



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:10 pm GMT

PDB ID : 5LEG
EMDB ID : EMD-4042
Title : Structure of the bacterial sex F pilus (pED208)
Authors : Costa, T.R.D.; Ilangovan, I.; Ukleja, M.; Redzej, A.; Santini, J.M.; Smith, T.K.; Egelman, E.H.; Waksman, G.
Deposited on : 2016-06-29
Resolution : 3.60 Å(reported)

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

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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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

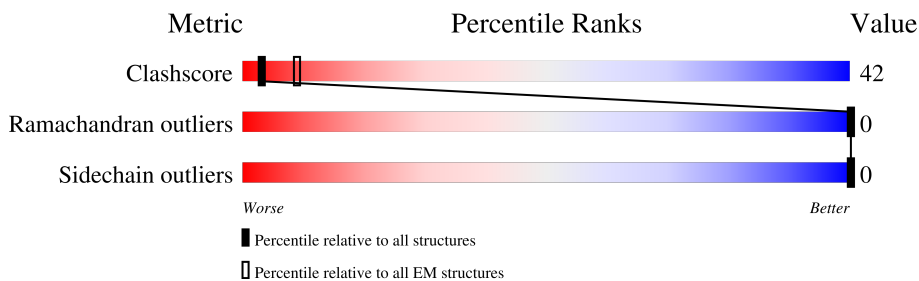
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1A	63	52% 44% .
1	1B	63	49% 48% .
1	1C	63	48% 49% .
1	1D	63	48% 49% .
1	1E	63	46% 51% .
1	1F	63	46% 51% .
1	1G	63	48% 49% .
1	1H	63	48% 49% .

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Mol	Chain	Length	Quality of chain	
1	1I	63	48%	49%
1	1J	63	46%	51%
1	1K	63	48%	49%
1	1L	63	51%	46%
1	1M	63	51%	46%
1	1N	63	8%	51%
1	1O	63	21%	52%
1	1P	63	49%	56%
1	2A	63	51%	46%
1	2B	63	46%	51%
1	2C	63	48%	49%
1	2D	63	48%	49%
1	2E	63	48%	49%
1	2F	63	46%	51%
1	2G	63	48%	49%
1	2H	63	48%	49%
1	2I	63	49%	48%
1	2J	63	51%	46%
1	2K	63	51%	46%
1	2L	63	51%	46%
1	2M	63	51%	46%
1	2N	63	8%	51%
1	2O	63	21%	52%
1	2P	63	49%	59%
1	3A	63	51%	46%



















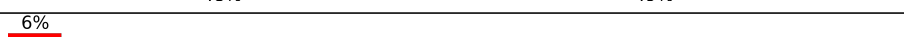


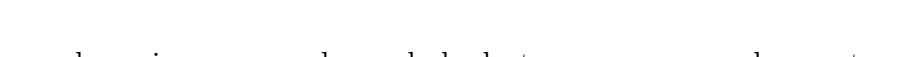
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Mol	Chain	Length	Quality of chain
1	3B	63	48% 49%
1	3C	63	48% 49%
1	3D	63	48% 49%
1	3E	63	48% 49%
1	3F	63	46% 51%
1	3G	63	44% 52%
1	3H	63	44% 52%
1	3I	63	46% 51%
1	3J	63	48% 49%
1	3K	63	48% 49%
1	3L	63	49% 48%
1	3M	63	49% 48%
1	3N	63	6% 51% 46%
1	3O	63	21% 51% 46%
1	3P	63	49% 59% 40%
1	4A	63	52% 44%
1	4B	63	49% 48%
1	4C	63	48% 49%
1	4D	63	51% 46%
1	4E	63	46% 51%
1	4F	63	43% 54%
1	4G	63	46% 51%
1	4H	63	48% 49%
1	4I	63	49% 48%
1	4J	63	51% 46%

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Mol	Chain	Length	Quality of chain
1	4K	63	
1	4L	63	
1	4M	63	
1	4N	63	
1	4O	63	
1	4P	63	
1	5A	63	
1	5B	63	
1	5C	63	
1	5D	63	
1	5E	63	
1	5F	63	
1	5G	63	
1	5H	63	
1	5I	63	
1	5J	63	
1	5K	63	
1	5L	63	
1	5M	63	
1	5N	63	
1	5O	63	
1	5P	63	

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	LHG	1A	101	-	-	X	-
2	LHG	1B	101	-	-	X	-
2	LHG	1C	101	-	-	X	-
2	LHG	1D	101	-	-	X	-
2	LHG	1E	101	-	-	X	-
2	LHG	1F	101	-	-	X	-
2	LHG	1G	101	-	-	X	-
2	LHG	1H	101	-	-	X	-
2	LHG	1I	101	-	-	X	-
2	LHG	1J	101	-	-	X	-
2	LHG	1K	101	-	-	X	-
2	LHG	1L	101	-	-	X	-
2	LHG	1M	101	-	-	X	-
2	LHG	1N	101	-	-	X	-
2	LHG	1O	101	-	-	X	-
2	LHG	2A	101	-	-	X	-
2	LHG	2B	101	-	-	X	-
2	LHG	2C	101	-	-	X	-
2	LHG	2D	101	-	-	X	-
2	LHG	2E	101	-	-	X	-
2	LHG	2F	101	-	-	X	-
2	LHG	2G	101	-	-	X	-
2	LHG	2H	101	-	-	X	-
2	LHG	2I	101	-	-	X	-
2	LHG	2J	101	-	-	X	-
2	LHG	2K	101	-	-	X	-
2	LHG	2L	101	-	-	X	-
2	LHG	2M	101	-	-	X	-
2	LHG	2N	101	-	-	X	-
2	LHG	2O	101	-	-	X	-
2	LHG	3A	101	-	-	X	-
2	LHG	3B	101	-	-	X	-
2	LHG	3C	101	-	-	X	-
2	LHG	3D	101	-	-	X	-
2	LHG	3E	101	-	-	X	-
2	LHG	3F	101	-	-	X	-
2	LHG	3G	101	-	-	X	-
2	LHG	3H	101	-	-	X	-
2	LHG	3I	101	-	-	X	-
2	LHG	3J	101	-	-	X	-
2	LHG	3K	101	-	-	X	-
2	LHG	3L	101	-	-	X	-
2	LHG	3M	101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LHG	3N	101	-	-	X	-
2	LHG	3O	101	-	-	X	-
2	LHG	4A	101	-	-	X	-
2	LHG	4B	101	-	-	X	-
2	LHG	4C	101	-	-	X	-
2	LHG	4D	101	-	-	X	-
2	LHG	4E	101	-	-	X	-
2	LHG	4F	101	-	-	X	-
2	LHG	4G	101	-	-	X	-
2	LHG	4H	101	-	-	X	-
2	LHG	4I	101	-	-	X	-
2	LHG	4J	101	-	-	X	-
2	LHG	4K	101	-	-	X	-
2	LHG	4L	101	-	-	X	-
2	LHG	4M	101	-	-	X	-
2	LHG	4N	101	-	-	X	-
2	LHG	4O	101	-	-	X	-
2	LHG	5A	101	-	-	X	-
2	LHG	5B	101	-	-	X	-
2	LHG	5C	101	-	-	X	-
2	LHG	5D	101	-	-	X	-
2	LHG	5E	101	-	-	X	-
2	LHG	5F	101	-	-	X	-
2	LHG	5G	101	-	-	X	-
2	LHG	5H	101	-	-	X	-
2	LHG	5I	101	-	-	X	-
2	LHG	5J	101	-	-	X	-
2	LHG	5K	101	-	-	X	-
2	LHG	5L	101	-	-	X	-
2	LHG	5M	101	-	-	X	-
2	LHG	5N	101	-	-	X	-
2	LHG	5O	101	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41355 atoms, of which 0 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 Pilin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	63	471	315	71	81	4	0	0
1	1B	63	471	315	71	81	4	0	0
1	1C	63	471	315	71	81	4	0	0
1	1D	63	471	315	71	81	4	0	0
1	1E	63	471	315	71	81	4	0	0
1	1F	63	471	315	71	81	4	0	0
1	1G	63	471	315	71	81	4	0	0
1	1H	63	471	315	71	81	4	0	0
1	1I	63	471	315	71	81	4	0	0
1	1J	63	471	315	71	81	4	0	0
1	1K	63	471	315	71	81	4	0	0
1	1L	63	471	315	71	81	4	0	0
1	1M	63	471	315	71	81	4	0	0
1	1N	63	471	315	71	81	4	0	0
1	1O	63	471	315	71	81	4	0	0
1	1P	63	471	315	71	81	4	0	0
1	2A	63	471	315	71	81	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2B	63	471	315	71	81	4	0	0
1	2C	63	471	315	71	81	4	0	0
1	2D	63	471	315	71	81	4	0	0
1	2E	63	471	315	71	81	4	0	0
1	2F	63	471	315	71	81	4	0	0
1	2G	63	471	315	71	81	4	0	0
1	2H	63	471	315	71	81	4	0	0
1	2I	63	471	315	71	81	4	0	0
1	2J	63	471	315	71	81	4	0	0
1	2K	63	471	315	71	81	4	0	0
1	2L	63	471	315	71	81	4	0	0
1	2M	63	471	315	71	81	4	0	0
1	2N	63	471	315	71	81	4	0	0
1	2O	63	471	315	71	81	4	0	0
1	2P	63	471	315	71	81	4	0	0
1	3A	63	471	315	71	81	4	0	0
1	3B	63	471	315	71	81	4	0	0
1	3C	63	471	315	71	81	4	0	0
1	3D	63	471	315	71	81	4	0	0
1	3E	63	471	315	71	81	4	0	0
1	3F	63	471	315	71	81	4	0	0

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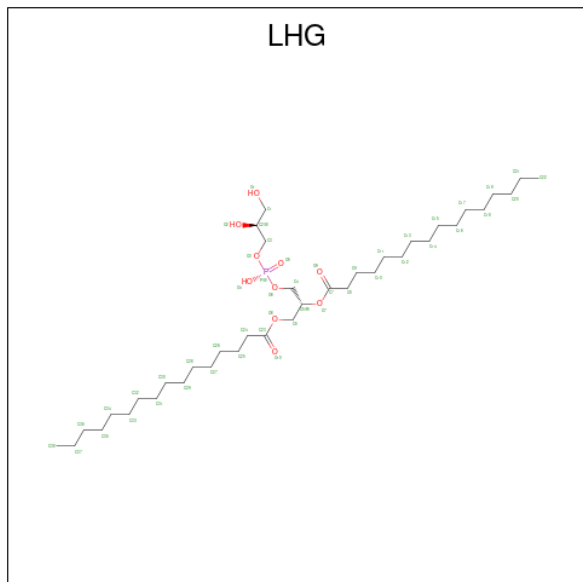
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3G	63	471	315	71	81	4	0	0
1	3H	63	471	315	71	81	4	0	0
1	3I	63	471	315	71	81	4	0	0
1	3J	63	471	315	71	81	4	0	0
1	3K	63	471	315	71	81	4	0	0
1	3L	63	471	315	71	81	4	0	0
1	3M	63	471	315	71	81	4	0	0
1	3N	63	471	315	71	81	4	0	0
1	3O	63	471	315	71	81	4	0	0
1	3P	63	471	315	71	81	4	0	0
1	4A	63	471	315	71	81	4	0	0
1	4B	63	471	315	71	81	4	0	0
1	4C	63	471	315	71	81	4	0	0
1	4D	63	471	315	71	81	4	0	0
1	4E	63	471	315	71	81	4	0	0
1	4F	63	471	315	71	81	4	0	0
1	4G	63	471	315	71	81	4	0	0
1	4H	63	471	315	71	81	4	0	0
1	4I	63	471	315	71	81	4	0	0
1	4J	63	471	315	71	81	4	0	0
1	4K	63	471	315	71	81	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4L	63	471	315	71	81	4	0	0
1	4M	63	471	315	71	81	4	0	0
1	4N	63	471	315	71	81	4	0	0
1	4O	63	471	315	71	81	4	0	0
1	4P	63	471	315	71	81	4	0	0
1	5A	63	471	315	71	81	4	0	0
1	5B	63	471	315	71	81	4	0	0
1	5C	63	471	315	71	81	4	0	0
1	5D	63	471	315	71	81	4	0	0
1	5E	63	471	315	71	81	4	0	0
1	5F	63	471	315	71	81	4	0	0
1	5G	63	471	315	71	81	4	0	0
1	5H	63	471	315	71	81	4	0	0
1	5I	63	471	315	71	81	4	0	0
1	5J	63	471	315	71	81	4	0	0
1	5K	63	471	315	71	81	4	0	0
1	5L	63	471	315	71	81	4	0	0
1	5M	63	471	315	71	81	4	0	0
1	5N	63	471	315	71	81	4	0	0
1	5O	63	471	315	71	81	4	0	0
1	5P	63	471	315	71	81	4	0	0

- Molecule 2 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	1A	1	49	38	10	1	0
2	1B	1	49	38	10	1	0
2	1C	1	49	38	10	1	0
2	1D	1	49	38	10	1	0
2	1E	1	49	38	10	1	0
2	1F	1	49	38	10	1	0
2	1G	1	49	38	10	1	0
2	1H	1	49	38	10	1	0
2	1I	1	49	38	10	1	0
2	1J	1	49	38	10	1	0
2	1K	1	49	38	10	1	0
2	1L	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	1M	1	49	38	10	1	0
2	1N	1	49	38	10	1	0
2	1O	1	49	38	10	1	0
2	2A	1	49	38	10	1	0
2	2B	1	49	38	10	1	0
2	2C	1	49	38	10	1	0
2	2D	1	49	38	10	1	0
2	2E	1	49	38	10	1	0
2	2F	1	49	38	10	1	0
2	2G	1	49	38	10	1	0
2	2H	1	49	38	10	1	0
2	2I	1	49	38	10	1	0
2	2J	1	49	38	10	1	0
2	2K	1	49	38	10	1	0
2	2L	1	49	38	10	1	0
2	2M	1	49	38	10	1	0
2	2N	1	49	38	10	1	0
2	2O	1	49	38	10	1	0
2	3A	1	49	38	10	1	0
2	3B	1	49	38	10	1	0
2	3C	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	3D	1	49	38	10	1	0
2	3E	1	49	38	10	1	0
2	3F	1	49	38	10	1	0
2	3G	1	49	38	10	1	0
2	3H	1	49	38	10	1	0
2	3I	1	49	38	10	1	0
2	3J	1	49	38	10	1	0
2	3K	1	49	38	10	1	0
2	3L	1	49	38	10	1	0
2	3M	1	49	38	10	1	0
2	3N	1	49	38	10	1	0
2	3O	1	49	38	10	1	0
2	4A	1	49	38	10	1	0
2	4B	1	49	38	10	1	0
2	4C	1	49	38	10	1	0
2	4D	1	49	38	10	1	0
2	4E	1	49	38	10	1	0
2	4F	1	49	38	10	1	0
2	4G	1	49	38	10	1	0
2	4H	1	49	38	10	1	0
2	4I	1	49	38	10	1	0

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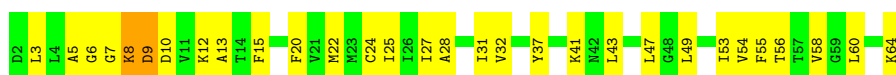
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	4J	1	Total 49	C 38	O 10	P 1	0
2	4K	1	Total 49	C 38	O 10	P 1	0
2	4L	1	Total 49	C 38	O 10	P 1	0
2	4M	1	Total 49	C 38	O 10	P 1	0
2	4N	1	Total 49	C 38	O 10	P 1	0
2	4O	1	Total 49	C 38	O 10	P 1	0
2	5A	1	Total 49	C 38	O 10	P 1	0
2	5B	1	Total 49	C 38	O 10	P 1	0
2	5C	1	Total 49	C 38	O 10	P 1	0
2	5D	1	Total 49	C 38	O 10	P 1	0
2	5E	1	Total 49	C 38	O 10	P 1	0
2	5F	1	Total 49	C 38	O 10	P 1	0
2	5G	1	Total 49	C 38	O 10	P 1	0
2	5H	1	Total 49	C 38	O 10	P 1	0
2	5I	1	Total 49	C 38	O 10	P 1	0
2	5J	1	Total 49	C 38	O 10	P 1	0
2	5K	1	Total 49	C 38	O 10	P 1	0
2	5L	1	Total 49	C 38	O 10	P 1	0
2	5M	1	Total 49	C 38	O 10	P 1	0
2	5N	1	Total 49	C 38	O 10	P 1	0
2	5O	1	Total 49	C 38	O 10	P 1	0

3 Residue-property plots [i](#)

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.

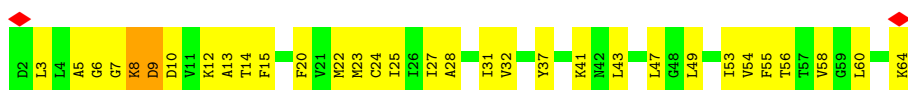
- Molecule 1: Pilin

Chain 1A: 



- Molecule 1: Pilin

Chain 1B: 



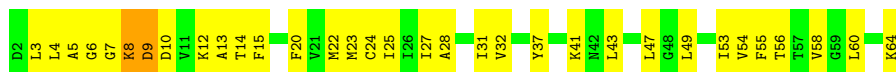
- Molecule 1: Pilin

Chain 1C: 



- Molecule 1: Pilin

Chain 1D: 

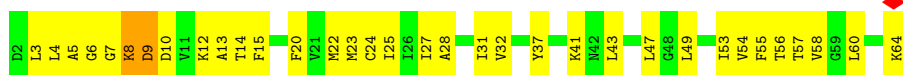


- Molecule 1: Pilin

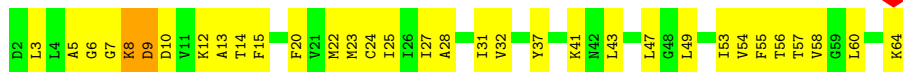
Chain 1E: 



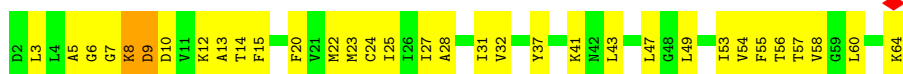
- Molecule 1: Pilin



● Molecule 1: Pilin



● Molecule 1: Pilin



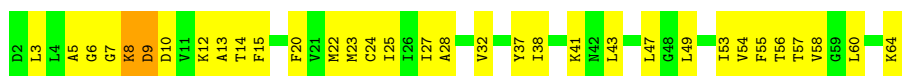
● Molecule 1: Pilin



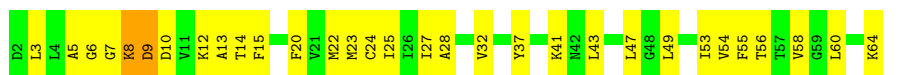
● Molecule 1: Pilin



● Molecule 1: Pilin

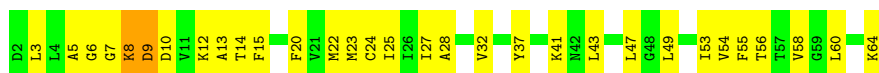


● Molecule 1: Pilin



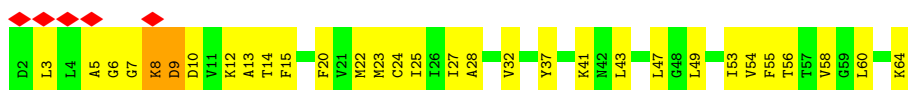
● Molecule 1: Pilin

Chain 1M:  51% 46%



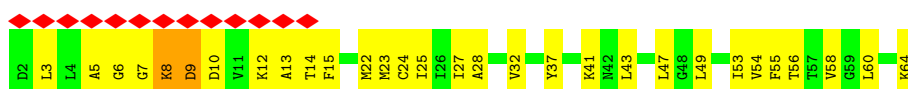
• Molecule 1: Pilin

Chain 1N:  8% 51% 46%



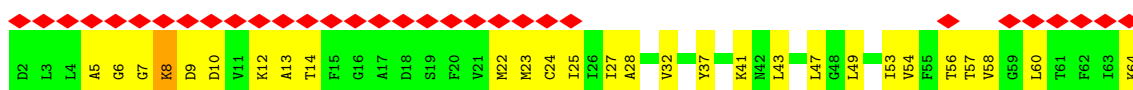
• Molecule 1: Pilin

Chain 1O:  21% 52% 44%



• Molecule 1: Pilin

Chain 1P:  49% 56% 43%



• Molecule 1: Pilin

Chain 2A:  51% 46%



• Molecule 1: Pilin

Chain 2B:  46% 51%

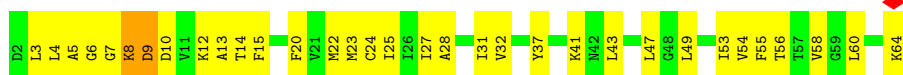


• Molecule 1: Pilin

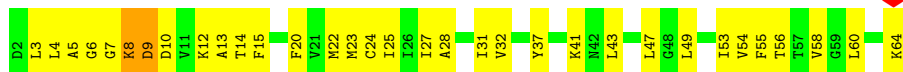
Chain 2C:  48% 49%



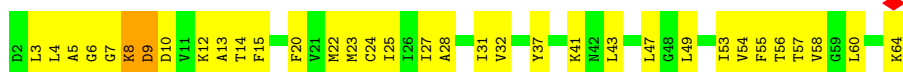
• Molecule 1: Pilin



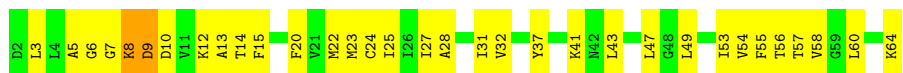
● Molecule 1: Pilin



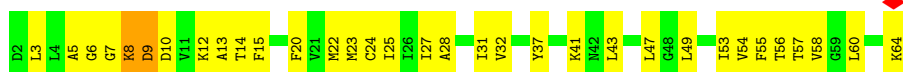
● Molecule 1: Pilin



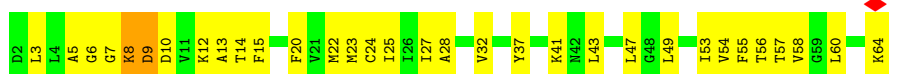
● Molecule 1: Pilin



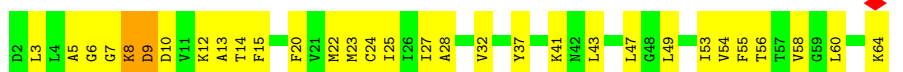
● Molecule 1: Pilin



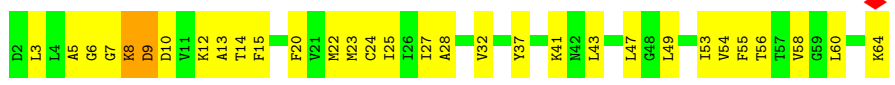
● Molecule 1: Pilin



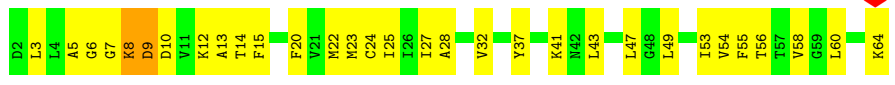
● Molecule 1: Pilin



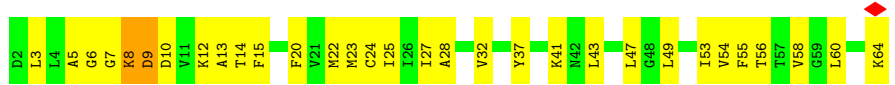
● Molecule 1: Pilin



● Molecule 1: Pilin



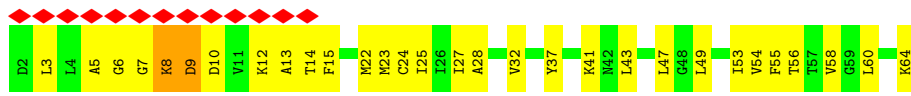
● Molecule 1: Pilin



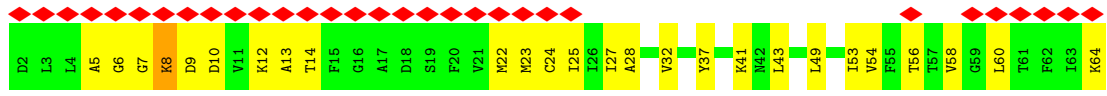
● Molecule 1: Pilin



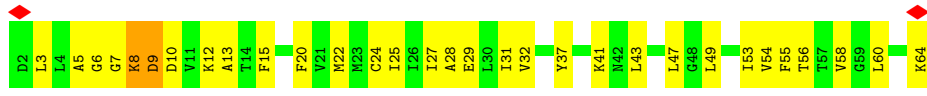
● Molecule 1: Pilin



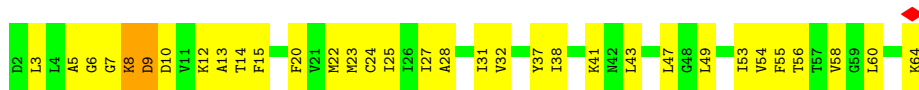
● Molecule 1: Pilin



● Molecule 1: Pilin



• Molecule 1: Pilin



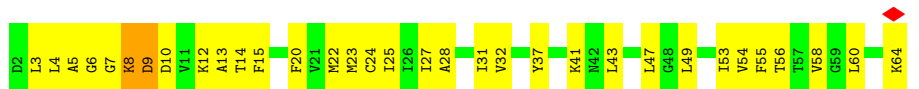
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



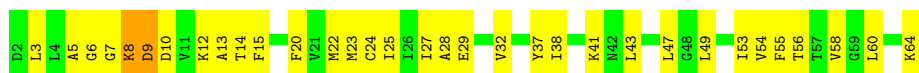
• Molecule 1: Pilin



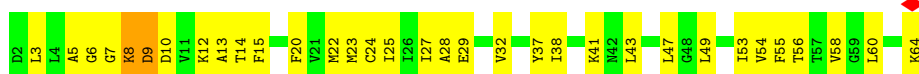
• Molecule 1: Pilin



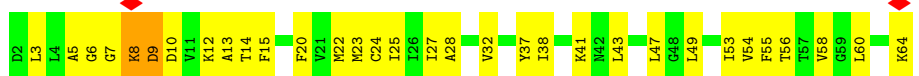
• Molecule 1: Pilin



• Molecule 1: Pilin



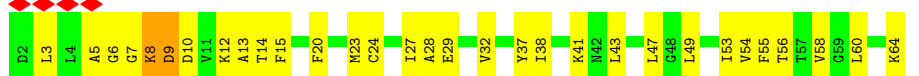
• Molecule 1: Pilin



• Molecule 1: Pilin



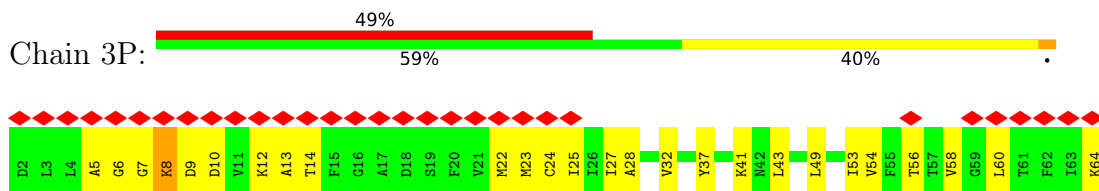
• Molecule 1: Pilin



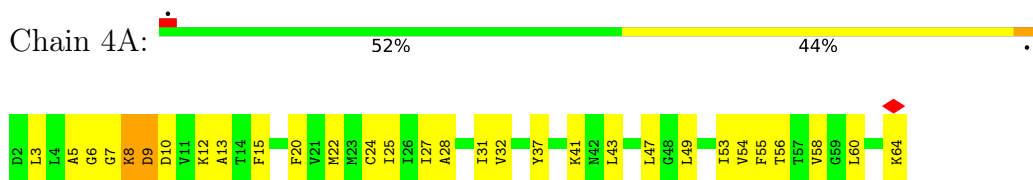
• Molecule 1: Pilin



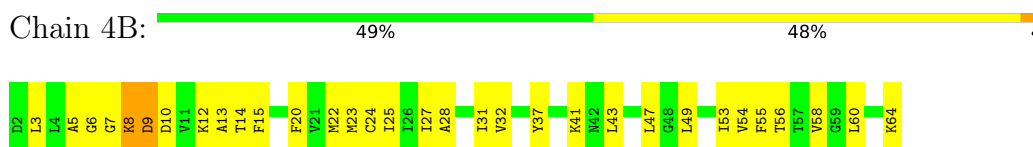
• Molecule 1: Pilin



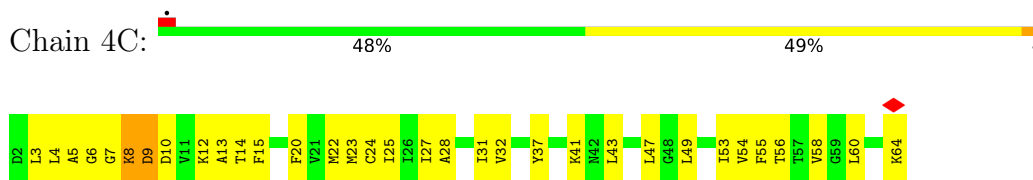
• Molecule 1: Pilin



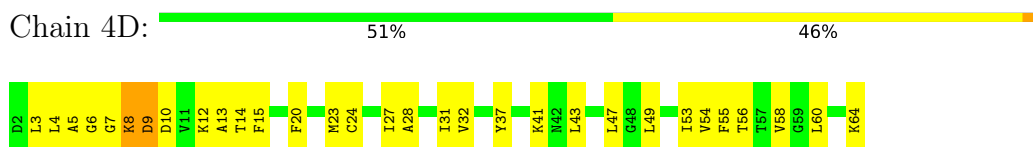
• Molecule 1: Pilin



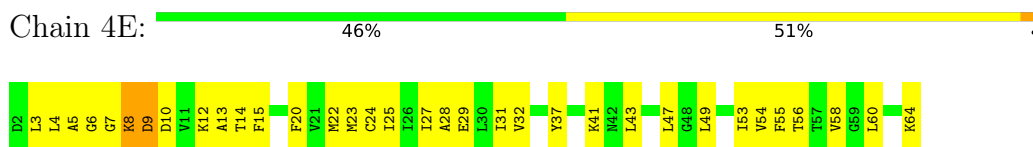
• Molecule 1: Pilin



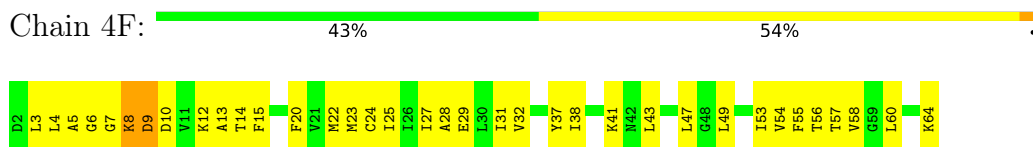
• Molecule 1: Pilin



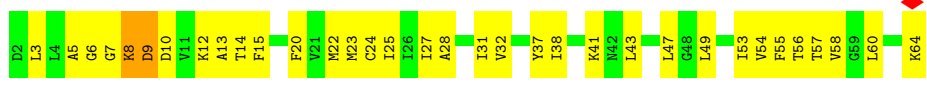
• Molecule 1: Pilin



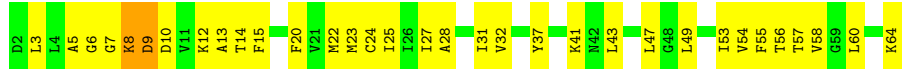
• Molecule 1: Pilin



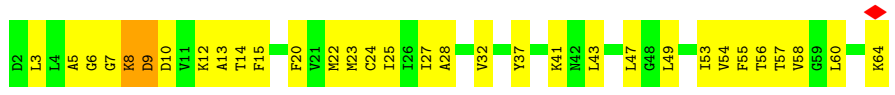
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



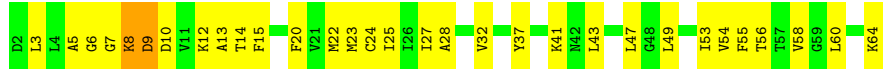
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



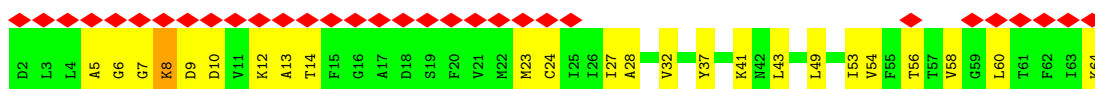
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



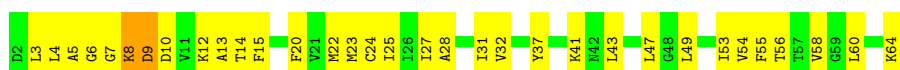
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin

Chain 5E:  46% 51%



• Molecule 1: Pilin

Chain 5F:  48% 49%



• Molecule 1: Pilin

Chain 5G:  49% 48%



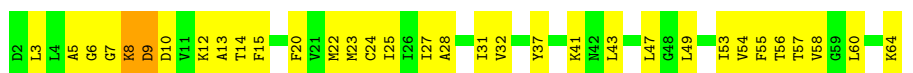
• Molecule 1: Pilin

Chain 5H:  49% 48%



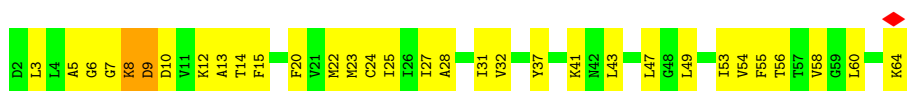
• Molecule 1: Pilin

Chain 5I:  48% 49%



• Molecule 1: Pilin

Chain 5J:  49% 48%



• Molecule 1: Pilin

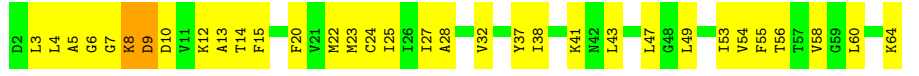
Chain 5K:  49% 48%



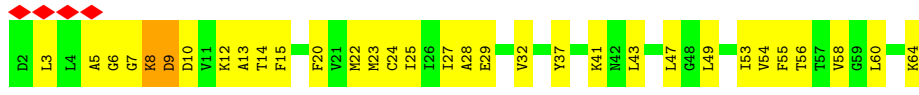
• Molecule 1: Pilin



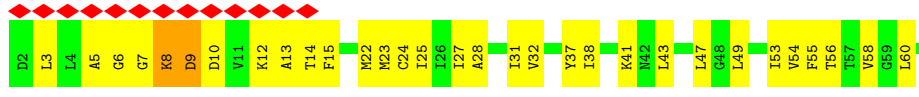
• Molecule 1: Pilin



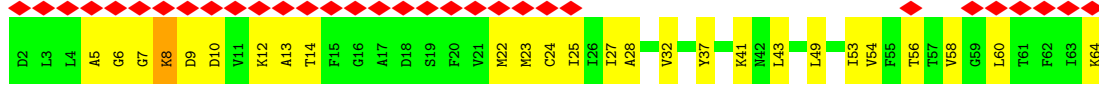
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=28.2°, rise=12.1 Å, axial sym=C5	Depositor
Number of segments used	43952	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	1.67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	76.360	Depositor
Minimum map value	-33.032	Depositor
Average map value	1.048	Depositor
Map value standard deviation	8.826	Depositor
Recommended contour level	10.5	Depositor
Map size (Å)	140.8, 140.8, 281.6	wwPDB
Map dimensions	128, 128, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	1A	0.40	0/475	0.52	0/642
1	1B	0.40	0/475	0.52	0/642
1	1C	0.40	0/475	0.52	0/642
1	1D	0.40	0/475	0.52	0/642
1	1E	0.40	0/475	0.52	0/642
1	1F	0.40	0/475	0.52	0/642
1	1G	0.40	0/475	0.52	0/642
1	1H	0.40	0/475	0.52	0/642
1	1I	0.40	0/475	0.52	0/642
1	1J	0.40	0/475	0.52	0/642
1	1K	0.40	0/475	0.52	0/642
1	1L	0.40	0/475	0.52	0/642
1	1M	0.40	0/475	0.52	0/642
1	1N	0.40	0/475	0.52	0/642
1	1O	0.40	0/475	0.52	0/642
1	1P	0.40	0/475	0.52	0/642
1	2A	0.40	0/475	0.52	0/642
1	2B	0.40	0/475	0.52	0/642
1	2C	0.40	0/475	0.52	0/642
1	2D	0.40	0/475	0.52	0/642
1	2E	0.40	0/475	0.52	0/642
1	2F	0.40	0/475	0.52	0/642
1	2G	0.40	0/475	0.52	0/642
1	2H	0.40	0/475	0.52	0/642
1	2I	0.40	0/475	0.52	0/642
1	2J	0.40	0/475	0.52	0/642
1	2K	0.40	0/475	0.52	0/642
1	2L	0.40	0/475	0.52	0/642
1	2M	0.40	0/475	0.52	0/642
1	2N	0.40	0/475	0.52	0/642
1	2O	0.40	0/475	0.52	0/642
1	2P	0.40	0/475	0.52	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3A	0.40	0/475	0.52	0/642
1	3B	0.40	0/475	0.52	0/642
1	3C	0.40	0/475	0.52	0/642
1	3D	0.40	0/475	0.52	0/642
1	3E	0.40	0/475	0.52	0/642
1	3F	0.40	0/475	0.52	0/642
1	3G	0.40	0/475	0.52	0/642
1	3H	0.40	0/475	0.52	0/642
1	3I	0.40	0/475	0.52	0/642
1	3J	0.40	0/475	0.52	0/642
1	3K	0.40	0/475	0.52	0/642
1	3L	0.40	0/475	0.52	0/642
1	3M	0.40	0/475	0.52	0/642
1	3N	0.41	0/475	0.52	0/642
1	3O	0.40	0/475	0.52	0/642
1	3P	0.41	0/475	0.52	0/642
1	4A	0.40	0/475	0.52	0/642
1	4B	0.40	0/475	0.52	0/642
1	4C	0.40	0/475	0.52	0/642
1	4D	0.40	0/475	0.52	0/642
1	4E	0.40	0/475	0.52	0/642
1	4F	0.40	0/475	0.52	0/642
1	4G	0.40	0/475	0.52	0/642
1	4H	0.40	0/475	0.52	0/642
1	4I	0.40	0/475	0.52	0/642
1	4J	0.40	0/475	0.52	0/642
1	4K	0.40	0/475	0.52	0/642
1	4L	0.40	0/475	0.52	0/642
1	4M	0.40	0/475	0.52	0/642
1	4N	0.41	0/475	0.52	0/642
1	4O	0.41	0/475	0.52	0/642
1	4P	0.41	0/475	0.52	0/642
1	5A	0.40	0/475	0.52	0/642
1	5B	0.40	0/475	0.52	0/642
1	5C	0.40	0/475	0.52	0/642
1	5D	0.40	0/475	0.52	0/642
1	5E	0.40	0/475	0.52	0/642
1	5F	0.40	0/475	0.52	0/642
1	5G	0.40	0/475	0.52	0/642
1	5H	0.40	0/475	0.52	0/642
1	5I	0.40	0/475	0.52	0/642
1	5J	0.40	0/475	0.52	0/642
1	5K	0.40	0/475	0.52	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5L	0.40	0/475	0.52	0/642
1	5M	0.40	0/475	0.52	0/642
1	5N	0.41	0/475	0.52	0/642
1	5O	0.40	0/475	0.52	0/642
1	5P	0.41	0/475	0.52	0/642
All	All	0.40	0/38000	0.52	0/51360

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1A	0	6
1	1B	0	6
1	1C	0	6
1	1D	0	6
1	1E	0	6
1	1F	0	6
1	1G	0	6
1	1H	0	6
1	1I	0	6
1	1J	0	6
1	1K	0	6
1	1L	0	6
1	1M	0	6
1	1N	0	6
1	1O	0	6
1	1P	0	6
1	2A	0	6
1	2B	0	6
1	2C	0	6
1	2D	0	6
1	2E	0	6
1	2F	0	6
1	2G	0	6
1	2H	0	6
1	2I	0	6
1	2J	0	6
1	2K	0	6
1	2L	0	6
1	2M	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	2N	0	6
1	2O	0	6
1	2P	0	6
1	3A	0	6
1	3B	0	6
1	3C	0	6
1	3D	0	6
1	3E	0	6
1	3F	0	6
1	3G	0	6
1	3H	0	6
1	3I	0	6
1	3J	0	6
1	3K	0	6
1	3L	0	6
1	3M	0	6
1	3N	0	6
1	3O	0	6
1	3P	0	6
1	4A	0	6
1	4B	0	6
1	4C	0	6
1	4D	0	6
1	4E	0	6
1	4F	0	6
1	4G	0	6
1	4H	0	6
1	4I	0	6
1	4J	0	6
1	4K	0	6
1	4L	0	6
1	4M	0	6
1	4N	0	6
1	4O	0	6
1	4P	0	6
1	5A	0	6
1	5B	0	6
1	5C	0	6
1	5D	0	6
1	5E	0	6
1	5F	0	6
1	5G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	5H	0	6
1	5I	0	6
1	5J	0	6
1	5K	0	6
1	5L	0	6
1	5M	0	6
1	5N	0	6
1	5O	0	6
1	5P	0	6
All	All	0	480

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 480 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	5	ALA	Peptide
1	1A	6	GLY	Peptide
1	1A	7	GLY	Peptide
1	1A	8	LYS	Peptide
1	1A	9	ASP	Peptide

