



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:22 AM UTC

PDB ID : 2MZI / pdb_00002mzi
BMRB ID : 25489
Title : NMR Solution Structure of the PRO Form of Human Matrilysin (proMMP-7)
in Complex with Anionic Membrane
Authors : Prior, S.H.; Van Doren, S.R.
Deposited on : 2015-02-12

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We welcome your comments at validation@mail.wwpdb.org

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

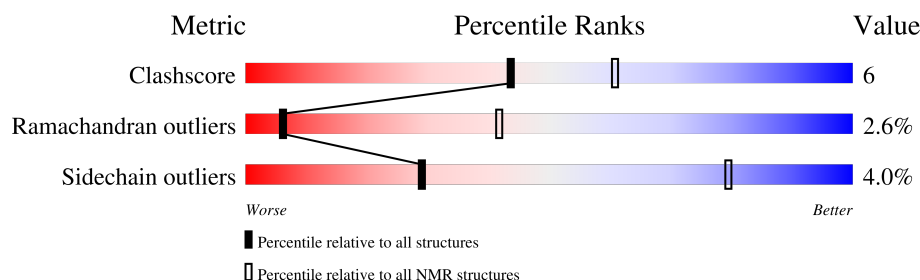
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 25%.

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	250	

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

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
5	A	C3S	431	20	-
5	A	C3S	432	20	-
5	A	C3S	433	20	-
5	A	C3S	434	20	-
5	A	C3S	435	20	-
5	A	C3S	436	20	-

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:75, A:82-A:244 (237)	1.20	5

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 8, 10, 11, 12, 15, 17, 18, 19
2	3, 6, 9, 13, 14, 16
3	1, 7, 20

3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10109 atoms, of which 2165 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrilysin.

Mol	Chain	Residues	Atoms						Trace
1	A	248	Total	C	H	N	O	S	0
			3847	1240	1895	339	364	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	GLU	engineered mutation	UNP P09237

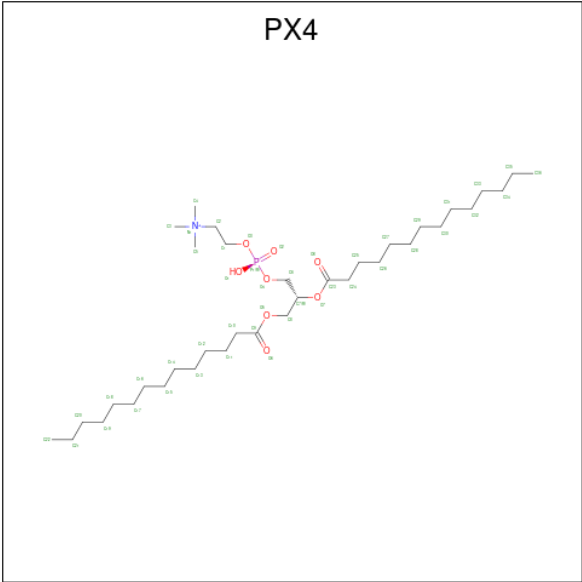
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

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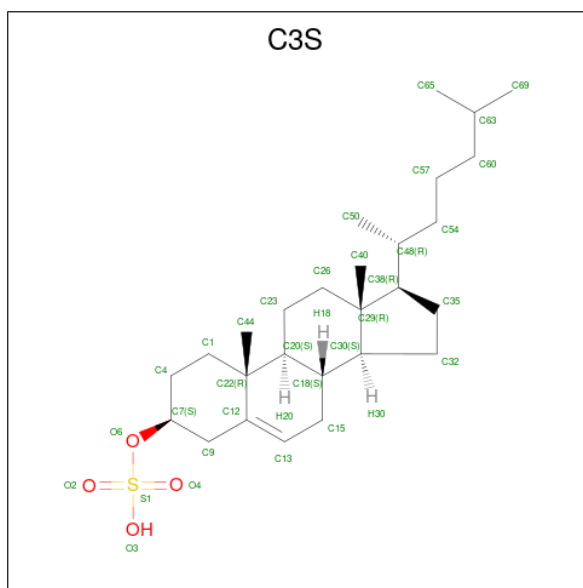
[illegible]

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Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

- Molecule 5 is CHOLEST-5-EN-3-YL HYDROGEN SULFATE (CCD ID: C3S) (formula: $C_{27}H_{46}O_4S$).



Mol	Chain	Residues	Atoms				
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1

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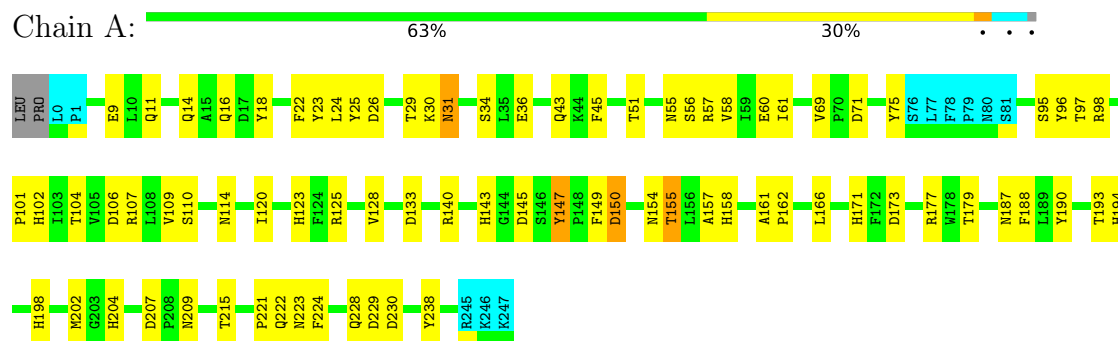
Mol	Chain	Residues	Atoms				
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

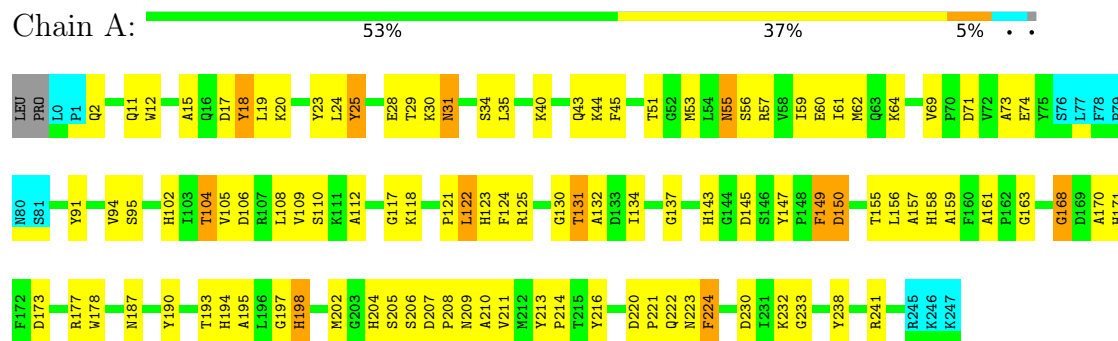
- Molecule 1: Matrilysin



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

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Matrilysin



5 Refinement protocol and experimental data overview

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

Of the 10000 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
HADDOCK	structure solution	2.1
GROMOS	refinement	4.5.7

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	797
Number of shifts mapped to atoms	797
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C3S, PX4, ZN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.56±0.00	0±0/1912 (0.0± 0.0%)	2.55±0.05	149±11/2587 (5.8± 0.4%)
All	All	0.56	0/38240 (0.0%)	2.55	2989/51740 (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	7.2±2.1
All	All	0	144

There are no bond-length outliers.

5 of 1161 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
1	A	149	PHE	CA-CB-CG	14.12	127.92	113.80	7	13
1	A	45	PHE	CA-CB-CG	13.65	127.45	113.80	2	14
1	A	218	ASN	CA-C-N	12.62	131.33	121.61	14	4
1	A	218	ASN	C-N-CA	12.62	131.33	121.61	14	4
1	A	102	HIS	CA-CB-CG	12.54	126.34	113.80	7	5

There are no chirality outliers.

5 of 60 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	238	TYR	Sidechain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	18	TYR	Sidechain	8
1	A	96	TYR	Sidechain	7
1	A	190	TYR	Sidechain	7
1	A	147	TYR	Sidechain	6

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	1861	1796	1796	4±2
4	A	5796	0	9072	122±10
5	A	192	270	272	3±2
All	All	157060	41320	222802	2461

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 6.

5 of 2413 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H50	4:A:427:PX4:H60	0.91	1.43	1	1
4:A:328:PX4:H39	4:A:351:PX4:H23	0.90	1.41	12	1
4:A:386:PX4:H42	4:A:417:PX4:H38	0.85	1.47	3	1
4:A:308:PX4:H17	4:A:326:PX4:H55	0.84	1.49	15	1
4:A:367:PX4:H16	4:A:399:PX4:H47	0.84	1.48	17	1

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	237/250 (95%)	211±3 (89±1%)	20±3 (8±1%)	6±1 (3±1%)	6	42
All	All	4740/5000 (95%)	4216 (89%)	401 (8%)	123 (3%)	6	42

5 of 22 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	31	ASN	18
1	A	147	TYR	18
1	A	150	ASP	16
1	A	25	TYR	11
1	A	224	PHE	11

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	195/208 (94%)	187±3 (96±1%)	8±3 (4±1%)	29	79
All	All	3900/4160 (94%)	3745 (96%)	155 (4%)	29	79

5 of 64 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	150	ASP	20
1	A	155	THR	12
1	A	177	ARG	7
1	A	75	TYR	6
1	A	179	THR	6

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 4 are monoatomic - leaving 132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	318	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	432	-	35,35,35	1.29±0.01	2±0 (5±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	388	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	435	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	383	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	436	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	376	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.64±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	395	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	434	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	391	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	431	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	392	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	433	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	340	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.64±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	330	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	305	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.64±0.00	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	318	-	51,53,53	1.51±0.15	9±3 (18±5%)
4	PX4	A	344	-	51,53,53	1.46±0.18	9±3 (16±6%)
4	PX4	A	405	-	51,53,53	1.57±0.14	10±3 (19±5%)
4	PX4	A	408	-	51,53,53	1.51±0.21	9±3 (16±6%)
4	PX4	A	386	-	51,53,53	1.52±0.12	10±2 (18±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	353	-	51,53,53	1.55±0.19	10±3 (19±6%)
4	PX4	A	361	-	51,53,53	1.49±0.18	9±3 (17±5%)
4	PX4	A	428	-	51,53,53	1.46±0.16	9±3 (17±5%)
4	PX4	A	345	-	51,53,53	1.51±0.16	9±2 (16±3%)
4	PX4	A	365	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	379	-	51,53,53	1.51±0.14	9±2 (17±4%)
4	PX4	A	308	-	51,53,53	1.50±0.16	8±2 (15±3%)
4	PX4	A	347	-	51,53,53	1.54±0.15	10±2 (19±4%)
4	PX4	A	368	-	51,53,53	1.49±0.12	8±2 (16±4%)
4	PX4	A	380	-	51,53,53	1.48±0.12	9±2 (16±3%)
4	PX4	A	413	-	51,53,53	1.52±0.16	10±3 (19±5%)
4	PX4	A	343	-	51,53,53	1.58±0.14	11±2 (20±4%)
4	PX4	A	373	-	51,53,53	1.49±0.17	9±2 (16±3%)
4	PX4	A	414	-	51,53,53	1.51±0.12	9±3 (18±5%)
4	PX4	A	315	-	51,53,53	1.47±0.12	9±2 (17±4%)
4	PX4	A	381	-	51,53,53	1.59±0.17	10±3 (20±5%)
5	C3S	A	432	-	51,55,55	2.46±0.22	20±4 (39±6%)
4	PX4	A	388	-	51,53,53	1.48±0.11	8±2 (16±4%)
4	PX4	A	335	-	51,53,53	1.56±0.14	10±3 (19±5%)
4	PX4	A	341	-	51,53,53	1.50±0.19	9±3 (17±5%)
5	C3S	A	435	-	51,55,55	2.39±0.27	21±4 (41±7%)
4	PX4	A	383	-	51,53,53	1.49±0.17	9±3 (17±6%)
4	PX4	A	355	-	51,53,53	1.51±0.16	9±3 (18±5%)
4	PX4	A	317	-	51,53,53	1.45±0.15	8±2 (16±4%)
4	PX4	A	332	-	51,53,53	1.52±0.14	8±2 (16±4%)
4	PX4	A	423	-	51,53,53	1.48±0.14	9±2 (17±3%)
4	PX4	A	427	-	51,53,53	1.52±0.18	9±3 (18±6%)
4	PX4	A	310	-	51,53,53	1.53±0.17	9±3 (17±5%)
4	PX4	A	333	-	51,53,53	1.50±0.19	9±3 (18±5%)
4	PX4	A	403	-	51,53,53	1.49±0.11	8±2 (16±4%)
4	PX4	A	377	-	51,53,53	1.53±0.14	9±2 (18±4%)
4	PX4	A	348	-	51,53,53	1.52±0.12	9±2 (17±4%)
4	PX4	A	357	-	51,53,53	1.60±0.15	10±2 (19±4%)
4	PX4	A	396	-	51,53,53	1.46±0.14	9±2 (17±4%)
4	PX4	A	407	-	51,53,53	1.52±0.16	9±3 (17±5%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	410	-	51,53,53	1.47±0.11	8±2 (16±4%)
4	PX4	A	336	-	51,53,53	1.56±0.18	9±3 (18±4%)
4	PX4	A	400	-	51,53,53	1.49±0.14	9±2 (17±4%)
4	PX4	A	351	-	51,53,53	1.45±0.15	8±2 (15±4%)
4	PX4	A	382	-	51,53,53	1.51±0.11	8±2 (16±3%)
4	PX4	A	387	-	51,53,53	1.56±0.12	10±2 (18±3%)
4	PX4	A	384	-	51,53,53	1.53±0.16	10±3 (19±5%)
4	PX4	A	337	-	51,53,53	1.49±0.16	8±3 (15±5%)
4	PX4	A	417	-	51,53,53	1.53±0.13	10±2 (18±4%)
4	PX4	A	324	-	51,53,53	1.51±0.17	10±2 (18±4%)
4	PX4	A	378	-	51,53,53	1.51±0.19	9±3 (18±6%)
4	PX4	A	358	-	51,53,53	1.48±0.18	9±3 (17±6%)
4	PX4	A	375	-	51,53,53	1.55±0.15	10±2 (19±4%)
4	PX4	A	429	-	51,53,53	1.51±0.14	9±2 (18±4%)
4	PX4	A	362	-	51,53,53	1.46±0.13	8±2 (15±4%)
5	C3S	A	436	-	51,55,55	2.39±0.26	18±3 (35±6%)
4	PX4	A	376	-	51,53,53	1.56±0.21	10±2 (19±4%)
4	PX4	A	409	-	51,53,53	1.56±0.15	10±3 (20±4%)
4	PX4	A	314	-	51,53,53	1.52±0.14	10±3 (18±5%)
4	PX4	A	339	-	51,53,53	1.44±0.14	8±2 (15±4%)
4	PX4	A	334	-	51,53,53	1.50±0.13	9±2 (17±3%)
4	PX4	A	309	-	51,53,53	1.55±0.15	9±2 (18±3%)
4	PX4	A	319	-	51,53,53	1.54±0.17	9±3 (18±5%)
4	PX4	A	425	-	51,53,53	1.49±0.14	9±2 (17±4%)
4	PX4	A	395	-	51,53,53	1.55±0.17	10±3 (18±5%)
4	PX4	A	390	-	51,53,53	1.49±0.12	9±2 (16±4%)
4	PX4	A	352	-	51,53,53	1.51±0.12	9±2 (17±3%)
4	PX4	A	416	-	51,53,53	1.55±0.16	10±3 (19±5%)
4	PX4	A	411	-	51,53,53	1.52±0.16	10±3 (19±5%)
4	PX4	A	398	-	51,53,53	1.50±0.14	9±3 (18±5%)
5	C3S	A	434	-	51,55,55	2.36±0.26	19±3 (37±5%)
4	PX4	A	391	-	51,53,53	1.49±0.12	9±2 (17±4%)
4	PX4	A	397	-	51,53,53	1.55±0.14	10±3 (19±6%)
5	C3S	A	431	-	51,55,55	2.37±0.33	20±4 (38±8%)
4	PX4	A	392	-	51,53,53	1.52±0.13	8±2 (16±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	326	-	51,53,53	1.53±0.13	9±2 (18±4%)
4	PX4	A	404	-	51,53,53	1.45±0.15	9±2 (16±4%)
4	PX4	A	313	-	51,53,53	1.51±0.14	9±2 (17±3%)
4	PX4	A	415	-	51,53,53	1.53±0.14	9±2 (18±4%)
4	PX4	A	402	-	51,53,53	1.55±0.15	9±2 (18±4%)
4	PX4	A	311	-	51,53,53	1.52±0.16	9±3 (18±6%)
4	PX4	A	364	-	51,53,53	1.53±0.14	9±3 (18±5%)
4	PX4	A	307	-	51,53,53	1.51±0.14	9±3 (17±5%)
4	PX4	A	360	-	51,53,53	1.51±0.16	9±2 (17±4%)
4	PX4	A	323	-	51,53,53	1.53±0.10	10±3 (19±5%)
4	PX4	A	327	-	51,53,53	1.42±0.17	8±3 (14±5%)
4	PX4	A	349	-	51,53,53	1.51±0.11	9±2 (17±3%)
4	PX4	A	363	-	51,53,53	1.47±0.15	9±3 (18±4%)
4	PX4	A	316	-	51,53,53	1.51±0.14	9±2 (17±4%)
4	PX4	A	367	-	51,53,53	1.53±0.14	9±3 (17±5%)
4	PX4	A	418	-	51,53,53	1.56±0.16	10±2 (19±3%)
4	PX4	A	385	-	51,53,53	1.52±0.13	9±2 (17±3%)
4	PX4	A	424	-	51,53,53	1.47±0.19	9±2 (17±3%)
4	PX4	A	370	-	51,53,53	1.52±0.13	9±2 (17±4%)
4	PX4	A	359	-	51,53,53	1.53±0.13	9±2 (18±4%)
5	C3S	A	433	-	51,55,55	2.37±0.21	20±3 (38±6%)
4	PX4	A	340	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	350	-	51,53,53	1.49±0.12	9±2 (16±4%)
4	PX4	A	369	-	51,53,53	1.47±0.09	9±2 (17±3%)
4	PX4	A	354	-	51,53,53	1.53±0.19	9±2 (17±3%)
4	PX4	A	421	-	51,53,53	1.54±0.18	9±3 (17±6%)
4	PX4	A	399	-	51,53,53	1.54±0.15	10±3 (19±5%)
4	PX4	A	321	-	51,53,53	1.51±0.12	9±2 (16±3%)
4	PX4	A	306	-	51,53,53	1.55±0.13	9±2 (18±4%)
4	PX4	A	420	-	51,53,53	1.49±0.14	8±2 (16±4%)
4	PX4	A	372	-	51,53,53	1.54±0.20	10±2 (18±4%)
4	PX4	A	330	-	51,53,53	1.57±0.12	10±3 (18±5%)
4	PX4	A	346	-	51,53,53	1.52±0.14	9±3 (18±5%)
4	PX4	A	305	-	51,53,53	1.48±0.09	8±2 (16±3%)
4	PX4	A	393	-	51,53,53	1.55±0.14	9±2 (18±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	422	-	51,53,53	1.47±0.13	8±2 (16±4%)
4	PX4	A	325	-	51,53,53	1.54±0.17	10±2 (18±4%)
4	PX4	A	426	-	51,53,53	1.45±0.16	8±2 (15±4%)
4	PX4	A	342	-	51,53,53	1.51±0.17	9±2 (18±4%)
4	PX4	A	356	-	51,53,53	1.58±0.15	10±2 (20±3%)
4	PX4	A	320	-	51,53,53	1.51±0.13	10±2 (18±3%)
4	PX4	A	374	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	412	-	51,53,53	1.49±0.17	9±2 (18±4%)
4	PX4	A	430	-	51,53,53	1.44±0.17	8±2 (15±4%)
4	PX4	A	389	-	51,53,53	1.49±0.13	9±2 (16±4%)
4	PX4	A	338	-	51,53,53	1.51±0.19	10±3 (19±5%)
4	PX4	A	406	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	328	-	51,53,53	1.56±0.18	11±3 (20±6%)
4	PX4	A	394	-	51,53,53	1.51±0.15	9±3 (17±5%)
4	PX4	A	322	-	51,53,53	1.54±0.13	10±2 (19±4%)
4	PX4	A	401	-	51,53,53	1.56±0.17	9±2 (17±3%)
4	PX4	A	366	-	51,53,53	1.45±0.14	8±2 (16±4%)
4	PX4	A	371	-	51,53,53	1.52±0.13	9±2 (18±4%)
4	PX4	A	329	-	51,53,53	1.45±0.14	9±2 (17±4%)
4	PX4	A	331	-	51,53,53	1.55±0.16	10±2 (19±4%)
4	PX4	A	312	-	51,53,53	1.49±0.16	9±3 (17±6%)
4	PX4	A	419	-	51,53,53	1.56±0.12	10±2 (19±4%)

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
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	418	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
5	C3S	A	434	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
4	PX4	A	377	-	-	1±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	315	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
5	C3S	A	432	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
5	C3S	A	435	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	328	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	1±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	364	-	-	0±0,49,49,49	-
4	PX4	A	323	-	-	0±0,49,49,49	-
4	PX4	A	305	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-
4	PX4	A	430	-	-	0±0,49,49,49	-
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	371	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	0±0,49,49,49	-
4	PX4	A	413	-	-	0±0,49,49,49	-
4	PX4	A	406	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	0±0,49,49,49	-
4	PX4	A	338	-	-	0±0,49,49,49	-
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	341	-	-	0±0,49,49,49	-
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	307	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
5	C3S	A	436	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	433	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	431	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
4	PX4	A	384	-	-	0±0,49,49,49	-

5 of 12 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	A	434	C3S	O6-S1	6.38	1.76	1.57	7	20
5	A	432	C3S	O6-S1	6.36	1.76	1.57	3	20
5	A	435	C3S	O6-S1	6.36	1.76	1.57	14	20
5	A	436	C3S	O6-S1	6.36	1.76	1.57	7	20
5	A	433	C3S	O6-S1	6.36	1.76	1.57	12	20

5 of 5450 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
5	A	432	C3S	C29-C38-C48	10.43	135.60	119.50	14	20
5	A	434	C3S	C29-C38-C48	9.47	134.12	119.50	15	16
5	A	433	C3S	O6-C7-C4	9.27	121.32	107.61	20	12
5	A	436	C3S	C50-C48-C38	8.98	126.36	112.88	16	17
5	A	431	C3S	C9-C12-C22	8.79	127.67	116.42	1	14

5 of 9 unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
5	A	431	C3S	C7	20
5	A	431	C3S	C48	20
5	A	432	C3S	C48	20
5	A	433	C3S	C48	20
5	A	434	C3S	C48	20

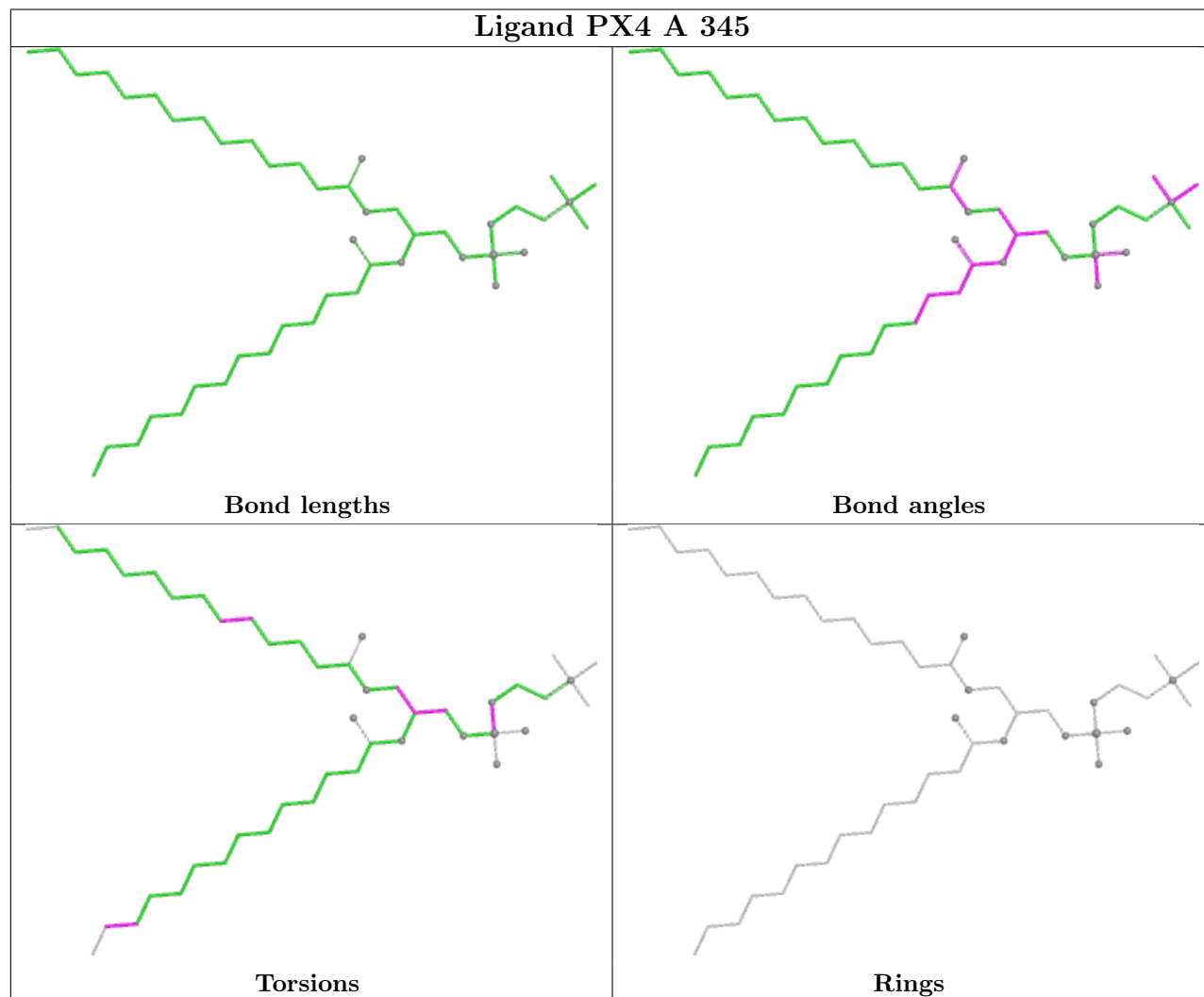
5 of 6 unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

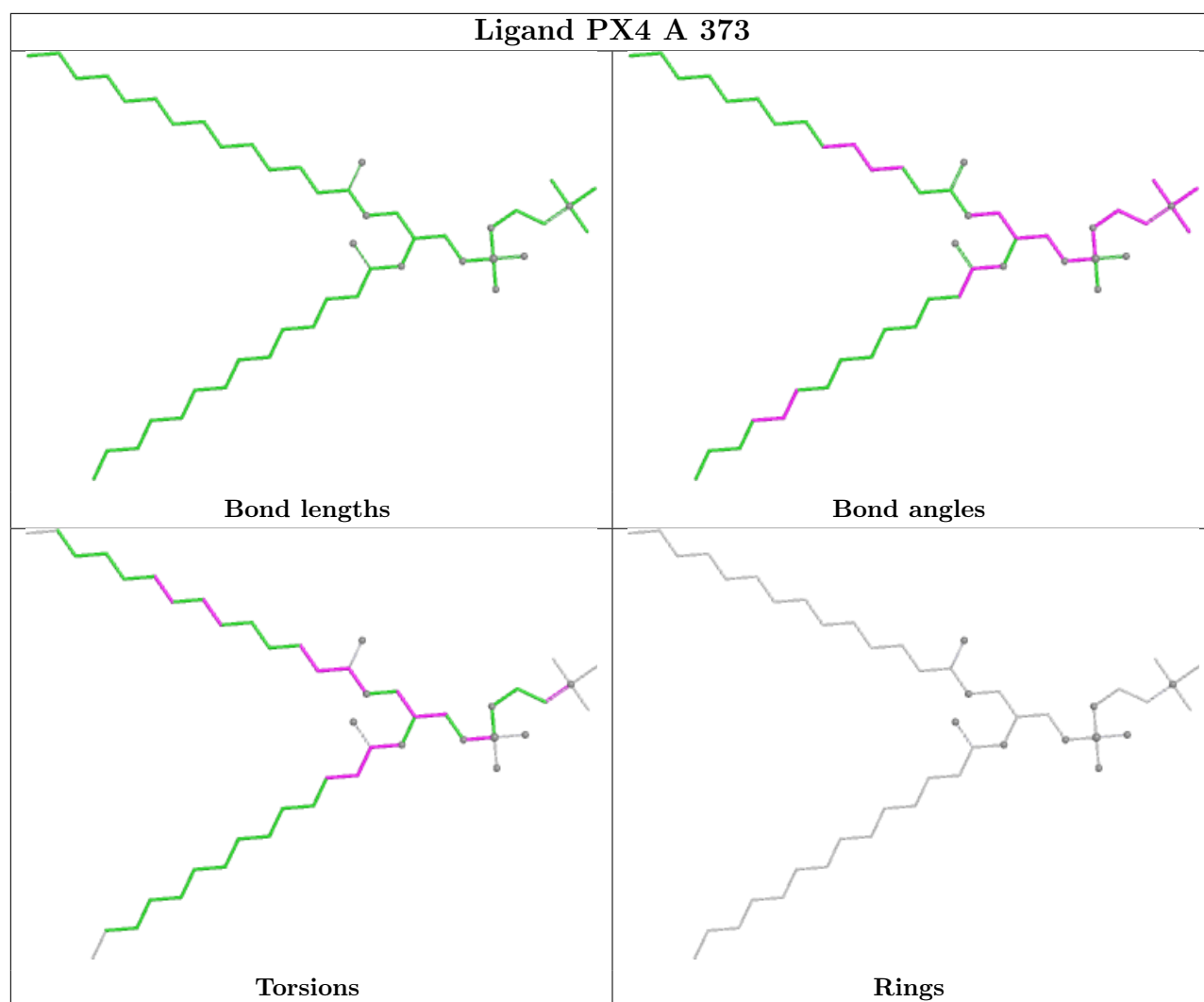
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	377	PX4	O8-C23-O7-C7	12
4	A	376	PX4	O8-C23-O7-C7	5
4	A	356	PX4	O8-C23-O7-C7	3
4	A	372	PX4	O8-C23-O7-C7	1
4	A	376	PX4	C24-C23-O7-C7	1

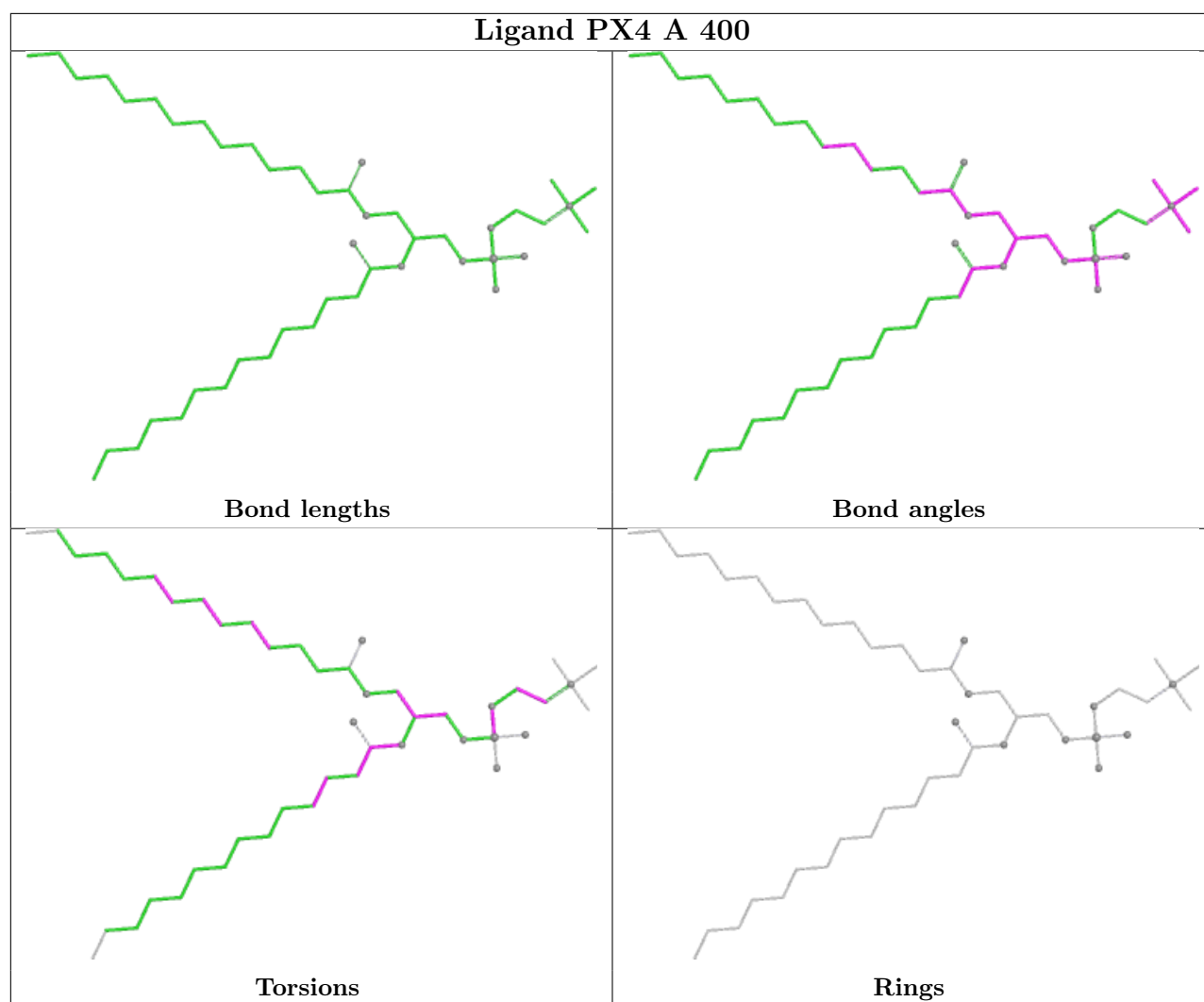
There are no ring outliers.

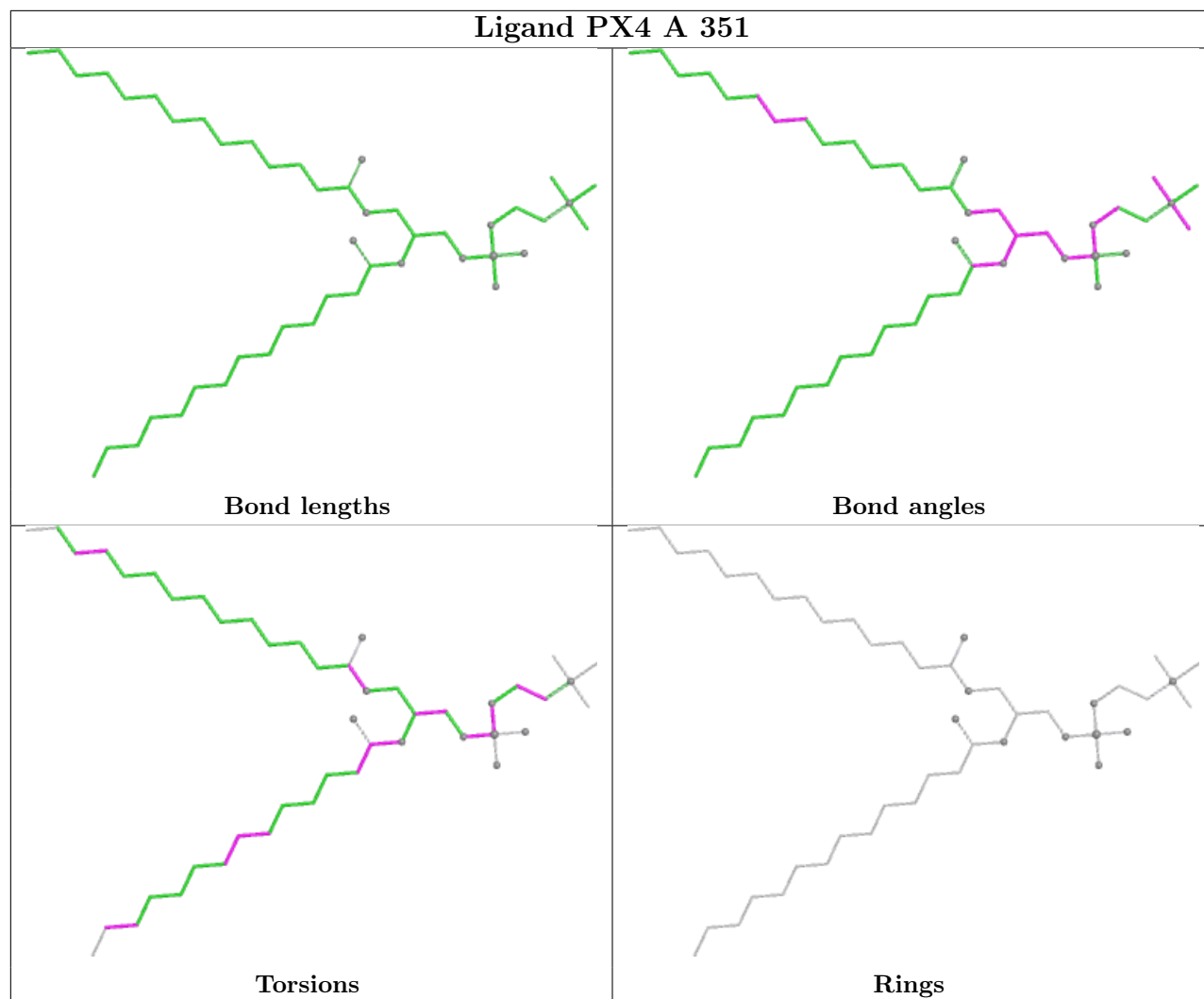
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

