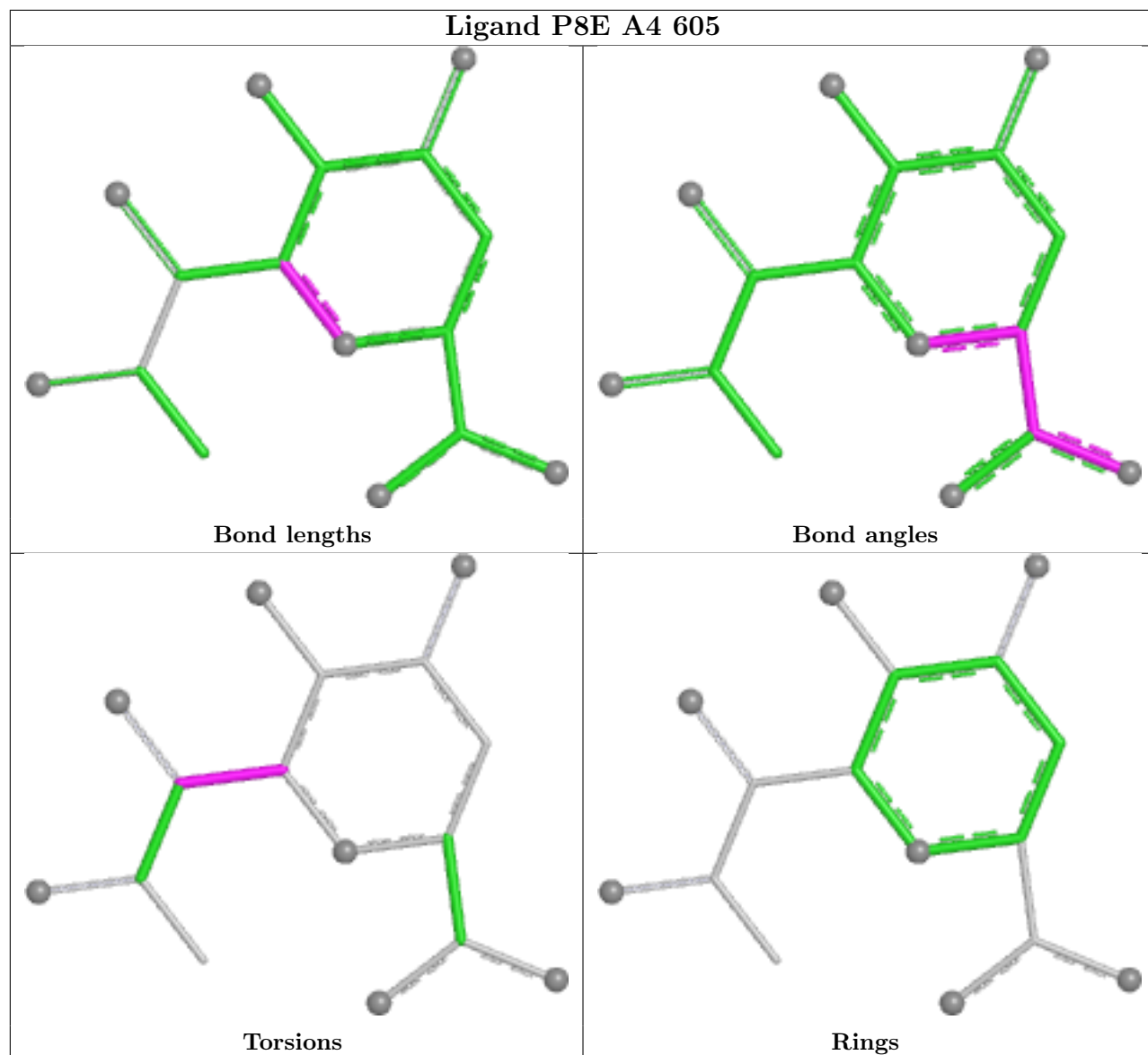


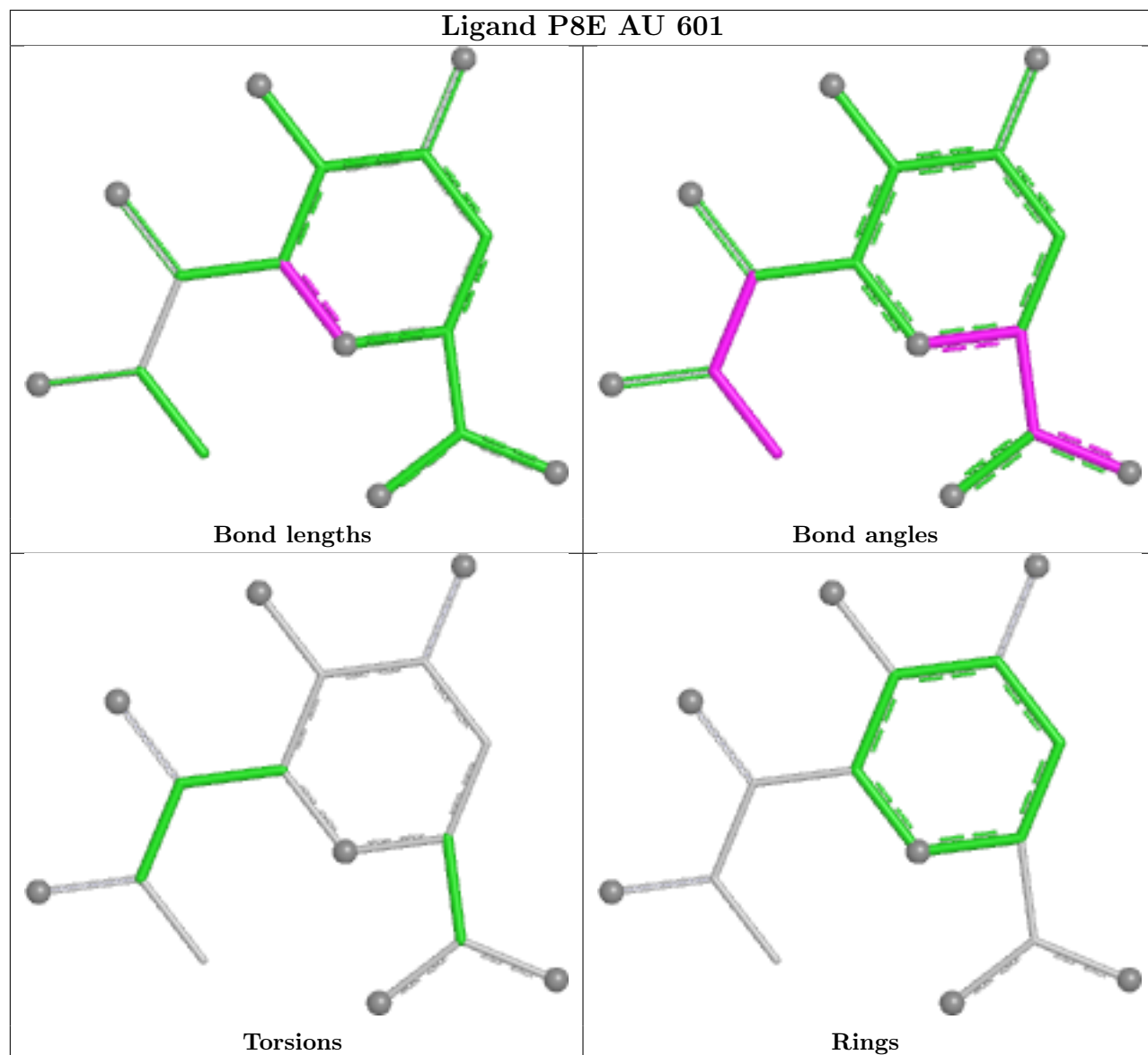


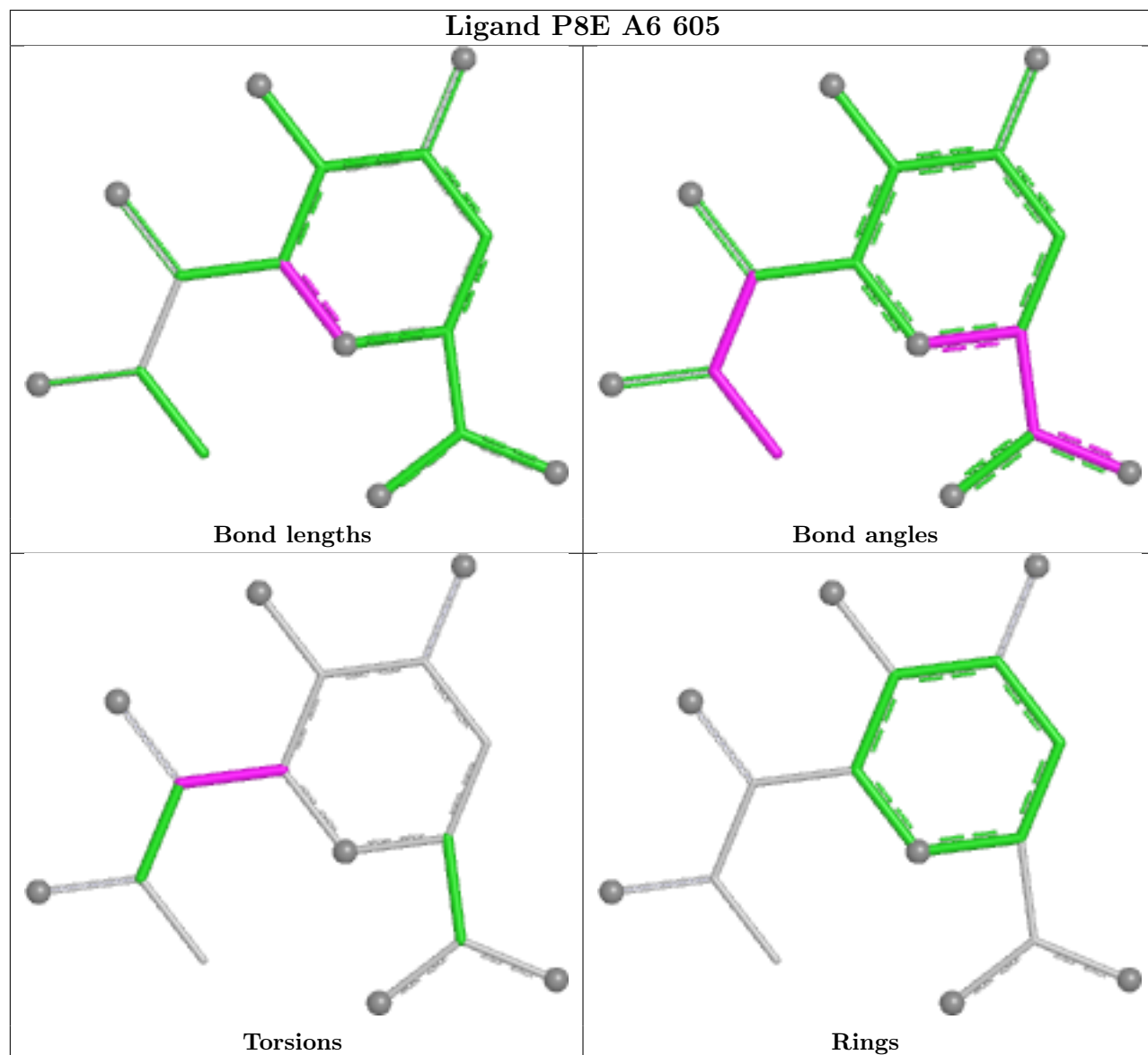


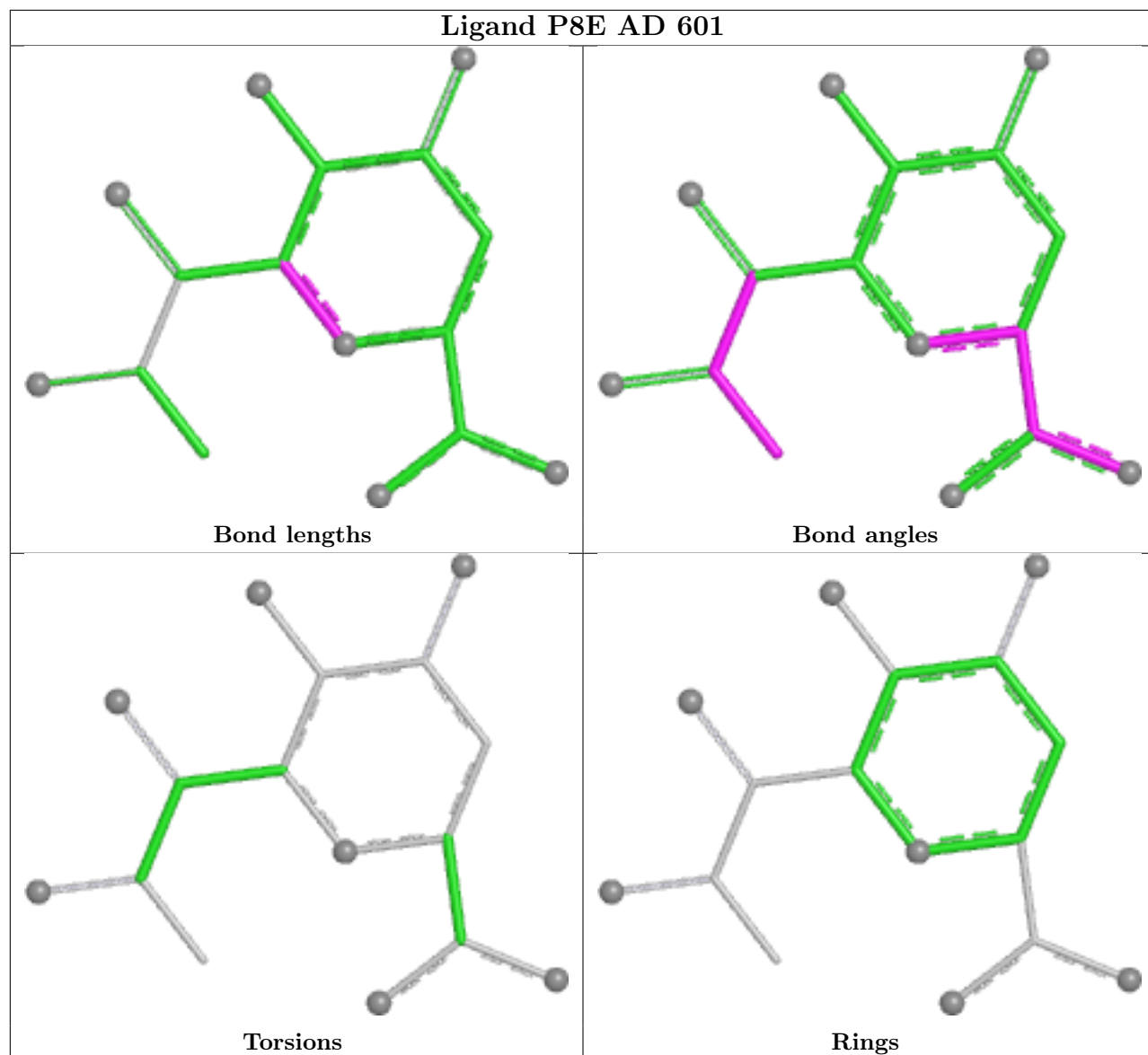


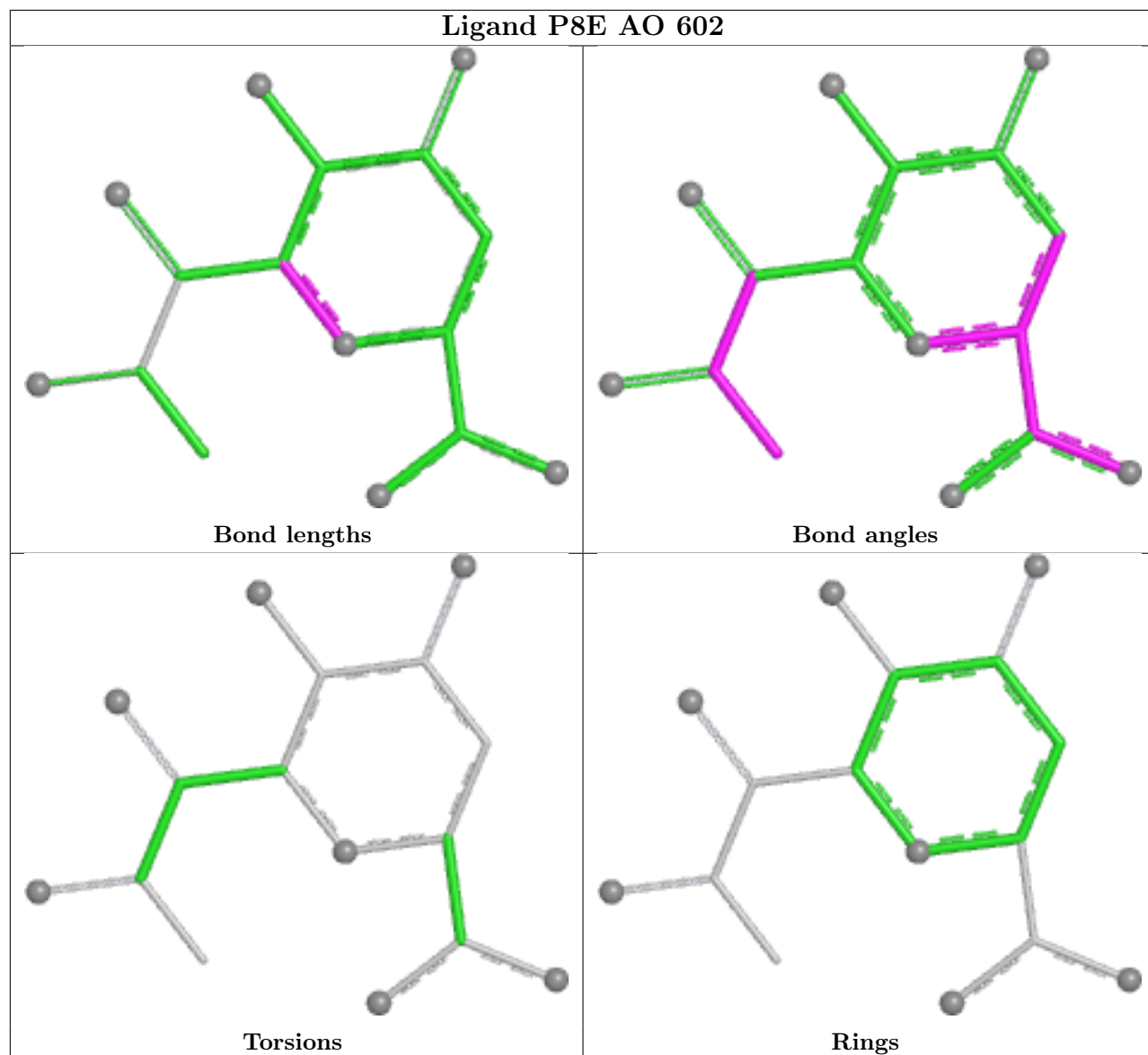


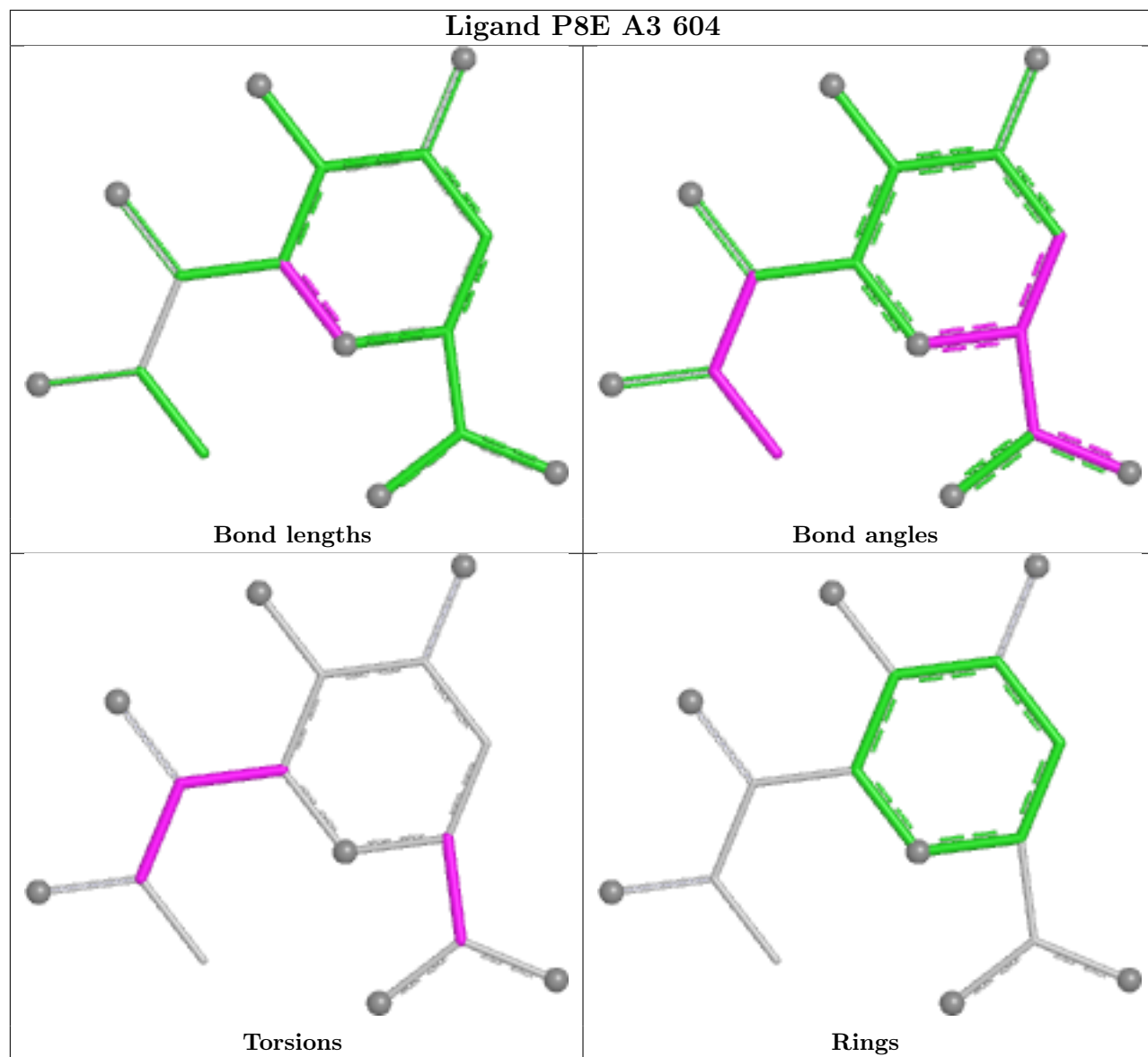


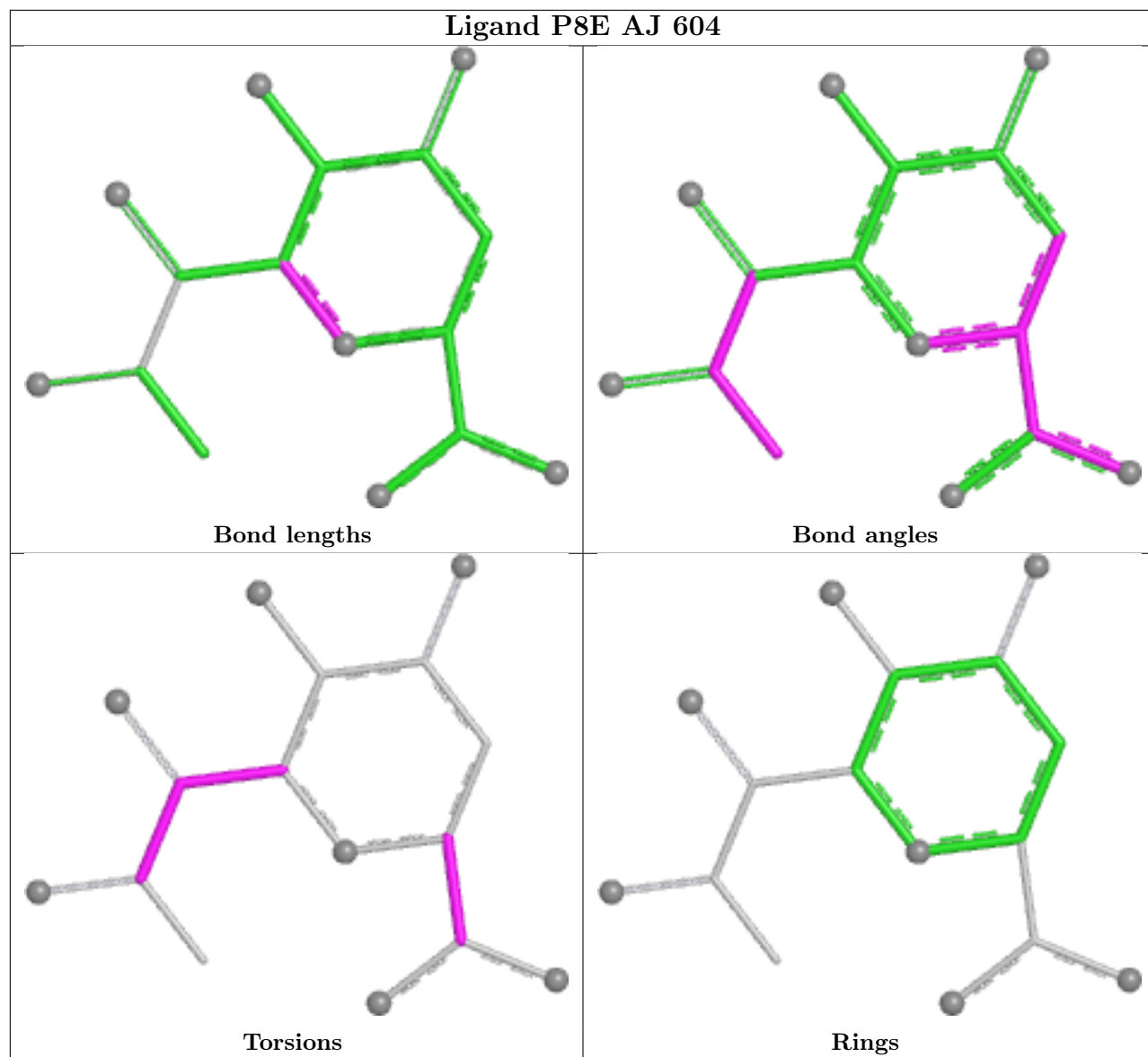


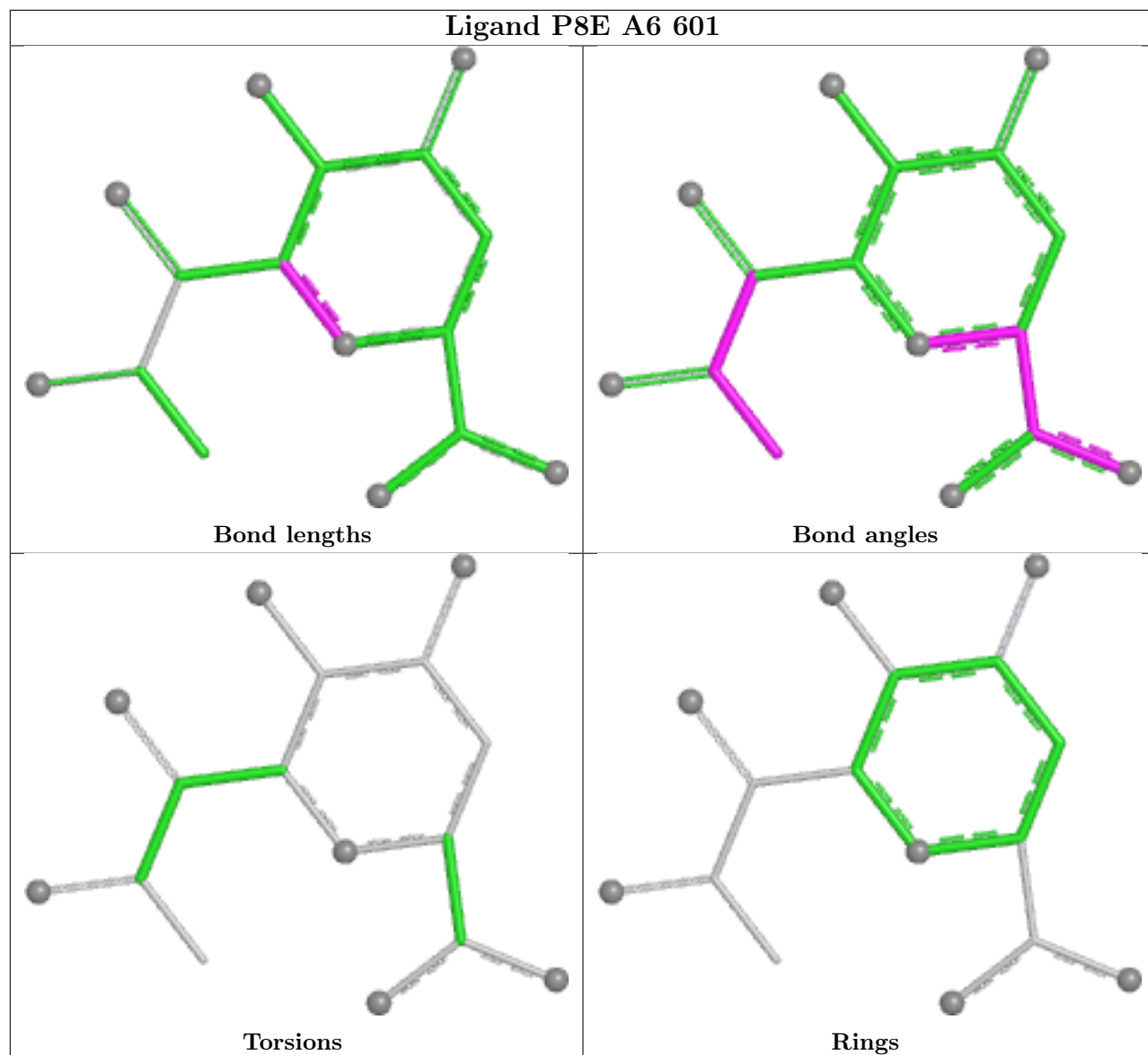


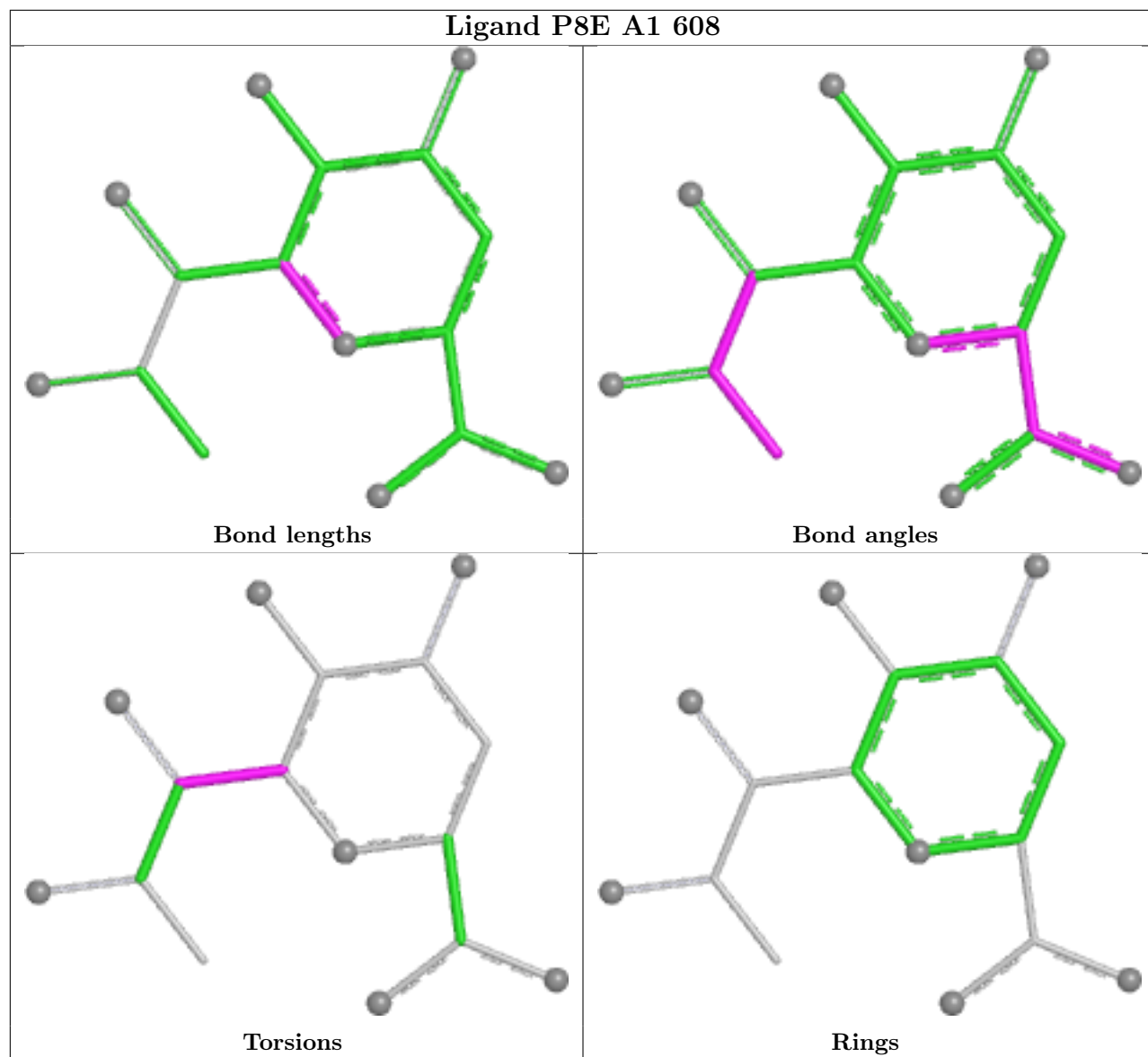


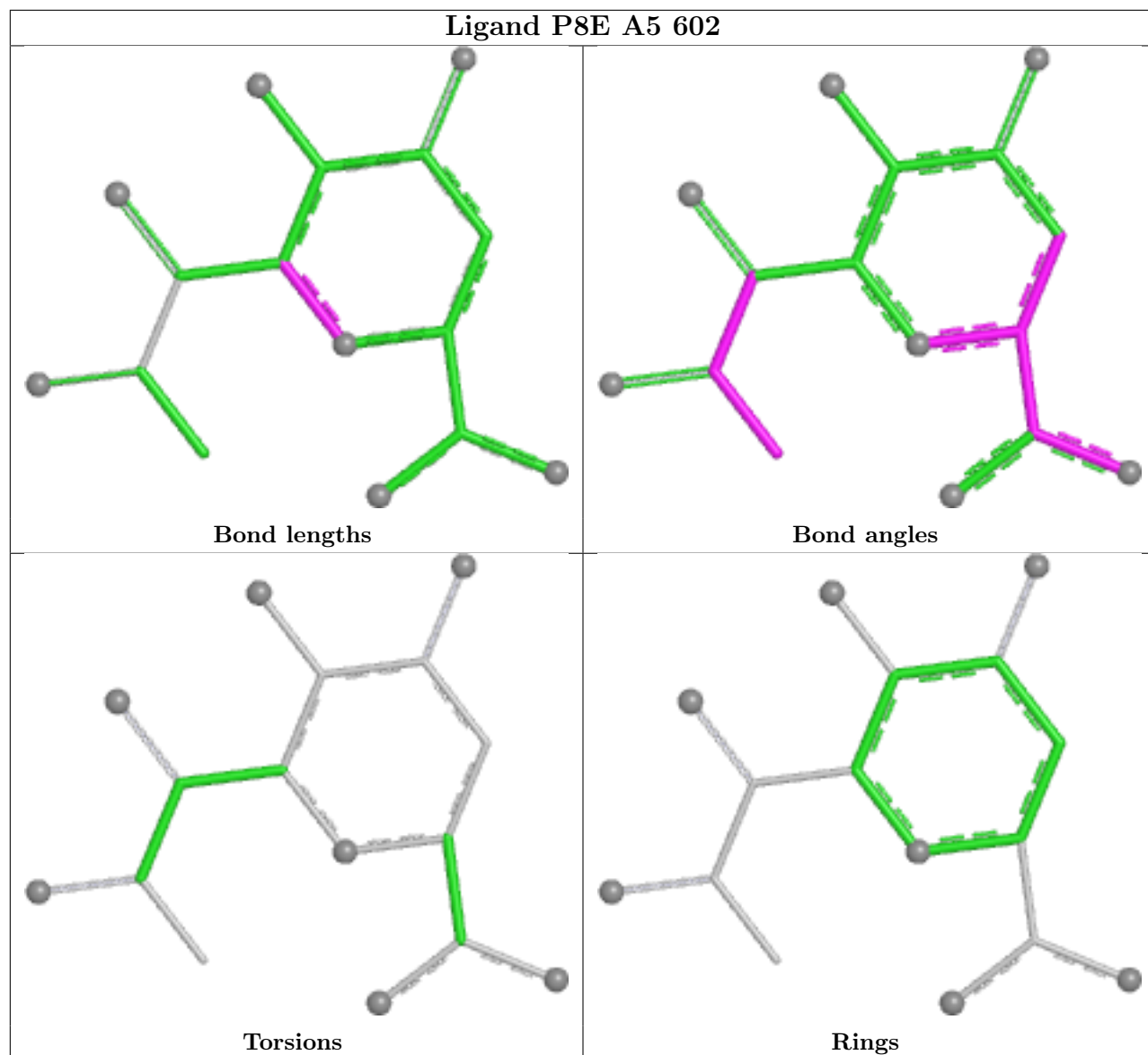


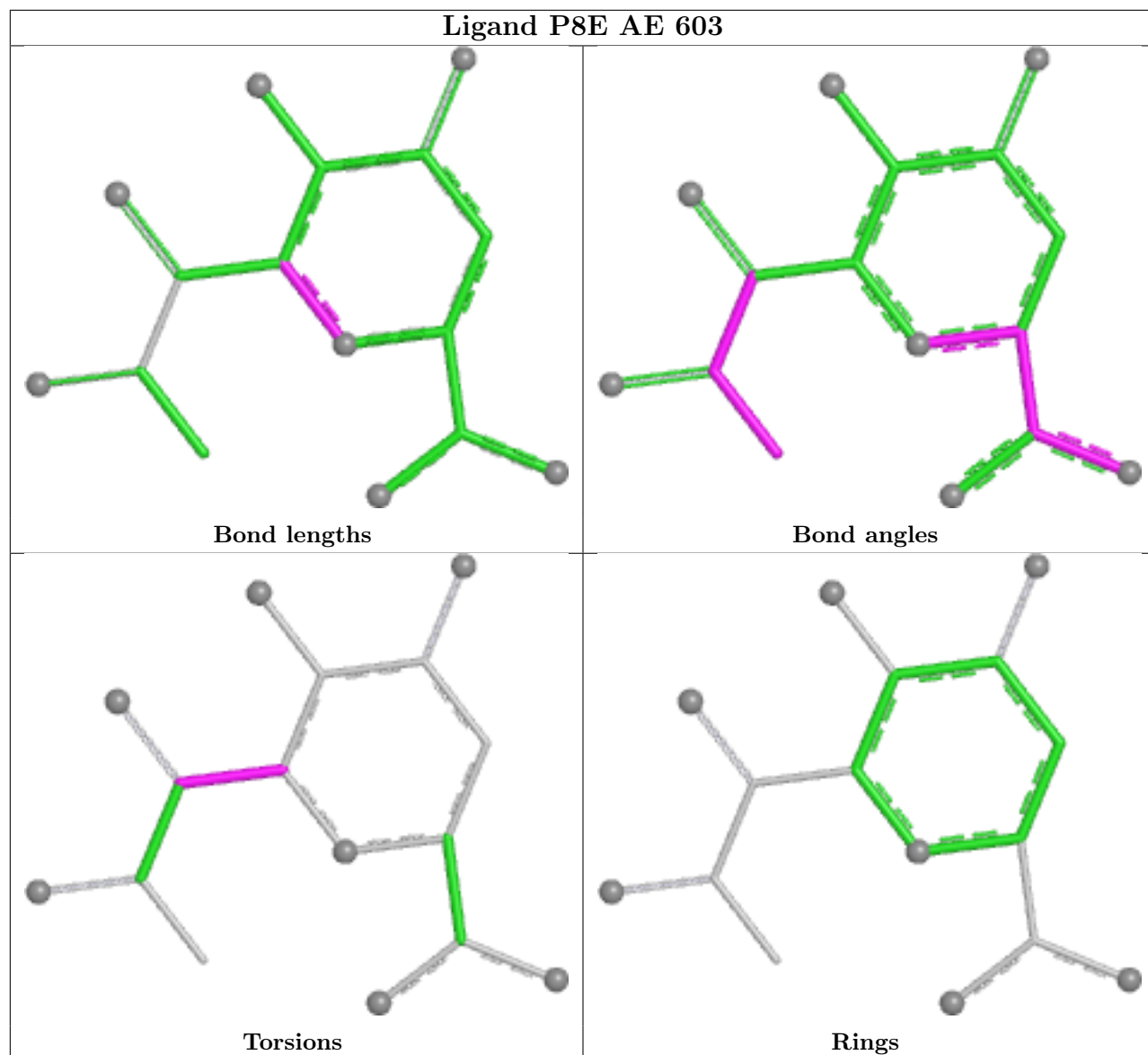


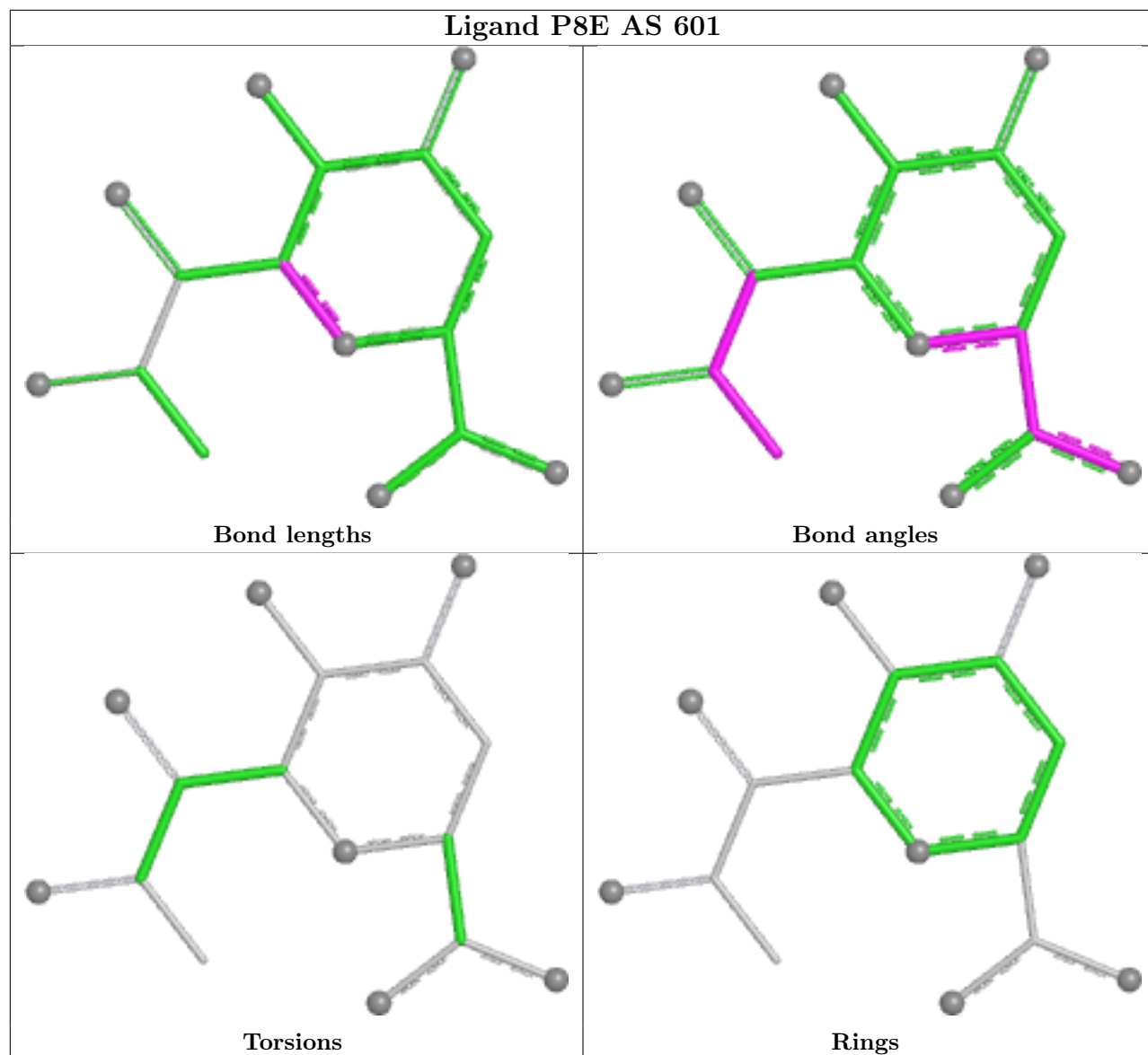


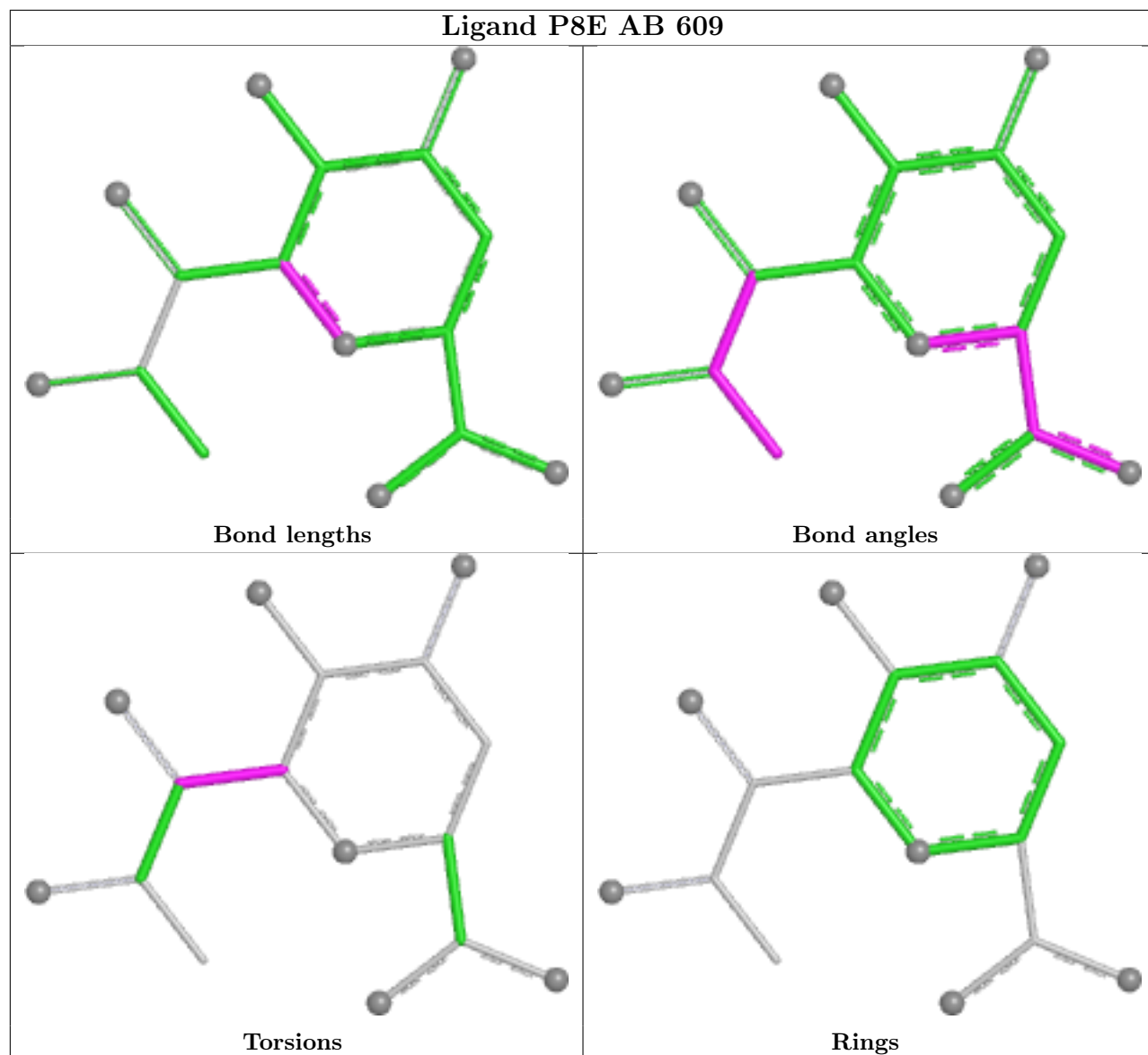


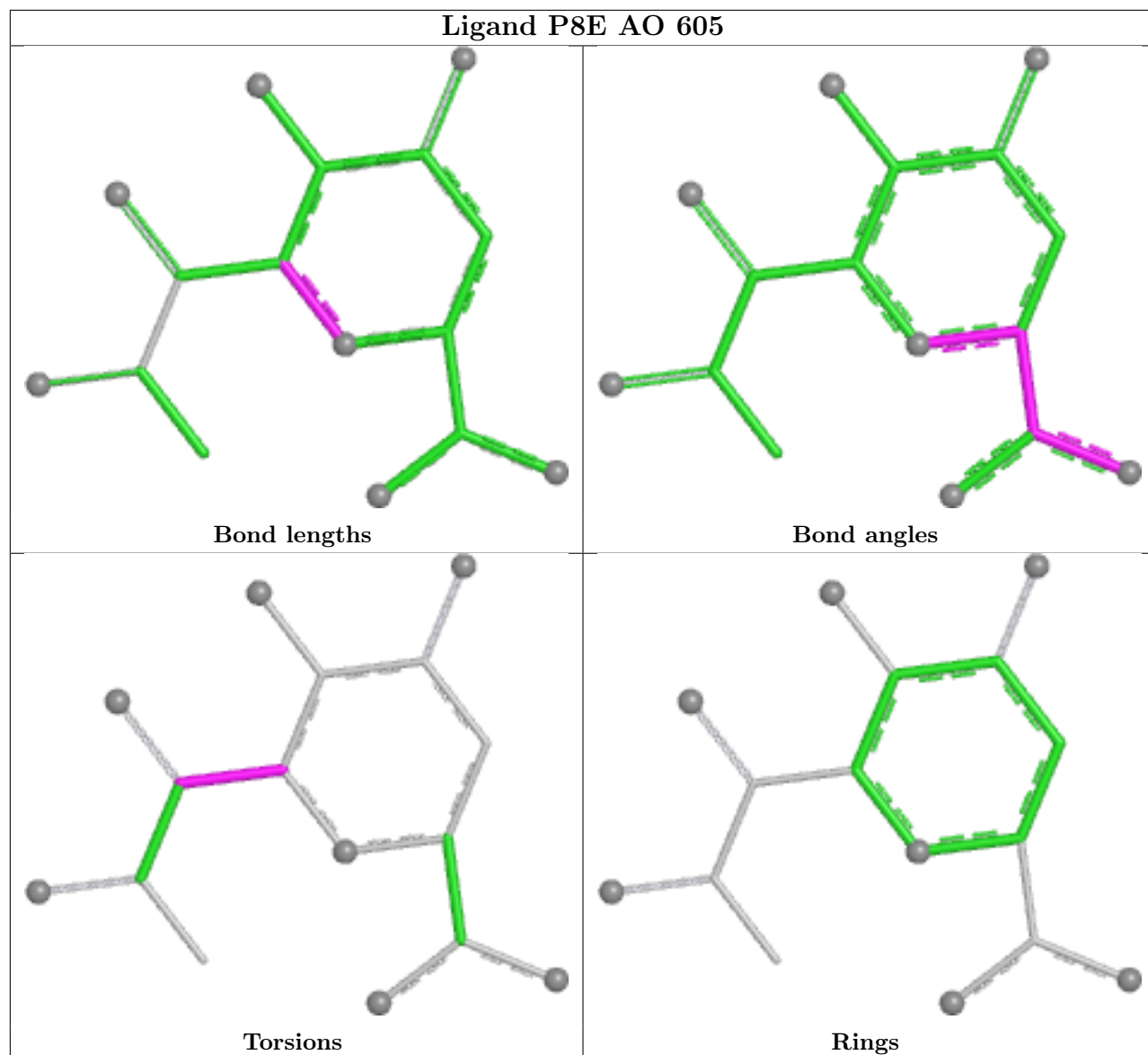


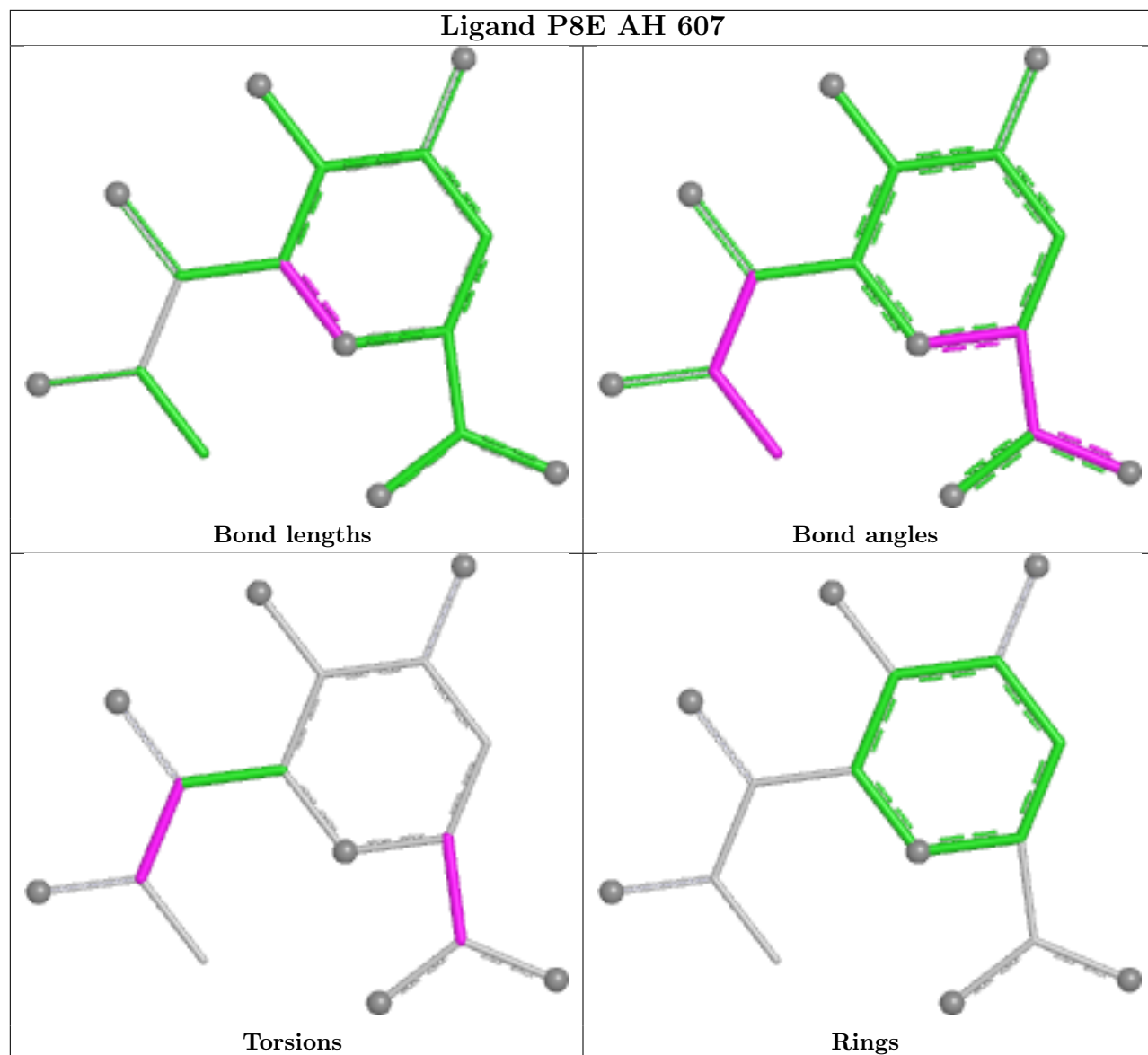


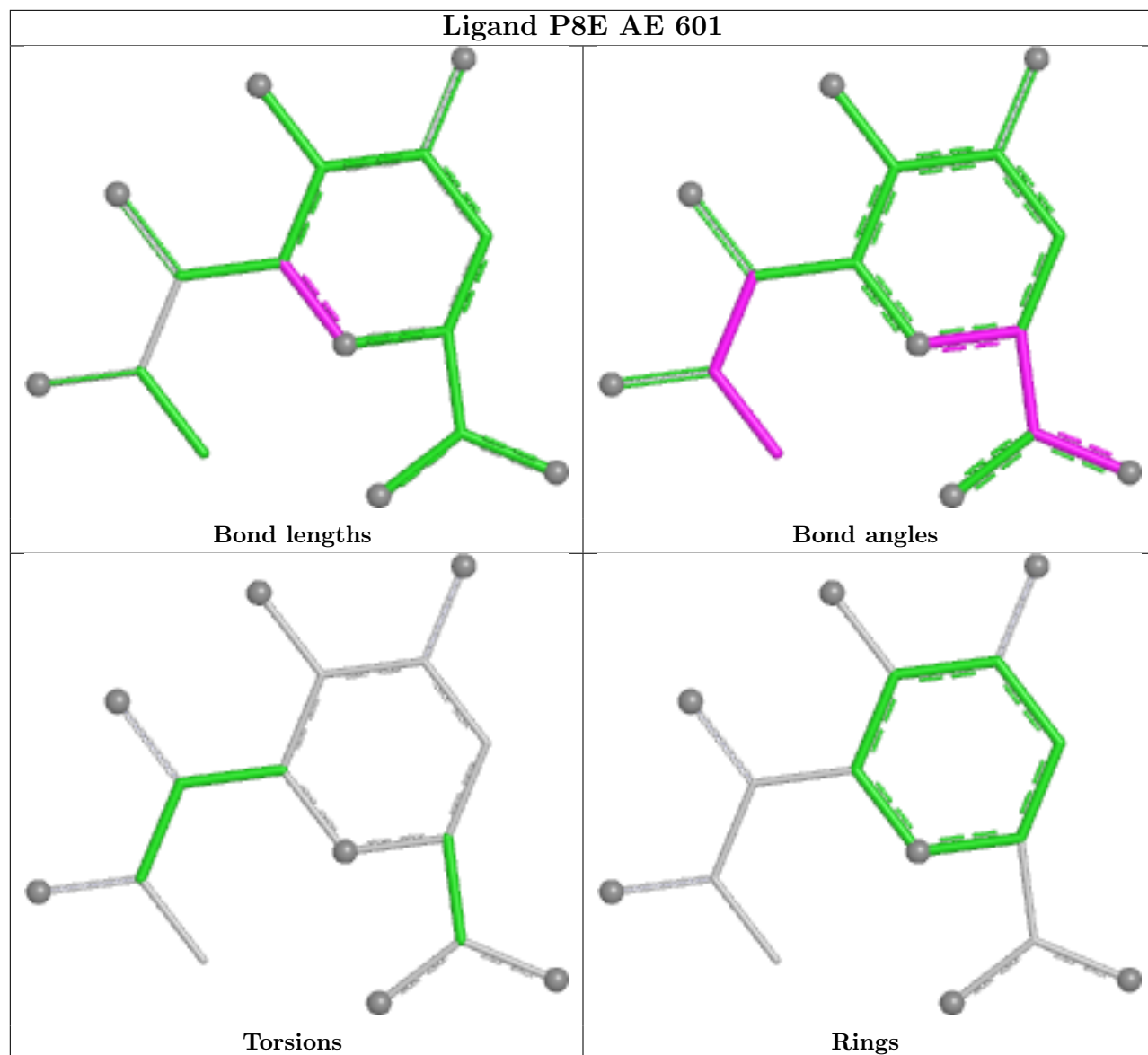


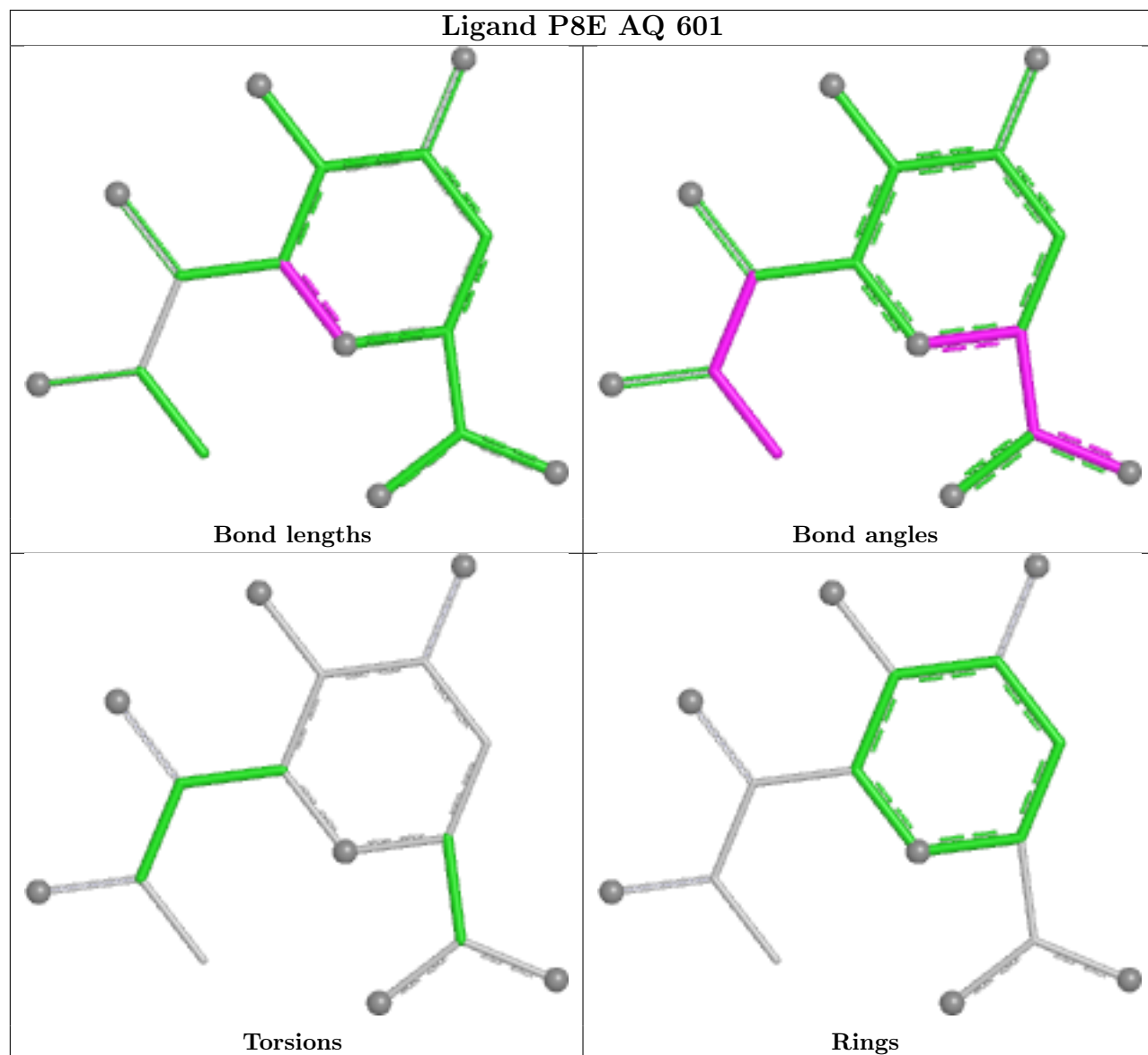


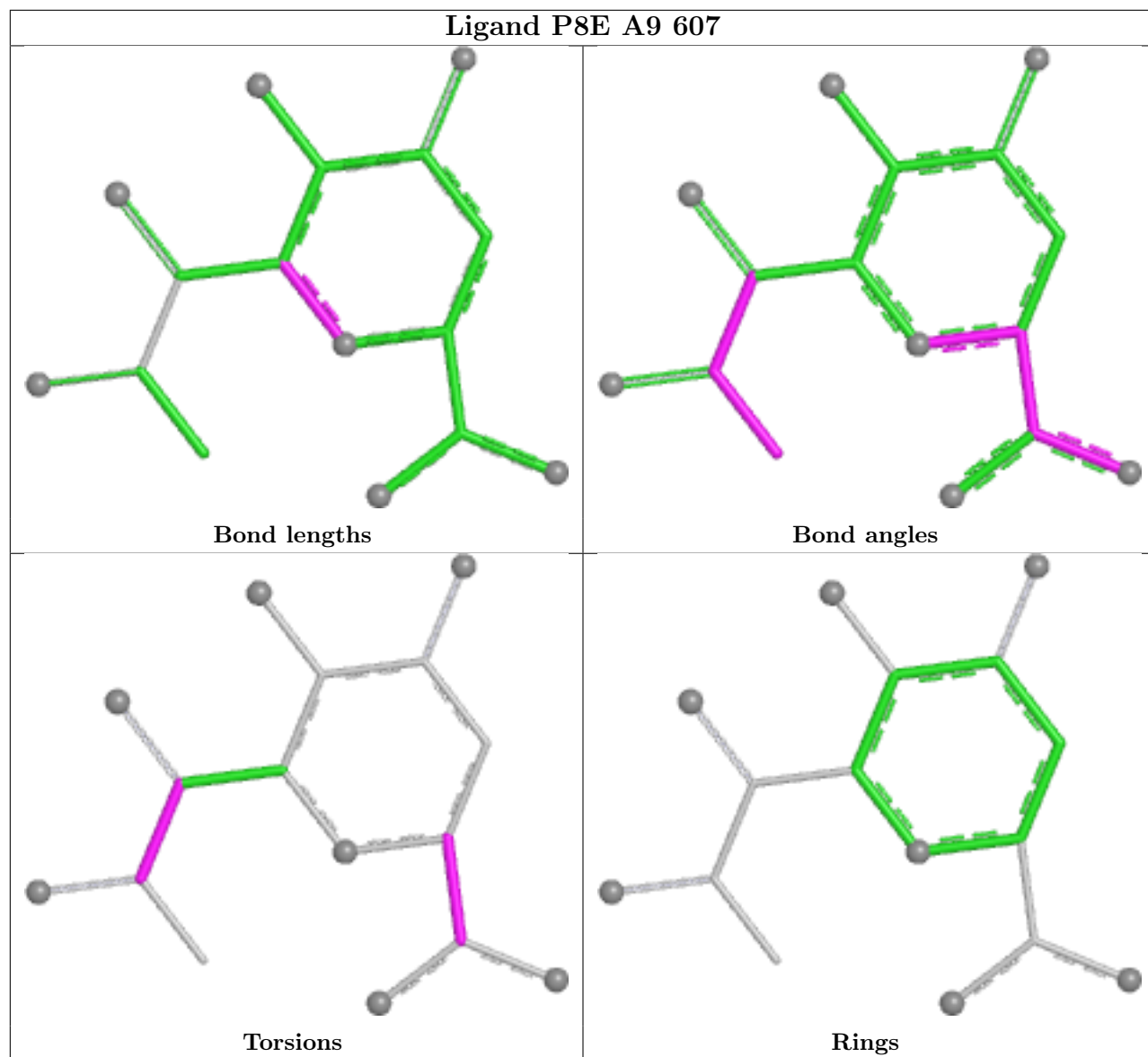


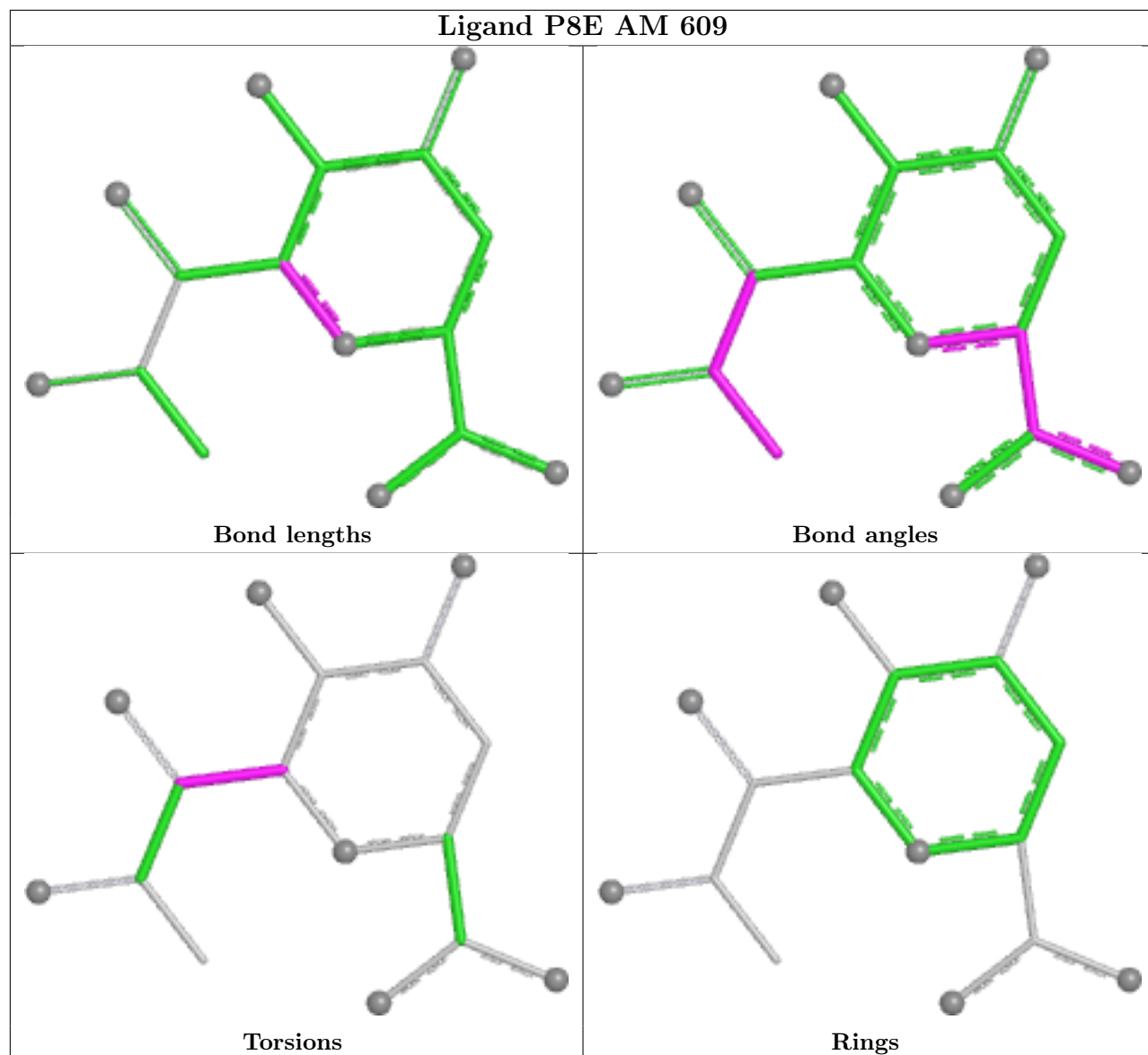


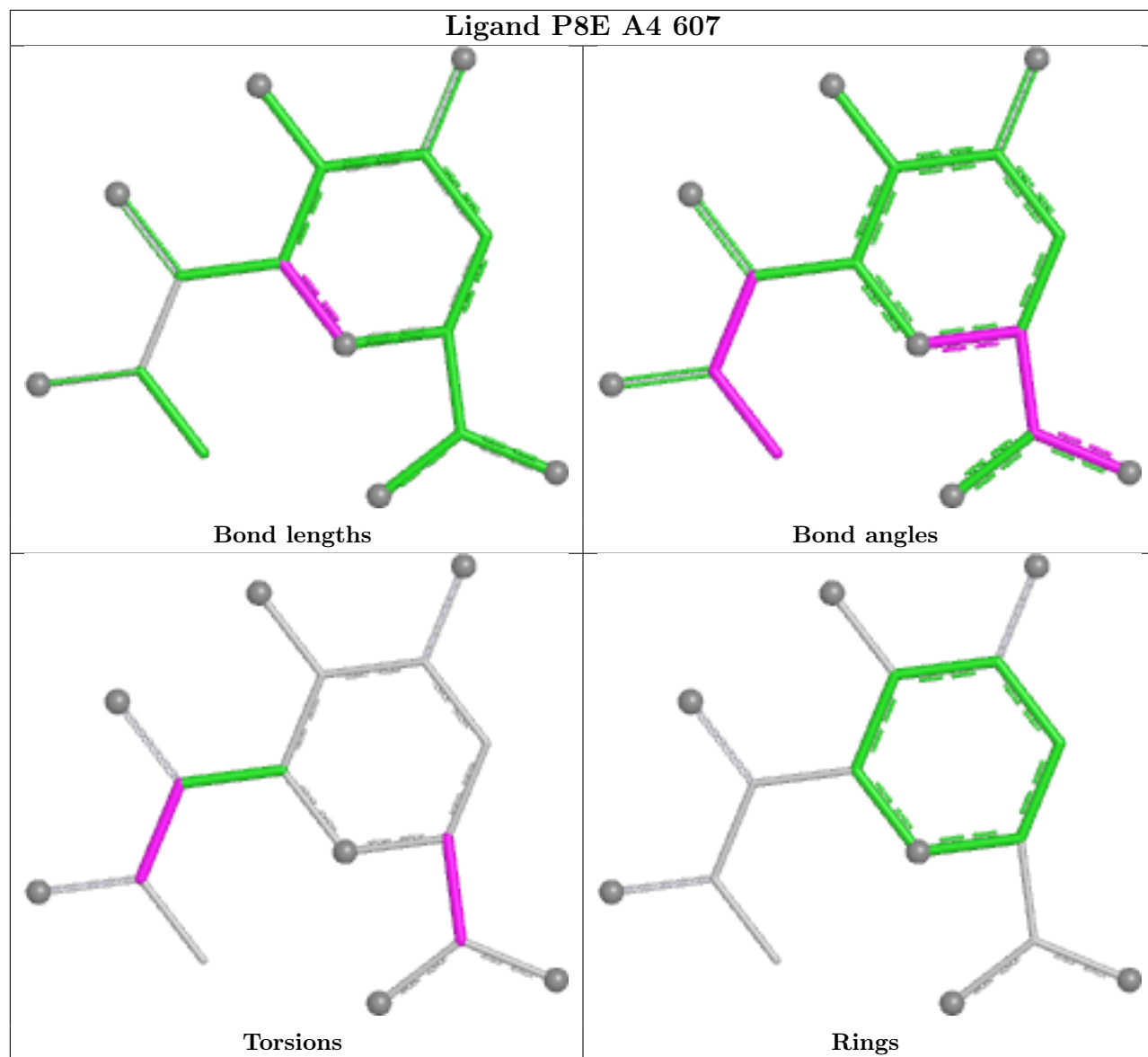


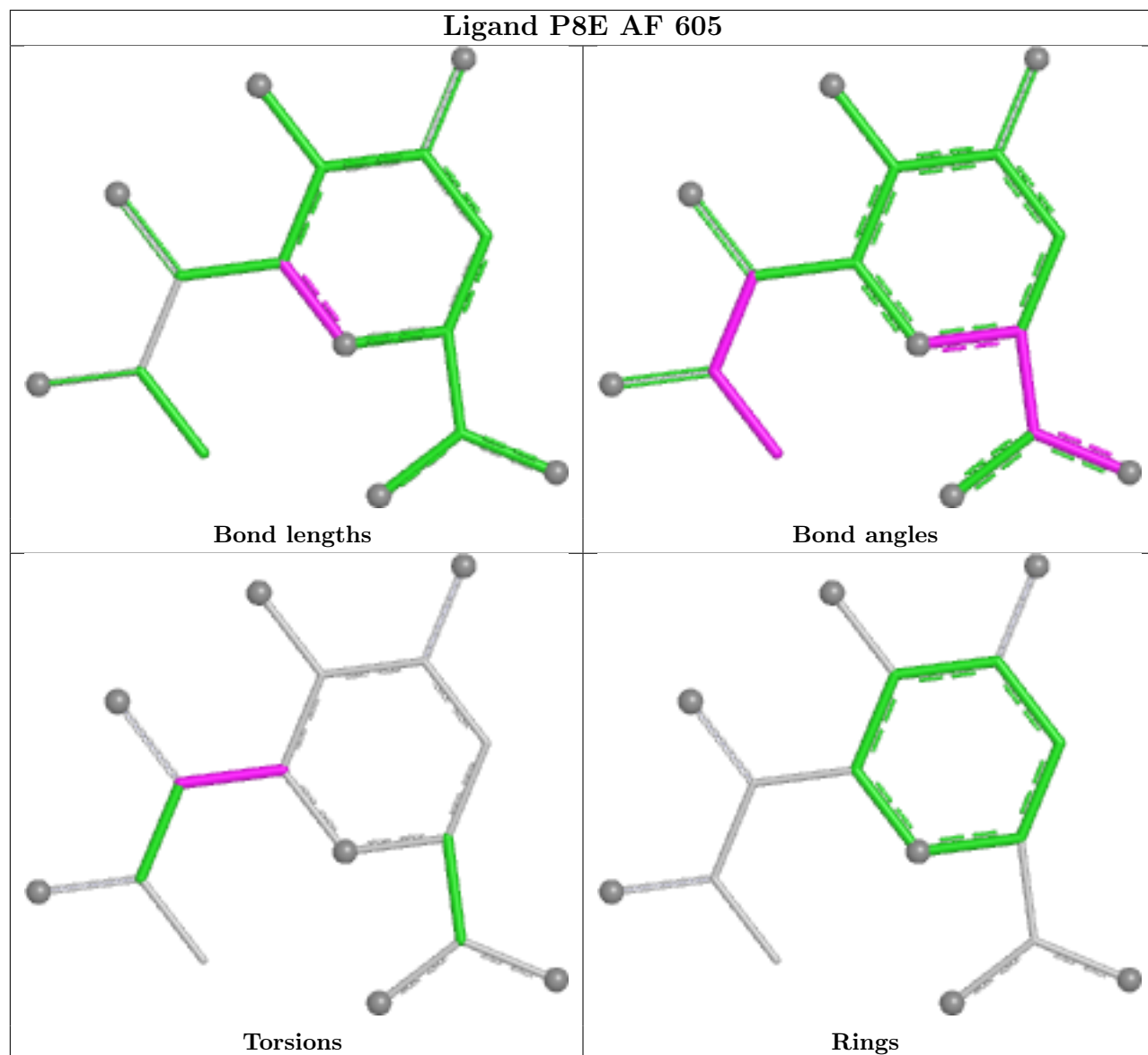


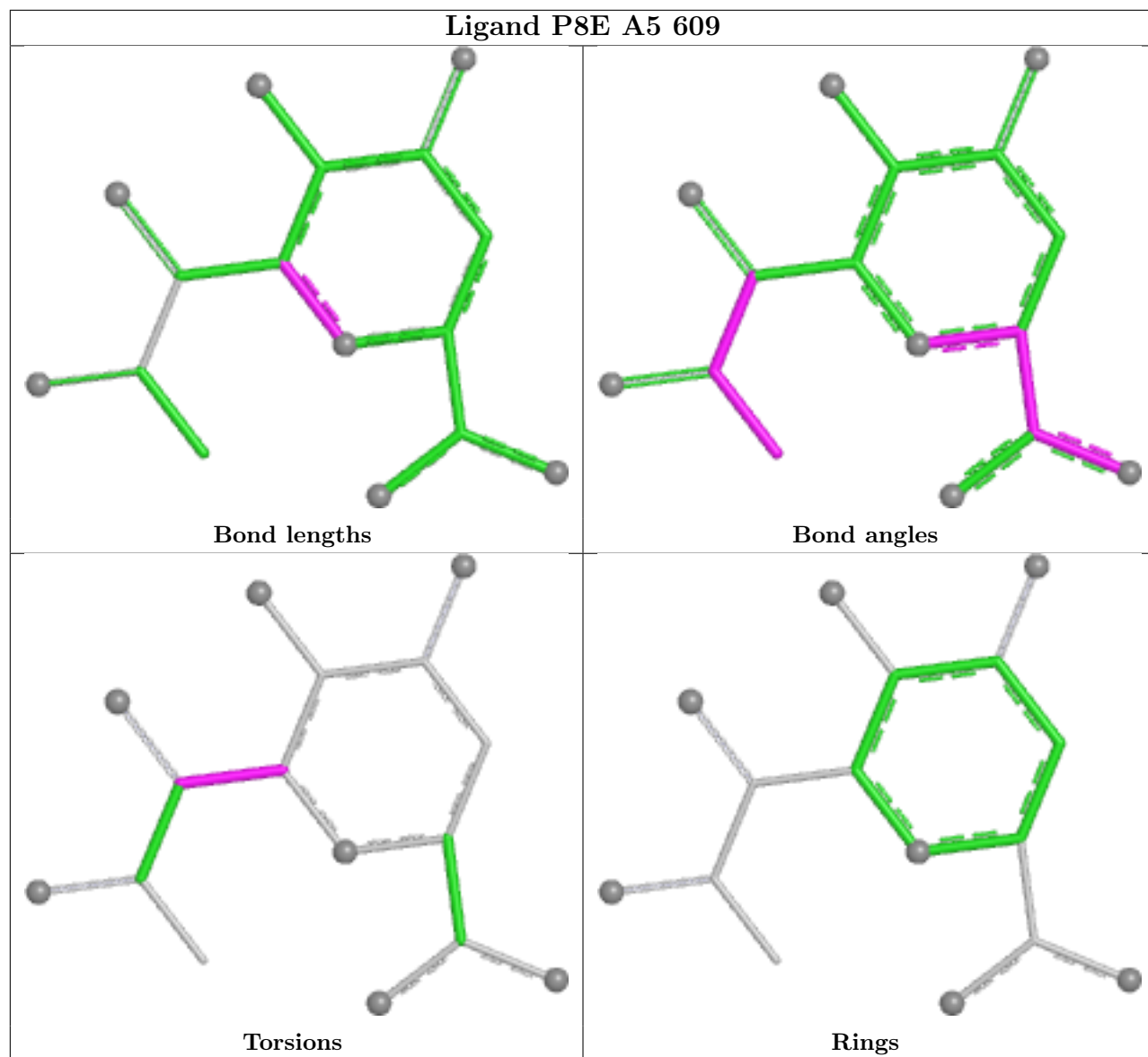


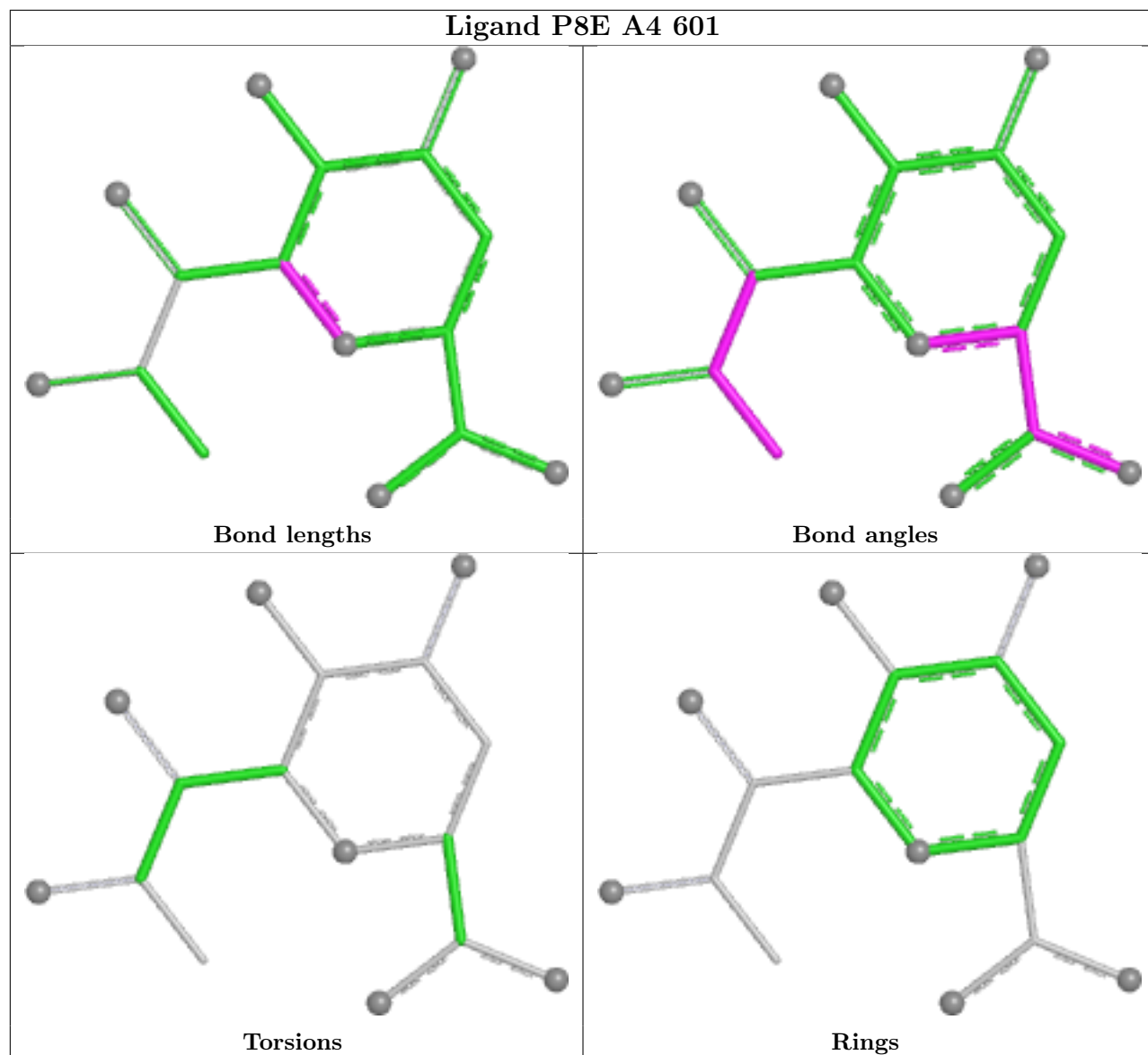


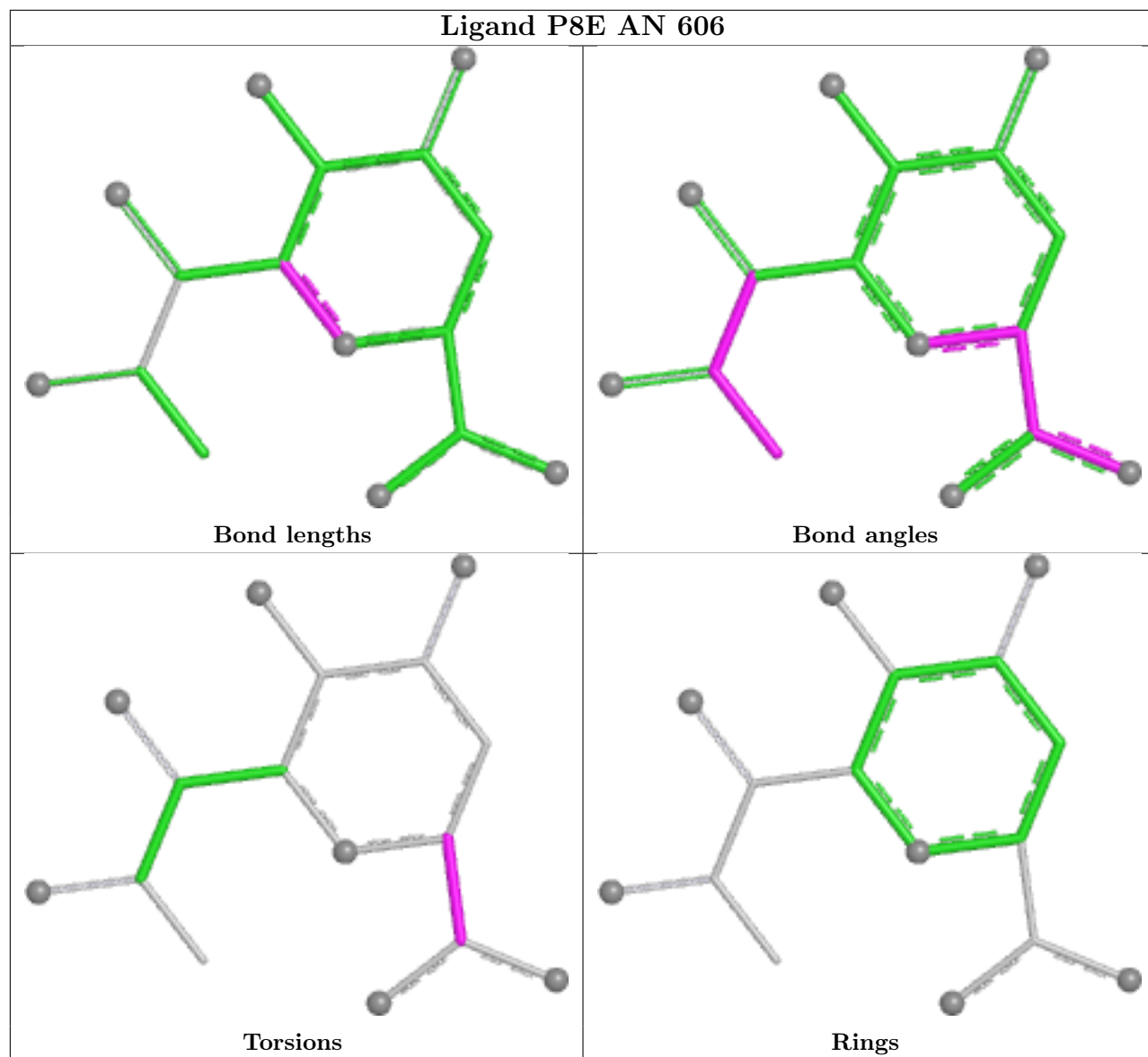


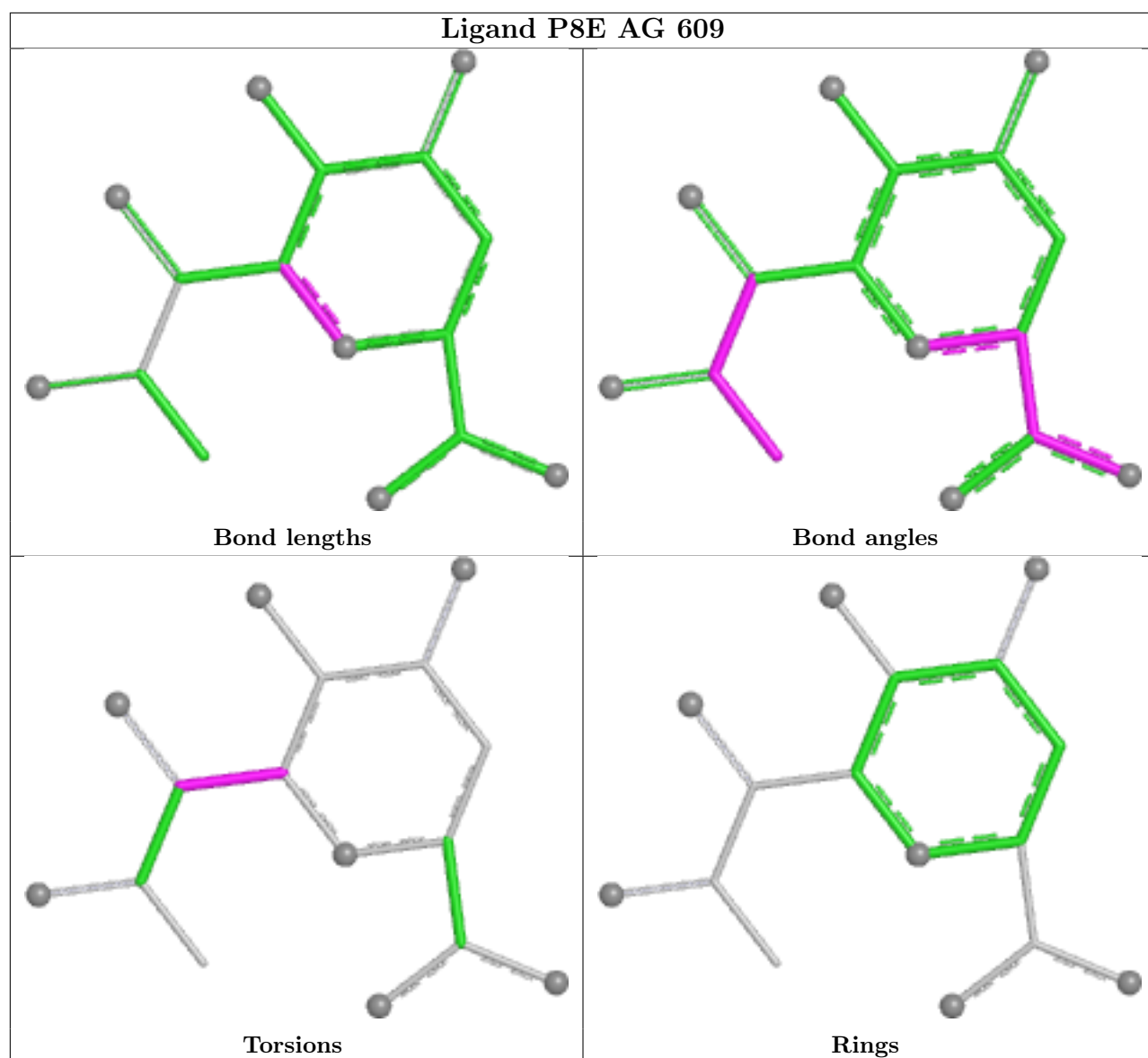


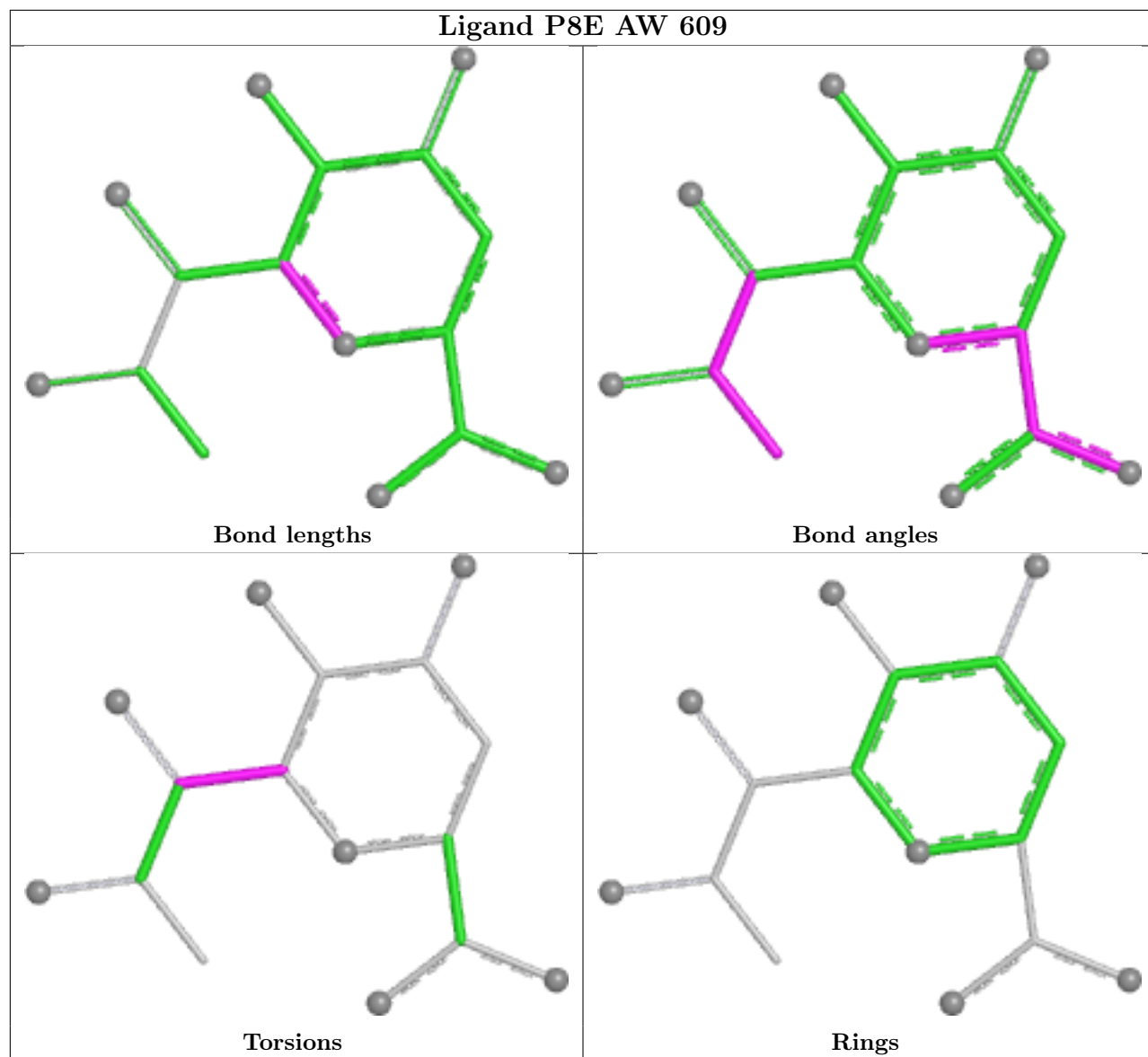


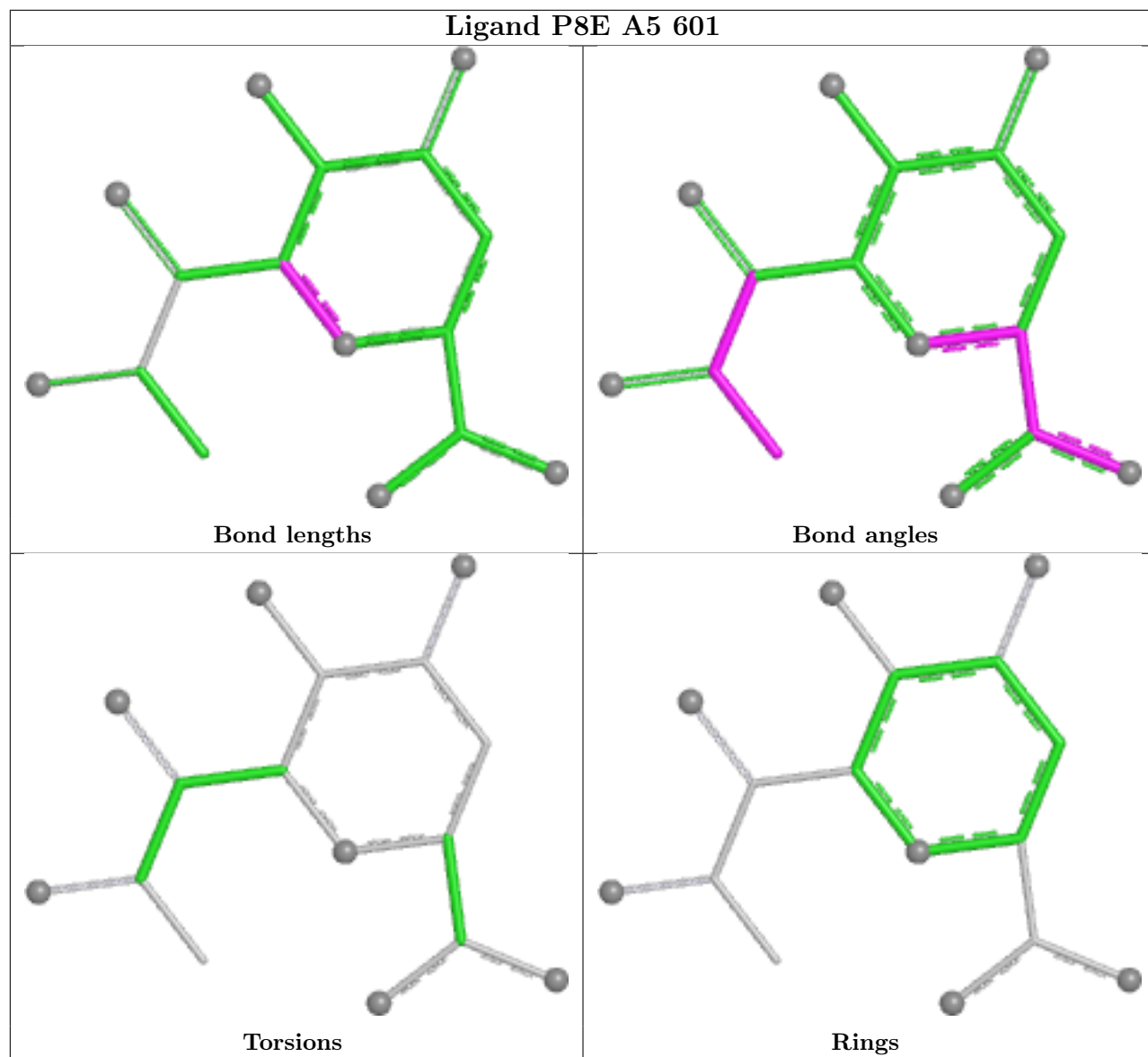


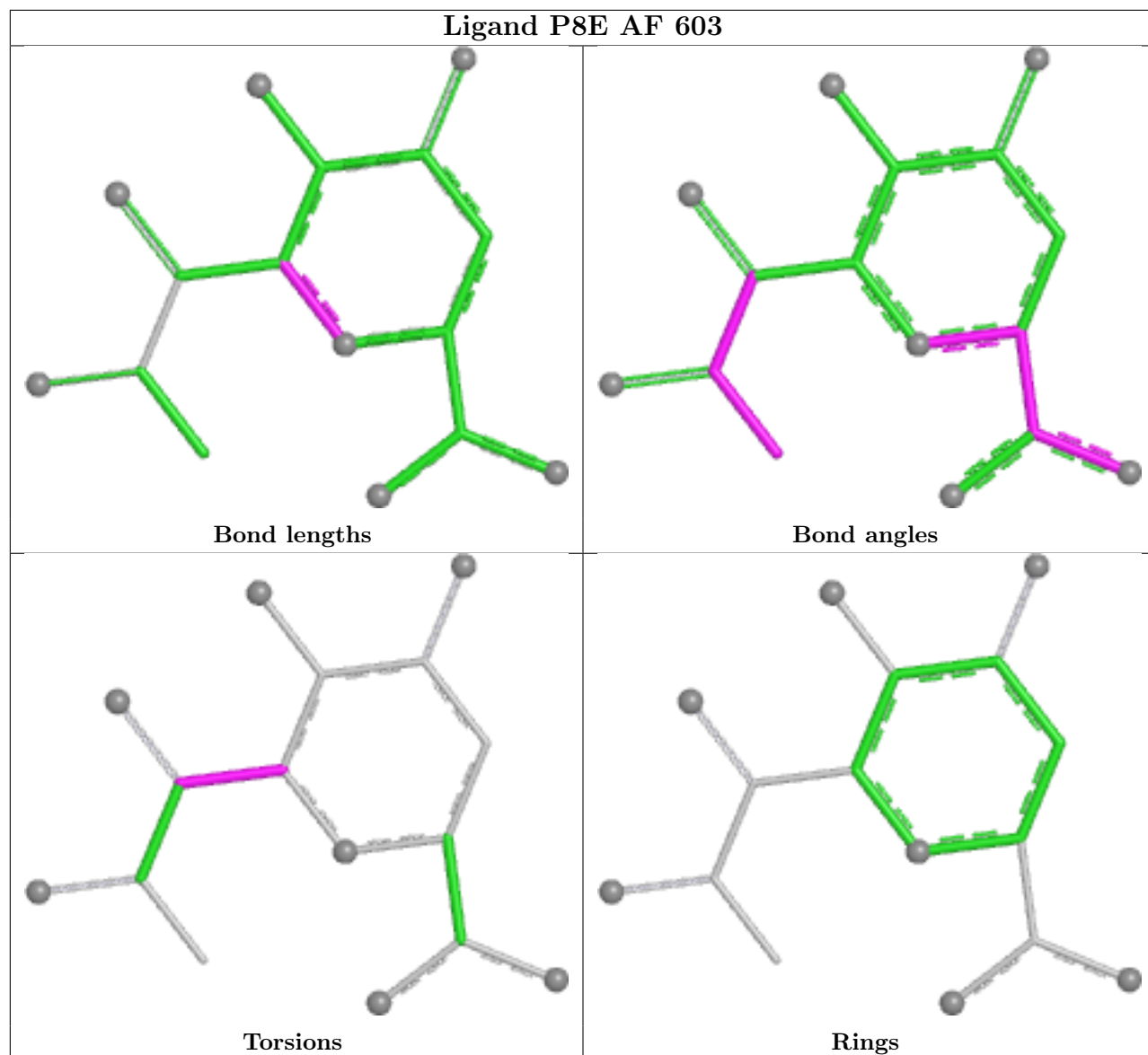


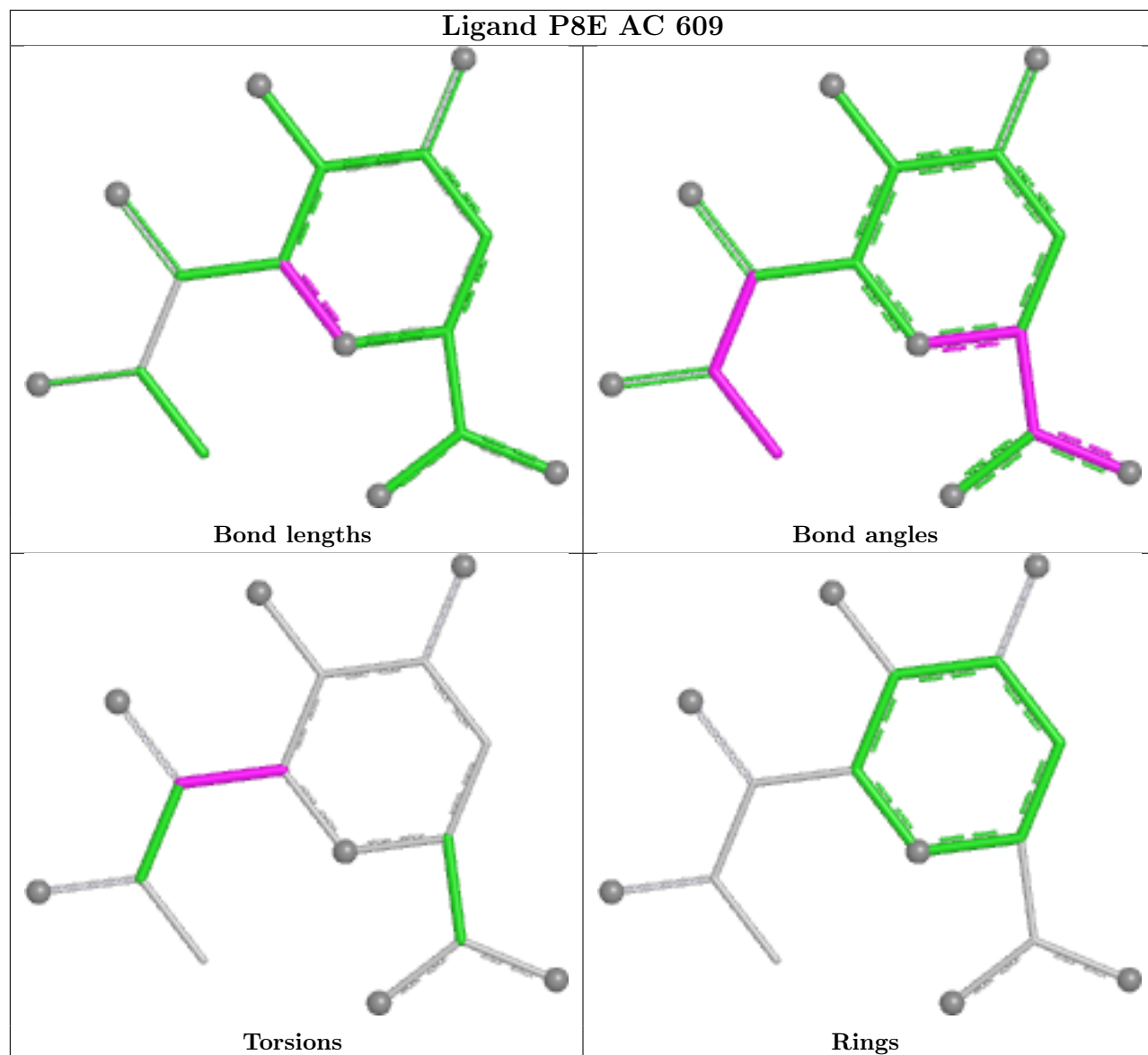


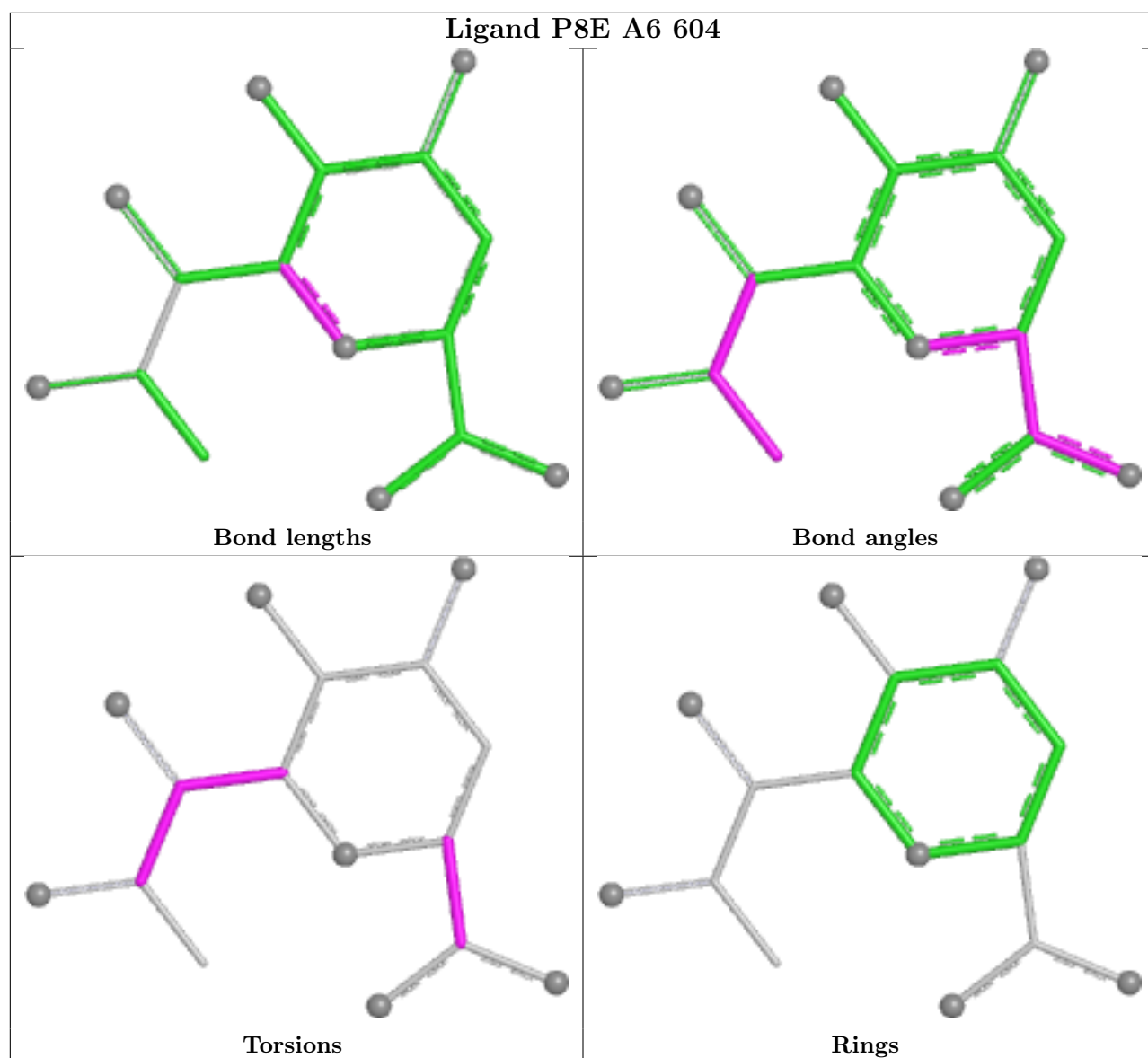


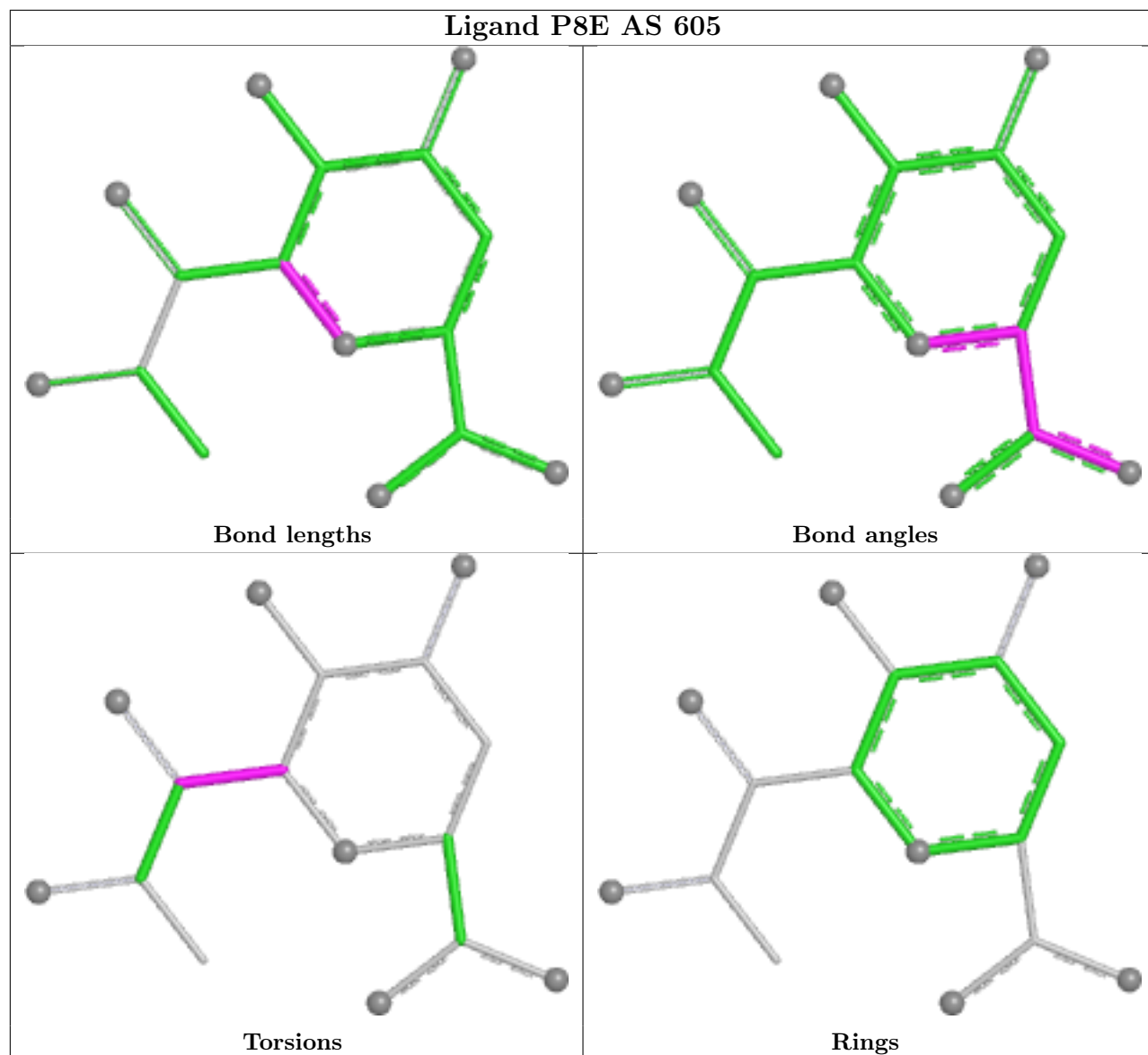


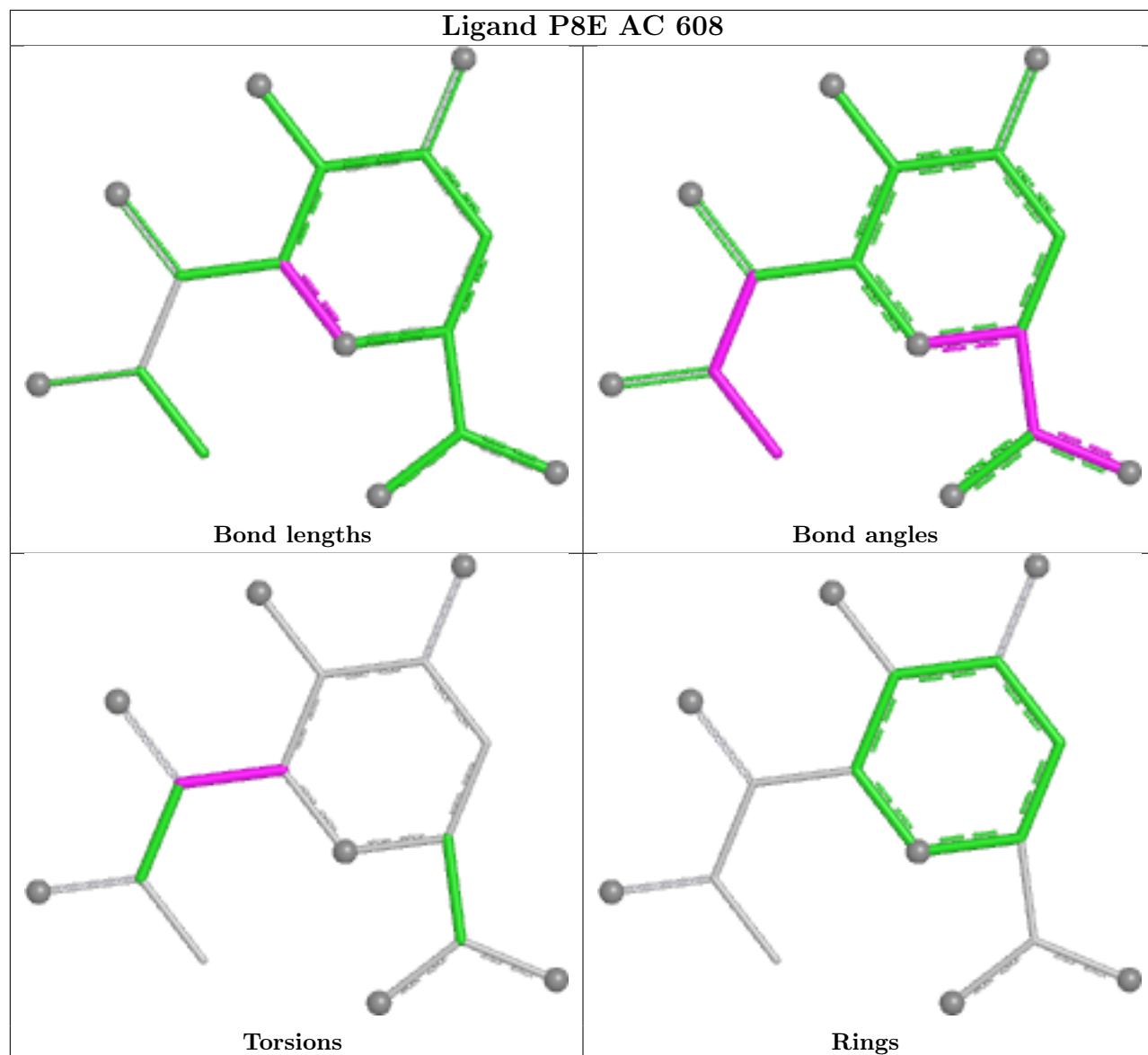


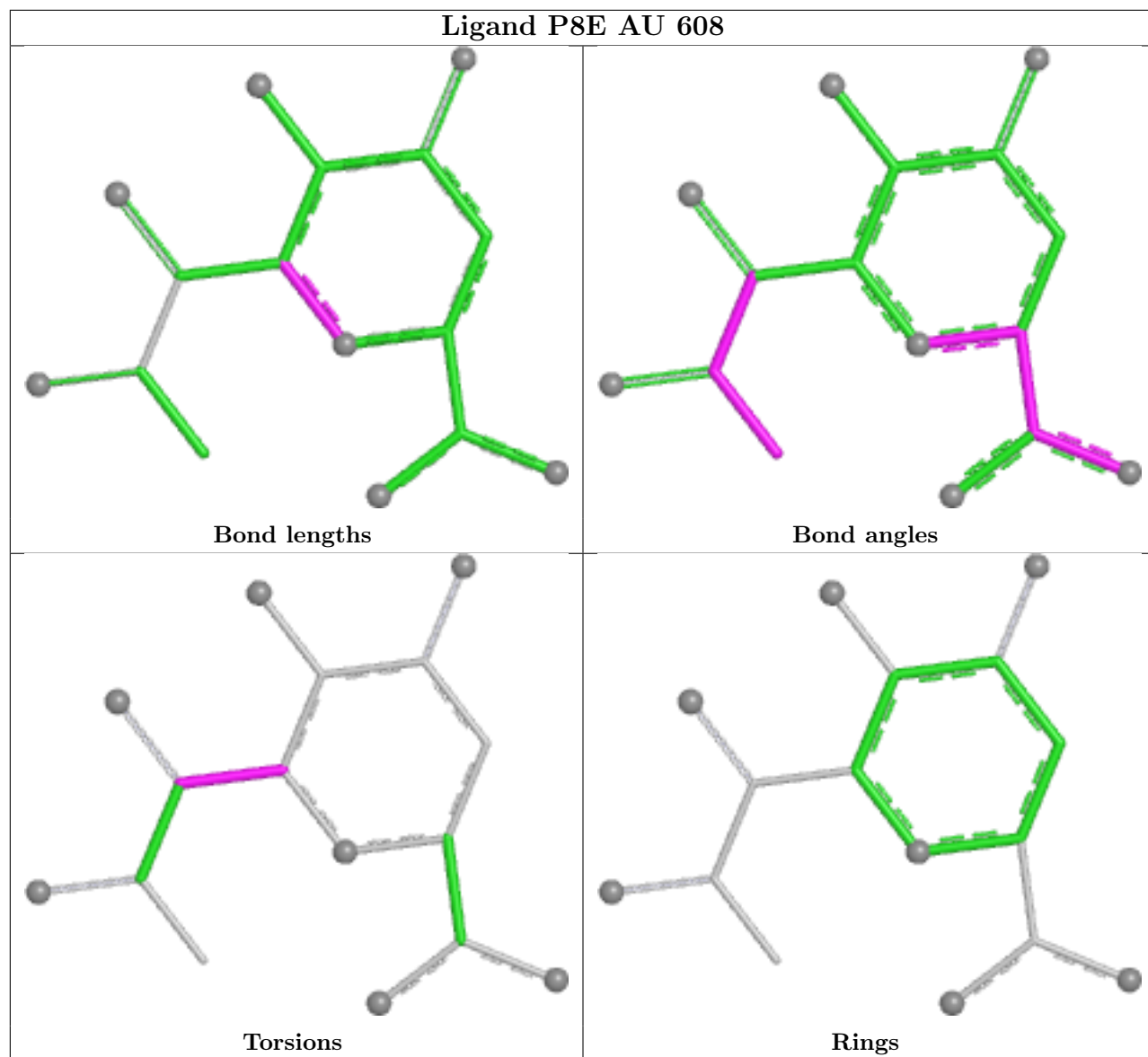


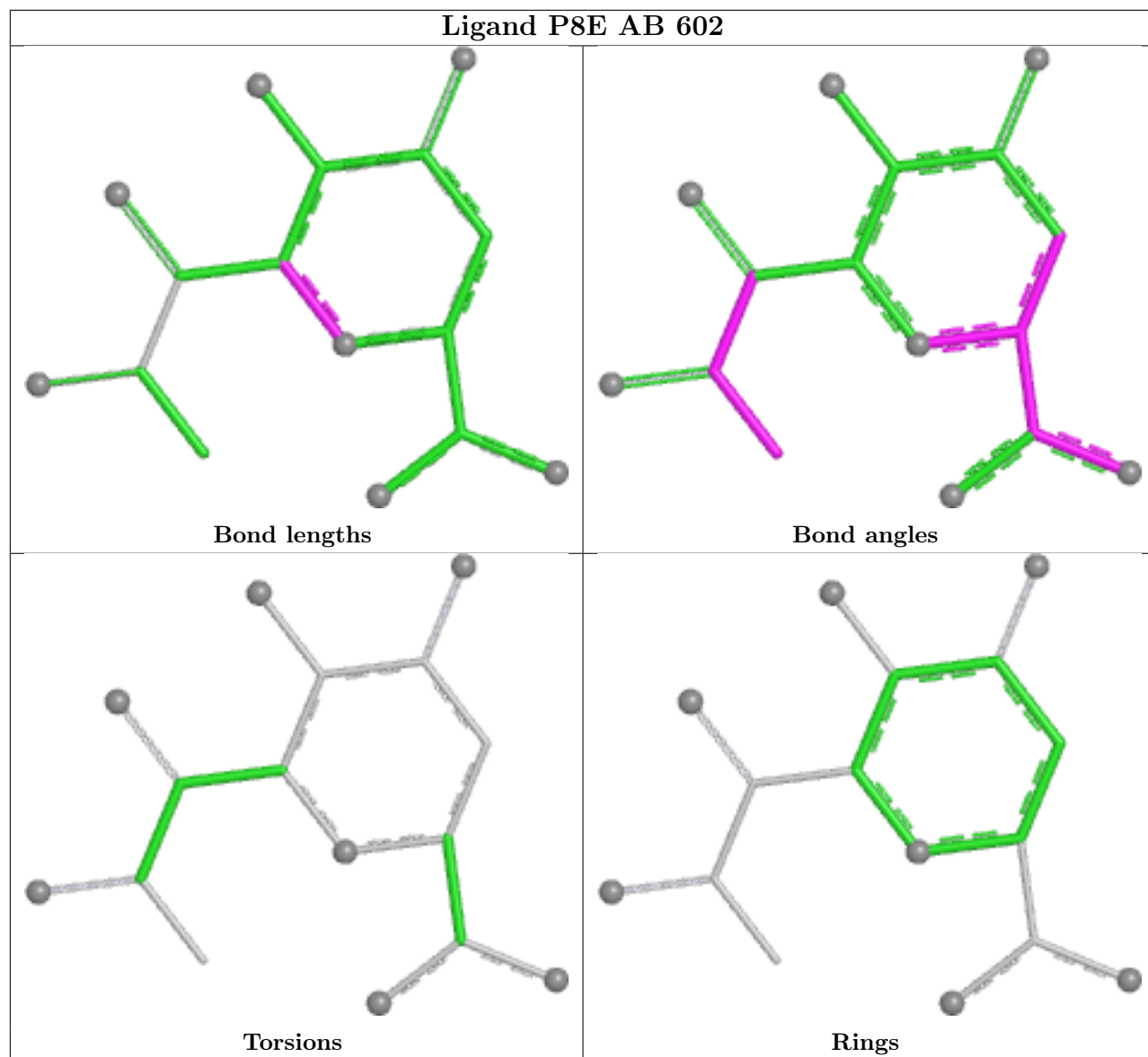


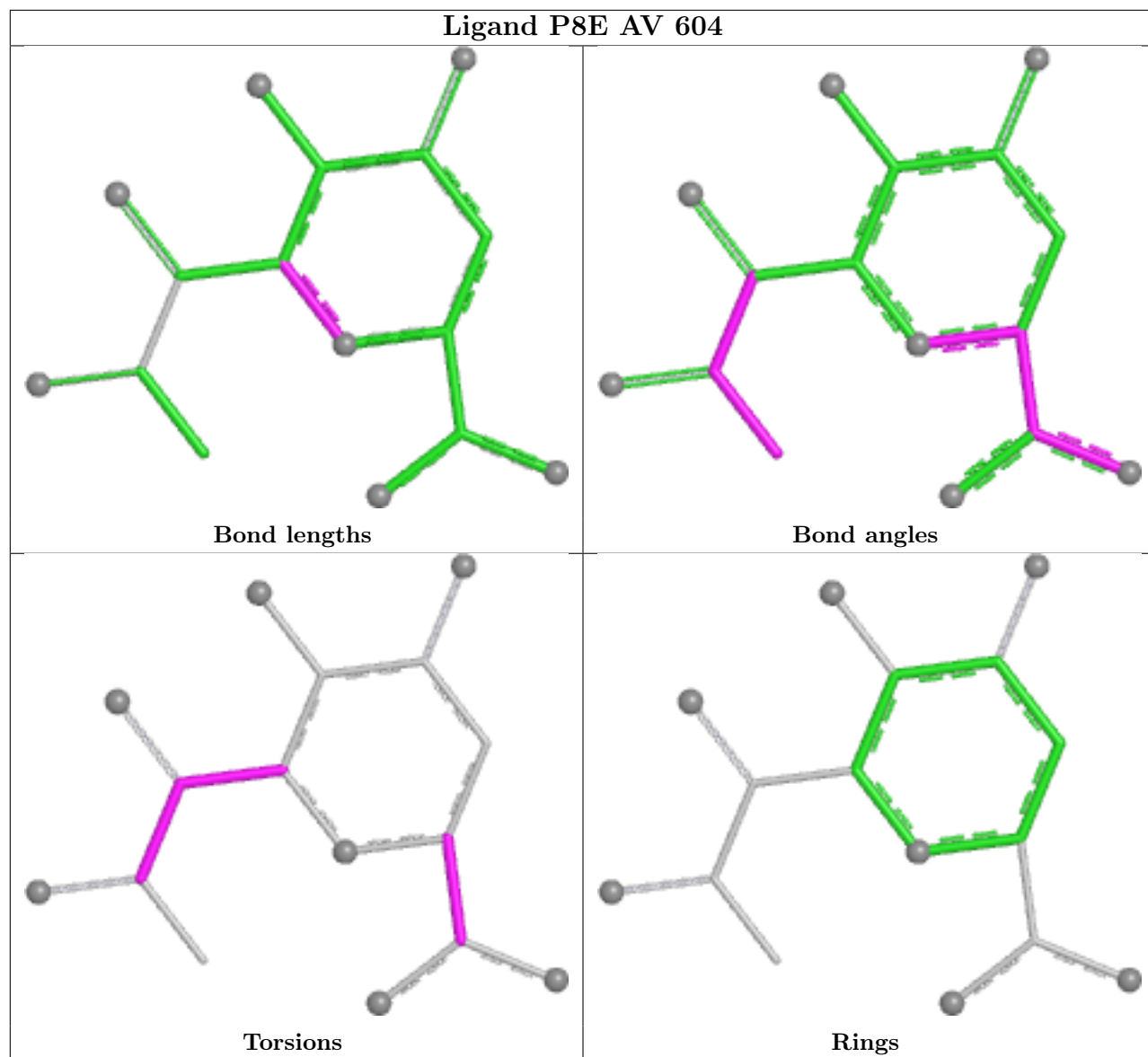


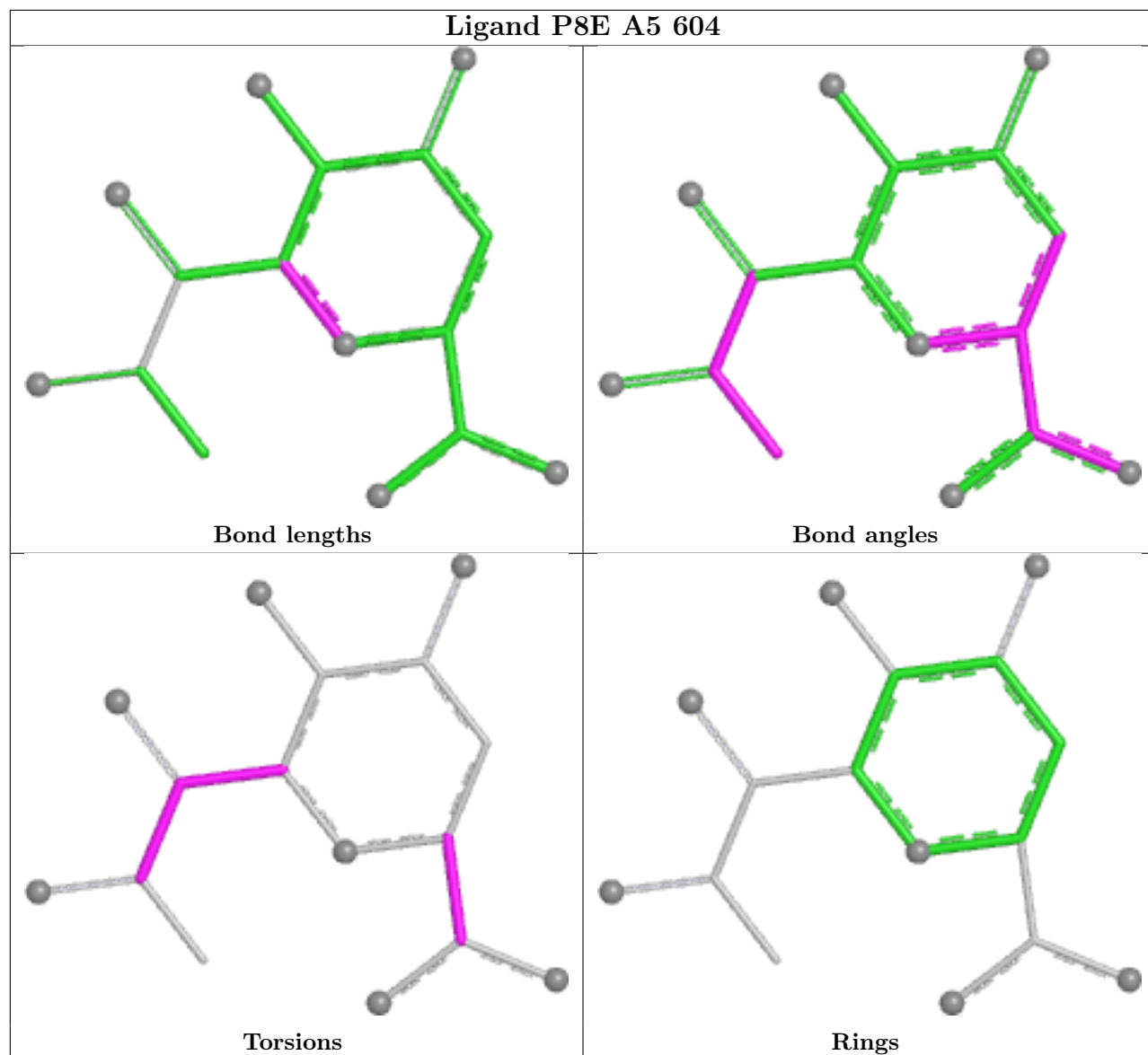


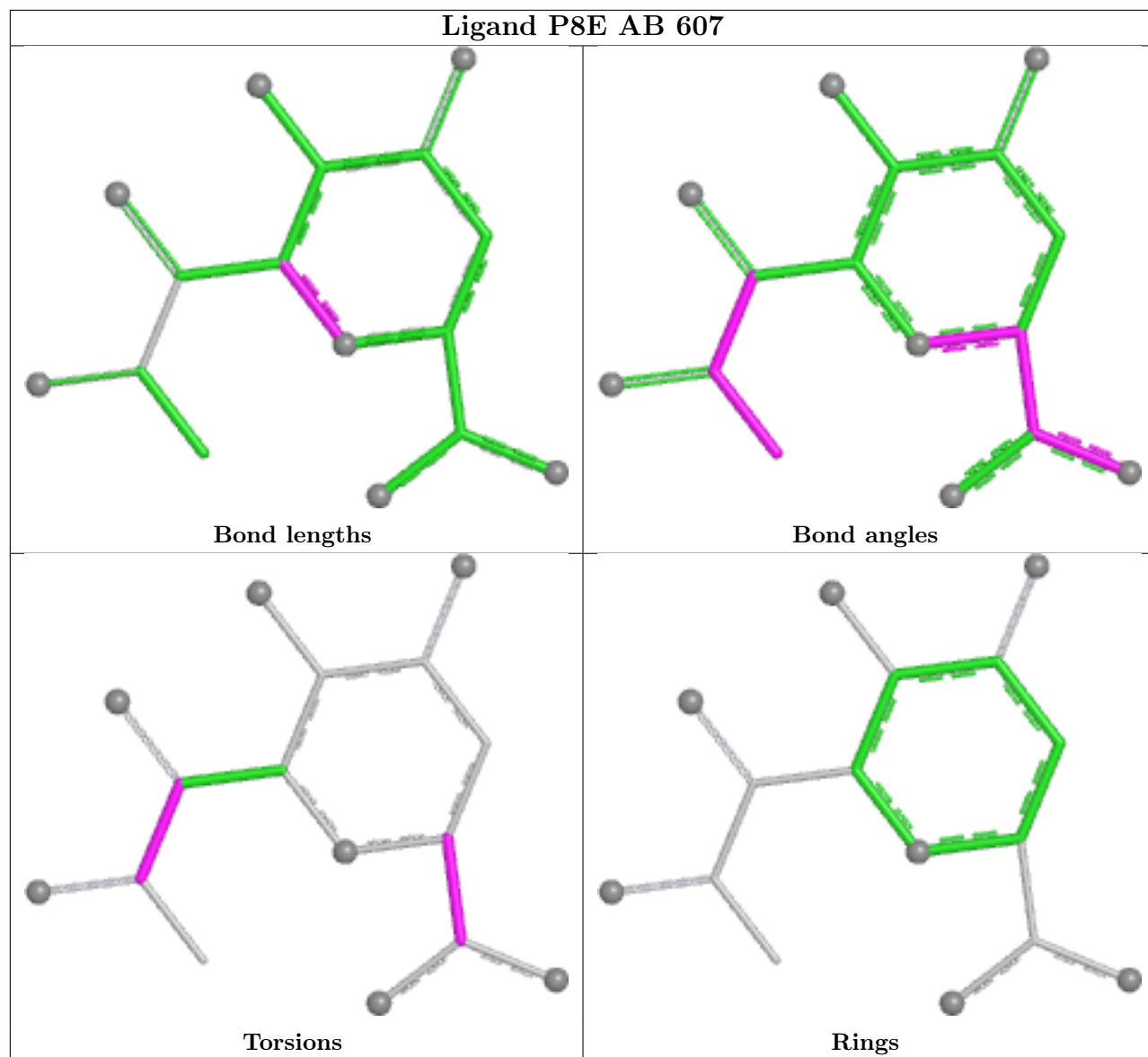


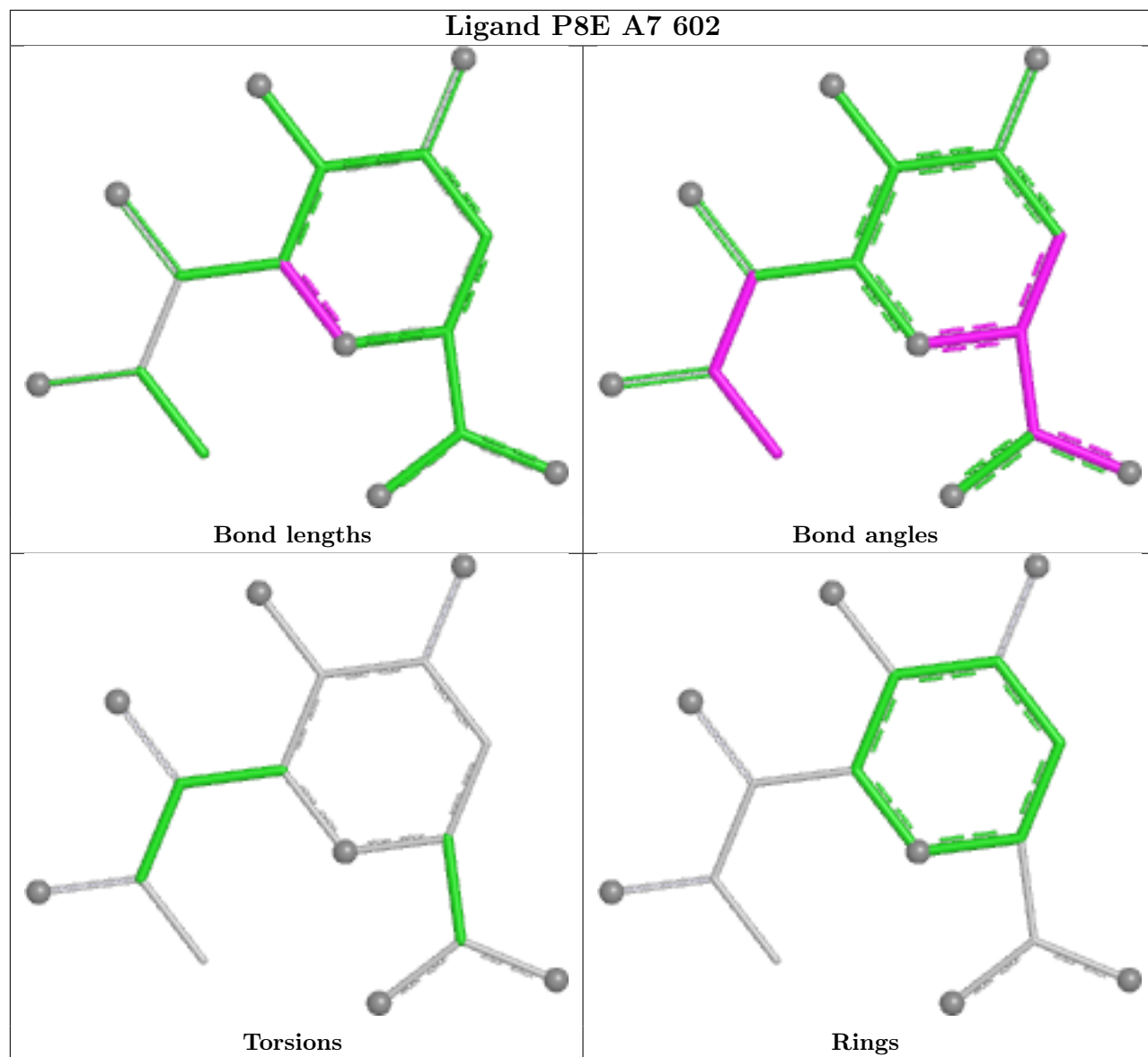


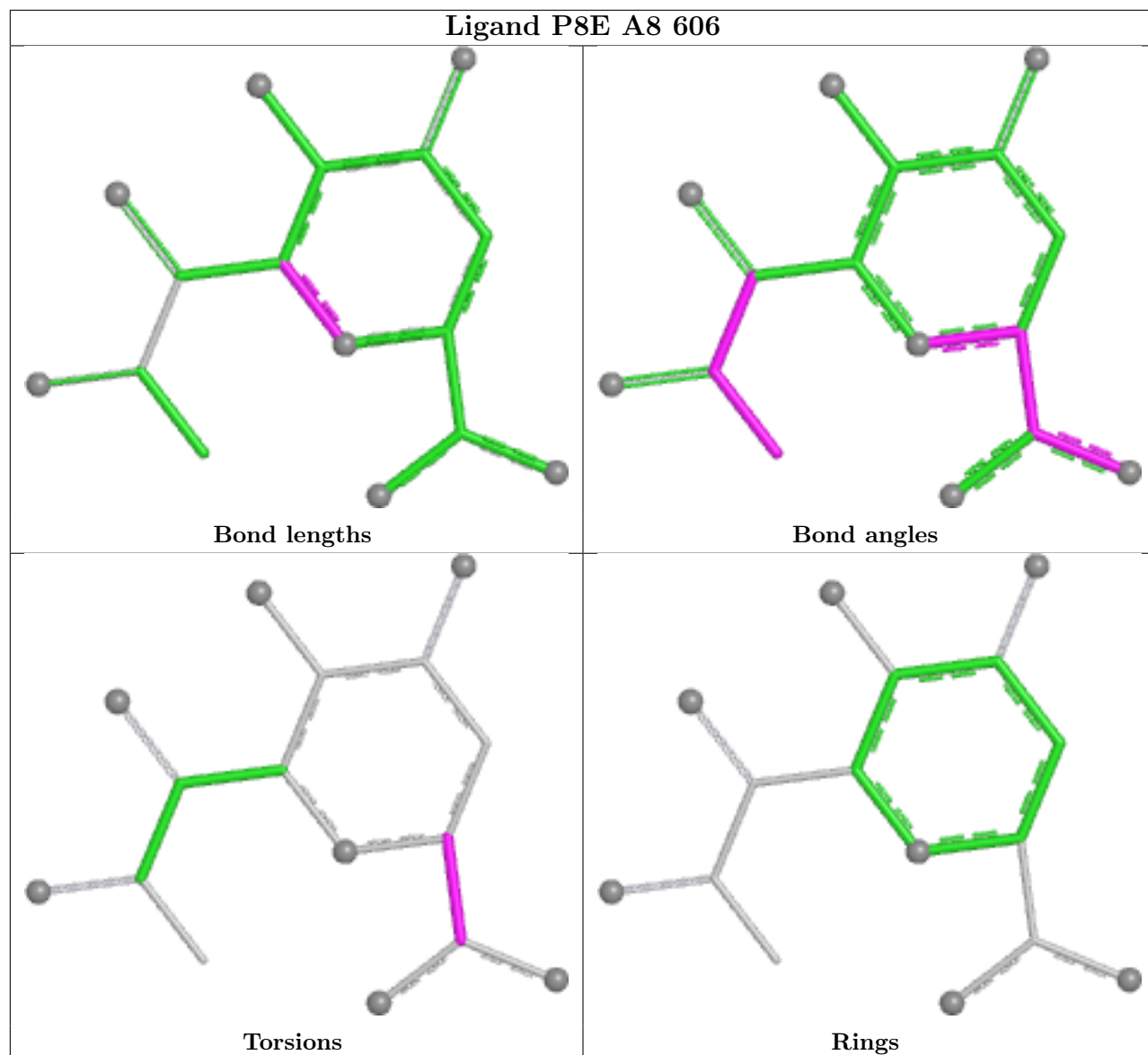


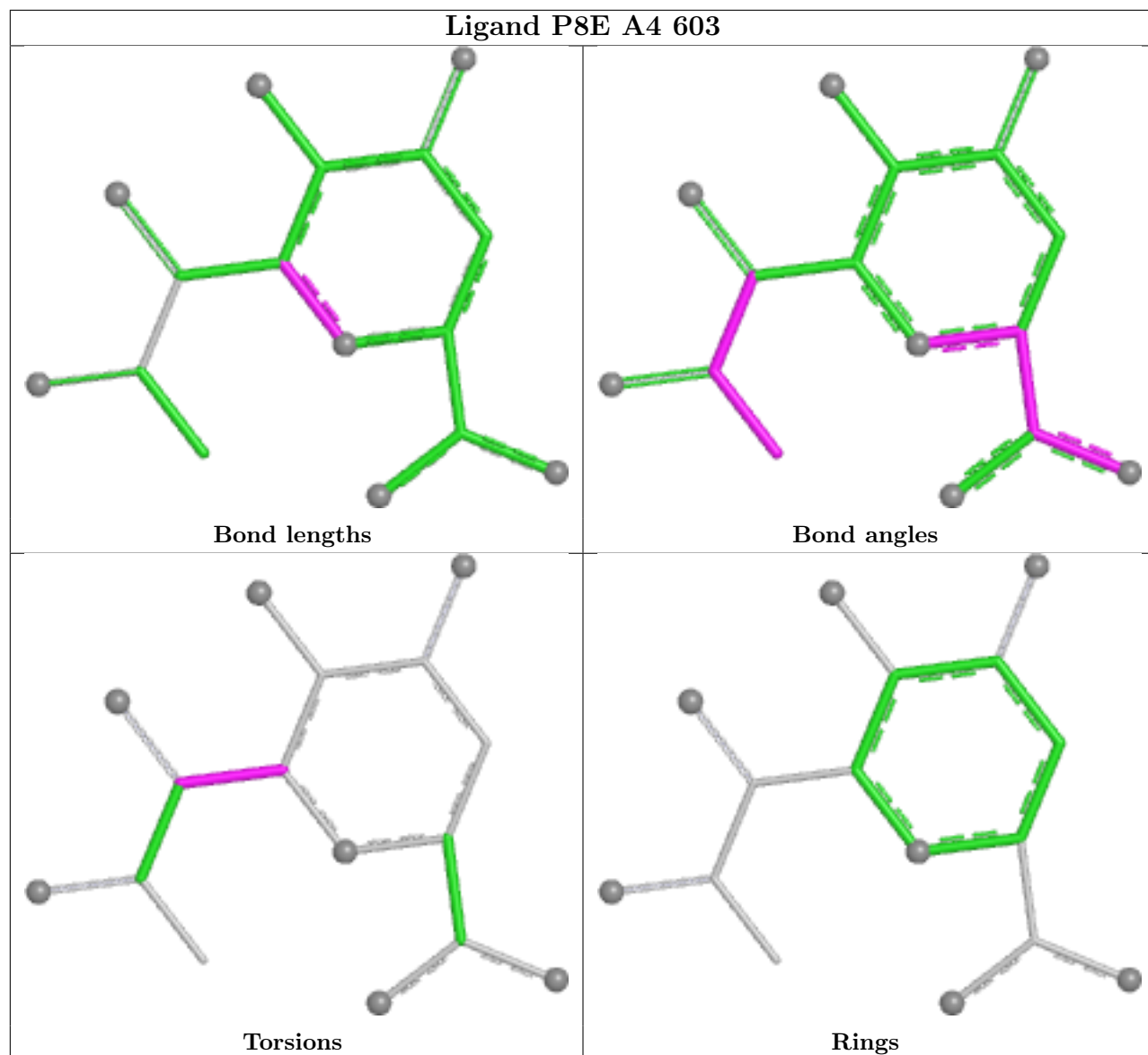


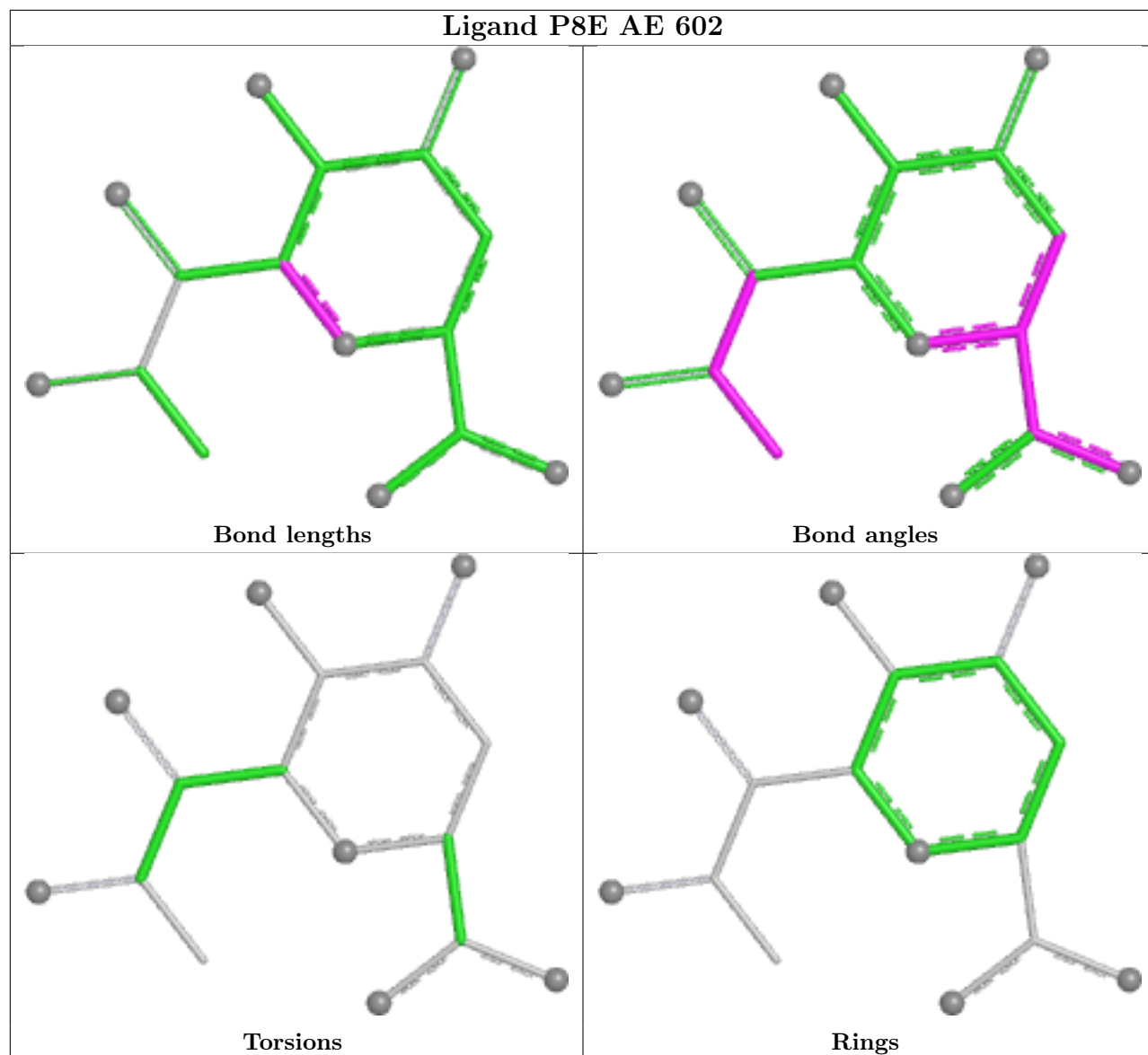


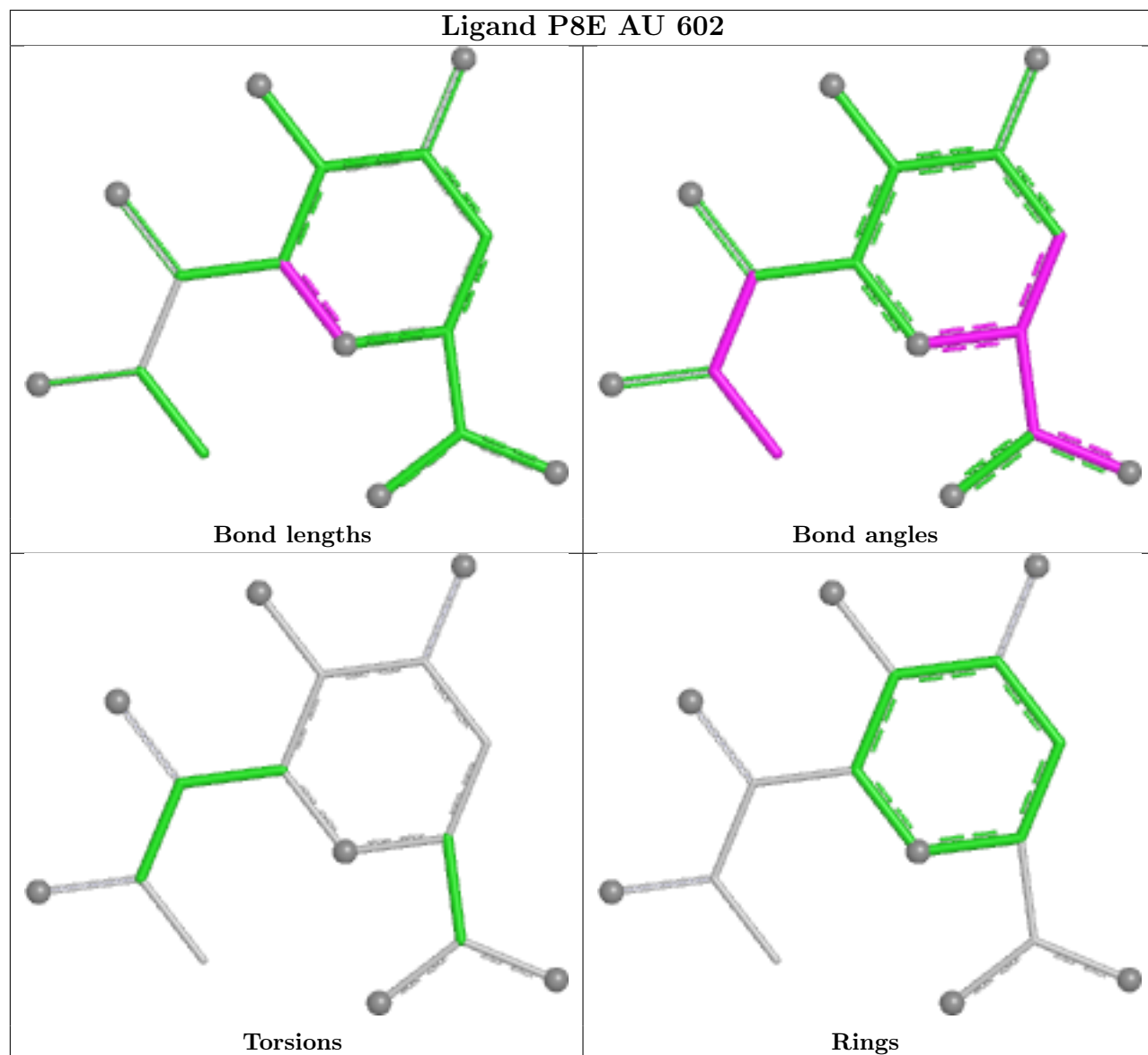


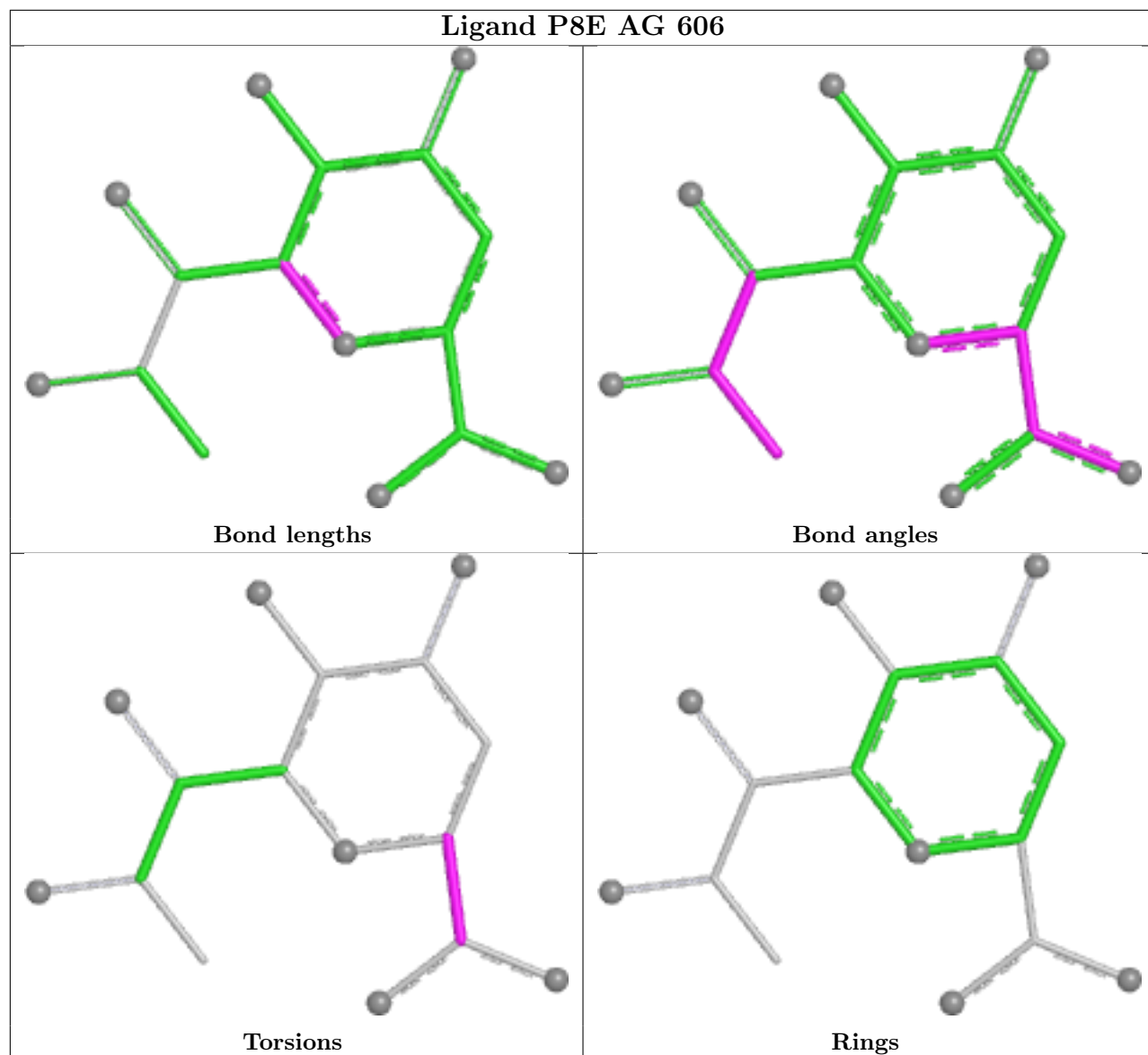