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	1A	471	0	520	42	0
1	1B	471	0	520	49	0
1	1C	471	0	520	49	0
1	1D	471	0	520	50	0
1	1E	471	0	520	52	0
1	1F	471	0	520	53	0
1	1G	471	0	520	53	0
1	1H	471	0	520	51	0
1	1I	471	0	520	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1J	471	0	520	48	0
1	1K	471	0	520	47	0
1	1L	471	0	520	43	0
1	1M	471	0	520	42	0
1	1N	471	0	520	43	0
1	1O	471	0	520	41	0
1	1P	471	0	520	22	0
1	2A	471	0	520	42	0
1	2B	471	0	520	50	0
1	2C	471	0	520	51	0
1	2D	471	0	520	49	0
1	2E	471	0	520	50	0
1	2F	471	0	520	51	0
1	2G	471	0	520	52	0
1	2H	471	0	520	51	0
1	2I	471	0	520	50	0
1	2J	471	0	520	45	0
1	2K	471	0	520	44	0
1	2L	471	0	520	43	0
1	2M	471	0	520	43	0
1	2N	471	0	520	43	0
1	2O	471	0	520	40	0
1	2P	471	0	520	20	0
1	3A	471	0	520	42	0
1	3B	471	0	520	49	0
1	3C	471	0	520	49	0
1	3D	471	0	520	51	0
1	3E	471	0	520	51	0
1	3F	471	0	520	52	0
1	3G	471	0	520	53	0
1	3H	471	0	520	54	0
1	3I	471	0	520	49	0
1	3J	471	0	520	47	0
1	3K	471	0	520	46	0
1	3L	471	0	520	44	0
1	3M	471	0	520	44	0
1	3N	471	0	520	44	0
1	3O	471	0	520	42	0
1	3P	471	0	520	20	0
1	4A	471	0	520	41	0
1	4B	471	0	520	48	0
1	4C	471	0	520	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4D	471	0	520	49	0
1	4E	471	0	520	53	0
1	4F	471	0	520	54	0
1	4G	471	0	520	53	0
1	4H	471	0	520	52	0
1	4I	471	0	520	51	0
1	4J	471	0	520	46	0
1	4K	471	0	520	45	0
1	4L	471	0	520	43	0
1	4M	471	0	520	42	0
1	4N	471	0	520	43	0
1	4O	471	0	520	41	0
1	4P	471	0	520	19	0
1	5A	471	0	520	40	0
1	5B	471	0	520	48	0
1	5C	471	0	520	51	0
1	5D	471	0	520	52	0
1	5E	471	0	520	53	0
1	5F	471	0	520	54	0
1	5G	471	0	520	54	0
1	5H	471	0	520	53	0
1	5I	471	0	520	52	0
1	5J	471	0	520	47	0
1	5K	471	0	520	46	0
1	5L	471	0	520	45	0
1	5M	471	0	520	45	0
1	5N	471	0	520	43	0
1	5O	471	0	520	42	0
1	5P	471	0	520	20	0
2	1A	49	0	74	23	0
2	1B	49	0	74	28	0
2	1C	49	0	74	28	0
2	1D	49	0	74	30	0
2	1E	49	0	74	30	0
2	1F	49	0	74	31	0
2	1G	49	0	74	31	0
2	1H	49	0	74	30	0
2	1I	49	0	74	30	0
2	1J	49	0	74	29	0
2	1K	49	0	74	29	0
2	1L	49	0	74	27	0
2	1M	49	0	74	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1N	49	0	74	25	0
2	1O	49	0	74	25	0
2	2A	49	0	74	22	0
2	2B	49	0	74	28	0
2	2C	49	0	74	29	0
2	2D	49	0	74	28	0
2	2E	49	0	74	29	0
2	2F	49	0	74	29	0
2	2G	49	0	74	29	0
2	2H	49	0	74	30	0
2	2I	49	0	74	29	0
2	2J	49	0	74	29	0
2	2K	49	0	74	28	0
2	2L	49	0	74	27	0
2	2M	49	0	74	26	0
2	2N	49	0	74	25	0
2	2O	49	0	74	24	0
2	3A	49	0	74	22	0
2	3B	49	0	74	27	0
2	3C	49	0	74	29	0
2	3D	49	0	74	30	0
2	3E	49	0	74	29	0
2	3F	49	0	74	29	0
2	3G	49	0	74	29	0
2	3H	49	0	74	30	0
2	3I	49	0	74	29	0
2	3J	49	0	74	28	0
2	3K	49	0	74	28	0
2	3L	49	0	74	27	0
2	3M	49	0	74	26	0
2	3N	49	0	74	26	0
2	3O	49	0	74	26	0
2	4A	49	0	74	22	0
2	4B	49	0	74	28	0
2	4C	49	0	74	28	0
2	4D	49	0	74	28	0
2	4E	49	0	74	30	0
2	4F	49	0	74	31	0
2	4G	49	0	74	30	0
2	4H	49	0	74	29	0
2	4I	49	0	74	30	0
2	4J	49	0	74	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4K	49	0	74	28	0
2	4L	49	0	74	27	0
2	4M	49	0	74	26	0
2	4N	49	0	74	26	0
2	4O	49	0	74	26	0
2	5A	49	0	74	22	0
2	5B	49	0	74	28	0
2	5C	49	0	74	29	0
2	5D	49	0	74	30	0
2	5E	49	0	74	30	0
2	5F	49	0	74	30	0
2	5G	49	0	74	30	0
2	5H	49	0	74	30	0
2	5I	49	0	74	29	0
2	5J	49	0	74	29	0
2	5K	49	0	74	28	0
2	5L	49	0	74	27	0
2	5M	49	0	74	25	0
2	5N	49	0	74	26	0
2	5O	49	0	74	25	0
All	All	41355	0	47150	3731	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 3731 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)
1:2J:47:LEU:HD22	2:2J:101:LHG:H102	1.34	1.10
1:1O:47:LEU:HD22	2:1O:101:LHG:H102	1.34	1.09
1:2F:47:LEU:HD22	2:2F:101:LHG:H102	1.34	1.09
1:2G:47:LEU:HD22	2:2G:101:LHG:H102	1.34	1.09
1:2H:47:LEU:HD22	2:2H:101:LHG:H102	1.34	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	1P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	2P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	3P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	4P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5A	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5B	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5C	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5D	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5F	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5G	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5H	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5I	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5J	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5K	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5M	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5N	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5O	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
1	5P	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
All	All	4880/5040 (97%)	4480 (92%)	400 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	1A	52/52 (100%)	52 (100%)	0	100	100
1	1B	52/52 (100%)	52 (100%)	0	100	100
1	1C	52/52 (100%)	52 (100%)	0	100	100
1	1D	52/52 (100%)	52 (100%)	0	100	100
1	1E	52/52 (100%)	52 (100%)	0	100	100
1	1F	52/52 (100%)	52 (100%)	0	100	100
1	1G	52/52 (100%)	52 (100%)	0	100	100
1	1H	52/52 (100%)	52 (100%)	0	100	100
1	1I	52/52 (100%)	52 (100%)	0	100	100
1	1J	52/52 (100%)	52 (100%)	0	100	100
1	1K	52/52 (100%)	52 (100%)	0	100	100
1	1L	52/52 (100%)	52 (100%)	0	100	100
1	1M	52/52 (100%)	52 (100%)	0	100	100
1	1N	52/52 (100%)	52 (100%)	0	100	100
1	1O	52/52 (100%)	52 (100%)	0	100	100
1	1P	52/52 (100%)	52 (100%)	0	100	100
1	2A	52/52 (100%)	52 (100%)	0	100	100
1	2B	52/52 (100%)	52 (100%)	0	100	100
1	2C	52/52 (100%)	52 (100%)	0	100	100
1	2D	52/52 (100%)	52 (100%)	0	100	100
1	2E	52/52 (100%)	52 (100%)	0	100	100
1	2F	52/52 (100%)	52 (100%)	0	100	100
1	2G	52/52 (100%)	52 (100%)	0	100	100
1	2H	52/52 (100%)	52 (100%)	0	100	100
1	2I	52/52 (100%)	52 (100%)	0	100	100
1	2J	52/52 (100%)	52 (100%)	0	100	100
1	2K	52/52 (100%)	52 (100%)	0	100	100
1	2L	52/52 (100%)	52 (100%)	0	100	100
1	2M	52/52 (100%)	52 (100%)	0	100	100
1	2N	52/52 (100%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2O	52/52 (100%)	52 (100%)	0	100	100
1	2P	52/52 (100%)	52 (100%)	0	100	100
1	3A	52/52 (100%)	52 (100%)	0	100	100
1	3B	52/52 (100%)	52 (100%)	0	100	100
1	3C	52/52 (100%)	52 (100%)	0	100	100
1	3D	52/52 (100%)	52 (100%)	0	100	100
1	3E	52/52 (100%)	52 (100%)	0	100	100
1	3F	52/52 (100%)	52 (100%)	0	100	100
1	3G	52/52 (100%)	52 (100%)	0	100	100
1	3H	52/52 (100%)	52 (100%)	0	100	100
1	3I	52/52 (100%)	52 (100%)	0	100	100
1	3J	52/52 (100%)	52 (100%)	0	100	100
1	3K	52/52 (100%)	52 (100%)	0	100	100
1	3L	52/52 (100%)	52 (100%)	0	100	100
1	3M	52/52 (100%)	52 (100%)	0	100	100
1	3N	52/52 (100%)	52 (100%)	0	100	100
1	3O	52/52 (100%)	52 (100%)	0	100	100
1	3P	52/52 (100%)	52 (100%)	0	100	100
1	4A	52/52 (100%)	52 (100%)	0	100	100
1	4B	52/52 (100%)	52 (100%)	0	100	100
1	4C	52/52 (100%)	52 (100%)	0	100	100
1	4D	52/52 (100%)	52 (100%)	0	100	100
1	4E	52/52 (100%)	52 (100%)	0	100	100
1	4F	52/52 (100%)	52 (100%)	0	100	100
1	4G	52/52 (100%)	52 (100%)	0	100	100
1	4H	52/52 (100%)	52 (100%)	0	100	100
1	4I	52/52 (100%)	52 (100%)	0	100	100
1	4J	52/52 (100%)	52 (100%)	0	100	100
1	4K	52/52 (100%)	52 (100%)	0	100	100
1	4L	52/52 (100%)	52 (100%)	0	100	100
1	4M	52/52 (100%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4N	52/52 (100%)	52 (100%)	0	100	100
1	4O	52/52 (100%)	52 (100%)	0	100	100
1	4P	52/52 (100%)	52 (100%)	0	100	100
1	5A	52/52 (100%)	52 (100%)	0	100	100
1	5B	52/52 (100%)	52 (100%)	0	100	100
1	5C	52/52 (100%)	52 (100%)	0	100	100
1	5D	52/52 (100%)	52 (100%)	0	100	100
1	5E	52/52 (100%)	52 (100%)	0	100	100
1	5F	52/52 (100%)	52 (100%)	0	100	100
1	5G	52/52 (100%)	52 (100%)	0	100	100
1	5H	52/52 (100%)	52 (100%)	0	100	100
1	5I	52/52 (100%)	52 (100%)	0	100	100
1	5J	52/52 (100%)	52 (100%)	0	100	100
1	5K	52/52 (100%)	52 (100%)	0	100	100
1	5L	52/52 (100%)	52 (100%)	0	100	100
1	5M	52/52 (100%)	52 (100%)	0	100	100
1	5N	52/52 (100%)	52 (100%)	0	100	100
1	5O	52/52 (100%)	52 (100%)	0	100	100
1	5P	52/52 (100%)	52 (100%)	0	100	100
All	All	4160/4160 (100%)	4160 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

75 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	LHG	2D	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2M	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	4C	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1E	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5J	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2L	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5M	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	3E	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3A	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2K	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3D	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4I	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	2I	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1C	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1K	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1H	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1A	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3M	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	4J	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3C	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2H	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3G	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LHG	4H	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4M	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	5C	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4G	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1G	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2N	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	3L	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2F	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3I	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	4D	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5H	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3N	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5I	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3B	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5K	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3H	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4B	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5G	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1L	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4F	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	3O	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	4E	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5A	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5B	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4K	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2G	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1J	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3K	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4O	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	2O	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	5D	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1M	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5O	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	1I	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	4A	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LHG	1N	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	3J	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	4L	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5F	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	5L	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	3F	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2A	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	5N	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	1F	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2C	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2E	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	5E	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1D	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2B	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	2J	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1B	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.59	2 (3%)
2	LHG	1O	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)
2	LHG	4N	101	-	48,48,48	0.60	1 (2%)	51,54,54	0.58	2 (3%)

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	LHG	2D	101	-	-	30/53/53/53	-
2	LHG	2M	101	-	-	31/53/53/53	-
2	LHG	4C	101	-	-	31/53/53/53	-
2	LHG	1E	101	-	-	30/53/53/53	-
2	LHG	5J	101	-	-	31/53/53/53	-
2	LHG	2L	101	-	-	31/53/53/53	-
2	LHG	5M	101	-	-	31/53/53/53	-
2	LHG	3E	101	-	-	30/53/53/53	-
2	LHG	3A	101	-	-	30/53/53/53	-
2	LHG	2K	101	-	-	31/53/53/53	-
2	LHG	3D	101	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LHG	4I	101	-	-	30/53/53/53	-
2	LHG	2I	101	-	-	30/53/53/53	-
2	LHG	1C	101	-	-	30/53/53/53	-
2	LHG	1K	101	-	-	31/53/53/53	-
2	LHG	1H	101	-	-	30/53/53/53	-
2	LHG	1A	101	-	-	31/53/53/53	-
2	LHG	3M	101	-	-	31/53/53/53	-
2	LHG	4J	101	-	-	31/53/53/53	-
2	LHG	3C	101	-	-	30/53/53/53	-
2	LHG	2H	101	-	-	30/53/53/53	-
2	LHG	3G	101	-	-	31/53/53/53	-
2	LHG	4H	101	-	-	30/53/53/53	-
2	LHG	4M	101	-	-	31/53/53/53	-
2	LHG	5C	101	-	-	31/53/53/53	-
2	LHG	4G	101	-	-	30/53/53/53	-
2	LHG	1G	101	-	-	31/53/53/53	-
2	LHG	2N	101	-	-	30/53/53/53	-
2	LHG	3L	101	-	-	31/53/53/53	-
2	LHG	2F	101	-	-	31/53/53/53	-
2	LHG	3I	101	-	-	31/53/53/53	-
2	LHG	4D	101	-	-	31/53/53/53	-
2	LHG	5H	101	-	-	30/53/53/53	-
2	LHG	3N	101	-	-	31/53/53/53	-
2	LHG	5I	101	-	-	30/53/53/53	-
2	LHG	3B	101	-	-	31/53/53/53	-
2	LHG	5K	101	-	-	31/53/53/53	-
2	LHG	3H	101	-	-	30/53/53/53	-
2	LHG	4B	101	-	-	30/53/53/53	-
2	LHG	5G	101	-	-	31/53/53/53	-
2	LHG	1L	101	-	-	31/53/53/53	-
2	LHG	4F	101	-	-	30/53/53/53	-
2	LHG	3O	101	-	-	31/53/53/53	-
2	LHG	4E	101	-	-	30/53/53/53	-
2	LHG	5A	101	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LHG	5B	101	-	-	30/53/53/53	-
2	LHG	4K	101	-	-	31/53/53/53	-
2	LHG	2G	101	-	-	31/53/53/53	-
2	LHG	1J	101	-	-	31/53/53/53	-
2	LHG	3K	101	-	-	31/53/53/53	-
2	LHG	4O	101	-	-	31/53/53/53	-
2	LHG	2O	101	-	-	31/53/53/53	-
2	LHG	5D	101	-	-	30/53/53/53	-
2	LHG	1M	101	-	-	31/53/53/53	-
2	LHG	5O	101	-	-	31/53/53/53	-
2	LHG	1I	101	-	-	30/53/53/53	-
2	LHG	4A	101	-	-	31/53/53/53	-
2	LHG	1N	101	-	-	31/53/53/53	-
2	LHG	3J	101	-	-	31/53/53/53	-
2	LHG	4L	101	-	-	31/53/53/53	-
2	LHG	5F	101	-	-	31/53/53/53	-
2	LHG	5L	101	-	-	31/53/53/53	-
2	LHG	3F	101	-	-	30/53/53/53	-
2	LHG	2A	101	-	-	31/53/53/53	-
2	LHG	5N	101	-	-	31/53/53/53	-
2	LHG	1F	101	-	-	30/53/53/53	-
2	LHG	2C	101	-	-	30/53/53/53	-
2	LHG	2E	101	-	-	30/53/53/53	-
2	LHG	5E	101	-	-	30/53/53/53	-
2	LHG	1D	101	-	-	30/53/53/53	-
2	LHG	2B	101	-	-	31/53/53/53	-
2	LHG	2J	101	-	-	31/53/53/53	-
2	LHG	1B	101	-	-	31/53/53/53	-
2	LHG	1O	101	-	-	31/53/53/53	-
2	LHG	4N	101	-	-	31/53/53/53	-

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4J	101	LHG	C16-C15	-3.49	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2L	101	LHG	C16-C15	-3.49	1.32	1.51
2	4I	101	LHG	C16-C15	-3.49	1.32	1.51
2	3J	101	LHG	C16-C15	-3.49	1.32	1.51
2	5J	101	LHG	C16-C15	-3.49	1.32	1.51

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5L	101	LHG	C17-C16-C15	2.34	126.29	114.42
2	4K	101	LHG	C17-C16-C15	2.33	126.28	114.42
2	2K	101	LHG	C17-C16-C15	2.33	126.27	114.42
2	2L	101	LHG	C17-C16-C15	2.33	126.25	114.42
2	5K	101	LHG	C17-C16-C15	2.33	126.24	114.42

There are no chirality outliers.

5 of 2297 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1A	101	LHG	O1-C1-C2-C3
2	1A	101	LHG	C4-O6-P-O5
2	1A	101	LHG	O9-C7-O7-C5
2	1B	101	LHG	O1-C1-C2-C3
2	1B	101	LHG	C4-O6-P-O5

There are no ring outliers.

75 monomers are involved in 2082 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2D	101	LHG	28	0
2	2M	101	LHG	26	0
2	4C	101	LHG	28	0
2	1E	101	LHG	30	0
2	5J	101	LHG	29	0
2	2L	101	LHG	27	0
2	5M	101	LHG	25	0
2	3E	101	LHG	29	0
2	3A	101	LHG	22	0
2	2K	101	LHG	28	0
2	3D	101	LHG	30	0
2	4I	101	LHG	30	0
2	2I	101	LHG	29	0

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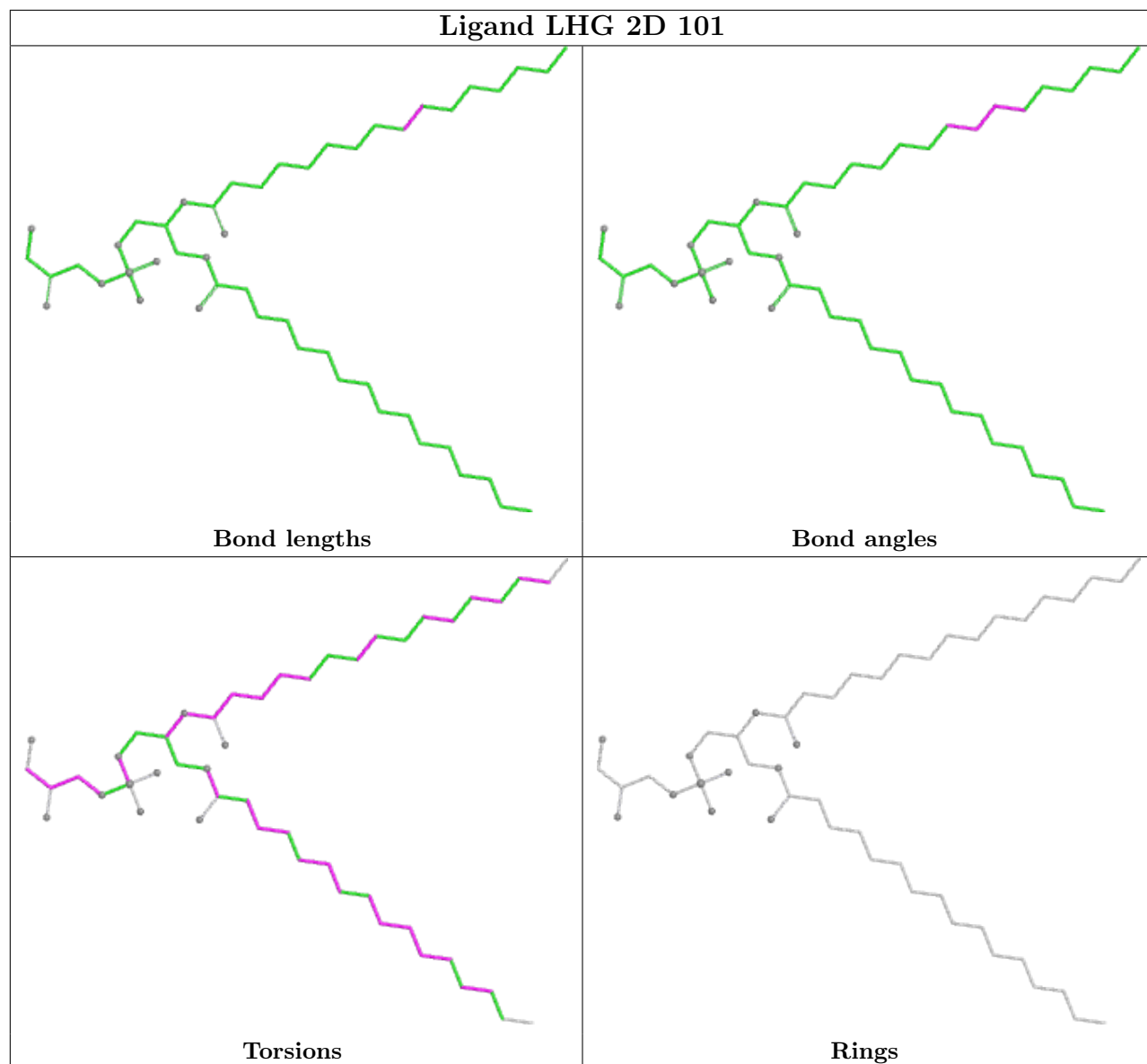
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1C	101	LHG	28	0
2	1K	101	LHG	29	0
2	1H	101	LHG	30	0
2	1A	101	LHG	23	0
2	3M	101	LHG	26	0
2	4J	101	LHG	28	0
2	3C	101	LHG	29	0
2	2H	101	LHG	30	0
2	3G	101	LHG	29	0
2	4H	101	LHG	29	0
2	4M	101	LHG	26	0
2	5C	101	LHG	29	0
2	4G	101	LHG	30	0
2	1G	101	LHG	31	0
2	2N	101	LHG	25	0
2	3L	101	LHG	27	0
2	2F	101	LHG	29	0
2	3I	101	LHG	29	0
2	4D	101	LHG	28	0
2	5H	101	LHG	30	0
2	3N	101	LHG	26	0
2	5I	101	LHG	29	0
2	3B	101	LHG	27	0
2	5K	101	LHG	28	0
2	3H	101	LHG	30	0
2	4B	101	LHG	28	0
2	5G	101	LHG	30	0
2	1L	101	LHG	27	0
2	4F	101	LHG	31	0
2	3O	101	LHG	26	0
2	4E	101	LHG	30	0
2	5A	101	LHG	22	0
2	5B	101	LHG	28	0
2	4K	101	LHG	28	0
2	2G	101	LHG	29	0
2	1J	101	LHG	29	0
2	3K	101	LHG	28	0
2	4O	101	LHG	26	0
2	2O	101	LHG	24	0
2	5D	101	LHG	30	0
2	1M	101	LHG	24	0
2	5O	101	LHG	25	0

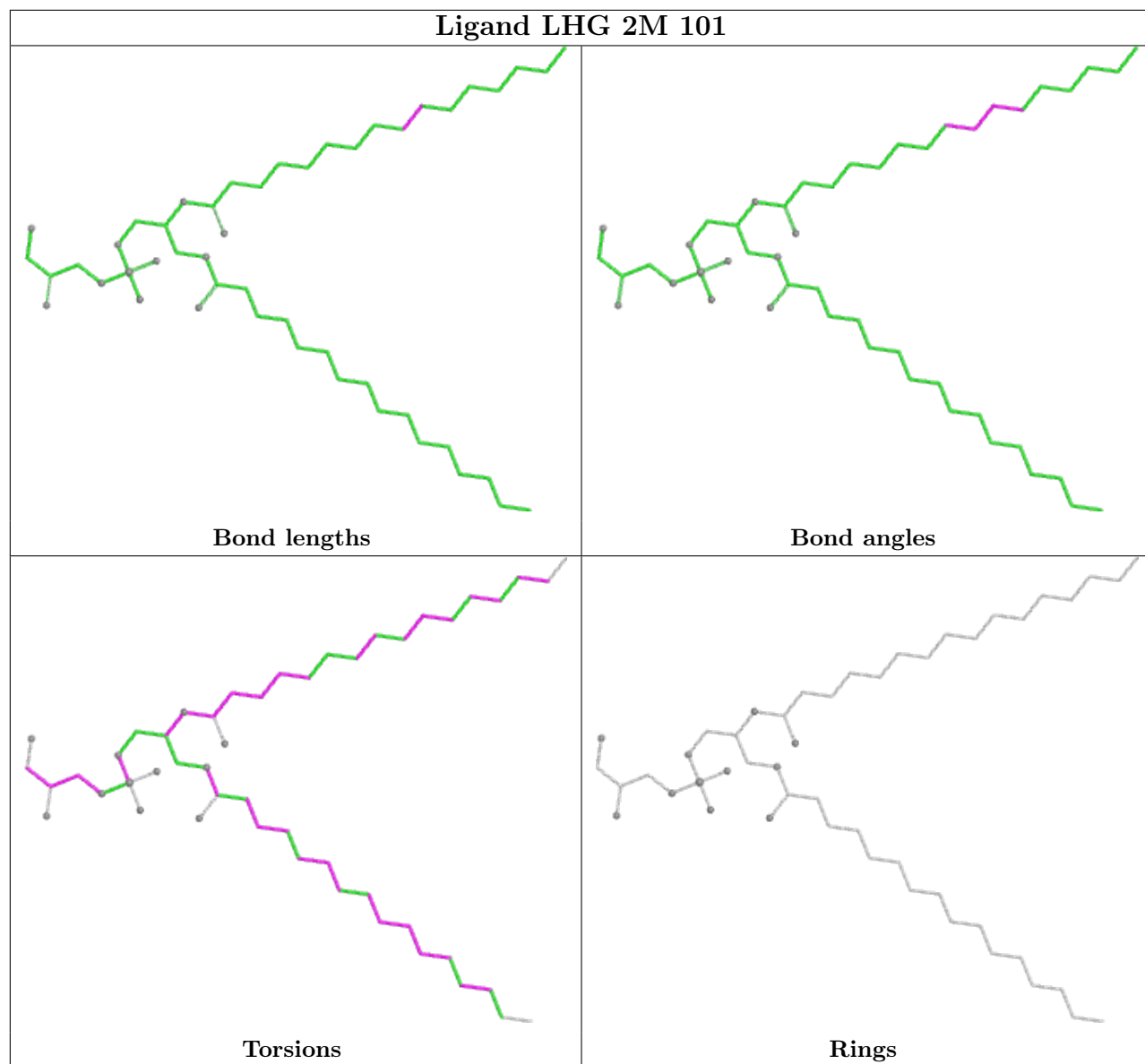
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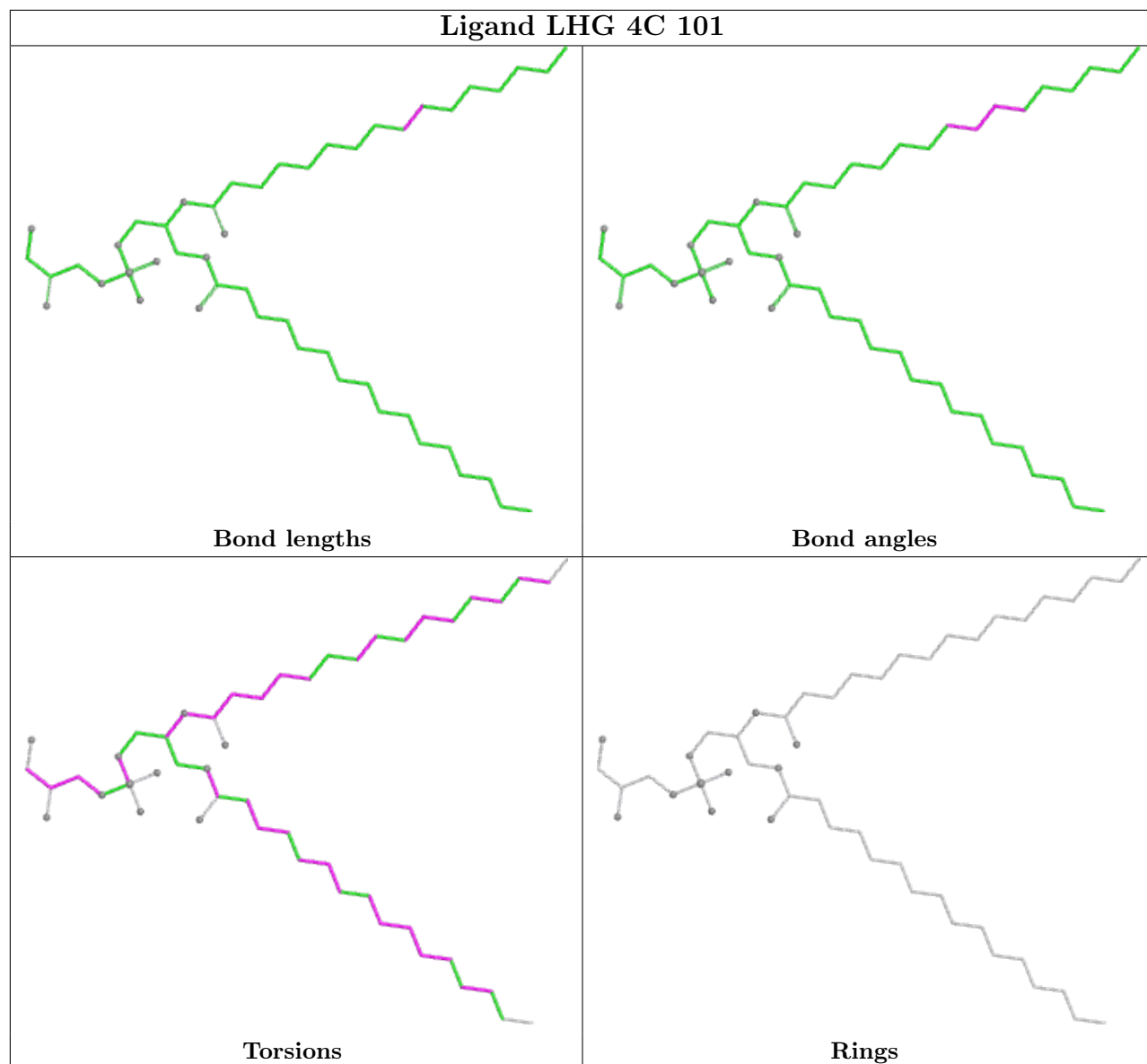
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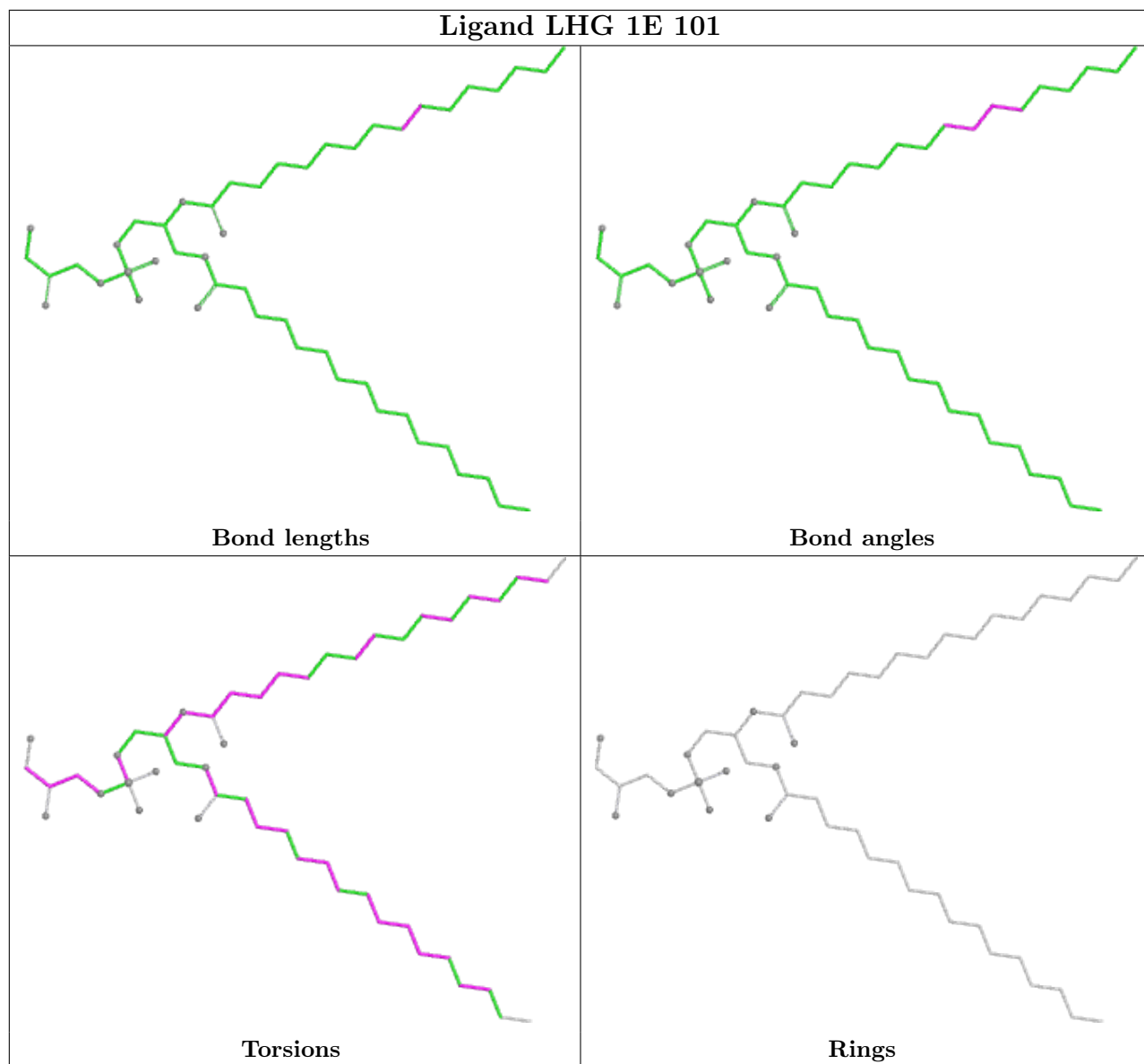
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1I	101	LHG	30	0
2	4A	101	LHG	22	0
2	1N	101	LHG	25	0
2	3J	101	LHG	28	0
2	4L	101	LHG	27	0
2	5F	101	LHG	30	0
2	5L	101	LHG	27	0
2	3F	101	LHG	29	0
2	2A	101	LHG	22	0
2	5N	101	LHG	26	0
2	1F	101	LHG	31	0
2	2C	101	LHG	29	0
2	2E	101	LHG	29	0
2	5E	101	LHG	30	0
2	1D	101	LHG	30	0
2	2B	101	LHG	28	0
2	2J	101	LHG	29	0
2	1B	101	LHG	28	0
2	1O	101	LHG	25	0
2	4N	101	LHG	26	0

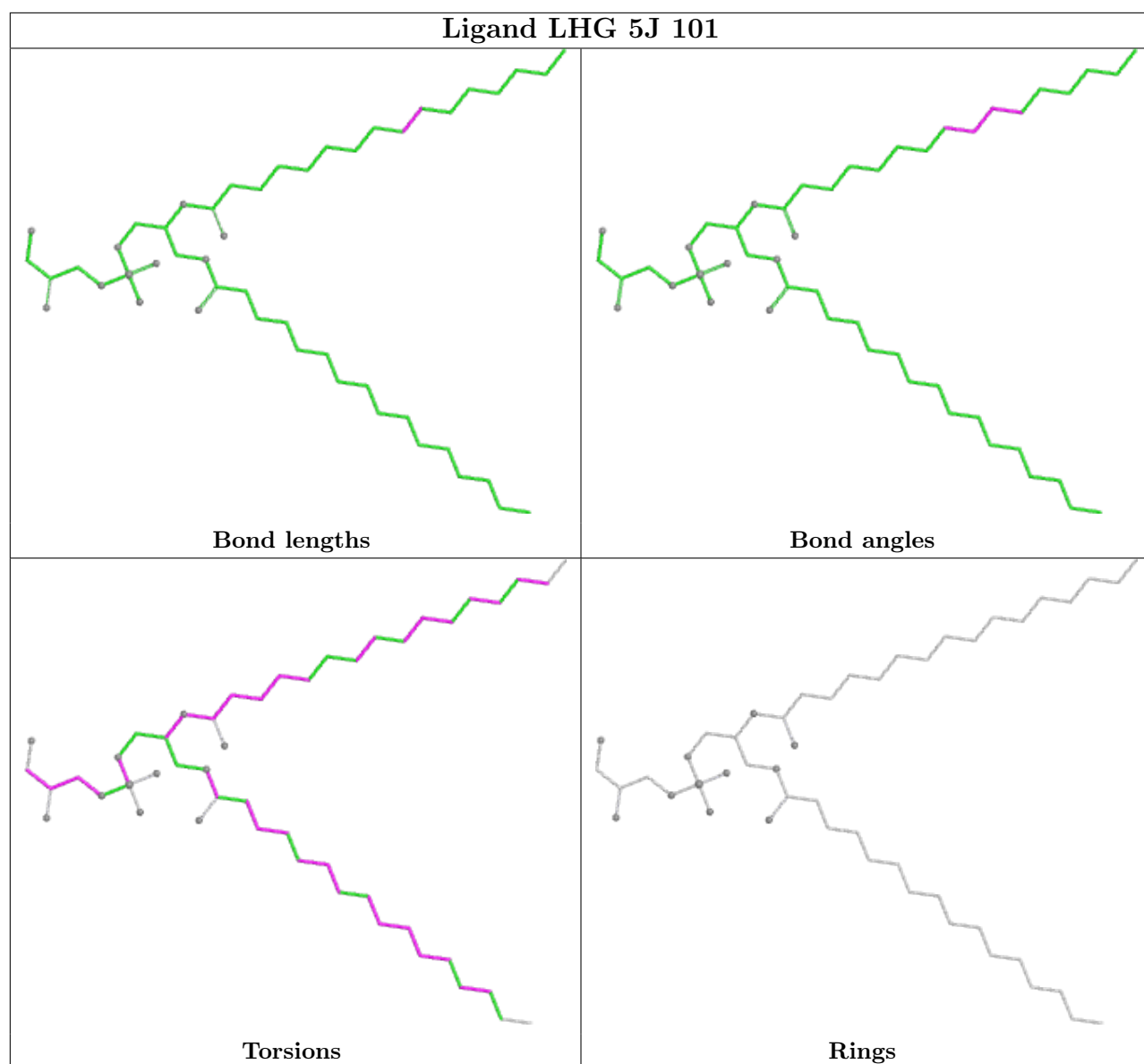
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

