



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 23, 2026 – 07:36 PM UTC

PDB ID : 6CM1 / pdb_00006cm1
BMRB ID : 30426
Title : MT1-MMP HPX Domain with Blade 2 Loop Bound to Nanodiscs
Authors : Marcink, T.C.; Van Doren, S.R.
Deposited on : 2018-03-02

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

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

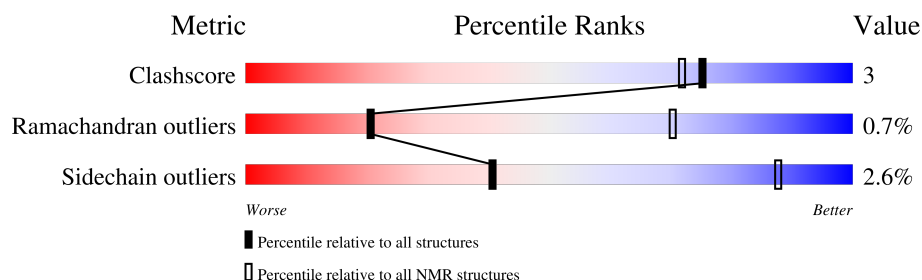
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 4%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	196	40% 59% .
2	B	211	33% 66% .
2	C	211	31% 67% .

2 Ensemble composition and analysis

This entry contains 15 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:316-A:511, B:55-B:265, C:55-C:262 (615)	1.54	10

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 8
2	9, 10, 11, 12
3	1, 2, 3, 4
4	13, 14, 15

3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35924 atoms, of which 20751 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix metalloproteinase-14.

Mol	Chain	Residues	Atoms						Trace
1	A	196	Total	C	H	N	O	S	0
			3202	1067	1565	277	284	9	

- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
2	B	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	
2	C	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	

There are 44 discrepancies between the modelled and reference sequences:

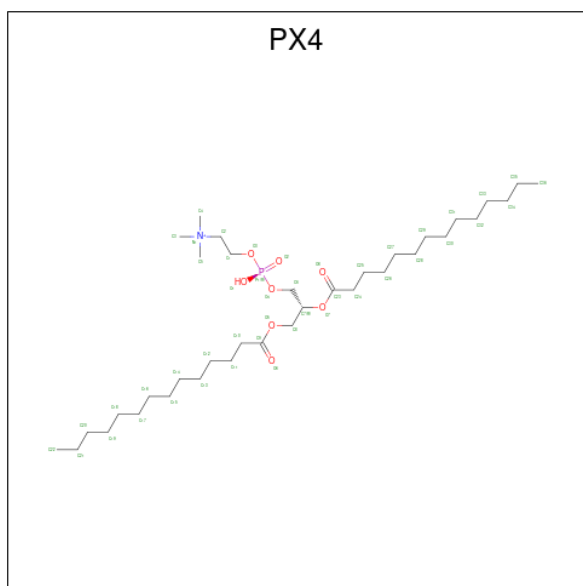
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PRO	-	insertion	UNP P02647
B	100	TYR	-	insertion	UNP P02647
B	101	LEU	-	insertion	UNP P02647
B	102	ASP	-	insertion	UNP P02647
B	103	ASP	-	insertion	UNP P02647
B	104	PHE	-	insertion	UNP P02647
B	105	GLN	-	insertion	UNP P02647
B	106	LYS	-	insertion	UNP P02647
B	107	LYS	-	insertion	UNP P02647
B	108	TRP	-	insertion	UNP P02647
B	109	GLN	-	insertion	UNP P02647
B	110	GLU	-	insertion	UNP P02647
B	111	GLU	-	insertion	UNP P02647
B	112	MET	-	insertion	UNP P02647
B	113	GLU	-	insertion	UNP P02647
B	114	LEU	-	insertion	UNP P02647
B	115	TYR	-	insertion	UNP P02647
B	116	ARG	-	insertion	UNP P02647
B	117	GLN	-	insertion	UNP P02647
B	118	LYS	-	insertion	UNP P02647
B	119	VAL	-	insertion	UNP P02647
B	120	GLU	-	insertion	UNP P02647
C	99	PRO	-	insertion	UNP P02647

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	TYR	-	insertion	UNP P02647
C	101	LEU	-	insertion	UNP P02647
C	102	ASP	-	insertion	UNP P02647
C	103	ASP	-	insertion	UNP P02647
C	104	PHE	-	insertion	UNP P02647
C	105	GLN	-	insertion	UNP P02647
C	106	LYS	-	insertion	UNP P02647
C	107	LYS	-	insertion	UNP P02647
C	108	TRP	-	insertion	UNP P02647
C	109	GLN	-	insertion	UNP P02647
C	110	GLU	-	insertion	UNP P02647
C	111	GLU	-	insertion	UNP P02647
C	112	MET	-	insertion	UNP P02647
C	113	GLU	-	insertion	UNP P02647
C	114	LEU	-	insertion	UNP P02647
C	115	TYR	-	insertion	UNP P02647
C	116	ARG	-	insertion	UNP P02647
C	117	GLN	-	insertion	UNP P02647
C	118	LYS	-	insertion	UNP P02647
C	119	VAL	-	insertion	UNP P02647
C	120	GLU	-	insertion	UNP P02647

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: C₃₆H₇₃NO₈P).



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Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	A	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1
3	B	1	118	36	72	1	8	1

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Mol	Chain	Residues	Atoms					
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Na
			1	1

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	
5	A	1	Total	Cl
			1	1

4 Residue-property plots

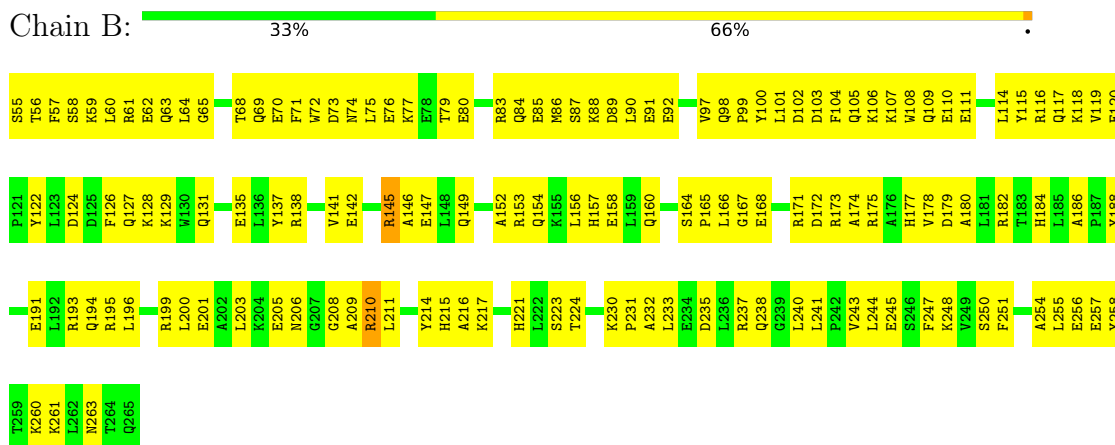
4.1 Average score per residue in the NMR ensemble

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

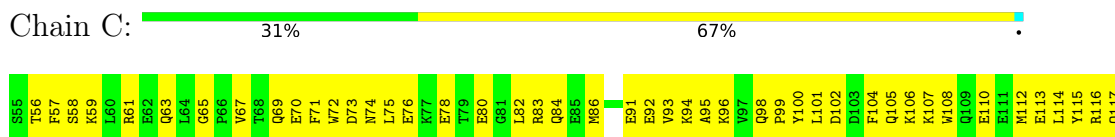
• Molecule 1: Matrix metalloproteinase-14

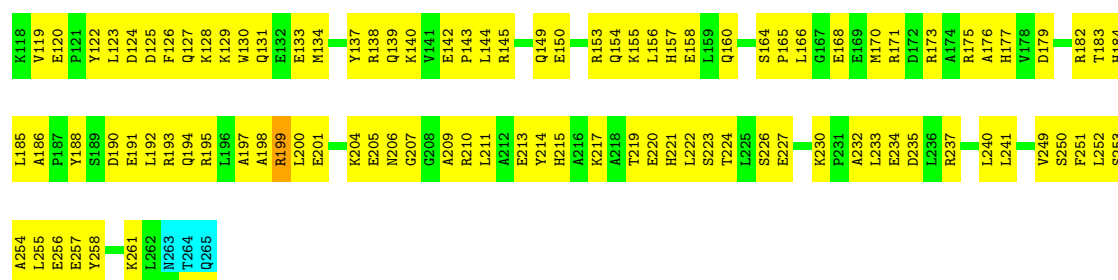


• Molecule 2: Apolipoprotein A-I



• Molecule 2: Apolipoprotein A-I



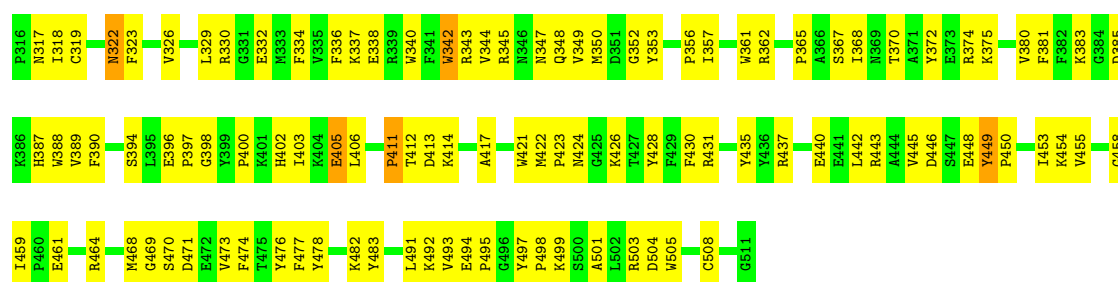


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

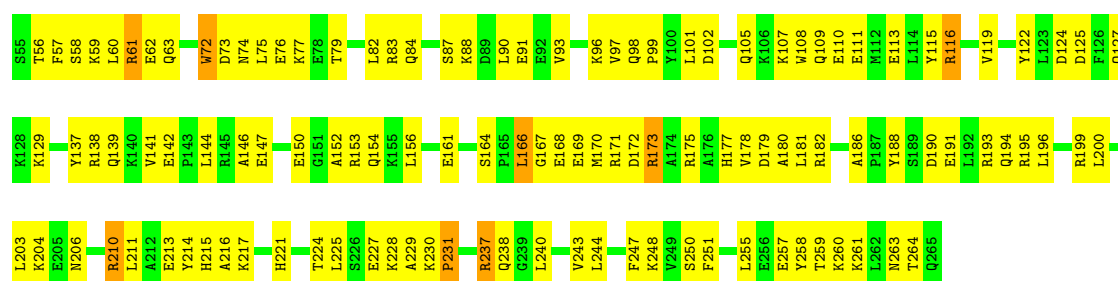
- Molecule 1: Matrix metalloproteinase-14

Chain A: 46% 52% .



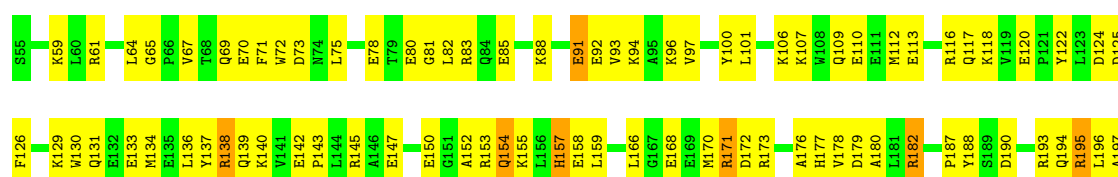
- Molecule 2: Apolipoprotein A-I

Chain B: 44% 53% .



- Molecule 2: Apolipoprotein A-I

Chain C: 45% 48% 5% .



A198	R199	L200	L203	N206	R210	L211	A212	E213	Y214	H215	A216	K217	A218	T219	E220	H221	L222	S226	K230	P231	A232	G239	L240	L241	P242	E245	S246	F247	K248	Y249	S250	F251	L252	E257	Y258	T259	K260	K261	L262	N263	T264	Q265
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 15 calculated structures, 15 were deposited, based on the following criterion: *all calculated structures submitted*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	structure calculation	HADDOCK2.1
NAMD	refinement	NAMD2.1 with CUDA GPU processing
NAMD	structure calculation	NAMD2.1 with CUDA GPU processing

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, PX4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.09±0.05	44±7/1696 (2.6± 0.4%)	2.38±0.04	102±10/2286 (4.4± 0.4%)
2	B	2.18±0.04	55±8/1784 (3.1± 0.4%)	2.63±0.05	155±12/2394 (6.5± 0.5%)
2	C	2.17±0.04	53±8/1760 (3.0± 0.5%)	2.63±0.04	150±10/2364 (6.4± 0.4%)
All	All	2.15	2290/78600 (2.9%)	2.55	6114/105660 (5.8%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	8.9±2.3
2	B	0.0±0.0	5.9±1.6
2	C	0.0±0.0	7.5±1.6
All	All	0	335

5 of 1555 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	152	ALA	N-CA	-11.49	1.32	1.46	12	3
2	B	172	ASP	CA-C	-10.13	1.42	1.53	12	1
2	C	95	ALA	N-CA	-10.01	1.34	1.46	15	1
1	A	477	PHE	CA-C	-10.00	1.39	1.52	15	2
2	C	221	HIS	ND1-CE1	9.78	1.42	1.32	14	4

5 of 2961 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	65	GLY	O-C-N	-21.37	113.38	121.07	15	5
1	A	503	ARG	NE-CZ-NH2	16.84	134.36	119.20	6	10
2	B	210	ARG	NE-CZ-NH2	15.39	133.06	119.20	11	9
2	B	153	ARG	NE-CZ-NH2	15.34	133.01	119.20	1	6
2	B	173	ARG	NE-CZ-NH2	15.17	132.85	119.20	12	8

There are no chirality outliers.

5 of 108 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	C	199	ARG	Sidechain	11
1	A	478	TYR	Sidechain	9
2	B	188	TYR	Sidechain	9
1	A	449	TYR	Sidechain	8
1	A	428	TYR	Sidechain	8

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1637	1565	1562	4±2
2	B	1753	1745	1742	4±2
2	C	1728	1724	1721	2±2
3	A	2484	3888	3888	35±5
3	B	4600	7200	7200	53±8
3	C	2944	4608	4608	29±5
All	All	227220	310950	310821	1651

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 3.

5 of 1237 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:402:HIS:CE1	3:A:649:PX4:H12	0.90	2.00	7	5
3:B:338:PX4:H4	3:B:343:PX4:O3	0.74	1.82	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:358:PX4:H9	3:C:361:PX4:O3	0.72	1.85	6	1
3:B:326:PX4:O3	3:B:355:PX4:H3	0.71	1.84	5	3
3:C:351:PX4:O4	3:C:351:PX4:H4	0.70	1.86	13	2

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/196 (99%)	176±3 (91±1%)	15±3 (8±1%)	3±1 (2±1%)	10	55
2	B	209/211 (99%)	205±2 (98±1%)	4±2 (2±1%)	0±0 (0±0%)	44	80
2	C	207/211 (98%)	202±2 (98±1%)	4±2 (2±1%)	1±1 (0±0%)	37	78
All	All	9150/9270 (99%)	8751 (96%)	338 (4%)	61 (1%)	20	70

5 of 34 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	448	GLU	5
1	A	367	SER	4
1	A	411	PRO	4
1	A	510	SER	3
2	C	65	GLY	3

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/169 (100%)	164±2 (97±1%)	5±2 (3±1%)	35	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	187/187 (100%)	182±1 (98±1%)	5±1 (2±1%)	42 88
2	C	184/187 (98%)	180±1 (98±1%)	4±1 (2±1%)	46 90
All	All	8100/8145 (99%)	7892 (97%)	208 (3%)	41 88

5 of 101 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	210	ARG	15
1	A	492	LYS	14
2	B	145	ARG	12
1	A	325	THR	8
1	A	368	ILE	8

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 220 ligands modelled in this entry, 2 are monoatomic - leaving 218 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	608	-	45,45,45	1.04±0.08	3±2 (6±3%)
3	PX4	A	631	-	45,45,45	1.11±0.12	3±2 (7±3%)
3	PX4	C	318	-	45,45,45	1.07±0.14	3±1 (5±2%)
3	PX4	B	351	-	45,45,45	1.07±0.14	3±2 (5±3%)
3	PX4	B	325	-	45,45,45	1.05±0.08	2±2 (5±3%)
3	PX4	C	362	-	45,45,45	1.09±0.13	3±2 (6±3%)
3	PX4	C	331	-	45,45,45	1.03±0.11	2±1 (5±2%)
3	PX4	C	350	-	45,45,45	1.09±0.11	3±1 (6±2%)
3	PX4	A	640	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	C	357	-	45,45,45	1.04±0.13	2±1 (5±2%)
3	PX4	A	620	-	45,45,45	1.04±0.10	3±1 (5±2%)
3	PX4	B	395	-	45,45,45	1.04±0.11	2±1 (4±2%)
3	PX4	C	335	-	45,45,45	1.14±0.12	3±1 (6±3%)
3	PX4	C	308	-	45,45,45	1.11±0.11	4±2 (8±3%)
3	PX4	C	338	-	45,45,45	1.03±0.11	3±2 (6±4%)
3	PX4	C	351	-	45,45,45	1.06±0.09	3±1 (6±2%)
3	PX4	A	606	-	45,45,45	1.10±0.10	4±2 (8±3%)
3	PX4	B	369	-	45,45,45	1.06±0.14	3±2 (6±4%)
3	PX4	A	637	-	45,45,45	1.06±0.10	3±2 (6±3%)
3	PX4	B	310	-	45,45,45	1.10±0.16	3±1 (6±3%)
3	PX4	B	363	-	45,45,45	1.04±0.11	2±1 (5±2%)
3	PX4	C	319	-	45,45,45	1.04±0.10	3±1 (5±2%)
3	PX4	B	330	-	45,45,45	1.09±0.09	3±1 (6±2%)
3	PX4	B	390	-	45,45,45	1.07±0.10	3±1 (7±3%)
3	PX4	B	394	-	45,45,45	1.09±0.12	3±2 (7±3%)
3	PX4	B	399	-	45,45,45	1.04±0.11	3±2 (6±3%)
3	PX4	A	621	-	45,45,45	1.04±0.10	3±1 (5±3%)
3	PX4	B	396	-	45,45,45	1.10±0.14	4±2 (8±3%)
3	PX4	C	312	-	45,45,45	1.08±0.11	3±2 (7±3%)
3	PX4	C	325	-	45,45,45	1.06±0.11	3±1 (6±2%)
3	PX4	C	309	-	45,45,45	1.10±0.17	3±2 (6±4%)
3	PX4	A	607	-	45,45,45	1.11±0.13	3±1 (6±2%)
3	PX4	B	385	-	45,45,45	1.10±0.12	3±1 (7±3%)
3	PX4	C	333	-	45,45,45	1.08±0.14	3±2 (6±3%)
3	PX4	C	311	-	45,45,45	1.06±0.09	3±1 (6±2%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	386	-	45,45,45	1.06±0.12	3±1 (6±3%)
3	PX4	B	368	-	45,45,45	1.10±0.09	3±1 (7±2%)
3	PX4	B	357	-	45,45,45	1.07±0.12	3±1 (6±3%)
3	PX4	B	344	-	45,45,45	1.07±0.12	4±2 (7±3%)
3	PX4	B	400	-	45,45,45	1.07±0.12	3±1 (6±3%)
3	PX4	B	375	-	45,45,45	1.02±0.08	3±1 (5±1%)
3	PX4	A	605	-	45,45,45	1.11±0.09	3±1 (7±2%)
3	PX4	A	653	-	45,45,45	1.11±0.13	4±2 (8±3%)
3	PX4	B	379	-	45,45,45	1.06±0.10	3±1 (7±2%)
3	PX4	C	306	-	45,45,45	1.10±0.12	3±1 (7±2%)
3	PX4	A	641	-	45,45,45	1.04±0.11	3±1 (5±2%)
3	PX4	C	347	-	45,45,45	1.08±0.14	3±1 (6±3%)
3	PX4	B	336	-	45,45,45	1.03±0.12	3±2 (5±4%)
3	PX4	C	313	-	45,45,45	1.04±0.12	2±2 (5±3%)
3	PX4	B	382	-	45,45,45	1.09±0.10	3±1 (7±2%)
3	PX4	B	309	-	45,45,45	1.07±0.10	3±1 (6±3%)
3	PX4	C	344	-	45,45,45	1.02±0.14	3±1 (5±3%)
3	PX4	C	343	-	45,45,45	1.09±0.10	3±1 (6±1%)
3	PX4	B	301	-	45,45,45	1.11±0.11	4±2 (7±3%)
3	PX4	C	358	-	45,45,45	1.03±0.10	3±1 (5±2%)
3	PX4	A	618	-	45,45,45	1.05±0.10	2±1 (5±2%)
3	PX4	C	345	-	45,45,45	1.09±0.13	3±2 (6±3%)
3	PX4	A	654	-	45,45,45	1.05±0.11	3±2 (6±3%)
3	PX4	A	646	-	45,45,45	1.03±0.07	2±1 (4±2%)
3	PX4	C	346	-	45,45,45	1.09±0.09	3±2 (5±3%)
3	PX4	B	350	-	45,45,45	1.09±0.08	3±1 (7±3%)
3	PX4	B	302	-	45,45,45	1.09±0.13	3±2 (7±4%)
3	PX4	A	614	-	45,45,45	1.10±0.09	3±1 (6±2%)
3	PX4	B	316	-	45,45,45	1.07±0.11	3±1 (7±3%)
3	PX4	A	602	-	45,45,45	1.08±0.11	3±2 (6±3%)
3	PX4	B	341	-	45,45,45	1.07±0.07	3±1 (5±3%)
3	PX4	A	644	-	45,45,45	1.03±0.13	3±2 (6±3%)
3	PX4	C	301	-	45,45,45	1.08±0.08	3±1 (7±2%)
3	PX4	A	611	-	45,45,45	1.08±0.09	3±1 (6±2%)
3	PX4	B	362	-	45,45,45	1.06±0.11	3±1 (6±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	393	-	45,45,45	1.11±0.14	3±2 (7±4%)
3	PX4	B	338	-	45,45,45	1.08±0.11	3±1 (6±1%)
3	PX4	C	339	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	B	333	-	45,45,45	1.09±0.11	3±1 (6±3%)
3	PX4	A	648	-	45,45,45	1.10±0.09	3±1 (7±2%)
3	PX4	A	652	-	45,45,45	1.05±0.07	3±1 (6±2%)
3	PX4	A	636	-	45,45,45	1.06±0.07	2±1 (5±2%)
3	PX4	A	639	-	45,45,45	1.13±0.14	4±2 (9±4%)
3	PX4	A	613	-	45,45,45	1.11±0.12	3±1 (7±2%)
3	PX4	C	302	-	45,45,45	1.05±0.07	3±1 (7±1%)
3	PX4	B	327	-	45,45,45	1.10±0.13	3±2 (7±3%)
3	PX4	A	643	-	45,45,45	1.04±0.13	3±2 (6±4%)
3	PX4	B	313	-	45,45,45	1.06±0.14	3±2 (6±3%)
3	PX4	A	601	-	45,45,45	1.10±0.08	3±1 (7±2%)
3	PX4	B	373	-	45,45,45	1.08±0.13	3±1 (5±2%)
3	PX4	B	381	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	A	626	-	45,45,45	1.05±0.14	2±1 (5±3%)
3	PX4	C	353	-	45,45,45	1.08±0.10	3±1 (7±2%)
3	PX4	B	397	-	45,45,45	1.07±0.11	3±1 (7±2%)
3	PX4	A	603	-	45,45,45	1.09±0.13	3±2 (6±3%)
3	PX4	B	355	-	45,45,45	1.11±0.12	4±2 (8±4%)
3	PX4	B	322	-	45,45,45	1.10±0.12	3±1 (7±2%)
3	PX4	B	354	-	45,45,45	1.08±0.08	3±1 (6±2%)
3	PX4	A	617	-	45,45,45	1.08±0.10	3±2 (7±4%)
3	PX4	A	627	-	45,45,45	1.11±0.12	4±1 (7±3%)
3	PX4	C	317	-	45,45,45	1.08±0.14	3±2 (6±4%)
3	PX4	A	642	-	45,45,45	1.08±0.09	3±1 (7±2%)
3	PX4	B	326	-	45,45,45	1.08±0.14	3±2 (6±4%)
3	PX4	B	392	-	45,45,45	1.05±0.11	3±1 (6±2%)
3	PX4	B	398	-	45,45,45	1.06±0.11	3±1 (6±2%)
3	PX4	B	365	-	45,45,45	1.06±0.14	3±2 (6±3%)
3	PX4	B	307	-	45,45,45	1.08±0.08	4±1 (8±3%)
3	PX4	C	354	-	45,45,45	1.11±0.09	3±1 (7±3%)
3	PX4	C	360	-	45,45,45	1.09±0.10	3±1 (7±2%)
3	PX4	B	345	-	45,45,45	1.09±0.14	3±2 (7±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	C	321	-	45,45,45	1.10±0.13	4±2 (8±4%)
3	PX4	B	339	-	45,45,45	1.05±0.09	3±1 (6±3%)
3	PX4	C	330	-	45,45,45	1.08±0.12	3±2 (7±4%)
3	PX4	B	323	-	45,45,45	1.08±0.13	3±2 (6±3%)
3	PX4	A	612	-	45,45,45	1.02±0.11	2±1 (5±2%)
3	PX4	C	356	-	45,45,45	1.05±0.16	3±2 (6±3%)
3	PX4	B	352	-	45,45,45	1.09±0.16	3±1 (6±3%)
3	PX4	B	359	-	45,45,45	1.08±0.09	3±1 (6±3%)
3	PX4	B	324	-	45,45,45	1.06±0.09	2±1 (5±2%)
3	PX4	B	311	-	45,45,45	1.15±0.12	4±1 (9±2%)
3	PX4	A	651	-	45,45,45	1.06±0.07	3±1 (7±2%)
3	PX4	C	349	-	45,45,45	1.05±0.12	3±2 (6±4%)
3	PX4	B	384	-	45,45,45	1.11±0.11	3±1 (7±3%)
3	PX4	A	630	-	45,45,45	1.05±0.09	3±2 (6±3%)
3	PX4	C	336	-	45,45,45	1.06±0.08	3±1 (6±2%)
3	PX4	C	332	-	45,45,45	1.06±0.11	3±1 (7±3%)
3	PX4	B	317	-	45,45,45	1.05±0.11	3±1 (6±2%)
3	PX4	B	366	-	45,45,45	1.02±0.11	3±1 (6±2%)
3	PX4	B	321	-	45,45,45	1.11±0.10	3±2 (7±3%)
3	PX4	C	337	-	45,45,45	1.07±0.09	3±2 (6±3%)
3	PX4	C	359	-	45,45,45	1.12±0.12	3±1 (6±3%)
3	PX4	B	349	-	45,45,45	1.09±0.06	3±1 (7±2%)
3	PX4	B	360	-	45,45,45	1.09±0.11	3±2 (7±3%)
3	PX4	B	329	-	45,45,45	1.12±0.11	4±1 (8±2%)
3	PX4	B	334	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	B	377	-	45,45,45	1.08±0.11	3±1 (7±3%)
3	PX4	C	305	-	45,45,45	1.09±0.13	3±2 (7±4%)
3	PX4	B	358	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	C	320	-	45,45,45	1.08±0.12	3±1 (5±2%)
3	PX4	C	327	-	45,45,45	1.06±0.08	3±1 (6±2%)
3	PX4	A	604	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	B	378	-	45,45,45	1.06±0.12	3±1 (6±2%)
3	PX4	B	391	-	45,45,45	1.04±0.07	2±1 (5±2%)
3	PX4	C	348	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	B	389	-	45,45,45	1.08±0.13	3±1 (6±2%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	632	-	45,45,45	1.07±0.16	3±1 (7±3%)
3	PX4	B	308	-	45,45,45	1.10±0.13	4±1 (8±2%)
3	PX4	B	374	-	45,45,45	1.08±0.14	3±2 (6±3%)
3	PX4	C	328	-	45,45,45	1.10±0.11	3±1 (7±2%)
3	PX4	B	305	-	45,45,45	1.09±0.08	3±1 (6±2%)
3	PX4	B	315	-	45,45,45	1.04±0.12	3±1 (6±2%)
3	PX4	A	628	-	45,45,45	1.05±0.11	3±2 (6±3%)
3	PX4	C	361	-	45,45,45	1.07±0.15	3±2 (5±3%)
3	PX4	B	383	-	45,45,45	1.10±0.13	4±2 (8±3%)
3	PX4	A	638	-	45,45,45	1.04±0.12	2±1 (5±3%)
3	PX4	A	623	-	45,45,45	1.03±0.13	2±2 (5±3%)
3	PX4	B	331	-	45,45,45	1.08±0.12	3±2 (6±3%)
3	PX4	A	619	-	45,45,45	1.07±0.12	3±1 (6±2%)
3	PX4	C	316	-	45,45,45	1.05±0.11	3±1 (6±2%)
3	PX4	C	355	-	45,45,45	1.11±0.11	4±2 (8±4%)
3	PX4	A	624	-	45,45,45	1.05±0.10	2±2 (5±3%)
3	PX4	B	361	-	45,45,45	1.09±0.11	3±2 (7±4%)
3	PX4	B	314	-	45,45,45	1.11±0.11	3±1 (6±2%)
3	PX4	C	342	-	45,45,45	1.04±0.13	3±1 (6±3%)
3	PX4	B	347	-	45,45,45	1.07±0.06	3±1 (7±2%)
3	PX4	C	322	-	45,45,45	1.05±0.13	3±1 (6±2%)
3	PX4	A	609	-	45,45,45	1.09±0.11	4±1 (7±3%)
3	PX4	C	303	-	45,45,45	1.08±0.17	3±2 (6±3%)
3	PX4	A	633	-	45,45,45	1.07±0.13	3±1 (5±3%)
3	PX4	A	616	-	45,45,45	1.08±0.11	3±1 (6±2%)
3	PX4	A	615	-	45,45,45	1.05±0.13	2±1 (5±3%)
3	PX4	C	329	-	45,45,45	1.16±0.12	4±2 (8±4%)
3	PX4	C	352	-	45,45,45	1.14±0.11	3±1 (7±2%)
3	PX4	A	625	-	45,45,45	1.08±0.11	3±2 (6±3%)
3	PX4	A	622	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	C	334	-	45,45,45	1.05±0.14	3±2 (6±3%)
3	PX4	C	340	-	45,45,45	1.06±0.09	3±1 (6±3%)
3	PX4	C	315	-	45,45,45	1.07±0.10	2±1 (5±2%)
3	PX4	A	649	-	45,45,45	1.08±0.12	3±1 (6±3%)
3	PX4	B	348	-	45,45,45	1.07±0.11	3±1 (6±2%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	634	-	45,45,45	1.04±0.10	3±1 (6±3%)
3	PX4	B	304	-	45,45,45	1.03±0.13	2±2 (5±3%)
3	PX4	C	363	-	45,45,45	1.09±0.12	3±2 (7±3%)
3	PX4	B	342	-	45,45,45	1.11±0.10	3±2 (6±3%)
3	PX4	C	314	-	45,45,45	1.06±0.11	2±1 (5±3%)
3	PX4	B	343	-	45,45,45	1.05±0.12	3±1 (5±3%)
3	PX4	B	303	-	45,45,45	1.02±0.14	3±2 (5±3%)
3	PX4	B	380	-	45,45,45	1.07±0.10	3±1 (6±2%)
3	PX4	B	353	-	45,45,45	1.10±0.13	3±1 (6±3%)
3	PX4	C	326	-	45,45,45	1.11±0.12	3±1 (7±3%)
3	PX4	A	645	-	45,45,45	1.11±0.09	3±1 (6±1%)
3	PX4	B	370	-	45,45,45	1.06±0.10	3±1 (5±2%)
3	PX4	B	346	-	45,45,45	1.09±0.12	3±1 (6±2%)
3	PX4	C	323	-	45,45,45	1.06±0.17	3±2 (6±4%)
3	PX4	A	650	-	45,45,45	1.07±0.08	3±1 (6±2%)
3	PX4	B	367	-	45,45,45	1.09±0.11	3±1 (5±3%)
3	PX4	B	318	-	45,45,45	1.04±0.11	3±2 (5±3%)
3	PX4	C	341	-	45,45,45	1.10±0.11	3±1 (7±2%)
3	PX4	B	371	-	45,45,45	1.05±0.12	3±2 (5±3%)
3	PX4	B	376	-	45,45,45	1.10±0.09	3±2 (7±3%)
3	PX4	B	319	-	45,45,45	1.08±0.10	3±1 (5±3%)
3	PX4	B	337	-	45,45,45	1.06±0.13	3±2 (7±3%)
3	PX4	A	610	-	45,45,45	1.07±0.12	3±2 (6±3%)
3	PX4	B	328	-	45,45,45	1.10±0.08	3±1 (7±2%)
3	PX4	C	324	-	45,45,45	1.04±0.09	2±2 (5±3%)
3	PX4	B	332	-	45,45,45	1.11±0.11	3±1 (7±3%)
3	PX4	B	364	-	45,45,45	1.07±0.14	3±2 (7±4%)
3	PX4	B	306	-	45,45,45	1.06±0.13	3±2 (6±3%)
3	PX4	C	364	-	45,45,45	1.10±0.11	3±2 (7±3%)
3	PX4	B	335	-	45,45,45	1.04±0.10	3±1 (5±2%)
3	PX4	B	387	-	45,45,45	1.06±0.11	3±2 (5±3%)
3	PX4	A	635	-	45,45,45	1.07±0.13	3±2 (7±4%)
3	PX4	C	307	-	45,45,45	1.10±0.16	3±2 (7±4%)
3	PX4	B	388	-	45,45,45	1.07±0.11	3±2 (6±3%)
3	PX4	A	629	-	45,45,45	1.07±0.10	3±1 (5±2%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	312	-	45,45,45	1.10±0.14	4±2 (8±4%)
3	PX4	B	320	-	45,45,45	1.08±0.11	3±1 (6±2%)
3	PX4	A	647	-	45,45,45	1.08±0.08	3±2 (7±3%)
3	PX4	C	310	-	45,45,45	1.06±0.11	3±1 (5±2%)
3	PX4	B	356	-	45,45,45	1.04±0.14	3±2 (5±3%)
3	PX4	B	340	-	45,45,45	1.10±0.13	3±2 (6±3%)
3	PX4	B	372	-	45,45,45	1.04±0.12	3±2 (6±3%)
3	PX4	C	304	-	45,45,45	1.12±0.10	3±2 (7±3%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	A	608	-	51,53,53	0.96±0.19	3±2 (4±3%)
3	PX4	A	631	-	51,53,53	0.95±0.10	2±1 (4±2%)
3	PX4	C	318	-	51,53,53	0.95±0.12	2±1 (4±2%)
3	PX4	B	351	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	B	325	-	51,53,53	0.95±0.12	2±2 (3±3%)
3	PX4	C	362	-	51,53,53	0.93±0.11	2±2 (4±3%)
3	PX4	C	331	-	51,53,53	0.92±0.11	2±1 (4±2%)
3	PX4	C	350	-	51,53,53	1.07±0.13	3±2 (6±3%)
3	PX4	A	640	-	51,53,53	0.98±0.09	2±1 (4±2%)
3	PX4	C	357	-	51,53,53	0.96±0.08	2±1 (4±2%)
3	PX4	A	620	-	51,53,53	0.93±0.12	2±1 (4±2%)
3	PX4	B	395	-	51,53,53	0.93±0.12	2±1 (4±2%)
3	PX4	C	335	-	51,53,53	0.99±0.11	3±2 (6±3%)
3	PX4	C	308	-	51,53,53	0.92±0.13	2±1 (3±2%)
3	PX4	C	338	-	51,53,53	0.96±0.12	2±1 (4±2%)
3	PX4	C	351	-	51,53,53	0.97±0.10	2±2 (4±3%)
3	PX4	A	606	-	51,53,53	0.92±0.10	2±2 (4±3%)
3	PX4	B	369	-	51,53,53	0.98±0.13	3±2 (5±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	A	637	-	51,53,53	0.95±0.08	2±1 (4±1%)
3	PX4	B	310	-	51,53,53	0.92±0.10	2±1 (3±1%)
3	PX4	B	363	-	51,53,53	0.97±0.10	2±1 (4±2%)
3	PX4	C	319	-	51,53,53	0.90±0.09	2±1 (3±1%)
3	PX4	B	330	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	B	390	-	51,53,53	0.91±0.10	2±1 (3±2%)
3	PX4	B	394	-	51,53,53	0.99±0.11	2±1 (4±2%)
3	PX4	B	399	-	51,53,53	0.96±0.11	2±1 (4±2%)
3	PX4	A	621	-	51,53,53	0.97±0.11	3±1 (5±2%)
3	PX4	B	396	-	51,53,53	0.99±0.10	2±1 (4±2%)
3	PX4	C	312	-	51,53,53	0.92±0.11	2±2 (4±4%)
3	PX4	C	325	-	51,53,53	0.98±0.07	3±1 (5±2%)
3	PX4	C	309	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	A	607	-	51,53,53	0.97±0.11	2±2 (4±3%)
3	PX4	B	385	-	51,53,53	1.01±0.16	3±1 (5±2%)
3	PX4	C	333	-	51,53,53	0.95±0.13	2±2 (4±3%)
3	PX4	C	311	-	51,53,53	1.00±0.10	2±1 (4±2%)
3	PX4	B	386	-	51,53,53	0.95±0.10	2±1 (3±2%)
3	PX4	B	368	-	51,53,53	0.97±0.14	2±1 (4±2%)
3	PX4	B	357	-	51,53,53	0.98±0.14	3±2 (5±4%)
3	PX4	B	344	-	51,53,53	1.00±0.10	2±1 (4±1%)
3	PX4	B	400	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	B	375	-	51,53,53	0.89±0.13	2±1 (3±2%)
3	PX4	A	605	-	51,53,53	0.97±0.12	3±1 (5±2%)
3	PX4	A	653	-	51,53,53	1.00±0.12	2±1 (4±2%)
3	PX4	B	379	-	51,53,53	0.96±0.11	2±2 (4±3%)
3	PX4	C	306	-	51,53,53	1.00±0.09	3±1 (5±2%)
3	PX4	A	641	-	51,53,53	0.91±0.12	2±1 (3±2%)
3	PX4	C	347	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	336	-	51,53,53	0.95±0.10	2±2 (3±2%)
3	PX4	C	313	-	51,53,53	0.98±0.09	2±2 (4±3%)
3	PX4	B	382	-	51,53,53	0.96±0.08	2±1 (4±2%)
3	PX4	B	309	-	51,53,53	0.99±0.13	3±1 (5±2%)
3	PX4	C	344	-	51,53,53	0.99±0.12	2±1 (4±2%)
3	PX4	C	343	-	51,53,53	0.93±0.09	2±2 (4±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	301	-	51,53,53	0.95±0.11	2±1 (3±2%)
3	PX4	C	358	-	51,53,53	0.99±0.10	2±1 (4±2%)
3	PX4	A	618	-	51,53,53	0.99±0.13	3±2 (6±3%)
3	PX4	C	345	-	51,53,53	0.95±0.13	2±1 (4±2%)
3	PX4	A	654	-	51,53,53	0.91±0.11	2±1 (3±2%)
3	PX4	A	646	-	51,53,53	0.91±0.14	2±1 (4±2%)
3	PX4	C	346	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	B	350	-	51,53,53	0.97±0.14	3±2 (5±4%)
3	PX4	B	302	-	51,53,53	0.90±0.11	2±1 (3±2%)
3	PX4	A	614	-	51,53,53	0.93±0.13	2±2 (4±3%)
3	PX4	B	316	-	51,53,53	0.91±0.14	2±1 (4±2%)
3	PX4	A	602	-	51,53,53	0.92±0.11	2±2 (4±3%)
3	PX4	B	341	-	51,53,53	1.05±0.12	3±1 (6±2%)
3	PX4	A	644	-	51,53,53	0.94±0.09	2±1 (4±1%)
3	PX4	C	301	-	51,53,53	0.95±0.09	2±2 (4±3%)
3	PX4	A	611	-	51,53,53	0.93±0.13	2±1 (3±1%)
3	PX4	B	362	-	51,53,53	0.95±0.10	2±2 (4±2%)
3	PX4	B	393	-	51,53,53	0.96±0.08	2±1 (4±1%)
3	PX4	B	338	-	51,53,53	0.91±0.12	2±1 (4±2%)
3	PX4	C	339	-	51,53,53	0.94±0.13	2±1 (3±2%)
3	PX4	B	333	-	51,53,53	0.95±0.10	2±2 (4±3%)
3	PX4	A	648	-	51,53,53	0.97±0.10	2±1 (4±2%)
3	PX4	A	652	-	51,53,53	0.99±0.10	3±1 (5±2%)
3	PX4	A	636	-	51,53,53	0.98±0.11	2±1 (4±2%)
3	PX4	A	639	-	51,53,53	0.93±0.08	2±1 (4±2%)
3	PX4	A	613	-	51,53,53	0.88±0.08	2±1 (3±1%)
3	PX4	C	302	-	51,53,53	0.98±0.13	3±2 (5±3%)
3	PX4	B	327	-	51,53,53	0.95±0.15	2±2 (4±3%)
3	PX4	A	643	-	51,53,53	0.97±0.08	2±2 (4±3%)
3	PX4	B	313	-	51,53,53	0.98±0.10	2±1 (4±2%)
3	PX4	A	601	-	51,53,53	0.97±0.14	3±1 (5±2%)
3	PX4	B	373	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	381	-	51,53,53	0.93±0.09	2±1 (3±2%)
3	PX4	A	626	-	51,53,53	0.96±0.15	2±2 (4±2%)
3	PX4	C	353	-	51,53,53	0.97±0.09	2±1 (4±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	397	-	51,53,53	0.94±0.12	2±1 (4±2%)
3	PX4	A	603	-	51,53,53	0.97±0.12	3±1 (5±2%)
3	PX4	B	355	-	51,53,53	0.94±0.13	2±1 (4±2%)
3	PX4	B	322	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	B	354	-	51,53,53	0.97±0.12	2±2 (4±3%)
3	PX4	A	617	-	51,53,53	0.98±0.12	2±1 (4±2%)
3	PX4	A	627	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	C	317	-	51,53,53	1.05±0.11	4±2 (7±3%)
3	PX4	A	642	-	51,53,53	0.98±0.11	3±2 (5±2%)
3	PX4	B	326	-	51,53,53	0.96±0.12	2±2 (4±3%)
3	PX4	B	392	-	51,53,53	0.96±0.09	3±1 (4±2%)
3	PX4	B	398	-	51,53,53	0.90±0.09	2±1 (3±2%)
3	PX4	B	365	-	51,53,53	0.94±0.13	2±1 (3±2%)
3	PX4	B	307	-	51,53,53	0.95±0.07	2±1 (4±2%)
3	PX4	C	354	-	51,53,53	0.98±0.11	3±1 (5±2%)
3	PX4	C	360	-	51,53,53	0.95±0.16	2±1 (3±2%)
3	PX4	B	345	-	51,53,53	0.93±0.10	2±1 (3±1%)
3	PX4	C	321	-	51,53,53	0.97±0.08	2±1 (4±2%)
3	PX4	B	339	-	51,53,53	0.91±0.12	2±1 (4±2%)
3	PX4	C	330	-	51,53,53	0.96±0.11	2±1 (4±1%)
3	PX4	B	323	-	51,53,53	0.90±0.08	2±1 (3±2%)
3	PX4	A	612	-	51,53,53	1.00±0.15	2±1 (4±2%)
3	PX4	C	356	-	51,53,53	0.94±0.12	2±2 (4±2%)
3	PX4	B	352	-	51,53,53	0.94±0.10	2±1 (3±2%)
3	PX4	B	359	-	51,53,53	0.95±0.10	2±2 (3±3%)
3	PX4	B	324	-	51,53,53	0.91±0.10	2±1 (4±2%)
3	PX4	B	311	-	51,53,53	0.96±0.08	2±1 (3±2%)
3	PX4	A	651	-	51,53,53	1.03±0.13	3±1 (6±2%)
3	PX4	C	349	-	51,53,53	1.00±0.14	3±2 (5±3%)
3	PX4	B	384	-	51,53,53	1.03±0.10	3±1 (5±2%)
3	PX4	A	630	-	51,53,53	0.92±0.11	2±1 (4±2%)
3	PX4	C	336	-	51,53,53	0.93±0.10	2±1 (4±2%)
3	PX4	C	332	-	51,53,53	0.97±0.14	2±2 (4±3%)
3	PX4	B	317	-	51,53,53	0.91±0.10	2±1 (3±2%)
3	PX4	B	366	-	51,53,53	0.93±0.09	2±1 (3±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	321	-	51,53,53	0.95±0.13	3±2 (5±3%)
3	PX4	C	337	-	51,53,53	0.93±0.11	2±1 (3±2%)
3	PX4	C	359	-	51,53,53	0.85±0.11	1±1 (2±2%)
3	PX4	B	349	-	51,53,53	0.95±0.10	2±1 (3±2%)
3	PX4	B	360	-	51,53,53	0.96±0.11	2±2 (3±3%)
3	PX4	B	329	-	51,53,53	0.95±0.13	2±1 (4±2%)
3	PX4	B	334	-	51,53,53	0.89±0.11	1±1 (2±2%)
3	PX4	B	377	-	51,53,53	0.94±0.11	2±1 (3±2%)
3	PX4	C	305	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	B	358	-	51,53,53	0.96±0.13	2±2 (4±3%)
3	PX4	C	320	-	51,53,53	1.00±0.10	3±1 (5±2%)
3	PX4	C	327	-	51,53,53	0.97±0.13	3±2 (5±3%)
3	PX4	A	604	-	51,53,53	0.96±0.09	3±1 (5±2%)
3	PX4	B	378	-	51,53,53	0.96±0.12	2±1 (4±2%)
3	PX4	B	391	-	51,53,53	0.91±0.13	2±2 (3±3%)
3	PX4	C	348	-	51,53,53	0.93±0.09	2±2 (4±3%)
3	PX4	B	389	-	51,53,53	0.96±0.09	2±1 (4±1%)
3	PX4	A	632	-	51,53,53	0.94±0.12	2±2 (4±3%)
3	PX4	B	308	-	51,53,53	0.93±0.16	2±2 (4±4%)
3	PX4	B	374	-	51,53,53	0.92±0.10	2±1 (4±2%)
3	PX4	C	328	-	51,53,53	0.95±0.11	2±1 (4±2%)
3	PX4	B	305	-	51,53,53	0.95±0.08	3±1 (5±2%)
3	PX4	B	315	-	51,53,53	0.99±0.12	2±1 (4±2%)
3	PX4	A	628	-	51,53,53	0.93±0.06	2±1 (4±2%)
3	PX4	C	361	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	383	-	51,53,53	1.02±0.08	3±1 (5±2%)
3	PX4	A	638	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	A	623	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	331	-	51,53,53	0.89±0.13	2±2 (3±3%)
3	PX4	A	619	-	51,53,53	0.93±0.09	2±1 (3±2%)
3	PX4	C	316	-	51,53,53	0.90±0.08	2±1 (3±2%)
3	PX4	C	355	-	51,53,53	0.99±0.12	3±1 (5±2%)
3	PX4	A	624	-	51,53,53	0.93±0.14	2±2 (4±3%)
3	PX4	B	361	-	51,53,53	0.94±0.11	2±2 (4±3%)
3	PX4	B	314	-	51,53,53	0.88±0.11	2±1 (3±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	342	-	51,53,53	0.92±0.11	2±1 (3±2%)
3	PX4	B	347	-	51,53,53	0.99±0.12	3±1 (4±1%)
3	PX4	C	322	-	51,53,53	0.96±0.10	2±1 (4±2%)
3	PX4	A	609	-	51,53,53	0.97±0.12	2±2 (4±3%)
3	PX4	C	303	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	A	633	-	51,53,53	0.94±0.10	2±1 (3±1%)
3	PX4	A	616	-	51,53,53	0.95±0.11	3±1 (5±2%)
3	PX4	A	615	-	51,53,53	0.93±0.11	2±1 (3±2%)
3	PX4	C	329	-	51,53,53	0.99±0.14	3±2 (5±3%)
3	PX4	C	352	-	51,53,53	0.95±0.08	2±1 (4±2%)
3	PX4	A	625	-	51,53,53	0.98±0.09	2±1 (3±2%)
3	PX4	A	622	-	51,53,53	0.97±0.14	3±1 (4±2%)
3	PX4	C	334	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	C	340	-	51,53,53	0.96±0.13	2±2 (4±3%)
3	PX4	C	315	-	51,53,53	0.97±0.10	3±1 (4±2%)
3	PX4	A	649	-	51,53,53	1.01±0.11	3±2 (5±3%)
3	PX4	B	348	-	51,53,53	0.99±0.10	3±1 (5±2%)
3	PX4	A	634	-	51,53,53	0.95±0.12	2±2 (4±3%)
3	PX4	B	304	-	51,53,53	0.94±0.10	2±1 (3±2%)
3	PX4	C	363	-	51,53,53	1.01±0.13	3±2 (5±3%)
3	PX4	B	342	-	51,53,53	0.99±0.13	3±2 (5±3%)
3	PX4	C	314	-	51,53,53	0.94±0.08	2±1 (3±2%)
3	PX4	B	343	-	51,53,53	0.95±0.09	2±2 (3±3%)
3	PX4	B	303	-	51,53,53	0.92±0.12	2±1 (4±2%)
3	PX4	B	380	-	51,53,53	0.98±0.12	3±2 (5±3%)
3	PX4	B	353	-	51,53,53	0.96±0.12	2±1 (4±2%)
3	PX4	C	326	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	A	645	-	51,53,53	0.90±0.14	2±2 (4±3%)
3	PX4	B	370	-	51,53,53	0.96±0.09	2±1 (4±2%)
3	PX4	B	346	-	51,53,53	0.88±0.07	1±1 (2±1%)
3	PX4	C	323	-	51,53,53	0.96±0.10	2±1 (4±2%)
3	PX4	A	650	-	51,53,53	0.94±0.12	2±1 (4±2%)
3	PX4	B	367	-	51,53,53	0.97±0.11	2±1 (4±1%)
3	PX4	B	318	-	51,53,53	0.94±0.12	2±1 (3±2%)
3	PX4	C	341	-	51,53,53	0.97±0.09	3±1 (4±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	371	-	51,53,53	0.96±0.12	2±1 (4±2%)
3	PX4	B	376	-	51,53,53	0.92±0.10	2±1 (4±2%)
3	PX4	B	319	-	51,53,53	1.00±0.10	3±2 (5±3%)
3	PX4	B	337	-	51,53,53	0.93±0.09	2±1 (4±2%)
3	PX4	A	610	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	B	328	-	51,53,53	0.95±0.07	2±1 (3±1%)
3	PX4	C	324	-	51,53,53	0.97±0.12	3±1 (4±2%)
3	PX4	B	332	-	51,53,53	0.96±0.15	3±2 (5±2%)
3	PX4	B	364	-	51,53,53	0.94±0.13	2±1 (3±2%)
3	PX4	B	306	-	51,53,53	1.00±0.12	3±1 (6±2%)
3	PX4	C	364	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	B	335	-	51,53,53	0.94±0.12	2±1 (4±2%)
3	PX4	B	387	-	51,53,53	0.89±0.10	2±1 (3±2%)
3	PX4	A	635	-	51,53,53	0.90±0.07	2±1 (3±1%)
3	PX4	C	307	-	51,53,53	0.94±0.09	2±1 (3±1%)
3	PX4	B	388	-	51,53,53	0.98±0.13	3±2 (4±3%)
3	PX4	A	629	-	51,53,53	0.88±0.13	2±1 (3±2%)
3	PX4	B	312	-	51,53,53	0.99±0.08	2±2 (4±2%)
3	PX4	B	320	-	51,53,53	0.99±0.13	3±2 (4±3%)
3	PX4	A	647	-	51,53,53	0.96±0.10	2±1 (4±2%)
3	PX4	C	310	-	51,53,53	1.03±0.14	3±1 (6±2%)
3	PX4	B	356	-	51,53,53	0.98±0.13	3±2 (5±3%)
3	PX4	B	340	-	51,53,53	0.92±0.09	2±1 (4±2%)
3	PX4	B	372	-	51,53,53	1.02±0.10	3±1 (6±2%)
3	PX4	C	304	-	51,53,53	0.96±0.15	3±2 (5±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
3	PX4	C	308	-	-	0±0,49,49,49	-
3	PX4	C	335	-	-	0±0,49,49,49	-
3	PX4	B	330	-	-	0±0,49,49,49	-
3	PX4	B	396	-	-	0±0,49,49,49	-
3	PX4	C	309	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	347	-	-	0±0,49,49,49	-
3	PX4	A	654	-	-	0±0,49,49,49	-
3	PX4	B	386	-	-	0±0,49,49,49	-
3	PX4	B	381	-	-	0±0,49,49,49	-
3	PX4	C	330	-	-	0±0,49,49,49	-
3	PX4	B	339	-	-	0±0,49,49,49	-
3	PX4	C	337	-	-	0±0,49,49,49	-
3	PX4	C	332	-	-	0±0,49,49,49	-
3	PX4	B	359	-	-	0±0,49,49,49	-
3	PX4	C	338	-	-	0±0,49,49,49	-
3	PX4	C	316	-	-	0±0,49,49,49	-
3	PX4	C	321	-	-	0±0,49,49,49	-
3	PX4	B	393	-	-	0±0,49,49,49	-
3	PX4	A	609	-	-	0±0,49,49,49	-
3	PX4	A	649	-	-	0±0,49,49,49	-
3	PX4	B	347	-	-	0±0,49,49,49	-
3	PX4	A	601	-	-	0±0,49,49,49	-
3	PX4	B	342	-	-	0±0,49,49,49	-
3	PX4	B	303	-	-	0±0,49,49,49	-
3	PX4	B	360	-	-	0±0,49,49,49	-
3	PX4	B	304	-	-	0±0,49,49,49	-
3	PX4	C	360	-	-	0±0,49,49,49	-
3	PX4	B	355	-	-	0±0,49,49,49	-
3	PX4	B	334	-	-	0±0,49,49,49	-
3	PX4	A	622	-	-	0±0,49,49,49	-
3	PX4	C	313	-	-	0±0,49,49,49	-
3	PX4	B	328	-	-	0±0,49,49,49	-
3	PX4	C	352	-	-	0±0,49,49,49	-
3	PX4	C	306	-	-	0±0,49,49,49	-
3	PX4	B	361	-	-	0±0,49,49,49	-
3	PX4	A	639	-	-	0±0,49,49,49	-
3	PX4	C	345	-	-	0±0,49,49,49	-
3	PX4	B	311	-	-	0±0,49,49,49	-
3	PX4	A	615	-	-	0±0,49,49,49	-
3	PX4	B	335	-	-	0±0,49,49,49	-
3	PX4	A	632	-	-	0±0,49,49,49	-
3	PX4	C	350	-	-	0±0,49,49,49	-
3	PX4	B	373	-	-	0±0,49,49,49	-
3	PX4	B	320	-	-	0±0,49,49,49	-
3	PX4	B	343	-	-	0±0,49,49,49	-
3	PX4	A	610	-	-	0±0,49,49,49	-
3	PX4	A	614	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	326	-	-	0±0,49,49,49	-
3	PX4	A	618	-	-	0±0,49,49,49	-
3	PX4	A	638	-	-	0±0,49,49,49	-
3	PX4	A	603	-	-	0±0,49,49,49	-
3	PX4	A	628	-	-	0±0,49,49,49	-
3	PX4	B	384	-	-	0±0,49,49,49	-
3	PX4	C	305	-	-	0±0,49,49,49	-
3	PX4	C	357	-	-	0±0,49,49,49	-
3	PX4	C	339	-	-	0±0,49,49,49	-
3	PX4	B	395	-	-	0±0,49,49,49	-
3	PX4	C	307	-	-	0±0,49,49,49	-
3	PX4	A	619	-	-	0±0,49,49,49	-
3	PX4	A	627	-	-	0±0,49,49,49	-
3	PX4	B	305	-	-	0±0,49,49,49	-
3	PX4	C	329	-	-	0±0,49,49,49	-
3	PX4	A	617	-	-	0±0,49,49,49	-
3	PX4	B	317	-	-	0±0,49,49,49	-
3	PX4	B	385	-	-	0±0,49,49,49	-
3	PX4	C	310	-	-	0±0,49,49,49	-
3	PX4	B	399	-	-	0±0,49,49,49	-
3	PX4	B	352	-	-	0±0,49,49,49	-
3	PX4	C	359	-	-	0±0,49,49,49	-
3	PX4	B	371	-	-	0±0,49,49,49	-
3	PX4	B	309	-	-	0±0,49,49,49	-
3	PX4	C	328	-	-	0±0,49,49,49	-
3	PX4	A	637	-	-	0±0,49,49,49	-
3	PX4	C	361	-	-	0±0,49,49,49	-
3	PX4	C	301	-	-	0±0,49,49,49	-
3	PX4	A	651	-	-	0±0,49,49,49	-
3	PX4	A	645	-	-	0±0,49,49,49	-
3	PX4	A	616	-	-	0±0,49,49,49	-
3	PX4	B	331	-	-	0±0,49,49,49	-
3	PX4	B	306	-	-	0±0,49,49,49	-
3	PX4	B	376	-	-	0±0,49,49,49	-
3	PX4	A	613	-	-	0±0,49,49,49	-
3	PX4	C	311	-	-	0±0,49,49,49	-
3	PX4	B	349	-	-	0±0,49,49,49	-
3	PX4	A	652	-	-	0±0,49,49,49	-
3	PX4	C	363	-	-	0±0,49,49,49	-
3	PX4	B	312	-	-	0±0,49,49,49	-
3	PX4	A	643	-	-	0±0,49,49,49	-
3	PX4	B	391	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	356	-	-	0±0,49,49,49	-
3	PX4	C	356	-	-	0±0,49,49,49	-
3	PX4	C	318	-	-	0±0,49,49,49	-
3	PX4	A	604	-	-	0±0,49,49,49	-
3	PX4	C	349	-	-	0±0,49,49,49	-
3	PX4	A	635	-	-	0±0,49,49,49	-
3	PX4	A	612	-	-	0±0,49,49,49	-
3	PX4	B	392	-	-	0±0,49,49,49	-
3	PX4	C	320	-	-	0±0,49,49,49	-
3	PX4	B	337	-	-	0±0,49,49,49	-
3	PX4	C	312	-	-	0±0,49,49,49	-
3	PX4	B	332	-	-	0±0,49,49,49	-
3	PX4	C	353	-	-	0±0,49,49,49	-
3	PX4	B	367	-	-	0±0,49,49,49	-
3	PX4	A	629	-	-	0±0,49,49,49	-
3	PX4	B	333	-	-	0±0,49,49,49	-
3	PX4	A	608	-	-	0±0,49,49,49	-
3	PX4	B	350	-	-	0±0,49,49,49	-
3	PX4	C	362	-	-	0±0,49,49,49	-
3	PX4	C	336	-	-	0±0,49,49,49	-
3	PX4	A	605	-	-	0±0,49,49,49	-
3	PX4	B	368	-	-	0±0,49,49,49	-
3	PX4	A	644	-	-	0±0,49,49,49	-
3	PX4	A	621	-	-	0±0,49,49,49	-
3	PX4	B	325	-	-	0±0,49,49,49	-
3	PX4	C	325	-	-	0±0,49,49,49	-
3	PX4	B	323	-	-	0±0,49,49,49	-
3	PX4	C	303	-	-	0±0,49,49,49	-
3	PX4	A	631	-	-	0±0,49,49,49	-
3	PX4	C	333	-	-	0±0,49,49,49	-
3	PX4	B	351	-	-	0±0,49,49,49	-
3	PX4	B	329	-	-	0±0,49,49,49	-
3	PX4	A	602	-	-	0±0,49,49,49	-
3	PX4	A	620	-	-	0±0,49,49,49	-
3	PX4	B	364	-	-	0±0,49,49,49	-
3	PX4	B	363	-	-	0±0,49,49,49	-
3	PX4	C	344	-	-	0±0,49,49,49	-
3	PX4	B	379	-	-	0±0,49,49,49	-
3	PX4	A	647	-	-	0±0,49,49,49	-
3	PX4	C	348	-	-	0±0,49,49,49	-
3	PX4	C	322	-	-	0±0,49,49,49	-
3	PX4	C	334	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	370	-	-	0±0,49,49,49	-
3	PX4	B	314	-	-	0±0,49,49,49	-
3	PX4	B	315	-	-	0±0,49,49,49	-
3	PX4	C	327	-	-	0±0,49,49,49	-
3	PX4	B	383	-	-	0±0,49,49,49	-
3	PX4	B	307	-	-	0±0,49,49,49	-
3	PX4	C	319	-	-	0±0,49,49,49	-
3	PX4	B	338	-	-	0±0,49,49,49	-
3	PX4	C	341	-	-	0±0,49,49,49	-
3	PX4	B	346	-	-	0±0,49,49,49	-
3	PX4	B	324	-	-	0±0,49,49,49	-
3	PX4	B	336	-	-	0±0,49,49,49	-
3	PX4	A	626	-	-	0±0,49,49,49	-
3	PX4	B	389	-	-	0±0,49,49,49	-
3	PX4	B	380	-	-	0±0,49,49,49	-
3	PX4	B	366	-	-	0±0,49,49,49	-
3	PX4	B	322	-	-	0±0,49,49,49	-
3	PX4	B	398	-	-	0±0,49,49,49	-
3	PX4	C	326	-	-	0±0,49,49,49	-
3	PX4	C	346	-	-	0±0,49,49,49	-
3	PX4	B	397	-	-	0±0,49,49,49	-
3	PX4	A	648	-	-	0±0,49,49,49	-
3	PX4	B	362	-	-	0±0,49,49,49	-
3	PX4	B	313	-	-	0±0,49,49,49	-
3	PX4	C	343	-	-	0±0,49,49,49	-
3	PX4	A	623	-	-	0±0,49,49,49	-
3	PX4	B	319	-	-	0±0,49,49,49	-
3	PX4	B	354	-	-	0±0,49,49,49	-
3	PX4	A	634	-	-	0±0,49,49,49	-
3	PX4	B	358	-	-	0±0,49,49,49	-
3	PX4	B	382	-	-	0±0,49,49,49	-
3	PX4	A	624	-	-	0±0,49,49,49	-
3	PX4	B	394	-	-	0±0,49,49,49	-
3	PX4	B	327	-	-	0±0,49,49,49	-
3	PX4	C	340	-	-	0±0,49,49,49	-
3	PX4	C	302	-	-	0±0,49,49,49	-
3	PX4	B	390	-	-	0±0,49,49,49	-
3	PX4	B	341	-	-	0±0,49,49,49	-
3	PX4	B	310	-	-	0±0,49,49,49	-
3	PX4	B	387	-	-	0±0,49,49,49	-
3	PX4	C	324	-	-	0±0,49,49,49	-
3	PX4	C	317	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	369	-	-	0±0,49,49,49	-
3	PX4	B	344	-	-	0±0,49,49,49	-
3	PX4	A	650	-	-	0±0,49,49,49	-
3	PX4	B	302	-	-	0±0,49,49,49	-
3	PX4	B	357	-	-	0±0,49,49,49	-
3	PX4	B	340	-	-	0±0,49,49,49	-
3	PX4	B	400	-	-	0±0,49,49,49	-
3	PX4	C	314	-	-	0±0,49,49,49	-
3	PX4	A	646	-	-	0±0,49,49,49	-
3	PX4	C	304	-	-	0±0,49,49,49	-
3	PX4	B	365	-	-	0±0,49,49,49	-
3	PX4	B	316	-	-	0±0,49,49,49	-
3	PX4	B	378	-	-	0±0,49,49,49	-
3	PX4	B	321	-	-	0±0,49,49,49	-
3	PX4	B	353	-	-	0±0,49,49,49	-
3	PX4	B	388	-	-	0±0,49,49,49	-
3	PX4	B	348	-	-	0±0,49,49,49	-
3	PX4	A	606	-	-	0±0,49,49,49	-
3	PX4	A	633	-	-	0±0,49,49,49	-
3	PX4	A	641	-	-	0±0,49,49,49	-
3	PX4	A	630	-	-	0±0,49,49,49	-
3	PX4	A	607	-	-	0±0,49,49,49	-
3	PX4	C	331	-	-	0±0,49,49,49	-
3	PX4	A	642	-	-	0±0,49,49,49	-
3	PX4	A	640	-	-	0±0,49,49,49	-
3	PX4	A	611	-	-	0±0,49,49,49	-
3	PX4	C	355	-	-	0±0,49,49,49	-
3	PX4	A	625	-	-	0±0,49,49,49	-
3	PX4	B	301	-	-	0±0,49,49,49	-
3	PX4	A	653	-	-	0±0,49,49,49	-
3	PX4	B	375	-	-	0±0,49,49,49	-
3	PX4	B	374	-	-	0±0,49,49,49	-
3	PX4	C	354	-	-	0±0,49,49,49	-
3	PX4	C	358	-	-	0±0,49,49,49	-
3	PX4	C	323	-	-	0±0,49,49,49	-
3	PX4	B	372	-	-	0±0,49,49,49	-
3	PX4	B	308	-	-	0±0,49,49,49	-
3	PX4	C	364	-	-	0±0,49,49,49	-
3	PX4	B	345	-	-	0±0,49,49,49	-
3	PX4	A	636	-	-	0±0,49,49,49	-
3	PX4	B	377	-	-	0±0,49,49,49	-
3	PX4	C	342	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	351	-	-	0±0,49,49,49	-
3	PX4	C	315	-	-	0±0,49,49,49	-
3	PX4	B	318	-	-	0±0,49,49,49	-

5 of 3857 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	322	PX4	C2-C1	5.97	1.69	1.51	1	5
3	B	352	PX4	C2-C1	5.78	1.68	1.51	2	6
3	B	313	PX4	C6-C7	5.46	1.67	1.50	7	6
3	B	357	PX4	C8-C7	5.44	1.67	1.50	10	5
3	A	611	PX4	C10-C9	5.39	1.66	1.50	3	5

5 of 3527 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	349	PX4	C7-O7-C23	5.89	103.71	117.80	4	6
3	A	653	PX4	O7-C23-C24	5.81	98.91	111.48	12	5
3	B	343	PX4	C7-O7-C23	5.60	104.38	117.80	4	5
3	C	318	PX4	C7-O7-C23	5.56	104.48	117.80	15	4
3	B	341	PX4	C7-O7-C23	5.54	104.54	117.80	11	9

There are no chirality outliers.

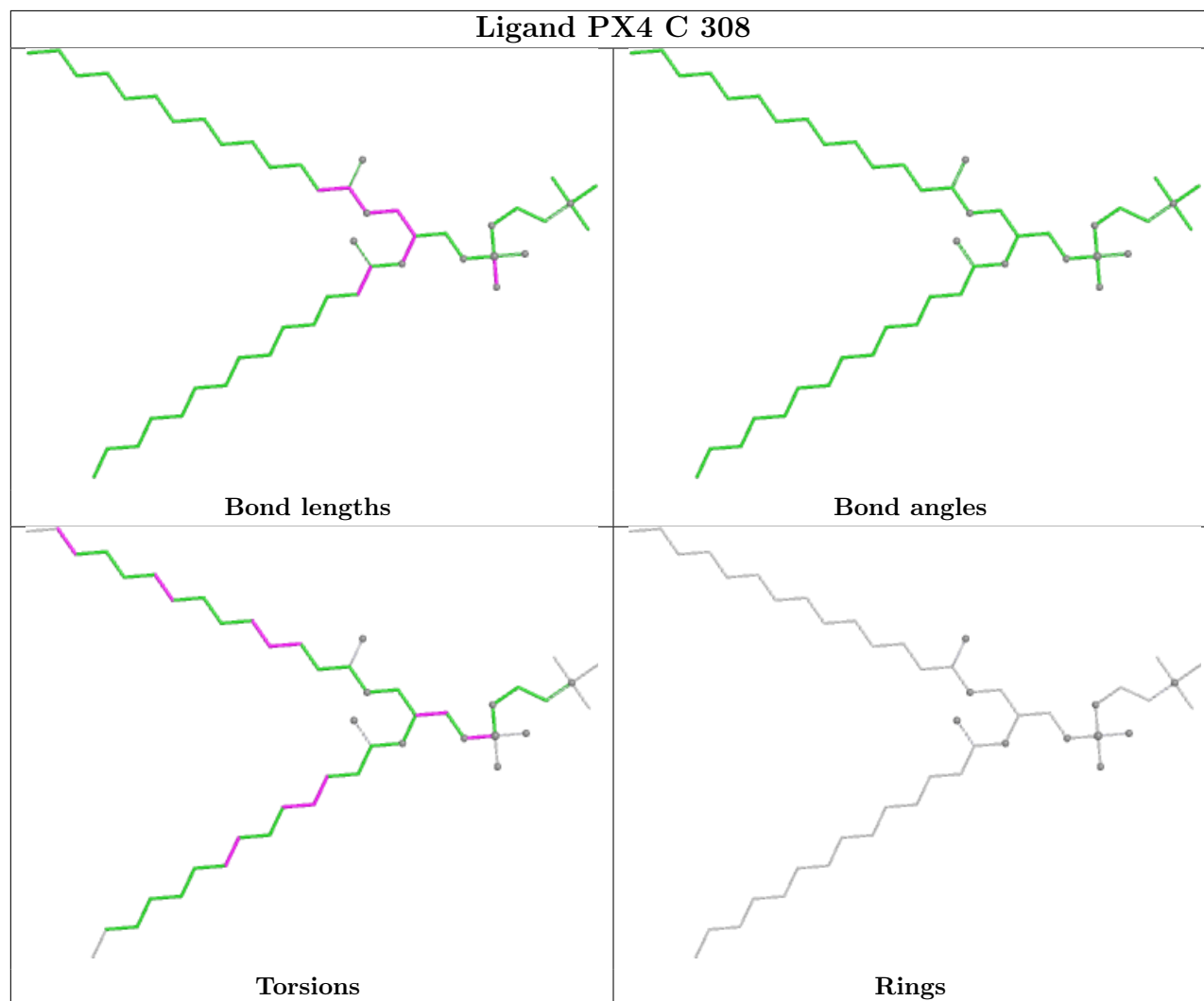
All unique torsion outliers are listed below.

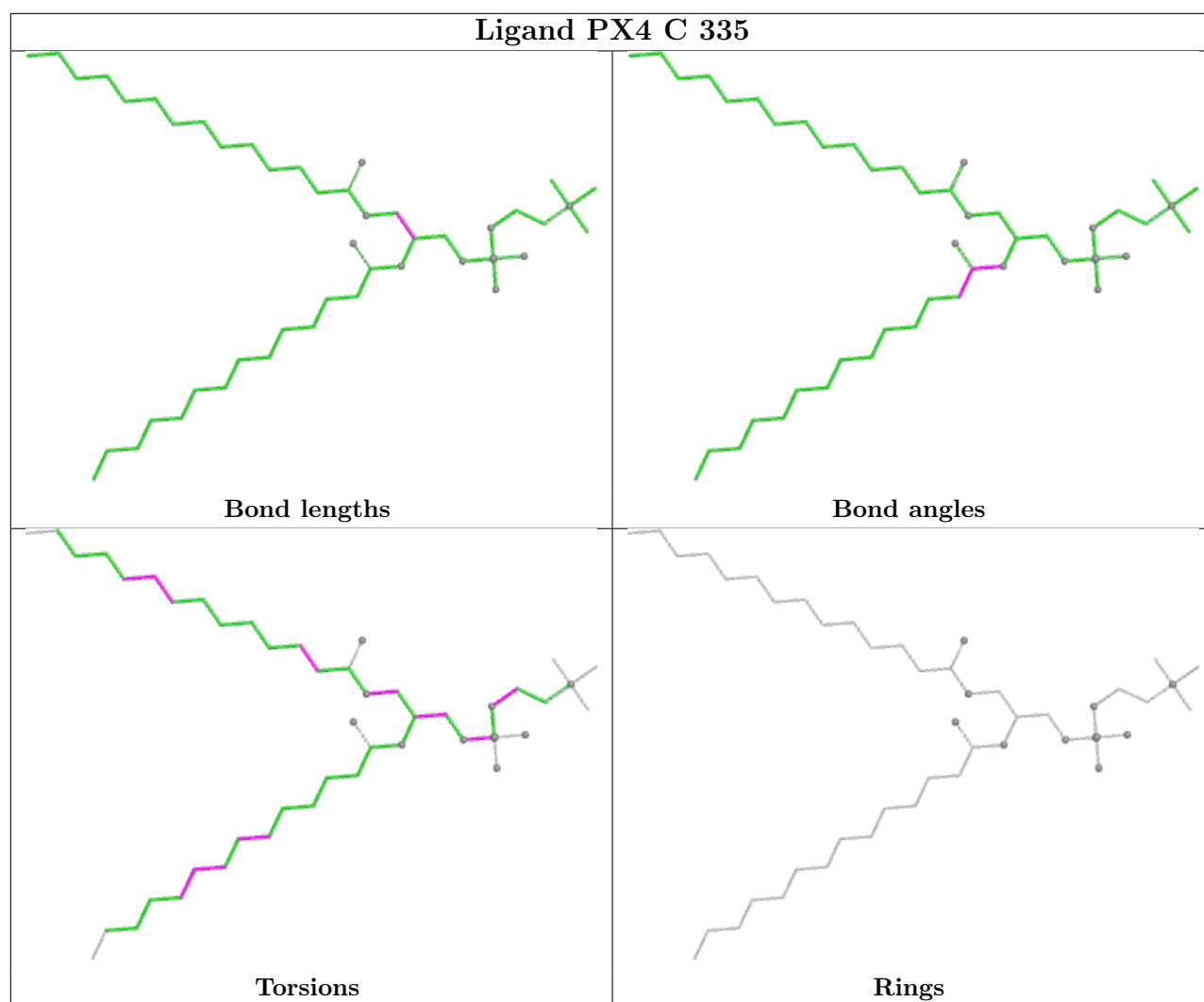
Mol	Chain	Res	Type	Atoms	Models (Total)
3	C	320	PX4	C7-C6-O4-P1	1

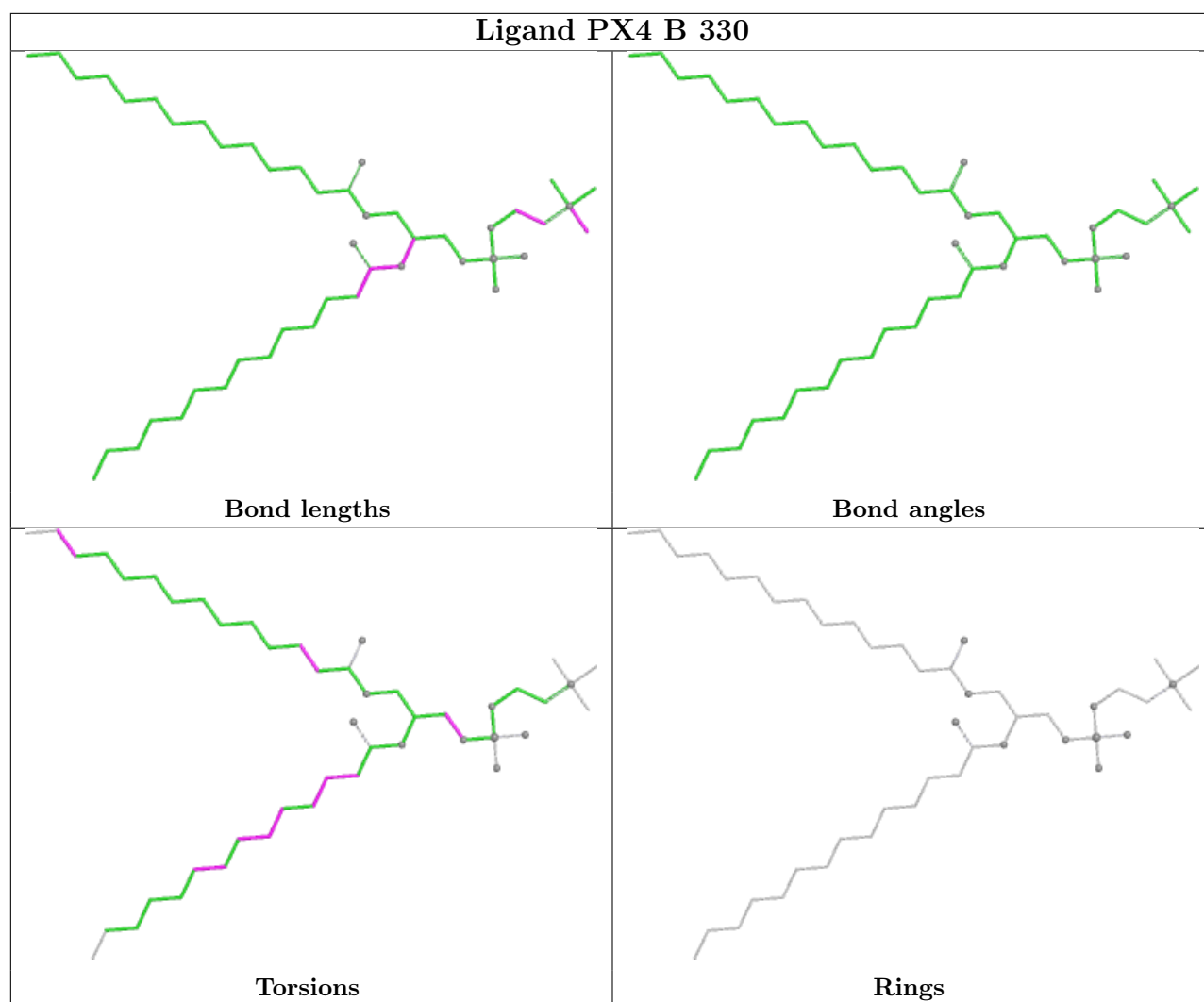
There are no ring outliers.

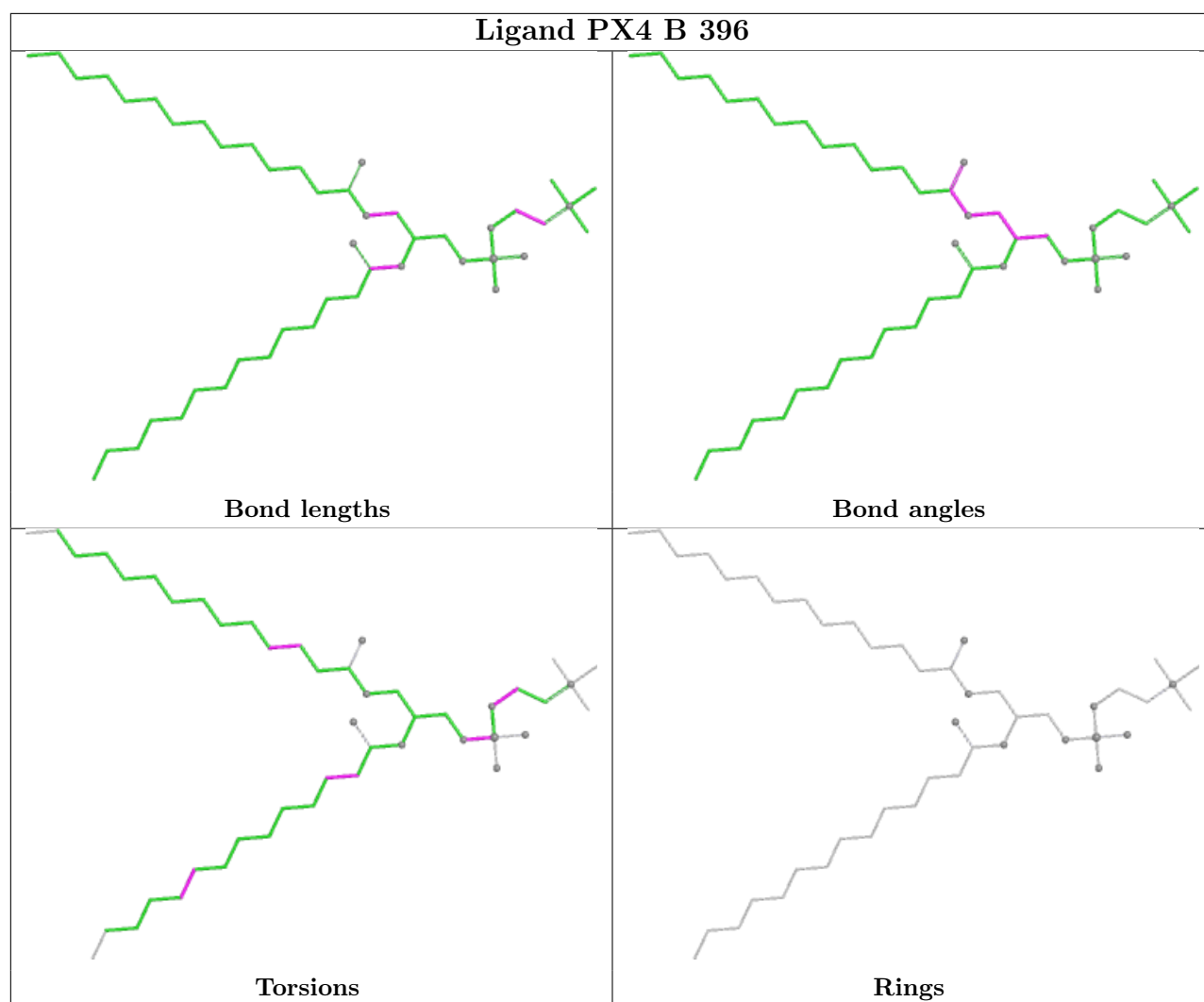
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

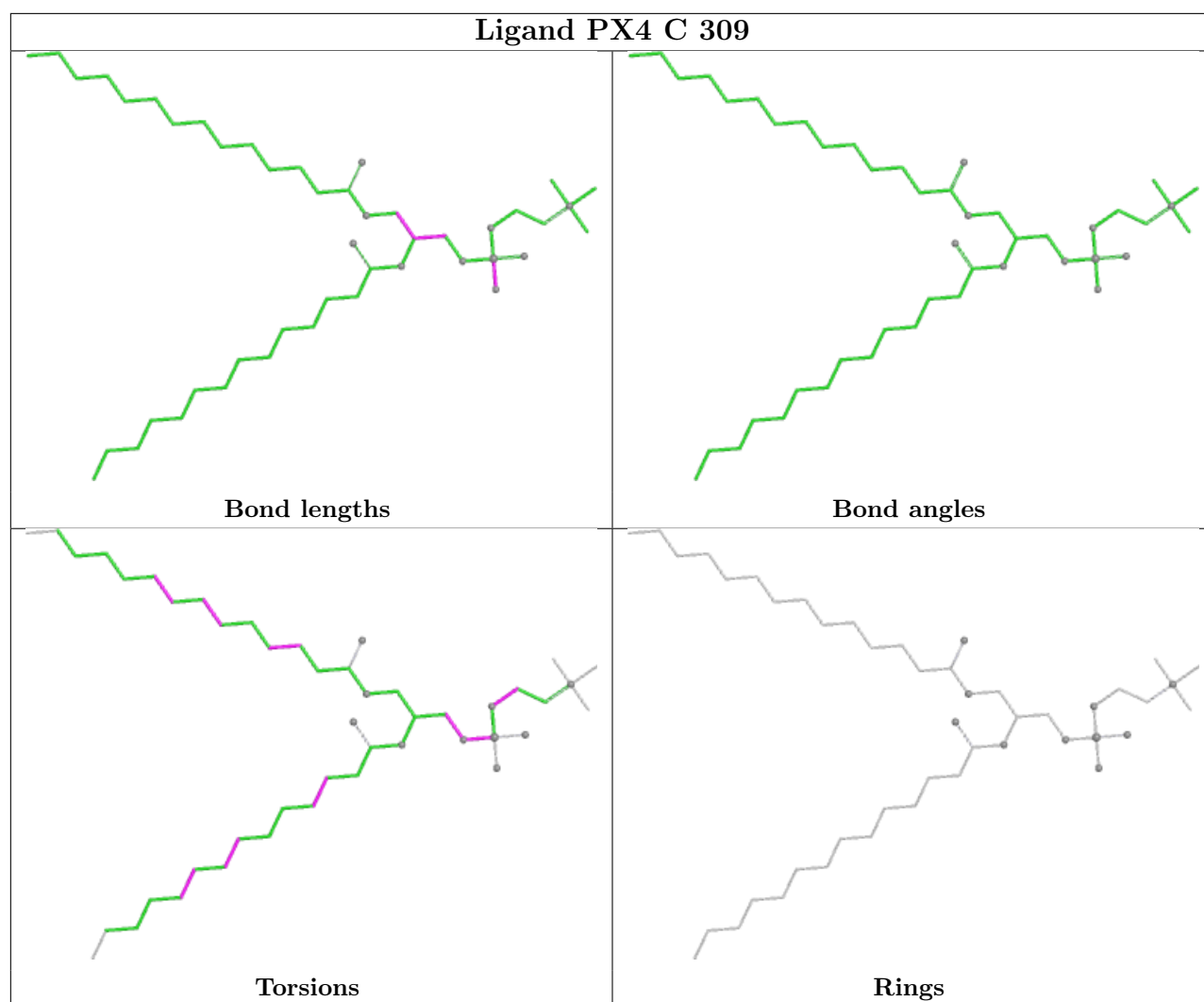
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