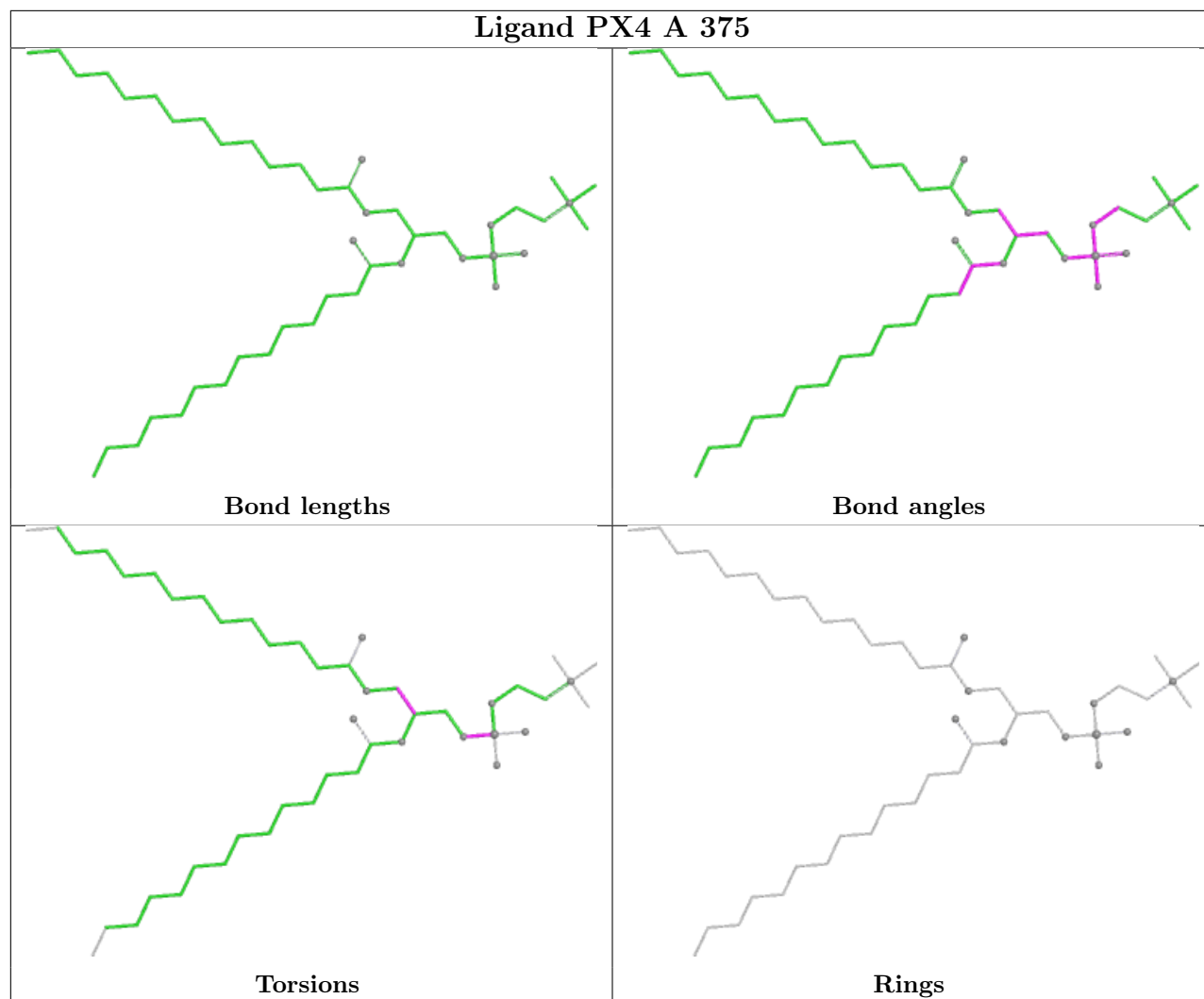


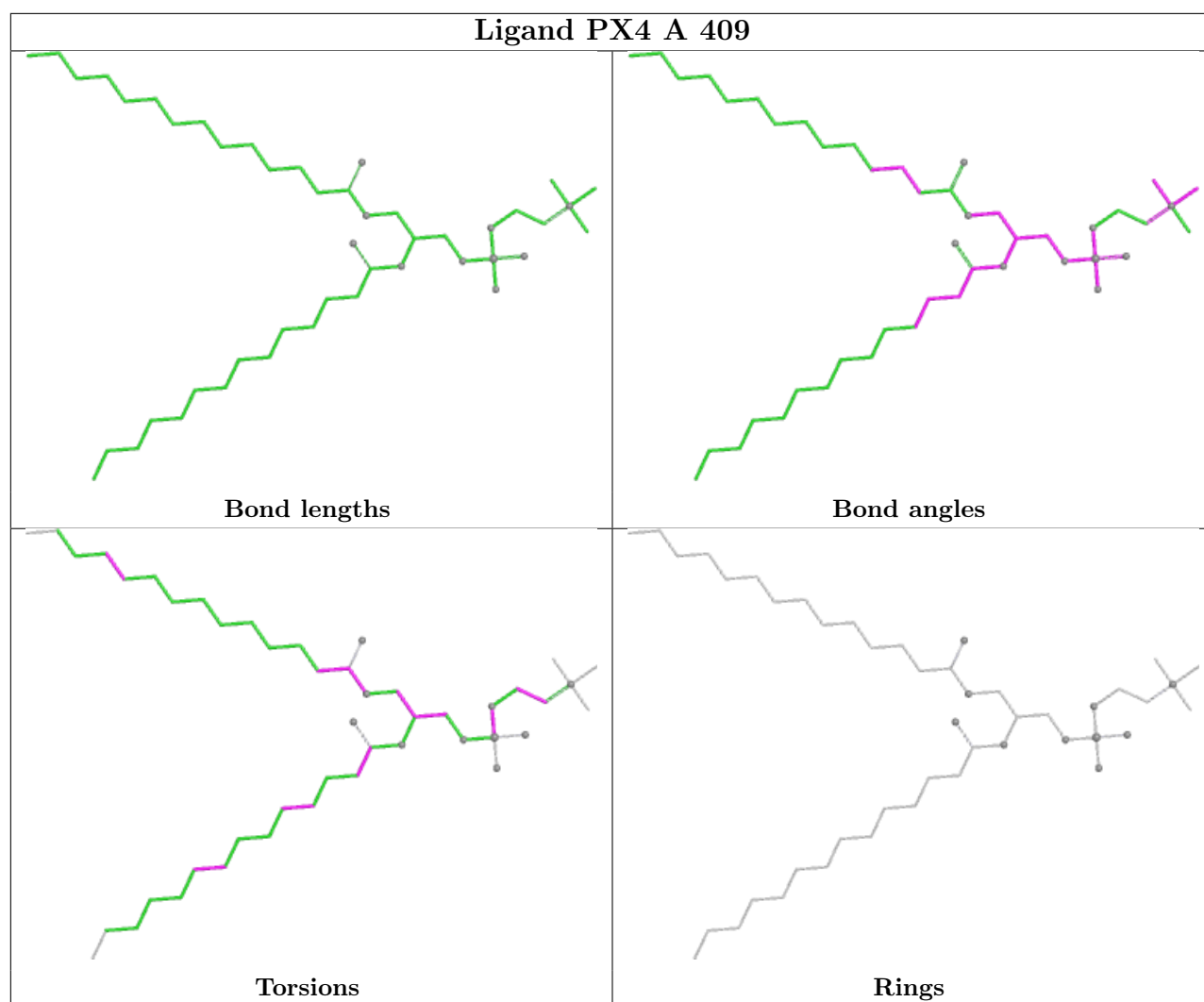


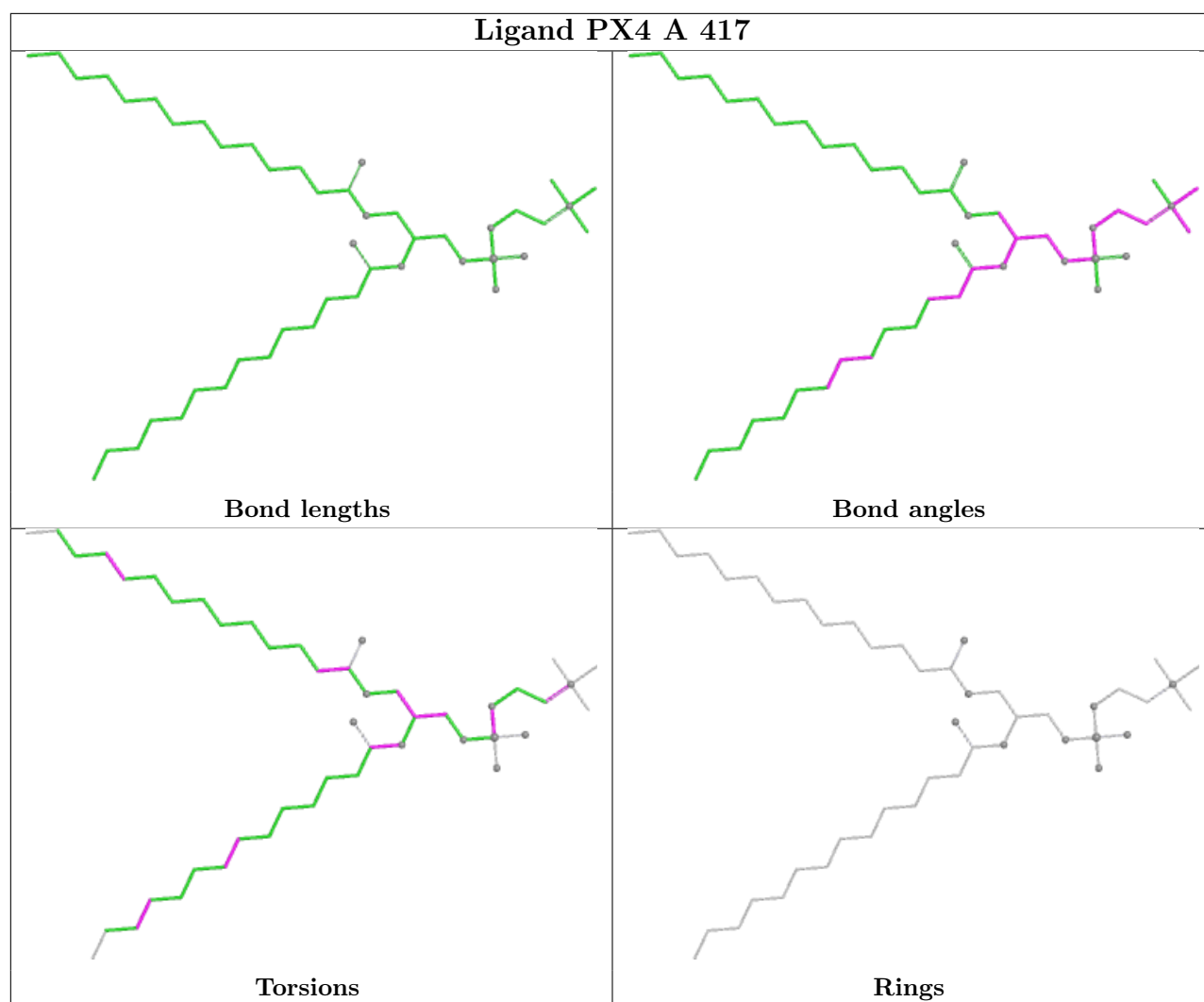


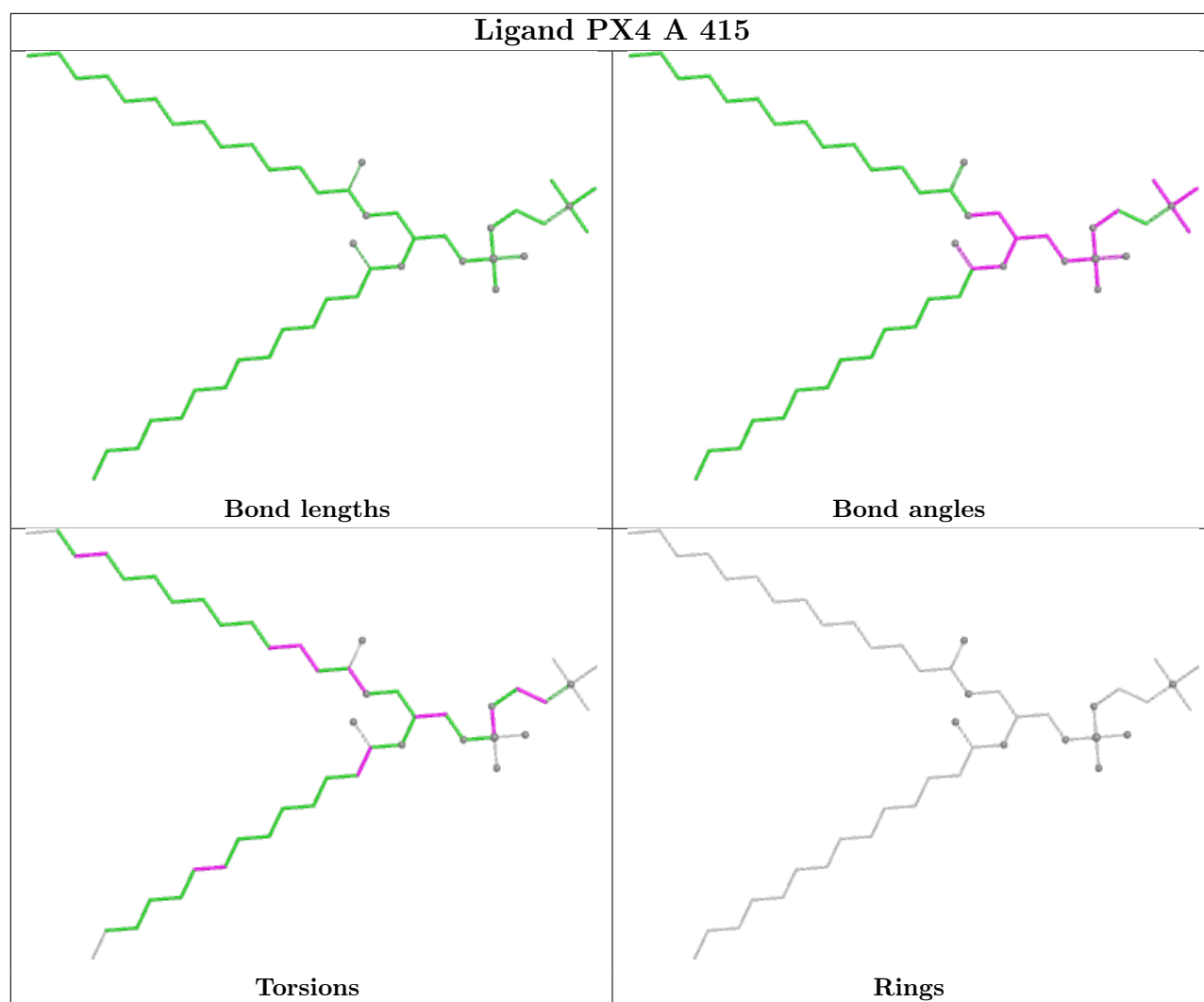


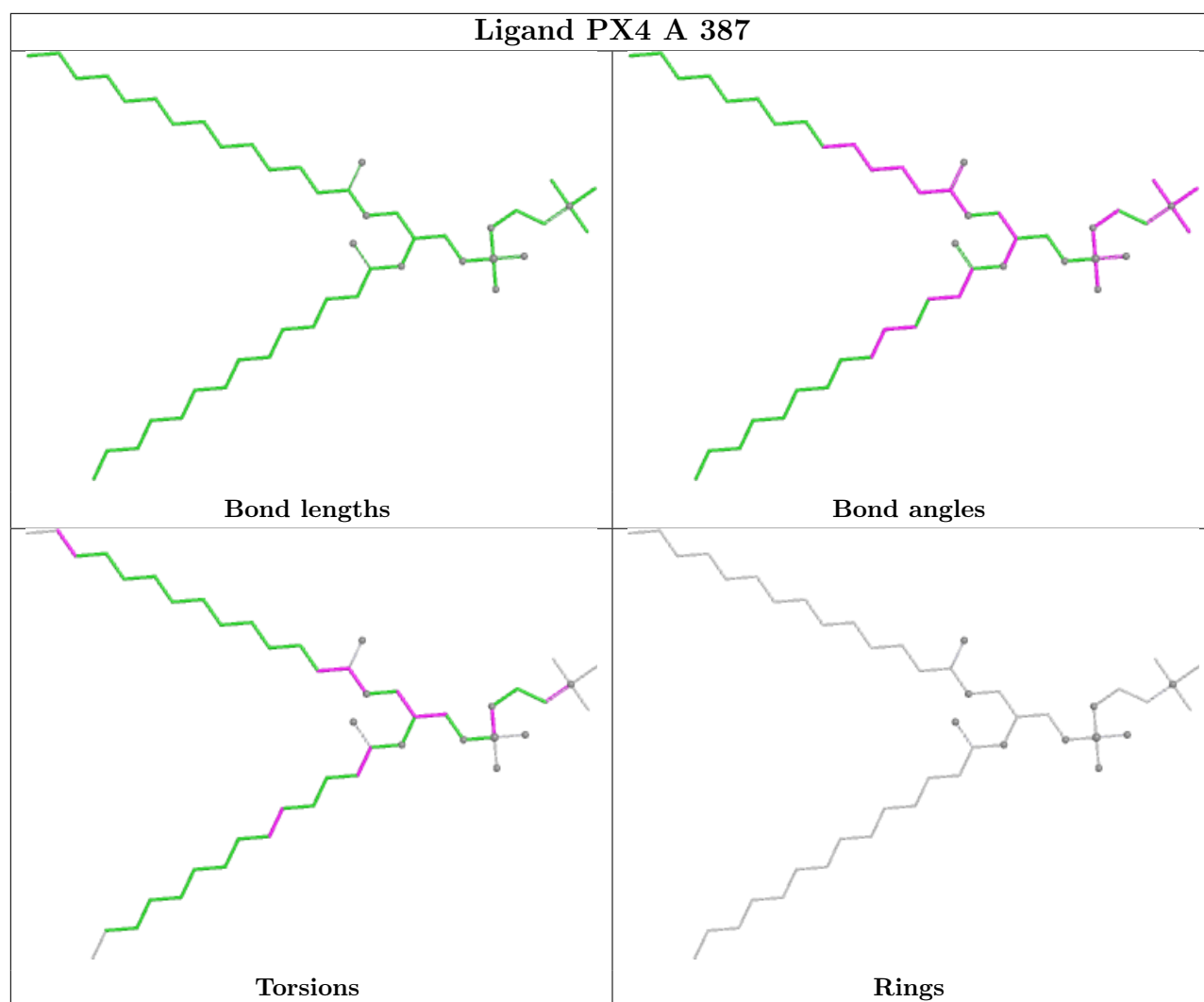
Ligand PX4 A 375

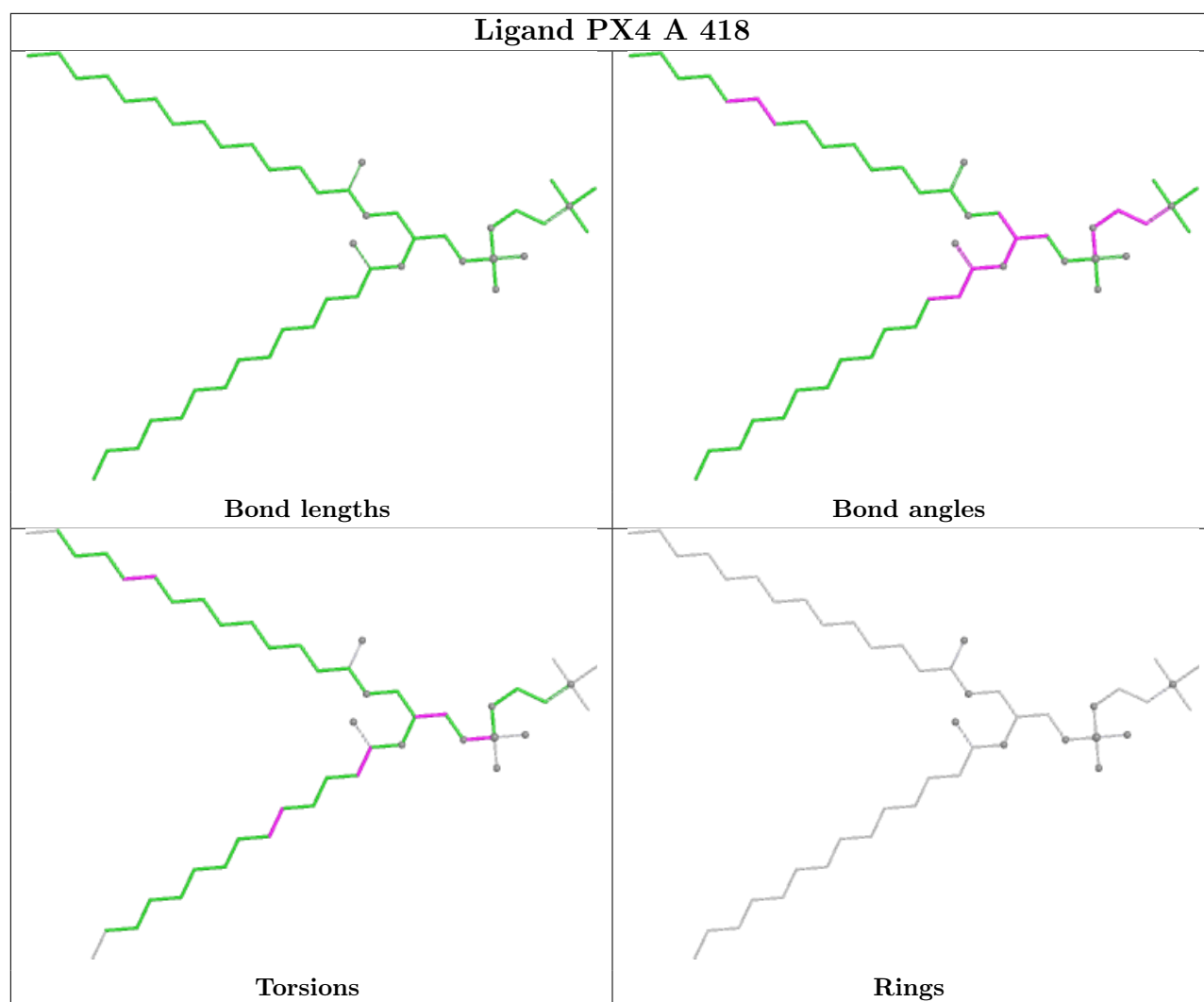


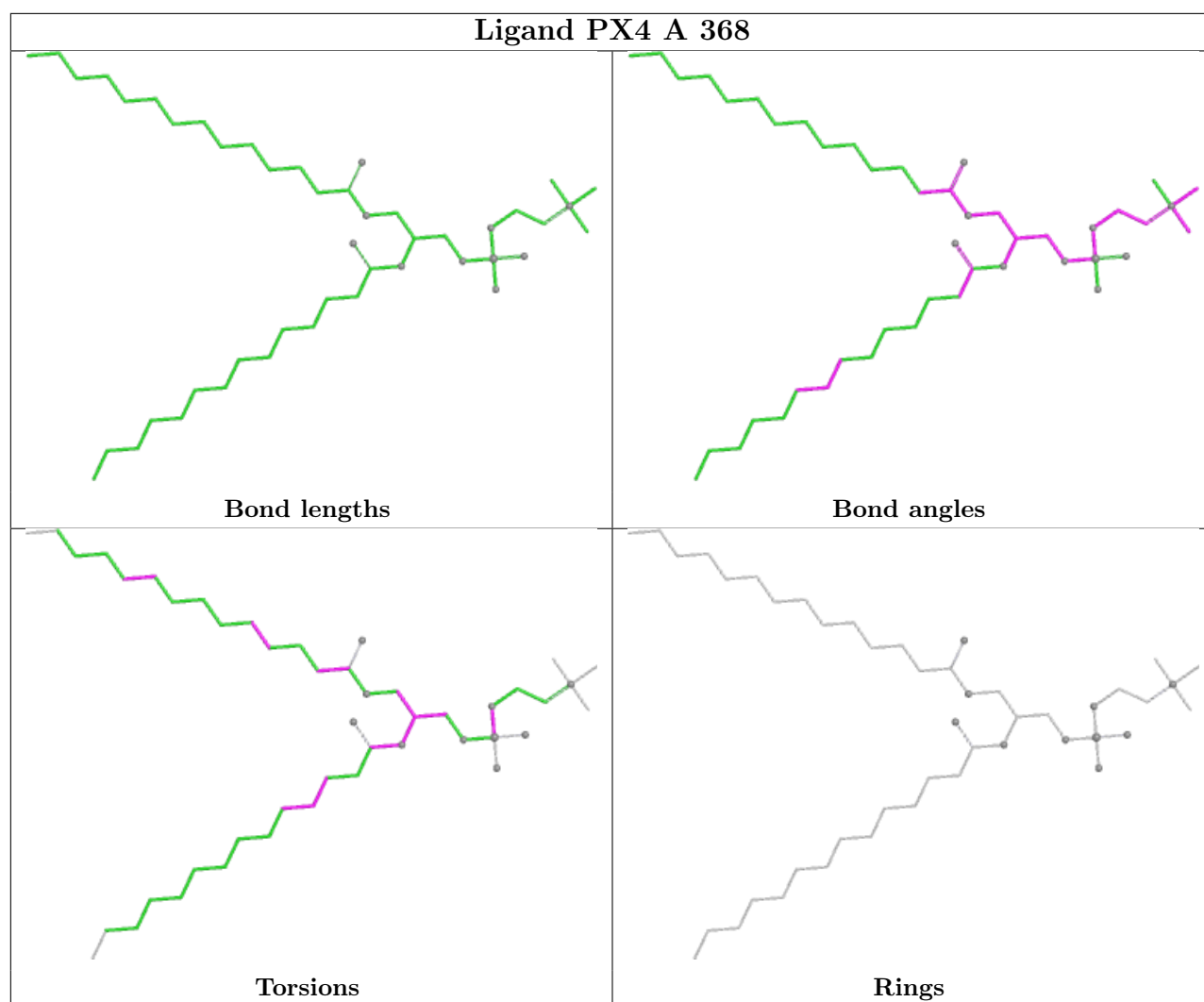


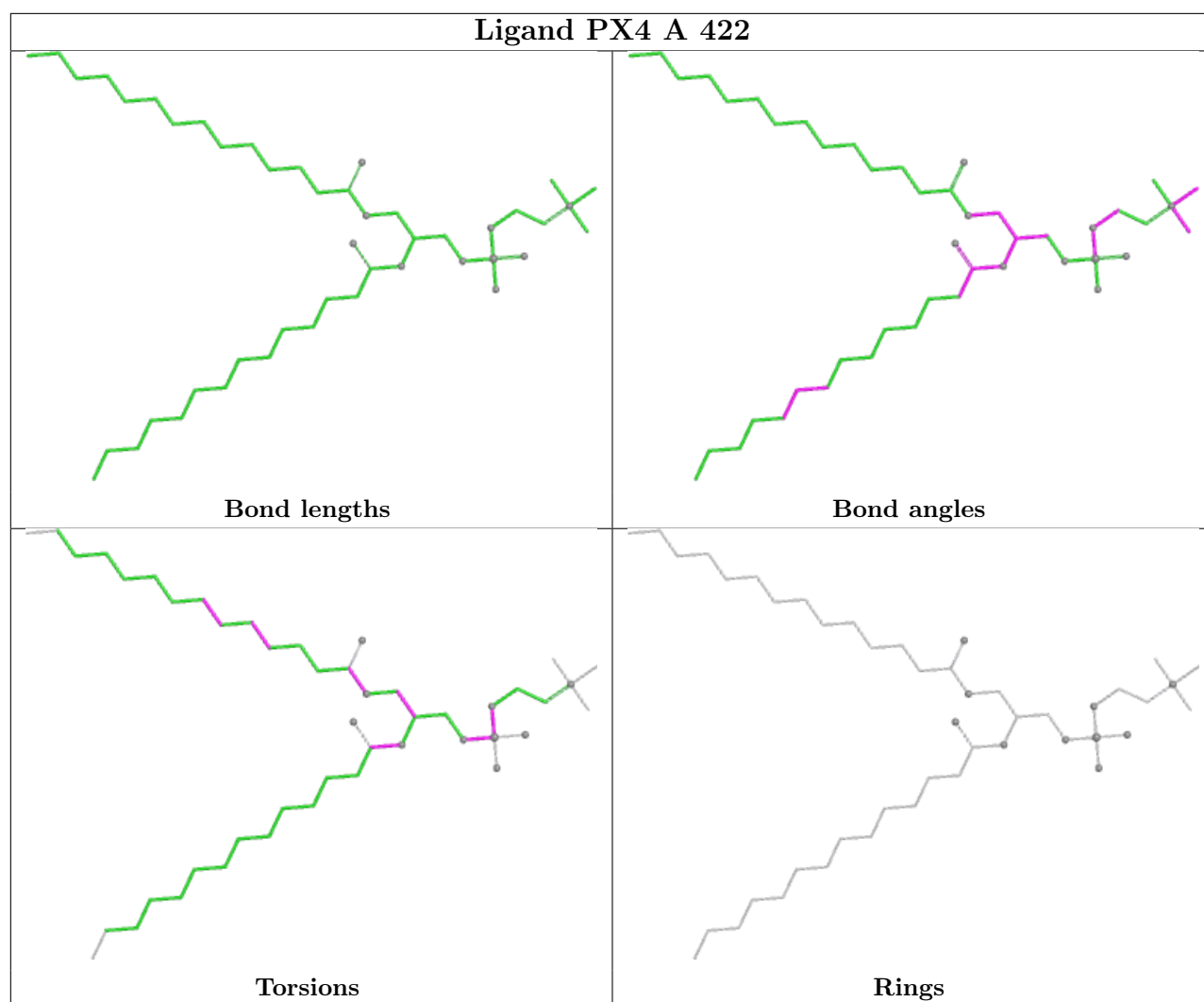


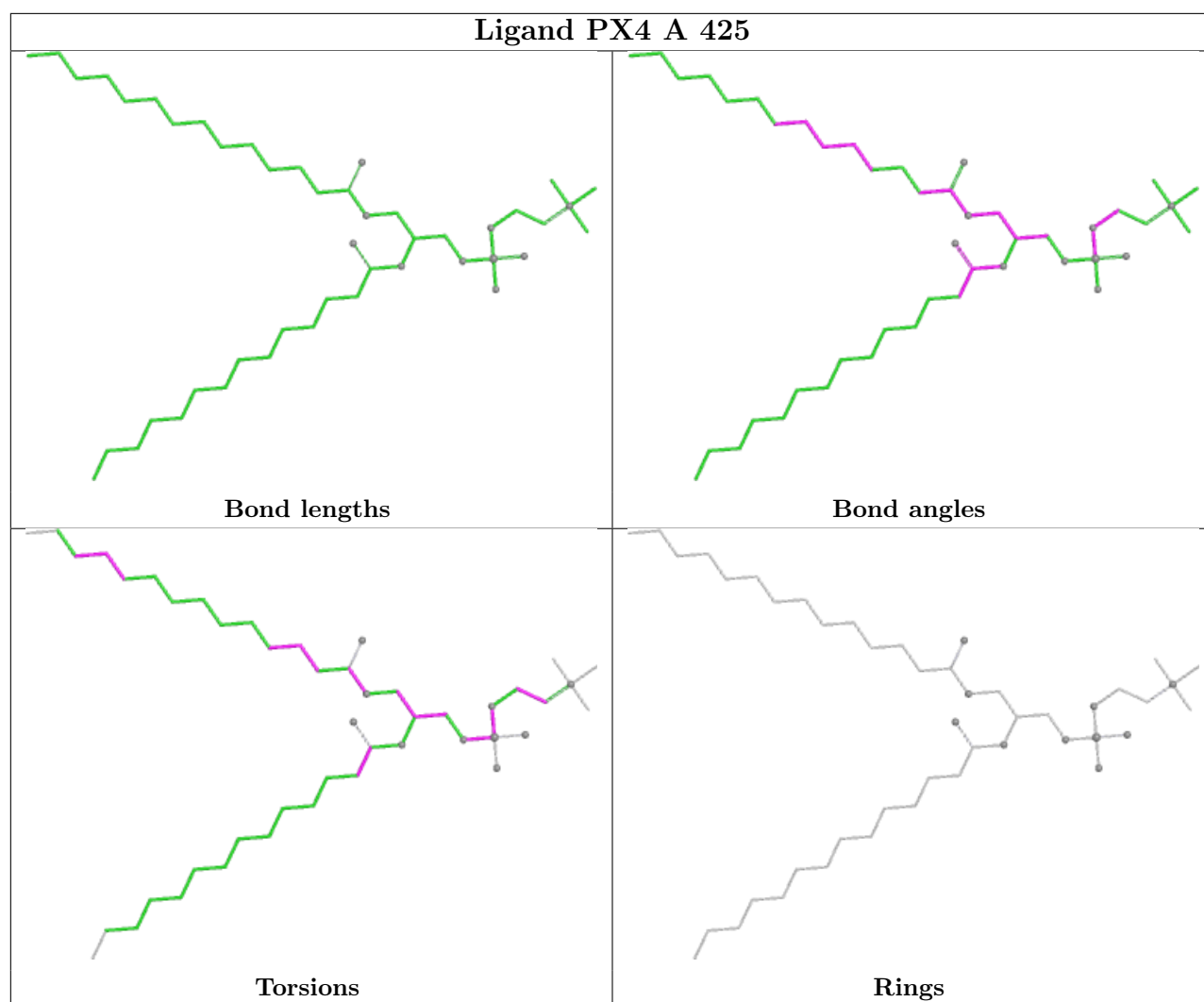


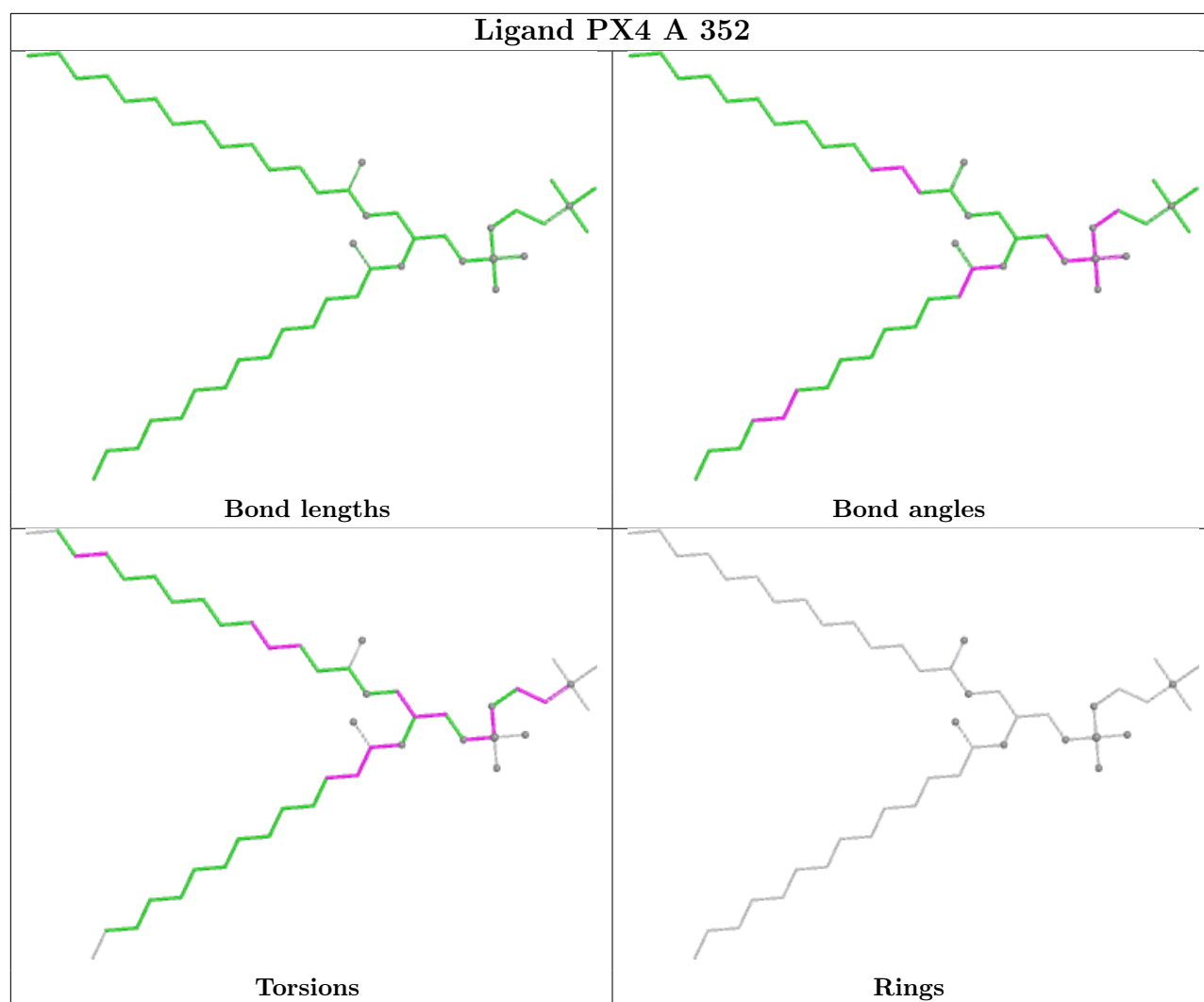


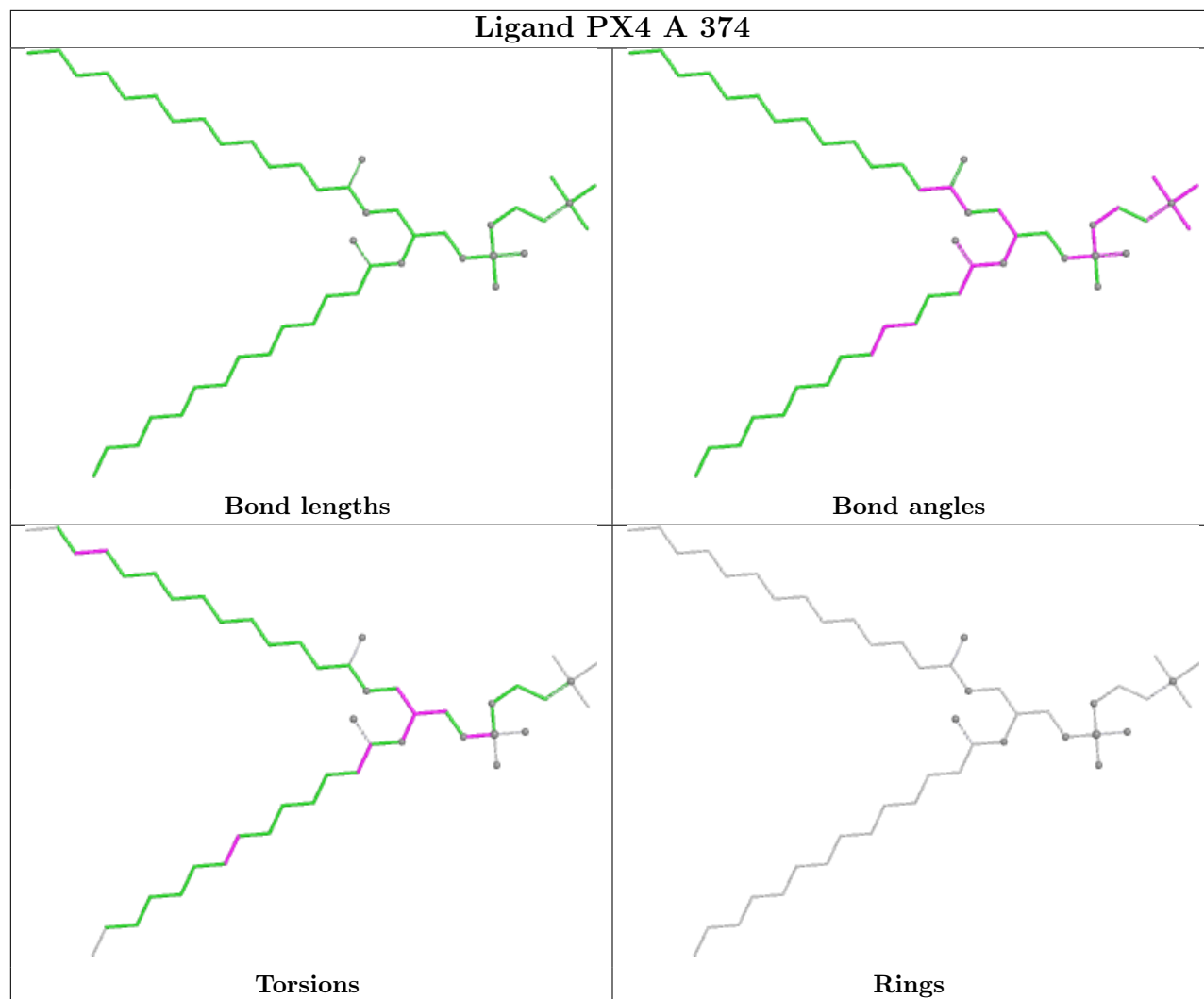




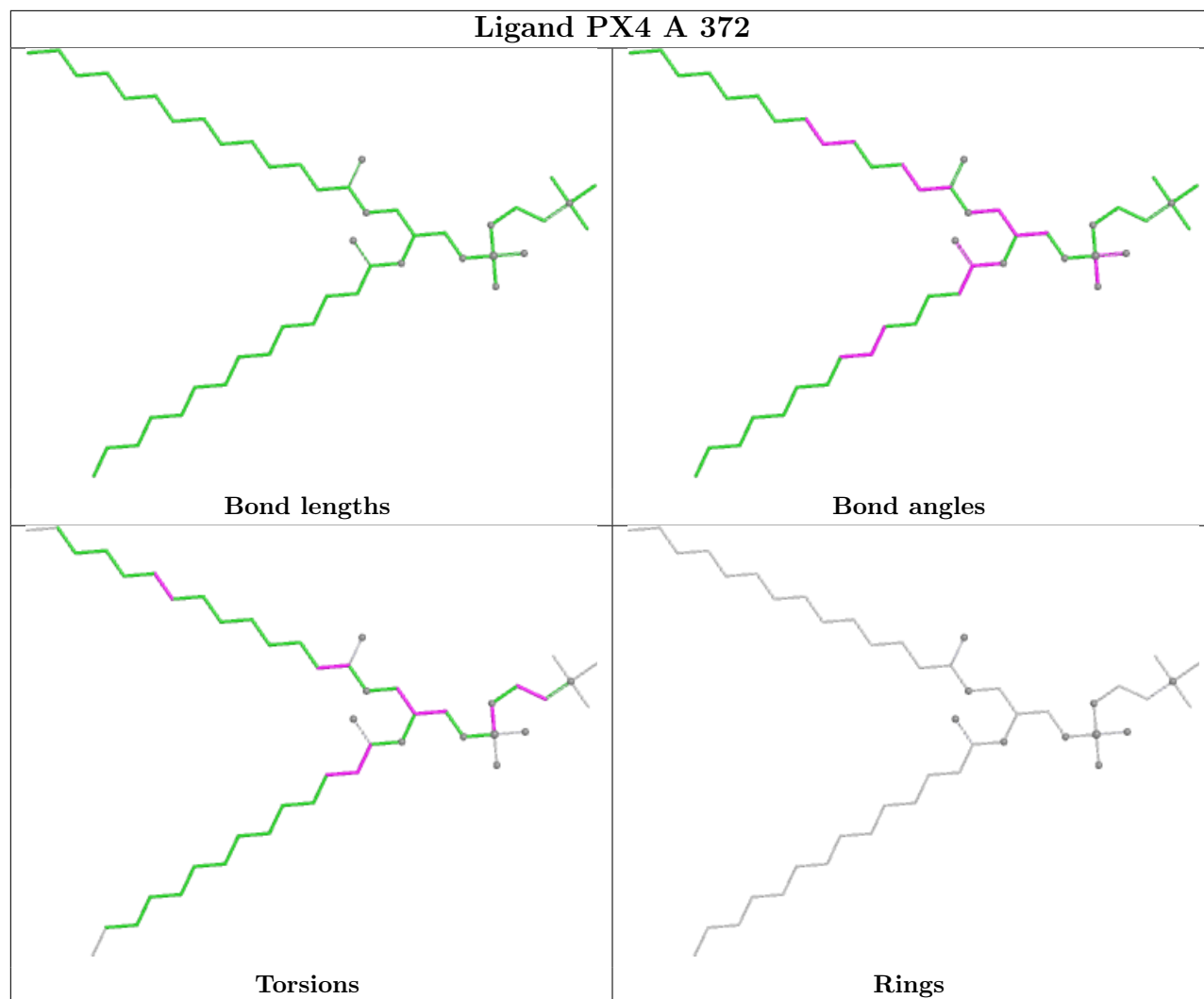


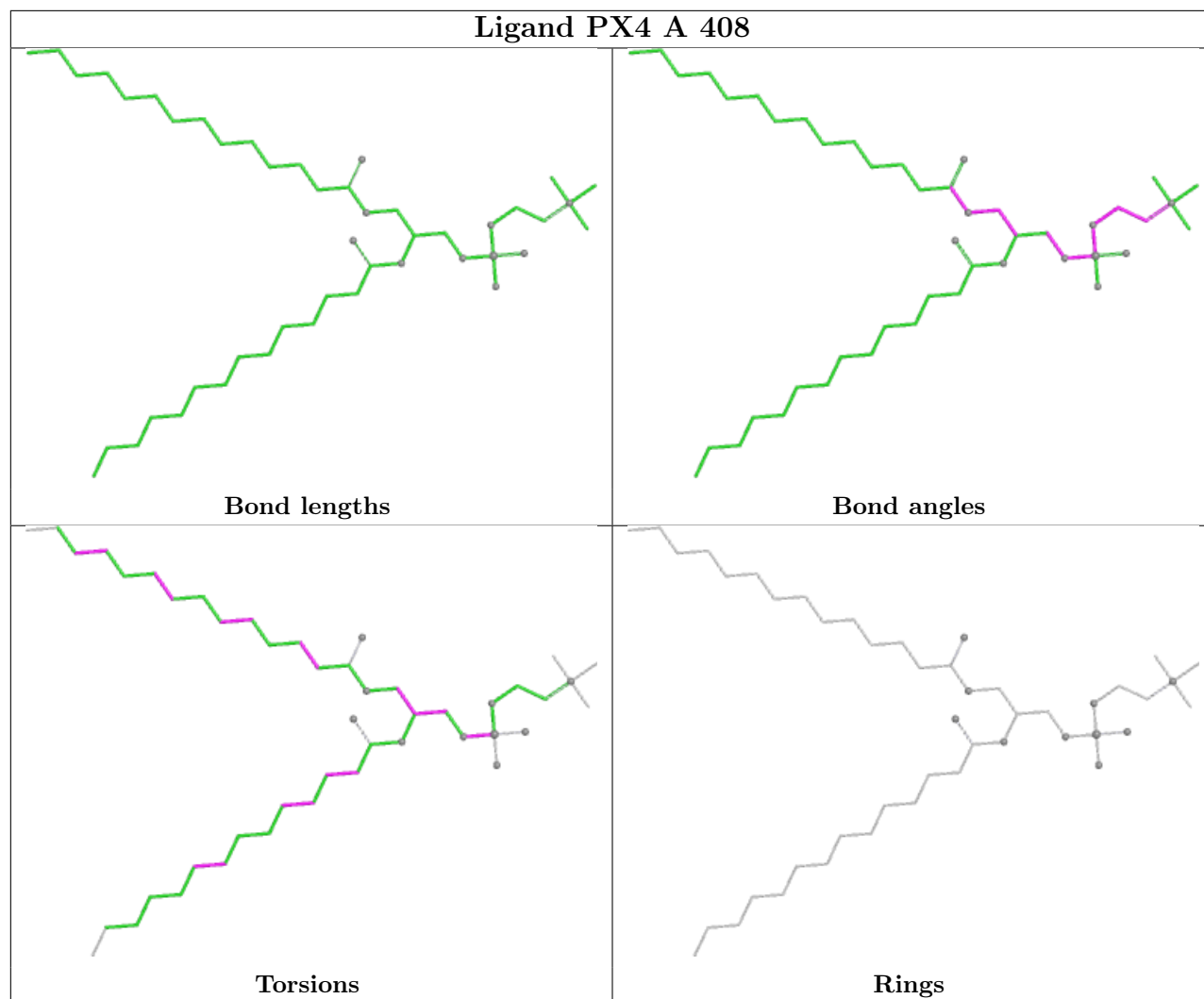


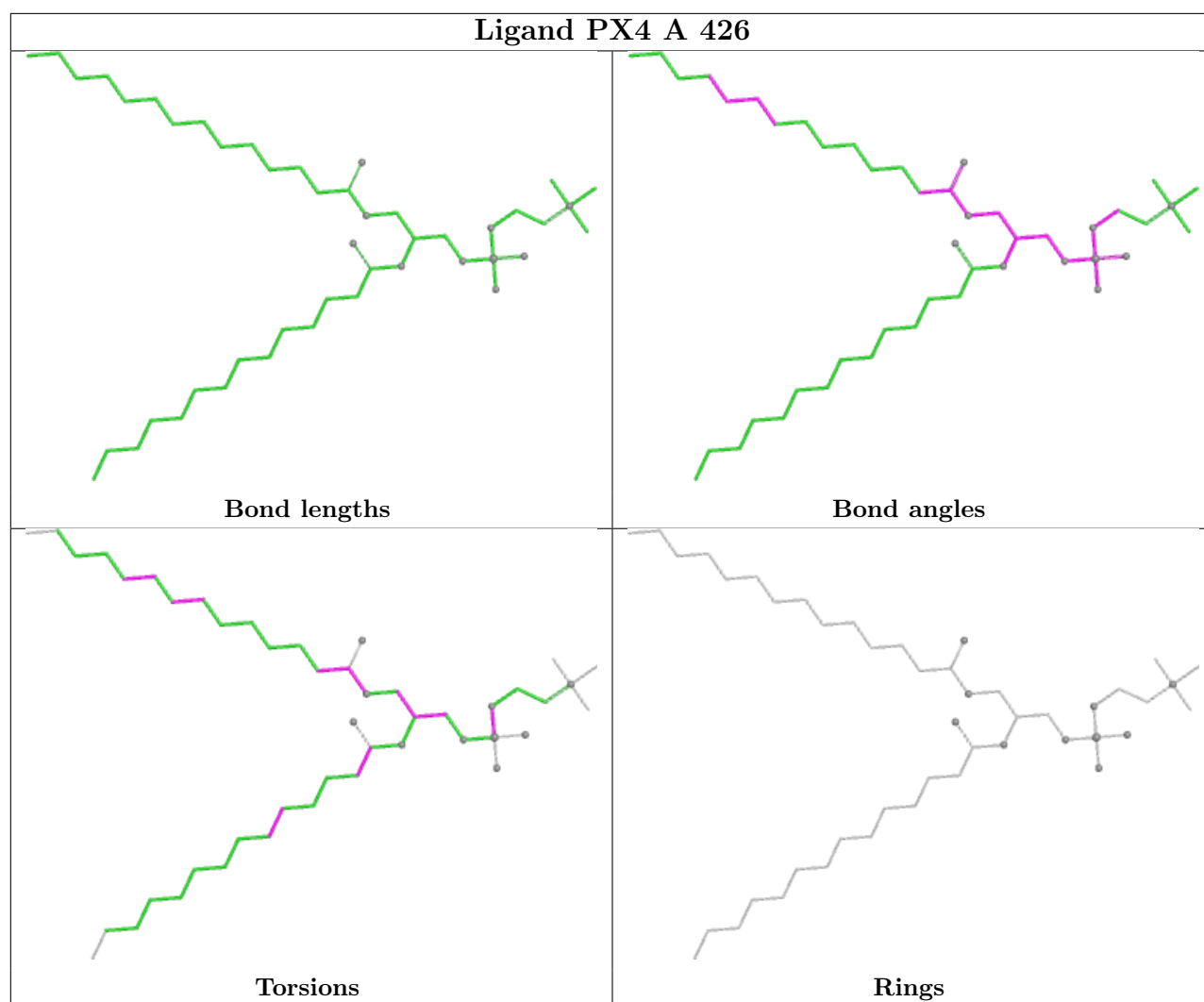




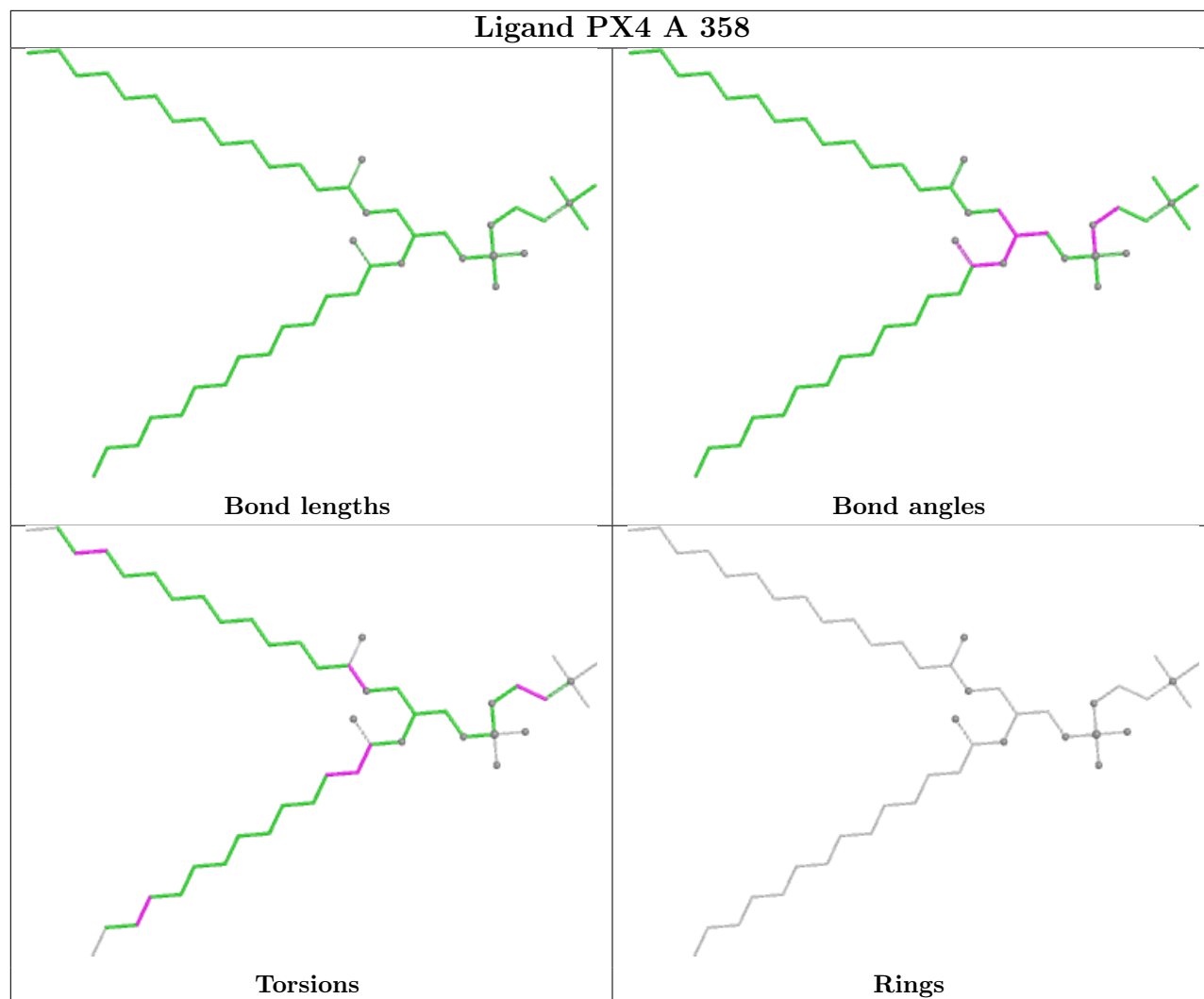
Ligand PX4 A 372



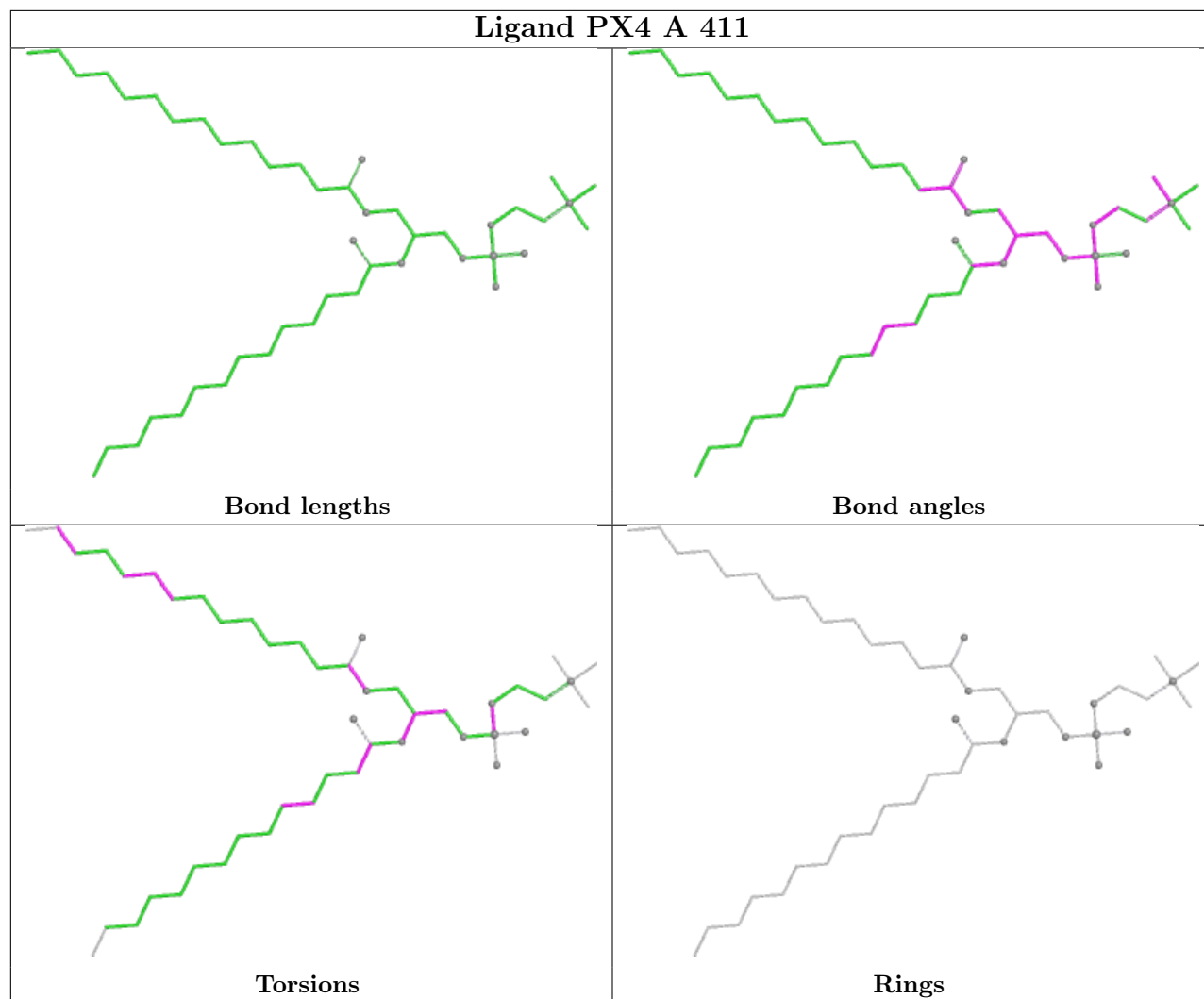




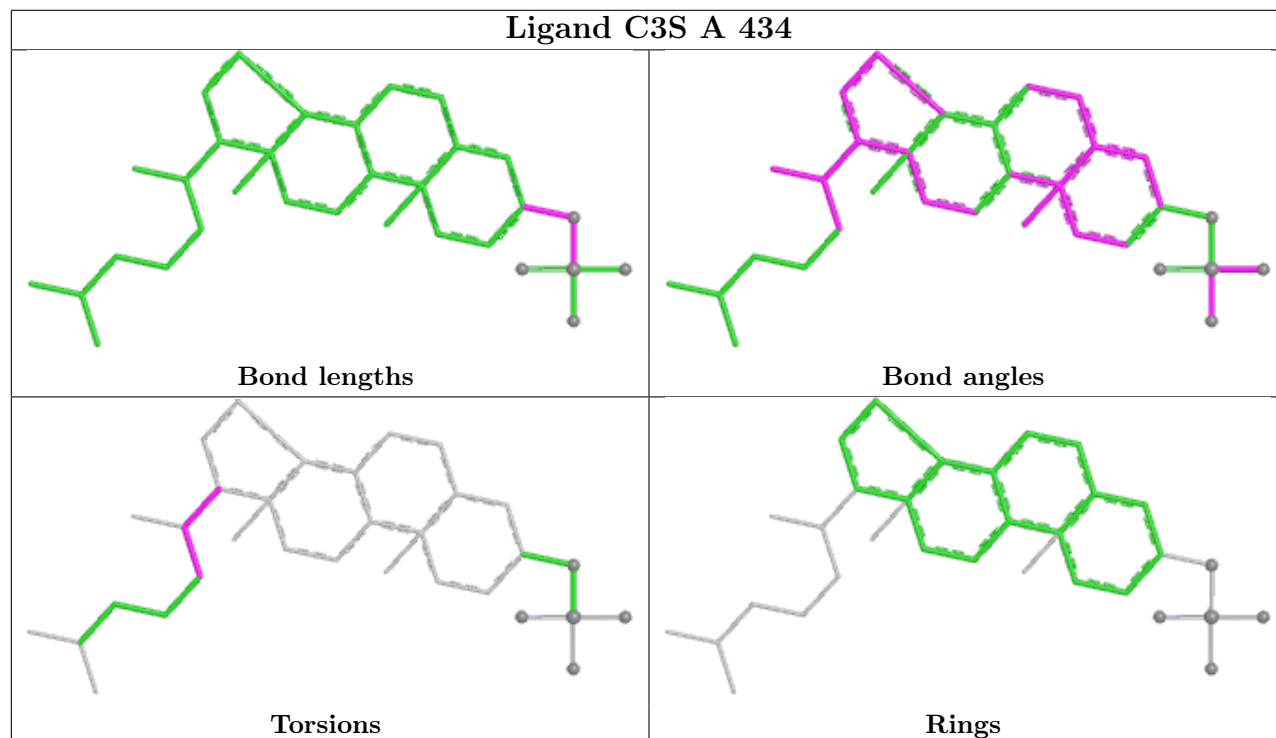
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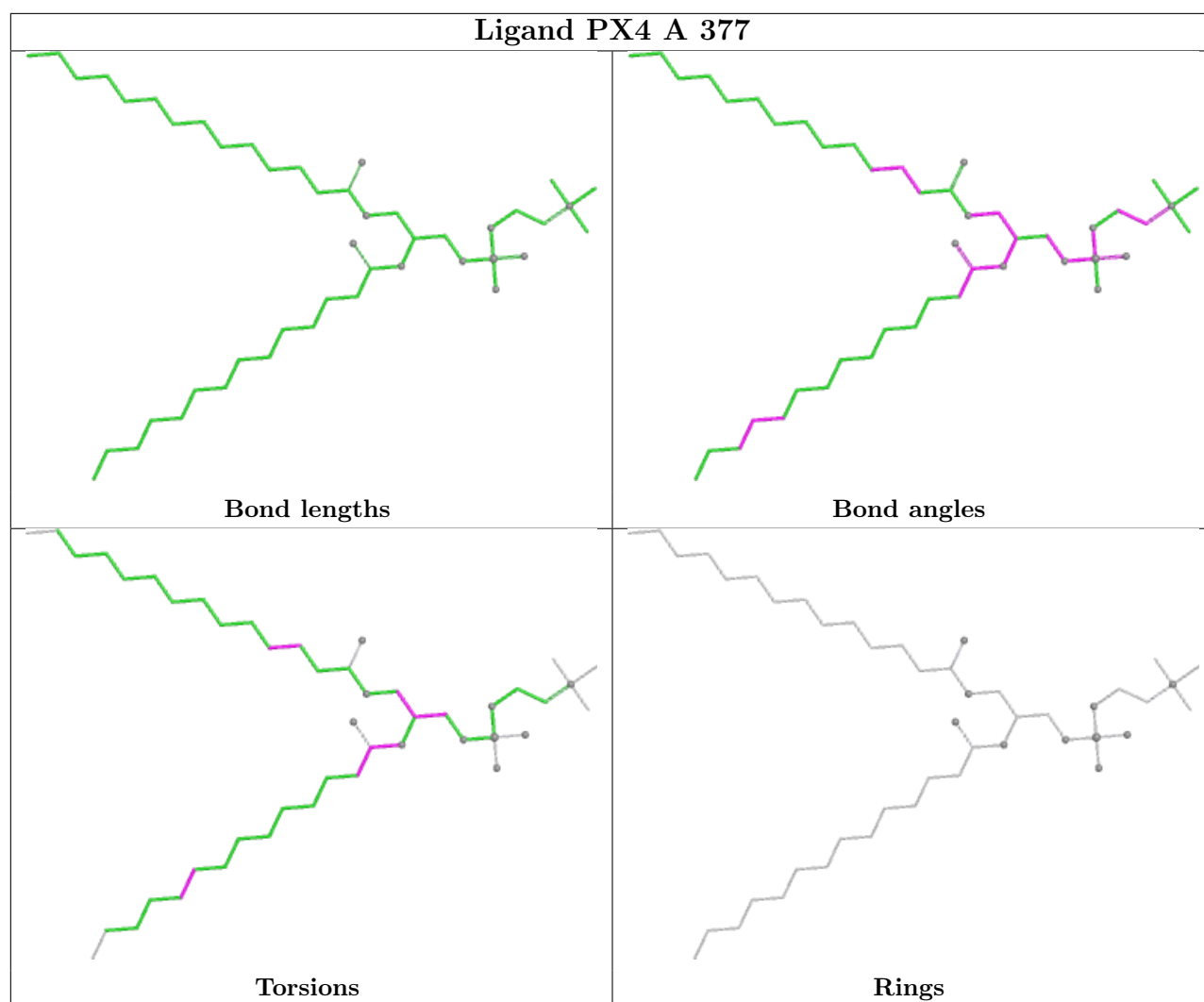


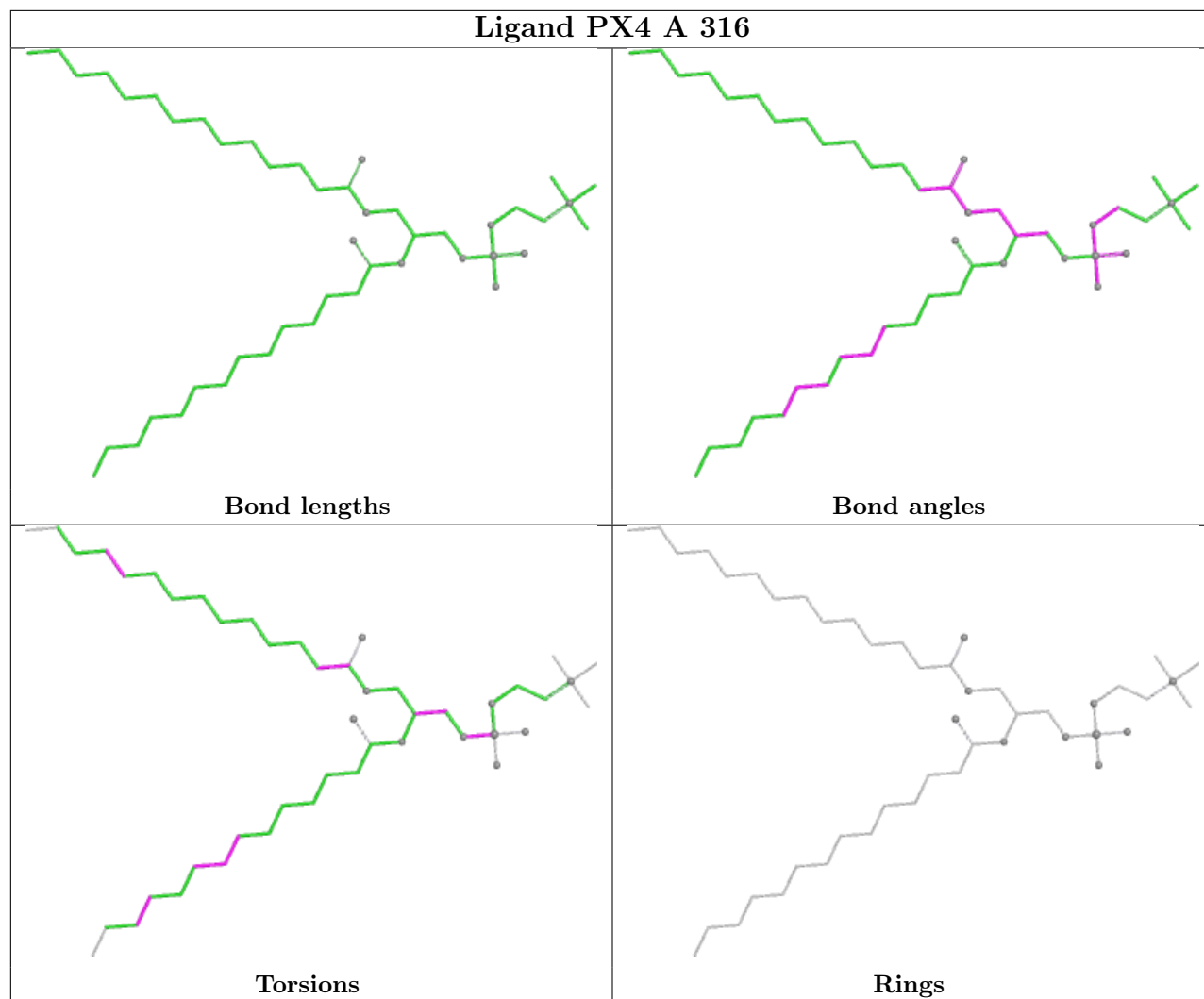
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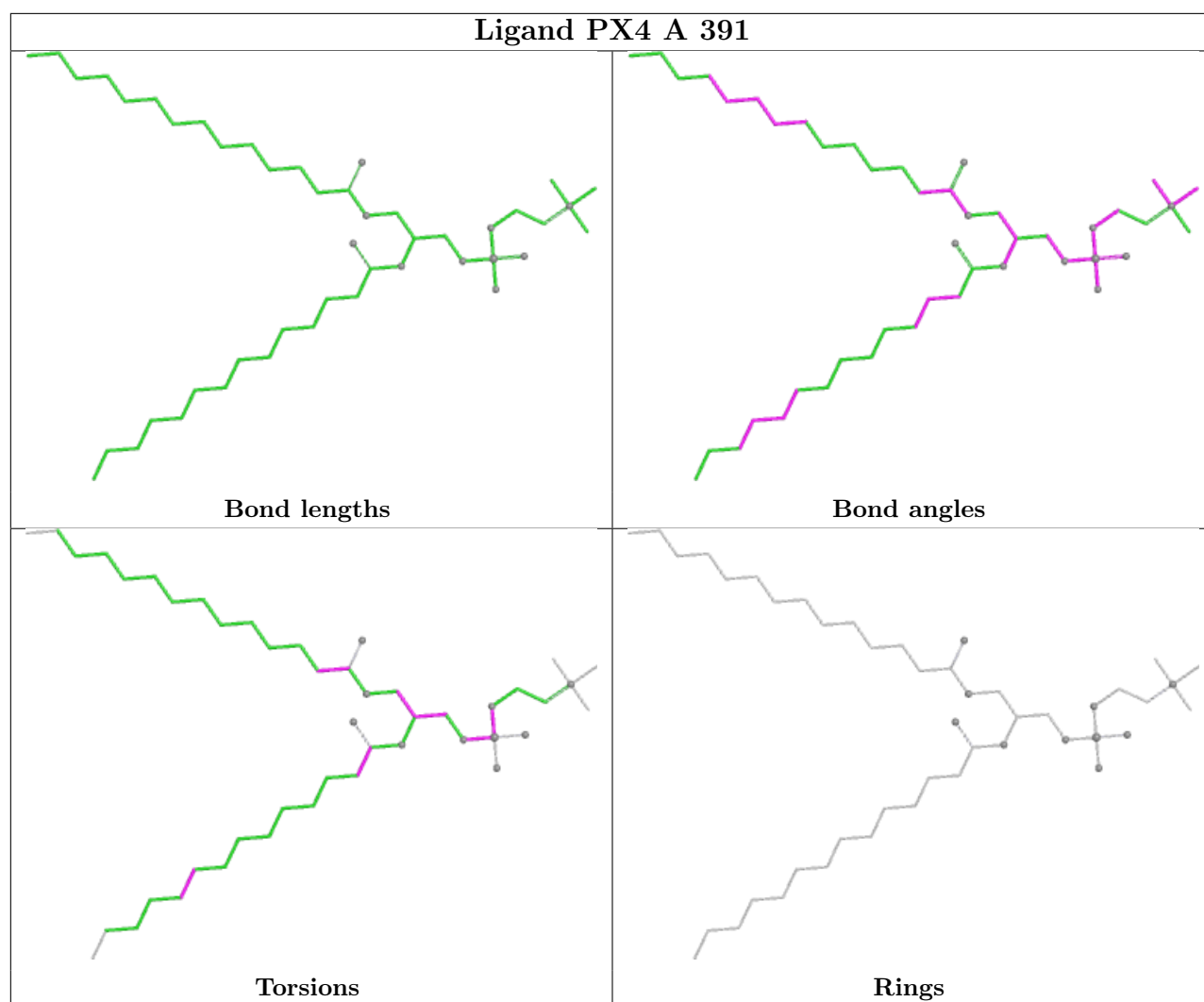