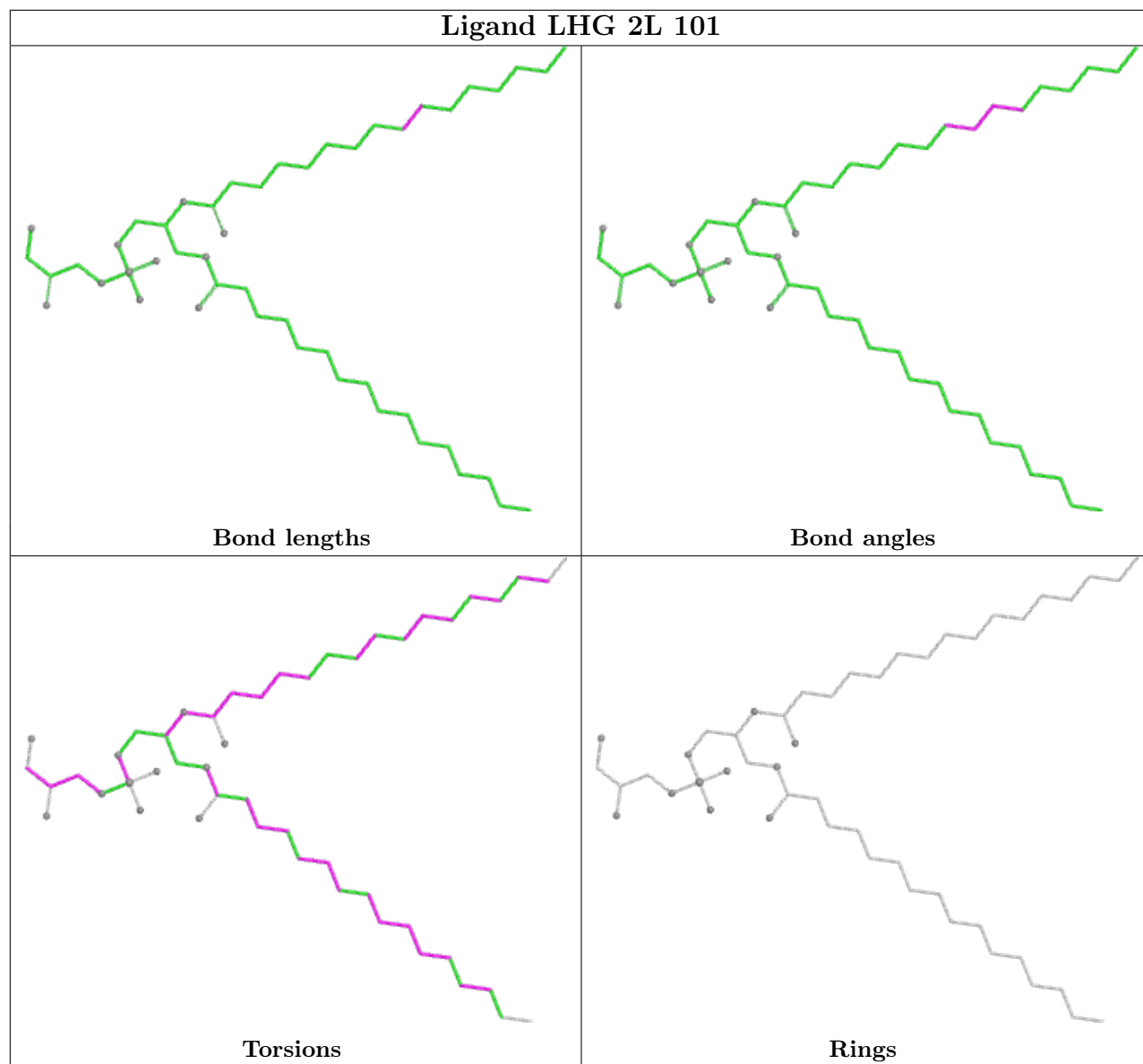


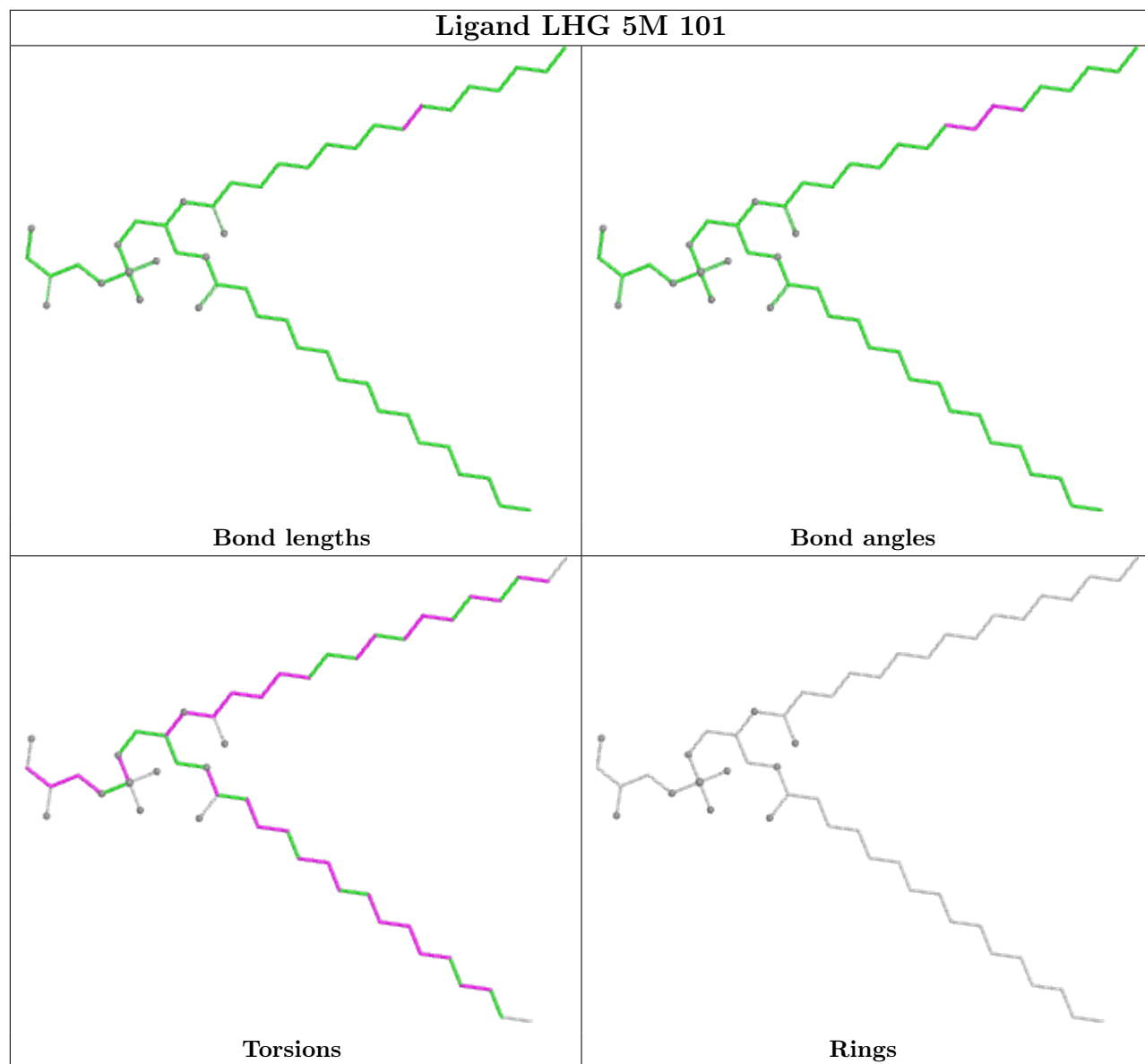


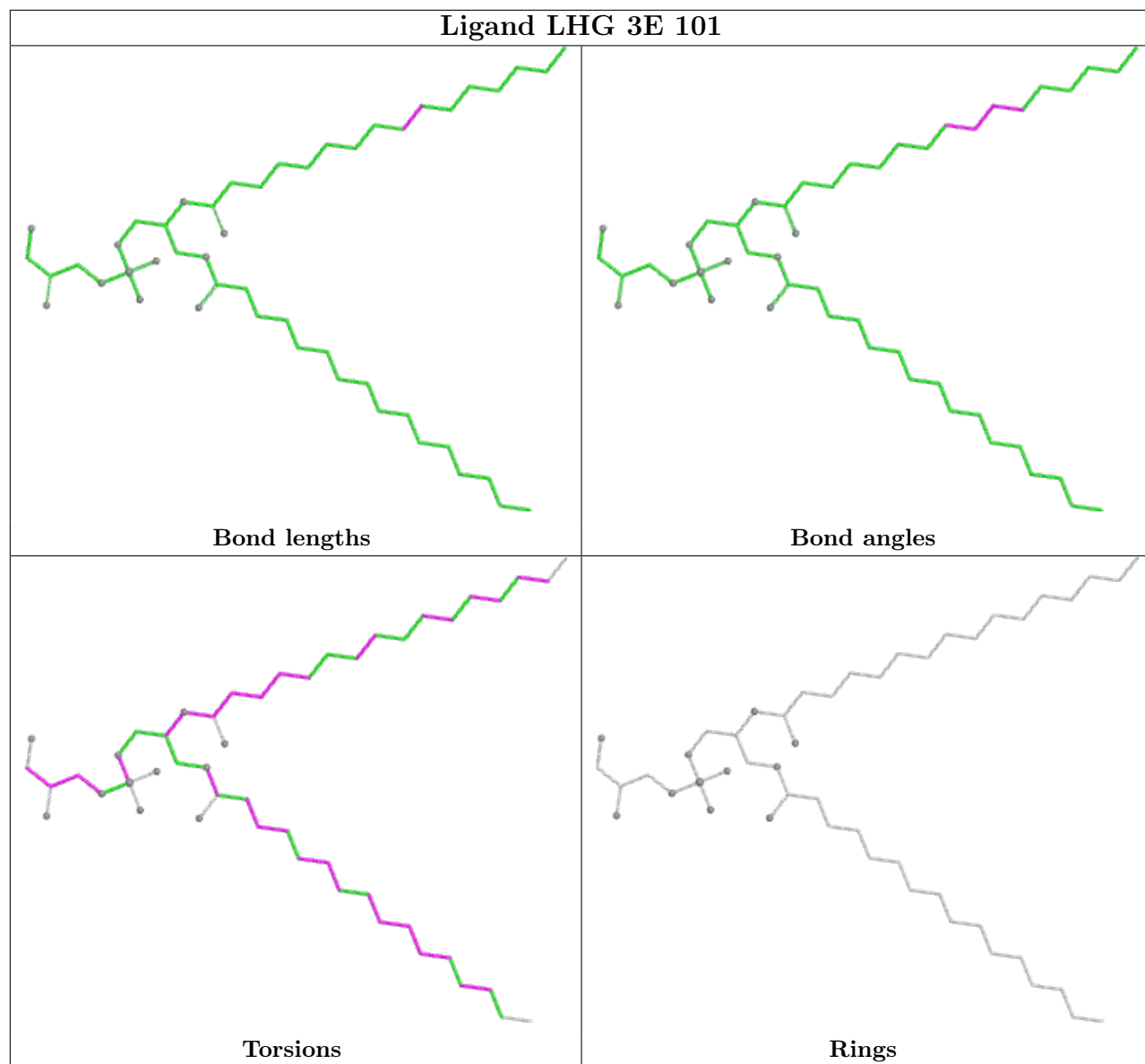


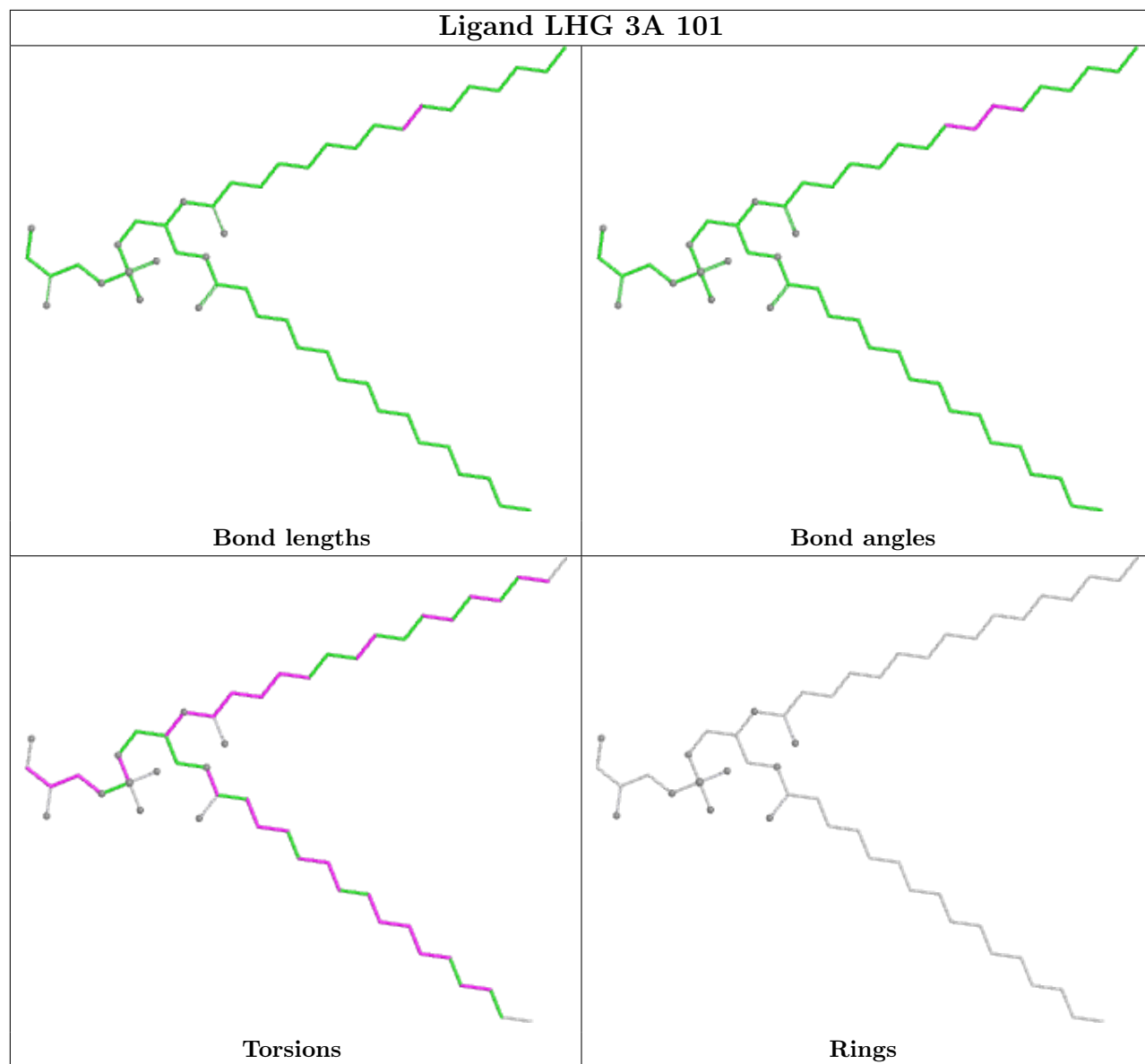


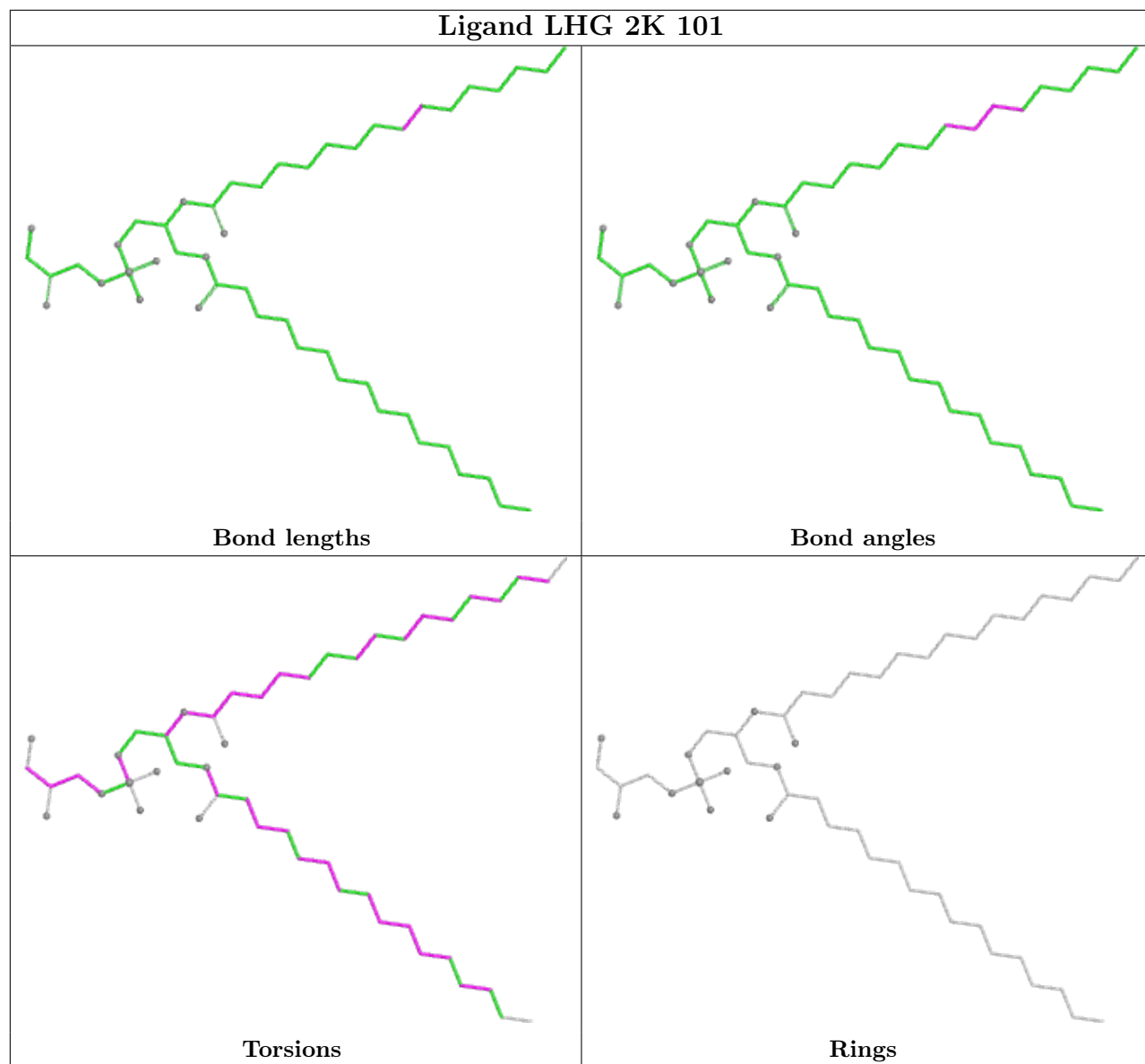


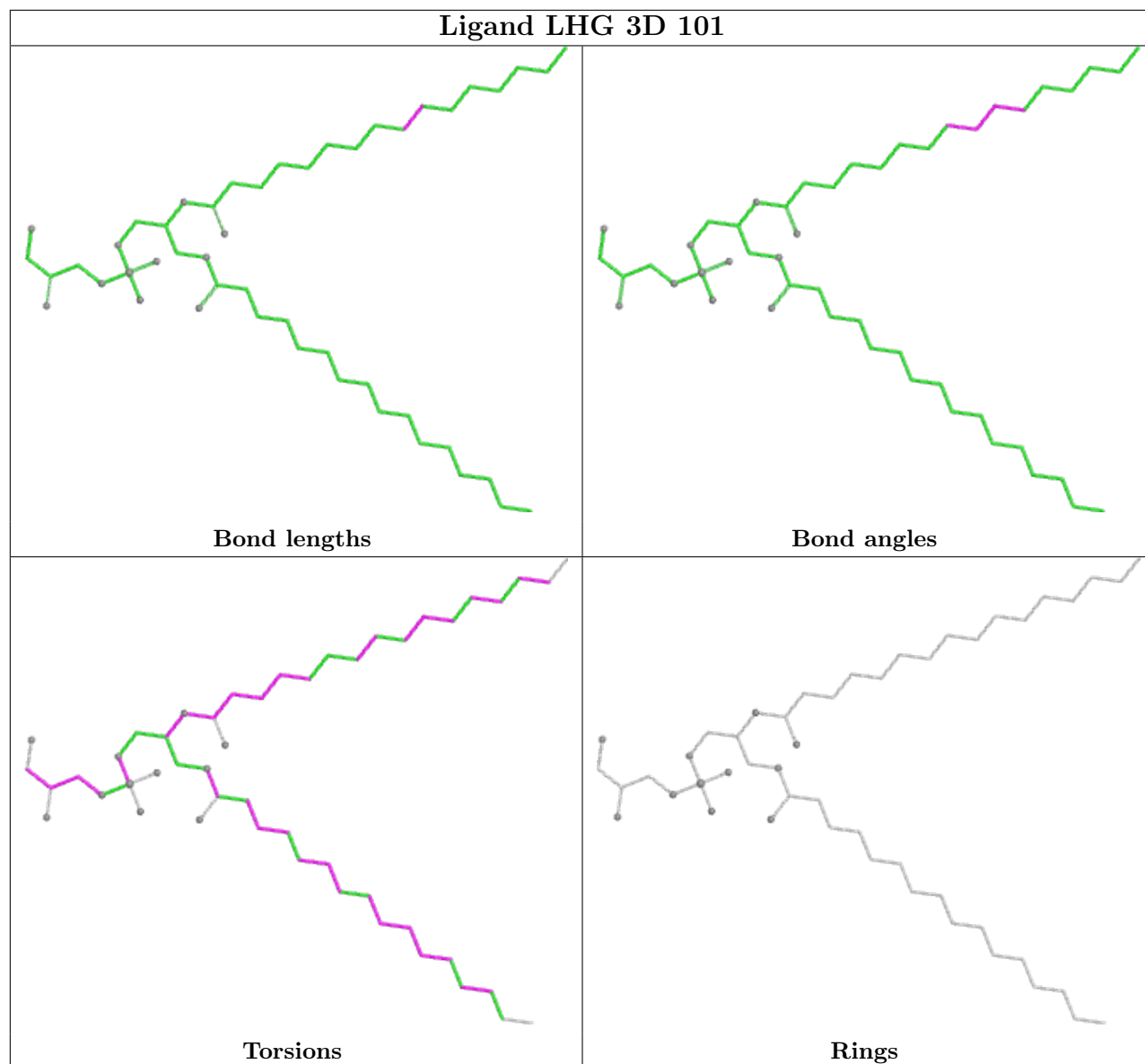


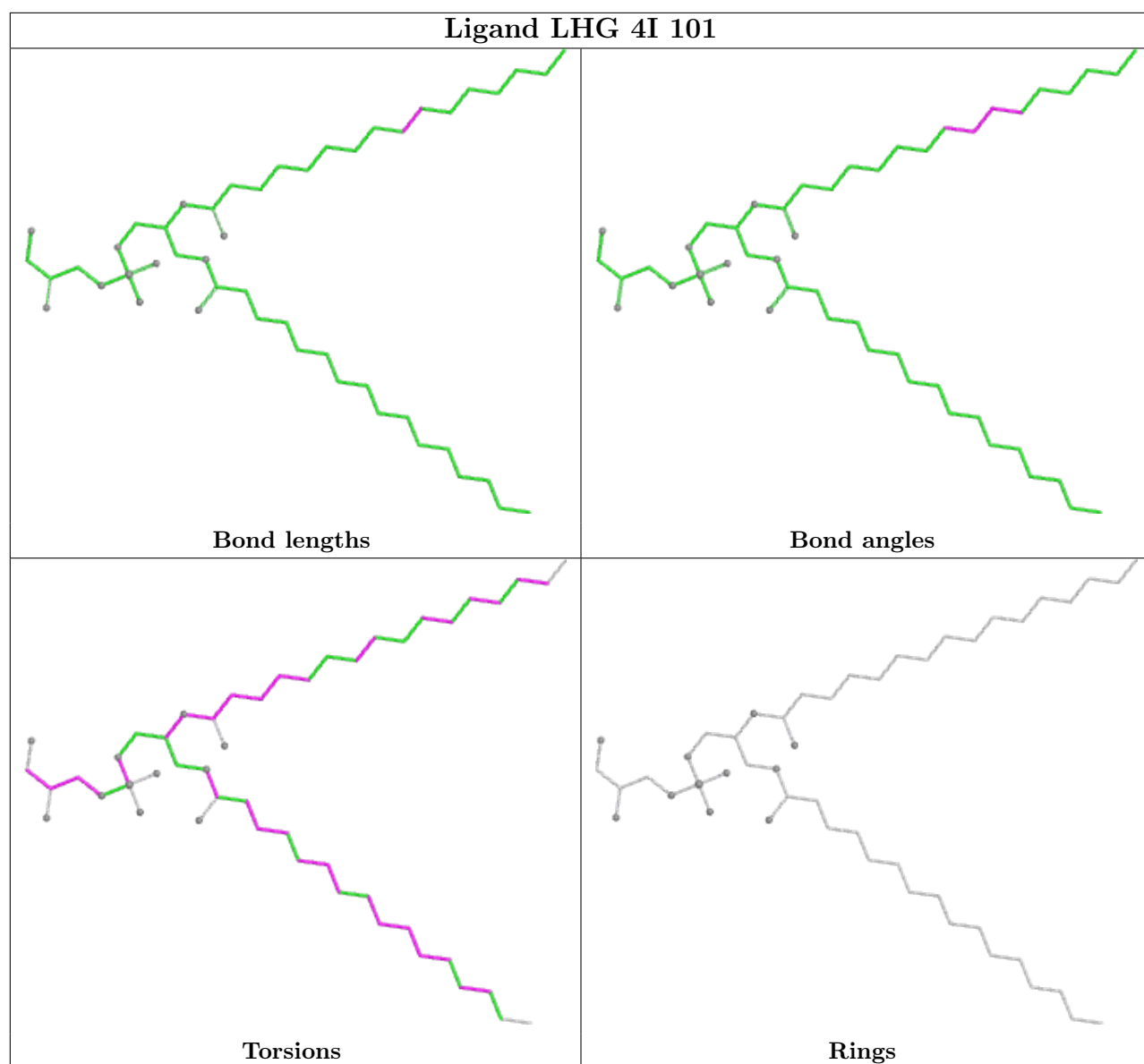


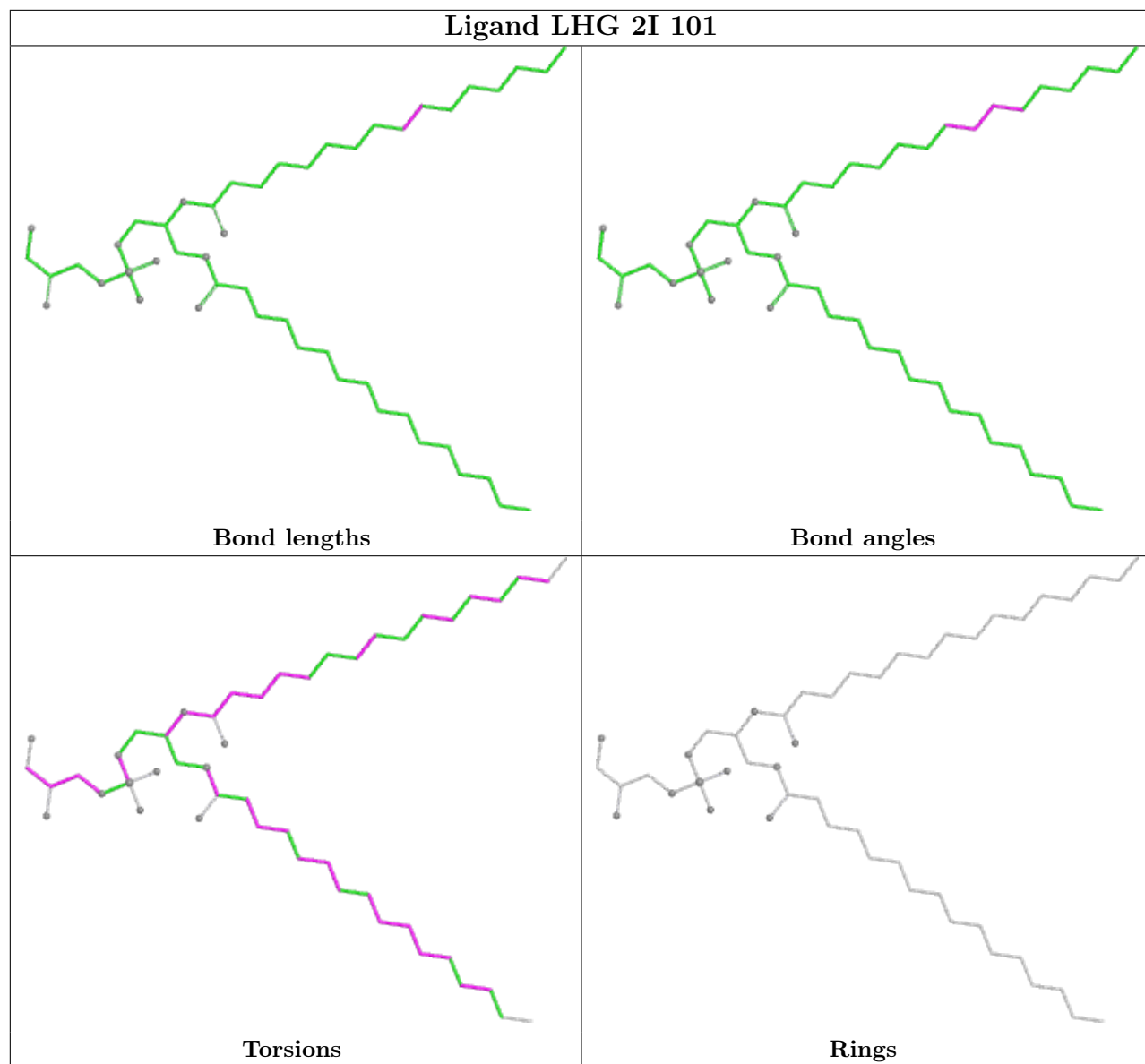


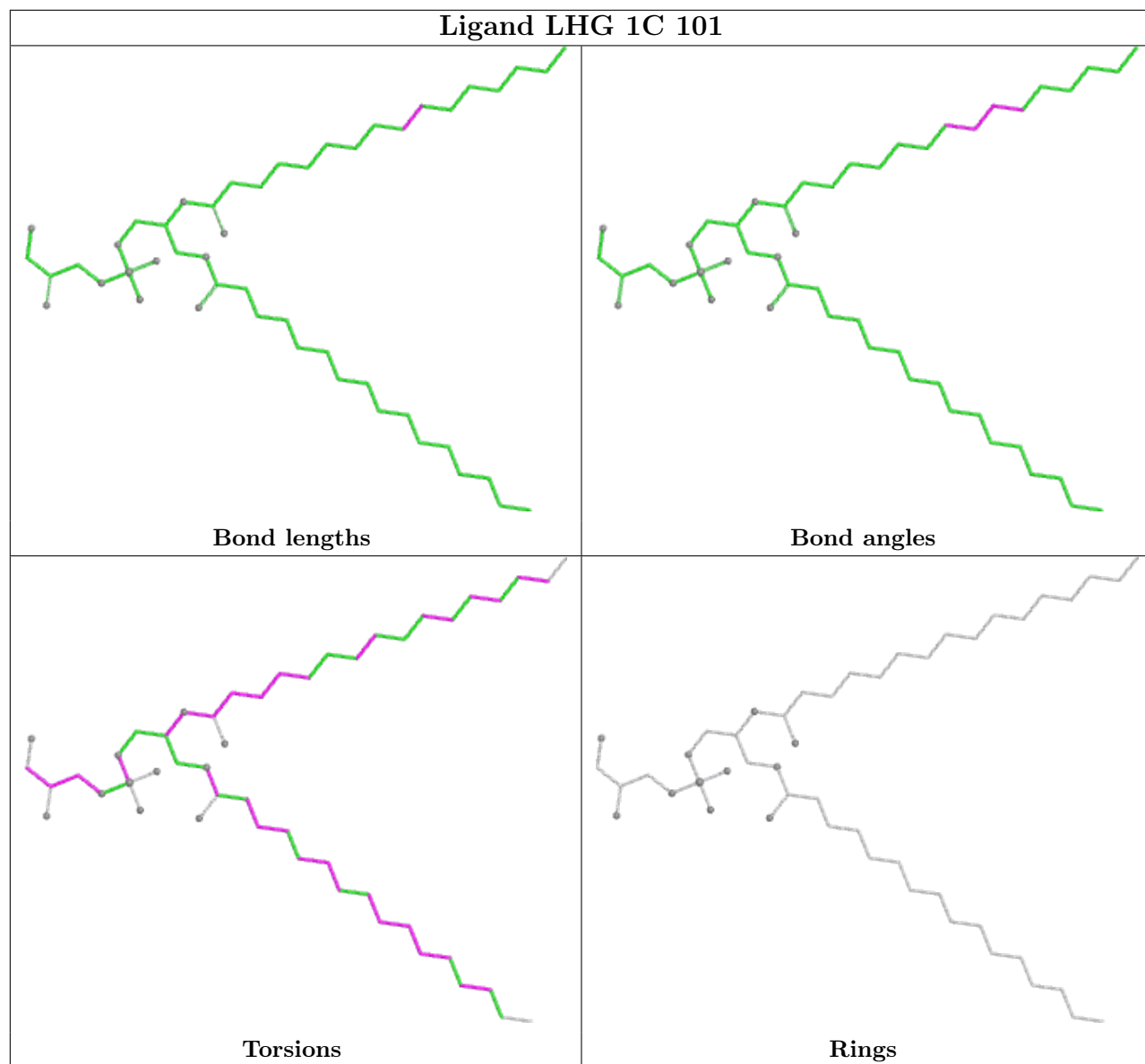


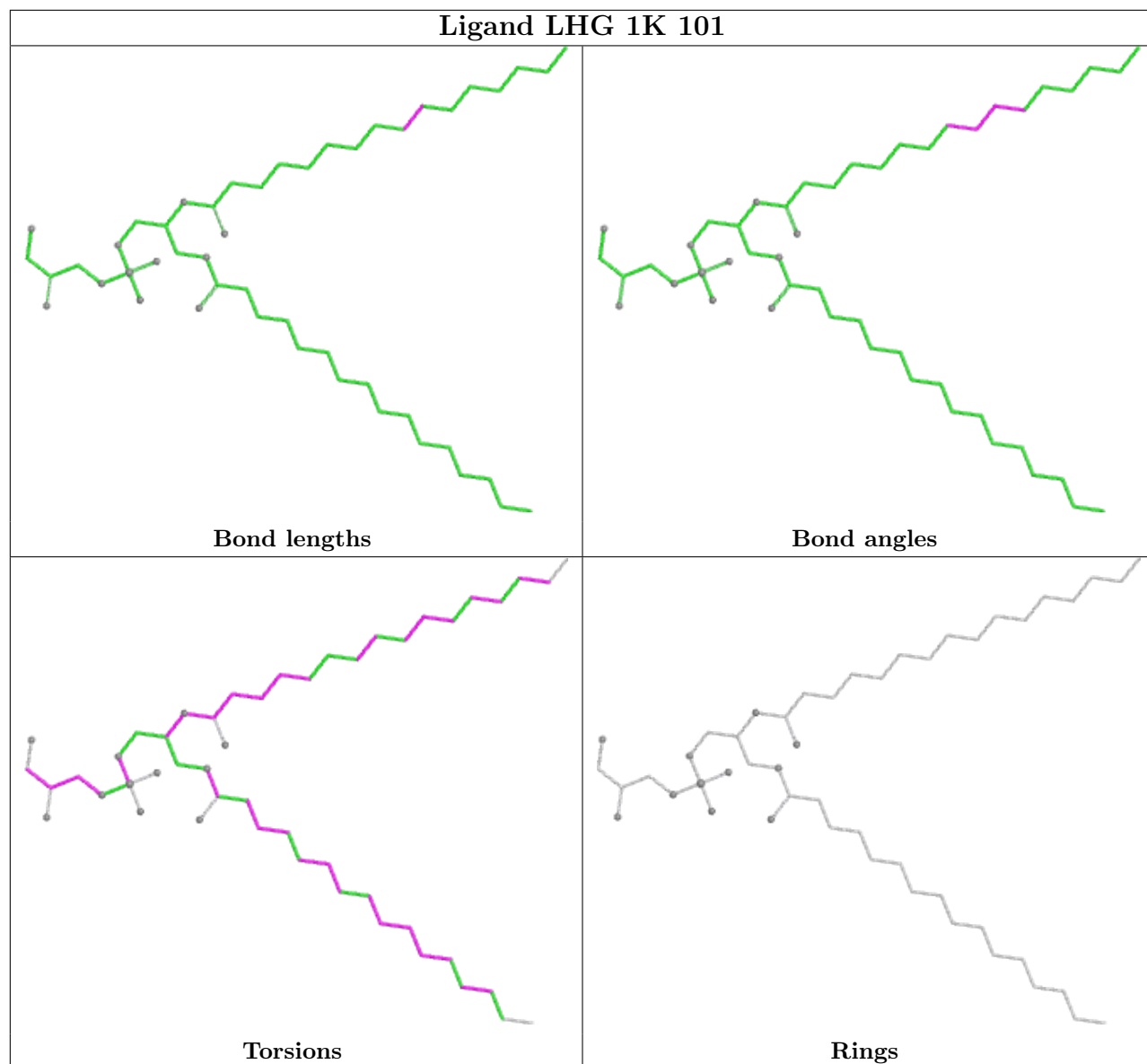


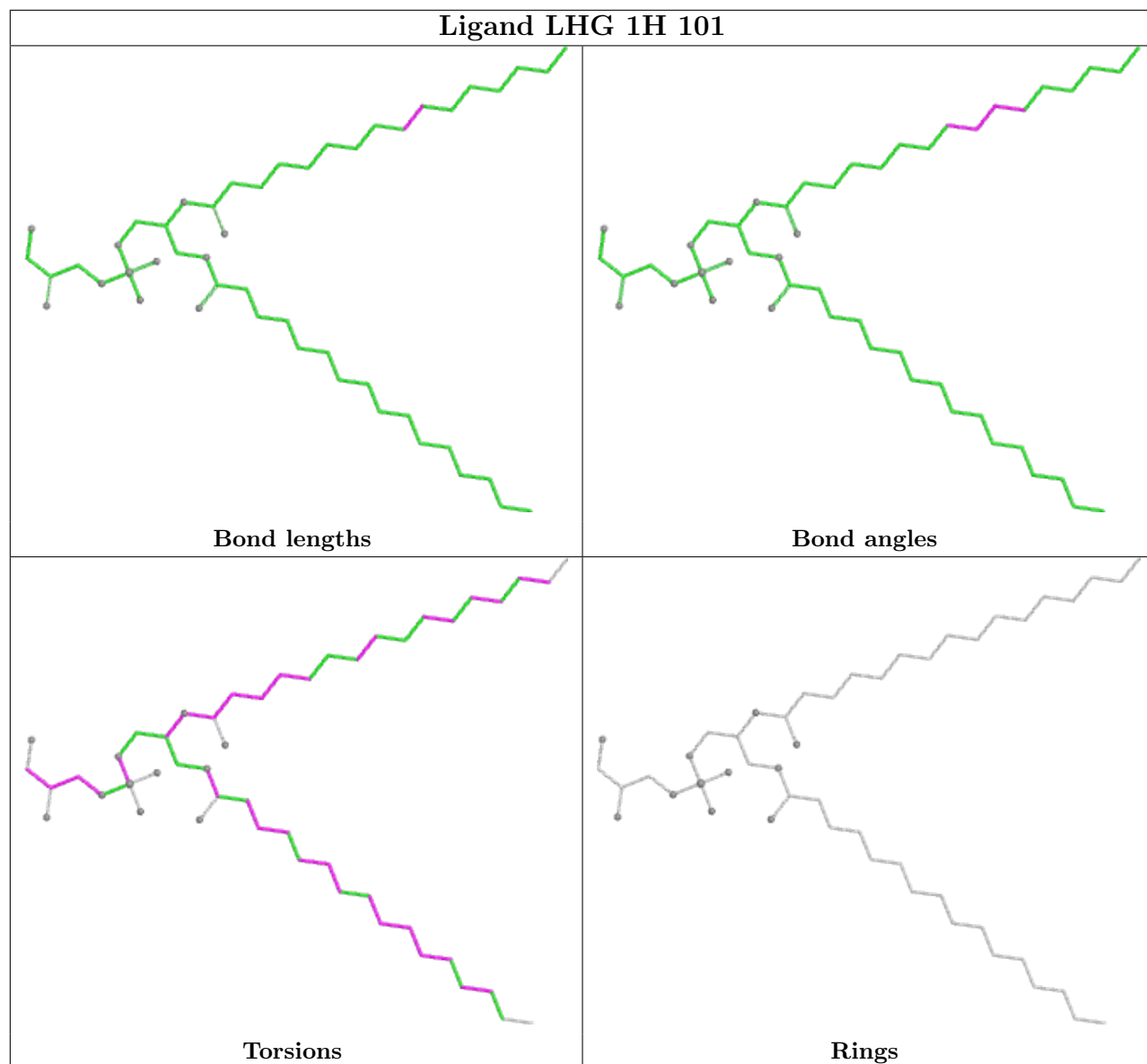


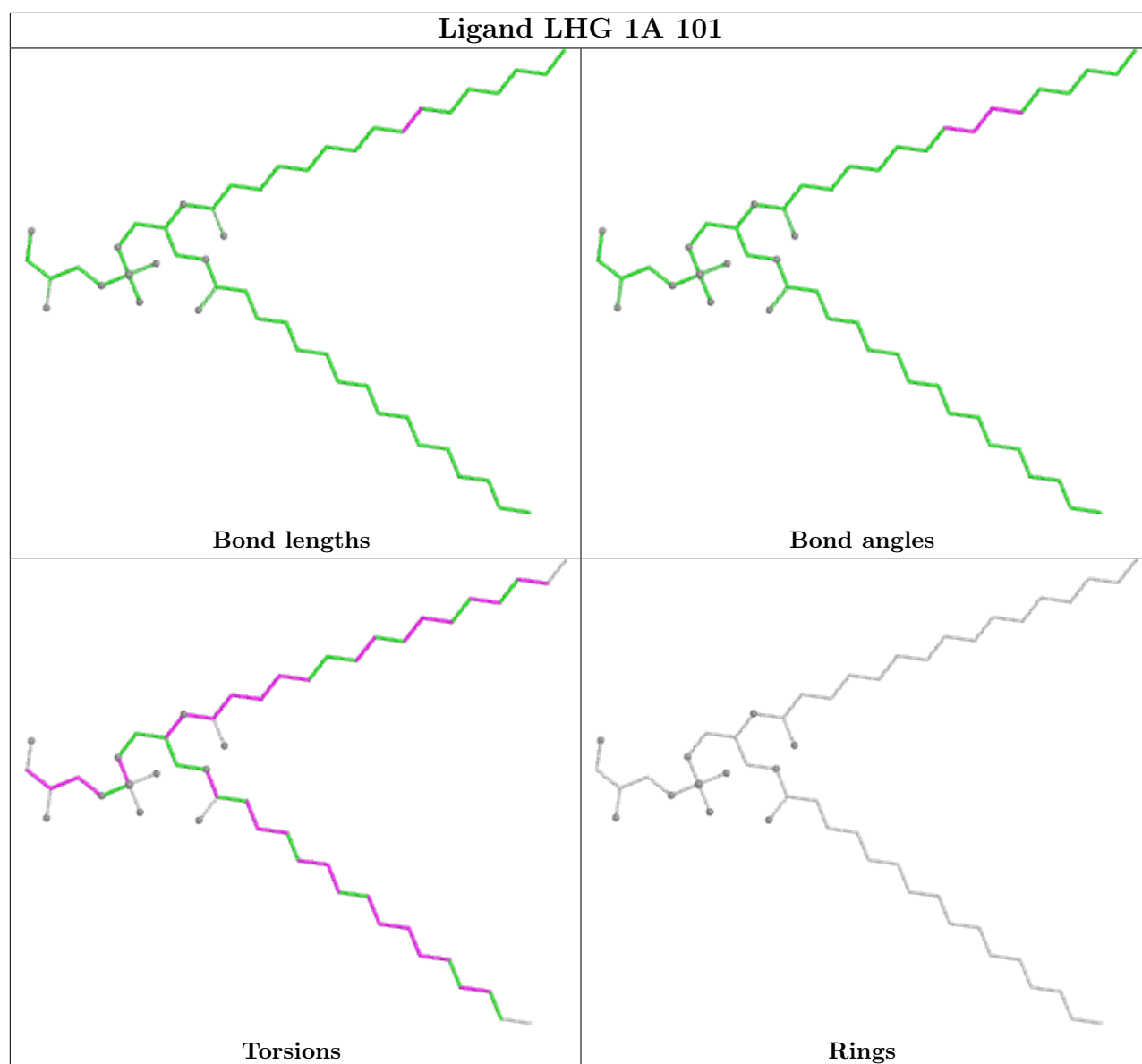


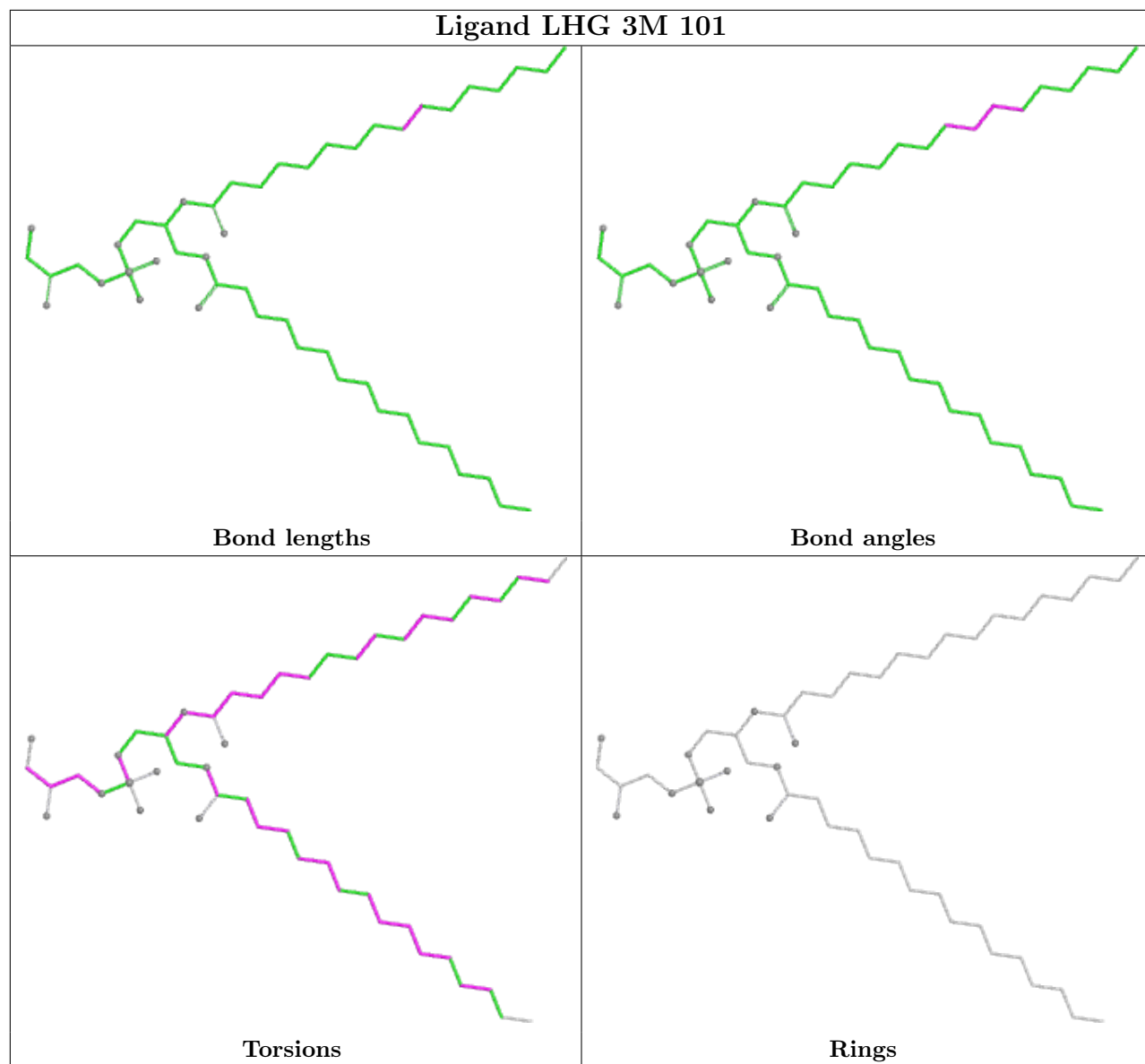


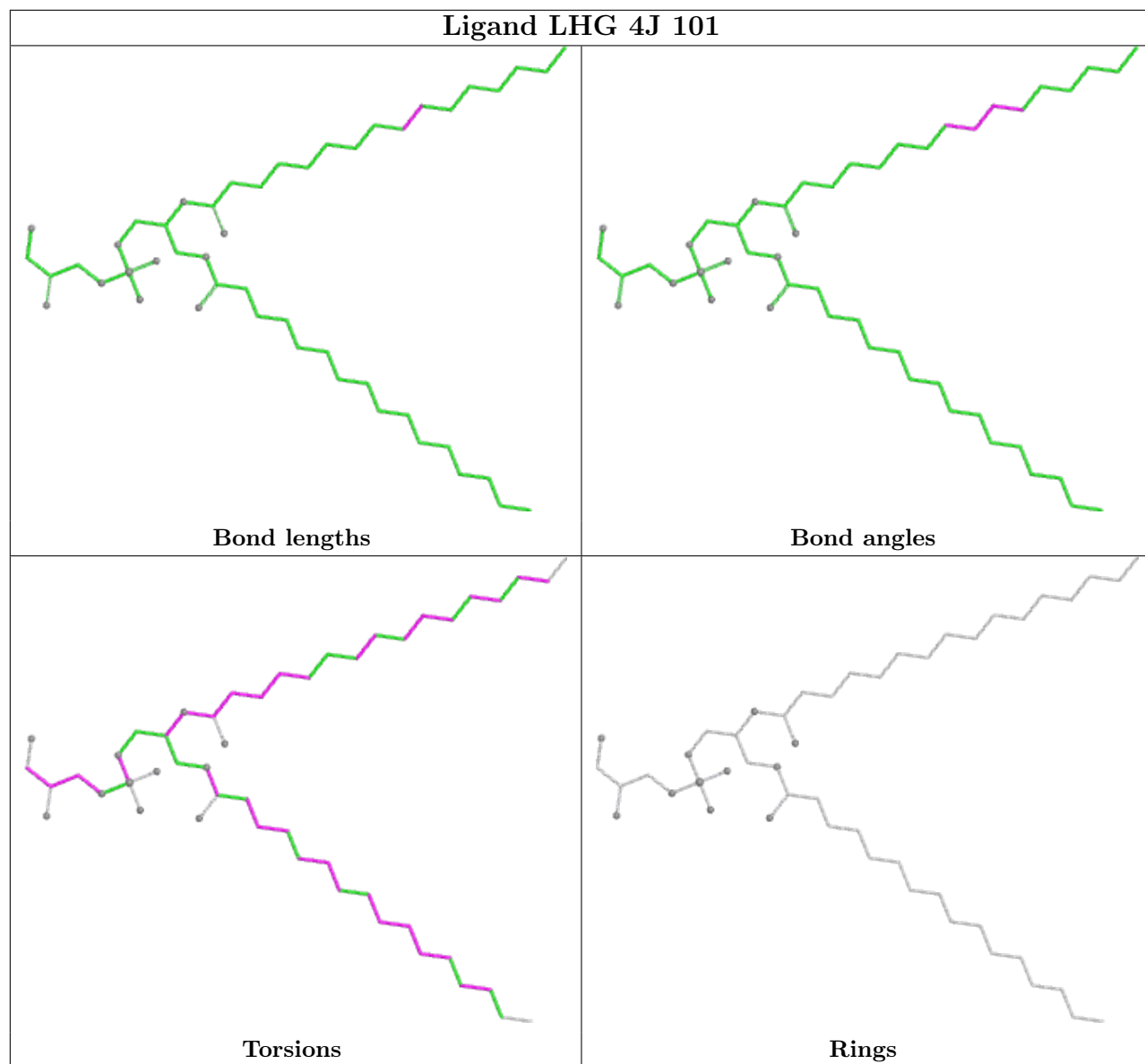


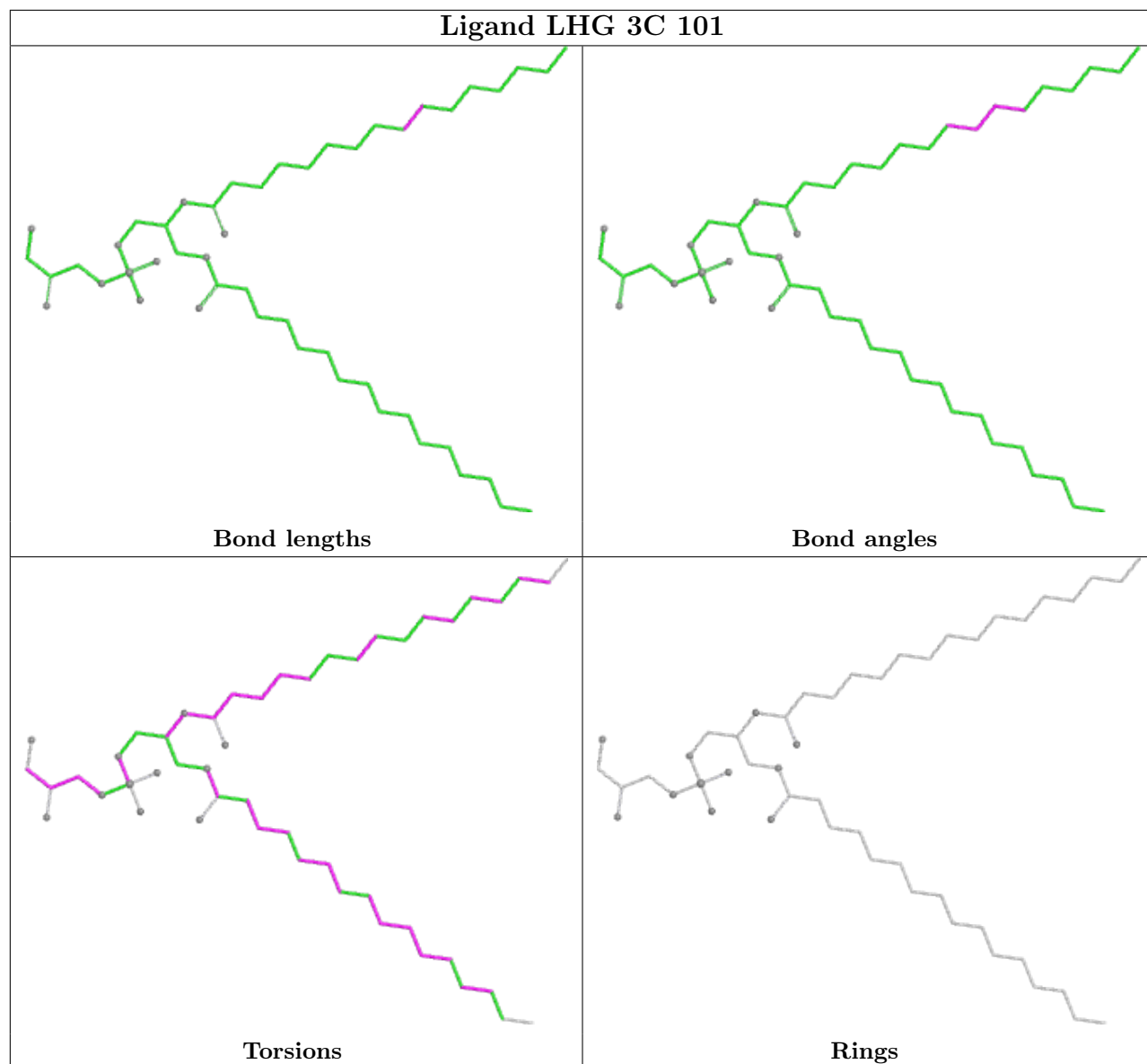


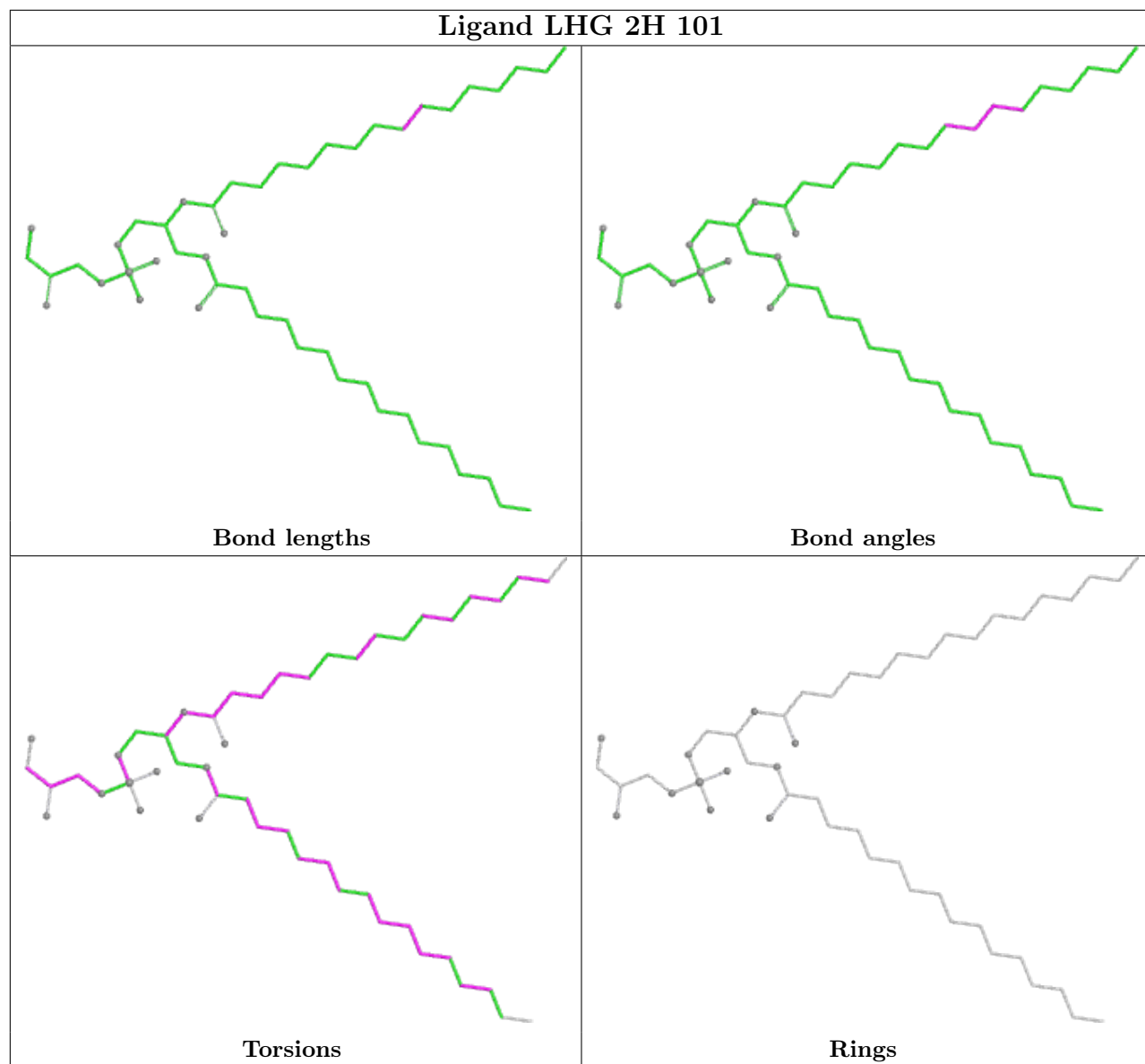


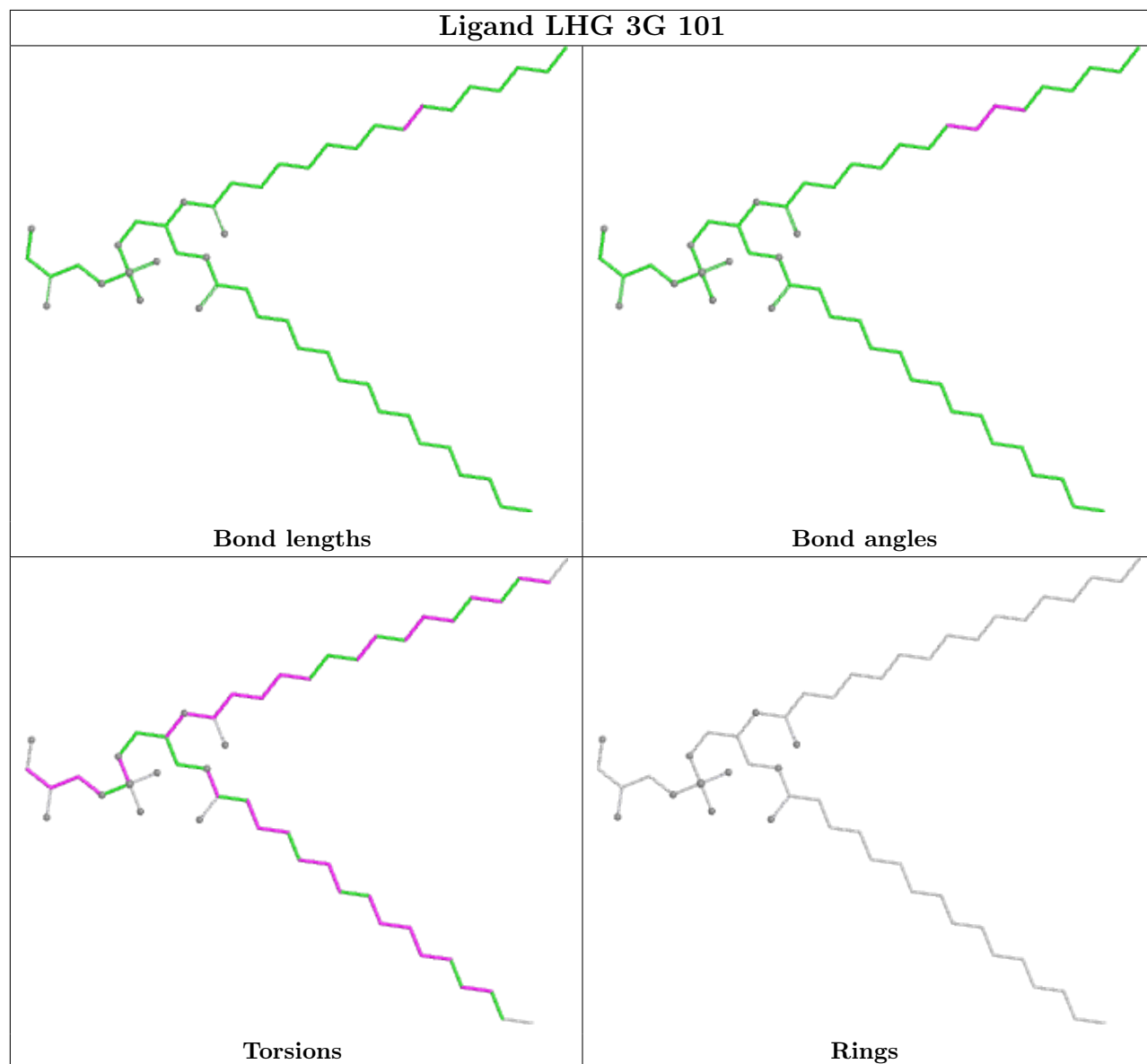


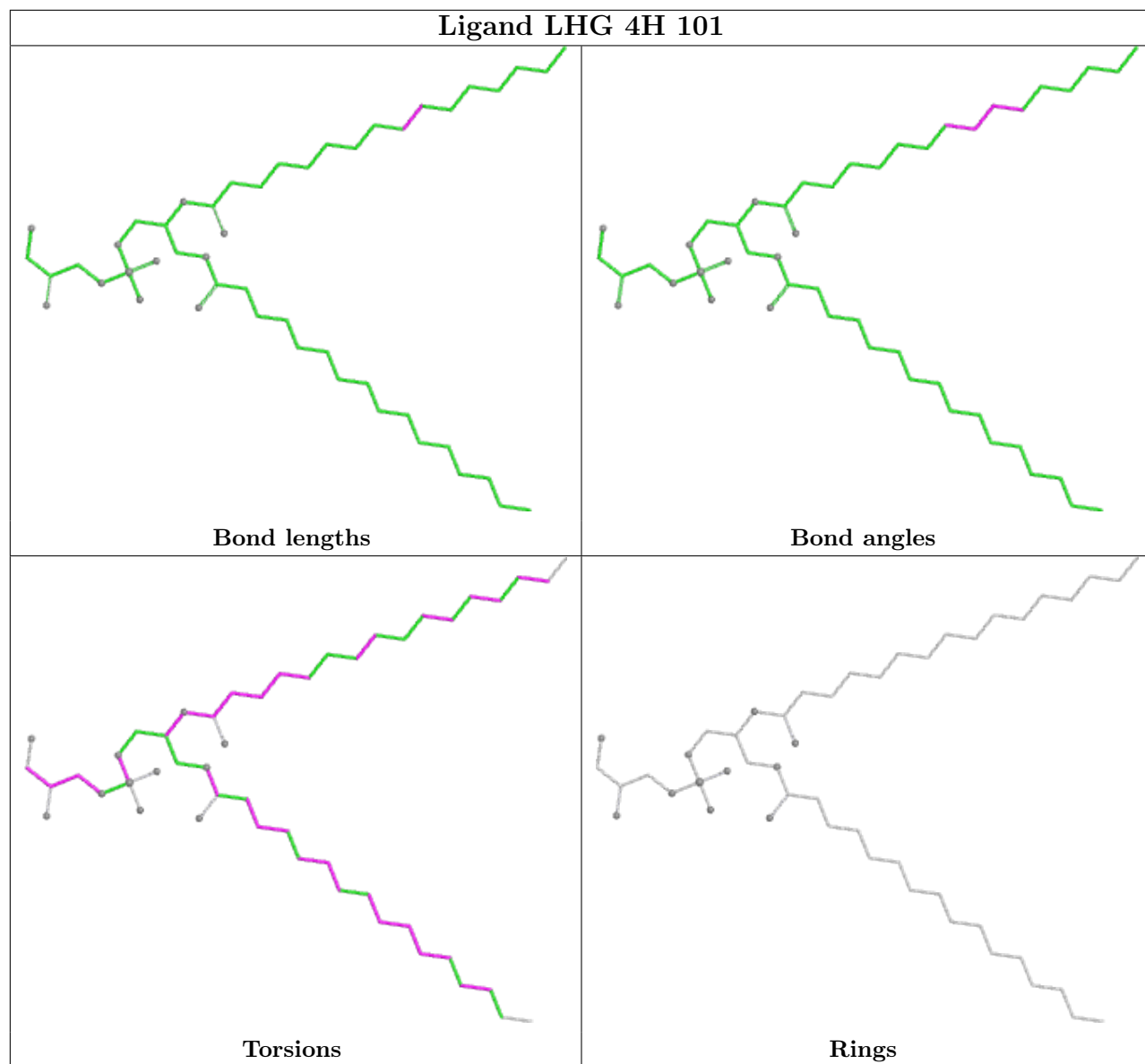


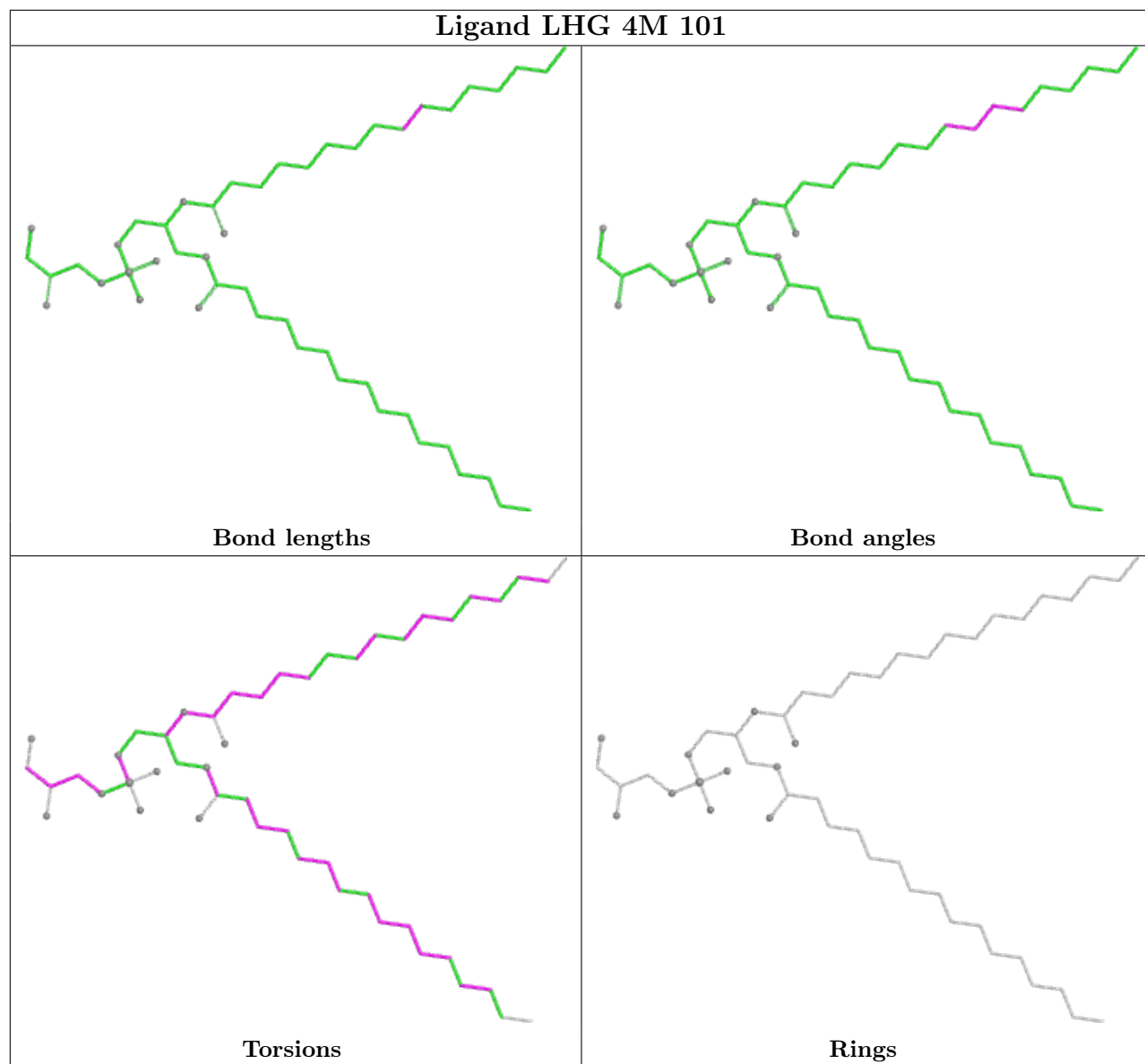


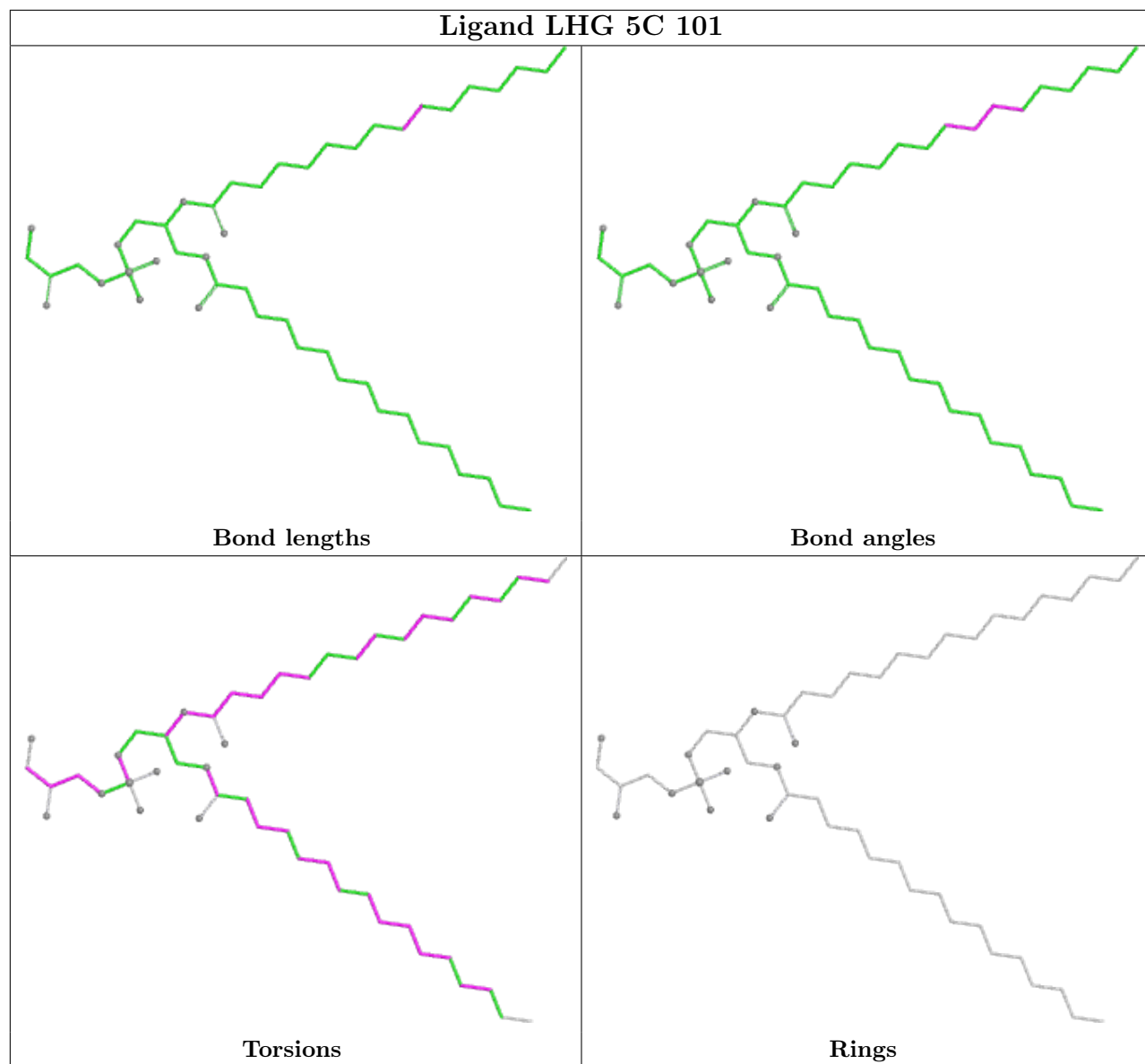


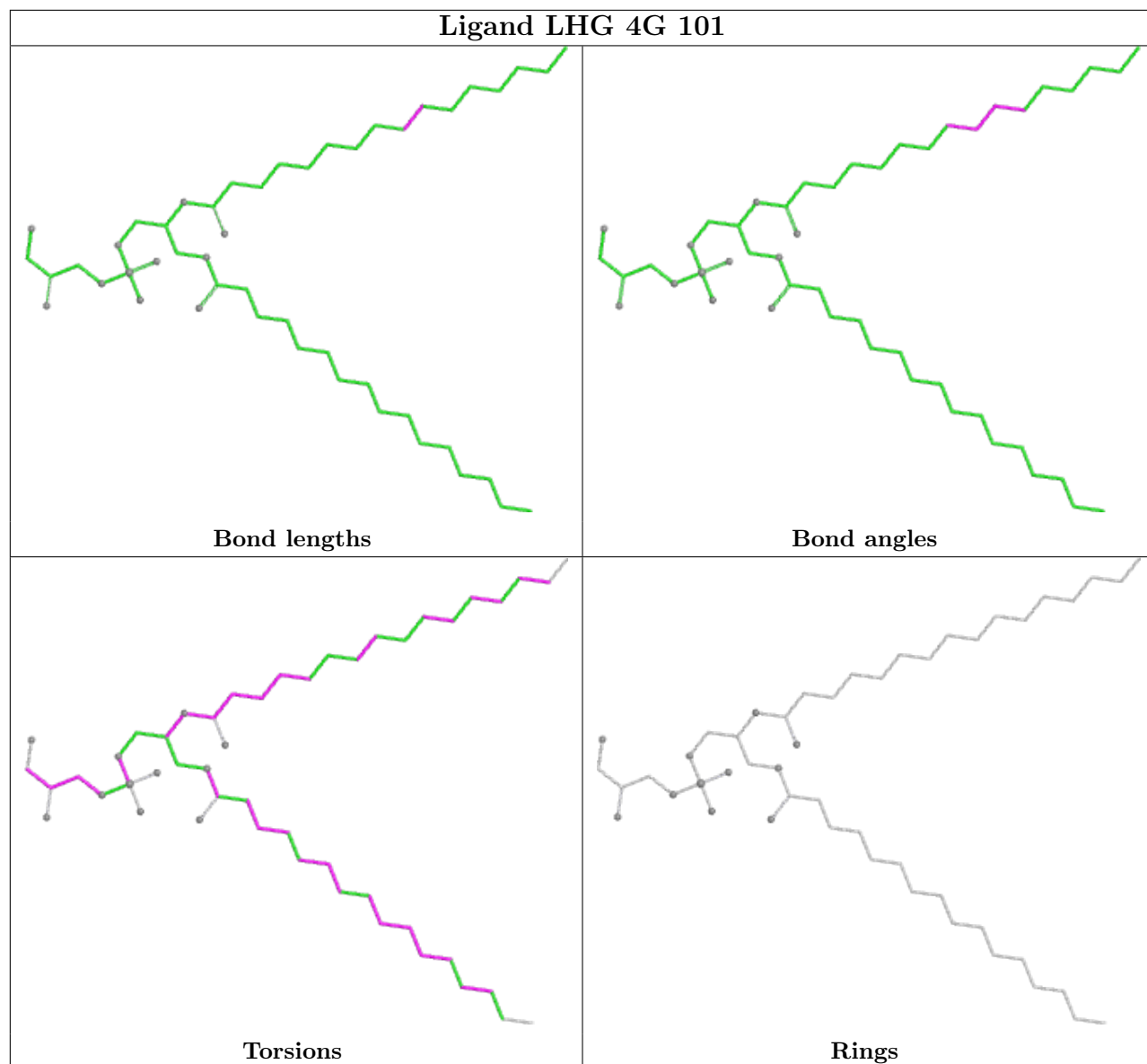


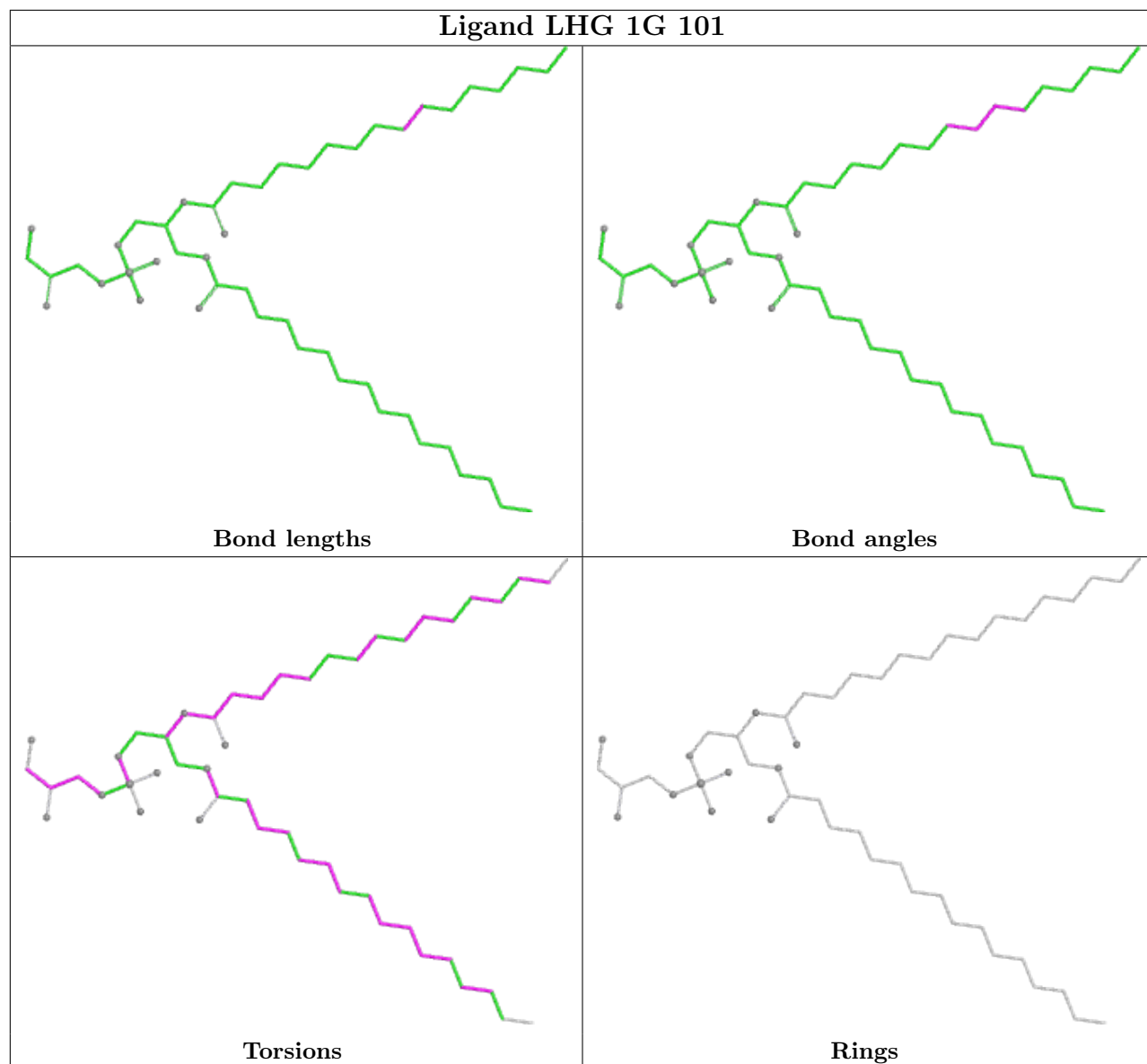


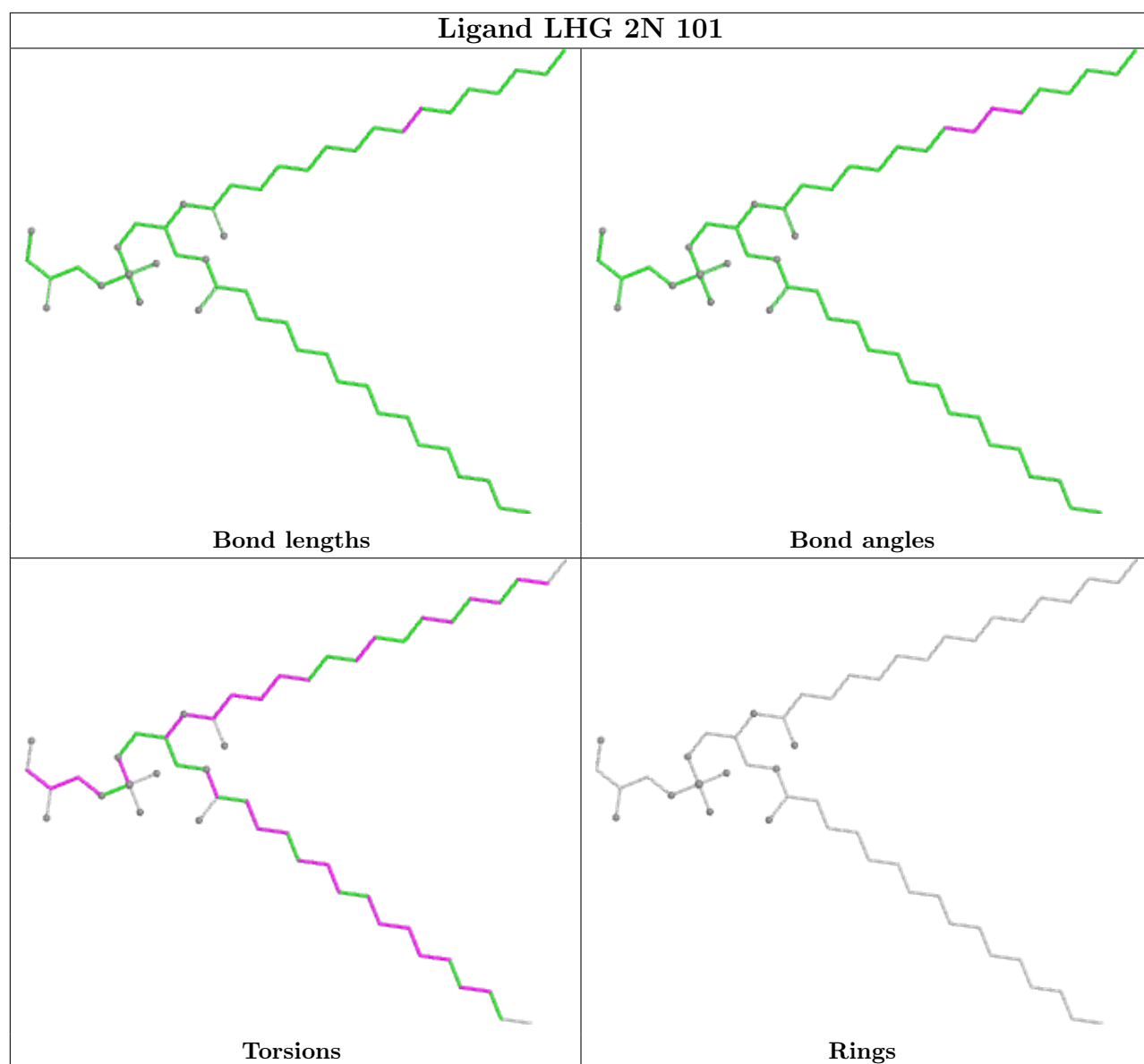


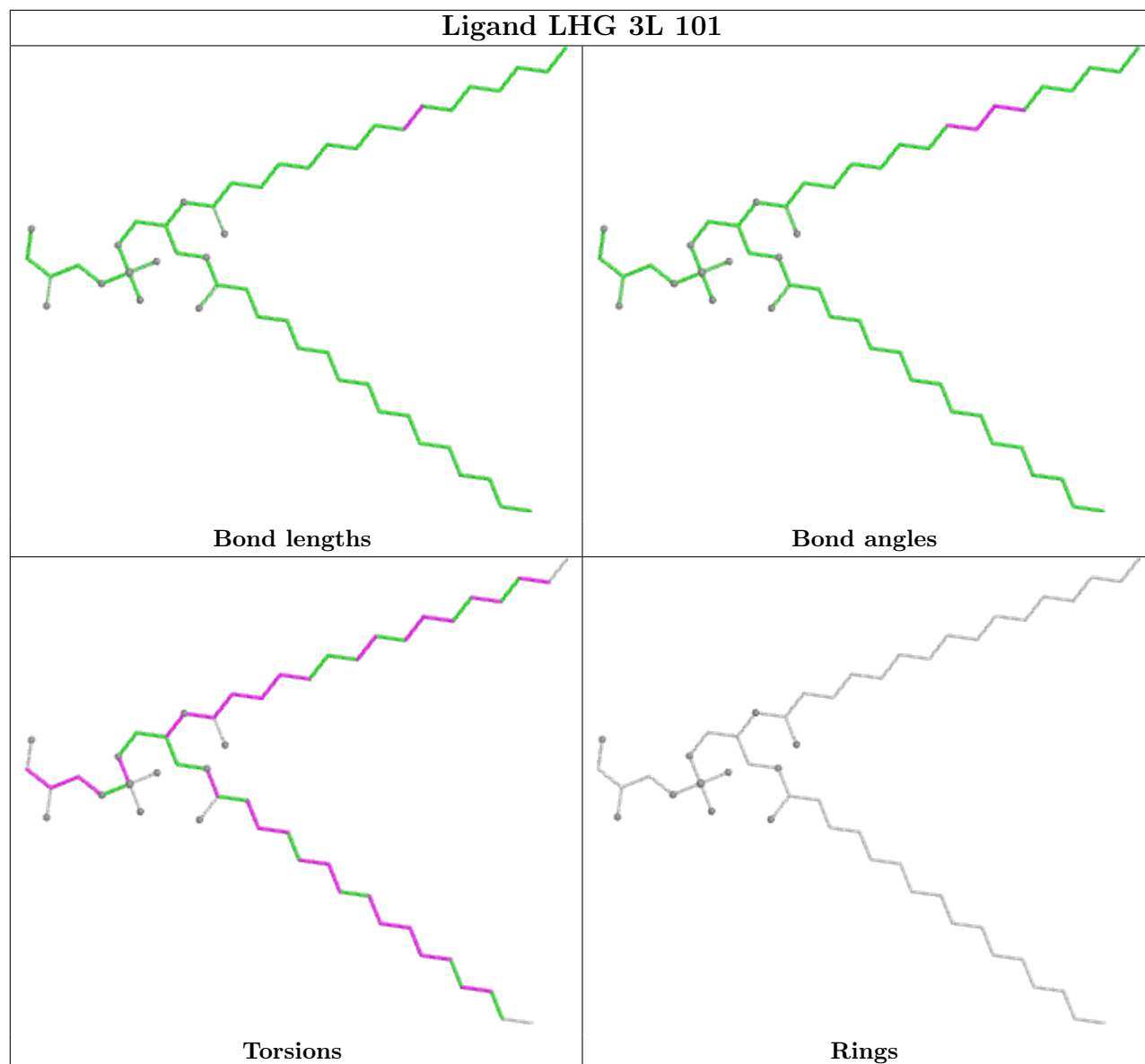


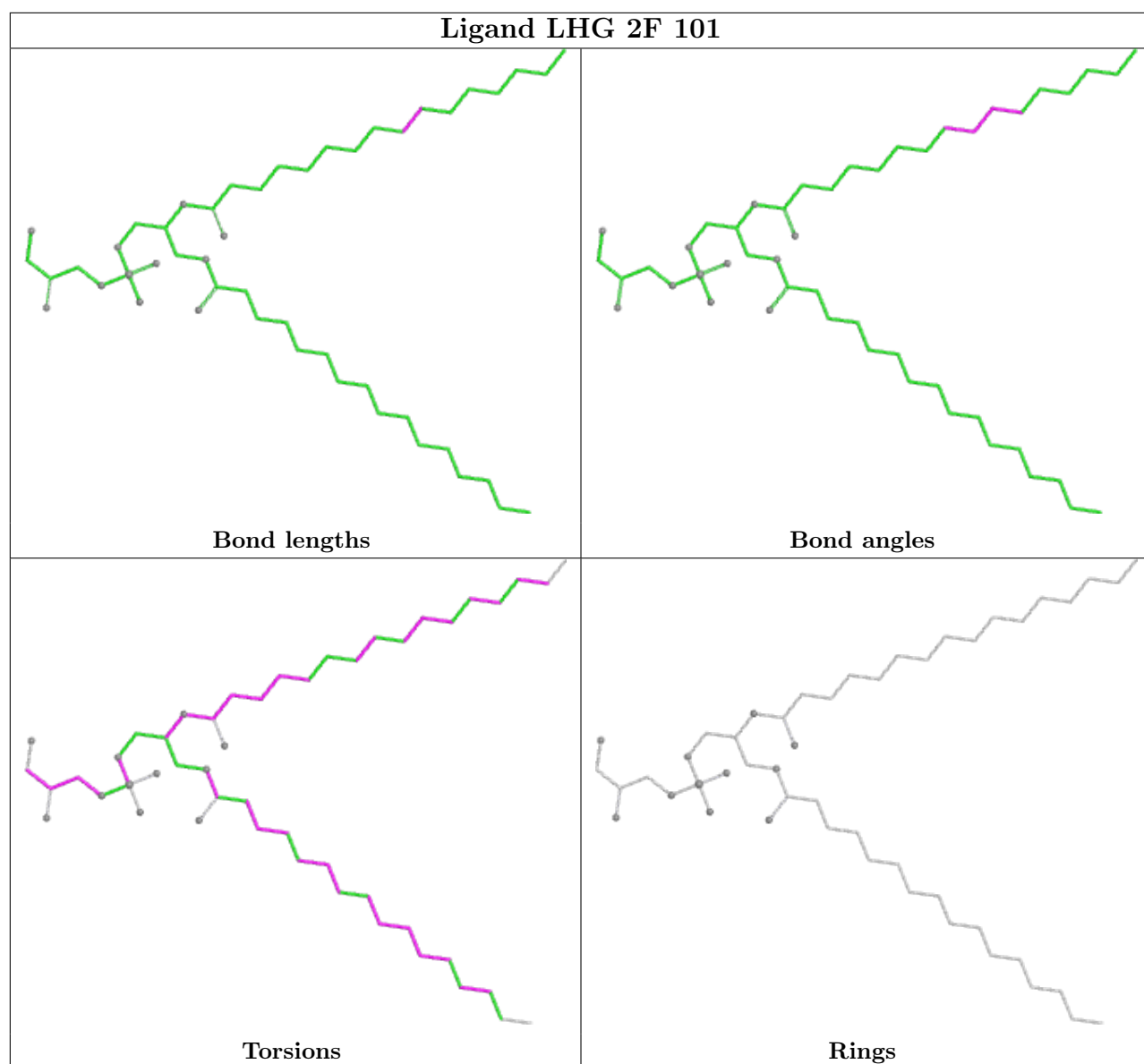


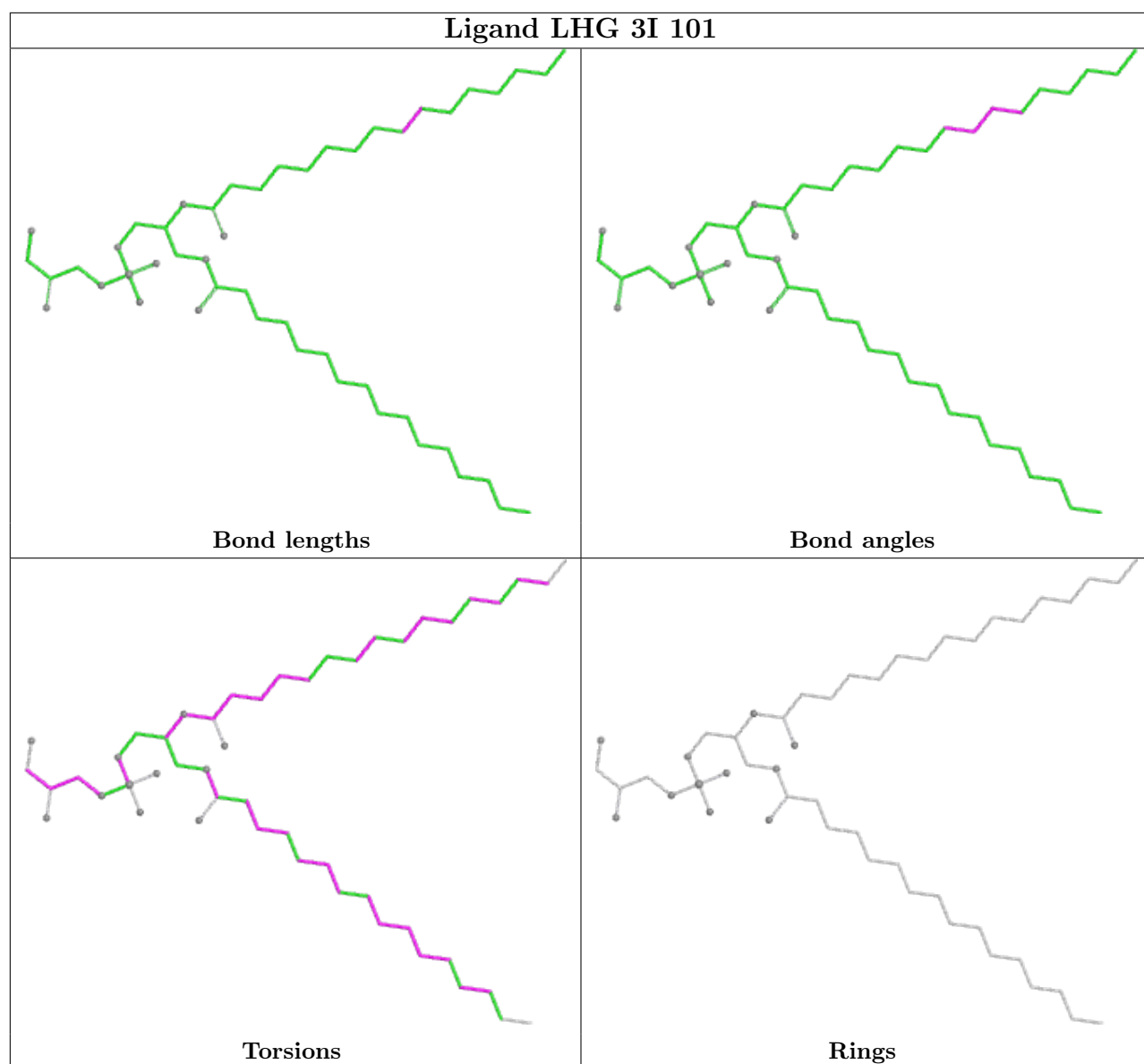