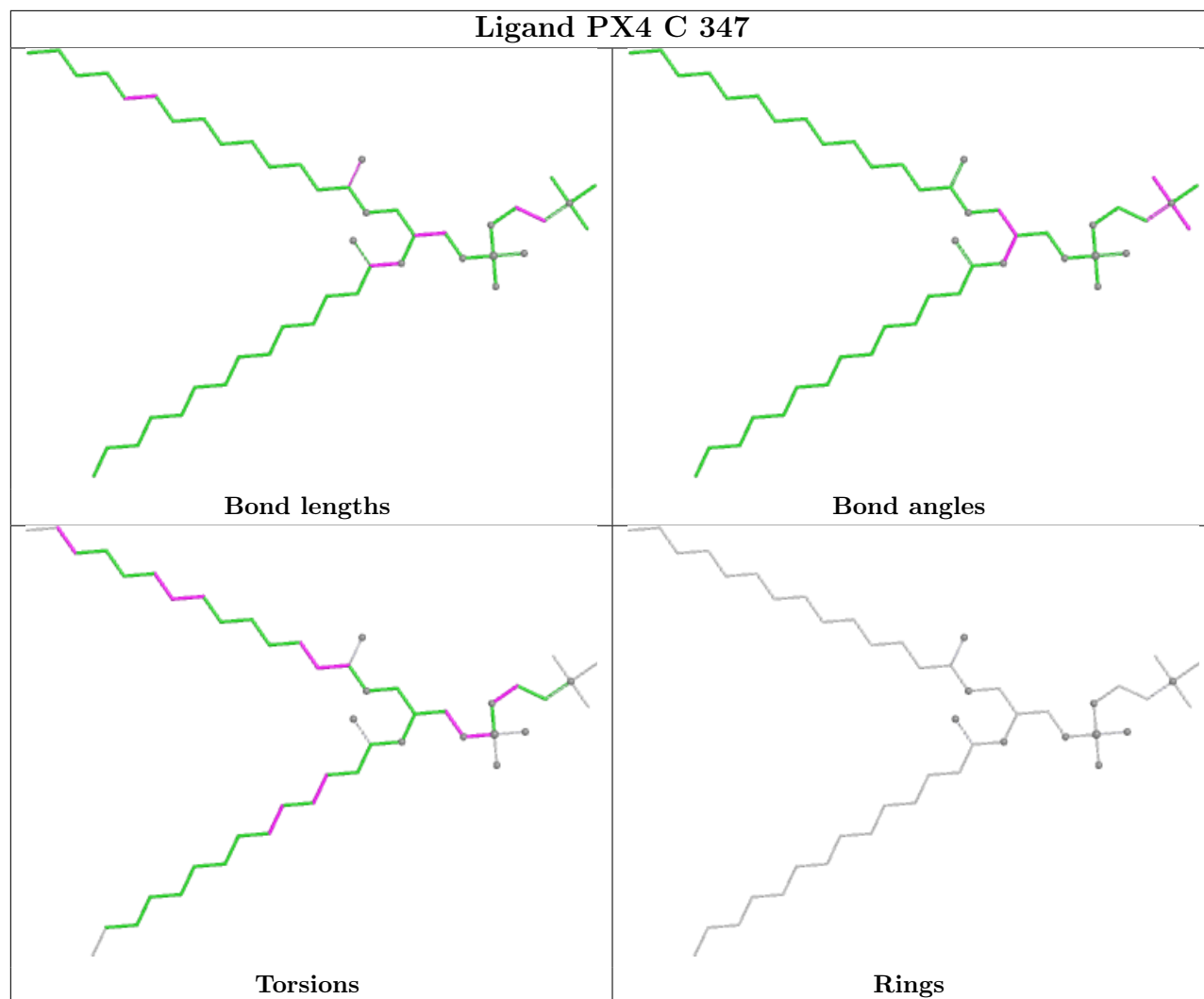


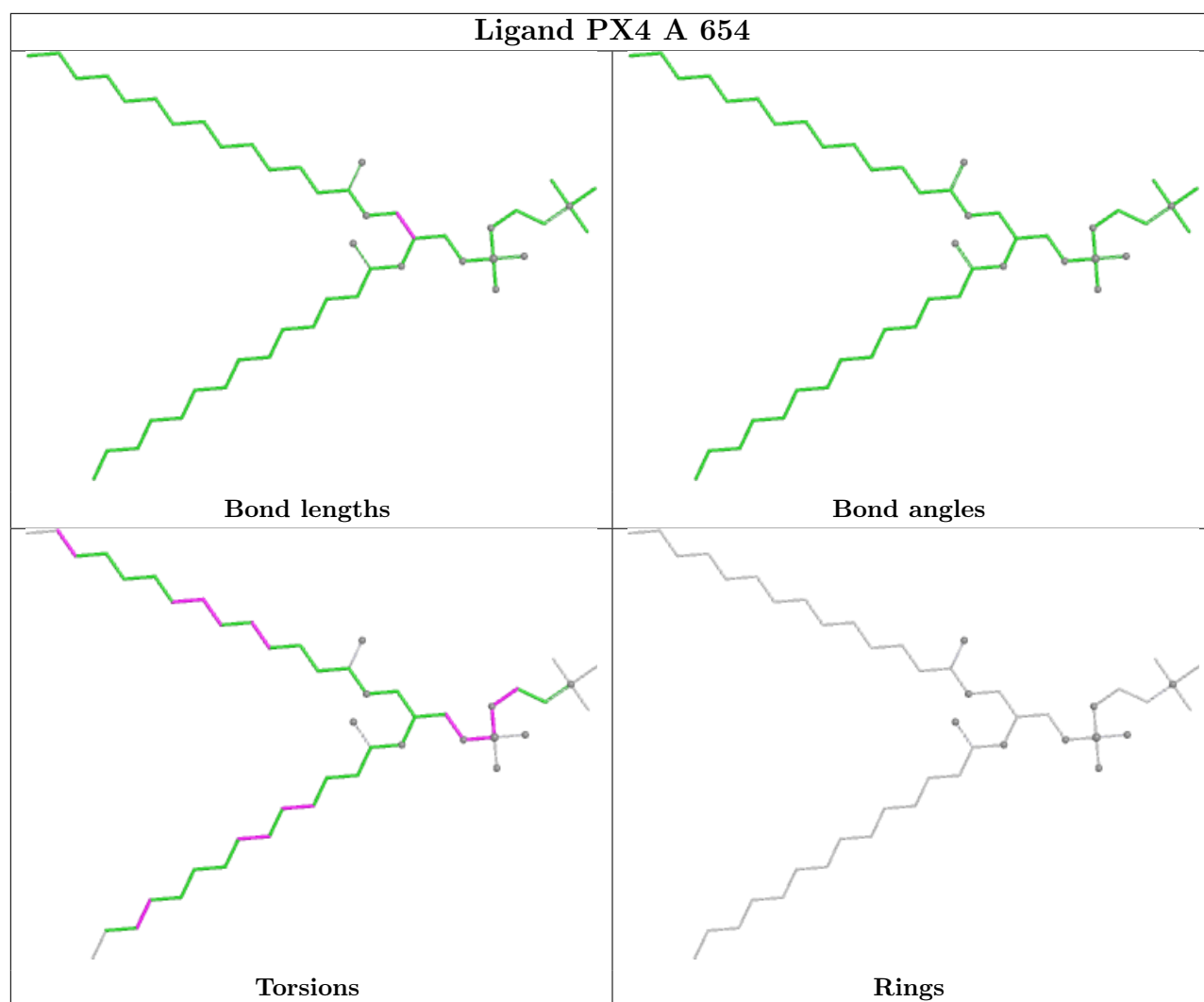


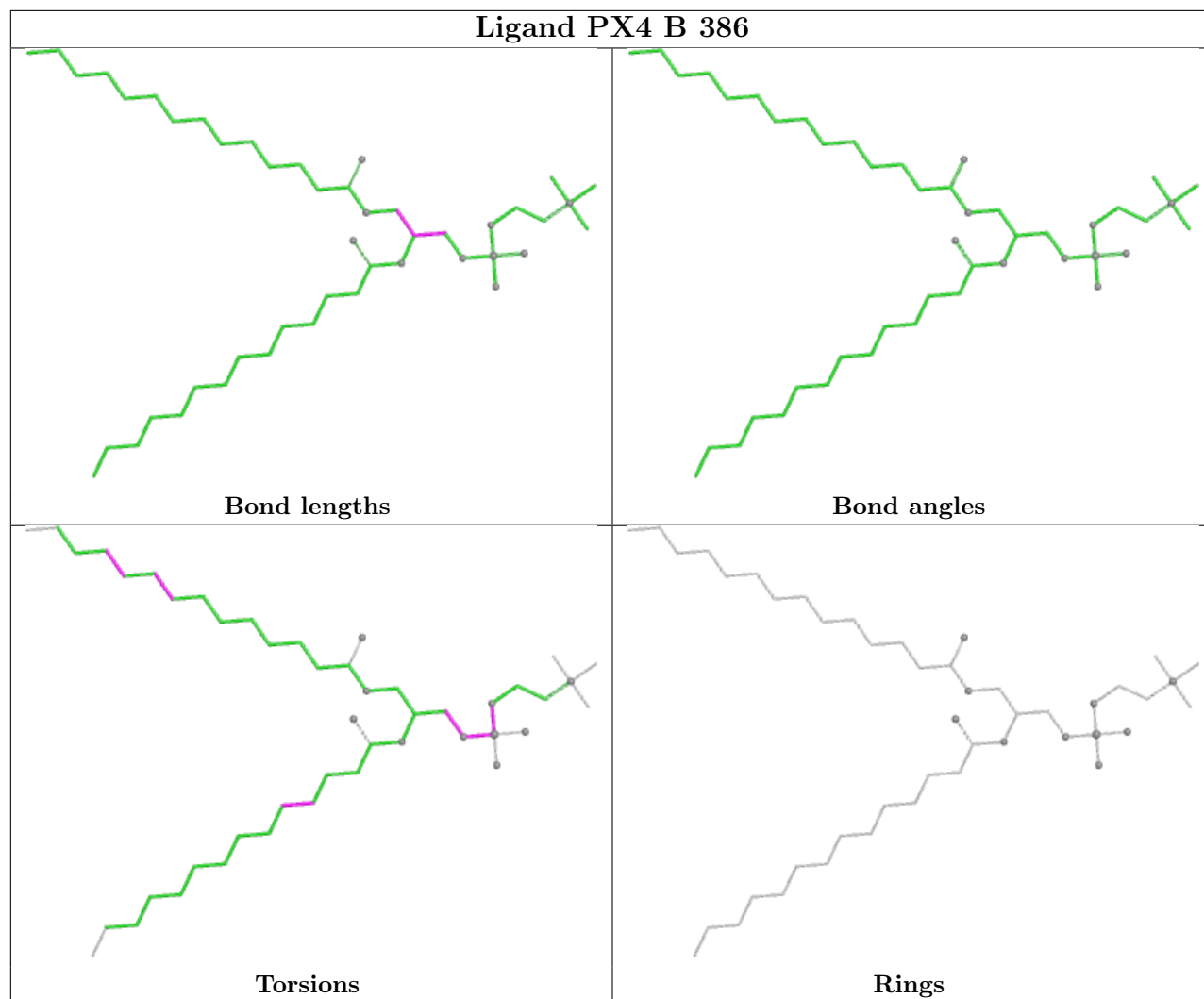


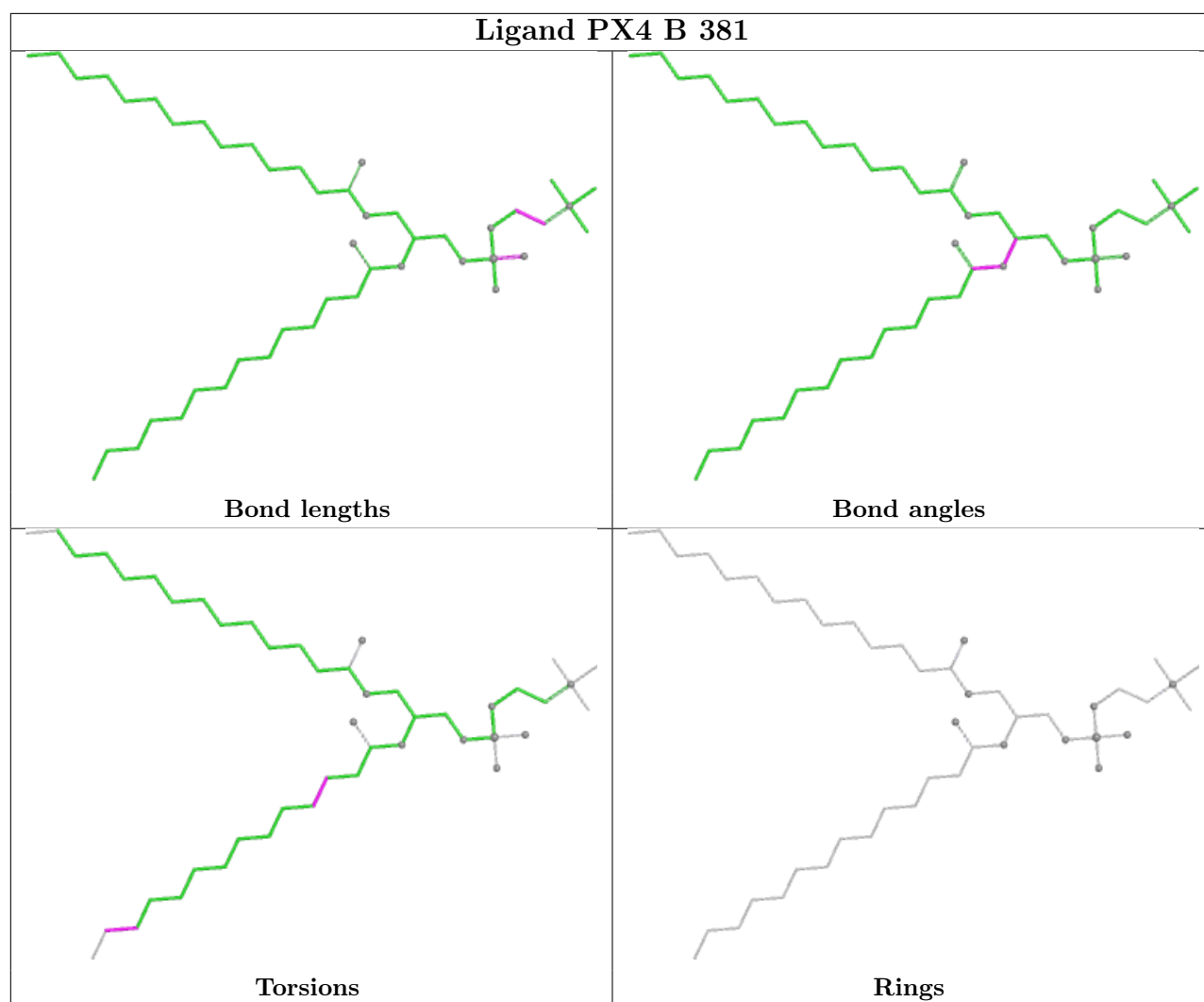


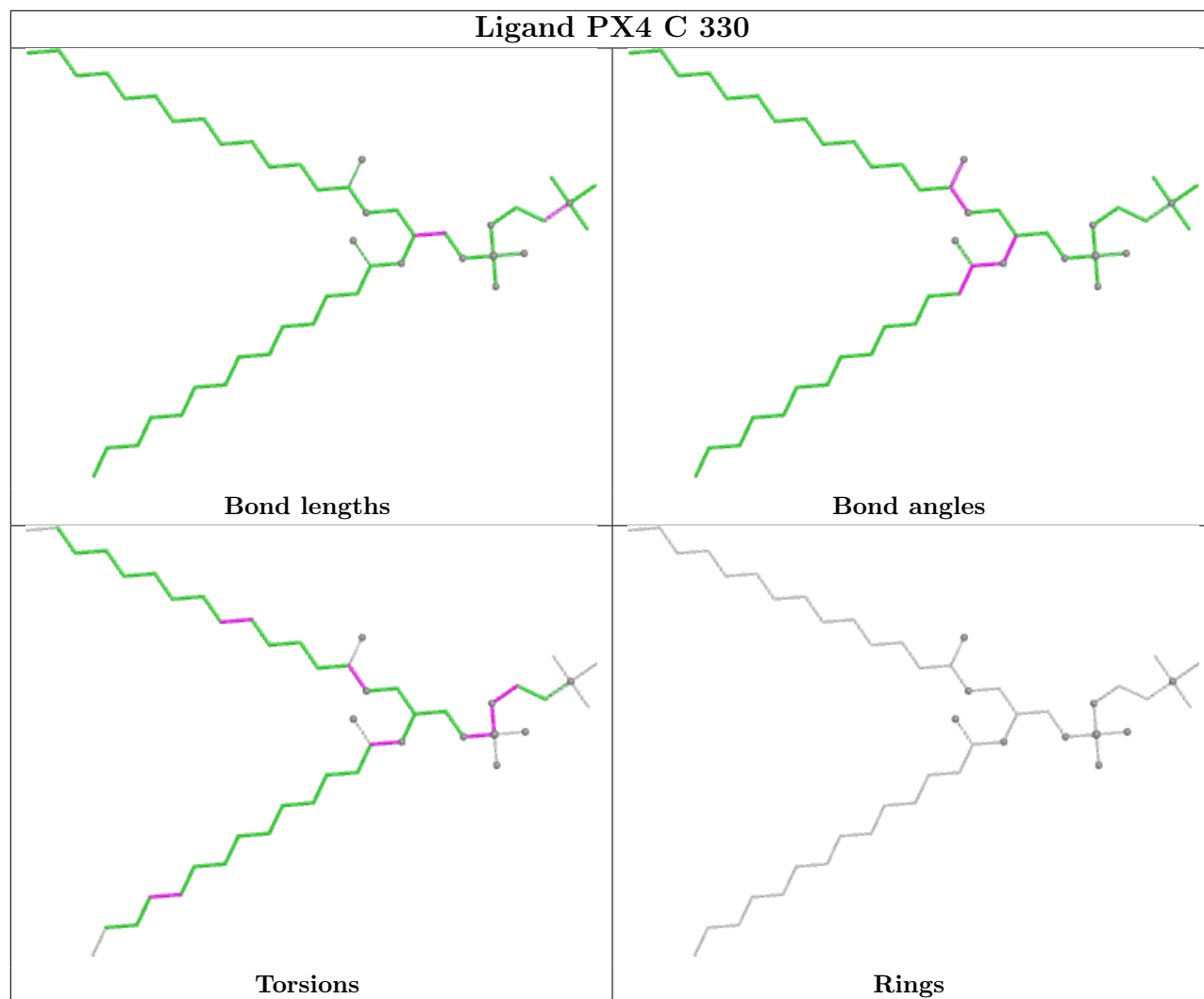
Ligand PX4 C 347

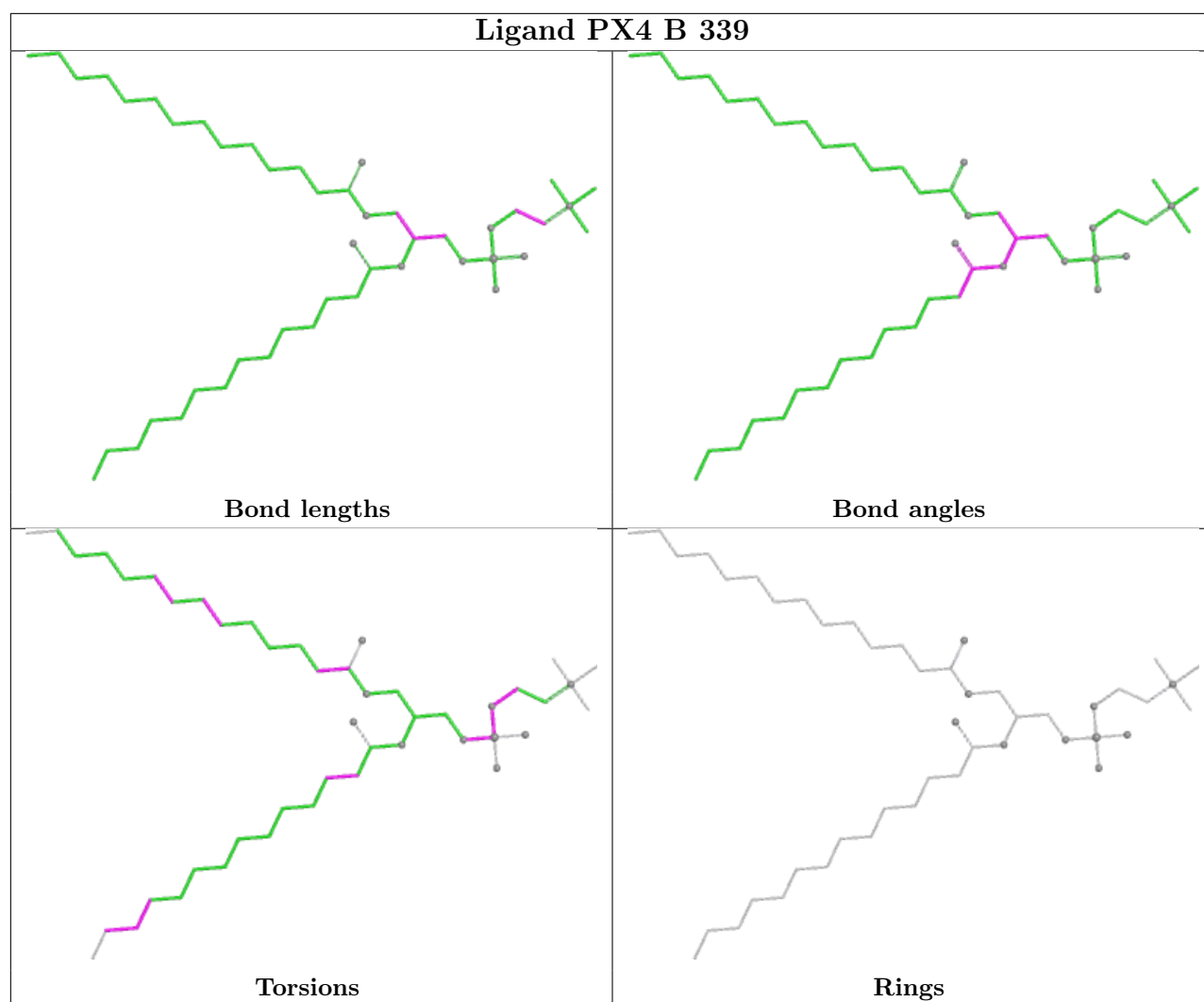




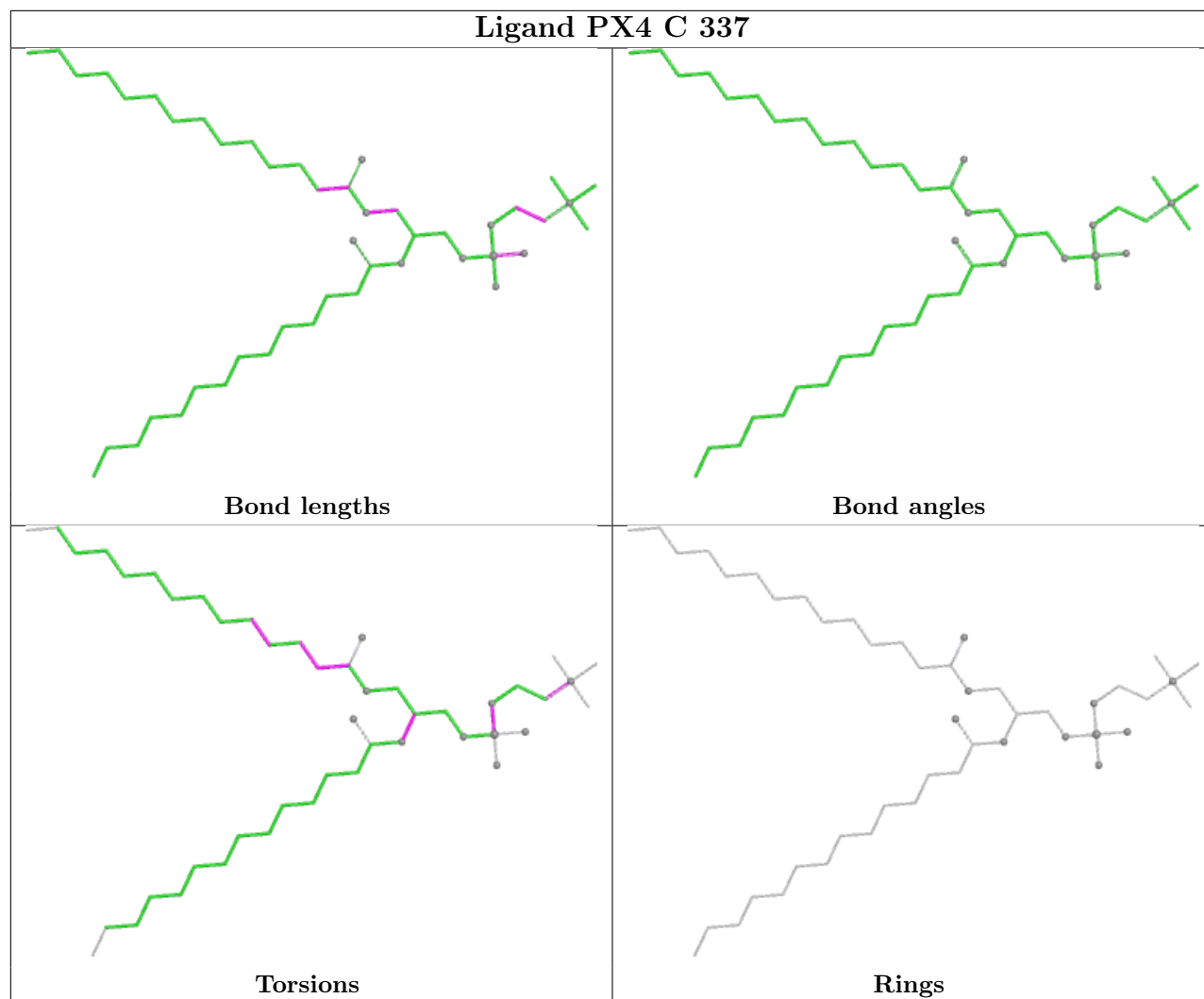


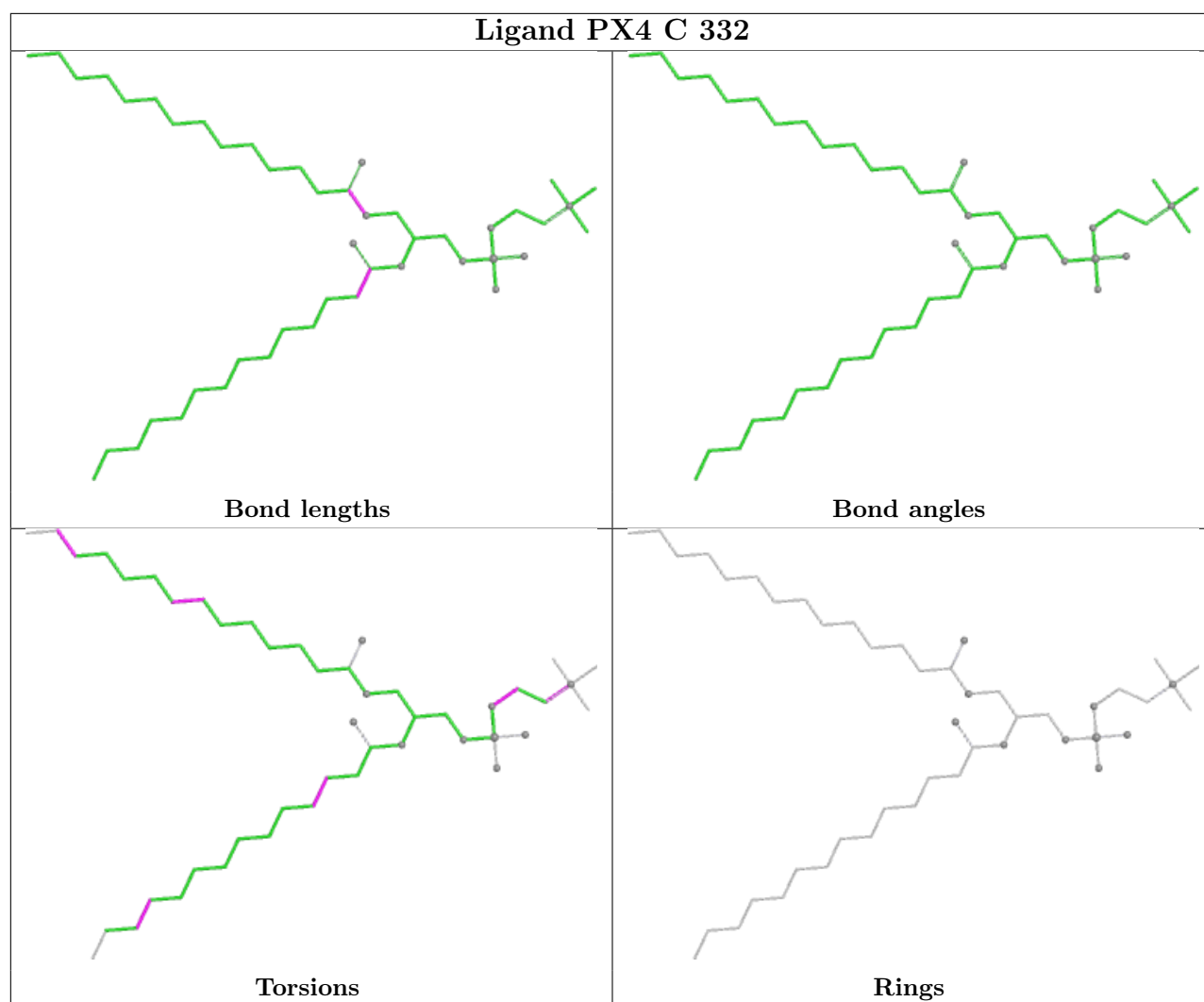




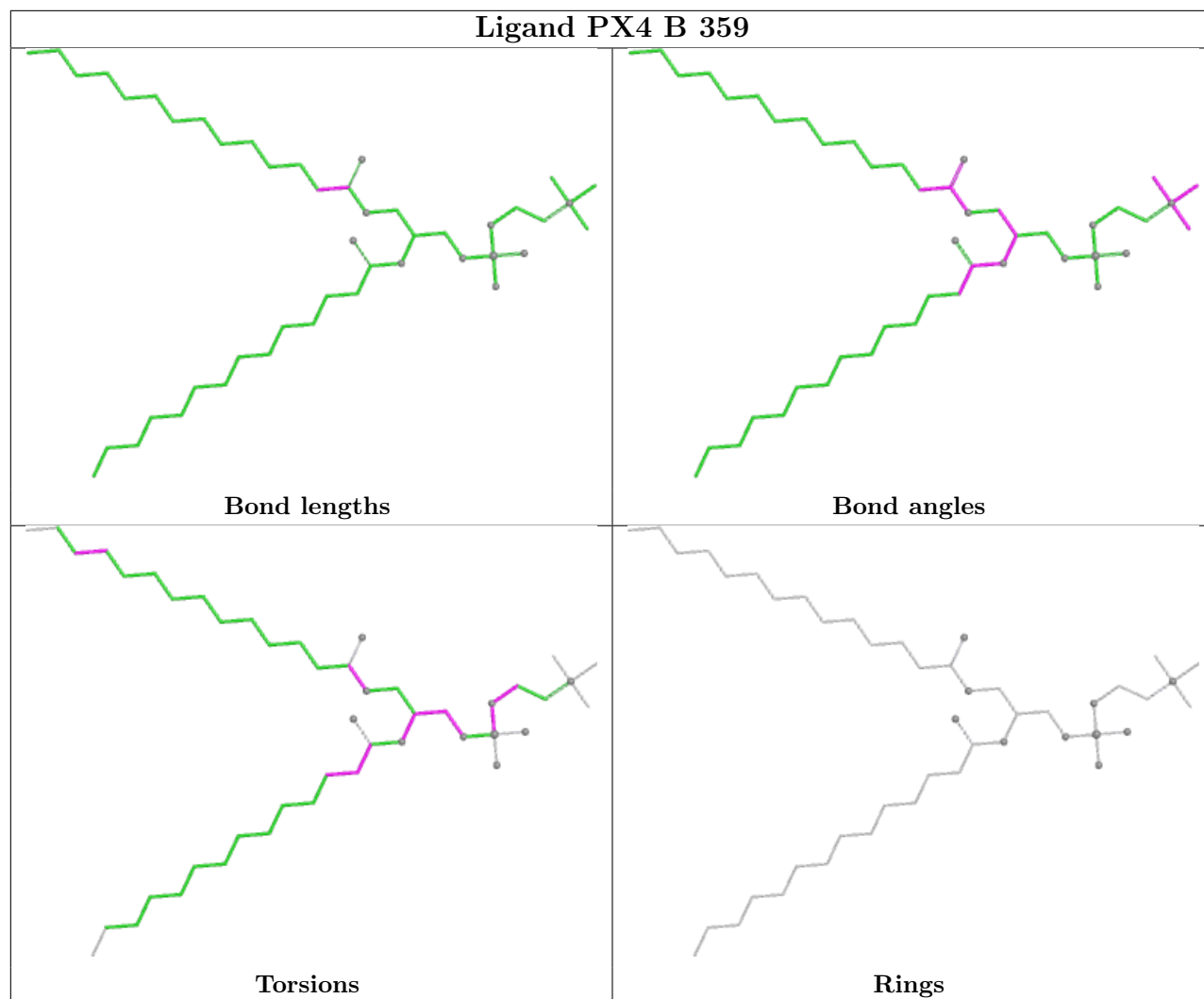


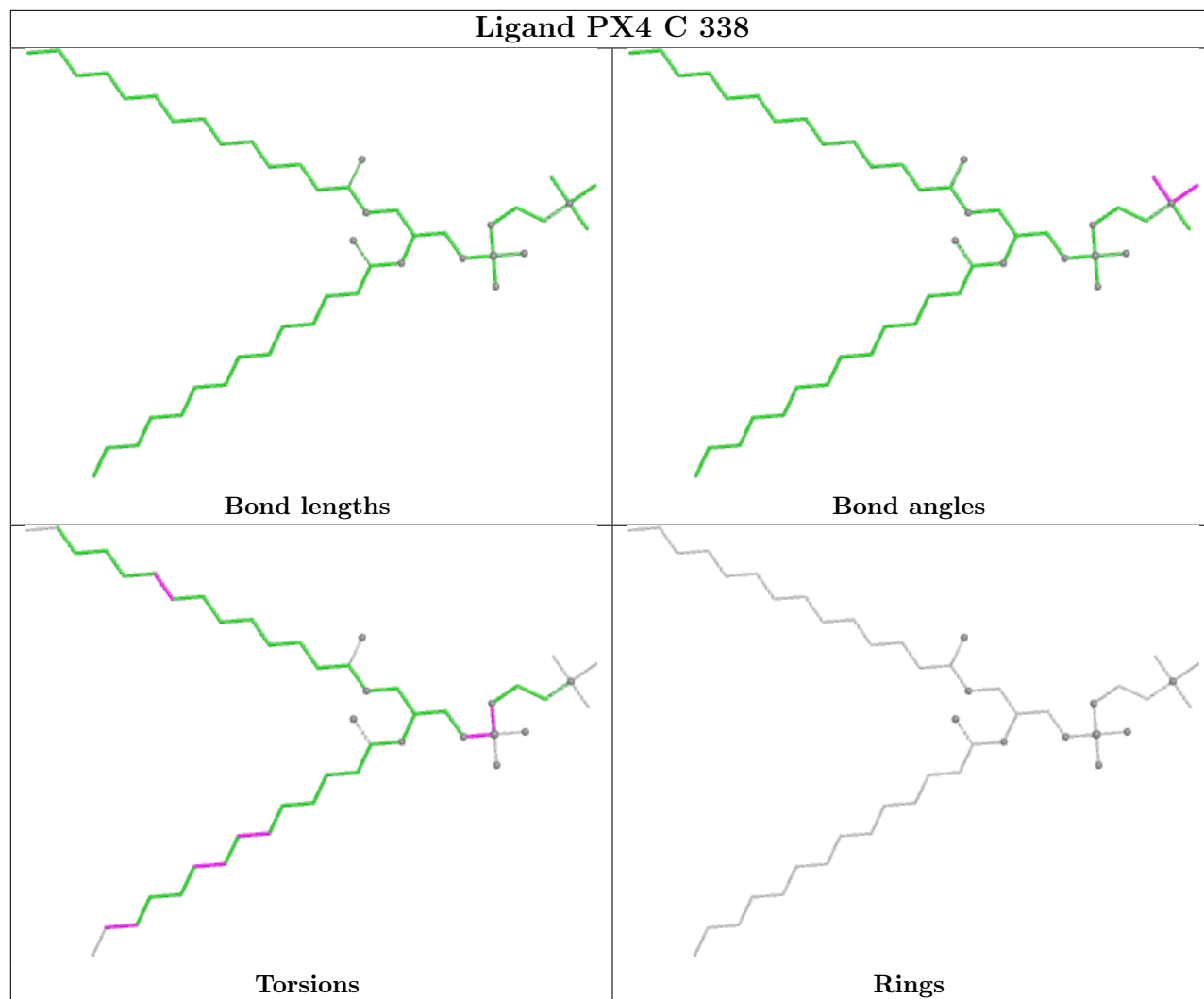
Ligand PX4 C 337

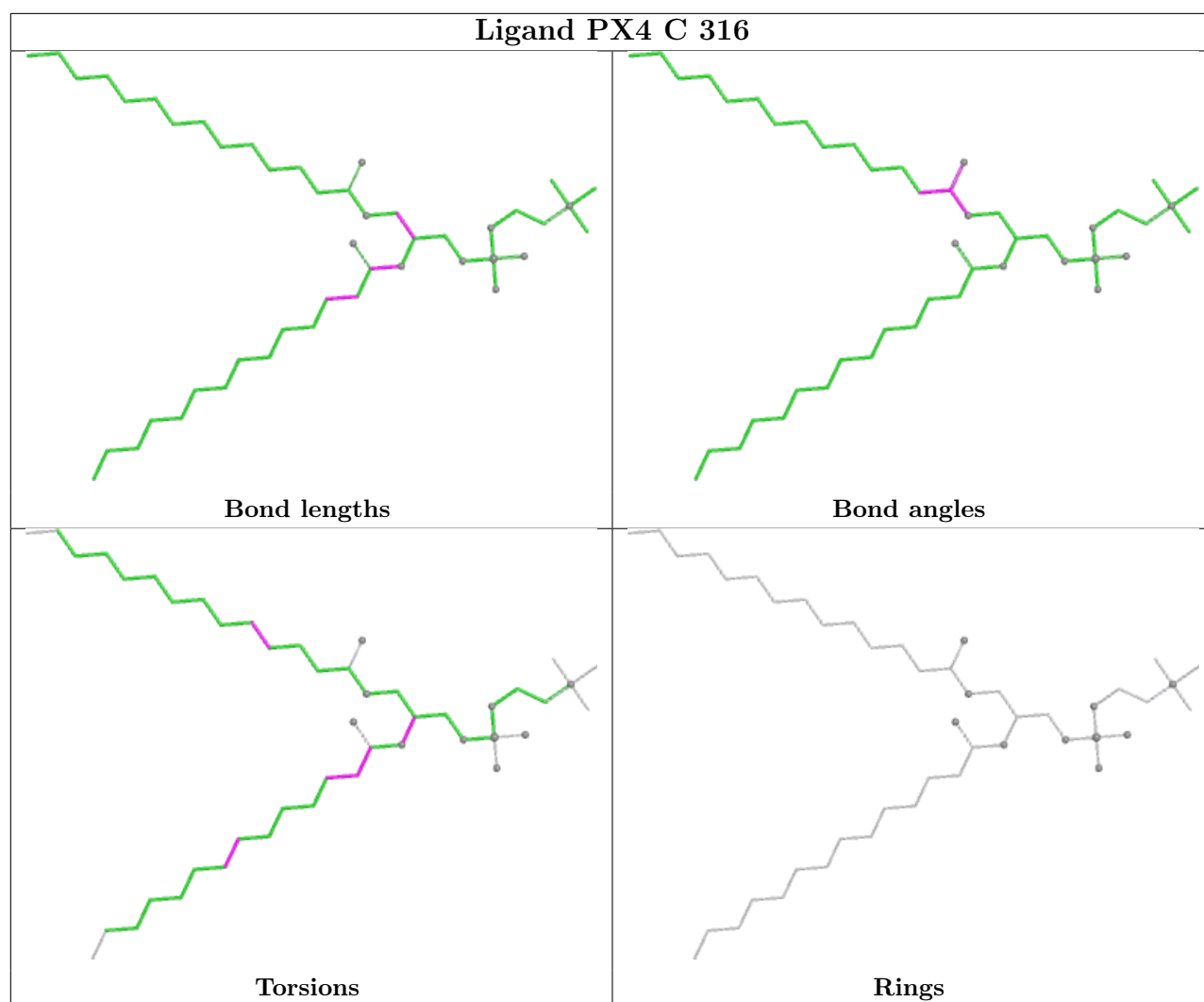


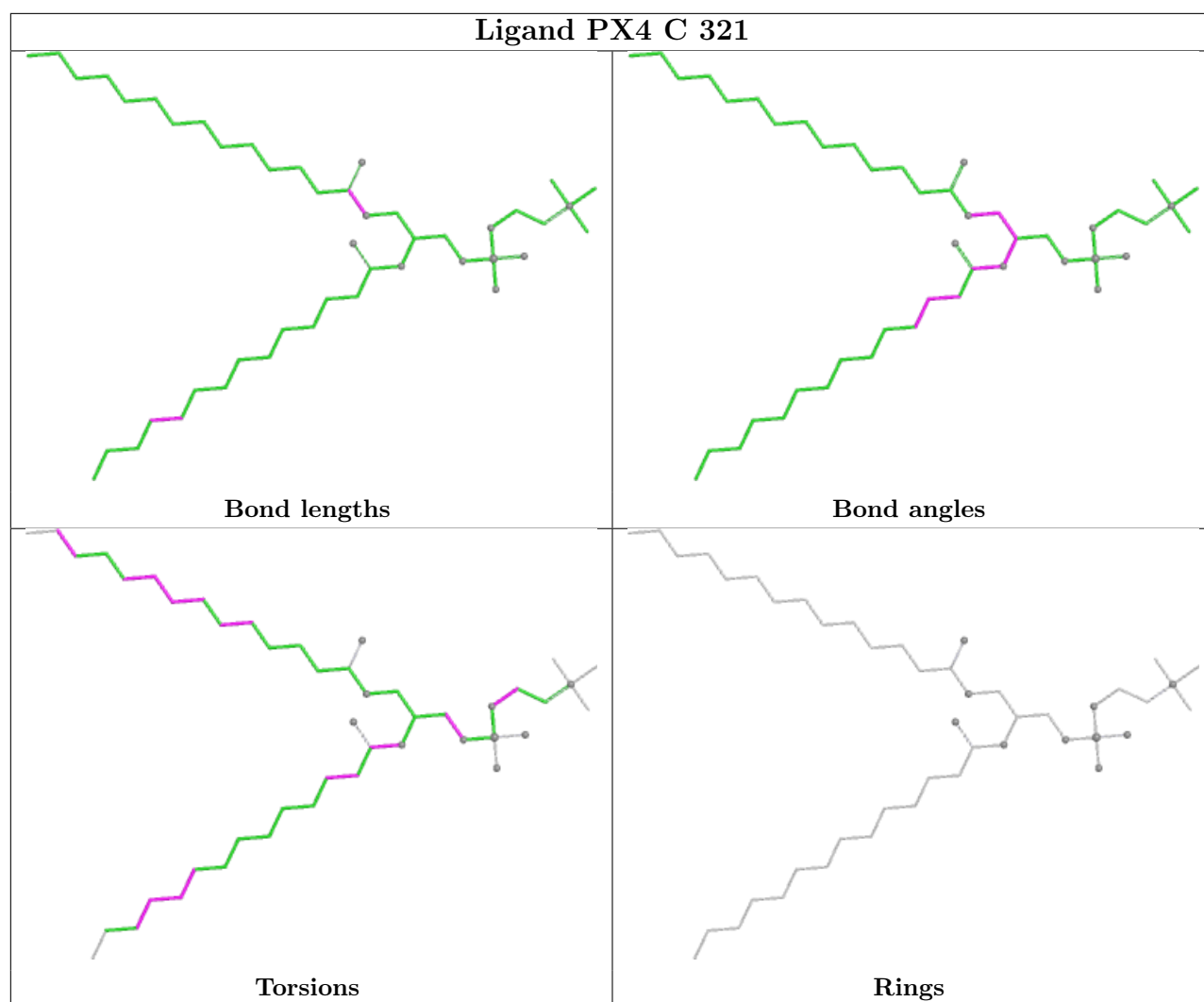


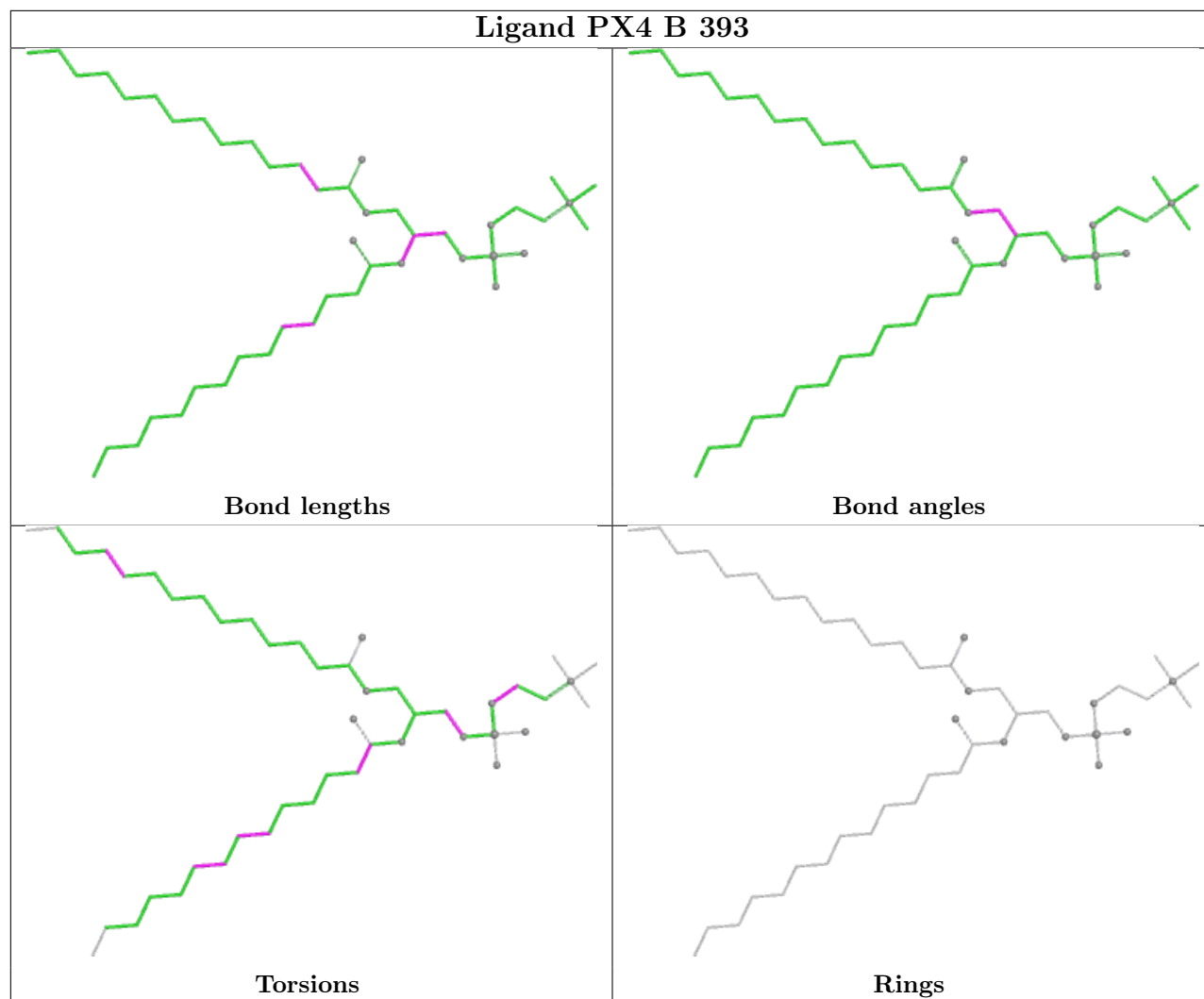
Ligand PX4 B 359

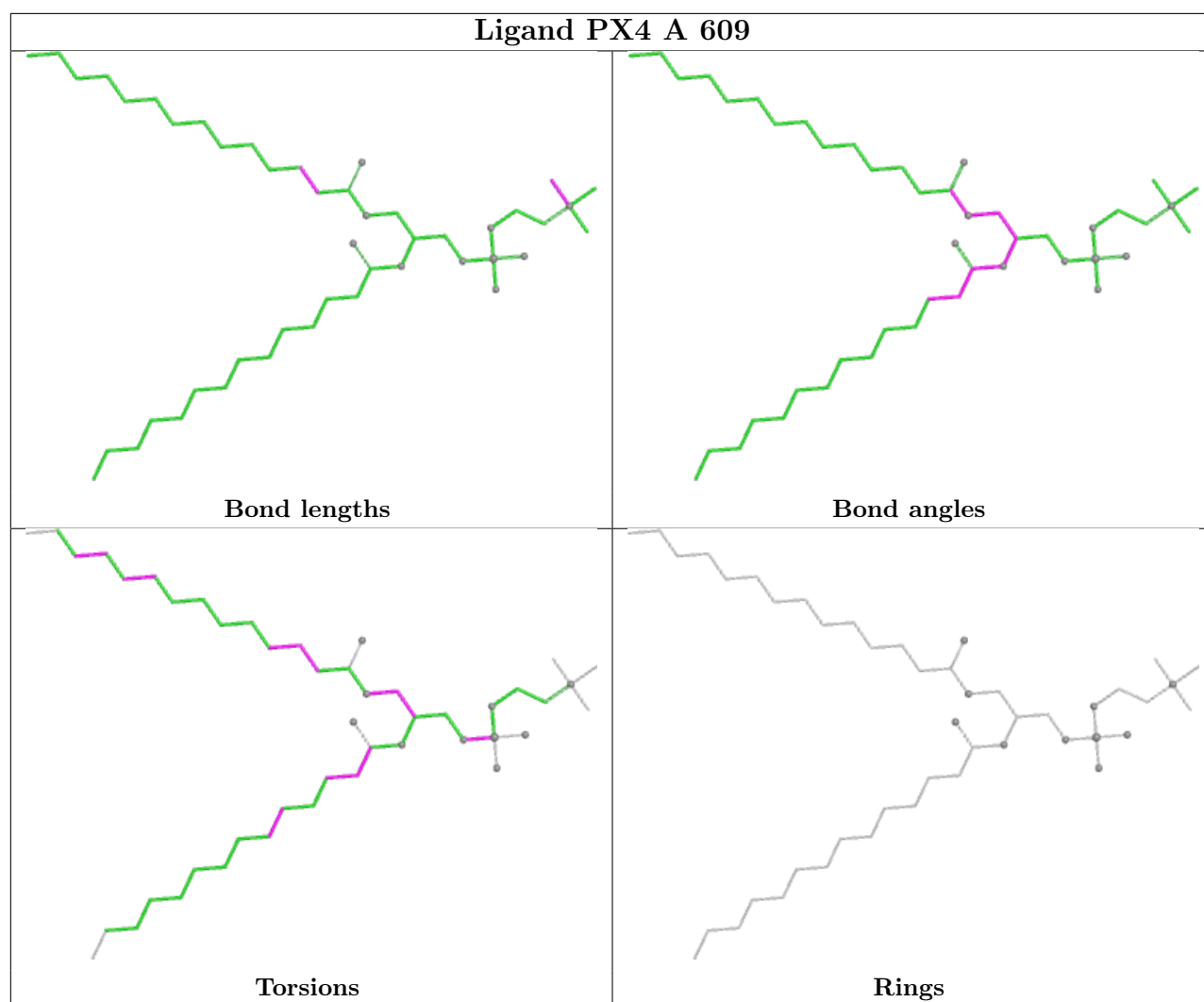


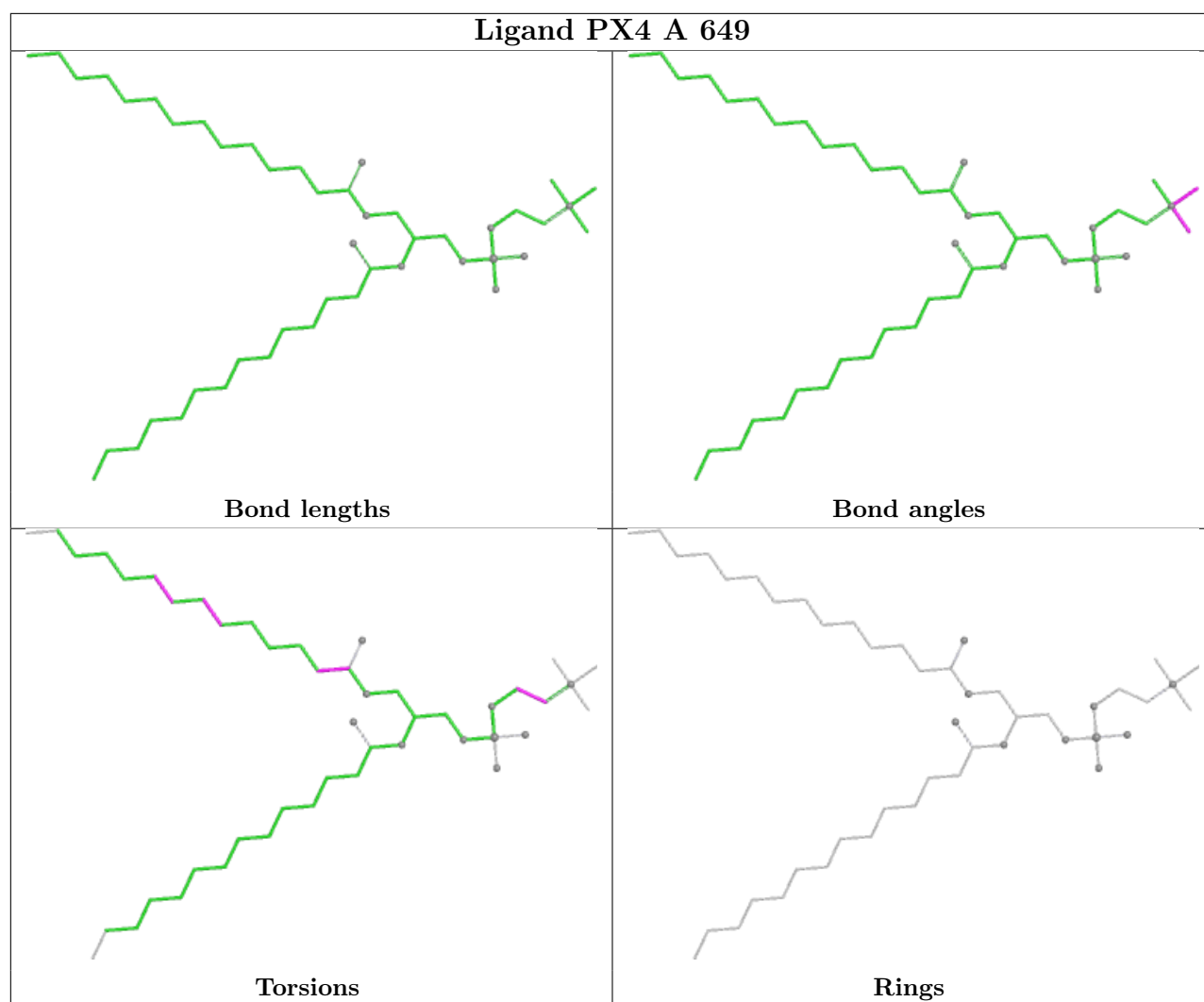


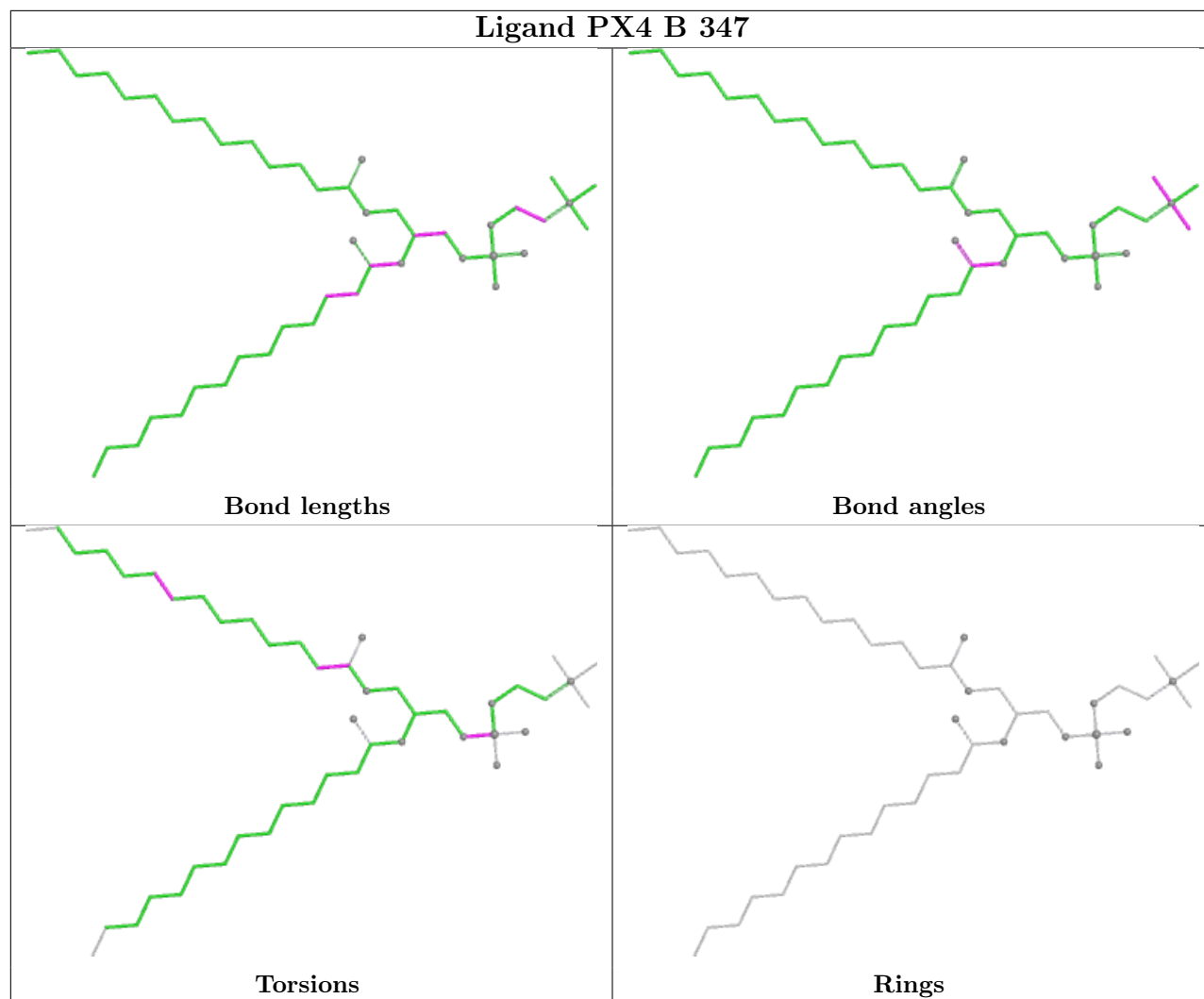


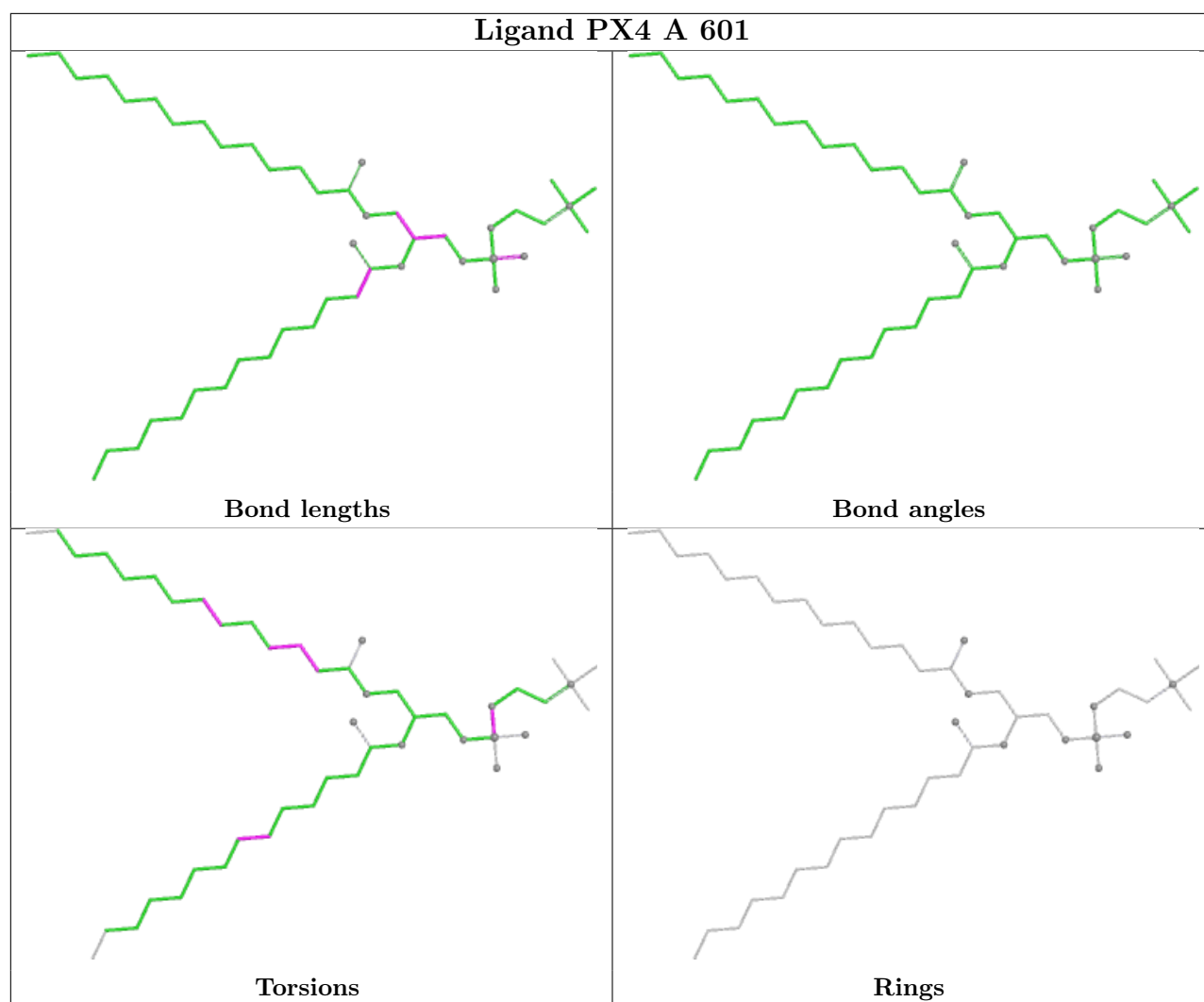




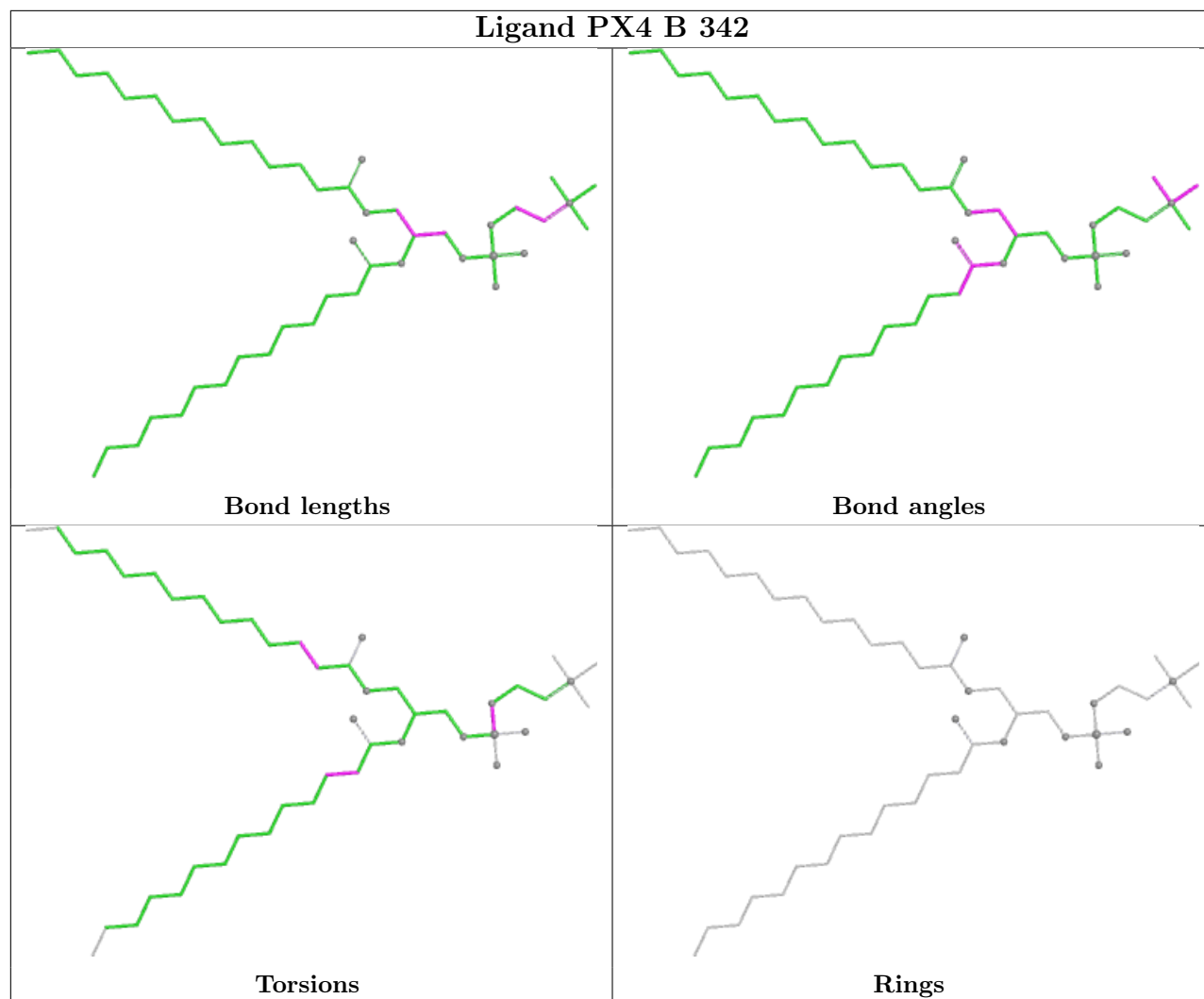


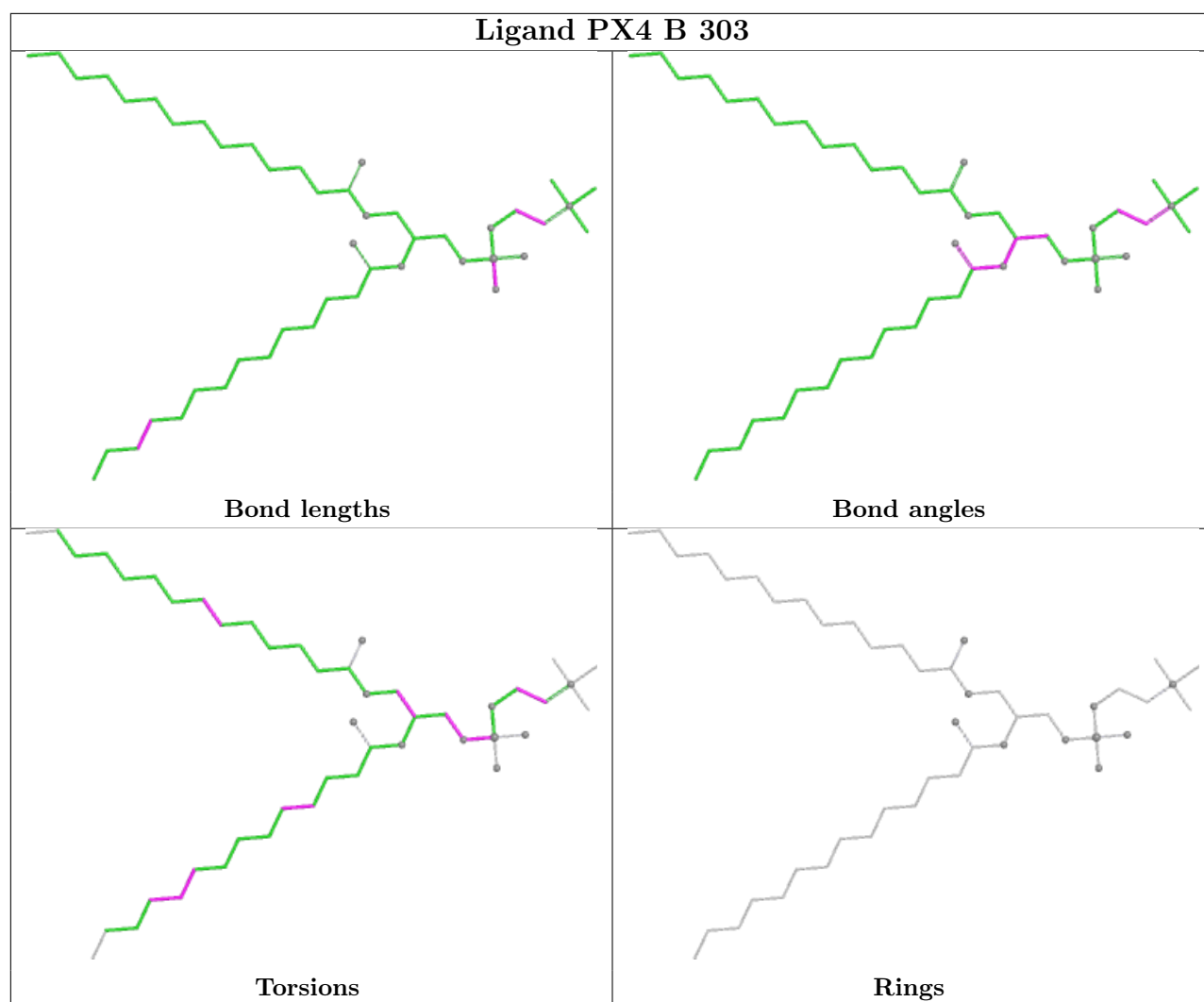


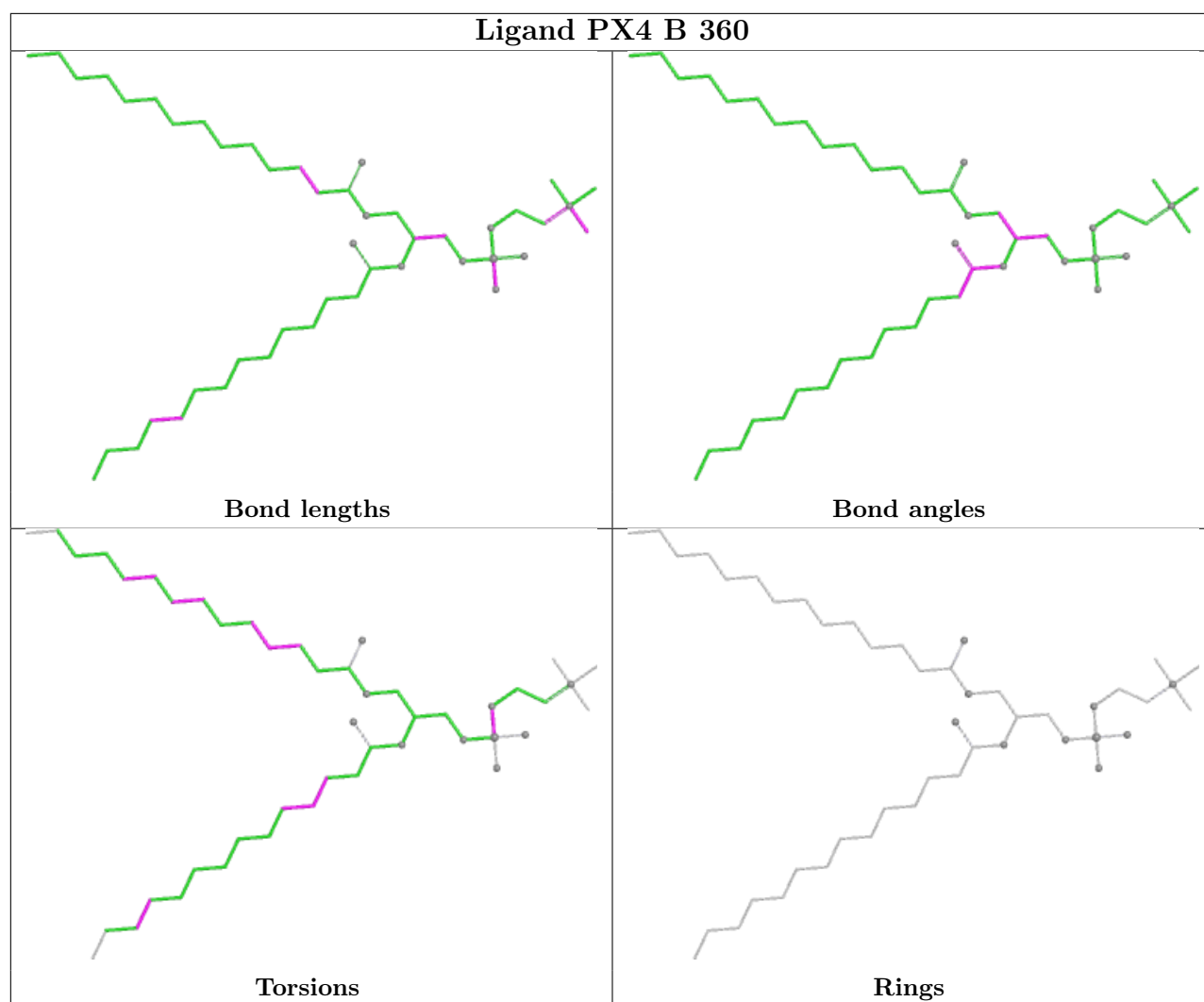


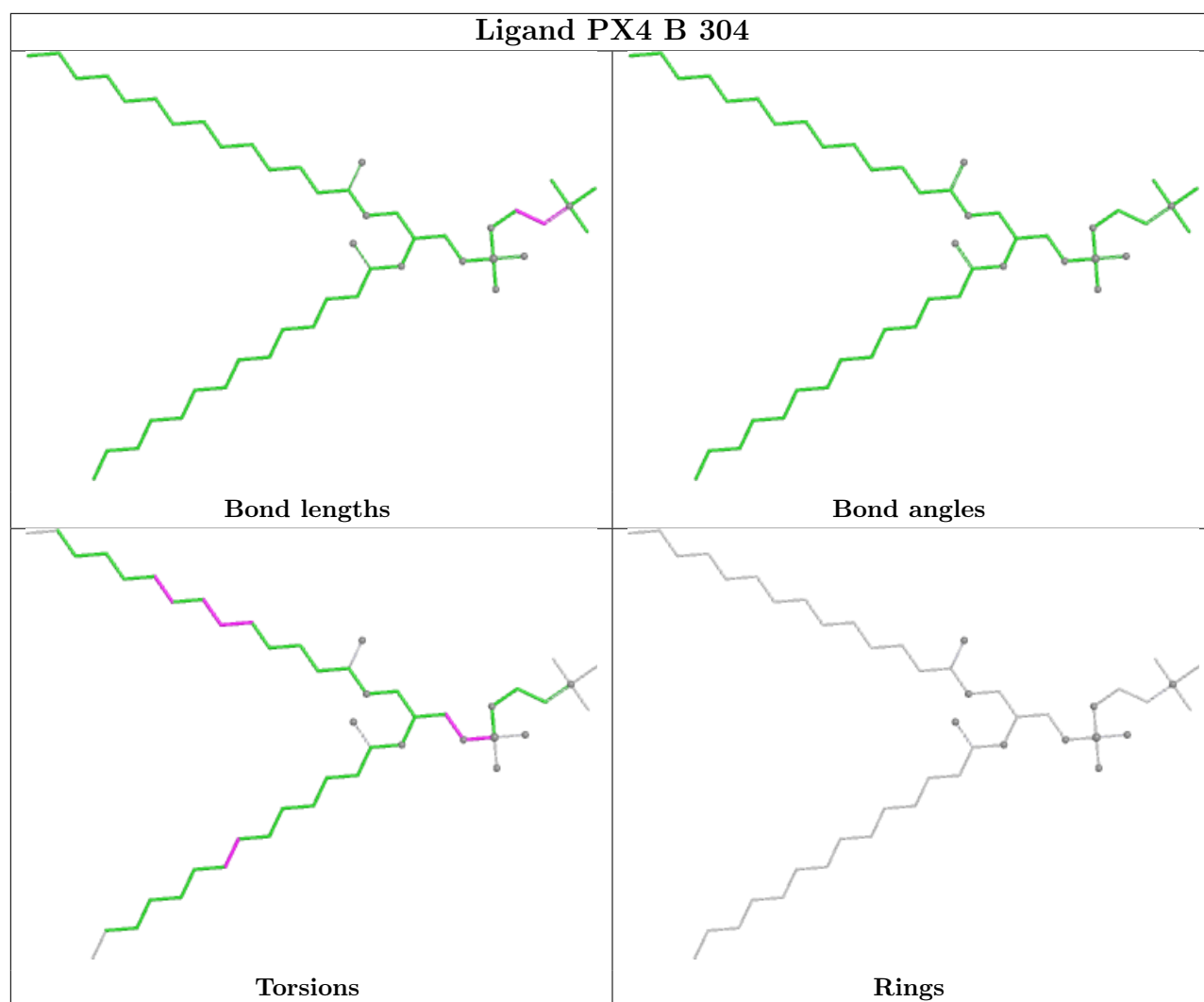


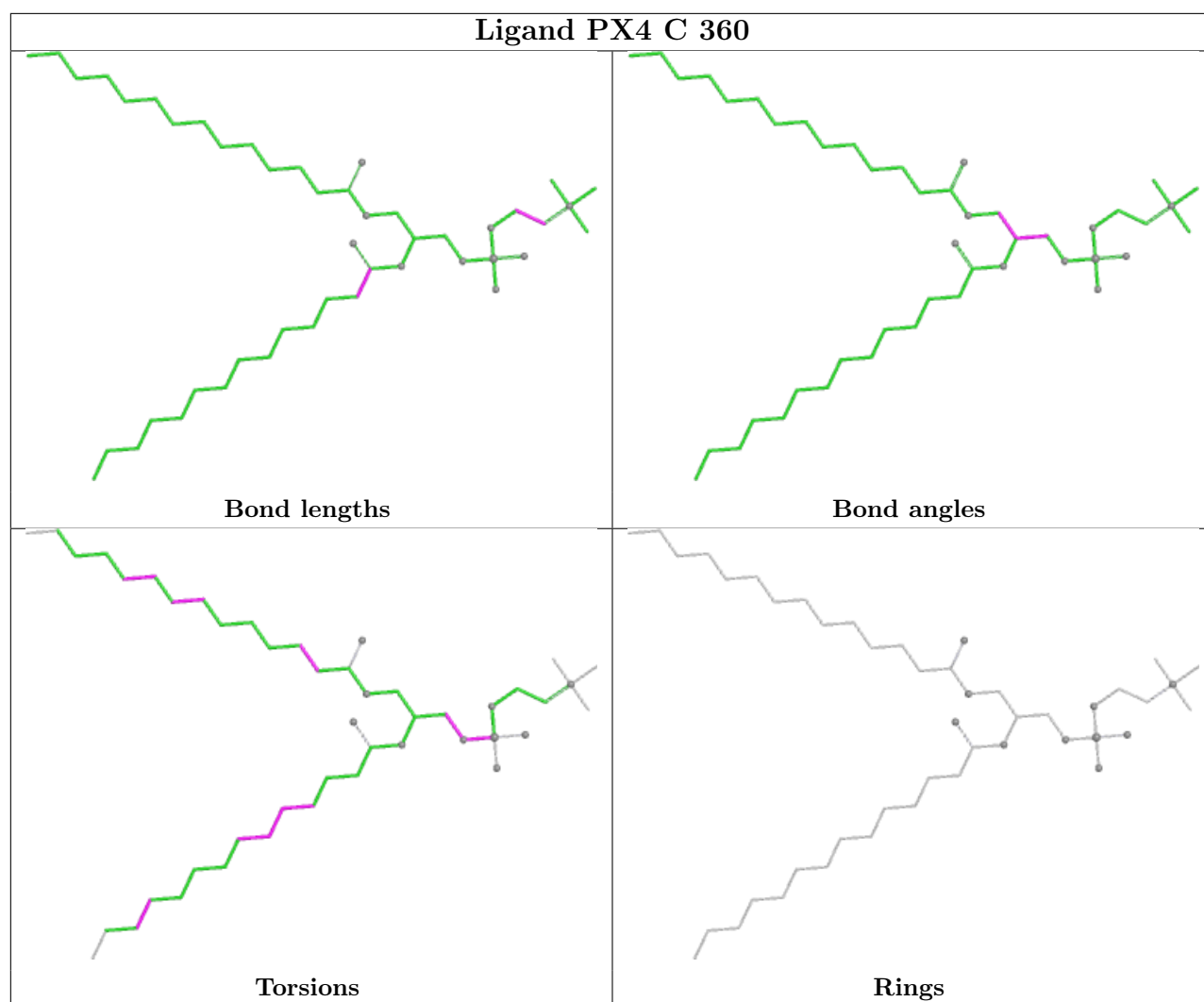
Ligand PX4 B 342

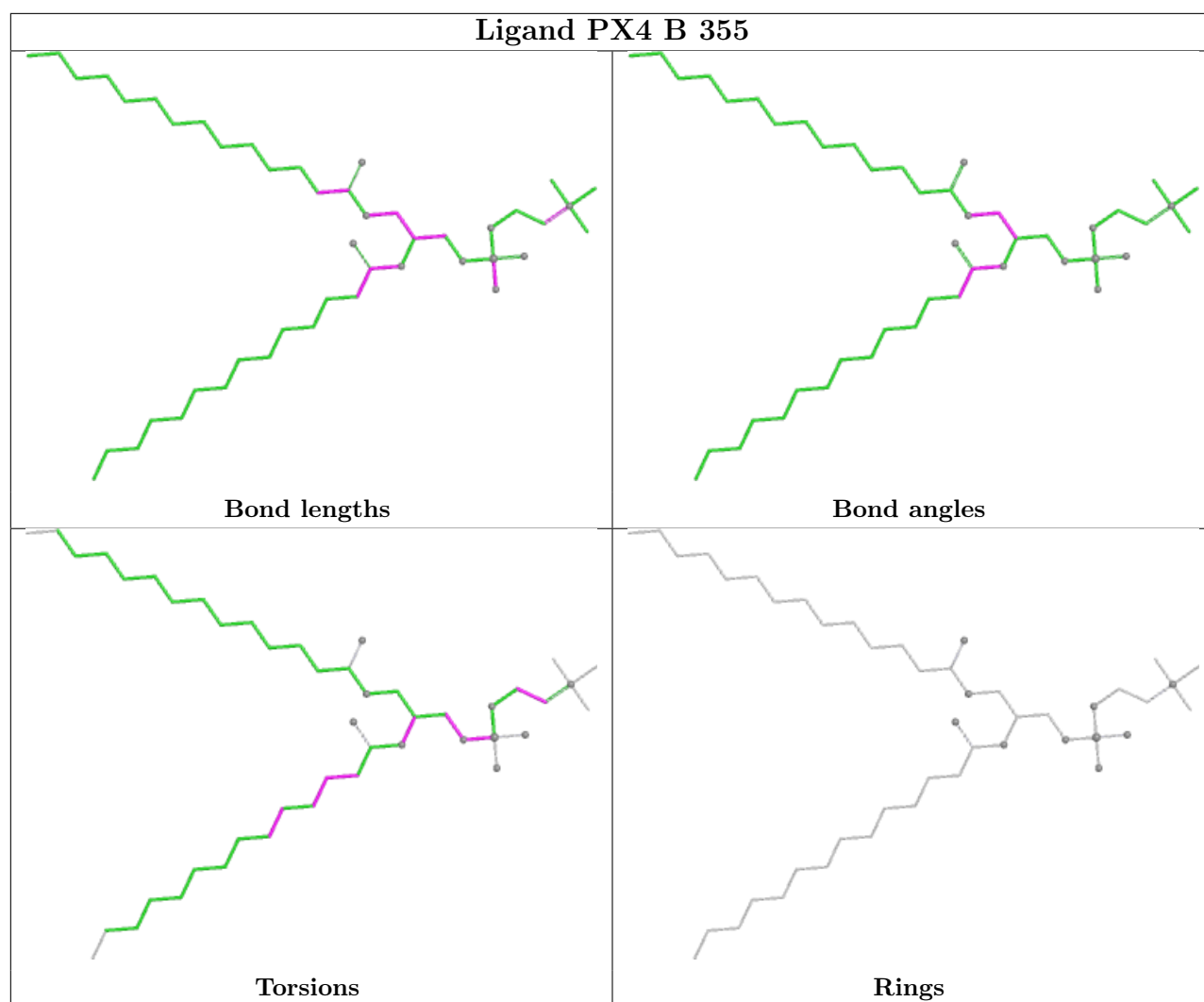


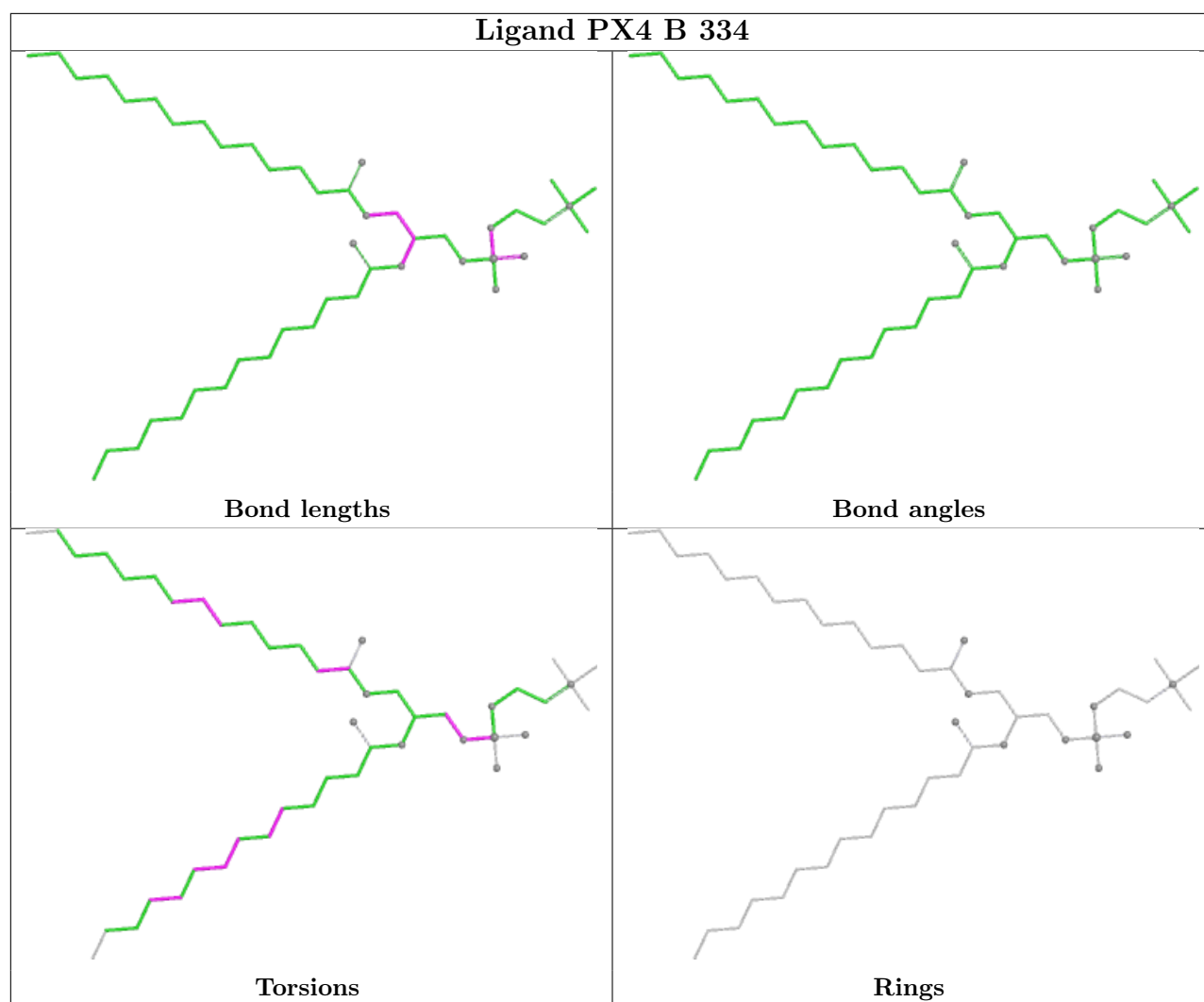


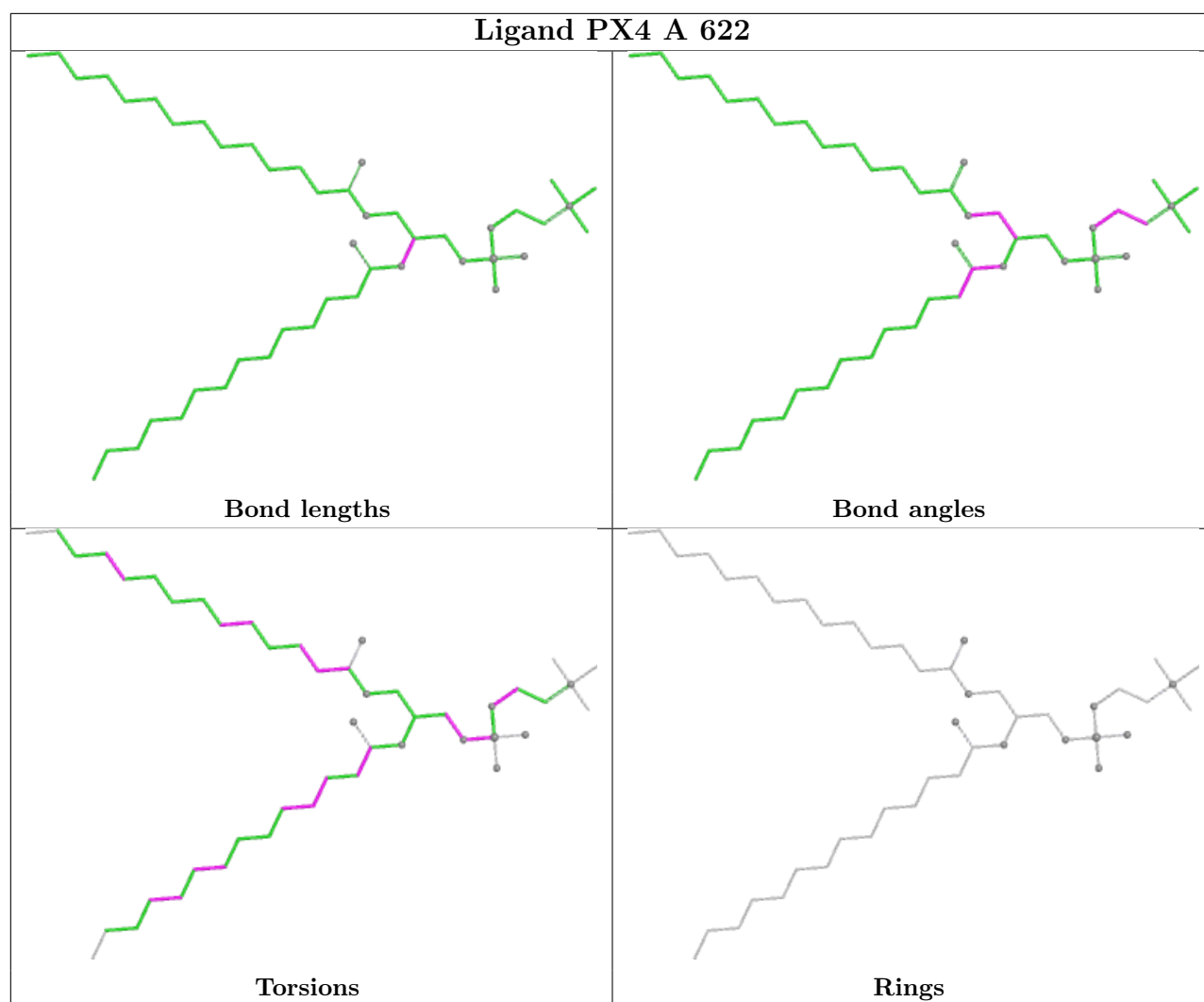


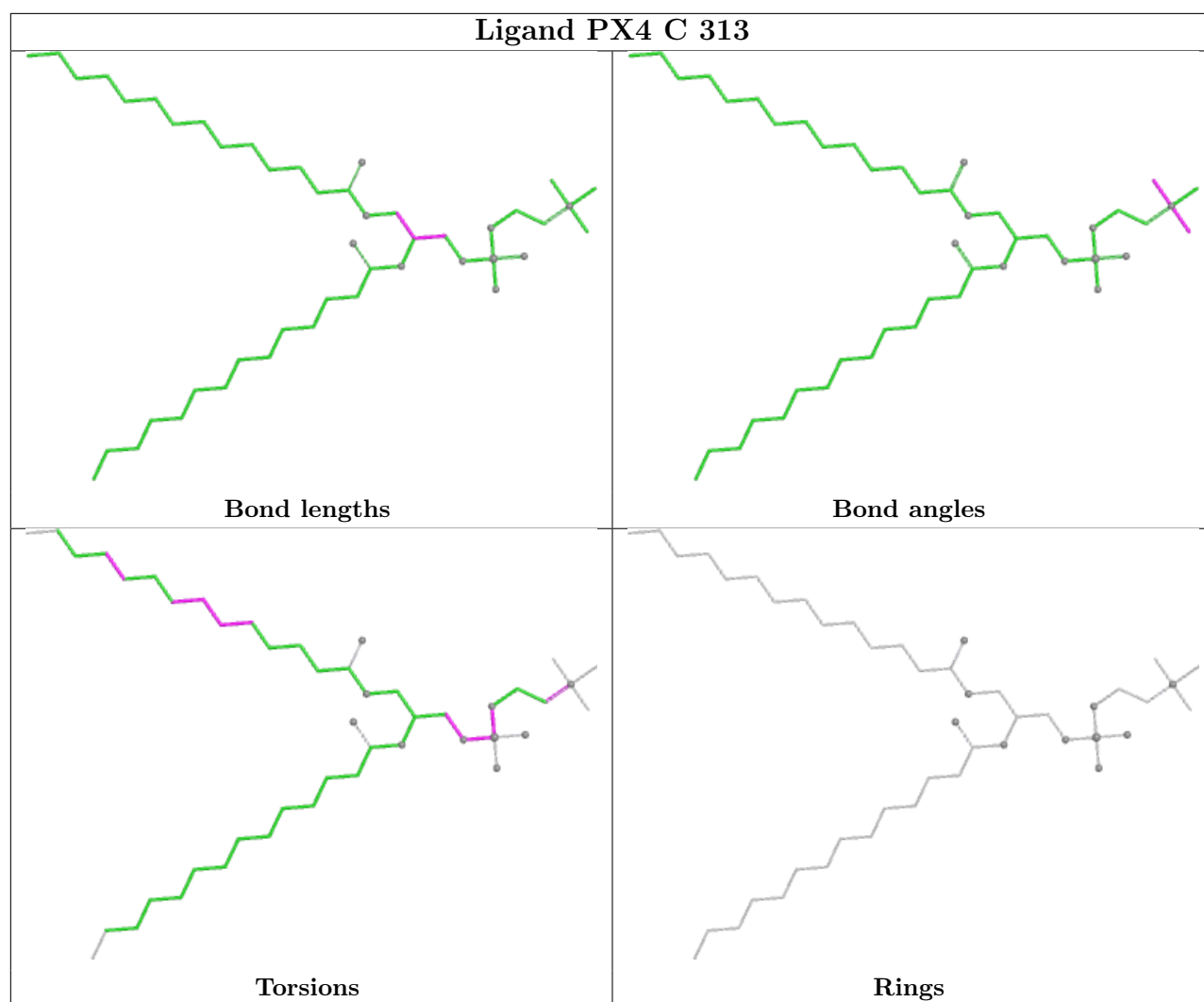


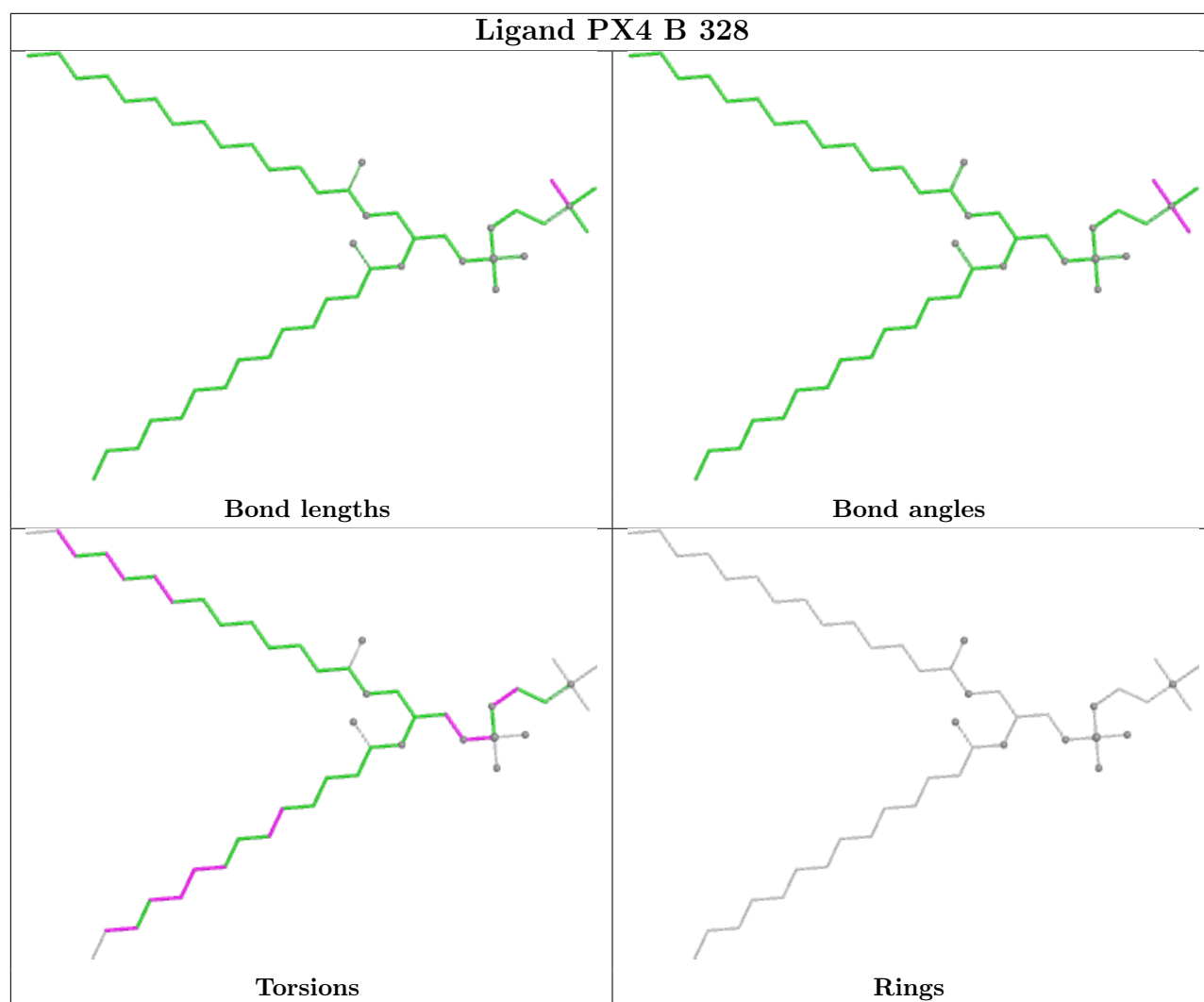


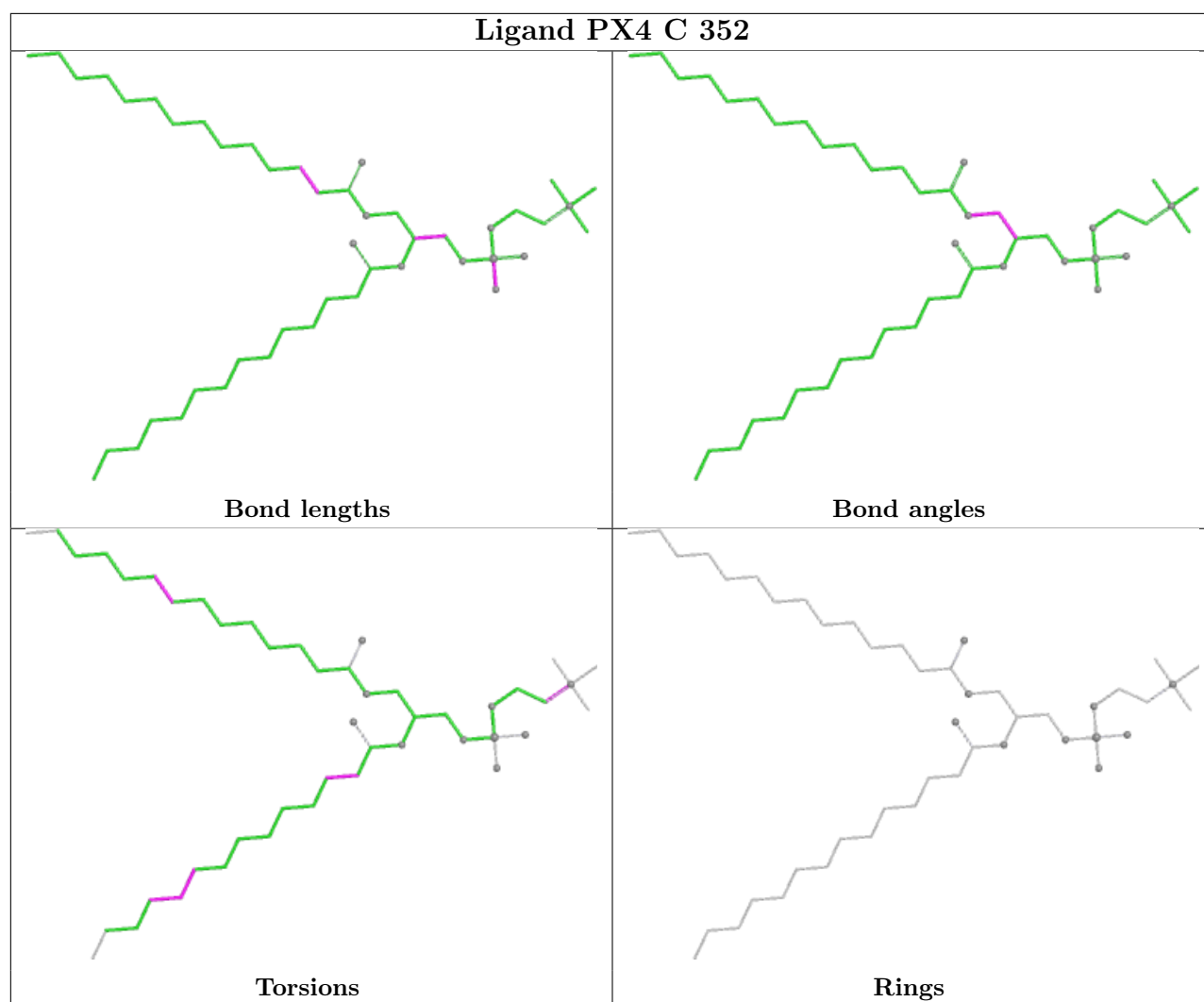


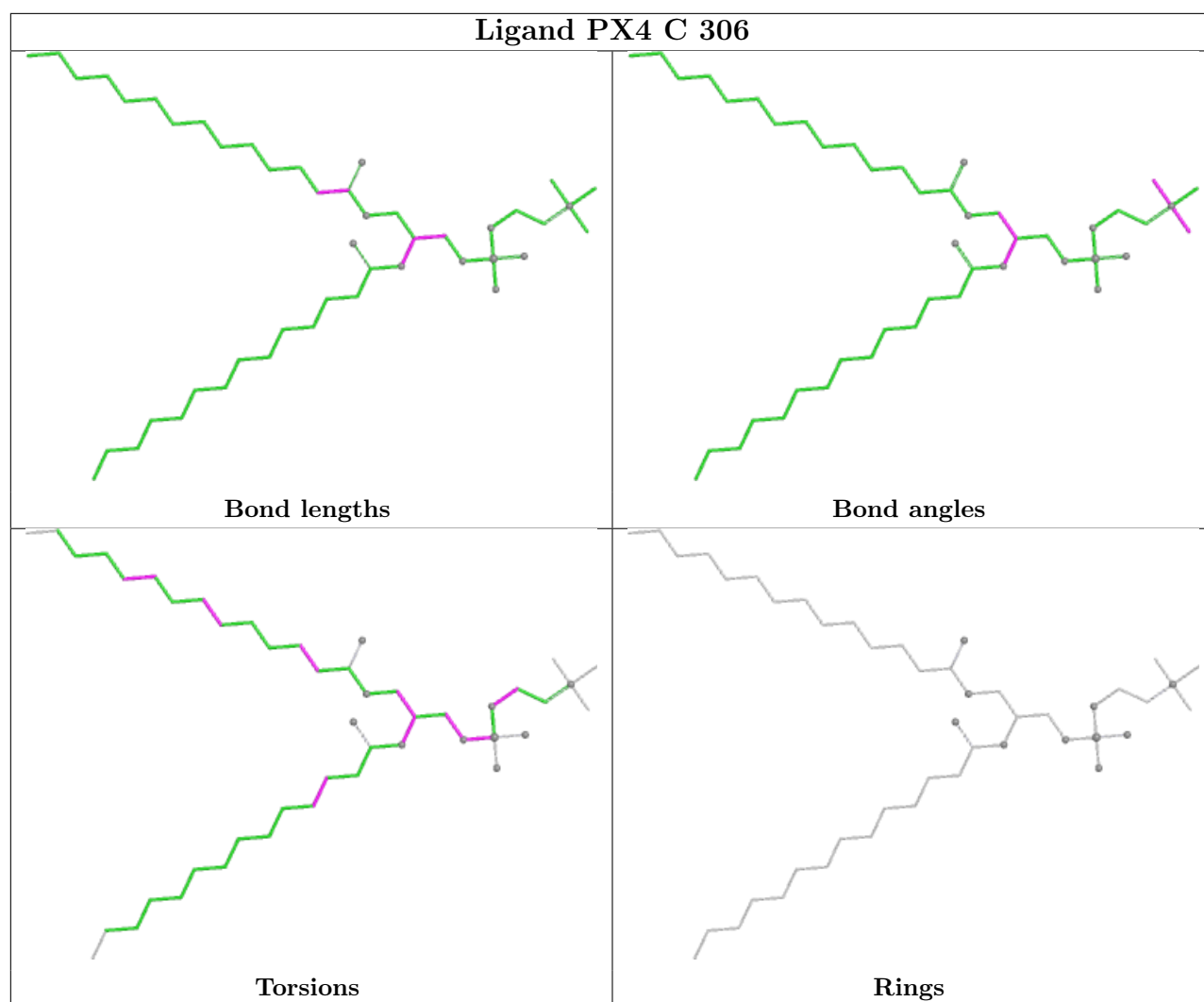


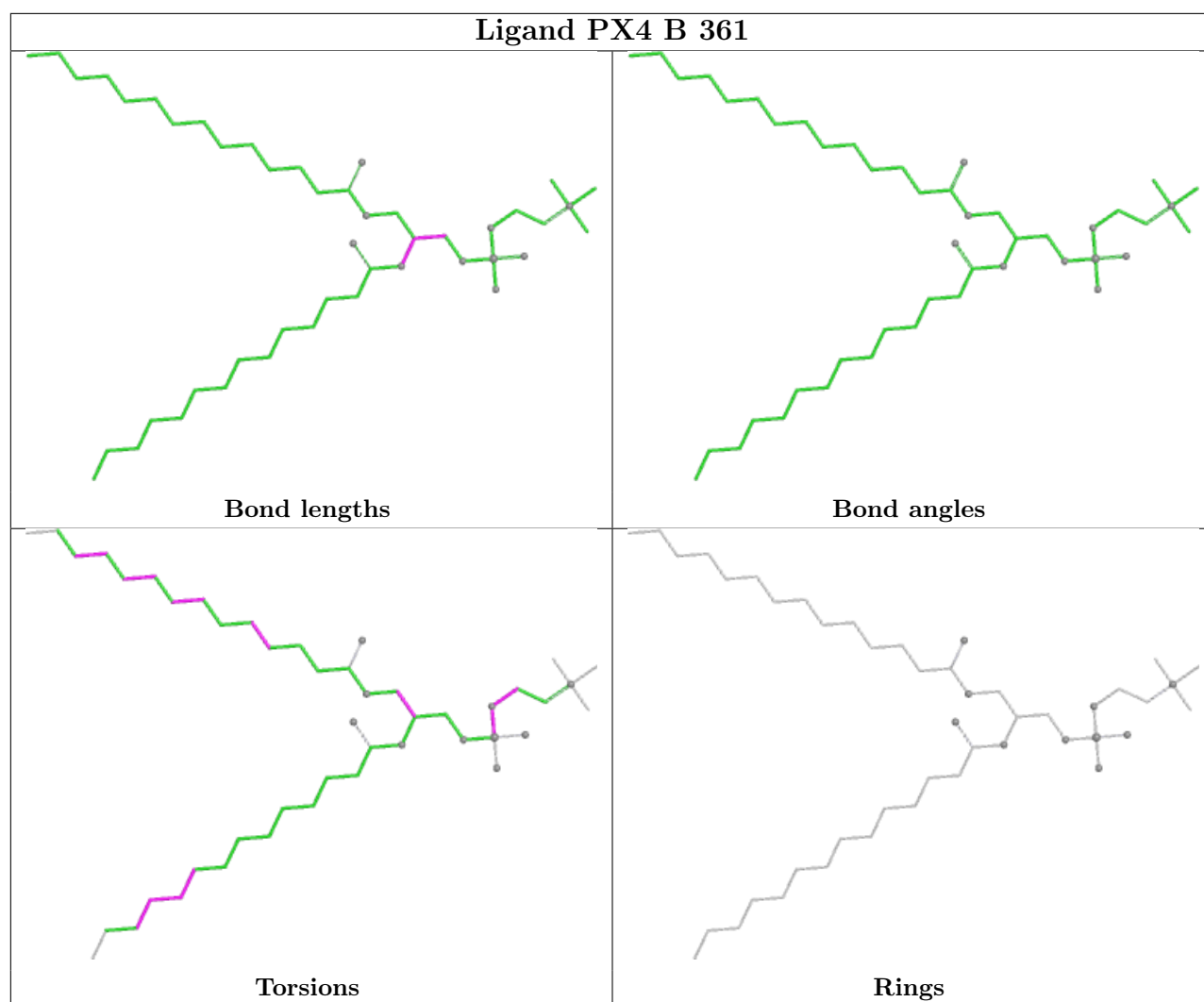


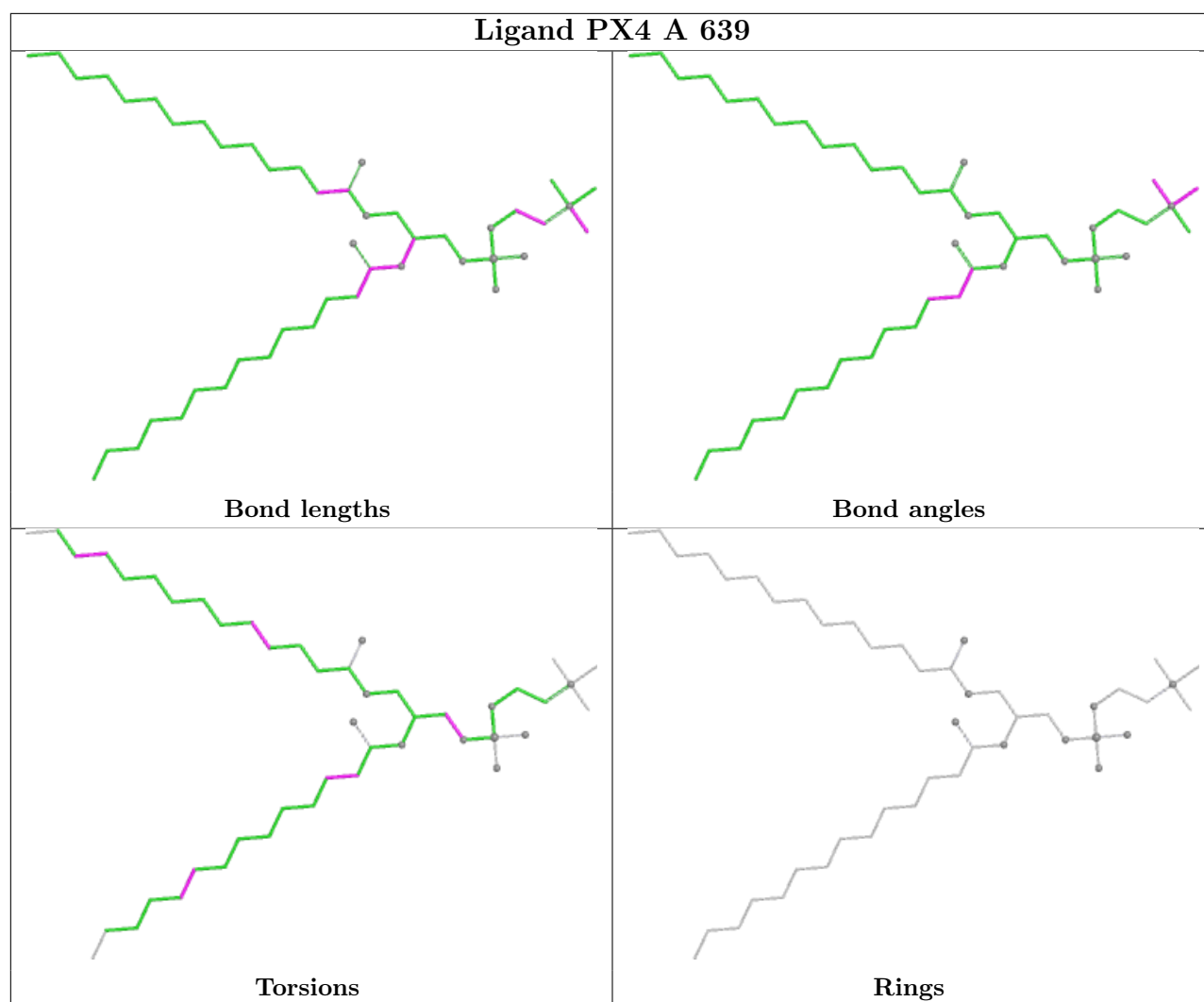


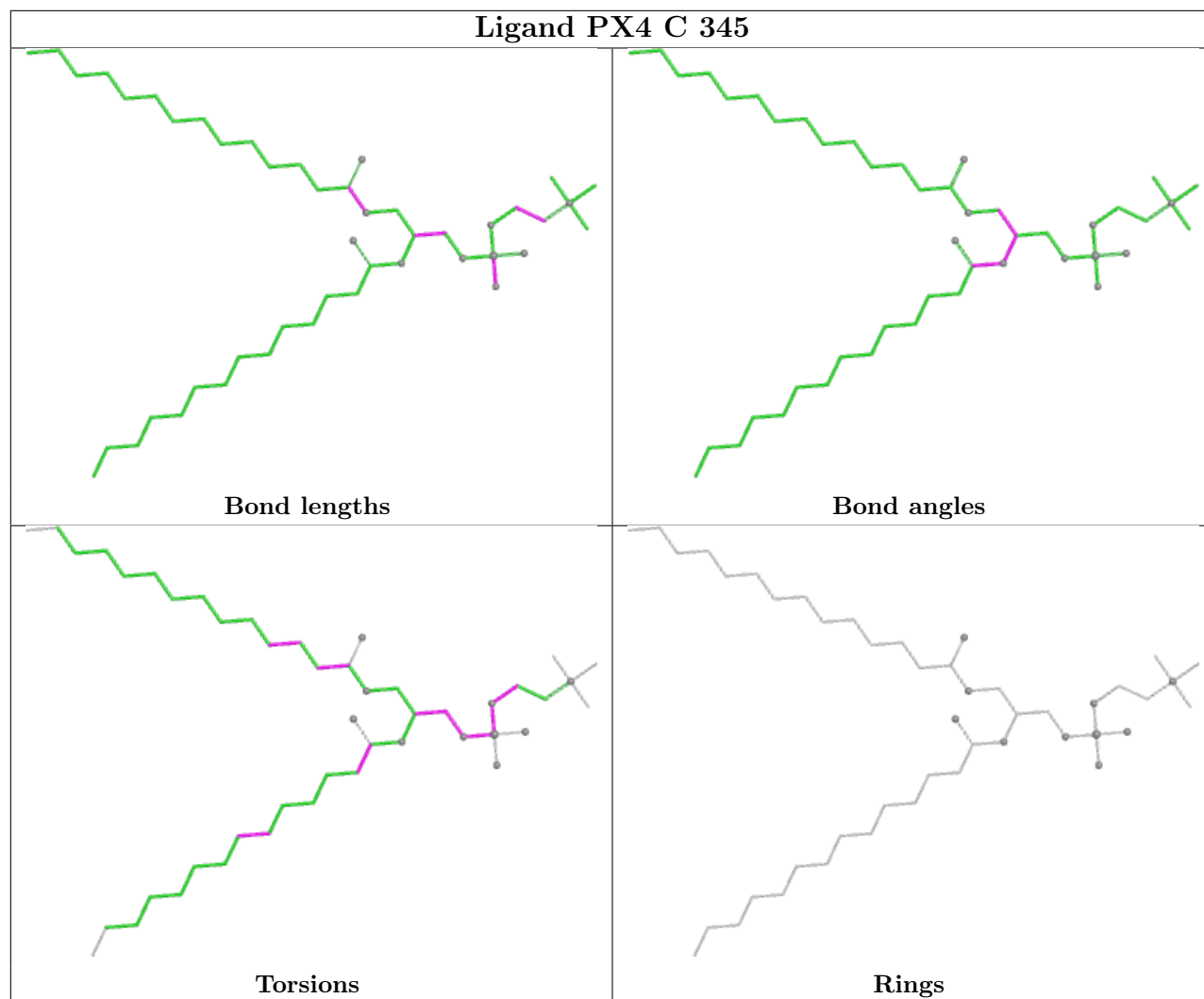


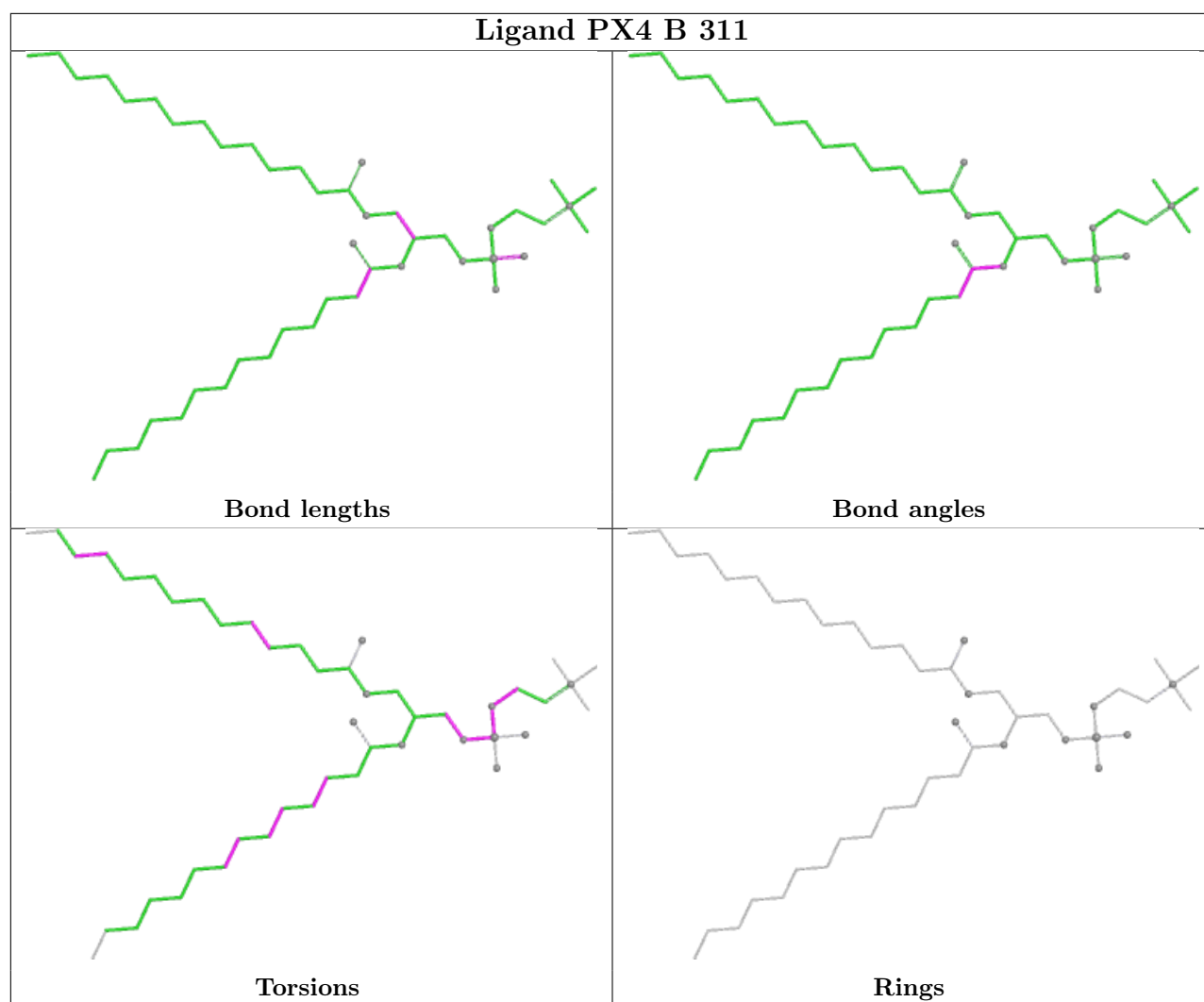


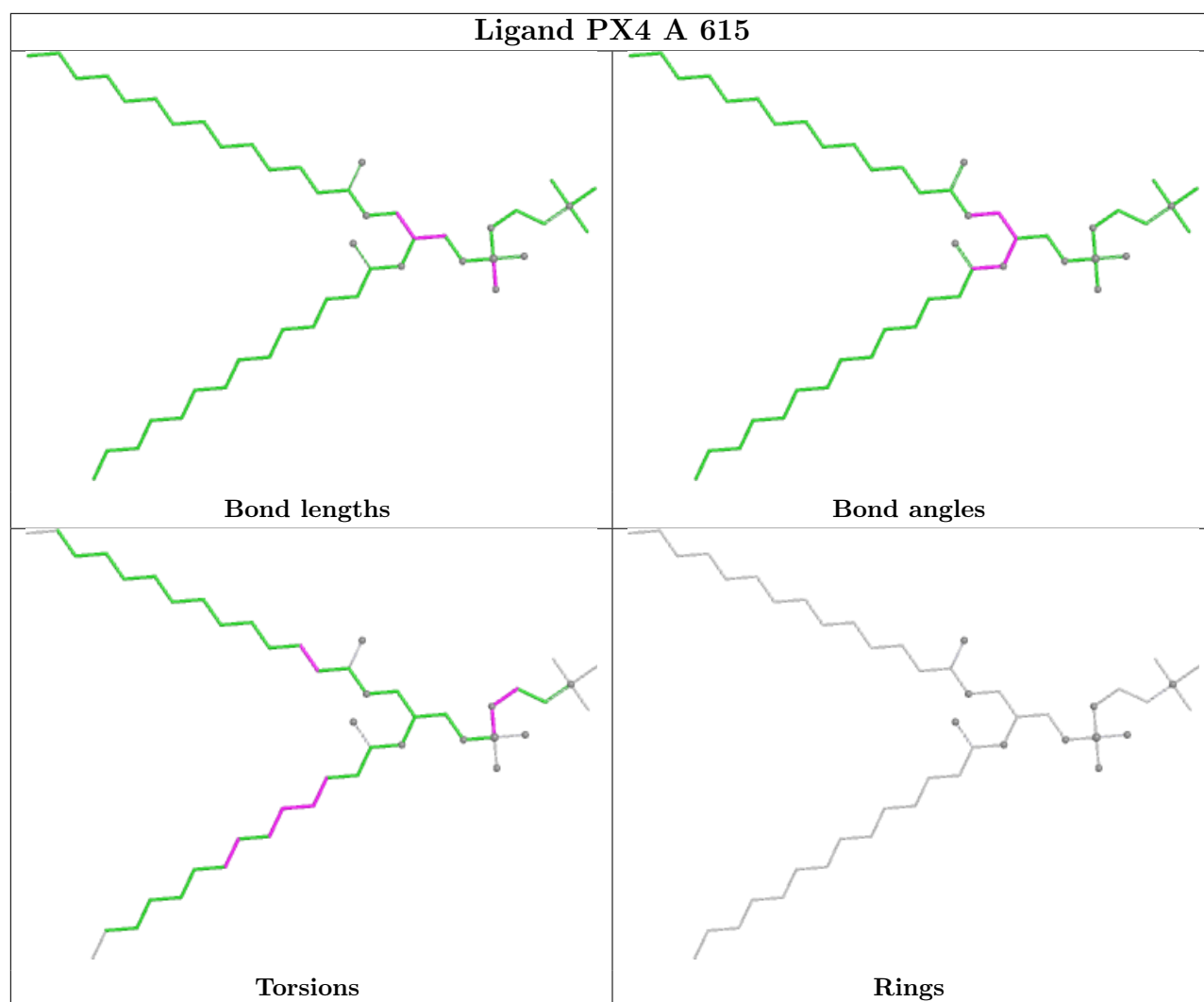


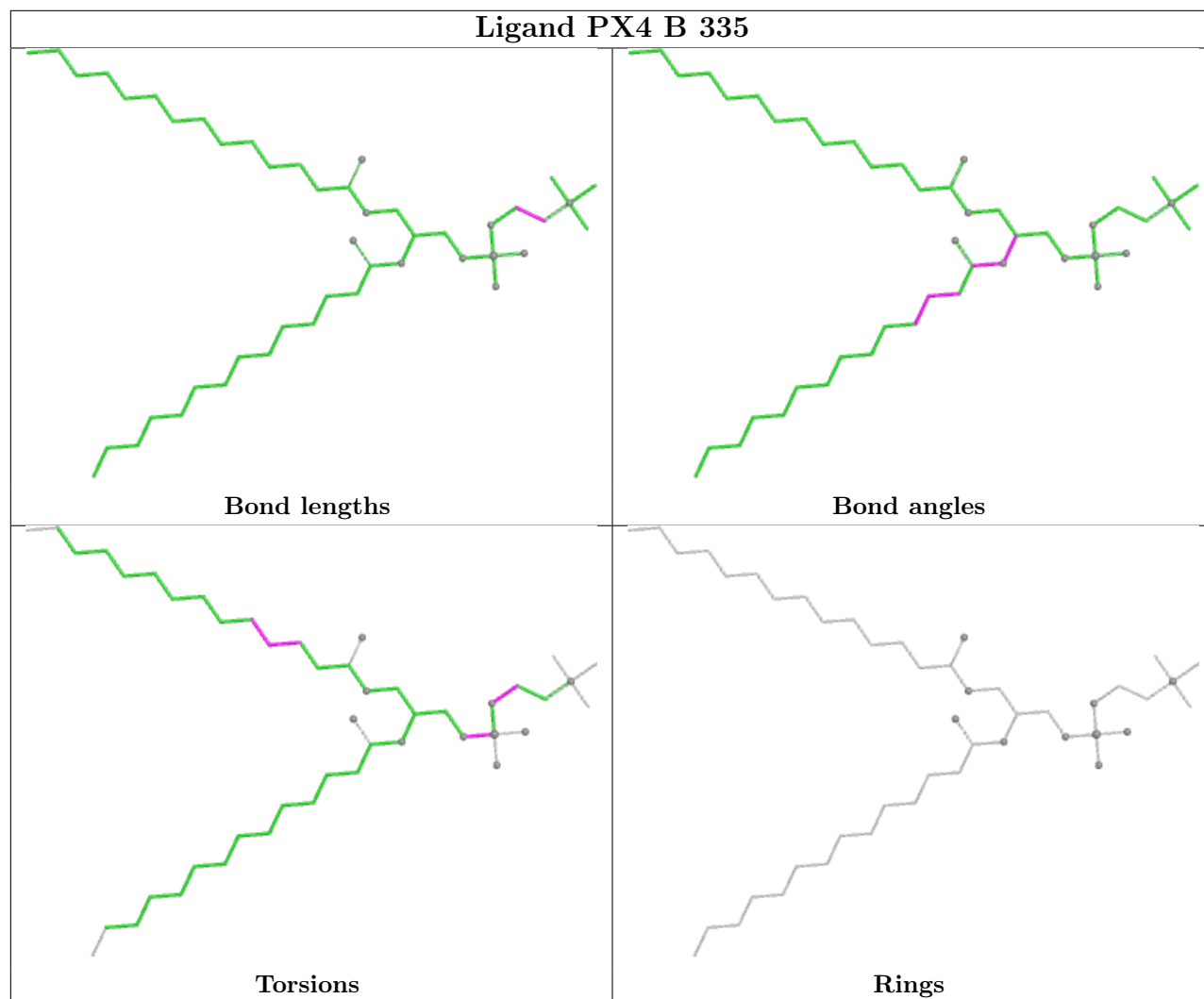


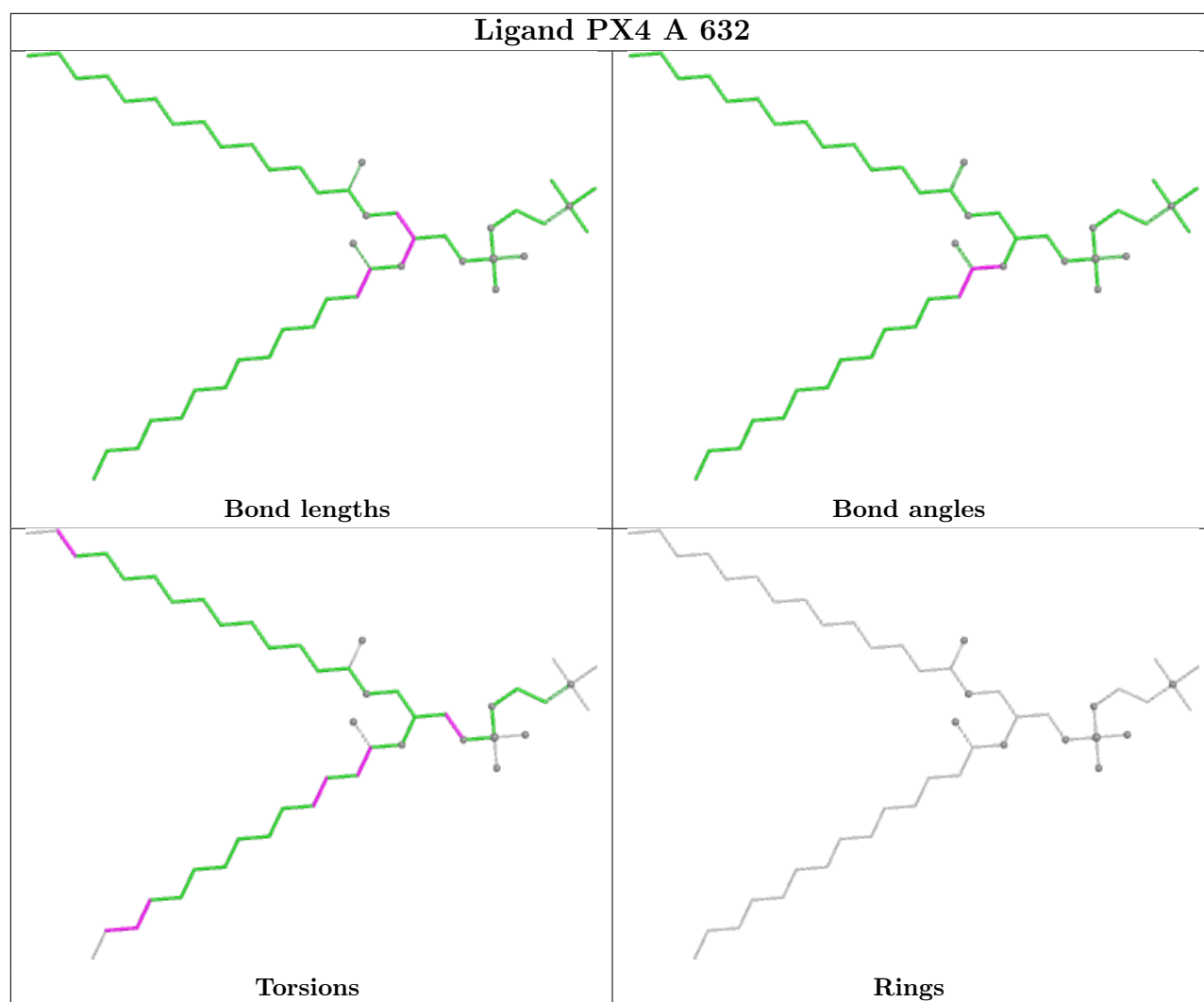