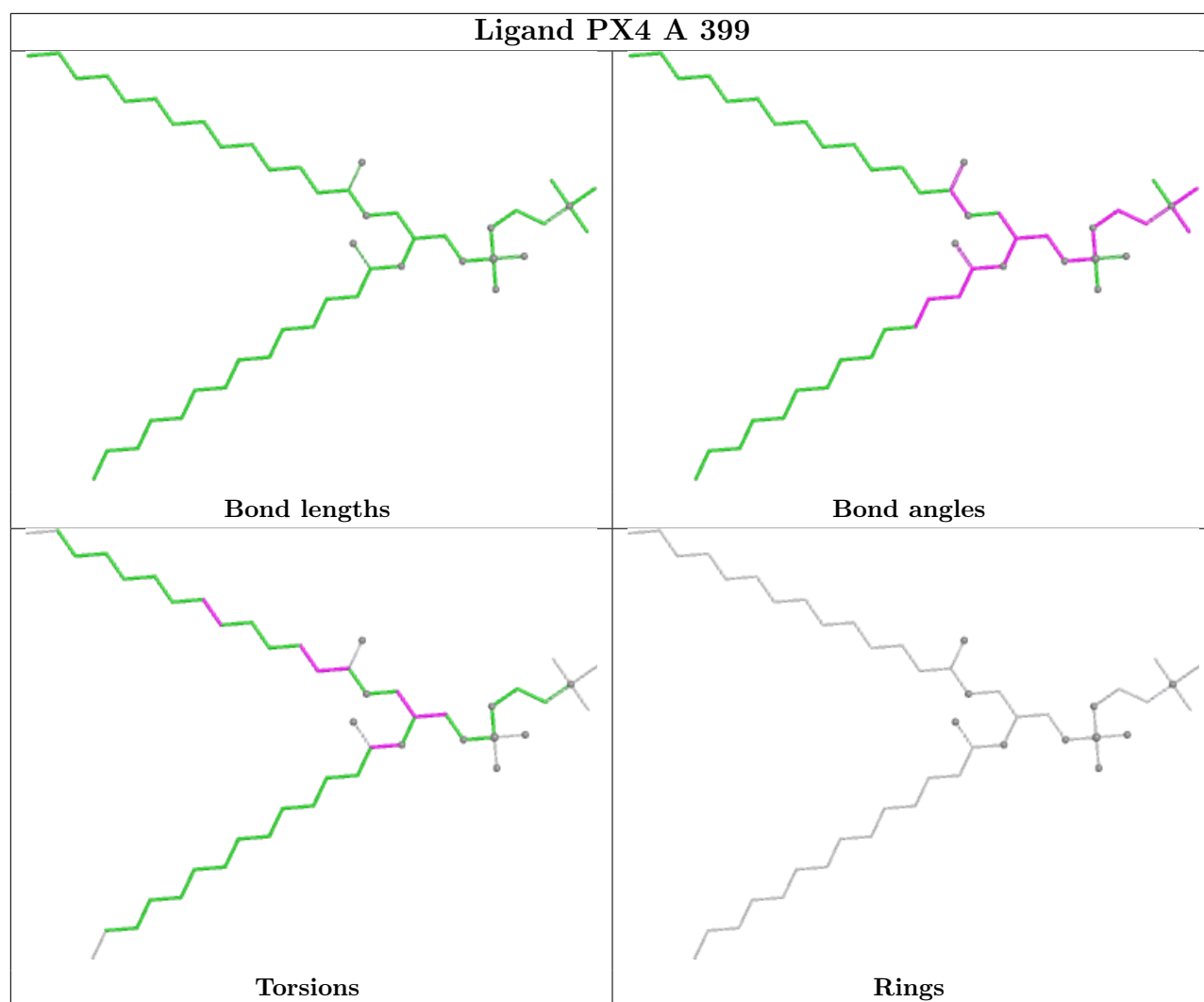
Ligand C3S A 434

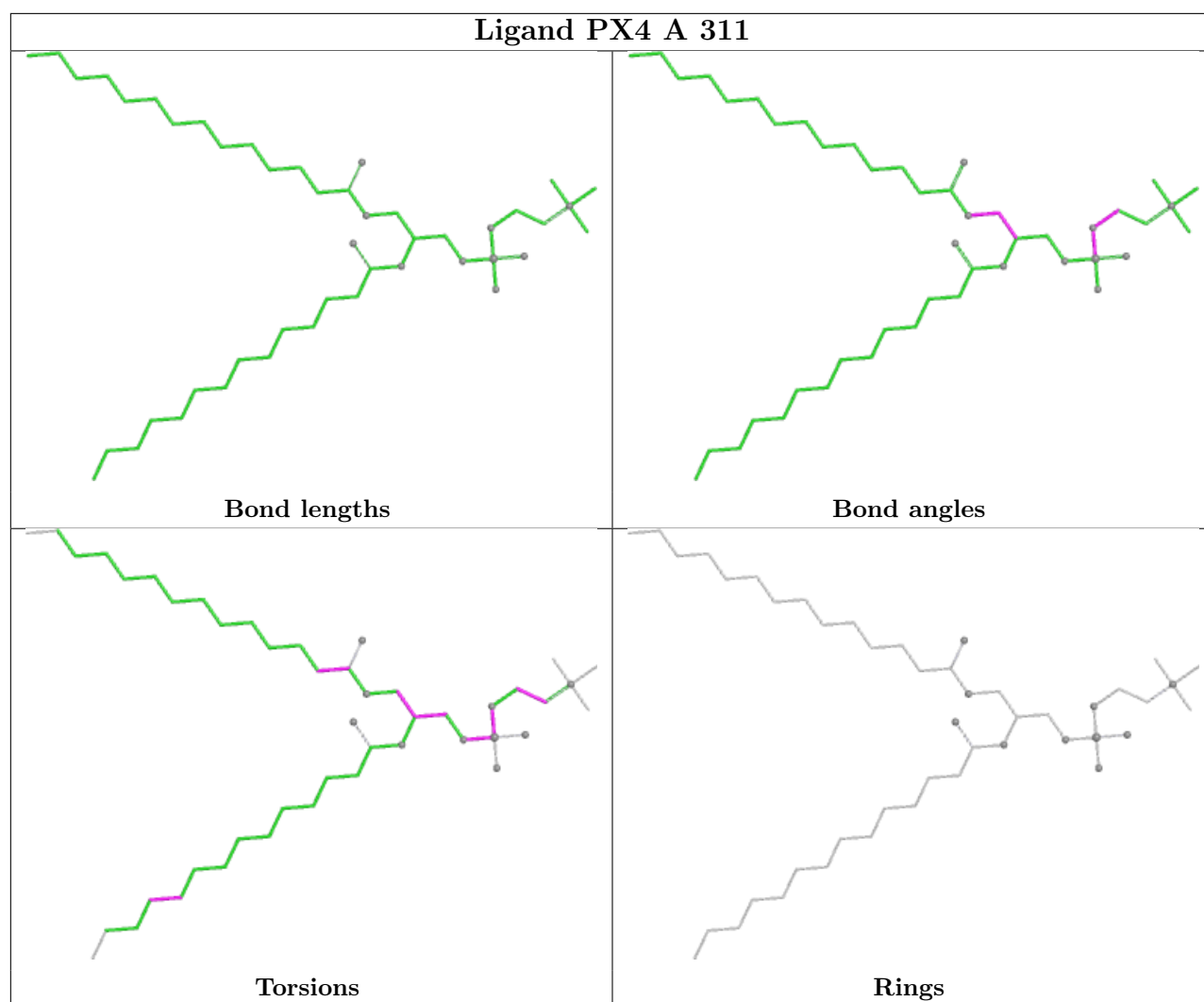


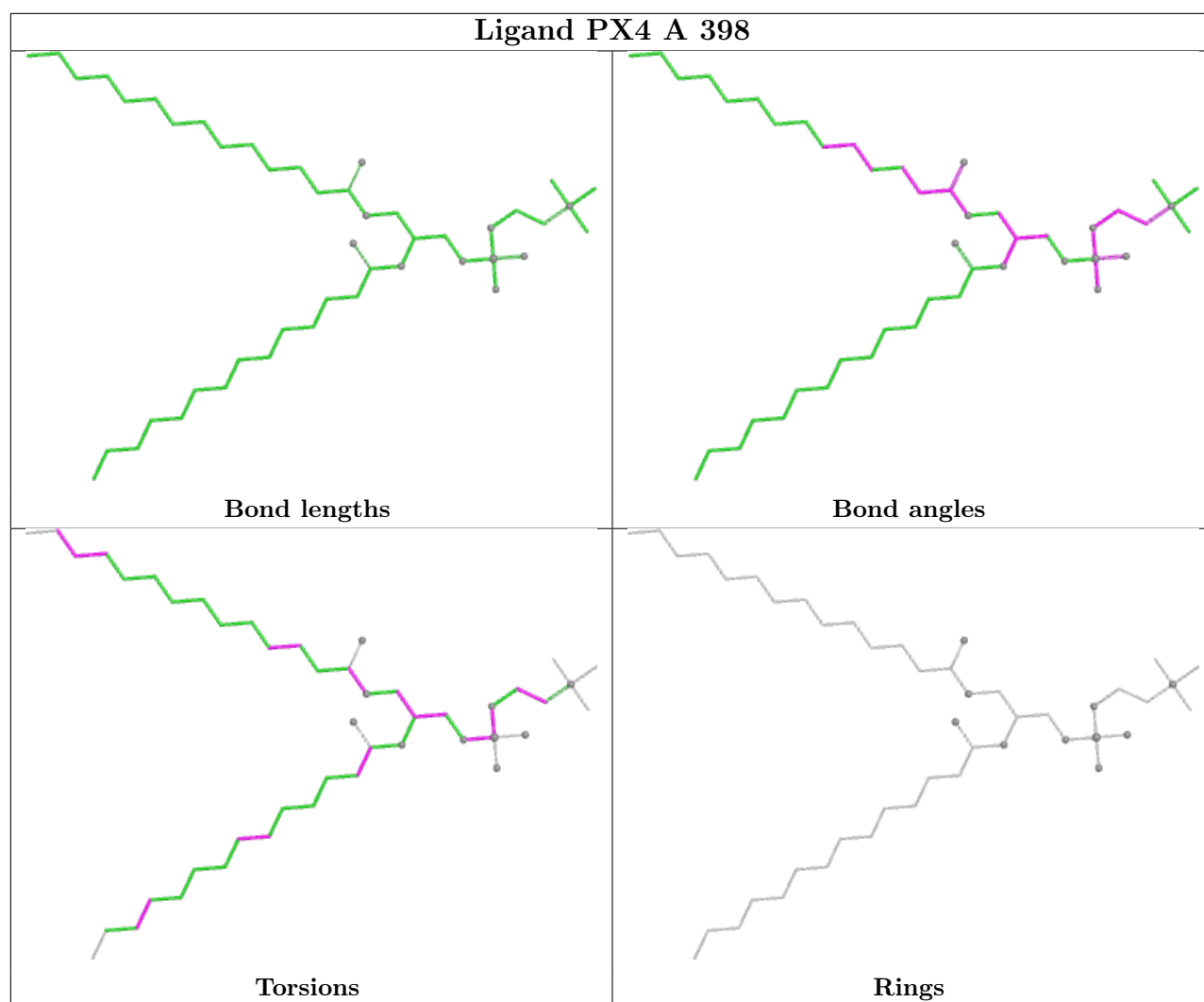


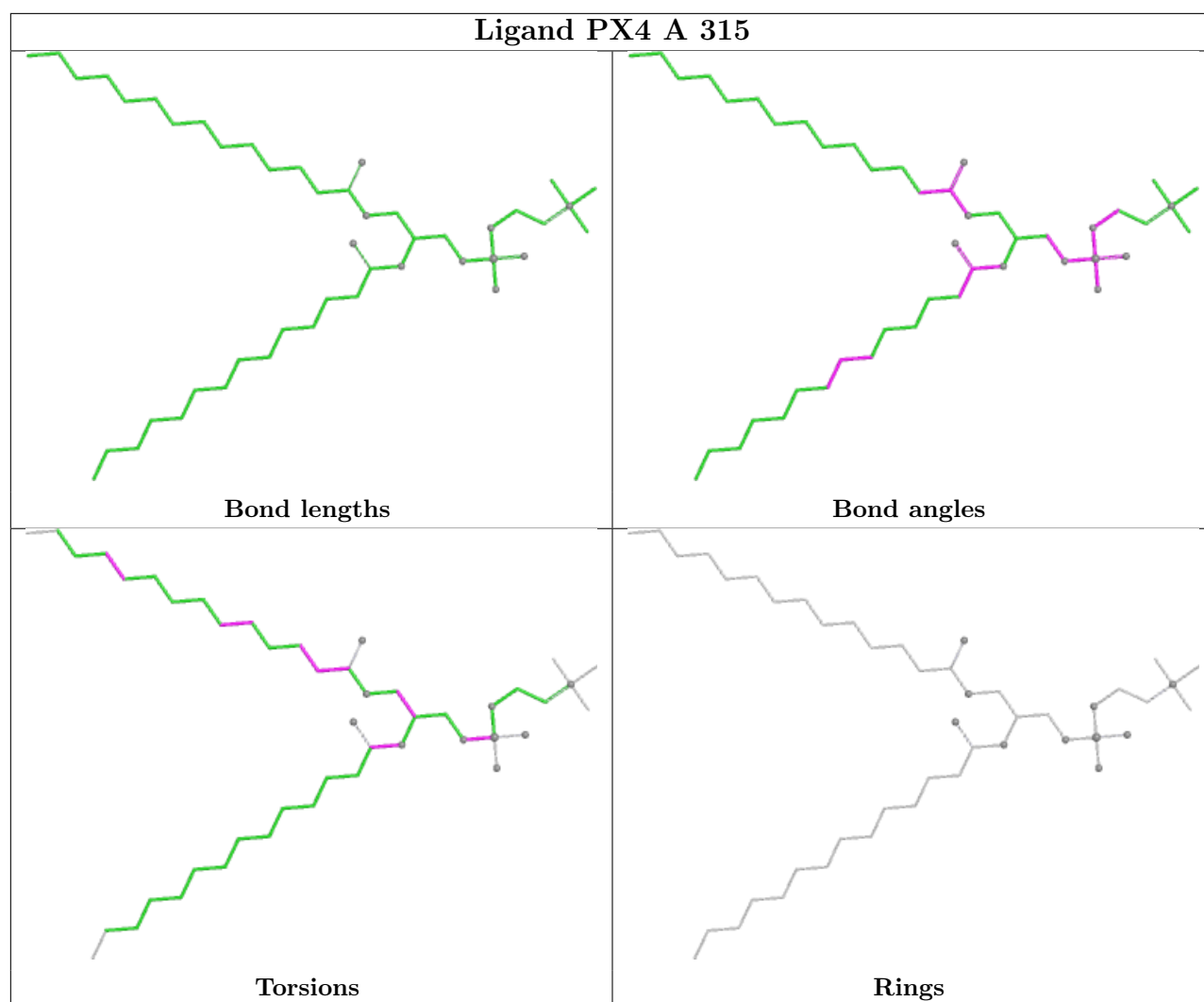


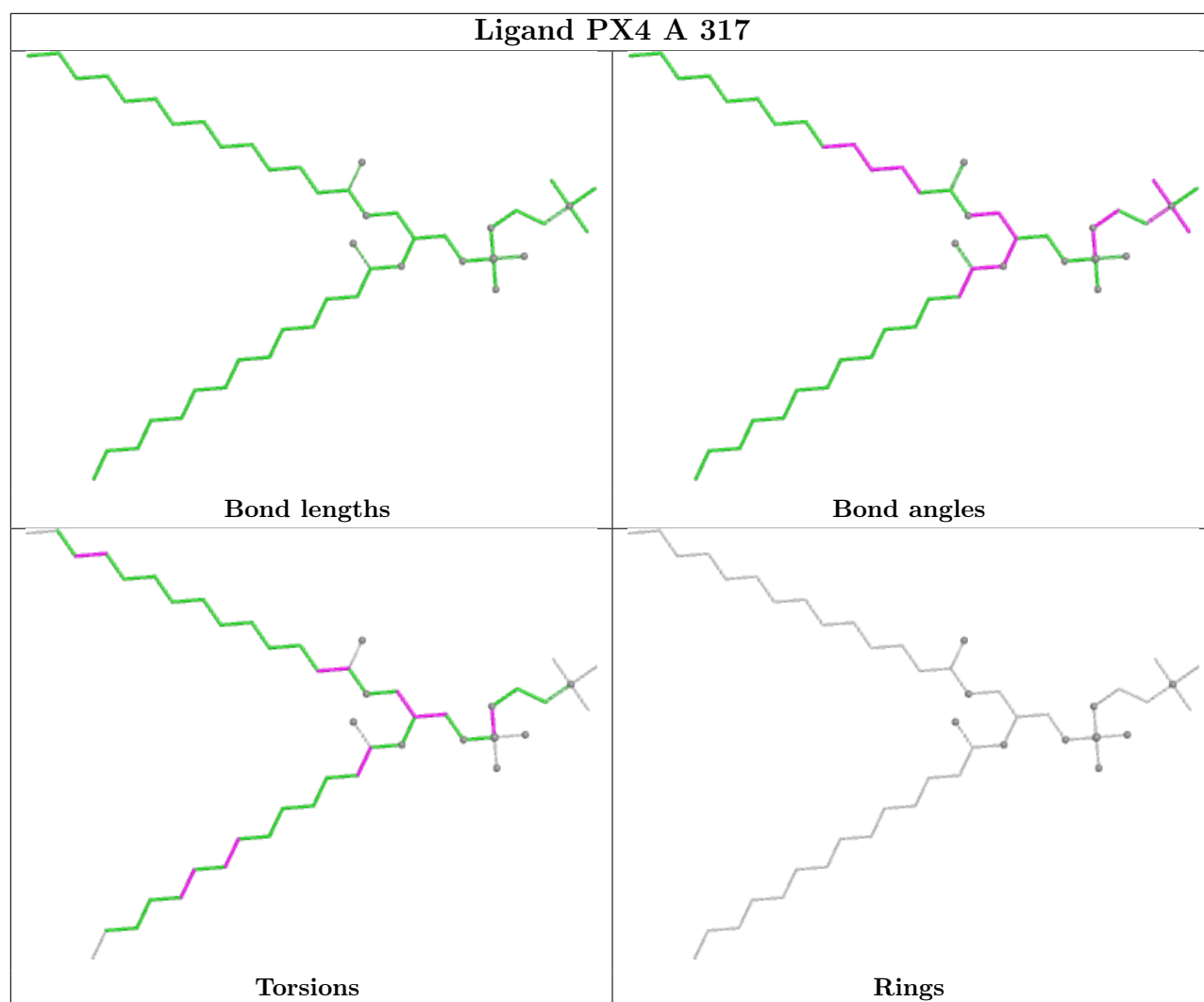


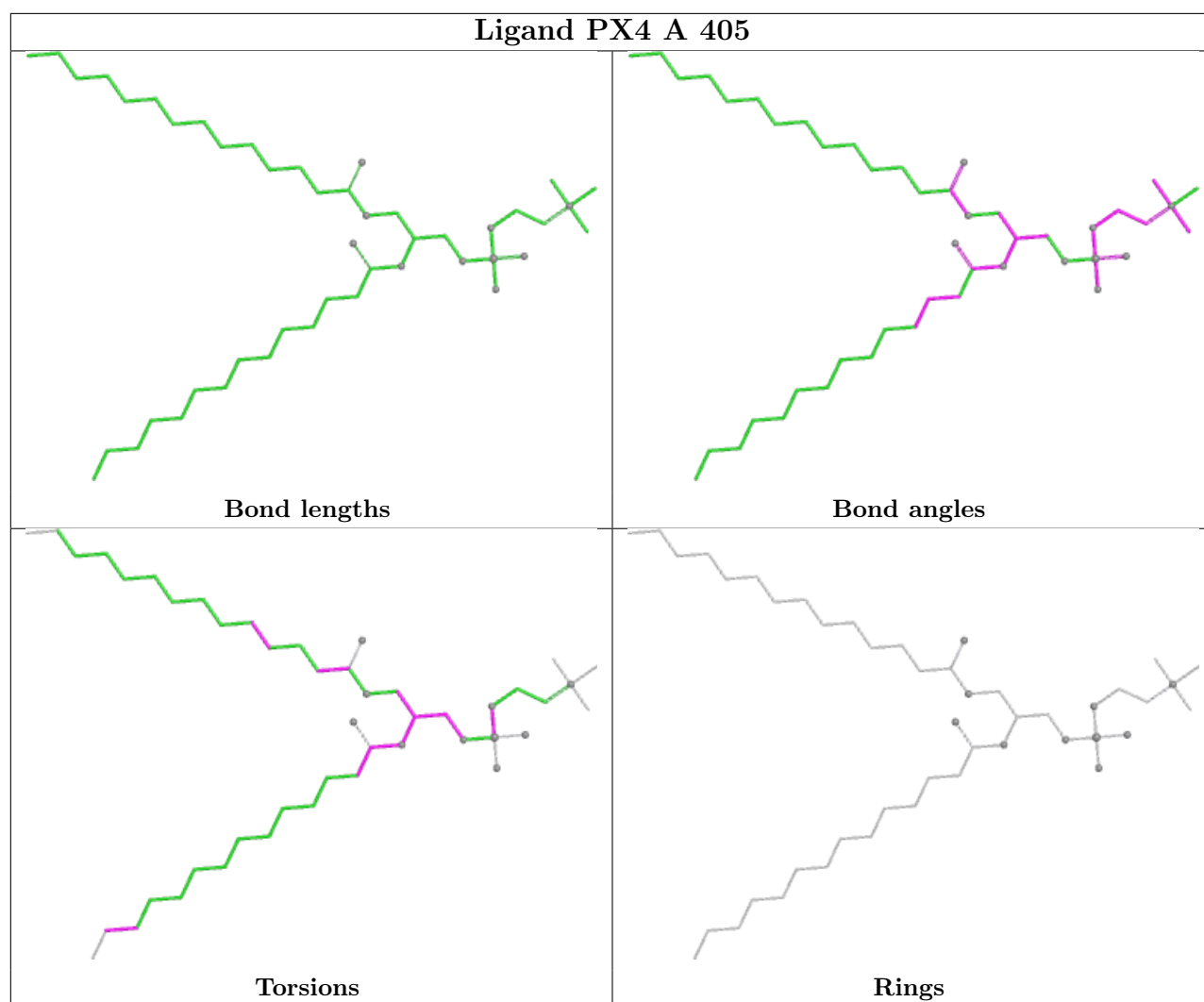


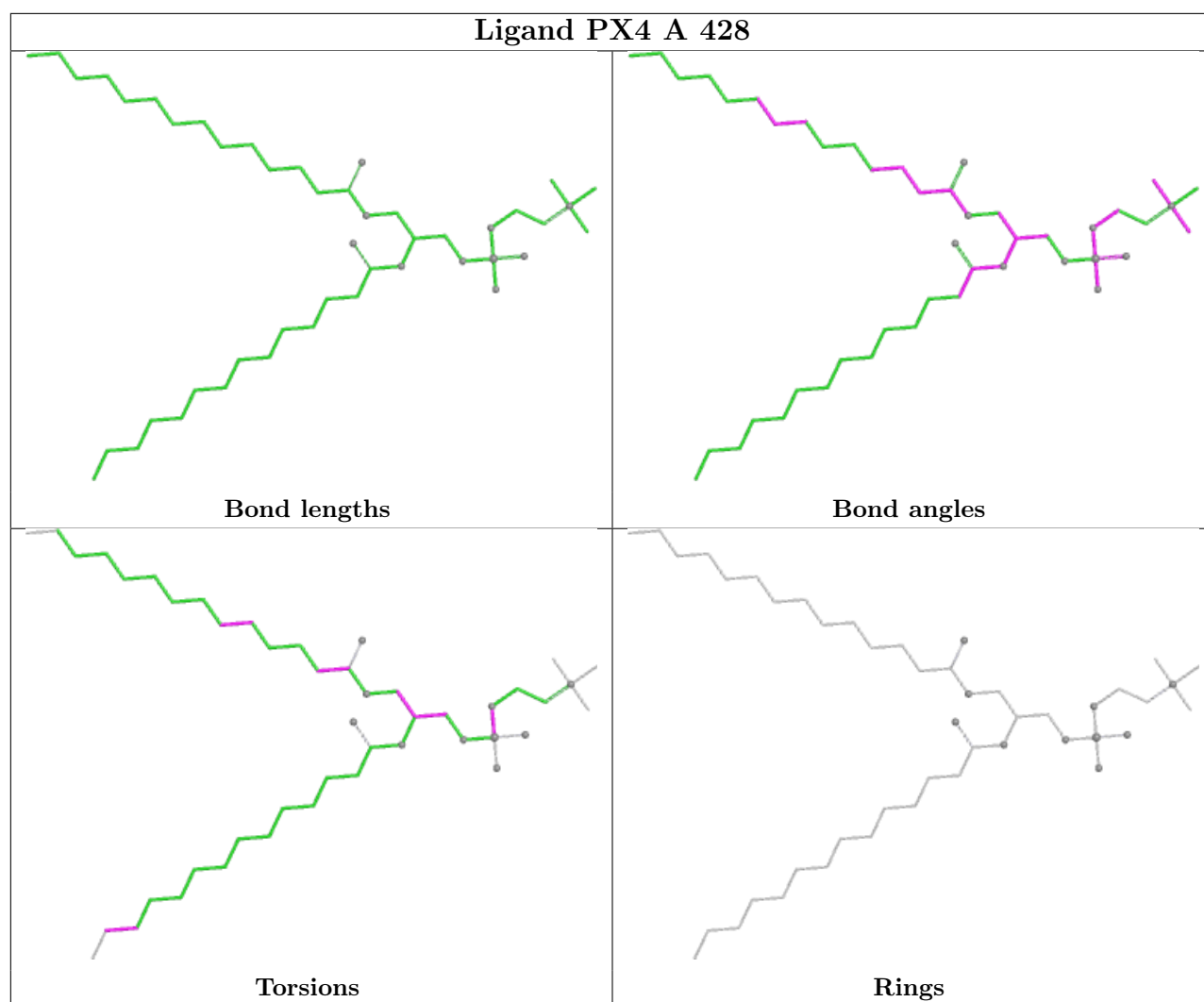


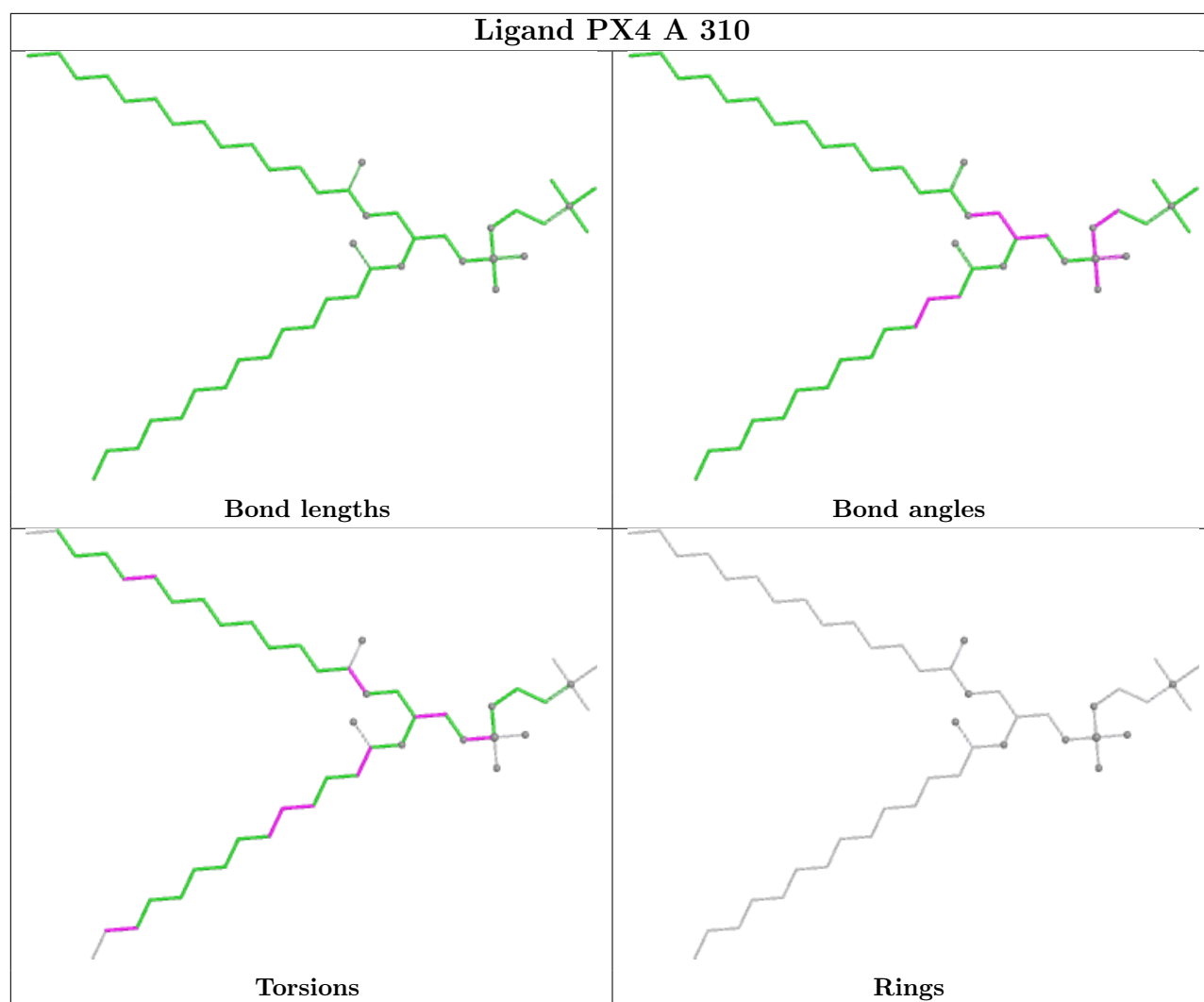




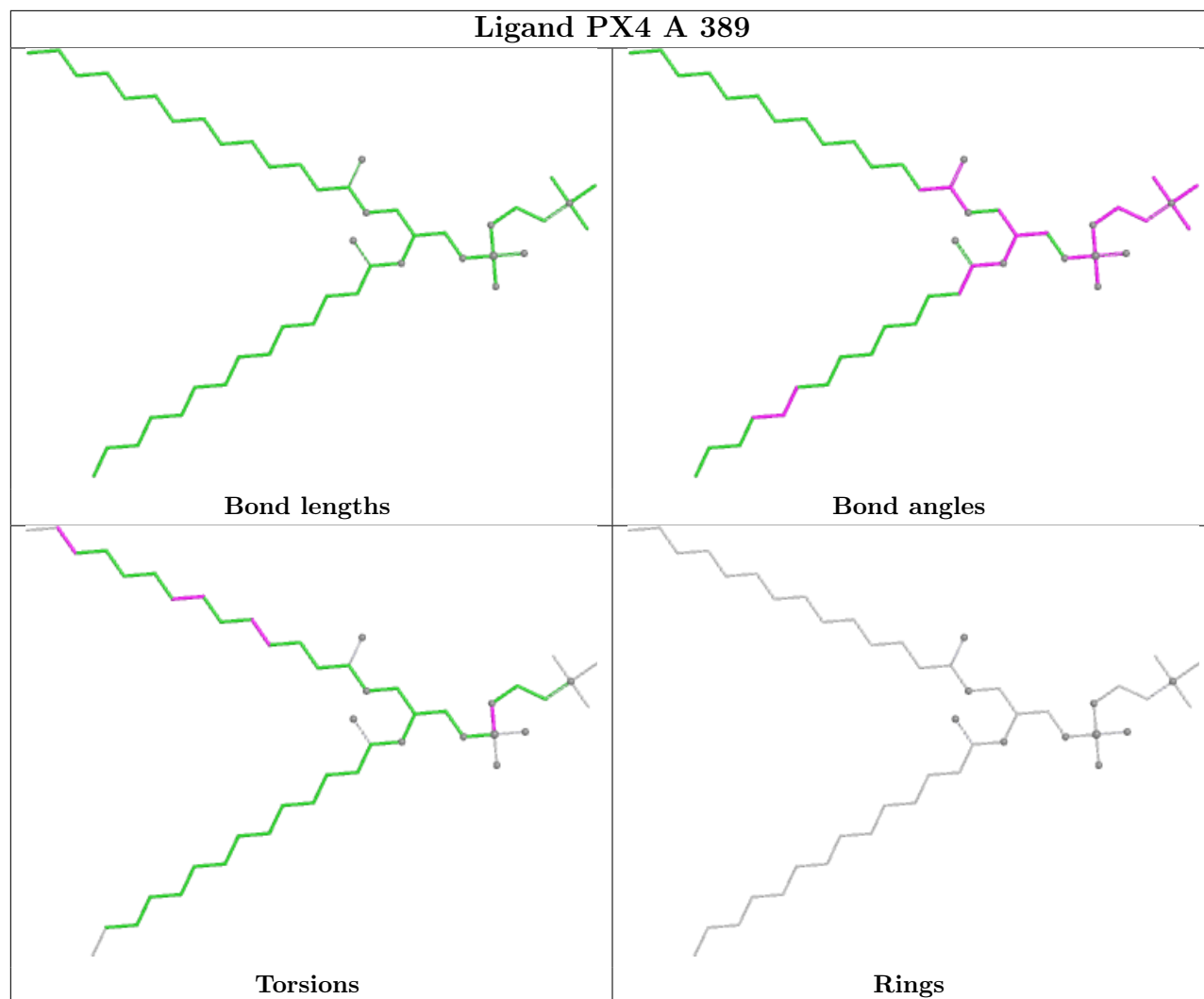




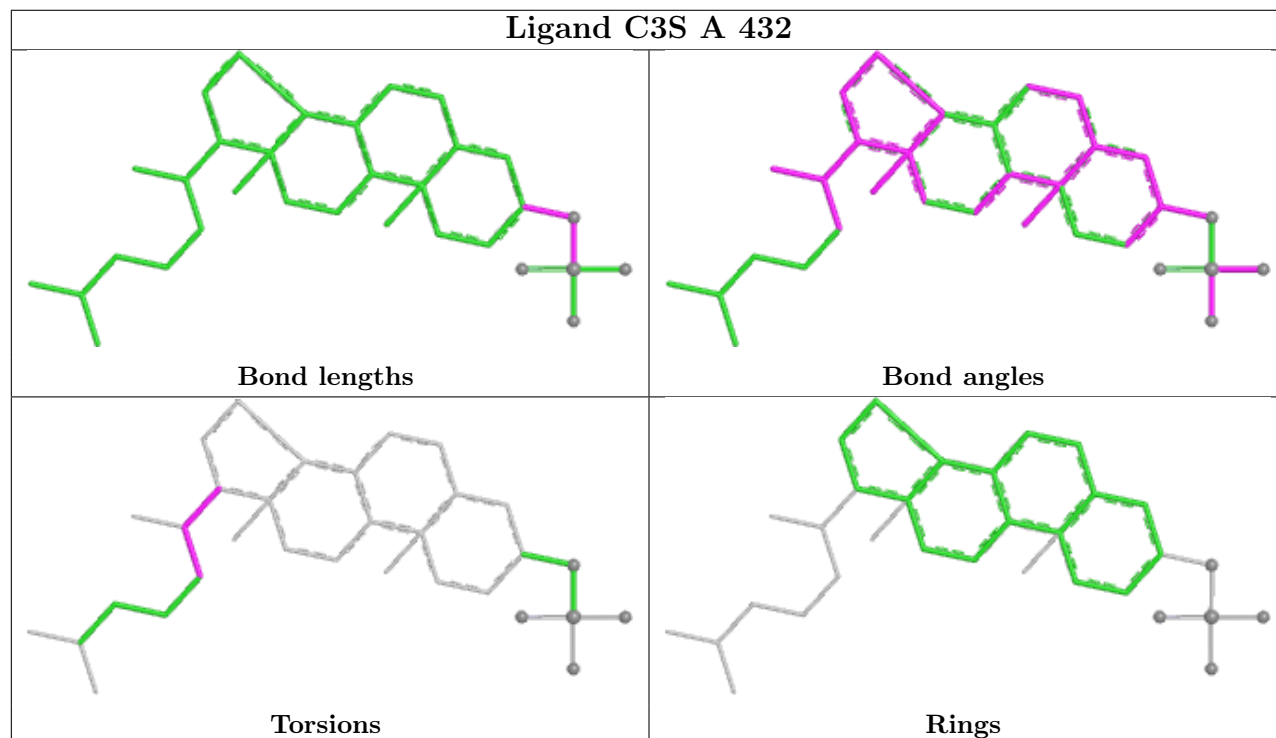


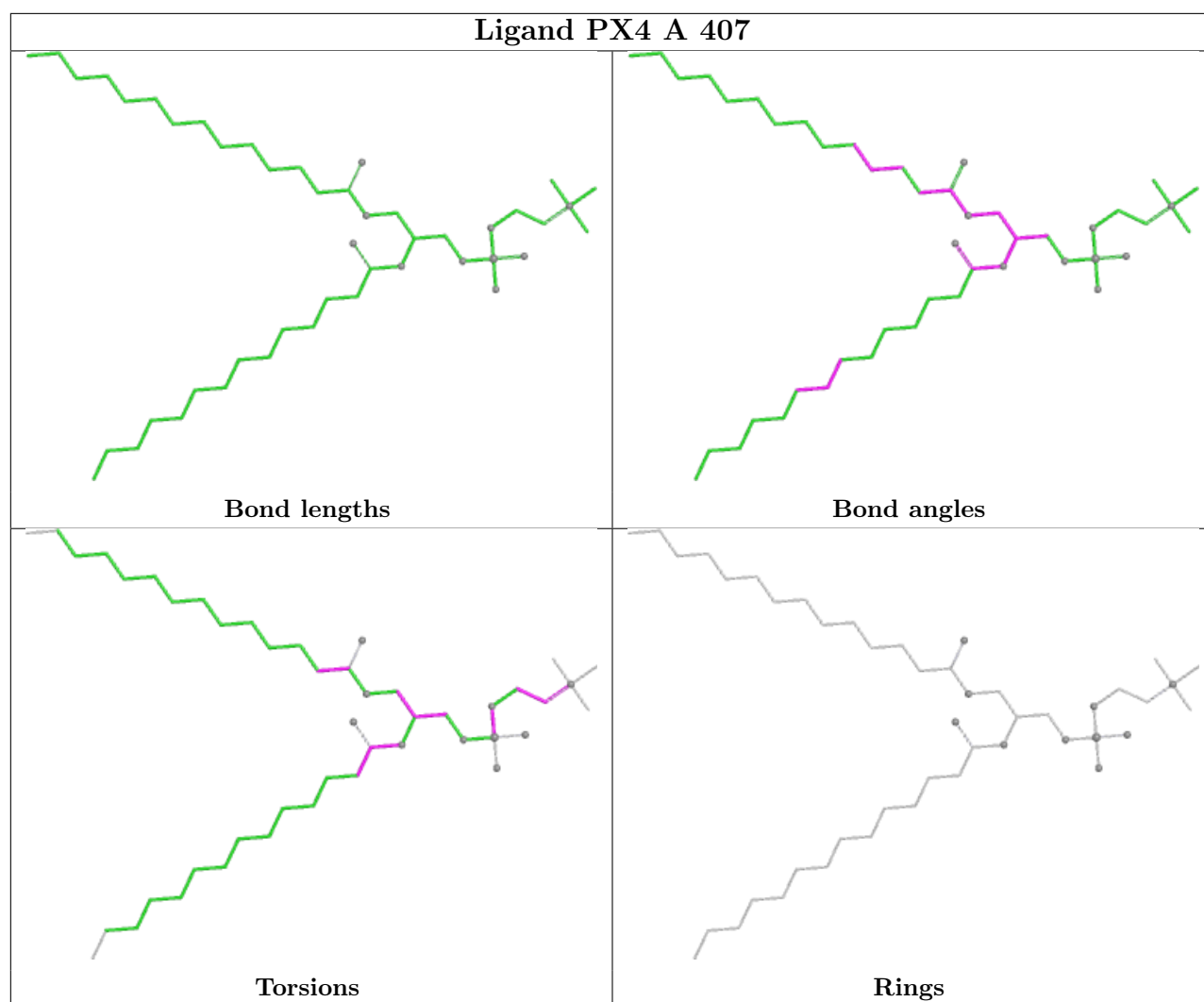


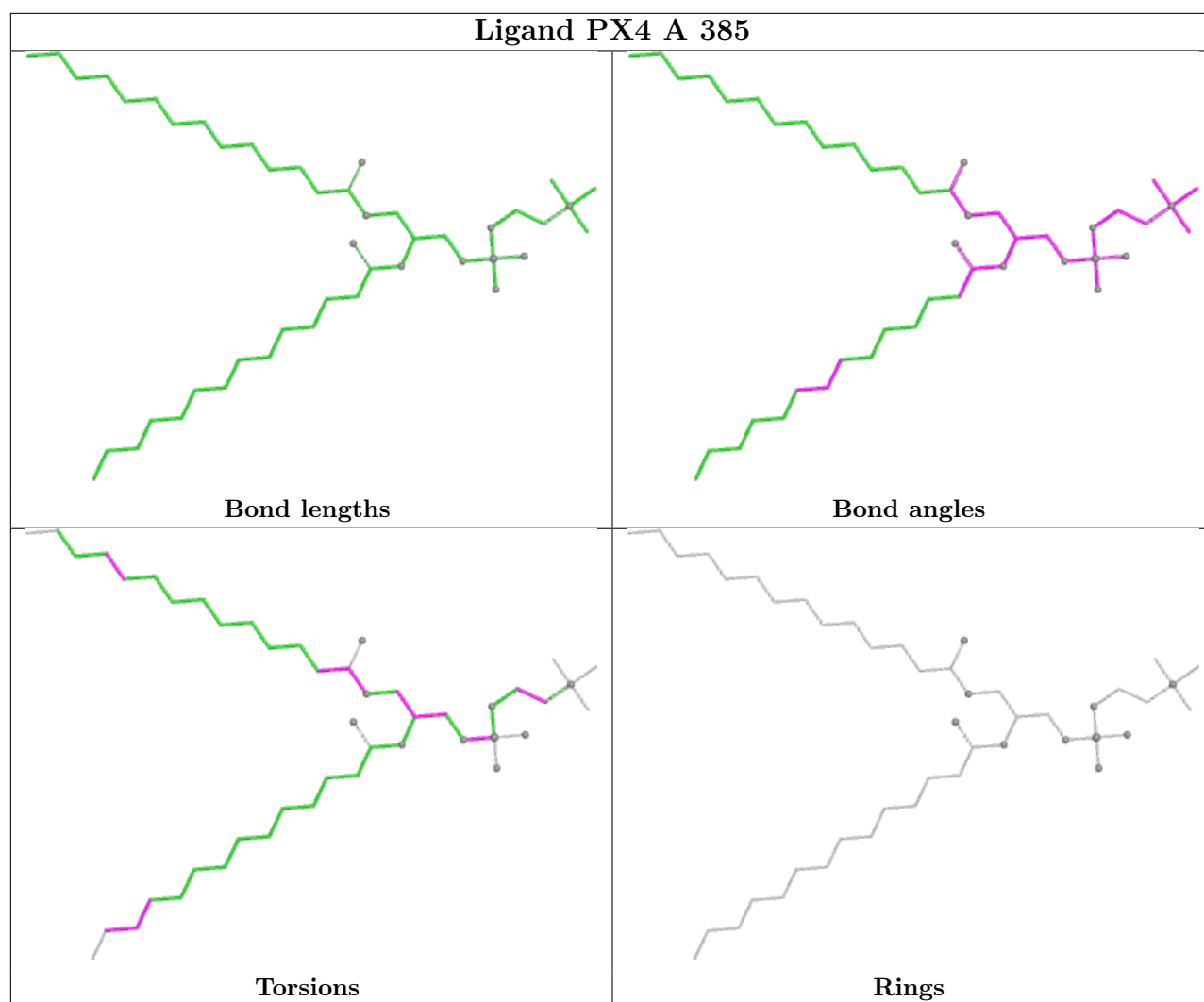
Ligand PX4 A 389

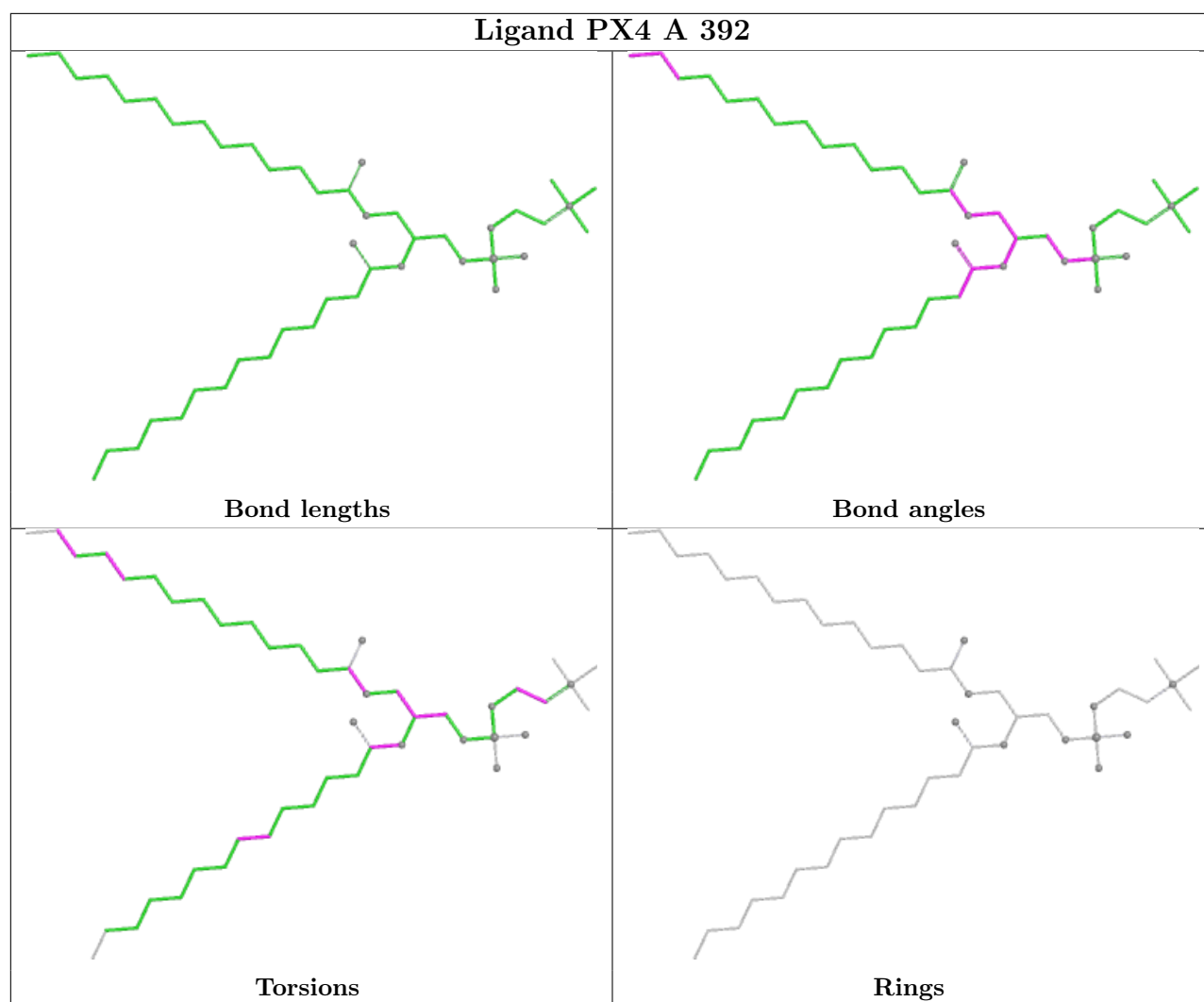


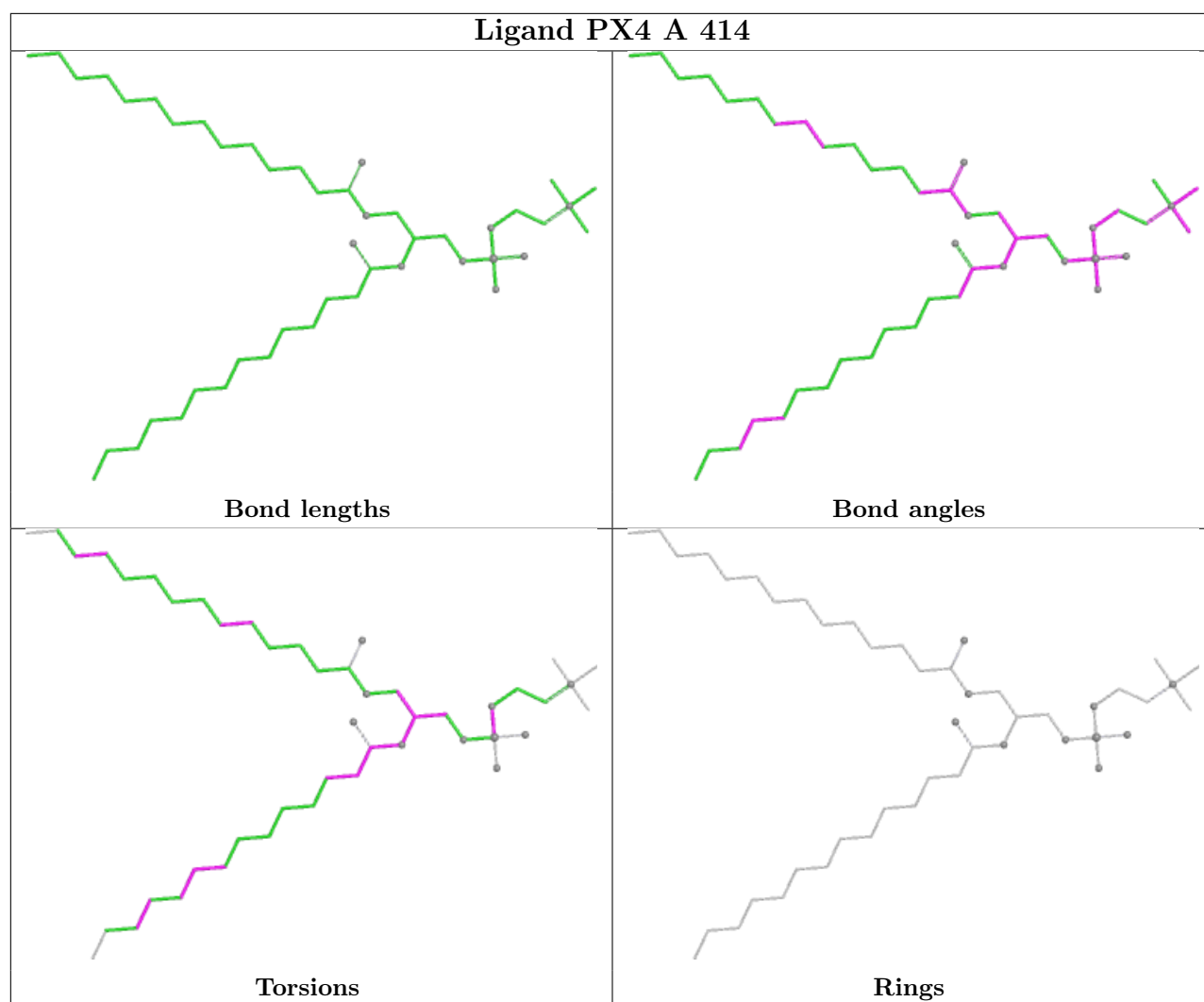
Ligand C3S A 432

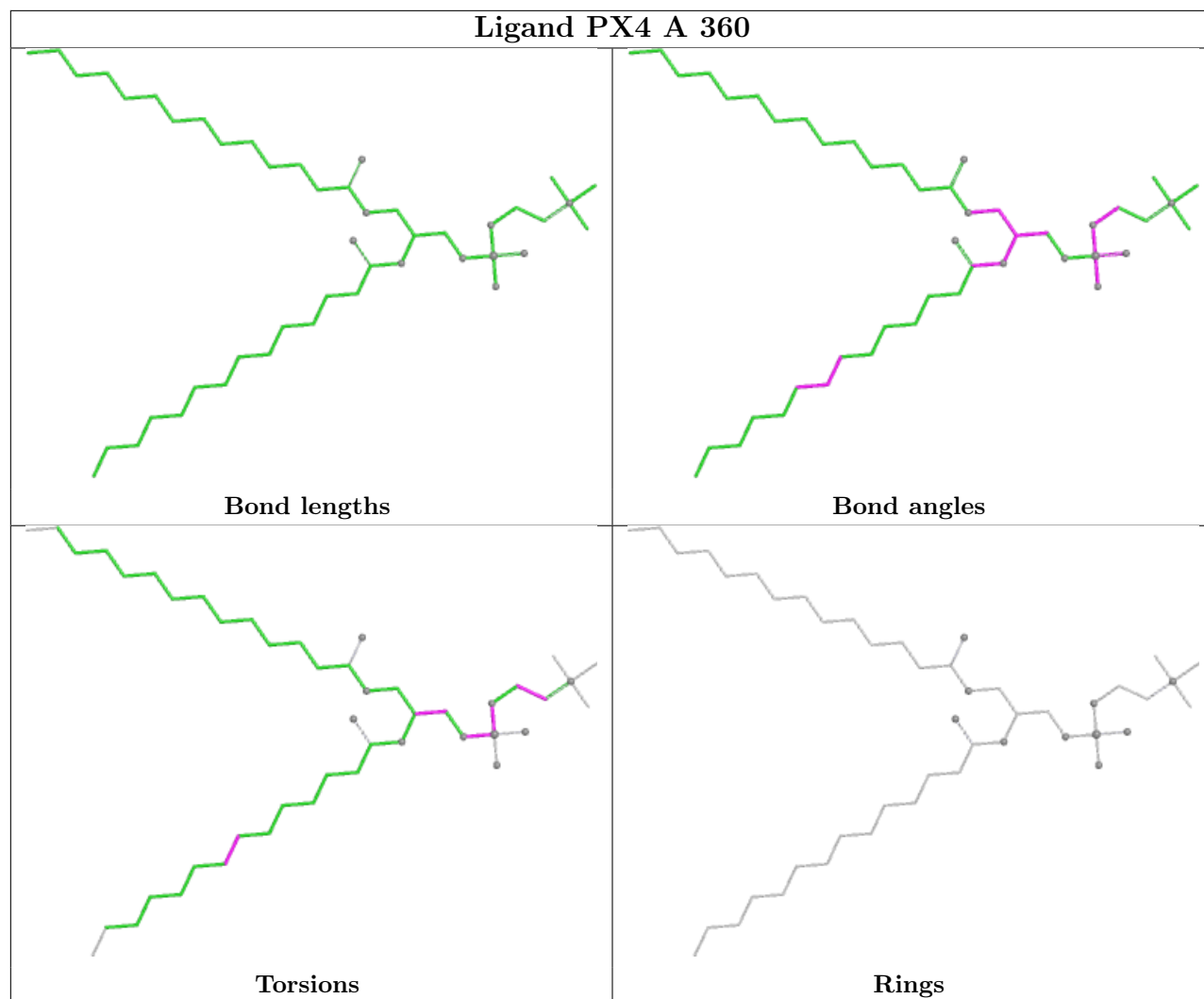




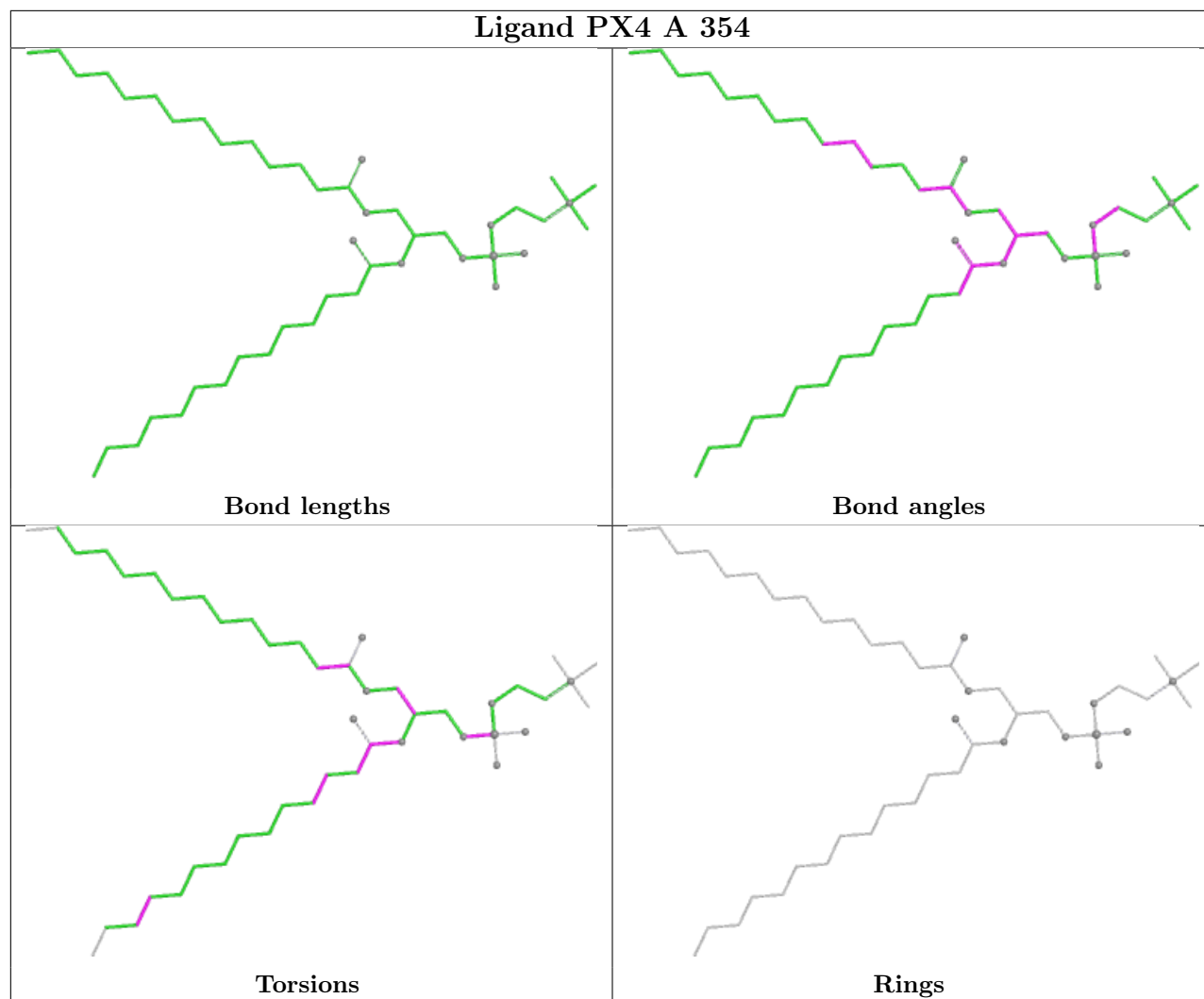


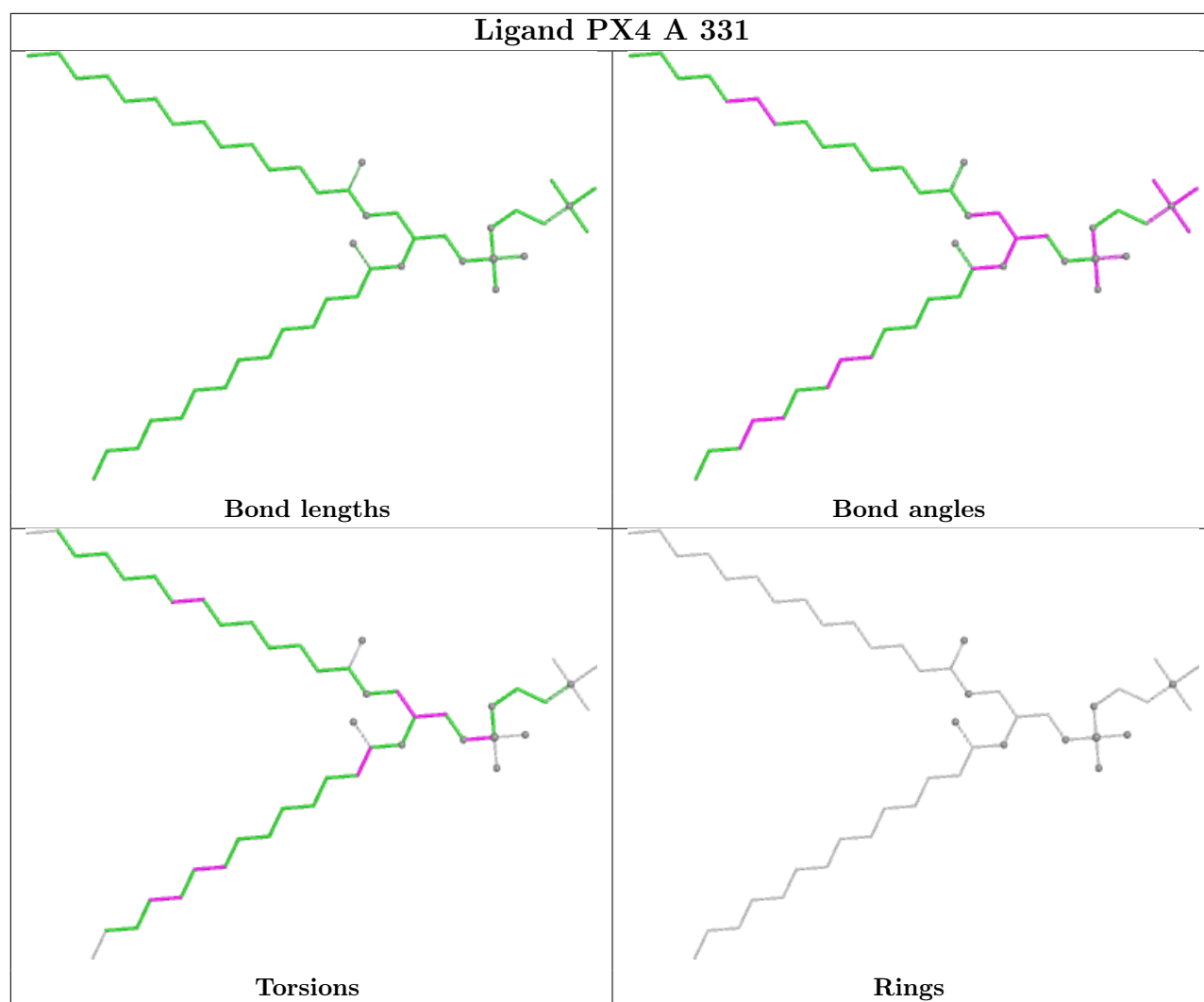


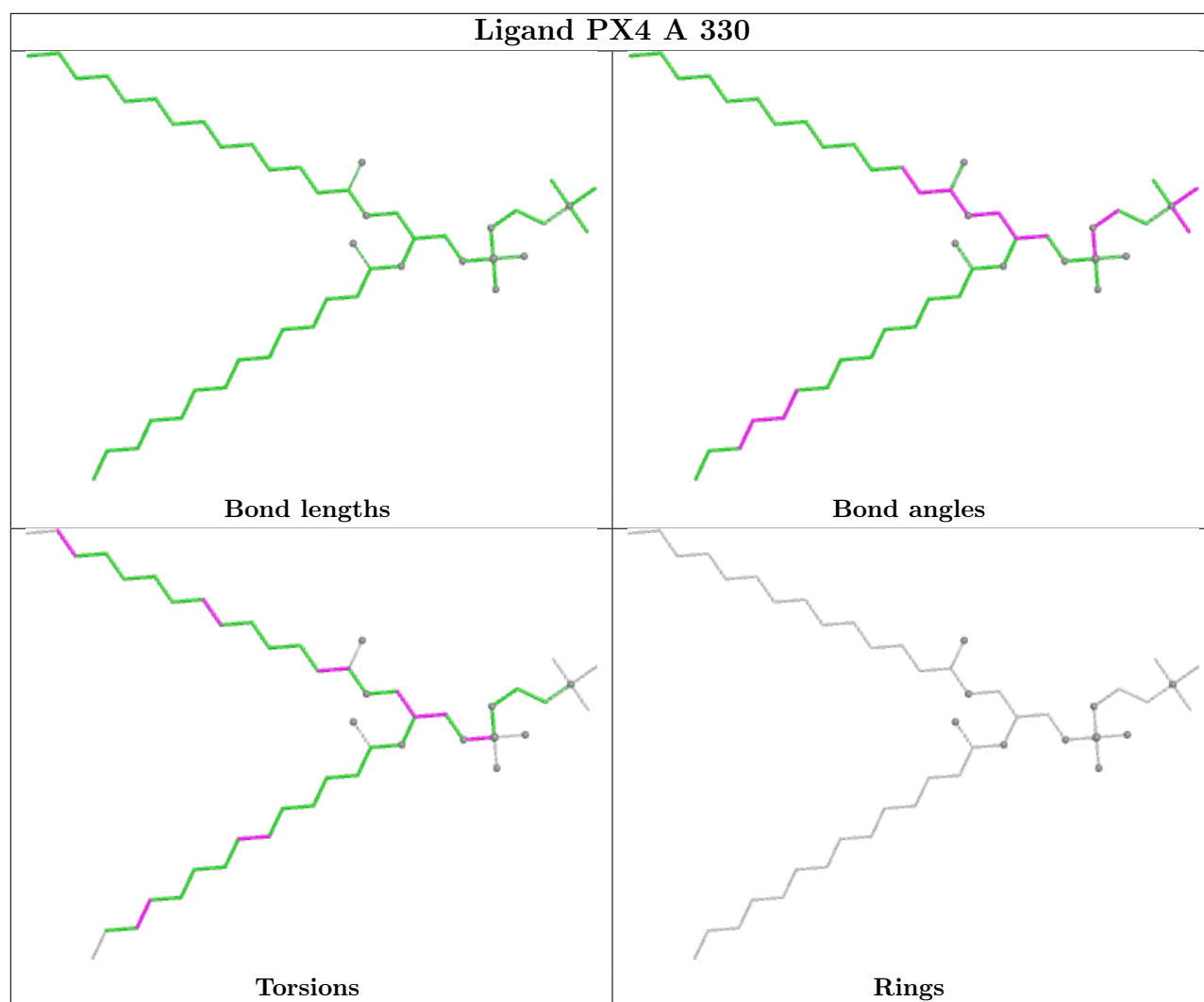


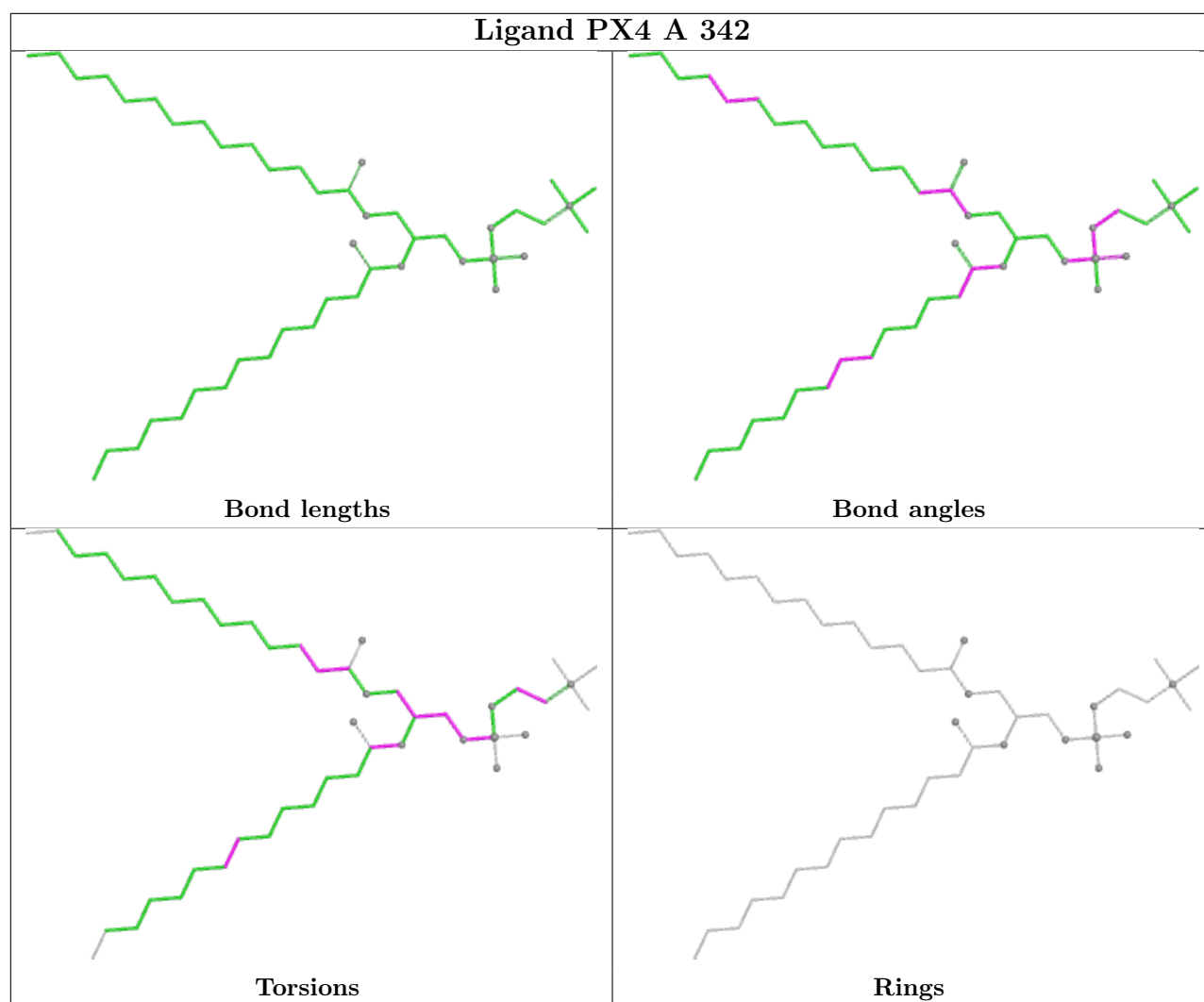


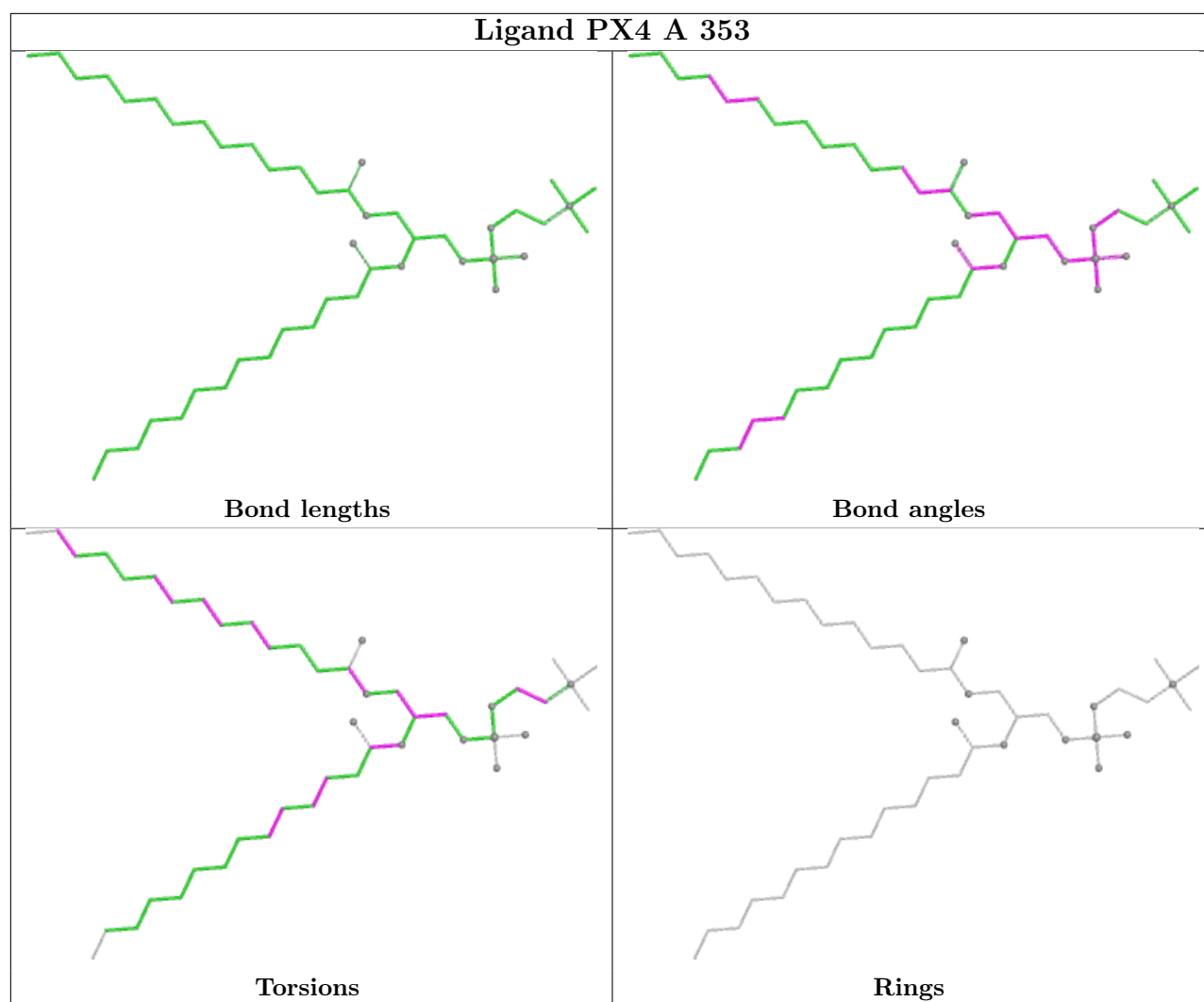
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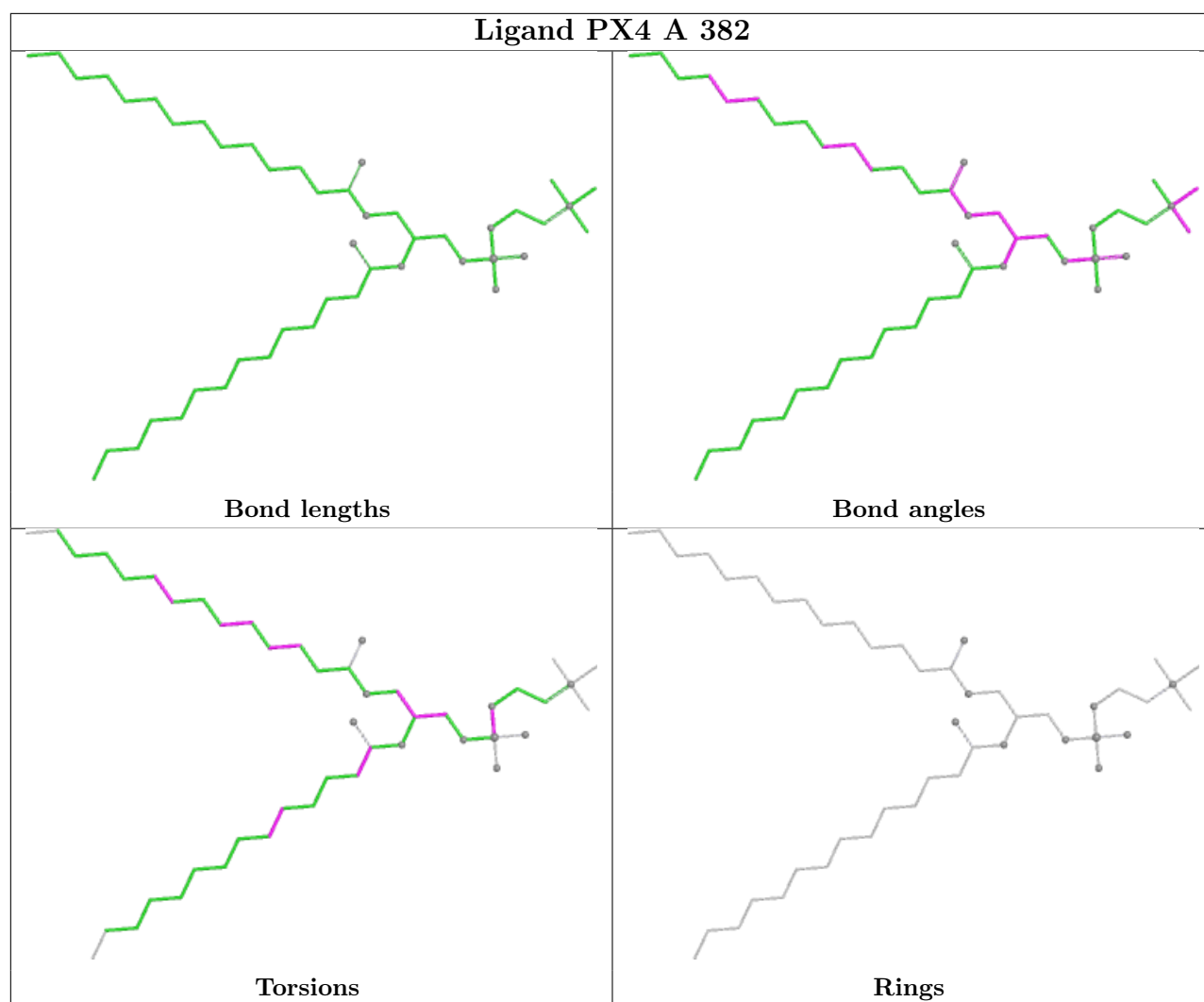




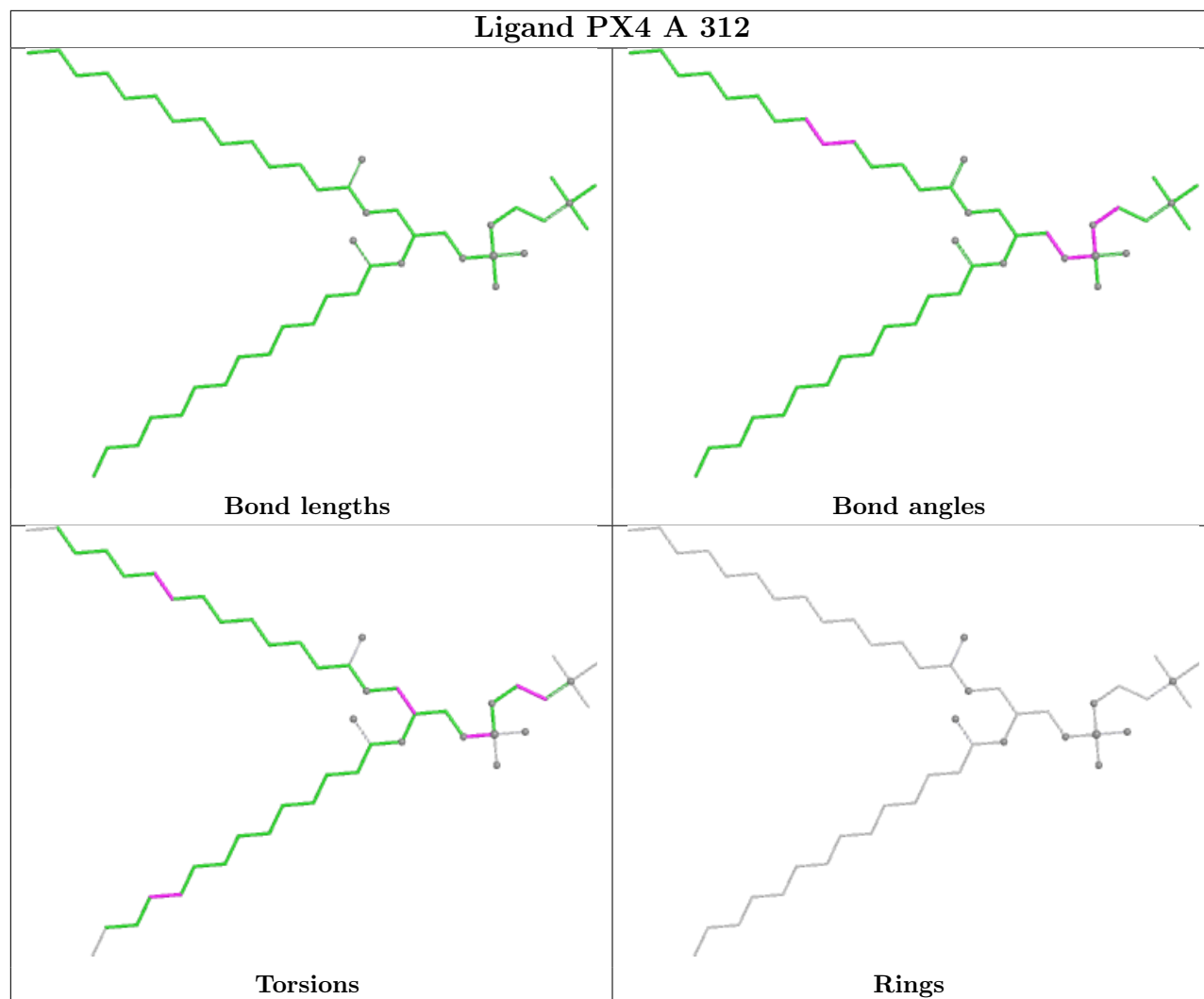




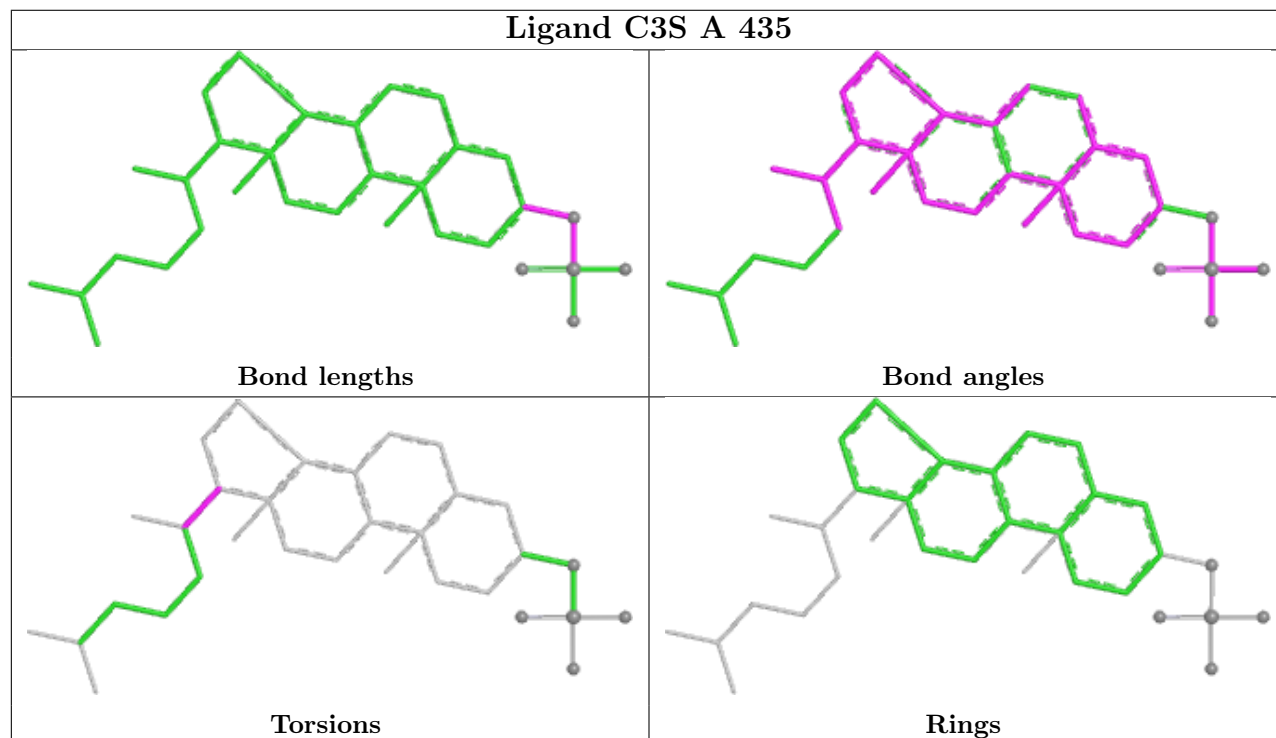


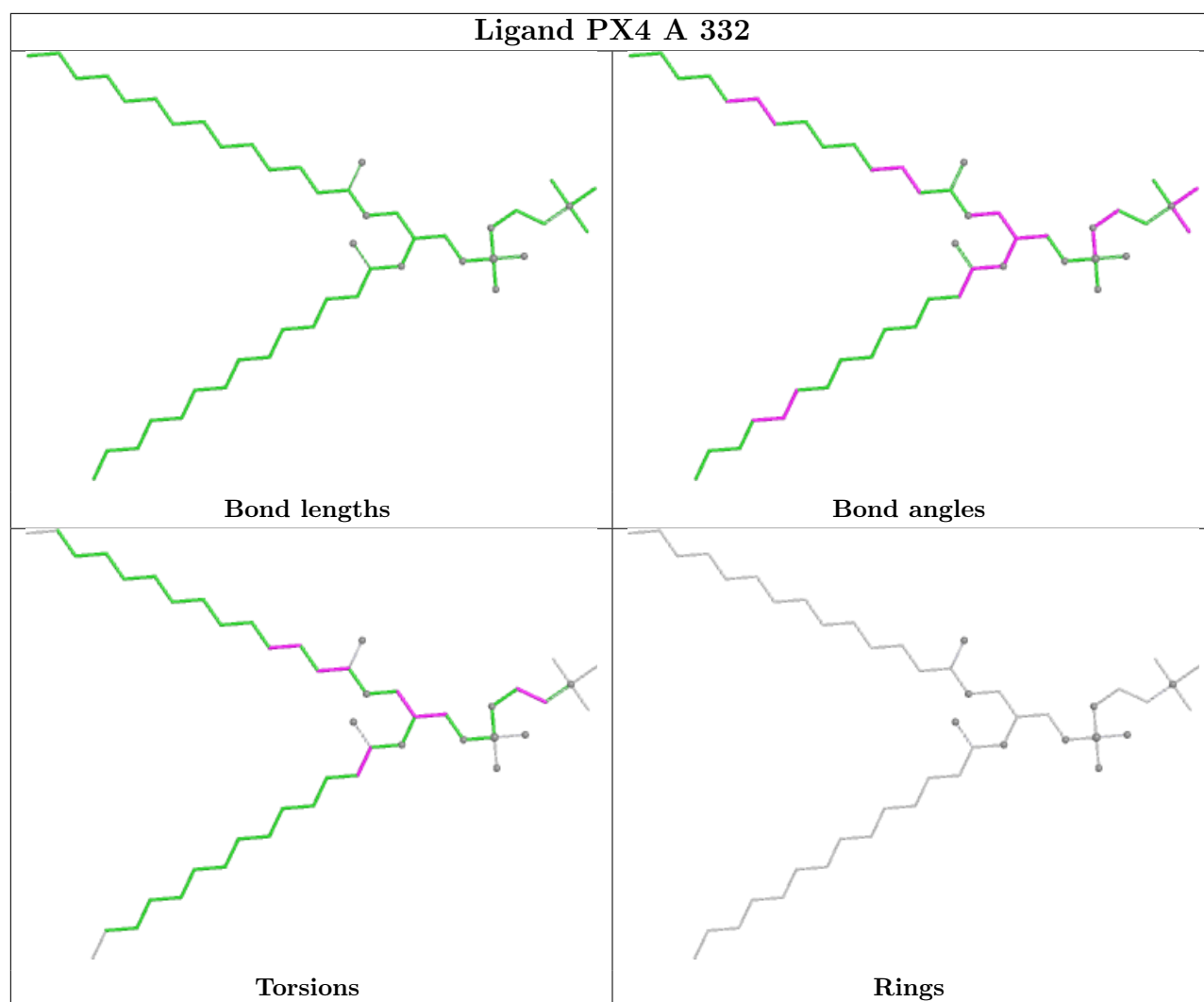


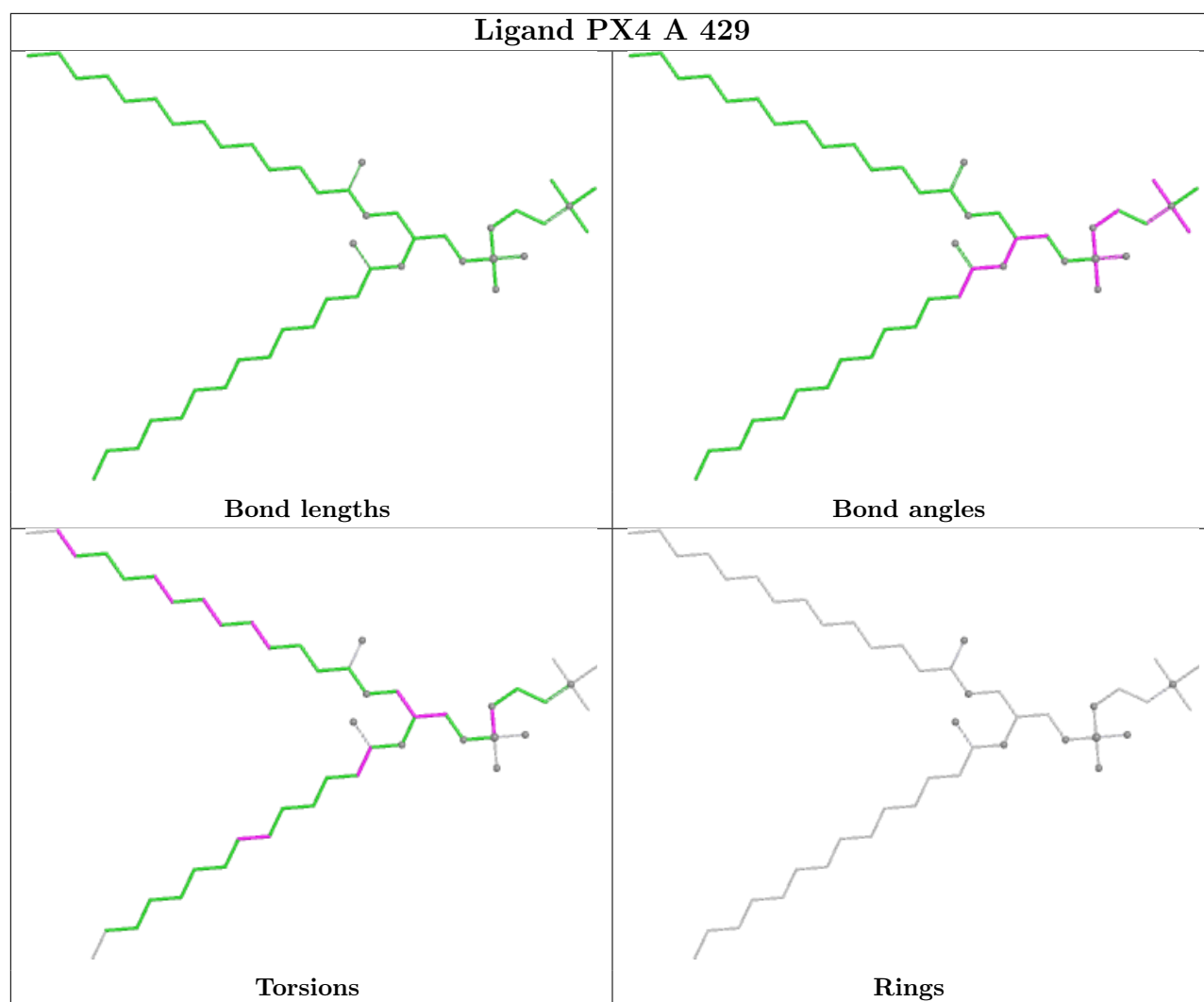
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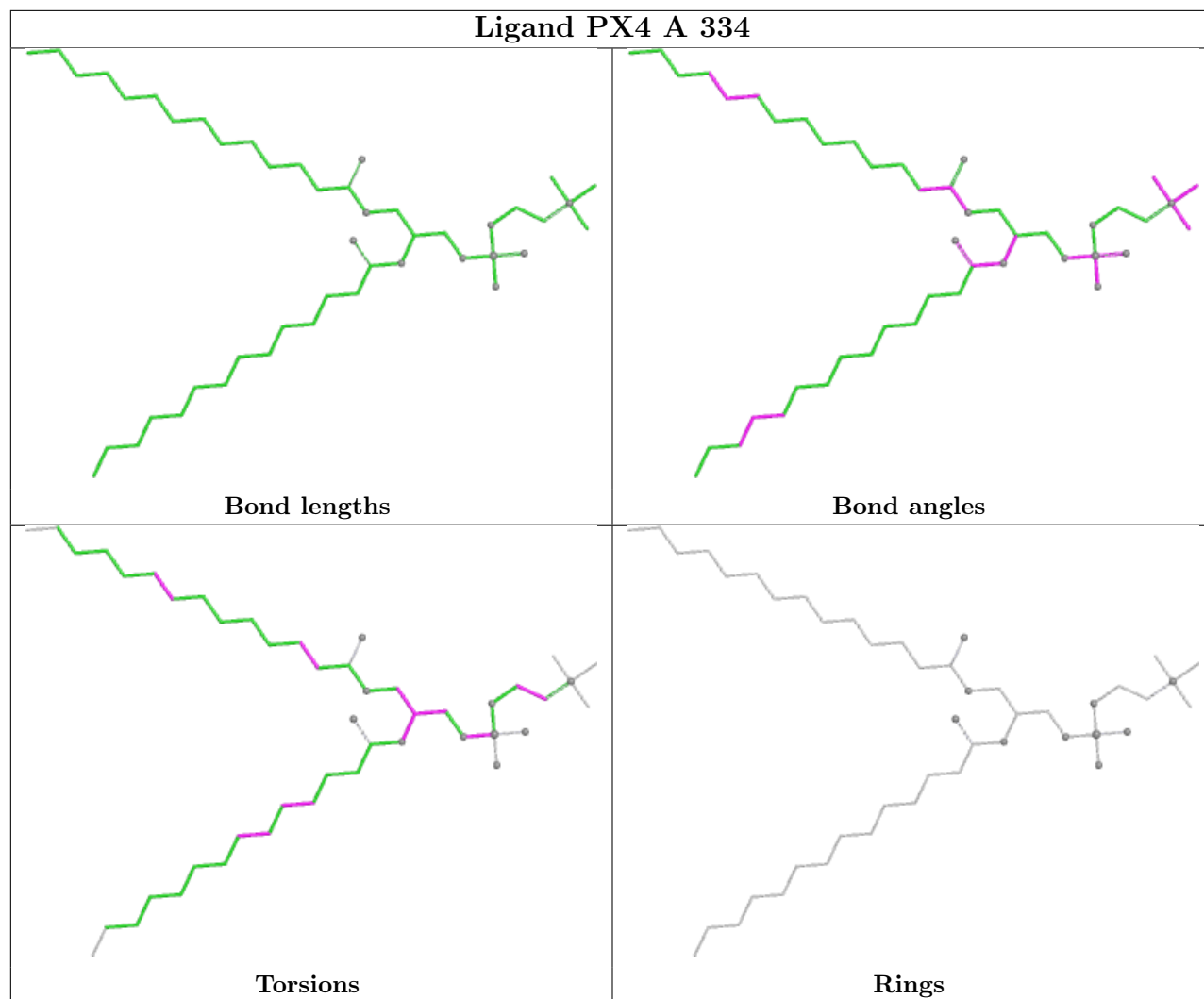
Ligand C3S A 435