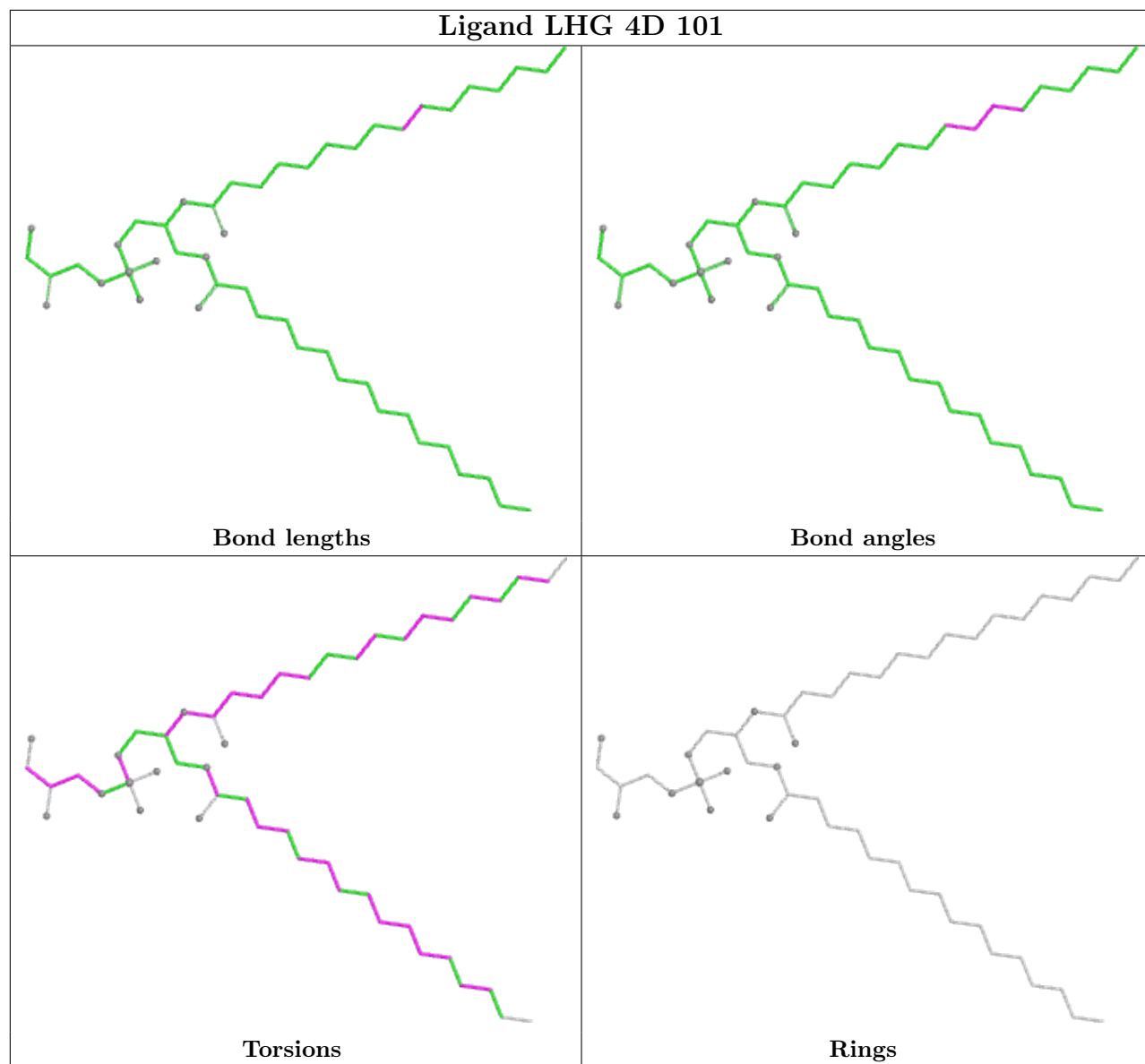


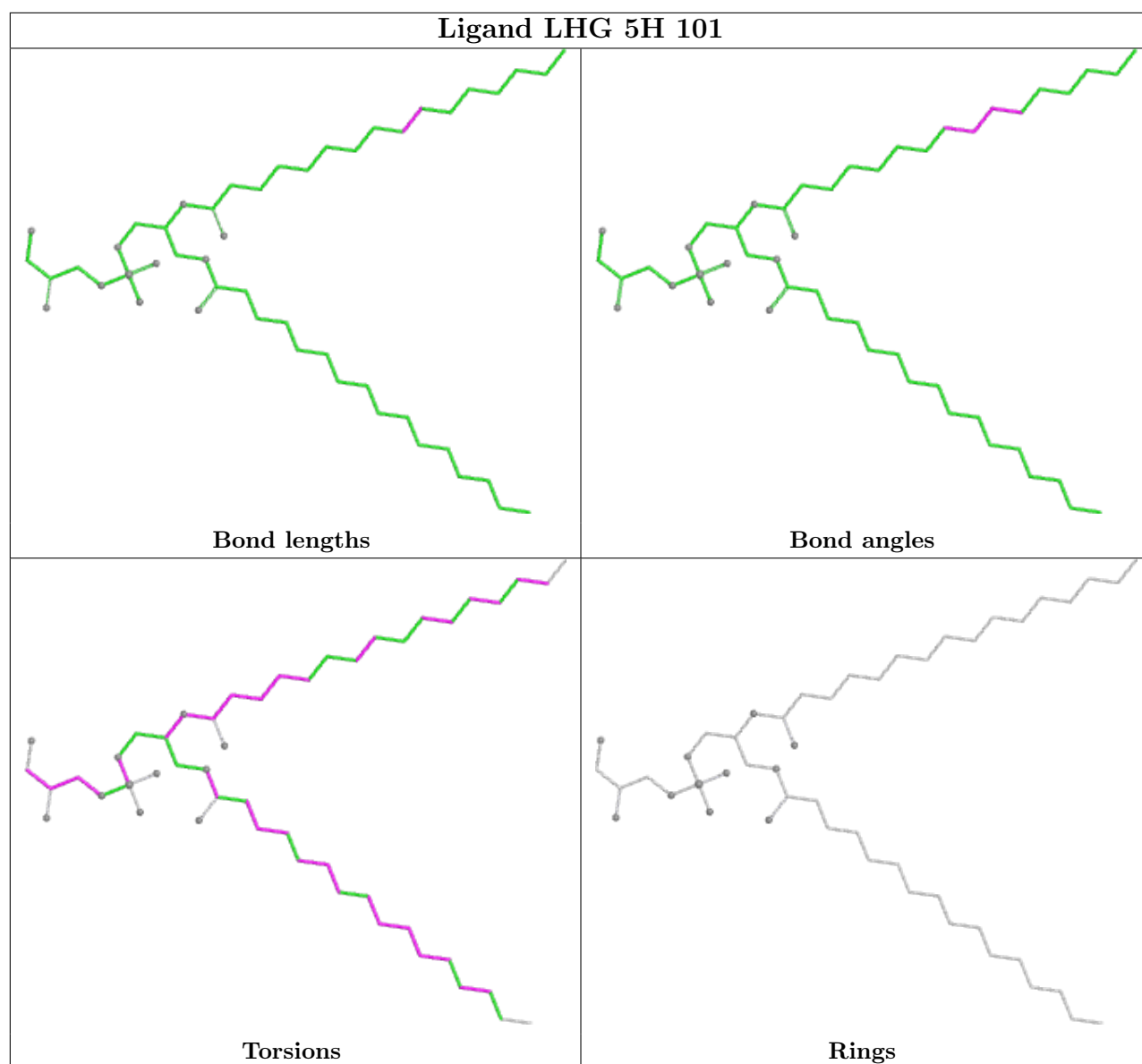


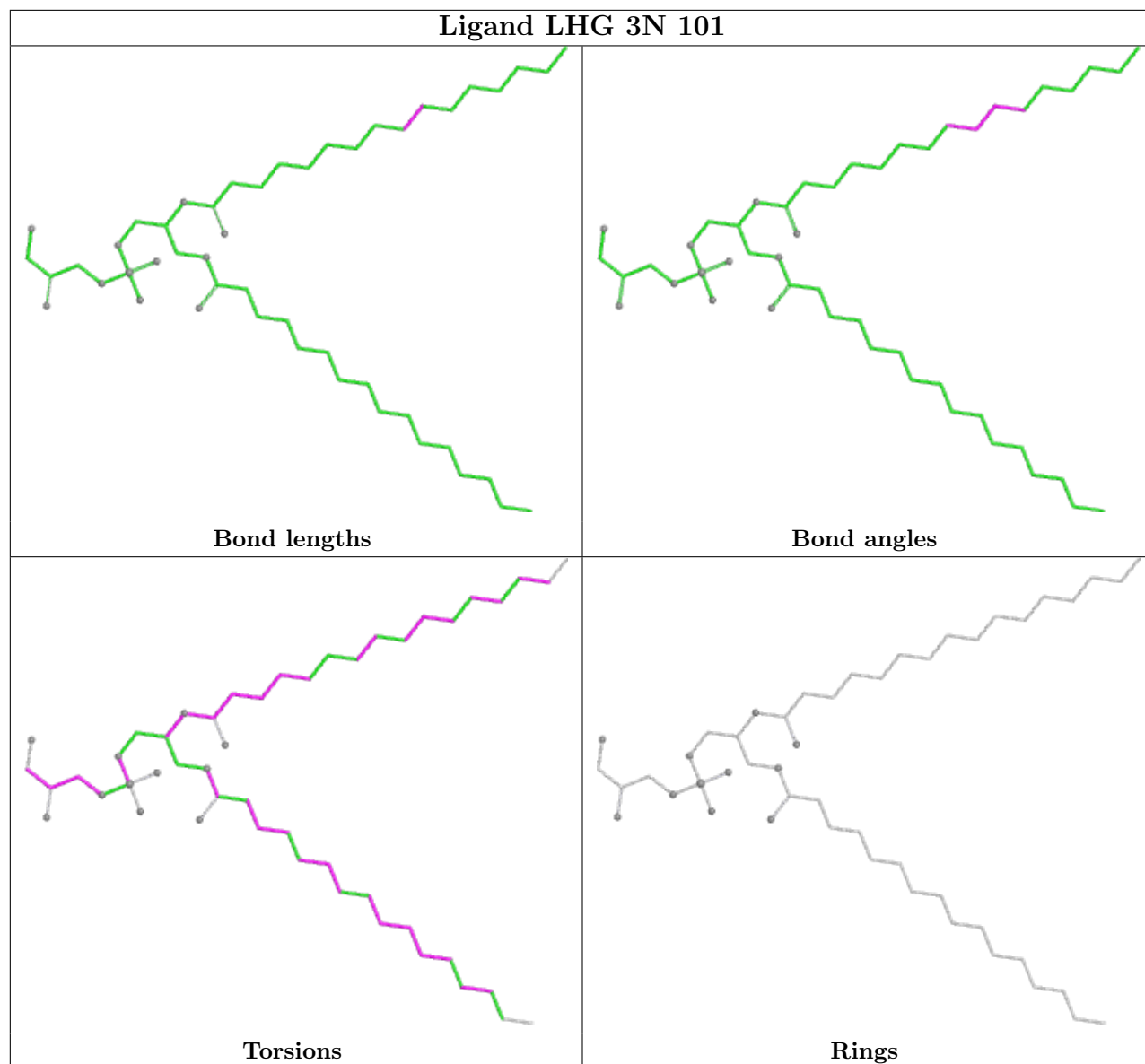


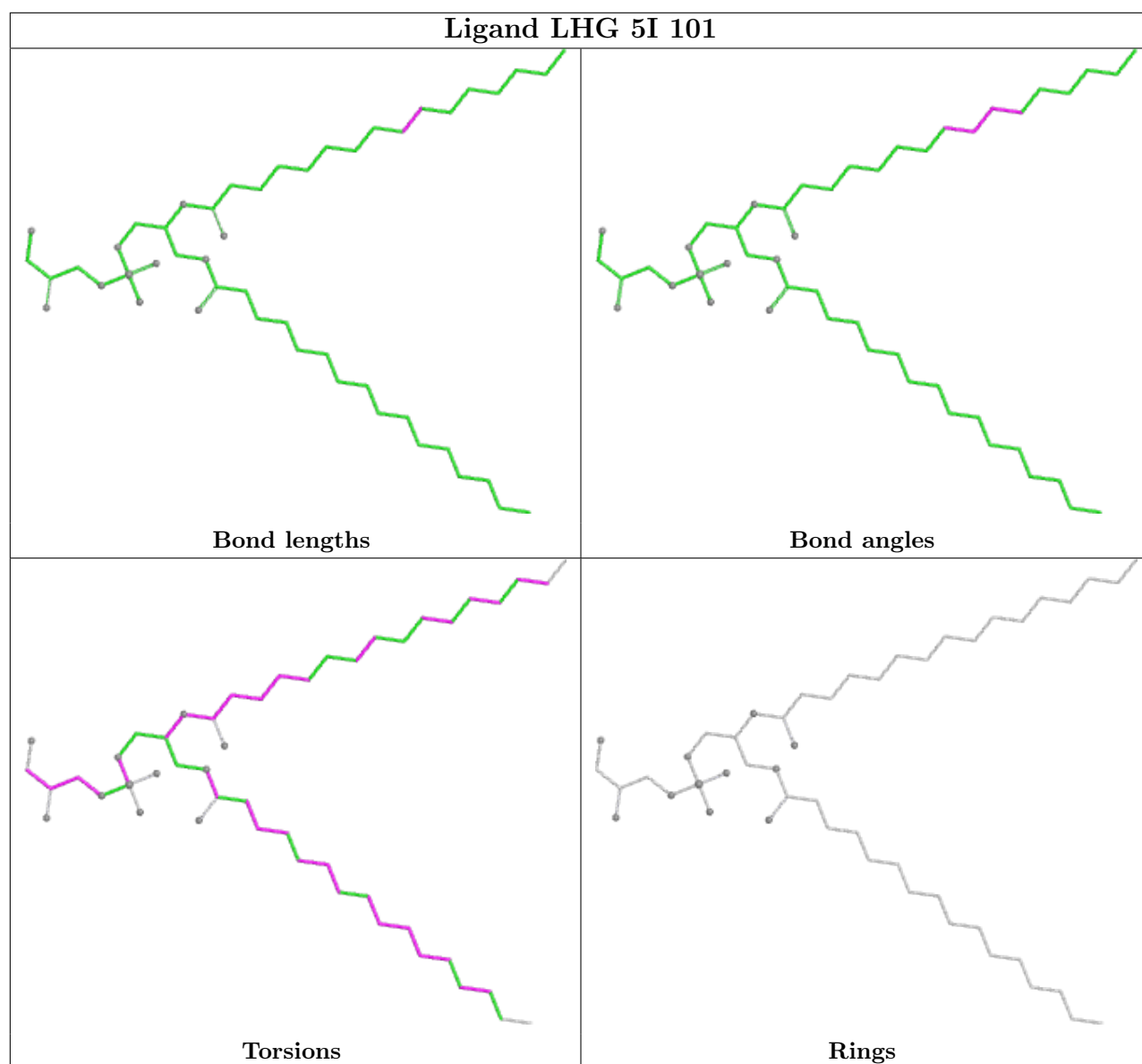


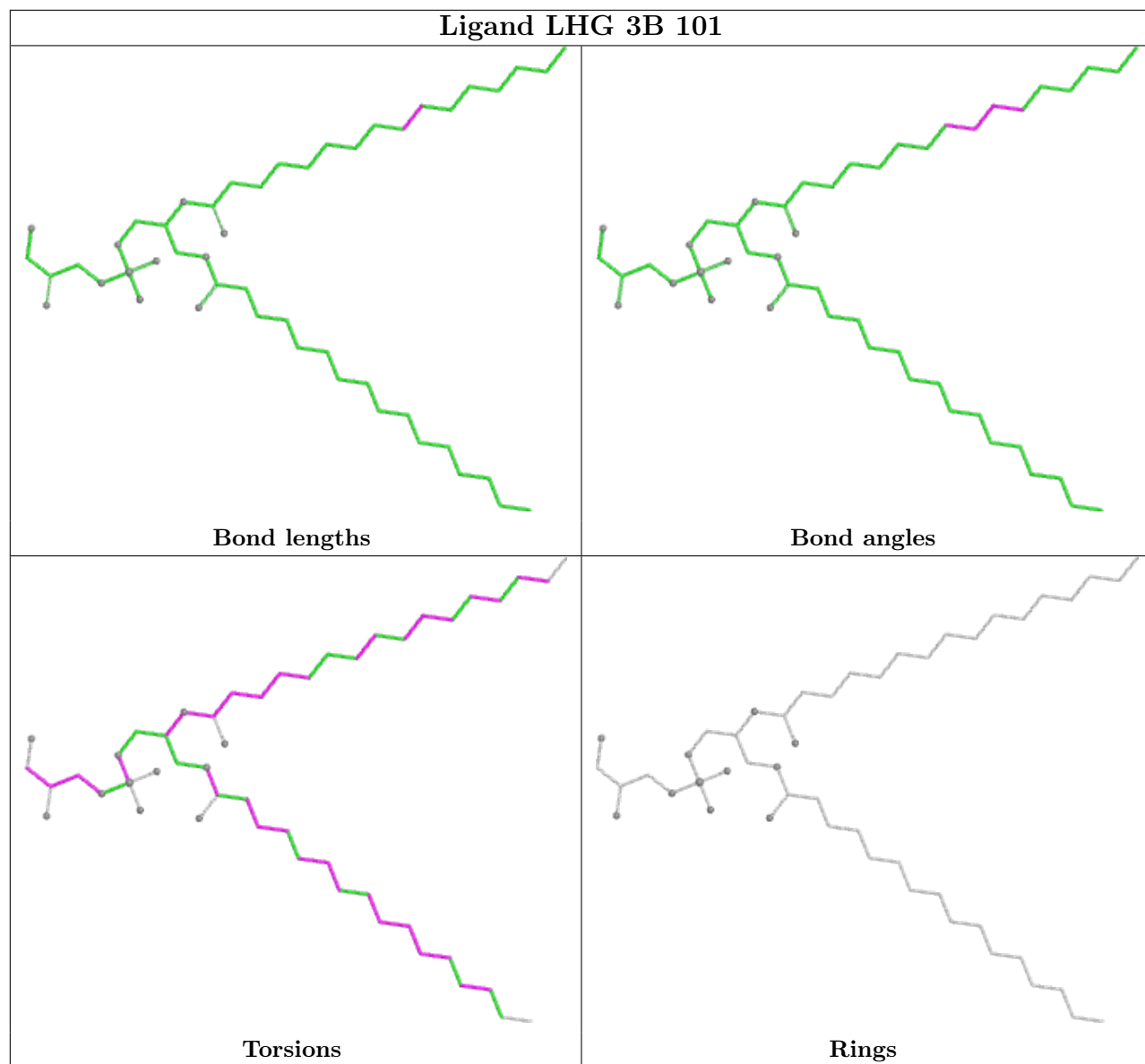


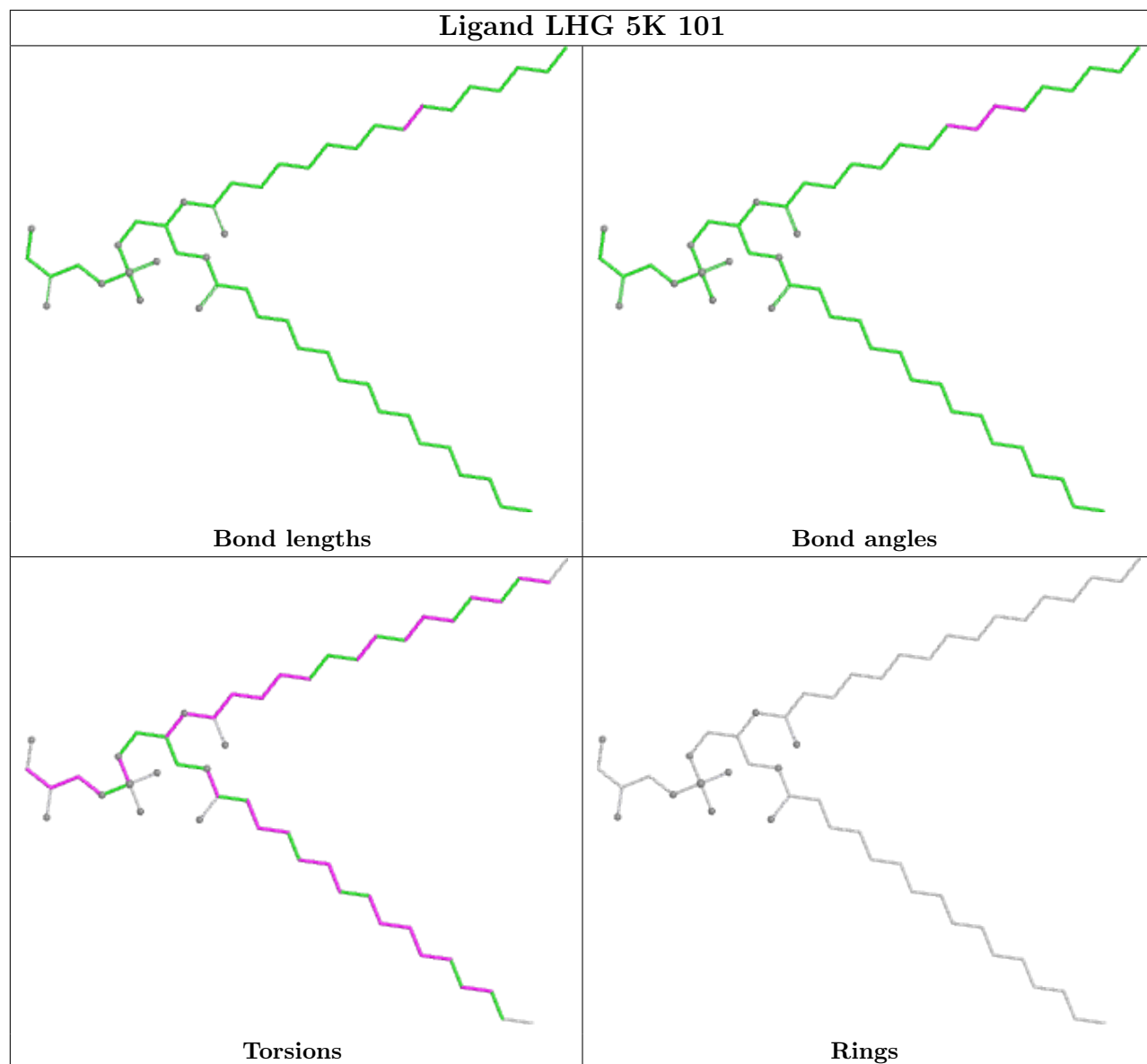


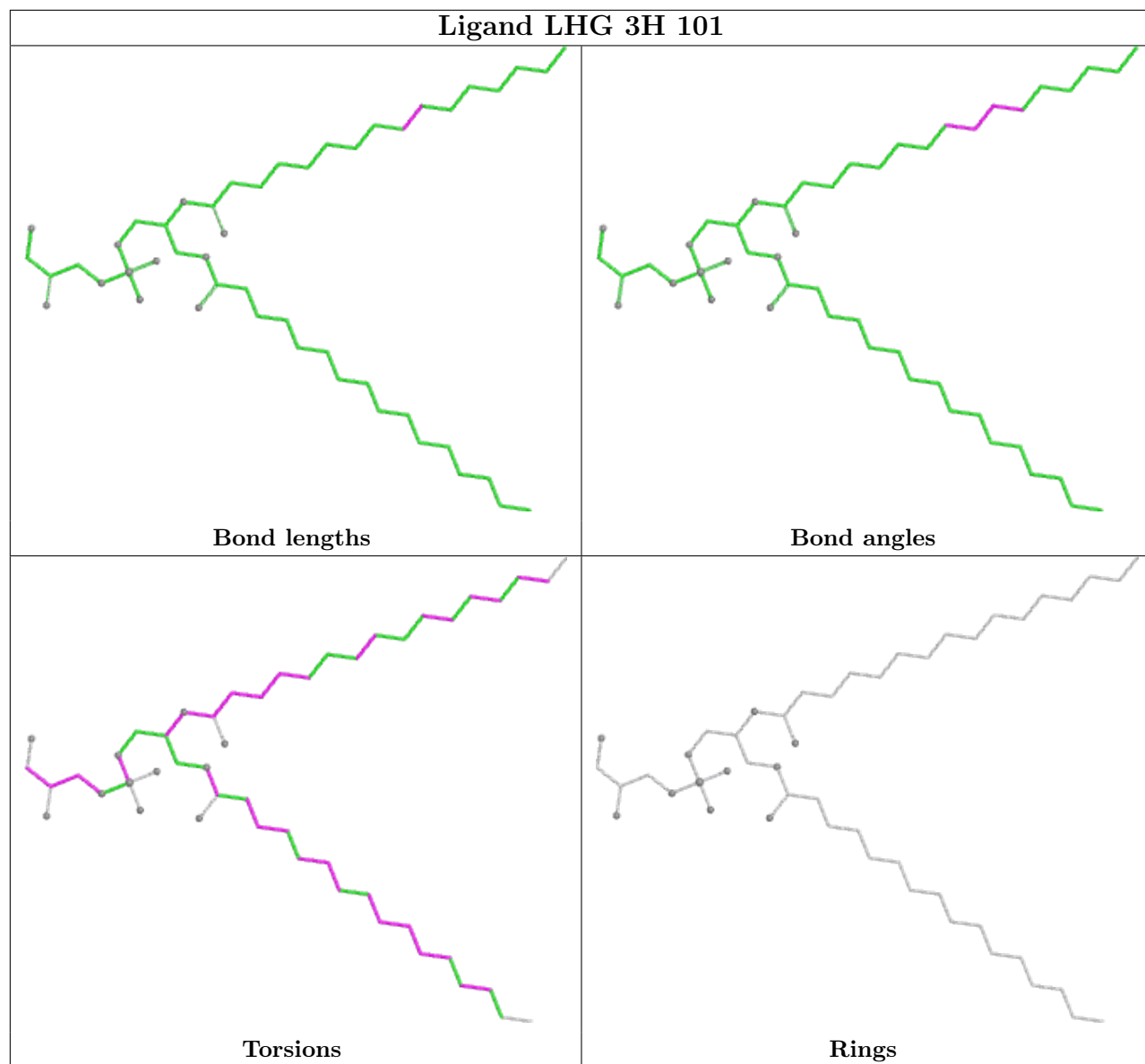


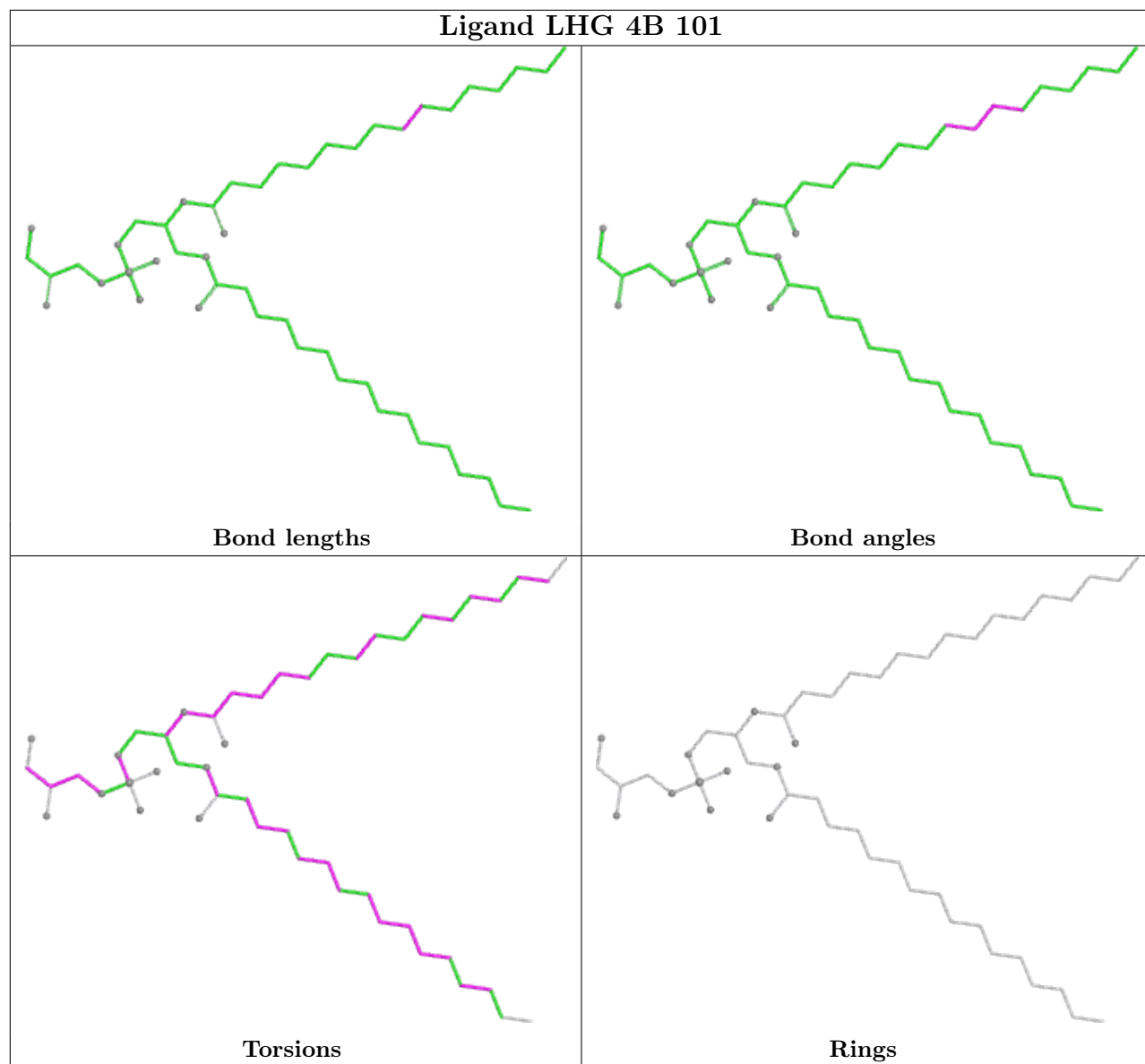


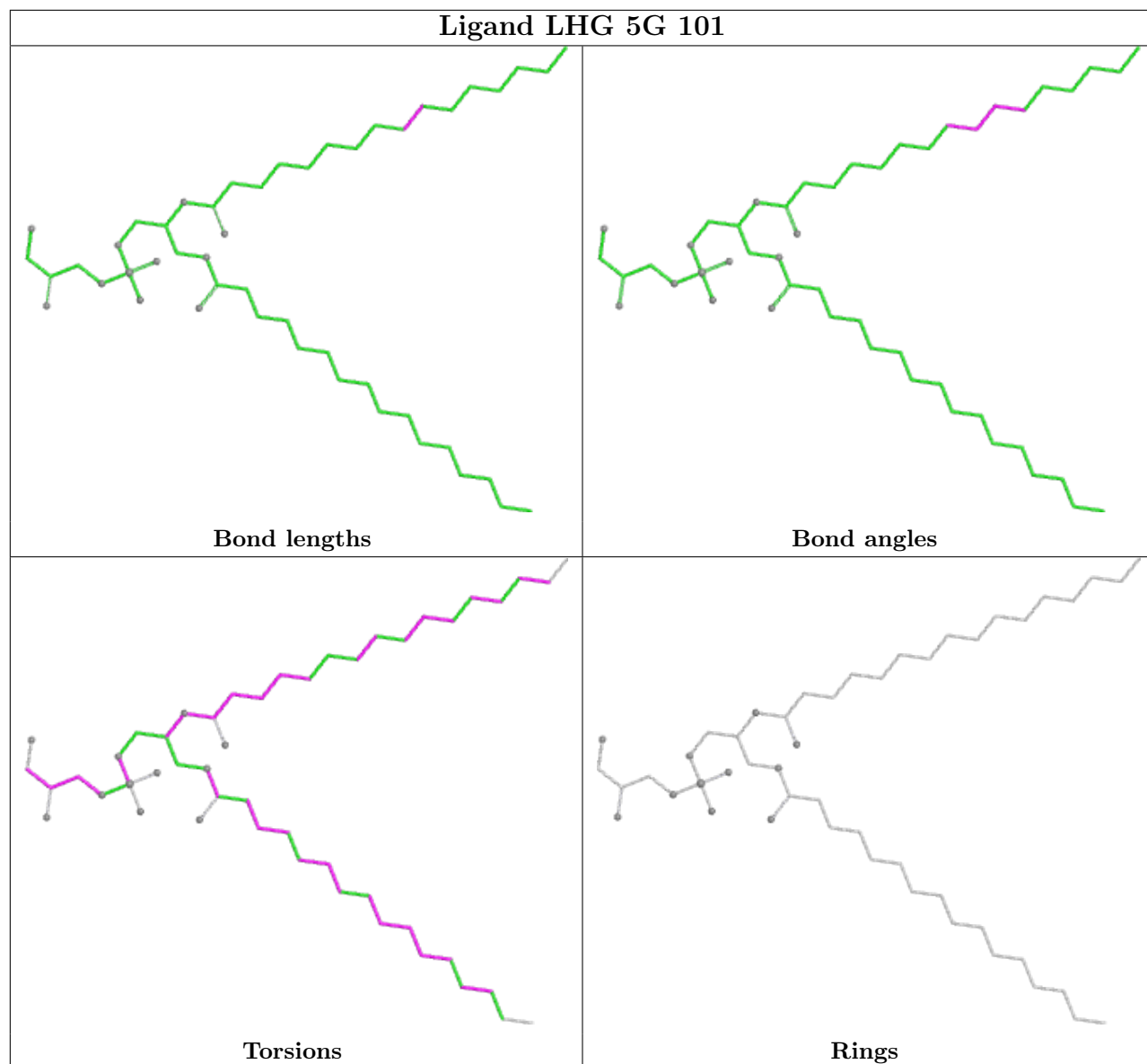


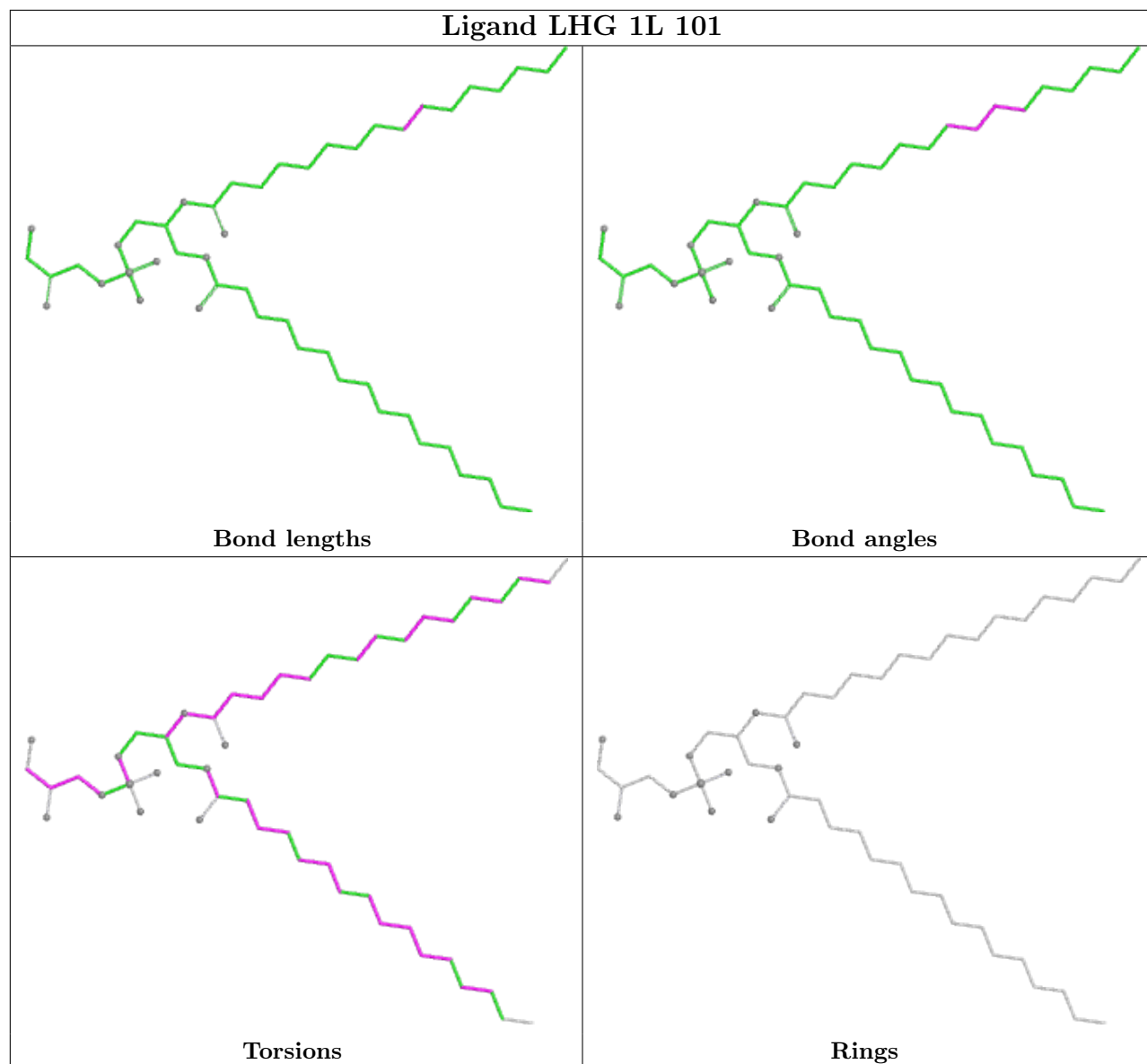


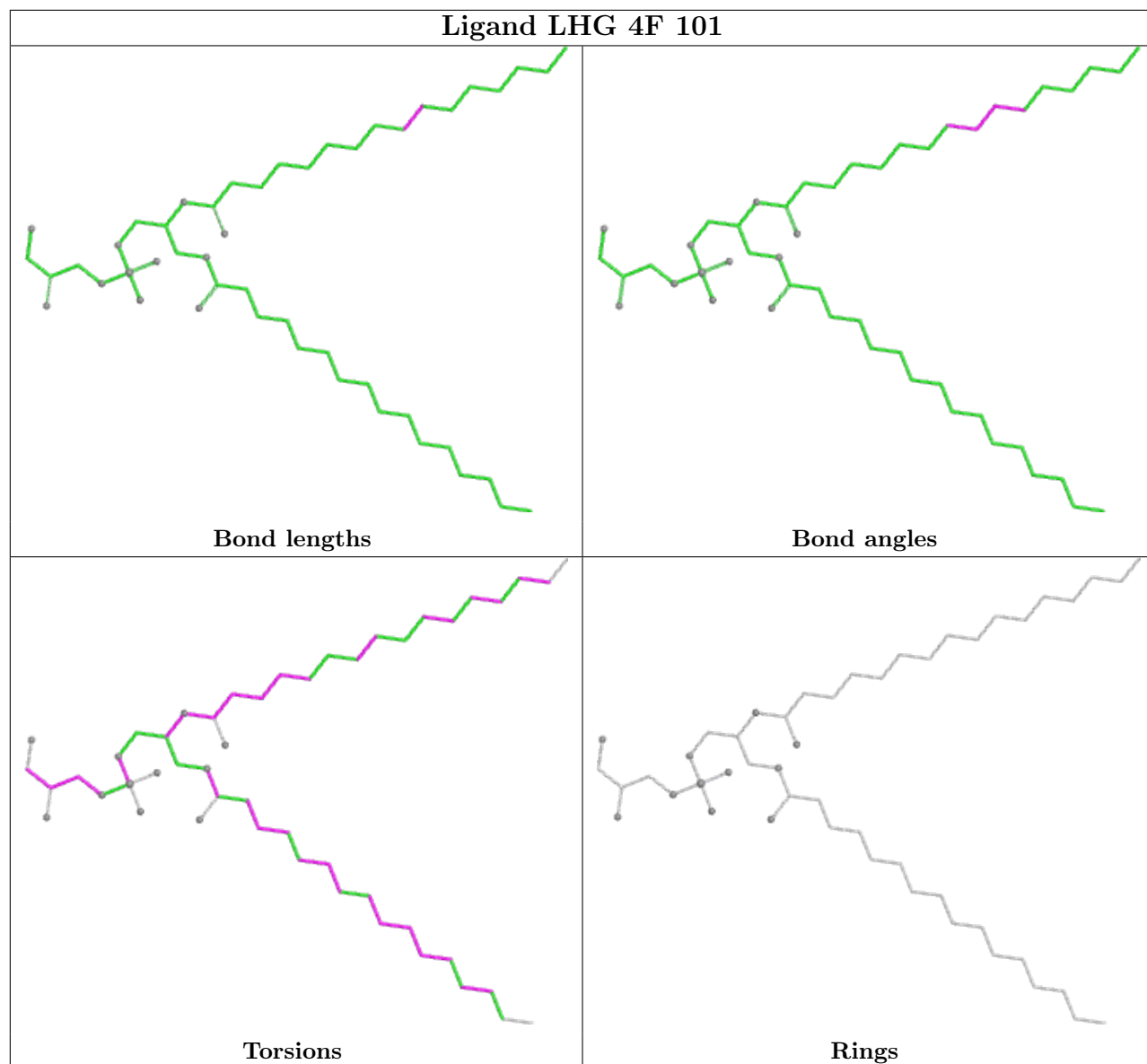


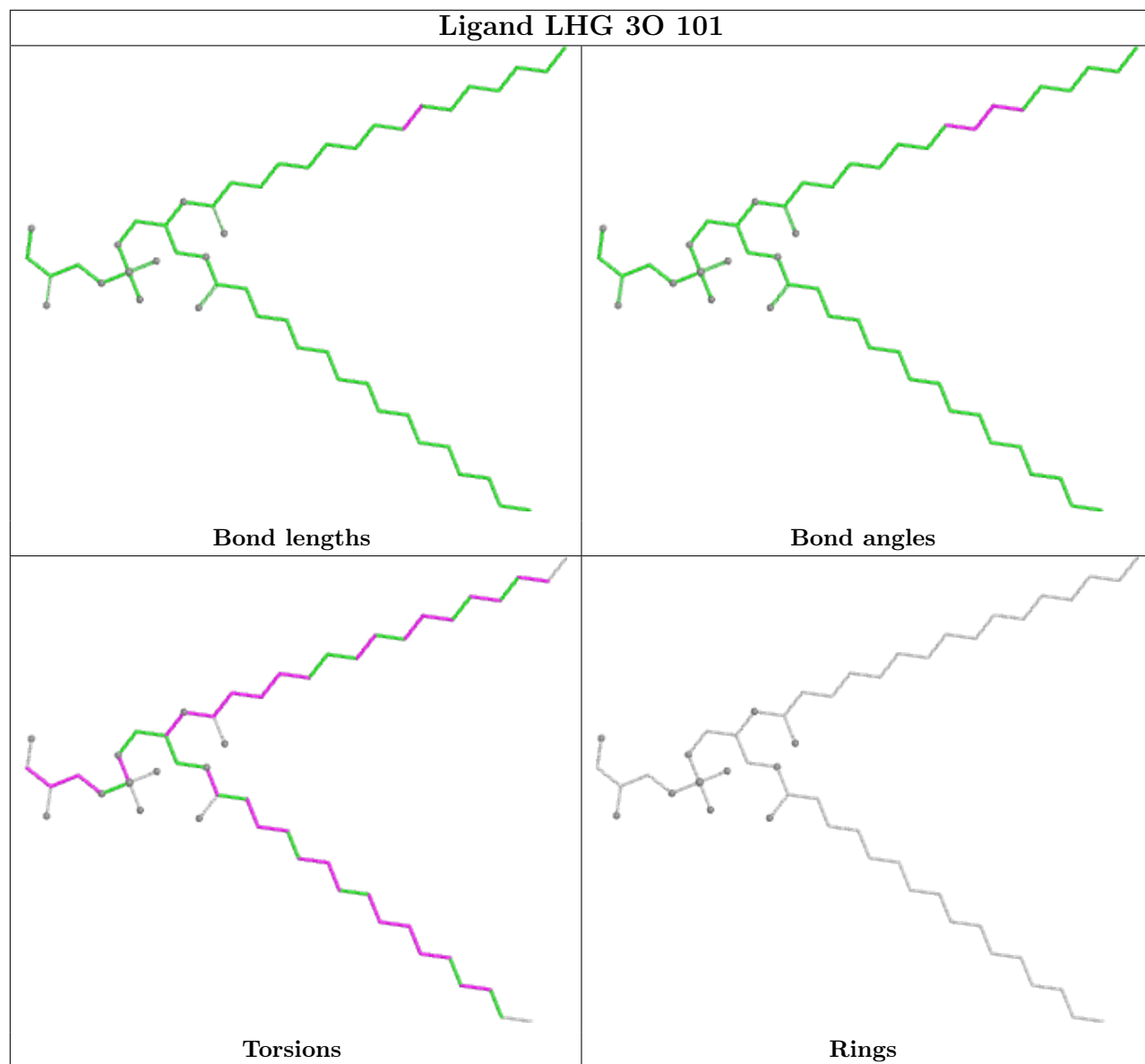


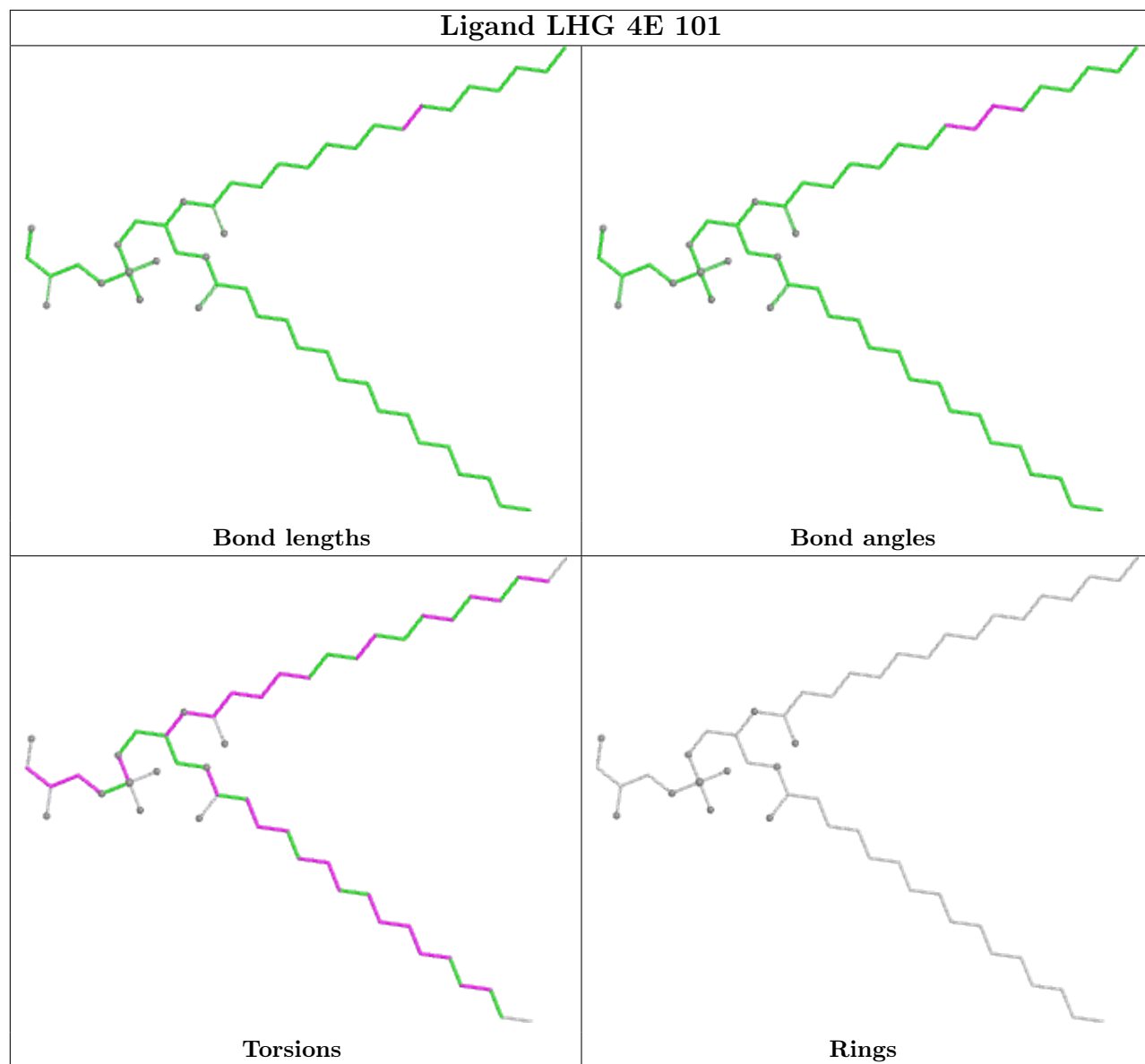


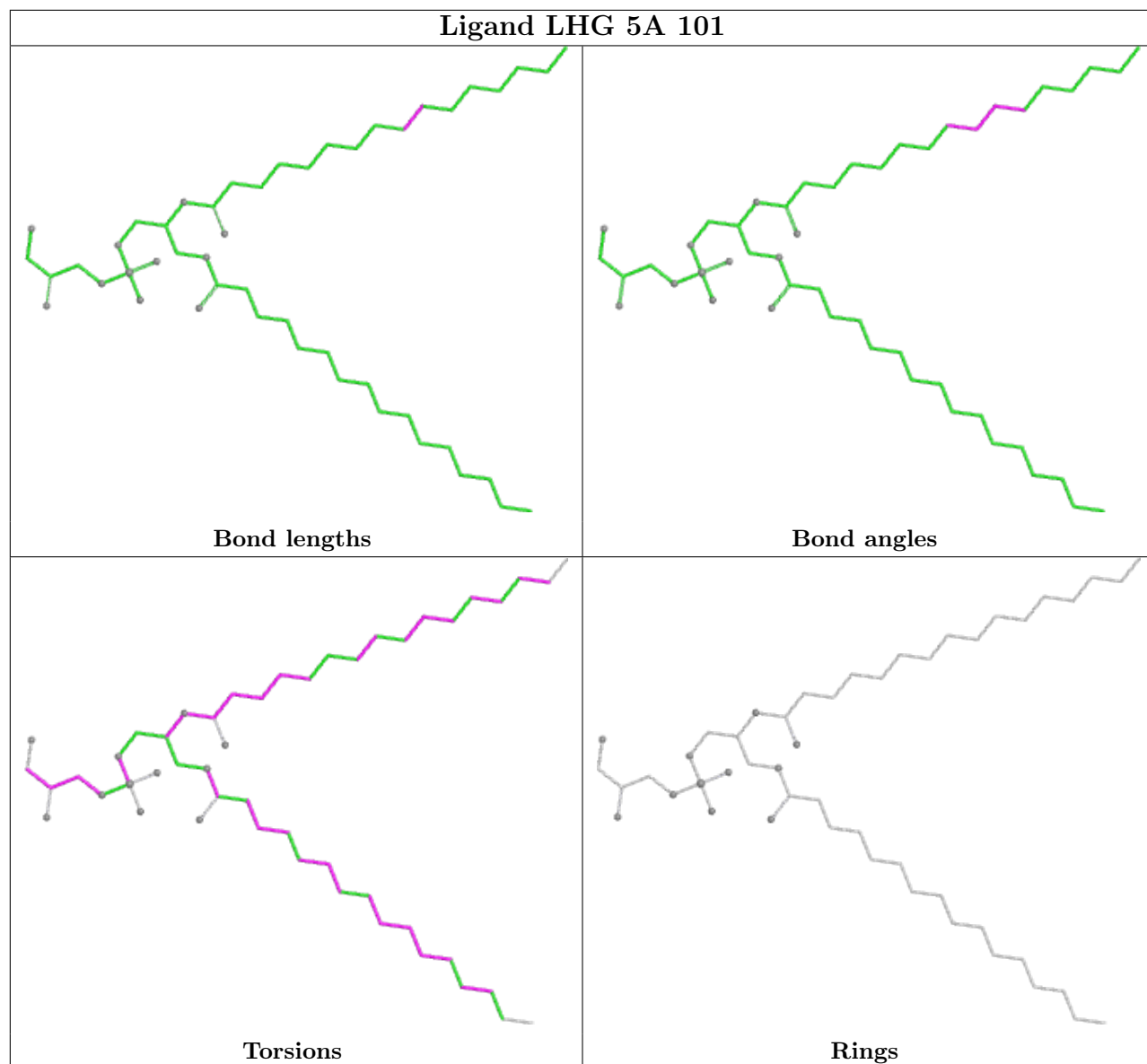


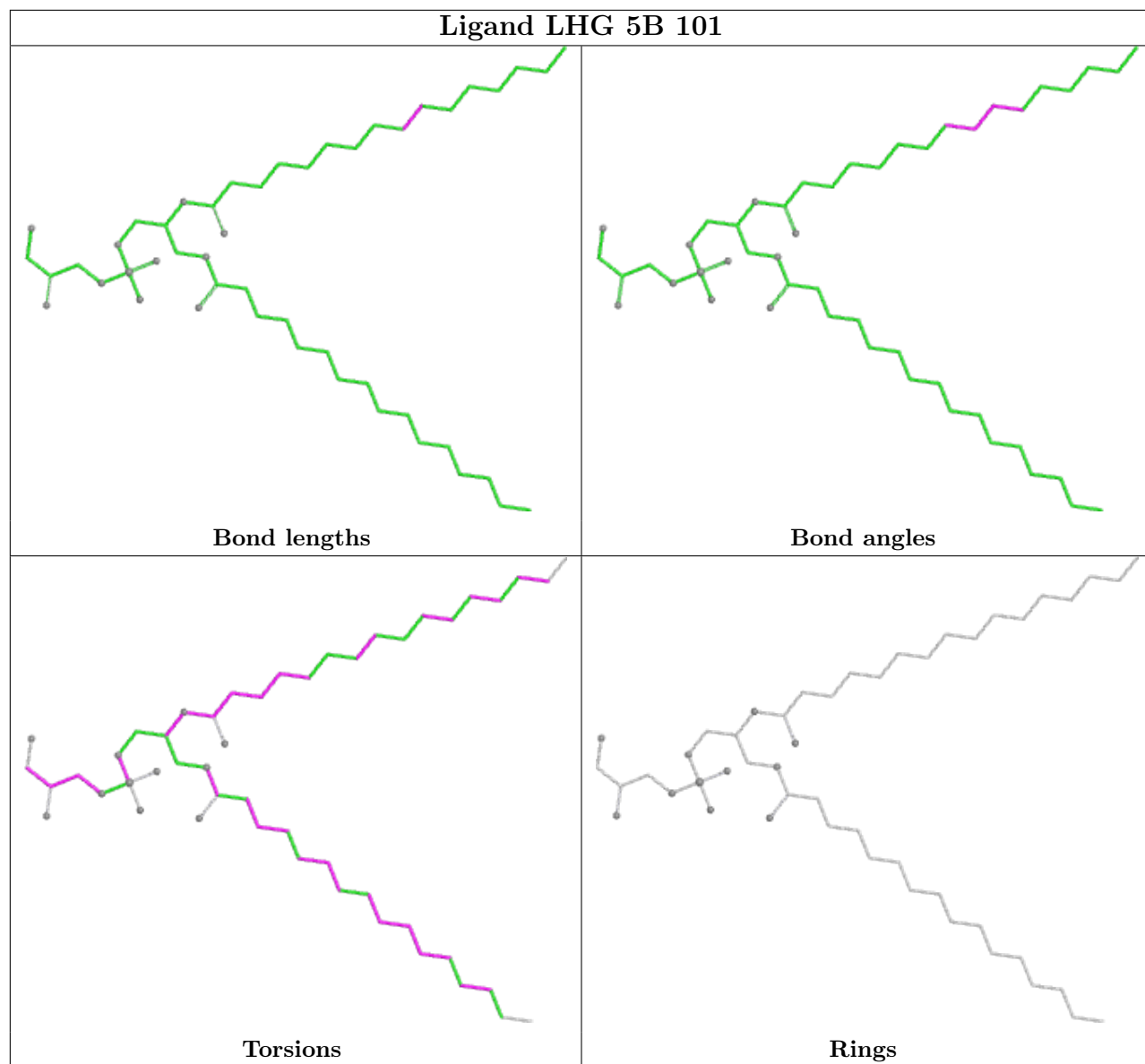


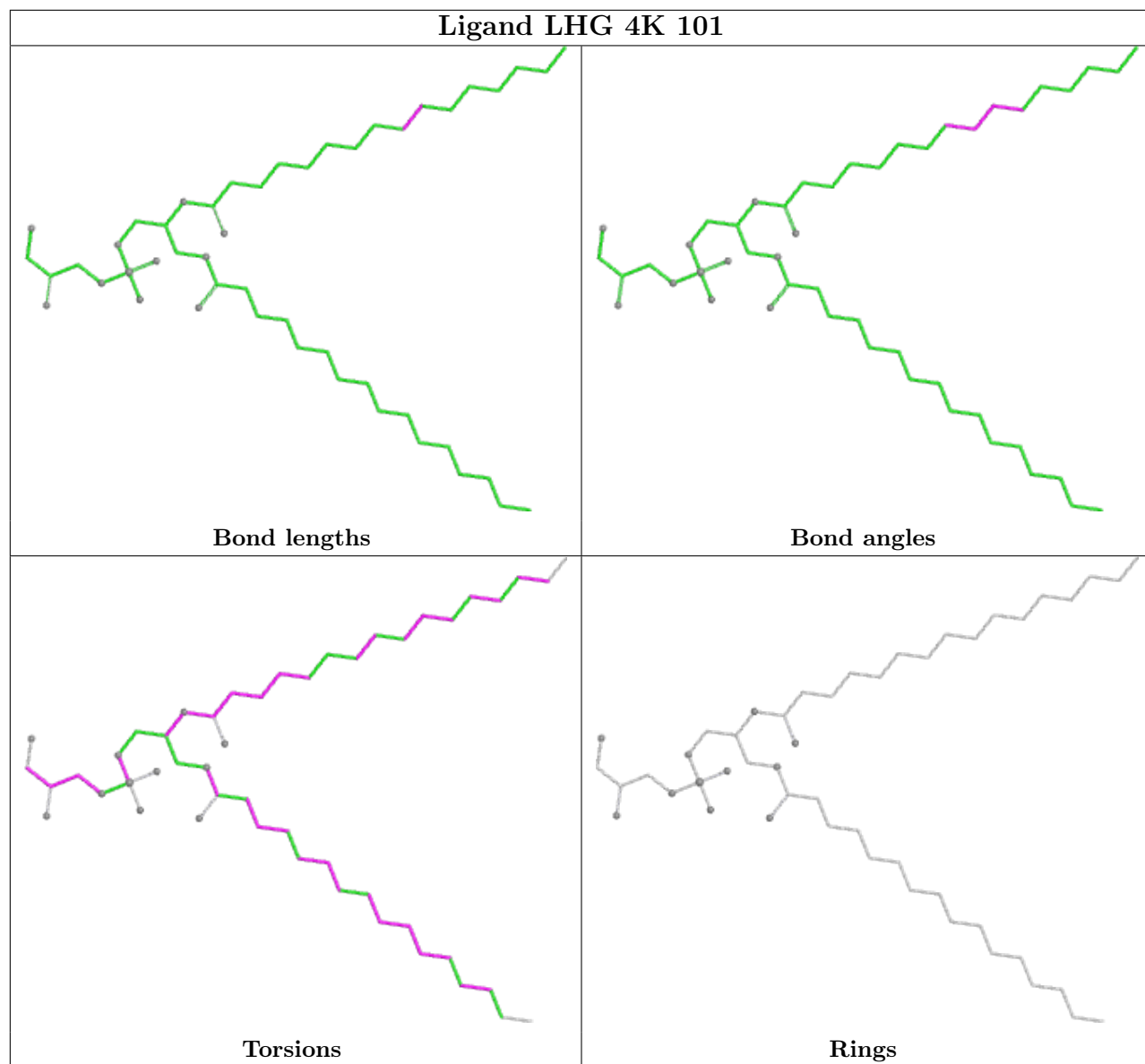


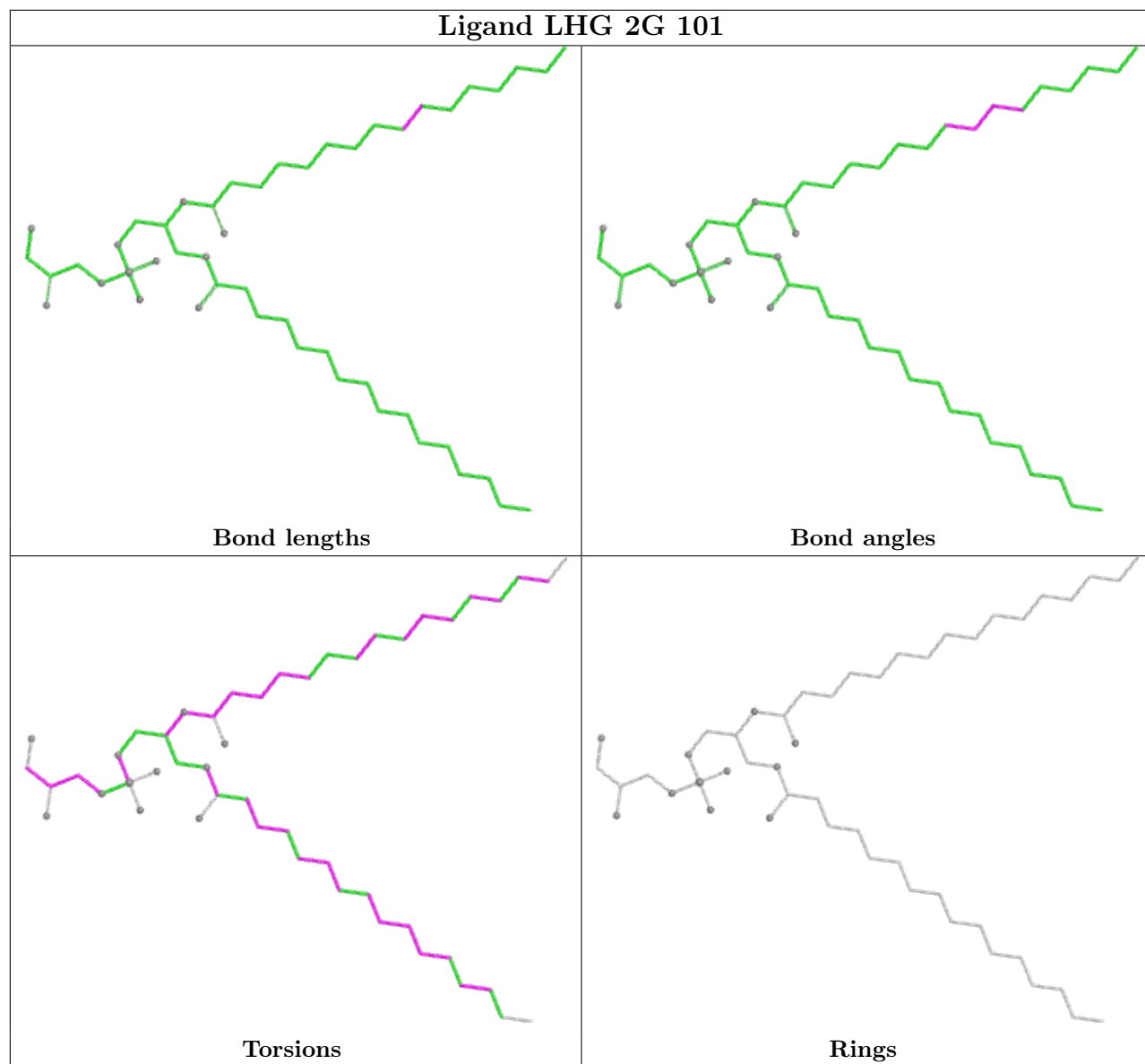


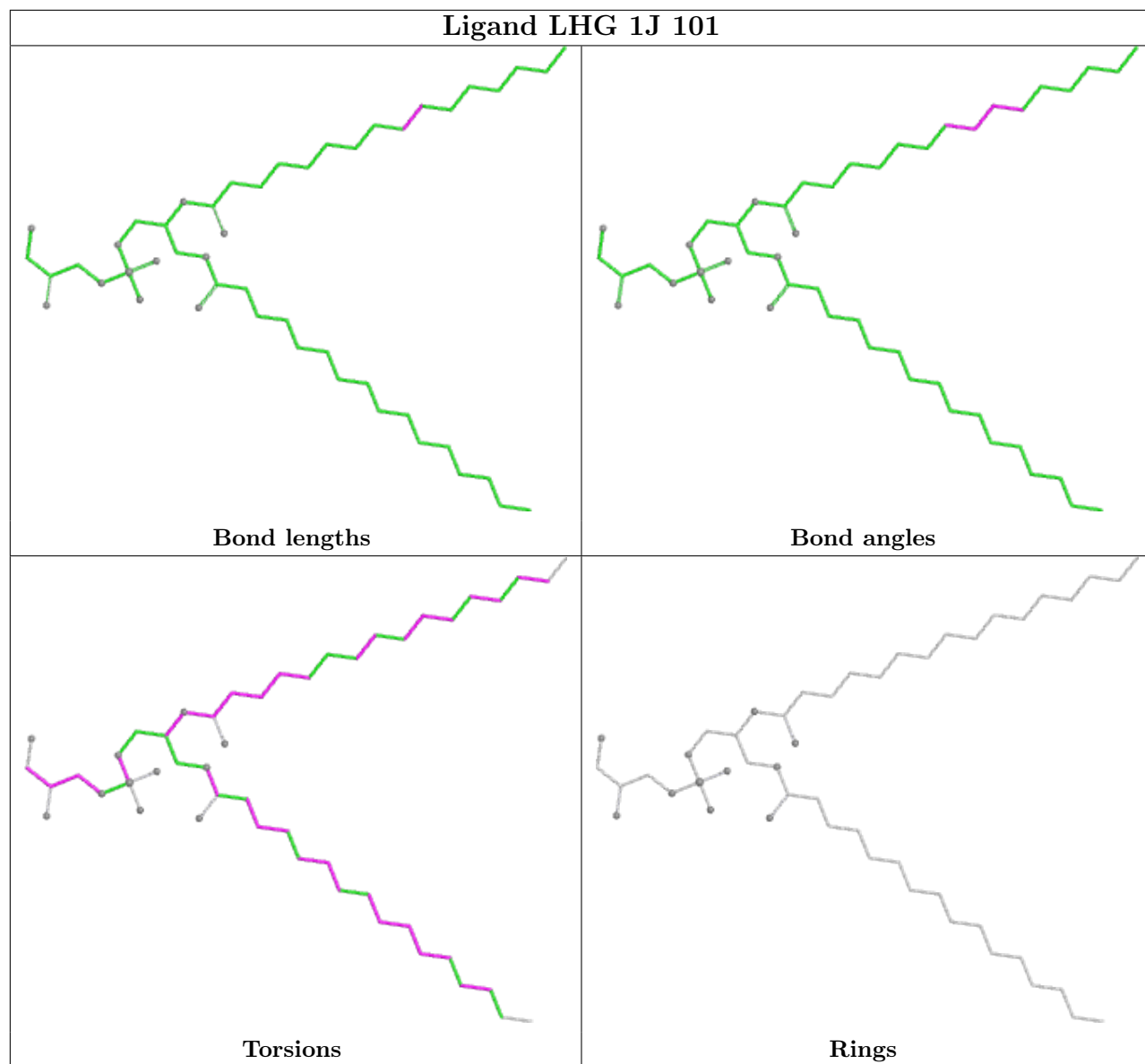


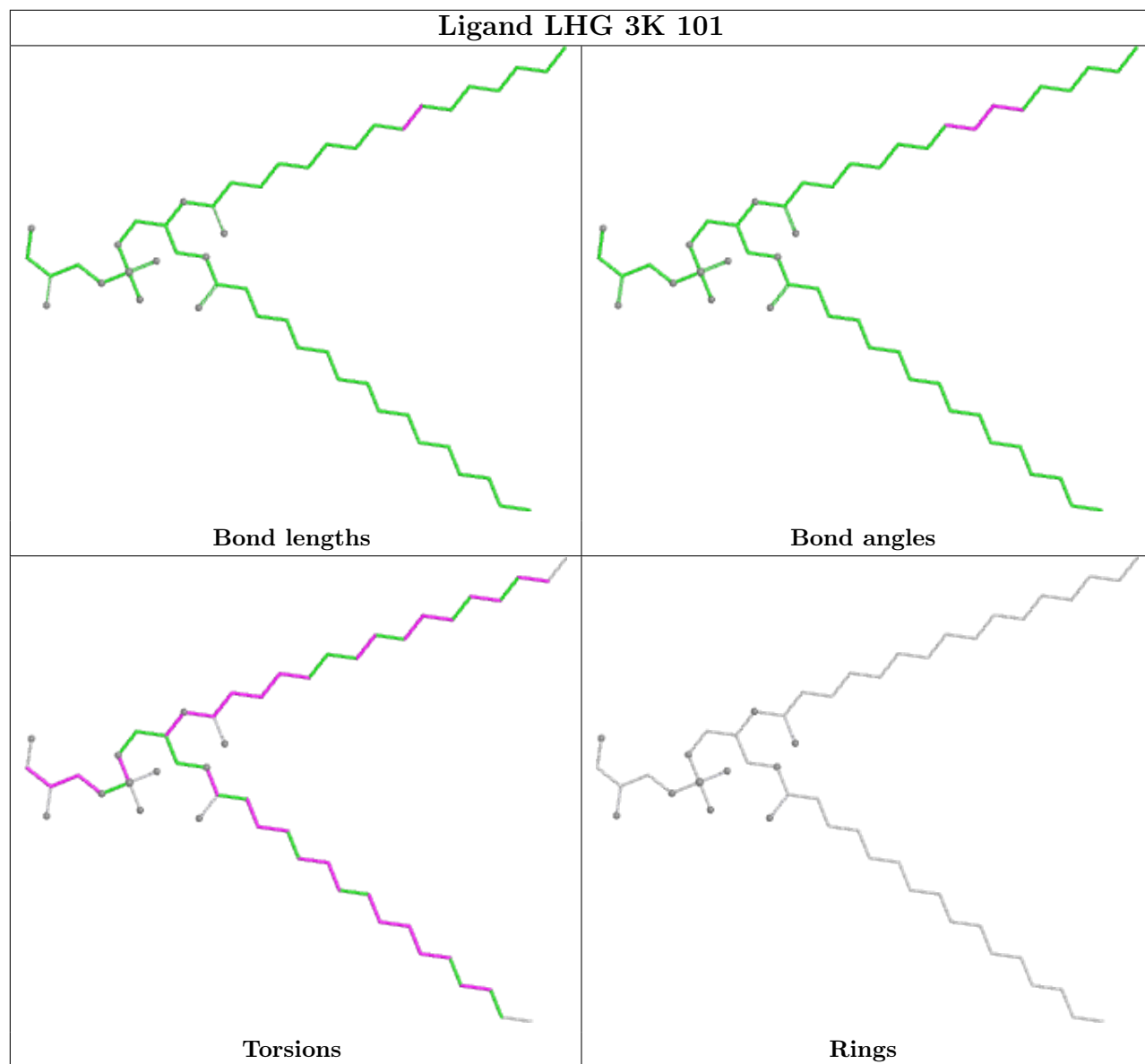


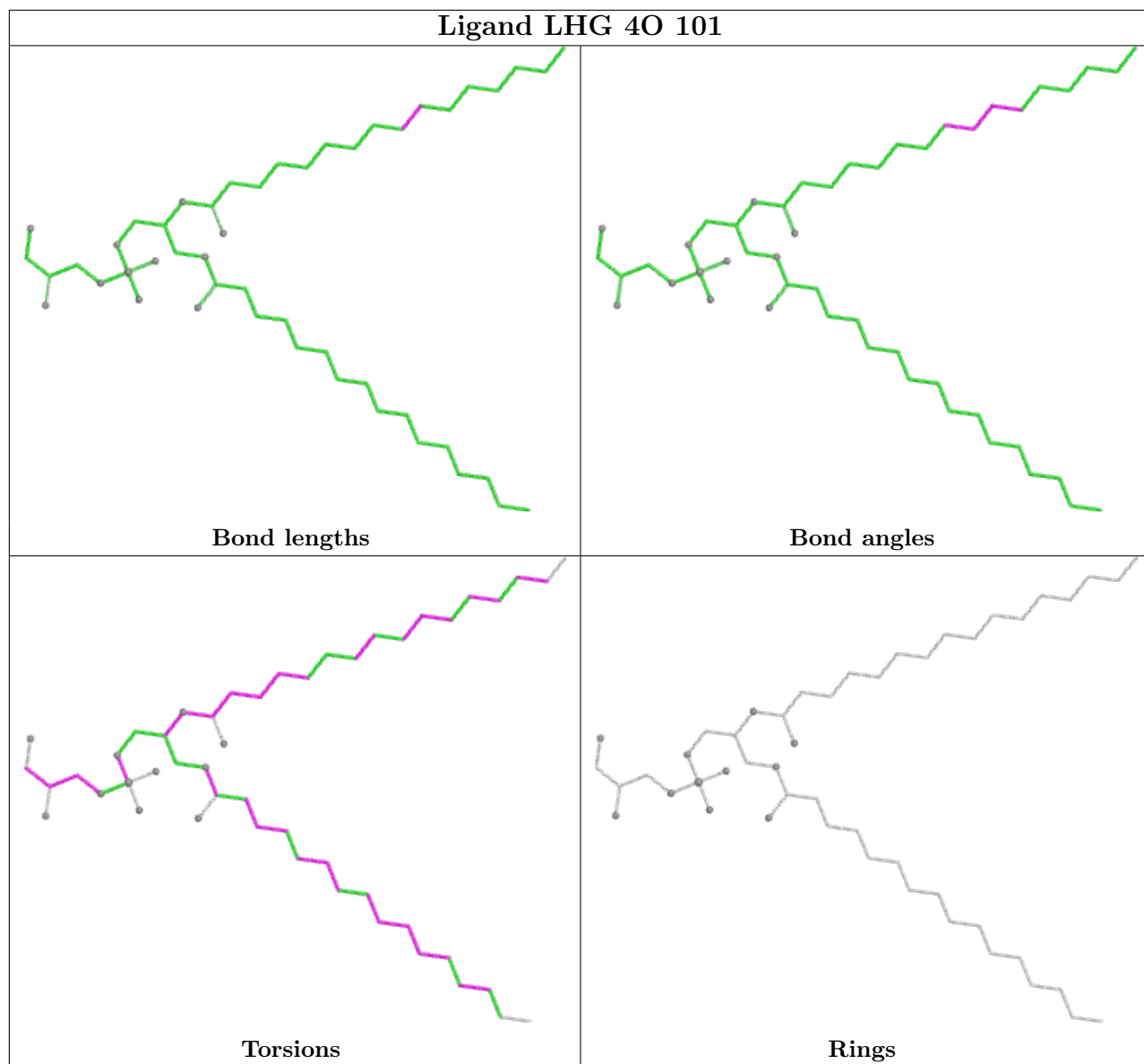


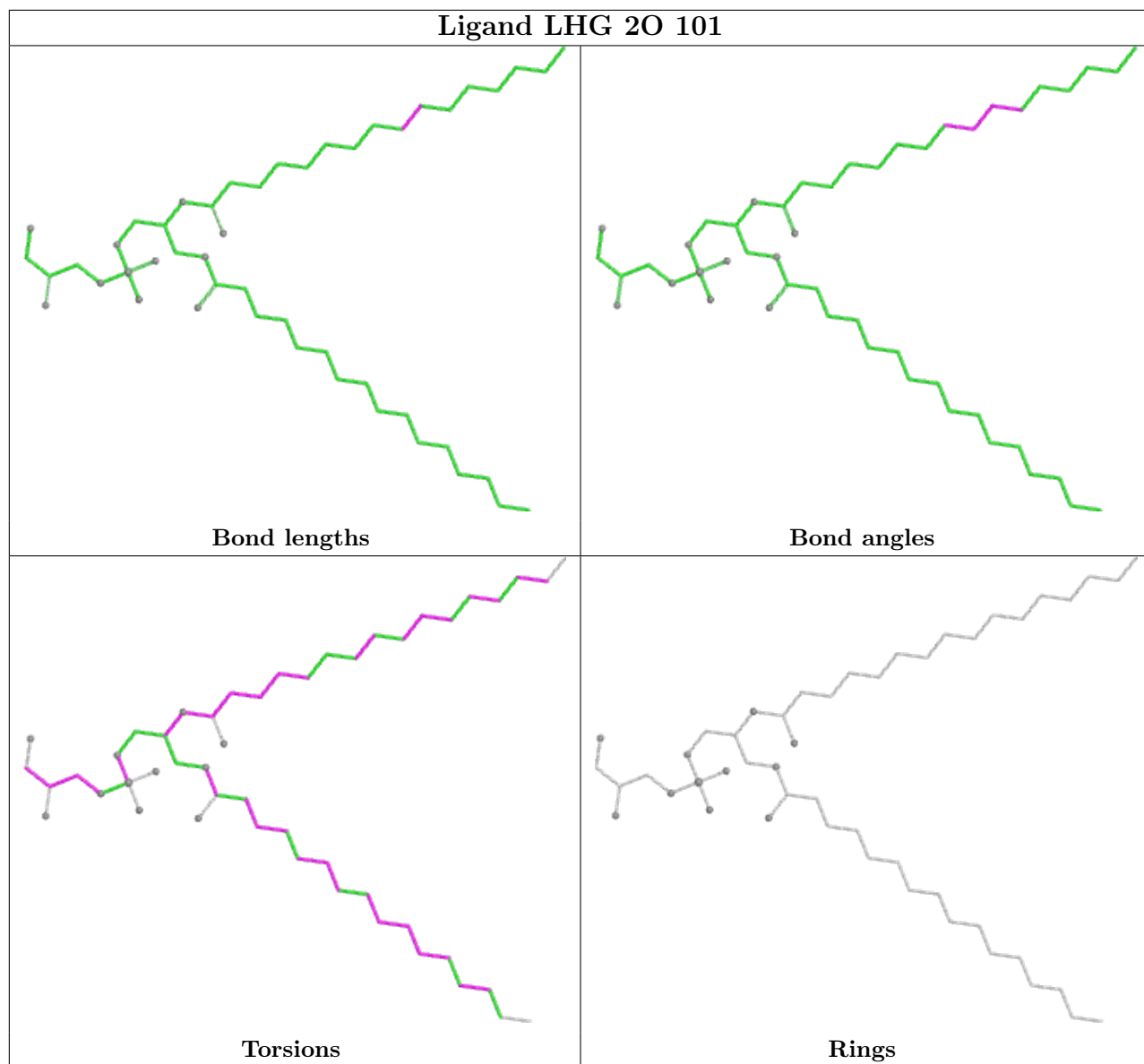


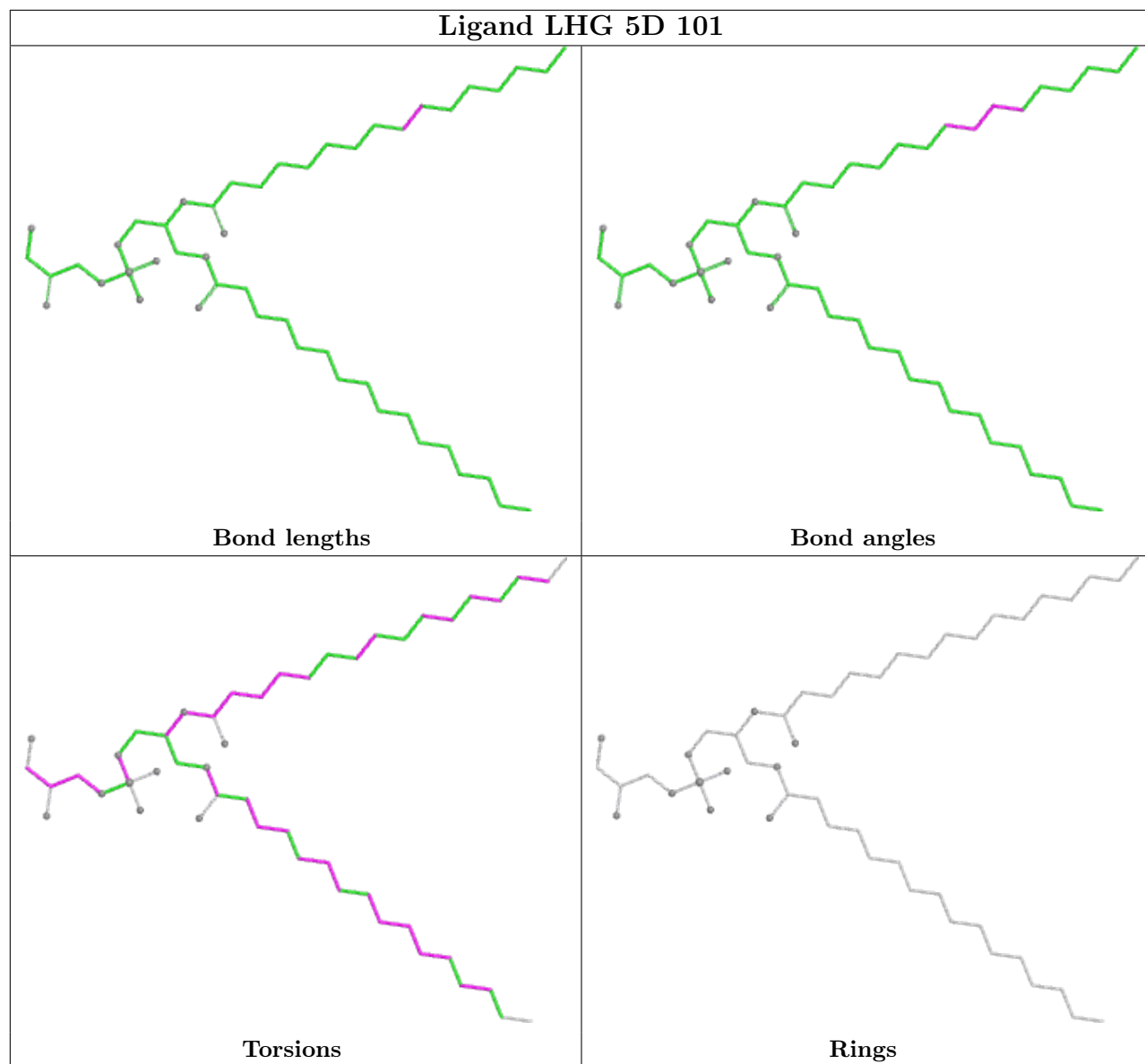


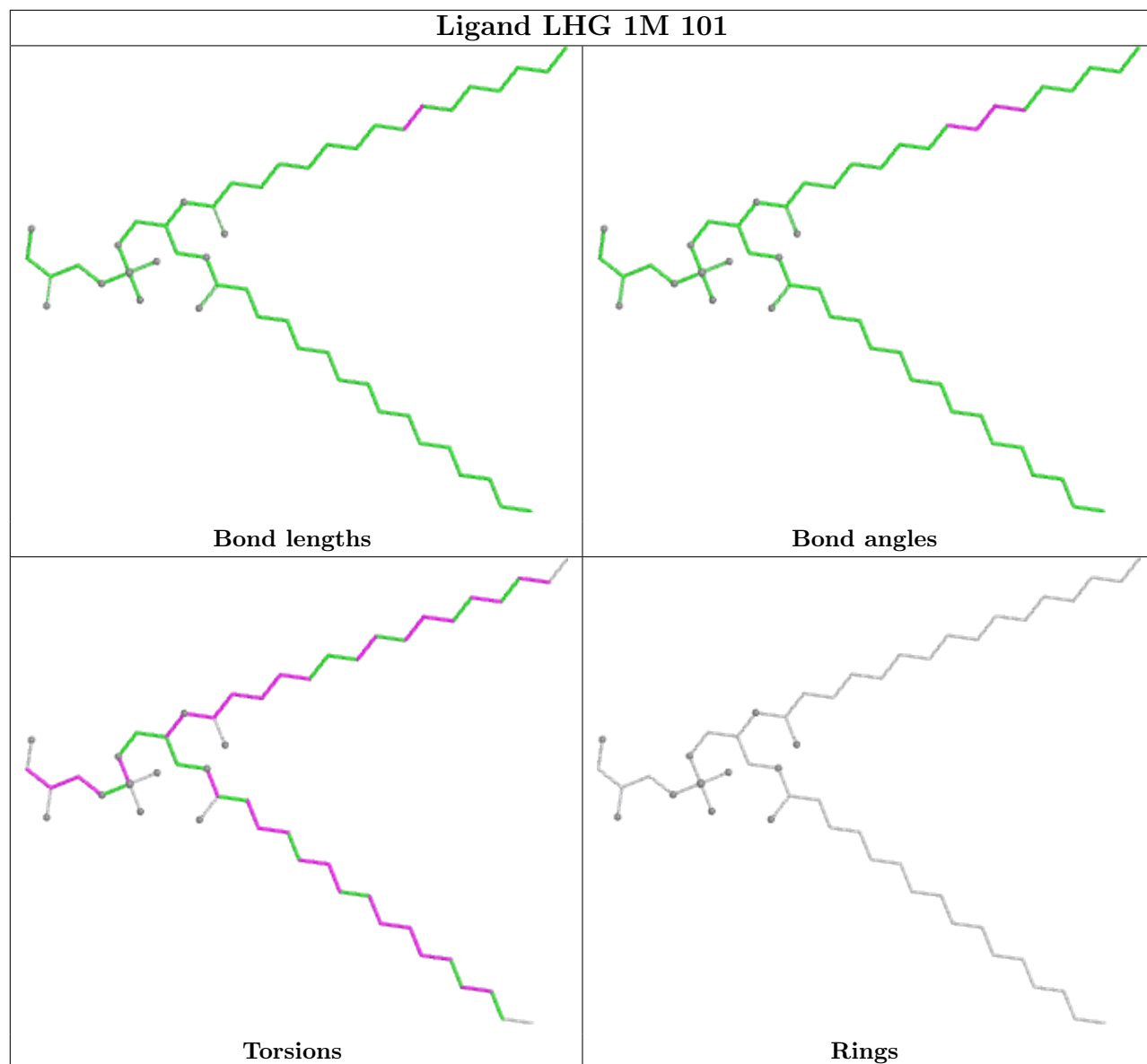


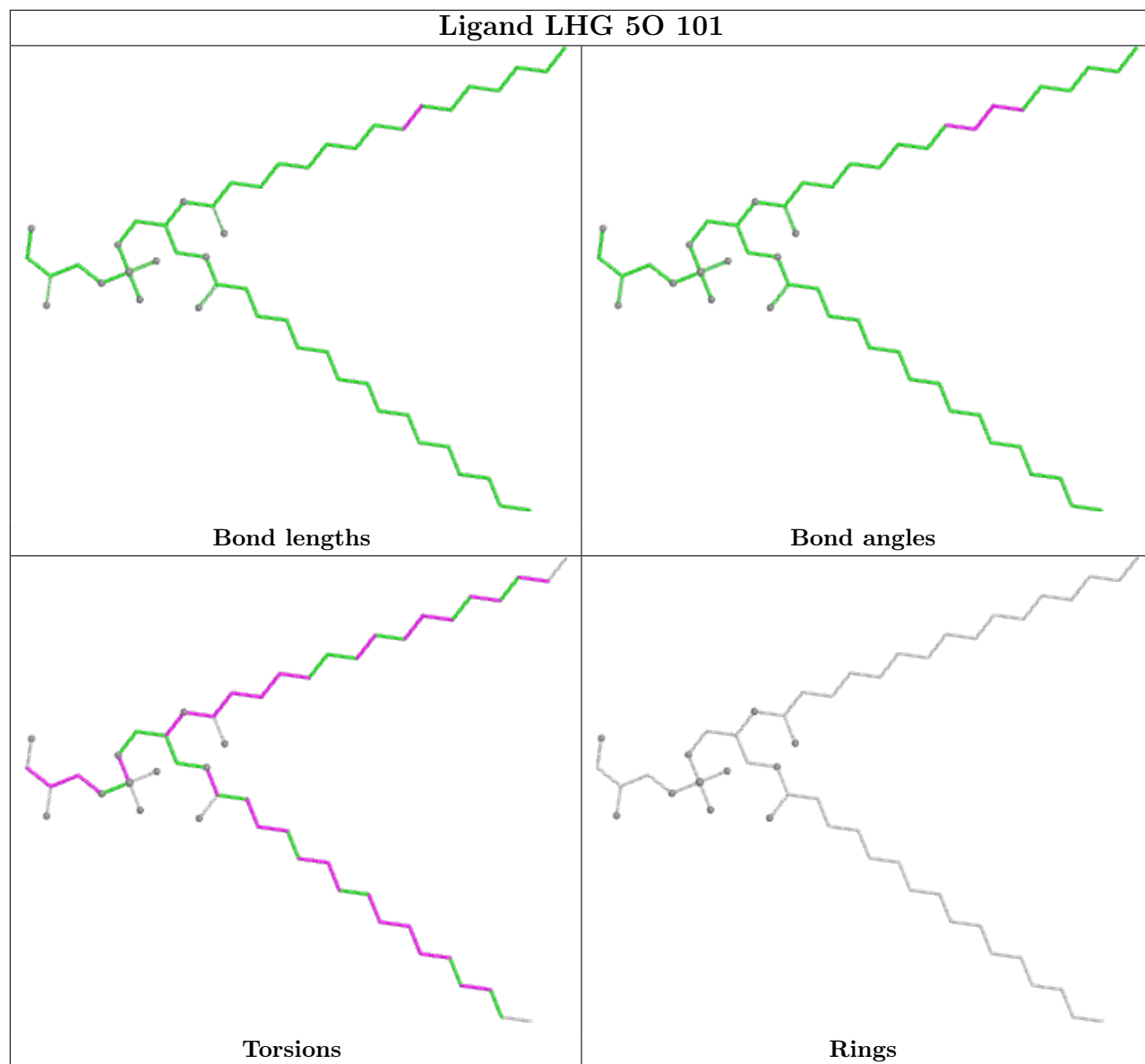


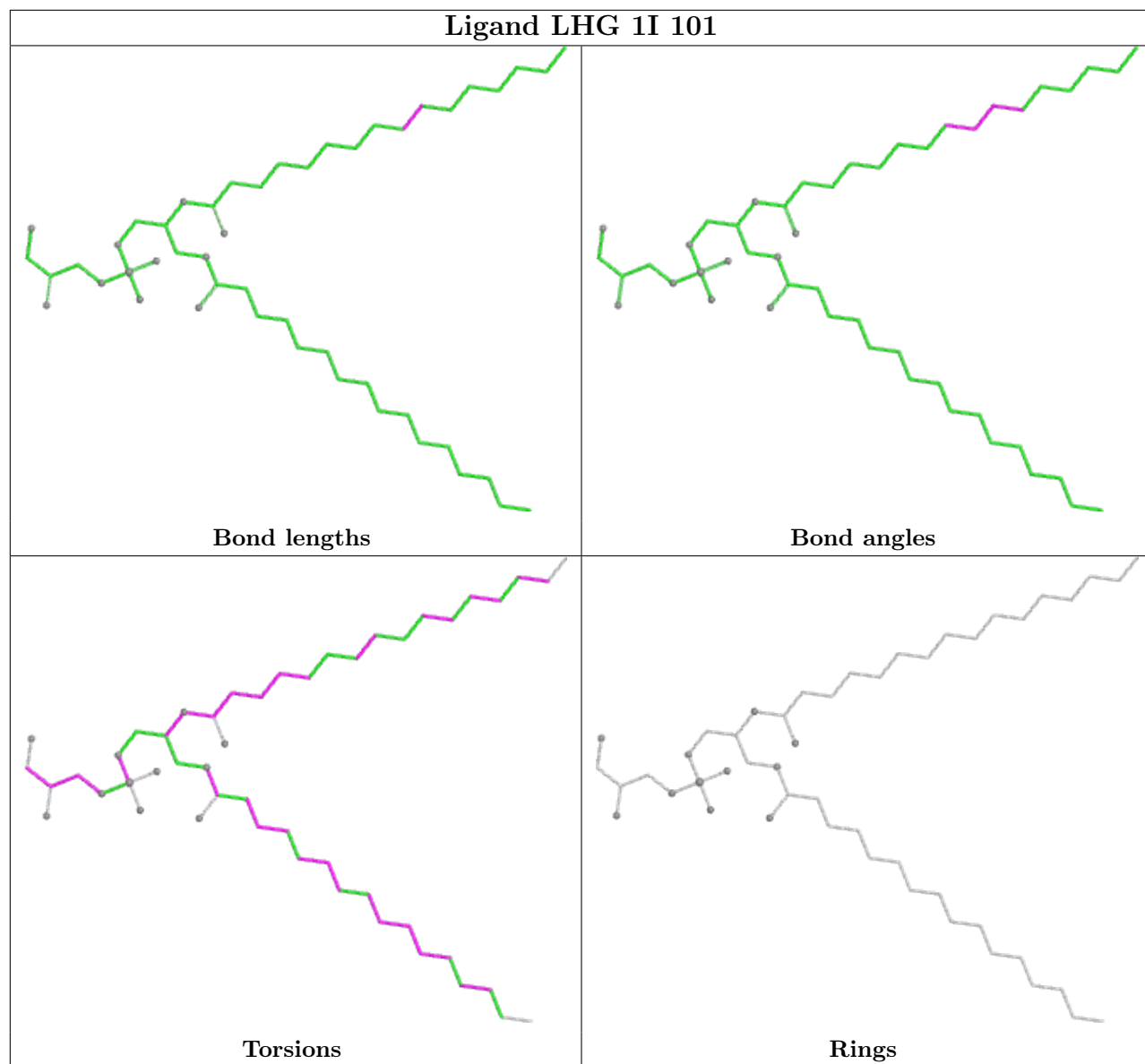


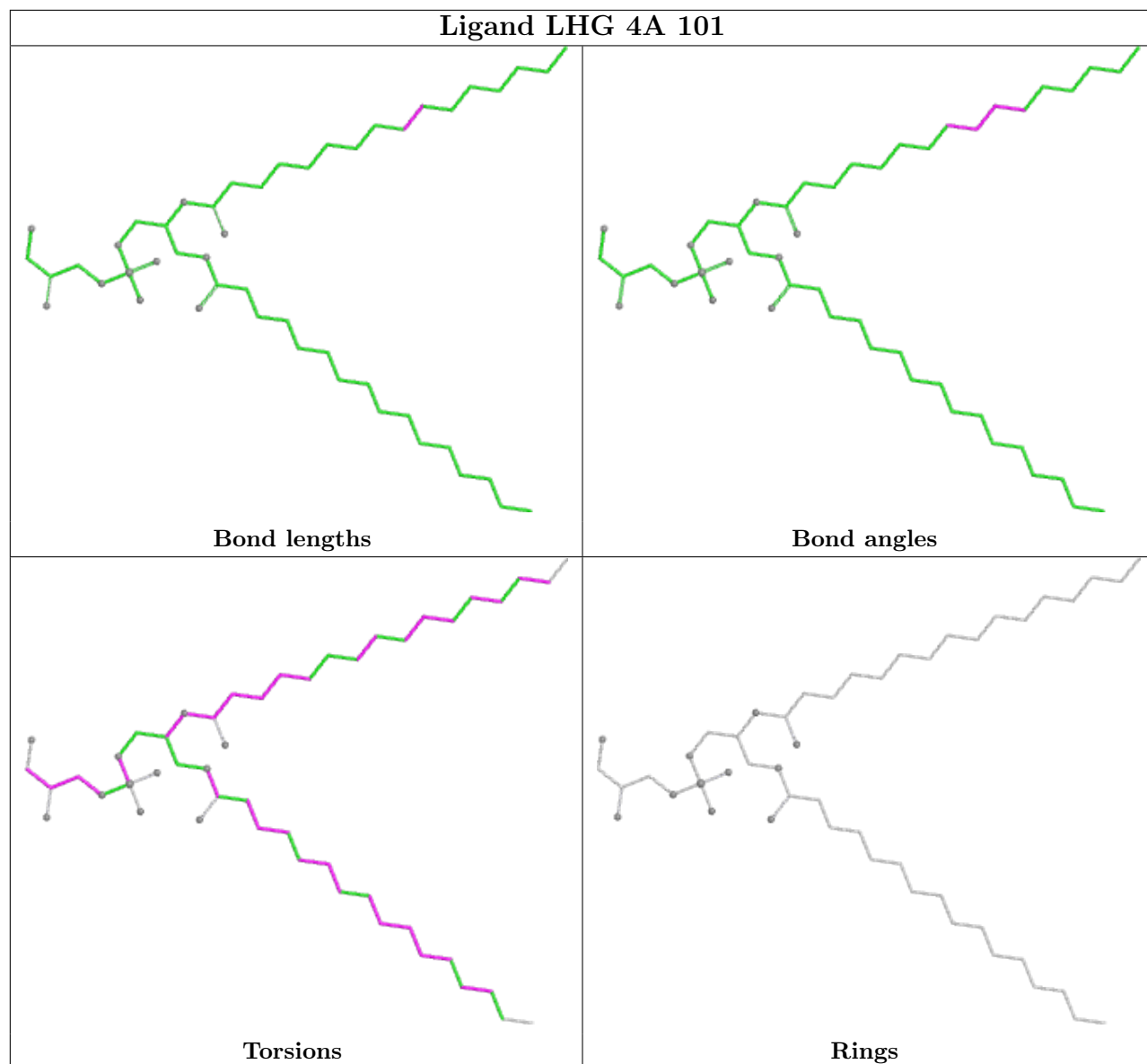