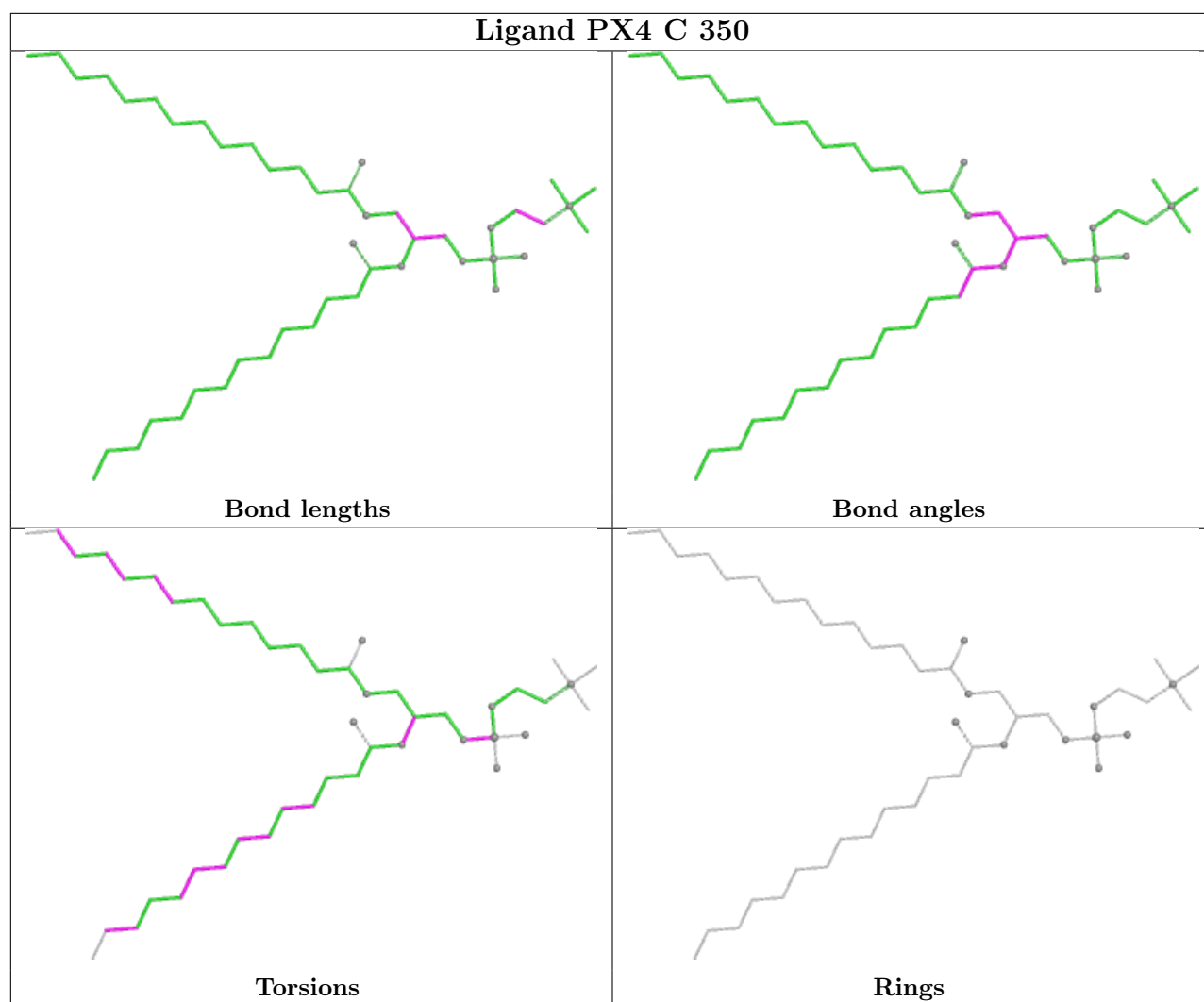


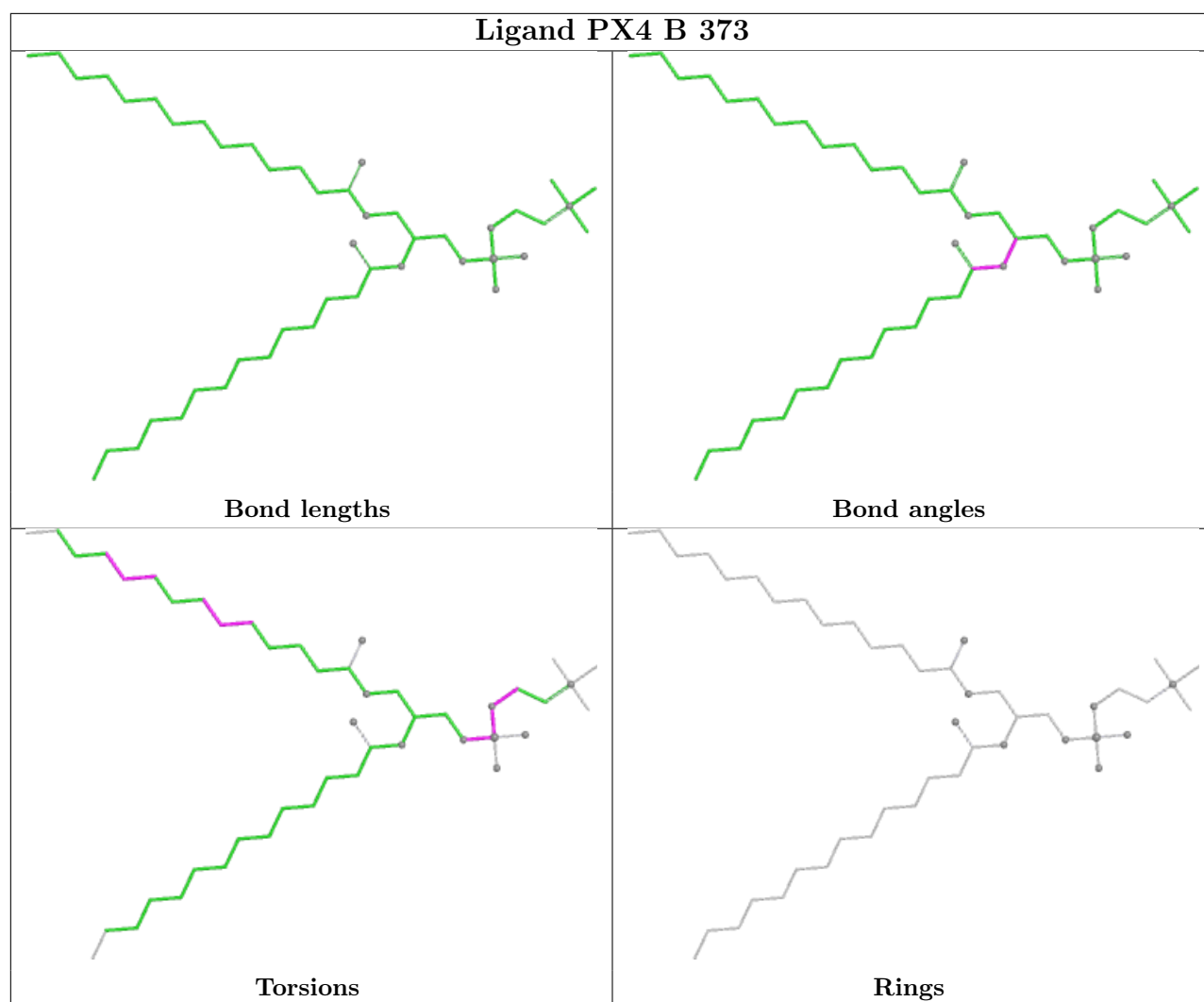




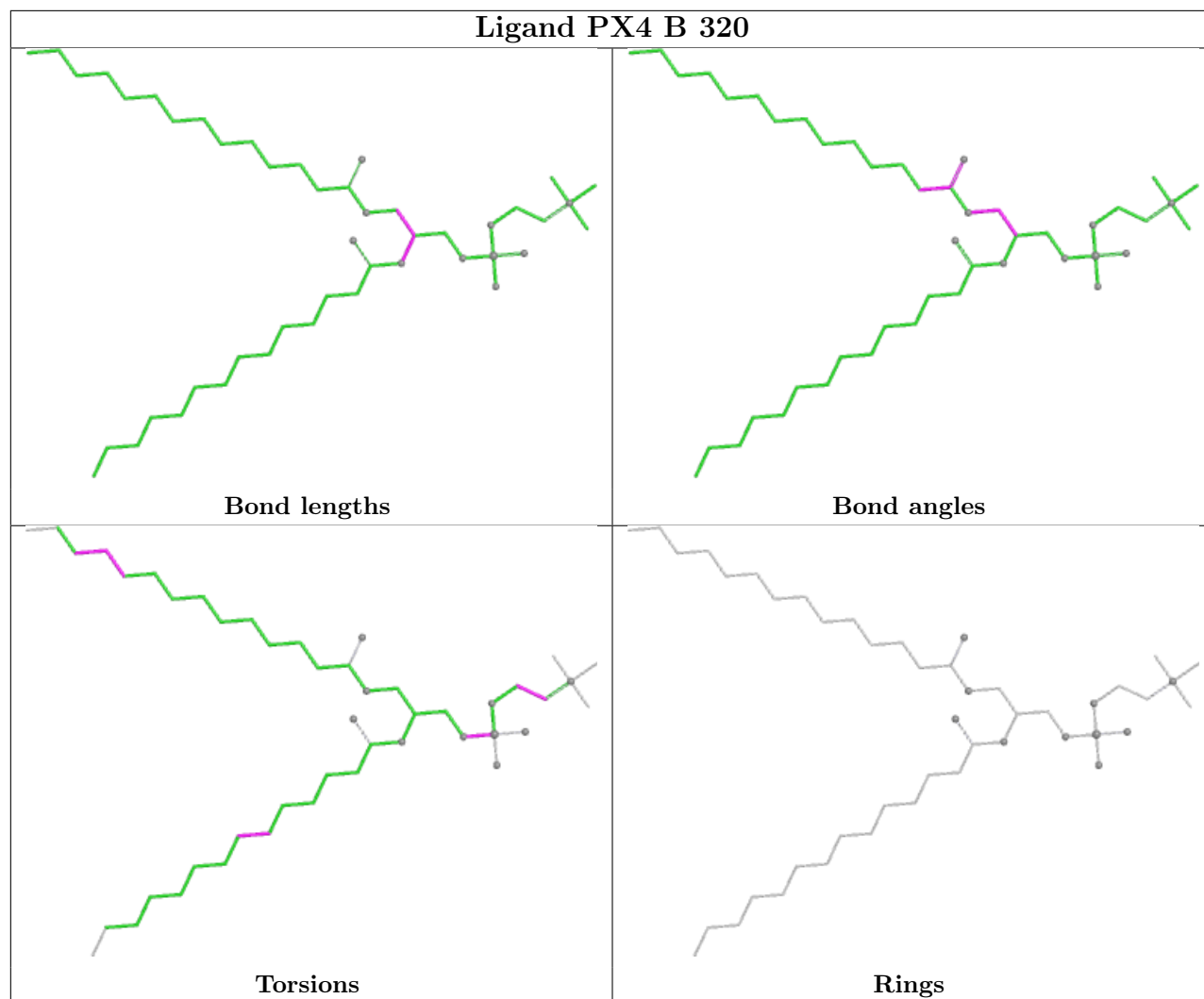


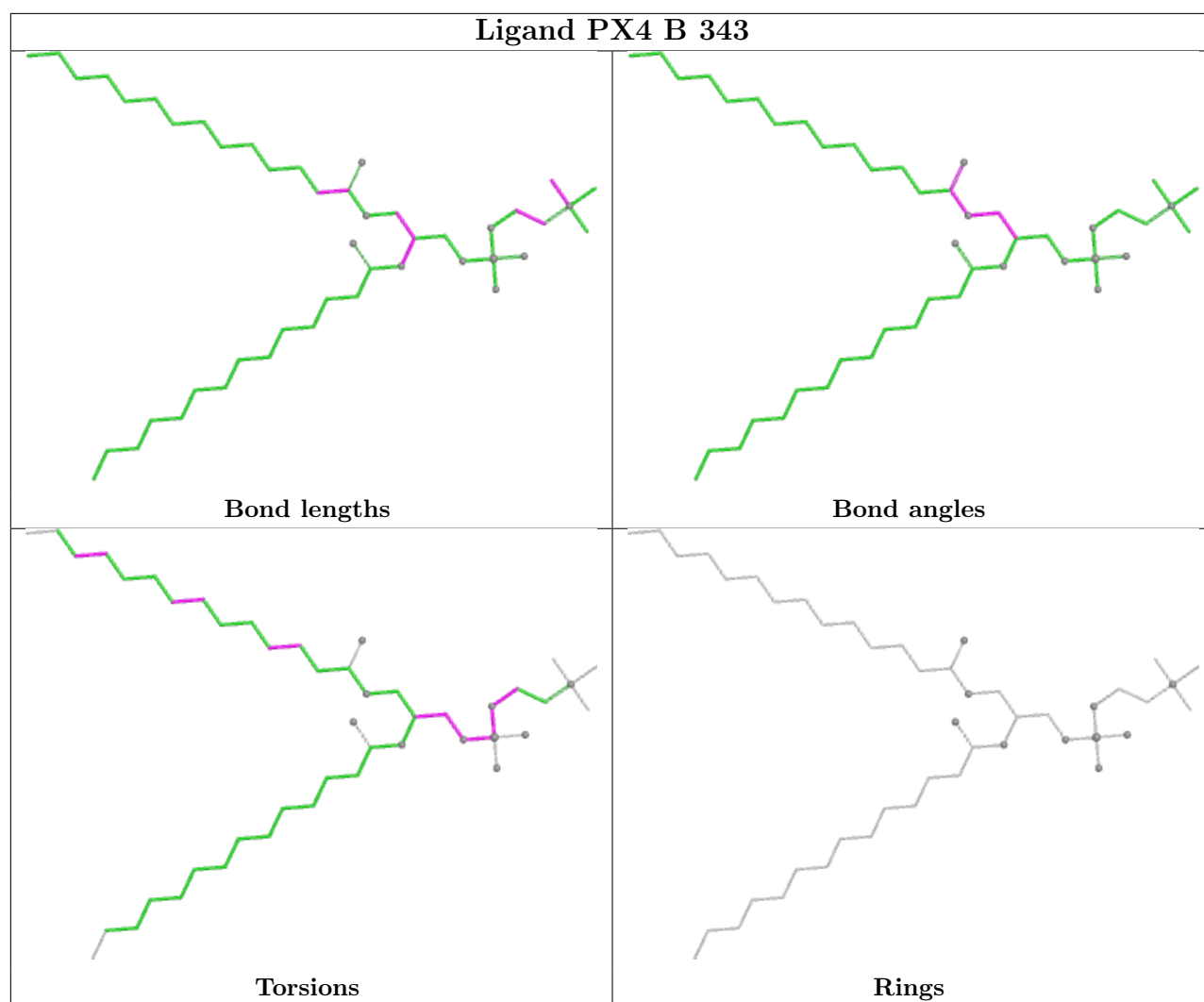


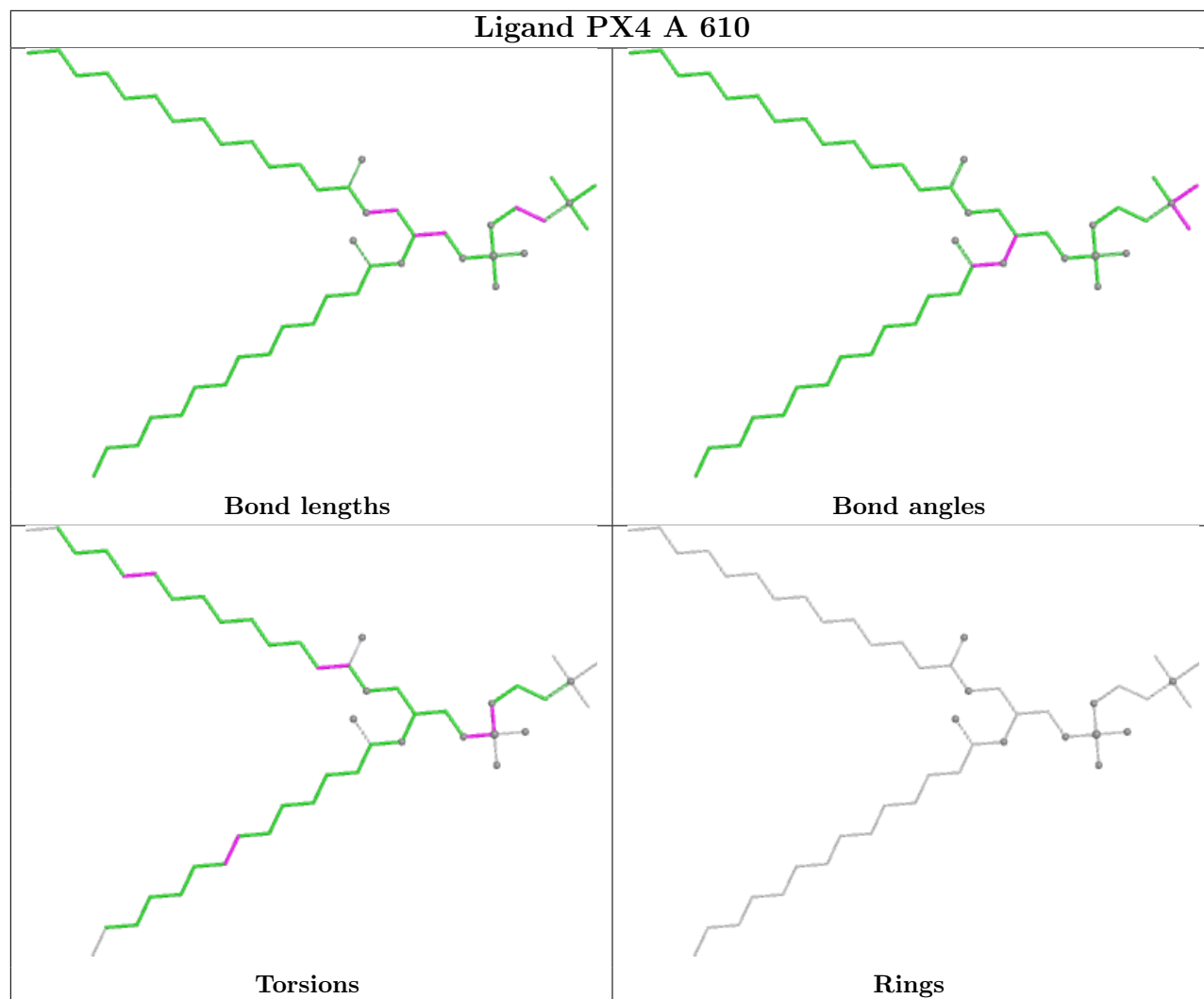


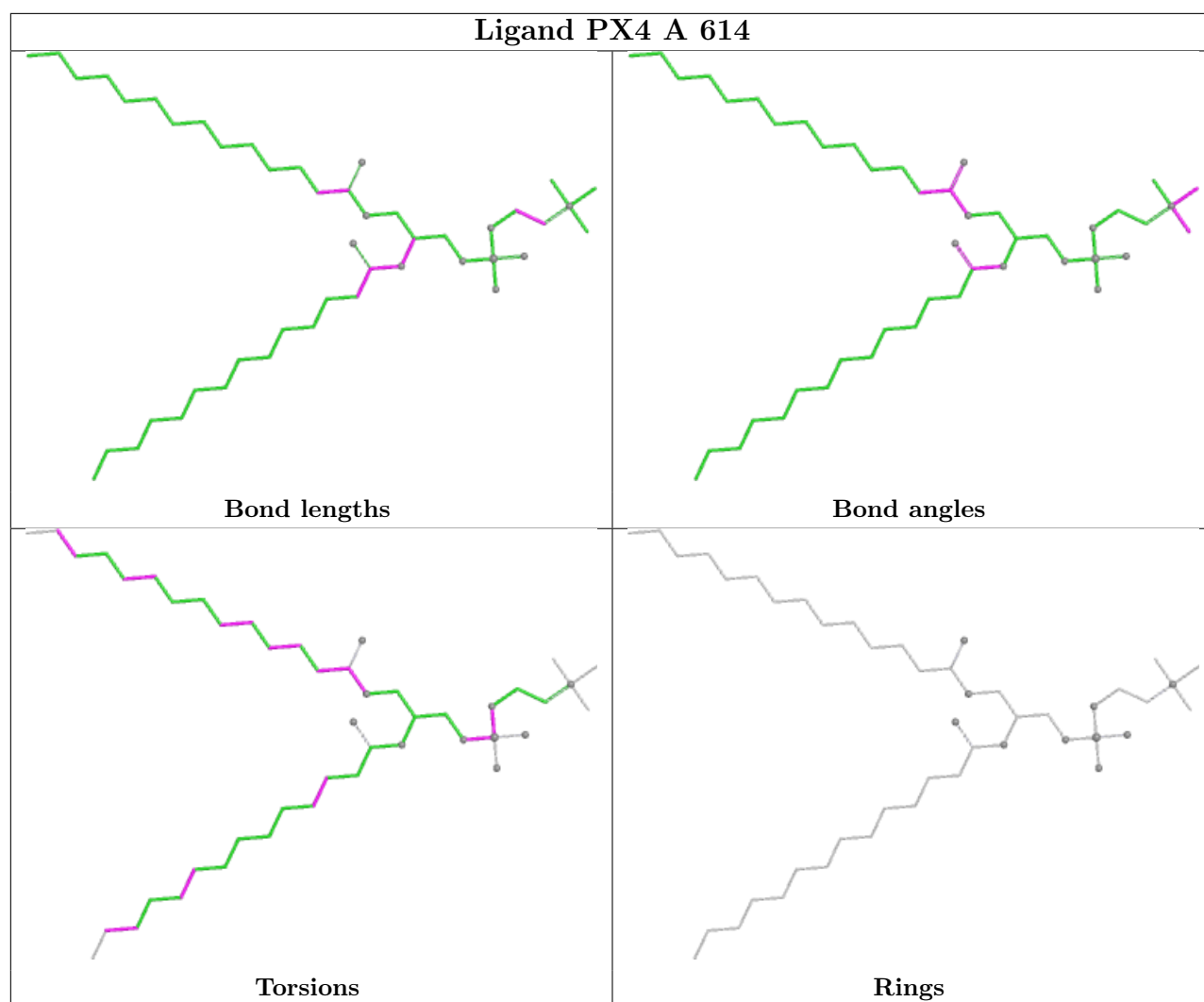


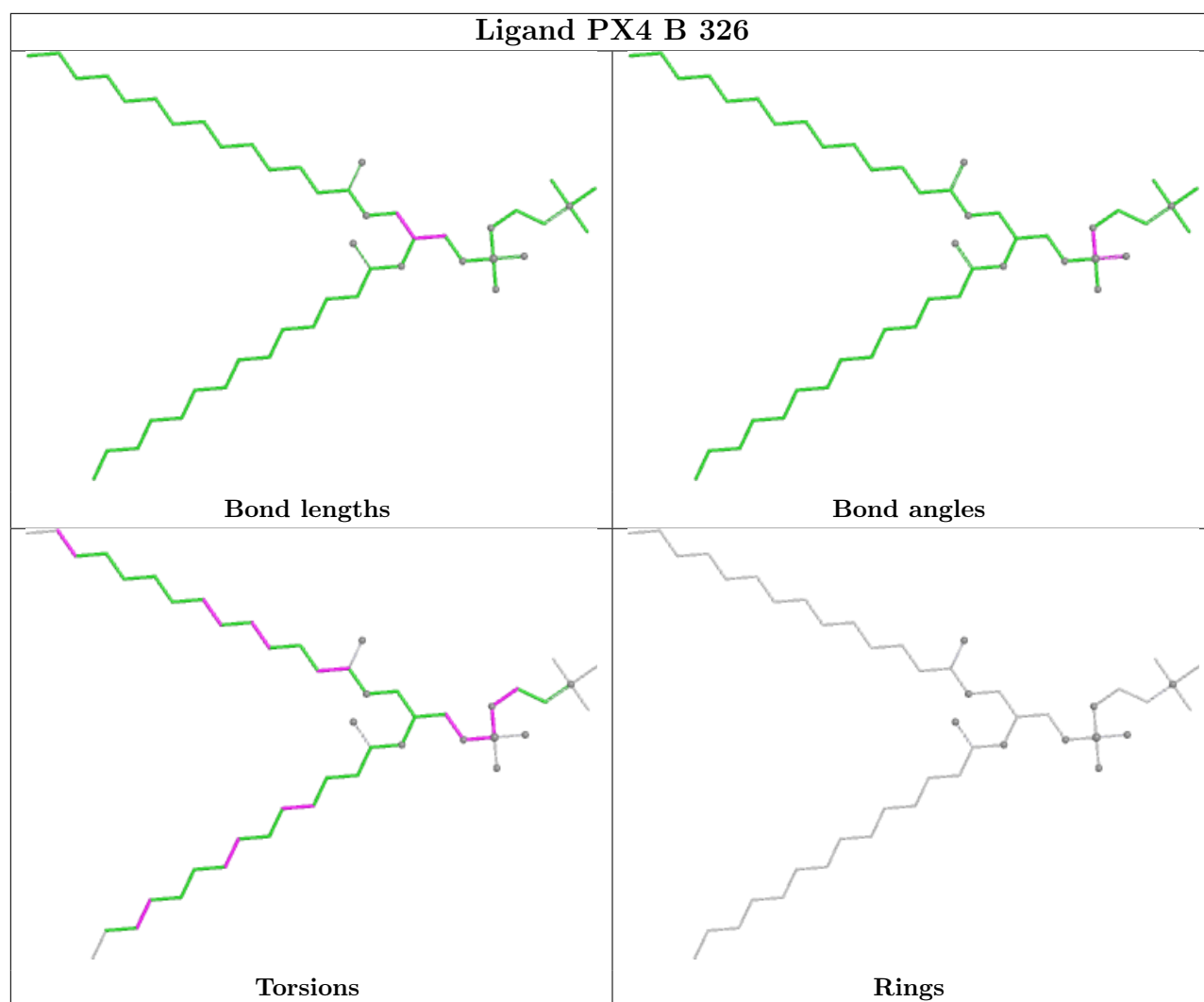
Ligand PX4 B 320

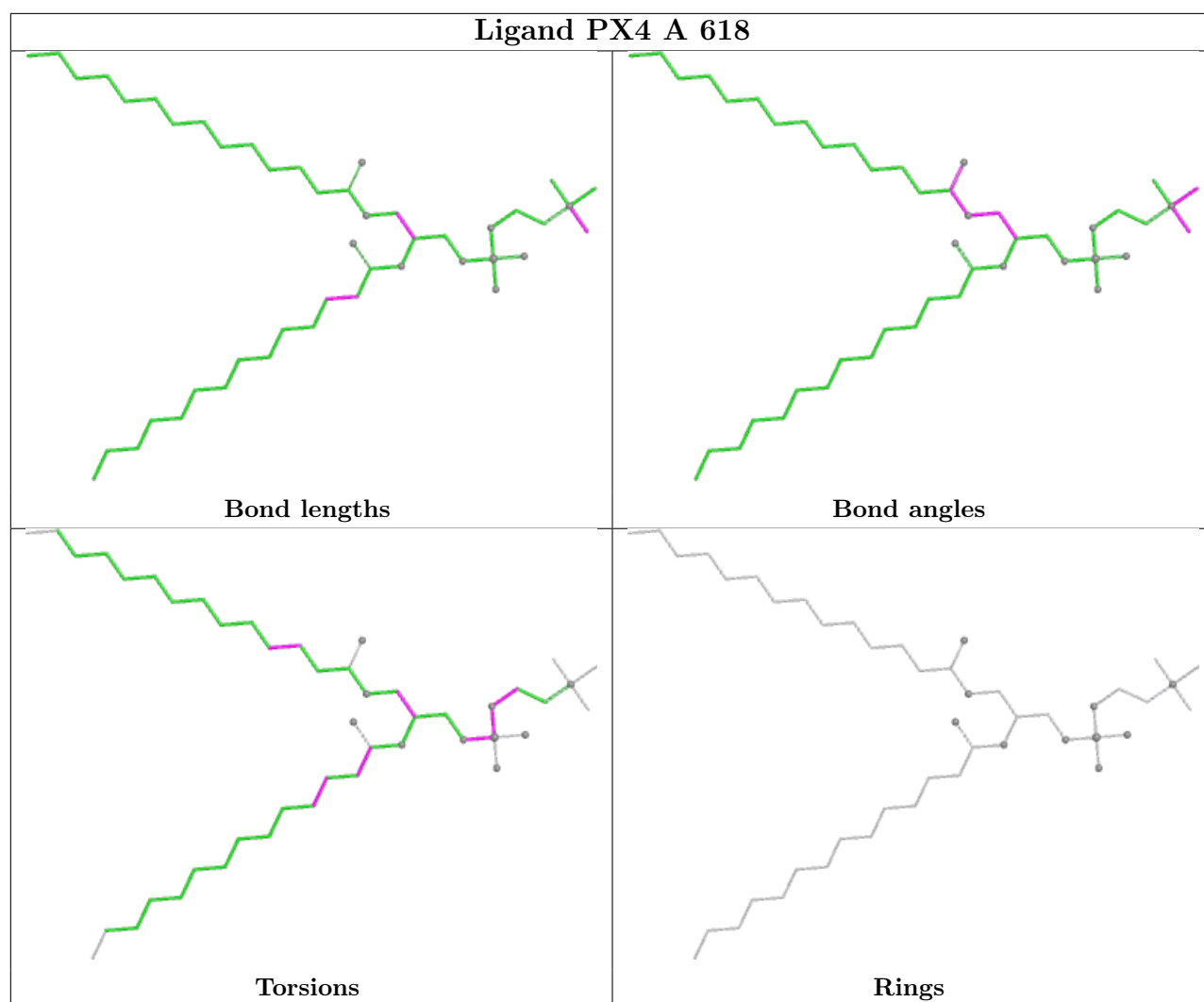


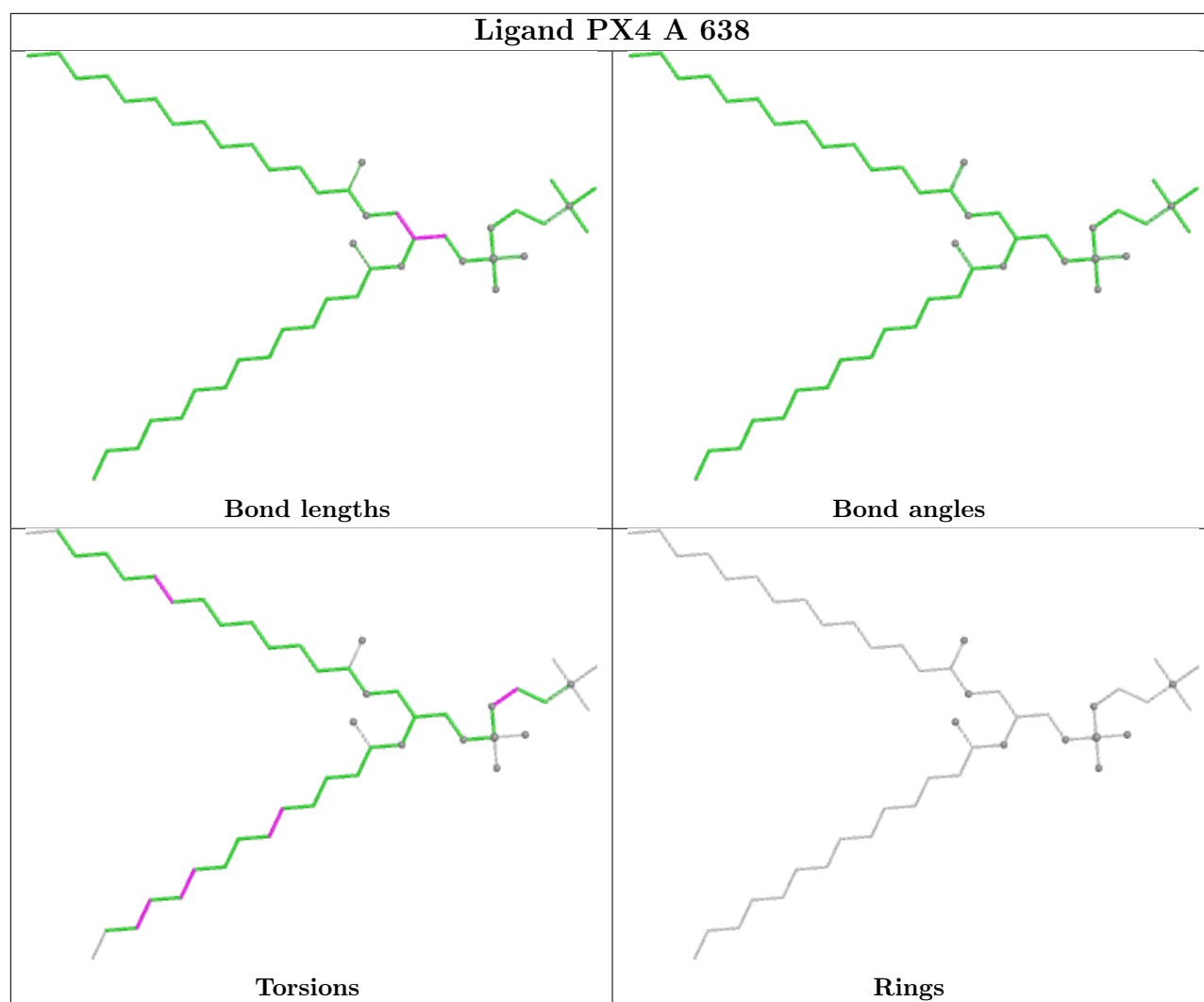


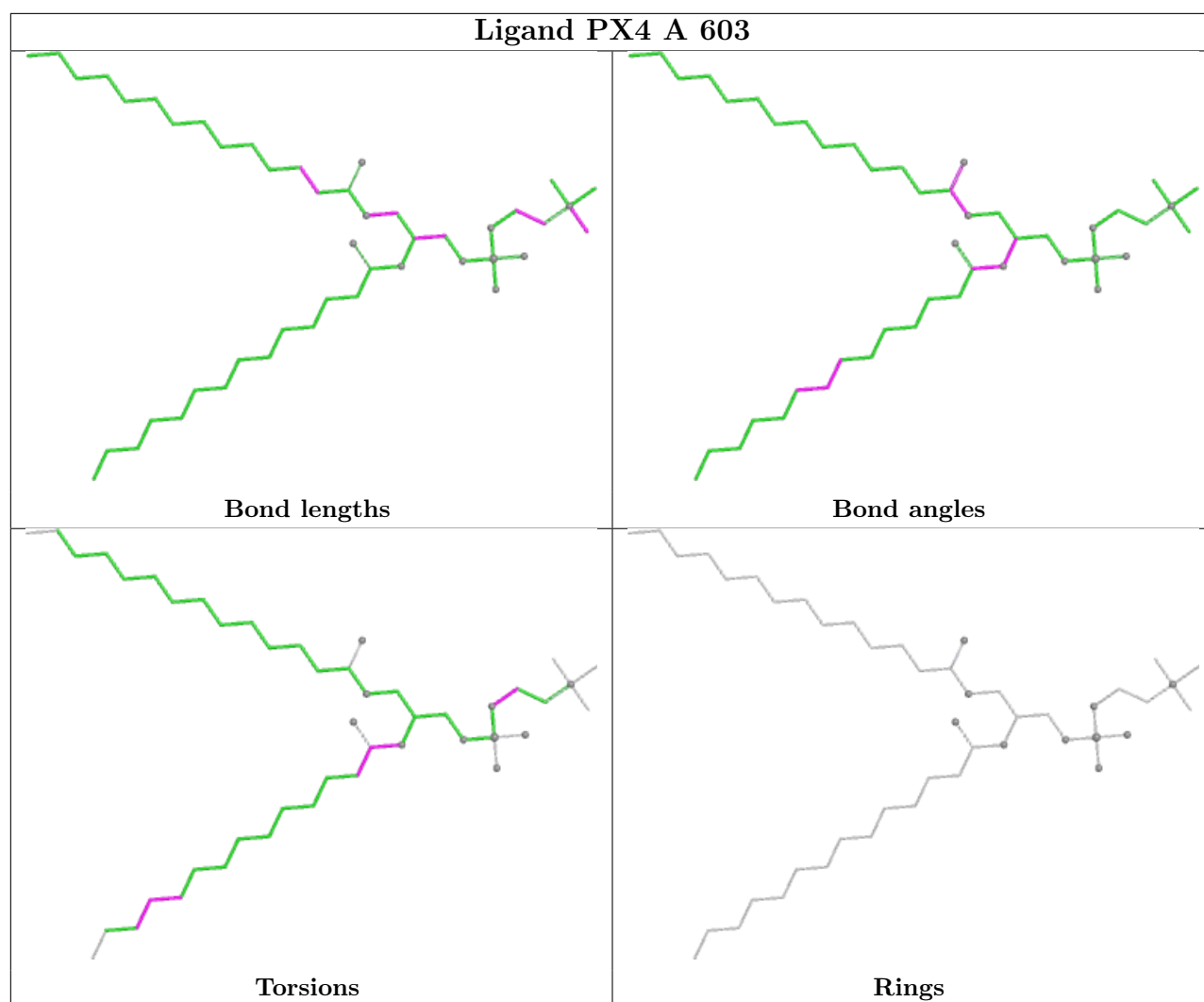


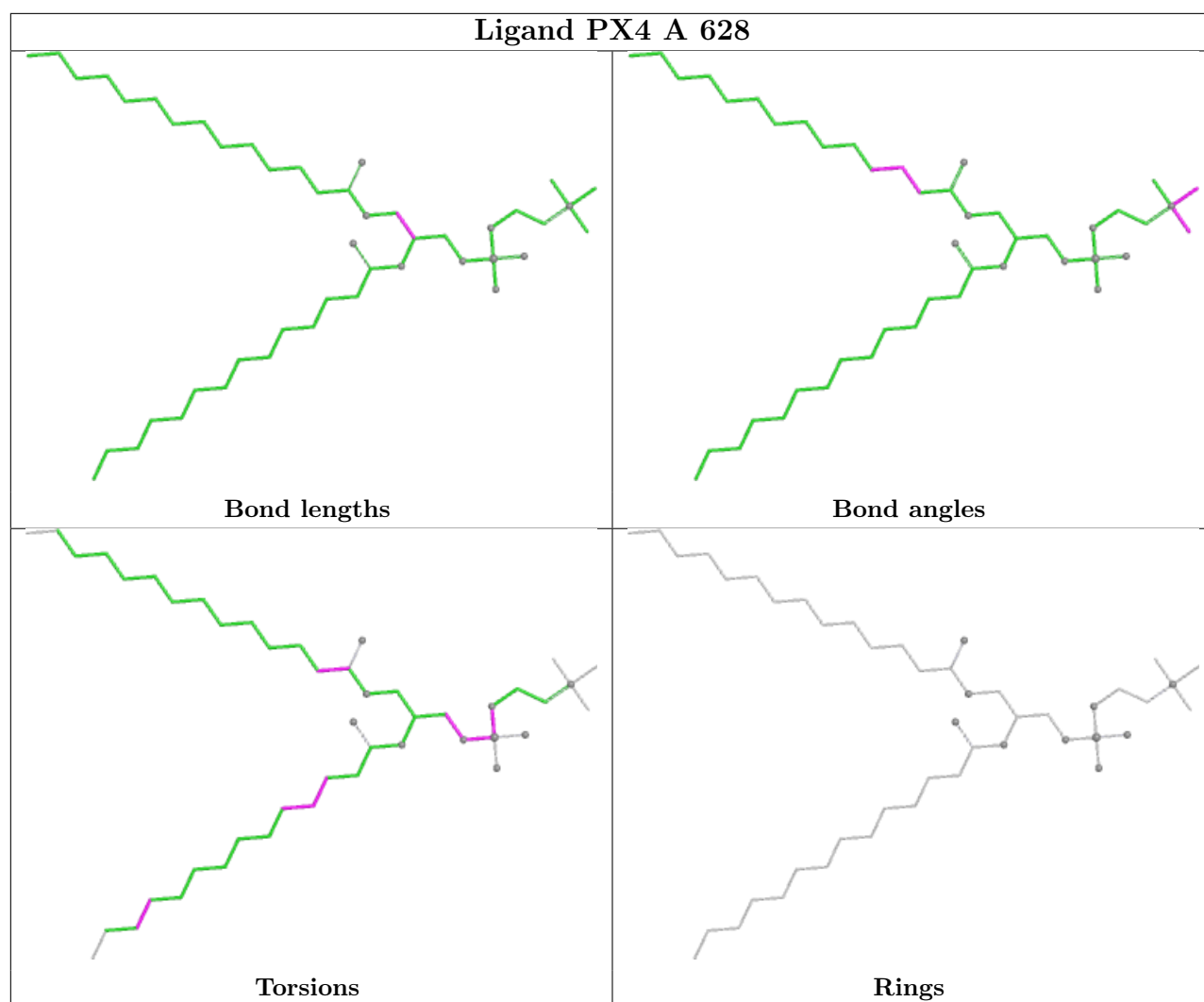




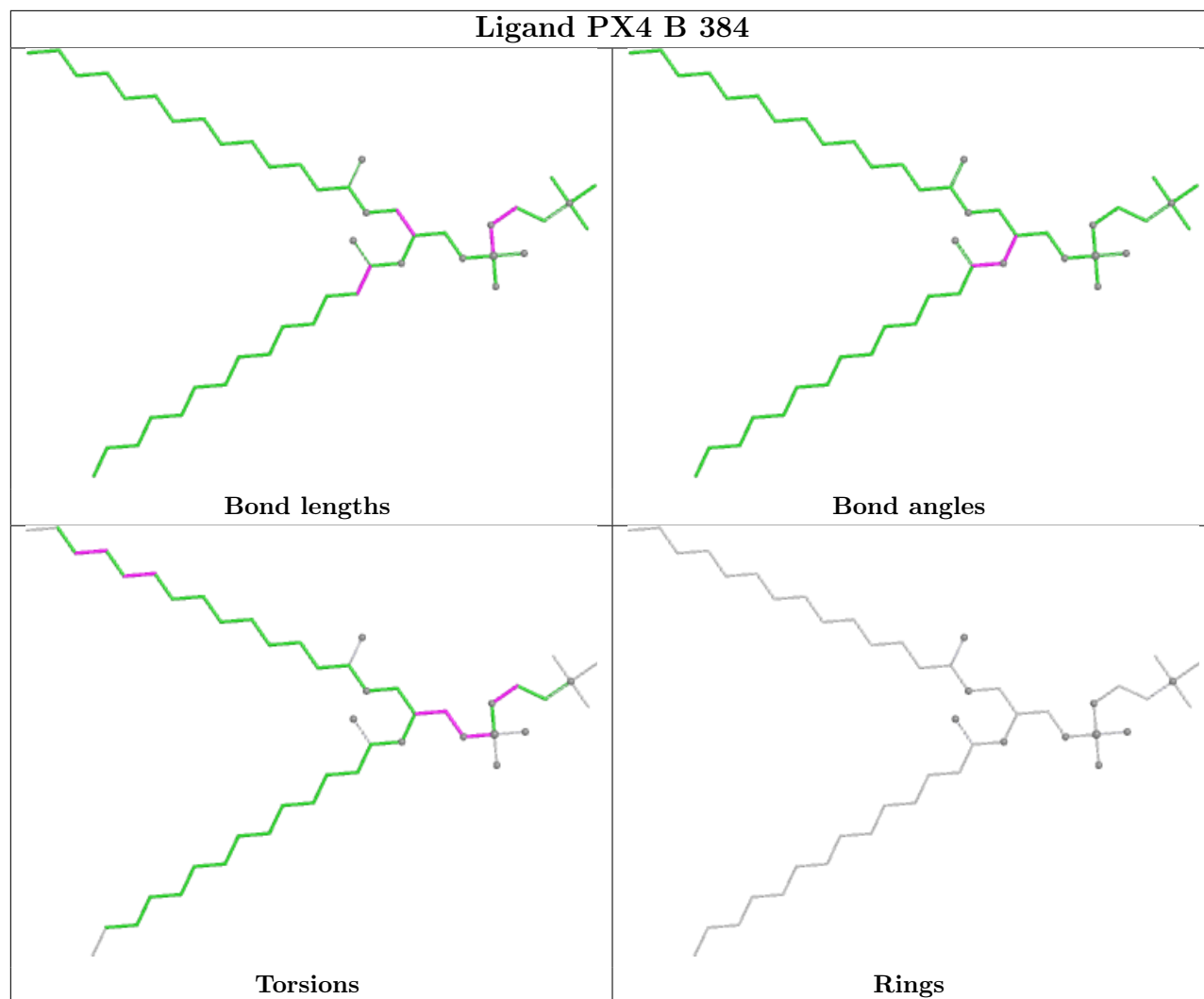




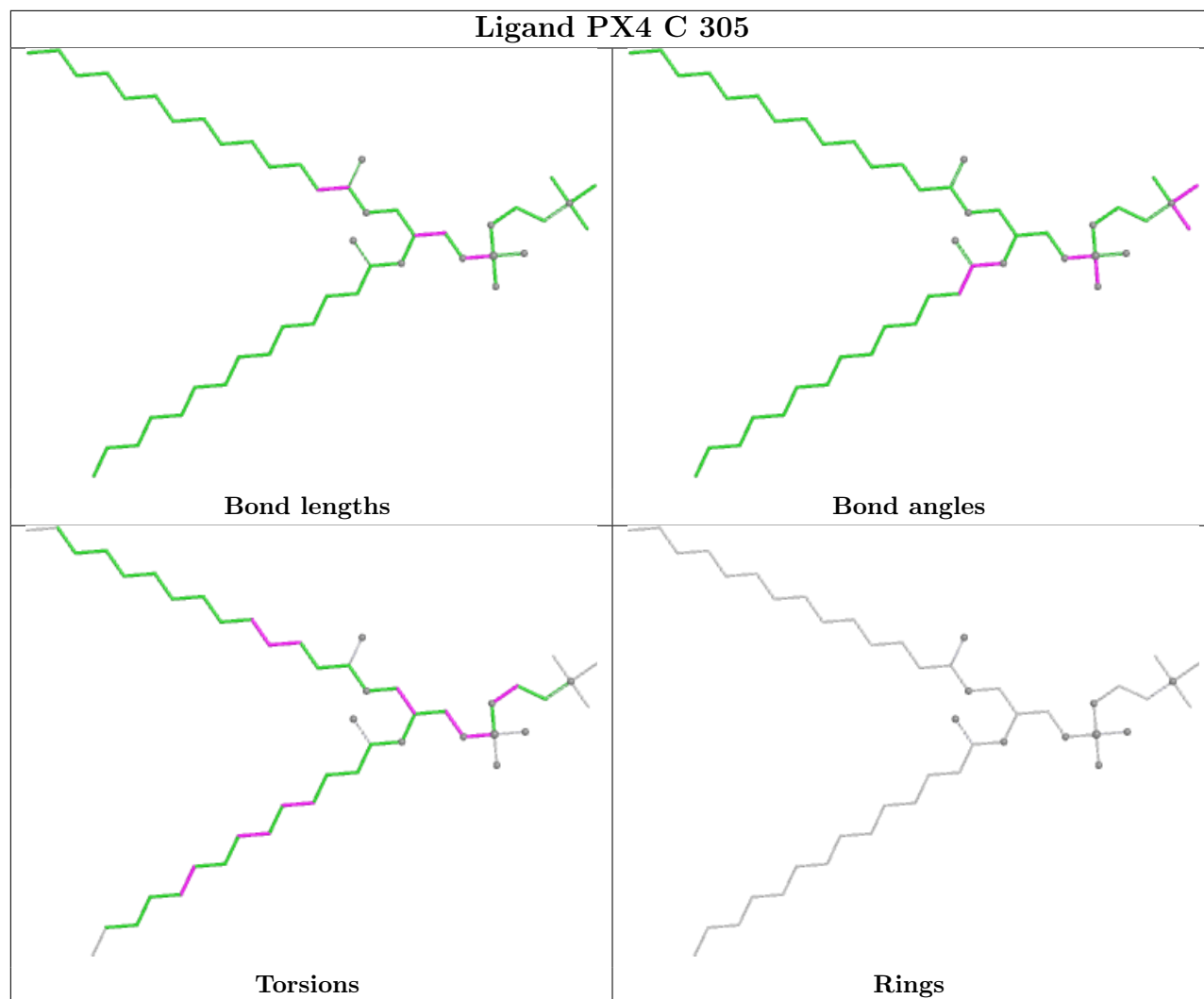


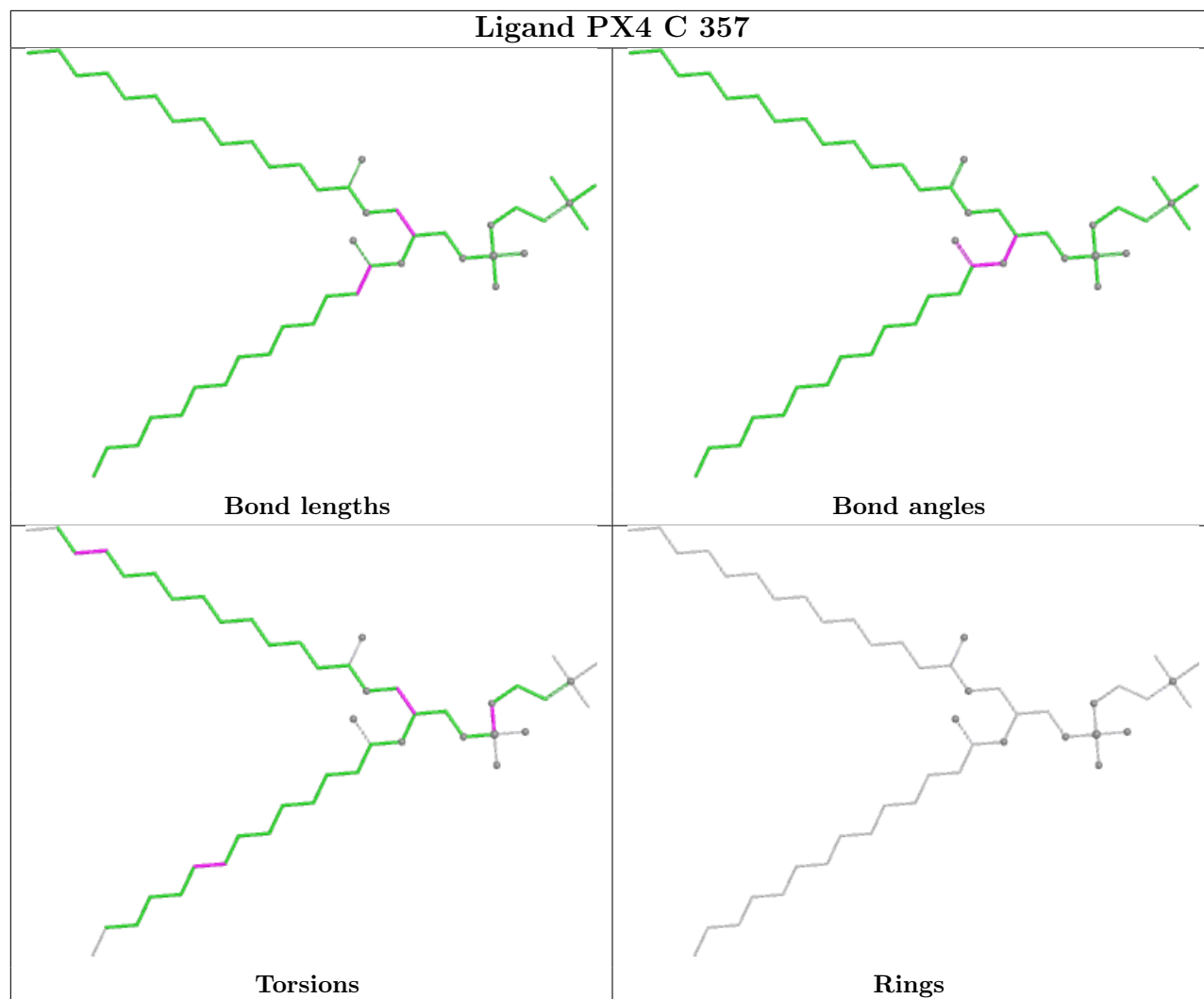


Ligand PX4 B 384

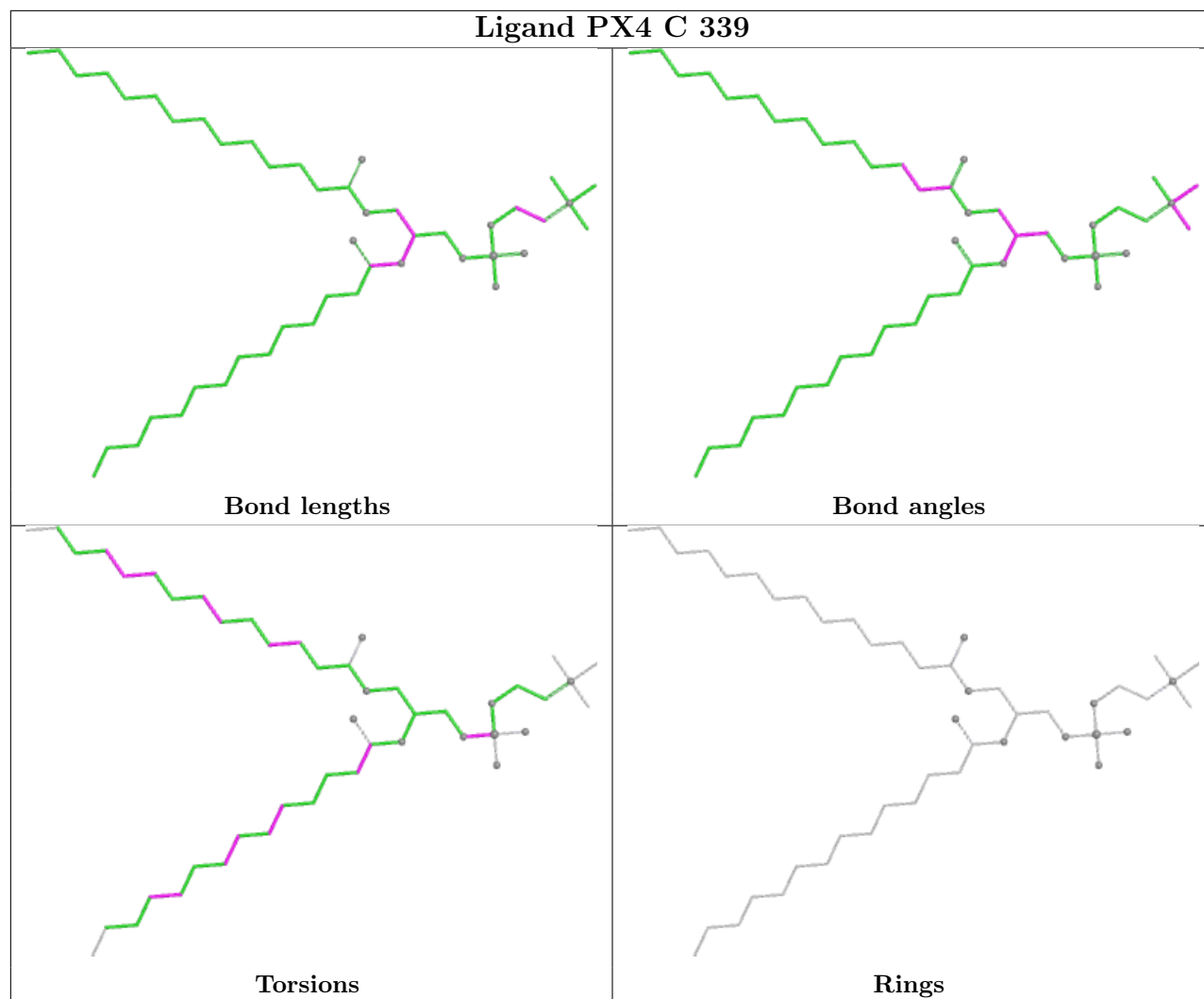


Ligand PX4 C 305

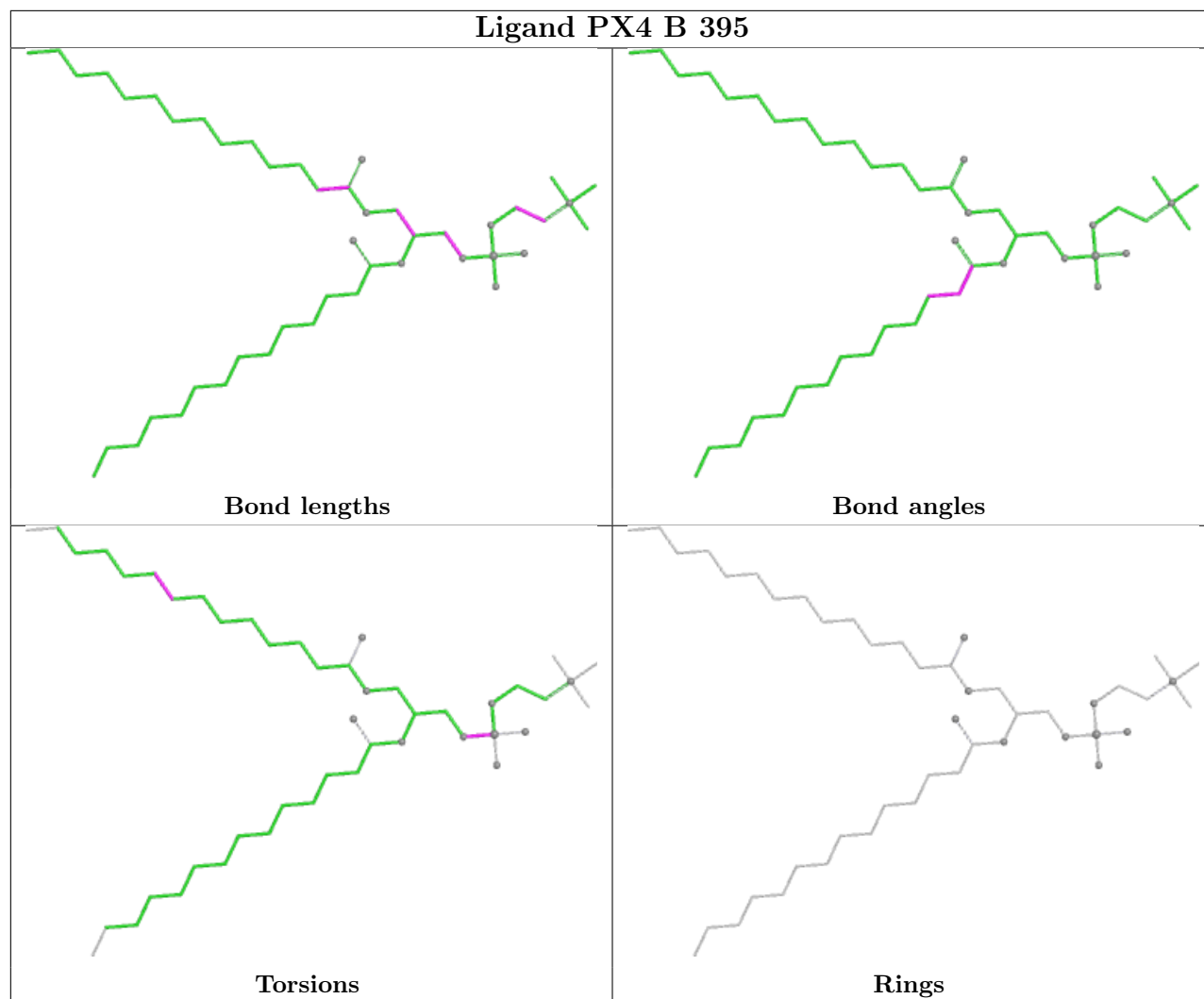


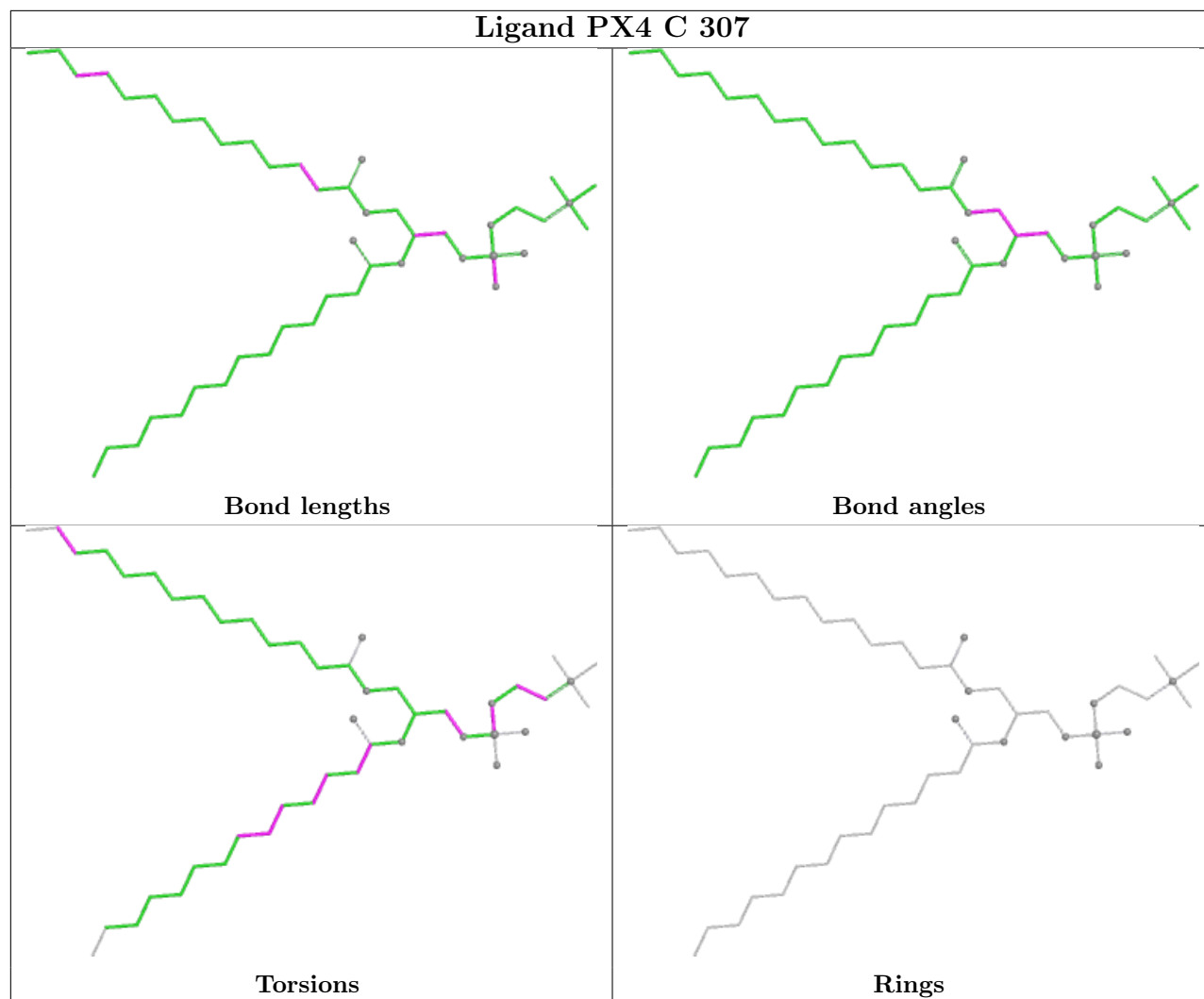


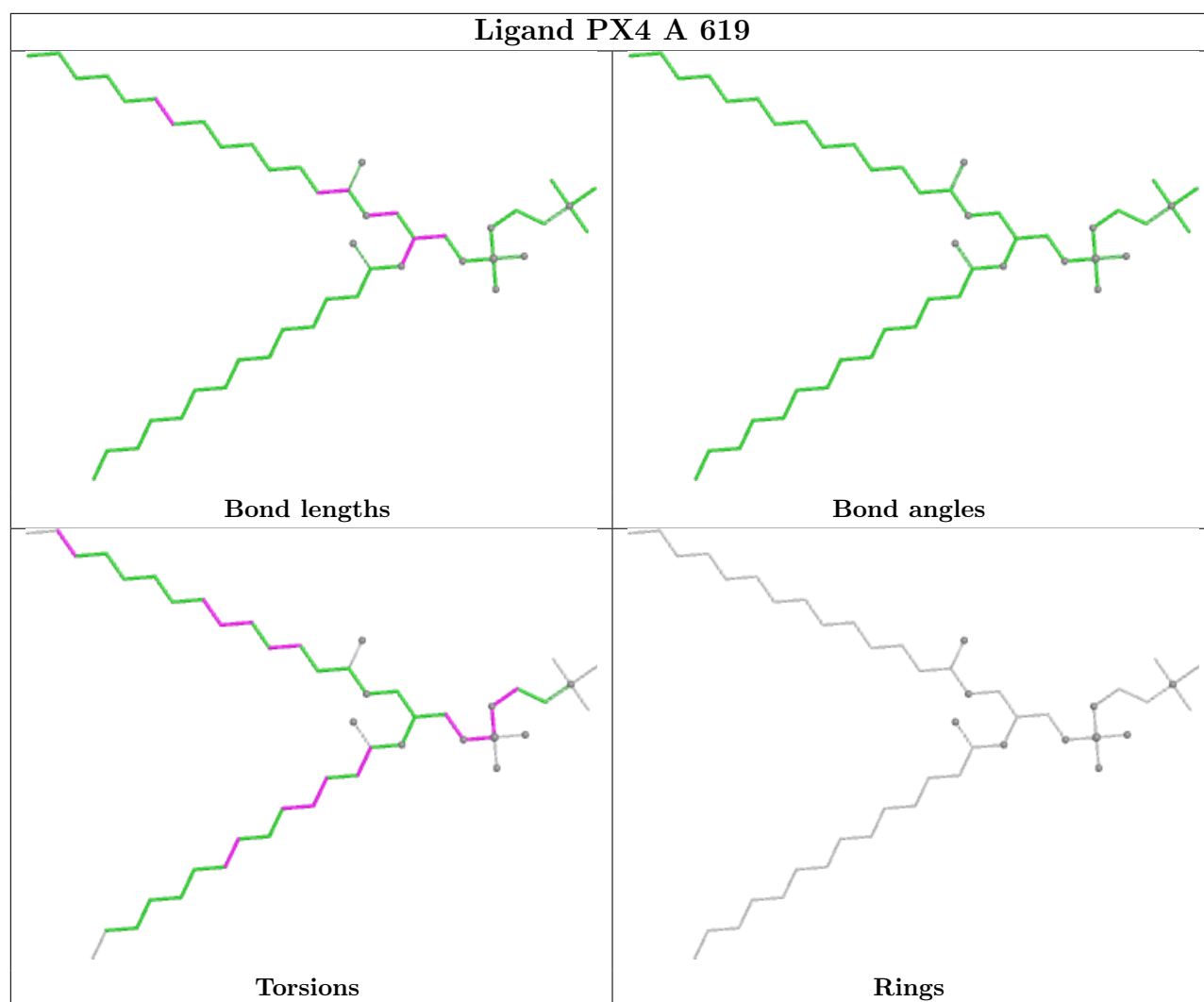
Ligand PX4 C 339

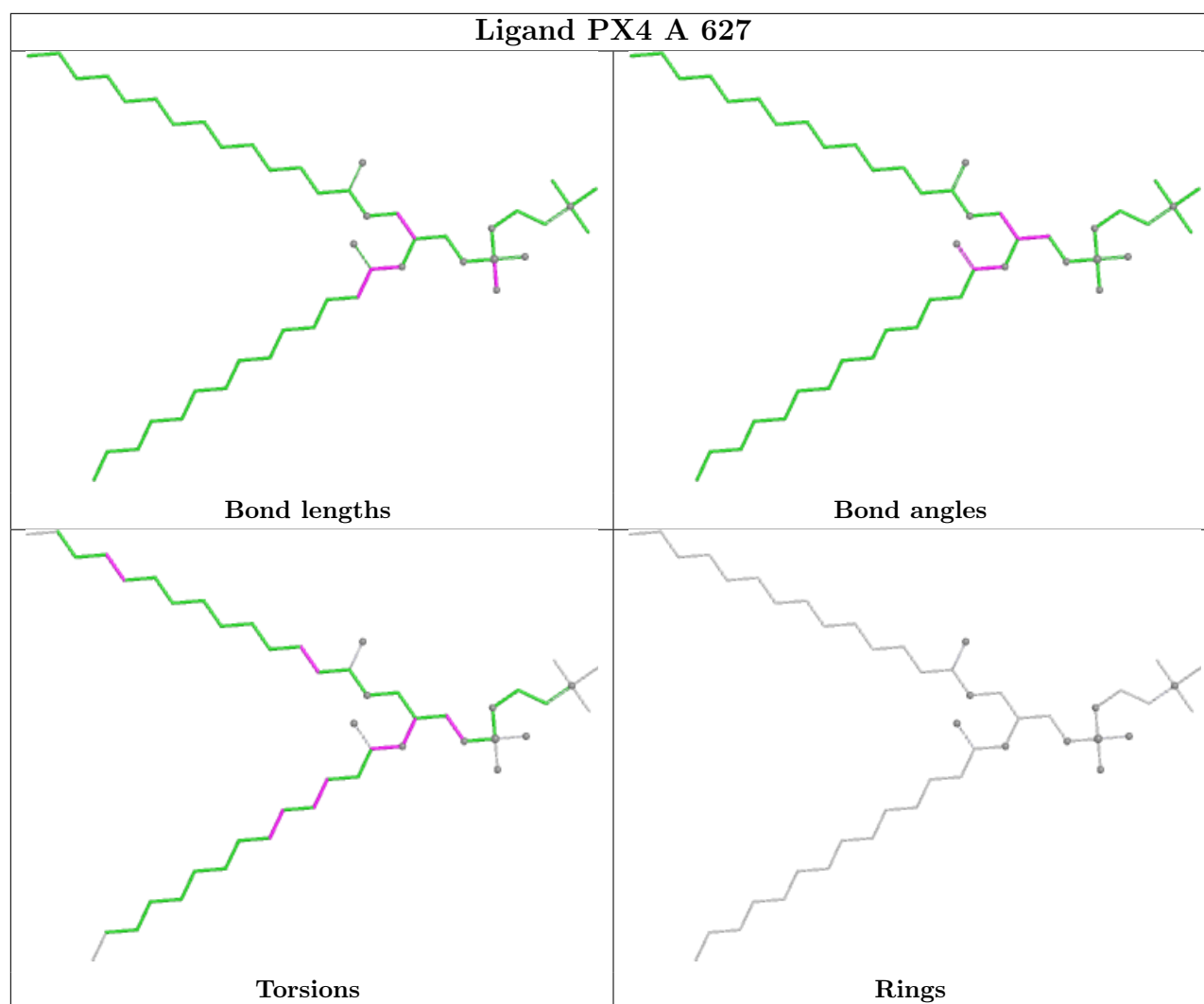


Ligand PX4 B 395

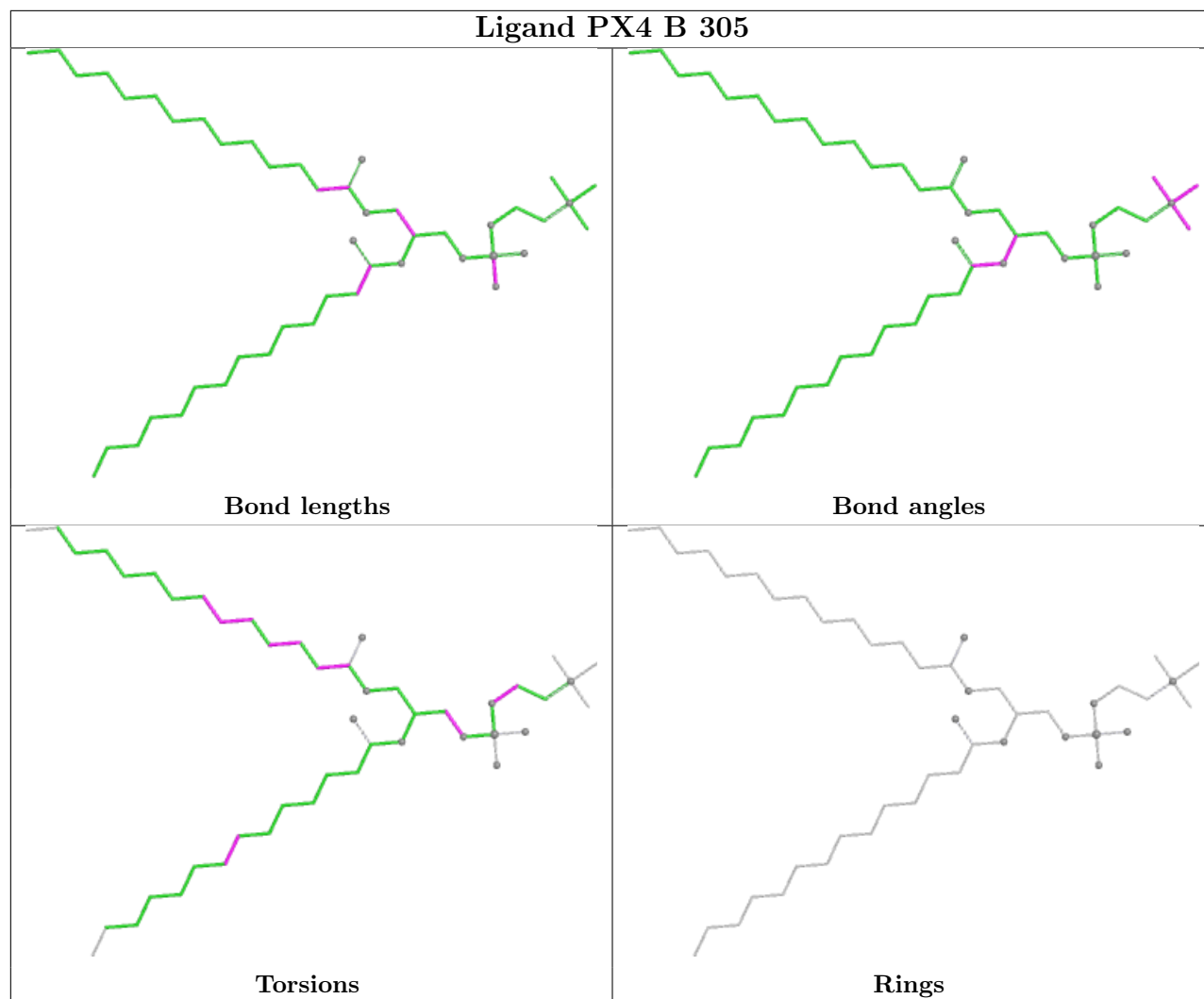


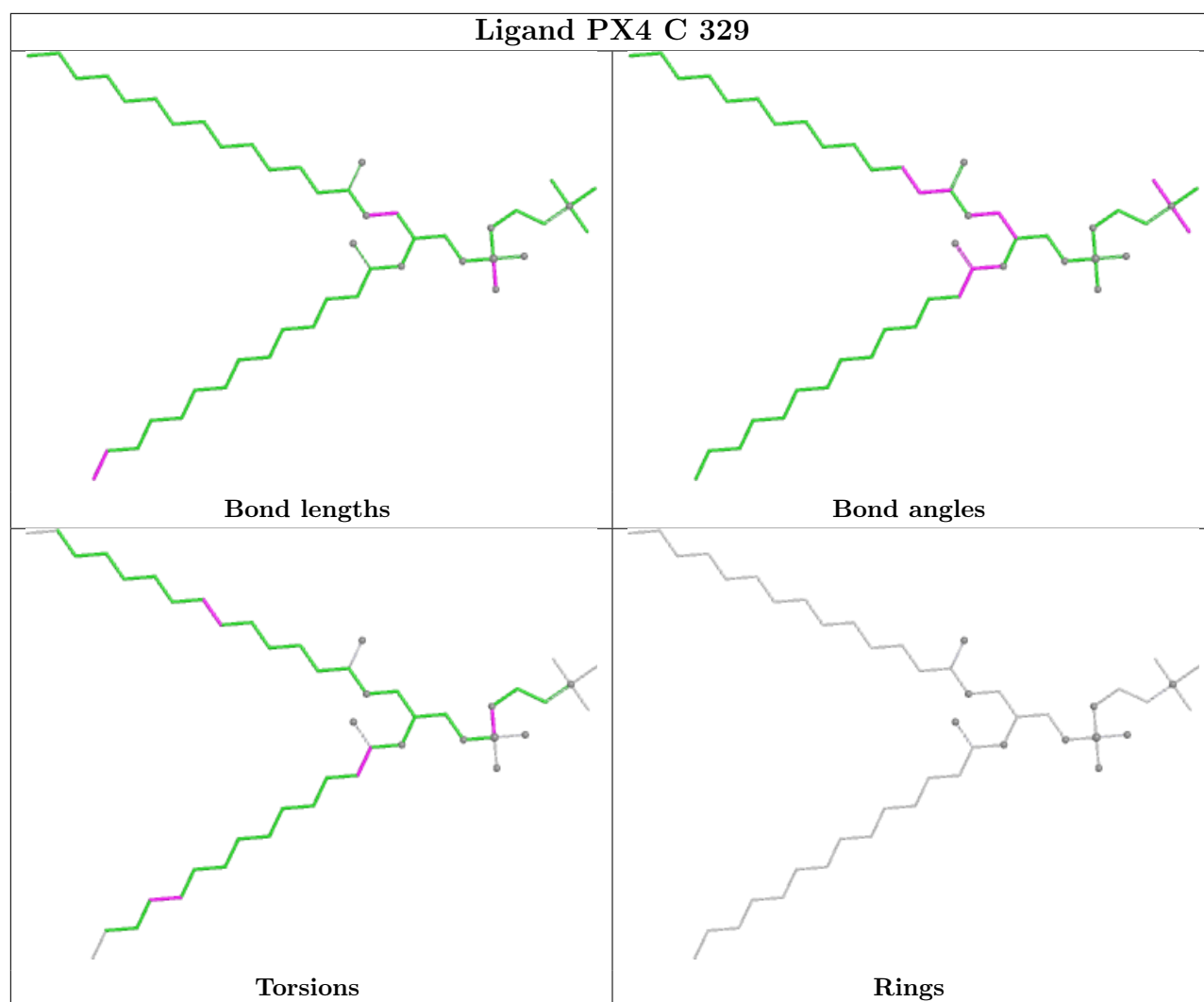


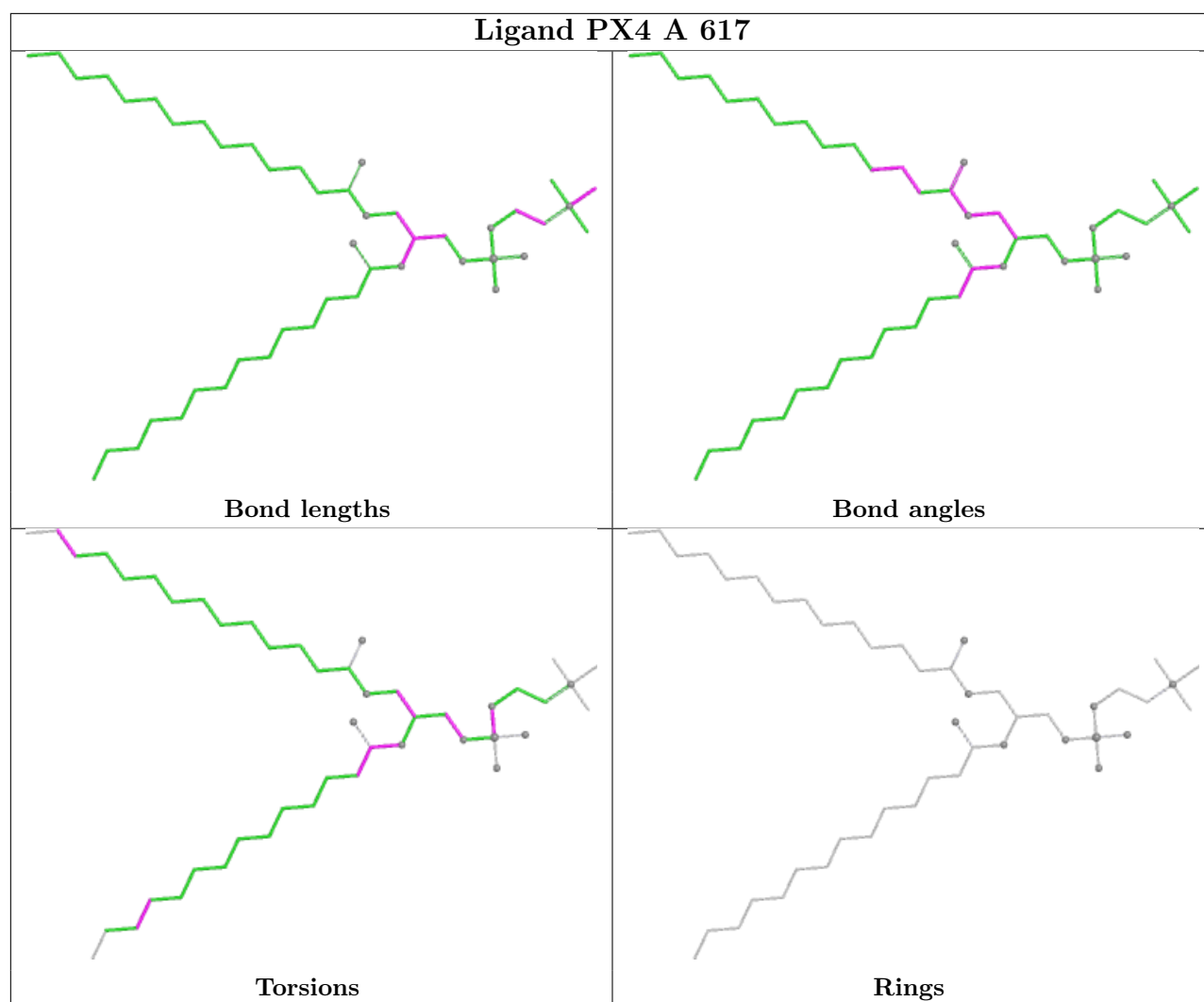




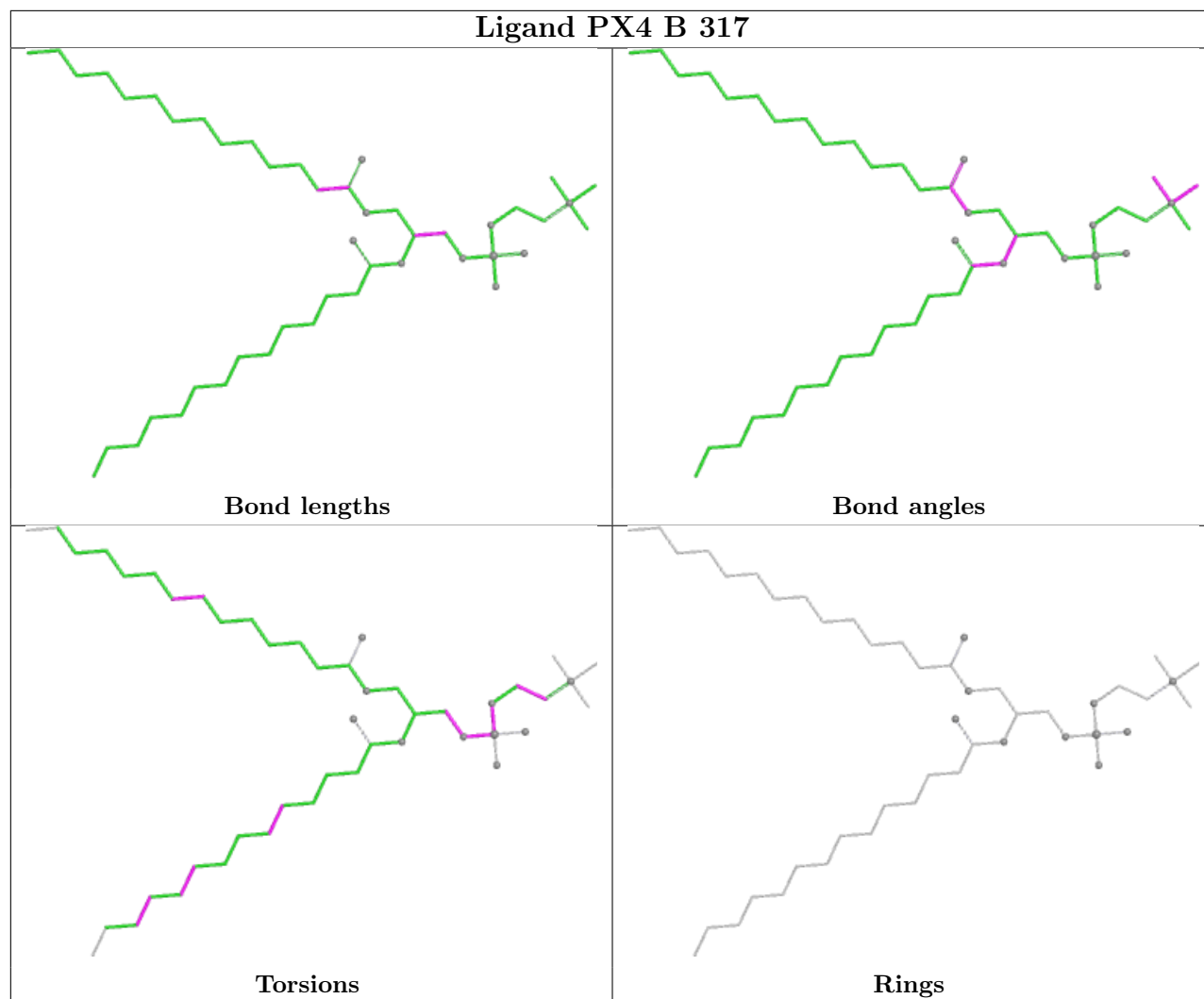
Ligand PX4 B 305

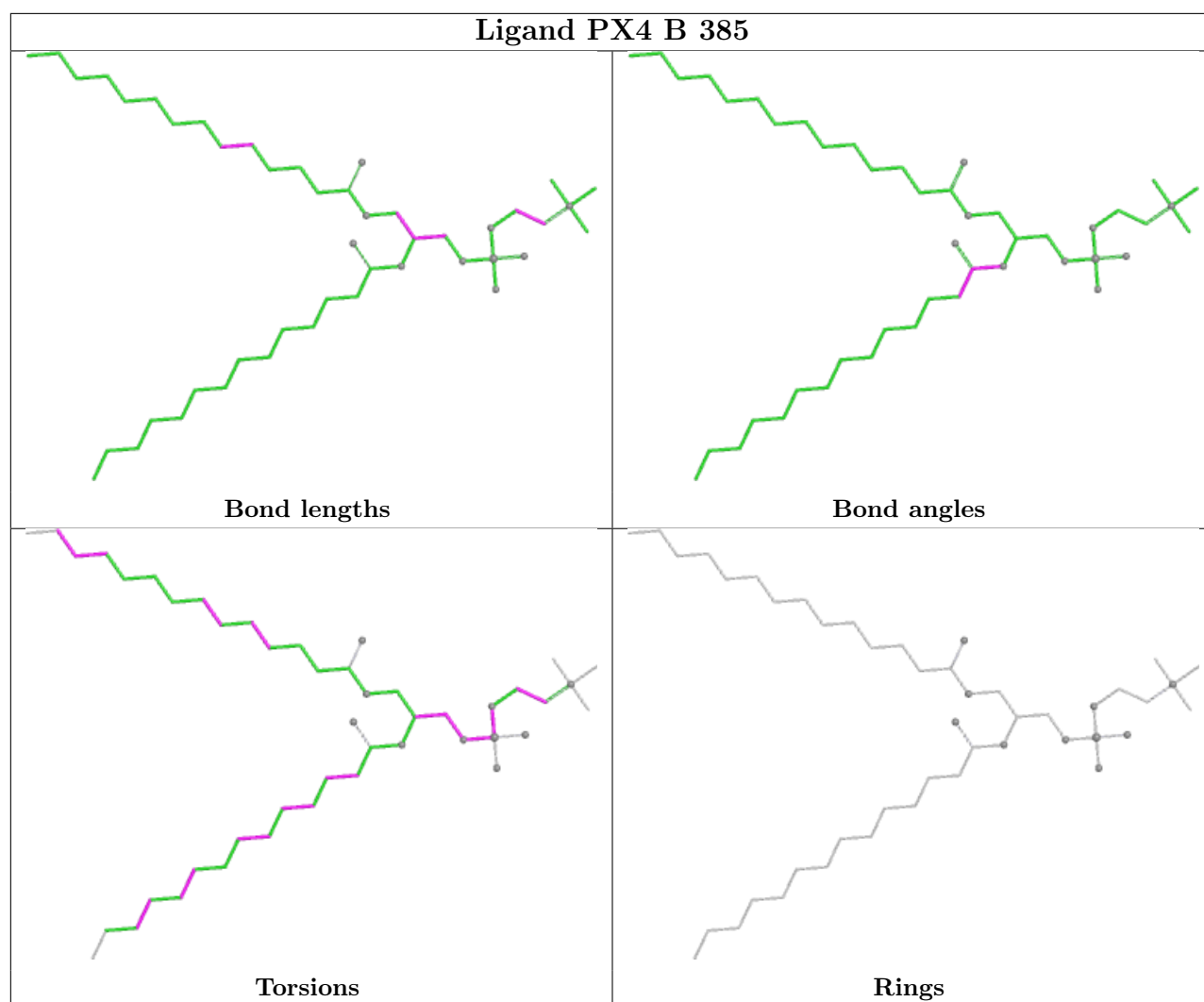


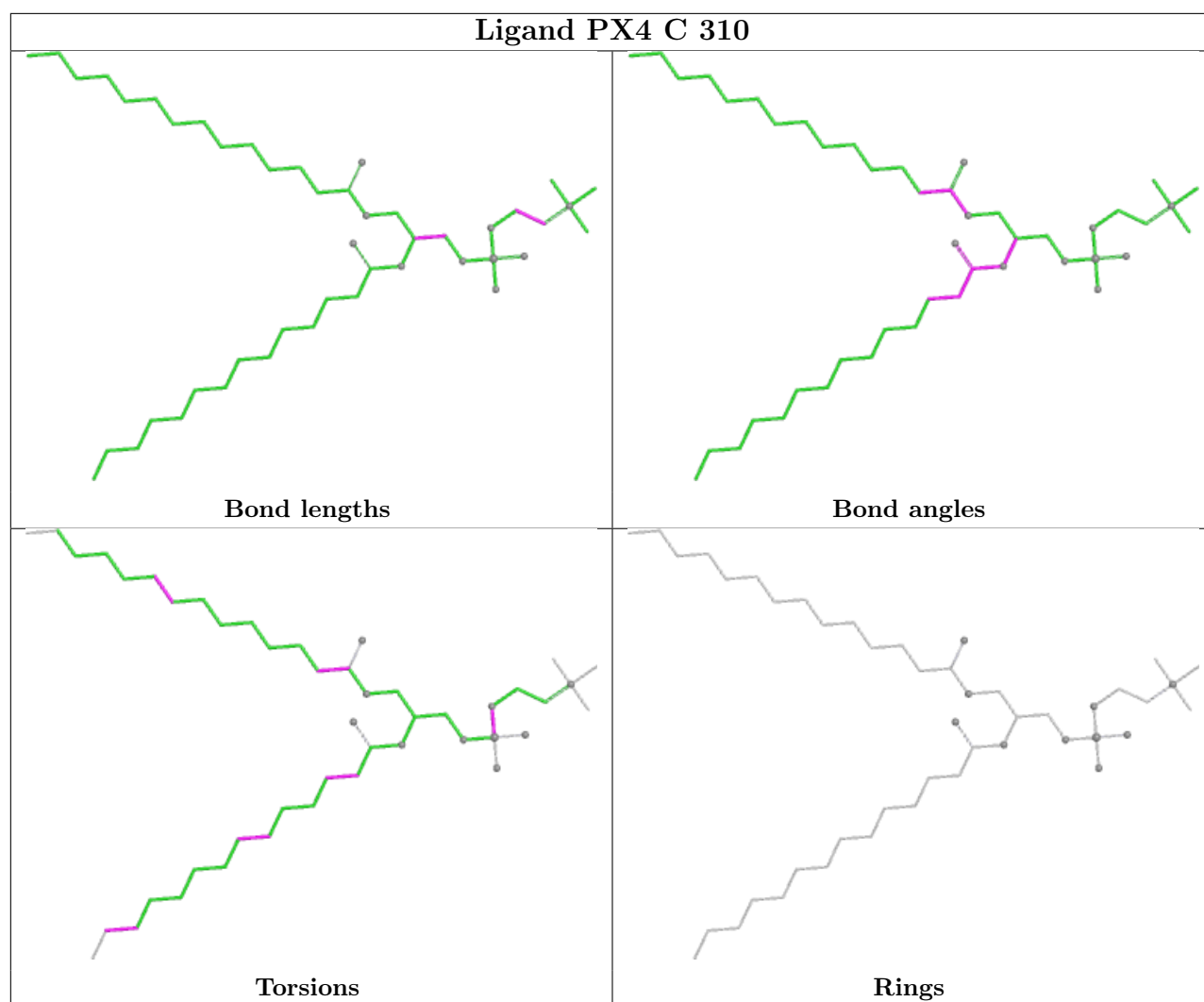


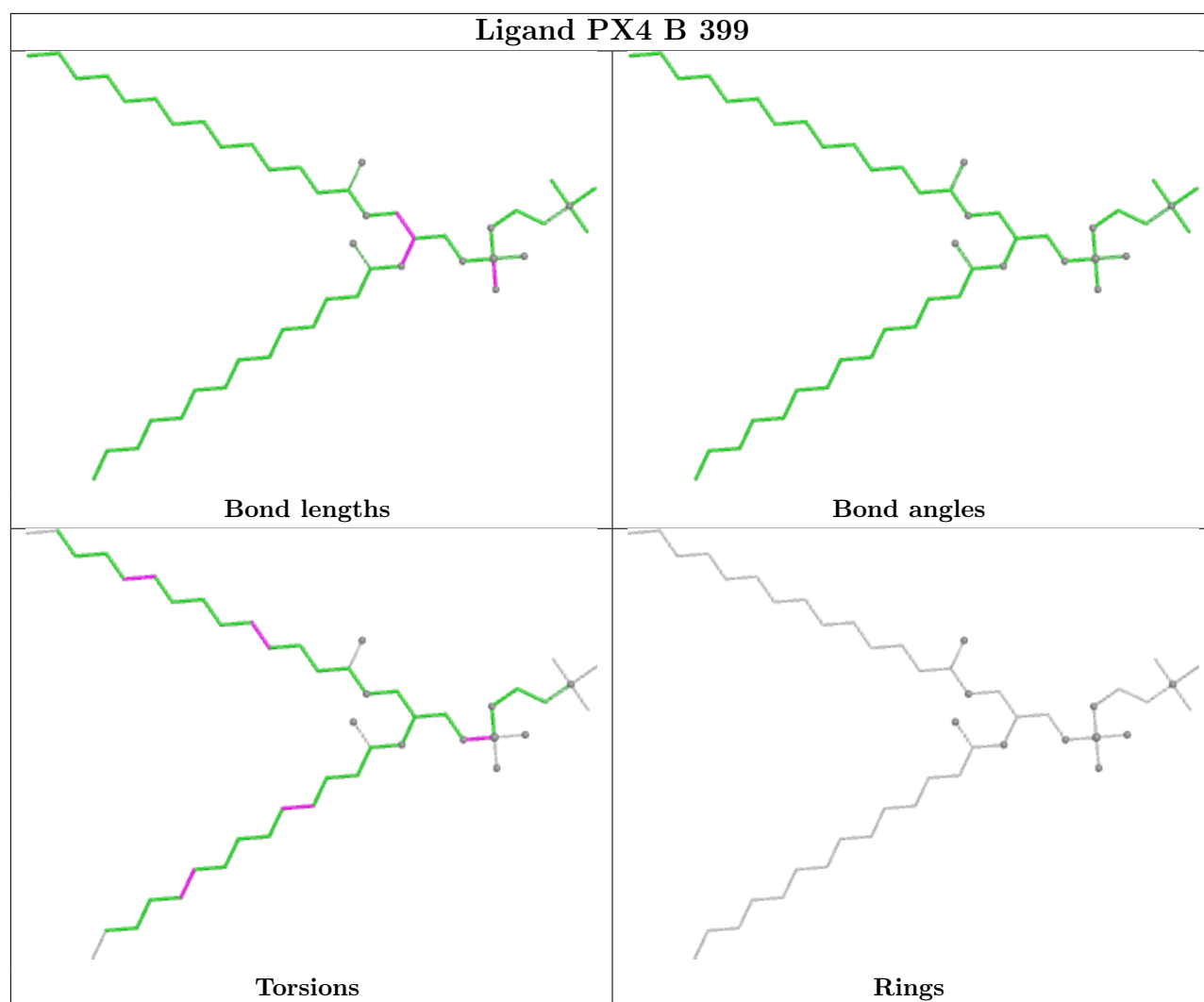


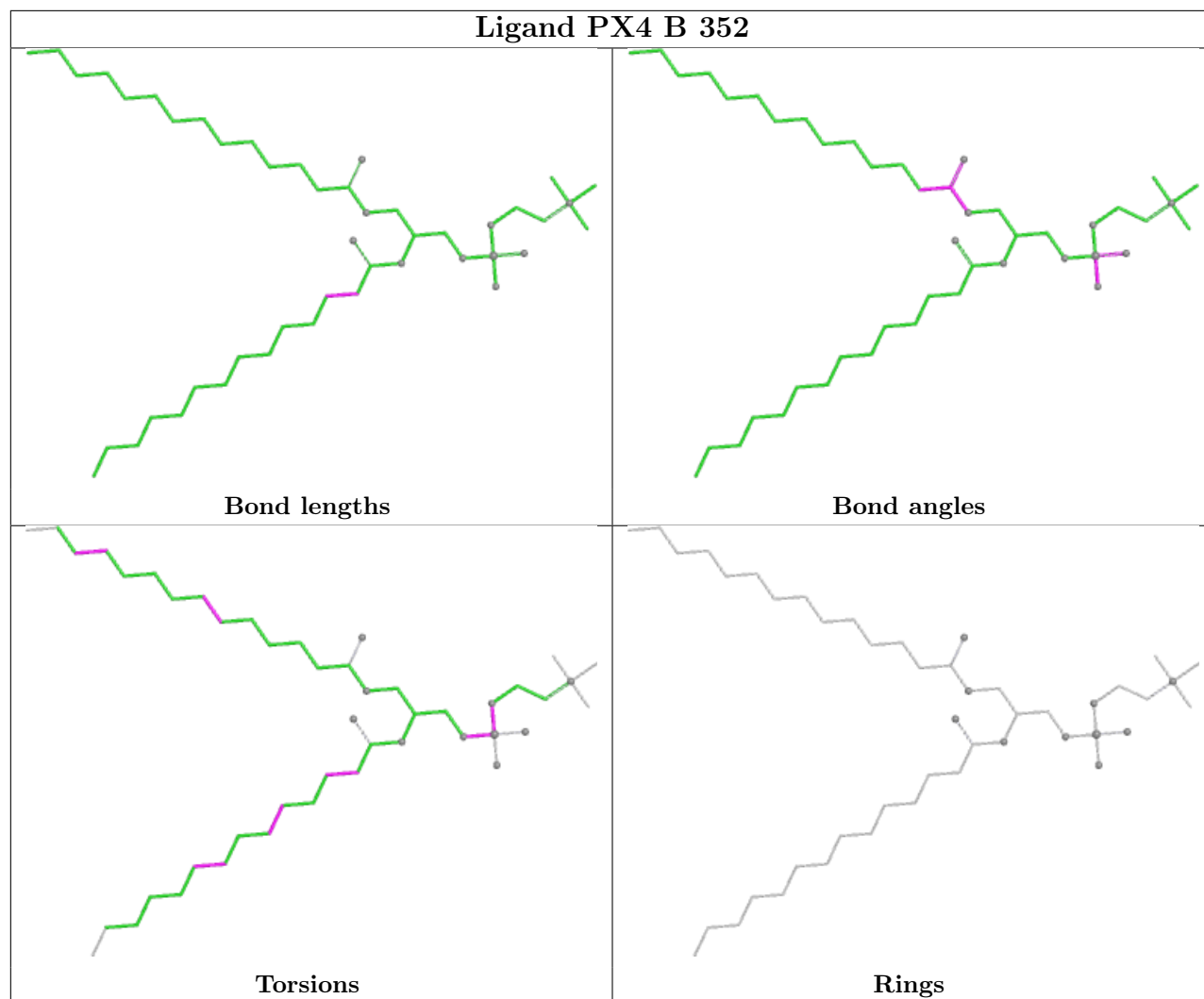
Ligand PX4 B 317

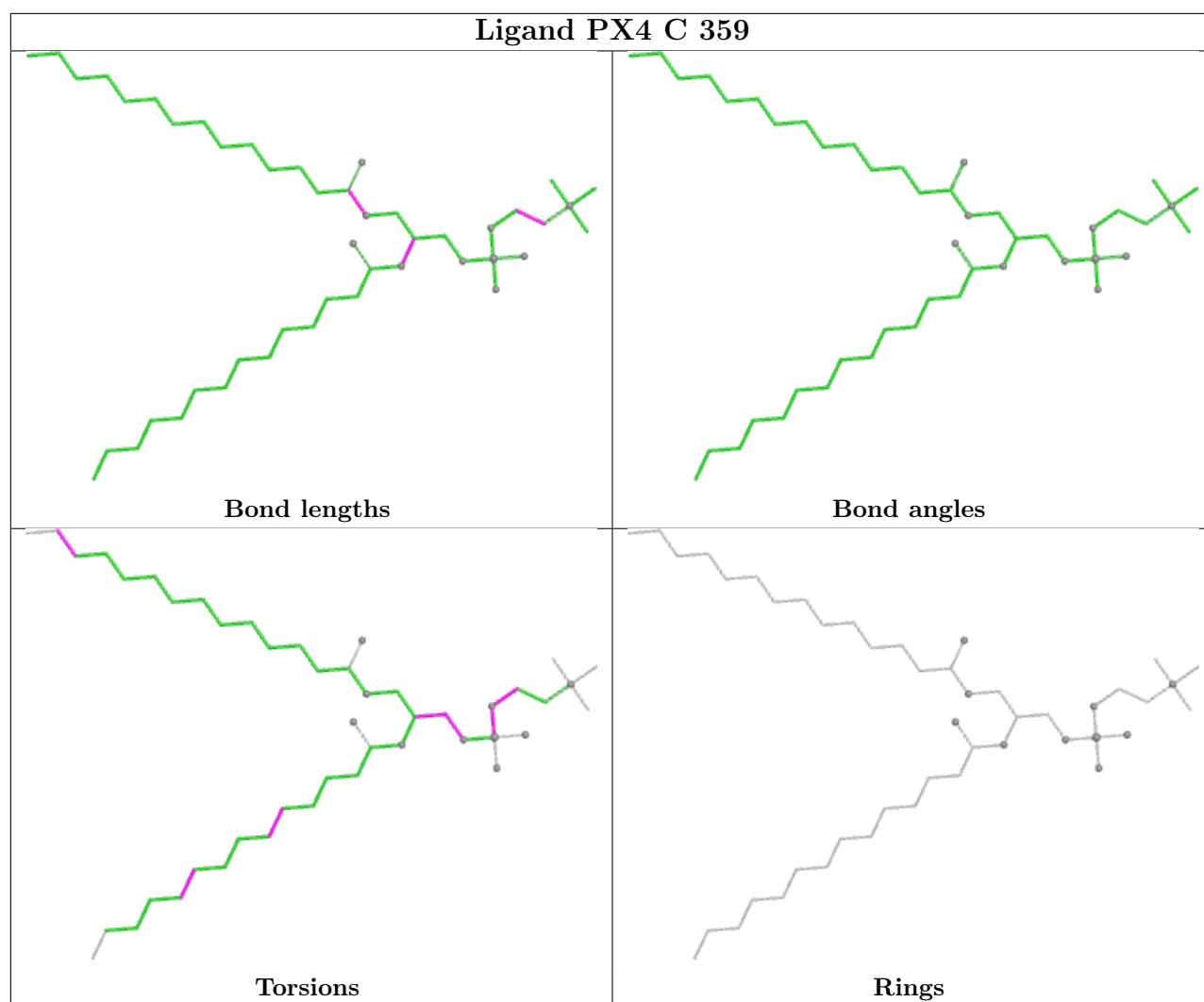




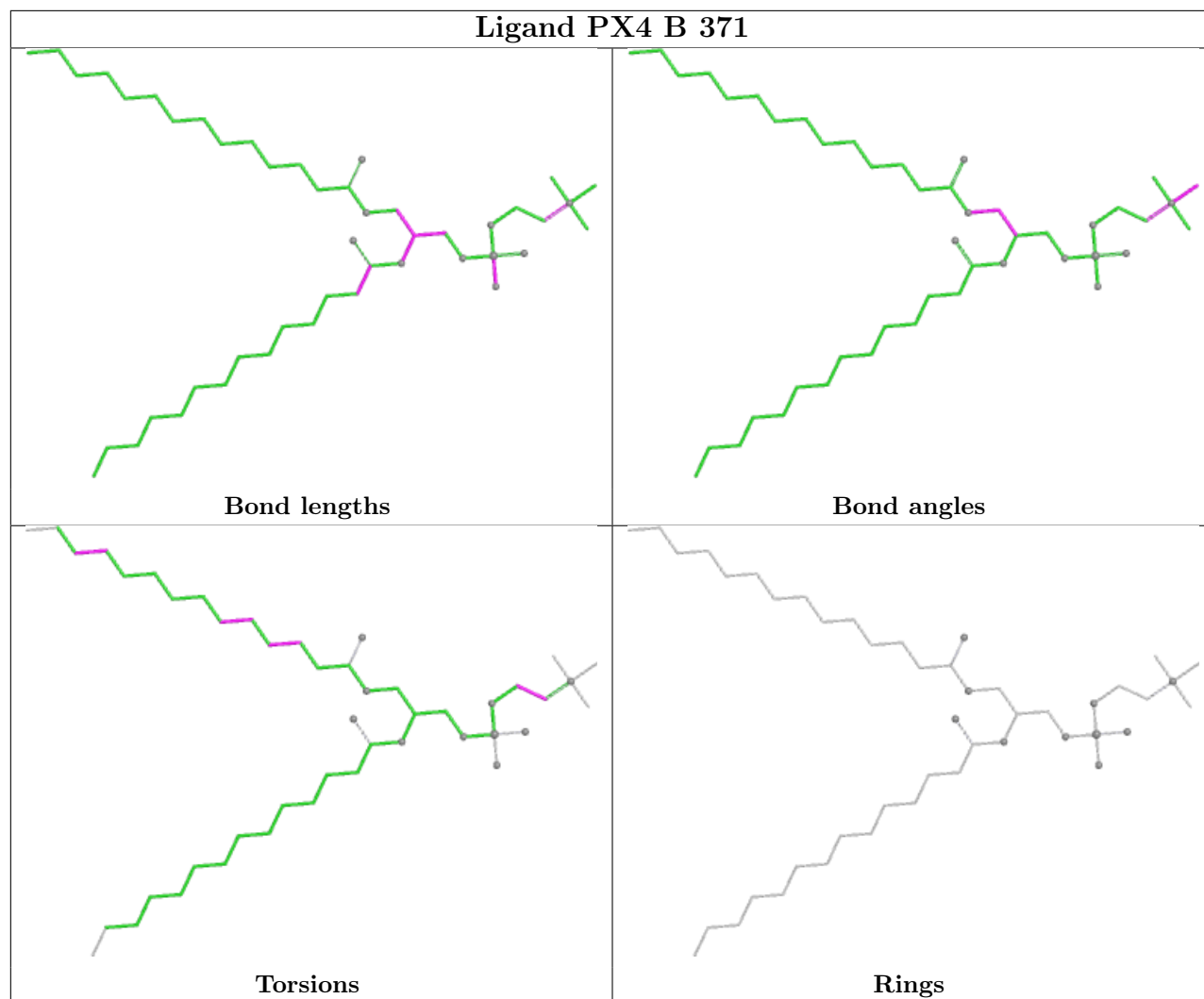


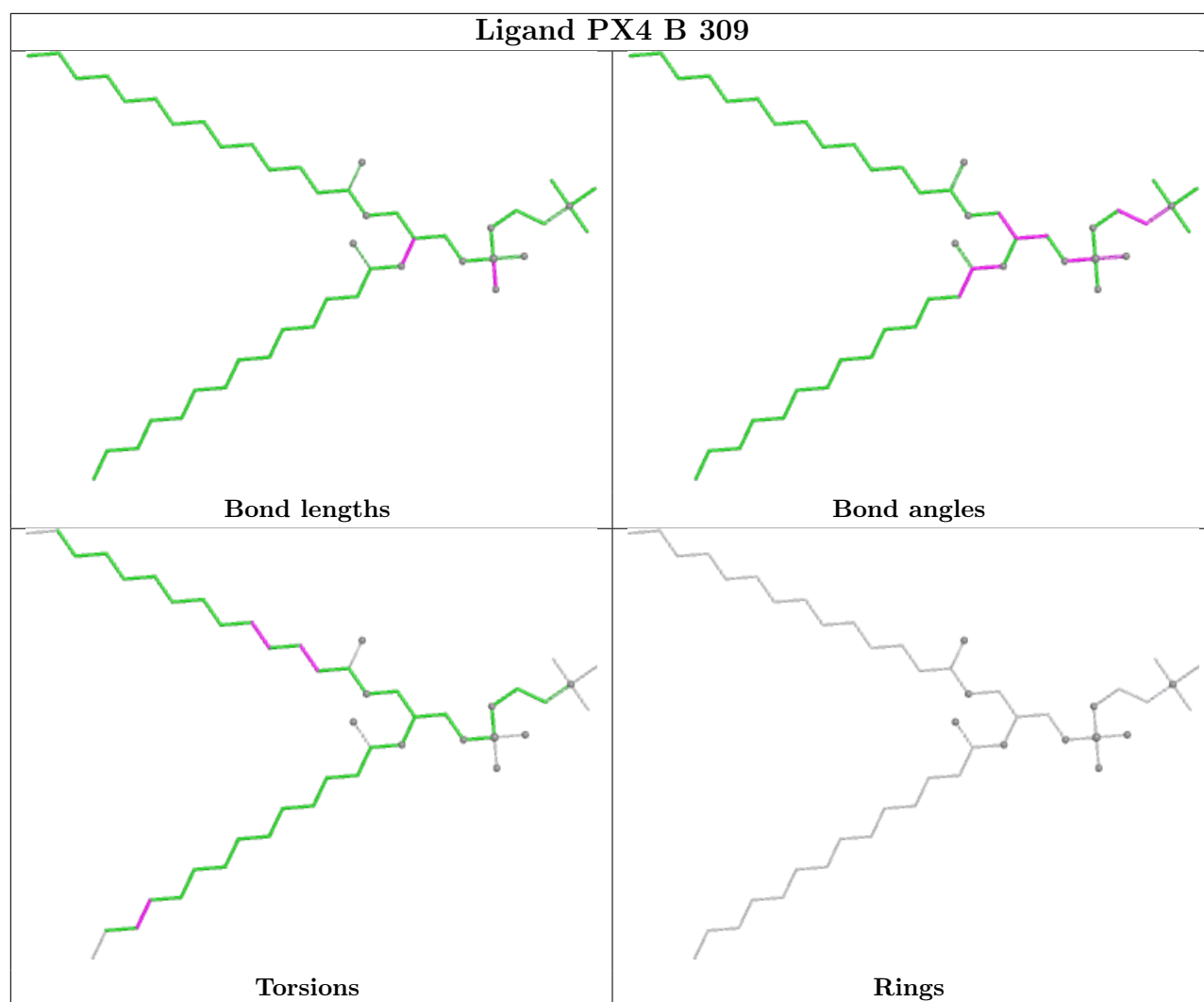




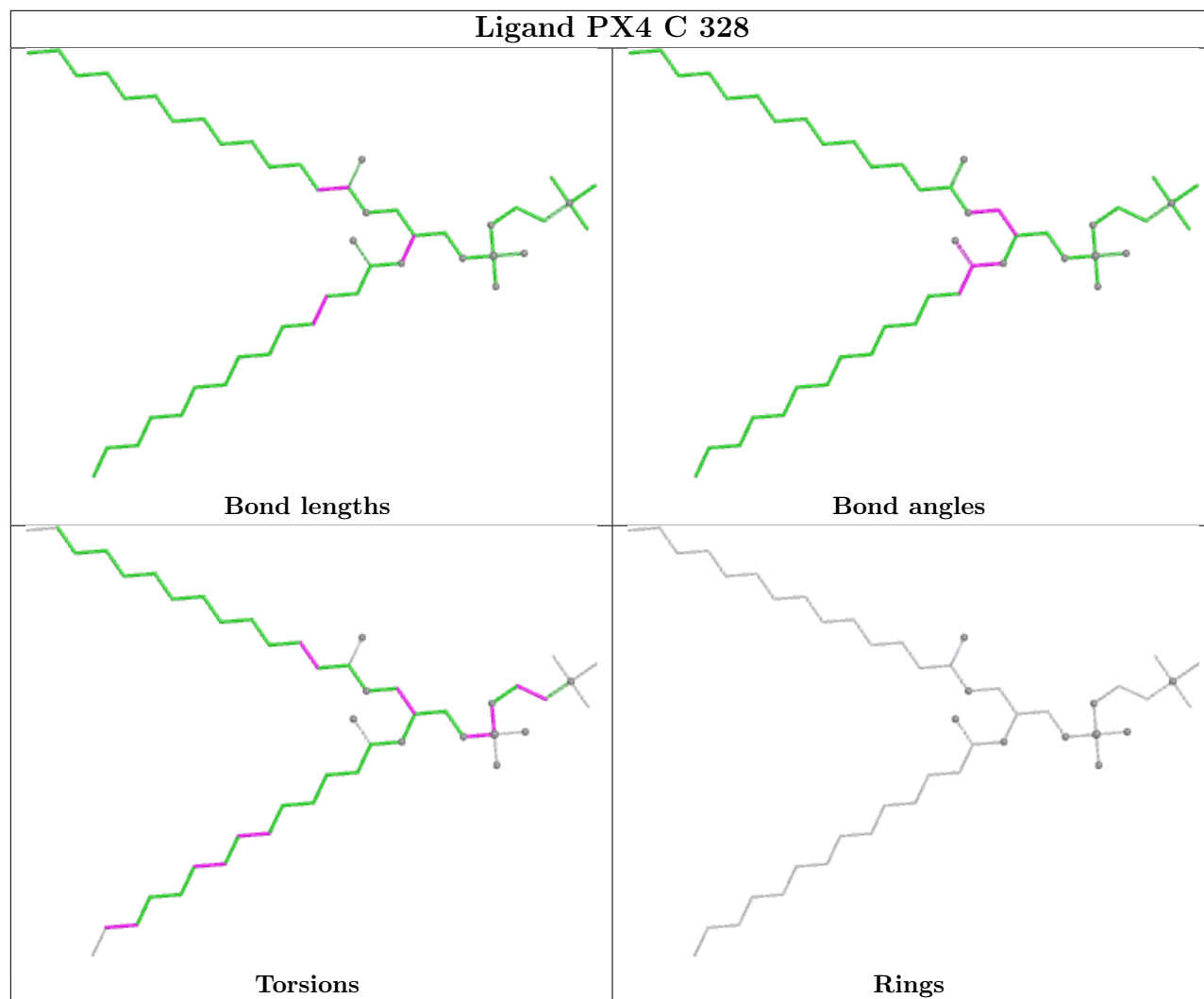


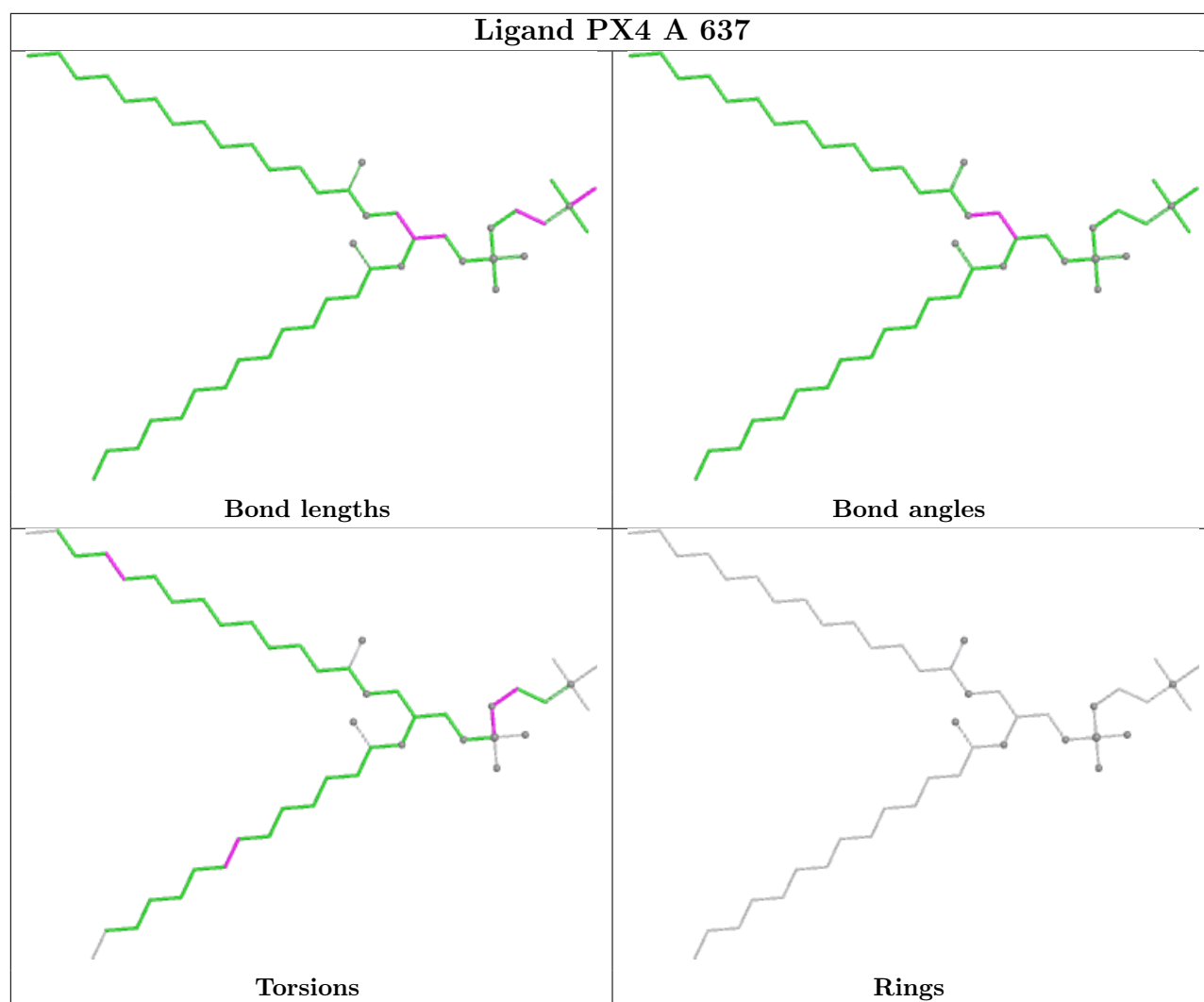
Ligand PX4 B 371



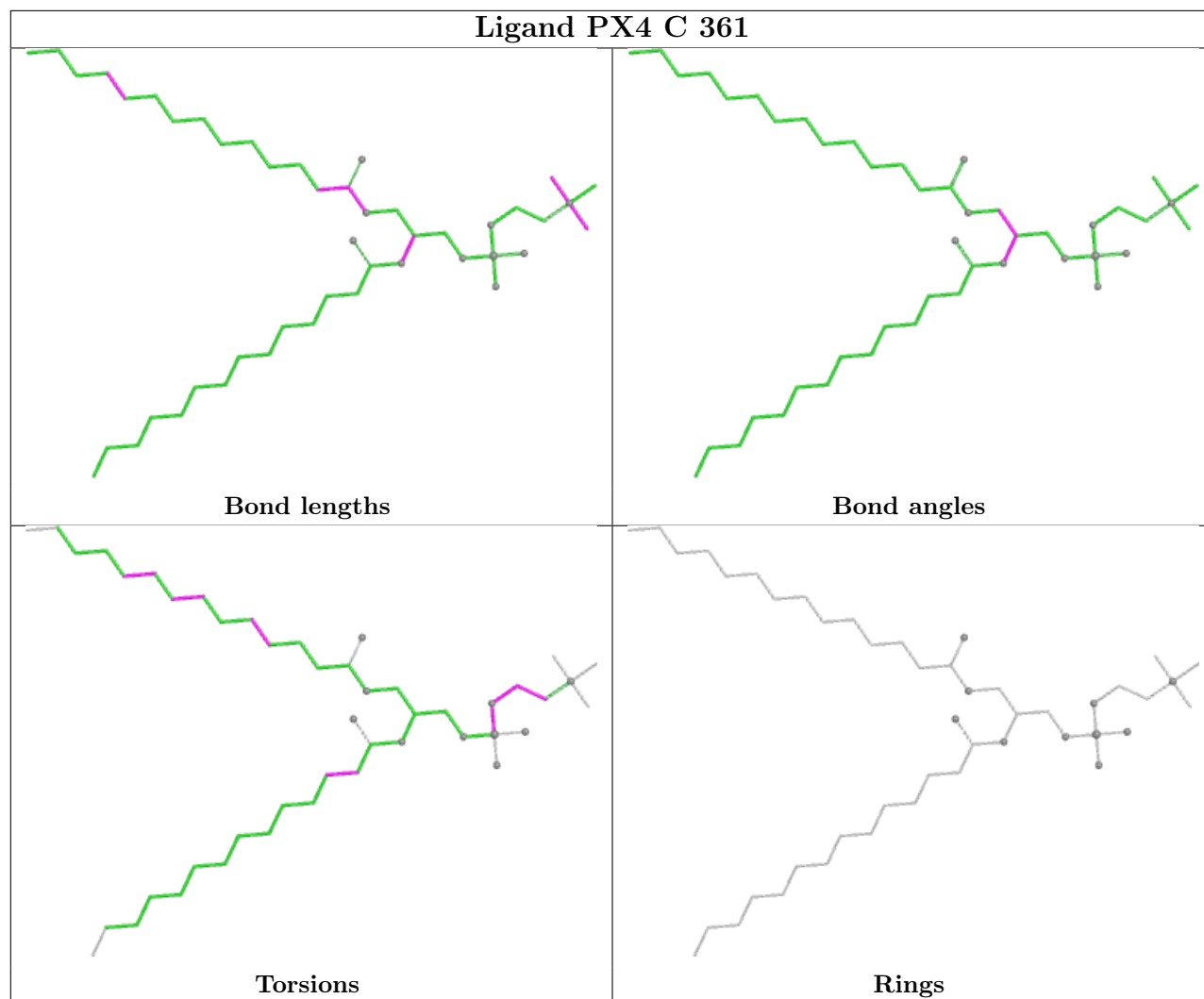


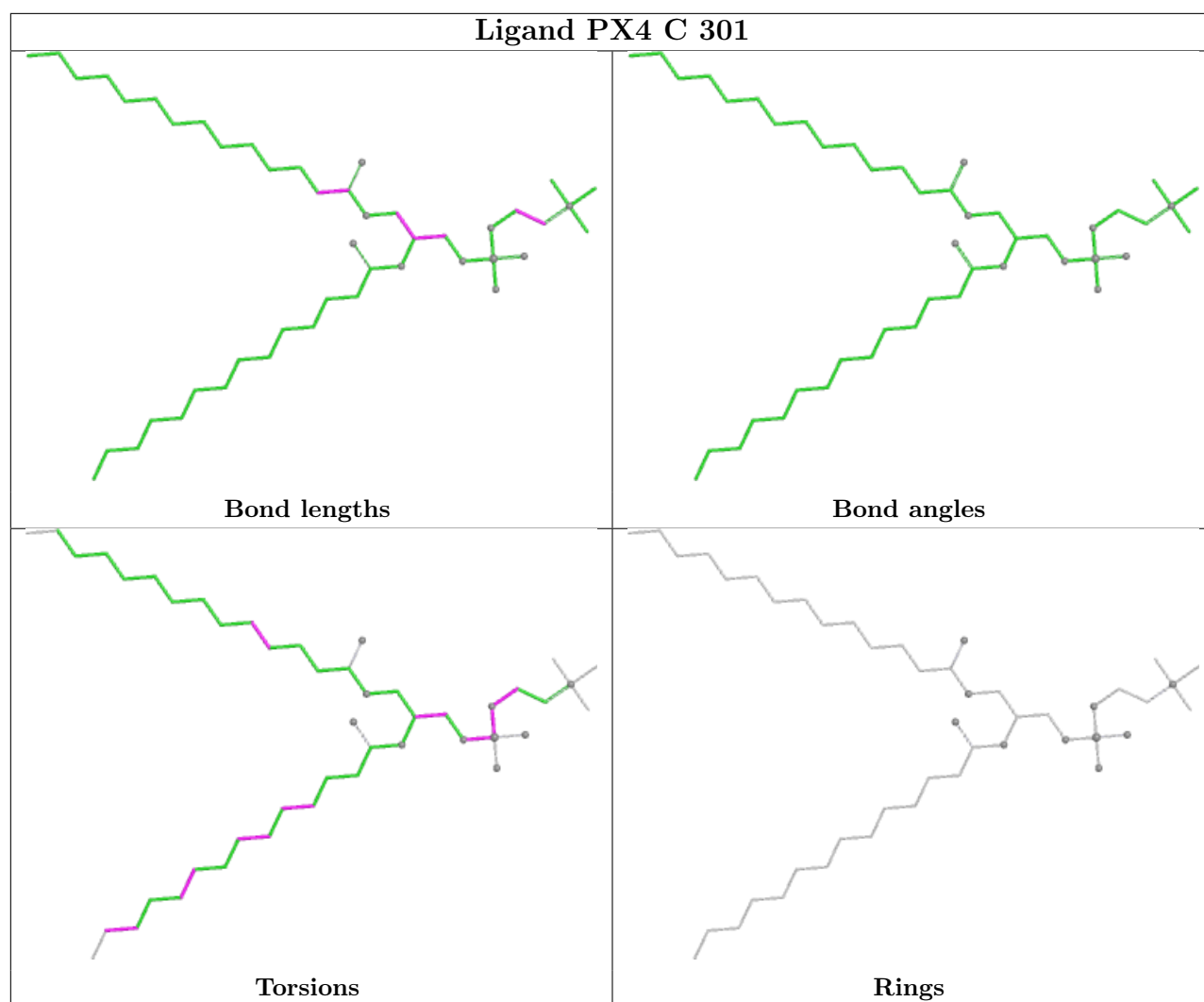