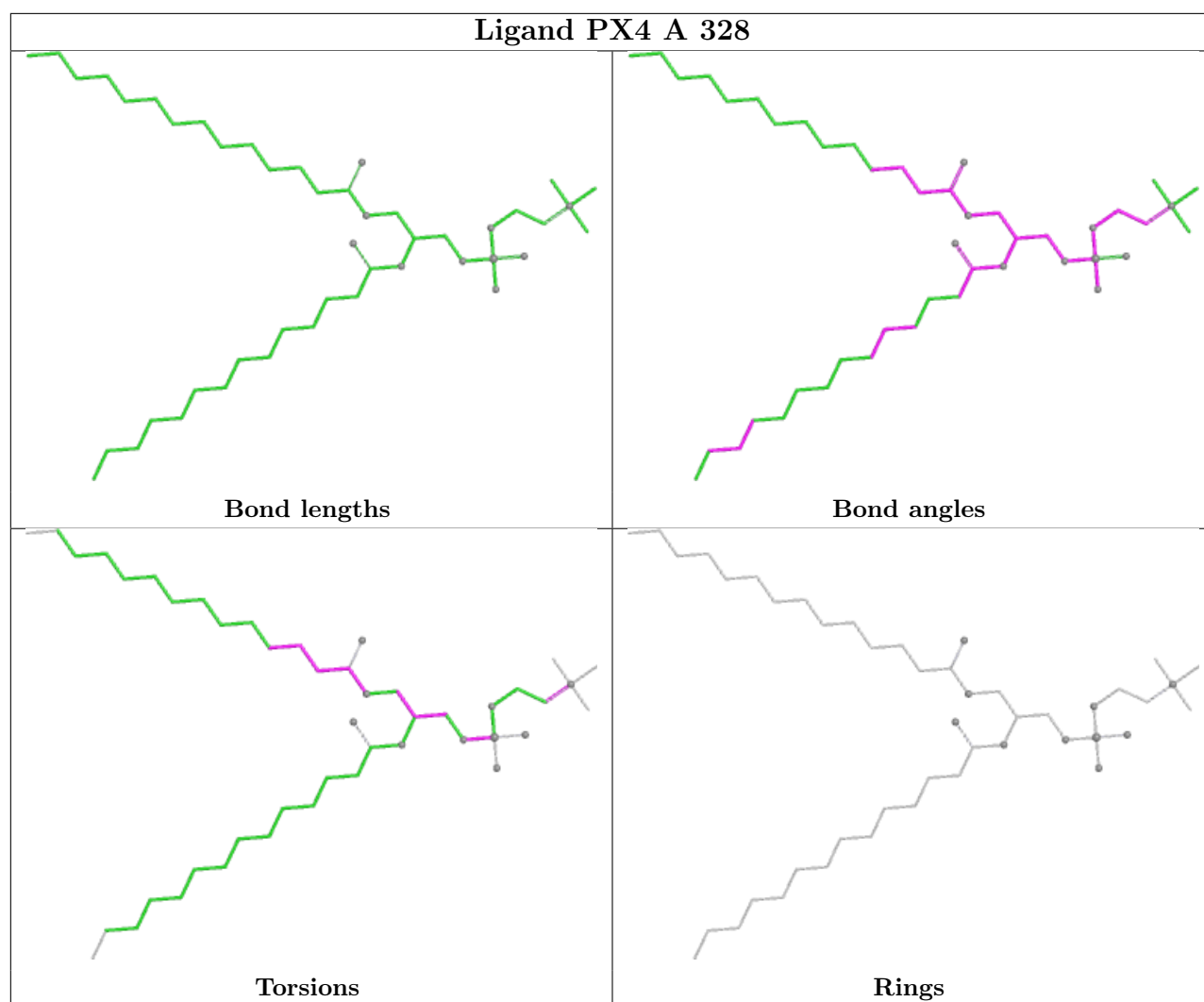


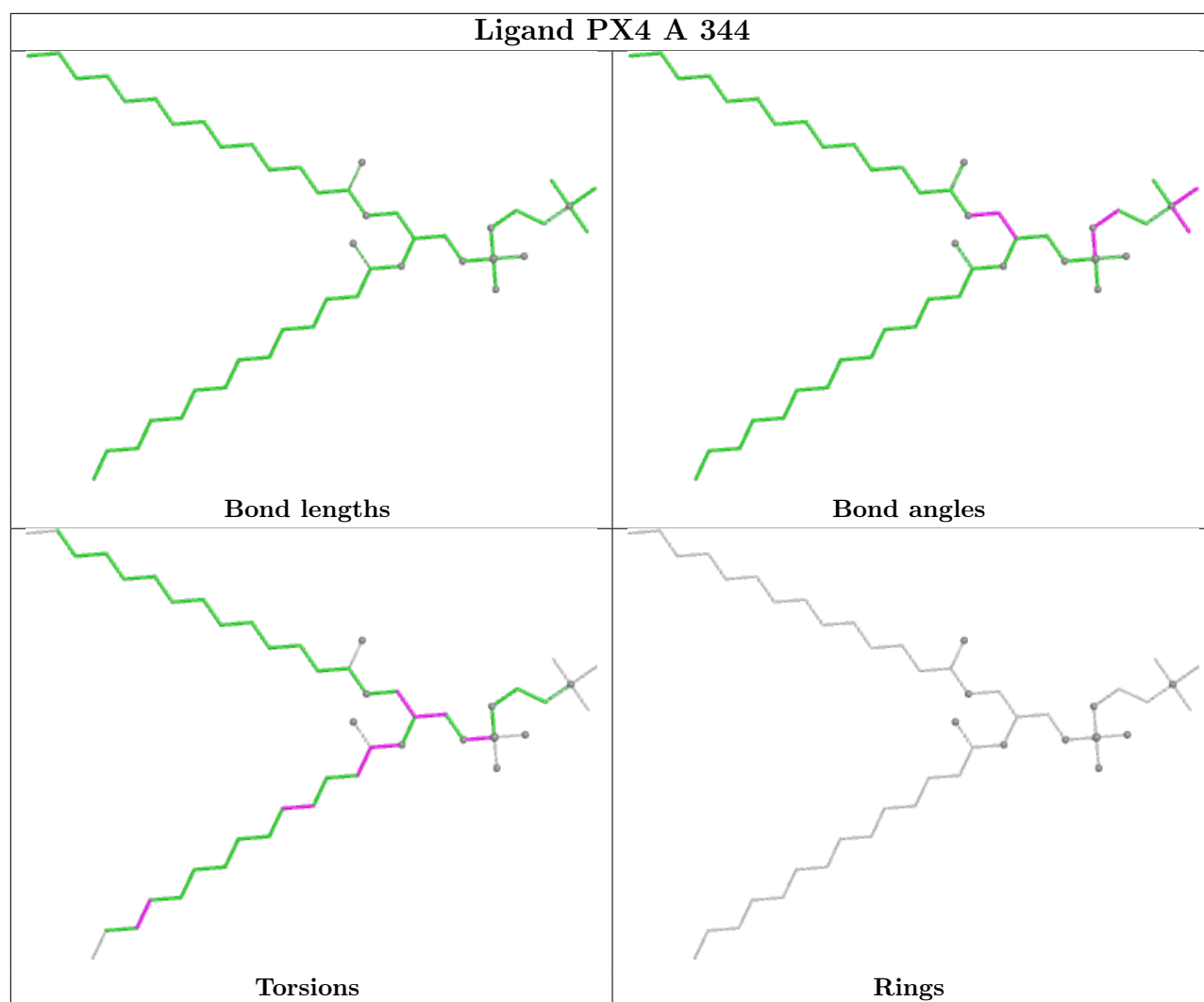


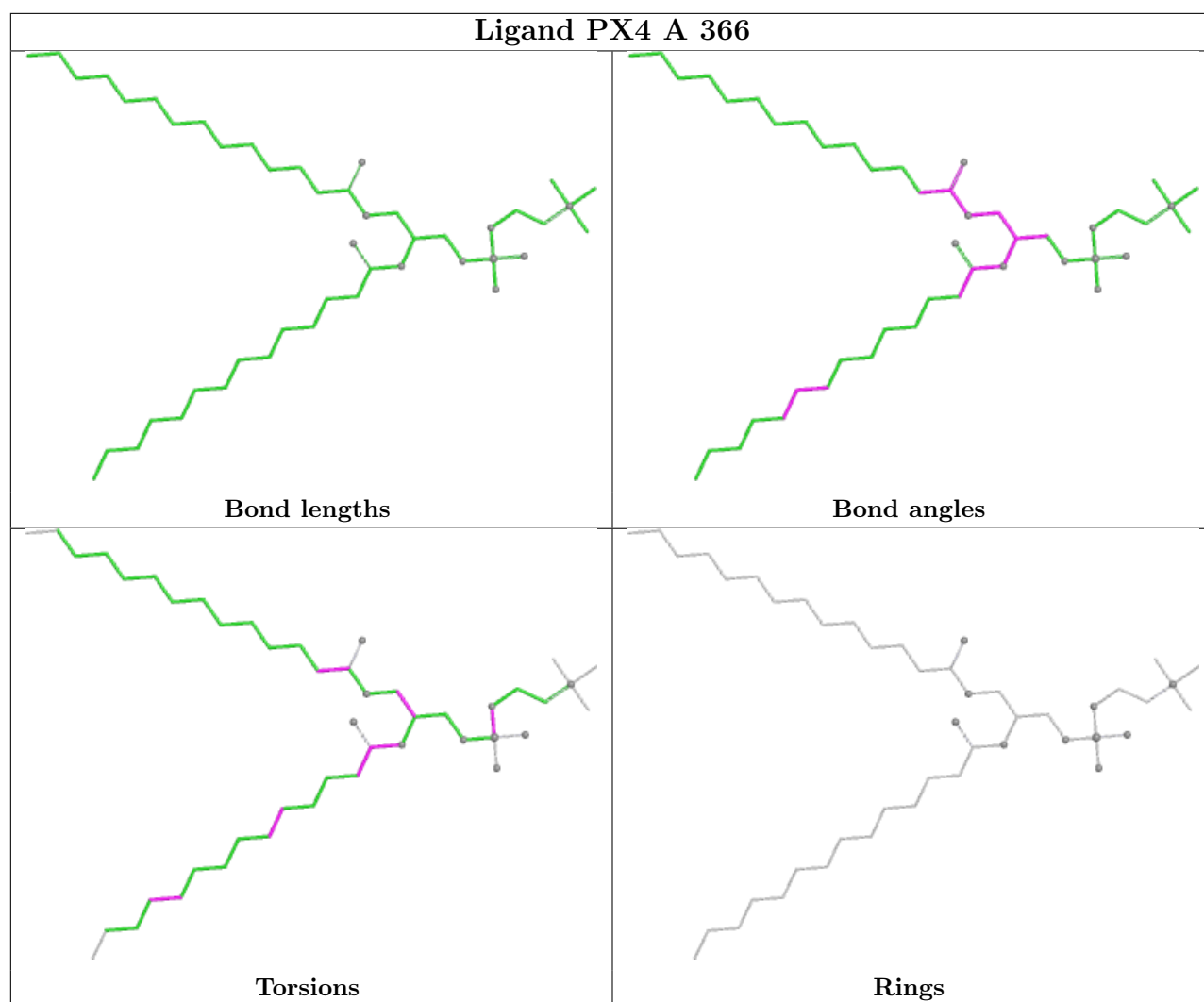


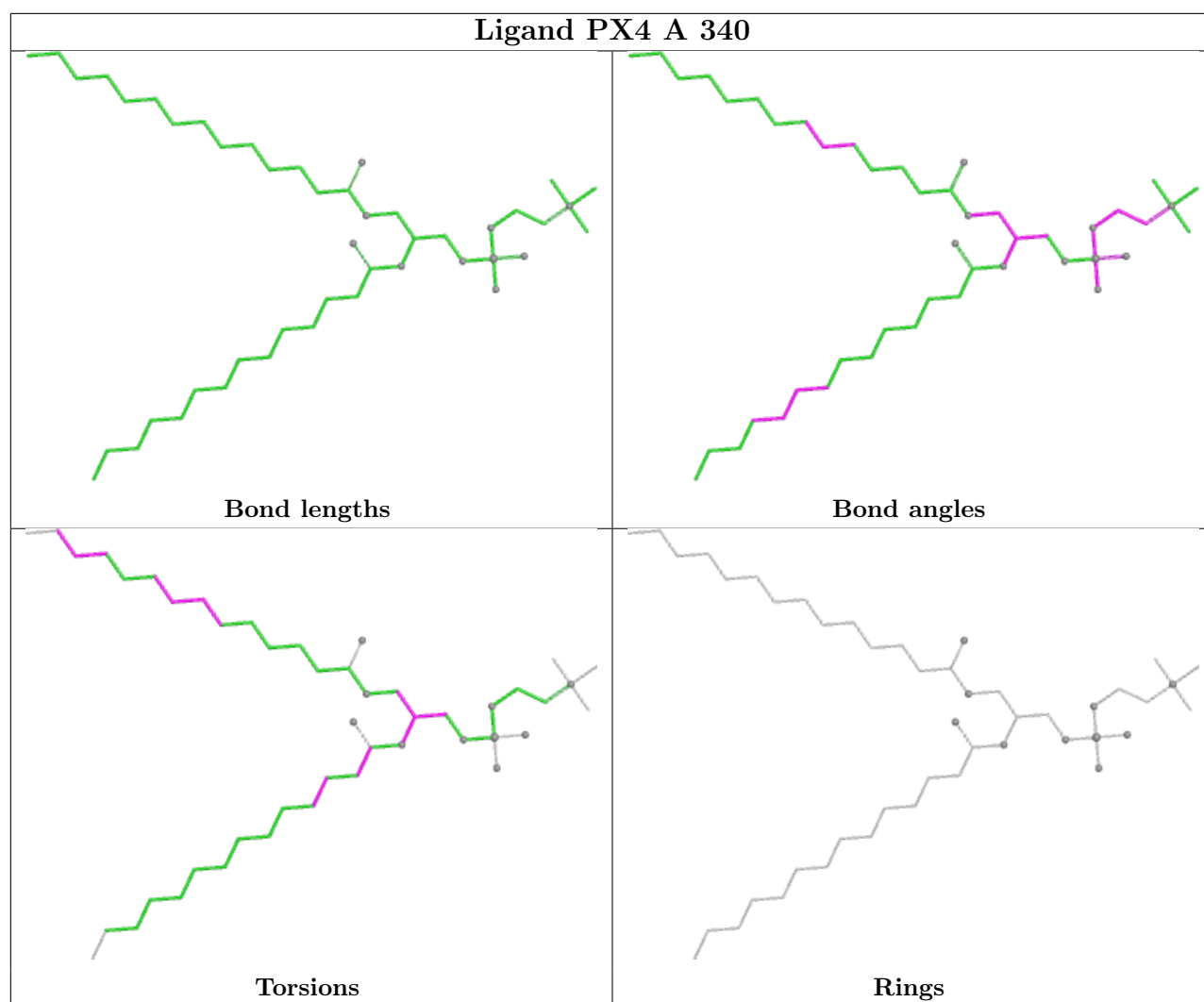
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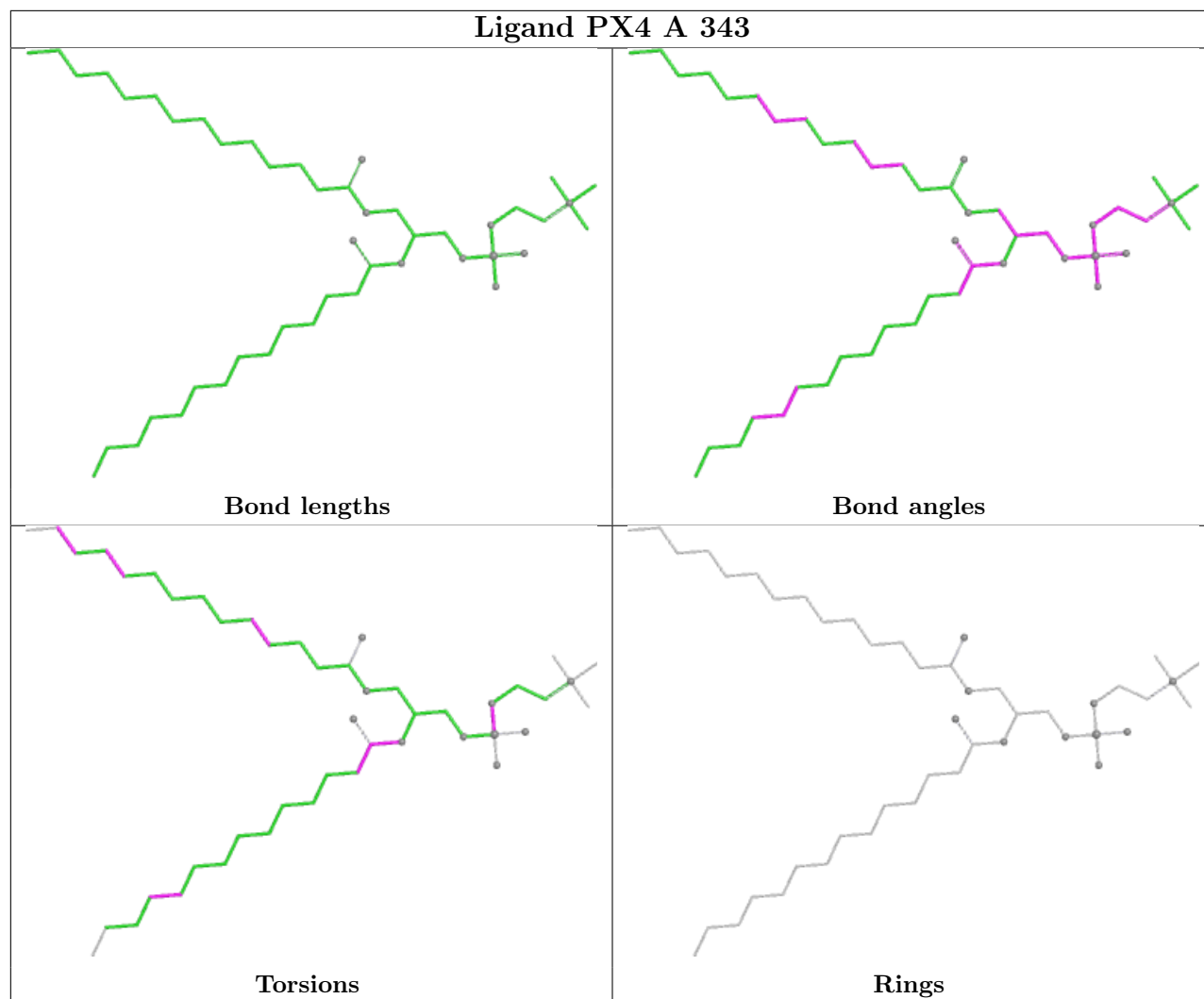




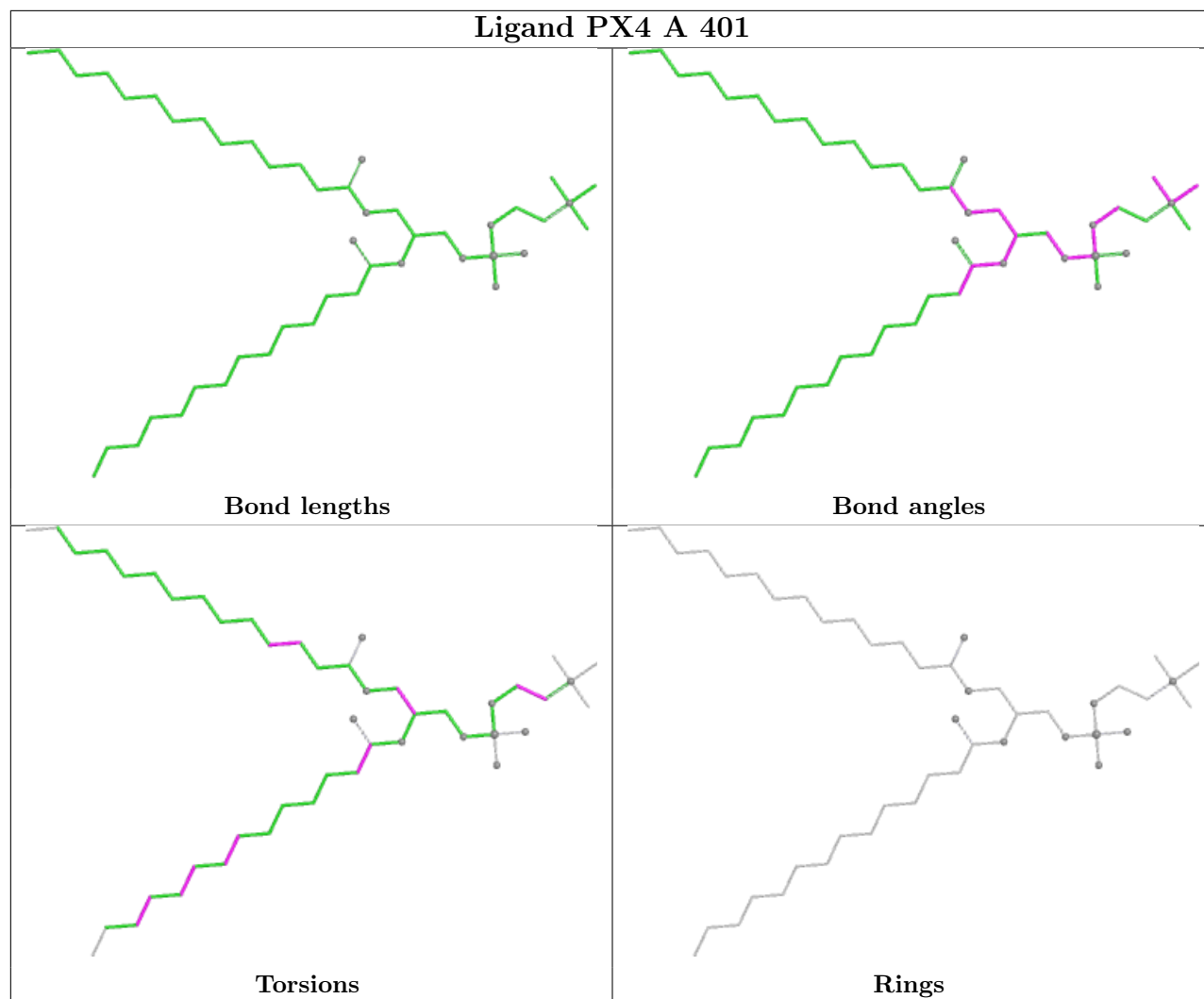




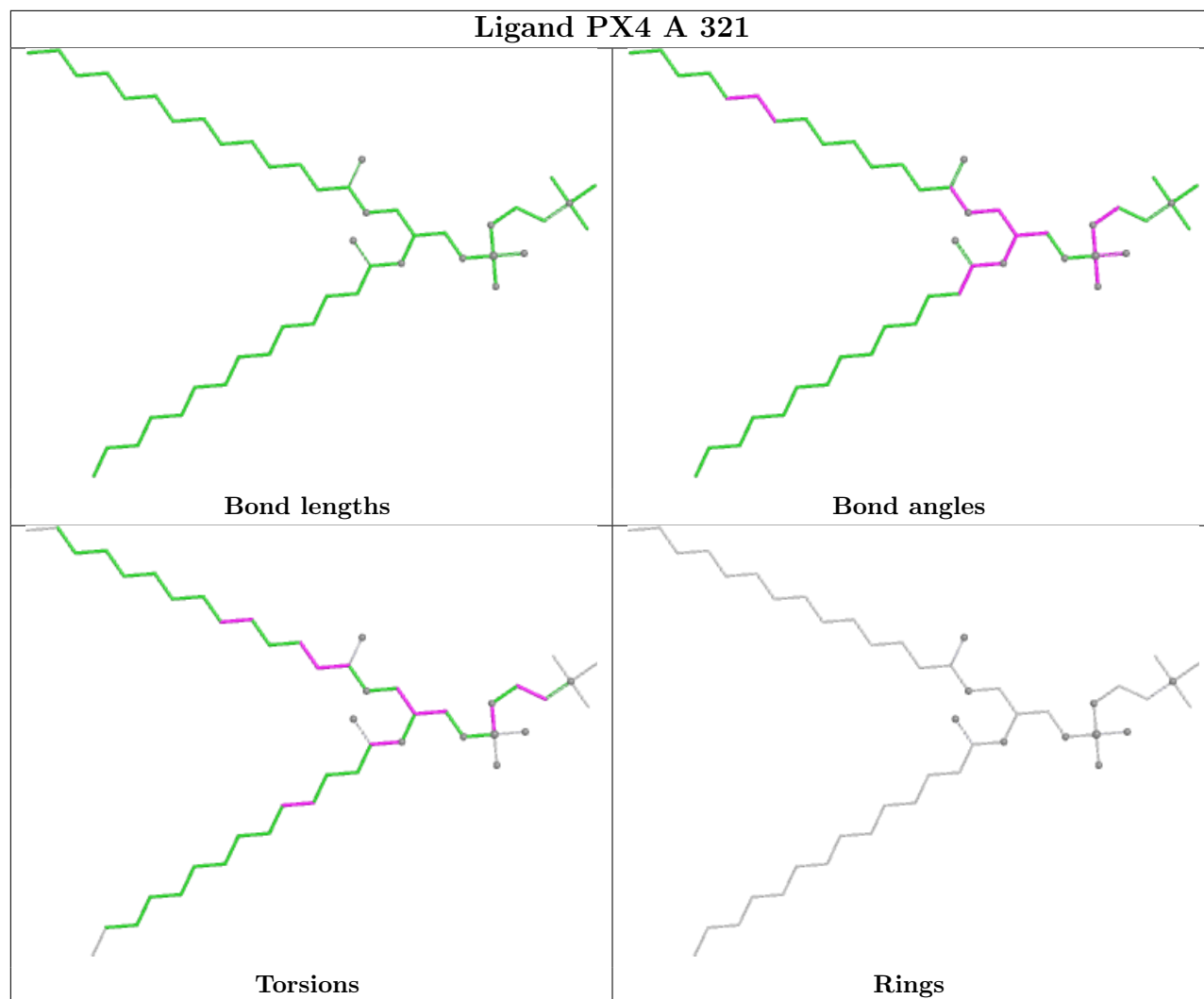
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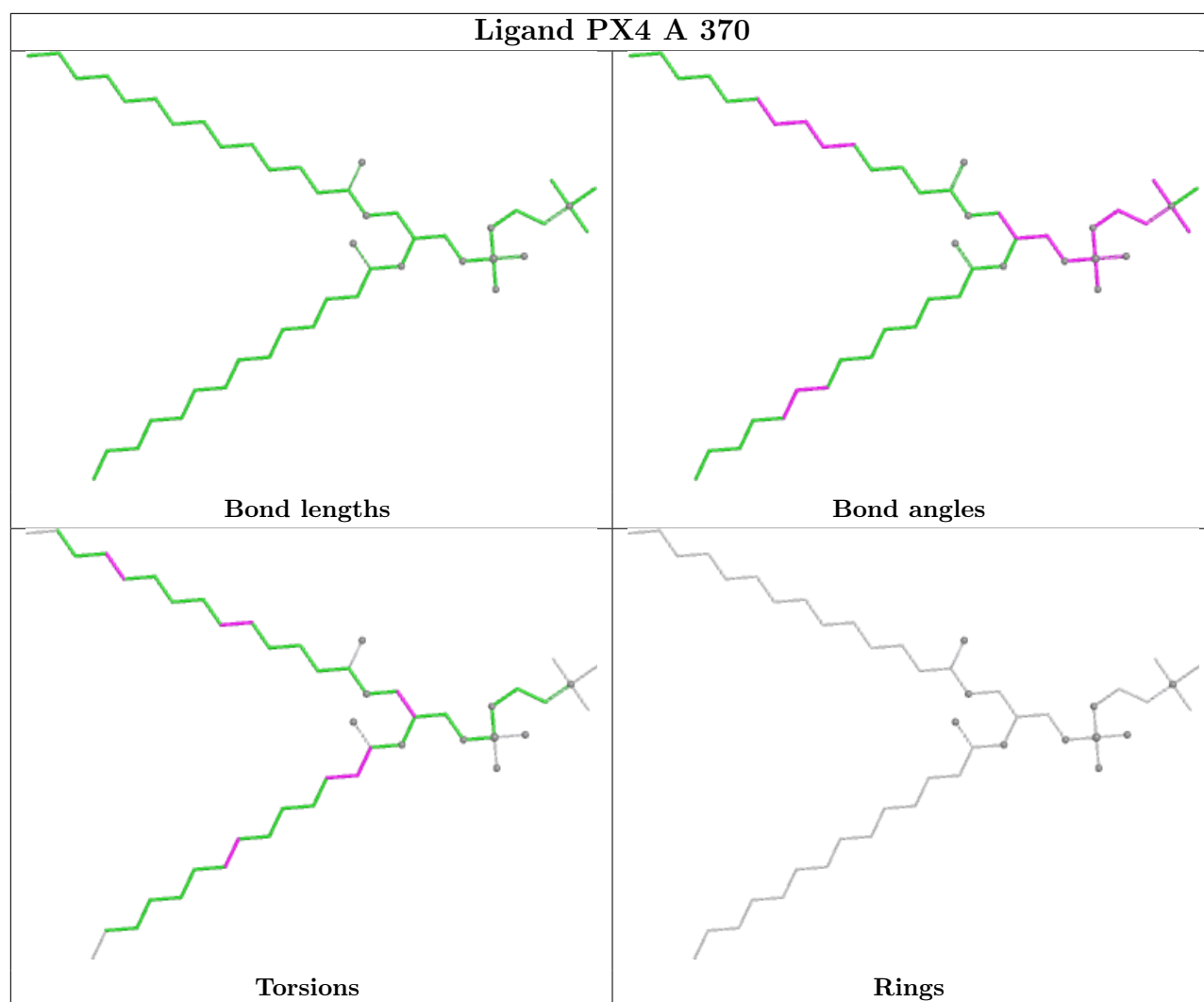


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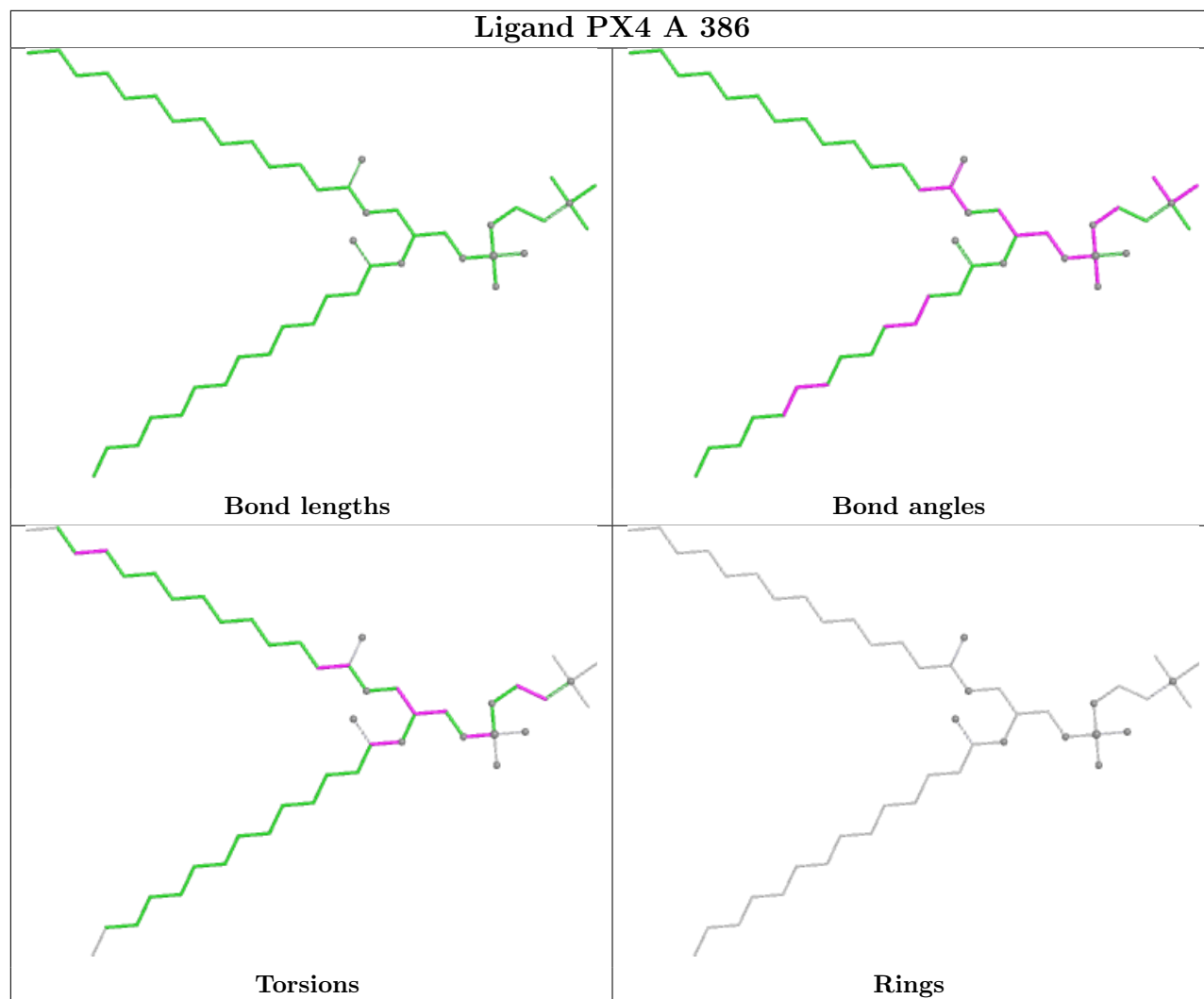


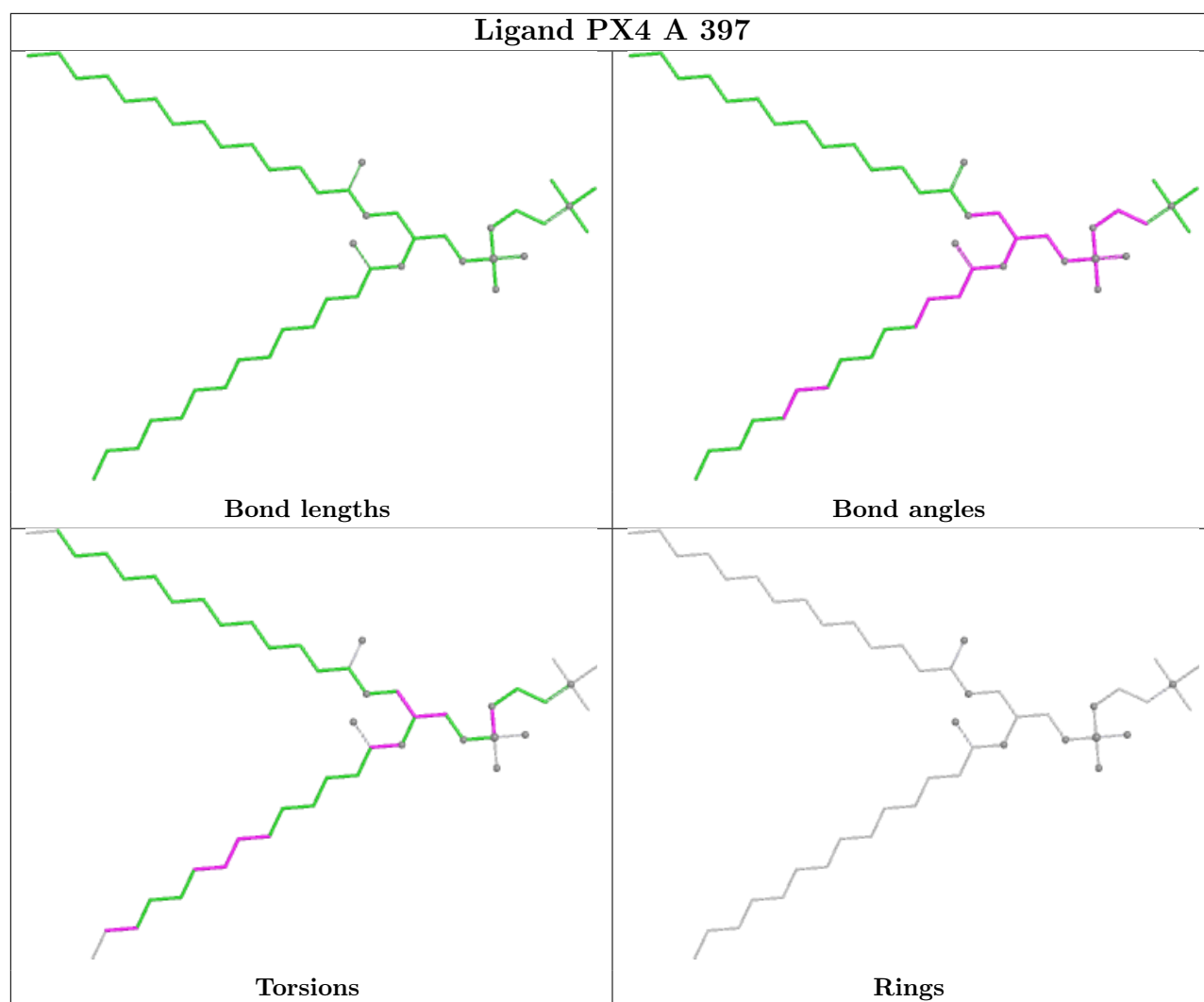
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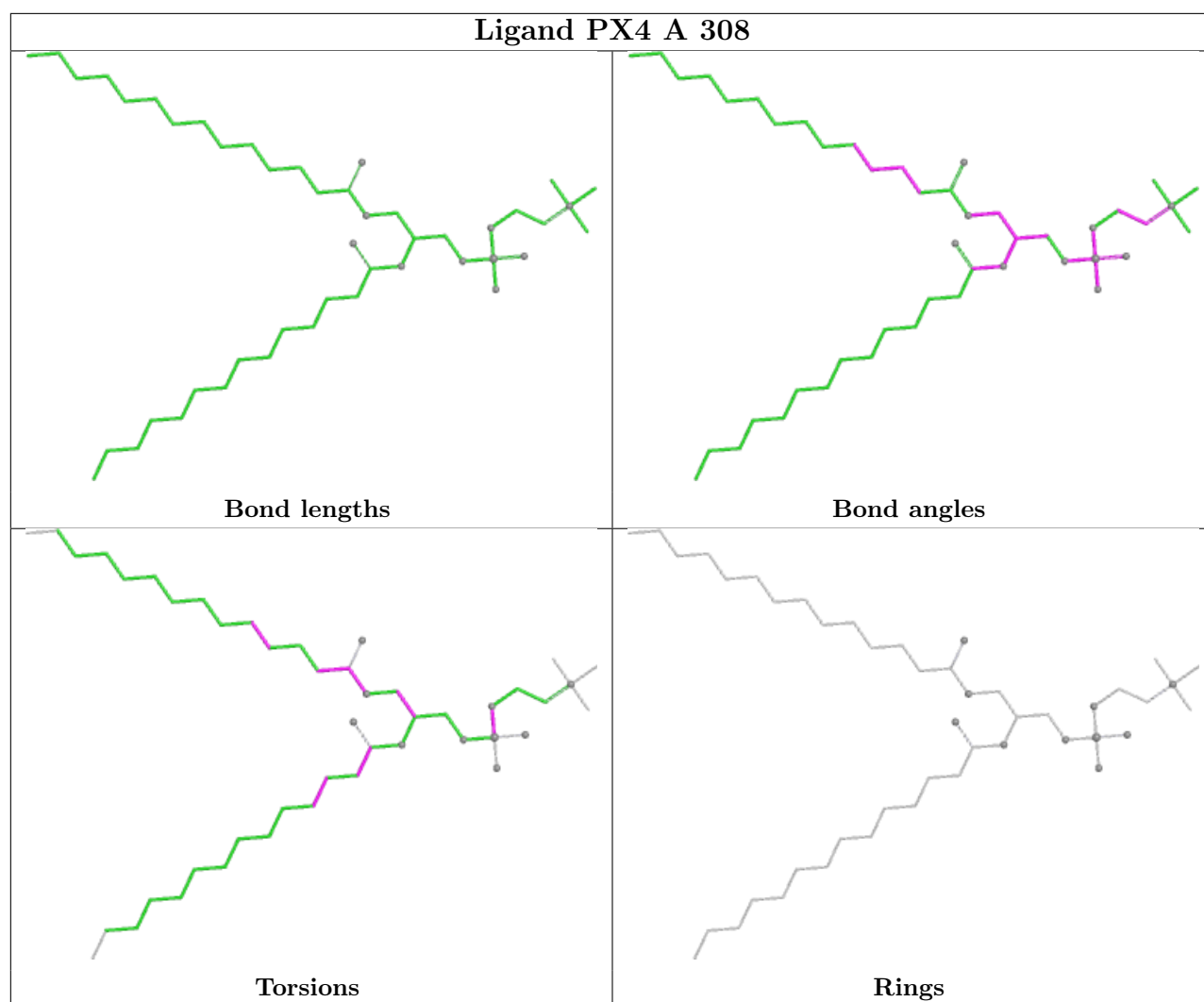


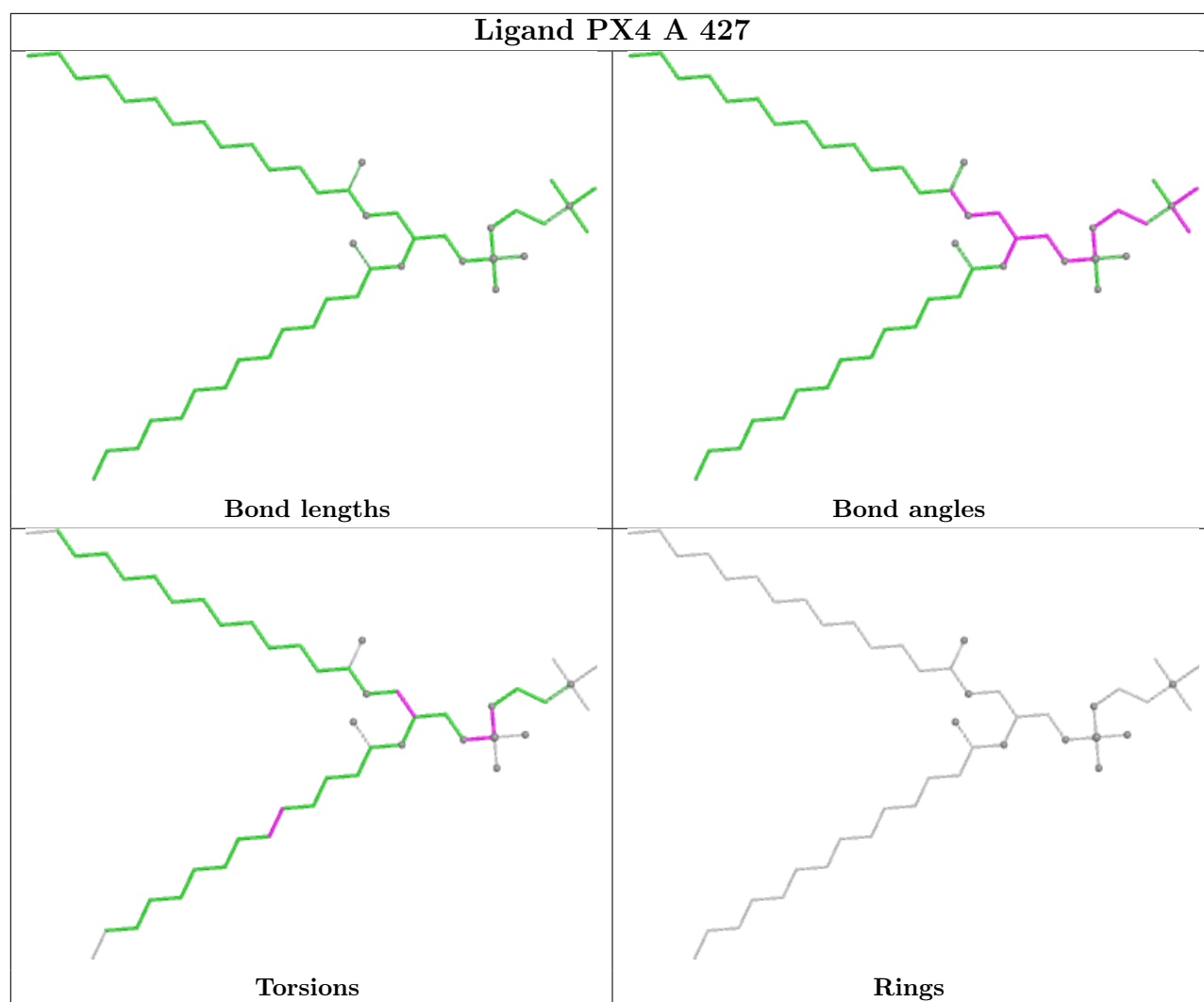


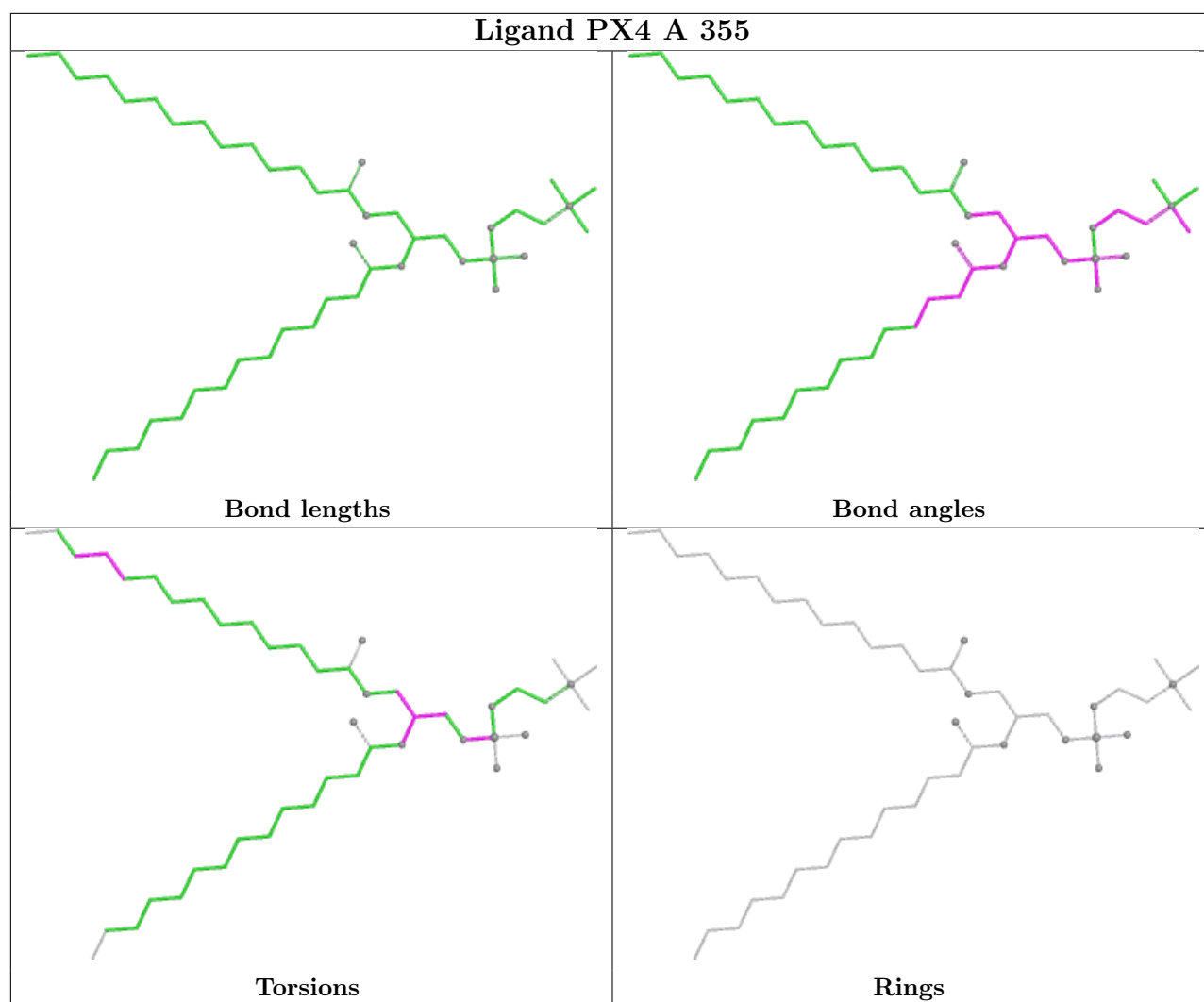
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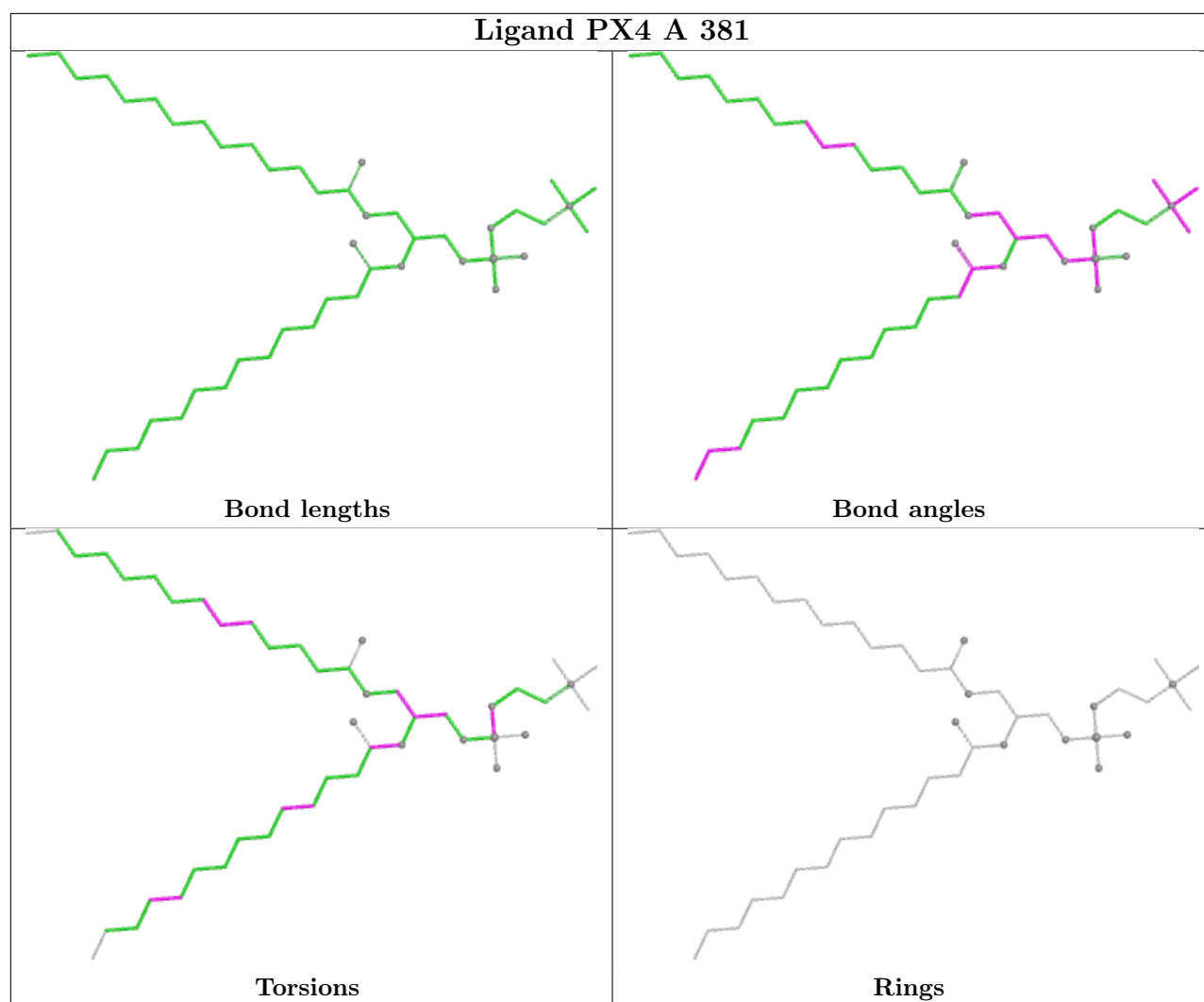