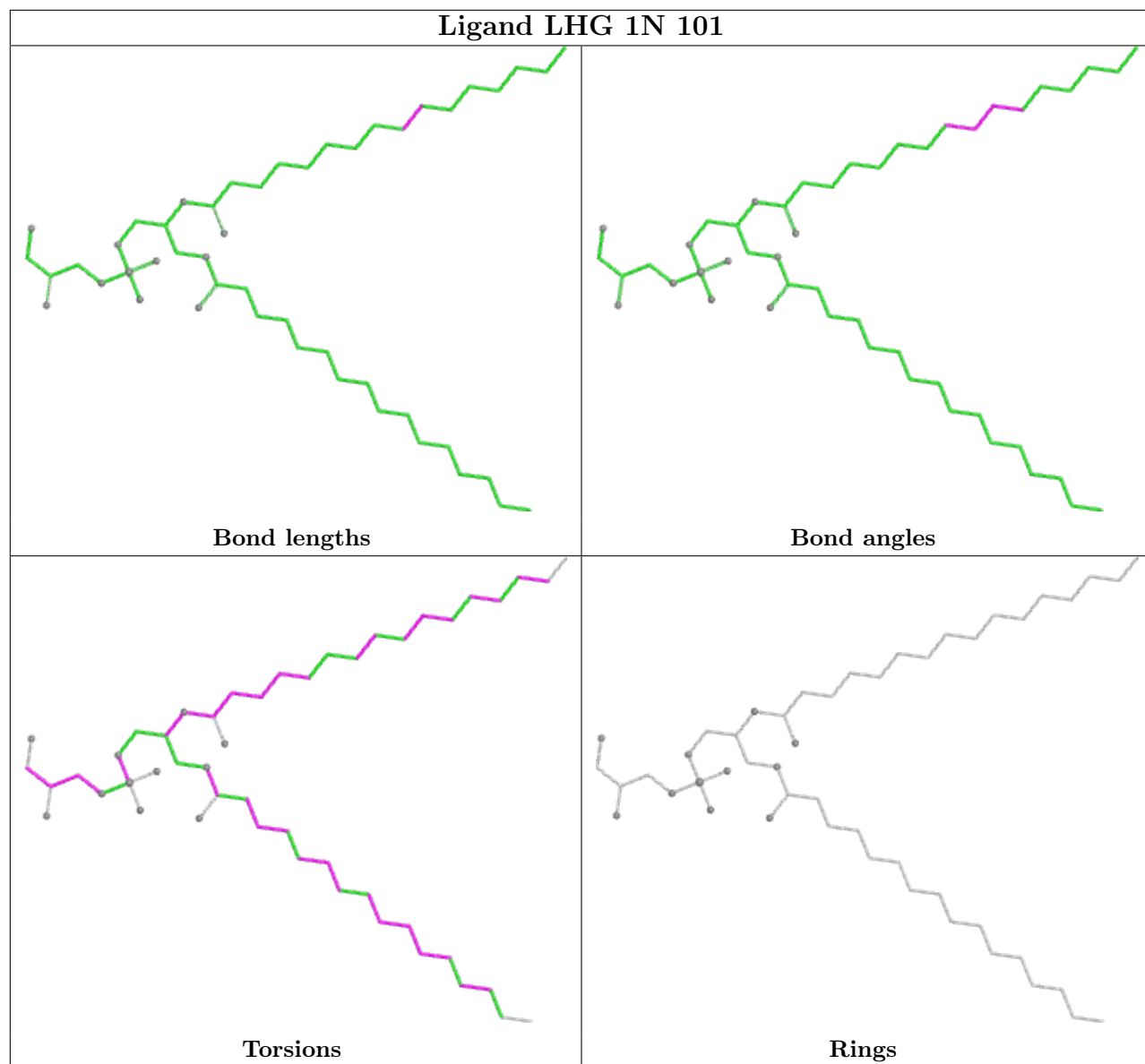


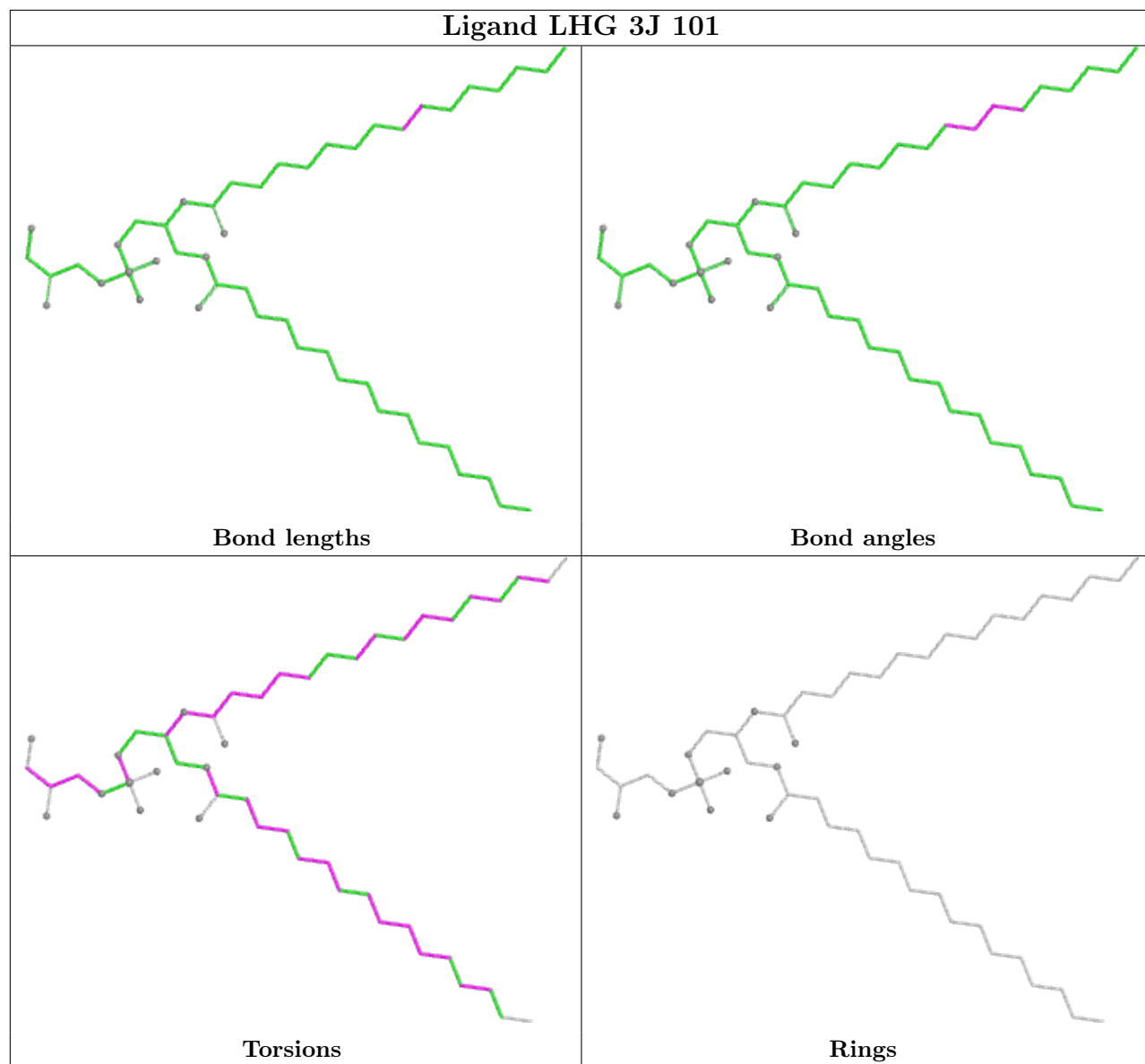


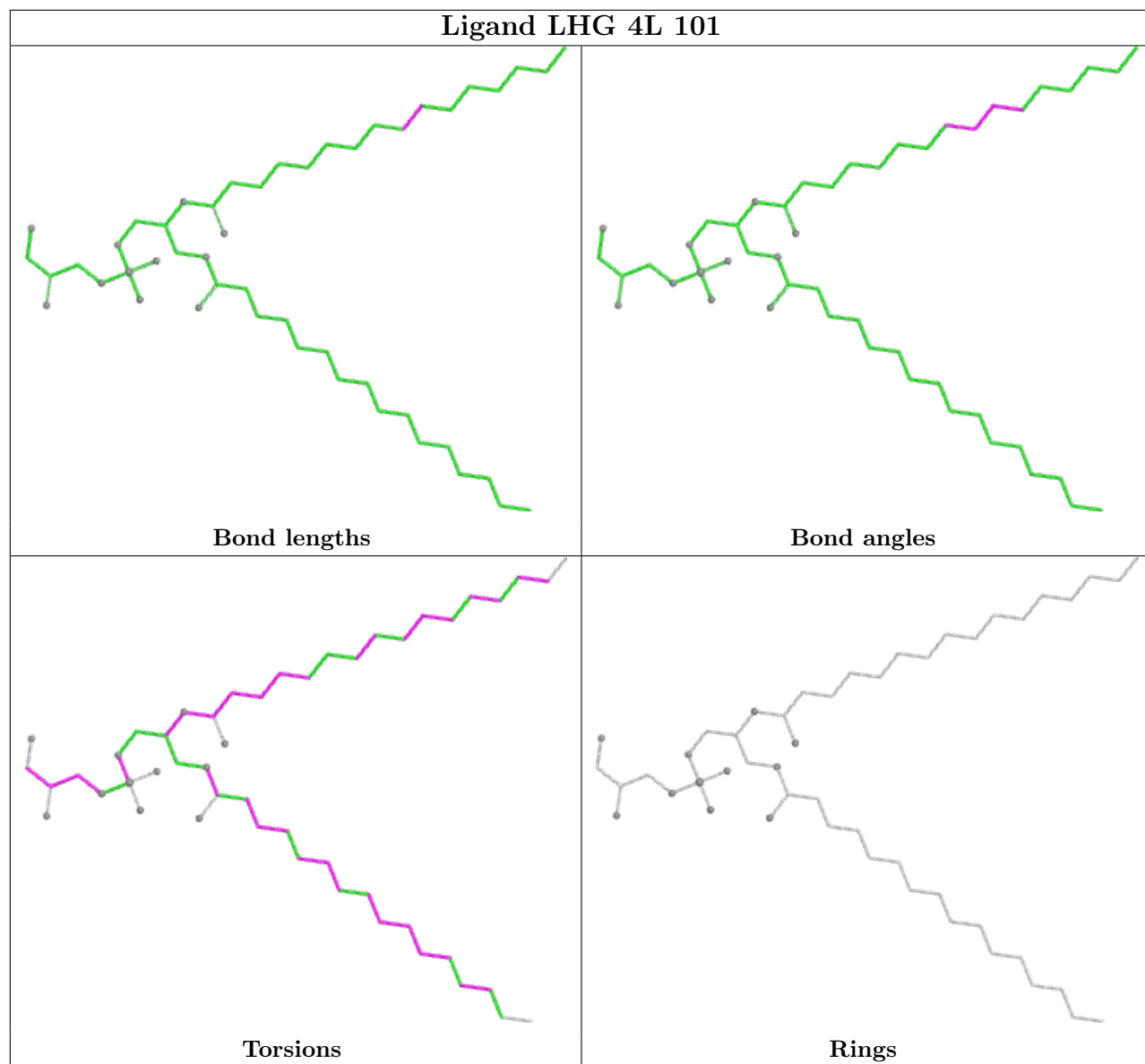


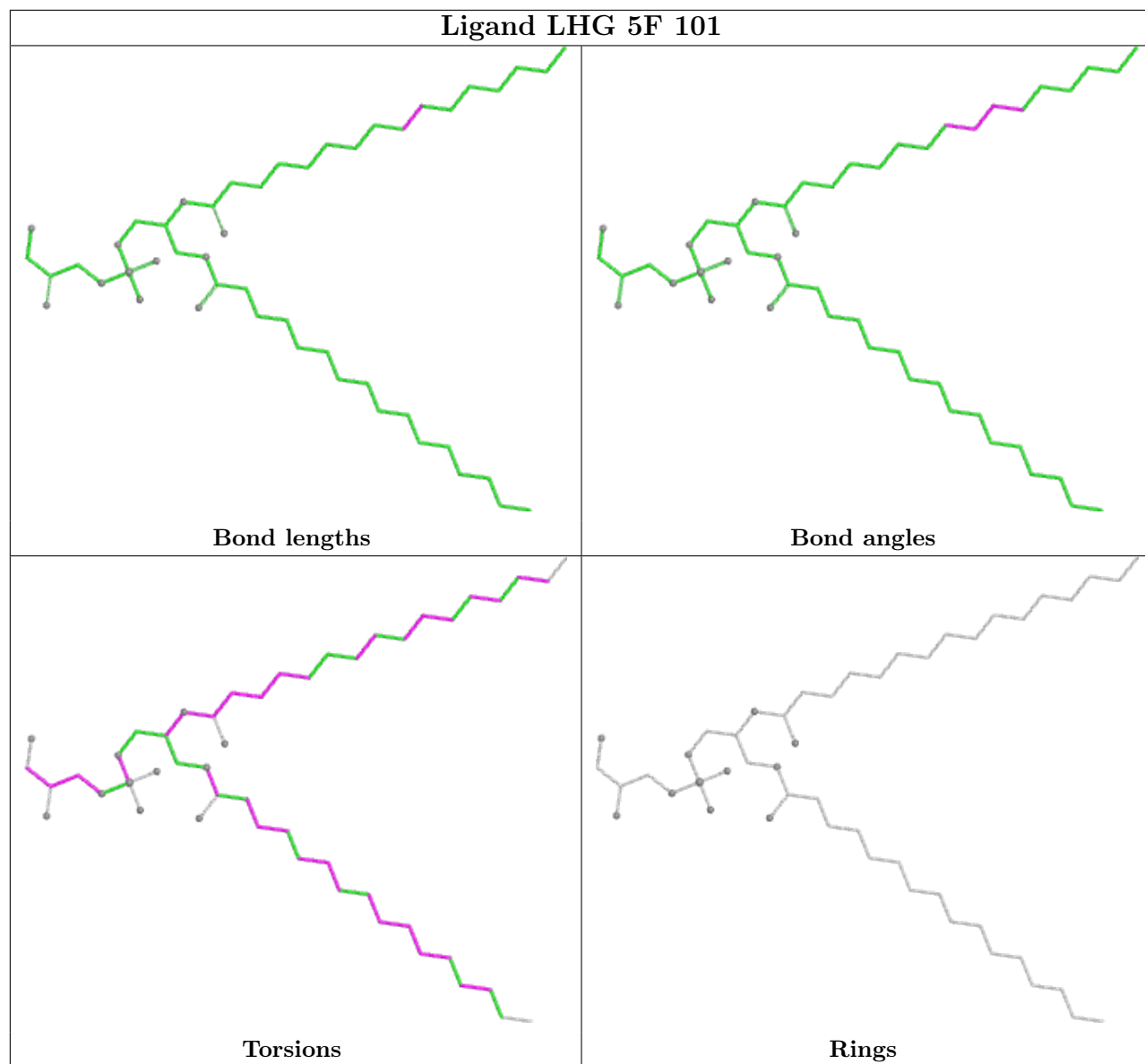


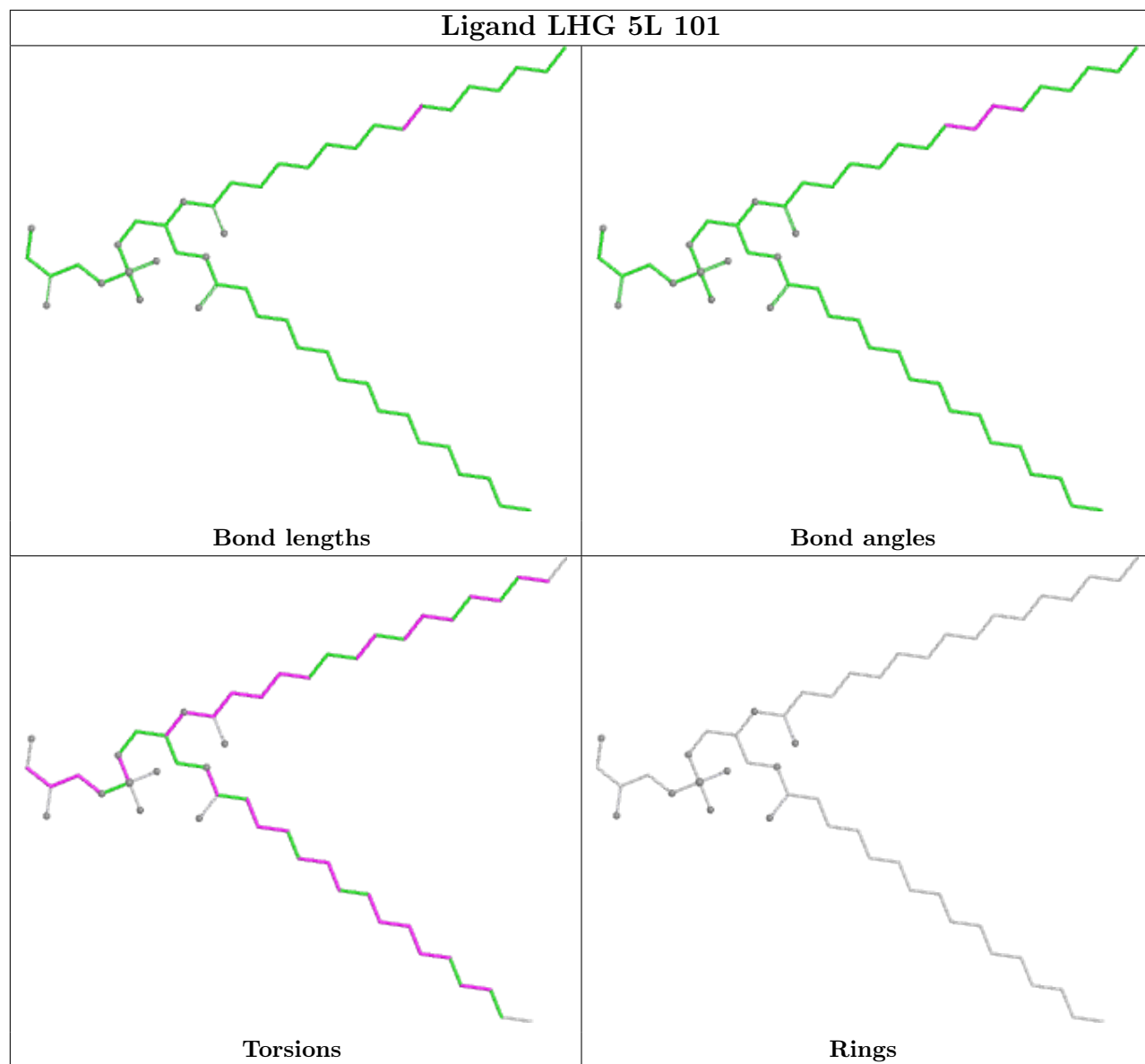


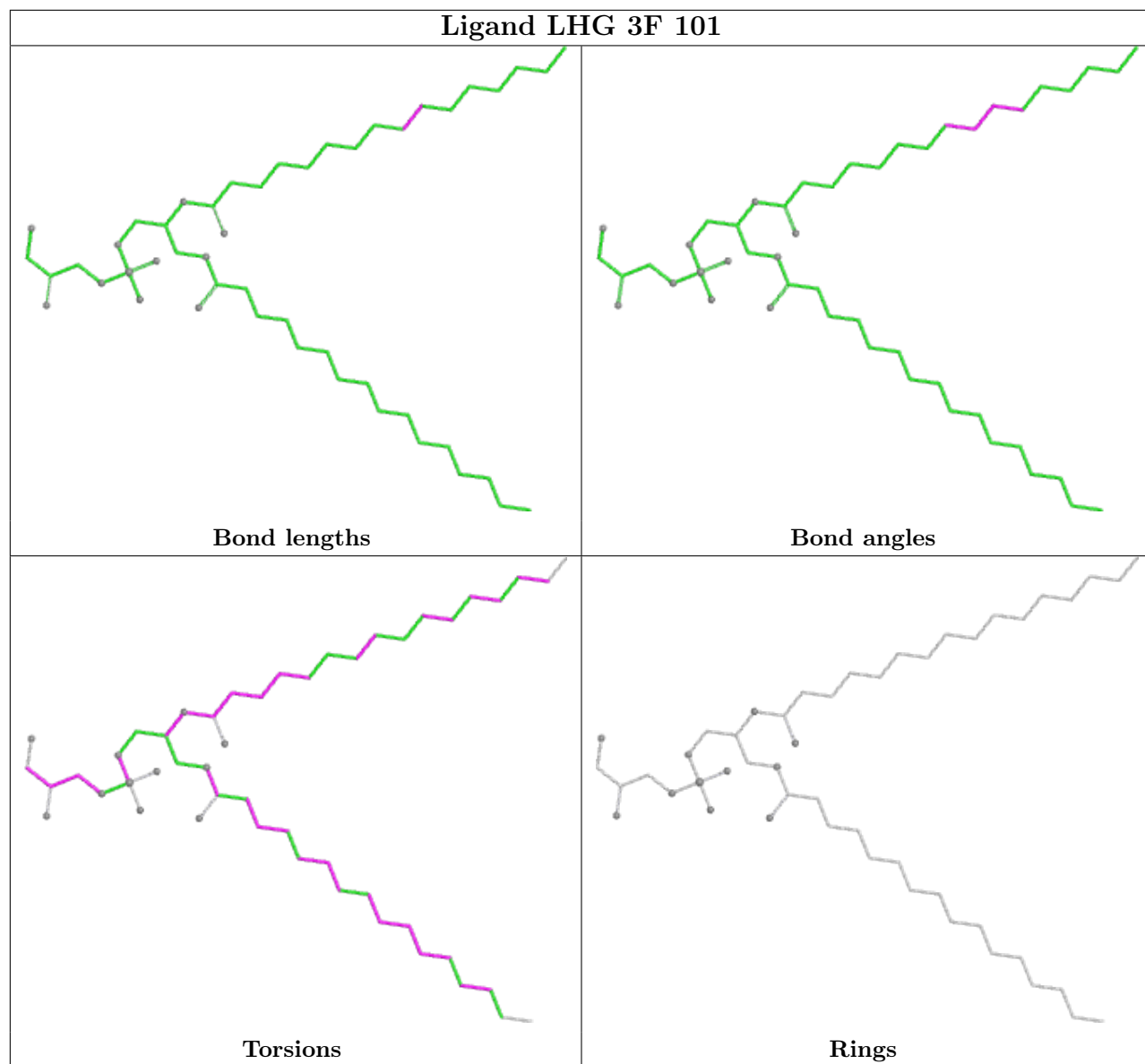


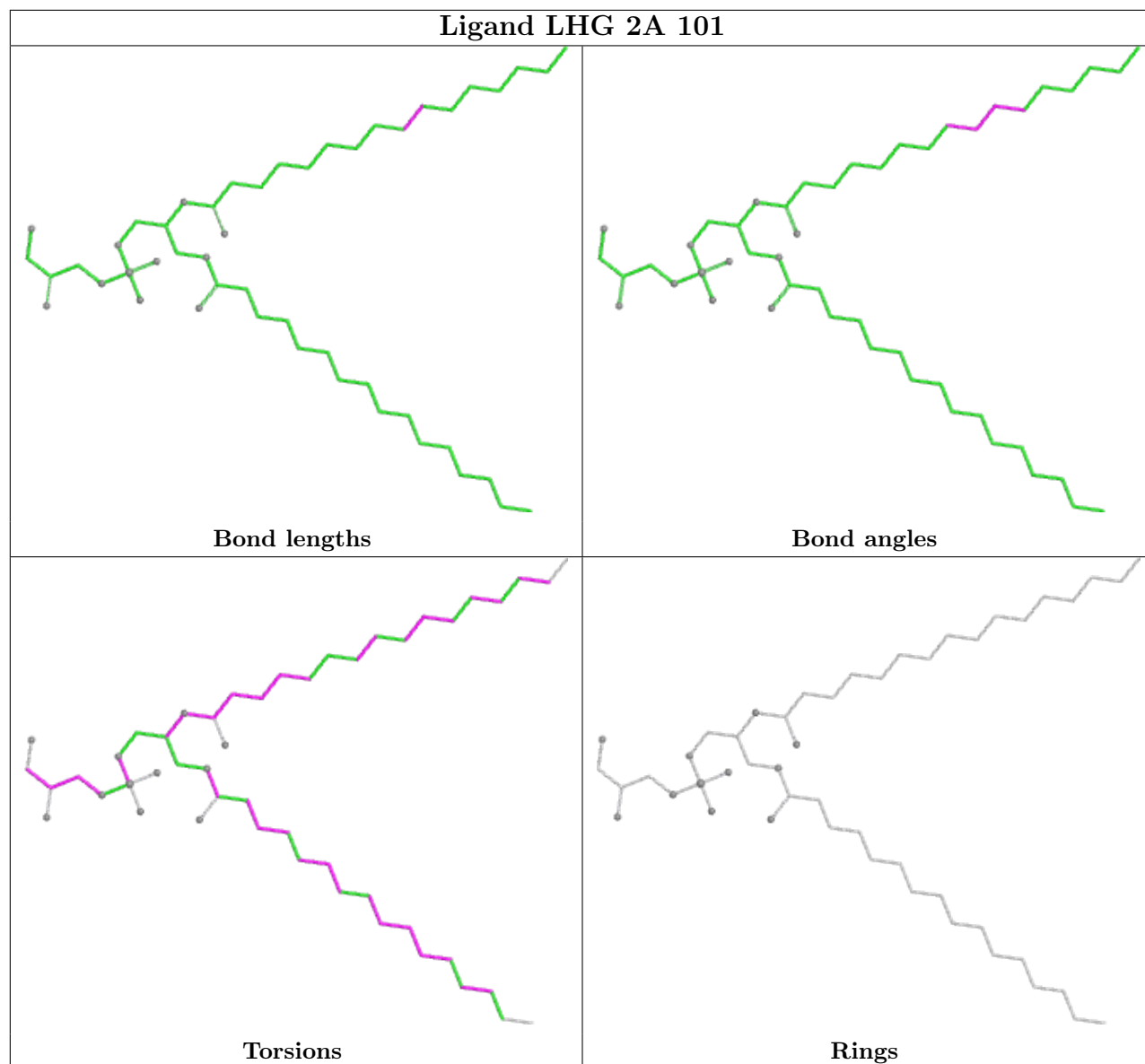


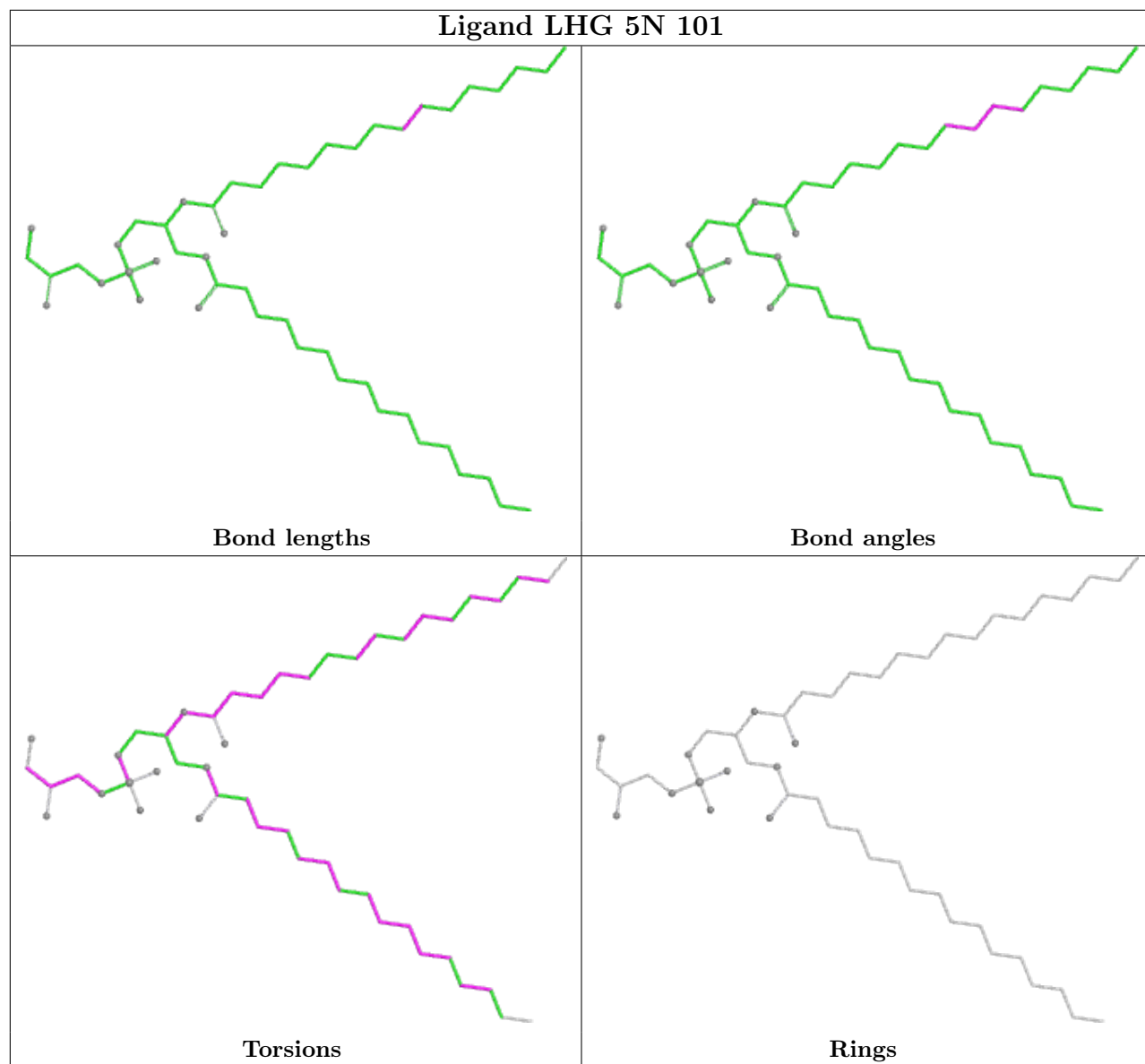


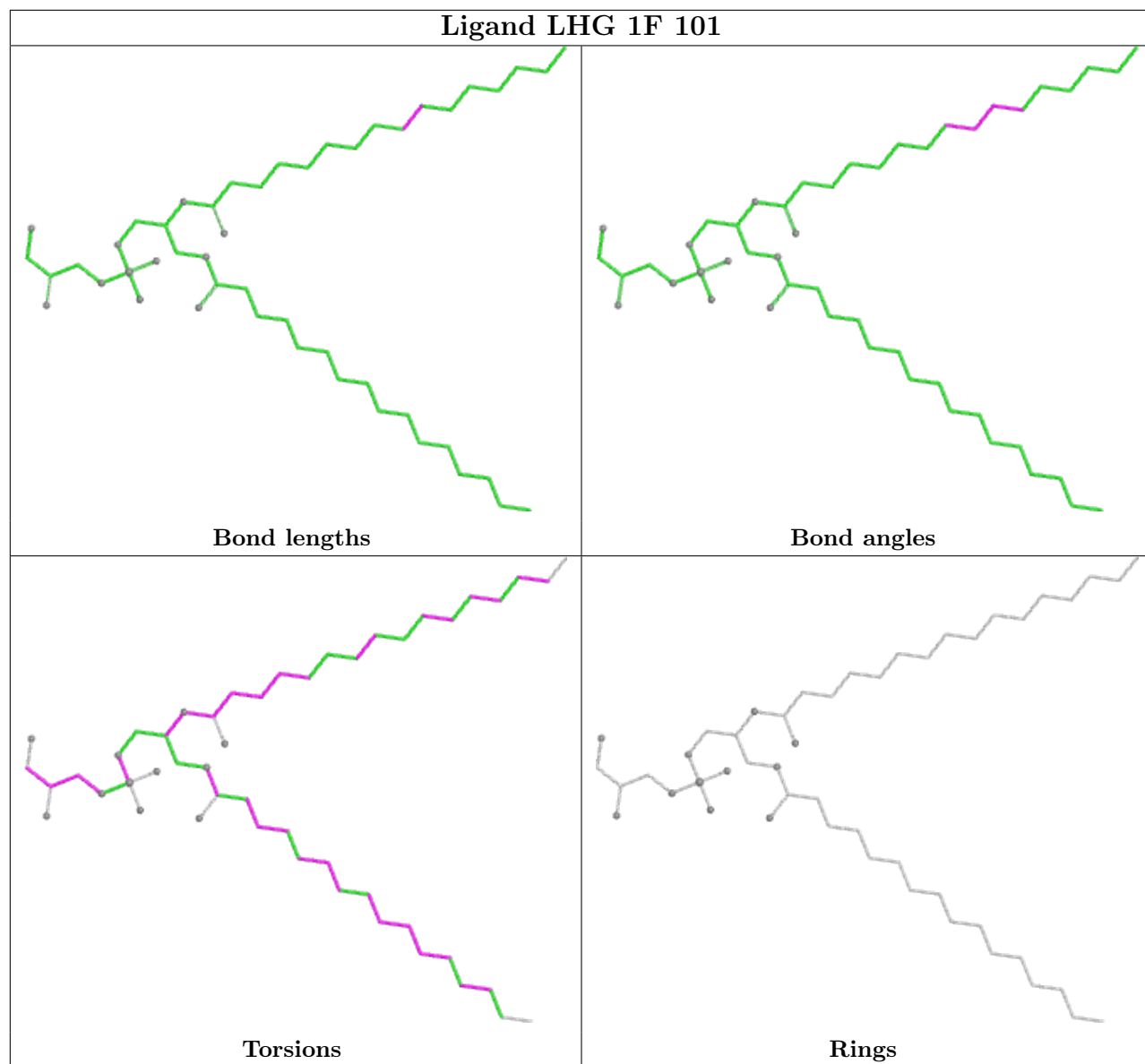


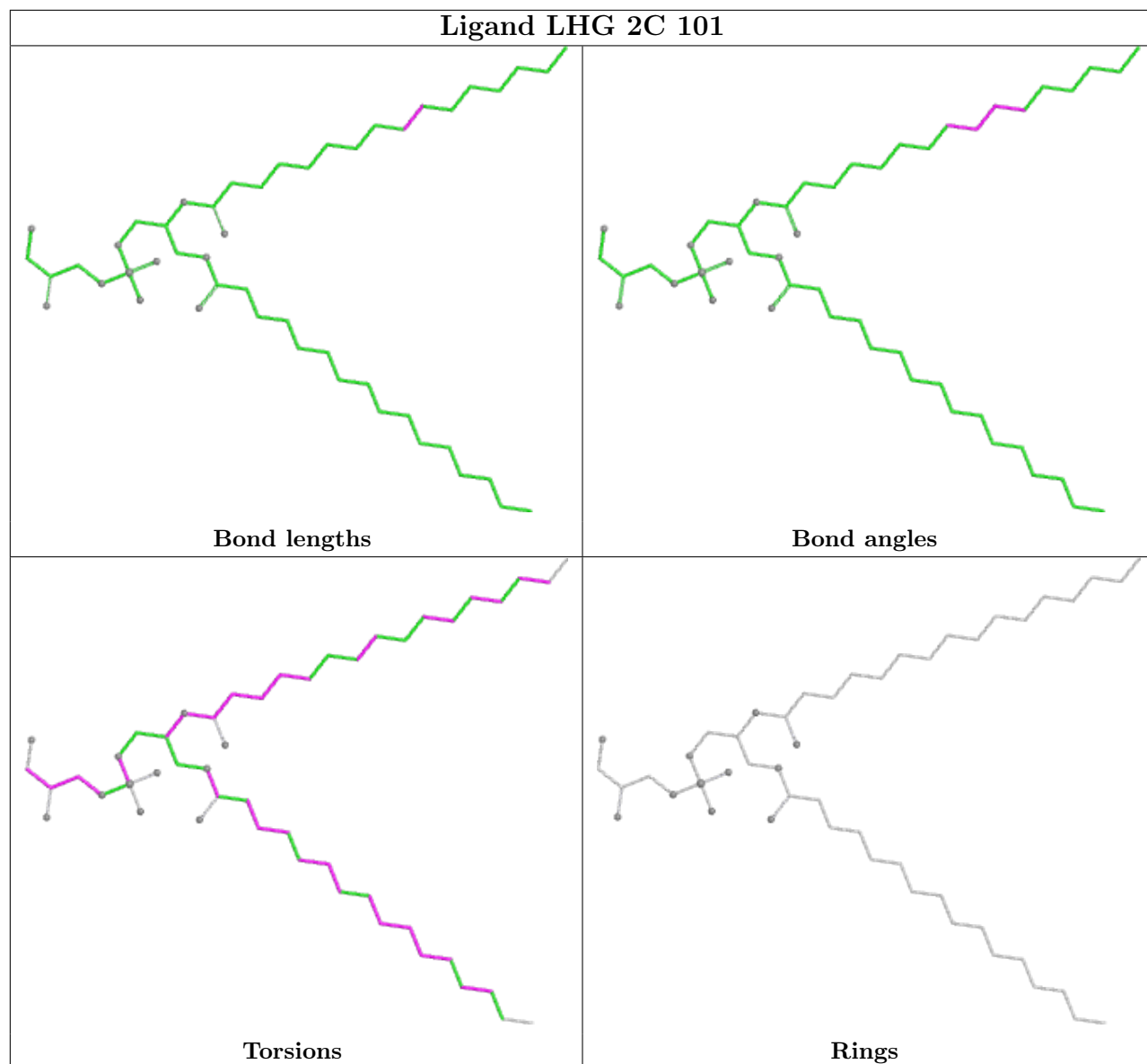


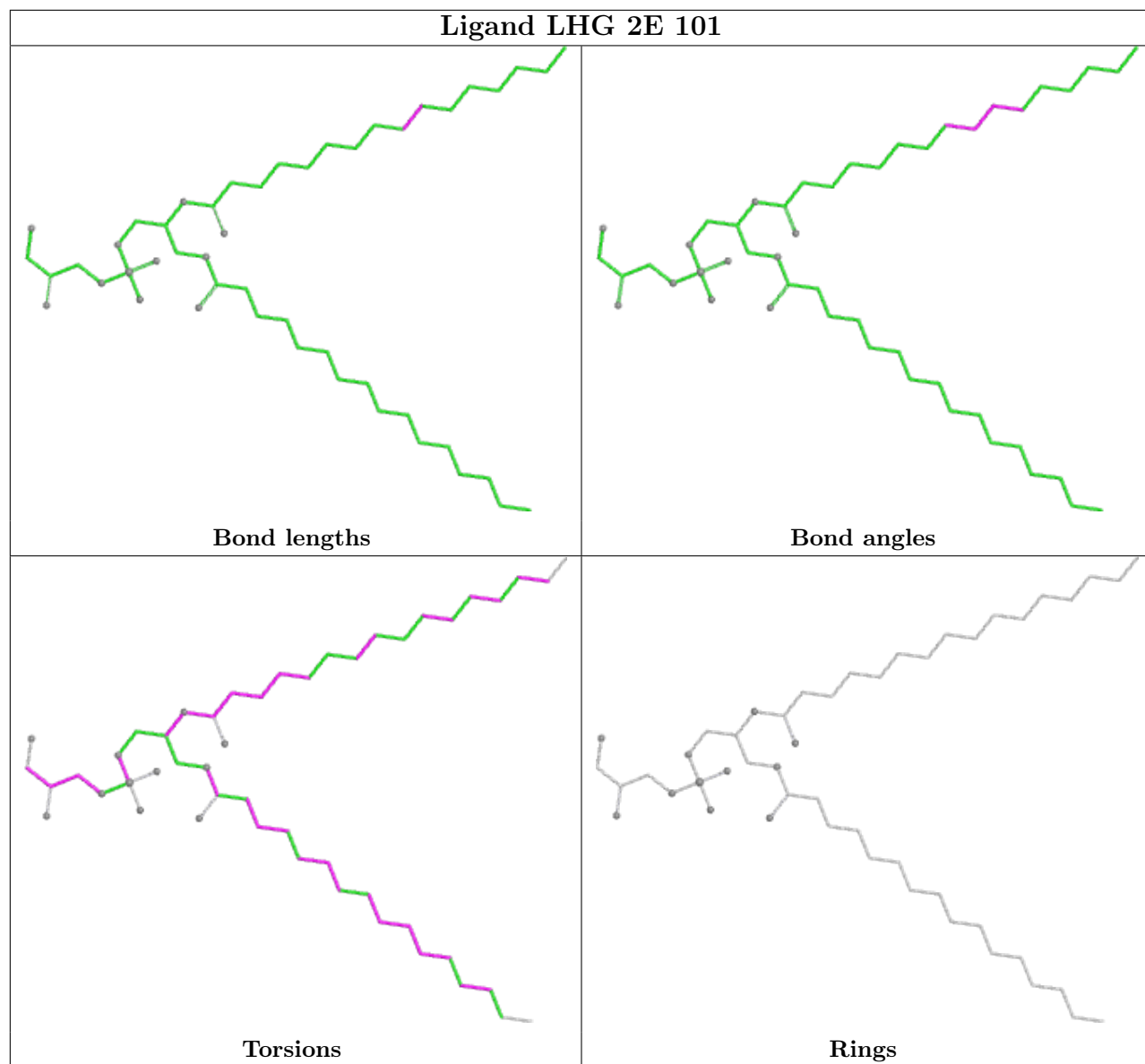


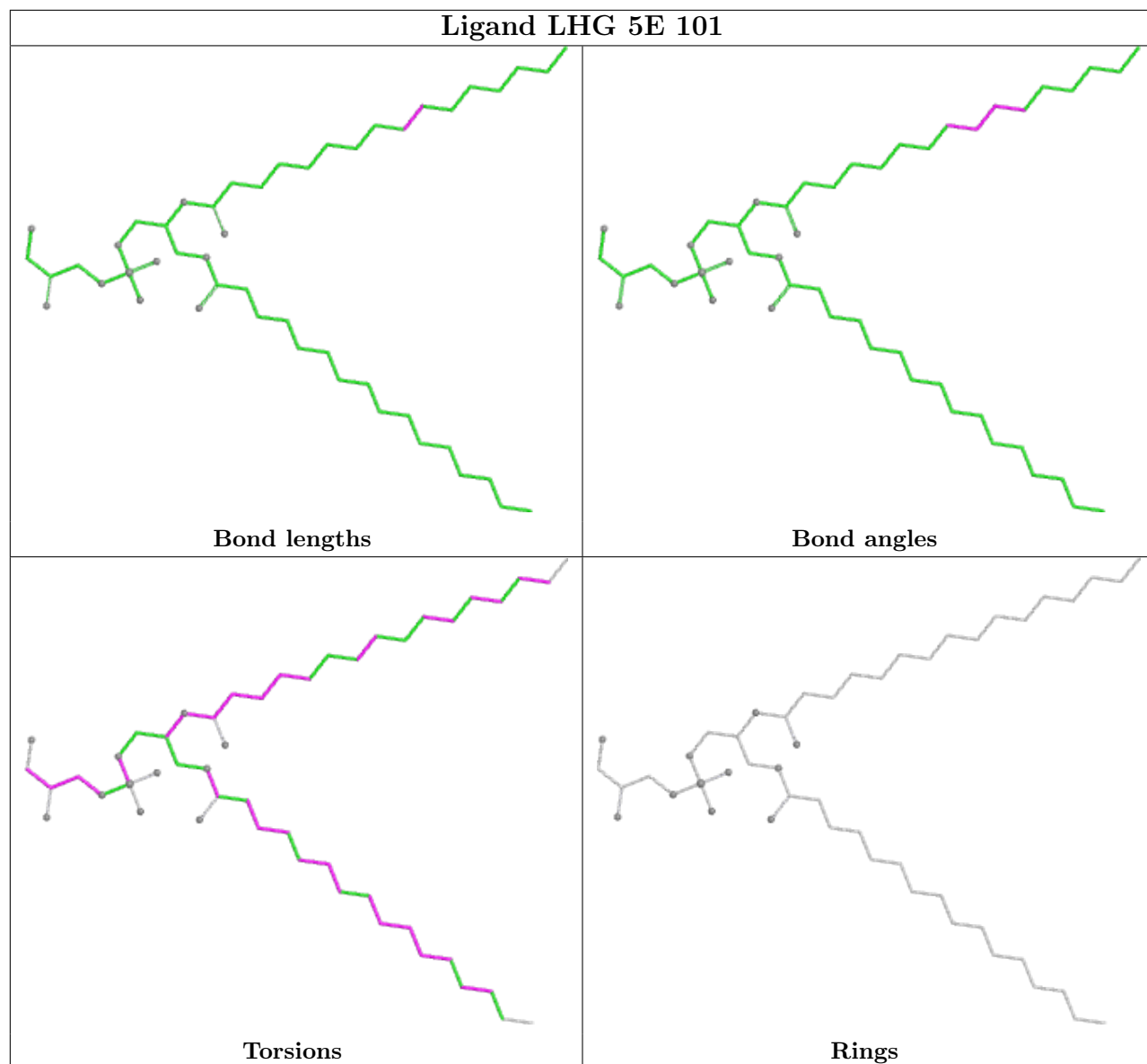


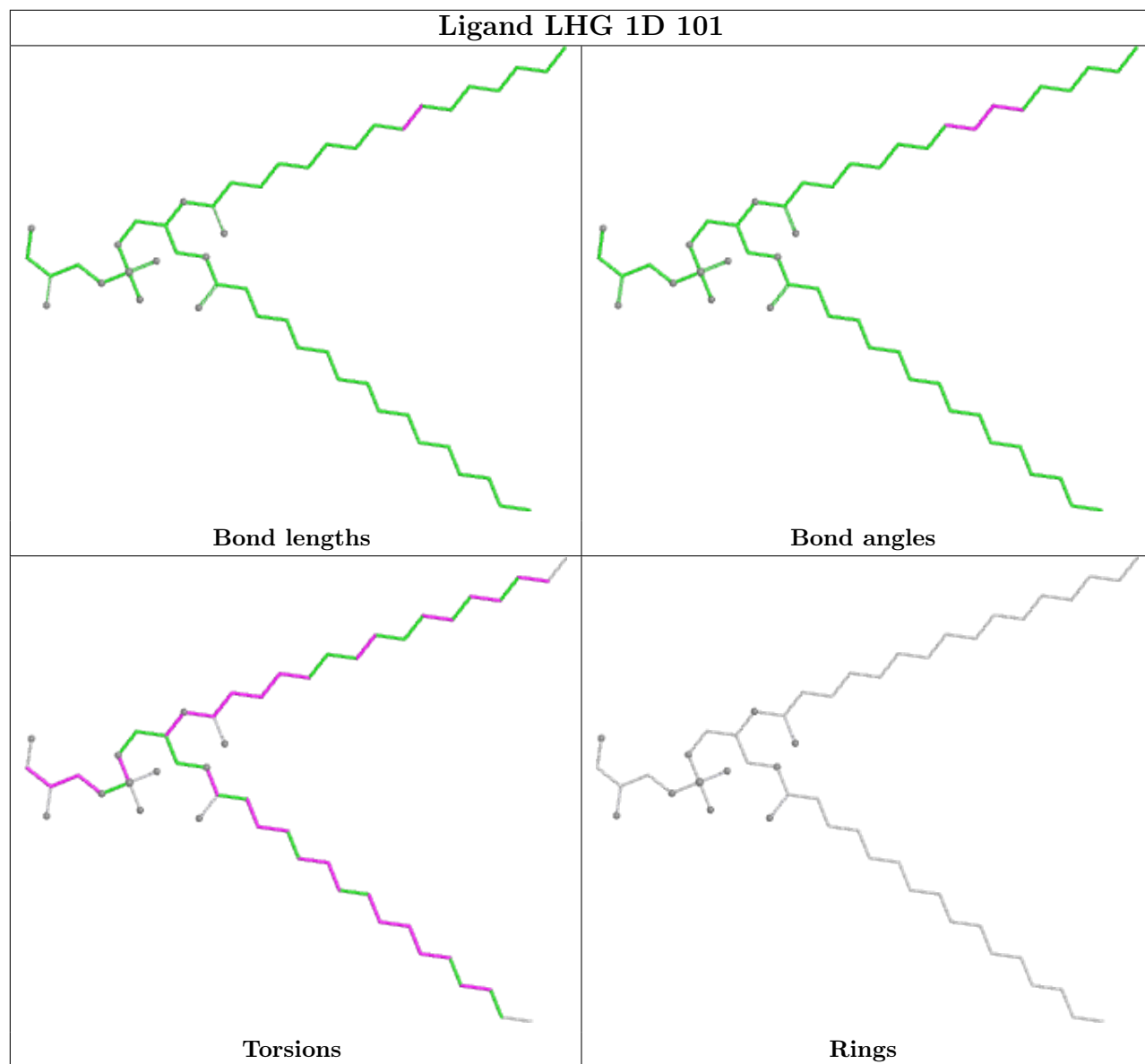


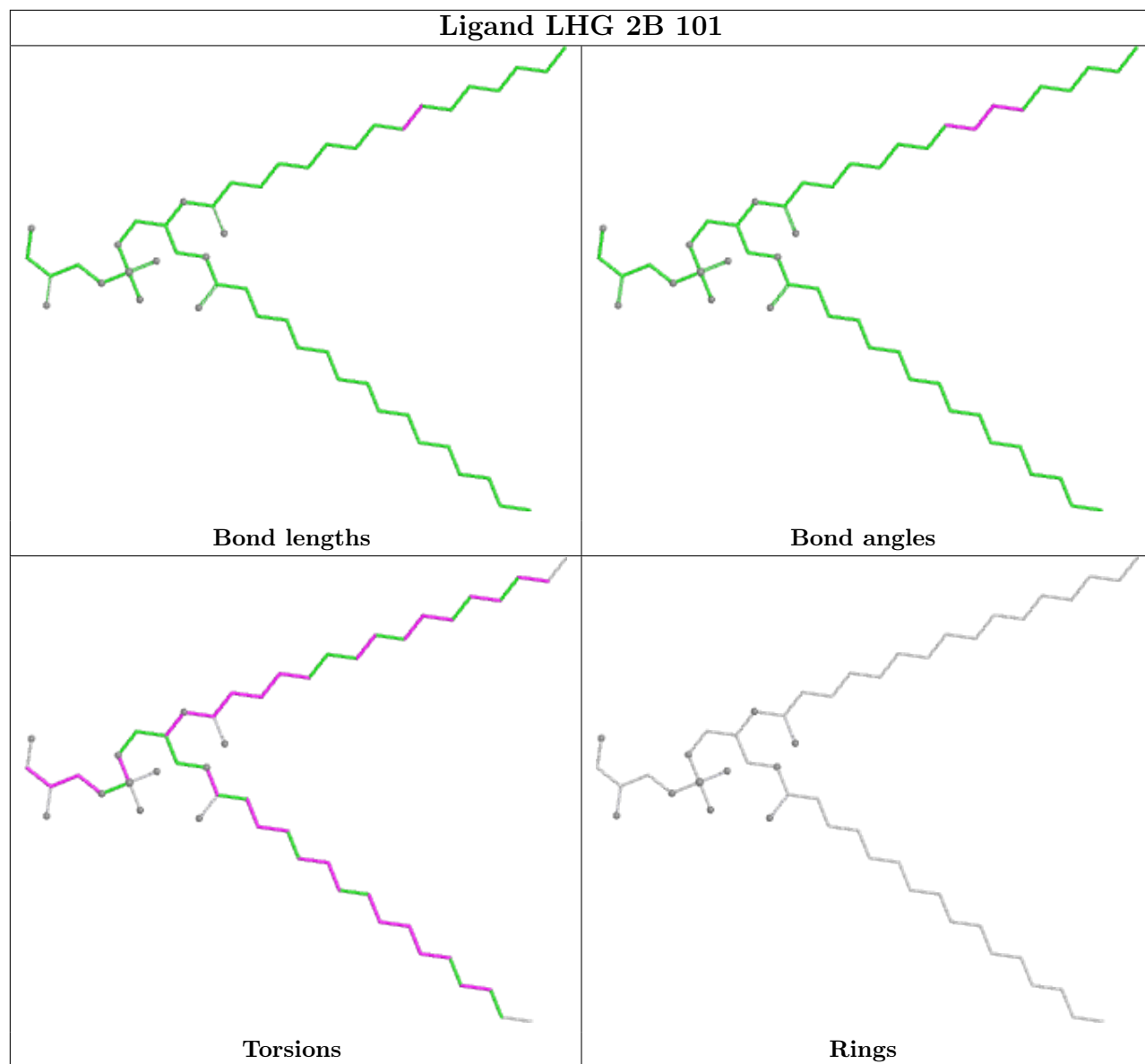


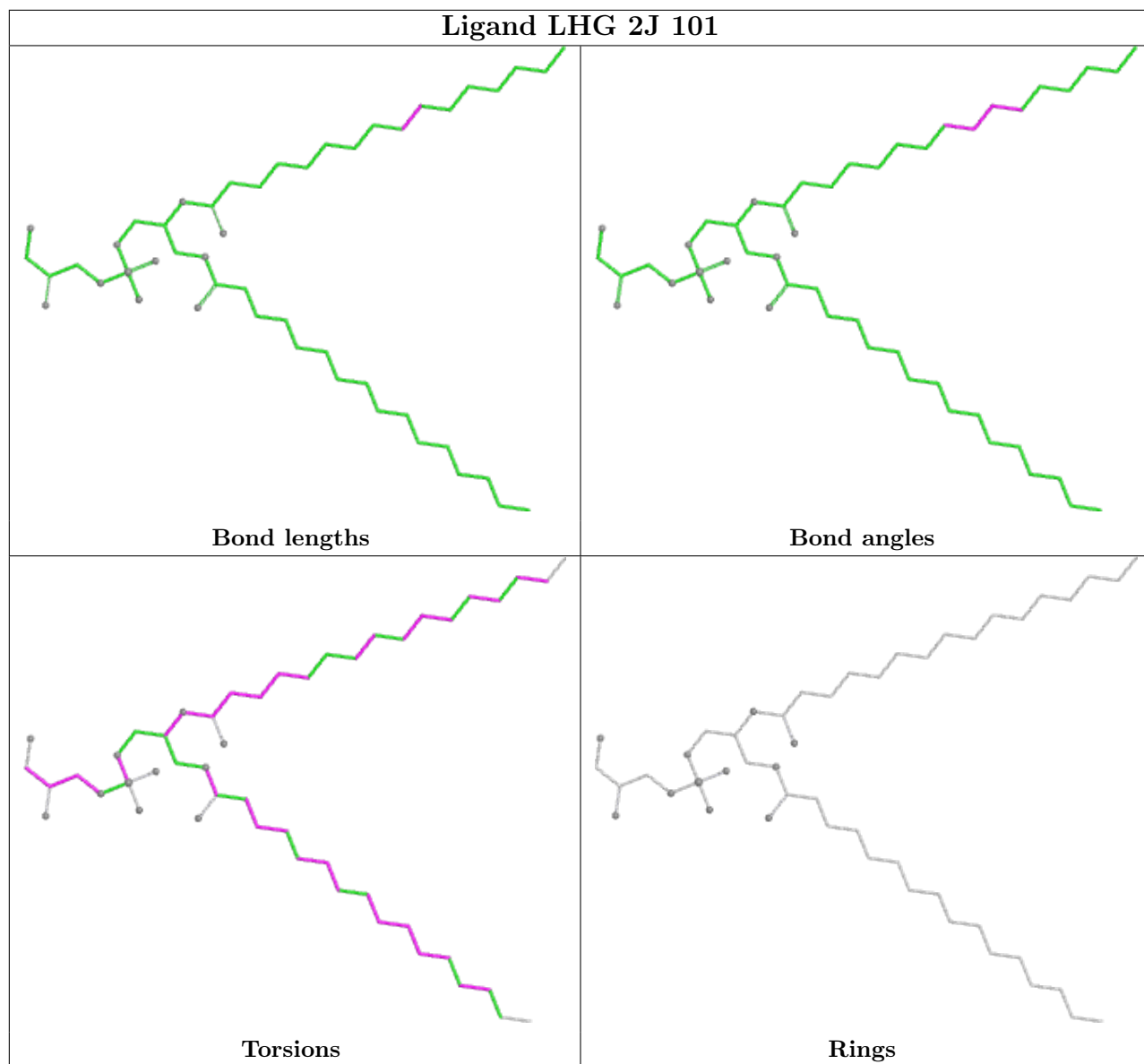


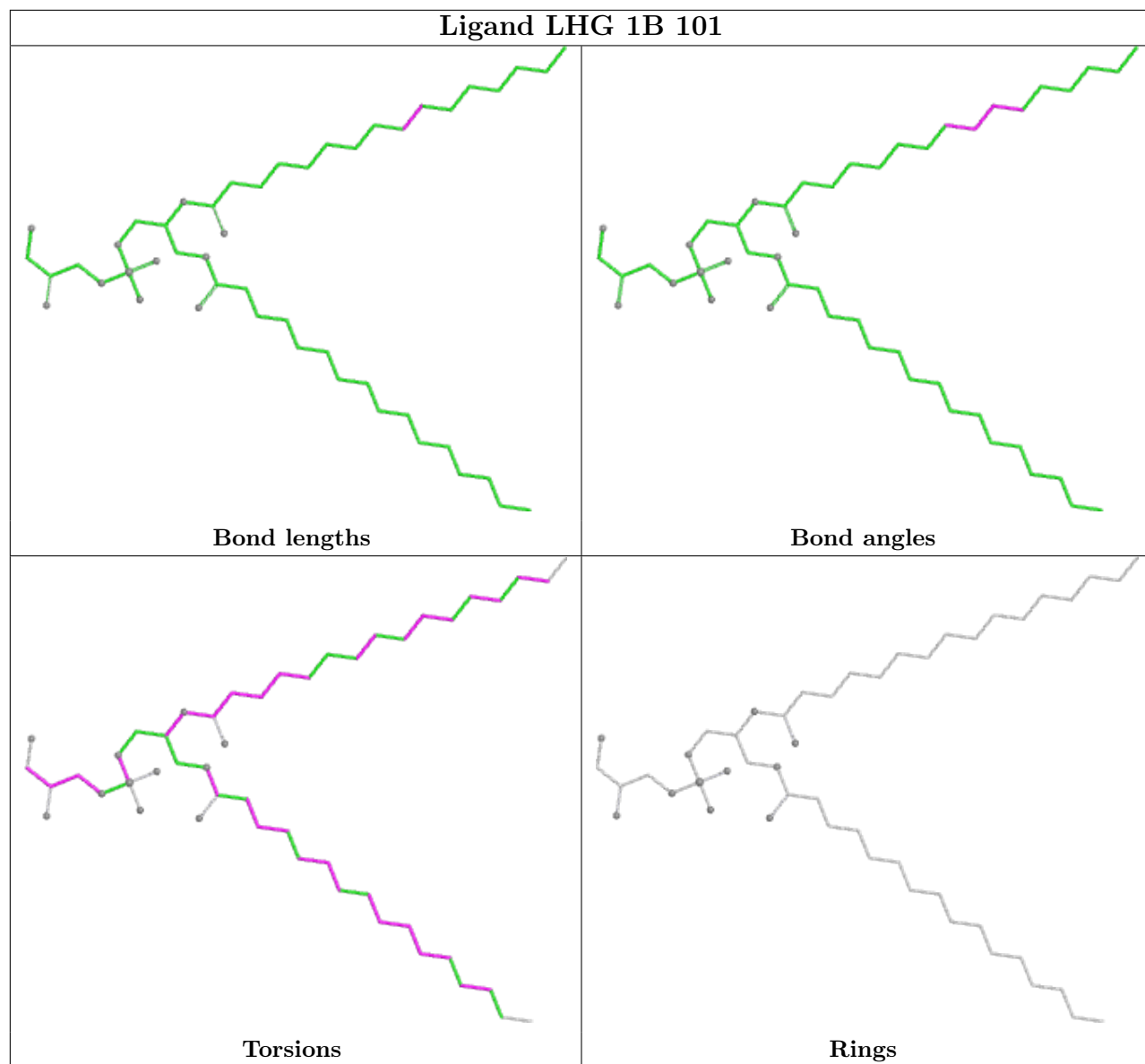


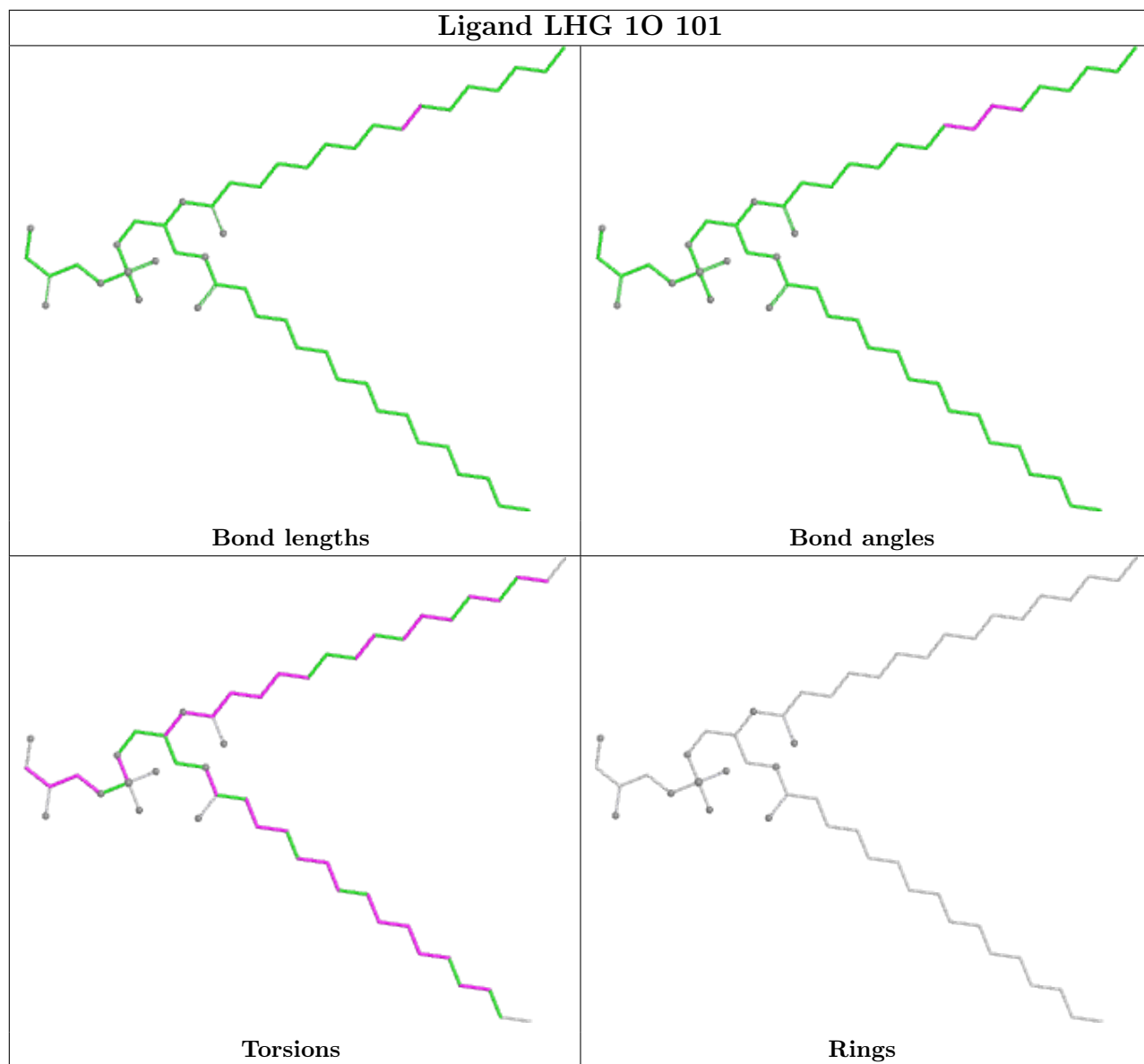


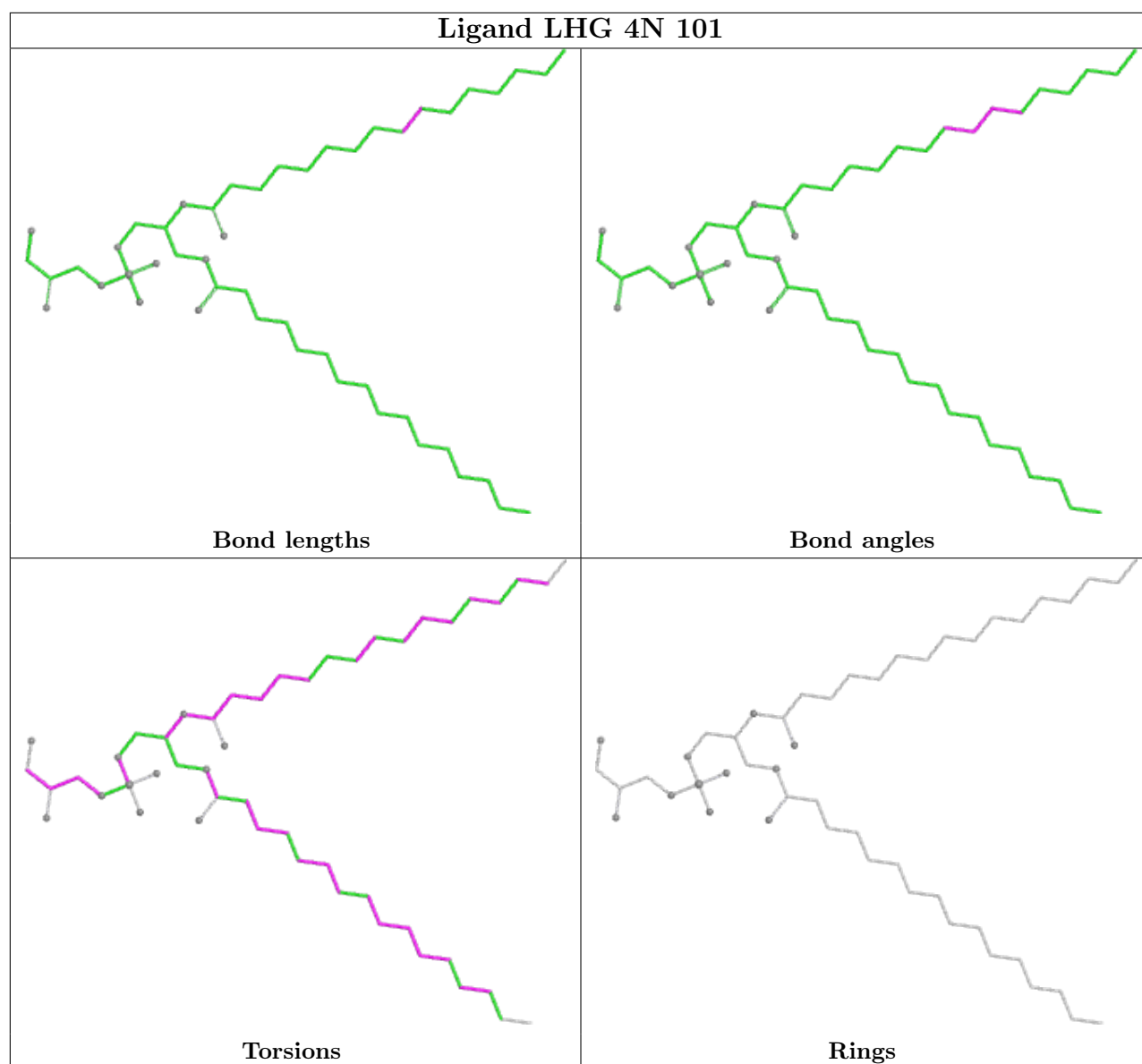












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

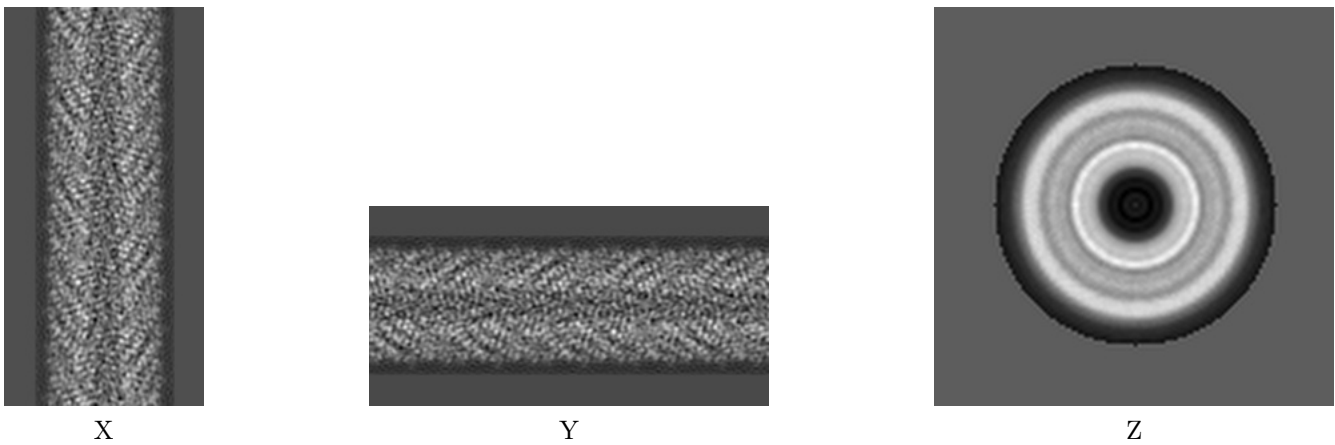
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4042. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

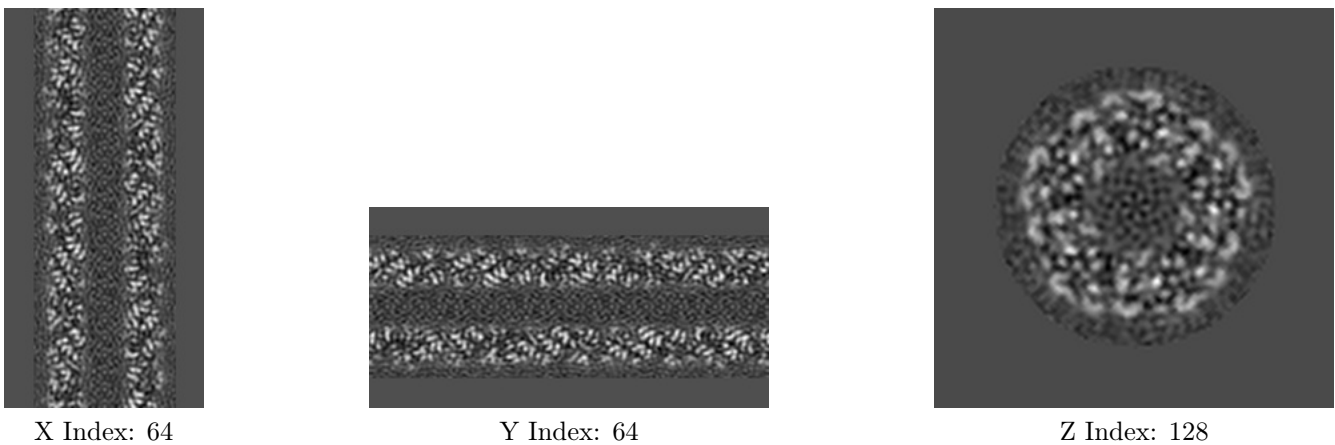
6.1.1 Primary map



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