Ligand PX4 C 328



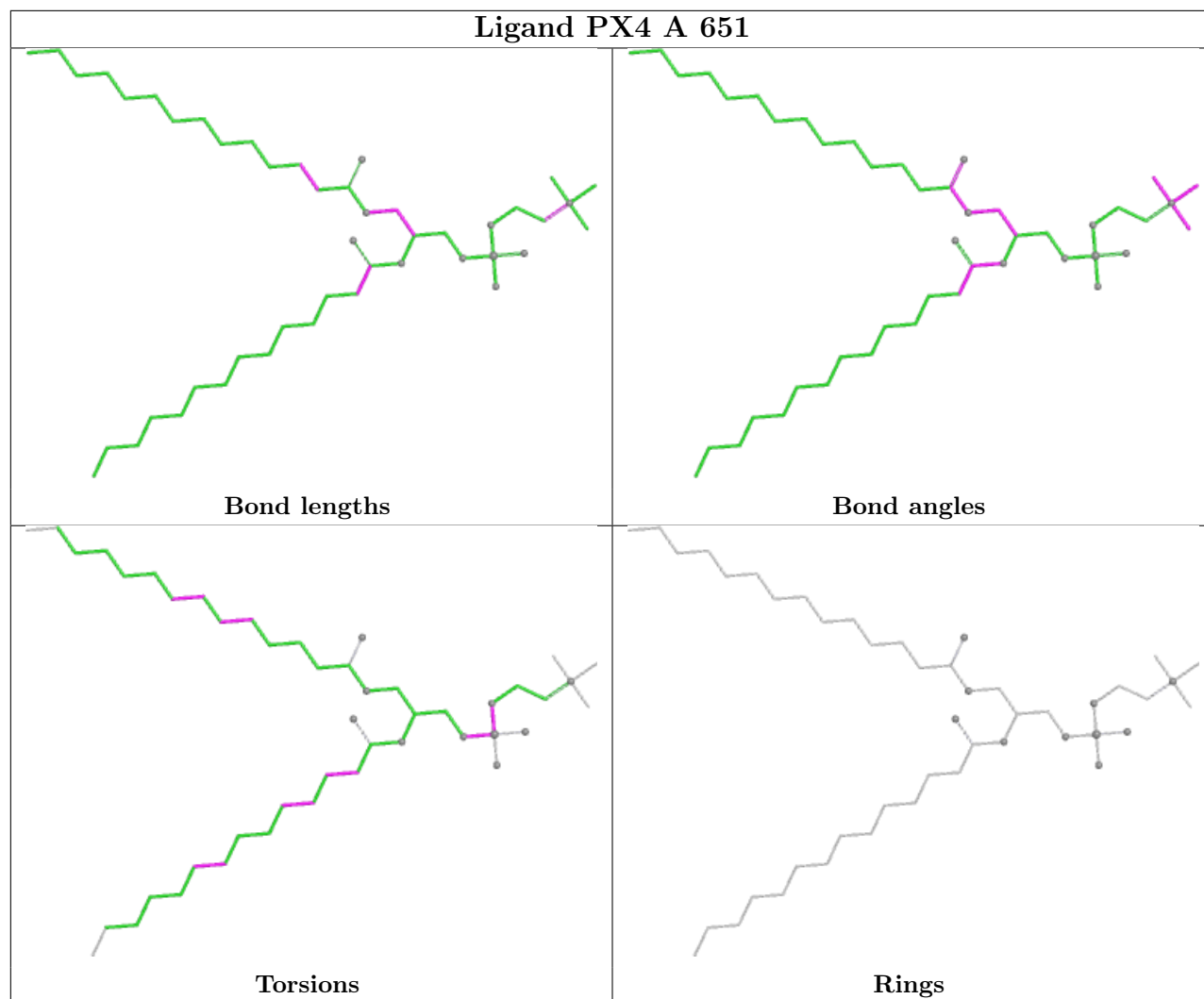


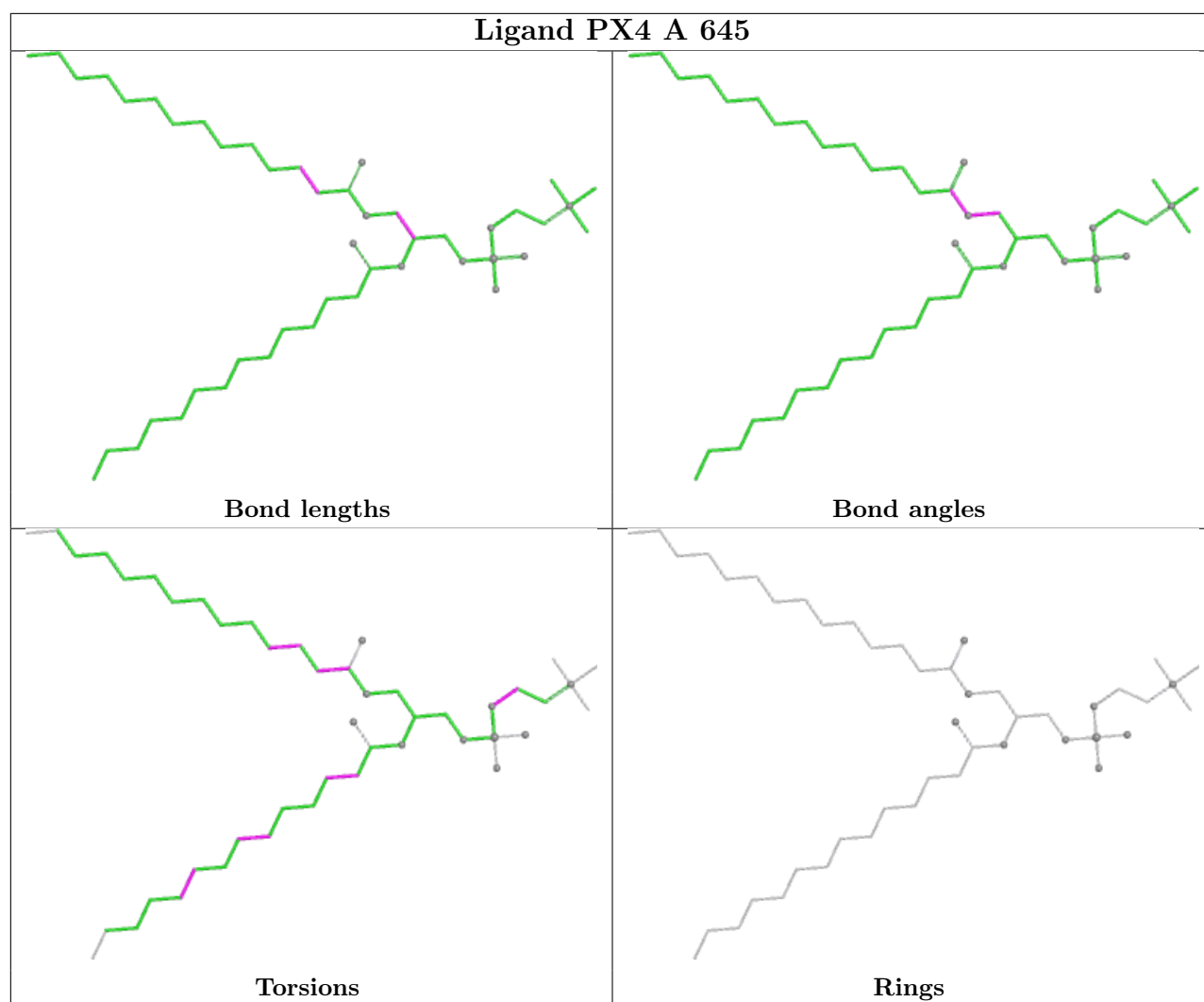
Ligand PX4 C 361

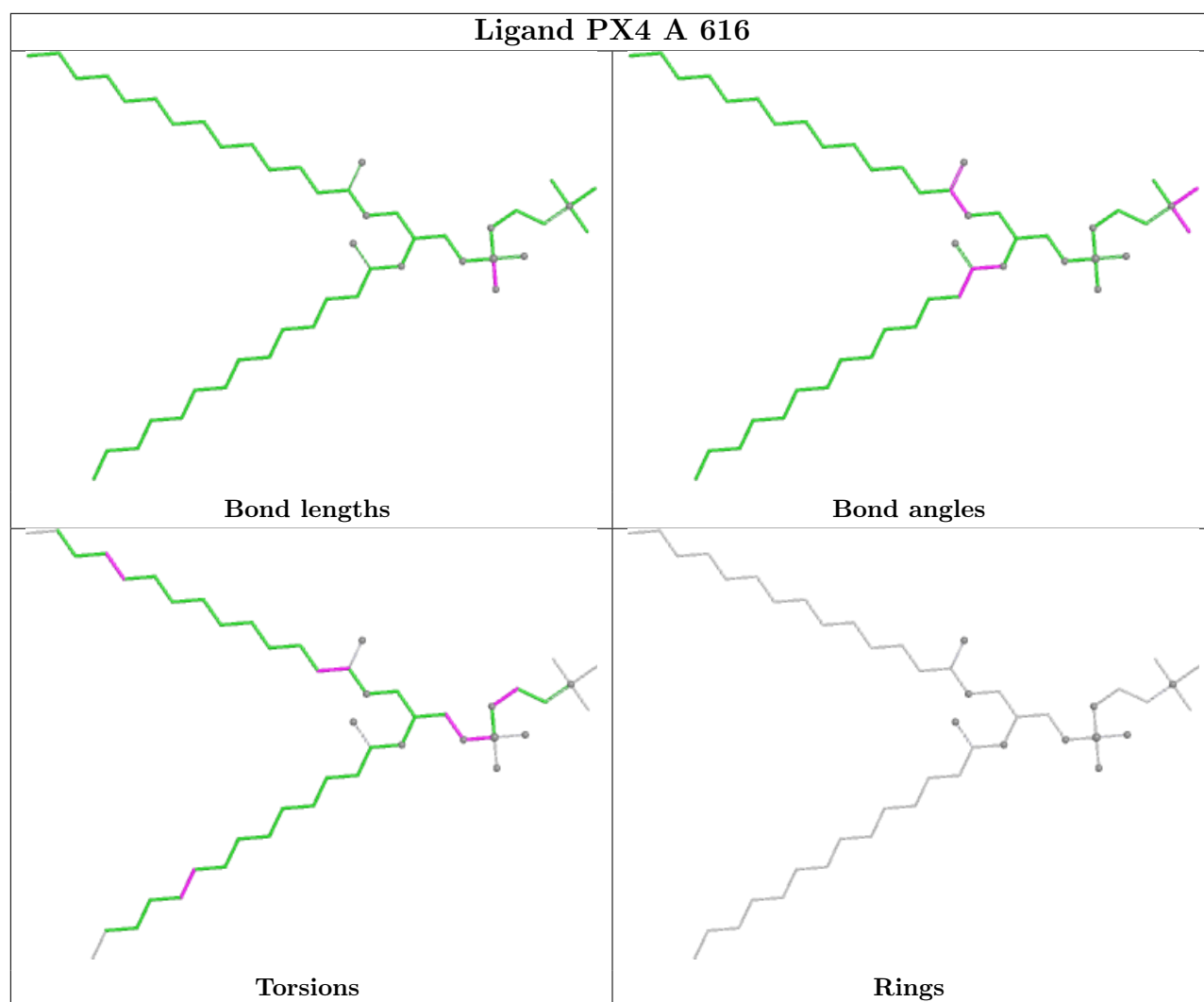




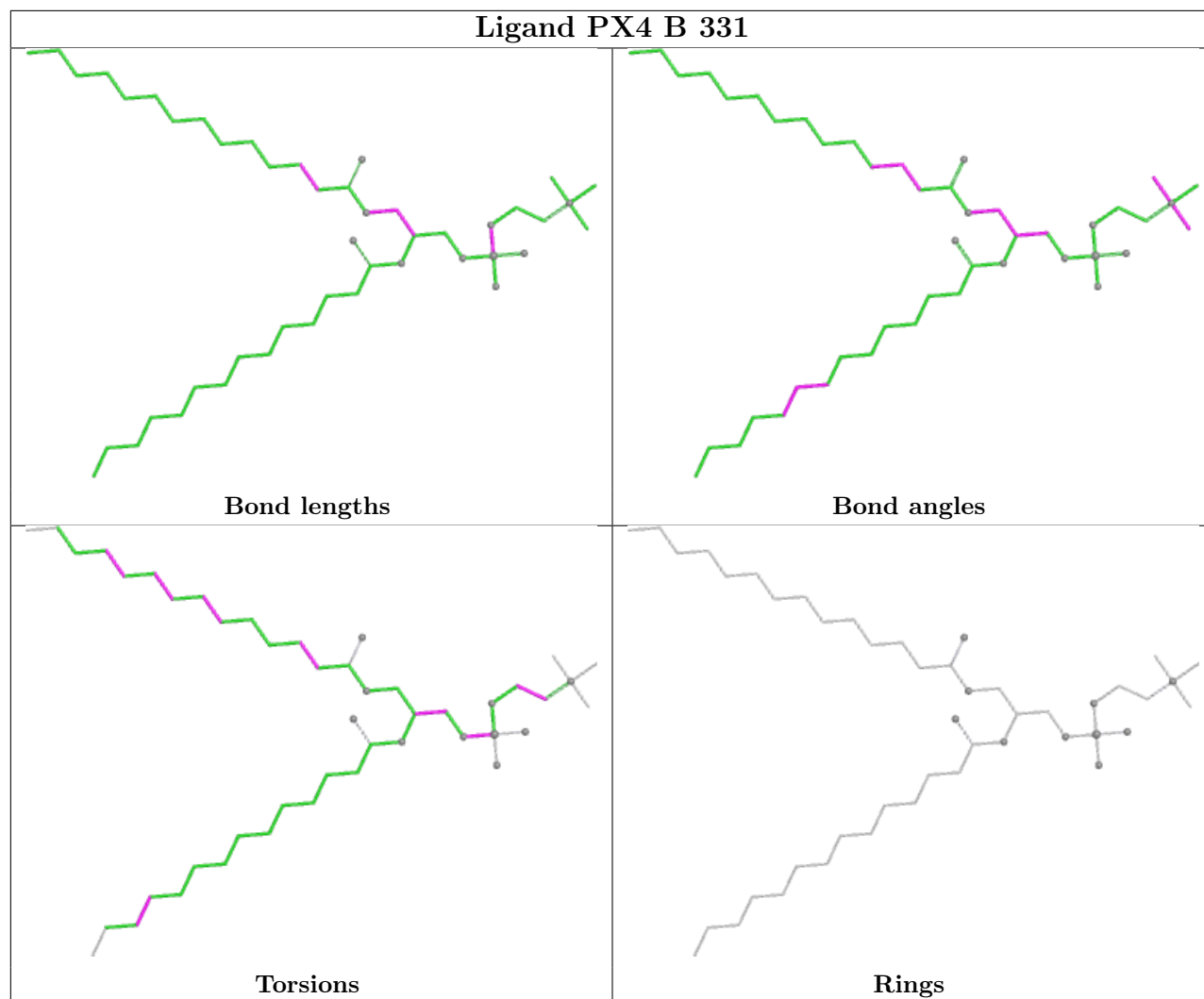
Ligand PX4 A 651



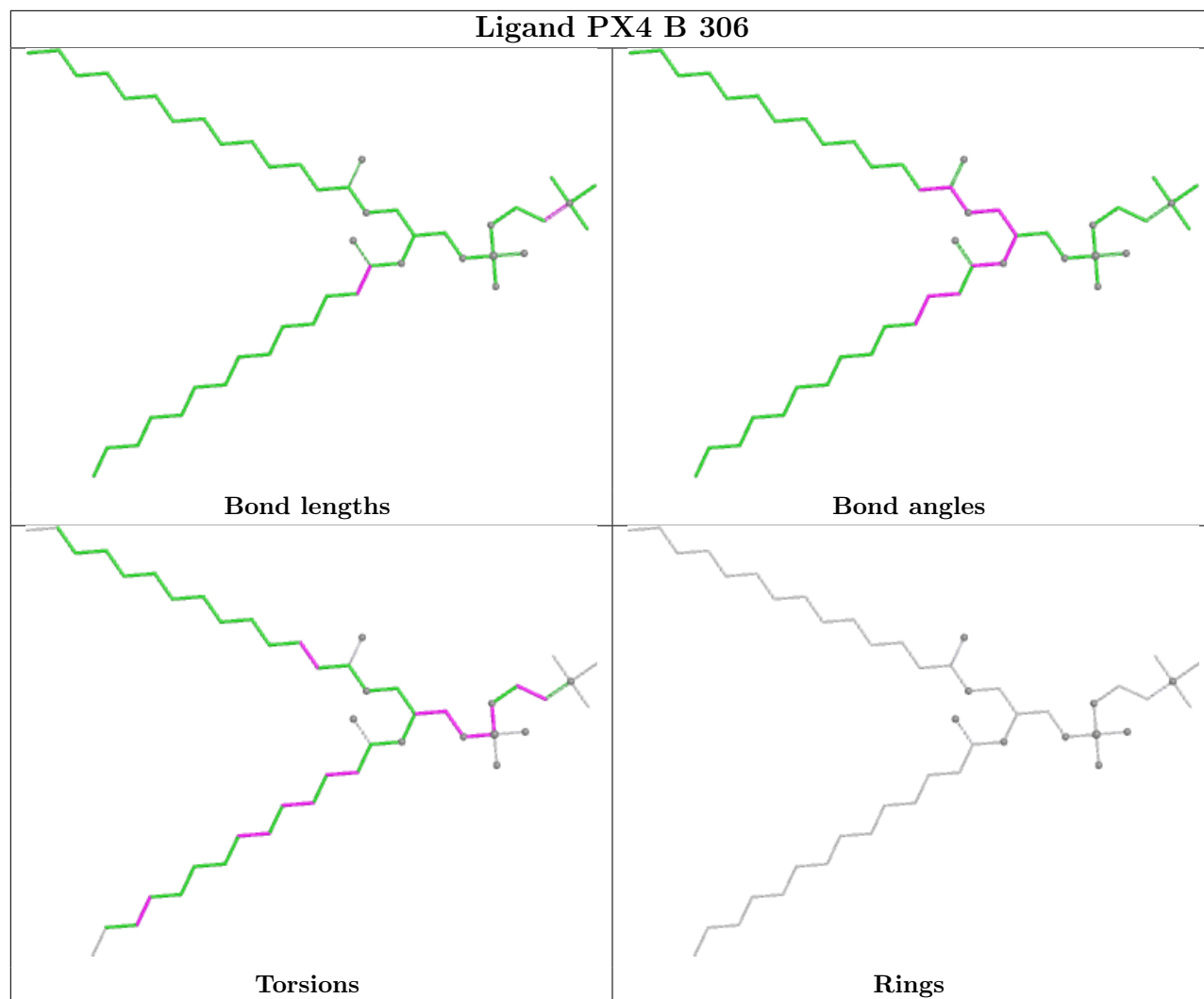




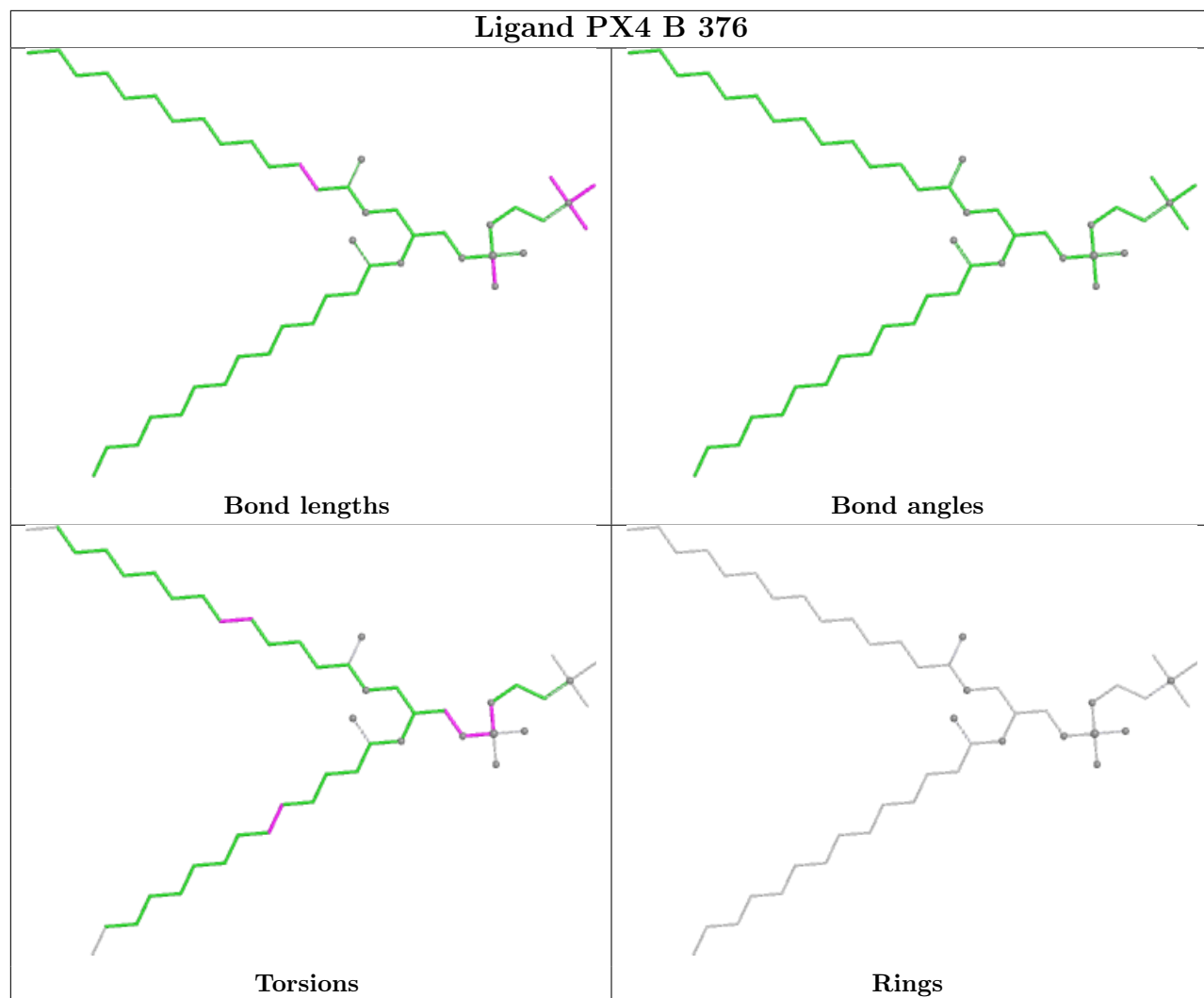
Ligand PX4 B 331



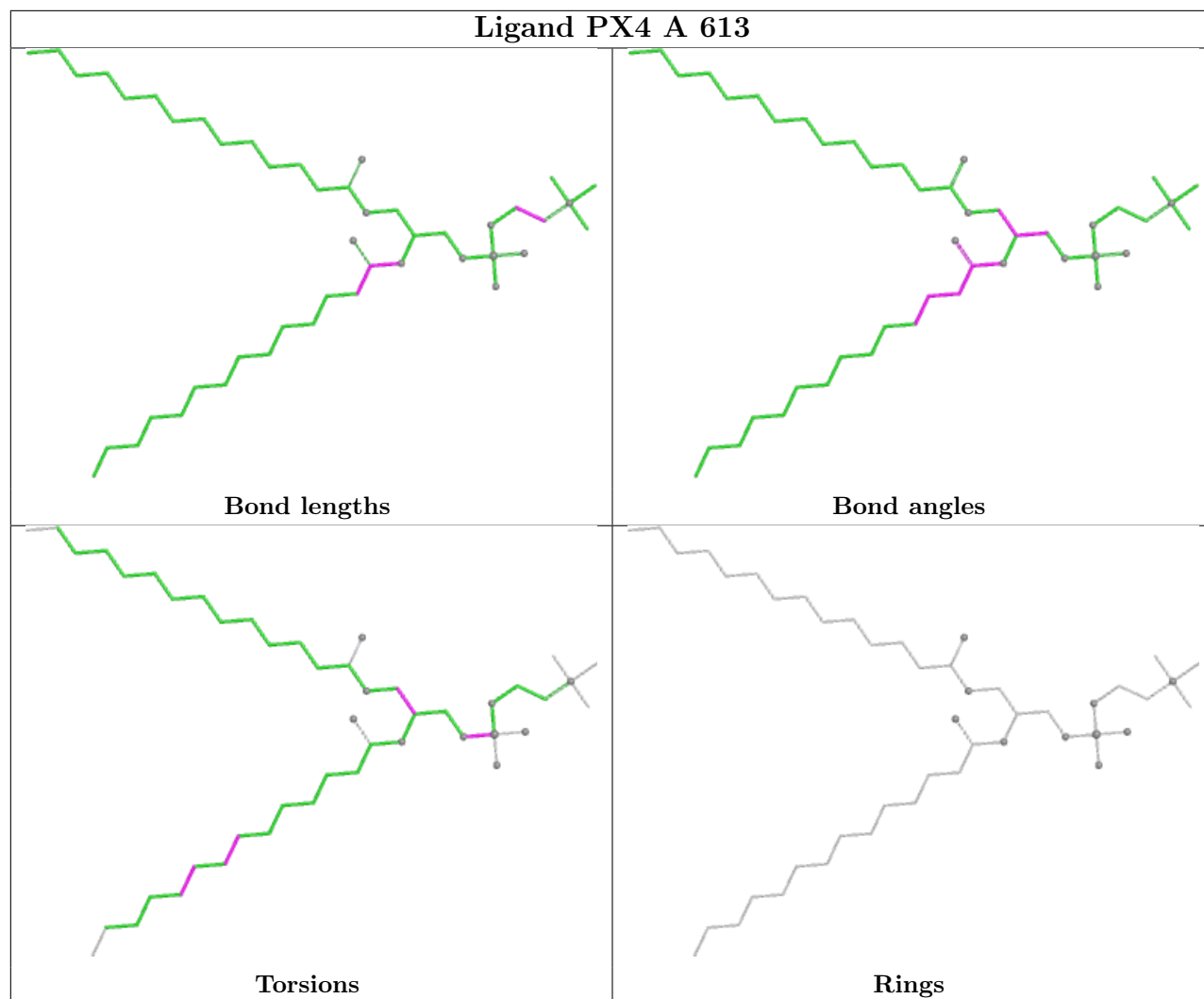
Ligand PX4 B 306



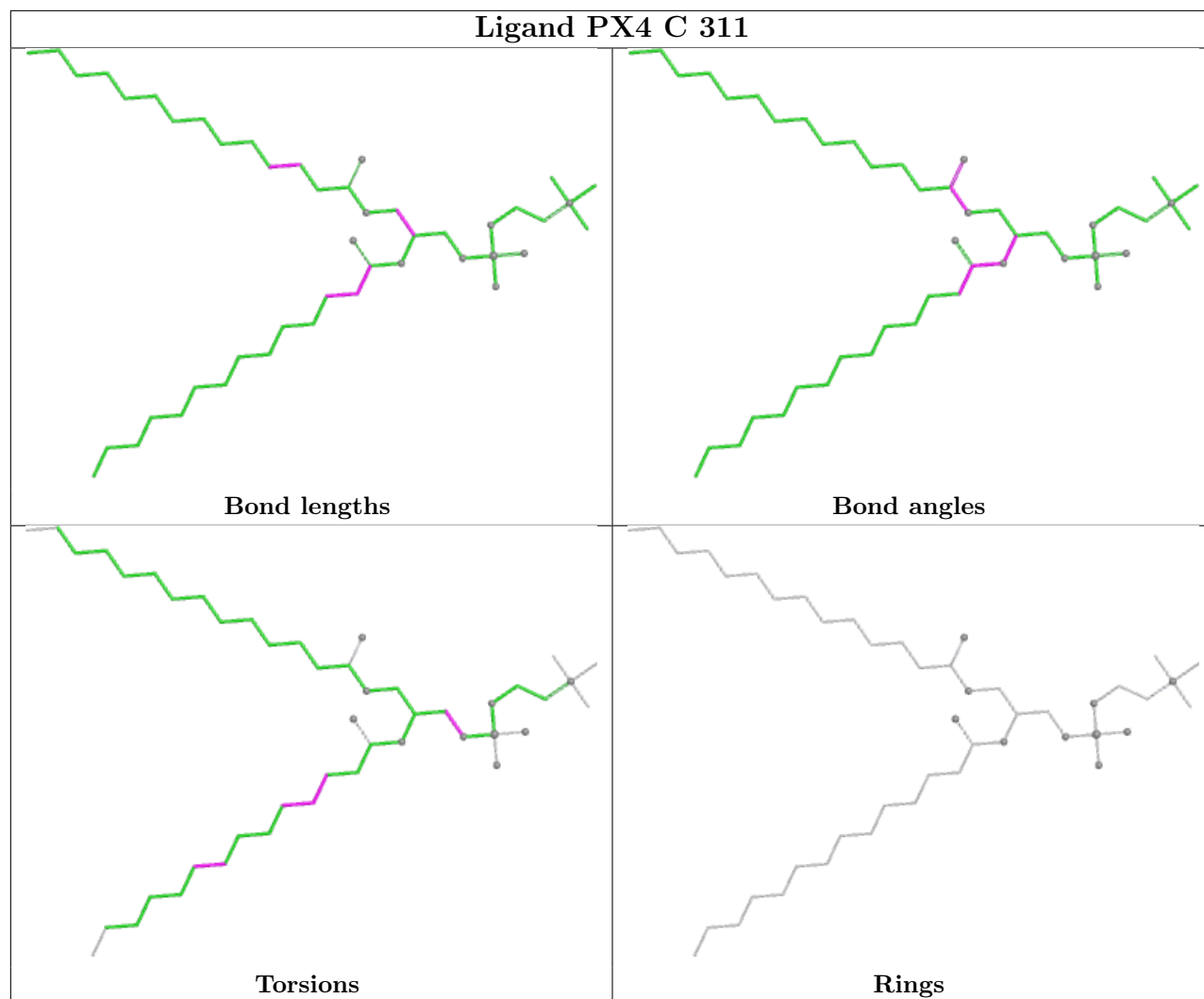
Ligand PX4 B 376

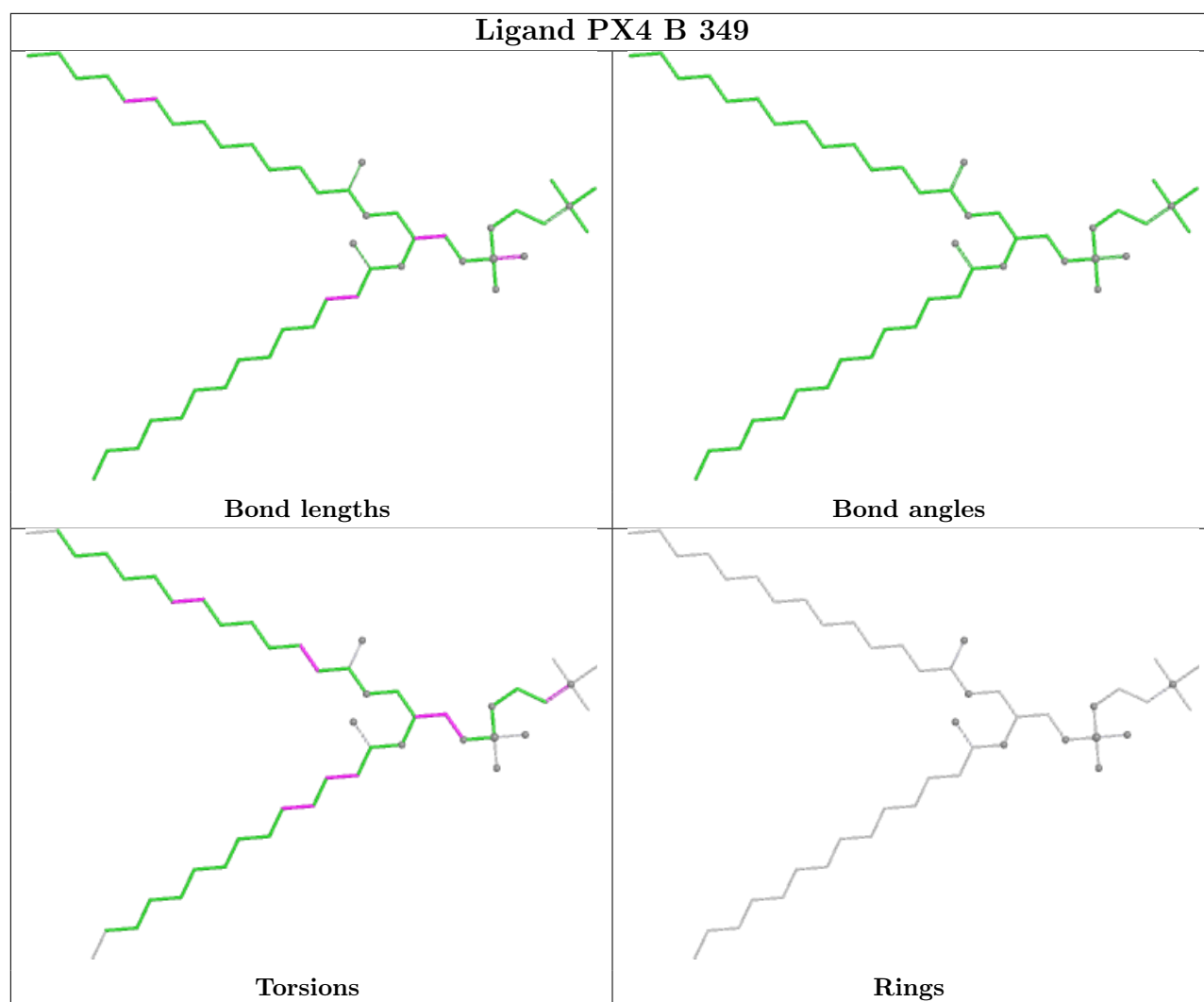


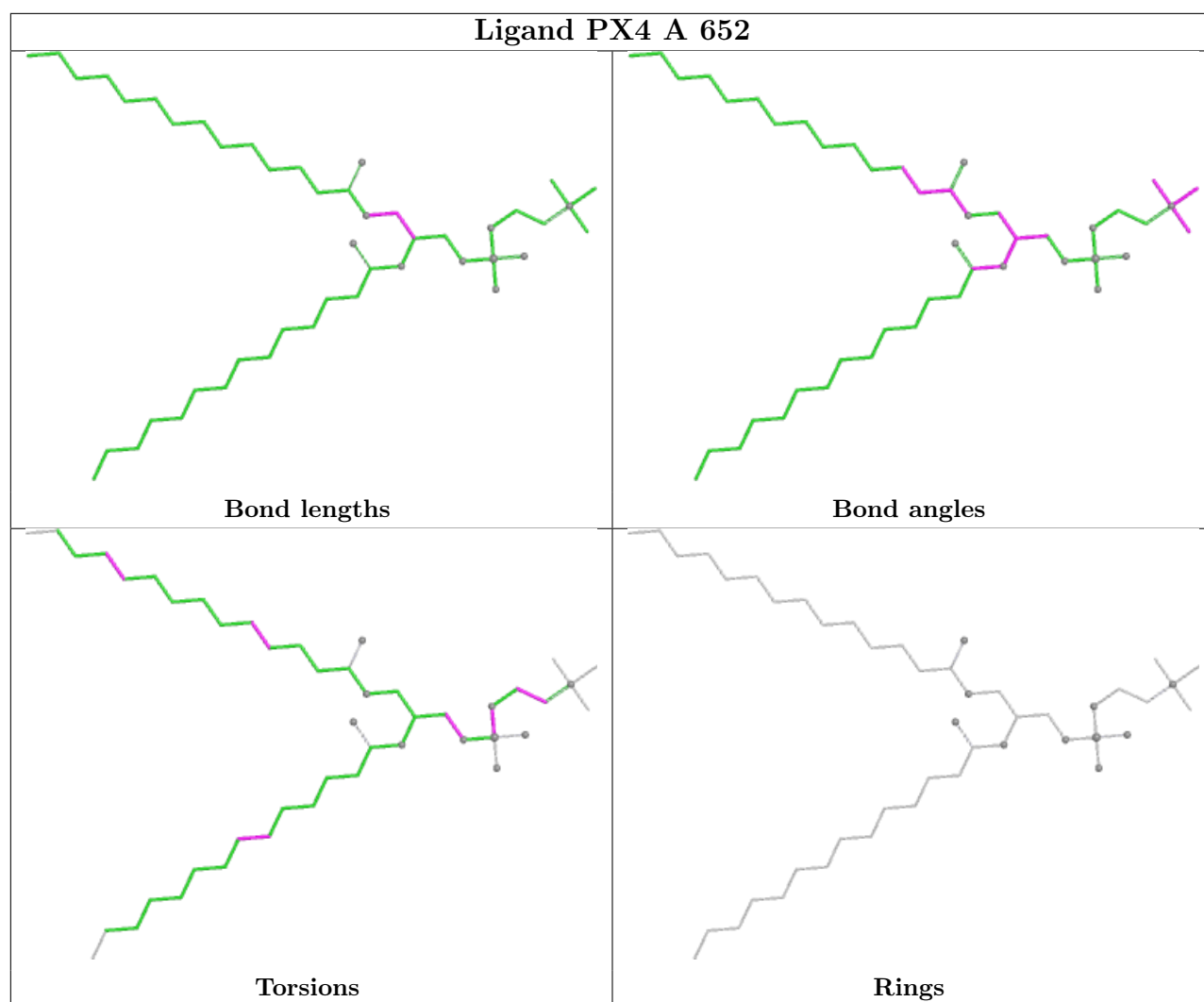
Ligand PX4 A 613



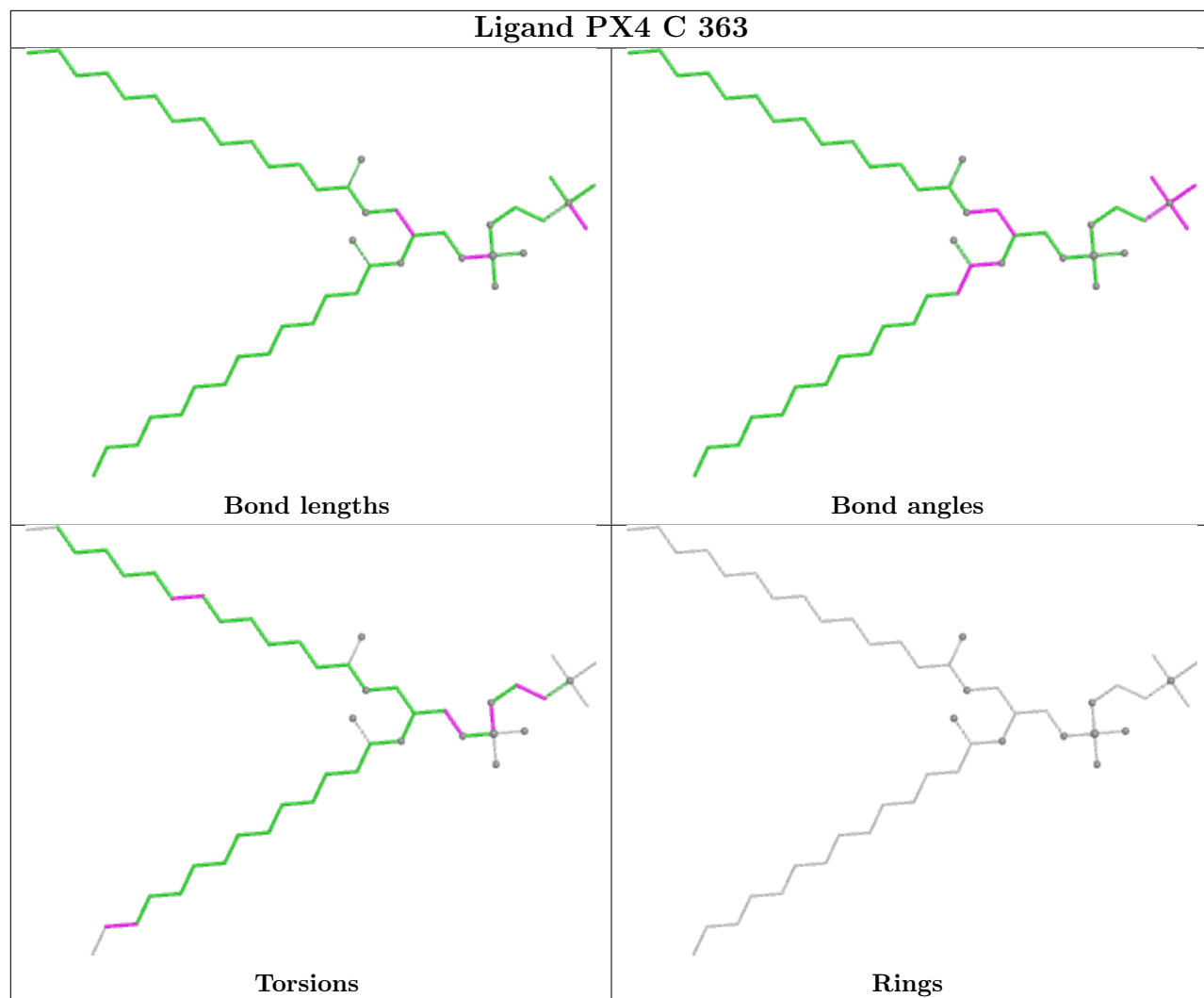
Ligand PX4 C 311



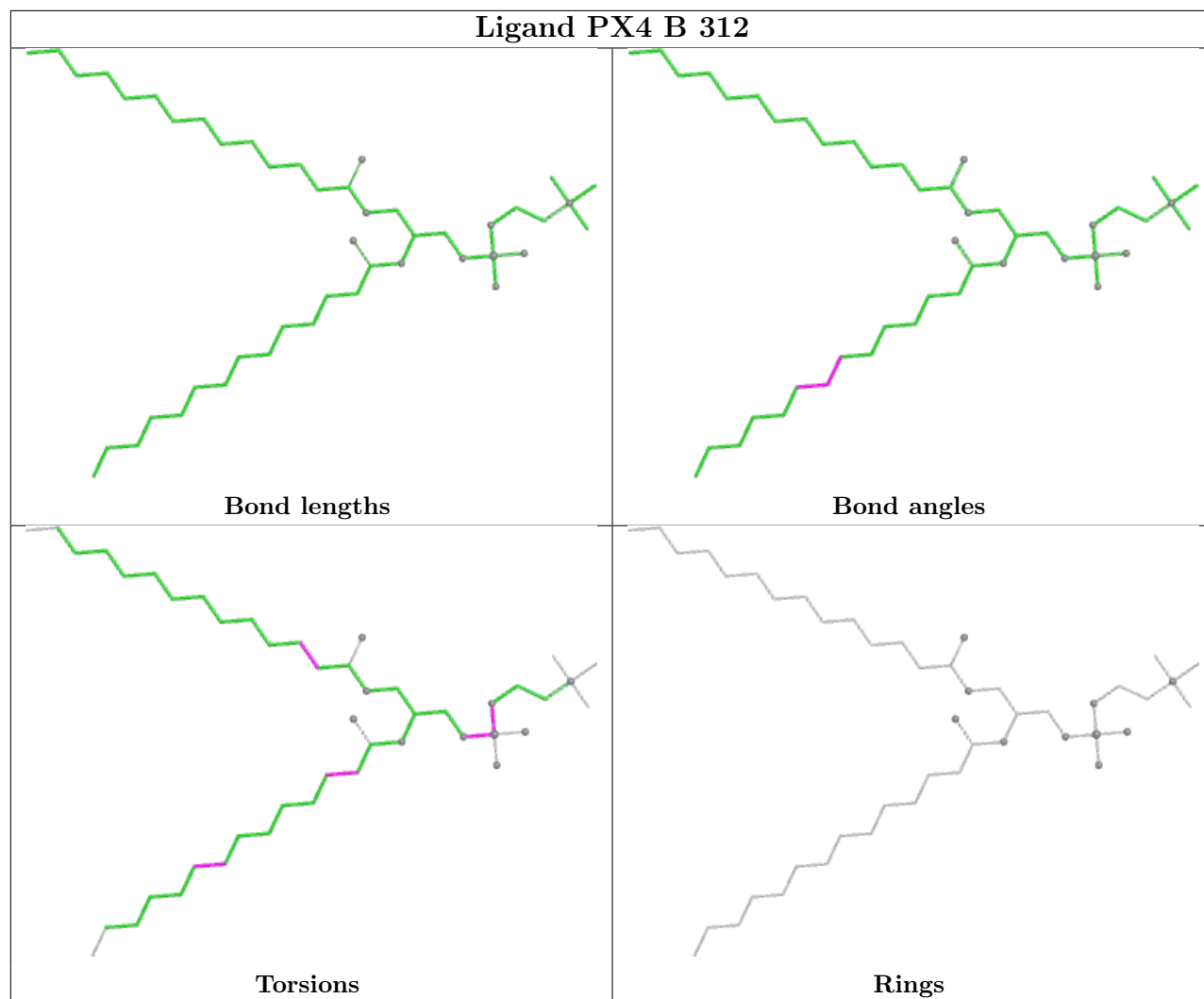




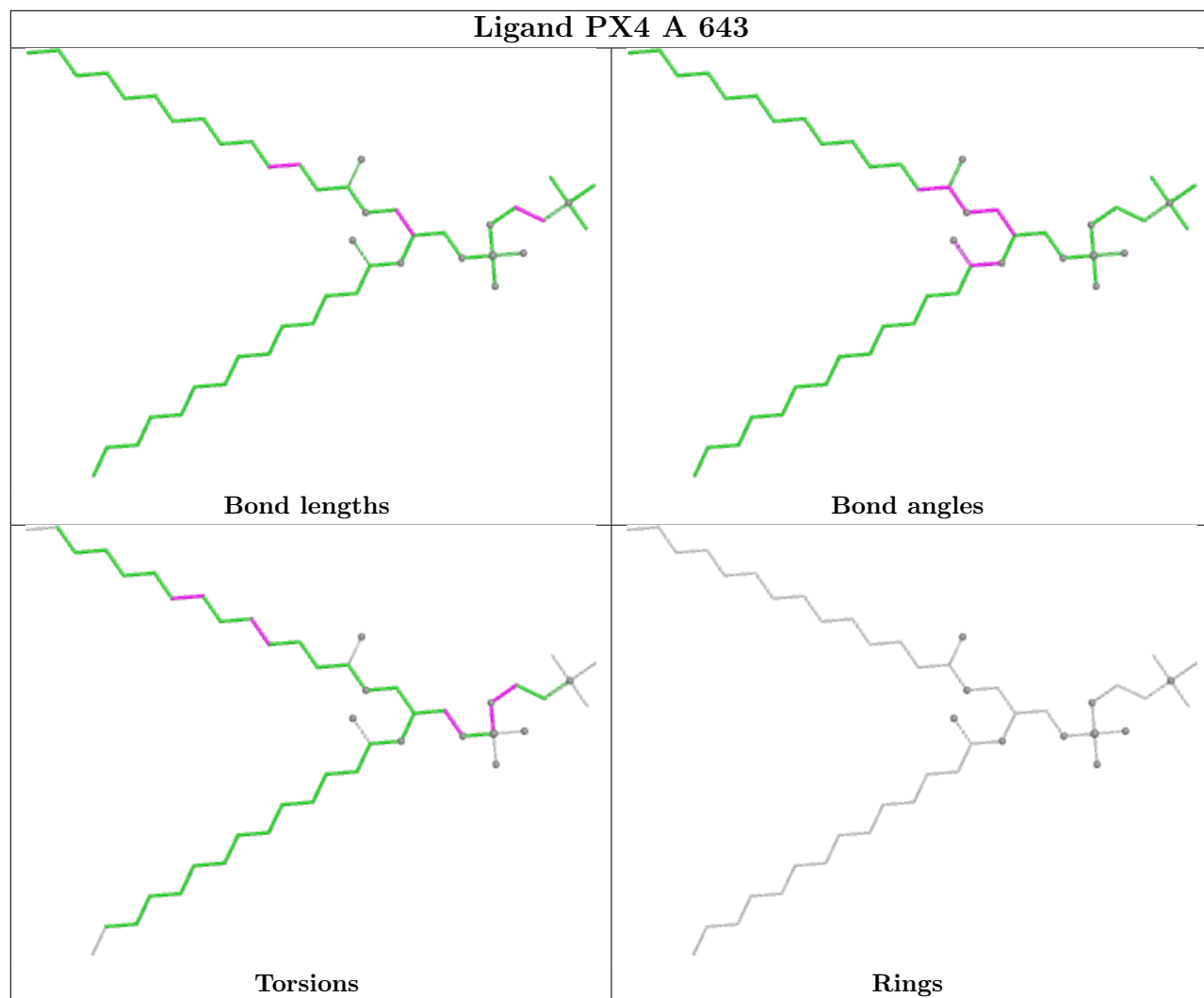
Ligand PX4 C 363



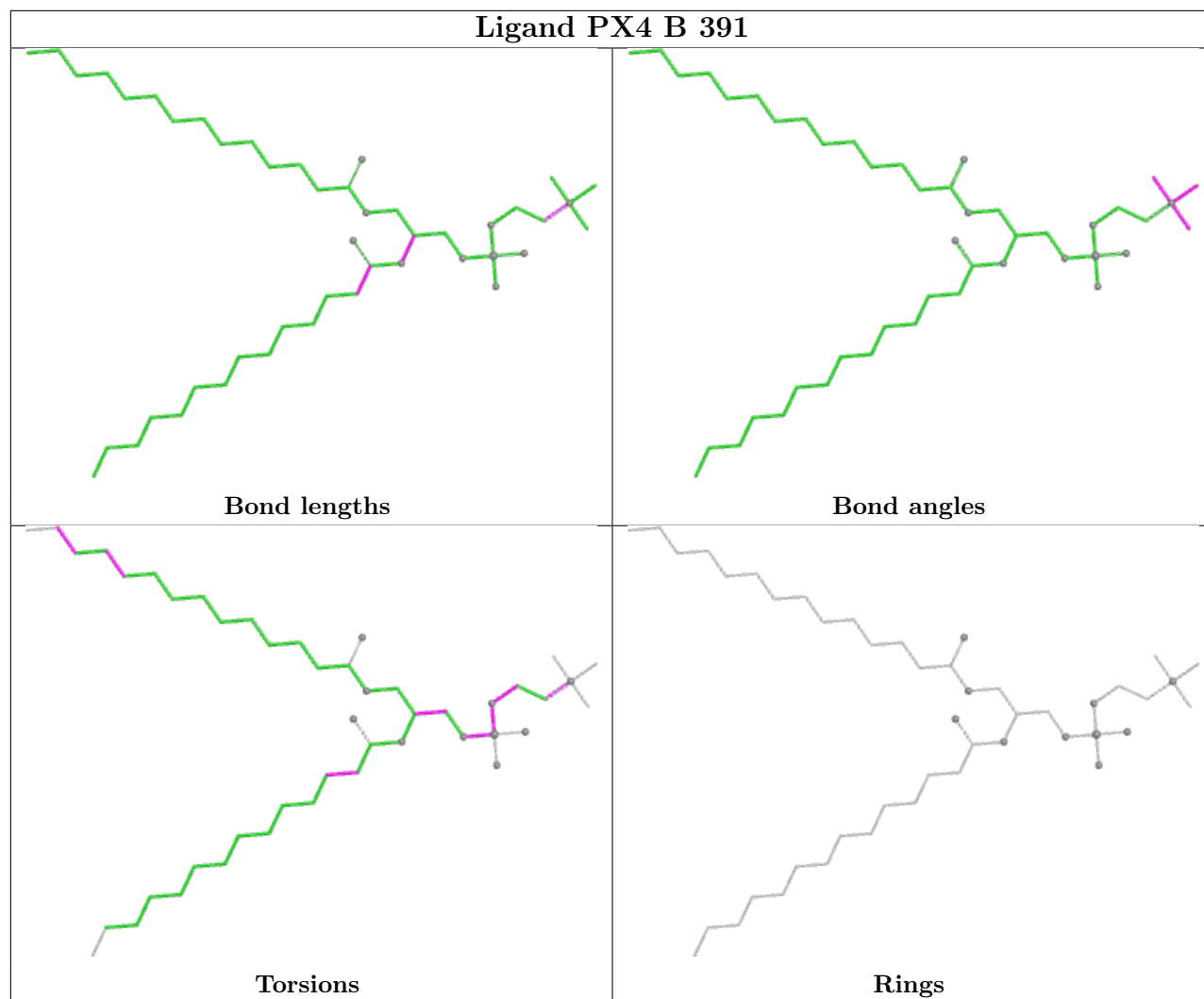
Ligand PX4 B 312

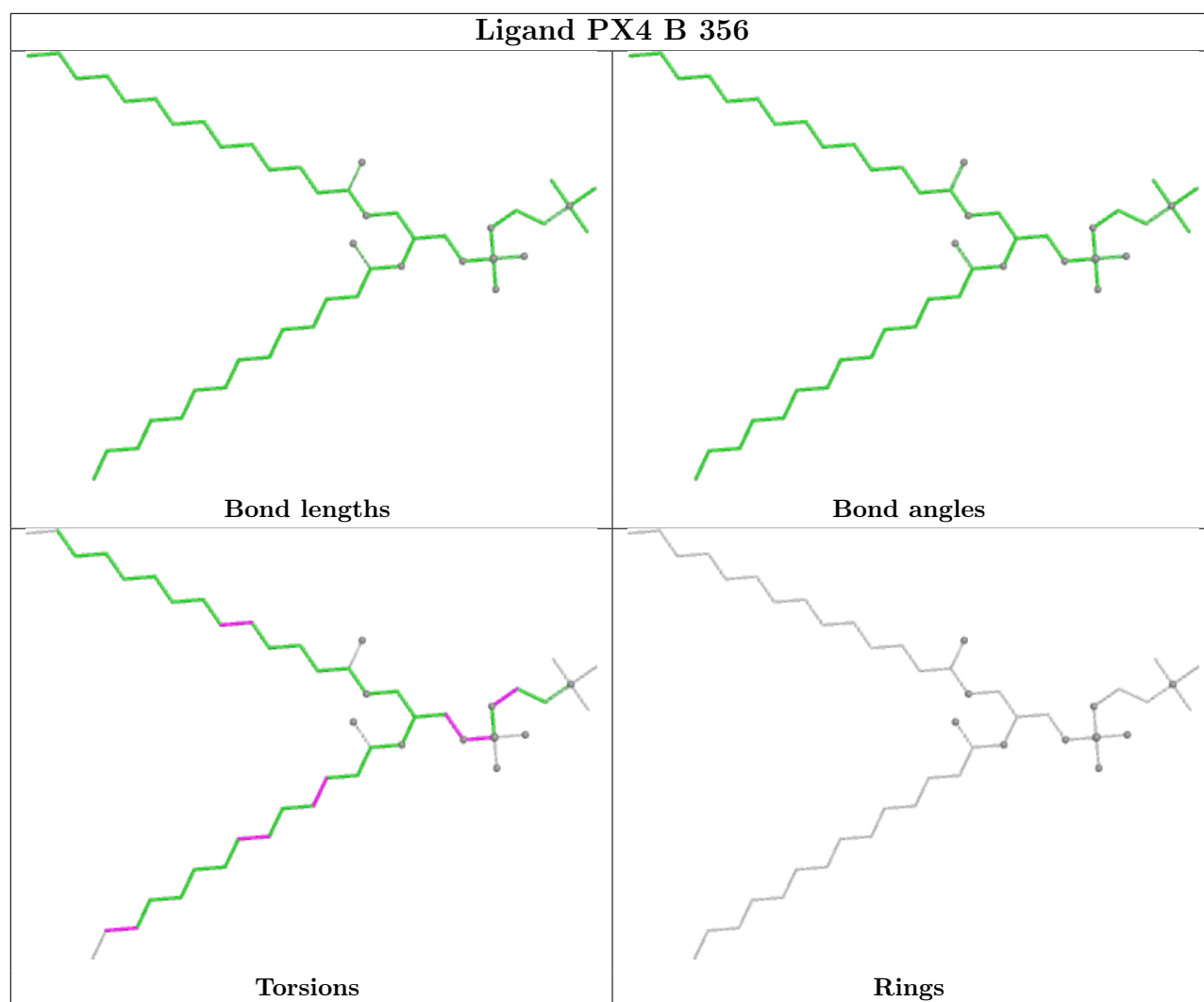


Ligand PX4 A 643

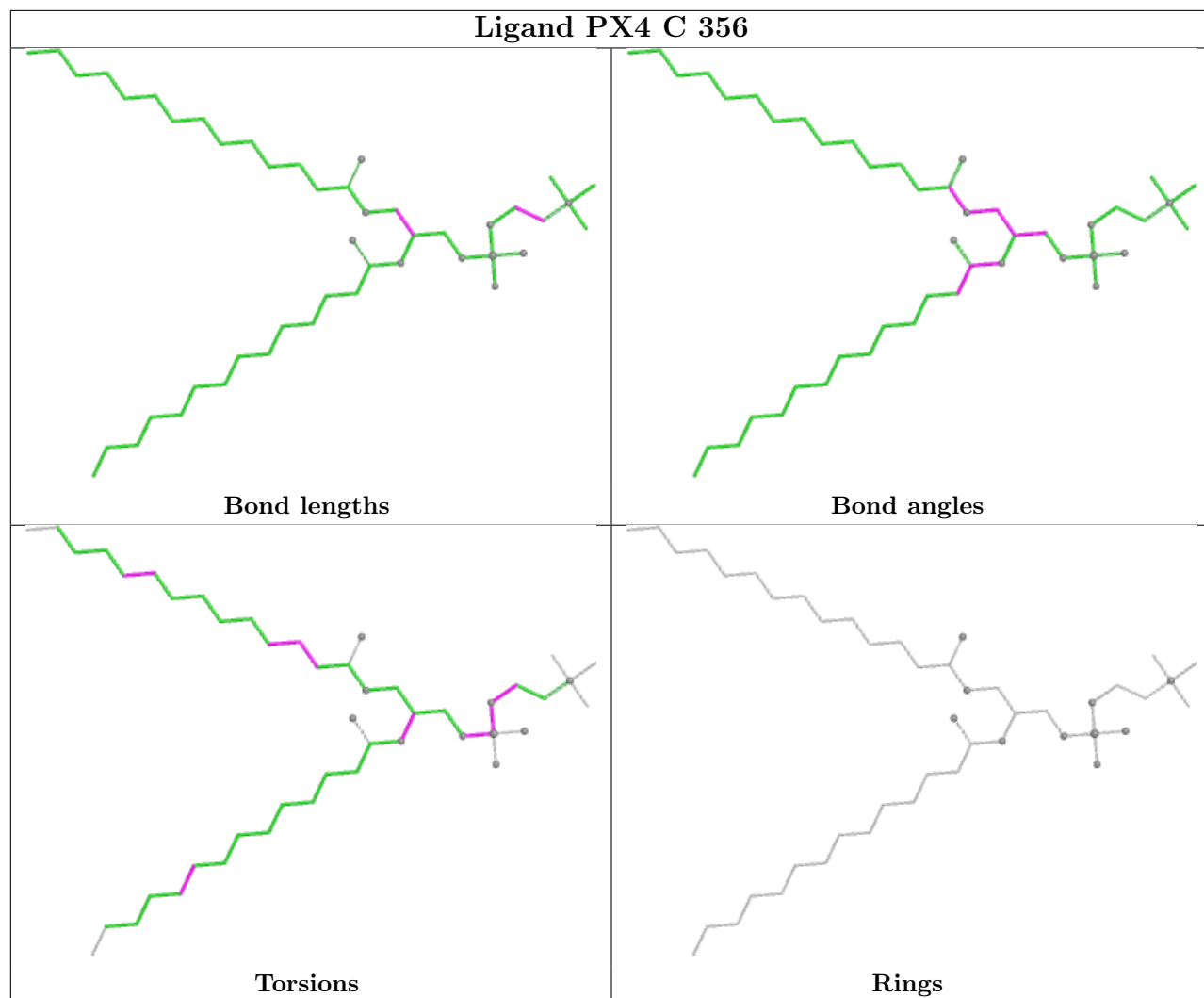


Ligand PX4 B 391

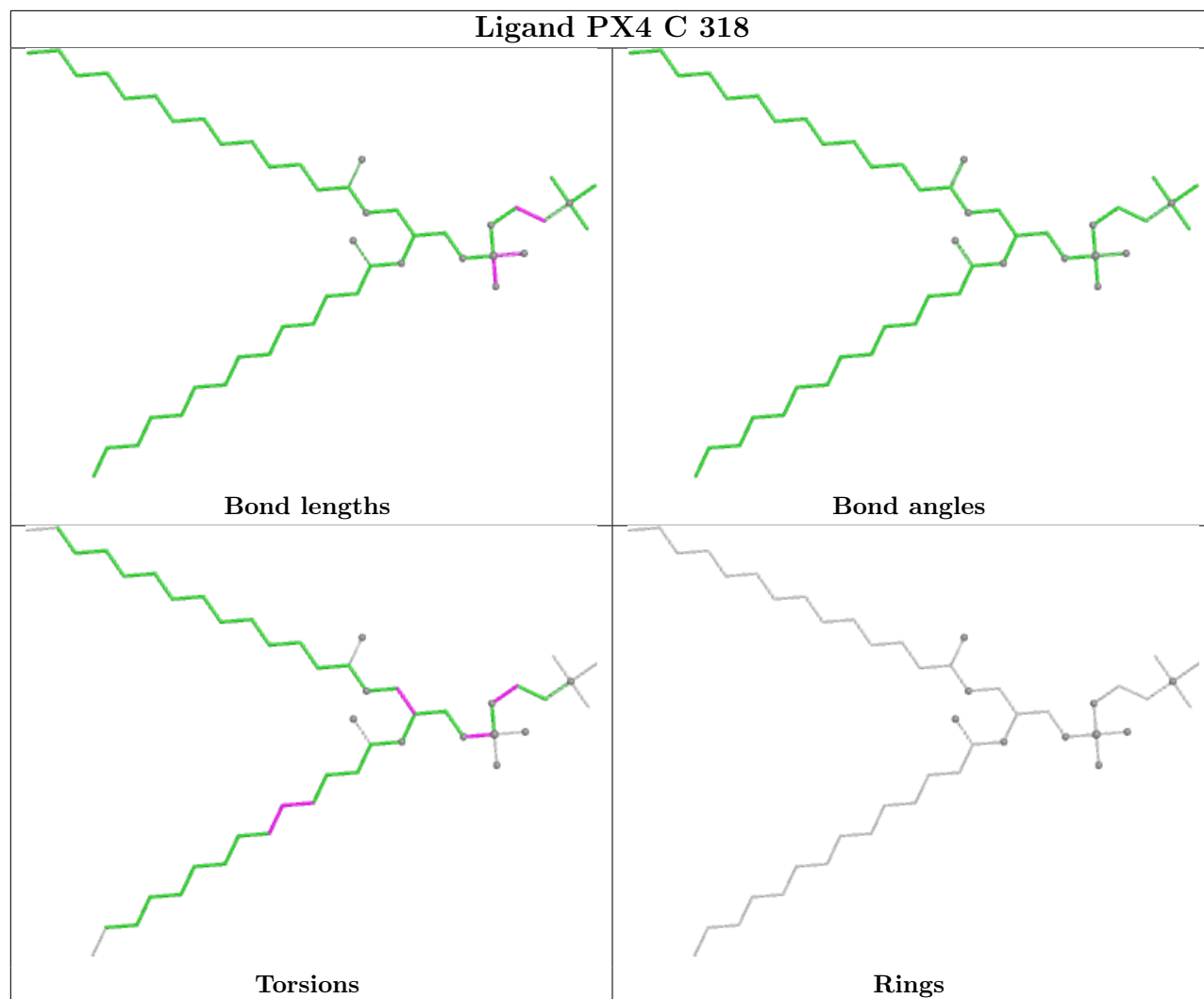


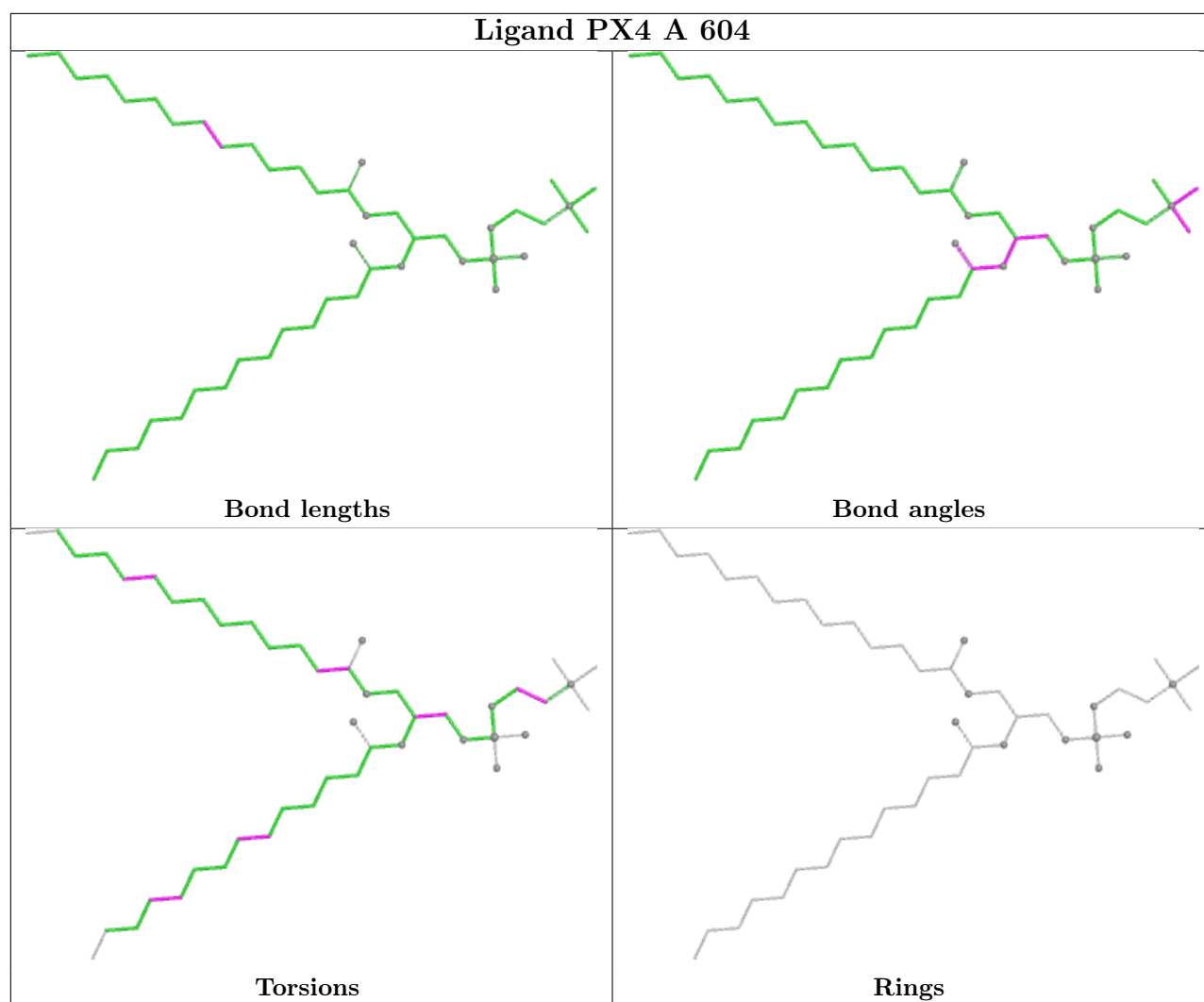


Ligand PX4 C 356

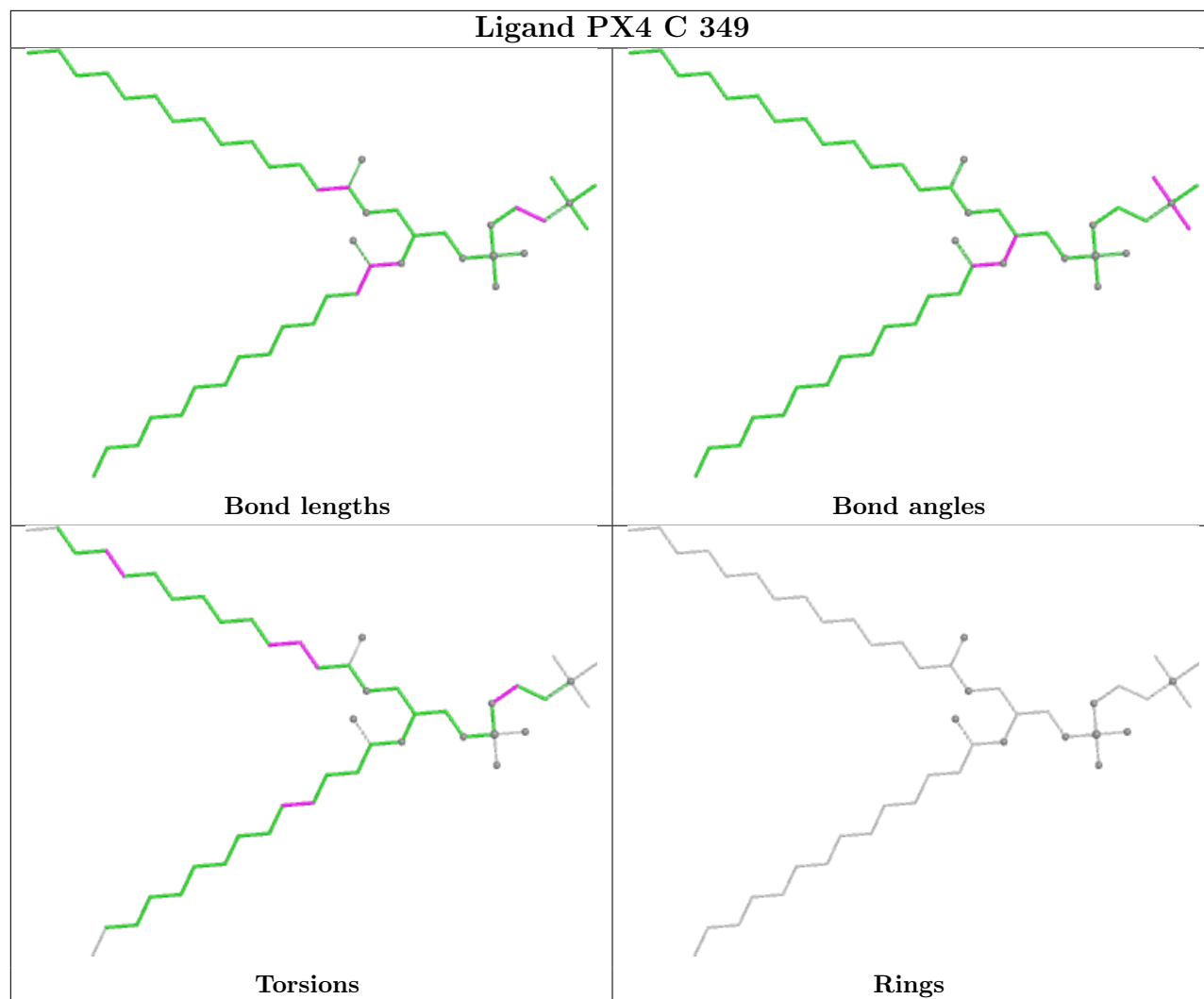


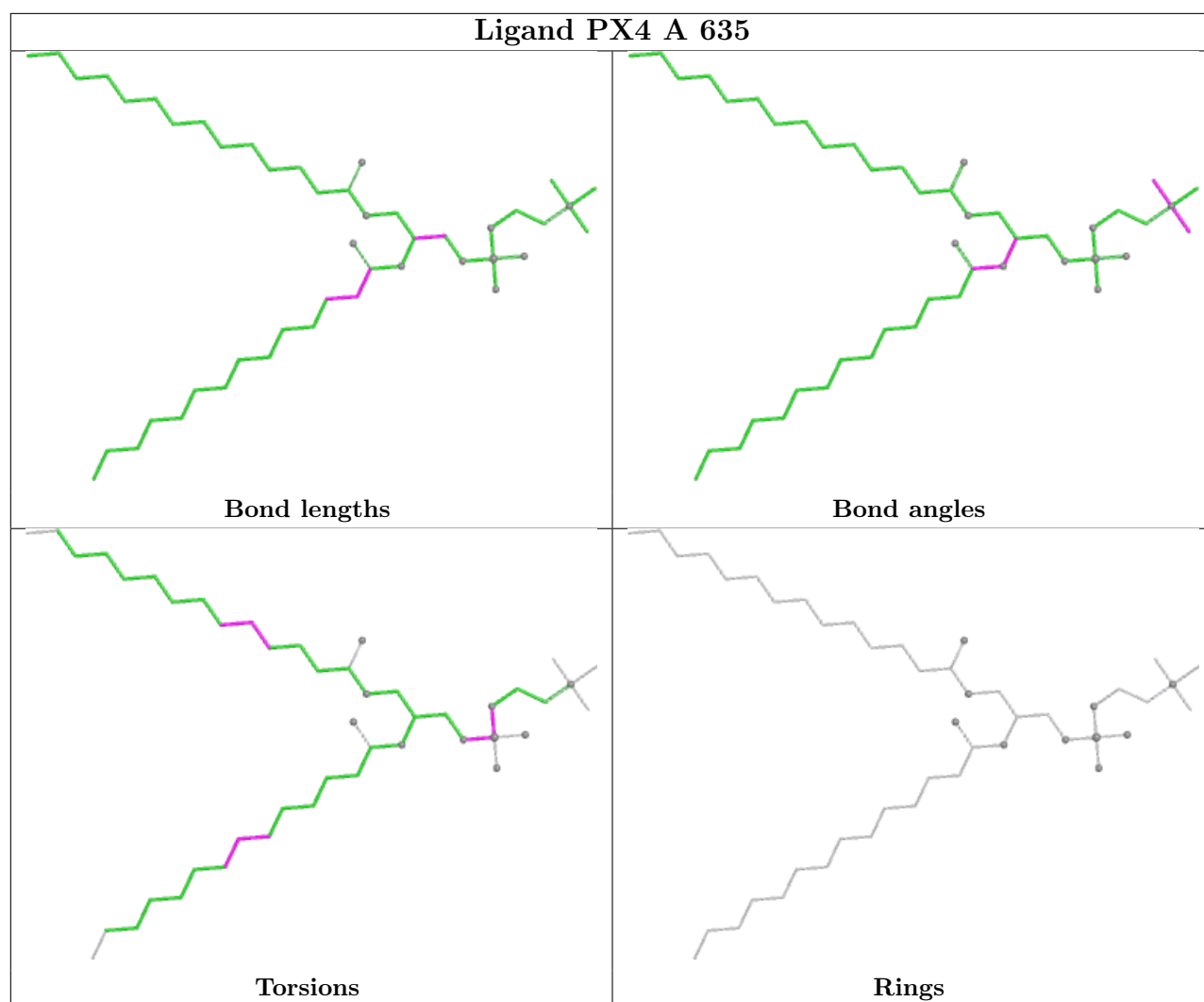
Ligand PX4 C 318

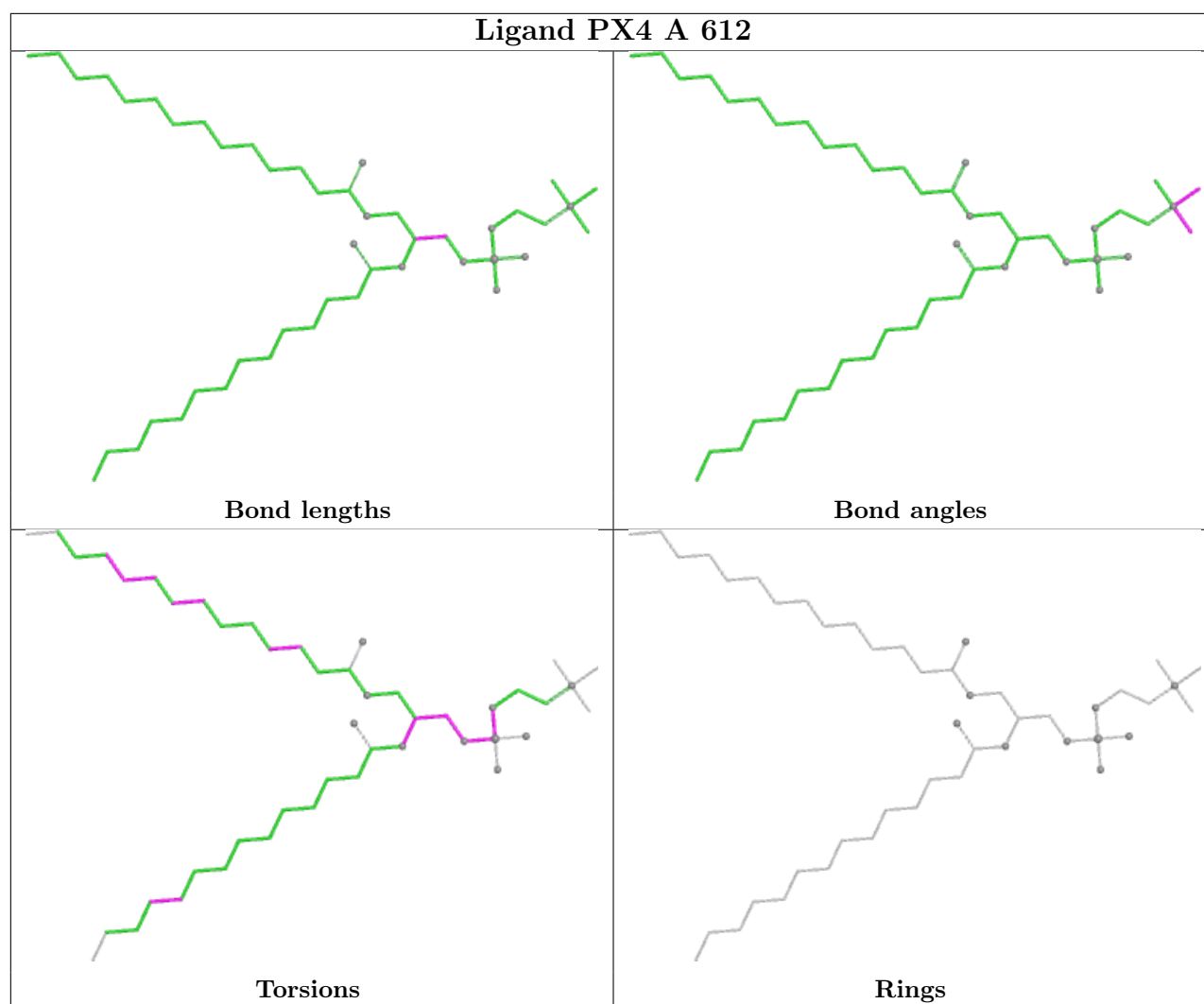




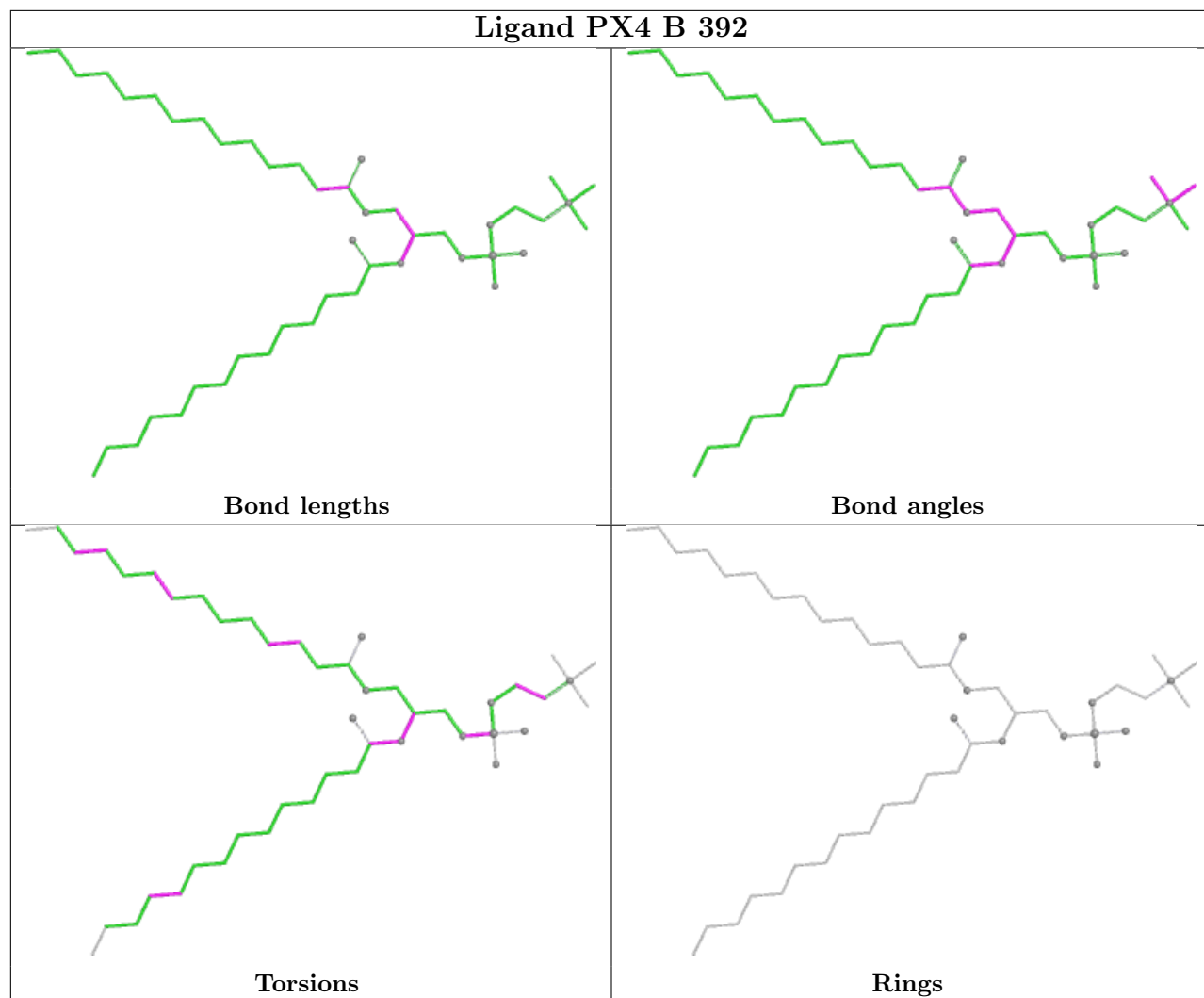
Ligand PX4 C 349



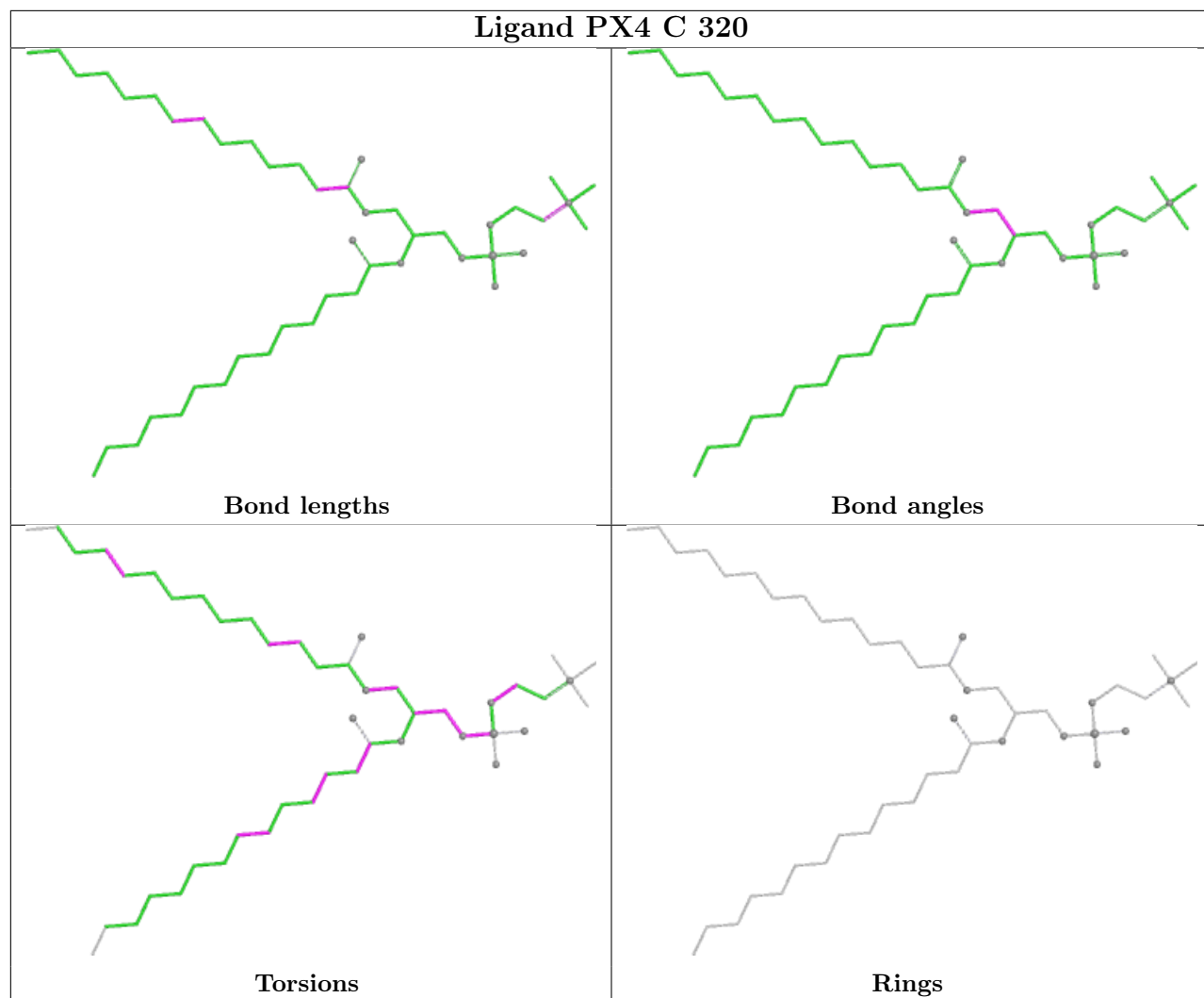




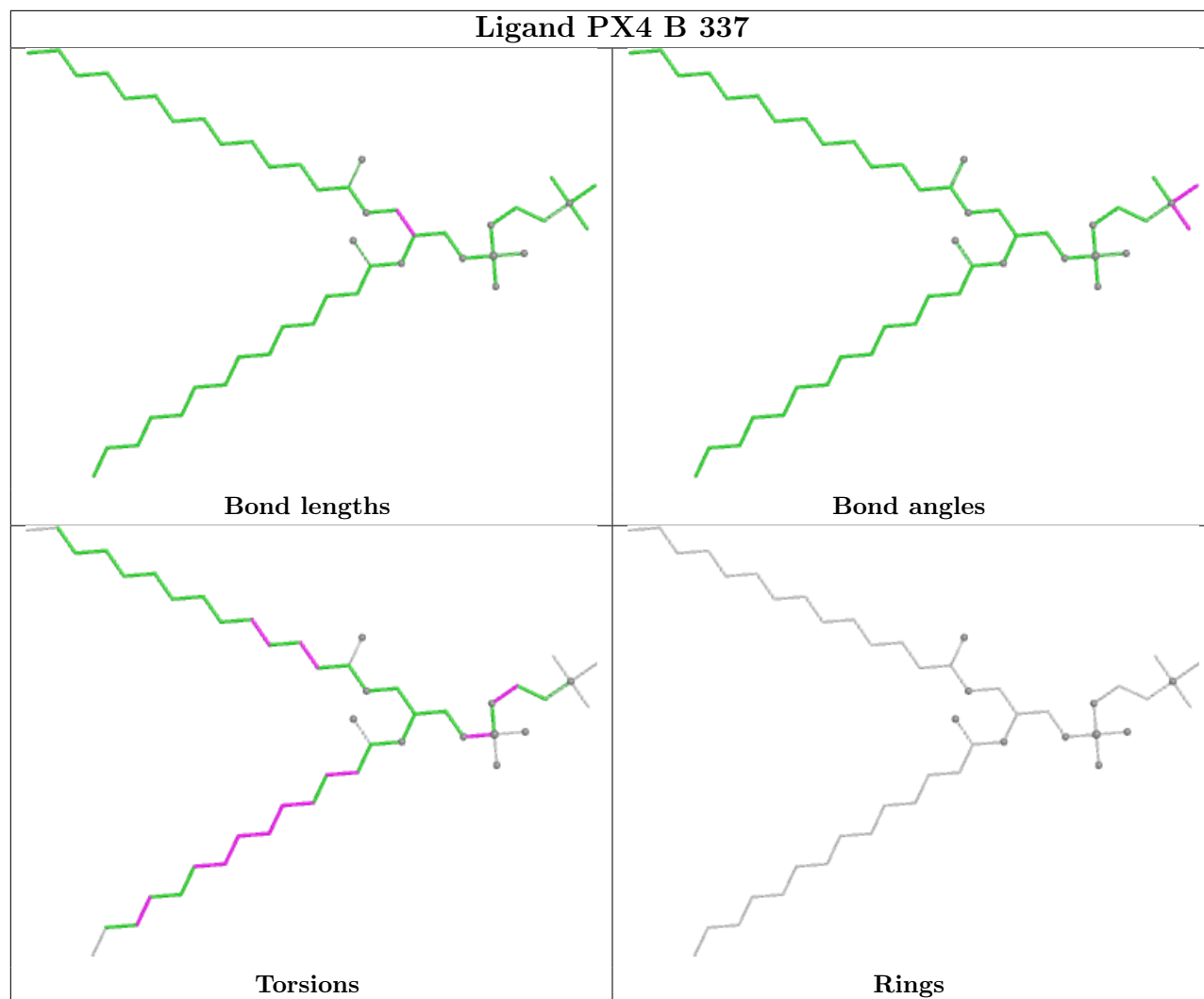
Ligand PX4 B 392



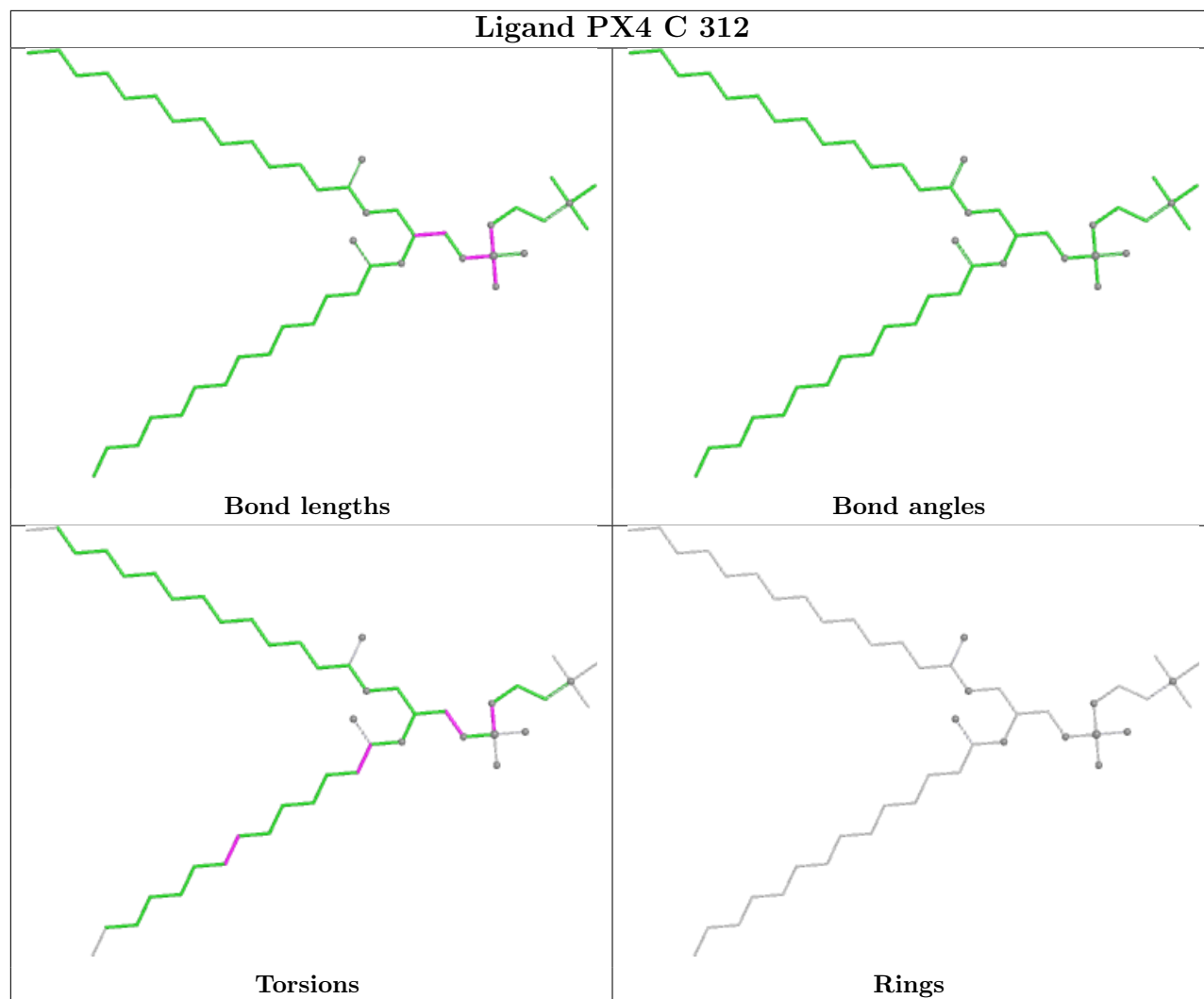
Ligand PX4 C 320

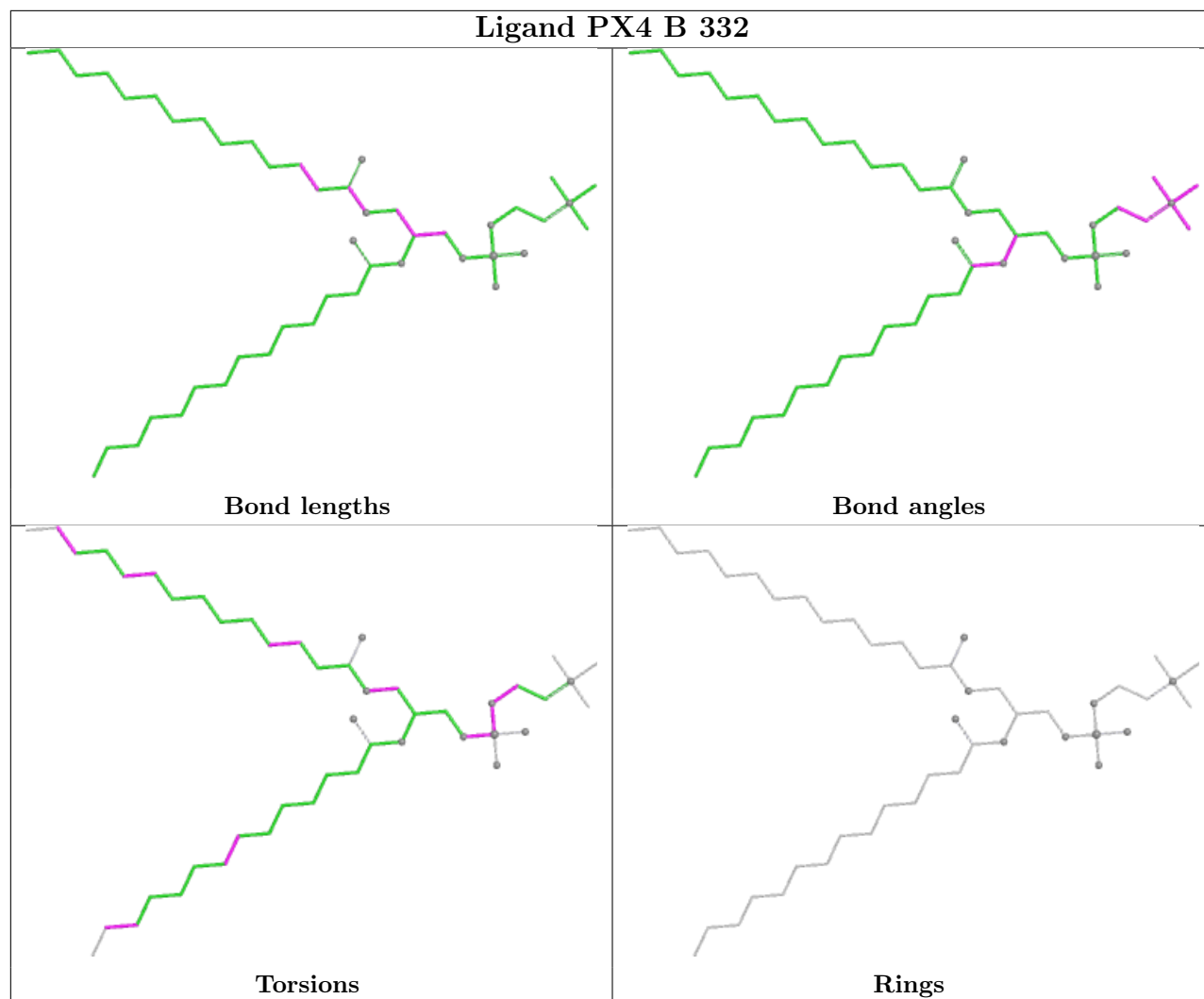


Ligand PX4 B 337

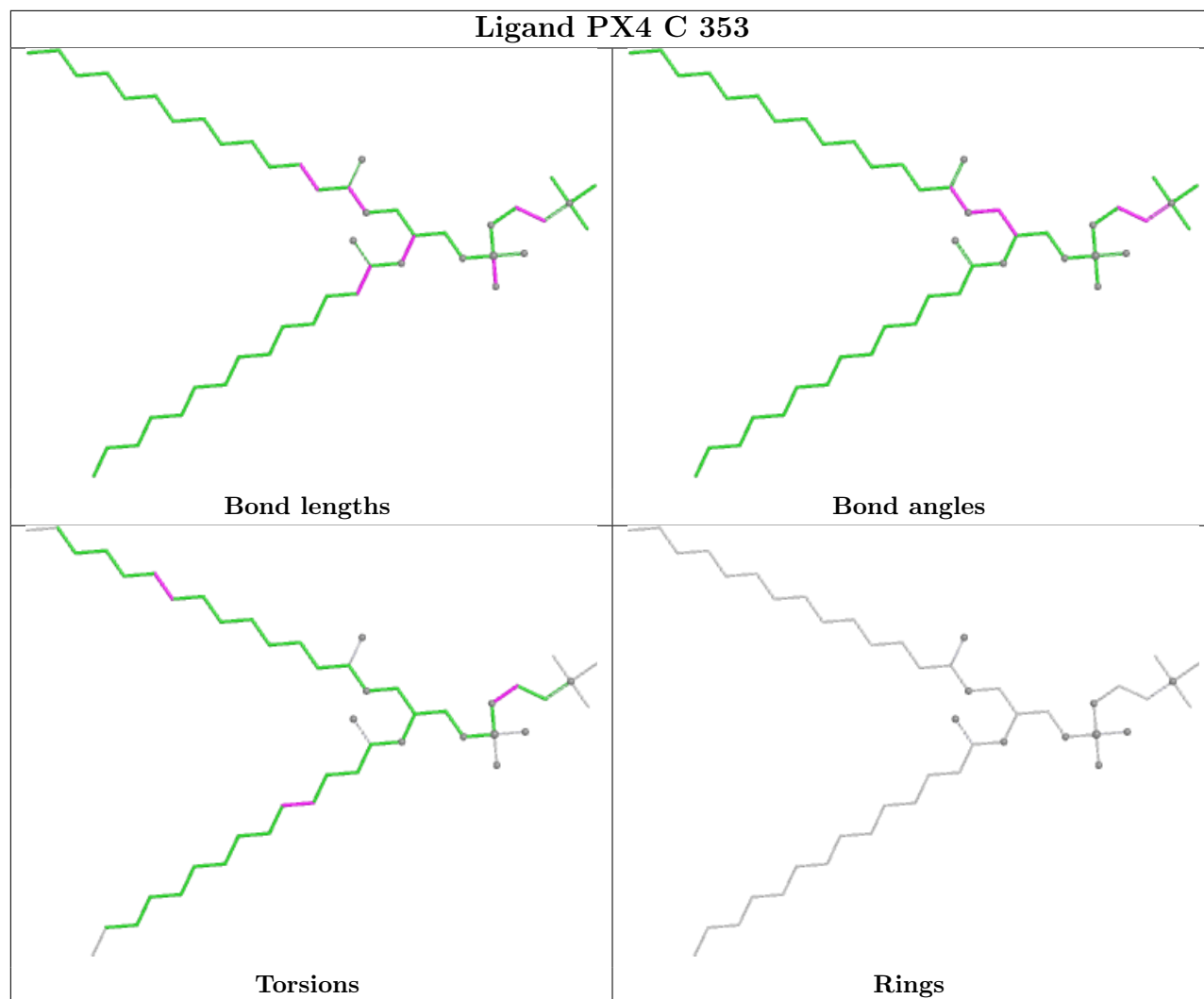


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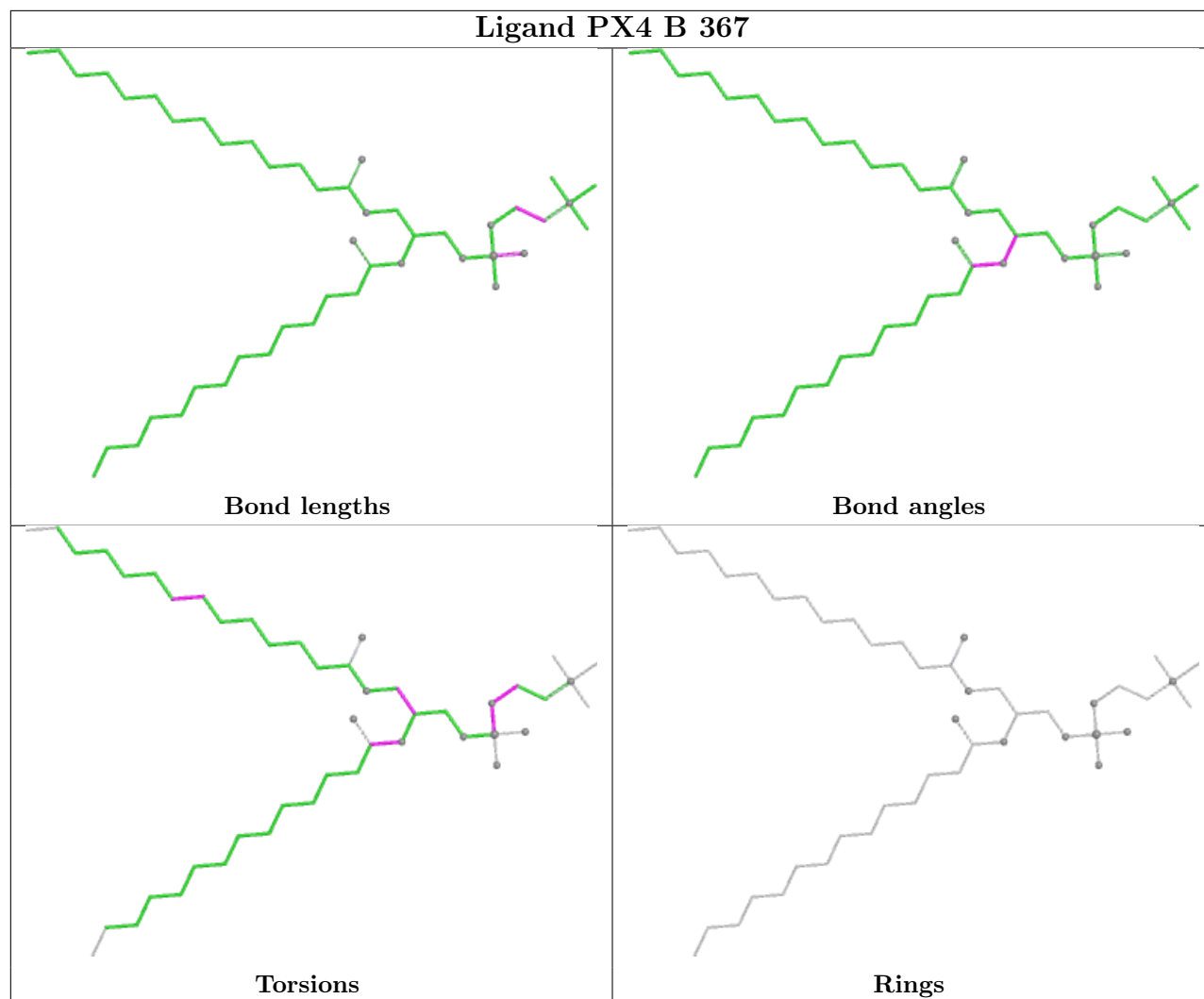