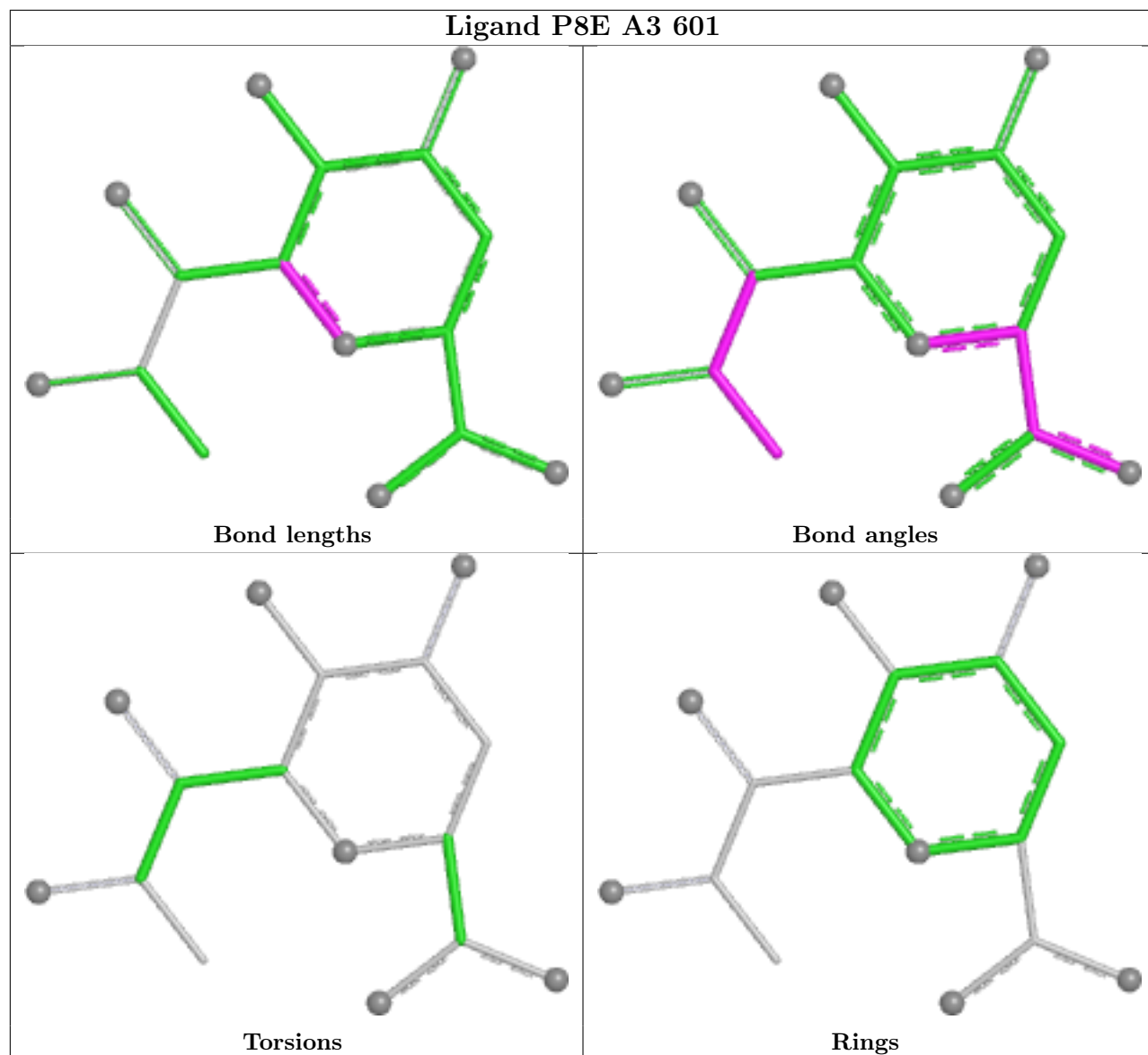


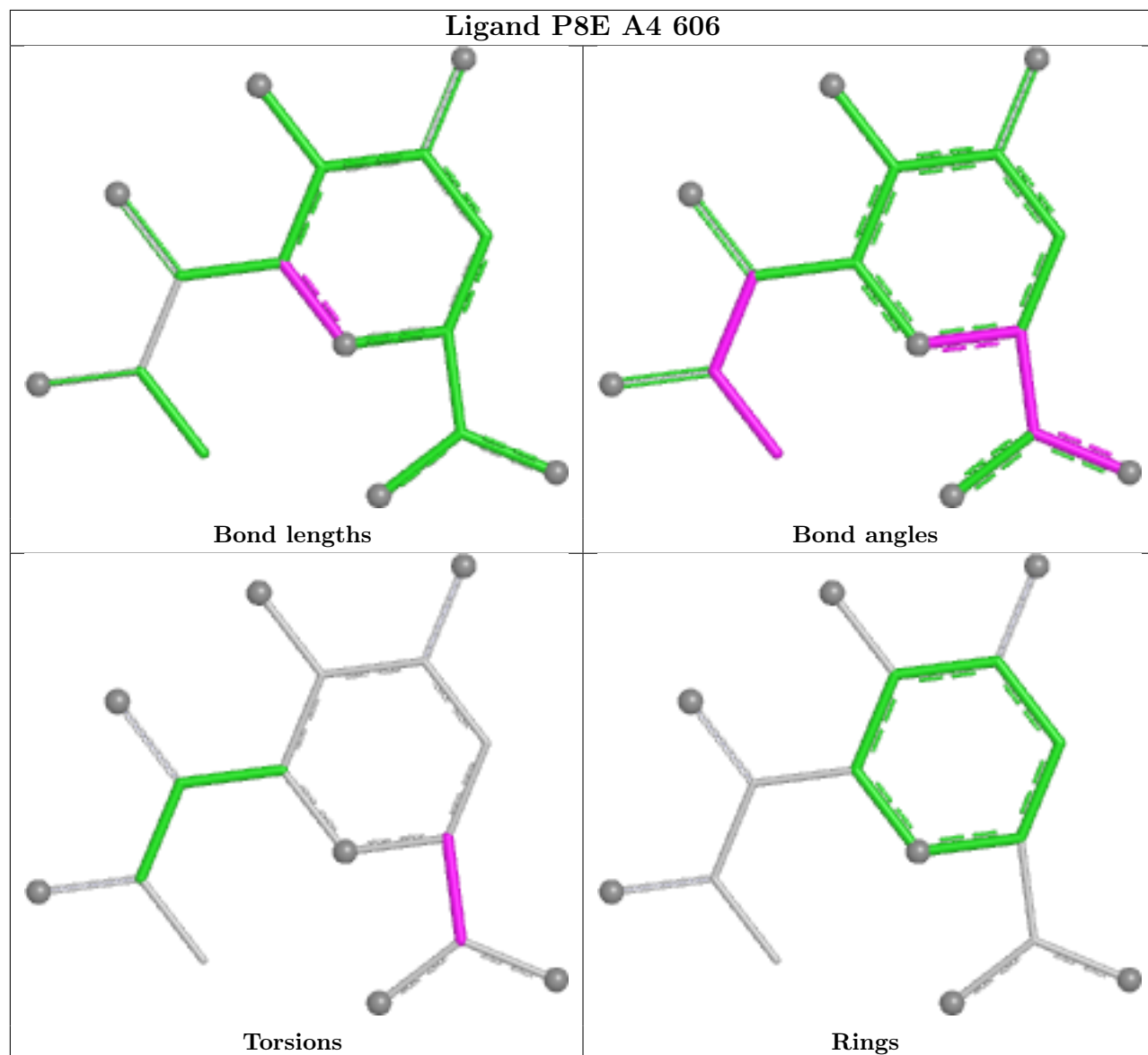


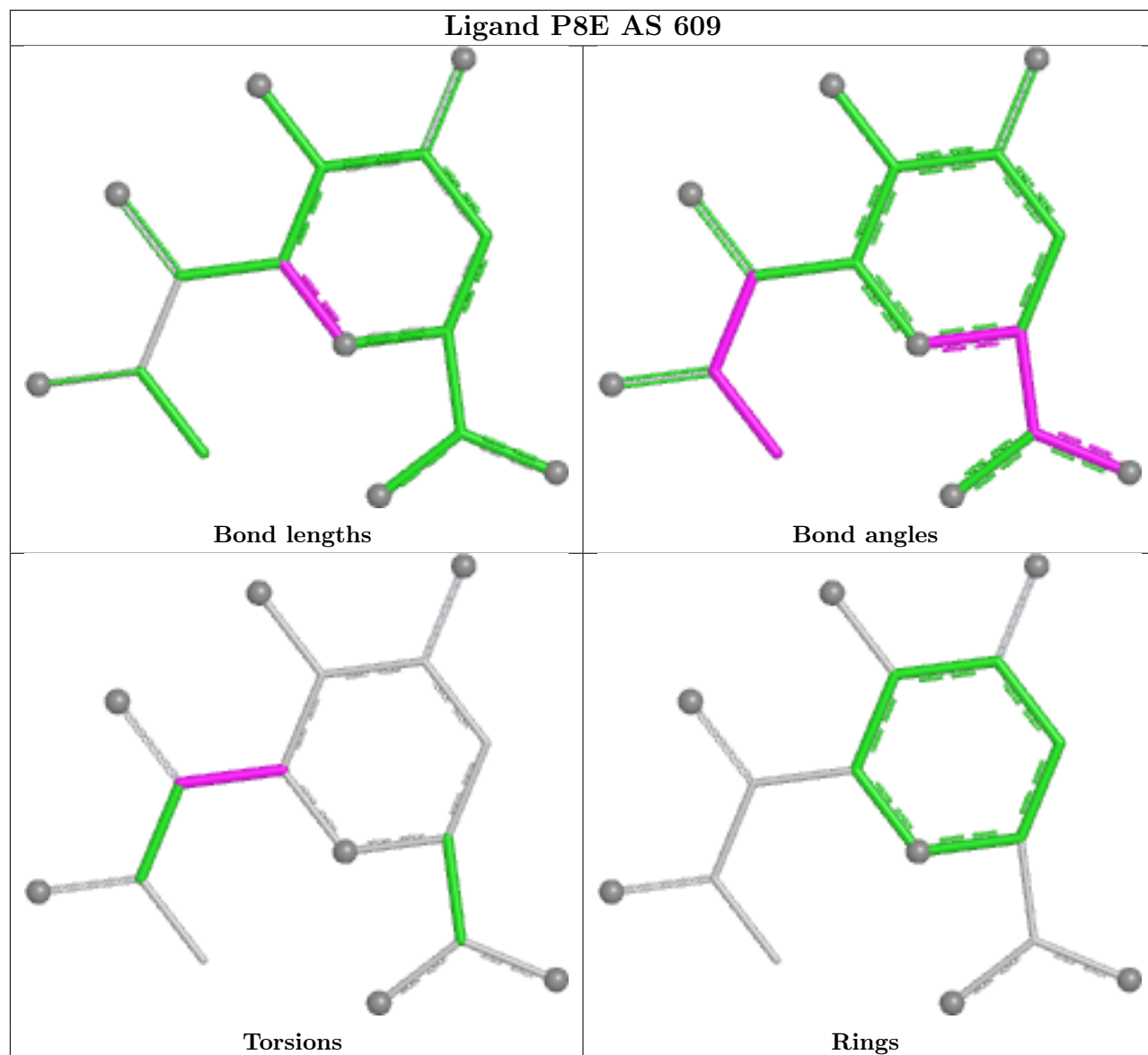


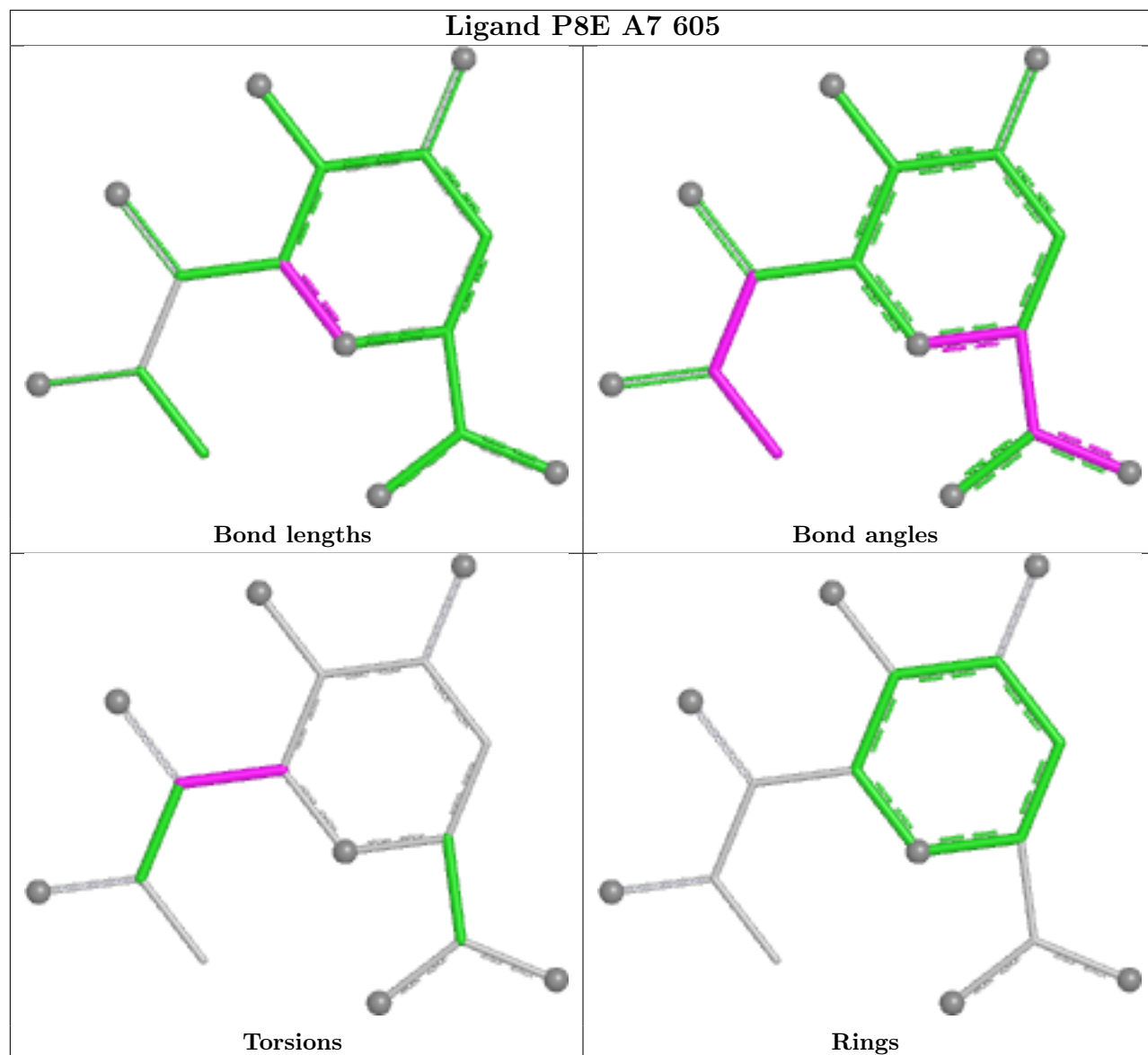


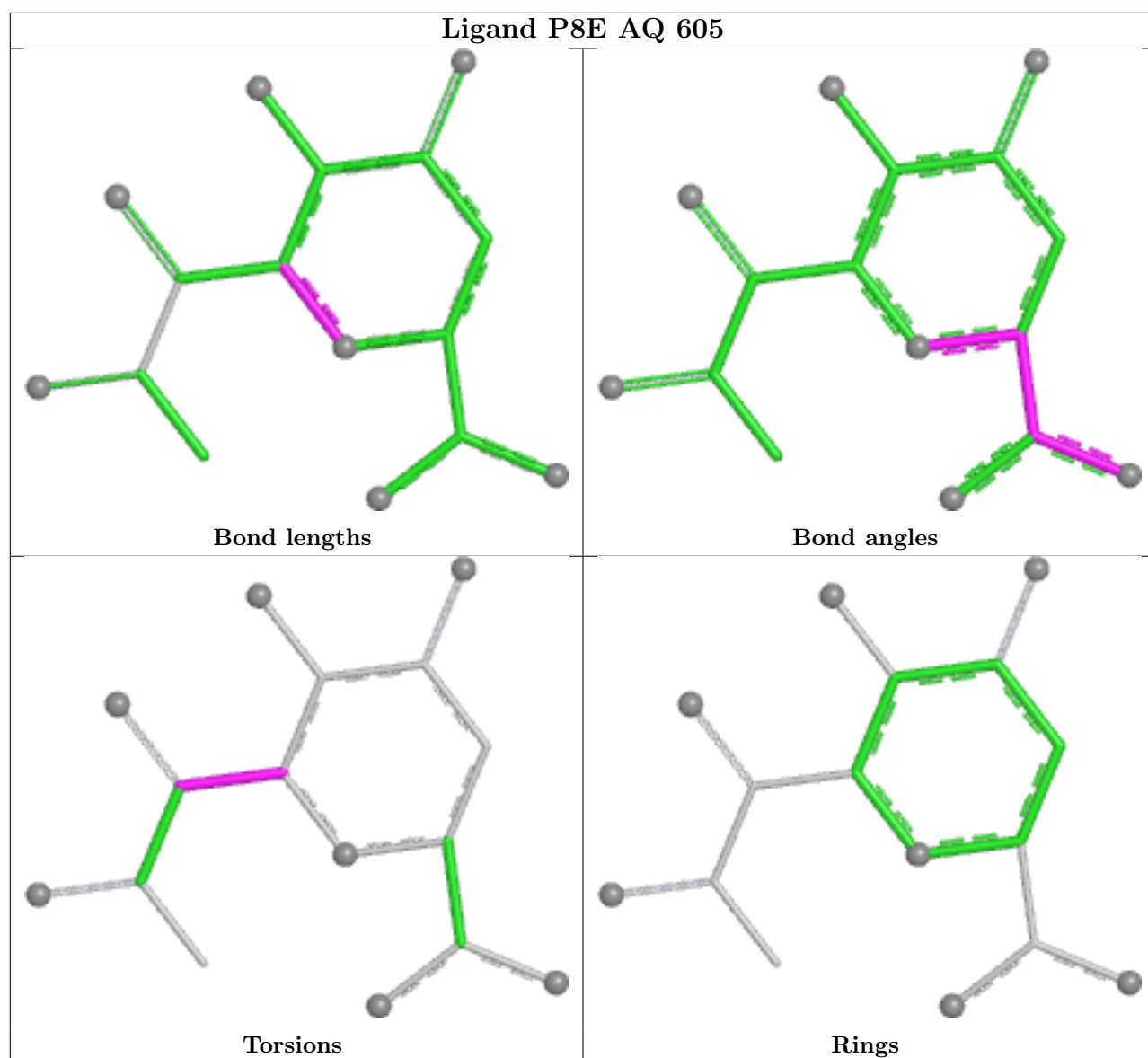


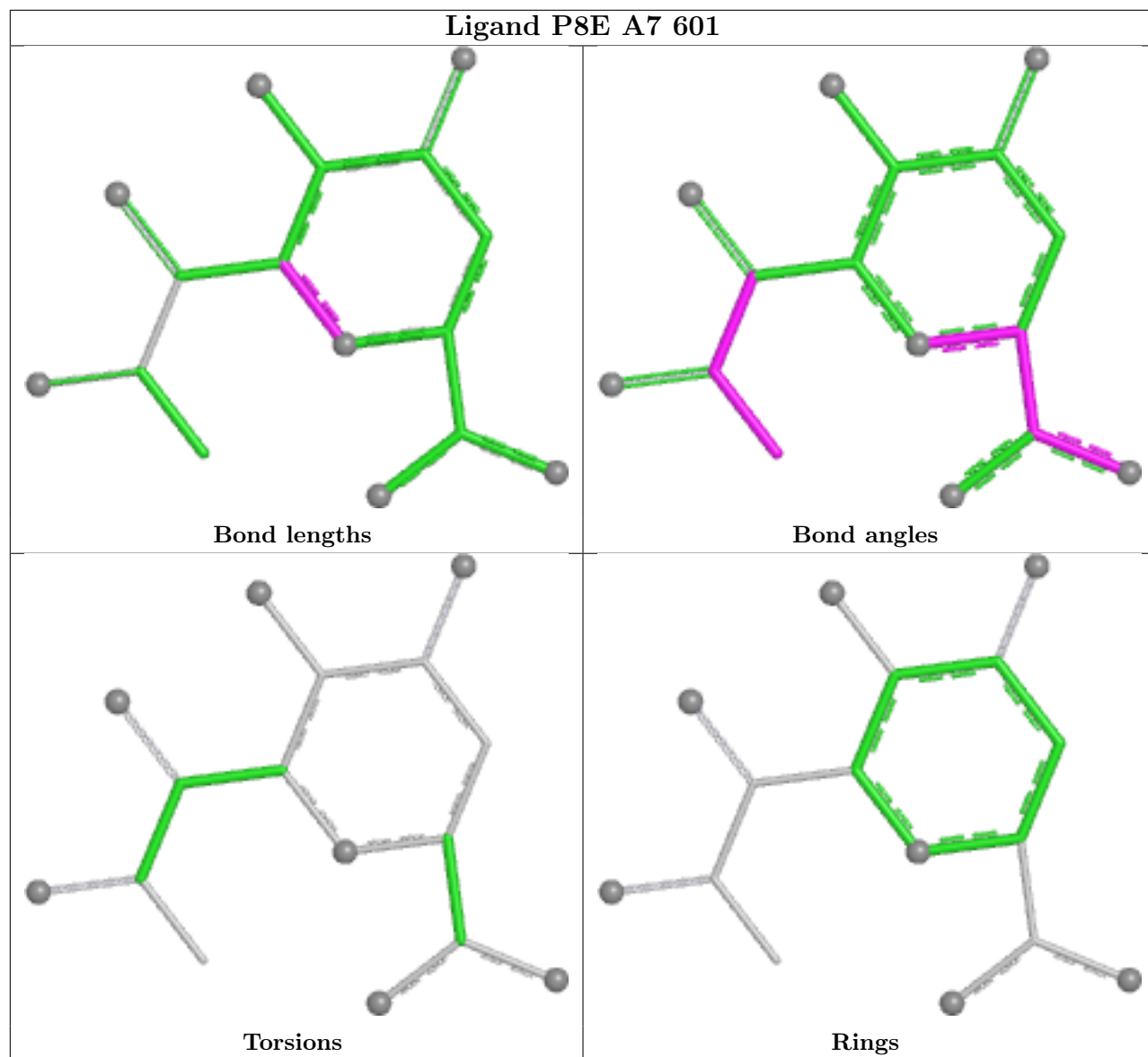


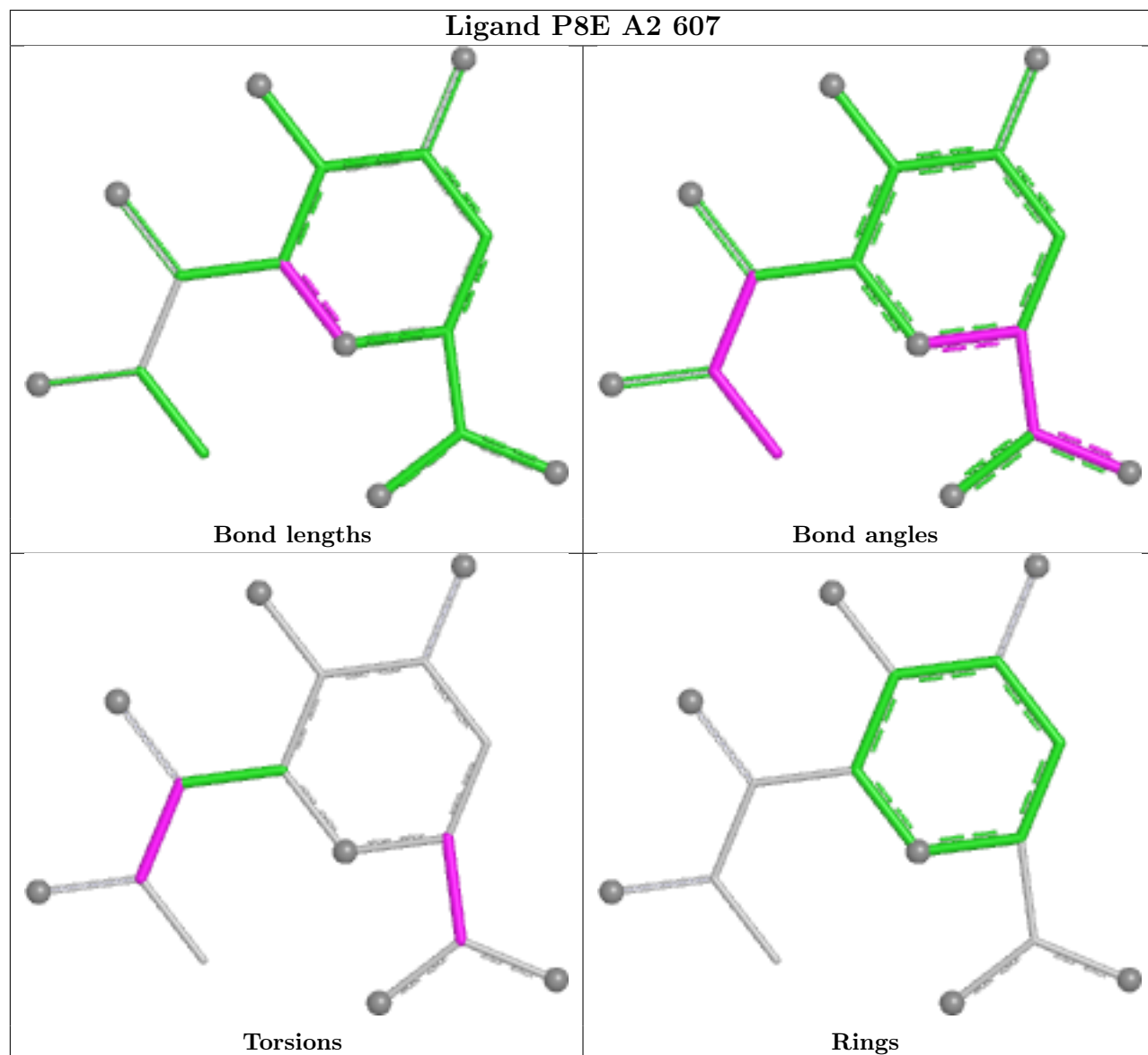


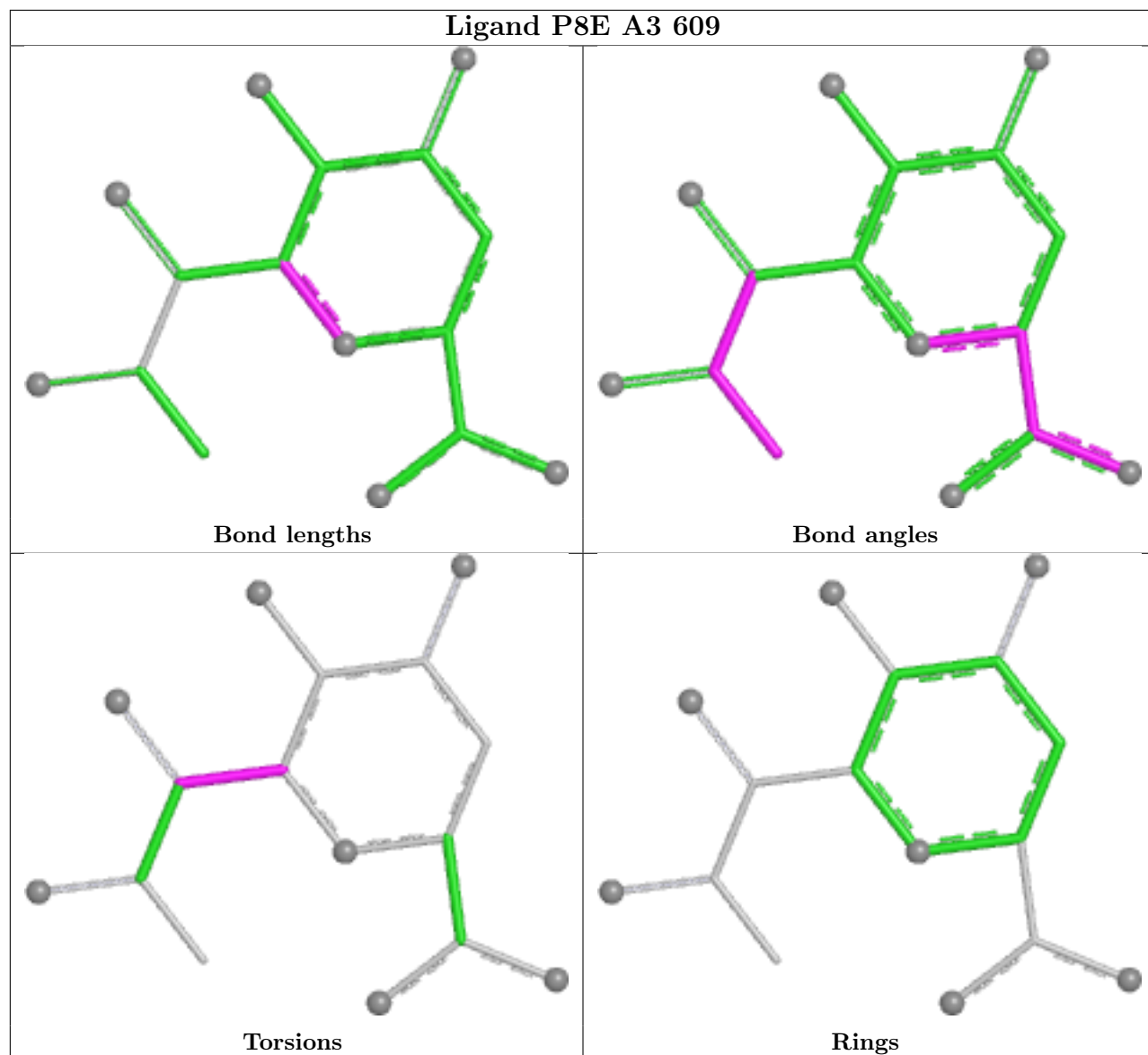


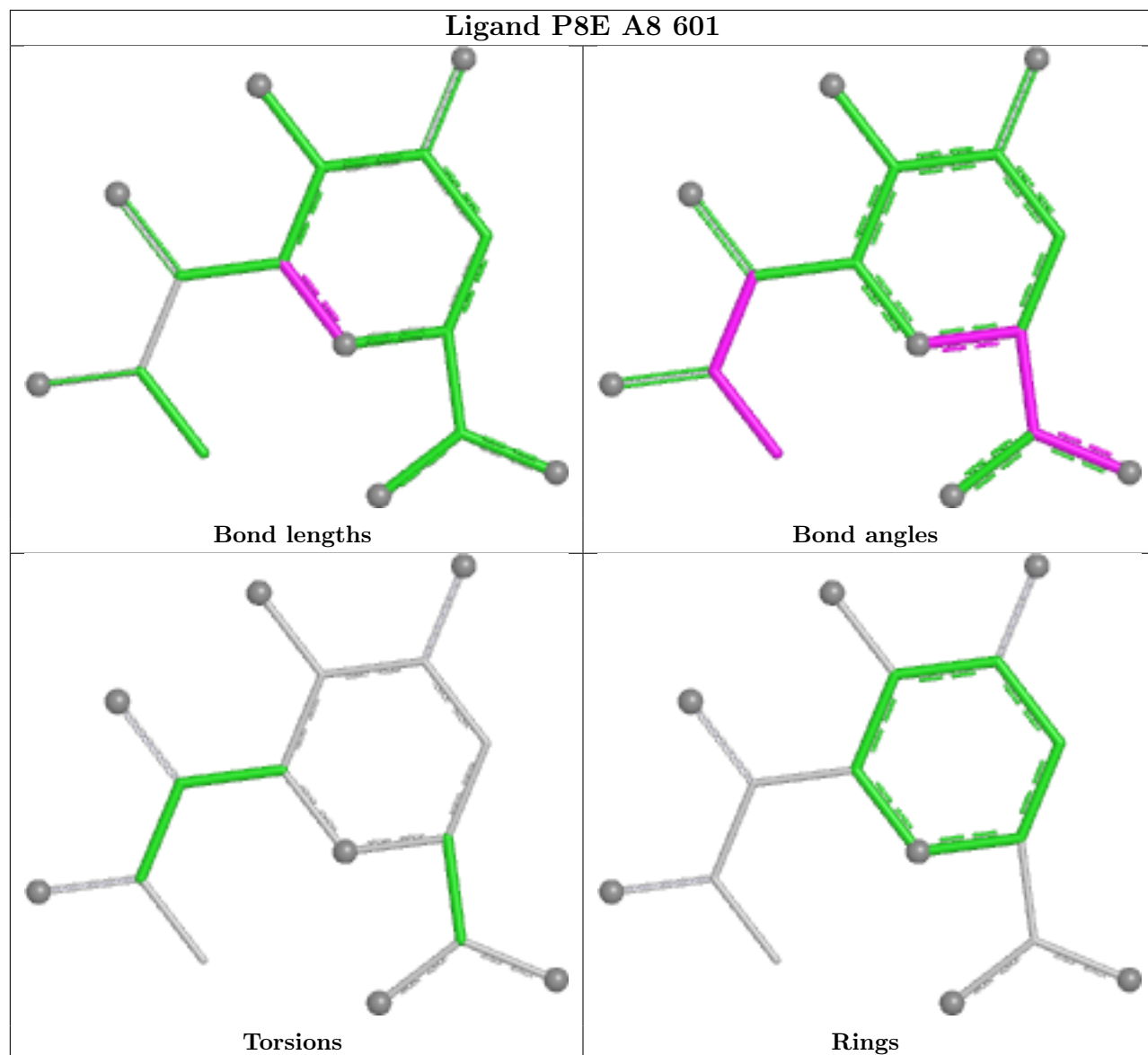


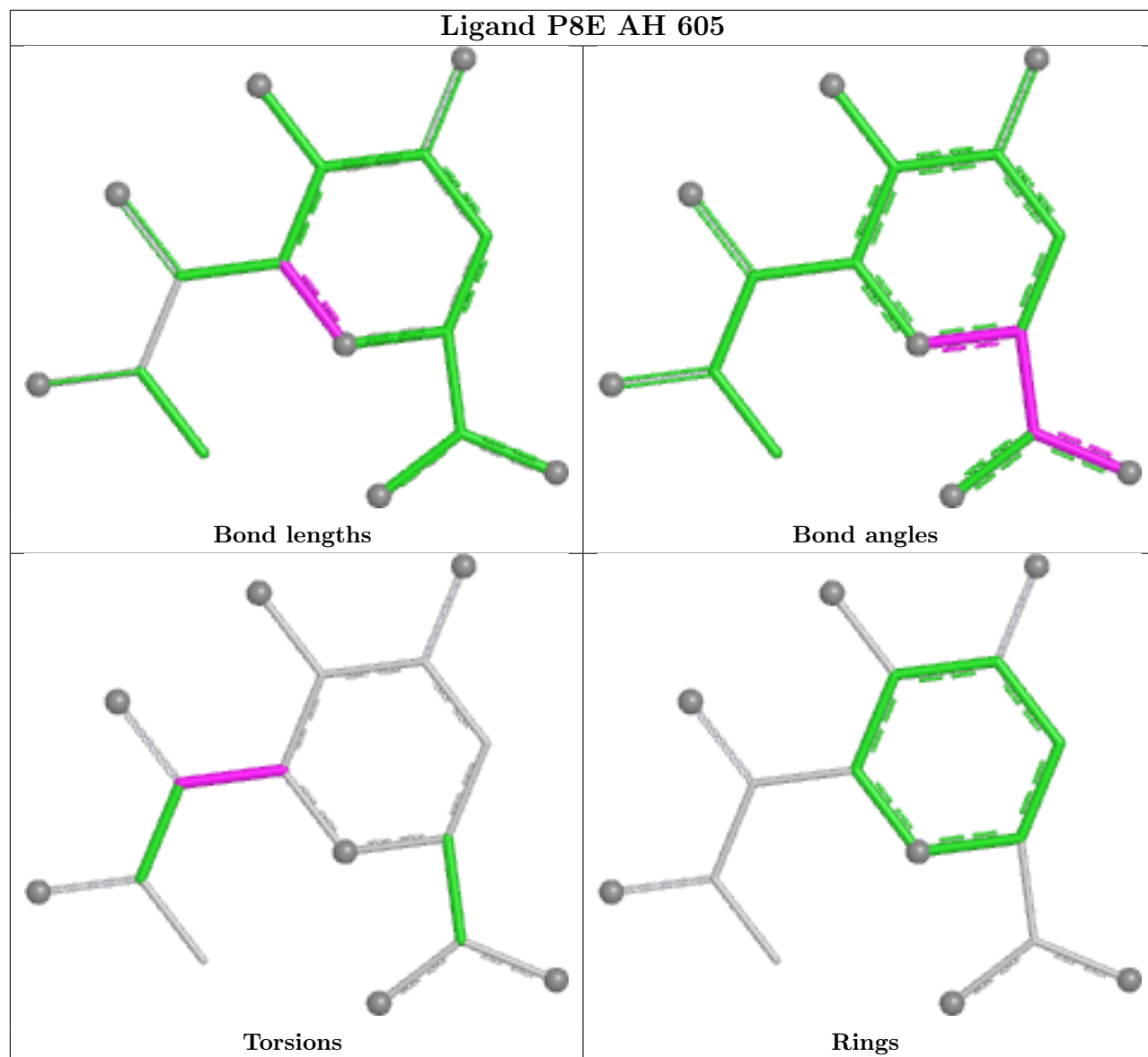


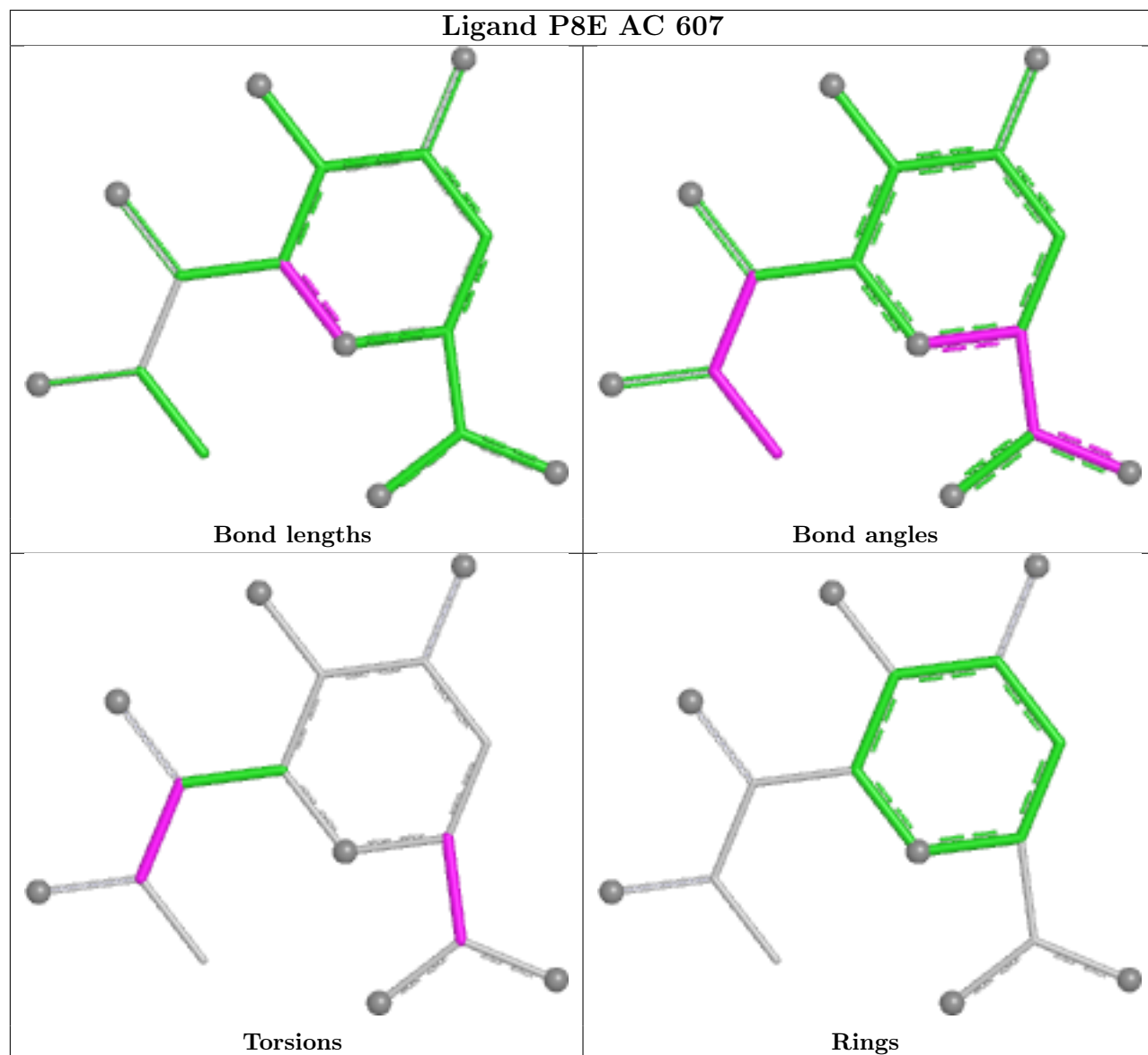


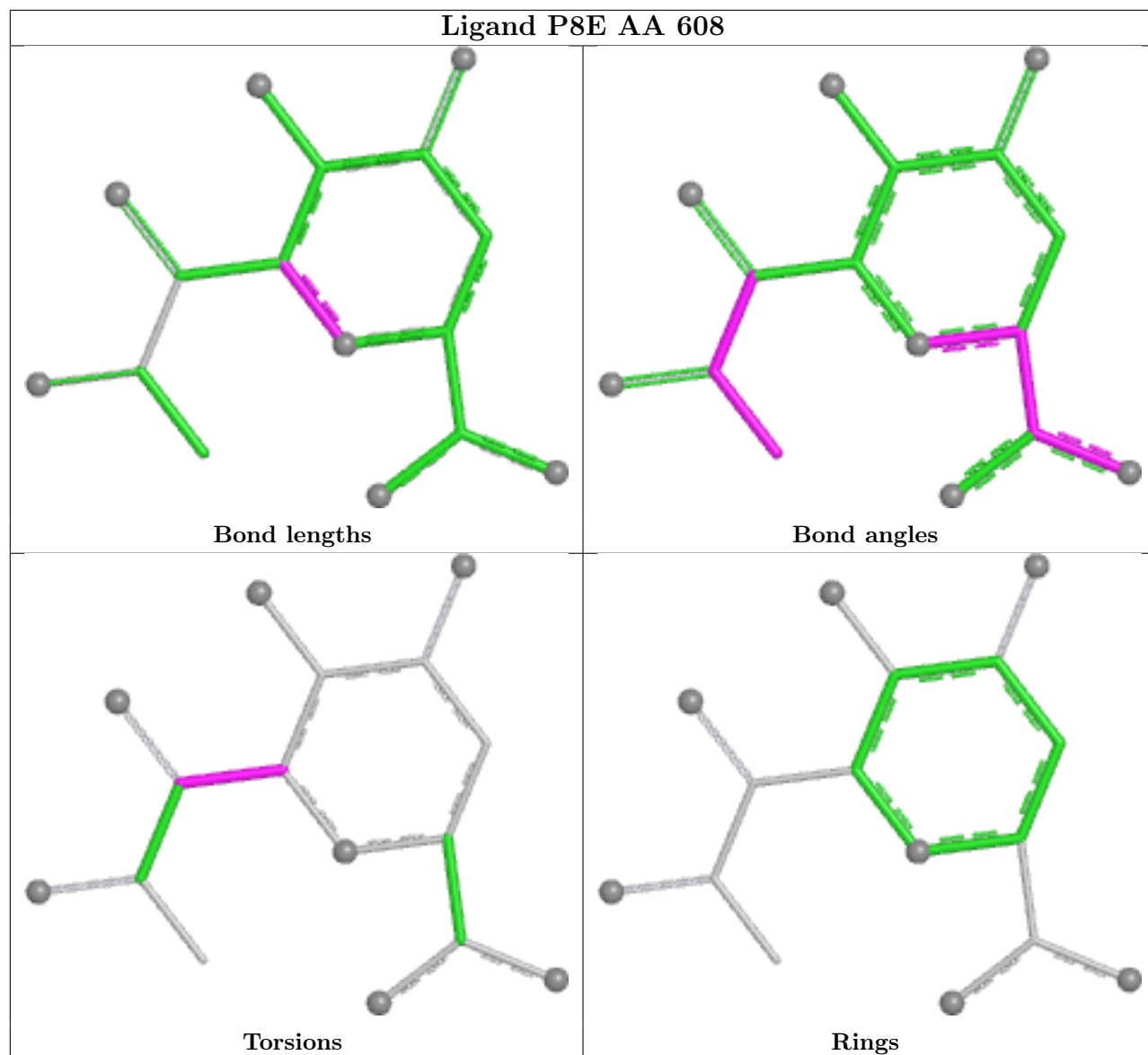


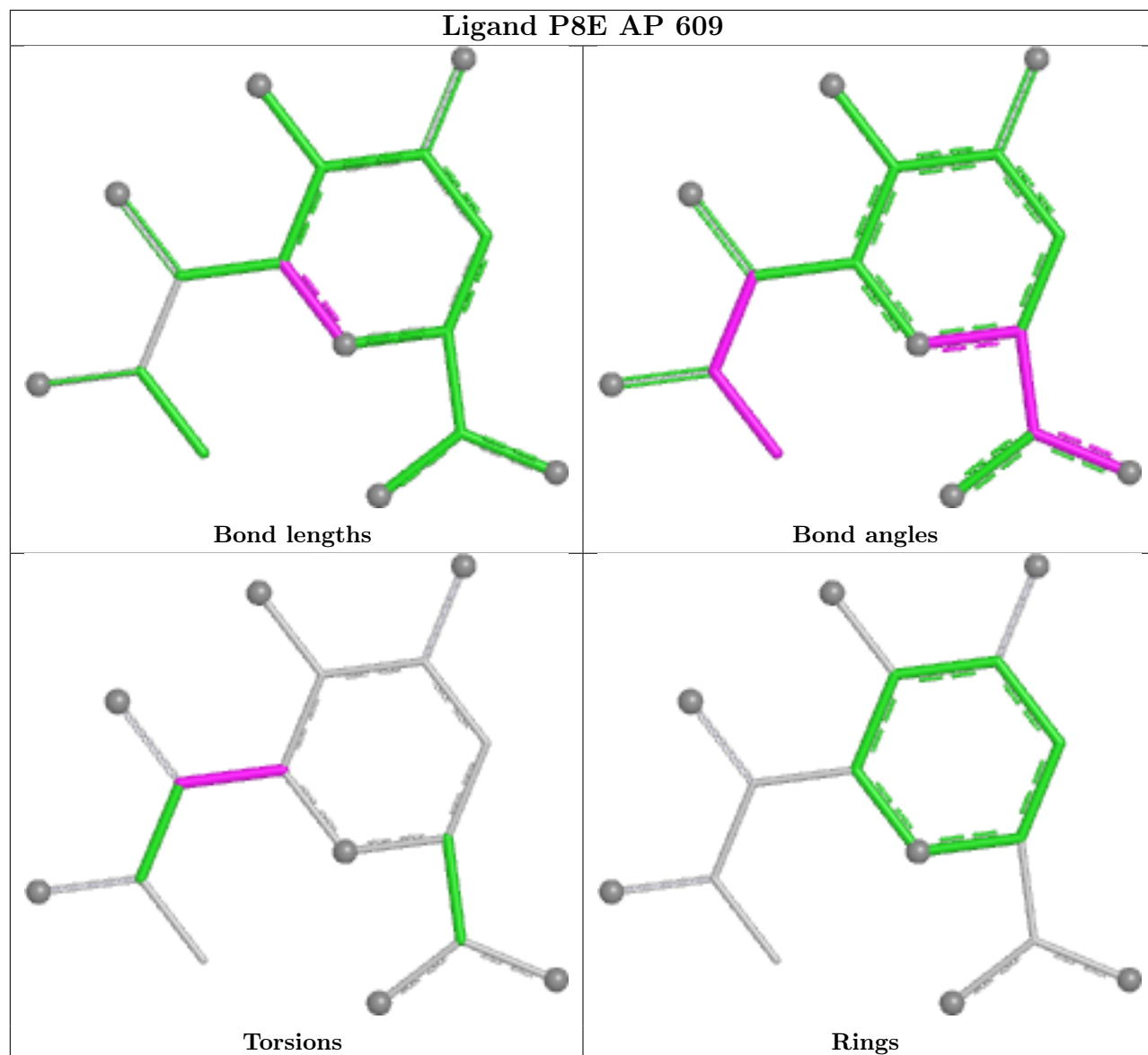


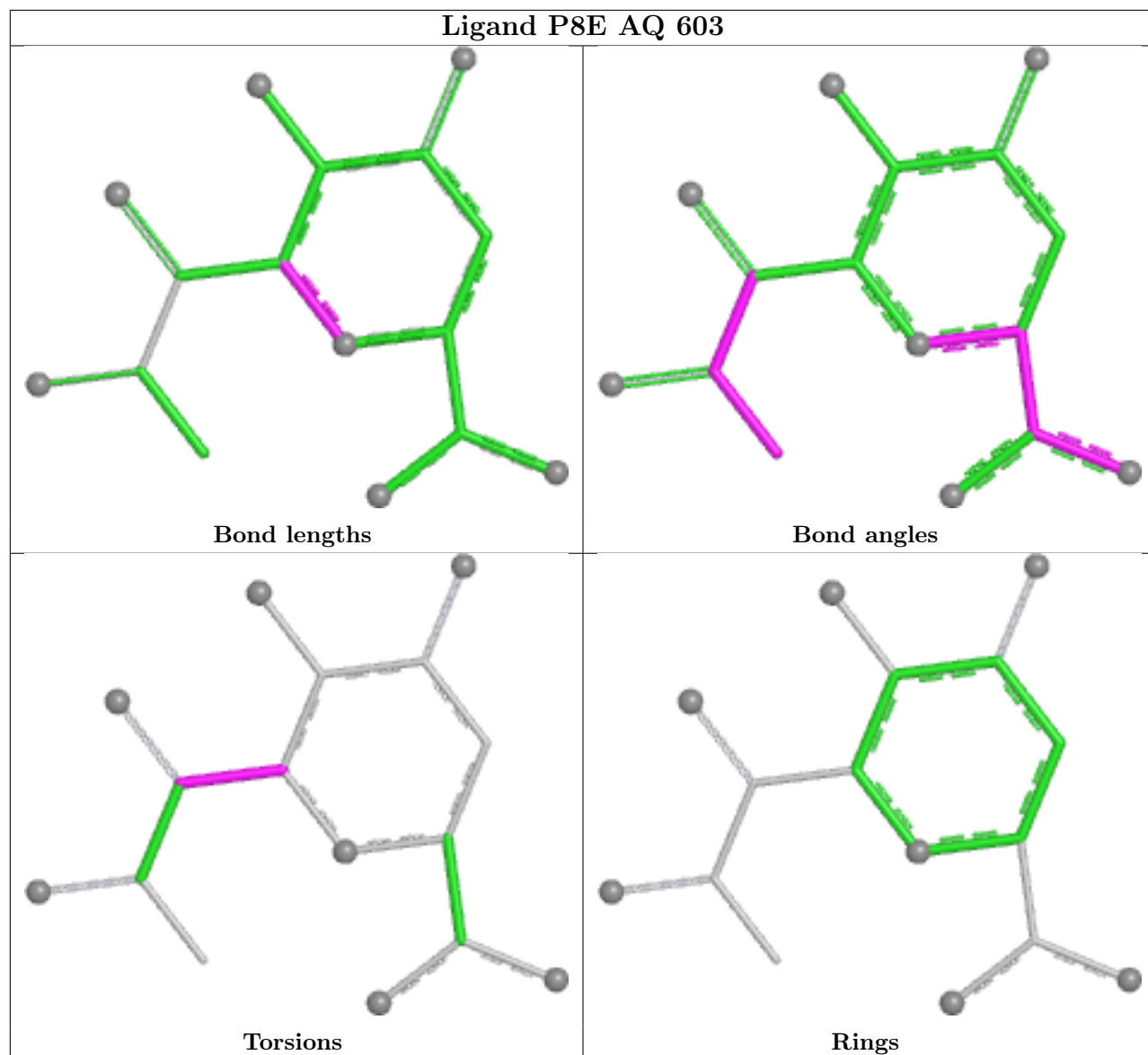


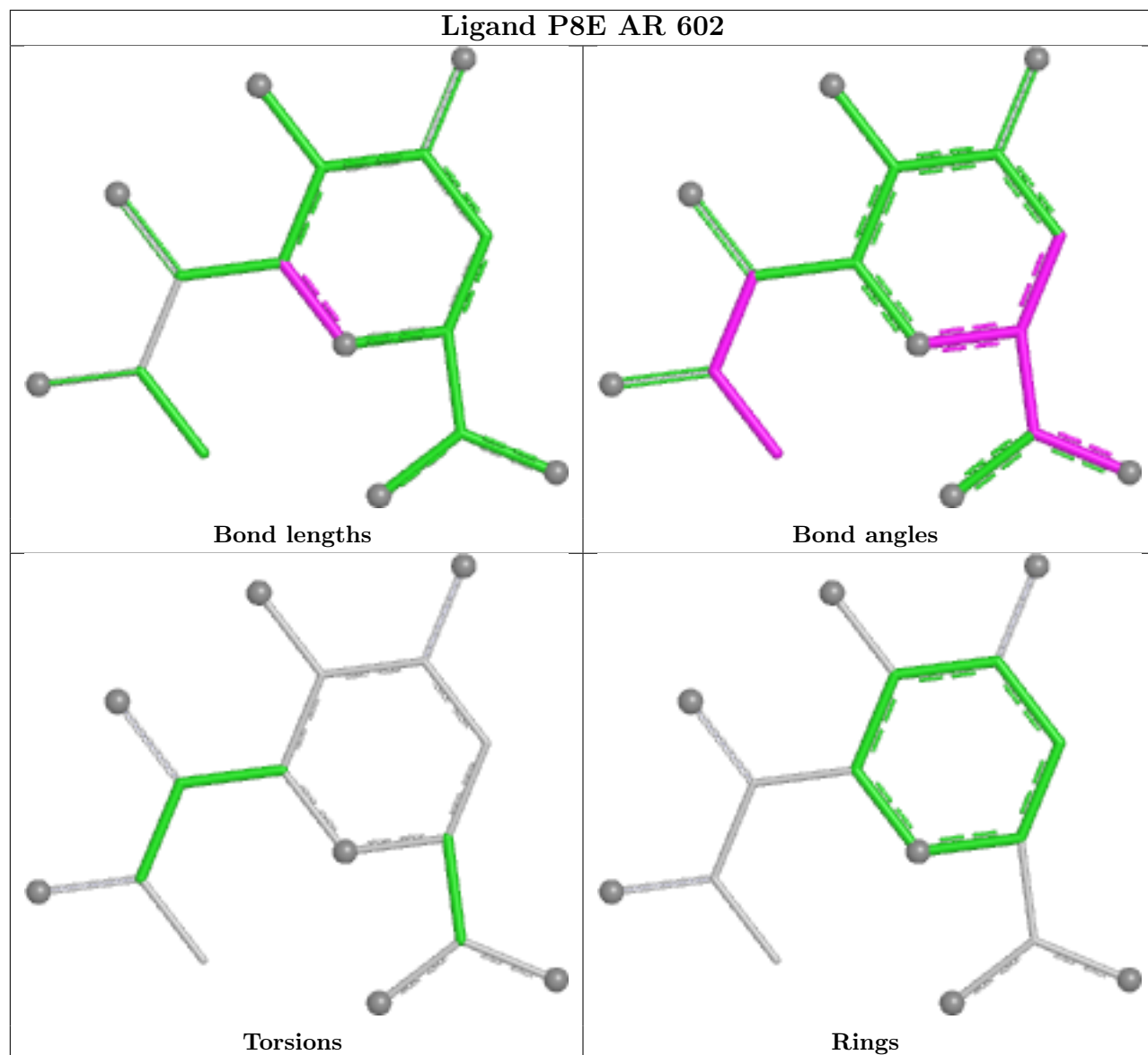


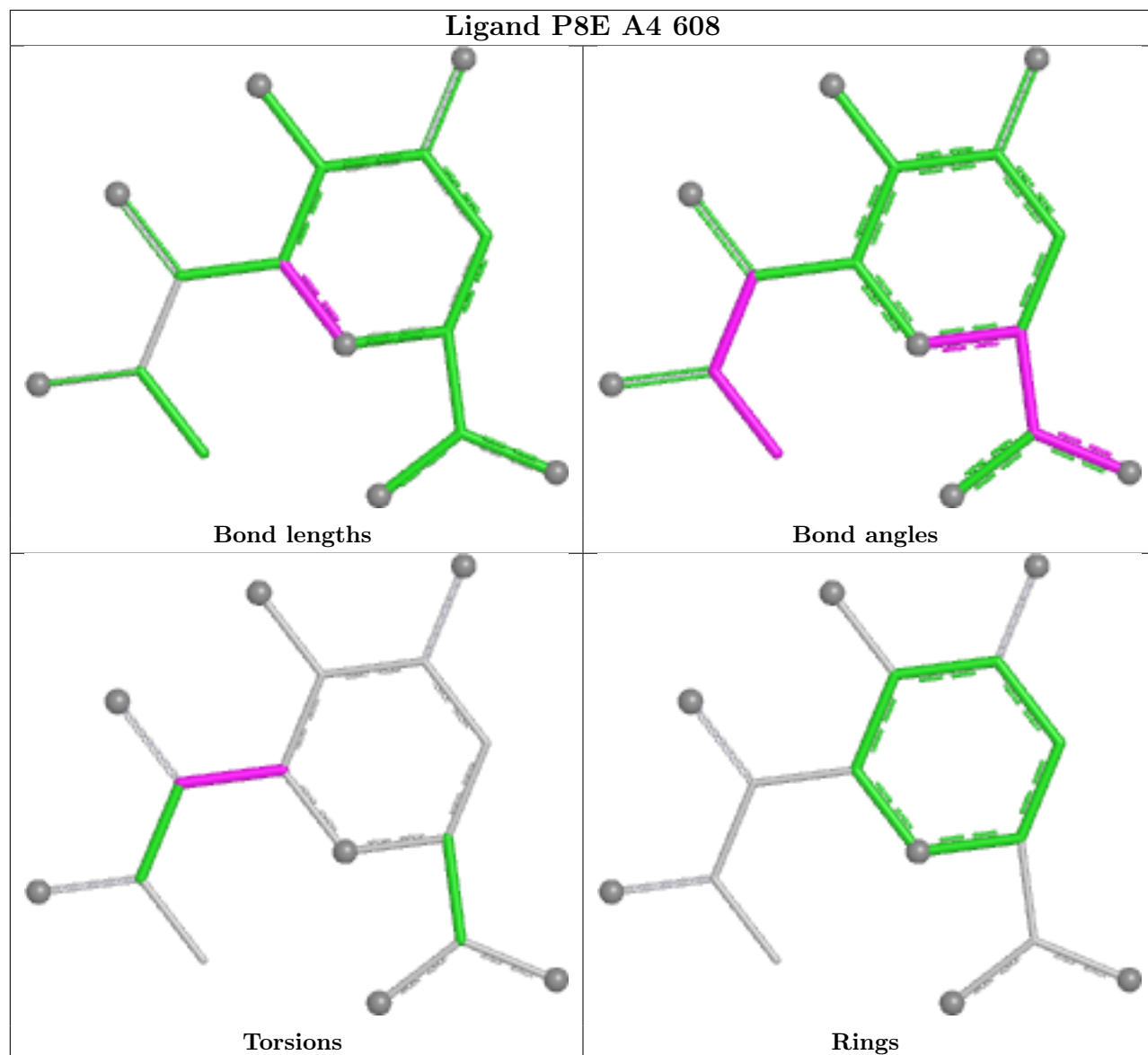


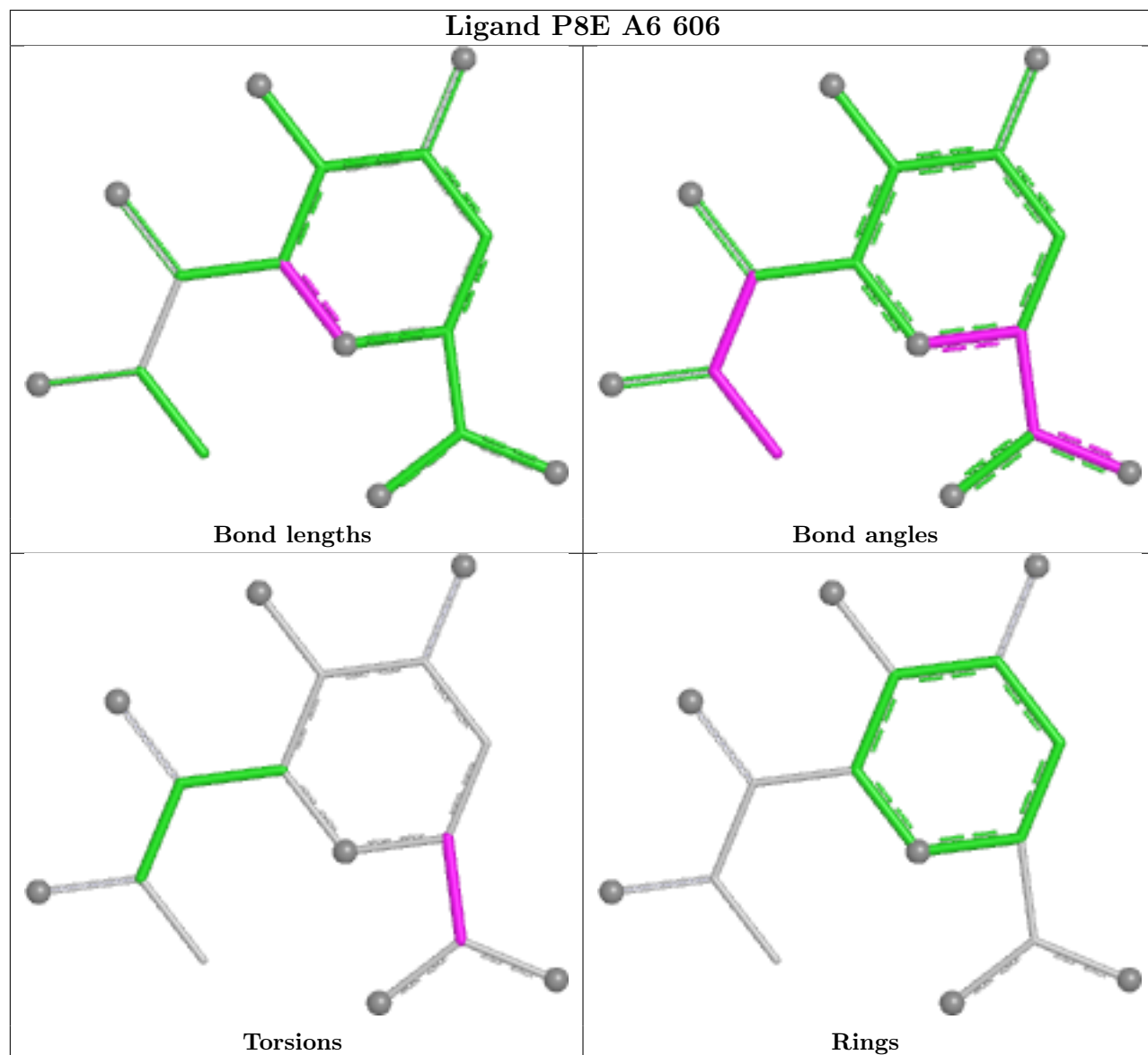


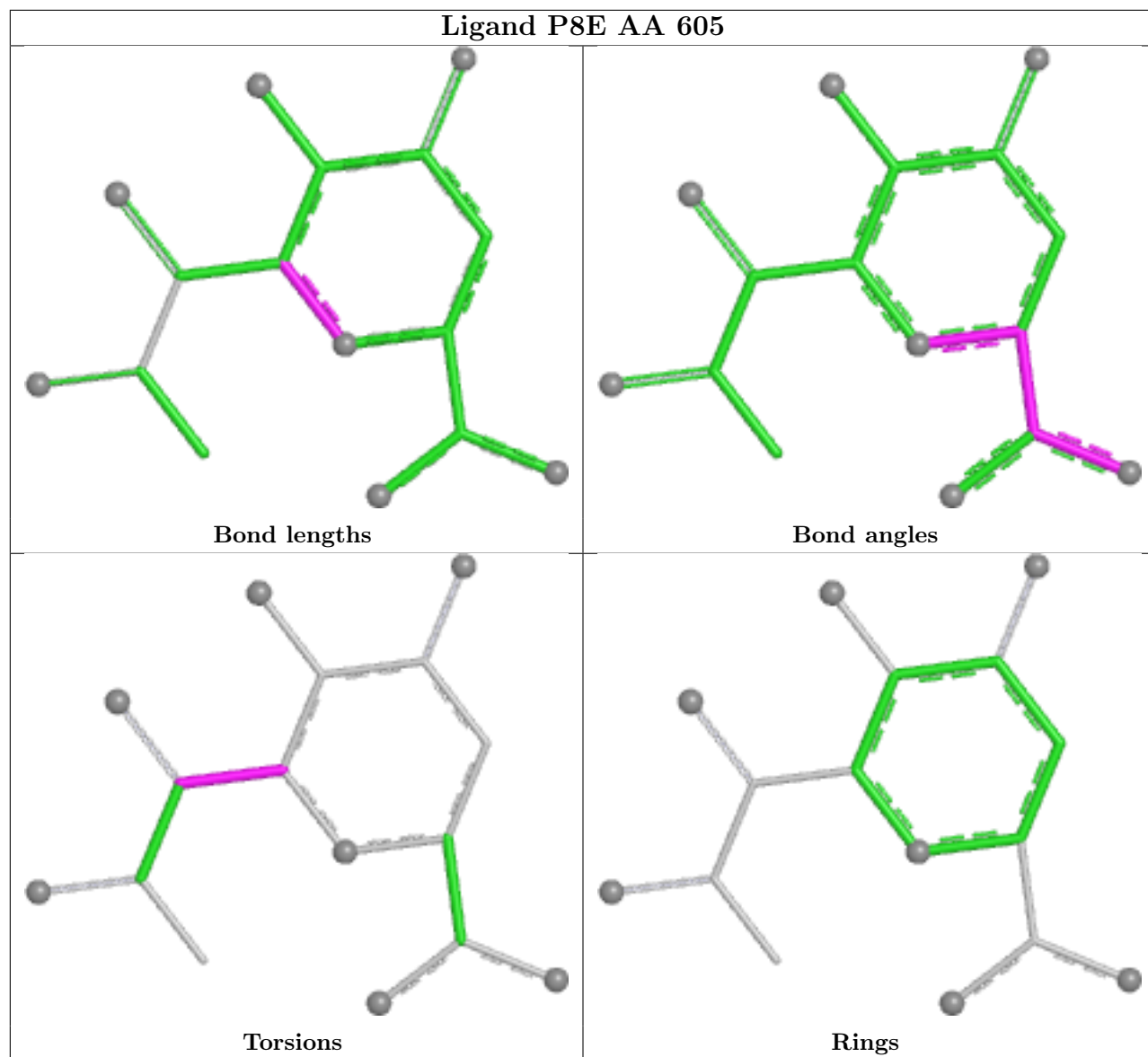


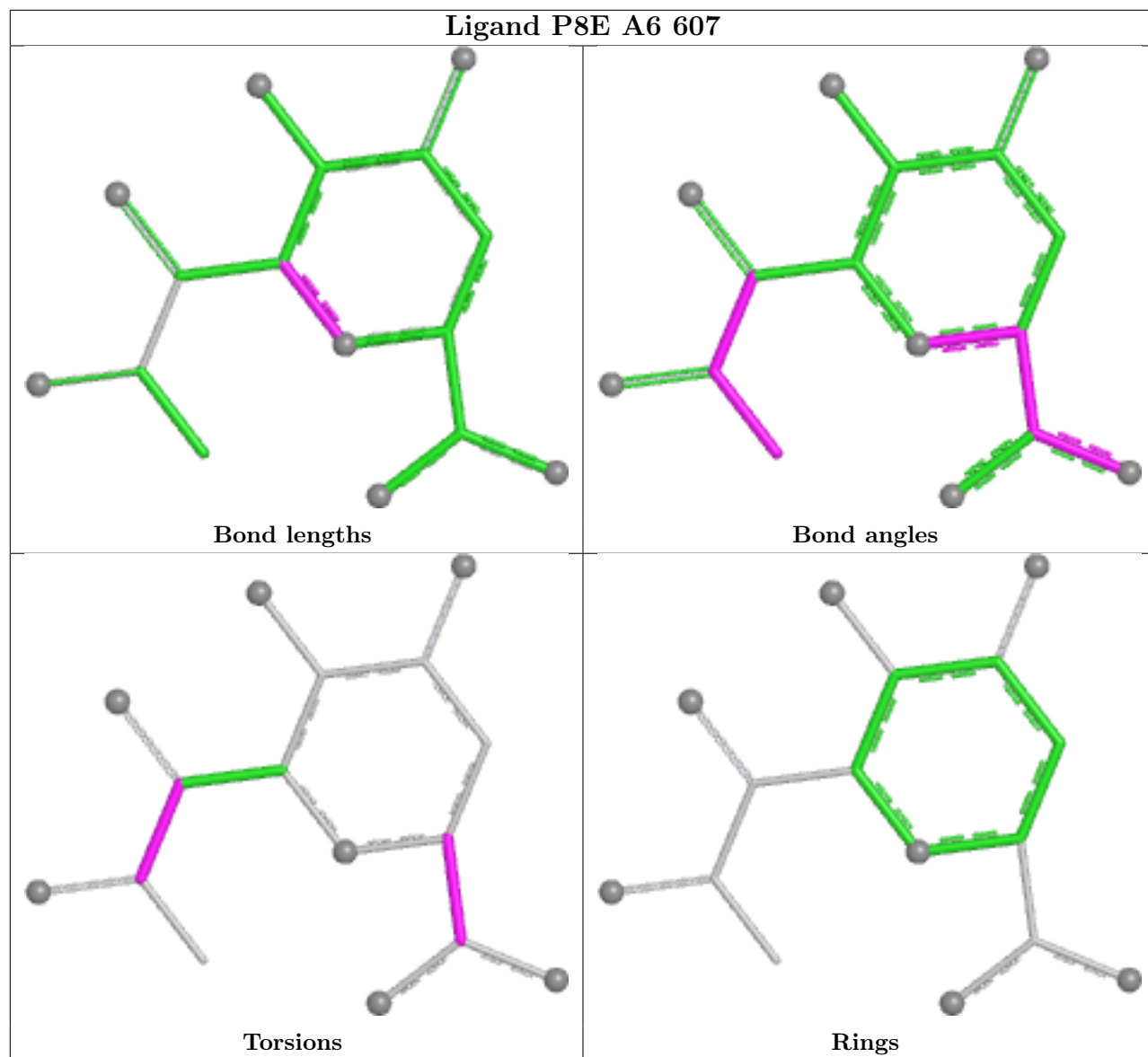


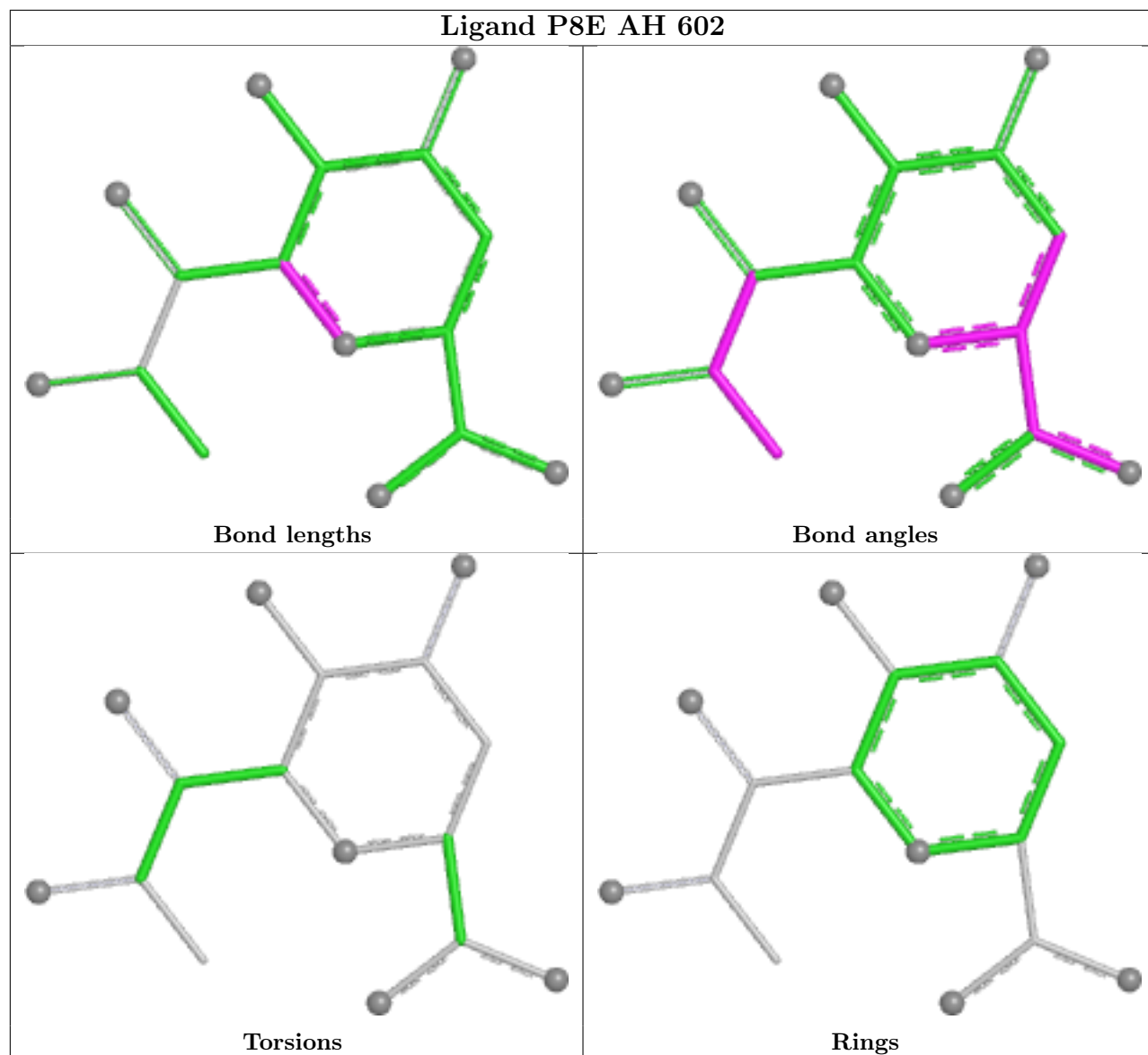


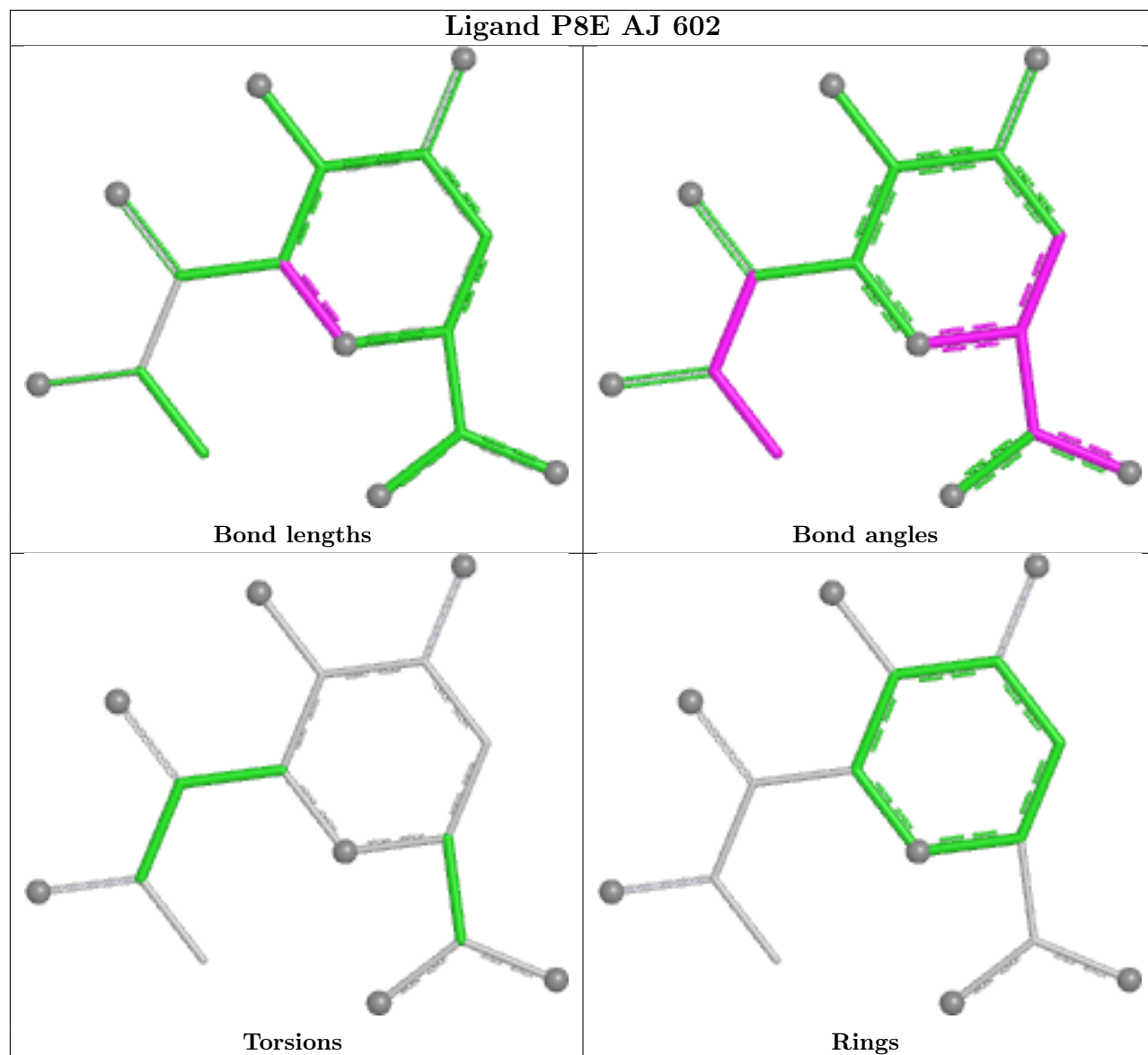


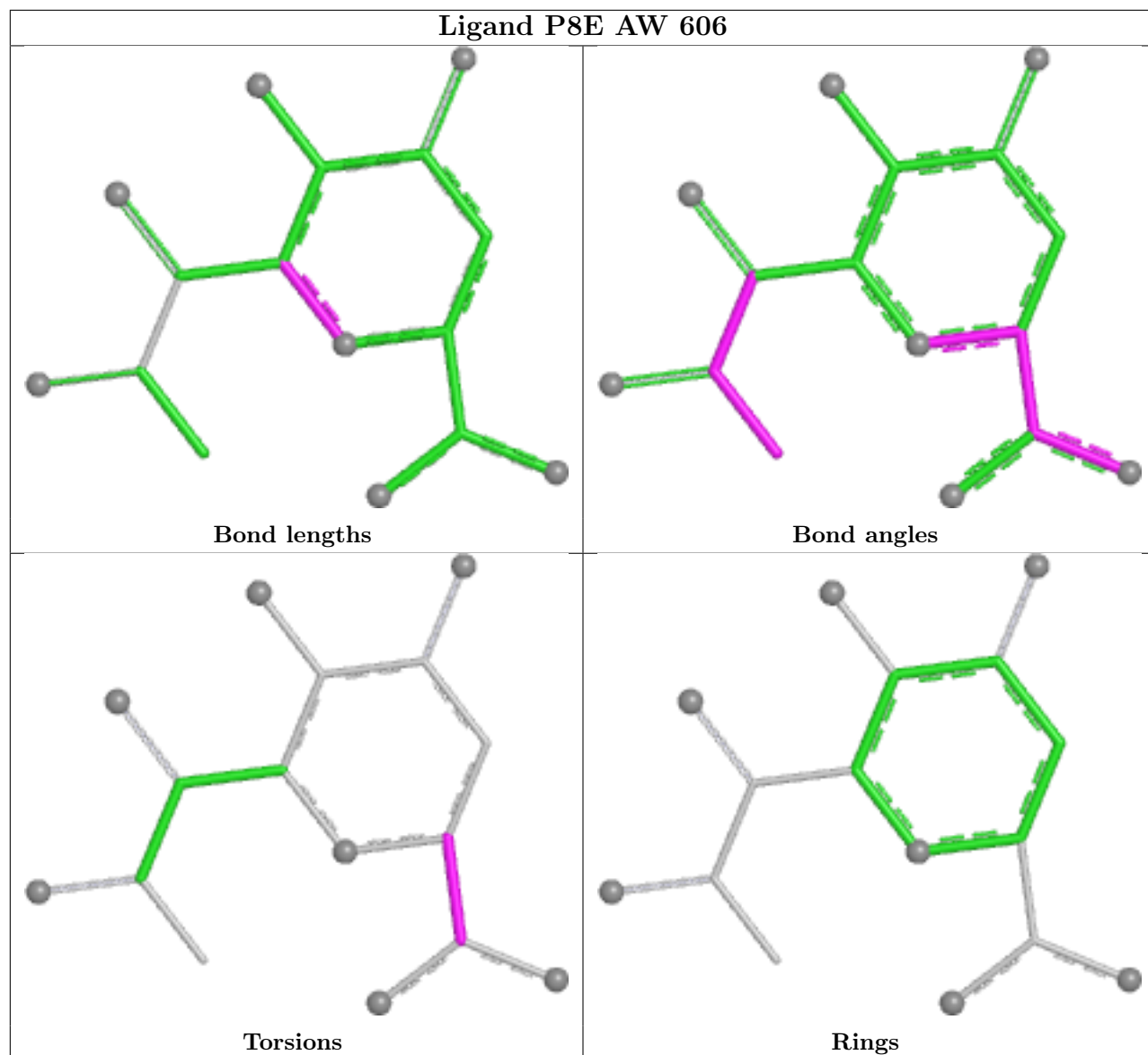


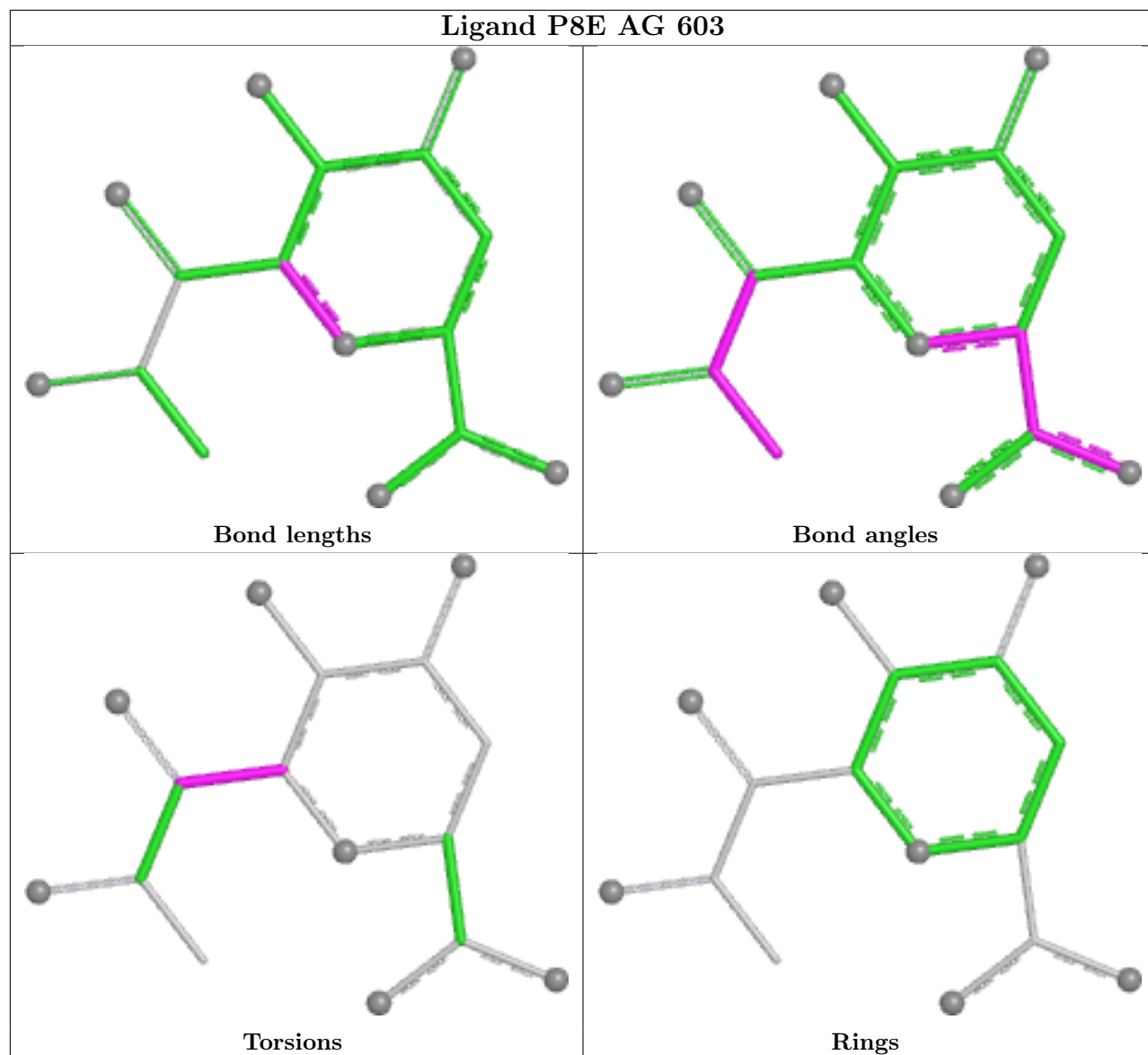


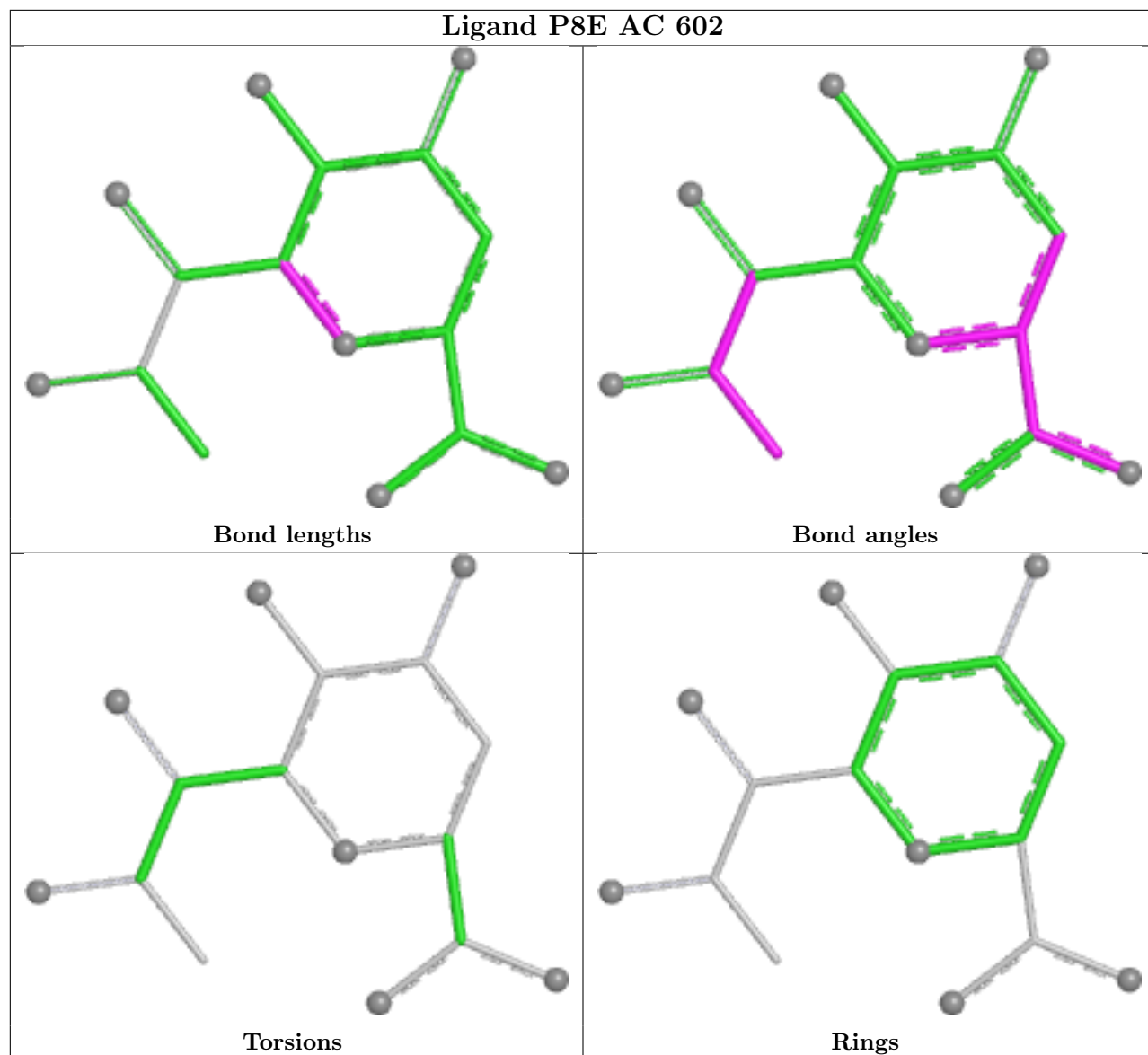


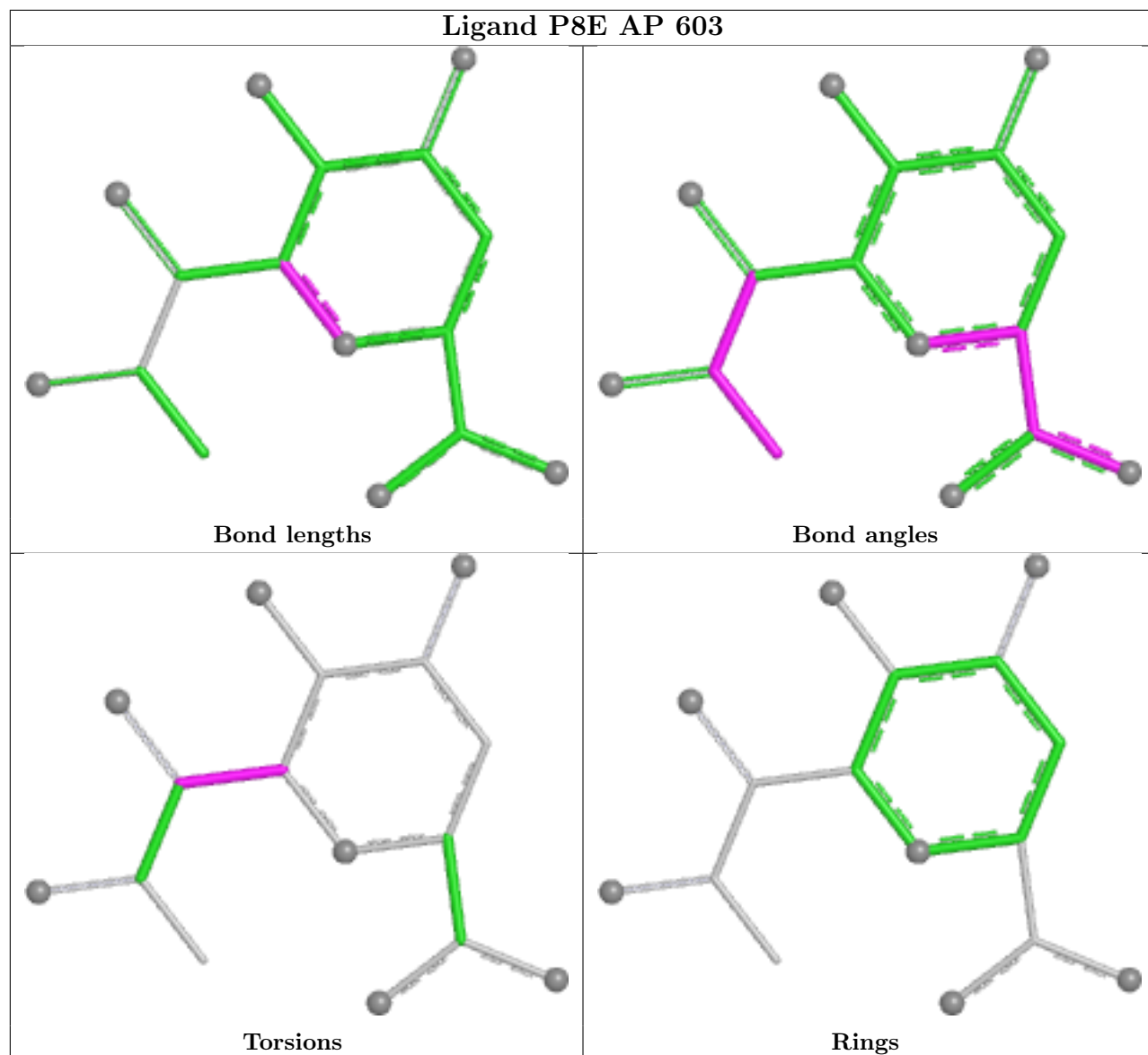


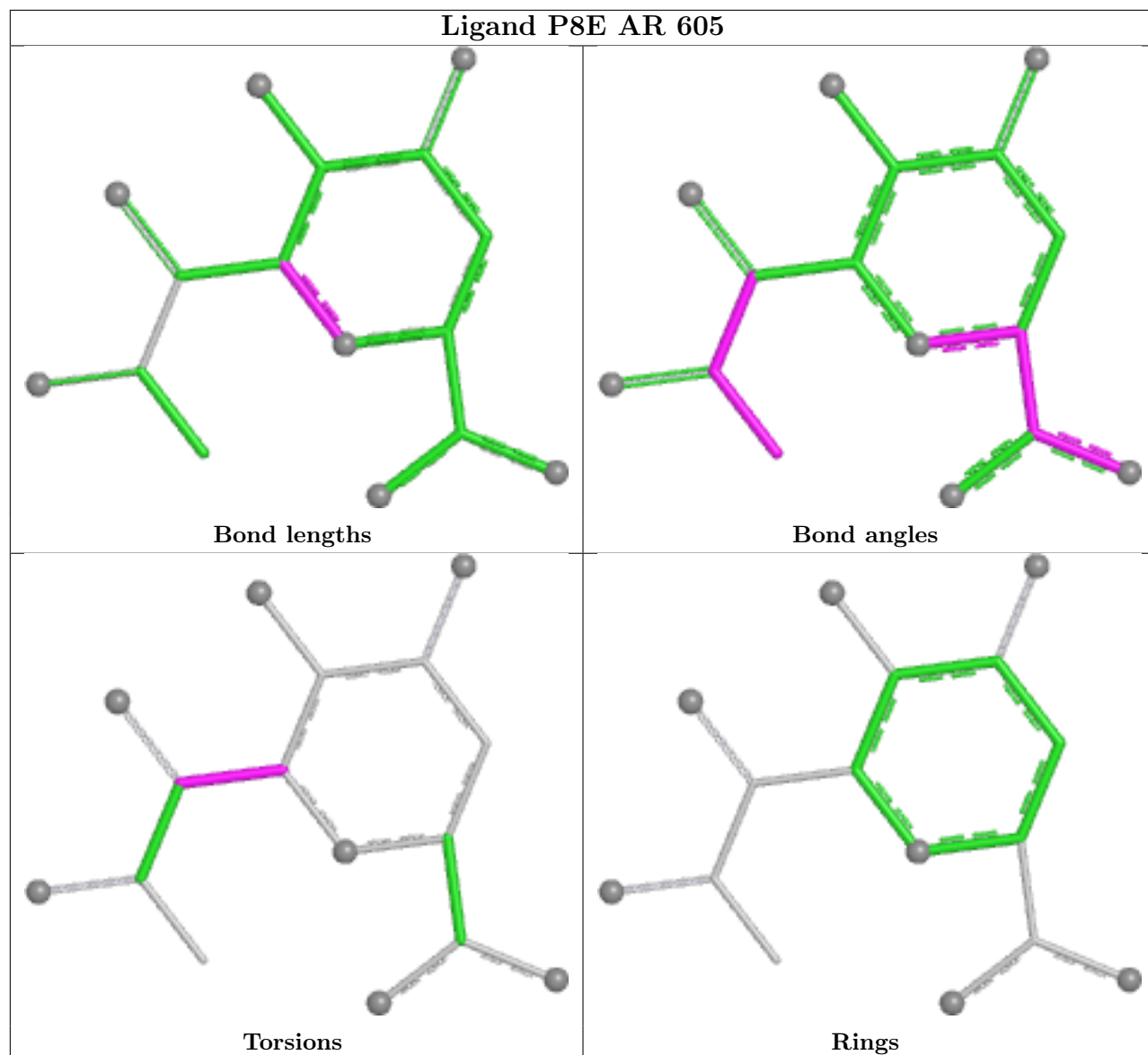


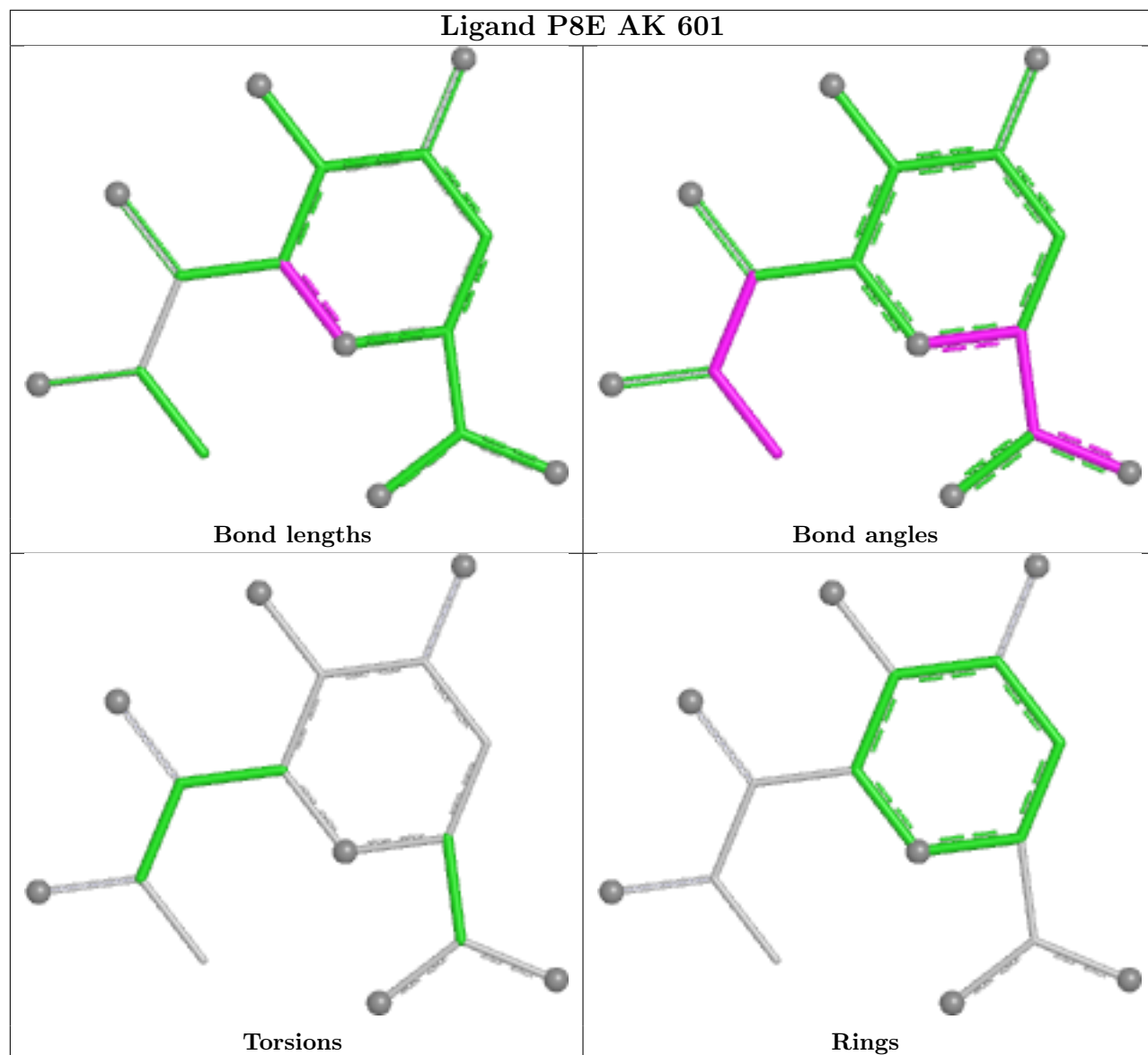


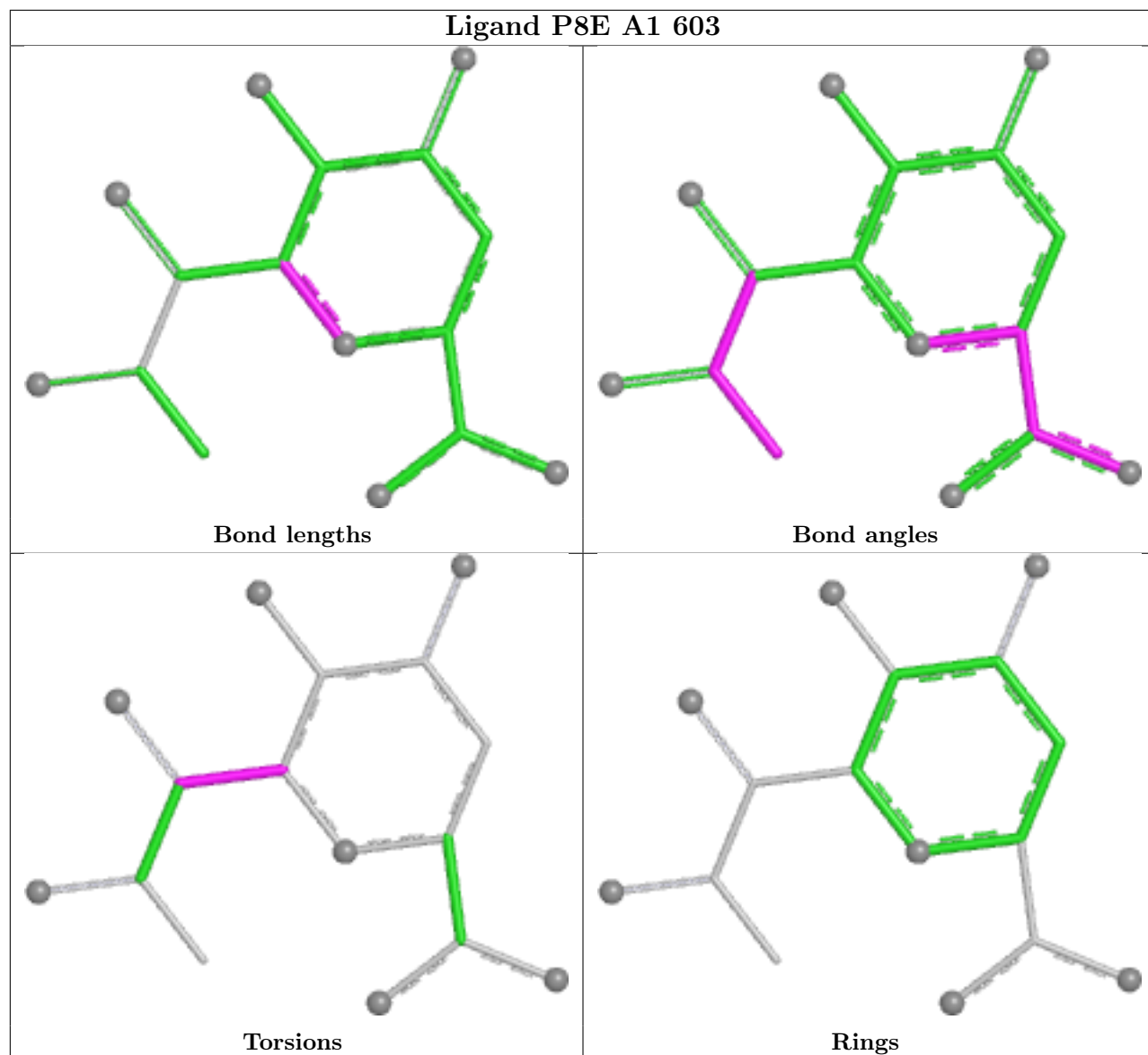


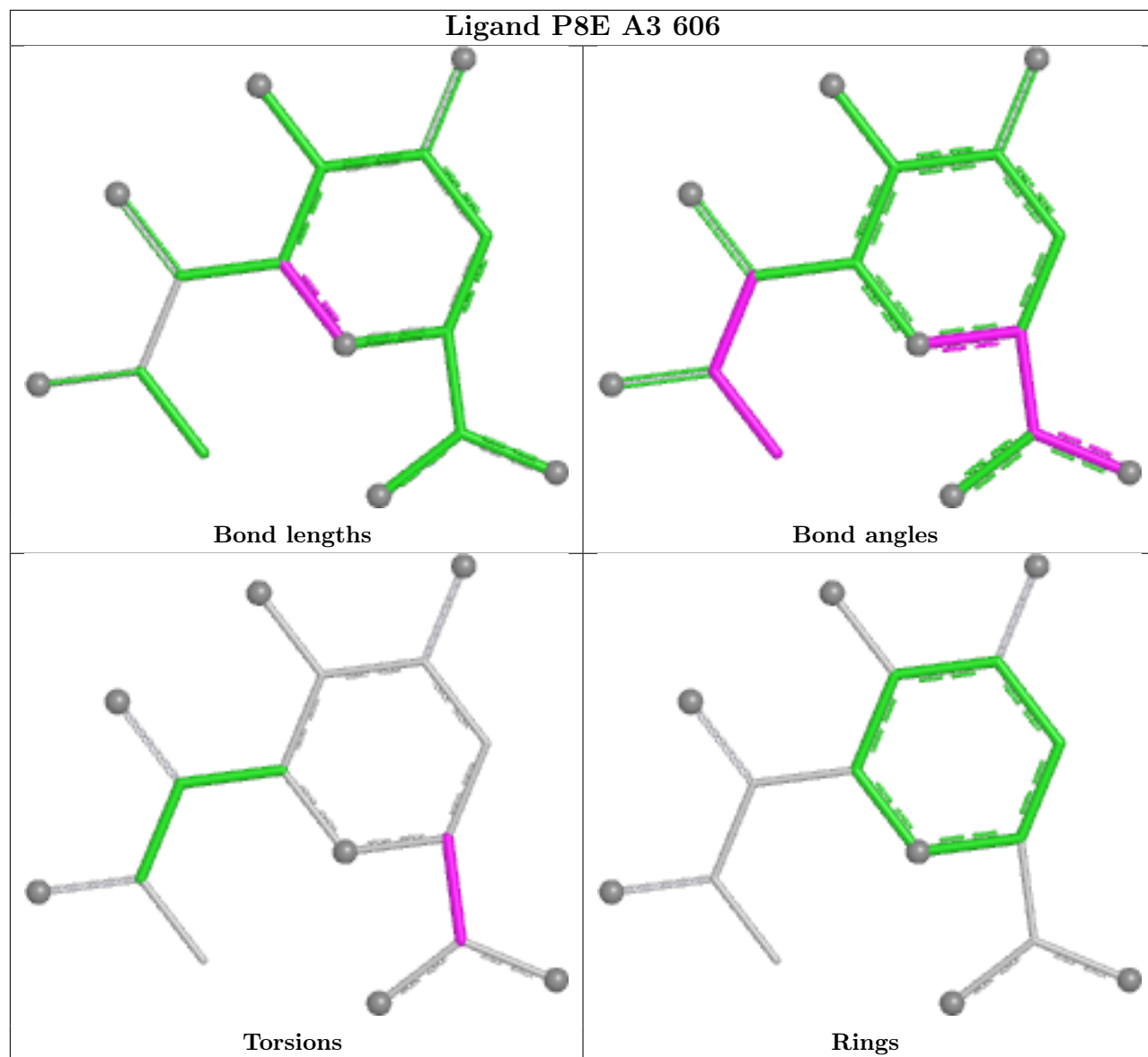


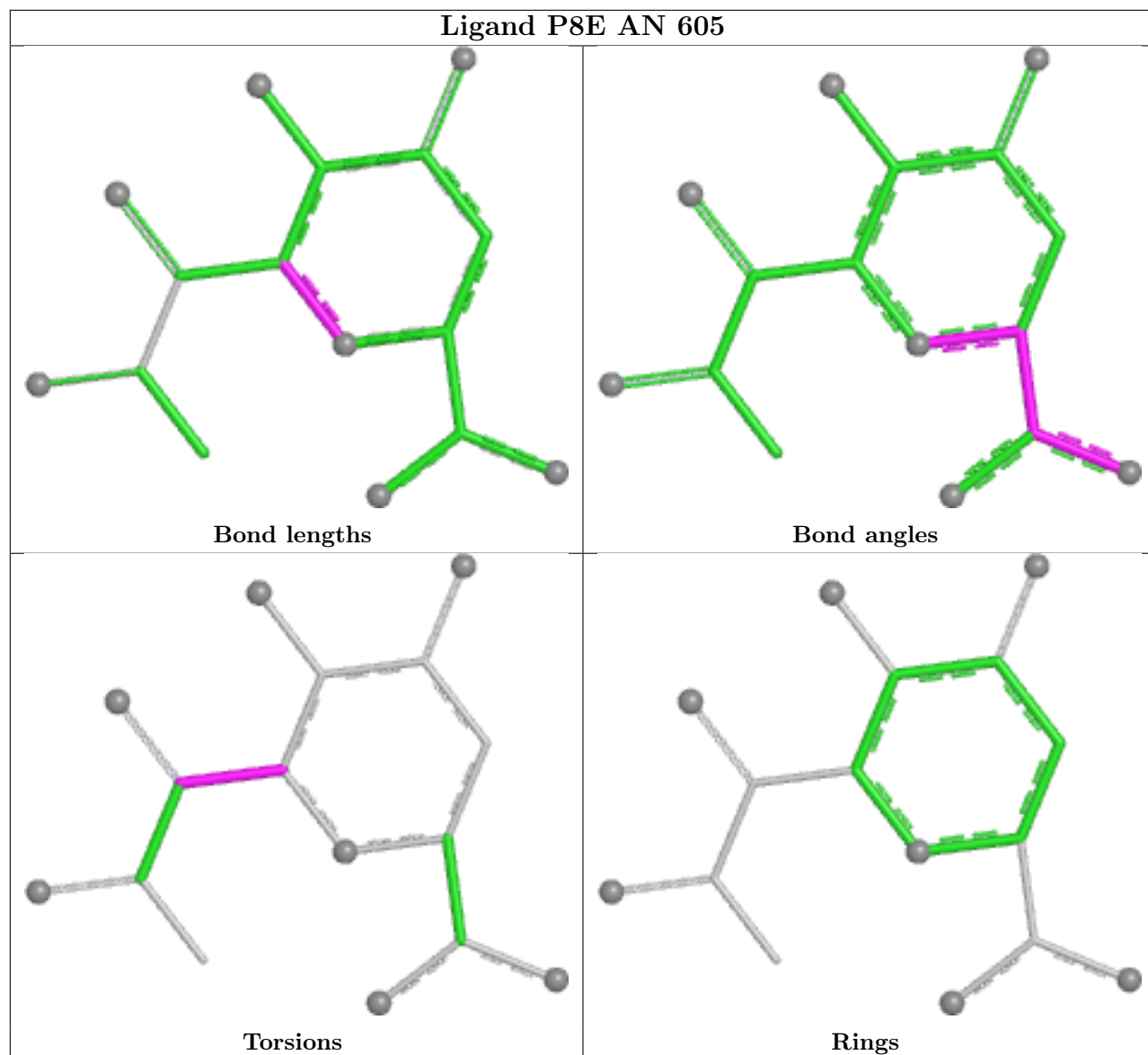


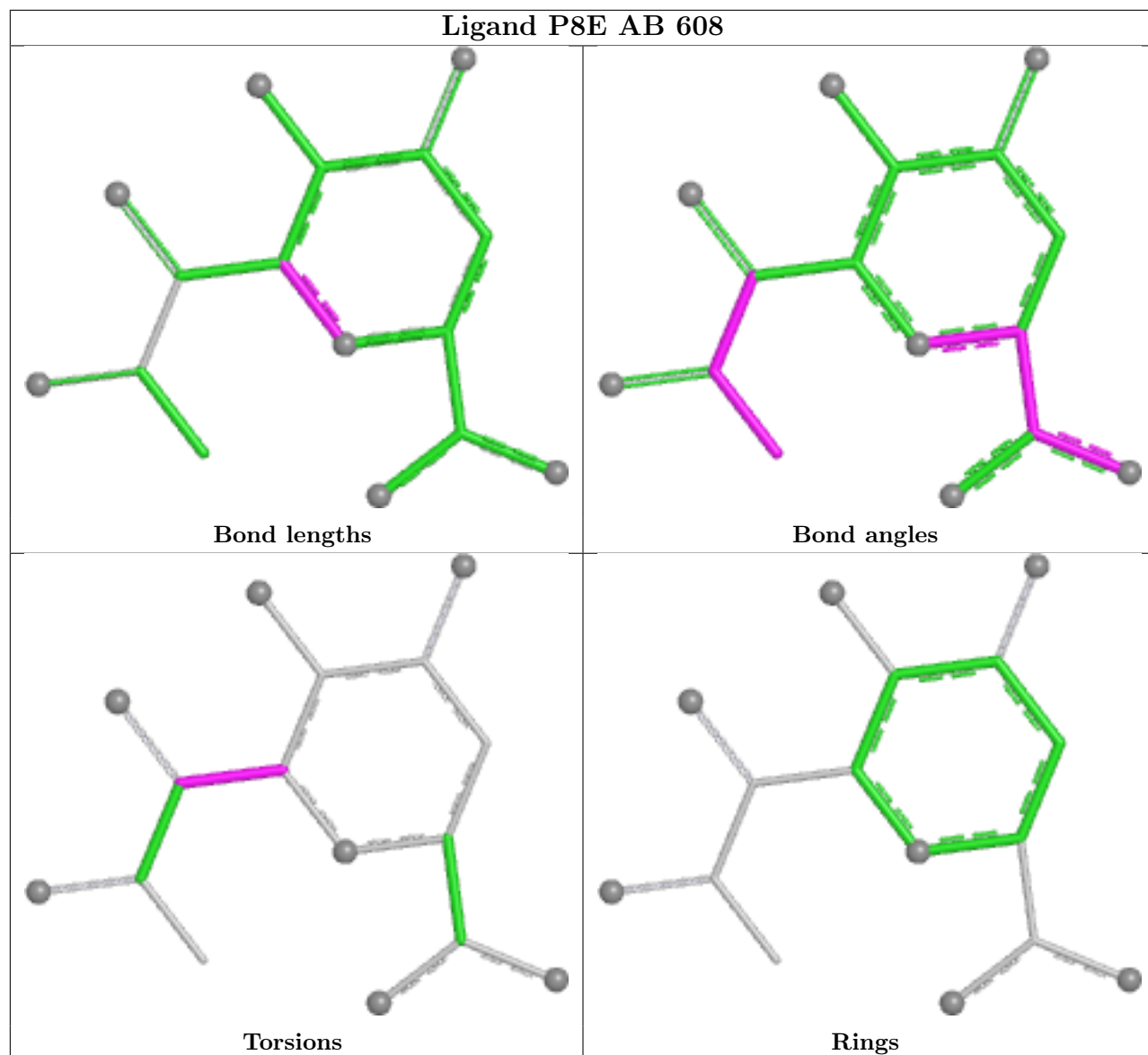


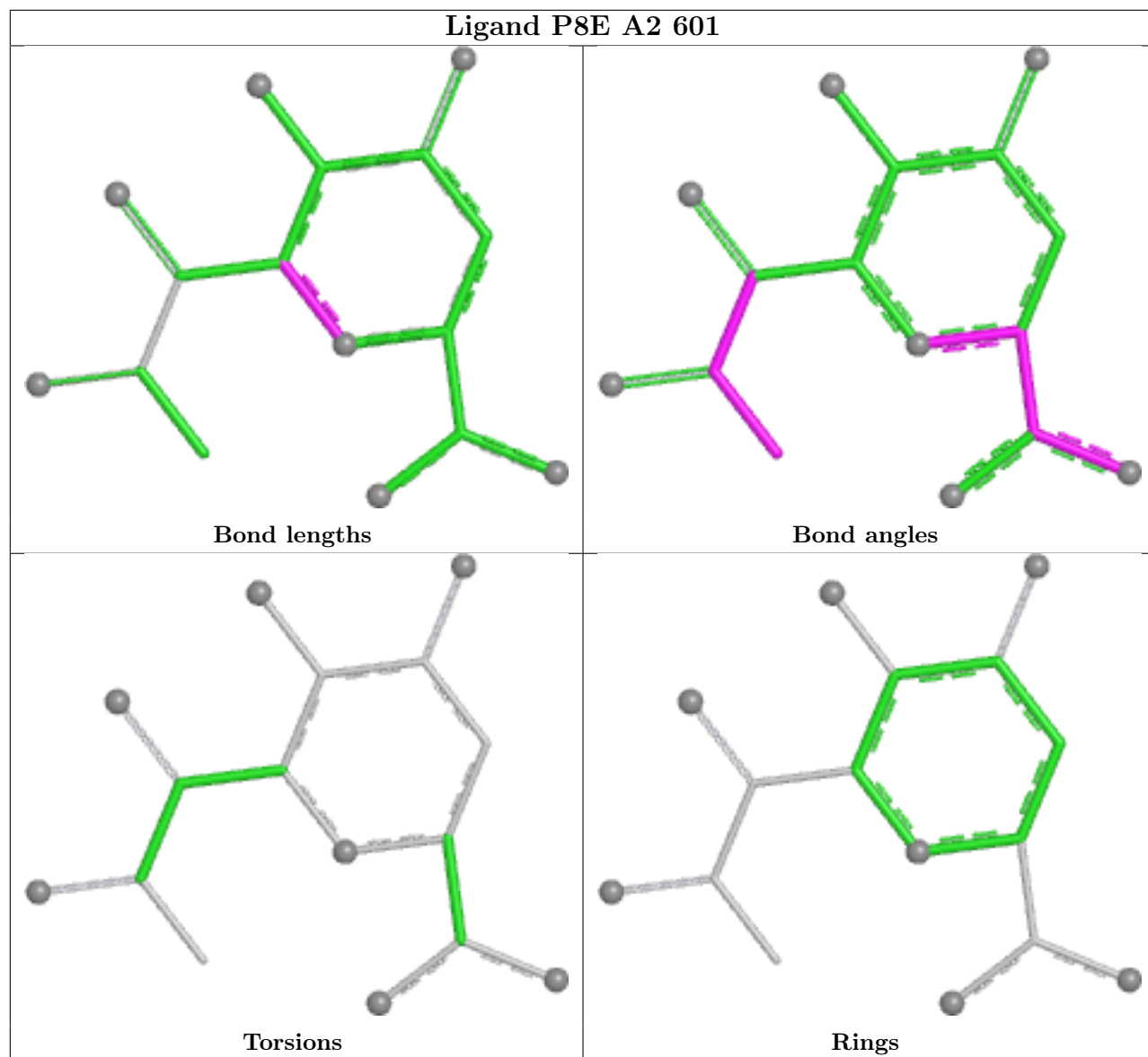


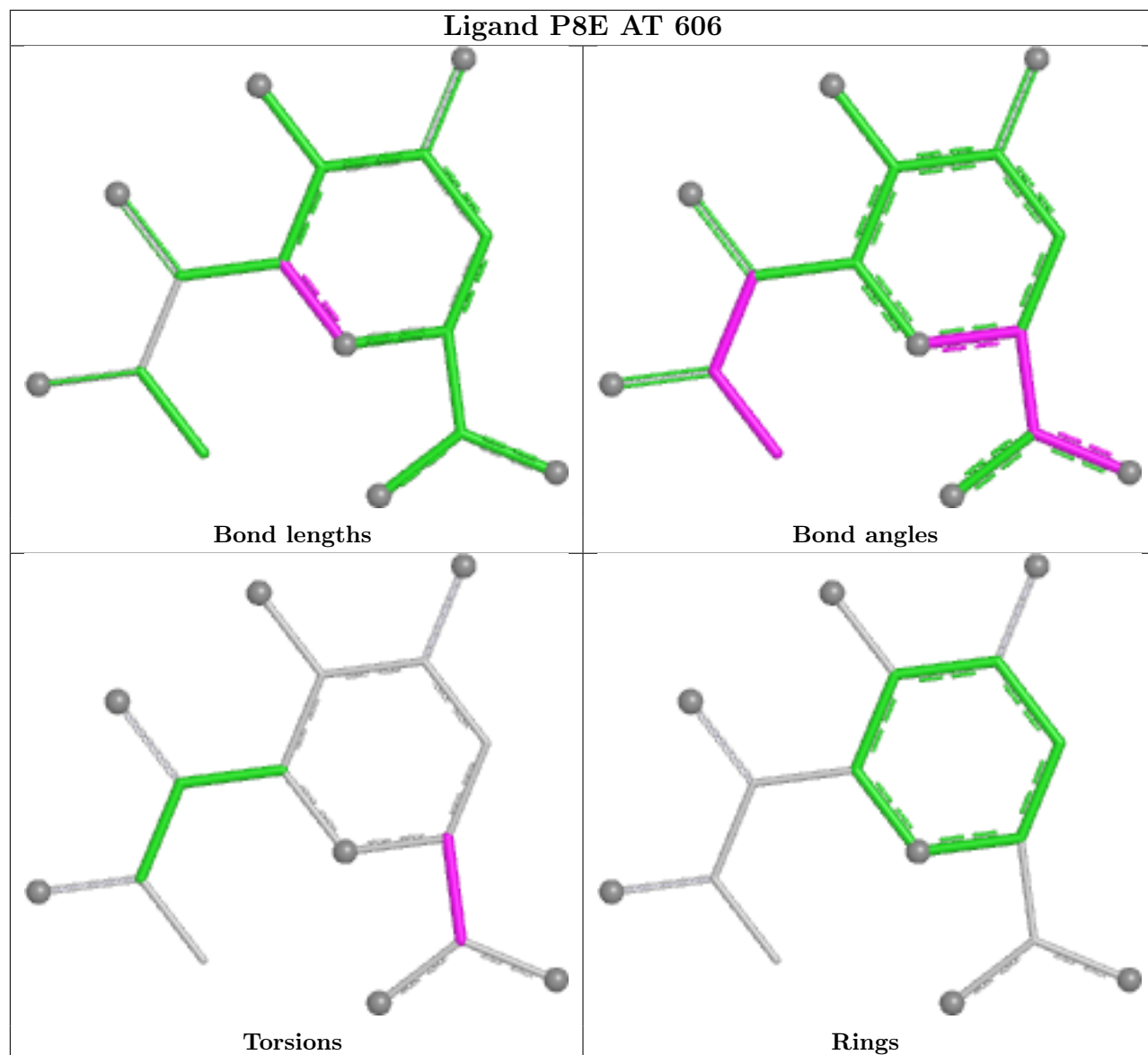


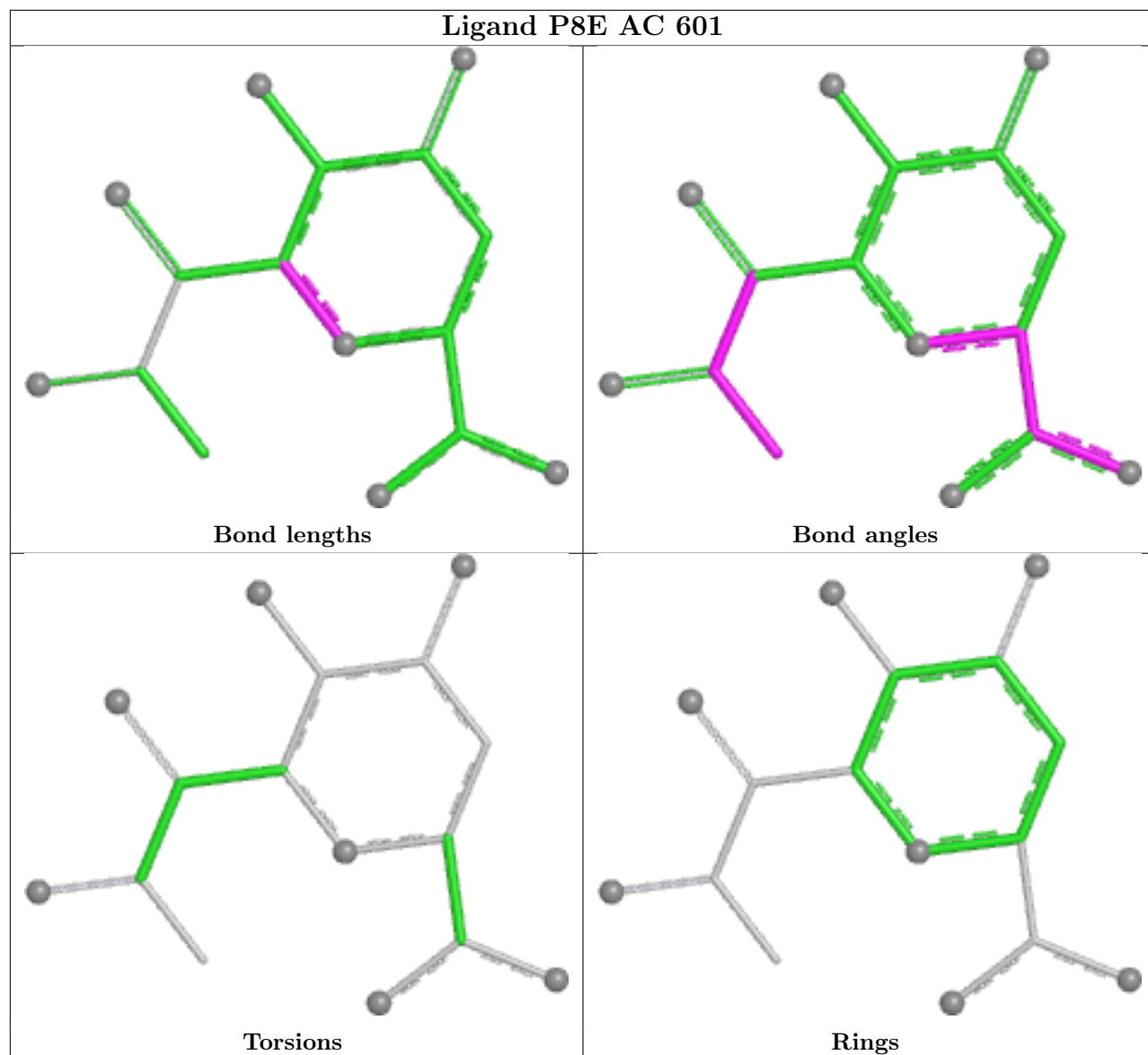


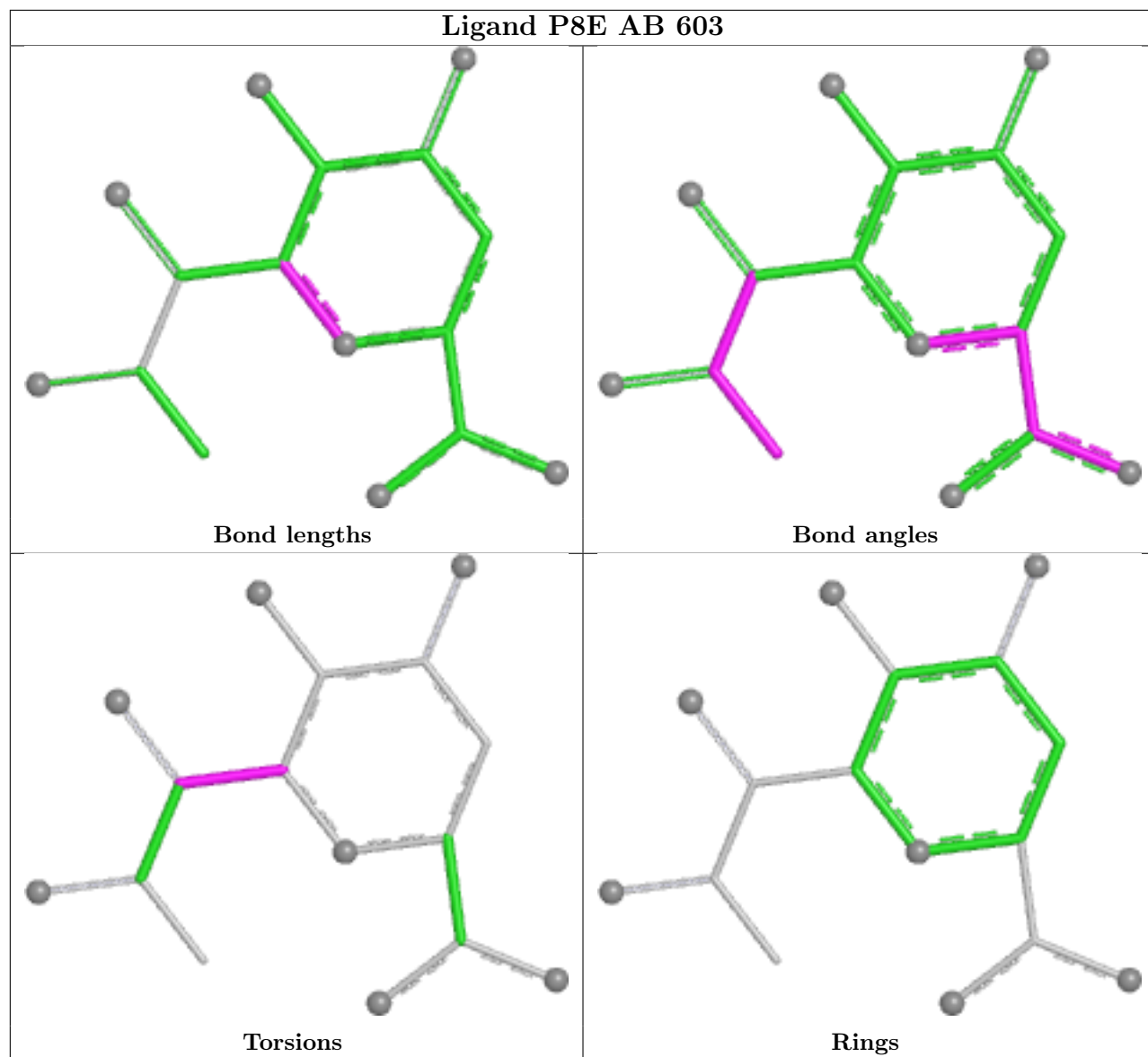


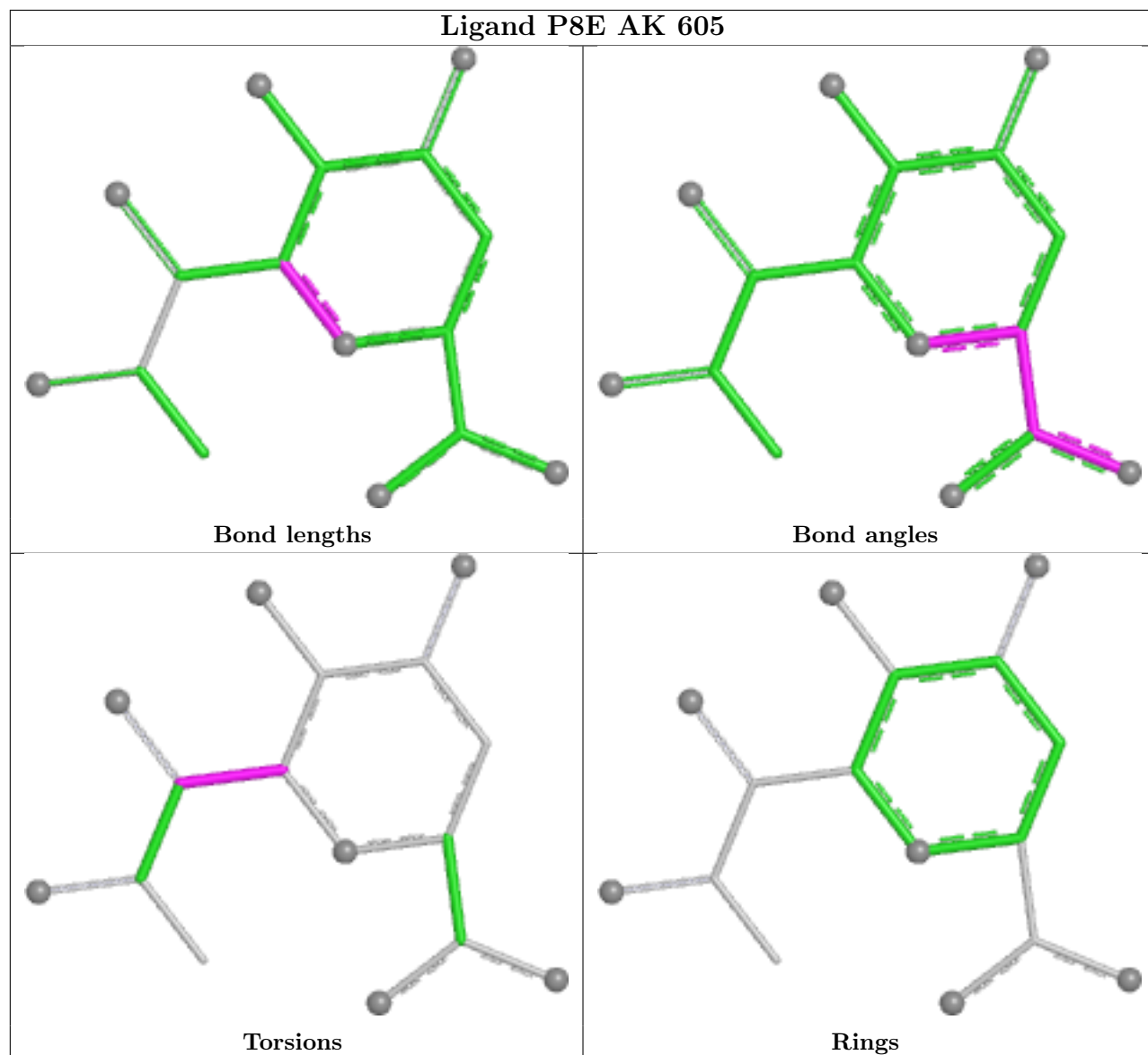


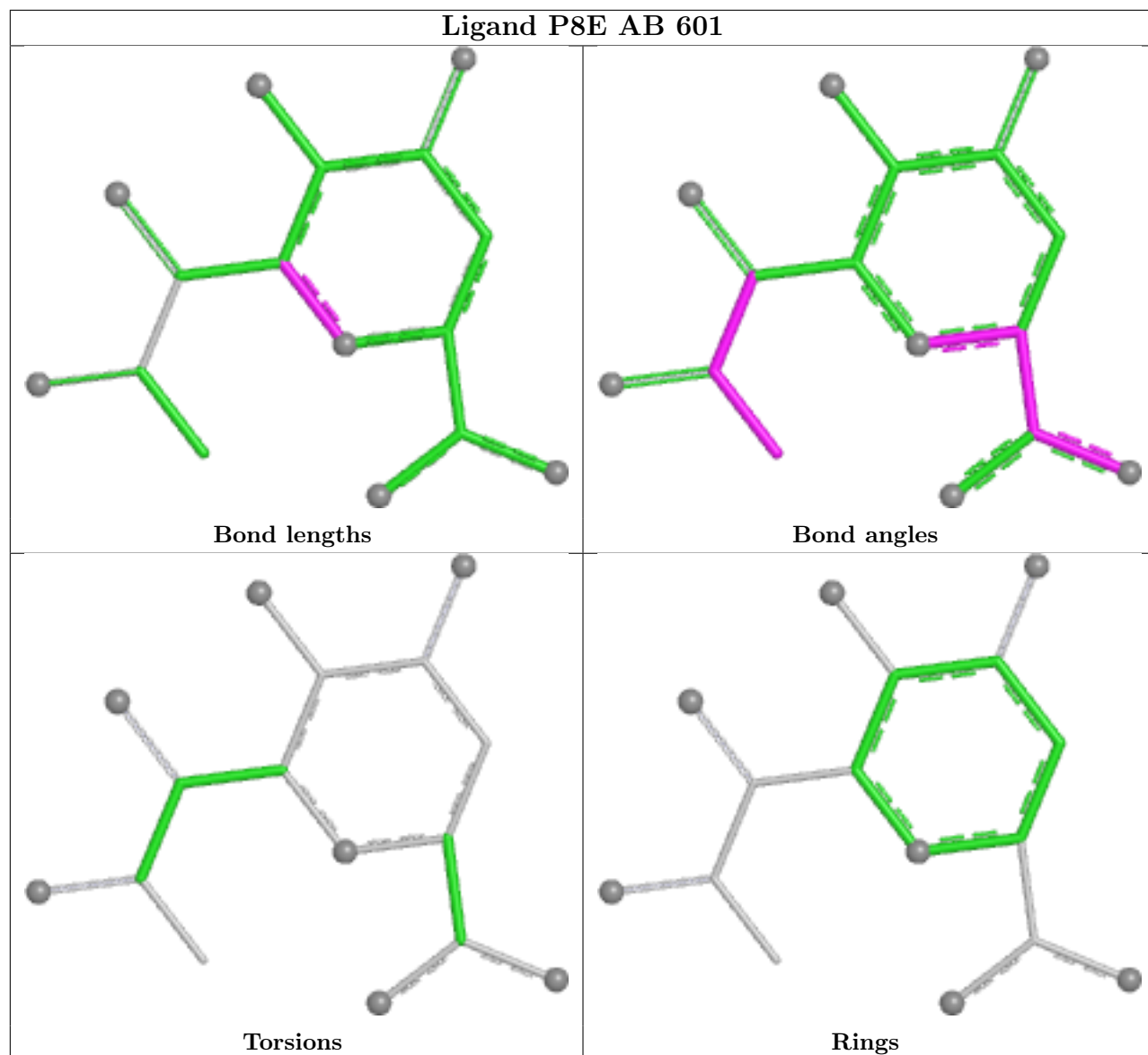


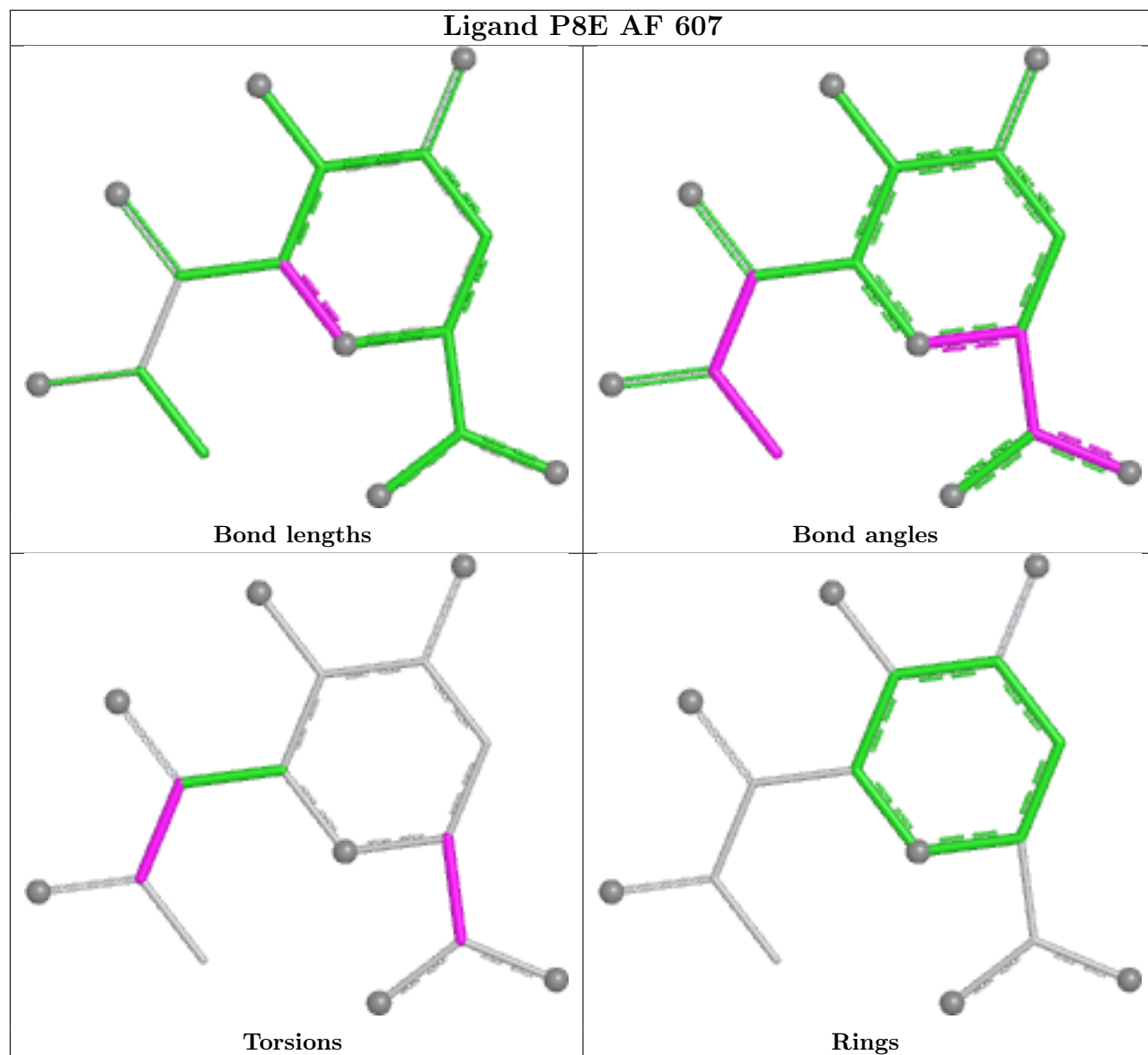


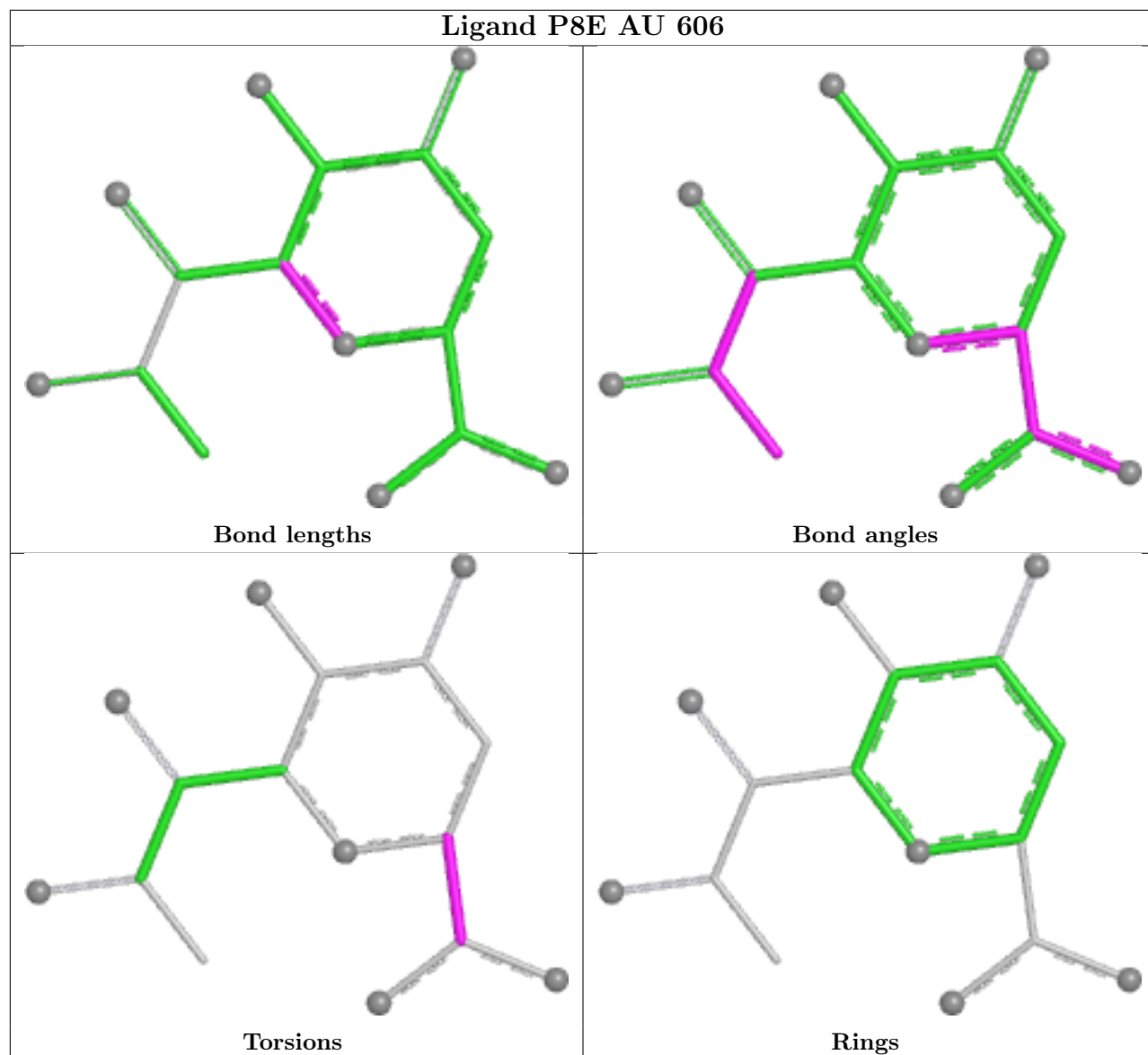


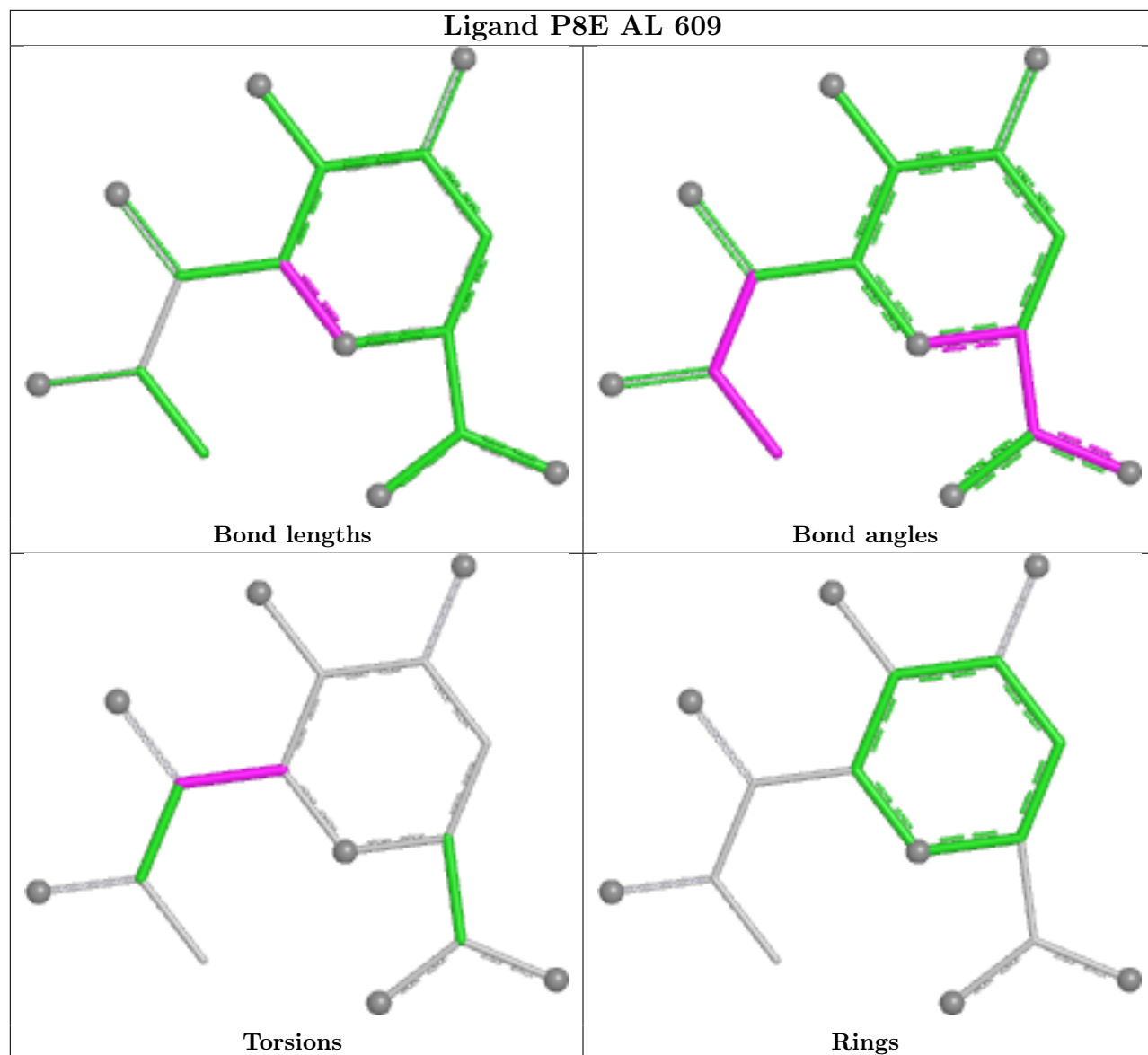


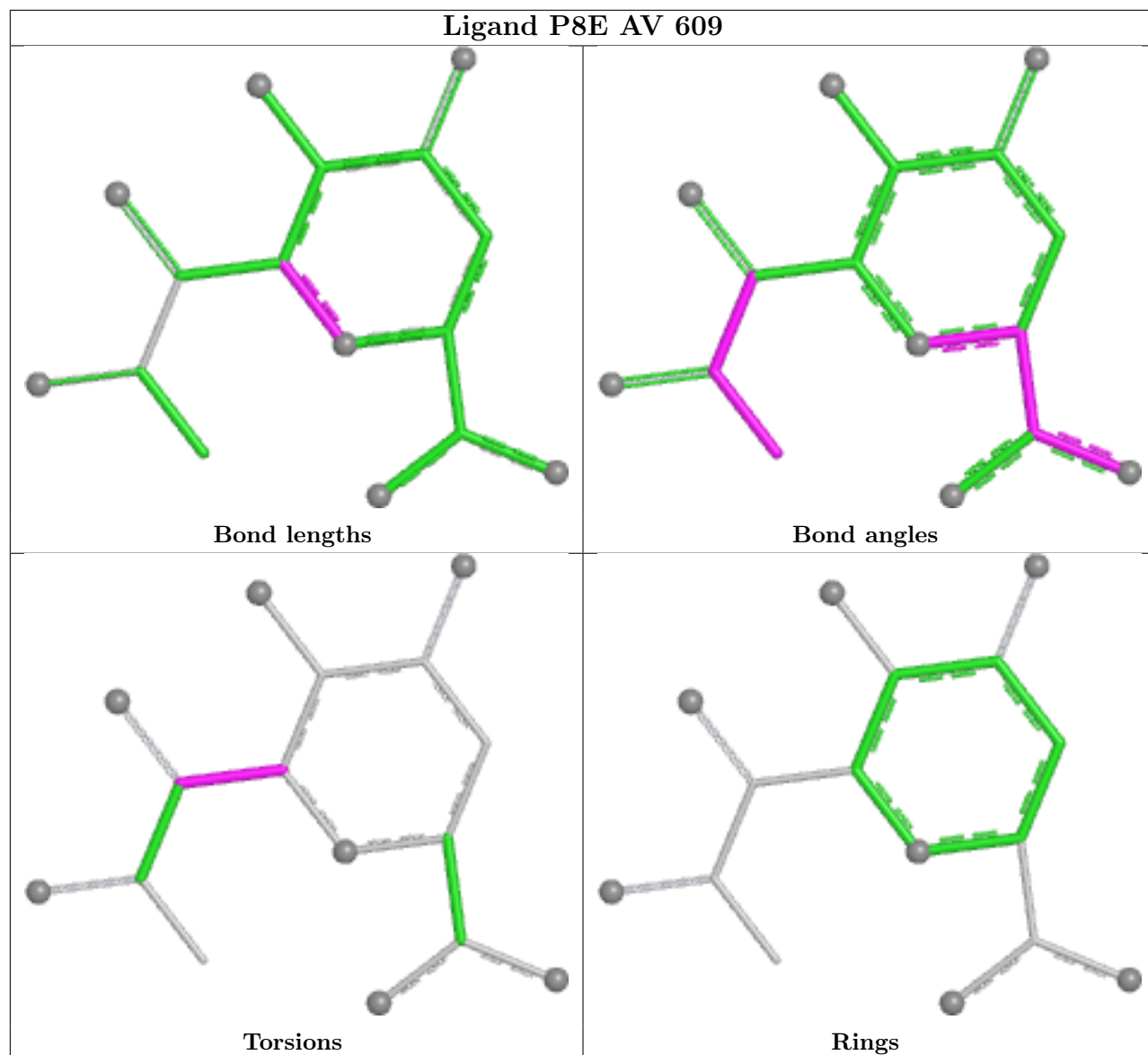


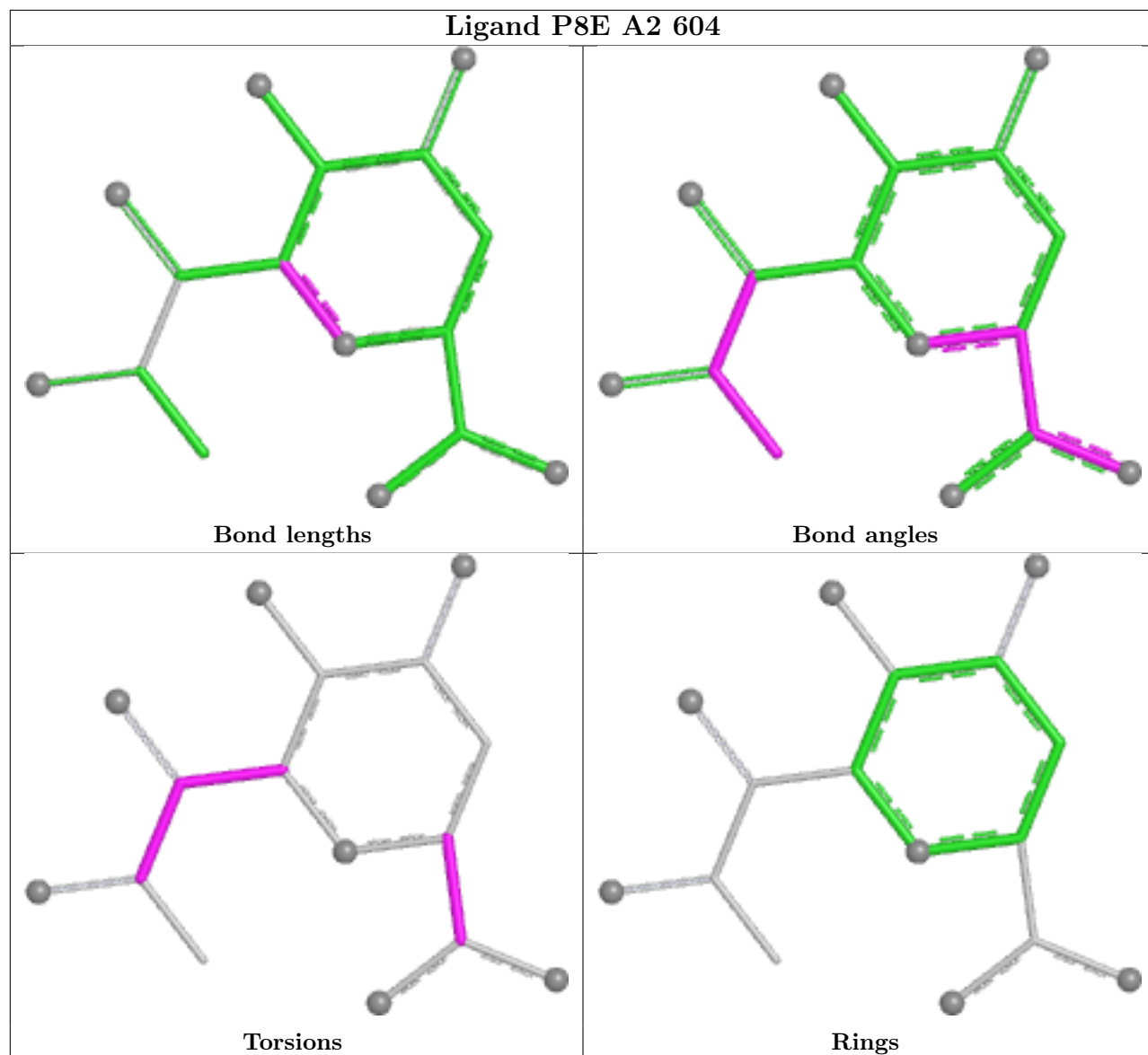


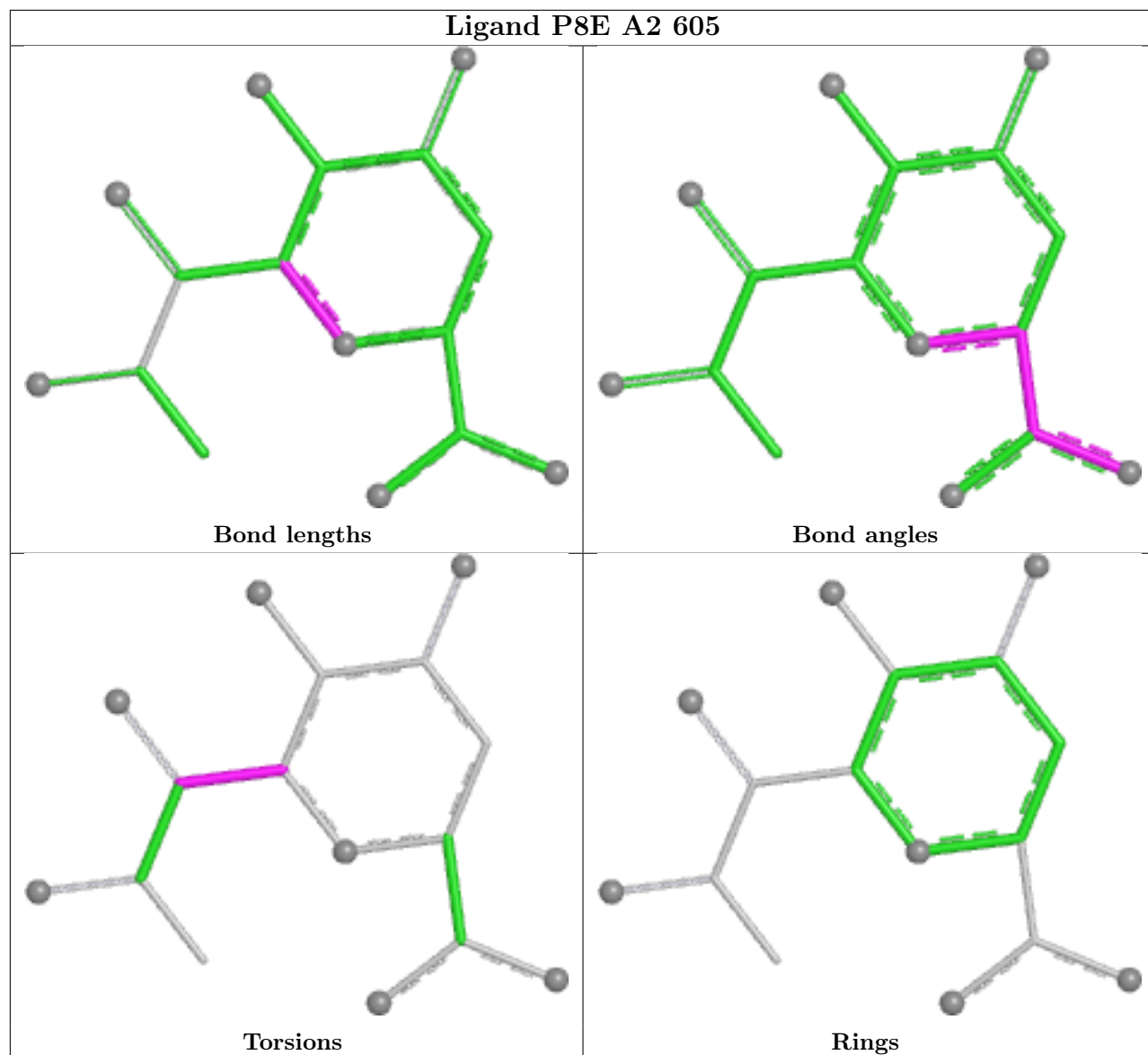