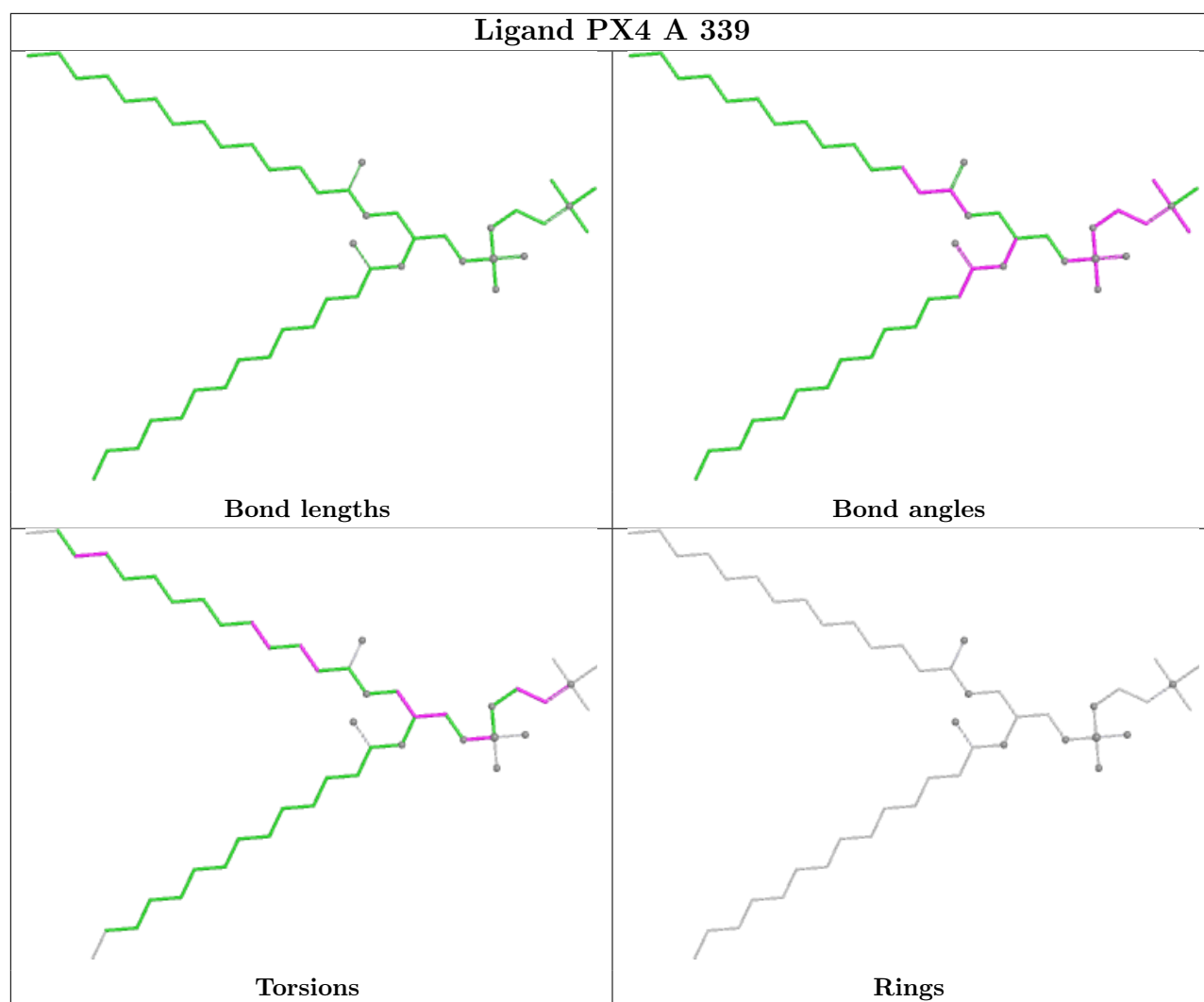




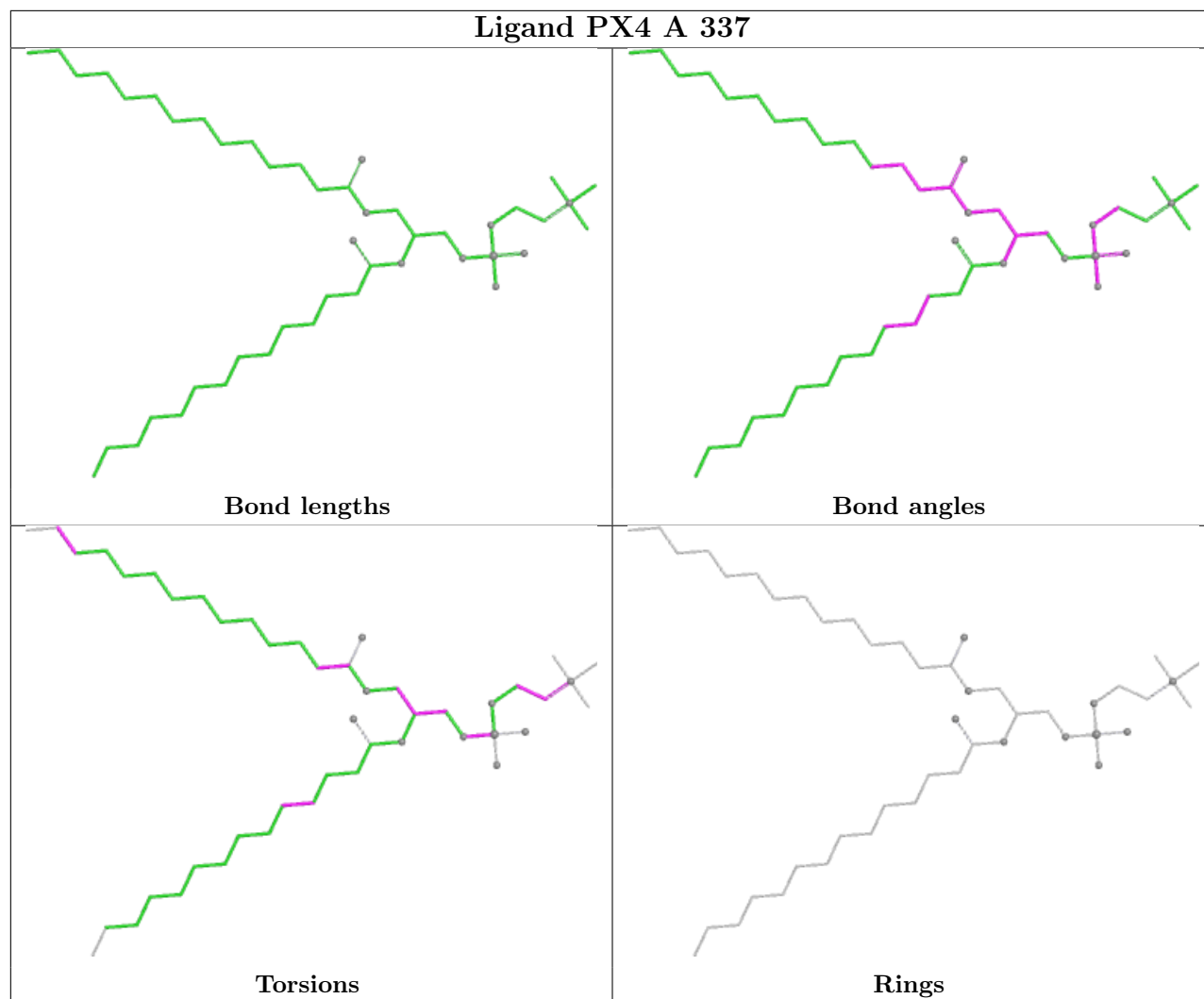


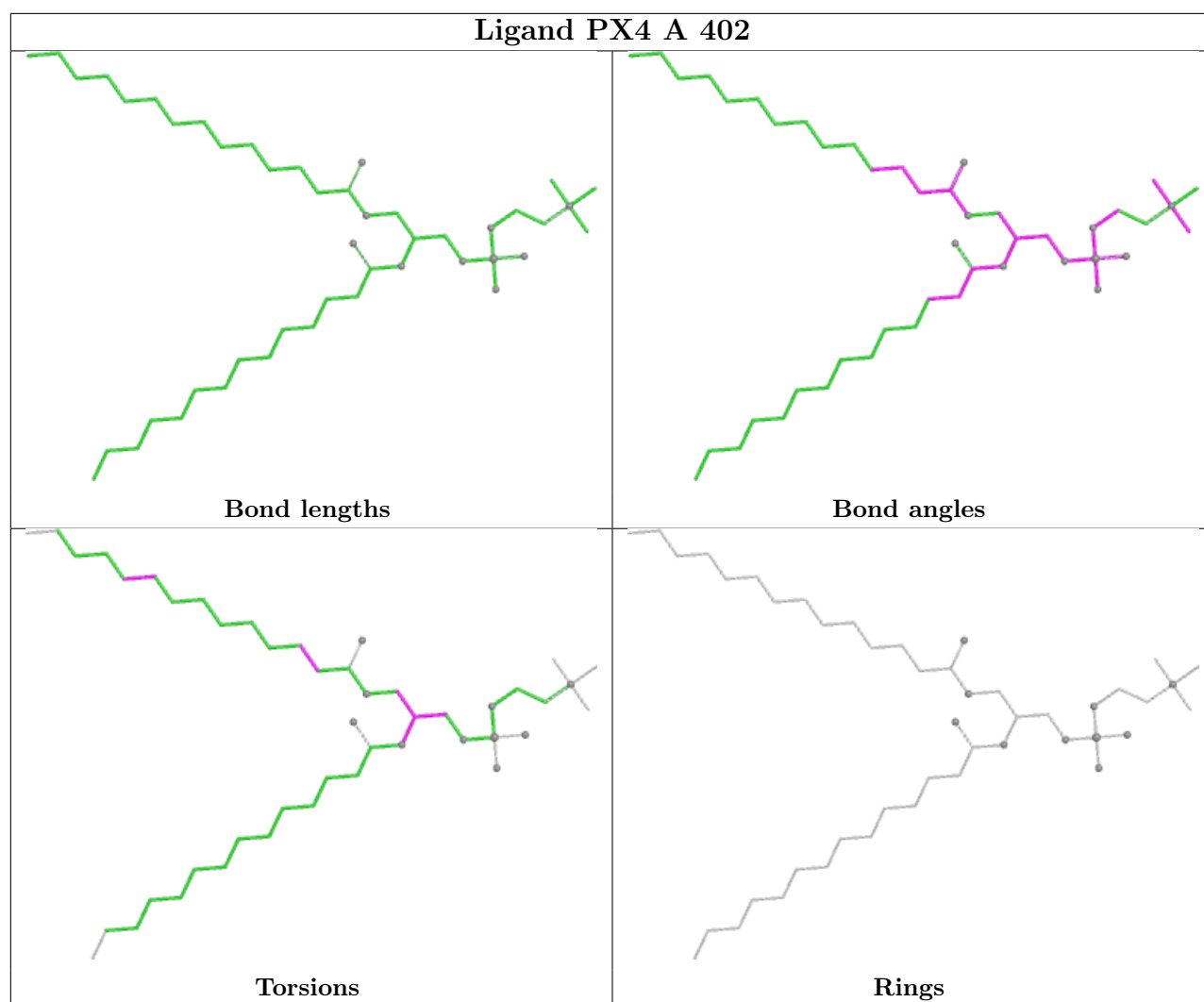


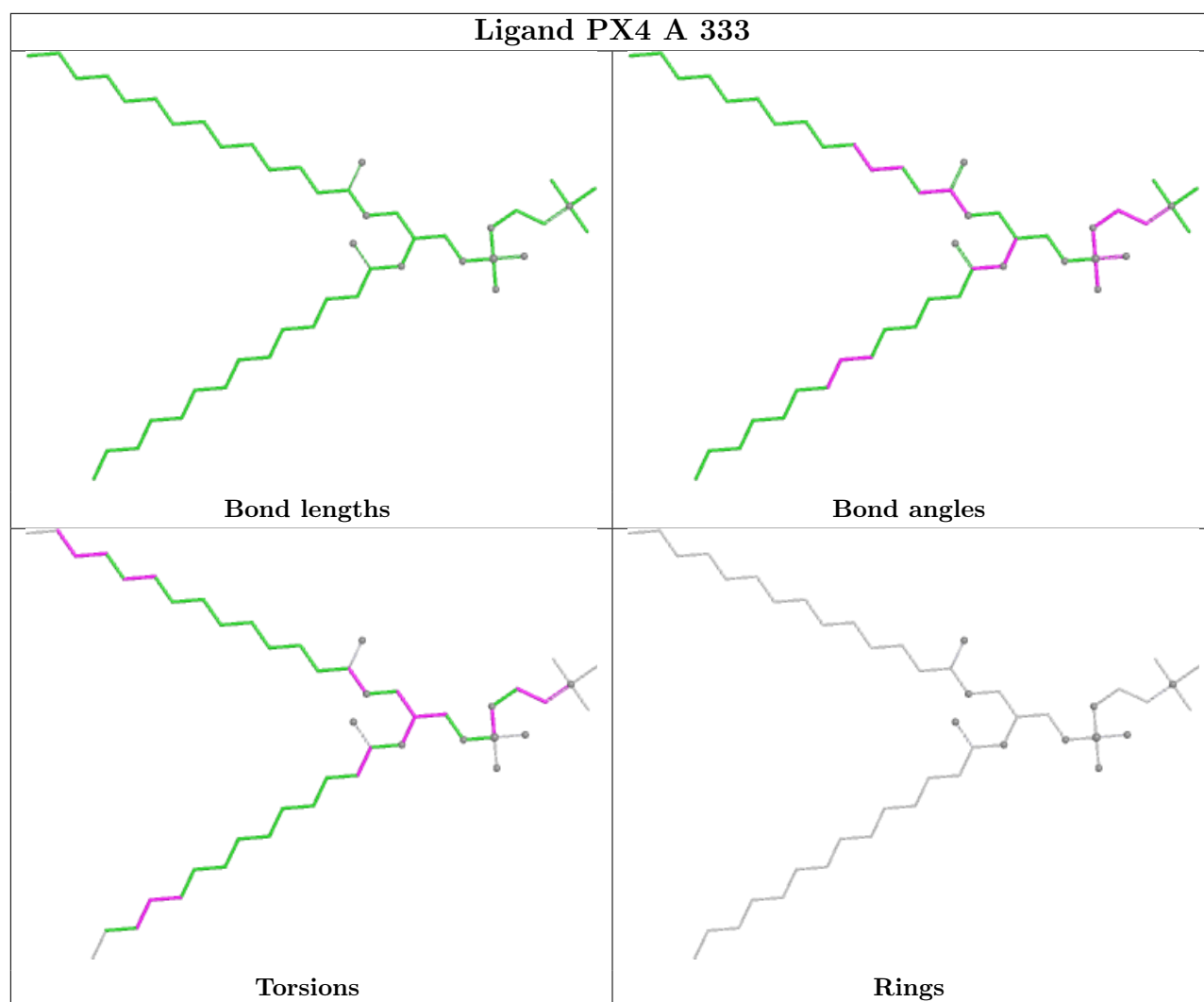




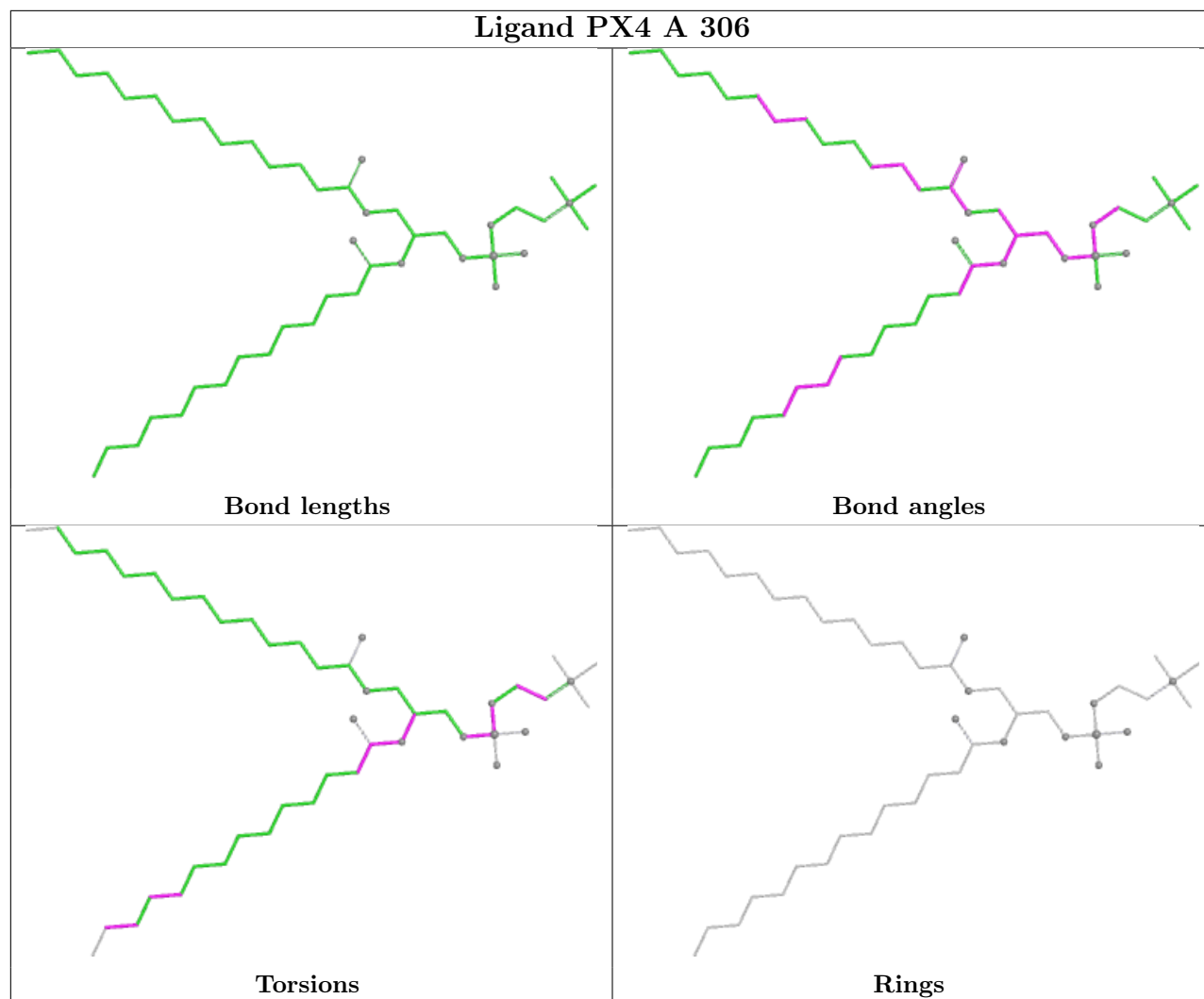
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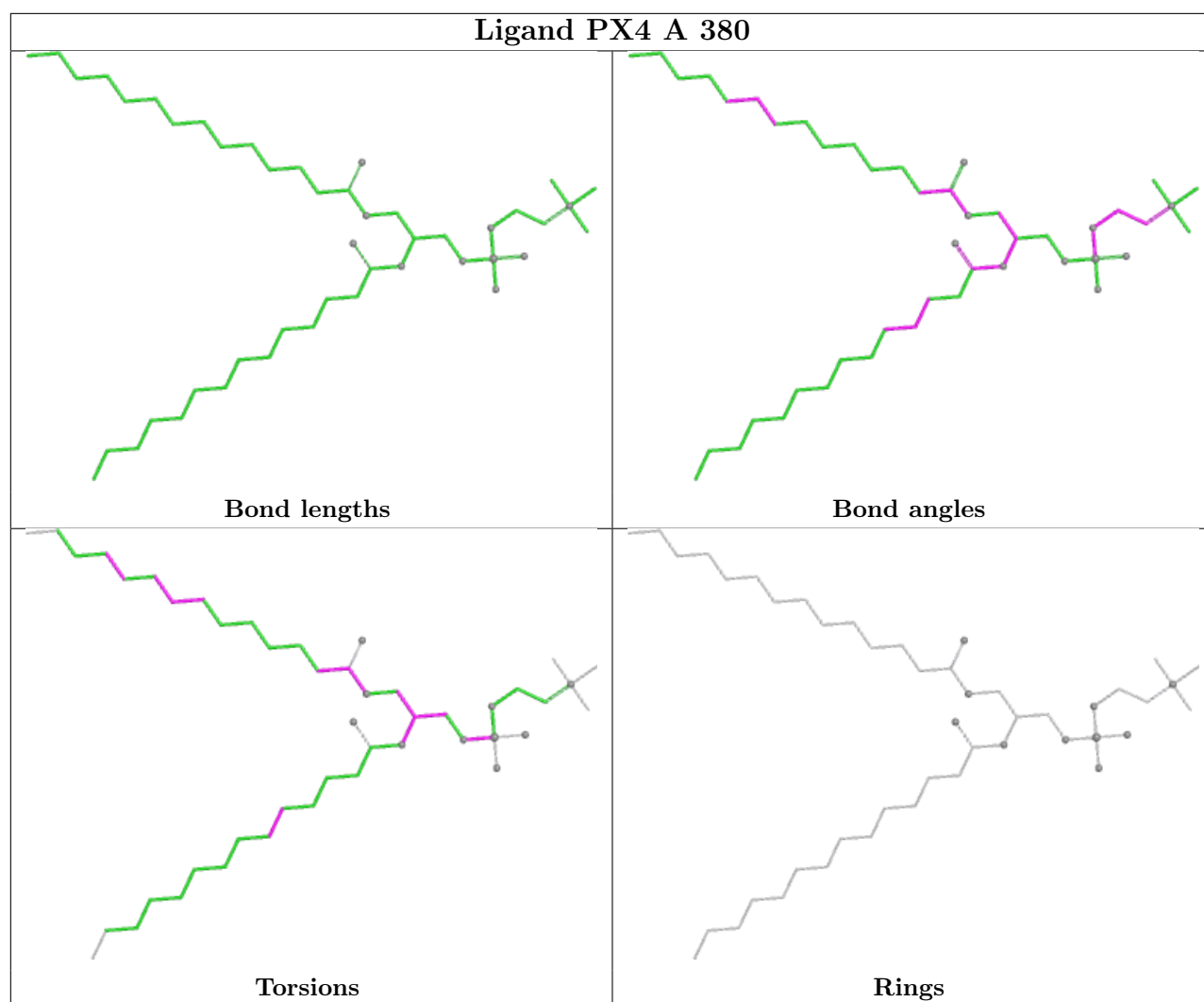


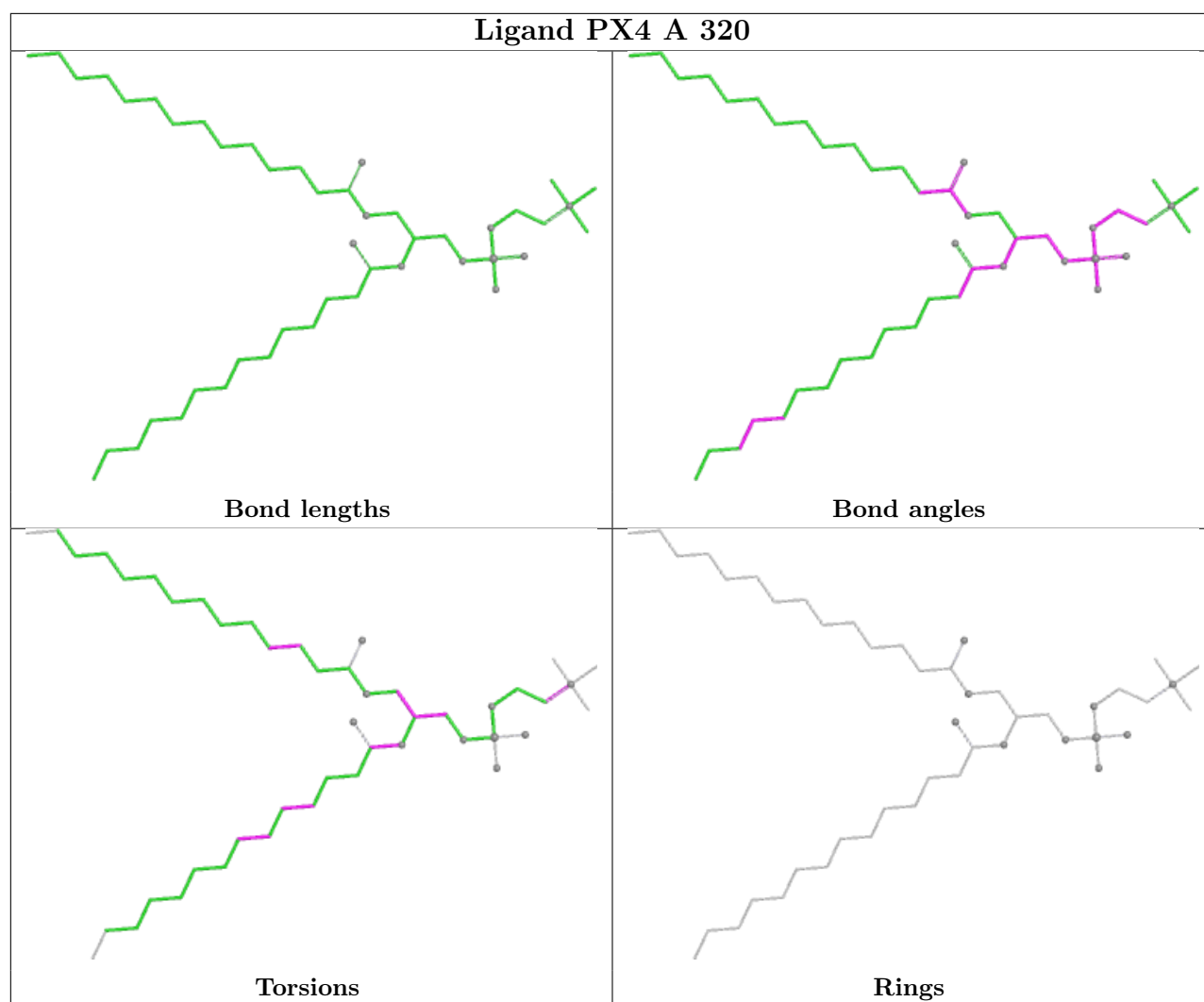


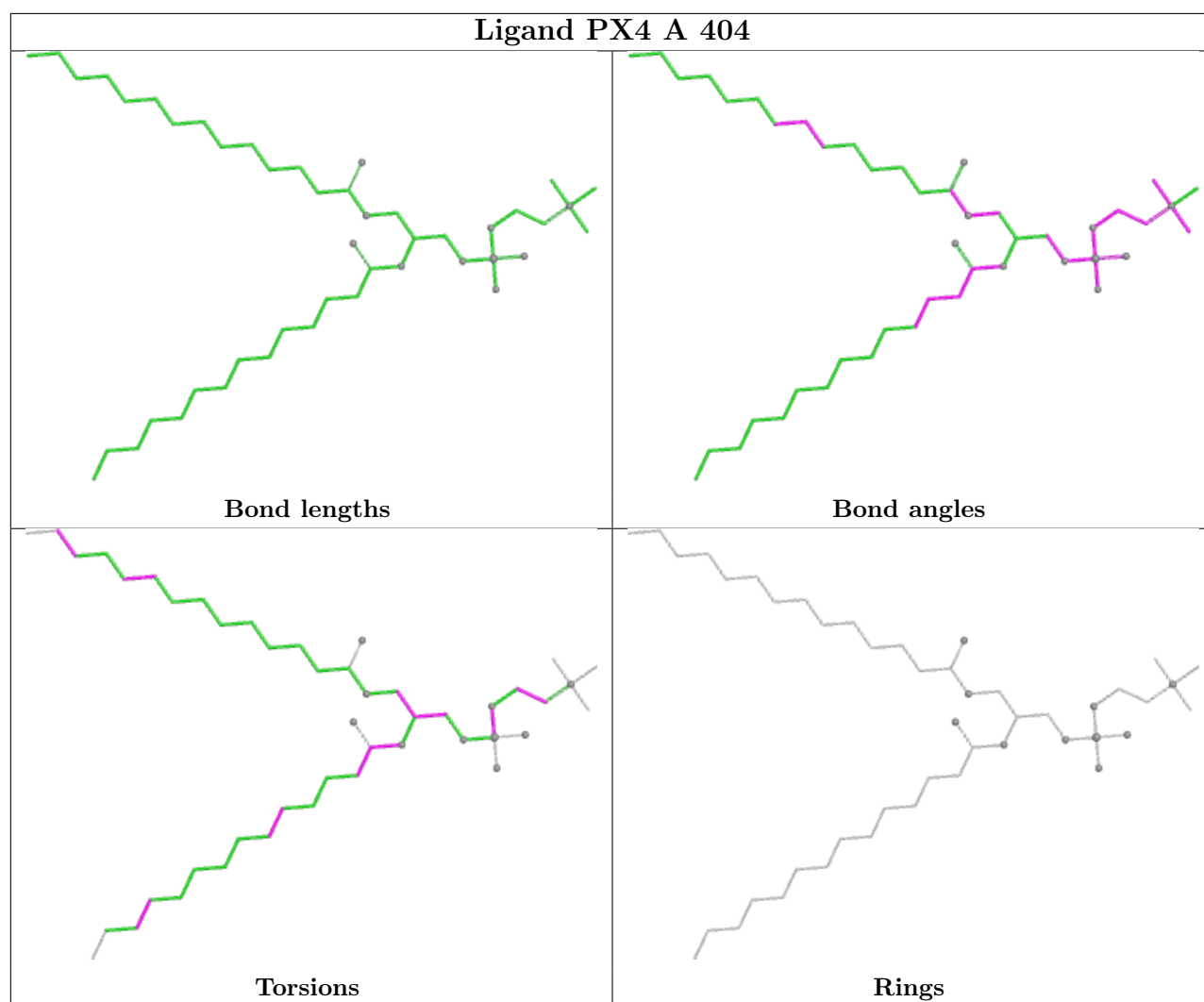


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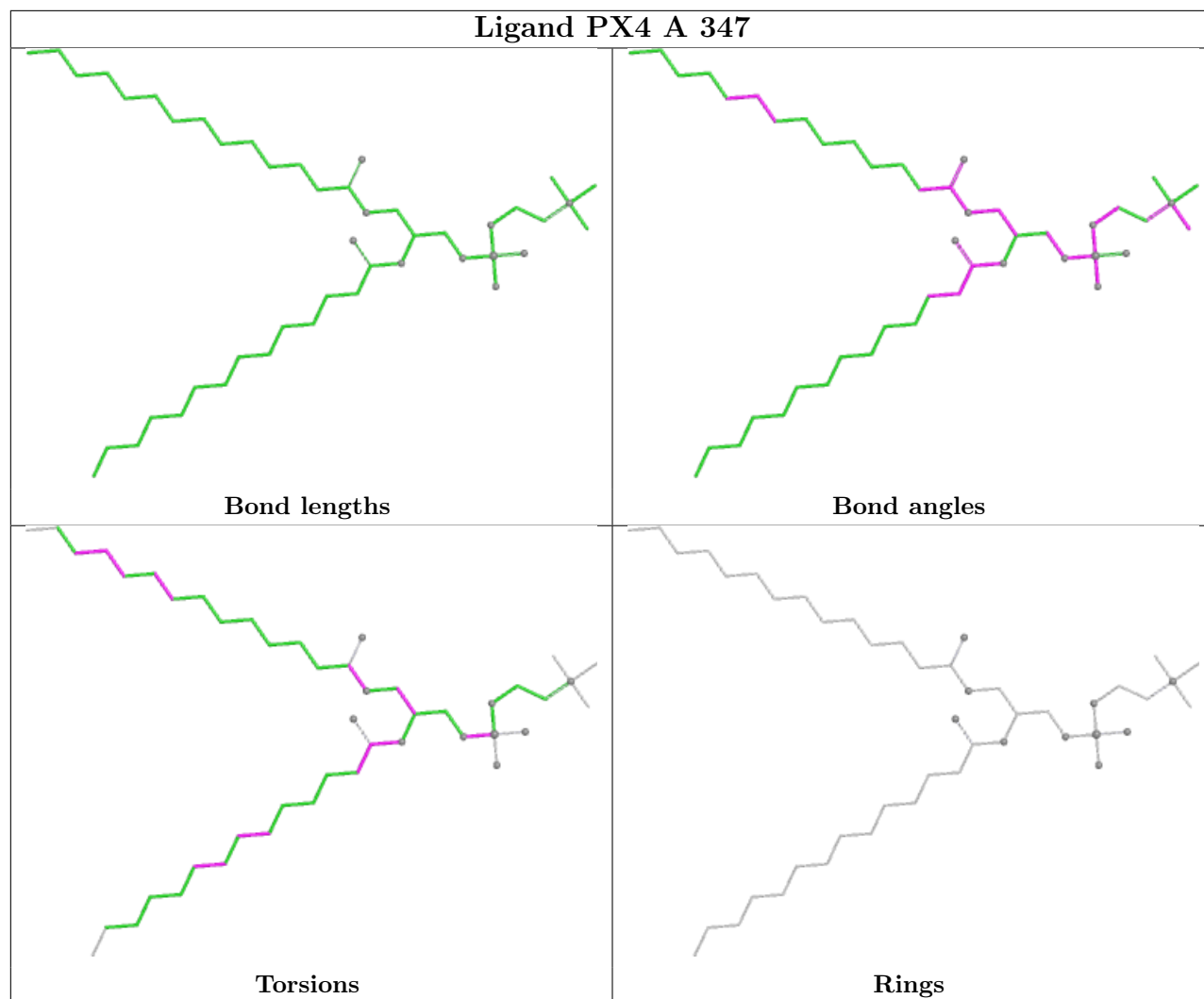




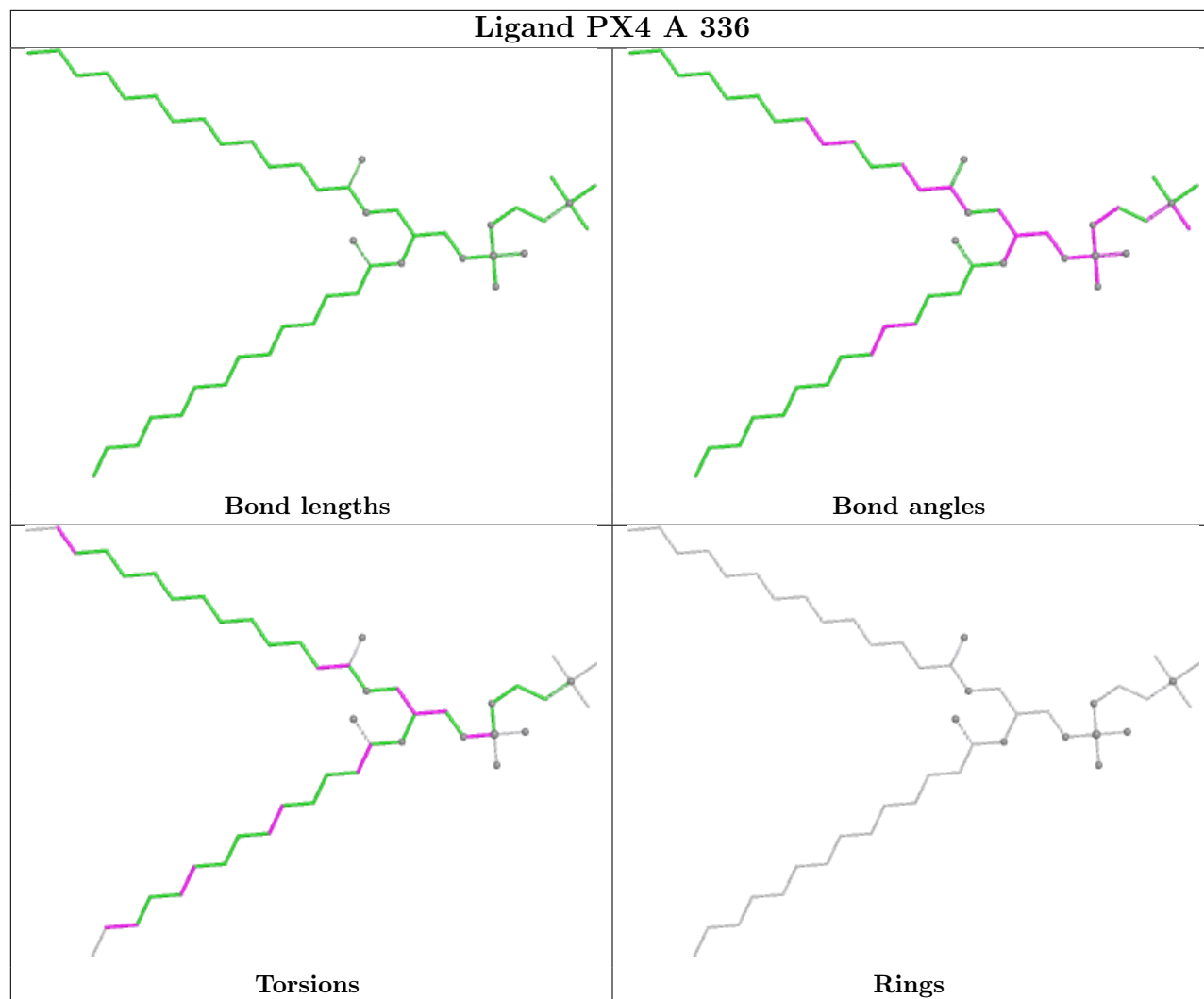




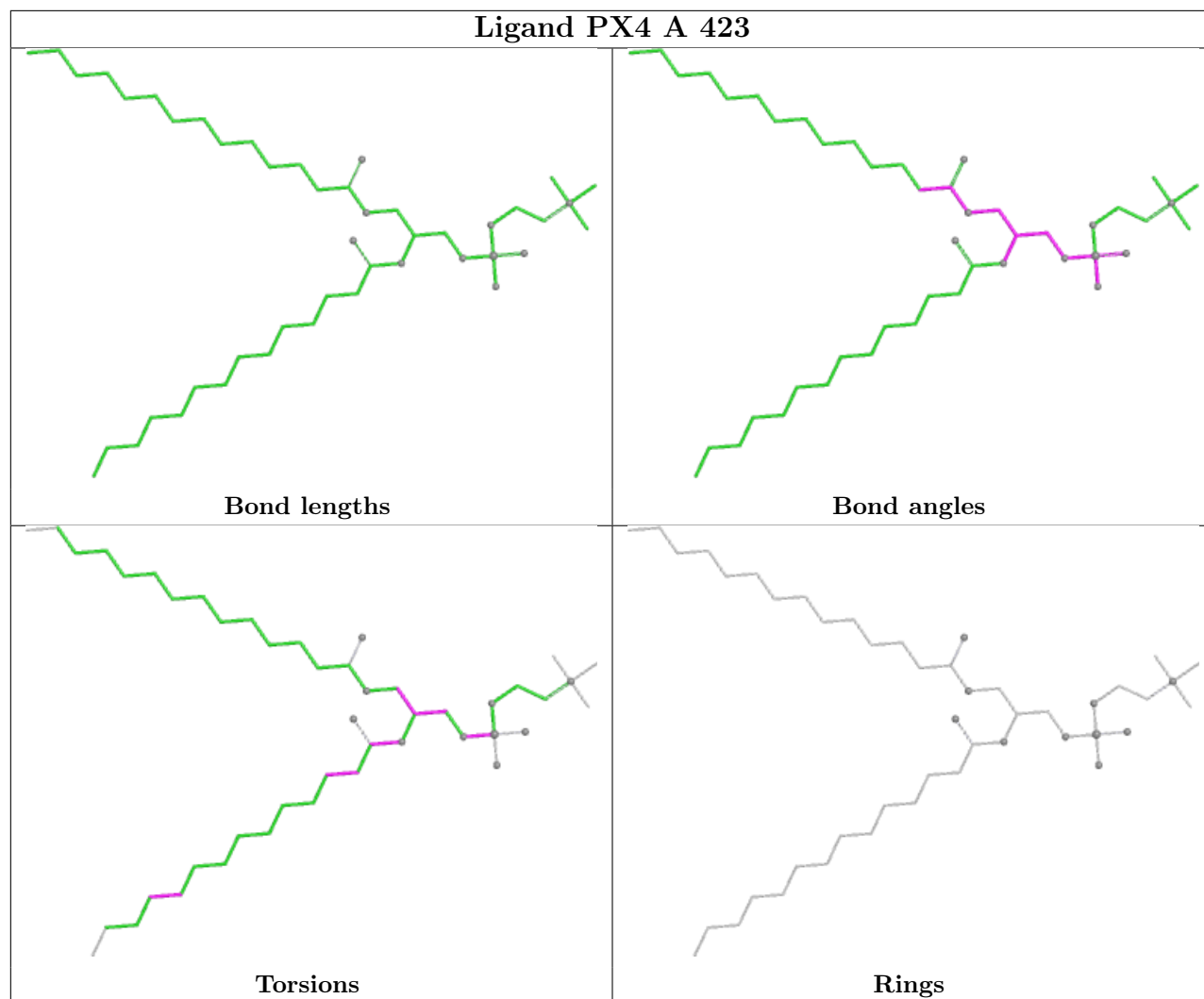
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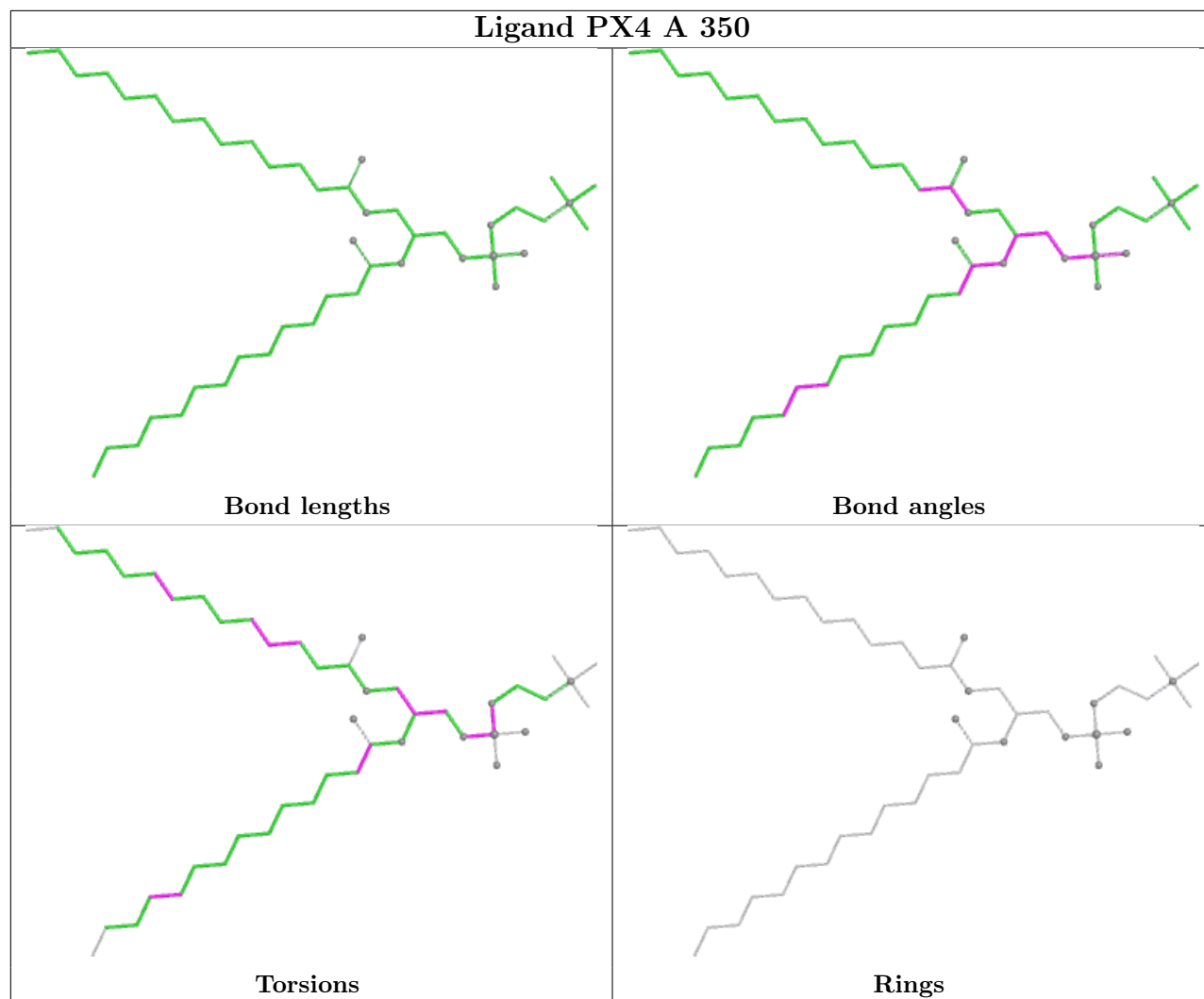
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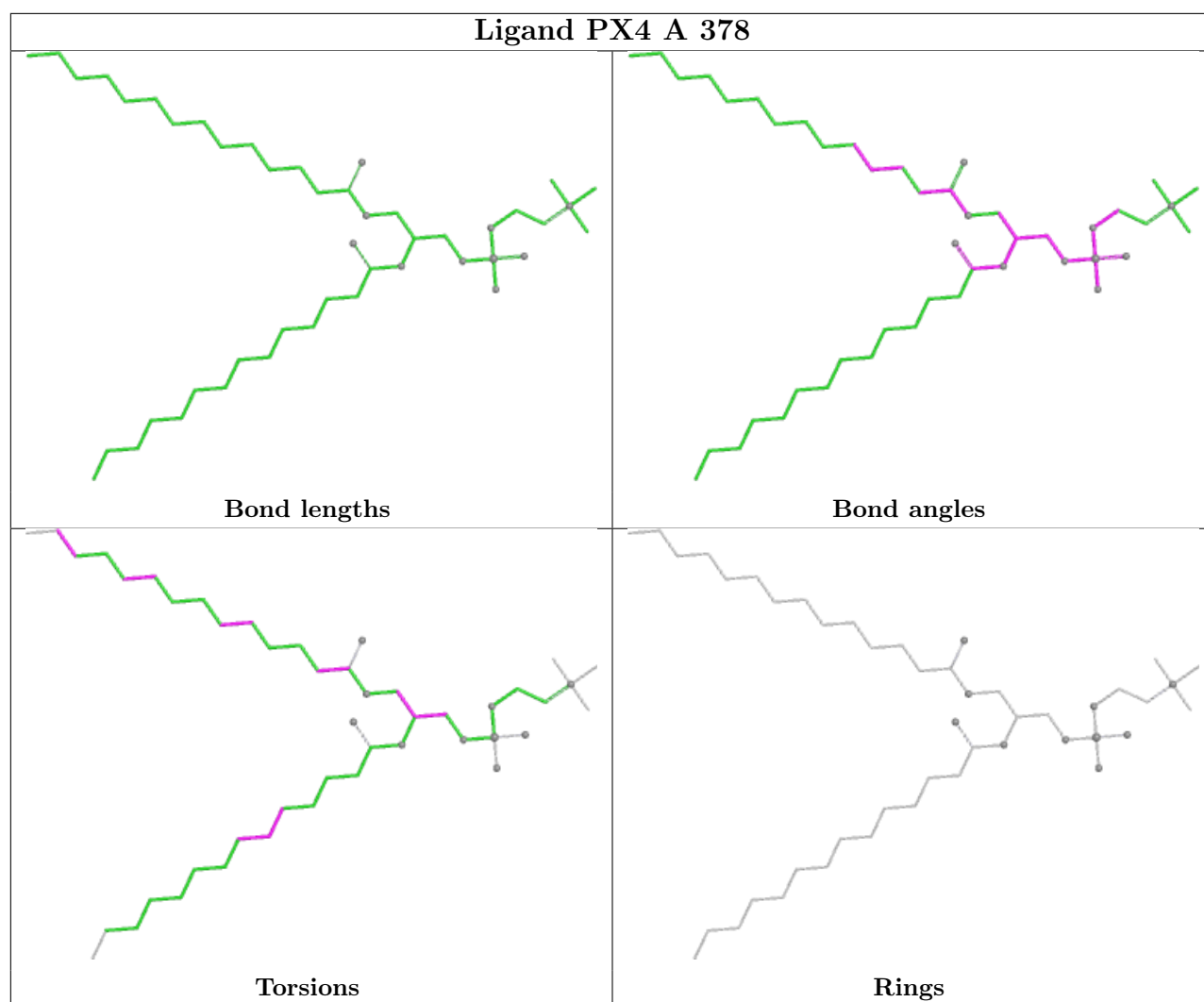


Ligand PX4 A 423

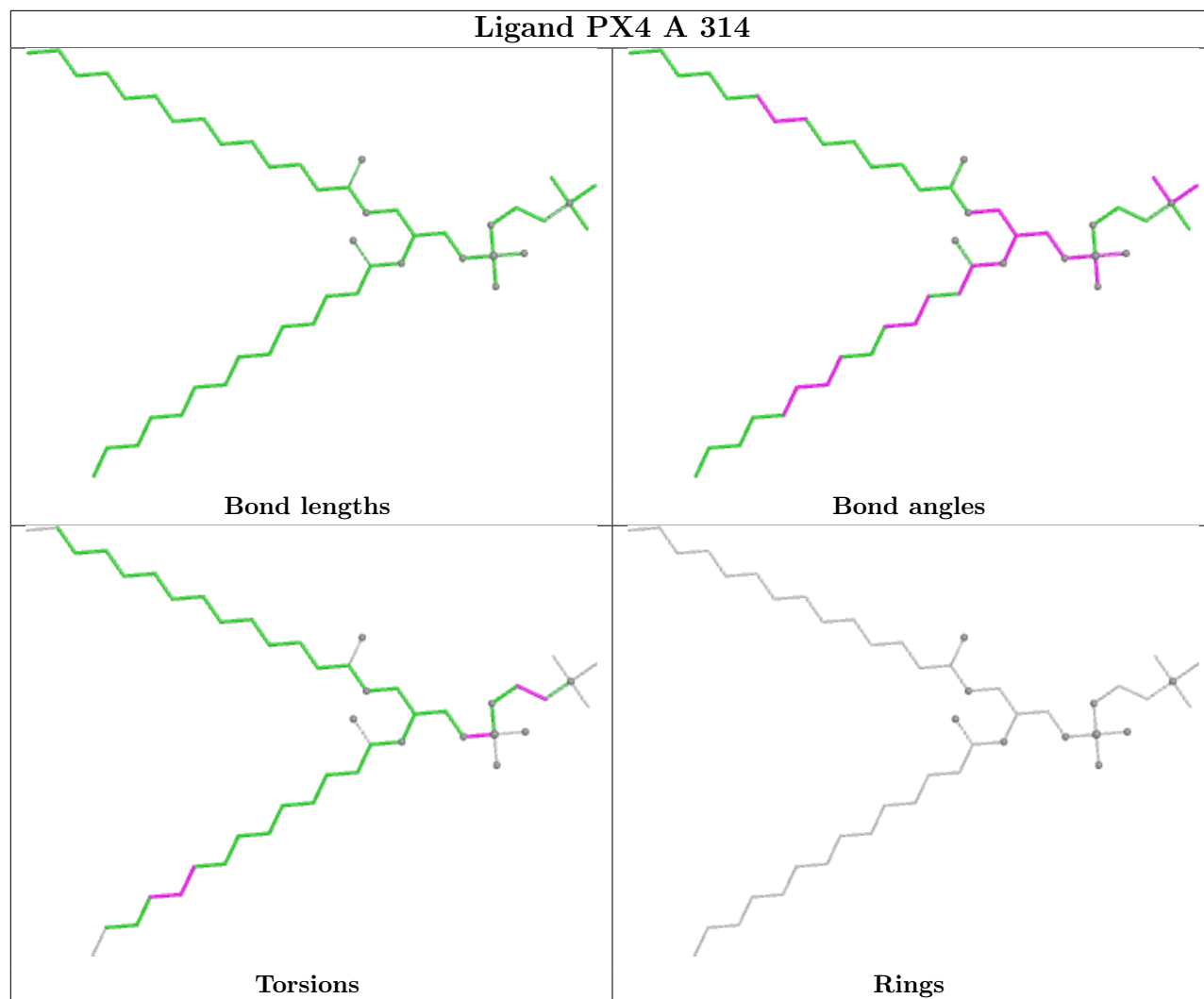


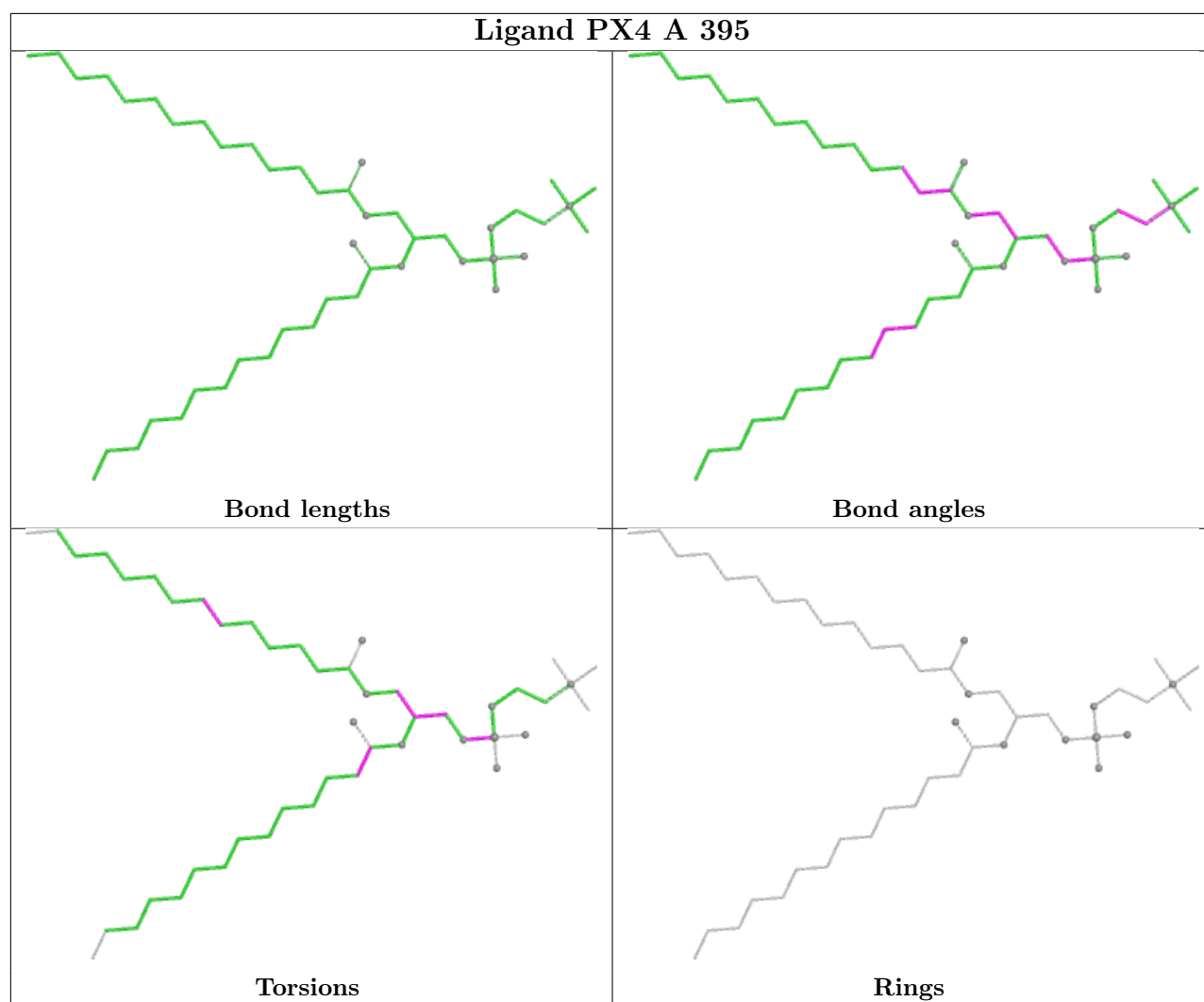
Ligand PX4 A 350

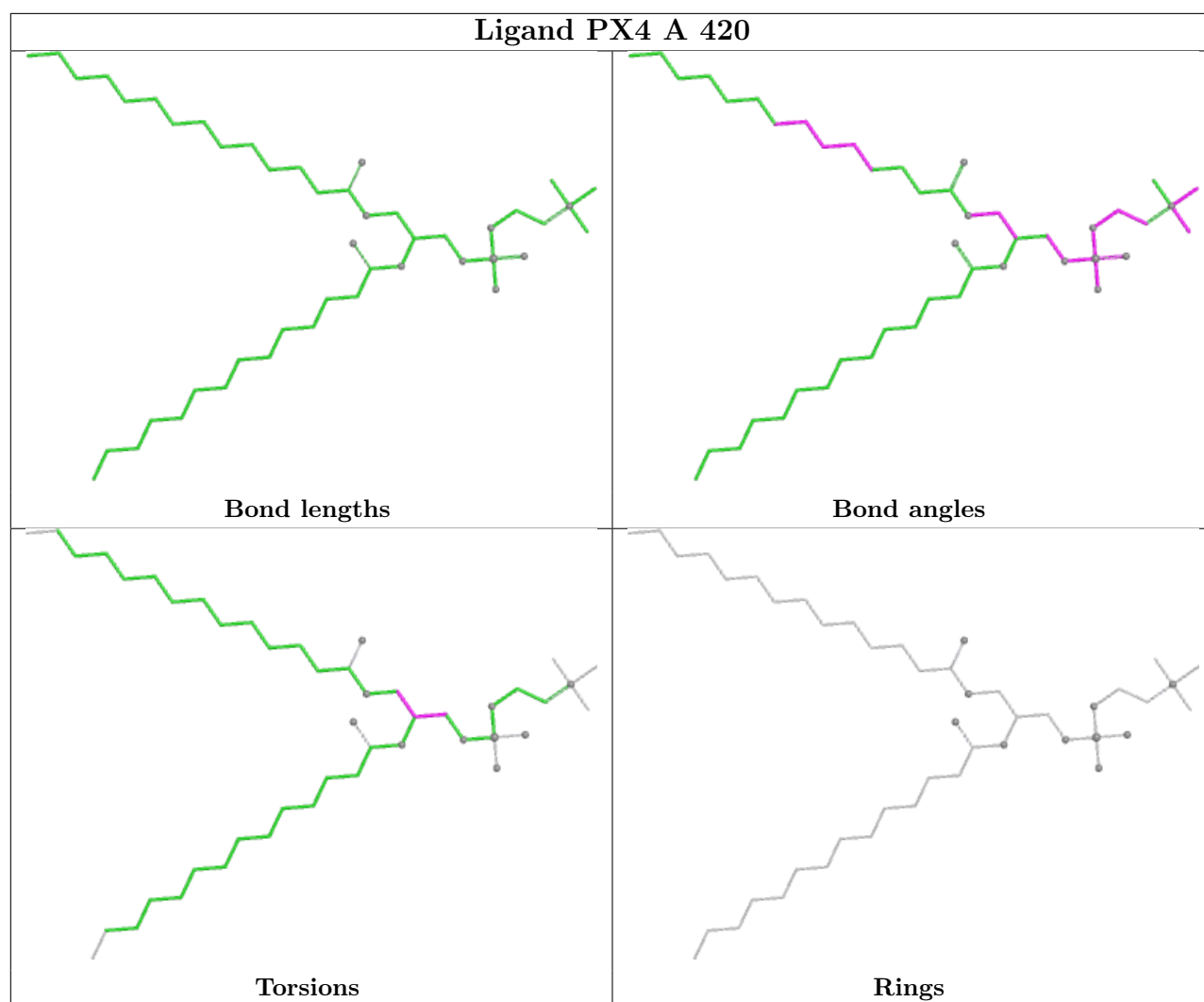


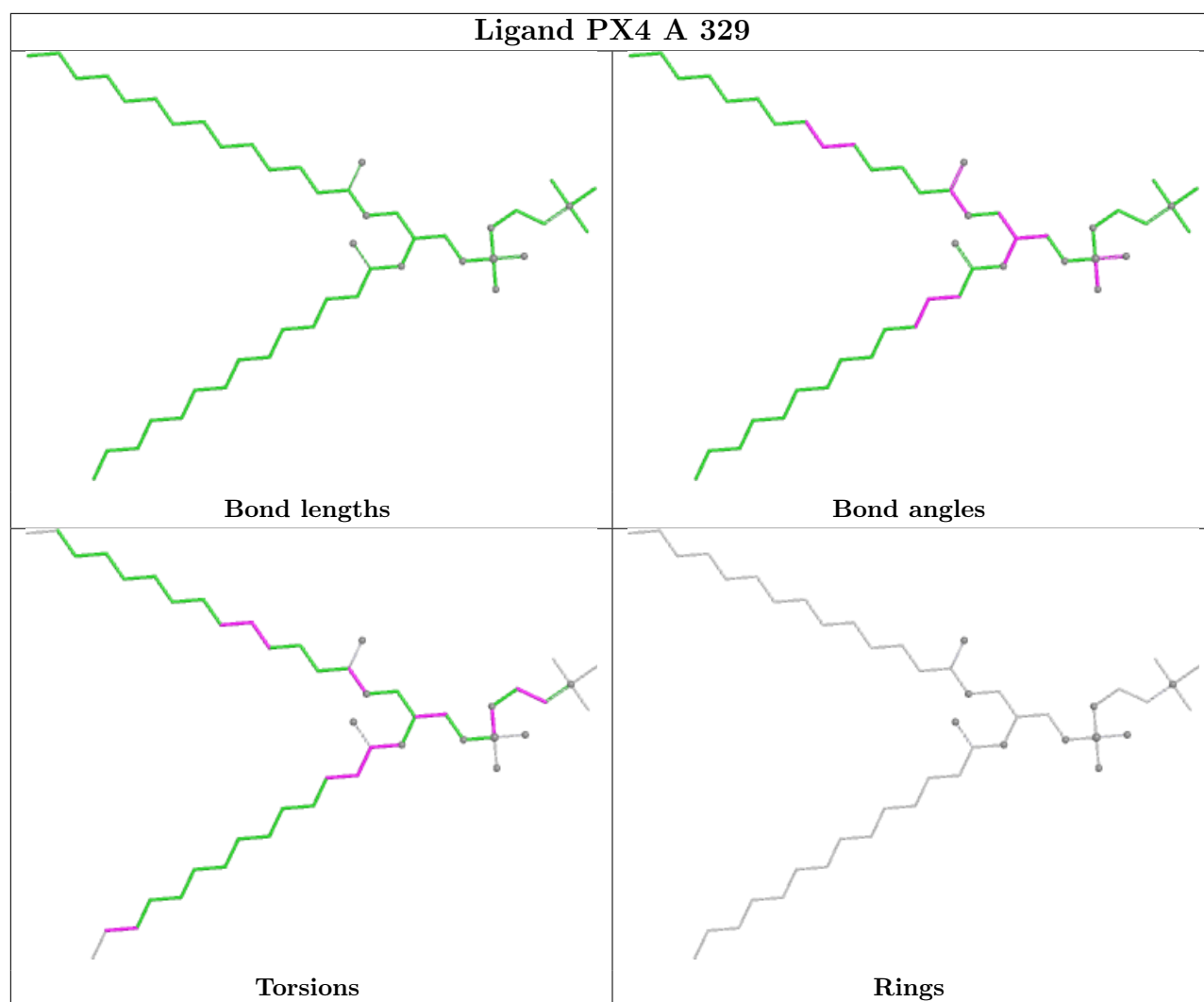


Ligand PX4 A 314

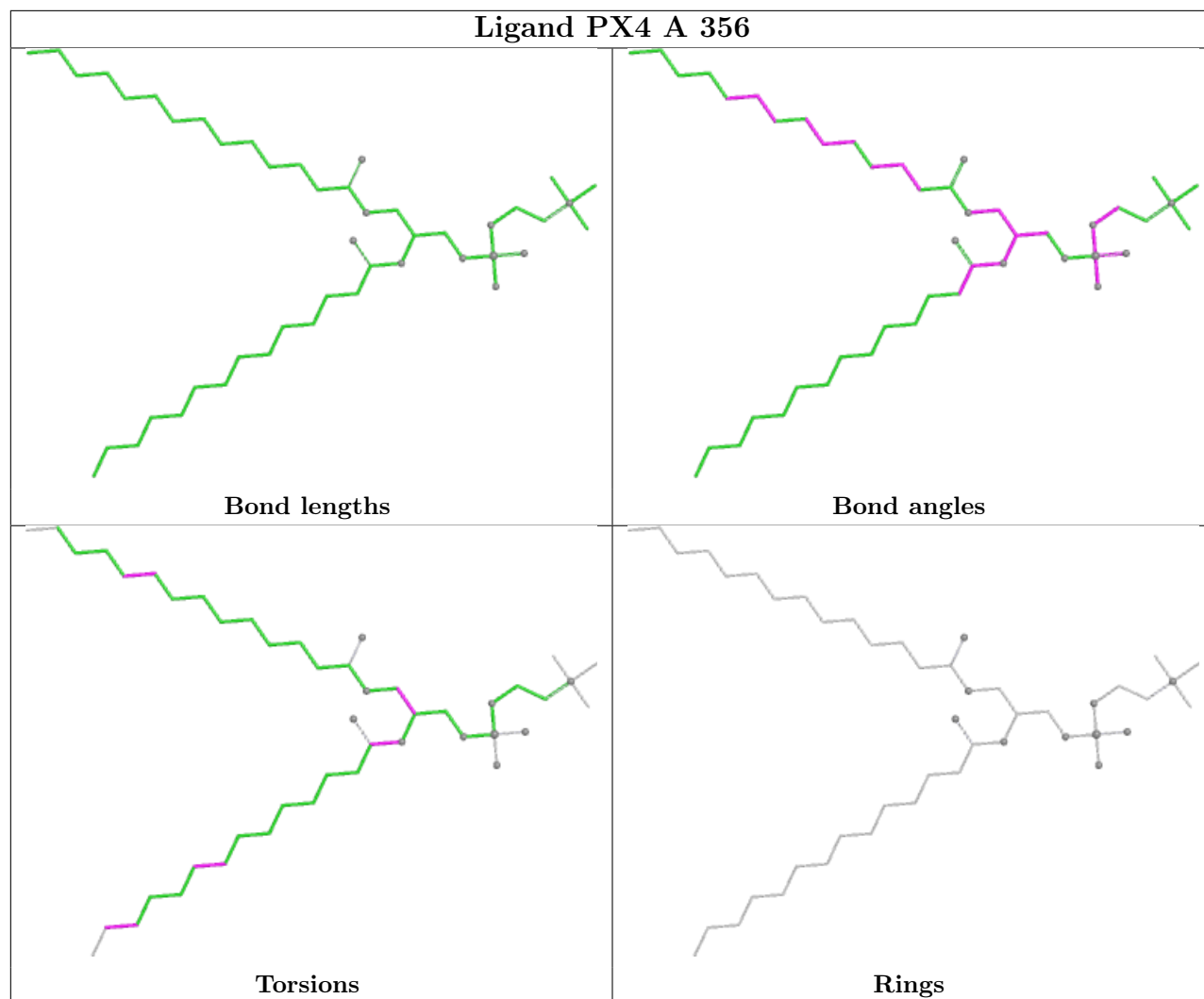




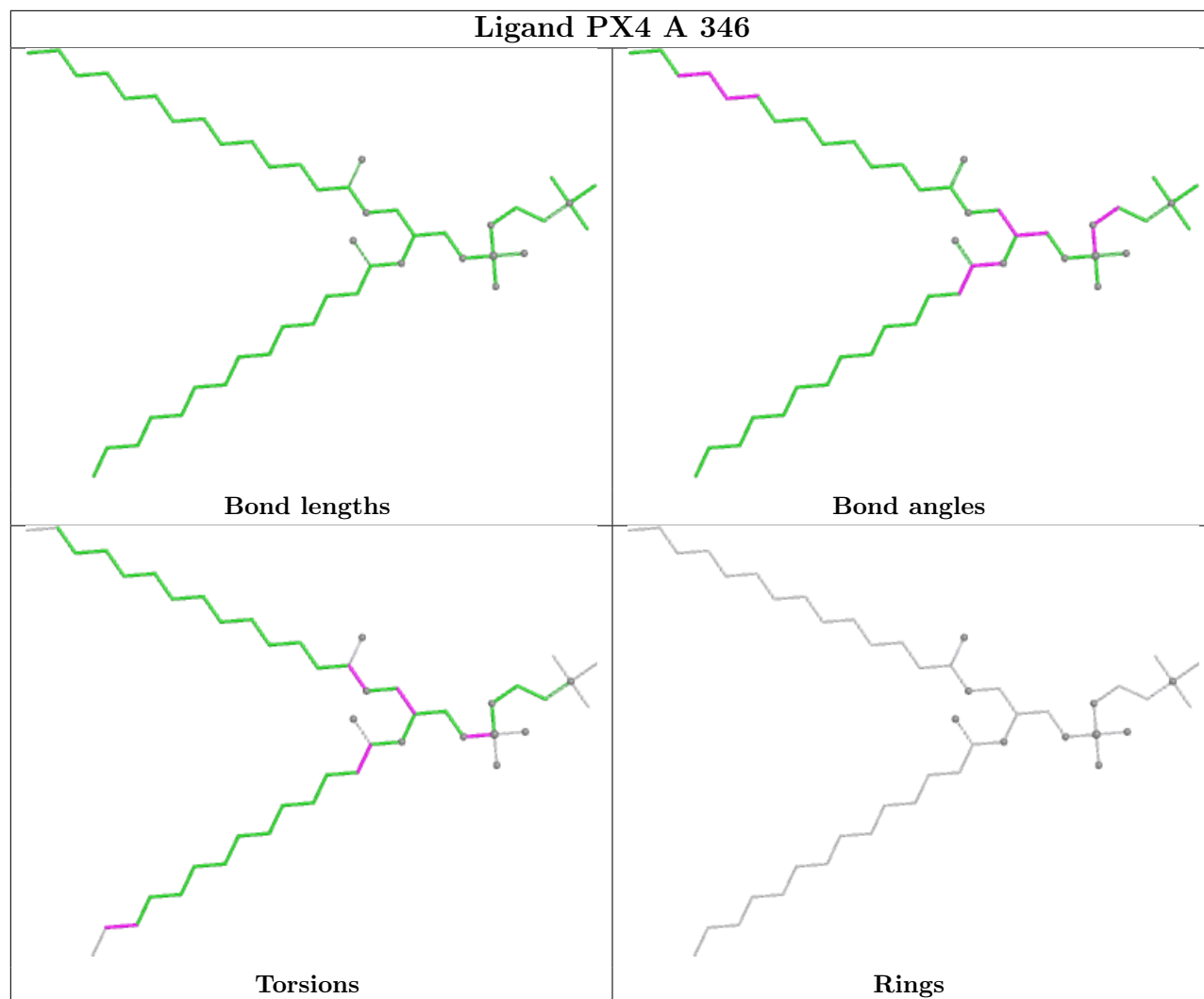




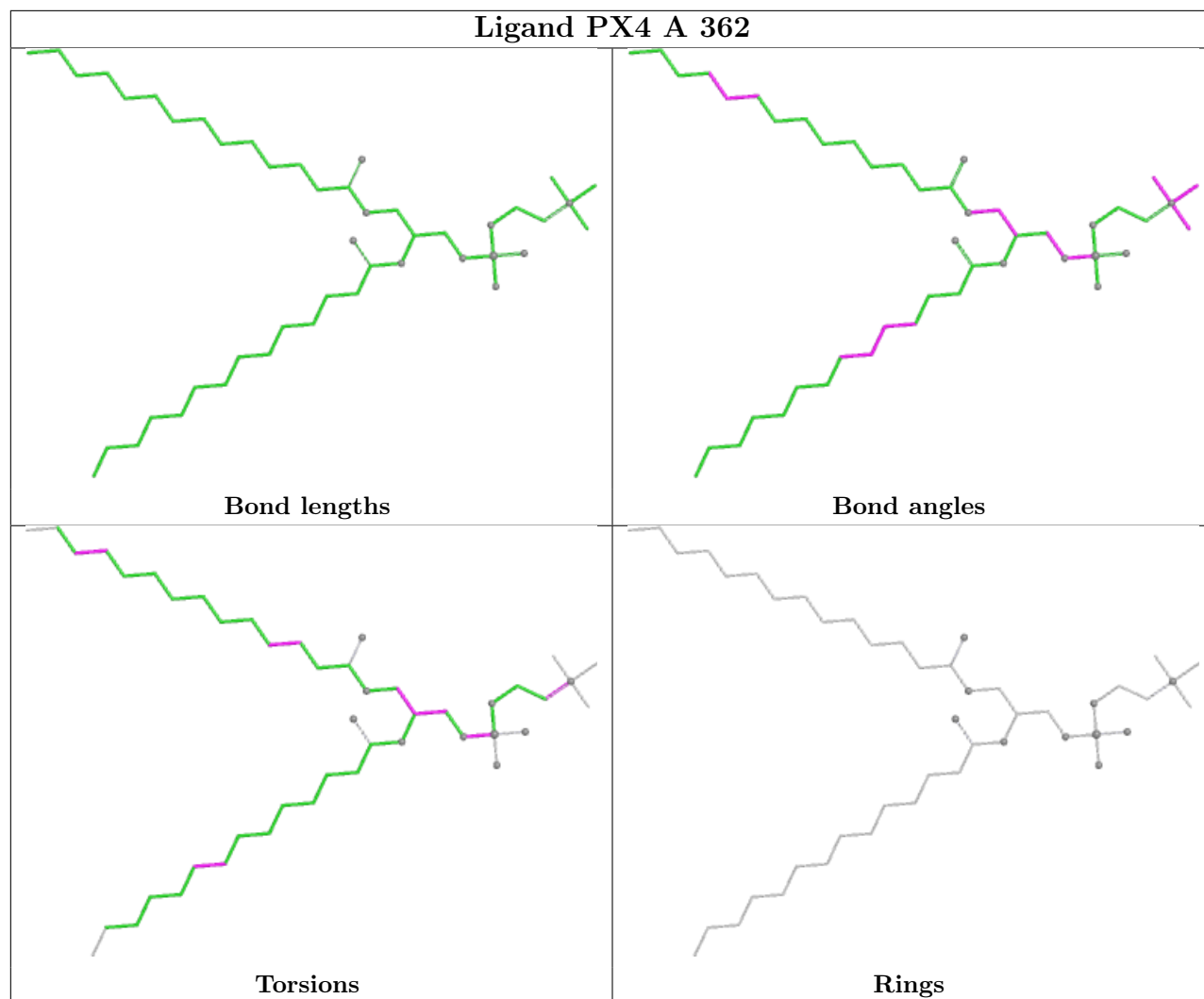
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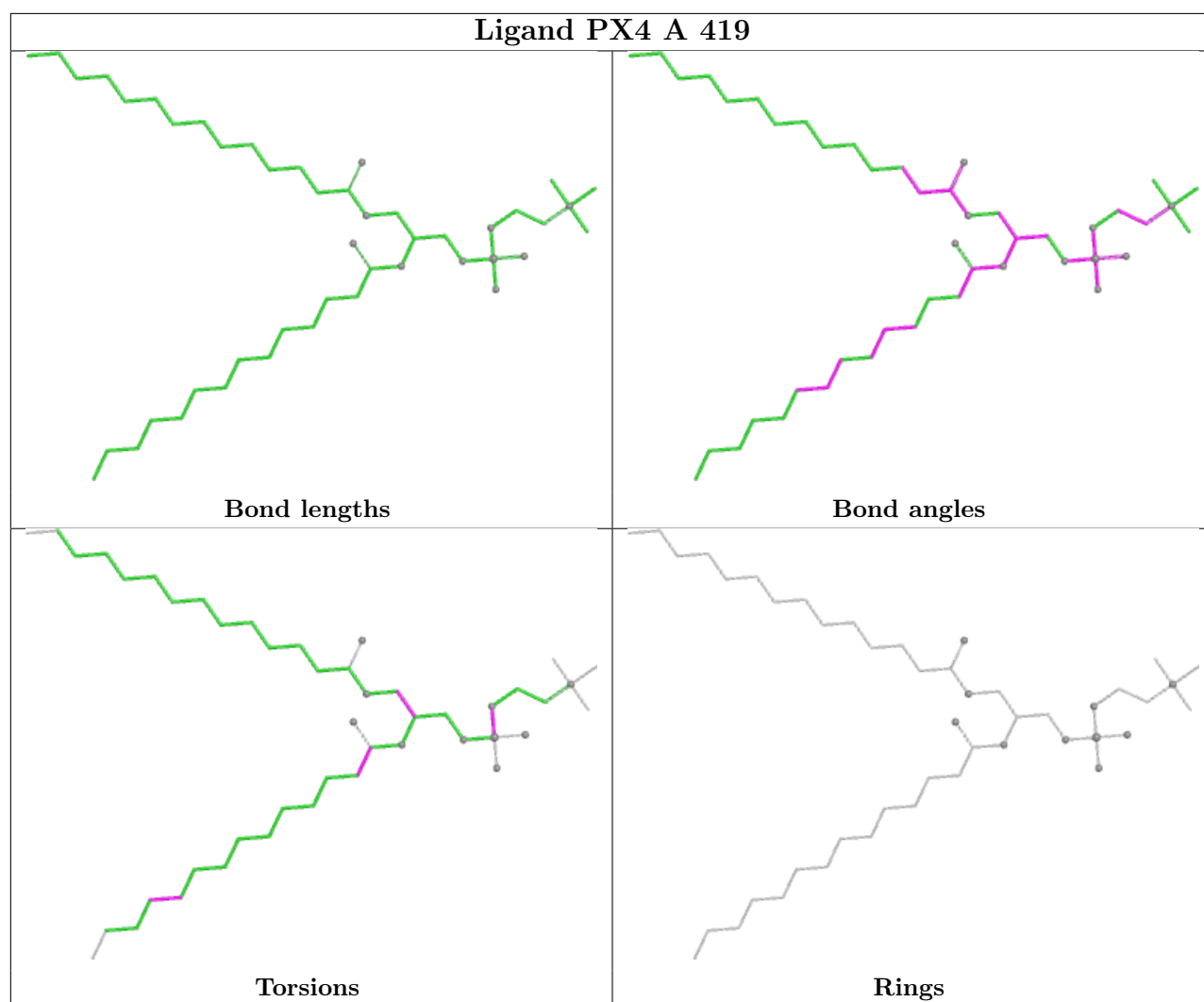