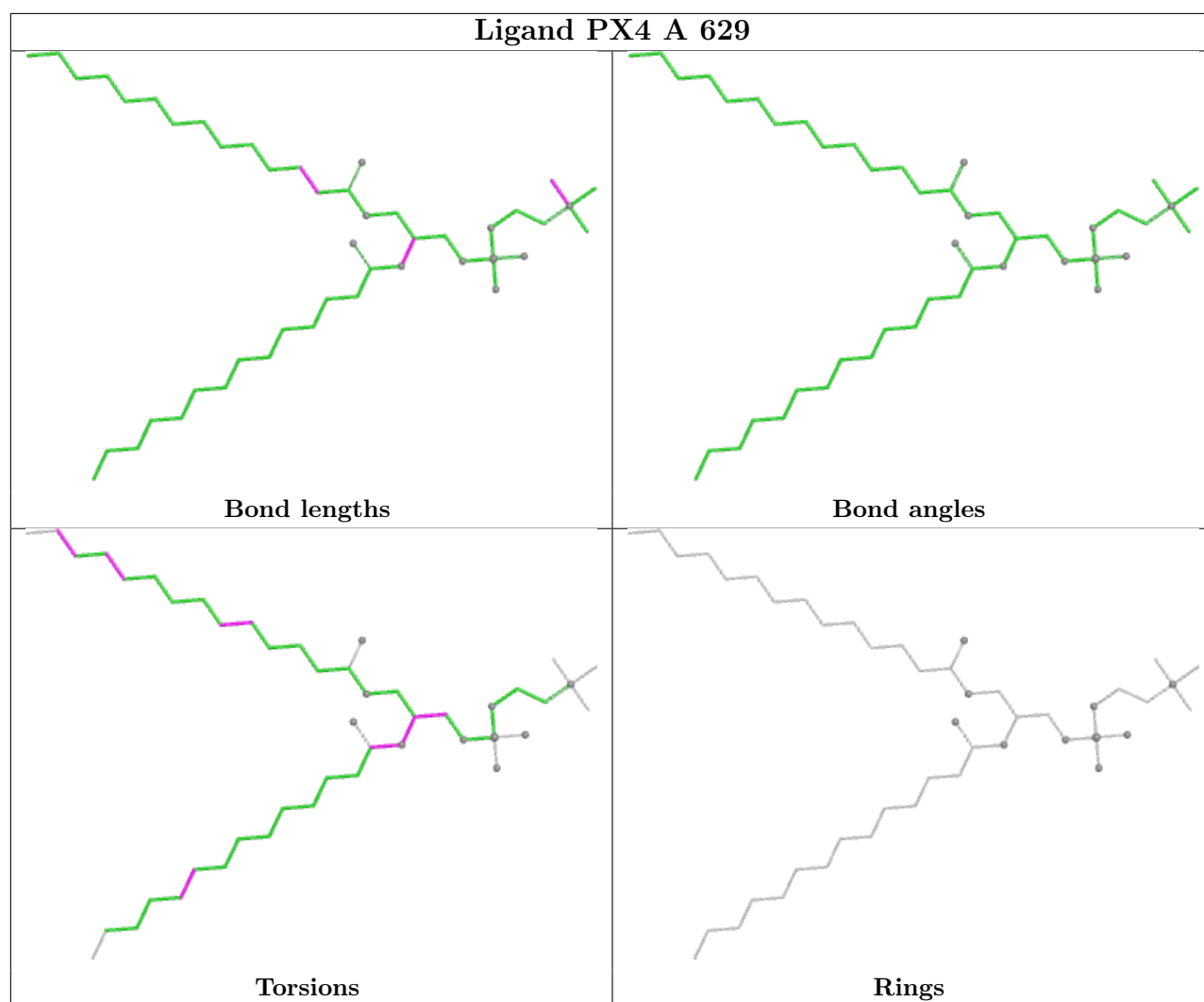


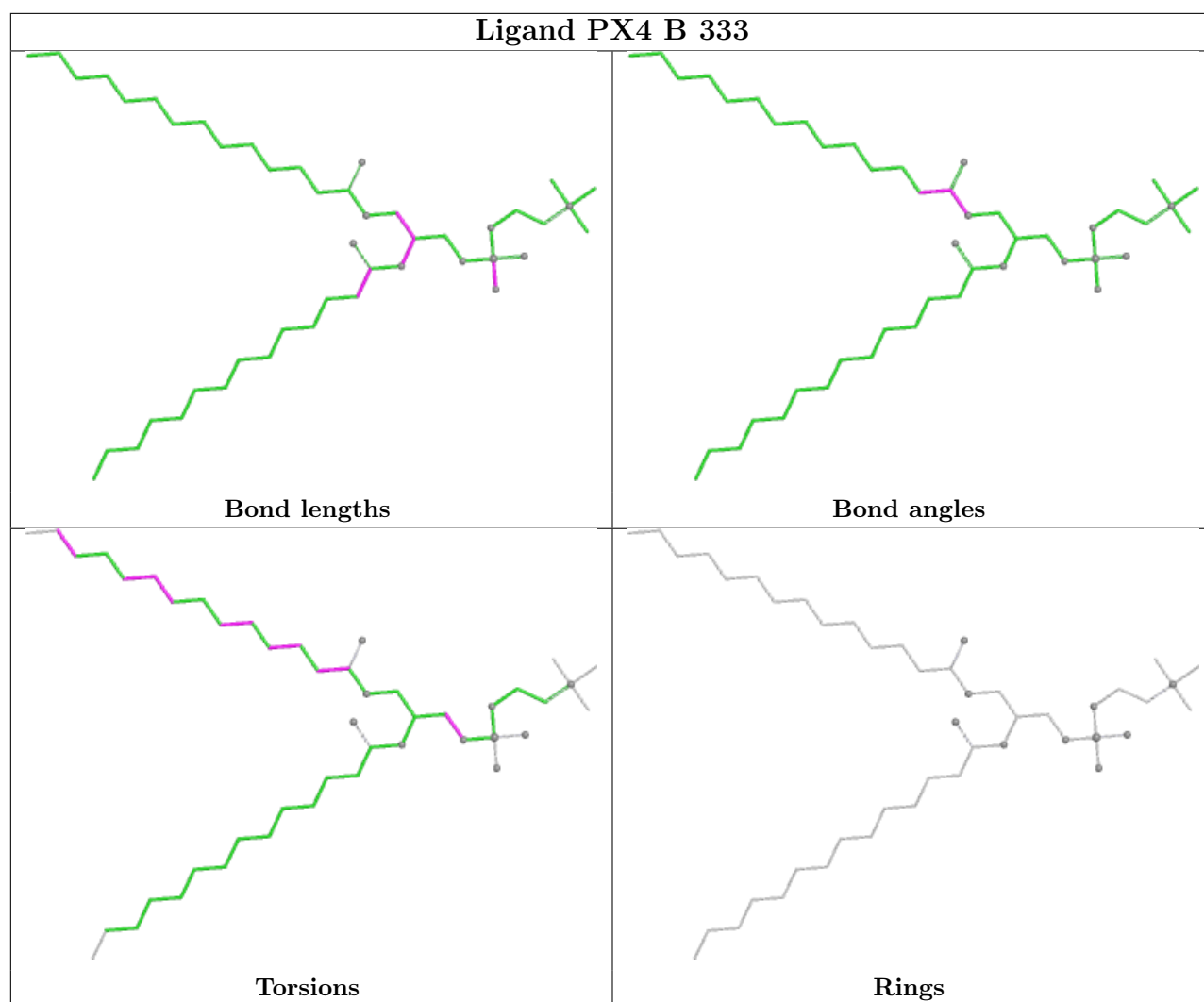
Ligand PX4 C 353

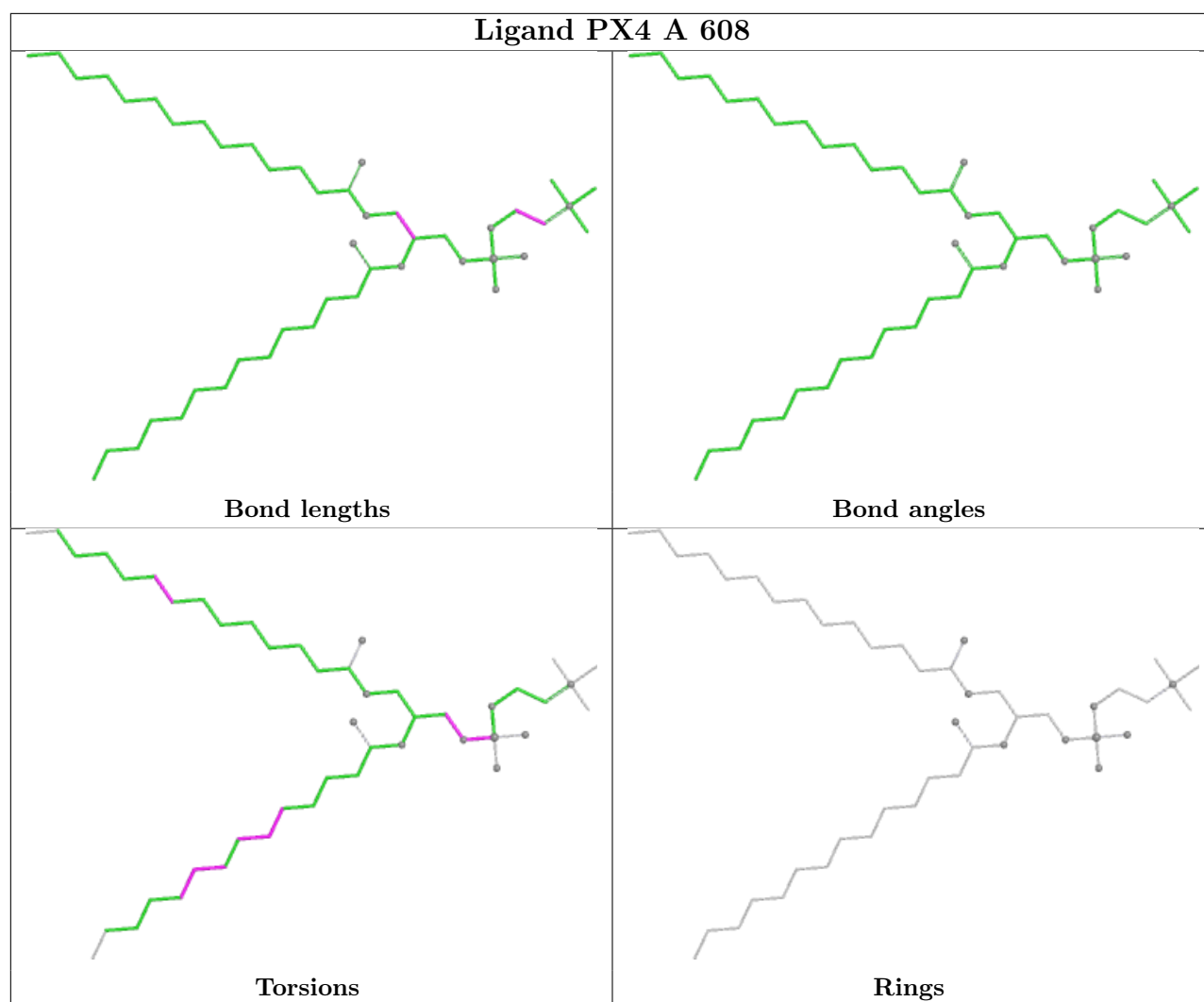


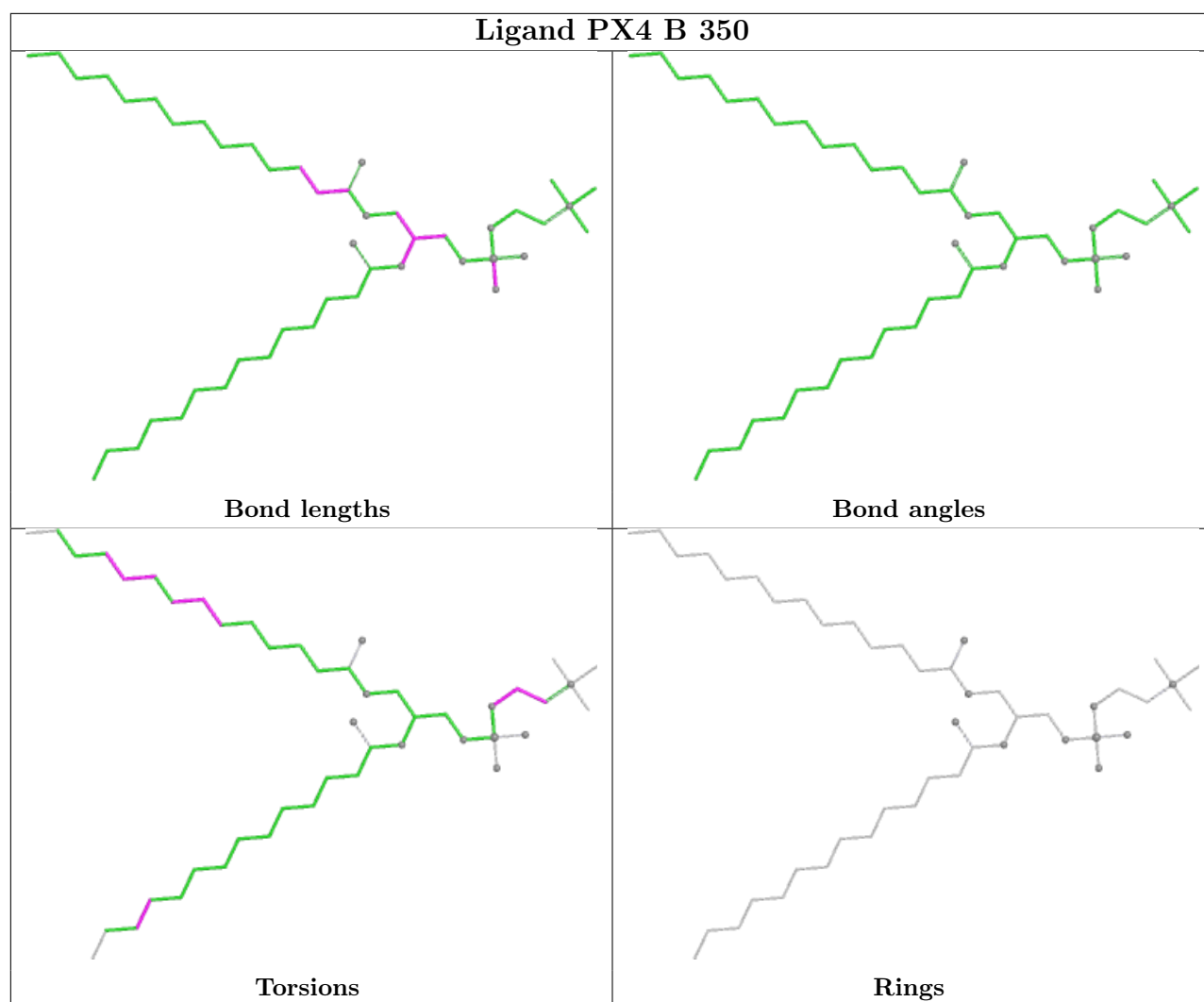
Ligand PX4 B 367



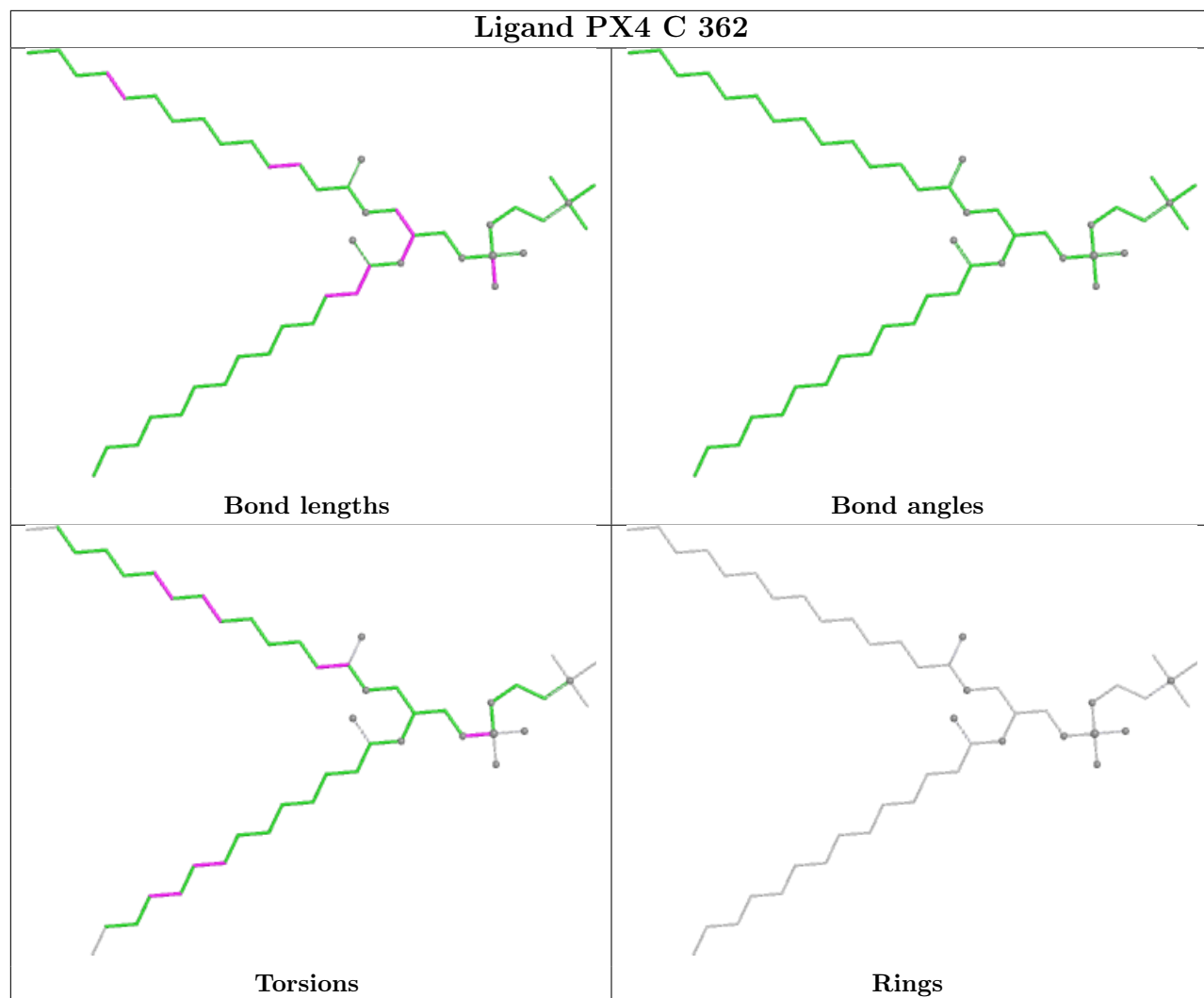




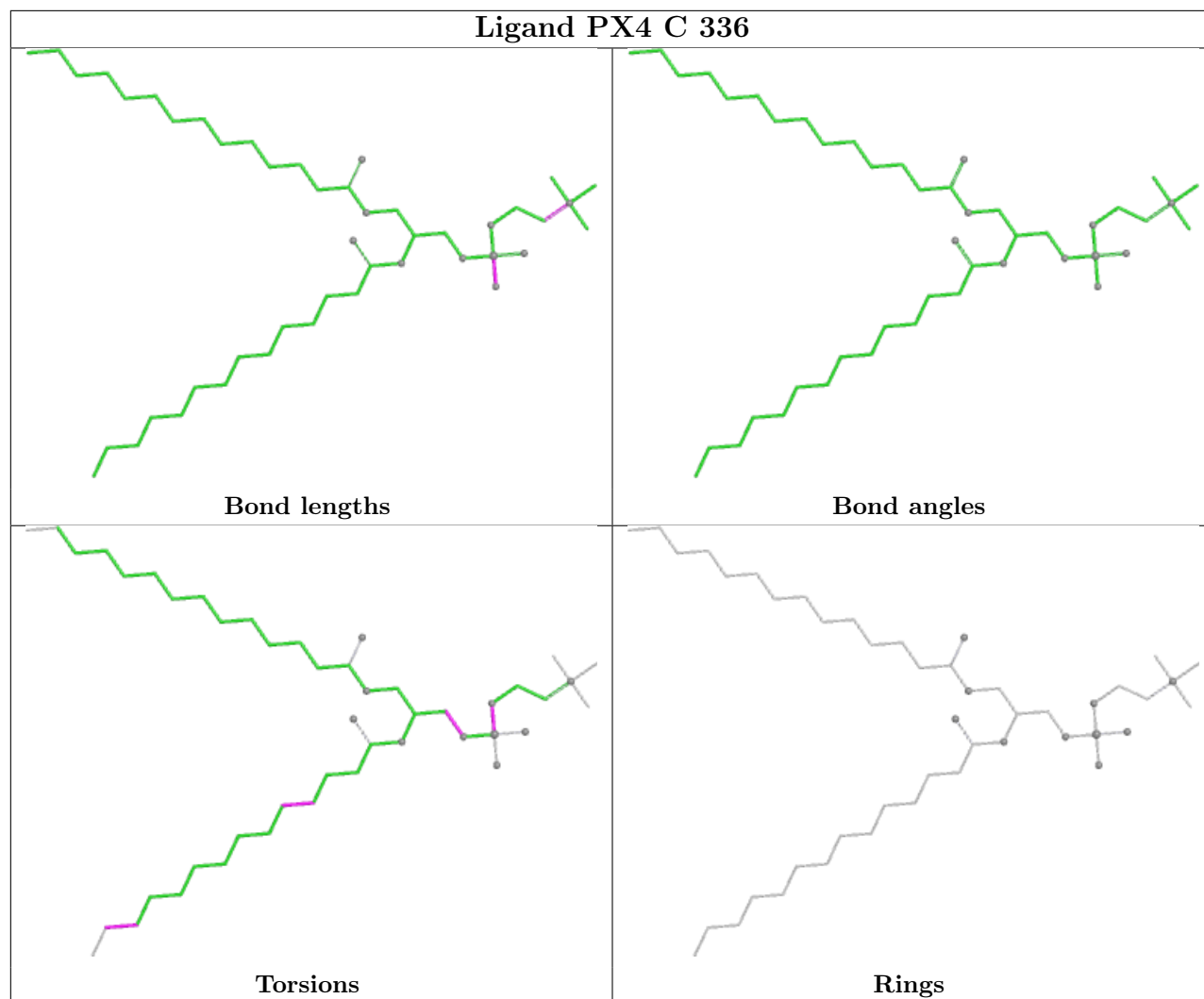


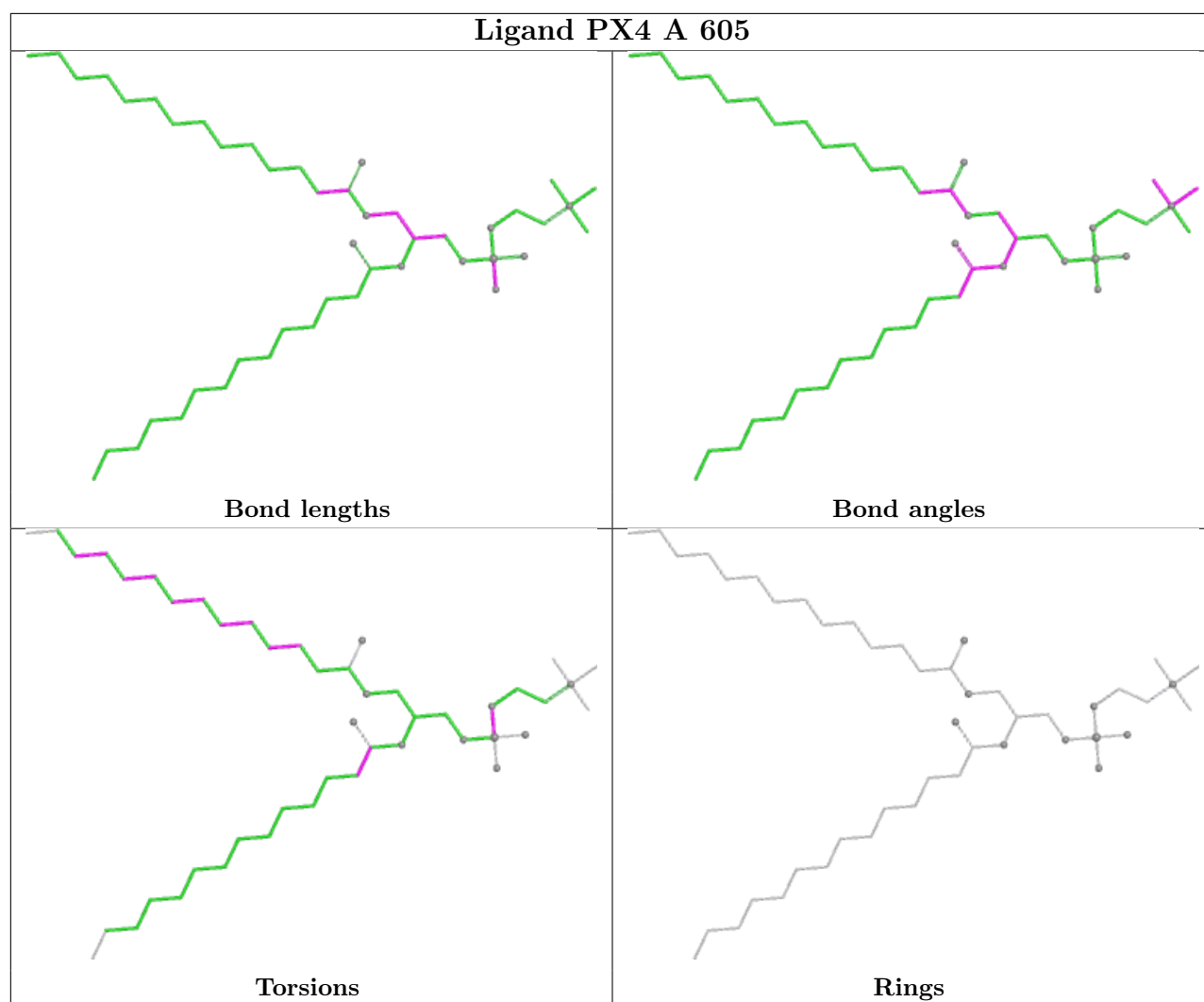


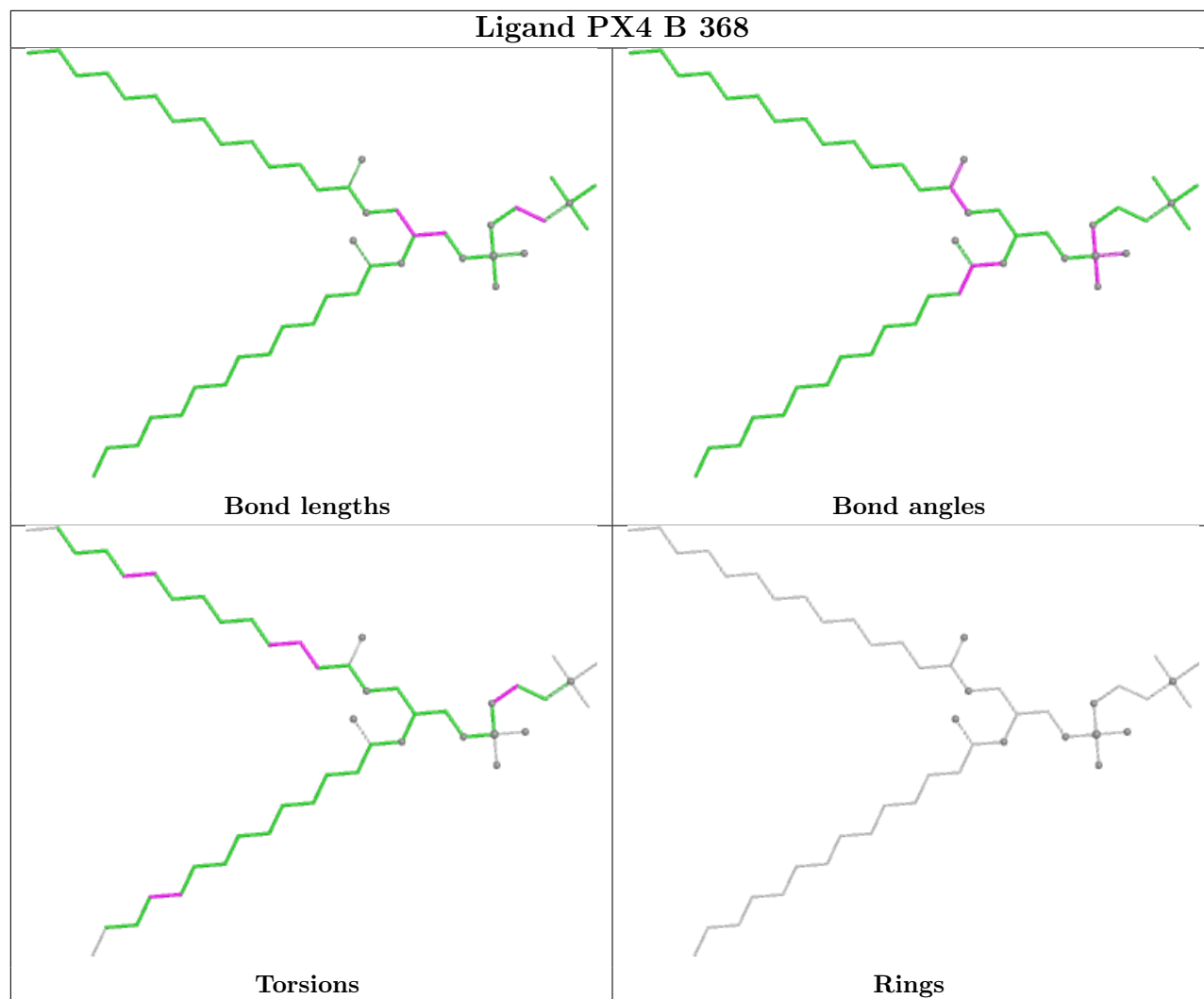
Ligand PX4 C 362



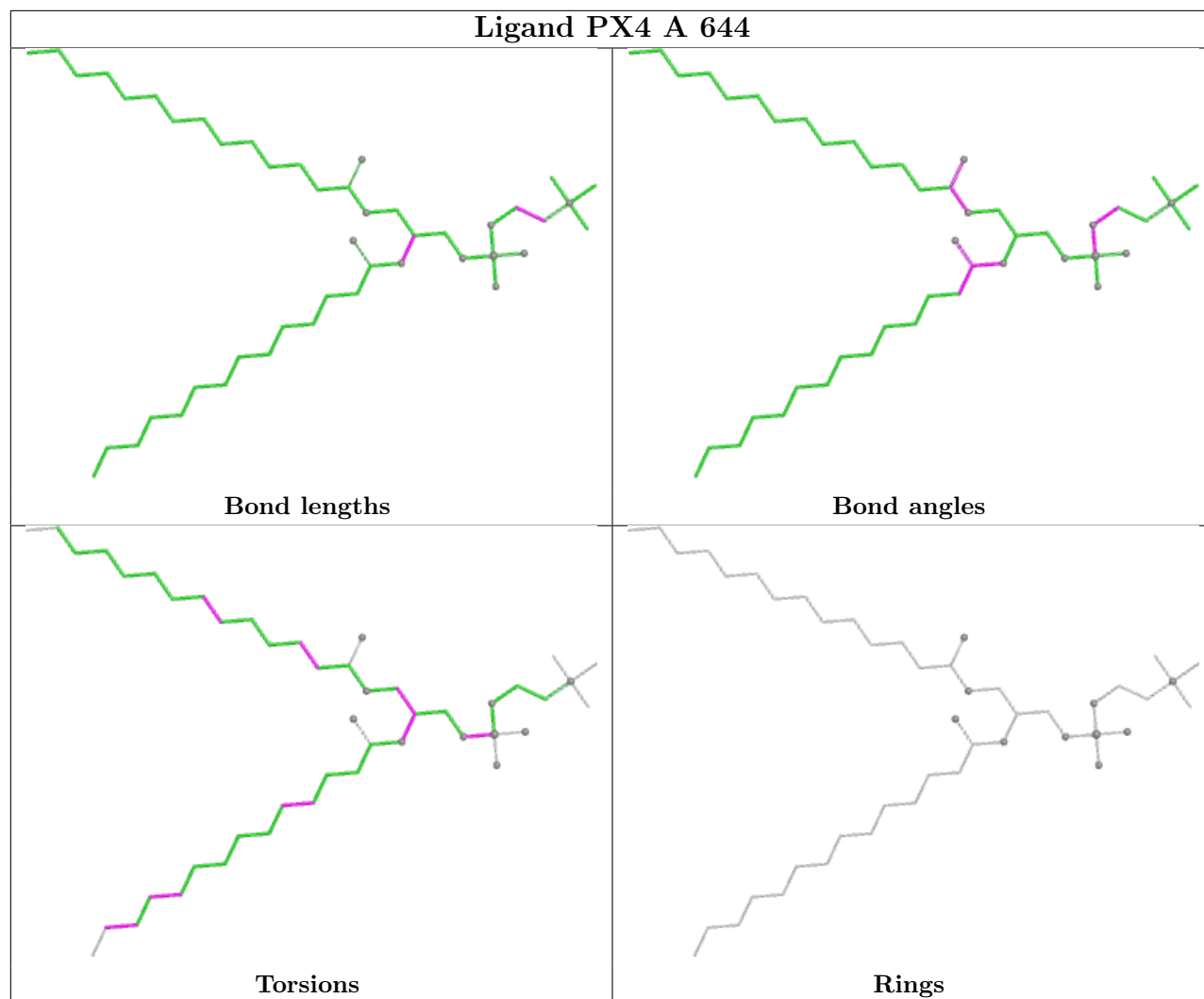
Ligand PX4 C 336



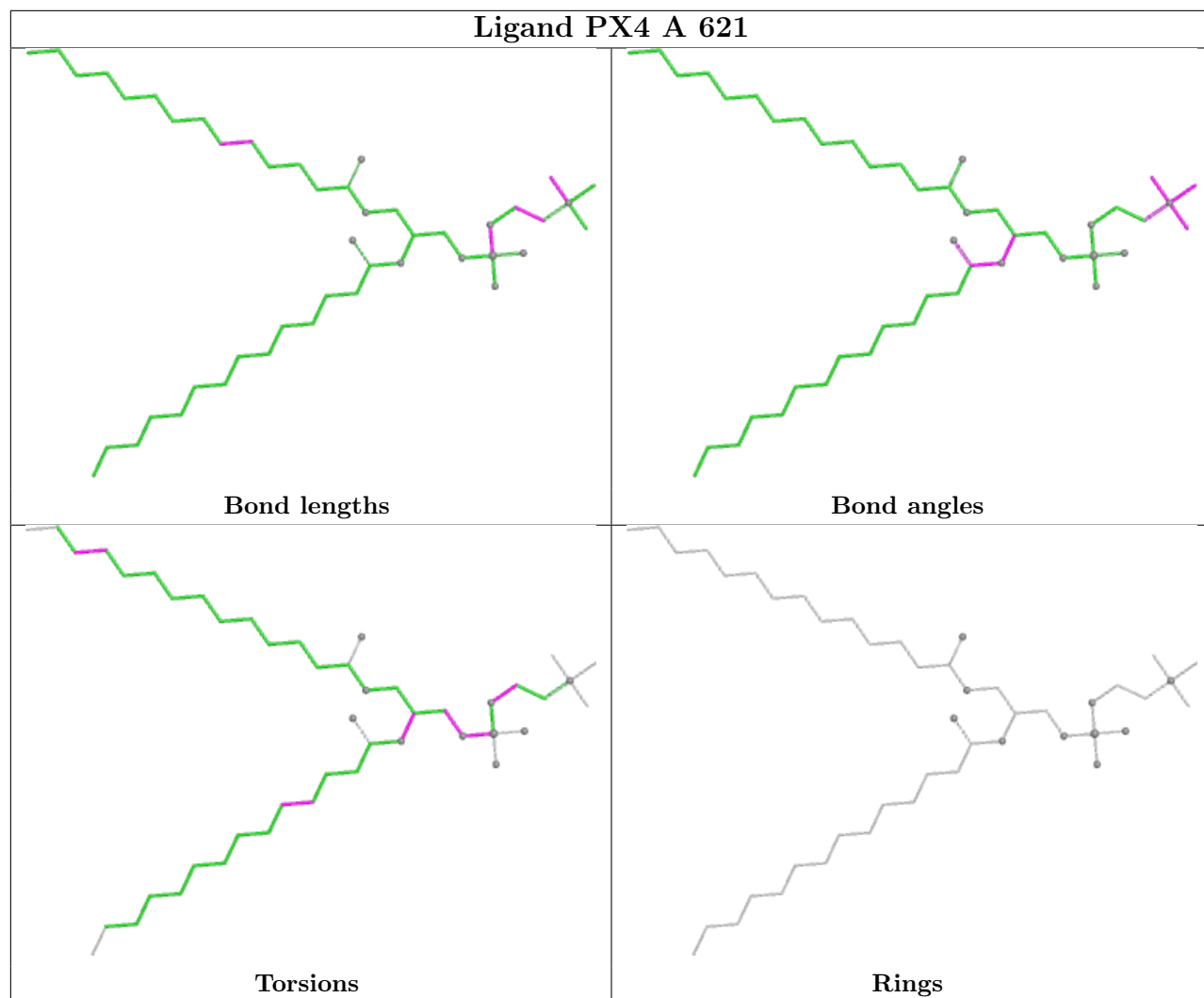


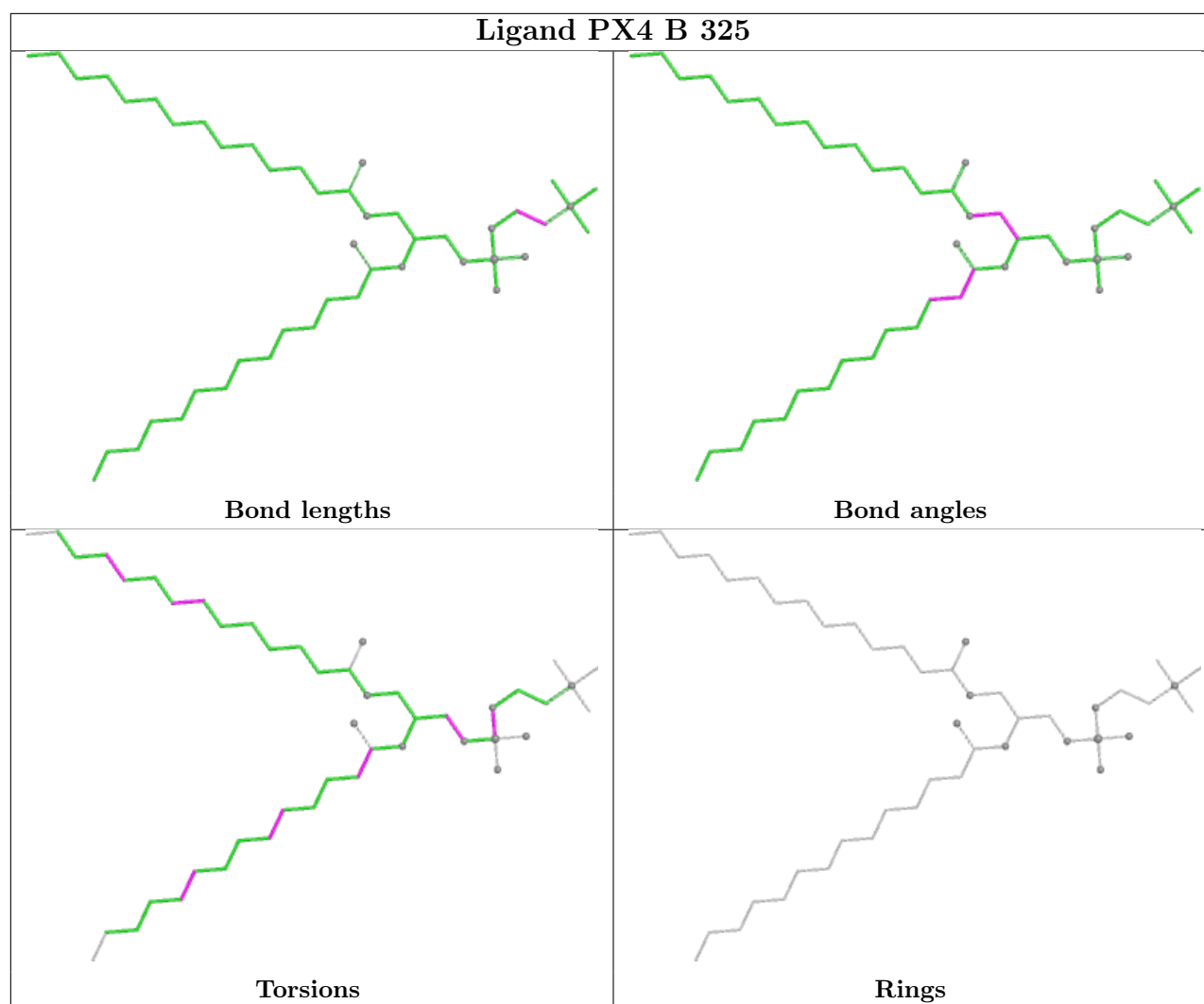


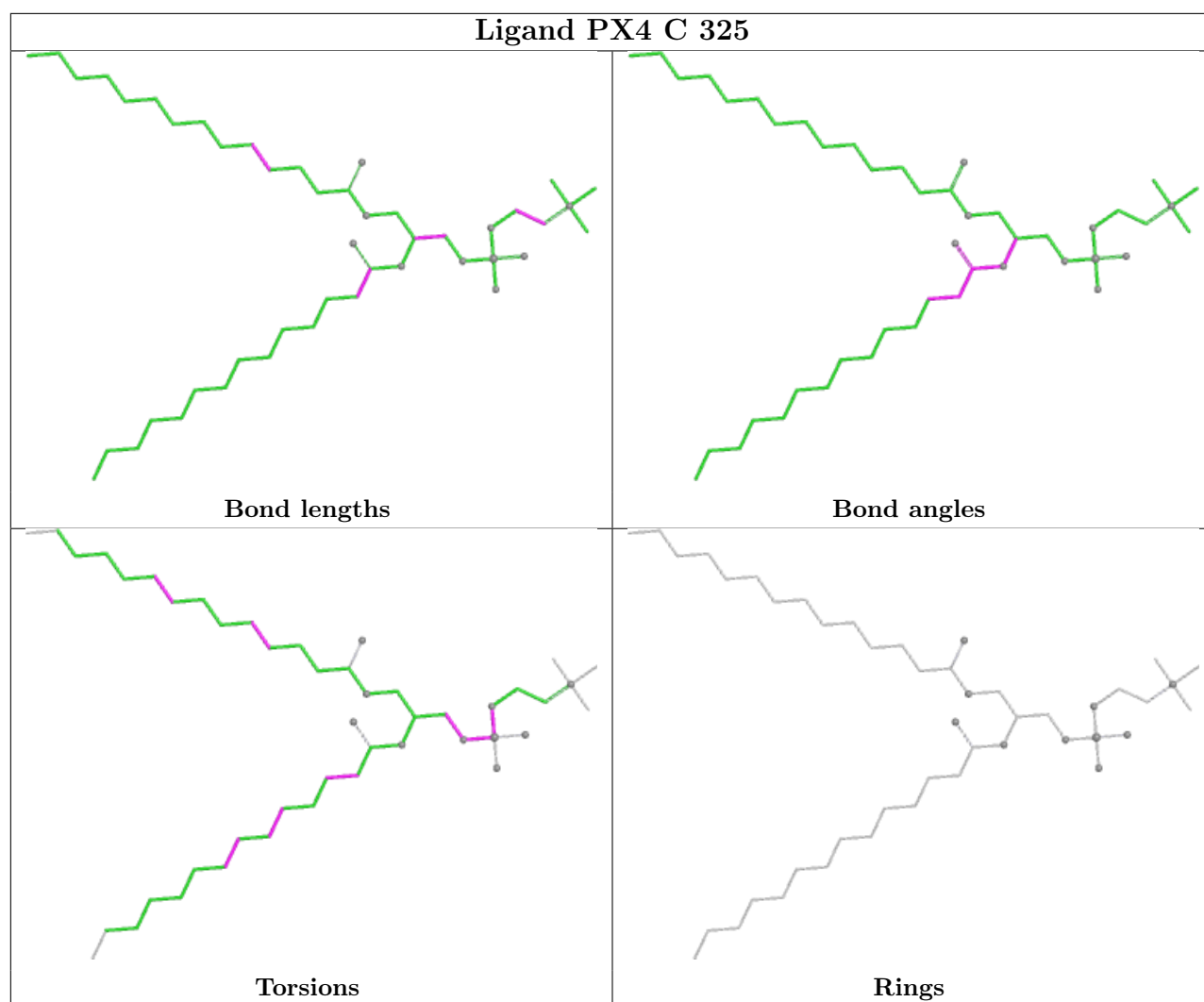
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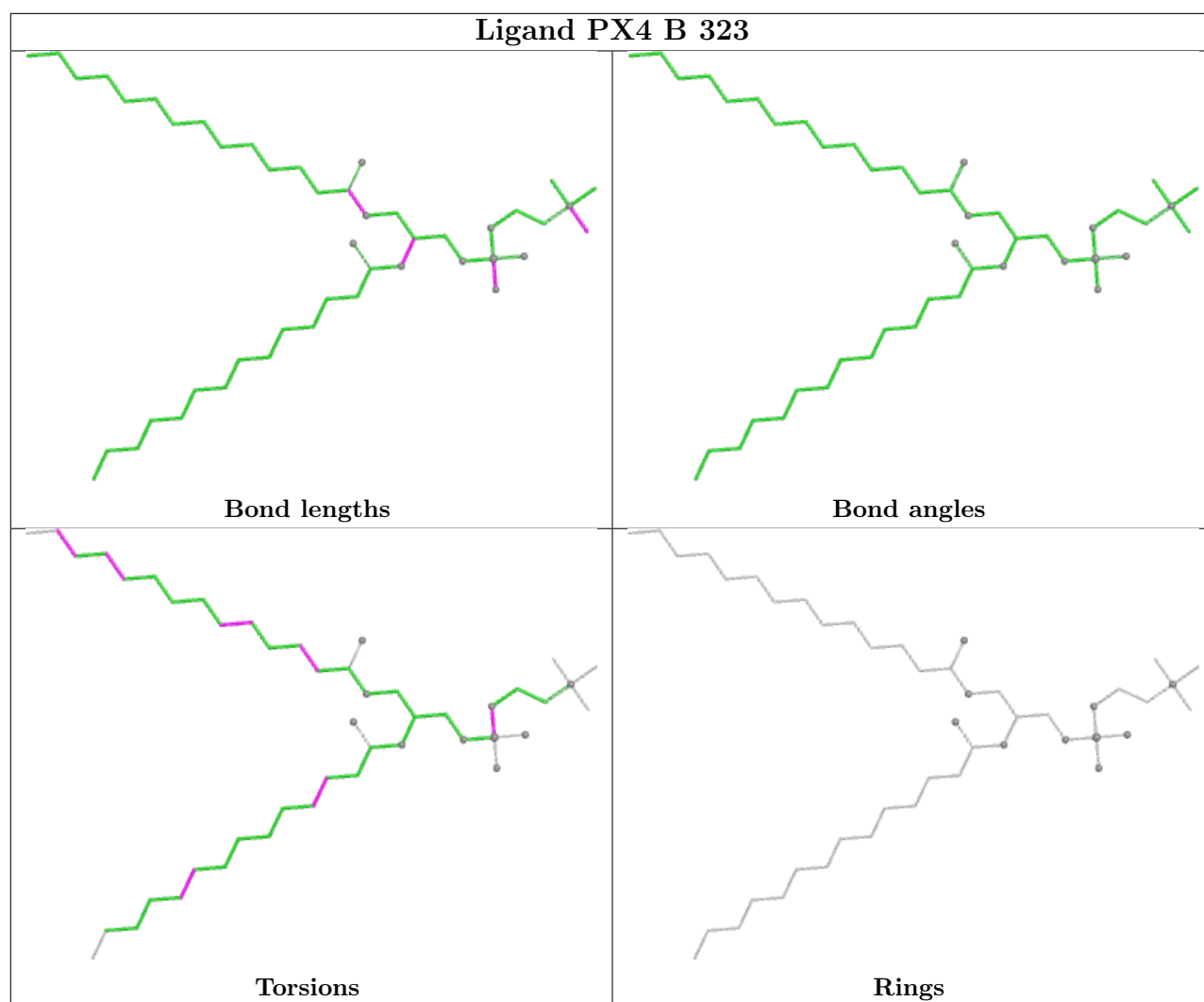


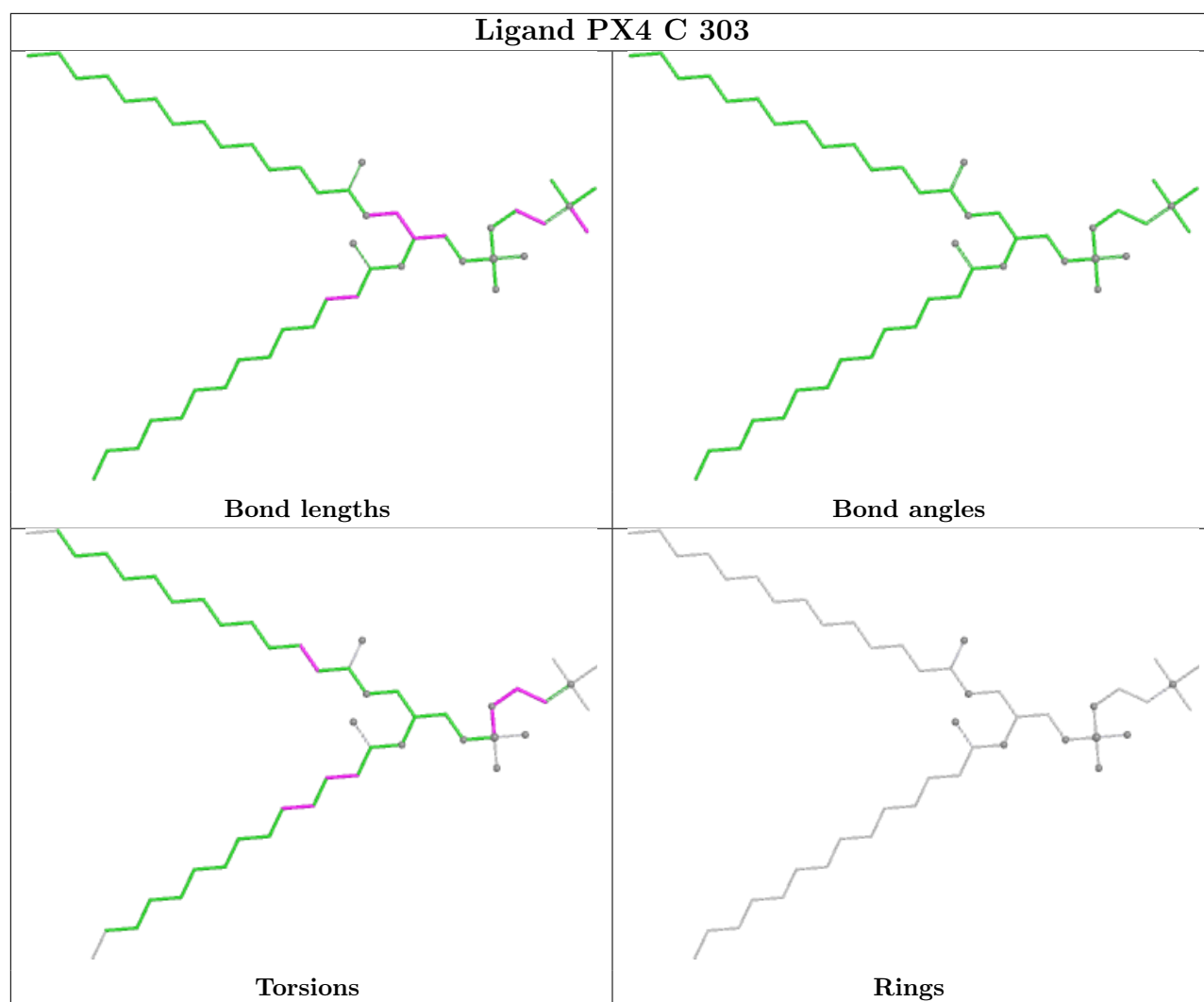
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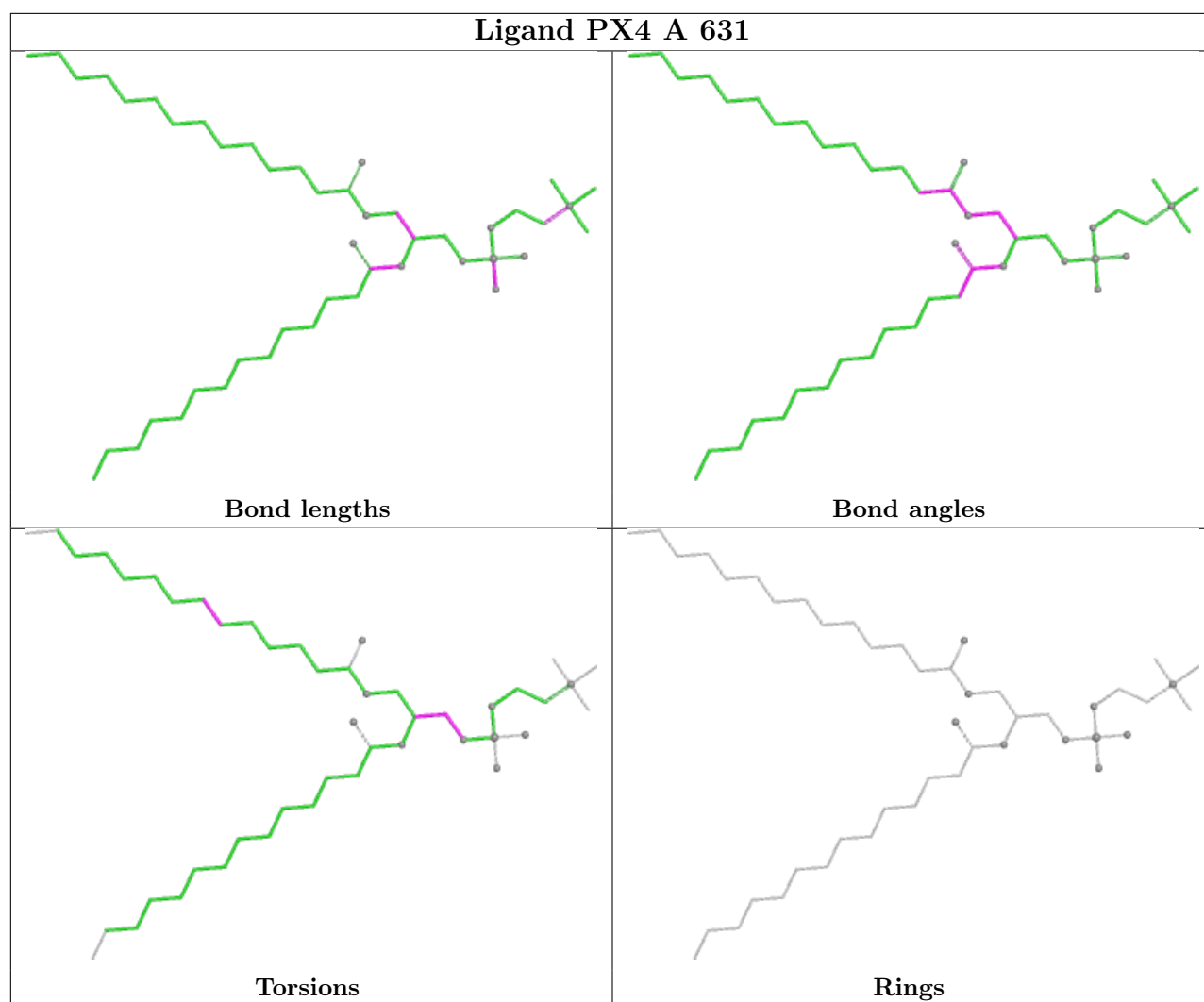




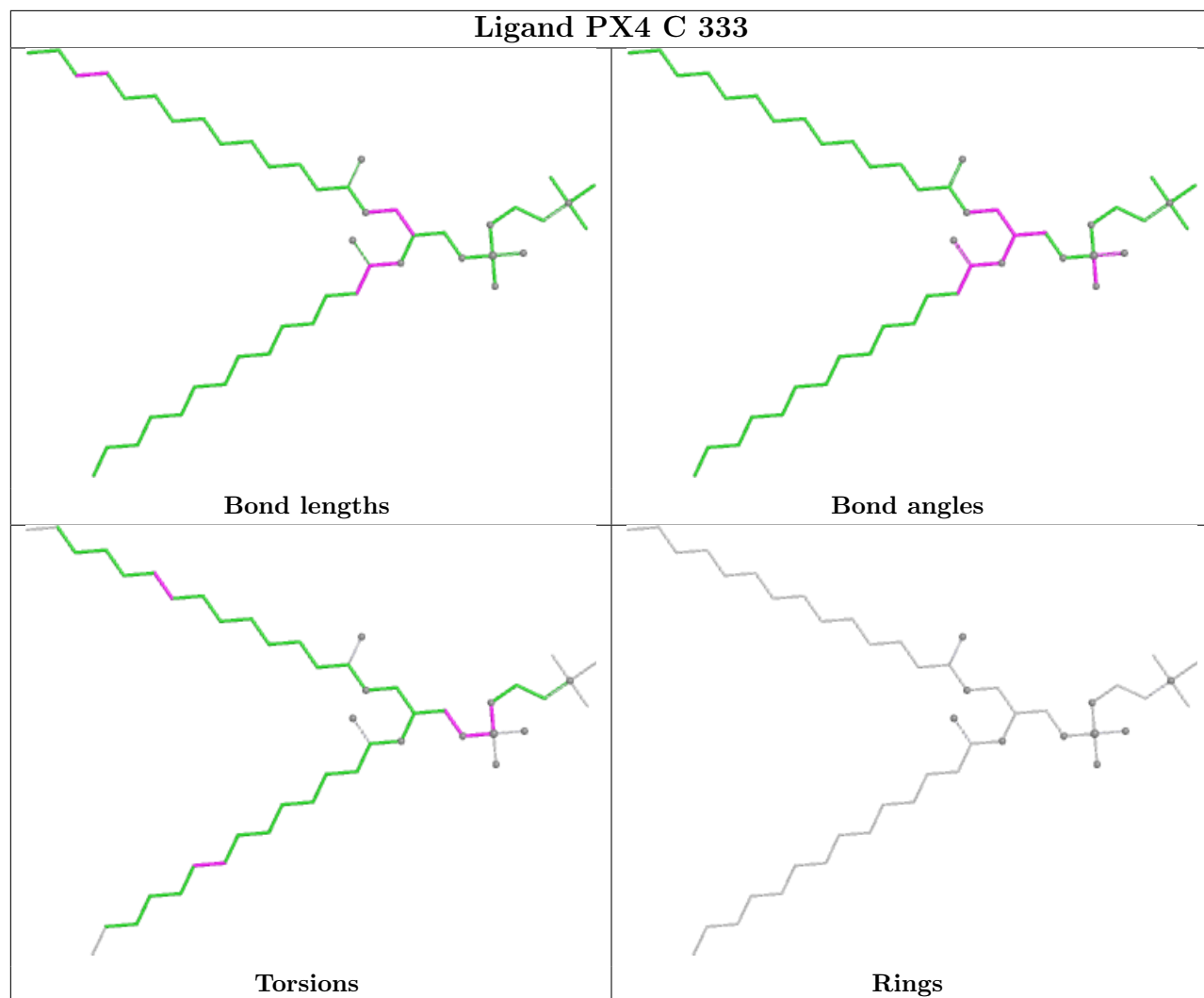




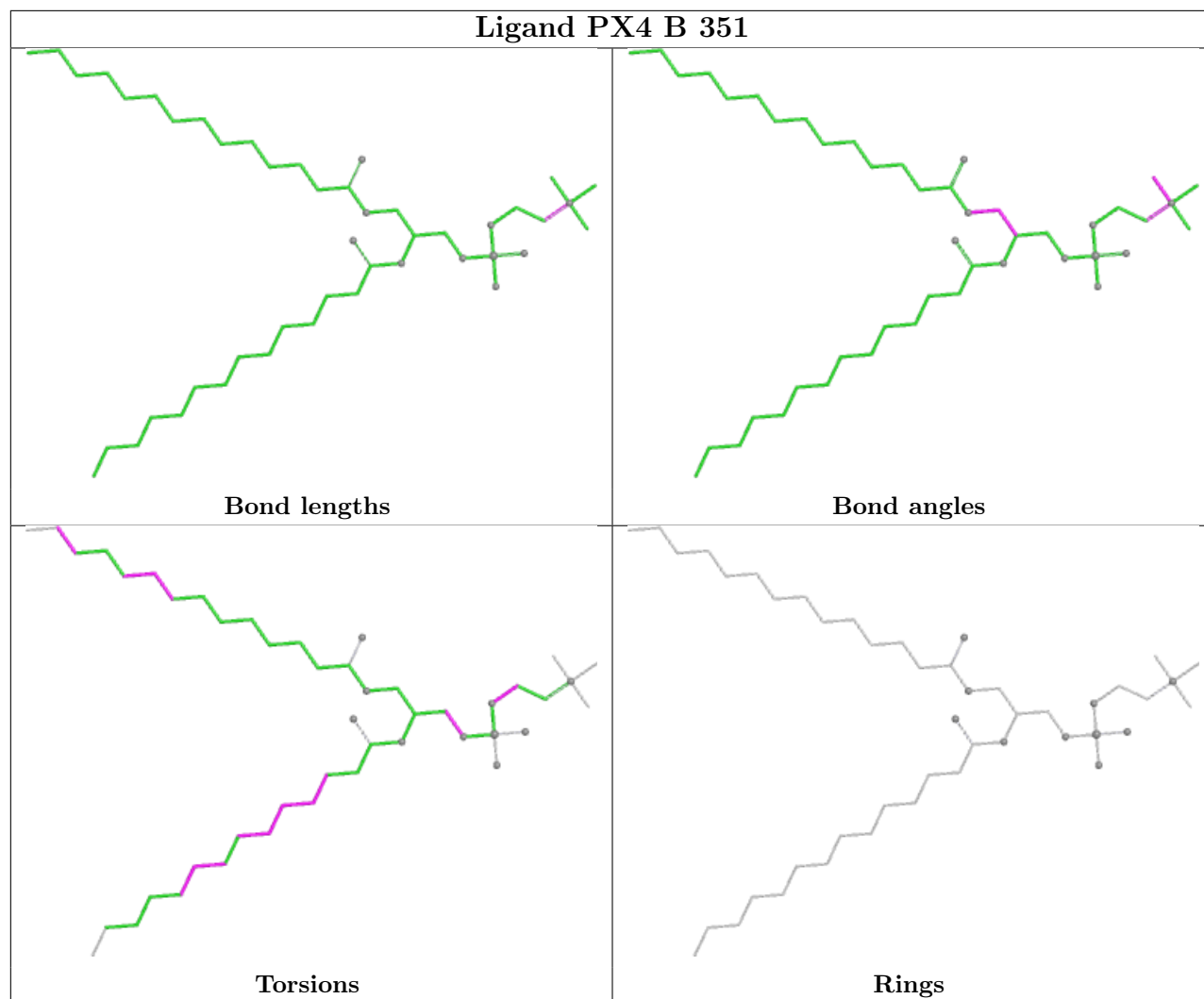




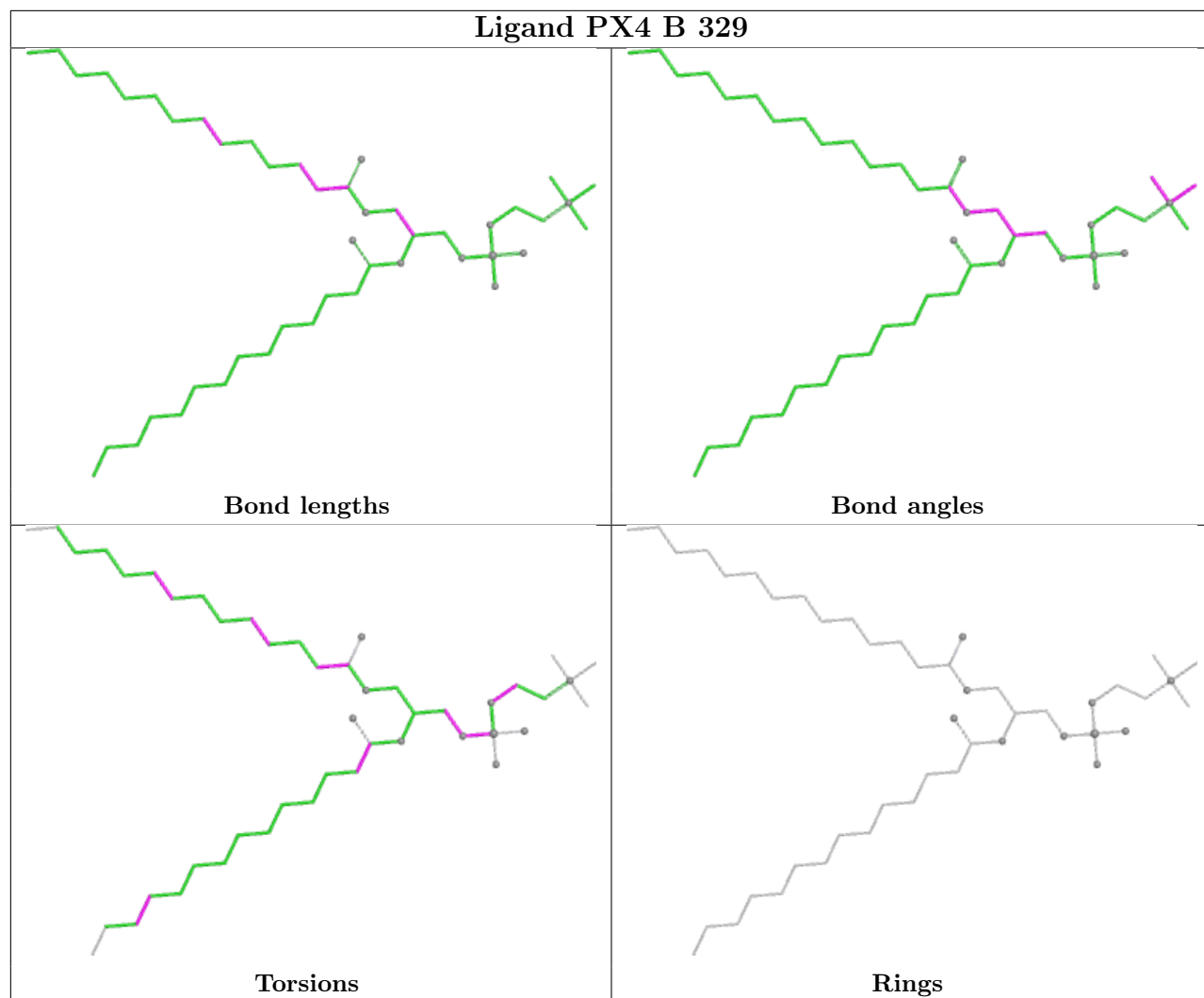
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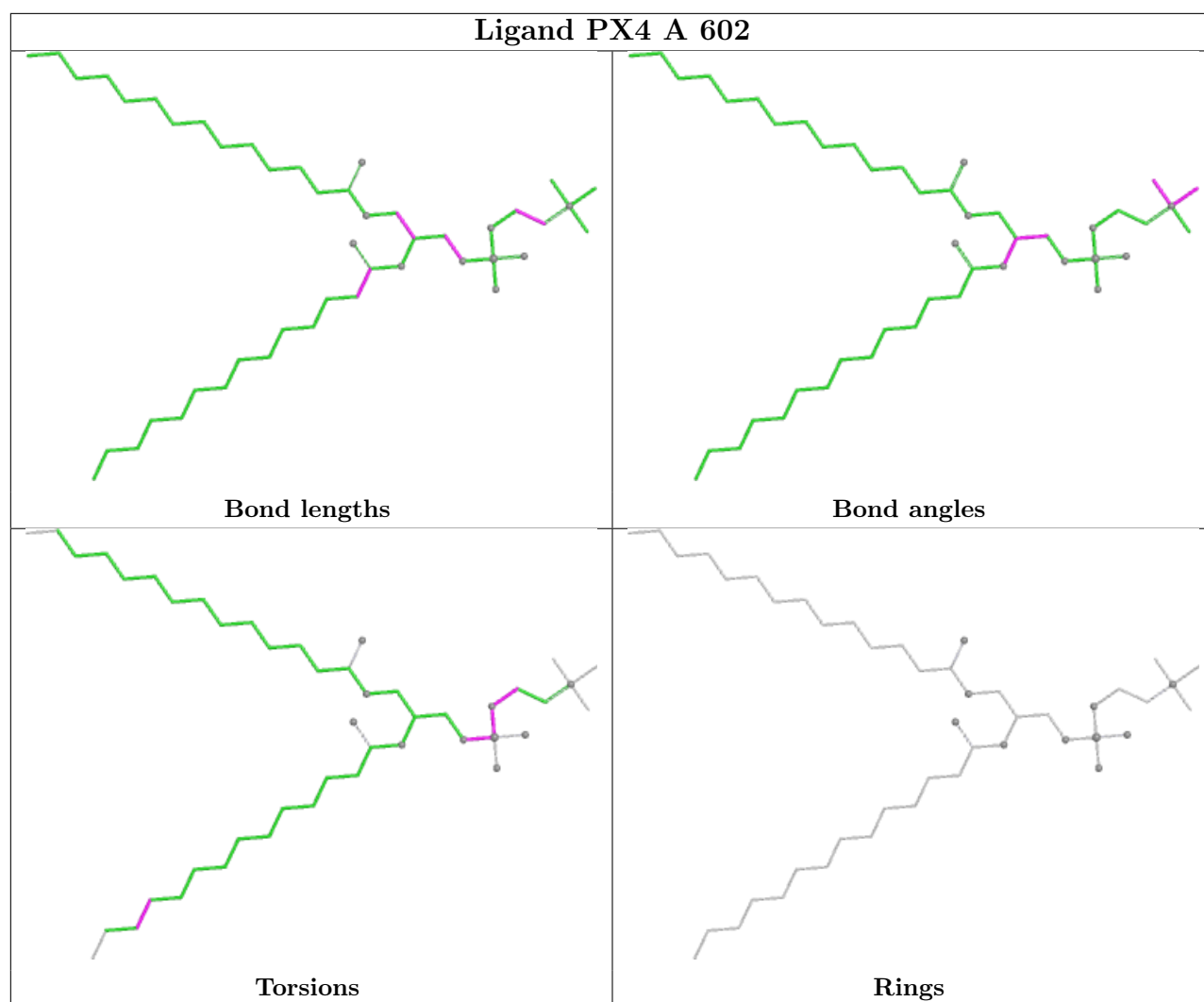


Ligand PX4 B 351

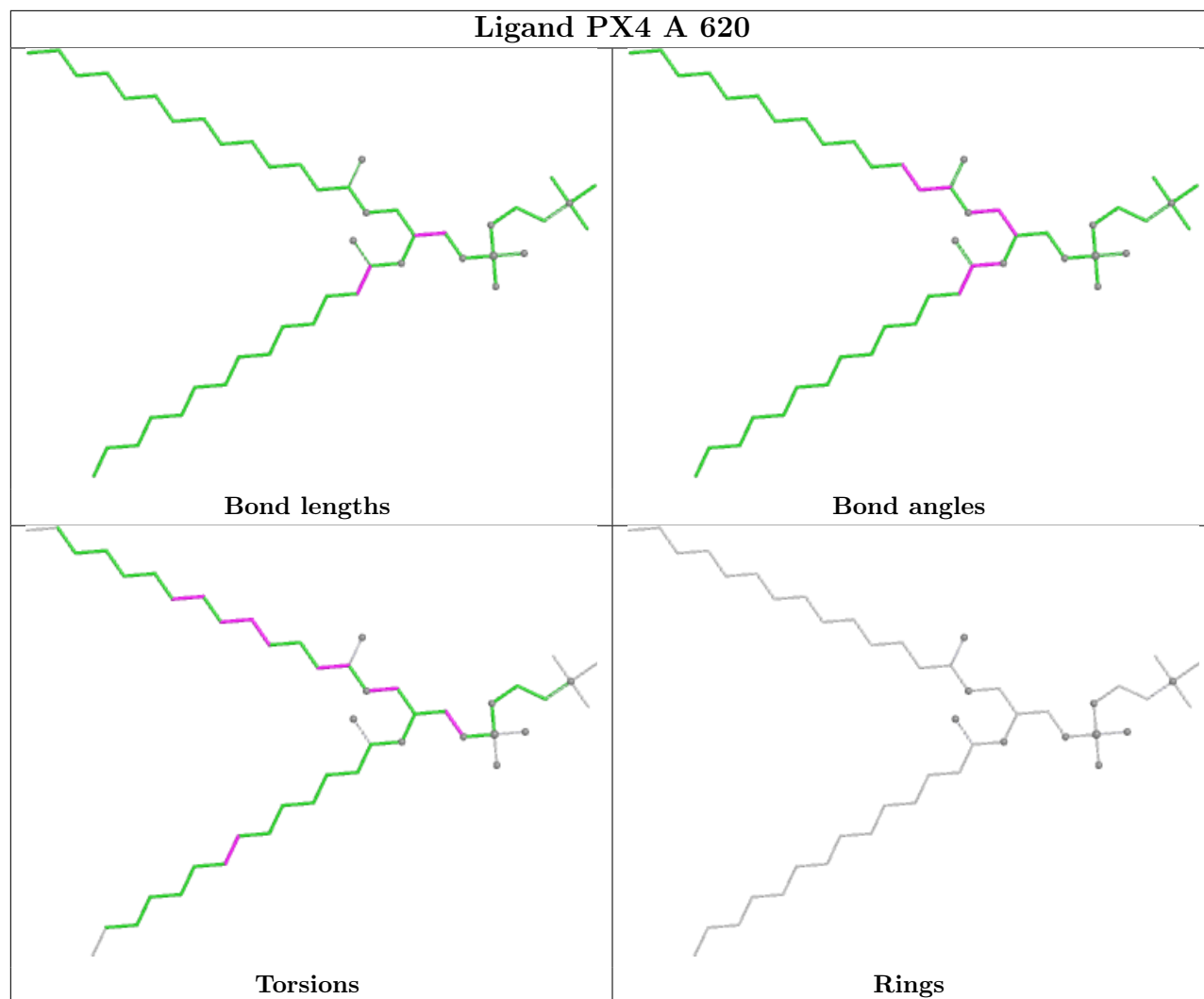


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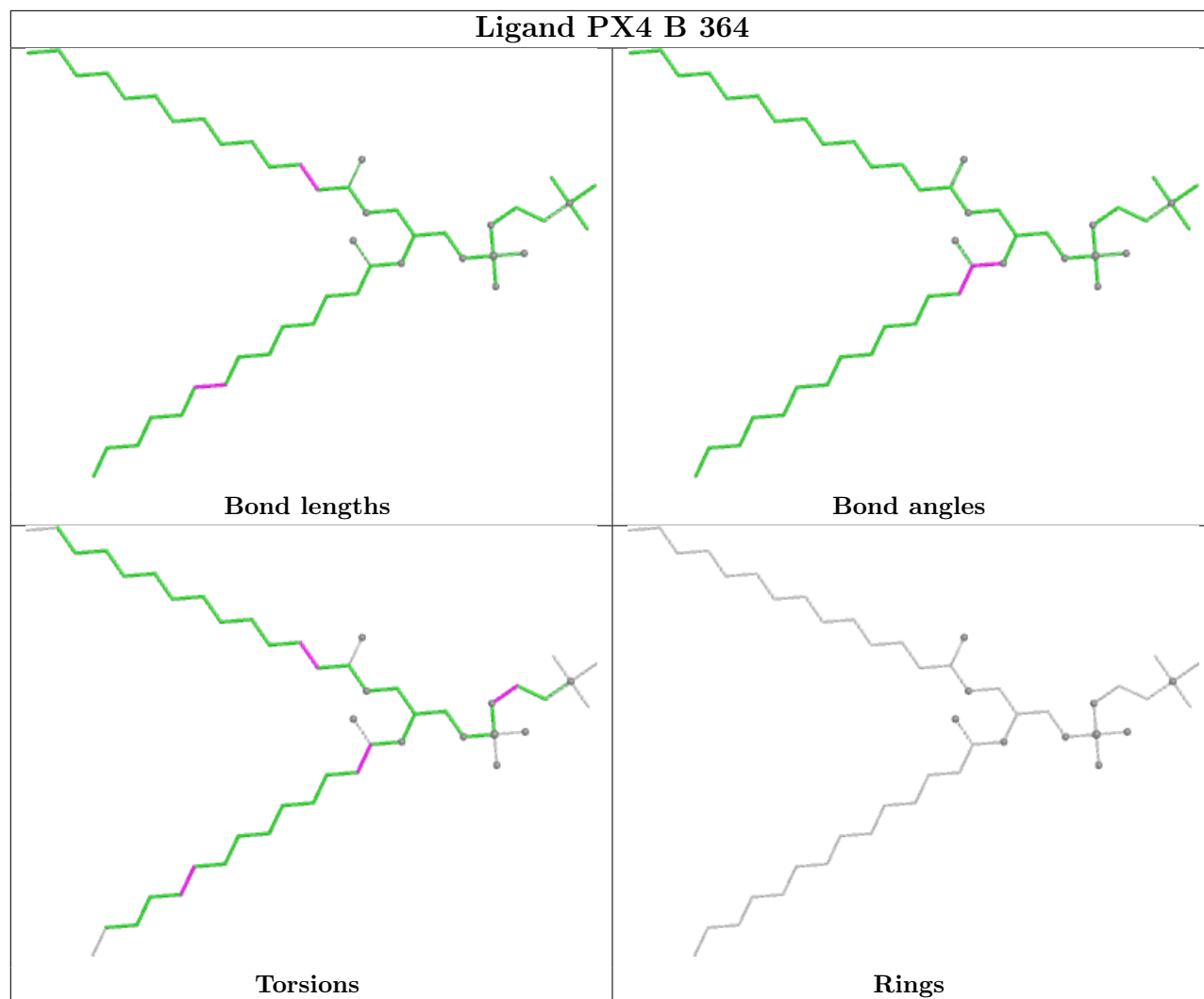




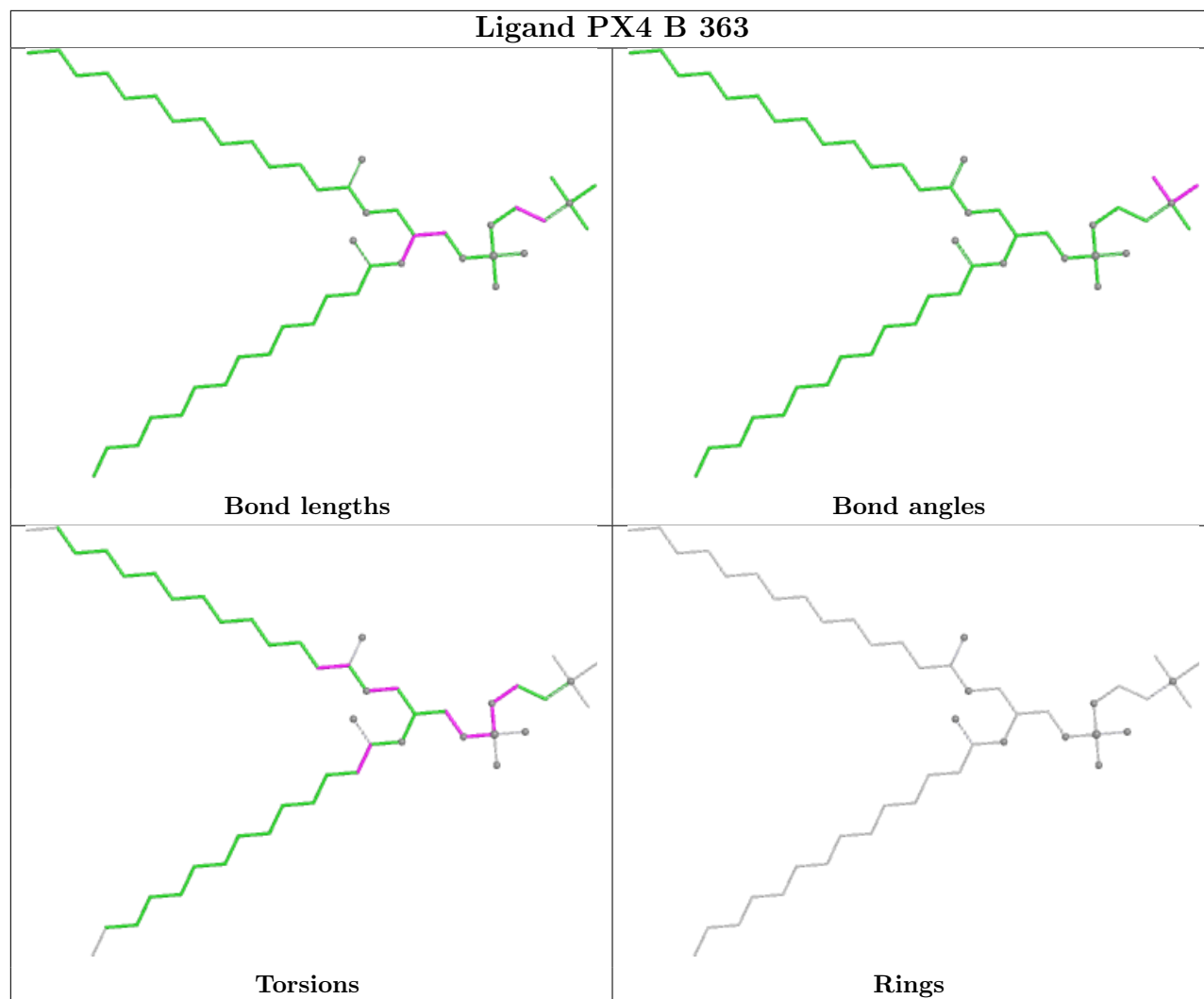
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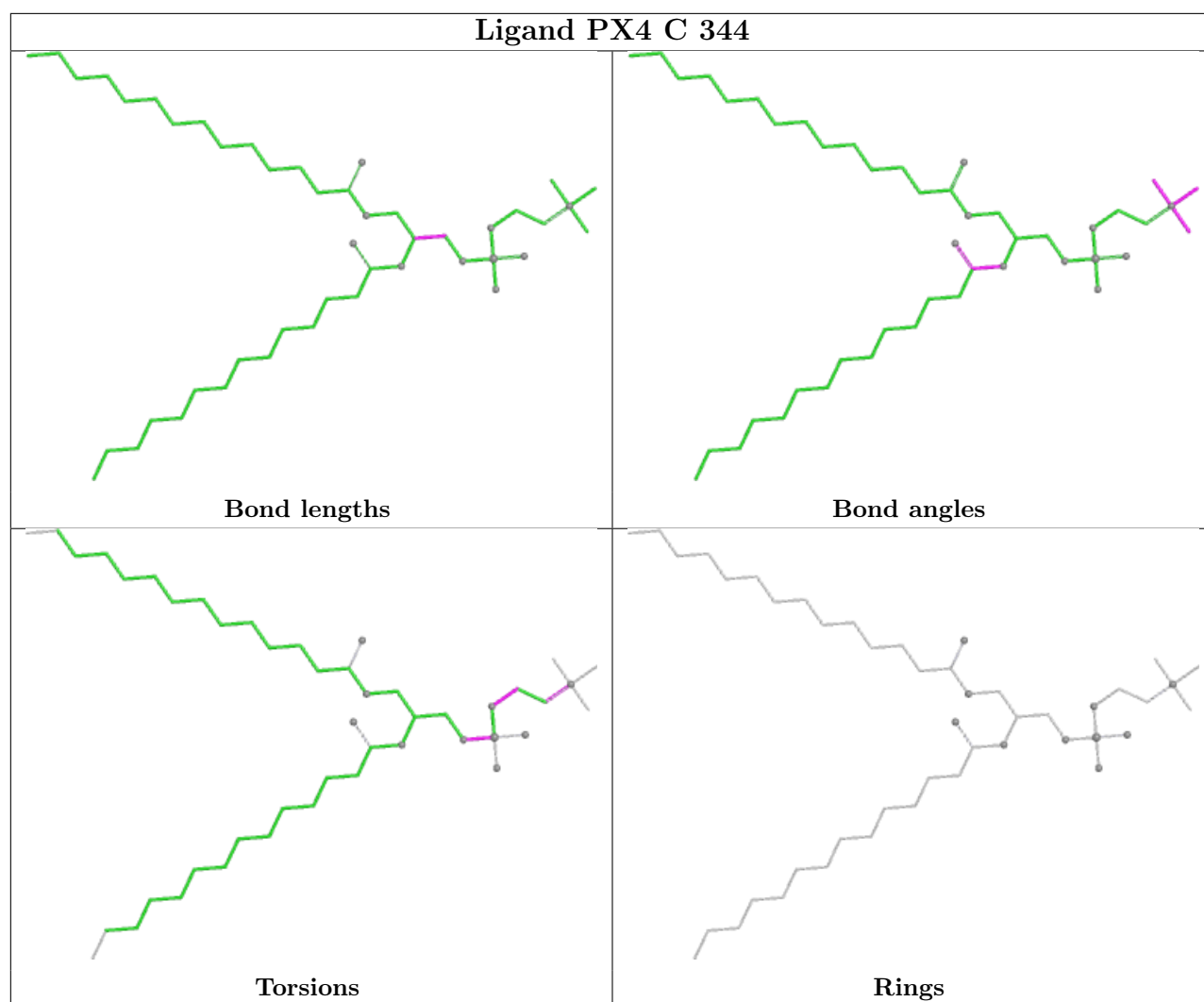


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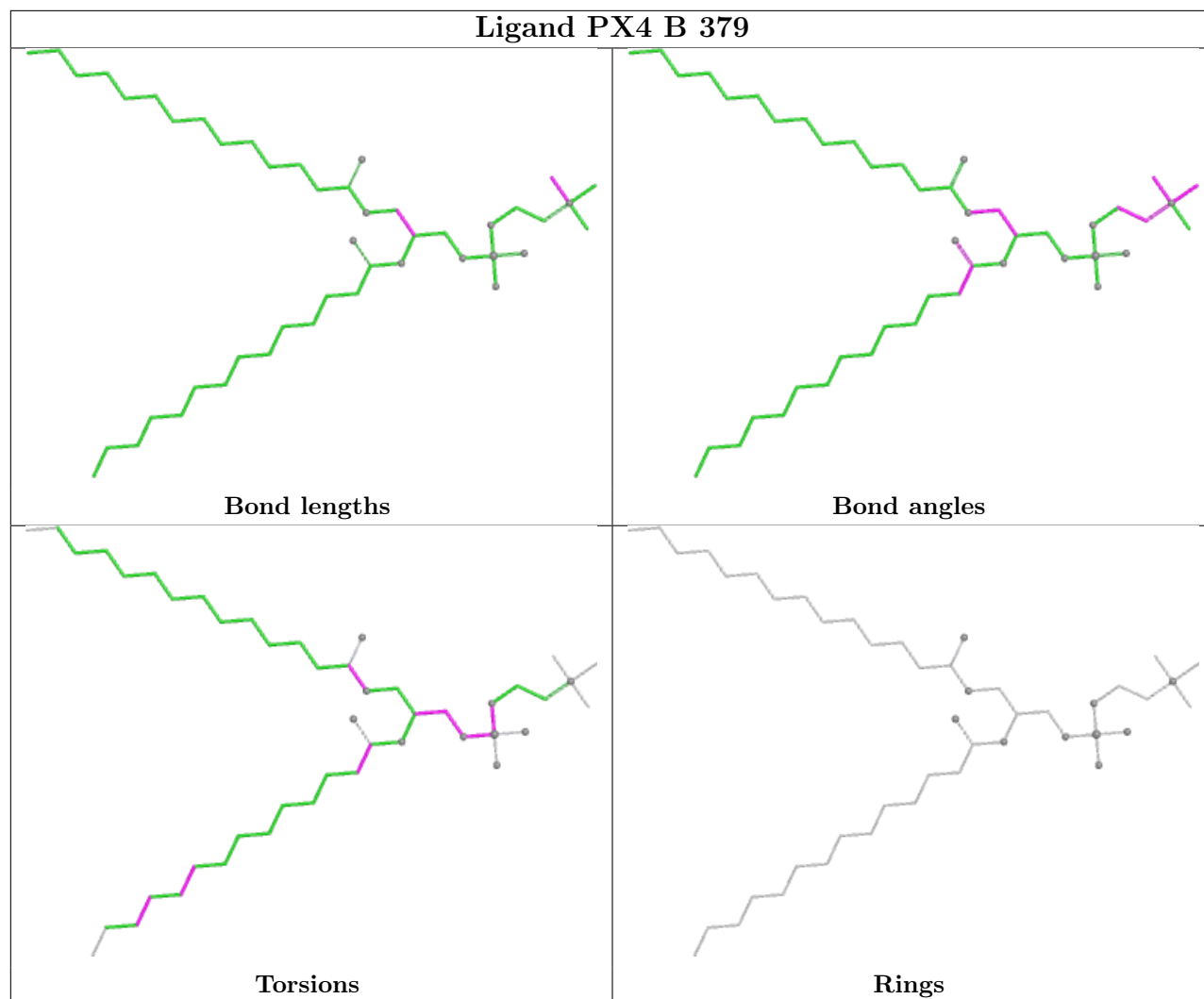


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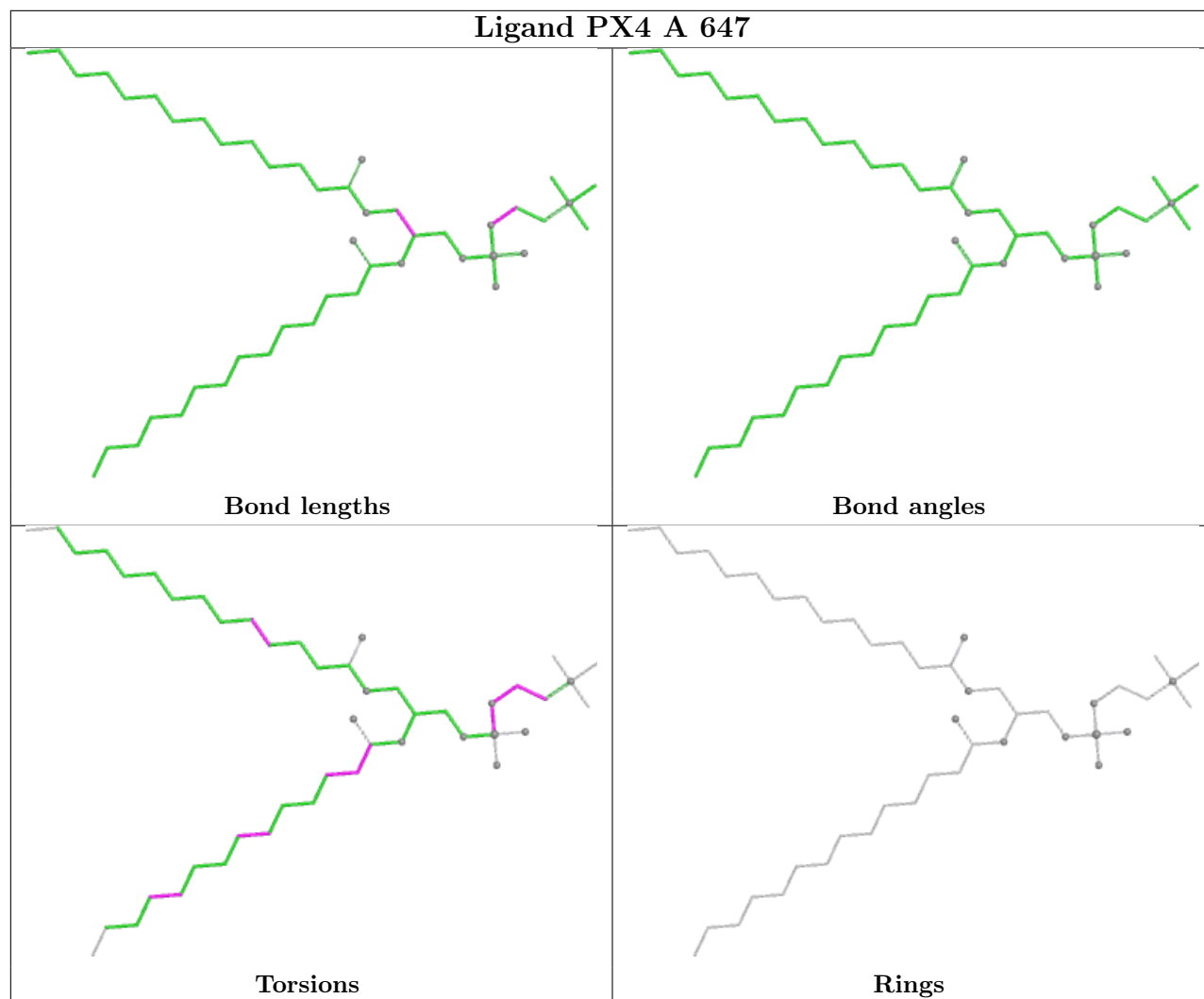




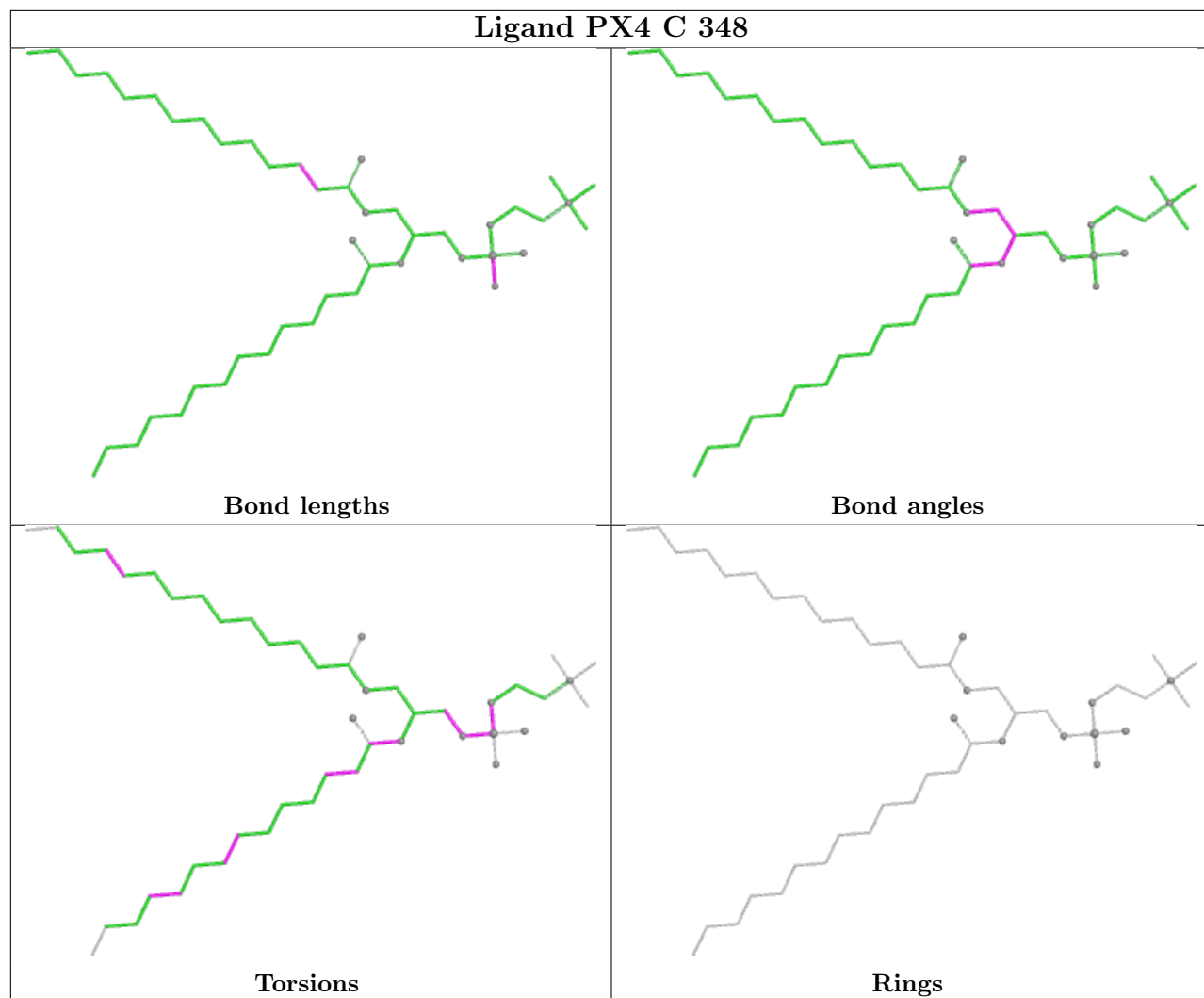
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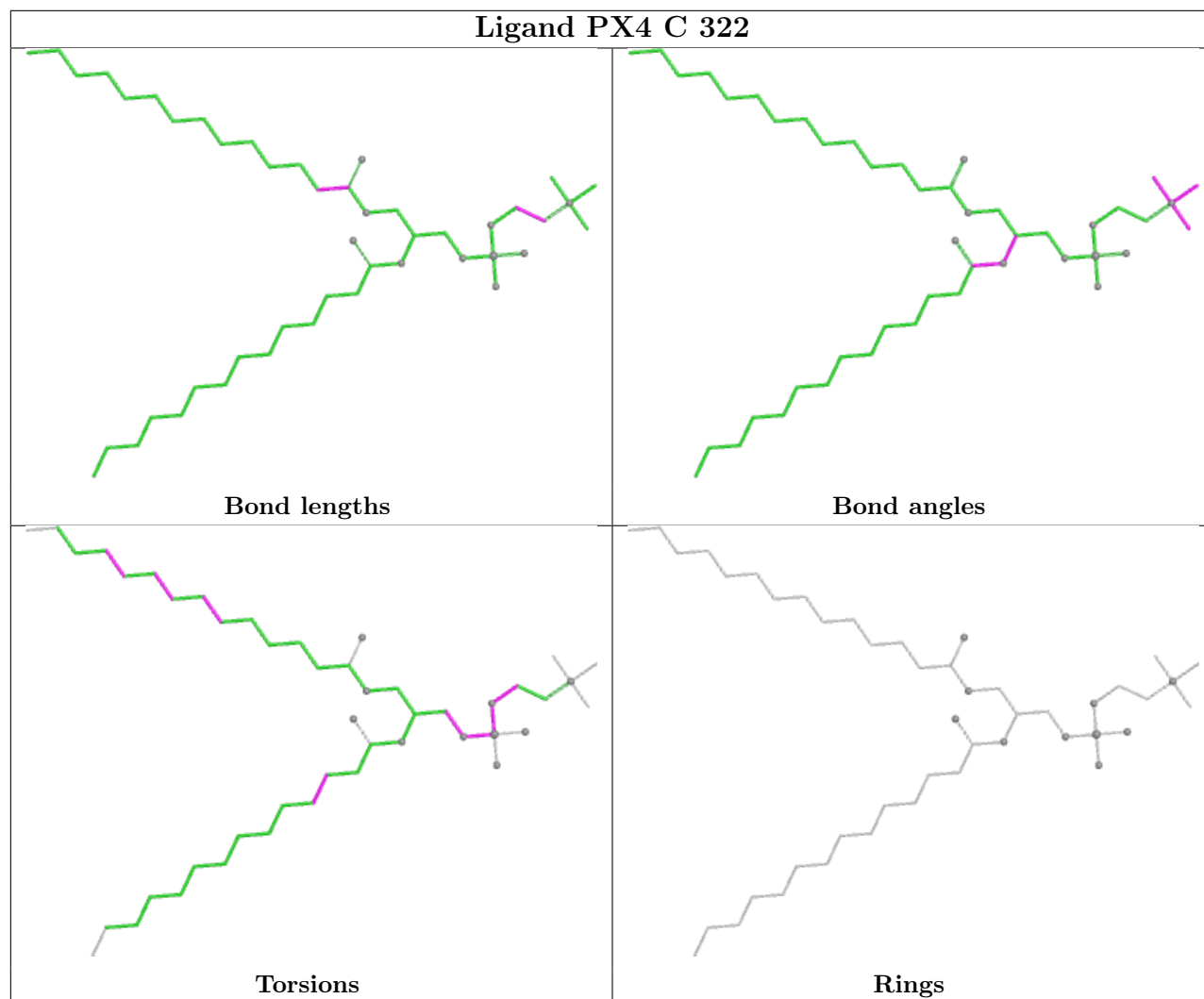
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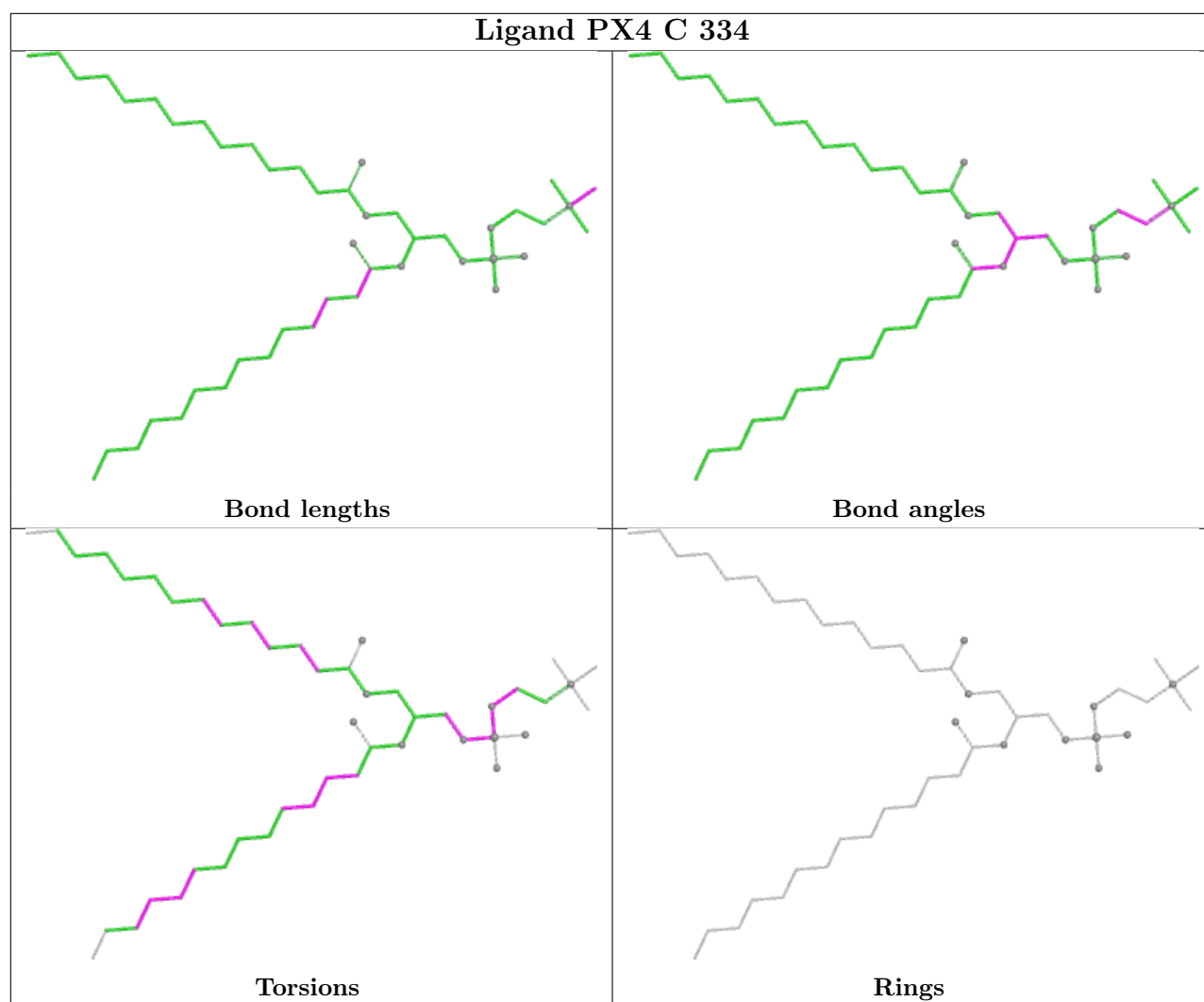