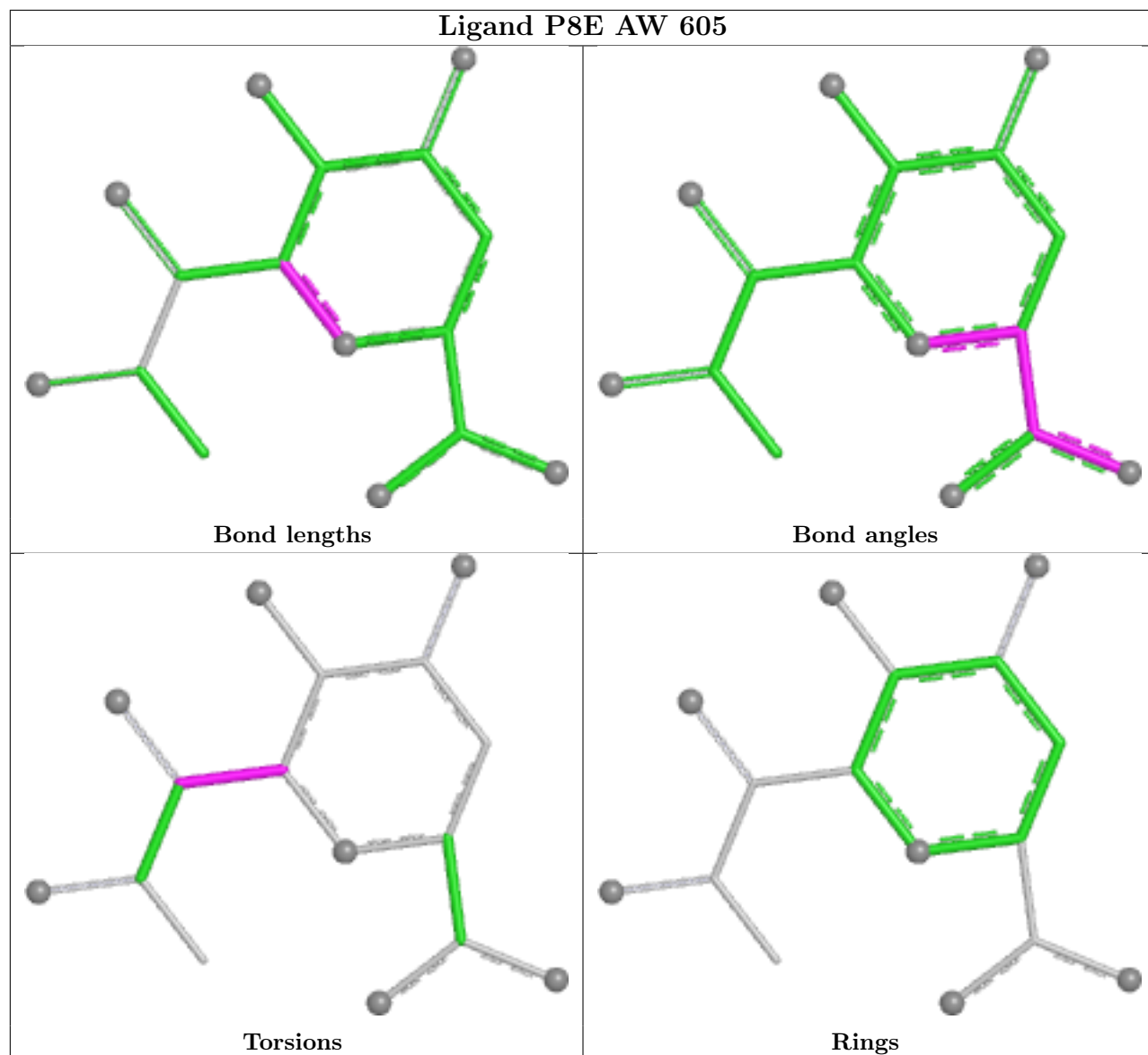


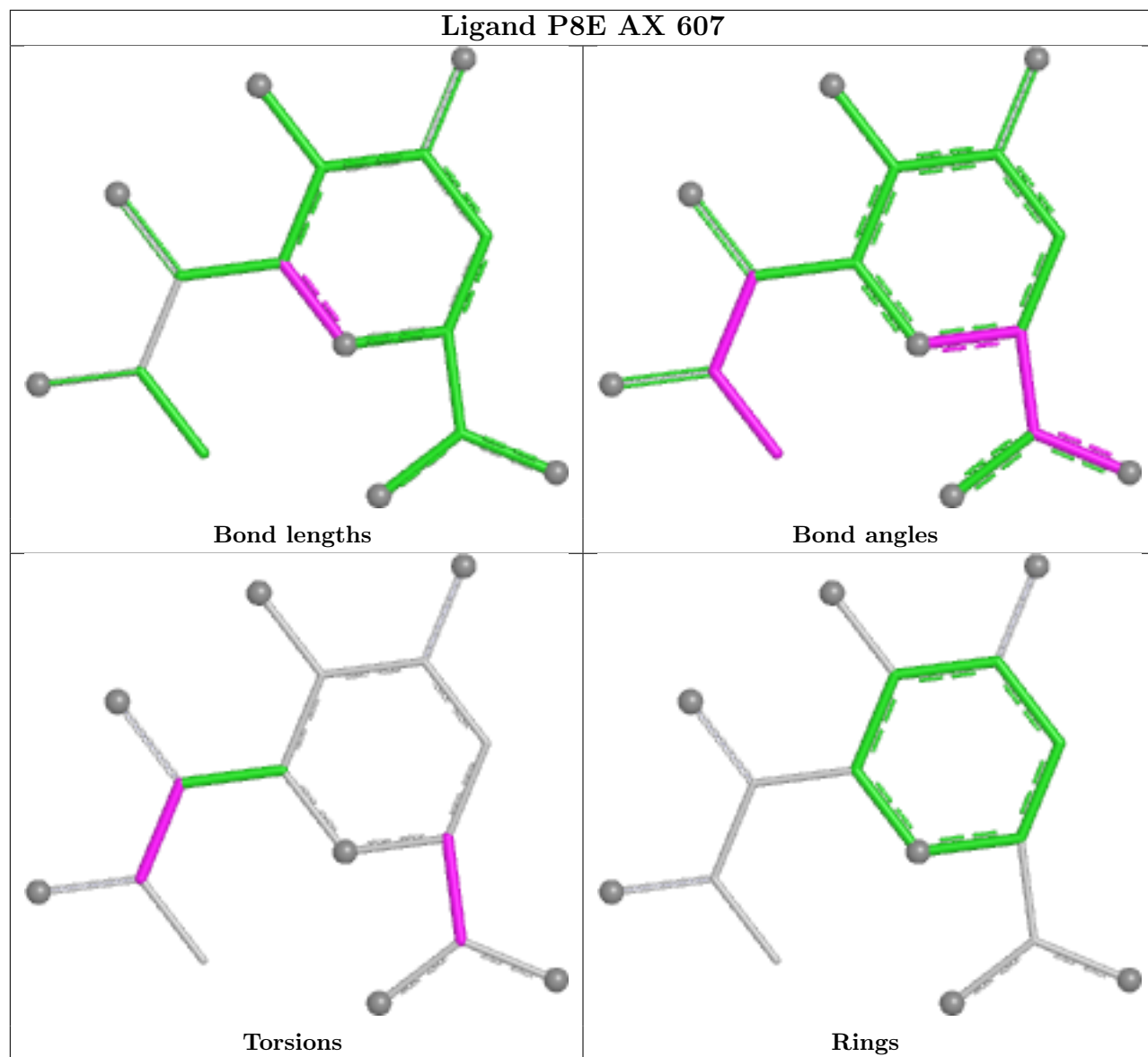


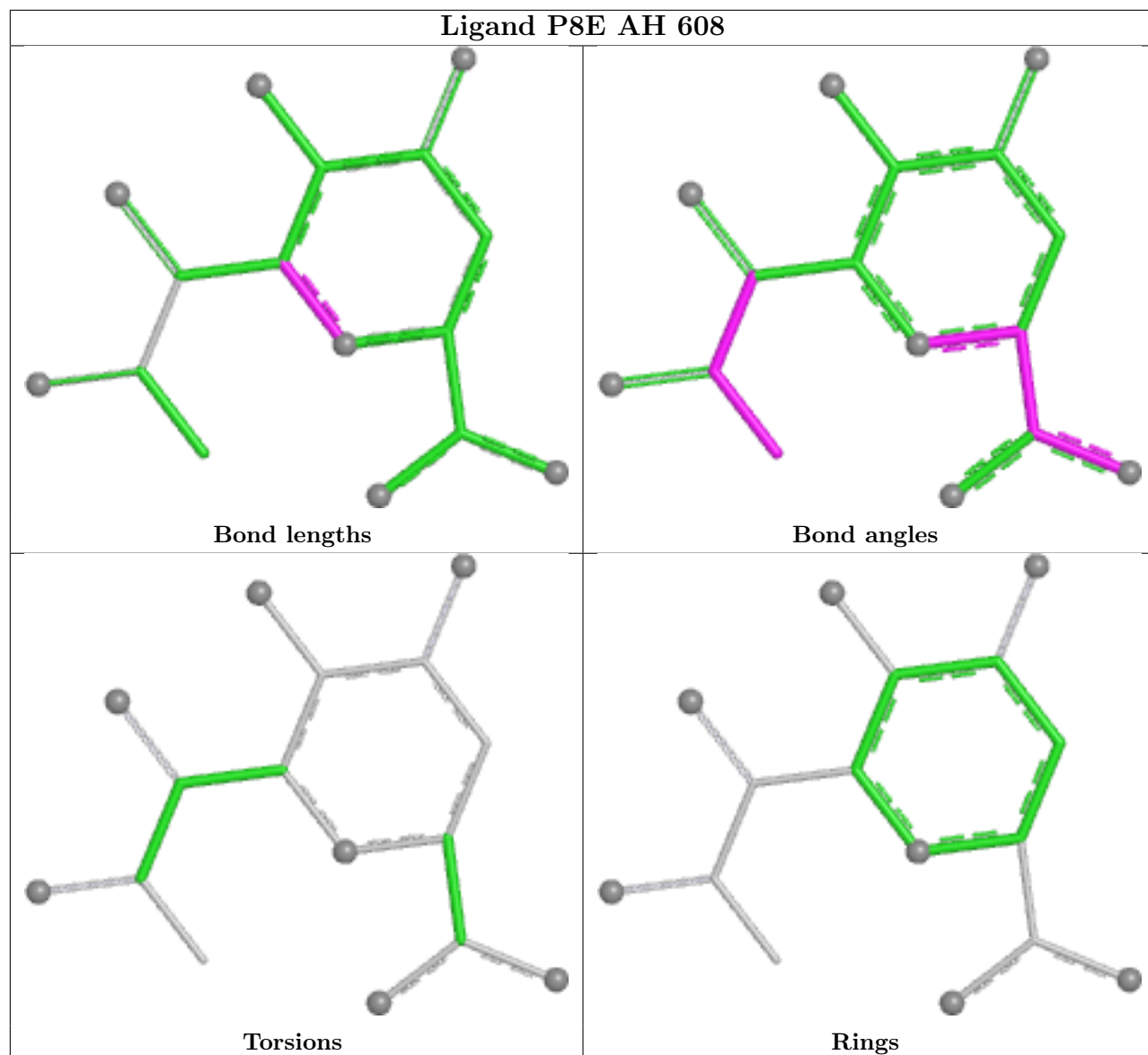


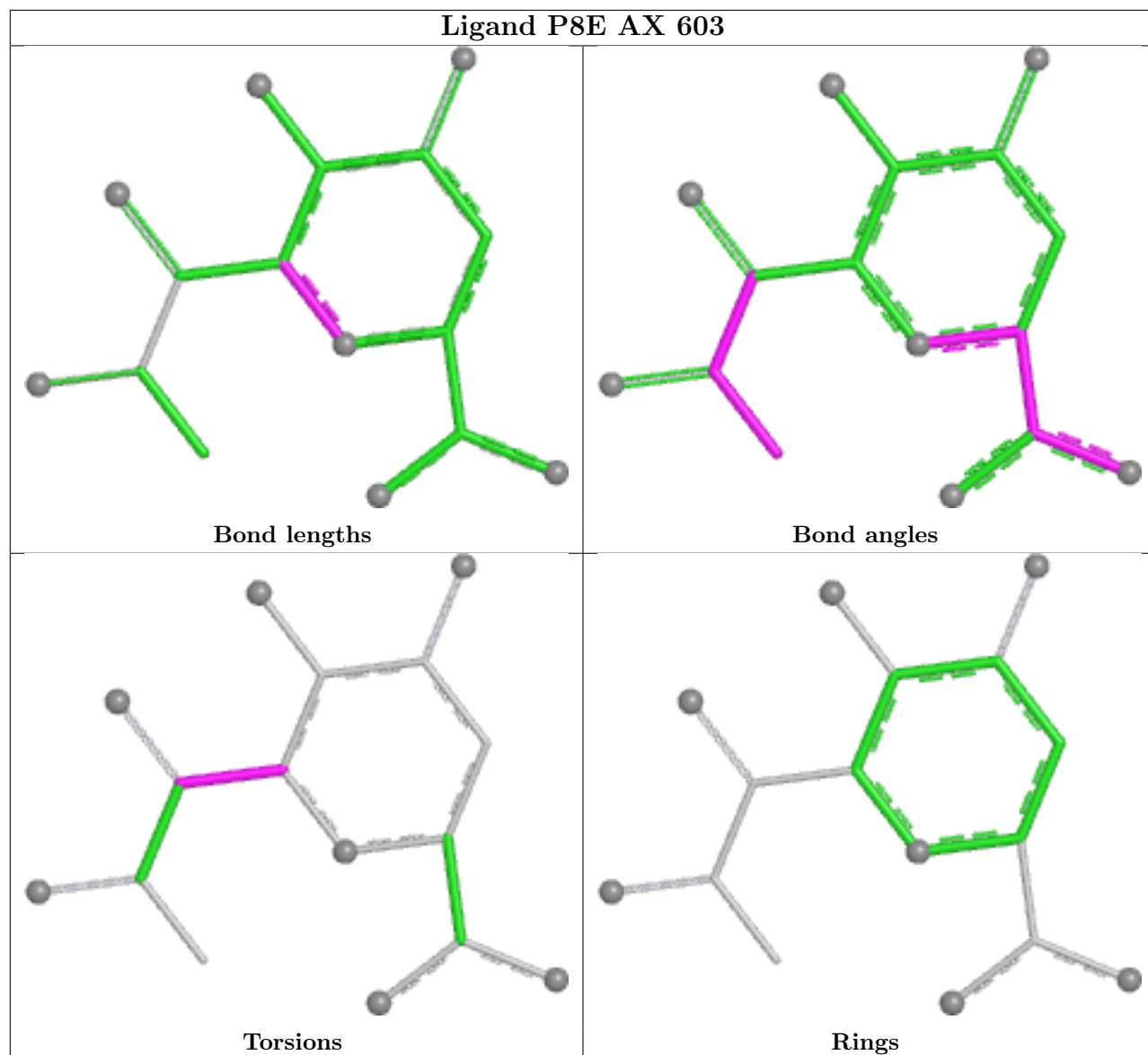


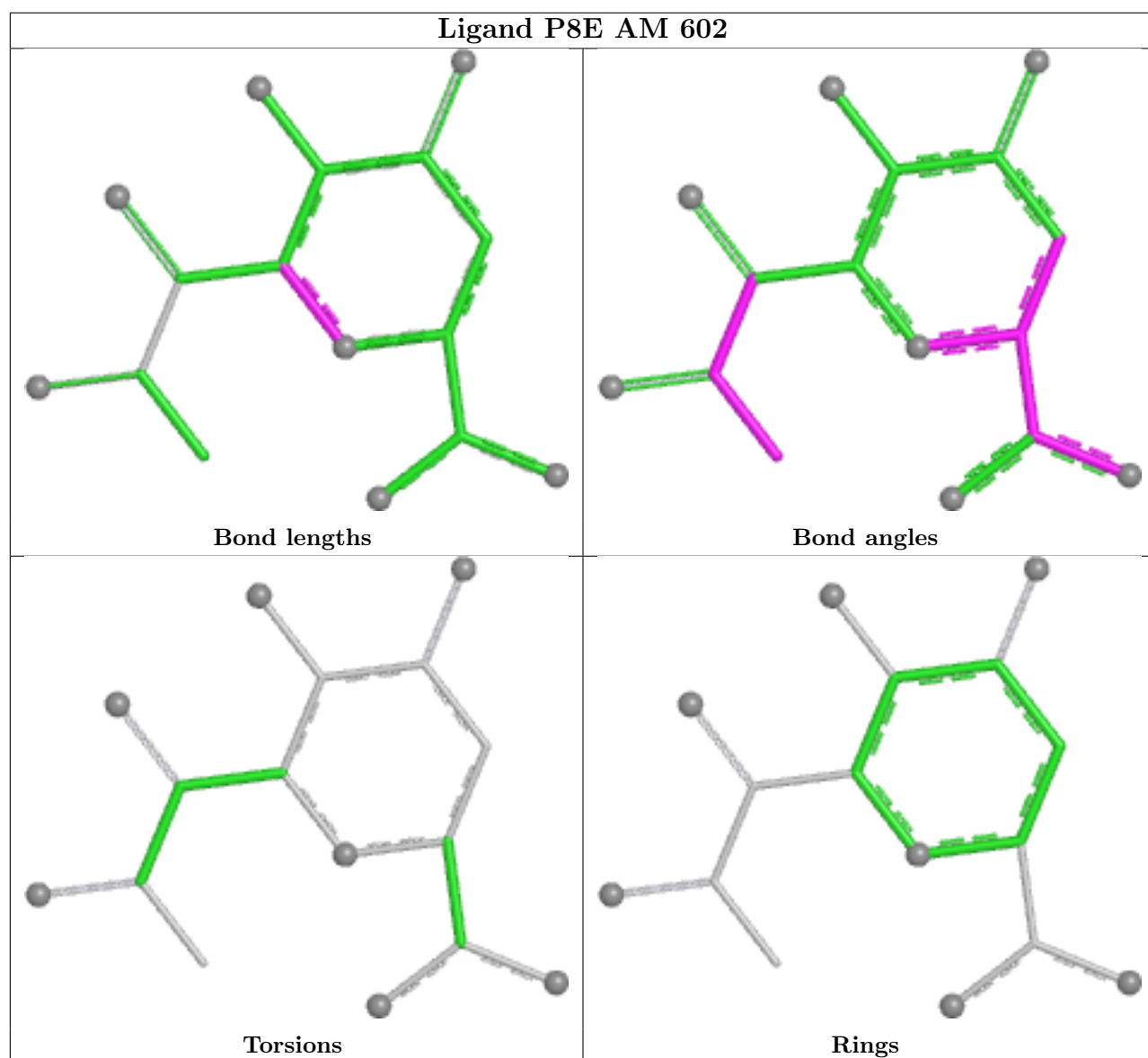


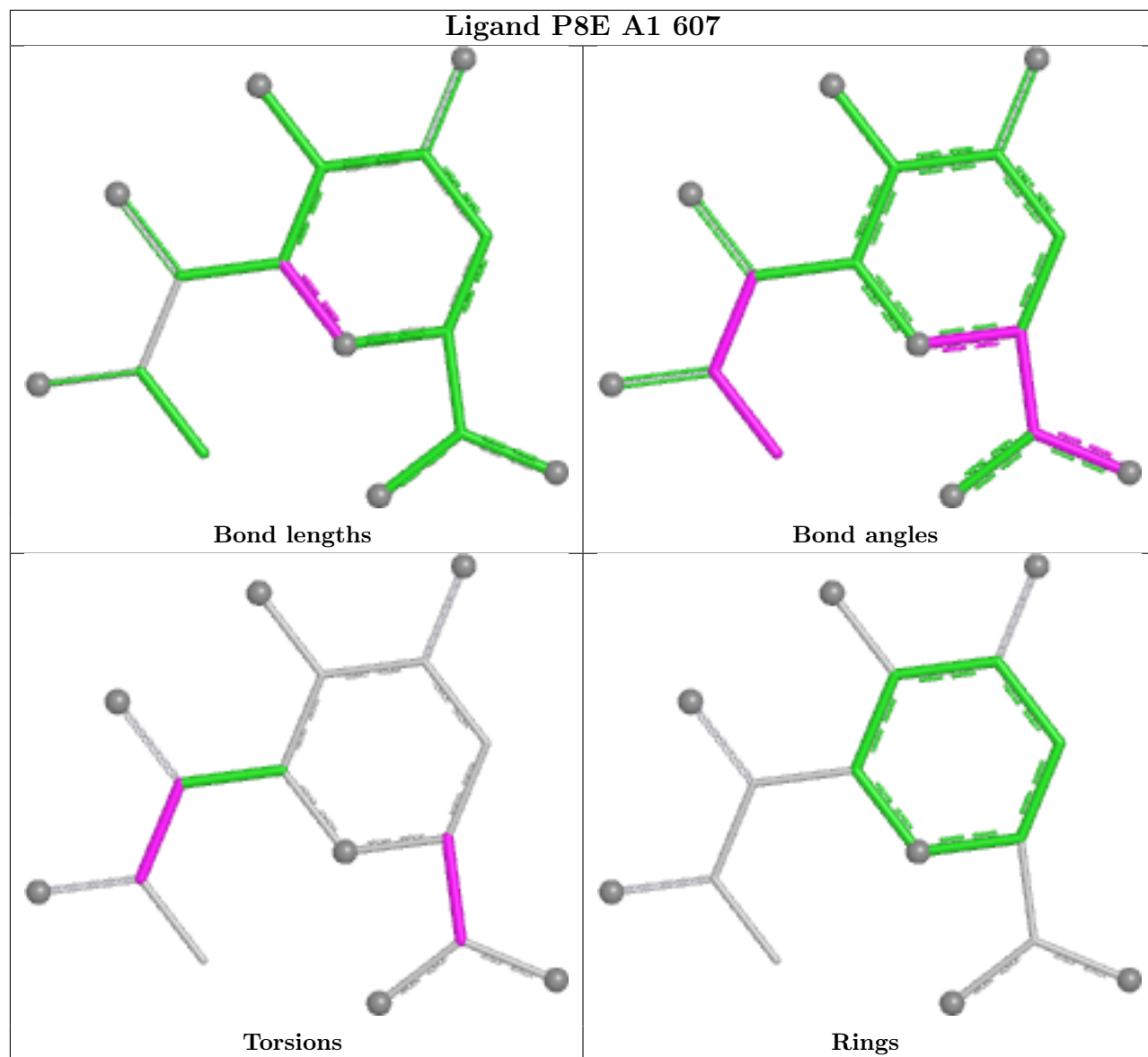


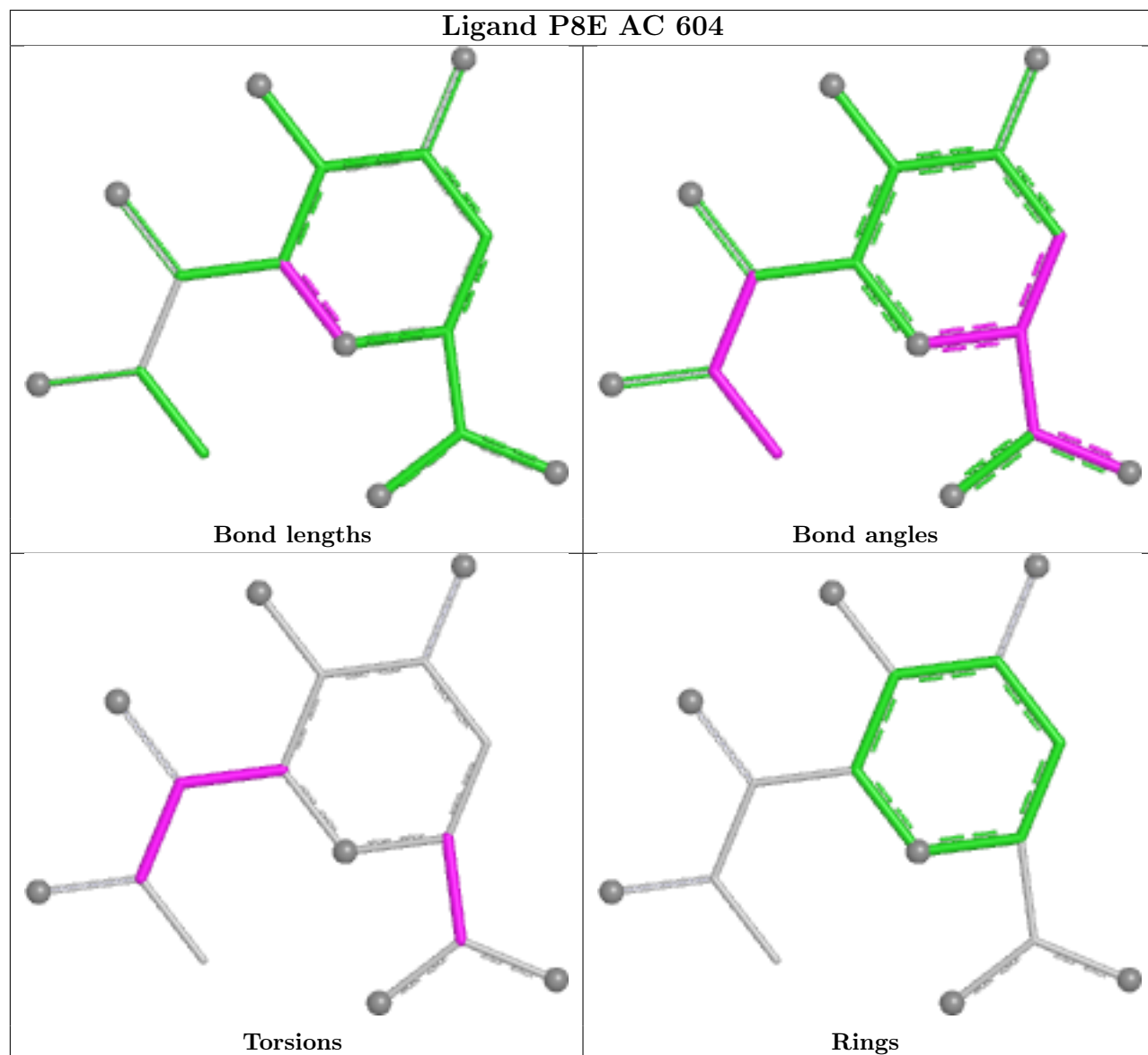


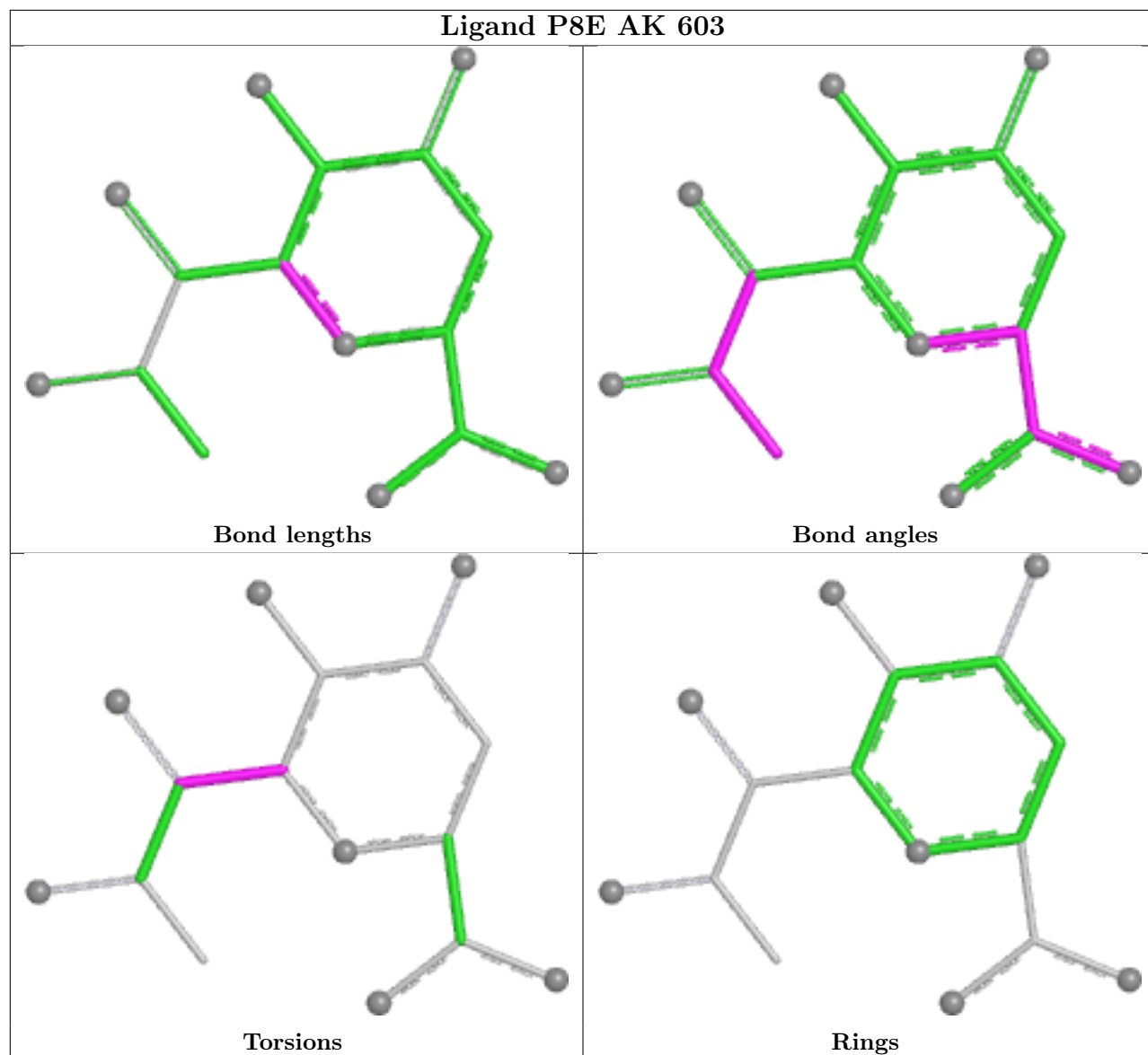


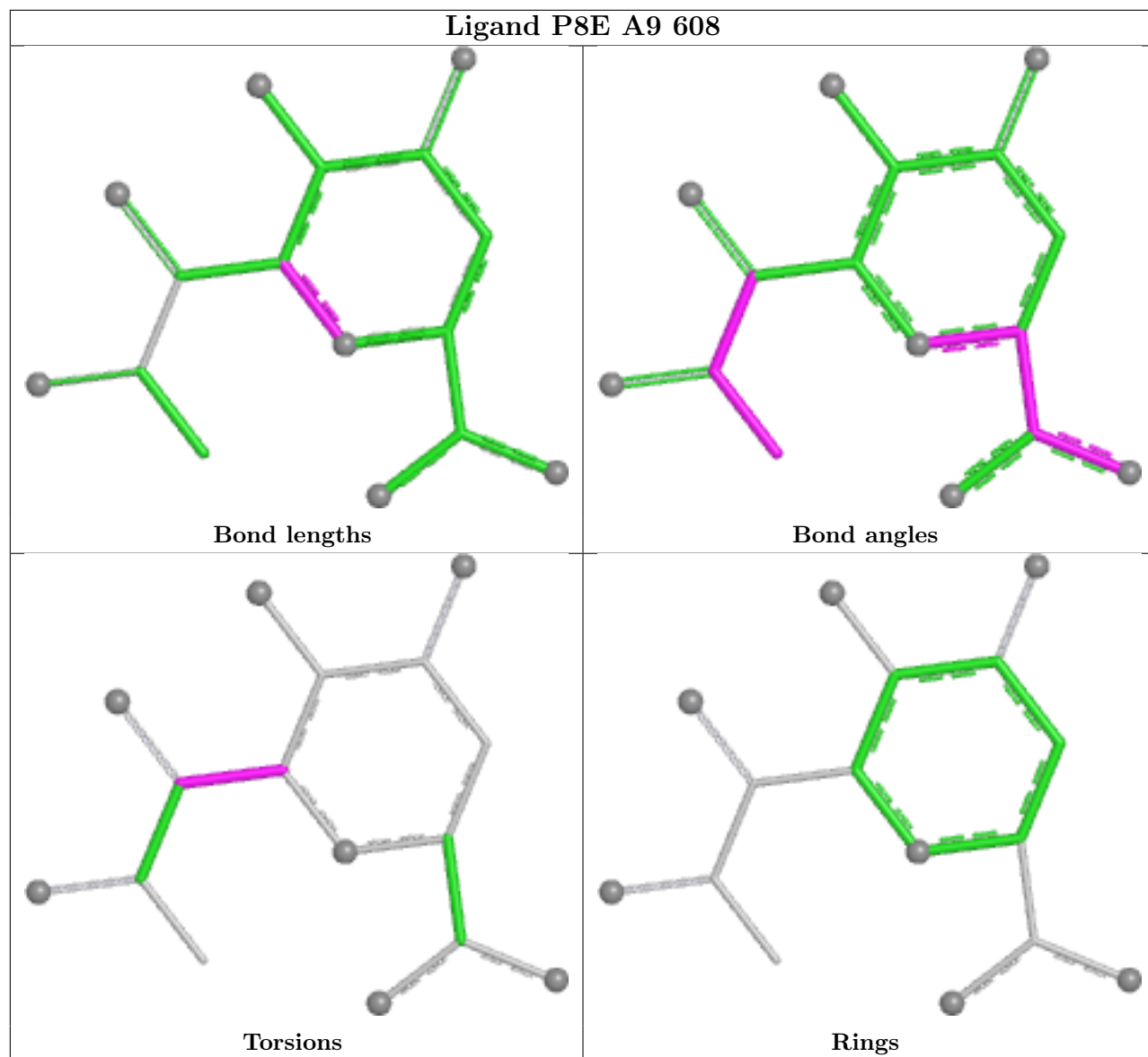


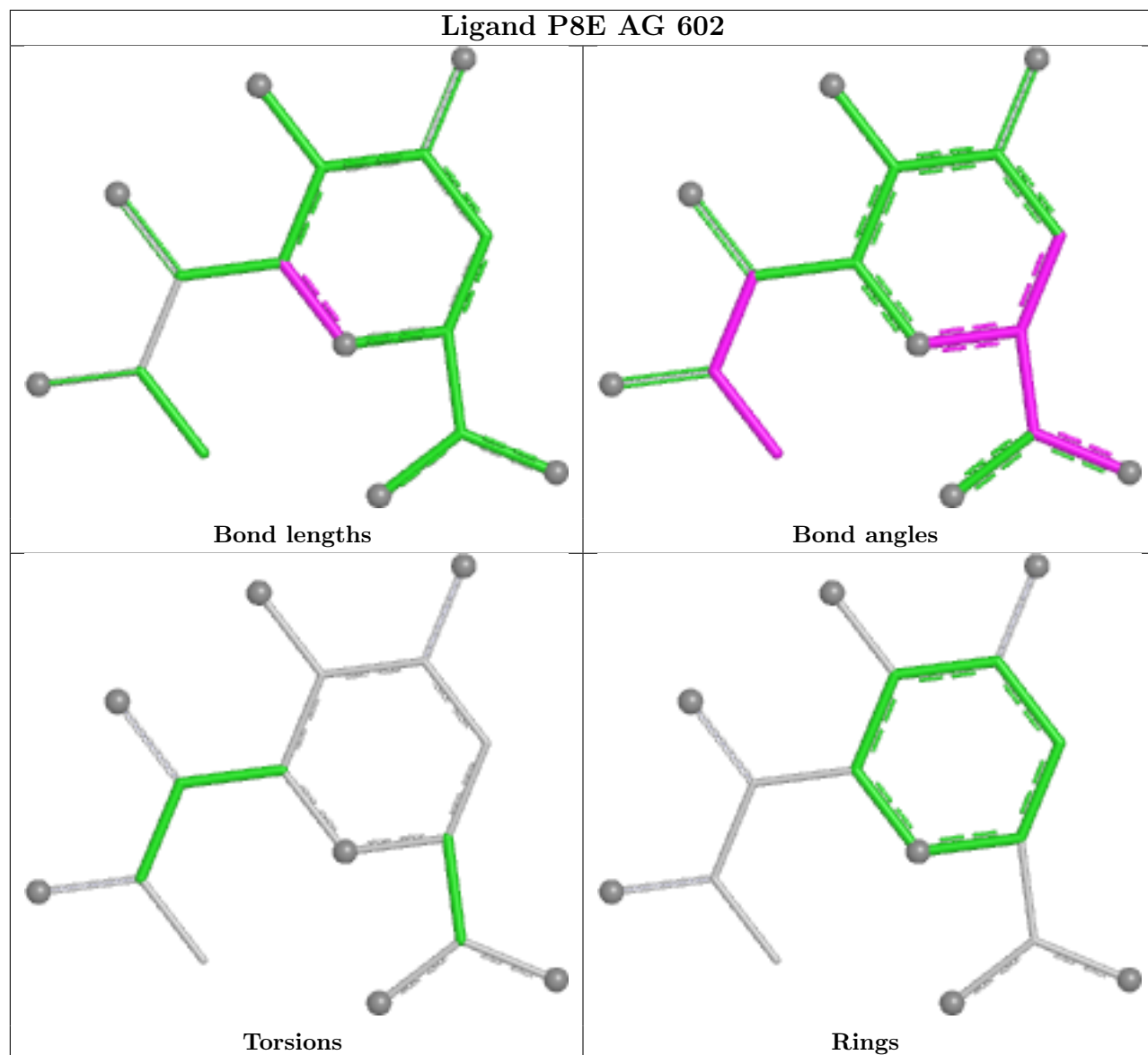


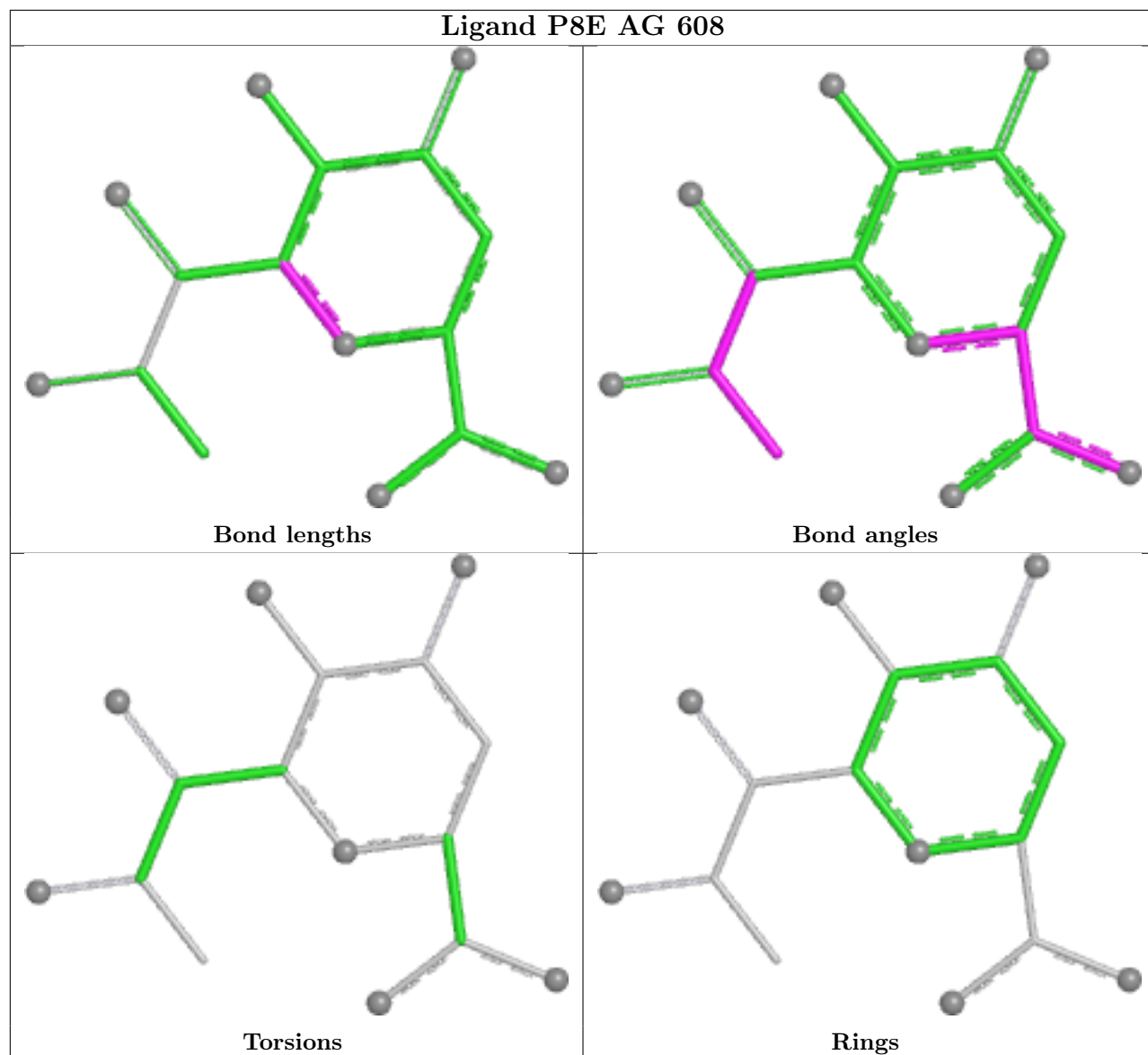


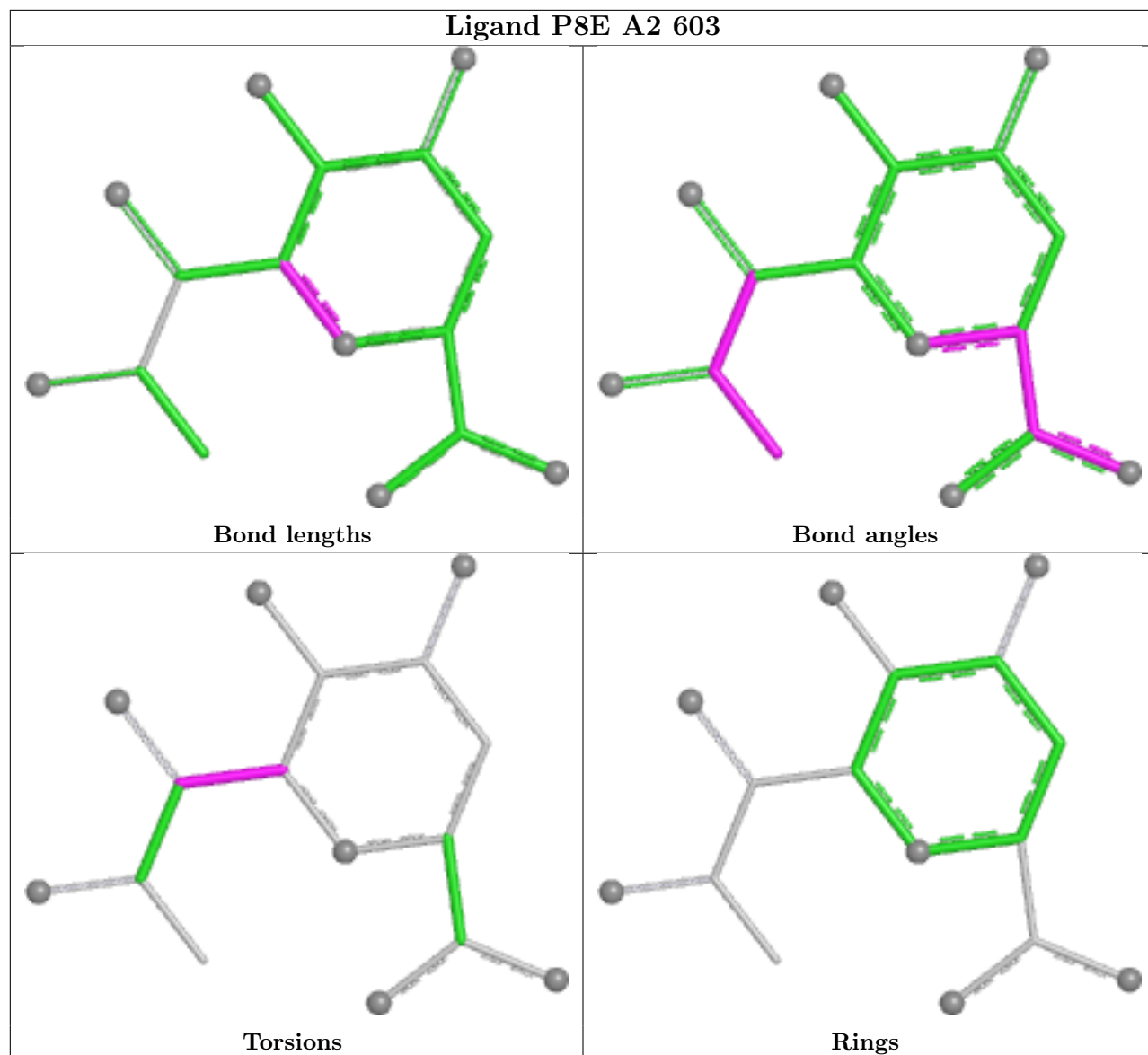


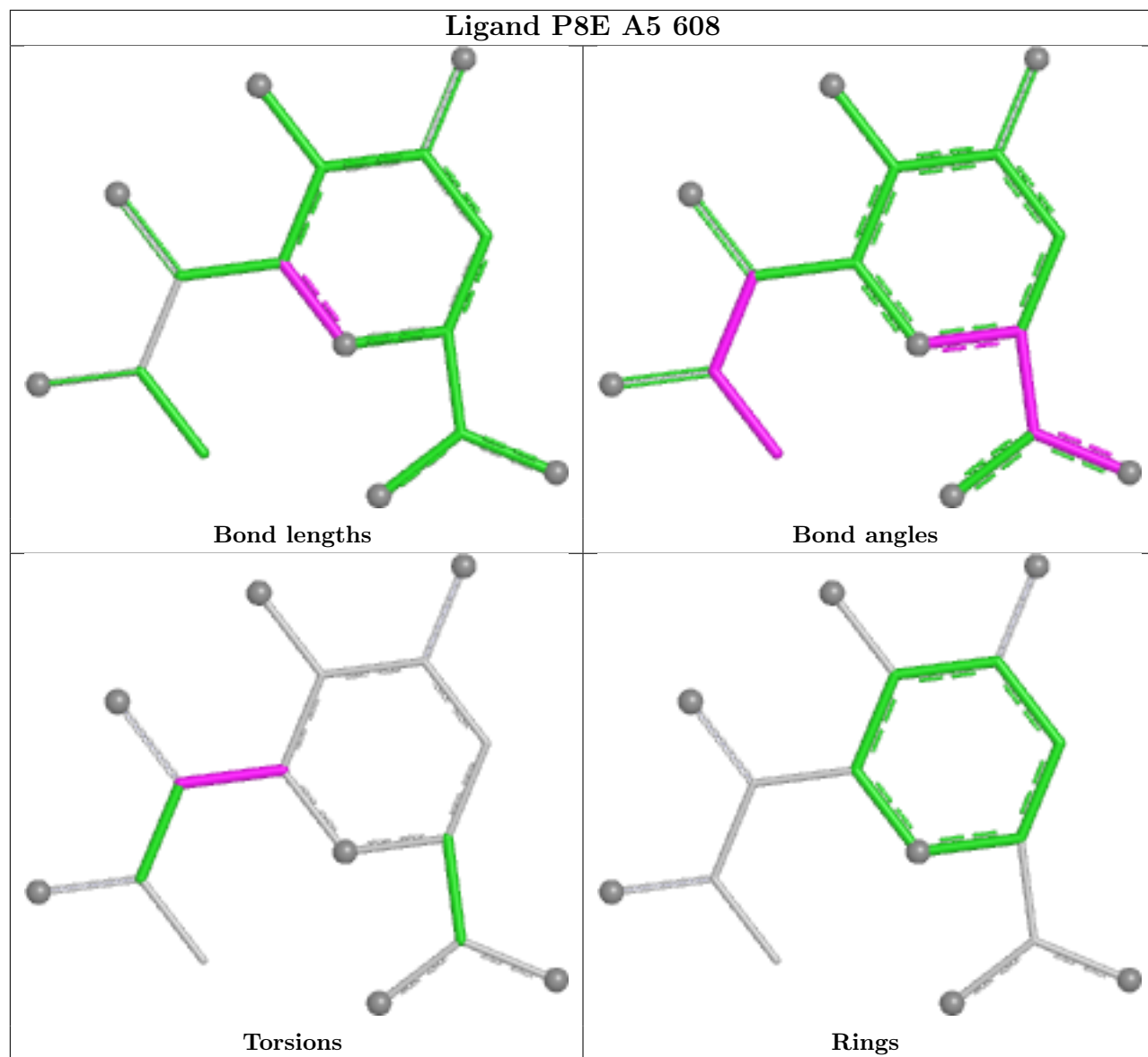


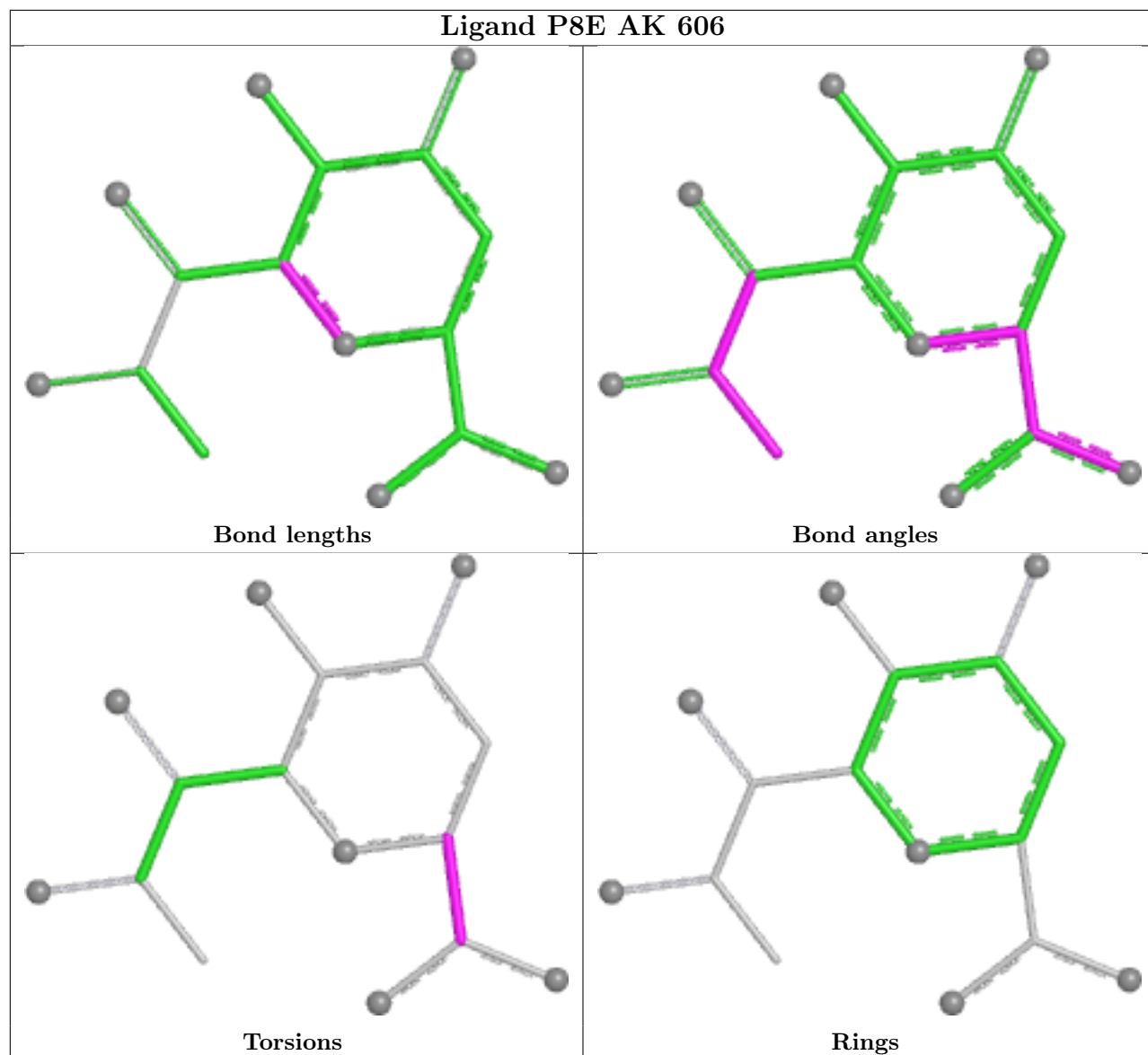


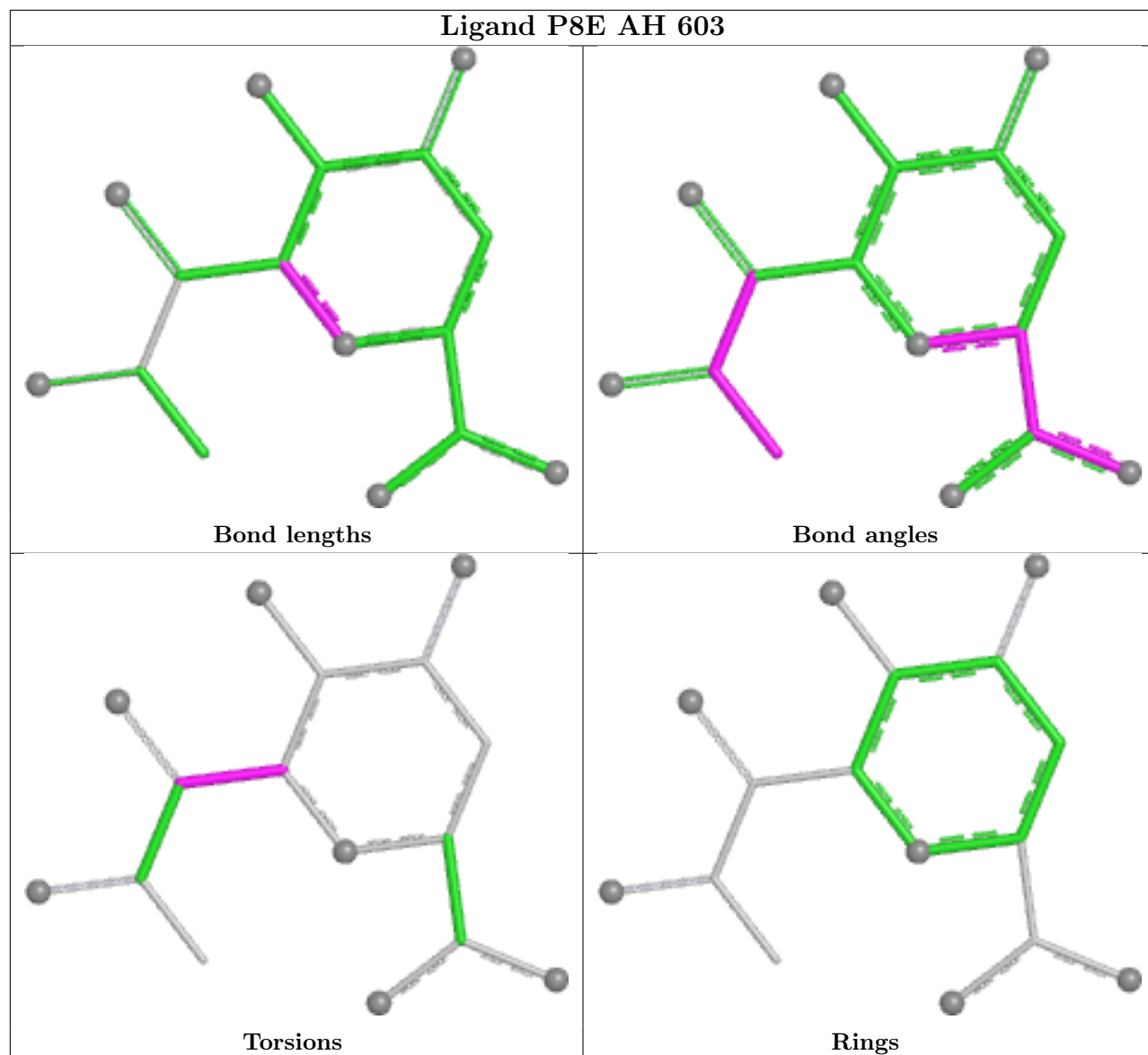


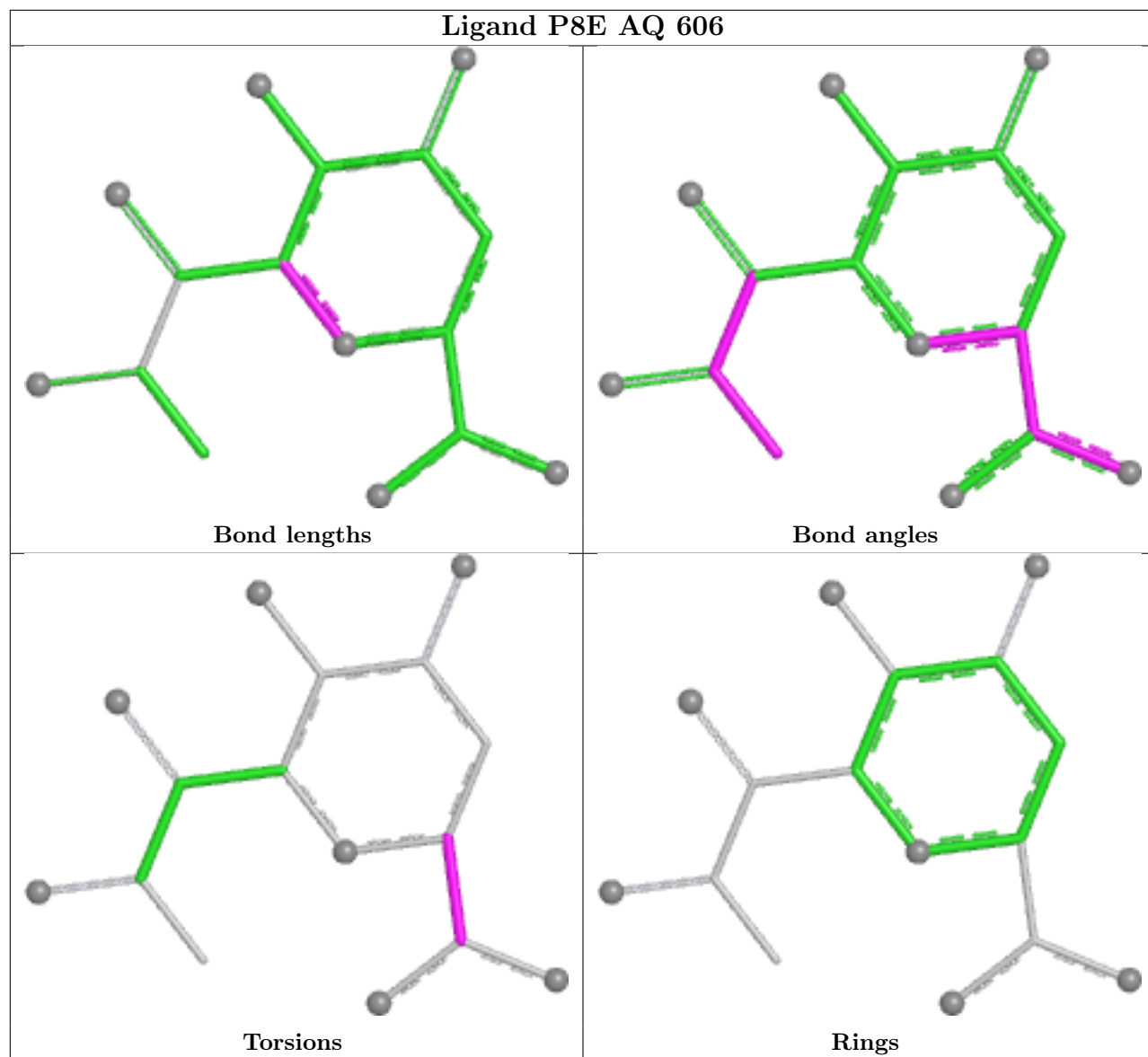


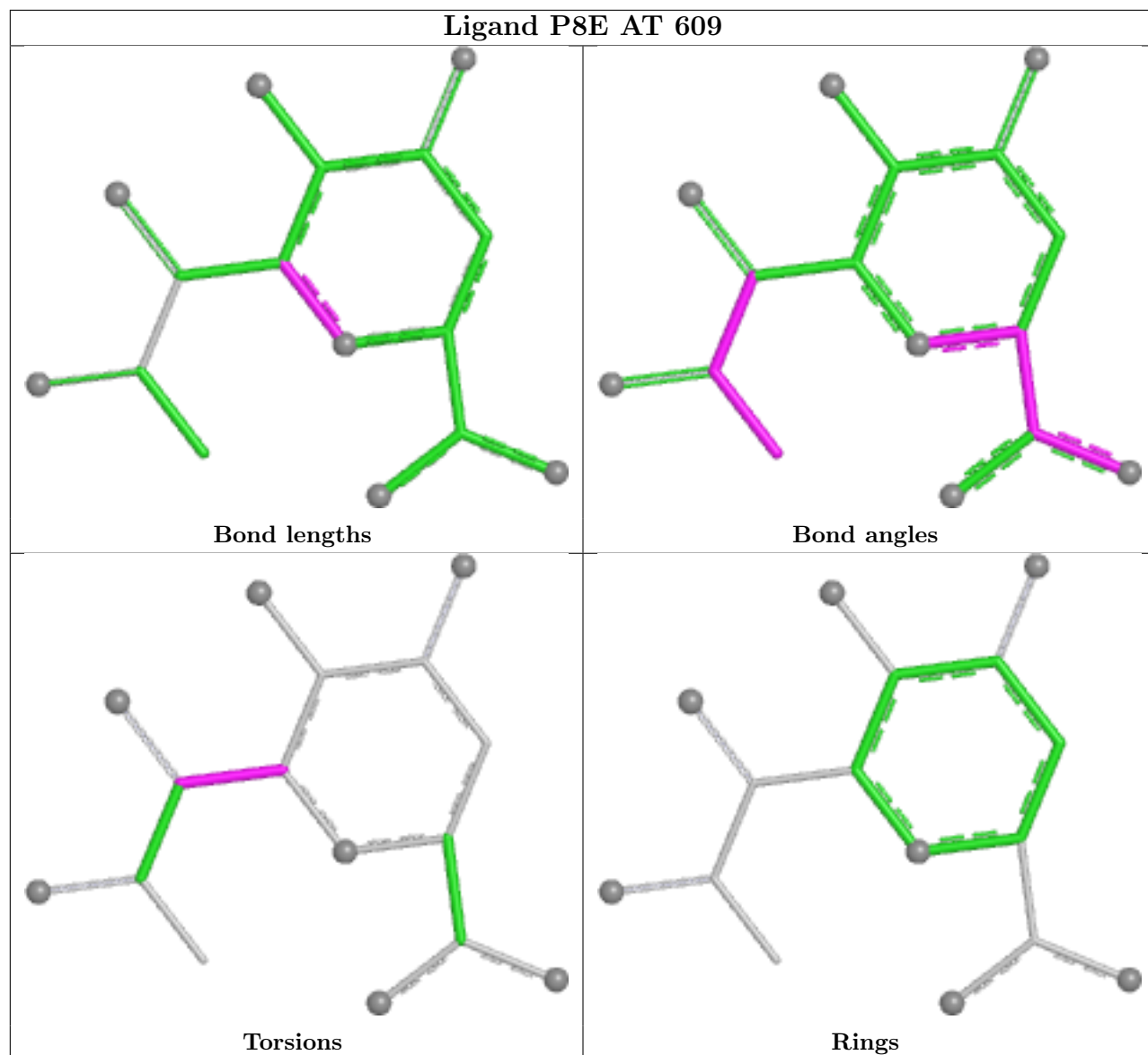


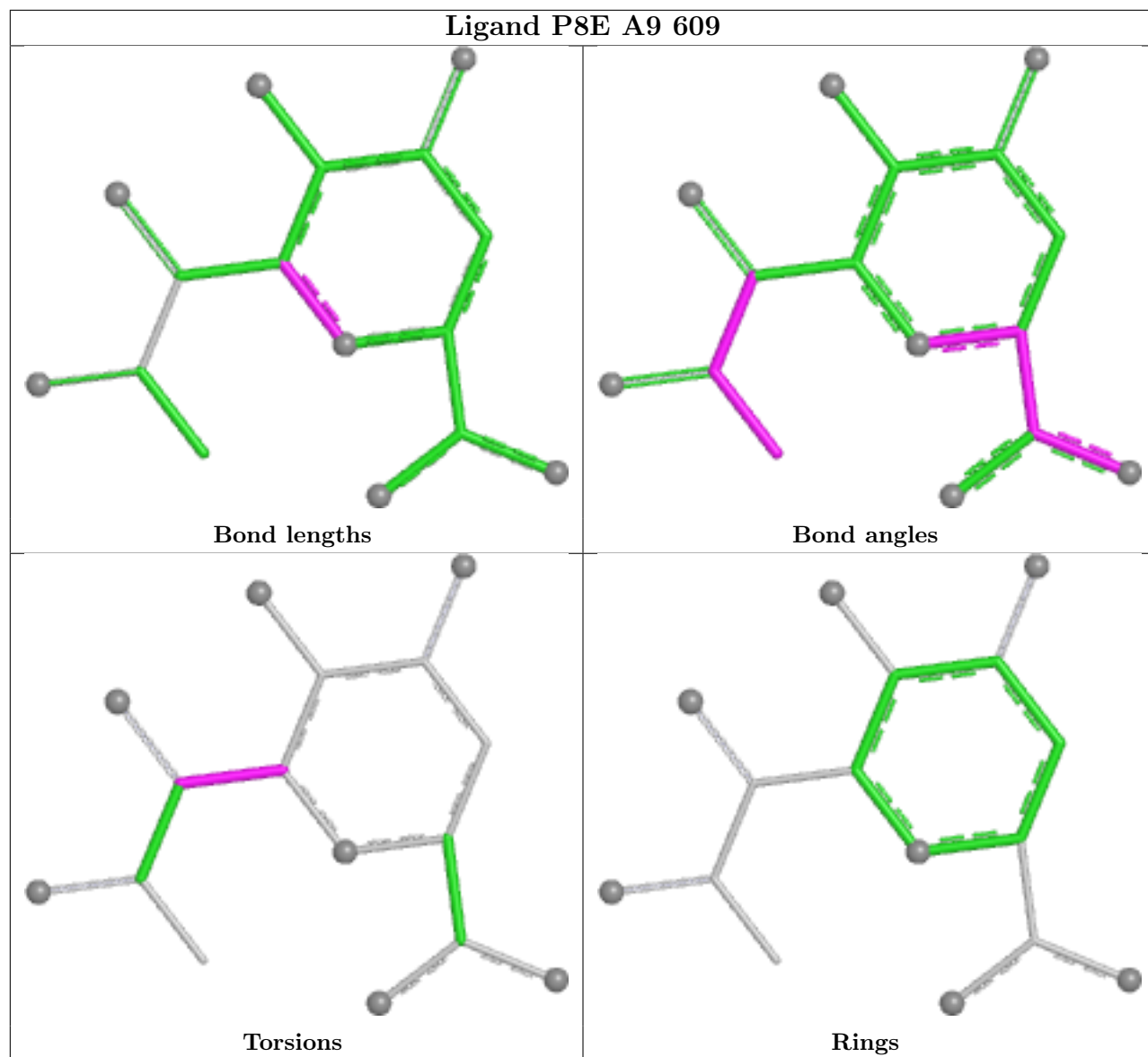


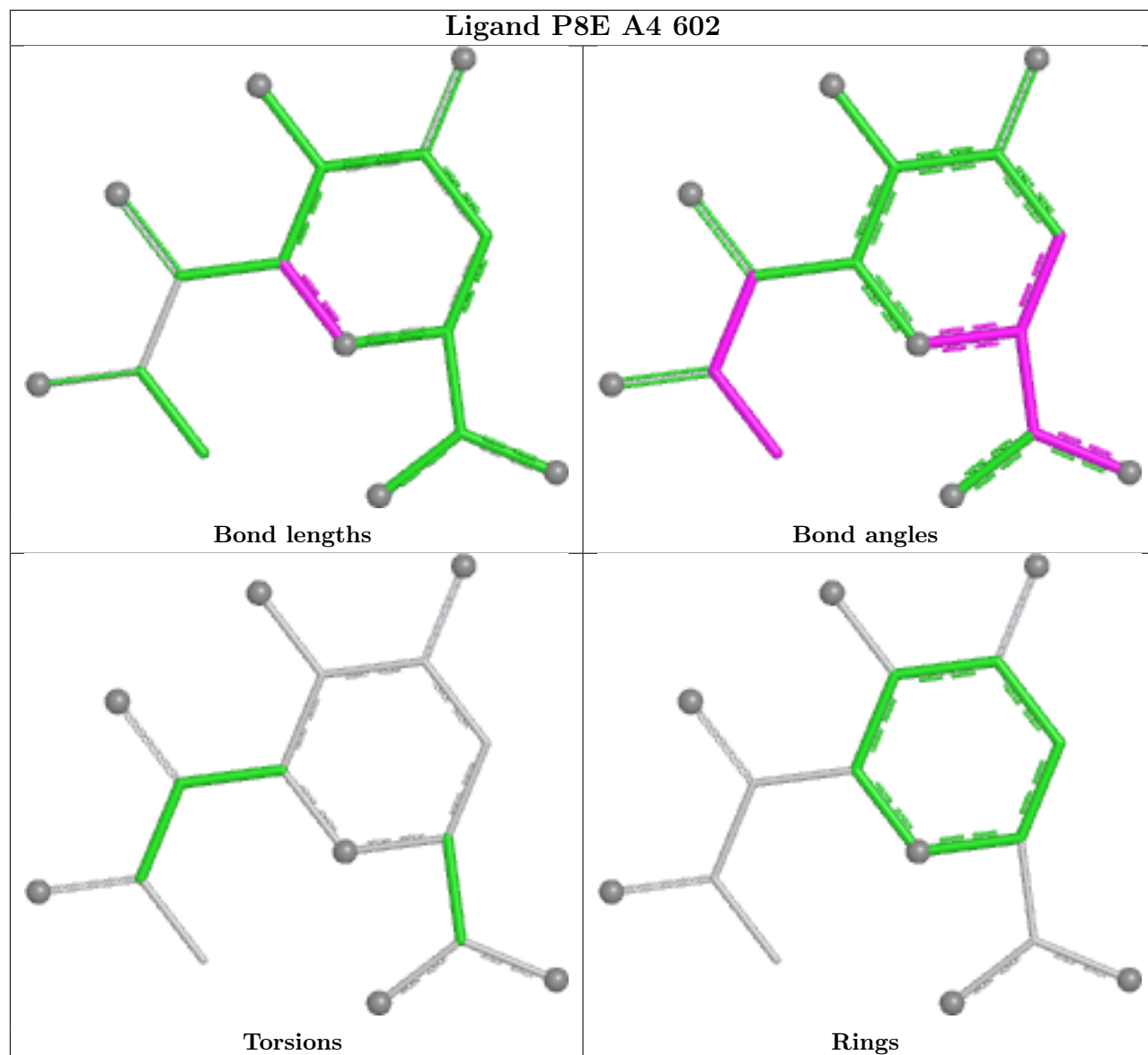


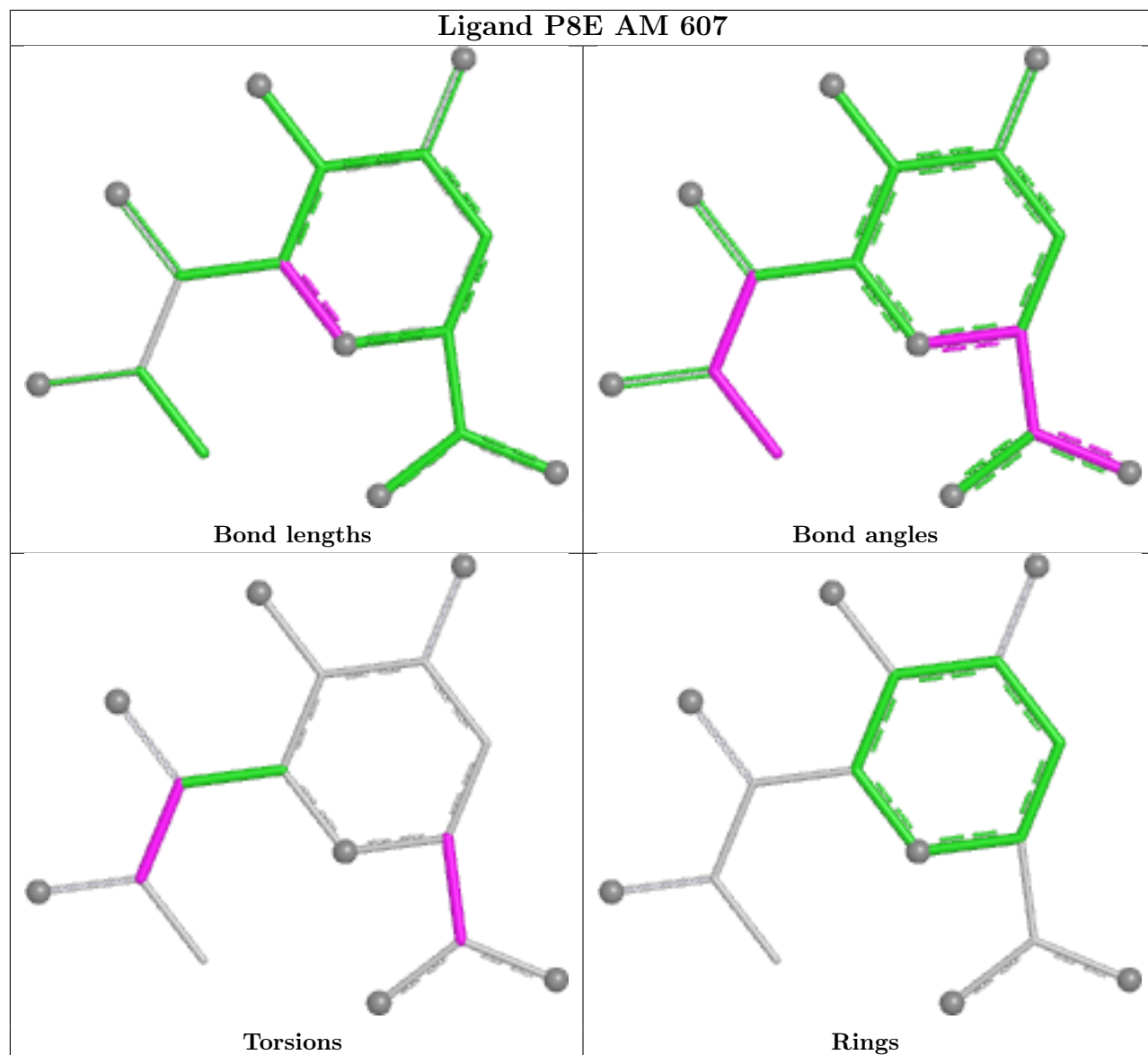


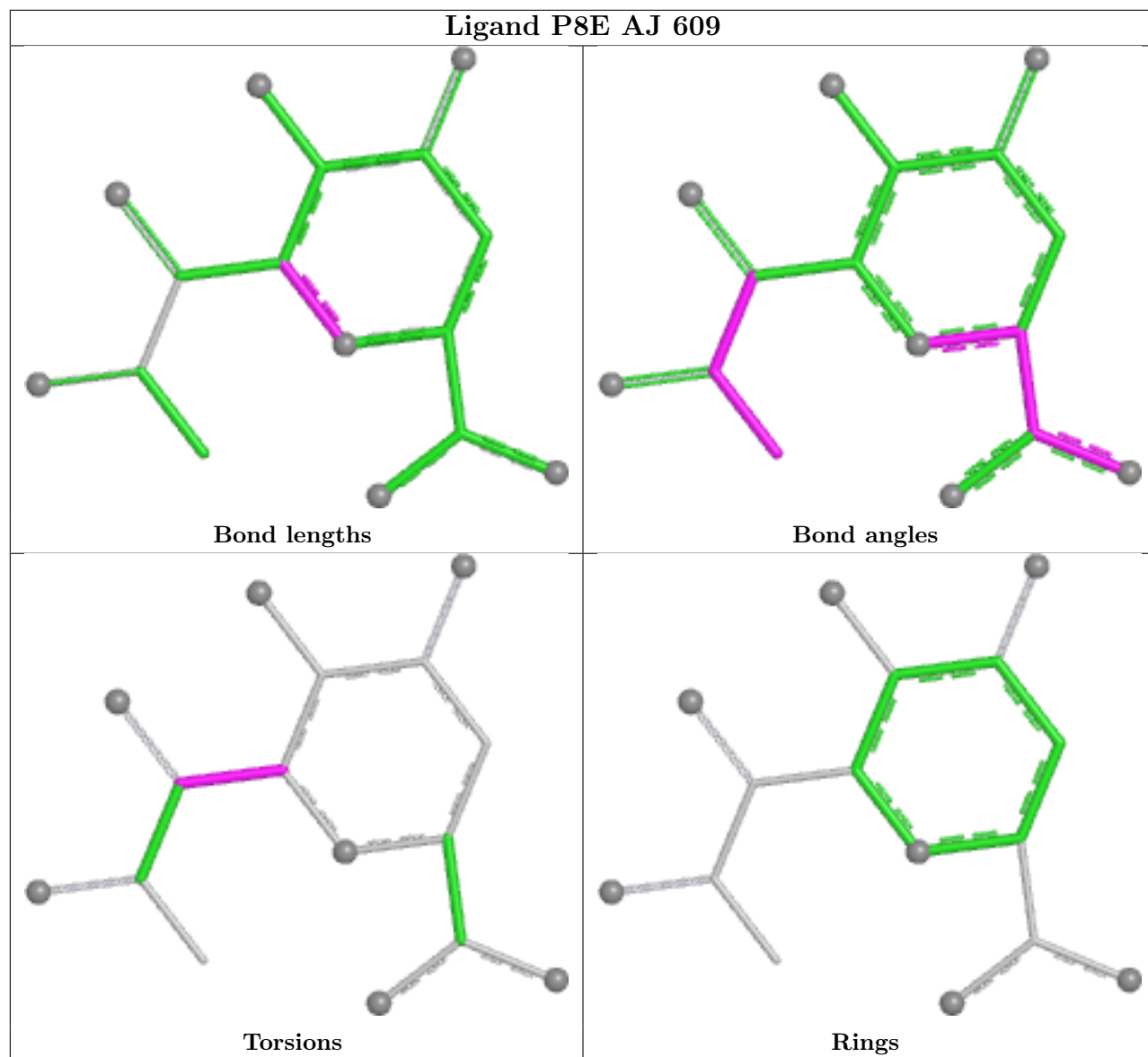


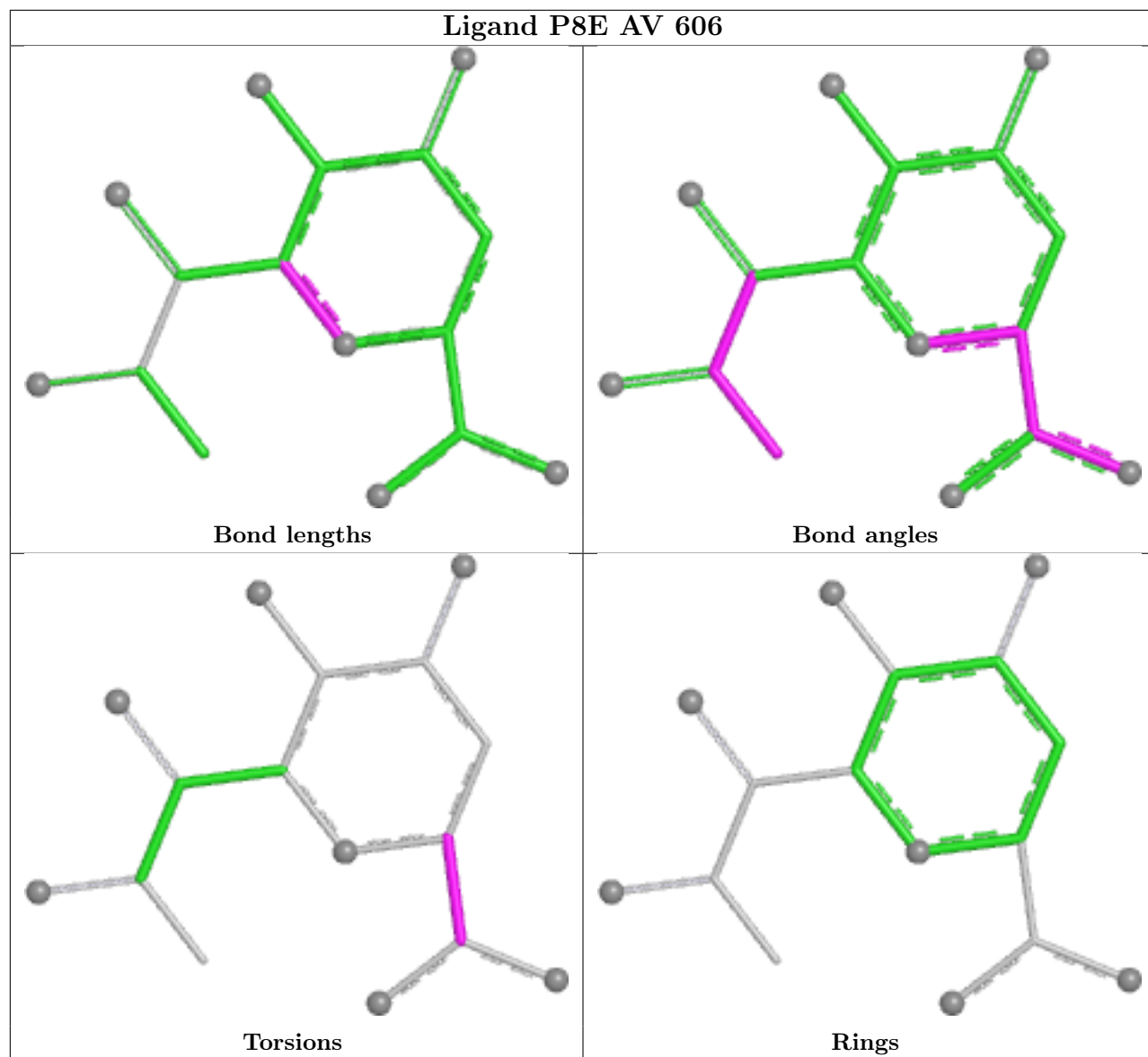


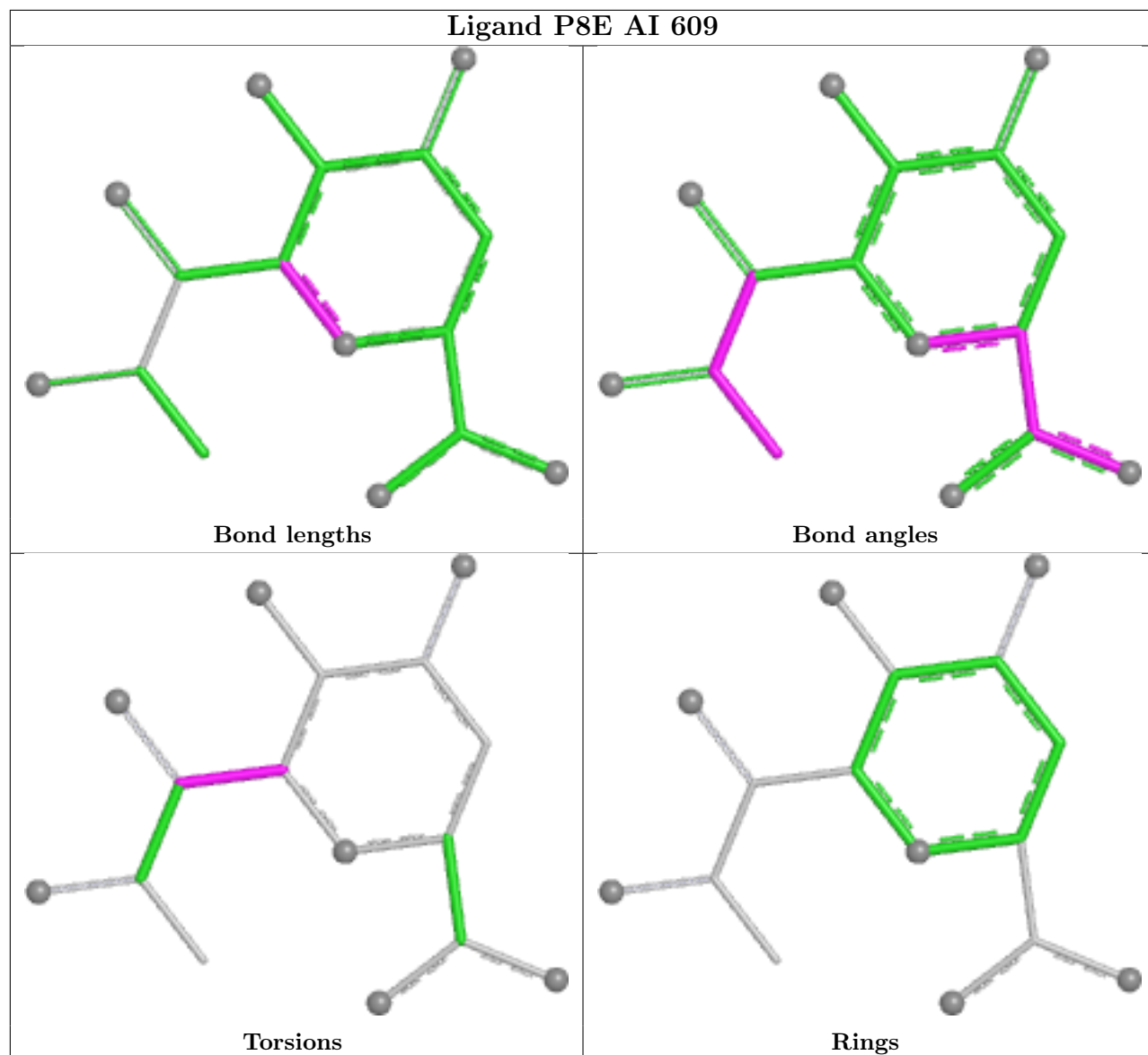


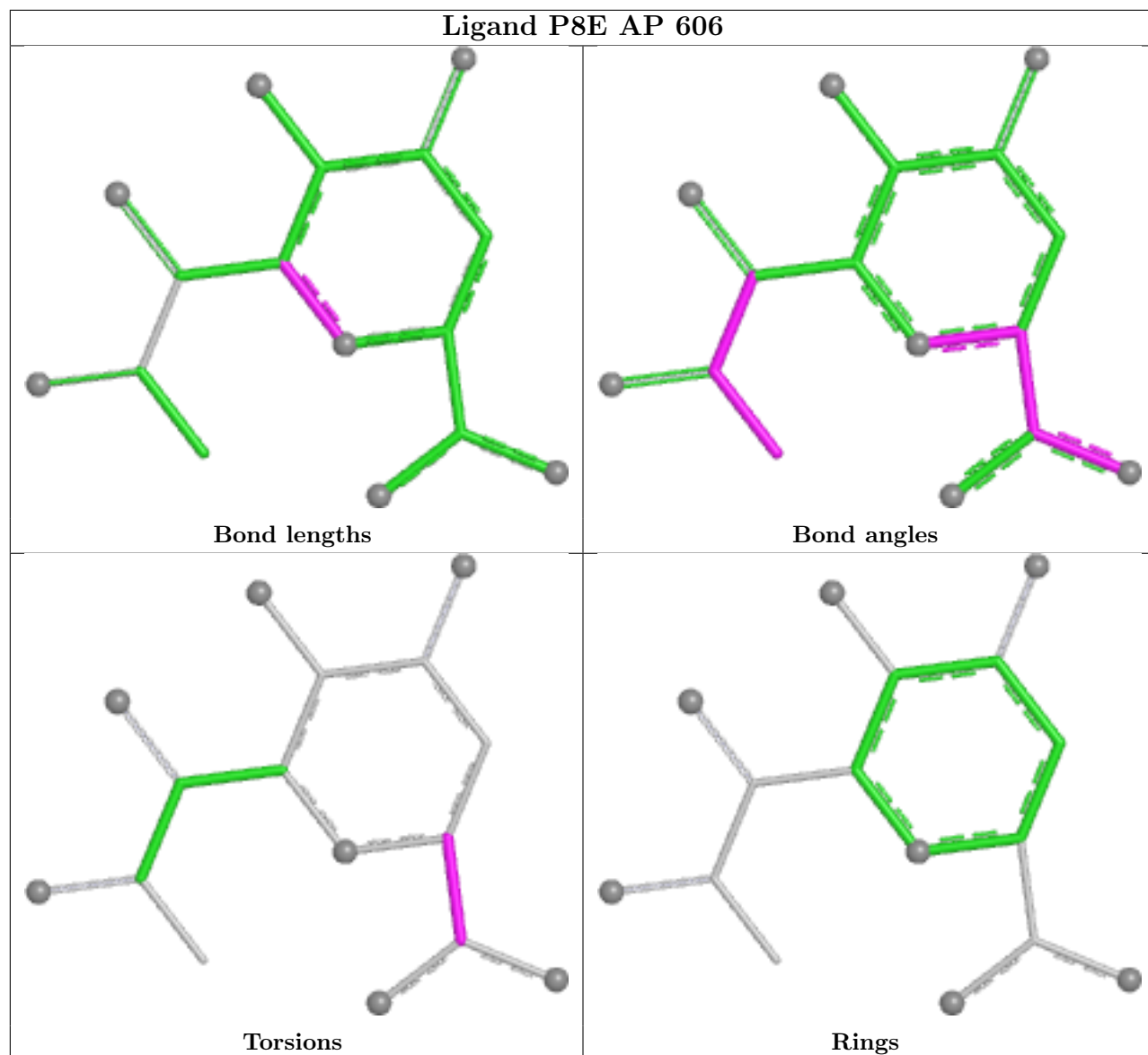


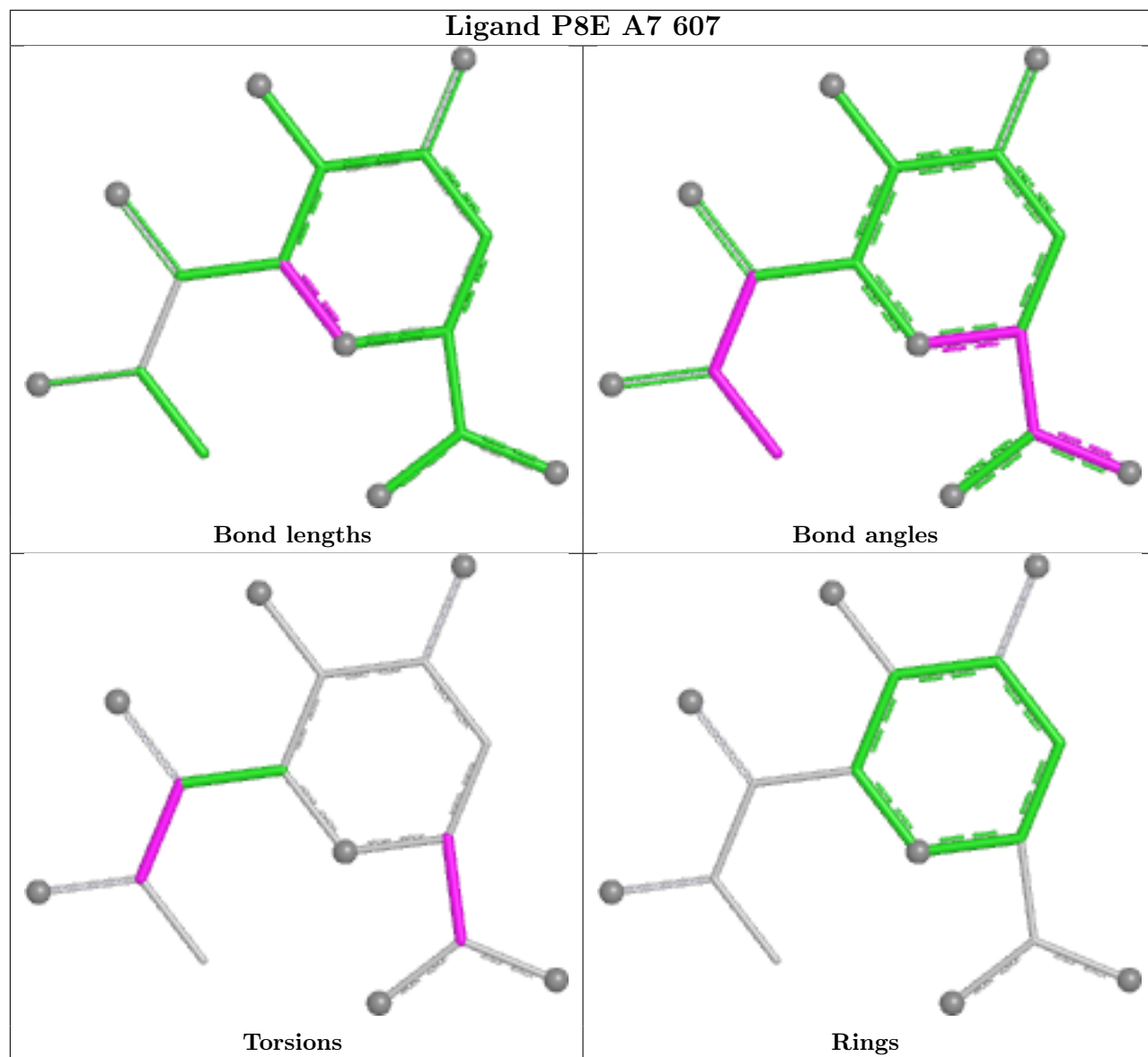


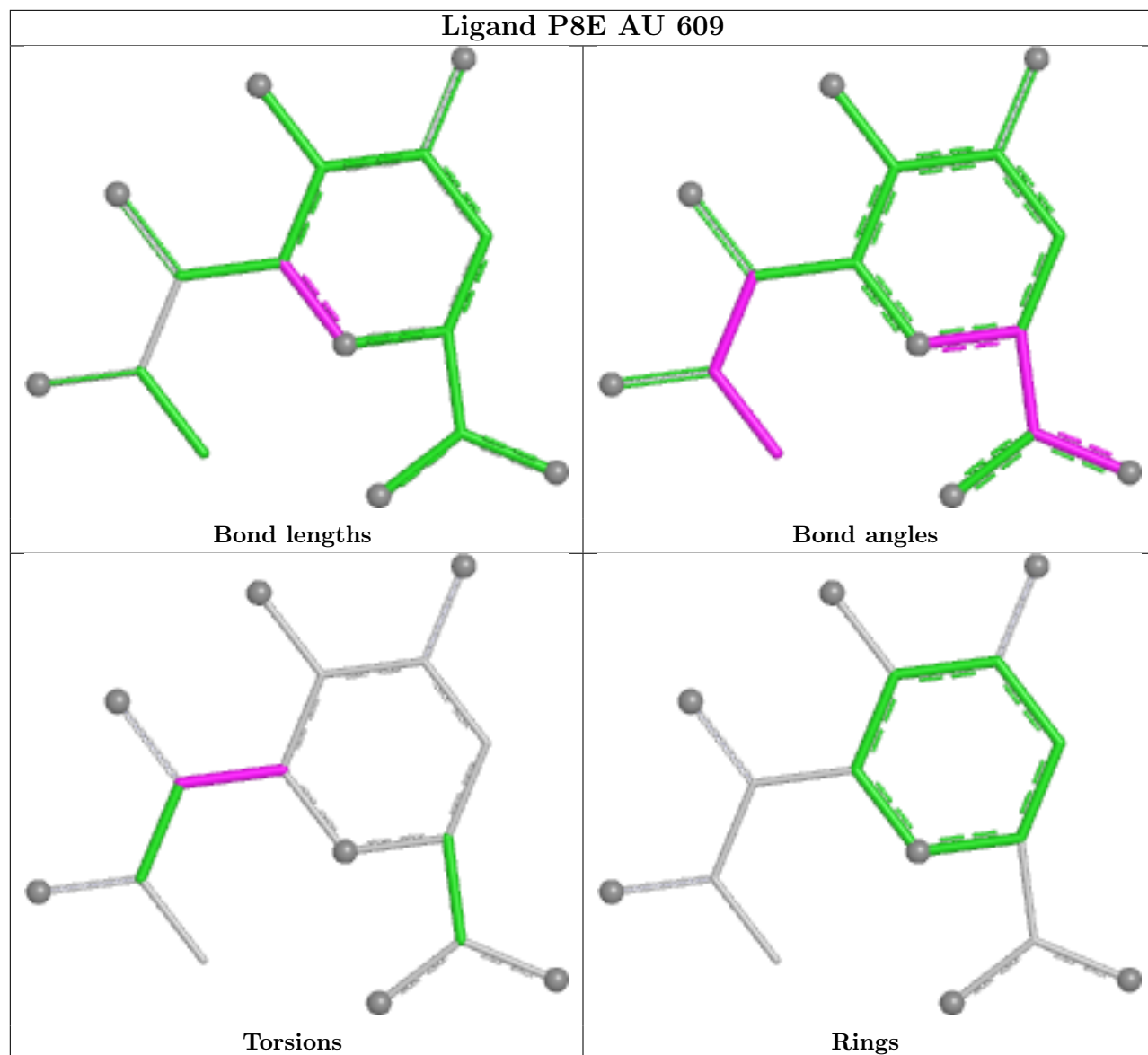


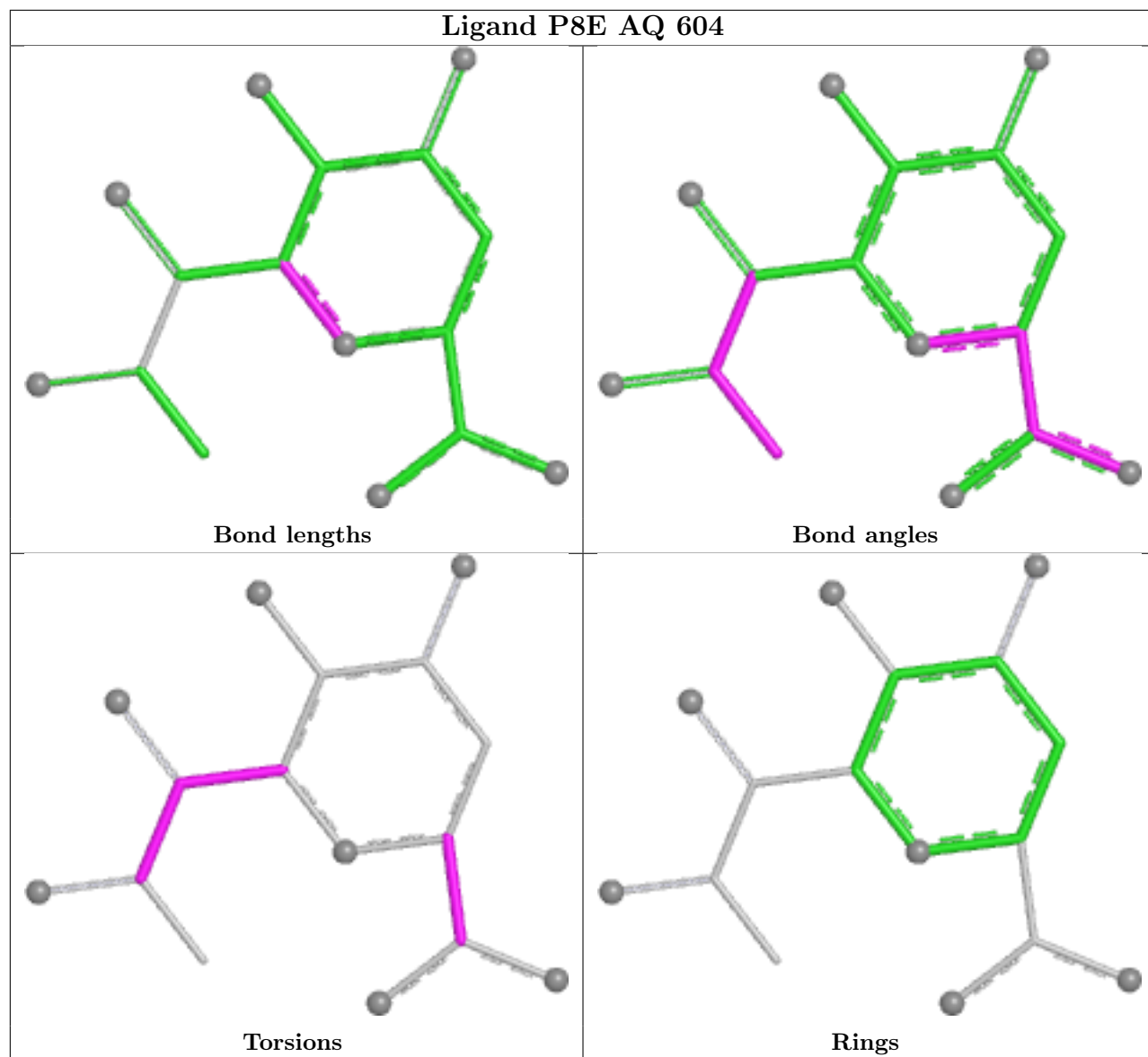


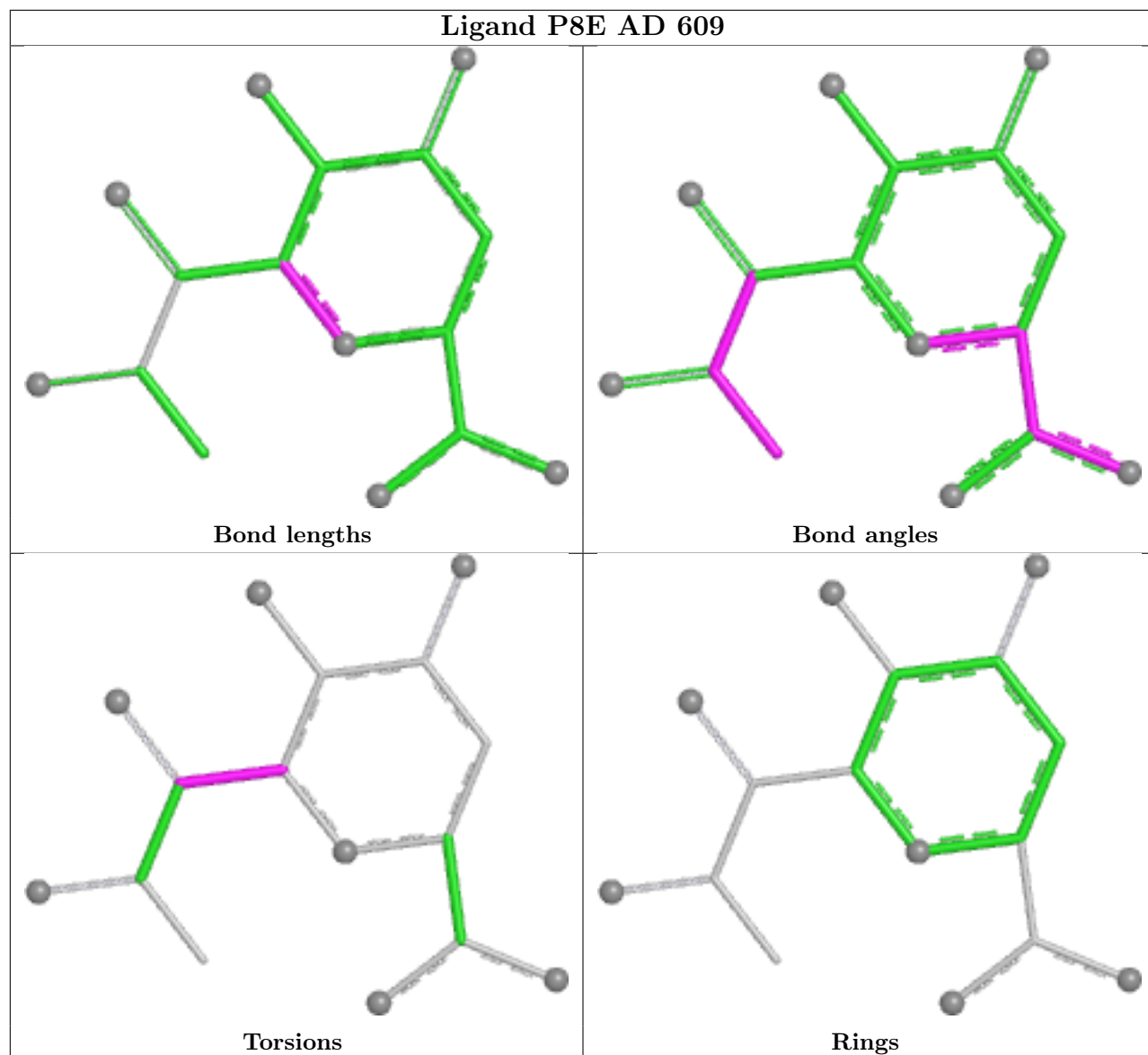


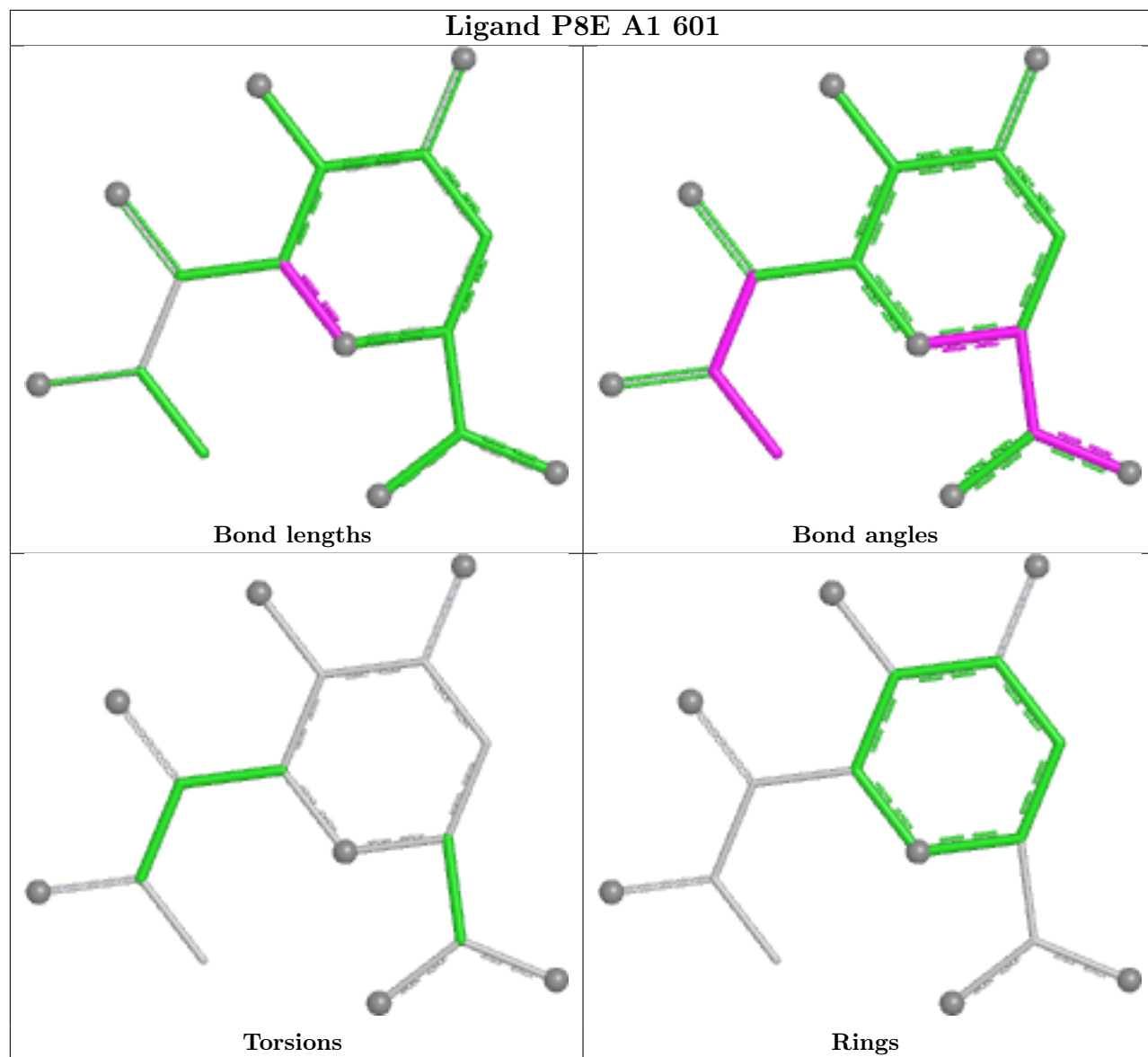


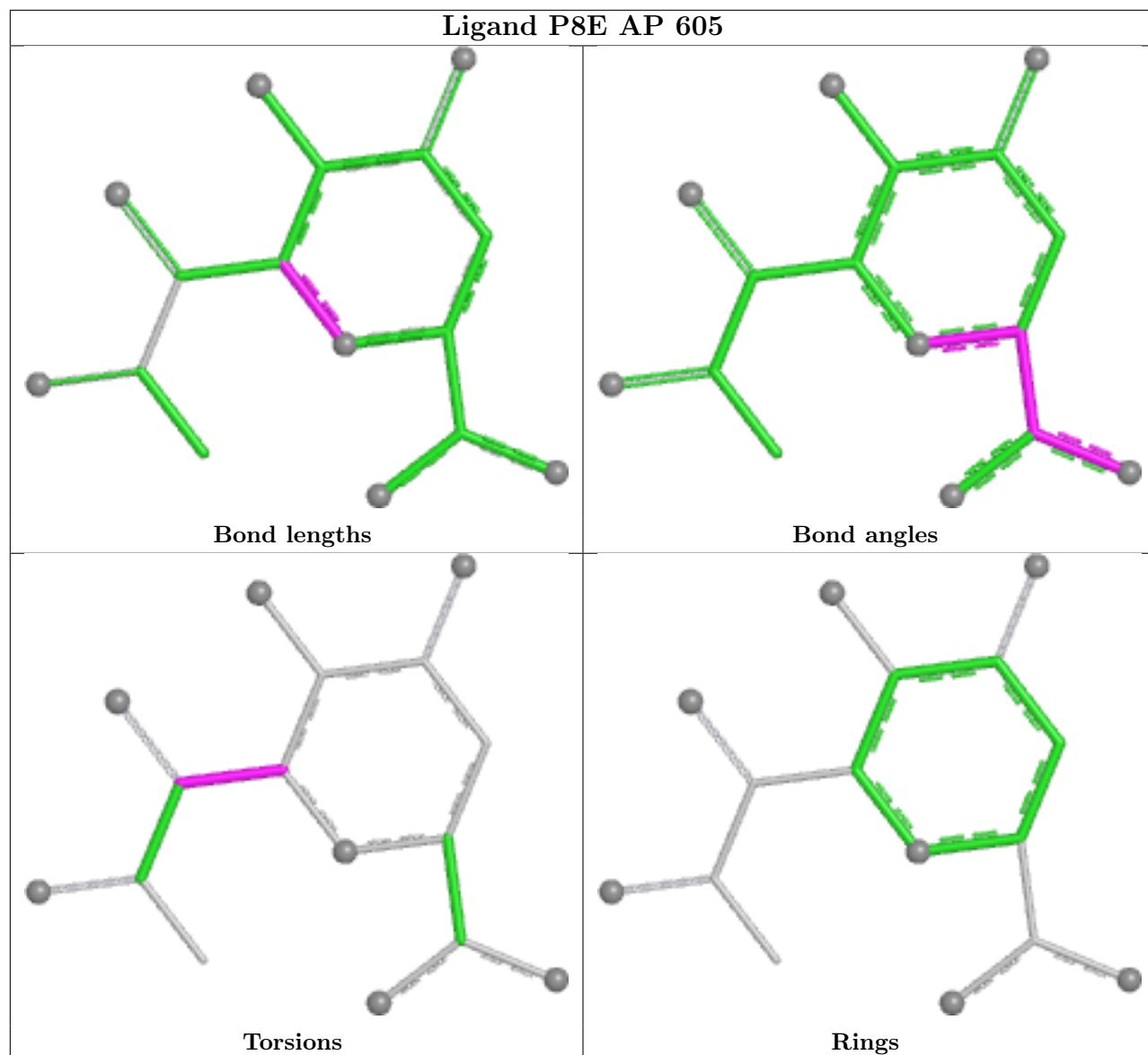


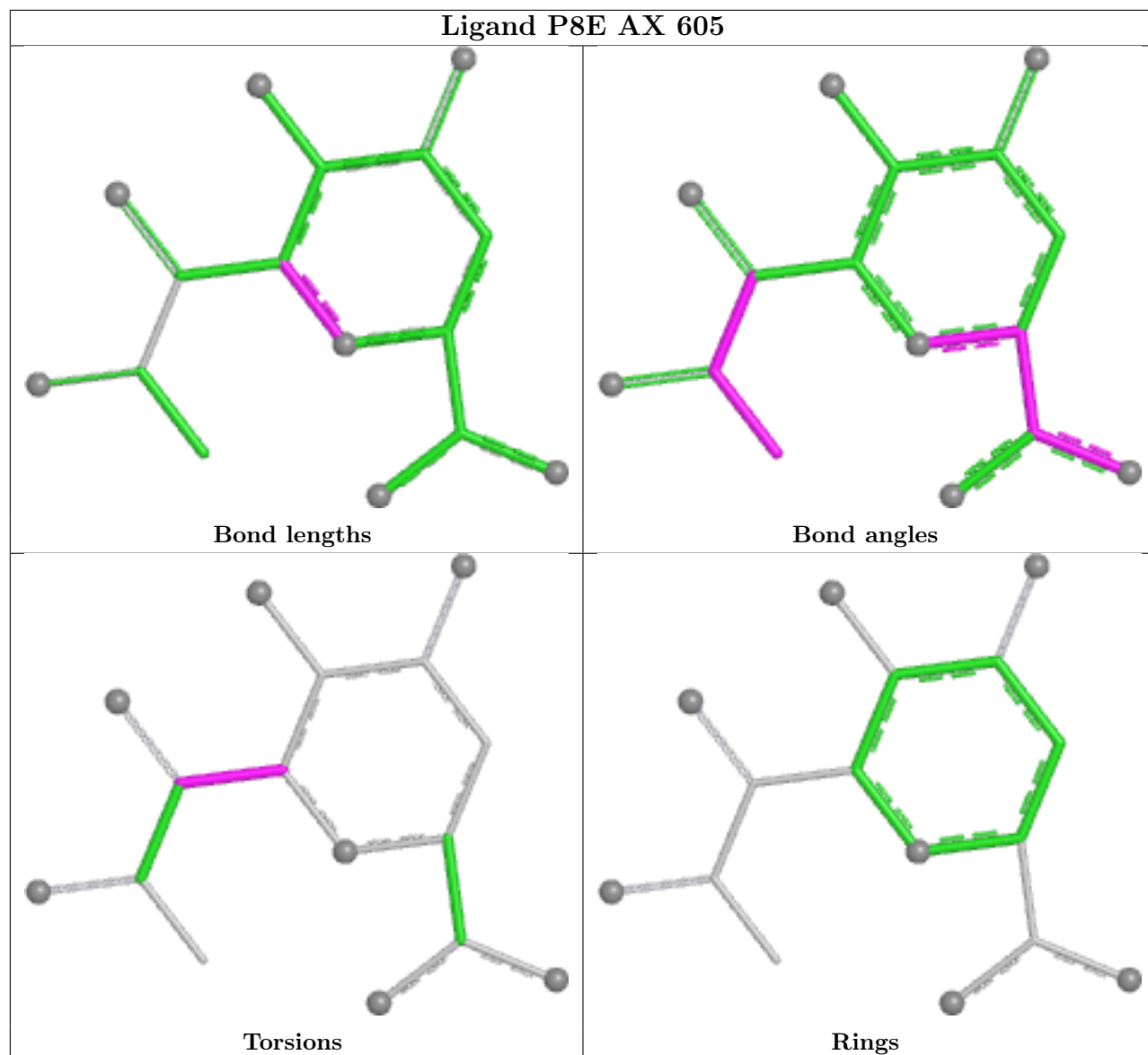


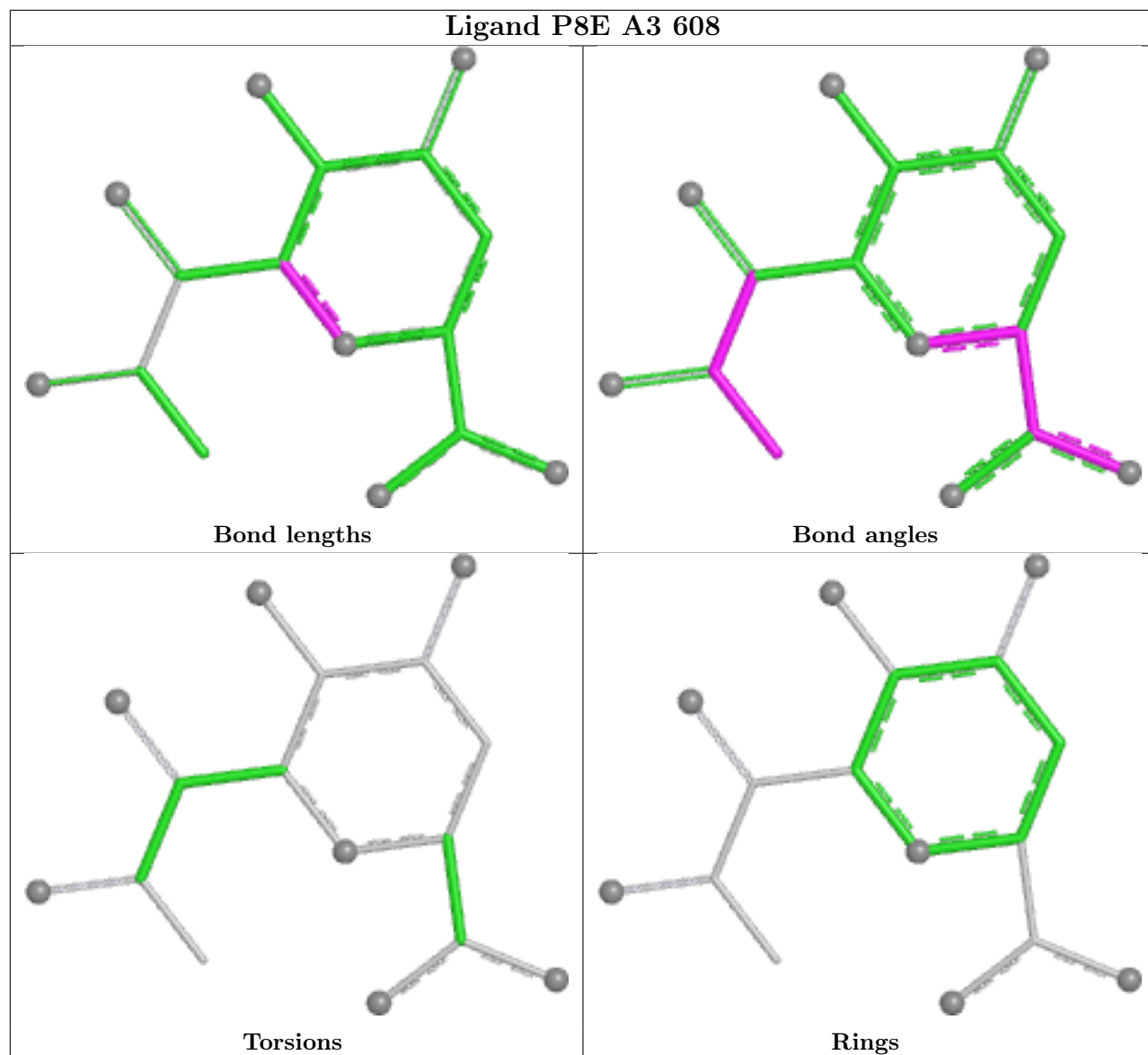


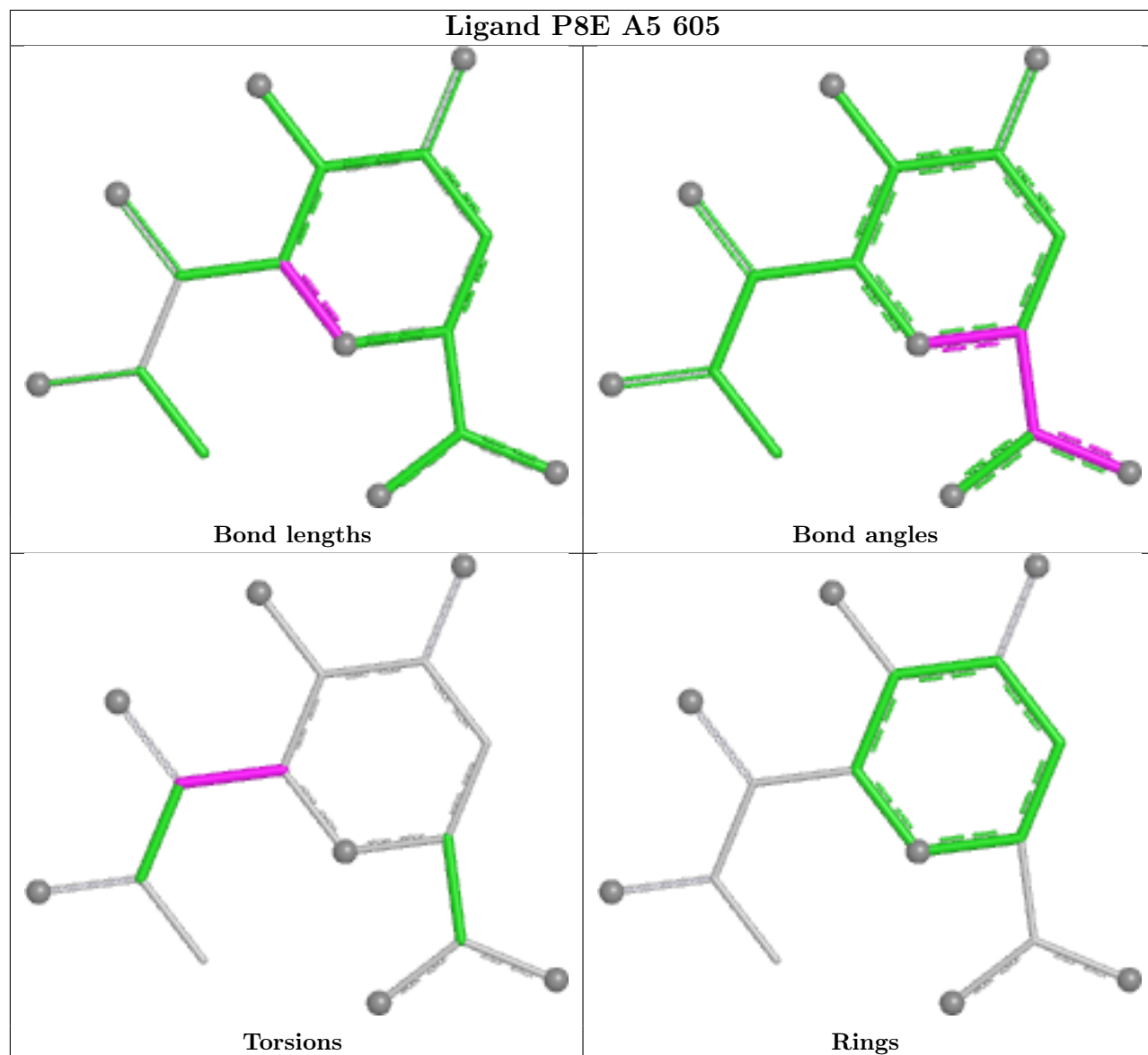


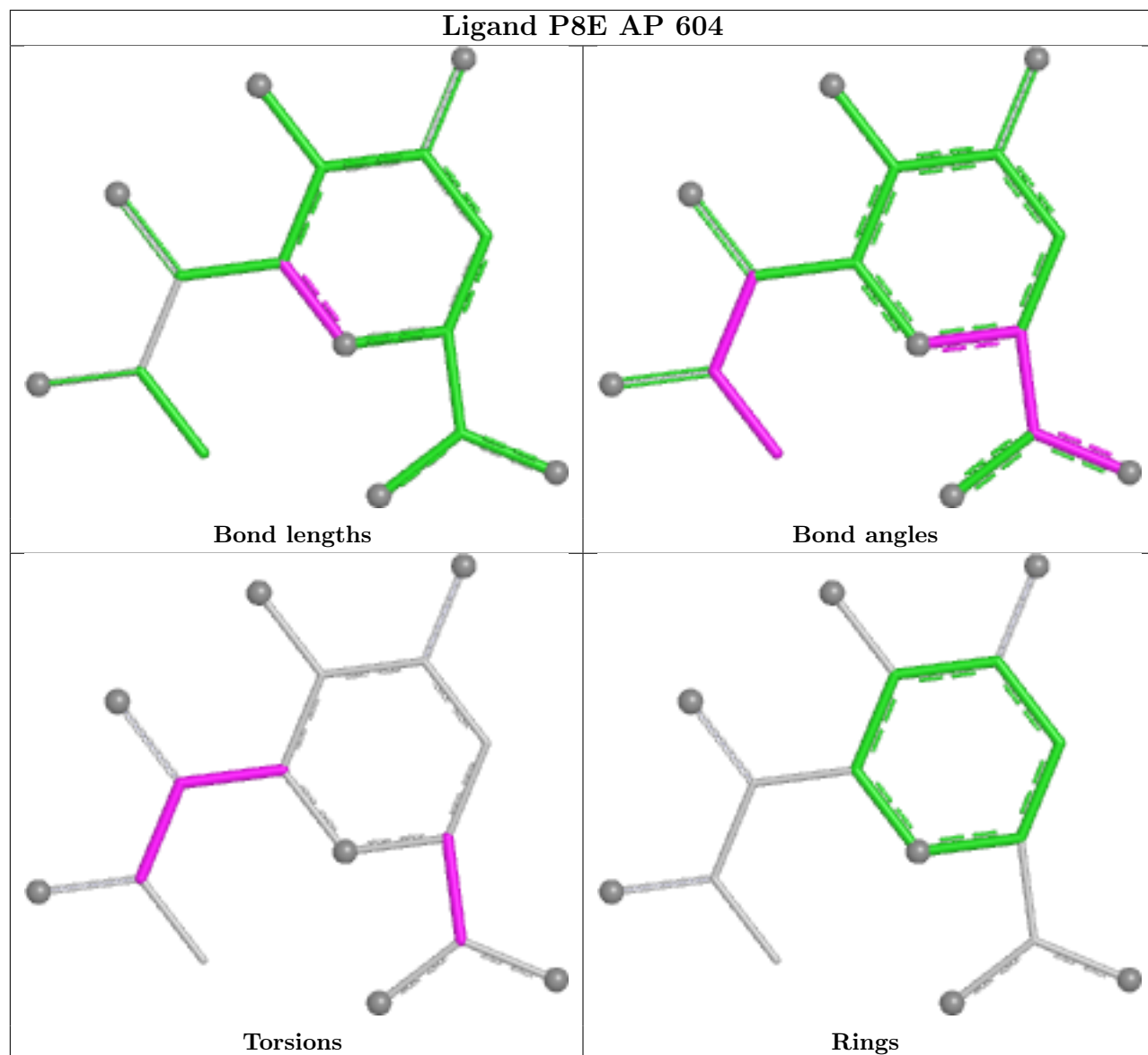


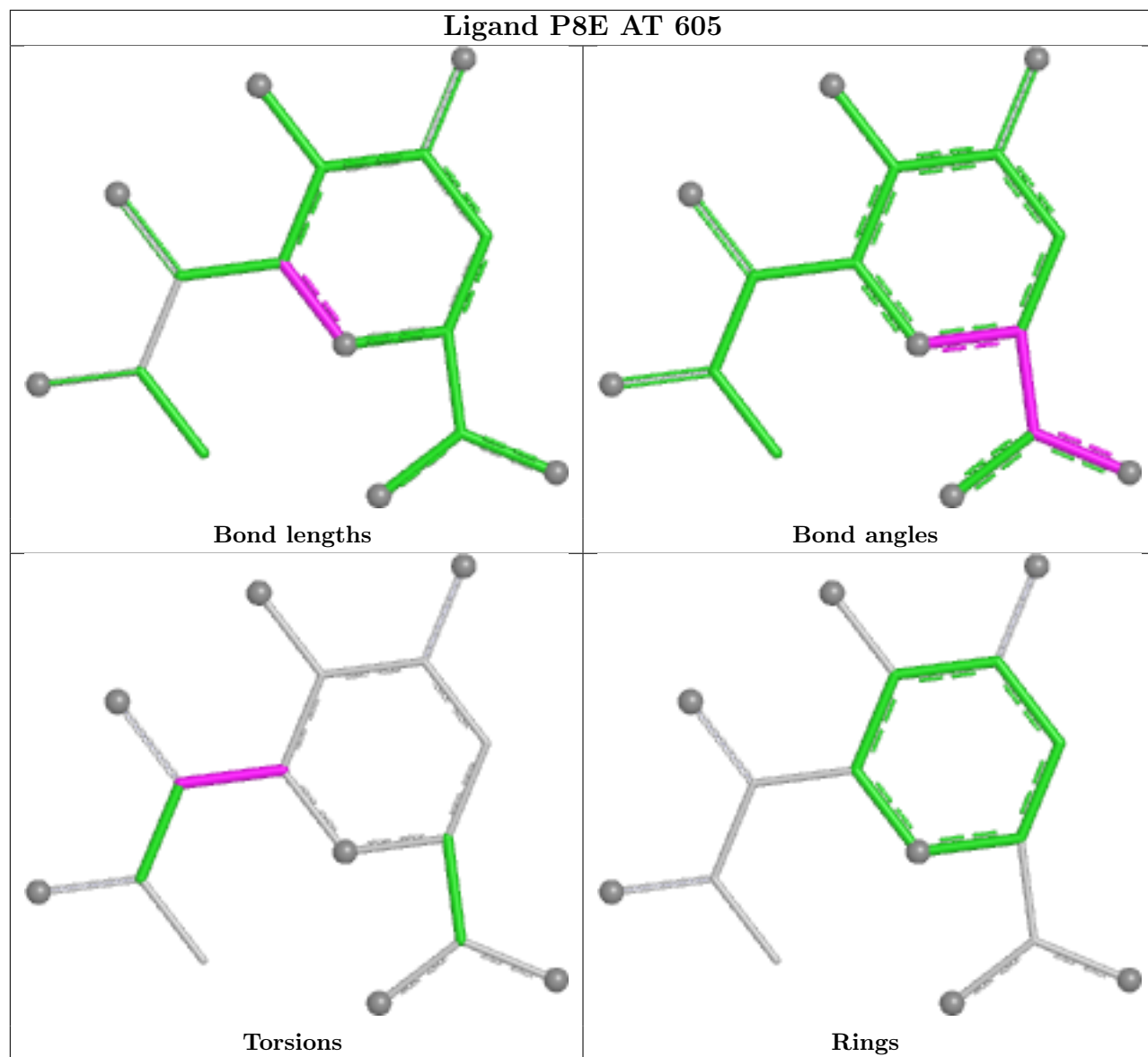


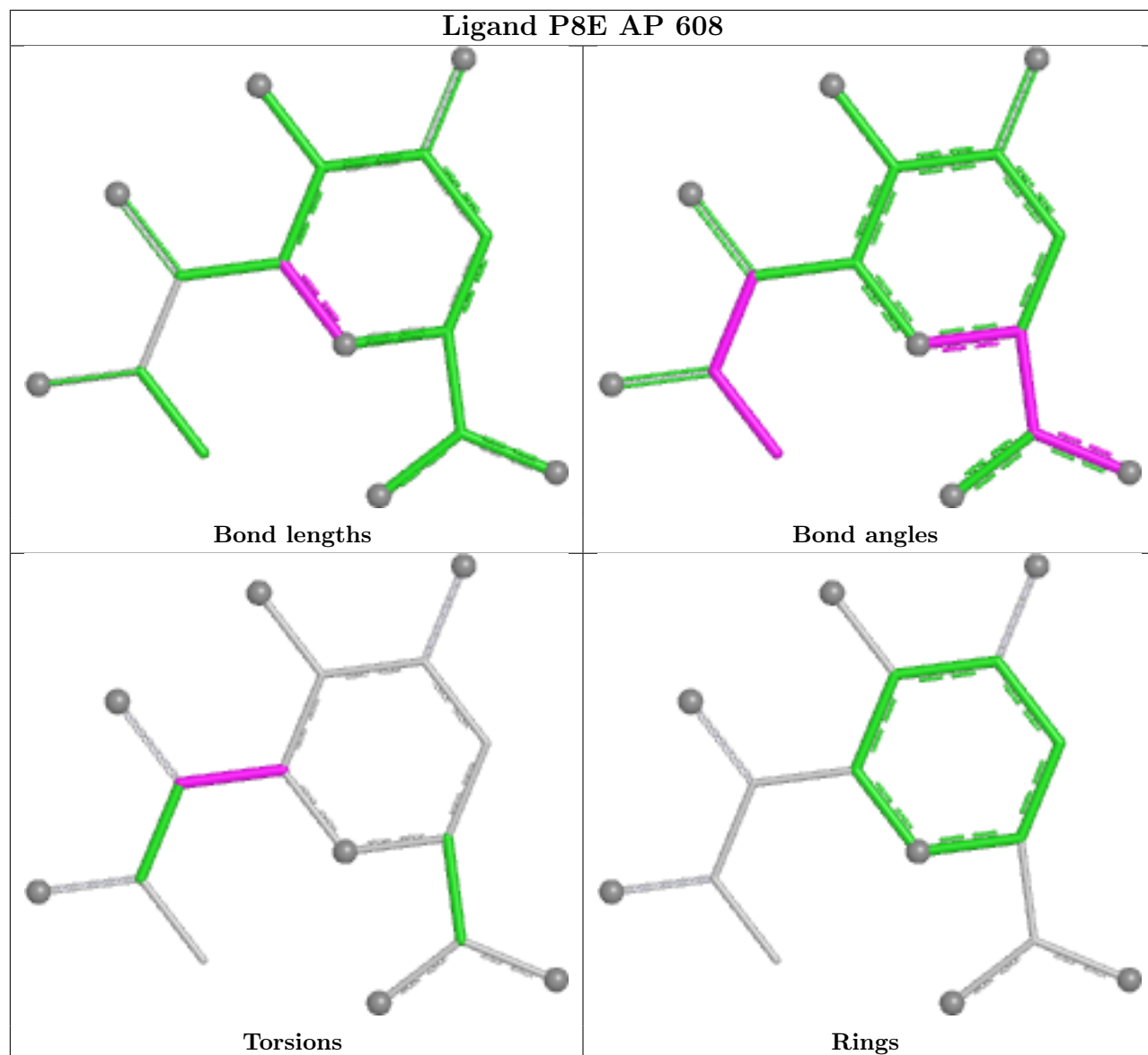


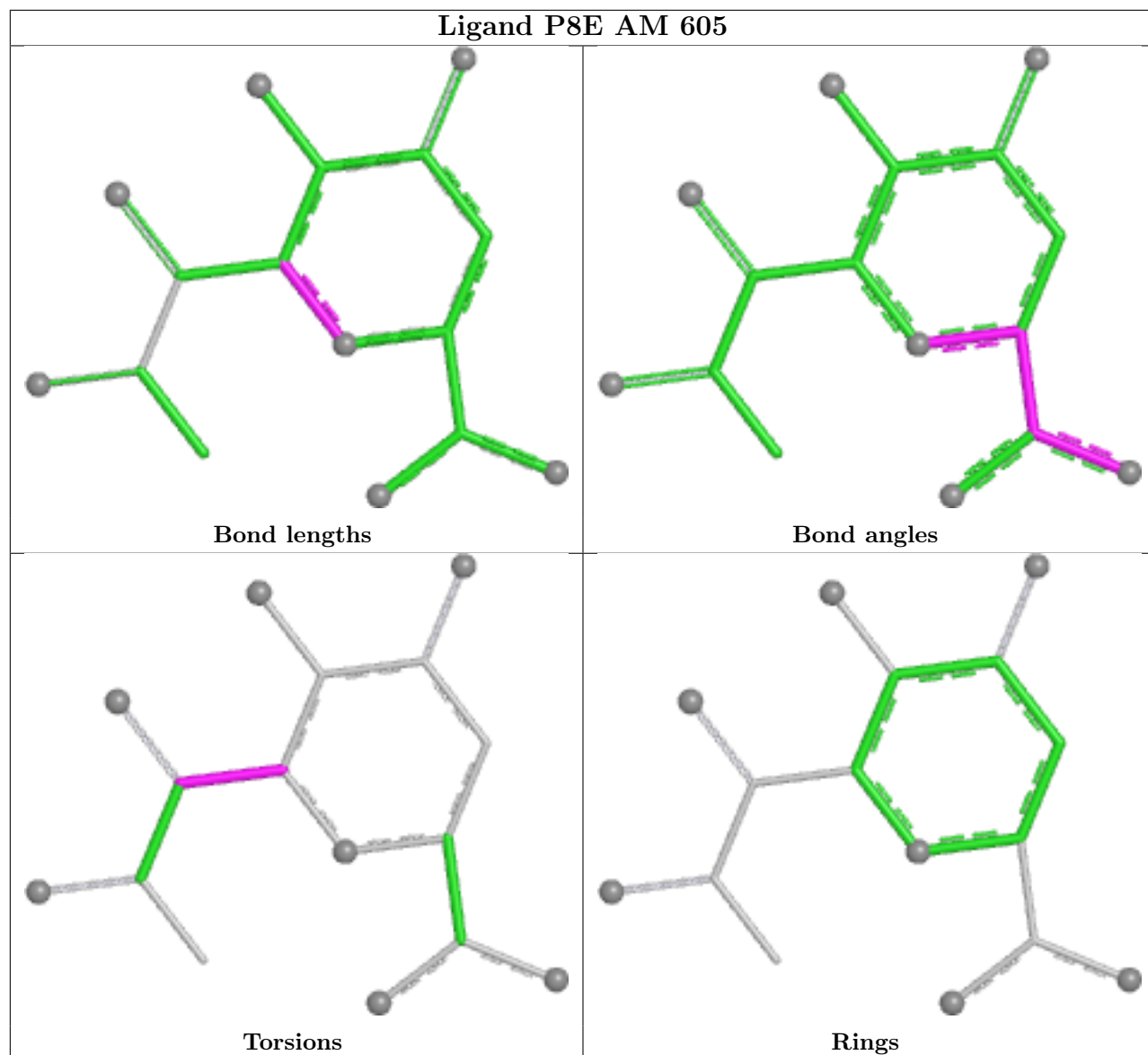


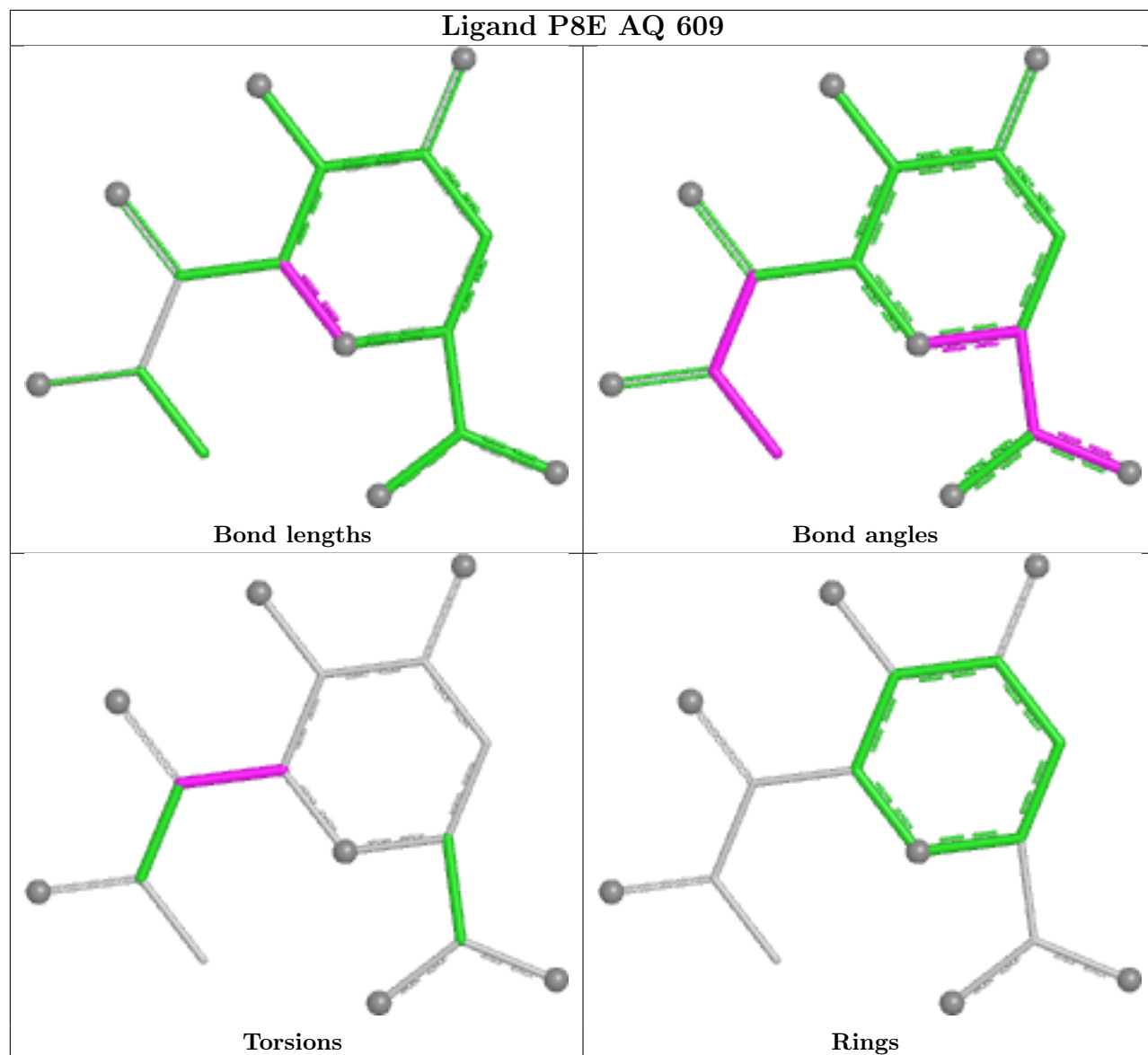


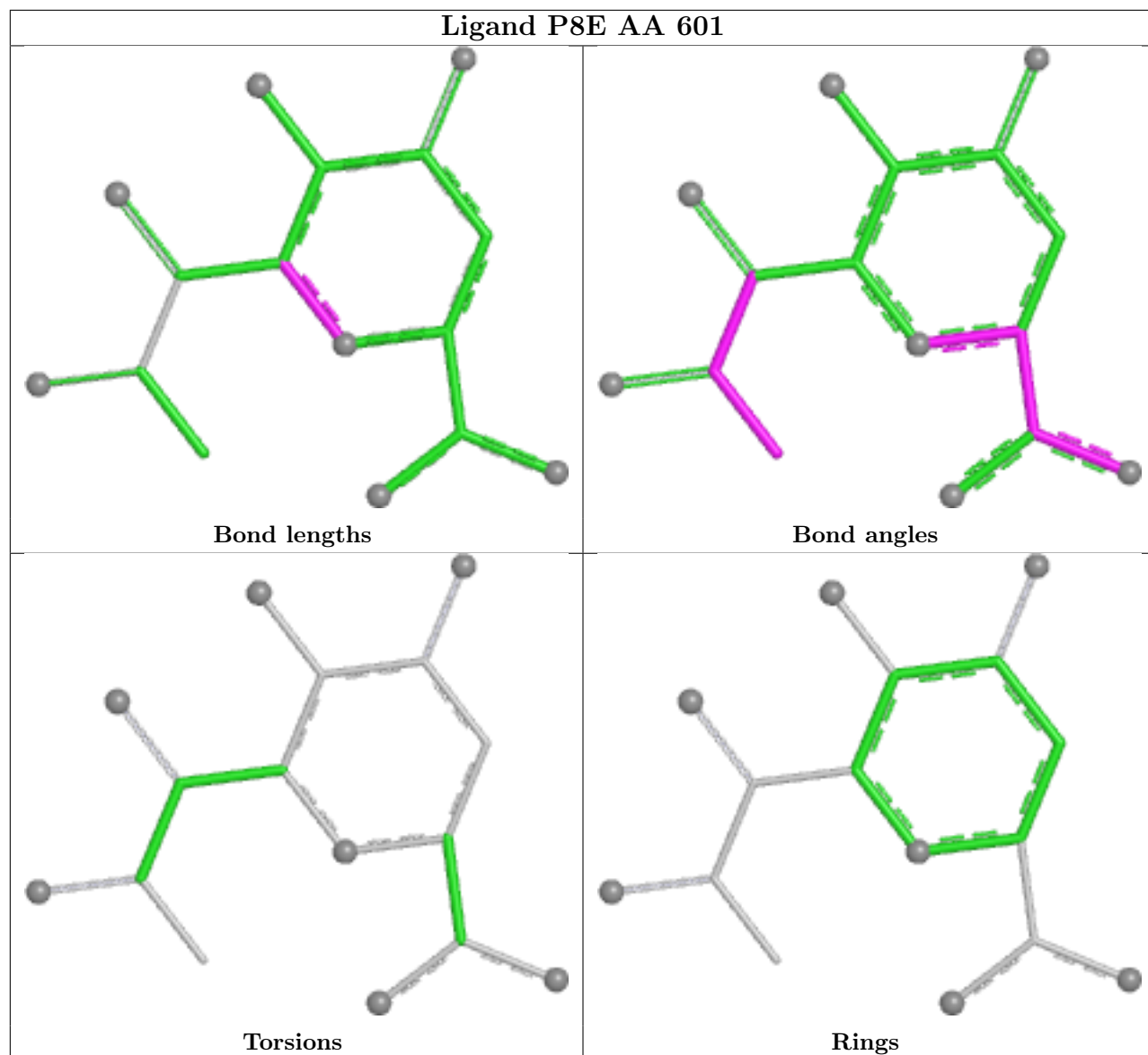


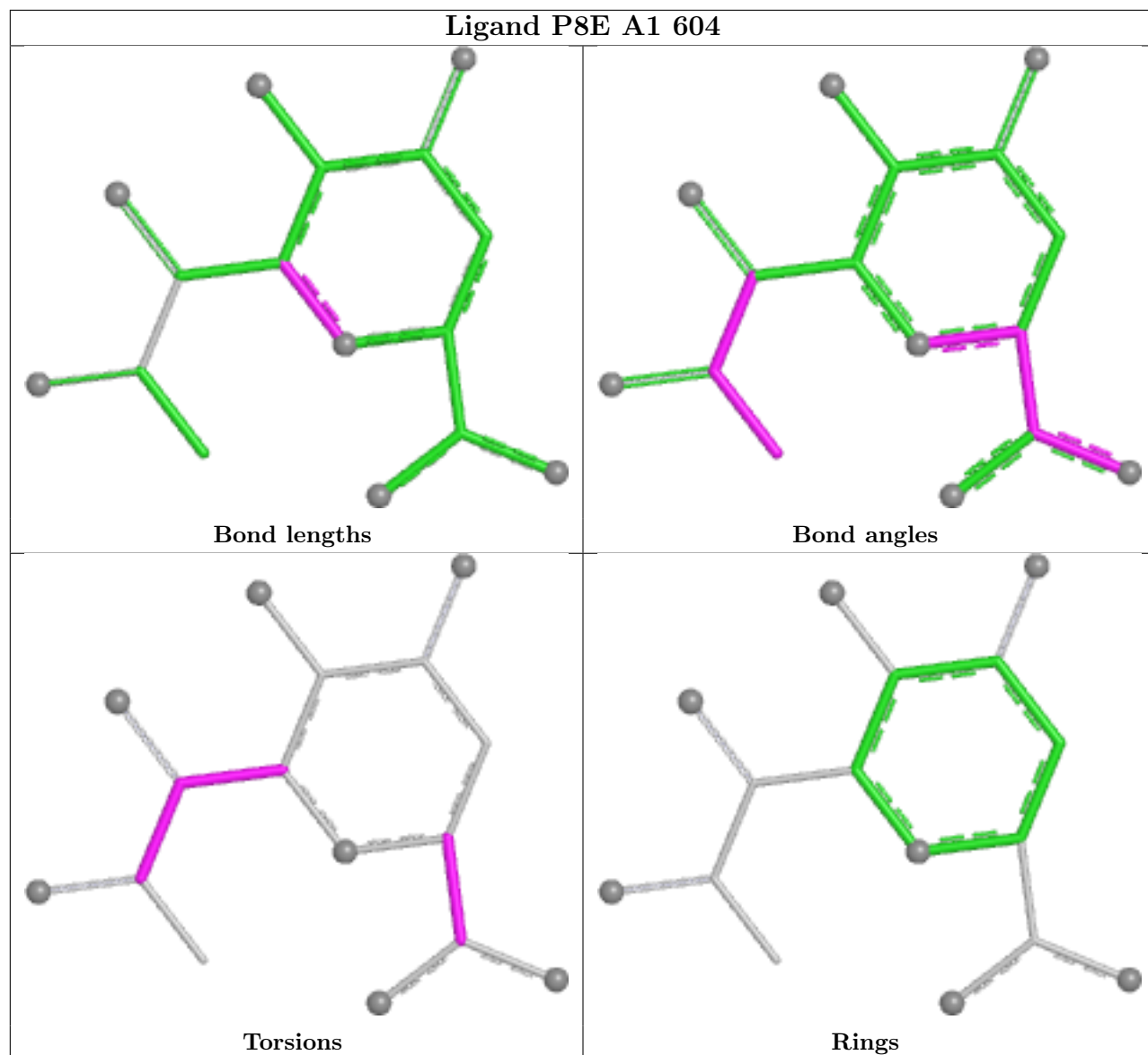


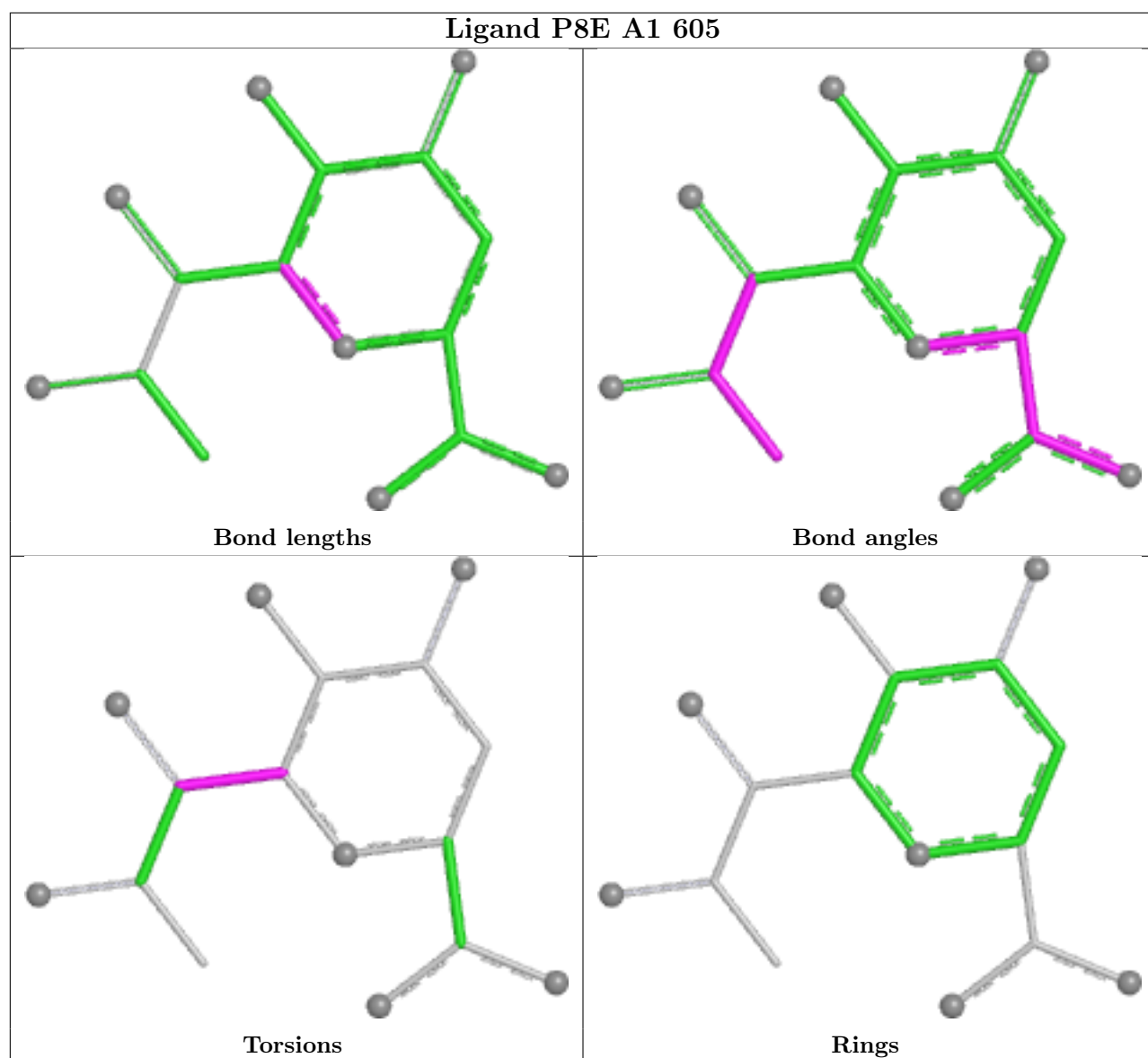


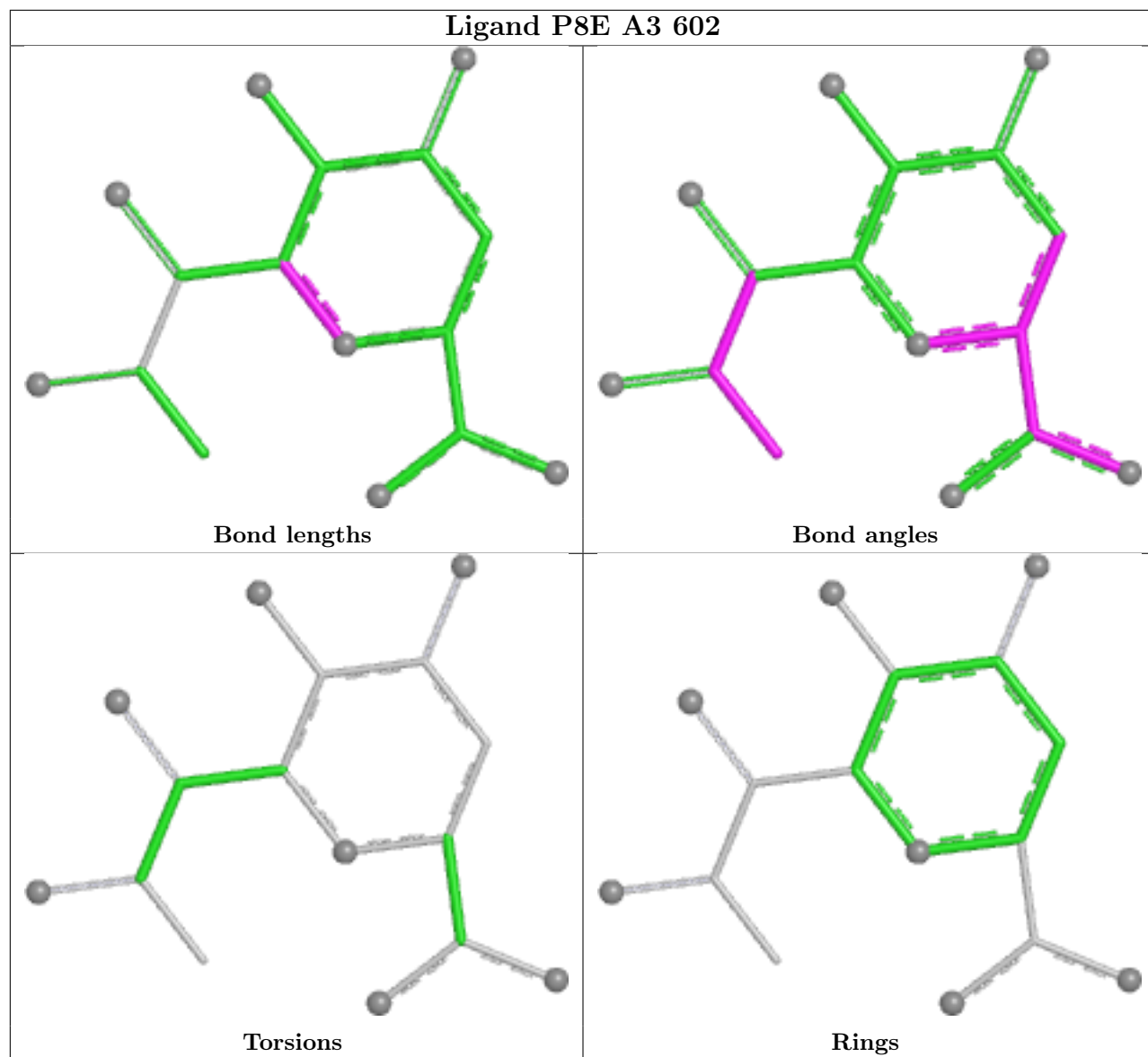


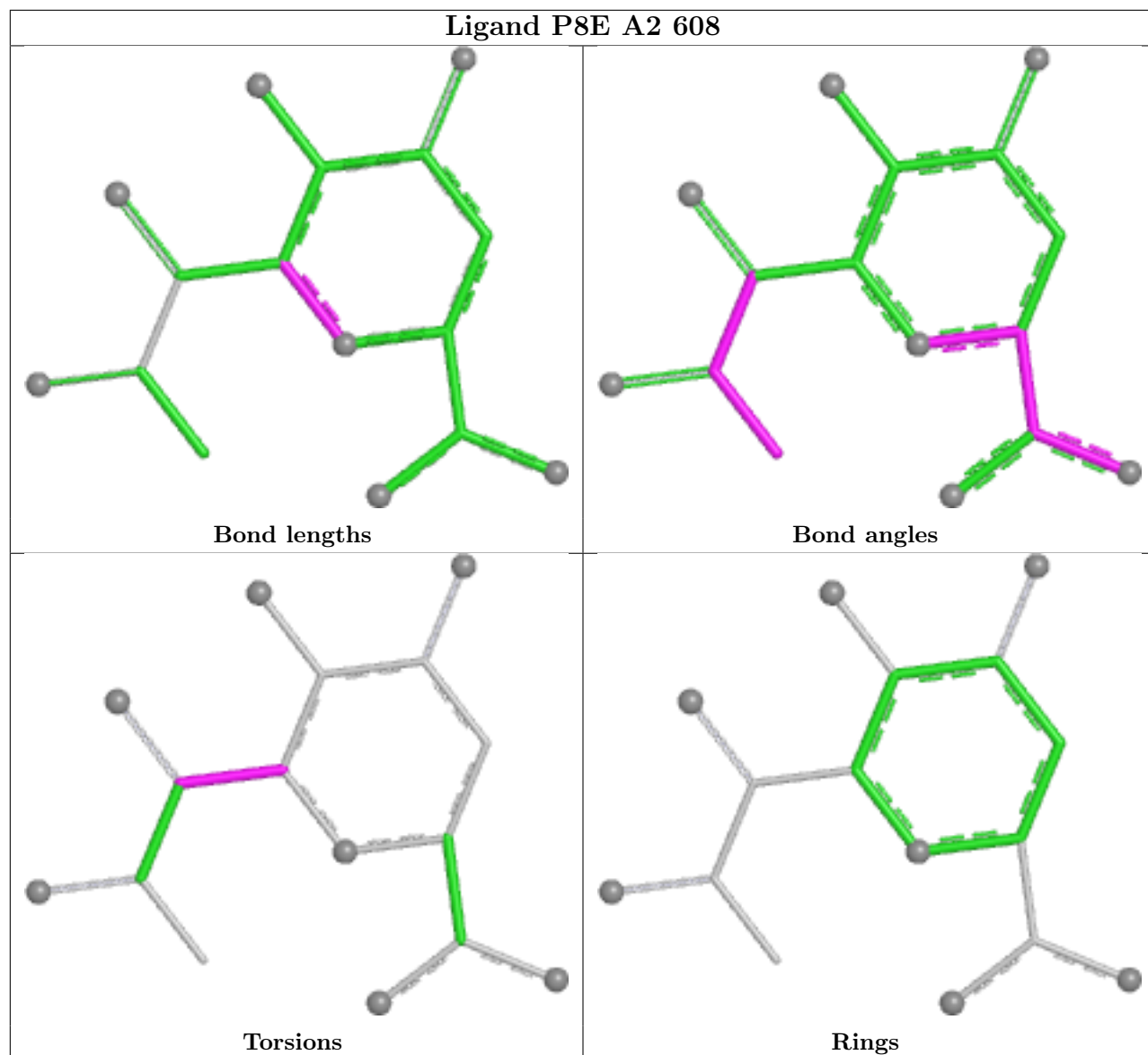