Ligand PX4 A 346

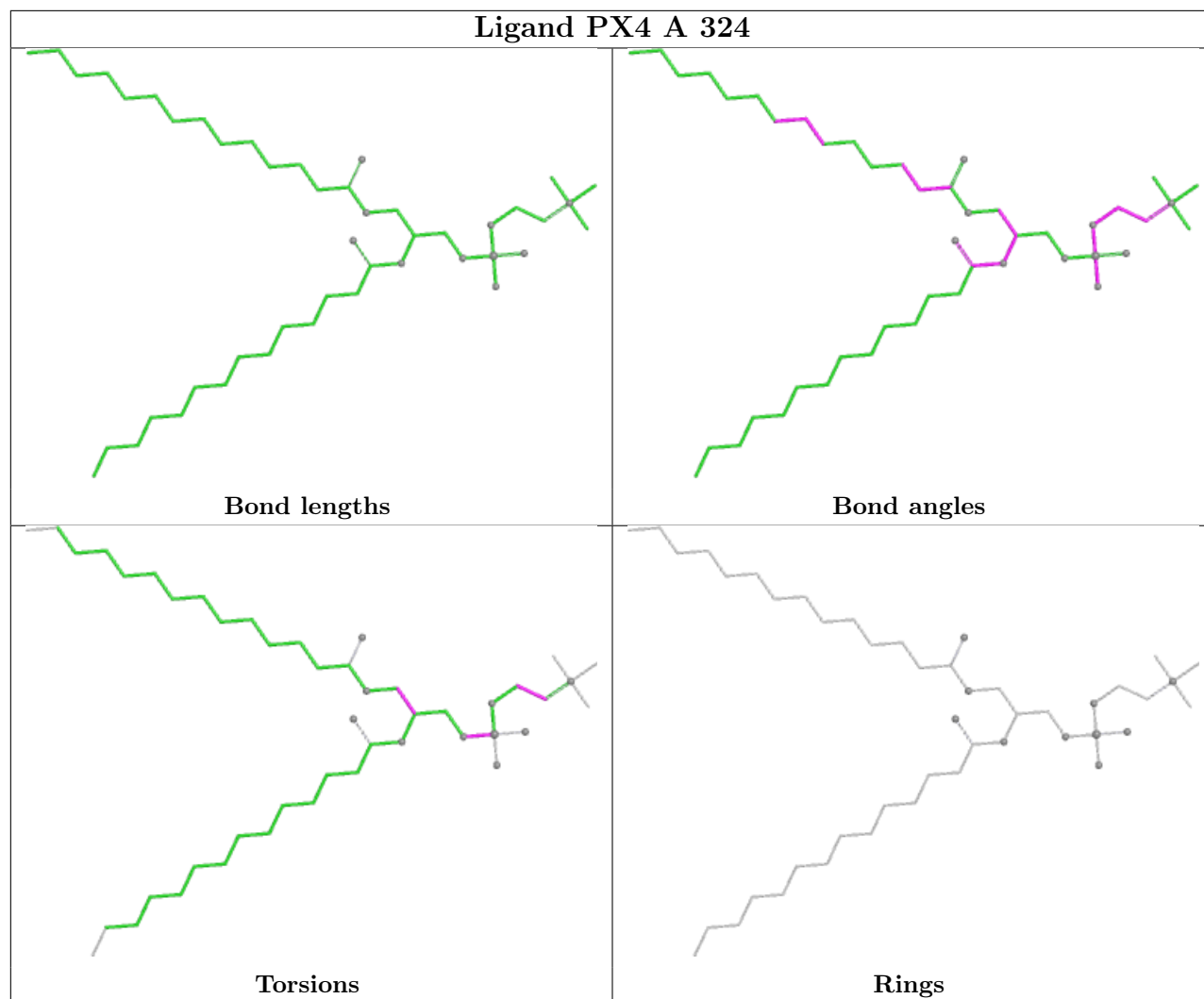


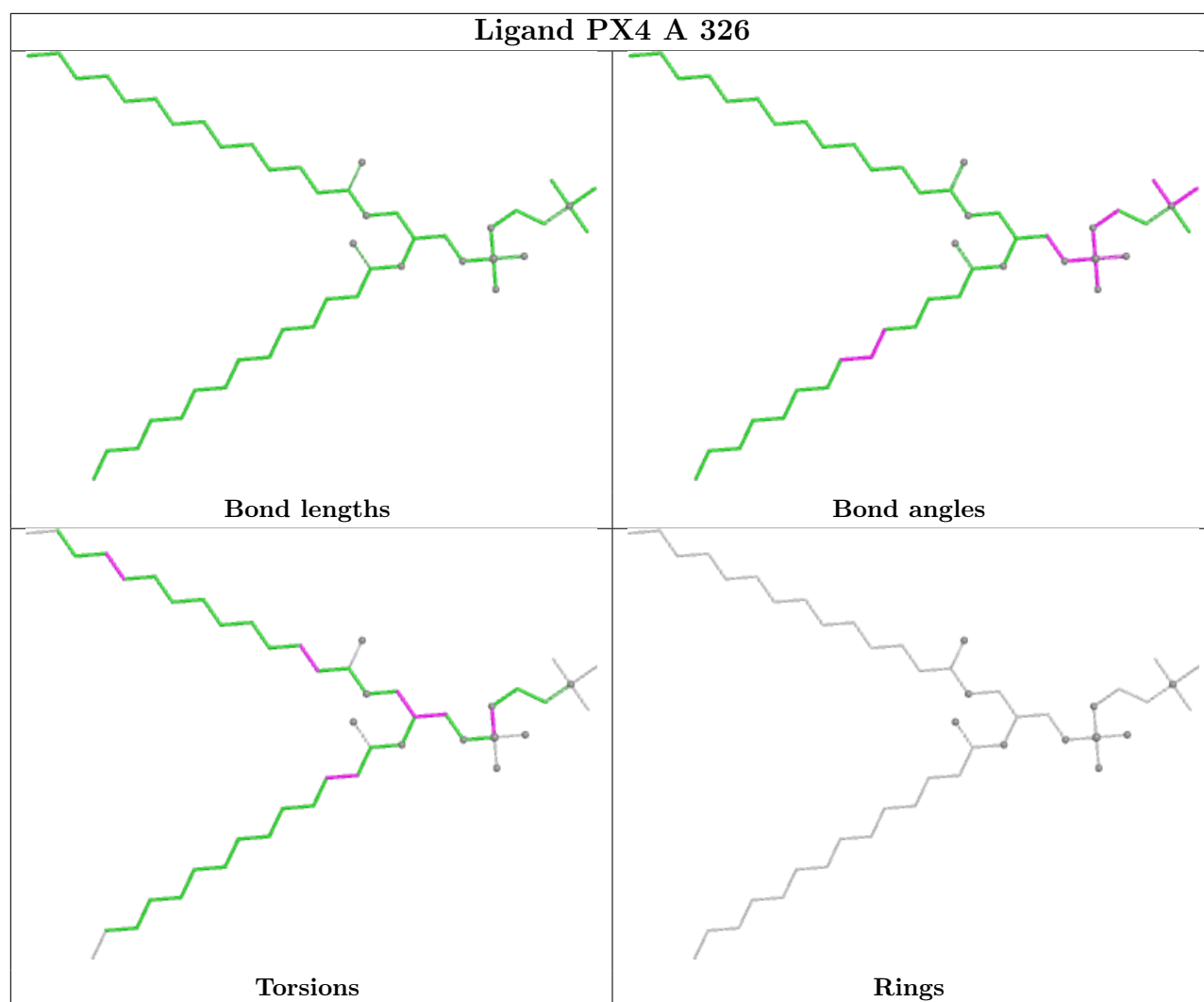
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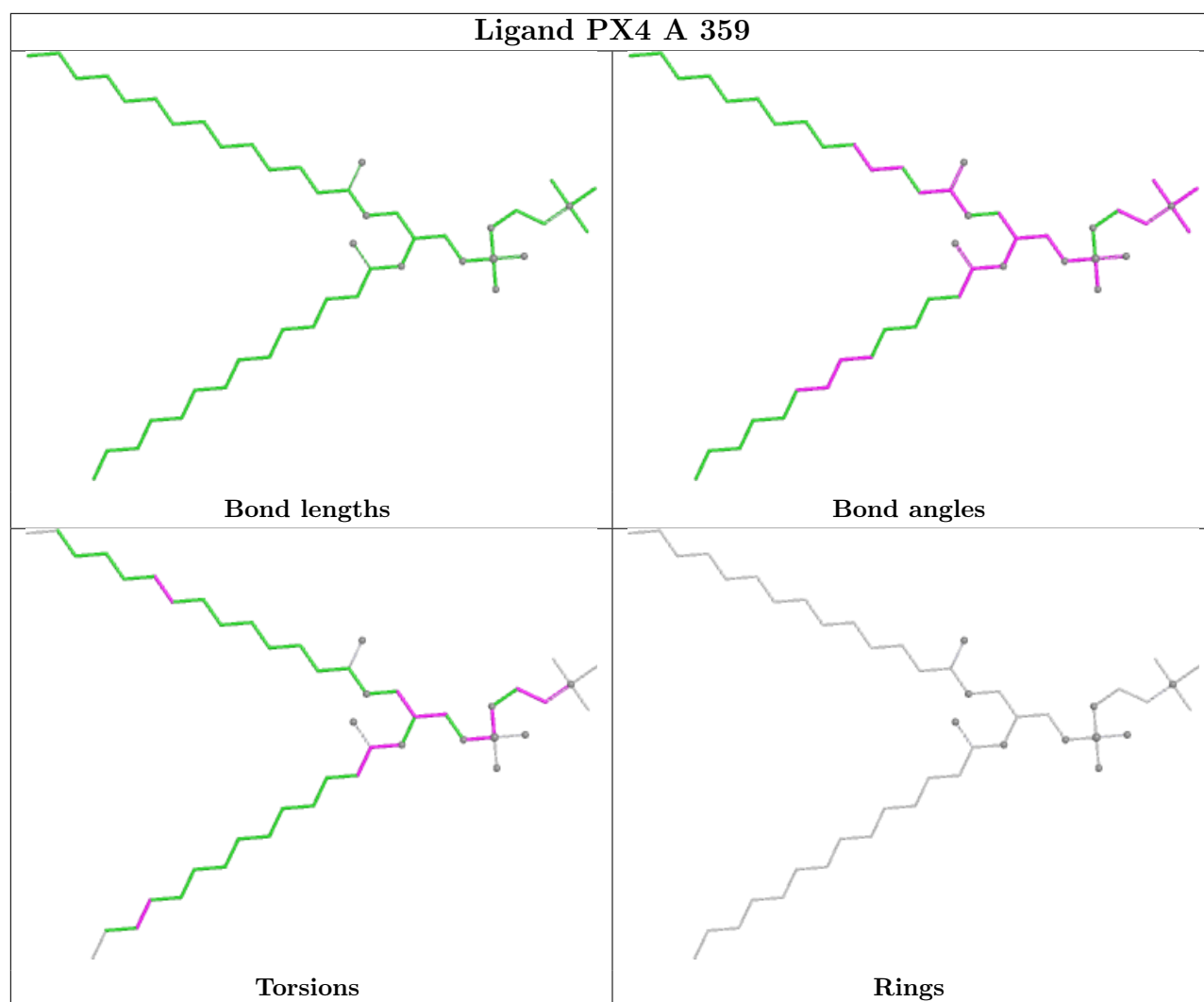




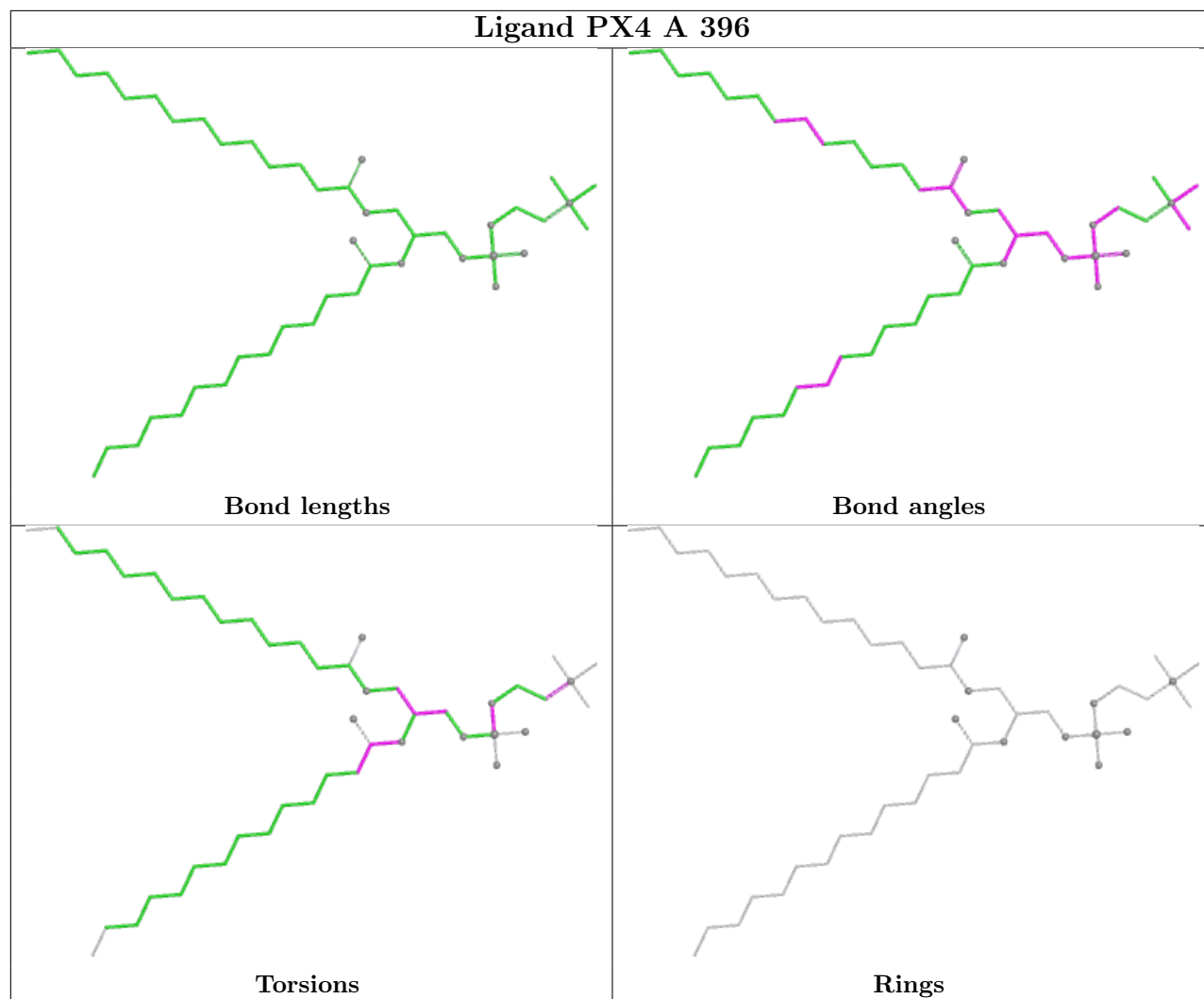
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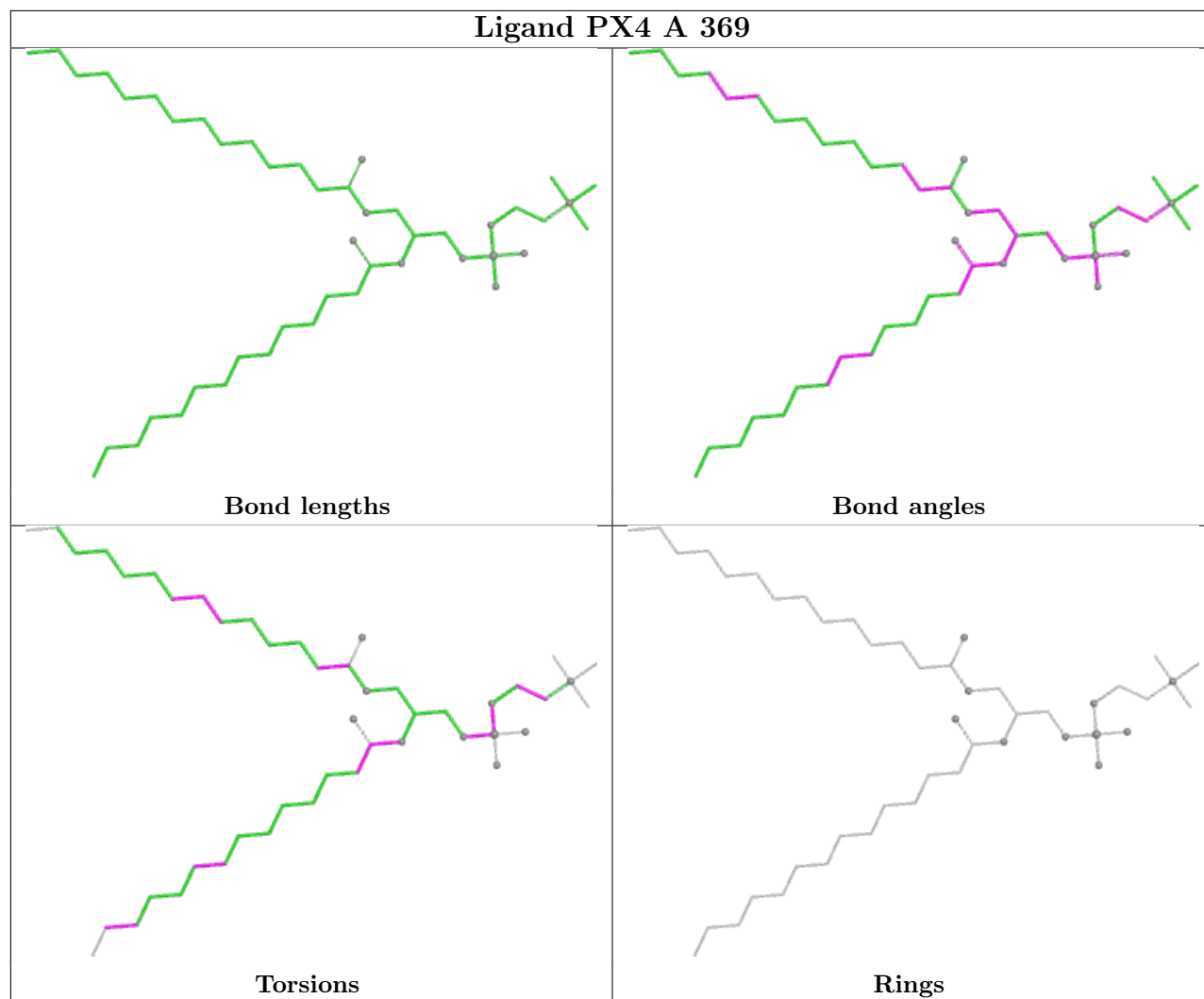


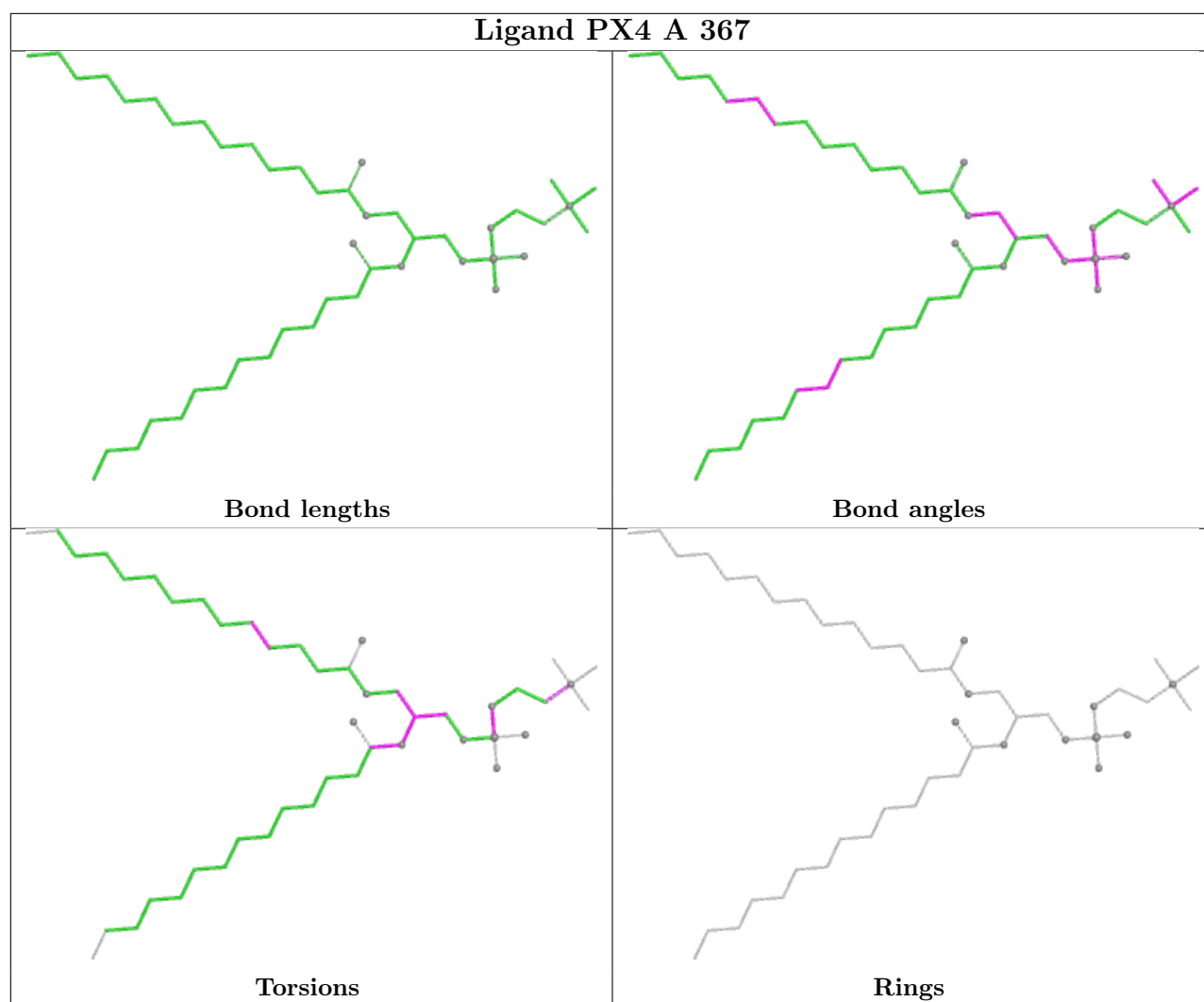


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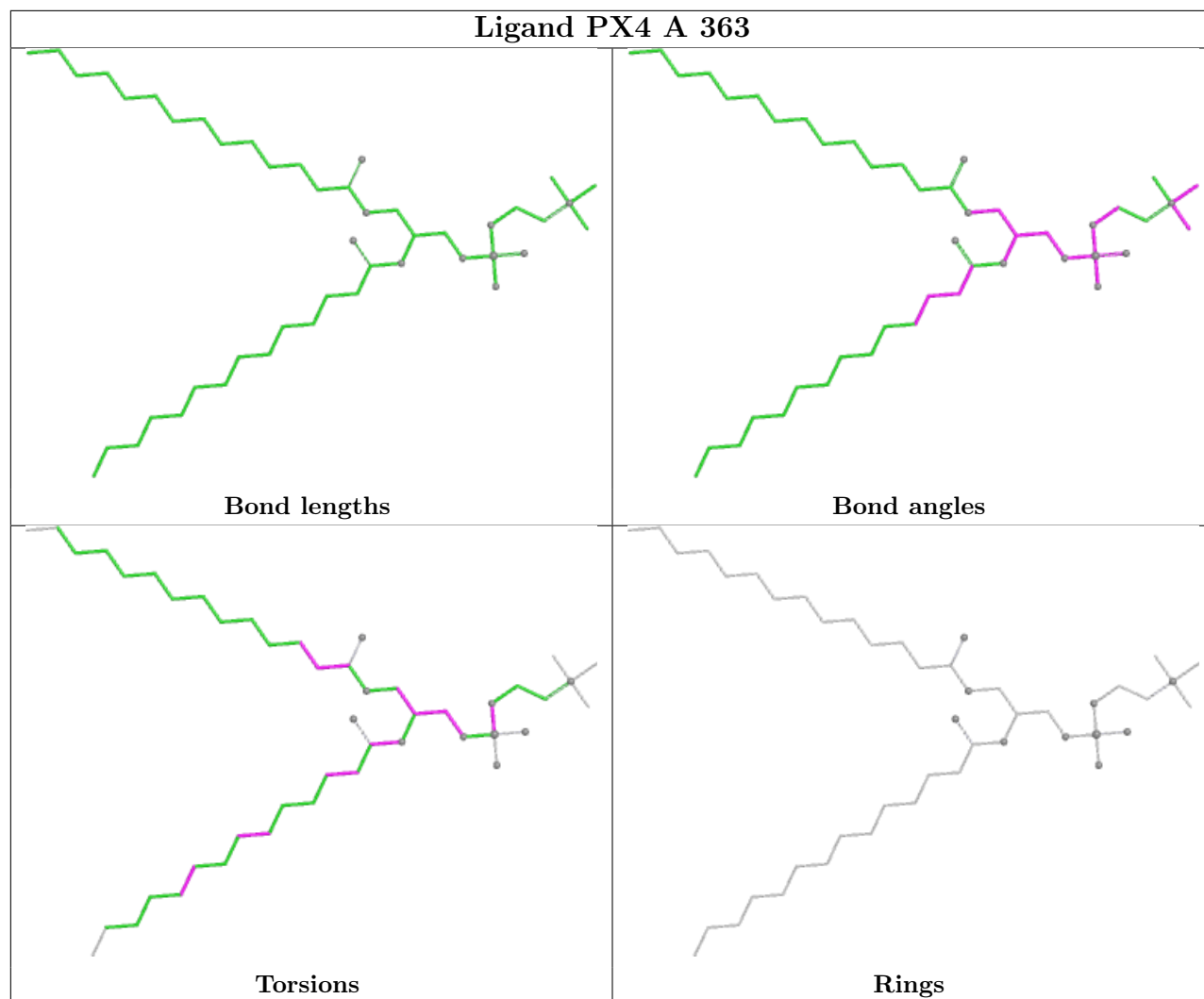


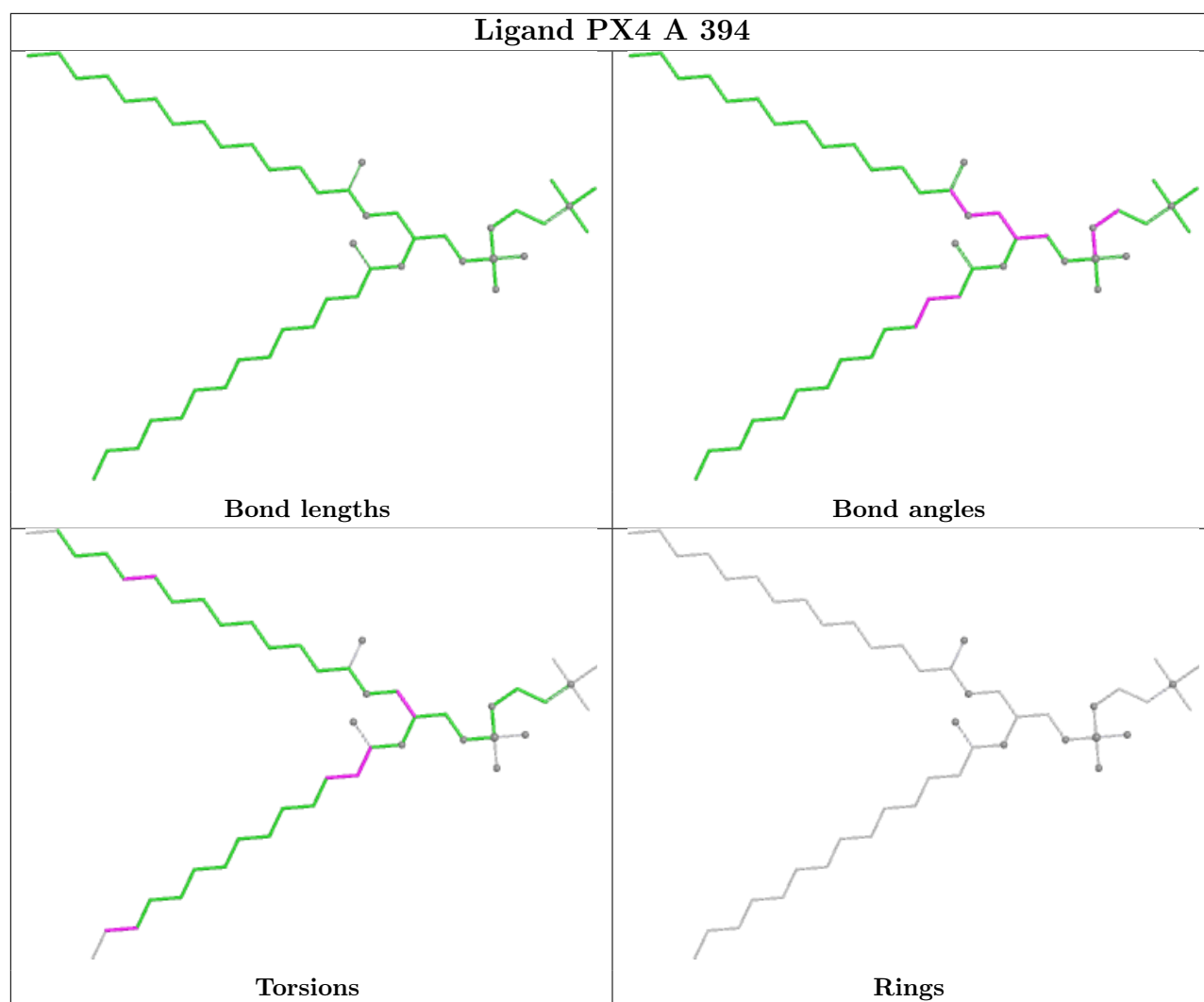
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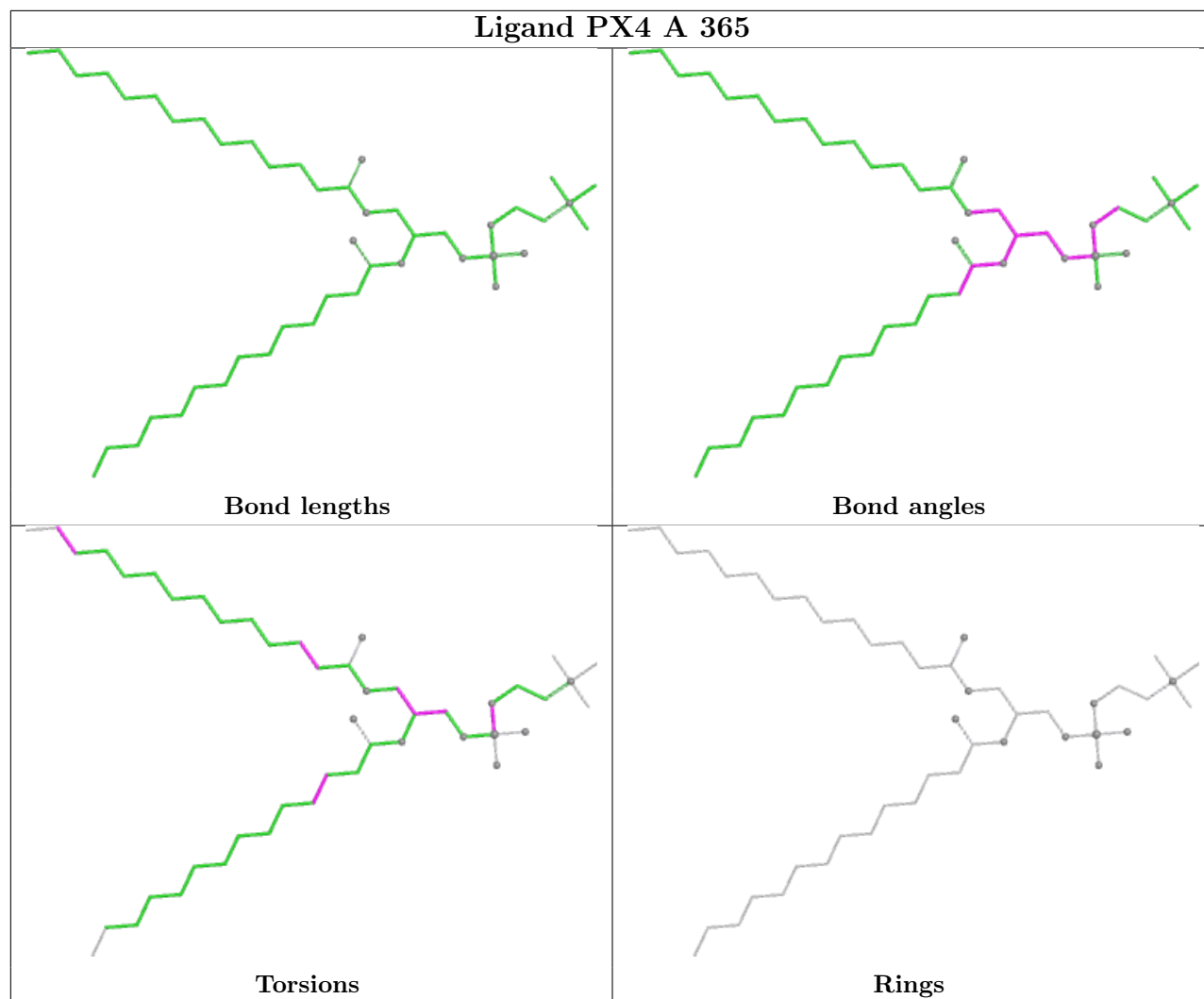


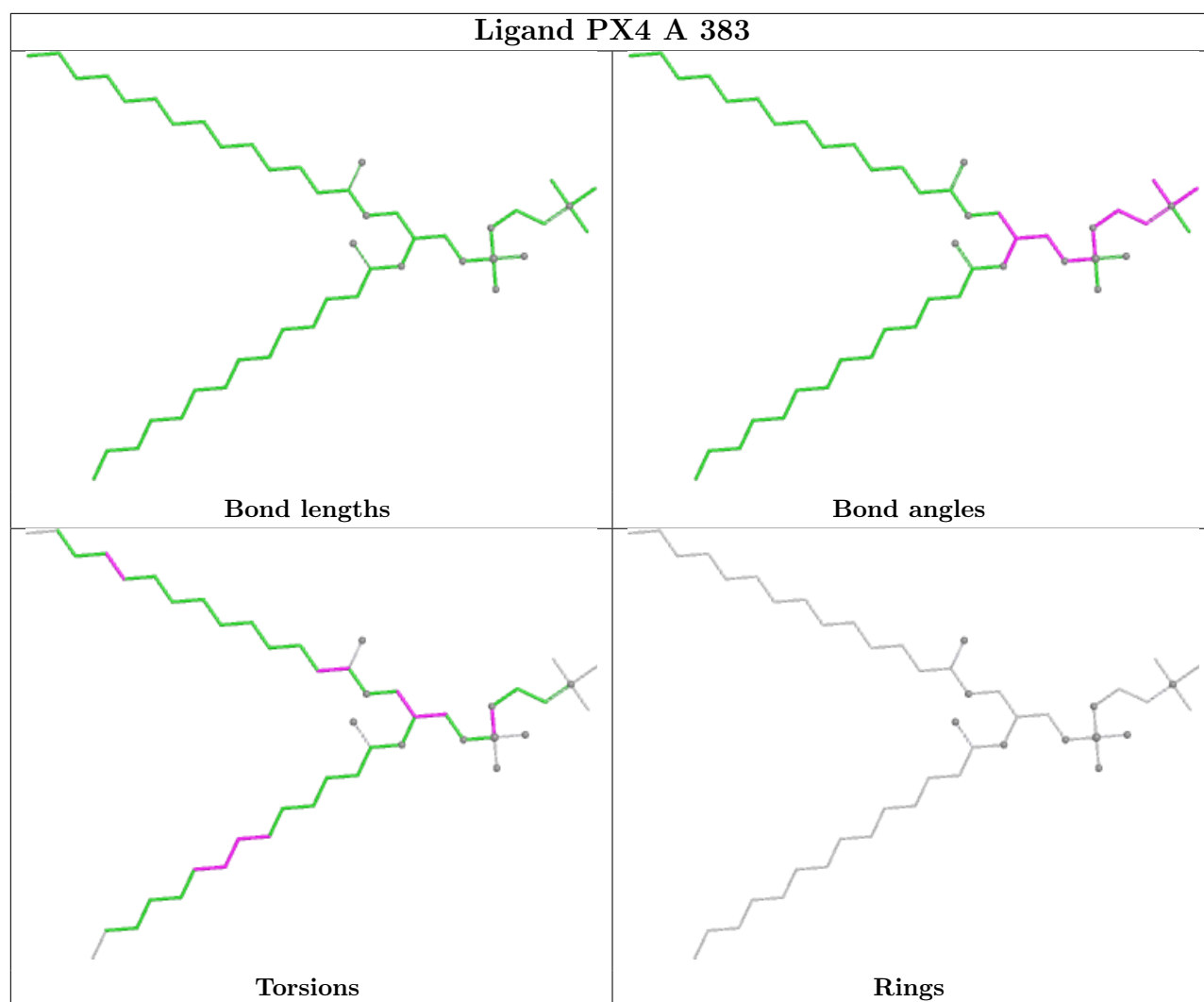
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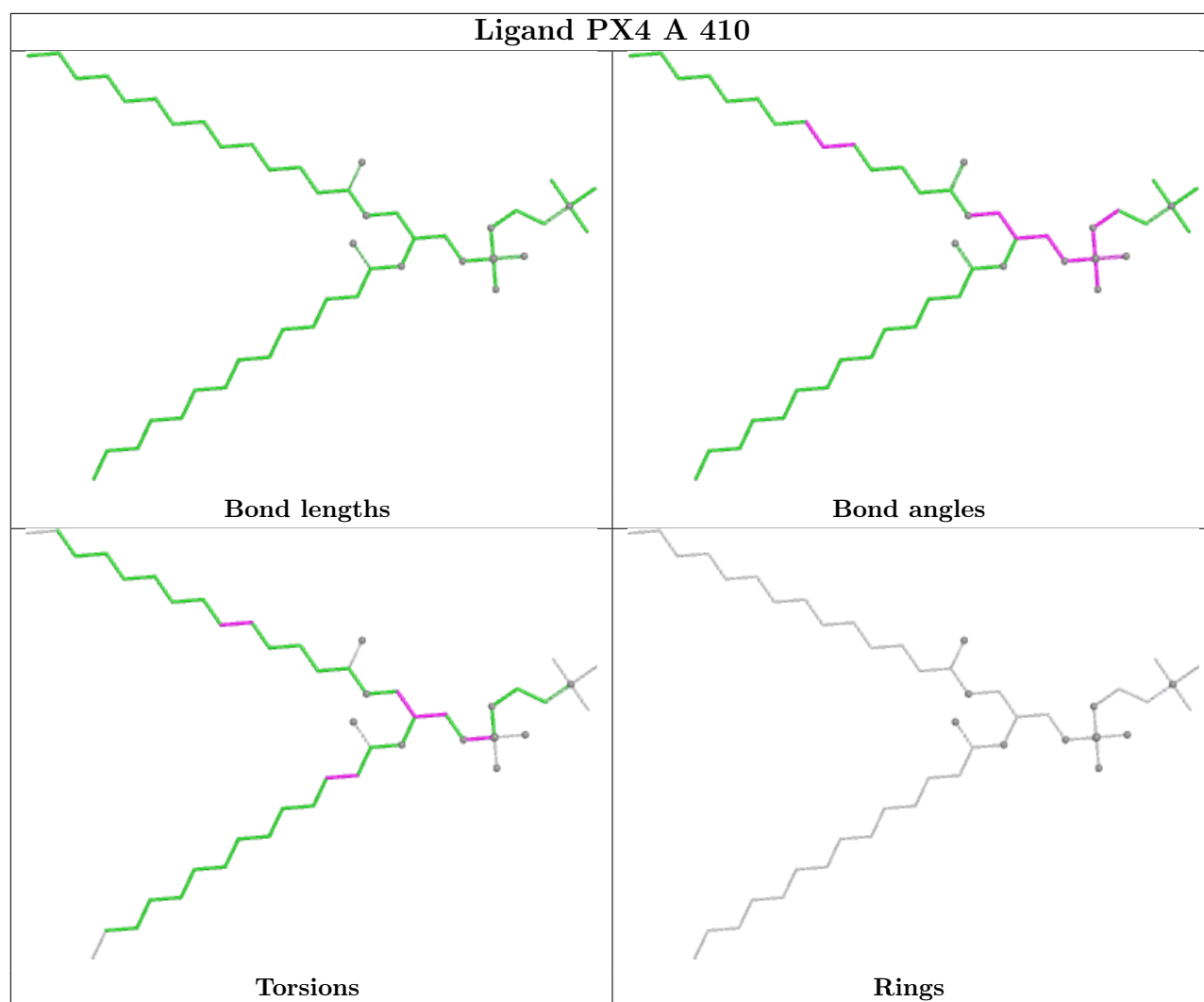




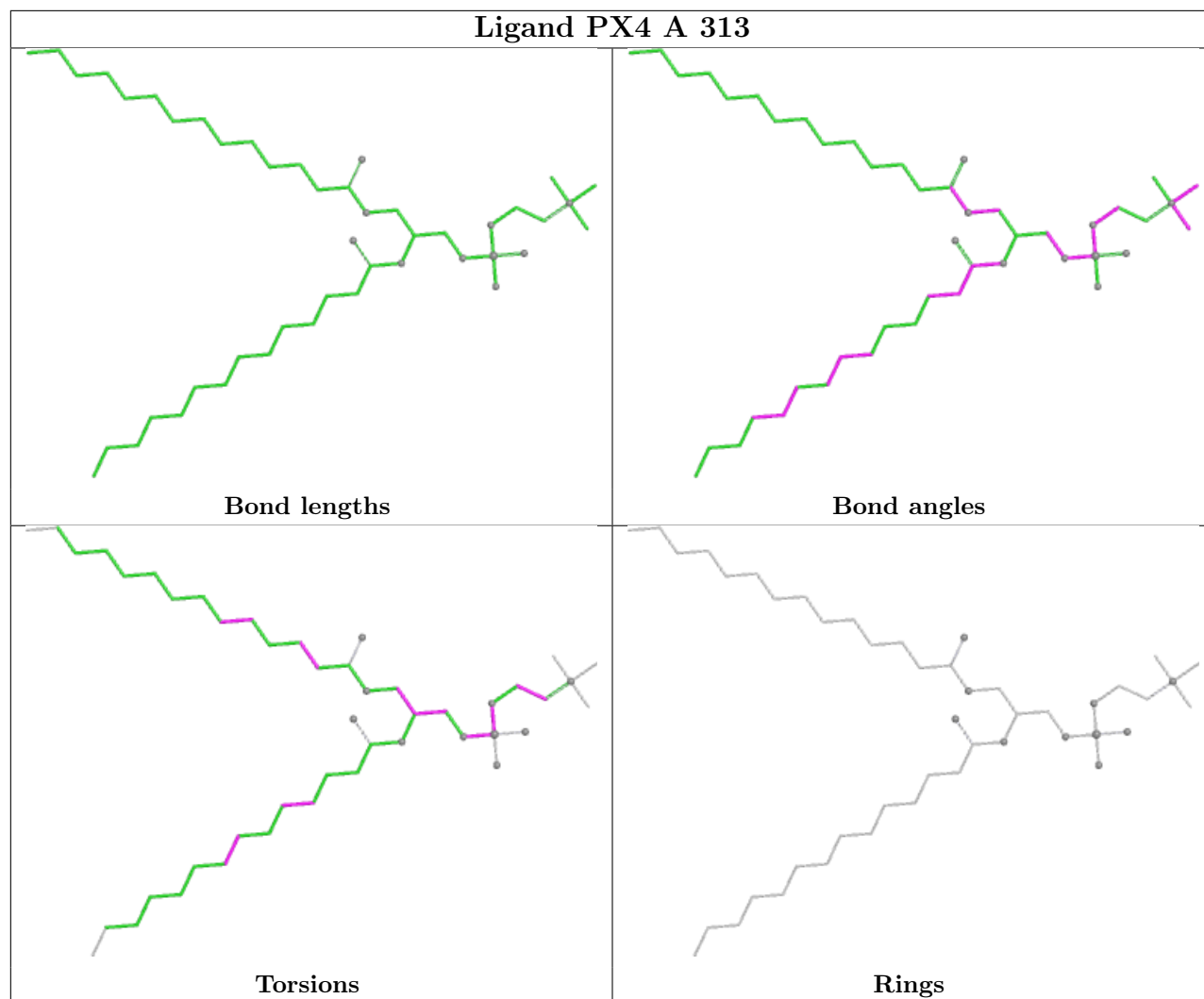
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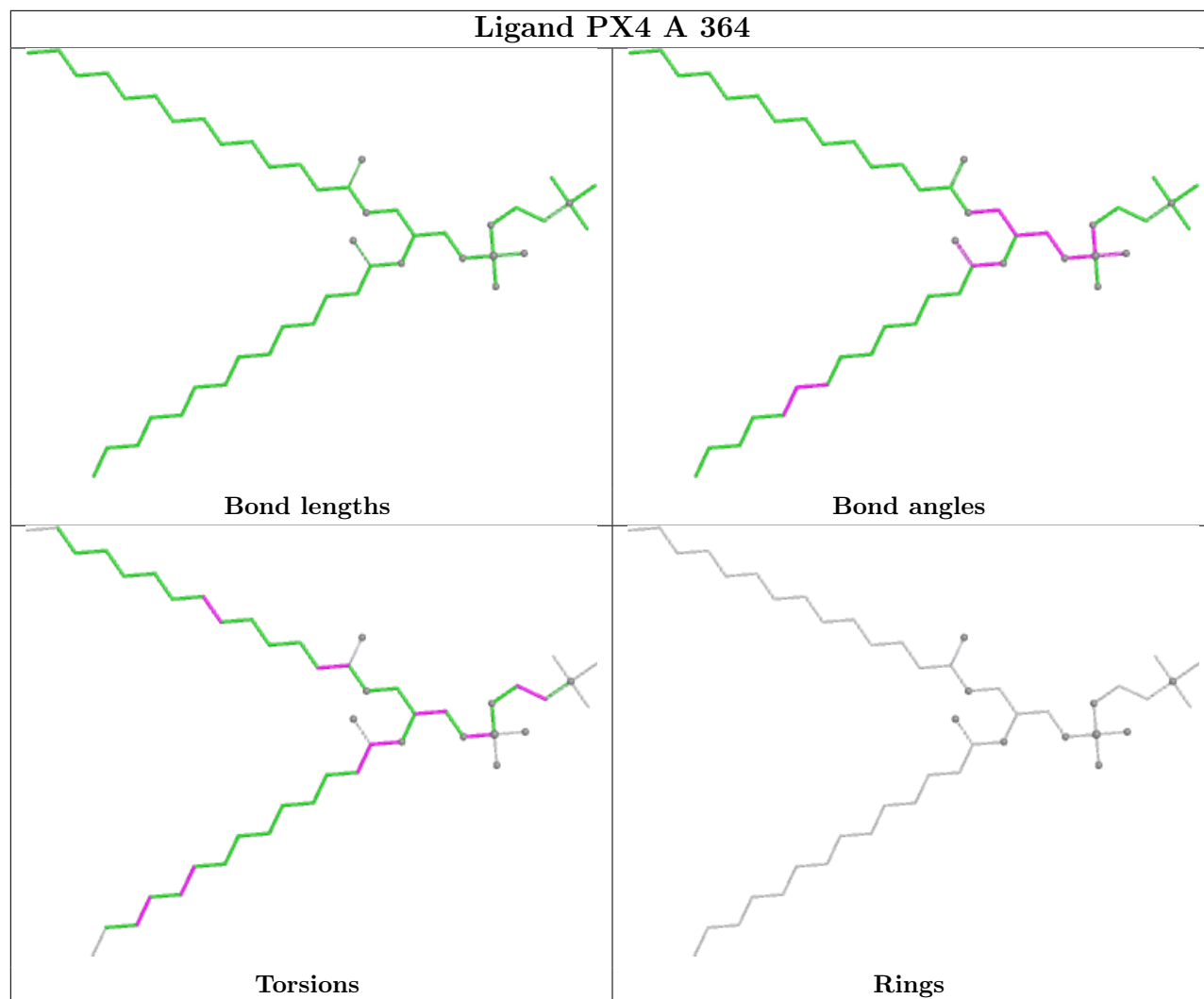