Ligand PX4 C 348

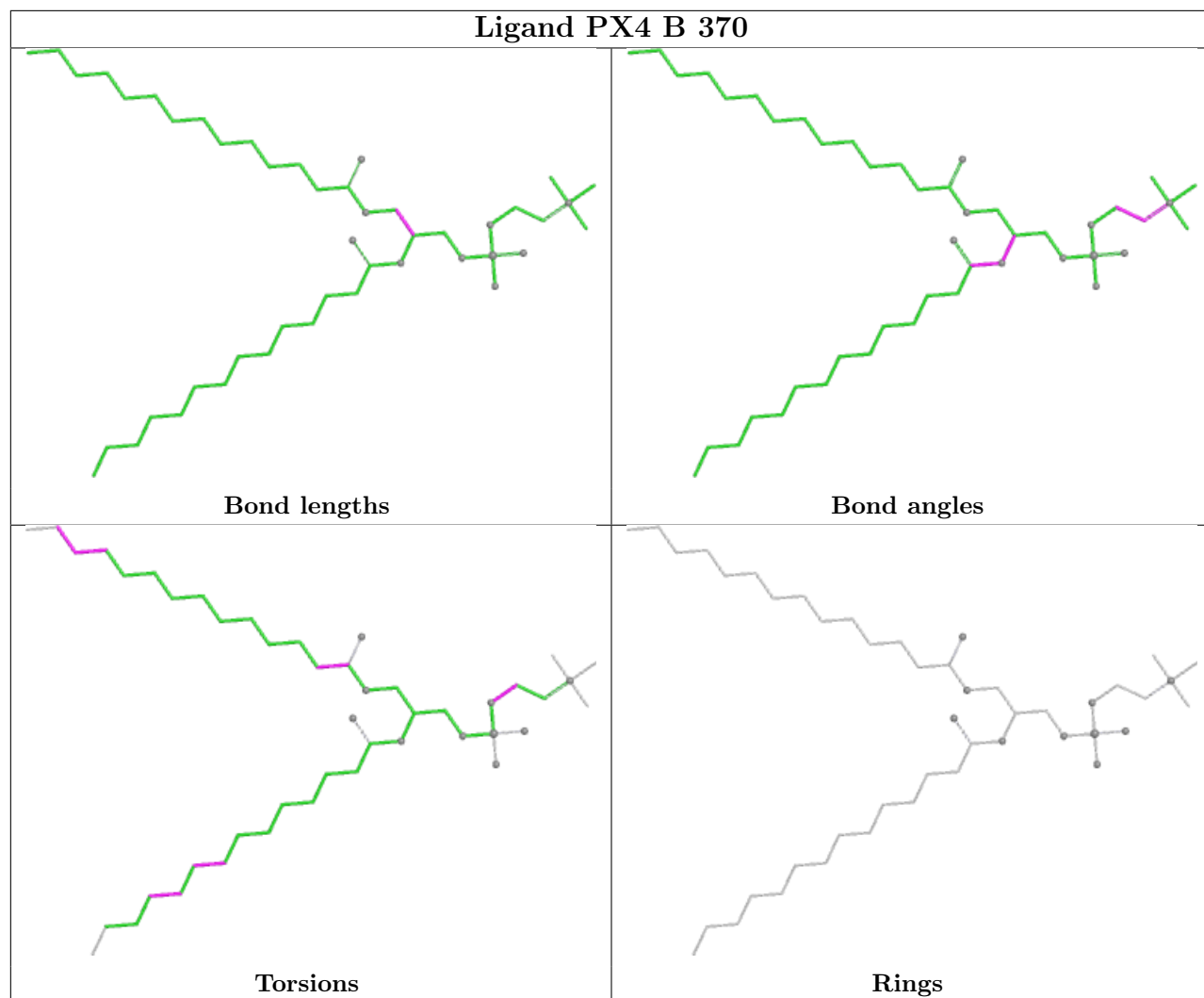


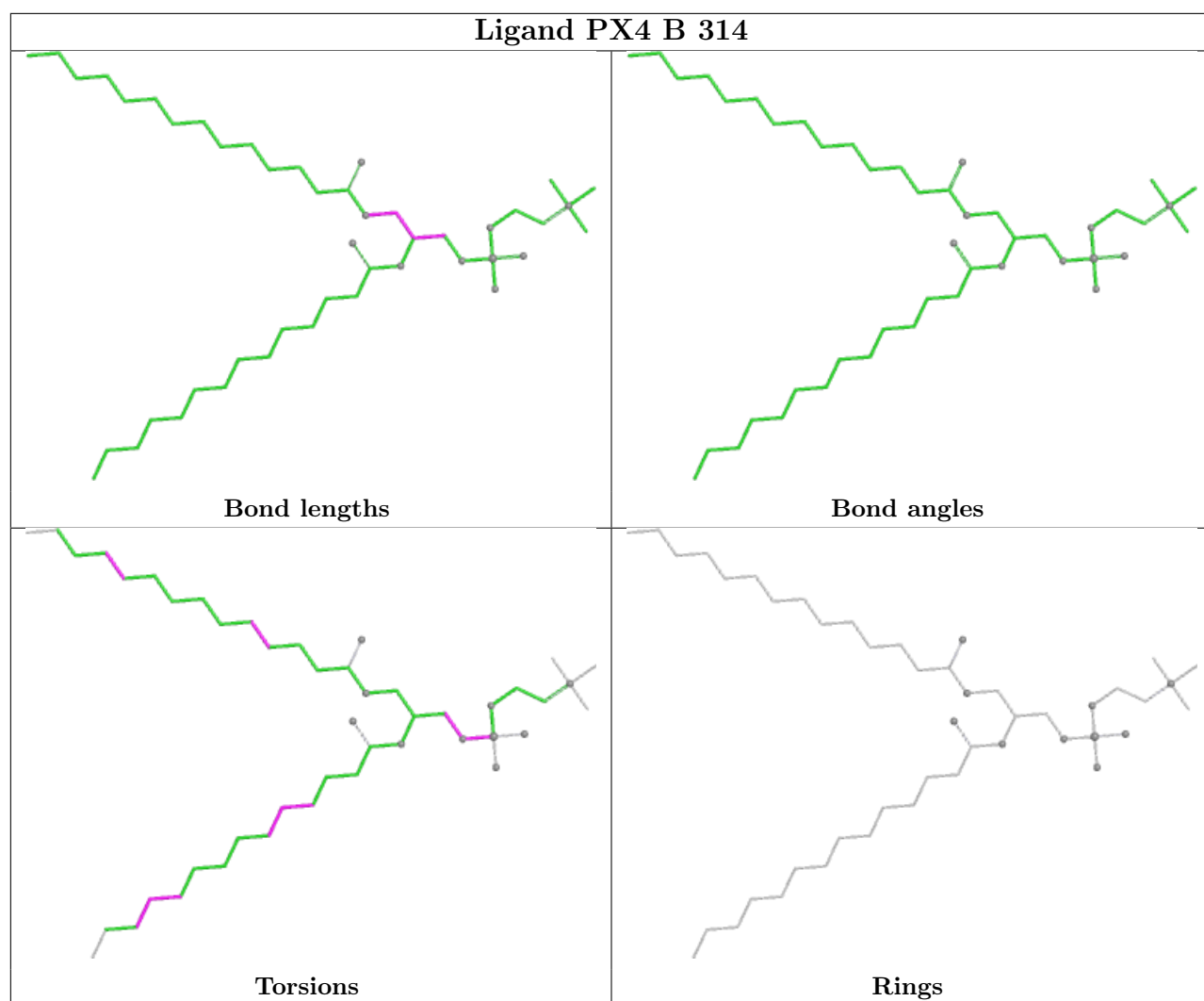
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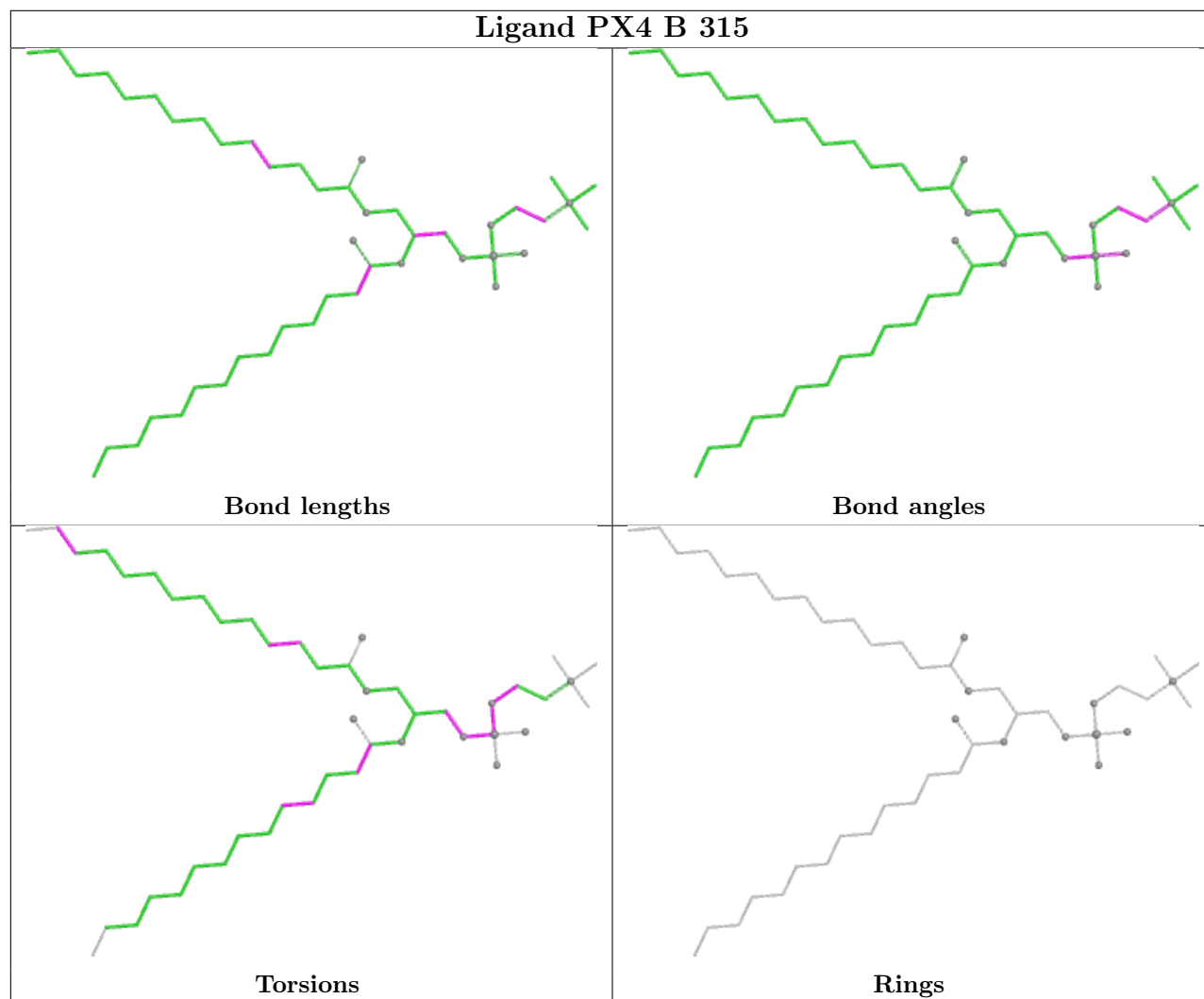


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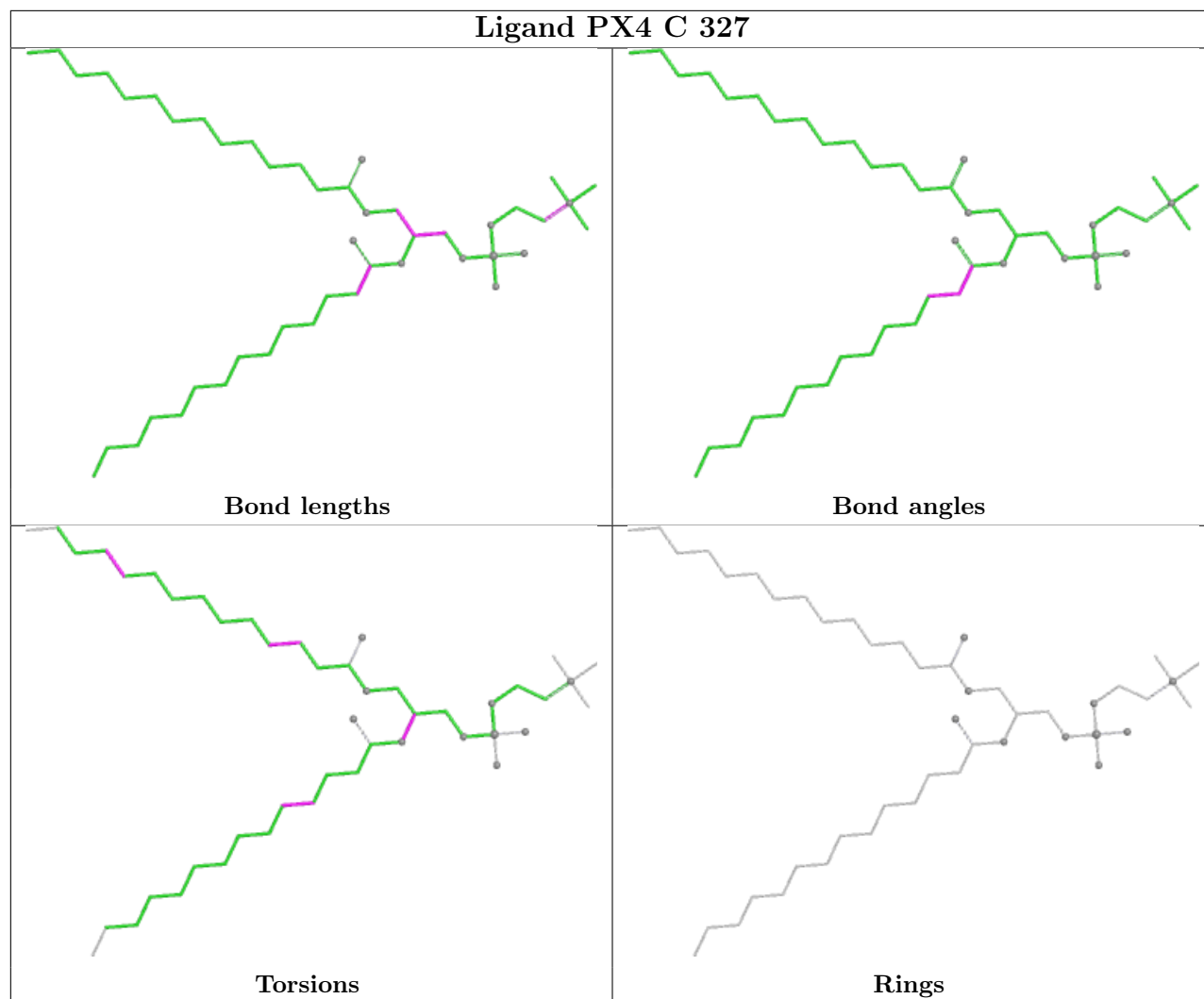




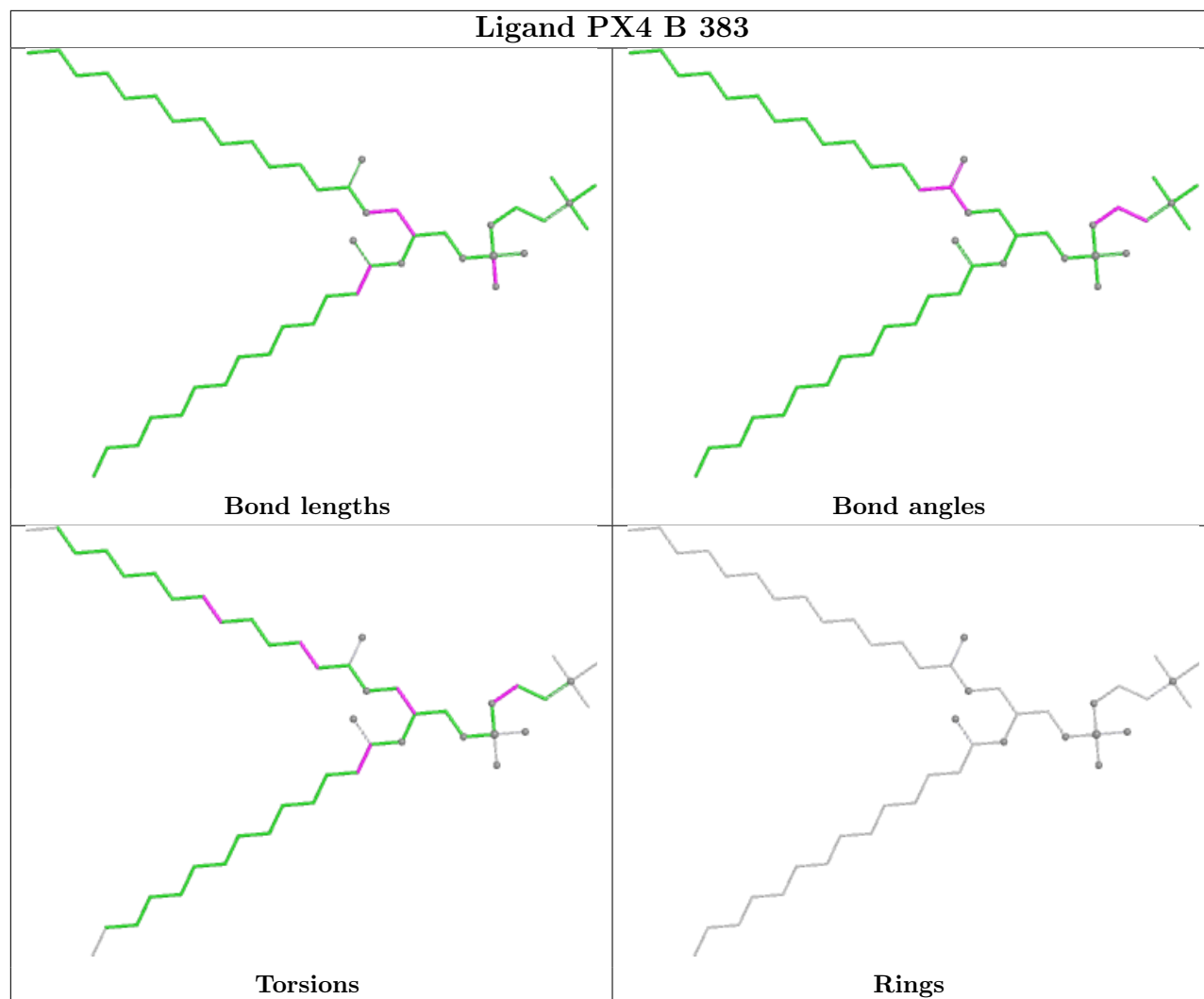
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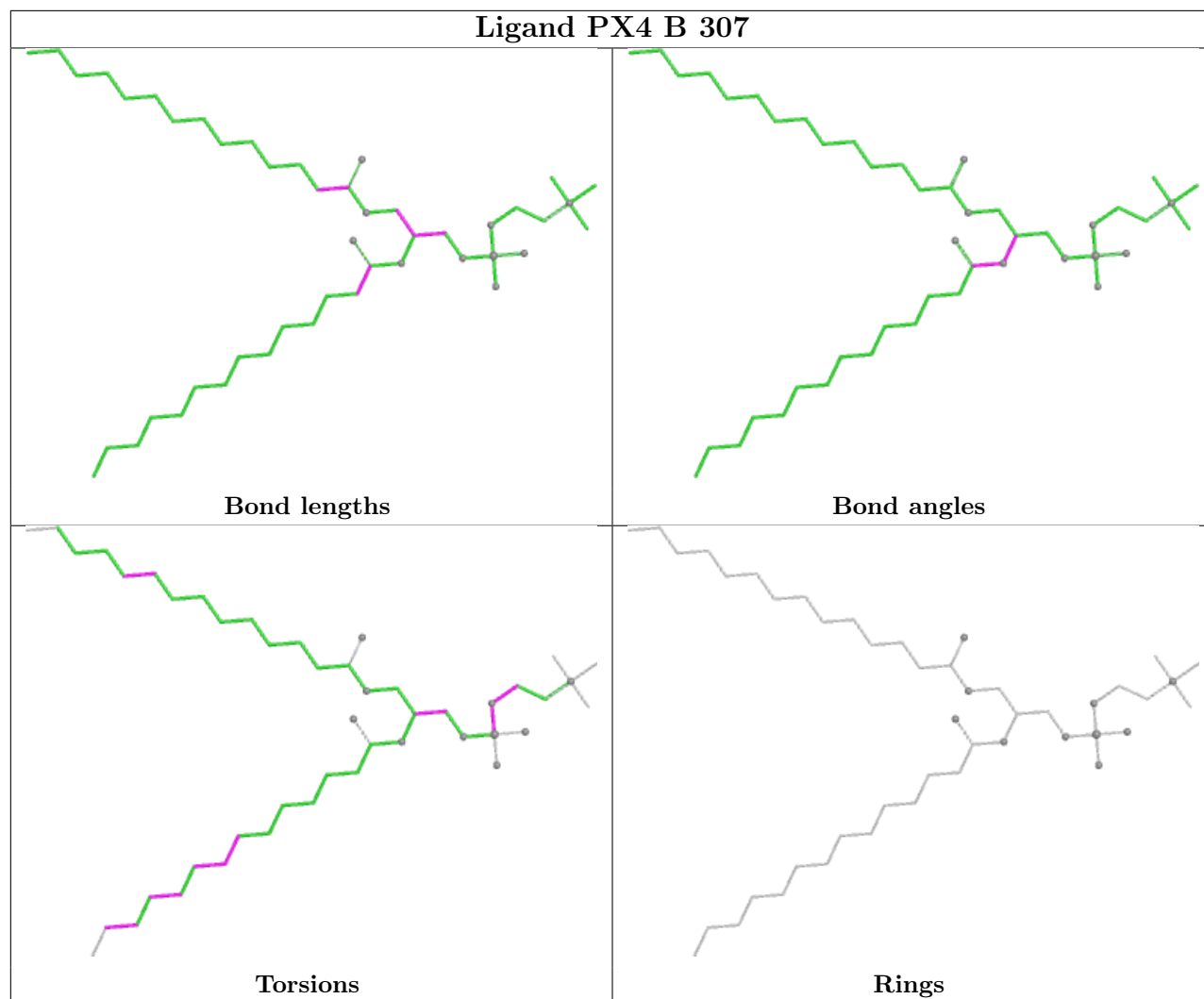
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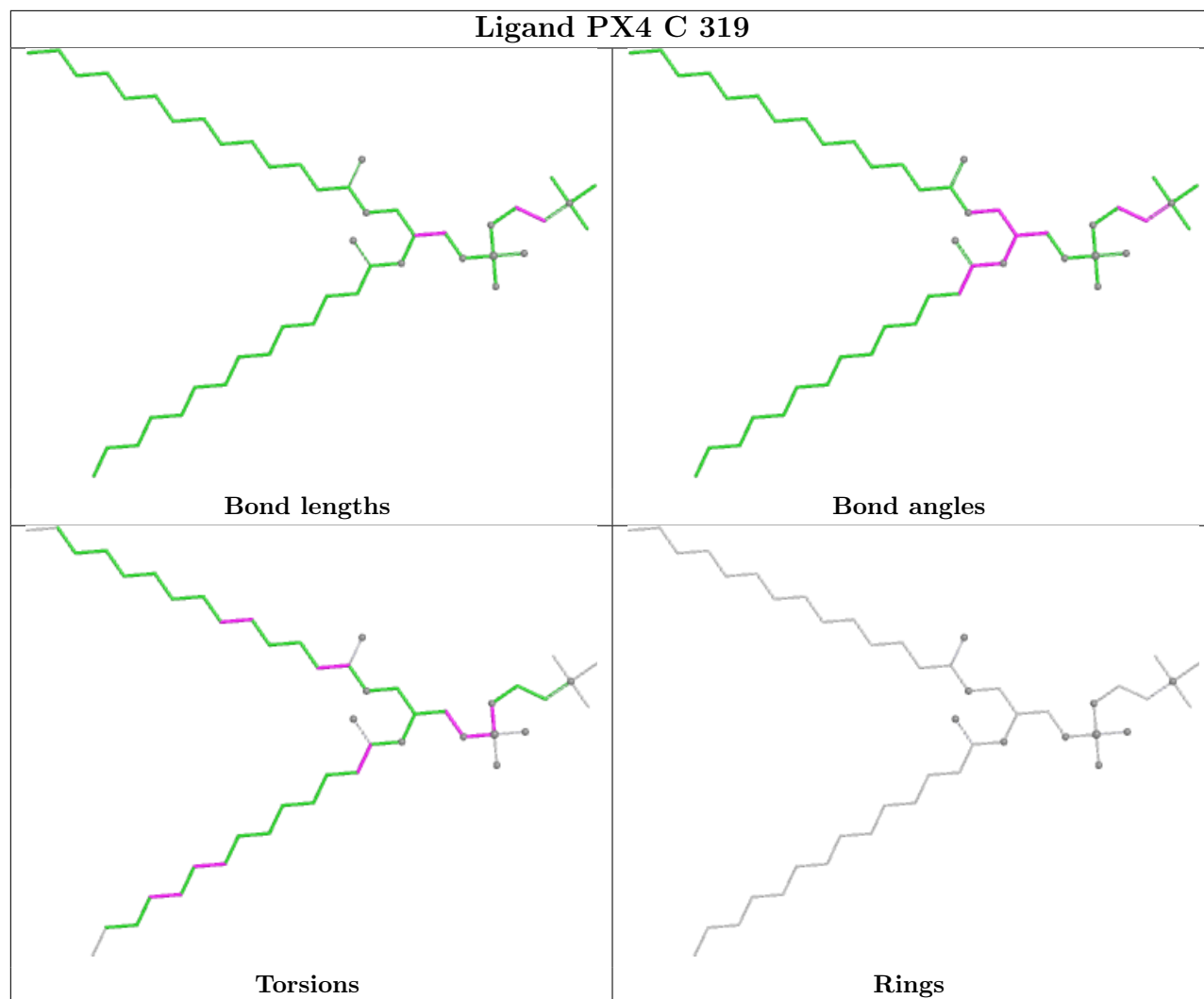
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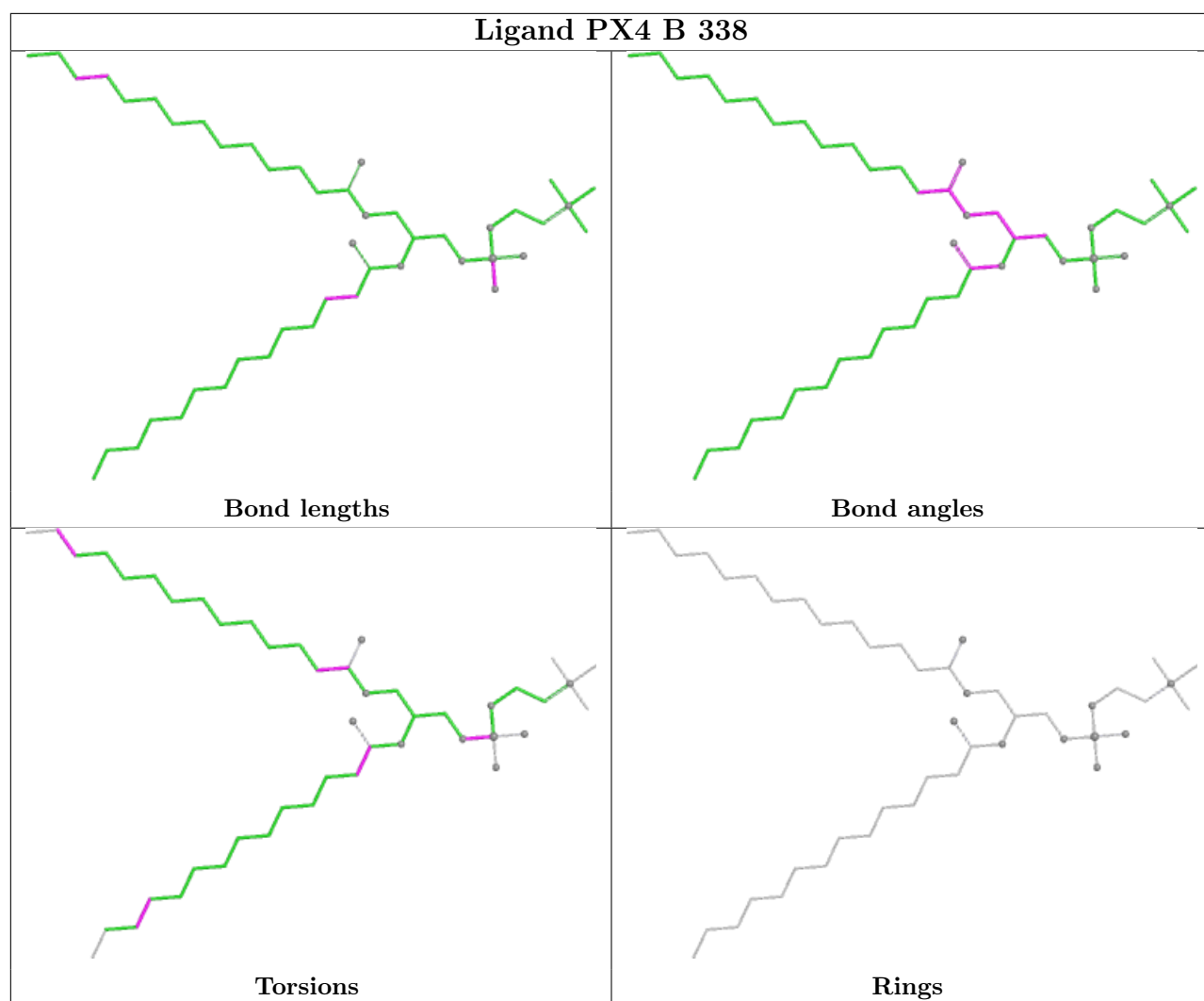


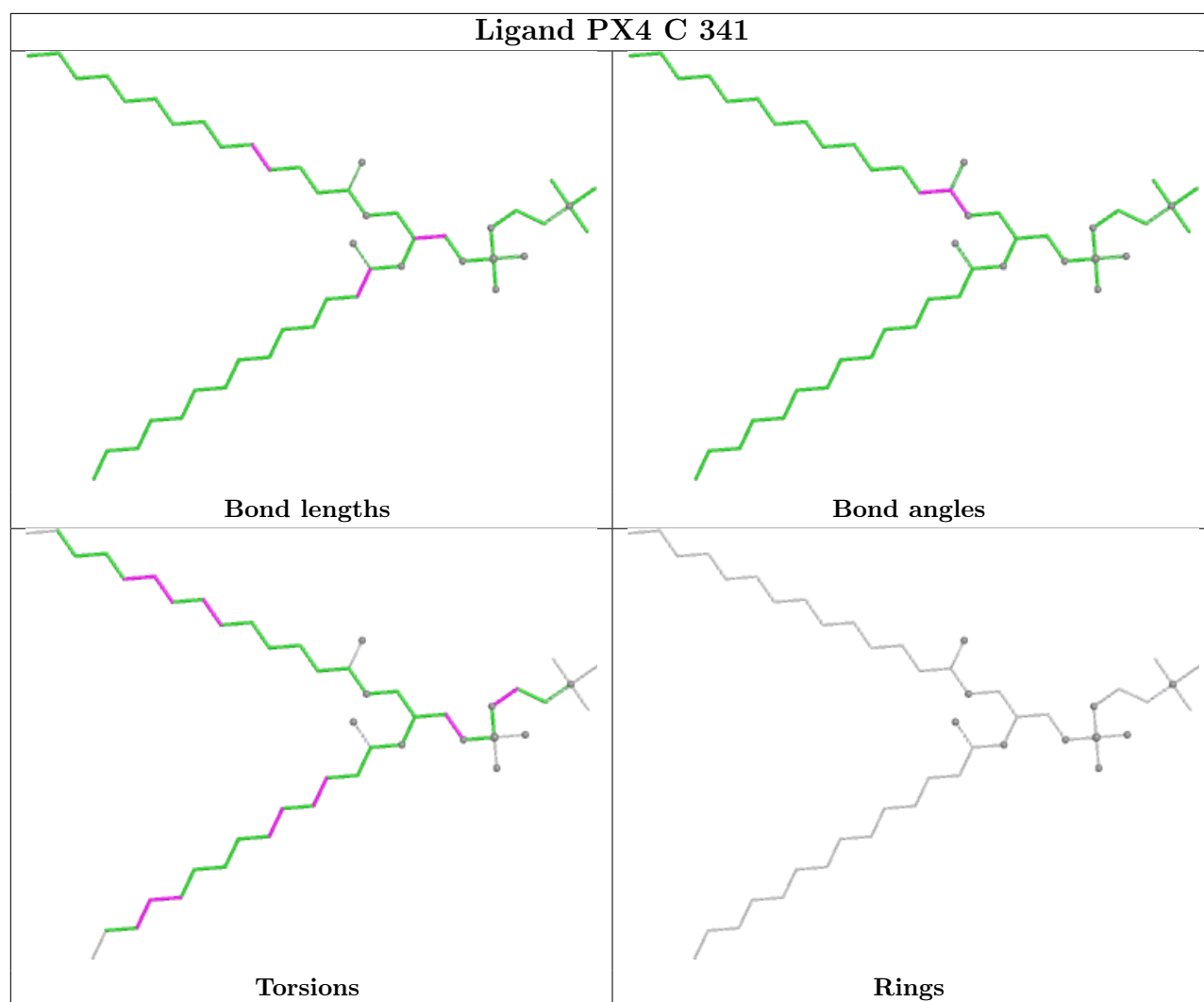
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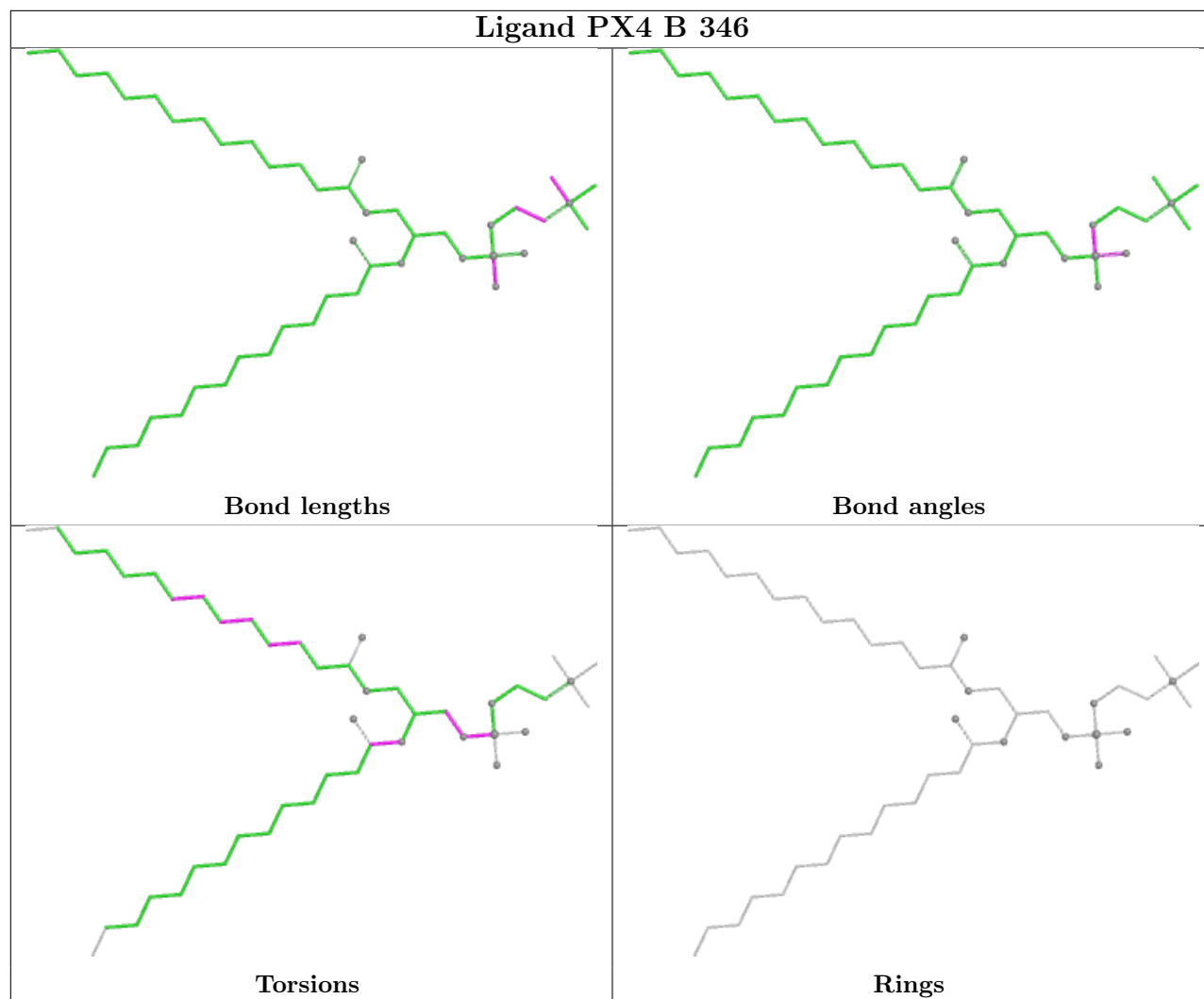
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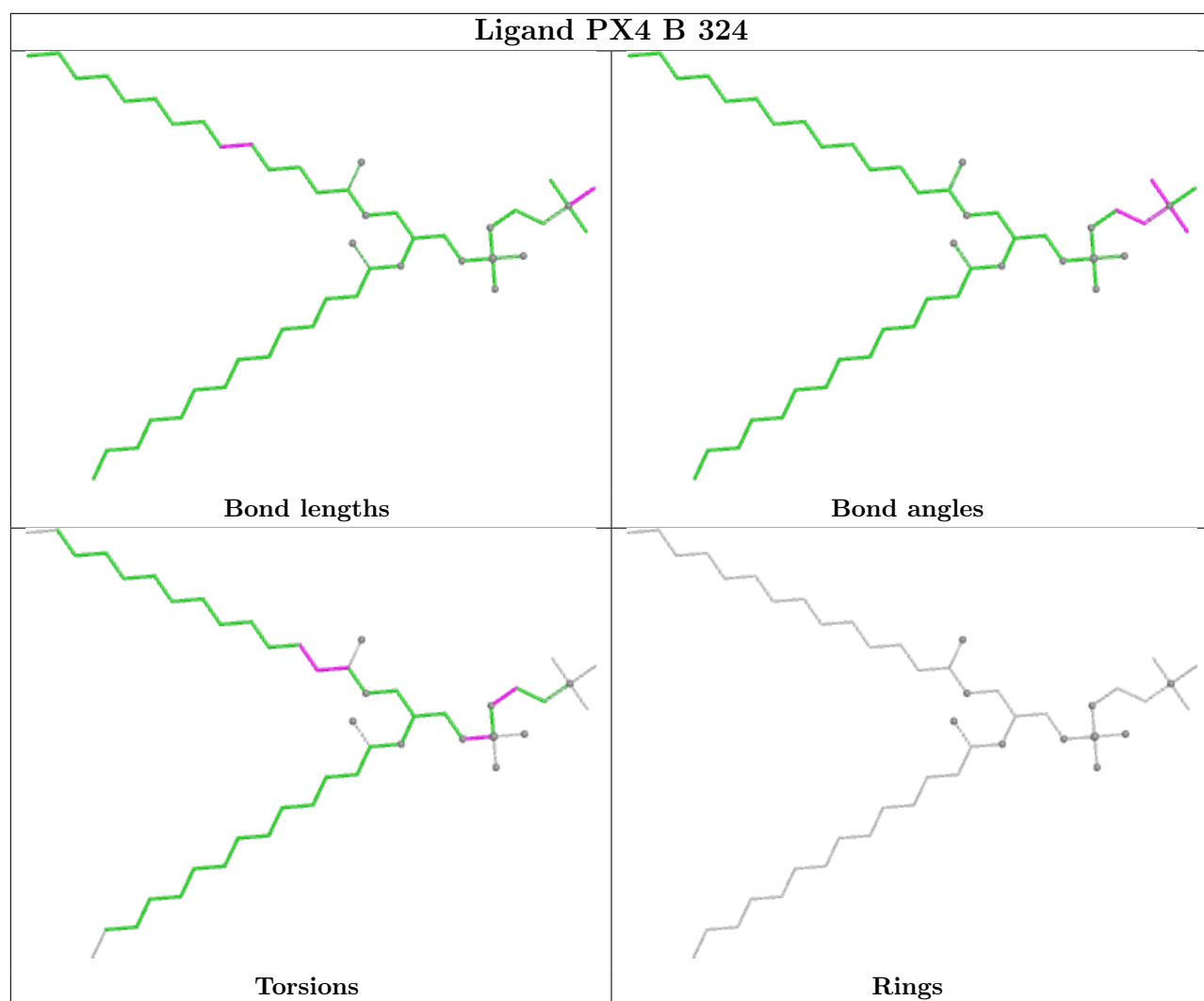




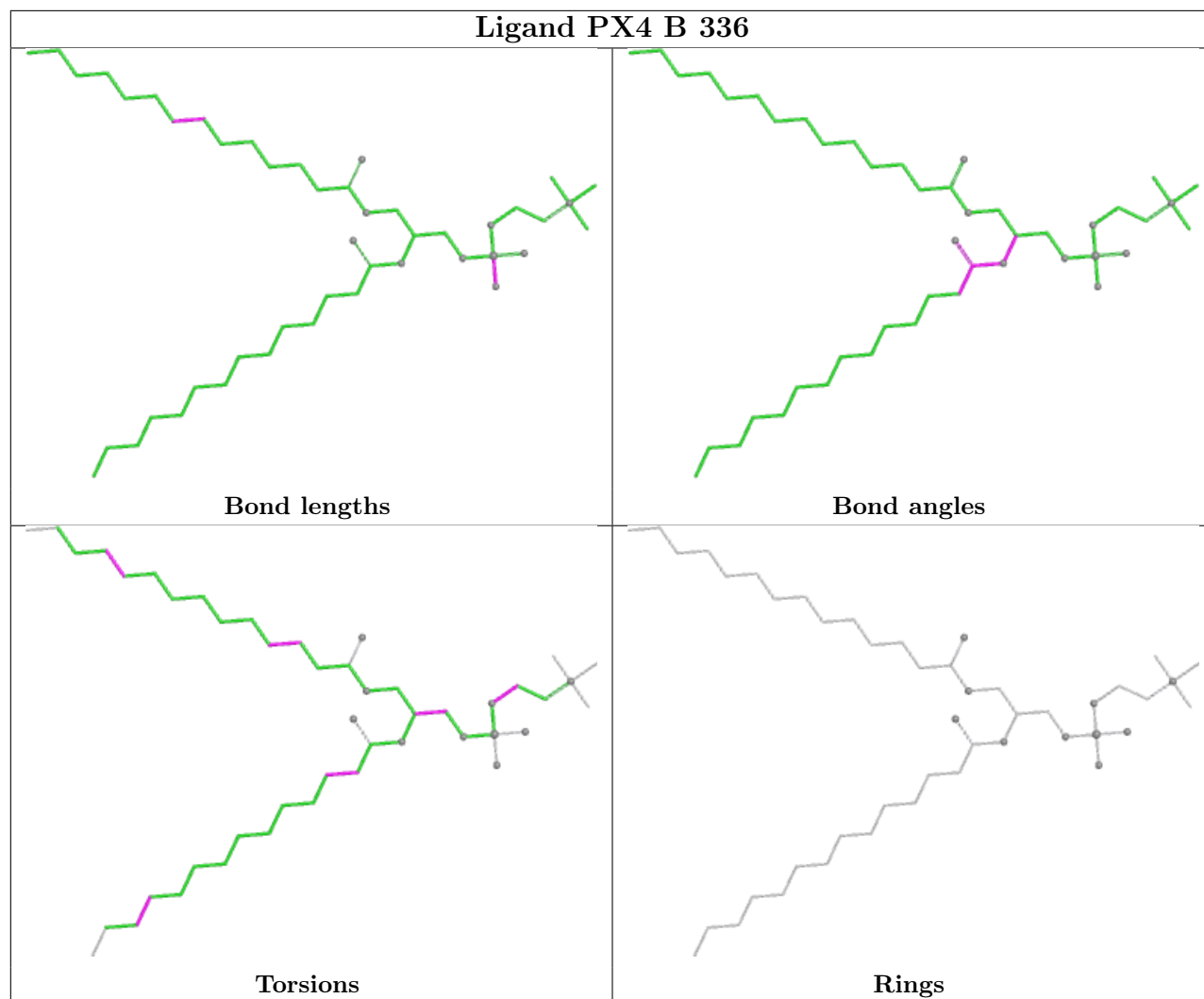


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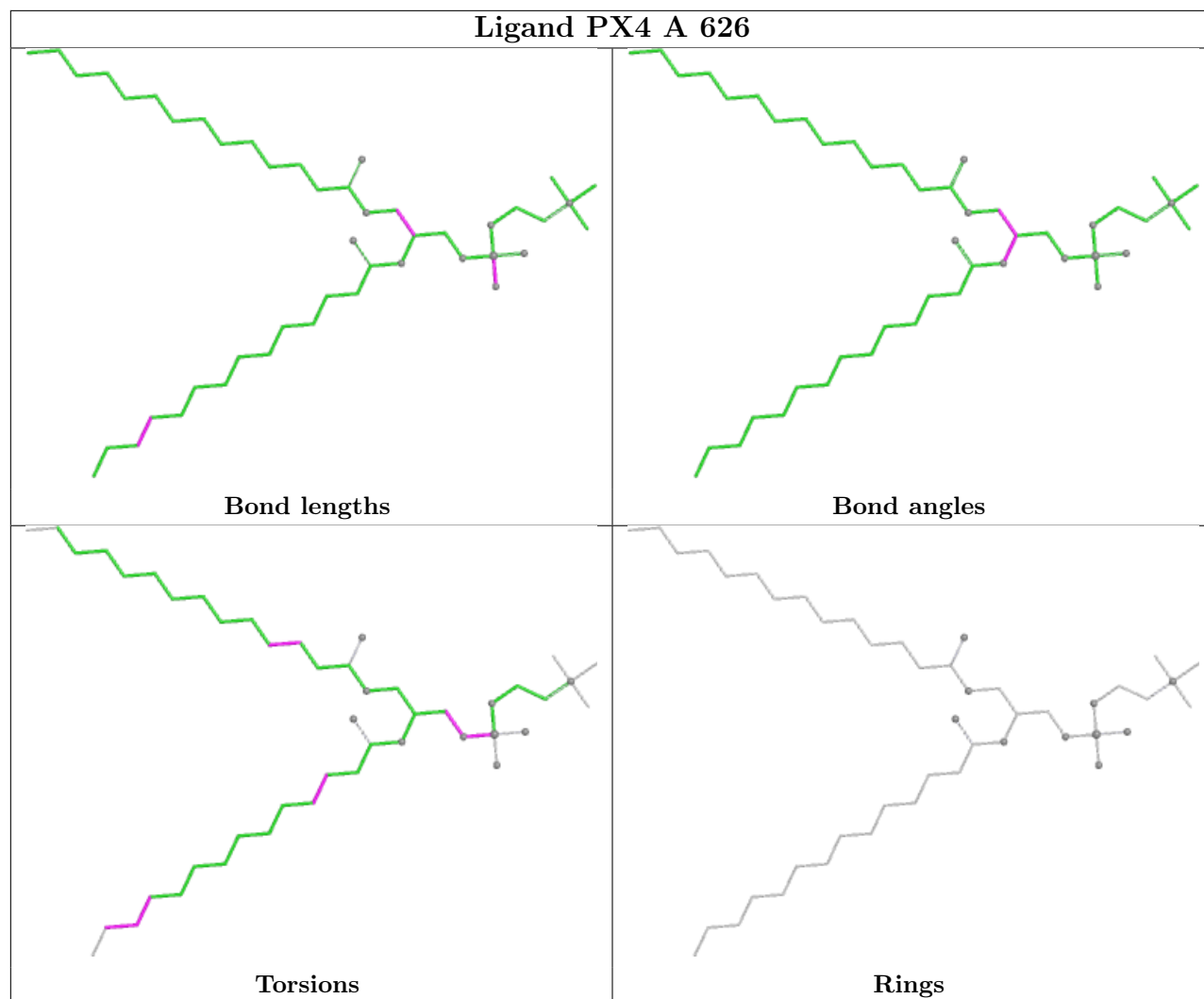


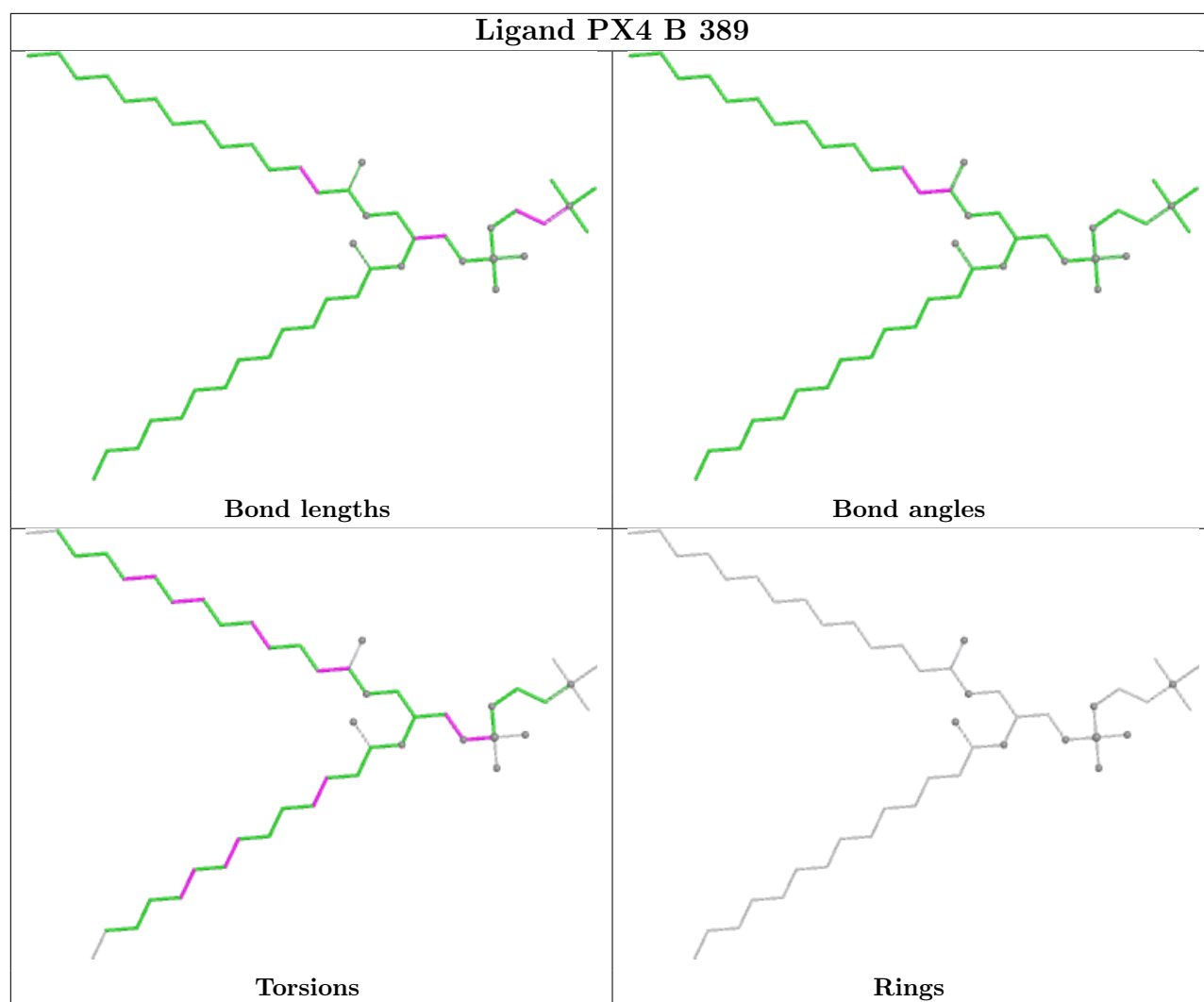


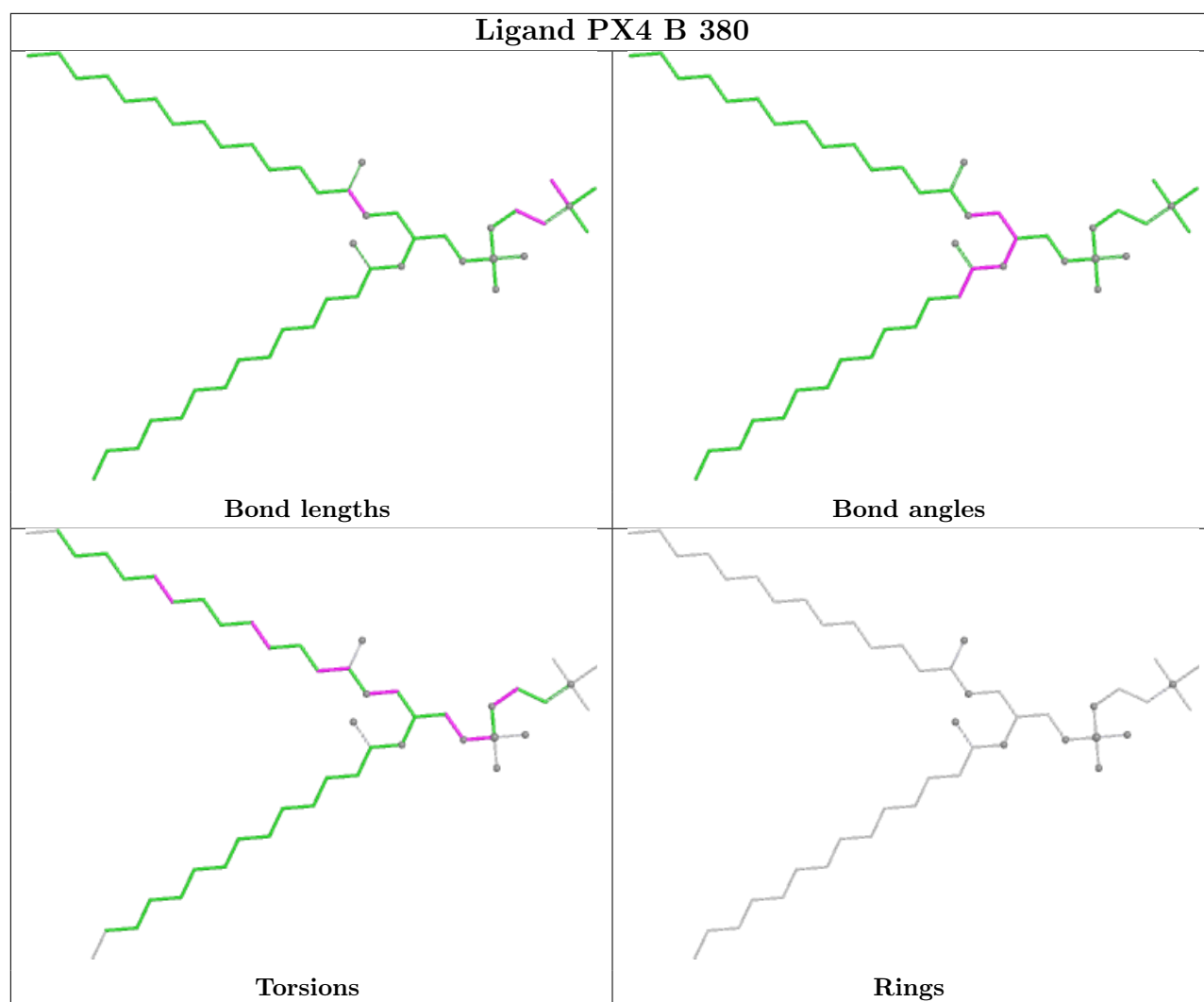
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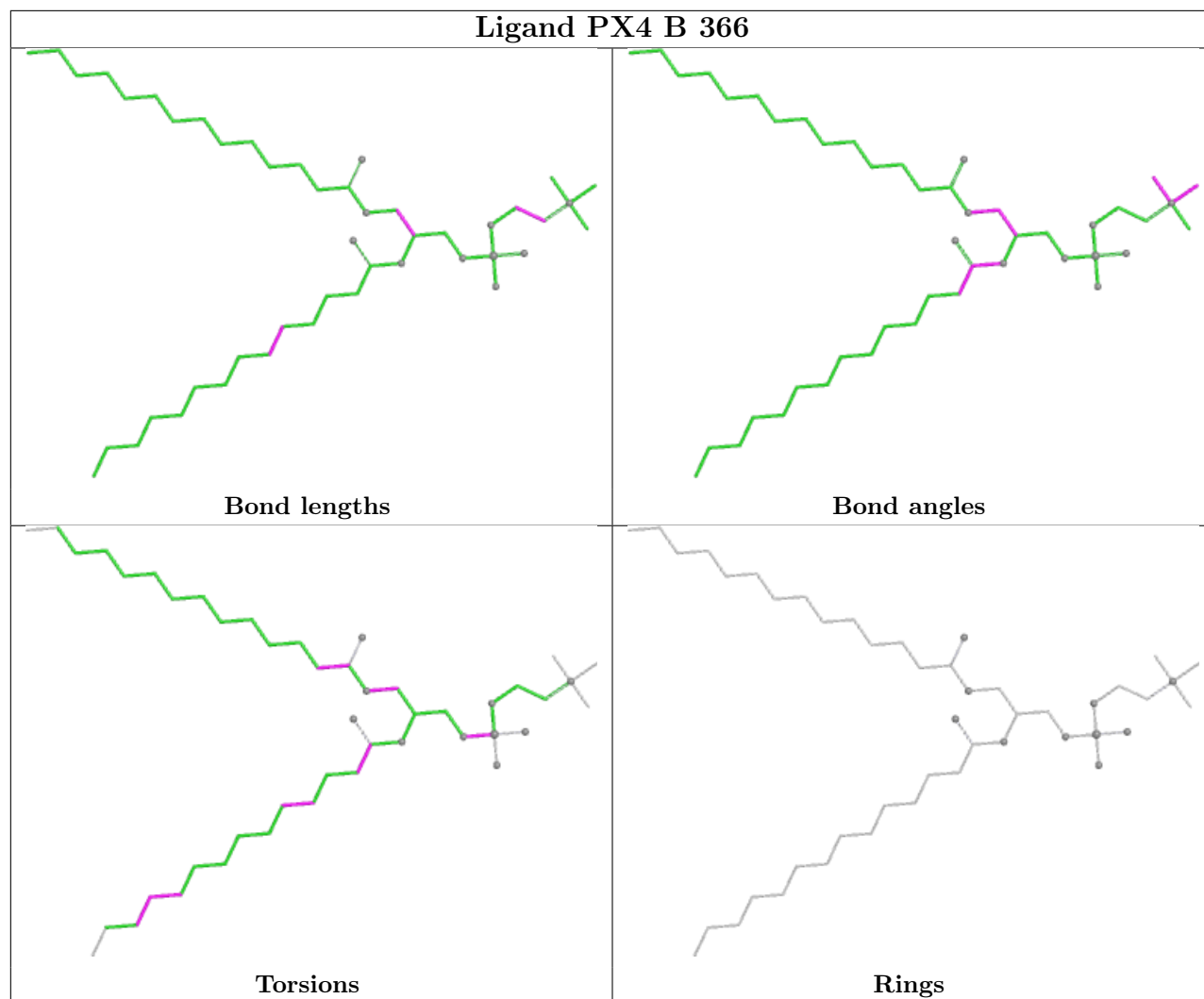
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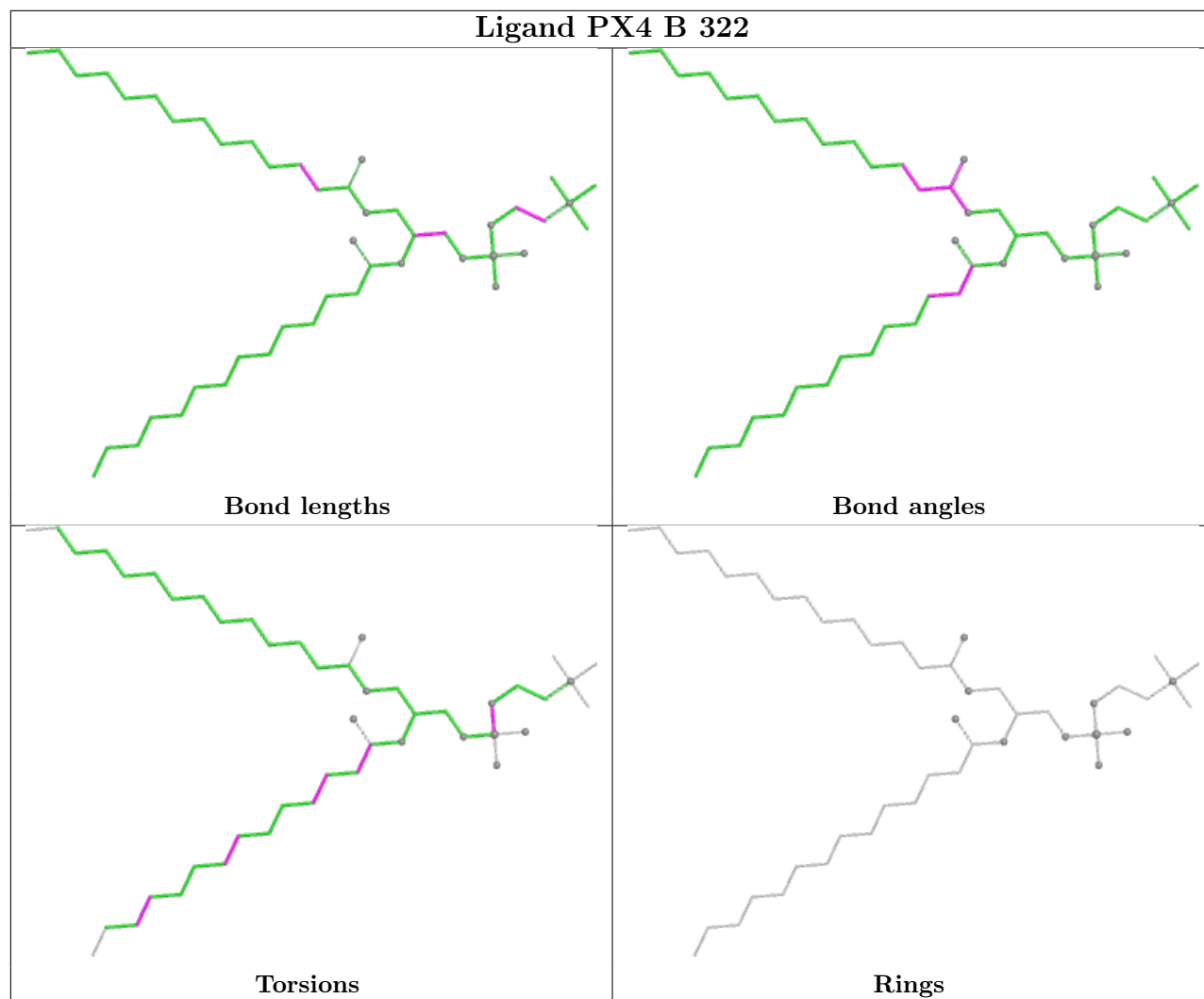


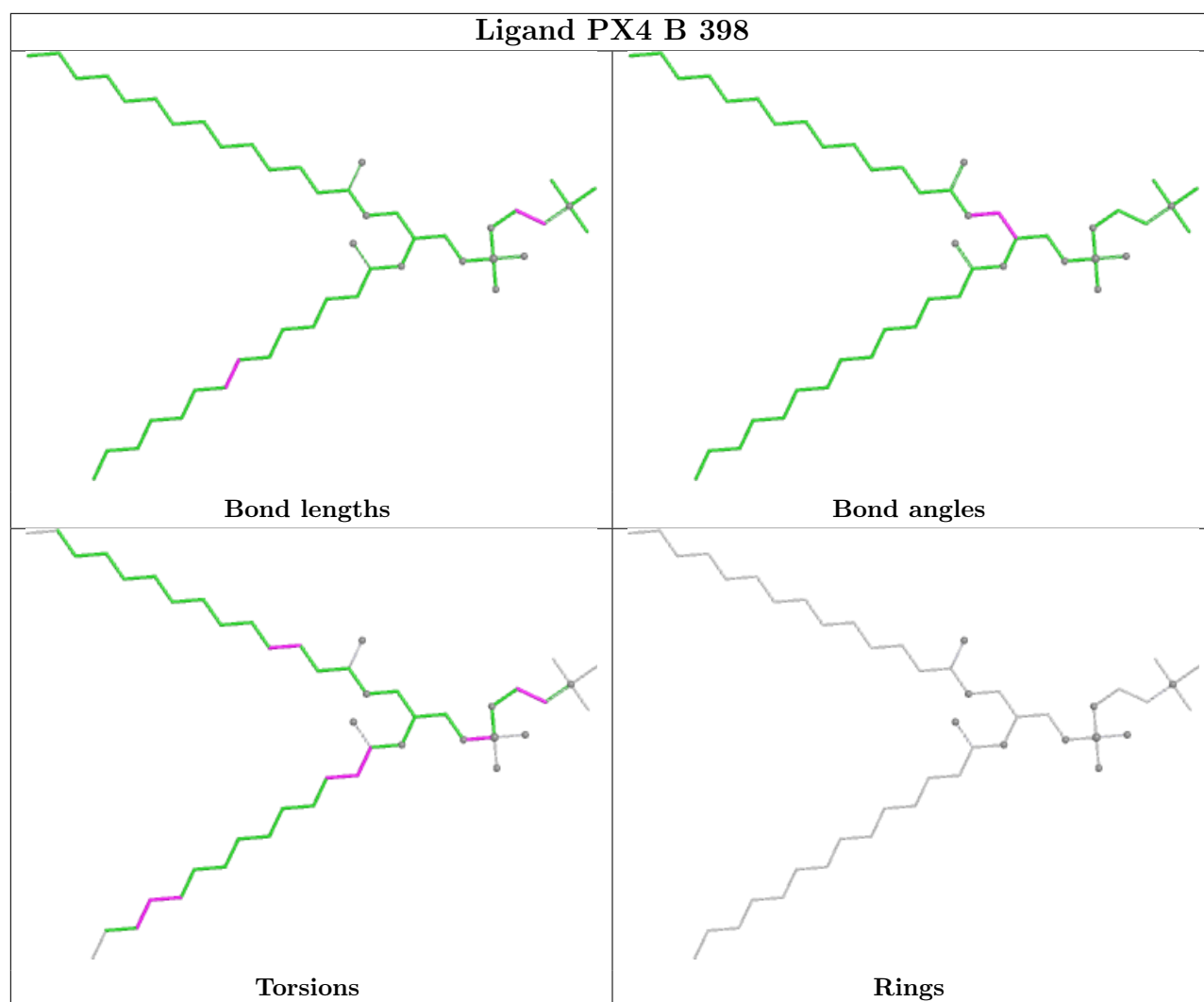


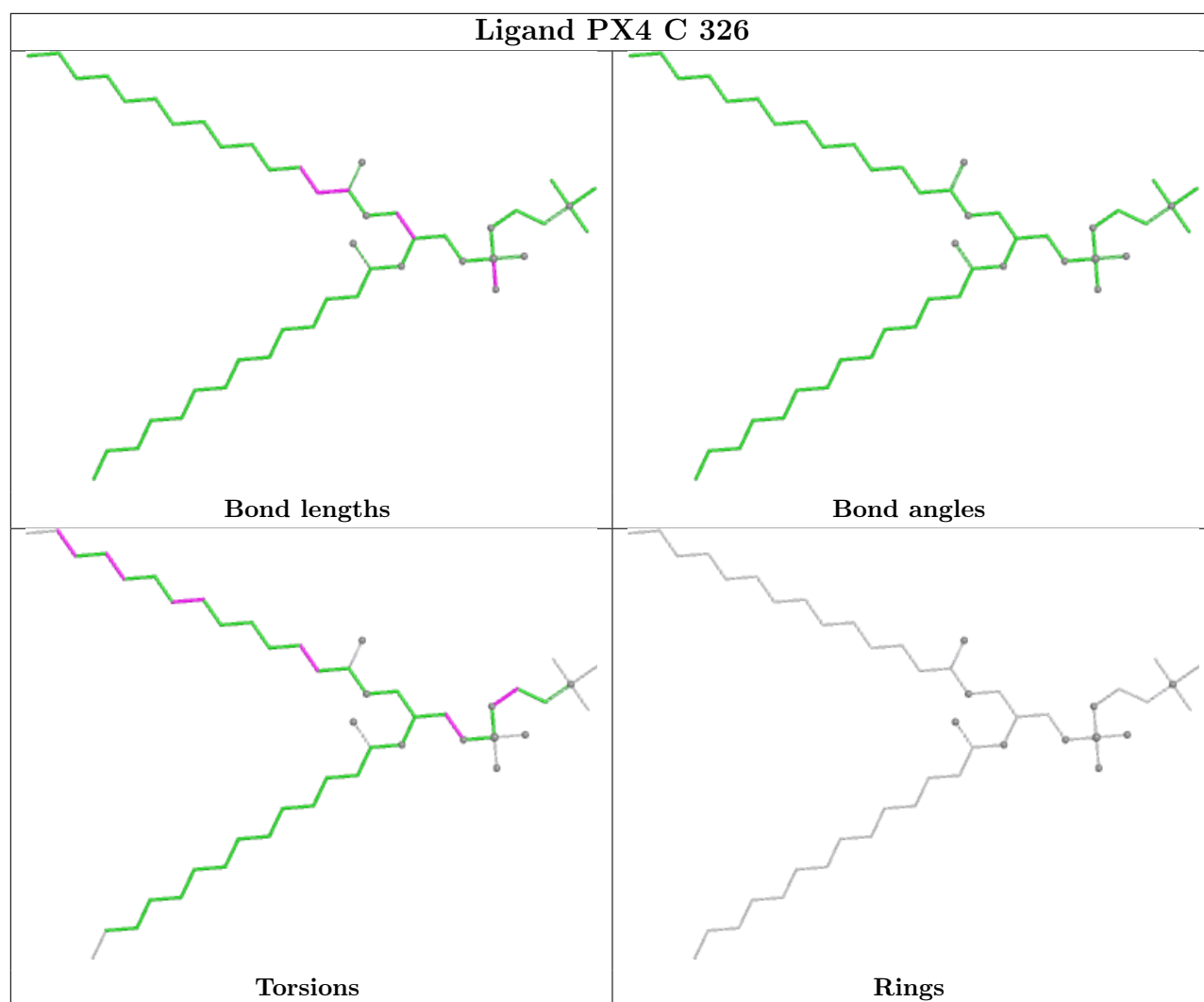
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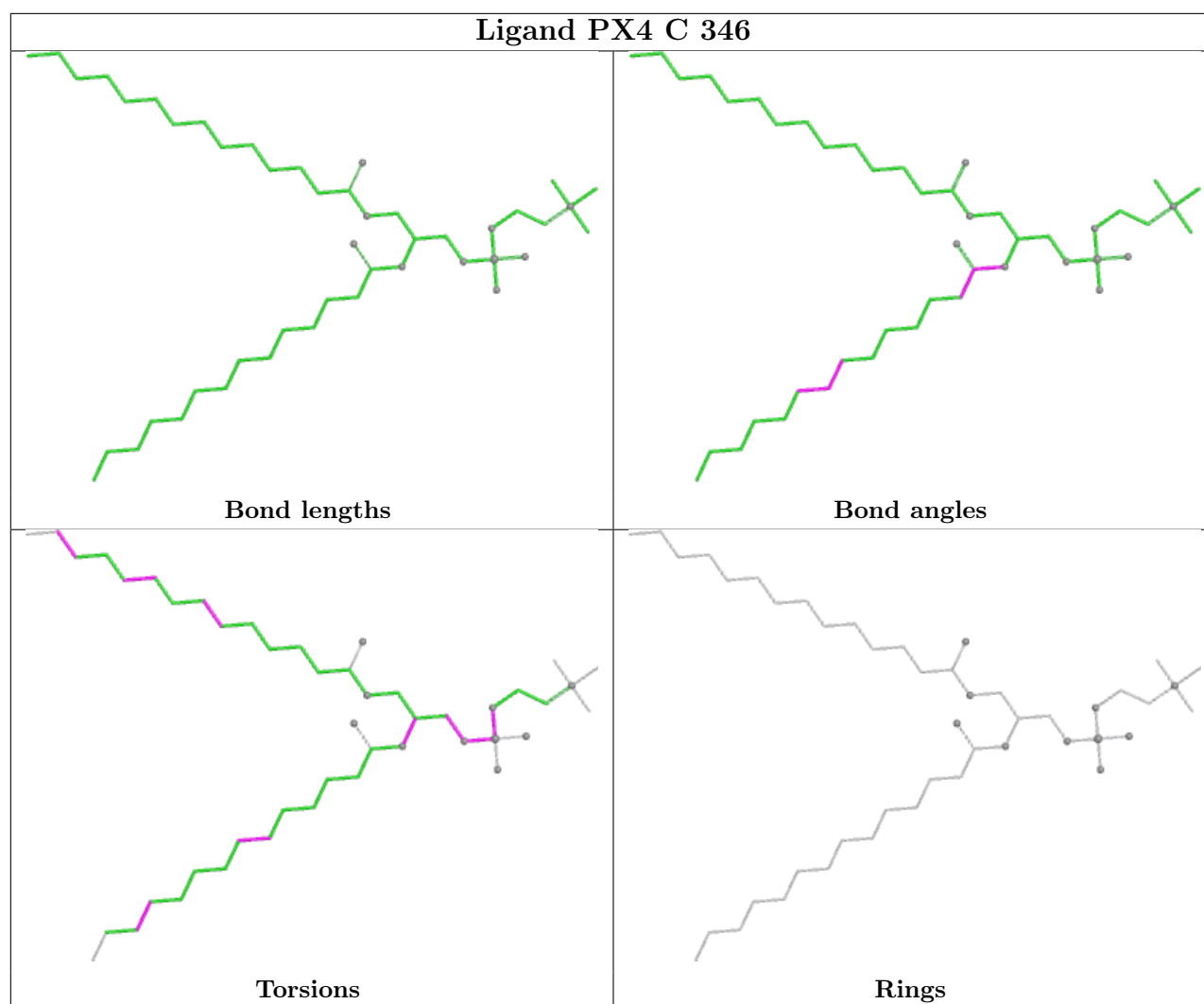


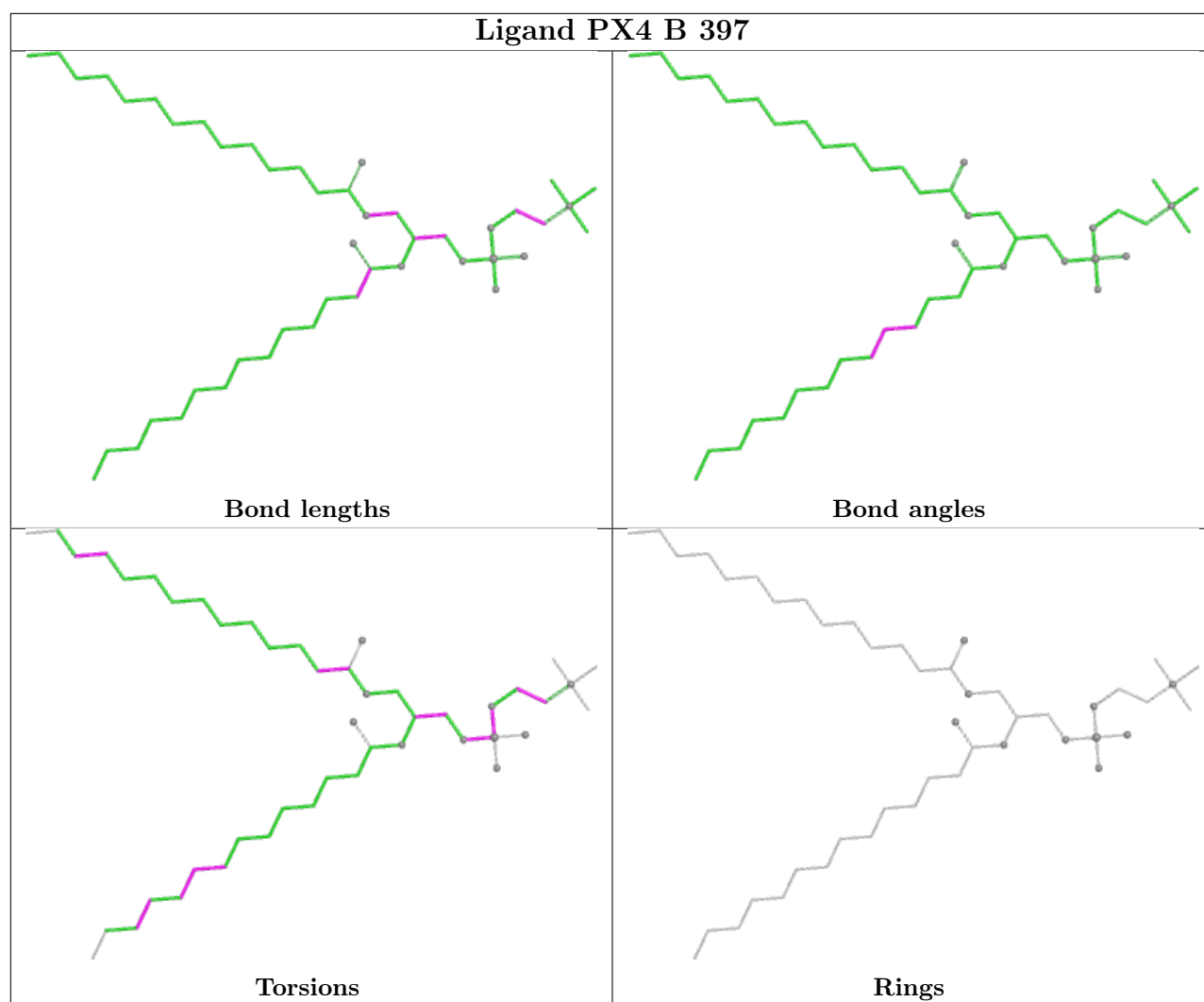
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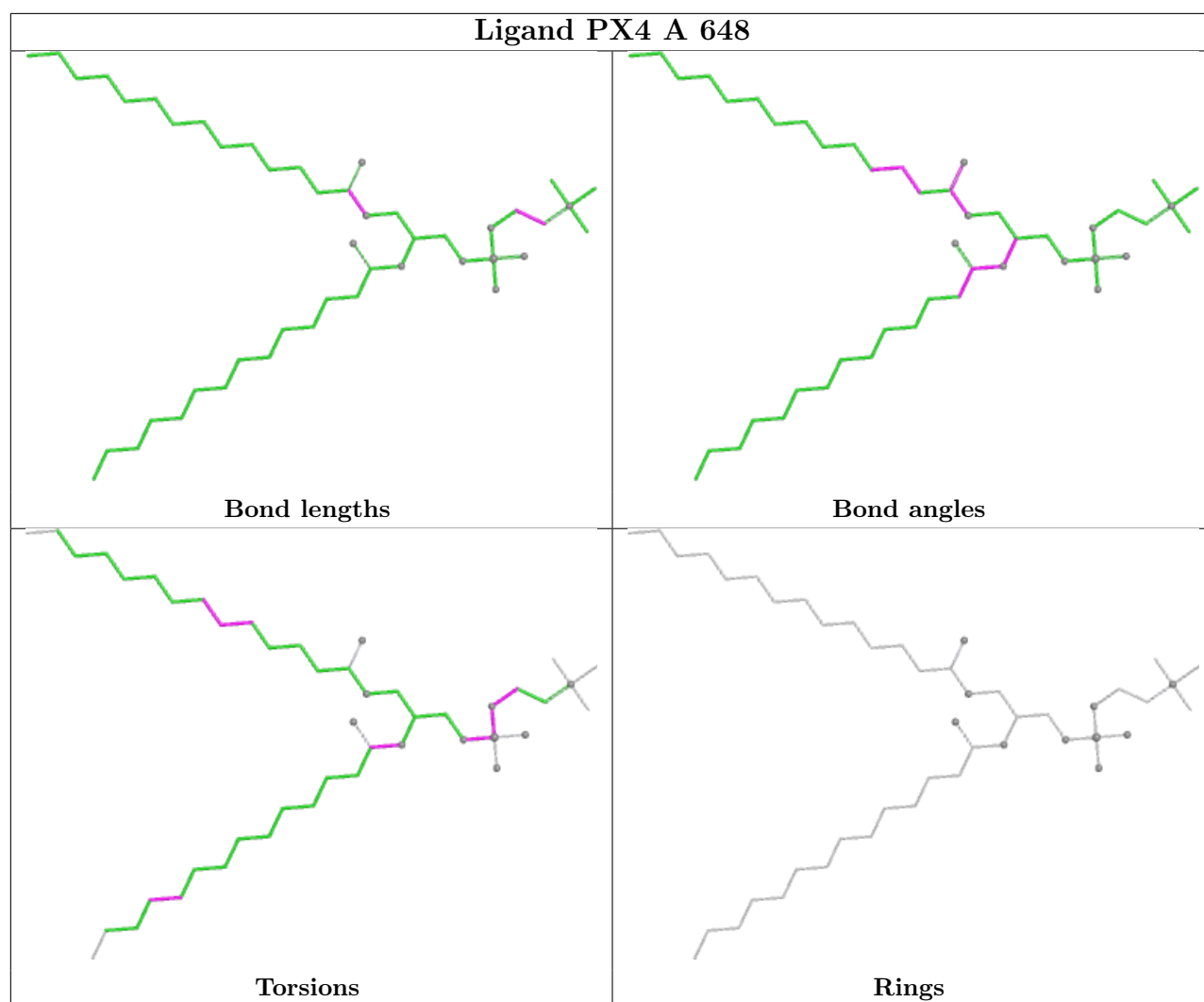


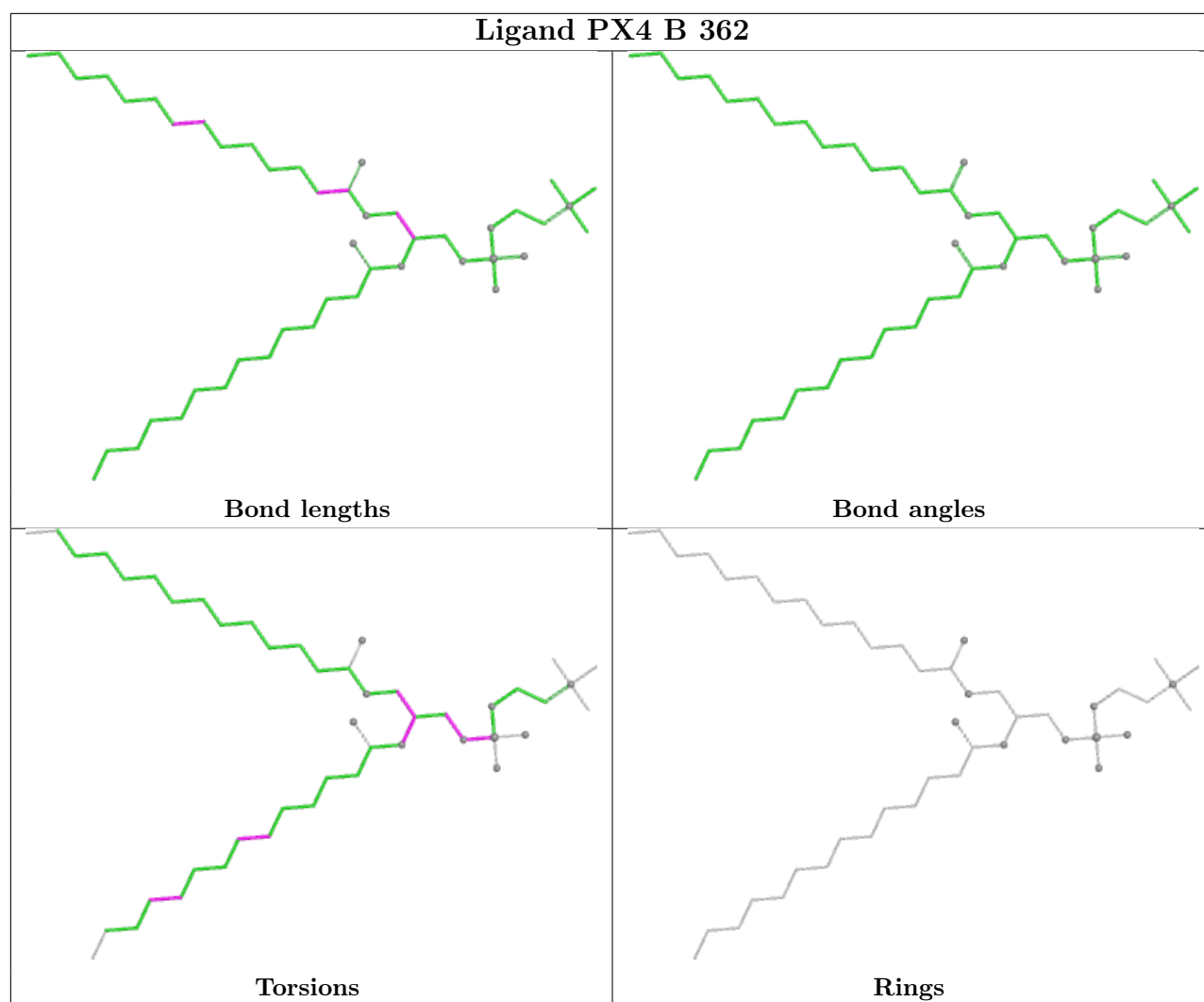


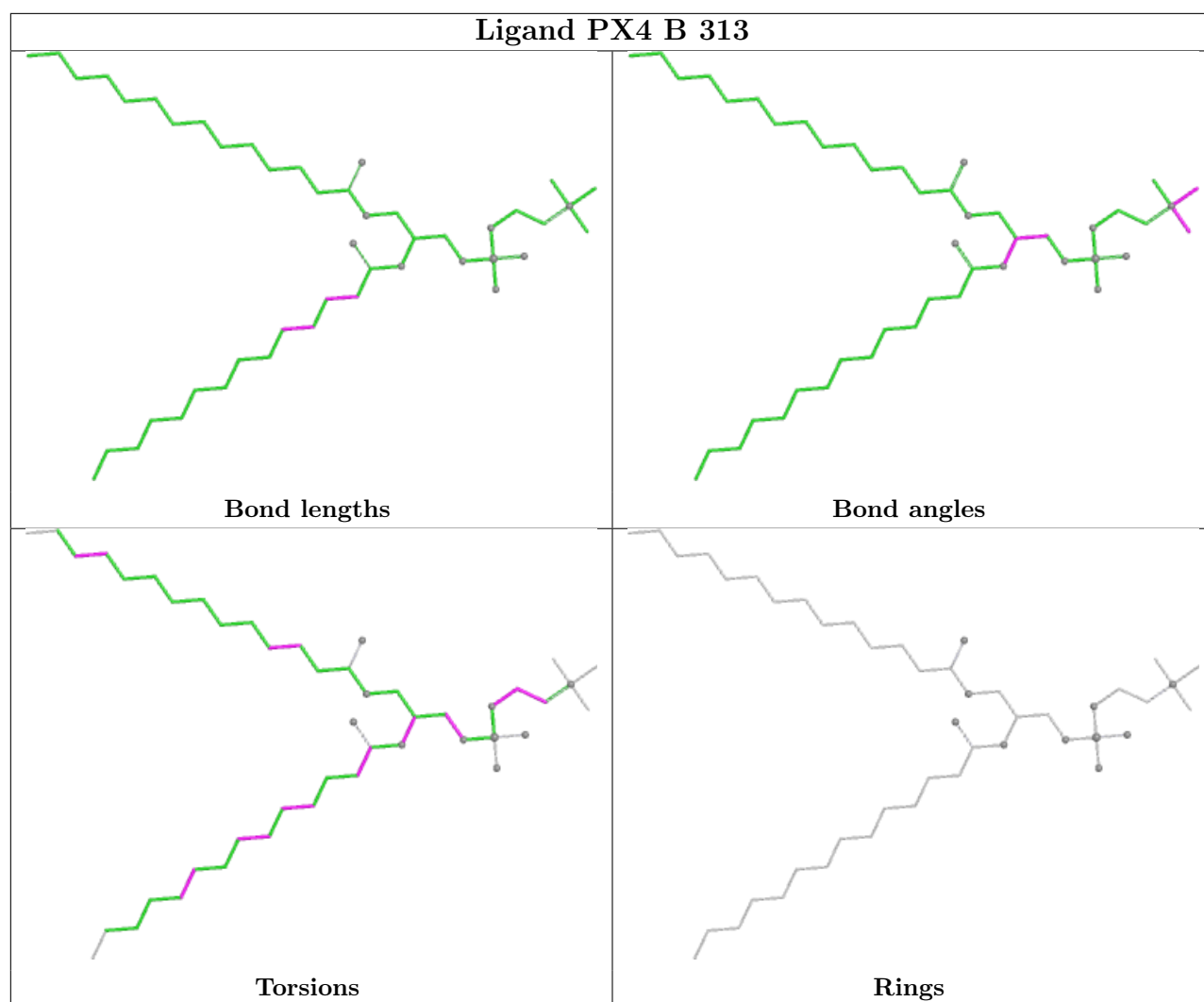




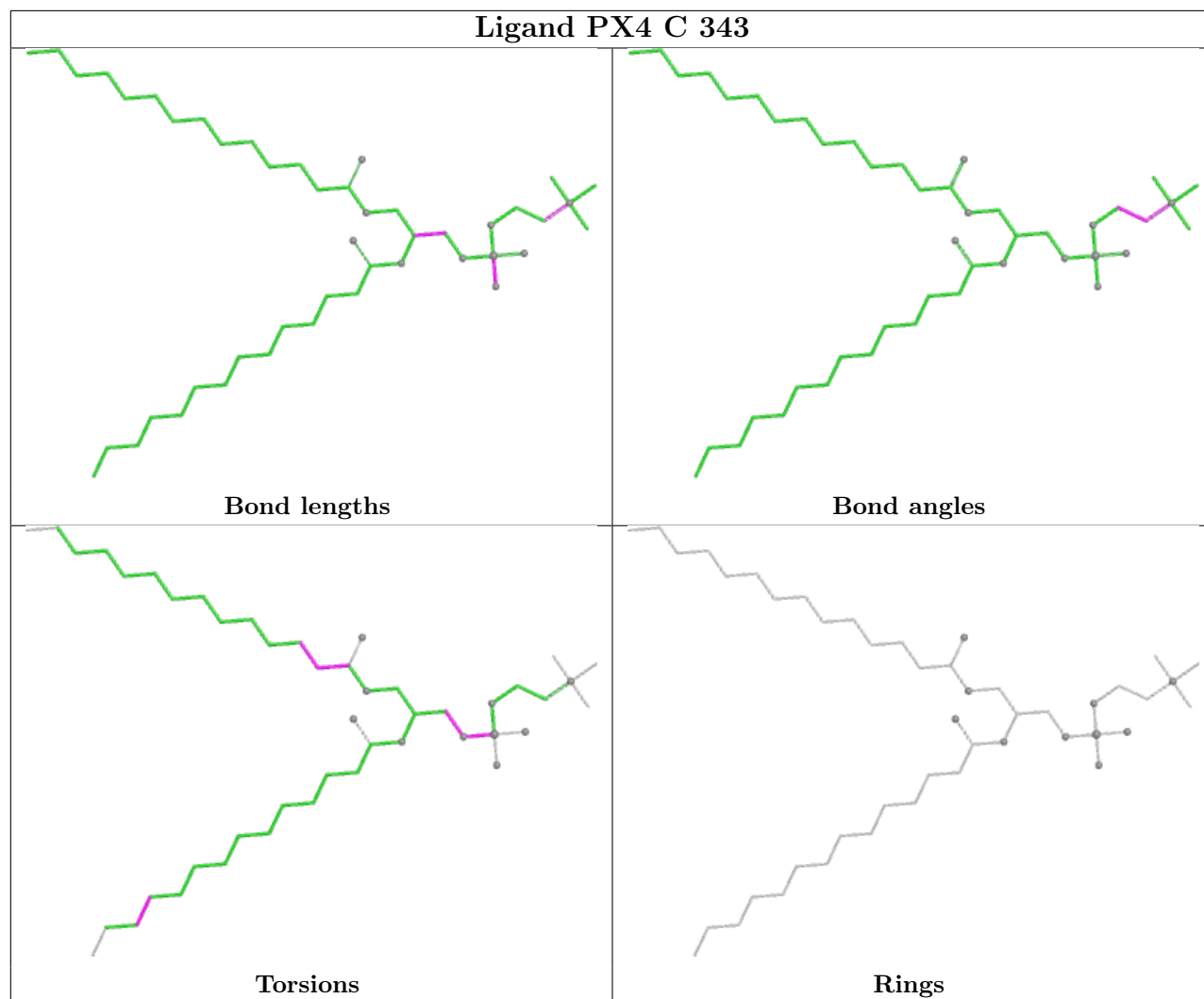


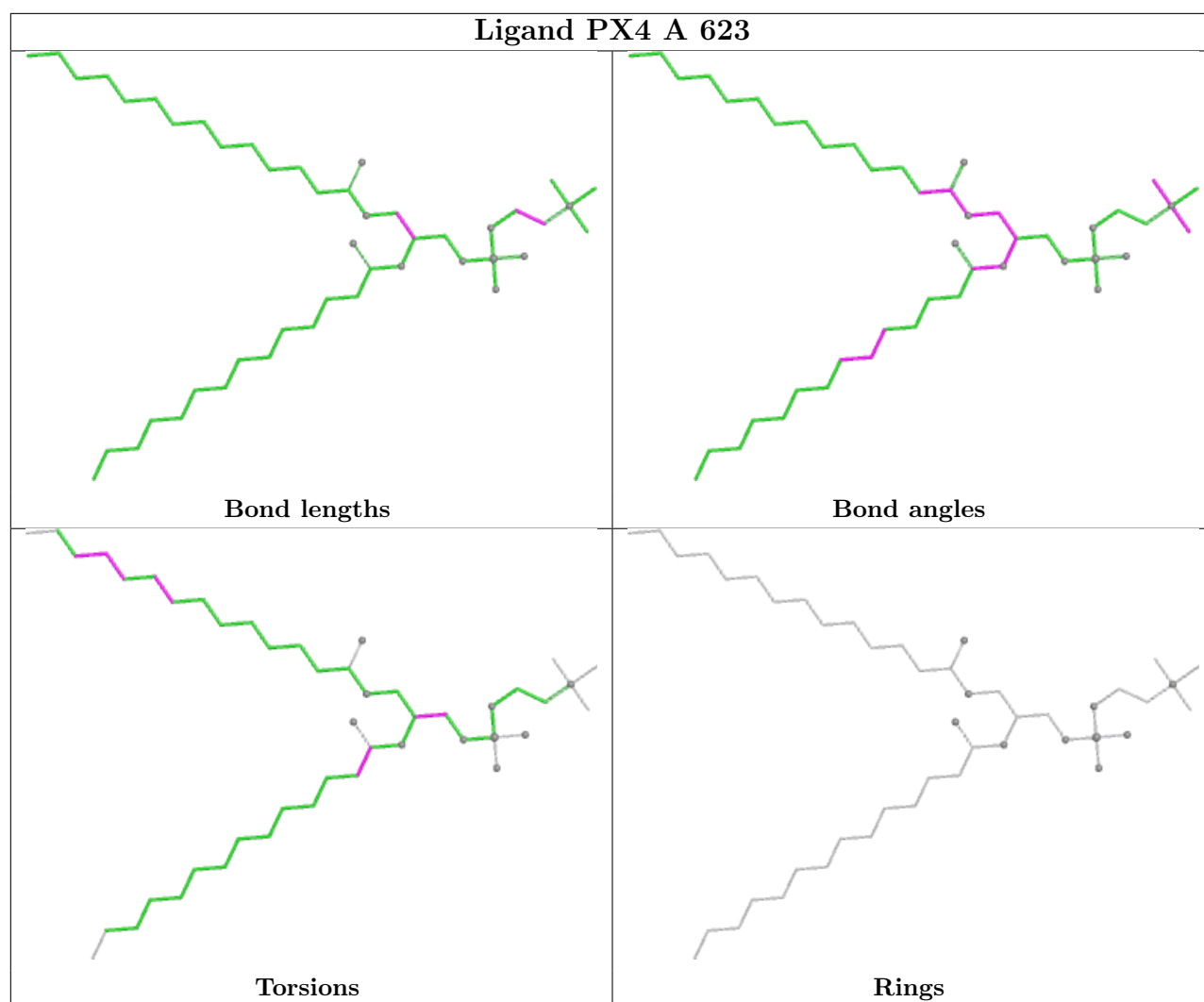


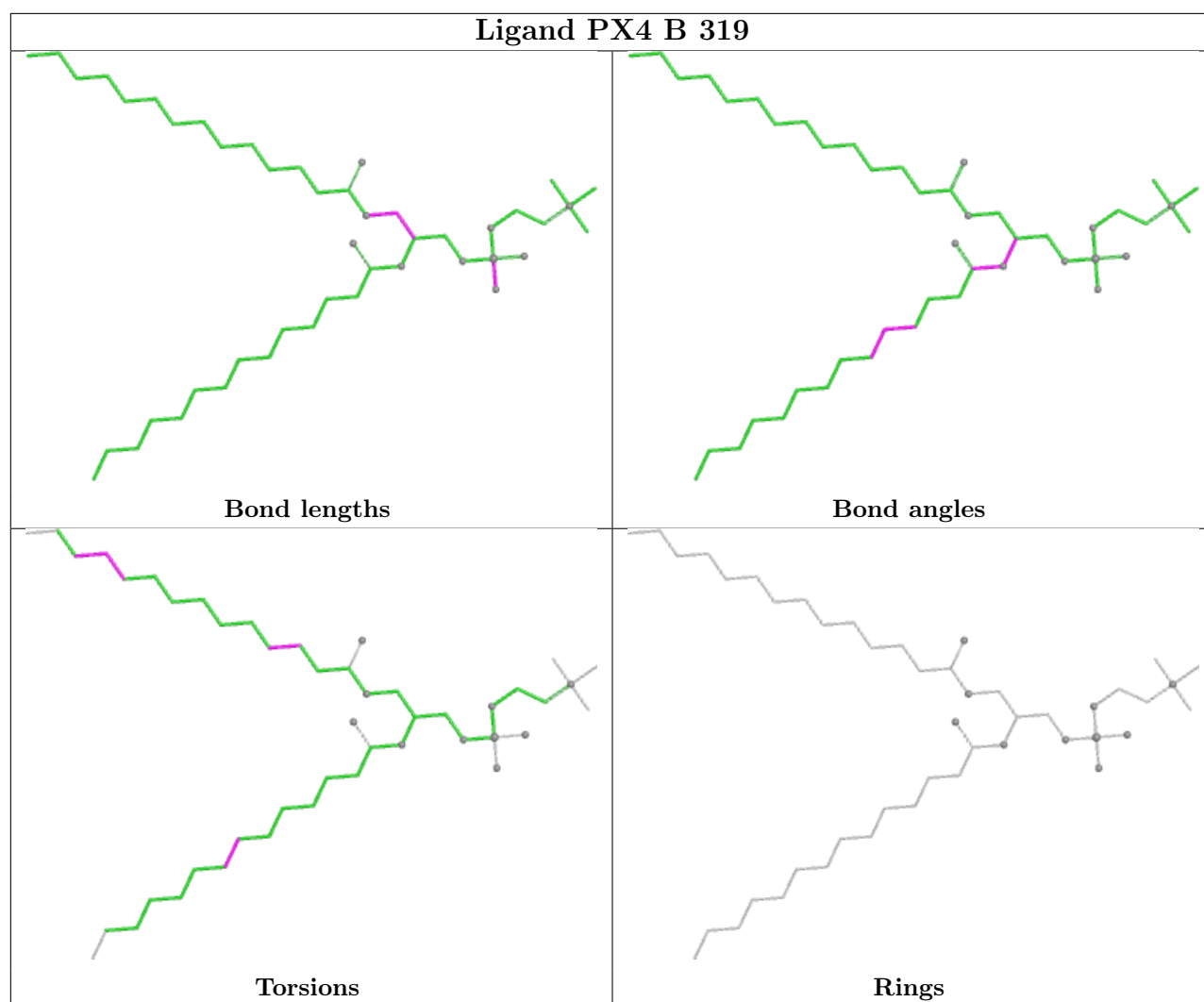




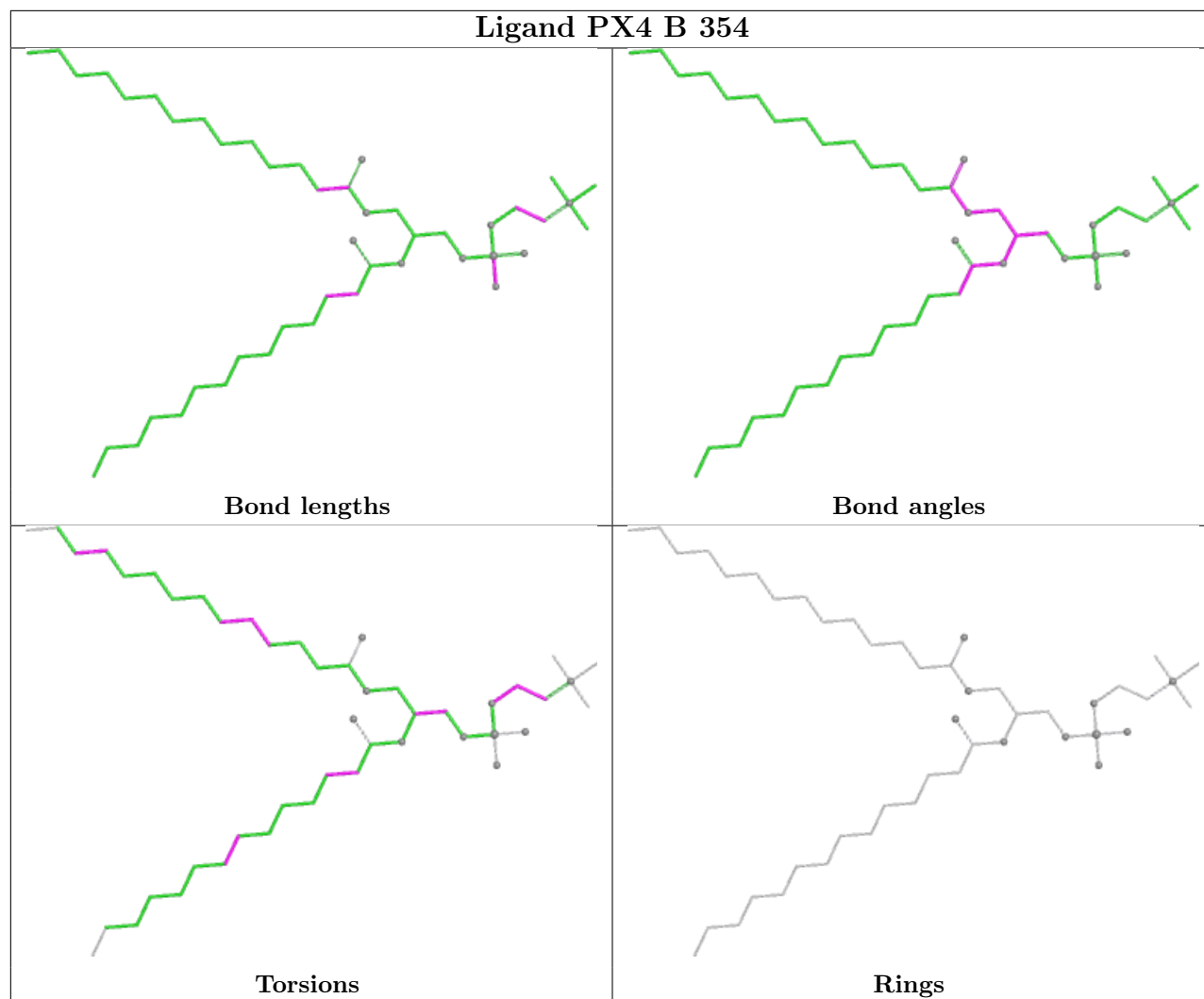
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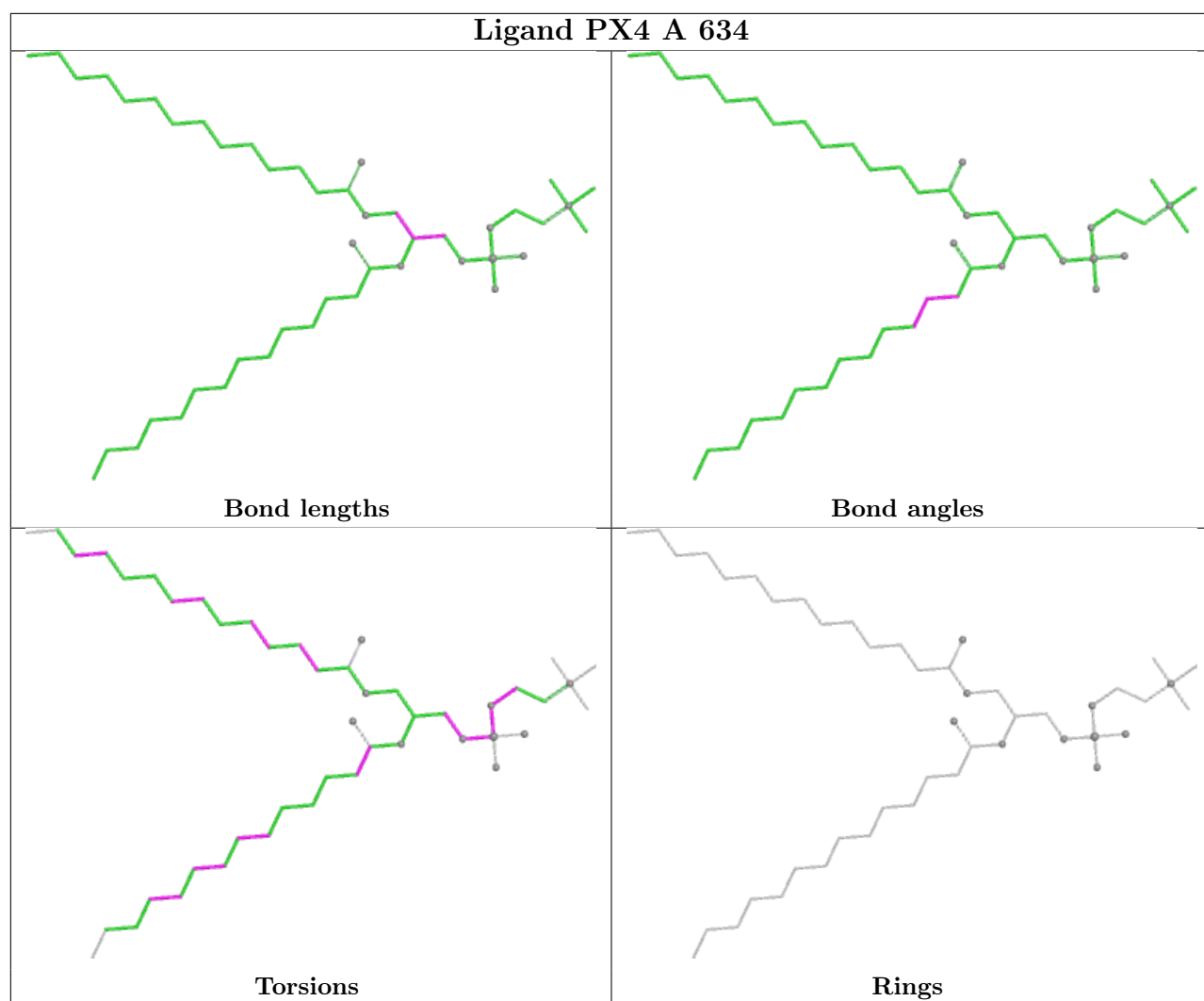