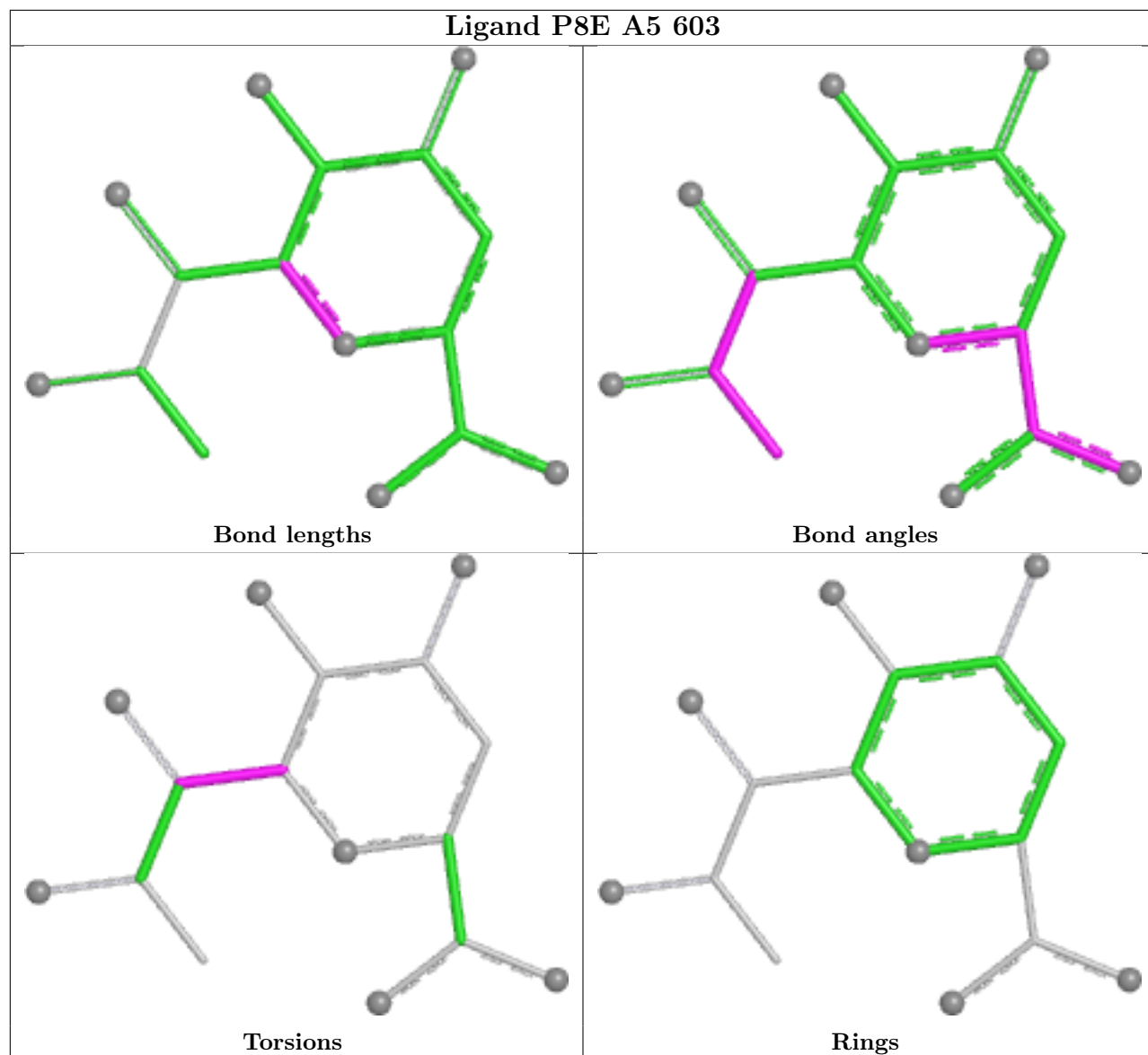


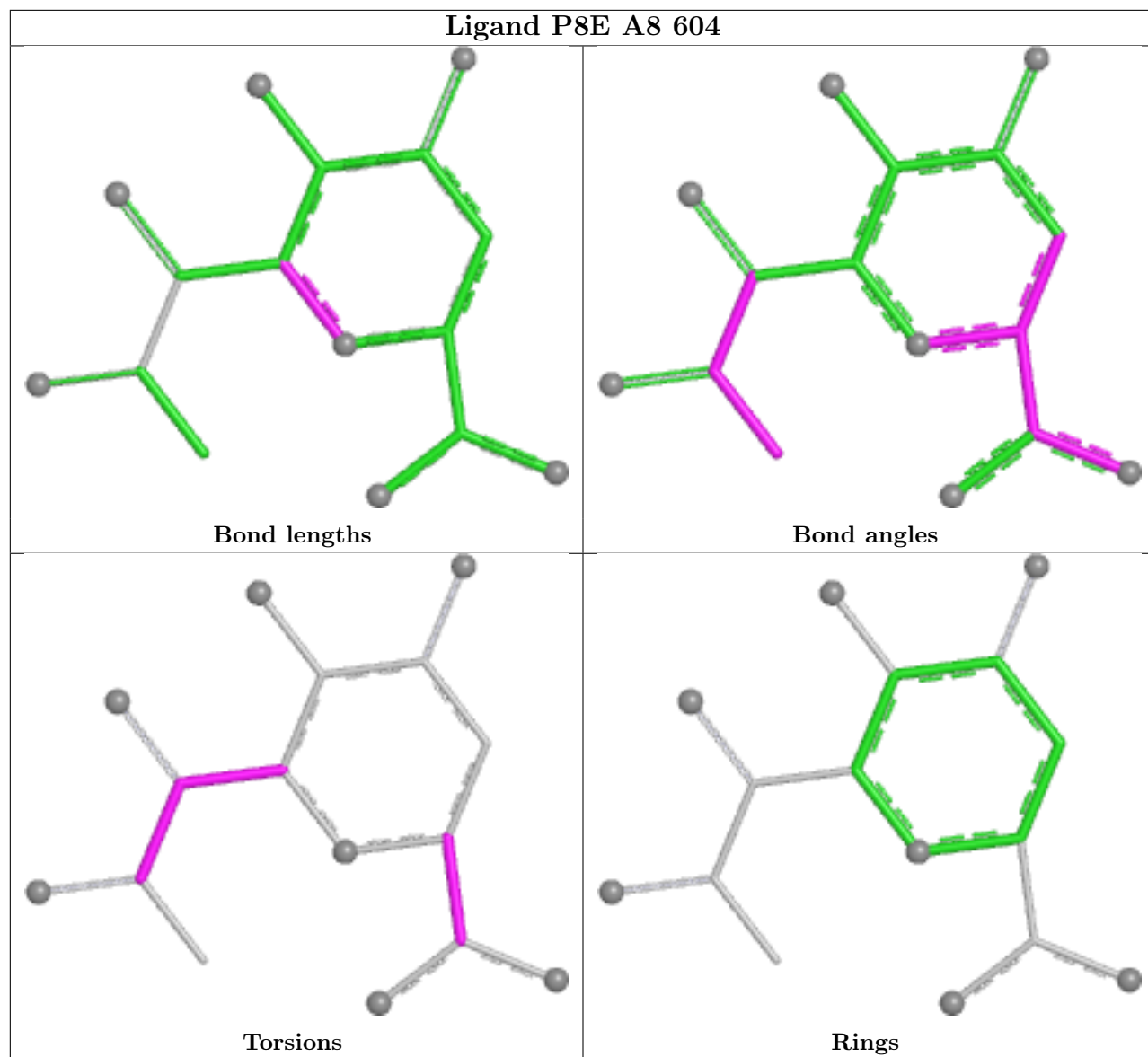


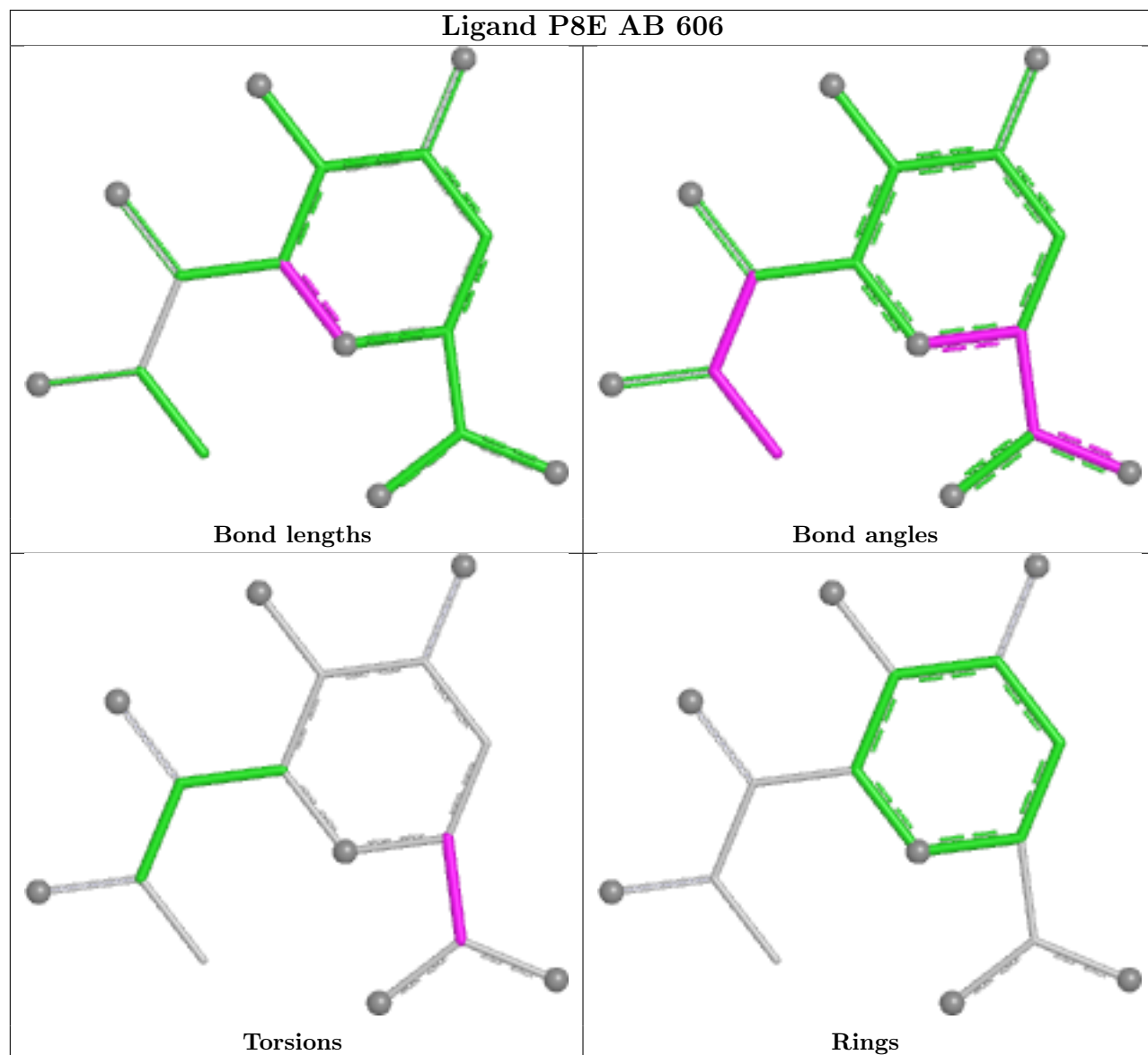


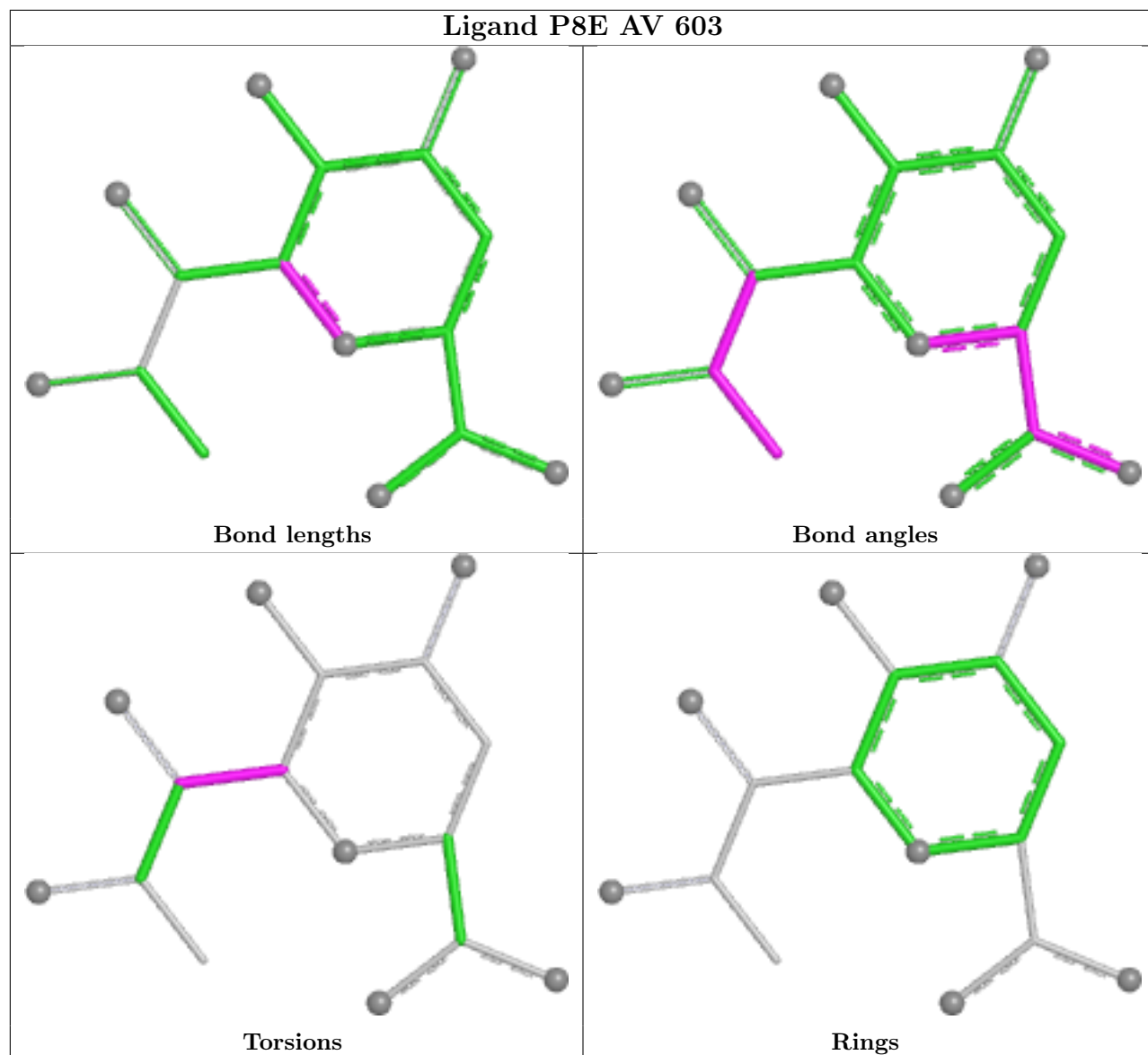


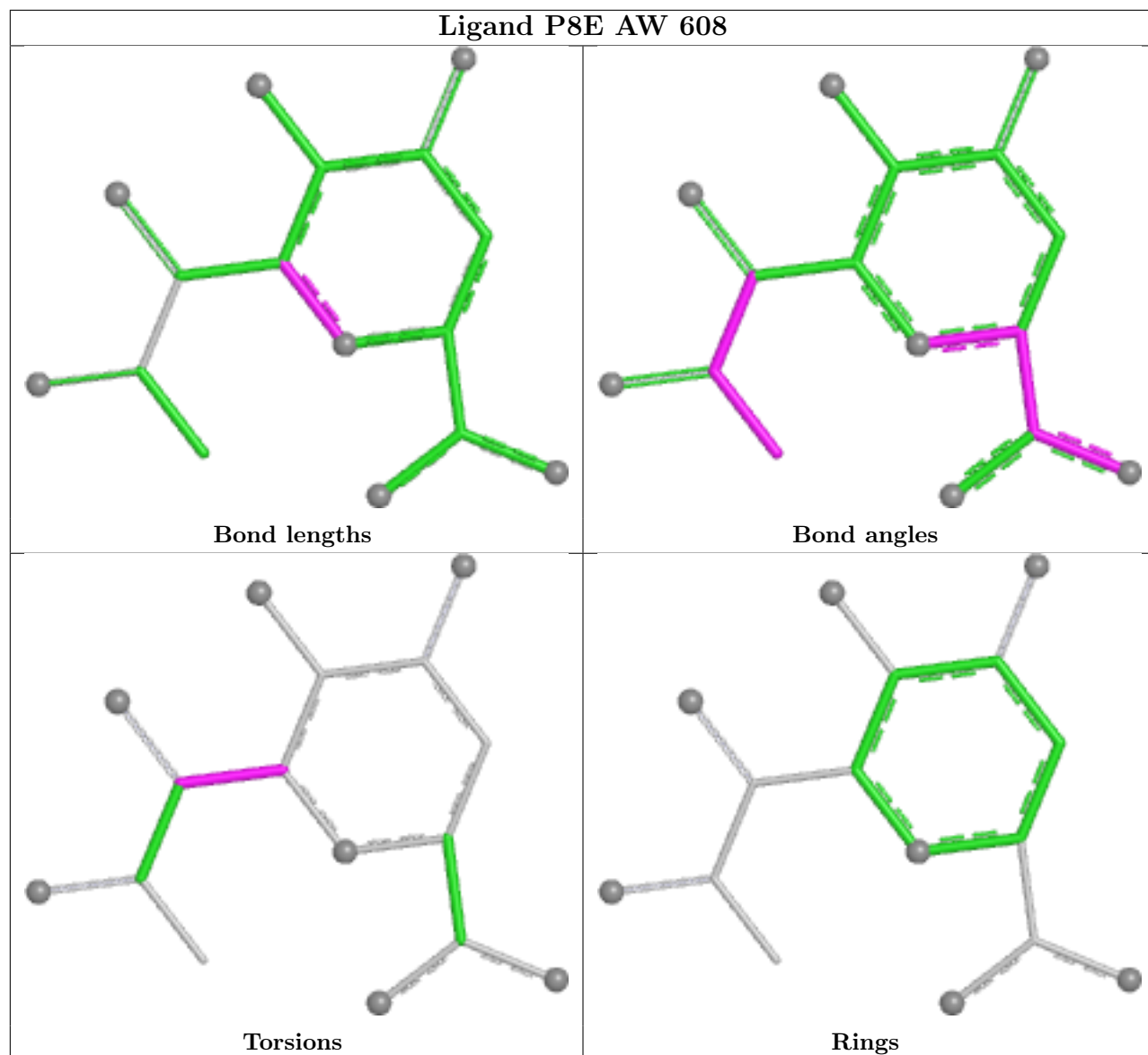


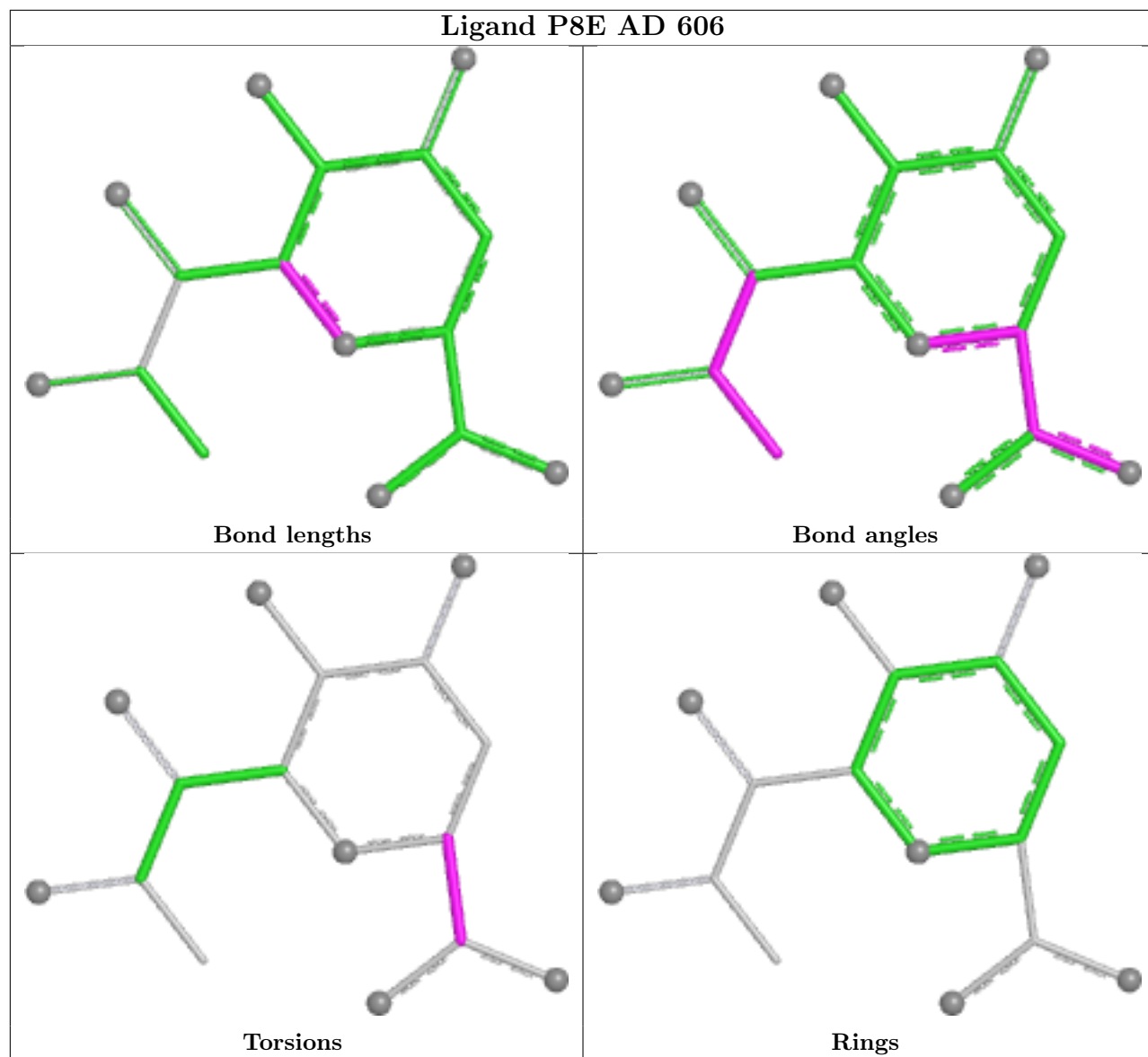


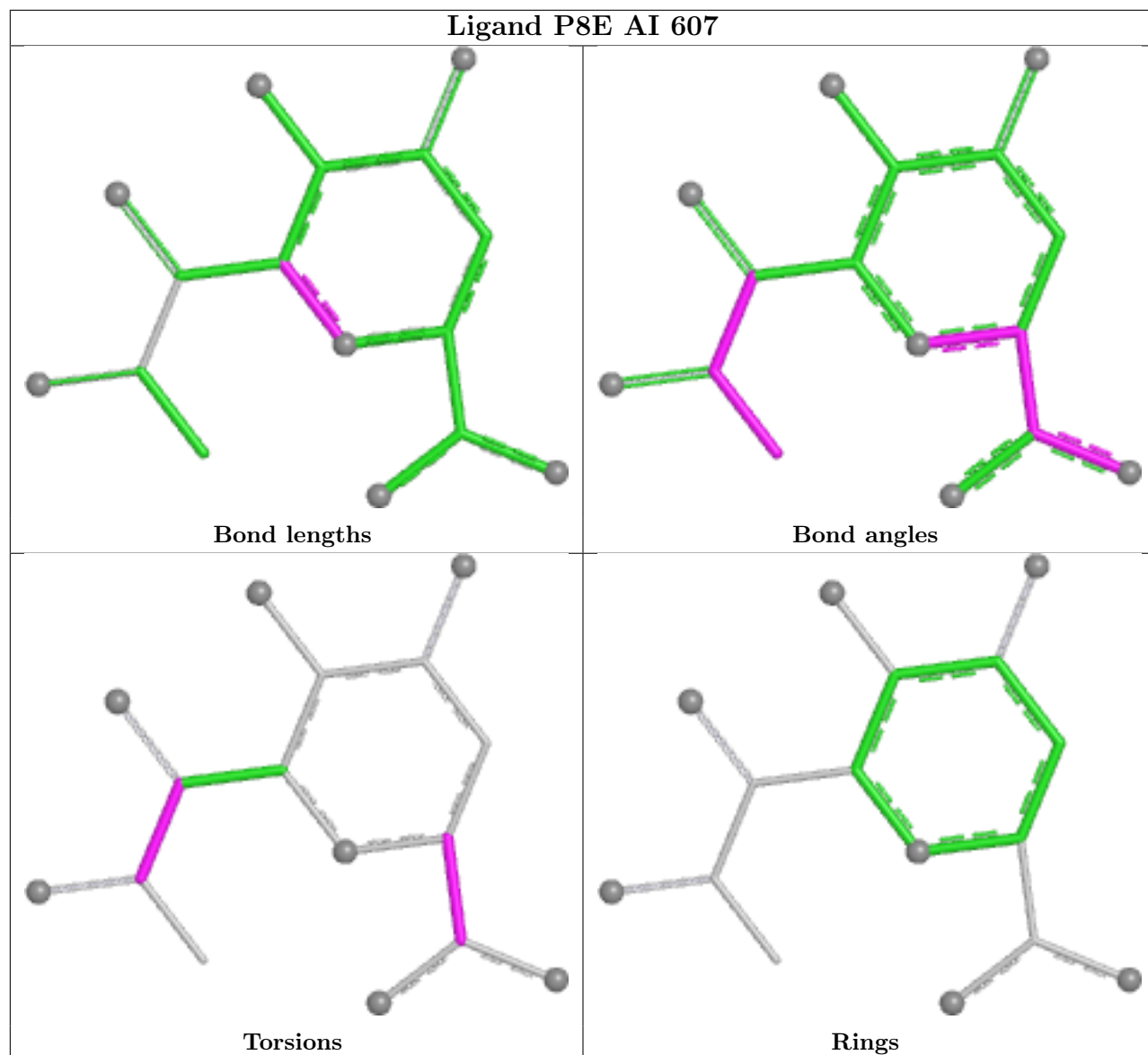


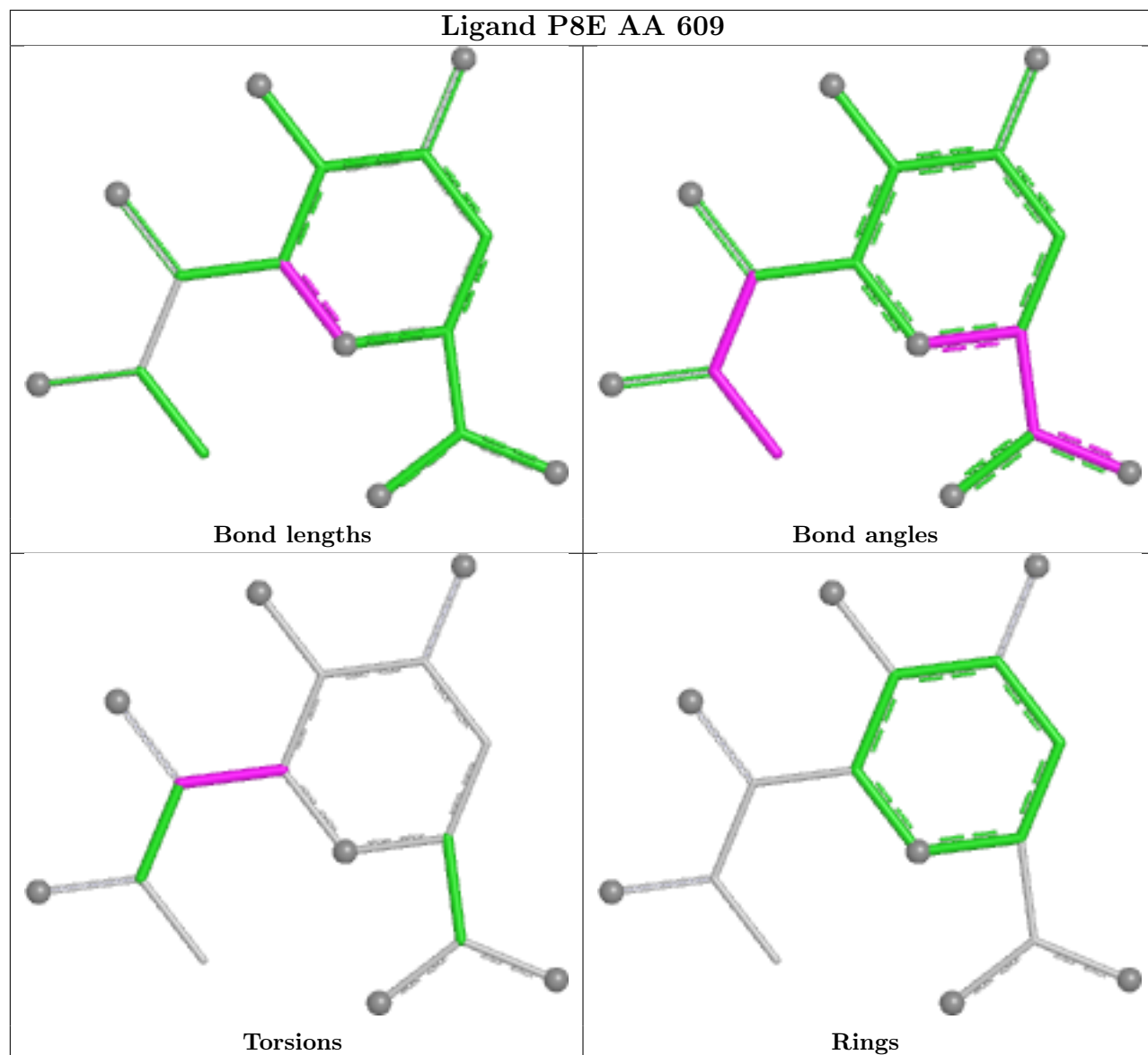


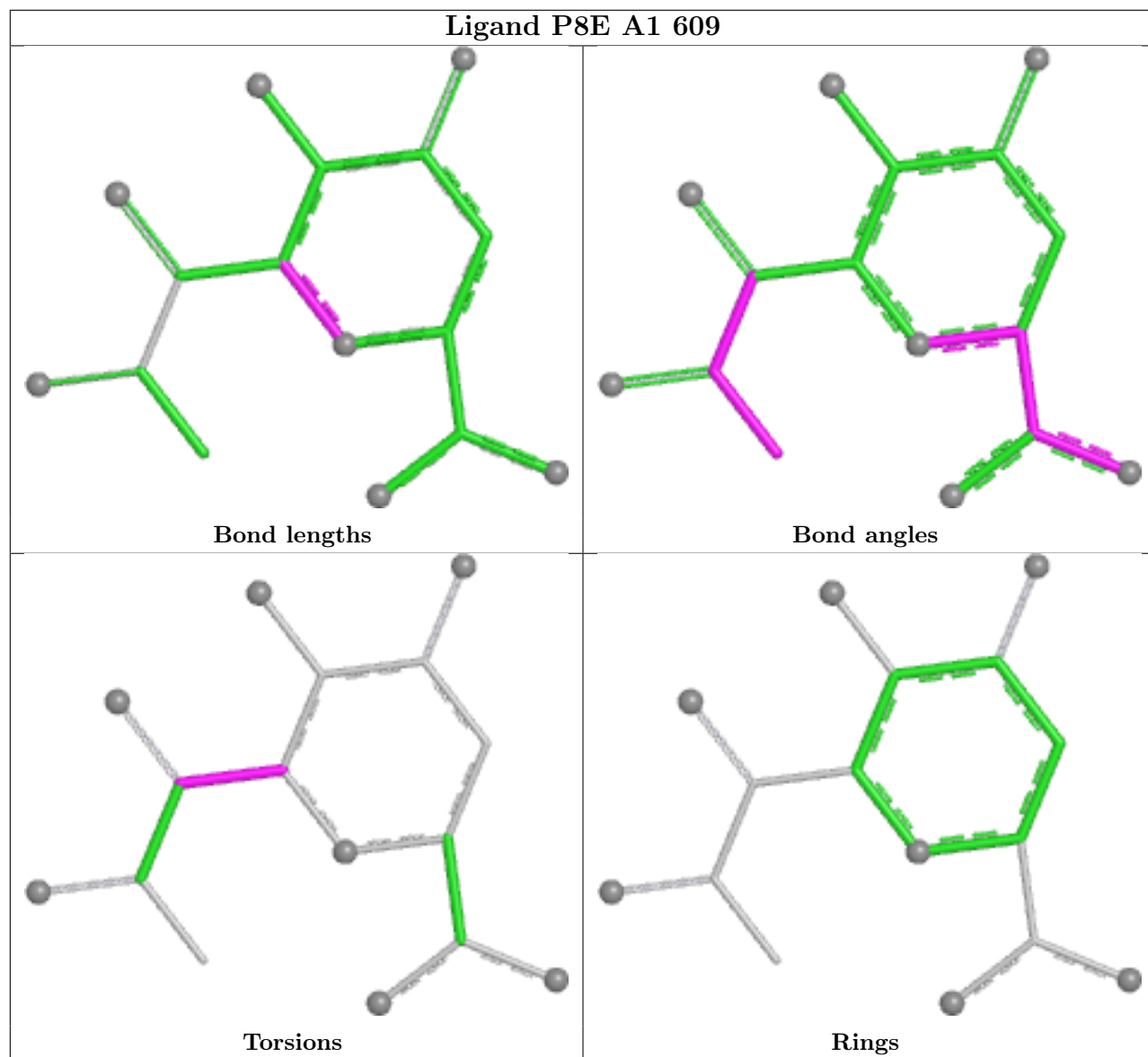


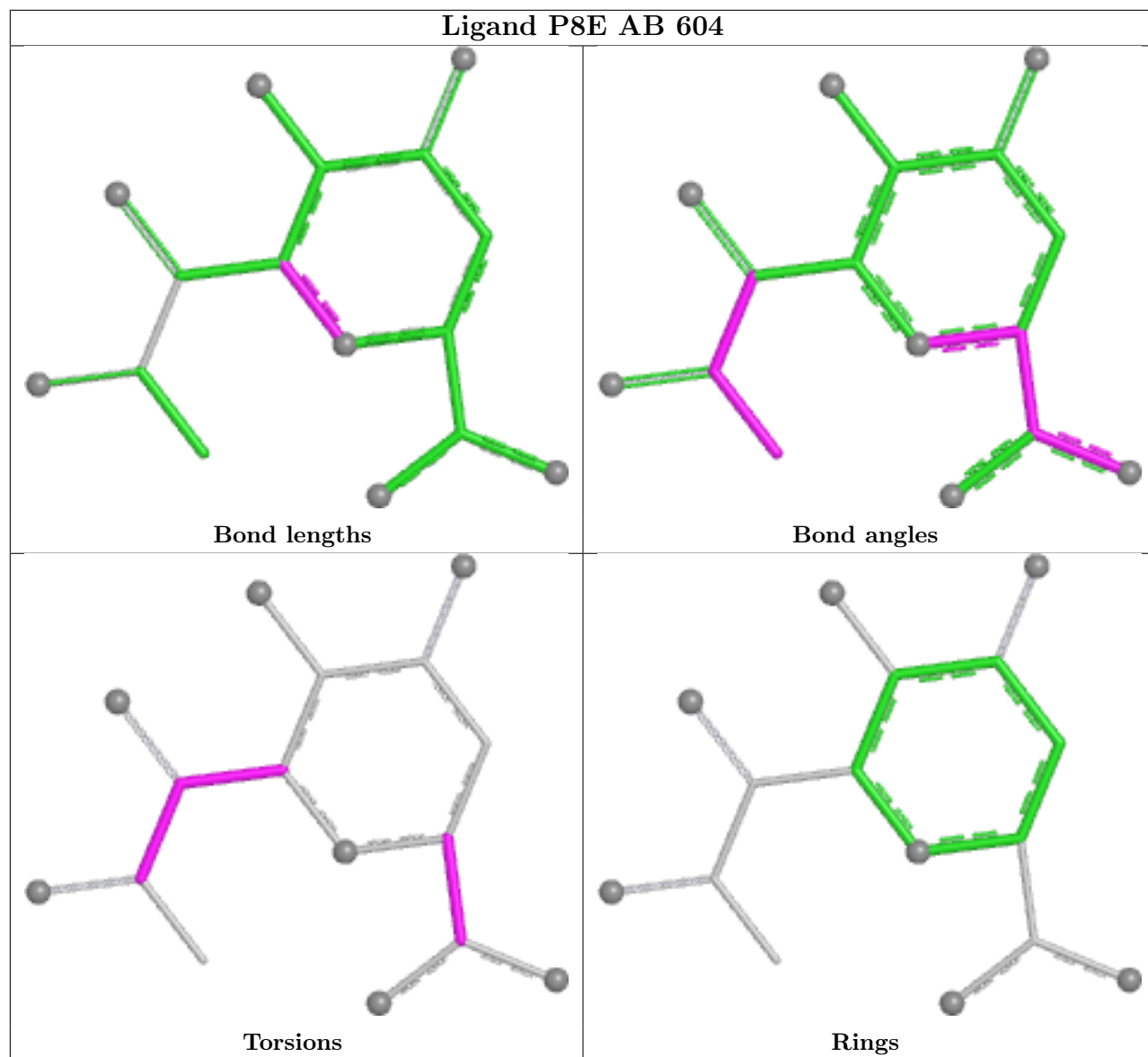


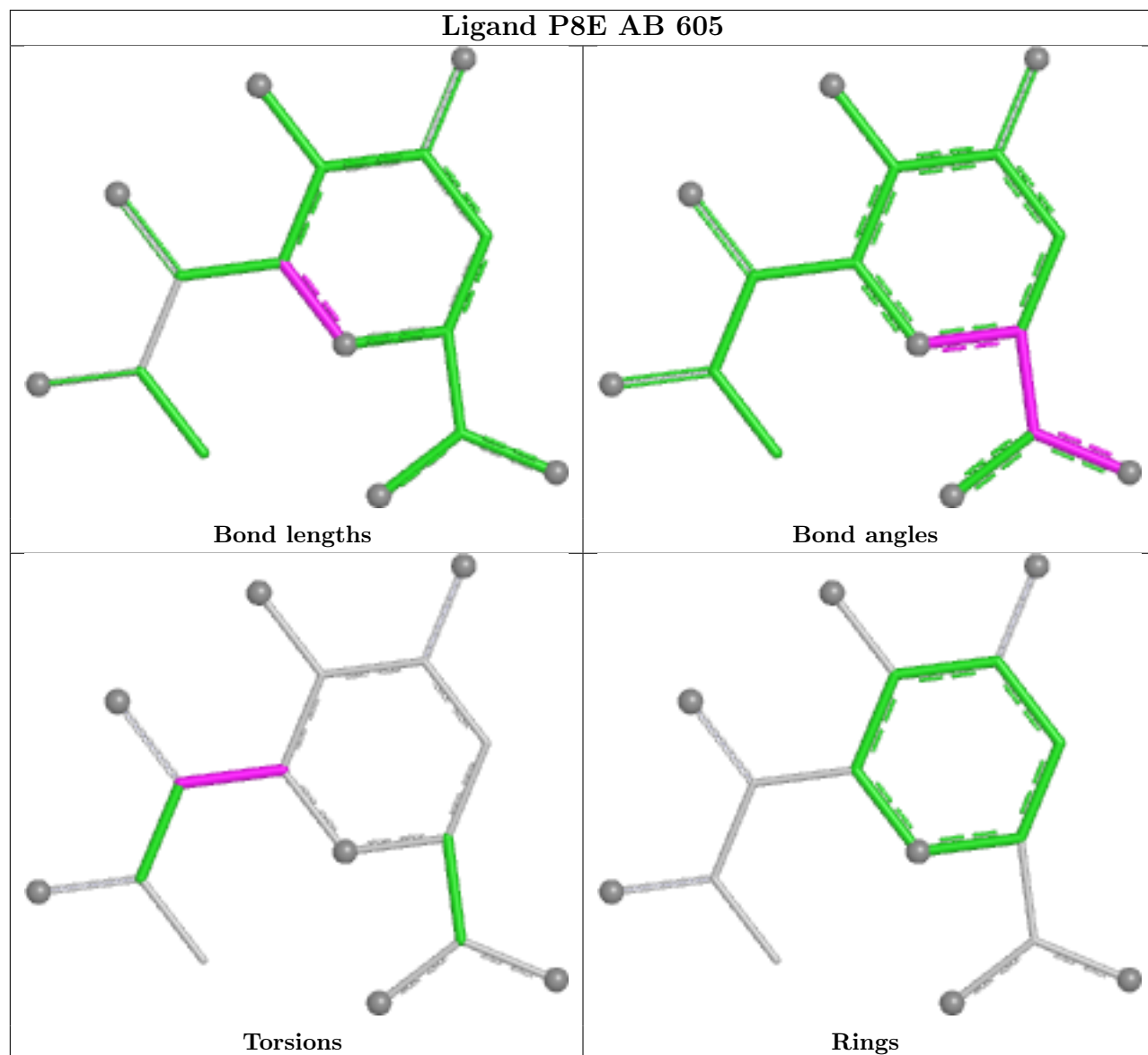


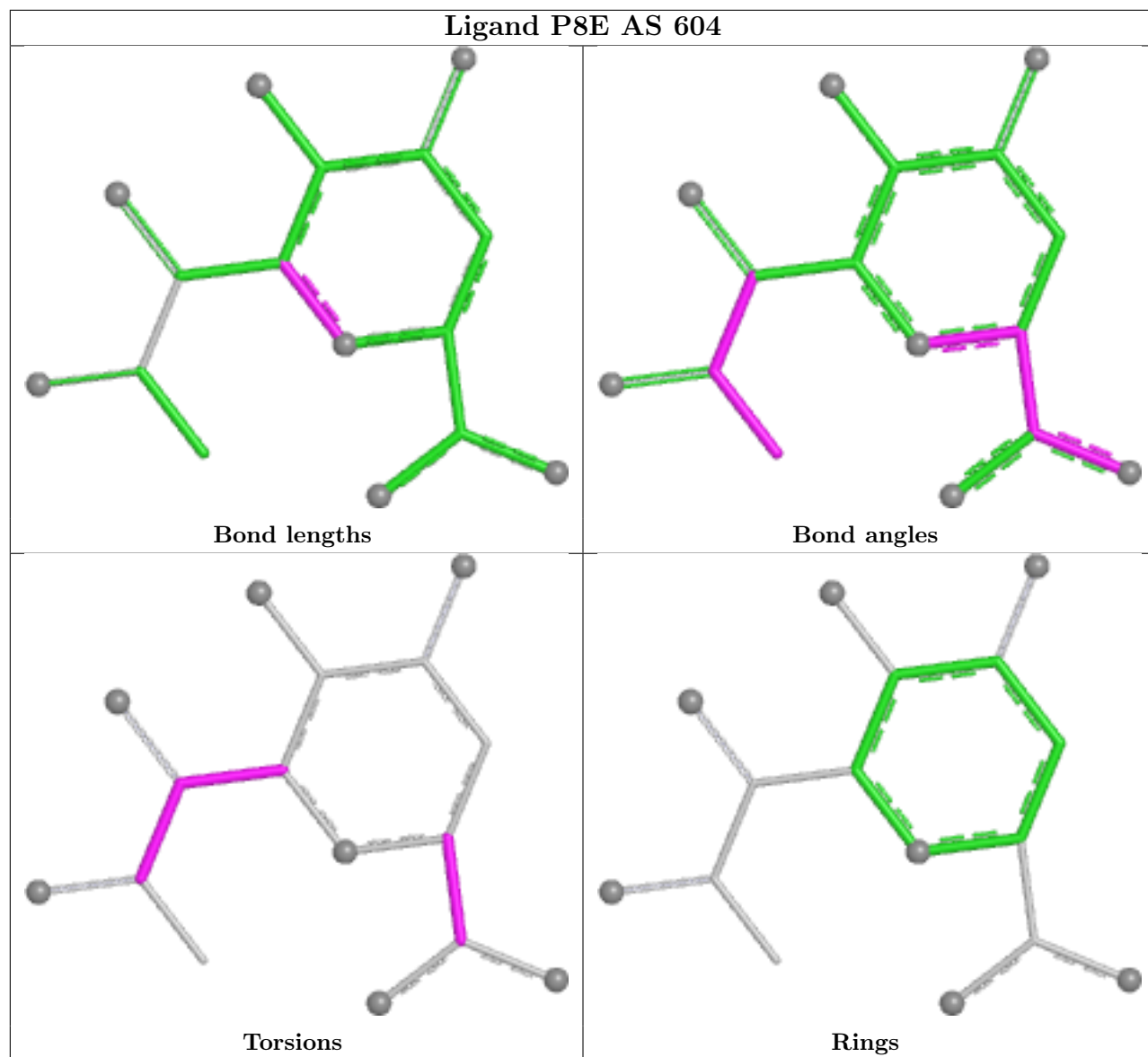


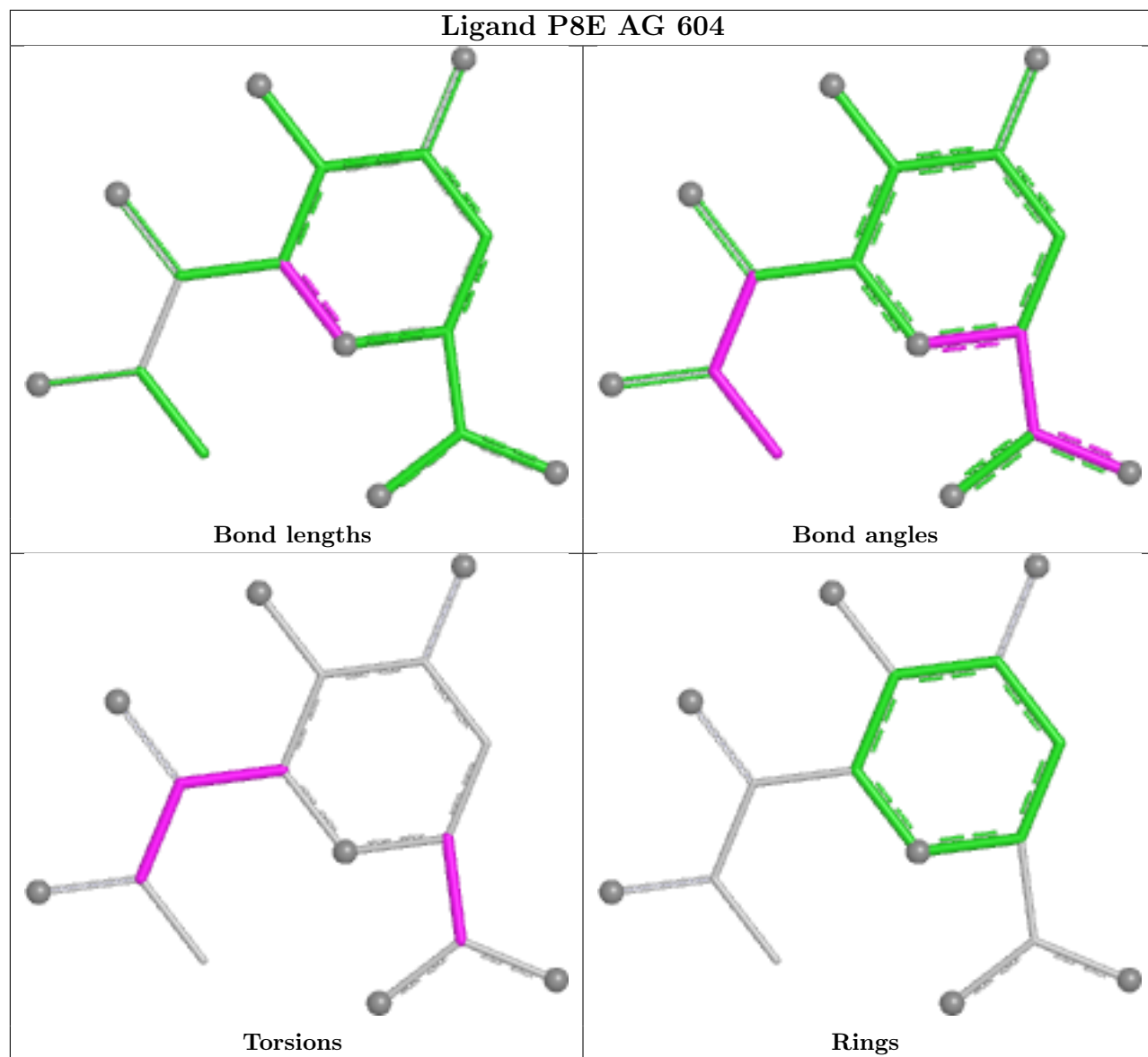


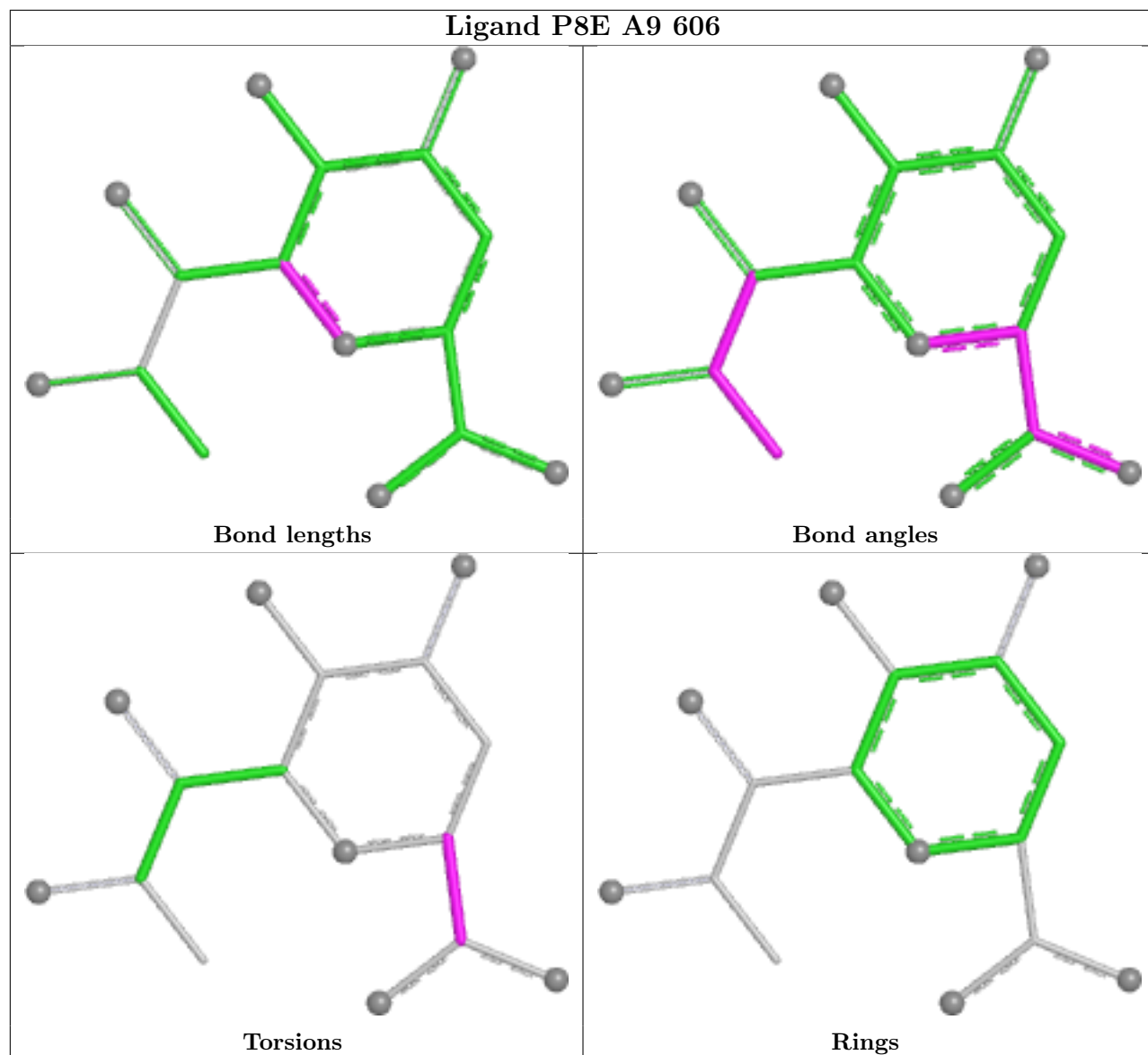


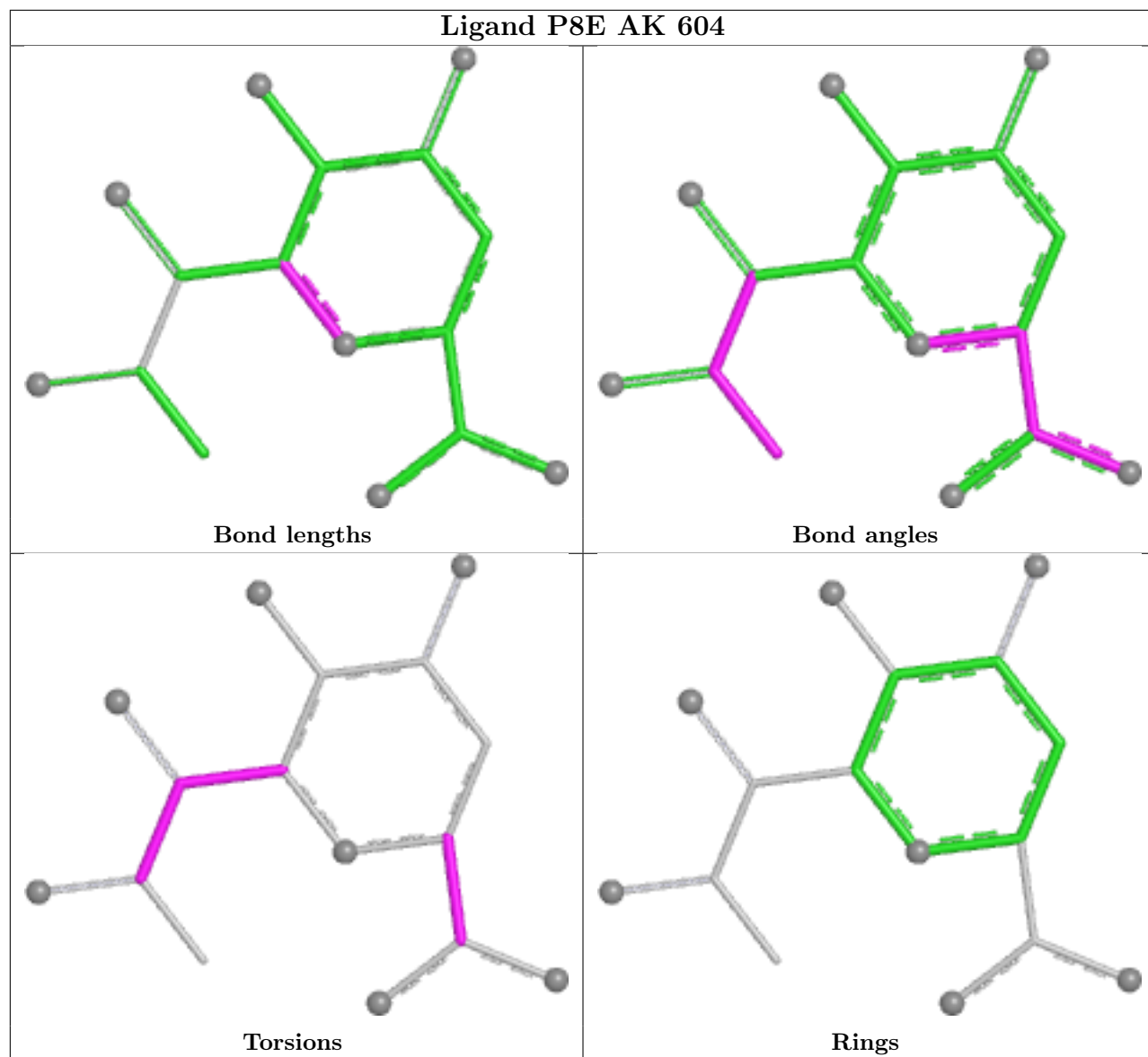


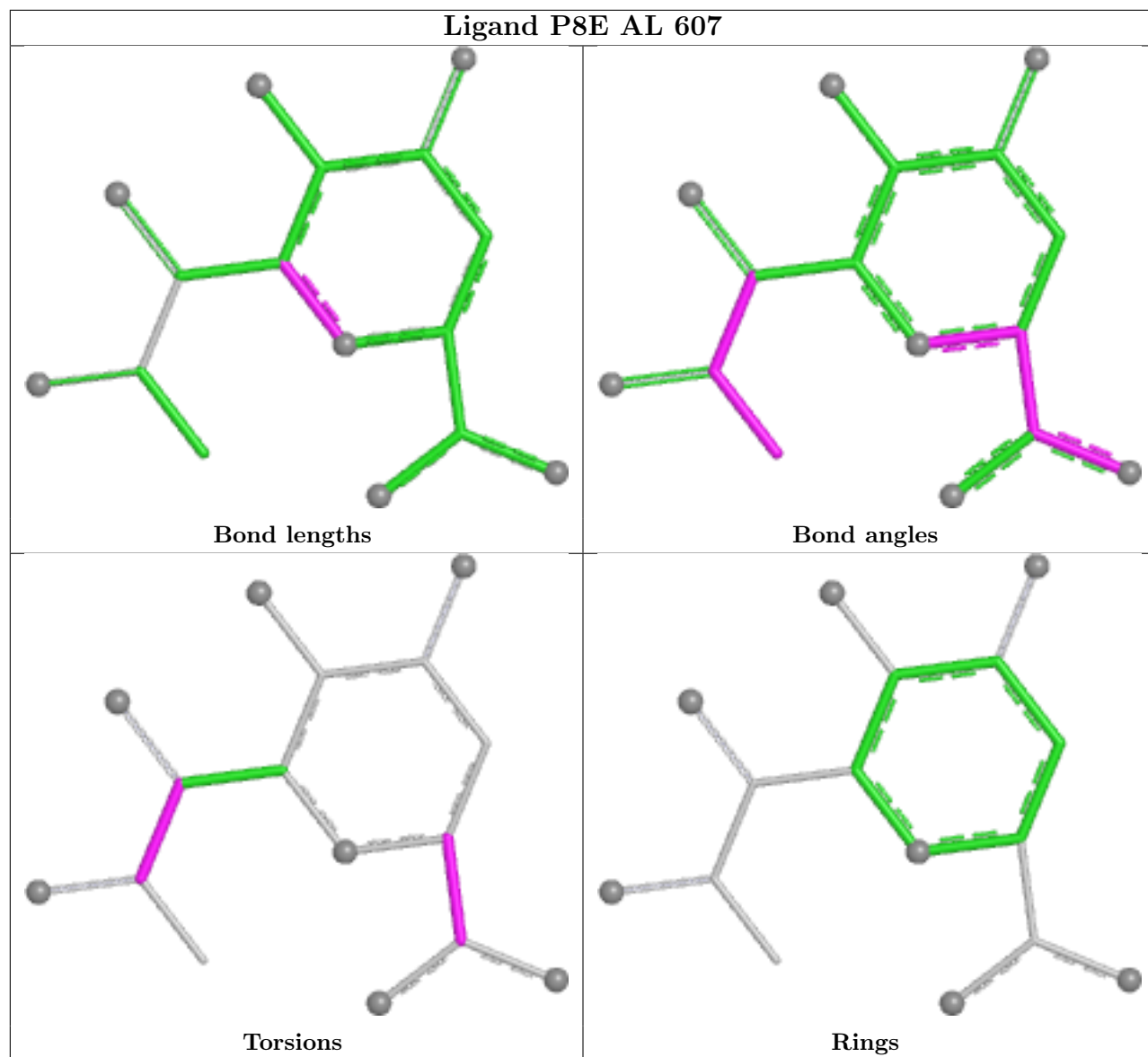


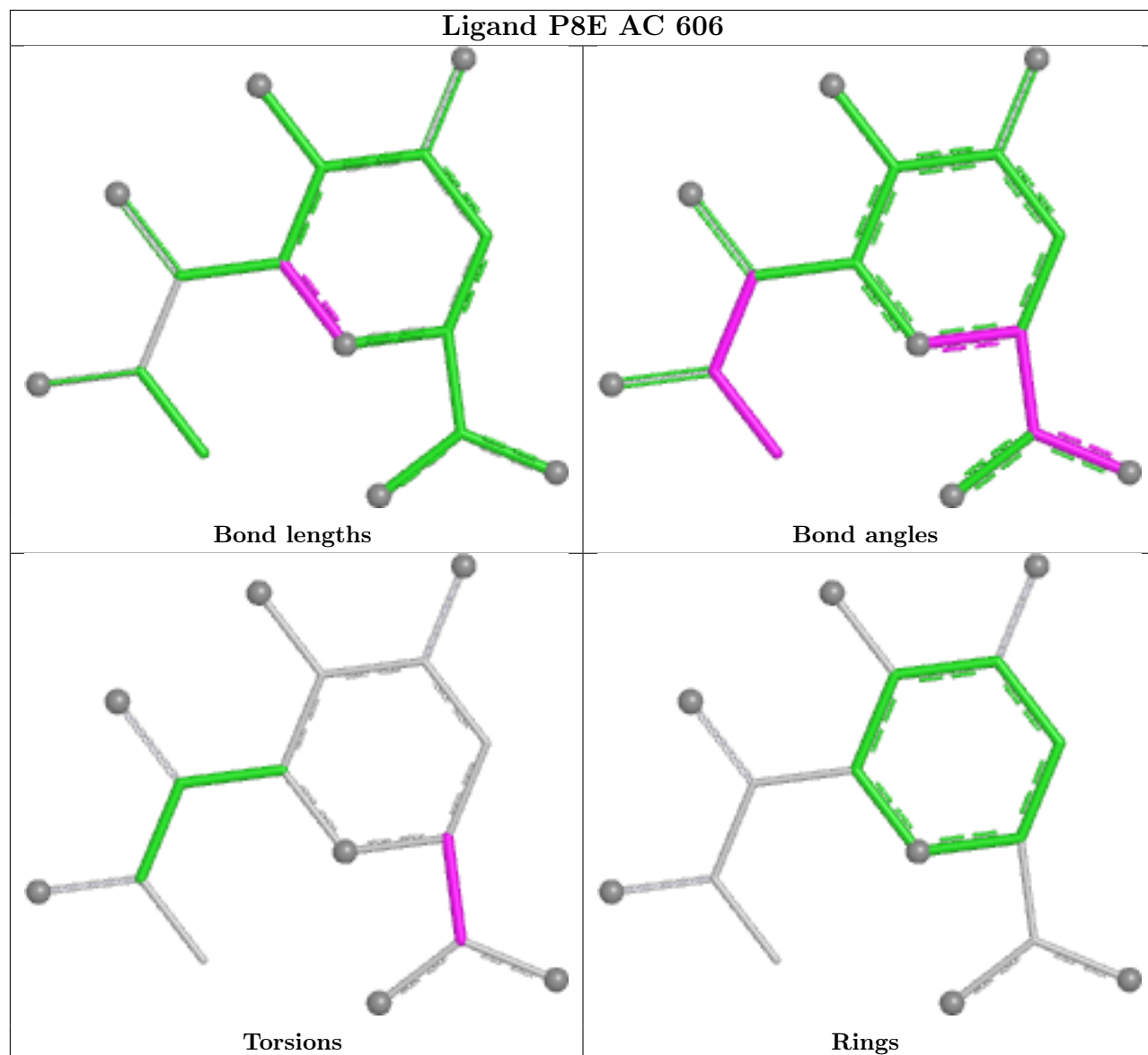


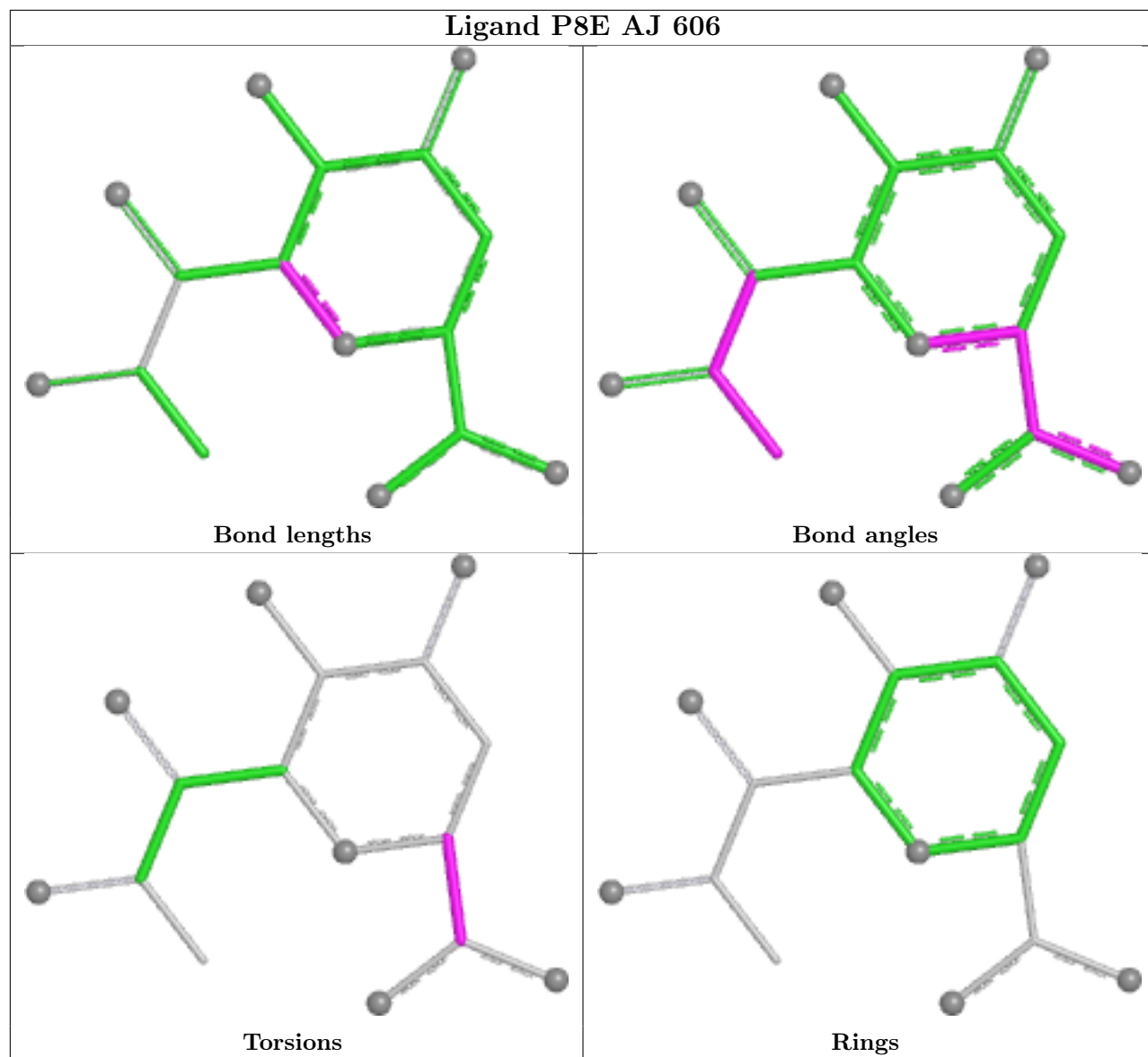


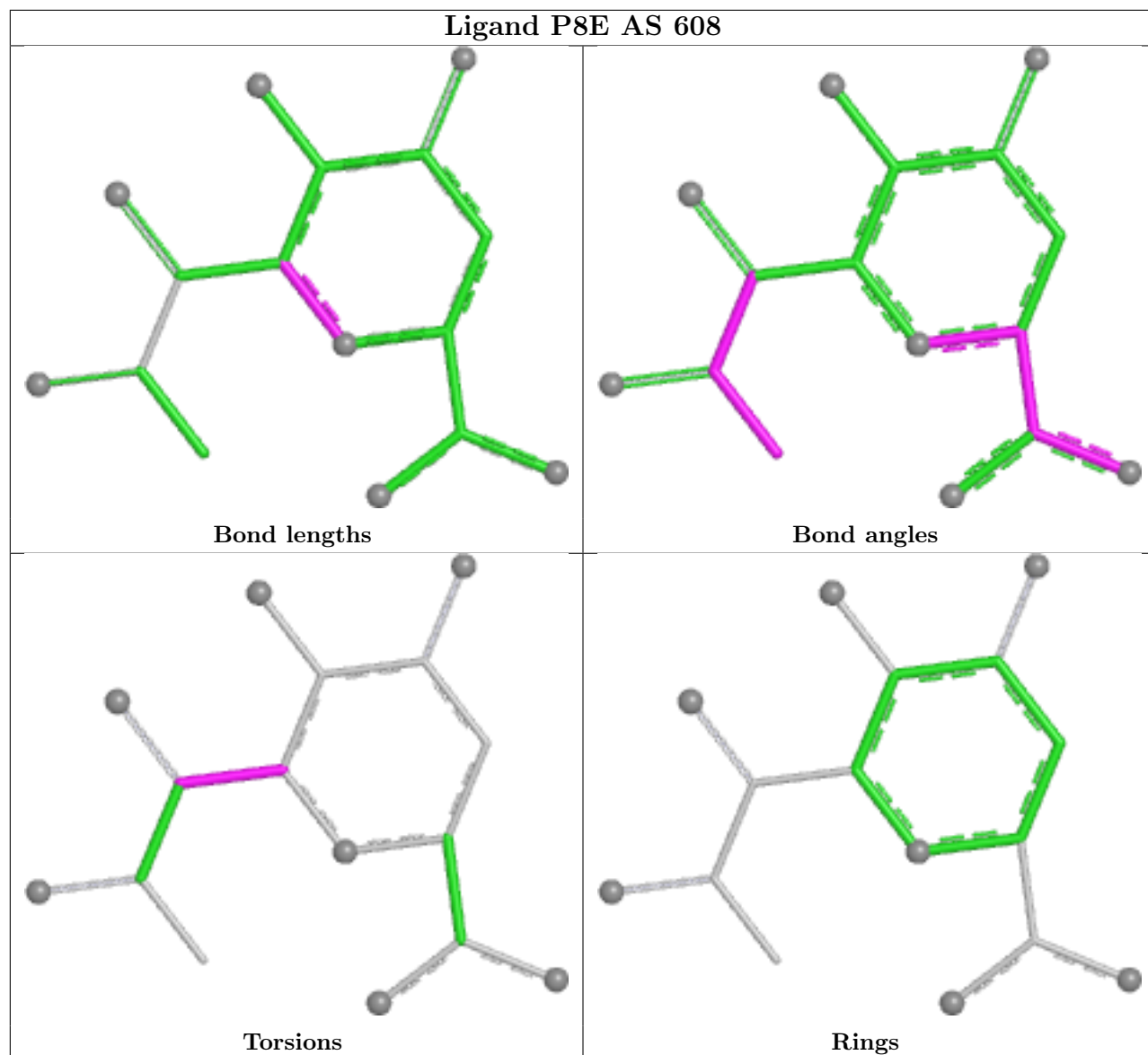


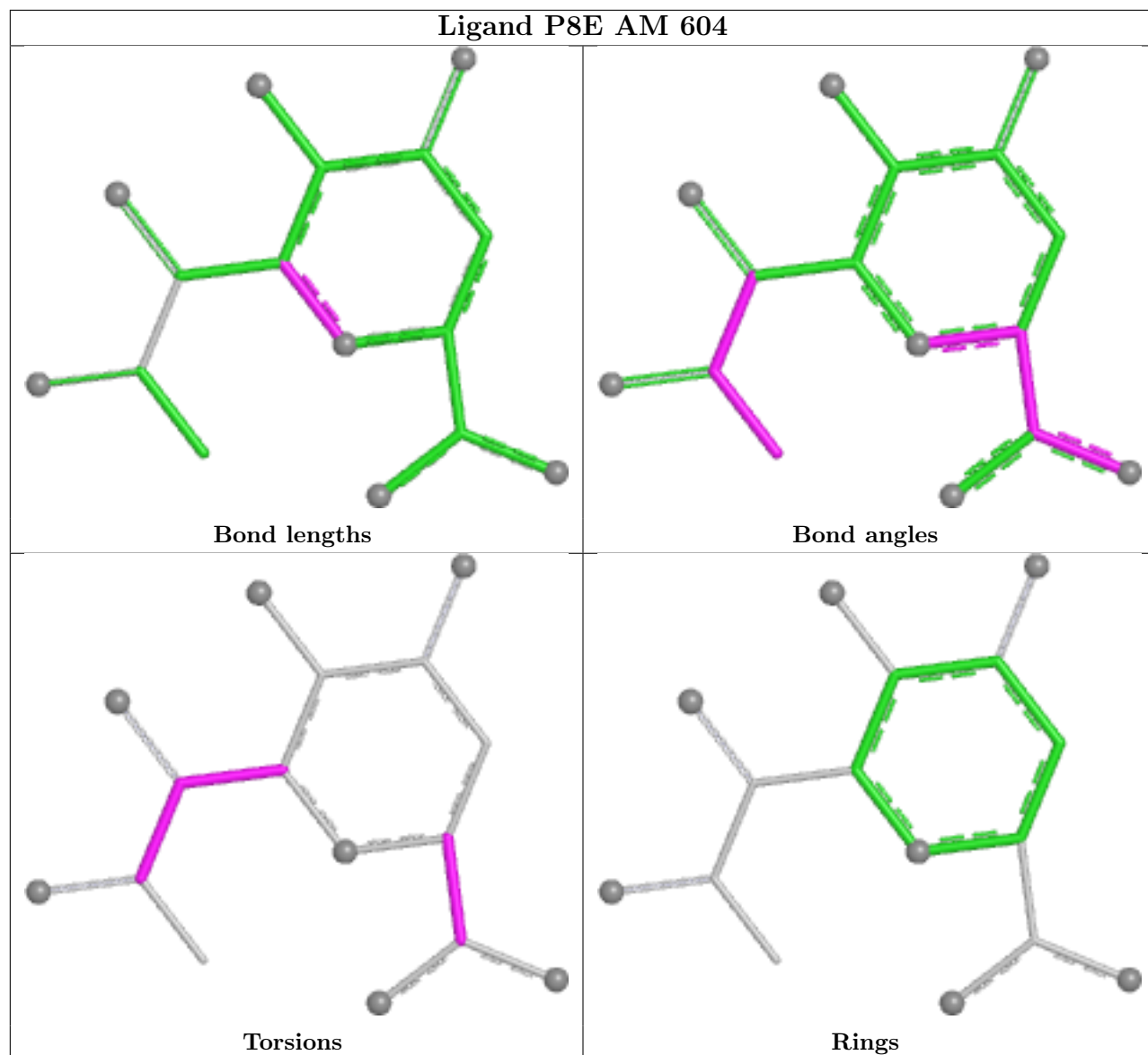


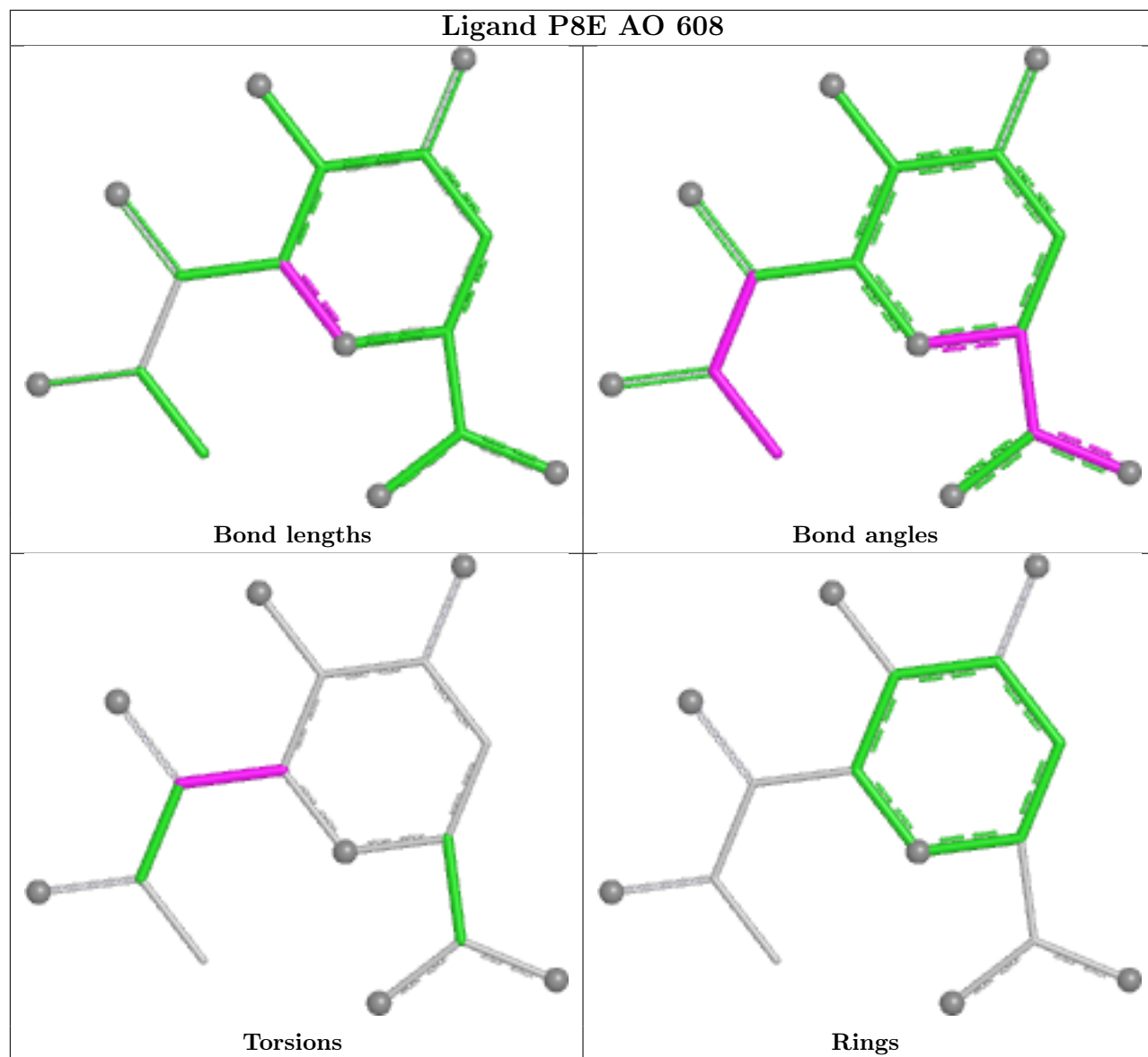


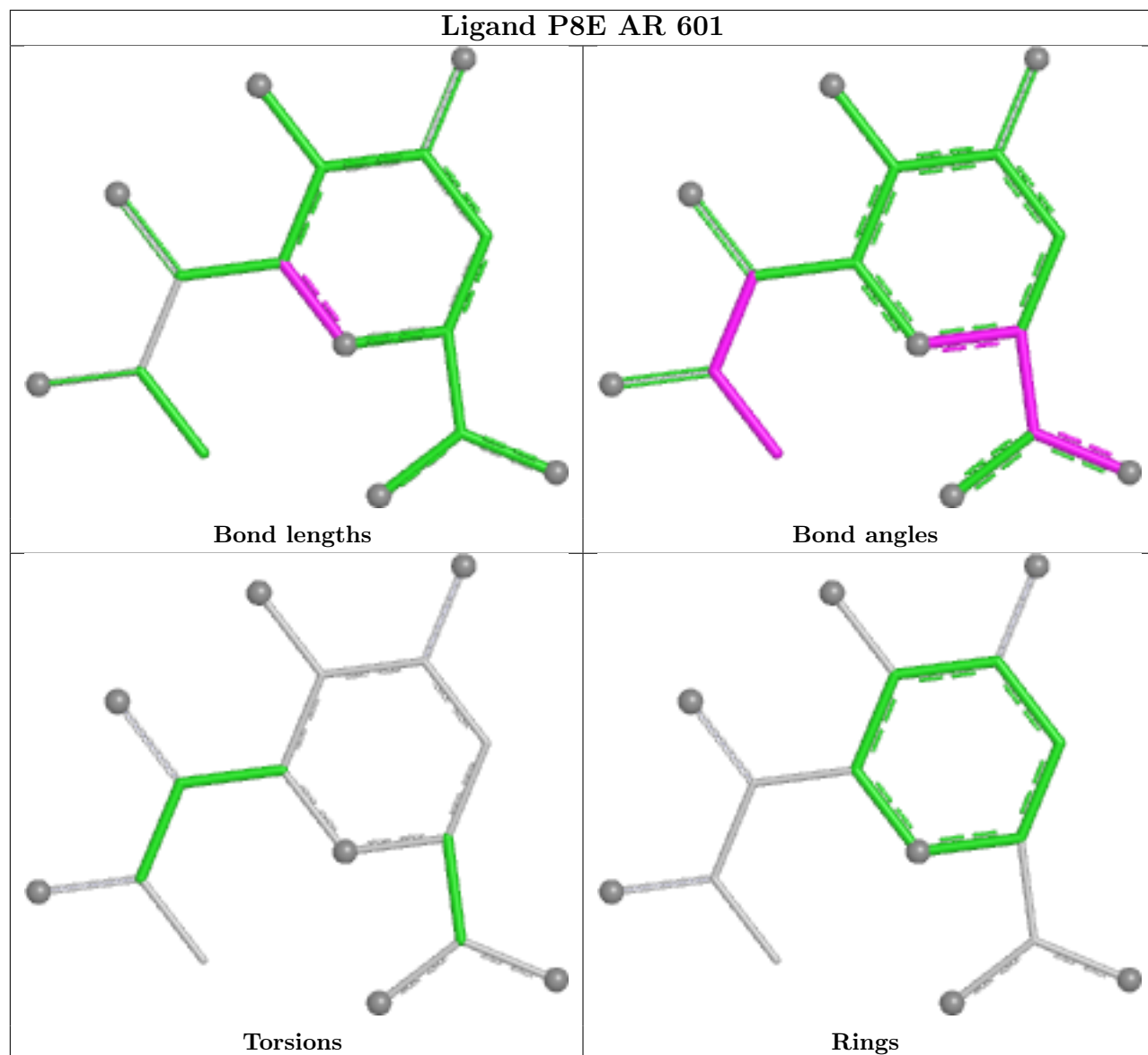


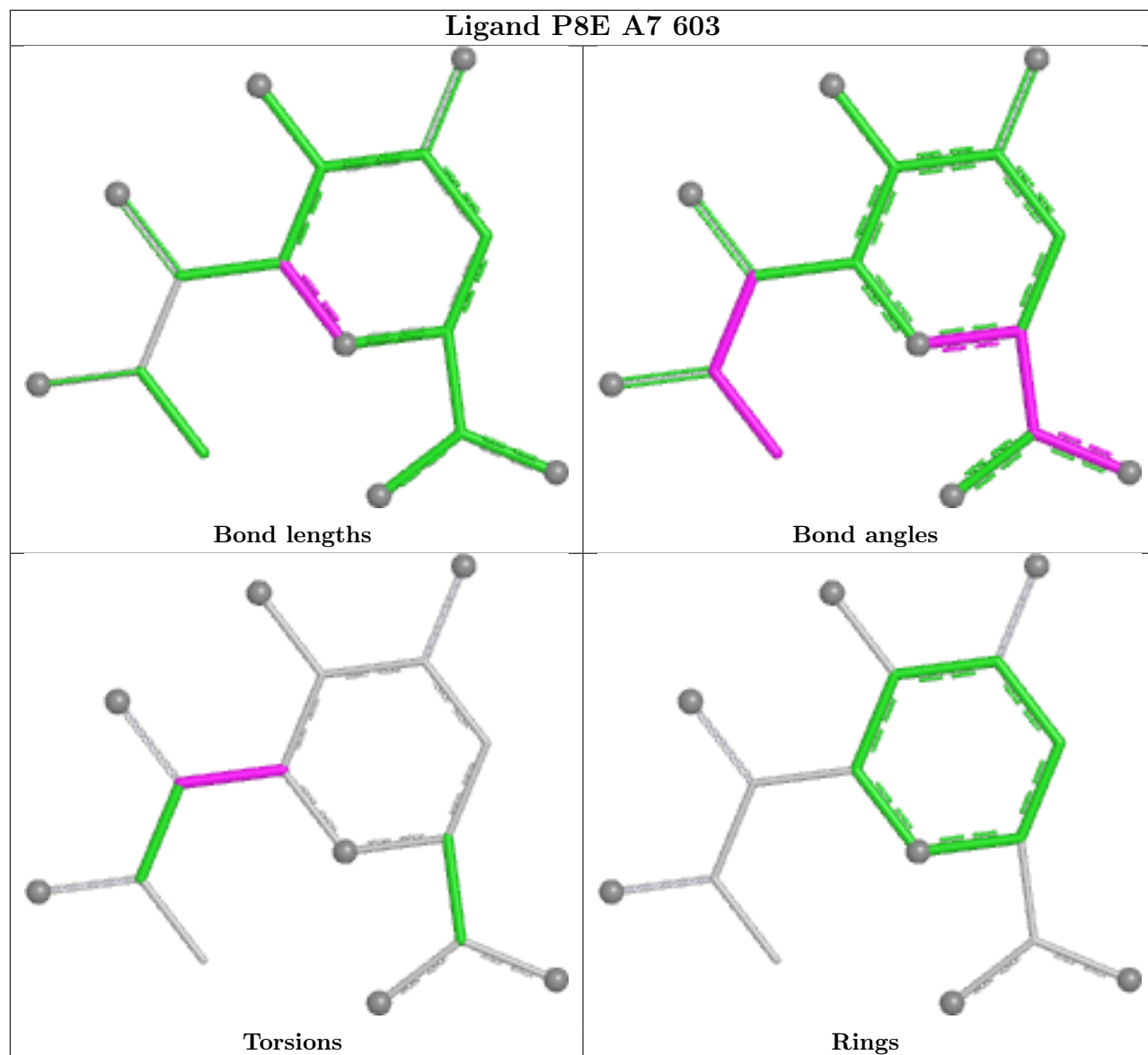


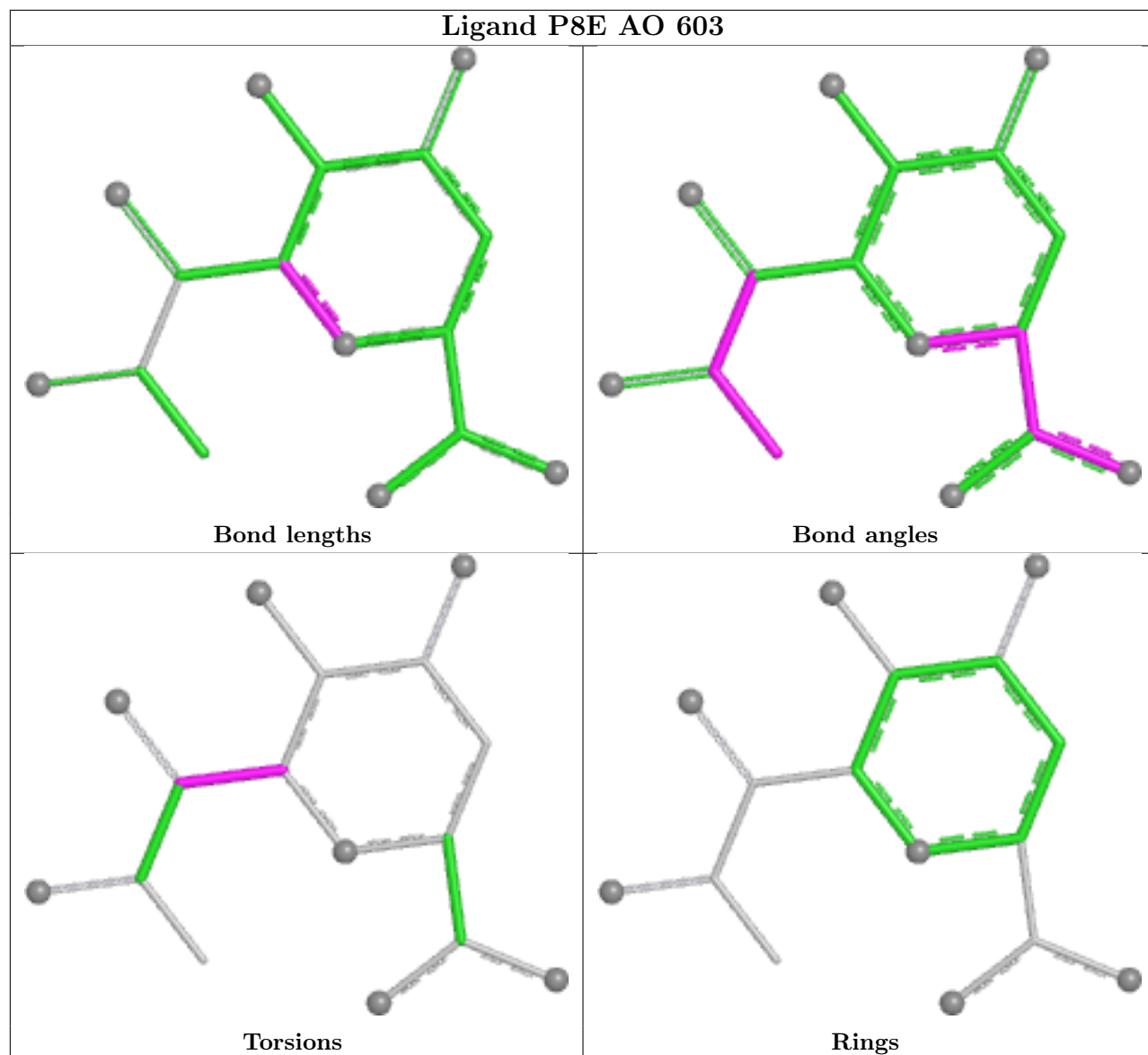


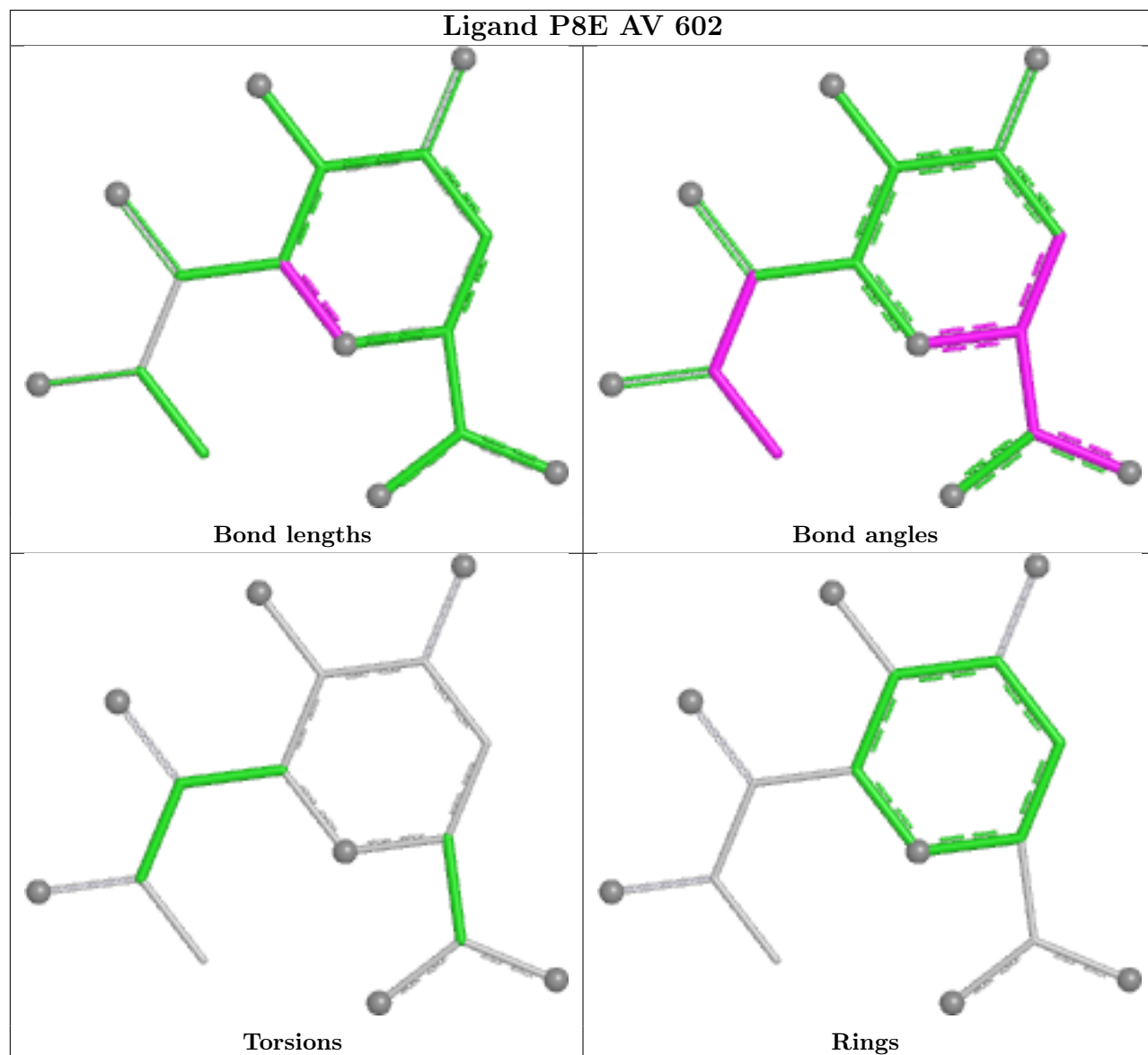


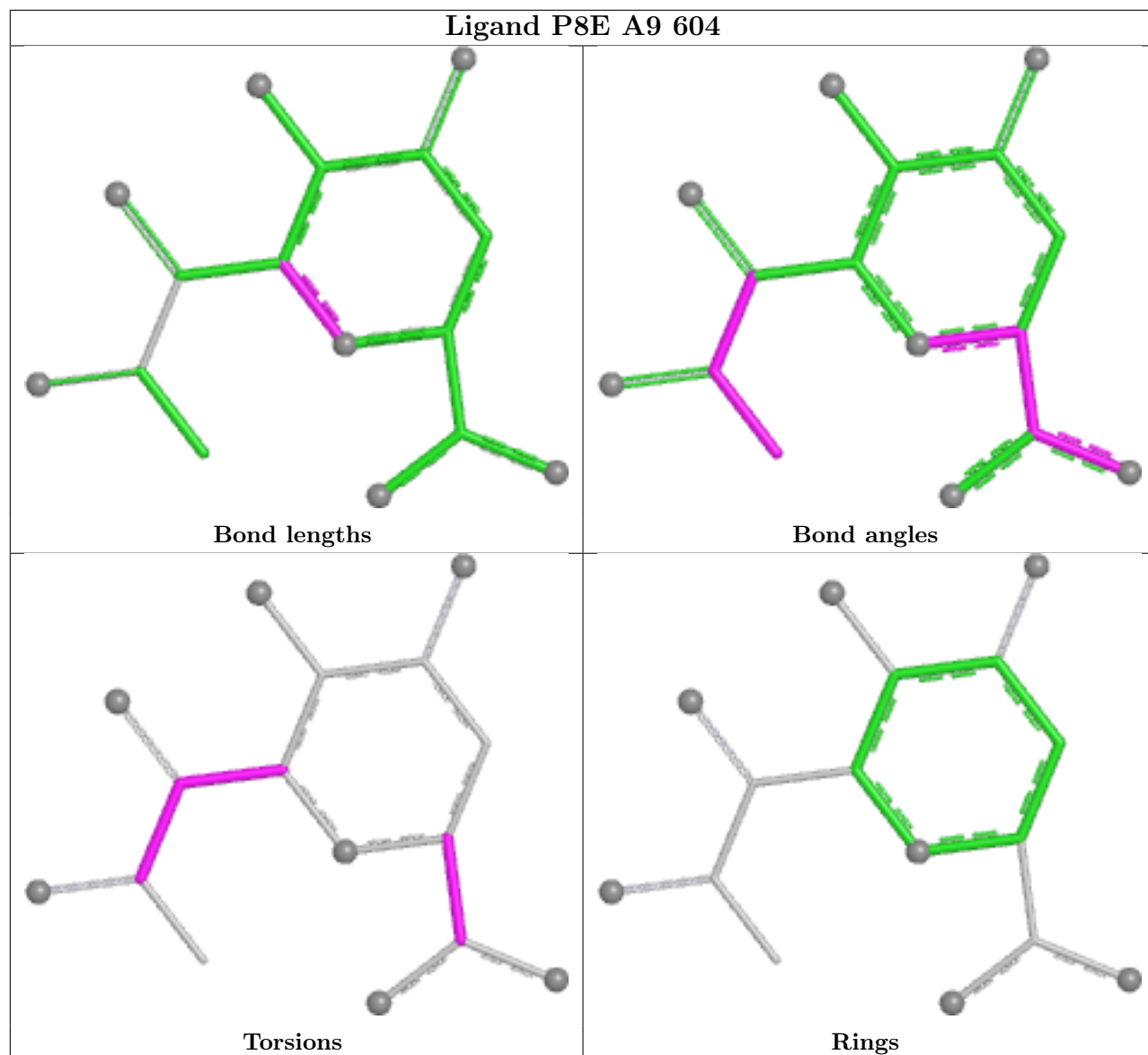


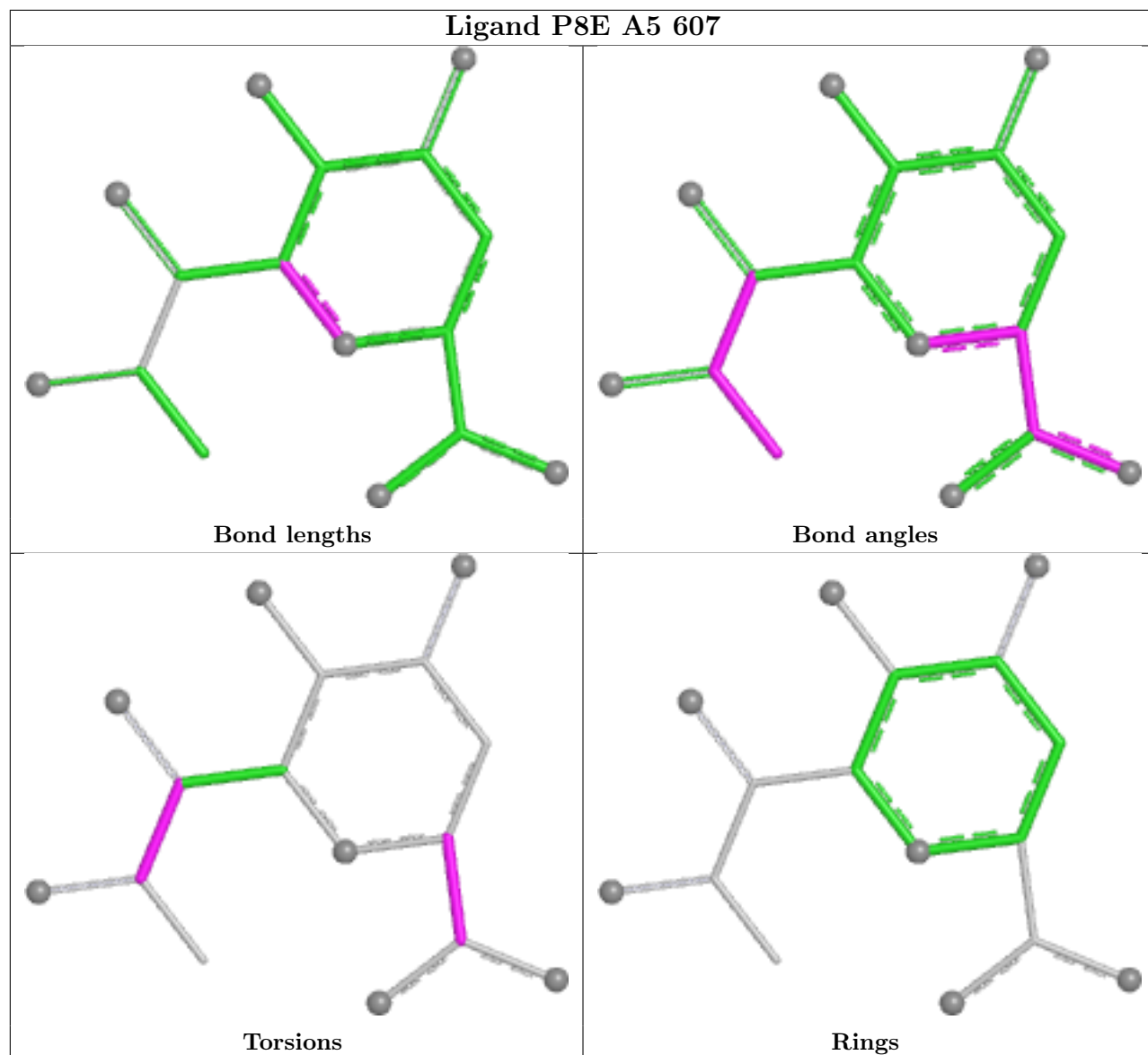


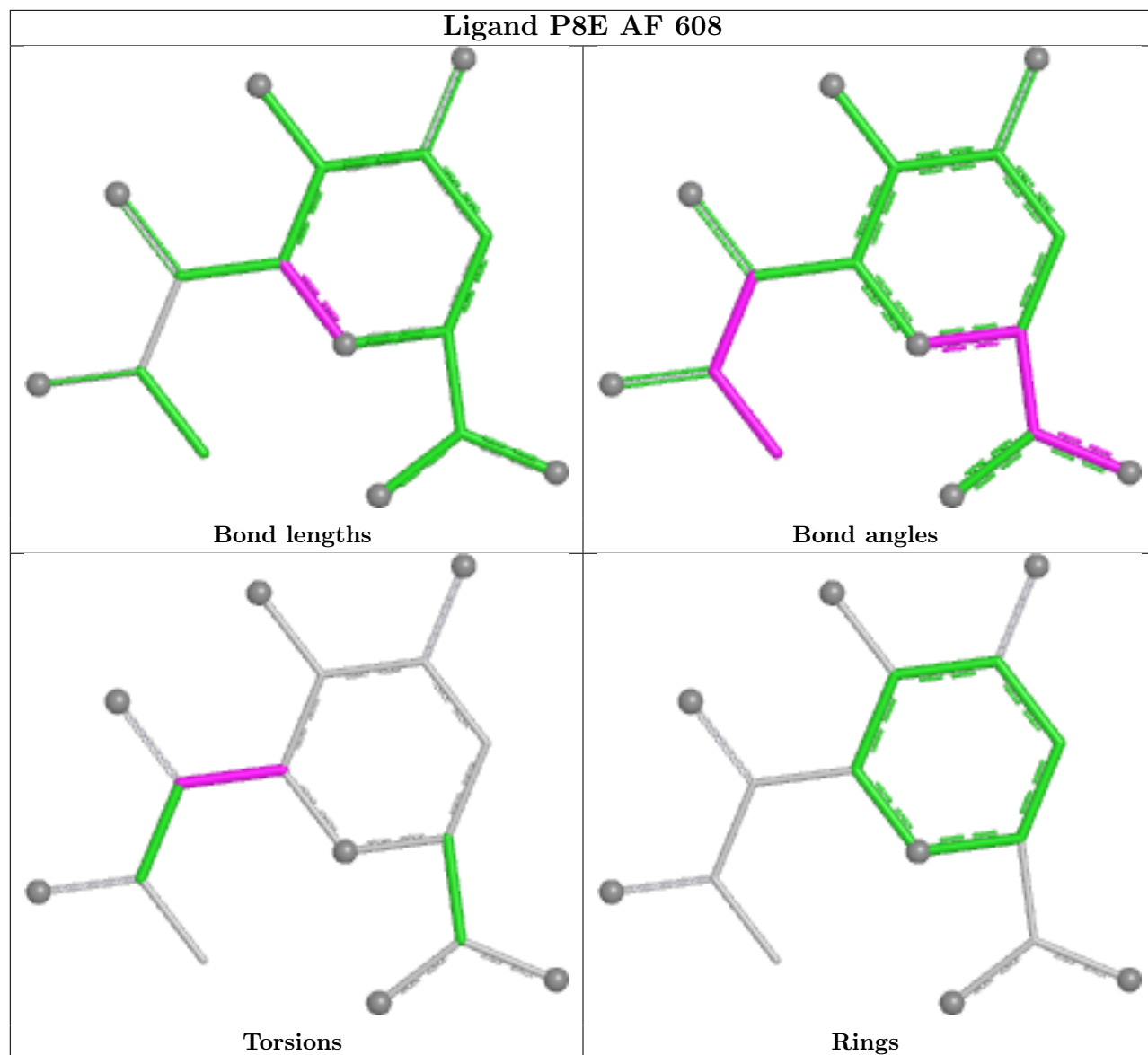


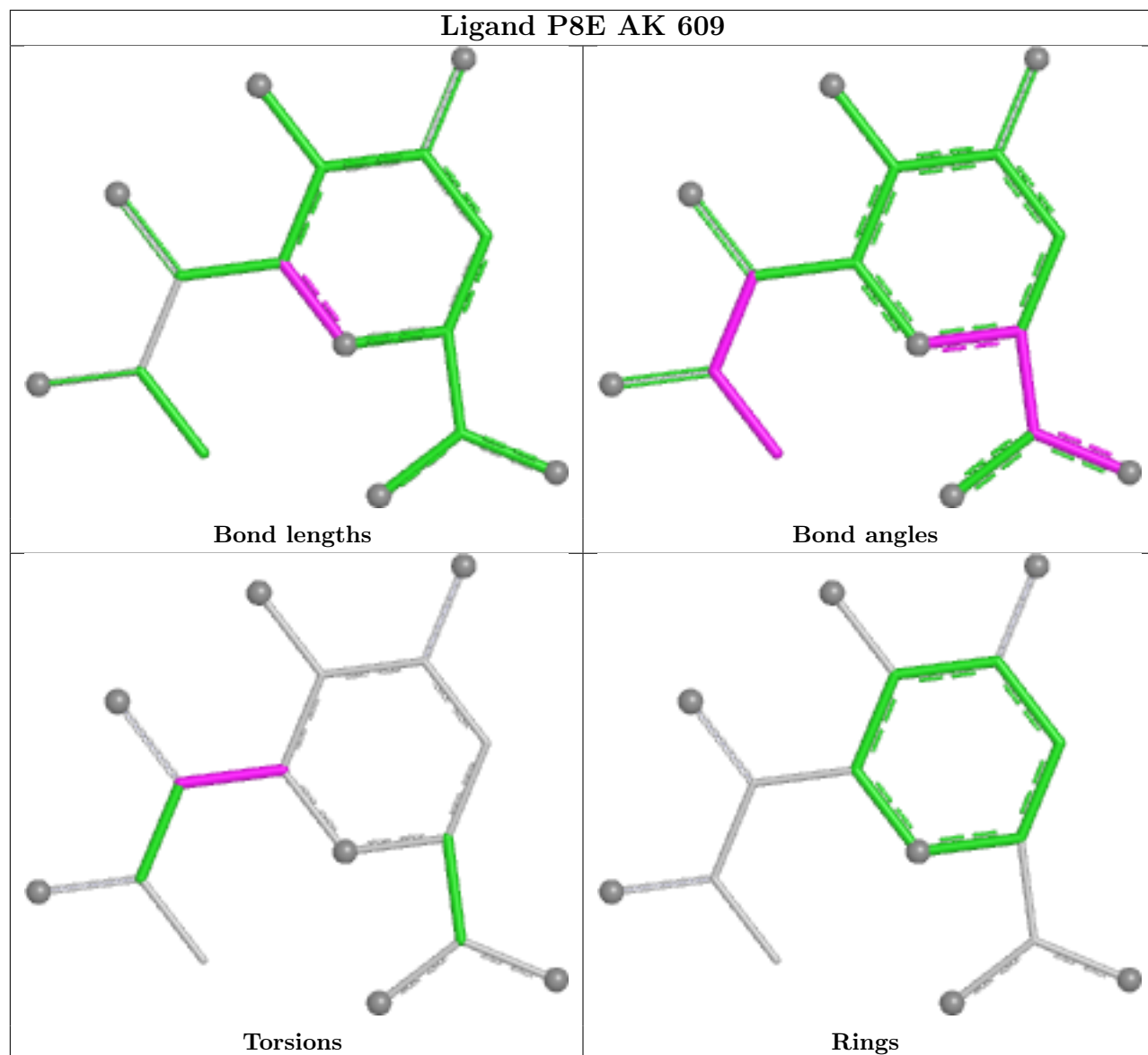


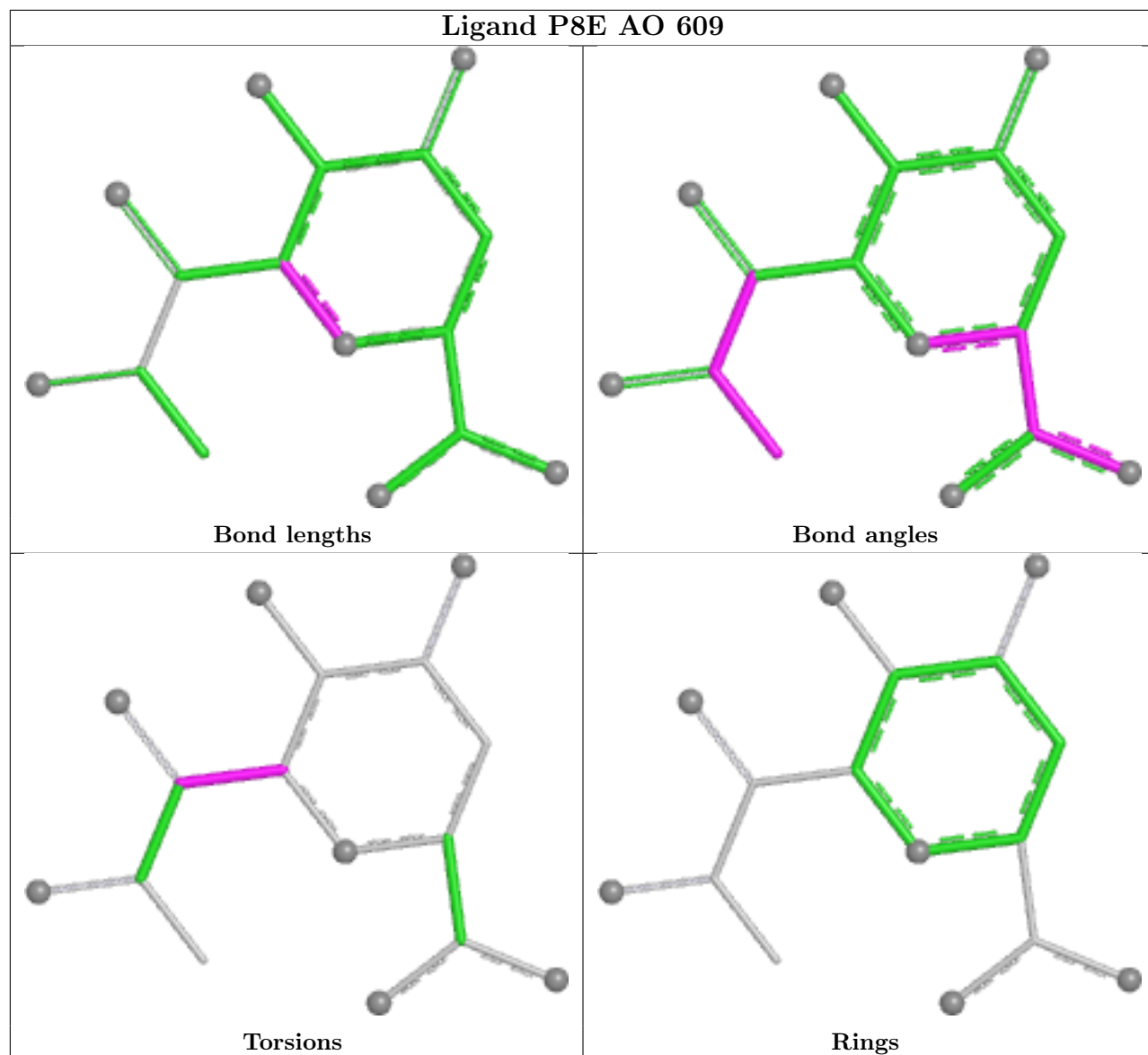


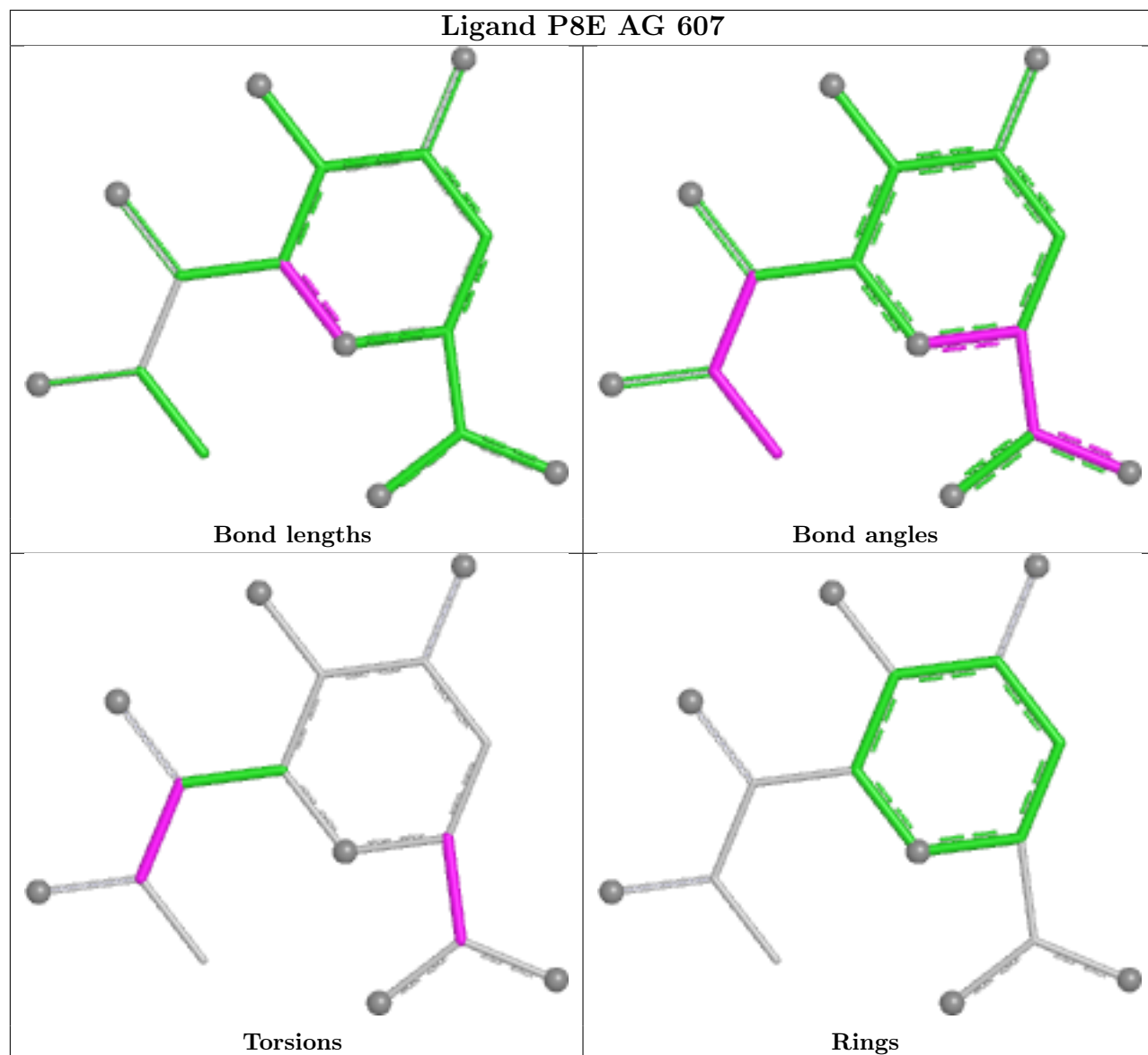


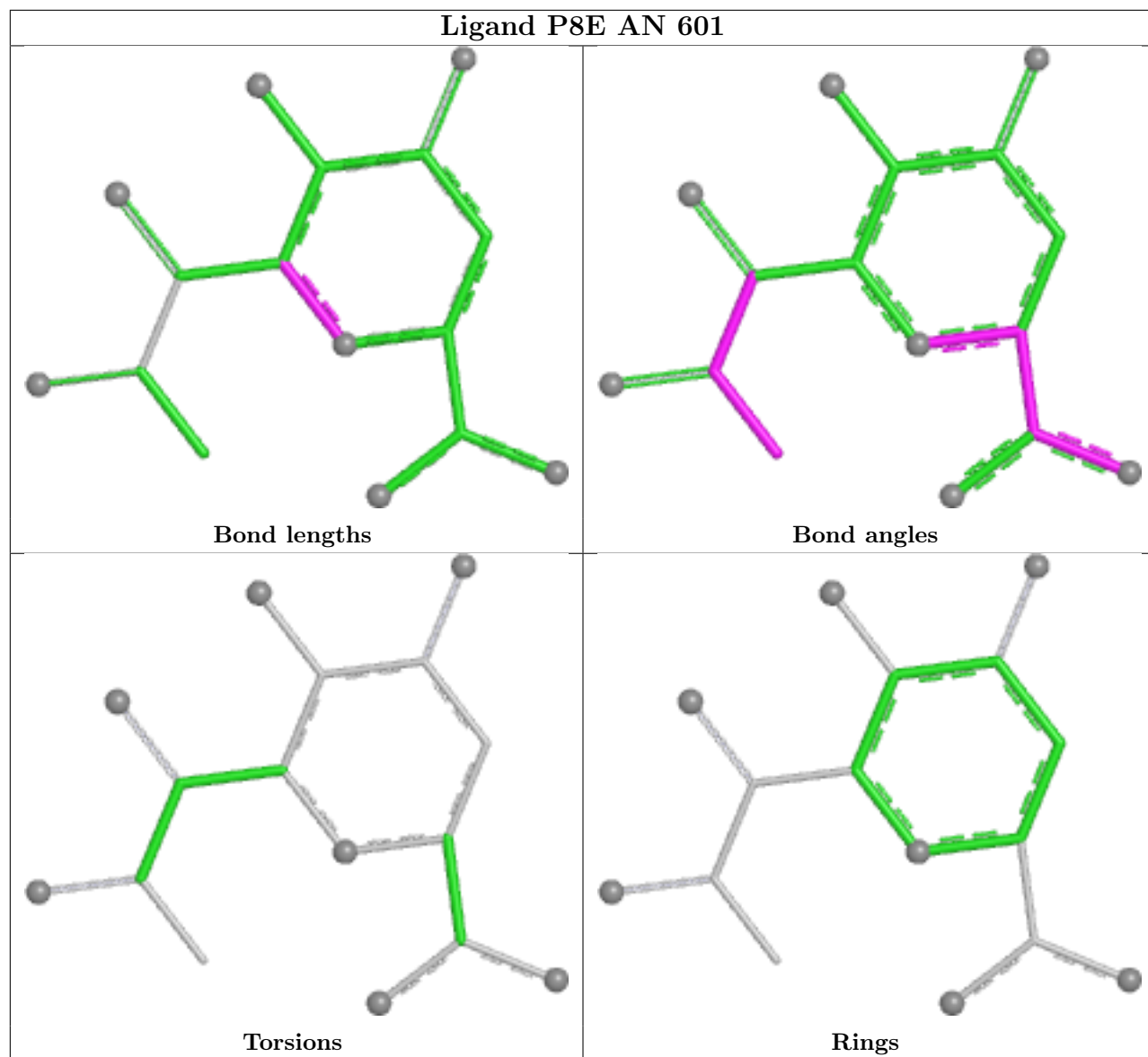


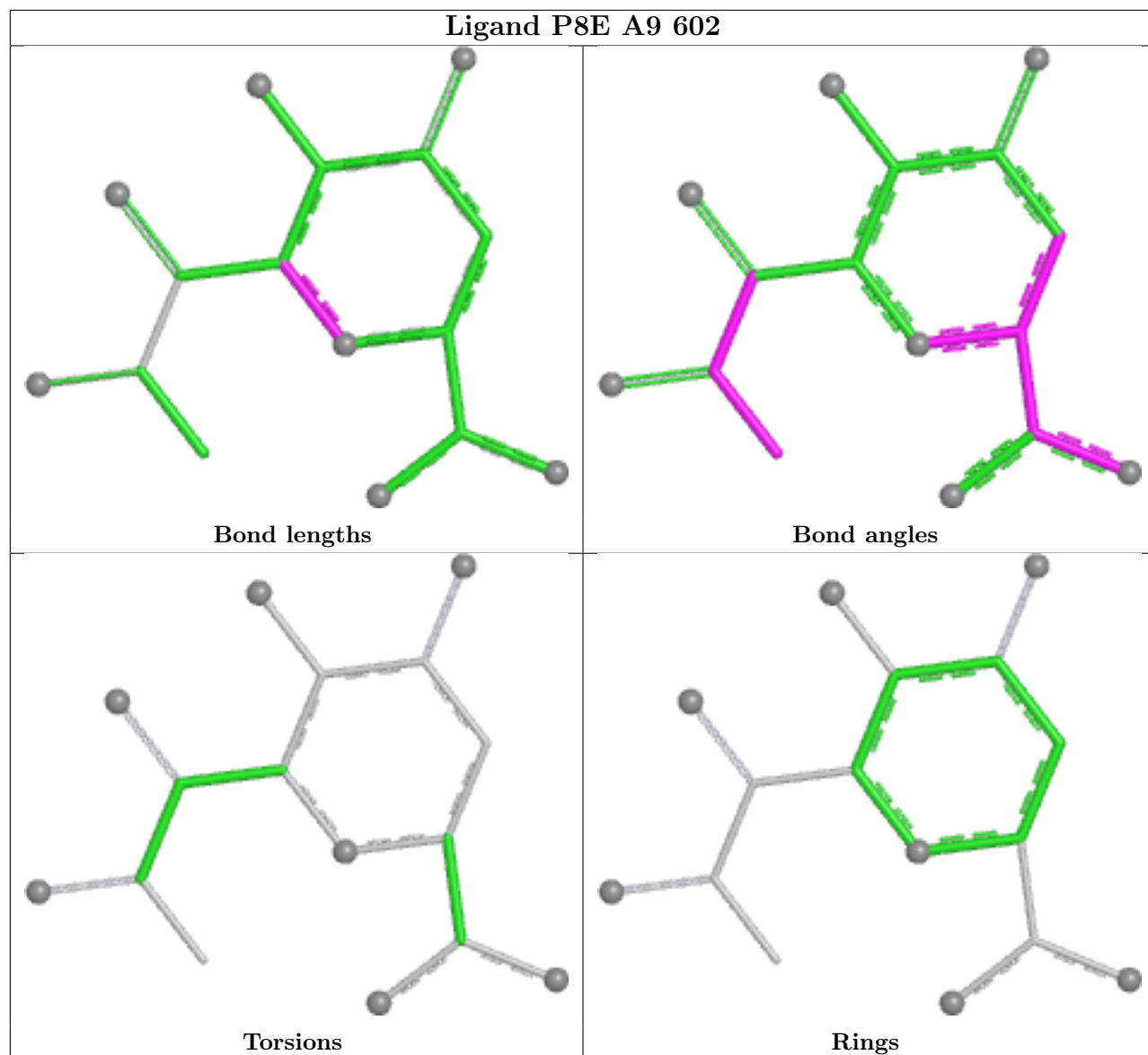


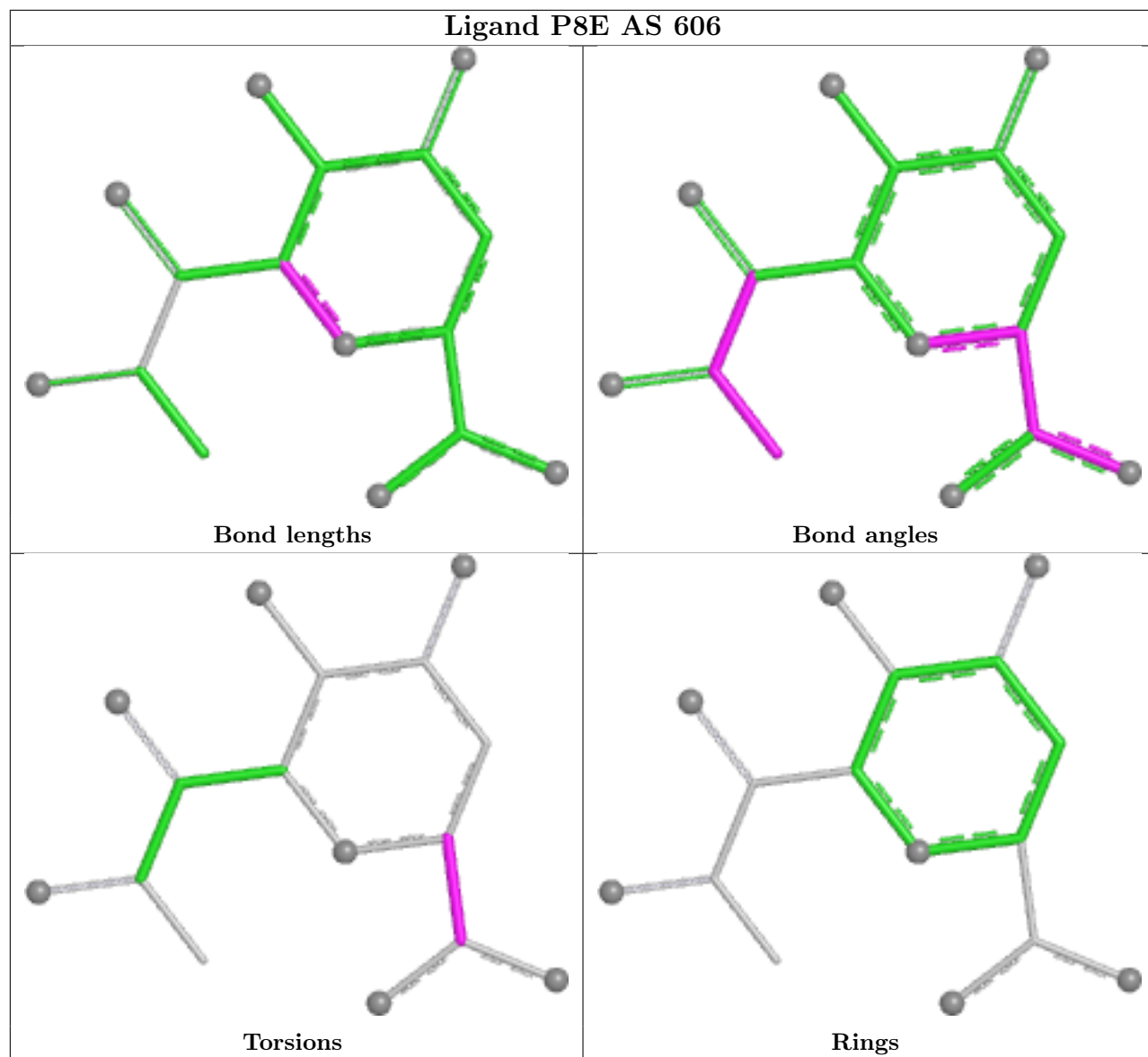


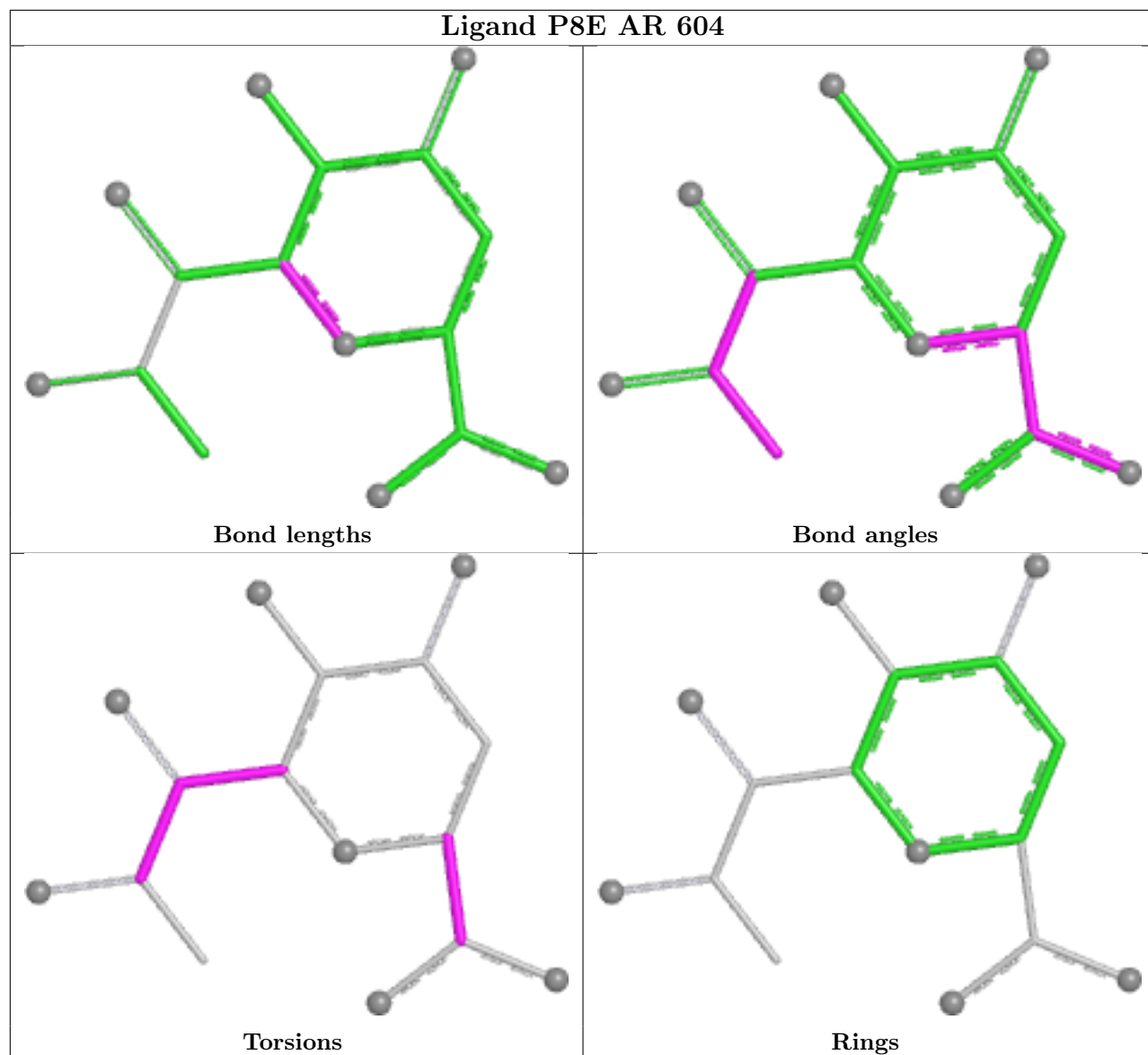


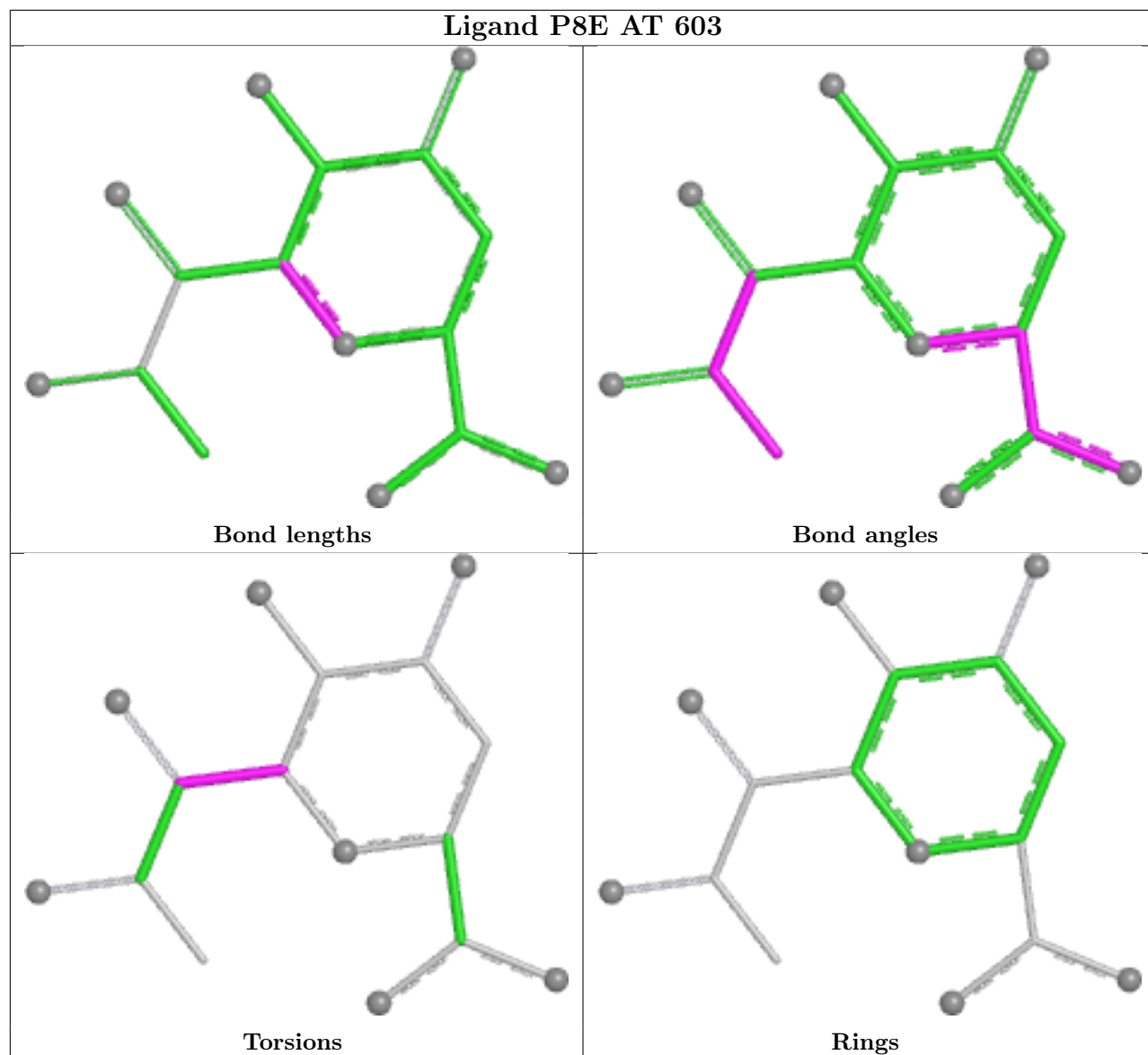


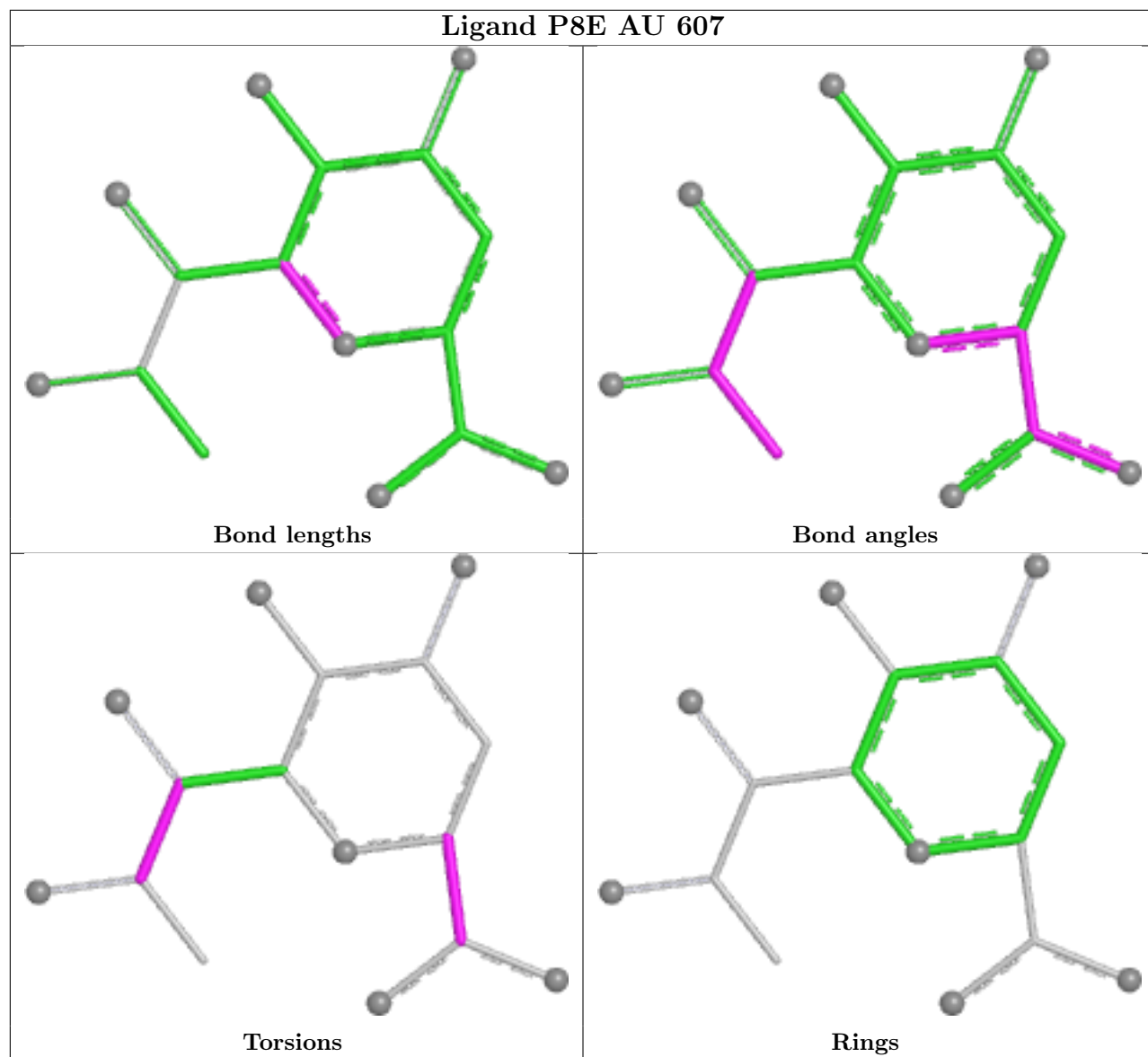


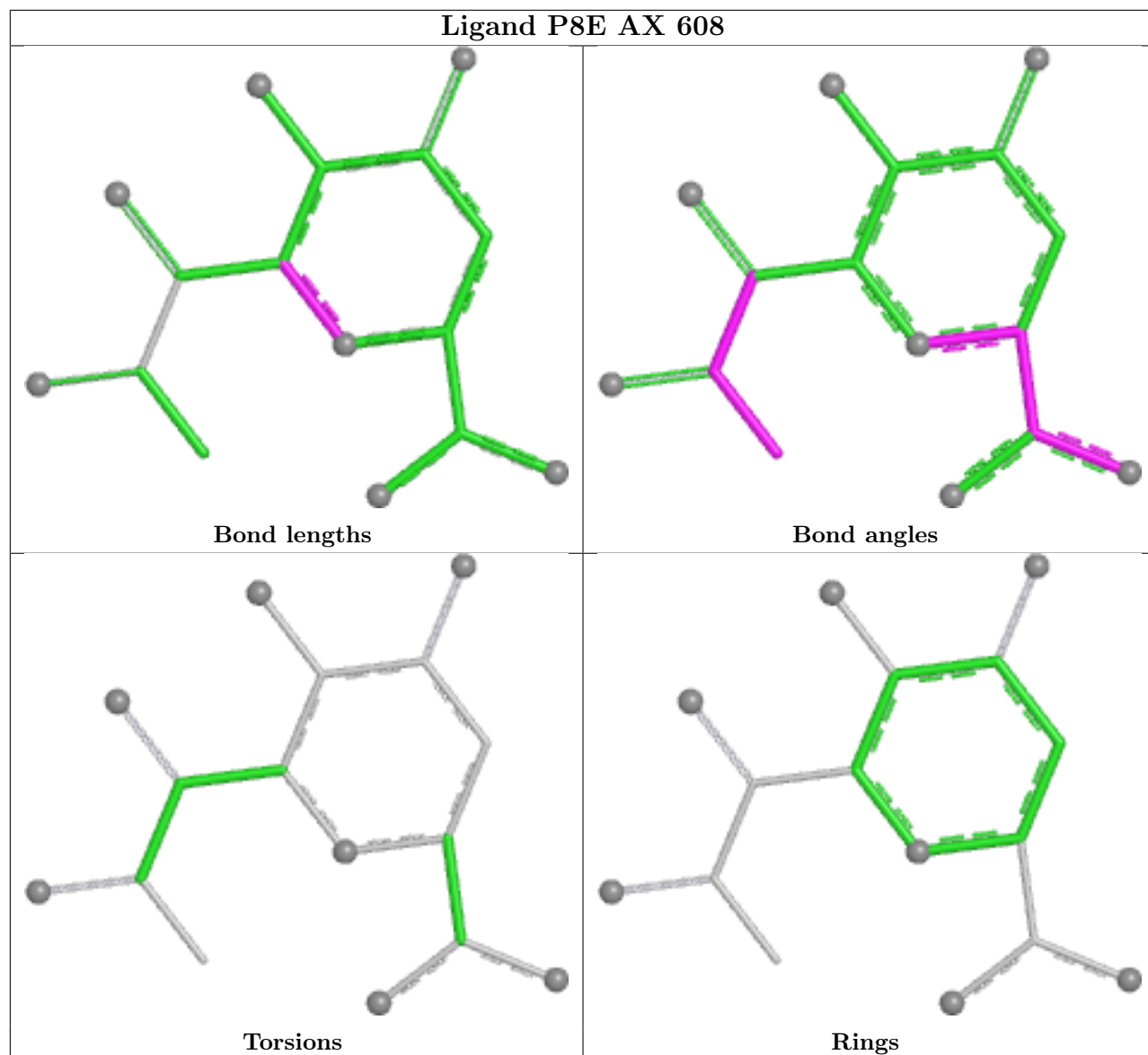


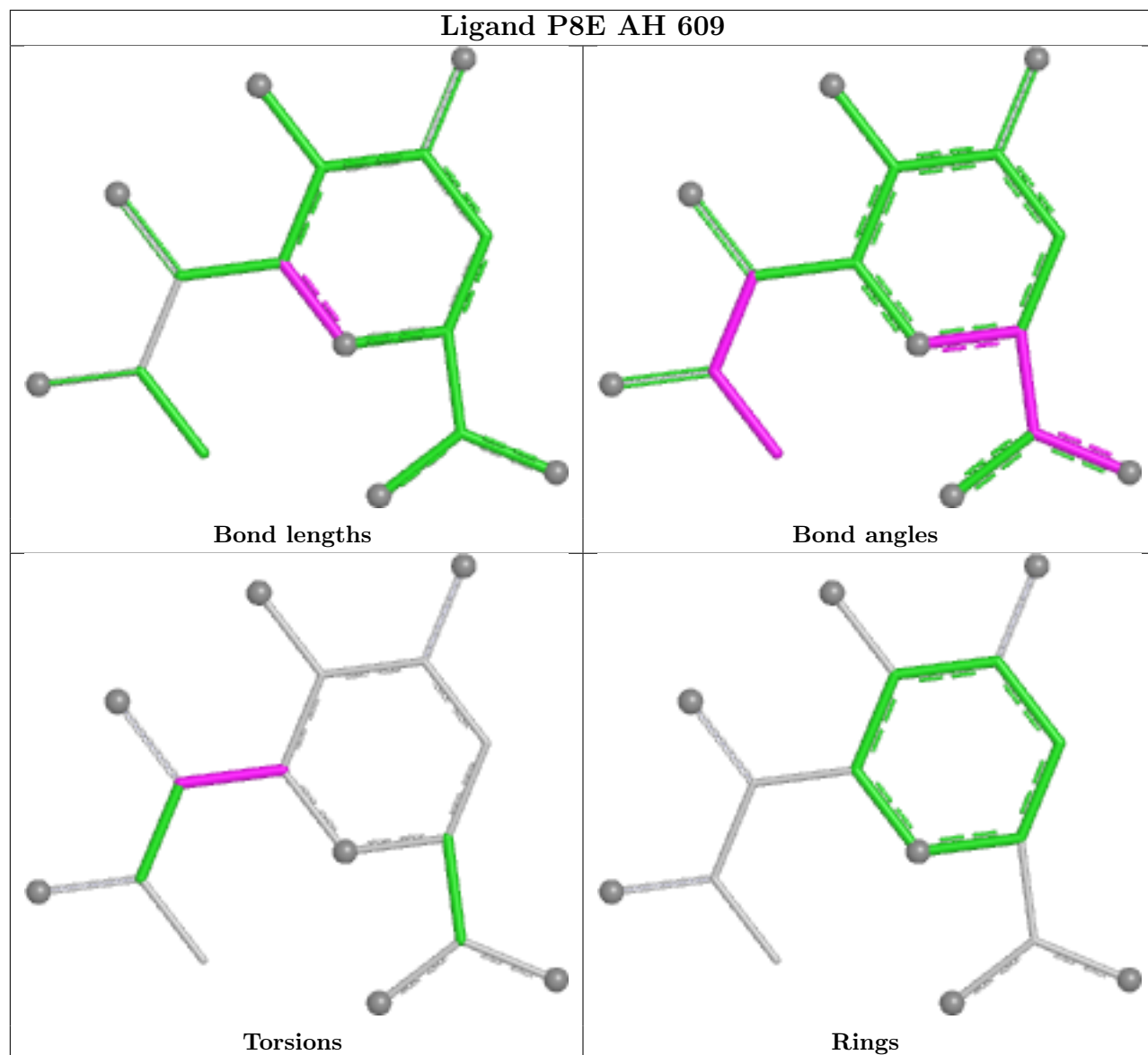


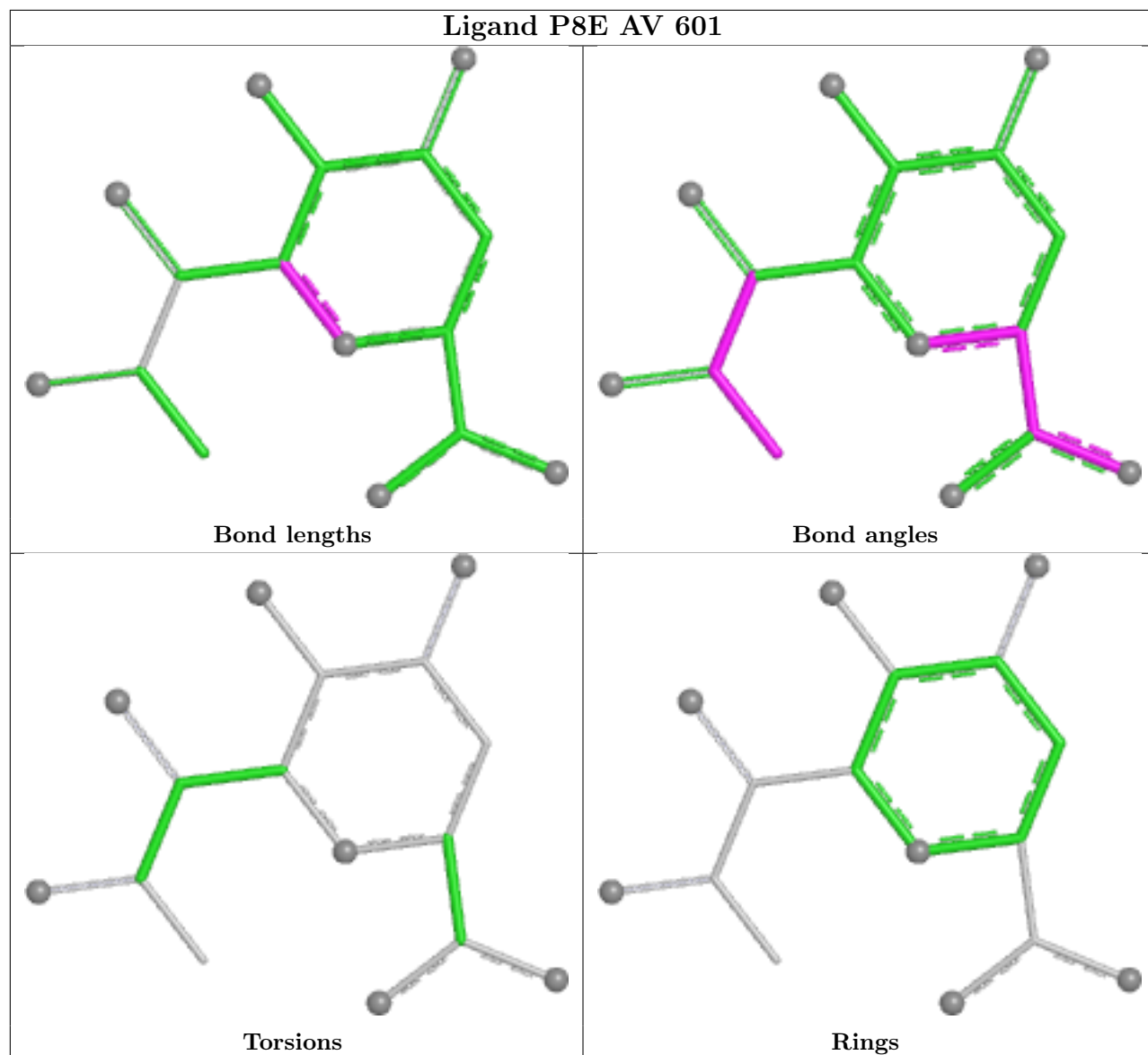


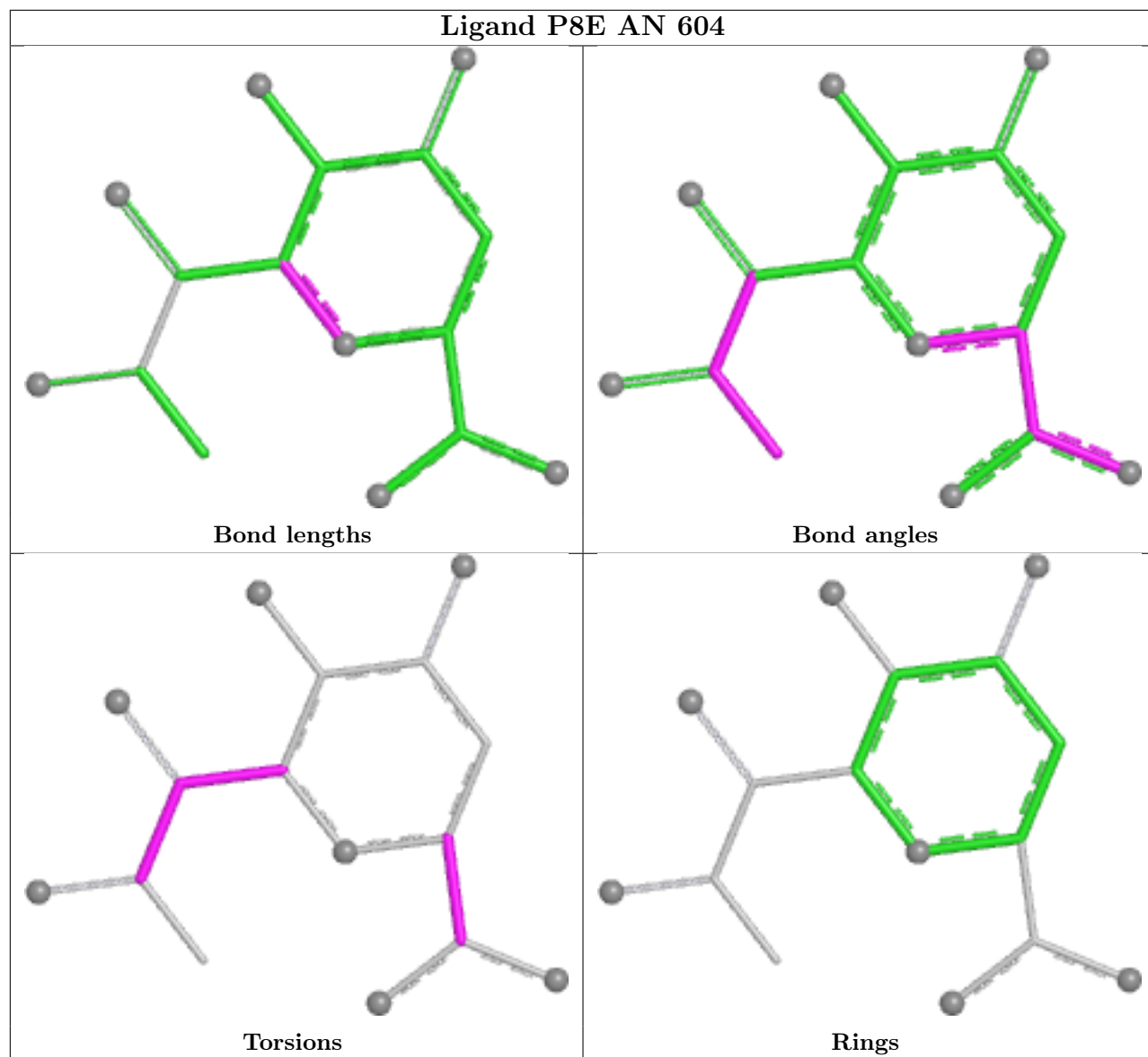


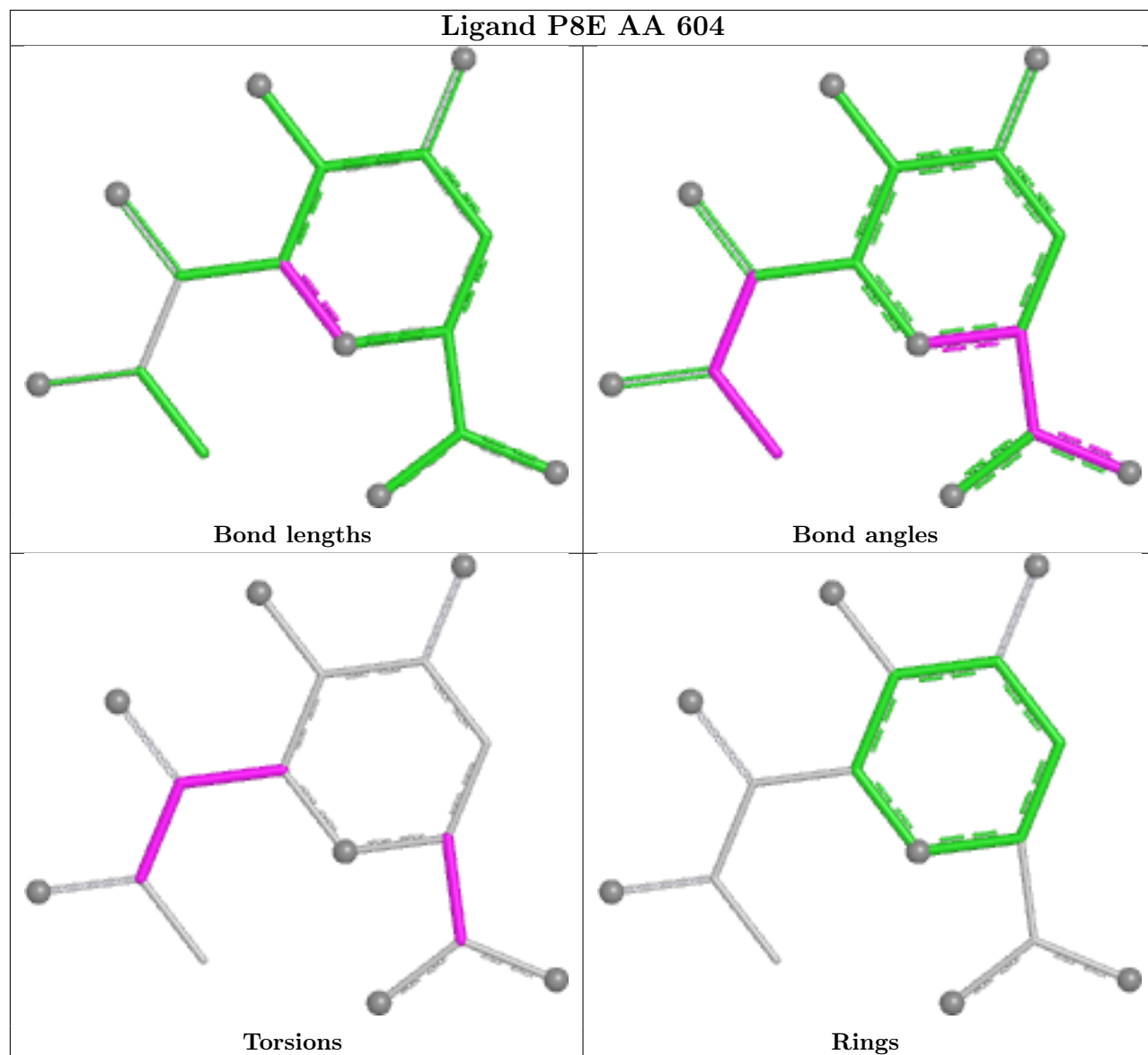


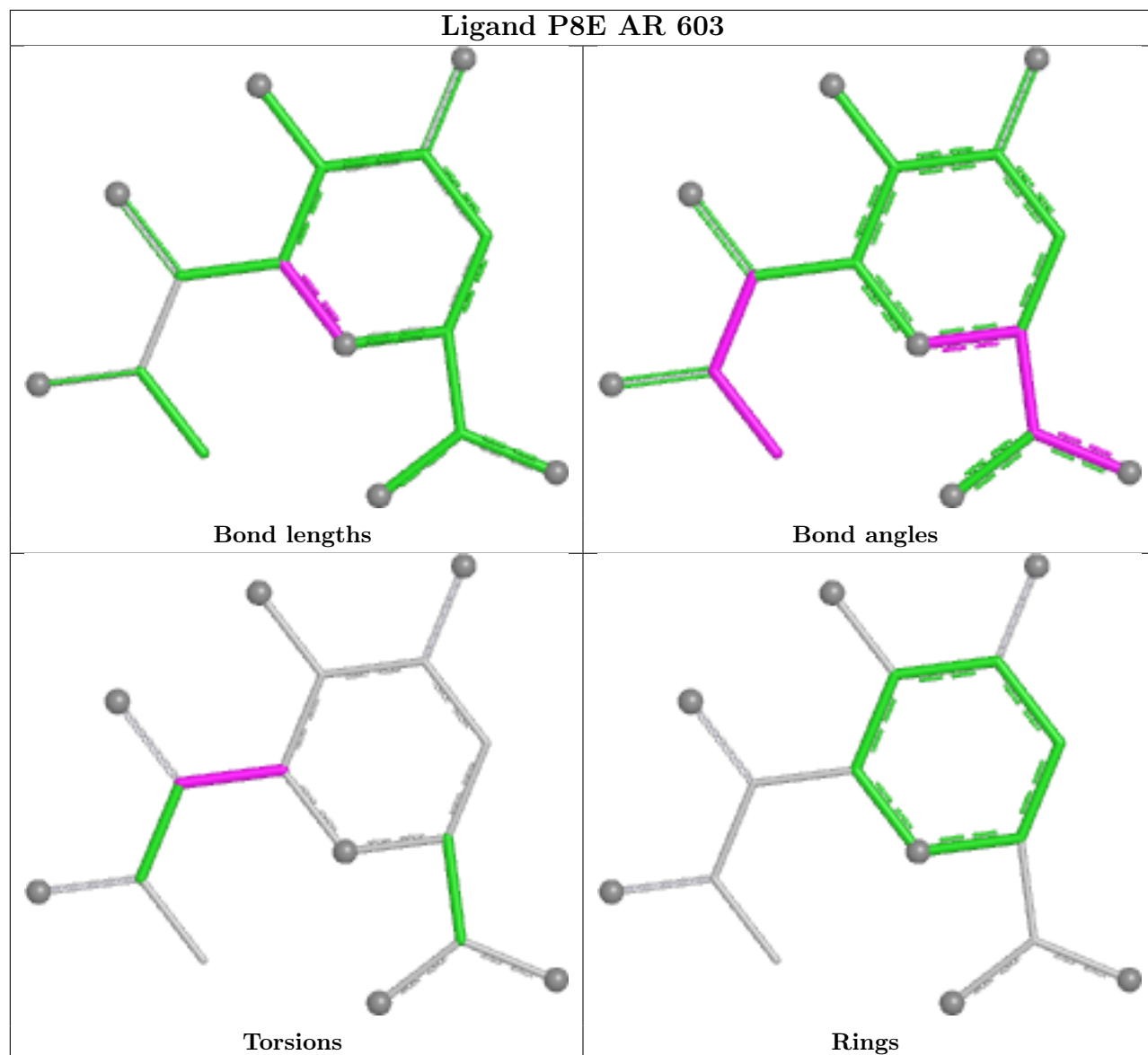


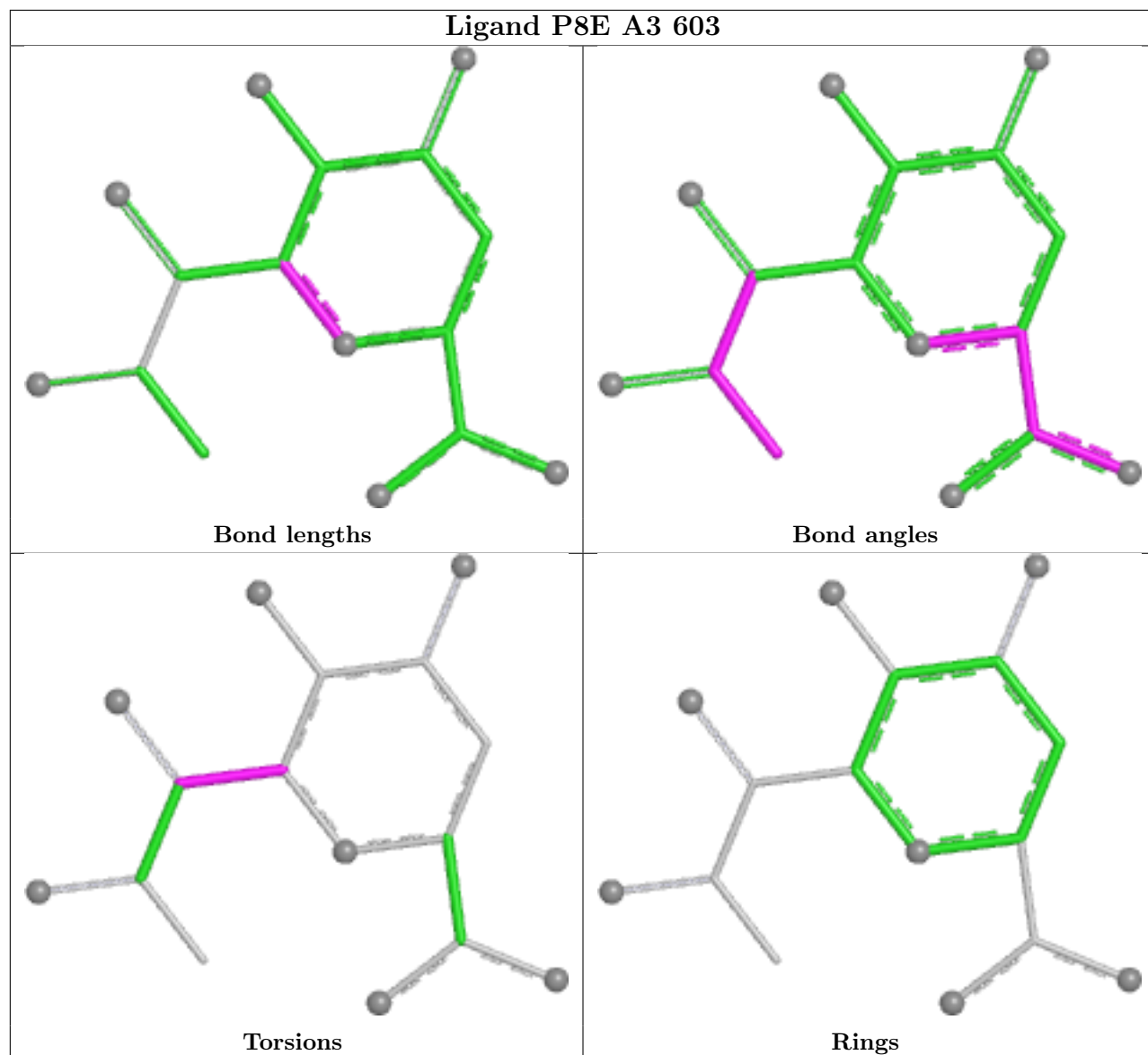


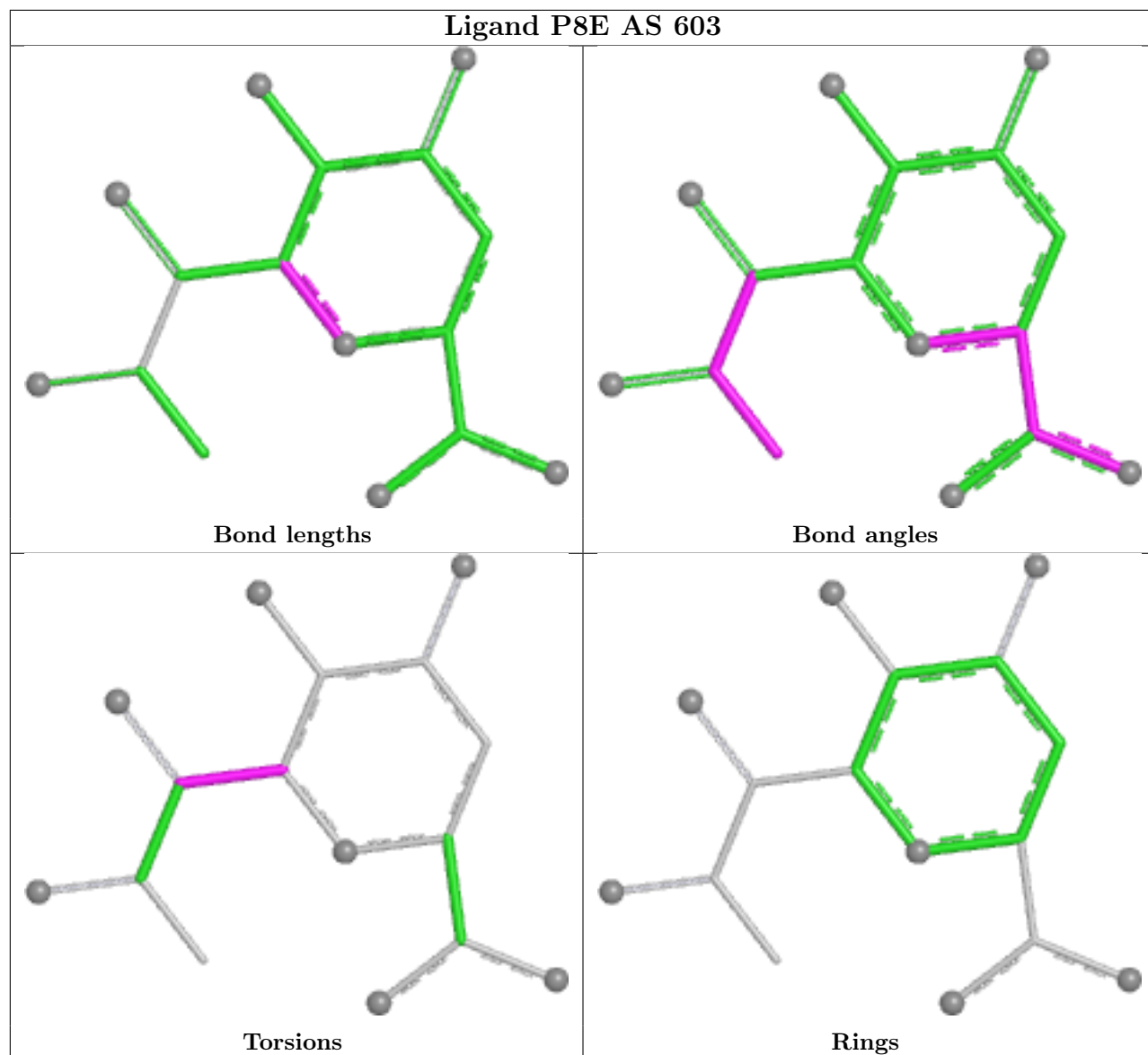


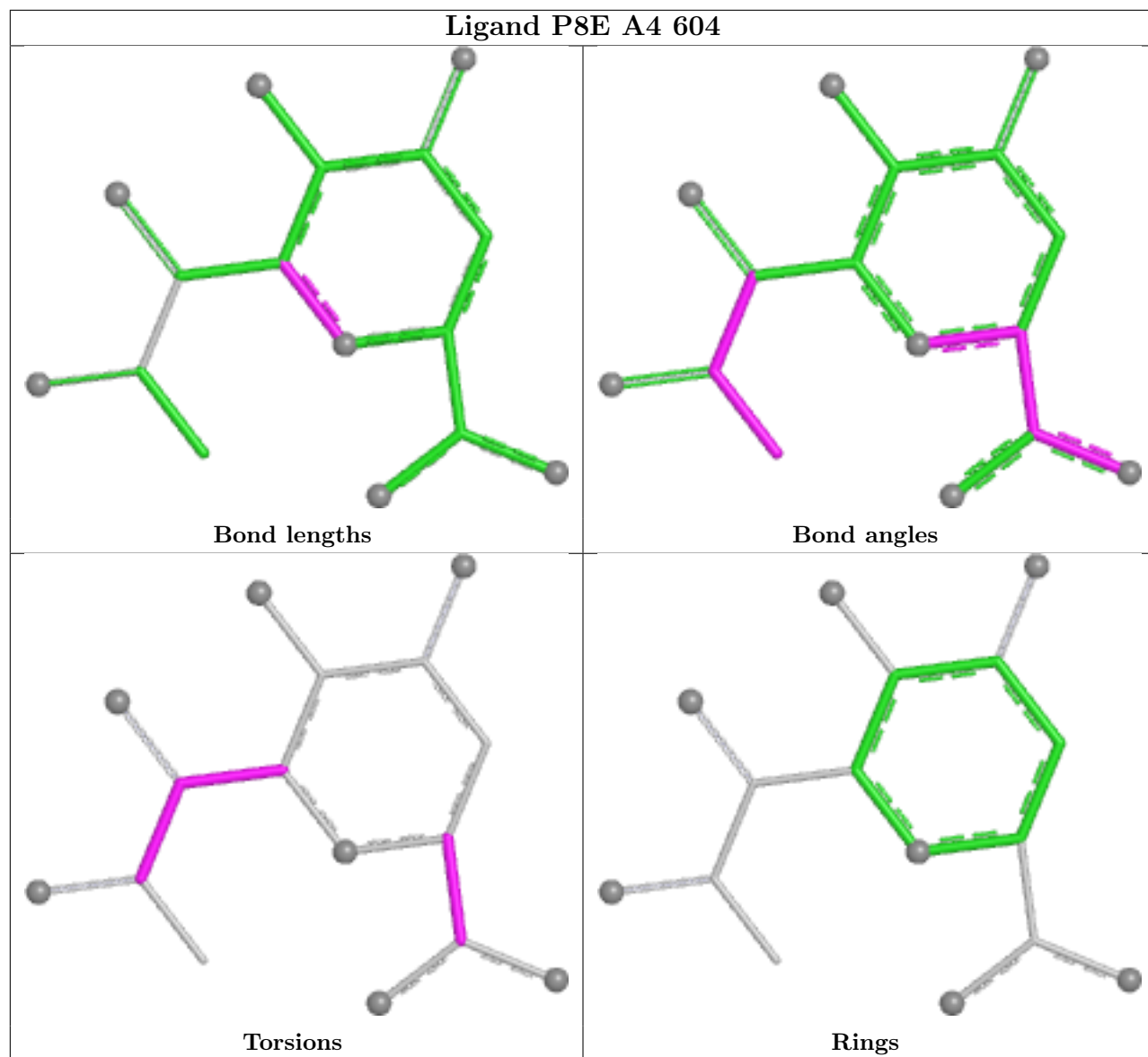


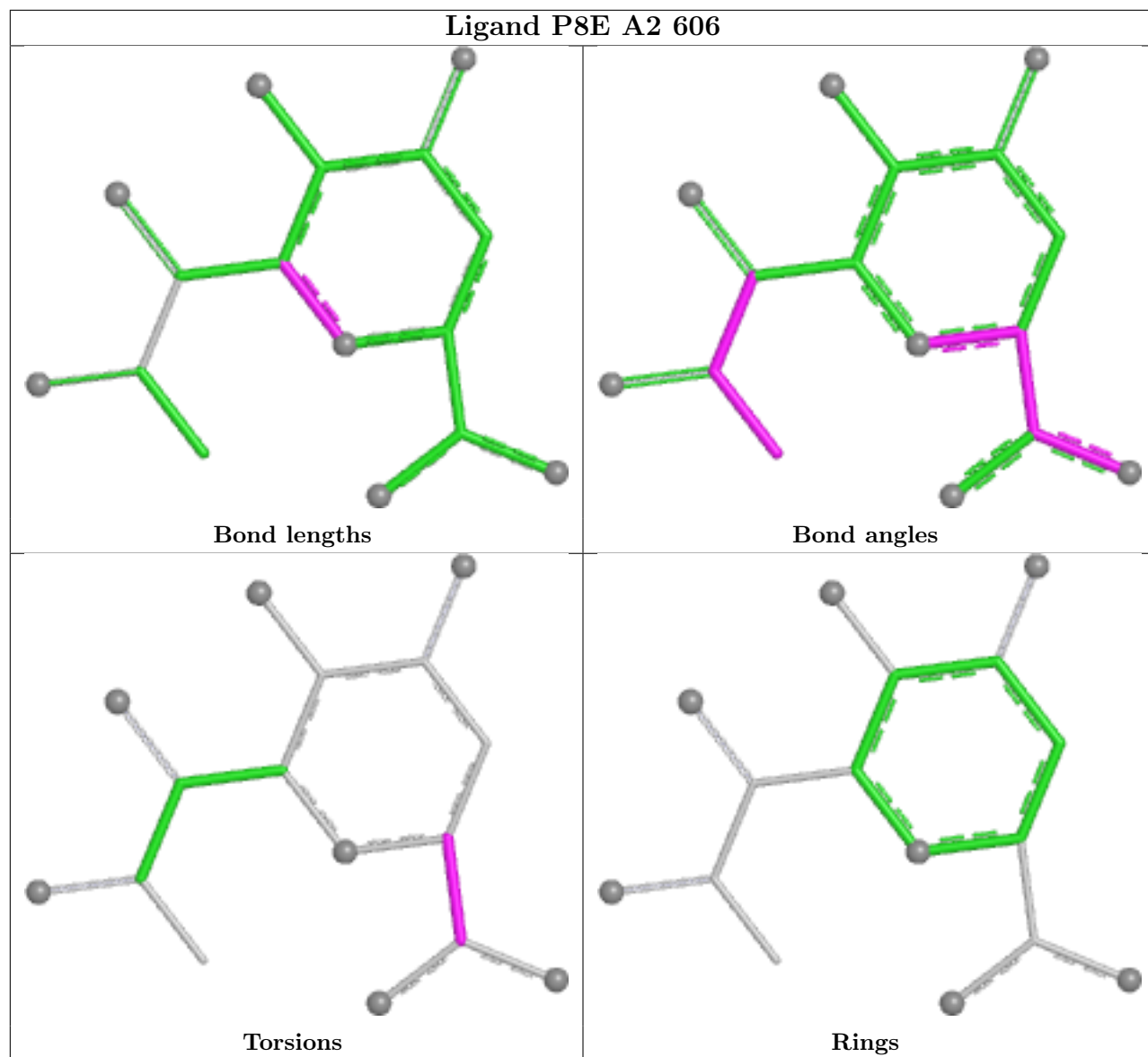


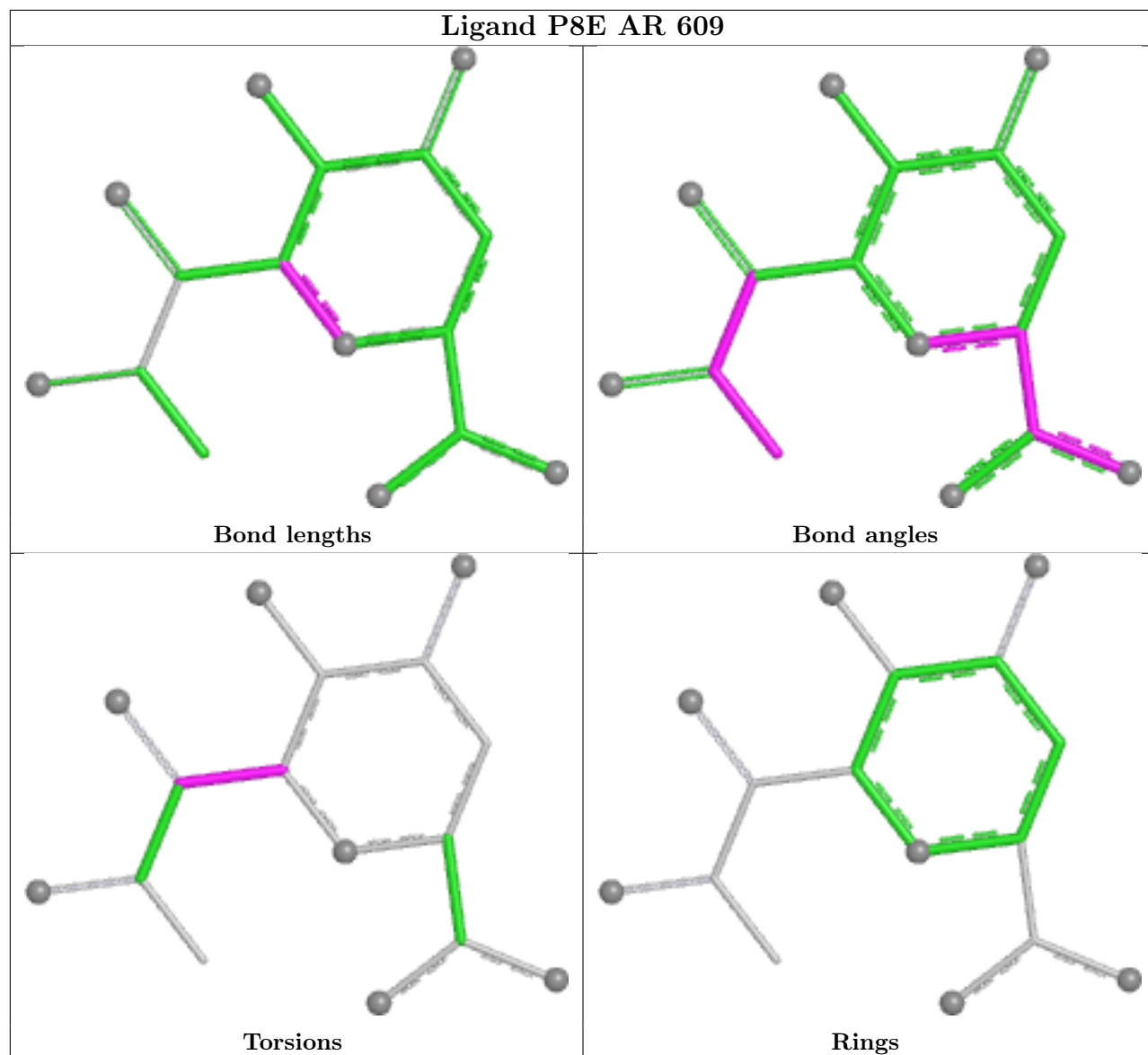


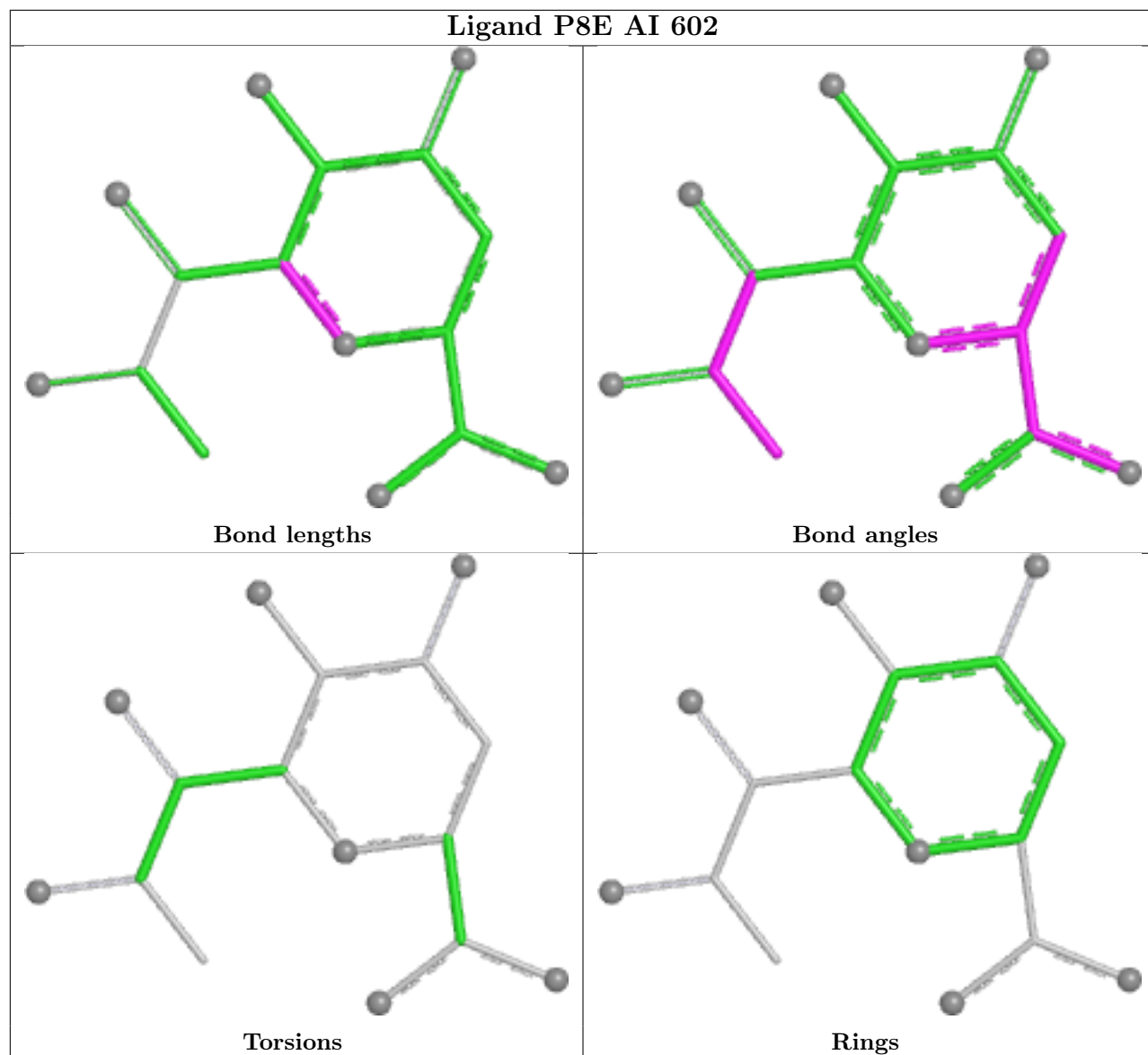


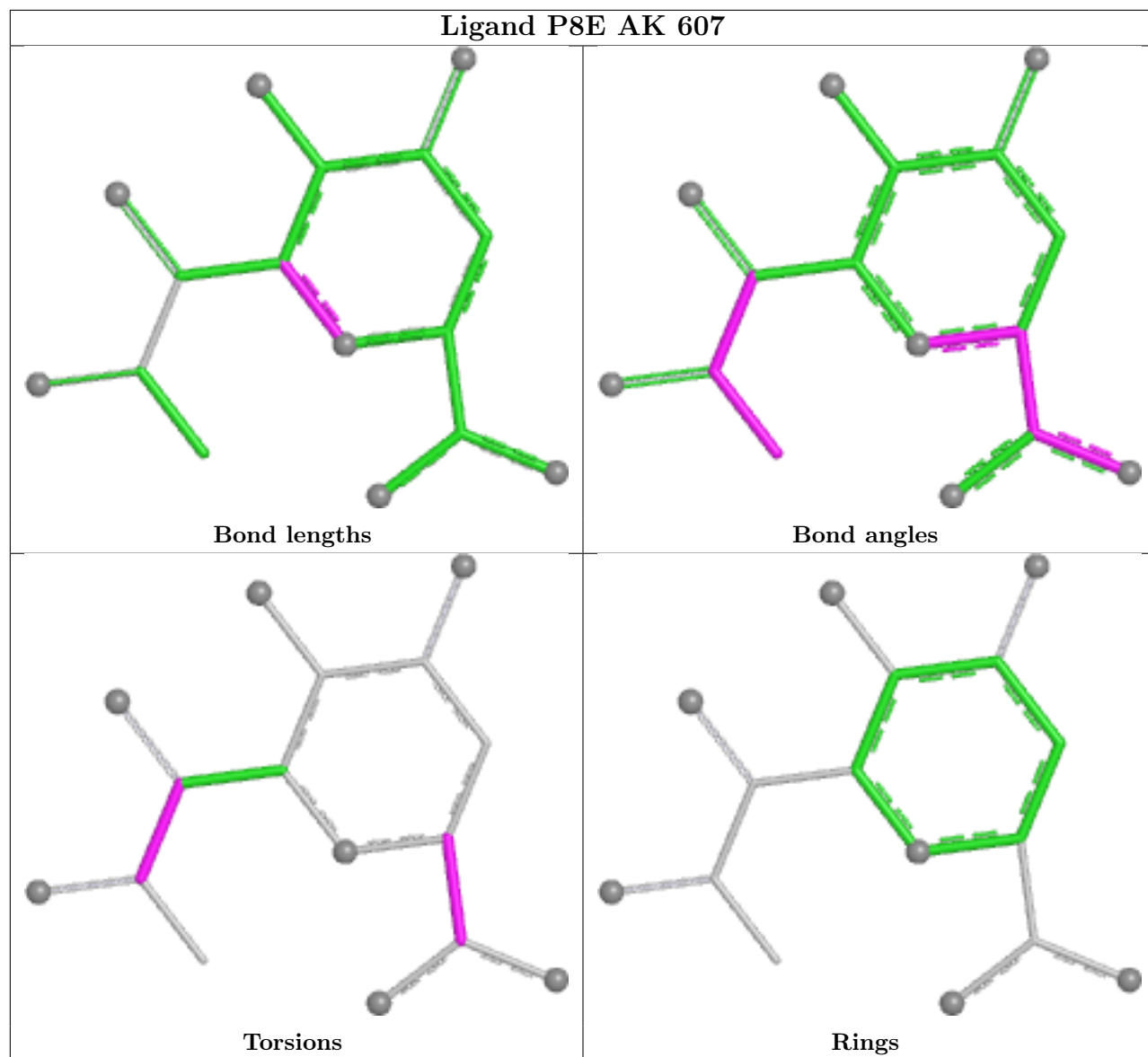


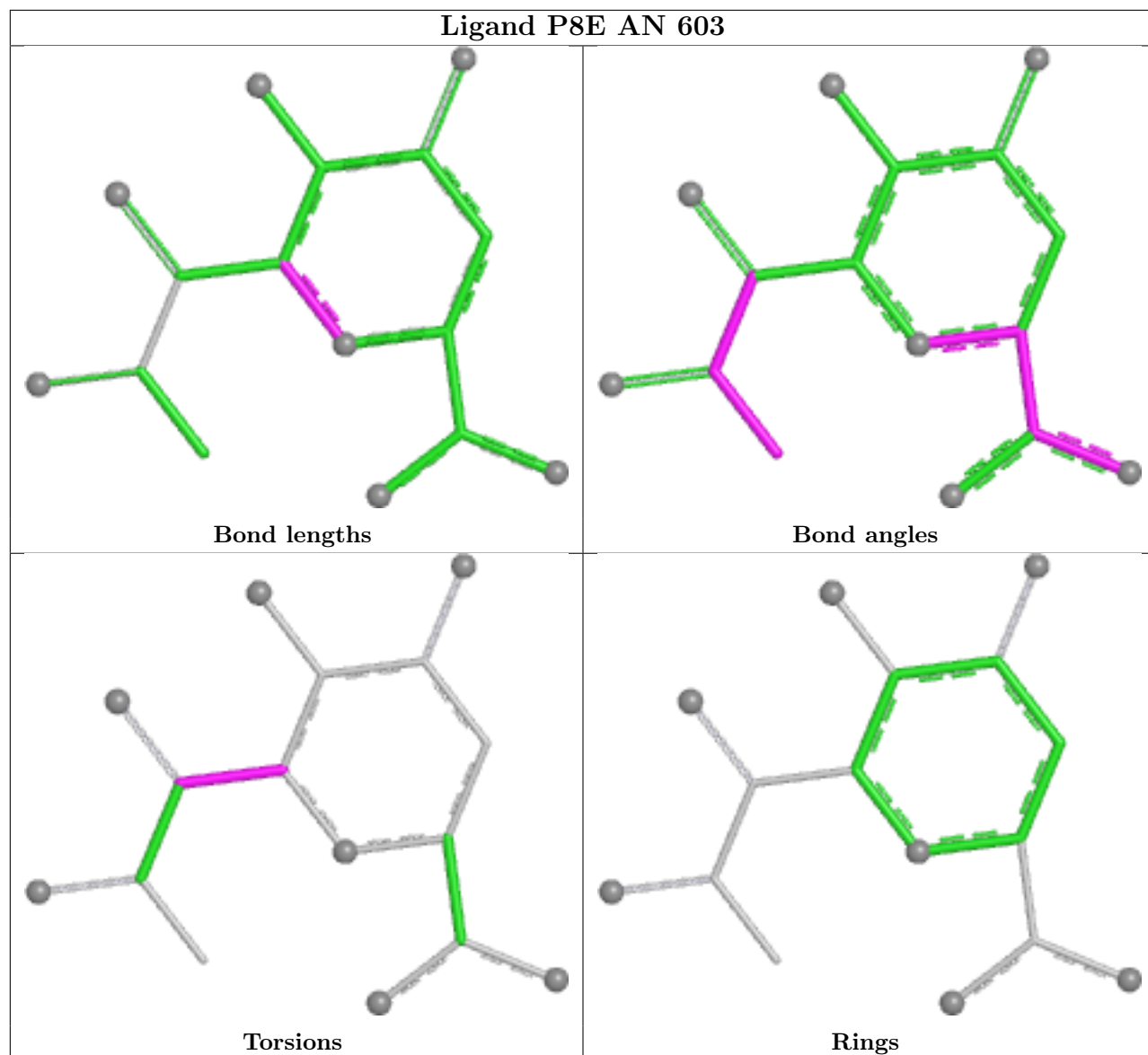


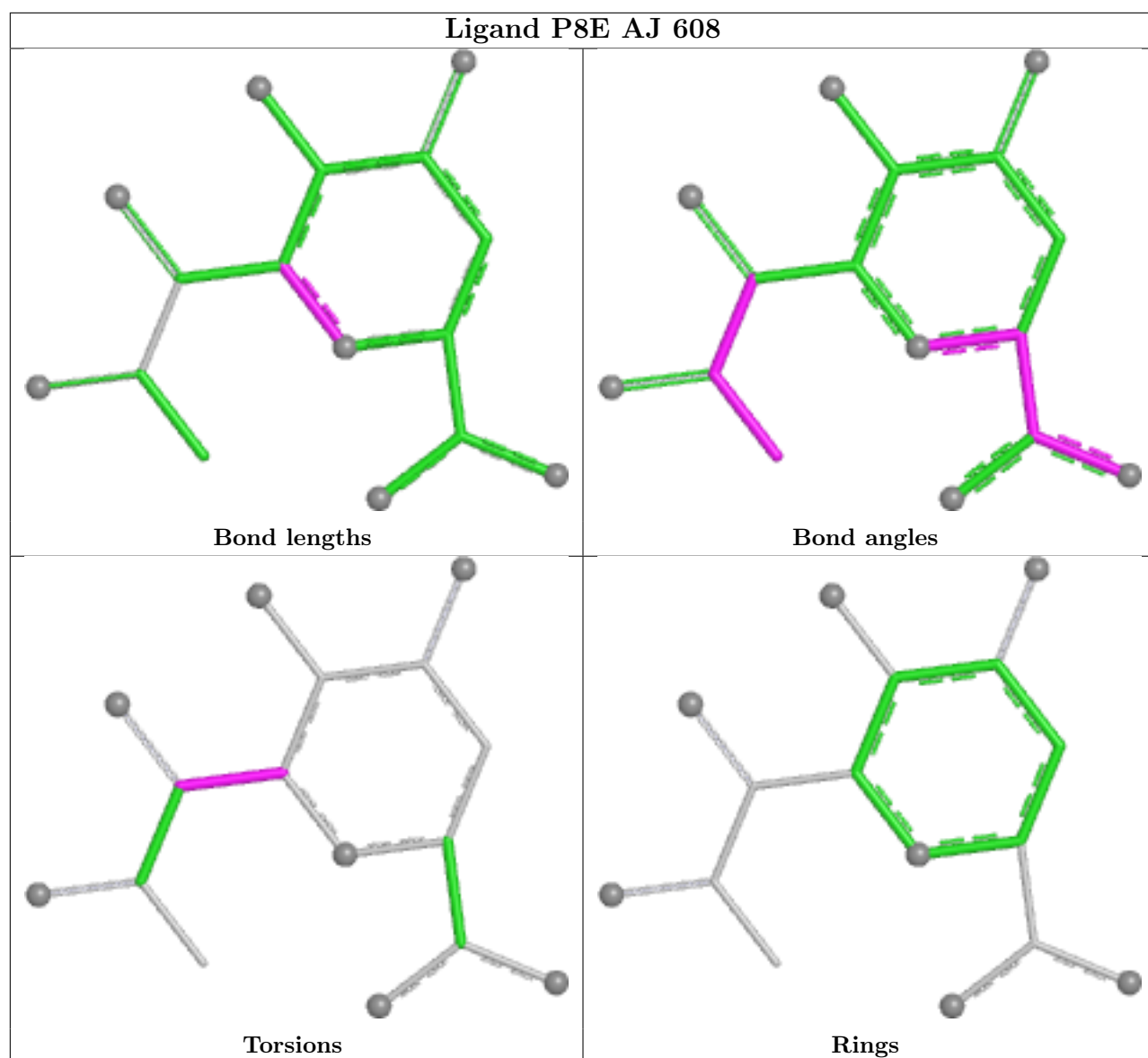


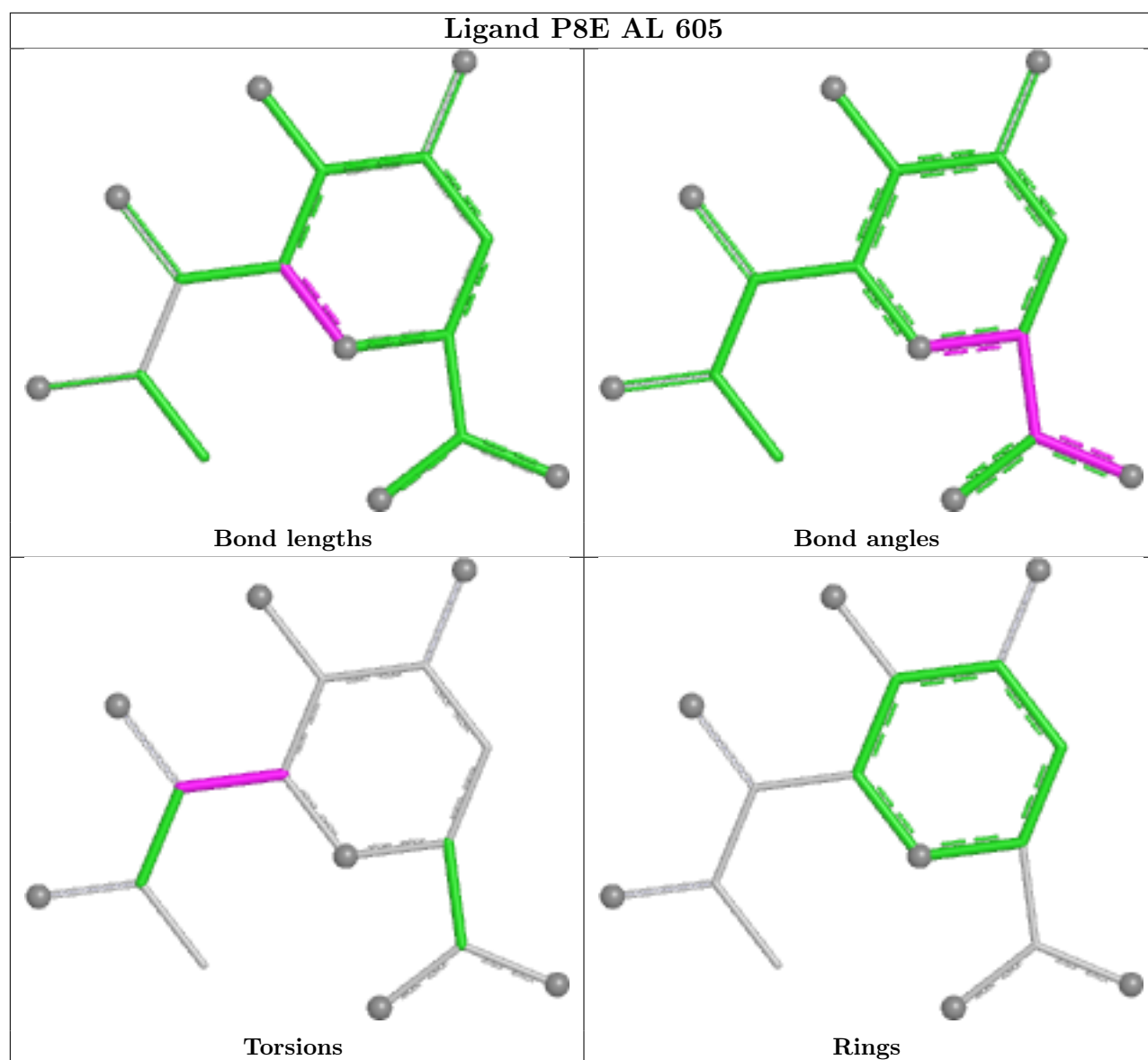


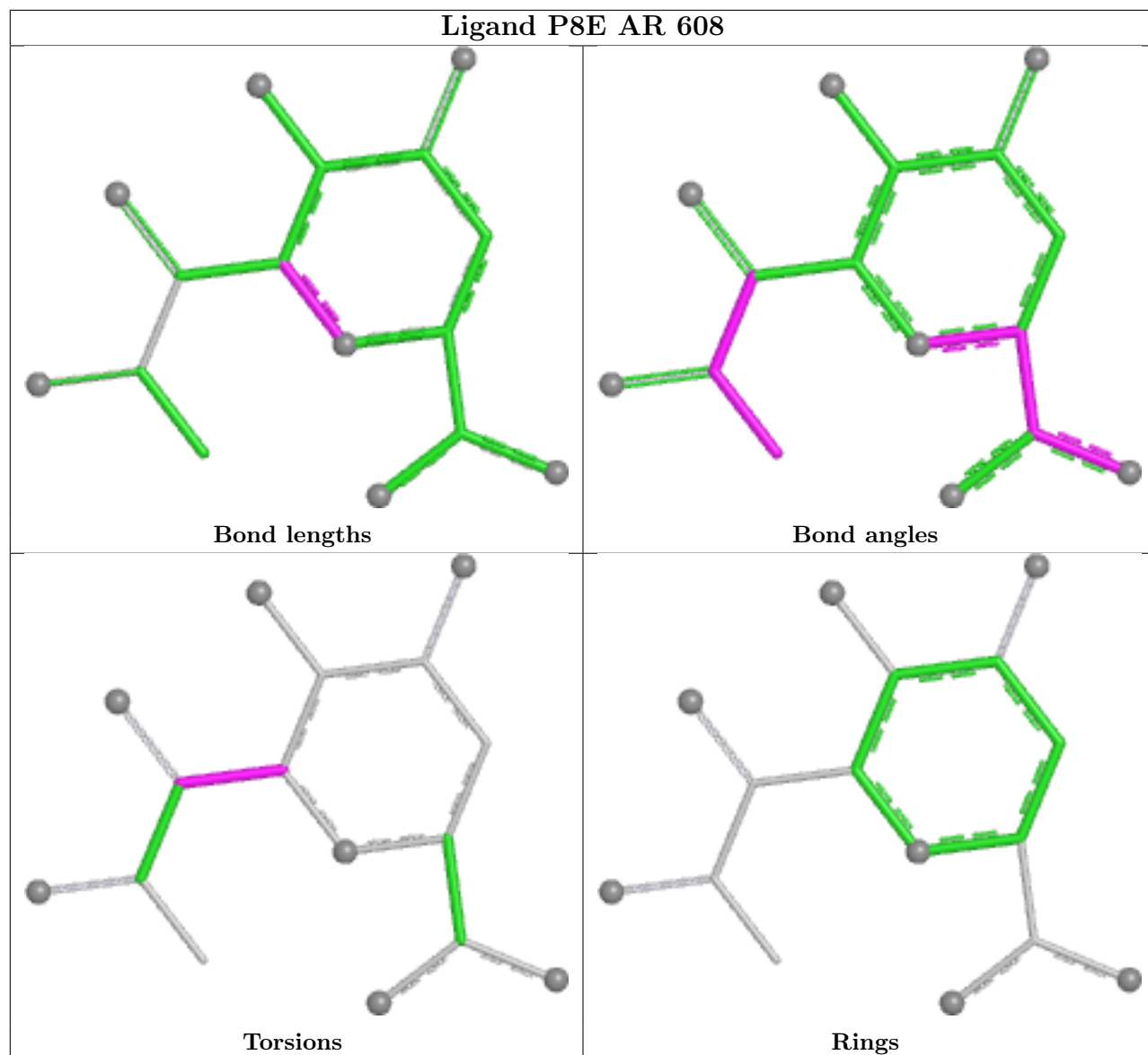


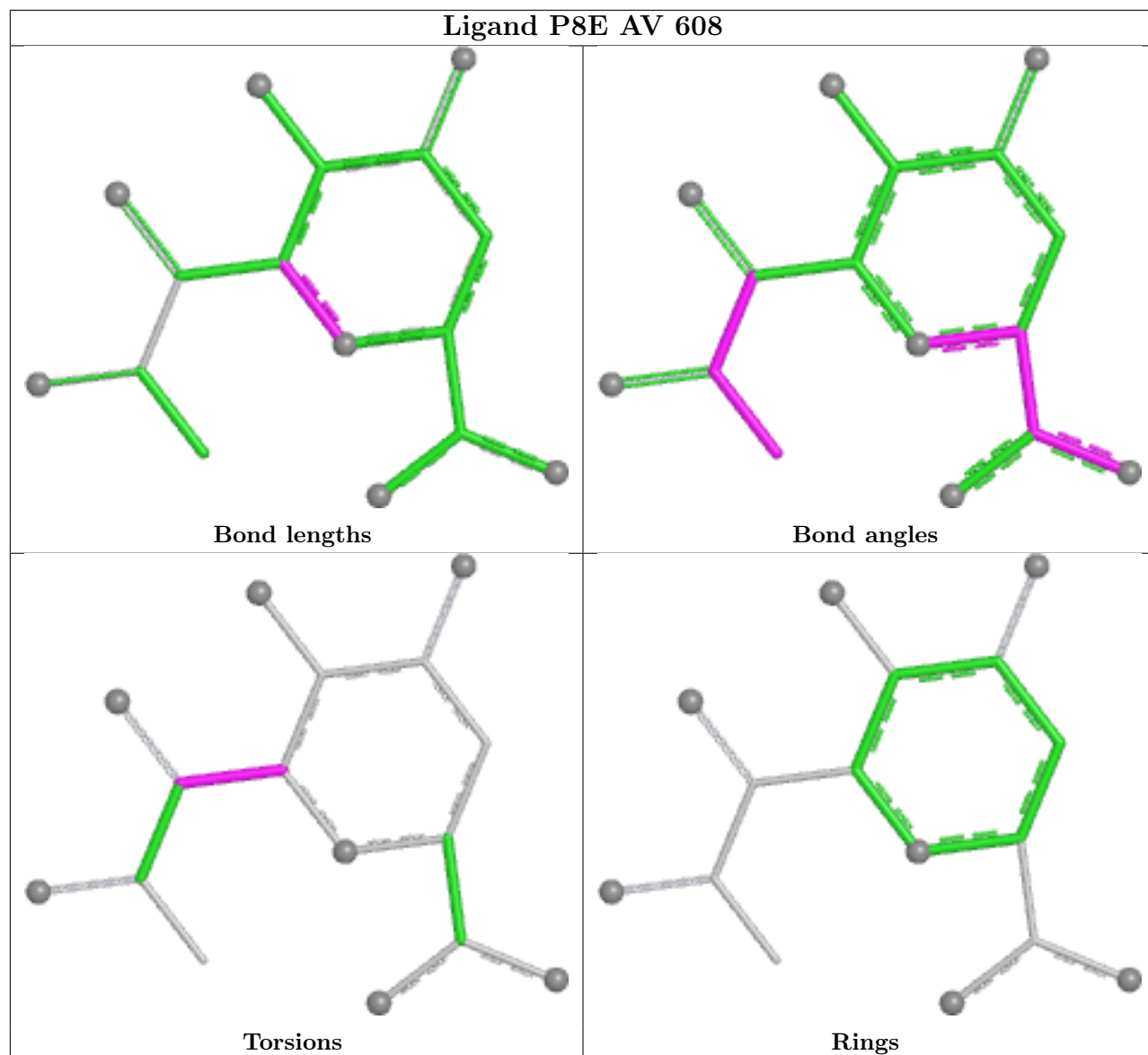


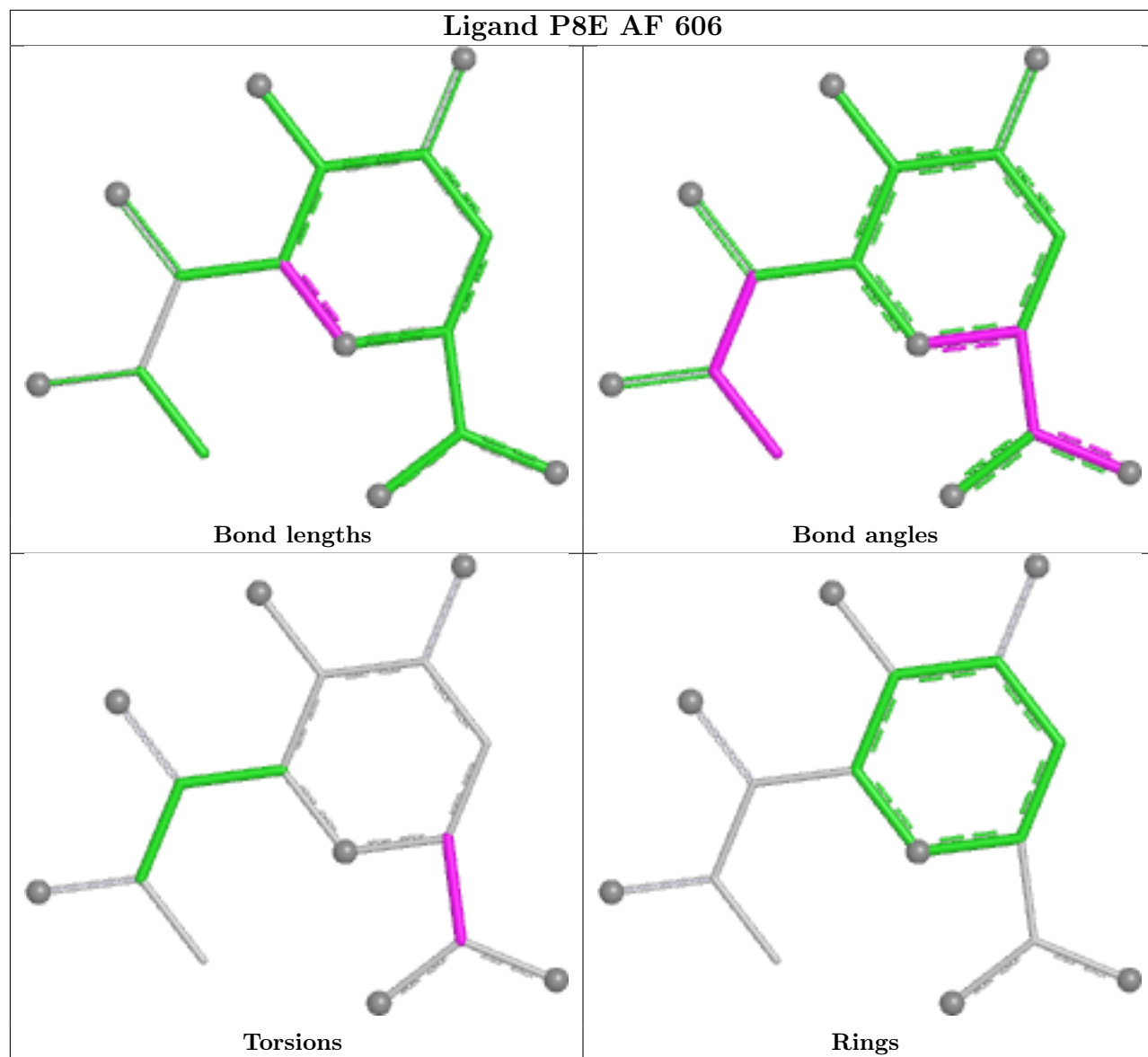


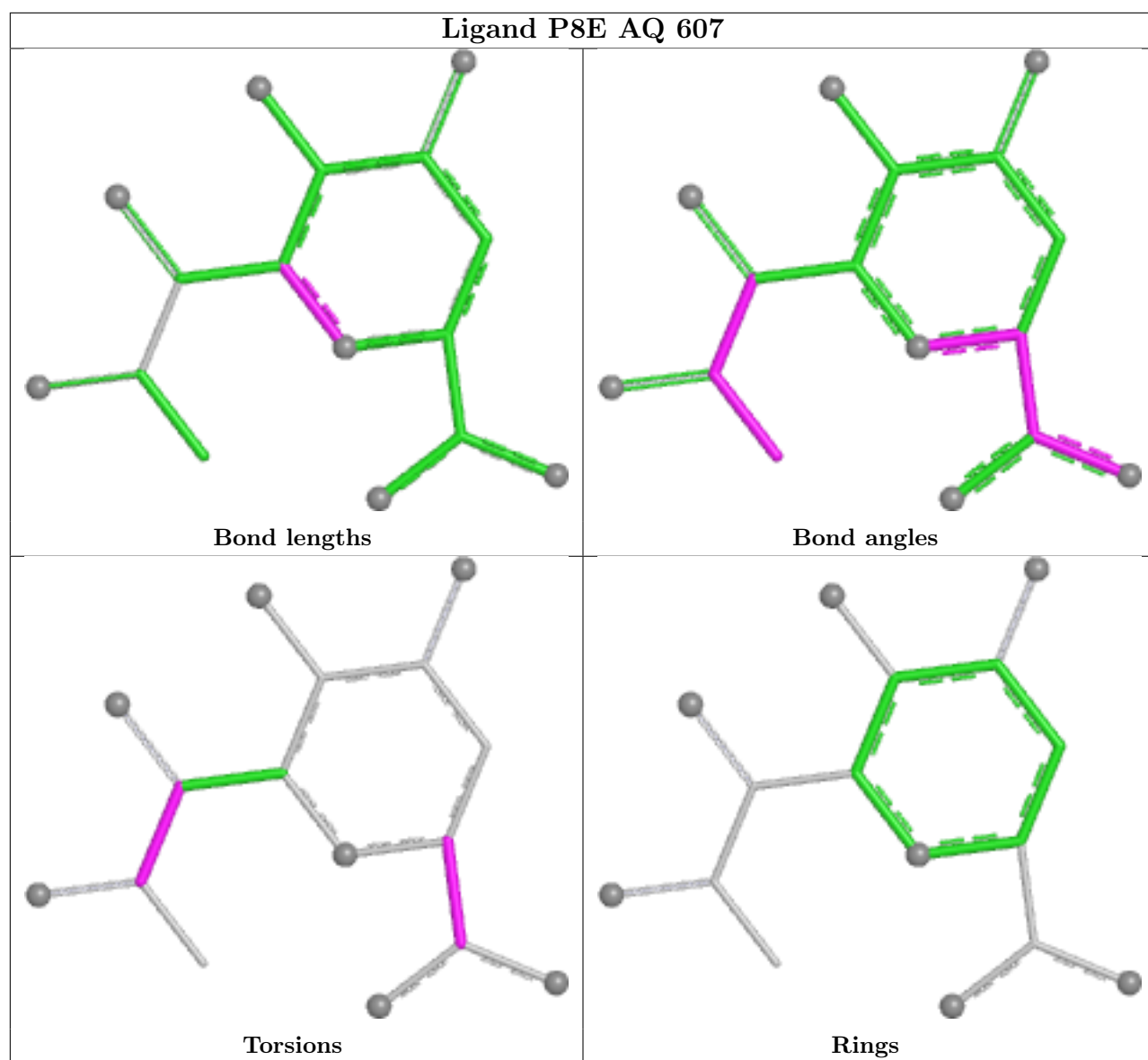


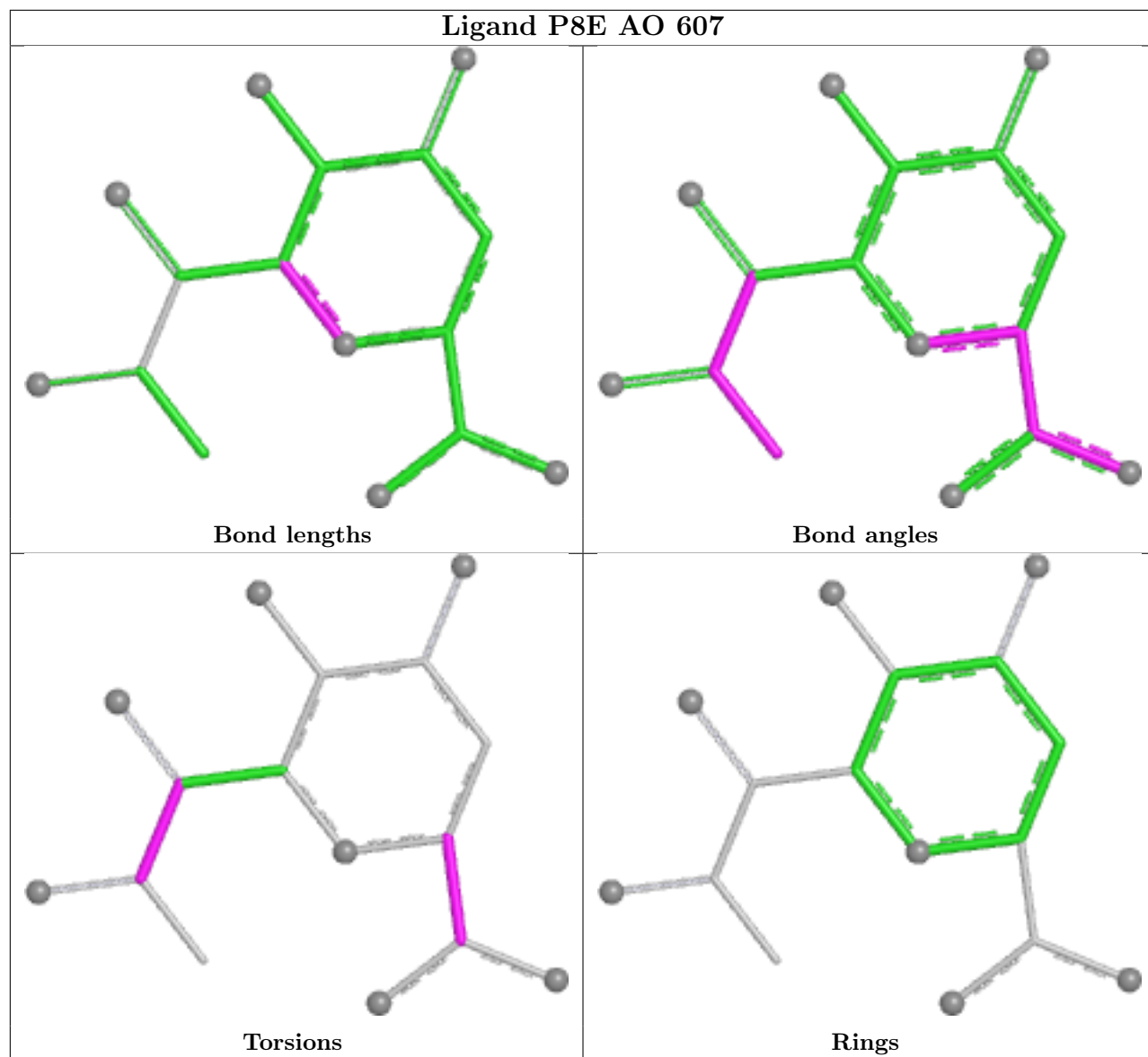


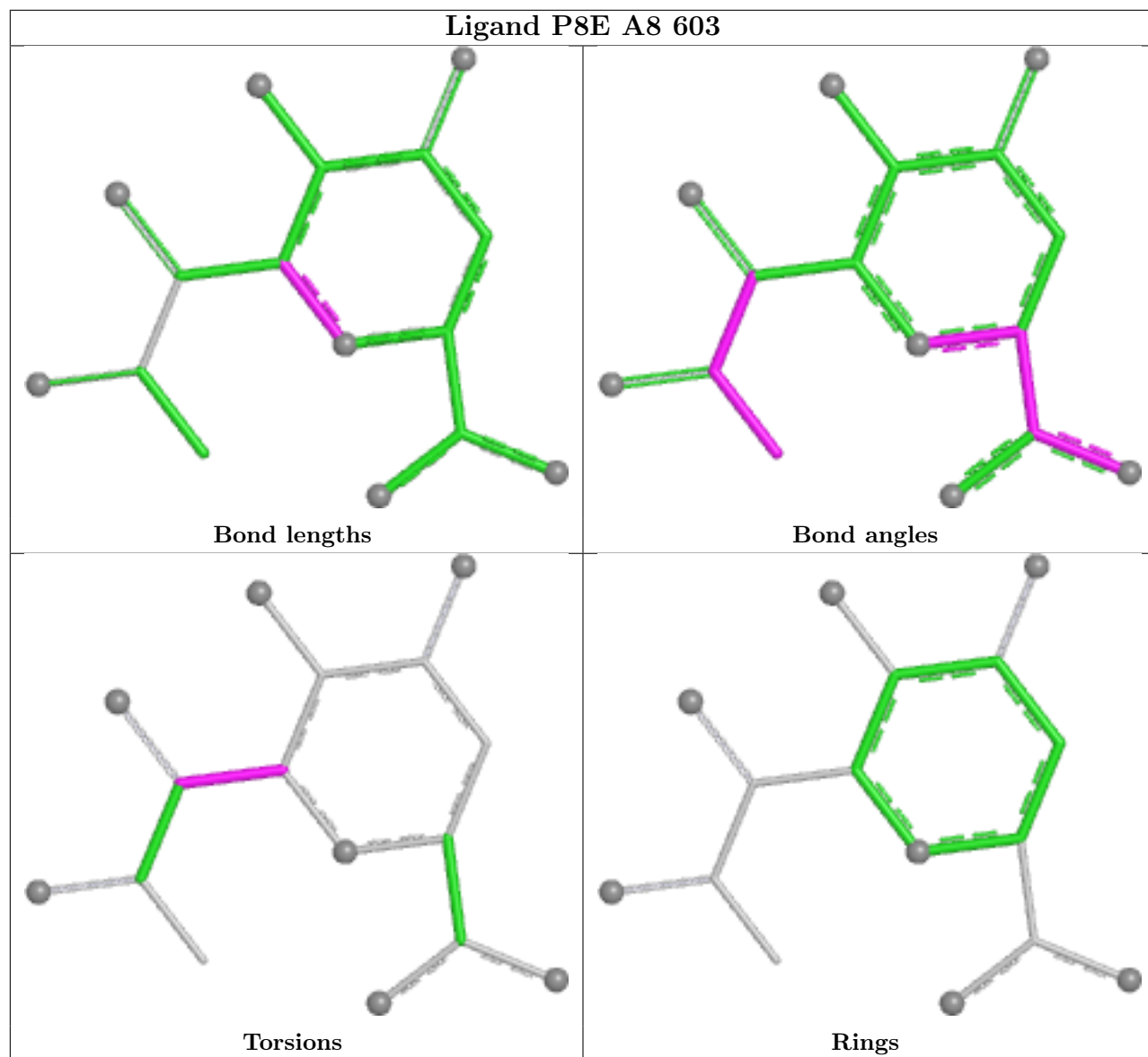


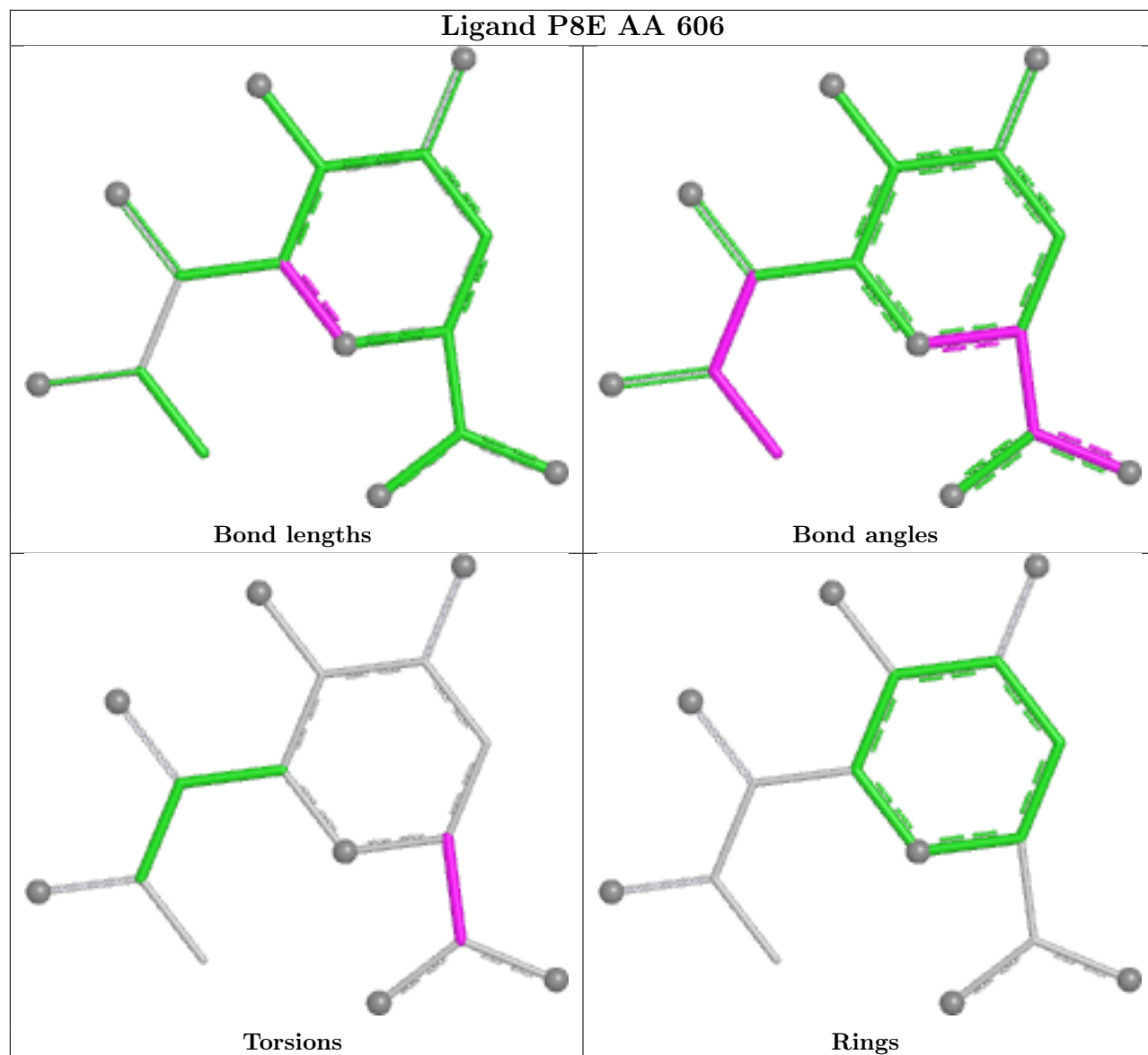


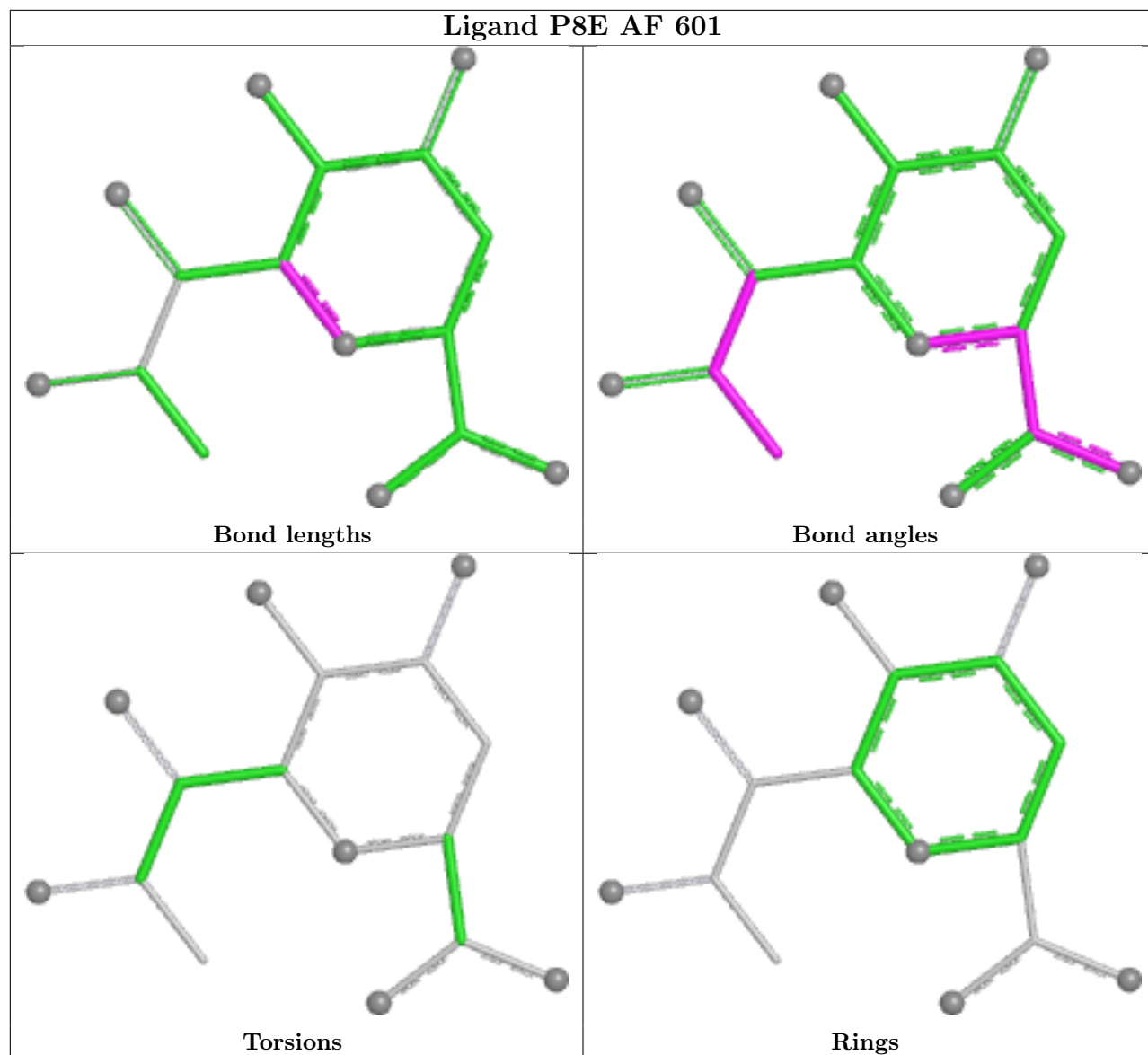


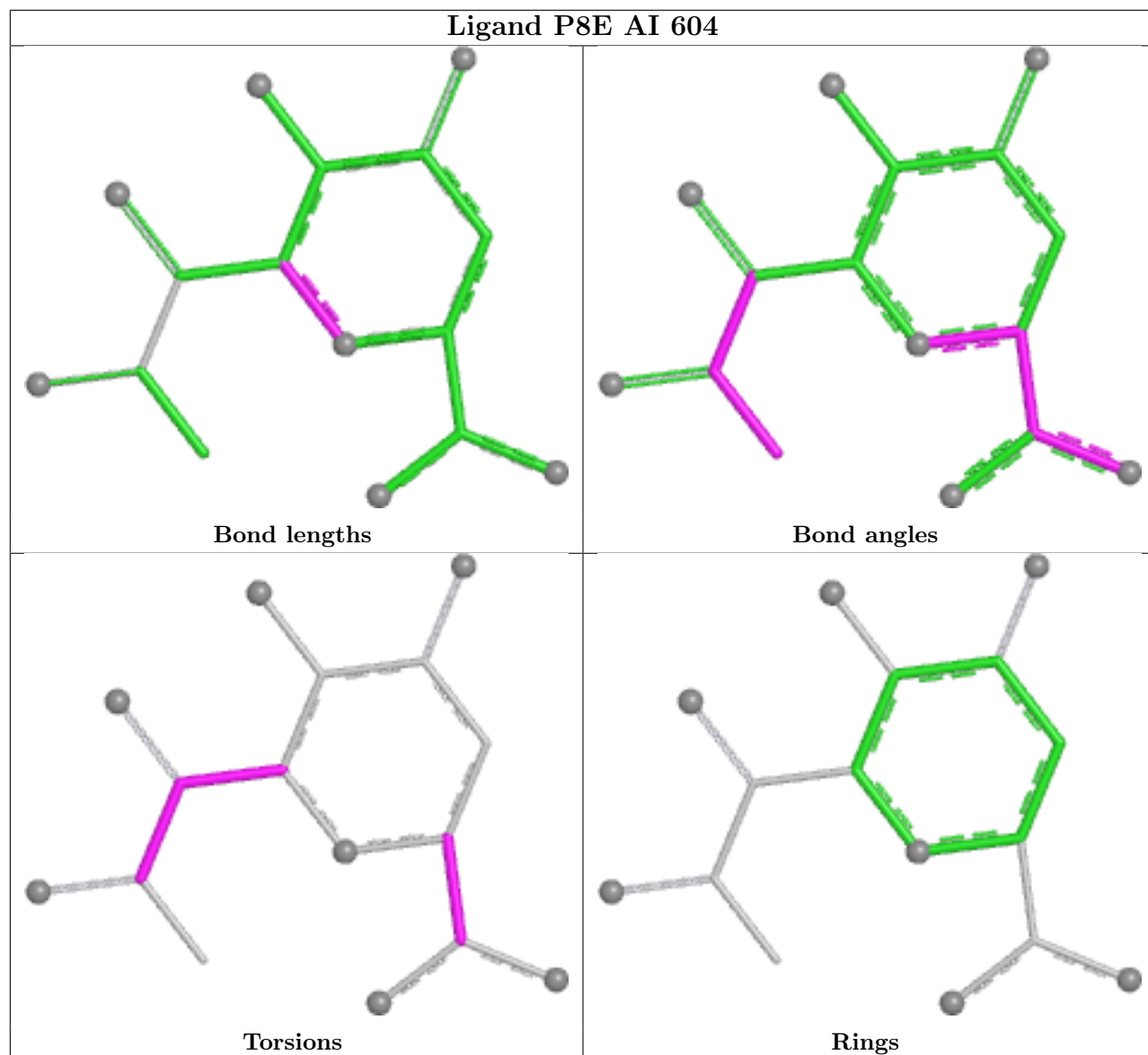


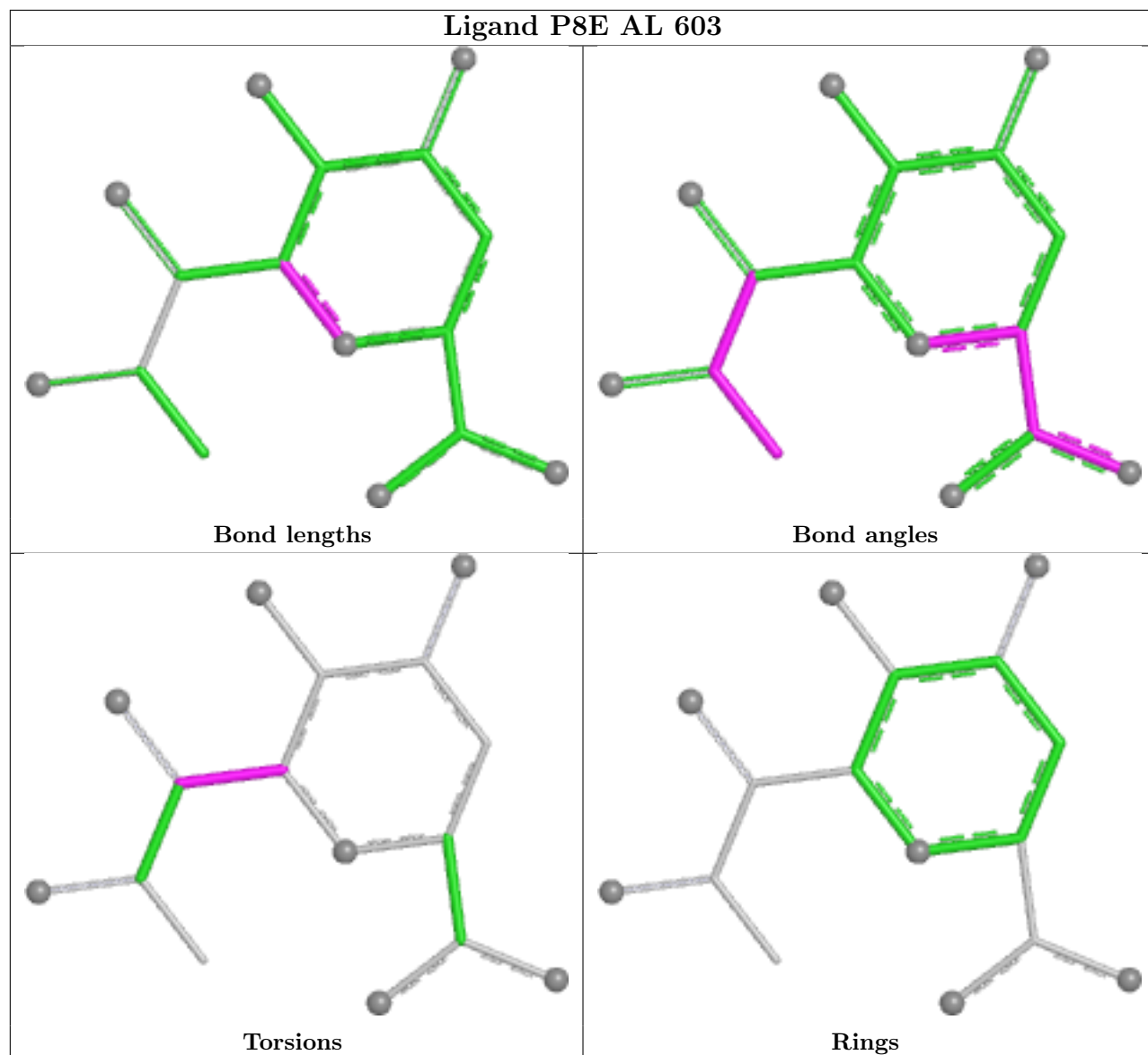


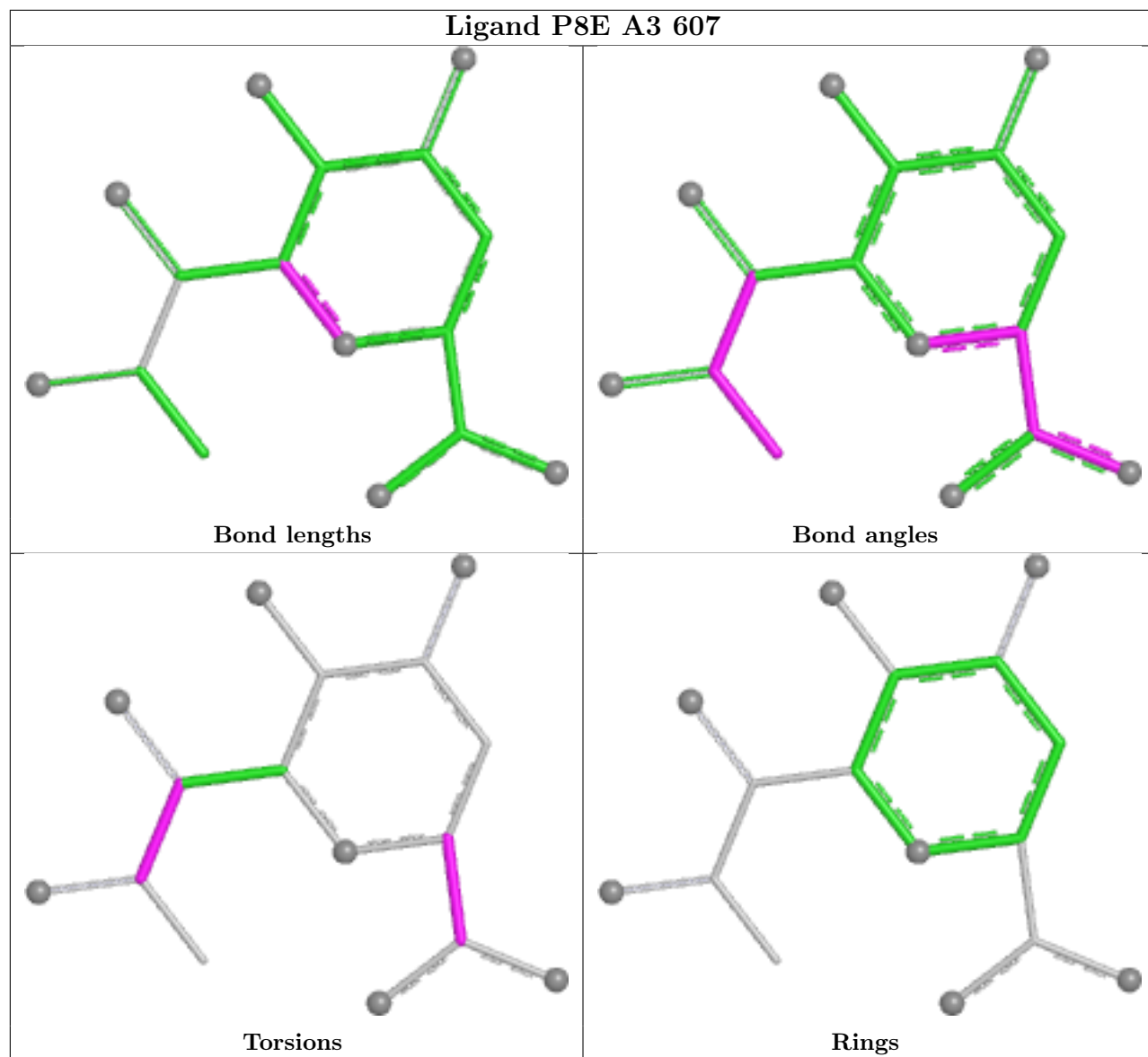


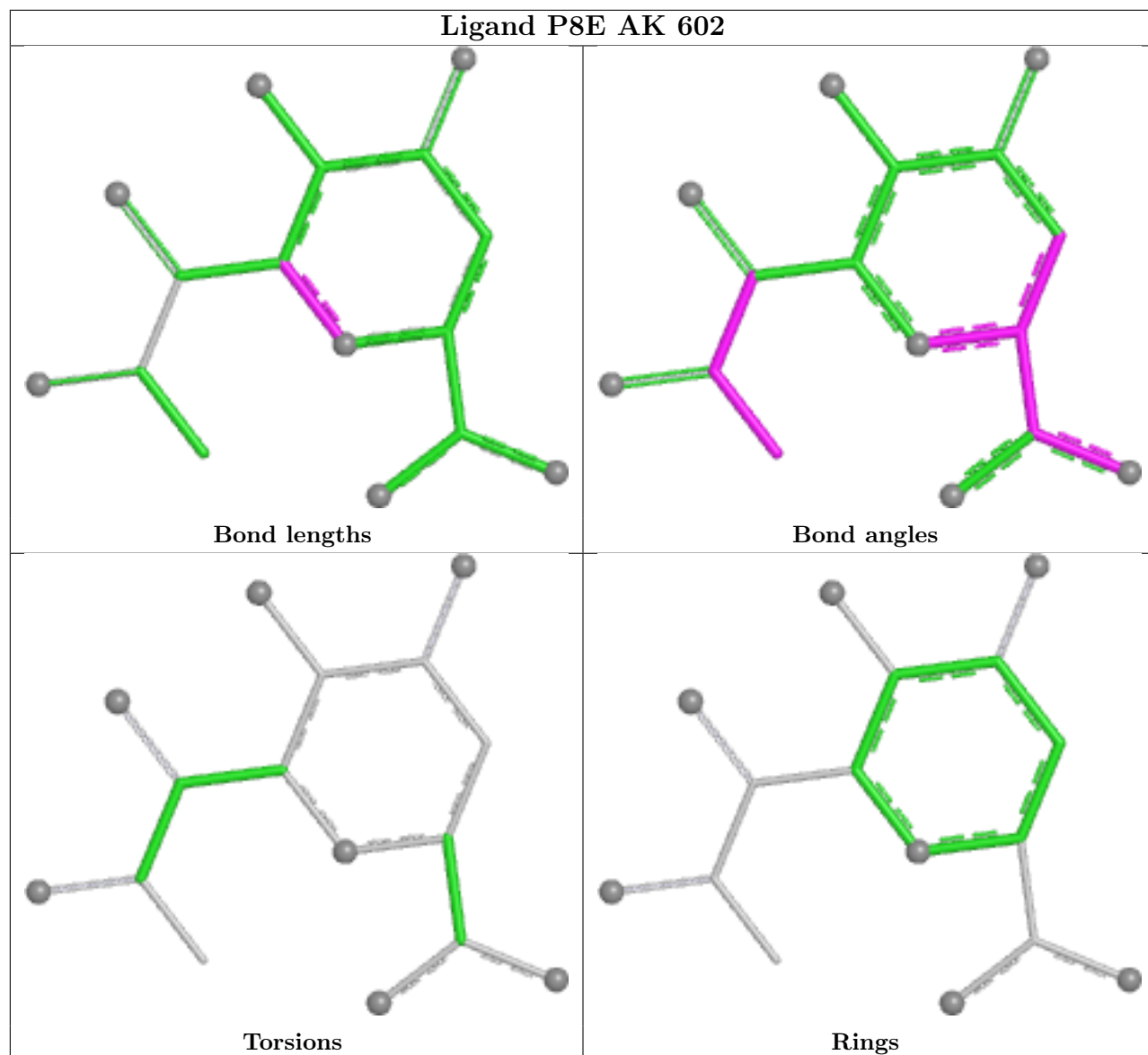


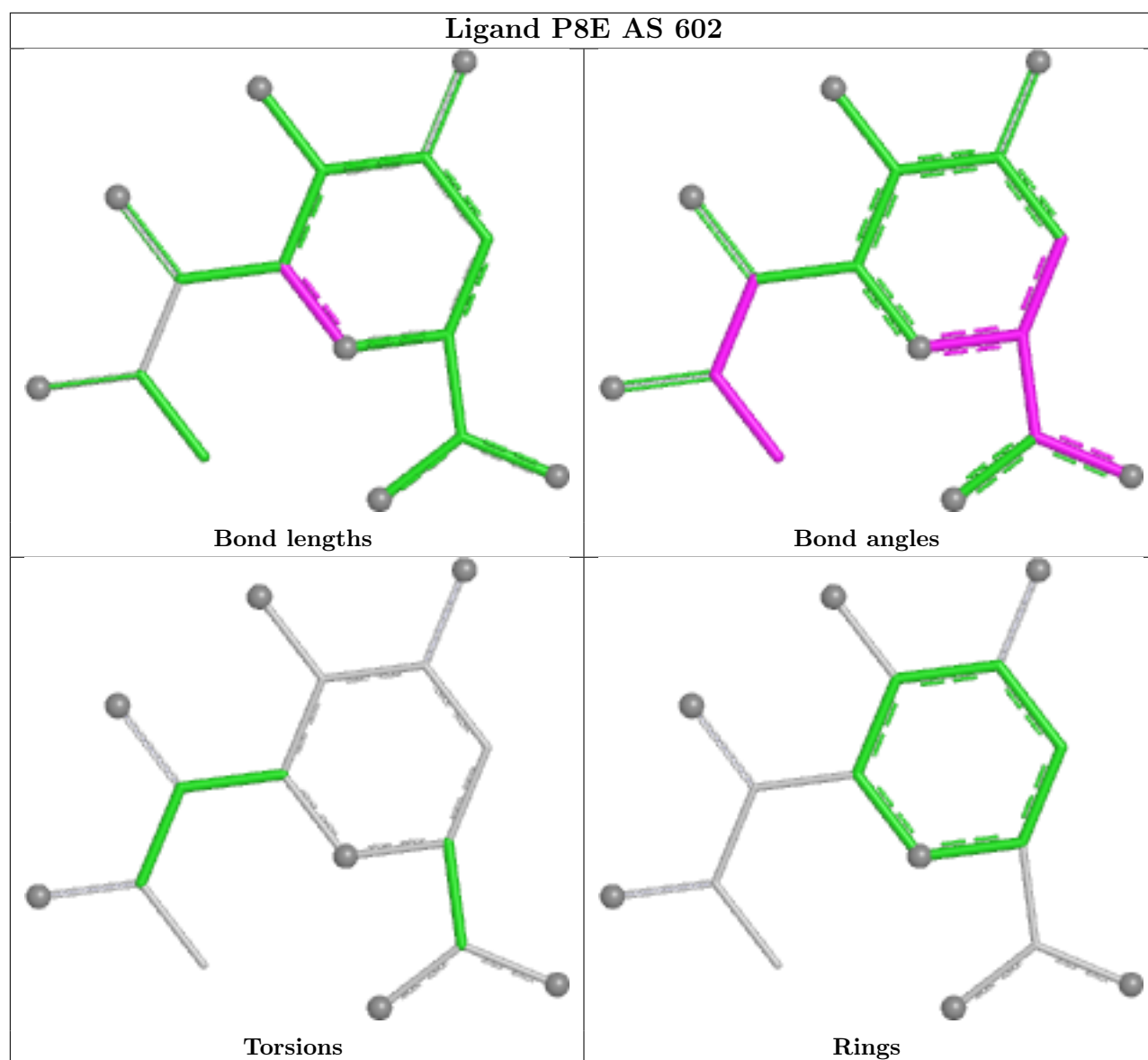


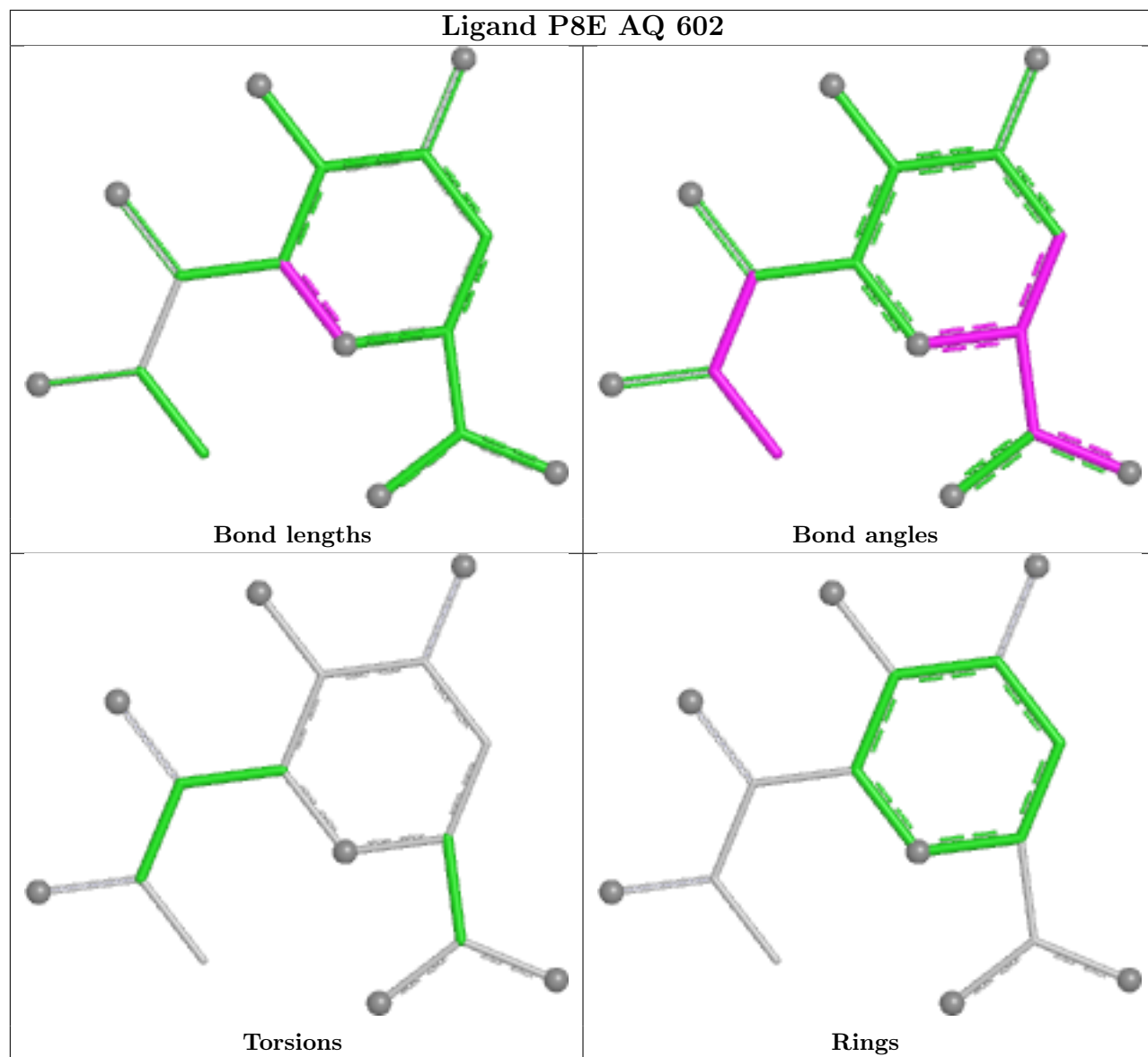


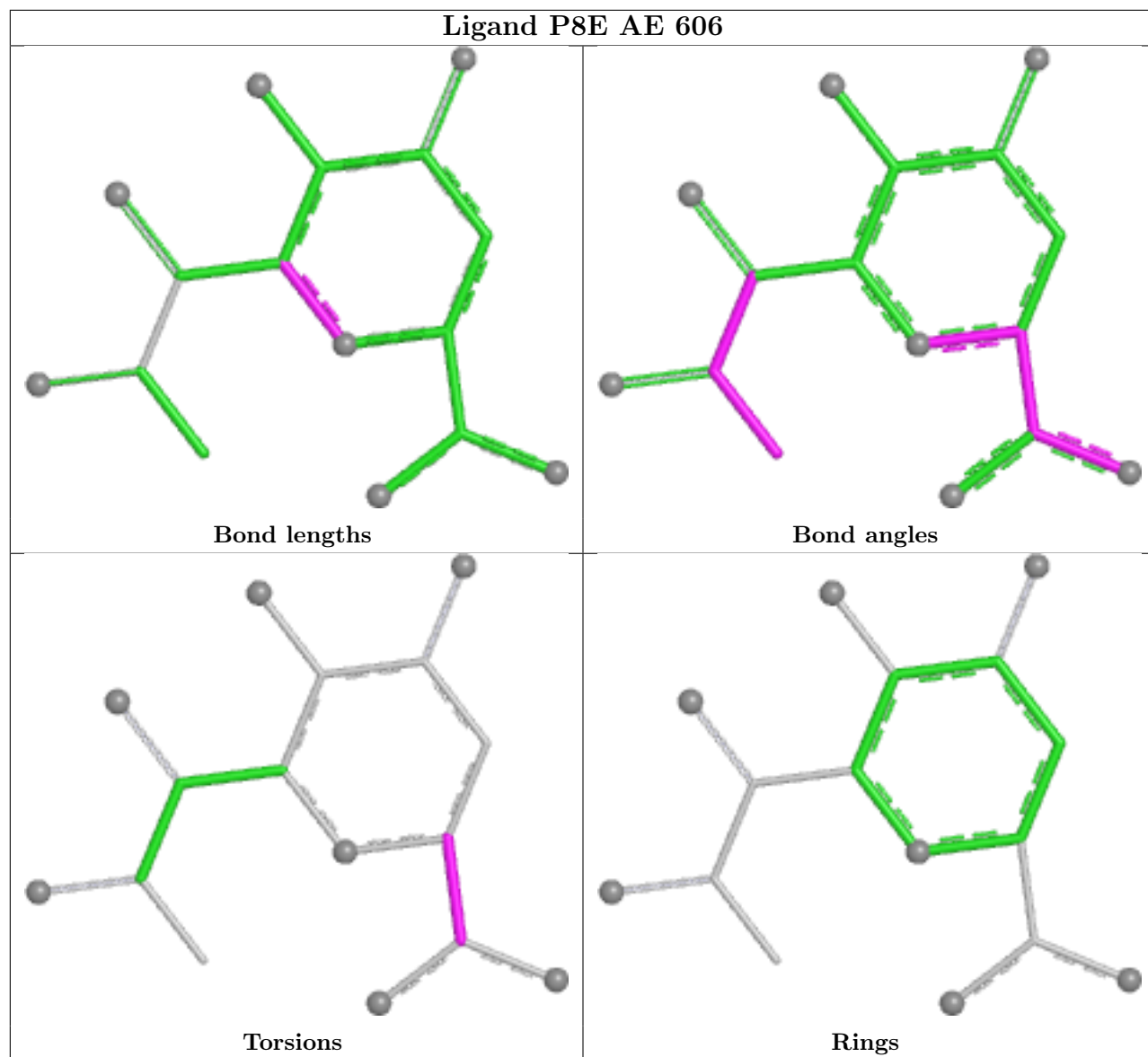


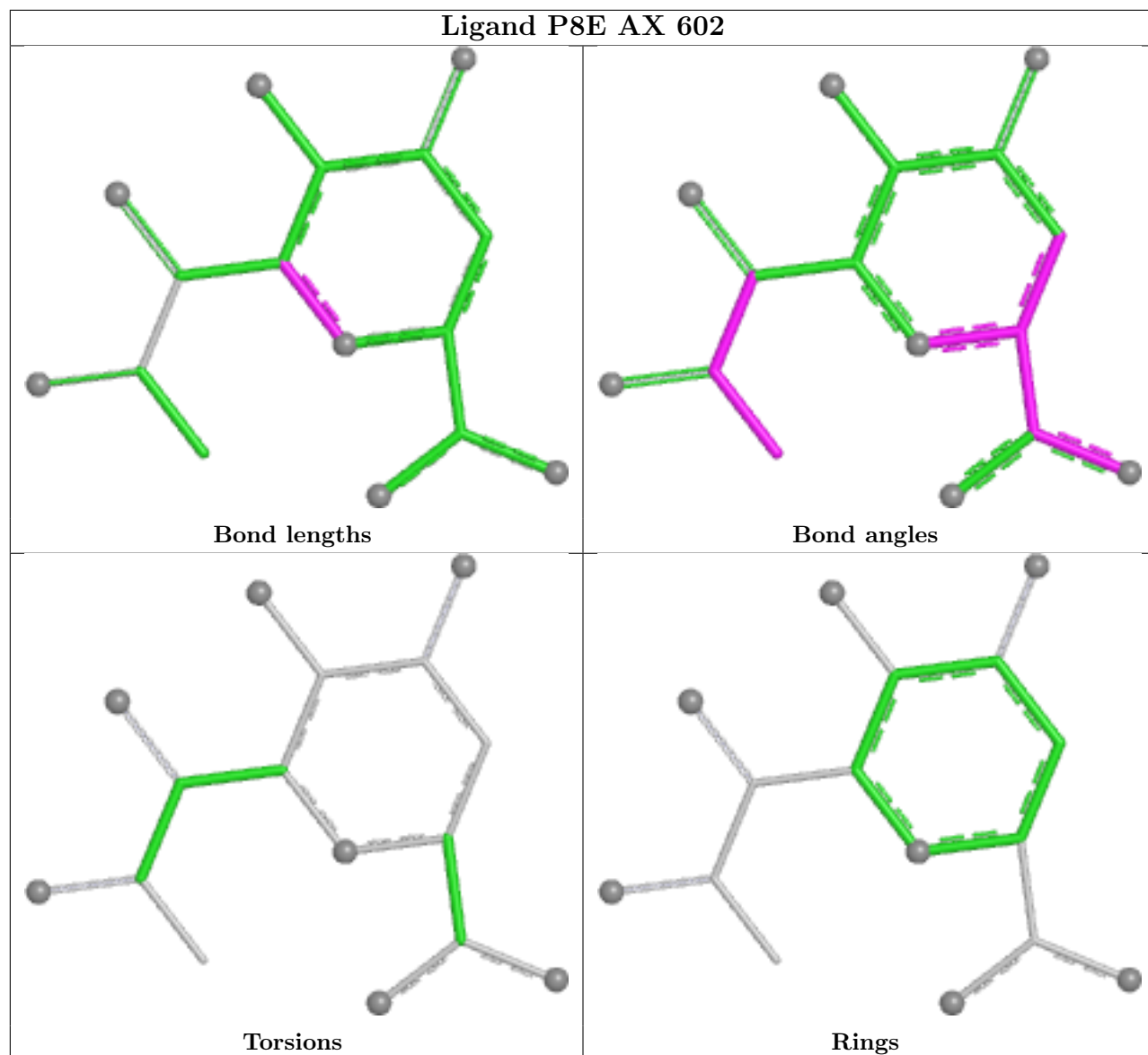


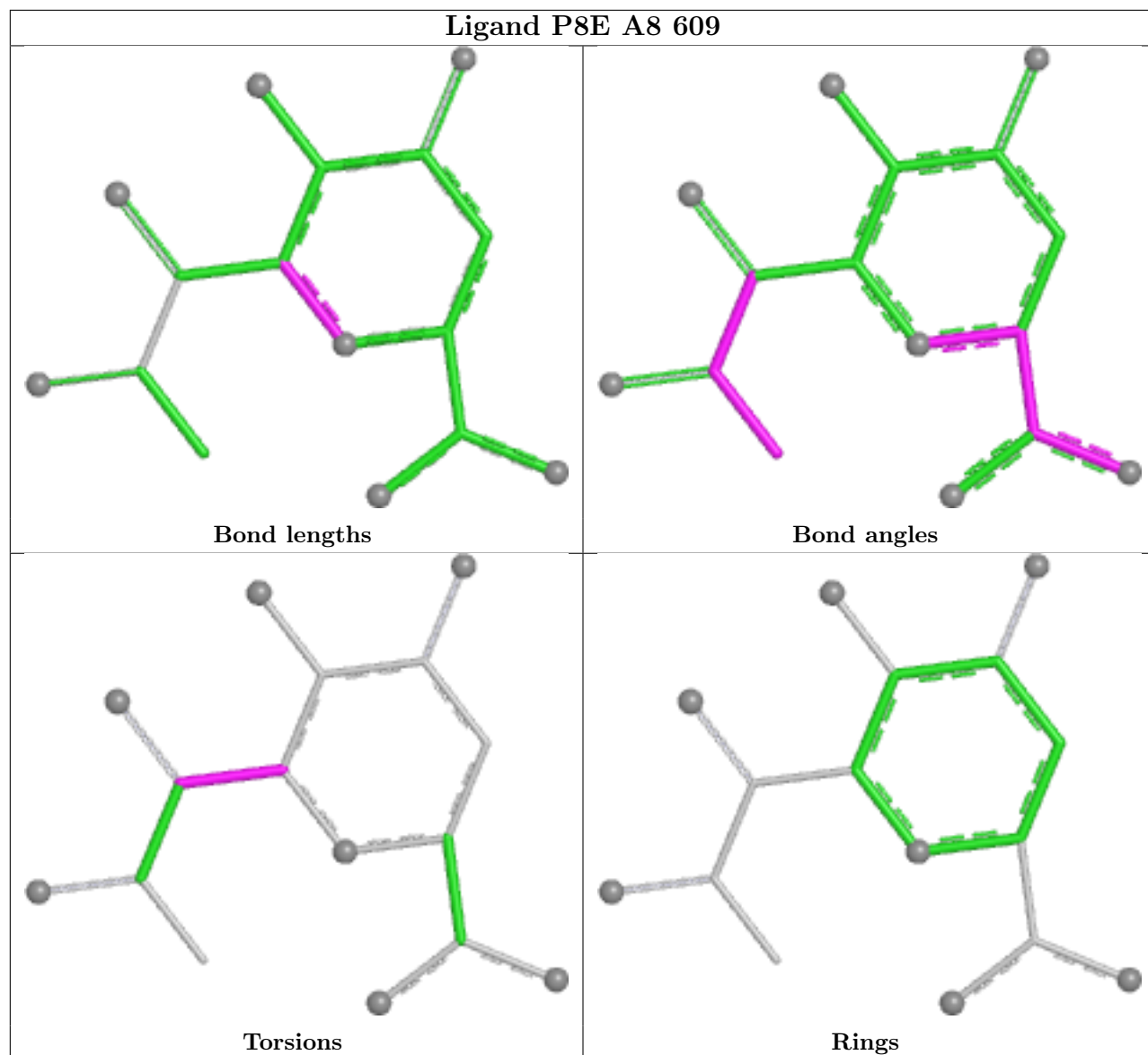


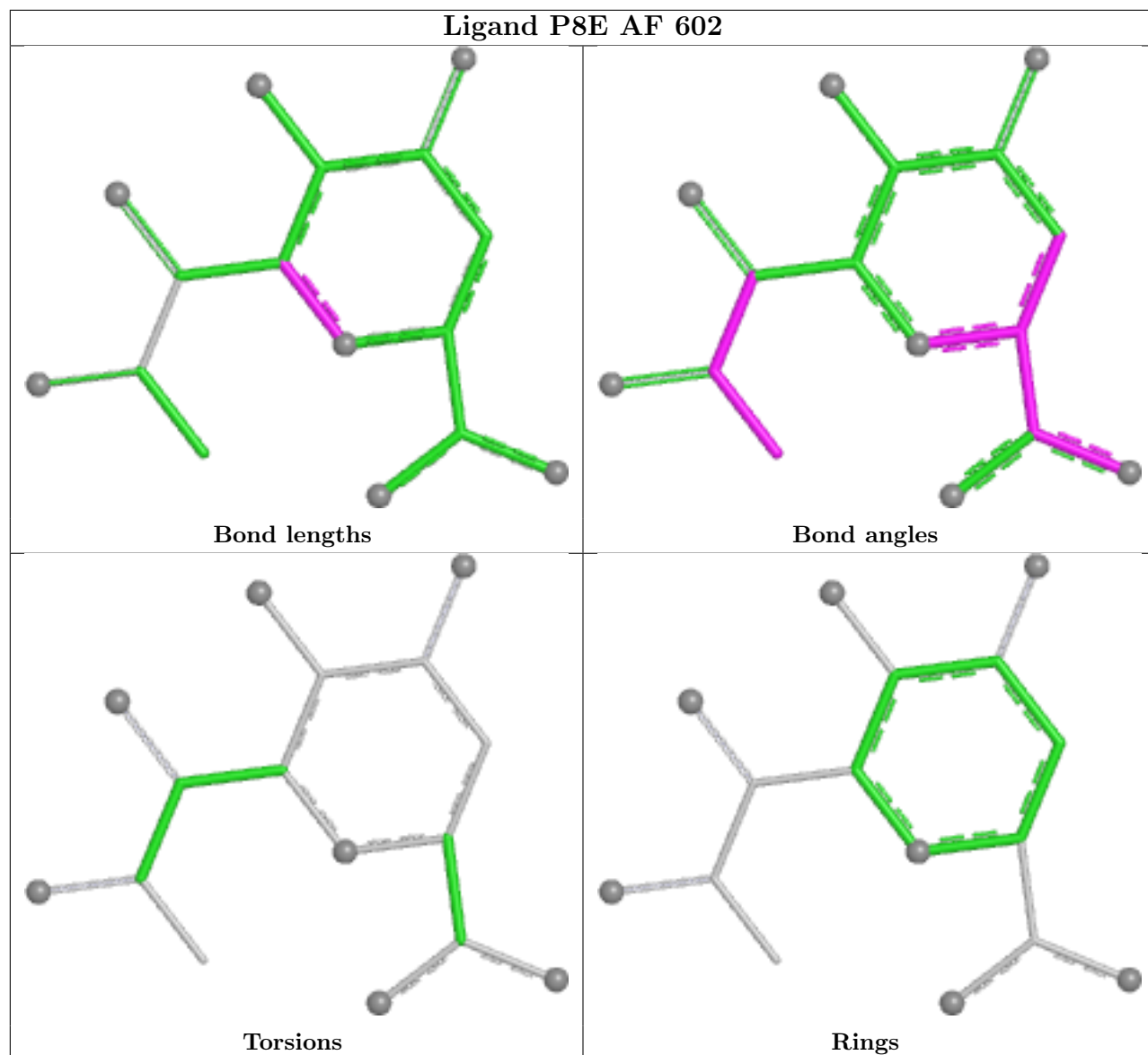


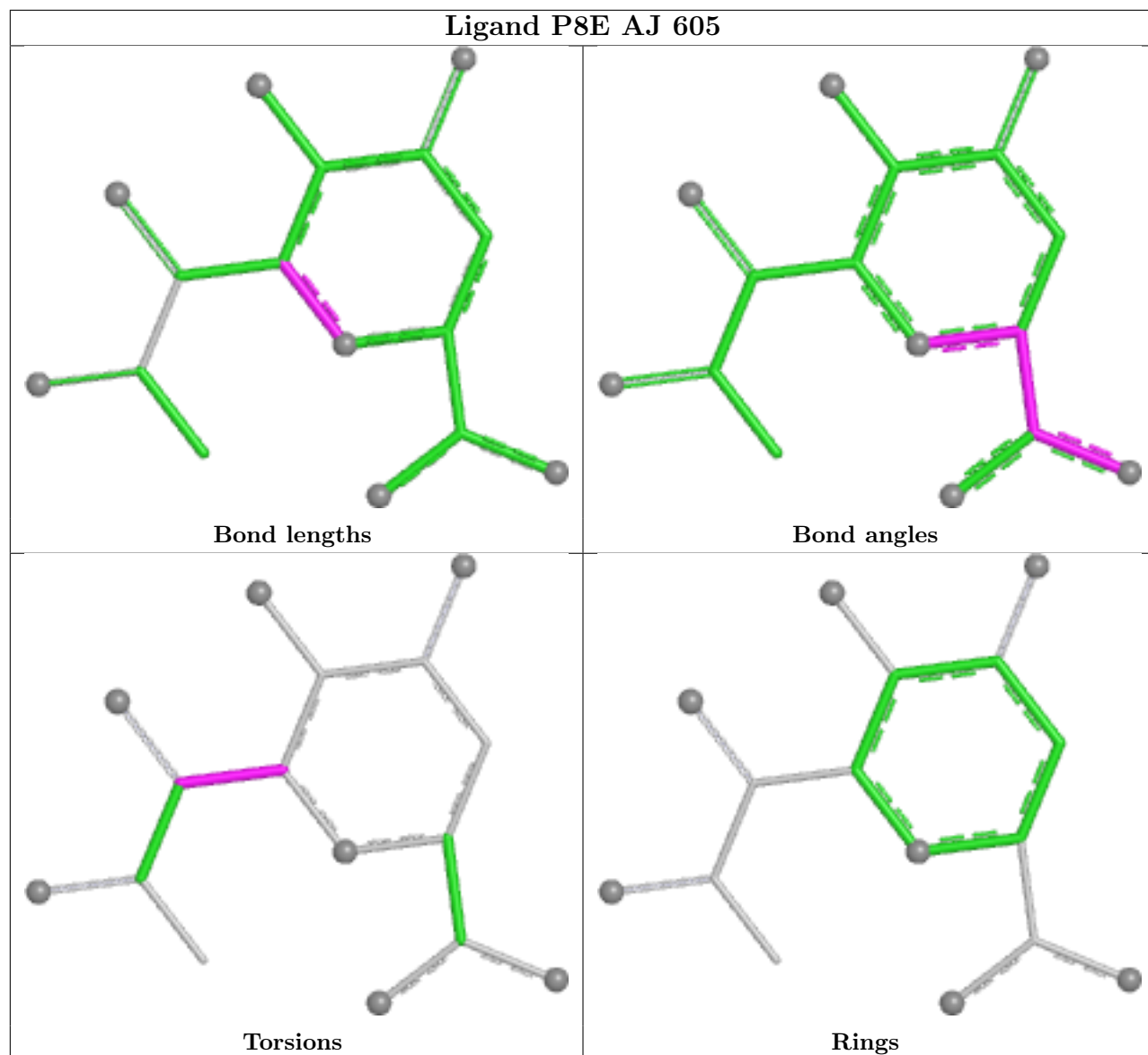


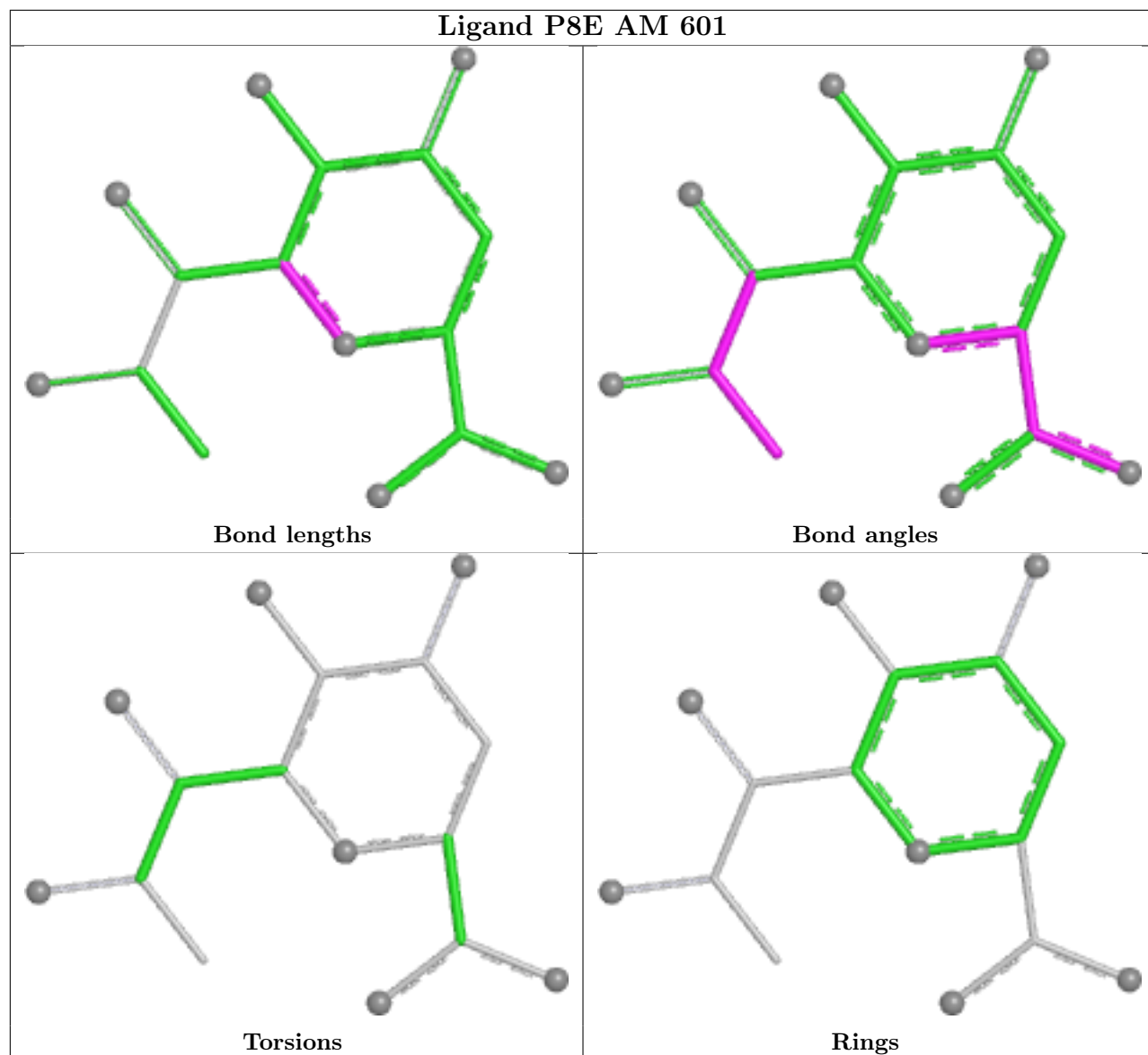


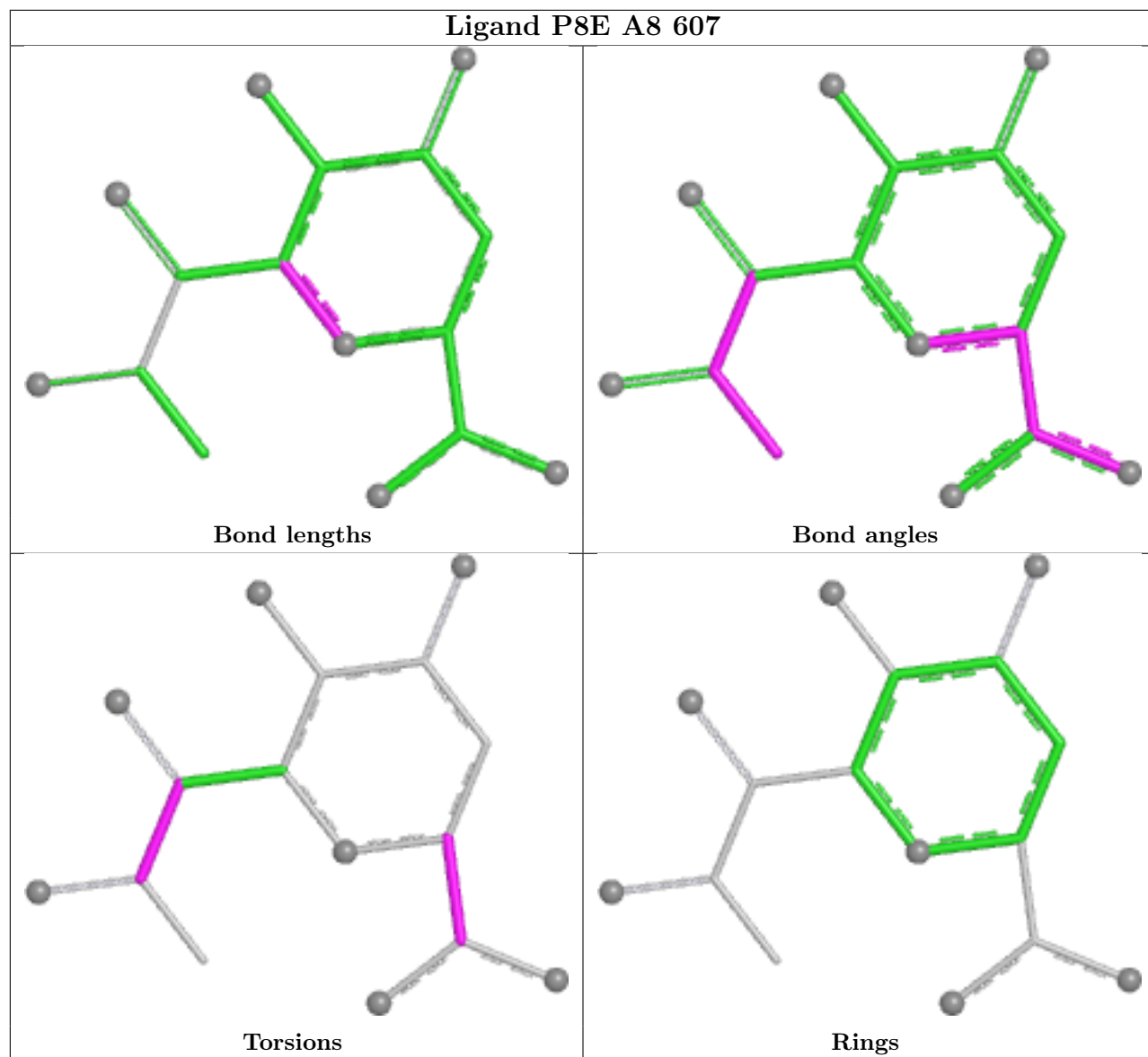


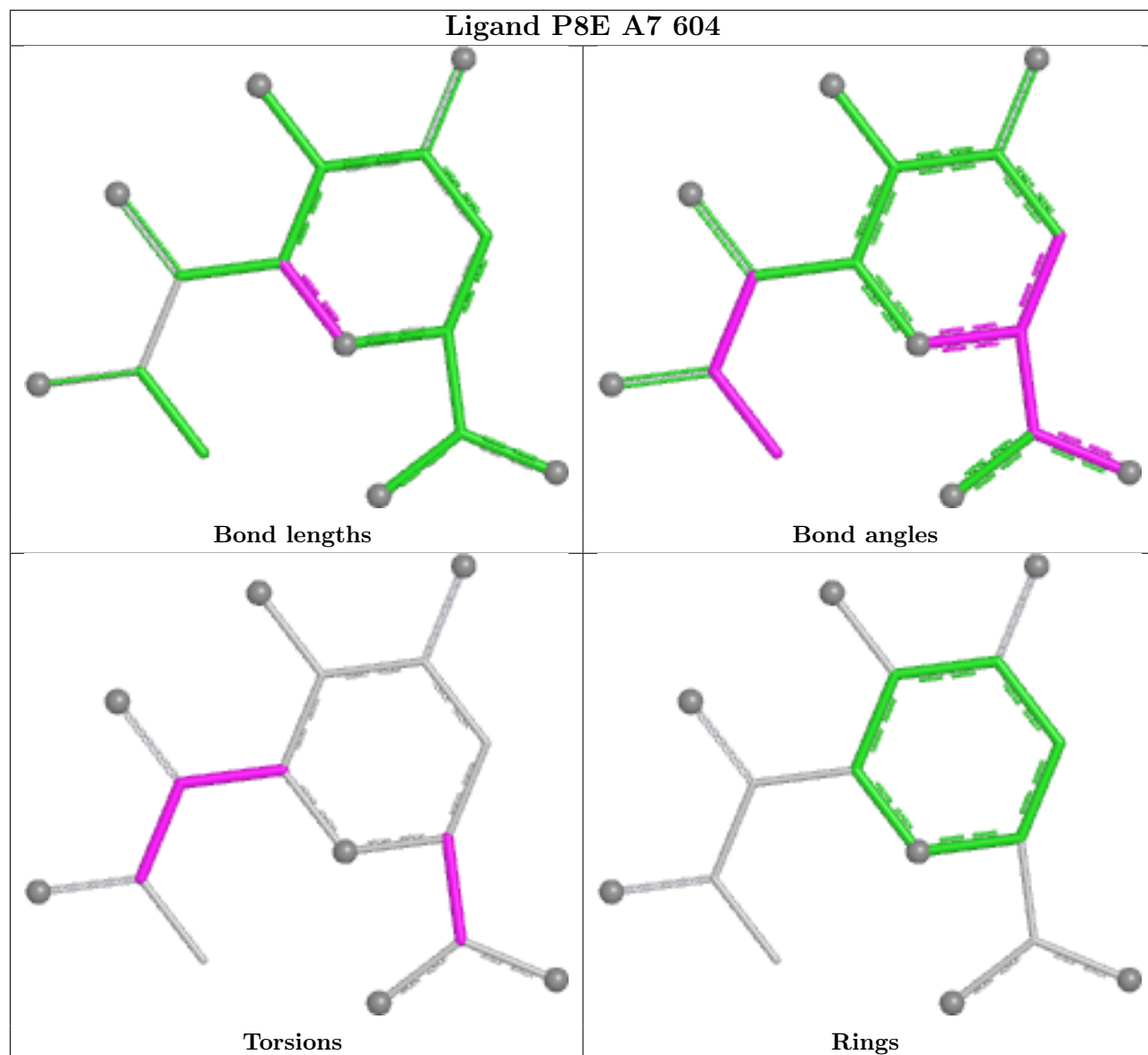


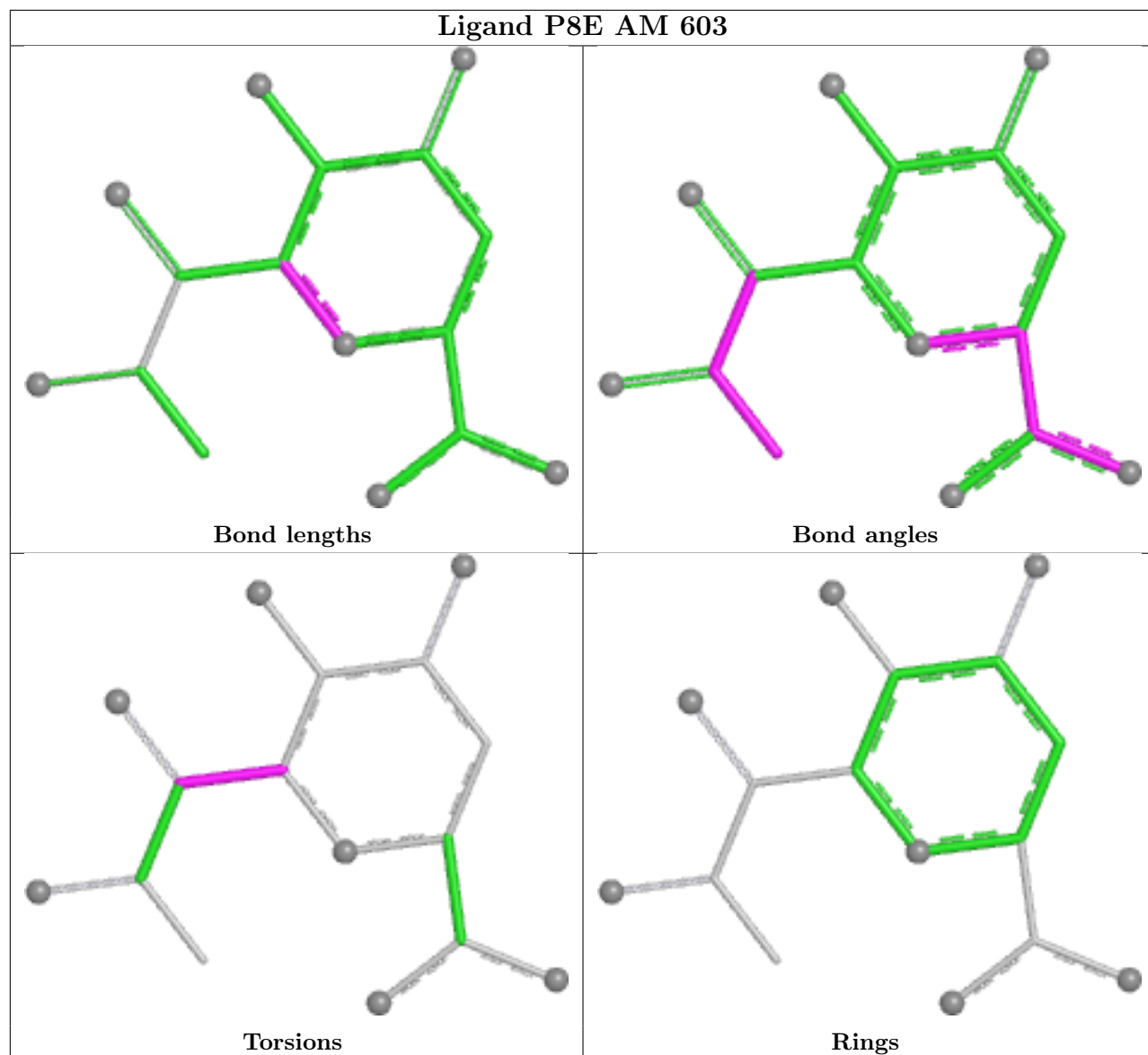


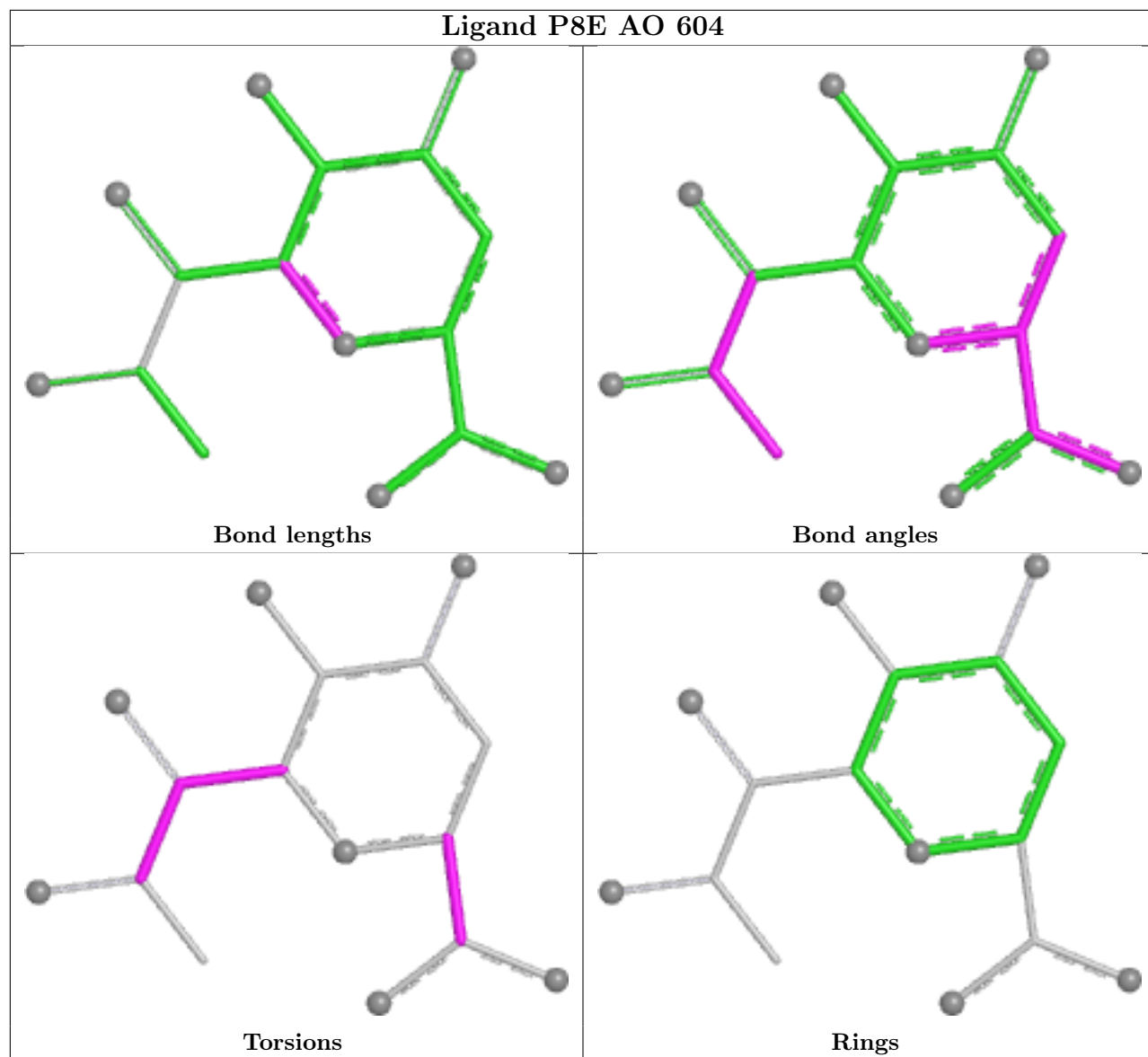


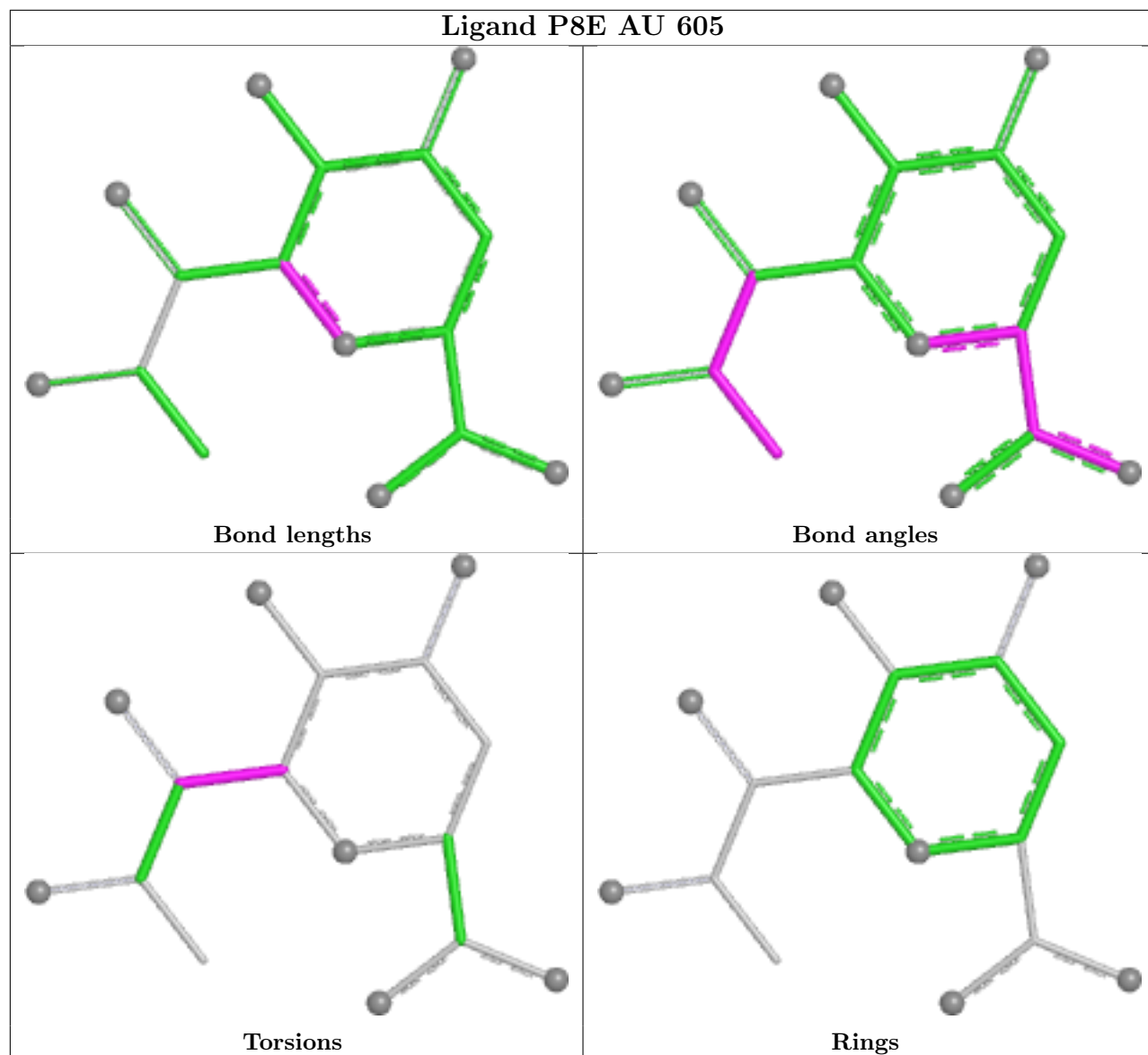




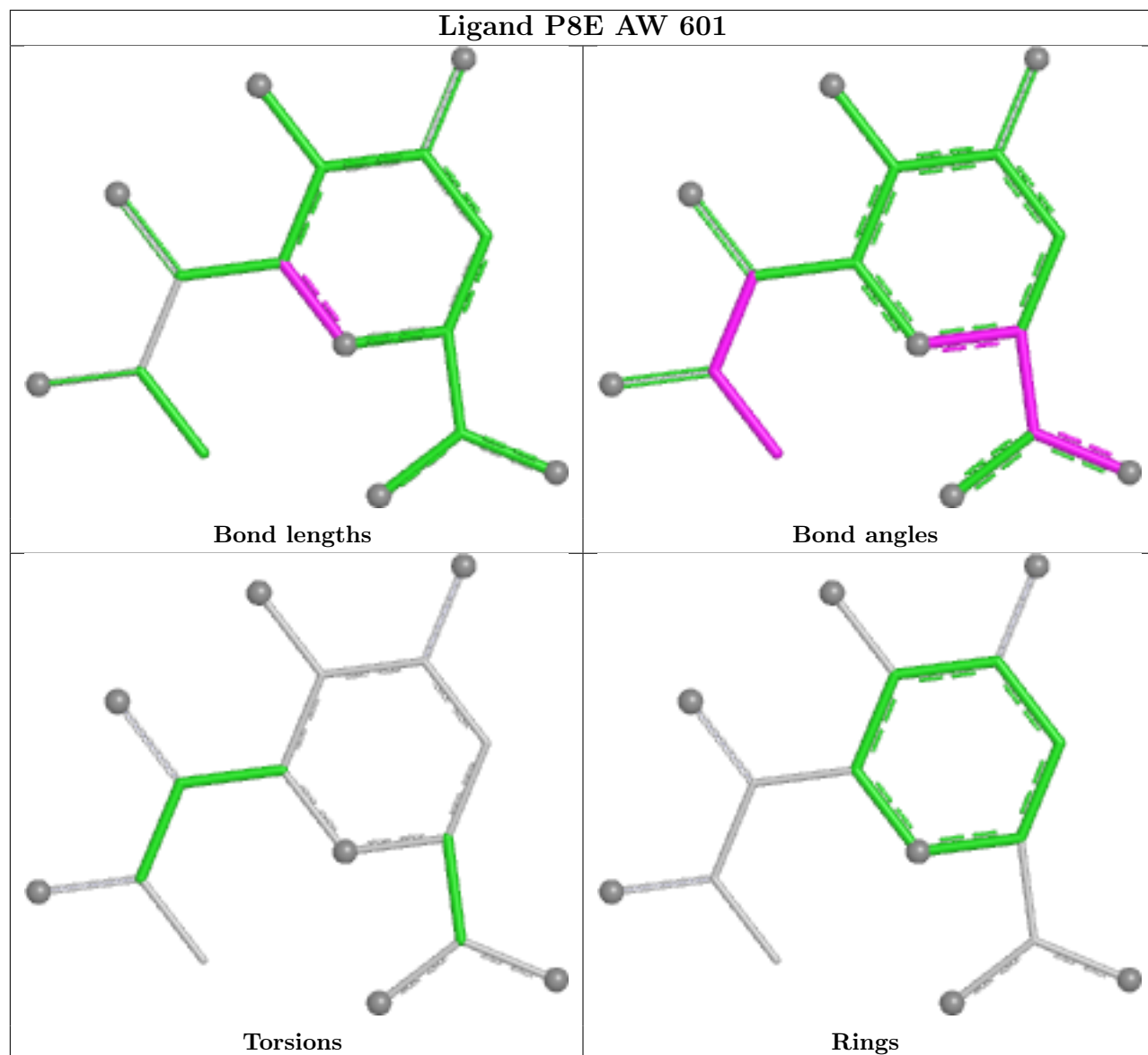


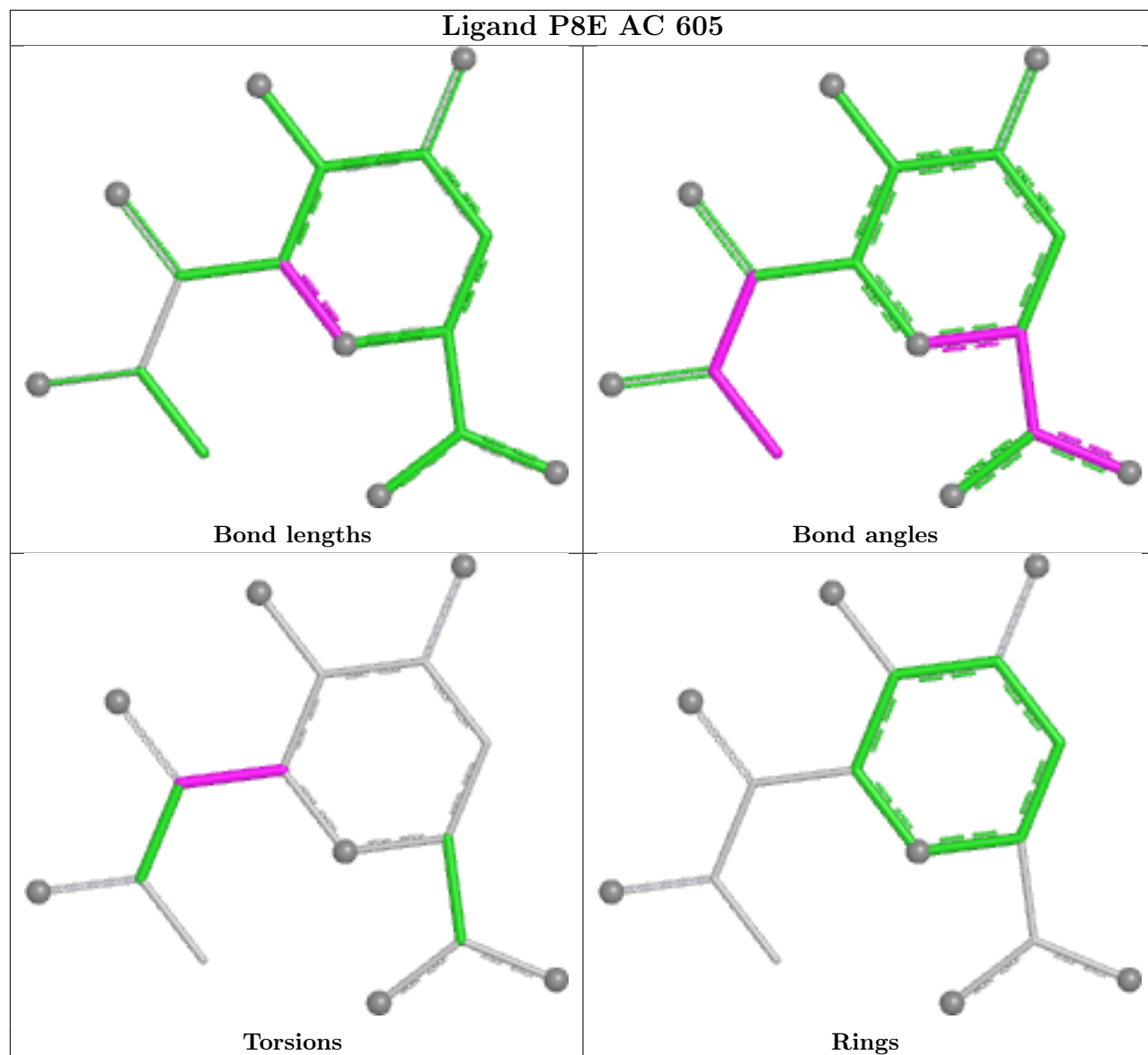


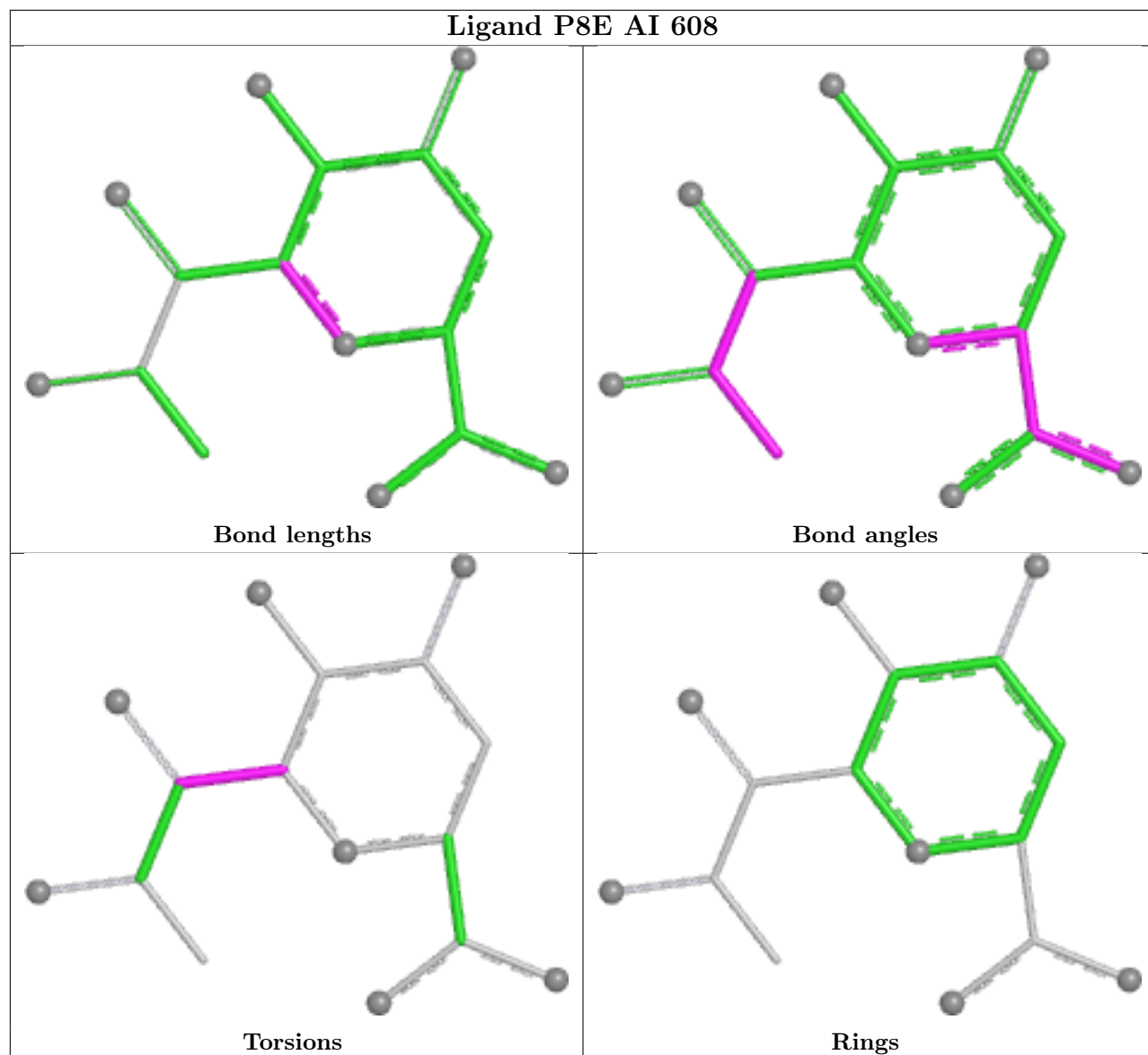


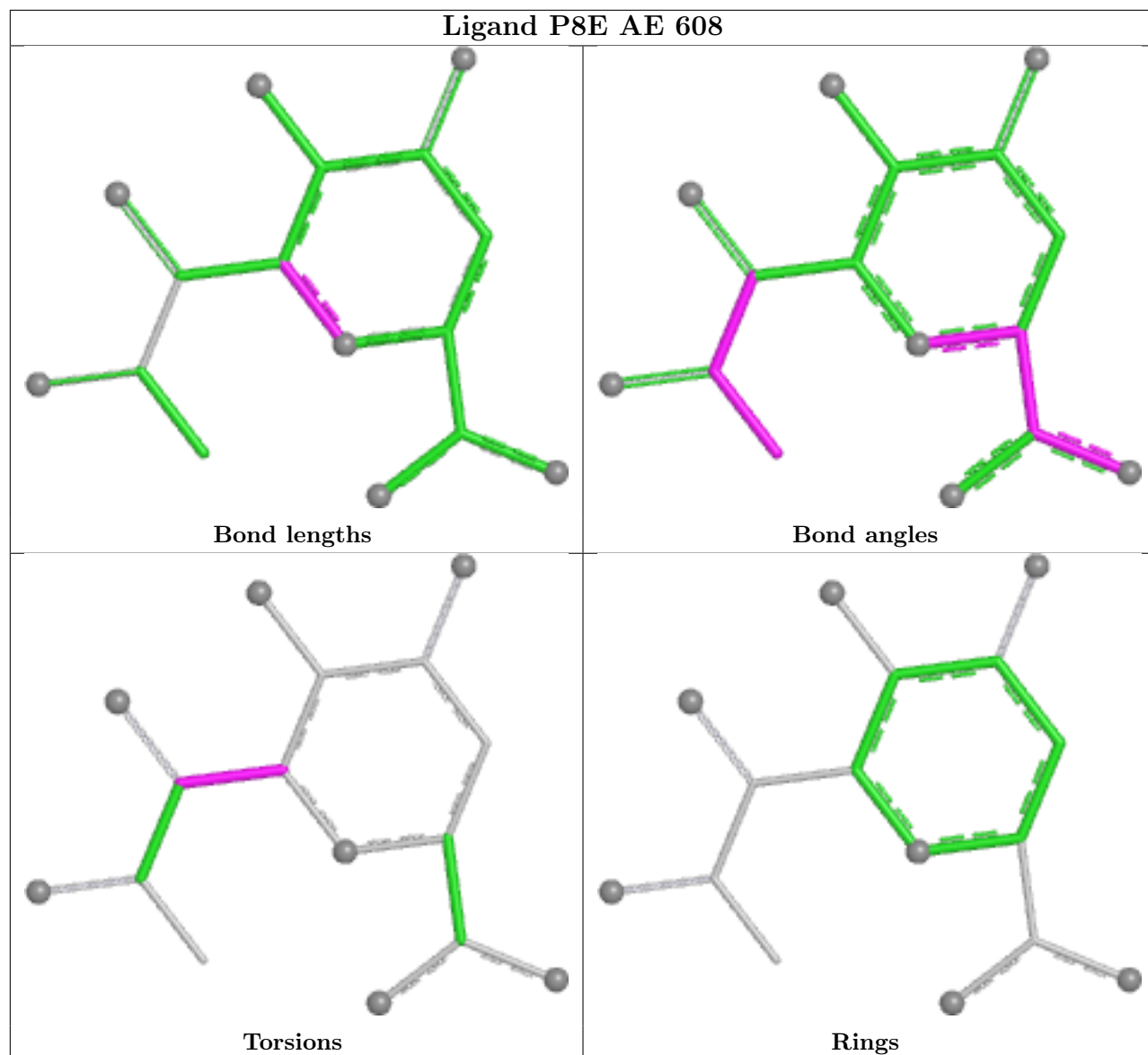


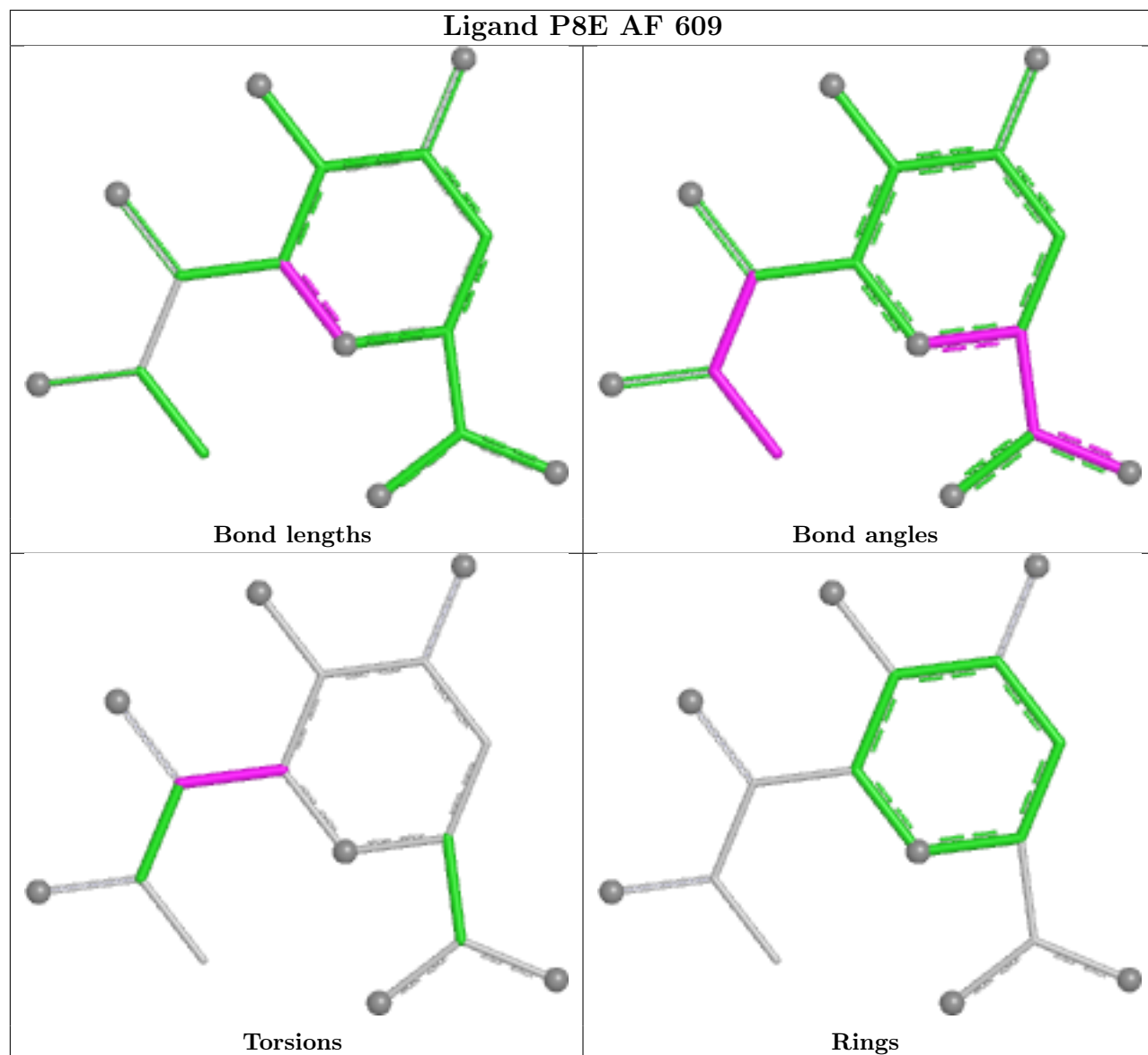
Ligand P8E AW 601

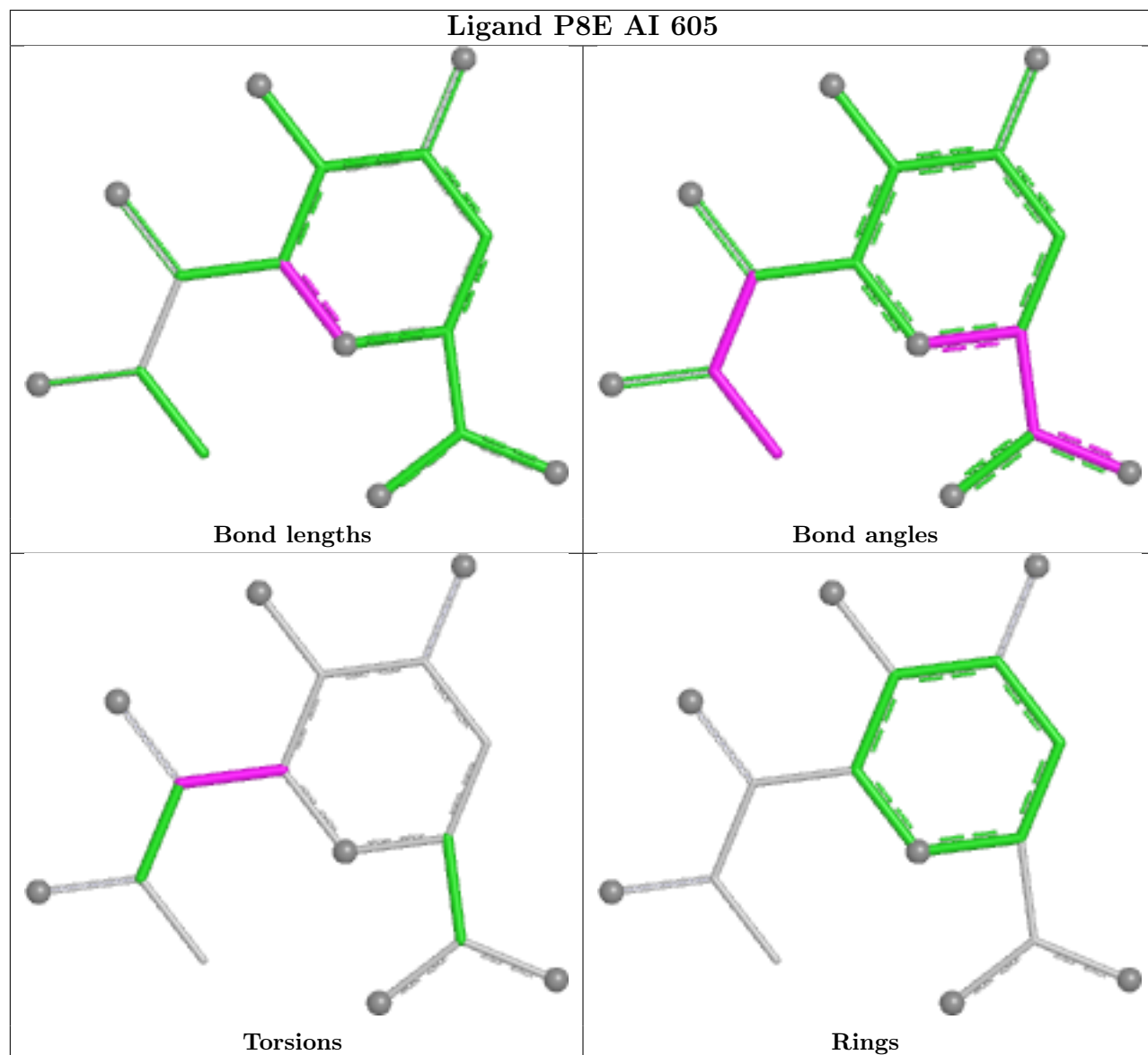


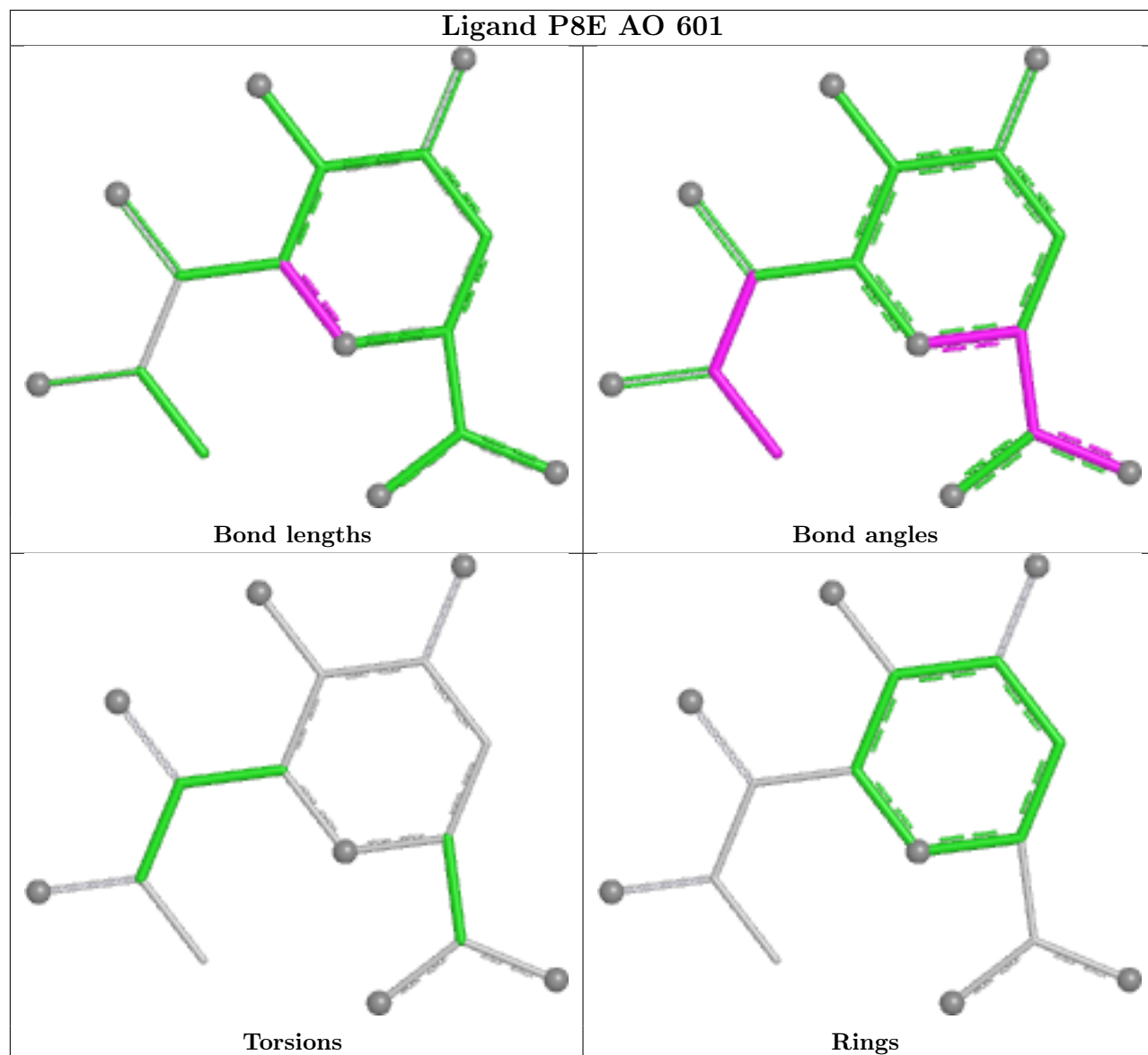


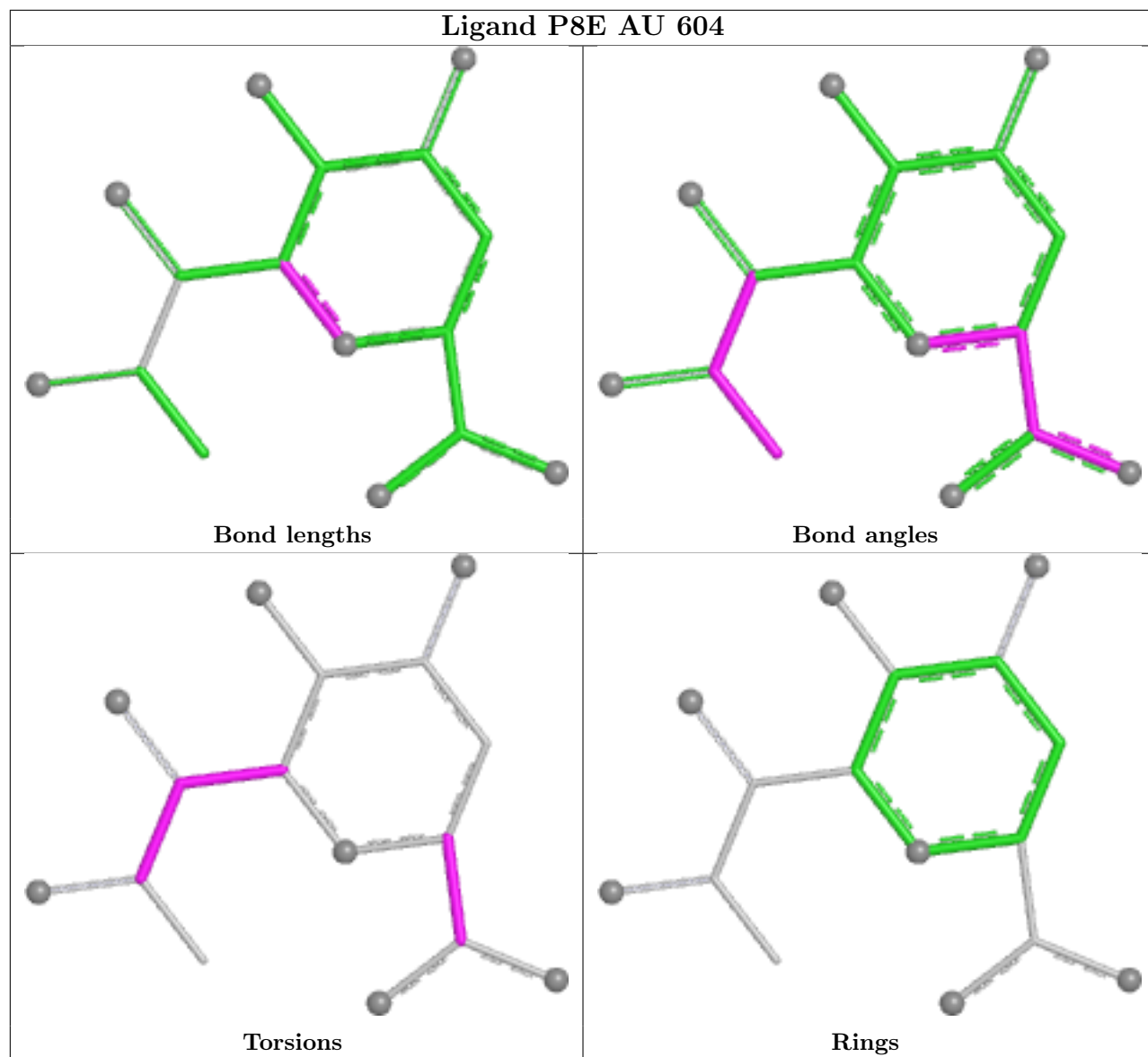


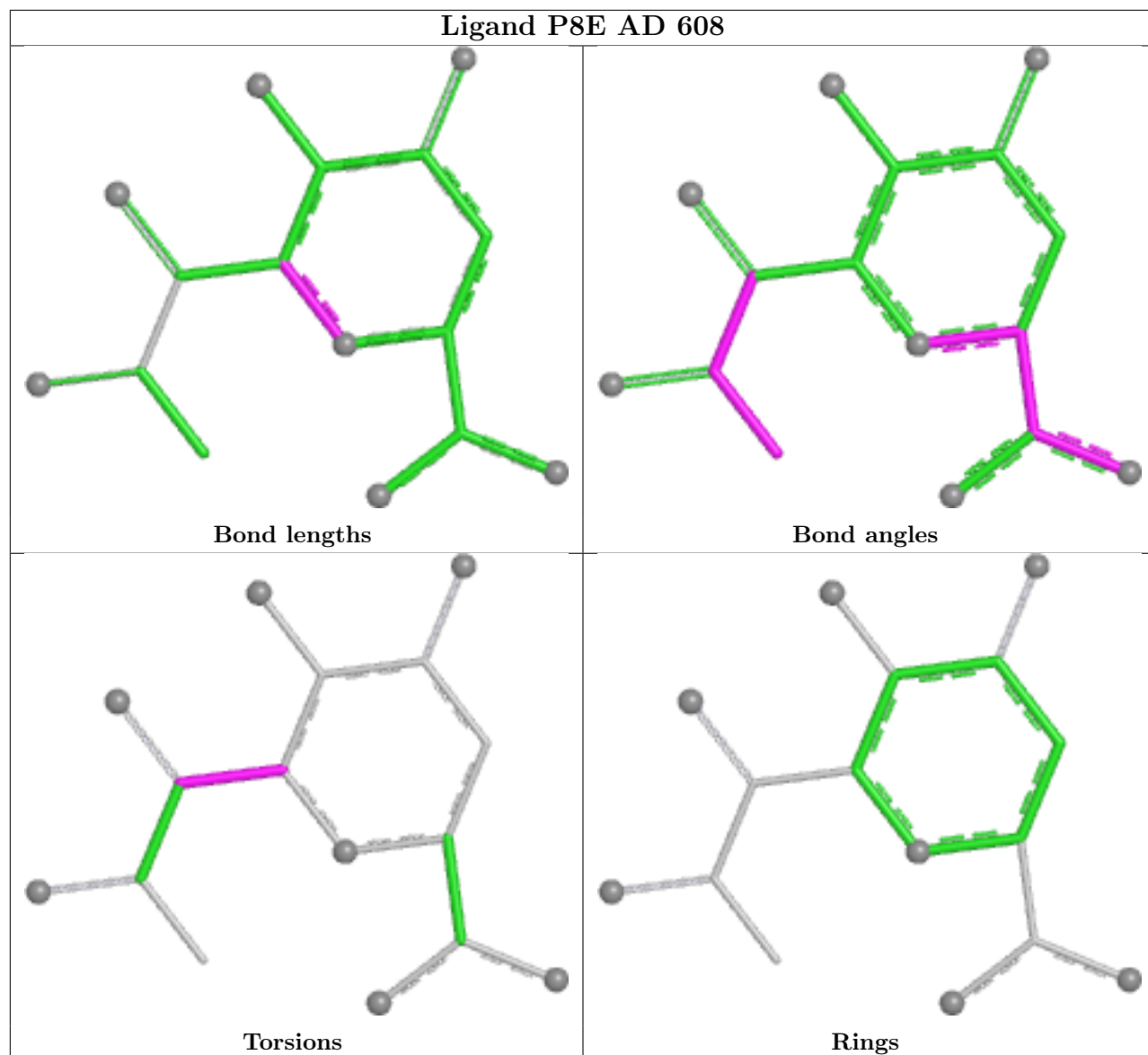


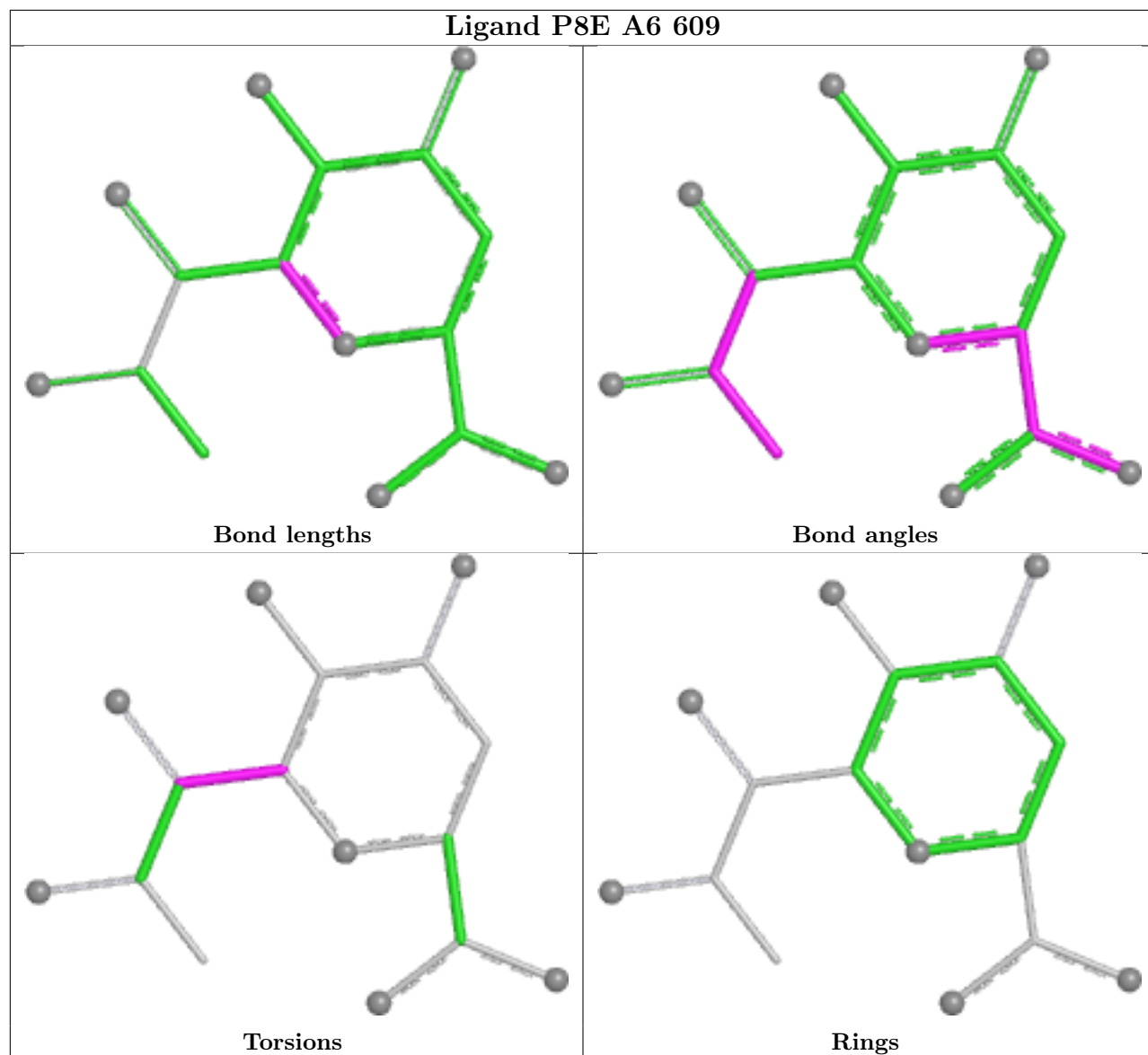


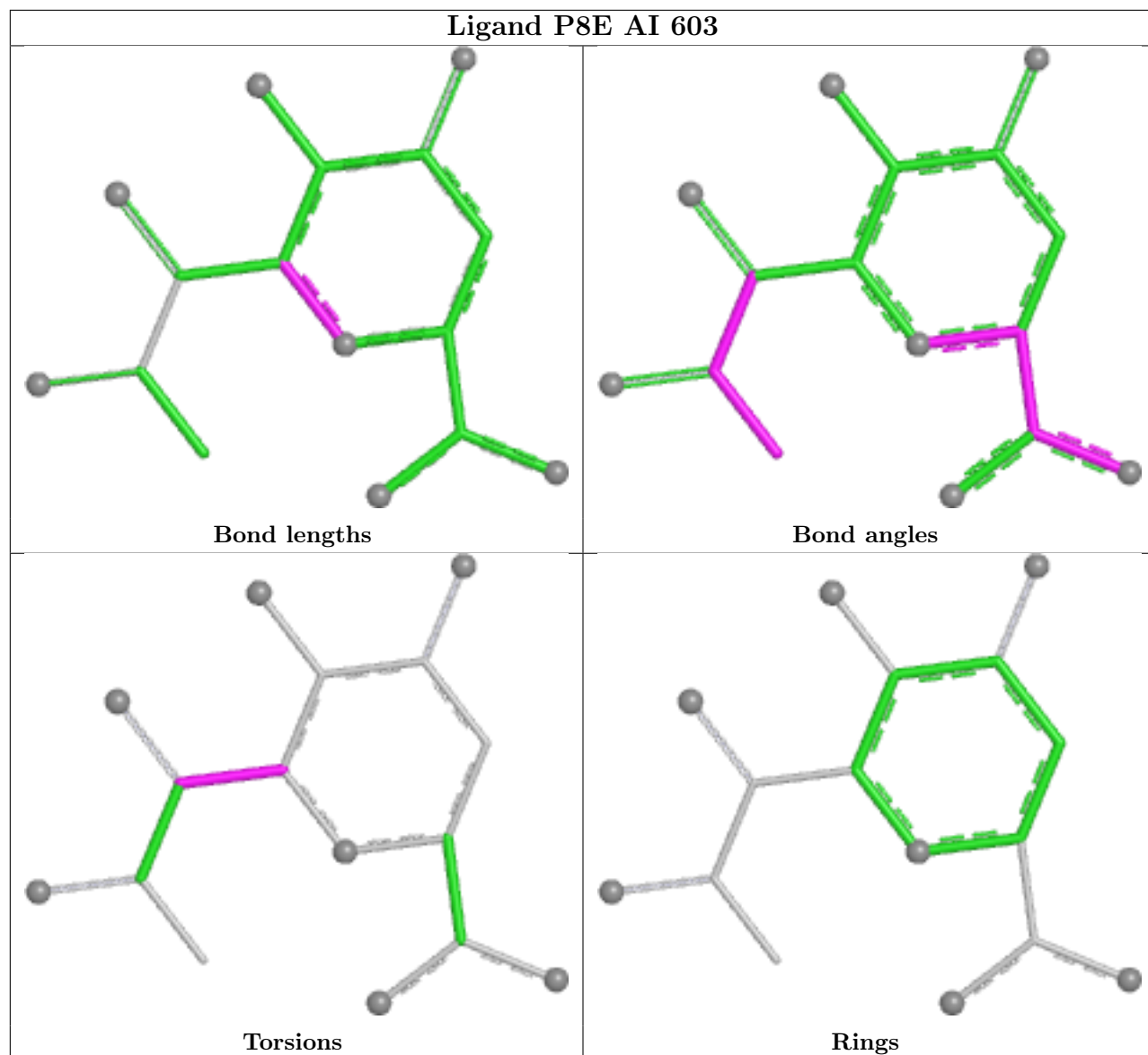


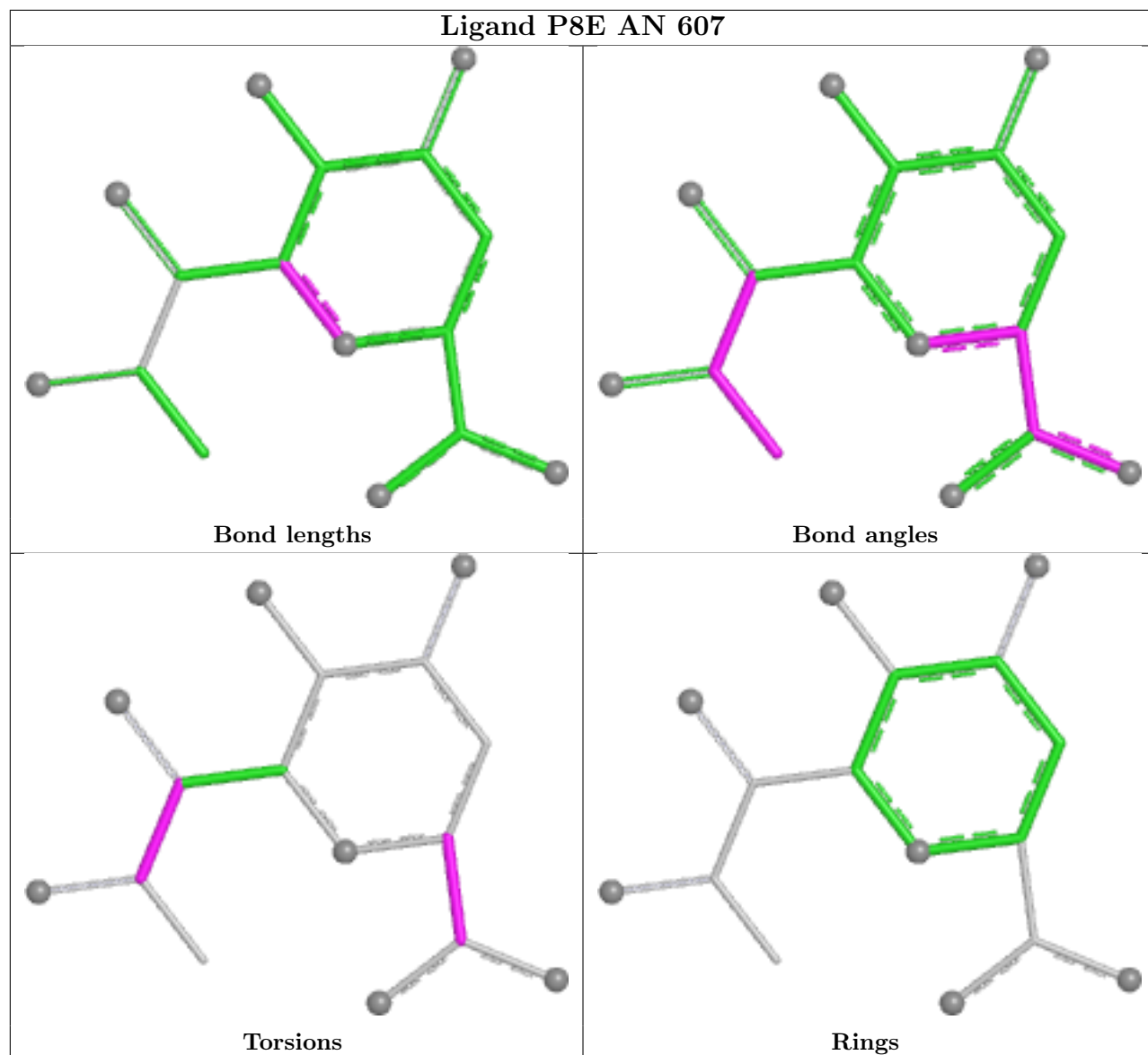


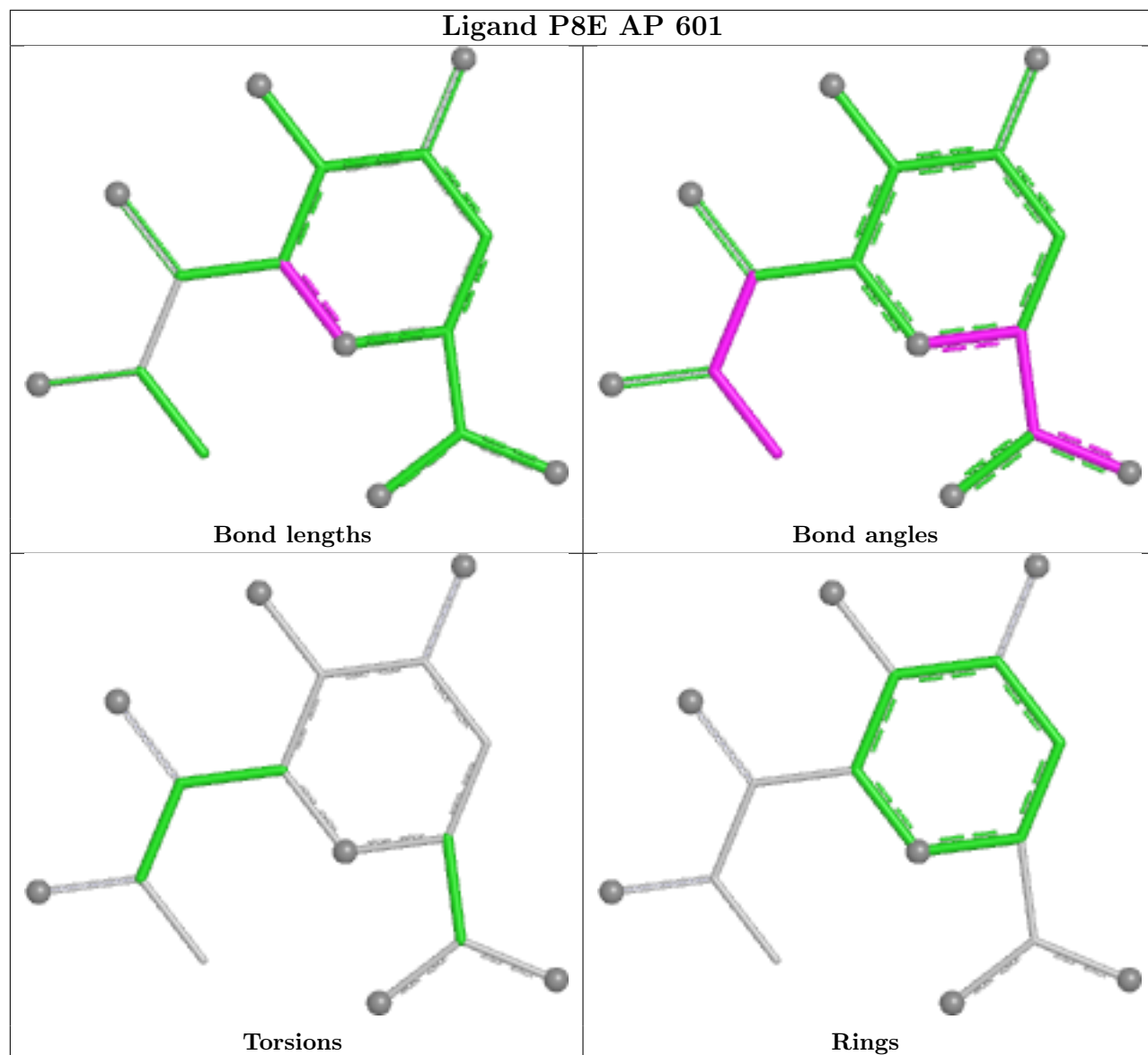


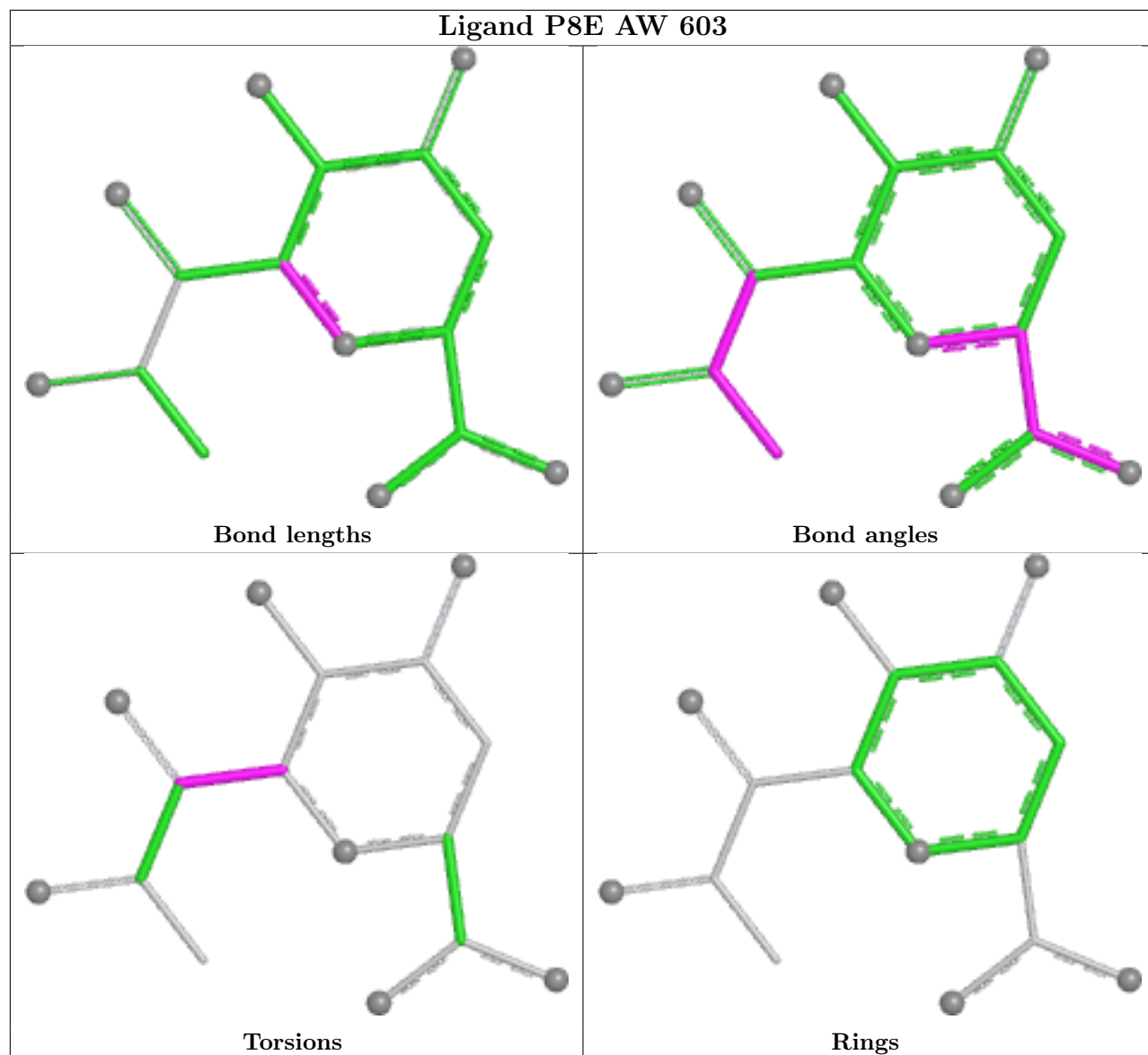


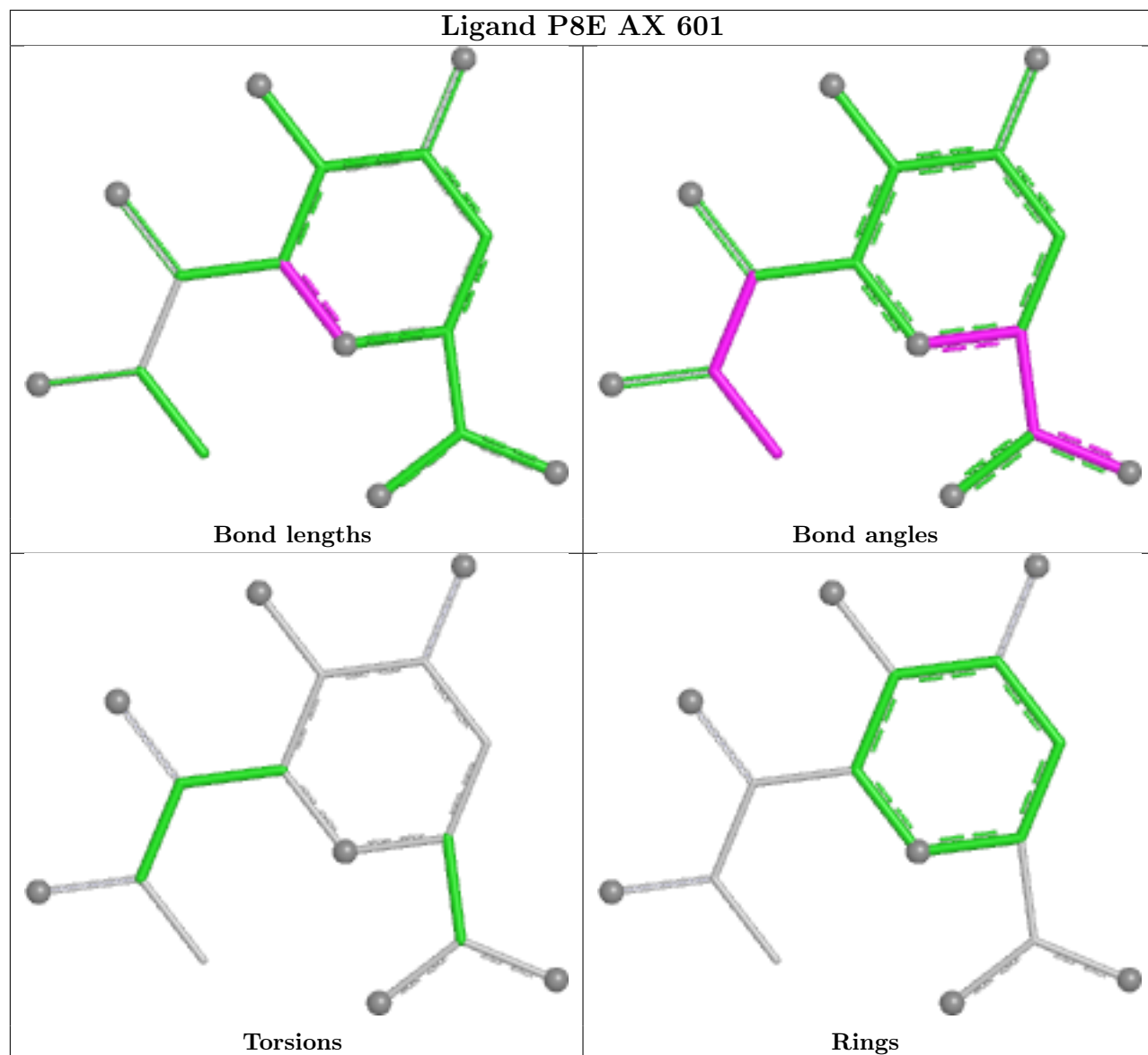


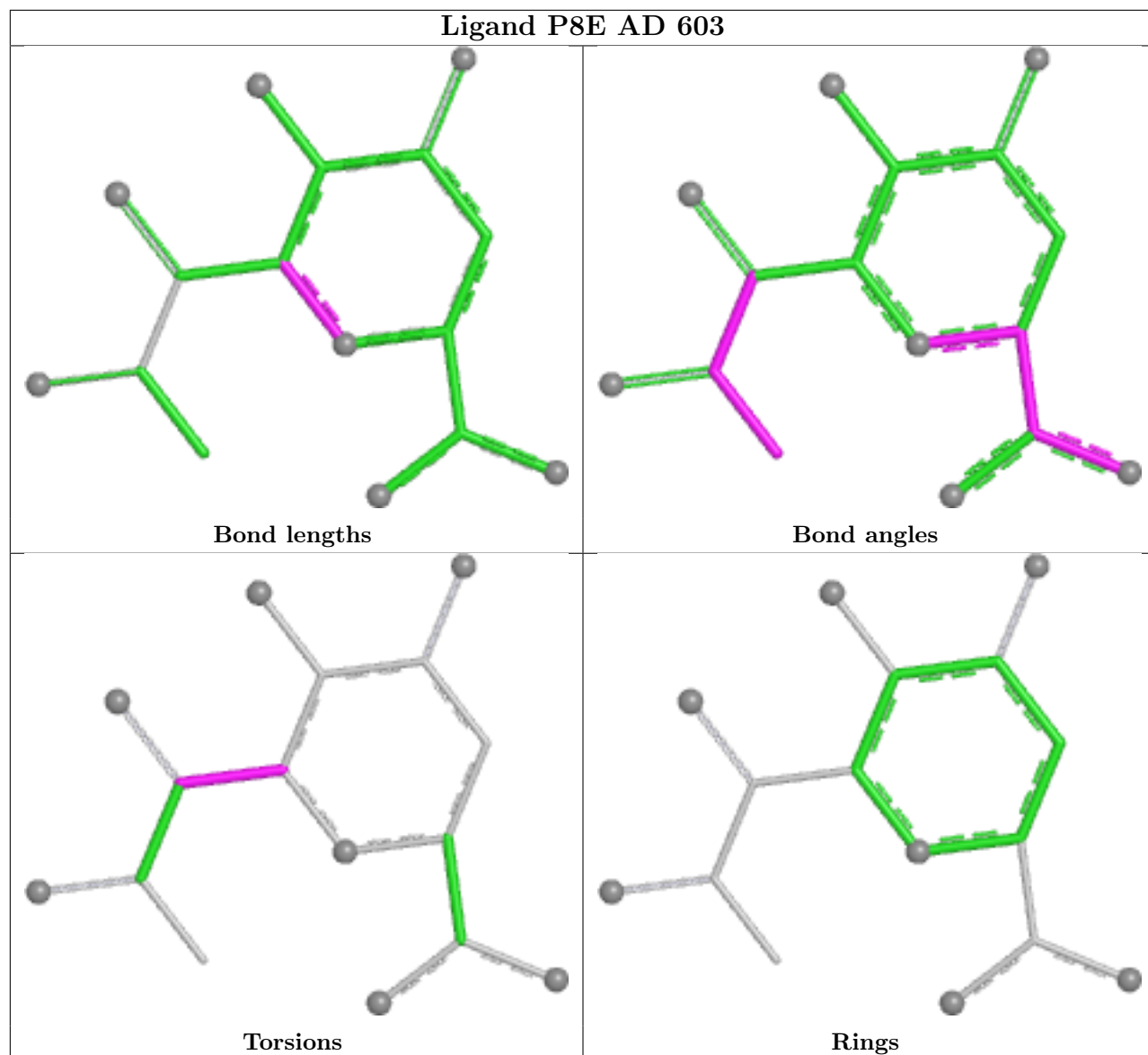


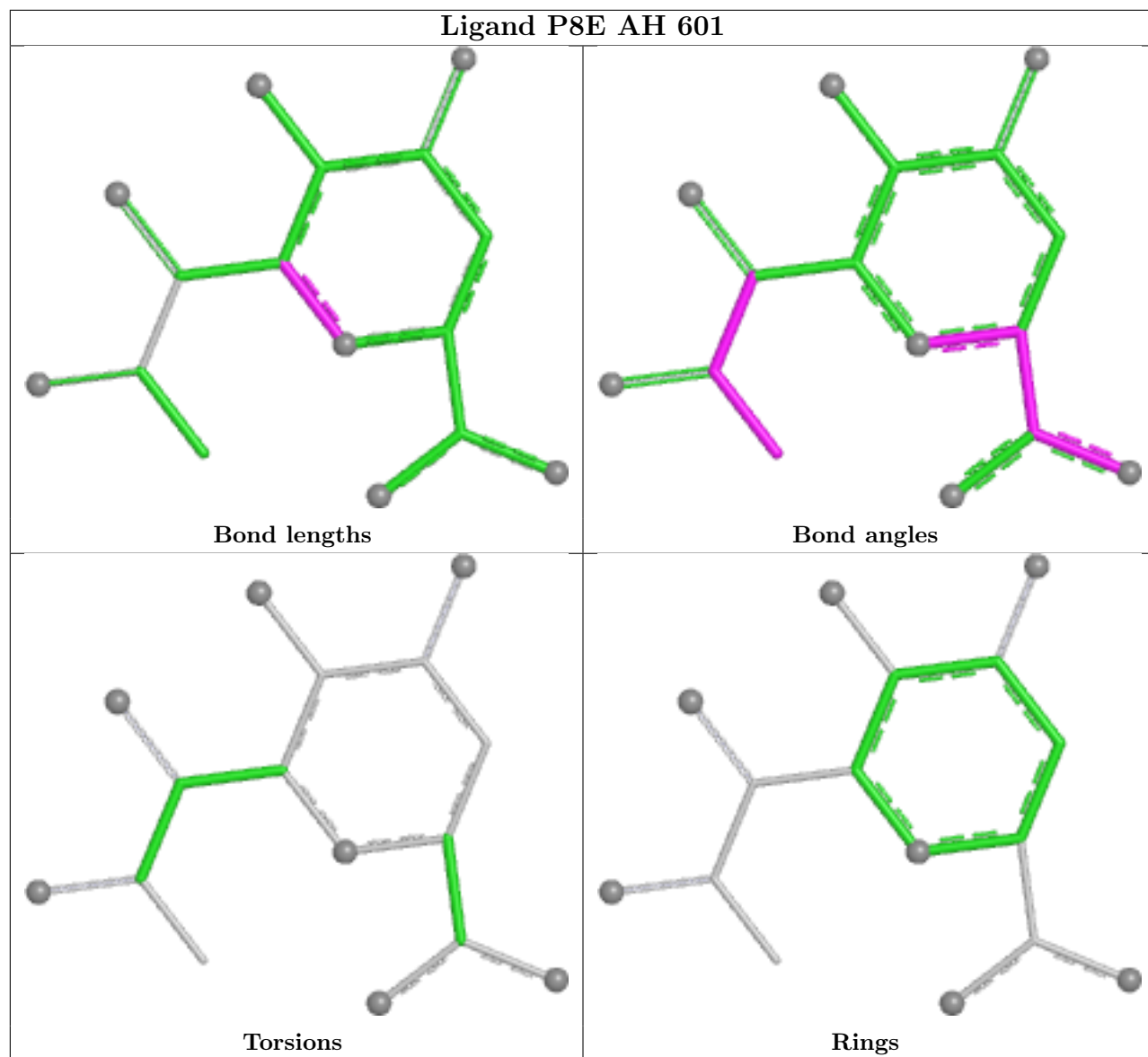


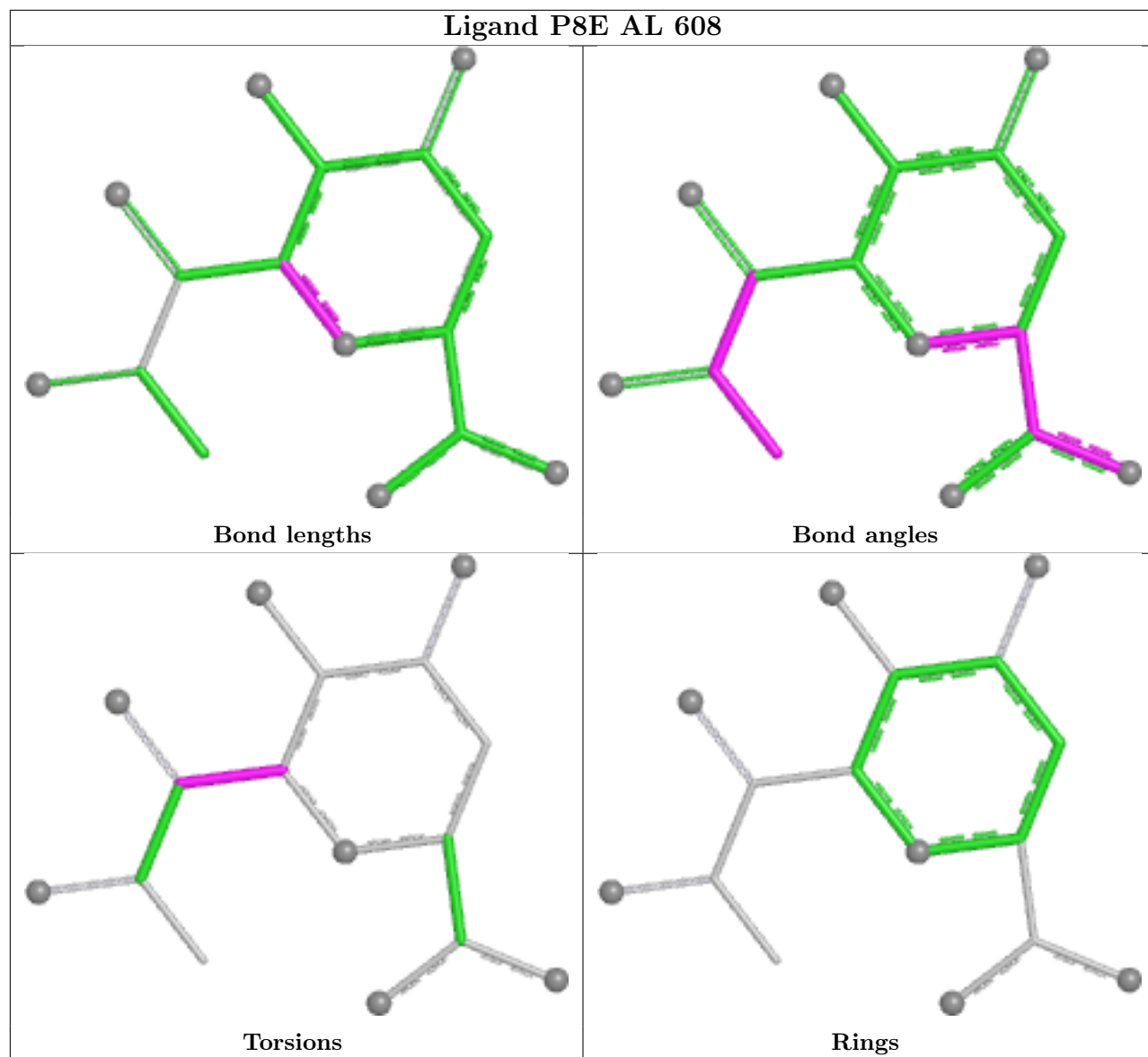


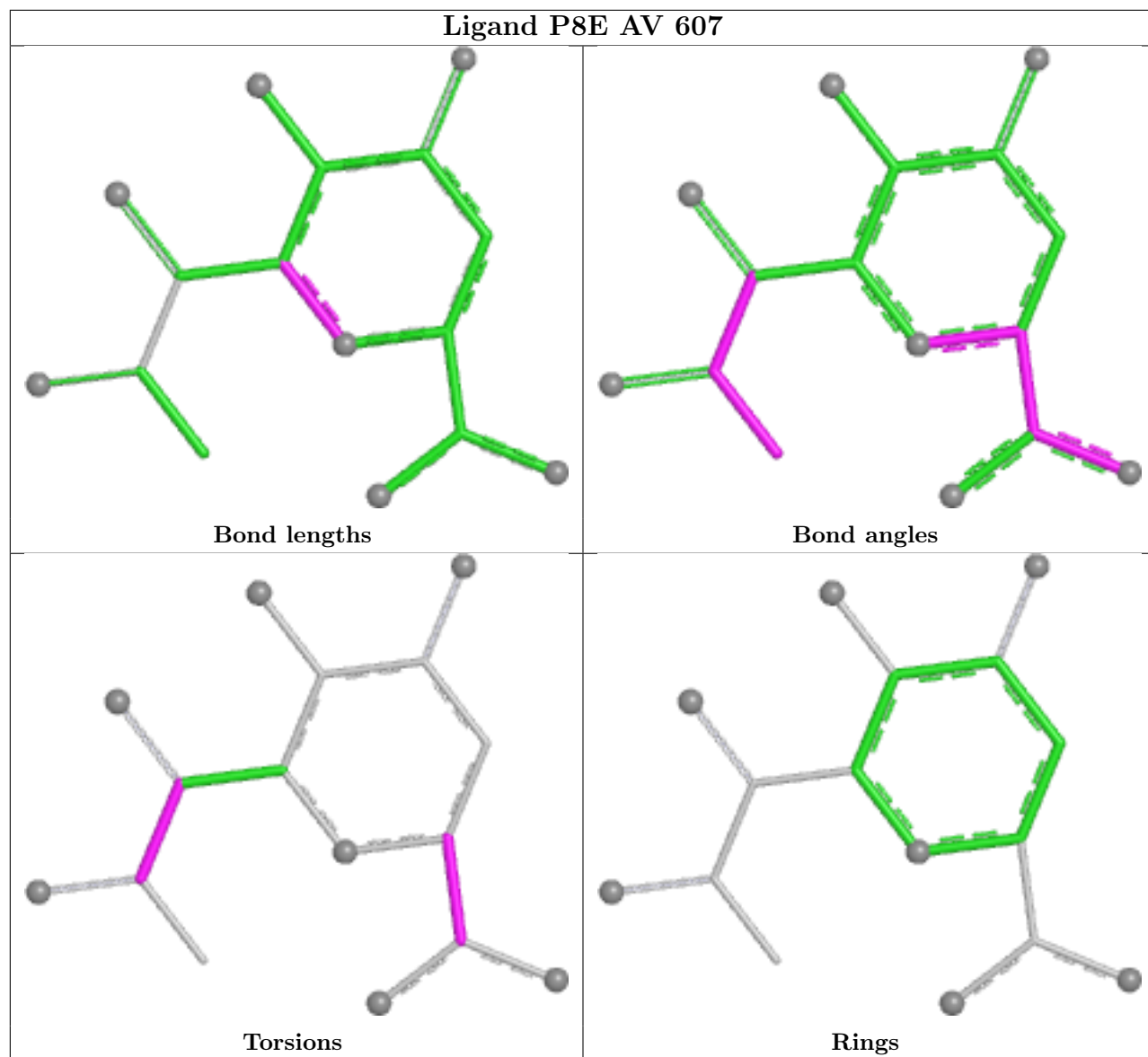


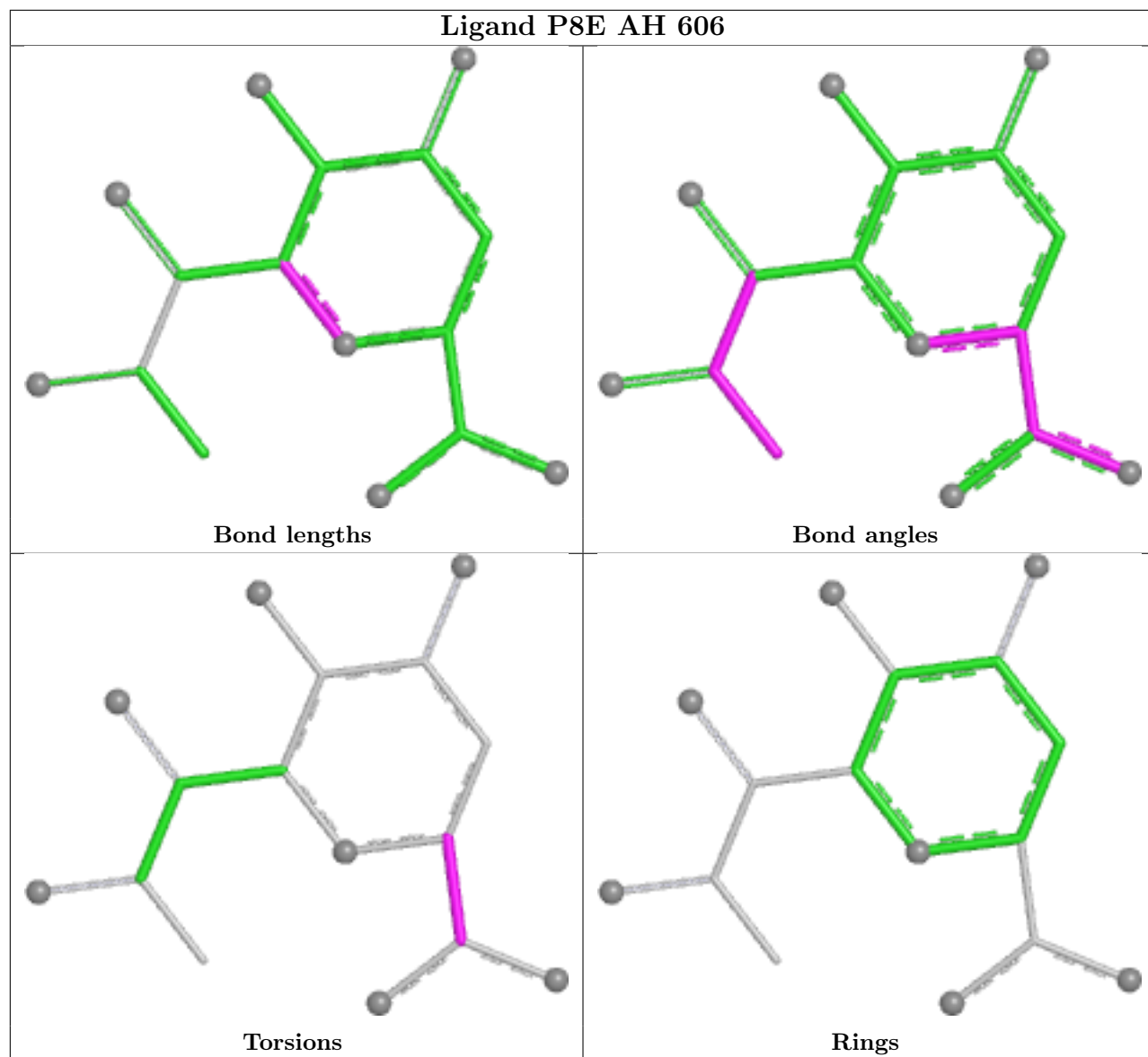


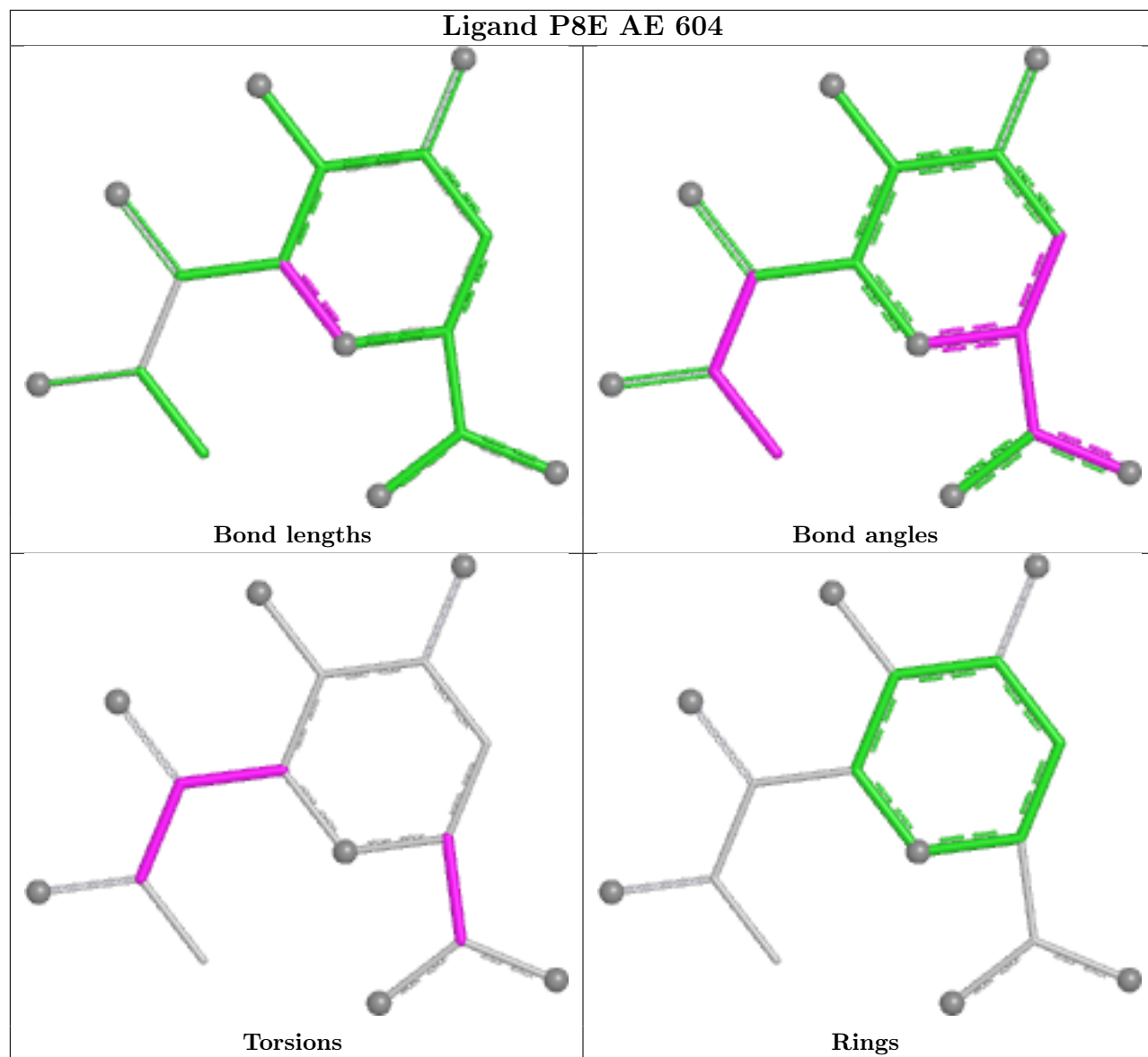


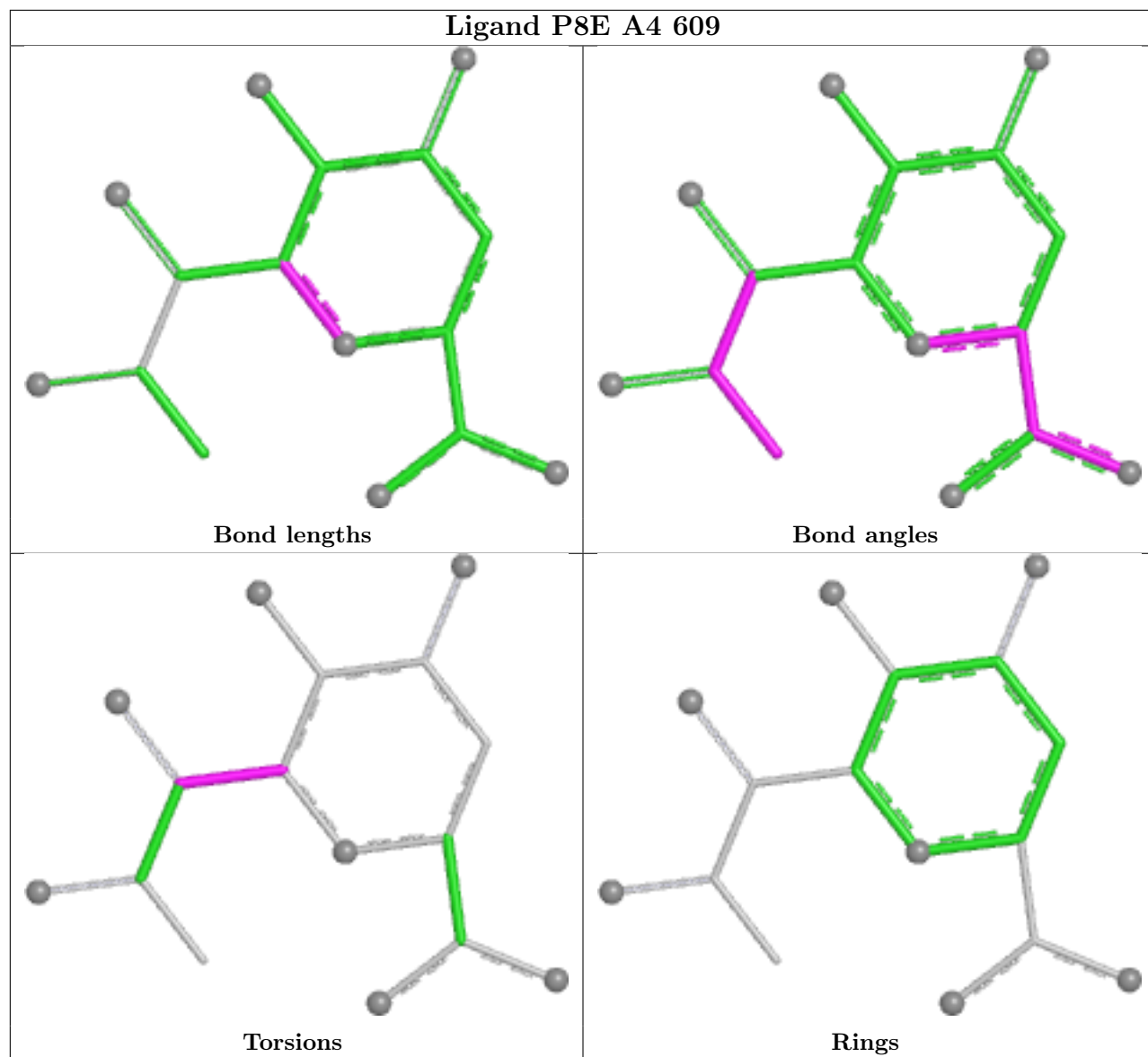


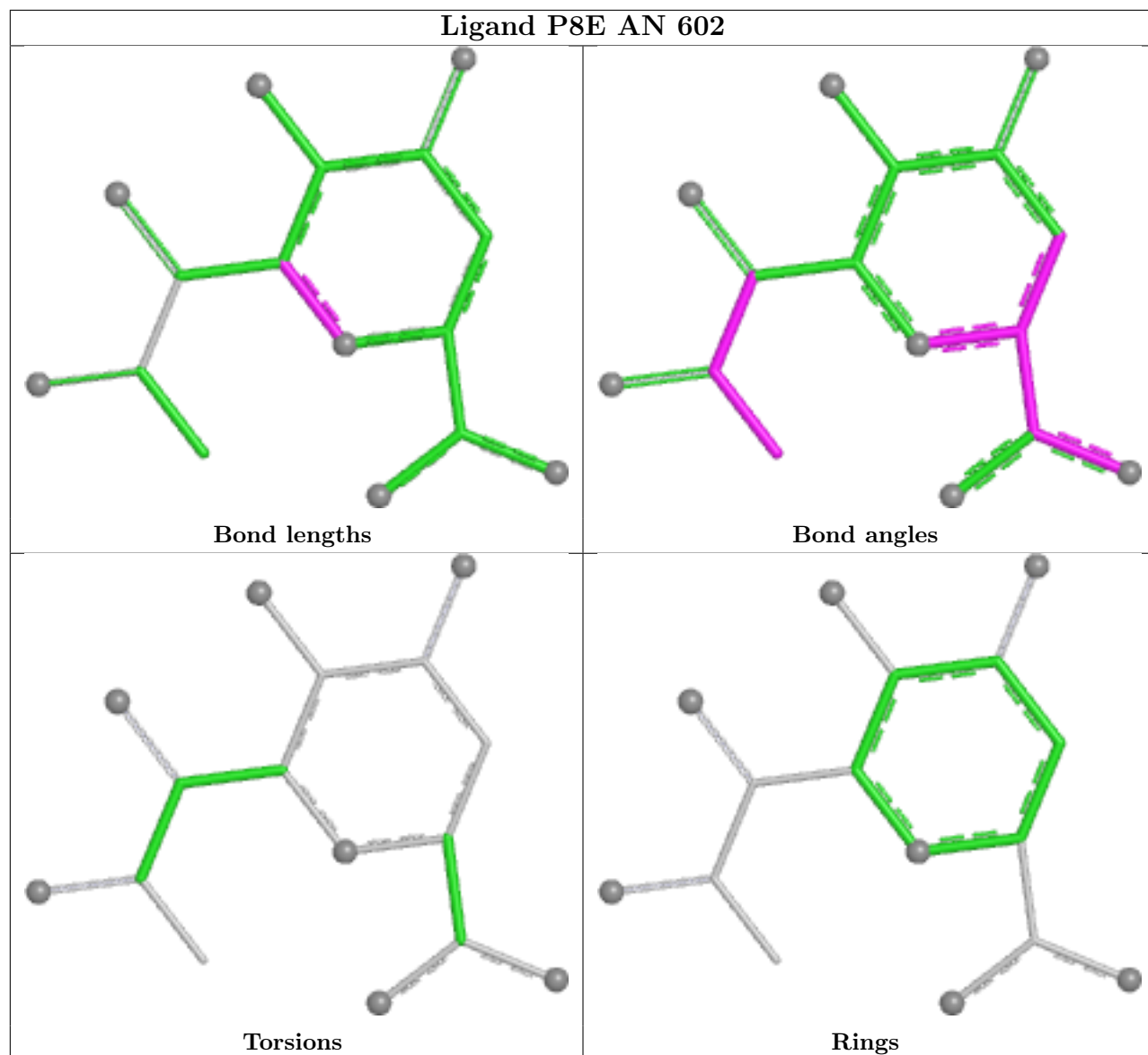


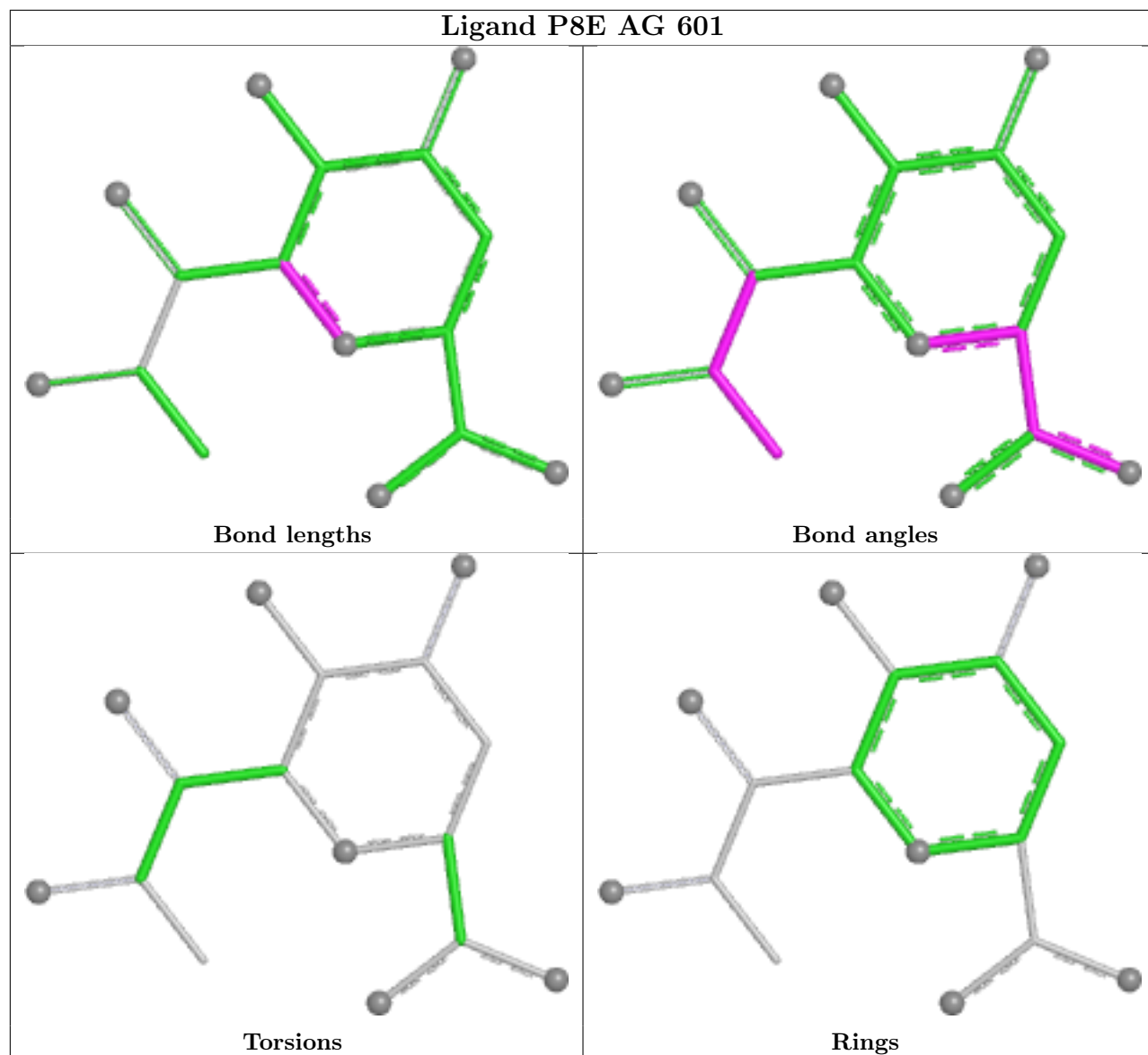


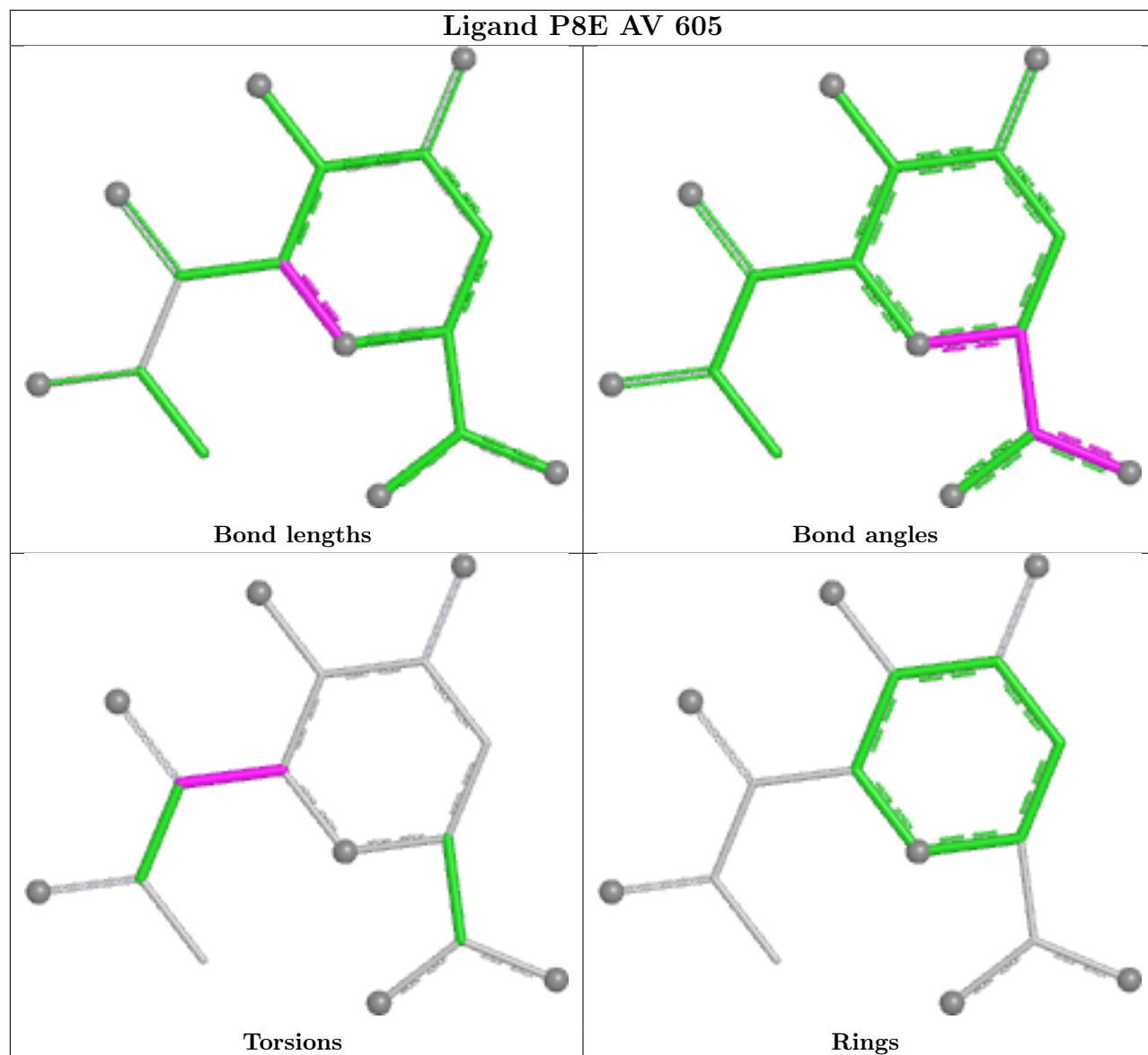


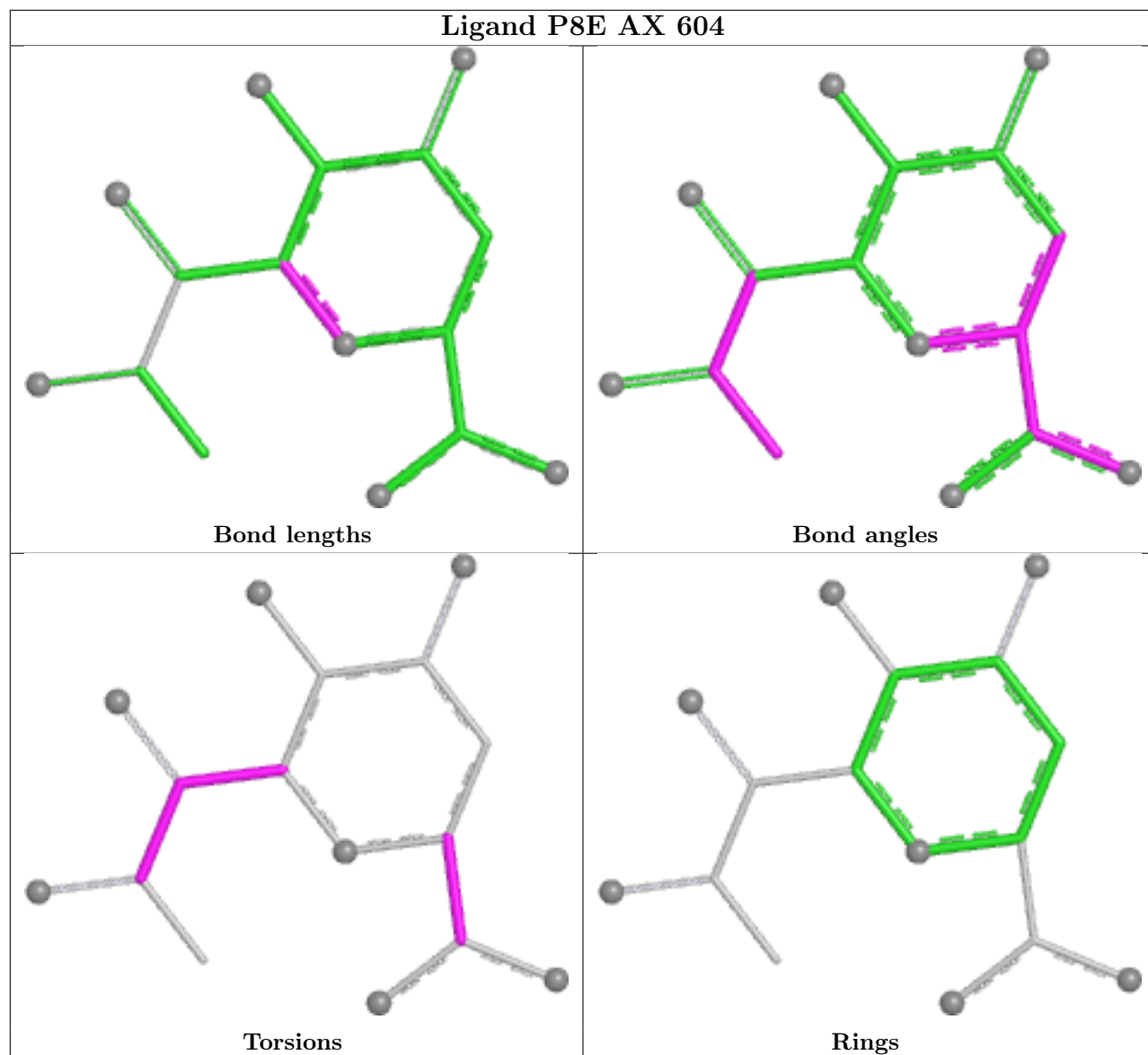


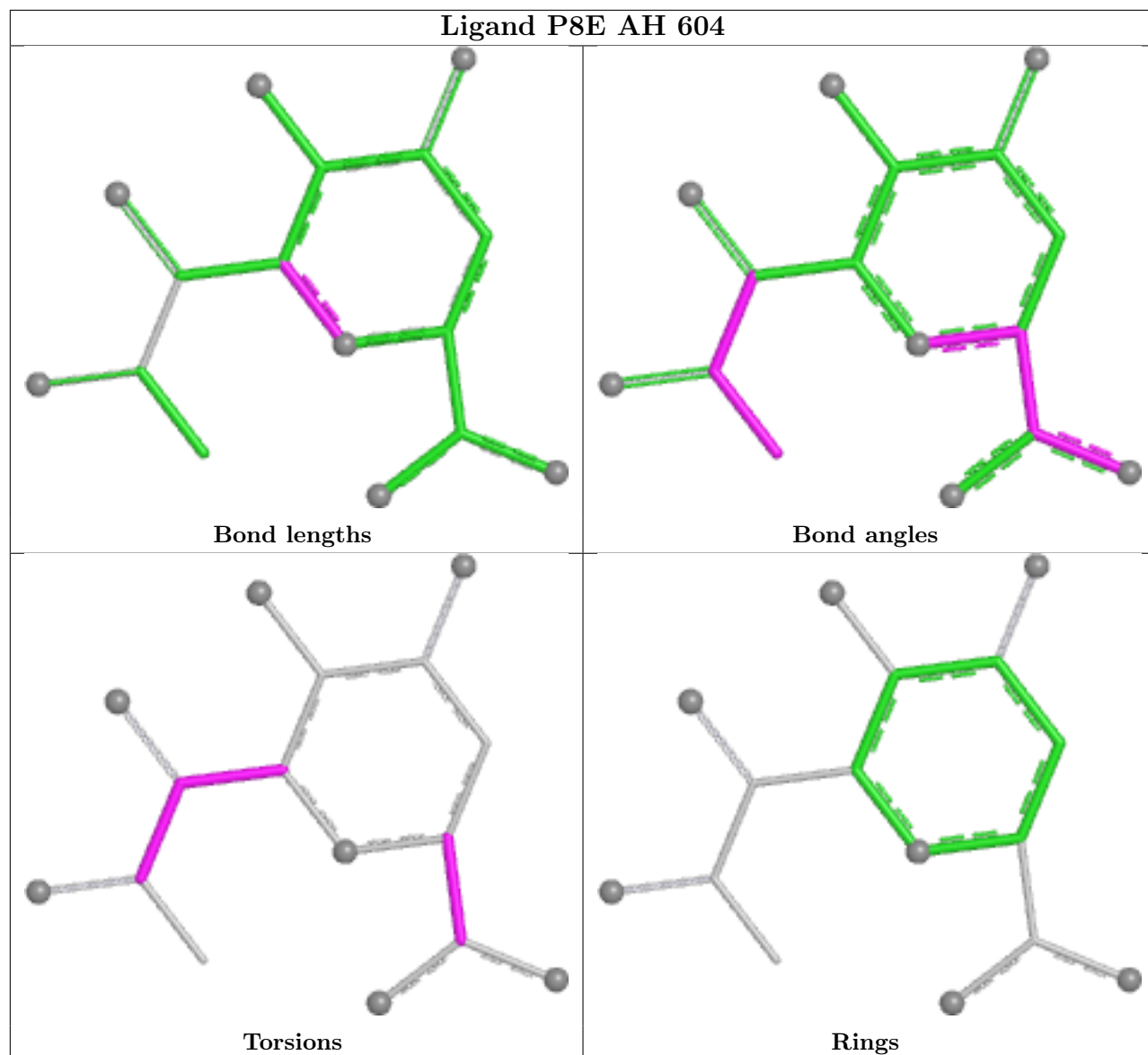


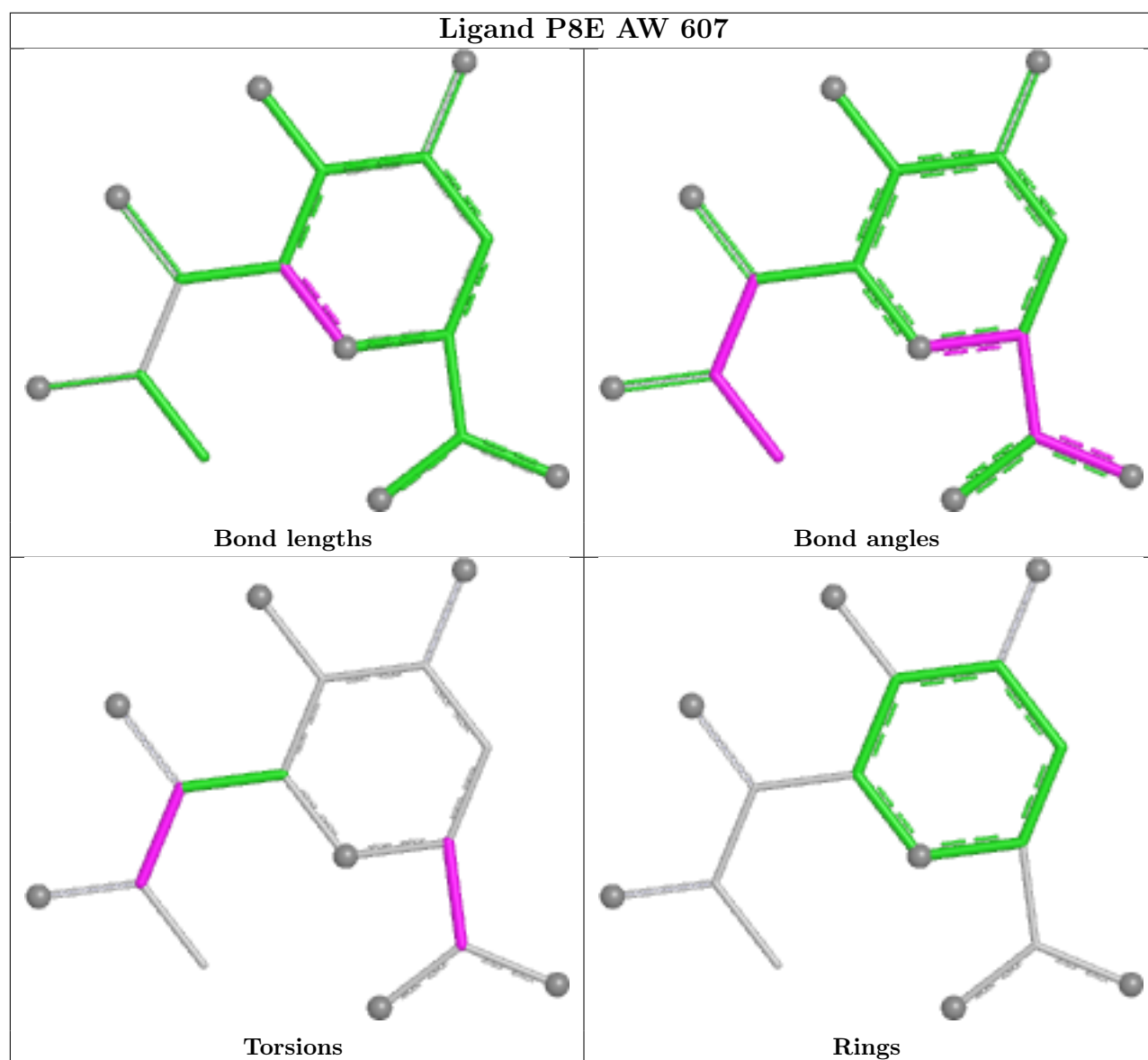


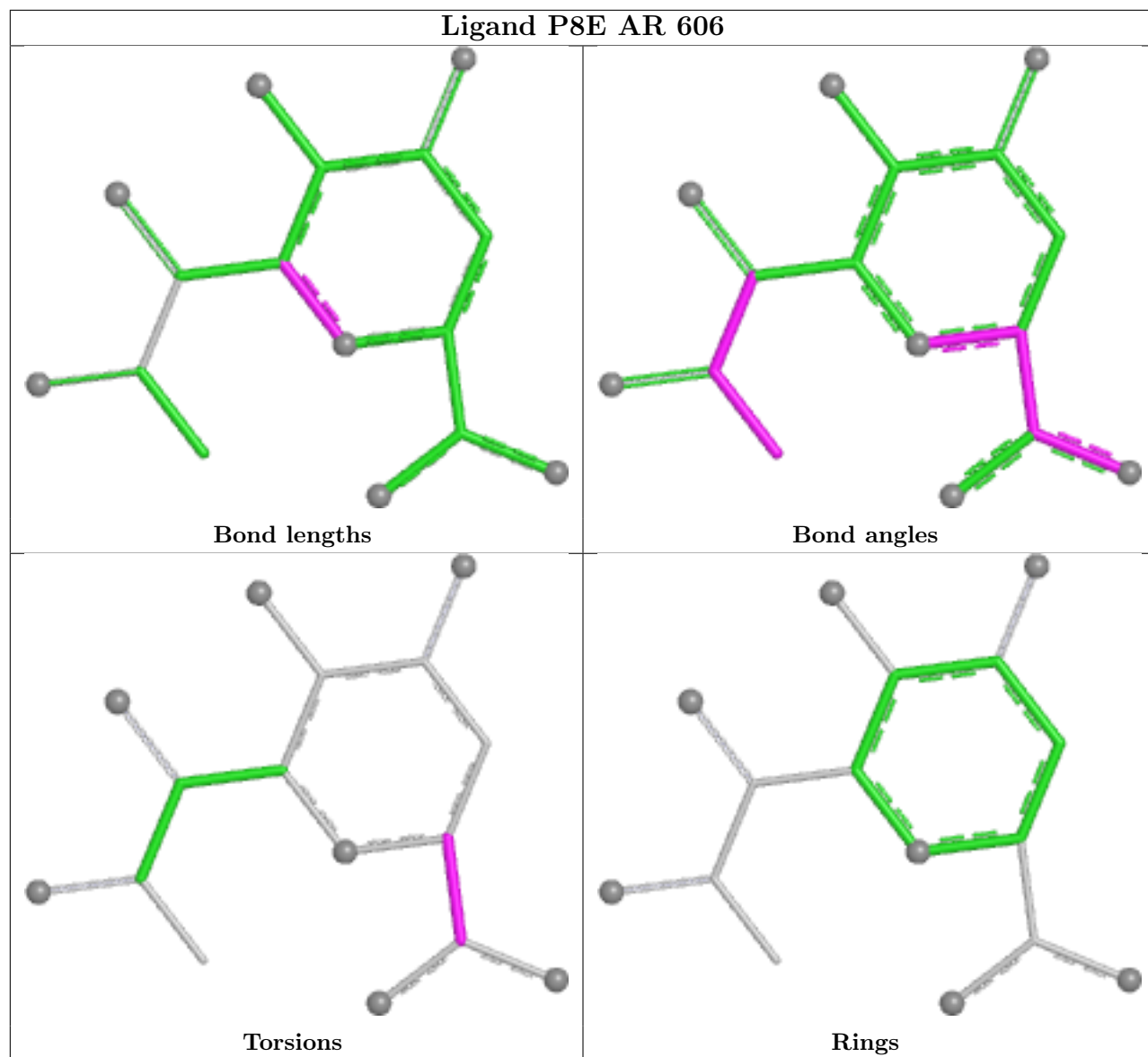


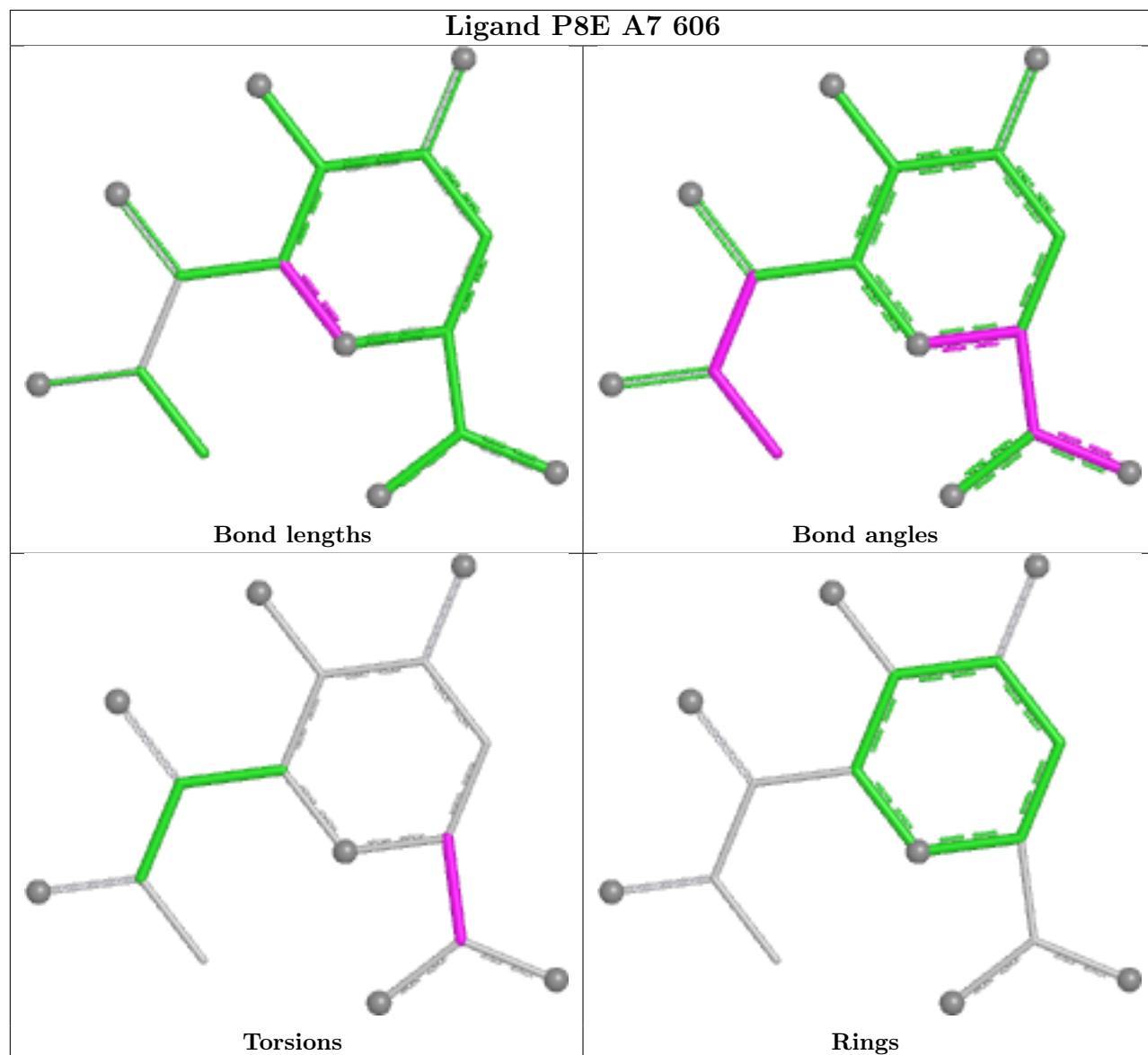


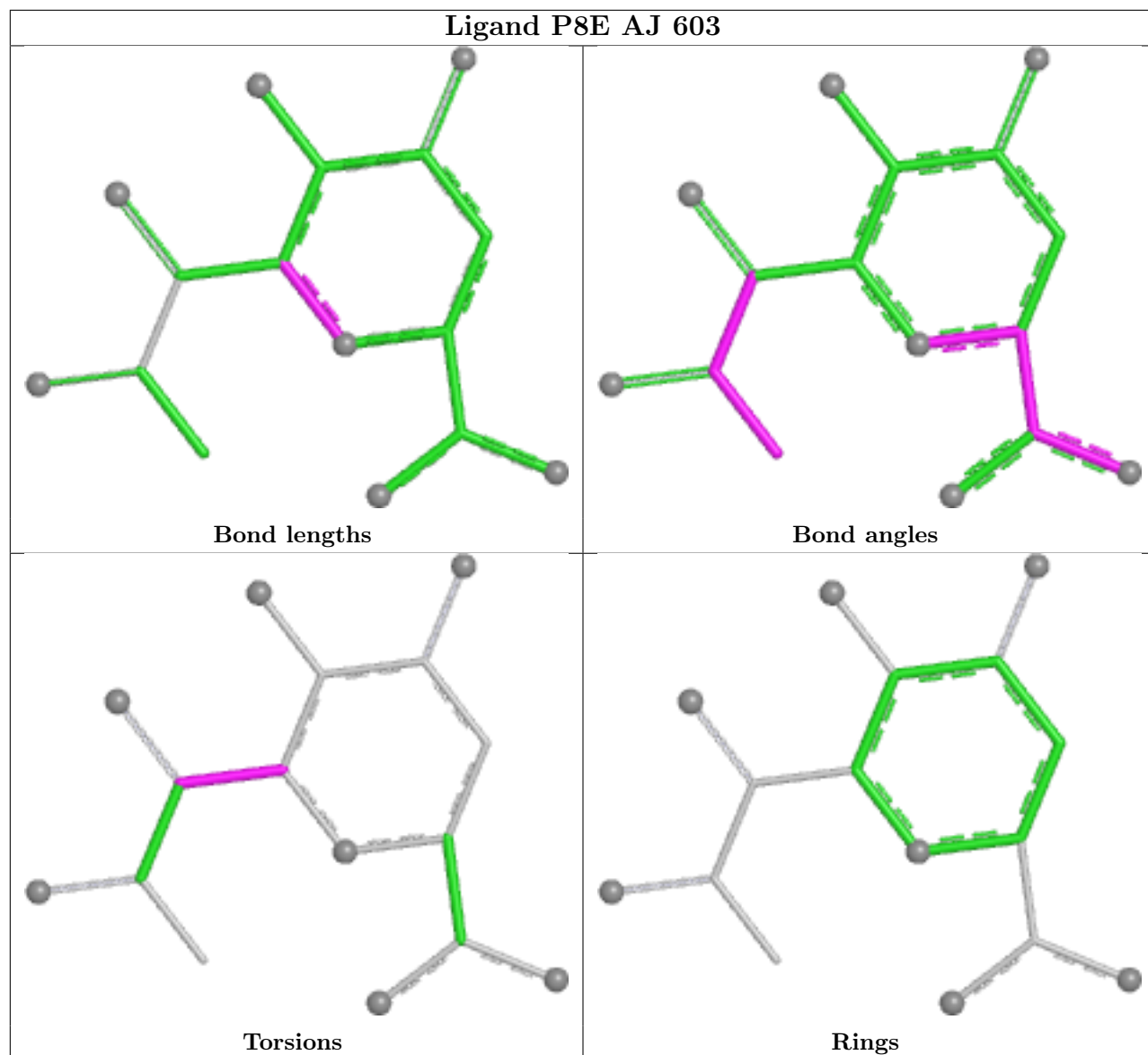


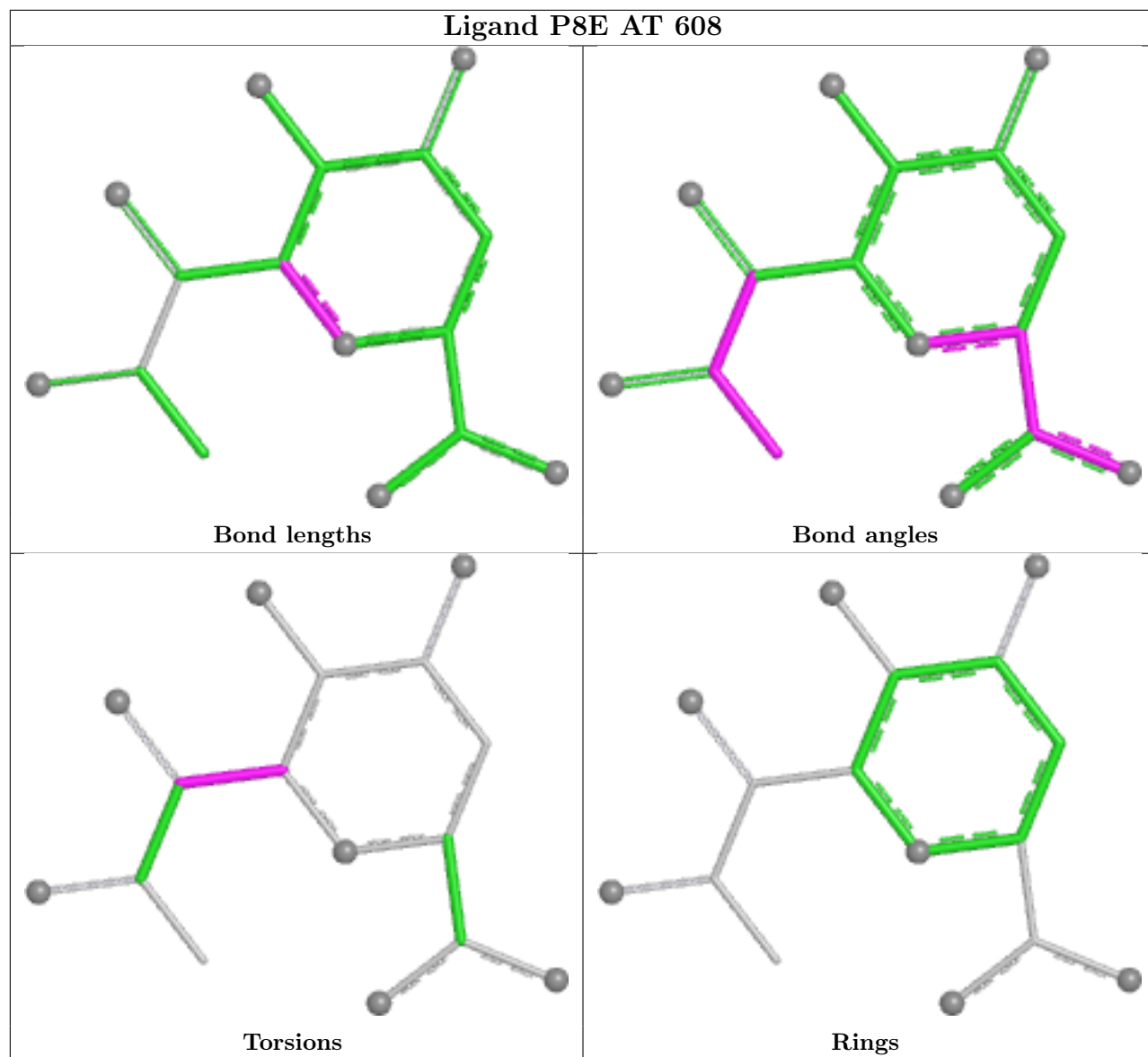


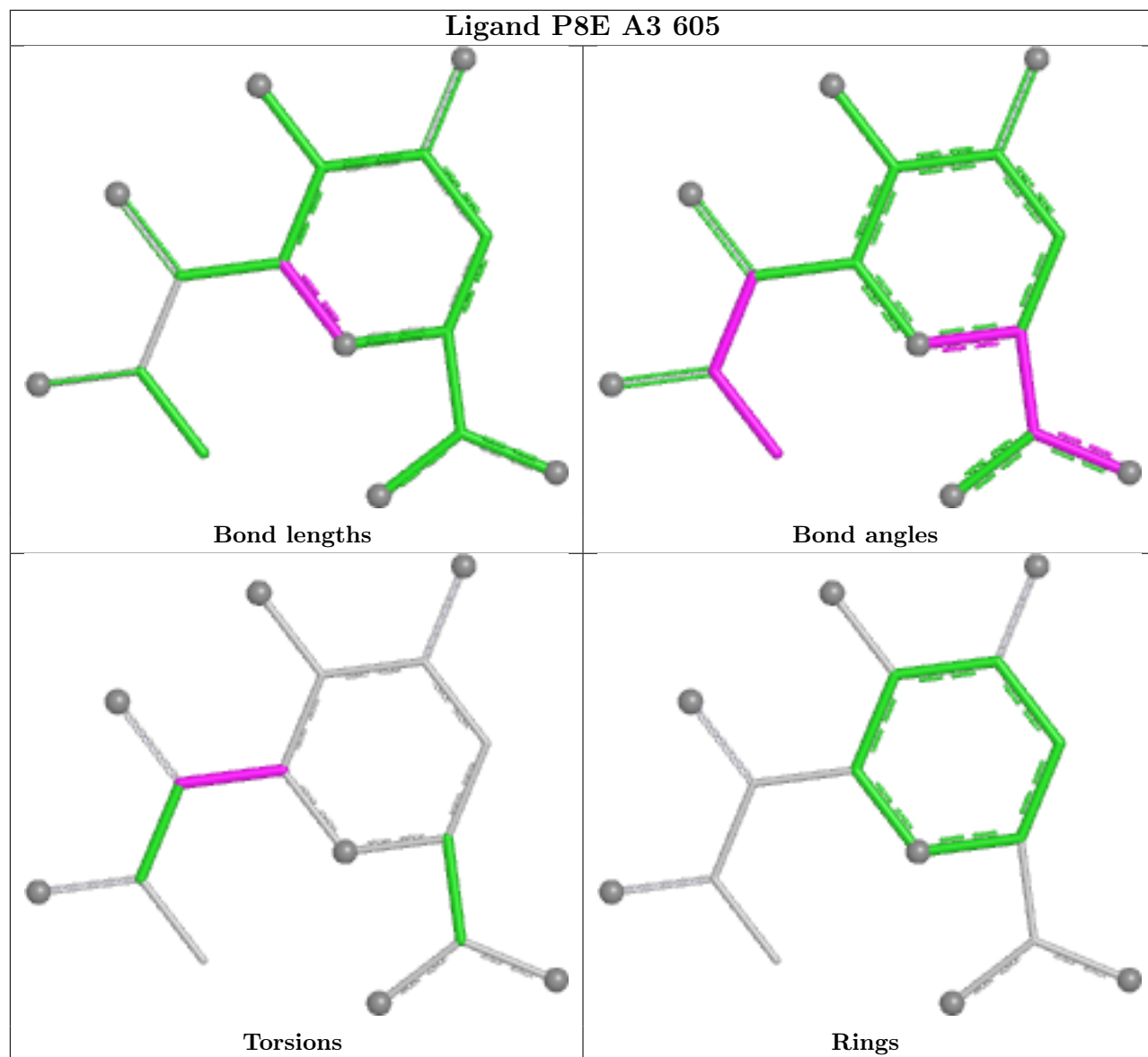


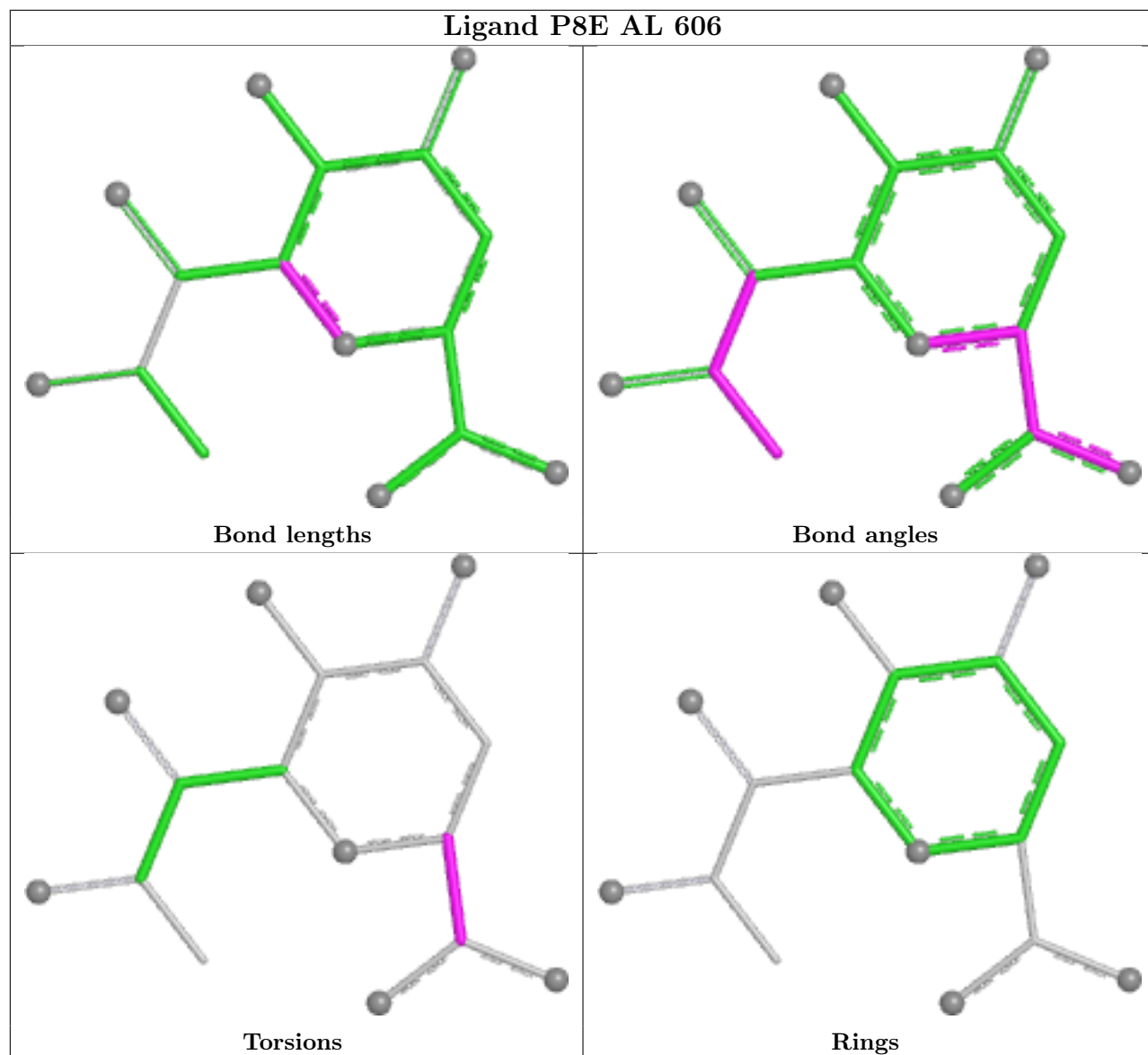


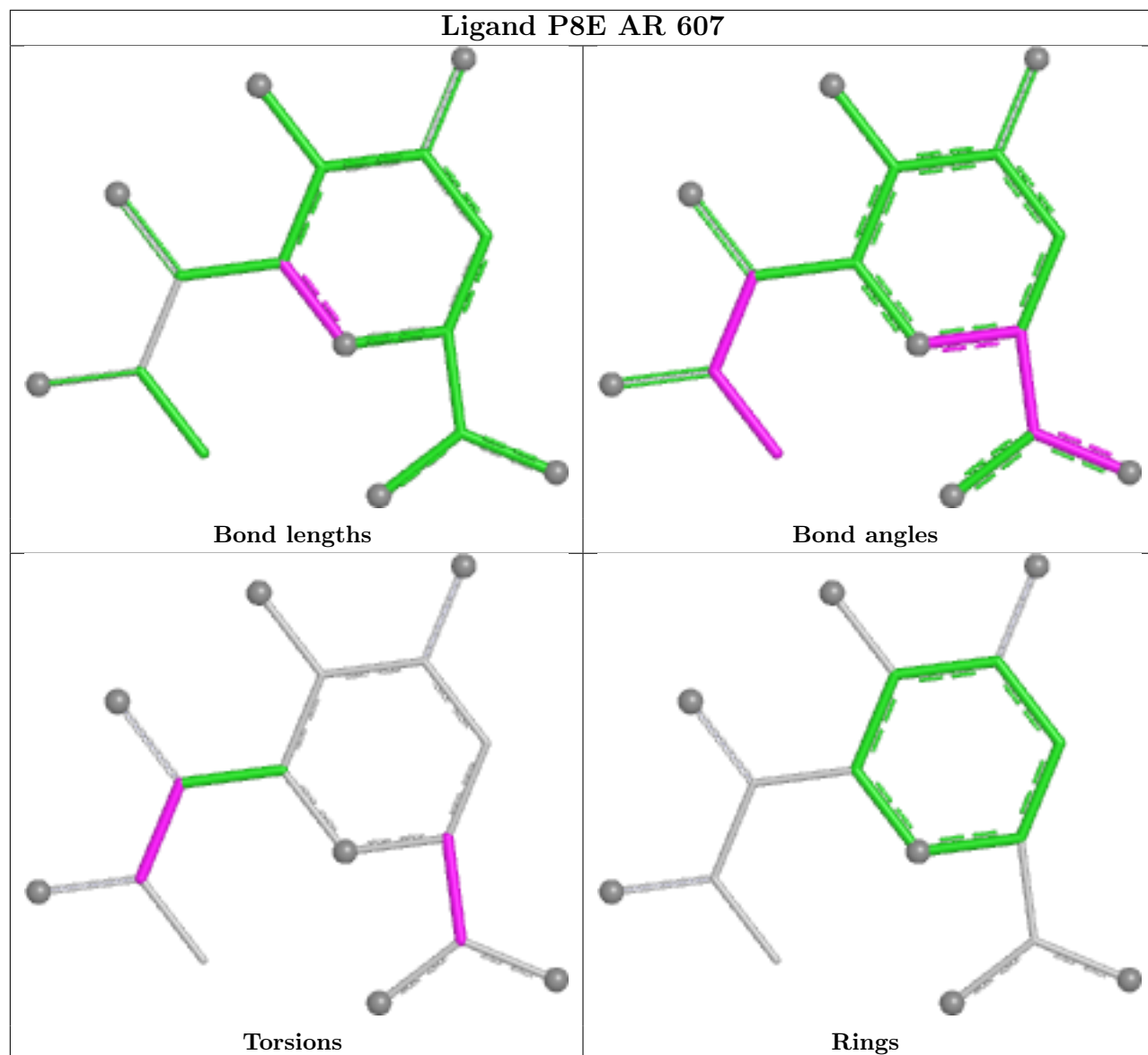


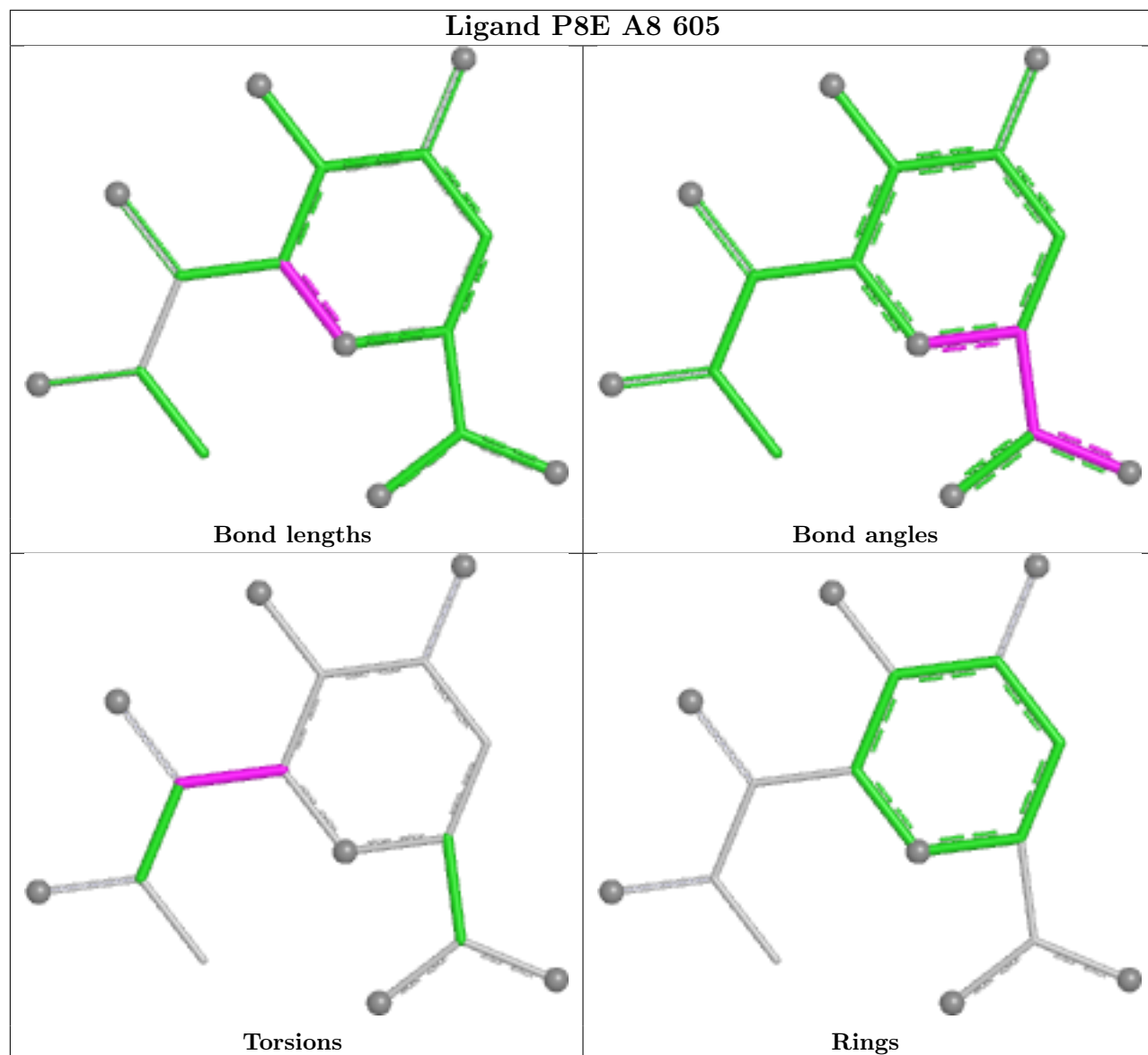


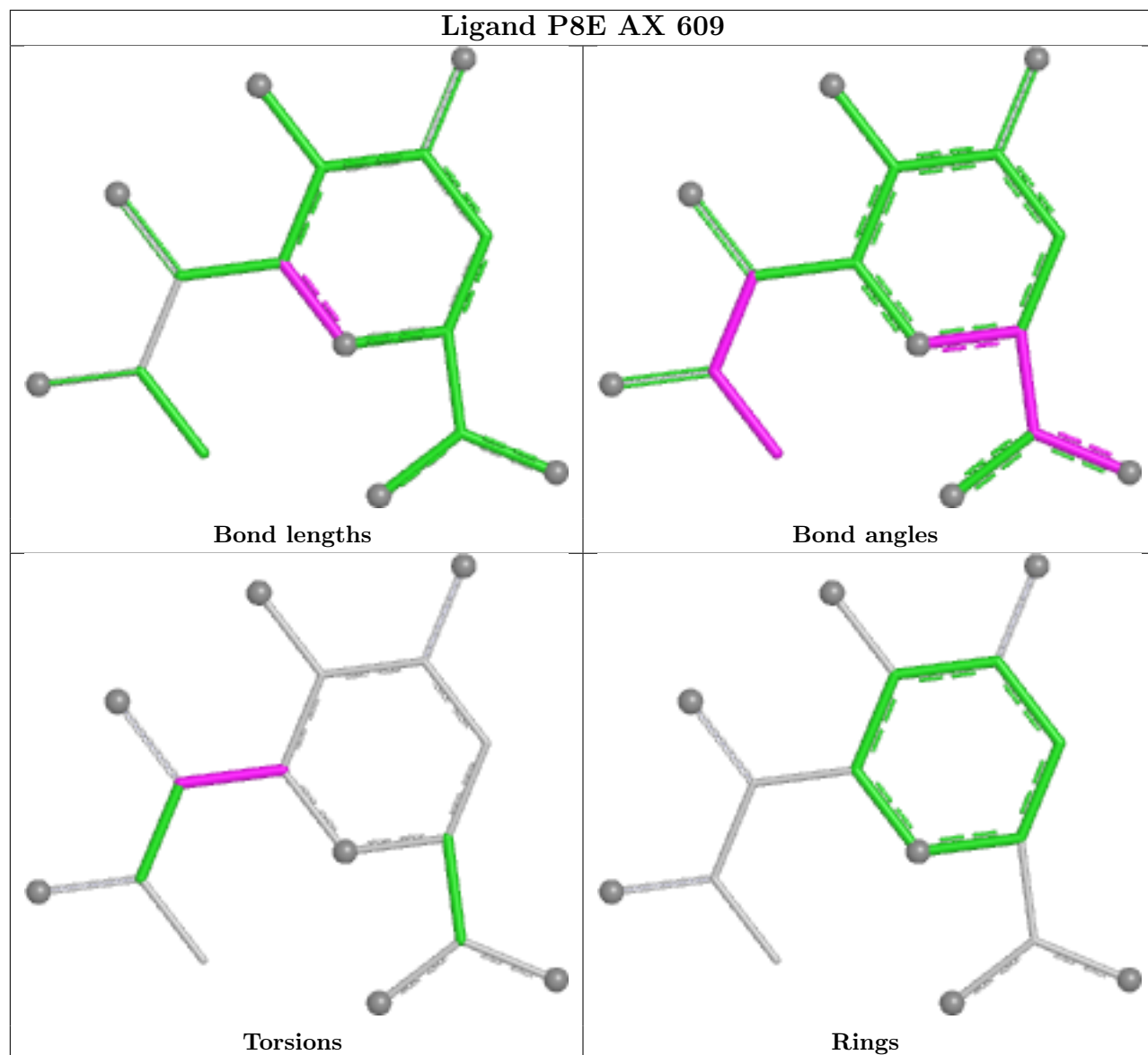


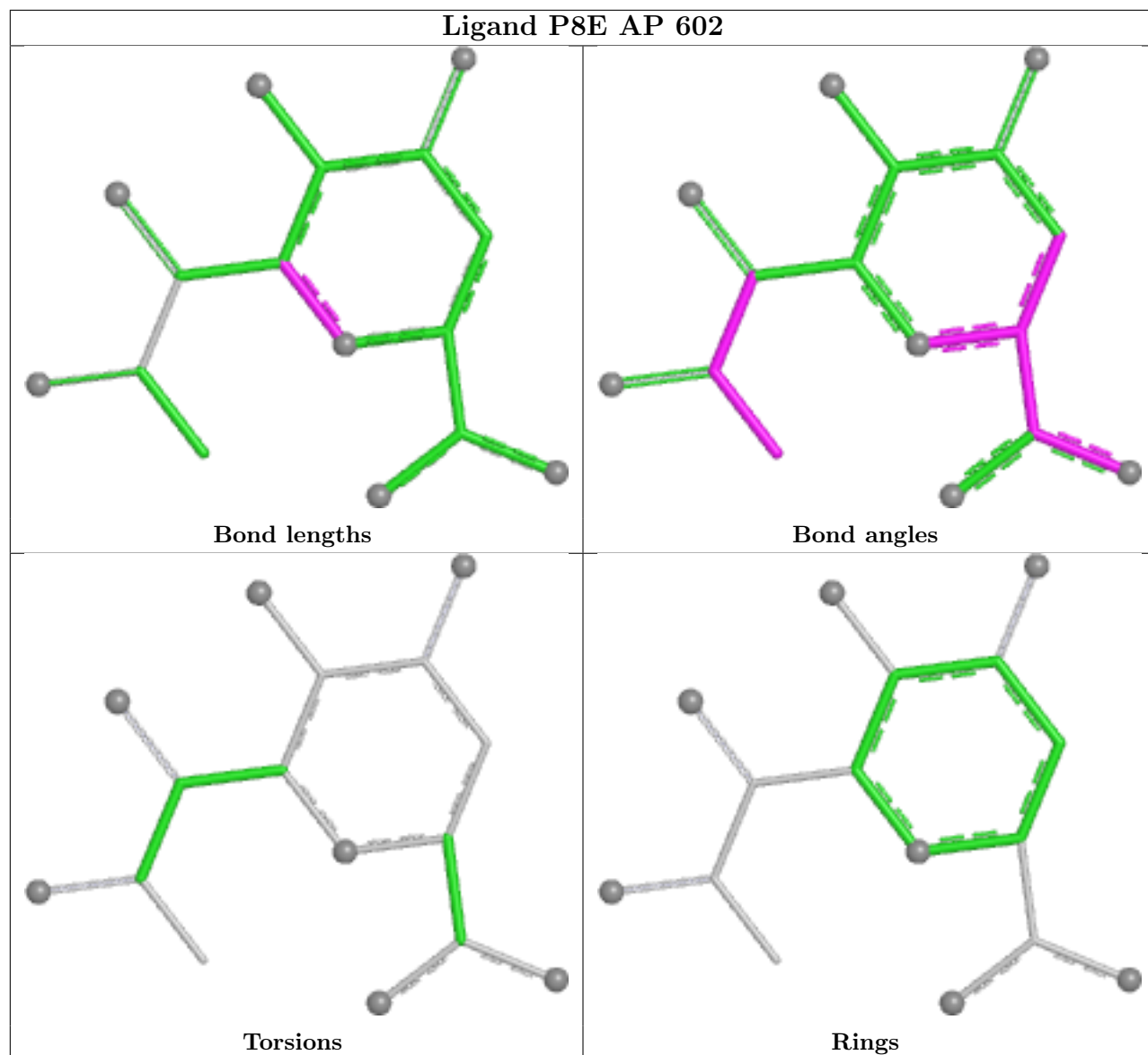


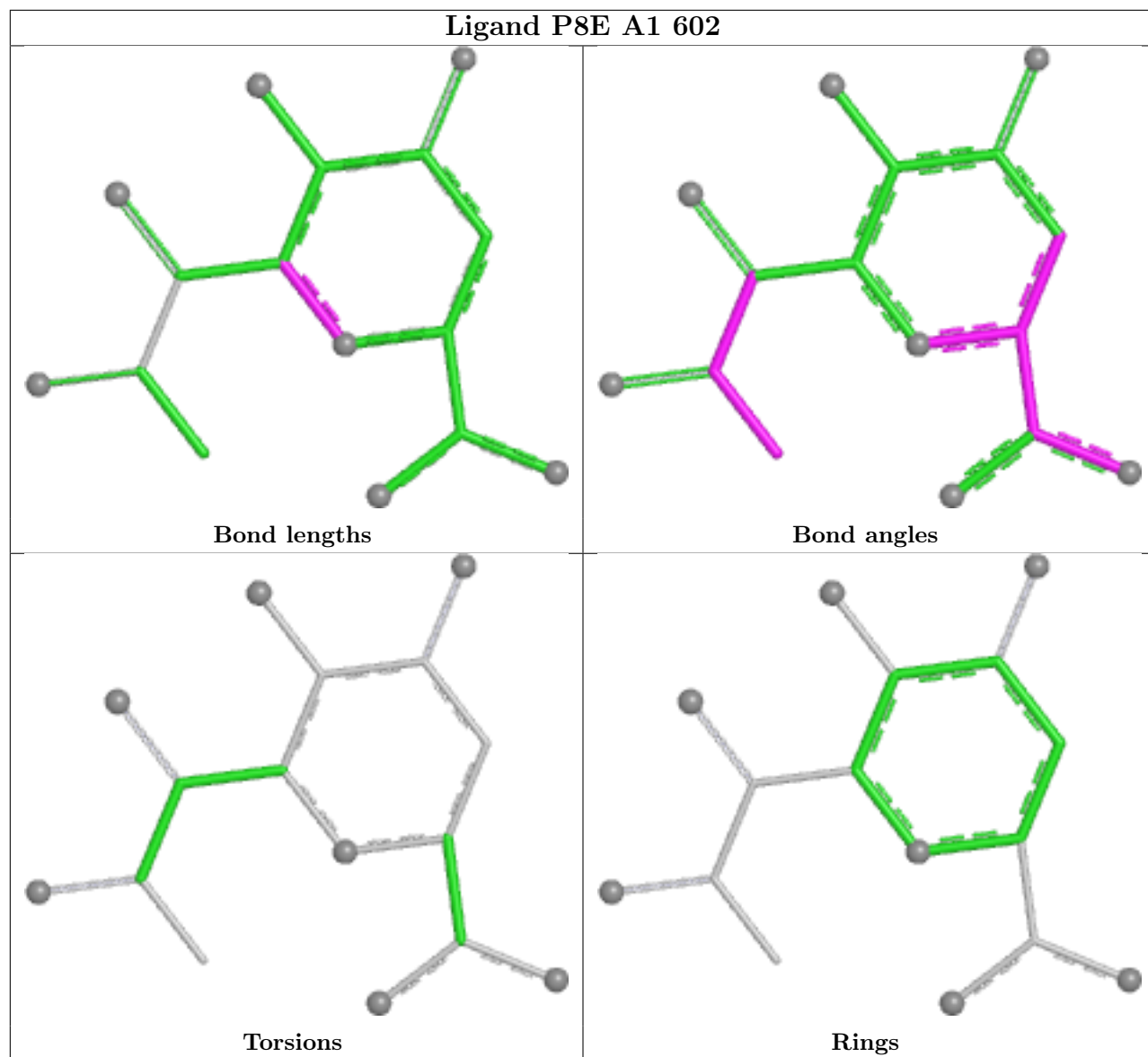


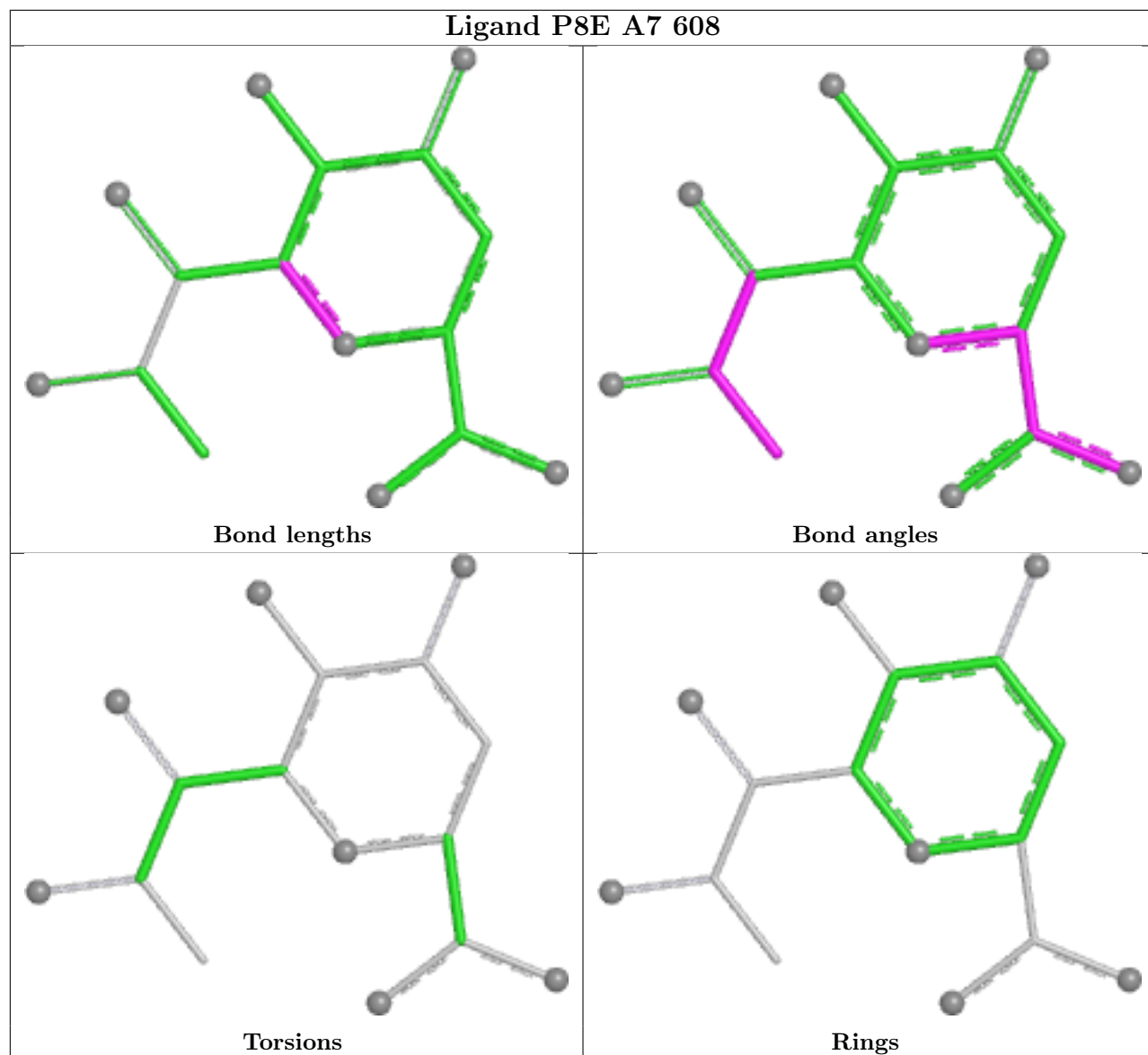


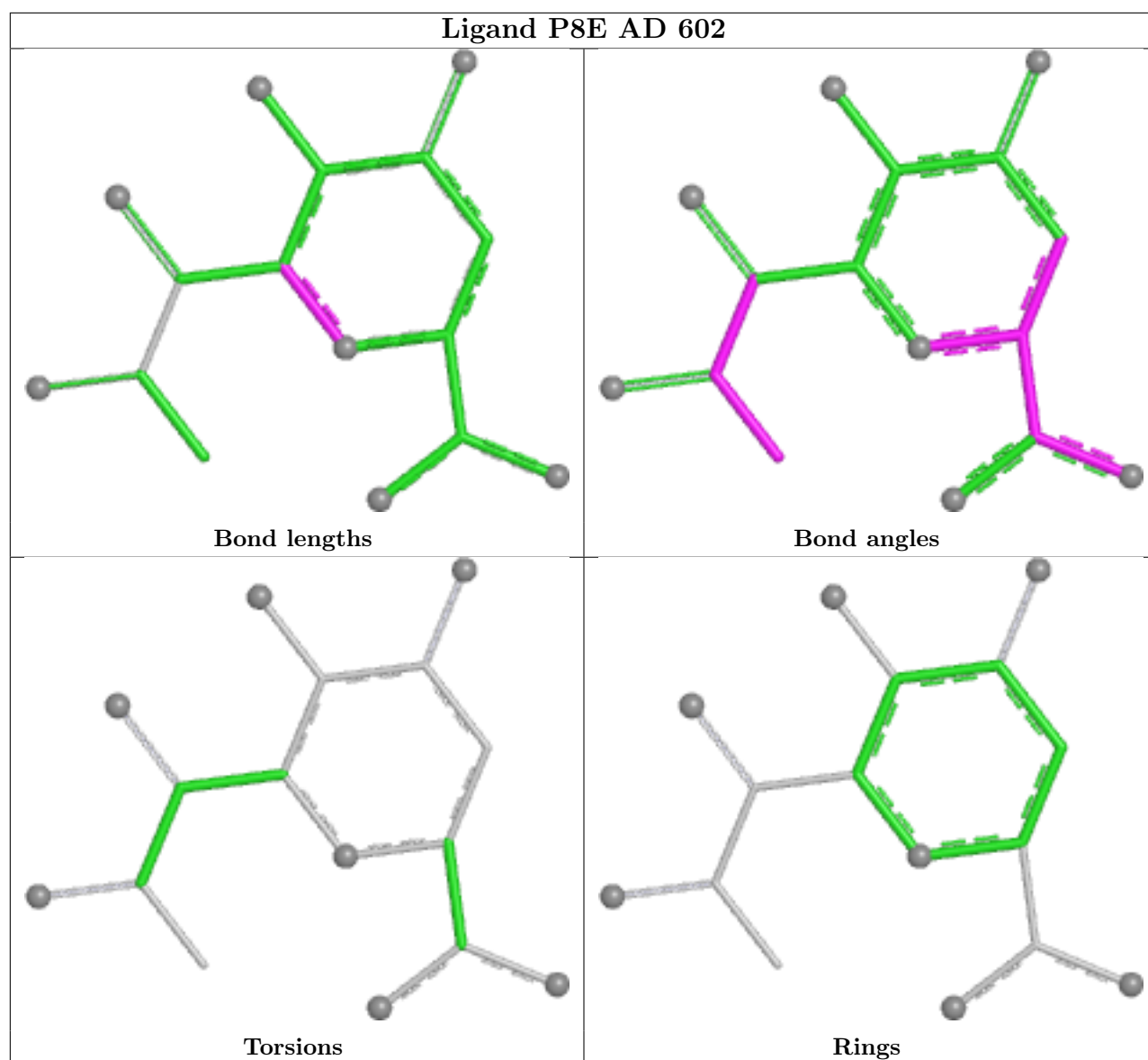












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

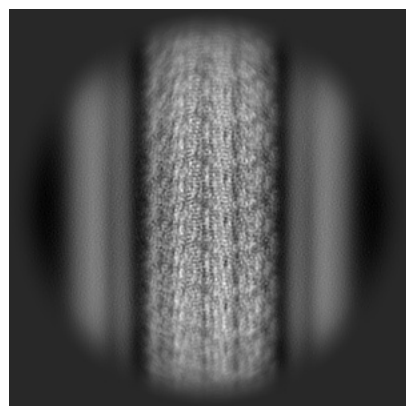
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72948. These allow visual inspection of the internal detail of the map and identification of artifacts.

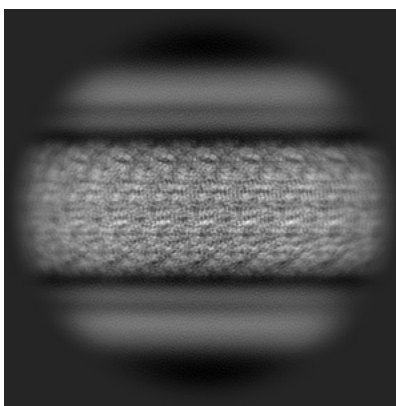
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

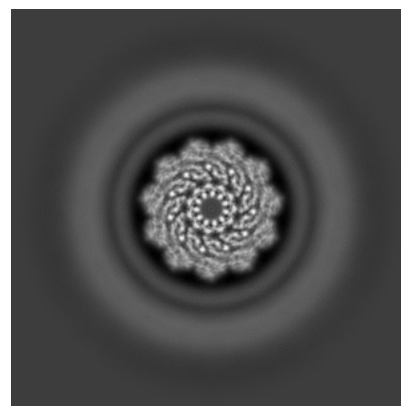
6.1.1 Primary map



X

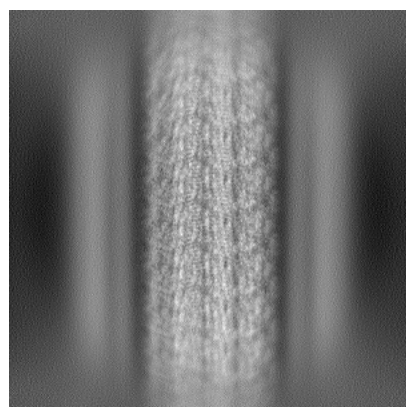


Y

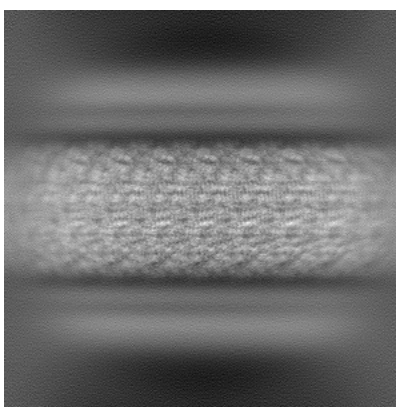


Z

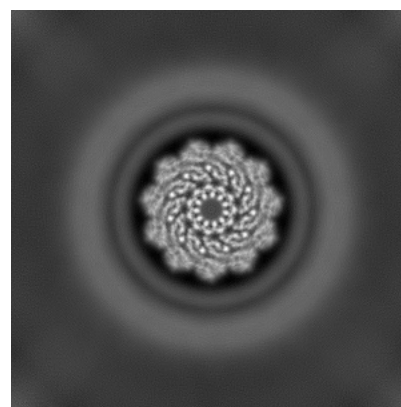
6.1.2 Raw map



X



Y

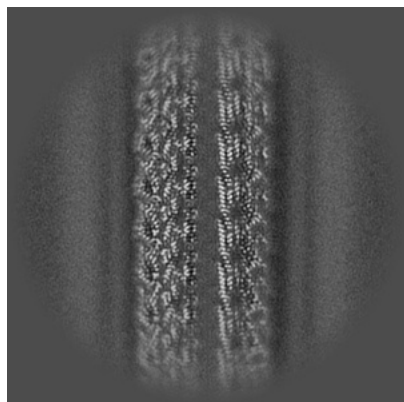


Z

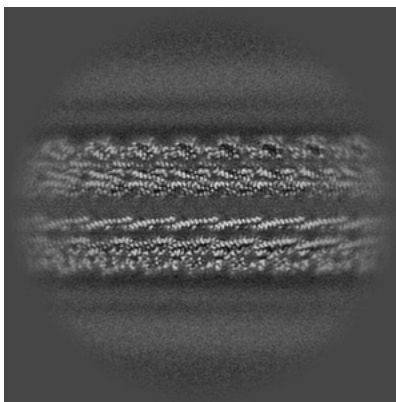
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

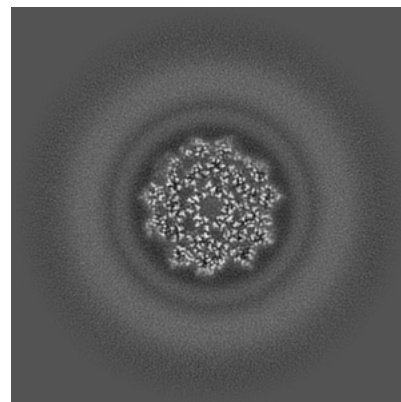
6.2.1 Primary map



X Index: 224

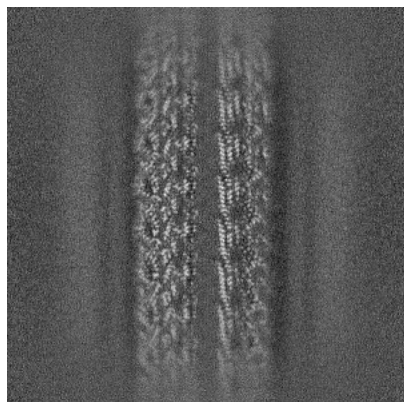


Y Index: 224

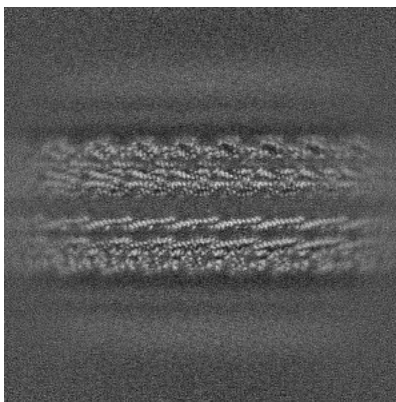


Z Index: 224

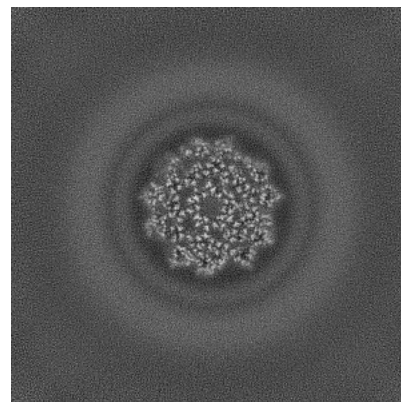
6.2.2 Raw map



X Index: 224



Y Index: 224

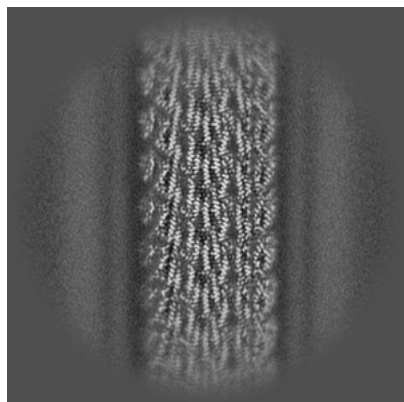


Z Index: 224

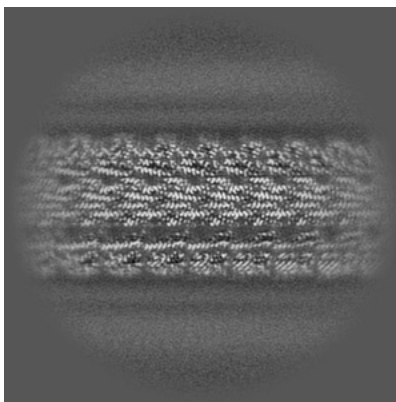
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

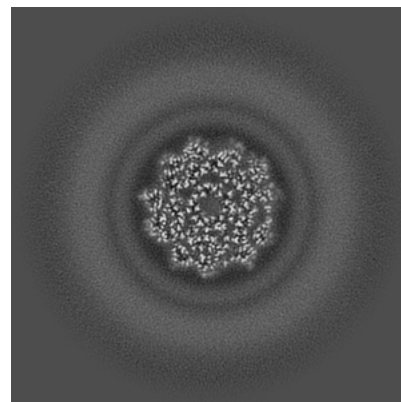
6.3.1 Primary map



X Index: 207

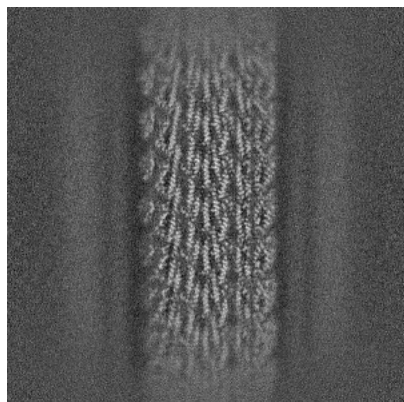


Y Index: 239

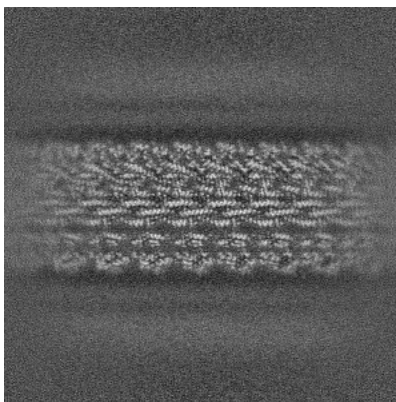


Z Index: 218

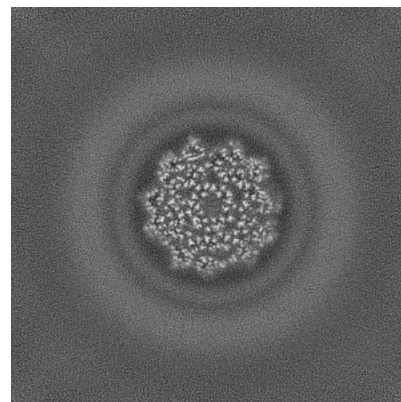
6.3.2 Raw map



X Index: 207



Y Index: 207

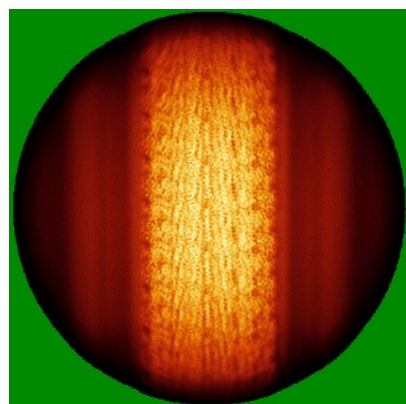


Z Index: 214

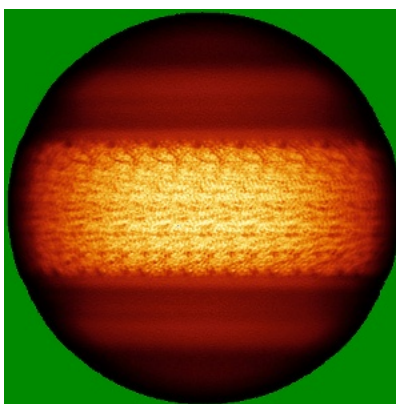
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

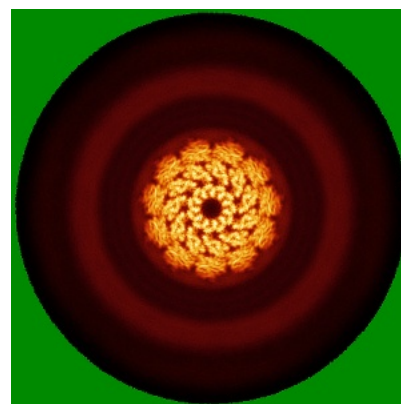
6.4.1 Primary map



X

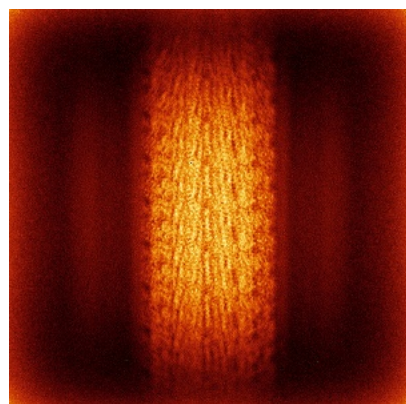


Y

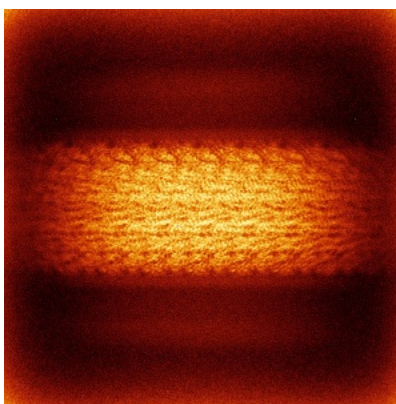


Z

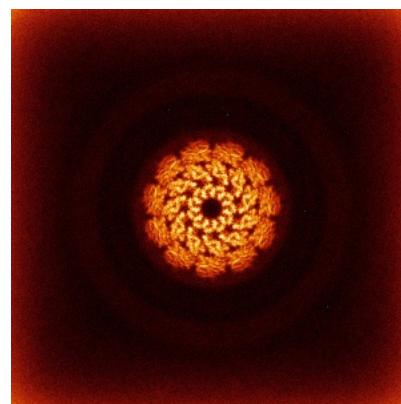
6.4.2 Raw map



X



Y

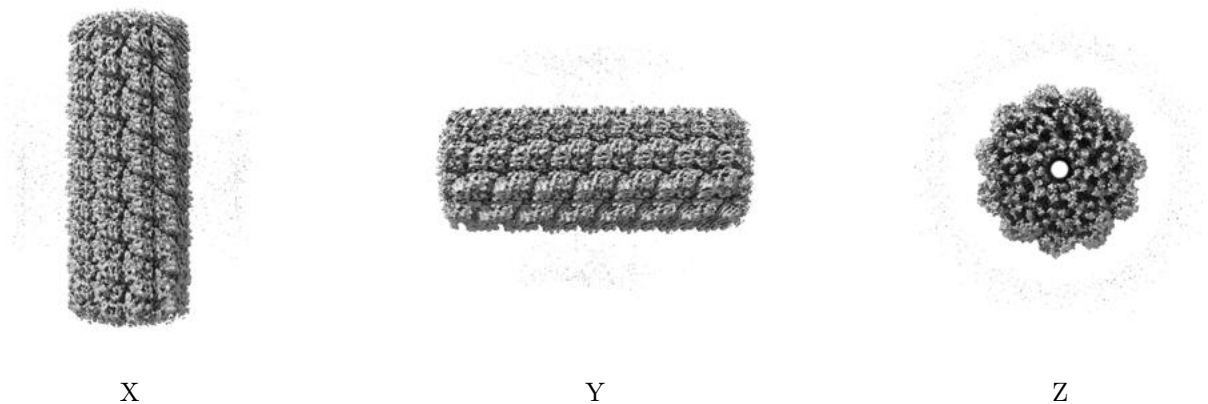


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

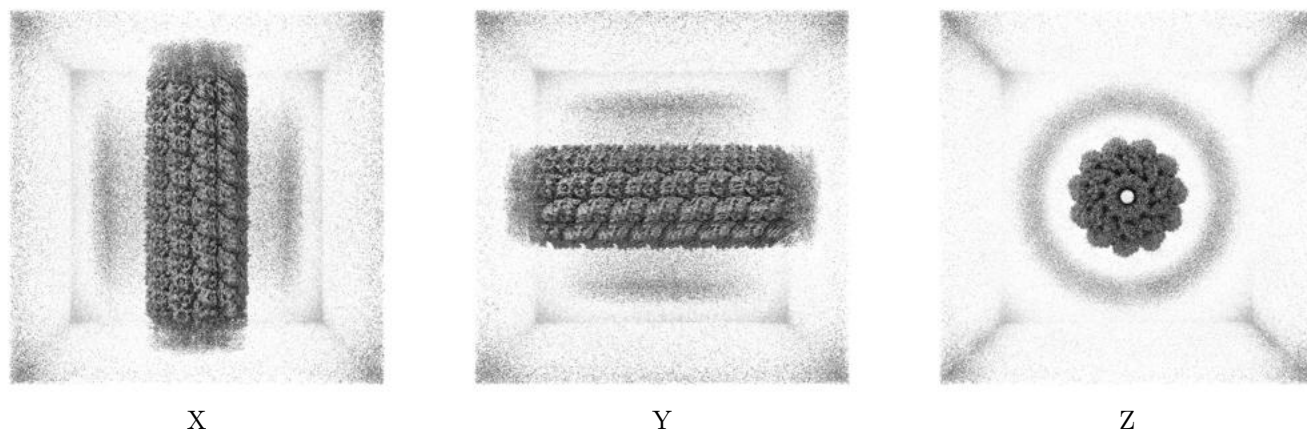
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.052. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

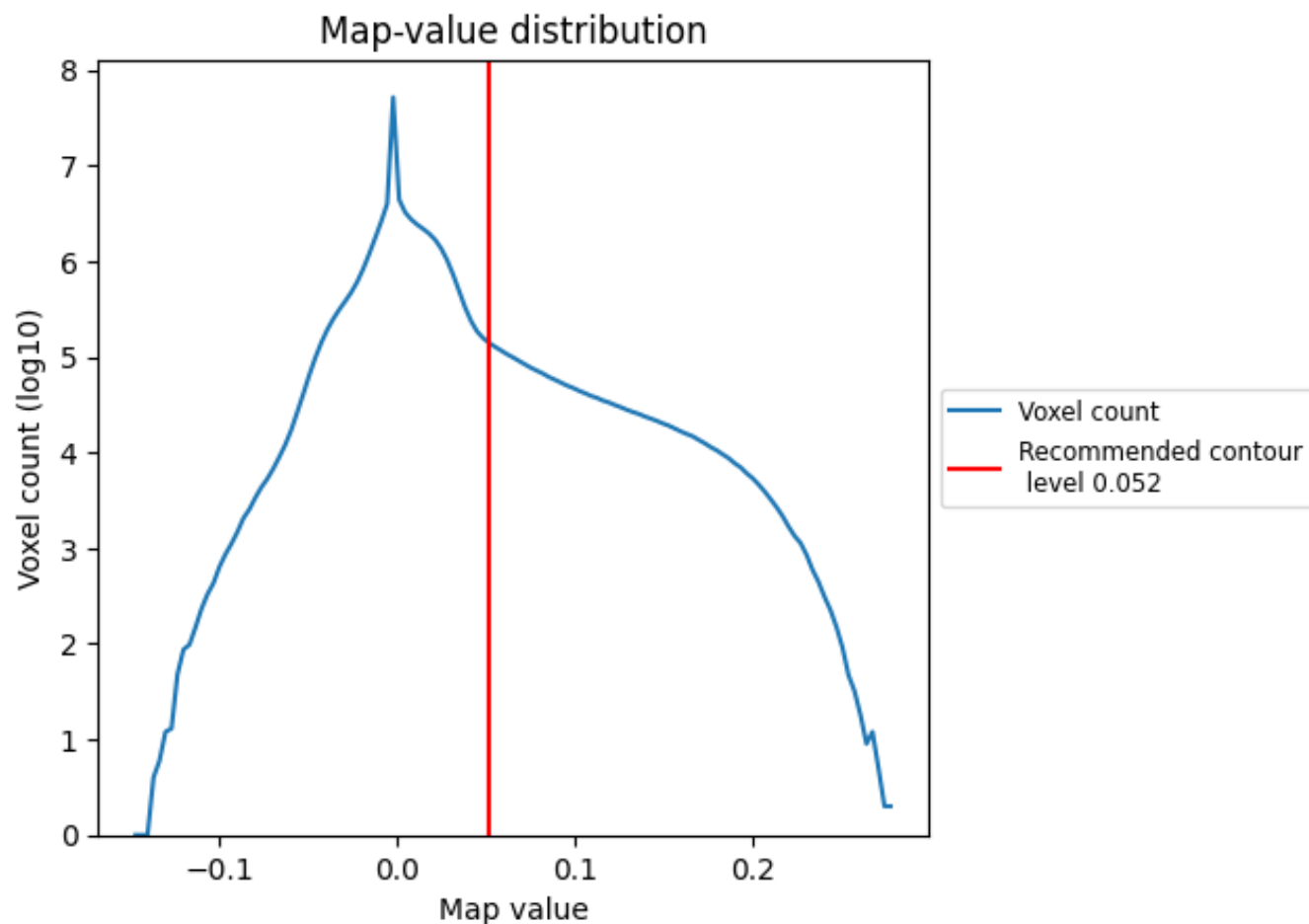
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

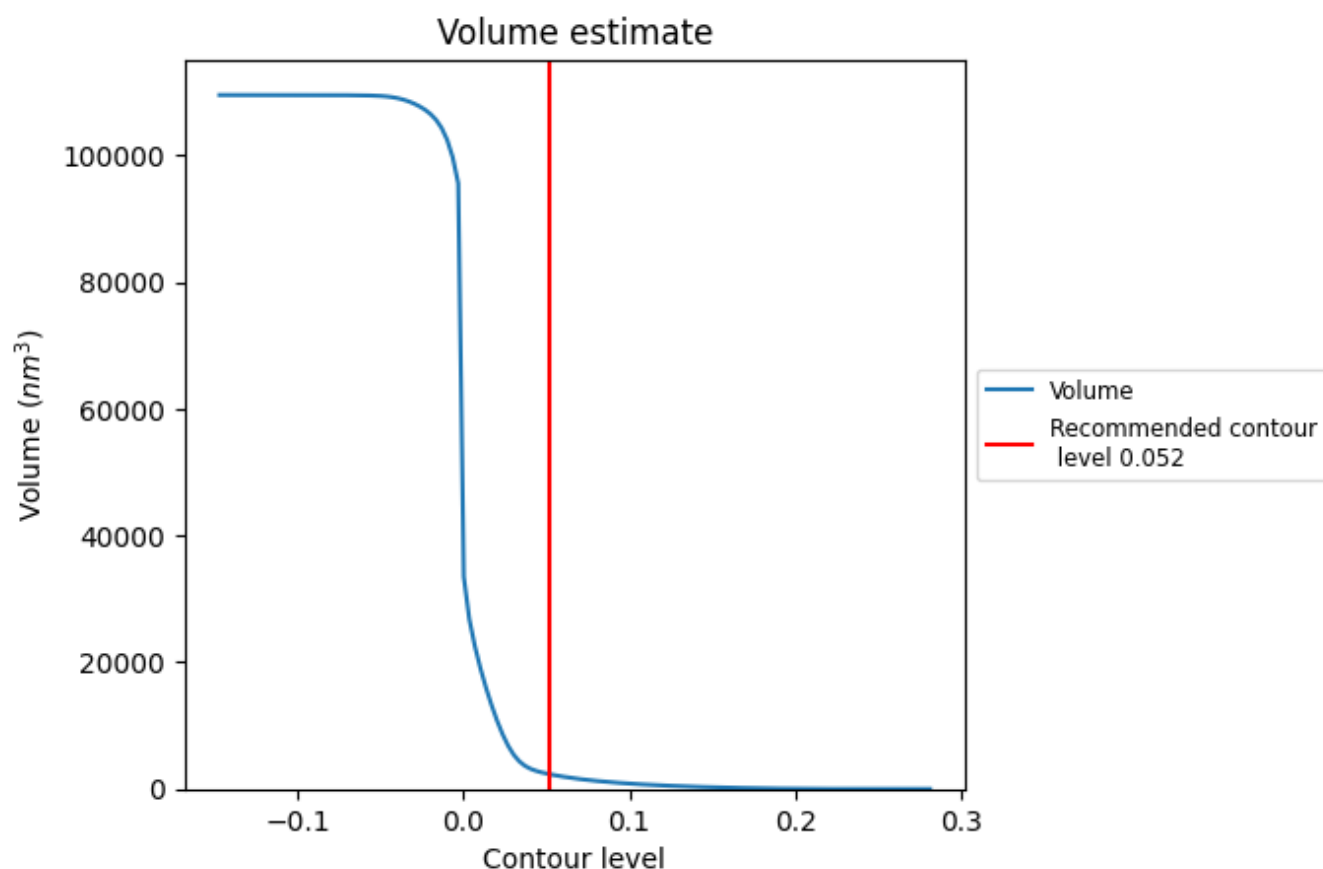
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

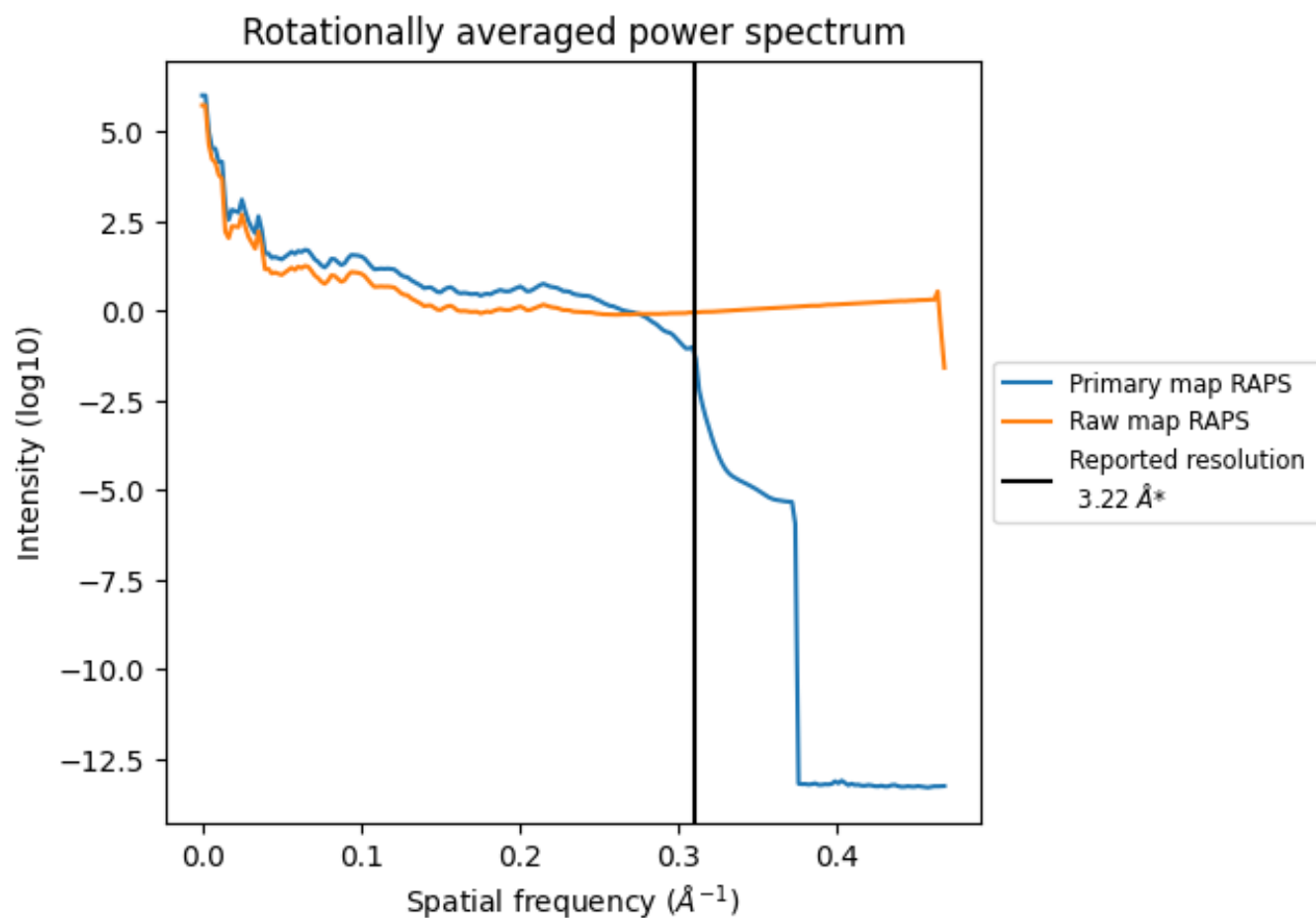
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2330 nm³; this corresponds to an approximate mass of 2105 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

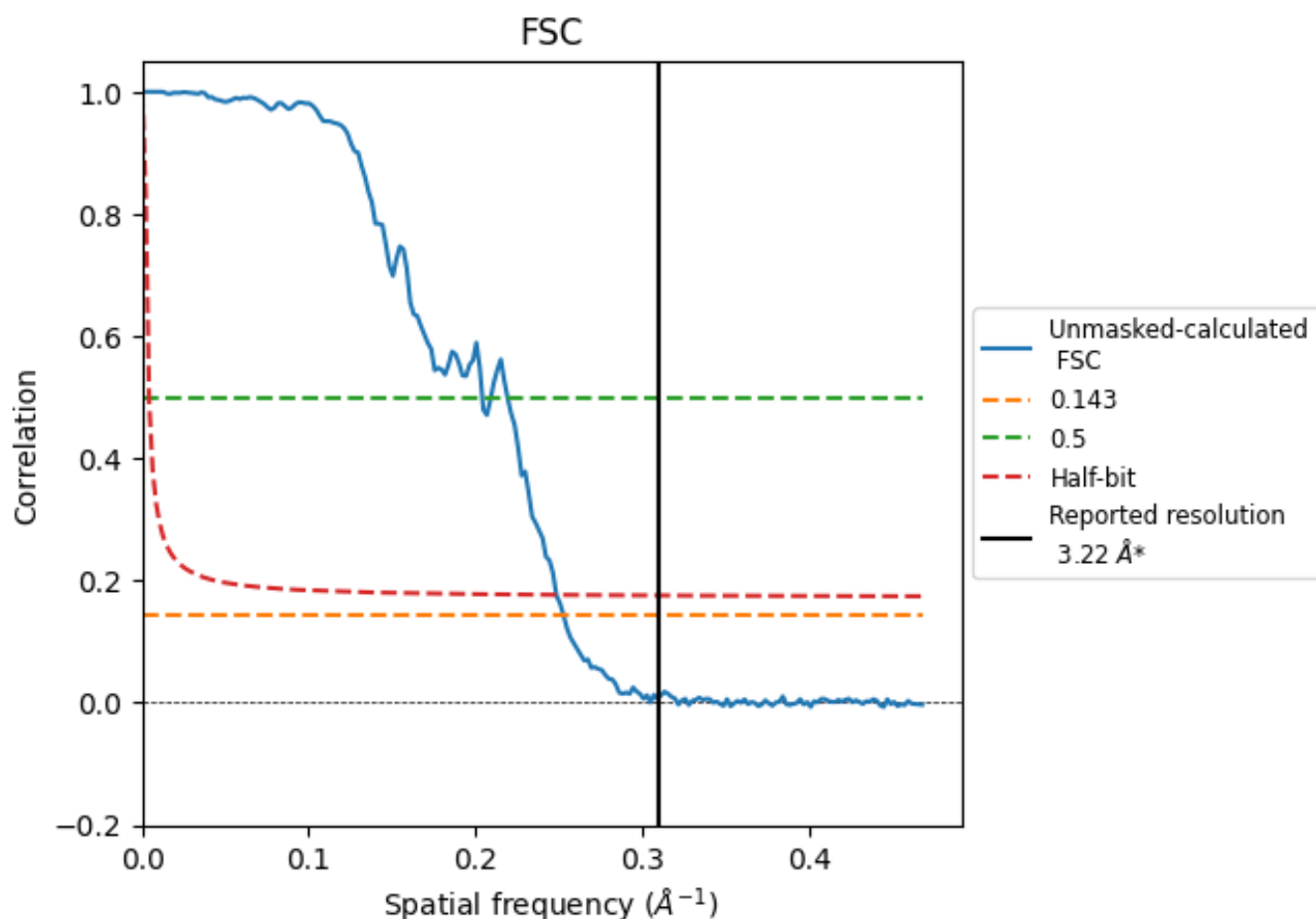


*Reported resolution corresponds to spatial frequency of 0.311 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

8.2 Resolution estimates [i](#)

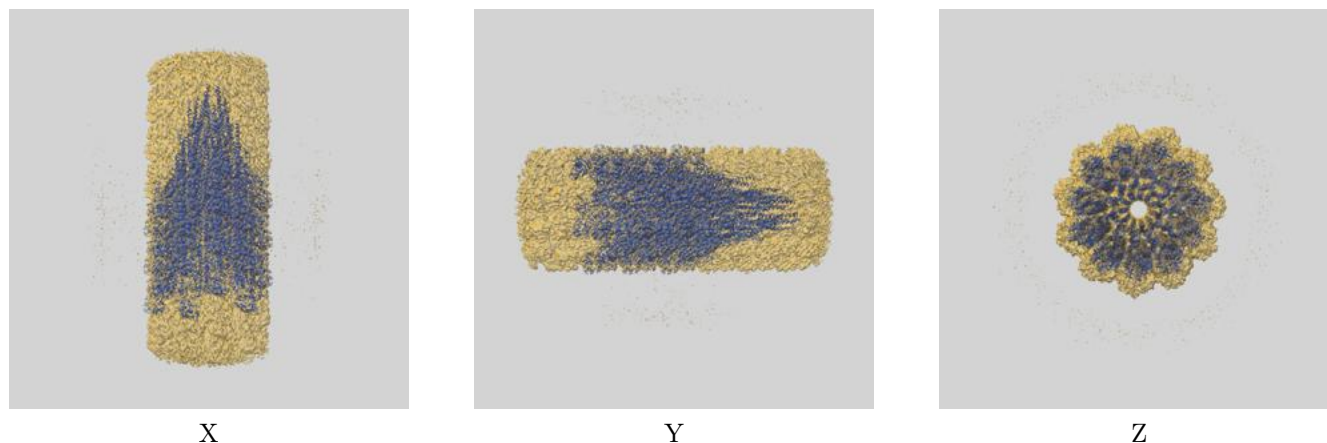
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	4.90	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.22 by more than 10 %

9 Map-model fit [i](#)

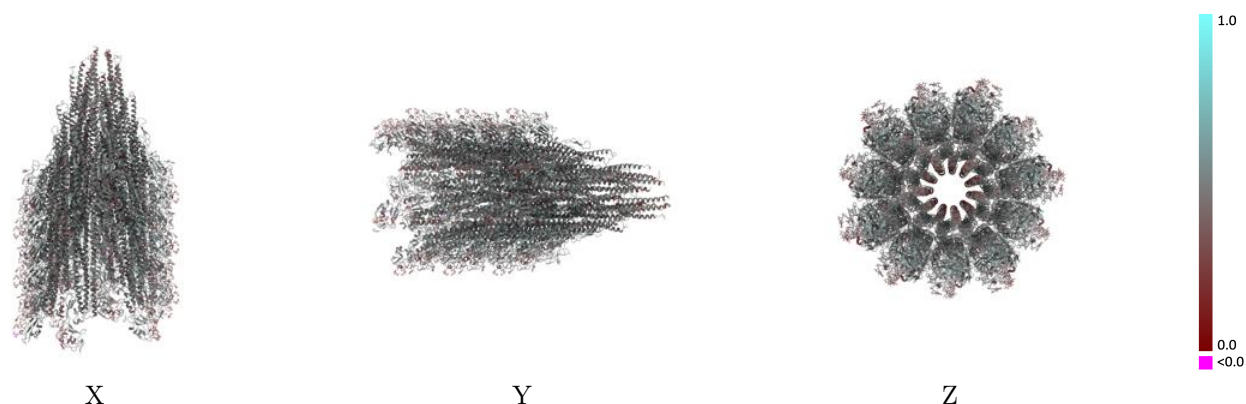
This section contains information regarding the fit between EMDB map EMD-72948 and PDB model 9YH1. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



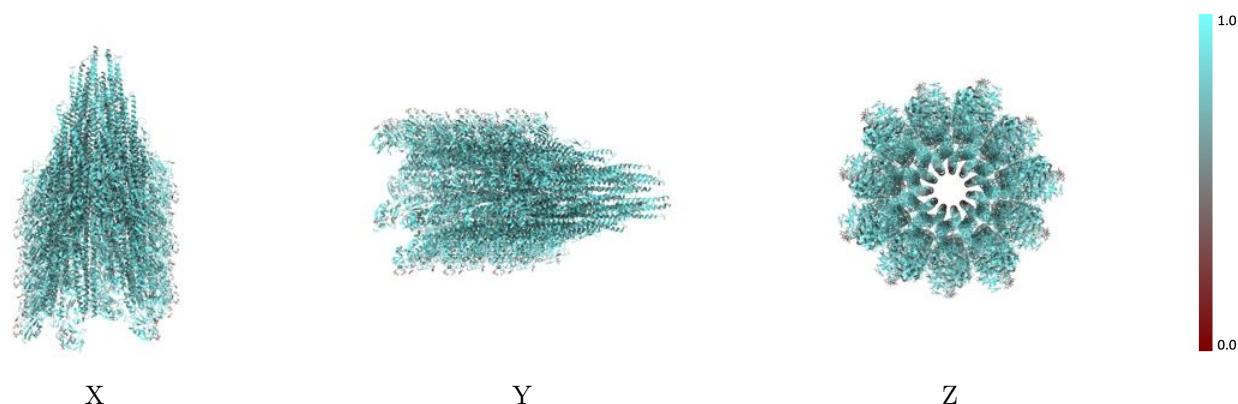
The images above show the 3D surface view of the map at the recommended contour level 0.052 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



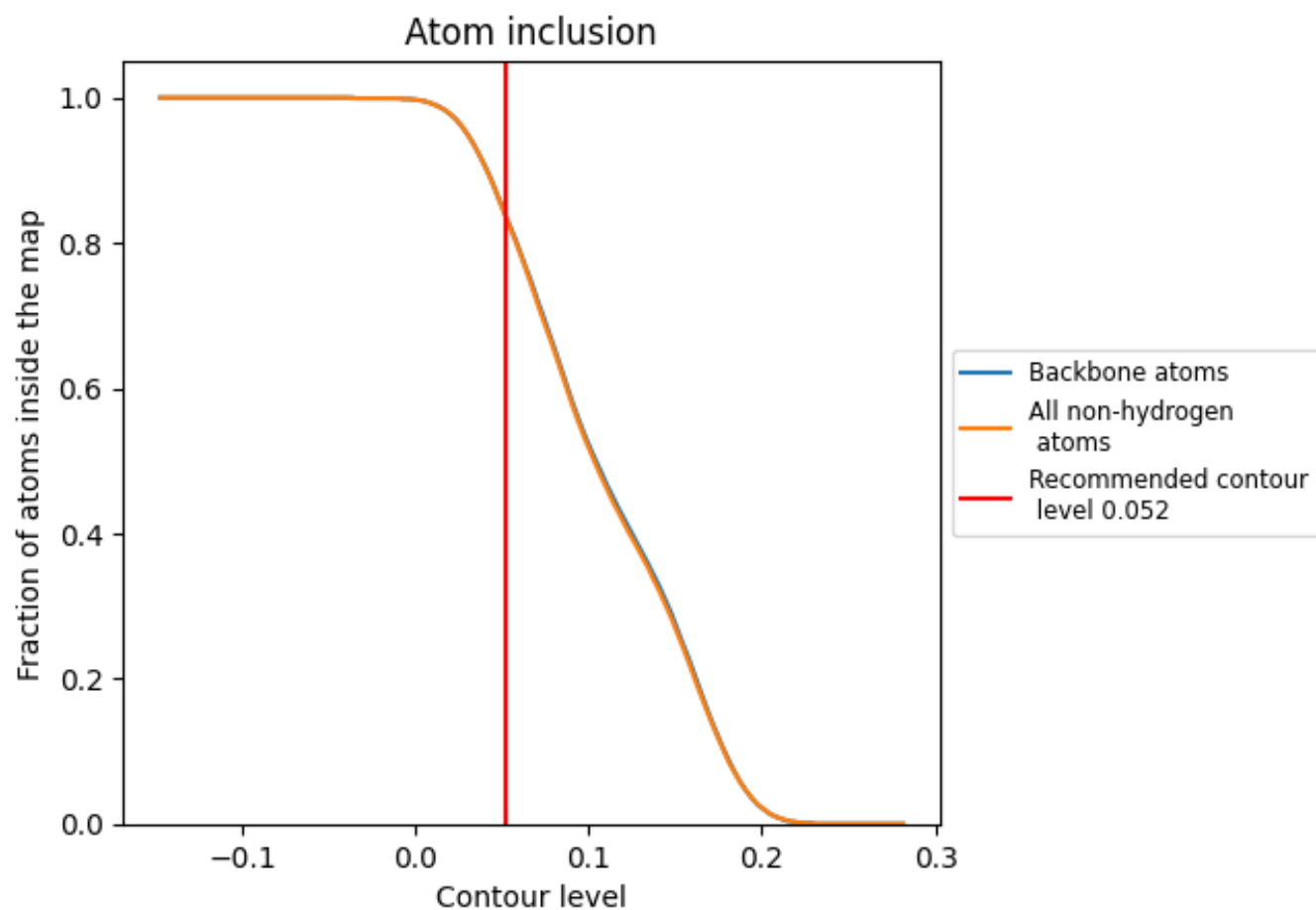
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.052).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.052) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.4740
A1	 0.8420	 0.4780
A2	 0.8450	 0.4800
A3	 0.8270	 0.4580
A4	 0.8390	 0.4740
A5	 0.8440	 0.4730
A6	 0.8450	 0.4790
A7	 0.8260	 0.4560
A8	 0.8420	 0.4720
A9	 0.8430	 0.4790
AA	 0.8380	 0.4710
AB	 0.8350	 0.4700
AC	 0.8380	 0.4680
AD	 0.8330	 0.4670
AE	 0.8300	 0.4630
AF	 0.8470	 0.4800
AG	 0.8520	 0.4800
AH	 0.8510	 0.4800
AI	 0.8500	 0.4790
AJ	 0.8380	 0.4710
AK	 0.8490	 0.4790
AL	 0.8420	 0.4690
AM	 0.8480	 0.4820
AN	 0.8510	 0.4810
AO	 0.8440	 0.4760
AP	 0.8520	 0.4770
AQ	 0.8470	 0.4810
AR	 0.8500	 0.4810
AS	 0.8510	 0.4780
AT	 0.8490	 0.4800
AU	 0.8470	 0.4770
AV	 0.8320	 0.4700
AW	 0.8420	 0.4750
AX	 0.8220	 0.4560