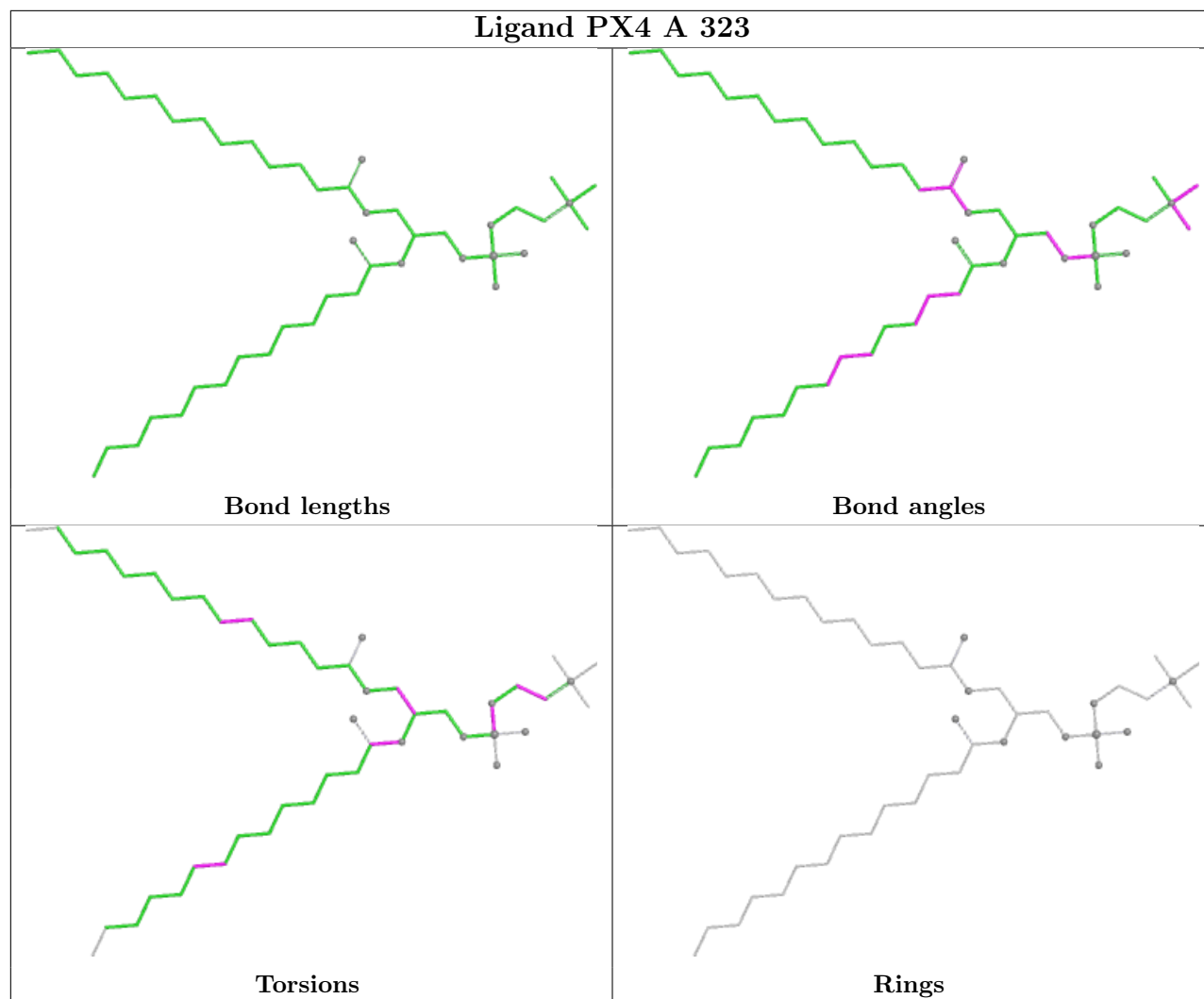
Ligand PX4 A 313

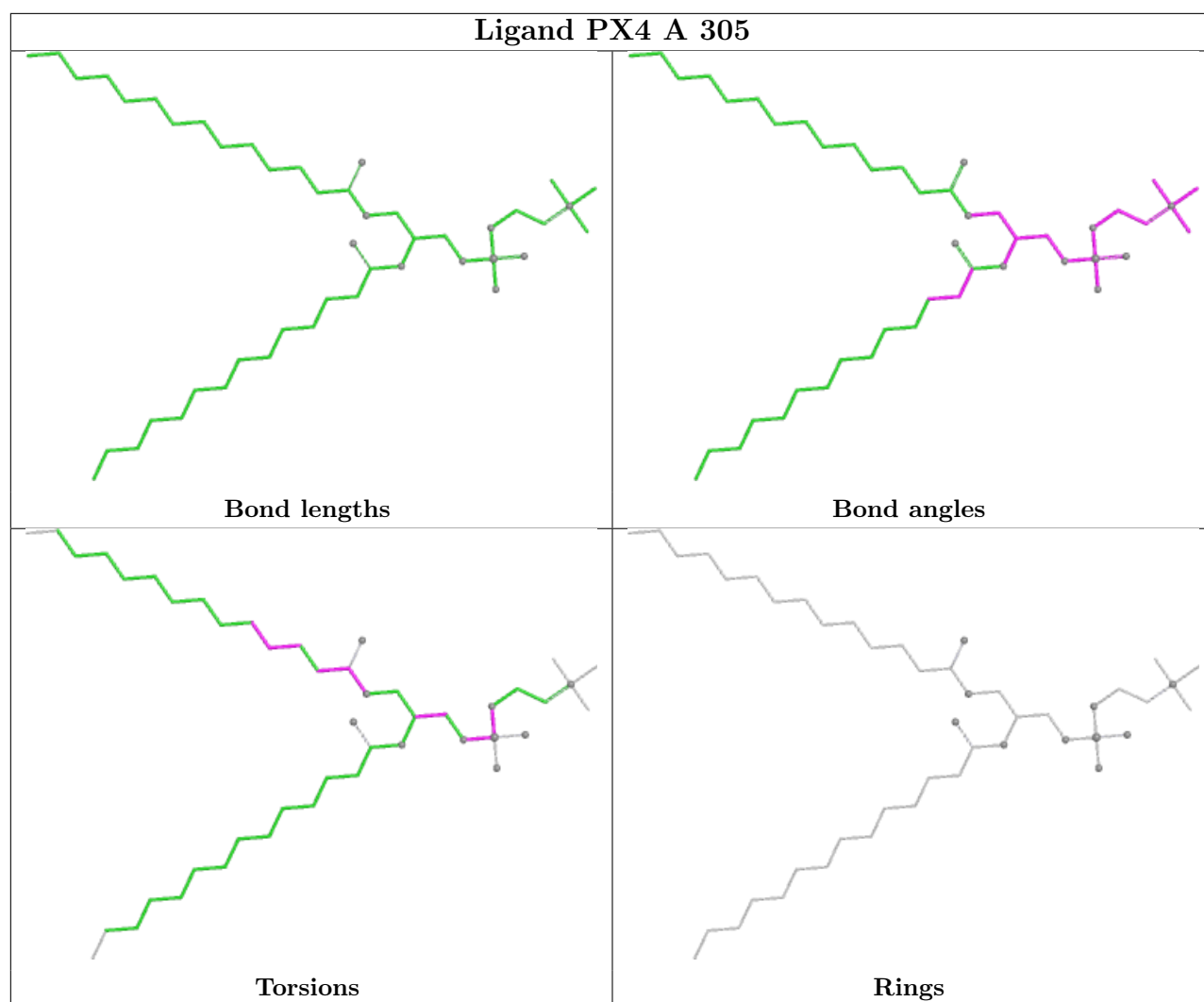


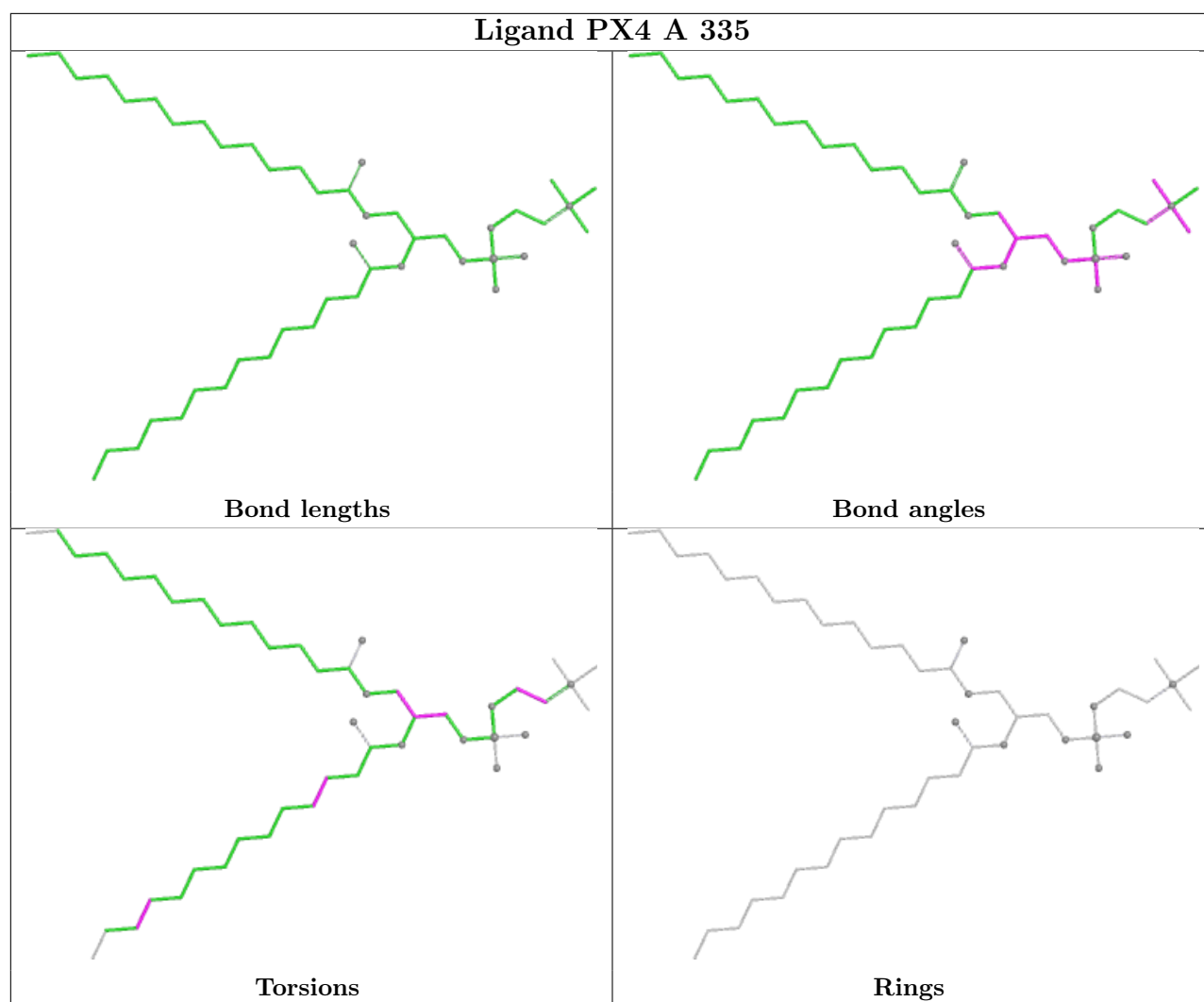
Ligand PX4 A 364



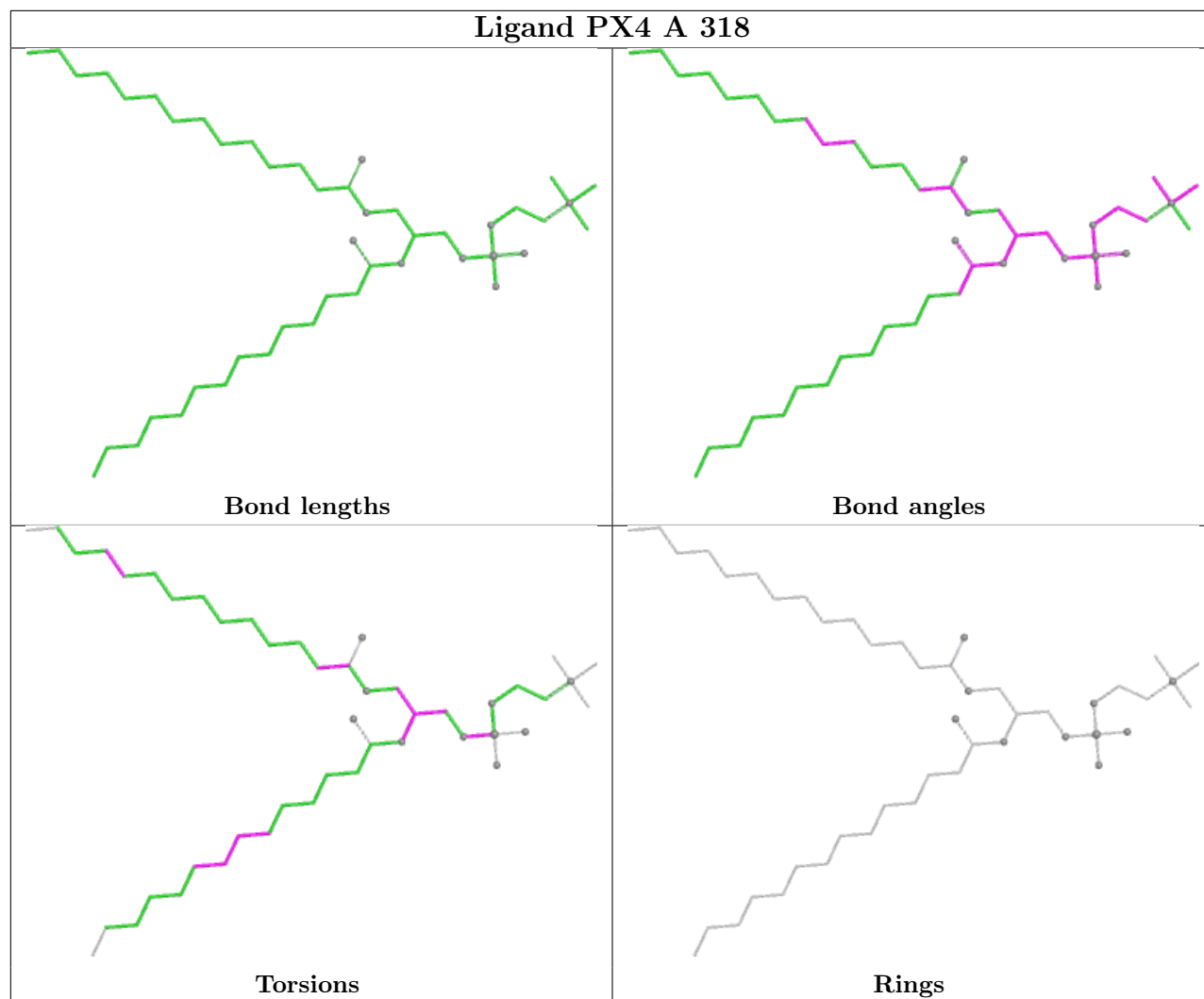
Ligand PX4 A 323



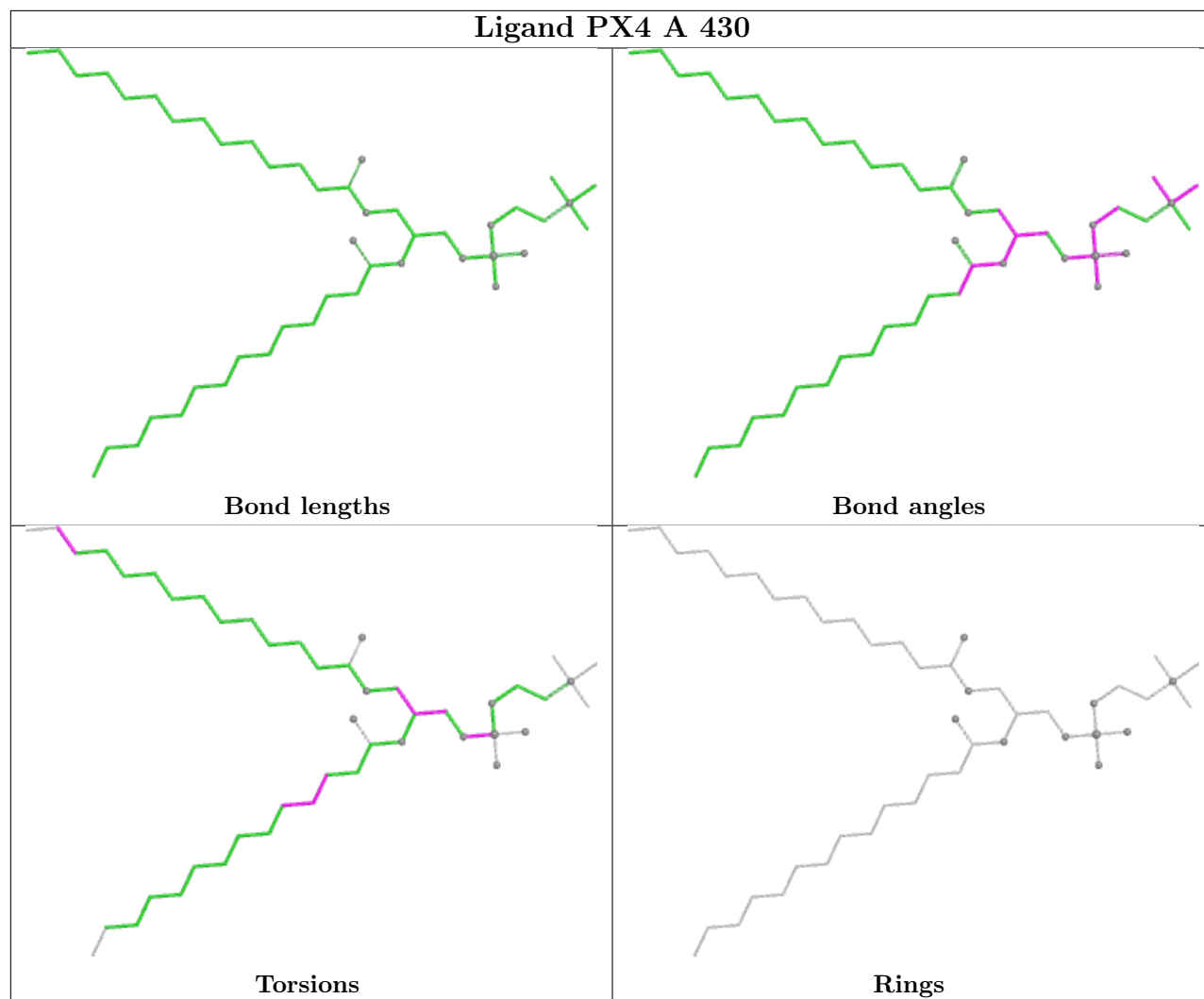


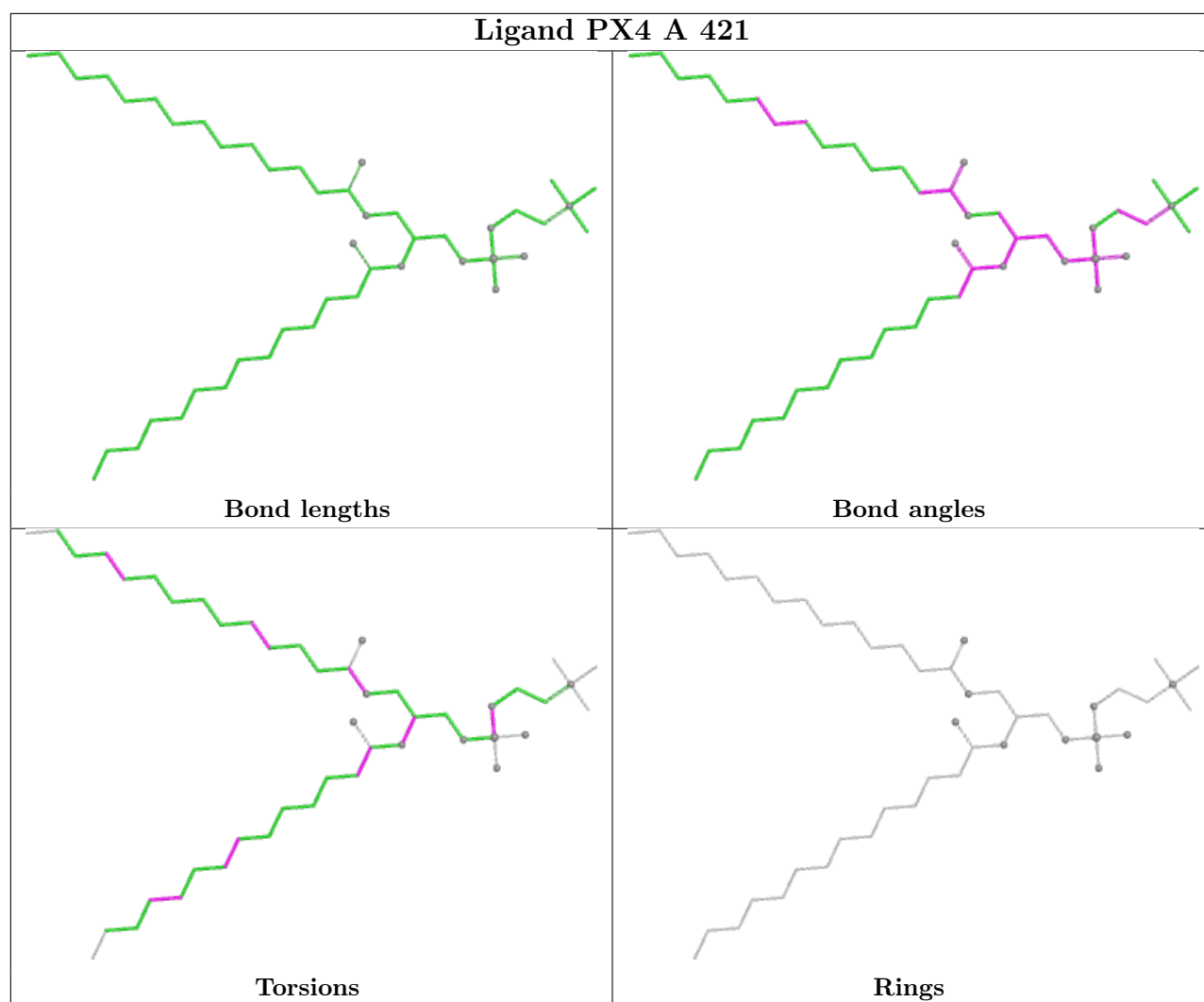


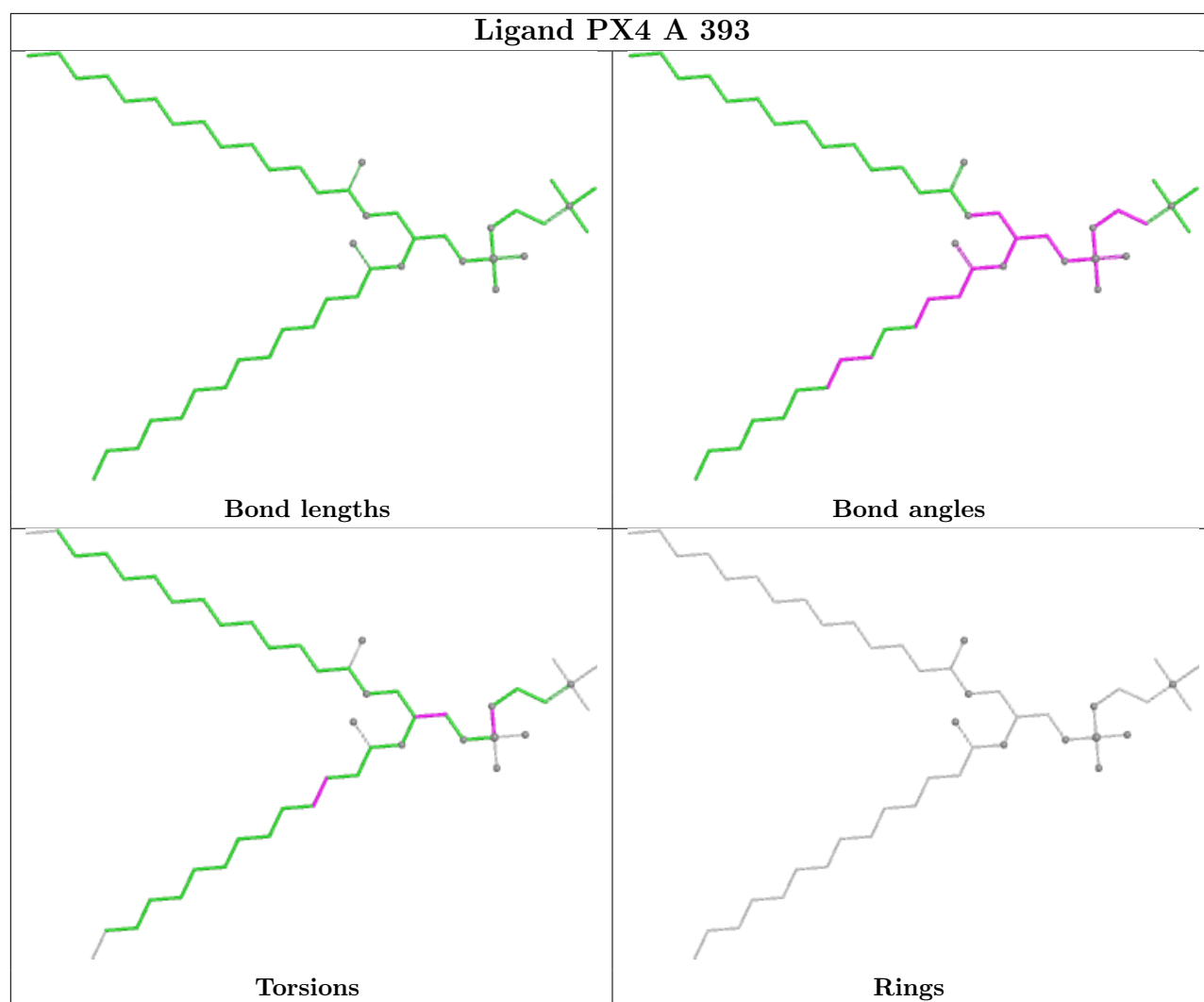
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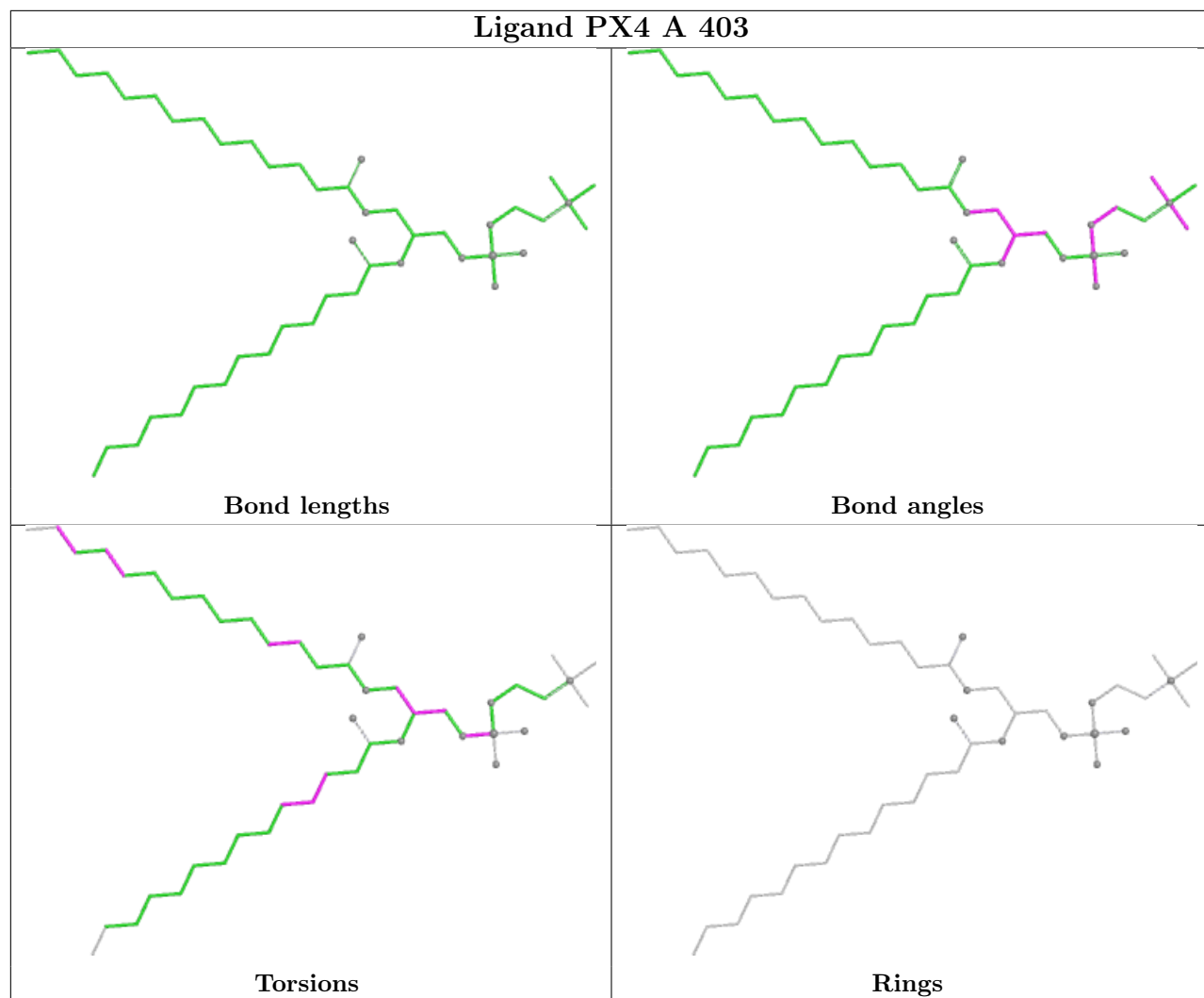
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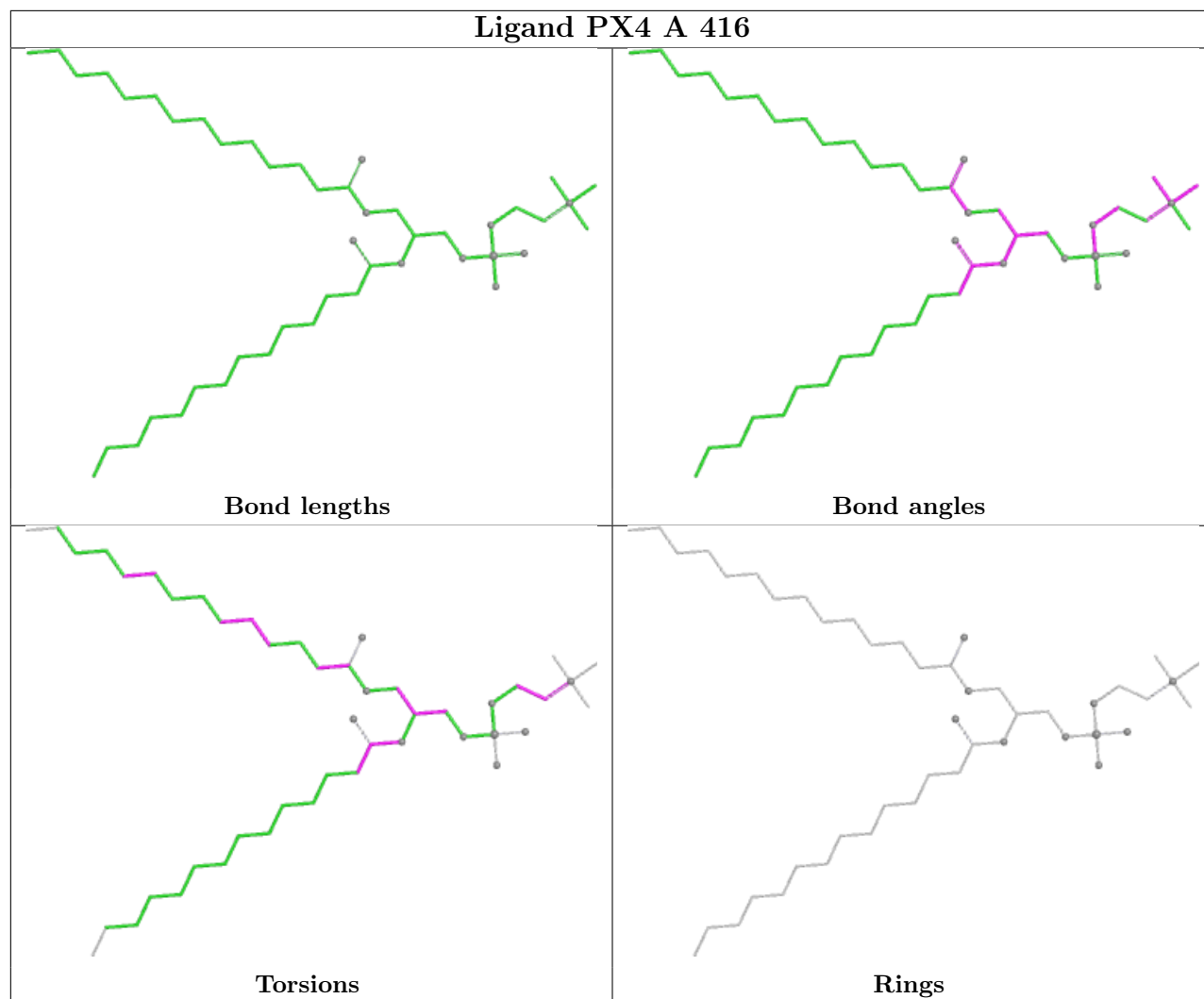


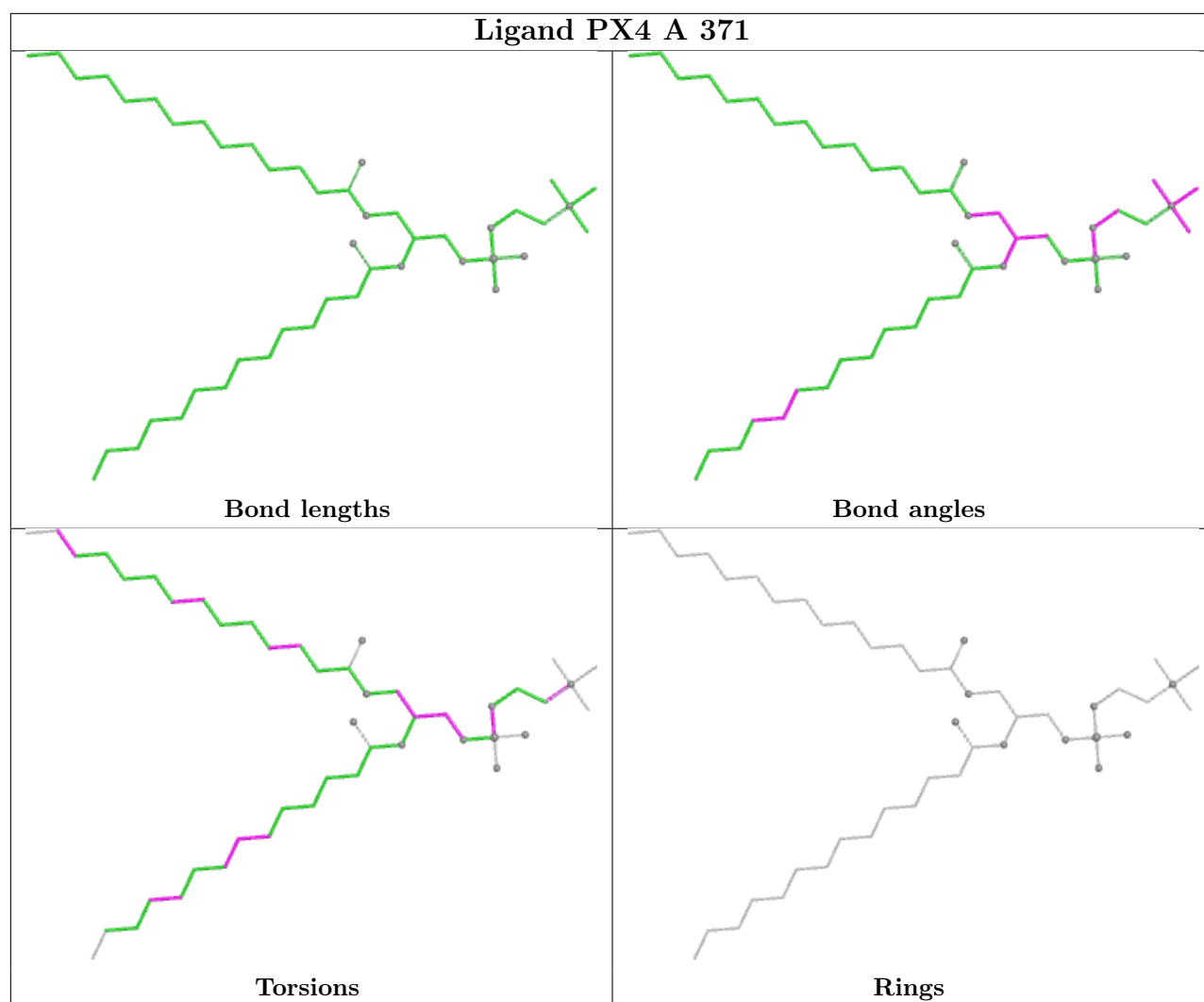


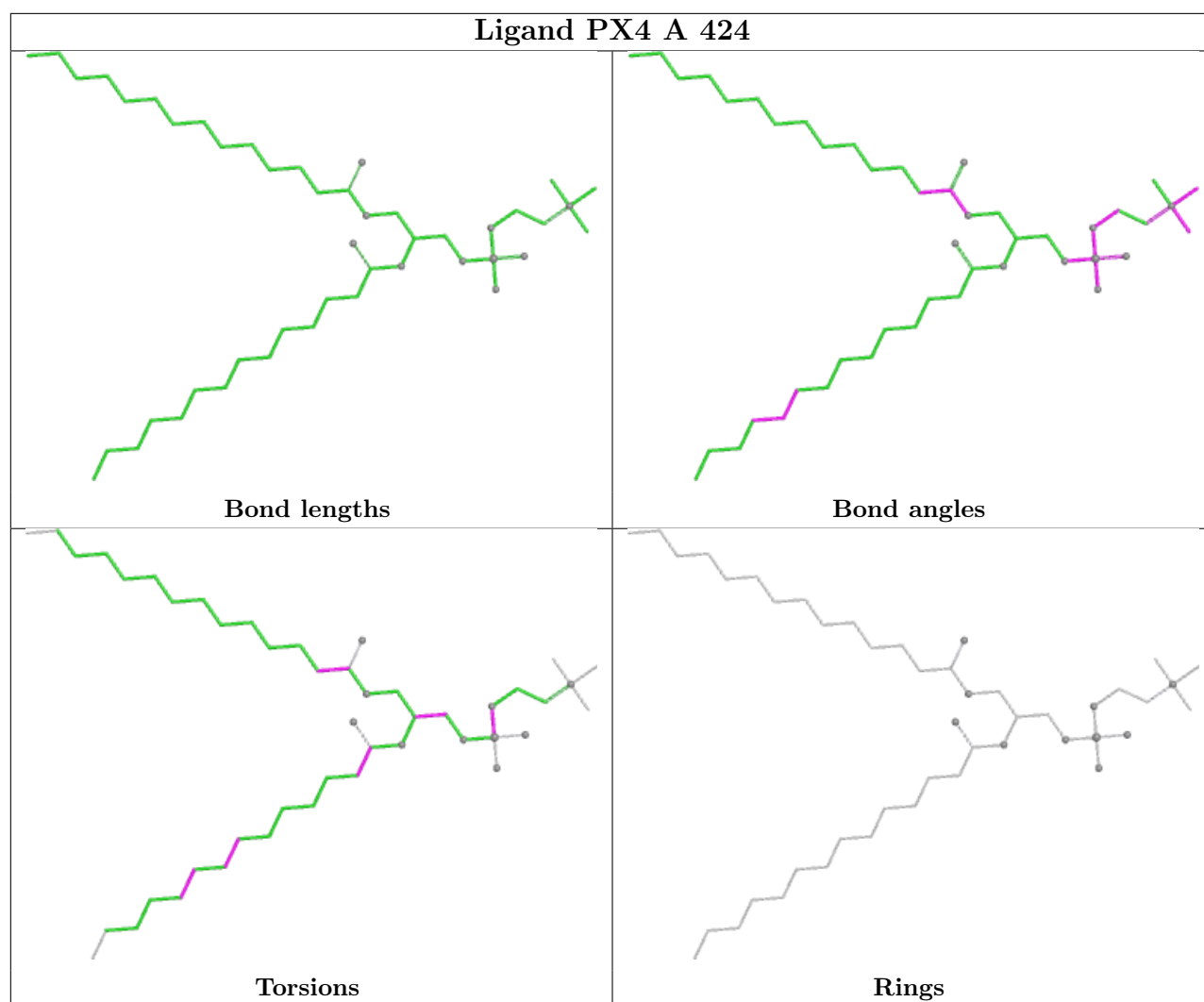
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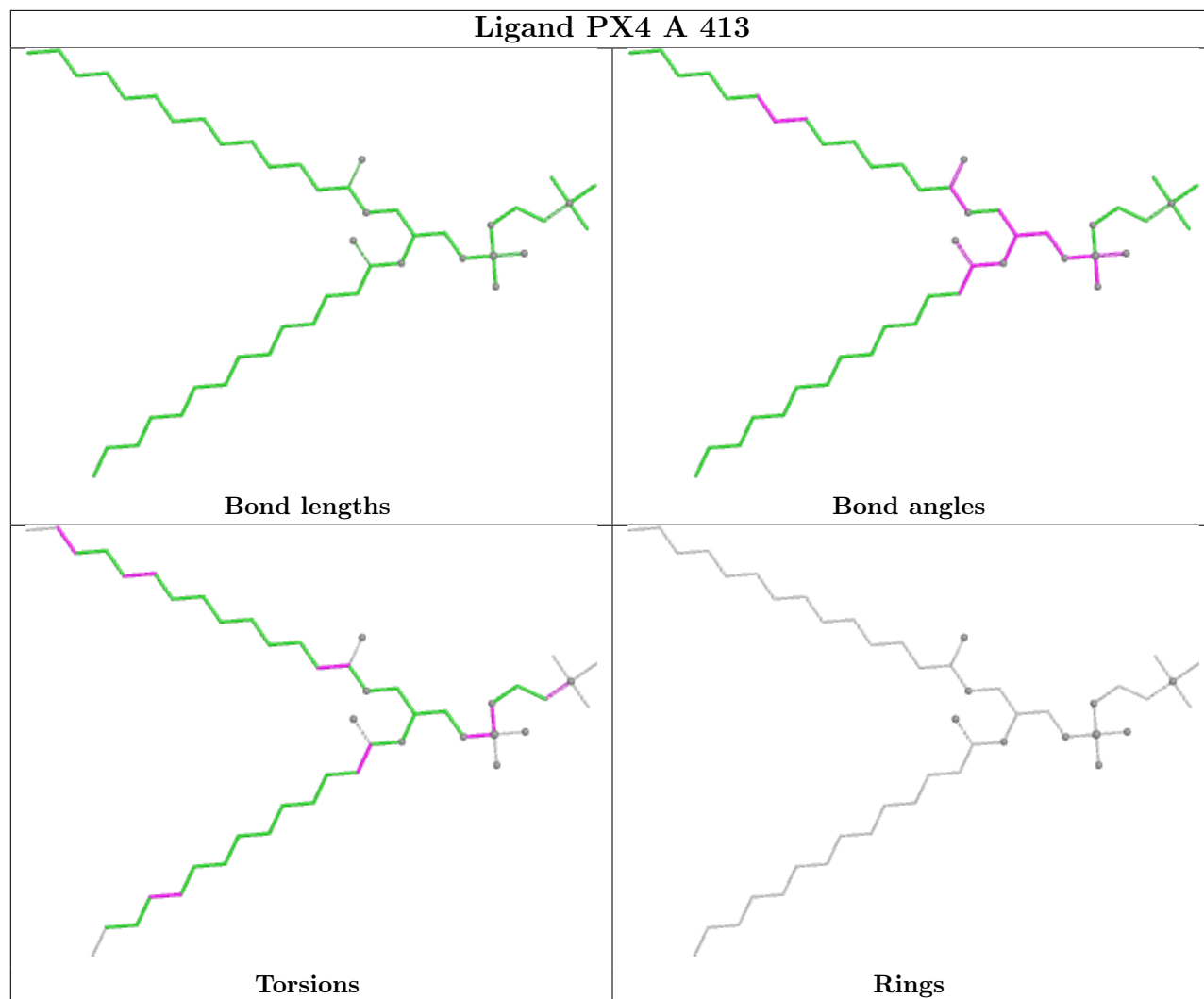
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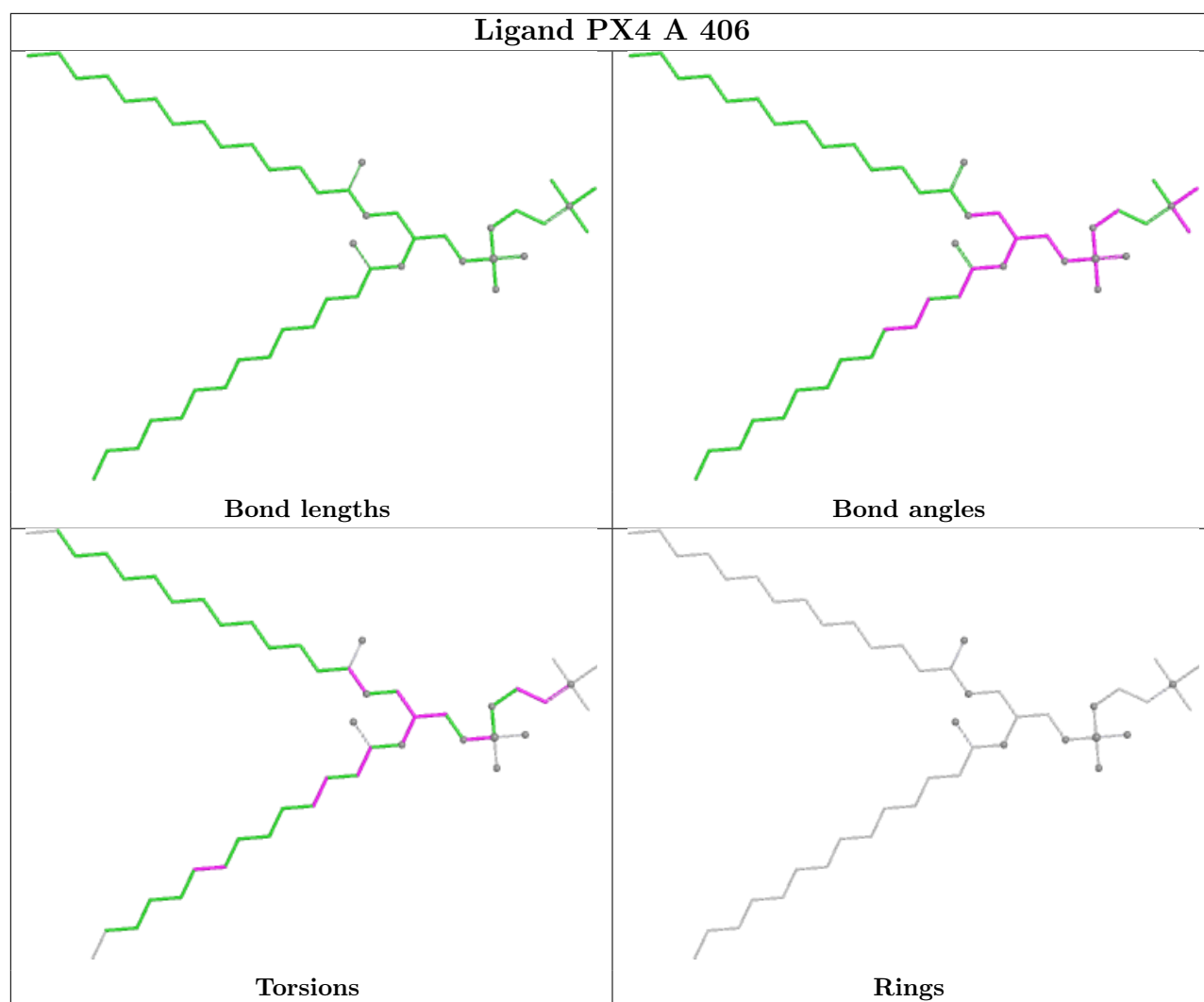


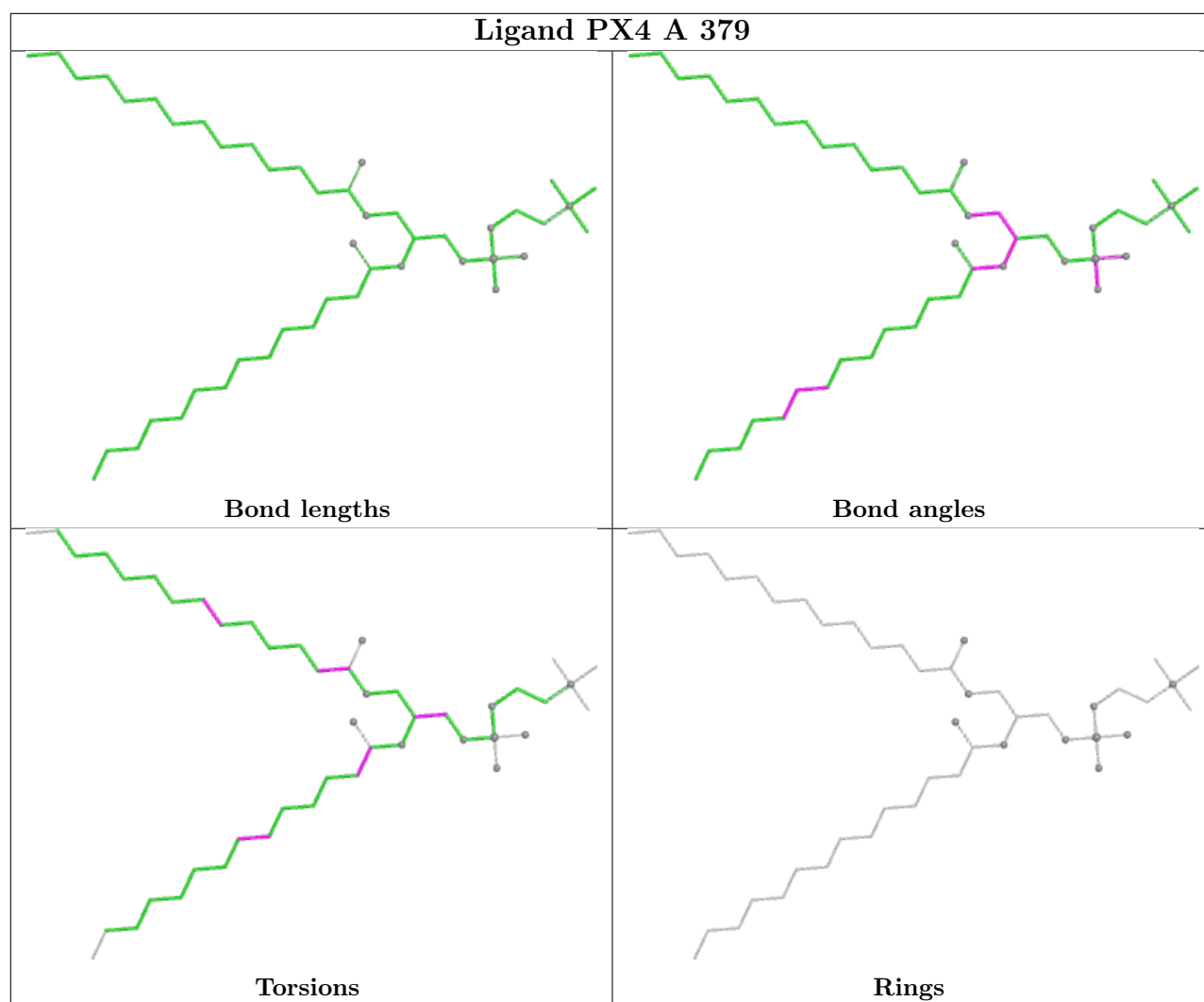


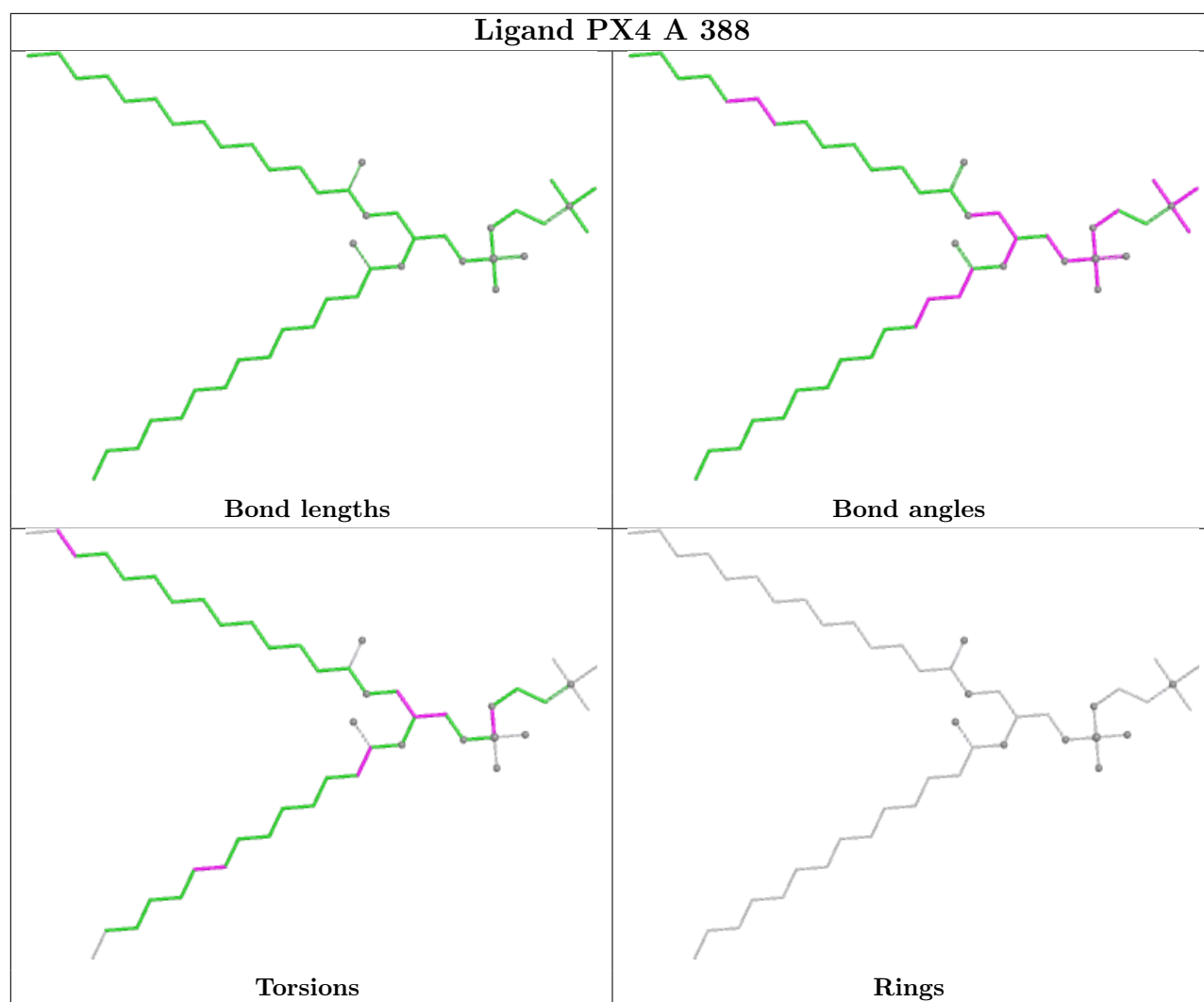


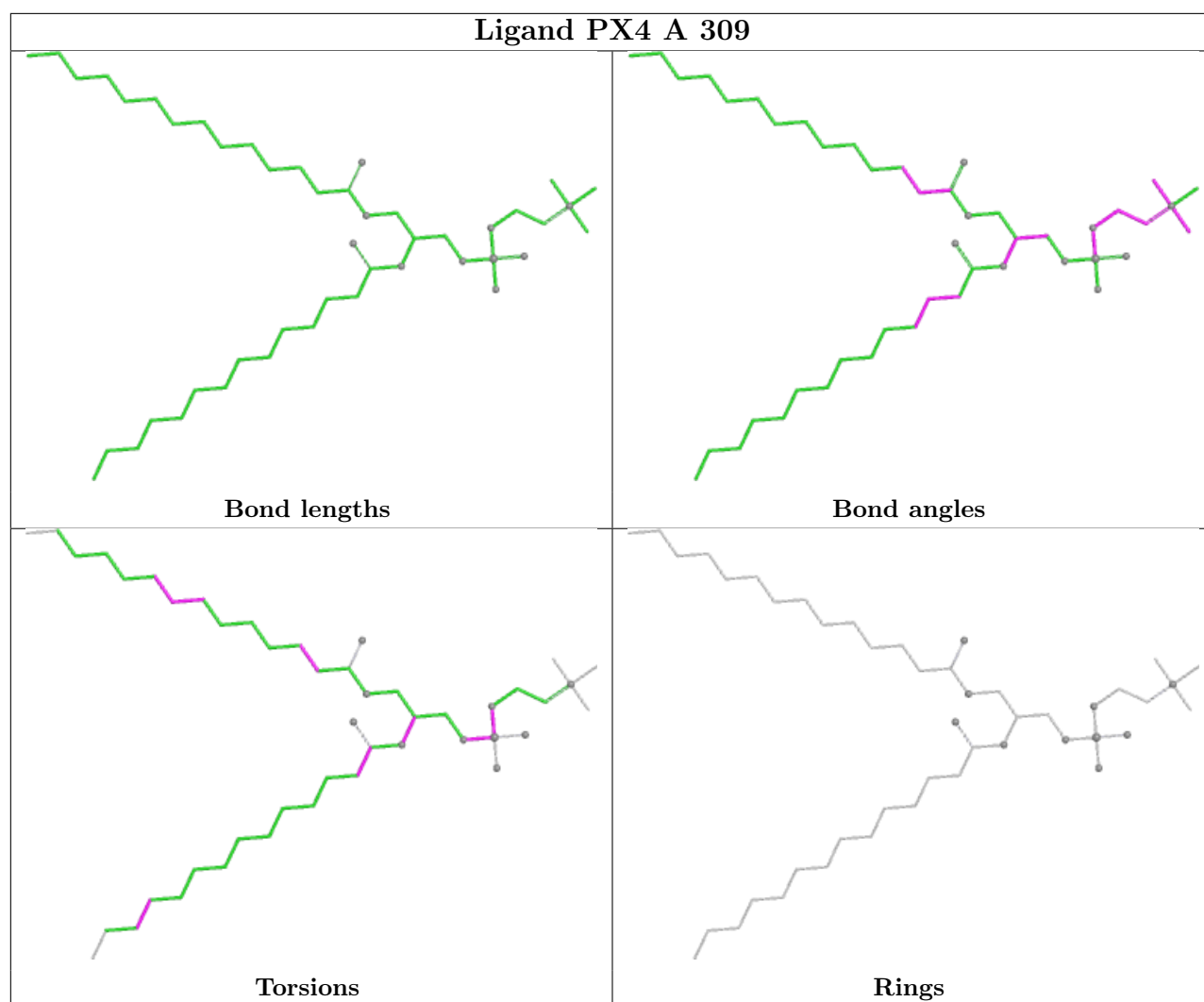
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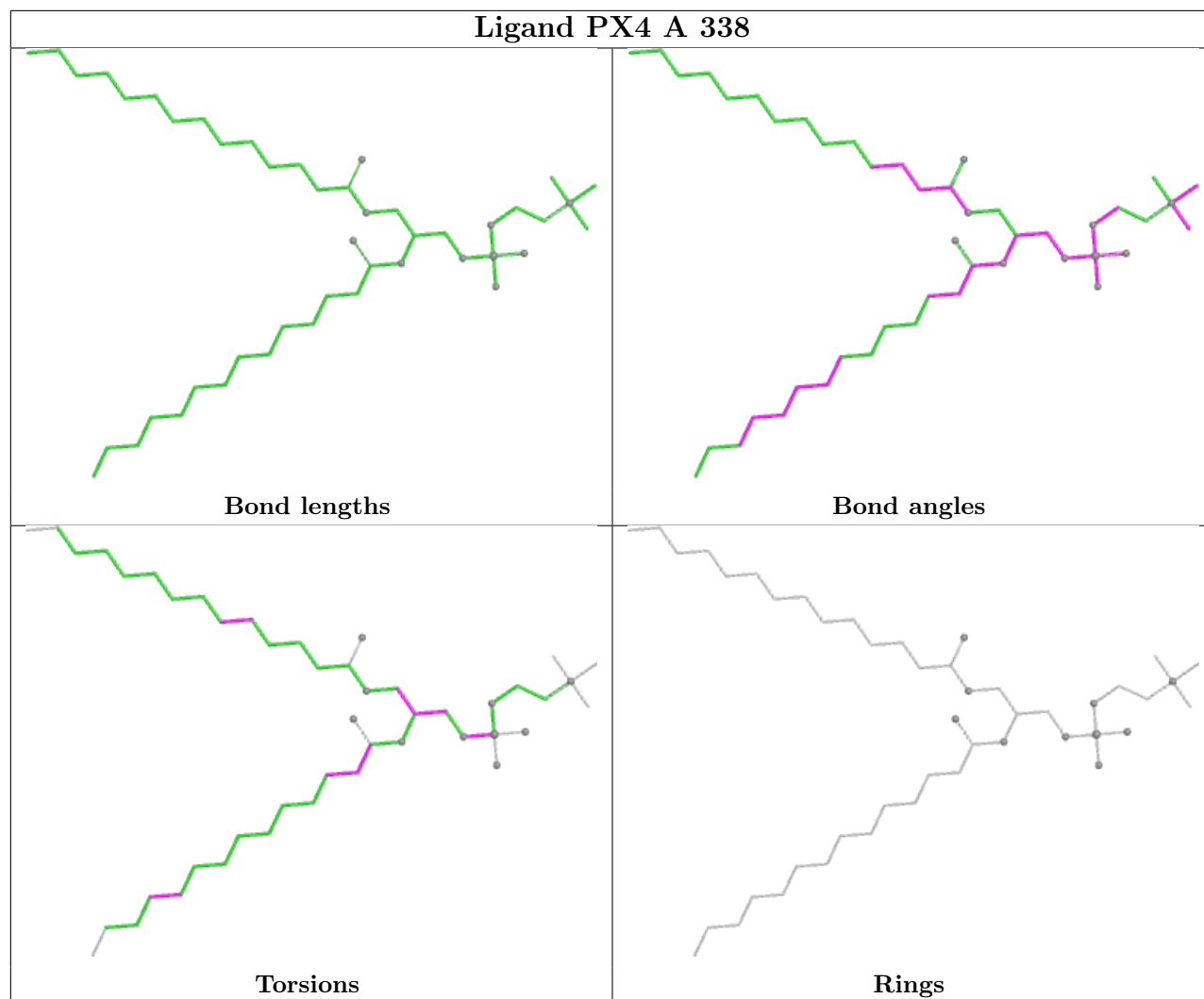




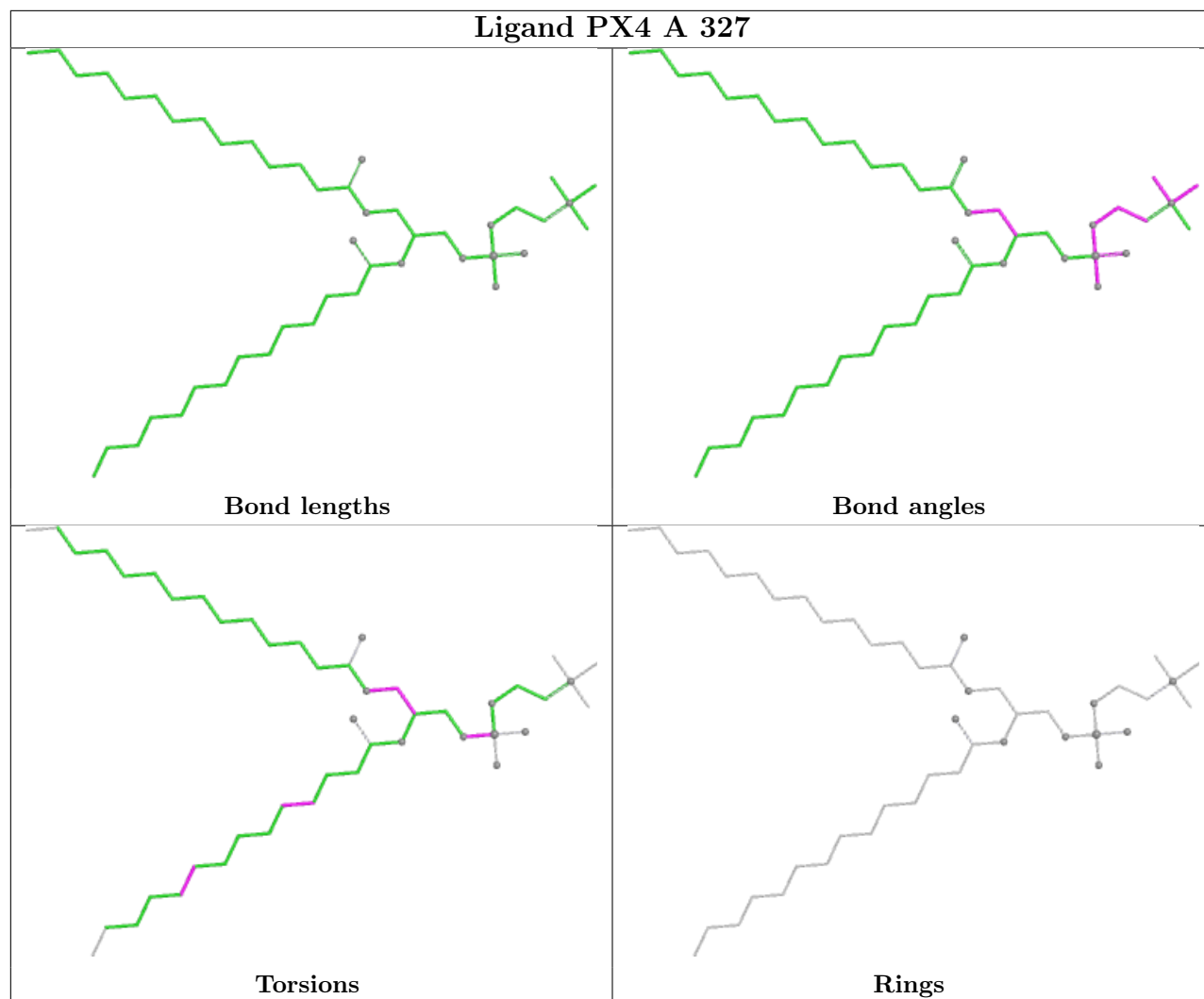




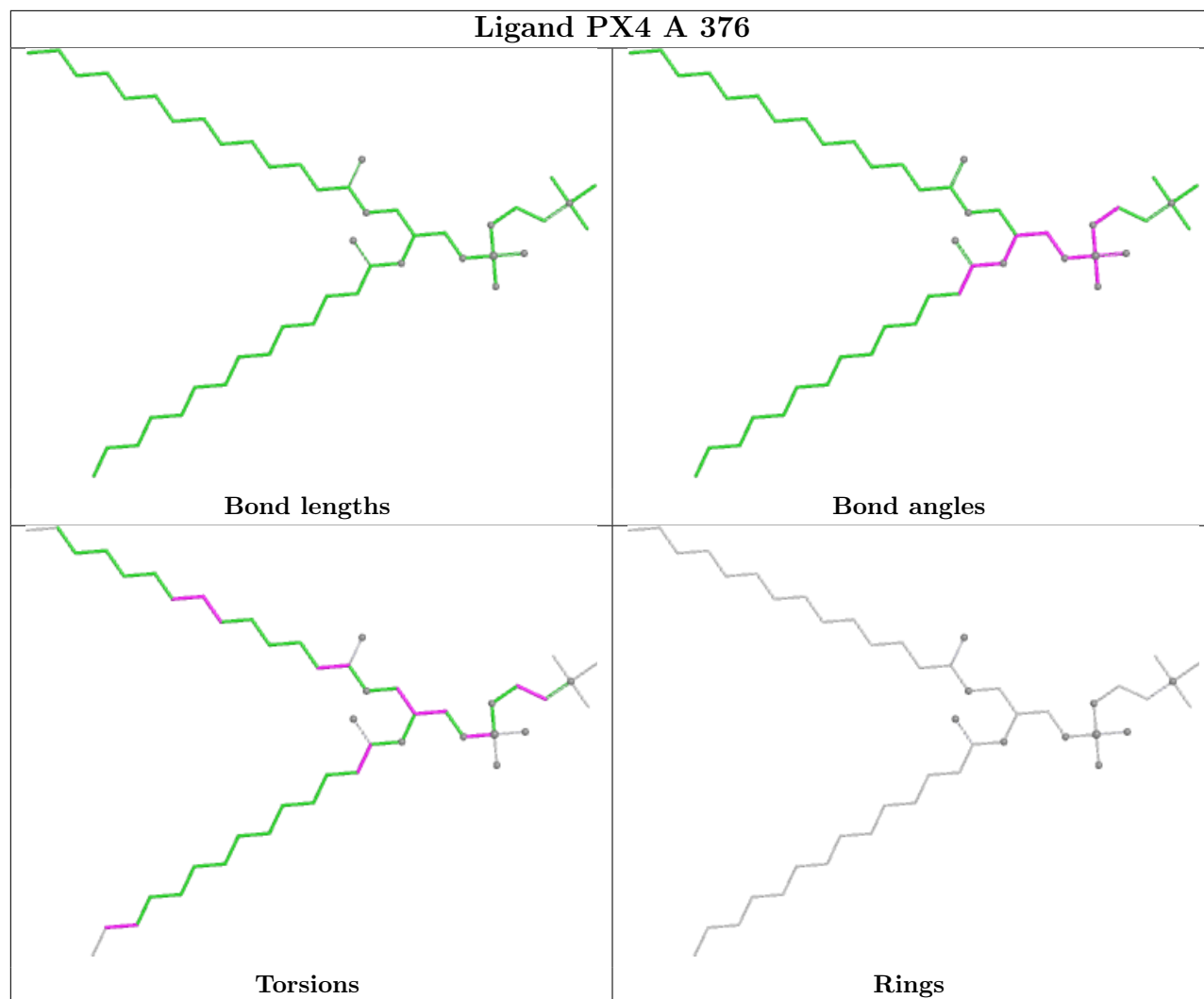
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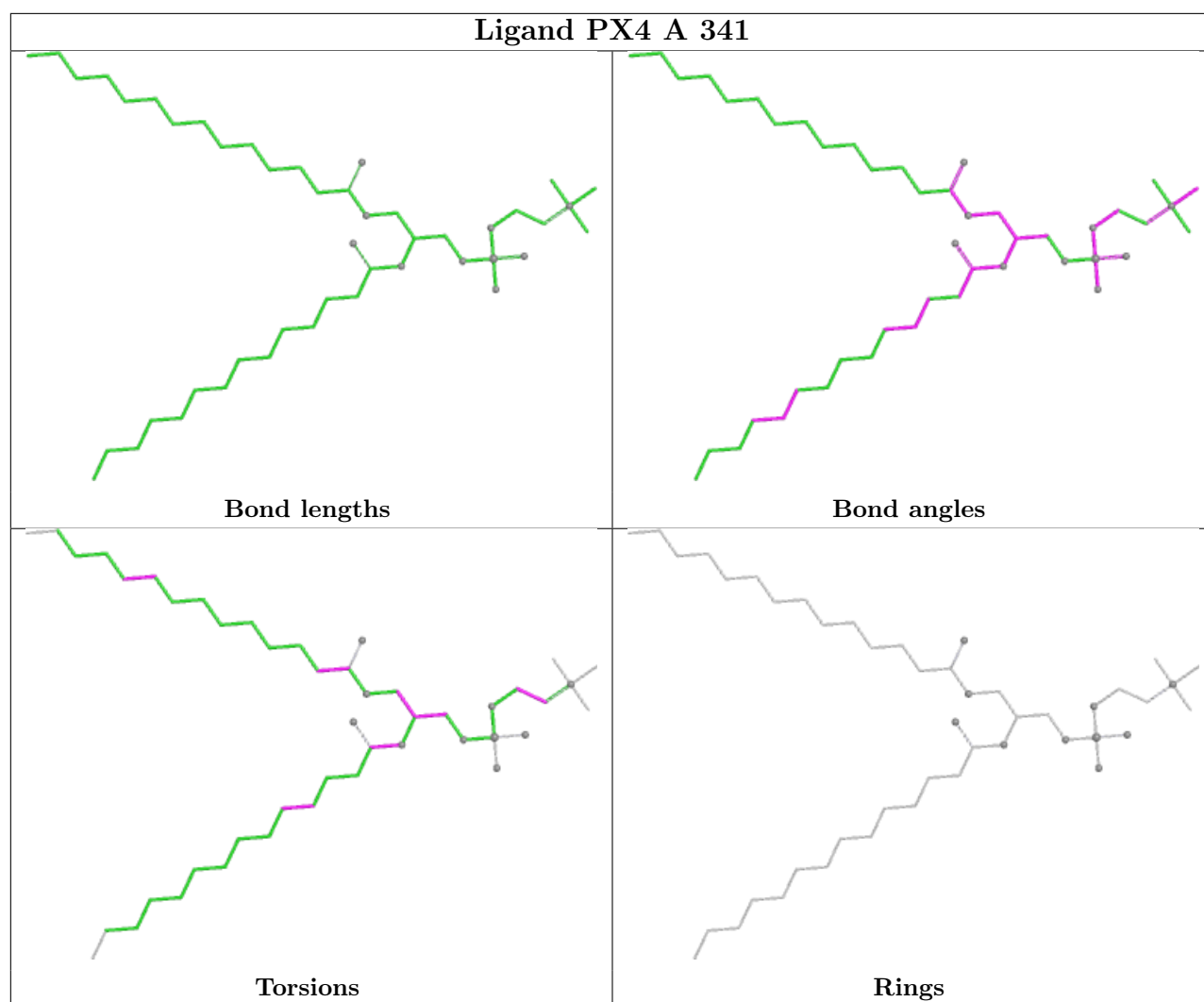


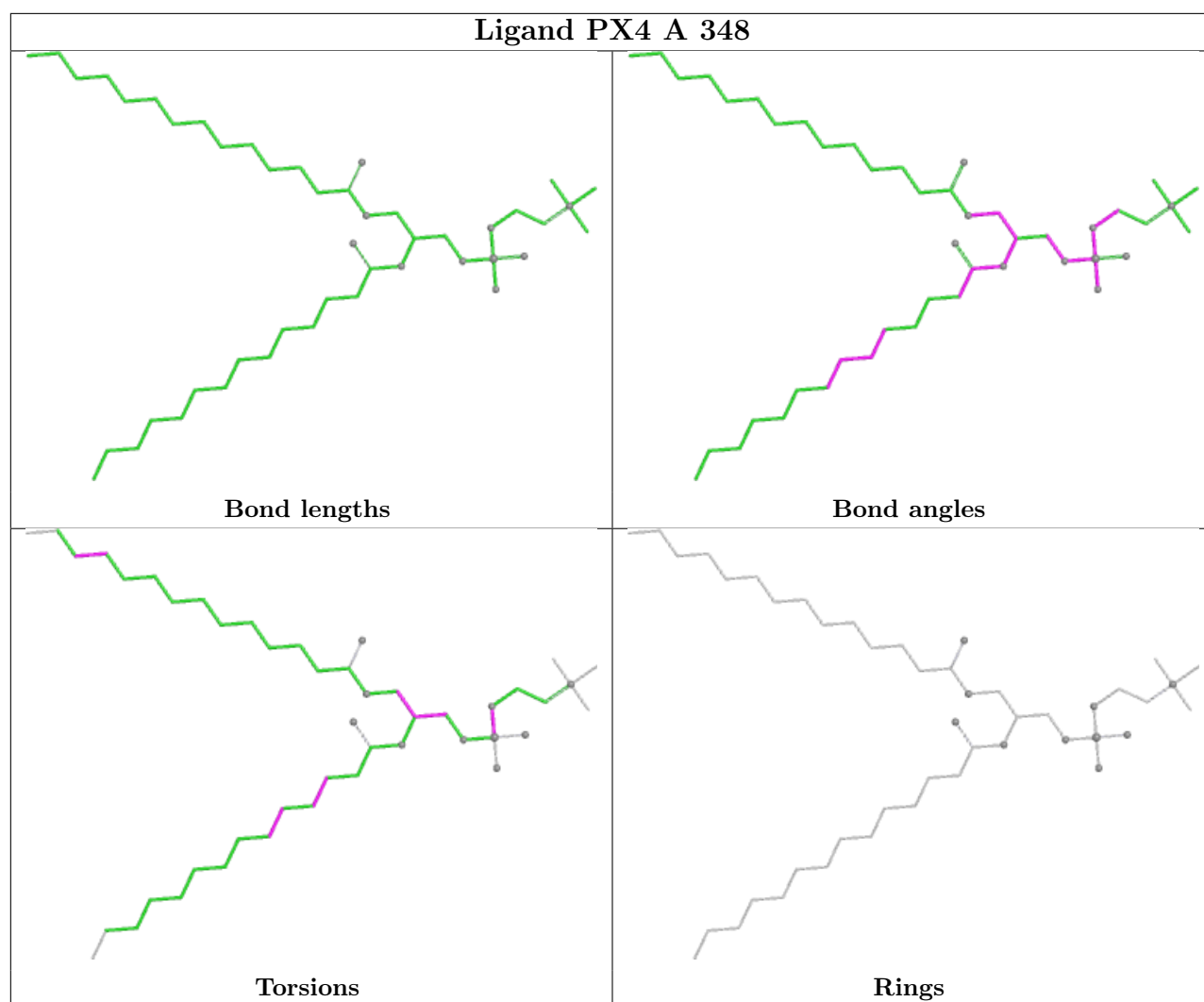
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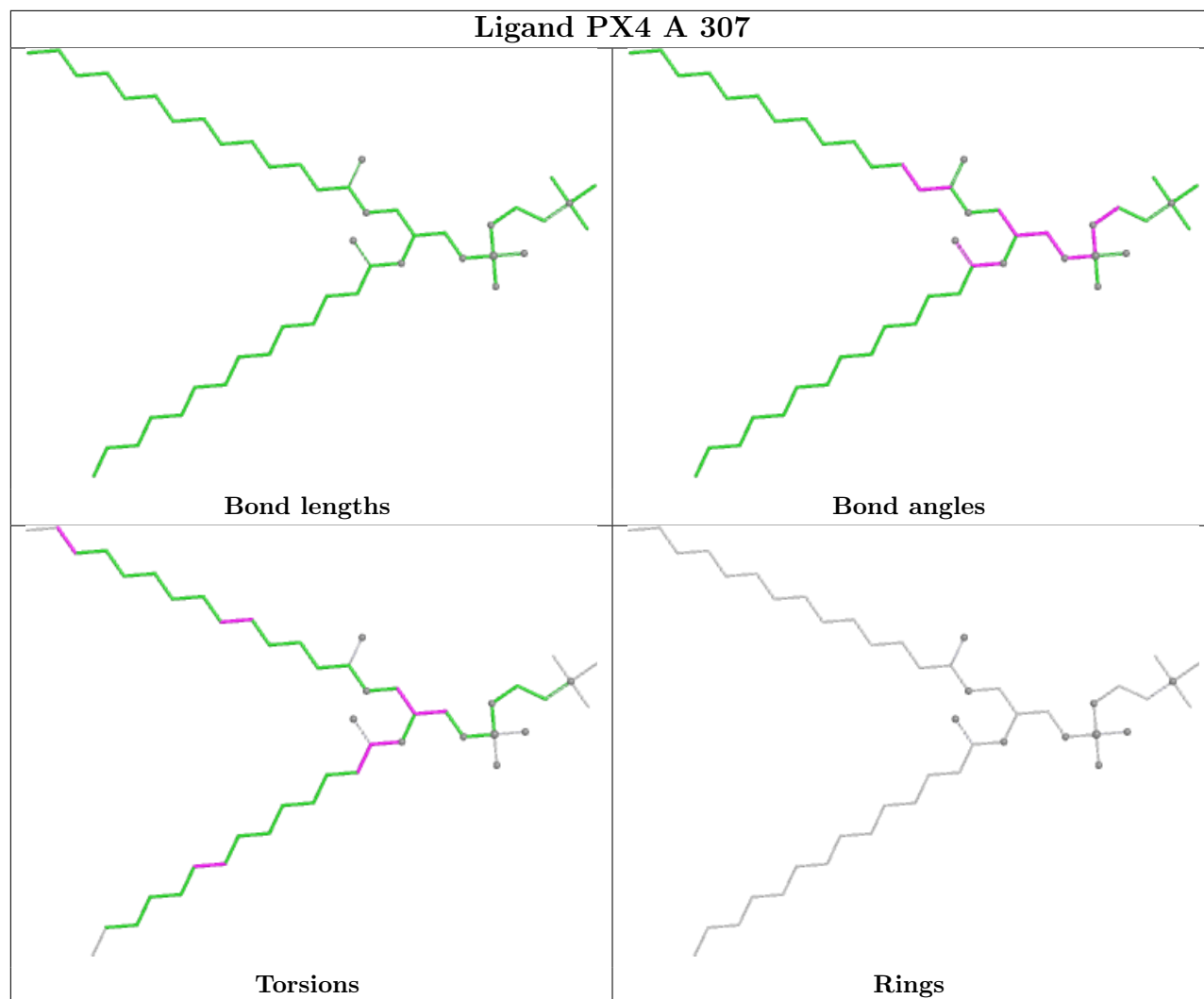
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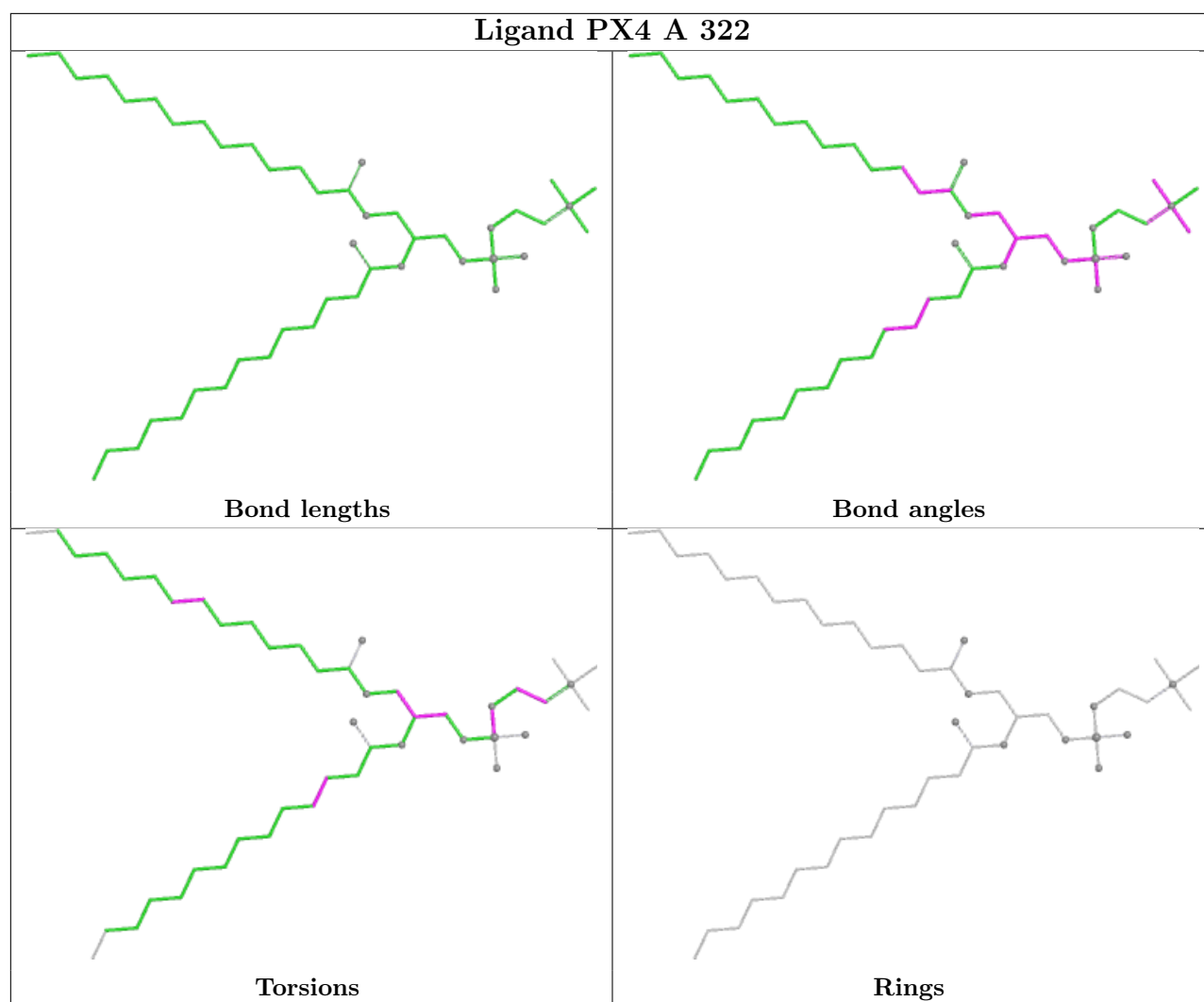


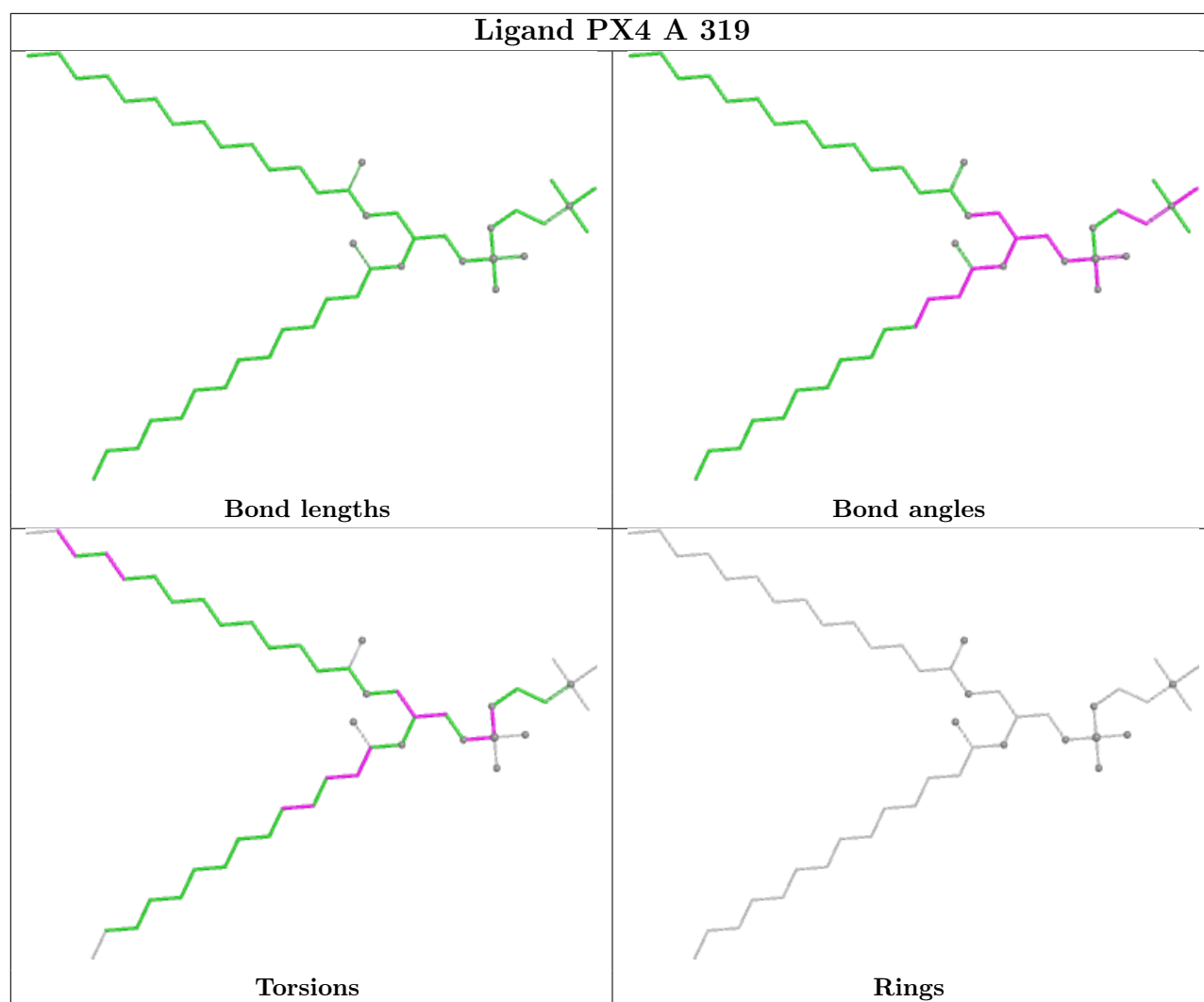


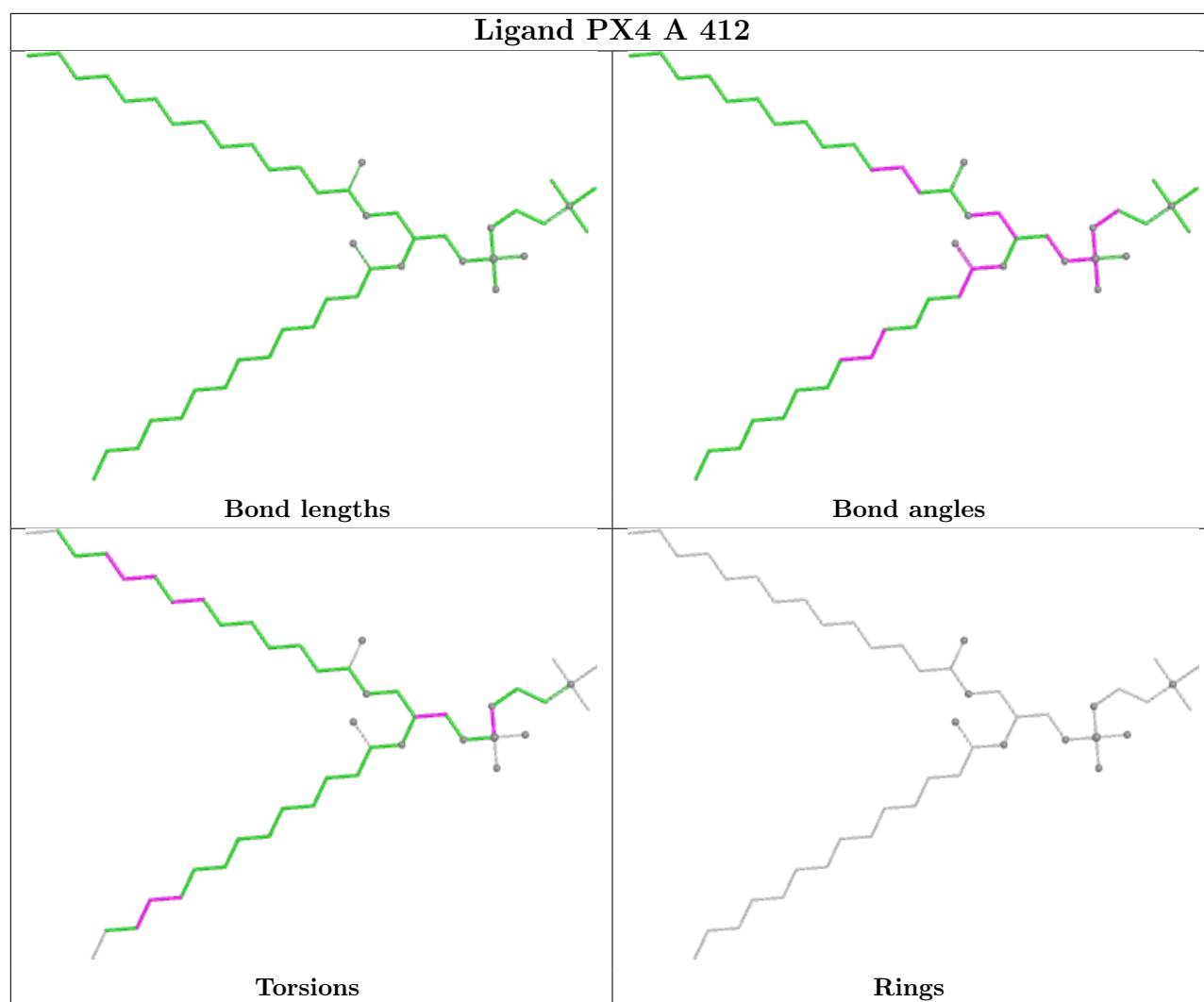


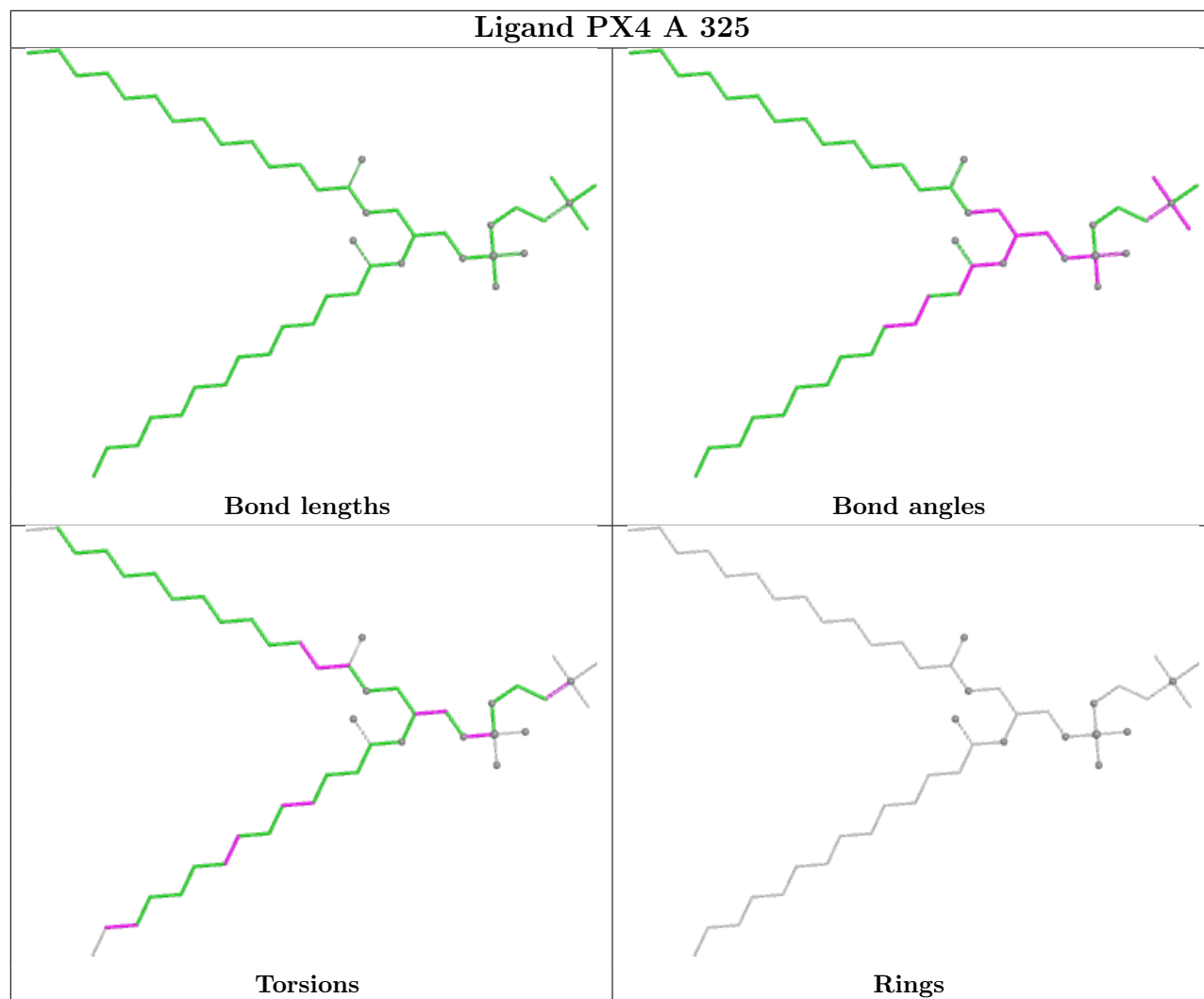
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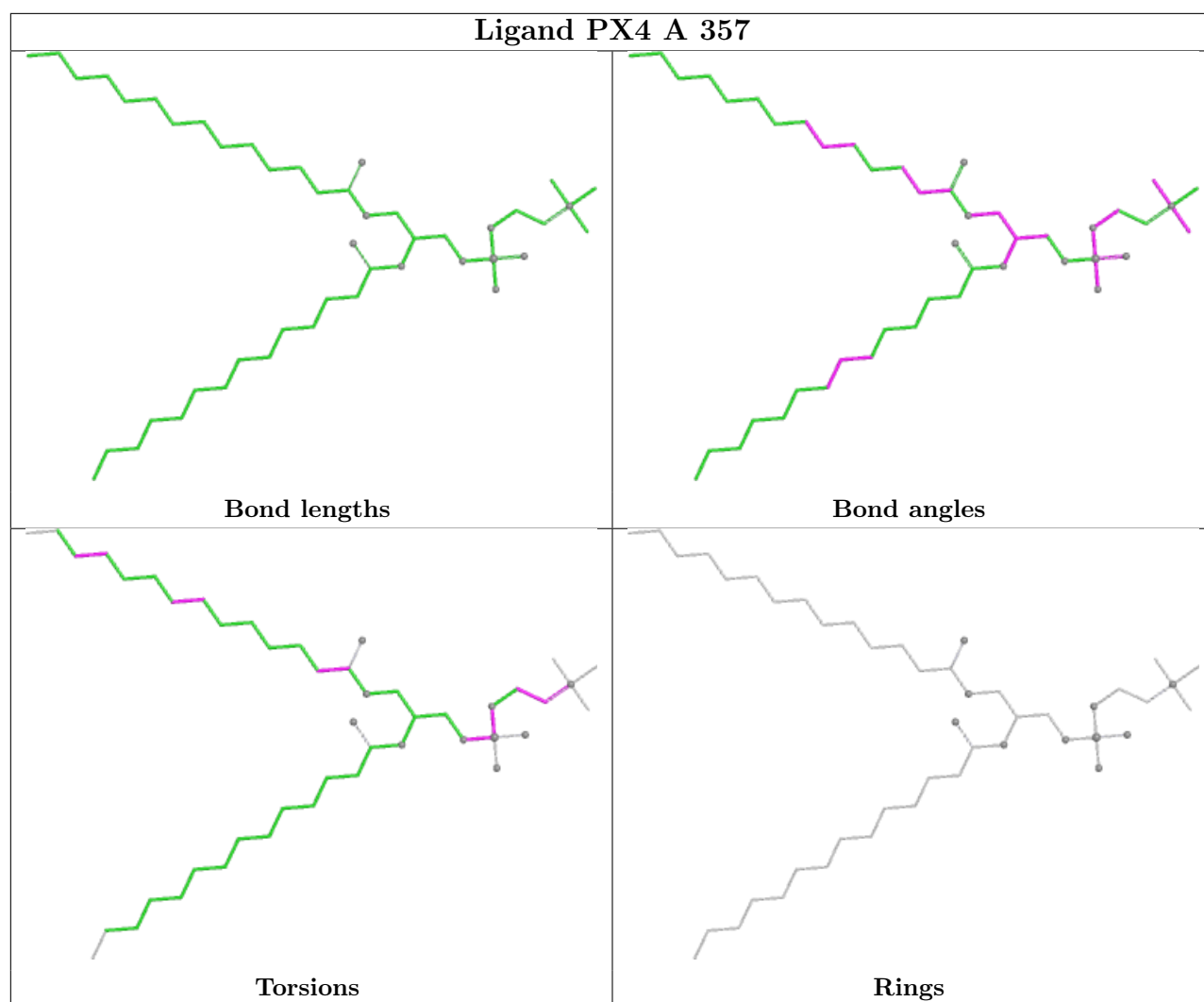


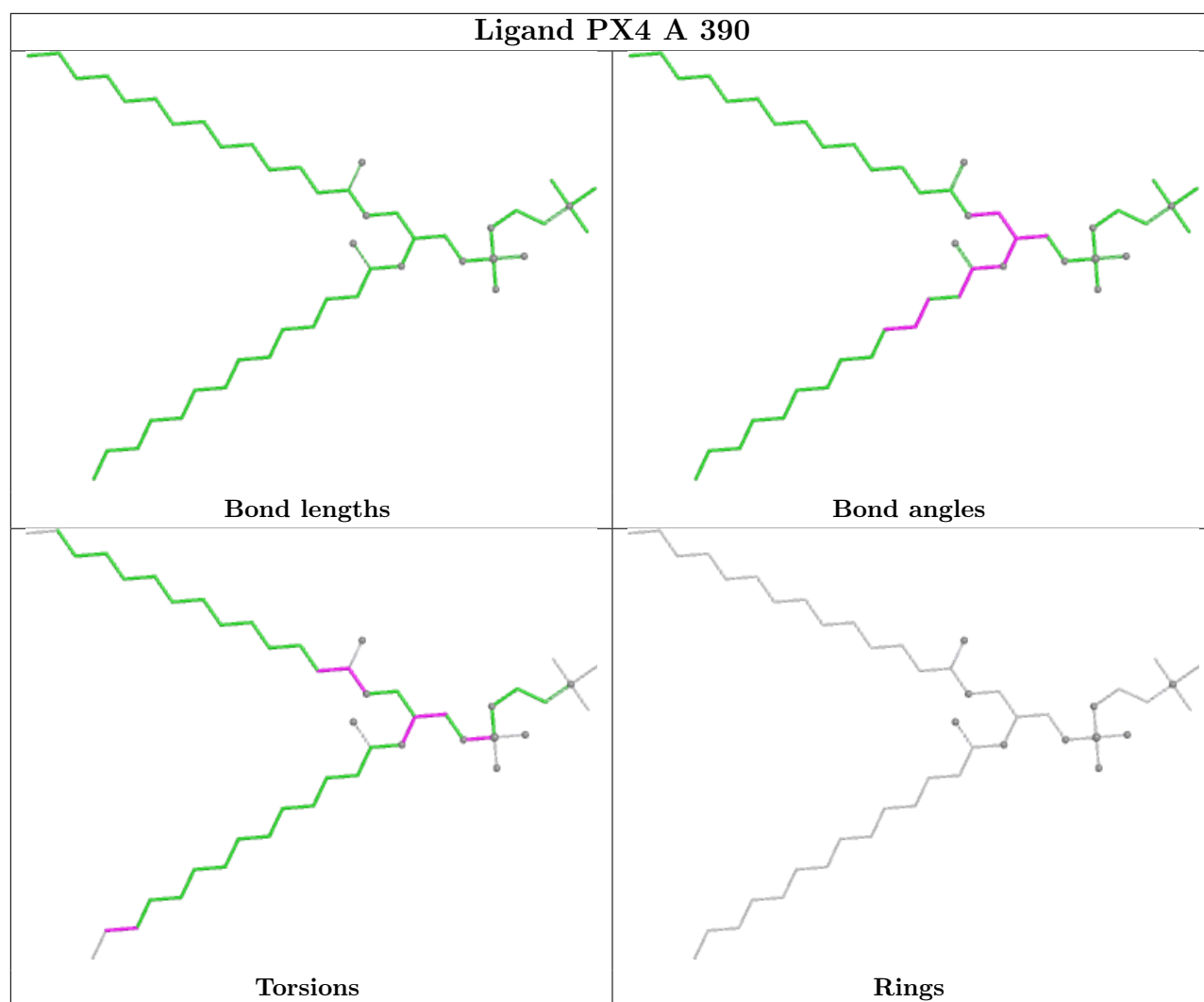


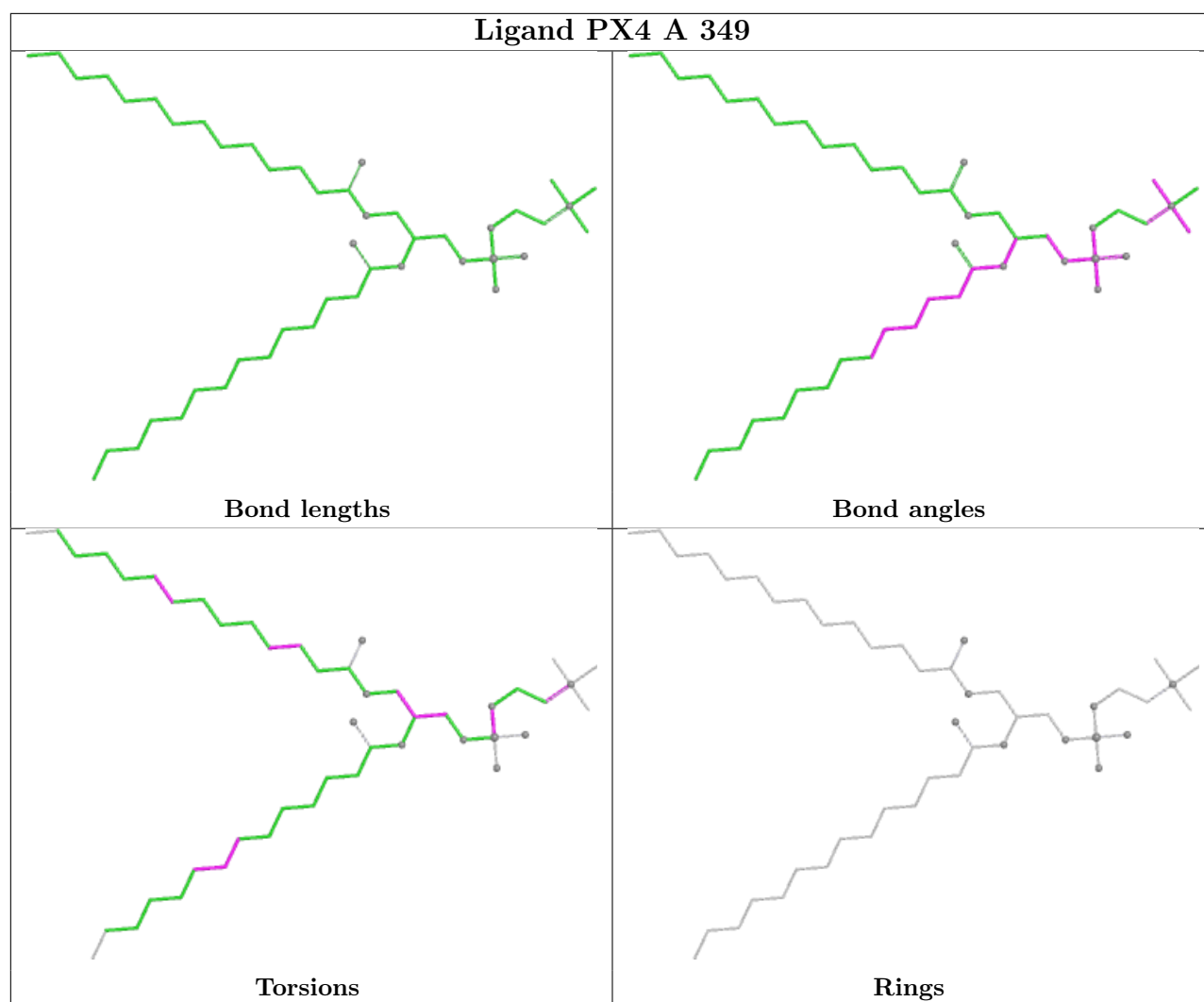




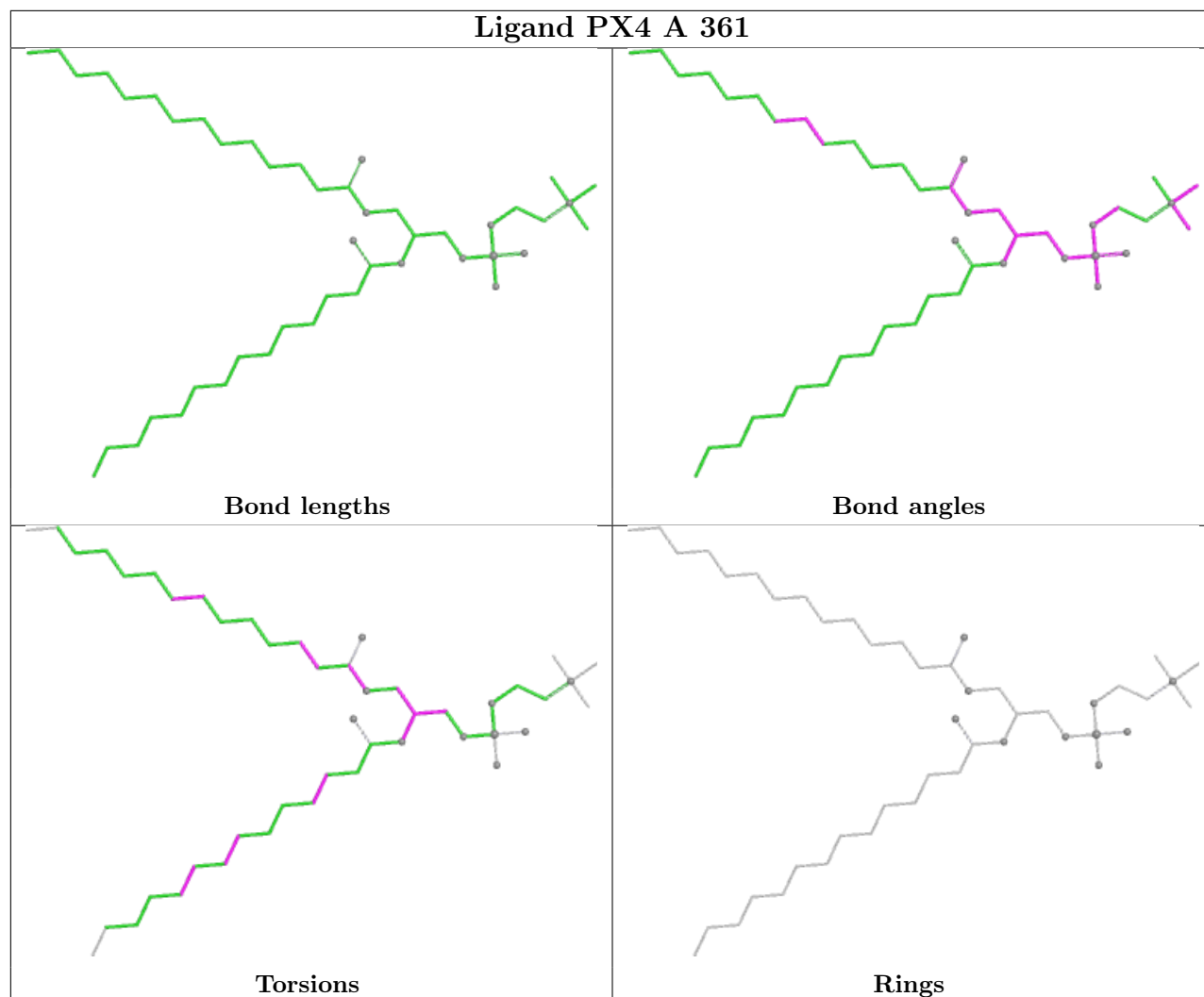




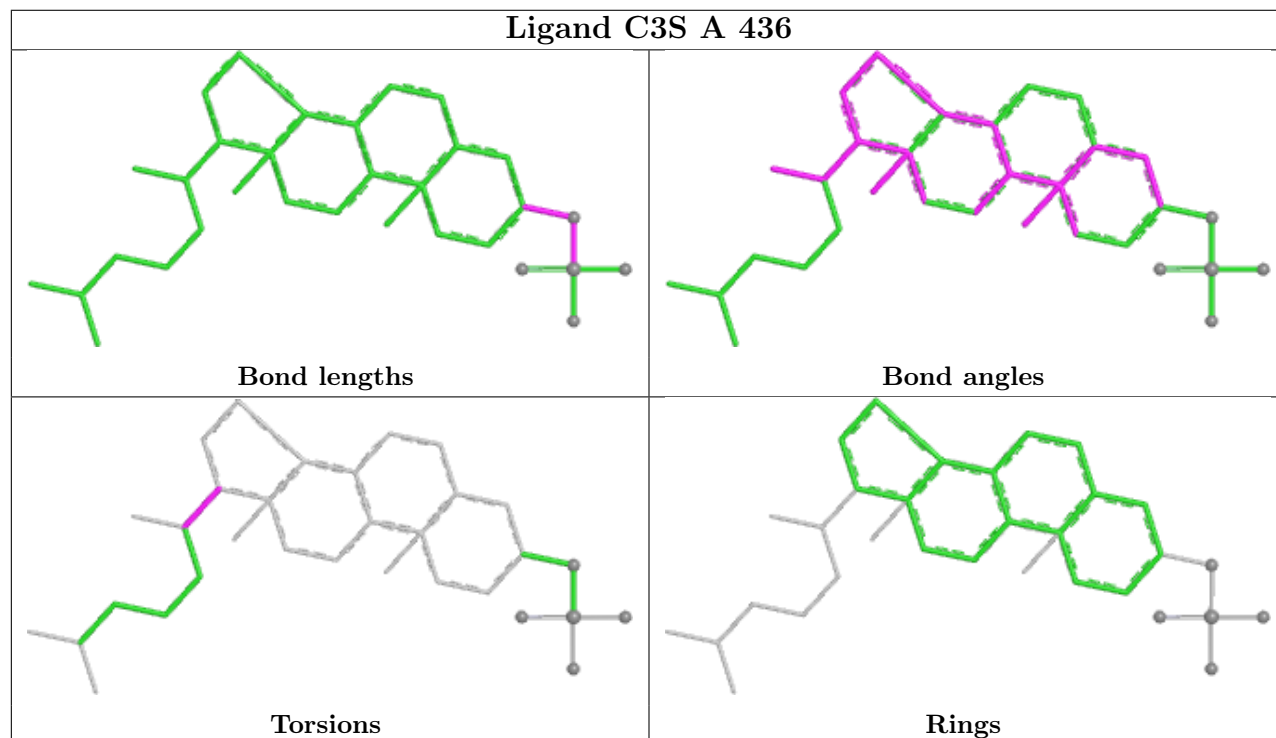




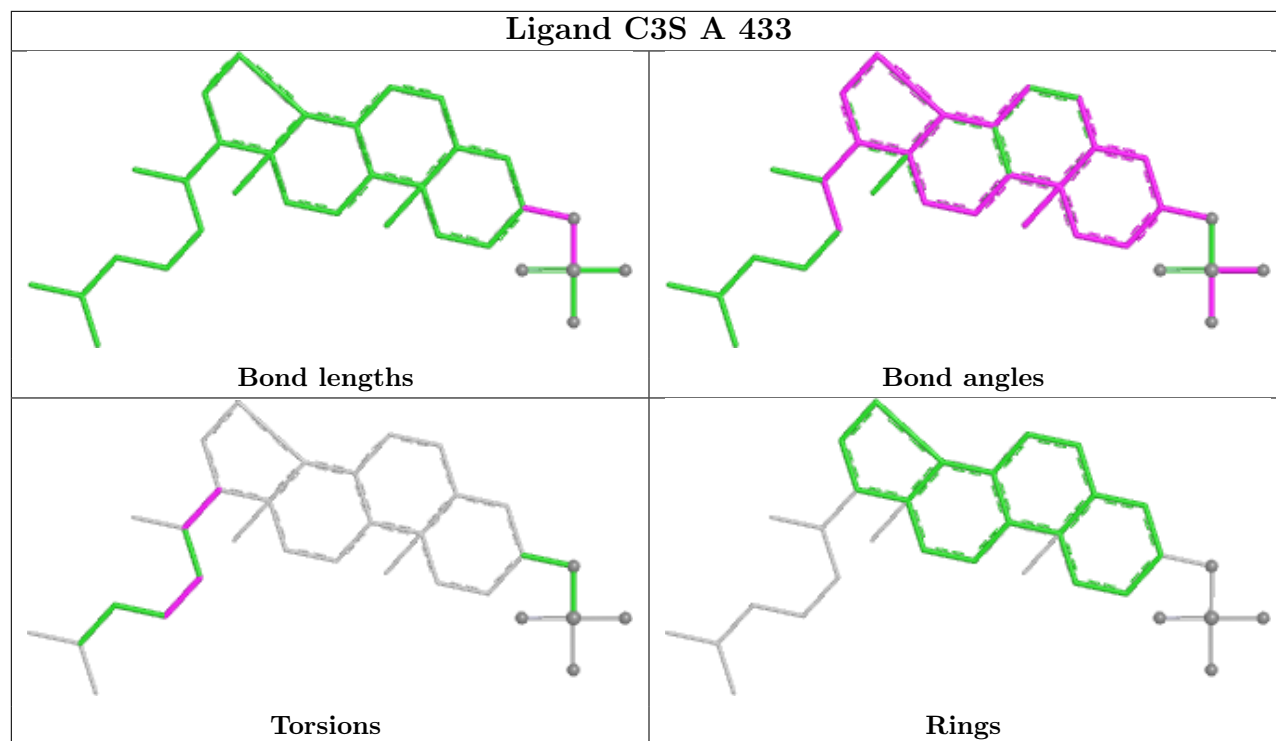
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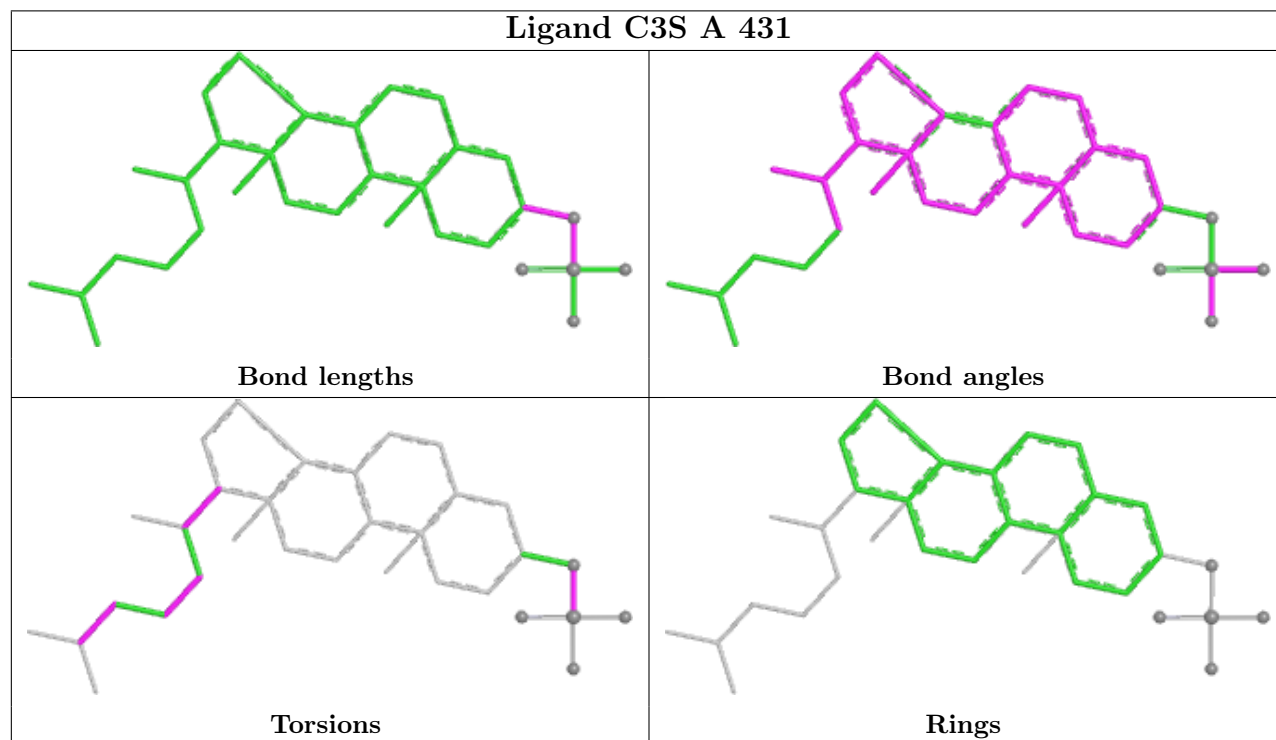
Ligand C3S A 436

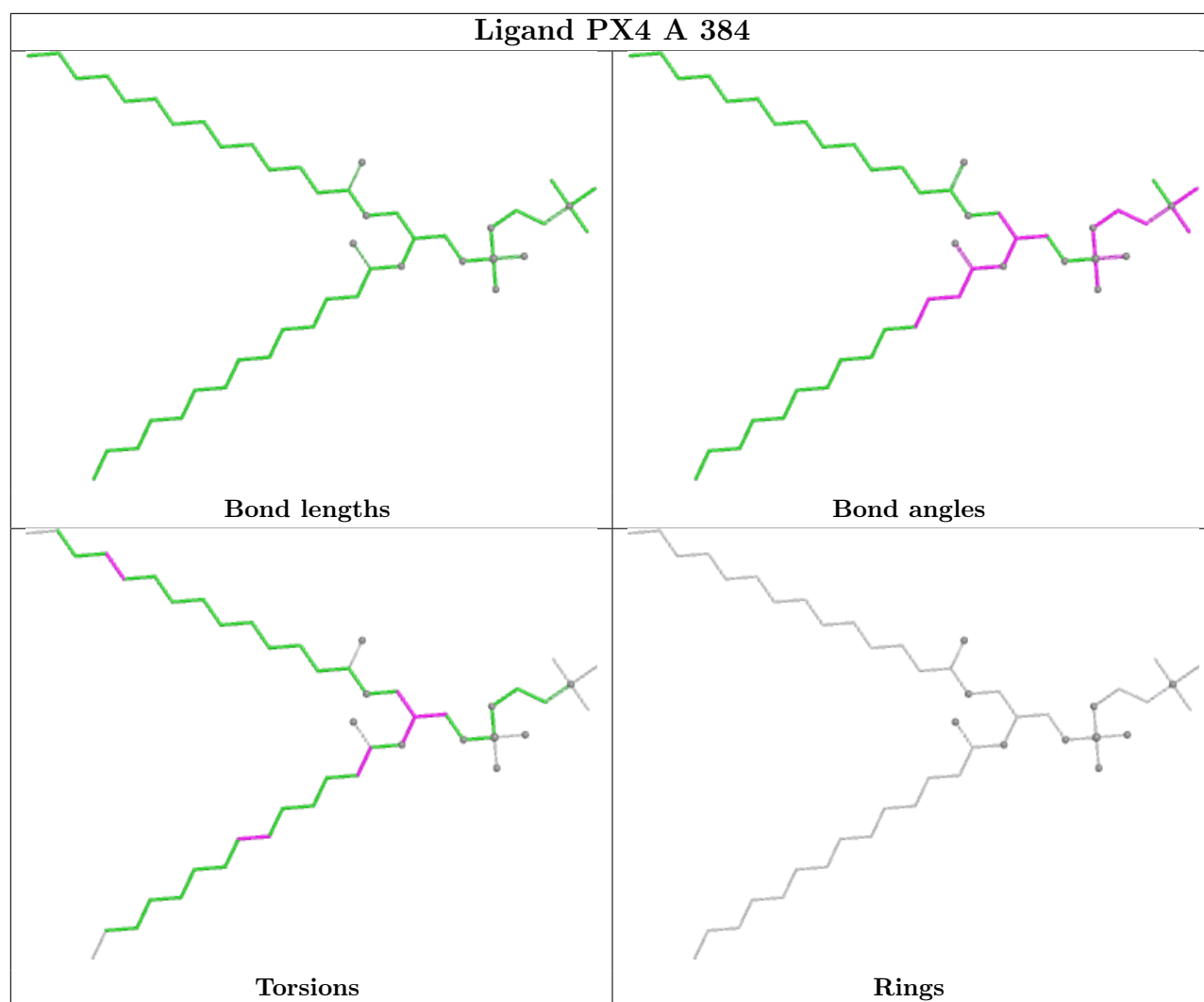


Ligand C3S A 433



Ligand C3S A 431





6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 25% for the well-defined parts and 24% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	797
Number of shifts mapped to atoms	797
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 [i](#)

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	188	0.12 ± 0.31	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 25%, i.e. 785 atoms were assigned a chemical shift out of a possible 3158. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	428/1186 (36%)	244/487 (50%)	0/474 (0%)	184/225 (82%)
Sidechain	344/1657 (21%)	295/1076 (27%)	45/517 (9%)	4/64 (6%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	13/315 (4%)	9/156 (6%)	0/146 (0%)	4/13 (31%)
Overall	785/3158 (25%)	548/1719 (32%)	45/1137 (4%)	192/302 (64%)

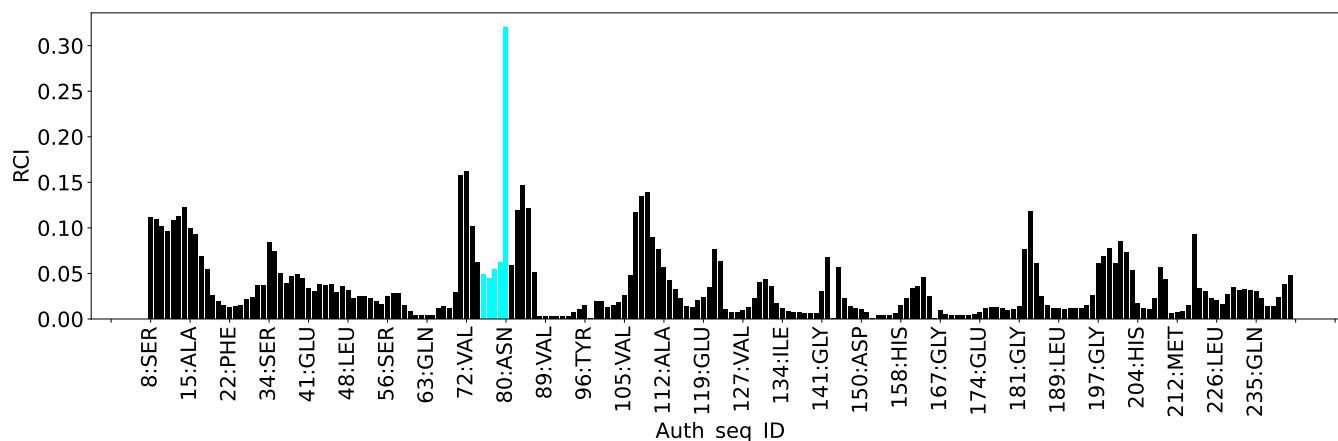
7.1.4 Statistically unusual chemical shifts [i](#)

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:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1188
Intra-residue ($ i-j =0$)	220
Sequential ($ i-j =1$)	340
Medium range ($ i-j >1$ and $ i-j <5$)	186
Long range ($ i-j \geq 5$)	305
Inter-chain	124
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	3.1
Number of long range restraints per residue ¹	0.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	18.4	0.2
0.2-0.5 (Medium)	48.8	0.5
>0.5 (Large)	145.3	38.77

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

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

9 Distance violation analysis ⓘ

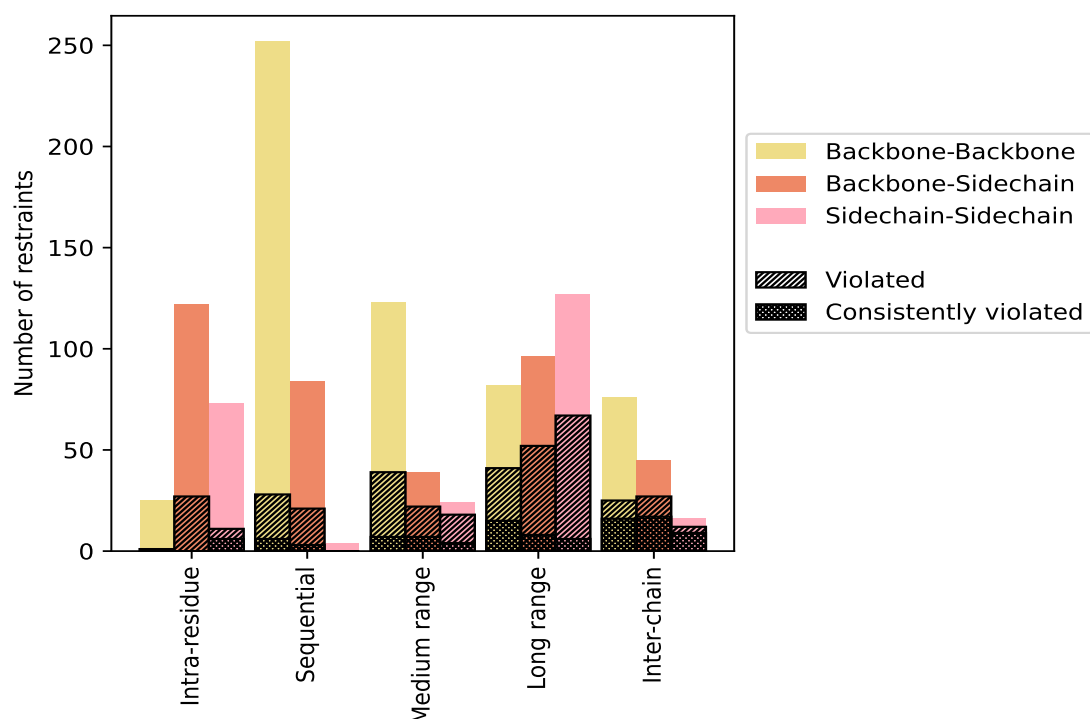
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	220	18.5	39	17.7	3.3	6	2.7	0.5
Backbone-Backbone	25	2.1	1	4.0	0.1	0	0.0	0.0
Backbone-Sidechain	122	10.3	27	22.1	2.3	0	0.0	0.0
Sidechain-Sidechain	73	6.1	11	15.1	0.9	6	8.2	0.5
Sequential ($i-j =1$)	340	28.6	49	14.4	4.1	9	2.6	0.8
Backbone-Backbone	252	21.2	28	11.1	2.4	6	2.4	0.5
Backbone-Sidechain	84	7.1	21	25.0	1.8	3	3.6	0.3
Sidechain-Sidechain	4	0.3	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	186	15.7	79	42.5	6.6	18	9.7	1.5
Backbone-Backbone	123	10.4	39	31.7	3.3	7	5.7	0.6
Backbone-Sidechain	39	3.3	22	56.4	1.9	7	17.9	0.6
Sidechain-Sidechain	24	2.0	18	75.0	1.5	4	16.7	0.3
Long range ($i-j \geq 5$)	305	25.7	160	52.5	13.5	29	9.5	2.4
Backbone-Backbone	82	6.9	41	50.0	3.5	15	18.3	1.3
Backbone-Sidechain	96	8.1	52	54.2	4.4	8	8.3	0.7
Sidechain-Sidechain	127	10.7	67	52.8	5.6	6	4.7	0.5
Inter-chain	124	10.4	53	42.7	4.5	34	27.4	2.9
Backbone-Backbone	76	6.4	25	32.9	2.1	16	21.1	1.3
Backbone-Sidechain	45	3.8	27	60.0	2.3	17	37.8	1.4
Sidechain-Sidechain	3	0.3	1	33.3	0.1	1	33.3	0.1
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1188	100.0	391	32.9	32.9	104	8.8	8.8
Backbone-Backbone	558	47.0	134	24.0	11.3	44	7.9	3.7
Backbone-Sidechain	386	32.5	149	38.6	12.5	35	9.1	2.9
Sidechain-Sidechain	244	20.5	108	44.3	9.1	25	10.2	2.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	17	17	36	92	53	215	4.16	36.22	6.47	1.35
2	17	20	40	82	53	212	4.09	36.18	6.48	1.0
3	16	18	33	87	53	207	4.13	34.66	6.4	1.25
4	15	24	34	103	51	227	3.59	30.06	5.86	1.2
5	10	17	39	90	52	208	4.09	38.15	6.56	1.25
6	13	20	40	84	52	209	4.14	36.54	6.46	1.28
7	16	16	43	103	57	235	3.94	34.73	6.23	1.36
8	11	23	38	80	52	204	3.9	31.8	6.24	1.02
9	13	20	43	89	54	219	3.95	36.82	6.3	1.09
10	14	18	40	80	58	210	4.38	38.77	6.81	1.09

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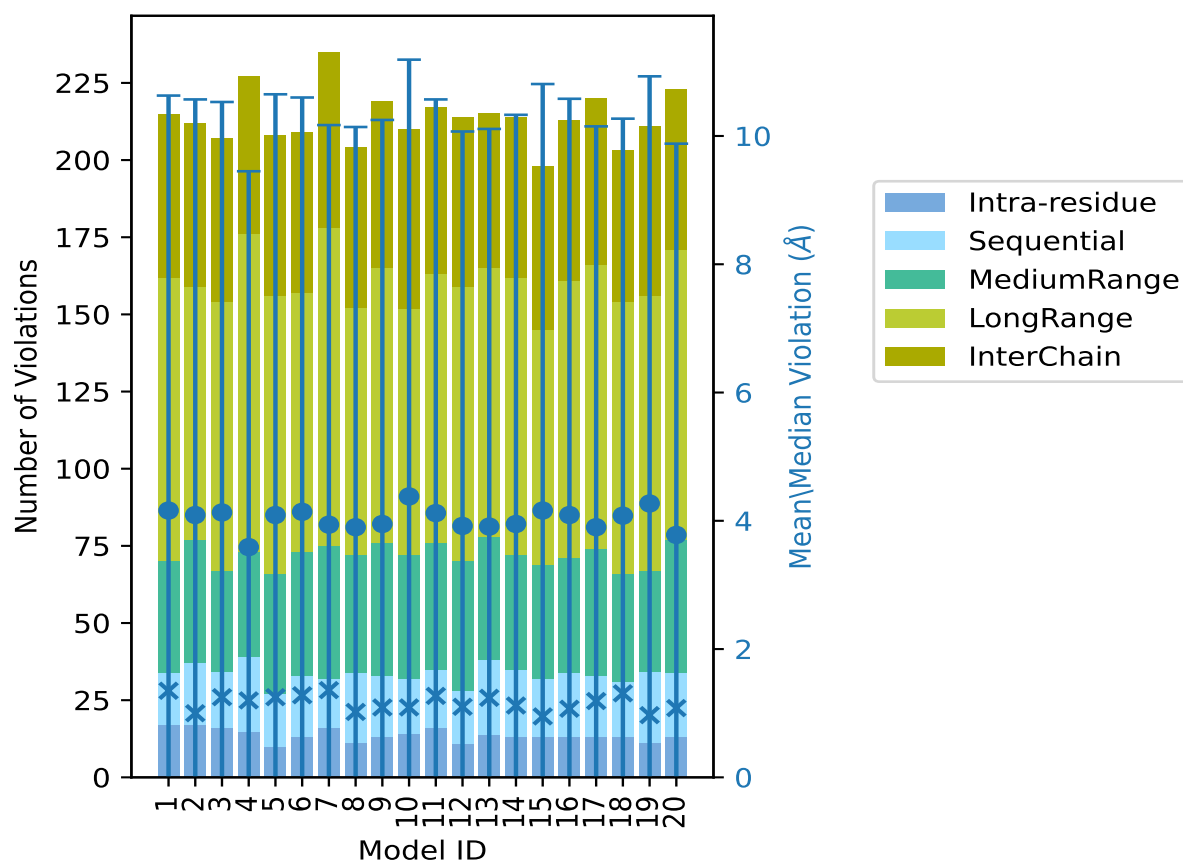
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	16	19	41	87	54	217	4.12	38.69	6.45	1.27
12	11	17	42	89	55	214	3.92	32.01	6.15	1.1
13	14	24	40	87	50	215	3.91	33.78	6.2	1.24
14	13	22	37	90	52	214	3.95	35.76	6.38	1.12
15	13	19	37	76	53	198	4.16	36.28	6.65	0.95
16	13	21	37	90	52	213	4.09	34.96	6.49	1.07
17	13	20	41	92	54	220	3.9	35.35	6.25	1.19
18	13	18	35	88	49	203	4.08	32.38	6.19	1.31
19	11	23	33	89	55	211	4.27	37.25	6.66	0.97
20	13	21	43	94	52	223	3.78	31.81	6.1	1.08

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

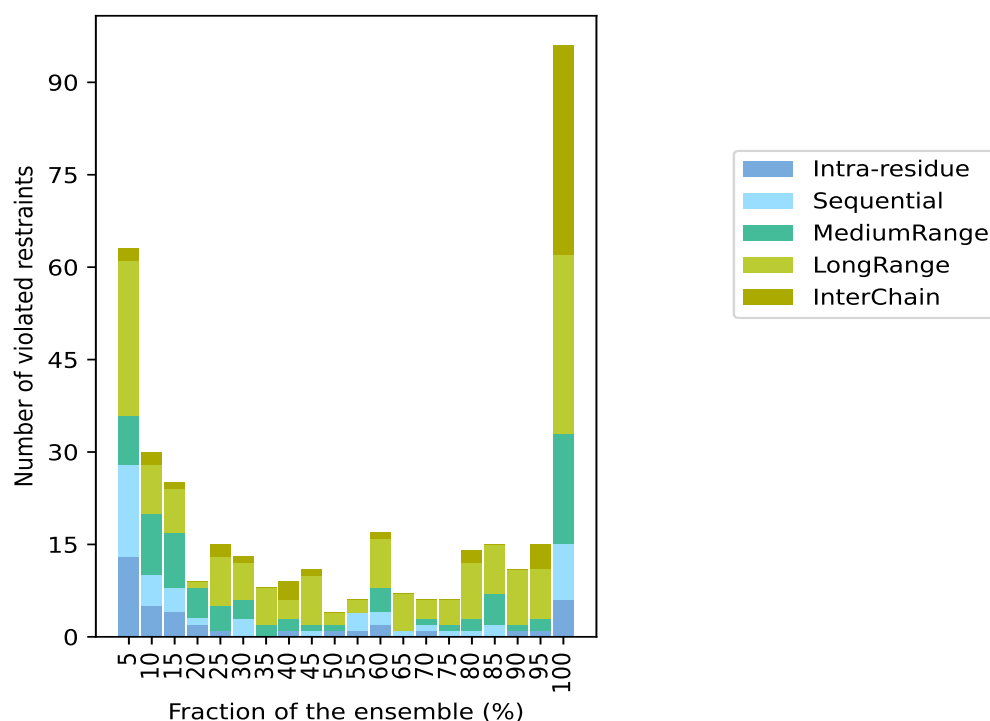
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 795(IR:181, SQ:291, MR:107, LR:145, IC:71) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
13	15	8	25	2	63	1	5.0
5	5	10	8	2	30	2	10.0
4	4	9	7	1	25	3	15.0
2	1	5	1	0	9	4	20.0
1	0	4	8	2	15	5	25.0
0	3	3	6	1	13	6	30.0
0	0	2	6	0	8	7	35.0
1	0	2	3	3	9	8	40.0
0	1	1	8	1	11	9	45.0
1	0	1	2	0	4	10	50.0
1	3	0	2	0	6	11	55.0
2	2	4	8	1	17	12	60.0
0	1	0	6	0	7	13	65.0
1	1	1	3	0	6	14	70.0
0	1	1	4	0	6	15	75.0
0	1	2	9	2	14	16	80.0
0	2	5	8	0	15	17	85.0
1	0	1	9	0	11	18	90.0
1	0	2	8	4	15	19	95.0
6	9	18	29	34	96	20	100.0

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

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

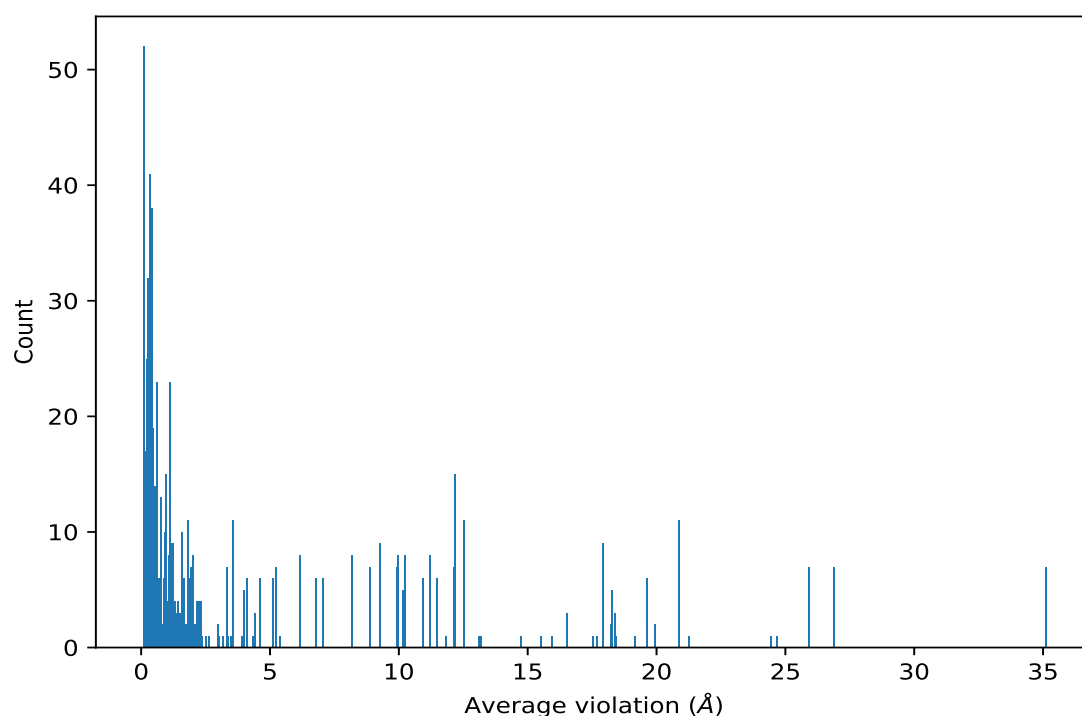
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,4)	1:33:A:ASN:H	4:320:A:PX4:C35	20	35.11	2.41	35.56
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	20	35.11	2.41	35.56
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	20	35.11	2.41	35.56
(3,4)	1:33:A:ASN:H	4:340:A:PX4:C35	20	35.11	2.41	35.56
(3,4)	1:33:A:ASN:H	4:352:A:PX4:C35	20	35.11	2.41	35.56
(3,4)	1:33:A:ASN:H	4:324:A:PX4:C35	20	35.11	2.41	35.56
(3,4)	1:33:A:ASN:H	4:309:A:PX4:C35	20	35.11	2.41	35.56
(3,5)	1:51:A:THR:H	4:338:A:PX4:C35	20	26.9	2.03	26.88
(3,5)	1:51:A:THR:H	4:322:A:PX4:C35	20	26.9	2.03	26.88
(3,5)	1:51:A:THR:H	4:307:A:PX4:C35	20	26.9	2.03	26.88
(3,5)	1:51:A:THR:H	4:348:A:PX4:C35	20	26.9	2.03	26.88
(3,5)	1:51:A:THR:H	4:330:A:PX4:C35	20	26.9	2.03	26.88
(3,5)	1:51:A:THR:H	4:317:A:PX4:C35	20	26.9	2.03	26.88
(3,5)	1:51:A:THR:H	4:332:A:PX4:C35	20	26.9	2.03	26.88
(3,1)	1:5:A:GLY:H	4:325:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:353:A:PX4:C35	20	25.93	1.87	25.9

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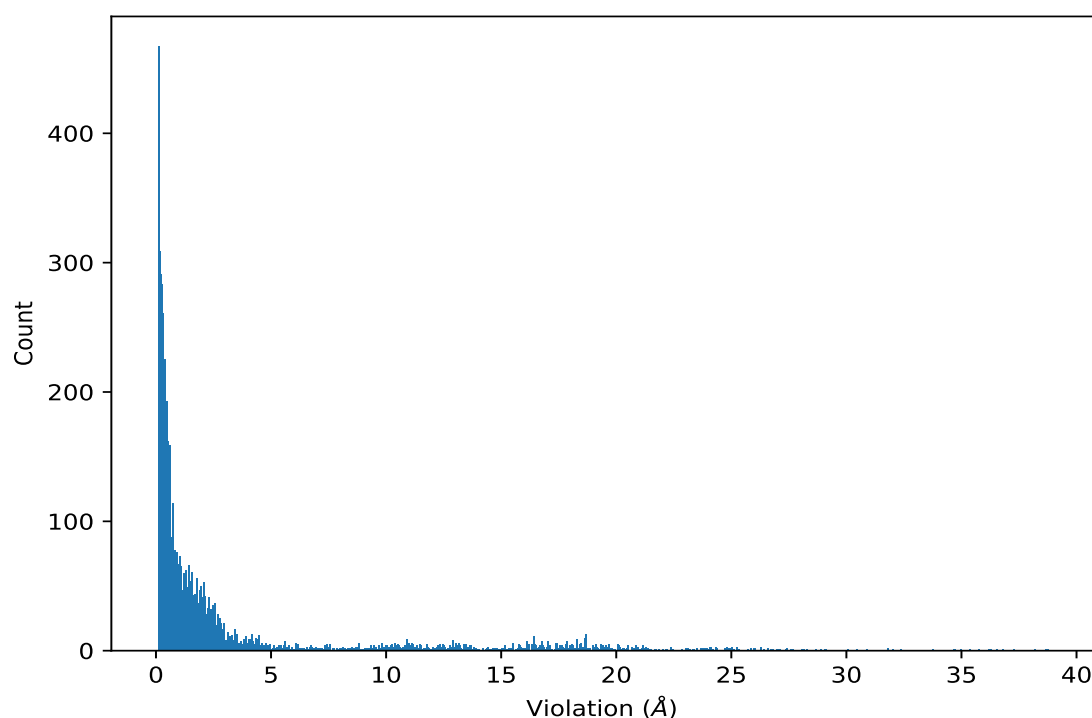
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1)	1:5:A:GLY:H	4:349:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:348:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:308:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:317:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:330:A:PX4:C35	20	25.93	1.87	25.9
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	20	24.69	0.98	24.88
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	20	24.44	0.49	24.34
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	20	21.26	0.45	21.19
(3,44)	1:34:A:SER:H	4:319:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:321:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:317:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:317:A:PX4:C3	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:310:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:319:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:317:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:321:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:353:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:321:A:PX4:C3	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:353:A:PX4:C4	20	20.86	1.82	21.04
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	20	19.95	0.65	20.13
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H13	20	19.95	0.65	20.13
(3,2)	1:21:A:ARG:H	4:320:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:348:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:340:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:352:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:324:A:PX4:C35	20	19.65	2.18	19.67
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	20	19.19	0.66	19.25

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	10	38.77
(3,4)	1:33:A:ASN:H	4:309:A:PX4:C35	11	38.69
(3,4)	1:33:A:ASN:H	4:340:A:PX4:C35	5	38.15
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	19	37.25
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	9	36.82
(3,4)	1:33:A:ASN:H	4:352:A:PX4:C35	6	36.54
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	15	36.28
(3,4)	1:33:A:ASN:H	4:320:A:PX4:C35	1	36.22
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	2	36.18
(3,4)	1:33:A:ASN:H	4:352:A:PX4:C35	14	35.76

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found