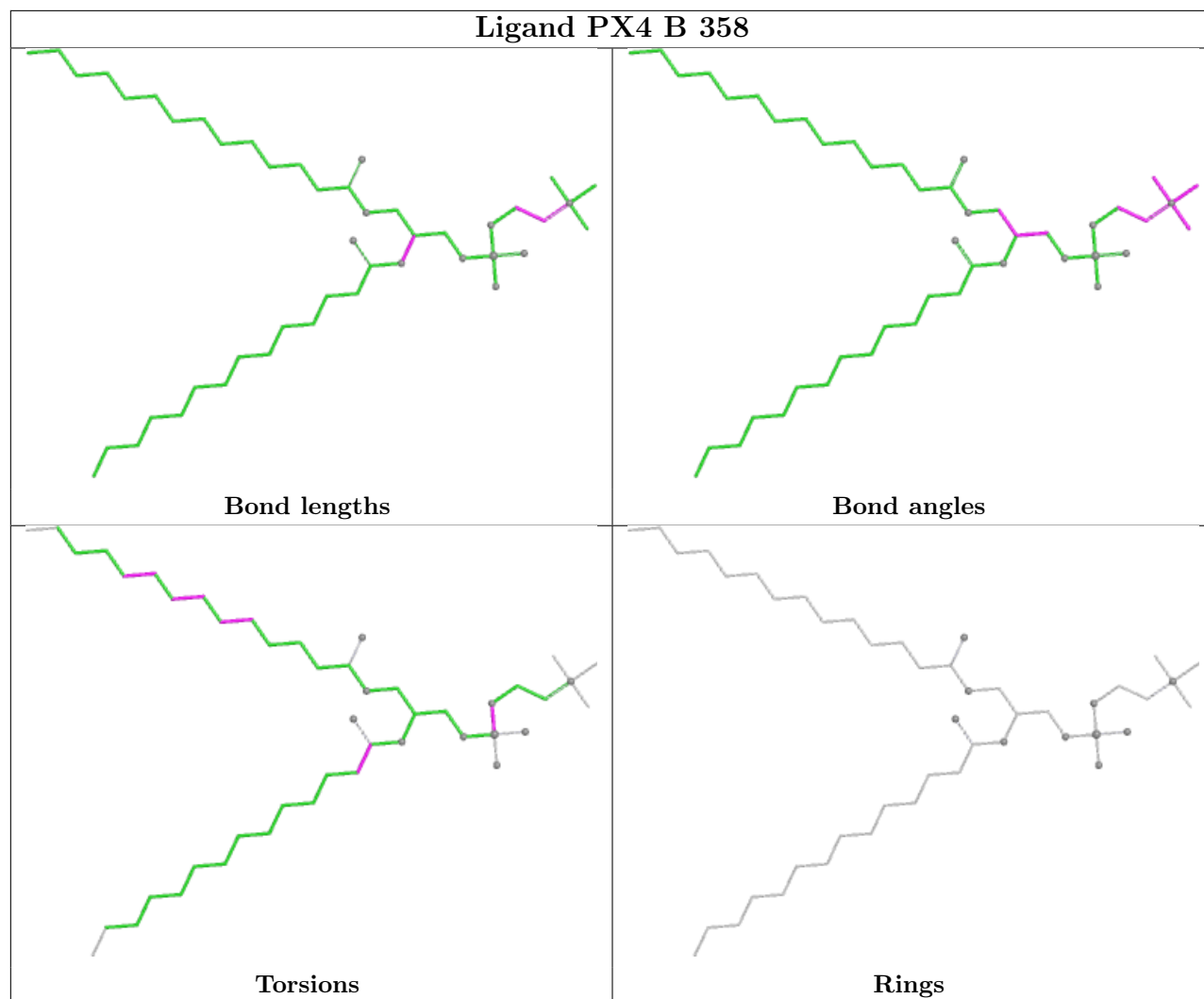


Ligand PX4 B 354

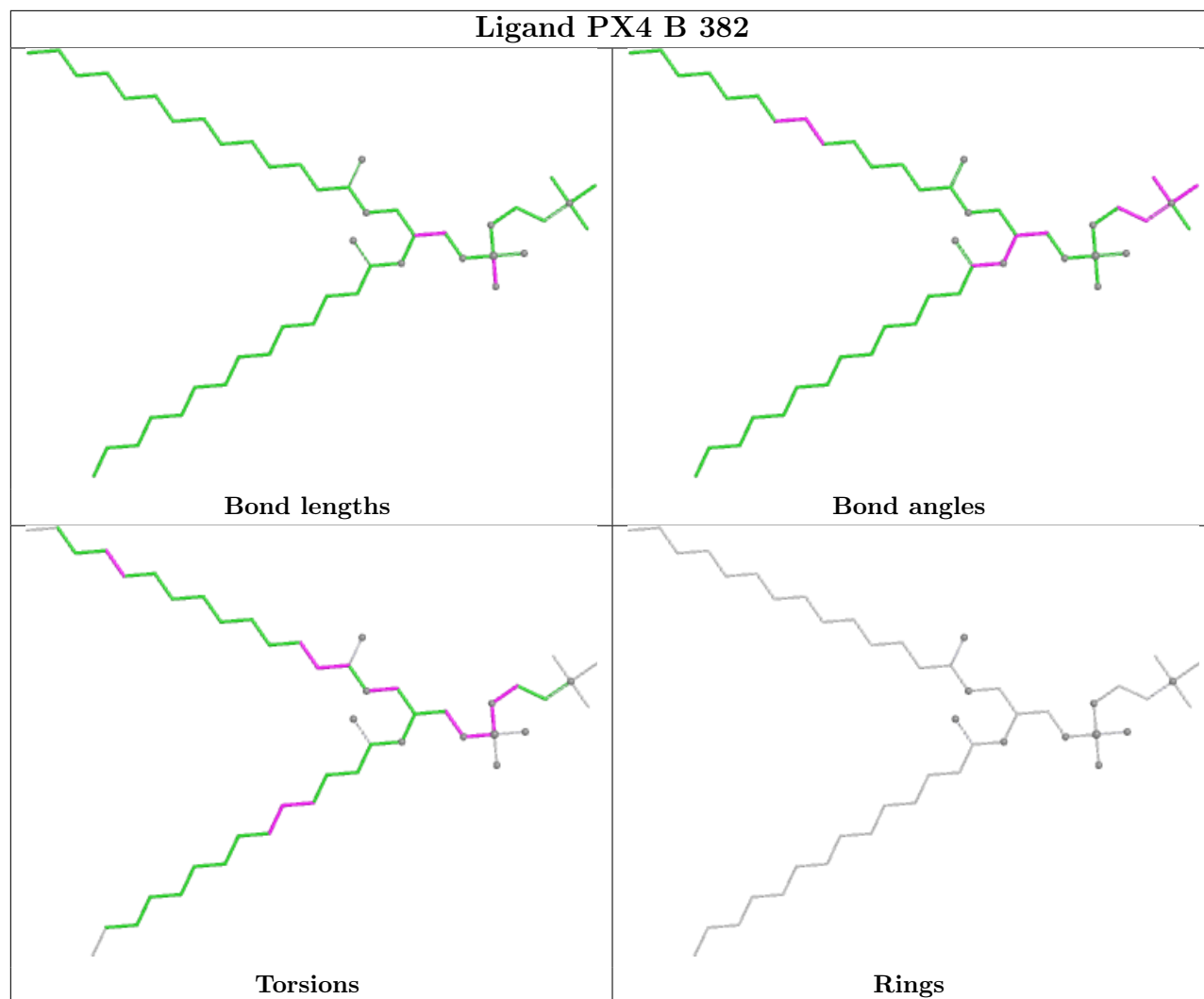


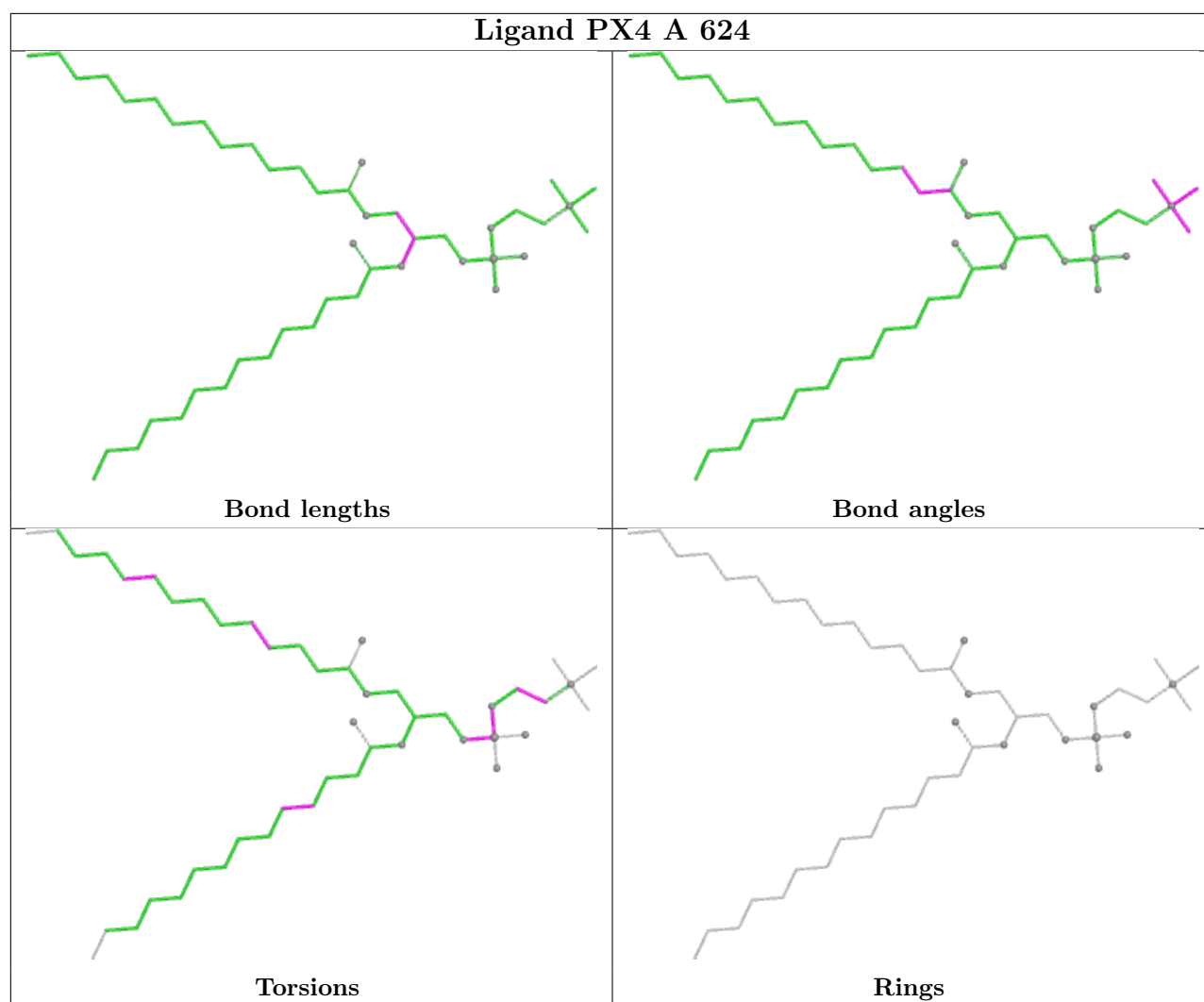


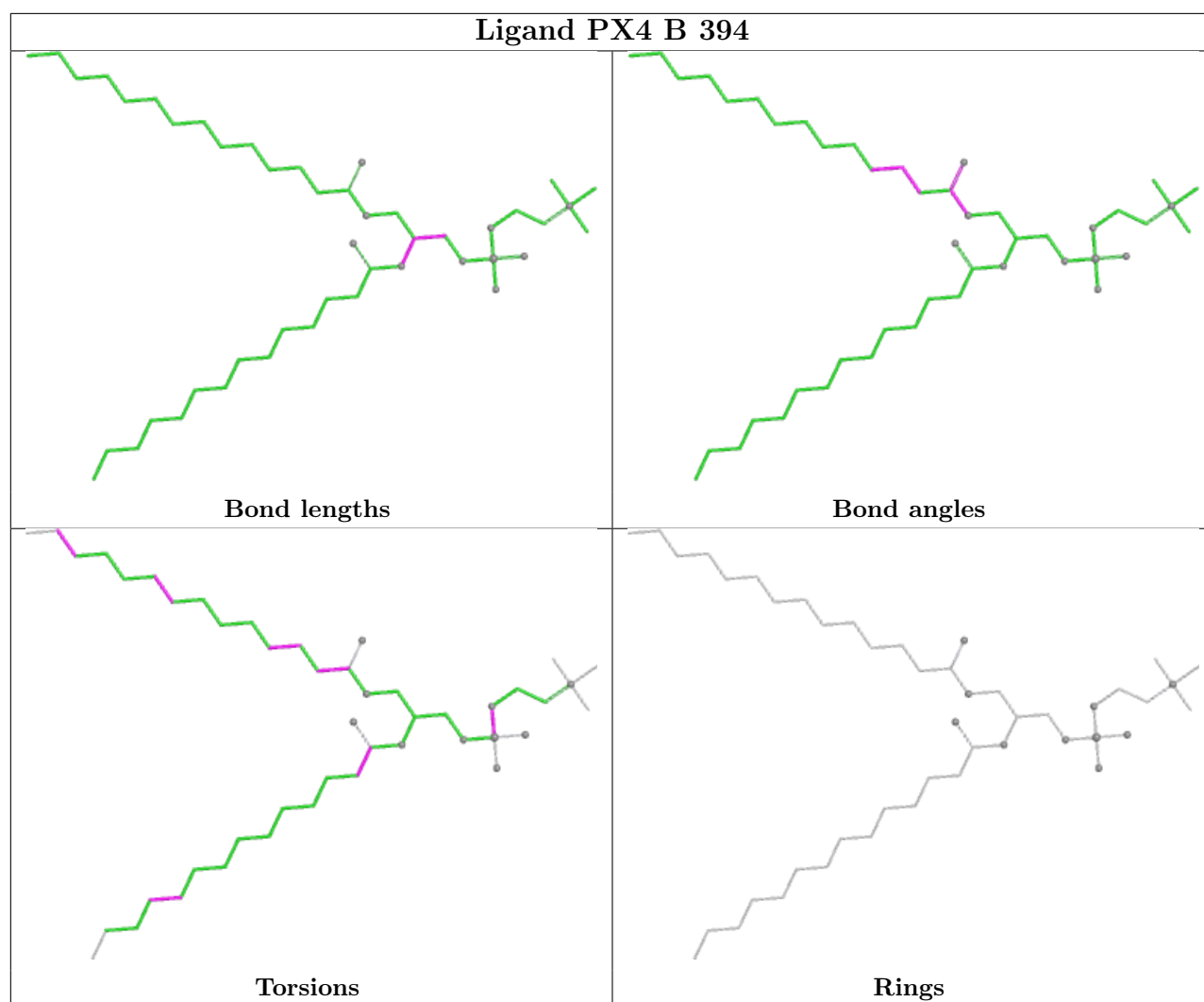
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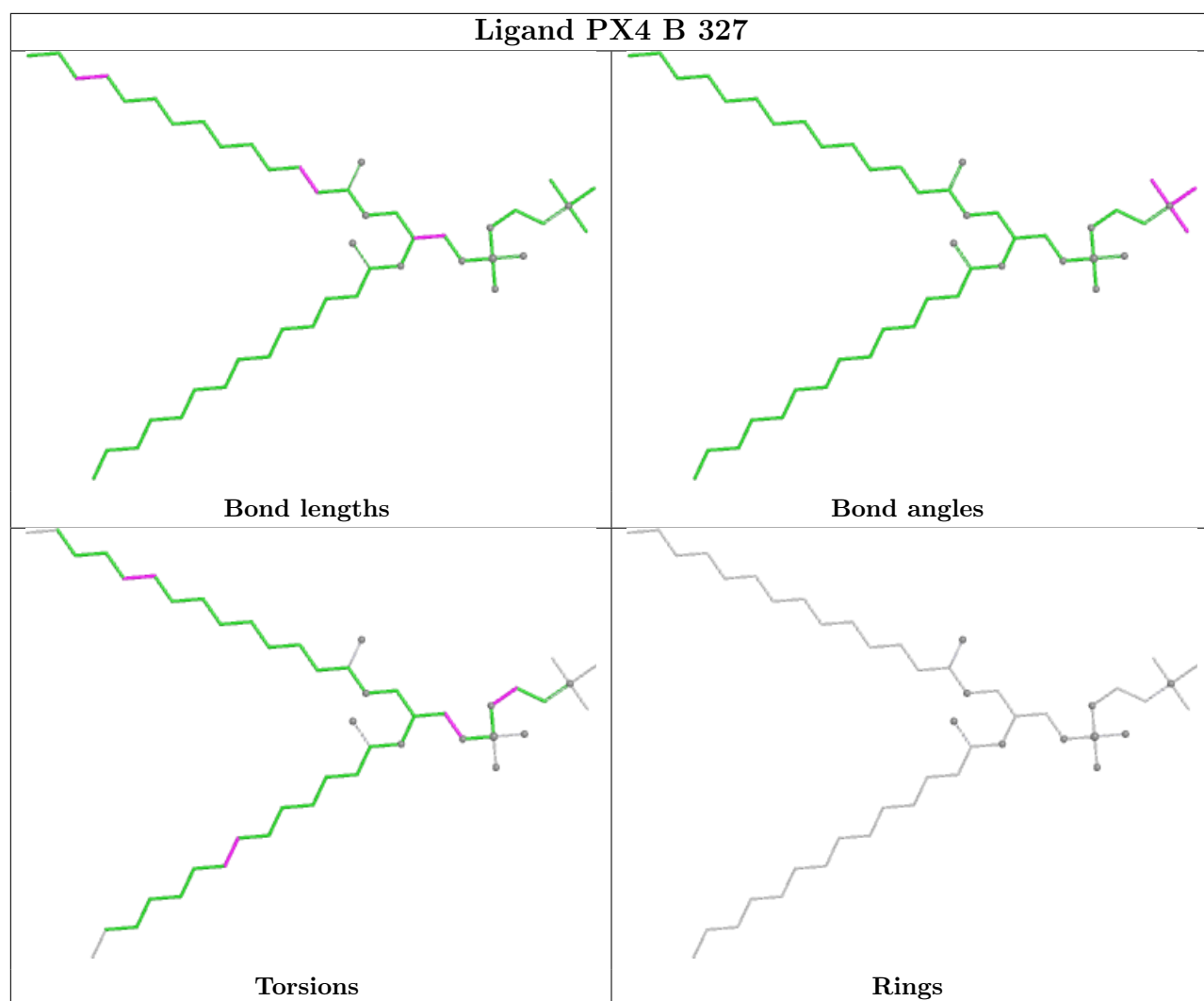


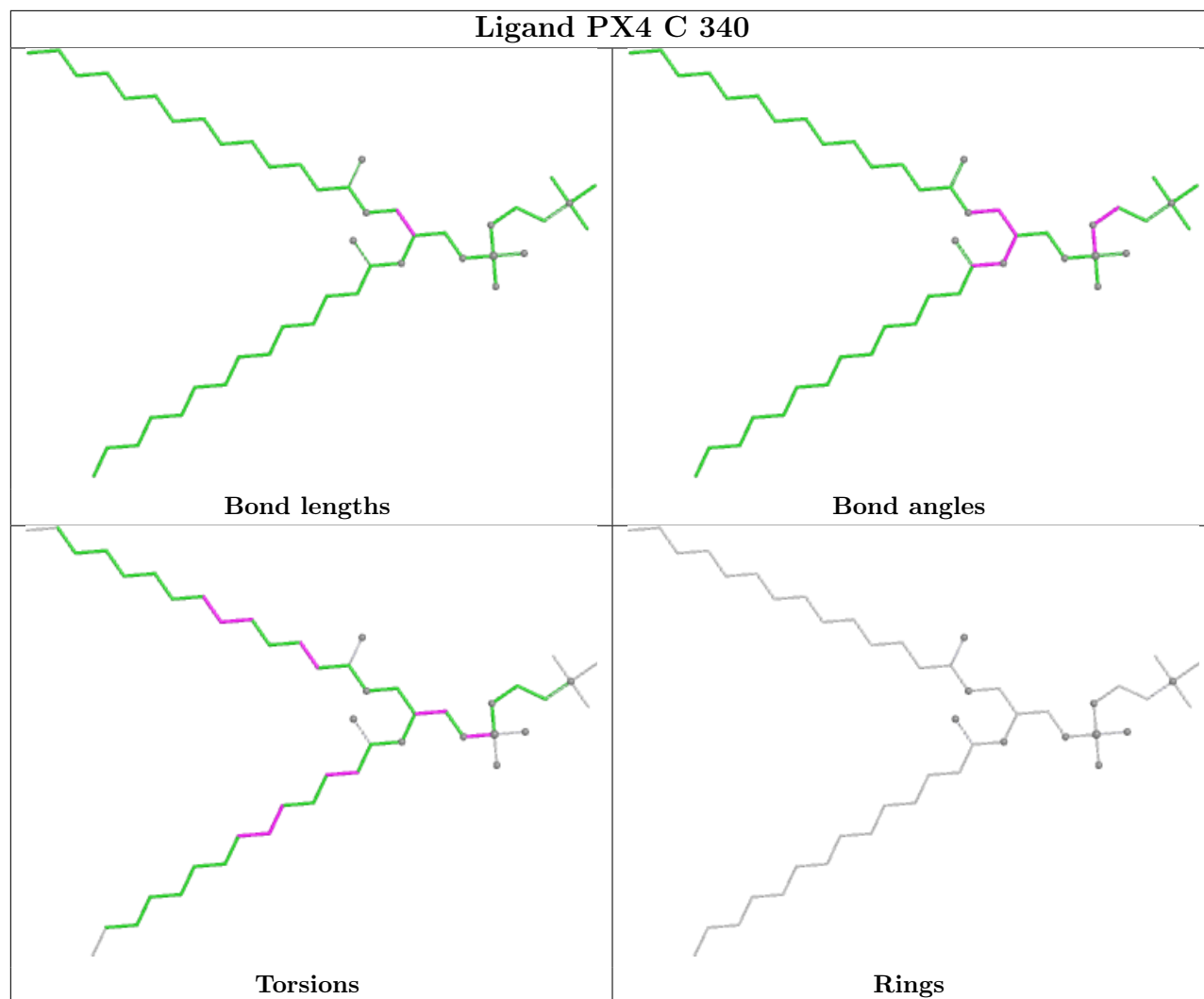
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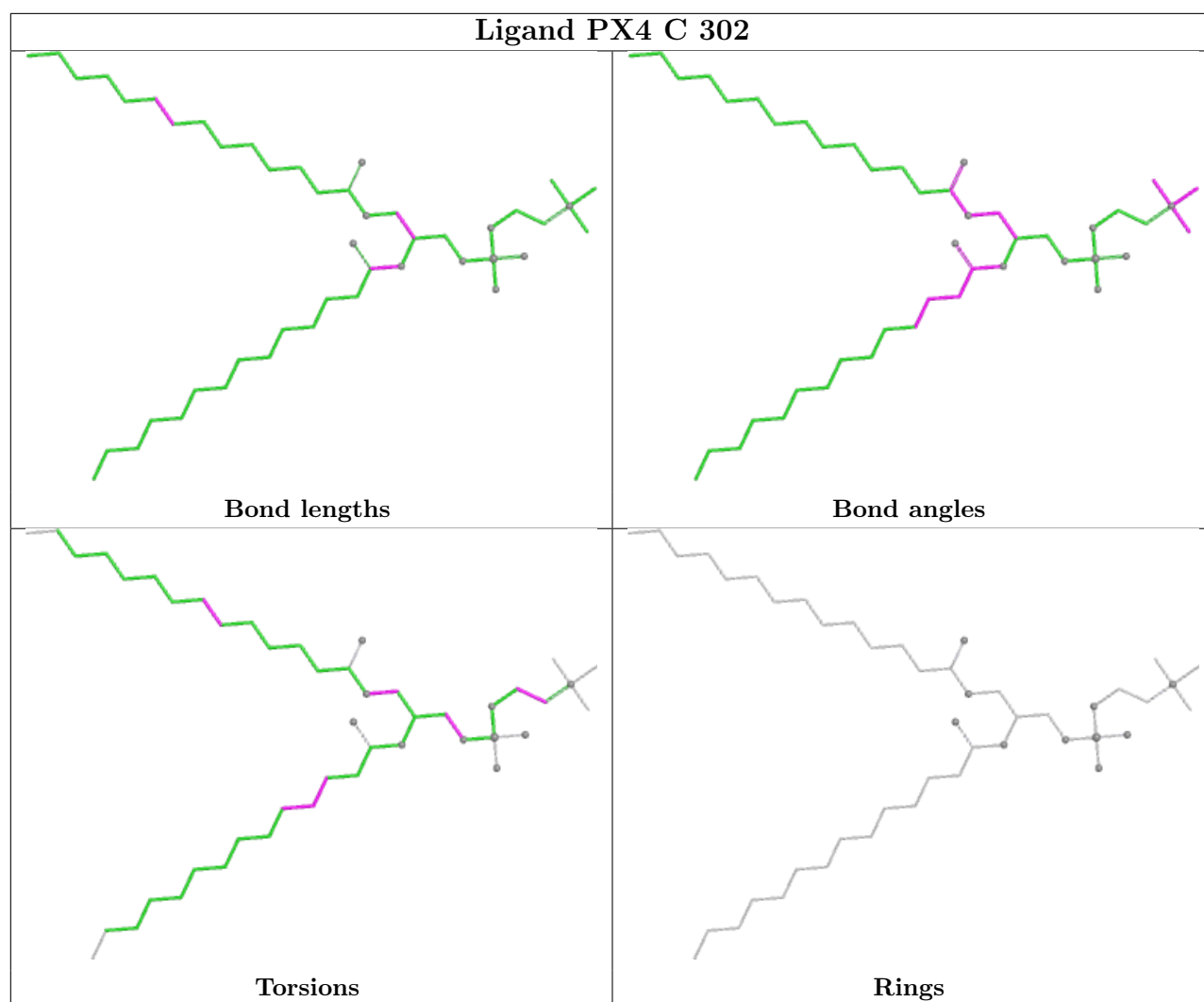




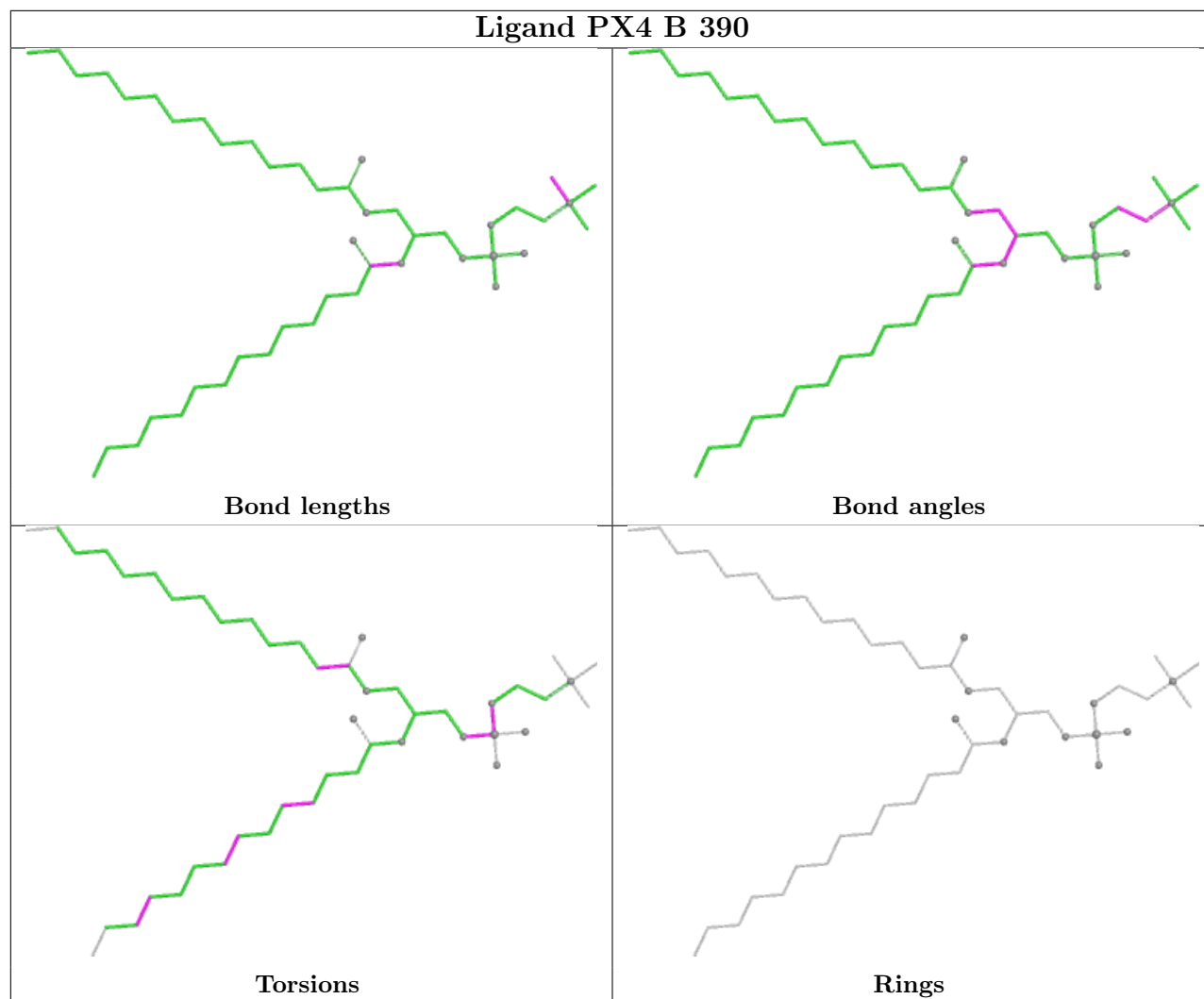


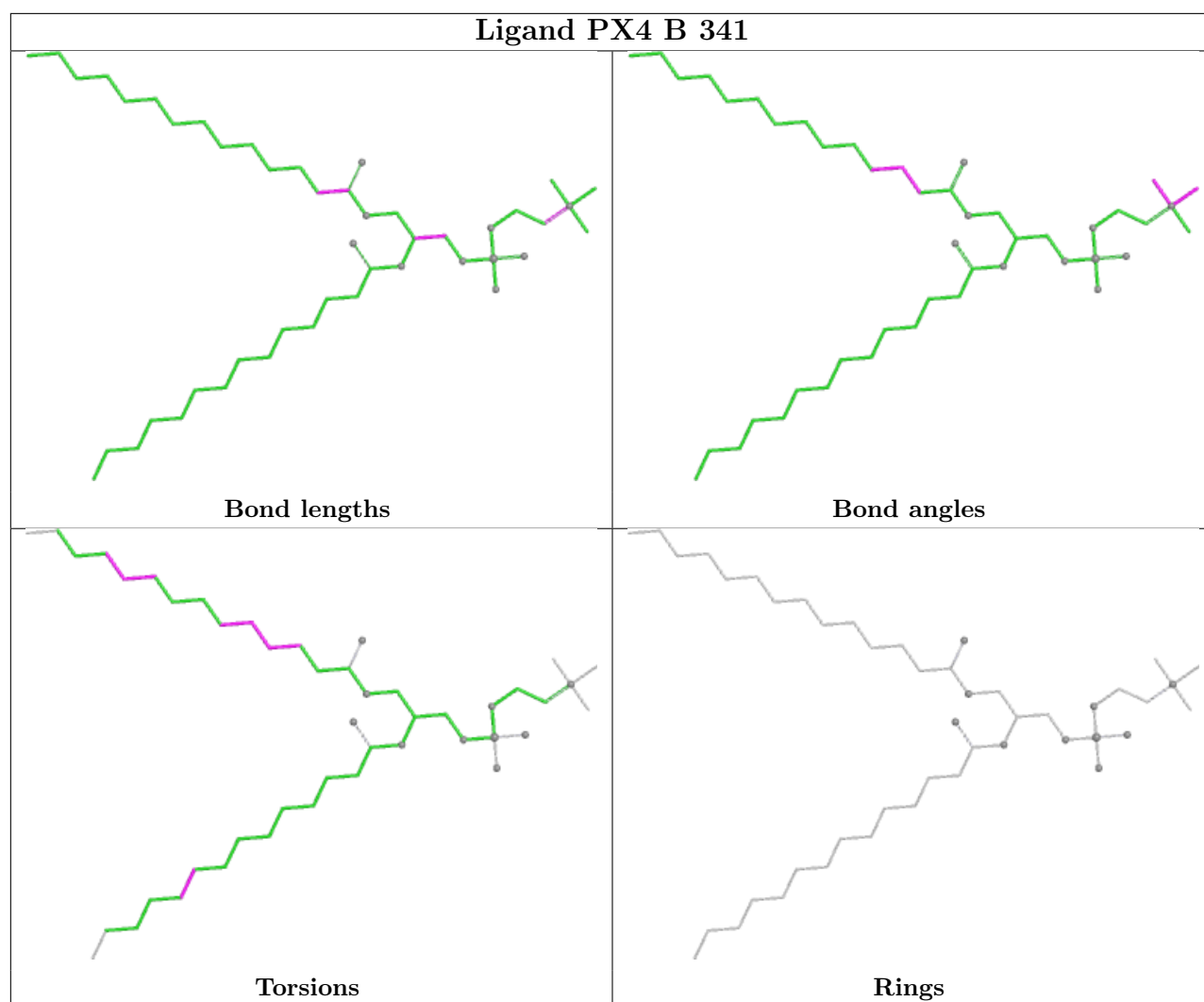


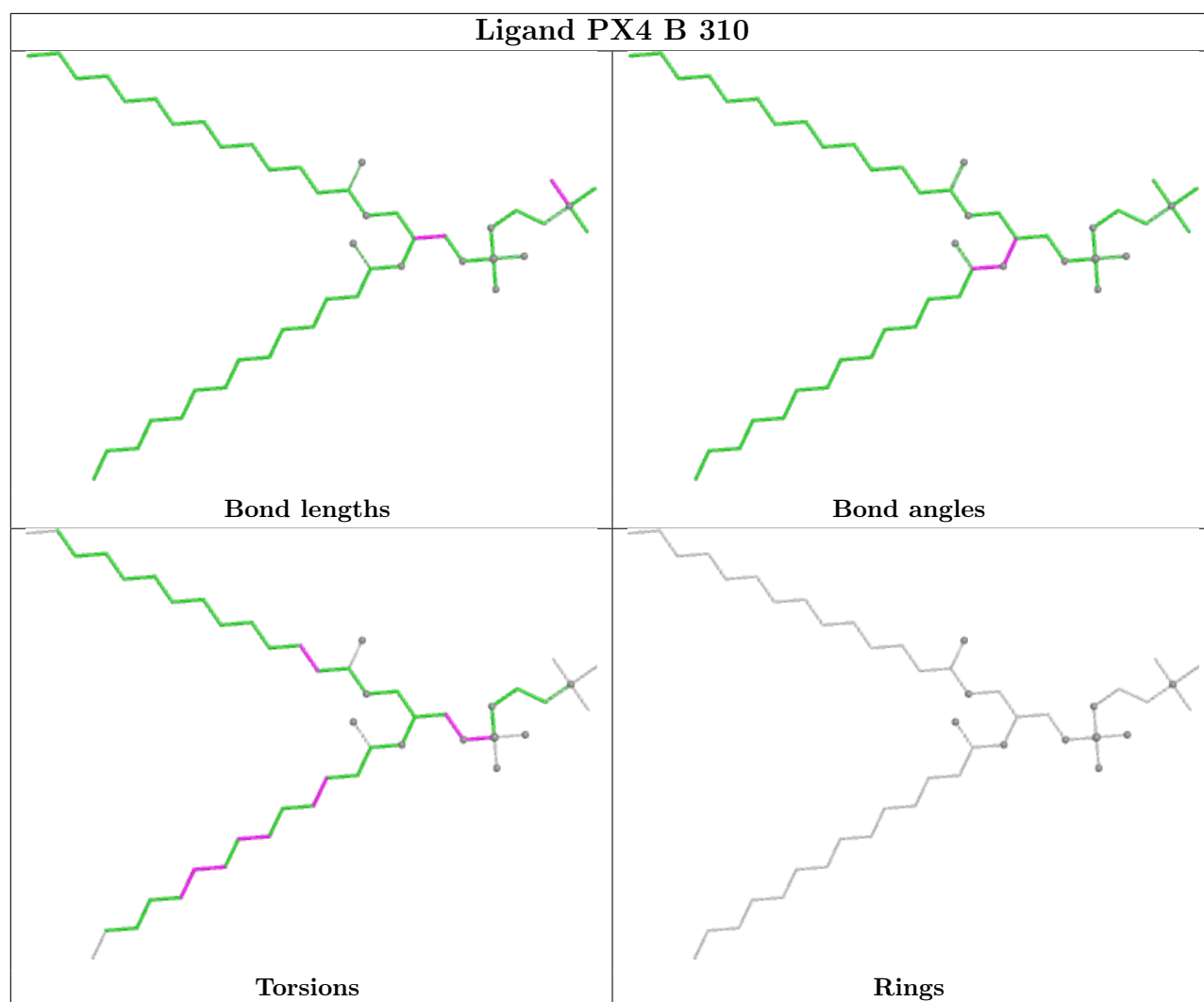




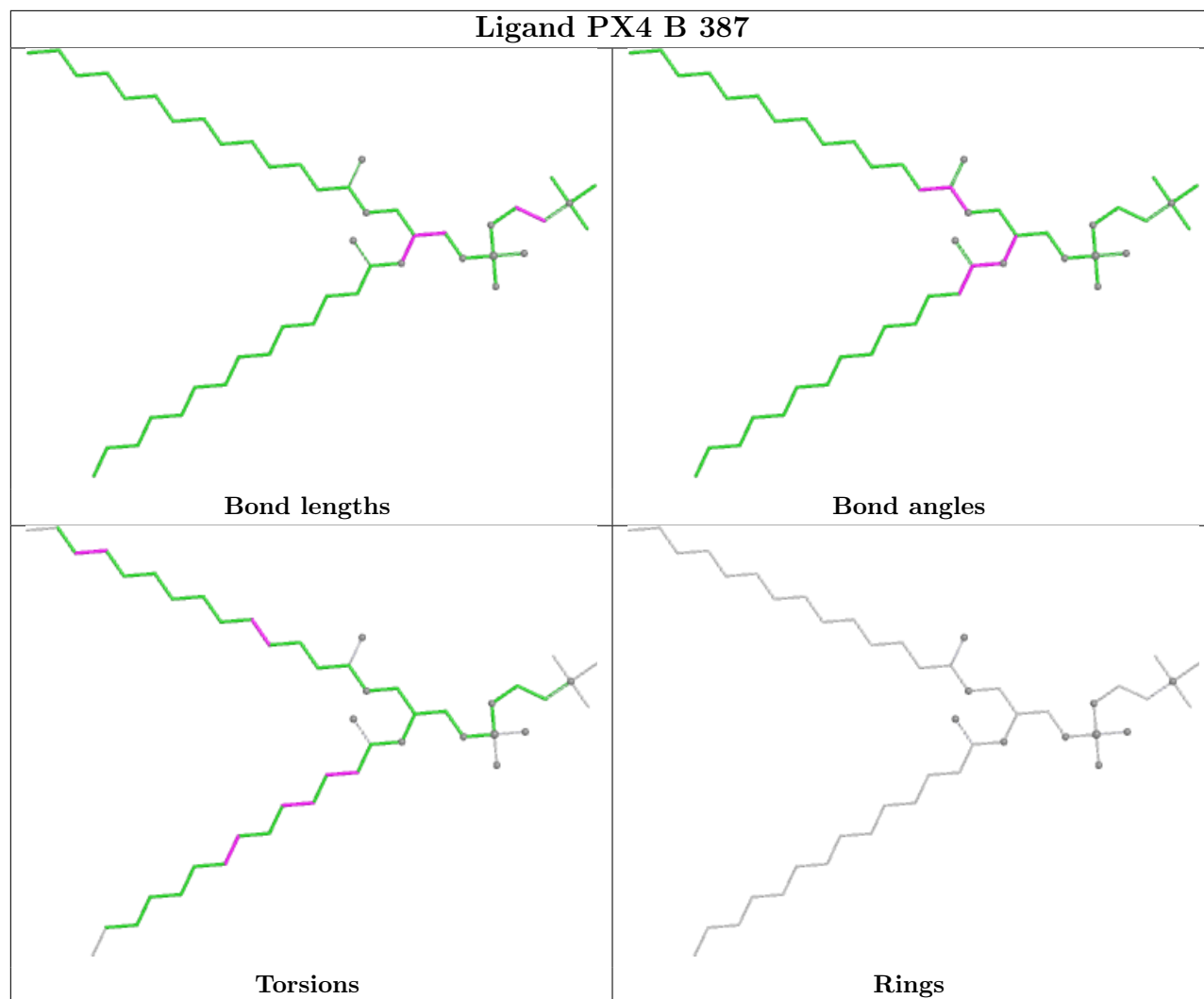
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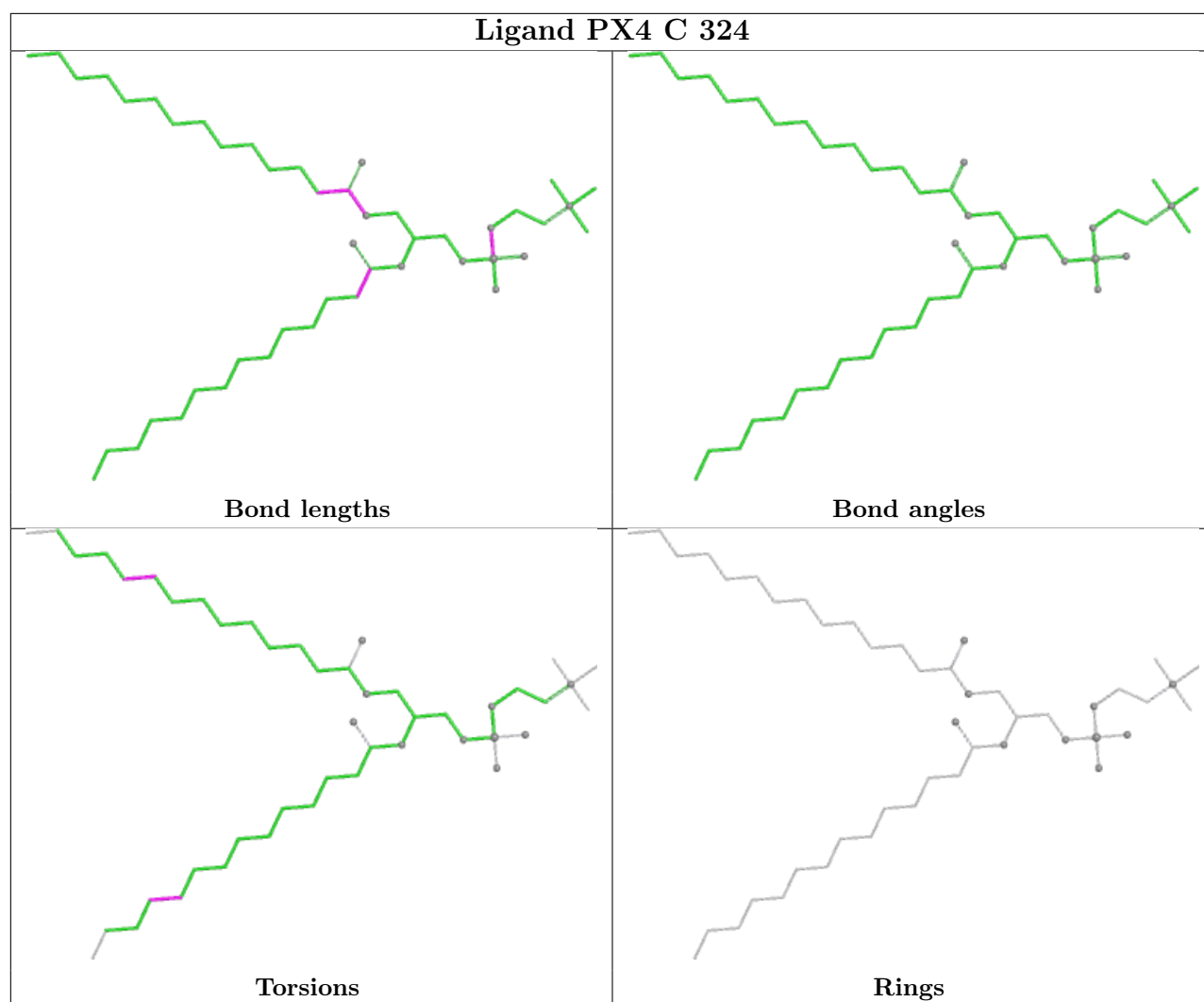




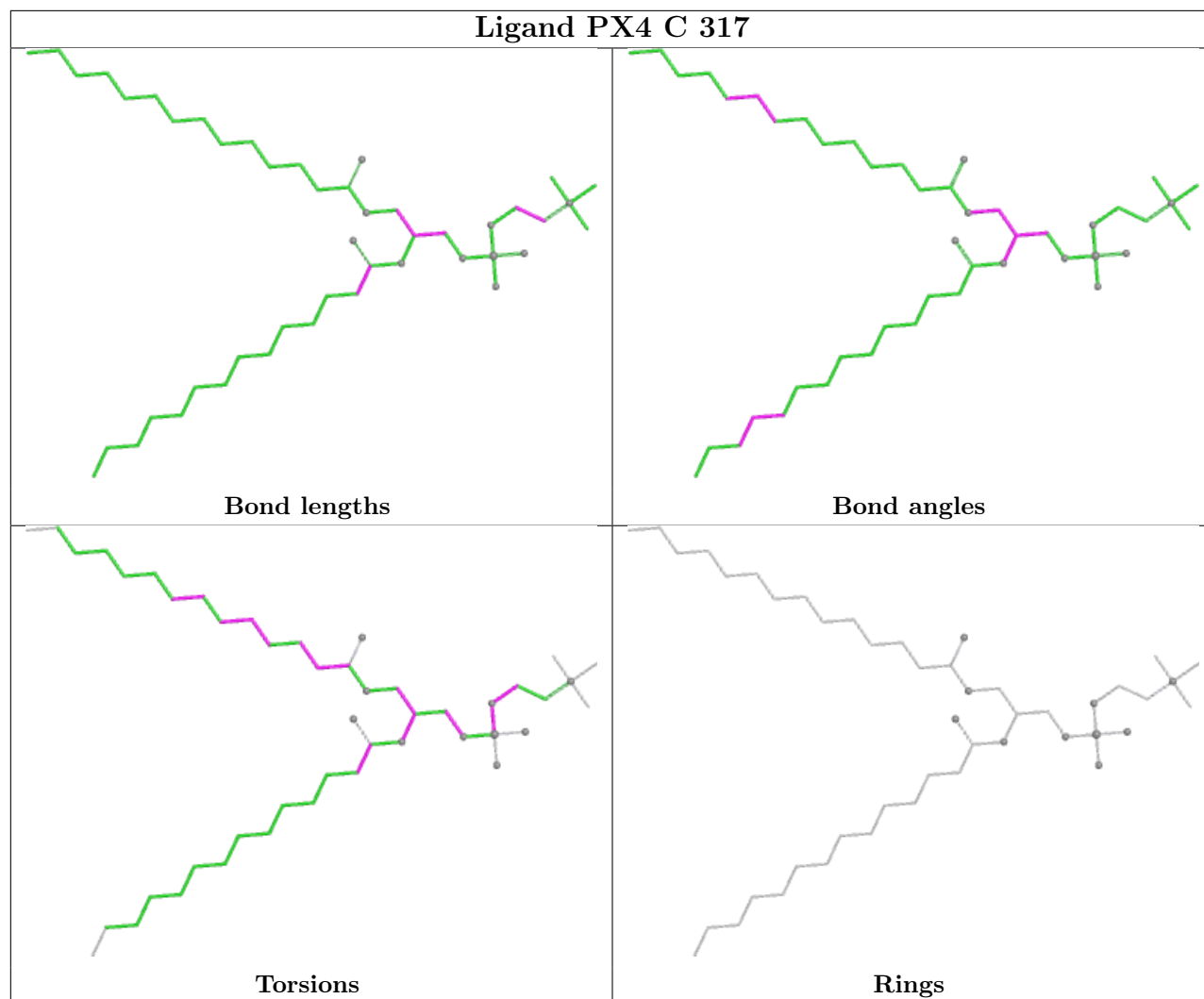


Ligand PX4 B 387

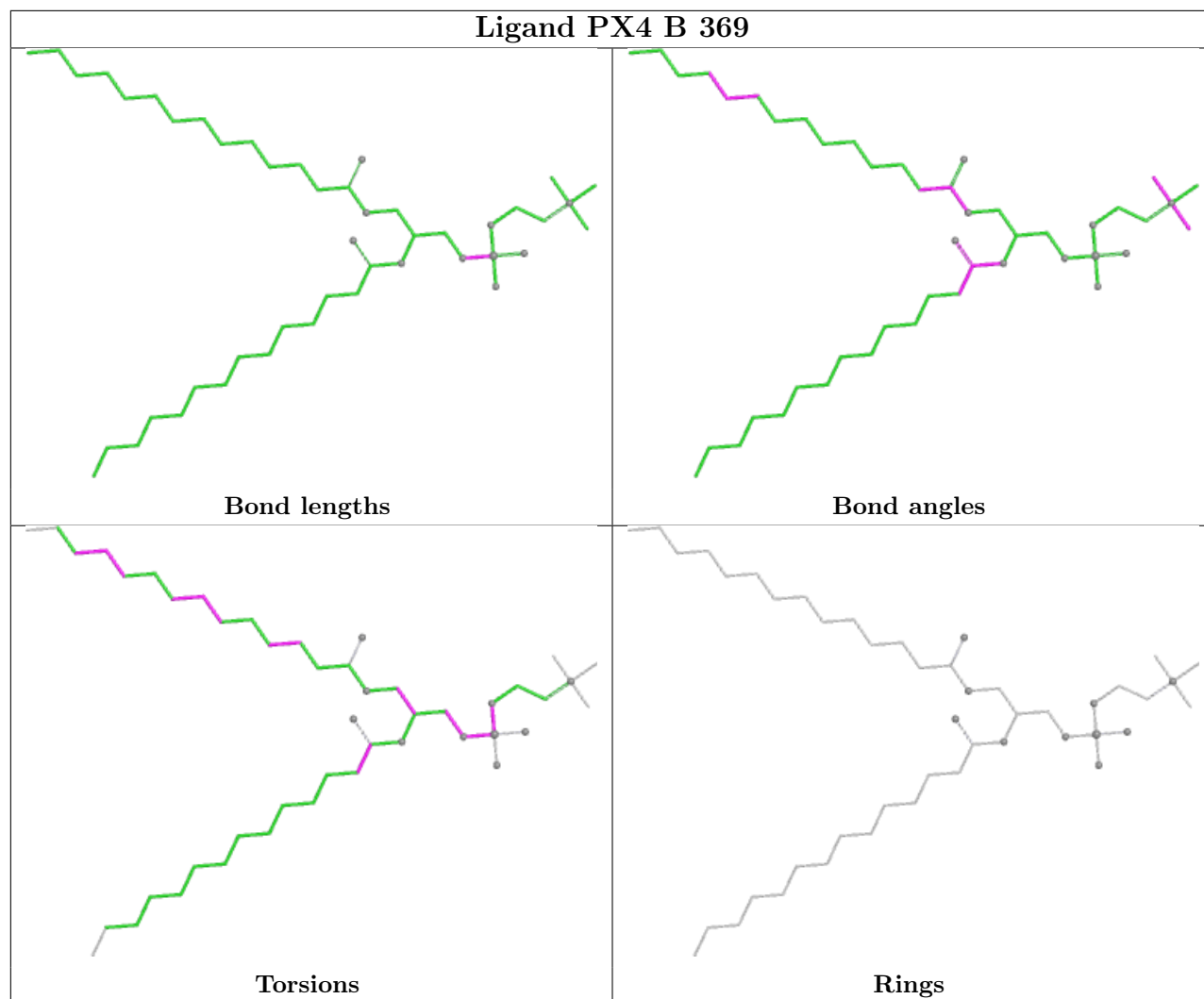


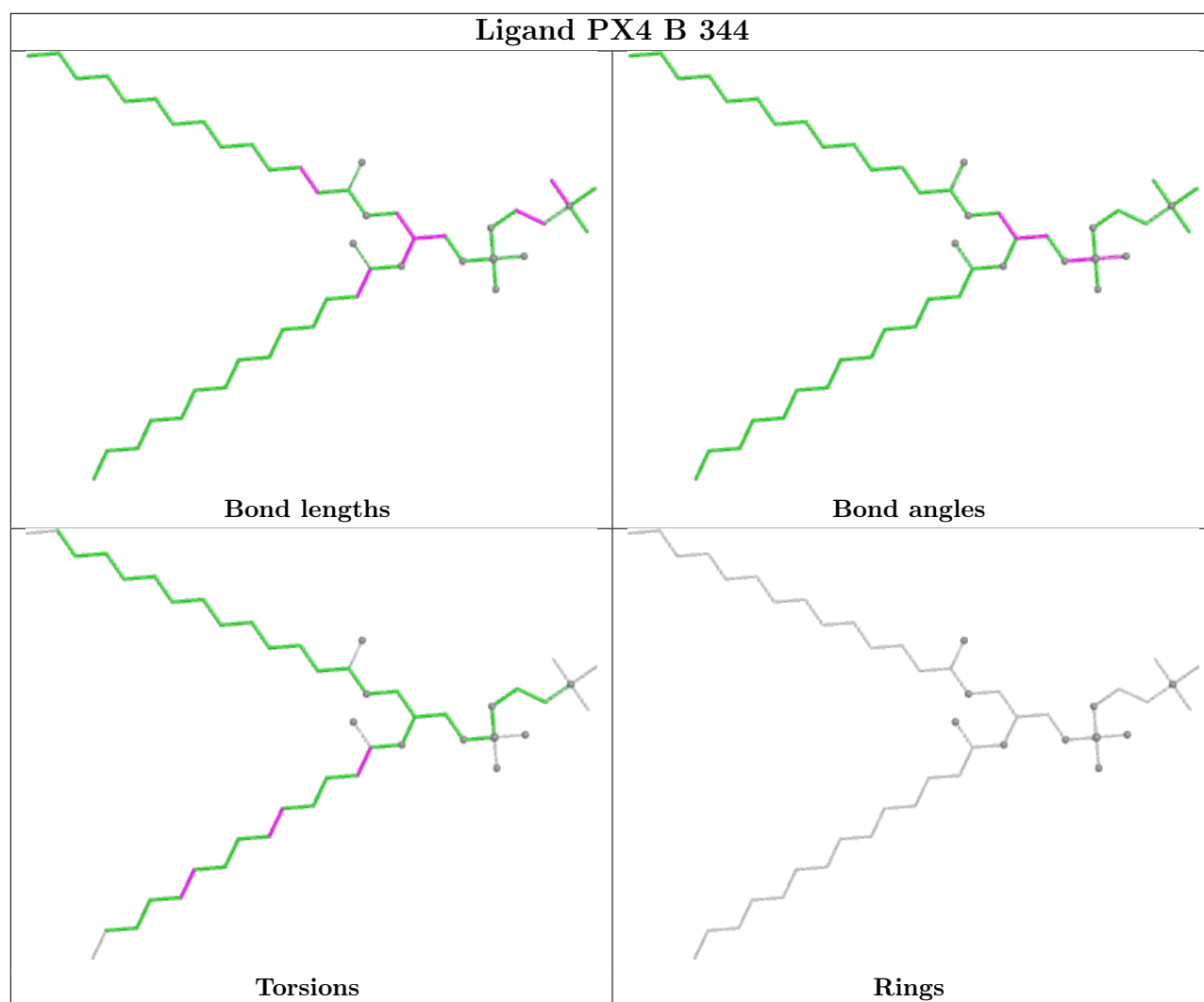


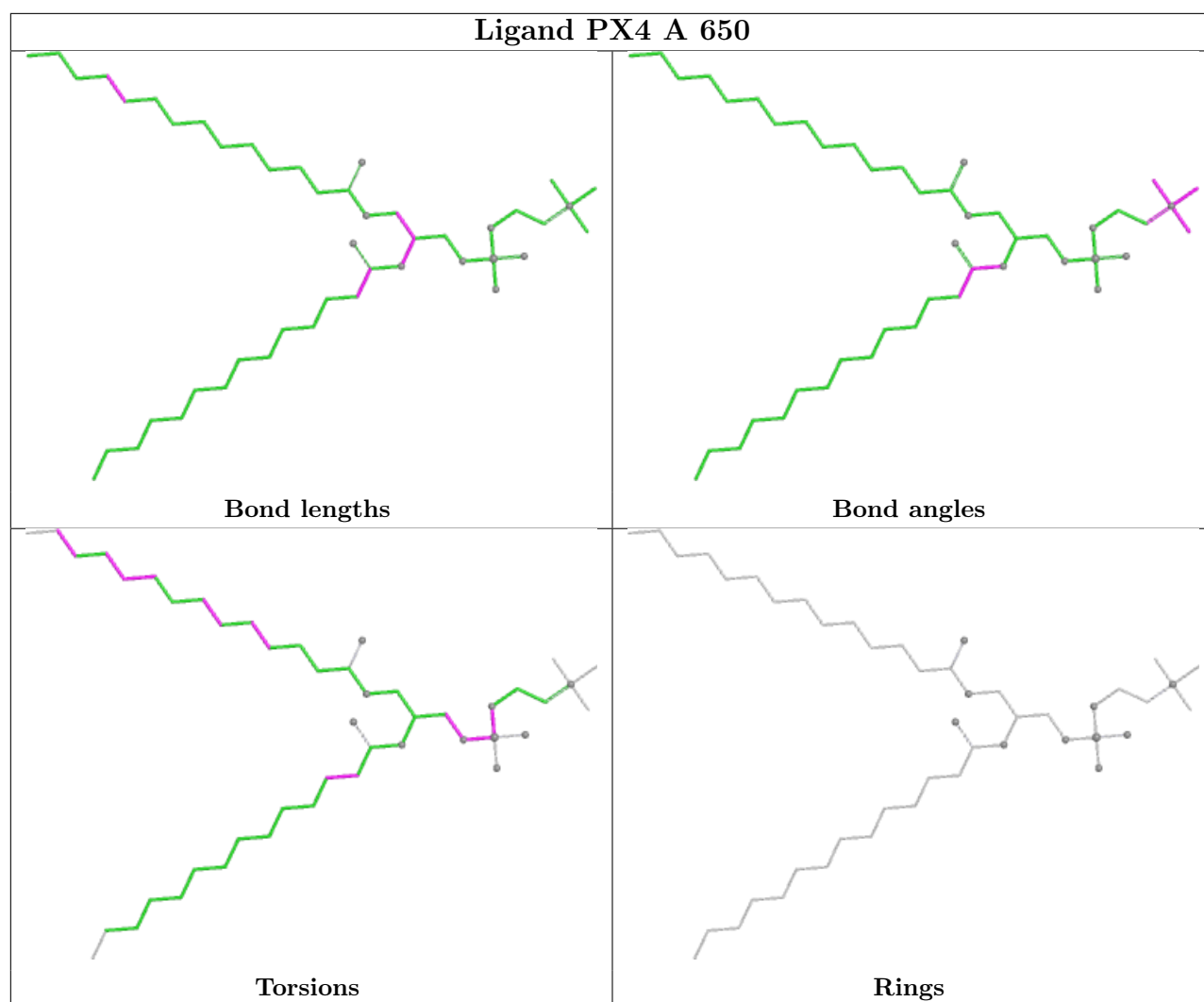
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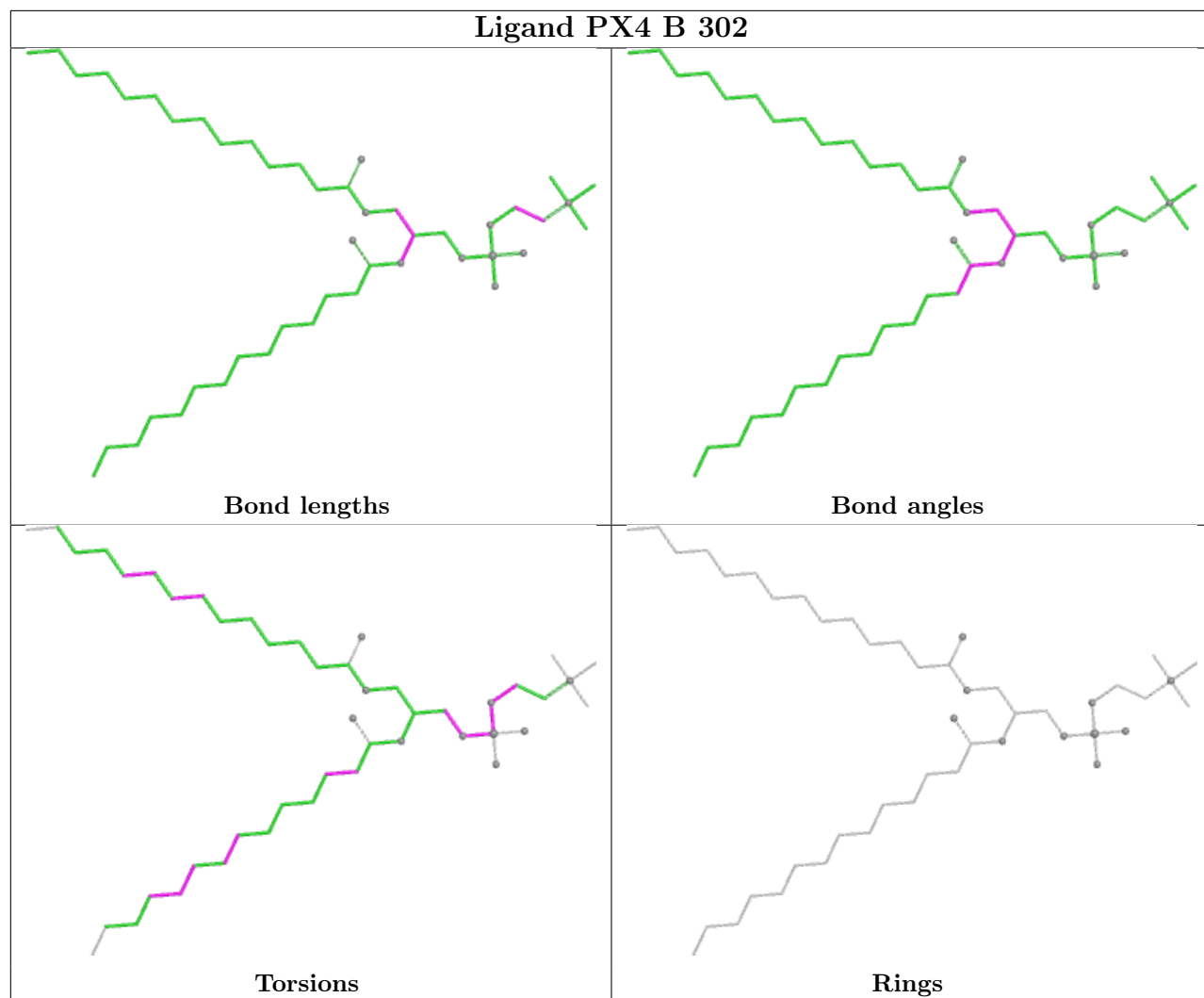


Ligand PX4 B 369

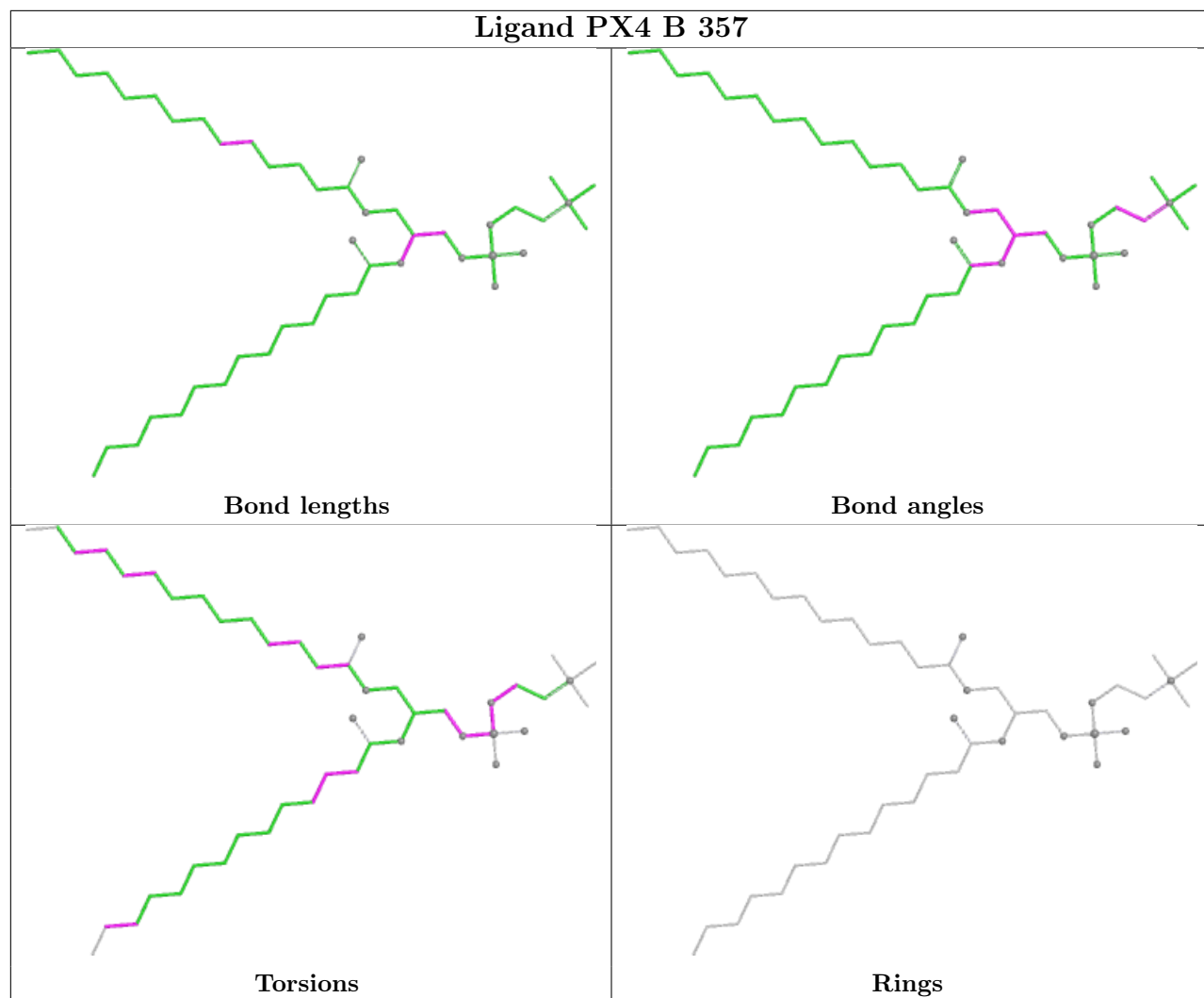


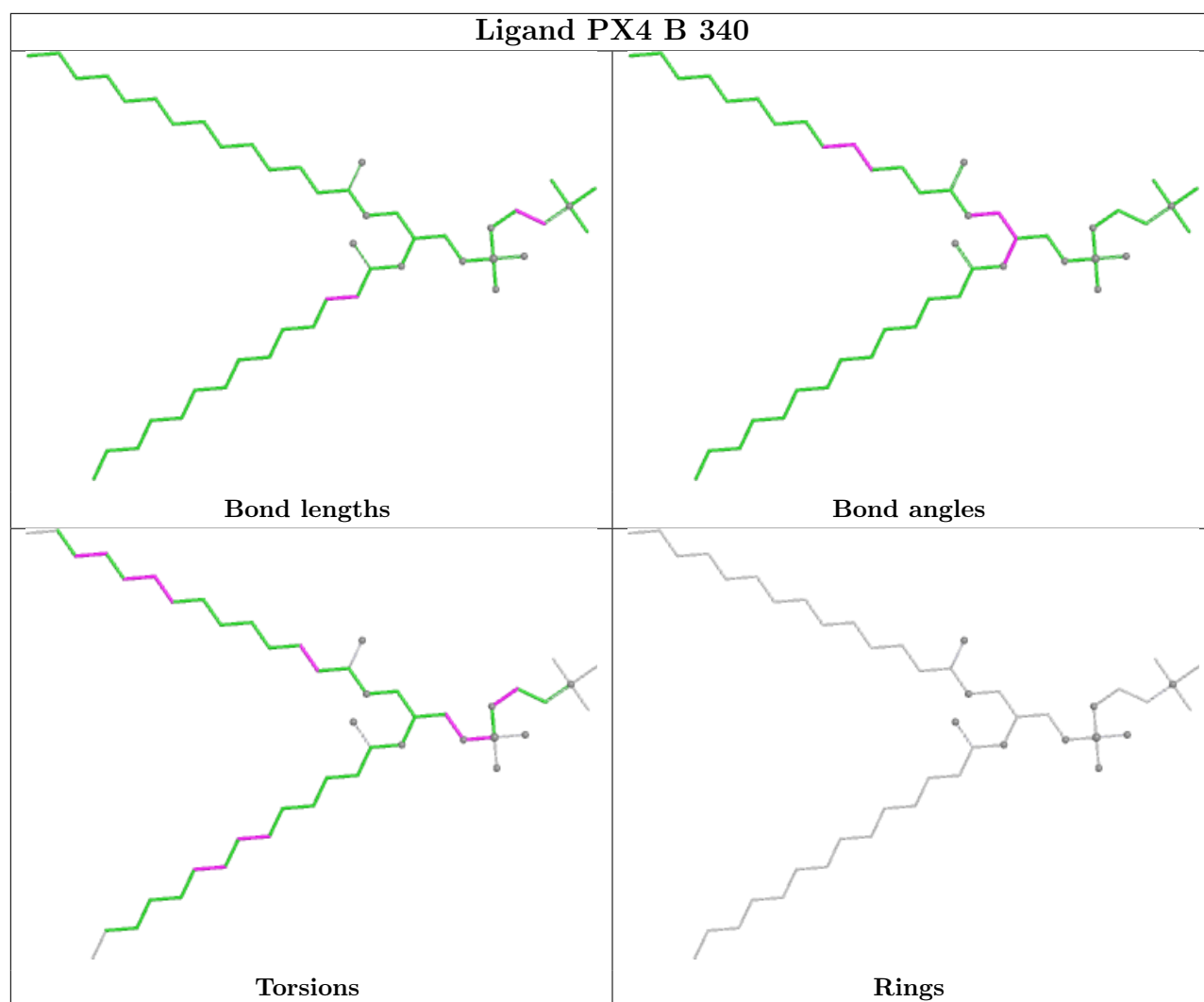


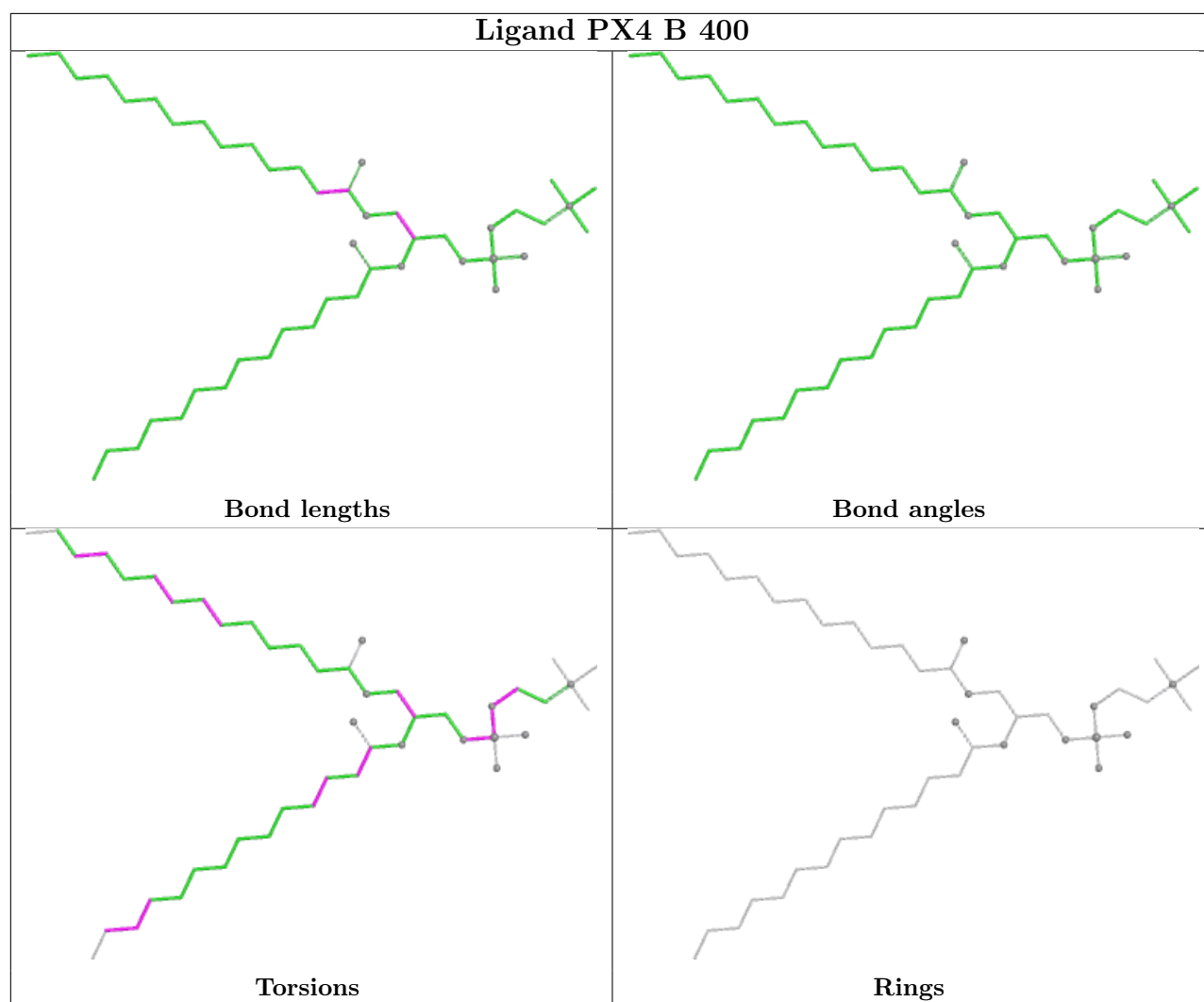




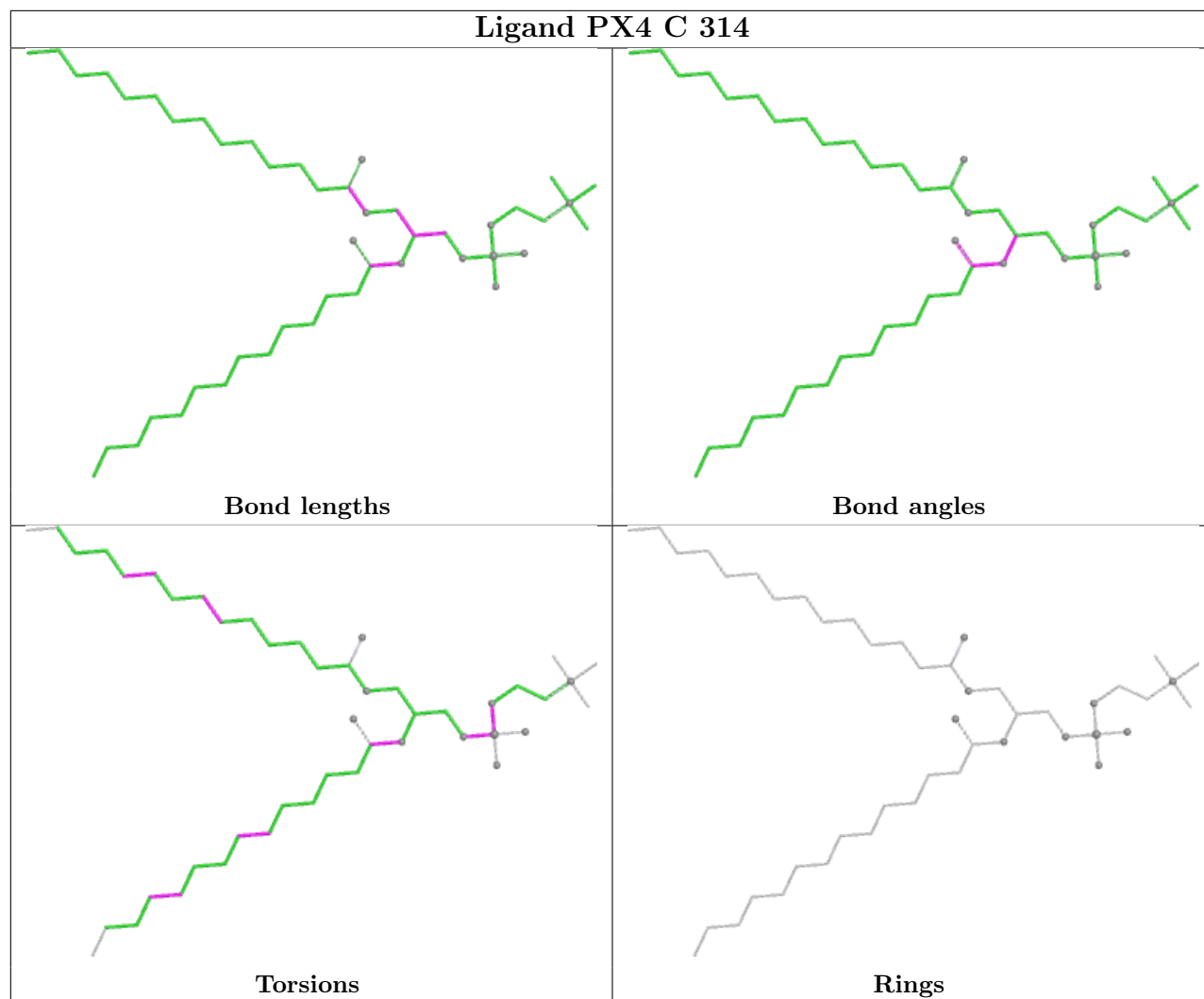
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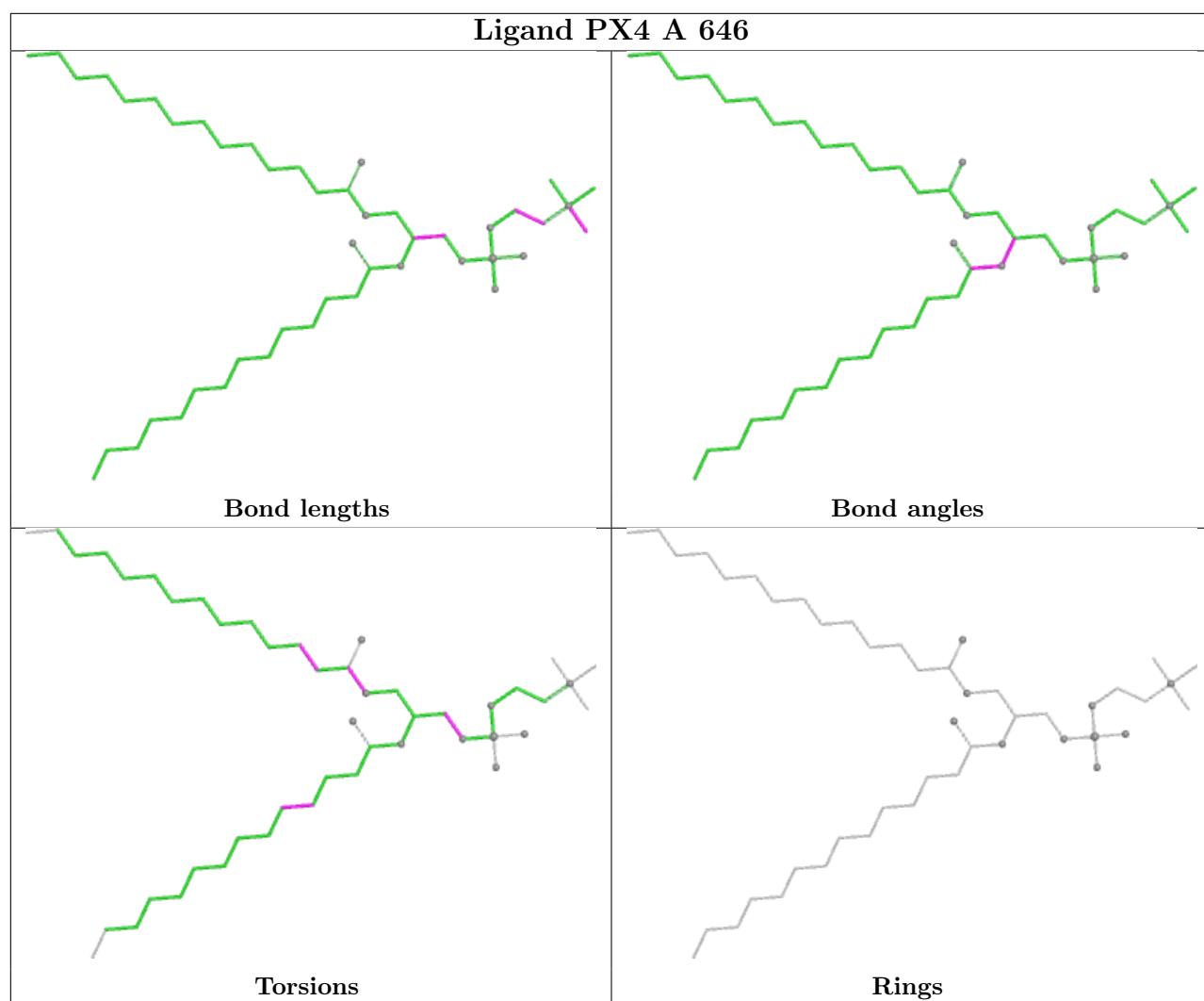


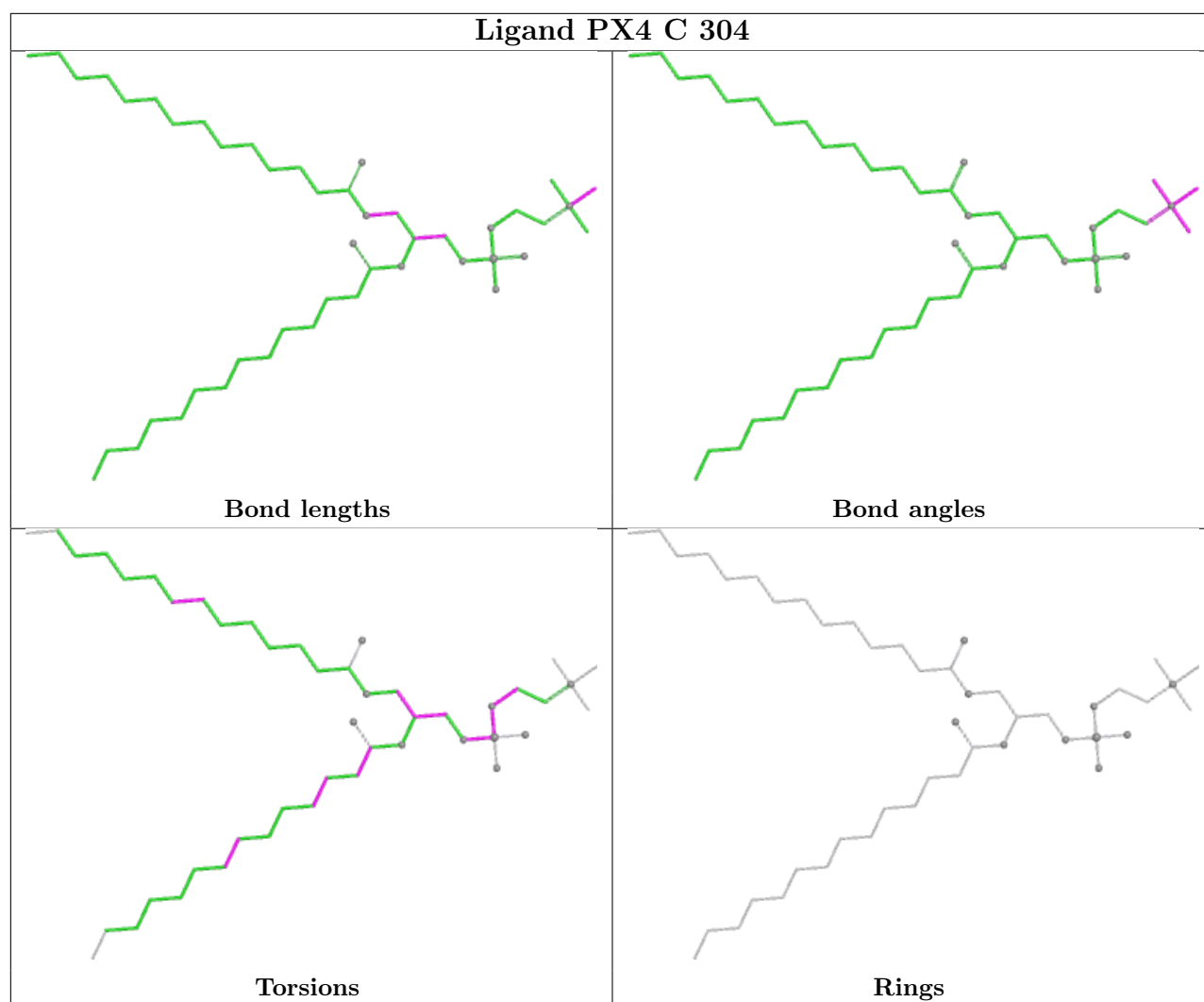




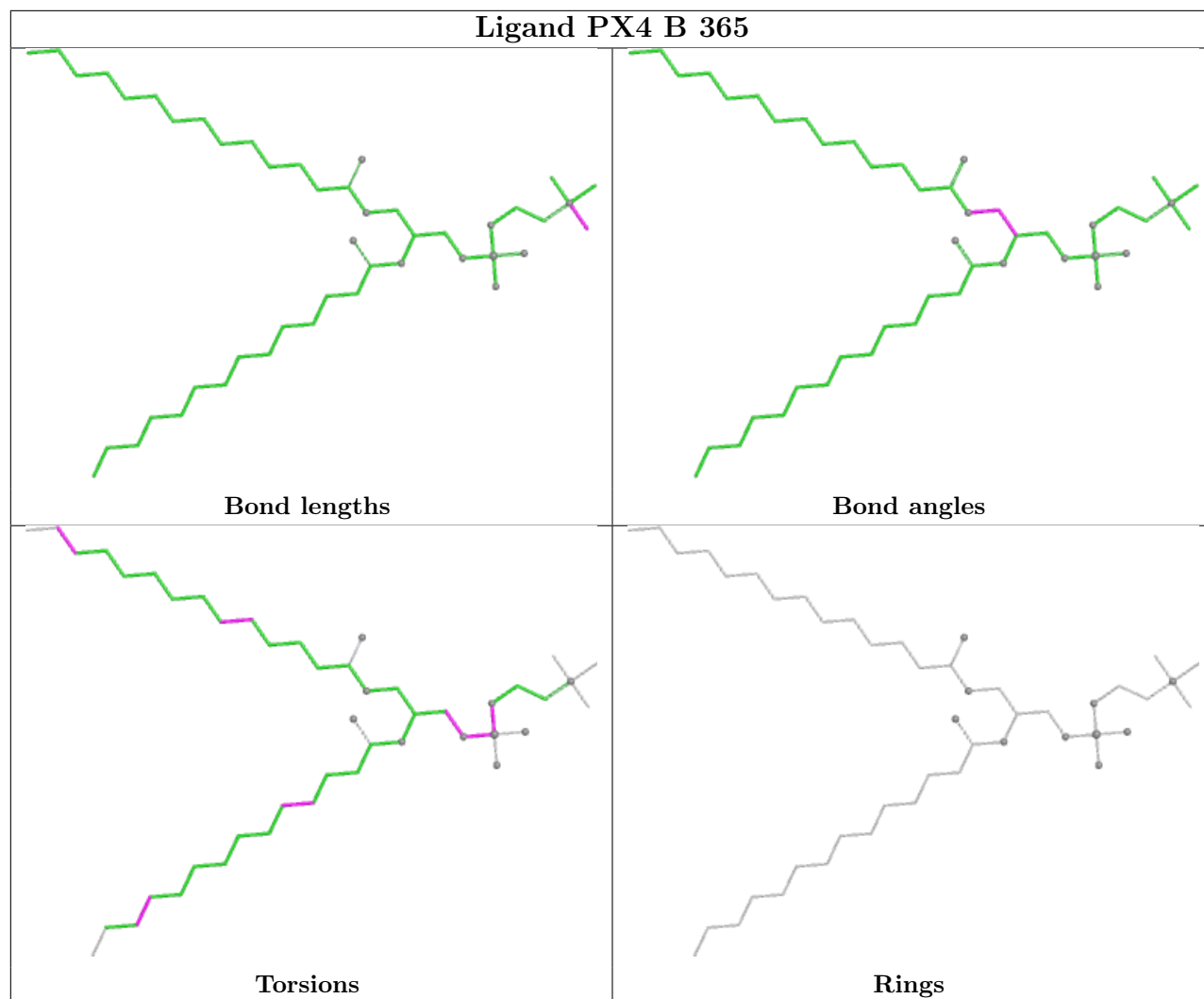
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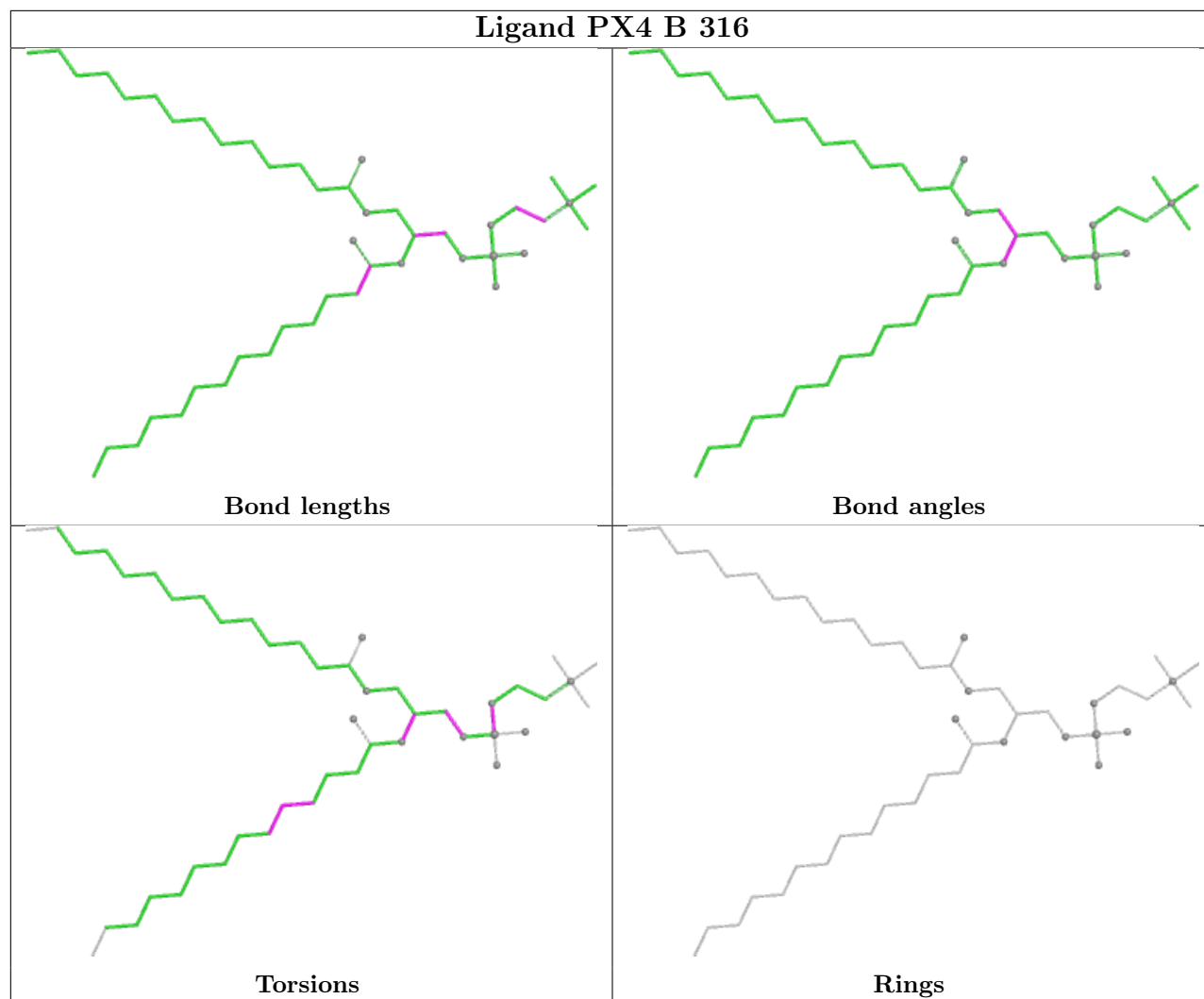


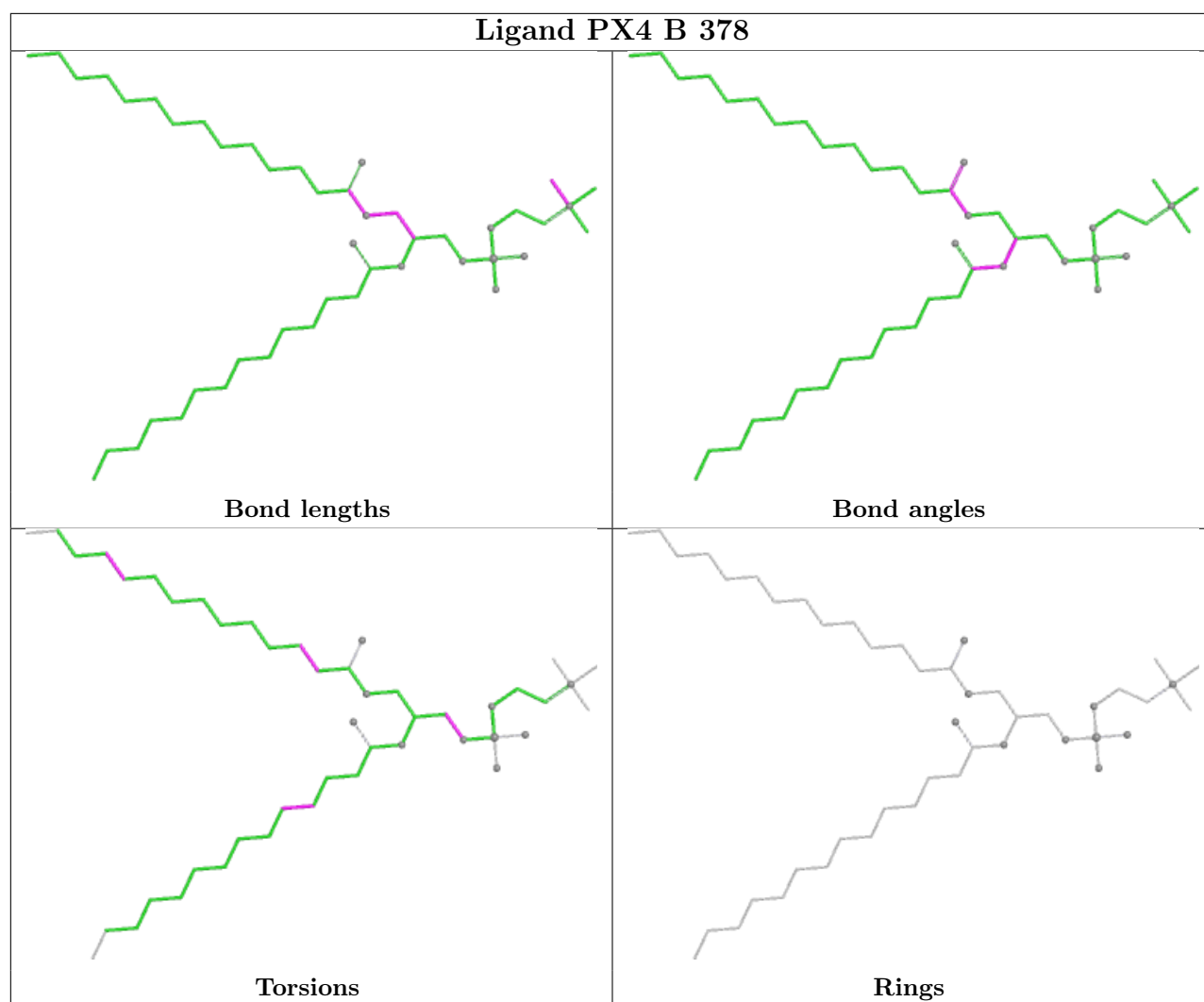


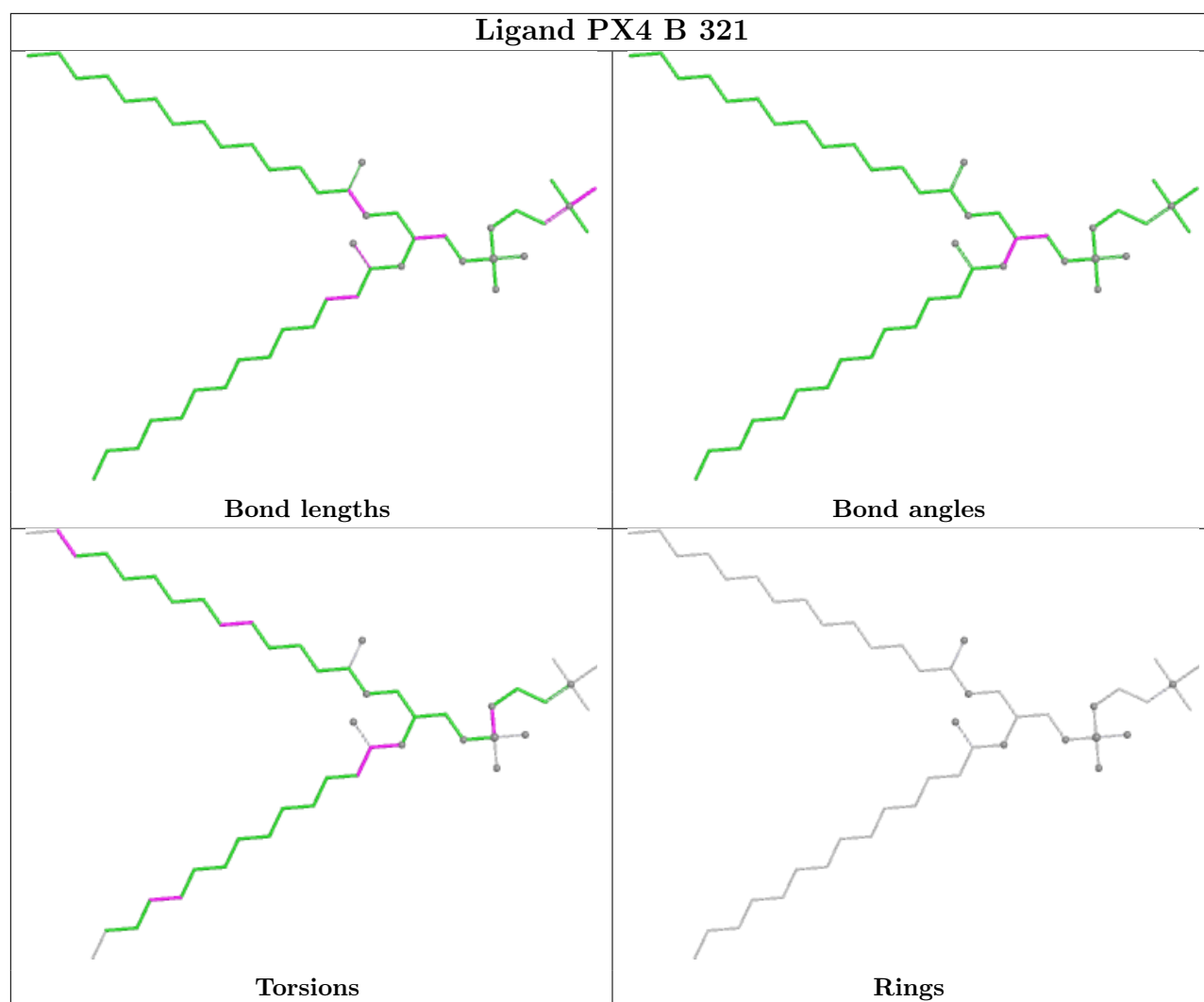
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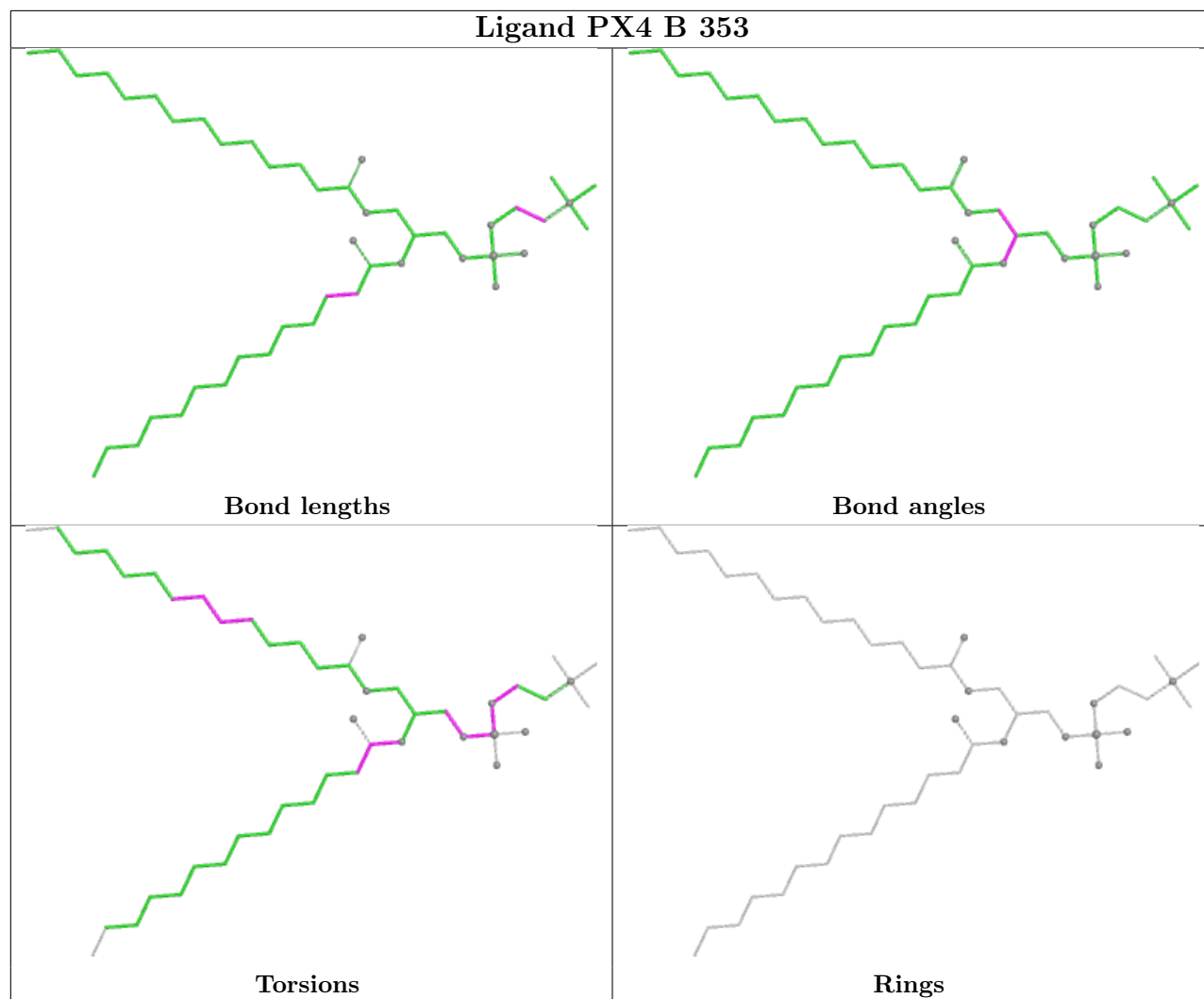
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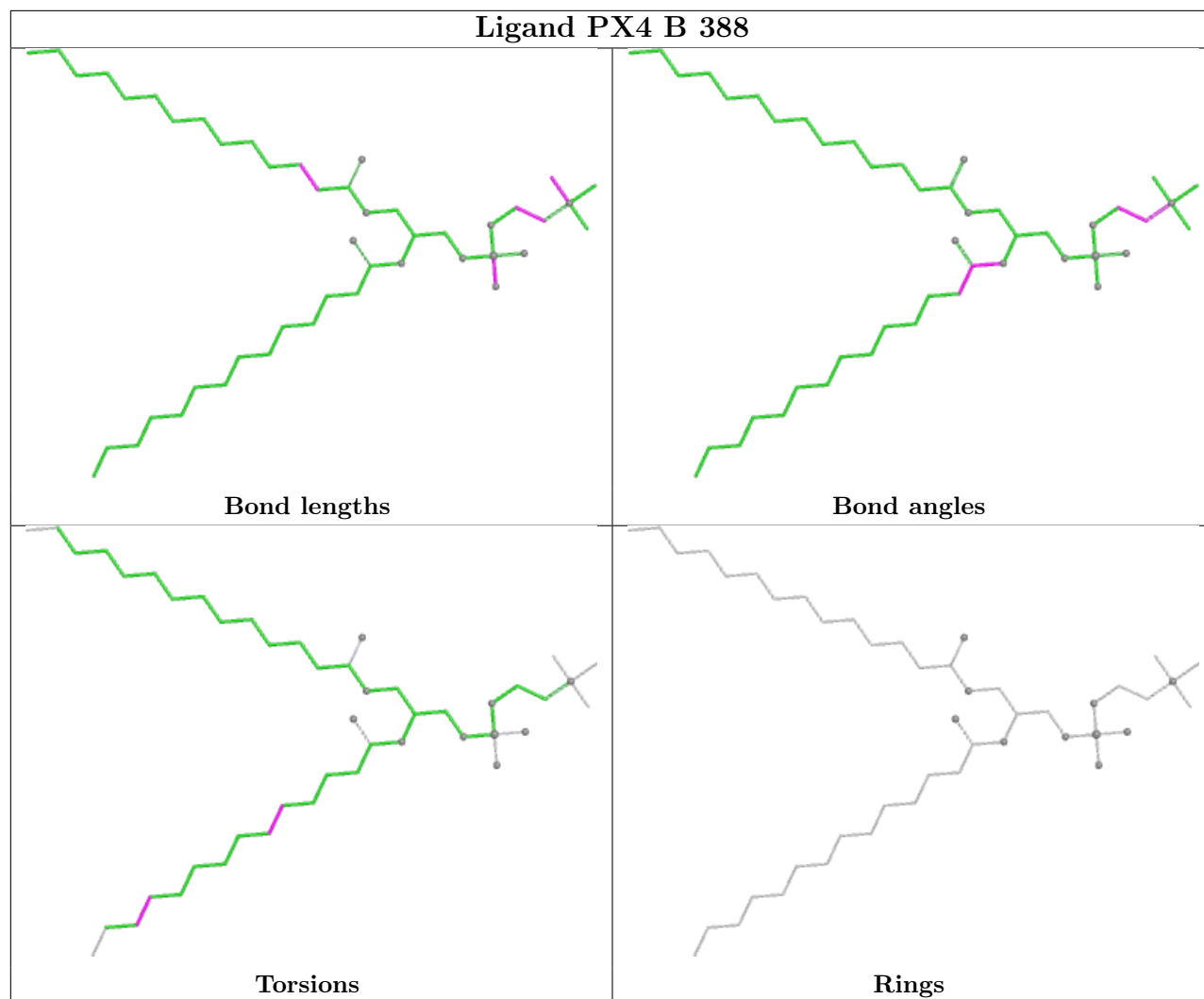