6.2 Central slices [i](#)

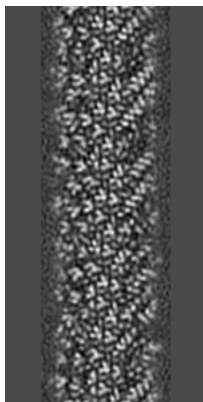
6.2.1 Primary map



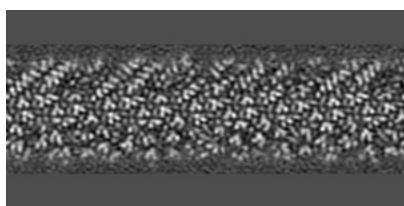
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

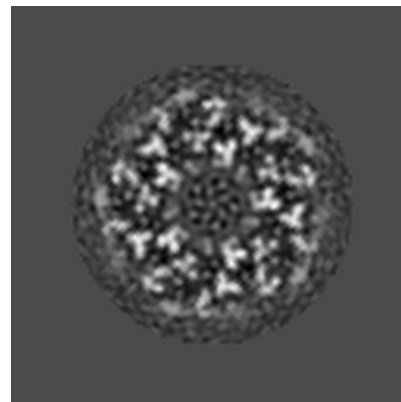
6.3.1 Primary map



X Index: 82



Y Index: 46

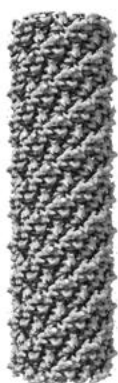


Z Index: 111

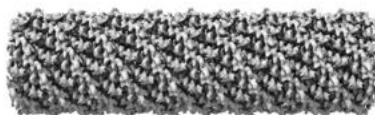
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

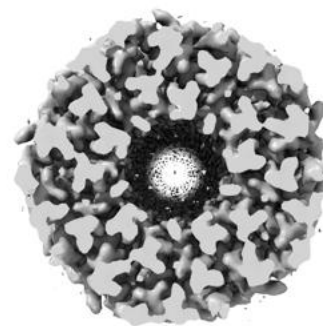
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

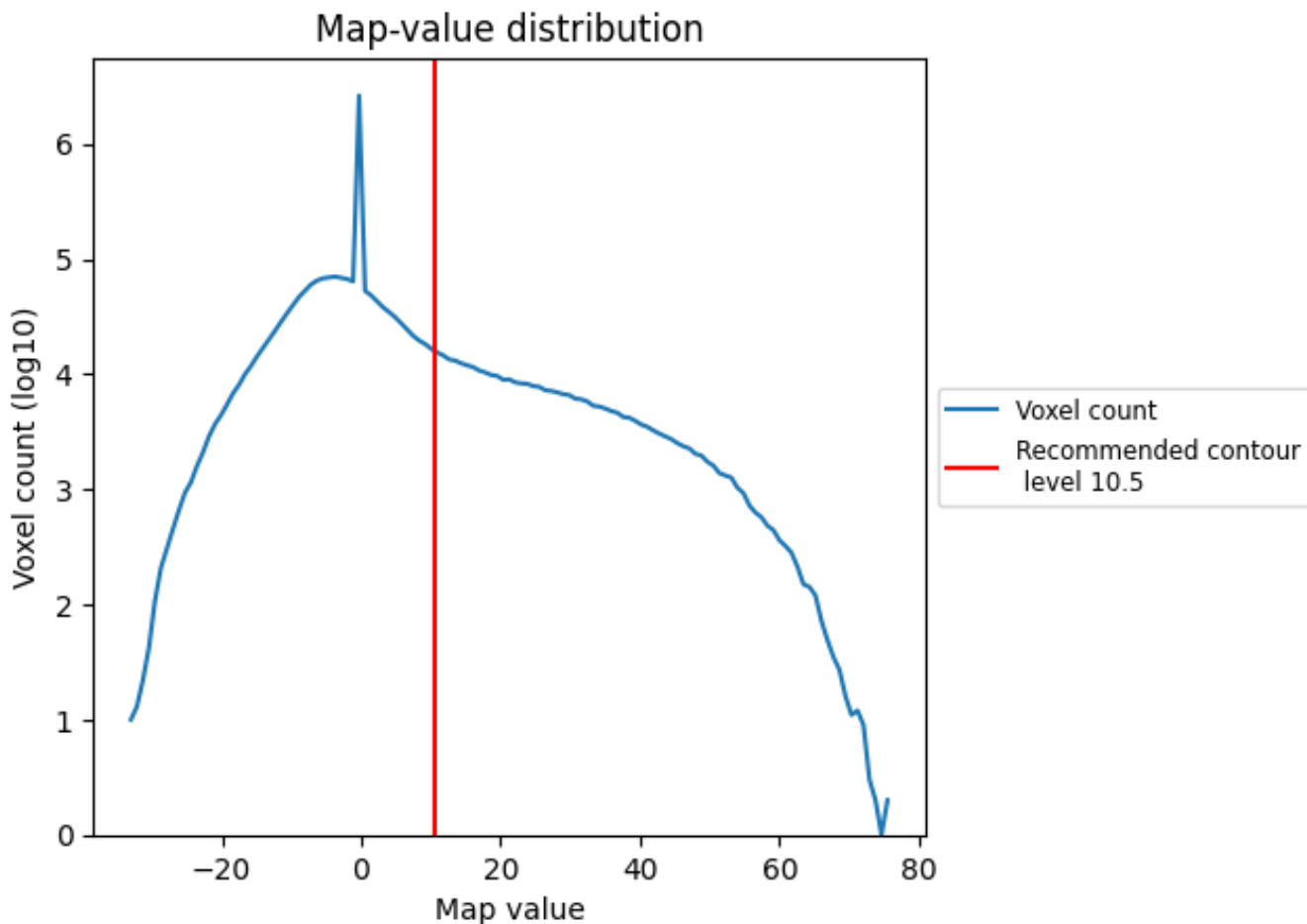
6.5 Mask visualisation

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

7 Map analysis [i](#)

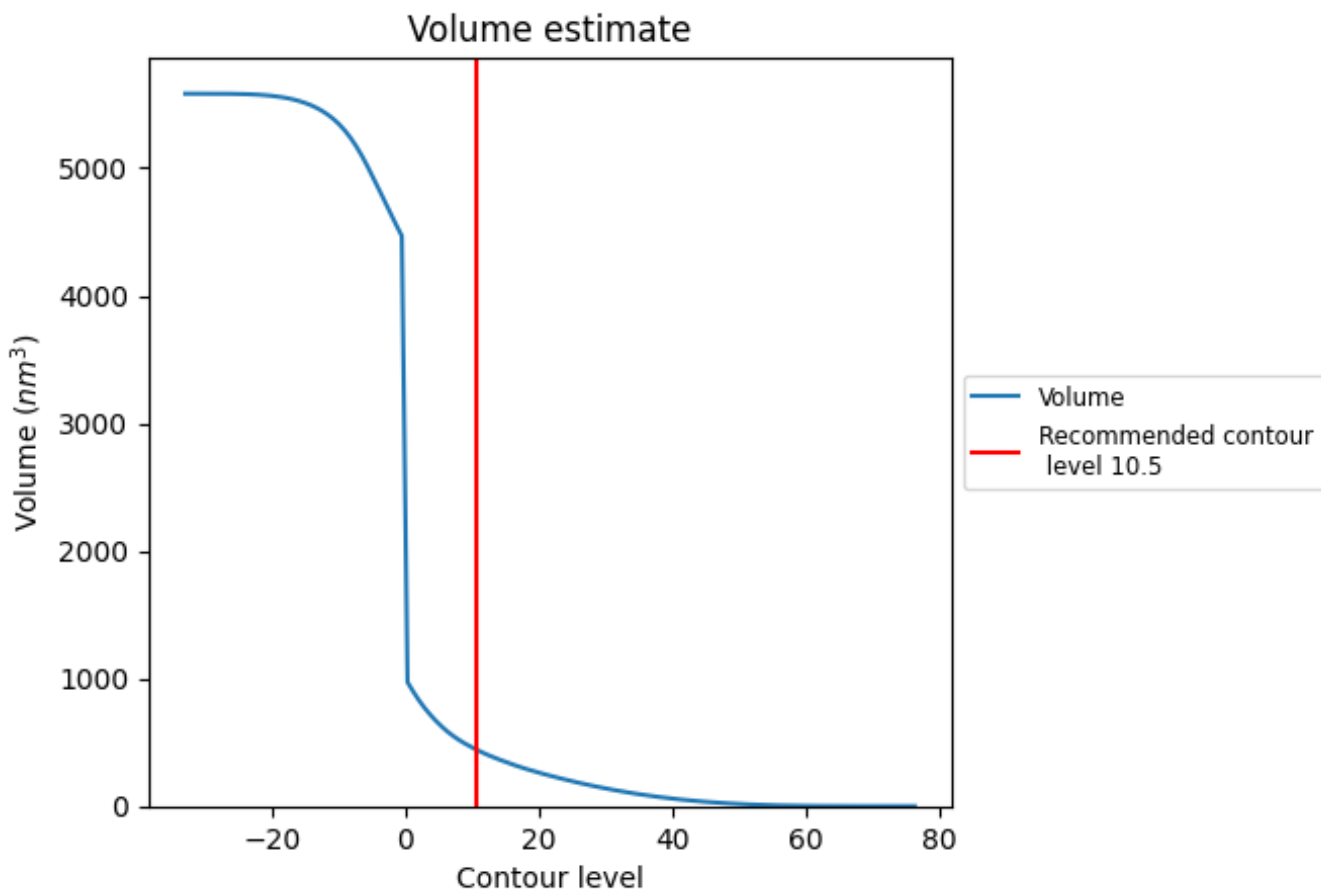
This section contains the results of statistical analysis of the map.

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 446 nm³; this corresponds to an approximate mass of 402 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 [\(i\)](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

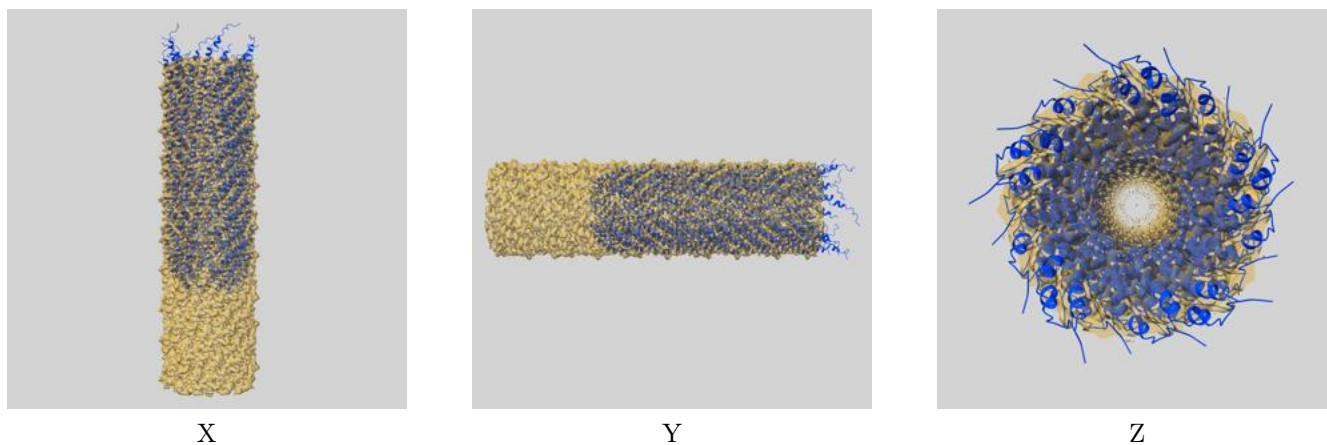
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

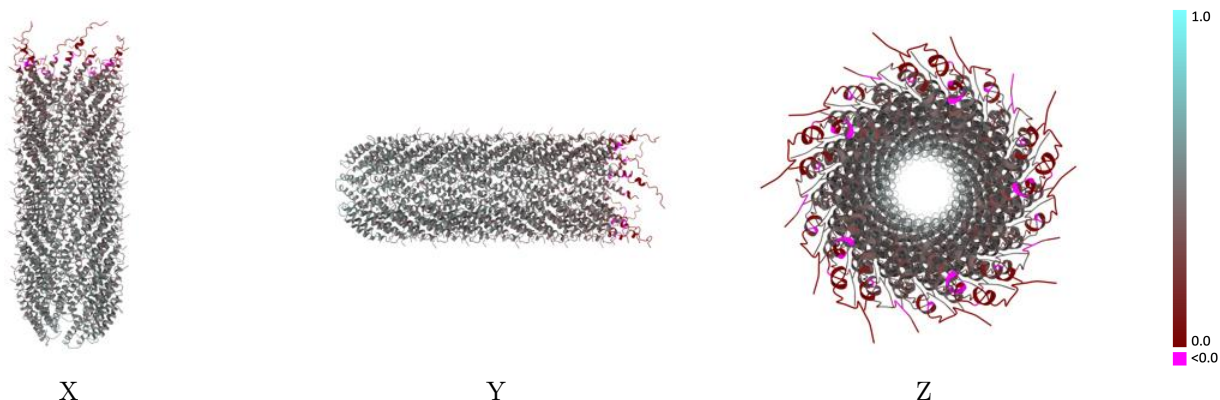
This section contains information regarding the fit between EMDB map EMD-4042 and PDB model 5LEG. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



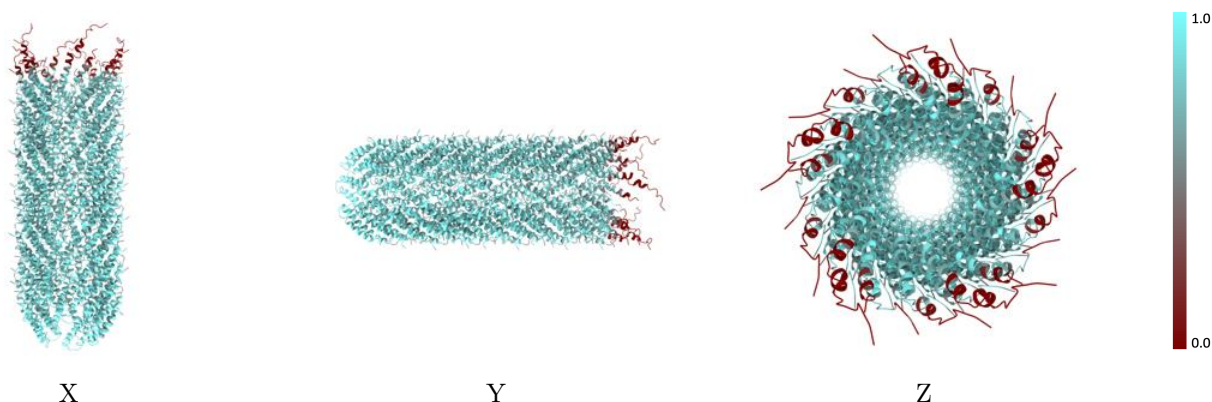
The images above show the 3D surface view of the map at the recommended contour level 10.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



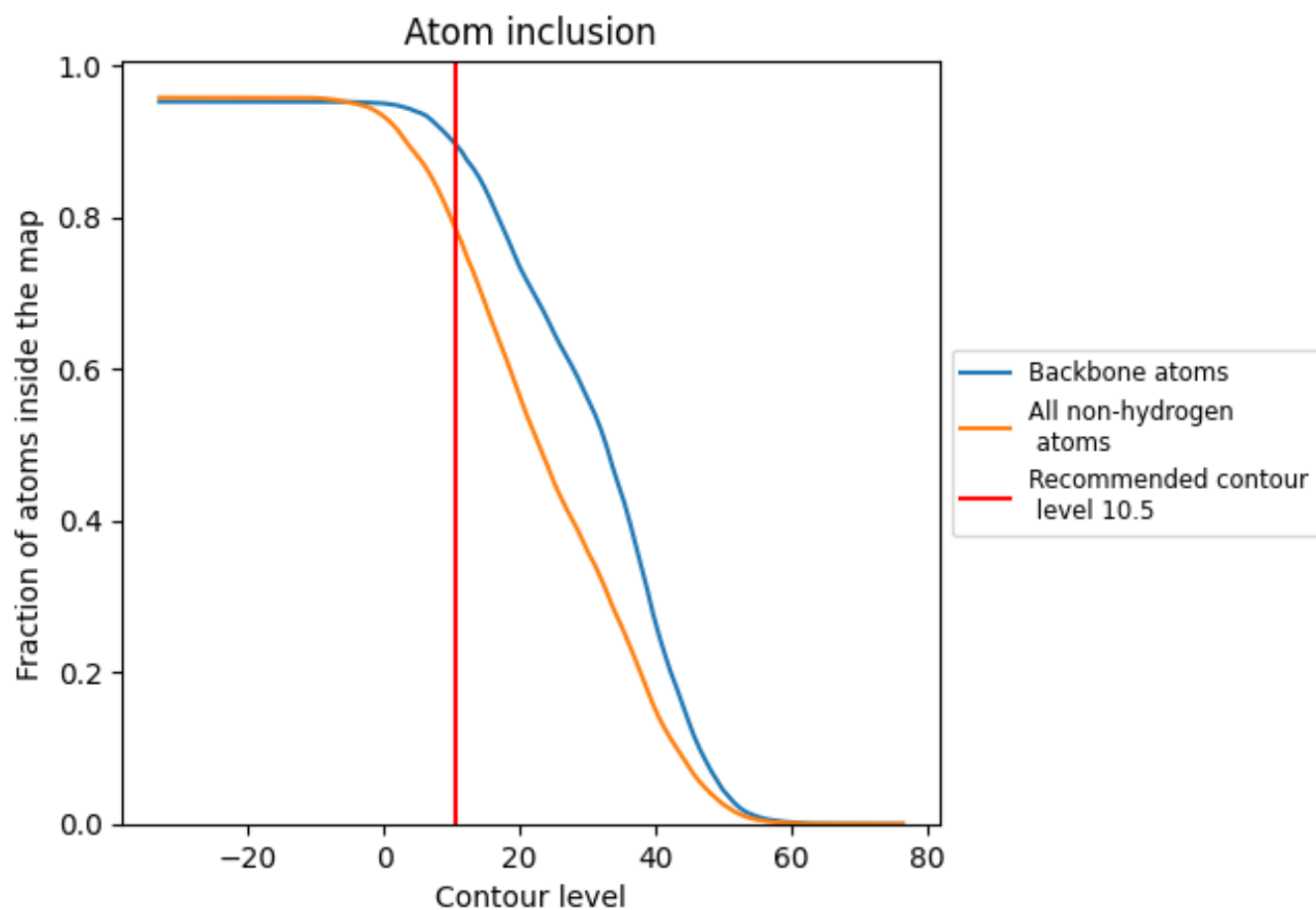
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (10.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.4390
1A	 0.8491	 0.4850
1B	 0.8375	 0.4850
1C	 0.8472	 0.4830
1D	 0.8433	 0.4870
1E	 0.8453	 0.4810
1F	 0.8433	 0.4810
1G	 0.8414	 0.4770
1H	 0.8279	 0.4730
1I	 0.8240	 0.4650
1J	 0.8182	 0.4520
1K	 0.8008	 0.4410
1L	 0.7892	 0.4290
1M	 0.7853	 0.4220
1N	 0.7195	 0.3880
1O	 0.6402	 0.3600
1P	 0.3953	 0.2170
2A	 0.8453	 0.4810
2B	 0.8491	 0.4830
2C	 0.8472	 0.4810
2D	 0.8414	 0.4780
2E	 0.8433	 0.4780
2F	 0.8530	 0.4800
2G	 0.8395	 0.4790
2H	 0.8337	 0.4710
2I	 0.8240	 0.4690
2J	 0.8240	 0.4580
2K	 0.8027	 0.4440
2L	 0.7911	 0.4260
2M	 0.7737	 0.4100
2N	 0.7157	 0.3820
2O	 0.6306	 0.3440
2P	 0.3868	 0.2040
3A	 0.8395	 0.4800
3B	 0.8511	 0.4790






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Chain	Atom inclusion	Q-score
3C	 0.8433	 0.4840
3D	 0.8491	 0.4790
3E	 0.8414	 0.4780
3F	 0.8472	 0.4780
3G	 0.8453	 0.4770
3H	 0.8375	 0.4700
3I	 0.8317	 0.4700
3J	 0.8317	 0.4640
3K	 0.8085	 0.4470
3L	 0.7969	 0.4320
3M	 0.7969	 0.4210
3N	 0.7369	 0.3880
3O	 0.6364	 0.3460
3P	 0.3910	 0.2090
4A	 0.8491	 0.4830
4B	 0.8375	 0.4810
4C	 0.8433	 0.4810
4D	 0.8472	 0.4770
4E	 0.8375	 0.4790
4F	 0.8337	 0.4760
4G	 0.8279	 0.4730
4H	 0.8375	 0.4730
4I	 0.8317	 0.4650
4J	 0.8143	 0.4560
4K	 0.8143	 0.4480
4L	 0.8008	 0.4420
4M	 0.7950	 0.4290
4N	 0.7331	 0.3930
4O	 0.6383	 0.3570
4P	 0.3932	 0.2160
5A	 0.8395	 0.4800
5B	 0.8472	 0.4840
5C	 0.8491	 0.4830
5D	 0.8414	 0.4770
5E	 0.8375	 0.4780
5F	 0.8317	 0.4750
5G	 0.8453	 0.4690
5H	 0.8279	 0.4690
5I	 0.8162	 0.4560
5J	 0.8066	 0.4500
5K	 0.8085	 0.4380
5L	 0.7911	 0.4290

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Chain	Atom inclusion	Q-score
5M	 0.7853	 0.4190
5N	 0.7253	 0.3890
5O	 0.6364	 0.3560
5P	 0.3953	 0.2150