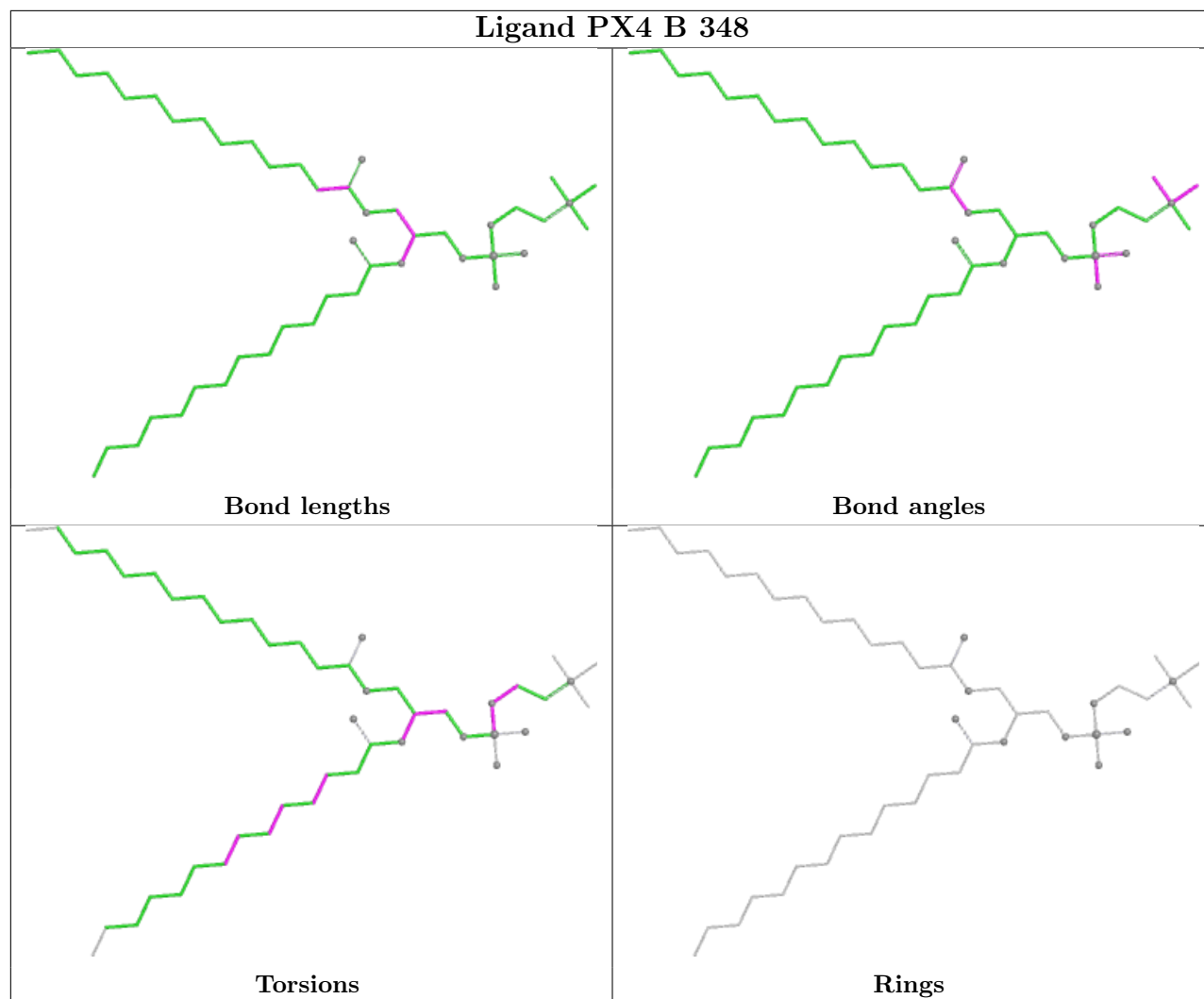
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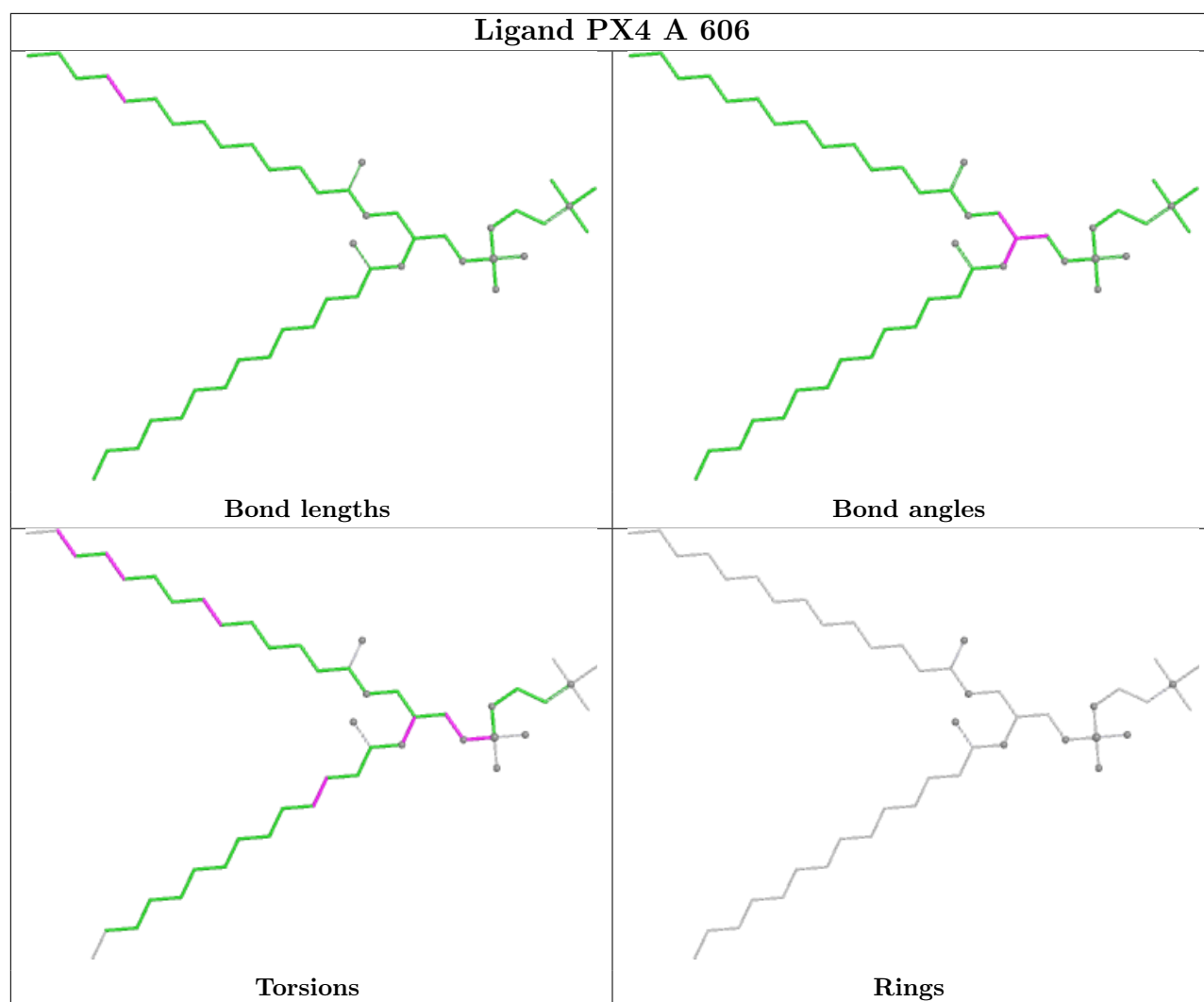


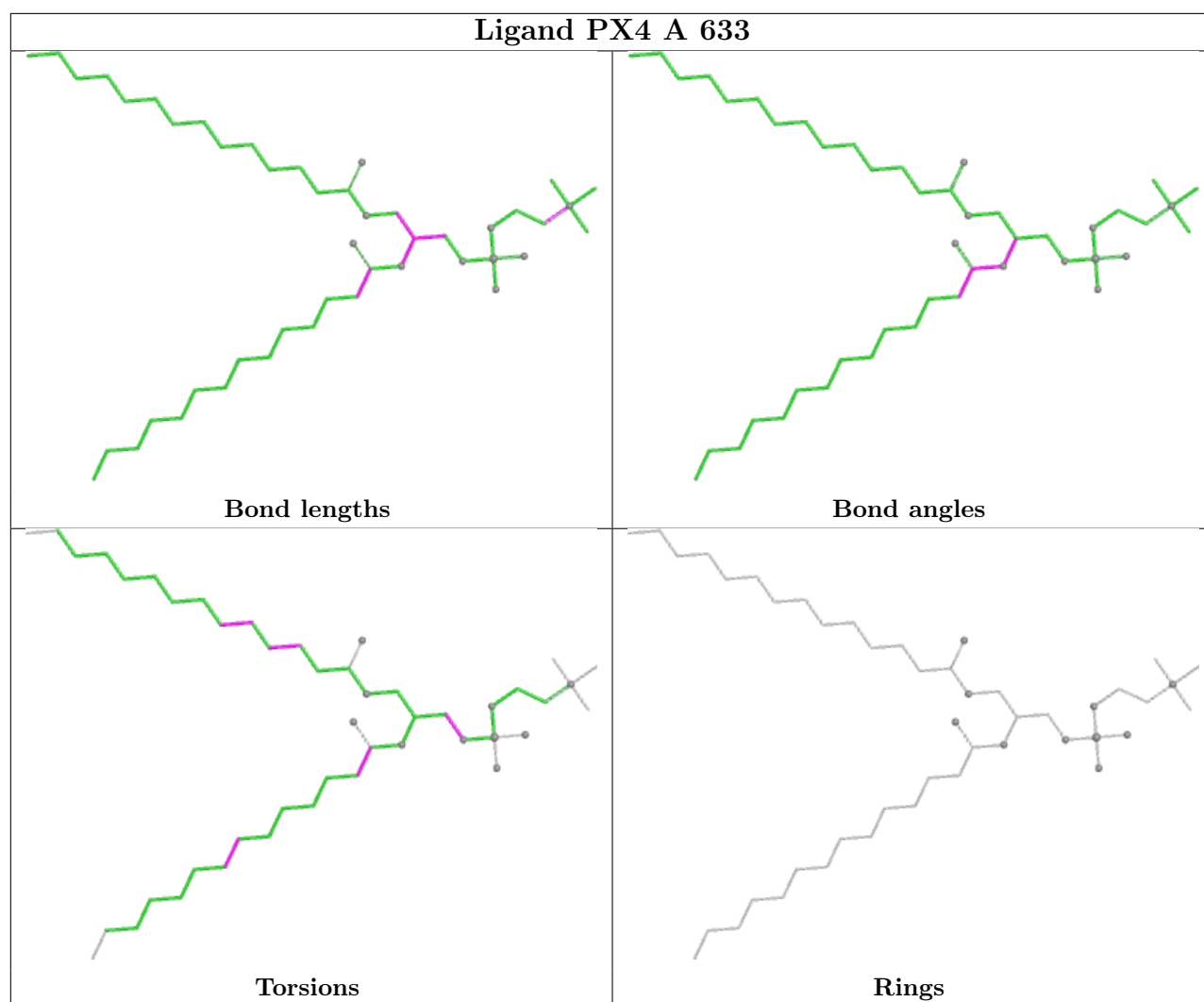
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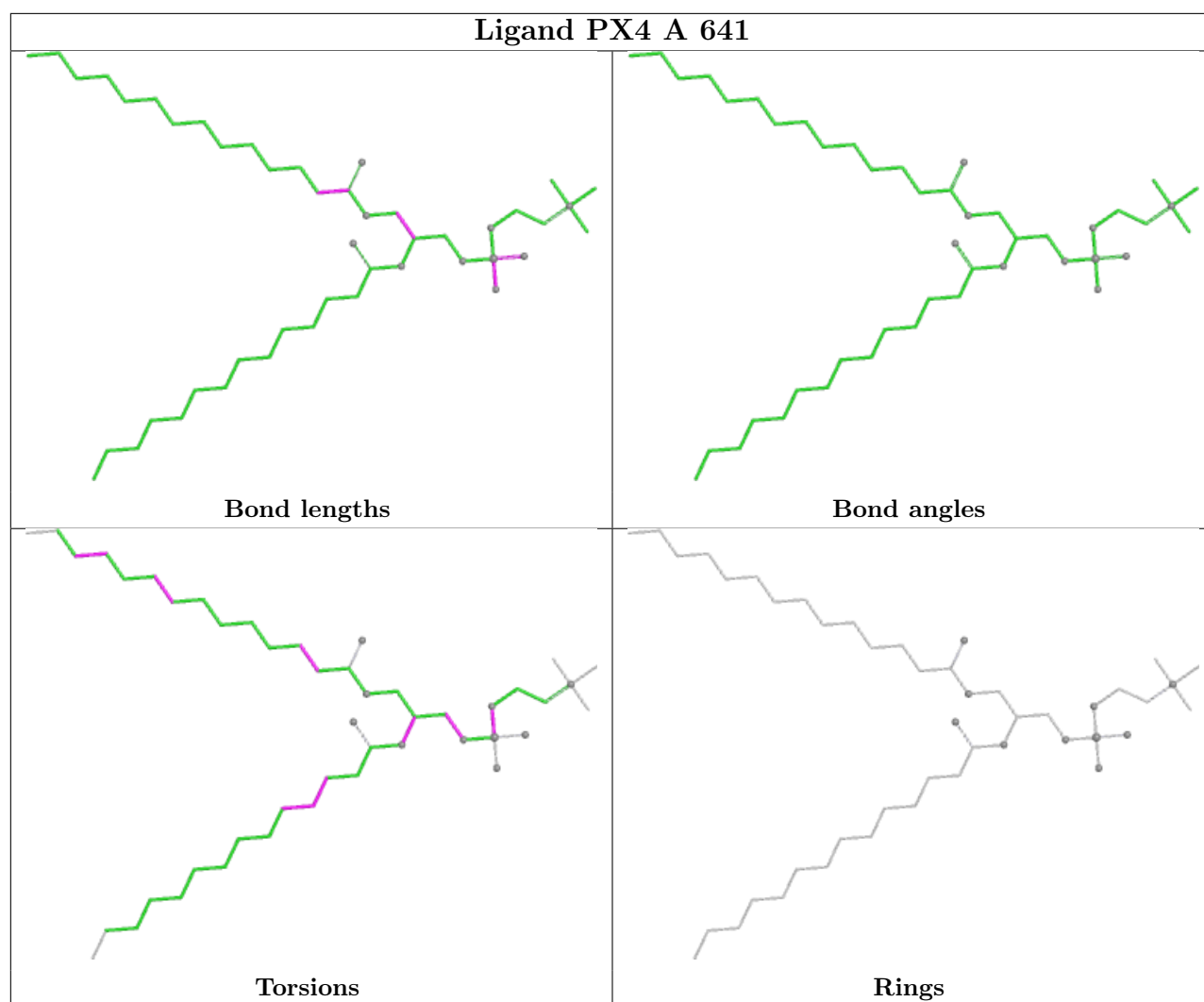


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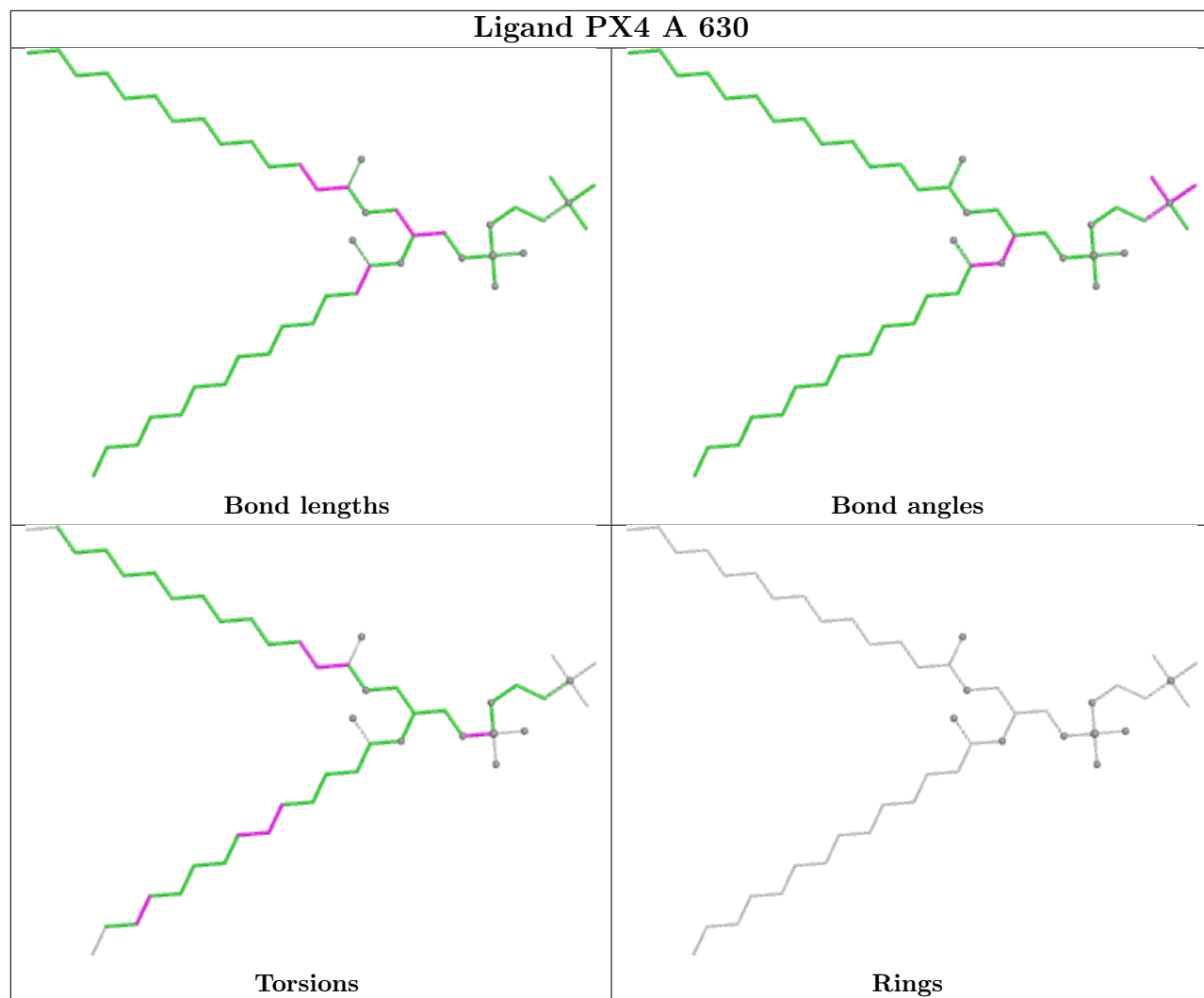


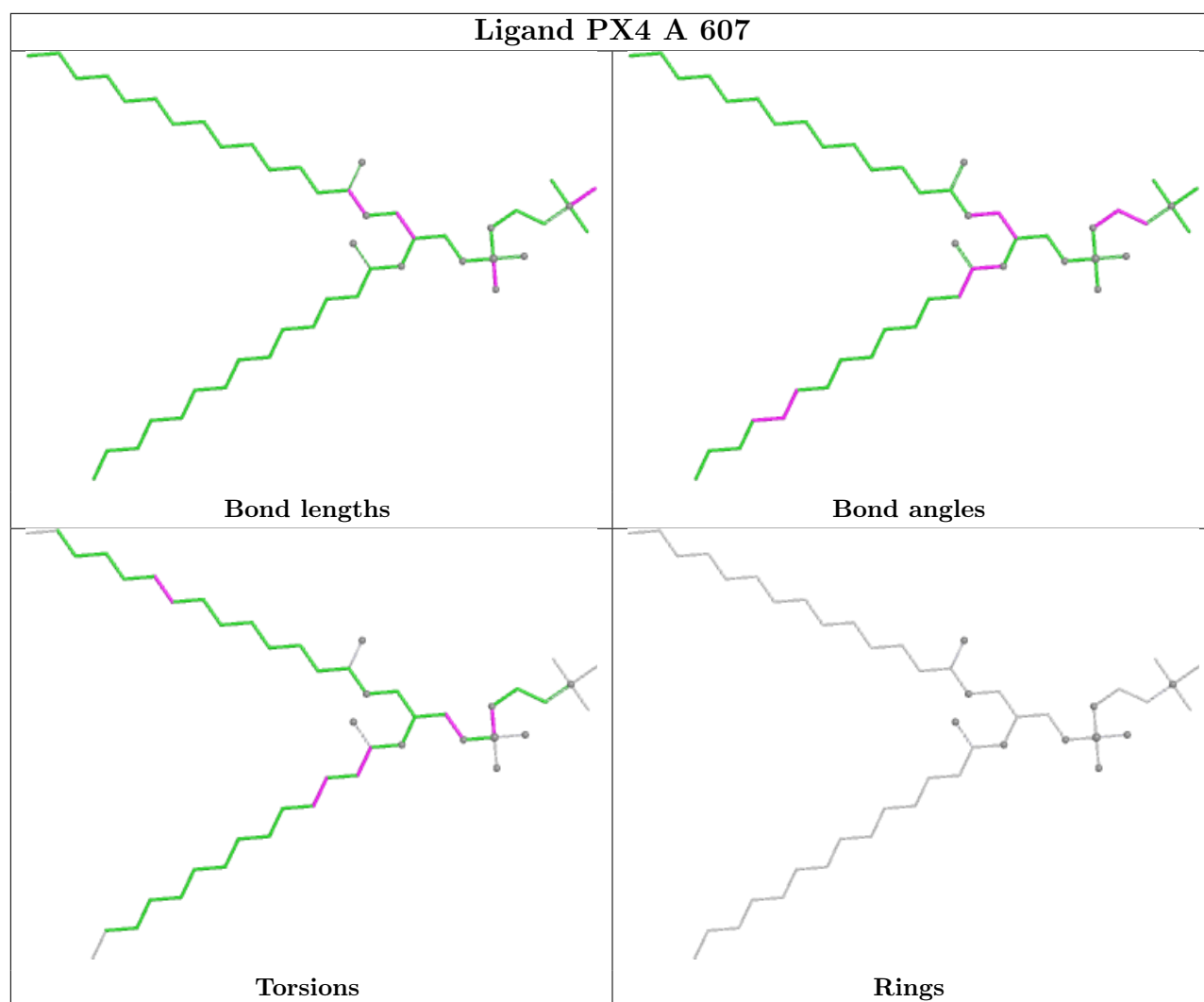




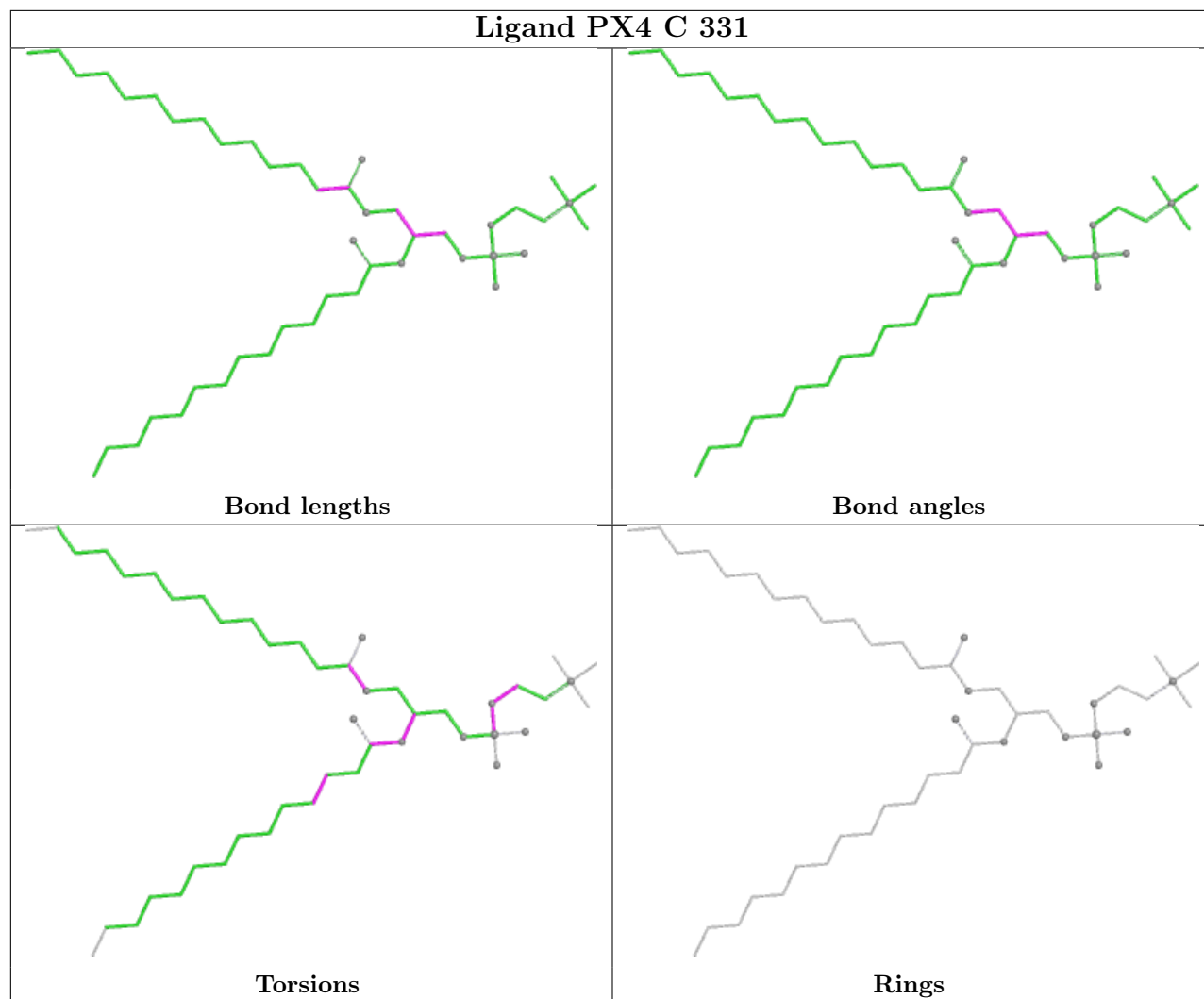


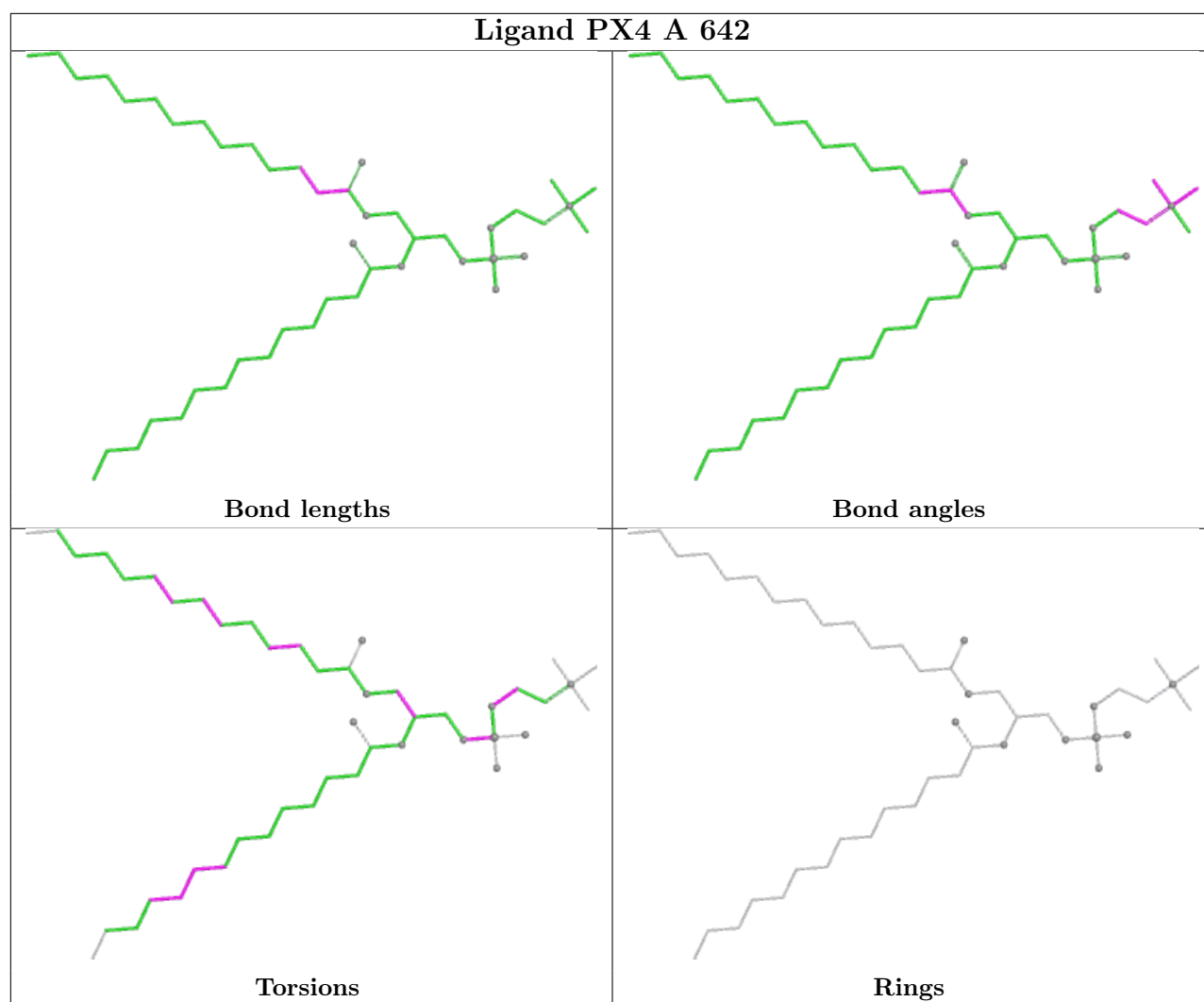
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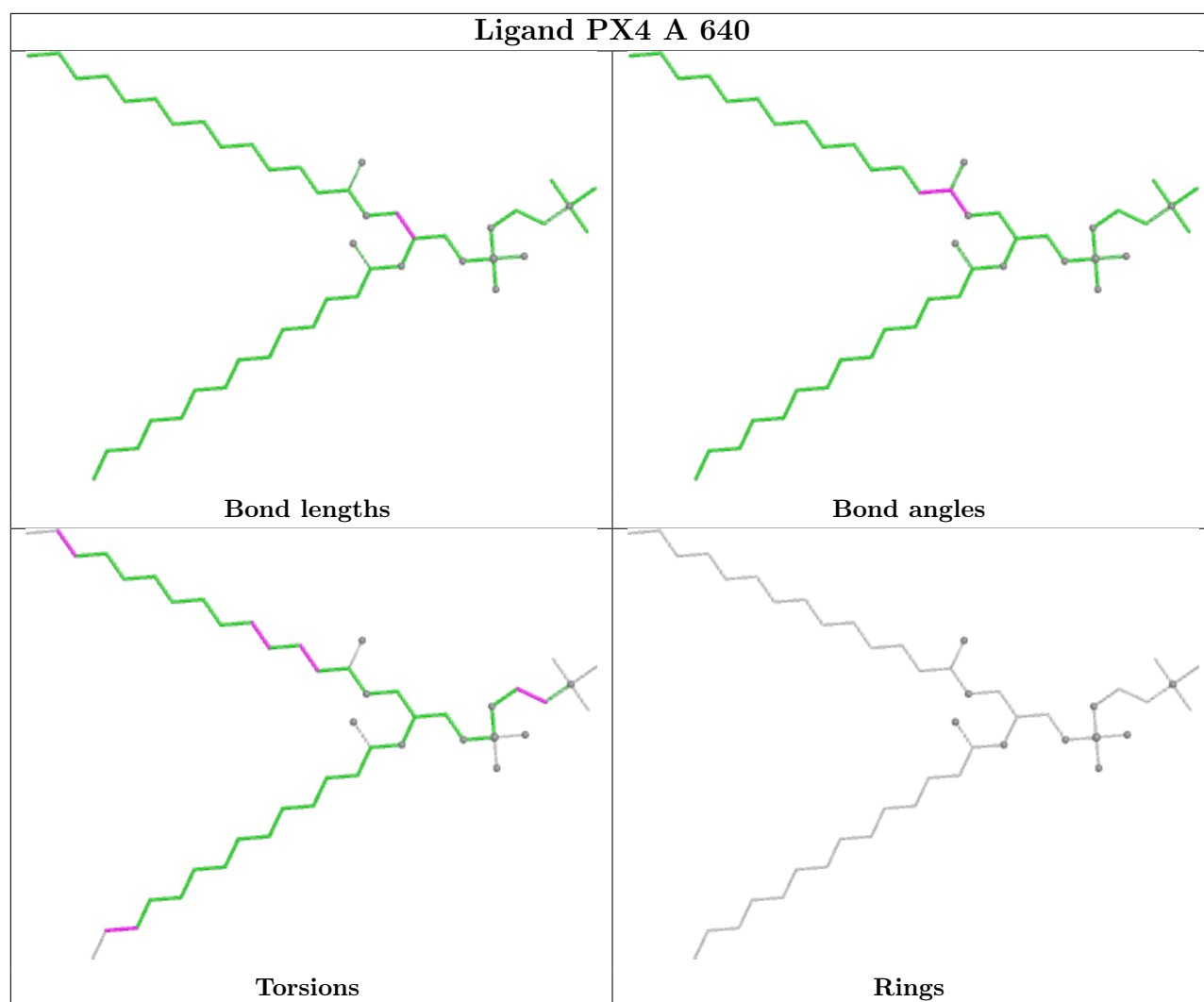


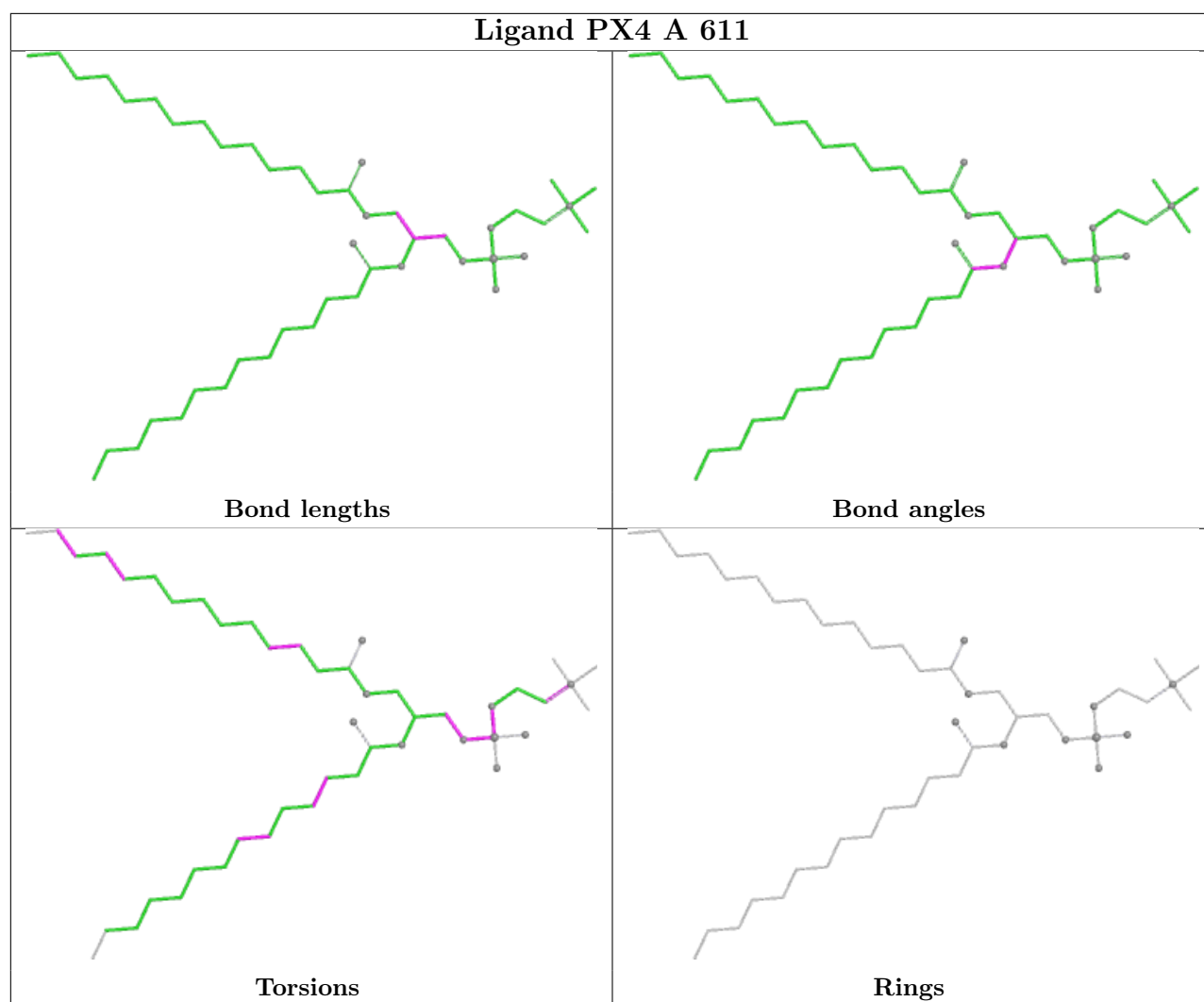


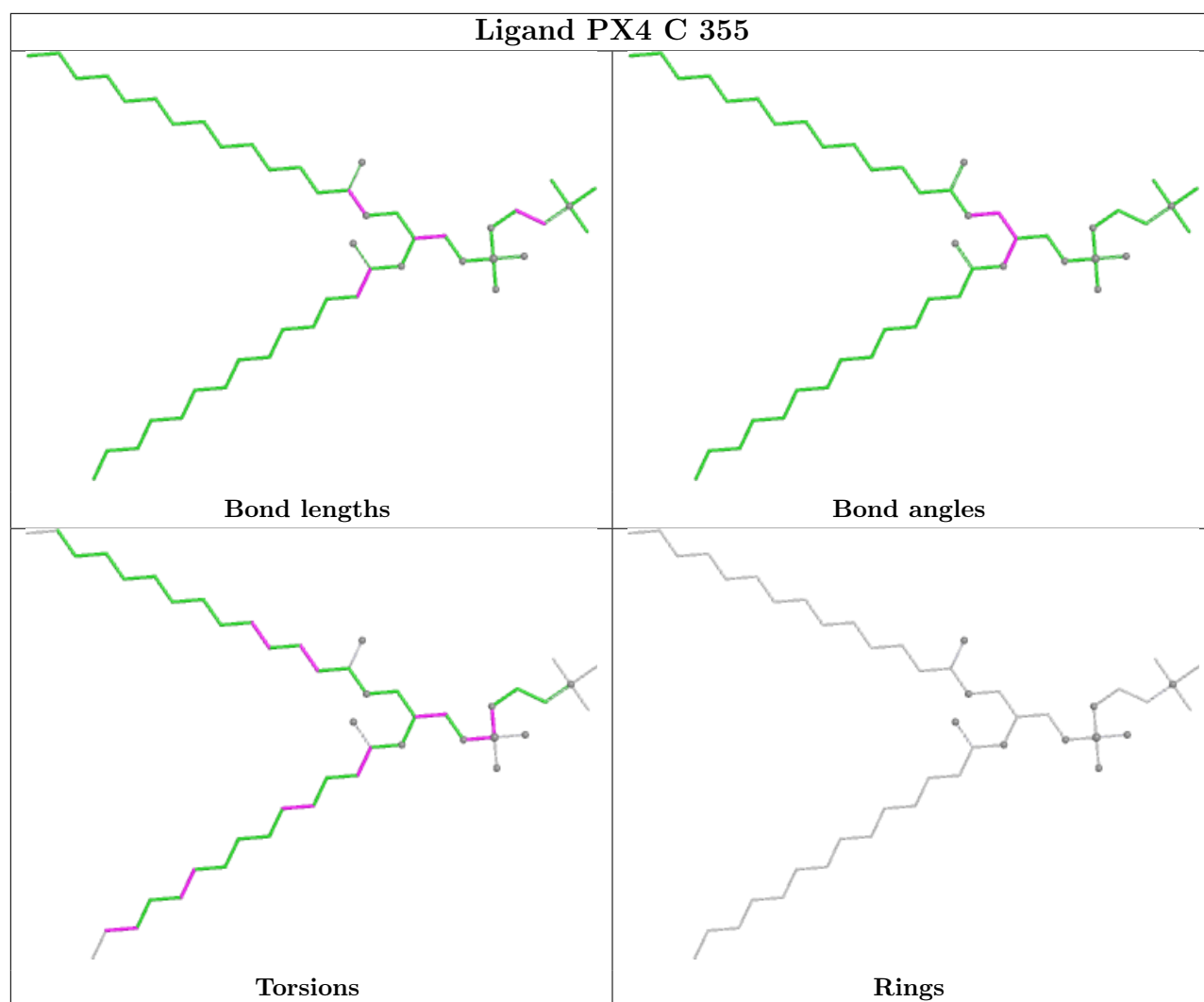
Ligand PX4 C 331

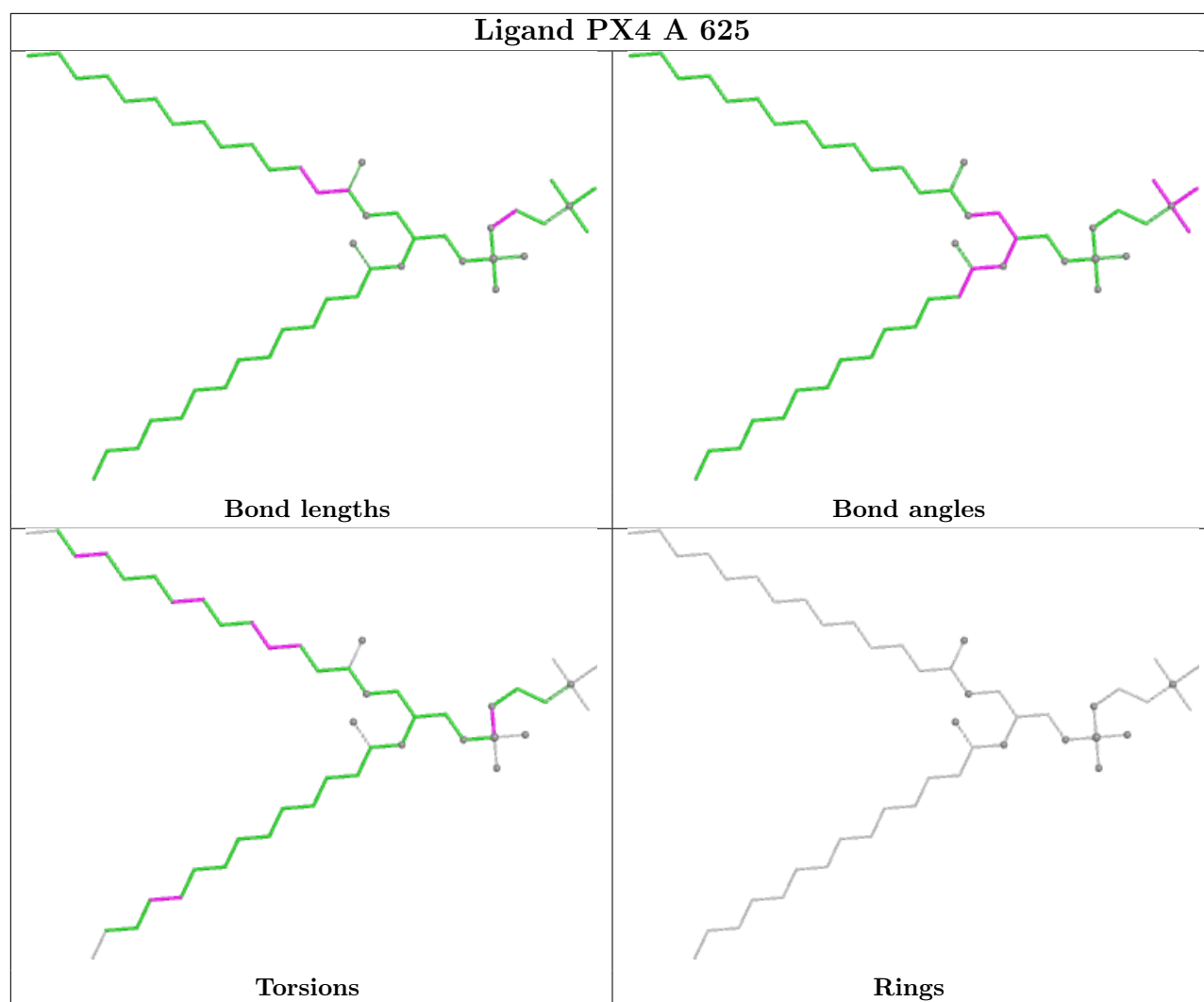


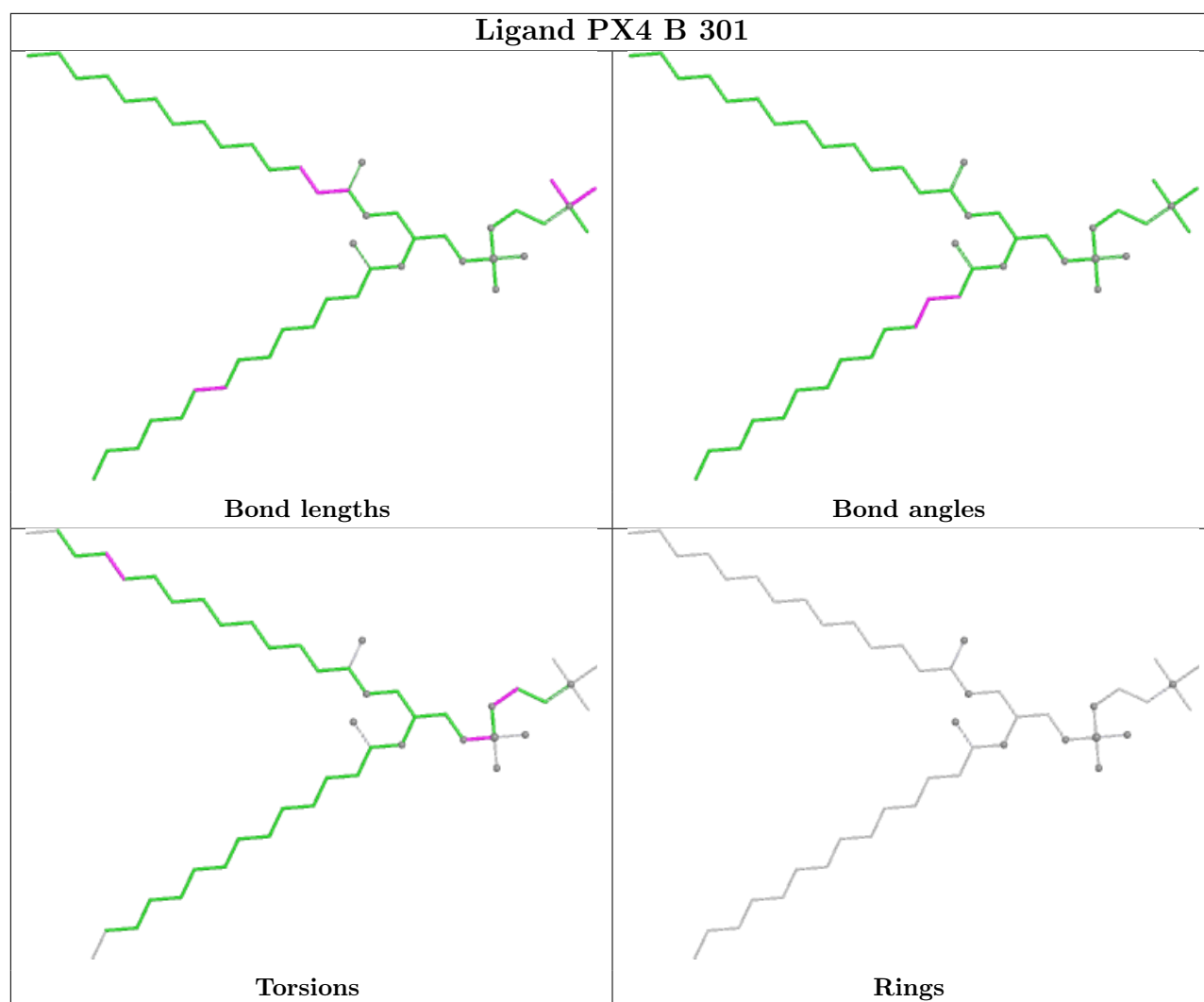


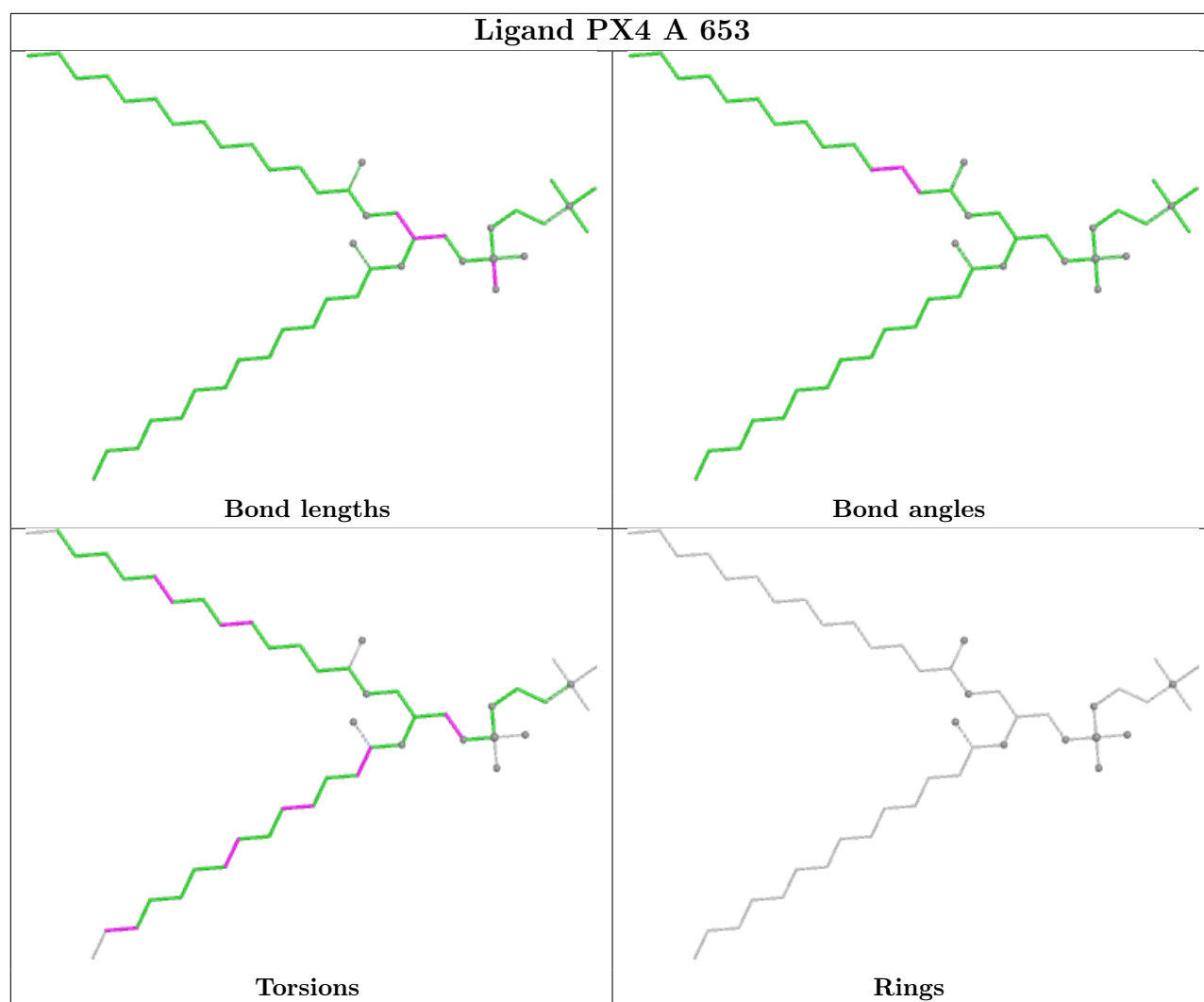




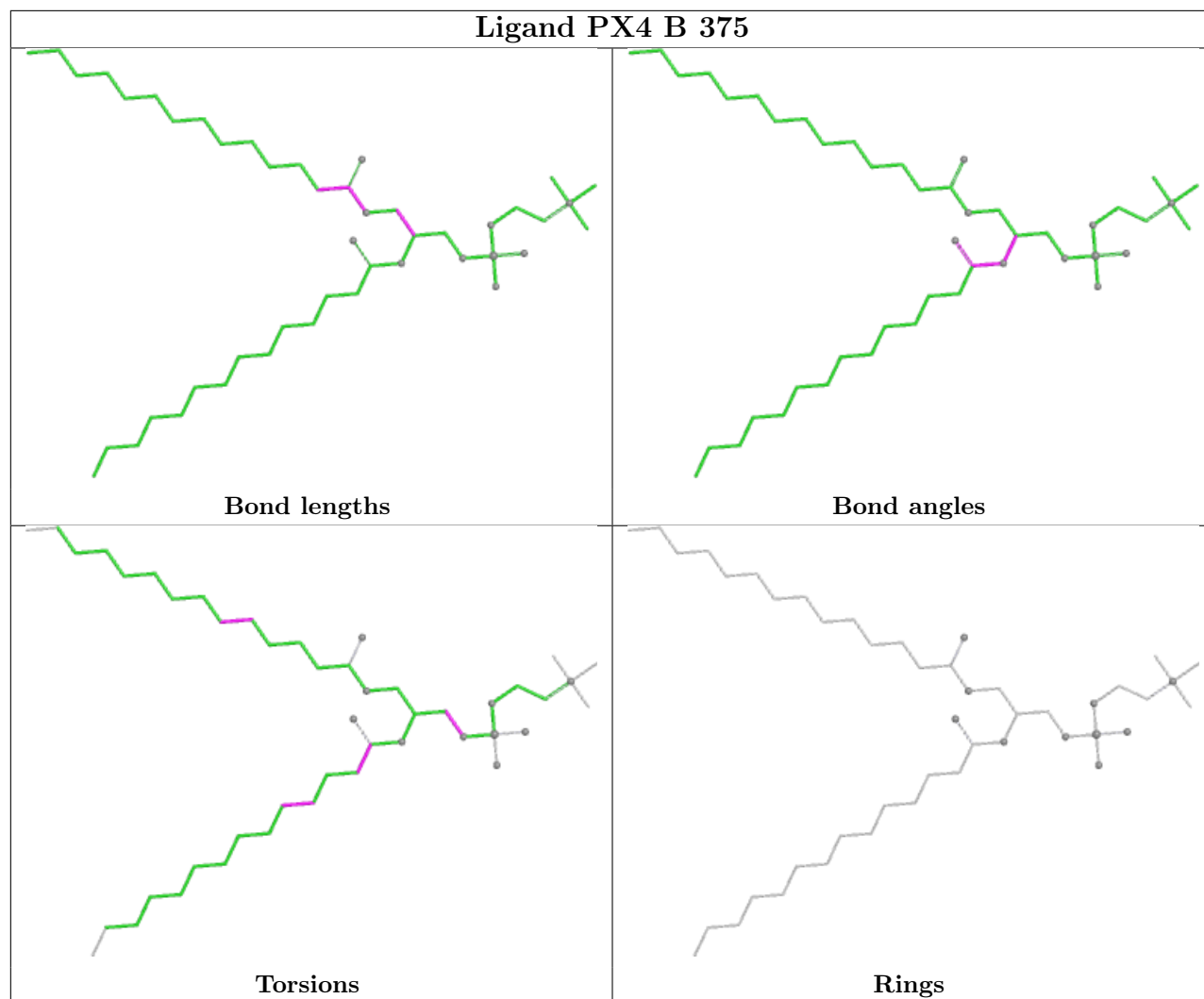




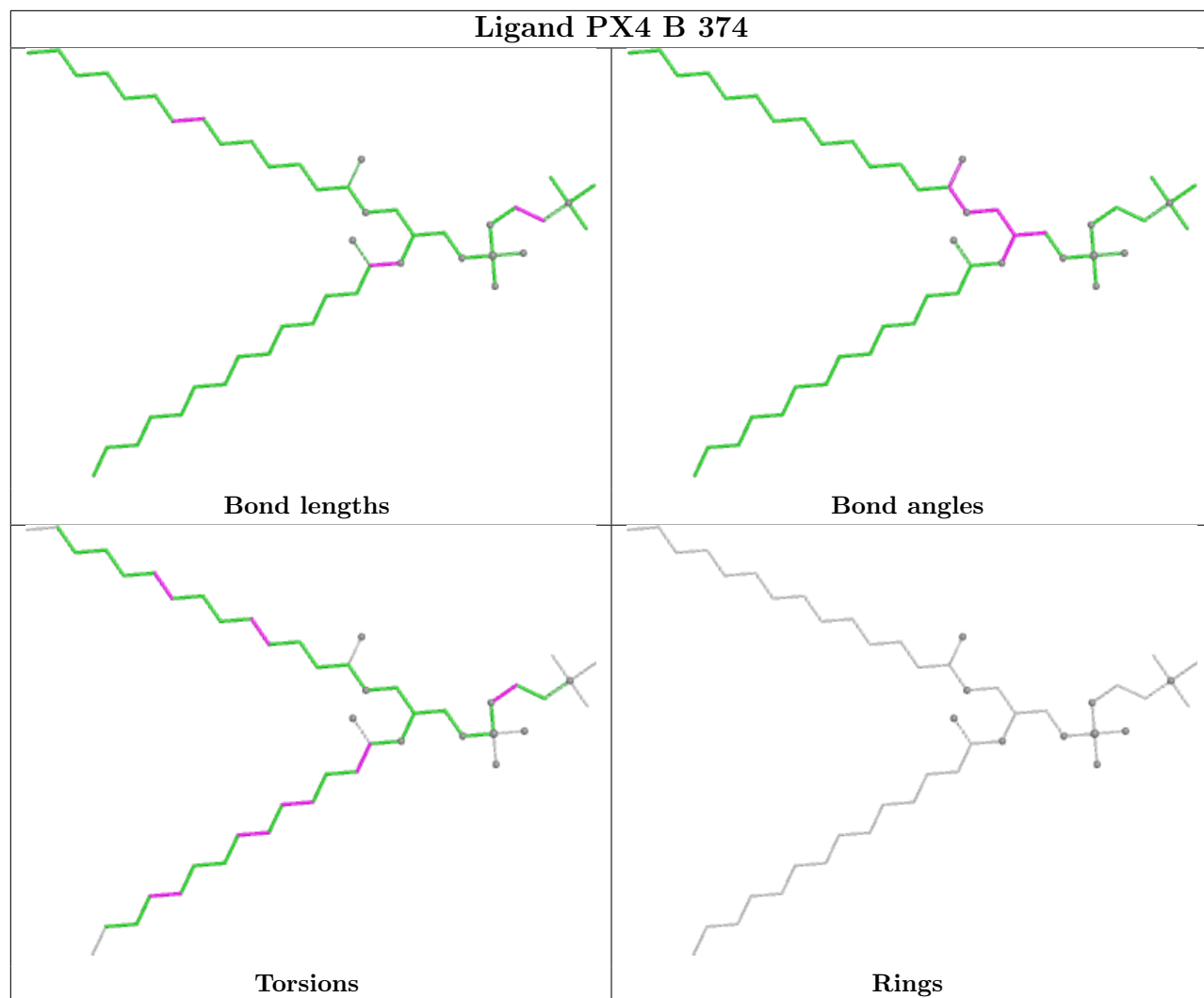


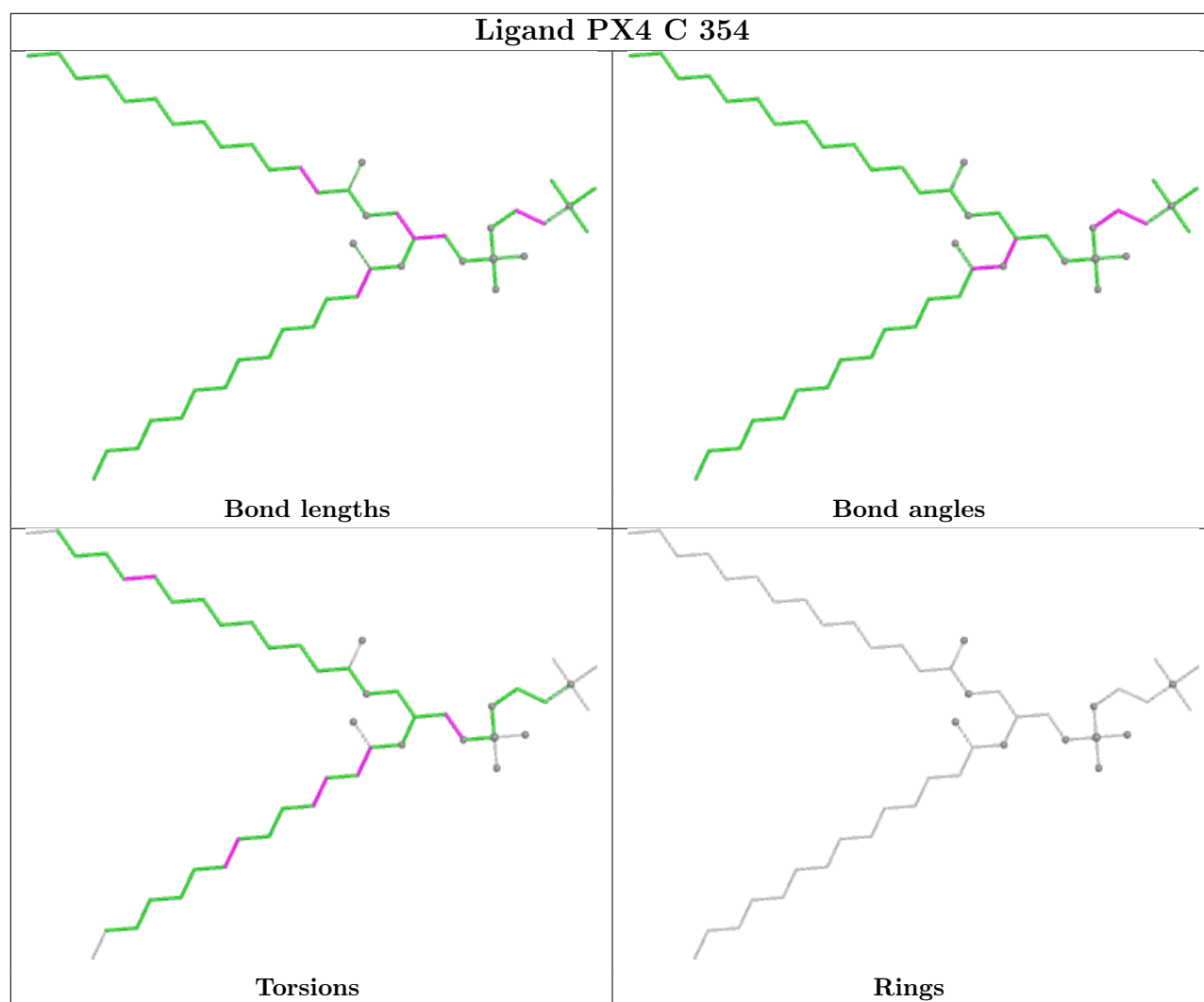


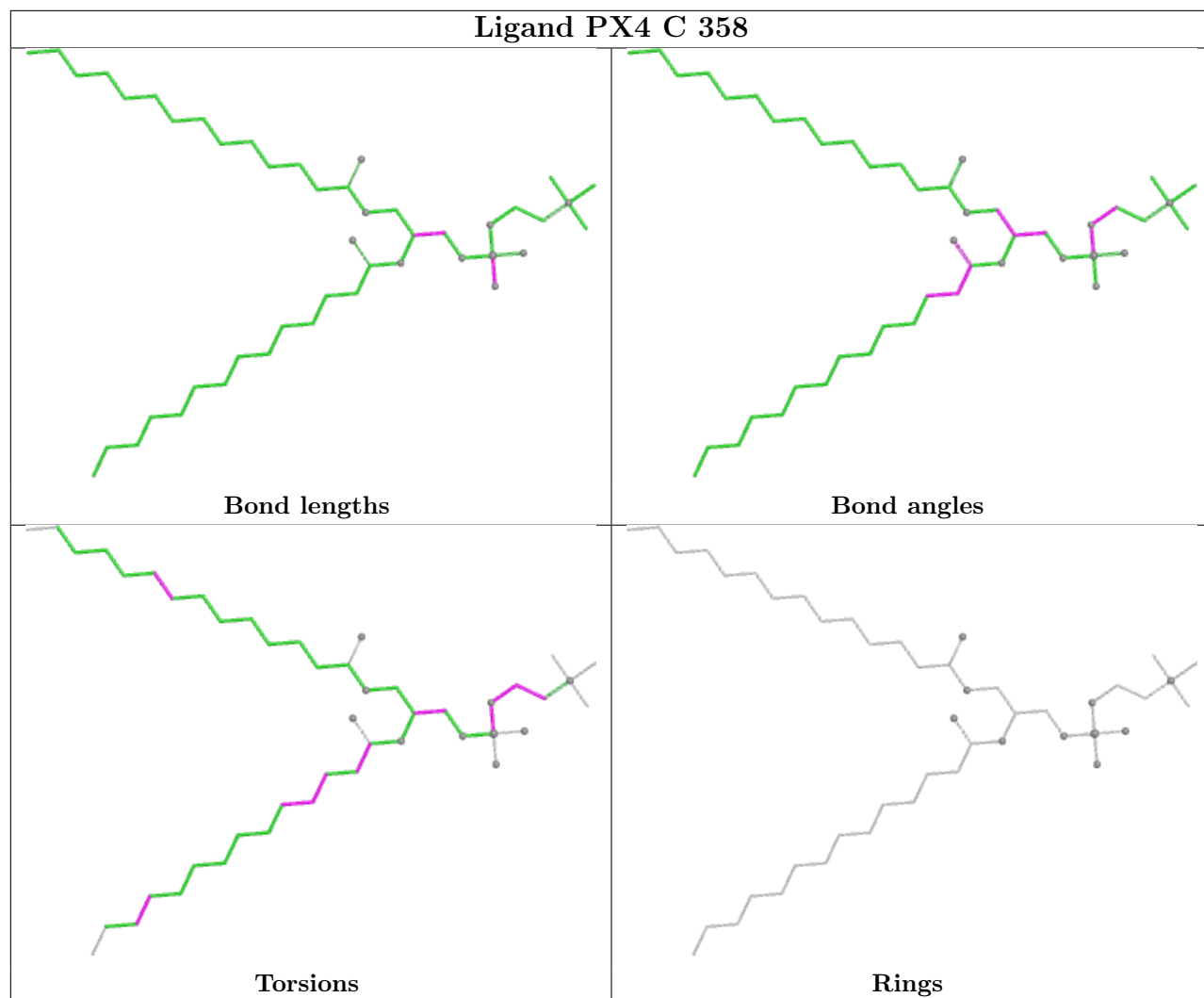
Ligand PX4 B 375



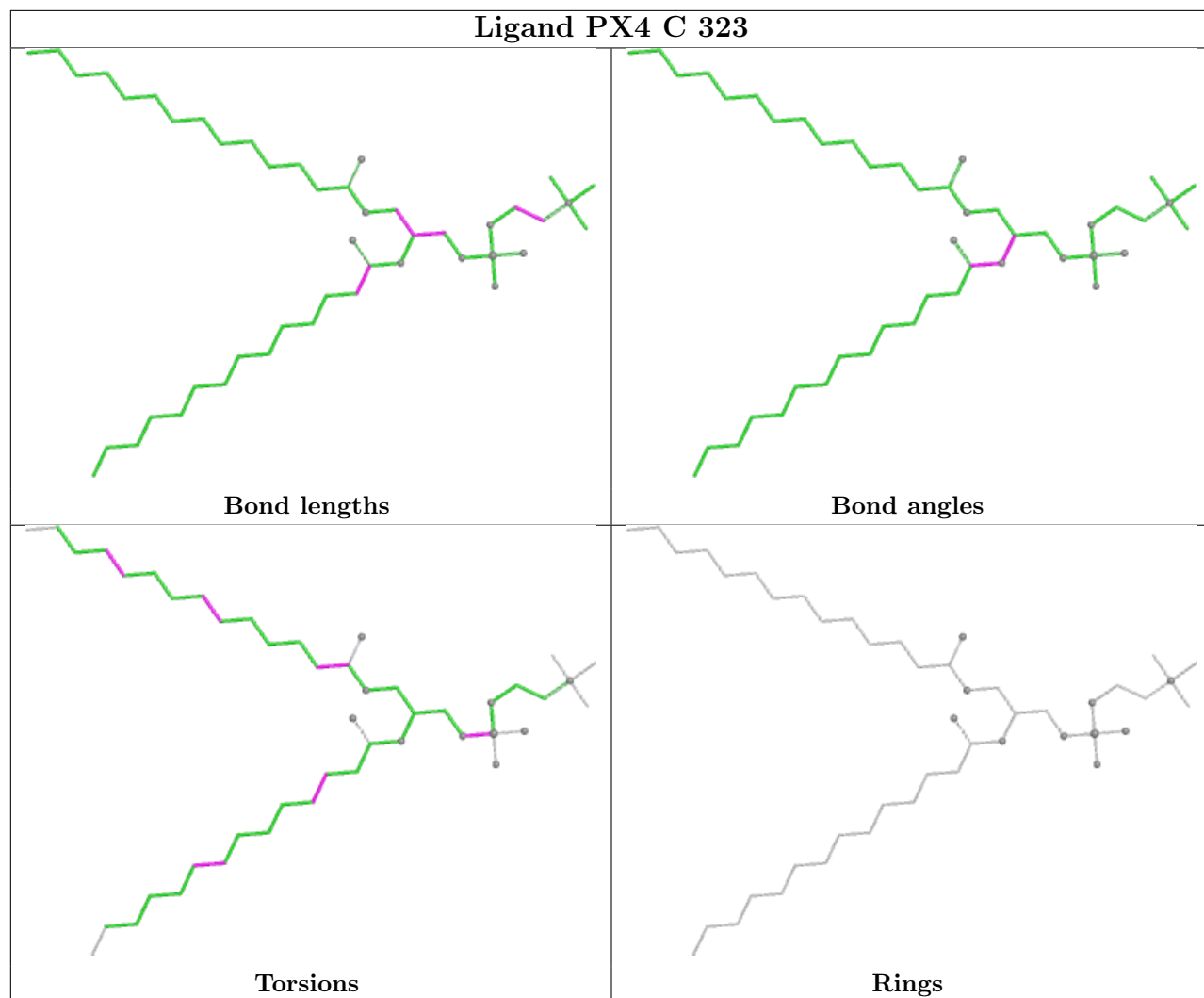
Ligand PX4 B 374



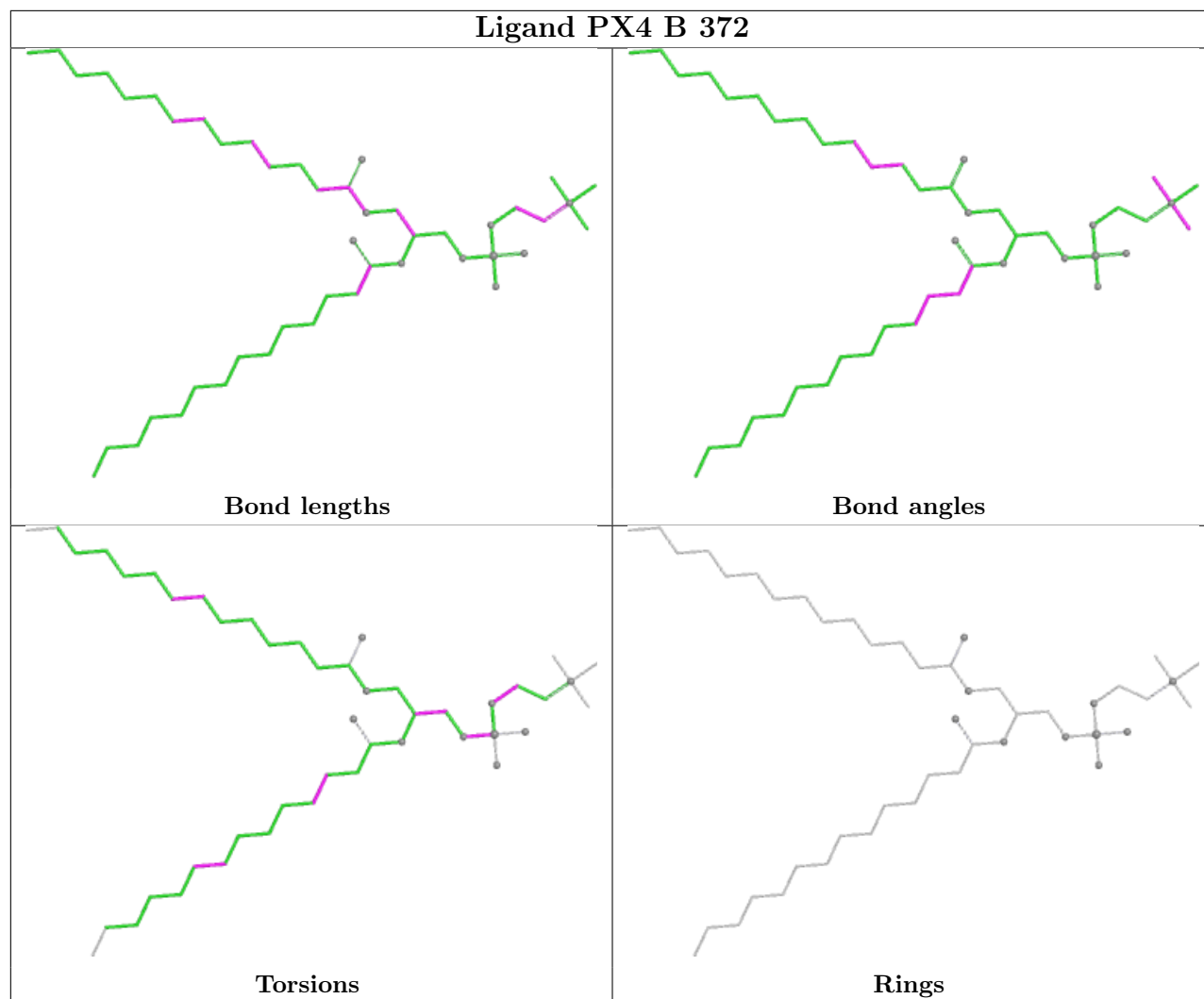


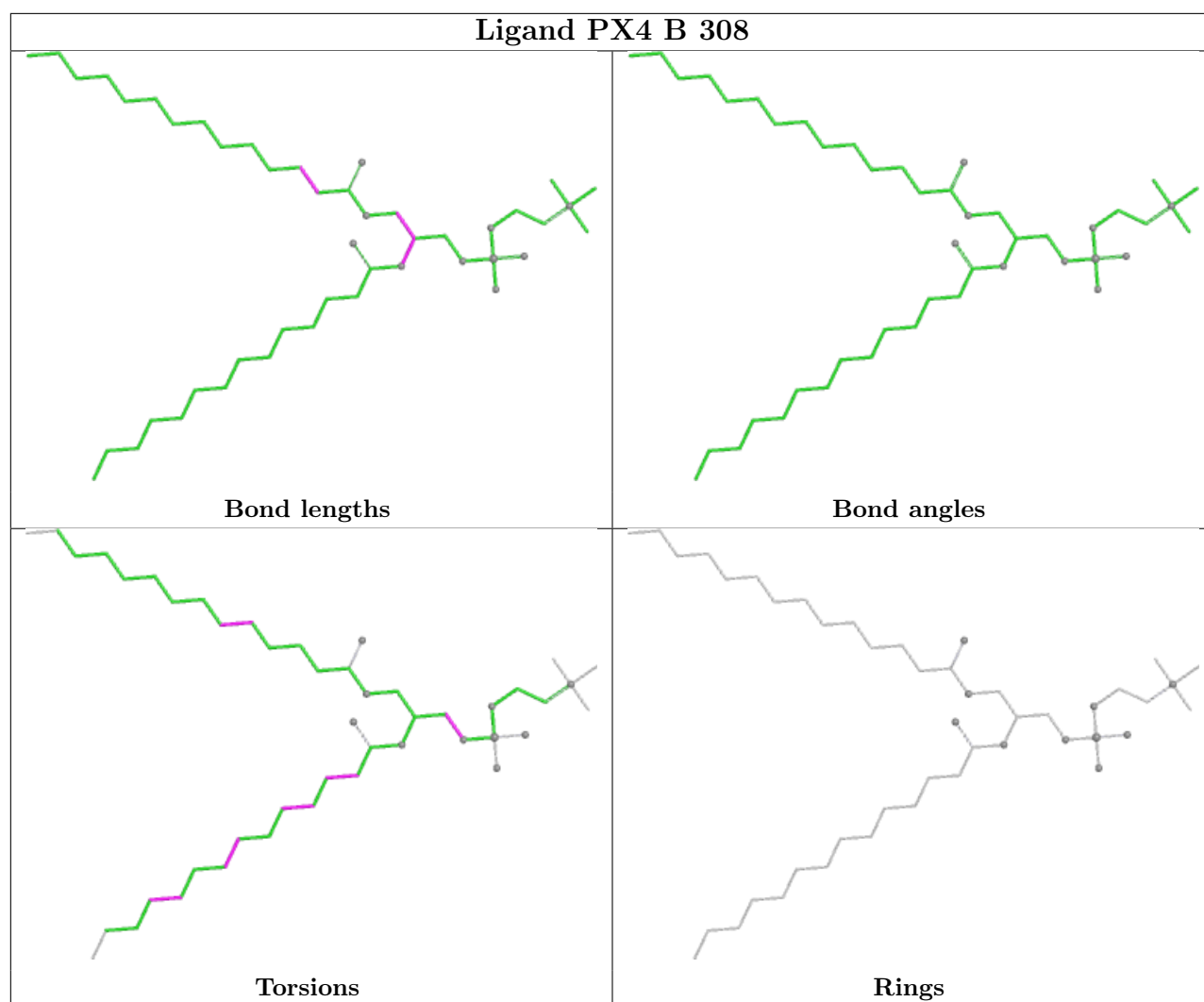


Ligand PX4 C 323

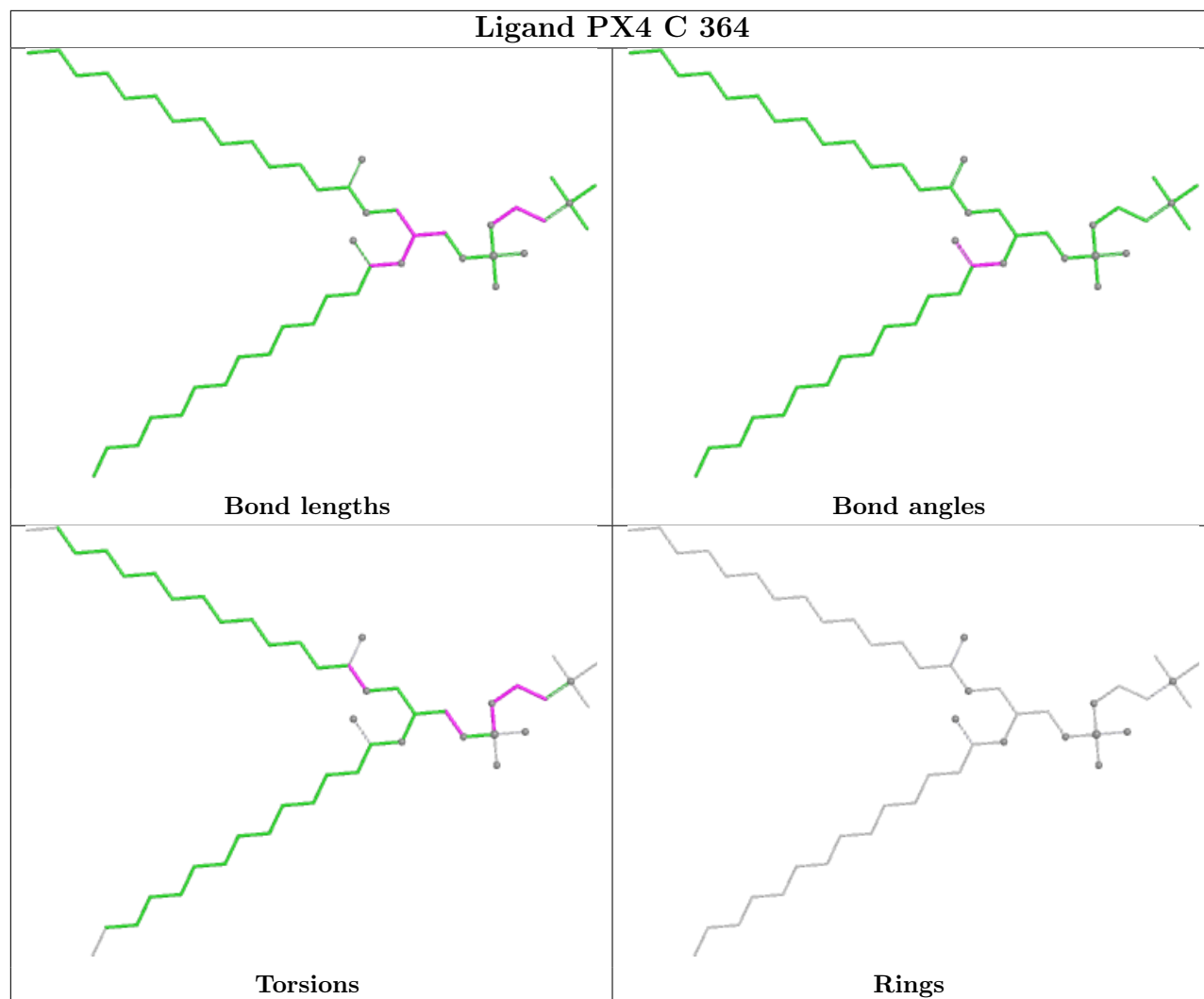


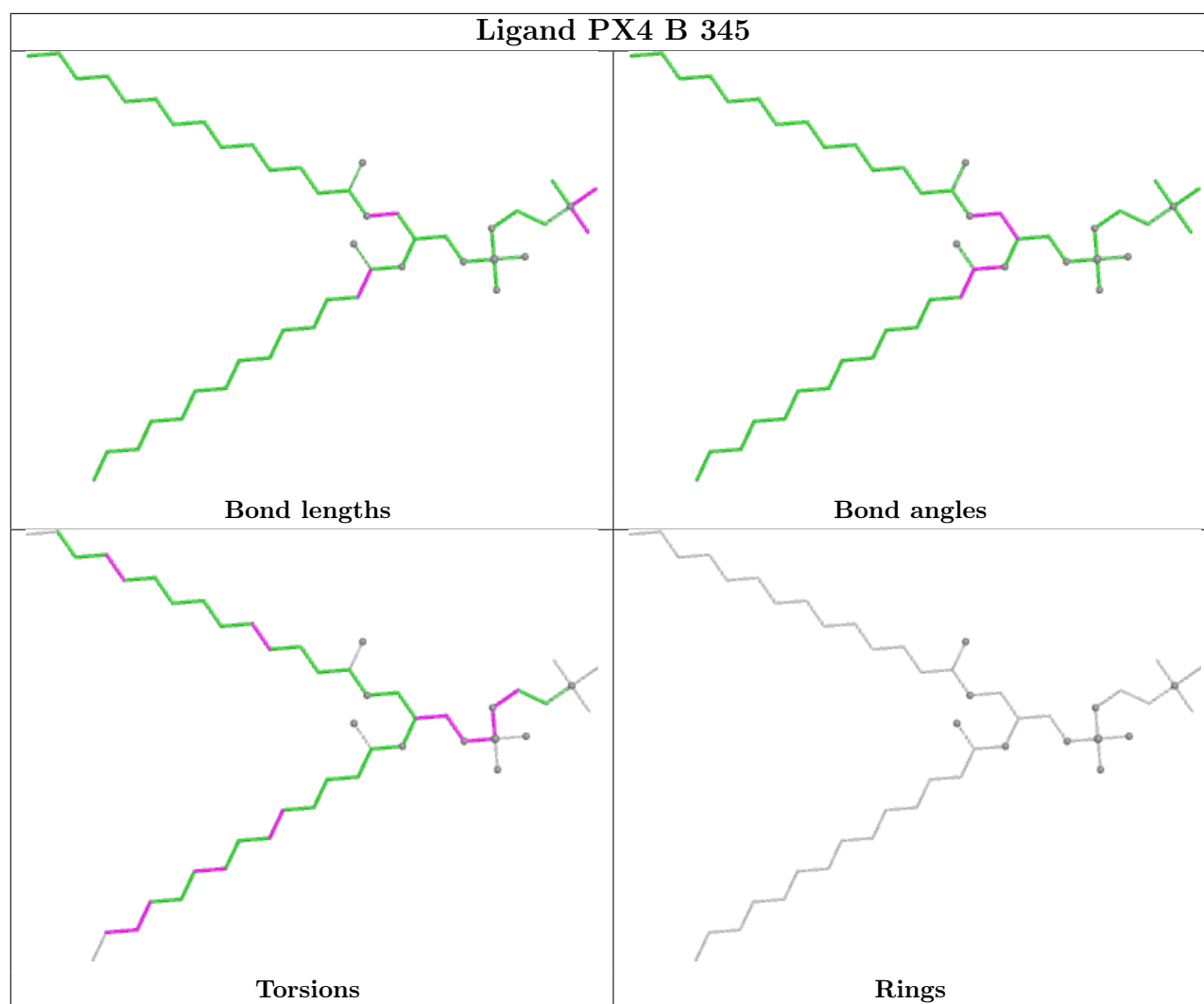
Ligand PX4 B 372

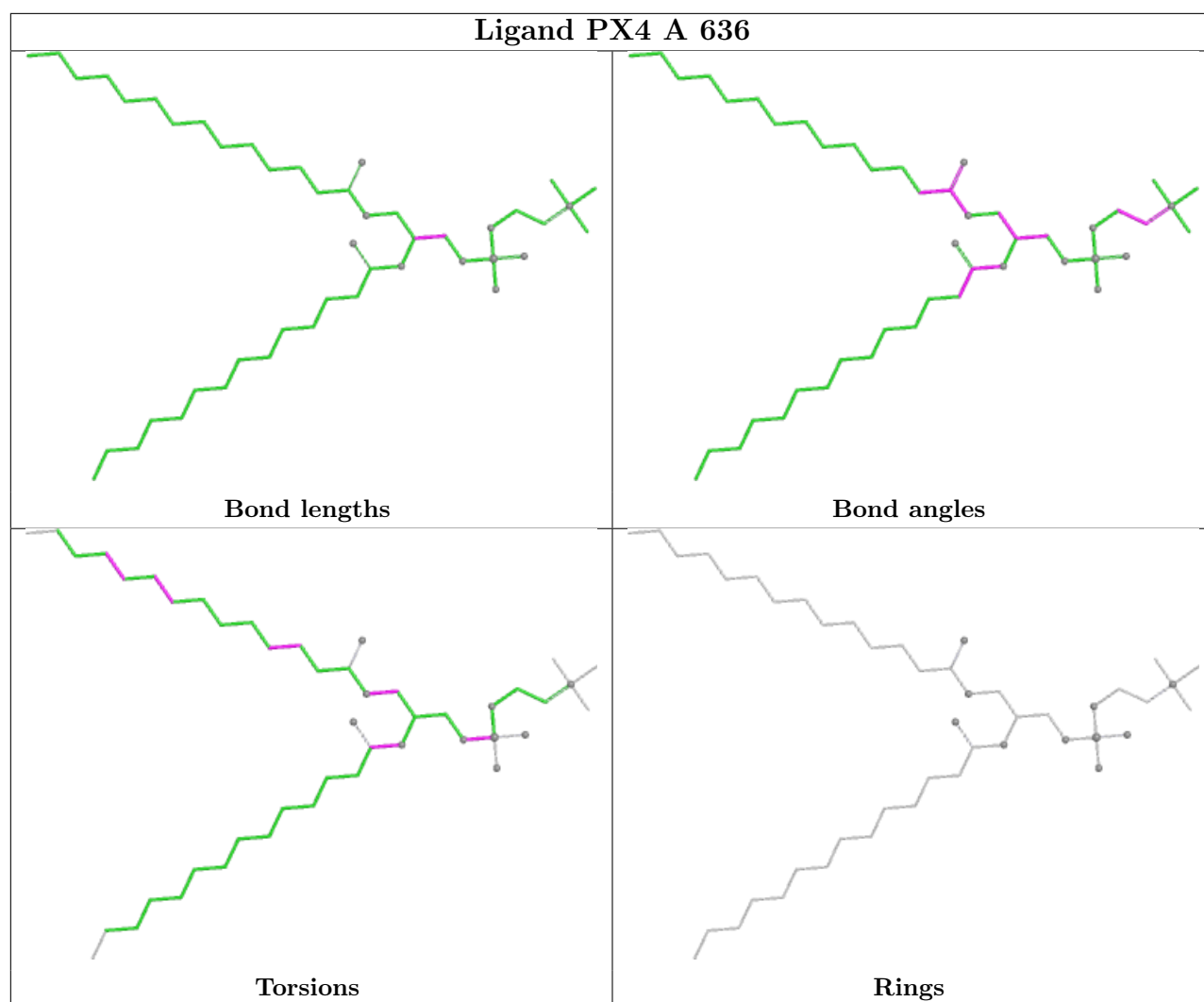




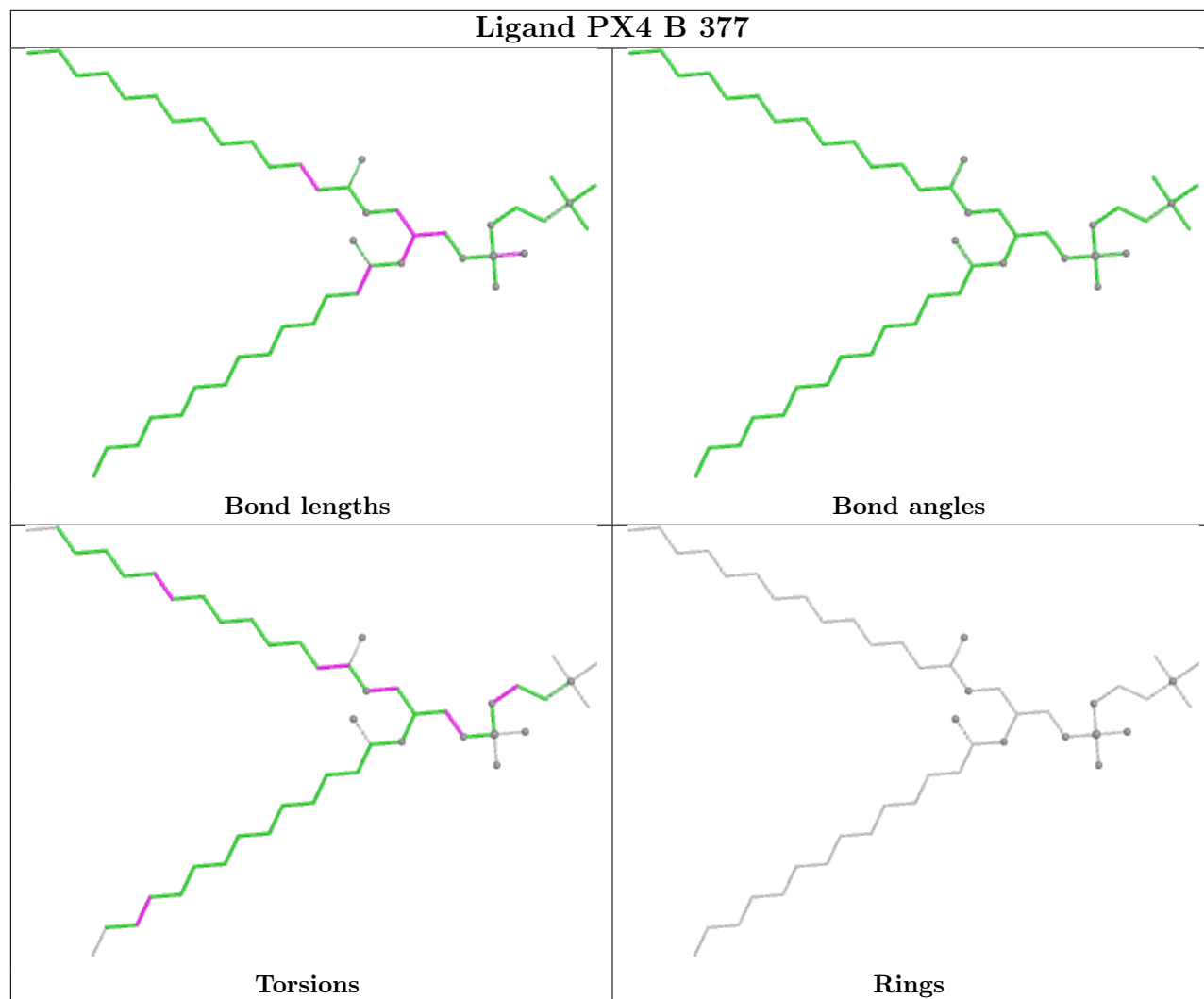
Ligand PX4 C 364

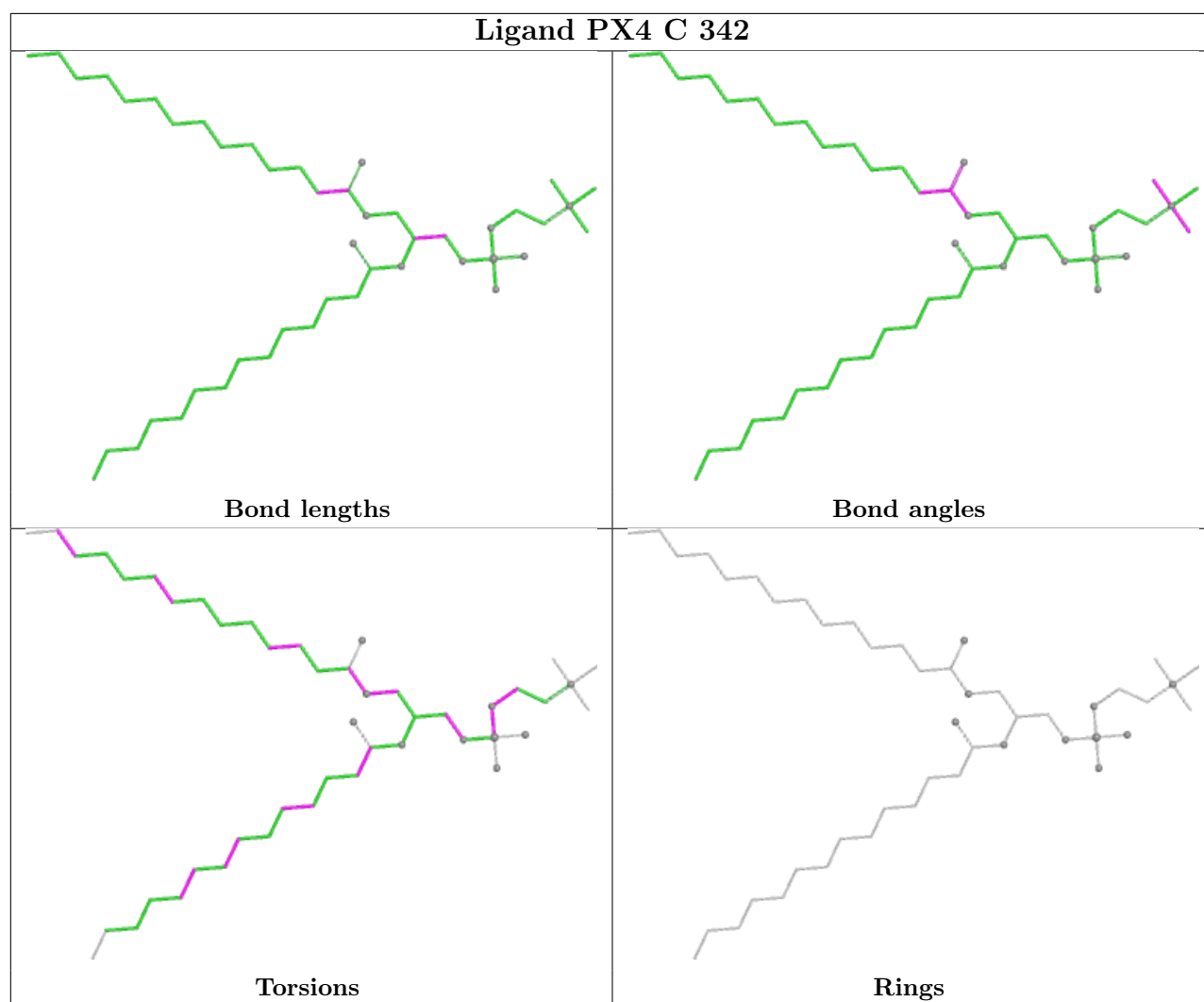




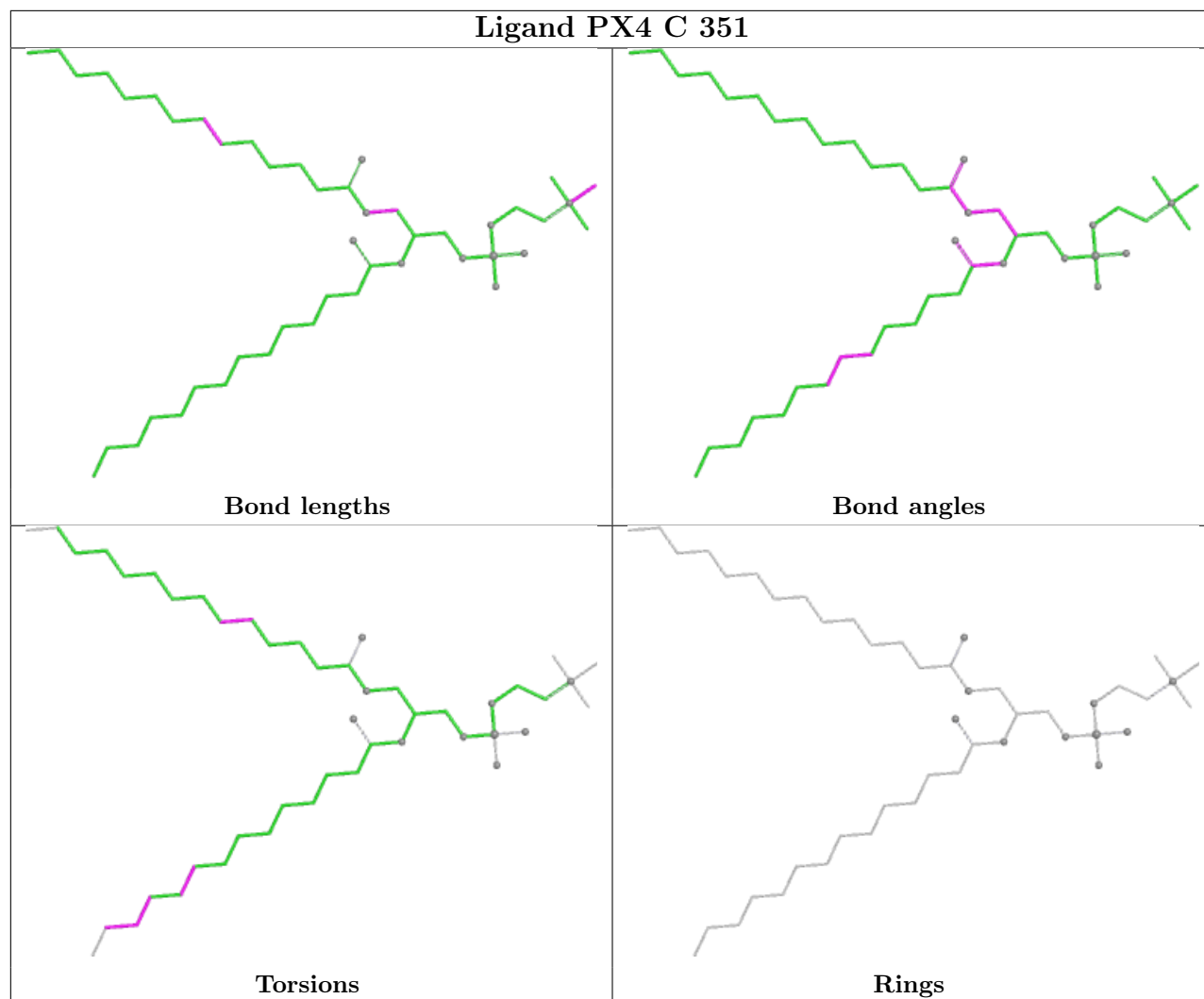


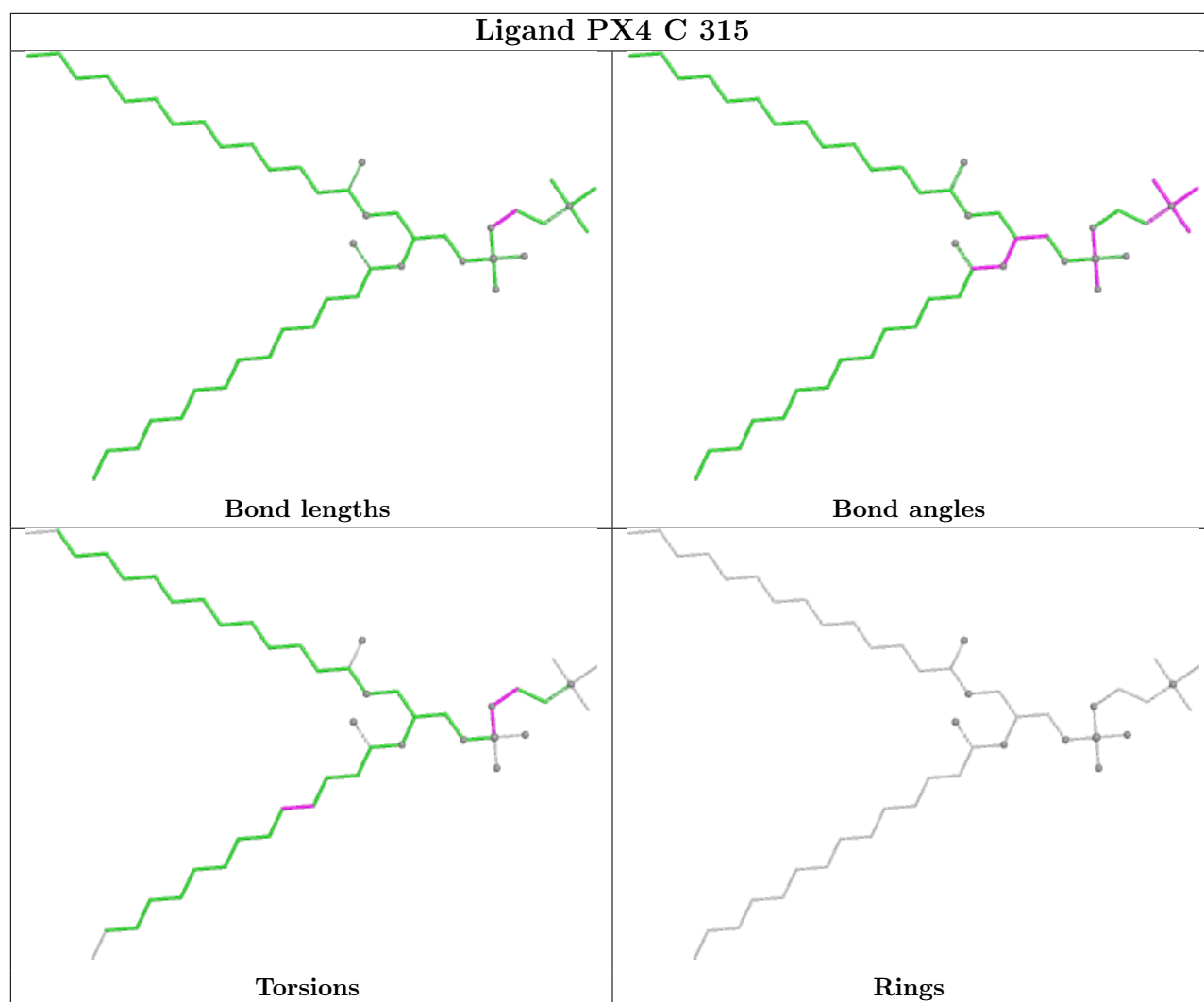
Ligand PX4 B 377

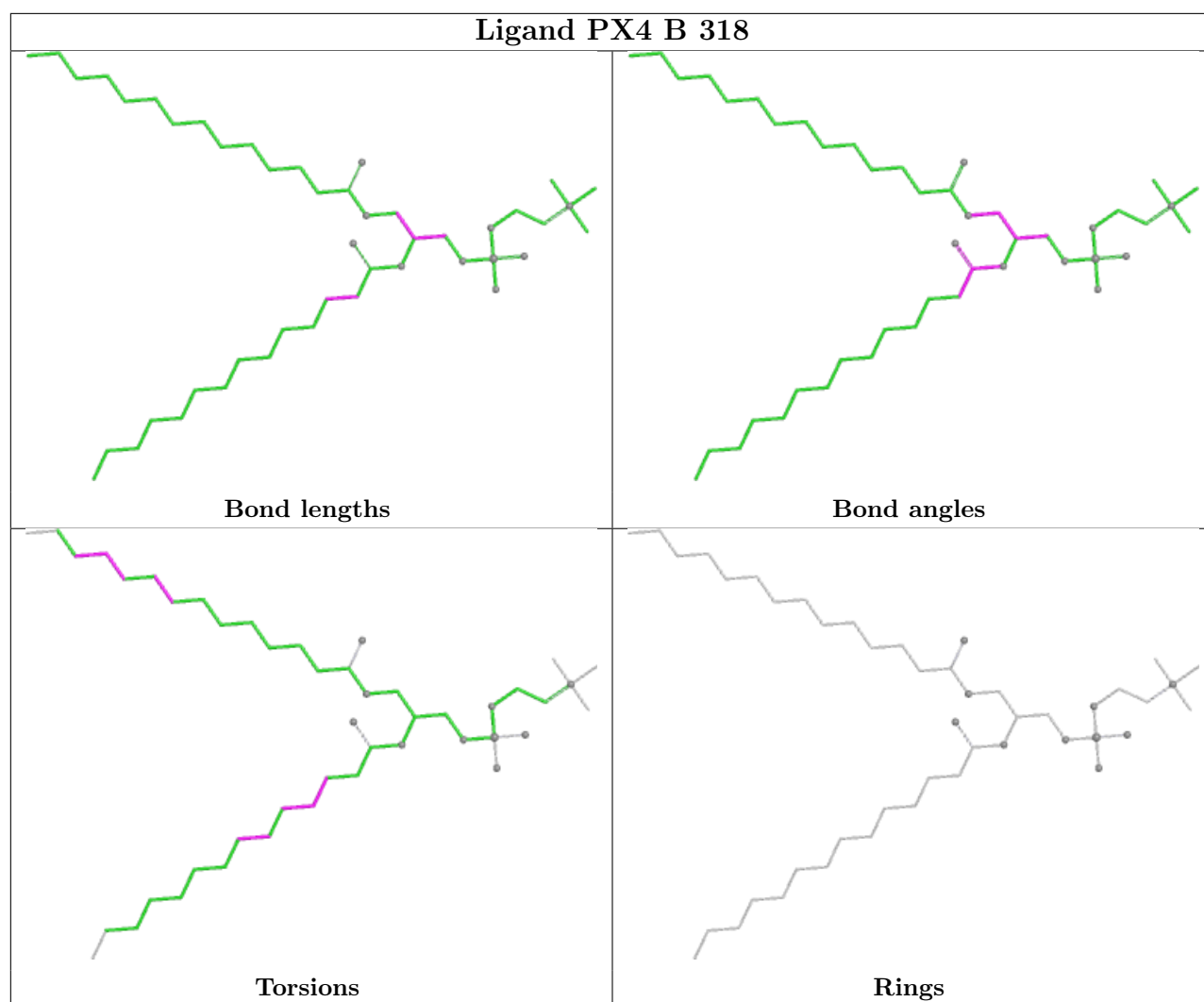




Ligand PX4 C 351







6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Deposition_nmr_coordinates_6Aug18.txt*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	92	1.11 ± 0.63	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 324 atoms were assigned a chemical shift out of a possible 8785. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	184/3048 (6%)	92/1233 (7%)	0/1230 (0%)	92/585 (16%)
Sidechain	140/4970 (3%)	105/3181 (3%)	35/1554 (2%)	0/235 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/767 (0%)	0/377 (0%)	0/364 (0%)	0/26 (0%)
Overall	324/8785 (4%)	197/4791 (4%)	35/3148 (1%)	92/846 (11%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:

