



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 17, 2020 – 01:19 am BST

PDB ID : 2MZH  
Title : NMR Solution Structure of the PRO Form of Human Matrilysin (proMMP-7)  
in Complex with Zwitterionic Membrane  
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Deposited on : 2015-02-12

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

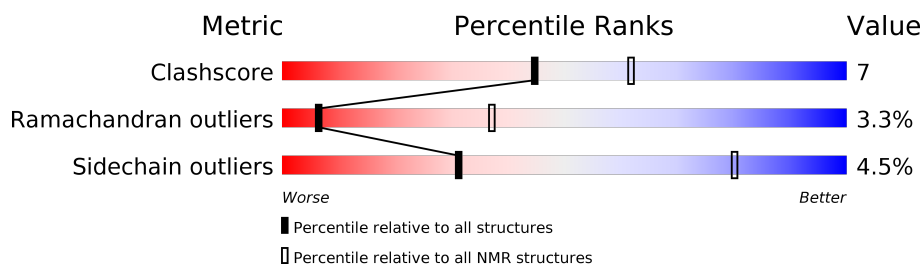
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 44%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	248	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 11 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:11-A:239 (229)	0.66	11

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 and 2 single-model clusters were found.

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

### 3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9696 atoms, of which 1898 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
			3850	1240	1898	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

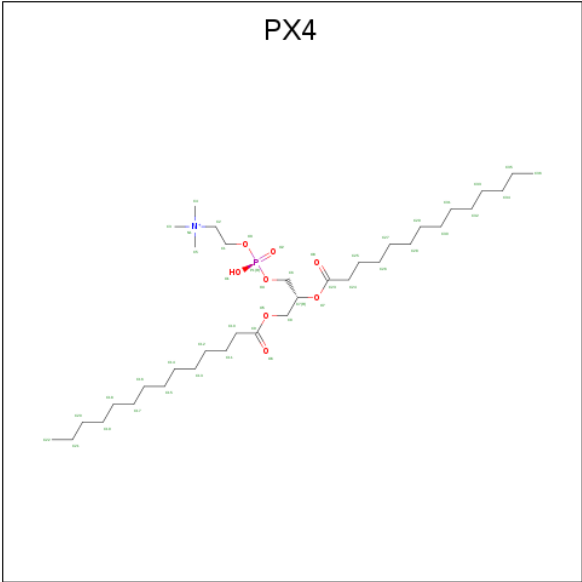
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



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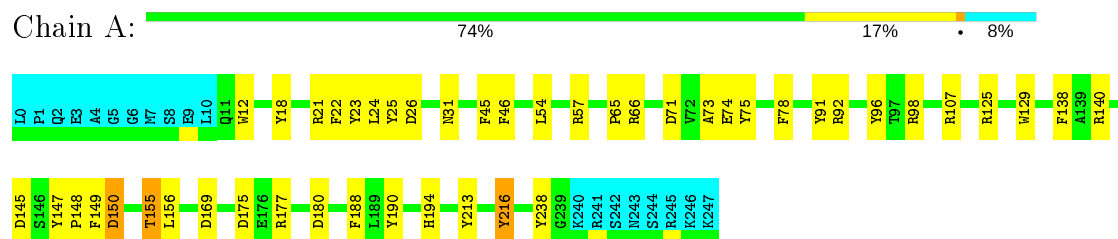
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

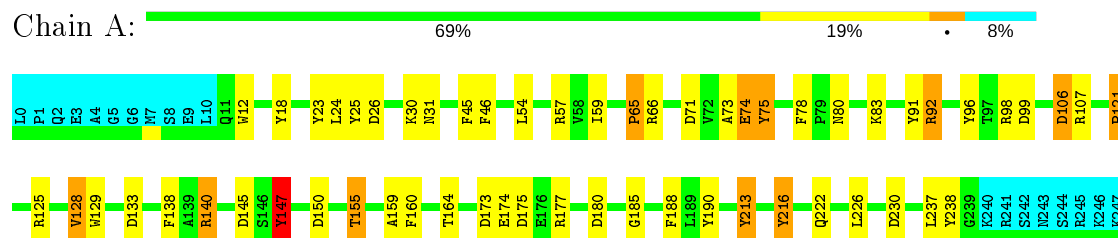


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

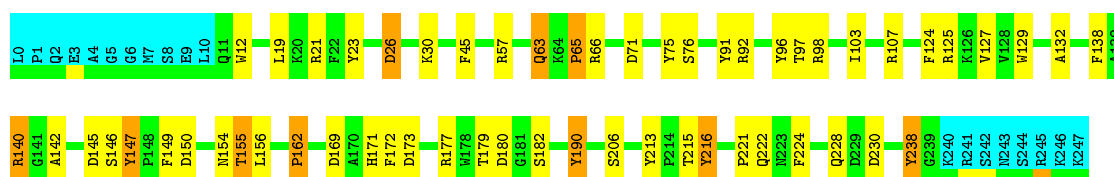
- Molecule 1: Matrilysin



#### 4.2.2 Score per residue for model 2

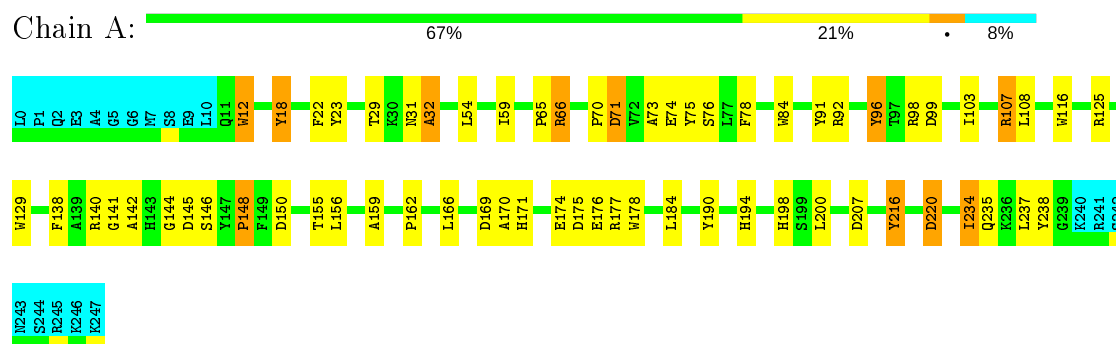
- Molecule 1: Matrilysin





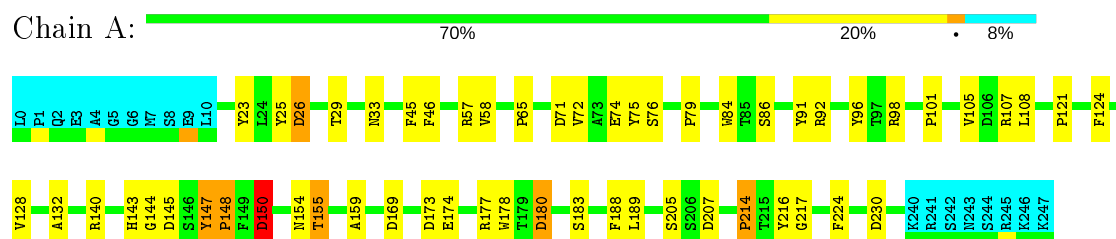
### 4.2.3 Score per residue for model 3

- Molecule 1: Matrilysin



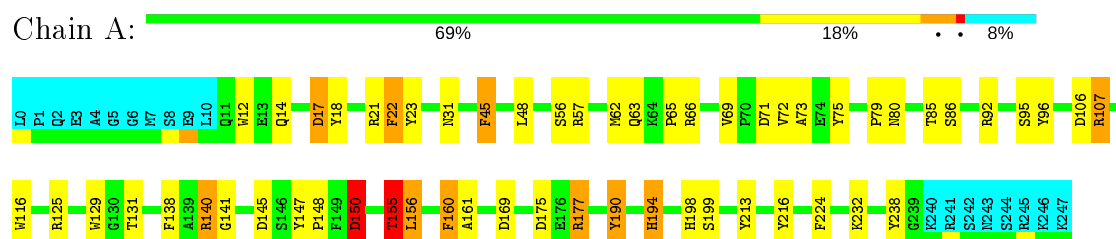
### 4.2.4 Score per residue for model 4

- Molecule 1: Matrilysin



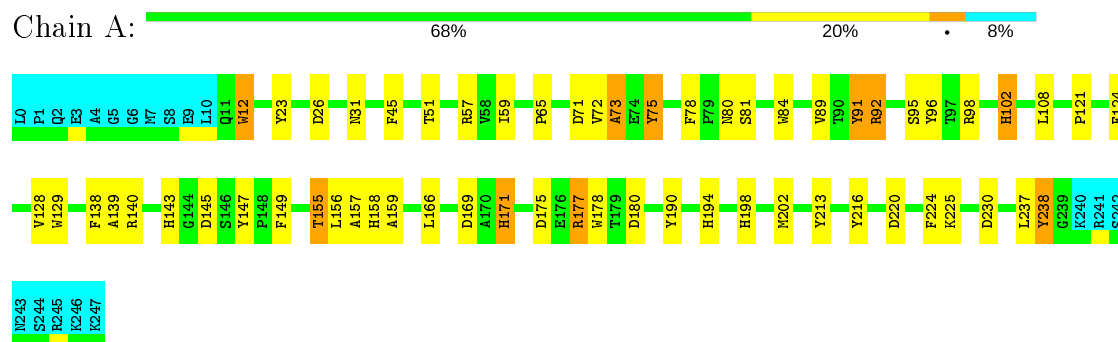
### 4.2.5 Score per residue for model 5

- Molecule 1: Matrilysin



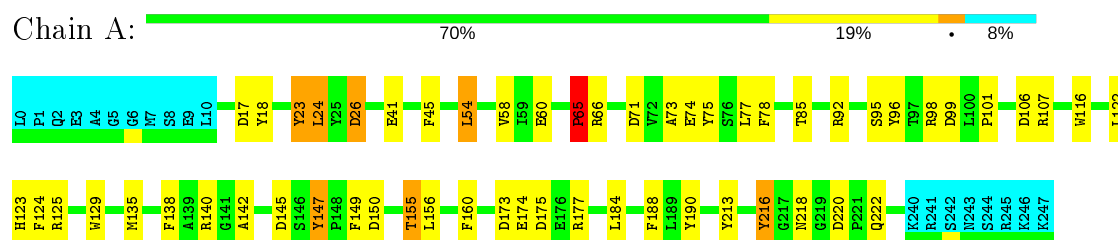
### 4.2.6 Score per residue for model 6

- Molecule 1: Matrilysin



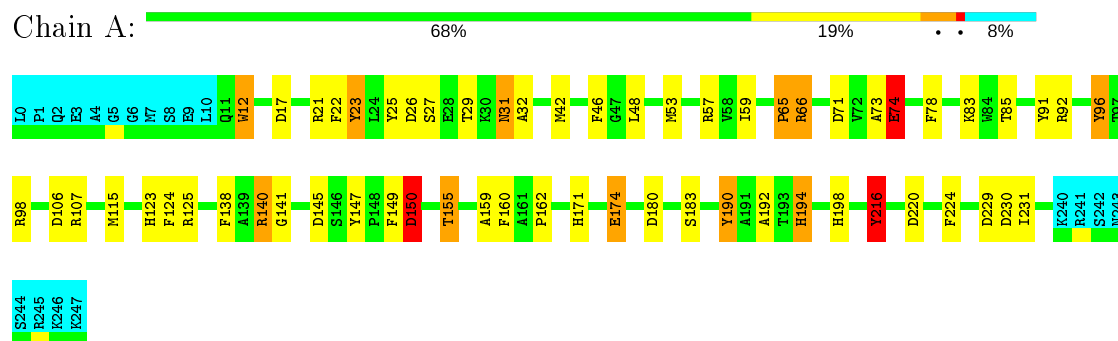
### 4.2.7 Score per residue for model 7

- Molecule 1: Matrilysin



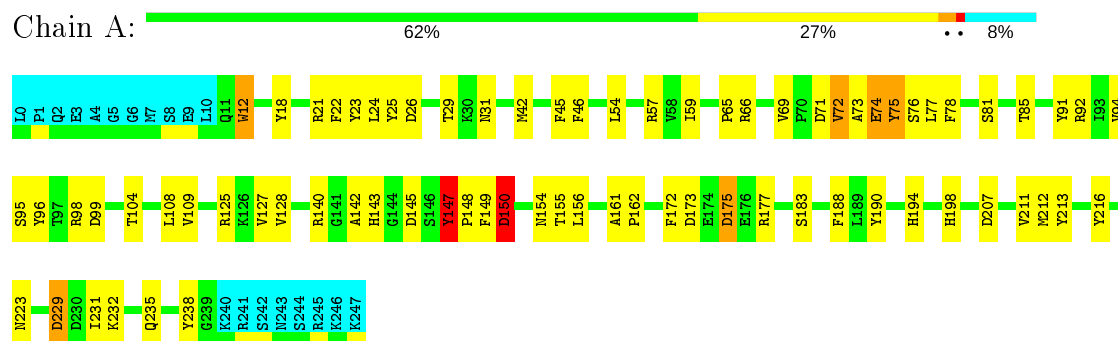
### 4.2.8 Score per residue for model 8

- Molecule 1: Matrilysin



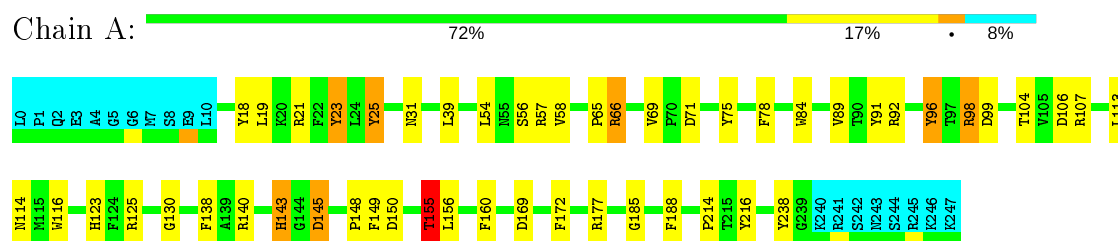
### 4.2.9 Score per residue for model 9

- Molecule 1: Matrilysin



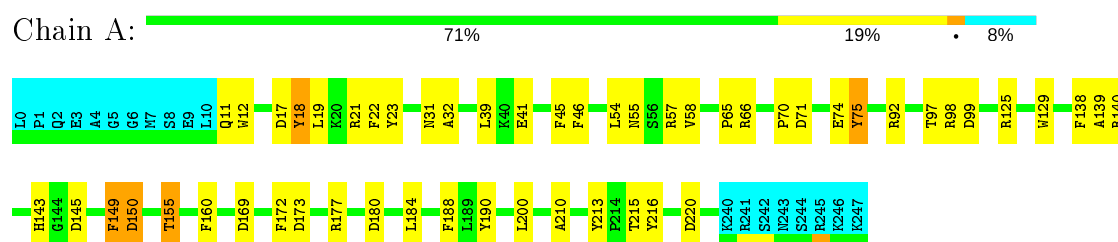
#### 4.2.10 Score per residue for model 10

- Molecule 1: Matrilysin



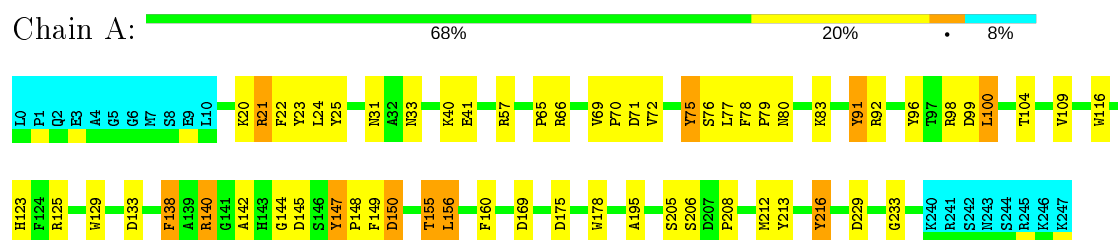
#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Matrilysin



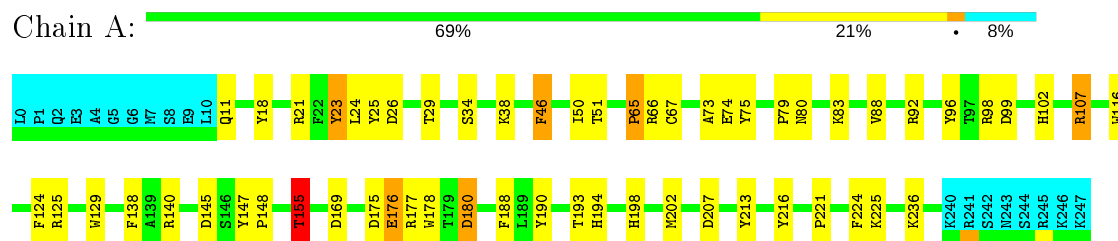
#### 4.2.12 Score per residue for model 12

- Molecule 1: Matrilysin



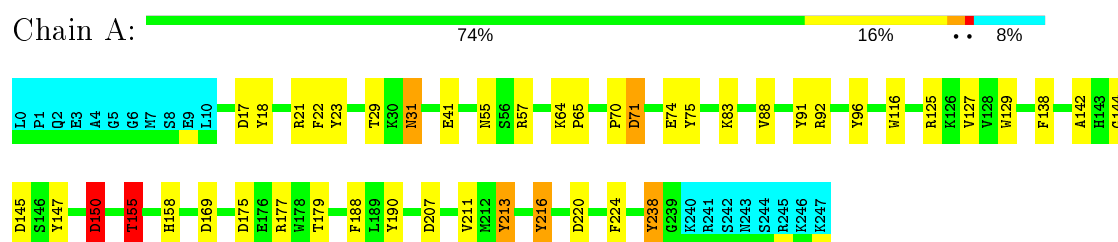
### 4.2.13 Score per residue for model 13

- Molecule 1: Matrilysin



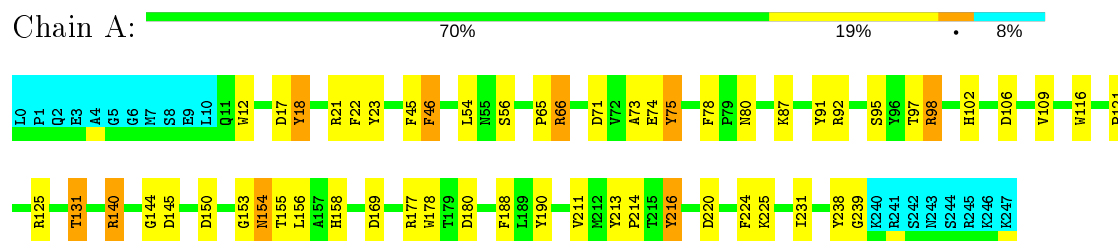
### 4.2.14 Score per residue for model 14

- Molecule 1: Matrilysin



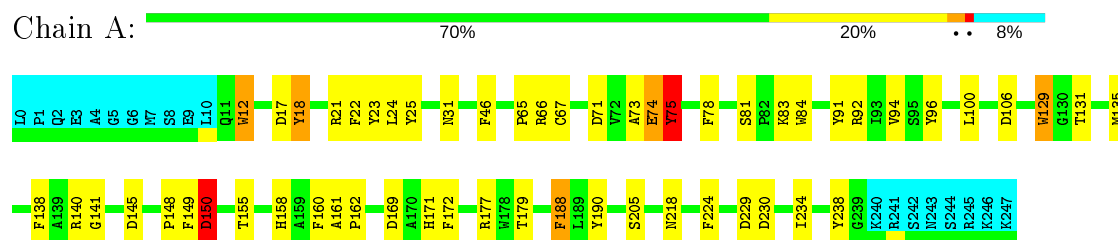
### 4.2.15 Score per residue for model 15

- Molecule 1: Matrilysin



### 4.2.16 Score per residue for model 16

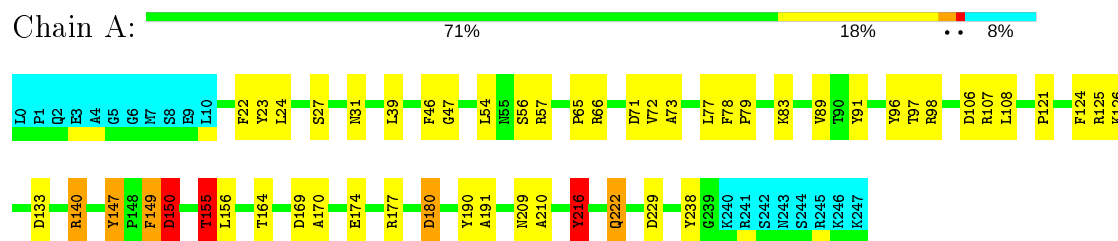
- Molecule 1: Matrilysin





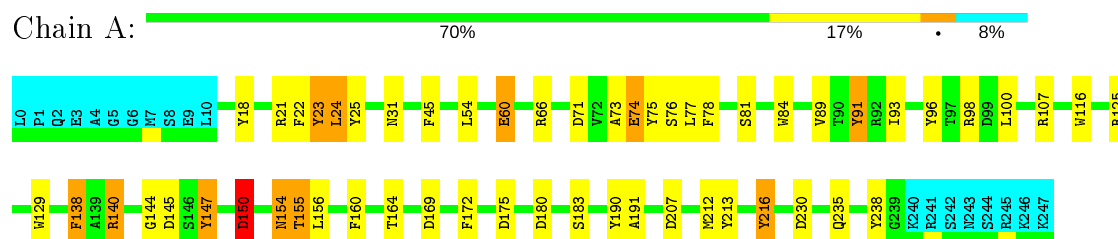
## 4.2.17 Score per residue for model 17

- Molecule 1: Matrilysin



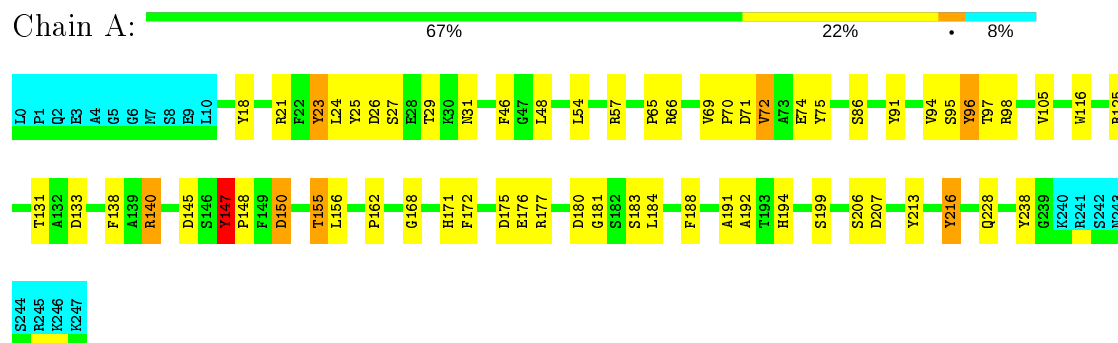
## 4.2.18 Score per residue for model 18

- Molecule 1: Matrilysin



## 4.2.19 Score per residue for model 19

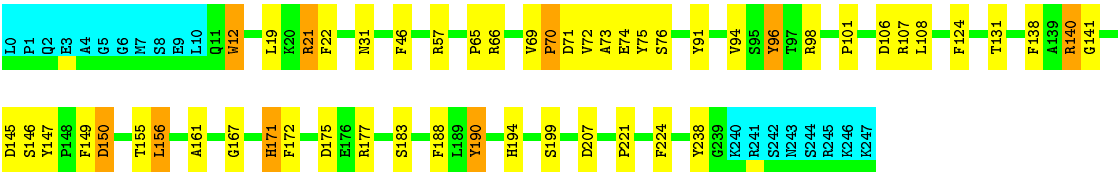
- Molecule 1: Matrilysin



## 4.2.20 Score per residue for model 20

- 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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1503
Number of shifts mapped to atoms	1503
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, 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	0.52±0.00	0±0/1858 ( 0.0± 0.0%)	2.04±0.04	58±6/2520 ( 2.3± 0.2%)
All	All	0.52	0/37160 ( 0.0%)	2.04	1156/50400 ( 2.3%)

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	6.8±2.3
All	All	0	135

There are no bond-length outliers.

All 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	140	ARG	NE-CZ-NH2	-20.93	109.84	120.30	5	9
1	A	75	TYR	CB-CG-CD2	-17.54	110.47	121.00	4	5
1	A	177	ARG	NE-CZ-NH2	-17.42	111.59	120.30	13	9
1	A	18	TYR	CB-CG-CD2	-17.28	110.63	121.00	7	9
1	A	98	ARG	NE-CZ-NH2	-16.76	111.92	120.30	18	8
1	A	140	ARG	NE-CZ-NH1	16.44	128.52	120.30	17	14
1	A	238	TYR	CB-CG-CD2	-16.14	111.32	121.00	3	5
1	A	107	ARG	NE-CZ-NH1	15.30	127.95	120.30	17	10
1	A	57	ARG	NE-CZ-NH1	15.19	127.90	120.30	2	8
1	A	125	ARG	NE-CZ-NH2	-15.00	112.80	120.30	12	9
1	A	213	TYR	CB-CG-CD2	-14.55	112.27	121.00	5	6
1	A	21	ARG	NE-CZ-NH1	13.74	127.17	120.30	20	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	71	ASP	CB-CG-OD2	13.22	130.19	118.30	2	13
1	A	230	ASP	CB-CG-OD2	12.96	129.97	118.30	18	3
1	A	57	ARG	NE-CZ-NH2	-12.71	113.94	120.30	17	8
1	A	125	ARG	NE-CZ-NH1	12.68	126.64	120.30	19	11
1	A	145	ASP	CB-CG-OD1	12.29	129.36	118.30	5	13
1	A	98	ARG	NE-CZ-NH1	12.08	126.34	120.30	17	10
1	A	91	TYR	CB-CG-CD2	-12.02	113.79	121.00	15	9
1	A	46	PHE	CB-CG-CD1	-12.01	112.39	120.80	17	7
1	A	71	ASP	CB-CG-OD1	12.00	129.10	118.30	10	15
1	A	21	ARG	NE-CZ-NH2	-11.95	114.32	120.30	2	9
1	A	92	ARG	NE-CZ-NH1	11.78	126.19	120.30	14	9
1	A	224	PHE	CB-CG-CD2	-11.73	112.59	120.80	20	4
1	A	66	ARG	NE-CZ-NH2	-11.67	114.47	120.30	3	8
1	A	91	TYR	CB-CG-CD1	-11.66	114.00	121.00	4	8
1	A	107	ARG	NE-CZ-NH2	-11.38	114.61	120.30	17	7
1	A	177	ARG	NE-CZ-NH1	11.36	125.98	120.30	9	10
1	A	22	PHE	CB-CG-CD2	-11.33	112.87	120.80	5	9
1	A	92	ARG	NE-CZ-NH2	-11.16	114.72	120.30	13	9
1	A	23	TYR	CB-CG-CD1	-11.14	114.31	121.00	4	6
1	A	145	ASP	CB-CG-OD2	10.92	128.13	118.30	3	13
1	A	45	PHE	CB-CG-CD1	-10.91	113.16	120.80	15	5
1	A	190	TYR	CB-CG-CD1	-10.71	114.58	121.00	5	6
1	A	91	TYR	CG-CD1-CE1	-10.61	112.81	121.30	6	2
1	A	213	TYR	CB-CG-CD1	-10.42	114.75	121.00	11	7
1	A	96	TYR	CB-CG-CD2	10.29	127.18	121.00	20	6
1	A	91	TYR	CG-CD2-CE2	-10.28	113.07	121.30	4	3
1	A	18	TYR	CB-CG-CD1	-10.21	114.88	121.00	9	4
1	A	150	ASP	CB-CG-OD1	10.19	127.47	118.30	18	4
1	A	138	PHE	CB-CG-CD2	-10.16	113.69	120.80	13	7
1	A	175	ASP	CB-CG-OD1	10.13	127.42	118.30	19	5
1	A	169	ASP	CB-CG-OD1	9.92	127.23	118.30	2	8
1	A	224	PHE	CB-CG-CD1	9.87	127.71	120.80	20	5
1	A	238	TYR	CB-CG-CD1	-9.84	115.09	121.00	5	9
1	A	96	TYR	CB-CG-CD1	-9.72	115.17	121.00	4	9
1	A	23	TYR	CB-CG-CD2	-9.72	115.17	121.00	1	9
1	A	188	PHE	CB-CG-CD2	-9.69	114.02	120.80	10	8
1	A	18	TYR	CG-CD2-CE2	-9.63	113.60	121.30	7	2
1	A	190	TYR	CB-CG-CD2	-9.42	115.35	121.00	16	7
1	A	66	ARG	NE-CZ-NH1	9.36	124.98	120.30	10	5
1	A	216	TYR	CB-CG-CD2	9.33	126.60	121.00	15	6
1	A	46	PHE	CB-CG-CD2	-9.26	114.32	120.80	13	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	155	THR	CA-CB-CG2	9.11	125.16	112.40	17	4
1	A	133	ASP	CB-CG-OD1	9.06	126.45	118.30	17	3
1	A	74	GLU	OE1-CD-OE2	-9.01	112.48	123.30	16	2
1	A	188	PHE	CB-CG-CD1	-8.98	114.52	120.80	15	5
1	A	71	ASP	OD1-CG-OD2	-8.96	106.27	123.30	19	15
1	A	220	ASP	CB-CG-OD2	-8.94	110.25	118.30	6	3
1	A	140	ARG	CD-NE-CZ	8.92	136.09	123.60	1	7
1	A	172	PHE	CB-CG-CD1	-8.86	114.60	120.80	18	4
1	A	29	THR	CA-CB-CG2	8.73	124.62	112.40	3	5
1	A	78	PHE	CB-CG-CD2	-8.71	114.70	120.80	8	4
1	A	216	TYR	CB-CG-CD1	-8.60	115.84	121.00	15	9
1	A	116	TRP	NE1-CE2-CD2	-8.59	98.71	107.30	5	6
1	A	150	ASP	CB-CG-OD2	8.57	126.02	118.30	16	4
1	A	172	PHE	CB-CG-CD2	-8.53	114.83	120.80	2	4
1	A	72	VAL	CA-CB-CG1	8.45	123.58	110.90	19	1
1	A	127	VAL	CA-CB-CG1	8.41	123.51	110.90	2	3
1	A	138	PHE	CB-CG-CD1	-8.40	114.92	120.80	18	6
1	A	106	ASP	CB-CG-OD2	8.39	125.85	118.30	15	6
1	A	94	VAL	CA-CB-CG2	8.39	123.48	110.90	20	2
1	A	145	ASP	OD1-CG-OD2	-8.31	107.51	123.30	5	15
1	A	213	TYR	CG-CD2-CE2	-8.20	114.74	121.30	18	3
1	A	149	PHE	CB-CG-CD1	-8.15	115.10	120.80	16	6
1	A	99	ASP	CB-CG-OD2	-8.12	110.99	118.30	11	7
1	A	159	ALA	CB-CA-C	8.12	122.27	110.10	3	4
1	A	207	ASP	CB-CG-OD2	-8.00	111.10	118.30	13	5
1	A	65	PRO	N-CA-CB	7.96	112.85	103.30	2	3
1	A	206	SER	CB-CA-C	7.94	125.18	110.10	12	1
1	A	169	ASP	CB-CG-OD2	7.91	125.42	118.30	12	6
1	A	210	ALA	CB-CA-C	-7.89	98.26	110.10	11	2
1	A	116	TRP	CE2-CD2-CG	7.86	113.59	107.30	5	4
1	A	91	TYR	CD1-CG-CD2	7.79	126.47	117.90	4	2
1	A	229	ASP	CB-CG-OD1	7.75	125.27	118.30	8	3
1	A	129	TRP	CD1-NE1-CE2	7.75	115.97	109.00	14	4
1	A	25	TYR	CG-CD1-CE1	-7.72	115.12	121.30	4	2
1	A	12	TRP	CB-CG-CD2	7.68	136.58	126.60	2	1
1	A	12	TRP	CD1-NE1-CE2	7.66	115.90	109.00	16	5
1	A	124	PHE	CB-CG-CD1	-7.66	115.44	120.80	4	4
1	A	75	TYR	CB-CG-CD1	7.65	125.59	121.00	4	6
1	A	18	TYR	CA-CB-CG	7.65	127.93	113.40	19	2
1	A	12	TRP	CD1-CG-CD2	-7.62	100.21	106.30	5	1
1	A	129	TRP	NE1-CE2-CD2	-7.60	99.70	107.30	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	116	TRP	CZ3-CH2-CZ2	-7.58	112.50	121.60	19	1
1	A	14	GLN	N-CA-CB	-7.55	97.01	110.60	5	1
1	A	79	PRO	N-CA-CB	7.54	112.35	103.30	13	1
1	A	106	ASP	CB-CG-OD1	-7.48	111.57	118.30	20	4
1	A	116	TRP	CH2-CZ2-CE2	7.48	124.88	117.40	19	1
1	A	78	PHE	CB-CG-CD1	7.44	126.01	120.80	3	3
1	A	75	TYR	CG-CD1-CE1	-7.41	115.37	121.30	4	3
1	A	116	TRP	CD1-NE1-CE2	7.41	115.67	109.00	5	6
1	A	98	ARG	NH1-CZ-NH2	7.41	127.55	119.40	4	1
1	A	131	THR	CA-CB-CG2	-7.40	102.05	112.40	15	1
1	A	17	ASP	CB-CG-OD2	7.39	124.95	118.30	14	3
1	A	214	PRO	N-CA-CB	7.34	112.10	103.30	10	1
1	A	66	ARG	CD-NE-CZ	7.29	133.80	123.60	5	5
1	A	149	PHE	CB-CG-CD2	-7.27	115.71	120.80	11	4
1	A	129	TRP	CE2-CD2-CG	7.27	113.11	107.30	1	2
1	A	98	ARG	CD-NE-CZ	7.25	133.75	123.60	2	3
1	A	150	ASP	CB-CA-C	7.24	124.87	110.40	14	7
1	A	18	TYR	CG-CD1-CE1	-7.21	115.53	121.30	15	2
1	A	164	THR	C-N-CA	7.21	137.45	122.30	18	1
1	A	96	TYR	CG-CD1-CE1	-7.20	115.54	121.30	4	6
1	A	140	ARG	NH1-CZ-NH2	7.18	127.30	119.40	5	4
1	A	238	TYR	CG-CD1-CE1	-7.18	115.56	121.30	16	5
1	A	69	VAL	CA-CB-CG2	7.13	121.59	110.90	20	4
1	A	147	TYR	CB-CG-CD2	7.11	125.27	121.00	5	3
1	A	17	ASP	CB-CG-OD1	7.09	124.68	118.30	7	3
1	A	180	ASP	CB-CA-C	7.09	124.58	110.40	4	2
1	A	238	TYR	CG-CD2-CE2	-7.09	115.63	121.30	16	2
1	A	91	TYR	CD1-CE1-CZ	7.08	126.17	119.80	6	3
1	A	108	LEU	CB-CG-CD1	7.08	123.04	111.00	4	4
1	A	116	TRP	NE1-CE2-CZ2	7.06	138.16	130.40	5	2
1	A	107	ARG	NH1-CZ-NH2	7.04	127.14	119.40	1	1
1	A	84	TRP	CD1-NE1-CE2	7.00	115.30	109.00	18	1
1	A	60	GLU	OE1-CD-OE2	-7.00	114.90	123.30	18	1
1	A	45	PHE	CB-CG-CD2	-6.99	115.91	120.80	9	5
1	A	191	ALA	CB-CA-C	-6.99	99.62	110.10	19	1
1	A	22	PHE	CB-CG-CD1	6.98	125.69	120.80	15	4
1	A	116	TRP	CE3-CZ3-CH2	-6.98	113.52	121.20	18	1
1	A	89	VAL	CA-CB-CG1	6.96	121.33	110.90	17	2
1	A	133	ASP	CB-CG-OD2	6.92	124.53	118.30	19	2
1	A	23	TYR	CD1-CE1-CZ	6.92	126.03	119.80	7	4
1	A	65	PRO	CA-N-CD	-6.91	101.83	111.50	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	TYR	CG-CD2-CE2	-6.90	115.78	121.30	13	1
1	A	18	TYR	CD1-CG-CD2	6.89	125.48	117.90	7	1
1	A	124	PHE	CB-CG-CD2	6.86	125.60	120.80	4	4
1	A	207	ASP	CB-CG-OD1	6.84	124.46	118.30	9	3
1	A	213	TYR	CD1-CG-CD2	6.84	125.43	117.90	12	1
1	A	220	ASP	CB-CG-OD1	-6.84	112.14	118.30	7	2
1	A	102	HIS	CA-CB-CG	6.83	125.22	113.60	6	1
1	A	31	ASN	N-CA-CB	6.80	122.84	110.60	14	2
1	A	73	ALA	C-N-CA	6.80	138.69	121.70	17	8
1	A	199	SER	N-CA-CB	-6.80	100.31	110.50	19	2
1	A	95	SER	CB-CA-C	6.79	123.01	110.10	15	4
1	A	70	PRO	N-CD-CG	6.79	113.38	103.20	19	1
1	A	57	ARG	CD-NE-CZ	6.79	133.10	123.60	9	4
1	A	116	TRP	CB-CG-CD2	6.78	135.41	126.60	19	1
1	A	125	ARG	CD-NE-CZ	6.78	133.09	123.60	13	4
1	A	190	TYR	N-CA-CB	-6.75	98.45	110.60	7	2
1	A	96	TYR	CG-CD2-CE2	-6.75	115.90	121.30	19	4
1	A	154	ASN	C-N-CA	6.72	138.50	121.70	9	3
1	A	150	ASP	OD1-CG-OD2	-6.69	110.58	123.30	20	1
1	A	161	ALA	N-CA-CB	-6.69	100.73	110.10	20	3
1	A	105	VAL	CA-CB-CG2	6.68	120.92	110.90	4	1
1	A	26	ASP	CB-CG-OD2	6.67	124.30	118.30	9	3
1	A	147	TYR	CB-CG-CD1	-6.66	117.00	121.00	5	3
1	A	96	TYR	CD1-CG-CD2	6.65	125.22	117.90	19	3
1	A	12	TRP	NE1-CE2-CD2	-6.64	100.66	107.30	20	5
1	A	183	SER	CB-CA-C	6.63	122.70	110.10	8	5
1	A	84	TRP	NE1-CE2-CD2	-6.60	100.70	107.30	18	1
1	A	171	HIS	CG-ND1-CE1	-6.59	97.14	105.70	16	1
1	A	69	VAL	CB-CA-C	6.57	123.89	111.40	10	1
1	A	25	TYR	CD1-CE1-CZ	6.57	125.71	119.80	4	2
1	A	25	TYR	CB-CG-CD2	-6.57	117.06	121.00	8	4
1	A	231	ILE	CA-CB-CG2	6.56	124.02	110.90	8	2
1	A	178	TRP	N-CA-CB	-6.55	98.80	110.60	4	1
1	A	86	SER	CB-CA-C	6.55	122.54	110.10	19	2
1	A	205	SER	N-CA-CB	-6.55	100.68	110.50	12	1
1	A	109	VAL	CA-CB-CG2	6.54	120.71	110.90	9	3
1	A	234	ILE	CA-CB-CG1	6.53	123.41	111.00	3	1
1	A	211	VAL	CG1-CB-CG2	-6.53	100.46	110.90	14	1
1	A	25	TYR	CB-CG-CD1	6.50	124.90	121.00	18	2
1	A	75	TYR	CD1-CE1-CZ	6.49	125.64	119.80	7	2
1	A	142	ALA	N-CA-CB	-6.49	101.02	110.10	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	LEU	C-N-CA	6.49	137.92	121.70	19	1
1	A	42	MET	CA-CB-CG	-6.48	102.28	113.30	8	1
1	A	160	PHE	CD1-CE1-CZ	-6.45	112.36	120.10	8	1
1	A	175	ASP	CB-CG-OD2	-6.45	112.50	118.30	9	2
1	A	45	PHE	CG-CD2-CE2	-6.44	113.71	120.80	5	1
1	A	88	VAL	CA-CB-CG2	6.44	120.56	110.90	13	1
1	A	92	ARG	NH1-CZ-NH2	6.41	126.45	119.40	1	1
1	A	85	THR	CA-CB-CG2	6.41	121.37	112.40	9	1
1	A	54	LEU	CB-CG-CD2	6.38	121.85	111.00	7	1
1	A	169	ASP	OD1-CG-OD2	-6.38	111.19	123.30	2	5
1	A	101	PRO	N-CD-CG	6.37	112.75	103.20	7	3
1	A	178	TRP	NE1-CE2-CZ2	6.36	137.40	130.40	3	1
1	A	96	TYR	CZ-CE2-CD2	-6.34	114.10	119.80	10	2
1	A	23	TYR	CG-CD1-CE1	-6.32	116.25	121.30	7	1
1	A	54	LEU	CB-CG-CD1	6.31	121.73	111.00	18	3
1	A	182	SER	C-N-CA	6.29	137.44	121.70	2	1
1	A	92	ARG	CD-NE-CZ	6.28	132.38	123.60	2	5
1	A	45	PHE	CZ-CE2-CD2	6.27	127.63	120.10	5	1
1	A	147	TYR	CG-CD2-CE2	-6.26	116.29	121.30	13	2
1	A	73	ALA	O-C-N	6.26	132.72	122.70	16	1
1	A	139	ALA	CB-CA-C	6.23	119.45	110.10	6	1
1	A	84	TRP	CH2-CZ2-CE2	6.23	123.63	117.40	4	2
1	A	213	TYR	N-CA-CB	-6.22	99.40	110.60	7	2
1	A	73	ALA	N-CA-CB	-6.21	101.41	110.10	1	2
1	A	84	TRP	CD1-CG-CD2	-6.20	101.34	106.30	3	1
1	A	89	VAL	CA-CB-CG2	6.20	120.20	110.90	10	2
1	A	173	ASP	CB-CG-OD1	6.19	123.87	118.30	4	3
1	A	193	THR	CA-CB-CG2	6.19	121.07	112.40	13	1
1	A	173	ASP	CB-CG-OD2	-6.19	112.73	118.30	7	3
1	A	12	TRP	CE2-CD2-CG	6.18	112.25	107.30	8	2
1	A	190	TYR	CA-CB-CG	6.18	125.14	113.40	14	4
1	A	160	PHE	CB-CG-CD1	-6.18	116.48	120.80	12	3
1	A	71	ASP	C-N-CA	6.16	137.10	121.70	1	2
1	A	190	TYR	CZ-CE2-CD2	-6.15	114.27	119.80	3	2
1	A	99	ASP	N-CA-CB	-6.13	99.57	110.60	7	2
1	A	130	GLY	O-C-N	6.12	132.49	122.70	10	1
1	A	144	GLY	C-N-CA	6.12	137.00	121.70	14	2
1	A	72	VAL	O-C-N	-6.09	112.95	122.70	12	2
1	A	96	TYR	CB-CA-C	6.08	122.56	110.40	7	2
1	A	238	TYR	CD1-CG-CD2	6.08	124.58	117.90	16	2
1	A	27	SER	N-CA-CB	-6.08	101.39	110.50	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	129	TRP	CA-CB-CG	6.07	125.24	113.70	12	1
1	A	26	ASP	CB-CG-OD1	6.07	123.76	118.30	1	3
1	A	70	PRO	N-CA-CB	6.07	110.58	103.30	14	3
1	A	156	LEU	CB-CA-C	6.06	121.71	110.20	20	1
1	A	200	LEU	CB-CG-CD1	6.02	121.23	111.00	3	1
1	A	74	GLU	CA-CB-CG	6.01	126.62	113.40	8	1
1	A	212	MET	CB-CA-C	6.00	122.41	110.40	18	2
1	A	84	TRP	NE1-CE2-CZ2	6.00	137.00	130.40	4	1
1	A	178	TRP	CB-CG-CD1	-6.00	119.20	127.00	12	1
1	A	32	ALA	N-CA-CB	-5.99	101.72	110.10	11	1
1	A	65	PRO	N-CD-CG	5.97	112.16	103.20	7	3
1	A	20	LYS	N-CA-CB	-5.97	99.86	110.60	12	1
1	A	58	VAL	O-C-N	-5.96	113.16	122.70	7	1
1	A	192	ALA	CB-CA-C	-5.96	101.16	110.10	19	1
1	A	91	TYR	CA-CB-CG	5.95	124.71	113.40	17	2
1	A	121	PRO	N-CA-CB	5.94	110.43	103.30	4	1
1	A	160	PHE	CB-CG-CD2	5.94	124.96	120.80	12	3
1	A	160	PHE	CG-CD1-CE1	5.93	127.33	120.80	8	2
1	A	129	TRP	CB-CG-CD2	5.93	134.31	126.60	1	2
1	A	104	THR	CA-CB-CG2	5.92	120.69	112.40	10	1
1	A	99	ASP	CB-CG-OD1	5.92	123.63	118.30	12	2
1	A	75	TYR	CG-CD2-CE2	-5.92	116.56	121.30	16	3
1	A	75	TYR	N-CA-CB	5.89	121.20	110.60	9	1
1	A	158	HIS	CB-CA-C	5.89	122.17	110.40	14	1
1	A	107	ARG	CD-NE-CZ	5.88	131.83	123.60	4	1
1	A	131	THR	C-N-CA	5.88	136.40	121.70	16	2
1	A	190	TYR	CG-CD2-CE2	-5.88	116.60	121.30	18	2
1	A	202	MET	CG-SD-CE	5.88	109.60	100.20	13	2
1	A	34	SER	N-CA-CB	-5.88	101.69	110.50	13	1
1	A	177	ARG	N-CA-CB	-5.86	100.06	110.60	4	1
1	A	123	HIS	CA-CB-CG	5.85	123.55	113.60	7	3
1	A	173	ASP	N-CA-CB	-5.84	100.08	110.60	9	1
1	A	29	THR	O-C-N	-5.84	113.35	122.70	14	1
1	A	140	ARG	C-N-CA	5.84	134.56	122.30	20	3
1	A	216	TYR	CG-CD2-CE2	-5.82	116.64	121.30	8	2
1	A	129	TRP	CG-CD2-CE3	-5.82	128.66	133.90	13	1
1	A	126	LYS	C-N-CA	5.81	136.24	121.70	17	1
1	A	41	GLU	CA-CB-CG	5.81	126.19	113.40	11	1
1	A	148	PRO	N-CA-CB	5.80	110.26	103.30	3	1
1	A	50	ILE	CA-CB-CG1	5.79	122.00	111.00	13	1
1	A	91	TYR	CZ-CE2-CD2	-5.79	114.59	119.80	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	178	TRP	NE1-CE2-CD2	-5.78	101.52	107.30	3	3
1	A	23	TYR	CZ-CE2-CD2	-5.78	114.60	119.80	18	1
1	A	55	ASN	O-C-N	-5.77	113.47	122.70	14	1
1	A	129	TRP	CB-CA-C	5.77	121.93	110.40	7	2
1	A	75	TYR	C-N-CA	5.76	136.10	121.70	19	3
1	A	39	LEU	CB-CG-CD1	5.76	120.79	111.00	10	2
1	A	97	THR	O-C-N	-5.76	113.49	122.70	15	1
1	A	58	VAL	CG1-CB-CG2	-5.75	101.70	110.90	7	2
1	A	70	PRO	C-N-CA	5.75	136.07	121.70	12	1
1	A	146	SER	N-CA-CB	-5.74	101.89	110.50	20	3
1	A	171	HIS	CB-CA-C	5.73	121.86	110.40	16	1
1	A	132	ALA	N-CA-CB	-5.72	102.09	110.10	2	1
1	A	180	ASP	CB-CG-OD2	5.72	123.45	118.30	19	1
1	A	213	TYR	CG-CD1-CE1	-5.71	116.73	121.30	11	1
1	A	161	ALA	CB-CA-C	5.71	118.66	110.10	16	1
1	A	87	LYS	CB-CG-CD	5.70	126.42	111.60	15	1
1	A	170	ALA	CB-CA-C	5.70	118.65	110.10	3	2
1	A	129	TRP	C-N-CA	5.68	134.24	122.30	12	1
1	A	81	SER	CB-CA-C	5.68	120.89	110.10	16	1
1	A	179	THR	CA-CB-OG1	5.68	120.92	109.00	14	1
1	A	229	ASP	CB-CG-OD2	5.67	123.41	118.30	12	2
1	A	159	ALA	O-C-N	5.67	131.76	122.70	3	1
1	A	76	SER	CB-CA-C	5.64	120.83	110.10	12	2
1	A	67	CYS	CA-CB-SG	5.63	124.14	114.00	16	1
1	A	178	TRP	CD1-NE1-CE2	5.63	114.07	109.00	3	2
1	A	178	TRP	CB-CG-CD2	5.62	133.91	126.60	12	1
1	A	12	TRP	CE3-CZ3-CH2	-5.60	115.04	121.20	6	1
1	A	116	TRP	CB-CG-CD1	-5.60	119.72	127.00	19	1
1	A	18	TYR	CD1-CE1-CZ	5.58	124.83	119.80	15	1
1	A	173	ASP	CA-CB-CG	5.58	125.67	113.40	11	1
1	A	58	VAL	CA-CB-CG2	5.57	119.26	110.90	11	2
1	A	75	TYR	CB-CA-C	5.57	121.54	110.40	14	1
1	A	194	HIS	CA-CB-CG	5.56	123.06	113.60	5	2
1	A	22	PHE	CD1-CE1-CZ	5.56	126.78	120.10	17	1
1	A	129	TRP	NE1-CE2-CZ2	5.56	136.51	130.40	3	2
1	A	147	TYR	CB-CA-C	5.55	121.50	110.40	1	2
1	A	100	LEU	CB-CA-C	5.55	120.74	110.20	18	1
1	A	18	TYR	CZ-CE2-CD2	5.54	124.79	119.80	7	2
1	A	162	PRO	N-CD-CG	5.54	111.52	103.20	9	1
1	A	41	GLU	O-C-N	-5.54	113.84	122.70	12	1
1	A	192	ALA	N-CA-CB	5.54	117.85	110.10	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	TRP	CB-CG-CD1	-5.53	119.81	127.00	2	1
1	A	221	PRO	N-CD-CG	5.53	111.49	103.20	2	1
1	A	108	LEU	CB-CG-CD2	5.52	120.39	111.00	9	2
1	A	222	GLN	CB-CG-CD	5.51	125.94	111.60	17	1
1	A	132	ALA	CB-CA-C	5.51	118.37	110.10	4	1
1	A	129	TRP	CE2-CD2-CE3	-5.51	112.09	118.70	1	2
1	A	27	SER	CB-CA-C	5.51	120.56	110.10	19	1
1	A	150	ASP	N-CA-CB	5.50	120.50	110.60	4	1
1	A	79	PRO	C-N-CA	5.50	135.44	121.70	4	3
1	A	206	SER	N-CA-CB	-5.49	102.27	110.50	2	2
1	A	162	PRO	C-N-CA	5.49	133.82	122.30	8	1
1	A	79	PRO	CA-N-CD	-5.49	103.82	111.50	13	1
1	A	194	HIS	N-CA-CB	-5.48	100.74	110.60	3	1
1	A	42	MET	O-C-N	-5.47	113.94	122.70	9	1
1	A	89	VAL	CG1-CB-CG2	-5.47	102.14	110.90	18	1
1	A	143	HIS	CA-CB-CG	5.47	122.91	113.60	9	4
1	A	174	GLU	OE1-CD-OE2	-5.47	116.73	123.30	8	2
1	A	237	LEU	CB-CG-CD2	5.47	120.30	111.00	6	1
1	A	176	GLU	OE1-CD-OE2	-5.46	116.74	123.30	3	2
1	A	178	TRP	CH2-CZ2-CE2	-5.46	111.94	117.40	15	1
1	A	148	PRO	N-CD-CG	5.46	111.39	103.20	4	2
1	A	142	ALA	CB-CA-C	5.46	118.29	110.10	9	1
1	A	48	LEU	CB-CG-CD2	-5.46	101.73	111.00	5	1
1	A	221	PRO	C-N-CA	5.44	135.30	121.70	13	1
1	A	160	PHE	CZ-CE2-CD2	-5.44	113.57	120.10	18	2
1	A	234	ILE	CA-CB-CG2	5.43	121.77	110.90	16	1
1	A	216	TYR	CG-CD1-CE1	-5.43	116.95	121.30	11	1
1	A	23	TYR	C-N-CA	5.43	135.27	121.70	5	1
1	A	85	THR	C-N-CA	5.43	135.27	121.70	5	1
1	A	156	LEU	CB-CG-CD2	5.43	120.23	111.00	12	1
1	A	30	LYS	C-N-CA	5.42	135.26	121.70	2	2
1	A	150	ASP	C-N-CA	5.41	133.67	122.30	1	1
1	A	12	TRP	NE1-CE2-CZ2	5.40	136.34	130.40	8	2
1	A	51	THR	CA-CB-OG1	5.40	120.34	109.00	13	1
1	A	72	VAL	CA-CB-CG2	5.40	118.99	110.90	5	2
1	A	97	THR	CA-CB-CG2	5.40	119.95	112.40	19	2
1	A	128	VAL	CA-CB-CG2	5.38	118.96	110.90	1	1
1	A	225	LYS	CB-CA-C	5.37	121.14	110.40	13	2
1	A	24	LEU	CB-CA-C	5.37	120.40	110.20	18	1
1	A	220	ASP	N-CA-CB	-5.37	100.94	110.60	3	1
1	A	208	PRO	N-CA-CB	5.37	109.74	103.30	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	TRP	CH2-CZ2-CE2	5.36	122.76	117.40	1	1
1	A	155	THR	CB-CA-C	5.36	126.08	111.60	5	1
1	A	226	LEU	CB-CA-C	-5.36	100.01	110.20	1	1
1	A	195	ALA	N-CA-CB	5.36	117.60	110.10	12	1
1	A	230	ASP	CB-CG-OD1	-5.36	113.48	118.30	2	2
1	A	158	HIS	CA-CB-CG	5.36	122.71	113.60	6	2
1	A	212	MET	CG-SD-CE	5.35	108.77	100.20	12	1
1	A	200	LEU	CB-CA-C	-5.35	100.03	110.20	11	1
1	A	213	TYR	CD1-CE1-CZ	5.34	124.61	119.80	11	1
1	A	21	ARG	O-C-N	-5.34	114.15	122.70	12	1
1	A	79	PRO	N-CD-CG	5.34	111.21	103.20	13	1
1	A	47	GLY	CA-C-O	-5.33	111.00	120.60	17	1
1	A	40	LYS	O-C-N	-5.33	114.17	122.70	12	1
1	A	124	PHE	CG-CD2-CE2	5.33	126.66	120.80	6	1
1	A	38	LYS	O-C-N	-5.33	114.18	122.70	13	1
1	A	191	ALA	N-CA-CB	-5.32	102.66	110.10	17	2
1	A	26	ASP	CB-CA-C	5.31	121.02	110.40	2	1
1	A	214	PRO	N-CA-C	5.31	125.91	112.10	4	1
1	A	218	ASN	CB-CA-C	5.30	121.01	110.40	16	1
1	A	67	CYS	O-C-N	-5.30	114.19	123.20	13	1
1	A	155	THR	OG1-CB-CG2	-5.30	97.80	110.00	18	1
1	A	235	GLN	O-C-N	-5.30	114.22	122.70	3	1
1	A	55	ASN	N-CA-CB	5.30	120.13	110.60	11	1
1	A	171	HIS	CA-CB-CG	5.29	122.59	113.60	20	1
1	A	228	GLN	N-CA-CB	-5.29	101.09	110.60	2	1
1	A	139	ALA	N-CA-CB	-5.28	102.71	110.10	11	1
1	A	180	ASP	CB-CG-OD1	-5.28	113.55	118.30	13	1
1	A	116	TRP	CD2-CE3-CZ3	5.28	125.66	118.80	18	1
1	A	24	LEU	N-CA-CB	5.27	120.93	110.40	7	1
1	A	22	PHE	C-N-CA	5.27	134.87	121.70	12	1
1	A	205	SER	CB-CA-C	5.25	120.08	110.10	16	1
1	A	125	ARG	CG-CD-NE	5.25	122.82	111.80	12	1
1	A	198	HIS	O-C-N	5.25	131.10	122.70	3	1
1	A	56	SER	N-CA-CB	-5.25	102.63	110.50	15	1
1	A	29	THR	OG1-CB-CG2	-5.24	97.95	110.00	8	1
1	A	46	PHE	CZ-CE2-CD2	-5.23	113.82	120.10	19	1
1	A	86	SER	C-N-CA	5.23	134.78	121.70	4	1
1	A	88	VAL	CA-CB-CG1	5.22	118.74	110.90	14	1
1	A	183	SER	N-CA-CB	5.22	118.33	110.50	20	1
1	A	188	PHE	CZ-CE2-CD2	-5.22	113.84	120.10	1	1
1	A	105	VAL	CA-CB-CG1	5.21	118.72	110.90	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	LEU	O-C-N	-5.21	114.36	122.70	20	1
1	A	224	PHE	N-CA-CB	-5.21	101.23	110.60	5	1
1	A	103	ILE	CB-CA-C	5.20	122.00	111.60	3	1
1	A	128	VAL	CB-CA-C	5.20	121.28	111.40	9	1
1	A	95	SER	C-N-CA	5.20	134.70	121.70	6	2
1	A	33	ASN	N-CA-CB	-5.20	101.25	110.60	4	1
1	A	102	HIS	C-N-CA	5.19	134.68	121.70	15	1
1	A	45	PHE	CA-CB-CG	5.19	126.35	113.90	18	1
1	A	32	ALA	CB-CA-C	-5.19	102.32	110.10	8	2
1	A	221	PRO	O-C-N	-5.19	114.40	122.70	20	1
1	A	226	LEU	CB-CG-CD2	5.18	119.81	111.00	1	1
1	A	159	ALA	N-CA-CB	5.18	117.35	110.10	6	1
1	A	133	ASP	N-CA-CB	5.18	119.92	110.60	17	1
1	A	156	LEU	CB-CG-CD1	5.17	119.80	111.00	9	1
1	A	59	ILE	CA-CB-CG1	5.16	120.81	111.00	1	1
1	A	160	PHE	O-C-N	-5.16	114.45	122.70	11	1
1	A	135	MET	CG-SD-CE	5.16	108.45	100.20	16	1
1	A	57	ARG	NH1-CZ-NH2	5.16	125.07	119.40	17	1
1	A	19	LEU	CB-CG-CD2	5.15	119.75	111.00	2	1
1	A	23	TYR	CD1-CG-CD2	5.15	123.56	117.90	13	1
1	A	213	TYR	CA-CB-CG	5.14	123.17	113.40	2	1
1	A	62	MET	CG-SD-CE	5.13	108.41	100.20	5	1
1	A	184	LEU	C-N-CA	5.13	133.06	122.30	19	1
1	A	156	LEU	N-CA-CB	5.12	120.65	110.40	18	1
1	A	121	PRO	N-CD-CG	5.11	110.86	103.20	1	1
1	A	115	MET	CA-CB-CG	5.11	121.98	113.30	8	1
1	A	171	HIS	N-CA-CB	-5.11	101.41	110.60	19	1
1	A	83	LYS	O-C-N	-5.11	114.53	122.70	17	1
1	A	74	GLU	CG-CD-OE1	5.10	128.50	118.30	16	1
1	A	64	LYS	CA-C-O	-5.09	109.42	120.10	14	1
1	A	213	TYR	CZ-CE2-CD2	5.08	124.38	119.80	18	1
1	A	162	PRO	N-CA-C	5.08	125.31	112.10	2	1
1	A	154	ASN	CB-CA-C	5.08	120.56	110.40	15	1
1	A	149	PHE	CG-CD2-CE2	-5.07	115.22	120.80	2	1
1	A	153	GLY	C-N-CA	5.07	134.37	121.70	15	1
1	A	41	GLU	OE1-CD-OE2	-5.07	117.22	123.30	14	1
1	A	19	LEU	N-CA-CB	-5.06	100.27	110.40	11	1
1	A	75	TYR	CA-CB-CG	5.06	123.02	113.40	6	1
1	A	77	LEU	CB-CG-CD1	5.06	119.60	111.00	7	1
1	A	19	LEU	CB-CG-CD1	5.06	119.59	111.00	10	1
1	A	156	LEU	N-CA-C	5.05	124.65	111.00	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	155	THR	C-N-CA	5.05	134.33	121.70	14	1
1	A	217	GLY	N-CA-C	5.05	125.72	113.10	4	1
1	A	158	HIS	ND1-CE1-NE2	5.04	121.00	109.90	16	1
1	A	215	THR	C-N-CA	5.04	134.30	121.70	11	1
1	A	77	LEU	CB-CA-C	5.03	119.76	110.20	17	1
1	A	51	THR	CA-CB-CG2	-5.02	105.37	112.40	6	1
1	A	78	PHE	CG-CD1-CE1	-5.02	115.28	120.80	8	1
1	A	33	ASN	O-C-N	-5.02	114.67	122.70	12	1
1	A	17	ASP	CB-CA-C	5.02	120.44	110.40	16	1
1	A	84	TRP	CB-CG-CD2	5.01	133.12	126.60	6	1
1	A	199	SER	C-N-CA	5.01	134.24	121.70	20	1
1	A	176	GLU	CG-CD-OE1	-5.00	108.29	118.30	19	1
1	A	94	VAL	CG1-CB-CG2	-5.00	102.89	110.90	9	1

There are no chirality outliers.

All 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	23	TYR	Sidechain,Peptide	9
1	A	238	TYR	Sidechain	6
1	A	147	TYR	Sidechain	6
1	A	216	TYR	Sidechain	6
1	A	96	TYR	Sidechain,Mainchain	6
1	A	140	ARG	Sidechain,Peptide	6
1	A	190	TYR	Sidechain	5
1	A	18	TYR	Sidechain	5
1	A	91	TYR	Sidechain	4
1	A	78	PHE	Sidechain	4
1	A	25	TYR	Sidechain	4
1	A	46	PHE	Sidechain	4
1	A	21	ARG	Sidechain	4
1	A	138	PHE	Sidechain	3
1	A	149	PHE	Sidechain	3
1	A	75	TYR	Sidechain	3
1	A	107	ARG	Sidechain	3
1	A	74	GLU	Peptide	3
1	A	160	PHE	Sidechain	2
1	A	102	HIS	Sidechain	2
1	A	71	ASP	Sidechain	2
1	A	213	TYR	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	188	PHE	Sidechain	2
1	A	185	GLY	Mainchain	2
1	A	194	HIS	Sidechain	2
1	A	73	ALA	Peptide	2
1	A	148	PRO	Peptide	2
1	A	233	GLY	Mainchain	1
1	A	100	LEU	Mainchain	1
1	A	171	HIS	Sidechain	1
1	A	97	THR	Mainchain	1
1	A	155	THR	Mainchain	1
1	A	172	PHE	Sidechain	1
1	A	66	ARG	Sidechain	1
1	A	131	THR	Mainchain	1
1	A	239	GLY	Mainchain	1
1	A	177	ARG	Sidechain	1
1	A	232	LYS	Mainchain	1
1	A	79	PRO	Peptide	1
1	A	124	PHE	Sidechain	1
1	A	224	PHE	Sidechain	1
1	A	22	PHE	Sidechain	1
1	A	113	LEU	Mainchain	1
1	A	121	PRO	Peptide	1
1	A	94	VAL	Mainchain	1
1	A	144	GLY	Peptide	1
1	A	128	VAL	Peptide	1
1	A	157	ALA	Peptide	1
1	A	72	VAL	Peptide	1
1	A	154	ASN	Peptide	1
1	A	83	LYS	Peptide	1
1	A	168	GLY	Peptide	1
1	A	45	PHE	Sidechain	1
1	A	181	GLY	Peptide	1
1	A	92	ARG	Sidechain	1
1	A	32	ALA	Mainchain	1
1	A	69	VAL	Mainchain	1
1	A	180	ASP	Mainchain	1

## 6.2 Too-close contacts

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	1805	1741	1741	2±2
4	A	5842	0	9144	125±14
All	All	153020	34820	217699	2534

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 7.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:320:PX4:H17	4:A:353:PX4:H16	0.96	1.32	10	1
4:A:373:PX4:H41	4:A:421:PX4:H66	0.96	1.37	1	1
4:A:389:PX4:H50	4:A:398:PX4:H22	0.95	1.37	2	1
4:A:313:PX4:H25	4:A:348:PX4:H64	0.95	1.39	6	1
4:A:313:PX4:H26	4:A:354:PX4:H50	0.94	1.35	5	1
4:A:349:PX4:H19	4:A:363:PX4:H21	0.93	1.41	16	1
4:A:382:PX4:H17	4:A:385:PX4:H49	0.92	1.38	1	1
4:A:361:PX4:H49	4:A:362:PX4:H22	0.91	1.41	4	1
4:A:329:PX4:H60	4:A:336:PX4:H49	0.89	1.42	14	1
4:A:378:PX4:H49	4:A:411:PX4:H54	0.89	1.43	18	1
4:A:369:PX4:H19	4:A:370:PX4:H22	0.86	1.47	14	1
4:A:336:PX4:H40	4:A:399:PX4:H33	0.86	1.45	15	1
4:A:308:PX4:H55	4:A:318:PX4:H27	0.86	1.46	7	1
4:A:381:PX4:H21	4:A:385:PX4:H54	0.85	1.48	16	1
4:A:324:PX4:H20	4:A:340:PX4:H54	0.85	1.48	16	1
4:A:374:PX4:H47	4:A:398:PX4:H19	0.85	1.48	2	1
4:A:325:PX4:H53	4:A:350:PX4:H54	0.85	1.48	14	1
4:A:328:PX4:H21	4:A:335:PX4:H16	0.84	1.45	6	2
4:A:386:PX4:H21	4:A:387:PX4:H17	0.83	1.50	15	2
4:A:336:PX4:H67	4:A:352:PX4:H58	0.83	1.49	14	1
4:A:324:PX4:H64	4:A:339:PX4:H26	0.83	1.48	12	1
4:A:320:PX4:H29	4:A:328:PX4:H37	0.82	1.50	3	1
4:A:355:PX4:H20	4:A:356:PX4:H17	0.81	1.52	11	2
4:A:376:PX4:H58	4:A:430:PX4:H32	0.81	1.52	11	1
4:A:315:PX4:H67	4:A:319:PX4:H16	0.81	1.51	2	1
4:A:376:PX4:H42	4:A:398:PX4:H59	0.80	1.52	17	1
4:A:375:PX4:H66	4:A:421:PX4:H44	0.80	1.52	14	1
4:A:377:PX4:H57	4:A:384:PX4:H59	0.80	1.51	3	1
4:A:373:PX4:H20	4:A:380:PX4:H54	0.80	1.53	15	1
4:A:385:PX4:H51	4:A:387:PX4:H49	0.80	1.53	14	1
4:A:305:PX4:H31	4:A:305:PX4:H53	0.80	1.51	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:328:PX4:H16	4:A:335:PX4:H20	0.80	1.50	14	1
4:A:348:PX4:H37	4:A:349:PX4:H31	0.80	1.50	19	1
4:A:387:PX4:H60	4:A:395:PX4:H29	0.80	1.51	17	1
4:A:381:PX4:H22	4:A:395:PX4:H53	0.80	1.53	9	1
4:A:386:PX4:H48	4:A:395:PX4:H21	0.79	1.54	2	1
4:A:337:PX4:H16	4:A:354:PX4:H16	0.79	1.54	20	1
4:A:324:PX4:H67	4:A:331:PX4:H34	0.79	1.54	17	1
4:A:398:PX4:H66	4:A:403:PX4:H40	0.79	1.52	15	1
4:A:405:PX4:H48	4:A:414:PX4:H22	0.78	1.55	14	1
4:A:371:PX4:H55	4:A:412:PX4:H16	0.78	1.56	17	1
4:A:401:PX4:H42	4:A:410:PX4:H40	0.78	1.54	19	1
4:A:424:PX4:H6	4:A:424:PX4:H14	0.78	1.55	19	1
4:A:371:PX4:H58	4:A:412:PX4:H49	0.78	1.56	15	1
1:A:140:ARG:CZ	4:A:330:PX4:H4	0.78	2.09	20	3
4:A:374:PX4:H19	4:A:383:PX4:H16	0.78	1.56	10	1
4:A:404:PX4:H61	4:A:414:PX4:H29	0.77	1.57	14	1
4:A:348:PX4:H42	4:A:374:PX4:H67	0.77	1.55	16	1
4:A:347:PX4:H22	4:A:354:PX4:H20	0.77	1.57	18	1
4:A:405:PX4:H15	4:A:414:PX4:H18	0.77	1.56	1	2
4:A:402:PX4:H60	4:A:427:PX4:H31	0.77	1.57	14	1
4:A:376:PX4:H66	4:A:425:PX4:H26	0.76	1.57	18	1
4:A:346:PX4:H52	4:A:346:PX4:H27	0.76	1.54	12	1
4:A:375:PX4:H21	4:A:421:PX4:H25	0.76	1.56	19	1
4:A:318:PX4:H68	4:A:322:PX4:H59	0.76	1.57	1	1
4:A:370:PX4:H41	4:A:377:PX4:H41	0.75	1.56	10	1
4:A:305:PX4:H16	4:A:328:PX4:H4	0.75	1.57	11	1
4:A:339:PX4:H48	4:A:355:PX4:H56	0.75	1.56	13	1
4:A:357:PX4:H17	4:A:358:PX4:H22	0.75	1.56	8	1
4:A:312:PX4:H32	4:A:327:PX4:H63	0.75	1.57	7	1
4:A:375:PX4:H6	4:A:375:PX4:H14	0.75	1.58	5	1
4:A:392:PX4:H55	4:A:409:PX4:H67	0.75	1.58	7	1
4:A:387:PX4:H55	4:A:395:PX4:H60	0.74	1.58	12	1
4:A:328:PX4:H58	4:A:335:PX4:H23	0.74	1.59	20	1
4:A:336:PX4:H51	4:A:344:PX4:H53	0.74	1.59	7	1
4:A:329:PX4:H57	4:A:346:PX4:H31	0.74	1.58	8	1
4:A:332:PX4:H16	4:A:340:PX4:H26	0.74	1.58	9	1
4:A:339:PX4:H16	4:A:355:PX4:H50	0.74	1.57	19	1
4:A:333:PX4:H51	4:A:348:PX4:H53	0.74	1.60	16	1
4:A:321:PX4:H16	4:A:330:PX4:H49	0.74	1.59	1	1
4:A:376:PX4:H27	4:A:383:PX4:H25	0.74	1.58	16	1
4:A:325:PX4:H67	4:A:376:PX4:H45	0.73	1.56	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:H52	4:A:402:PX4:H31	0.73	1.58	12	1
4:A:313:PX4:H26	4:A:356:PX4:H28	0.73	1.61	6	1
4:A:348:PX4:H27	4:A:349:PX4:H48	0.73	1.59	7	2
4:A:396:PX4:H54	4:A:396:PX4:H24	0.73	1.59	10	1
4:A:376:PX4:H46	4:A:430:PX4:H17	0.72	1.61	13	4
4:A:383:PX4:H19	4:A:398:PX4:H50	0.72	1.61	13	1
4:A:307:PX4:H70	4:A:309:PX4:H21	0.72	1.61	15	1
4:A:370:PX4:H20	4:A:419:PX4:H51	0.72	1.61	9	2
4:A:330:PX4:H24	4:A:331:PX4:H27	0.72	1.60	14	1
4:A:424:PX4:H49	4:A:430:PX4:H25	0.72	1.61	6	1
4:A:379:PX4:H37	4:A:427:PX4:H37	0.72	1.61	7	1
4:A:328:PX4:H38	4:A:351:PX4:H34	0.72	1.59	2	1
4:A:388:PX4:H41	4:A:402:PX4:H32	0.72	1.61	8	1
4:A:378:PX4:H62	4:A:380:PX4:H34	0.72	1.62	13	1
4:A:404:PX4:H23	4:A:412:PX4:H48	0.72	1.62	18	1
4:A:368:PX4:H1	4:A:368:PX4:H22	0.72	1.61	1	1
4:A:352:PX4:H27	4:A:416:PX4:H44	0.72	1.59	14	1
4:A:329:PX4:H19	4:A:338:PX4:H24	0.72	1.62	12	1
4:A:352:PX4:H17	4:A:365:PX4:H22	0.72	1.60	1	1
4:A:310:PX4:H55	4:A:363:PX4:H51	0.72	1.62	10	1
4:A:362:PX4:H39	4:A:379:PX4:H39	0.71	1.61	13	1
4:A:379:PX4:H21	4:A:427:PX4:H16	0.71	1.60	20	1
4:A:325:PX4:H65	4:A:325:PX4:H33	0.71	1.60	13	1
4:A:334:PX4:H67	4:A:341:PX4:H35	0.71	1.61	17	1
4:A:324:PX4:H42	4:A:324:PX4:H62	0.71	1.61	10	1
4:A:370:PX4:H44	4:A:378:PX4:H40	0.71	1.60	5	1
4:A:328:PX4:H49	4:A:335:PX4:H28	0.71	1.63	8	1
4:A:336:PX4:H15	4:A:351:PX4:H58	0.71	1.62	8	1
4:A:378:PX4:H59	4:A:379:PX4:H37	0.71	1.61	16	1
4:A:368:PX4:H58	4:A:376:PX4:H57	0.71	1.60	3	1
4:A:332:PX4:H38	4:A:340:PX4:H67	0.70	1.62	8	1
4:A:329:PX4:H22	4:A:351:PX4:H53	0.70	1.62	20	1
4:A:348:PX4:H49	4:A:356:PX4:H49	0.70	1.63	8	1
4:A:407:PX4:H37	4:A:423:PX4:H41	0.70	1.61	13	1
4:A:401:PX4:H16	4:A:427:PX4:H47	0.70	1.63	6	2
4:A:407:PX4:H32	4:A:423:PX4:H29	0.70	1.61	19	1
4:A:308:PX4:H24	4:A:315:PX4:H17	0.70	1.61	7	2
4:A:308:PX4:H65	4:A:314:PX4:H61	0.70	1.62	18	1
4:A:312:PX4:H62	4:A:317:PX4:H64	0.70	1.64	19	1
4:A:342:PX4:H19	4:A:351:PX4:H22	0.70	1.62	18	1
4:A:381:PX4:H60	4:A:387:PX4:H35	0.70	1.63	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H58	4:A:424:PX4:H30	0.70	1.62	8	1
4:A:406:PX4:H23	4:A:408:PX4:H39	0.70	1.62	5	1
4:A:380:PX4:H20	4:A:411:PX4:H47	0.69	1.61	13	1
4:A:306:PX4:H63	4:A:333:PX4:H59	0.69	1.62	6	1
4:A:390:PX4:H48	4:A:399:PX4:H49	0.69	1.64	20	1
4:A:425:PX4:H25	4:A:430:PX4:H21	0.69	1.64	20	1
4:A:324:PX4:H72	4:A:355:PX4:H67	0.69	1.64	10	1
4:A:392:PX4:H66	4:A:402:PX4:H62	0.69	1.62	6	1
4:A:337:PX4:H20	4:A:346:PX4:H26	0.69	1.64	15	1
4:A:353:PX4:H63	4:A:360:PX4:H49	0.69	1.62	9	1
4:A:384:PX4:H16	4:A:400:PX4:H20	0.69	1.65	9	1
4:A:309:PX4:H67	4:A:399:PX4:H67	0.69	1.64	8	1
4:A:380:PX4:H17	4:A:381:PX4:O6	0.69	1.88	7	2
4:A:372:PX4:O2	4:A:373:PX4:H18	0.69	1.87	7	1
4:A:391:PX4:H52	4:A:400:PX4:H57	0.69	1.64	14	1
4:A:316:PX4:H68	4:A:317:PX4:H30	0.69	1.63	20	1
4:A:344:PX4:H57	4:A:346:PX4:H31	0.69	1.64	10	1
4:A:334:PX4:H15	4:A:341:PX4:H16	0.69	1.64	6	1
4:A:393:PX4:H39	4:A:400:PX4:H40	0.69	1.64	2	1
4:A:424:PX4:H35	4:A:425:PX4:H67	0.69	1.63	3	1
4:A:317:PX4:H46	4:A:343:PX4:H17	0.69	1.65	6	1
4:A:328:PX4:H57	4:A:335:PX4:H31	0.68	1.65	17	1
4:A:377:PX4:H22	4:A:378:PX4:H16	0.68	1.64	20	1
4:A:394:PX4:H38	4:A:418:PX4:H27	0.68	1.64	14	1
4:A:373:PX4:H33	4:A:421:PX4:H72	0.68	1.64	14	1
4:A:392:PX4:H59	4:A:418:PX4:H27	0.68	1.65	8	1
4:A:403:PX4:H56	4:A:404:PX4:H62	0.68	1.64	12	1
4:A:305:PX4:H28	4:A:335:PX4:H28	0.68	1.65	4	1
4:A:377:PX4:H16	4:A:378:PX4:H20	0.68	1.66	10	2
4:A:373:PX4:H54	4:A:381:PX4:H52	0.68	1.66	7	1
4:A:376:PX4:H22	4:A:390:PX4:H25	0.68	1.64	7	1
4:A:332:PX4:H22	4:A:340:PX4:H25	0.68	1.65	20	1
4:A:331:PX4:H61	4:A:346:PX4:H60	0.68	1.65	15	1
4:A:388:PX4:H20	4:A:395:PX4:H17	0.68	1.66	7	2
4:A:384:PX4:H20	4:A:400:PX4:H16	0.68	1.66	4	5
4:A:417:PX4:H46	4:A:426:PX4:H19	0.68	1.66	2	1
4:A:419:PX4:H37	4:A:426:PX4:H66	0.68	1.65	4	1
4:A:308:PX4:H64	4:A:372:PX4:H42	0.67	1.64	5	1
4:A:386:PX4:H66	4:A:402:PX4:H33	0.67	1.64	15	1
4:A:378:PX4:H42	4:A:387:PX4:H31	0.67	1.65	17	1
4:A:379:PX4:H28	4:A:427:PX4:H28	0.67	1.65	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:H29	4:A:355:PX4:H33	0.67	1.65	10	1
4:A:394:PX4:H23	4:A:412:PX4:H49	0.67	1.65	10	1
4:A:409:PX4:H65	4:A:410:PX4:H65	0.67	1.66	18	1
4:A:305:PX4:H25	4:A:320:PX4:H33	0.67	1.64	2	1
4:A:337:PX4:H46	4:A:346:PX4:H48	0.67	1.66	17	1
4:A:386:PX4:H62	4:A:402:PX4:H29	0.67	1.67	16	1
4:A:345:PX4:H46	4:A:354:PX4:H16	0.67	1.65	19	1
4:A:369:PX4:H47	4:A:370:PX4:H25	0.67	1.66	19	1
4:A:333:PX4:H35	4:A:339:PX4:H67	0.67	1.65	12	1
4:A:384:PX4:H17	4:A:393:PX4:H20	0.67	1.65	14	1
4:A:390:PX4:H17	4:A:397:PX4:H66	0.67	1.65	8	1
4:A:384:PX4:H28	4:A:400:PX4:H52	0.67	1.65	12	1
4:A:337:PX4:H61	4:A:355:PX4:H40	0.67	1.67	18	1
4:A:307:PX4:H21	4:A:363:PX4:H26	0.67	1.65	7	1
4:A:325:PX4:H31	4:A:349:PX4:H59	0.67	1.65	1	1
4:A:305:PX4:H51	4:A:362:PX4:H48	0.67	1.67	12	1
4:A:417:PX4:H69	4:A:426:PX4:H40	0.67	1.66	12	1
4:A:400:PX4:H49	4:A:425:PX4:H27	0.67	1.66	12	1
4:A:419:PX4:H22	4:A:426:PX4:H50	0.67	1.66	18	1
4:A:355:PX4:H21	4:A:356:PX4:H15	0.67	1.67	7	1
4:A:399:PX4:H19	4:A:408:PX4:H14	0.67	1.65	1	2
4:A:413:PX4:H29	4:A:422:PX4:H24	0.67	1.67	4	1
4:A:309:PX4:H19	4:A:366:PX4:H49	0.67	1.64	5	1
4:A:405:PX4:H19	4:A:420:PX4:H21	0.67	1.64	5	1
4:A:306:PX4:H59	4:A:311:PX4:H55	0.67	1.67	15	1
4:A:339:PX4:H9	4:A:340:PX4:H51	0.66	1.66	14	1
4:A:384:PX4:H28	4:A:400:PX4:H58	0.66	1.65	19	1
4:A:376:PX4:H24	4:A:429:PX4:H31	0.66	1.64	10	1
4:A:308:PX4:H70	4:A:382:PX4:H39	0.66	1.67	5	1
4:A:401:PX4:H25	4:A:427:PX4:H48	0.66	1.67	18	1
4:A:336:PX4:H45	4:A:399:PX4:H29	0.66	1.66	15	1
4:A:388:PX4:H54	4:A:389:PX4:H48	0.66	1.64	7	1
4:A:379:PX4:H71	4:A:380:PX4:H45	0.66	1.66	4	1
4:A:347:PX4:H72	4:A:351:PX4:H21	0.66	1.67	2	1
4:A:337:PX4:H67	4:A:355:PX4:H40	0.66	1.67	2	1
4:A:348:PX4:H60	4:A:355:PX4:H32	0.66	1.66	10	1
4:A:316:PX4:H19	4:A:334:PX4:H66	0.66	1.65	18	1
4:A:327:PX4:H39	4:A:360:PX4:H32	0.66	1.67	18	1
4:A:334:PX4:H26	4:A:341:PX4:H22	0.66	1.68	17	1
4:A:305:PX4:H38	4:A:322:PX4:H26	0.66	1.67	13	1
4:A:373:PX4:H20	4:A:380:PX4:H20	0.66	1.68	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:309:PX4:H67	4:A:383:PX4:H66	0.66	1.67	9	1
4:A:369:PX4:O8	4:A:391:PX4:H5	0.66	1.90	2	1
4:A:330:PX4:H15	4:A:331:PX4:H18	0.66	1.68	20	1
4:A:338:PX4:H32	4:A:346:PX4:H67	0.66	1.66	14	1
4:A:423:PX4:H17	4:A:424:PX4:H24	0.66	1.65	16	1
4:A:393:PX4:H58	4:A:408:PX4:H41	0.66	1.67	9	1
4:A:329:PX4:H27	4:A:347:PX4:H54	0.66	1.67	1	1
4:A:384:PX4:H60	4:A:393:PX4:H29	0.65	1.67	4	1
4:A:318:PX4:H28	4:A:319:PX4:H65	0.65	1.68	20	1
4:A:325:PX4:H63	4:A:341:PX4:H59	0.65	1.68	20	1
4:A:336:PX4:H62	4:A:366:PX4:H16	0.65	1.67	8	1
4:A:354:PX4:H22	4:A:356:PX4:H29	0.65	1.69	4	1
4:A:309:PX4:H27	4:A:366:PX4:H23	0.65	1.68	4	1
4:A:332:PX4:H20	4:A:340:PX4:H16	0.65	1.67	11	4
4:A:308:PX4:H17	4:A:318:PX4:H49	0.65	1.68	16	1
4:A:411:PX4:H36	4:A:419:PX4:H54	0.65	1.68	5	1
4:A:392:PX4:H17	4:A:409:PX4:H61	0.65	1.67	15	3
4:A:383:PX4:H45	4:A:412:PX4:H63	0.65	1.68	3	1
4:A:371:PX4:H69	4:A:389:PX4:H45	0.65	1.66	2	1
4:A:417:PX4:H57	4:A:427:PX4:H63	0.65	1.67	3	1
4:A:384:PX4:H68	4:A:386:PX4:H55	0.65	1.68	1	1
4:A:381:PX4:H46	4:A:385:PX4:H16	0.65	1.67	14	1
4:A:313:PX4:H60	4:A:348:PX4:H20	0.65	1.67	13	1
4:A:326:PX4:H14	4:A:343:PX4:H15	0.65	1.68	4	1
4:A:370:PX4:H17	4:A:419:PX4:H47	0.65	1.65	2	1
4:A:401:PX4:H64	4:A:410:PX4:H33	0.65	1.67	18	1
4:A:314:PX4:H28	4:A:354:PX4:H56	0.65	1.69	4	1
4:A:376:PX4:H51	4:A:430:PX4:H48	0.65	1.68	7	1
4:A:380:PX4:H29	4:A:381:PX4:H32	0.65	1.69	3	1
4:A:322:PX4:H29	4:A:332:PX4:H28	0.65	1.67	5	1
4:A:328:PX4:H62	4:A:332:PX4:H29	0.65	1.68	14	1
4:A:404:PX4:H21	4:A:405:PX4:H40	0.65	1.69	9	1
4:A:338:PX4:H66	4:A:400:PX4:H38	0.65	1.68	4	1
4:A:325:PX4:H39	4:A:382:PX4:H41	0.65	1.69	20	1
4:A:322:PX4:H21	4:A:332:PX4:H49	0.64	1.68	8	1
4:A:322:PX4:H39	4:A:340:PX4:H21	0.64	1.67	8	1
4:A:418:PX4:H67	4:A:420:PX4:H72	0.64	1.67	10	1
4:A:401:PX4:H69	4:A:417:PX4:H44	0.64	1.67	13	1
4:A:409:PX4:H21	4:A:416:PX4:H21	0.64	1.67	13	1
4:A:384:PX4:H25	4:A:400:PX4:H16	0.64	1.69	12	1
4:A:319:PX4:H43	4:A:407:PX4:H33	0.64	1.68	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:347:PX4:H20	4:A:355:PX4:H47	0.64	1.69	2	1
4:A:359:PX4:H28	4:A:407:PX4:H37	0.64	1.67	2	1
4:A:423:PX4:H55	4:A:426:PX4:H22	0.64	1.70	2	1
4:A:328:PX4:H60	4:A:328:PX4:H39	0.64	1.67	3	1
4:A:333:PX4:H39	4:A:389:PX4:H67	0.64	1.68	3	1
4:A:330:PX4:H68	4:A:331:PX4:H42	0.64	1.68	1	1
4:A:387:PX4:H53	4:A:387:PX4:H33	0.64	1.70	14	1
4:A:424:PX4:H34	4:A:424:PX4:H62	0.64	1.69	8	1
4:A:336:PX4:H67	4:A:360:PX4:H63	0.64	1.69	16	1
4:A:372:PX4:H46	4:A:428:PX4:H59	0.64	1.70	5	1
4:A:313:PX4:H46	4:A:348:PX4:H54	0.64	1.69	18	1
4:A:342:PX4:H36	4:A:351:PX4:H49	0.64	1.69	7	1
4:A:409:PX4:H19	4:A:410:PX4:H51	0.64	1.70	8	1
4:A:385:PX4:H47	4:A:387:PX4:H16	0.64	1.68	16	1
4:A:306:PX4:H24	4:A:313:PX4:H38	0.64	1.69	7	1
4:A:347:PX4:H68	4:A:351:PX4:H70	0.64	1.69	16	1
4:A:325:PX4:H44	4:A:382:PX4:H35	0.64	1.69	20	1
4:A:316:PX4:H47	4:A:325:PX4:H55	0.64	1.69	16	1
4:A:393:PX4:H48	4:A:394:PX4:C25	0.64	2.22	6	1
4:A:321:PX4:H16	4:A:330:PX4:H19	0.64	1.68	20	1
4:A:422:PX4:H19	4:A:431:PX4:H49	0.64	1.67	4	1
4:A:329:PX4:H37	4:A:336:PX4:H32	0.64	1.69	2	1
4:A:336:PX4:H43	4:A:399:PX4:H23	0.64	1.70	17	1
4:A:411:PX4:H18	4:A:427:PX4:H49	0.64	1.70	10	2
4:A:390:PX4:H26	4:A:398:PX4:H66	0.64	1.68	13	1
4:A:375:PX4:H28	4:A:413:PX4:H66	0.64	1.70	16	1
4:A:330:PX4:H53	4:A:331:PX4:H21	0.64	1.69	12	1
4:A:307:PX4:H64	4:A:396:PX4:H64	0.63	1.70	5	1
4:A:329:PX4:H28	4:A:338:PX4:H62	0.63	1.70	18	1
4:A:369:PX4:H64	4:A:391:PX4:H29	0.63	1.70	7	1
4:A:400:PX4:H49	4:A:408:PX4:H11	0.63	1.68	20	1
4:A:409:PX4:H18	4:A:416:PX4:H14	0.63	1.70	15	1
4:A:413:PX4:H65	4:A:383:PX4:H63	0.63	1.70	1	1
4:A:408:PX4:H51	4:A:415:PX4:H59	0.63	1.69	14	1
4:A:399:PX4:H37	4:A:408:PX4:H67	0.63	1.70	18	1
4:A:379:PX4:H38	4:A:427:PX4:H71	0.63	1.70	4	1
4:A:380:PX4:H17	4:A:381:PX4:H18	0.63	1.69	2	1
4:A:318:PX4:H62	4:A:340:PX4:H28	0.63	1.70	15	1
4:A:335:PX4:H21	4:A:342:PX4:H47	0.63	1.68	8	1
4:A:407:PX4:H1	4:A:417:PX4:H8	0.63	1.70	16	1
4:A:321:PX4:H33	4:A:331:PX4:H62	0.63	1.70	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H67	4:A:370:PX4:H39	0.63	1.71	11	1
4:A:317:PX4:H27	4:A:318:PX4:H17	0.63	1.70	2	1
4:A:355:PX4:H59	4:A:356:PX4:H65	0.63	1.70	14	1
4:A:417:PX4:O2	4:A:419:PX4:H10	0.63	1.94	16	1
4:A:373:PX4:H65	4:A:380:PX4:H65	0.63	1.71	9	1
4:A:372:PX4:H36	4:A:421:PX4:H38	0.63	1.70	7	1
4:A:333:PX4:H18	4:A:356:PX4:H56	0.63	1.69	14	1
4:A:337:PX4:H19	4:A:344:PX4:H50	0.63	1.70	18	1
4:A:389:PX4:H54	4:A:398:PX4:H26	0.63	1.69	2	1
4:A:326:PX4:H52	4:A:343:PX4:H47	0.63	1.69	1	1
4:A:371:PX4:H68	4:A:412:PX4:H63	0.63	1.71	5	1
4:A:307:PX4:H56	4:A:310:PX4:H53	0.63	1.70	12	1
4:A:371:PX4:H68	4:A:388:PX4:H28	0.63	1.69	7	1
4:A:317:PX4:O6	4:A:318:PX4:H11	0.63	1.94	17	1
4:A:392:PX4:H25	4:A:393:PX4:H47	0.62	1.69	1	1
4:A:391:PX4:H24	4:A:425:PX4:H49	0.62	1.70	18	1
4:A:378:PX4:H65	4:A:411:PX4:H59	0.62	1.70	9	1
4:A:414:PX4:H34	4:A:431:PX4:H25	0.62	1.71	8	1
4:A:421:PX4:H58	4:A:428:PX4:H21	0.62	1.70	13	1
4:A:374:PX4:H51	4:A:385:PX4:H58	0.62	1.71	7	1
4:A:358:PX4:H70	4:A:408:PX4:H70	0.62	1.70	16	1
4:A:345:PX4:H62	4:A:354:PX4:H30	0.62	1.72	19	1
4:A:337:PX4:H36	4:A:338:PX4:H44	0.62	1.72	9	1
4:A:308:PX4:H4	4:A:319:PX4:O3	0.62	1.94	11	1
1:A:142:ALA:HB2	4:A:321:PX4:H7	0.62	1.70	3	1
4:A:336:PX4:H48	4:A:352:PX4:H13	0.62	1.71	9	1
4:A:374:PX4:H46	4:A:382:PX4:H16	0.62	1.72	13	1
4:A:403:PX4:H27	4:A:403:PX4:H49	0.62	1.72	20	1
4:A:380:PX4:H20	4:A:411:PX4:H49	0.62	1.71	7	1
4:A:384:PX4:H39	4:A:400:PX4:H33	0.62	1.70	19	1
4:A:371:PX4:H48	4:A:404:PX4:H18	0.62	1.72	16	1
4:A:347:PX4:H31	4:A:355:PX4:H26	0.61	1.71	19	1
4:A:396:PX4:H23	4:A:405:PX4:H56	0.61	1.70	19	1
4:A:404:PX4:H56	4:A:405:PX4:H49	0.61	1.72	13	2
4:A:327:PX4:H31	4:A:353:PX4:H65	0.61	1.69	18	1
4:A:305:PX4:H60	4:A:362:PX4:H59	0.61	1.69	4	1
4:A:350:PX4:H50	4:A:363:PX4:H51	0.61	1.70	15	1
4:A:406:PX4:H25	4:A:409:PX4:H34	0.61	1.72	3	1
4:A:423:PX4:H38	4:A:424:PX4:H34	0.61	1.71	3	1
4:A:387:PX4:H32	4:A:387:PX4:H48	0.61	1.72	14	1
4:A:333:PX4:H69	4:A:371:PX4:H70	0.61	1.70	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:348:PX4:H35	4:A:363:PX4:H54	0.61	1.70	8	1
4:A:319:PX4:H22	4:A:327:PX4:H65	0.61	1.72	17	1
4:A:403:PX4:H48	4:A:412:PX4:H17	0.61	1.72	14	1
4:A:324:PX4:H37	4:A:382:PX4:H37	0.61	1.72	16	1
4:A:375:PX4:H47	4:A:421:PX4:H27	0.61	1.72	16	1
4:A:394:PX4:H53	4:A:402:PX4:H30	0.61	1.71	6	1
4:A:371:PX4:H58	4:A:404:PX4:H28	0.61	1.72	4	1
4:A:402:PX4:H52	4:A:392:PX4:H54	0.61	1.73	1	1
4:A:368:PX4:H62	4:A:390:PX4:H34	0.61	1.71	5	1
4:A:369:PX4:H55	4:A:391:PX4:H22	0.61	1.72	11	1
4:A:385:PX4:H26	4:A:387:PX4:H24	0.61	1.71	13	1
4:A:405:PX4:H62	4:A:414:PX4:H29	0.61	1.71	6	1
4:A:401:PX4:H23	4:A:427:PX4:H31	0.61	1.72	7	1
4:A:402:PX4:H65	4:A:392:PX4:H66	0.61	1.73	1	1
4:A:345:PX4:H38	4:A:365:PX4:H33	0.61	1.72	12	1
4:A:325:PX4:H48	4:A:339:PX4:H61	0.61	1.71	17	1
4:A:386:PX4:O8	4:A:394:PX4:H13	0.61	1.96	12	1
4:A:359:PX4:H48	4:A:367:PX4:H23	0.61	1.72	2	1
4:A:386:PX4:H39	4:A:387:PX4:H36	0.61	1.71	2	1
4:A:354:PX4:H23	4:A:356:PX4:H57	0.61	1.72	20	1
4:A:361:PX4:H40	4:A:364:PX4:H37	0.61	1.72	20	1
4:A:320:PX4:H65	4:A:328:PX4:H57	0.61	1.71	13	1
4:A:371:PX4:H53	4:A:388:PX4:H17	0.61	1.72	6	1
4:A:342:PX4:H39	4:A:357:PX4:H43	0.61	1.73	12	1
4:A:308:PX4:H36	4:A:312:PX4:H41	0.61	1.73	18	1
4:A:423:PX4:H34	4:A:424:PX4:H34	0.61	1.71	19	1
4:A:342:PX4:H31	4:A:358:PX4:H39	0.61	1.73	2	1
4:A:329:PX4:H14	4:A:351:PX4:H15	0.61	1.73	1	1
4:A:341:PX4:H47	4:A:341:PX4:H28	0.60	1.73	17	1
4:A:338:PX4:H30	4:A:347:PX4:H56	0.60	1.73	17	1
4:A:307:PX4:H8	4:A:310:PX4:O3	0.60	1.95	10	1
4:A:307:PX4:H61	4:A:311:PX4:H28	0.60	1.72	7	1
4:A:377:PX4:H68	4:A:391:PX4:H58	0.60	1.73	10	1
4:A:307:PX4:H43	4:A:405:PX4:H57	0.60	1.73	13	1
4:A:347:PX4:H29	4:A:356:PX4:H63	0.60	1.73	16	1
4:A:373:PX4:H17	4:A:380:PX4:H49	0.60	1.74	12	1
4:A:368:PX4:H63	4:A:376:PX4:H43	0.60	1.71	15	1
4:A:383:PX4:H38	4:A:389:PX4:H49	0.60	1.71	10	1
4:A:377:PX4:H58	4:A:387:PX4:H22	0.60	1.72	16	1
4:A:419:PX4:H20	4:A:426:PX4:H16	0.60	1.73	2	5
4:A:394:PX4:H48	4:A:402:PX4:H27	0.60	1.73	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:419:PX4:H32	4:A:424:PX4:H38	0.60	1.73	9	1
4:A:308:PX4:H51	4:A:318:PX4:H25	0.60	1.73	3	1
4:A:308:PX4:H23	4:A:319:PX4:H48	0.60	1.72	16	1
4:A:385:PX4:H15	4:A:387:PX4:H19	0.60	1.71	6	1
4:A:354:PX4:H63	4:A:356:PX4:H42	0.60	1.71	9	1
4:A:321:PX4:H52	4:A:330:PX4:H28	0.60	1.72	15	1
4:A:313:PX4:H17	4:A:348:PX4:H52	0.60	1.74	1	1
4:A:369:PX4:H66	4:A:425:PX4:H69	0.60	1.74	1	1
4:A:388:PX4:O2	4:A:389:PX4:H8	0.60	1.96	7	1
4:A:378:PX4:H50	4:A:411:PX4:H15	0.60	1.73	8	1
4:A:341:PX4:H59	4:A:350:PX4:H58	0.60	1.74	7	1
4:A:325:PX4:O6	4:A:349:PX4:H9	0.60	1.97	11	1
4:A:335:PX4:H67	4:A:353:PX4:H38	0.60	1.72	15	1
4:A:342:PX4:H32	4:A:351:PX4:H53	0.60	1.71	16	1
4:A:377:PX4:H59	4:A:386:PX4:H20	0.60	1.72	16	1
4:A:318:PX4:H50	4:A:323:PX4:H49	0.60	1.72	6	1
4:A:336:PX4:H30	4:A:351:PX4:H60	0.60	1.74	18	1
4:A:352:PX4:H41	4:A:358:PX4:H57	0.60	1.74	18	1
4:A:373:PX4:H57	4:A:380:PX4:H55	0.60	1.72	8	1
4:A:387:PX4:H18	4:A:387:PX4:H1	0.60	1.72	12	1
4:A:324:PX4:H47	4:A:339:PX4:H15	0.60	1.73	9	1
4:A:370:PX4:H47	4:A:419:PX4:H17	0.59	1.74	17	2
4:A:309:PX4:H35	4:A:366:PX4:H42	0.59	1.72	18	1
4:A:309:PX4:H38	4:A:357:PX4:H70	0.59	1.74	4	1
4:A:392:PX4:H19	4:A:393:PX4:H49	0.59	1.74	4	1
4:A:379:PX4:H62	4:A:380:PX4:H37	0.59	1.74	2	1
4:A:385:PX4:H15	4:A:387:PX4:H20	0.59	1.72	1	2
4:A:377:PX4:H58	4:A:378:PX4:H31	0.59	1.71	13	1
4:A:354:PX4:H65	4:A:364:PX4:H39	0.59	1.71	7	1
4:A:384:PX4:H48	4:A:400:PX4:H19	0.59	1.74	7	1
4:A:375:PX4:H57	4:A:382:PX4:H50	0.59	1.73	20	1
4:A:351:PX4:H61	4:A:358:PX4:H66	0.59	1.72	17	1
4:A:378:PX4:H17	4:A:385:PX4:H19	0.59	1.74	13	1
4:A:348:PX4:H63	4:A:356:PX4:H32	0.59	1.74	6	1
4:A:317:PX4:H40	4:A:318:PX4:H53	0.59	1.72	11	1
4:A:394:PX4:H33	4:A:418:PX4:H26	0.59	1.74	15	1
4:A:323:PX4:H33	4:A:375:PX4:H43	0.59	1.74	1	1
4:A:348:PX4:H25	4:A:349:PX4:H22	0.59	1.73	3	1
4:A:375:PX4:H52	4:A:382:PX4:H19	0.59	1.74	14	1
4:A:418:PX4:H17	4:A:427:PX4:H23	0.59	1.73	16	2
4:A:382:PX4:H38	4:A:421:PX4:H30	0.59	1.75	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:311:PX4:H71	4:A:404:PX4:H69	0.59	1.73	5	1
4:A:345:PX4:H38	4:A:395:PX4:H42	0.59	1.74	18	1
4:A:405:PX4:H26	4:A:431:PX4:H27	0.59	1.74	18	1
4:A:321:PX4:H16	4:A:330:PX4:H21	0.59	1.75	11	1
4:A:332:PX4:H43	4:A:375:PX4:H43	0.59	1.74	15	1
4:A:397:PX4:H37	4:A:403:PX4:H36	0.59	1.75	14	1
4:A:375:PX4:H27	4:A:421:PX4:H41	0.59	1.73	16	1
4:A:413:PX4:H26	4:A:431:PX4:H17	0.59	1.73	16	1
4:A:369:PX4:H62	4:A:391:PX4:H33	0.59	1.74	5	1
4:A:337:PX4:H27	4:A:344:PX4:H51	0.59	1.73	6	1
4:A:418:PX4:H52	4:A:427:PX4:H33	0.59	1.73	15	1
4:A:314:PX4:H24	4:A:354:PX4:H46	0.59	1.73	19	1
4:A:305:PX4:H41	4:A:321:PX4:H67	0.59	1.75	6	1
4:A:342:PX4:H28	4:A:358:PX4:H35	0.59	1.74	11	1
4:A:383:PX4:H61	4:A:390:PX4:H31	0.59	1.75	14	1
4:A:313:PX4:H19	4:A:354:PX4:H23	0.59	1.74	19	1
4:A:371:PX4:H26	4:A:418:PX4:H50	0.59	1.73	10	1
4:A:325:PX4:H19	4:A:349:PX4:H53	0.59	1.73	9	1
4:A:424:PX4:H33	4:A:426:PX4:H55	0.59	1.72	4	1
4:A:313:PX4:H34	4:A:364:PX4:H34	0.59	1.73	3	1
4:A:312:PX4:H19	4:A:327:PX4:H54	0.59	1.75	19	1
4:A:420:PX4:H16	4:A:428:PX4:H47	0.58	1.75	16	2
4:A:344:PX4:H16	4:A:345:PX4:H17	0.58	1.74	9	1
4:A:306:PX4:H47	4:A:364:PX4:H33	0.58	1.74	9	1
4:A:413:PX4:H42	4:A:431:PX4:H28	0.58	1.75	4	1
4:A:379:PX4:H19	4:A:427:PX4:H20	0.58	1.75	2	1
4:A:368:PX4:H61	4:A:376:PX4:H56	0.58	1.73	17	1
4:A:378:PX4:H45	4:A:380:PX4:H35	0.58	1.75	10	1
4:A:369:PX4:H3	4:A:370:PX4:H18	0.58	1.74	5	1
4:A:401:PX4:H57	4:A:417:PX4:H48	0.58	1.74	6	1
4:A:333:PX4:H24	4:A:339:PX4:H53	0.58	1.73	14	1
4:A:369:PX4:H52	4:A:391:PX4:H22	0.58	1.75	10	1
4:A:339:PX4:H48	4:A:355:PX4:H60	0.58	1.73	6	1
4:A:409:PX4:H18	4:A:416:PX4:O6	0.58	1.98	18	1
4:A:320:PX4:H60	4:A:328:PX4:H56	0.58	1.75	7	1
4:A:382:PX4:H52	4:A:389:PX4:H54	0.58	1.74	11	1
4:A:337:PX4:H19	4:A:346:PX4:H28	0.58	1.74	2	1
4:A:402:PX4:H48	4:A:418:PX4:H26	0.58	1.74	17	1
4:A:312:PX4:H59	4:A:317:PX4:H61	0.58	1.74	19	1
4:A:389:PX4:H27	4:A:403:PX4:H49	0.58	1.76	8	1
4:A:313:PX4:H36	4:A:364:PX4:H33	0.58	1.76	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:305:PX4:H17	4:A:362:PX4:O7	0.58	1.99	5	1
4:A:398:PX4:H39	4:A:429:PX4:H41	0.58	1.74	5	1
4:A:344:PX4:H49	4:A:345:PX4:H49	0.58	1.75	18	1
4:A:313:PX4:H19	4:A:348:PX4:H65	0.58	1.73	11	1
4:A:384:PX4:H66	4:A:395:PX4:H35	0.58	1.74	2	1
4:A:343:PX4:H37	4:A:343:PX4:H69	0.58	1.74	15	1
4:A:392:PX4:H23	4:A:399:PX4:H21	0.58	1.73	15	1
4:A:357:PX4:H41	4:A:408:PX4:H58	0.58	1.75	14	1
4:A:346:PX4:H62	4:A:346:PX4:H38	0.58	1.76	19	1
4:A:341:PX4:H34	4:A:408:PX4:H66	0.58	1.76	13	1
4:A:369:PX4:H27	4:A:370:PX4:H34	0.58	1.76	11	1
4:A:376:PX4:H34	4:A:398:PX4:H72	0.58	1.76	4	1
4:A:401:PX4:H48	4:A:410:PX4:H19	0.58	1.75	15	1
4:A:362:PX4:H28	4:A:365:PX4:H49	0.58	1.76	14	1
4:A:419:PX4:H21	4:A:426:PX4:H20	0.58	1.76	7	1
4:A:413:PX4:H56	4:A:421:PX4:H17	0.58	1.74	4	1
4:A:332:PX4:H16	4:A:340:PX4:C10	0.58	2.29	20	1
4:A:373:PX4:H17	4:A:380:PX4:H46	0.58	1.75	17	1
4:A:372:PX4:H17	4:A:428:PX4:H22	0.58	1.74	14	1
4:A:327:PX4:H41	4:A:353:PX4:H41	0.58	1.74	8	1
4:A:392:PX4:H16	4:A:393:PX4:H15	0.58	1.75	8	1
4:A:337:PX4:H31	4:A:344:PX4:H55	0.58	1.76	6	1
4:A:375:PX4:H27	4:A:429:PX4:H20	0.58	1.76	18	1
4:A:370:PX4:H31	4:A:377:PX4:H35	0.58	1.76	4	1
4:A:374:PX4:H26	4:A:429:PX4:H34	0.58	1.75	3	1
4:A:325:PX4:H20	4:A:348:PX4:H24	0.58	1.76	13	2
4:A:327:PX4:H24	4:A:353:PX4:H31	0.58	1.75	19	1
4:A:386:PX4:H52	4:A:394:PX4:H2	0.58	1.74	5	1
4:A:368:PX4:H14	4:A:429:PX4:H14	0.57	1.75	6	2
4:A:338:PX4:H54	4:A:351:PX4:H24	0.57	1.74	7	1
4:A:353:PX4:H39	4:A:362:PX4:H68	0.57	1.76	20	1
4:A:311:PX4:H49	4:A:363:PX4:H31	0.57	1.76	1	1
4:A:392:PX4:H56	4:A:409:PX4:H54	0.57	1.76	9	1
4:A:423:PX4:H47	4:A:426:PX4:H17	0.57	1.75	3	1
4:A:357:PX4:H17	4:A:358:PX4:H20	0.57	1.75	14	1
4:A:312:PX4:H14	4:A:319:PX4:H15	0.57	1.76	19	1
4:A:357:PX4:H40	4:A:358:PX4:H37	0.57	1.75	8	1
4:A:334:PX4:H48	4:A:343:PX4:H19	0.57	1.77	10	1
4:A:379:PX4:H53	4:A:418:PX4:H55	0.57	1.76	16	1
4:A:377:PX4:H14	4:A:378:PX4:O1	0.57	1.99	9	1
4:A:401:PX4:H71	4:A:401:PX4:H39	0.57	1.75	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H23	4:A:393:PX4:H27	0.57	1.75	1	1
4:A:394:PX4:H66	4:A:400:PX4:H34	0.57	1.75	8	1
4:A:338:PX4:H31	4:A:346:PX4:H29	0.57	1.75	18	1
4:A:374:PX4:H10	4:A:382:PX4:H18	0.57	1.75	20	1
4:A:407:PX4:H34	4:A:423:PX4:H28	0.57	1.75	20	1
4:A:378:PX4:H59	4:A:411:PX4:H24	0.57	1.76	20	1
4:A:391:PX4:H56	4:A:425:PX4:H67	0.57	1.76	14	1
4:A:305:PX4:H24	4:A:320:PX4:H59	0.57	1.77	10	1
4:A:328:PX4:H19	4:A:335:PX4:H16	0.57	1.76	15	2
4:A:369:PX4:H59	4:A:391:PX4:H28	0.57	1.77	20	1
4:A:330:PX4:H46	4:A:331:PX4:H7	0.57	1.75	1	1
4:A:328:PX4:H16	4:A:342:PX4:H57	0.57	1.75	17	1
4:A:418:PX4:H64	4:A:428:PX4:H66	0.57	1.77	16	1
4:A:326:PX4:H16	4:A:327:PX4:C26	0.57	2.29	9	1
4:A:417:PX4:H51	4:A:419:PX4:H49	0.57	1.77	4	1
4:A:338:PX4:H71	4:A:425:PX4:H66	0.57	1.77	14	1
4:A:378:PX4:H58	4:A:380:PX4:H32	0.57	1.76	8	1
4:A:381:PX4:C11	4:A:385:PX4:H54	0.57	2.26	16	1
4:A:333:PX4:H34	4:A:339:PX4:H55	0.57	1.76	9	1
4:A:357:PX4:H34	4:A:429:PX4:H39	0.57	1.76	9	1
4:A:390:PX4:H20	4:A:430:PX4:H55	0.57	1.75	17	1
4:A:331:PX4:H60	4:A:346:PX4:H65	0.57	1.76	7	1
4:A:377:PX4:H42	4:A:419:PX4:H51	0.57	1.77	11	1
4:A:389:PX4:H32	4:A:403:PX4:H29	0.57	1.77	2	1
4:A:315:PX4:H67	4:A:319:PX4:H32	0.57	1.75	19	1
4:A:397:PX4:H12	4:A:397:PX4:H14	0.57	1.76	8	1
4:A:319:PX4:H62	4:A:429:PX4:H71	0.57	1.76	13	1
4:A:368:PX4:H35	4:A:429:PX4:H64	0.57	1.77	12	1
4:A:372:PX4:H21	4:A:421:PX4:H48	0.57	1.77	2	1
4:A:331:PX4:H50	4:A:347:PX4:H18	0.57	1.75	15	1
4:A:317:PX4:H36	4:A:319:PX4:H56	0.57	1.76	1	1
4:A:352:PX4:H4	4:A:365:PX4:H15	0.57	1.76	1	1
4:A:392:PX4:H55	4:A:402:PX4:H63	0.57	1.76	17	1
4:A:414:PX4:H53	4:A:422:PX4:H25	0.57	1.75	14	1
4:A:372:PX4:H55	4:A:373:PX4:H34	0.57	1.76	19	1
4:A:325:PX4:H21	4:A:349:PX4:H46	0.57	1.75	16	1
4:A:388:PX4:H51	4:A:412:PX4:H46	0.57	1.76	6	1
4:A:313:PX4:H29	4:A:364:PX4:H40	0.57	1.77	2	1
4:A:342:PX4:H38	4:A:358:PX4:H21	0.56	1.77	17	1
4:A:391:PX4:H3	4:A:425:PX4:H14	0.56	1.77	17	1
4:A:330:PX4:H17	4:A:331:PX4:H20	0.56	1.78	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:318:PX4:H1	4:A:323:PX4:H18	0.56	1.77	8	2
4:A:418:PX4:H17	4:A:427:PX4:H19	0.56	1.75	8	1
4:A:337:PX4:H25	4:A:337:PX4:H58	0.56	1.76	12	1
4:A:338:PX4:H28	4:A:346:PX4:H56	0.56	1.76	11	1
4:A:330:PX4:H66	4:A:346:PX4:H64	0.56	1.78	18	1
4:A:348:PX4:H64	4:A:354:PX4:H33	0.56	1.76	9	1
4:A:308:PX4:H48	4:A:315:PX4:H51	0.56	1.76	11	1
4:A:309:PX4:H20	4:A:357:PX4:H54	0.56	1.78	20	1
4:A:338:PX4:H24	4:A:346:PX4:H24	0.56	1.77	15	1
4:A:320:PX4:H23	4:A:353:PX4:H65	0.56	1.76	3	1
4:A:351:PX4:H42	4:A:391:PX4:H71	0.56	1.76	3	1
4:A:335:PX4:O2	4:A:342:PX4:H4	0.56	2.00	14	1
4:A:404:PX4:H65	4:A:414:PX4:H33	0.56	1.77	14	1
4:A:412:PX4:H30	4:A:420:PX4:H63	0.56	1.76	14	1
4:A:305:PX4:H11	4:A:362:PX4:O6	0.56	2.00	10	1
4:A:311:PX4:H58	4:A:405:PX4:H36	0.56	1.77	13	1
4:A:326:PX4:H16	4:A:327:PX4:H50	0.56	1.77	9	1
4:A:341:PX4:H65	4:A:343:PX4:H45	0.56	1.75	20	1
4:A:414:PX4:H59	4:A:422:PX4:H47	0.56	1.78	15	1
4:A:377:PX4:H60	4:A:391:PX4:H49	0.56	1.77	5	1
4:A:392:PX4:H44	4:A:399:PX4:H39	0.56	1.77	6	1
4:A:334:PX4:H48	4:A:343:PX4:H20	0.56	1.76	12	1
4:A:416:PX4:H55	4:A:422:PX4:H52	0.56	1.77	9	1
4:A:354:PX4:O6	4:A:355:PX4:H17	0.56	2.00	20	1
4:A:321:PX4:H3	4:A:328:PX4:H11	0.56	1.77	8	1
4:A:318:PX4:H16	4:A:323:PX4:H14	0.56	1.78	9	1
4:A:338:PX4:H69	4:A:384:PX4:H34	0.56	1.77	4	1
4:A:355:PX4:H48	4:A:356:PX4:H50	0.56	1.78	2	1
4:A:332:PX4:H16	4:A:340:PX4:H19	0.56	1.77	20	1
4:A:393:PX4:H48	4:A:394:PX4:H49	0.56	1.78	6	1
4:A:371:PX4:H41	4:A:420:PX4:H35	0.56	1.77	11	1
4:A:413:PX4:H60	4:A:421:PX4:O6	0.56	2.00	4	1
4:A:310:PX4:H59	4:A:349:PX4:H21	0.56	1.78	2	1
4:A:320:PX4:H23	4:A:320:PX4:H58	0.56	1.77	1	1
4:A:361:PX4:H38	4:A:427:PX4:H38	0.56	1.77	5	1
4:A:377:PX4:H47	4:A:378:PX4:H24	0.56	1.78	12	1
4:A:372:PX4:H16	4:A:373:PX4:H25	0.56	1.76	4	1
4:A:411:PX4:H56	4:A:427:PX4:H60	0.56	1.77	2	1
4:A:376:PX4:H19	4:A:383:PX4:H22	0.56	1.77	17	1
4:A:377:PX4:H68	4:A:378:PX4:H35	0.56	1.77	14	1
4:A:413:PX4:H25	4:A:431:PX4:H52	0.56	1.78	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:H13	4:A:319:PX4:O2	0.56	2.01	11	1
4:A:404:PX4:H47	4:A:405:PX4:H16	0.56	1.78	11	1
4:A:417:PX4:O4	4:A:419:PX4:H8	0.56	2.00	4	1
4:A:414:PX4:H20	4:A:422:PX4:H37	0.56	1.78	20	1
4:A:328:PX4:O4	4:A:335:PX4:H16	0.56	2.01	17	1
4:A:426:PX4:H57	4:A:426:PX4:H25	0.56	1.78	19	1
4:A:346:PX4:H39	4:A:358:PX4:H70	0.56	1.77	5	1
4:A:391:PX4:C12	4:A:425:PX4:H48	0.56	2.31	4	1
4:A:409:PX4:H21	4:A:410:PX4:H46	0.56	1.79	2	1
4:A:324:PX4:H70	4:A:374:PX4:H66	0.55	1.78	11	1
4:A:357:PX4:H56	4:A:358:PX4:H65	0.55	1.76	20	1
4:A:413:PX4:H71	4:A:429:PX4:H21	0.55	1.78	13	1
4:A:319:PX4:H25	4:A:367:PX4:H34	0.55	1.78	9	1
4:A:309:PX4:O6	4:A:366:PX4:H17	0.55	2.02	15	2
4:A:396:PX4:H35	4:A:414:PX4:H38	0.55	1.77	2	1
4:A:374:PX4:H17	4:A:398:PX4:O1	0.55	2.02	2	1
4:A:373:PX4:H61	4:A:385:PX4:H45	0.55	1.78	3	1
4:A:308:PX4:H56	4:A:340:PX4:H45	0.55	1.78	1	1
4:A:372:PX4:H54	4:A:421:PX4:H56	0.55	1.78	17	1
1:A:48:LEU:HD23	1:A:53:MET:SD	0.55	2.41	8	1
4:A:316:PX4:H28	4:A:325:PX4:H60	0.55	1.76	13	1
4:A:331:PX4:H21	4:A:339:PX4:H23	0.55	1.78	11	1
4:A:423:PX4:H51	4:A:426:PX4:H57	0.55	1.77	11	1
4:A:386:PX4:H4	4:A:400:PX4:O1	0.55	2.01	17	1
4:A:370:PX4:H48	4:A:419:PX4:H17	0.55	1.78	13	1
4:A:391:PX4:H37	4:A:425:PX4:H34	0.55	1.78	13	1
4:A:315:PX4:H21	4:A:322:PX4:H48	0.55	1.78	4	1
4:A:396:PX4:H18	4:A:398:PX4:H55	0.55	1.77	20	1
4:A:409:PX4:H20	4:A:416:PX4:H16	0.55	1.78	12	3
4:A:399:PX4:H46	4:A:408:PX4:H59	0.55	1.78	8	1
4:A:387:PX4:H53	4:A:395:PX4:H21	0.55	1.78	16	1
4:A:396:PX4:H67	4:A:405:PX4:H72	0.55	1.79	11	1
4:A:403:PX4:H56	4:A:405:PX4:H56	0.55	1.76	3	1
4:A:320:PX4:H72	4:A:362:PX4:H64	0.55	1.78	17	1
4:A:360:PX4:H67	4:A:360:PX4:H28	0.55	1.78	14	1
4:A:371:PX4:H19	4:A:418:PX4:H48	0.55	1.79	19	1
4:A:348:PX4:H36	4:A:349:PX4:H65	0.55	1.76	10	1
4:A:371:PX4:H34	4:A:418:PX4:H68	0.55	1.78	10	1
4:A:326:PX4:H18	4:A:327:PX4:H49	0.55	1.76	18	1
4:A:308:PX4:H57	4:A:318:PX4:H46	0.55	1.78	7	1
4:A:323:PX4:H64	4:A:331:PX4:H45	0.55	1.78	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:305:PX4:H42	4:A:305:PX4:H61	0.55	1.77	11	1
4:A:357:PX4:H21	4:A:358:PX4:H27	0.55	1.78	4	1
4:A:374:PX4:H47	4:A:398:PX4:C10	0.55	2.28	2	1
4:A:385:PX4:H12	4:A:387:PX4:H16	0.55	1.77	2	1
4:A:357:PX4:H55	4:A:358:PX4:H61	0.55	1.78	20	1
4:A:375:PX4:H13	4:A:429:PX4:H16	0.55	1.77	17	1
4:A:318:PX4:H69	4:A:373:PX4:H40	0.55	1.77	14	1
4:A:329:PX4:H19	4:A:338:PX4:H47	0.55	1.79	8	1
4:A:382:PX4:H17	4:A:385:PX4:H58	0.55	1.77	13	1
4:A:404:PX4:H49	4:A:405:PX4:H52	0.55	1.77	16	1
4:A:388:PX4:H61	4:A:388:PX4:H34	0.55	1.79	12	1
4:A:378:PX4:C25	4:A:411:PX4:H54	0.55	2.28	18	1
4:A:384:PX4:H69	4:A:393:PX4:H39	0.55	1.78	4	1
4:A:375:PX4:H28	4:A:429:PX4:H24	0.55	1.77	4	1
4:A:419:PX4:H56	4:A:426:PX4:H32	0.55	1.79	2	1
4:A:429:PX4:H4	4:A:429:PX4:H19	0.55	1.77	2	1
4:A:327:PX4:H38	4:A:353:PX4:H37	0.55	1.77	8	1
4:A:369:PX4:H24	4:A:370:PX4:H27	0.55	1.77	16	1
4:A:329:PX4:H30	4:A:351:PX4:H24	0.55	1.79	9	1
4:A:378:PX4:H8	4:A:385:PX4:O2	0.55	2.02	20	1
4:A:322:PX4:O2	4:A:361:PX4:H4	0.55	2.02	15	1
4:A:384:PX4:H26	4:A:400:PX4:H23	0.55	1.79	3	1
4:A:389:PX4:H50	4:A:395:PX4:H52	0.55	1.79	1	1
4:A:392:PX4:H28	4:A:409:PX4:H58	0.55	1.79	8	1
4:A:369:PX4:H34	4:A:400:PX4:H27	0.55	1.78	16	1
4:A:329:PX4:H67	4:A:338:PX4:H62	0.55	1.78	9	1
4:A:328:PX4:H48	4:A:335:PX4:H22	0.55	1.79	1	1
4:A:348:PX4:H26	4:A:349:PX4:H30	0.55	1.79	17	1
4:A:312:PX4:H23	4:A:327:PX4:H55	0.55	1.77	14	1
4:A:346:PX4:H46	4:A:347:PX4:H17	0.55	1.78	13	1
4:A:318:PX4:H48	4:A:323:PX4:H53	0.55	1.79	20	1
4:A:378:PX4:H54	4:A:385:PX4:H28	0.55	1.79	15	1
4:A:384:PX4:H21	4:A:400:PX4:H26	0.54	1.79	8	1
4:A:369:PX4:H60	4:A:391:PX4:H25	0.54	1.79	16	1
4:A:320:PX4:H17	4:A:353:PX4:H49	0.54	1.79	12	1
4:A:312:PX4:H19	4:A:359:PX4:H15	0.54	1.78	9	1
4:A:318:PX4:H8	4:A:324:PX4:H23	0.54	1.79	7	1
4:A:324:PX4:H38	4:A:340:PX4:H39	0.54	1.79	15	1
4:A:374:PX4:H15	4:A:383:PX4:H49	0.54	1.79	16	1
4:A:372:PX4:H44	4:A:421:PX4:H37	0.54	1.80	5	1
4:A:317:PX4:H21	4:A:318:PX4:H5	0.54	1.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:335:PX4:H70	4:A:391:PX4:H66	0.54	1.79	7	1
4:A:328:PX4:H16	4:A:335:PX4:H18	0.54	1.79	1	1
4:A:377:PX4:H33	4:A:411:PX4:H34	0.54	1.79	8	1
4:A:308:PX4:H4	4:A:319:PX4:O2	0.54	2.03	6	1
4:A:368:PX4:H62	4:A:429:PX4:H30	0.54	1.77	12	1
4:A:332:PX4:H19	4:A:340:PX4:H16	0.54	1.78	18	1
4:A:393:PX4:H27	4:A:400:PX4:H27	0.54	1.80	2	1
4:A:321:PX4:H27	4:A:338:PX4:H49	0.54	1.80	15	1
4:A:312:PX4:H19	4:A:327:PX4:H57	0.54	1.78	17	1
4:A:396:PX4:H33	4:A:396:PX4:H65	0.54	1.79	14	1
4:A:357:PX4:H46	4:A:358:PX4:H48	0.54	1.80	7	1
4:A:391:PX4:H17	4:A:400:PX4:H47	0.54	1.80	11	2
4:A:371:PX4:H25	4:A:418:PX4:H53	0.54	1.78	14	1
4:A:320:PX4:H72	4:A:353:PX4:H70	0.54	1.79	7	1
4:A:379:PX4:H66	4:A:380:PX4:H42	0.54	1.80	3	1
4:A:376:PX4:H51	4:A:430:PX4:H57	0.54	1.79	8	1
4:A:383:PX4:H58	4:A:429:PX4:H31	0.54	1.80	12	1
4:A:332:PX4:H39	4:A:340:PX4:H29	0.54	1.80	15	1
4:A:329:PX4:H51	4:A:338:PX4:H25	0.54	1.80	14	1
4:A:424:PX4:H46	4:A:426:PX4:H54	0.54	1.78	16	1
4:A:324:PX4:H52	4:A:339:PX4:H17	0.54	1.78	18	1
4:A:377:PX4:H43	4:A:378:PX4:H71	0.54	1.80	7	1
4:A:355:PX4:H9	4:A:355:PX4:O2	0.54	2.02	2	1
4:A:396:PX4:H15	4:A:397:PX4:O1	0.54	2.02	14	1
4:A:320:PX4:C8	4:A:353:PX4:H16	0.54	2.21	10	1
4:A:414:PX4:H45	4:A:421:PX4:H49	0.54	1.80	9	1
4:A:388:PX4:H62	4:A:412:PX4:H64	0.54	1.80	11	1
4:A:371:PX4:H47	4:A:404:PX4:H20	0.54	1.80	2	1
4:A:392:PX4:H30	4:A:393:PX4:H17	0.54	1.80	20	1
4:A:350:PX4:H26	4:A:357:PX4:H20	0.54	1.80	15	1
4:A:321:PX4:H46	4:A:328:PX4:H48	0.54	1.78	17	1
4:A:312:PX4:H39	4:A:319:PX4:H16	0.54	1.79	16	1
4:A:338:PX4:H16	4:A:346:PX4:H47	0.54	1.80	12	1
4:A:357:PX4:H2	4:A:358:PX4:O6	0.54	2.03	12	1
4:A:324:PX4:H30	4:A:339:PX4:H62	0.54	1.78	18	1
4:A:384:PX4:H66	4:A:386:PX4:H47	0.54	1.79	18	1
4:A:407:PX4:H49	4:A:416:PX4:H13	0.54	1.78	18	1
4:A:364:PX4:H55	4:A:412:PX4:H43	0.54	1.78	7	1
4:A:316:PX4:O6	4:A:324:PX4:H19	0.54	2.03	4	1
4:A:370:PX4:H19	4:A:419:PX4:H47	0.54	1.79	1	1
4:A:404:PX4:H59	4:A:414:PX4:H19	0.54	1.78	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:328:PX4:H20	4:A:342:PX4:H55	0.54	1.79	5	1
4:A:369:PX4:H47	4:A:370:PX4:H21	0.54	1.80	15	2
4:A:316:PX4:H36	4:A:343:PX4:H39	0.54	1.79	9	1
4:A:399:PX4:H10	4:A:408:PX4:O4	0.54	2.02	7	1
4:A:376:PX4:H16	4:A:383:PX4:H47	0.54	1.79	20	2
4:A:341:PX4:H38	4:A:358:PX4:H35	0.54	1.79	3	1
4:A:371:PX4:H46	4:A:412:PX4:H16	0.54	1.80	1	1
4:A:401:PX4:H52	4:A:417:PX4:H49	0.54	1.80	1	1
4:A:390:PX4:H20	4:A:398:PX4:H62	0.53	1.79	19	1
1:A:84:TRP:CE2	1:A:162:PRO:HB3	0.53	2.38	16	1
4:A:306:PX4:H48	4:A:364:PX4:H27	0.53	1.78	18	1
4:A:392:PX4:O2	4:A:409:PX4:H9	0.53	2.01	17	1
4:A:306:PX4:O2	4:A:313:PX4:H10	0.53	2.02	14	1
4:A:344:PX4:H24	4:A:344:PX4:H59	0.53	1.79	8	1
4:A:309:PX4:O2	4:A:366:PX4:H12	0.53	2.02	5	1
4:A:334:PX4:H56	4:A:341:PX4:H21	0.53	1.78	12	1
4:A:390:PX4:O3	4:A:390:PX4:H18	0.53	2.03	18	1
1:A:142:ALA:O	4:A:335:PX4:H6	0.53	2.03	2	1
4:A:348:PX4:H41	4:A:397:PX4:H40	0.53	1.77	2	1
4:A:312:PX4:H48	4:A:326:PX4:H54	0.53	1.79	15	1
4:A:333:PX4:H61	4:A:348:PX4:H54	0.53	1.81	3	1
4:A:326:PX4:H56	4:A:343:PX4:H51	0.53	1.79	1	1
4:A:322:PX4:H20	4:A:332:PX4:H17	0.53	1.79	14	1
4:A:316:PX4:H70	4:A:390:PX4:H45	0.53	1.80	13	1
4:A:409:PX4:H59	4:A:416:PX4:H24	0.53	1.80	16	1
4:A:325:PX4:H23	4:A:356:PX4:H65	0.53	1.80	6	1
4:A:331:PX4:H48	4:A:355:PX4:H53	0.53	1.80	9	1
4:A:337:PX4:H50	4:A:355:PX4:H22	0.53	1.81	2	1
4:A:305:PX4:H62	4:A:362:PX4:H55	0.53	1.78	20	1
4:A:333:PX4:H17	4:A:339:PX4:H64	0.53	1.80	17	1
4:A:331:PX4:H60	4:A:347:PX4:H51	0.53	1.81	14	1
4:A:305:PX4:H27	4:A:305:PX4:H53	0.53	1.80	8	1
4:A:305:PX4:H39	4:A:330:PX4:H27	0.53	1.79	8	1
4:A:312:PX4:H69	4:A:383:PX4:H69	0.53	1.80	13	1
4:A:370:PX4:H36	4:A:425:PX4:H67	0.53	1.78	5	1
4:A:325:PX4:H8	4:A:350:PX4:O8	0.53	2.03	6	1
4:A:404:PX4:H22	4:A:412:PX4:H16	0.53	1.80	18	1
4:A:381:PX4:H62	4:A:385:PX4:H61	0.53	1.79	11	1
4:A:345:PX4:H67	4:A:354:PX4:H44	0.53	1.80	15	1
4:A:319:PX4:H34	4:A:407:PX4:H39	0.53	1.79	15	1
4:A:377:PX4:H48	4:A:386:PX4:H7	0.53	1.81	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:402:PX4:H63	4:A:418:PX4:H29	0.53	1.81	14	1
4:A:414:PX4:H51	4:A:431:PX4:H24	0.53	1.80	14	1
4:A:316:PX4:H19	4:A:324:PX4:H26	0.53	1.81	8	1
4:A:324:PX4:H60	4:A:340:PX4:H56	0.53	1.79	5	1
4:A:409:PX4:H17	4:A:410:PX4:H48	0.53	1.80	15	1
4:A:391:PX4:H39	4:A:425:PX4:H68	0.53	1.80	3	1
4:A:404:PX4:H14	4:A:412:PX4:O1	0.53	2.04	1	1
4:A:388:PX4:H54	4:A:395:PX4:H53	0.53	1.80	17	1
4:A:361:PX4:H60	4:A:427:PX4:H45	0.53	1.80	17	1
4:A:373:PX4:H65	4:A:380:PX4:H63	0.53	1.80	8	1
4:A:308:PX4:H23	4:A:359:PX4:H65	0.53	1.79	13	1
4:A:424:PX4:H54	4:A:430:PX4:H41	0.53	1.81	16	1
4:A:369:PX4:H32	4:A:378:PX4:H31	0.53	1.81	6	1
4:A:381:PX4:H28	4:A:382:PX4:H25	0.53	1.80	18	1
4:A:377:PX4:H35	4:A:411:PX4:H19	0.53	1.79	9	1
4:A:411:PX4:H32	4:A:417:PX4:H64	0.53	1.79	20	1
4:A:329:PX4:H48	4:A:351:PX4:H50	0.53	1.79	3	1
4:A:326:PX4:H32	4:A:353:PX4:H34	0.53	1.79	16	1
4:A:337:PX4:H16	4:A:354:PX4:C7	0.53	2.30	20	1
4:A:388:PX4:H1	4:A:412:PX4:H49	0.53	1.79	20	1
4:A:359:PX4:H16	4:A:367:PX4:H18	0.53	1.80	19	1
4:A:329:PX4:O6	4:A:351:PX4:H17	0.53	2.03	16	1
4:A:321:PX4:H49	4:A:330:PX4:H24	0.53	1.78	5	1
4:A:305:PX4:H53	4:A:362:PX4:H17	0.53	1.81	9	1
4:A:413:PX4:H60	4:A:429:PX4:H52	0.53	1.79	9	1
4:A:369:PX4:H49	4:A:370:PX4:H27	0.53	1.81	11	1
4:A:317:PX4:H29	4:A:323:PX4:H38	0.53	1.81	13	1
4:A:320:PX4:H49	4:A:362:PX4:H47	0.53	1.80	14	1
4:A:305:PX4:H68	4:A:321:PX4:H62	0.53	1.80	19	1
4:A:396:PX4:H25	4:A:405:PX4:H51	0.53	1.80	6	1
4:A:380:PX4:H30	4:A:385:PX4:H36	0.53	1.80	12	1
4:A:335:PX4:H23	4:A:342:PX4:H53	0.53	1.81	9	1
4:A:355:PX4:H24	4:A:356:PX4:H30	0.53	1.80	9	1
4:A:344:PX4:H60	4:A:366:PX4:H60	0.53	1.79	7	1
4:A:339:PX4:H21	4:A:355:PX4:H57	0.53	1.81	7	1
4:A:331:PX4:H62	4:A:339:PX4:H31	0.53	1.78	11	1
4:A:377:PX4:H51	4:A:386:PX4:H11	0.53	1.80	20	1
4:A:307:PX4:H4	4:A:363:PX4:O6	0.53	2.04	1	1
4:A:369:PX4:H56	4:A:425:PX4:H55	0.52	1.81	14	1
4:A:321:PX4:H59	4:A:328:PX4:H60	0.52	1.79	13	1
4:A:316:PX4:H38	4:A:375:PX4:H71	0.52	1.80	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:349:PX4:H60	4:A:350:PX4:H61	0.52	1.80	5	1
4:A:316:PX4:H43	4:A:318:PX4:H26	0.52	1.81	18	1
4:A:346:PX4:H52	4:A:347:PX4:H53	0.52	1.82	2	1
4:A:380:PX4:O6	4:A:381:PX4:H9	0.52	2.02	2	1
4:A:385:PX4:H60	4:A:386:PX4:H32	0.52	1.82	15	1
1:A:147:TYR:HB3	1:A:148:PRO:HD2	0.52	1.82	19	2
4:A:386:PX4:H19	4:A:395:PX4:H34	0.52	1.81	13	1
4:A:409:PX4:H30	4:A:417:PX4:H26	0.52	1.81	16	1
4:A:383:PX4:H28	4:A:389:PX4:H67	0.52	1.81	12	1
4:A:376:PX4:H35	4:A:383:PX4:H29	0.52	1.81	11	1
4:A:398:PX4:H66	4:A:403:PX4:C20	0.52	2.33	15	1
4:A:305:PX4:H33	4:A:321:PX4:H55	0.52	1.81	1	1
4:A:385:PX4:H51	4:A:387:PX4:C25	0.52	2.32	14	1
4:A:423:PX4:H25	4:A:424:PX4:H22	0.52	1.81	13	1
4:A:309:PX4:H20	4:A:366:PX4:H20	0.52	1.80	16	1
4:A:409:PX4:H30	4:A:410:PX4:H69	0.52	1.81	9	1
4:A:379:PX4:H58	4:A:380:PX4:H27	0.52	1.81	11	1
4:A:321:PX4:H43	4:A:338:PX4:H49	0.52	1.79	20	1
4:A:416:PX4:H56	4:A:422:PX4:H60	0.52	1.80	1	1
4:A:414:PX4:H56	4:A:422:PX4:H29	0.52	1.80	14	1
4:A:348:PX4:H19	4:A:349:PX4:H17	0.52	1.80	19	1
4:A:330:PX4:O2	4:A:339:PX4:H3	0.52	2.05	5	1
4:A:377:PX4:H65	4:A:384:PX4:H62	0.52	1.80	12	1
4:A:377:PX4:H16	4:A:387:PX4:H5	0.52	1.81	7	1
4:A:329:PX4:H72	4:A:344:PX4:H27	0.52	1.81	11	1
4:A:305:PX4:H33	4:A:328:PX4:H62	0.52	1.81	15	1
4:A:319:PX4:H34	4:A:312:PX4:H37	0.52	1.82	1	1
4:A:387:PX4:H56	4:A:395:PX4:H51	0.52	1.82	8	1
4:A:305:PX4:H37	4:A:328:PX4:H65	0.52	1.81	5	1
4:A:391:PX4:O6	4:A:400:PX4:H6	0.52	2.05	6	1
4:A:336:PX4:H20	4:A:358:PX4:H15	0.52	1.81	18	1
4:A:370:PX4:H27	4:A:377:PX4:H30	0.52	1.81	9	1
4:A:422:PX4:H16	4:A:431:PX4:H20	0.52	1.80	19	5
4:A:383:PX4:H37	4:A:389:PX4:H17	0.52	1.81	10	2
4:A:352:PX4:H20	4:A:360:PX4:H46	0.52	1.81	6	1
4:A:325:PX4:H23	4:A:349:PX4:H56	0.52	1.79	9	1
4:A:308:PX4:H21	4:A:315:PX4:H49	0.52	1.82	7	1
4:A:307:PX4:O6	4:A:348:PX4:H11	0.52	2.03	11	1
4:A:316:PX4:H18	4:A:324:PX4:H19	0.52	1.81	2	1
4:A:324:PX4:H50	4:A:339:PX4:H50	0.52	1.80	2	1
4:A:311:PX4:O8	4:A:364:PX4:H47	0.52	2.05	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H50	4:A:382:PX4:H16	0.52	1.80	6	1
4:A:374:PX4:H18	4:A:382:PX4:H56	0.52	1.82	18	1
4:A:370:PX4:H43	4:A:411:PX4:H39	0.52	1.80	9	1
4:A:324:PX4:H32	4:A:413:PX4:H43	0.52	1.81	9	1
4:A:309:PX4:H33	4:A:366:PX4:H71	0.52	1.81	11	1
4:A:374:PX4:H57	4:A:398:PX4:H31	0.52	1.80	4	1
4:A:377:PX4:H49	4:A:378:PX4:H24	0.52	1.80	2	1
4:A:369:PX4:H6	4:A:419:PX4:O1	0.52	2.05	1	1
4:A:396:PX4:H30	4:A:414:PX4:H53	0.52	1.82	17	1
4:A:306:PX4:H66	4:A:364:PX4:H35	0.52	1.81	10	1
4:A:392:PX4:H47	4:A:409:PX4:H58	0.52	1.79	10	1
4:A:388:PX4:H28	4:A:394:PX4:H51	0.52	1.82	13	1
4:A:406:PX4:H36	4:A:409:PX4:H33	0.52	1.82	15	1
4:A:372:PX4:H15	4:A:428:PX4:H7	0.52	1.80	8	1
4:A:369:PX4:H65	4:A:400:PX4:H52	0.52	1.82	6	1
4:A:404:PX4:O8	4:A:420:PX4:H3	0.52	2.05	18	1
4:A:333:PX4:H21	4:A:356:PX4:H53	0.52	1.82	7	1
4:A:409:PX4:C8	4:A:416:PX4:H14	0.52	2.34	15	1
4:A:342:PX4:H27	4:A:351:PX4:H16	0.52	1.80	10	1
4:A:392:PX4:H16	4:A:393:PX4:H9	0.52	1.82	10	1
4:A:320:PX4:H21	4:A:353:PX4:H24	0.52	1.80	16	1
4:A:388:PX4:H49	4:A:389:PX4:H16	0.52	1.81	16	1
4:A:368:PX4:H29	4:A:413:PX4:H56	0.52	1.82	5	1
4:A:336:PX4:H54	4:A:344:PX4:H49	0.52	1.82	6	1
4:A:312:PX4:H23	4:A:359:PX4:H19	0.52	1.82	18	1
4:A:370:PX4:H26	4:A:370:PX4:H55	0.52	1.82	7	1
4:A:377:PX4:H59	4:A:384:PX4:H57	0.52	1.81	15	1
4:A:394:PX4:H46	4:A:402:PX4:H24	0.52	1.82	15	1
4:A:318:PX4:H17	4:A:323:PX4:H20	0.52	1.80	1	1
4:A:345:PX4:O6	4:A:352:PX4:H7	0.52	2.05	1	1
4:A:333:PX4:H40	4:A:355:PX4:H57	0.52	1.82	1	1
4:A:384:PX4:H56	4:A:395:PX4:H27	0.52	1.82	1	1
4:A:369:PX4:H72	4:A:391:PX4:H57	0.51	1.82	5	1
4:A:321:PX4:H31	4:A:335:PX4:H25	0.51	1.81	12	1
4:A:336:PX4:H8	4:A:344:PX4:O1	0.51	2.05	12	1
4:A:377:PX4:H21	4:A:378:PX4:H25	0.51	1.81	11	1
4:A:419:PX4:H36	4:A:424:PX4:H34	0.51	1.83	4	1
4:A:322:PX4:H22	4:A:332:PX4:H13	0.51	1.80	2	1
4:A:399:PX4:H51	4:A:408:PX4:H57	0.51	1.82	15	1
4:A:312:PX4:O2	4:A:327:PX4:H13	0.51	2.06	14	1
4:A:338:PX4:H36	4:A:346:PX4:H72	0.51	1.82	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:H51	4:A:346:PX4:H23	0.51	1.81	16	1
4:A:370:PX4:H21	4:A:425:PX4:H51	0.51	1.81	16	1
4:A:381:PX4:H25	4:A:382:PX4:H47	0.51	1.81	9	1
4:A:329:PX4:H19	4:A:338:PX4:H28	0.51	1.82	7	1
4:A:375:PX4:H9	4:A:421:PX4:O6	0.51	2.05	7	1
4:A:347:PX4:H8	4:A:355:PX4:O6	0.51	2.05	11	1
4:A:369:PX4:O8	4:A:391:PX4:H11	0.51	2.05	19	1
4:A:392:PX4:H54	4:A:409:PX4:H49	0.51	1.81	18	1
4:A:354:PX4:H21	4:A:355:PX4:H22	0.51	1.82	9	1
4:A:392:PX4:H62	4:A:418:PX4:H44	0.51	1.81	4	1
4:A:384:PX4:H49	4:A:386:PX4:H7	0.51	1.80	2	1
4:A:331:PX4:H57	4:A:347:PX4:H52	0.51	1.82	15	1
4:A:334:PX4:H62	4:A:341:PX4:H55	0.51	1.81	17	1
4:A:392:PX4:H26	4:A:399:PX4:H29	0.51	1.83	13	1
4:A:322:PX4:H24	4:A:332:PX4:H17	0.51	1.82	7	2
4:A:353:PX4:H66	4:A:362:PX4:H67	0.51	1.82	18	1
4:A:317:PX4:H24	4:A:323:PX4:H30	0.51	1.81	9	1
4:A:338:PX4:H3	4:A:342:PX4:O2	0.51	2.05	7	1
4:A:318:PX4:H1	4:A:323:PX4:O3	0.51	2.05	11	1
4:A:399:PX4:H44	4:A:402:PX4:H39	0.51	1.81	4	1
4:A:337:PX4:C7	4:A:354:PX4:H16	0.51	2.31	20	1
4:A:312:PX4:H39	4:A:327:PX4:H70	0.51	1.80	14	1
4:A:352:PX4:H29	4:A:416:PX4:H39	0.51	1.82	14	1
4:A:333:PX4:H36	4:A:339:PX4:H40	0.51	1.82	19	1
4:A:316:PX4:H51	4:A:317:PX4:H49	0.51	1.81	16	1
4:A:373:PX4:O2	4:A:373:PX4:H6	0.51	2.06	16	1
4:A:409:PX4:H17	4:A:410:PX4:H15	0.51	1.81	16	1
4:A:311:PX4:H16	4:A:364:PX4:H5	0.51	1.82	5	1
4:A:383:PX4:H49	4:A:429:PX4:H11	0.51	1.81	5	1
4:A:320:PX4:H30	4:A:321:PX4:H63	0.51	1.83	9	1
4:A:314:PX4:H44	4:A:345:PX4:H63	0.51	1.82	11	1
4:A:305:PX4:H17	4:A:362:PX4:H13	0.51	1.82	20	1
4:A:335:PX4:H54	4:A:342:PX4:H17	0.51	1.82	15	1
4:A:373:PX4:H24	4:A:380:PX4:H58	0.51	1.82	15	1
4:A:404:PX4:H43	4:A:405:PX4:H34	0.51	1.82	15	1
4:A:379:PX4:H53	4:A:380:PX4:H32	0.51	1.82	3	1
4:A:321:PX4:O2	4:A:332:PX4:H5	0.51	2.06	8	2
4:A:358:PX4:H32	4:A:399:PX4:H70	0.51	1.83	14	1
4:A:329:PX4:O6	4:A:338:PX4:H17	0.51	2.05	10	1
4:A:371:PX4:H9	4:A:420:PX4:O2	0.51	2.06	9	1
4:A:354:PX4:H62	4:A:364:PX4:H39	0.51	1.83	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:401:PX4:H47	4:A:410:PX4:H16	0.51	1.81	2	1
4:A:392:PX4:O2	4:A:409:PX4:H48	0.51	2.05	15	1
4:A:329:PX4:H27	4:A:347:PX4:C28	0.51	2.35	1	1
4:A:397:PX4:H30	4:A:403:PX4:H27	0.51	1.82	17	1
4:A:308:PX4:H39	4:A:322:PX4:H65	0.51	1.81	14	1
4:A:307:PX4:H46	4:A:310:PX4:H10	0.51	1.82	12	1
4:A:347:PX4:H26	4:A:355:PX4:H53	0.51	1.83	18	1
4:A:352:PX4:H31	4:A:366:PX4:H63	0.51	1.82	4	1
4:A:336:PX4:H30	4:A:352:PX4:H35	0.51	1.82	20	1
4:A:328:PX4:C10	4:A:335:PX4:H16	0.51	2.35	15	1
4:A:312:PX4:H45	4:A:423:PX4:H43	0.51	1.82	10	1
4:A:320:PX4:H59	4:A:328:PX4:H21	0.51	1.81	13	1
4:A:368:PX4:H25	4:A:424:PX4:H19	0.51	1.83	13	1
4:A:328:PX4:H23	4:A:342:PX4:H59	0.51	1.82	16	1
4:A:392:PX4:H55	4:A:410:PX4:H68	0.51	1.82	6	1
4:A:320:PX4:O8	4:A:362:PX4:H4	0.51	2.06	12	1
4:A:348:PX4:H49	4:A:356:PX4:H20	0.51	1.82	18	1
4:A:330:PX4:H46	4:A:331:PX4:H9	0.51	1.83	4	1
4:A:360:PX4:H28	4:A:426:PX4:H70	0.51	1.83	2	1
4:A:369:PX4:O1	4:A:377:PX4:H18	0.51	2.06	20	1
4:A:333:PX4:H22	4:A:356:PX4:H53	0.51	1.81	1	1
4:A:406:PX4:H32	4:A:409:PX4:H31	0.51	1.81	17	1
4:A:335:PX4:H55	4:A:342:PX4:H17	0.51	1.83	14	1
4:A:383:PX4:H38	4:A:389:PX4:C25	0.51	2.36	10	1
4:A:336:PX4:H28	4:A:358:PX4:H63	0.51	1.83	16	1
4:A:341:PX4:H50	4:A:350:PX4:H54	0.51	1.82	5	1
4:A:394:PX4:H7	4:A:395:PX4:H18	0.51	1.82	12	1
4:A:313:PX4:H33	4:A:354:PX4:H52	0.51	1.83	7	1
4:A:350:PX4:H44	4:A:390:PX4:H70	0.51	1.81	11	1
4:A:391:PX4:H27	4:A:400:PX4:H52	0.51	1.83	11	1
4:A:306:PX4:H61	4:A:313:PX4:H48	0.51	1.82	15	1
4:A:362:PX4:H34	4:A:362:PX4:H63	0.51	1.83	3	1
4:A:348:PX4:H58	4:A:356:PX4:H30	0.50	1.83	13	1
4:A:374:PX4:H30	4:A:398:PX4:H29	0.50	1.84	5	1
4:A:346:PX4:H55	4:A:346:PX4:H32	0.50	1.82	6	1
4:A:396:PX4:H39	4:A:414:PX4:H57	0.50	1.83	12	1
4:A:347:PX4:H19	4:A:355:PX4:H51	0.50	1.82	9	1
4:A:420:PX4:H26	4:A:428:PX4:H31	0.50	1.83	20	1
4:A:329:PX4:H49	4:A:336:PX4:H5	0.50	1.82	15	1
4:A:346:PX4:H13	4:A:347:PX4:O4	0.50	2.05	3	1
4:A:337:PX4:H70	4:A:402:PX4:H38	0.50	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:408:PX4:H48	4:A:415:PX4:H55	0.50	1.84	14	1
4:A:321:PX4:H51	4:A:335:PX4:H23	0.50	1.83	13	1
4:A:394:PX4:H61	4:A:394:PX4:H28	0.50	1.82	16	1
4:A:398:PX4:O6	4:A:398:PX4:H10	0.50	2.06	6	1
4:A:337:PX4:H20	4:A:345:PX4:H55	0.50	1.84	18	1
4:A:346:PX4:H20	4:A:347:PX4:H14	0.50	1.81	9	1
4:A:324:PX4:C22	4:A:375:PX4:H39	0.50	2.36	4	1
4:A:349:PX4:H55	4:A:363:PX4:H49	0.50	1.83	20	1
4:A:369:PX4:H40	4:A:391:PX4:H64	0.50	1.82	3	1
4:A:328:PX4:H44	4:A:342:PX4:H63	0.50	1.81	19	1
4:A:305:PX4:O6	4:A:362:PX4:H15	0.50	2.06	8	1
4:A:347:PX4:H43	4:A:388:PX4:H66	0.50	1.84	13	1
4:A:329:PX4:H16	4:A:351:PX4:H47	0.50	1.83	7	2
4:A:393:PX4:H50	4:A:402:PX4:H27	0.50	1.82	6	1
4:A:327:PX4:H36	4:A:360:PX4:H29	0.50	1.83	18	1
4:A:407:PX4:H32	4:A:423:PX4:H34	0.50	1.82	7	1
4:A:386:PX4:H72	4:A:402:PX4:H38	0.50	1.81	19	1
4:A:362:PX4:H71	4:A:411:PX4:H40	0.50	1.83	10	1
4:A:375:PX4:H15	4:A:421:PX4:H20	0.50	1.82	16	1
4:A:377:PX4:H33	4:A:378:PX4:H30	0.50	1.83	6	1
4:A:307:PX4:H60	4:A:310:PX4:H20	0.50	1.83	18	1
4:A:317:PX4:H41	4:A:382:PX4:H43	0.50	1.83	11	1
4:A:413:PX4:H50	4:A:431:PX4:H51	0.50	1.84	4	1
4:A:409:PX4:H28	4:A:416:PX4:H55	0.50	1.82	15	1
4:A:413:PX4:H17	4:A:421:PX4:H46	0.50	1.83	17	1
4:A:419:PX4:H45	4:A:419:PX4:H71	0.50	1.84	19	1
4:A:313:PX4:H5	4:A:348:PX4:O2	0.50	2.07	8	1
4:A:397:PX4:H41	4:A:398:PX4:H34	0.50	1.83	16	1
4:A:311:PX4:H64	4:A:412:PX4:H34	0.50	1.83	5	1
4:A:407:PX4:H18	4:A:422:PX4:H15	0.50	1.84	12	1
4:A:391:PX4:H28	4:A:425:PX4:H52	0.50	1.84	2	1
4:A:312:PX4:H16	4:A:319:PX4:H53	0.50	1.82	20	1
4:A:349:PX4:H66	4:A:382:PX4:H45	0.50	1.84	20	1
4:A:404:PX4:H71	4:A:422:PX4:H45	0.50	1.83	20	1
4:A:424:PX4:H46	4:A:430:PX4:H19	0.50	1.83	15	1
1:A:194:HIS:CD2	1:A:198:HIS:CE1	0.50	3.00	8	4
4:A:372:PX4:O2	4:A:428:PX4:H4	0.50	2.07	10	1
4:A:308:PX4:H71	4:A:340:PX4:H27	0.50	1.83	16	1
4:A:331:PX4:O6	4:A:339:PX4:H4	0.50	2.06	6	1
4:A:339:PX4:H16	4:A:355:PX4:H55	0.50	1.82	11	1
4:A:396:PX4:H65	4:A:396:PX4:H33	0.50	1.83	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H31	4:A:346:PX4:H34	0.50	1.84	20	1
4:A:345:PX4:H38	4:A:352:PX4:H72	0.50	1.84	20	1
4:A:424:PX4:O8	4:A:430:PX4:H4	0.50	2.07	3	1
4:A:384:PX4:H67	4:A:393:PX4:H42	0.50	1.84	17	1
4:A:413:PX4:H37	4:A:428:PX4:H31	0.50	1.82	17	1
4:A:349:PX4:H41	4:A:405:PX4:H67	0.50	1.84	14	1
4:A:305:PX4:H56	4:A:361:PX4:H62	0.50	1.84	14	1
4:A:351:PX4:H42	4:A:391:PX4:H44	0.50	1.83	19	1
4:A:417:PX4:H64	4:A:427:PX4:H69	0.50	1.83	8	1
4:A:321:PX4:H52	4:A:335:PX4:H25	0.50	1.83	5	1
4:A:344:PX4:H34	4:A:345:PX4:H66	0.50	1.82	5	1
4:A:359:PX4:H59	4:A:364:PX4:H50	0.50	1.83	5	1
4:A:318:PX4:H60	4:A:403:PX4:H44	0.50	1.83	18	1
4:A:382:PX4:H26	4:A:385:PX4:H53	0.50	1.83	18	1
4:A:399:PX4:H26	4:A:408:PX4:H14	0.50	1.82	7	1
4:A:374:PX4:O6	4:A:398:PX4:H14	0.50	2.07	2	1
4:A:333:PX4:H29	4:A:355:PX4:H62	0.50	1.84	1	1
4:A:307:PX4:H42	4:A:403:PX4:H55	0.50	1.82	1	1
4:A:318:PX4:H26	4:A:319:PX4:H48	0.50	1.83	17	1
4:A:384:PX4:H57	4:A:400:PX4:H27	0.50	1.84	14	1
4:A:338:PX4:O2	4:A:346:PX4:H3	0.50	2.06	16	1
4:A:318:PX4:O2	4:A:324:PX4:H7	0.50	2.07	12	1
4:A:320:PX4:H51	4:A:327:PX4:H26	0.50	1.84	18	1
4:A:387:PX4:H63	4:A:395:PX4:H56	0.50	1.84	11	1
4:A:307:PX4:H5	4:A:310:PX4:H48	0.50	1.84	15	1
4:A:388:PX4:H35	4:A:393:PX4:H40	0.50	1.82	15	1
4:A:379:PX4:H52	4:A:381:PX4:H23	0.50	1.84	17	1
4:A:328:PX4:H25	4:A:342:PX4:H50	0.50	1.83	19	1
4:A:334:PX4:H56	4:A:341:PX4:H16	0.50	1.83	10	1
4:A:332:PX4:O8	4:A:340:PX4:H13	0.50	2.06	5	1
4:A:373:PX4:H57	4:A:382:PX4:H34	0.50	1.84	6	1
4:A:326:PX4:H28	4:A:343:PX4:H63	0.50	1.84	12	1
4:A:370:PX4:C9	4:A:419:PX4:H47	0.50	2.37	9	1
4:A:380:PX4:H69	4:A:381:PX4:H38	0.50	1.84	2	1
4:A:406:PX4:H8	4:A:409:PX4:H16	0.50	1.82	2	1
4:A:334:PX4:H48	4:A:343:PX4:H23	0.50	1.82	20	1
4:A:360:PX4:H60	4:A:360:PX4:H28	0.50	1.84	3	1
4:A:316:PX4:H32	4:A:325:PX4:H67	0.49	1.83	17	1
4:A:343:PX4:H50	4:A:353:PX4:H26	0.49	1.84	17	1
4:A:338:PX4:H24	4:A:347:PX4:H61	0.49	1.84	8	1
4:A:410:PX4:H53	4:A:417:PX4:H42	0.49	1.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:399:PX4:H16	4:A:408:PX4:H46	0.49	1.84	10	2
4:A:388:PX4:H32	4:A:402:PX4:H32	0.49	1.83	13	1
4:A:373:PX4:H32	4:A:421:PX4:H28	0.49	1.83	5	1
4:A:348:PX4:H66	4:A:356:PX4:H35	0.49	1.82	12	1
4:A:401:PX4:H60	4:A:417:PX4:H54	0.49	1.83	12	1
4:A:390:PX4:H15	4:A:399:PX4:O1	0.49	2.07	20	1
4:A:329:PX4:H25	4:A:342:PX4:H33	0.49	1.84	3	1
4:A:347:PX4:H44	4:A:355:PX4:H35	0.49	1.82	8	1
4:A:312:PX4:H50	4:A:317:PX4:H20	0.49	1.82	5	1
4:A:371:PX4:H72	4:A:388:PX4:H37	0.49	1.82	11	1
4:A:378:PX4:H48	4:A:380:PX4:H21	0.49	1.83	1	1
4:A:348:PX4:H28	4:A:349:PX4:H22	0.49	1.84	19	1
4:A:320:PX4:H49	4:A:362:PX4:H46	0.49	1.83	13	1
4:A:370:PX4:H16	4:A:425:PX4:H46	0.49	1.83	16	1
4:A:347:PX4:H70	4:A:378:PX4:H70	0.49	1.82	18	1
4:A:413:PX4:H33	4:A:428:PX4:H33	0.49	1.83	4	1
4:A:376:PX4:H42	4:A:390:PX4:H42	0.49	1.84	15	1
4:A:359:PX4:H69	4:A:364:PX4:H61	0.49	1.84	1	1
4:A:330:PX4:H30	4:A:330:PX4:H56	0.49	1.84	13	1
4:A:384:PX4:H22	4:A:400:PX4:H49	0.49	1.83	16	1
4:A:333:PX4:H21	4:A:356:PX4:H61	0.49	1.84	9	1
4:A:349:PX4:H43	4:A:415:PX4:H43	0.49	1.82	7	1
4:A:371:PX4:H63	4:A:412:PX4:H20	0.49	1.84	4	1
4:A:321:PX4:H22	4:A:330:PX4:O5	0.49	2.08	20	1
4:A:347:PX4:H39	4:A:355:PX4:H69	0.49	1.85	20	1
4:A:388:PX4:H70	4:A:395:PX4:H72	0.49	1.83	15	1
4:A:313:PX4:H33	4:A:314:PX4:H22	0.49	1.84	10	1
4:A:319:PX4:H56	4:A:359:PX4:H23	0.49	1.84	9	1
4:A:321:PX4:H22	4:A:335:PX4:H23	0.49	1.85	7	1
4:A:348:PX4:H19	4:A:349:PX4:H9	0.49	1.85	7	1
4:A:381:PX4:H30	4:A:381:PX4:H59	0.49	1.85	11	1
4:A:313:PX4:O6	4:A:356:PX4:H23	0.49	2.07	3	1
4:A:387:PX4:H59	4:A:395:PX4:H59	0.49	1.85	19	1
4:A:333:PX4:H50	4:A:348:PX4:H48	0.49	1.84	13	1
4:A:364:PX4:H60	4:A:414:PX4:H43	0.49	1.84	6	1
4:A:391:PX4:H29	4:A:425:PX4:H63	0.49	1.83	18	1
4:A:423:PX4:H48	4:A:426:PX4:H47	0.49	1.85	11	1
4:A:338:PX4:H59	4:A:351:PX4:H32	0.49	1.83	15	1
4:A:311:PX4:O2	4:A:364:PX4:H9	0.49	2.08	15	1
4:A:310:PX4:H27	4:A:311:PX4:H35	0.49	1.84	1	1
4:A:377:PX4:H50	4:A:391:PX4:H46	0.49	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:388:PX4:H23	4:A:412:PX4:H61	0.49	1.83	14	1
4:A:339:PX4:O1	4:A:355:PX4:H11	0.49	2.08	19	2
4:A:376:PX4:H16	4:A:383:PX4:H48	0.49	1.83	19	1
4:A:305:PX4:H8	4:A:365:PX4:O6	0.49	2.06	8	1
4:A:369:PX4:H9	4:A:370:PX4:O2	0.49	2.07	5	1
4:A:381:PX4:H22	4:A:395:PX4:C27	0.49	2.33	9	1
4:A:346:PX4:H64	4:A:347:PX4:H30	0.49	1.83	7	1
4:A:371:PX4:H64	4:A:403:PX4:H53	0.49	1.83	11	1
4:A:323:PX4:H47	4:A:339:PX4:H5	0.49	1.84	4	1
4:A:337:PX4:H62	4:A:339:PX4:H37	0.49	1.85	17	1
4:A:392:PX4:H36	4:A:393:PX4:H60	0.49	1.85	17	1
4:A:377:PX4:H46	4:A:386:PX4:H12	0.49	1.85	8	1
4:A:371:PX4:H52	4:A:404:PX4:H25	0.49	1.85	5	1
4:A:337:PX4:H55	4:A:354:PX4:H19	0.49	1.84	3	2
4:A:337:PX4:H19	4:A:344:PX4:C26	0.49	2.36	18	1
4:A:386:PX4:O1	4:A:387:PX4:H9	0.49	2.08	7	1
4:A:399:PX4:H61	4:A:425:PX4:H35	0.49	1.84	7	1
4:A:329:PX4:H40	4:A:338:PX4:H60	0.49	1.84	11	1
4:A:404:PX4:H9	4:A:420:PX4:O3	0.49	2.07	4	1
4:A:392:PX4:H50	4:A:409:PX4:H58	0.49	1.84	2	1
4:A:309:PX4:H28	4:A:406:PX4:H41	0.49	1.85	2	1
4:A:384:PX4:O6	4:A:408:PX4:H8	0.49	2.08	2	1
4:A:420:PX4:H7	4:A:420:PX4:H15	0.49	1.85	1	1
4:A:402:PX4:H66	4:A:418:PX4:H42	0.49	1.84	8	1
4:A:305:PX4:H36	4:A:361:PX4:H62	0.49	1.85	10	1
4:A:313:PX4:H26	4:A:354:PX4:C26	0.49	2.25	5	1
4:A:376:PX4:H52	4:A:430:PX4:H17	0.49	1.83	5	1
4:A:326:PX4:H49	4:A:343:PX4:H17	0.49	1.84	12	1
4:A:320:PX4:H32	4:A:321:PX4:H56	0.49	1.83	18	1
4:A:330:PX4:H55	4:A:331:PX4:H51	0.49	1.83	18	1
4:A:316:PX4:H38	4:A:317:PX4:H18	0.49	1.84	9	1
4:A:309:PX4:H26	4:A:366:PX4:H50	0.49	1.84	7	1
4:A:377:PX4:O8	4:A:387:PX4:H8	0.49	2.08	7	1
4:A:332:PX4:H29	4:A:340:PX4:H48	0.49	1.84	20	1
4:A:314:PX4:H45	4:A:365:PX4:H59	0.49	1.84	15	1
4:A:425:PX4:H17	4:A:430:PX4:H14	0.49	1.85	3	2
4:A:329:PX4:H54	4:A:336:PX4:H19	0.49	1.84	14	1
4:A:389:PX4:H3	4:A:403:PX4:H2	0.49	1.85	8	1
4:A:390:PX4:H36	4:A:429:PX4:H38	0.49	1.85	10	1
4:A:336:PX4:H51	4:A:366:PX4:H50	0.49	1.85	13	1
4:A:362:PX4:H19	4:A:365:PX4:H16	0.49	1.85	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:381:PX4:H48	4:A:387:PX4:H31	0.49	1.85	12	1
4:A:354:PX4:H35	4:A:355:PX4:H69	0.49	1.84	9	1
4:A:418:PX4:H17	4:A:427:PX4:H22	0.49	1.85	11	1
4:A:305:PX4:H16	4:A:328:PX4:H6	0.49	1.85	1	1
4:A:399:PX4:O6	4:A:408:PX4:H9	0.49	2.07	1	1
4:A:373:PX4:H61	4:A:380:PX4:H59	0.48	1.85	8	1
4:A:399:PX4:H2	4:A:408:PX4:H6	0.48	1.84	13	1
4:A:350:PX4:H61	4:A:363:PX4:H61	0.48	1.84	16	1
4:A:353:PX4:H48	4:A:362:PX4:H50	0.48	1.84	16	1
4:A:401:PX4:O6	4:A:418:PX4:H10	0.48	2.08	16	1
4:A:360:PX4:H20	4:A:367:PX4:H49	0.48	1.85	12	1
4:A:369:PX4:H53	4:A:369:PX4:H20	0.48	1.84	11	1
4:A:338:PX4:H18	4:A:338:PX4:H13	0.48	1.85	4	1
4:A:388:PX4:H57	4:A:412:PX4:H54	0.48	1.83	15	1
4:A:318:PX4:H67	4:A:332:PX4:H60	0.48	1.83	3	1
4:A:330:PX4:H71	4:A:335:PX4:H42	0.48	1.84	1	1
4:A:316:PX4:H49	4:A:341:PX4:H61	0.48	1.85	8	1
4:A:369:PX4:H48	4:A:425:PX4:H55	0.48	1.84	10	1
4:A:336:PX4:H41	4:A:384:PX4:H37	0.48	1.84	10	1
4:A:339:PX4:H53	4:A:355:PX4:H56	0.48	1.84	15	1
4:A:306:PX4:H23	4:A:314:PX4:H49	0.48	1.85	17	1
4:A:396:PX4:H23	4:A:396:PX4:H57	0.48	1.84	8	1
4:A:390:PX4:H22	4:A:430:PX4:H52	0.48	1.86	8	1
4:A:320:PX4:H38	4:A:328:PX4:H36	0.48	1.84	10	1
4:A:379:PX4:H62	4:A:380:PX4:H38	0.48	1.86	10	1
4:A:403:PX4:H48	4:A:412:PX4:H57	0.48	1.85	16	1
4:A:370:PX4:O1	4:A:426:PX4:H10	0.48	2.09	12	1
4:A:305:PX4:O8	4:A:362:PX4:H11	0.48	2.08	9	1
4:A:344:PX4:H40	4:A:401:PX4:H39	0.48	1.84	7	1
4:A:396:PX4:H30	4:A:414:PX4:H55	0.48	1.84	7	1
4:A:307:PX4:H15	4:A:307:PX4:H12	0.48	1.84	19	1
4:A:384:PX4:H35	4:A:400:PX4:H30	0.48	1.84	19	1
4:A:306:PX4:H4	4:A:354:PX4:O3	0.48	2.07	8	1
4:A:388:PX4:H18	4:A:395:PX4:O7	0.48	2.08	10	1
4:A:396:PX4:O2	4:A:414:PX4:H7	0.48	2.09	10	1
4:A:381:PX4:O8	4:A:382:PX4:H11	0.48	2.08	11	2
1:A:93:ILE:N	1:A:93:ILE:HD12	0.48	2.24	18	1
4:A:391:PX4:H19	4:A:425:PX4:H23	0.48	1.85	11	1
4:A:319:PX4:H26	4:A:327:PX4:H61	0.48	1.85	2	1
4:A:320:PX4:H49	4:A:362:PX4:H50	0.48	1.83	20	1
4:A:425:PX4:C13	4:A:430:PX4:H21	0.48	2.36	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H24	4:A:314:PX4:H19	0.48	1.84	3	1
4:A:359:PX4:H20	4:A:367:PX4:H9	0.48	1.85	3	1
4:A:400:PX4:H8	4:A:425:PX4:H23	0.48	1.85	1	1
4:A:322:PX4:H48	4:A:332:PX4:H55	0.48	1.84	14	1
4:A:334:PX4:H3	4:A:334:PX4:C9	0.48	2.39	14	1
4:A:317:PX4:H52	4:A:343:PX4:H25	0.48	1.85	16	1
4:A:374:PX4:H10	4:A:374:PX4:O4	0.48	2.07	18	1
4:A:399:PX4:O6	4:A:408:PX4:H3	0.48	2.07	9	1
4:A:348:PX4:H4	4:A:349:PX4:O1	0.48	2.09	11	1
4:A:326:PX4:C6	4:A:343:PX4:H15	0.48	2.37	4	1
4:A:375:PX4:H56	4:A:382:PX4:H26	0.48	1.85	2	1
4:A:336:PX4:H19	4:A:351:PX4:H57	0.48	1.85	17	2
4:A:383:PX4:H34	4:A:398:PX4:H17	0.48	1.84	17	1
4:A:309:PX4:H27	4:A:416:PX4:H43	0.48	1.86	14	1
4:A:318:PX4:H60	4:A:340:PX4:H23	0.48	1.85	19	1
4:A:402:PX4:H72	4:A:410:PX4:H35	0.48	1.85	19	1
4:A:314:PX4:H18	4:A:361:PX4:H18	0.48	1.85	8	1
4:A:334:PX4:H40	4:A:425:PX4:H41	0.48	1.85	10	1
4:A:305:PX4:H16	4:A:321:PX4:H55	0.48	1.84	20	1
4:A:336:PX4:H46	4:A:344:PX4:H12	0.48	1.85	20	1
4:A:391:PX4:H31	4:A:400:PX4:H49	0.48	1.85	3	1
4:A:369:PX4:H14	4:A:370:PX4:H21	0.48	1.86	17	1
4:A:392:PX4:P1	4:A:409:PX4:H11	0.48	2.48	19	1
4:A:369:PX4:H63	4:A:391:PX4:H51	0.48	1.86	10	1
4:A:333:PX4:H11	4:A:339:PX4:O8	0.48	2.09	18	1
4:A:324:PX4:H63	4:A:339:PX4:H57	0.48	1.86	9	1
4:A:407:PX4:H28	4:A:423:PX4:H30	0.48	1.85	7	1
1:A:98:ARG:NH2	4:A:331:PX4:O1	0.48	2.46	20	1
4:A:321:PX4:H49	4:A:332:PX4:H19	0.48	1.85	14	1
4:A:355:PX4:H25	4:A:356:PX4:H47	0.48	1.84	19	1
4:A:308:PX4:H19	4:A:315:PX4:H49	0.48	1.86	8	1
4:A:387:PX4:O6	4:A:387:PX4:H7	0.48	2.09	6	1
4:A:327:PX4:H55	4:A:360:PX4:H24	0.48	1.86	18	1
4:A:320:PX4:H42	4:A:351:PX4:H42	0.48	1.84	7	1
4:A:379:PX4:H37	4:A:427:PX4:H68	0.48	1.86	2	1
4:A:335:PX4:H64	4:A:341:PX4:H29	0.48	1.84	15	1
4:A:331:PX4:H64	4:A:347:PX4:H60	0.48	1.85	15	1
4:A:406:PX4:H10	4:A:416:PX4:O6	0.48	2.08	3	1
4:A:412:PX4:H67	4:A:389:PX4:H41	0.48	1.85	1	1
4:A:306:PX4:H17	4:A:313:PX4:H24	0.48	1.85	17	1
4:A:334:PX4:H59	4:A:341:PX4:H27	0.48	1.86	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:420:PX4:H22	4:A:428:PX4:H22	0.48	1.84	16	1
4:A:374:PX4:H27	4:A:383:PX4:H54	0.48	1.84	9	1
4:A:375:PX4:H5	4:A:421:PX4:O6	0.48	2.09	17	1
4:A:372:PX4:H45	4:A:429:PX4:H60	0.48	1.86	14	1
4:A:325:PX4:H16	4:A:349:PX4:H51	0.48	1.85	19	1
4:A:348:PX4:H35	4:A:363:PX4:C28	0.48	2.37	8	1
4:A:394:PX4:H66	4:A:400:PX4:C17	0.48	2.39	8	1
4:A:329:PX4:H68	4:A:337:PX4:H23	0.48	1.85	16	1
4:A:370:PX4:H60	4:A:426:PX4:H32	0.48	1.84	5	1
4:A:344:PX4:H30	4:A:345:PX4:H30	0.48	1.86	6	1
4:A:352:PX4:H47	4:A:365:PX4:H25	0.48	1.86	15	1
1:A:22:PHE:CE2	1:A:66:ARG:CZ	0.48	2.96	3	1
4:A:361:PX4:H58	4:A:362:PX4:H32	0.48	1.86	3	1
4:A:382:PX4:H58	4:A:395:PX4:H60	0.48	1.85	1	1
4:A:324:PX4:H71	4:A:331:PX4:H34	0.47	1.86	10	1
4:A:407:PX4:H29	4:A:423:PX4:H20	0.47	1.86	16	1
4:A:371:PX4:H69	4:A:389:PX4:H59	0.47	1.86	6	1
4:A:381:PX4:H66	4:A:385:PX4:H64	0.47	1.85	12	1
4:A:413:PX4:H37	4:A:428:PX4:H32	0.47	1.86	12	1
4:A:381:PX4:H25	4:A:382:PX4:H48	0.47	1.85	18	1
4:A:330:PX4:H68	4:A:342:PX4:H72	0.47	1.83	4	1
4:A:369:PX4:H57	4:A:391:PX4:H46	0.47	1.86	2	1
4:A:384:PX4:H6	4:A:393:PX4:O2	0.47	2.08	20	1
4:A:326:PX4:H10	4:A:326:PX4:H17	0.47	1.86	1	1
4:A:348:PX4:H19	4:A:349:PX4:C9	0.47	2.39	14	1
4:A:346:PX4:H66	4:A:346:PX4:H42	0.47	1.85	19	1
4:A:321:PX4:H40	4:A:347:PX4:H63	0.47	1.86	19	1
4:A:424:PX4:H46	4:A:430:PX4:H23	0.47	1.86	10	1
4:A:420:PX4:H22	4:A:428:PX4:C11	0.47	2.39	16	1
4:A:308:PX4:H37	4:A:315:PX4:H23	0.47	1.84	6	1
4:A:425:PX4:H17	4:A:425:PX4:H10	0.47	1.86	12	1
4:A:327:PX4:H59	4:A:360:PX4:H27	0.47	1.85	18	1
4:A:376:PX4:H64	4:A:430:PX4:H67	0.47	1.86	7	1
4:A:306:PX4:H27	4:A:314:PX4:H47	0.47	1.84	4	1
4:A:312:PX4:H49	4:A:318:PX4:H19	0.47	1.86	3	1
4:A:383:PX4:H30	4:A:389:PX4:H17	0.47	1.85	3	1
4:A:335:PX4:H20	4:A:342:PX4:H46	0.47	1.85	1	1
4:A:366:PX4:H35	4:A:409:PX4:H40	0.47	1.86	1	1
4:A:330:PX4:H28	4:A:331:PX4:H32	0.47	1.85	14	1
4:A:331:PX4:H50	4:A:347:PX4:H24	0.47	1.85	8	1
4:A:362:PX4:H20	4:A:365:PX4:H16	0.47	1.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:329:PX4:H13	4:A:338:PX4:O6	0.47	2.09	12	1
4:A:348:PX4:H12	4:A:349:PX4:H22	0.47	1.84	18	1
4:A:366:PX4:O6	4:A:366:PX4:H12	0.47	2.08	18	1
4:A:370:PX4:H49	4:A:424:PX4:H59	0.47	1.85	18	1
4:A:380:PX4:H52	4:A:385:PX4:H46	0.47	1.87	9	1
4:A:384:PX4:H56	4:A:393:PX4:H25	0.47	1.86	4	1
4:A:404:PX4:H25	4:A:412:PX4:H19	0.47	1.86	4	1
4:A:341:PX4:H51	4:A:350:PX4:H14	0.47	1.87	15	1
4:A:360:PX4:H60	4:A:360:PX4:C14	0.47	2.39	3	1
4:A:341:PX4:H45	4:A:408:PX4:H65	0.47	1.86	14	1
4:A:318:PX4:H47	4:A:323:PX4:H49	0.47	1.85	19	1
4:A:386:PX4:H36	4:A:387:PX4:H57	0.47	1.86	19	1
4:A:406:PX4:O2	4:A:415:PX4:H14	0.47	2.09	16	1
4:A:305:PX4:H27	4:A:362:PX4:H54	0.47	1.86	6	1
4:A:363:PX4:H43	4:A:405:PX4:H42	0.47	1.85	6	1
4:A:336:PX4:H43	4:A:400:PX4:H62	0.47	1.84	9	1
4:A:309:PX4:H68	4:A:357:PX4:H33	0.47	1.86	4	1
4:A:370:PX4:H47	4:A:419:PX4:H19	0.47	1.85	20	1
4:A:389:PX4:O6	4:A:403:PX4:H7	0.47	2.10	3	1
4:A:321:PX4:H37	4:A:347:PX4:H58	0.47	1.86	10	1
4:A:413:PX4:O6	4:A:428:PX4:H11	0.47	2.10	10	1
4:A:329:PX4:H17	4:A:338:PX4:H17	0.47	1.86	16	1
4:A:401:PX4:H30	4:A:410:PX4:H39	0.47	1.86	16	1
4:A:328:PX4:H25	4:A:335:PX4:H57	0.47	1.85	11	1
4:A:399:PX4:H31	4:A:409:PX4:H53	0.47	1.87	2	1
4:A:332:PX4:H29	4:A:340:PX4:H26	0.47	1.87	15	1
4:A:357:PX4:H38	4:A:408:PX4:H62	0.47	1.87	14	1
4:A:305:PX4:H47	4:A:362:PX4:H52	0.47	1.85	19	1
4:A:327:PX4:H40	4:A:343:PX4:H63	0.47	1.87	8	1
4:A:369:PX4:H49	4:A:370:PX4:H26	0.47	1.86	8	1
4:A:376:PX4:H21	4:A:383:PX4:H21	0.47	1.85	8	1
4:A:342:PX4:H13	4:A:342:PX4:H14	0.47	1.86	10	1
4:A:374:PX4:C10	4:A:383:PX4:H16	0.47	2.37	10	1
4:A:394:PX4:H64	4:A:400:PX4:H38	0.47	1.87	13	1
4:A:349:PX4:H21	4:A:363:PX4:H17	0.47	1.86	6	1
4:A:311:PX4:H56	4:A:315:PX4:H31	0.47	1.85	20	1
4:A:321:PX4:H34	4:A:330:PX4:H57	0.47	1.87	20	1
4:A:344:PX4:O6	4:A:344:PX4:H4	0.47	2.09	20	1
4:A:361:PX4:H36	4:A:364:PX4:H33	0.47	1.87	20	1
4:A:337:PX4:H57	4:A:337:PX4:H23	0.47	1.85	3	1
4:A:403:PX4:H52	4:A:405:PX4:H53	0.47	1.85	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:382:PX4:H35	4:A:421:PX4:H30	0.47	1.87	17	1
4:A:392:PX4:H20	4:A:393:PX4:H46	0.47	1.86	14	1
4:A:310:PX4:H68	4:A:397:PX4:H44	0.47	1.86	14	1
4:A:392:PX4:H68	4:A:394:PX4:H45	0.47	1.86	14	1
4:A:392:PX4:H55	4:A:402:PX4:H51	0.47	1.84	14	1
4:A:383:PX4:H19	4:A:398:PX4:H16	0.47	1.86	19	1
4:A:411:PX4:H17	4:A:411:PX4:H10	0.47	1.86	19	1
4:A:411:PX4:H18	4:A:427:PX4:H58	0.47	1.87	19	1
4:A:321:PX4:H31	4:A:335:PX4:H38	0.47	1.86	8	1
4:A:387:PX4:H58	4:A:388:PX4:H68	0.47	1.87	10	1
4:A:328:PX4:H19	4:A:342:PX4:H61	0.47	1.86	10	1
4:A:375:PX4:H9	4:A:429:PX4:O4	0.47	2.08	10	1
4:A:377:PX4:H54	4:A:378:PX4:H27	0.47	1.86	13	1
4:A:375:PX4:H16	4:A:382:PX4:H24	0.47	1.85	13	1
4:A:333:PX4:H11	4:A:339:PX4:H48	0.47	1.86	16	1
4:A:392:PX4:H57	4:A:402:PX4:H19	0.47	1.87	16	1
4:A:316:PX4:H50	4:A:317:PX4:H50	0.47	1.86	5	1
4:A:419:PX4:H35	4:A:426:PX4:H58	0.47	1.86	5	1
4:A:337:PX4:H47	4:A:346:PX4:H23	0.47	1.86	12	1
4:A:406:PX4:H17	4:A:415:PX4:H21	0.47	1.87	18	1
4:A:377:PX4:H69	4:A:378:PX4:H35	0.47	1.87	18	1
4:A:318:PX4:H43	4:A:422:PX4:H67	0.47	1.87	9	1
4:A:380:PX4:H24	4:A:411:PX4:H52	0.47	1.86	7	1
4:A:306:PX4:H60	4:A:313:PX4:H57	0.47	1.85	7	1
4:A:320:PX4:H61	4:A:362:PX4:H58	0.47	1.85	7	1
4:A:405:PX4:H15	4:A:414:PX4:O4	0.47	2.09	11	2
4:A:361:PX4:H43	4:A:411:PX4:H64	0.47	1.87	11	1
4:A:406:PX4:H38	4:A:417:PX4:H33	0.47	1.86	11	1
4:A:336:PX4:H52	4:A:352:PX4:H53	0.47	1.85	20	1
4:A:379:PX4:H28	4:A:401:PX4:H24	0.47	1.86	20	1
4:A:320:PX4:H16	4:A:328:PX4:H52	0.47	1.87	15	1
4:A:340:PX4:H69	4:A:387:PX4:H70	0.47	1.86	15	1
4:A:314:PX4:O2	4:A:354:PX4:H11	0.47	2.09	3	1
4:A:339:PX4:H44	4:A:381:PX4:H66	0.47	1.86	1	1
4:A:344:PX4:H23	4:A:345:PX4:H26	0.47	1.86	17	1
4:A:338:PX4:H40	4:A:346:PX4:H35	0.47	1.86	19	1
4:A:309:PX4:H24	4:A:366:PX4:H53	0.47	1.87	5	1
4:A:368:PX4:H28	4:A:429:PX4:H51	0.47	1.87	5	1
4:A:322:PX4:H45	4:A:332:PX4:H58	0.47	1.87	12	1
4:A:403:PX4:H58	4:A:412:PX4:H55	0.47	1.86	9	1
4:A:375:PX4:H6	4:A:375:PX4:H15	0.47	1.87	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:410:PX4:H25	4:A:423:PX4:H71	0.47	1.85	11	1
4:A:321:PX4:H52	4:A:328:PX4:H47	0.47	1.87	20	1
4:A:330:PX4:H32	4:A:332:PX4:H23	0.47	1.87	20	1
4:A:322:PX4:H20	4:A:332:PX4:O7	0.47	2.09	1	1
4:A:417:PX4:O8	4:A:419:PX4:H11	0.47	2.08	17	1
4:A:307:PX4:H17	4:A:363:PX4:O6	0.47	2.10	19	1
4:A:378:PX4:H13	4:A:385:PX4:O2	0.47	2.09	8	1
4:A:310:PX4:H50	4:A:363:PX4:H16	0.47	1.86	10	1
4:A:381:PX4:H27	4:A:385:PX4:H37	0.47	1.86	10	1
4:A:342:PX4:H20	4:A:351:PX4:O5	0.47	2.09	16	1
4:A:374:PX4:O6	4:A:398:PX4:H6	0.47	2.10	16	1
4:A:429:PX4:H61	4:A:431:PX4:H65	0.47	1.87	16	1
4:A:377:PX4:H53	4:A:395:PX4:H41	0.47	1.87	5	1
4:A:385:PX4:H59	4:A:387:PX4:H53	0.47	1.85	12	1
4:A:306:PX4:H7	4:A:313:PX4:O2	0.47	2.10	9	1
4:A:329:PX4:H36	4:A:358:PX4:H44	0.47	1.85	9	1
4:A:419:PX4:H23	4:A:426:PX4:H48	0.47	1.85	9	1
4:A:321:PX4:H41	4:A:338:PX4:H60	0.47	1.87	7	1
4:A:309:PX4:H64	4:A:363:PX4:H59	0.47	1.86	2	1
4:A:312:PX4:H65	4:A:319:PX4:H68	0.47	1.86	20	1
4:A:401:PX4:H16	4:A:427:PX4:H48	0.47	1.86	20	1
4:A:337:PX4:H52	4:A:356:PX4:H25	0.47	1.85	3	1
4:A:348:PX4:H16	4:A:349:PX4:H10	0.47	1.85	17	2
4:A:321:PX4:H32	4:A:330:PX4:H64	0.47	1.87	19	1
4:A:392:PX4:H27	4:A:393:PX4:H61	0.47	1.85	8	1
4:A:337:PX4:H45	4:A:388:PX4:H36	0.47	1.86	13	1
4:A:391:PX4:O7	4:A:400:PX4:H17	0.47	2.10	13	1
4:A:347:PX4:H22	4:A:355:PX4:H48	0.47	1.87	5	1
4:A:357:PX4:H17	4:A:358:PX4:H21	0.47	1.87	5	1
4:A:344:PX4:H56	4:A:366:PX4:H67	0.47	1.87	6	1
4:A:369:PX4:H21	4:A:377:PX4:H46	0.47	1.85	12	1
4:A:321:PX4:H25	4:A:335:PX4:H32	0.47	1.87	18	1
4:A:329:PX4:H20	4:A:347:PX4:H55	0.47	1.85	7	1
4:A:331:PX4:H17	4:A:339:PX4:H14	0.47	1.85	7	1
4:A:334:PX4:H22	4:A:353:PX4:H37	0.47	1.86	7	1
4:A:323:PX4:O2	4:A:324:PX4:H11	0.47	2.10	4	1
4:A:318:PX4:H17	4:A:323:PX4:H24	0.47	1.85	3	1
4:A:403:PX4:H16	4:A:412:PX4:H8	0.47	1.86	1	1
4:A:369:PX4:H14	4:A:370:PX4:C11	0.46	2.40	17	1
4:A:309:PX4:H67	4:A:363:PX4:H62	0.46	1.87	14	1
4:A:377:PX4:H47	4:A:395:PX4:H39	0.46	1.86	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:359:PX4:H19	4:A:367:PX4:H20	0.46	1.86	13	1
4:A:396:PX4:H48	4:A:422:PX4:H46	0.46	1.86	13	1
4:A:333:PX4:H34	4:A:339:PX4:H39	0.46	1.87	16	1
4:A:383:PX4:H57	4:A:429:PX4:H32	0.46	1.86	6	1
4:A:397:PX4:O8	4:A:398:PX4:H56	0.46	2.10	11	1
4:A:334:PX4:H27	4:A:351:PX4:H28	0.46	1.85	4	1
4:A:388:PX4:O6	4:A:394:PX4:H7	0.46	2.10	2	1
4:A:390:PX4:H20	4:A:430:PX4:H51	0.46	1.86	2	1
4:A:325:PX4:H23	4:A:333:PX4:H22	0.46	1.86	20	1
4:A:424:PX4:H21	4:A:425:PX4:H55	0.46	1.86	15	1
4:A:322:PX4:H66	4:A:372:PX4:H39	0.46	1.87	1	1
4:A:361:PX4:H28	4:A:427:PX4:H44	0.46	1.87	17	1
4:A:307:PX4:H16	4:A:311:PX4:H14	0.46	1.87	19	2
4:A:393:PX4:H51	4:A:402:PX4:H27	0.46	1.87	8	1
4:A:325:PX4:H22	4:A:333:PX4:H47	0.46	1.87	6	1
4:A:316:PX4:H20	4:A:325:PX4:H57	0.46	1.86	9	1
4:A:369:PX4:H69	4:A:393:PX4:H43	0.46	1.88	9	1
4:A:313:PX4:H62	4:A:403:PX4:H35	0.46	1.87	11	1
4:A:369:PX4:H55	4:A:400:PX4:H59	0.46	1.86	20	1
4:A:402:PX4:H22	4:A:392:PX4:H53	0.46	1.87	1	1
4:A:336:PX4:H66	4:A:366:PX4:H14	0.46	1.88	17	1
4:A:382:PX4:H38	4:A:421:PX4:H32	0.46	1.86	10	1
4:A:318:PX4:H69	4:A:373:PX4:H70	0.46	1.87	13	1
4:A:372:PX4:H48	4:A:421:PX4:H53	0.46	1.87	13	1
4:A:416:PX4:H53	4:A:417:PX4:H21	0.46	1.86	16	1
4:A:309:PX4:H53	4:A:357:PX4:H55	0.46	1.87	18	1
4:A:418:PX4:H19	4:A:427:PX4:H22	0.46	1.87	18	1
4:A:306:PX4:H17	4:A:313:PX4:H22	0.46	1.87	7	1
4:A:392:PX4:H50	4:A:409:PX4:H59	0.46	1.86	11	1
4:A:361:PX4:H30	4:A:365:PX4:H61	0.46	1.86	2	1
4:A:430:PX4:O6	4:A:430:PX4:H2	0.46	2.10	15	1
4:A:386:PX4:H57	4:A:394:PX4:H46	0.46	1.86	3	1
4:A:399:PX4:H25	4:A:408:PX4:H14	0.46	1.88	17	1
4:A:320:PX4:H16	4:A:362:PX4:H5	0.46	1.87	14	1
4:A:306:PX4:H31	4:A:314:PX4:H47	0.46	1.88	19	1
4:A:358:PX4:H40	4:A:399:PX4:H70	0.46	1.88	12	1
4:A:340:PX4:H69	4:A:382:PX4:H65	0.46	1.87	11	1
4:A:406:PX4:H25	4:A:416:PX4:H22	0.46	1.86	11	1
4:A:406:PX4:H36	4:A:408:PX4:H31	0.46	1.88	2	1
4:A:343:PX4:H45	4:A:390:PX4:H44	0.46	1.88	15	1
4:A:413:PX4:H20	4:A:421:PX4:H51	0.46	1.87	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:333:PX4:H41	4:A:347:PX4:H33	0.46	1.86	1	1
4:A:321:PX4:H26	4:A:347:PX4:H46	0.46	1.87	10	1
4:A:305:PX4:H18	4:A:362:PX4:H3	0.46	1.87	13	1
4:A:314:PX4:H31	4:A:354:PX4:H57	0.46	1.86	13	1
4:A:308:PX4:H22	4:A:359:PX4:H59	0.46	1.88	13	1
4:A:391:PX4:H53	4:A:400:PX4:H55	0.46	1.88	12	2
4:A:383:PX4:H45	4:A:388:PX4:H54	0.46	1.88	5	1
4:A:307:PX4:H60	4:A:311:PX4:H32	0.46	1.86	6	1
4:A:316:PX4:H53	4:A:316:PX4:H31	0.46	1.88	18	1
4:A:373:PX4:H42	4:A:421:PX4:H39	0.46	1.87	4	1
4:A:326:PX4:H41	4:A:424:PX4:H43	0.46	1.87	2	1
4:A:318:PX4:H49	4:A:340:PX4:H5	0.46	1.87	15	1
4:A:324:PX4:H24	4:A:325:PX4:H50	0.46	1.87	3	1
4:A:305:PX4:H29	4:A:321:PX4:H51	0.46	1.88	1	1
4:A:328:PX4:O2	4:A:335:PX4:H14	0.46	2.10	17	1
4:A:392:PX4:C10	4:A:393:PX4:H46	0.46	2.41	14	1
4:A:393:PX4:H29	4:A:394:PX4:H59	0.46	1.87	13	1
4:A:401:PX4:H14	4:A:410:PX4:O2	0.46	2.10	13	1
4:A:357:PX4:H54	4:A:358:PX4:H45	0.46	1.86	16	1
4:A:372:PX4:H72	4:A:379:PX4:H70	0.46	1.88	12	1
4:A:378:PX4:H8	4:A:380:PX4:O1	0.46	2.11	9	1
4:A:389:PX4:H42	4:A:404:PX4:H69	0.46	1.88	4	1
4:A:315:PX4:H51	4:A:318:PX4:H56	0.46	1.87	15	1
4:A:313:PX4:H38	4:A:306:PX4:H27	0.46	1.87	1	1
4:A:337:PX4:H23	4:A:344:PX4:H51	0.46	1.86	1	1
4:A:369:PX4:H52	4:A:425:PX4:H51	0.46	1.88	17	1
4:A:305:PX4:H33	4:A:305:PX4:H59	0.46	1.87	19	1
4:A:323:PX4:H58	4:A:340:PX4:H22	0.46	1.88	19	1
4:A:372:PX4:H19	4:A:421:PX4:H16	0.46	1.87	16	1
4:A:336:PX4:O6	4:A:358:PX4:H17	0.46	2.11	5	1
4:A:337:PX4:H48	4:A:346:PX4:H56	0.46	1.85	5	1
4:A:401:PX4:H22	4:A:410:PX4:H19	0.46	1.87	6	1
4:A:380:PX4:H2	4:A:385:PX4:O6	0.46	2.09	18	1
4:A:351:PX4:H70	4:A:357:PX4:H47	0.46	1.86	7	1
4:A:420:PX4:H26	4:A:428:PX4:H27	0.46	1.87	20	1
4:A:321:PX4:H14	4:A:330:PX4:O5	0.46	2.10	15	1
4:A:336:PX4:H72	4:A:365:PX4:H45	0.46	1.87	15	1
4:A:419:PX4:H10	4:A:426:PX4:O2	0.46	2.11	15	1
4:A:334:PX4:H38	4:A:400:PX4:H64	0.46	1.87	1	1
4:A:391:PX4:H15	4:A:400:PX4:O7	0.46	2.11	17	1
4:A:393:PX4:H65	4:A:400:PX4:H40	0.46	1.88	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:368:PX4:H54	4:A:430:PX4:H20	0.46	1.87	19	1
4:A:377:PX4:H59	4:A:391:PX4:H50	0.46	1.88	8	1
4:A:393:PX4:H28	4:A:394:PX4:H56	0.46	1.88	10	1
4:A:424:PX4:H53	4:A:430:PX4:H27	0.46	1.88	13	1
4:A:403:PX4:H34	4:A:403:PX4:H61	0.46	1.85	16	1
4:A:338:PX4:H45	4:A:347:PX4:H71	0.46	1.88	9	1
4:A:396:PX4:H11	4:A:403:PX4:O6	0.46	2.10	9	1
4:A:335:PX4:H58	4:A:353:PX4:H42	0.46	1.87	7	1
4:A:316:PX4:H3	4:A:324:PX4:O2	0.46	2.11	11	1
4:A:348:PX4:H38	4:A:349:PX4:H30	0.46	1.86	4	1
4:A:384:PX4:H52	4:A:400:PX4:H20	0.46	1.88	2	1
4:A:341:PX4:H55	4:A:357:PX4:H24	0.46	1.88	15	1
4:A:352:PX4:H3	4:A:365:PX4:O4	0.46	2.11	15	1
4:A:337:PX4:H51	4:A:347:PX4:H22	0.46	1.88	17	1
1:A:129:TRP:CD2	4:A:313:PX4:H1	0.46	2.46	16	1
4:A:409:PX4:H71	4:A:410:PX4:H63	0.46	1.87	5	1
4:A:409:PX4:H28	4:A:417:PX4:H23	0.46	1.88	6	1
4:A:401:PX4:H36	4:A:410:PX4:H36	0.46	1.88	18	1
4:A:414:PX4:H10	4:A:422:PX4:O8	0.46	2.11	9	1
4:A:311:PX4:H32	4:A:396:PX4:H43	0.46	1.88	7	1
4:A:399:PX4:H26	4:A:408:PX4:C6	0.46	2.40	7	1
4:A:333:PX4:H26	4:A:339:PX4:H58	0.46	1.87	15	1
4:A:340:PX4:H59	4:A:355:PX4:H67	0.46	1.88	1	1
4:A:384:PX4:H17	4:A:393:PX4:H22	0.46	1.87	1	1
4:A:329:PX4:H40	4:A:391:PX4:H67	0.46	1.88	17	1
4:A:399:PX4:H18	4:A:408:PX4:H1	0.46	1.88	17	1
4:A:313:PX4:H66	4:A:349:PX4:H39	0.46	1.87	19	1
1:A:129:TRP:CG	4:A:313:PX4:H1	0.46	2.46	16	1
4:A:322:PX4:H58	4:A:332:PX4:H61	0.46	1.87	5	1
4:A:392:PX4:H34	4:A:399:PX4:H39	0.46	1.87	5	1
4:A:399:PX4:C9	4:A:408:PX4:H3	0.46	2.41	6	1
4:A:381:PX4:H23	4:A:385:PX4:H41	0.46	1.88	12	1
4:A:318:PX4:H43	4:A:431:PX4:H38	0.46	1.87	18	1
4:A:328:PX4:H14	4:A:335:PX4:H21	0.46	1.87	9	1
4:A:336:PX4:H18	4:A:358:PX4:H15	0.46	1.86	7	1
4:A:329:PX4:H70	4:A:402:PX4:H39	0.46	1.88	7	1
4:A:323:PX4:H54	4:A:340:PX4:H48	0.46	1.87	11	1
4:A:371:PX4:H63	4:A:403:PX4:H49	0.46	1.87	2	1
4:A:374:PX4:H49	4:A:382:PX4:O5	0.46	2.11	2	1
4:A:366:PX4:H45	4:A:417:PX4:H34	0.46	1.88	15	1
4:A:417:PX4:O1	4:A:417:PX4:H17	0.46	2.11	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:H24	4:A:346:PX4:H35	0.46	1.87	3	1
4:A:329:PX4:H33	4:A:384:PX4:H42	0.45	1.88	13	1
4:A:336:PX4:H27	4:A:341:PX4:H26	0.45	1.87	6	1
4:A:362:PX4:H71	4:A:365:PX4:H65	0.45	1.88	6	1
4:A:313:PX4:H24	4:A:354:PX4:H55	0.45	1.87	11	1
4:A:358:PX4:H35	4:A:399:PX4:H68	0.45	1.86	15	1
4:A:344:PX4:H16	4:A:345:PX4:H47	0.45	1.88	1	1
4:A:327:PX4:H20	4:A:353:PX4:H52	0.45	1.88	17	1
4:A:390:PX4:H48	4:A:430:PX4:H59	0.45	1.88	19	1
4:A:392:PX4:H60	4:A:402:PX4:H58	0.45	1.88	8	1
4:A:306:PX4:H71	4:A:364:PX4:H39	0.45	1.88	10	1
4:A:380:PX4:O6	4:A:381:PX4:H6	0.45	2.12	10	1
4:A:407:PX4:H37	4:A:423:PX4:C21	0.45	2.38	13	1
4:A:321:PX4:H32	4:A:330:PX4:H63	0.45	1.87	5	1
4:A:317:PX4:H32	4:A:323:PX4:H33	0.45	1.87	18	1
4:A:331:PX4:H66	4:A:380:PX4:H43	0.45	1.87	9	1
4:A:424:PX4:H59	4:A:425:PX4:H39	0.45	1.86	9	1
4:A:347:PX4:H20	4:A:355:PX4:H17	0.45	1.87	7	1
4:A:405:PX4:H58	4:A:406:PX4:H59	0.45	1.87	7	1
4:A:375:PX4:H11	4:A:413:PX4:H54	0.45	1.87	11	1
4:A:321:PX4:H17	4:A:328:PX4:H49	0.45	1.88	4	1
4:A:337:PX4:H23	4:A:337:PX4:H57	0.45	1.86	2	1
4:A:390:PX4:H52	4:A:399:PX4:H15	0.45	1.87	2	1
4:A:372:PX4:H9	4:A:372:PX4:H15	0.45	1.88	20	1
4:A:310:PX4:H19	4:A:307:PX4:H55	0.45	1.88	1	1
4:A:308:PX4:H31	4:A:315:PX4:H26	0.45	1.89	17	1
4:A:357:PX4:H15	4:A:358:PX4:O5	0.45	2.10	17	1
4:A:374:PX4:O1	4:A:375:PX4:H15	0.45	2.11	17	1
4:A:319:PX4:H42	4:A:340:PX4:H45	0.45	1.88	14	1
4:A:315:PX4:H68	4:A:318:PX4:H23	0.45	1.88	8	1
4:A:373:PX4:H64	4:A:381:PX4:H34	0.45	1.87	8	1
4:A:394:PX4:H63	4:A:400:PX4:H33	0.45	1.88	8	1
1:A:12:TRP:CE3	1:A:59:ILE:HD11	0.45	2.47	6	3
4:A:407:PX4:O6	4:A:407:PX4:H7	0.45	2.11	10	1
4:A:313:PX4:H55	4:A:333:PX4:H53	0.45	1.89	9	1
4:A:407:PX4:H1	4:A:423:PX4:O1	0.45	2.10	7	1
4:A:401:PX4:C36	4:A:401:PX4:H39	0.45	2.41	2	1
4:A:391:PX4:H31	4:A:425:PX4:H56	0.45	1.89	2	1
4:A:371:PX4:H17	4:A:404:PX4:O6	0.45	2.11	15	1
4:A:311:PX4:H3	4:A:364:PX4:O8	0.45	2.12	14	1
4:A:382:PX4:H17	4:A:385:PX4:H56	0.45	1.88	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H43	4:A:404:PX4:H25	0.45	1.89	8	1
4:A:369:PX4:H60	4:A:369:PX4:H30	0.45	1.89	13	1
4:A:357:PX4:H55	4:A:358:PX4:H55	0.45	1.87	12	1
4:A:384:PX4:H26	4:A:400:PX4:H21	0.45	1.86	12	1
4:A:337:PX4:H60	4:A:356:PX4:H32	0.45	1.87	7	1
4:A:318:PX4:O2	4:A:323:PX4:H14	0.45	2.10	2	1
4:A:358:PX4:H42	4:A:399:PX4:H64	0.45	1.87	2	1
4:A:406:PX4:H23	4:A:416:PX4:H20	0.45	1.87	2	1
4:A:316:PX4:H5	4:A:325:PX4:O6	0.45	2.11	20	1
4:A:334:PX4:H25	4:A:341:PX4:H25	0.45	1.88	20	1
4:A:380:PX4:H5	4:A:411:PX4:O8	0.45	2.11	20	1
4:A:369:PX4:H30	4:A:369:PX4:H64	0.45	1.89	15	1
4:A:374:PX4:H26	4:A:375:PX4:H29	0.45	1.89	15	1
4:A:384:PX4:H58	4:A:393:PX4:H30	0.45	1.89	17	1
4:A:405:PX4:O2	4:A:414:PX4:H6	0.45	2.11	17	1
4:A:361:PX4:H60	4:A:427:PX4:C22	0.45	2.41	17	1
4:A:322:PX4:H70	4:A:372:PX4:H37	0.45	1.88	8	1
4:A:369:PX4:C27	4:A:391:PX4:H22	0.45	2.40	10	1
4:A:409:PX4:H21	4:A:410:PX4:H47	0.45	1.88	16	1
4:A:370:PX4:H69	4:A:426:PX4:H34	0.45	1.89	12	1
4:A:396:PX4:H5	4:A:403:PX4:O6	0.45	2.10	18	1
4:A:337:PX4:H17	4:A:346:PX4:H21	0.45	1.89	7	1
4:A:349:PX4:H69	4:A:350:PX4:H66	0.45	1.87	7	1
4:A:375:PX4:H5	4:A:429:PX4:O8	0.45	2.12	7	1
4:A:335:PX4:H72	4:A:343:PX4:H68	0.45	1.89	4	1
4:A:360:PX4:H71	4:A:360:PX4:H20	0.45	1.87	2	1
4:A:340:PX4:H41	4:A:428:PX4:H41	0.45	1.89	14	1
4:A:382:PX4:H47	4:A:387:PX4:H46	0.45	1.89	19	1
4:A:316:PX4:H19	4:A:324:PX4:H28	0.45	1.88	5	1
4:A:370:PX4:C10	4:A:419:PX4:H51	0.45	2.38	9	1
4:A:347:PX4:H11	4:A:355:PX4:H17	0.45	1.89	4	1
4:A:377:PX4:H23	4:A:411:PX4:H25	0.45	1.88	20	1
4:A:410:PX4:H21	4:A:410:PX4:H54	0.45	1.87	15	1
4:A:403:PX4:H51	4:A:412:PX4:H52	0.45	1.87	15	1
4:A:425:PX4:O6	4:A:430:PX4:H16	0.45	2.11	15	1
4:A:373:PX4:H54	4:A:381:PX4:H53	0.45	1.88	3	1
4:A:378:PX4:H4	4:A:381:PX4:O3	0.45	2.12	1	1
4:A:338:PX4:H25	4:A:346:PX4:H21	0.45	1.87	10	1
4:A:310:PX4:H67	4:A:363:PX4:H24	0.45	1.88	10	1
4:A:376:PX4:H17	4:A:390:PX4:H19	0.45	1.89	10	1
4:A:411:PX4:H34	4:A:426:PX4:H35	0.45	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:329:PX4:H4	4:A:338:PX4:O1	0.45	2.11	16	1
4:A:319:PX4:H70	4:A:375:PX4:H43	0.45	1.88	5	1
4:A:368:PX4:H4	4:A:429:PX4:O1	0.45	2.11	18	1
4:A:337:PX4:H25	4:A:346:PX4:H35	0.45	1.88	9	1
4:A:357:PX4:C15	4:A:429:PX4:H44	0.45	2.41	9	1
4:A:306:PX4:H46	4:A:313:PX4:O8	0.45	2.12	11	1
4:A:369:PX4:H1	4:A:370:PX4:O2	0.45	2.11	4	1
4:A:388:PX4:H54	4:A:412:PX4:H54	0.45	1.88	3	1
4:A:323:PX4:H15	4:A:339:PX4:H5	0.45	1.89	17	1
4:A:314:PX4:H32	4:A:345:PX4:H25	0.45	1.88	19	1
4:A:361:PX4:H46	4:A:362:PX4:H23	0.45	1.88	19	1
4:A:312:PX4:H46	4:A:317:PX4:C6	0.45	2.42	10	1
4:A:340:PX4:H28	4:A:340:PX4:H9	0.45	1.88	10	1
4:A:336:PX4:H24	4:A:351:PX4:H50	0.45	1.89	5	1
1:A:100:LEU:HB3	1:A:104:THR:HG21	0.45	1.89	12	1
4:A:332:PX4:H56	4:A:410:PX4:H44	0.45	1.89	18	1
4:A:333:PX4:H55	4:A:333:PX4:H19	0.45	1.86	18	1
4:A:313:PX4:H26	4:A:348:PX4:H60	0.45	1.88	7	1
4:A:405:PX4:H60	4:A:396:PX4:H27	0.45	1.87	1	1
4:A:376:PX4:H19	4:A:383:PX4:C11	0.45	2.41	17	1
4:A:305:PX4:H21	4:A:328:PX4:H17	0.45	1.89	13	1
4:A:389:PX4:H3	4:A:403:PX4:O1	0.45	2.12	13	1
4:A:338:PX4:H55	4:A:346:PX4:H64	0.45	1.88	16	1
4:A:374:PX4:H24	4:A:398:PX4:H16	0.45	1.89	16	1
4:A:372:PX4:H16	4:A:373:PX4:C11	0.45	2.42	6	1
4:A:316:PX4:H19	4:A:334:PX4:C34	0.45	2.39	18	1
4:A:306:PX4:H21	4:A:314:PX4:H15	0.45	1.89	7	1
4:A:367:PX4:H45	4:A:421:PX4:H68	0.45	1.88	4	1
4:A:391:PX4:H44	4:A:400:PX4:H62	0.45	1.89	3	1
4:A:360:PX4:H43	4:A:401:PX4:H45	0.45	1.87	3	1
4:A:370:PX4:H53	4:A:424:PX4:H20	0.45	1.89	3	1
4:A:305:PX4:H22	4:A:328:PX4:H9	0.45	1.89	17	1
4:A:372:PX4:H5	4:A:380:PX4:O1	0.45	2.11	17	1
4:A:349:PX4:H16	4:A:363:PX4:H47	0.45	1.88	8	1
4:A:312:PX4:H26	4:A:327:PX4:H60	0.45	1.89	13	1
4:A:328:PX4:H58	4:A:342:PX4:H66	0.45	1.89	5	1
4:A:339:PX4:H33	4:A:347:PX4:H35	0.45	1.88	5	1
4:A:399:PX4:O2	4:A:408:PX4:H12	0.45	2.11	6	1
4:A:389:PX4:H24	4:A:403:PX4:H24	0.45	1.87	12	1
4:A:322:PX4:H37	4:A:332:PX4:H62	0.45	1.88	7	1
4:A:337:PX4:H40	4:A:388:PX4:H44	0.45	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:376:PX4:H17	4:A:390:PX4:H24	0.45	1.89	11	1
4:A:328:PX4:C30	4:A:335:PX4:H23	0.45	2.36	20	1
4:A:326:PX4:O1	4:A:343:PX4:H15	0.44	2.13	14	1
4:A:324:PX4:H51	4:A:339:PX4:H49	0.44	1.89	5	1
4:A:394:PX4:H40	4:A:402:PX4:H18	0.44	1.88	5	1
4:A:389:PX4:O1	4:A:398:PX4:H3	0.44	2.13	12	1
4:A:368:PX4:H65	4:A:376:PX4:H62	0.44	1.88	7	1
4:A:392:PX4:H30	4:A:394:PX4:H60	0.44	1.89	4	1
4:A:381:PX4:H34	4:A:387:PX4:H38	0.44	1.89	2	1
4:A:392:PX4:H34	4:A:393:PX4:H69	0.44	1.89	15	1
4:A:336:PX4:H22	4:A:351:PX4:H57	0.44	1.89	1	1
4:A:368:PX4:C1	4:A:368:PX4:H22	0.44	2.39	1	1
4:A:318:PX4:H64	4:A:332:PX4:H64	0.44	1.89	19	1
4:A:399:PX4:H23	4:A:408:PX4:H24	0.44	1.88	8	1
4:A:326:PX4:H4	4:A:353:PX4:O6	0.44	2.10	16	1
4:A:422:PX4:H59	4:A:431:PX4:H32	0.44	1.89	5	1
4:A:392:PX4:H68	4:A:394:PX4:H31	0.44	1.89	7	1
4:A:393:PX4:H4	4:A:402:PX4:O2	0.44	2.12	11	1
4:A:352:PX4:H27	4:A:366:PX4:H60	0.44	1.90	4	1
4:A:354:PX4:H26	4:A:356:PX4:H34	0.44	1.89	4	1
4:A:390:PX4:H17	4:A:399:PX4:H48	0.44	1.90	20	1
4:A:343:PX4:H30	4:A:350:PX4:H36	0.44	1.88	3	1
4:A:354:PX4:H35	4:A:354:PX4:H61	0.44	1.89	3	1
4:A:319:PX4:H64	4:A:429:PX4:H72	0.44	1.89	17	1
4:A:419:PX4:H30	4:A:424:PX4:H16	0.44	1.89	14	1
4:A:376:PX4:H19	4:A:390:PX4:H31	0.44	1.90	8	1
1:A:143:HIS:CE1	1:A:145:ASP:OD2	0.44	2.69	10	1
4:A:368:PX4:H28	4:A:431:PX4:H53	0.44	1.88	16	1
1:A:140:ARG:NE	1:A:175:ASP:OD1	0.44	2.46	5	1
4:A:403:PX4:H47	4:A:412:PX4:H17	0.44	1.89	5	1
4:A:329:PX4:O6	4:A:338:PX4:H11	0.44	2.13	12	1
4:A:319:PX4:H22	4:A:327:PX4:H58	0.44	1.88	11	1
4:A:379:PX4:H57	4:A:381:PX4:H32	0.44	1.89	11	1
4:A:396:PX4:H34	4:A:414:PX4:H60	0.44	1.89	11	1
4:A:316:PX4:H49	4:A:317:PX4:H46	0.44	1.89	20	1
4:A:336:PX4:H43	4:A:399:PX4:H57	0.44	1.88	15	1
4:A:329:PX4:H36	4:A:338:PX4:H67	0.44	1.90	15	1
4:A:394:PX4:H34	4:A:412:PX4:H39	0.44	1.89	3	1
4:A:341:PX4:H17	4:A:350:PX4:H20	0.44	1.90	1	1
4:A:379:PX4:H13	4:A:379:PX4:O3	0.44	2.12	14	1
4:A:308:PX4:H5	4:A:359:PX4:H53	0.44	1.89	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:331:PX4:H66	4:A:346:PX4:H69	0.44	1.89	10	1
4:A:378:PX4:C22	4:A:380:PX4:H35	0.44	2.41	10	1
4:A:327:PX4:H53	4:A:327:PX4:H5	0.44	1.89	13	1
4:A:348:PX4:H38	4:A:349:PX4:H33	0.44	1.89	7	1
4:A:306:PX4:H27	4:A:313:PX4:H22	0.44	1.88	20	1
4:A:338:PX4:H24	4:A:346:PX4:H60	0.44	1.90	20	1
4:A:312:PX4:O6	4:A:327:PX4:H12	0.44	2.12	15	1
4:A:320:PX4:H4	4:A:353:PX4:H46	0.44	1.88	15	1
4:A:377:PX4:H14	4:A:387:PX4:H11	0.44	1.89	15	1
4:A:376:PX4:H55	4:A:430:PX4:H19	0.44	1.88	1	1
4:A:337:PX4:H42	4:A:388:PX4:H45	0.44	1.89	14	1
4:A:379:PX4:H17	4:A:380:PX4:H11	0.44	1.88	8	1
4:A:336:PX4:H55	4:A:345:PX4:H26	0.44	1.90	16	1
4:A:309:PX4:H58	4:A:357:PX4:H16	0.44	1.89	6	1
4:A:369:PX4:H29	4:A:378:PX4:H29	0.44	1.88	9	1
4:A:380:PX4:O6	4:A:411:PX4:H14	0.44	2.13	7	1
4:A:405:PX4:O6	4:A:420:PX4:H17	0.44	2.12	20	1
4:A:306:PX4:H58	4:A:348:PX4:H63	0.44	1.88	15	1
4:A:332:PX4:H59	4:A:340:PX4:H24	0.44	1.88	3	1
4:A:331:PX4:H40	4:A:340:PX4:H68	0.44	1.90	17	1
4:A:387:PX4:H62	4:A:395:PX4:H52	0.44	1.90	13	1
4:A:368:PX4:H58	4:A:383:PX4:H63	0.44	1.88	5	1
4:A:334:PX4:H36	4:A:353:PX4:H40	0.44	1.88	6	1
4:A:307:PX4:H49	4:A:310:PX4:O3	0.44	2.13	18	1
4:A:396:PX4:H61	4:A:396:PX4:H29	0.44	1.90	11	1
4:A:375:PX4:H24	4:A:429:PX4:H24	0.44	1.89	11	1
4:A:363:PX4:H26	4:A:364:PX4:H68	0.44	1.88	4	1
4:A:315:PX4:O8	4:A:340:PX4:H5	0.44	2.13	20	1
4:A:338:PX4:H5	4:A:351:PX4:O6	0.44	2.13	15	1
4:A:419:PX4:H16	4:A:426:PX4:H19	0.44	1.89	14	1
4:A:390:PX4:H26	4:A:430:PX4:H57	0.44	1.90	14	1
4:A:422:PX4:H34	4:A:431:PX4:H44	0.44	1.89	8	1
4:A:320:PX4:H71	4:A:342:PX4:H72	0.44	1.88	10	1
4:A:359:PX4:H39	4:A:367:PX4:H64	0.44	1.88	13	1
4:A:319:PX4:H71	4:A:431:PX4:H71	0.44	1.89	12	1
4:A:330:PX4:H37	4:A:380:PX4:H44	0.44	1.88	12	1
4:A:375:PX4:H66	4:A:421:PX4:H71	0.44	1.88	18	1
4:A:411:PX4:H33	4:A:427:PX4:H67	0.44	1.90	18	1
4:A:309:PX4:H52	4:A:357:PX4:H59	0.44	1.89	2	1
4:A:305:PX4:H21	4:A:321:PX4:H71	0.44	1.88	20	1
4:A:308:PX4:H57	4:A:318:PX4:H28	0.44	1.90	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:314:PX4:H8	4:A:364:PX4:O6	0.44	2.13	15	1
4:A:310:PX4:H33	4:A:359:PX4:H31	0.44	1.89	1	1
4:A:315:PX4:H70	4:A:319:PX4:O8	0.44	2.12	1	1
4:A:388:PX4:H16	4:A:395:PX4:H50	0.44	1.90	17	1
4:A:419:PX4:H27	4:A:426:PX4:H55	0.44	1.88	14	1
4:A:333:PX4:H3	4:A:339:PX4:H70	0.44	1.89	8	1
4:A:347:PX4:H13	4:A:355:PX4:H18	0.44	1.90	16	1
4:A:333:PX4:H25	4:A:355:PX4:H66	0.44	1.89	6	1
4:A:348:PX4:H57	4:A:348:PX4:H51	0.44	1.52	12	1
4:A:385:PX4:O1	4:A:387:PX4:H14	0.44	2.13	9	1
4:A:326:PX4:H32	4:A:326:PX4:H64	0.44	1.90	7	1
4:A:366:PX4:O6	4:A:366:PX4:H7	0.44	2.13	7	1
4:A:399:PX4:H46	4:A:408:PX4:H57	0.44	1.89	3	1
4:A:315:PX4:H35	4:A:373:PX4:H43	0.44	1.89	1	1
4:A:337:PX4:H41	4:A:354:PX4:H43	0.44	1.90	14	1
4:A:318:PX4:H8	4:A:324:PX4:H21	0.44	1.89	19	1
4:A:376:PX4:H55	4:A:430:PX4:H61	0.44	1.88	8	1
4:A:315:PX4:H49	4:A:322:PX4:H50	0.44	1.88	10	1
4:A:322:PX4:H42	4:A:323:PX4:H65	0.44	1.89	10	1
4:A:404:PX4:H57	4:A:404:PX4:H62	0.44	1.35	10	1
4:A:377:PX4:H62	4:A:378:PX4:H35	0.44	1.90	13	1
4:A:430:PX4:H42	4:A:430:PX4:H35	0.44	1.37	16	1
4:A:372:PX4:H19	4:A:421:PX4:O8	0.44	2.13	5	1
4:A:417:PX4:H68	4:A:427:PX4:H69	0.44	1.90	6	1
4:A:324:PX4:H60	4:A:339:PX4:H22	0.44	1.89	12	1
4:A:413:PX4:H64	4:A:429:PX4:H47	0.44	1.89	12	1
4:A:320:PX4:H46	4:A:353:PX4:H52	0.44	1.90	18	1
4:A:384:PX4:H53	4:A:386:PX4:H46	0.44	1.89	18	1
4:A:378:PX4:H34	4:A:385:PX4:H30	0.44	1.90	9	1
4:A:333:PX4:H32	4:A:339:PX4:H61	0.44	1.90	3	1
4:A:397:PX4:H59	4:A:398:PX4:H68	0.43	1.90	17	1
4:A:377:PX4:O8	4:A:387:PX4:H9	0.43	2.13	5	1
4:A:428:PX4:H48	4:A:428:PX4:H54	0.43	1.62	5	1
4:A:336:PX4:H30	4:A:358:PX4:H31	0.43	1.89	6	1
4:A:419:PX4:H38	4:A:419:PX4:H44	0.43	1.53	12	1
4:A:401:PX4:H65	4:A:401:PX4:H38	0.43	1.90	18	1
4:A:419:PX4:H25	4:A:426:PX4:H23	0.43	1.90	7	1
4:A:321:PX4:H42	4:A:342:PX4:H63	0.43	1.89	11	1
4:A:379:PX4:H66	4:A:380:PX4:H36	0.43	1.90	11	1
4:A:406:PX4:H32	4:A:408:PX4:H30	0.43	1.88	11	1
4:A:346:PX4:H32	4:A:346:PX4:H63	0.43	1.89	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:329:PX4:H11	4:A:346:PX4:O1	0.43	2.13	20	1
4:A:334:PX4:H50	4:A:341:PX4:H53	0.43	1.90	15	1
4:A:413:PX4:H60	4:A:413:PX4:H67	0.43	1.52	1	1
4:A:323:PX4:H63	4:A:340:PX4:H56	0.43	1.89	14	1
4:A:370:PX4:H22	4:A:419:PX4:H54	0.43	1.90	10	1
4:A:309:PX4:H7	4:A:366:PX4:O7	0.43	2.12	13	1
4:A:389:PX4:H37	4:A:403:PX4:H63	0.43	1.90	13	1
4:A:373:PX4:O2	4:A:380:PX4:H14	0.43	2.12	16	1
4:A:334:PX4:H20	4:A:342:PX4:H25	0.43	1.89	6	1
4:A:389:PX4:H60	4:A:395:PX4:H55	0.43	1.90	6	1
4:A:321:PX4:H46	4:A:328:PX4:H51	0.43	1.91	12	1
4:A:365:PX4:H26	4:A:365:PX4:H20	0.43	1.48	12	1
4:A:347:PX4:H19	4:A:355:PX4:C26	0.43	2.43	9	1
4:A:368:PX4:H48	4:A:429:PX4:H47	0.43	1.89	4	1
4:A:376:PX4:H54	4:A:430:PX4:H52	0.43	1.89	15	1
4:A:388:PX4:H31	4:A:388:PX4:H37	0.43	1.58	3	1
4:A:321:PX4:H36	4:A:333:PX4:H44	0.43	1.90	1	1
4:A:334:PX4:C13	4:A:341:PX4:H22	0.43	2.42	17	1
4:A:351:PX4:H42	4:A:391:PX4:C22	0.43	2.43	19	1
4:A:396:PX4:H53	4:A:414:PX4:H50	0.43	1.90	10	1
4:A:379:PX4:H27	4:A:401:PX4:C12	0.43	2.43	16	1
4:A:419:PX4:H28	4:A:426:PX4:H48	0.43	1.88	16	1
4:A:307:PX4:H36	4:A:307:PX4:H41	0.43	1.54	6	1
4:A:339:PX4:H21	4:A:355:PX4:H61	0.43	1.90	12	1
4:A:312:PX4:H31	4:A:319:PX4:H54	0.43	1.89	9	1
4:A:314:PX4:H20	4:A:354:PX4:H51	0.43	1.90	7	1
4:A:374:PX4:H33	4:A:382:PX4:H28	0.43	1.90	11	1
4:A:340:PX4:O6	4:A:340:PX4:H2	0.43	2.14	2	1
4:A:399:PX4:H22	4:A:408:PX4:O7	0.43	2.14	15	1
1:A:98:ARG:CZ	4:A:355:PX4:H13	0.43	2.44	15	1
4:A:349:PX4:H53	4:A:350:PX4:H46	0.43	1.89	1	1
4:A:387:PX4:H1	4:A:387:PX4:H18	0.43	1.90	14	1
4:A:386:PX4:H20	4:A:395:PX4:H19	0.43	1.90	10	1
4:A:374:PX4:H25	4:A:429:PX4:H28	0.43	1.90	13	1
4:A:378:PX4:H38	4:A:387:PX4:H40	0.43	1.90	16	1
4:A:305:PX4:H47	4:A:362:PX4:O6	0.43	2.13	6	1
4:A:346:PX4:H27	4:A:346:PX4:C27	0.43	2.37	12	1
4:A:390:PX4:O6	4:A:390:PX4:H6	0.43	2.13	9	1
4:A:413:PX4:H16	4:A:431:PX4:H15	0.43	1.91	9	1
4:A:410:PX4:H54	4:A:410:PX4:H49	0.43	1.60	11	1
4:A:313:PX4:H29	4:A:364:PX4:H29	0.43	1.91	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:O4	4:A:346:PX4:H16	0.43	2.13	2	1
4:A:354:PX4:O6	4:A:356:PX4:H26	0.43	2.14	2	1
4:A:374:PX4:H62	4:A:374:PX4:H39	0.43	1.90	2	1
4:A:402:PX4:H50	4:A:402:PX4:H57	0.43	1.62	20	1
4:A:358:PX4:H39	4:A:399:PX4:H64	0.43	1.90	15	1
4:A:419:PX4:H29	4:A:426:PX4:H29	0.43	1.89	1	1
4:A:362:PX4:O2	4:A:365:PX4:H11	0.43	2.14	14	1
4:A:381:PX4:H42	4:A:381:PX4:H35	0.43	1.41	14	1
4:A:397:PX4:H47	4:A:415:PX4:H10	0.43	1.91	19	1
4:A:308:PX4:H57	4:A:318:PX4:H48	0.43	1.90	10	1
4:A:317:PX4:H33	4:A:318:PX4:H23	0.43	1.91	13	1
4:A:324:PX4:C10	4:A:340:PX4:H54	0.43	2.34	16	1
4:A:350:PX4:H29	4:A:350:PX4:H53	0.43	1.88	5	1
4:A:333:PX4:H20	4:A:356:PX4:H55	0.43	1.90	6	1
4:A:314:PX4:H53	4:A:315:PX4:H72	0.43	1.90	18	1
4:A:331:PX4:H16	4:A:331:PX4:H47	0.43	1.64	18	1
4:A:320:PX4:H56	4:A:362:PX4:H54	0.43	1.91	7	1
4:A:373:PX4:H54	4:A:375:PX4:H55	0.43	1.89	4	1
4:A:338:PX4:H8	4:A:351:PX4:O6	0.43	2.14	20	1
4:A:338:PX4:H50	4:A:342:PX4:H52	0.43	1.90	20	1
4:A:359:PX4:H21	4:A:367:PX4:H16	0.43	1.91	3	1
4:A:322:PX4:H64	4:A:332:PX4:H65	0.43	1.91	17	1
4:A:321:PX4:H14	4:A:330:PX4:O8	0.43	2.13	19	1
4:A:334:PX4:H52	4:A:334:PX4:H39	0.43	1.90	19	1
4:A:364:PX4:H38	4:A:420:PX4:H63	0.43	1.89	19	1
4:A:329:PX4:H65	4:A:346:PX4:H40	0.43	1.89	8	1
4:A:375:PX4:H27	4:A:421:PX4:H37	0.43	1.90	16	1
4:A:373:PX4:H67	4:A:375:PX4:H66	0.43	1.89	6	1
4:A:378:PX4:H15	4:A:380:PX4:H3	0.43	1.90	18	1
4:A:341:PX4:H52	4:A:350:PX4:H19	0.43	1.90	7	1
4:A:338:PX4:C35	4:A:384:PX4:H34	0.43	2.43	4	1
4:A:383:PX4:H4	4:A:398:PX4:O1	0.43	2.12	4	1
4:A:383:PX4:H35	4:A:397:PX4:H30	0.43	1.88	2	1
4:A:306:PX4:C10	4:A:314:PX4:H17	0.43	2.43	20	1
4:A:381:PX4:H55	4:A:387:PX4:H54	0.43	1.89	20	1
4:A:305:PX4:H4	4:A:361:PX4:O8	0.43	2.13	15	1
4:A:369:PX4:H45	4:A:378:PX4:H42	0.43	1.89	15	1
4:A:422:PX4:H19	4:A:431:PX4:H24	0.43	1.91	15	1
4:A:329:PX4:H66	4:A:338:PX4:H43	0.43	1.90	3	1
4:A:379:PX4:H47	4:A:380:PX4:H5	0.43	1.89	17	1
4:A:321:PX4:H19	4:A:330:PX4:H69	0.43	1.88	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:349:PX4:H50	4:A:350:PX4:H51	0.43	1.90	14	1
4:A:311:PX4:H16	4:A:363:PX4:H27	0.43	1.90	19	1
4:A:312:PX4:H72	4:A:317:PX4:H68	0.43	1.89	10	1
4:A:369:PX4:H58	4:A:391:PX4:H48	0.43	1.90	10	1
4:A:384:PX4:C13	4:A:391:PX4:H57	0.43	2.43	13	1
4:A:334:PX4:H49	4:A:341:PX4:H16	0.43	1.89	16	1
4:A:344:PX4:H9	4:A:345:PX4:O6	0.43	2.13	16	1
4:A:316:PX4:H17	4:A:317:PX4:H22	0.43	1.89	6	1
4:A:346:PX4:H42	4:A:355:PX4:H31	0.43	1.89	6	1
4:A:369:PX4:H20	4:A:377:PX4:H22	0.43	1.90	12	1
1:A:12:TRP:CZ2	1:A:54:LEU:HD22	0.43	2.49	9	1
1:A:73:ALA:HB1	1:A:78:PHE:CZ	0.43	2.49	9	1
1:A:74:GLU:HG3	1:A:75:TYR:H	0.43	1.74	1	2
4:A:320:PX4:H66	4:A:362:PX4:H62	0.43	1.91	7	1
4:A:413:PX4:H26	4:A:421:PX4:H50	0.43	1.89	7	1
4:A:305:PX4:O8	4:A:328:PX4:H9	0.43	2.13	11	1
4:A:414:PX4:H58	4:A:422:PX4:H58	0.43	1.89	11	1
4:A:407:PX4:H16	4:A:422:PX4:H3	0.43	1.91	4	1
4:A:359:PX4:H35	4:A:359:PX4:H30	0.43	1.65	2	1
4:A:419:PX4:H61	4:A:425:PX4:H59	0.43	1.90	2	1
4:A:305:PX4:H47	4:A:321:PX4:H65	0.43	1.90	20	1
4:A:403:PX4:H21	4:A:403:PX4:H28	0.43	1.55	20	1
4:A:386:PX4:H7	4:A:400:PX4:O6	0.43	2.14	3	1
4:A:364:PX4:H35	4:A:405:PX4:H41	0.43	1.90	3	1
4:A:424:PX4:H24	4:A:425:PX4:H55	0.43	1.90	3	1
4:A:379:PX4:H64	4:A:381:PX4:H35	0.43	1.90	17	1
4:A:398:PX4:H58	4:A:398:PX4:H65	0.43	1.44	14	1
4:A:334:PX4:H59	4:A:334:PX4:H39	0.43	1.89	19	1
4:A:332:PX4:H31	4:A:340:PX4:H57	0.43	1.90	10	1
4:A:423:PX4:H35	4:A:424:PX4:H64	0.43	1.89	13	1
4:A:332:PX4:H45	4:A:381:PX4:H40	0.43	1.90	6	1
4:A:384:PX4:H58	4:A:394:PX4:H53	0.43	1.91	9	1
4:A:376:PX4:H53	4:A:383:PX4:H55	0.43	1.90	7	1
4:A:394:PX4:O2	4:A:394:PX4:H7	0.43	2.13	11	1
4:A:384:PX4:O8	4:A:386:PX4:H3	0.43	2.14	3	2
4:A:328:PX4:H19	4:A:335:PX4:H48	0.43	1.91	2	1
4:A:391:PX4:H20	4:A:391:PX4:H6	0.43	1.89	2	1
4:A:329:PX4:H21	4:A:351:PX4:H17	0.43	1.90	20	1
4:A:352:PX4:C1	4:A:365:PX4:H17	0.43	2.44	15	1
4:A:423:PX4:H40	4:A:423:PX4:H34	0.43	1.65	1	1
4:A:372:PX4:H16	4:A:373:PX4:H22	0.43	1.91	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:316:PX4:H63	4:A:316:PX4:H68	0.43	1.61	10	1
4:A:431:PX4:H56	4:A:431:PX4:H62	0.43	1.53	10	1
4:A:318:PX4:H60	4:A:318:PX4:H54	0.43	1.67	13	1
4:A:407:PX4:H20	4:A:423:PX4:O6	0.43	2.13	5	1
4:A:393:PX4:H48	4:A:394:PX4:H48	0.43	1.91	6	1
4:A:312:PX4:H30	4:A:319:PX4:H49	0.43	1.90	18	1
4:A:415:PX4:H57	4:A:415:PX4:H62	0.43	1.53	18	1
4:A:375:PX4:H1	4:A:421:PX4:O3	0.43	2.13	18	1
4:A:305:PX4:H57	4:A:305:PX4:H51	0.43	1.73	9	1
4:A:383:PX4:H30	4:A:397:PX4:H27	0.43	1.91	4	1
4:A:399:PX4:H63	4:A:399:PX4:H56	0.43	1.53	4	1
4:A:422:PX4:H25	4:A:431:PX4:H37	0.43	1.90	4	1
4:A:328:PX4:H65	4:A:342:PX4:H71	0.43	1.91	17	1
4:A:337:PX4:H25	4:A:356:PX4:H21	0.43	1.91	17	1
4:A:402:PX4:H31	4:A:402:PX4:H38	0.43	1.44	14	1
4:A:396:PX4:H17	4:A:414:PX4:H16	0.43	1.91	19	1
4:A:377:PX4:H64	4:A:386:PX4:H32	0.43	1.91	12	1
4:A:336:PX4:H71	4:A:344:PX4:H42	0.43	1.91	4	1
4:A:413:PX4:H22	4:A:413:PX4:H28	0.43	1.68	3	1
4:A:424:PX4:H27	4:A:429:PX4:H59	0.42	1.91	19	1
4:A:357:PX4:H47	4:A:358:PX4:H16	0.42	1.90	8	1
4:A:369:PX4:H29	4:A:370:PX4:H40	0.42	1.89	8	1
4:A:382:PX4:H43	4:A:398:PX4:H43	0.42	1.92	13	1
4:A:309:PX4:H16	4:A:357:PX4:H51	0.42	1.91	5	1
4:A:378:PX4:H60	4:A:380:PX4:H28	0.42	1.91	5	1
4:A:372:PX4:H22	4:A:421:PX4:H50	0.42	1.91	5	1
4:A:313:PX4:H30	4:A:348:PX4:H68	0.42	1.91	6	1
4:A:414:PX4:H29	4:A:431:PX4:H19	0.42	1.91	9	1
4:A:421:PX4:H27	4:A:421:PX4:H22	0.42	1.61	2	1
4:A:329:PX4:H53	4:A:336:PX4:H47	0.42	1.91	3	1
4:A:306:PX4:H50	4:A:364:PX4:H23	0.42	1.91	17	1
4:A:328:PX4:H30	4:A:328:PX4:H35	0.42	1.49	14	1
4:A:383:PX4:H31	4:A:398:PX4:H26	0.42	1.91	14	1
4:A:373:PX4:H66	4:A:382:PX4:H38	0.42	1.91	8	1
4:A:388:PX4:H23	4:A:394:PX4:H17	0.42	1.92	10	1
1:A:96:TYR:OH	4:A:333:PX4:H2	0.42	2.14	10	1
4:A:371:PX4:H52	4:A:412:PX4:H21	0.42	1.92	13	1
4:A:387:PX4:H30	4:A:395:PX4:H35	0.42	1.91	13	1
4:A:392:PX4:H51	4:A:402:PX4:H15	0.42	1.91	16	1
4:A:336:PX4:H68	4:A:366:PX4:H67	0.42	1.90	12	1
4:A:323:PX4:H70	4:A:428:PX4:H68	0.42	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H57	4:A:386:PX4:H55	0.42	1.91	9	1
4:A:371:PX4:H36	4:A:427:PX4:H44	0.42	1.92	7	1
4:A:341:PX4:H23	4:A:358:PX4:H37	0.42	1.92	11	1
4:A:346:PX4:H34	4:A:346:PX4:H27	0.42	1.56	11	1
4:A:402:PX4:H67	4:A:427:PX4:H37	0.42	1.91	11	1
4:A:417:PX4:H6	4:A:423:PX4:O8	0.42	2.14	4	1
4:A:307:PX4:H12	4:A:310:PX4:O4	0.42	2.13	20	1
4:A:377:PX4:C11	4:A:378:PX4:H16	0.42	2.40	20	1
4:A:325:PX4:H28	4:A:325:PX4:H63	0.42	1.90	3	1
4:A:333:PX4:H42	4:A:395:PX4:H62	0.42	1.91	3	1
4:A:399:PX4:H36	4:A:408:PX4:H36	0.42	1.91	1	1
4:A:418:PX4:H7	4:A:427:PX4:O2	0.42	2.14	1	1
4:A:403:PX4:C21	4:A:403:PX4:H63	0.42	2.44	17	1
4:A:352:PX4:H24	4:A:366:PX4:H20	0.42	1.91	14	1
4:A:408:PX4:H18	4:A:415:PX4:H27	0.42	1.91	14	1
4:A:386:PX4:O1	4:A:387:PX4:H7	0.42	2.14	8	1
4:A:337:PX4:H63	4:A:346:PX4:H39	0.42	1.91	10	1
4:A:408:PX4:H30	4:A:408:PX4:H36	0.42	1.62	13	1
4:A:318:PX4:H58	4:A:318:PX4:H65	0.42	1.66	16	1
4:A:388:PX4:H55	4:A:389:PX4:H53	0.42	1.91	16	1
4:A:419:PX4:H27	4:A:424:PX4:H56	0.42	1.90	16	1
4:A:429:PX4:H31	4:A:429:PX4:H25	0.42	1.61	16	1
4:A:325:PX4:H65	4:A:325:PX4:H42	0.42	1.91	5	1
4:A:352:PX4:O2	4:A:365:PX4:H10	0.42	2.14	5	1
4:A:388:PX4:H25	4:A:394:PX4:O6	0.42	2.15	5	1
4:A:314:PX4:H37	4:A:365:PX4:H58	0.42	1.90	12	1
4:A:404:PX4:H57	4:A:412:PX4:H23	0.42	1.90	12	1
4:A:369:PX4:H56	4:A:369:PX4:H31	0.42	1.90	9	1
4:A:317:PX4:H18	4:A:318:PX4:H8	0.42	1.91	11	1
4:A:320:PX4:C15	4:A:328:PX4:H37	0.42	2.36	3	1
4:A:336:PX4:H39	4:A:358:PX4:H65	0.42	1.90	3	1
4:A:365:PX4:H70	4:A:379:PX4:H45	0.42	1.92	1	1
4:A:420:PX4:H21	4:A:420:PX4:H27	0.42	1.56	1	1
4:A:333:PX4:H25	4:A:356:PX4:H53	0.42	1.90	17	1
4:A:389:PX4:O7	4:A:398:PX4:H15	0.42	2.15	17	1
4:A:419:PX4:H36	4:A:419:PX4:H41	0.42	1.61	14	1
4:A:421:PX4:H66	4:A:421:PX4:H34	0.42	1.90	14	1
4:A:404:PX4:H33	4:A:420:PX4:H55	0.42	1.90	8	1
4:A:384:PX4:H29	4:A:400:PX4:H30	0.42	1.91	10	1
4:A:411:PX4:H54	4:A:411:PX4:H61	0.42	1.76	10	1
4:A:391:PX4:H8	4:A:400:PX4:O2	0.42	2.14	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H56	4:A:395:PX4:H34	0.42	1.90	6	1
4:A:322:PX4:H16	4:A:332:PX4:H47	0.42	1.92	7	1
4:A:374:PX4:O3	4:A:429:PX4:H5	0.42	2.14	7	1
4:A:386:PX4:H31	4:A:387:PX4:H31	0.42	1.89	7	1
4:A:310:PX4:H58	4:A:363:PX4:H32	0.42	1.92	4	1
4:A:397:PX4:O5	4:A:398:PX4:H52	0.42	2.14	2	1
4:A:307:PX4:H54	4:A:310:PX4:H18	0.42	1.89	20	1
4:A:404:PX4:H23	4:A:418:PX4:H20	0.42	1.91	15	1
4:A:318:PX4:H71	4:A:322:PX4:H55	0.42	1.90	3	1
4:A:399:PX4:O6	4:A:408:PX4:H7	0.42	2.14	3	1
4:A:411:PX4:O2	4:A:381:PX4:H11	0.42	2.15	1	1
4:A:378:PX4:H62	4:A:411:PX4:H54	0.42	1.91	17	1
4:A:369:PX4:O8	4:A:391:PX4:H8	0.42	2.14	8	1
4:A:382:PX4:H48	4:A:382:PX4:H55	0.42	1.58	13	1
4:A:316:PX4:H23	4:A:339:PX4:H55	0.42	1.92	16	1
4:A:406:PX4:H12	4:A:415:PX4:O6	0.42	2.15	16	1
4:A:418:PX4:H38	4:A:418:PX4:H31	0.42	1.60	5	1
4:A:403:PX4:O4	4:A:412:PX4:H8	0.42	2.14	6	1
4:A:400:PX4:H54	4:A:425:PX4:H35	0.42	1.91	6	1
4:A:376:PX4:C19	4:A:397:PX4:H67	0.42	2.44	4	1
4:A:376:PX4:H60	4:A:430:PX4:H22	0.42	1.90	4	1
1:A:63:GLN:HA	1:A:63:GLN:HE21	0.42	1.75	2	1
4:A:322:PX4:H52	4:A:332:PX4:H47	0.42	1.91	15	1
4:A:346:PX4:H58	4:A:346:PX4:H64	0.42	1.62	15	1
4:A:364:PX4:H23	4:A:364:PX4:H30	0.42	1.64	15	1
1:A:234:ILE:HG23	1:A:237:LEU:HD12	0.42	1.90	3	1
4:A:321:PX4:C24	4:A:328:PX4:H48	0.42	2.45	17	1
4:A:379:PX4:H60	4:A:381:PX4:H31	0.42	1.90	17	1
4:A:307:PX4:H16	4:A:311:PX4:O1	0.42	2.15	19	1
4:A:342:PX4:H37	4:A:342:PX4:H32	0.42	1.63	8	1
4:A:426:PX4:H67	4:A:426:PX4:H35	0.42	1.90	8	1
4:A:379:PX4:H65	4:A:385:PX4:H41	0.42	1.91	10	1
4:A:305:PX4:O6	4:A:362:PX4:H4	0.42	2.14	13	1
4:A:313:PX4:H62	4:A:313:PX4:H69	0.42	1.64	16	1
4:A:318:PX4:H22	4:A:319:PX4:H58	0.42	1.90	5	1
4:A:399:PX4:H20	4:A:408:PX4:H14	0.42	1.89	6	1
4:A:306:PX4:H21	4:A:364:PX4:H21	0.42	1.92	12	1
4:A:370:PX4:O1	4:A:426:PX4:H5	0.42	2.15	18	1
4:A:397:PX4:H21	4:A:398:PX4:H48	0.42	1.91	9	1
4:A:383:PX4:H69	4:A:429:PX4:H31	0.42	1.92	9	1
4:A:315:PX4:H66	4:A:318:PX4:H23	0.42	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:373:PX4:H37	4:A:421:PX4:H36	0.42	1.90	2	1
4:A:399:PX4:H7	4:A:408:PX4:O4	0.42	2.15	20	1
4:A:379:PX4:H25	4:A:427:PX4:H48	0.42	1.91	15	1
4:A:320:PX4:H19	4:A:353:PX4:H61	0.42	1.90	3	1
4:A:333:PX4:H18	4:A:333:PX4:H9	0.42	1.91	3	1
4:A:420:PX4:H36	4:A:420:PX4:H53	0.42	1.92	3	1
4:A:384:PX4:O6	4:A:408:PX4:H11	0.42	2.15	9	2
4:A:330:PX4:H49	4:A:331:PX4:H16	0.42	1.92	10	1
4:A:374:PX4:H45	4:A:375:PX4:H24	0.42	1.91	13	1
4:A:405:PX4:H59	4:A:405:PX4:H52	0.42	1.66	13	1
4:A:416:PX4:H39	4:A:416:PX4:H34	0.42	1.53	13	1
4:A:414:PX4:H65	4:A:422:PX4:H56	0.42	1.92	5	1
4:A:413:PX4:H48	4:A:413:PX4:H55	0.42	1.59	18	1
4:A:311:PX4:H22	4:A:359:PX4:H50	0.42	1.92	7	1
4:A:392:PX4:H55	4:A:409:PX4:C34	0.42	2.39	7	1
4:A:374:PX4:H58	4:A:382:PX4:H58	0.42	1.92	11	1
4:A:389:PX4:H23	4:A:403:PX4:H21	0.42	1.91	11	1
4:A:326:PX4:H29	4:A:360:PX4:H70	0.42	1.91	4	1
4:A:331:PX4:H27	4:A:331:PX4:H34	0.42	1.60	4	1
4:A:321:PX4:H64	4:A:321:PX4:H59	0.42	1.61	15	1
4:A:318:PX4:H20	4:A:319:PX4:H11	0.42	1.91	3	1
4:A:386:PX4:H25	4:A:387:PX4:H54	0.42	1.91	3	1
4:A:318:PX4:C8	4:A:323:PX4:H20	0.42	2.45	1	1
4:A:403:PX4:H51	4:A:404:PX4:H55	0.42	1.91	1	1
4:A:428:PX4:H21	4:A:428:PX4:H28	0.42	1.61	1	1
4:A:321:PX4:H16	4:A:330:PX4:H20	0.42	1.91	17	1
4:A:370:PX4:H51	4:A:419:PX4:H17	0.42	1.90	17	1
4:A:421:PX4:H37	4:A:421:PX4:H45	0.42	1.62	17	1
4:A:431:PX4:H28	4:A:431:PX4:H33	0.42	1.49	17	1
4:A:388:PX4:H14	4:A:395:PX4:O1	0.42	2.15	8	1
4:A:336:PX4:H16	4:A:336:PX4:O3	0.42	2.15	13	1
4:A:371:PX4:H17	4:A:404:PX4:H22	0.42	1.91	5	1
4:A:371:PX4:H16	4:A:388:PX4:H6	0.42	1.91	6	1
4:A:374:PX4:H37	4:A:374:PX4:H45	0.42	1.60	12	2
4:A:381:PX4:H55	4:A:381:PX4:H61	0.42	1.45	12	1
4:A:332:PX4:C10	4:A:340:PX4:H16	0.42	2.45	18	2
4:A:372:PX4:H37	4:A:372:PX4:H45	0.42	1.74	18	1
4:A:379:PX4:H24	4:A:411:PX4:H18	0.42	1.92	9	1
4:A:315:PX4:H69	4:A:315:PX4:H62	0.42	1.40	11	1
4:A:335:PX4:H19	4:A:342:PX4:H58	0.42	1.90	11	1
4:A:365:PX4:H41	4:A:379:PX4:H40	0.42	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:363:PX4:H68	4:A:374:PX4:H59	0.42	1.91	20	1
4:A:305:PX4:H25	4:A:328:PX4:H55	0.42	1.91	15	1
4:A:387:PX4:H32	4:A:395:PX4:H35	0.42	1.92	3	1
4:A:338:PX4:H16	4:A:347:PX4:C26	0.42	2.45	17	1
4:A:391:PX4:H51	4:A:400:PX4:H22	0.42	1.92	17	1
4:A:309:PX4:H42	4:A:352:PX4:H69	0.42	1.92	14	1
4:A:329:PX4:H65	4:A:329:PX4:H58	0.42	1.58	14	1
4:A:328:PX4:H14	4:A:335:PX4:O2	0.42	2.15	19	1
4:A:343:PX4:H43	4:A:425:PX4:H36	0.42	1.92	19	1
4:A:349:PX4:H40	4:A:349:PX4:H33	0.42	1.61	19	1
4:A:321:PX4:H48	4:A:335:PX4:H31	0.42	1.90	8	1
4:A:376:PX4:C12	4:A:429:PX4:H31	0.42	2.41	10	1
4:A:329:PX4:H66	4:A:337:PX4:H67	0.42	1.90	16	1
4:A:334:PX4:H61	4:A:334:PX4:H54	0.42	1.20	16	1
4:A:341:PX4:H38	4:A:341:PX4:H61	0.42	1.92	16	1
4:A:342:PX4:H13	4:A:342:PX4:O8	0.42	2.15	5	1
4:A:400:PX4:H60	4:A:400:PX4:H67	0.42	1.57	6	1
1:A:59:ILE:HD12	1:A:59:ILE:H	0.42	1.73	9	1
4:A:405:PX4:H13	4:A:414:PX4:O6	0.42	2.15	11	1
4:A:305:PX4:O6	4:A:362:PX4:H13	0.42	2.15	4	1
4:A:330:PX4:H58	4:A:347:PX4:H47	0.42	1.90	4	1
4:A:373:PX4:H49	4:A:421:PX4:H20	0.42	1.91	2	1
4:A:325:PX4:H68	4:A:341:PX4:H68	0.42	1.92	20	1
4:A:409:PX4:H25	4:A:409:PX4:H61	0.42	1.89	20	1
4:A:341:PX4:H54	4:A:350:PX4:H16	0.42	1.92	15	1
4:A:351:PX4:H29	4:A:351:PX4:H24	0.42	1.41	15	1
4:A:386:PX4:H31	4:A:386:PX4:H26	0.42	1.49	15	1
4:A:355:PX4:H67	4:A:355:PX4:H60	0.42	1.54	1	1
4:A:328:PX4:H53	4:A:335:PX4:H28	0.42	1.91	14	1
4:A:372:PX4:H54	4:A:372:PX4:H61	0.42	1.47	14	1
4:A:375:PX4:H17	4:A:421:PX4:H22	0.42	1.91	14	1
4:A:368:PX4:H17	4:A:429:PX4:H47	0.42	1.92	14	1
4:A:373:PX4:H51	4:A:381:PX4:H20	0.42	1.90	19	1
4:A:390:PX4:H22	4:A:398:PX4:H69	0.42	1.91	10	1
4:A:360:PX4:H36	4:A:360:PX4:H29	0.42	1.66	13	1
4:A:325:PX4:H29	4:A:348:PX4:H23	0.42	1.90	16	1
4:A:337:PX4:H47	4:A:346:PX4:H19	0.42	1.90	16	1
4:A:312:PX4:H61	4:A:312:PX4:H66	0.42	1.60	5	1
1:A:143:HIS:NE2	1:A:171:HIS:CE1	0.42	2.87	6	1
4:A:312:PX4:H9	4:A:312:PX4:O1	0.42	2.15	6	1
4:A:344:PX4:H26	4:A:345:PX4:H26	0.42	1.90	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:320:PX4:H14	4:A:353:PX4:O8	0.42	2.14	18	1
4:A:359:PX4:H36	4:A:359:PX4:H29	0.42	1.36	11	1
4:A:412:PX4:H25	4:A:412:PX4:H20	0.42	1.49	11	1
4:A:332:PX4:H54	4:A:332:PX4:H61	0.42	1.65	20	1
4:A:360:PX4:H14	4:A:360:PX4:H9	0.42	1.91	20	1
4:A:308:PX4:H48	4:A:315:PX4:H53	0.42	1.92	15	1
4:A:386:PX4:H48	4:A:395:PX4:H22	0.42	1.91	15	1
4:A:374:PX4:H68	4:A:398:PX4:H44	0.42	1.91	3	1
4:A:404:PX4:H8	4:A:405:PX4:O6	0.42	2.15	3	1
4:A:330:PX4:H60	4:A:331:PX4:H29	0.42	1.92	1	1
4:A:305:PX4:H60	4:A:305:PX4:H55	0.41	1.64	17	1
4:A:331:PX4:H15	4:A:339:PX4:O1	0.41	2.15	17	1
4:A:330:PX4:H56	4:A:330:PX4:H30	0.41	1.92	19	1
4:A:396:PX4:H17	4:A:414:PX4:C7	0.41	2.45	19	1
4:A:363:PX4:H69	4:A:415:PX4:H50	0.41	1.90	8	1
4:A:338:PX4:H3	4:A:342:PX4:O3	0.41	2.15	13	1
4:A:363:PX4:H62	4:A:363:PX4:H68	0.41	1.37	13	1
4:A:376:PX4:H31	4:A:383:PX4:C15	0.41	2.46	16	1
4:A:387:PX4:H17	4:A:395:PX4:H20	0.41	1.90	16	1
4:A:328:PX4:H36	4:A:338:PX4:H57	0.41	1.92	5	1
4:A:431:PX4:H46	4:A:431:PX4:H53	0.41	1.68	12	1
4:A:368:PX4:H29	4:A:431:PX4:H55	0.41	1.92	12	1
4:A:333:PX4:H30	4:A:333:PX4:H35	0.41	1.65	7	1
4:A:338:PX4:H4	4:A:351:PX4:O2	0.41	2.15	7	1
4:A:338:PX4:H44	4:A:400:PX4:H42	0.41	1.92	11	1
4:A:354:PX4:H41	4:A:354:PX4:H36	0.41	1.59	4	1
4:A:370:PX4:H57	4:A:430:PX4:H33	0.41	1.92	2	1
4:A:337:PX4:H62	4:A:347:PX4:H36	0.41	1.92	20	1
4:A:351:PX4:H35	4:A:391:PX4:H43	0.41	1.92	20	1
4:A:307:PX4:H52	4:A:310:PX4:H52	0.41	1.91	15	1
4:A:329:PX4:H53	4:A:336:PX4:C24	0.41	2.45	3	1
4:A:370:PX4:H31	4:A:370:PX4:H38	0.41	1.69	3	1
4:A:344:PX4:H39	4:A:344:PX4:H34	0.41	1.59	1	1
4:A:403:PX4:H72	4:A:397:PX4:H32	0.41	1.91	1	1
4:A:364:PX4:H38	4:A:412:PX4:H42	0.41	1.91	14	1
4:A:389:PX4:O6	4:A:403:PX4:H1	0.41	2.15	19	1
4:A:410:PX4:H62	4:A:410:PX4:H30	0.41	1.92	8	1
4:A:425:PX4:H32	4:A:425:PX4:H25	0.41	1.62	10	1
4:A:305:PX4:O1	4:A:362:PX4:H13	0.41	2.15	13	1
4:A:388:PX4:H22	4:A:394:PX4:H17	0.41	1.91	13	1
4:A:407:PX4:H14	4:A:416:PX4:H51	0.41	1.91	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PX4:C26	4:A:419:PX4:H24	0.41	2.45	18	1
4:A:381:PX4:H56	4:A:395:PX4:H56	0.41	1.92	9	1
4:A:335:PX4:H48	4:A:342:PX4:H49	0.41	1.92	7	1
4:A:397:PX4:H21	4:A:397:PX4:H28	0.41	1.51	11	1
4:A:379:PX4:H51	4:A:380:PX4:H24	0.41	1.92	4	1
4:A:326:PX4:H51	4:A:343:PX4:H17	0.41	1.91	2	1
4:A:331:PX4:H44	4:A:335:PX4:H45	0.41	1.92	15	1
4:A:406:PX4:H23	4:A:416:PX4:H22	0.41	1.92	15	1
4:A:419:PX4:H65	4:A:426:PX4:H39	0.41	1.92	3	1
4:A:337:PX4:H17	4:A:346:PX4:H24	0.41	1.91	1	1
4:A:366:PX4:H69	4:A:366:PX4:H62	0.41	1.39	17	1
4:A:384:PX4:H51	4:A:386:PX4:H47	0.41	1.92	14	1
4:A:338:PX4:H6	4:A:342:PX4:O4	0.41	2.14	19	1
4:A:335:PX4:H37	4:A:391:PX4:H69	0.41	1.91	10	1
4:A:355:PX4:H35	4:A:356:PX4:H55	0.41	1.92	13	1
4:A:414:PX4:H52	4:A:431:PX4:H22	0.41	1.92	13	1
4:A:314:PX4:H54	4:A:361:PX4:H19	0.41	1.92	16	1
4:A:417:PX4:H3	4:A:423:PX4:H49	0.41	1.90	16	1
4:A:310:PX4:H19	4:A:310:PX4:H26	0.41	1.57	5	1
4:A:317:PX4:H11	4:A:343:PX4:H18	0.41	1.91	5	1
4:A:381:PX4:H72	4:A:381:PX4:H64	0.41	1.44	6	1
4:A:329:PX4:H34	4:A:351:PX4:H50	0.41	1.90	12	1
4:A:311:PX4:H72	4:A:412:PX4:H38	0.41	1.91	11	1
4:A:317:PX4:H22	4:A:324:PX4:H26	0.41	1.91	4	1
4:A:326:PX4:H14	4:A:343:PX4:C6	0.41	2.44	4	1
4:A:343:PX4:H69	4:A:343:PX4:H39	0.41	1.91	4	1
4:A:341:PX4:O6	4:A:351:PX4:H9	0.41	2.15	4	1
4:A:360:PX4:H14	4:A:360:PX4:H66	0.41	1.92	2	1
4:A:308:PX4:H34	4:A:308:PX4:H39	0.41	1.62	20	1
4:A:322:PX4:H36	4:A:332:PX4:H53	0.41	1.91	20	1
4:A:352:PX4:H50	4:A:352:PX4:H57	0.41	1.70	20	1
4:A:378:PX4:H46	4:A:411:PX4:O1	0.41	2.15	20	1
4:A:396:PX4:H63	4:A:396:PX4:H68	0.41	1.48	15	1
4:A:379:PX4:H53	4:A:420:PX4:H43	0.41	1.91	1	1
4:A:383:PX4:H54	4:A:429:PX4:H24	0.41	1.91	1	1
4:A:346:PX4:H52	4:A:346:PX4:H47	0.41	1.65	17	1
4:A:350:PX4:H33	4:A:350:PX4:H39	0.41	1.70	17	1
4:A:360:PX4:H48	4:A:360:PX4:H55	0.41	1.69	14	1
4:A:346:PX4:H47	4:A:347:PX4:H18	0.41	1.92	19	1
4:A:350:PX4:H48	4:A:350:PX4:H26	0.41	1.93	19	1
4:A:401:PX4:H15	4:A:410:PX4:C8	0.41	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:378:PX4:H3	4:A:385:PX4:O4	0.41	2.14	8	1
4:A:308:PX4:H19	4:A:319:PX4:H15	0.41	1.92	16	1
4:A:315:PX4:H12	4:A:315:PX4:H14	0.41	1.92	16	1
4:A:340:PX4:H70	4:A:380:PX4:H69	0.41	1.92	16	1
4:A:349:PX4:H48	4:A:350:PX4:H54	0.41	1.91	16	1
4:A:306:PX4:H19	4:A:314:PX4:H17	0.41	1.93	20	2
4:A:312:PX4:H3	4:A:319:PX4:O1	0.41	2.15	6	1
4:A:348:PX4:H60	4:A:356:PX4:H61	0.41	1.90	18	1
4:A:386:PX4:H66	4:A:394:PX4:H62	0.41	1.92	18	1
4:A:411:PX4:H36	4:A:426:PX4:H42	0.41	1.92	18	1
4:A:403:PX4:H3	4:A:412:PX4:O1	0.41	2.16	18	1
4:A:368:PX4:H19	4:A:429:PX4:H50	0.41	1.93	7	1
4:A:387:PX4:H25	4:A:395:PX4:H40	0.41	1.93	7	1
4:A:370:PX4:H45	4:A:370:PX4:H37	0.41	1.46	11	1
4:A:372:PX4:H48	4:A:372:PX4:H55	0.41	1.55	11	1
4:A:418:PX4:H47	4:A:427:PX4:H19	0.41	1.91	11	1
4:A:346:PX4:H62	4:A:346:PX4:H69	0.41	1.59	4	1
4:A:329:PX4:H30	4:A:329:PX4:H23	0.41	1.67	20	1
4:A:322:PX4:H40	4:A:332:PX4:H56	0.41	1.92	20	1
4:A:381:PX4:H21	4:A:385:PX4:H25	0.41	1.92	15	1
4:A:340:PX4:H59	4:A:340:PX4:H52	0.41	1.55	3	1
4:A:381:PX4:H2	4:A:381:PX4:H18	0.41	1.92	3	1
4:A:315:PX4:H72	4:A:319:PX4:H27	0.41	1.93	19	1
4:A:350:PX4:H71	4:A:350:PX4:H65	0.41	1.57	19	1
4:A:332:PX4:H33	4:A:340:PX4:H63	0.41	1.92	8	1
4:A:404:PX4:H26	4:A:404:PX4:H20	0.41	1.65	8	1
4:A:400:PX4:H15	4:A:400:PX4:H13	0.41	1.91	10	1
4:A:375:PX4:H52	4:A:382:PX4:H50	0.41	1.92	16	1
4:A:397:PX4:H59	4:A:397:PX4:H52	0.41	1.66	5	1
4:A:337:PX4:H71	4:A:346:PX4:H41	0.41	1.90	6	1
4:A:424:PX4:H24	4:A:430:PX4:H33	0.41	1.92	6	1
4:A:306:PX4:H70	4:A:389:PX4:H41	0.41	1.91	12	1
4:A:312:PX4:H33	4:A:367:PX4:H37	0.41	1.92	18	1
4:A:414:PX4:H22	4:A:431:PX4:H28	0.41	1.92	18	1
1:A:194:HIS:CD2	1:A:198:HIS:NE2	0.41	2.89	9	1
4:A:307:PX4:H21	4:A:363:PX4:C13	0.41	2.39	7	1
4:A:312:PX4:C9	4:A:319:PX4:H17	0.41	2.46	7	1
4:A:371:PX4:H16	4:A:418:PX4:H20	0.41	1.90	11	1
4:A:358:PX4:H19	4:A:358:PX4:H26	0.41	1.57	4	1
4:A:361:PX4:H45	4:A:427:PX4:H70	0.41	1.91	4	1
4:A:361:PX4:H50	4:A:361:PX4:H57	0.41	1.66	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:396:PX4:H29	4:A:396:PX4:H36	0.41	1.61	2	1
4:A:384:PX4:H48	4:A:400:PX4:O6	0.41	2.16	2	1
4:A:371:PX4:H22	4:A:404:PX4:H25	0.41	1.91	2	1
4:A:372:PX4:H14	4:A:373:PX4:H2	0.41	1.92	20	1
4:A:388:PX4:H1	4:A:412:PX4:C25	0.41	2.46	20	1
4:A:318:PX4:H58	4:A:340:PX4:H23	0.41	1.92	3	1
4:A:333:PX4:H44	4:A:389:PX4:H63	0.41	1.91	3	1
1:A:83:LYS:CD	1:A:237:LEU:HD22	0.41	2.46	1	1
4:A:313:PX4:H65	4:A:313:PX4:H58	0.41	1.50	19	1
4:A:312:PX4:H51	4:A:319:PX4:H46	0.41	1.92	19	1
4:A:418:PX4:H51	4:A:418:PX4:H56	0.41	1.47	19	1
4:A:401:PX4:H18	4:A:427:PX4:O7	0.41	2.16	8	1
4:A:323:PX4:H55	4:A:340:PX4:H52	0.41	1.91	10	1
4:A:360:PX4:H53	4:A:367:PX4:H50	0.41	1.92	10	1
4:A:390:PX4:H31	4:A:429:PX4:H34	0.41	1.93	10	1
4:A:347:PX4:H38	4:A:355:PX4:H37	0.41	1.93	13	1
4:A:392:PX4:H21	4:A:409:PX4:H57	0.41	1.92	5	1
4:A:311:PX4:H51	4:A:311:PX4:H56	0.41	1.50	6	1
4:A:322:PX4:H31	4:A:322:PX4:H26	0.41	1.56	6	1
4:A:406:PX4:H11	4:A:416:PX4:O6	0.41	2.15	6	1
4:A:362:PX4:H72	4:A:426:PX4:H44	0.41	1.93	12	1
4:A:339:PX4:H11	4:A:340:PX4:H48	0.41	1.92	7	1
4:A:347:PX4:H45	4:A:412:PX4:H70	0.41	1.92	7	1
4:A:314:PX4:H36	4:A:345:PX4:H29	0.41	1.91	11	1
4:A:322:PX4:H34	4:A:332:PX4:H17	0.41	1.91	11	1
4:A:346:PX4:H67	4:A:346:PX4:H36	0.41	1.93	2	1
4:A:373:PX4:H55	4:A:380:PX4:H62	0.41	1.92	2	1
4:A:365:PX4:H36	4:A:365:PX4:H41	0.41	1.50	20	1
4:A:309:PX4:H55	4:A:309:PX4:H60	0.41	1.57	15	1
4:A:332:PX4:H25	4:A:340:PX4:H22	0.41	1.90	15	1
4:A:352:PX4:H17	4:A:365:PX4:C11	0.41	2.41	1	1
4:A:381:PX4:H17	4:A:385:PX4:H21	0.41	1.92	1	1
4:A:344:PX4:H51	4:A:346:PX4:H24	0.41	1.93	17	1
4:A:346:PX4:H59	4:A:347:PX4:H57	0.41	1.92	17	1
4:A:336:PX4:O6	4:A:358:PX4:H15	0.41	2.16	17	1
4:A:395:PX4:H32	4:A:395:PX4:H25	0.41	1.45	17	1
4:A:376:PX4:H7	4:A:376:PX4:O1	0.41	2.15	14	1
4:A:384:PX4:H4	4:A:393:PX4:O5	0.41	2.15	8	1
4:A:342:PX4:H62	4:A:342:PX4:H69	0.41	1.69	10	1
4:A:386:PX4:H38	4:A:386:PX4:H32	0.41	1.59	10	1
1:A:98:ARG:NH1	4:A:330:PX4:O1	0.41	2.53	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:329:PX4:H63	4:A:344:PX4:H52	0.41	1.92	13	1
4:A:336:PX4:H57	4:A:336:PX4:H62	0.41	1.72	13	1
4:A:336:PX4:H62	4:A:366:PX4:H49	0.41	1.93	13	1
4:A:386:PX4:H36	4:A:386:PX4:H29	0.41	1.63	16	1
4:A:398:PX4:H20	4:A:398:PX4:H25	0.41	1.57	16	1
4:A:327:PX4:H35	4:A:334:PX4:H39	0.41	1.91	6	1
4:A:331:PX4:H63	4:A:347:PX4:H22	0.41	1.93	6	1
4:A:310:PX4:H68	4:A:363:PX4:H25	0.41	1.92	6	1
4:A:430:PX4:O6	4:A:430:PX4:H12	0.41	2.15	18	1
4:A:316:PX4:H10	4:A:333:PX4:H15	0.41	1.93	9	1
4:A:318:PX4:H39	4:A:319:PX4:H65	0.41	1.91	9	1
4:A:307:PX4:H24	4:A:311:PX4:H47	0.41	1.92	11	1
4:A:321:PX4:H30	4:A:321:PX4:H23	0.41	1.68	11	1
4:A:308:PX4:H68	4:A:322:PX4:H70	0.41	1.93	20	1
1:A:116:TRP:CH2	1:A:211:VAL:HG11	0.41	2.50	15	1
4:A:329:PX4:H65	4:A:337:PX4:H36	0.41	1.92	15	1
4:A:384:PX4:O6	4:A:394:PX4:H68	0.41	2.14	15	1
4:A:328:PX4:H27	4:A:342:PX4:H55	0.41	1.92	17	1
4:A:333:PX4:H44	4:A:374:PX4:H68	0.41	1.93	17	1
4:A:360:PX4:H32	4:A:360:PX4:H50	0.41	1.93	19	1
4:A:330:PX4:H33	4:A:332:PX4:H35	0.41	1.91	10	1
4:A:331:PX4:H43	4:A:387:PX4:H63	0.41	1.92	10	1
4:A:318:PX4:H68	4:A:318:PX4:H63	0.41	1.62	13	1
4:A:334:PX4:H23	4:A:335:PX4:H66	0.41	1.91	13	1
4:A:338:PX4:H41	4:A:338:PX4:H36	0.41	1.55	13	1
4:A:368:PX4:H67	4:A:424:PX4:H62	0.41	1.92	13	1
4:A:376:PX4:H45	4:A:376:PX4:H37	0.41	1.43	13	1
4:A:347:PX4:H69	4:A:351:PX4:H31	0.41	1.92	5	1
4:A:351:PX4:H33	4:A:391:PX4:H68	0.41	1.92	5	1
4:A:351:PX4:H37	4:A:391:PX4:H65	0.41	1.92	5	1
4:A:326:PX4:H11	4:A:353:PX4:O6	0.41	2.15	6	1
4:A:339:PX4:C7	4:A:355:PX4:H58	0.41	2.46	6	1
4:A:308:PX4:H10	4:A:359:PX4:O8	0.41	2.15	6	1
4:A:317:PX4:H17	4:A:318:PX4:H4	0.41	1.93	18	1
4:A:324:PX4:H49	4:A:339:PX4:H15	0.41	1.93	18	1
4:A:409:PX4:H68	4:A:410:PX4:H69	0.41	1.92	18	1
4:A:324:PX4:H44	4:A:398:PX4:H37	0.41	1.93	11	1
4:A:347:PX4:H30	4:A:356:PX4:H59	0.41	1.92	11	1
4:A:374:PX4:H18	4:A:398:PX4:H19	0.41	1.92	4	1
4:A:340:PX4:H32	4:A:421:PX4:H43	0.41	1.92	2	1
4:A:360:PX4:H50	4:A:360:PX4:H57	0.41	1.70	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:377:PX4:H63	4:A:377:PX4:H68	0.41	1.75	15	1
4:A:403:PX4:H55	4:A:404:PX4:H51	0.41	1.93	15	1
4:A:387:PX4:H27	4:A:387:PX4:H33	0.41	1.70	1	1
4:A:321:PX4:H26	4:A:330:PX4:H54	0.41	1.93	17	1
4:A:344:PX4:H49	4:A:344:PX4:H54	0.41	1.48	17	1
4:A:357:PX4:H28	4:A:357:PX4:H22	0.41	1.61	17	1
4:A:379:PX4:H59	4:A:428:PX4:H64	0.41	1.93	17	1
4:A:388:PX4:H17	4:A:388:PX4:H13	0.41	1.93	17	1
4:A:402:PX4:H18	4:A:418:PX4:H27	0.41	1.92	17	1
4:A:384:PX4:H2	4:A:393:PX4:O4	0.41	2.15	14	1
4:A:390:PX4:H36	4:A:390:PX4:H29	0.41	1.61	19	1
4:A:406:PX4:H25	4:A:409:PX4:H32	0.41	1.92	19	1
4:A:326:PX4:H52	4:A:326:PX4:H22	0.41	1.93	19	1
4:A:349:PX4:H14	4:A:363:PX4:C6	0.41	2.46	19	1
1:A:72:VAL:HG13	1:A:74:GLU:HB3	0.41	1.91	19	1
4:A:373:PX4:H58	4:A:381:PX4:H54	0.41	1.92	10	1
4:A:391:PX4:H33	4:A:391:PX4:H40	0.41	1.65	10	1
4:A:399:PX4:H25	4:A:399:PX4:H20	0.41	1.61	10	1
4:A:388:PX4:H54	4:A:388:PX4:H49	0.41	1.51	10	1
4:A:423:PX4:H64	4:A:423:PX4:H58	0.41	1.67	10	1
4:A:339:PX4:H51	4:A:355:PX4:H64	0.41	1.92	13	1
4:A:338:PX4:H65	4:A:338:PX4:H71	0.41	1.49	16	1
4:A:307:PX4:H33	4:A:363:PX4:H41	0.41	1.92	16	1
4:A:369:PX4:H20	4:A:369:PX4:H26	0.41	1.51	16	1
4:A:374:PX4:H26	4:A:374:PX4:H31	0.41	1.60	16	1
4:A:376:PX4:H55	4:A:429:PX4:H45	0.41	1.92	16	1
4:A:411:PX4:H34	4:A:426:PX4:H31	0.41	1.93	16	1
4:A:325:PX4:O2	4:A:349:PX4:H4	0.41	2.15	5	1
4:A:391:PX4:H31	4:A:391:PX4:H26	0.41	1.50	5	1
4:A:409:PX4:O4	4:A:409:PX4:H9	0.41	2.16	5	1
4:A:415:PX4:H29	4:A:415:PX4:H24	0.41	1.59	5	1
4:A:389:PX4:H32	4:A:389:PX4:H37	0.41	1.36	6	1
4:A:330:PX4:H15	4:A:331:PX4:O4	0.41	2.16	6	1
4:A:375:PX4:H68	4:A:421:PX4:H27	0.41	1.91	12	1
4:A:312:PX4:H54	4:A:312:PX4:H60	0.41	1.64	18	1
4:A:381:PX4:H69	4:A:381:PX4:H62	0.41	1.60	18	1
4:A:349:PX4:H69	4:A:375:PX4:H33	0.41	1.93	9	1
4:A:326:PX4:H71	4:A:326:PX4:H64	0.41	1.67	7	1
4:A:338:PX4:H36	4:A:338:PX4:H29	0.41	1.29	7	1
4:A:312:PX4:H44	4:A:318:PX4:H36	0.41	1.93	4	1
4:A:383:PX4:H35	4:A:389:PX4:H17	0.41	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:313:PX4:H52	4:A:333:PX4:H55	0.41	1.93	2	1
4:A:374:PX4:H17	4:A:398:PX4:H8	0.41	1.91	20	1
4:A:345:PX4:H40	4:A:345:PX4:H34	0.41	1.67	15	1
4:A:366:PX4:H41	4:A:366:PX4:H36	0.41	1.69	15	1
4:A:378:PX4:H3	4:A:385:PX4:H17	0.41	1.92	3	1
4:A:423:PX4:H55	4:A:426:PX4:H26	0.41	1.92	3	1
4:A:378:PX4:H26	4:A:387:PX4:H29	0.41	1.93	1	1
4:A:384:PX4:H60	4:A:395:PX4:H35	0.41	1.92	17	1
4:A:394:PX4:H8	4:A:395:PX4:O2	0.41	2.16	17	1
4:A:352:PX4:H35	4:A:352:PX4:H29	0.41	1.69	14	1
4:A:305:PX4:H13	4:A:362:PX4:O1	0.41	2.16	19	1
4:A:309:PX4:H34	4:A:309:PX4:H40	0.41	1.69	8	1
4:A:307:PX4:H25	4:A:313:PX4:H52	0.41	1.92	8	1
4:A:350:PX4:H61	4:A:350:PX4:H55	0.41	1.66	8	1
4:A:326:PX4:H41	4:A:360:PX4:H27	0.41	1.92	8	1
4:A:393:PX4:H34	4:A:400:PX4:H42	0.41	1.92	8	1
4:A:315:PX4:H54	4:A:319:PX4:H45	0.41	1.91	10	1
4:A:346:PX4:H59	4:A:347:PX4:H56	0.41	1.92	13	1
4:A:382:PX4:O8	4:A:398:PX4:H5	0.41	2.16	13	1
4:A:391:PX4:H58	4:A:400:PX4:H62	0.41	1.93	13	1
4:A:305:PX4:C29	4:A:320:PX4:H54	0.41	2.46	16	1
4:A:349:PX4:H55	4:A:349:PX4:H60	0.41	1.79	12	1
4:A:429:PX4:H64	4:A:429:PX4:H59	0.41	1.63	18	1
4:A:405:PX4:H31	4:A:405:PX4:H26	0.41	1.32	9	1
4:A:358:PX4:H55	4:A:358:PX4:H60	0.41	1.60	7	1
4:A:383:PX4:H26	4:A:398:PX4:H53	0.41	1.93	7	1
4:A:341:PX4:H38	4:A:341:PX4:H31	0.41	1.65	11	1
4:A:341:PX4:H60	4:A:341:PX4:H67	0.41	1.60	11	1
4:A:372:PX4:H25	4:A:421:PX4:H26	0.41	1.90	2	1
4:A:375:PX4:H16	4:A:382:PX4:H3	0.41	1.92	20	1
4:A:348:PX4:H37	4:A:348:PX4:H32	0.41	1.63	15	1
4:A:392:PX4:H37	4:A:392:PX4:H31	0.41	1.61	15	1
4:A:414:PX4:H63	4:A:422:PX4:H53	0.41	1.93	15	1
4:A:312:PX4:O1	4:A:327:PX4:H13	0.40	2.15	17	1
4:A:329:PX4:H47	4:A:338:PX4:H24	0.40	1.92	17	1
4:A:313:PX4:H36	4:A:314:PX4:H27	0.40	1.92	14	1
4:A:368:PX4:H44	4:A:429:PX4:H67	0.40	1.92	14	1
4:A:387:PX4:H38	4:A:387:PX4:H31	0.40	1.55	14	1
4:A:430:PX4:H49	4:A:430:PX4:H54	0.40	1.55	19	1
4:A:312:PX4:H35	4:A:312:PX4:H30	0.40	1.53	10	1
4:A:370:PX4:H66	4:A:425:PX4:H66	0.40	1.93	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:377:PX4:C35	4:A:391:PX4:H58	0.40	2.44	10	1
4:A:336:PX4:H34	4:A:336:PX4:H27	0.40	1.57	13	1
4:A:415:PX4:H28	4:A:415:PX4:H21	0.40	1.50	16	1
4:A:362:PX4:H70	4:A:362:PX4:H39	0.40	1.93	6	1
4:A:326:PX4:O6	4:A:327:PX4:H14	0.40	2.16	18	1
4:A:336:PX4:H25	4:A:351:PX4:H57	0.40	1.91	9	1
4:A:413:PX4:H25	4:A:431:PX4:H50	0.40	1.92	9	1
4:A:329:PX4:O5	4:A:338:PX4:H24	0.40	2.16	7	1
4:A:399:PX4:C10	4:A:408:PX4:H14	0.40	2.46	7	1
4:A:321:PX4:H30	4:A:321:PX4:H35	0.40	1.64	11	1
4:A:361:PX4:H59	4:A:365:PX4:C16	0.40	2.45	11	1
4:A:307:PX4:H23	4:A:307:PX4:H30	0.40	1.72	4	1
4:A:354:PX4:C28	4:A:354:PX4:H25	0.40	2.46	4	1
4:A:318:PX4:H41	4:A:319:PX4:H38	0.40	1.93	2	1
4:A:353:PX4:H36	4:A:353:PX4:H41	0.40	1.67	2	1
4:A:419:PX4:H30	4:A:424:PX4:H33	0.40	1.93	2	1
4:A:370:PX4:H47	4:A:419:PX4:O6	0.40	2.16	15	1
4:A:377:PX4:H27	4:A:411:PX4:H31	0.40	1.92	3	1
4:A:397:PX4:H32	4:A:397:PX4:H37	0.40	1.70	3	1
4:A:375:PX4:H5	4:A:413:PX4:H58	0.40	1.92	1	1
4:A:379:PX4:H33	4:A:427:PX4:H32	0.40	1.93	1	1
4:A:385:PX4:H28	4:A:387:PX4:H30	0.40	1.93	1	1
4:A:352:PX4:H2	4:A:352:PX4:H12	0.40	1.62	17	1
4:A:406:PX4:C13	4:A:409:PX4:H32	0.40	2.45	19	1
4:A:415:PX4:H30	4:A:415:PX4:H35	0.40	1.73	19	1
4:A:310:PX4:C28	4:A:363:PX4:H51	0.40	2.40	10	1
4:A:348:PX4:H54	4:A:356:PX4:H48	0.40	1.94	16	1
4:A:368:PX4:H48	4:A:429:PX4:H49	0.40	1.92	5	1
4:A:352:PX4:H43	4:A:409:PX4:H43	0.40	1.93	5	1
4:A:384:PX4:H26	4:A:391:PX4:H56	0.40	1.91	6	1
4:A:331:PX4:H41	4:A:339:PX4:H45	0.40	1.91	18	1
4:A:357:PX4:H63	4:A:357:PX4:H68	0.40	1.48	9	1
4:A:429:PX4:H52	4:A:429:PX4:H59	0.40	1.60	7	1
4:A:309:PX4:H56	4:A:309:PX4:H62	0.40	1.71	11	1
4:A:372:PX4:H34	4:A:373:PX4:H41	0.40	1.94	4	1
4:A:306:PX4:H72	4:A:348:PX4:H35	0.40	1.93	20	1
4:A:379:PX4:H48	4:A:379:PX4:H55	0.40	1.74	20	1
4:A:316:PX4:H54	4:A:316:PX4:H49	0.40	1.64	15	1
4:A:389:PX4:H47	4:A:398:PX4:H17	0.40	1.91	15	1
4:A:307:PX4:H17	4:A:363:PX4:H22	0.40	1.92	1	1
4:A:329:PX4:H63	4:A:338:PX4:H38	0.40	1.92	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:393:PX4:H5	4:A:402:PX4:O1	0.40	2.17	14	1
4:A:423:PX4:H59	4:A:426:PX4:H54	0.40	1.93	14	1
4:A:320:PX4:H37	4:A:328:PX4:H33	0.40	1.92	19	1
4:A:393:PX4:O6	4:A:408:PX4:H5	0.40	2.16	19	1
4:A:394:PX4:H27	4:A:394:PX4:H34	0.40	1.44	19	1
4:A:402:PX4:H64	4:A:410:PX4:H63	0.40	1.93	19	1
4:A:408:PX4:H68	4:A:408:PX4:H63	0.40	1.74	19	1
4:A:368:PX4:H72	4:A:430:PX4:H27	0.40	1.92	19	1
4:A:370:PX4:H23	4:A:377:PX4:H26	0.40	1.93	8	1
4:A:391:PX4:H45	4:A:391:PX4:H37	0.40	1.71	8	1
4:A:328:PX4:H39	4:A:328:PX4:H34	0.40	1.57	10	1
4:A:332:PX4:H30	4:A:332:PX4:H23	0.40	1.69	10	1
4:A:349:PX4:H14	4:A:363:PX4:O1	0.40	2.17	10	1
4:A:395:PX4:H59	4:A:412:PX4:H58	0.40	1.92	10	1
4:A:315:PX4:H64	4:A:315:PX4:H72	0.40	1.56	13	1
4:A:305:PX4:H19	4:A:328:PX4:H52	0.40	1.93	16	1
4:A:326:PX4:H40	4:A:353:PX4:H42	0.40	1.93	16	1
4:A:378:PX4:O7	4:A:381:PX4:H11	0.40	2.16	5	1
4:A:384:PX4:H57	4:A:384:PX4:H51	0.40	1.77	5	1
4:A:328:PX4:O5	4:A:335:PX4:H14	0.40	2.16	6	1
4:A:306:PX4:H54	4:A:349:PX4:H29	0.40	1.94	9	1
4:A:414:PX4:H27	4:A:414:PX4:H33	0.40	1.54	9	1
4:A:312:PX4:O2	4:A:327:PX4:H3	0.40	2.16	7	1
4:A:354:PX4:H28	4:A:354:PX4:H21	0.40	1.20	7	1
4:A:318:PX4:H41	4:A:421:PX4:H69	0.40	1.92	7	1
4:A:312:PX4:H52	4:A:317:PX4:H22	0.40	1.93	11	1
4:A:386:PX4:H38	4:A:387:PX4:H35	0.40	1.92	11	1
4:A:330:PX4:O2	4:A:339:PX4:H9	0.40	2.16	4	1
4:A:330:PX4:H15	4:A:331:PX4:C8	0.40	2.44	20	1
4:A:391:PX4:H30	4:A:391:PX4:H35	0.40	1.70	20	1
1:A:213:TYR:CG	1:A:214:PRO:HD2	0.40	2.51	15	1
4:A:420:PX4:H35	4:A:420:PX4:H30	0.40	1.61	3	1
4:A:334:PX4:H50	4:A:334:PX4:H57	0.40	1.73	1	1
4:A:323:PX4:H59	4:A:340:PX4:H56	0.40	1.93	17	1
4:A:342:PX4:H16	4:A:351:PX4:H22	0.40	1.92	17	1
4:A:383:PX4:H65	4:A:429:PX4:H36	0.40	1.94	17	1
4:A:318:PX4:H28	4:A:318:PX4:H22	0.40	1.65	19	1
4:A:325:PX4:H56	4:A:349:PX4:H58	0.40	1.93	19	1
4:A:419:PX4:O4	4:A:426:PX4:H10	0.40	2.16	19	1
4:A:420:PX4:H33	4:A:420:PX4:H28	0.40	1.75	8	1
4:A:321:PX4:H54	4:A:335:PX4:H23	0.40	1.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H34	4:A:375:PX4:H21	0.40	1.93	10	1
4:A:384:PX4:H58	4:A:395:PX4:H27	0.40	1.93	13	1
4:A:305:PX4:H56	4:A:362:PX4:H56	0.40	1.93	16	1
1:A:129:TRP:CE2	4:A:313:PX4:H3	0.40	2.51	5	1
4:A:310:PX4:H31	4:A:310:PX4:H38	0.40	1.73	5	1
4:A:406:PX4:H34	4:A:406:PX4:H27	0.40	1.53	5	1
4:A:341:PX4:O6	4:A:357:PX4:H5	0.40	2.16	6	1
4:A:346:PX4:H52	4:A:347:PX4:H49	0.40	1.92	6	1
4:A:353:PX4:H15	4:A:353:PX4:O8	0.40	2.15	6	1
4:A:318:PX4:H44	4:A:375:PX4:H42	0.40	1.92	6	1
4:A:330:PX4:C27	4:A:331:PX4:H21	0.40	2.42	12	1
4:A:418:PX4:H2	4:A:427:PX4:O1	0.40	2.16	9	1
4:A:423:PX4:H55	4:A:426:PX4:C11	0.40	2.44	2	1
4:A:316:PX4:H9	4:A:316:PX4:H14	0.40	1.92	3	1
4:A:318:PX4:H17	4:A:323:PX4:H23	0.40	1.92	1	1
4:A:343:PX4:H54	4:A:353:PX4:H30	0.40	1.94	17	1
4:A:366:PX4:H53	4:A:366:PX4:H58	0.40	1.66	17	1
4:A:341:PX4:H27	4:A:341:PX4:H34	0.40	1.64	19	1
4:A:385:PX4:H53	4:A:385:PX4:H46	0.40	1.32	19	1
4:A:316:PX4:H59	4:A:317:PX4:H52	0.40	1.93	8	1
4:A:354:PX4:H21	4:A:354:PX4:H50	0.40	1.94	13	1
4:A:373:PX4:H48	4:A:375:PX4:H52	0.40	1.94	13	1
4:A:316:PX4:H47	4:A:325:PX4:C28	0.40	2.45	16	1
4:A:344:PX4:H47	4:A:344:PX4:H52	0.40	1.30	16	1
4:A:314:PX4:H47	4:A:364:PX4:H20	0.40	1.93	16	1
4:A:398:PX4:H67	4:A:398:PX4:H60	0.40	1.69	16	1
4:A:413:PX4:O1	4:A:428:PX4:H11	0.40	2.17	16	1
4:A:313:PX4:H34	4:A:364:PX4:H30	0.40	1.94	6	1
4:A:390:PX4:H26	4:A:397:PX4:H59	0.40	1.94	6	1
4:A:408:PX4:H28	4:A:416:PX4:H36	0.40	1.94	6	1
4:A:374:PX4:H71	4:A:398:PX4:H35	0.40	1.93	12	1
4:A:315:PX4:H39	4:A:388:PX4:H57	0.40	1.93	18	1
4:A:405:PX4:H19	4:A:414:PX4:H24	0.40	1.93	18	1
4:A:420:PX4:H63	4:A:420:PX4:H68	0.40	1.43	18	1
4:A:316:PX4:H20	4:A:325:PX4:H50	0.40	1.92	9	1
4:A:331:PX4:H46	4:A:331:PX4:H16	0.40	1.64	9	1
4:A:345:PX4:H53	4:A:354:PX4:H53	0.40	1.94	9	1
4:A:416:PX4:H58	4:A:417:PX4:H21	0.40	1.94	11	1
4:A:343:PX4:H54	4:A:353:PX4:H27	0.40	1.93	4	1
4:A:370:PX4:H30	4:A:377:PX4:H35	0.40	1.93	4	1
4:A:378:PX4:H69	4:A:380:PX4:H38	0.40	1.94	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:365:PX4:H45	4:A:379:PX4:H43	0.40	1.92	4	1
4:A:431:PX4:H72	4:A:431:PX4:H64	0.40	1.74	2	1
4:A:332:PX4:H34	4:A:340:PX4:H53	0.40	1.93	20	1
4:A:368:PX4:H44	4:A:368:PX4:H38	0.40	1.58	20	1
4:A:341:PX4:H31	4:A:341:PX4:H26	0.40	1.62	15	1
4:A:397:PX4:H56	4:A:397:PX4:H50	0.40	1.67	3	1
4:A:318:PX4:H2	4:A:323:PX4:H1	0.40	1.94	1	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	229/248 (92%)	202±3 (88±1%)	20±3 (9±1%)	8±2 (3±1%)	6	37
All	All	4580/4960 (92%)	4036 (88%)	391 (9%)	153 (3%)	6	37

All 32 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	155	THR	20
1	A	65	PRO	17
1	A	31	ASN	15
1	A	150	ASP	13
1	A	74	GLU	11
1	A	147	TYR	11
1	A	24	LEU	9
1	A	80	ASN	6
1	A	76	SER	5
1	A	75	TYR	5
1	A	141	GLY	5
1	A	121	PRO	3
1	A	144	GLY	3
1	A	56	SER	3
1	A	148	PRO	3

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Mol	Chain	Res	Type	Models (Total)
1	A	162	PRO	3
1	A	81	SER	2
1	A	72	VAL	2
1	A	166	LEU	2
1	A	70	PRO	2
1	A	154	ASN	2
1	A	73	ALA	1
1	A	211	VAL	1
1	A	103	ILE	1
1	A	164	THR	1
1	A	142	ALA	1
1	A	232	LYS	1
1	A	214	PRO	1
1	A	11	GLN	1
1	A	215	THR	1
1	A	167	GLY	1
1	A	216	TYR	1

### 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	190/206 (92%)	182±3 (96±2%)	9±3 (4±2%)	31	80
All	All	3800/4120 (92%)	3630 (96%)	170 (4%)	31	80

All 60 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	155	THR	13
1	A	150	ASP	13
1	A	156	LEU	11
1	A	216	TYR	11
1	A	180	ASP	9
1	A	26	ASP	7
1	A	177	ARG	6
1	A	175	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	174	GLU	5
1	A	138	PHE	5
1	A	66	ARG	5
1	A	54	LEU	5
1	A	171	HIS	4
1	A	222	GLN	4
1	A	83	LYS	4
1	A	12	TRP	4
1	A	77	LEU	3
1	A	184	LEU	3
1	A	220	ASP	2
1	A	230	ASP	2
1	A	179	THR	2
1	A	85	THR	2
1	A	63	GLN	2
1	A	235	GLN	2
1	A	65	PRO	2
1	A	60	GLU	2
1	A	128	VAL	2
1	A	131	THR	2
1	A	114	ASN	1
1	A	106	ASP	1
1	A	75	TYR	1
1	A	213	TYR	1
1	A	189	LEU	1
1	A	225	LYS	1
1	A	223	ASN	1
1	A	209	ASN	1
1	A	164	THR	1
1	A	224	PHE	1
1	A	218	ASN	1
1	A	123	HIS	1
1	A	39	LEU	1
1	A	72	VAL	1
1	A	97	THR	1
1	A	100	LEU	1
1	A	92	ARG	1
1	A	205	SER	1
1	A	48	LEU	1
1	A	176	GLU	1
1	A	41	GLU	1
1	A	228	GLN	1

*Continued on next page...*

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Mol	Chain	Res	Type	Models (Total)
1	A	11	GLN	1
1	A	81	SER	1
1	A	231	ILE	1
1	A	207	ASP	1
1	A	148	PRO	1
1	A	17	ASP	1
1	A	71	ASP	1
1	A	135	MET	1
1	A	104	THR	1
1	A	122	LEU	1

### 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 carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

Of 131 ligands modelled in this entry, 4 are monoatomic - leaving 127 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	392	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.63±0.00	0±0 (0±0%)



Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	403	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.63±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	343	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	431	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.63±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	369	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	305	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.63±0.01	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	392	-	51,53,53	1.53±0.14	0±1 (0±1%)
4	PX4	A	340	-	51,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	407	-	51,53,53	1.51±0.16	0±1 (0±1%)
4	PX4	A	405	-	51,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	403	-	51,53,53	1.52±0.13	0±0 (0±0%)
4	PX4	A	317	-	51,53,53	1.47±0.16	0±0 (0±0%)
4	PX4	A	310	-	51,53,53	1.50±0.10	0±1 (0±0%)
4	PX4	A	333	-	51,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	337	-	51,53,53	1.55±0.17	0±1 (0±1%)
4	PX4	A	376	-	51,53,53	1.54±0.19	0±0 (0±0%)
4	PX4	A	323	-	51,53,53	1.44±0.12	0±0 (0±0%)
4	PX4	A	429	-	51,53,53	1.45±0.18	0±0 (0±0%)
4	PX4	A	359	-	51,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	410	-	51,53,53	1.51±0.17	0±0 (0±0%)
4	PX4	A	307	-	51,53,53	1.50±0.17	0±0 (0±0%)
4	PX4	A	380	-	51,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	399	-	51,53,53	1.44±0.17	0±0 (0±0%)
4	PX4	A	328	-	51,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	319	-	51,53,53	1.55±0.15	0±0 (0±0%)
4	PX4	A	327	-	51,53,53	1.45±0.15	0±0 (0±0%)
4	PX4	A	424	-	51,53,53	1.43±0.14	0±0 (0±0%)
4	PX4	A	316	-	51,53,53	1.53±0.10	0±0 (0±0%)
4	PX4	A	330	-	51,53,53	1.49±0.17	0±0 (0±0%)
4	PX4	A	391	-	51,53,53	1.50±0.14	0±0 (0±0%)
4	PX4	A	430	-	51,53,53	1.48±0.17	0±1 (0±0%)
4	PX4	A	355	-	51,53,53	1.54±0.12	0±1 (0±0%)
4	PX4	A	326	-	51,53,53	1.55±0.13	0±0 (0±0%)
4	PX4	A	320	-	51,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	358	-	51,53,53	1.48±0.11	0±0 (0±0%)
4	PX4	A	374	-	51,53,53	1.53±0.10	0±0 (0±0%)
4	PX4	A	384	-	51,53,53	1.55±0.18	0±0 (0±0%)
4	PX4	A	413	-	51,53,53	1.46±0.14	0±0 (0±0%)
4	PX4	A	381	-	51,53,53	1.51±0.15	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	387	-	51,53,53	1.42±0.11	0±0 (0±0%)
4	PX4	A	419	-	51,53,53	1.51±0.15	0±0 (0±0%)
4	PX4	A	365	-	51,53,53	1.45±0.16	0±0 (0±0%)
4	PX4	A	347	-	51,53,53	1.45±0.11	0±0 (0±0%)
4	PX4	A	357	-	51,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	428	-	51,53,53	1.52±0.16	0±0 (0±0%)
4	PX4	A	362	-	51,53,53	1.44±0.14	0±0 (0±0%)
4	PX4	A	397	-	51,53,53	1.48±0.07	0±0 (0±0%)
4	PX4	A	425	-	51,53,53	1.50±0.14	0±0 (0±0%)
4	PX4	A	409	-	51,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	324	-	51,53,53	1.50±0.14	0±0 (0±0%)
4	PX4	A	408	-	51,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	344	-	51,53,53	1.48±0.08	0±0 (0±0%)
4	PX4	A	411	-	51,53,53	1.55±0.12	0±0 (0±0%)
4	PX4	A	343	-	51,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	389	-	51,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	366	-	51,53,53	1.45±0.13	0±0 (0±0%)
4	PX4	A	394	-	51,53,53	1.43±0.14	0±0 (0±0%)
4	PX4	A	311	-	51,53,53	1.56±0.13	0±0 (0±0%)
4	PX4	A	417	-	51,53,53	1.45±0.15	0±0 (0±0%)
4	PX4	A	334	-	51,53,53	1.48±0.11	0±0 (0±0%)
4	PX4	A	351	-	51,53,53	1.52±0.15	0±0 (0±0%)
4	PX4	A	415	-	51,53,53	1.53±0.12	0±0 (0±0%)
4	PX4	A	412	-	51,53,53	1.51±0.17	0±0 (0±0%)
4	PX4	A	346	-	51,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	426	-	51,53,53	1.45±0.17	0±0 (0±0%)
4	PX4	A	309	-	51,53,53	1.46±0.11	0±0 (0±0%)
4	PX4	A	364	-	51,53,53	1.45±0.12	0±0 (0±0%)
4	PX4	A	431	-	51,53,53	1.53±0.13	0±0 (0±0%)
4	PX4	A	361	-	51,53,53	1.51±0.11	0±0 (0±0%)
4	PX4	A	341	-	51,53,53	1.47±0.09	0±0 (0±0%)
4	PX4	A	321	-	51,53,53	1.51±0.18	0±0 (0±0%)
4	PX4	A	390	-	51,53,53	1.53±0.17	0±1 (0±1%)
4	PX4	A	427	-	51,53,53	1.47±0.13	0±0 (0±0%)
4	PX4	A	313	-	51,53,53	1.50±0.14	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	402	-	51,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	370	-	51,53,53	1.53±0.14	0±0 (0±0%)
4	PX4	A	414	-	51,53,53	1.54±0.13	0±1 (0±1%)
4	PX4	A	375	-	51,53,53	1.45±0.17	0±0 (0±0%)
4	PX4	A	385	-	51,53,53	1.53±0.17	0±0 (0±0%)
4	PX4	A	422	-	51,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	418	-	51,53,53	1.52±0.08	0±0 (0±0%)
4	PX4	A	393	-	51,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	372	-	51,53,53	1.55±0.16	0±0 (0±0%)
4	PX4	A	404	-	51,53,53	1.43±0.12	0±0 (0±0%)
4	PX4	A	354	-	51,53,53	1.50±0.17	0±0 (0±0%)
4	PX4	A	382	-	51,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	367	-	51,53,53	1.51±0.18	0±0 (0±0%)
4	PX4	A	349	-	51,53,53	1.54±0.13	0±0 (0±0%)
4	PX4	A	312	-	51,53,53	1.55±0.17	0±0 (0±0%)
4	PX4	A	378	-	51,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	338	-	51,53,53	1.46±0.08	0±0 (0±0%)
4	PX4	A	373	-	51,53,53	1.55±0.18	0±0 (0±0%)
4	PX4	A	332	-	51,53,53	1.51±0.15	0±0 (0±0%)
4	PX4	A	383	-	51,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	379	-	51,53,53	1.47±0.21	0±0 (0±0%)
4	PX4	A	377	-	51,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	369	-	51,53,53	1.52±0.19	0±1 (0±1%)
4	PX4	A	314	-	51,53,53	1.52±0.11	0±0 (0±0%)
4	PX4	A	306	-	51,53,53	1.53±0.16	0±0 (0±0%)
4	PX4	A	406	-	51,53,53	1.52±0.14	0±0 (0±0%)
4	PX4	A	325	-	51,53,53	1.49±0.16	0±1 (0±1%)
4	PX4	A	305	-	51,53,53	1.48±0.15	0±1 (0±1%)
4	PX4	A	421	-	51,53,53	1.53±0.15	0±0 (0±0%)
4	PX4	A	329	-	51,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	315	-	51,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	371	-	51,53,53	1.46±0.12	0±0 (0±0%)
4	PX4	A	420	-	51,53,53	1.51±0.14	0±0 (0±0%)
4	PX4	A	322	-	51,53,53	1.47±0.13	0±0 (0±0%)
4	PX4	A	352	-	51,53,53	1.49±0.19	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	350	-	51,53,53	1.43±0.18	0±0 (0±0%)
4	PX4	A	318	-	51,53,53	1.53±0.13	0±0 (0±0%)
4	PX4	A	308	-	51,53,53	1.44±0.11	0±0 (0±0%)
4	PX4	A	335	-	51,53,53	1.50±0.11	0±0 (0±0%)
4	PX4	A	363	-	51,53,53	1.54±0.13	0±0 (0±0%)
4	PX4	A	348	-	51,53,53	1.51±0.13	0±0 (0±0%)
4	PX4	A	368	-	51,53,53	1.52±0.13	0±0 (0±0%)
4	PX4	A	345	-	51,53,53	1.49±0.10	0±0 (0±0%)
4	PX4	A	423	-	51,53,53	1.52±0.17	0±0 (0±0%)
4	PX4	A	353	-	51,53,53	1.55±0.16	0±0 (0±0%)
4	PX4	A	416	-	51,53,53	1.43±0.10	0±0 (0±0%)
4	PX4	A	356	-	51,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	388	-	51,53,53	1.53±0.17	0±1 (0±0%)
4	PX4	A	360	-	51,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	401	-	51,53,53	1.51±0.17	0±0 (0±0%)
4	PX4	A	395	-	51,53,53	1.54±0.12	0±0 (0±0%)
4	PX4	A	398	-	51,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	386	-	51,53,53	1.52±0.14	0±0 (0±0%)
4	PX4	A	331	-	51,53,53	1.50±0.18	0±0 (0±0%)
4	PX4	A	336	-	51,53,53	1.48±0.17	0±0 (0±0%)
4	PX4	A	400	-	51,53,53	1.45±0.17	0±0 (0±0%)
4	PX4	A	396	-	51,53,53	1.46±0.12	0±0 (0±0%)
4	PX4	A	339	-	51,53,53	1.46±0.14	0±0 (0±0%)
4	PX4	A	342	-	51,53,53	1.48±0.12	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	377	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	328	-	-	0±0,49,49,49	-
4	PX4	A	341	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
4	PX4	A	305	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	431	-	-	0±0,49,49,49	-
4	PX4	A	384	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	307	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	430	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	418	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	1±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	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	329	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	315	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	371	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	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	338	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-

There are no bond-length outliers.

All 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
4	A	343	PX4	C8-C7-C6	7.96	92.97	111.79	16	1
4	A	392	PX4	C7-O7-C23	7.71	136.78	117.79	11	1
4	A	384	PX4	C5-N1-C4	7.66	89.28	108.97	6	1
4	A	369	PX4	C8-C7-C6	7.48	94.09	111.79	12	6
4	A	356	PX4	C8-C7-C6	7.31	94.49	111.79	5	3
4	A	398	PX4	C8-C7-C6	7.11	94.98	111.79	15	1
4	A	426	PX4	O7-C23-O8	7.08	106.60	123.70	12	1
4	A	307	PX4	C8-C7-C6	6.98	95.28	111.79	8	1
4	A	349	PX4	O5-C8-C7	6.96	128.70	108.43	8	3
4	A	384	PX4	C8-C7-C6	6.94	95.37	111.79	7	1
4	A	319	PX4	O5-C8-C7	6.93	128.62	108.43	19	1
4	A	331	PX4	C8-C7-C6	6.93	95.40	111.79	19	1
4	A	337	PX4	O7-C23-C24	6.93	126.43	111.50	16	1
4	A	311	PX4	C7-O7-C23	6.90	134.79	117.79	15	1
4	A	407	PX4	O7-C23-C24	6.87	126.31	111.50	10	1
4	A	403	PX4	C8-C7-C6	6.84	95.61	111.79	14	4
4	A	391	PX4	O5-C8-C7	6.83	128.31	108.43	14	2
4	A	331	PX4	C7-O7-C23	6.80	134.53	117.79	16	1
4	A	373	PX4	O7-C23-C24	6.73	126.00	111.50	13	2
4	A	406	PX4	O7-C23-C24	6.72	125.98	111.50	9	1
4	A	419	PX4	P1-O3-C1	6.57	89.26	121.59	13	1
4	A	321	PX4	C8-C7-C6	6.54	96.31	111.79	11	2
4	A	337	PX4	O5-C8-C7	6.52	127.42	108.43	18	2
4	A	386	PX4	O5-C8-C7	6.49	127.33	108.43	7	2
4	A	377	PX4	C8-C7-C6	6.48	96.46	111.79	8	1
4	A	420	PX4	C8-C7-C6	6.47	96.49	111.79	9	1
4	A	309	PX4	C4-N1-C3	6.43	92.43	108.97	12	1
4	A	370	PX4	O7-C23-C24	6.40	125.28	111.50	4	1
4	A	326	PX4	O5-C8-C7	6.39	127.04	108.43	9	1
4	A	363	PX4	O7-C23-C24	6.32	125.13	111.50	10	3
4	A	390	PX4	C4-N1-C3	6.29	92.79	108.97	8	1
4	A	390	PX4	C8-C7-C6	6.29	96.92	111.79	1	3
4	A	318	PX4	O5-C8-C7	6.26	126.65	108.43	1	3
4	A	306	PX4	C8-C7-C6	6.21	97.09	111.79	7	3
4	A	408	PX4	P1-O3-C1	6.21	91.04	121.59	11	1
4	A	414	PX4	O7-C23-C24	6.20	124.87	111.50	8	2
4	A	324	PX4	C8-C7-C6	6.20	97.13	111.79	8	2
4	A	341	PX4	C8-C7-C6	6.19	97.15	111.79	7	1
4	A	352	PX4	O7-C23-C24	6.17	124.81	111.50	18	1
4	A	357	PX4	C8-C7-C6	6.15	97.24	111.79	3	1
4	A	424	PX4	C8-C7-C6	6.14	97.27	111.79	14	1
4	A	418	PX4	C8-C7-C6	6.14	97.27	111.79	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	O7-C23-C24	6.12	124.68	111.50	15	1
4	A	403	PX4	O5-C8-C7	6.11	126.21	108.43	12	2
4	A	392	PX4	O7-C23-C24	6.09	124.62	111.50	6	1
4	A	337	PX4	C8-C7-C6	6.09	97.39	111.79	5	1
4	A	417	PX4	C8-C7-C6	6.09	97.39	111.79	9	1
4	A	428	PX4	C8-C7-C6	6.07	97.42	111.79	5	2
4	A	393	PX4	O3-P1-O2	6.05	85.42	109.07	16	1
4	A	351	PX4	O5-C8-C7	6.04	126.01	108.43	7	1
4	A	372	PX4	C8-C7-C6	6.03	97.52	111.79	17	2
4	A	376	PX4	O3-P1-O2	6.02	85.56	109.07	7	1
4	A	384	PX4	C7-O7-C23	6.01	132.59	117.79	15	1
4	A	355	PX4	O7-C23-C24	6.01	124.45	111.50	16	1
4	A	352	PX4	C8-C7-C6	6.00	97.60	111.79	16	1
4	A	330	PX4	O7-C23-C24	5.99	124.41	111.50	9	1
4	A	312	PX4	O5-C8-C7	5.98	125.85	108.43	12	1
4	A	392	PX4	C8-C7-C6	5.98	97.65	111.79	17	2
4	A	393	PX4	C8-C7-C6	5.98	97.66	111.79	11	1
4	A	369	PX4	O7-C23-C24	5.97	124.37	111.50	16	1
4	A	385	PX4	C8-C7-C6	5.97	97.68	111.79	20	2
4	A	430	PX4	O7-C23-C24	5.95	124.33	111.50	3	1
4	A	311	PX4	O5-C8-C7	5.93	125.70	108.43	16	4
4	A	418	PX4	O5-C8-C7	5.93	125.69	108.43	8	1
4	A	321	PX4	O7-C23-C24	5.91	124.25	111.50	10	2
4	A	316	PX4	C8-C7-C6	5.90	97.82	111.79	4	3
4	A	305	PX4	O7-C23-C24	5.90	124.22	111.50	3	2
4	A	325	PX4	O7-C23-O8	5.89	109.48	123.70	4	1
4	A	390	PX4	O7-C23-C24	5.87	124.16	111.50	4	1
4	A	412	PX4	O5-C8-C7	5.86	125.50	108.43	14	2
4	A	430	PX4	O5-C8-C7	5.83	125.40	108.43	3	2
4	A	350	PX4	C8-C7-C6	5.83	98.00	111.79	15	2
4	A	366	PX4	O5-C8-C7	5.82	125.37	108.43	5	1
4	A	313	PX4	O3-P1-O2	5.80	86.41	109.07	11	1
4	A	379	PX4	C8-C7-C6	5.79	98.09	111.79	19	2
4	A	407	PX4	C8-C7-C6	5.77	98.14	111.79	3	4
4	A	319	PX4	C8-C7-C6	5.77	98.15	111.79	1	4
4	A	305	PX4	O7-C23-O8	5.76	109.78	123.70	12	1
4	A	356	PX4	O5-C8-C7	5.76	125.19	108.43	11	1
4	A	328	PX4	C8-C7-C6	5.76	98.17	111.79	11	2
4	A	310	PX4	C8-C7-C6	5.75	98.18	111.79	7	1
4	A	341	PX4	O5-C8-C7	5.75	125.16	108.43	15	1
4	A	369	PX4	O5-C8-C7	5.74	125.15	108.43	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	320	PX4	O7-C23-C24	5.74	123.86	111.50	4	2
4	A	370	PX4	C7-O7-C23	5.73	131.89	117.79	9	1
4	A	410	PX4	O5-C8-C7	5.73	125.10	108.43	18	1
4	A	424	PX4	O7-C23-C24	5.72	123.83	111.50	9	1
4	A	415	PX4	O7-C23-O8	5.71	109.89	123.70	10	1
4	A	430	PX4	C8-C7-C6	5.71	98.28	111.79	18	1
4	A	310	PX4	O7-C23-C24	5.71	123.81	111.50	1	1
4	A	400	PX4	O5-C8-C7	5.71	125.06	108.43	9	1
4	A	391	PX4	C7-O7-C23	5.71	131.85	117.79	1	1
4	A	396	PX4	C8-C7-C6	5.70	98.30	111.79	2	2
4	A	410	PX4	C8-C7-C6	5.70	98.31	111.79	5	1
4	A	372	PX4	O7-C23-O8	5.69	109.94	123.70	15	1
4	A	407	PX4	O7-C23-O8	5.69	109.95	123.70	10	1
4	A	313	PX4	O7-C23-C24	5.68	123.75	111.50	5	2
4	A	325	PX4	O7-C23-C24	5.66	123.69	111.50	8	1
4	A	401	PX4	O7-C23-C24	5.65	123.68	111.50	9	2
4	A	317	PX4	O5-C8-C7	5.65	124.88	108.43	19	2
4	A	407	PX4	O5-C8-C7	5.65	124.89	108.43	1	2
4	A	343	PX4	O5-C9-O6	5.64	109.37	123.59	4	1
4	A	423	PX4	O7-C23-C24	5.63	123.64	111.50	5	2
4	A	397	PX4	C7-O7-C23	5.63	131.65	117.79	20	1
4	A	388	PX4	O5-C8-C7	5.62	124.80	108.43	9	1
4	A	353	PX4	O7-C23-C24	5.61	123.59	111.50	17	1
4	A	354	PX4	O7-C23-O8	5.61	110.15	123.70	3	1
4	A	406	PX4	O5-C8-C7	5.60	124.74	108.43	7	1
4	A	307	PX4	O7-C23-C24	5.59	123.56	111.50	16	1
4	A	372	PX4	O7-C23-C24	5.59	123.55	111.50	13	1
4	A	399	PX4	P1-O3-C1	5.59	94.09	121.59	15	1
4	A	388	PX4	C5-N1-C4	5.58	94.63	108.97	11	1
4	A	417	PX4	O5-C8-C7	5.58	124.67	108.43	13	2
4	A	379	PX4	O7-C23-C24	5.58	123.52	111.50	4	1
4	A	367	PX4	O7-C23-C24	5.58	123.52	111.50	17	1
4	A	388	PX4	C8-C7-C6	5.57	98.62	111.79	9	2
4	A	318	PX4	O7-C23-C24	5.57	123.50	111.50	16	1
4	A	397	PX4	O5-C8-C7	5.57	124.64	108.43	5	1
4	A	337	PX4	C26-C25-C24	5.56	93.19	113.19	13	1
4	A	429	PX4	C5-N1-C3	5.56	94.67	108.97	7	1
4	A	355	PX4	C8-C7-C6	5.56	98.63	111.79	10	2
4	A	313	PX4	O5-C8-C7	5.55	124.58	108.43	19	1
4	A	395	PX4	C5-N1-C4	5.54	94.74	108.97	3	1
4	A	306	PX4	O7-C23-C24	5.53	123.41	111.50	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	305	PX4	P1-O3-C1	5.52	94.40	121.59	12	1
4	A	410	PX4	O7-C23-C24	5.52	123.40	111.50	6	2
4	A	386	PX4	O7-C23-C24	5.52	123.39	111.50	4	1
4	A	431	PX4	C8-C7-C6	5.52	98.74	111.79	1	1
4	A	342	PX4	C8-C7-C6	5.52	98.74	111.79	8	2
4	A	382	PX4	O5-C9-O6	5.51	109.68	123.59	15	1
4	A	382	PX4	C8-C7-C6	5.50	98.78	111.79	8	1
4	A	312	PX4	O7-C23-O8	5.50	110.41	123.70	1	1
4	A	325	PX4	O5-C8-C7	5.50	124.44	108.43	11	2
4	A	403	PX4	O7-C23-C24	5.50	123.36	111.50	13	2
4	A	362	PX4	C8-C7-C6	5.49	98.81	111.79	4	1
4	A	319	PX4	C5-N1-C3	5.48	123.07	108.97	8	1
4	A	319	PX4	C7-O7-C23	5.48	131.28	117.79	20	2
4	A	346	PX4	O3-P1-O2	5.47	87.68	109.07	1	1
4	A	400	PX4	O7-C23-C24	5.47	123.30	111.50	19	2
4	A	414	PX4	C8-C7-C6	5.47	98.86	111.79	11	1
4	A	376	PX4	O7-C23-C24	5.46	123.27	111.50	3	3
4	A	405	PX4	C4-N1-C3	5.46	94.94	108.97	8	1
4	A	373	PX4	C8-C7-C6	5.45	98.90	111.79	16	1
4	A	427	PX4	C8-C7-C6	5.44	98.92	111.79	14	1
4	A	331	PX4	O7-C23-C24	5.44	123.23	111.50	18	1
4	A	348	PX4	O5-C8-C7	5.42	124.20	108.43	8	1
4	A	346	PX4	O5-C8-C7	5.42	124.20	108.43	15	1
4	A	314	PX4	C8-C7-C6	5.42	98.98	111.79	13	1
4	A	351	PX4	C8-C7-C6	5.41	98.99	111.79	12	1
4	A	404	PX4	O7-C23-O8	5.41	110.63	123.70	17	1
4	A	419	PX4	O7-C23-C24	5.40	123.14	111.50	14	2
4	A	322	PX4	O5-C8-C7	5.39	124.11	108.43	14	1
4	A	415	PX4	C8-C7-C6	5.37	99.08	111.79	20	2
4	A	347	PX4	O7-C23-C24	5.37	123.08	111.50	17	1
4	A	340	PX4	C7-O7-C23	5.37	131.01	117.79	12	1
4	A	326	PX4	C4-N1-C3	5.36	95.19	108.97	6	2
4	A	347	PX4	C7-O7-C23	5.36	130.98	117.79	4	1
4	A	310	PX4	O5-C8-C7	5.36	124.02	108.43	12	1
4	A	386	PX4	C7-O7-C23	5.35	130.97	117.79	14	1
4	A	416	PX4	O7-C23-C24	5.34	123.01	111.50	7	1
4	A	410	PX4	O7-C23-O8	5.33	110.81	123.70	17	1
4	A	314	PX4	C7-O7-C23	5.33	130.91	117.79	18	1
4	A	355	PX4	O7-C23-O8	5.33	110.83	123.70	16	1
4	A	396	PX4	O5-C8-C7	5.32	123.92	108.43	16	1
4	A	395	PX4	O7-C23-C24	5.32	122.97	111.50	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	307	PX4	O5-C8-C7	5.32	123.92	108.43	10	1
4	A	380	PX4	O5-C8-C7	5.32	123.92	108.43	1	1
4	A	345	PX4	C8-C7-C6	5.32	99.22	111.79	20	1
4	A	389	PX4	O7-C23-C24	5.31	122.95	111.50	14	1
4	A	404	PX4	C8-C7-C6	5.31	99.24	111.79	17	1
4	A	316	PX4	P1-O3-C1	5.31	95.46	121.59	9	1
4	A	431	PX4	O5-C8-C7	5.31	123.88	108.43	17	1
4	A	335	PX4	C8-C7-C6	5.30	99.25	111.79	7	1
4	A	344	PX4	O7-C23-C24	5.29	122.90	111.50	12	1
4	A	358	PX4	C7-O7-C23	5.28	130.79	117.79	7	1
4	A	405	PX4	O7-C23-C24	5.28	122.87	111.50	5	1
4	A	348	PX4	C8-C7-C6	5.27	99.32	111.79	18	1
4	A	396	PX4	O7-C23-C24	5.26	122.85	111.50	12	1
4	A	413	PX4	O7-C23-C24	5.26	122.84	111.50	8	1
4	A	421	PX4	O5-C8-C7	5.26	123.75	108.43	18	1
4	A	387	PX4	O5-C8-C7	5.24	123.69	108.43	15	1
4	A	389	PX4	O5-C8-C7	5.24	123.69	108.43	12	2
4	A	412	PX4	C7-O7-C23	5.24	104.89	117.79	20	1
4	A	340	PX4	C8-C7-C6	5.24	99.40	111.79	18	1
4	A	364	PX4	C8-C7-C6	5.23	99.41	111.79	9	1
4	A	323	PX4	C5-N1-C3	5.23	95.53	108.97	7	2
4	A	389	PX4	C8-C7-C6	5.23	99.43	111.79	6	1
4	A	335	PX4	O7-C23-C24	5.22	122.76	111.50	8	1
4	A	414	PX4	C7-O7-C23	5.22	130.65	117.79	17	2
4	A	354	PX4	C8-C7-C6	5.22	99.44	111.79	16	1
4	A	374	PX4	O3-P1-O2	5.22	88.68	109.07	7	1
4	A	393	PX4	O5-C8-C7	5.22	123.61	108.43	13	1
4	A	366	PX4	C8-C7-C6	5.22	99.45	111.79	12	1
4	A	422	PX4	C7-O7-C23	5.21	130.62	117.79	18	1
4	A	421	PX4	C8-C7-C6	5.21	99.46	111.79	12	1
4	A	336	PX4	O7-C23-C24	5.21	122.73	111.50	13	1
4	A	361	PX4	O7-C23-C24	5.21	122.72	111.50	13	1
4	A	345	PX4	O7-C23-C24	5.21	122.72	111.50	18	1
4	A	422	PX4	O7-C23-C24	5.21	122.72	111.50	5	1
4	A	372	PX4	O5-C8-C7	5.20	123.58	108.43	2	1
4	A	402	PX4	O5-C8-C7	5.20	123.58	108.43	1	1
4	A	411	PX4	O5-C8-C7	5.20	123.57	108.43	14	2
4	A	364	PX4	P1-O3-C1	5.20	95.98	121.59	17	1
4	A	398	PX4	C4-N1-C3	5.20	95.60	108.97	13	1
4	A	349	PX4	C8-C7-C6	5.20	99.49	111.79	16	1
4	A	339	PX4	O7-C23-C24	5.20	122.70	111.50	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	382	PX4	O5-C8-C7	5.19	123.54	108.43	20	2
4	A	315	PX4	O7-C23-C24	5.19	122.68	111.50	3	1
4	A	319	PX4	O3-P1-O2	5.19	88.80	109.07	7	1
4	A	332	PX4	C8-C7-C6	5.19	99.52	111.79	2	1
4	A	346	PX4	C7-O7-C23	5.18	105.04	117.79	5	1
4	A	422	PX4	C8-C7-C6	5.17	99.55	111.79	6	1
4	A	369	PX4	O7-C23-O8	5.17	111.21	123.70	16	1
4	A	374	PX4	P1-O3-C1	5.17	96.14	121.59	10	1
4	A	391	PX4	C8-C7-C6	5.17	99.57	111.79	16	1
4	A	310	PX4	O7-C23-O8	5.17	111.22	123.70	1	1
4	A	312	PX4	O7-C23-C24	5.16	122.62	111.50	10	2
4	A	325	PX4	C8-C7-C6	5.16	99.59	111.79	20	1
4	A	380	PX4	C8-C7-C6	5.15	99.61	111.79	11	1
4	A	333	PX4	C5-N1-C3	5.14	95.75	108.97	17	1
4	A	357	PX4	C5-N1-C4	5.14	95.76	108.97	6	1
4	A	383	PX4	O5-C8-C7	5.14	123.38	108.43	17	1
4	A	332	PX4	O5-C8-C7	5.13	123.38	108.43	7	1
4	A	314	PX4	O7-C23-O8	5.13	111.31	123.70	18	1
4	A	326	PX4	P1-O3-C1	5.13	96.34	121.59	12	1
4	A	392	PX4	O5-C8-C7	5.13	123.36	108.43	1	2
4	A	356	PX4	C7-O7-C23	5.13	130.41	117.79	20	1
4	A	383	PX4	C5-N1-C3	5.12	95.80	108.97	15	1
4	A	379	PX4	O5-C8-C7	5.12	123.34	108.43	15	1
4	A	374	PX4	C8-C7-C6	5.11	99.70	111.79	9	2
4	A	322	PX4	C7-O7-C23	5.11	130.37	117.79	5	1
4	A	373	PX4	C26-C25-C24	5.11	94.83	113.19	3	1
4	A	427	PX4	P1-O3-C1	5.11	96.45	121.59	1	1
4	A	421	PX4	O5-C9-O6	5.10	110.71	123.59	14	1
4	A	412	PX4	O7-C23-C24	5.10	122.49	111.50	13	1
4	A	321	PX4	O5-C8-C7	5.09	123.26	108.43	18	1
4	A	367	PX4	P1-O4-C6	5.09	91.82	121.68	19	1
4	A	429	PX4	C8-C7-C6	5.09	99.75	111.79	11	2
4	A	425	PX4	O7-C23-C24	5.08	122.45	111.50	8	1
4	A	390	PX4	P1-O3-C1	5.08	96.57	121.59	1	1
4	A	427	PX4	O5-C8-C7	5.08	123.23	108.43	12	1
4	A	341	PX4	C7-O7-C23	5.08	130.30	117.79	1	1
4	A	376	PX4	O5-C8-C7	5.08	123.21	108.43	1	1
4	A	344	PX4	C8-C7-C6	5.07	99.79	111.79	11	1
4	A	396	PX4	O7-C7-C8	5.07	126.76	108.40	13	1
4	A	426	PX4	O7-C23-C24	5.07	122.42	111.50	12	1
4	A	383	PX4	O7-C23-O8	5.06	111.48	123.70	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	395	PX4	O5-C8-C7	5.06	123.15	108.43	16	1
4	A	333	PX4	O5-C8-C7	5.05	123.12	108.43	9	1
4	A	353	PX4	O5-C8-C7	5.04	123.11	108.43	2	1
4	A	327	PX4	C8-C7-C6	5.04	99.86	111.79	1	1
4	A	340	PX4	O7-C7-C8	5.04	126.64	108.40	9	1
4	A	384	PX4	P1-O3-C1	5.04	96.78	121.59	16	1
4	A	423	PX4	C5-N1-C4	5.04	96.02	108.97	6	1
4	A	350	PX4	O7-C23-C24	5.03	122.34	111.50	1	1
4	A	420	PX4	C5-N1-C4	5.03	121.90	108.97	19	1
4	A	325	PX4	C5-N1-C4	5.02	96.06	108.97	11	1
4	A	405	PX4	C8-C7-C6	5.02	99.92	111.79	10	1
4	A	363	PX4	C8-C7-C6	5.02	99.92	111.79	11	1
4	A	343	PX4	C7-O7-C23	5.01	130.14	117.79	11	1
4	A	352	PX4	O5-C8-C7	5.01	123.03	108.43	13	1
4	A	423	PX4	O5-C8-C7	5.01	123.02	108.43	12	1
4	A	370	PX4	C8-C7-C6	5.01	99.94	111.79	14	1
4	A	334	PX4	O7-C23-C24	5.01	122.29	111.50	17	1
4	A	338	PX4	O5-C8-C7	5.00	123.00	108.43	5	1
4	A	381	PX4	C8-C7-C6	5.00	99.95	111.79	4	1
4	A	394	PX4	C8-C7-C6	5.00	99.96	111.79	9	1

There are no chirality outliers.

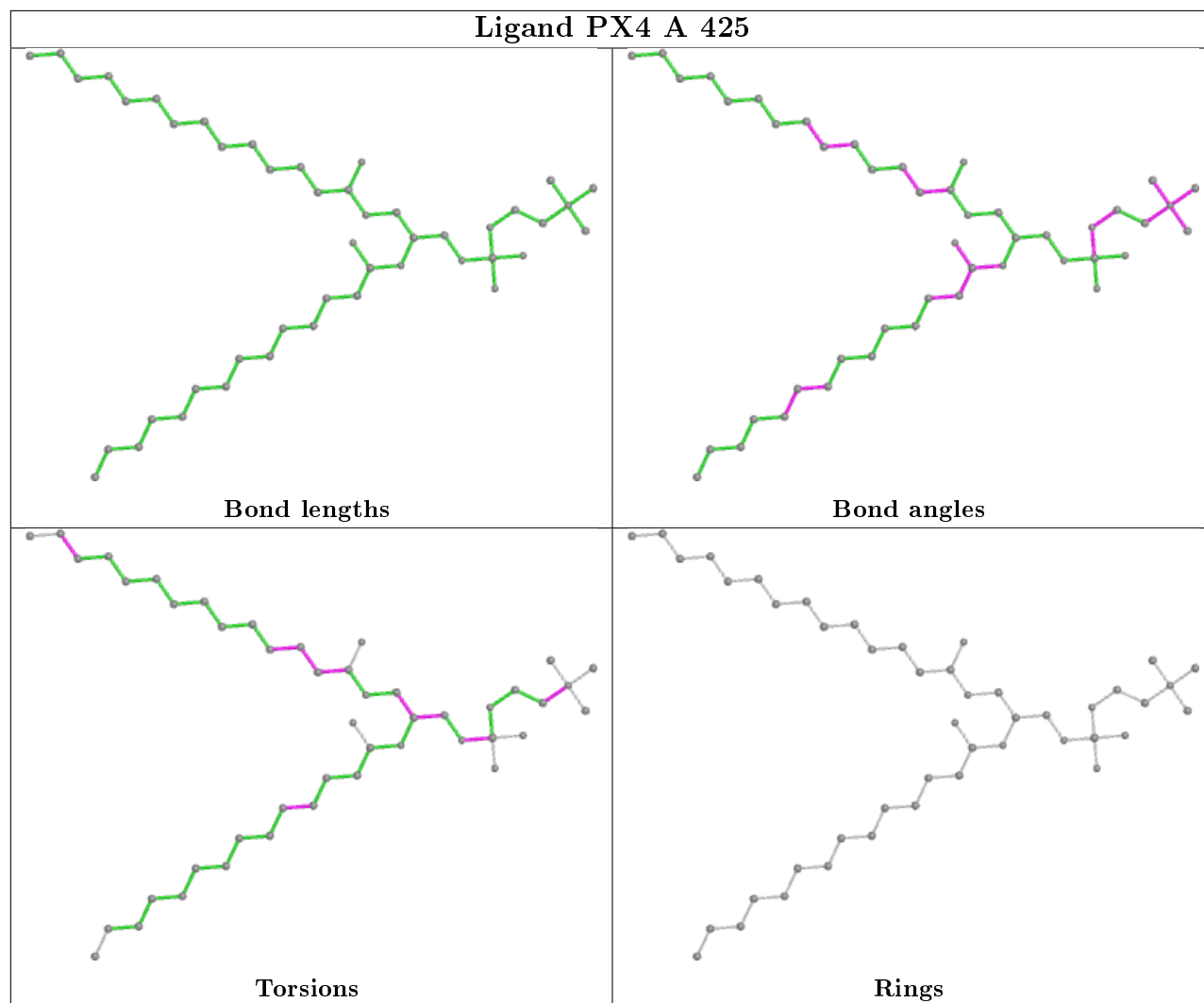
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

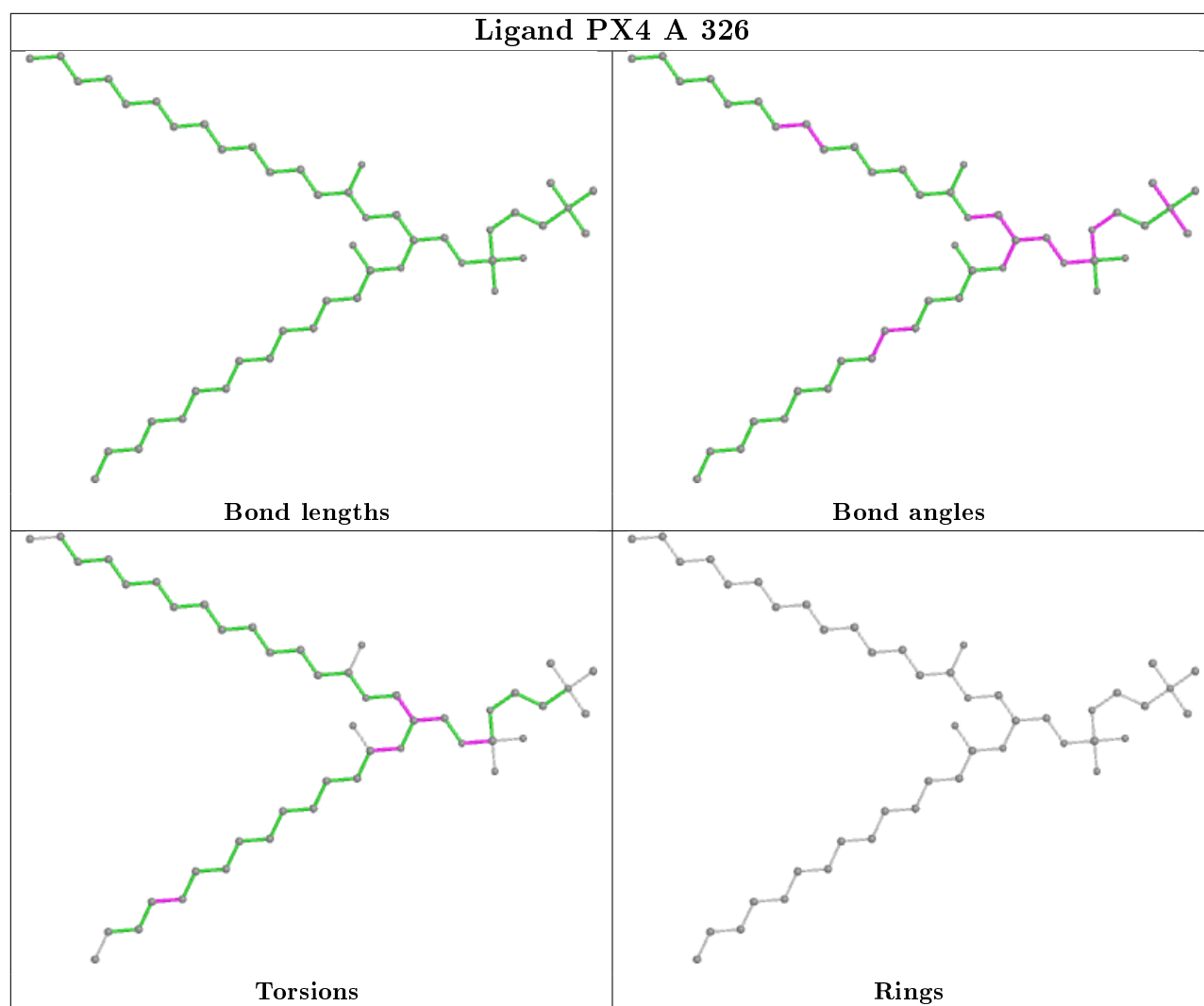
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	414	PX4	O8-C23-O7-C7	4
4	A	331	PX4	O8-C23-O7-C7	2
4	A	323	PX4	O8-C23-O7-C7	1
4	A	321	PX4	O8-C23-O7-C7	1

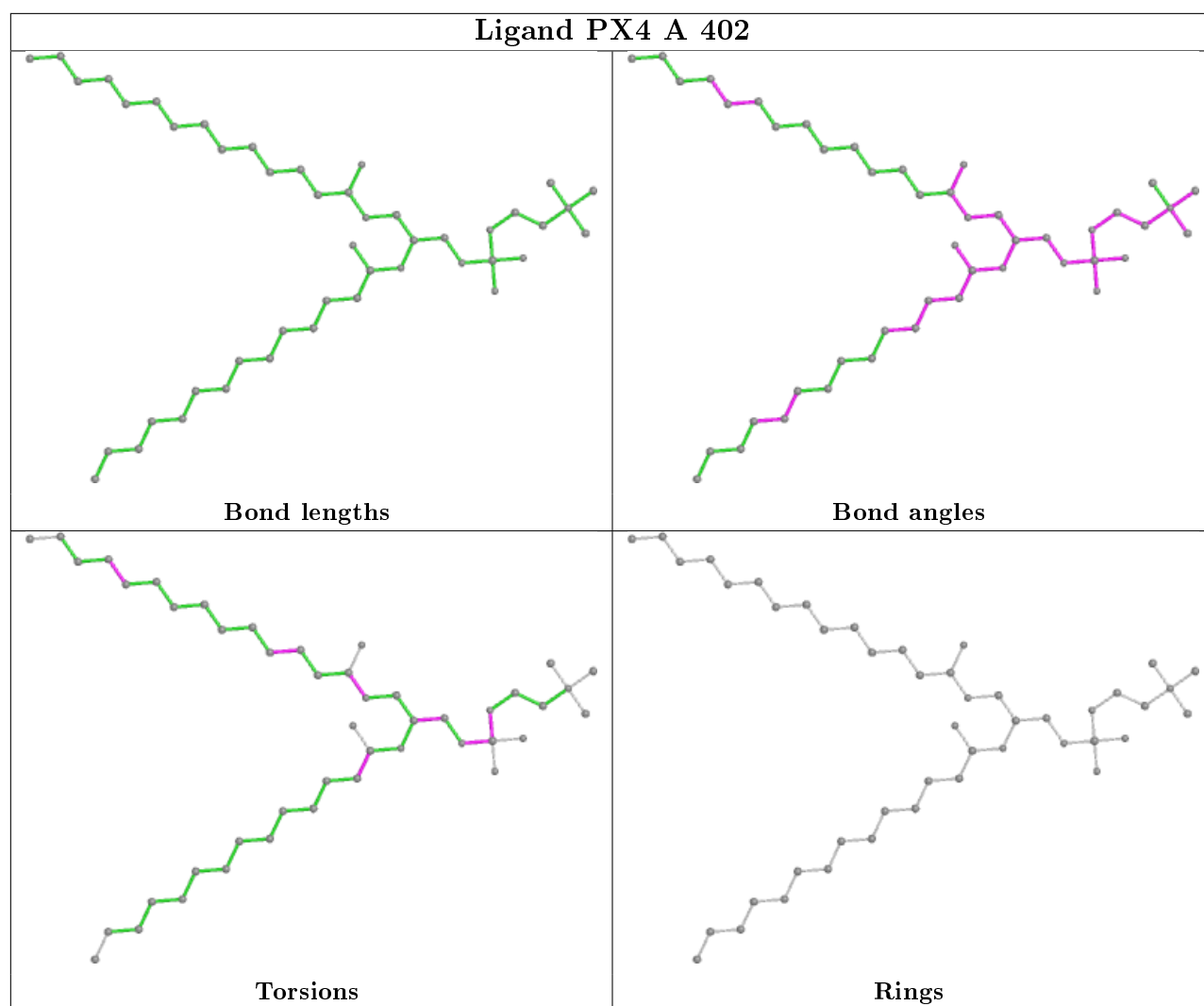
There are no ring outliers.

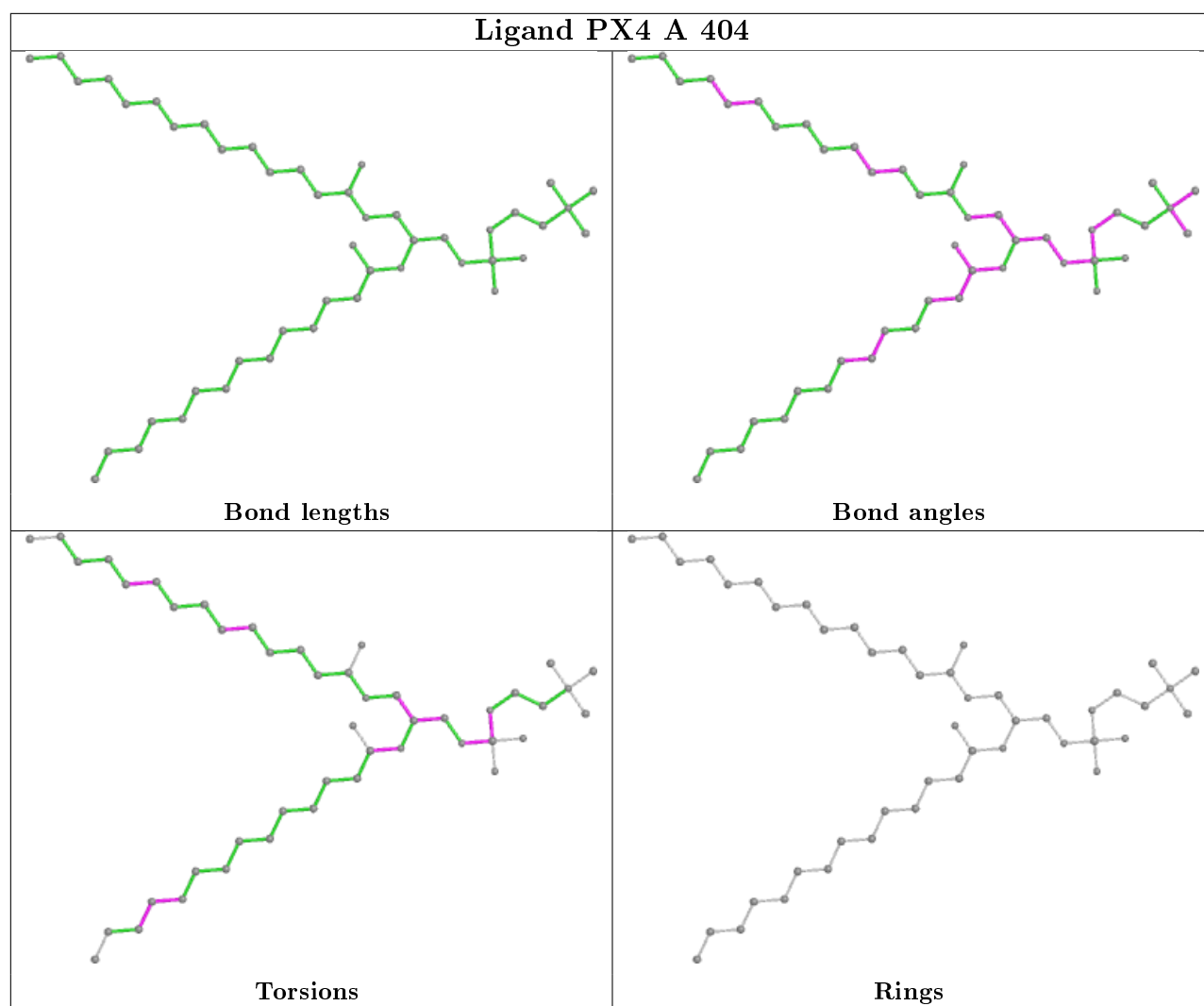
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

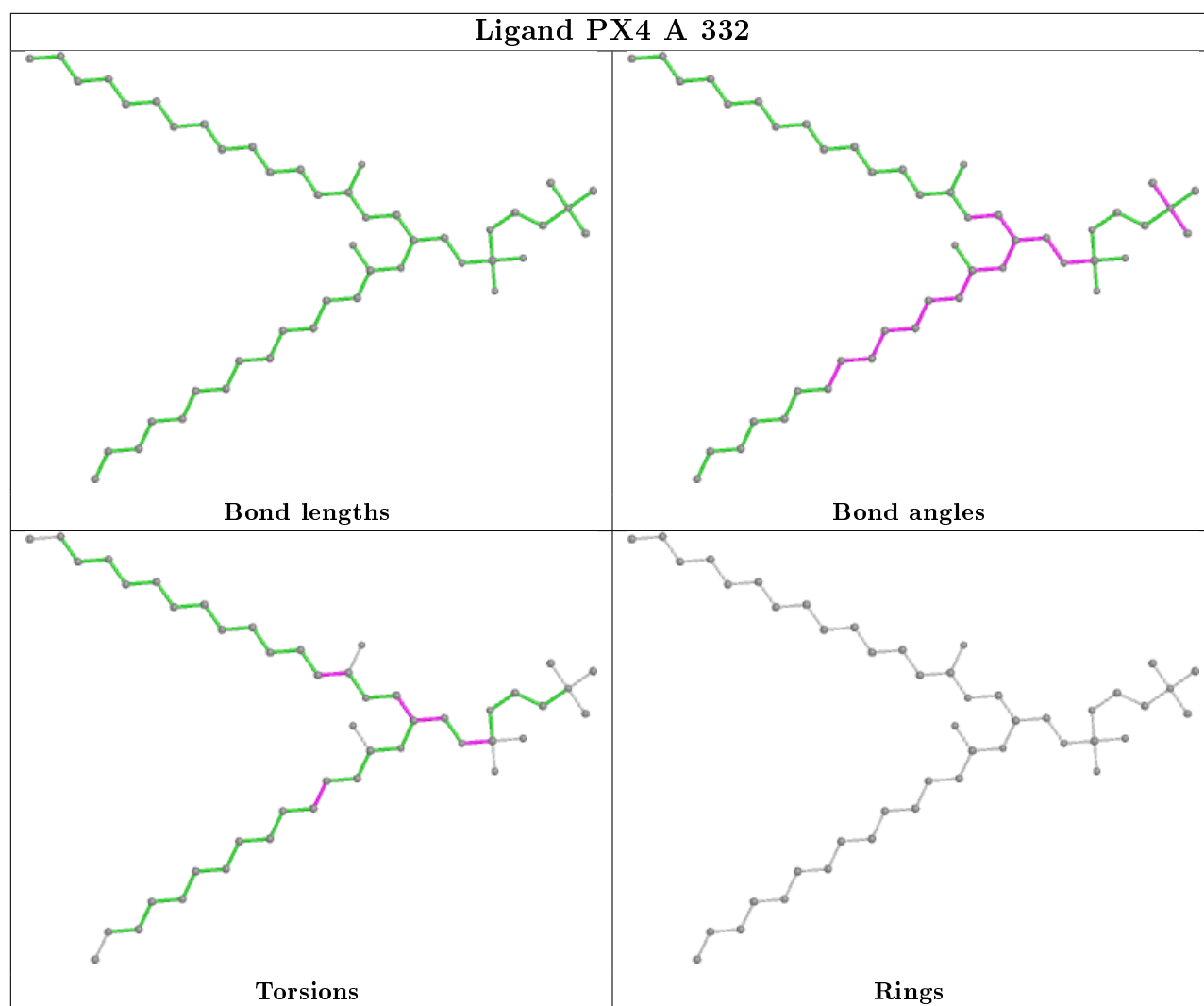
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

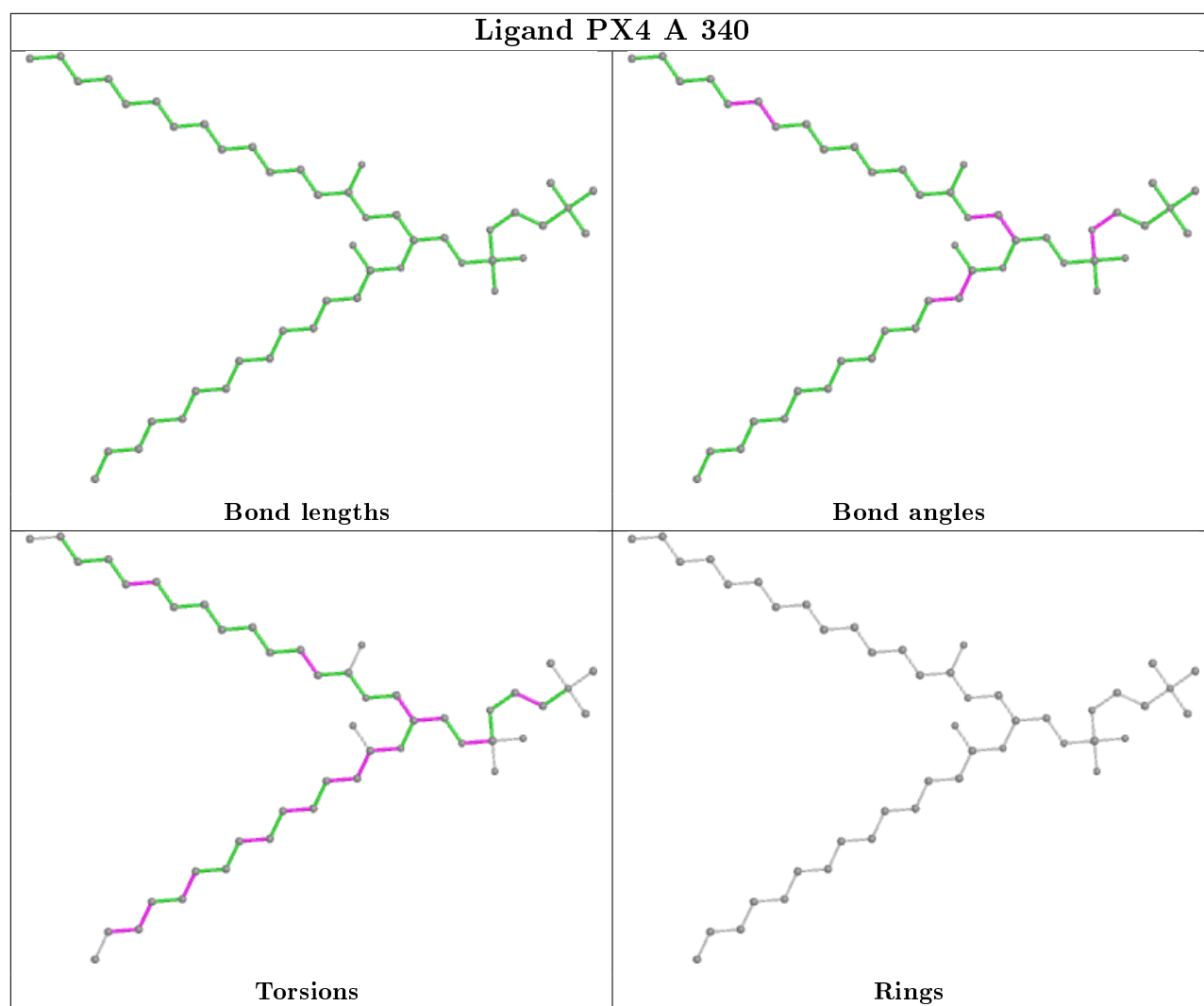


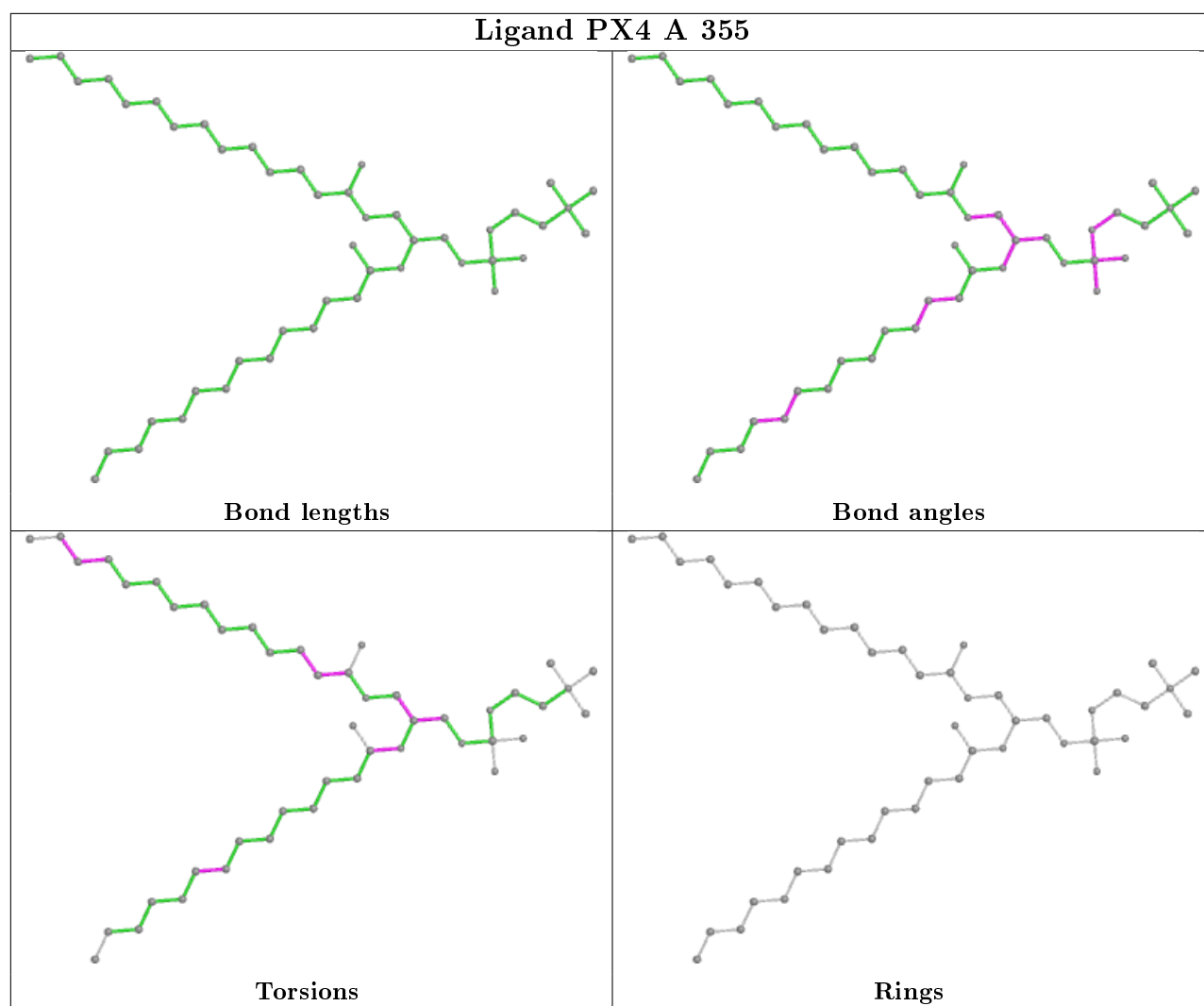




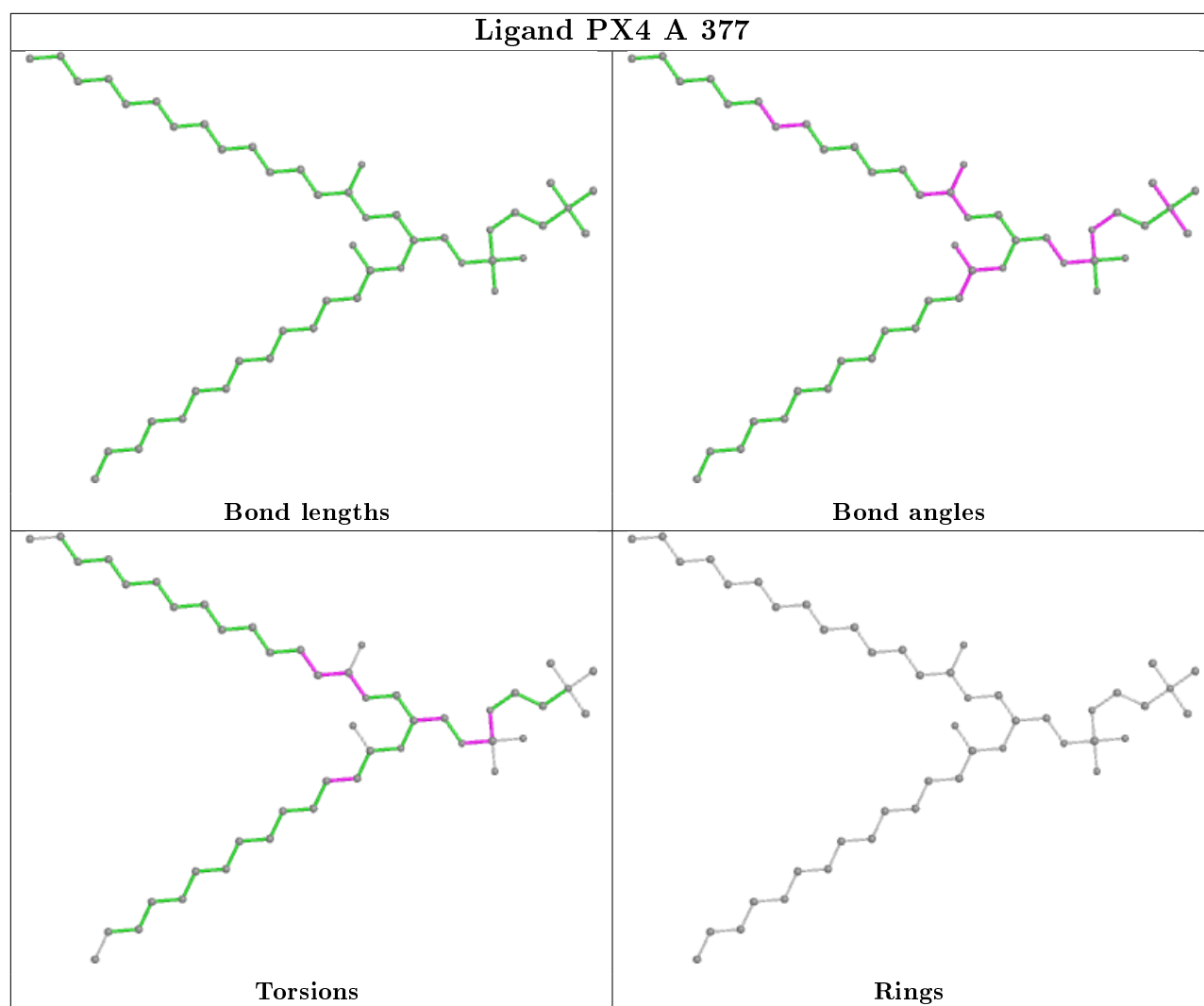


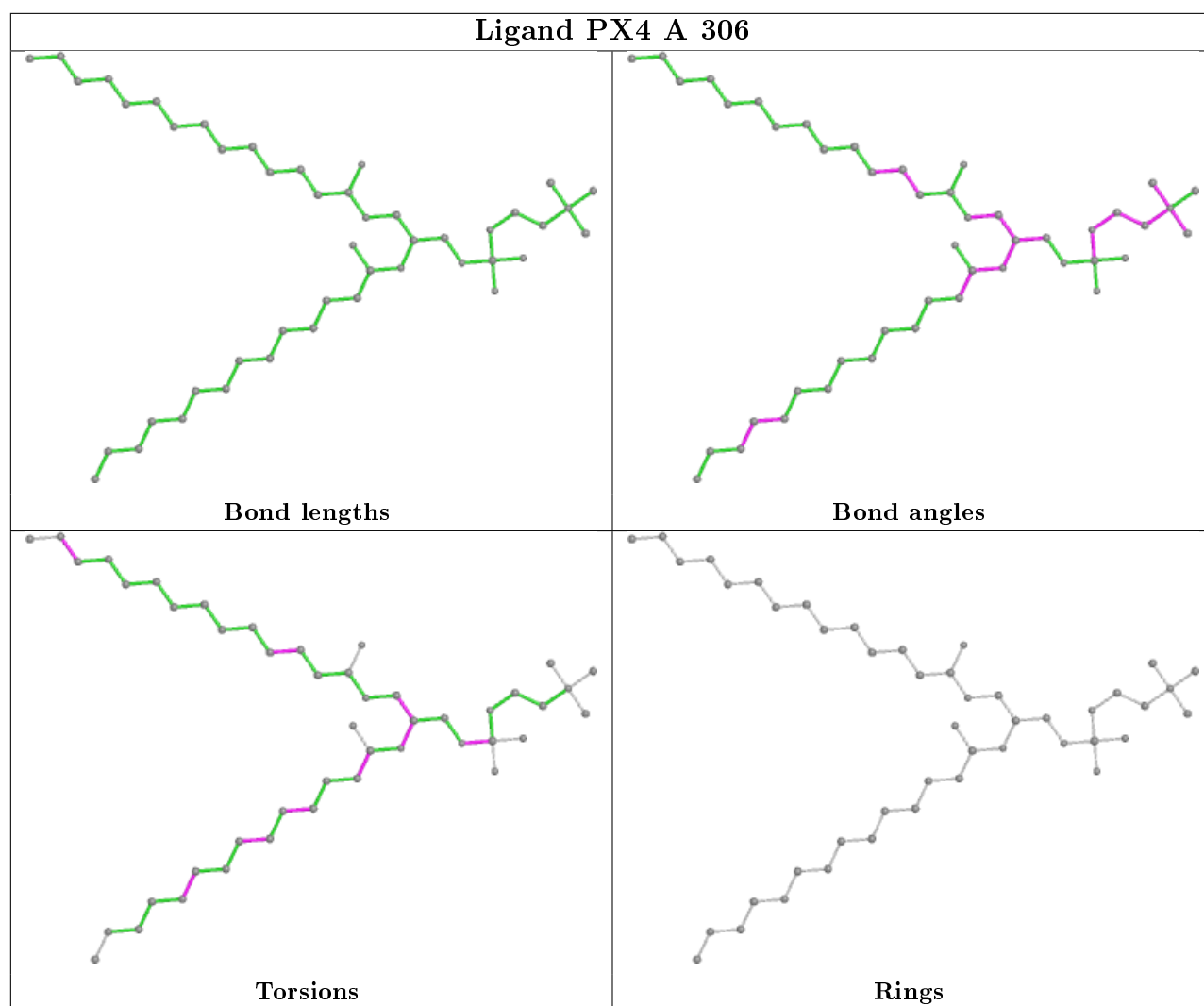


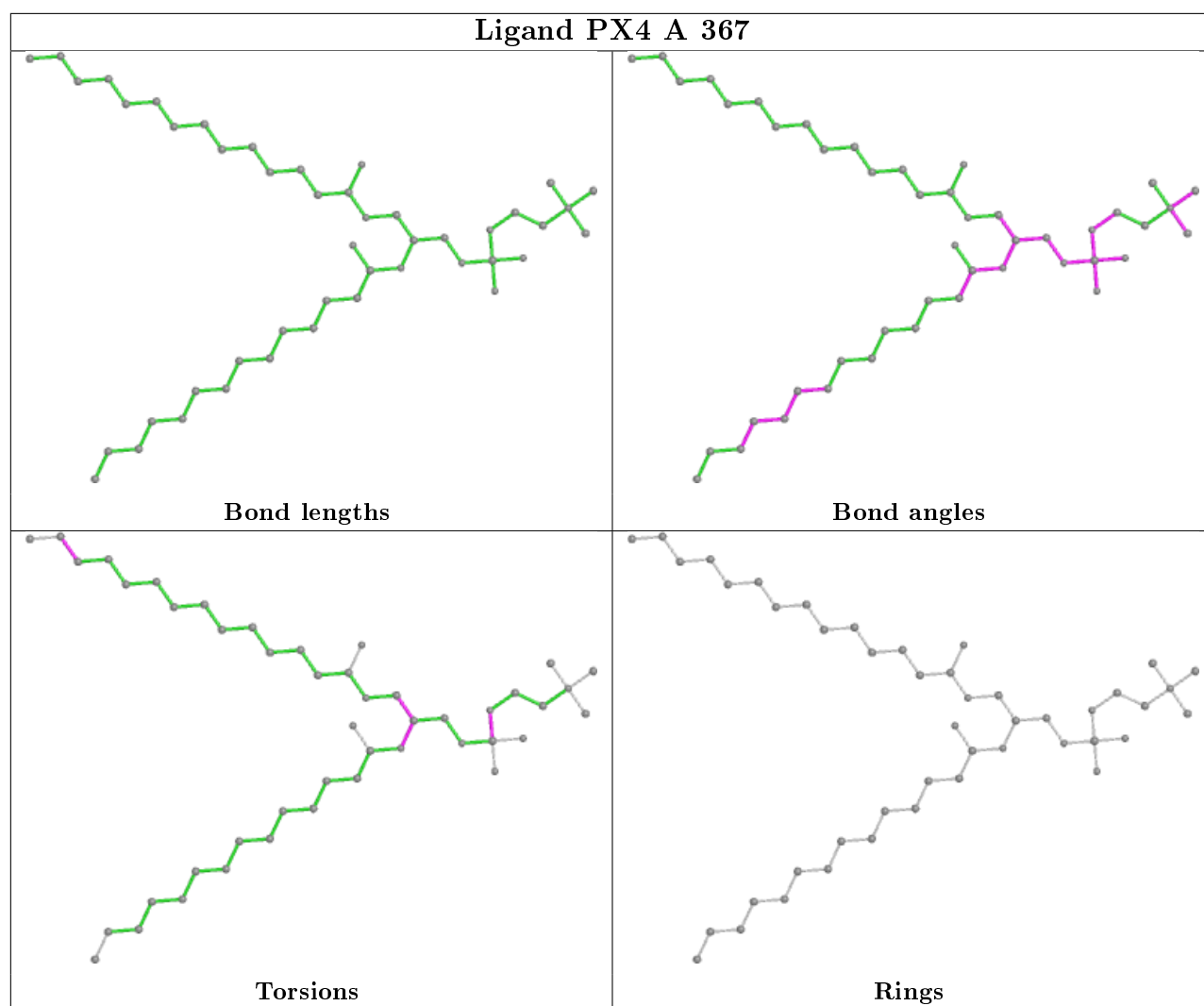


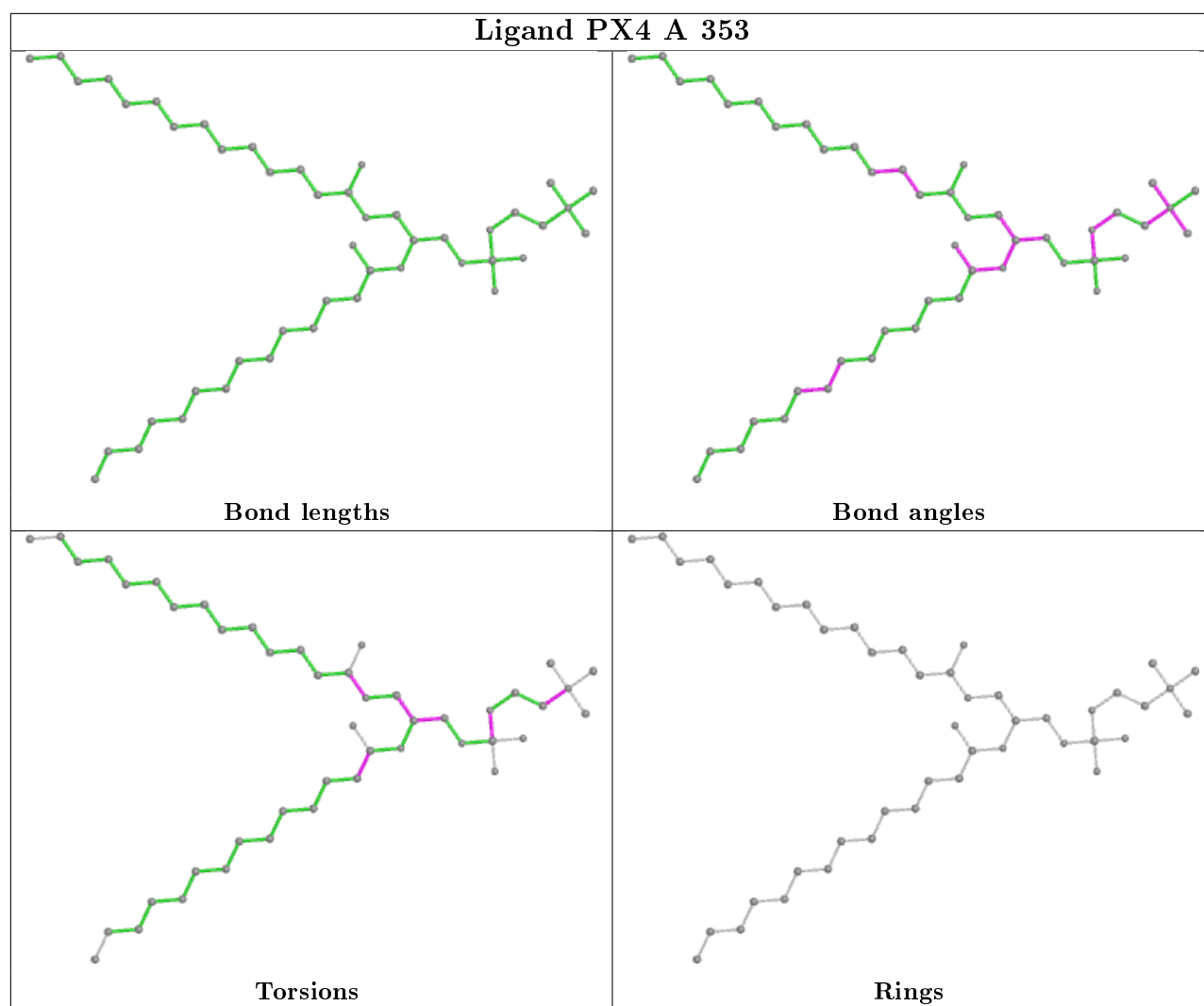


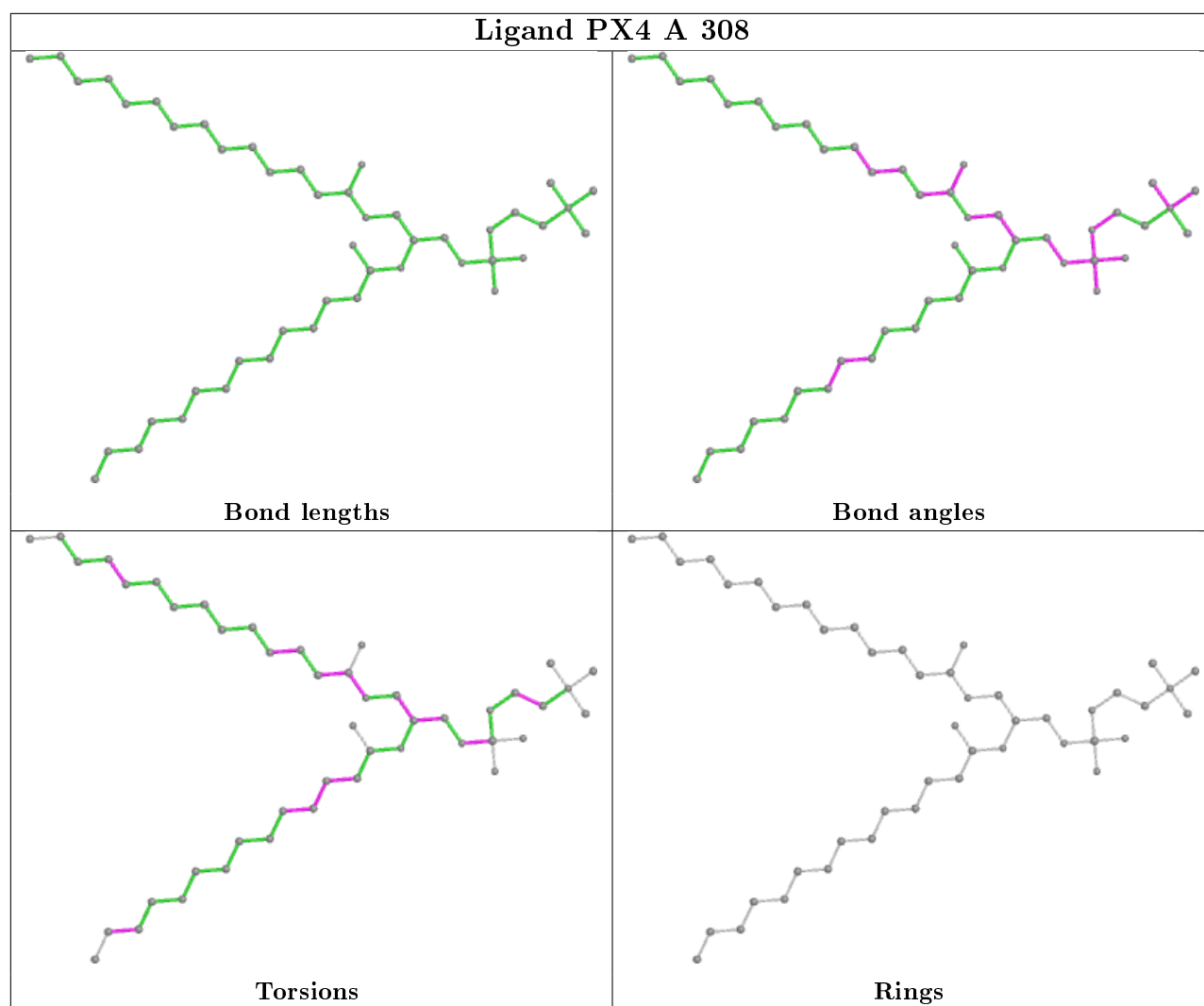


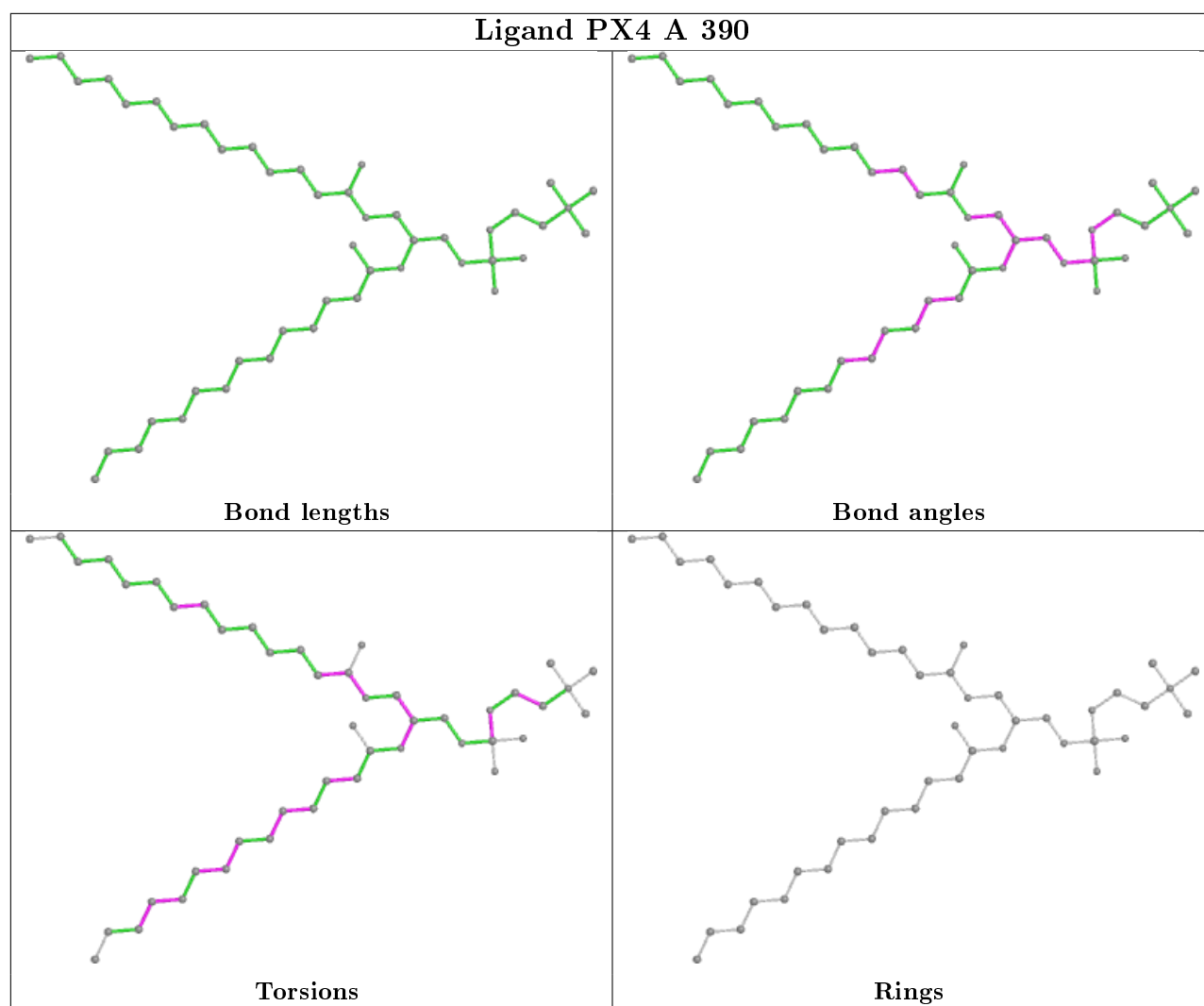


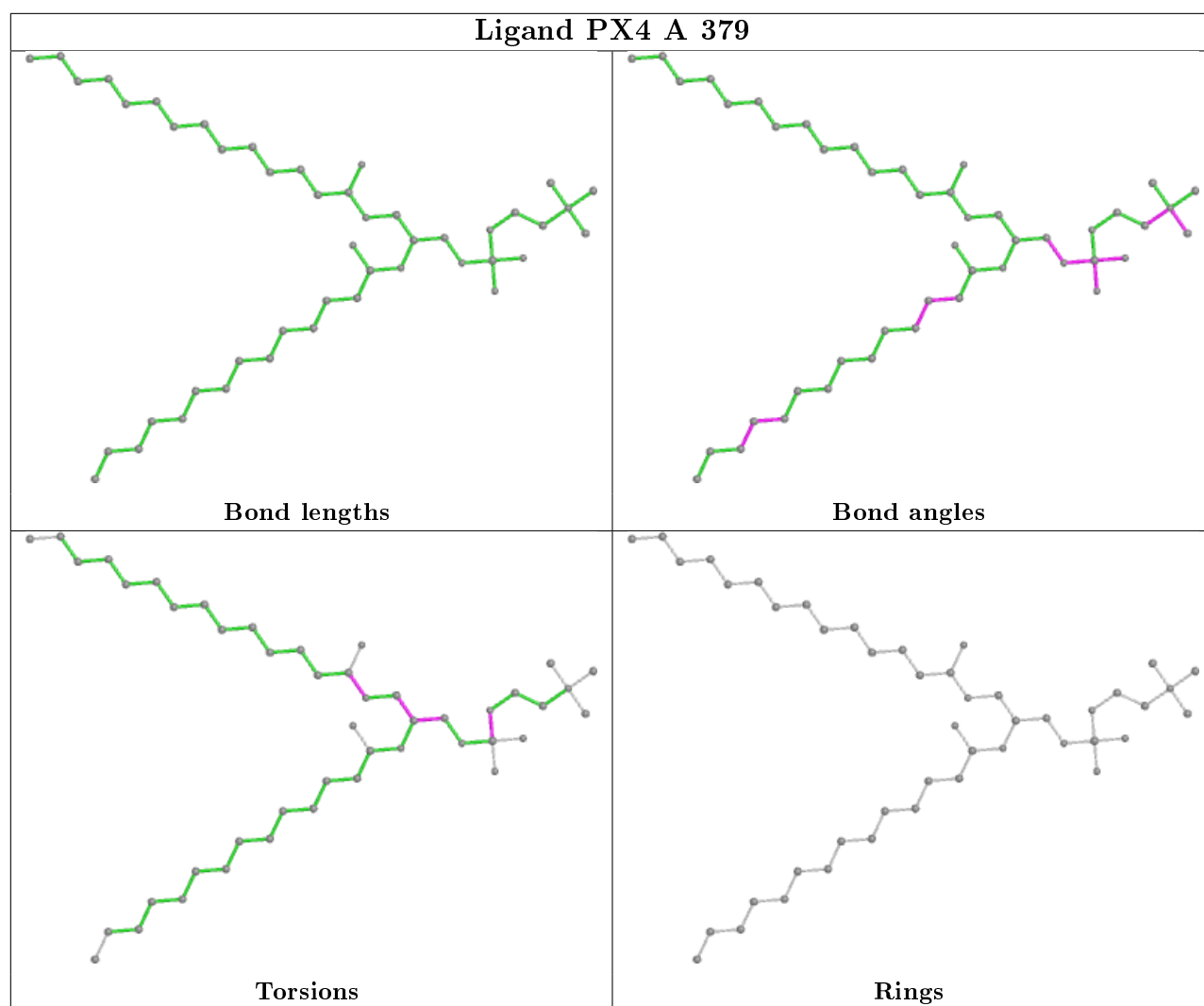


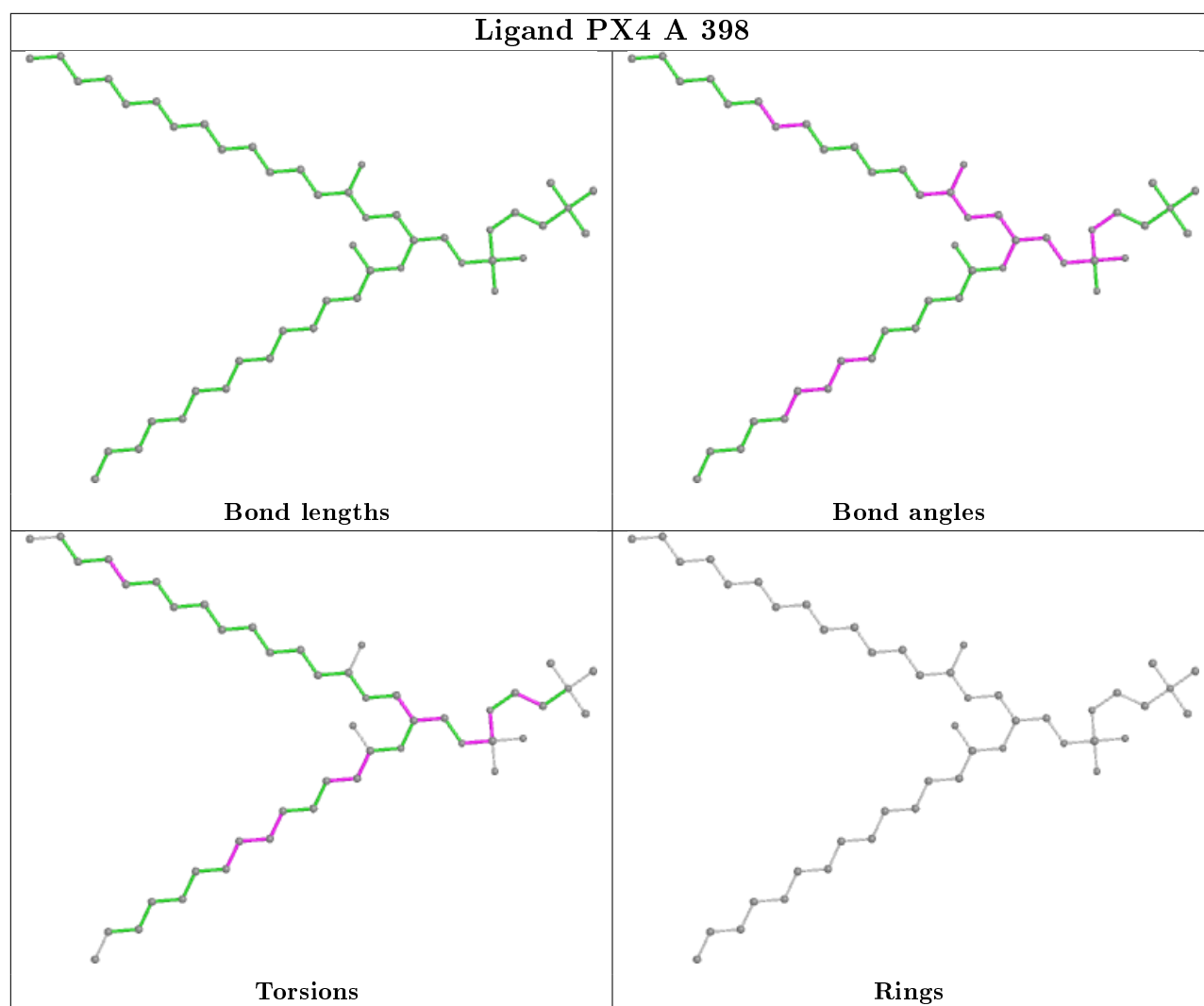




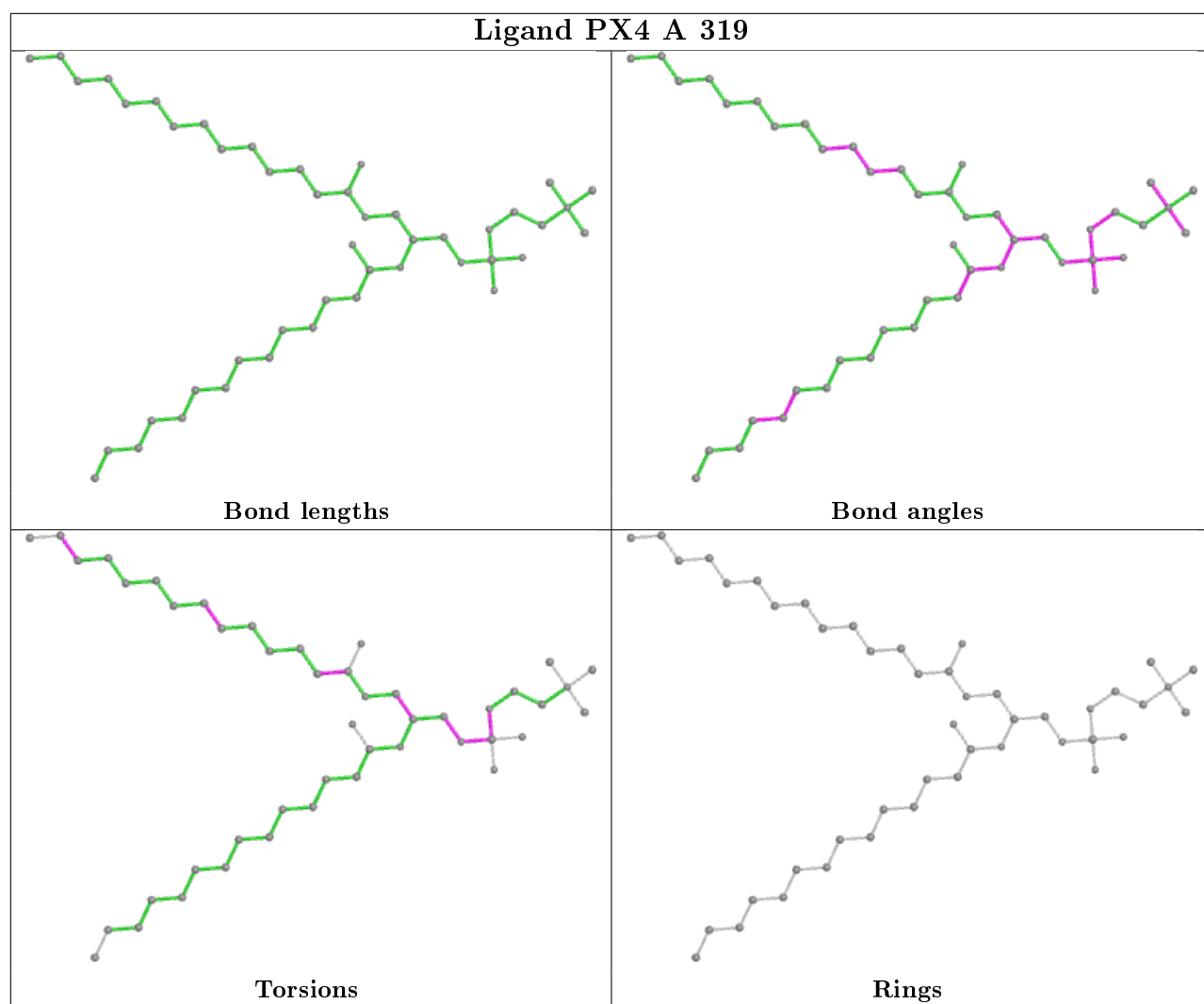


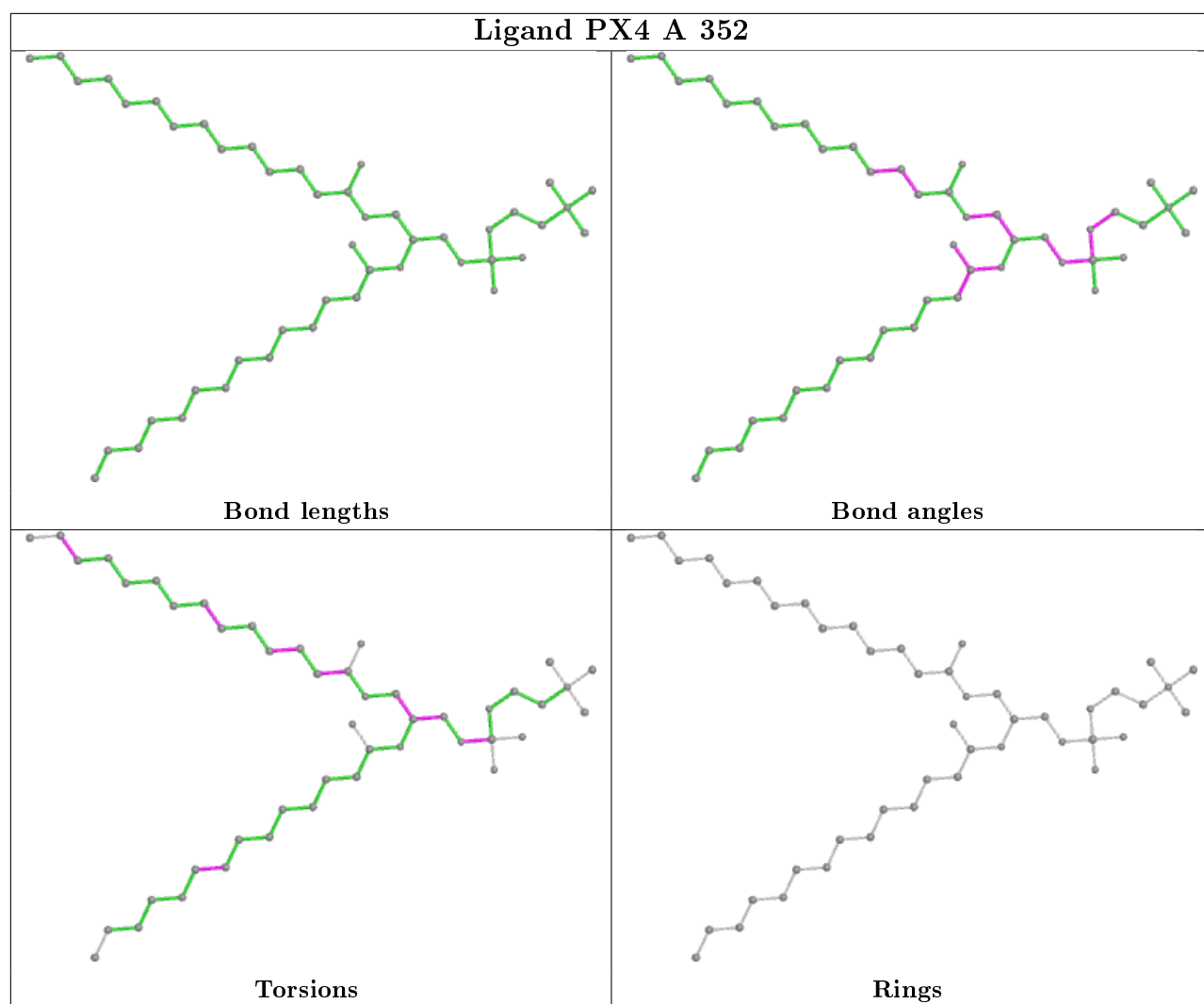


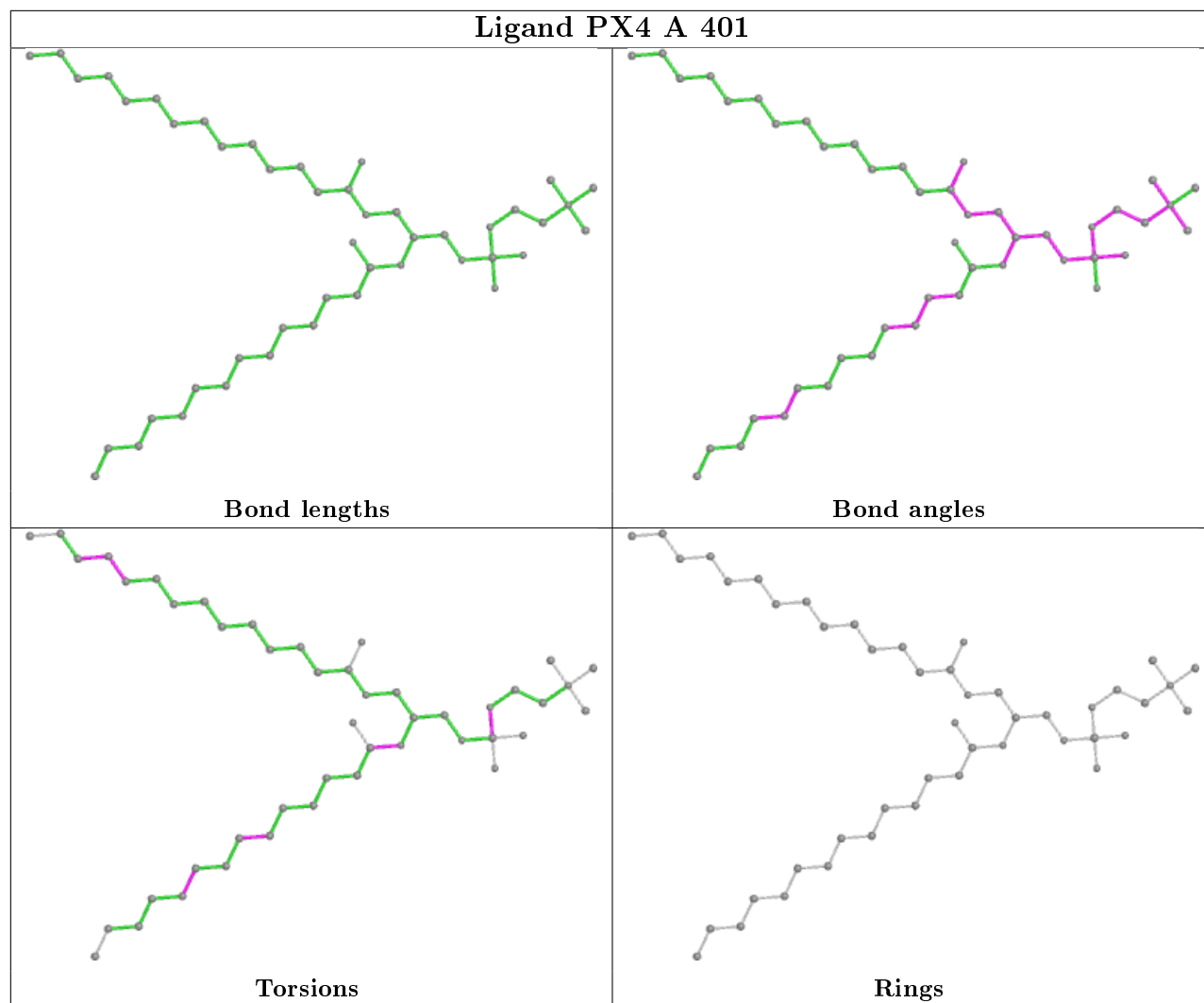


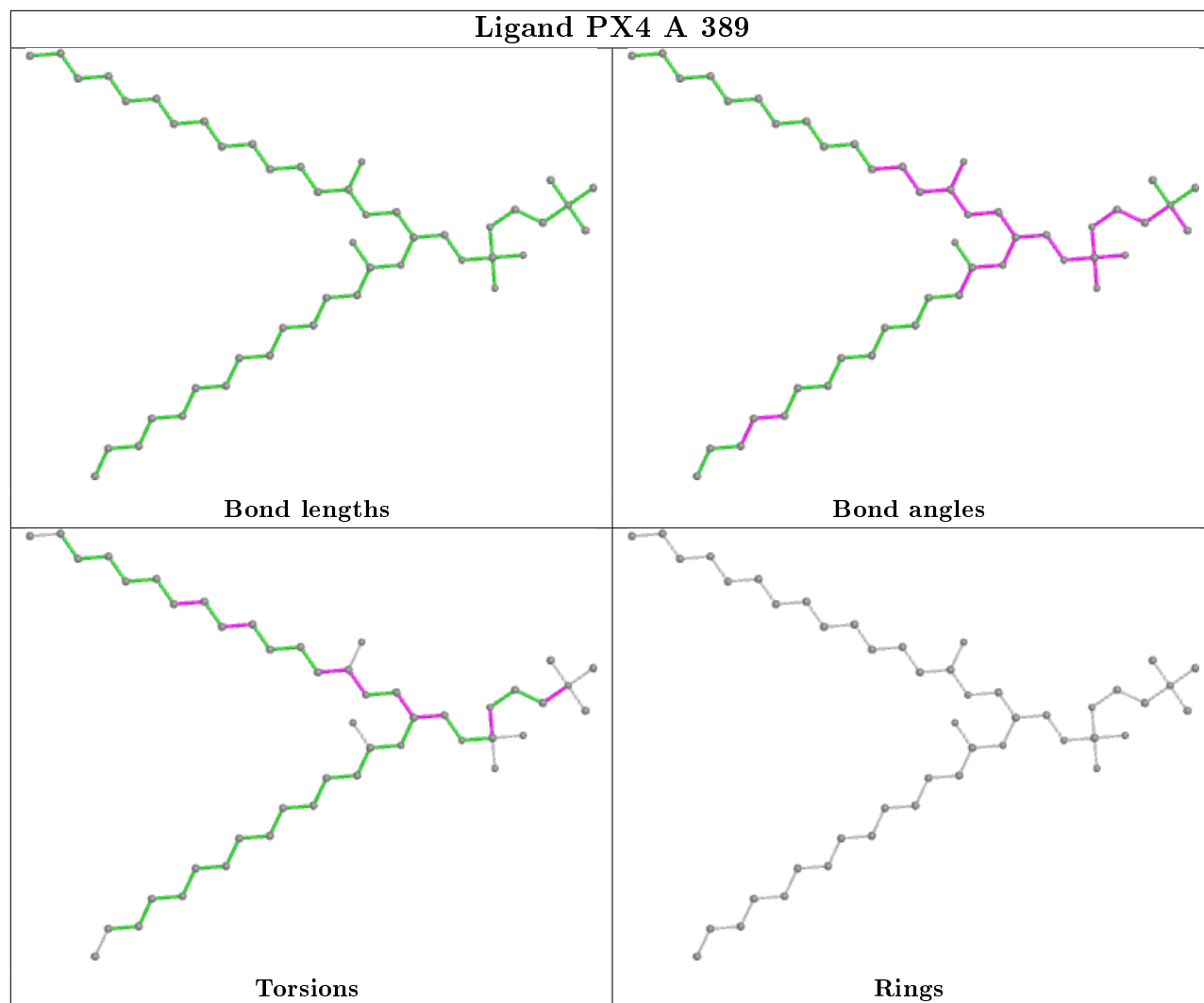


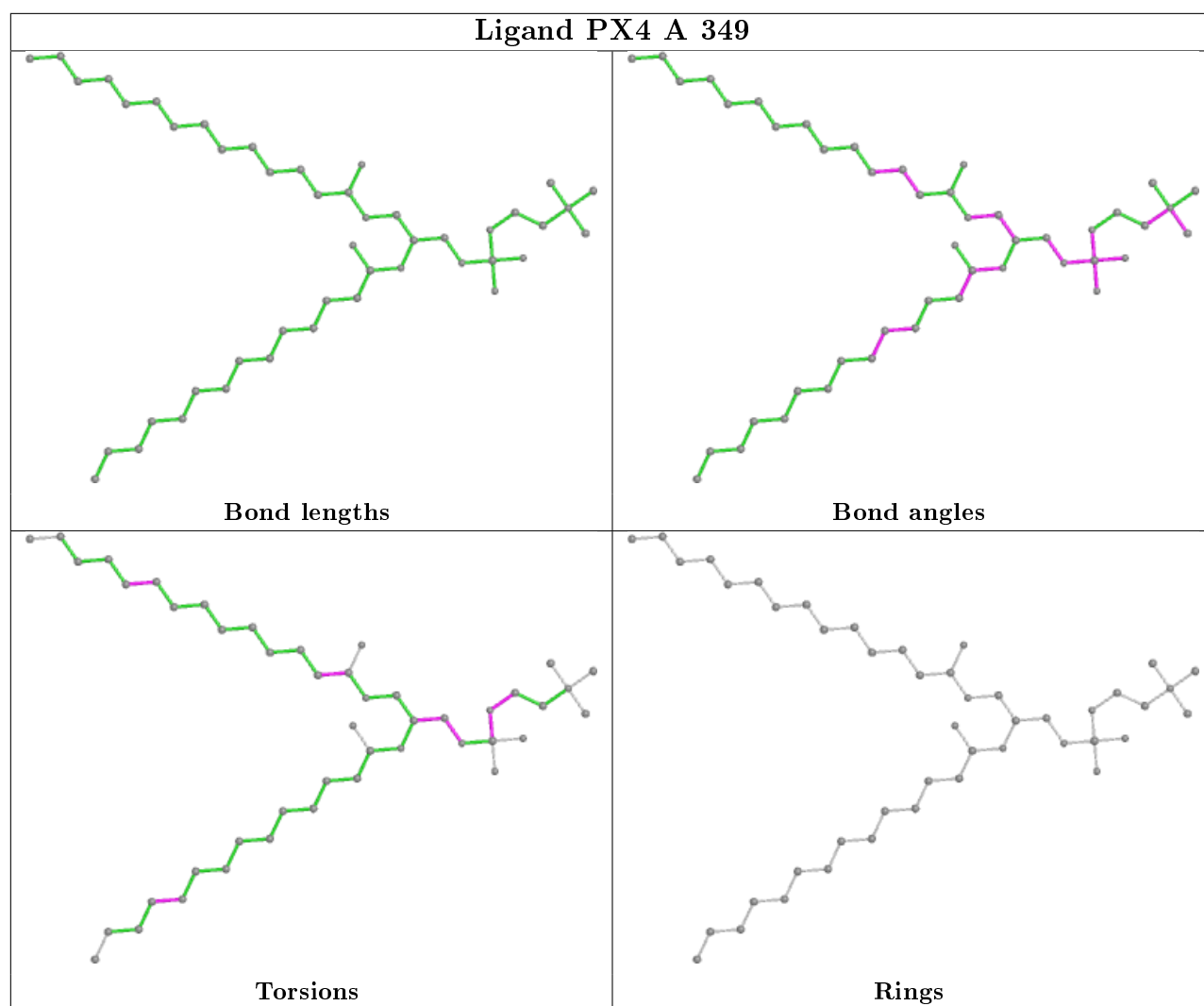


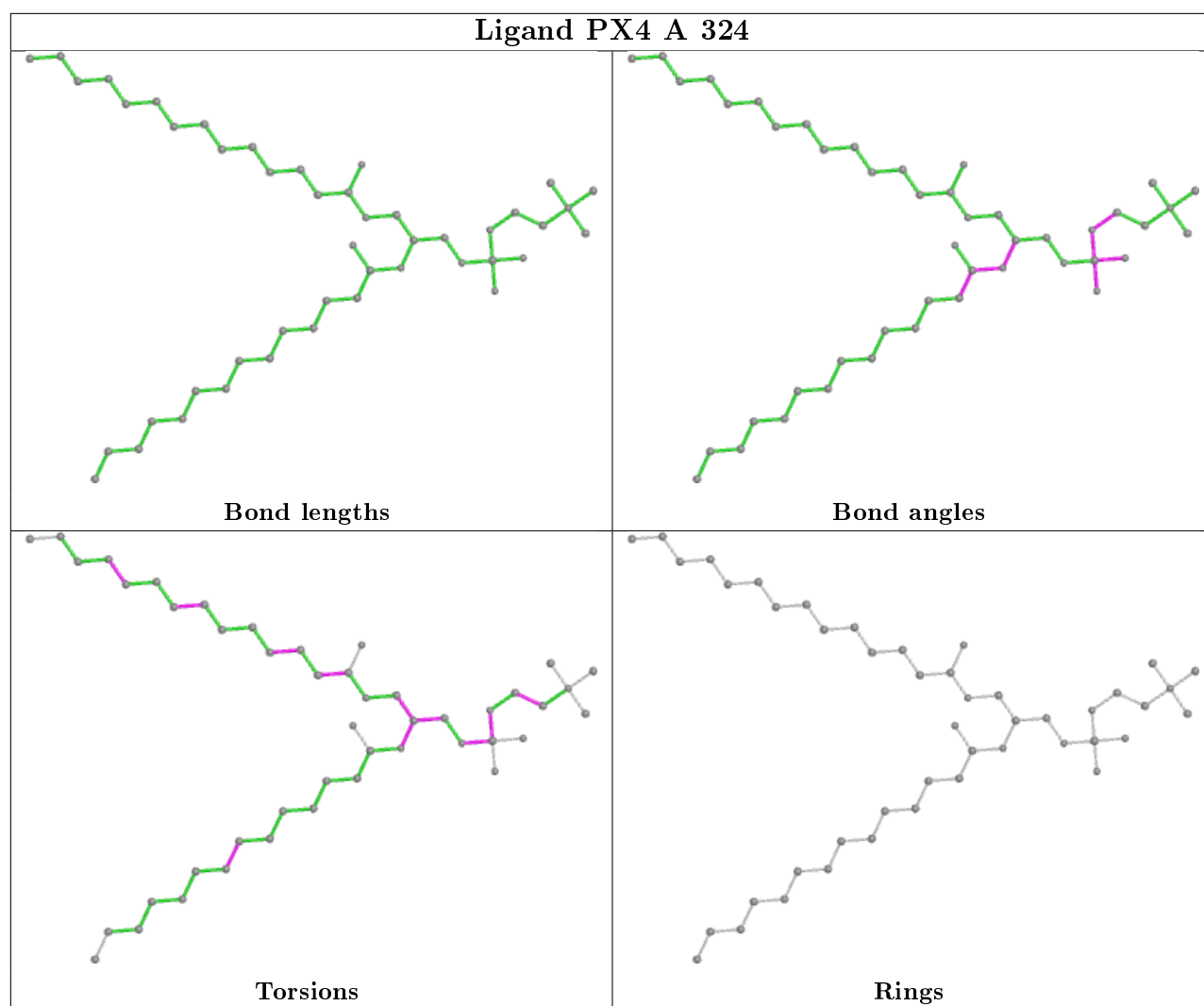


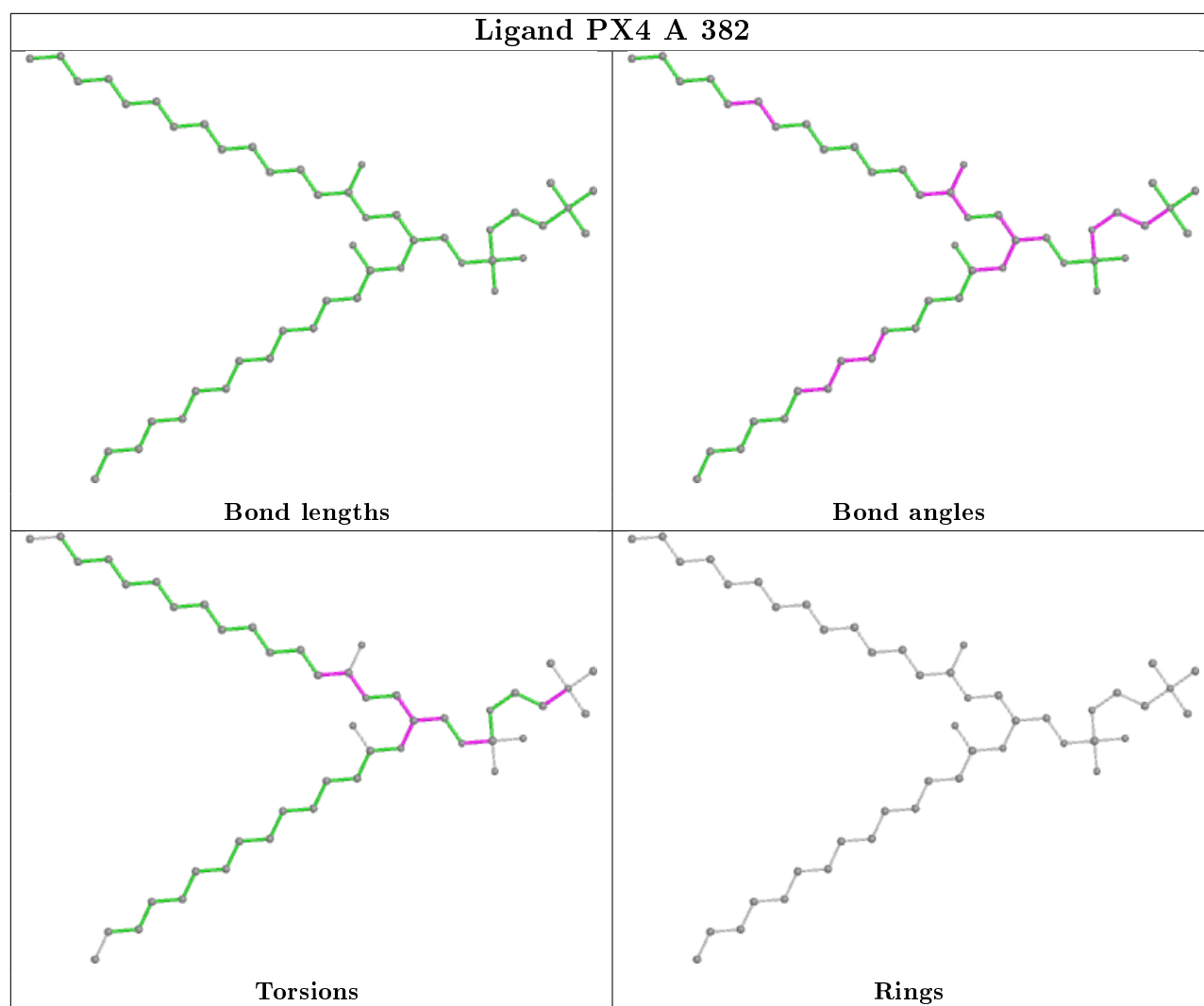


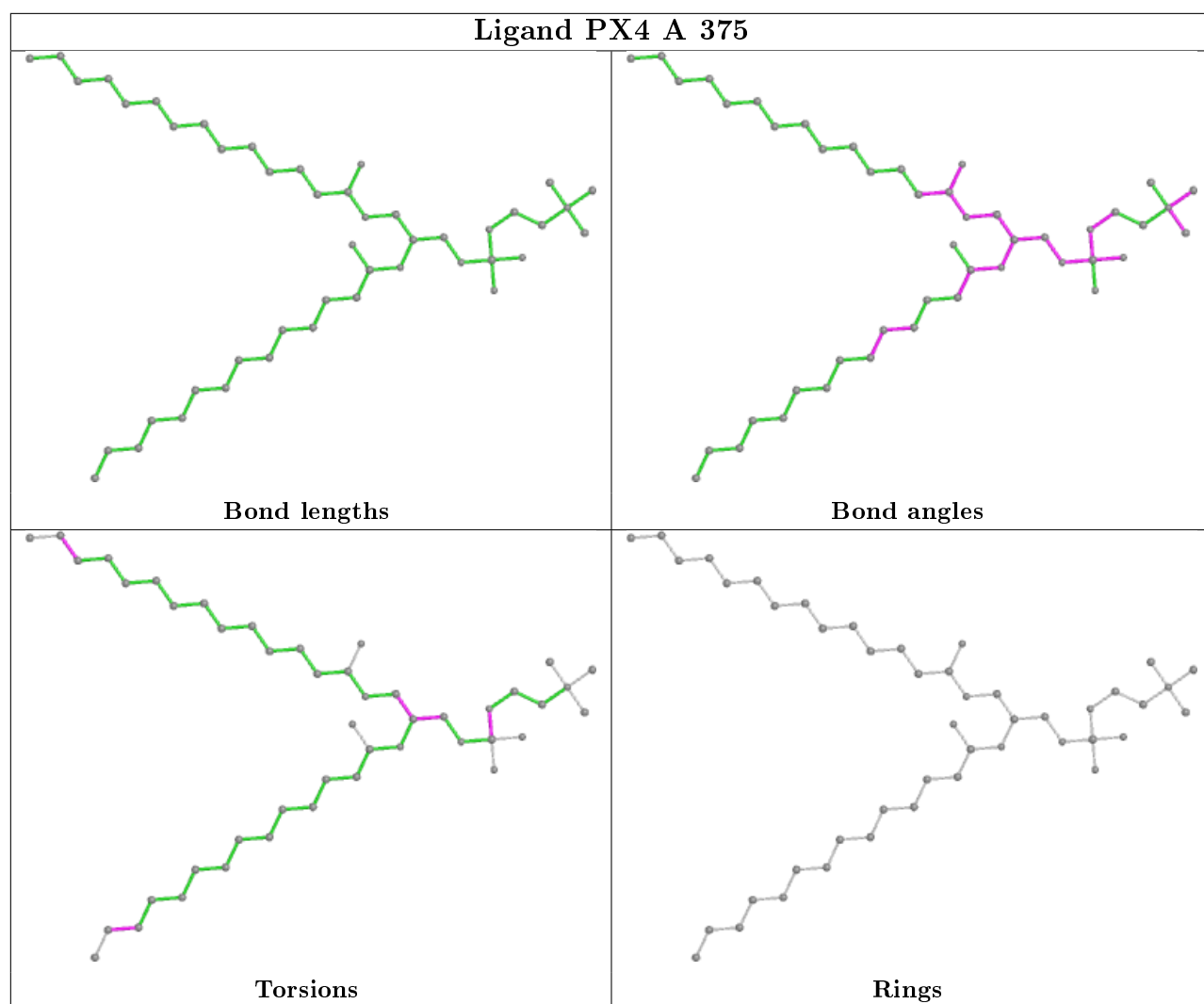




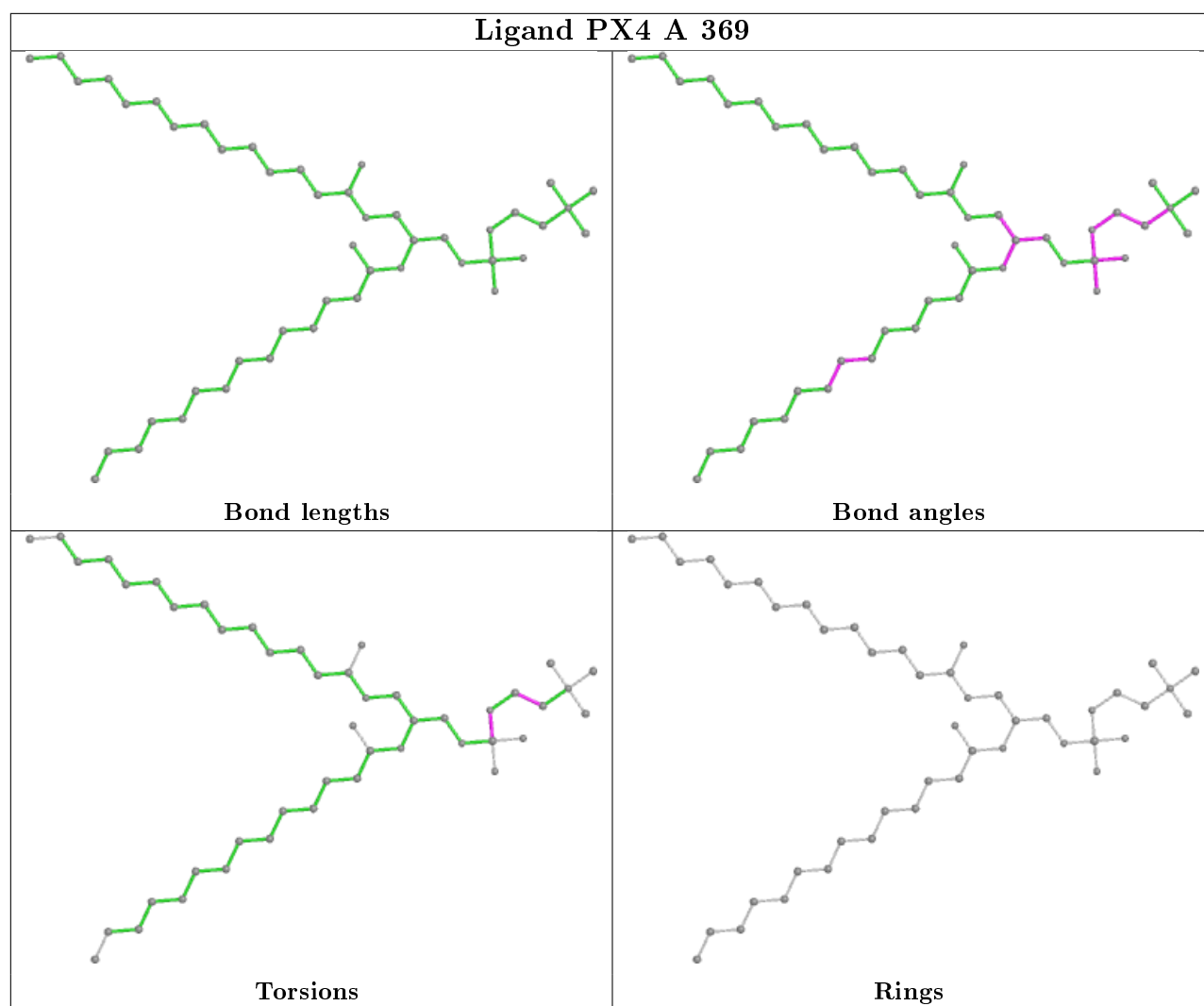


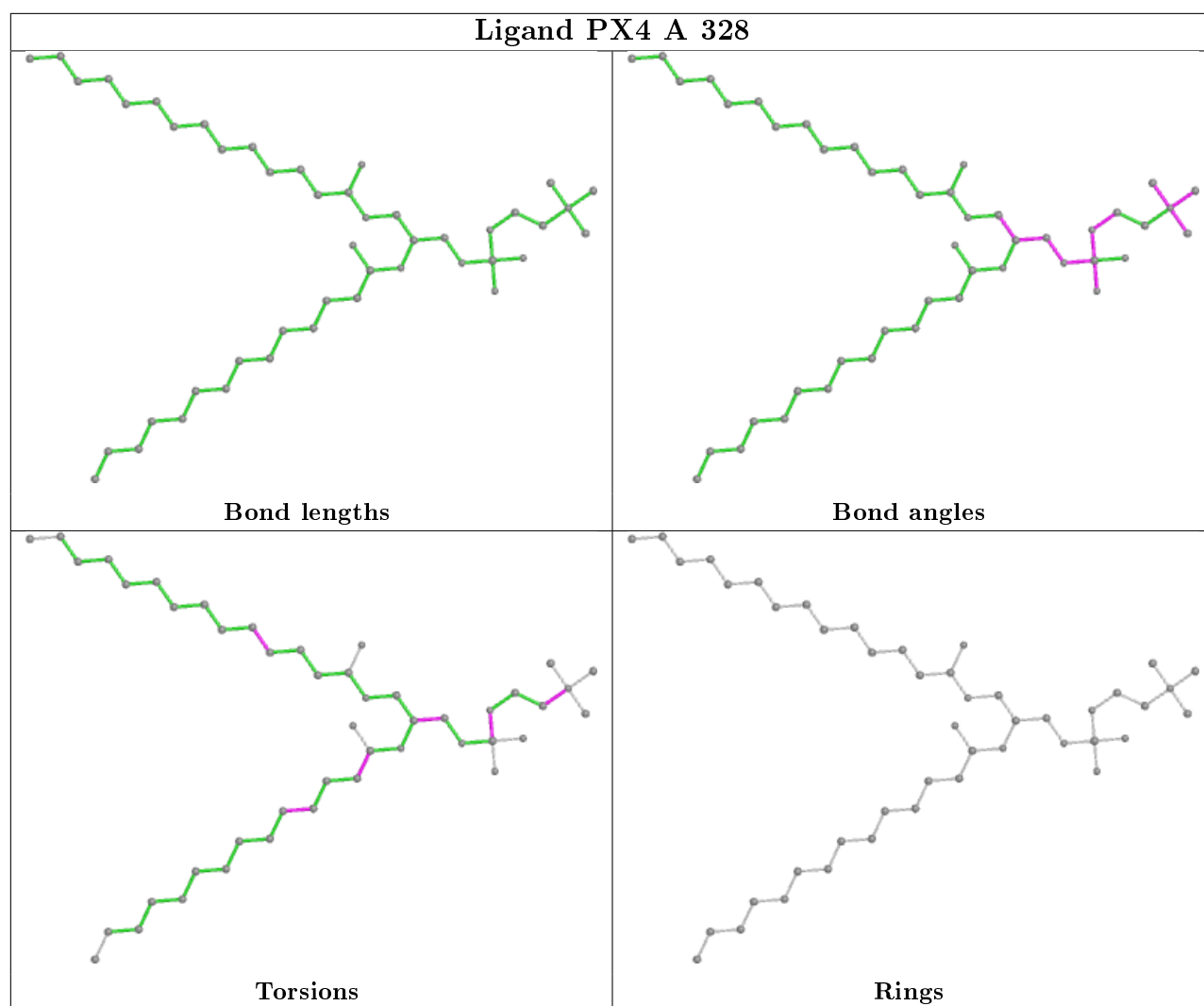


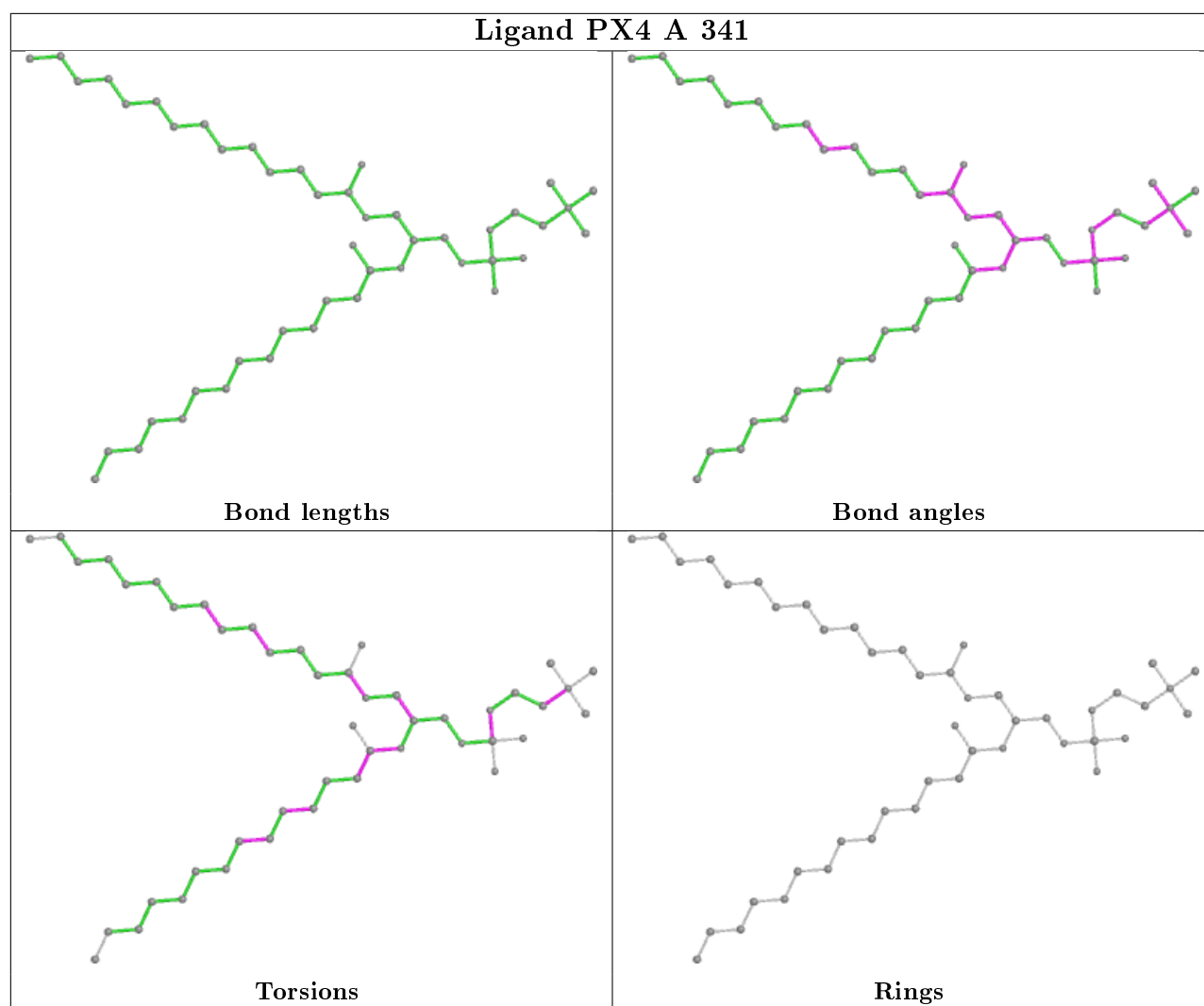


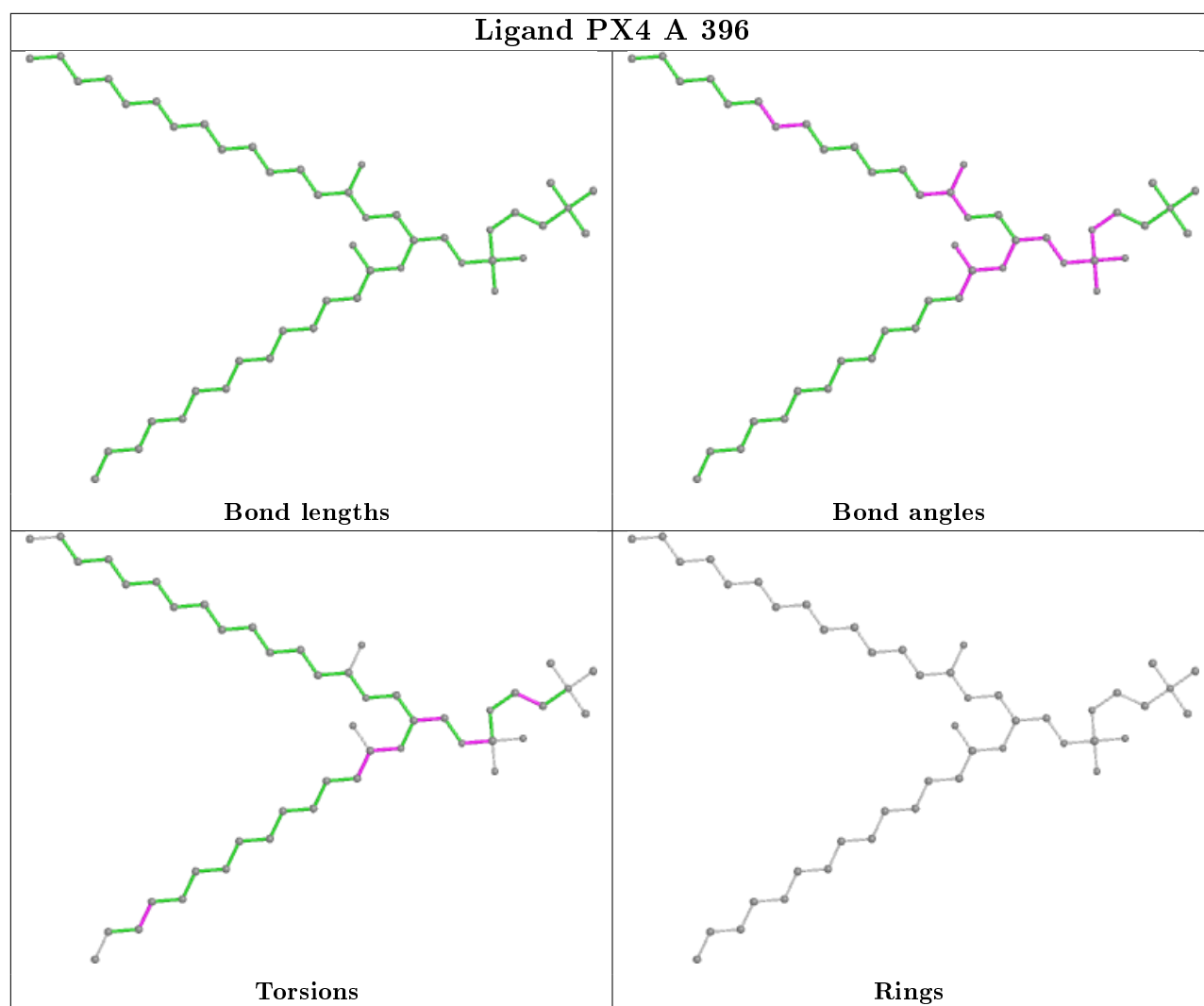


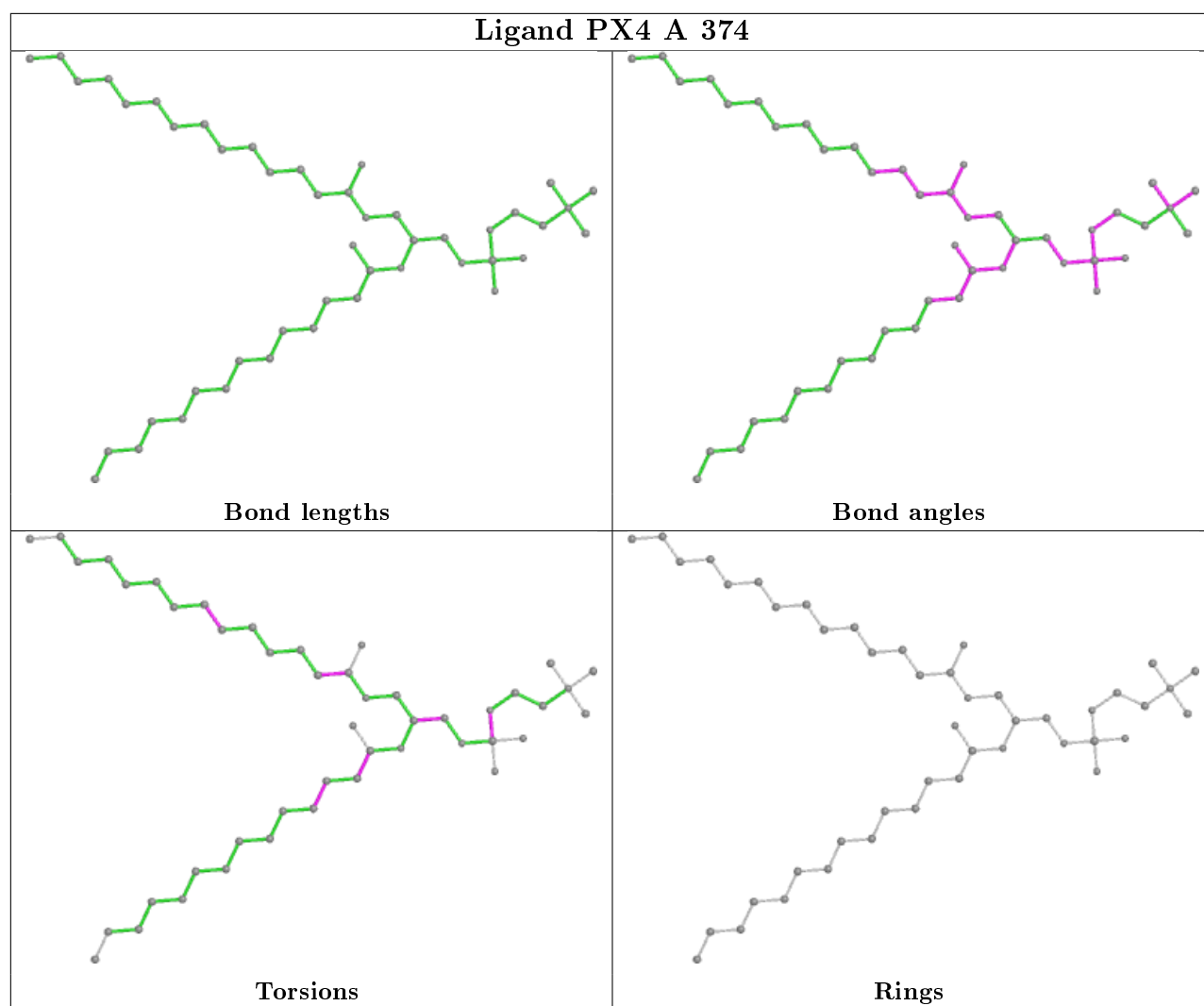


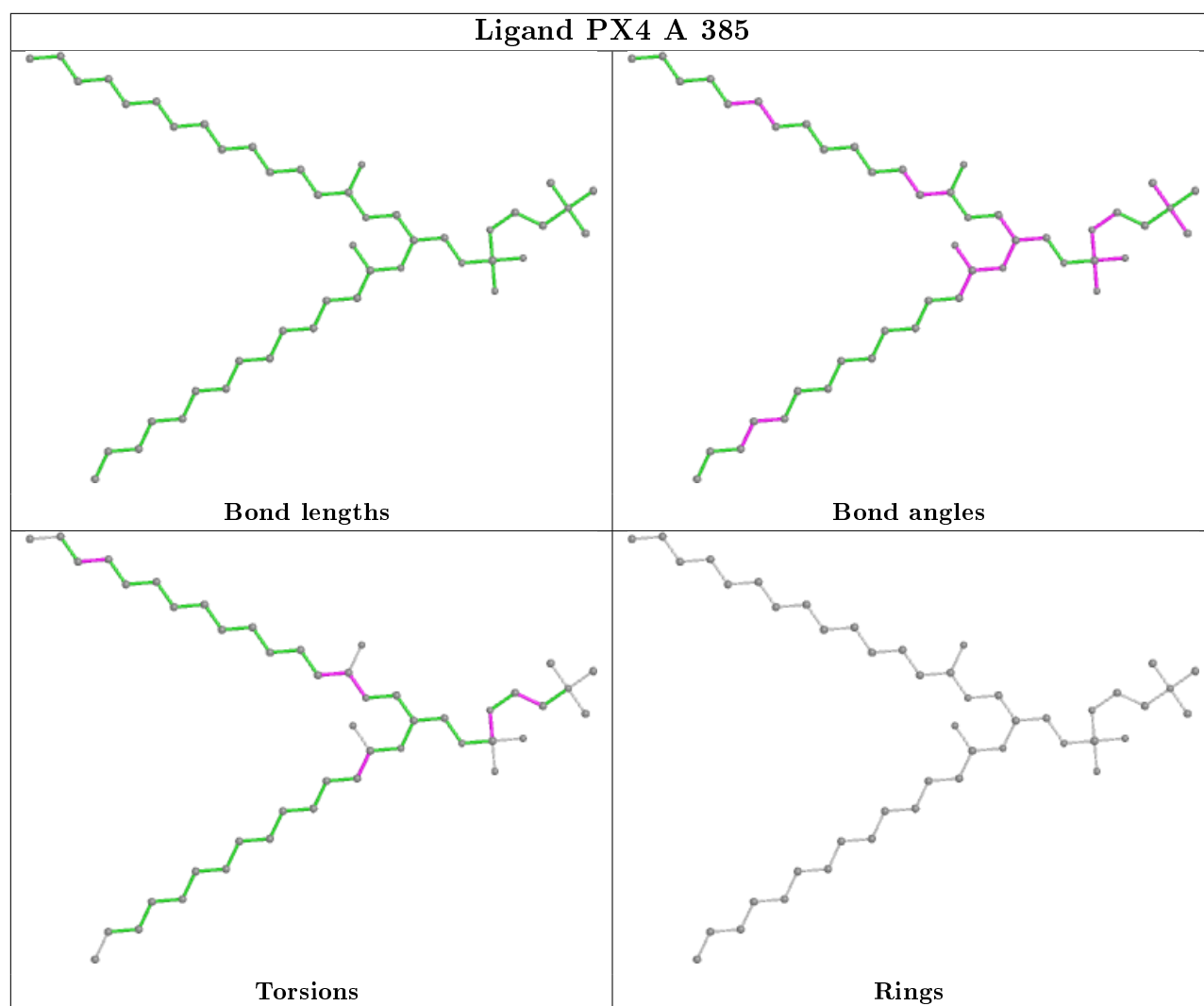


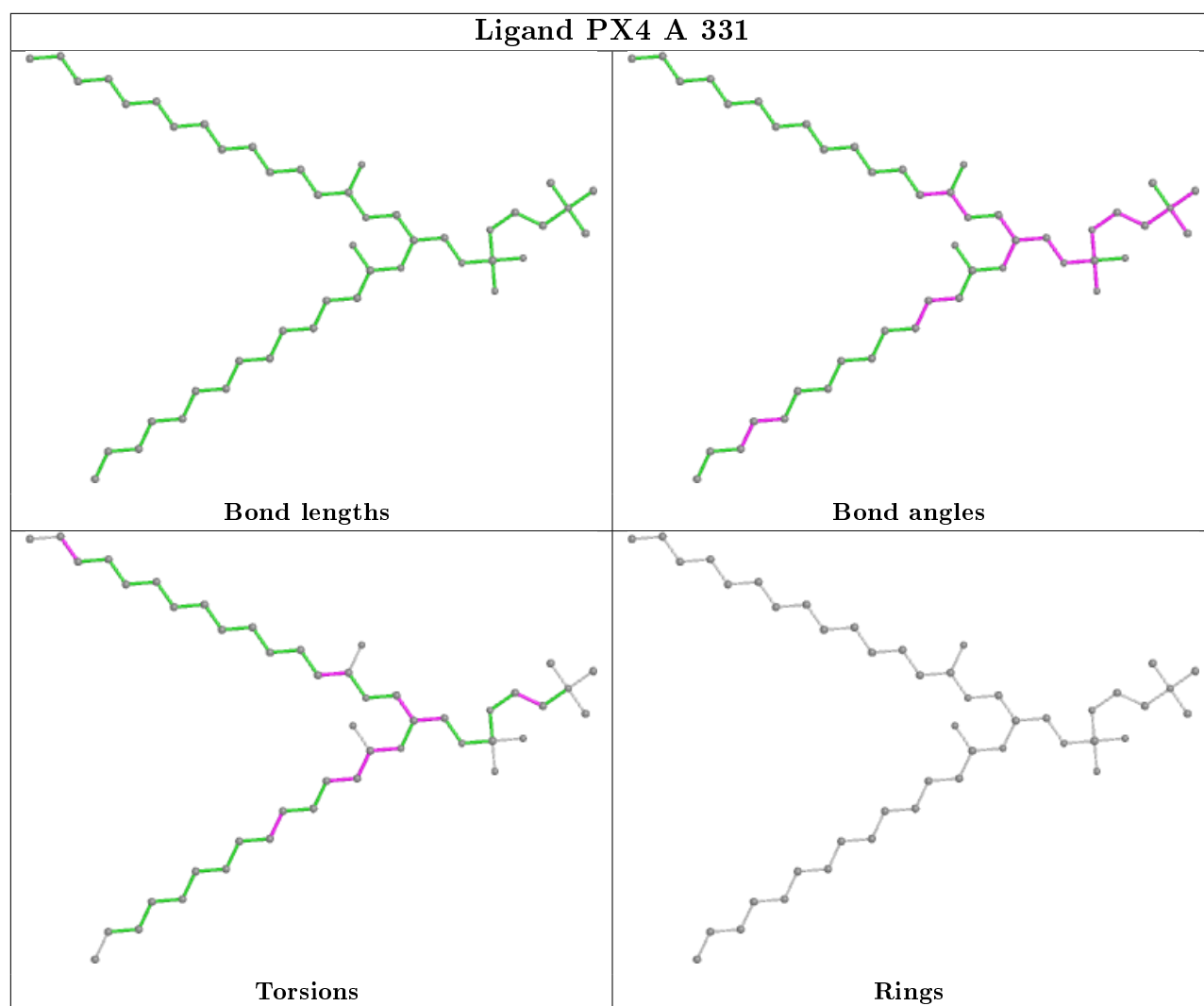


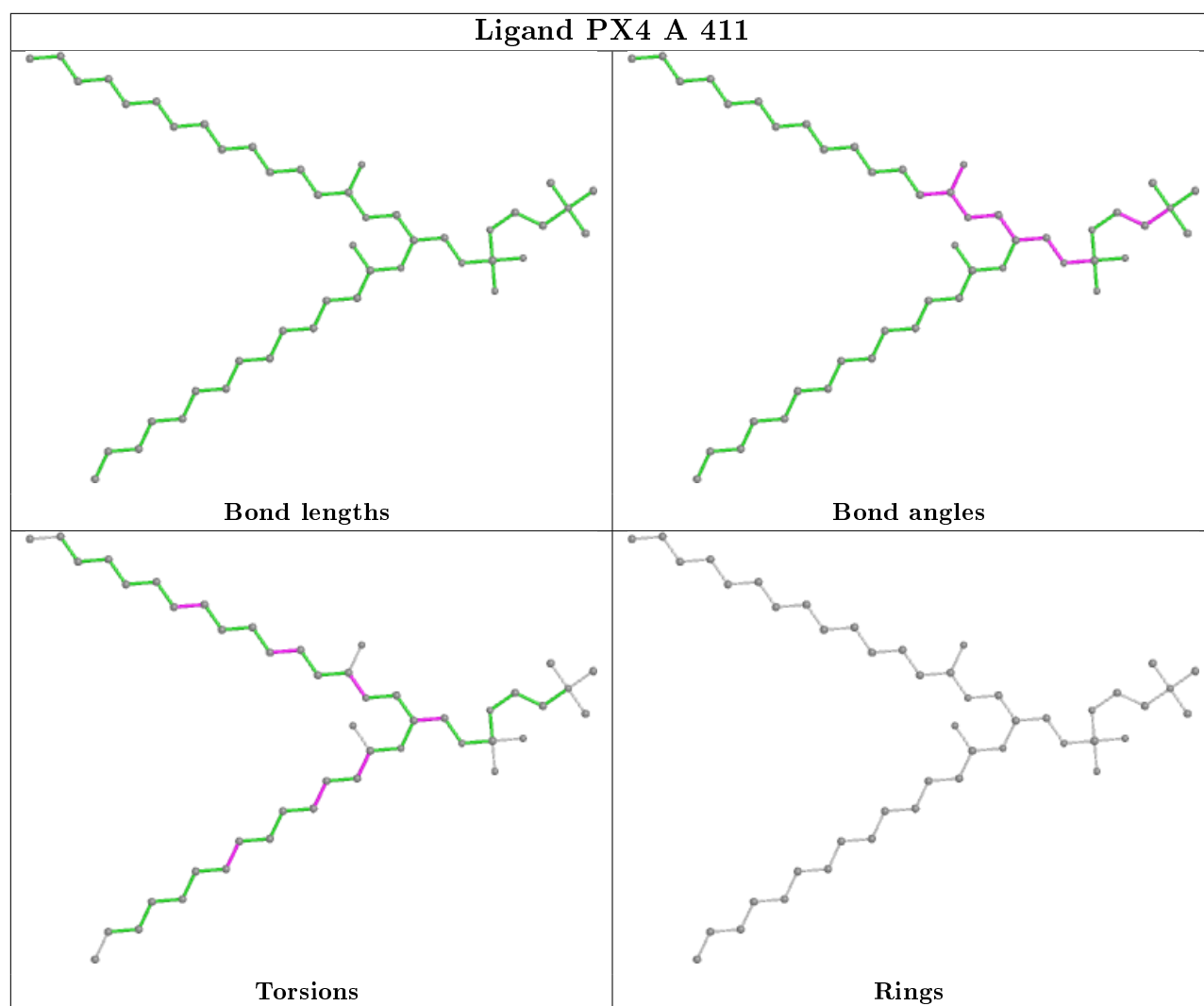




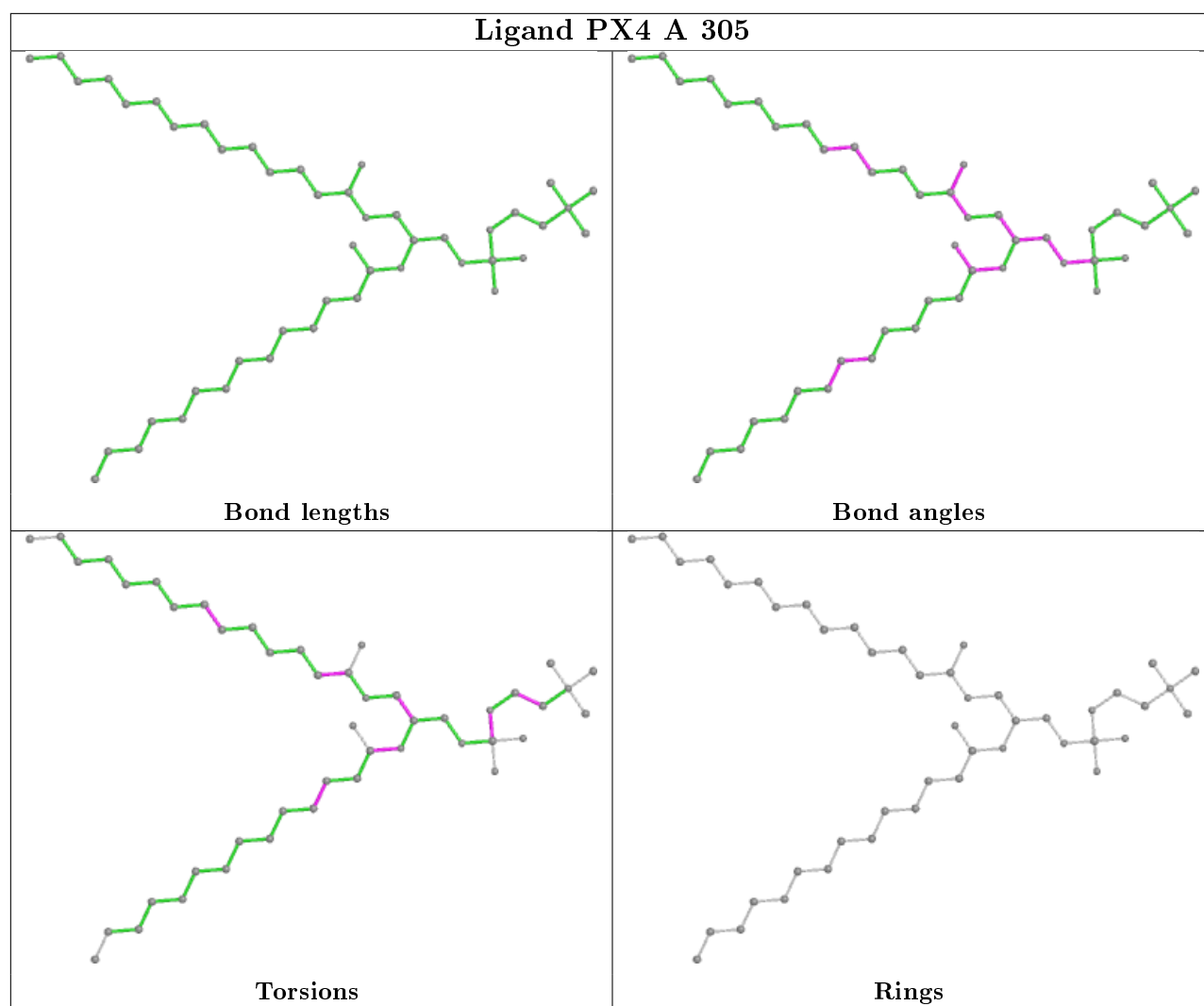


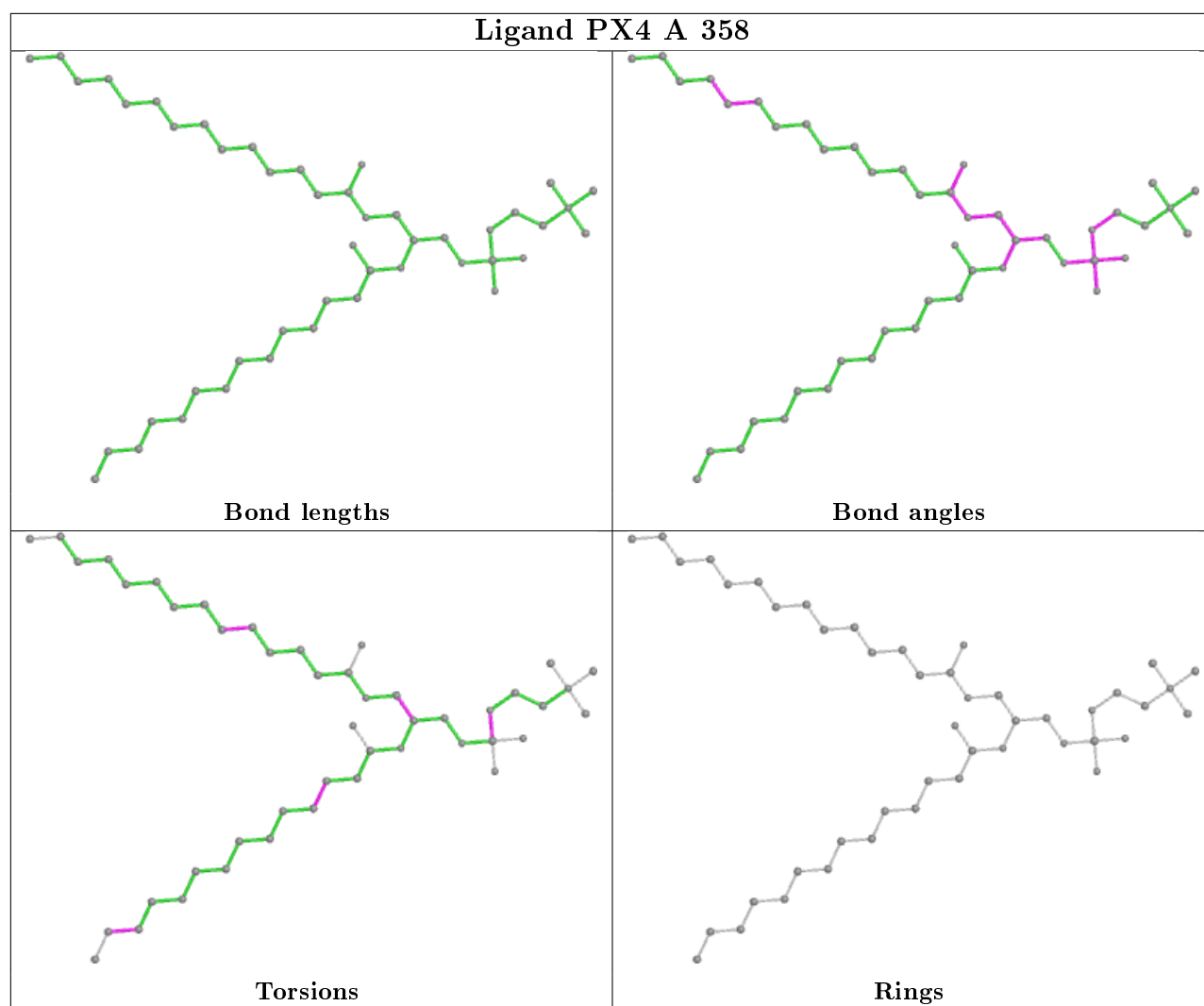


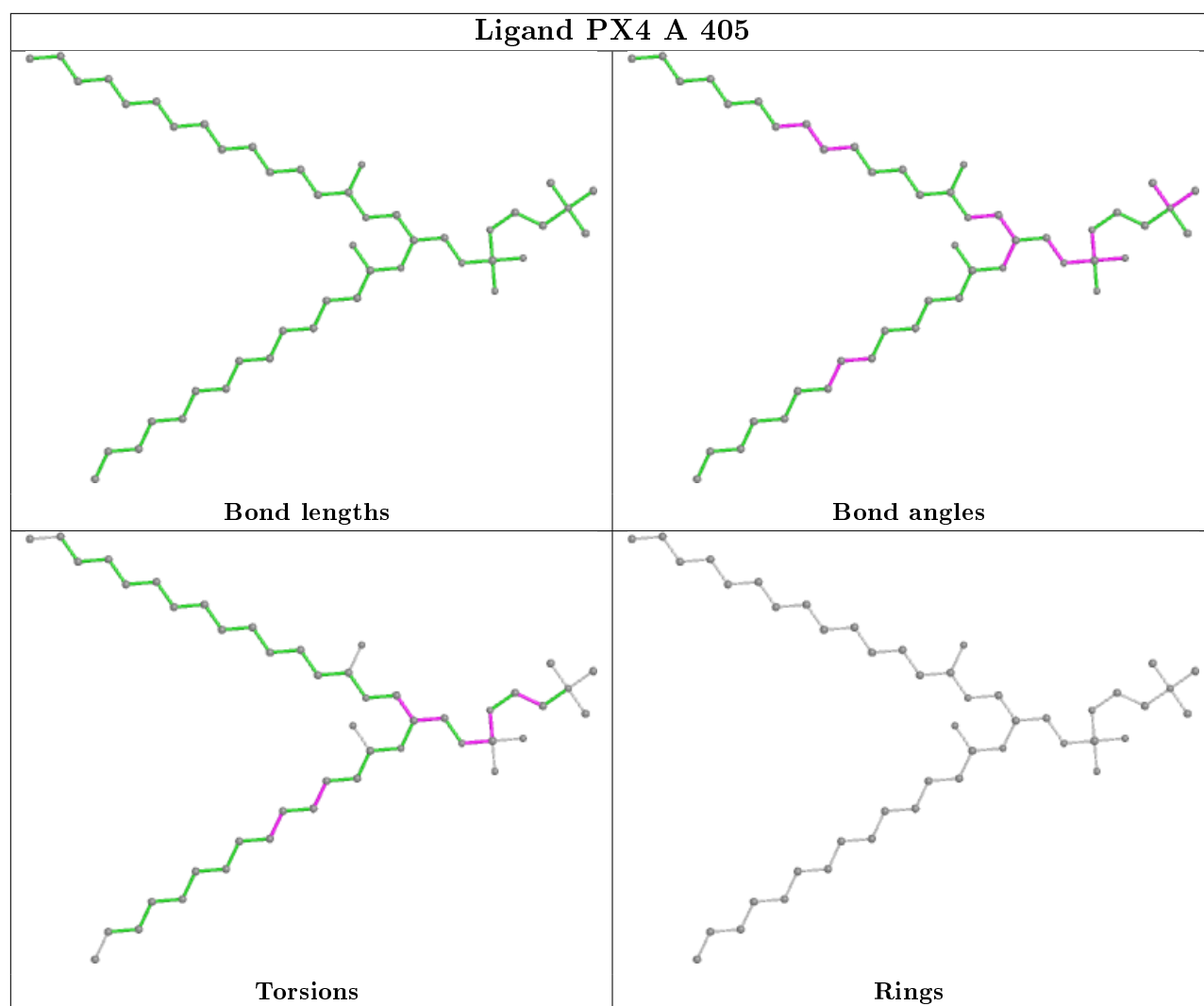


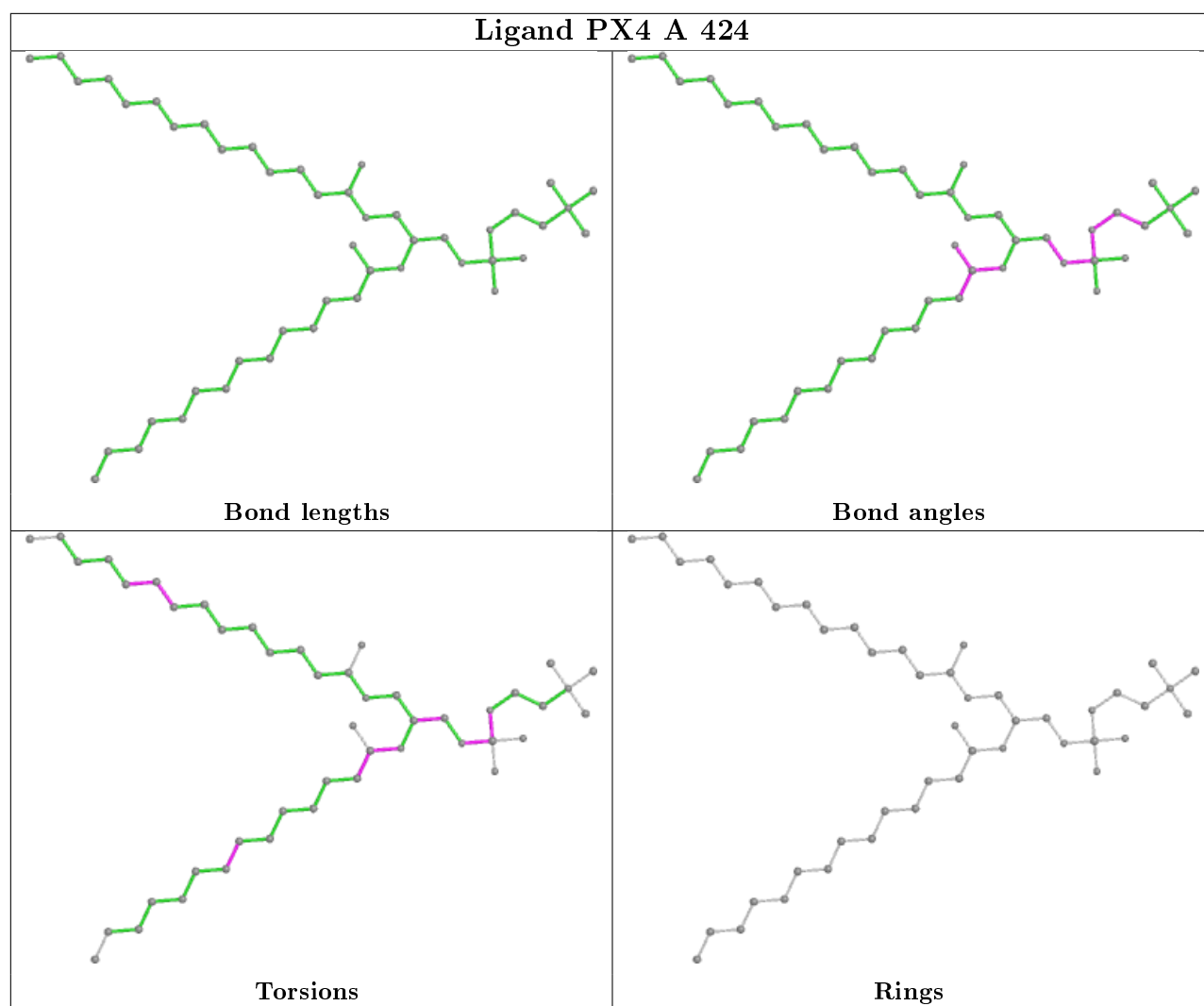


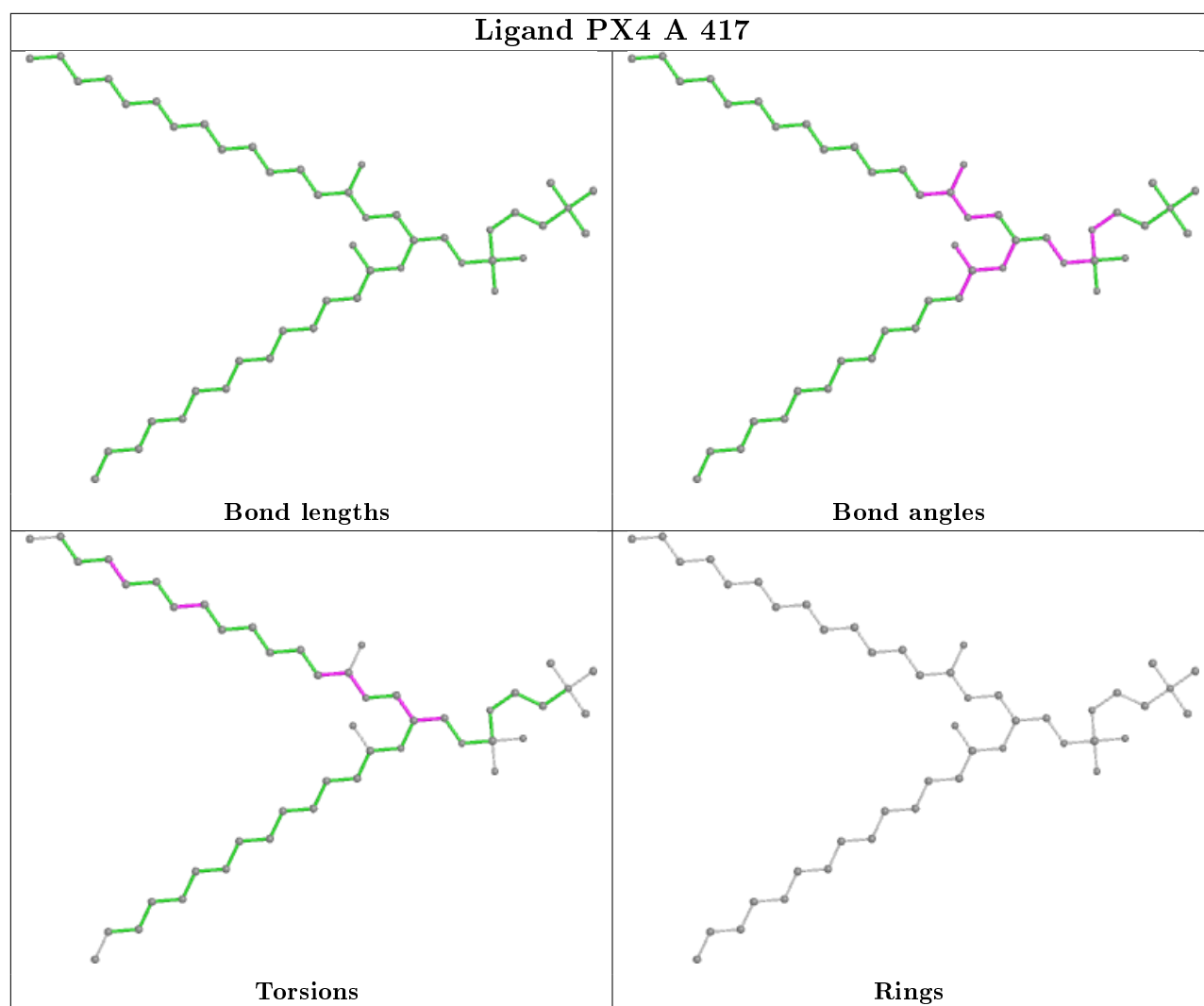


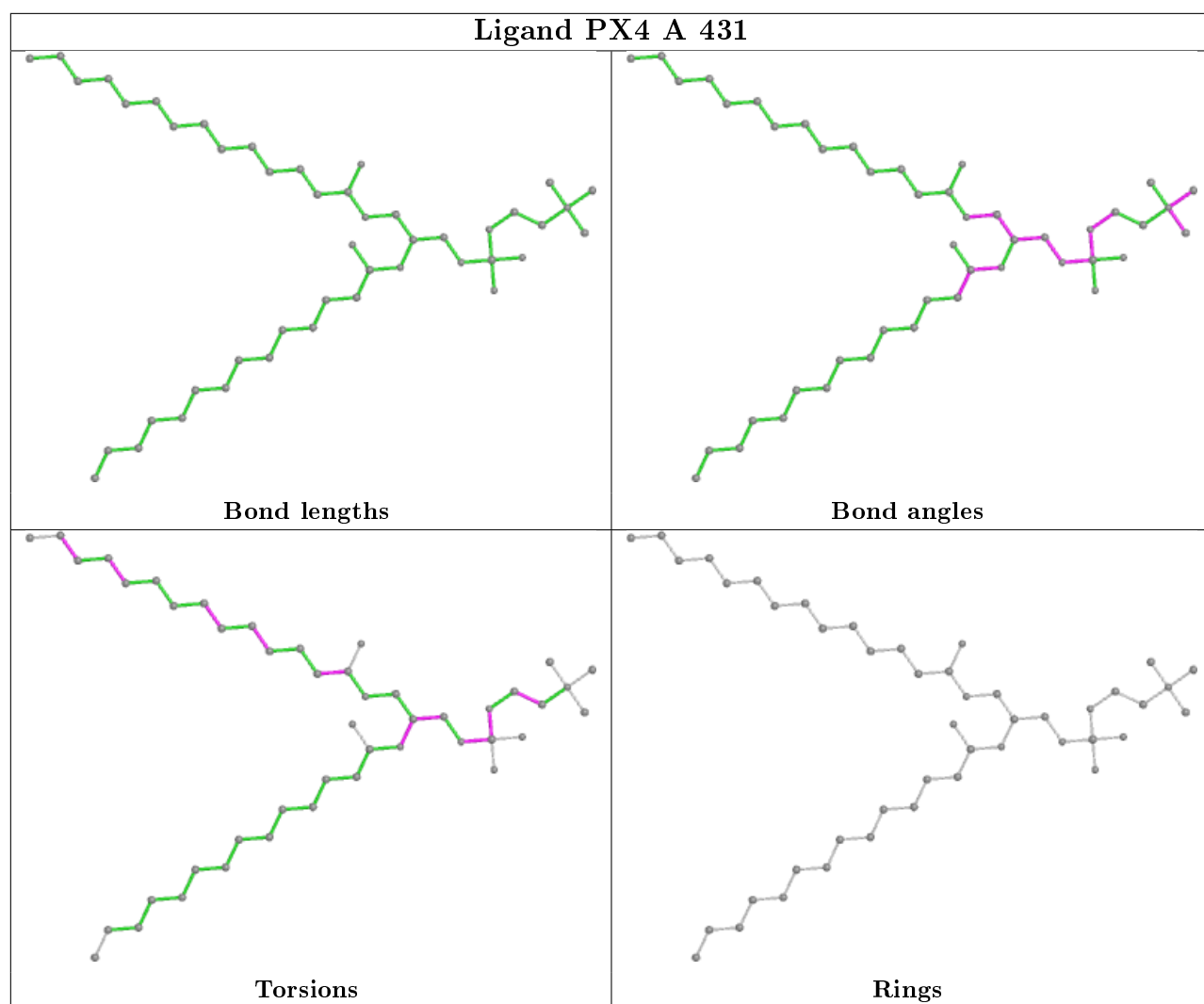


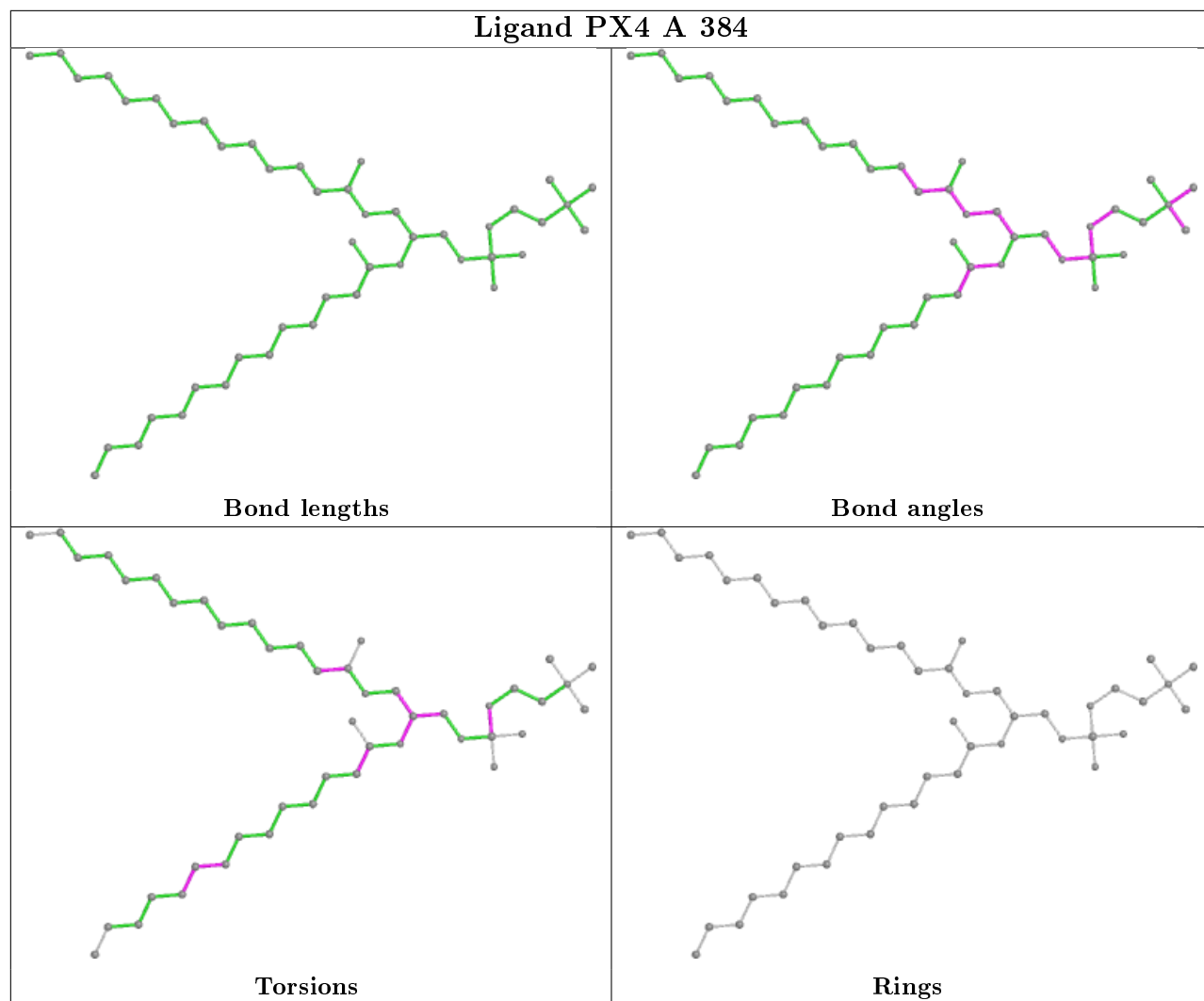


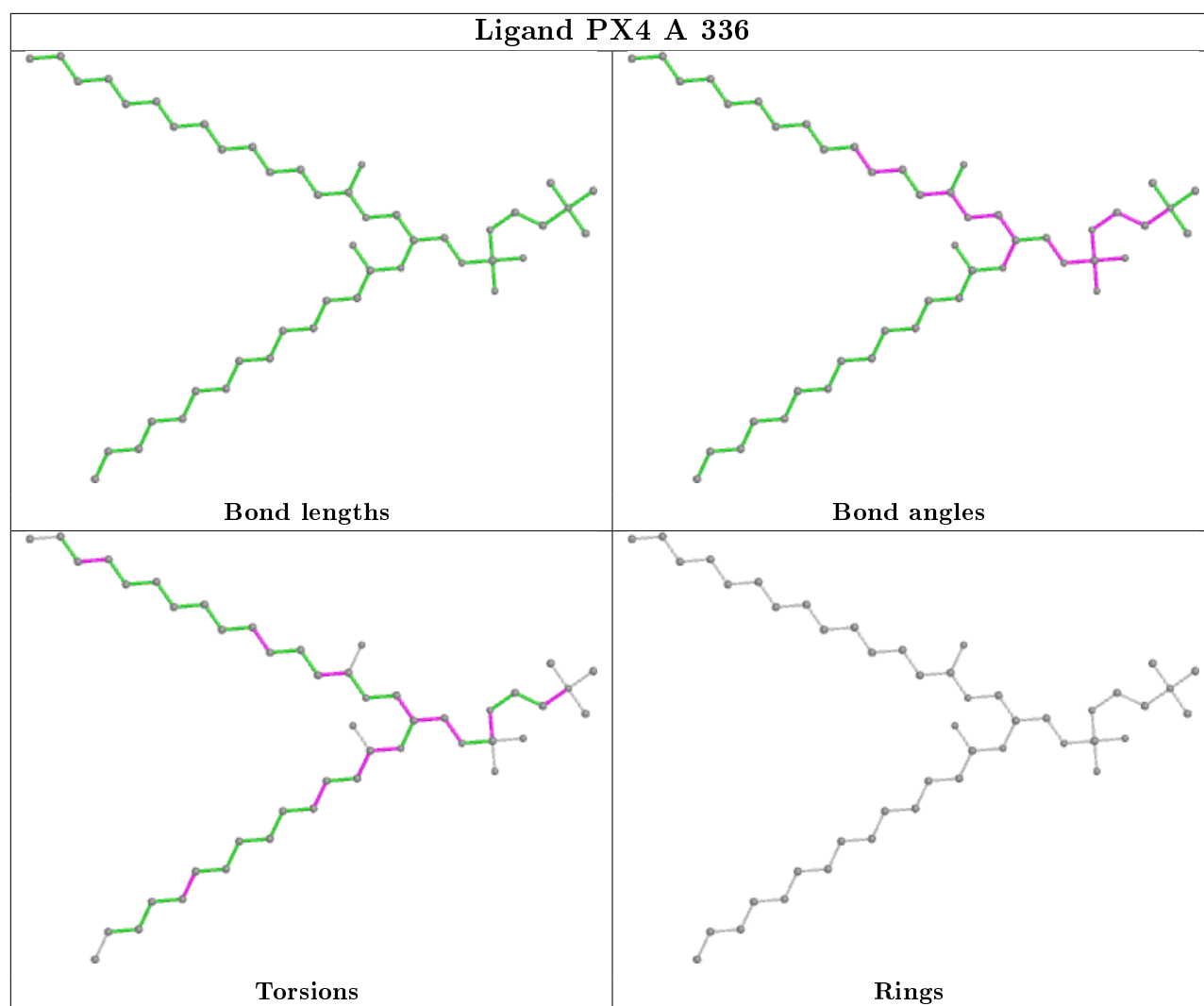




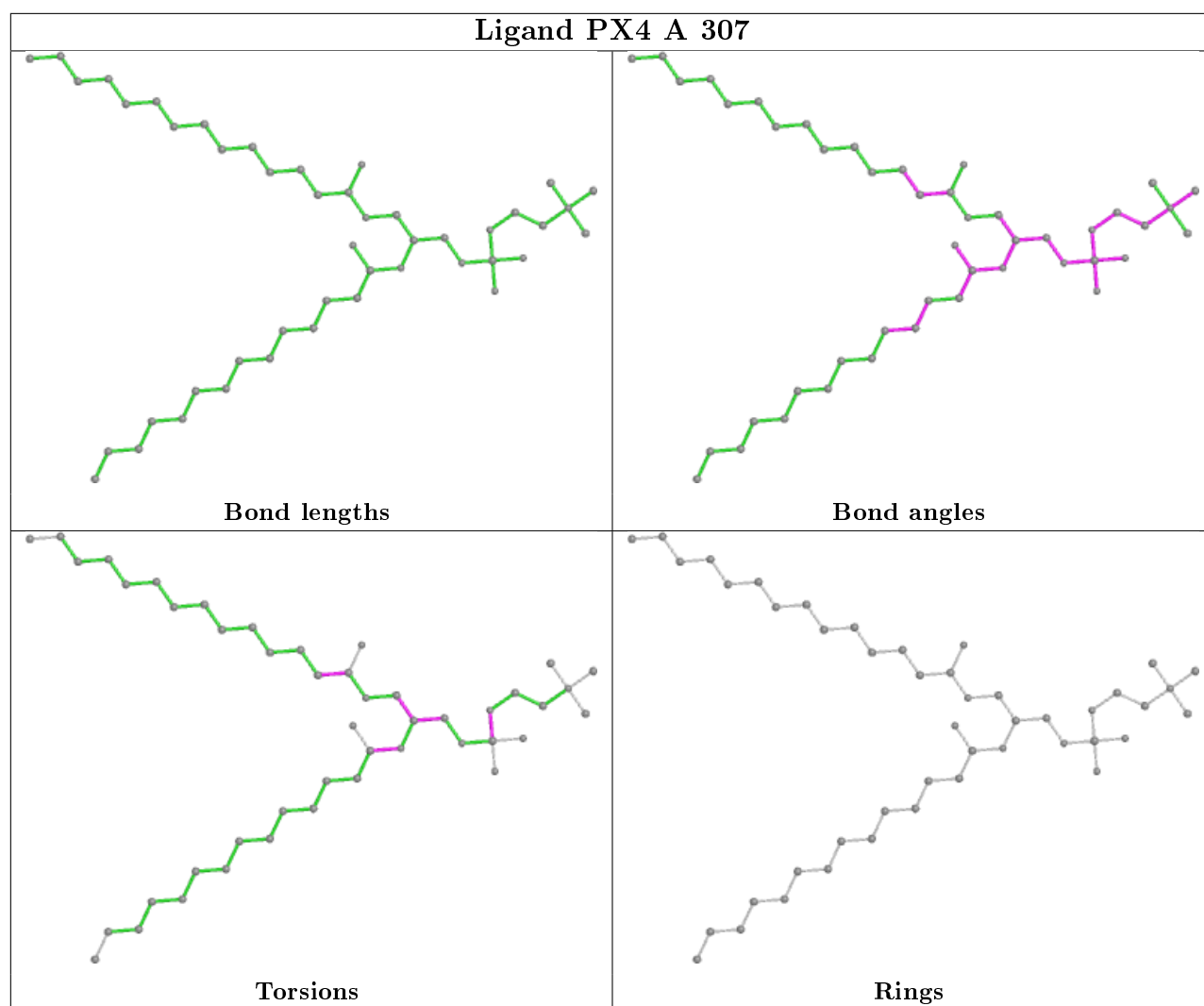


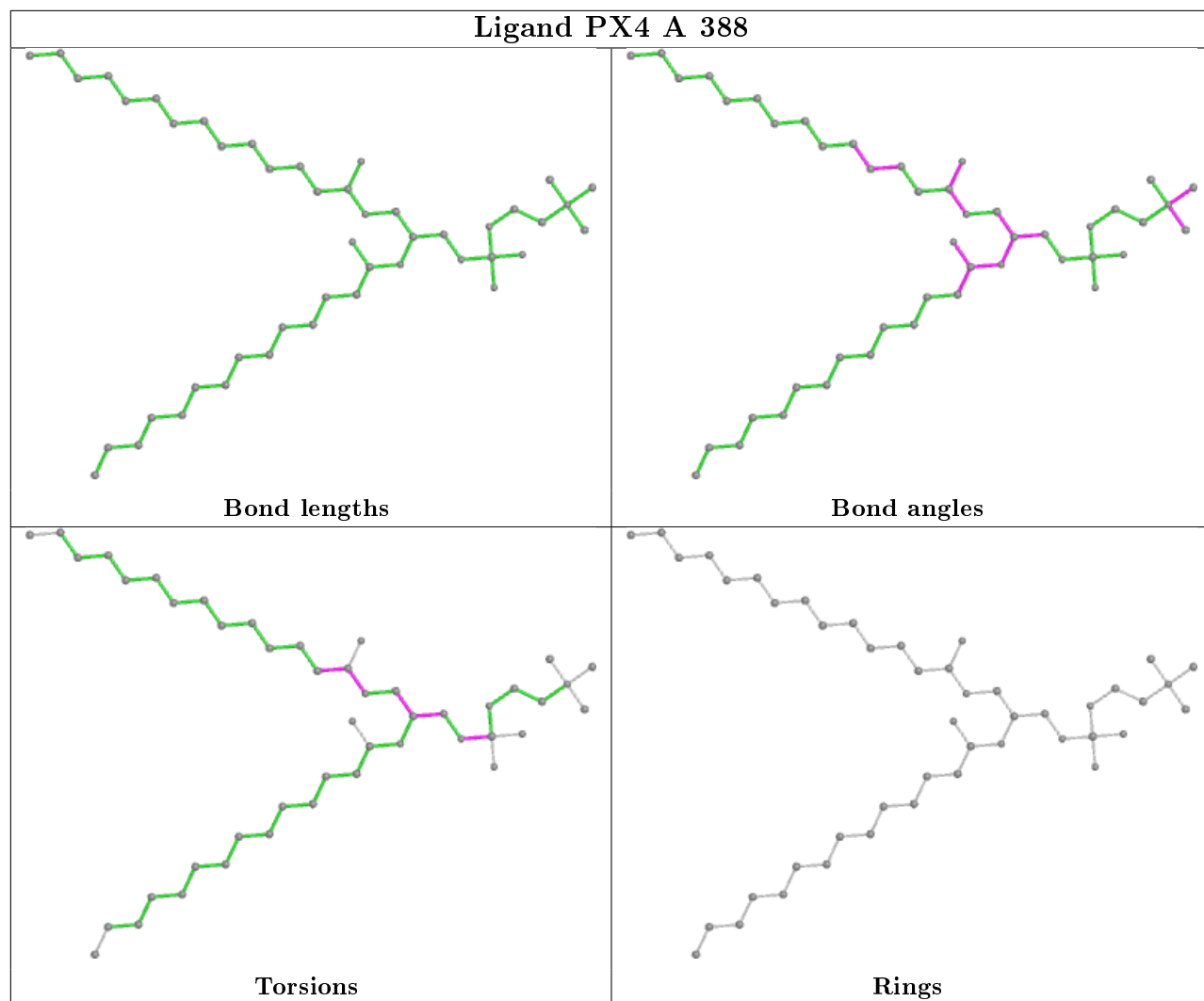


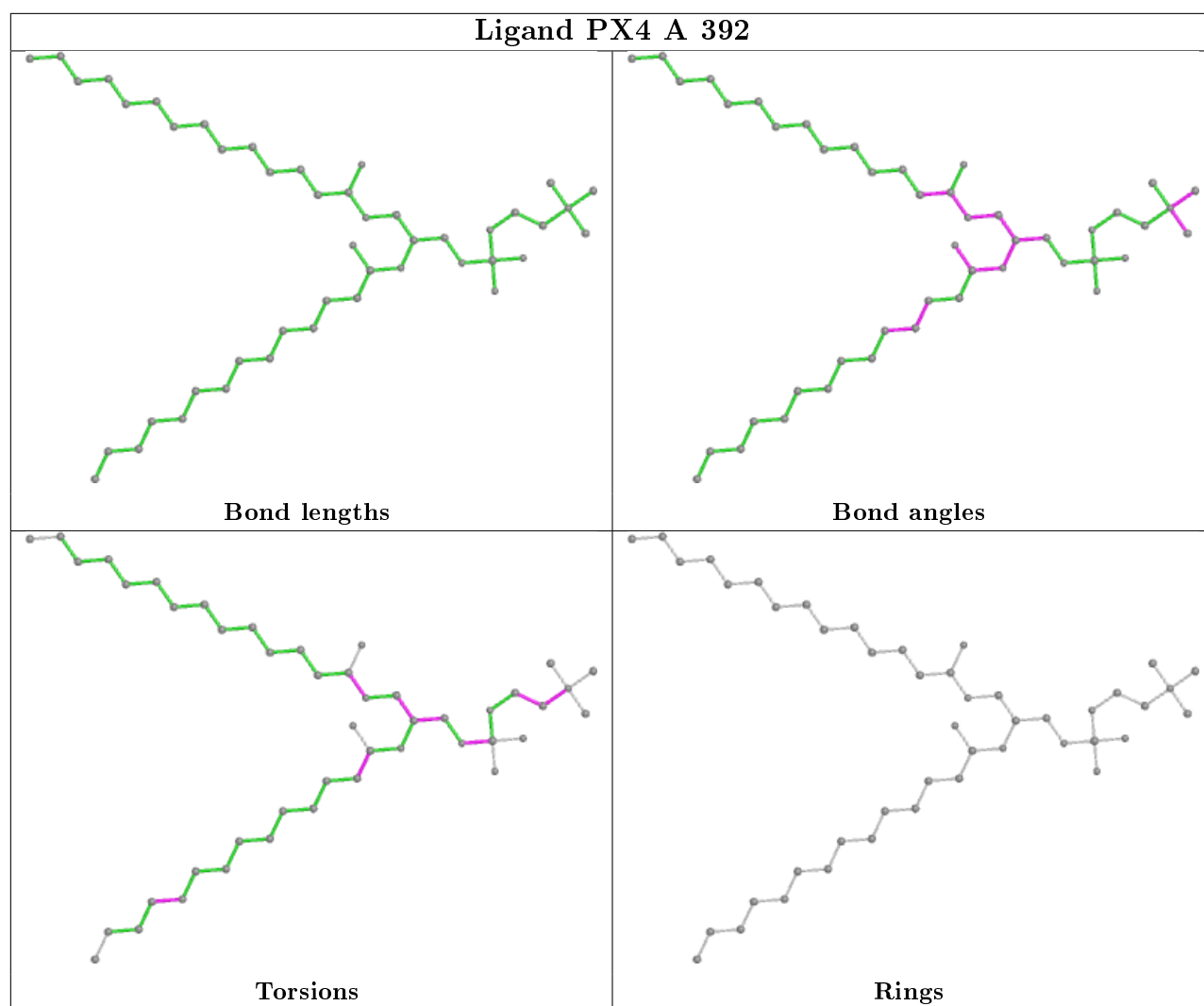


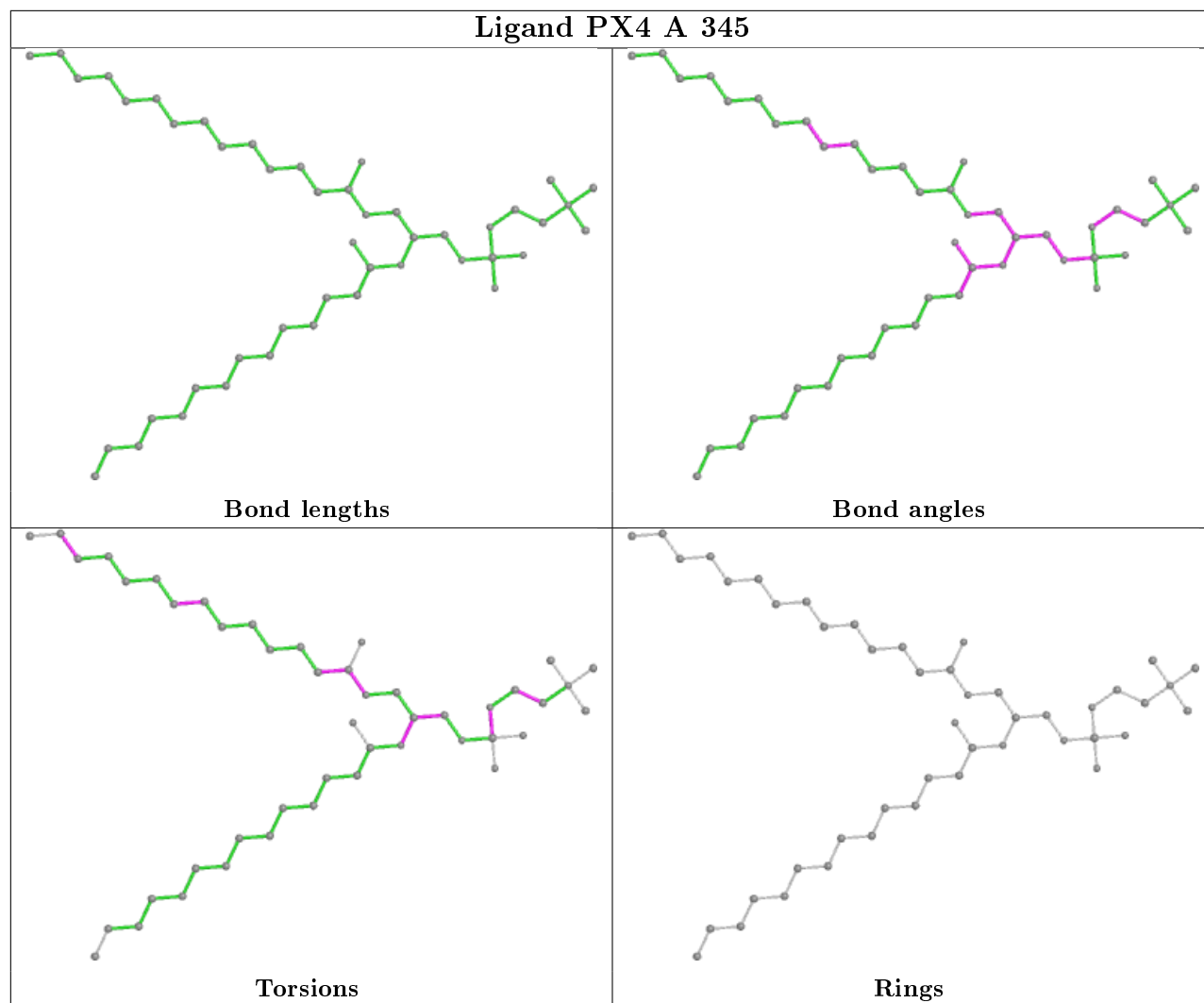


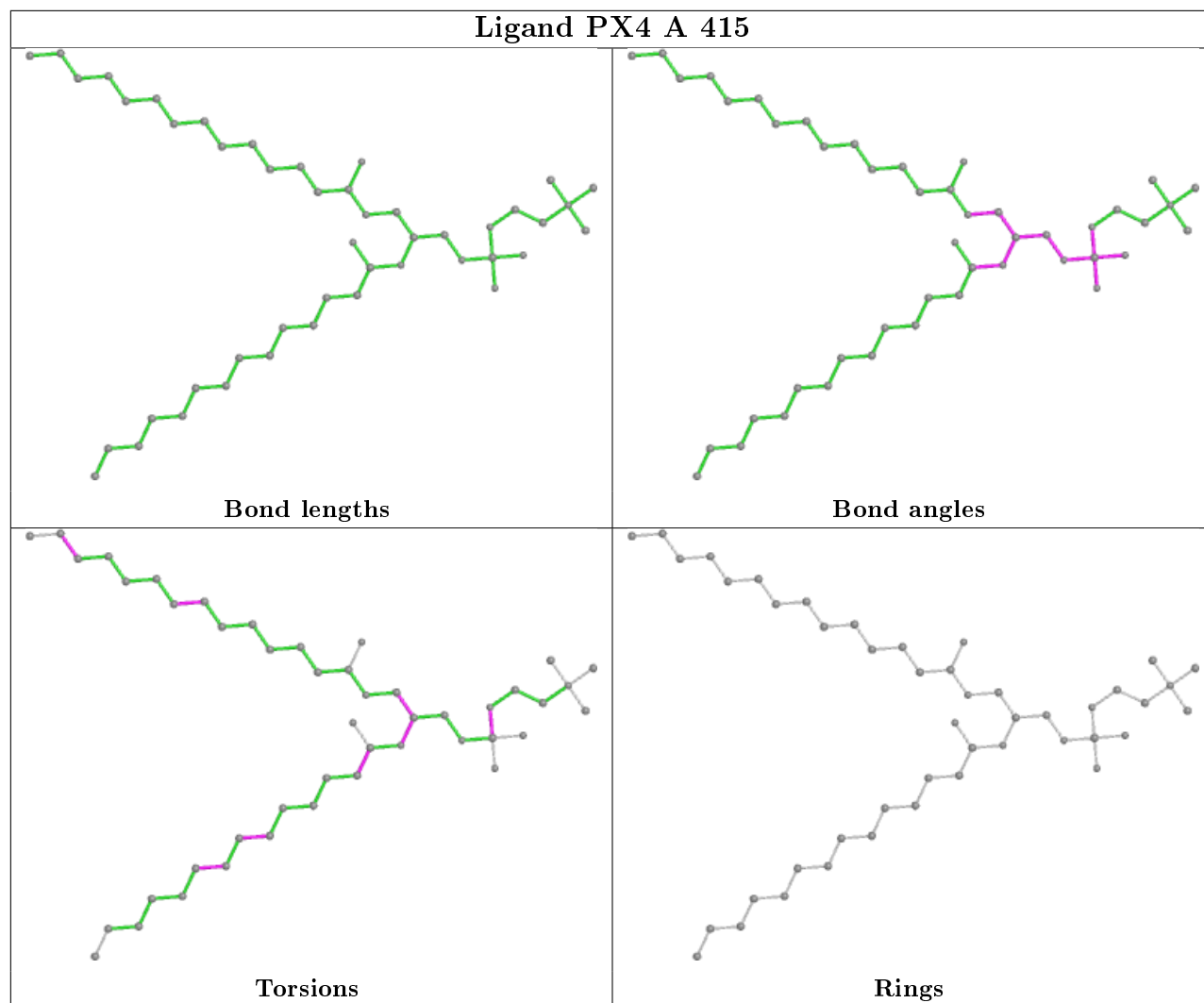


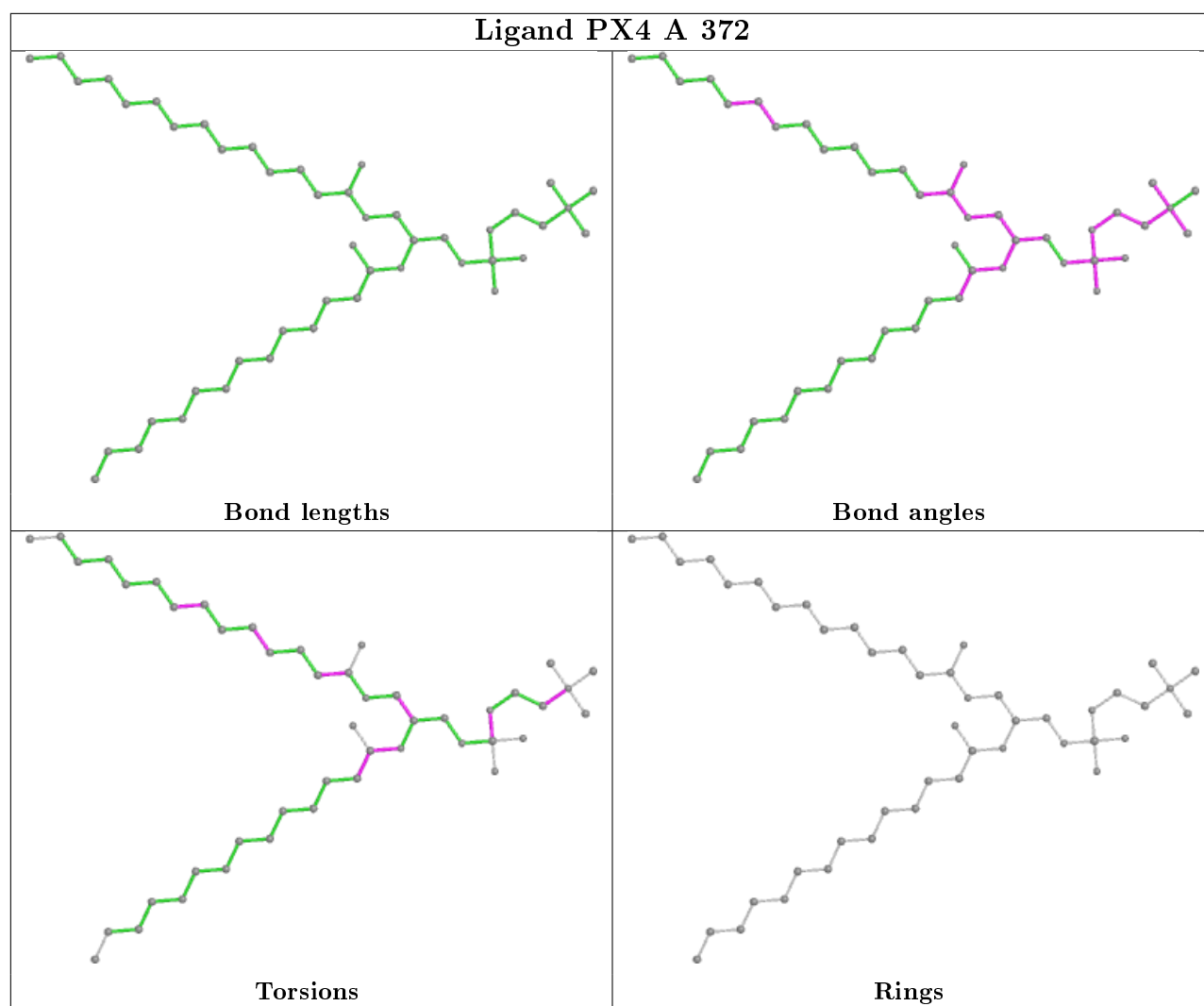


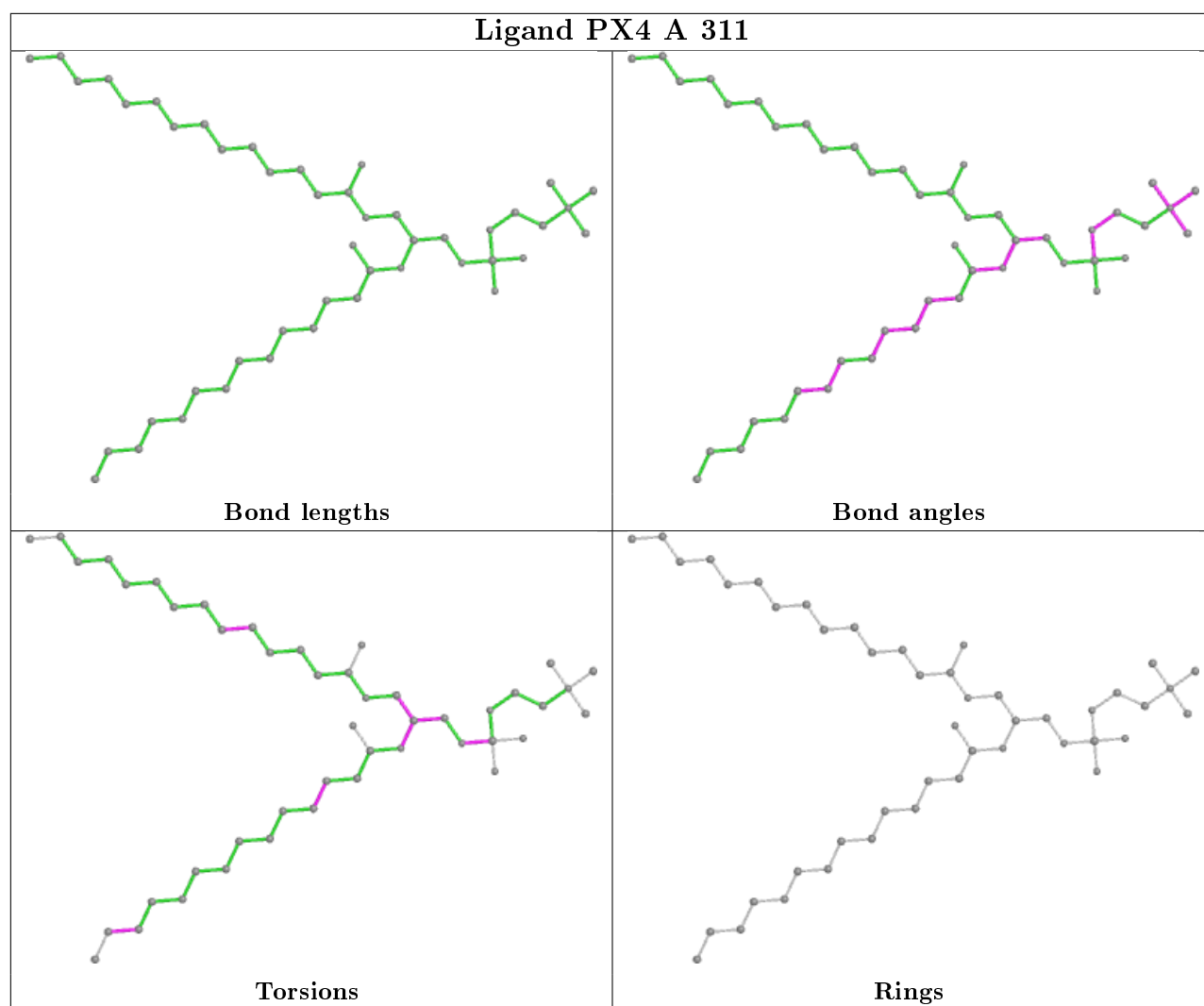




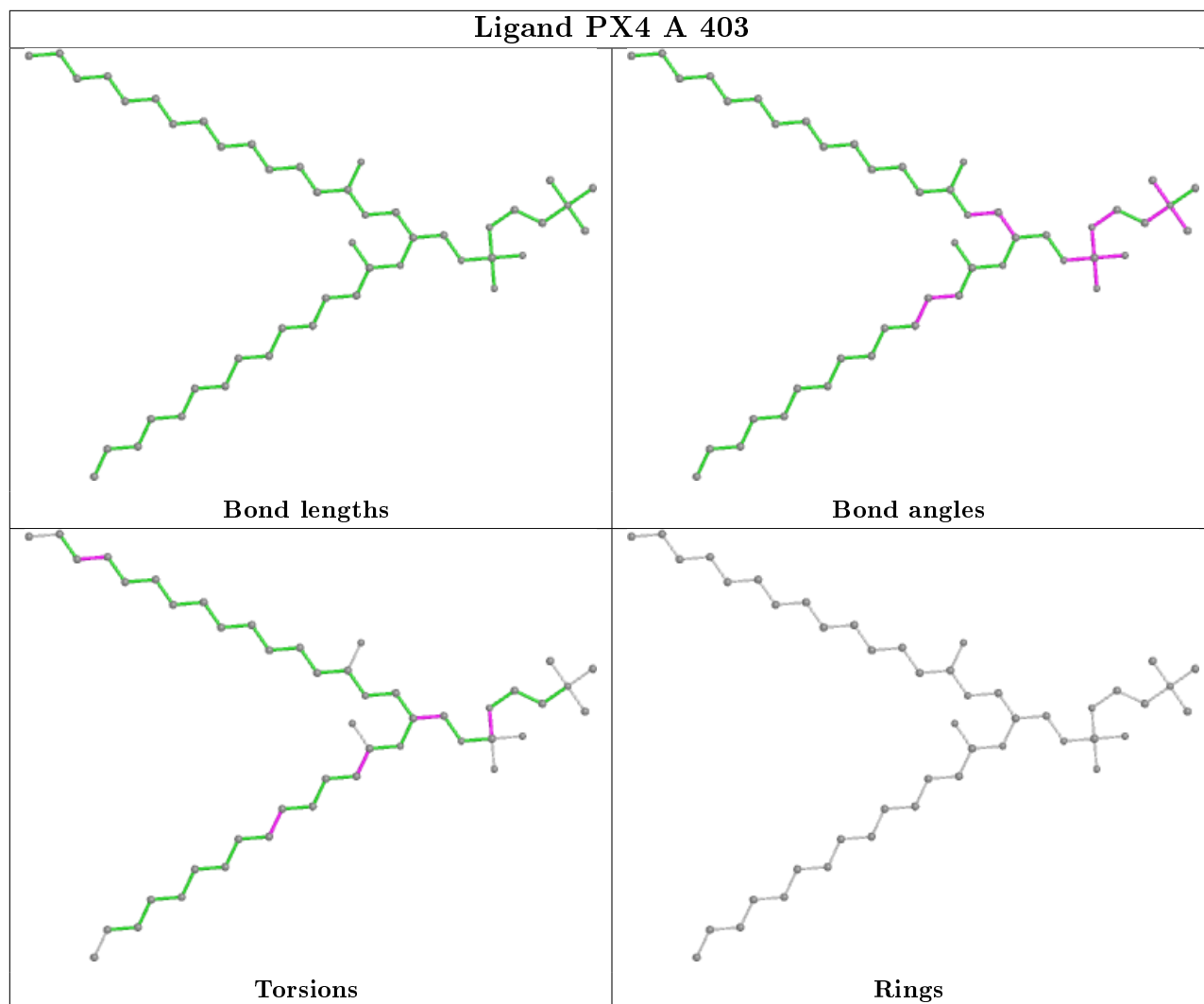




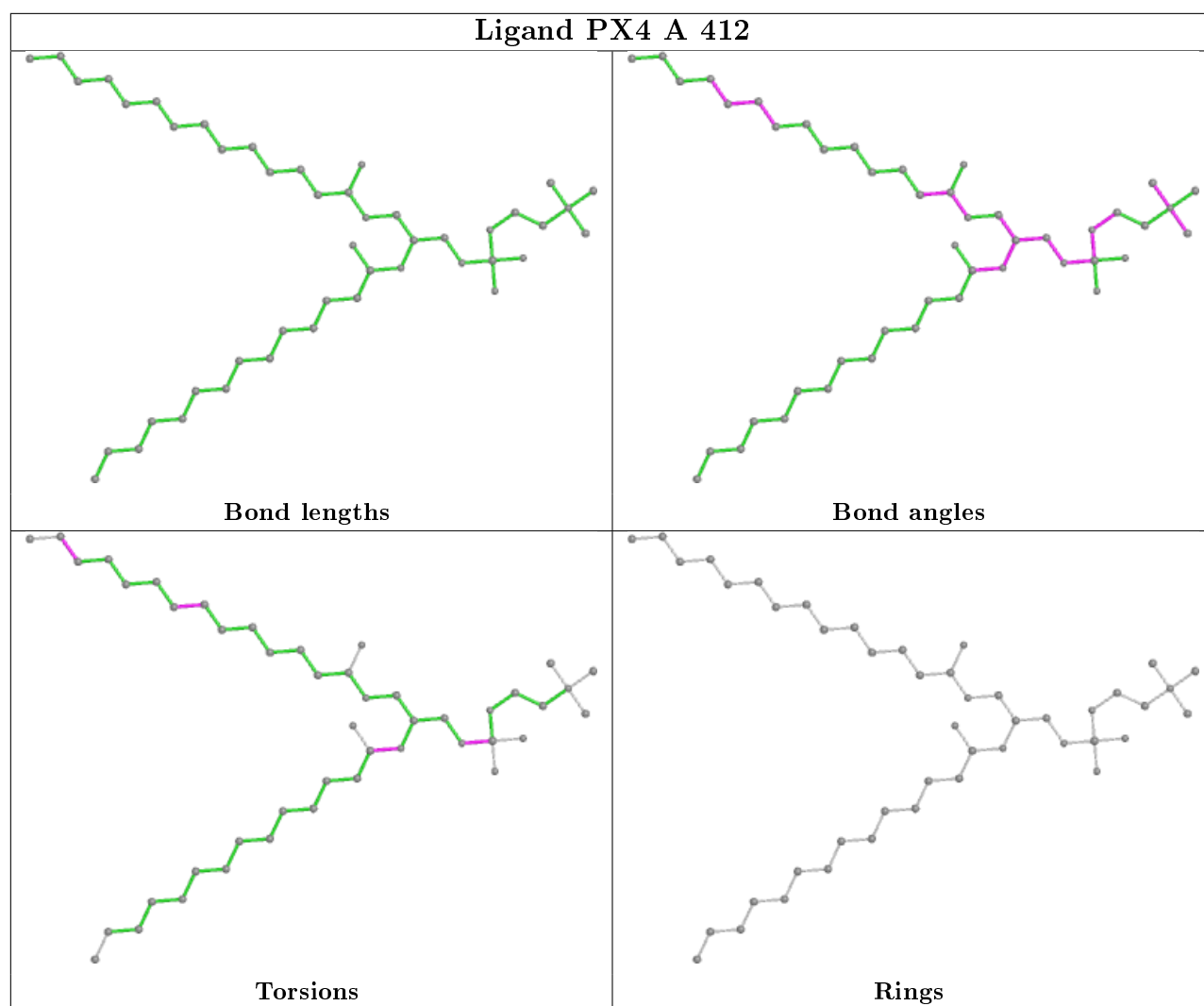


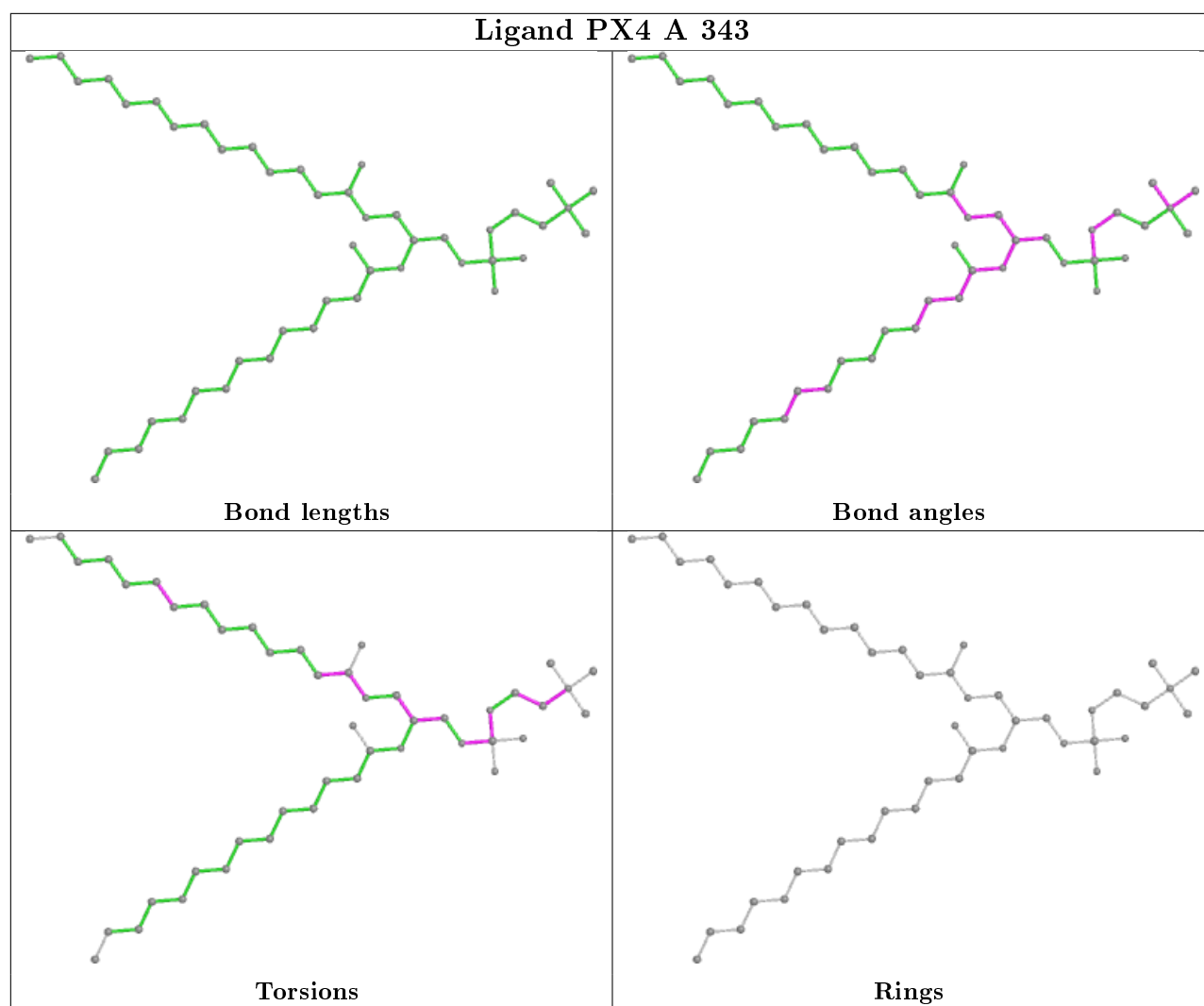


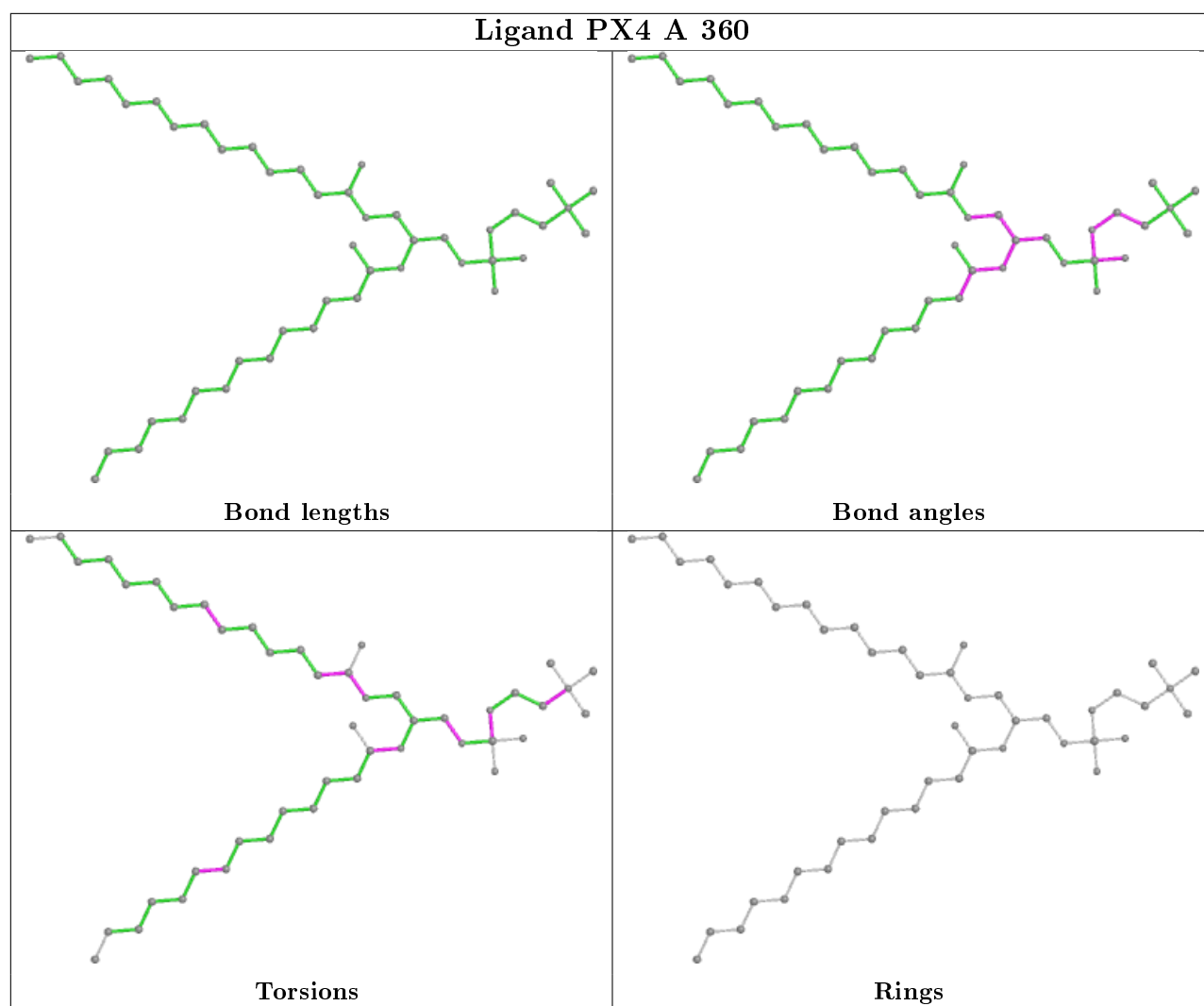
## Ligand PX4 A 403

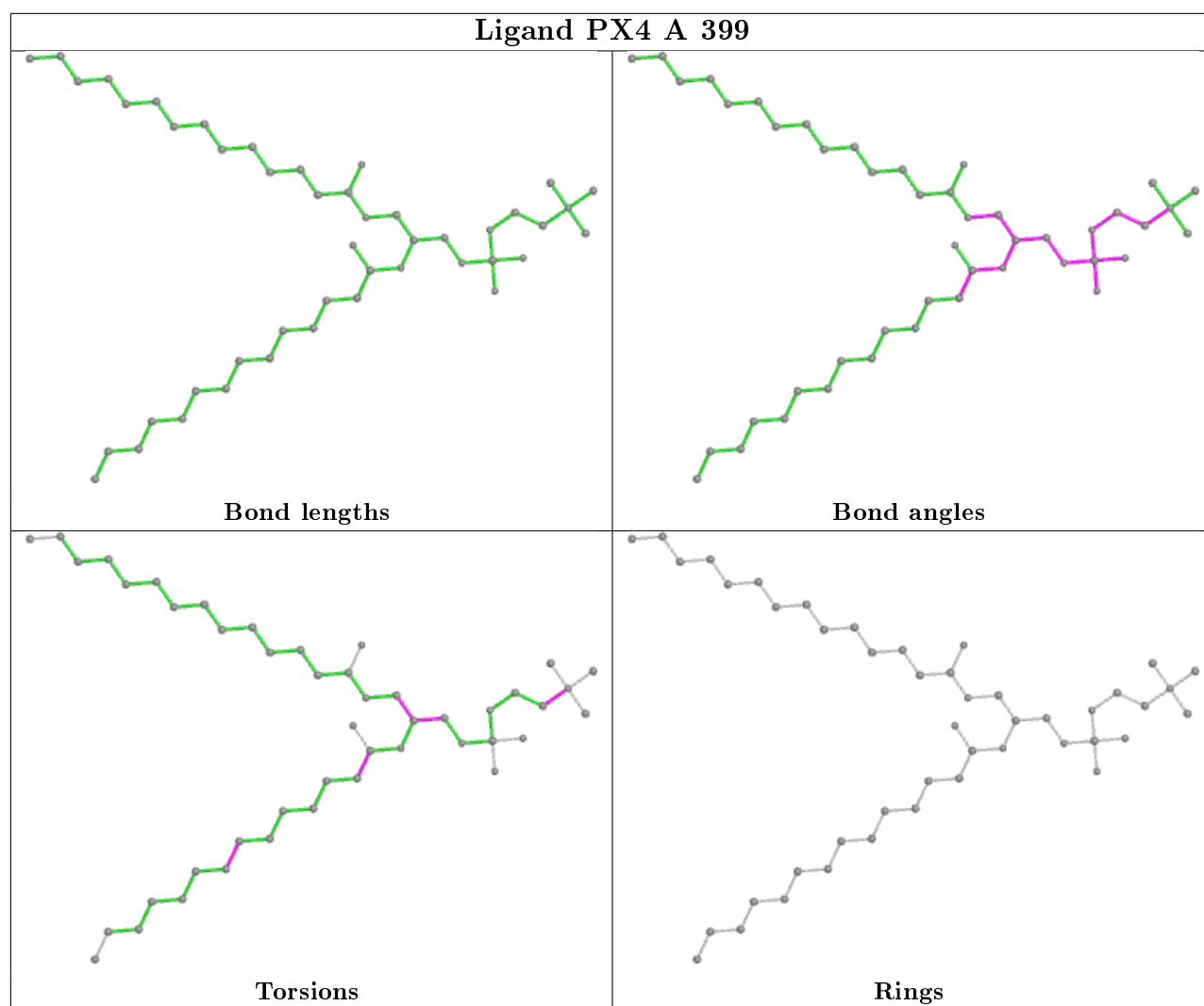


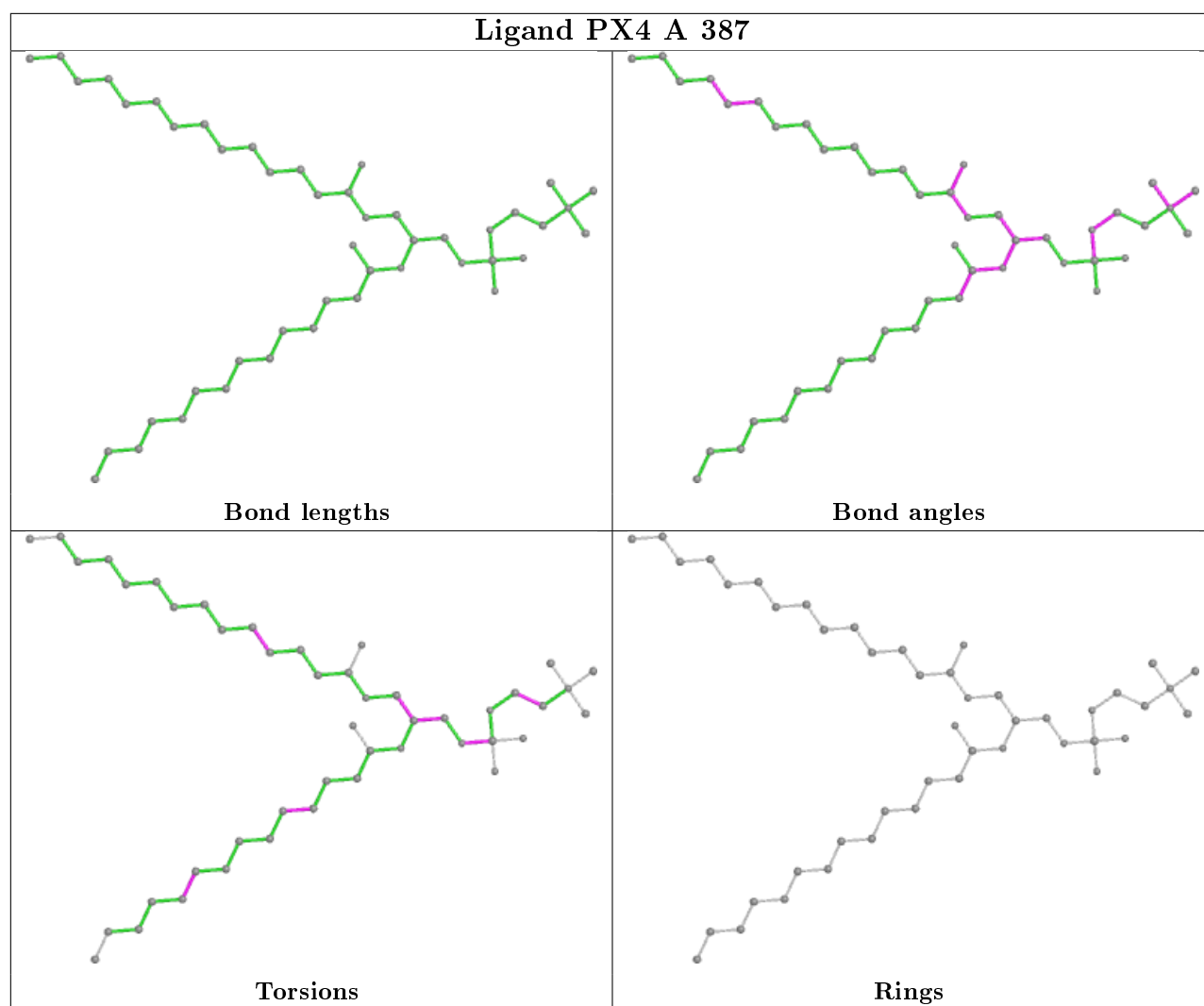


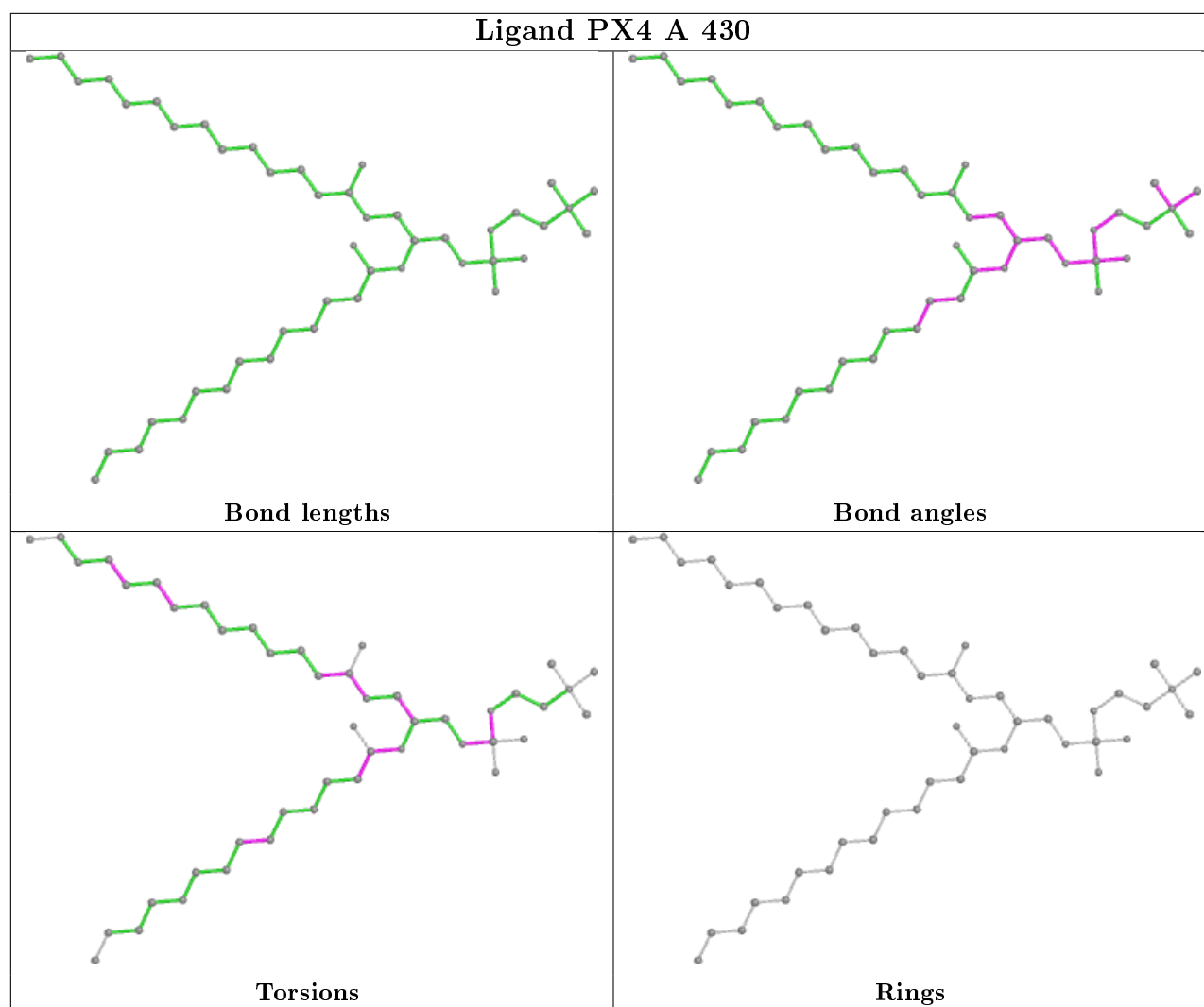


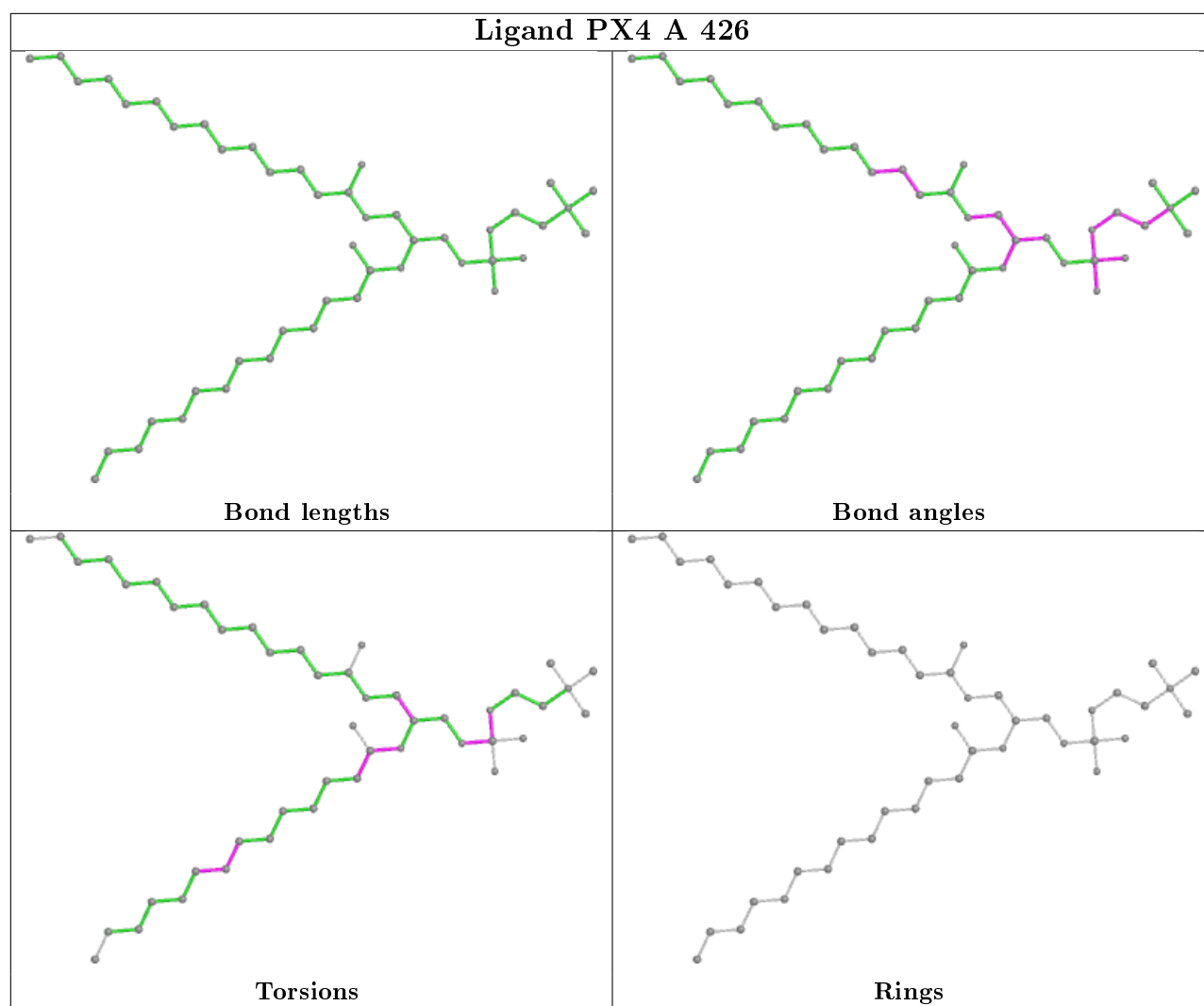


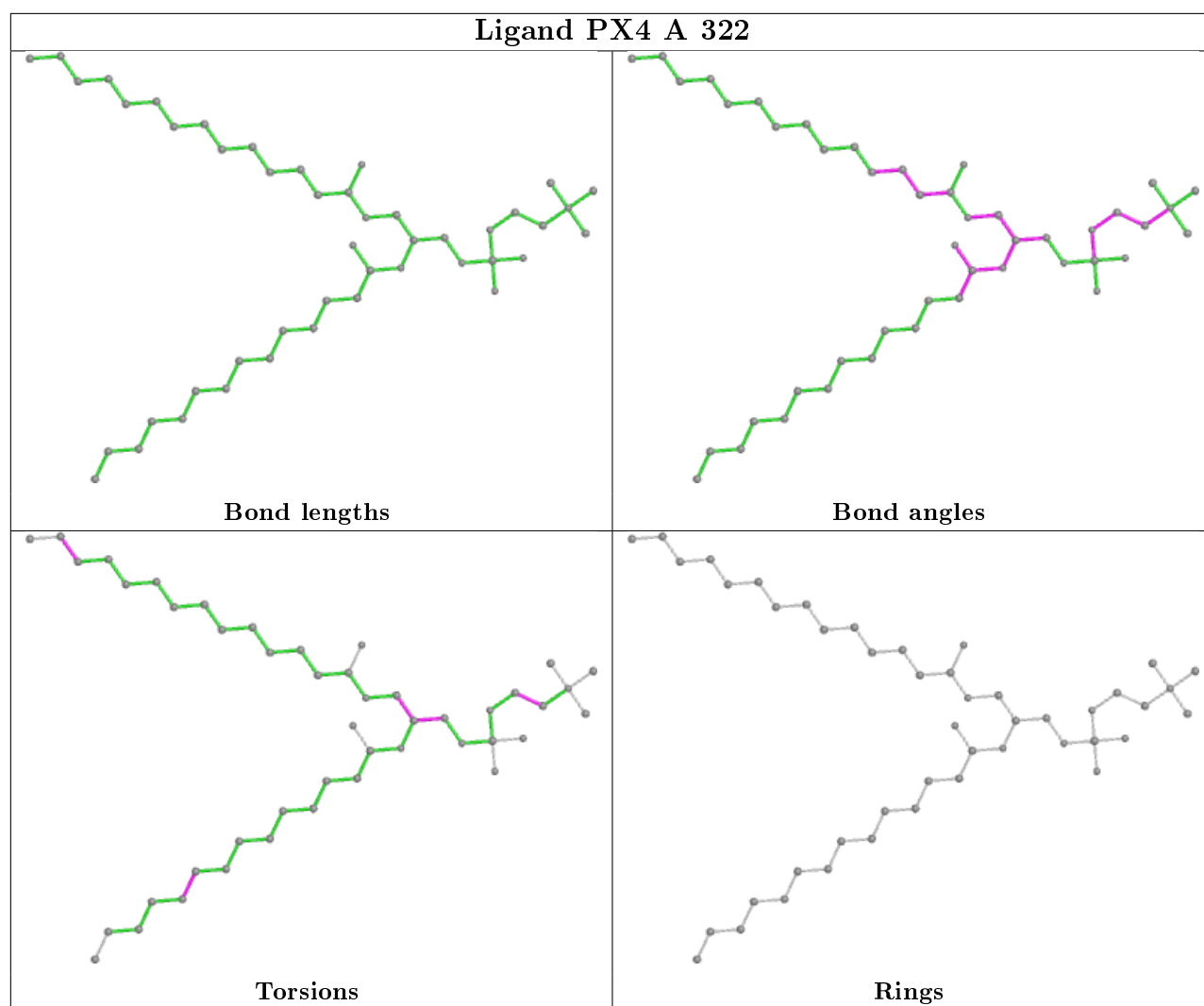




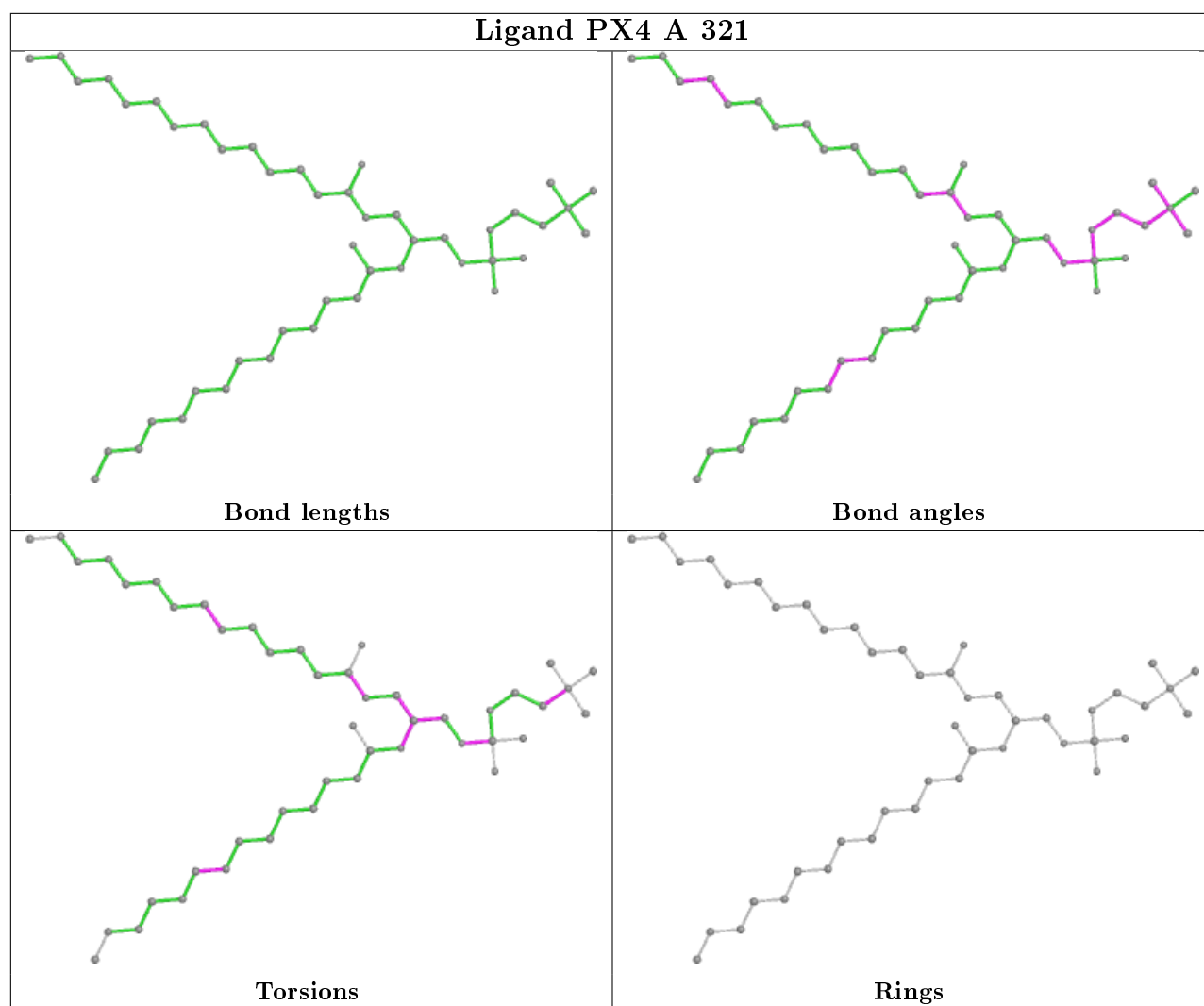


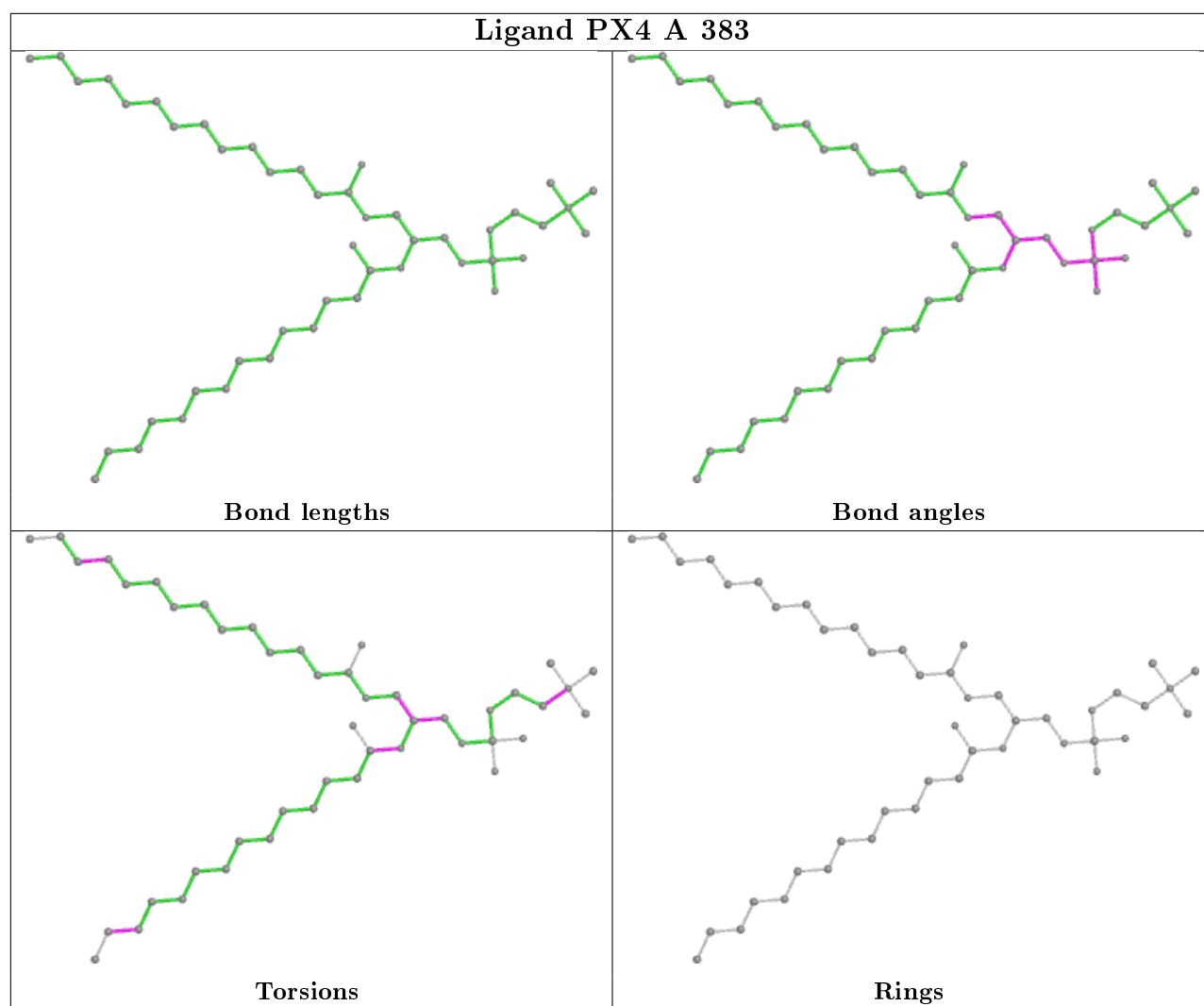


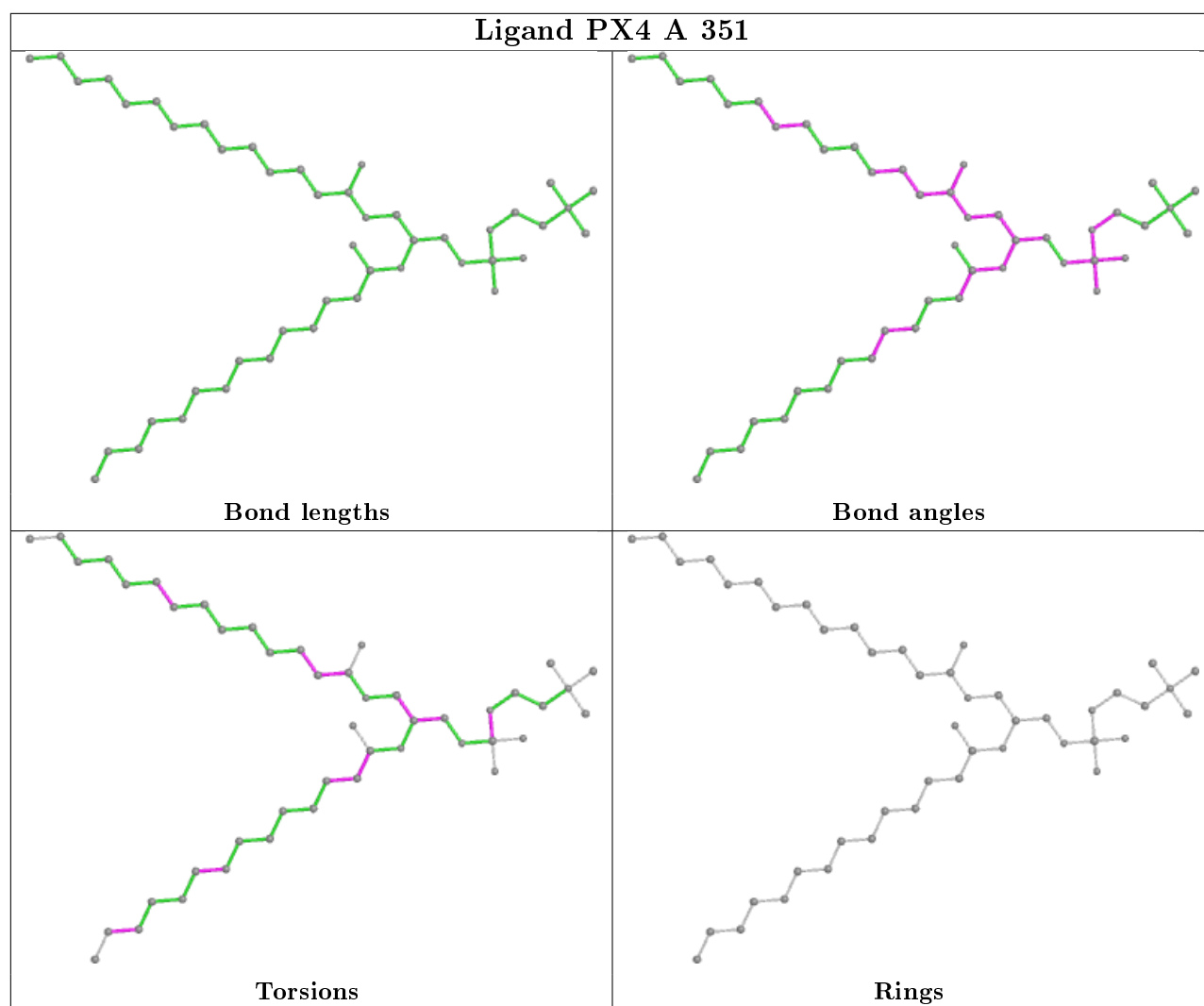




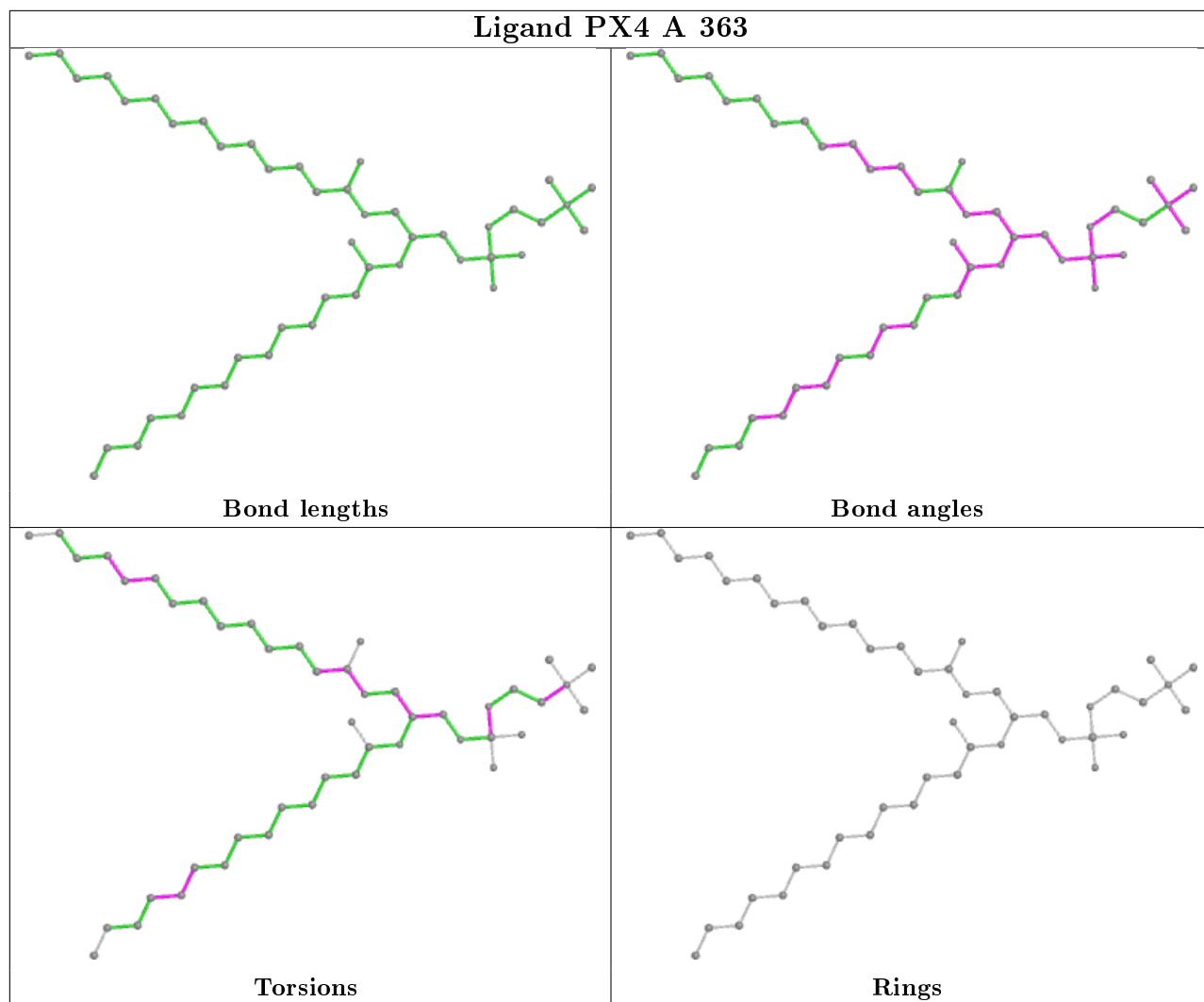


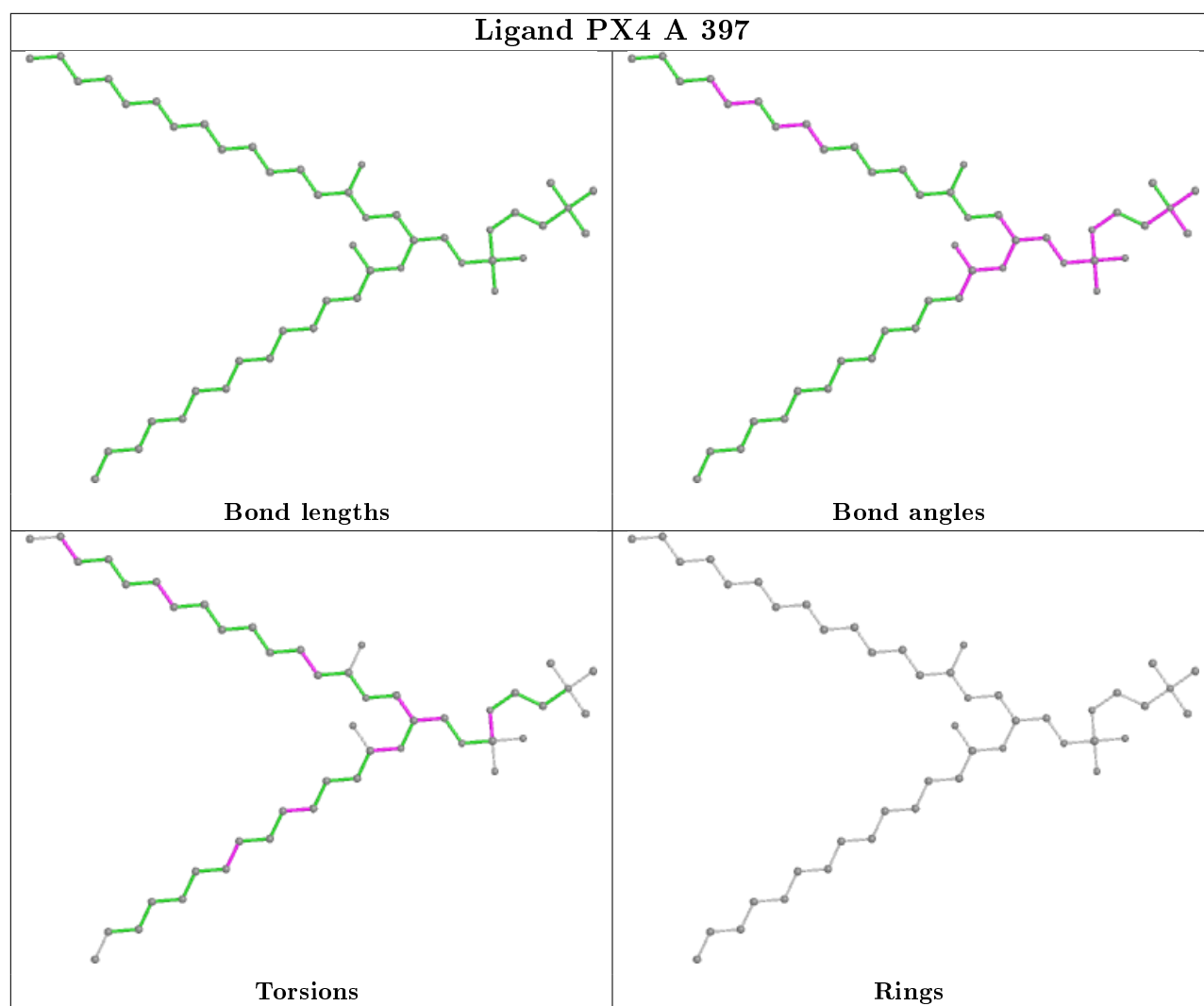


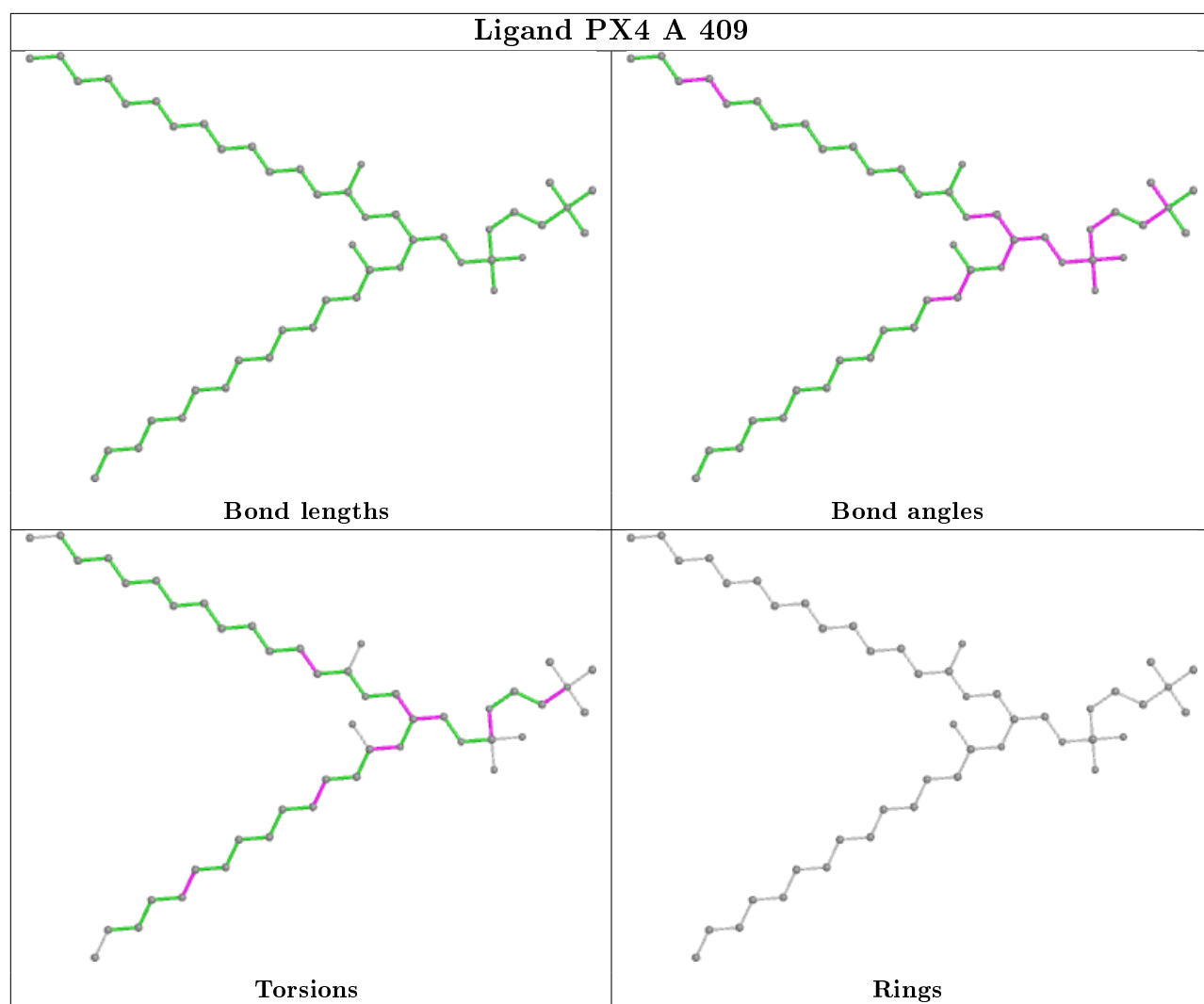


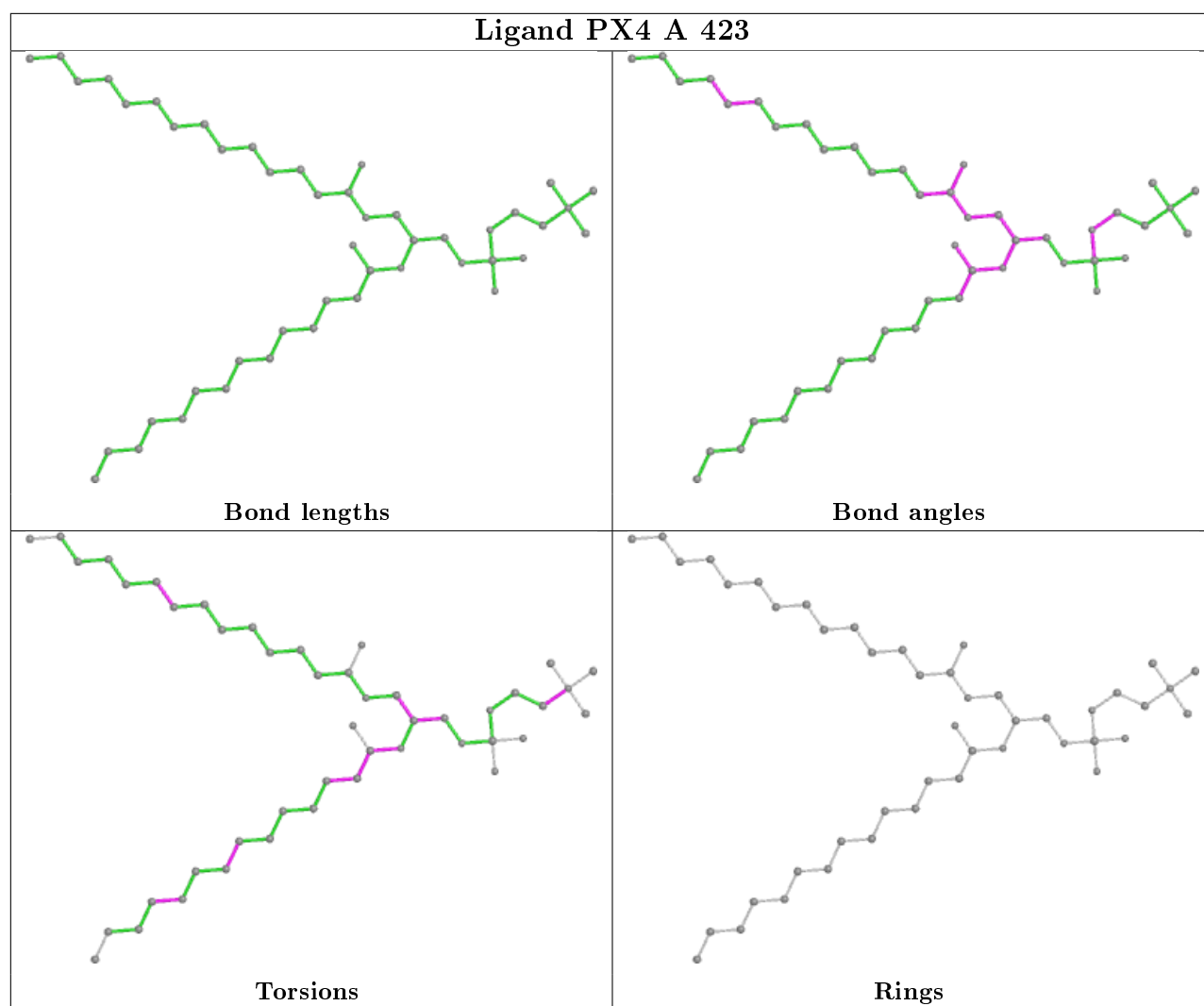


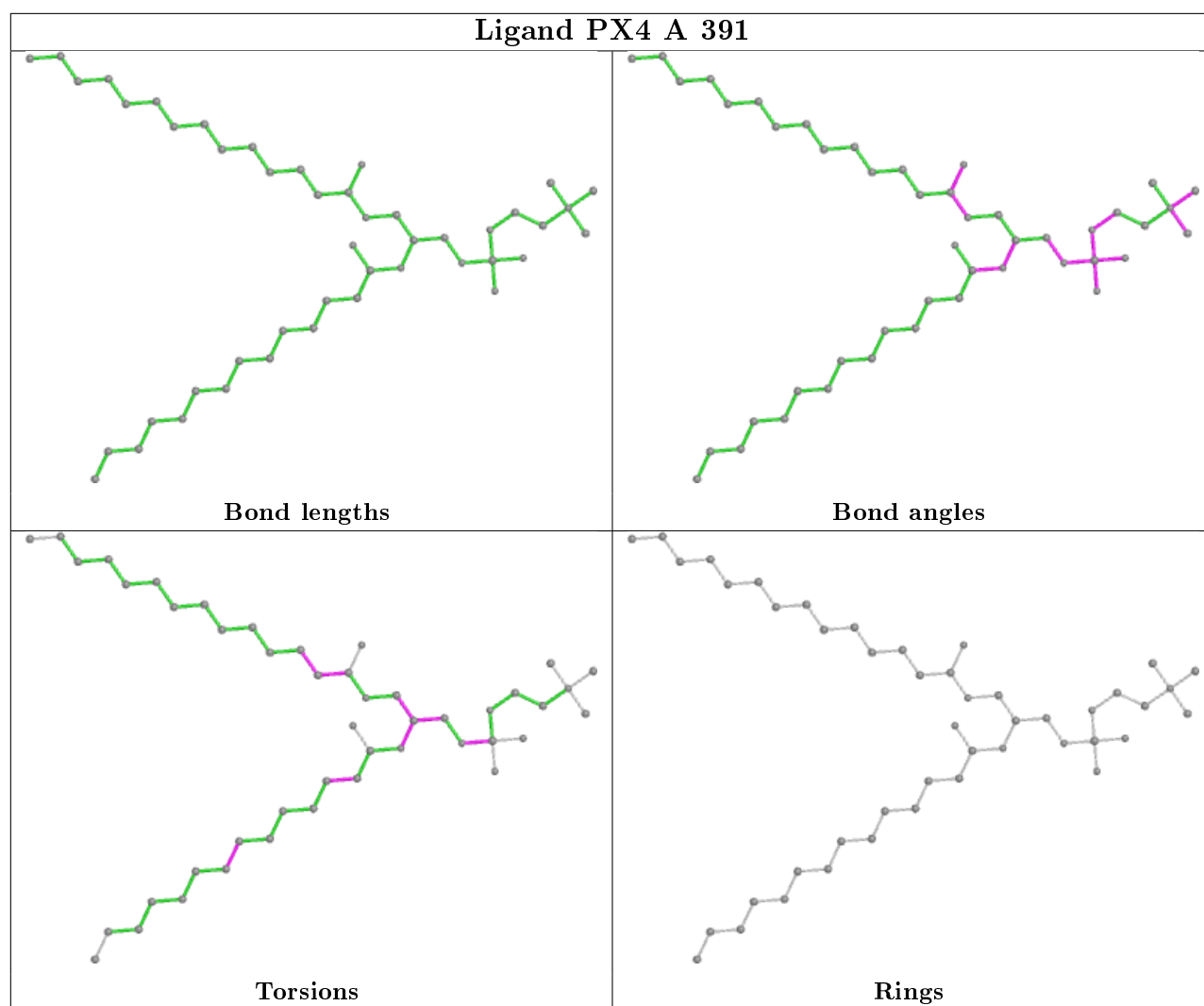
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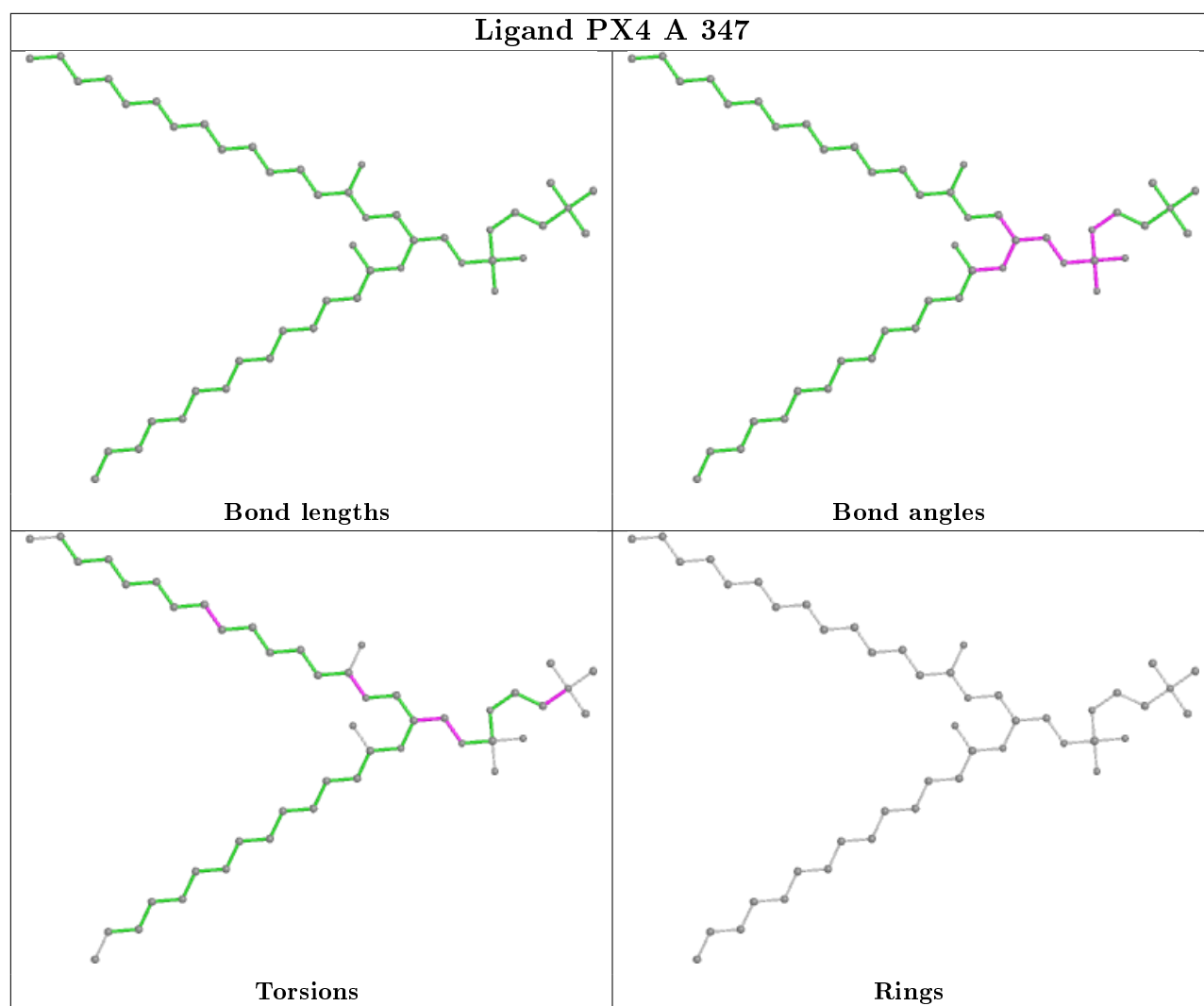


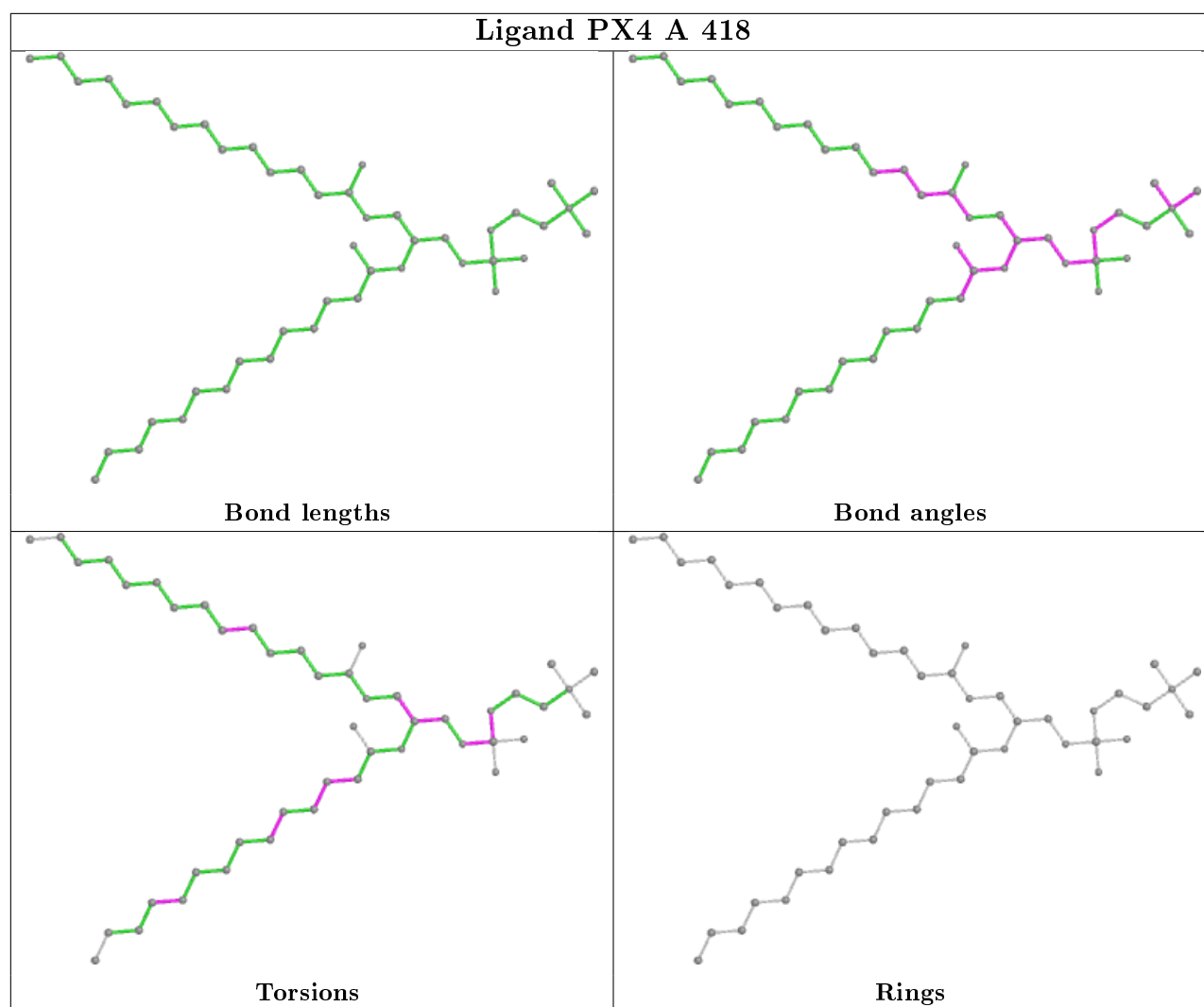


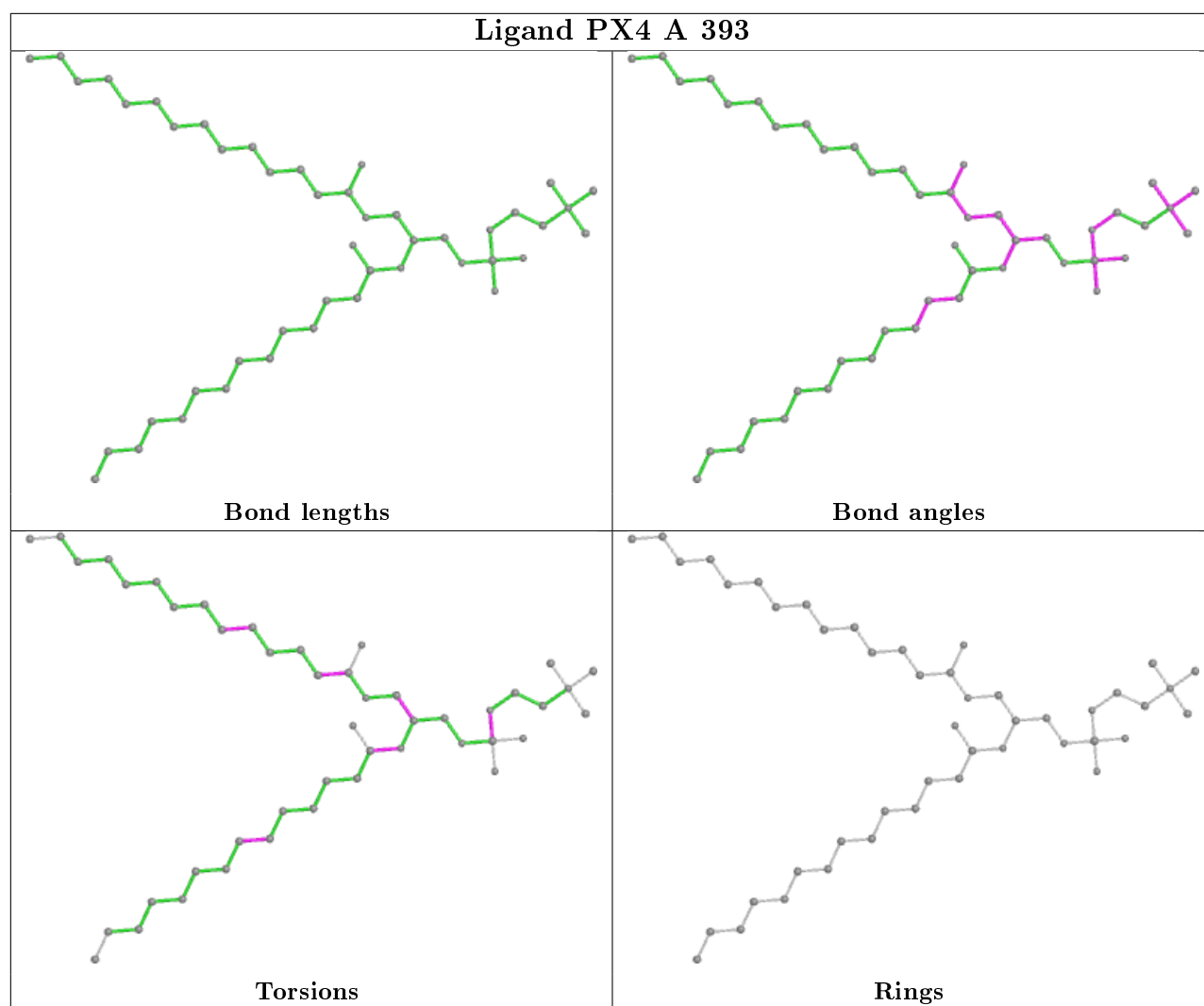


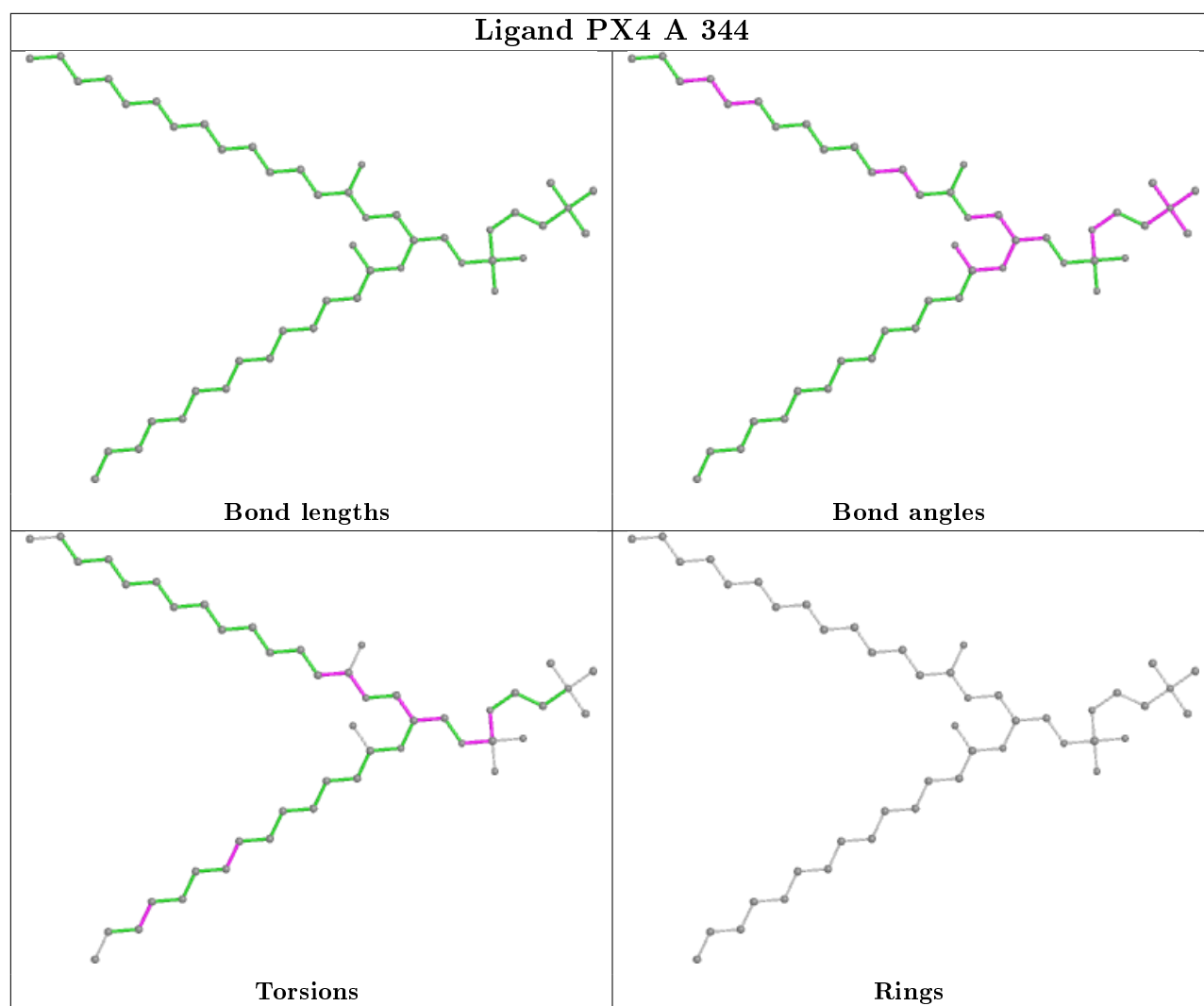


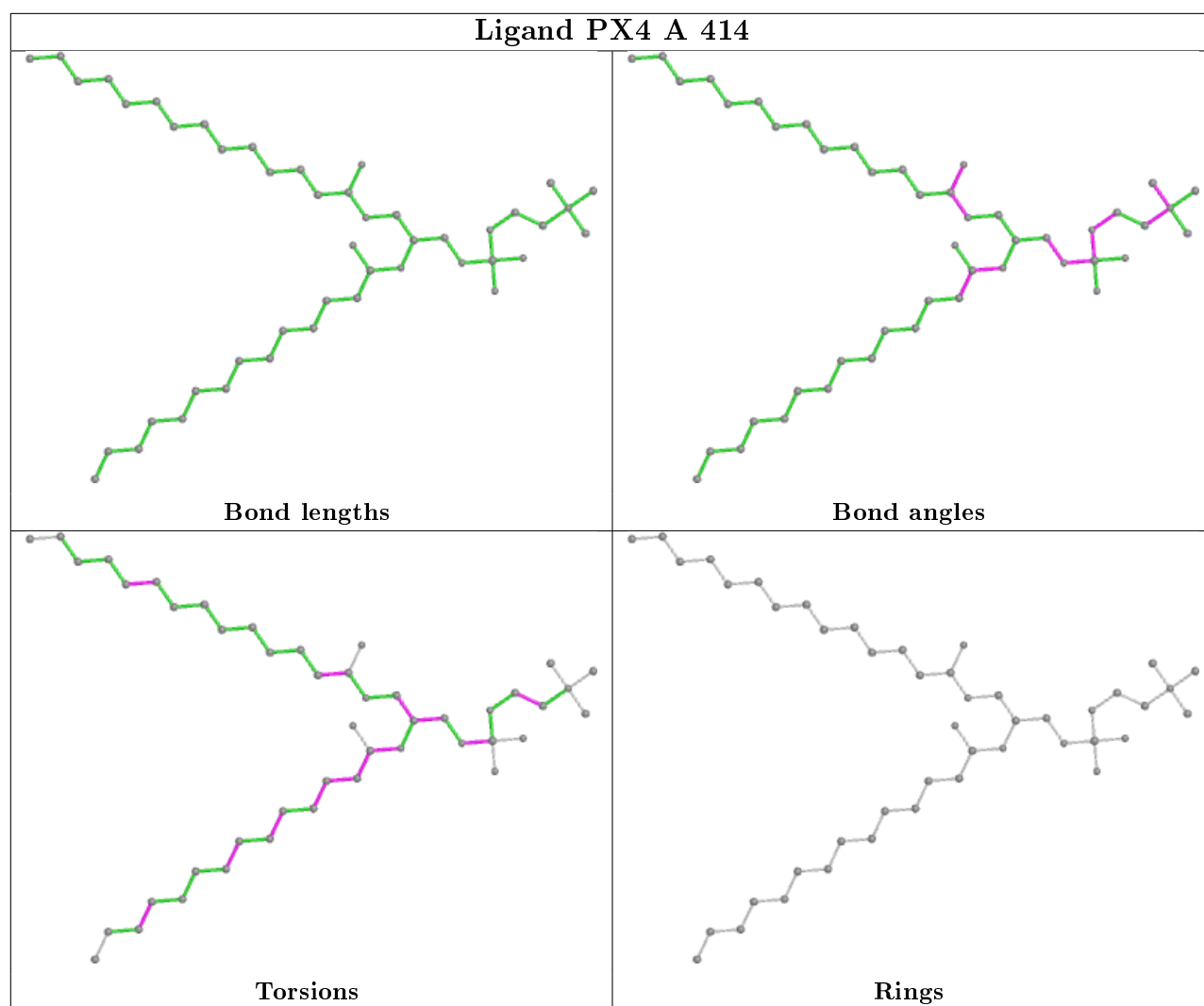


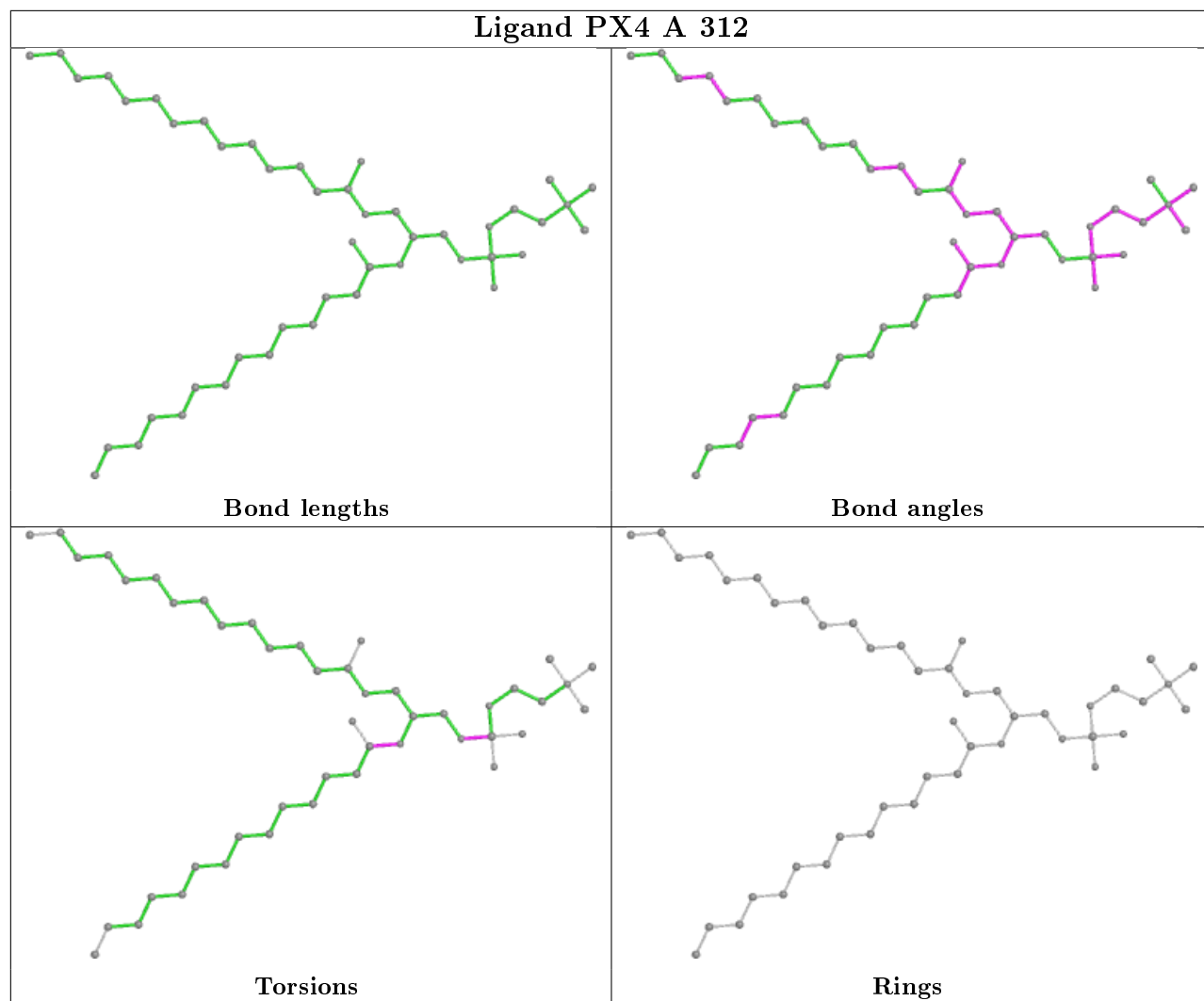


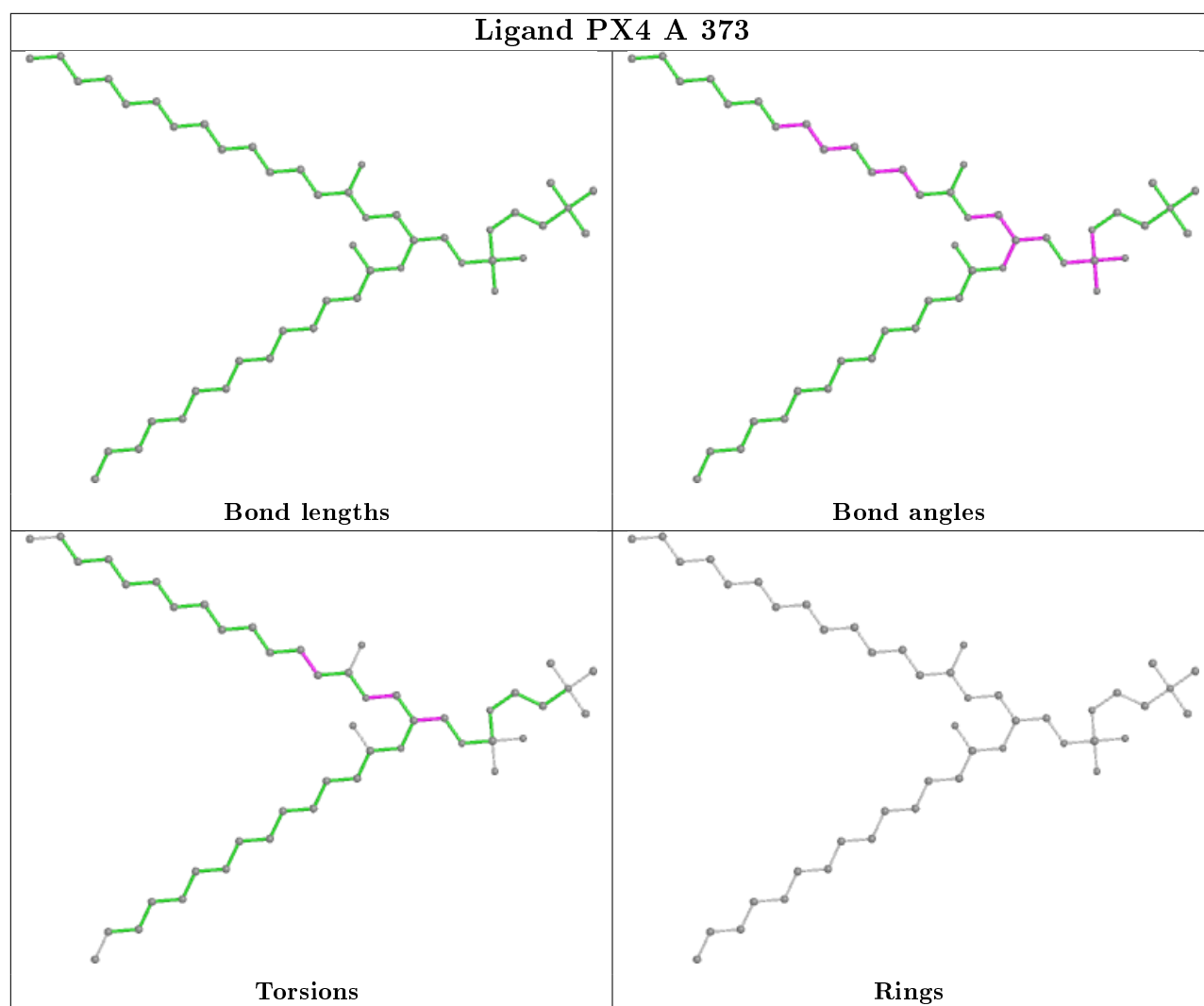


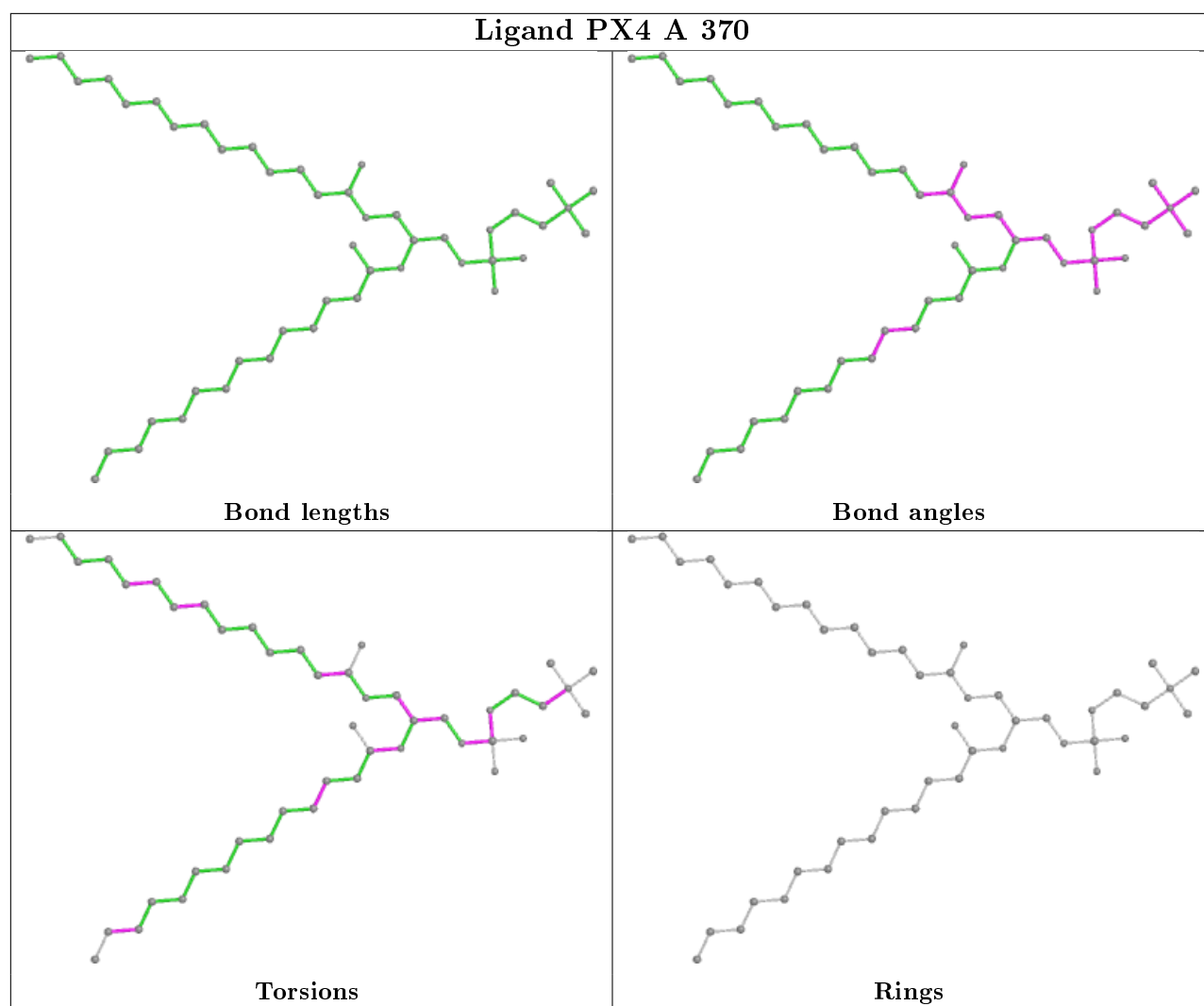




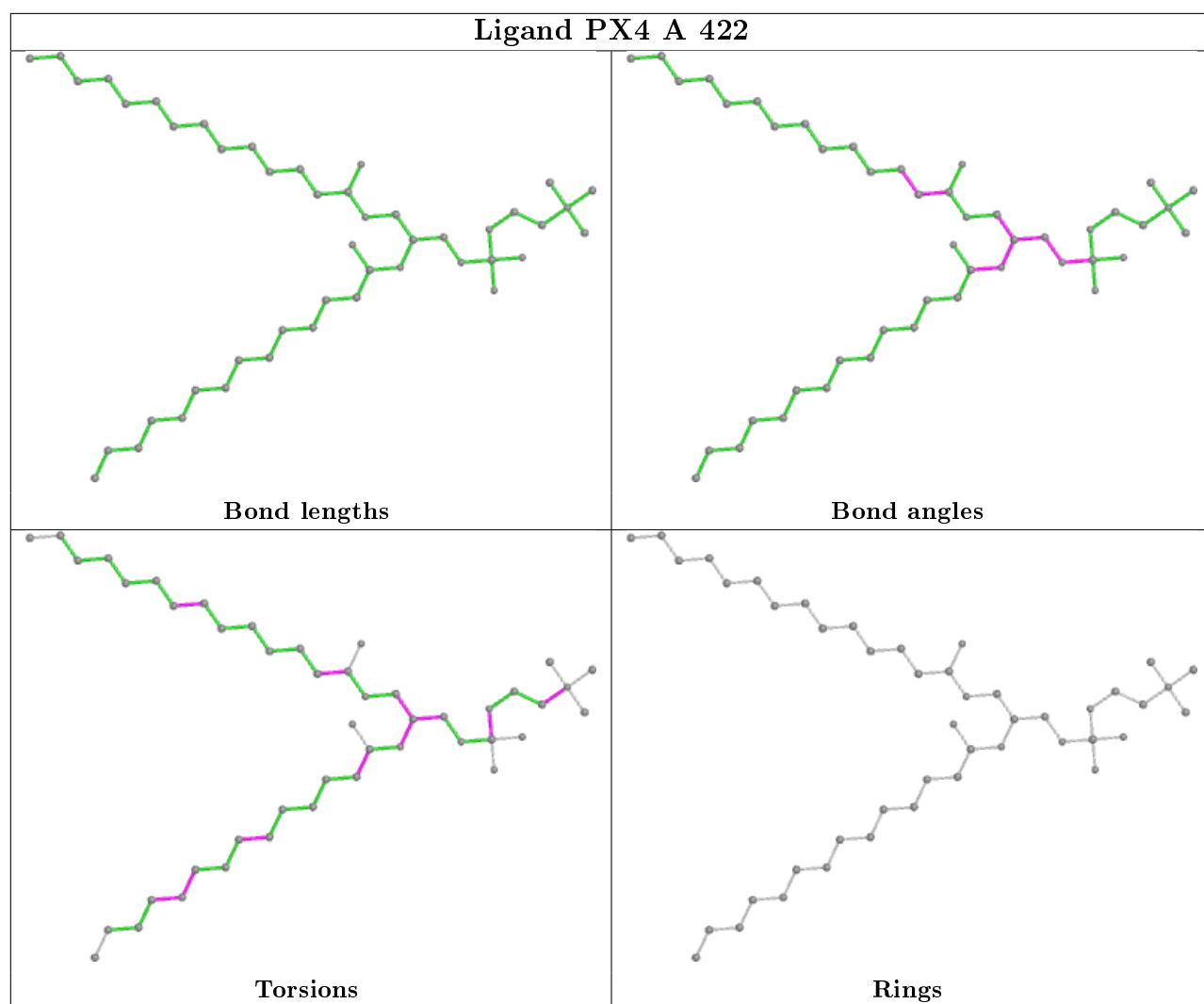


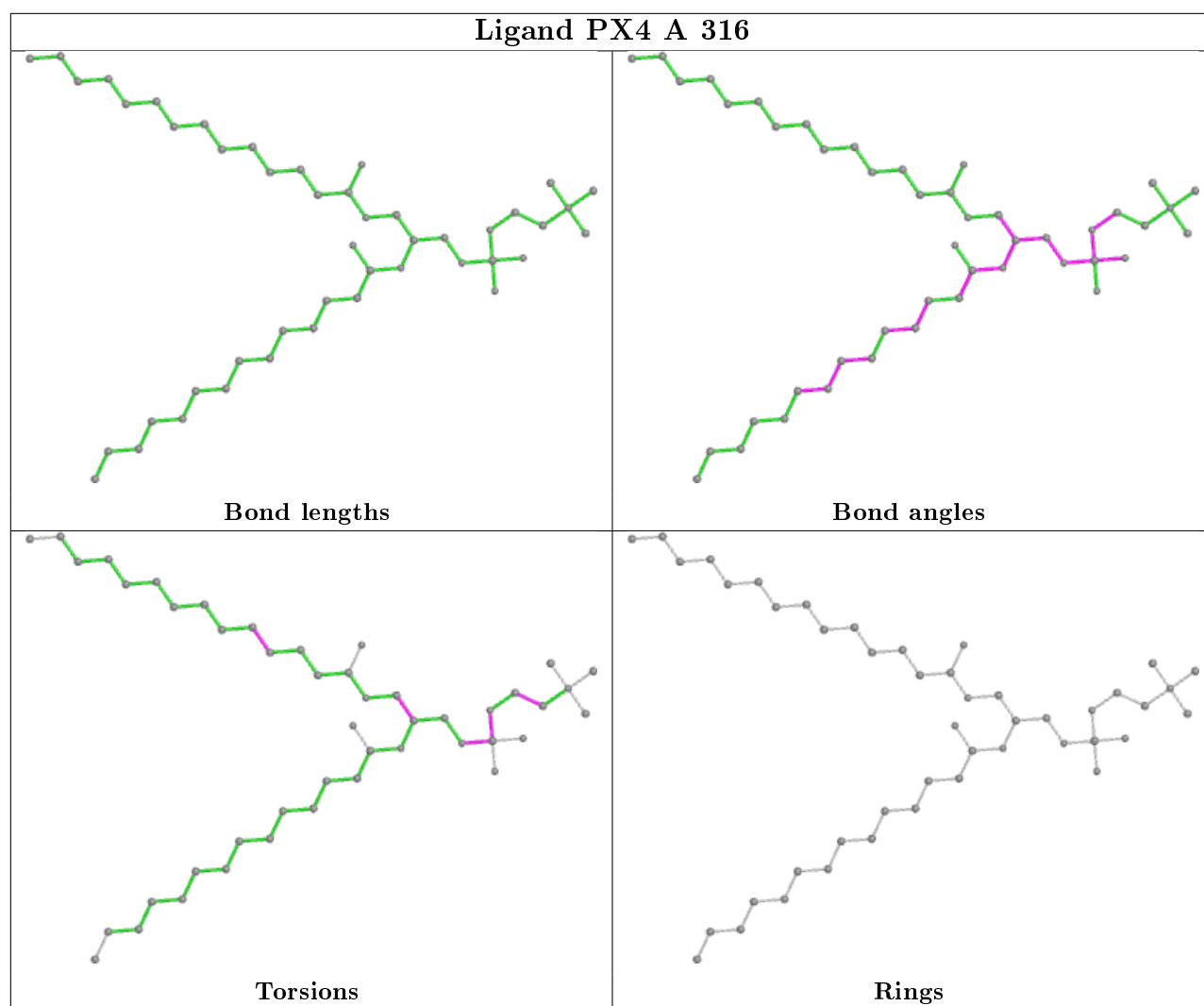


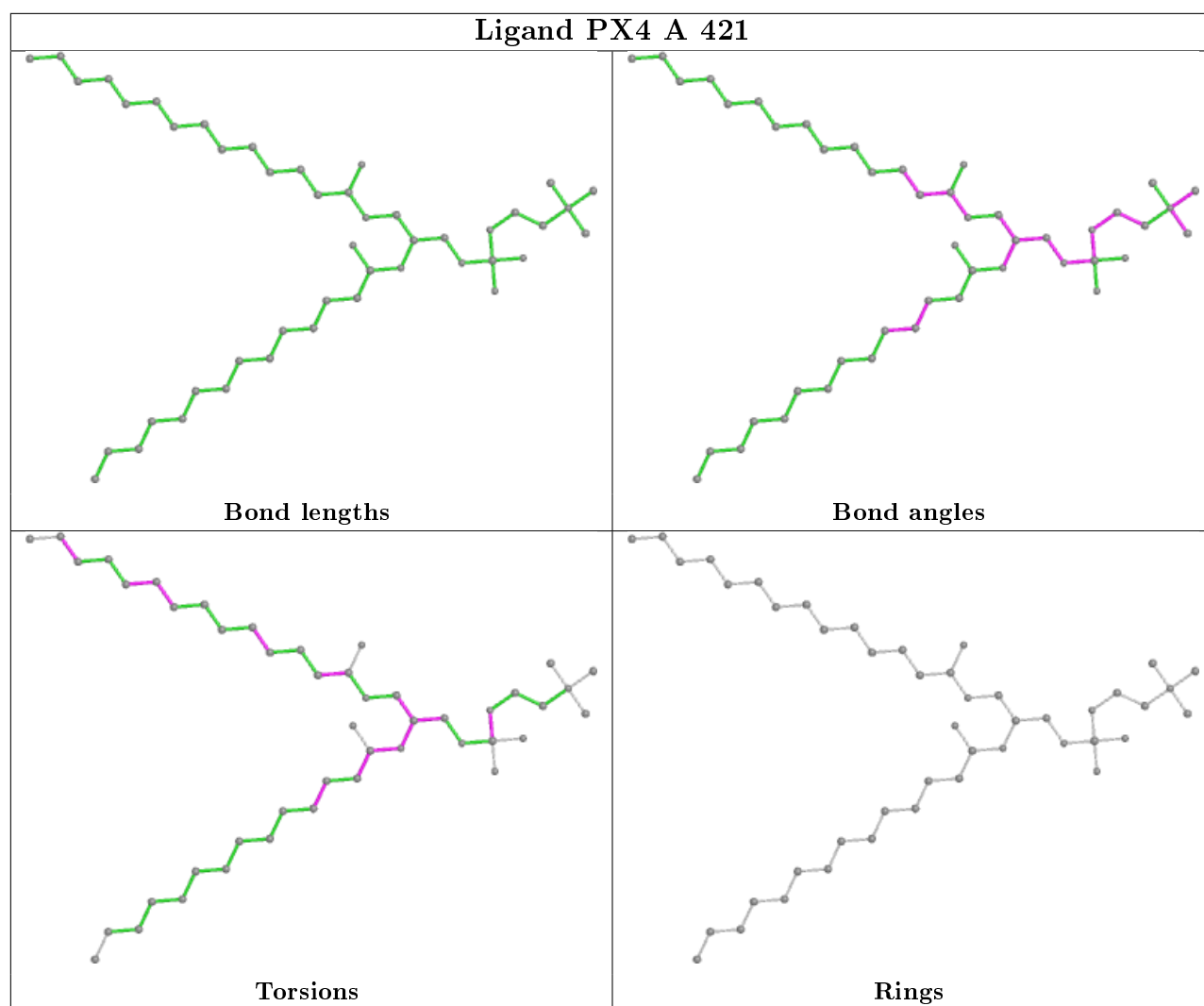


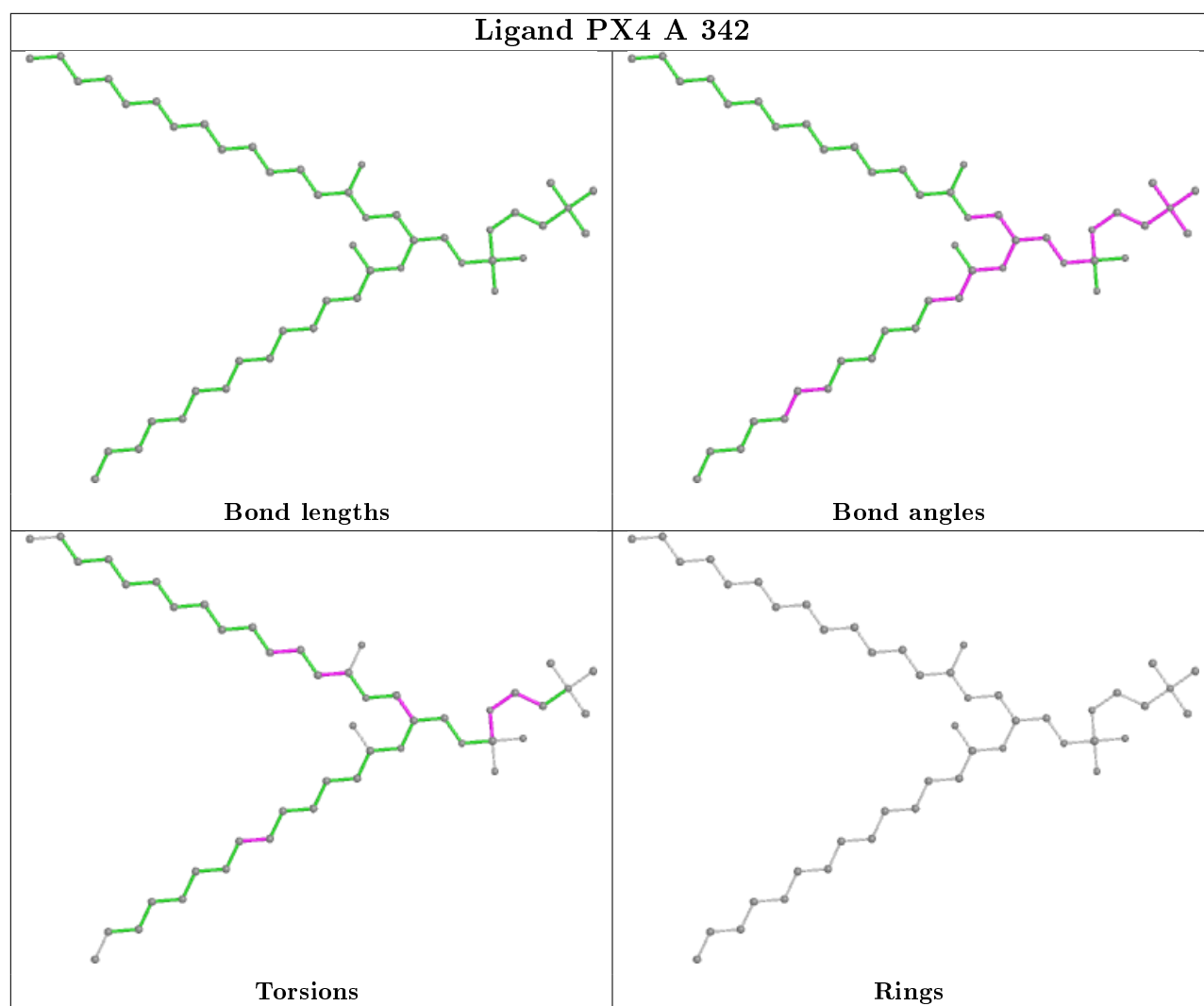


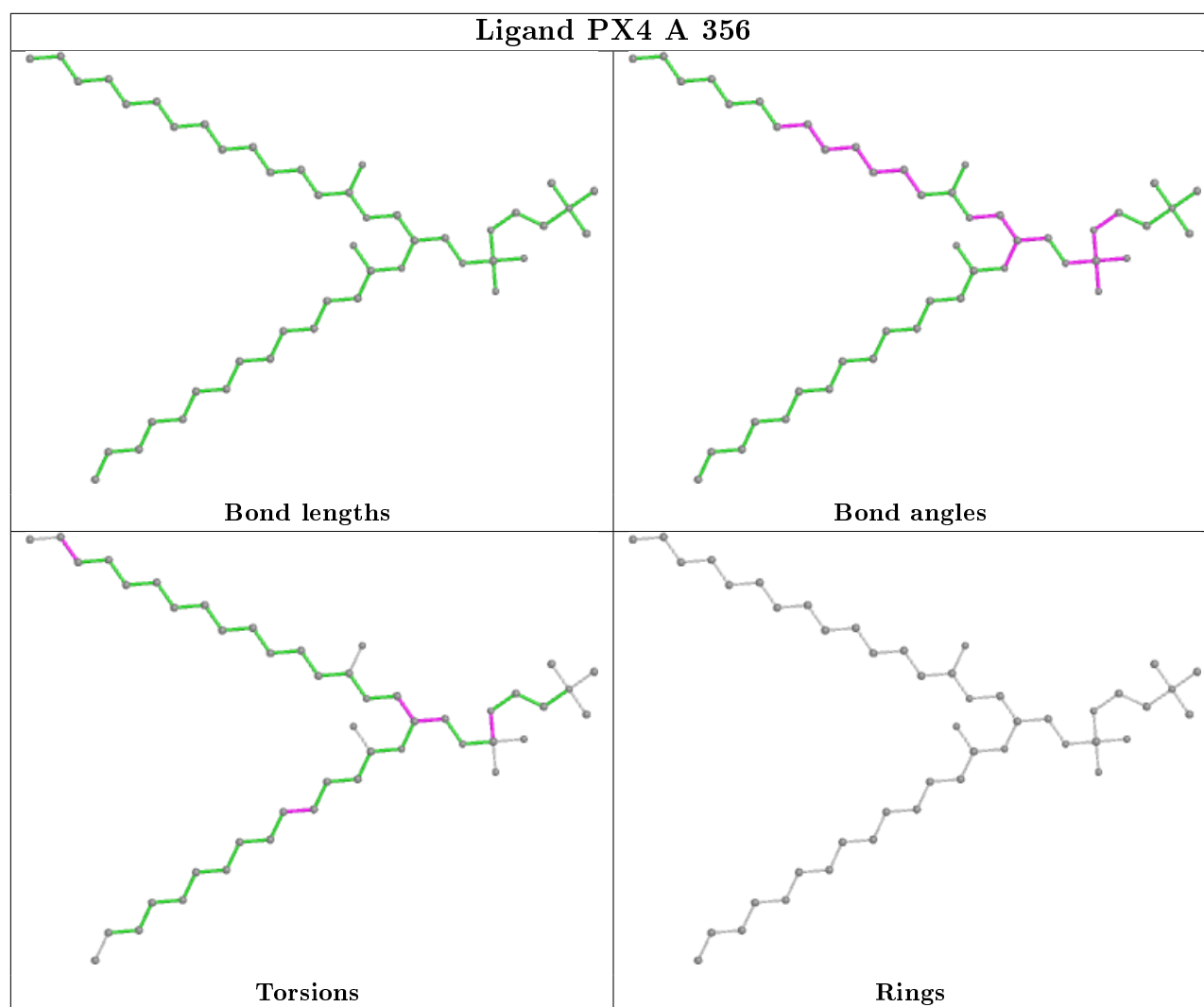


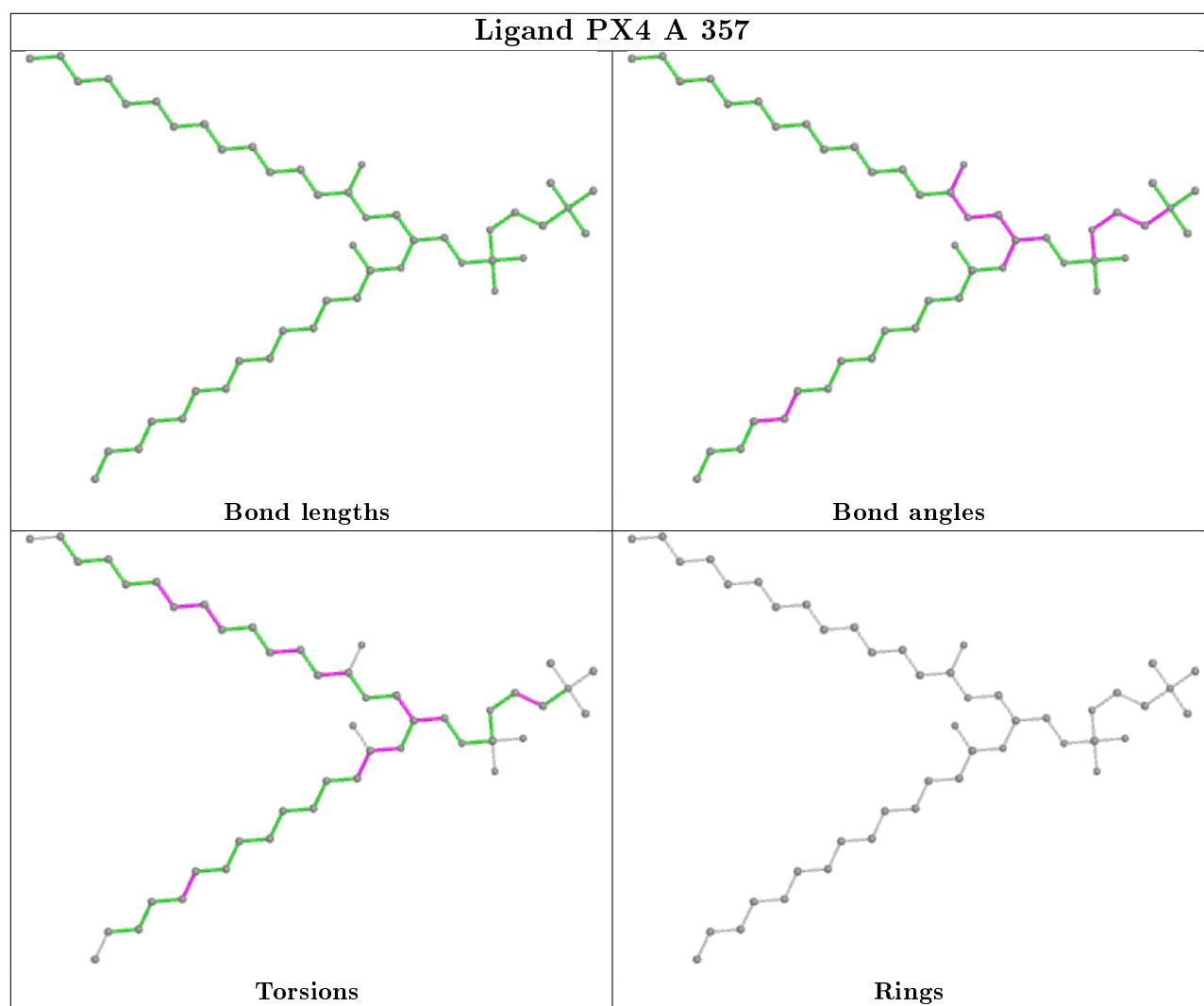


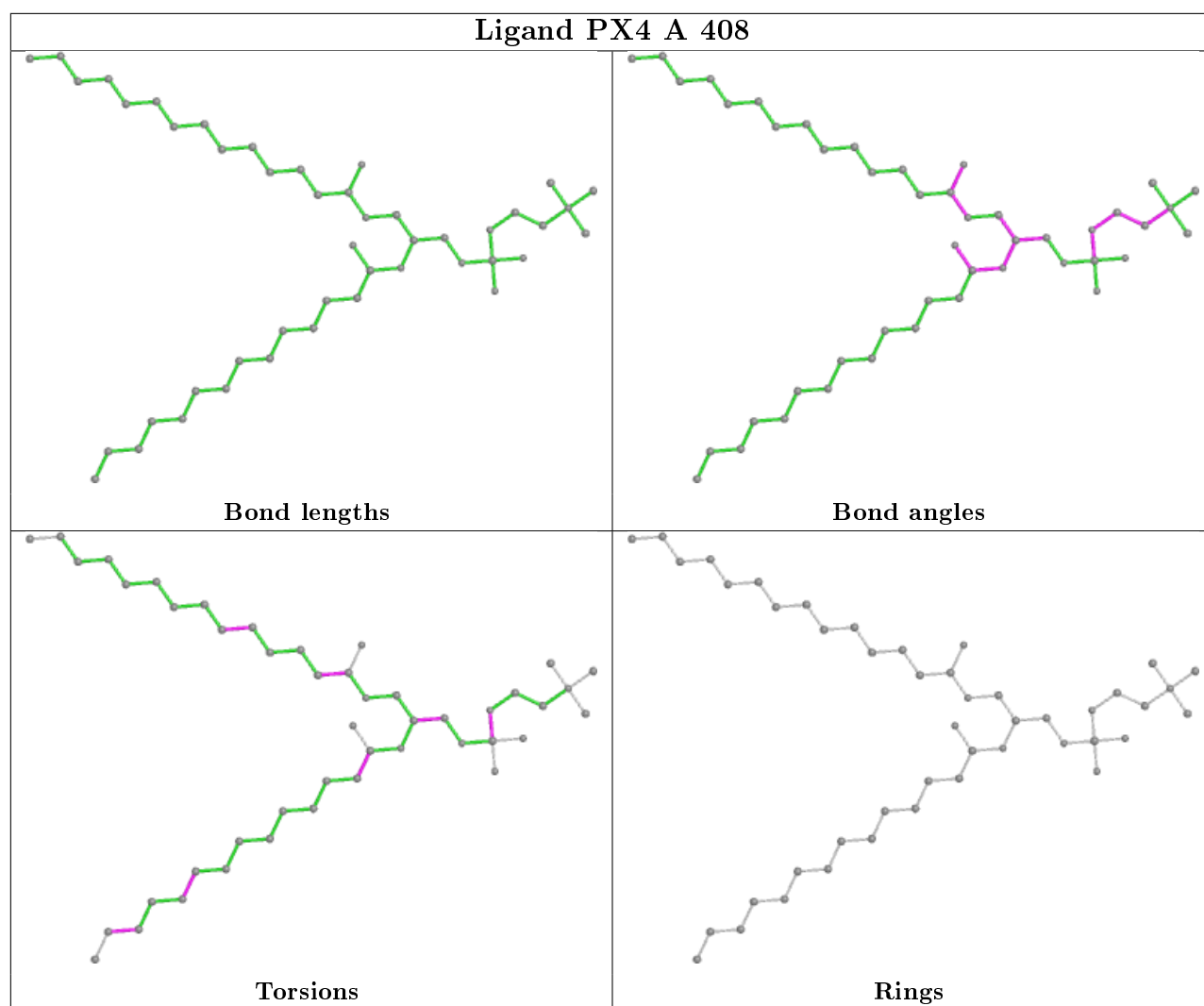


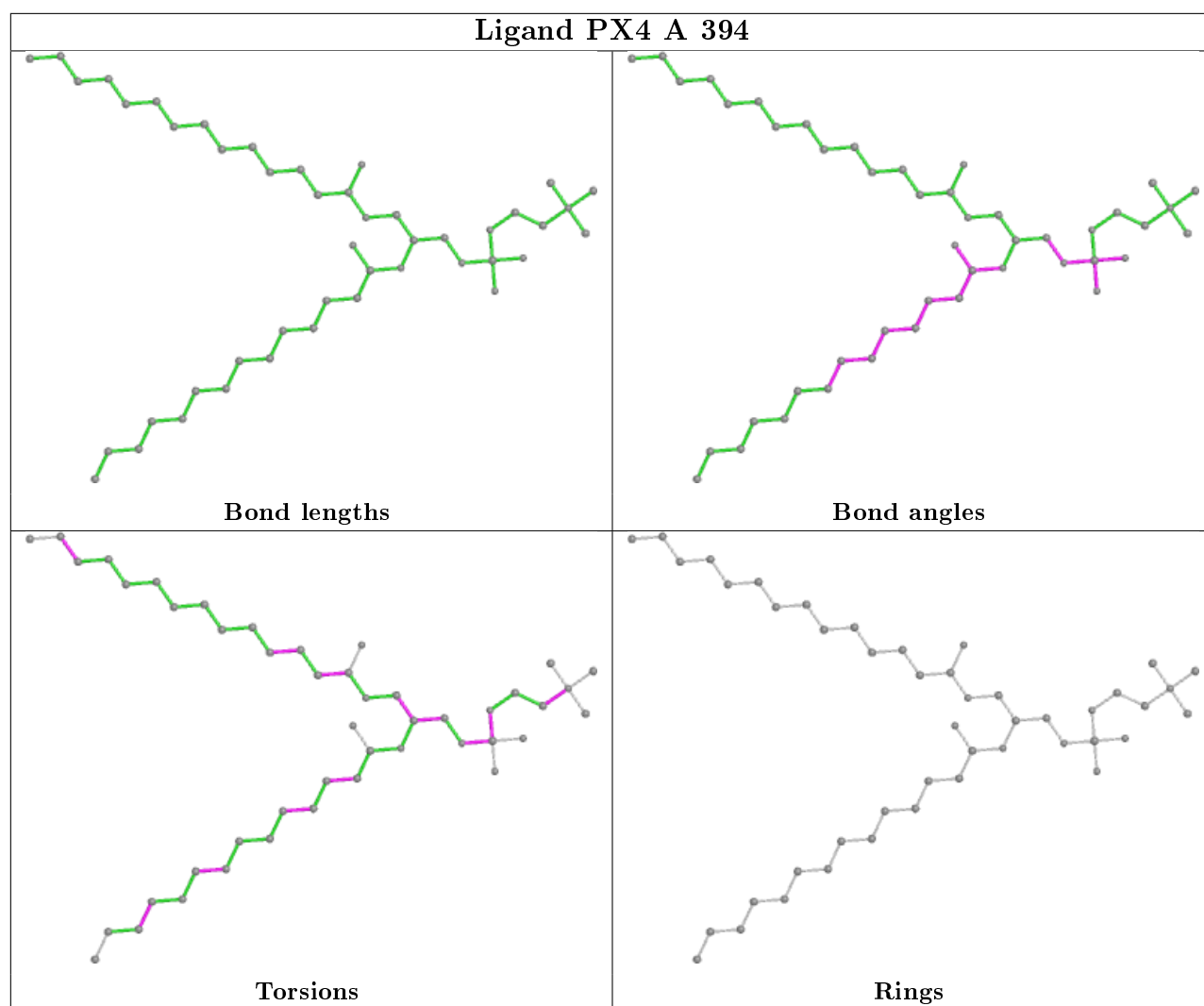




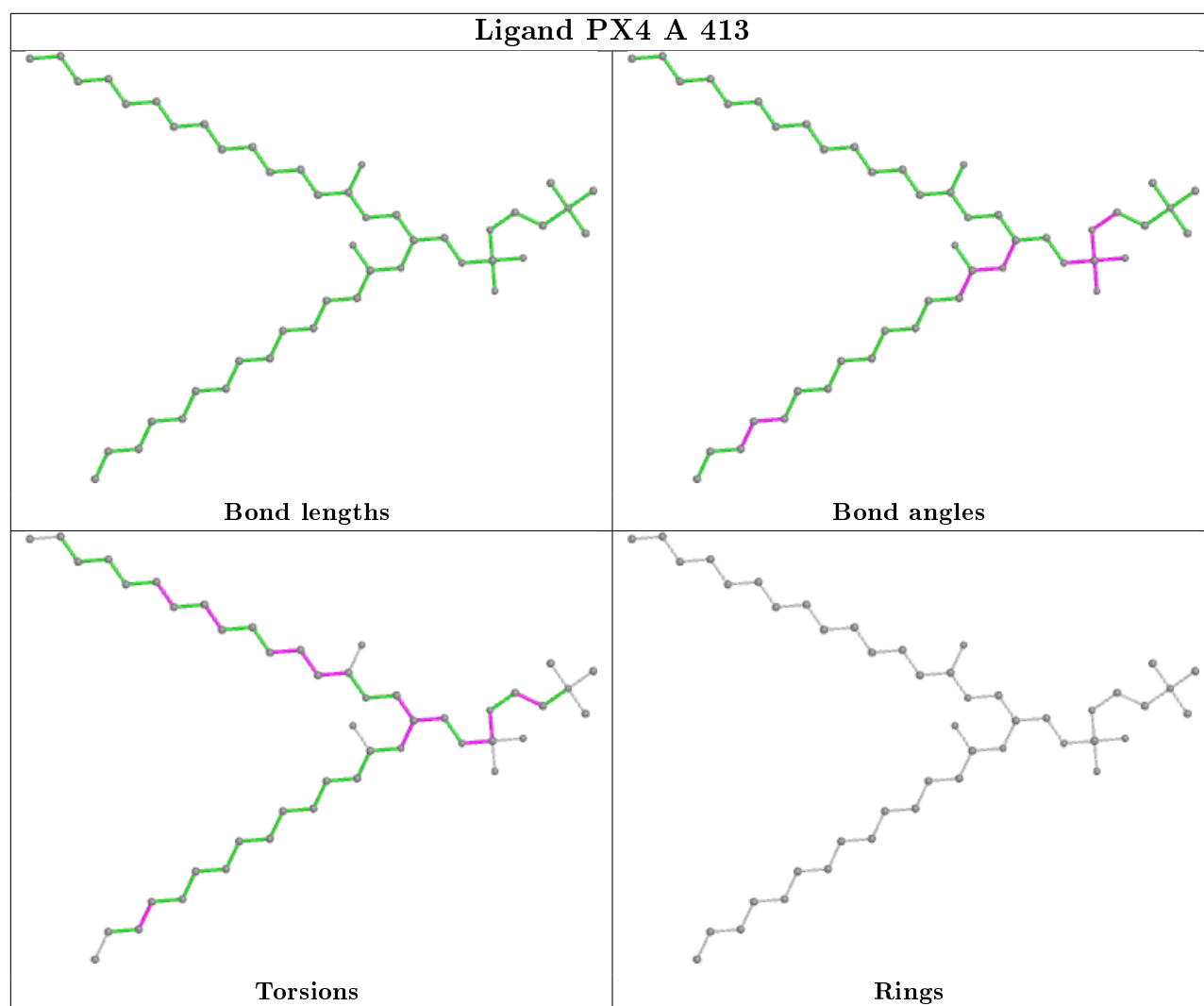


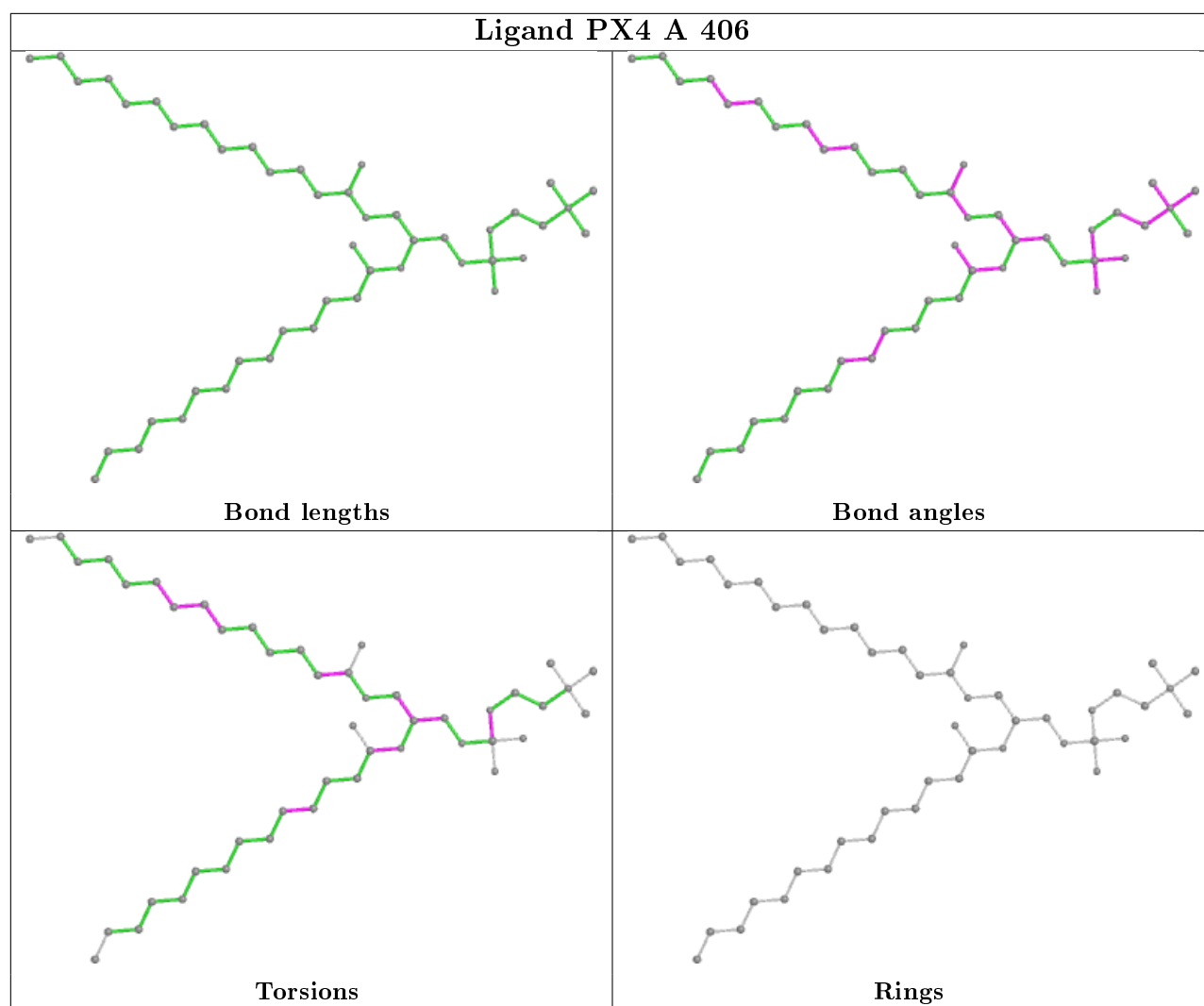


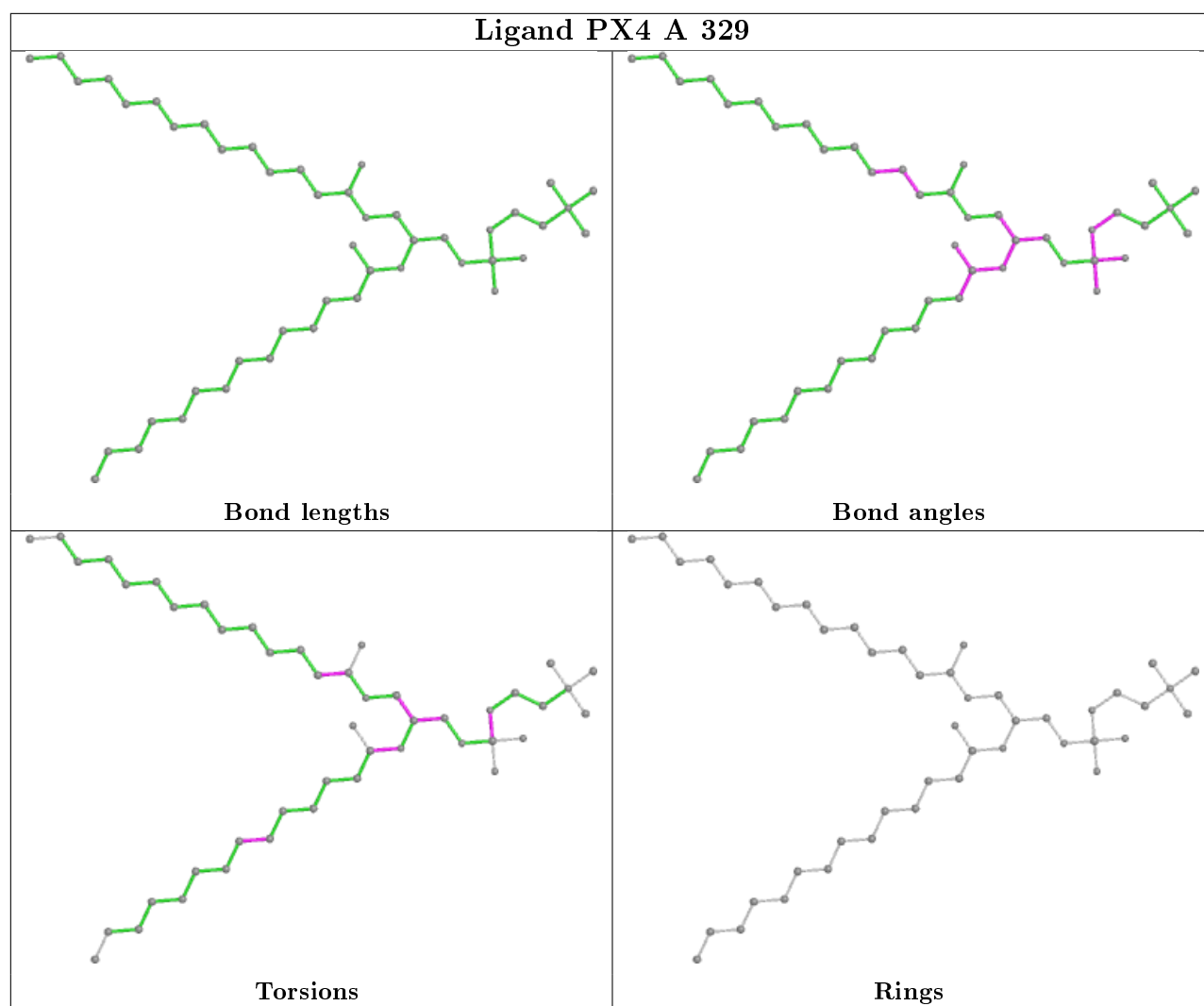


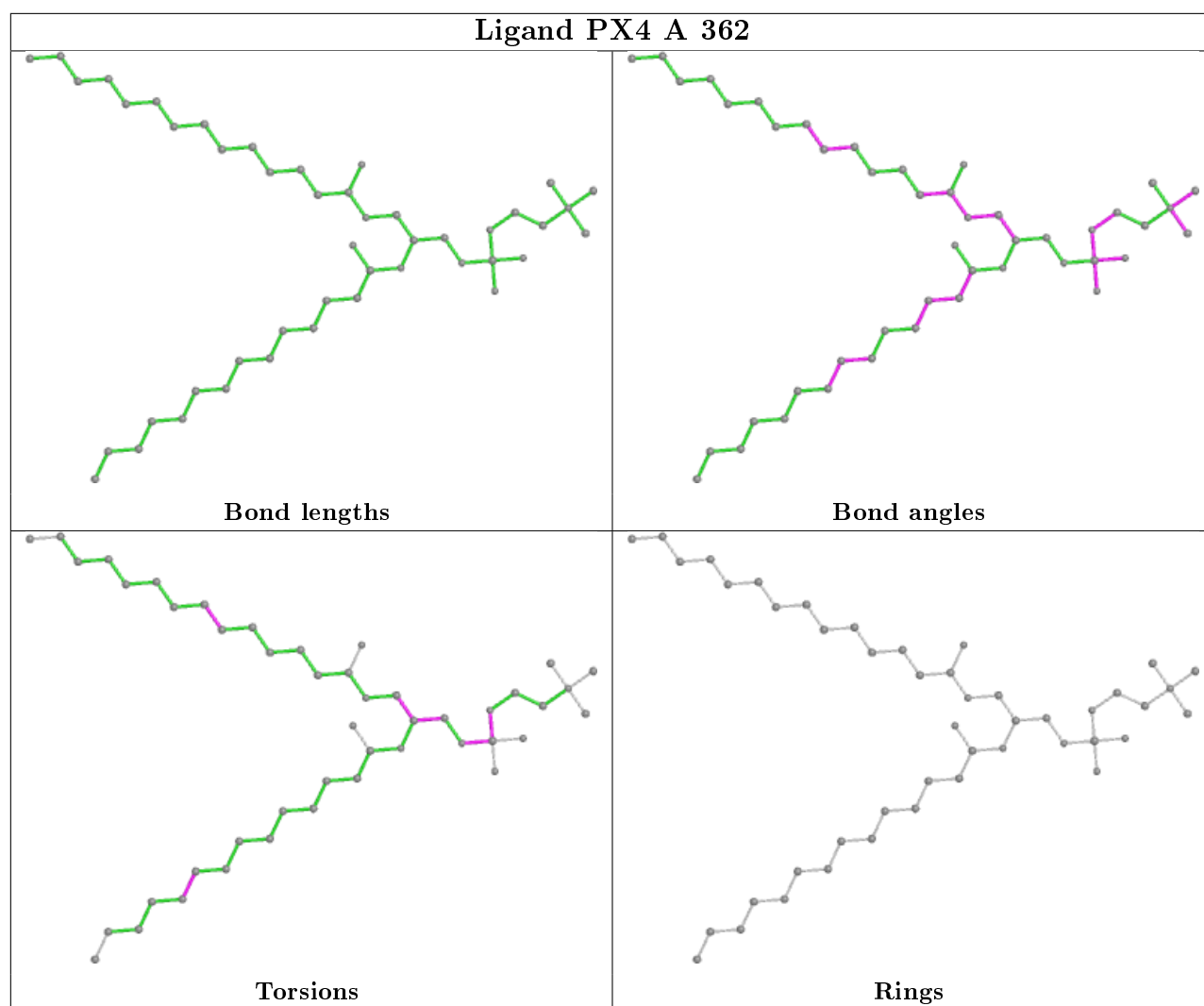


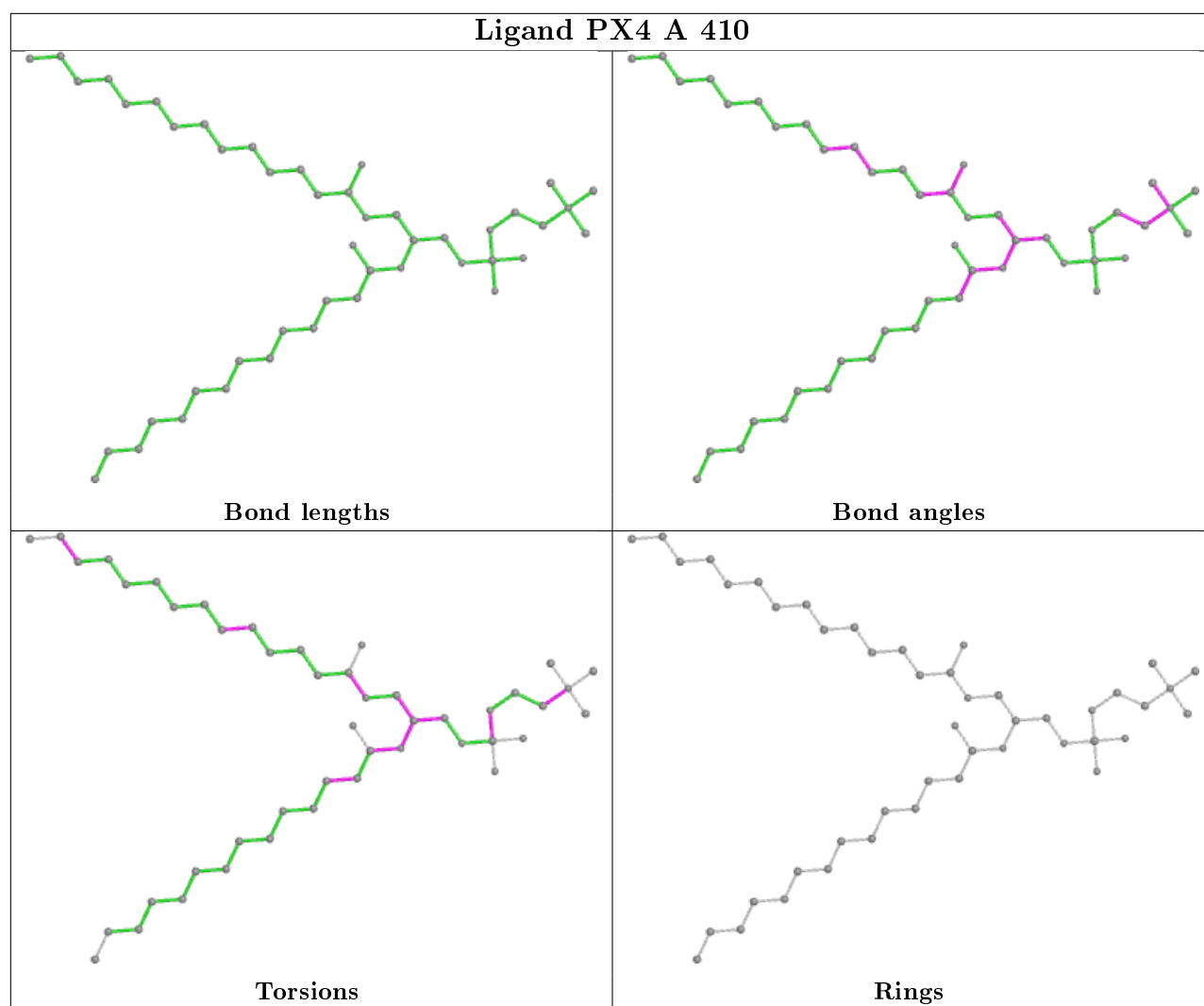


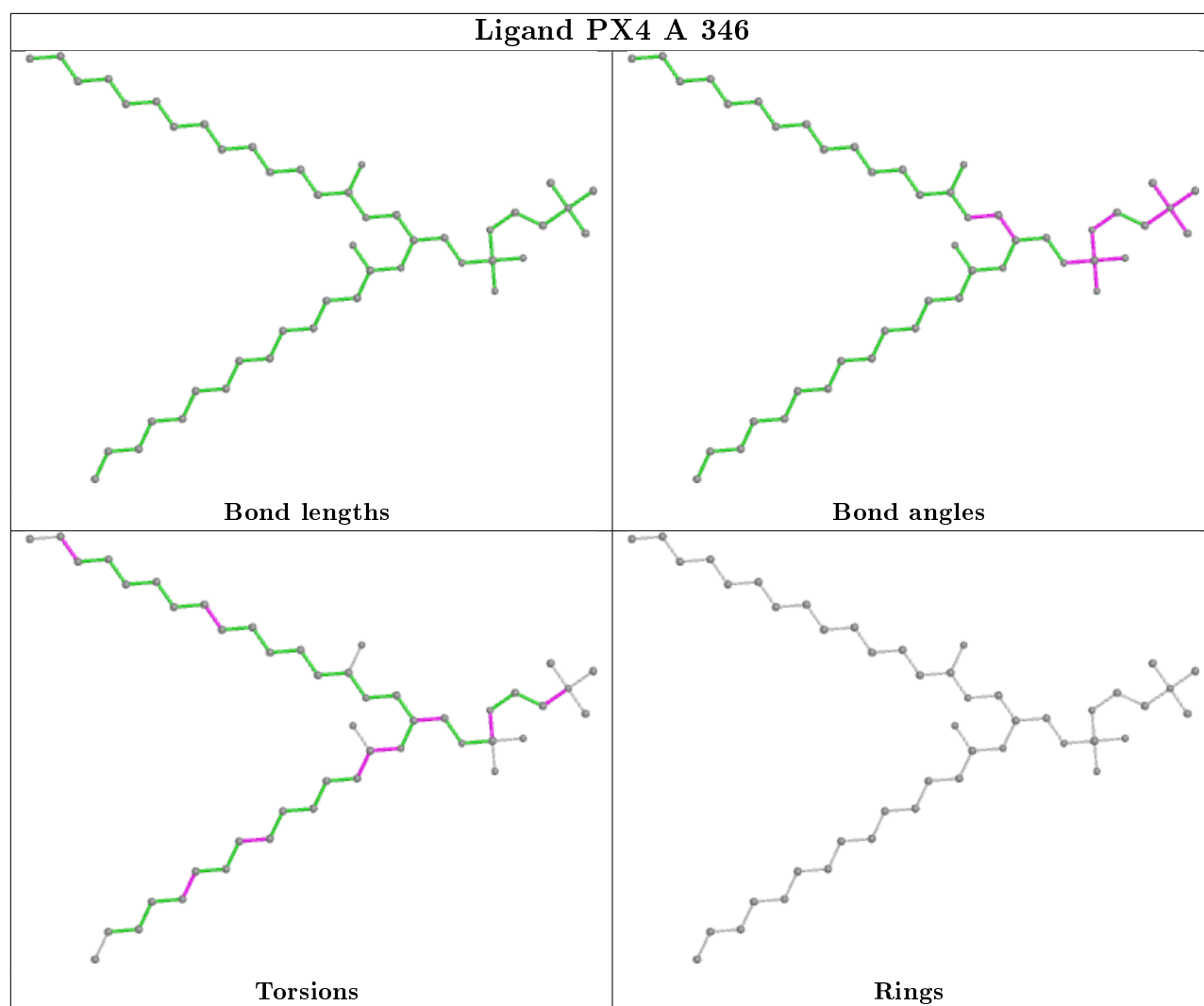


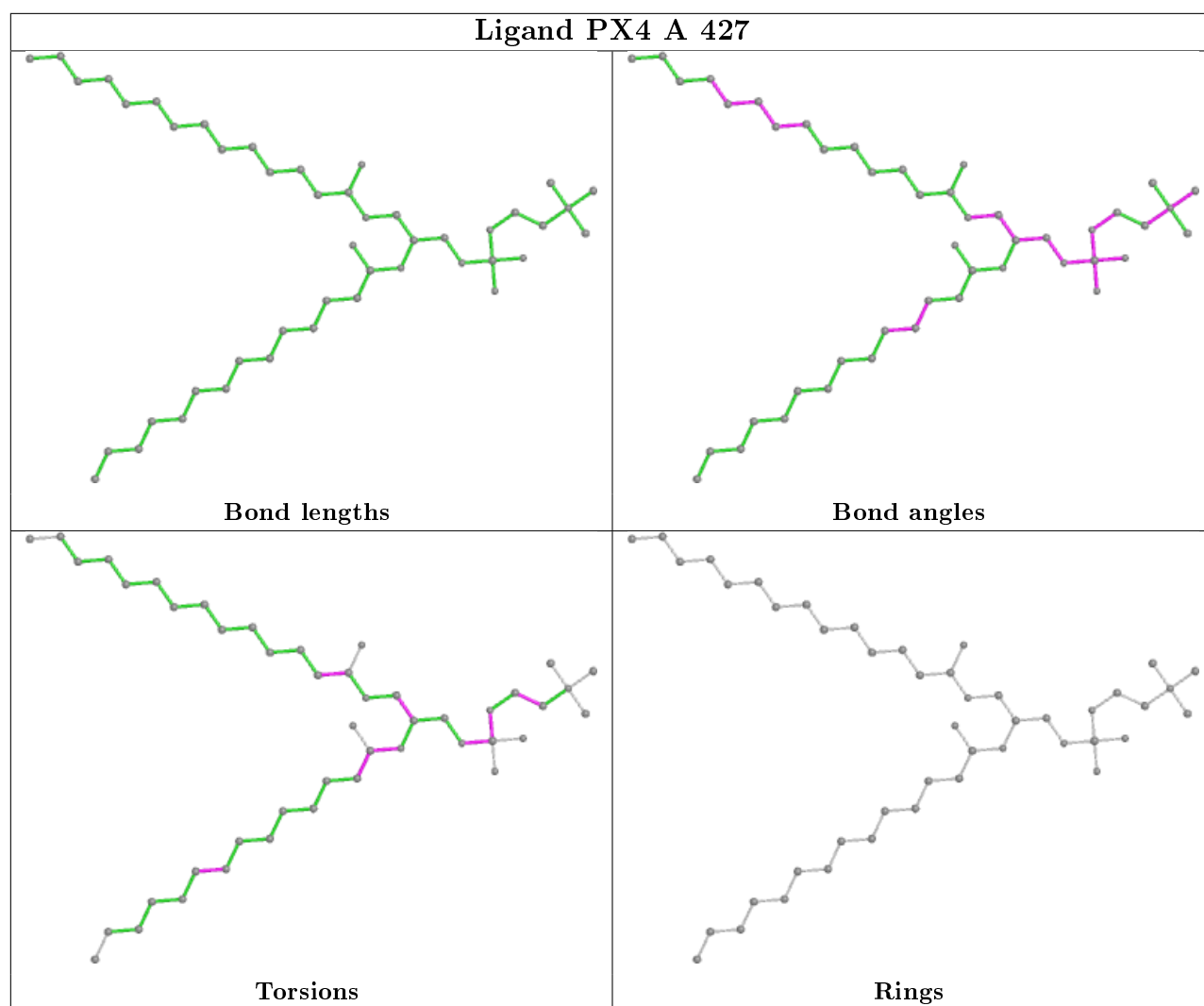


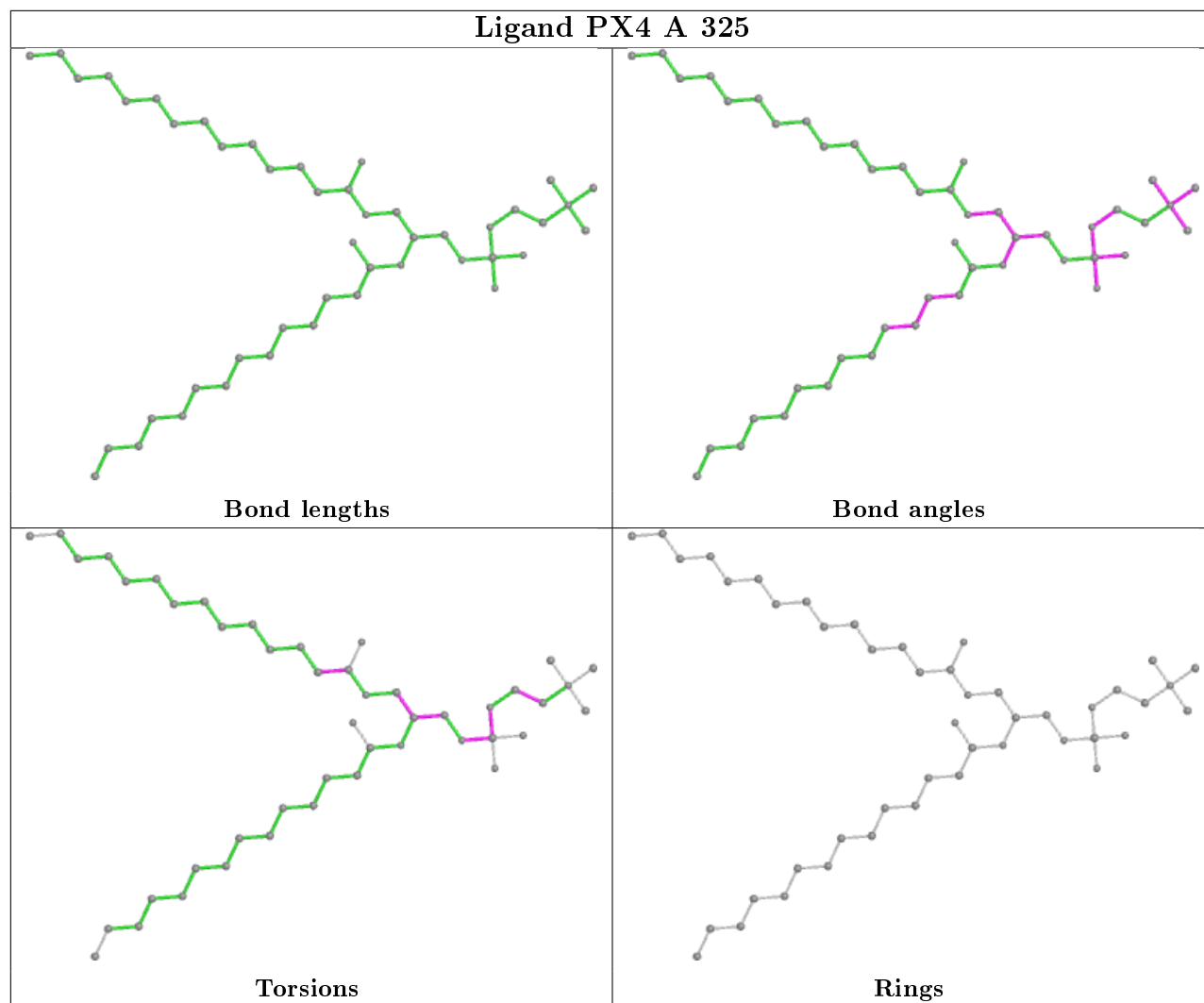




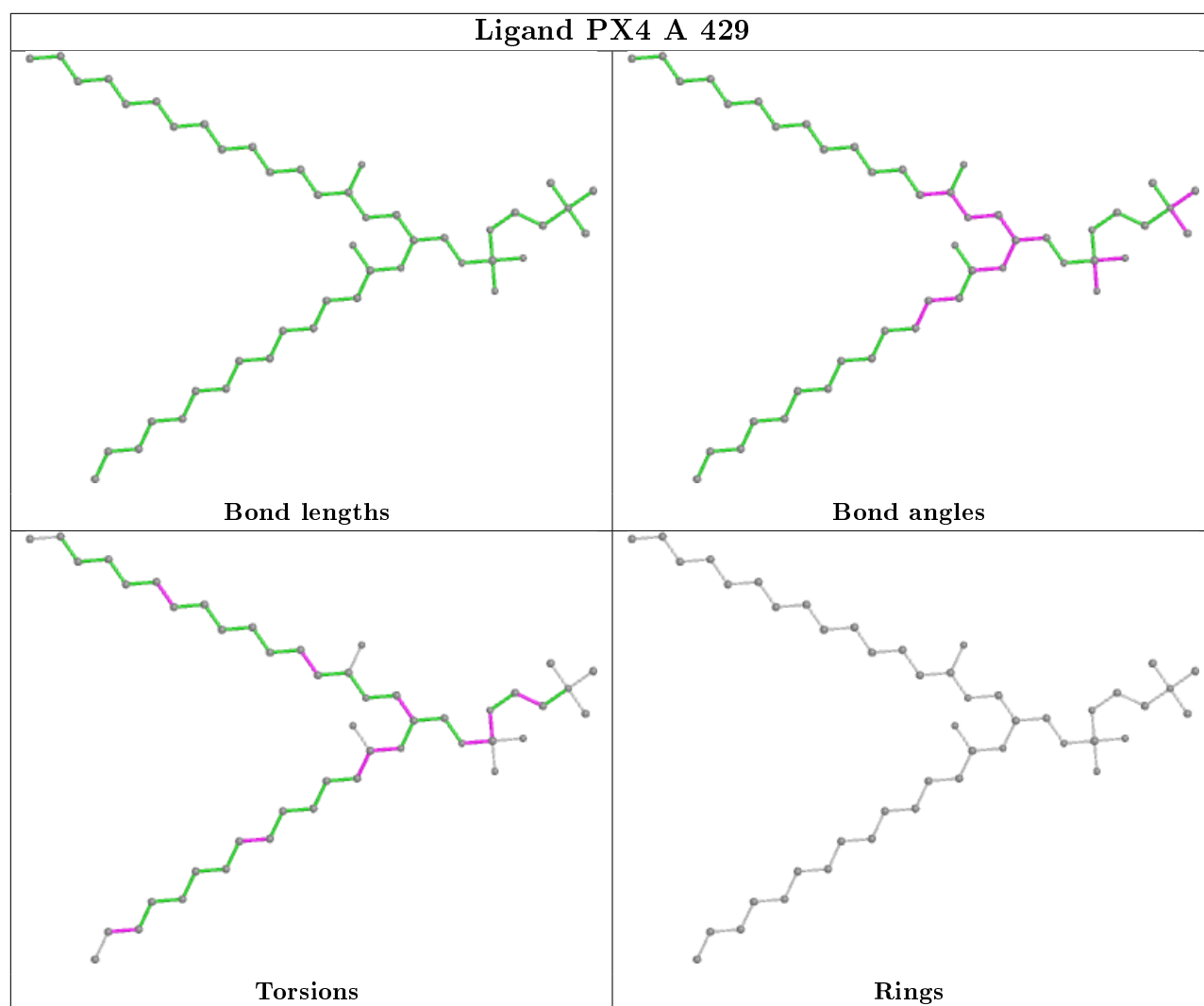


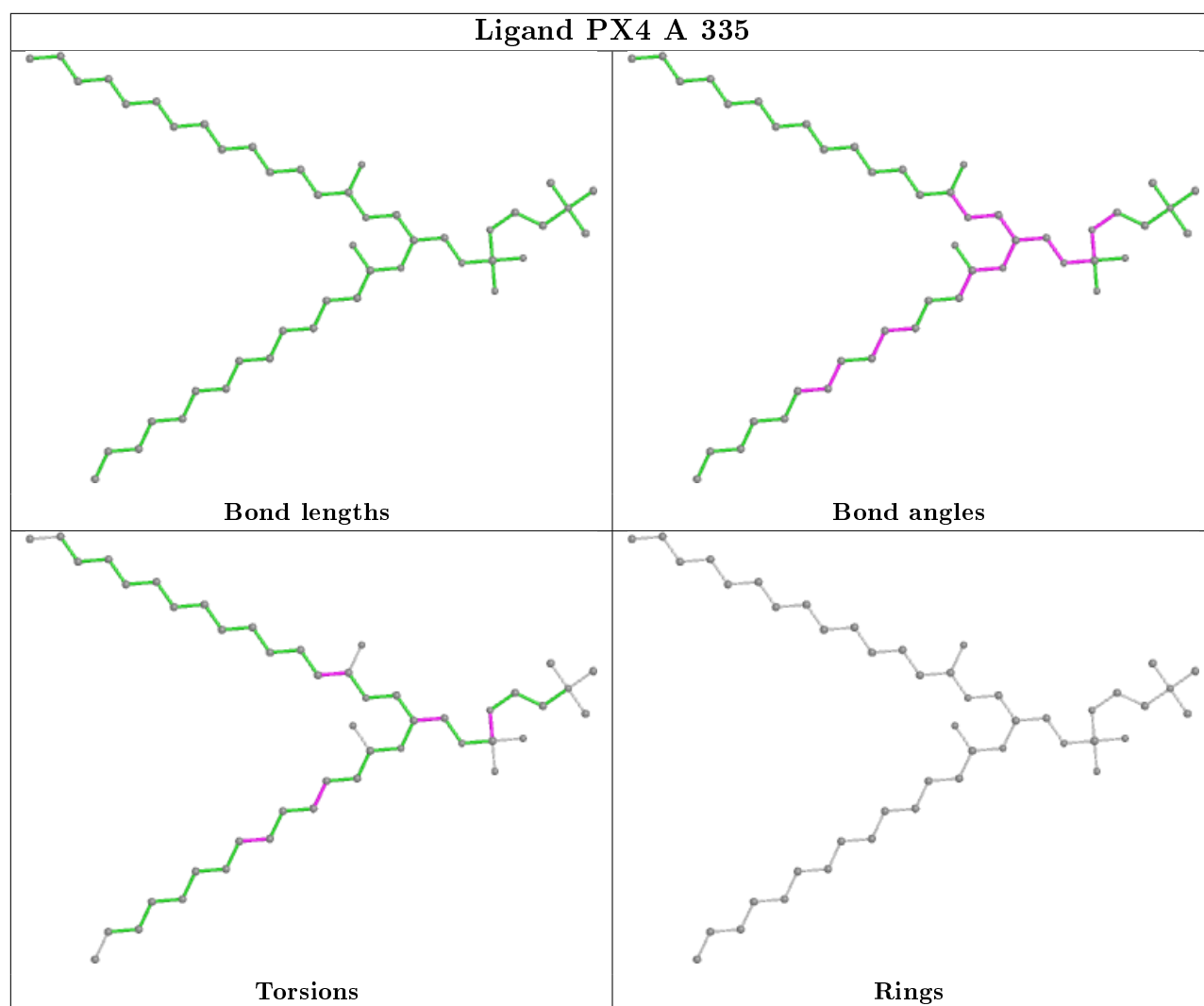


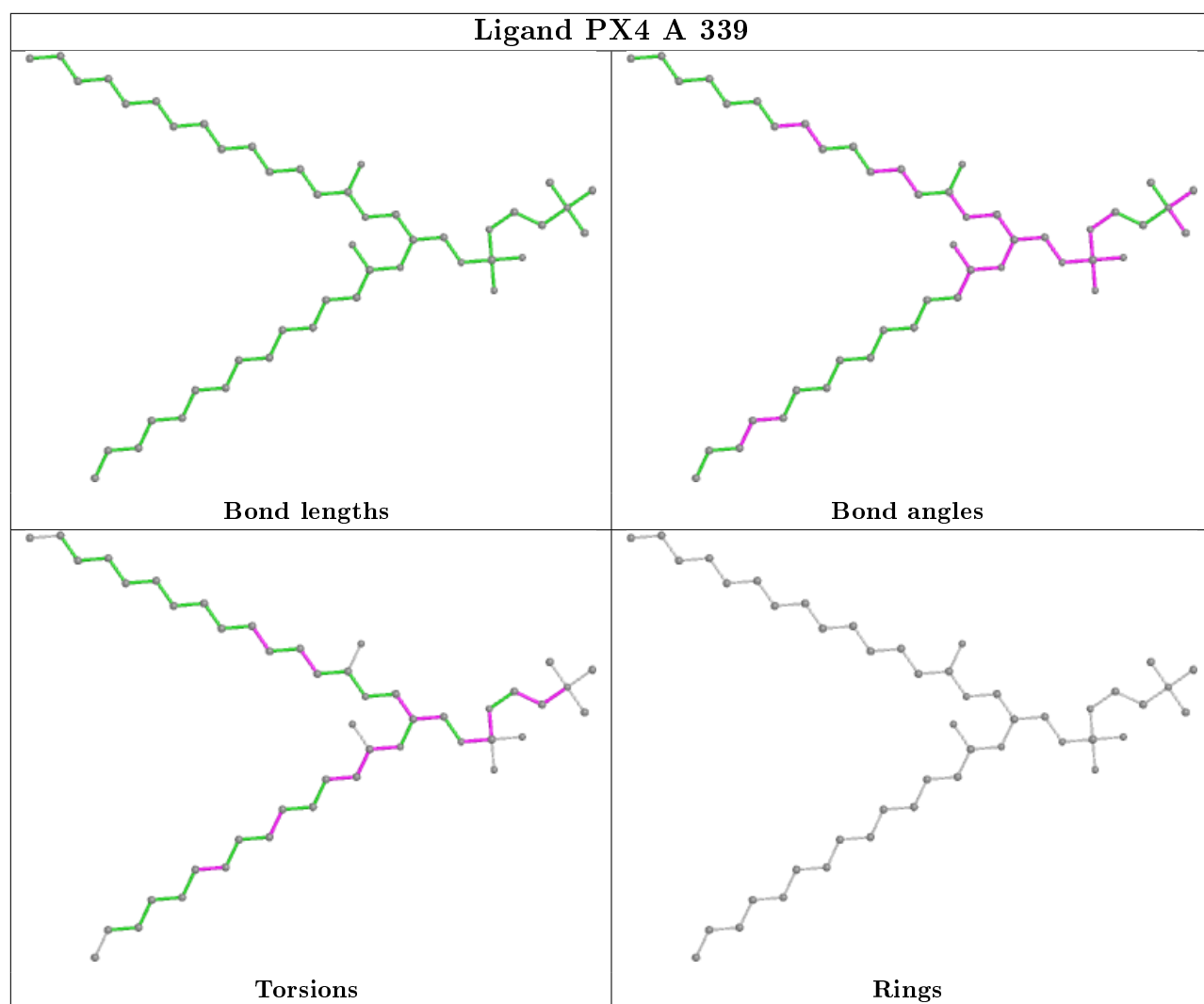


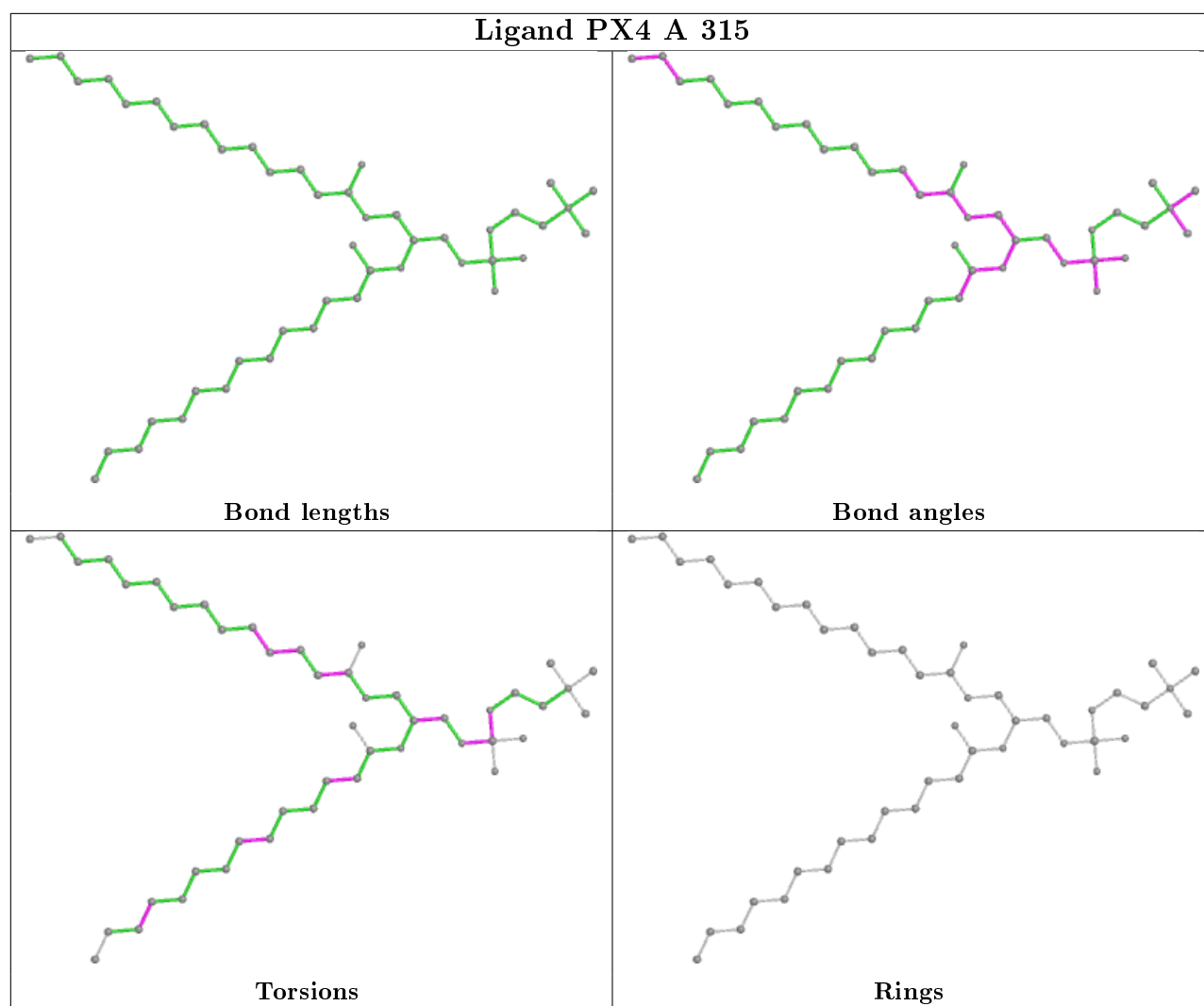


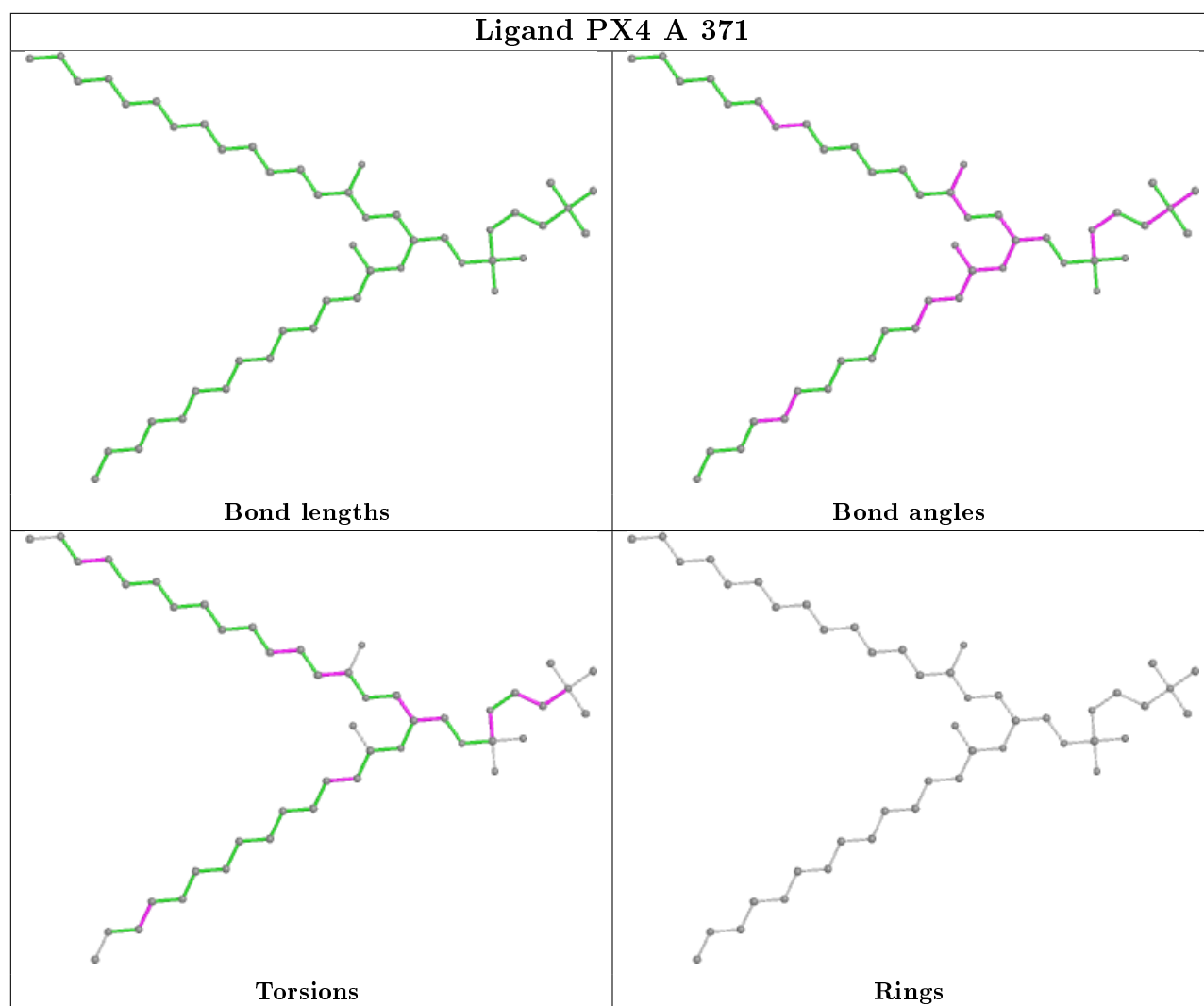


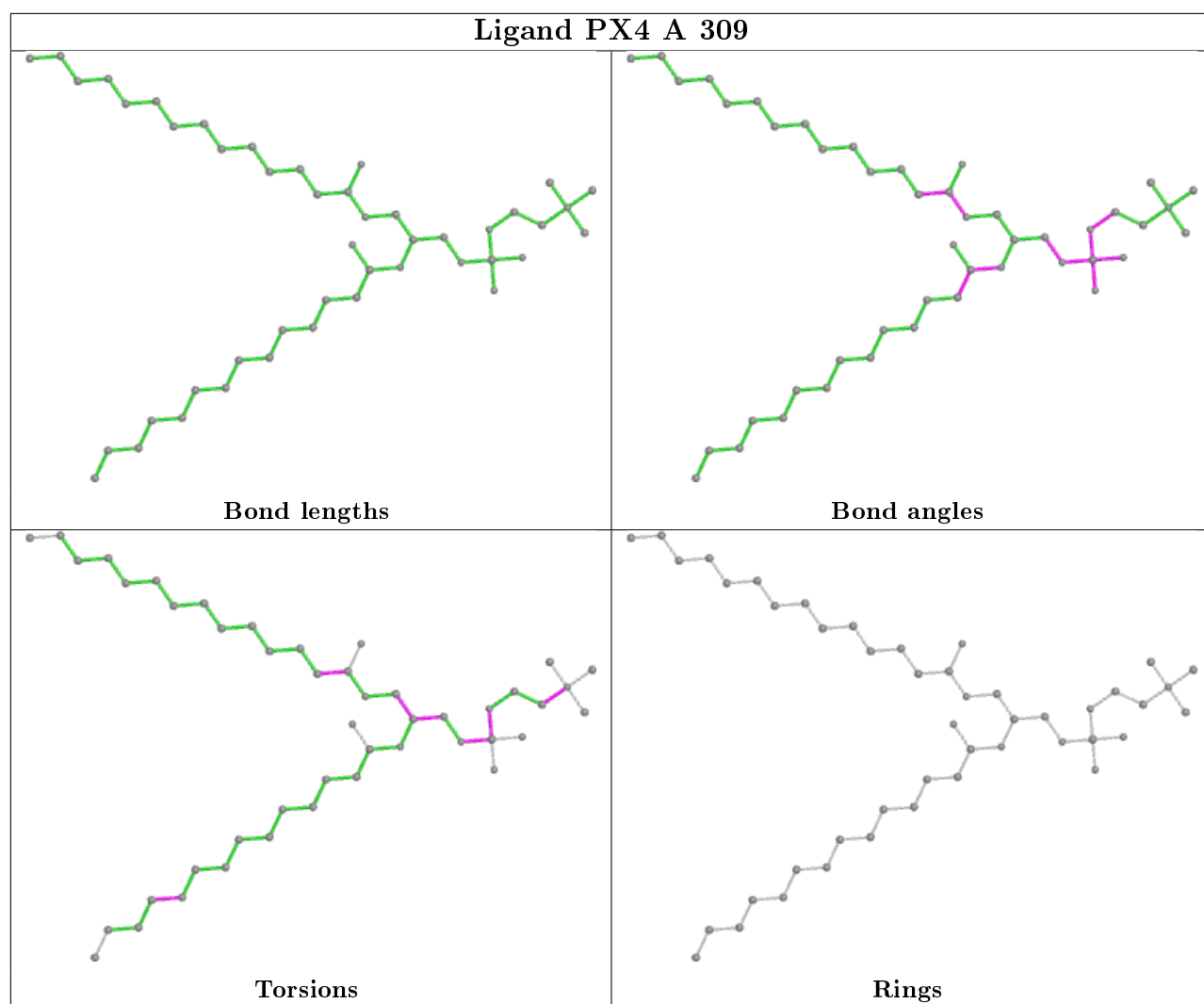


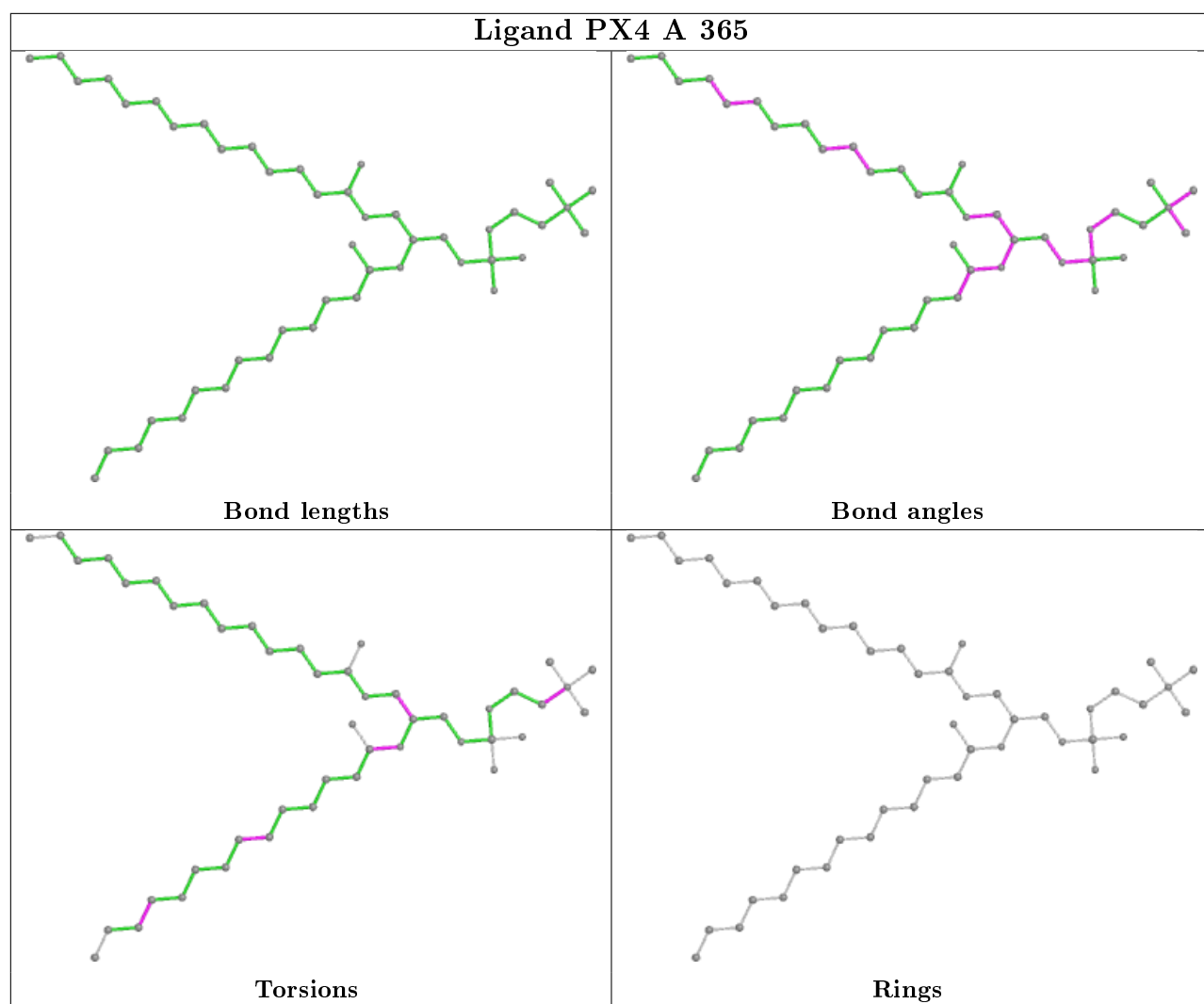


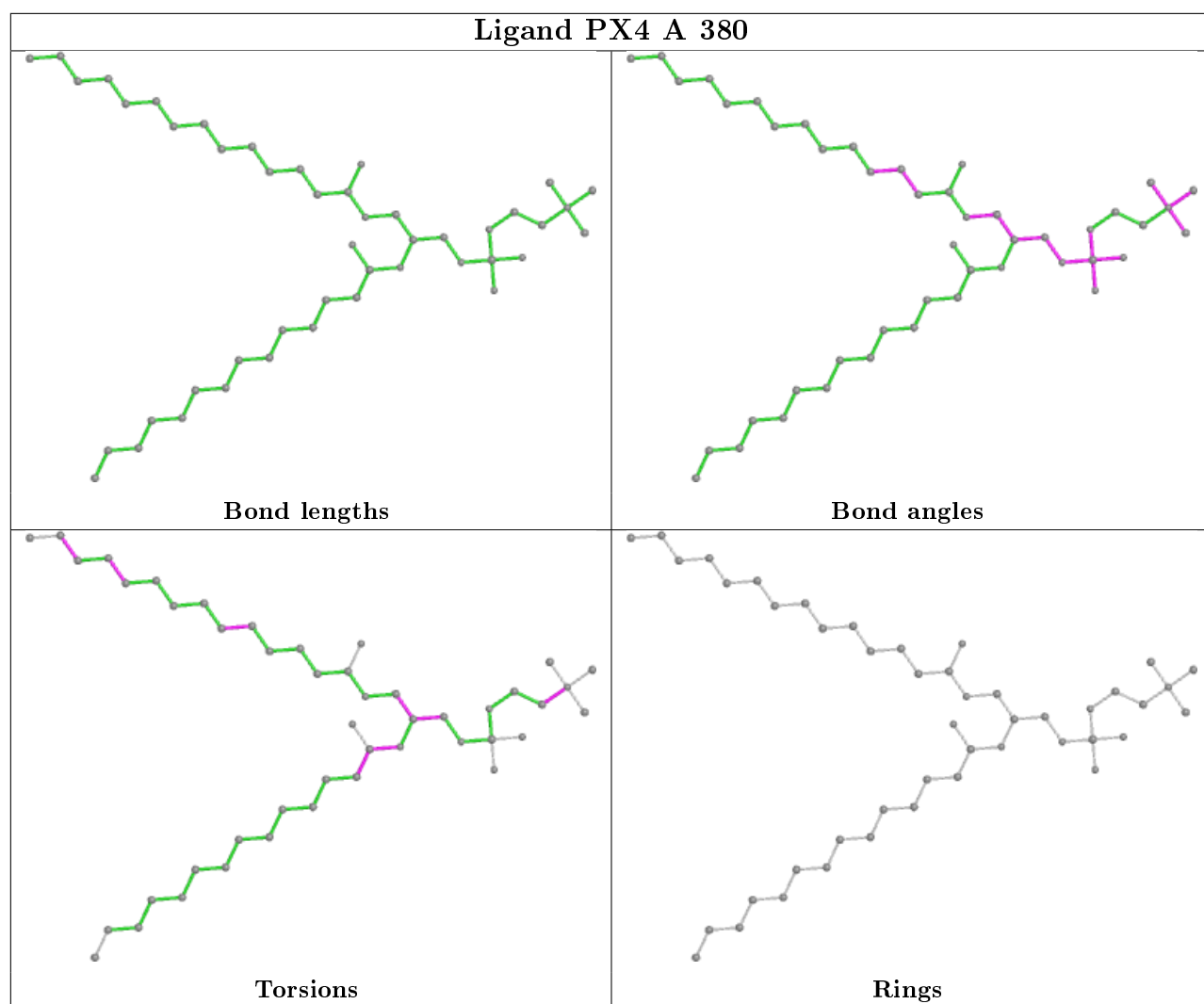




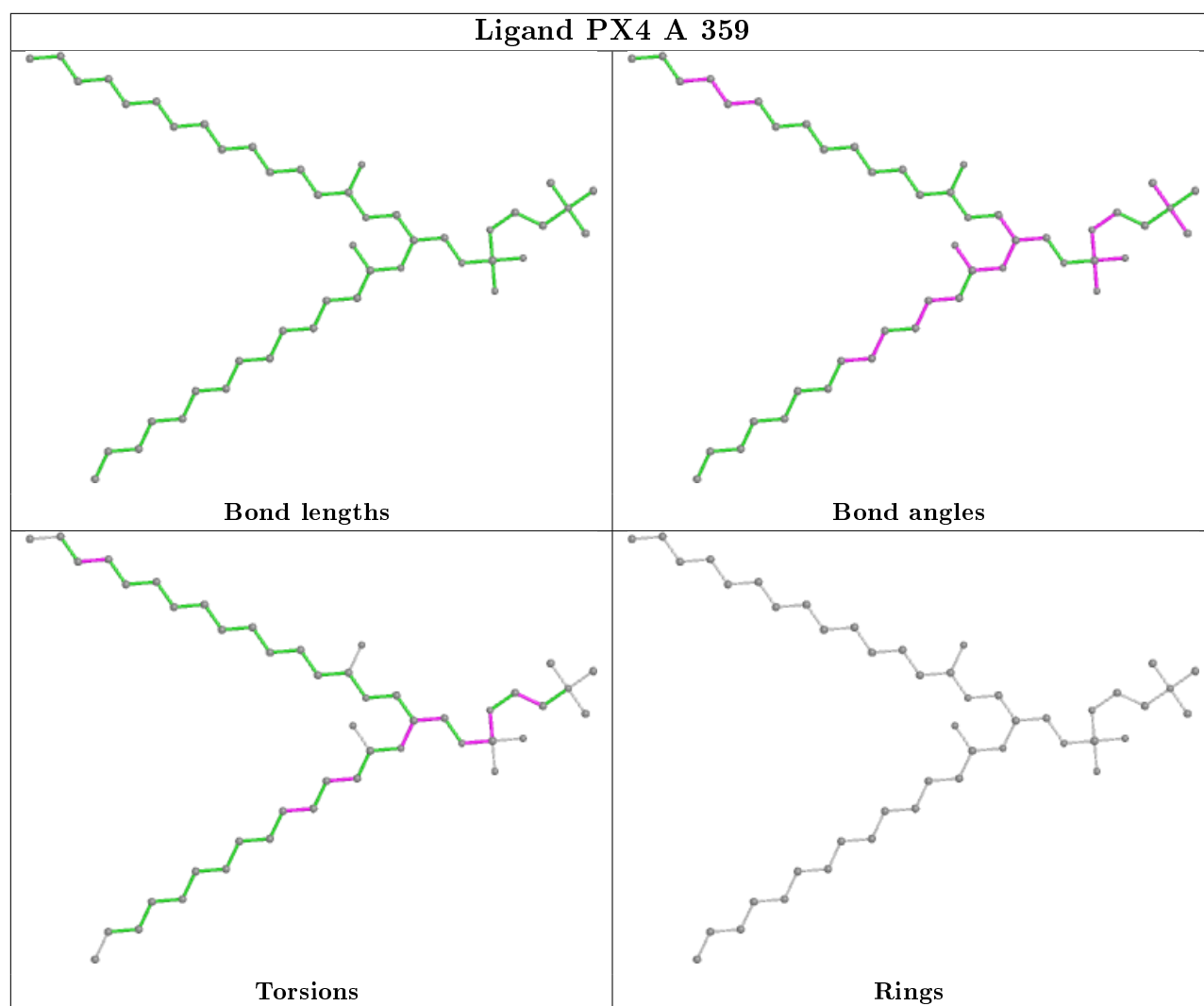


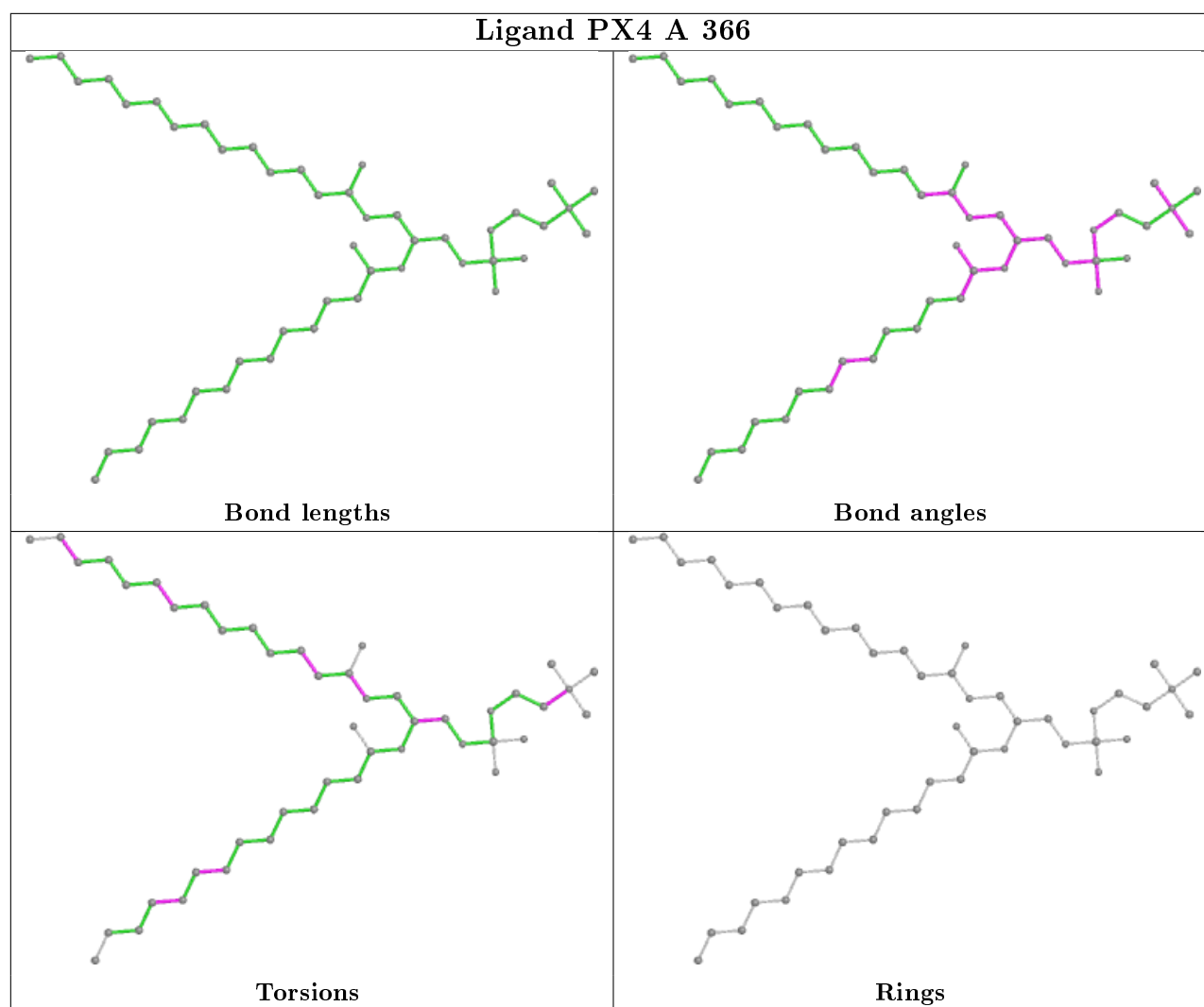


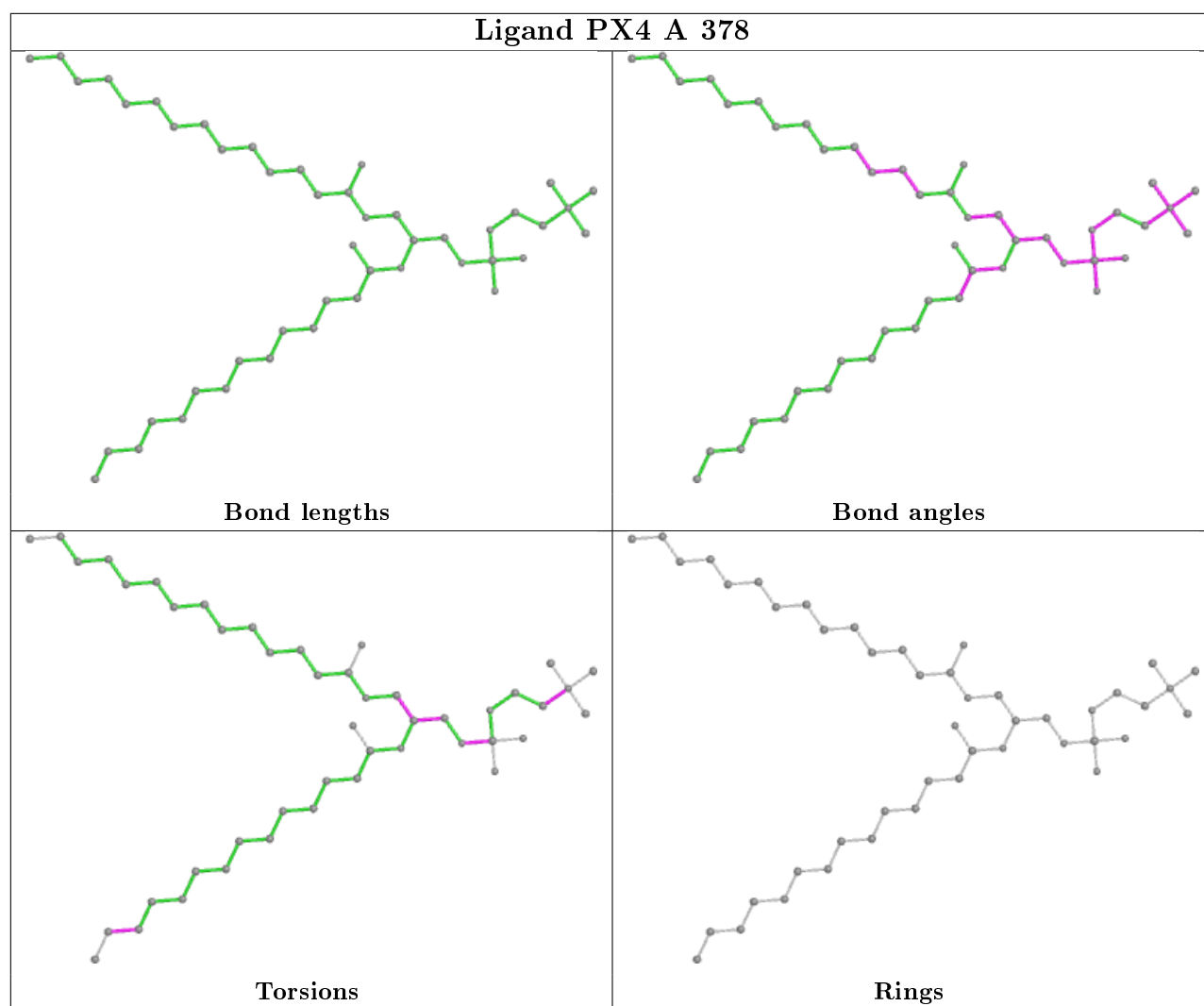


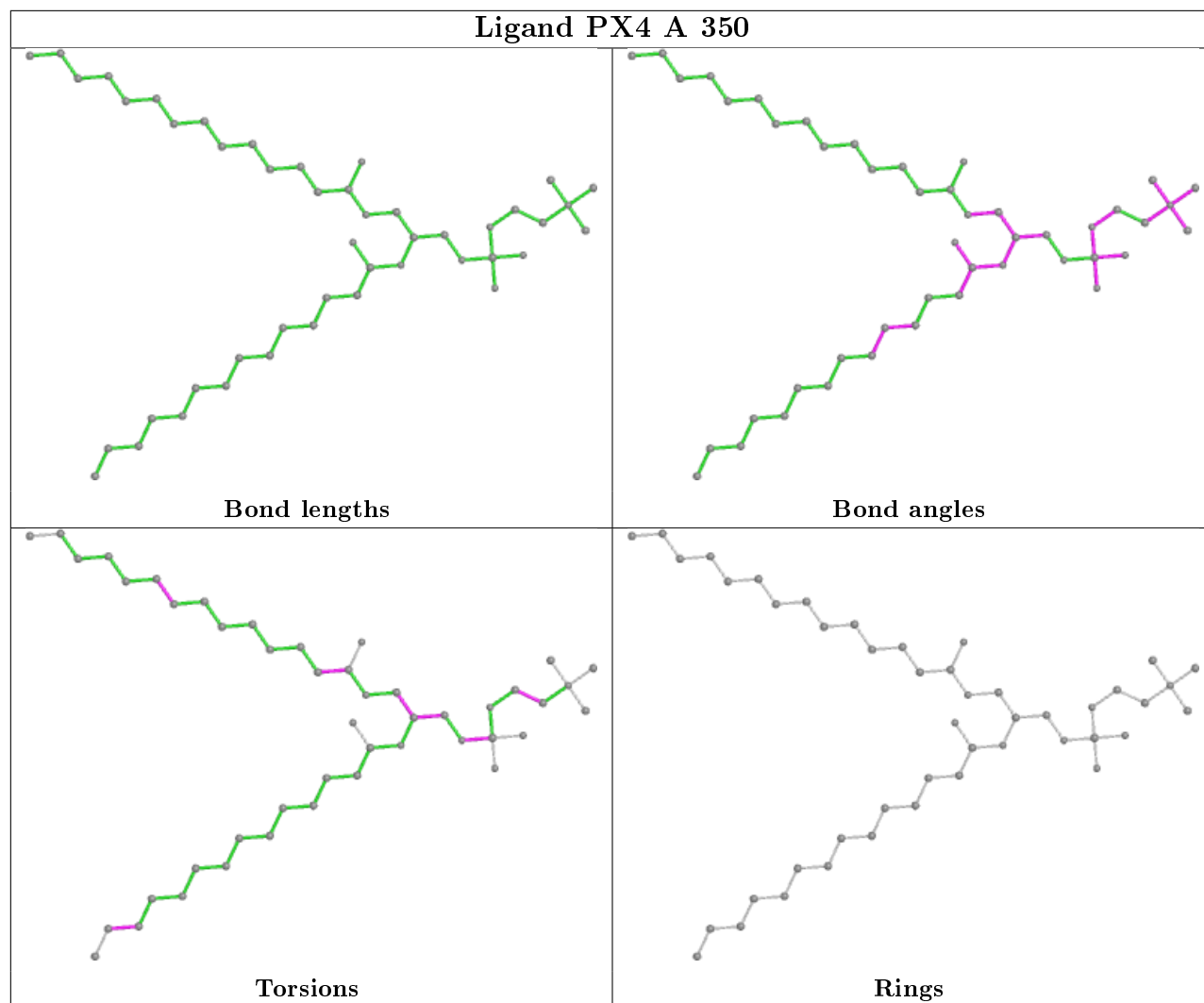


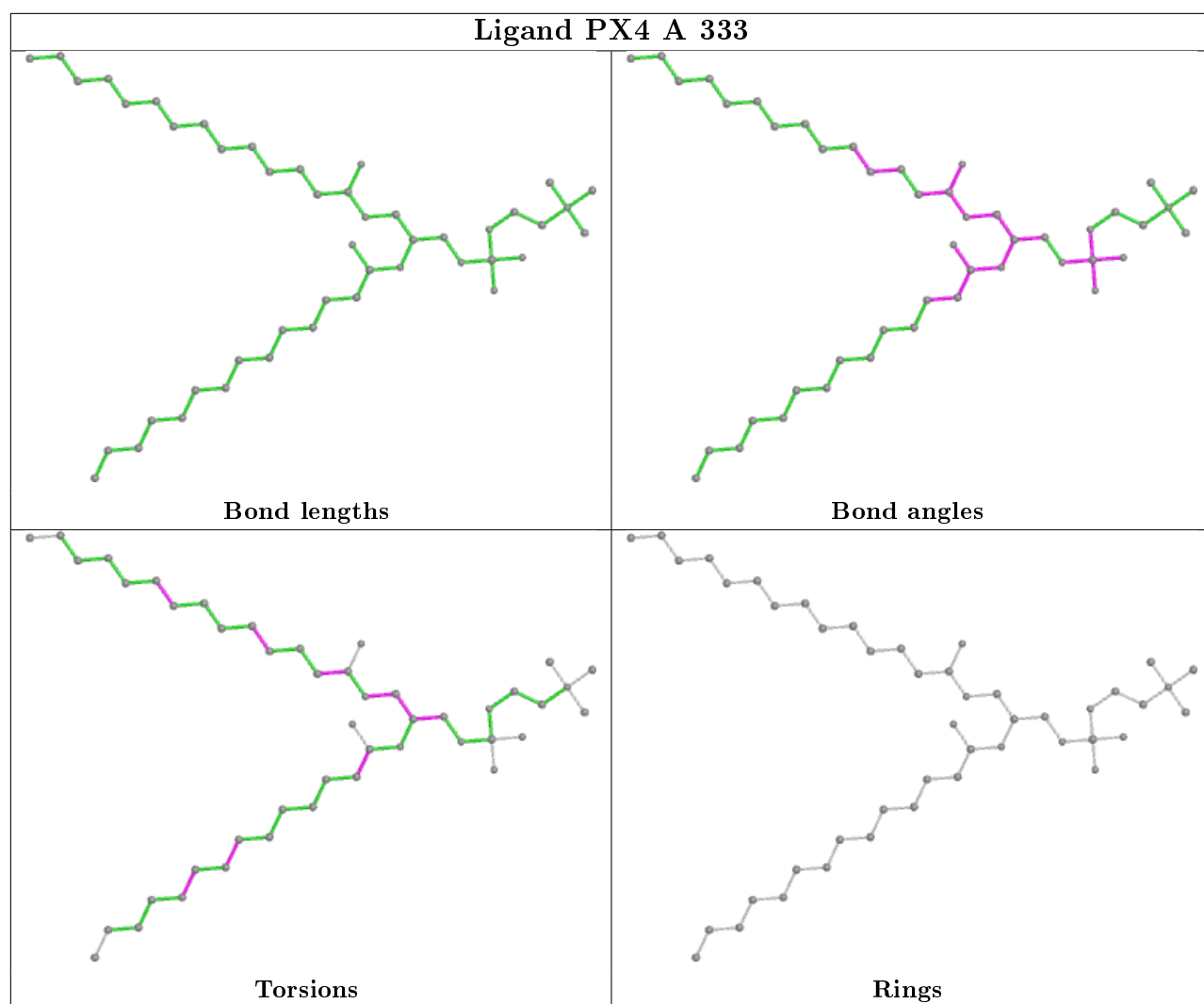


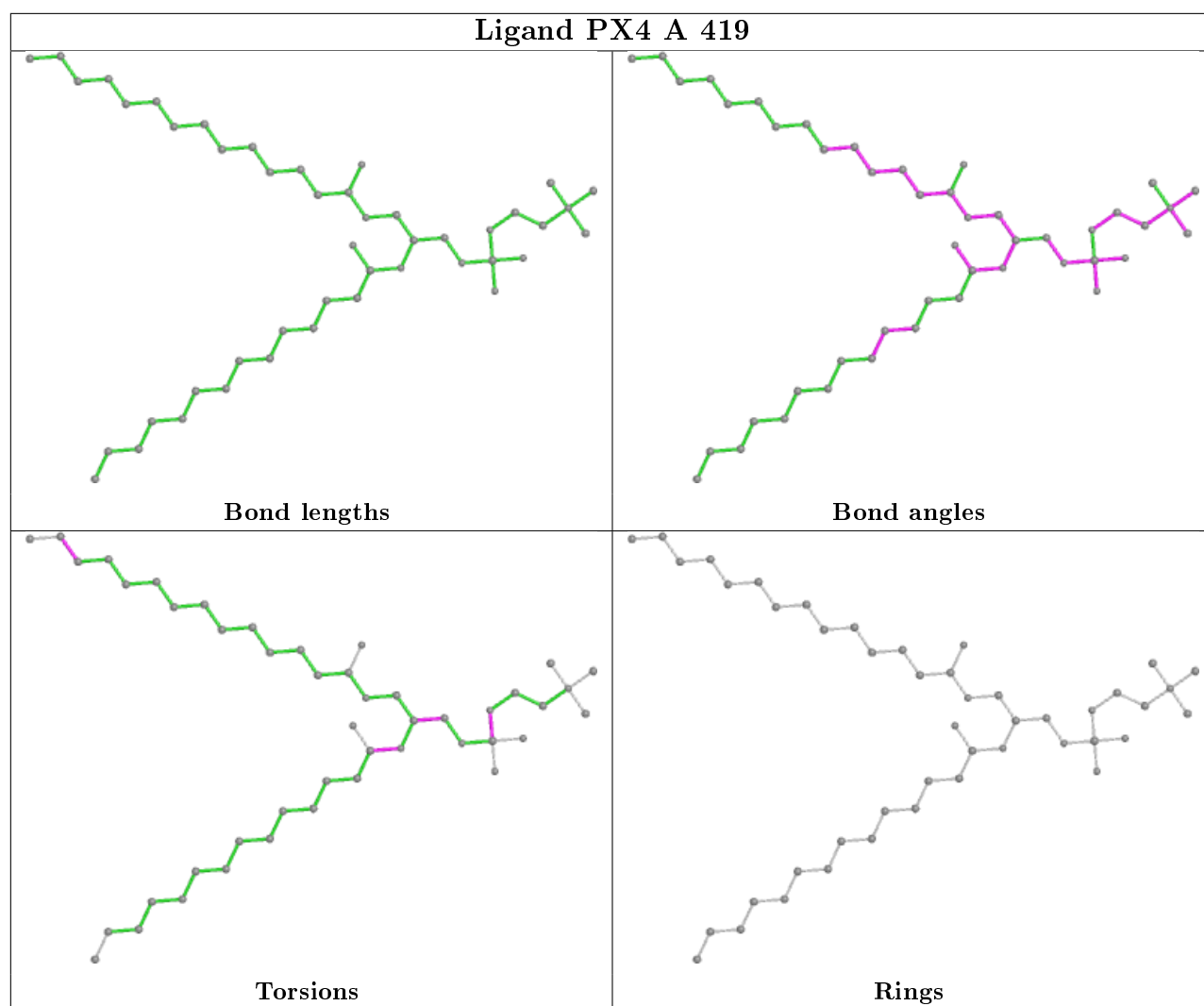


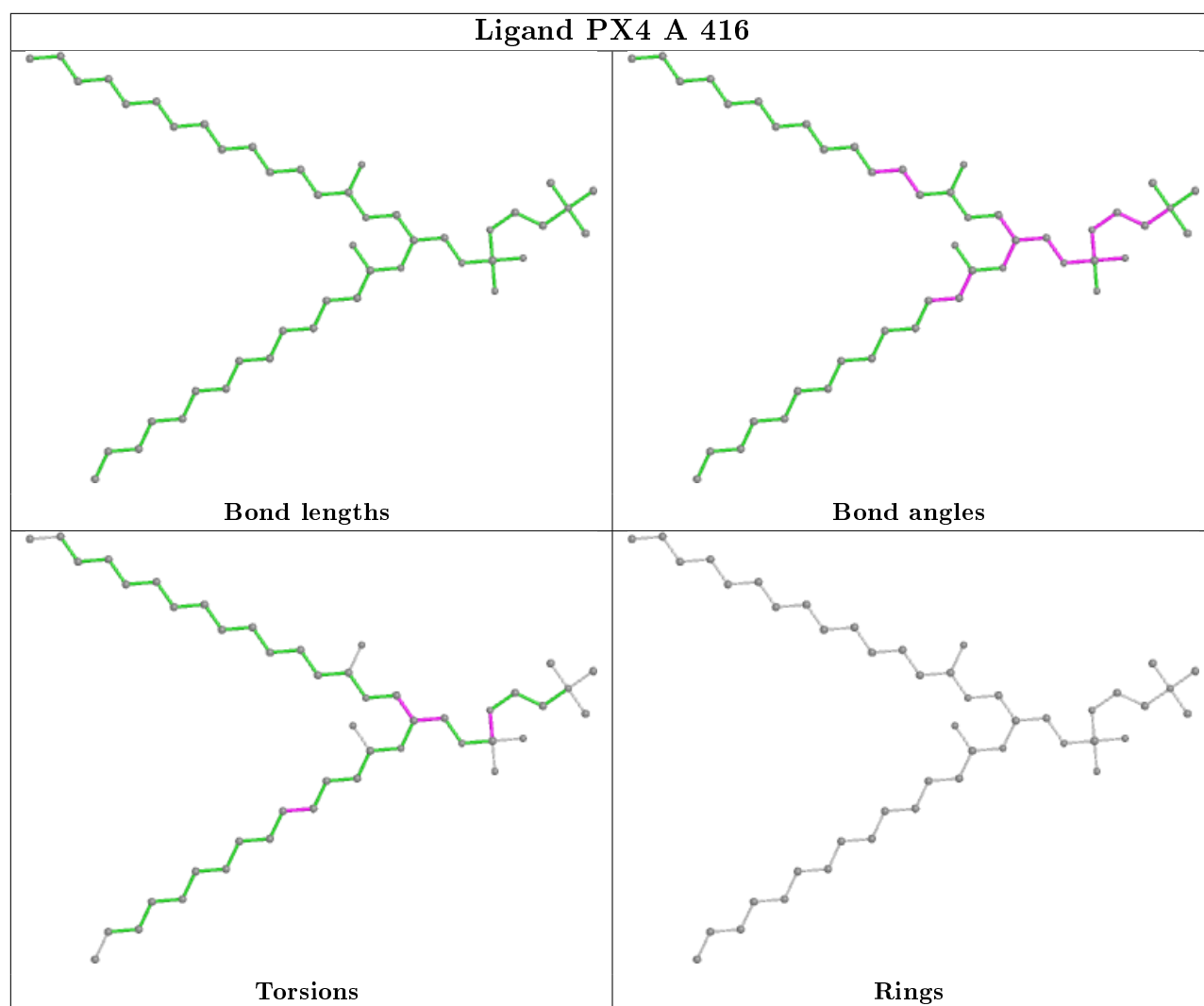


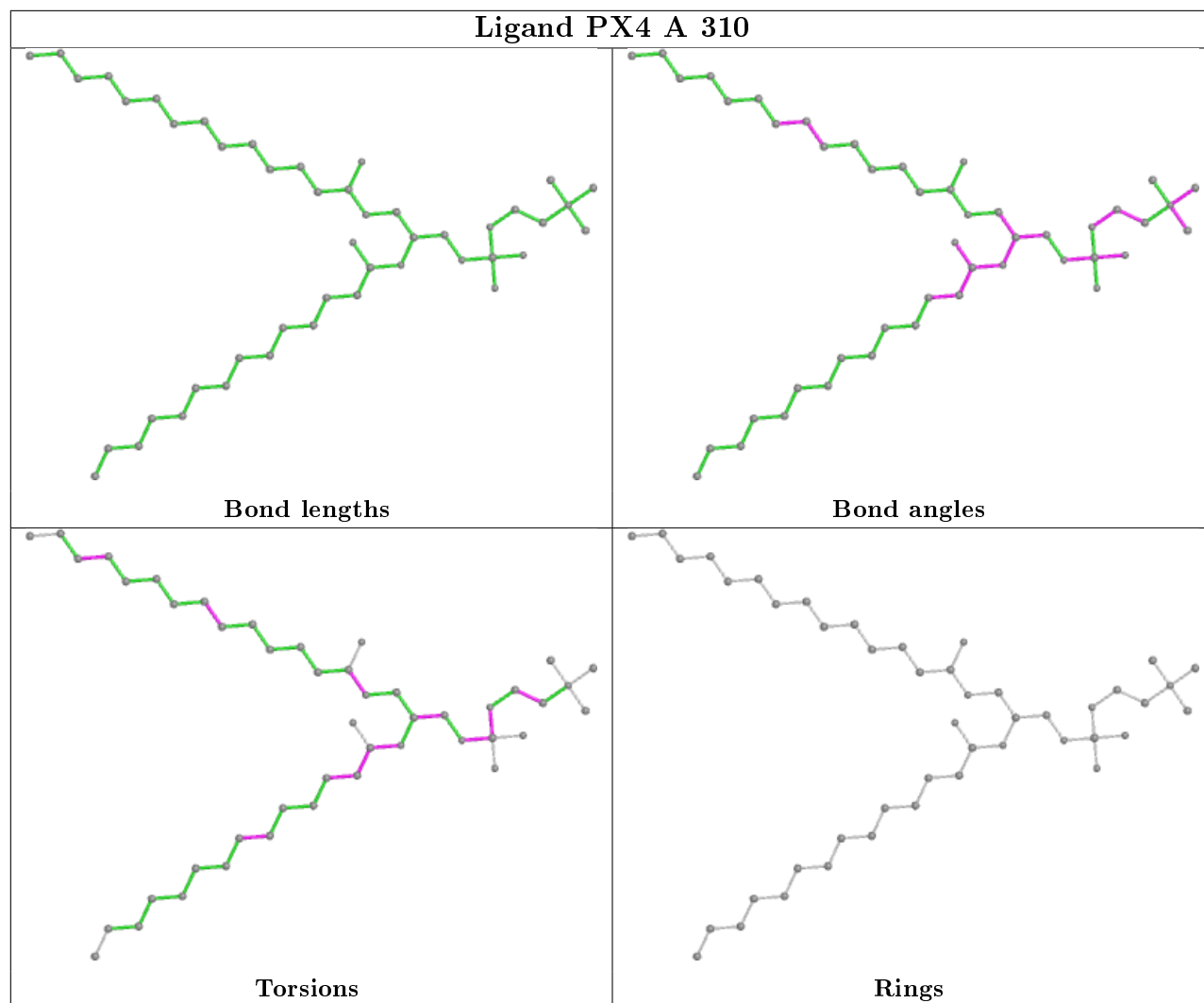




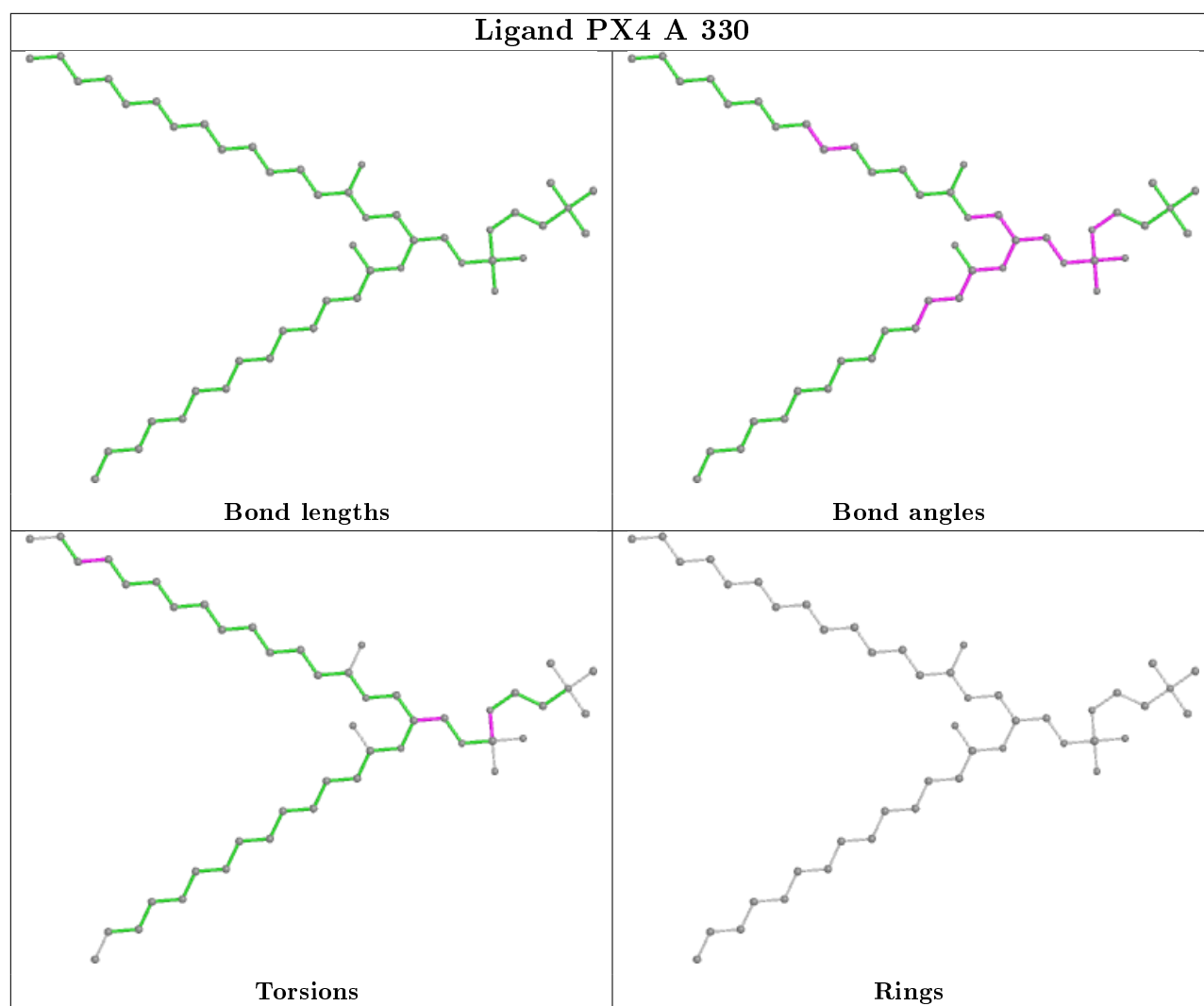


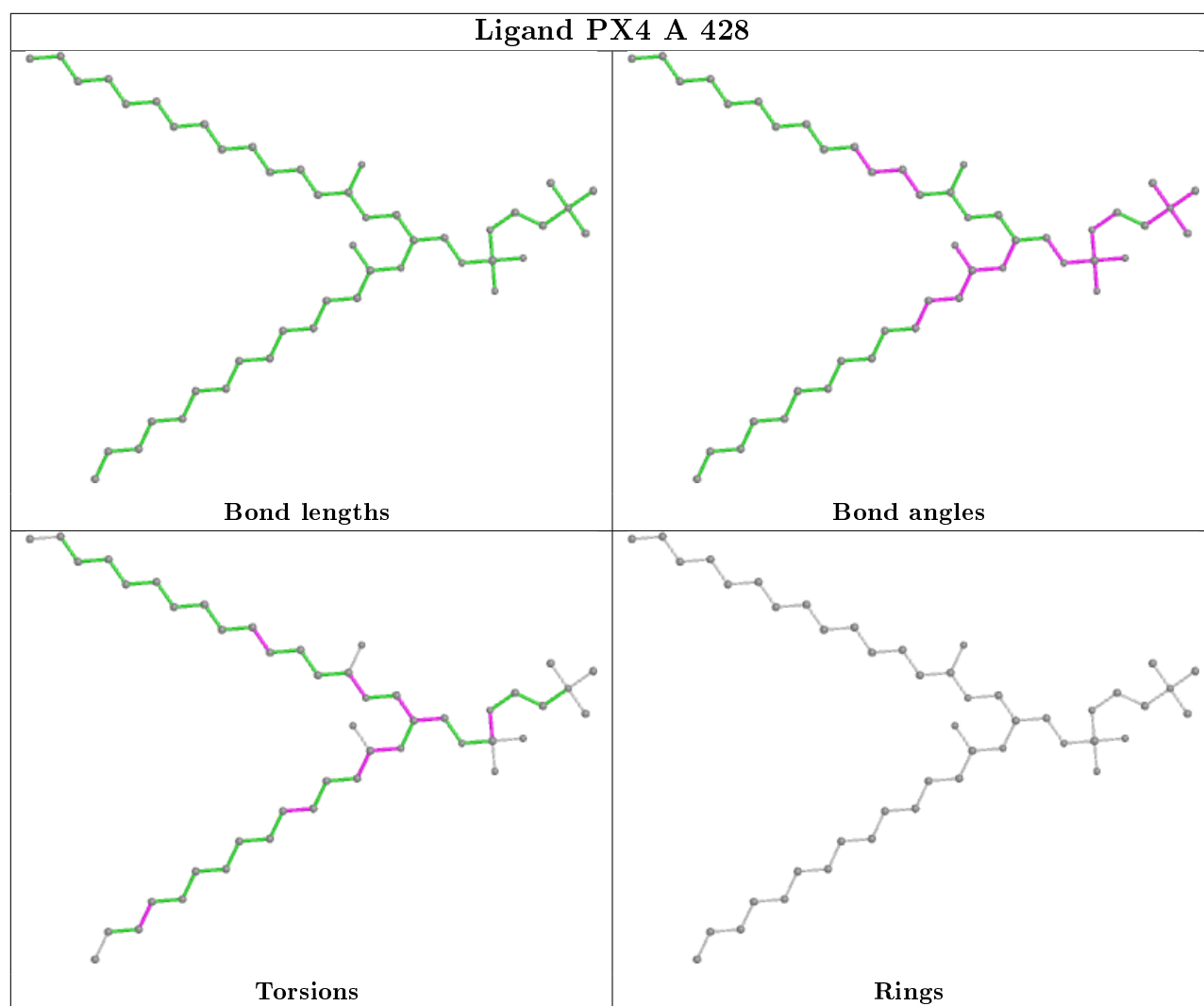


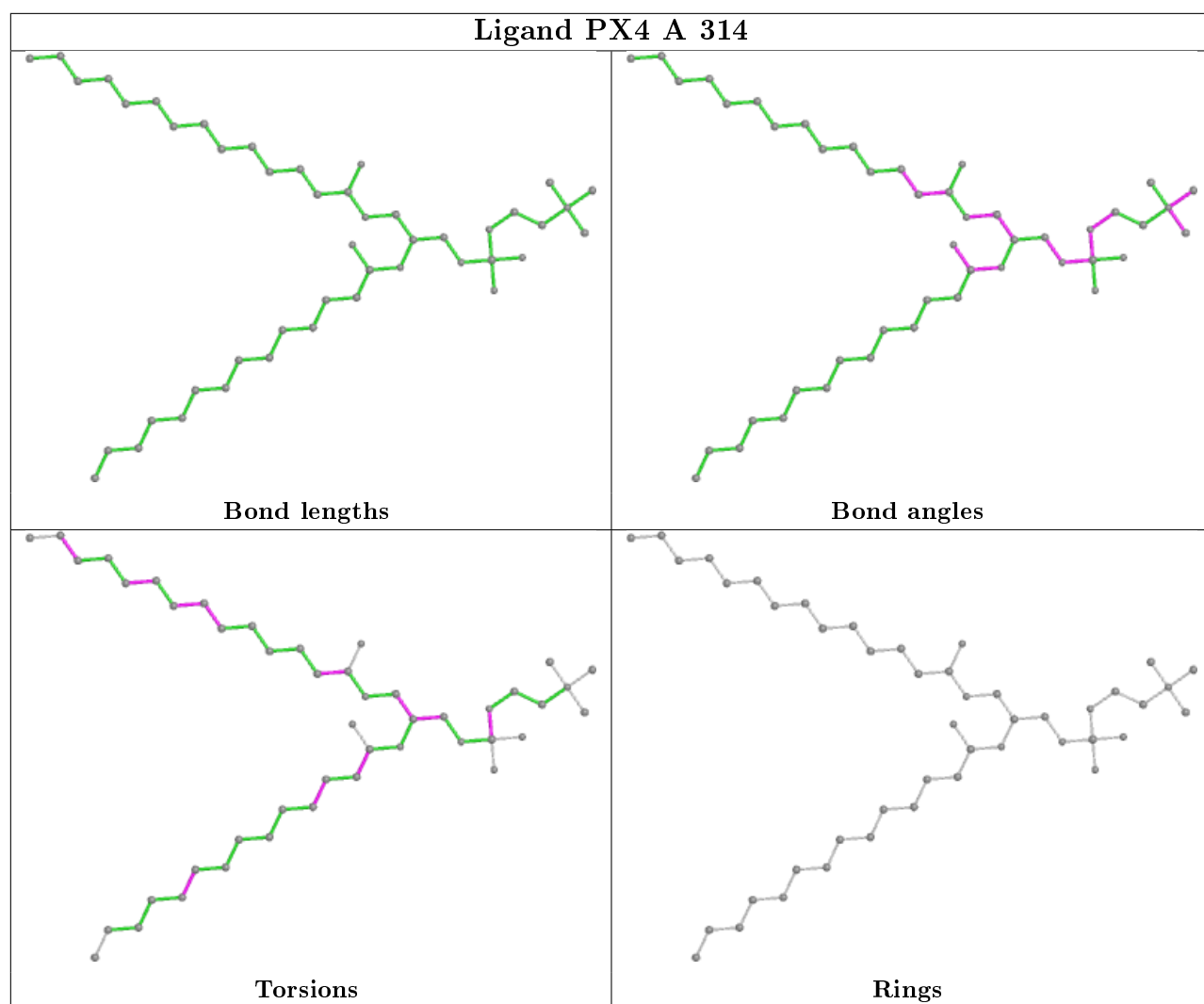


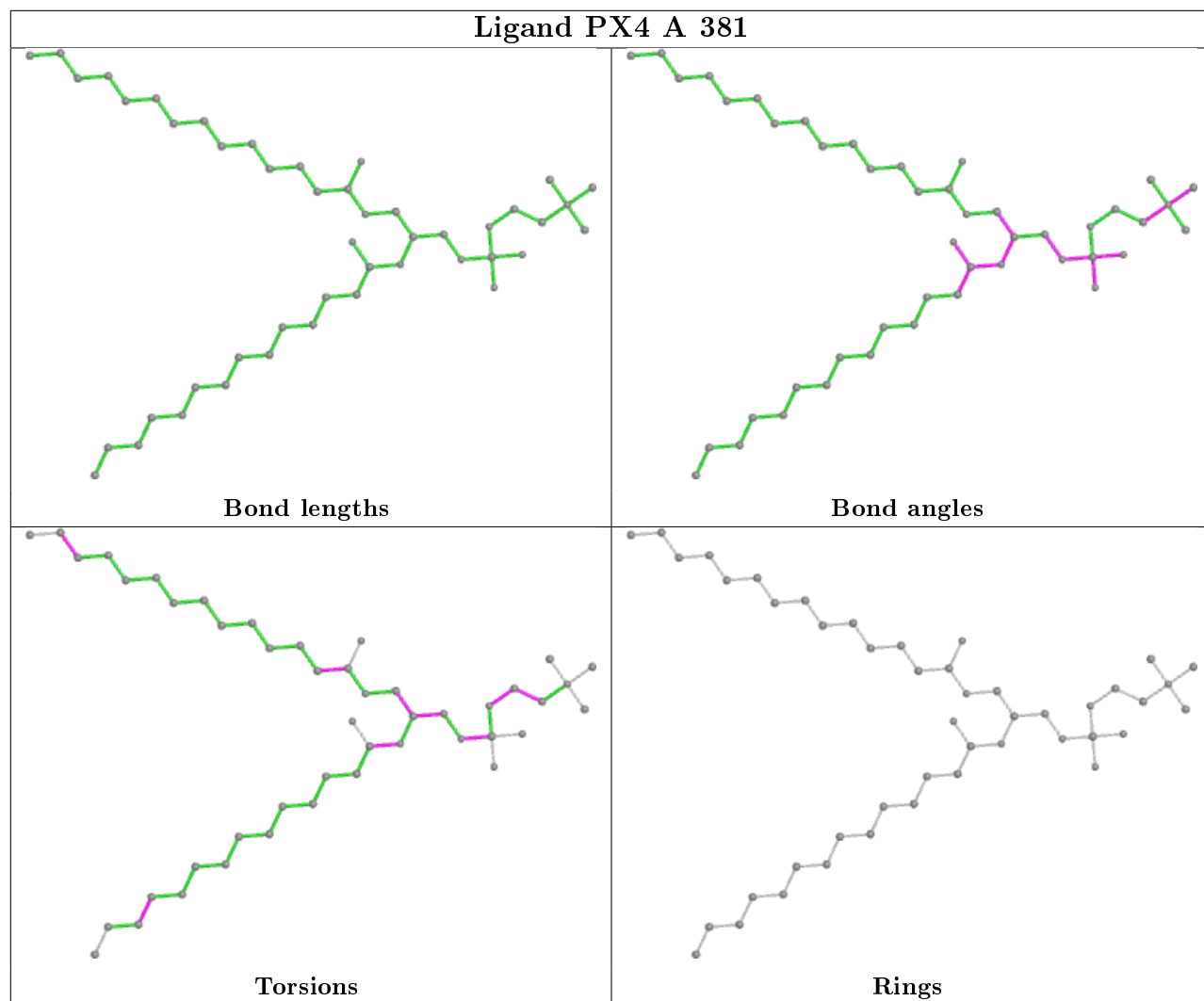


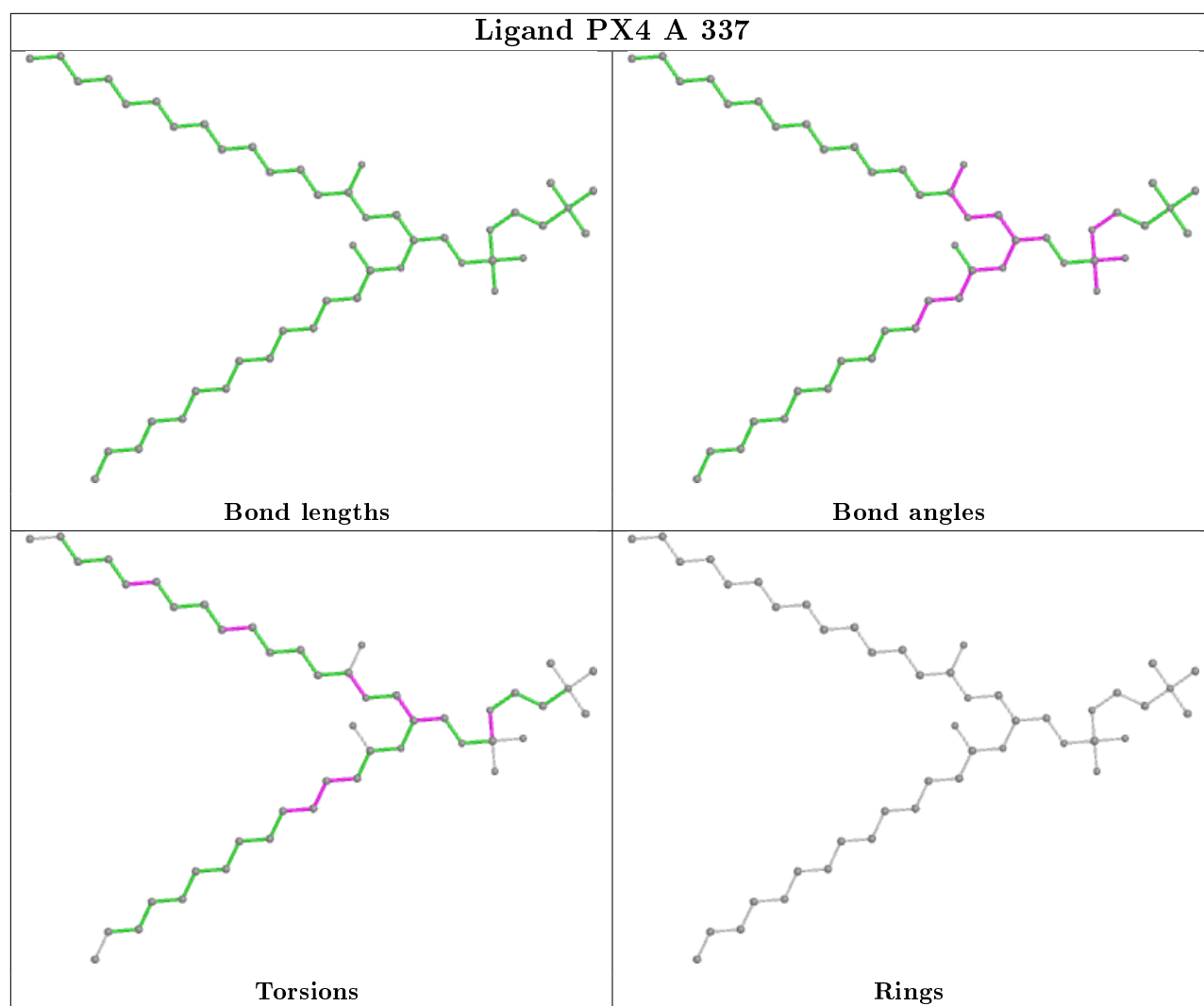


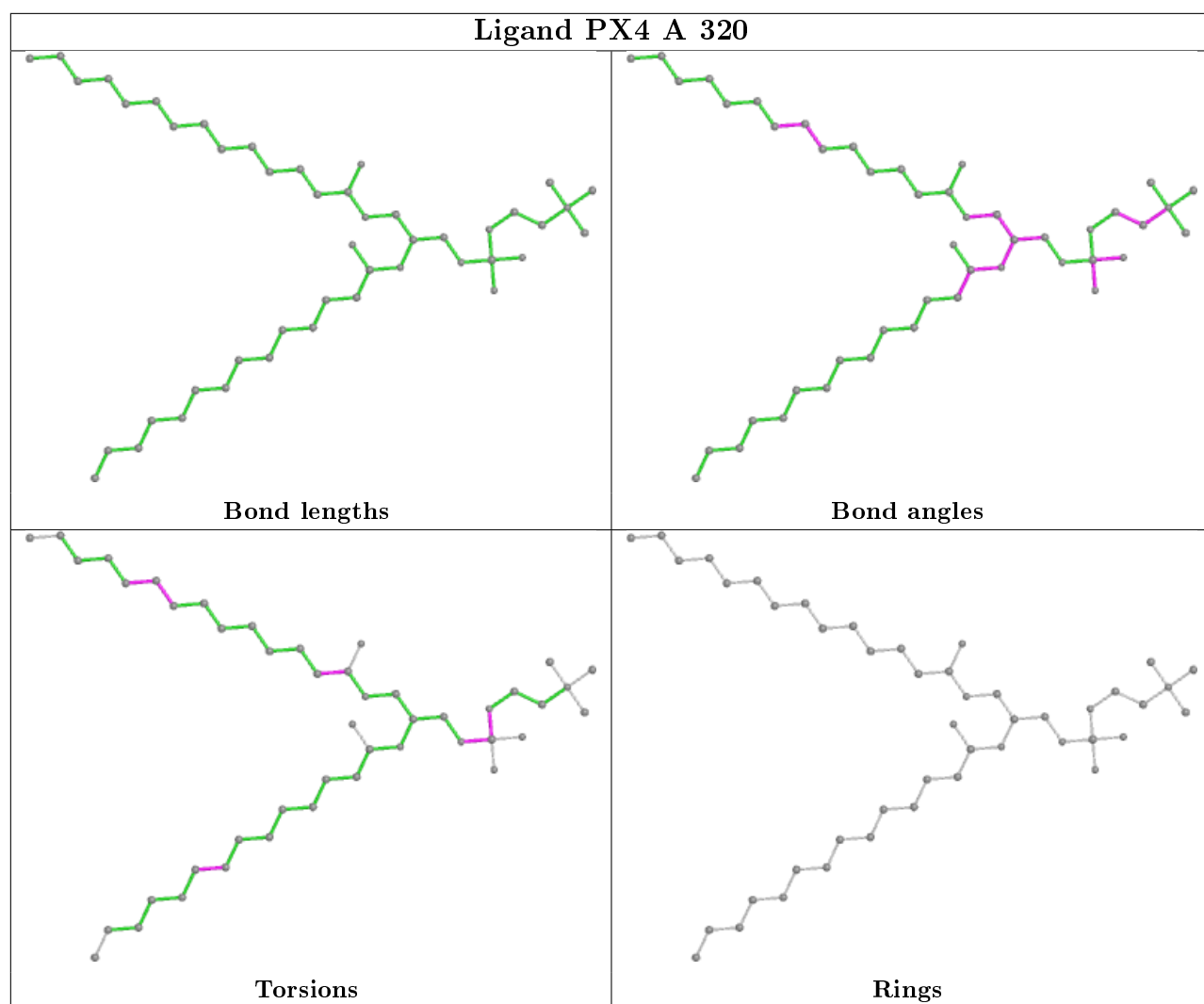


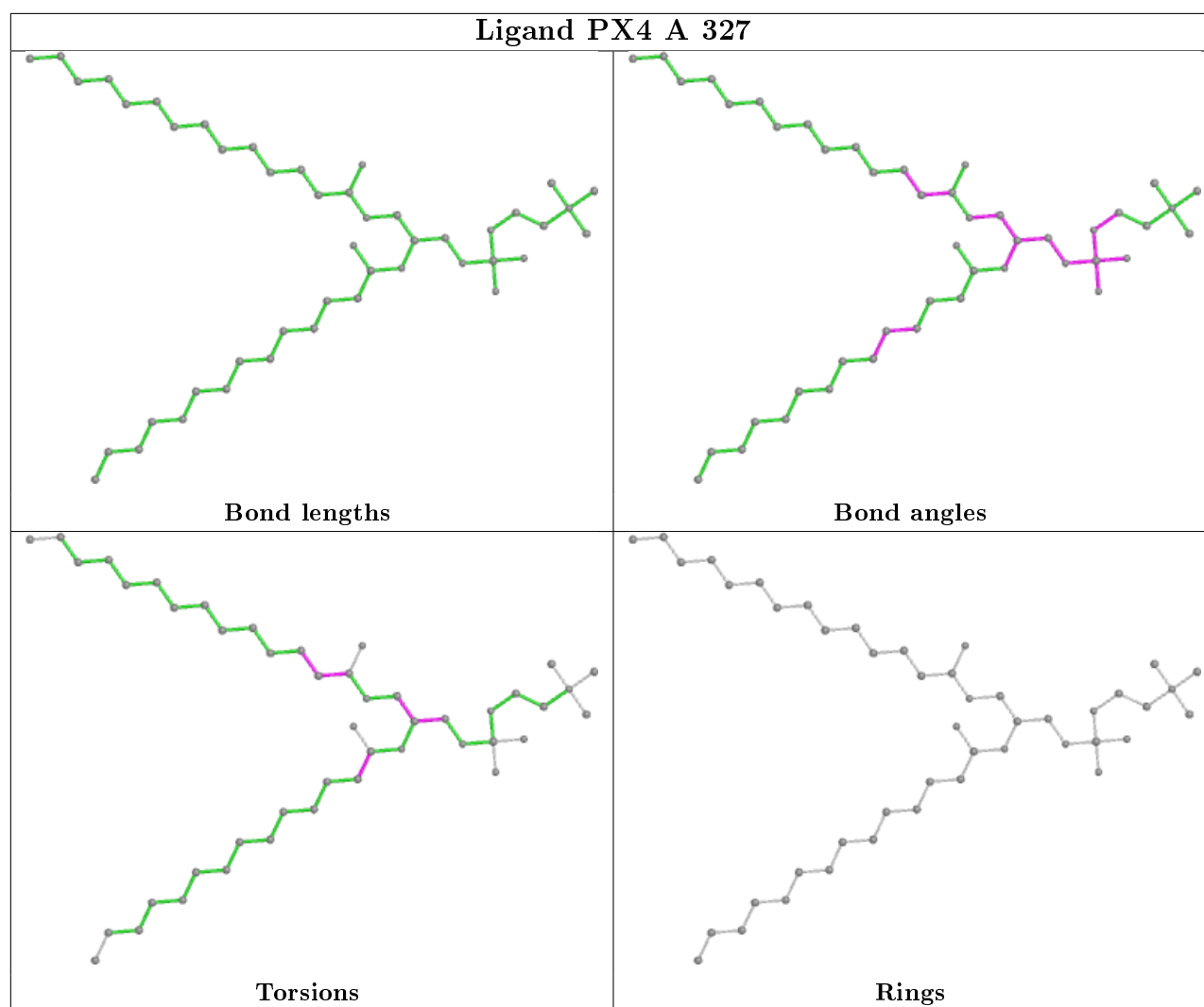


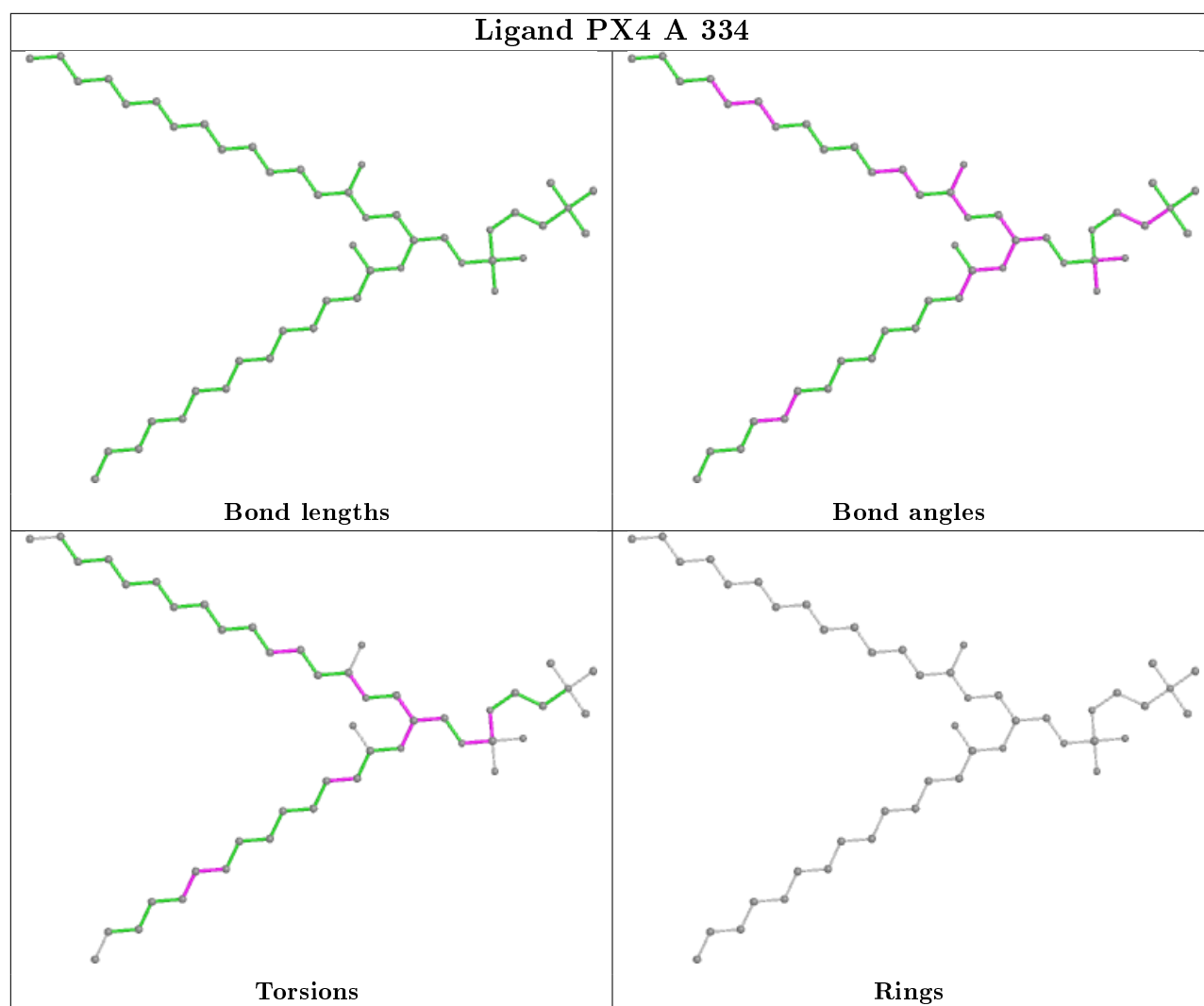




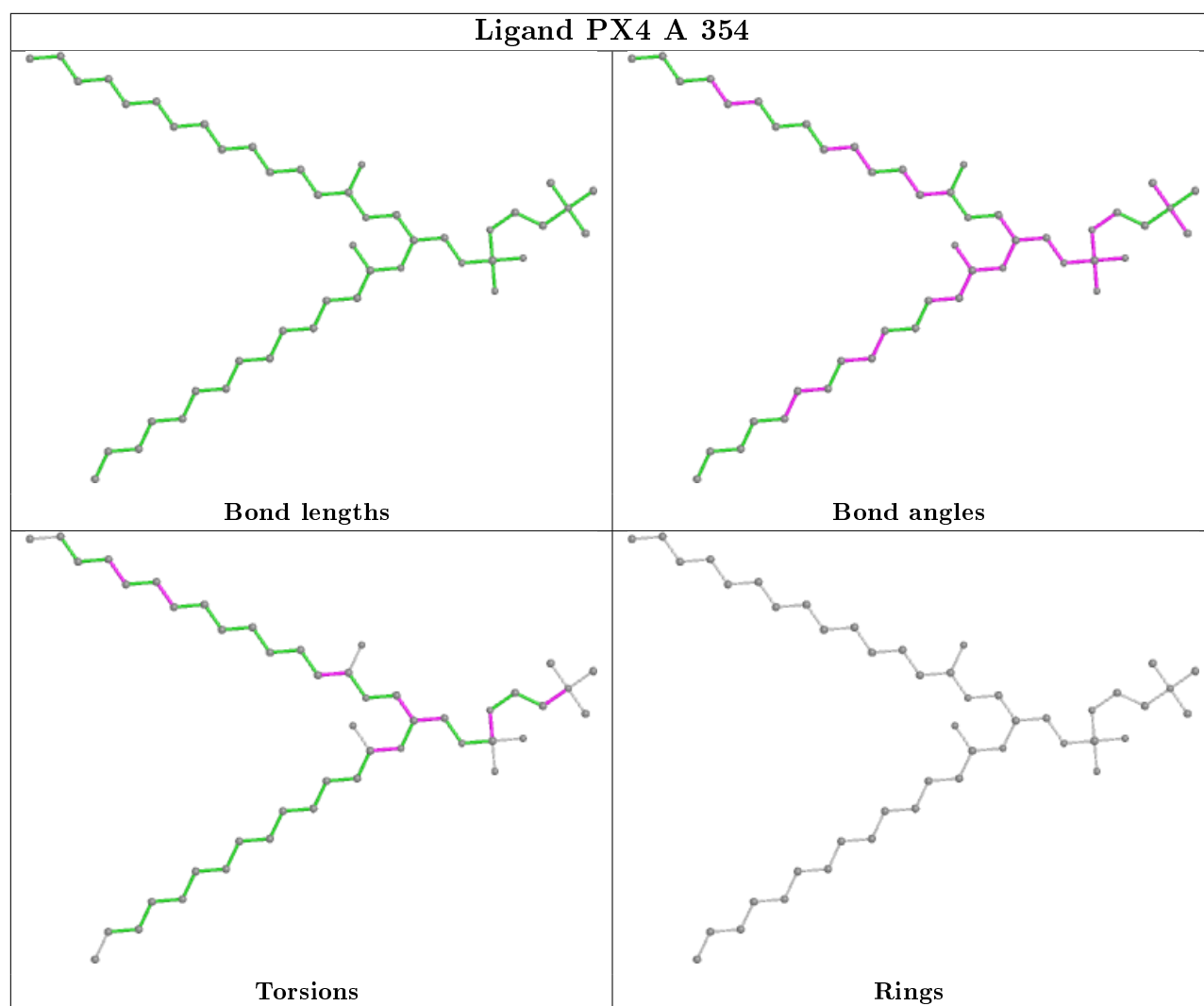


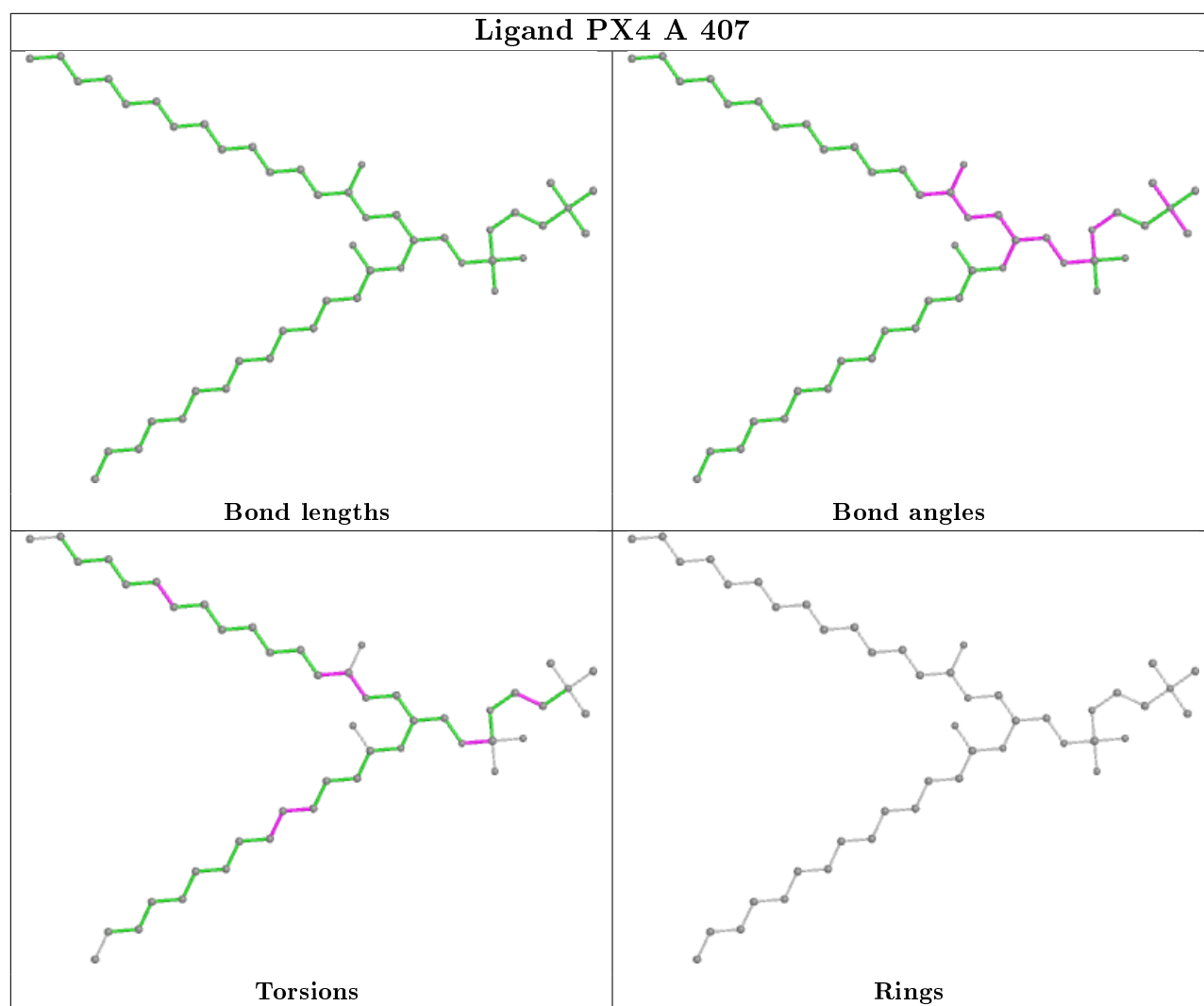


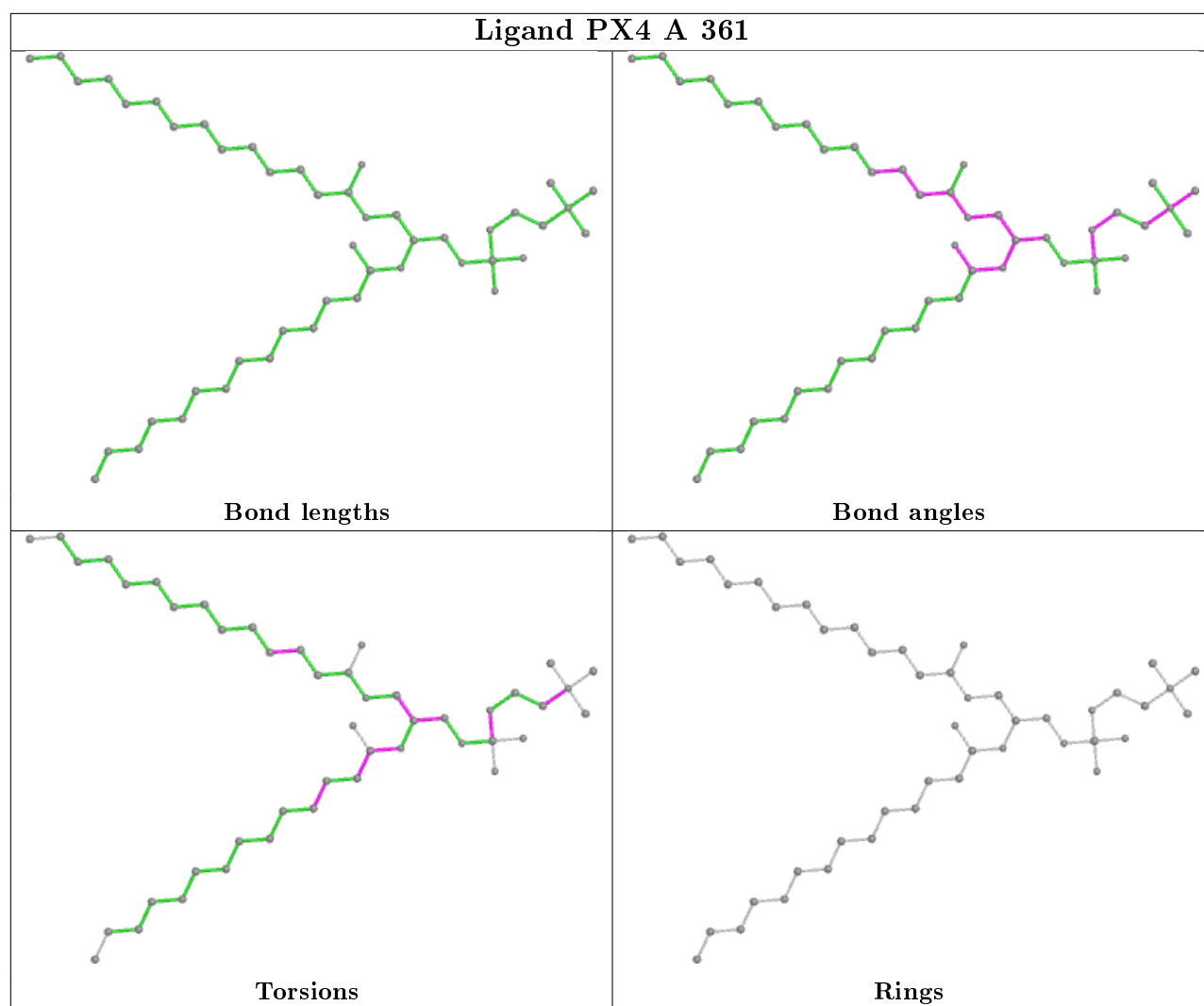


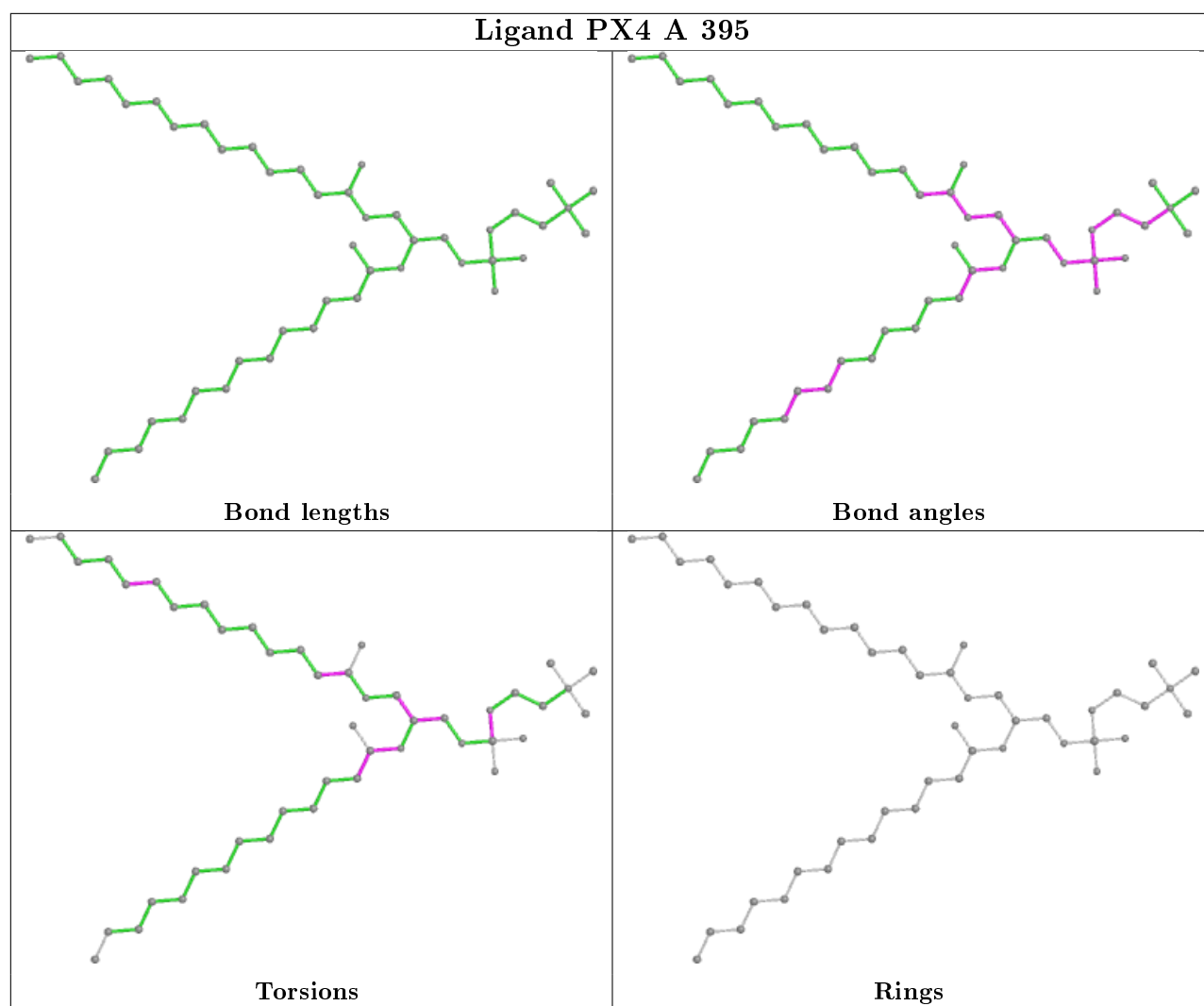


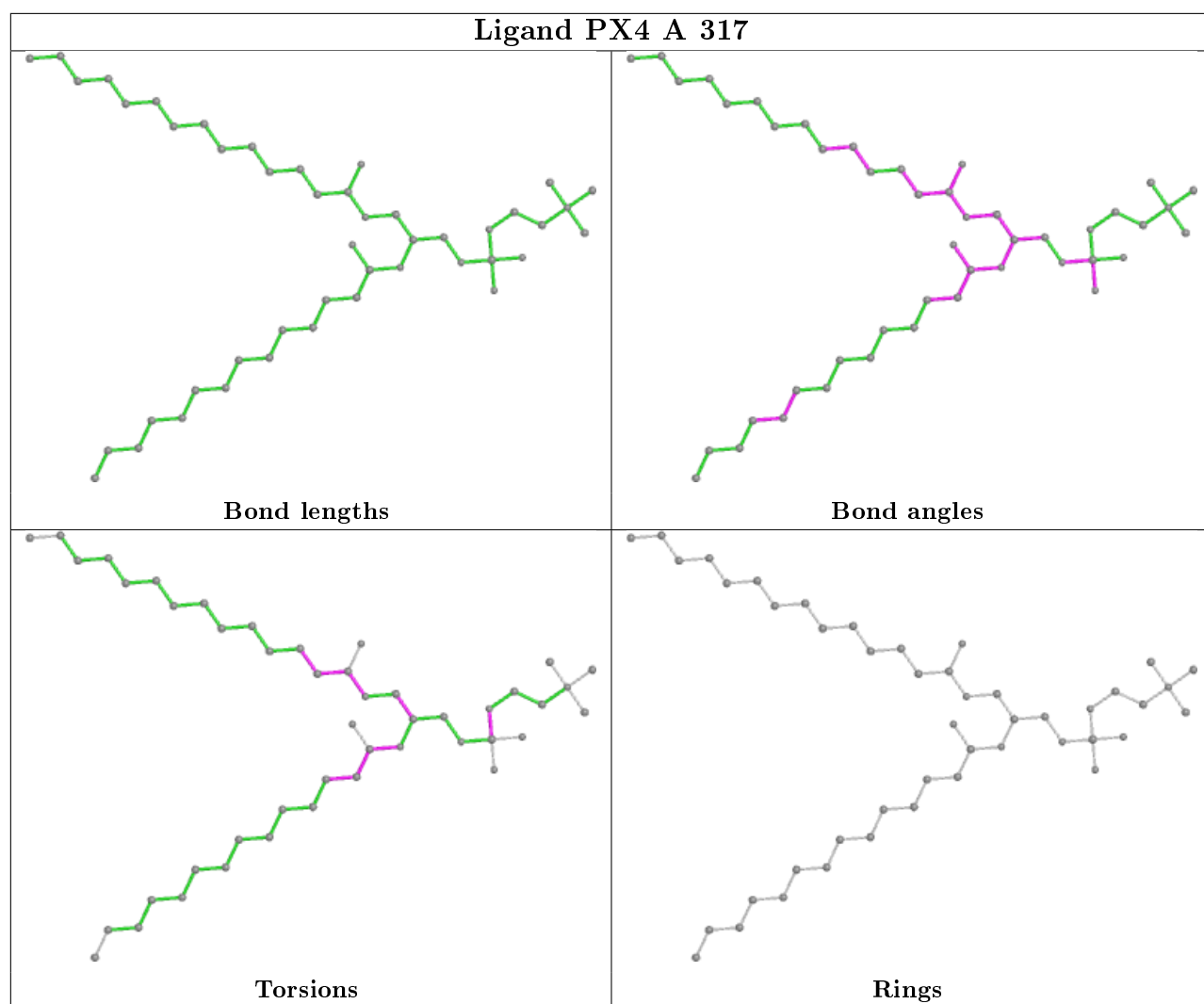


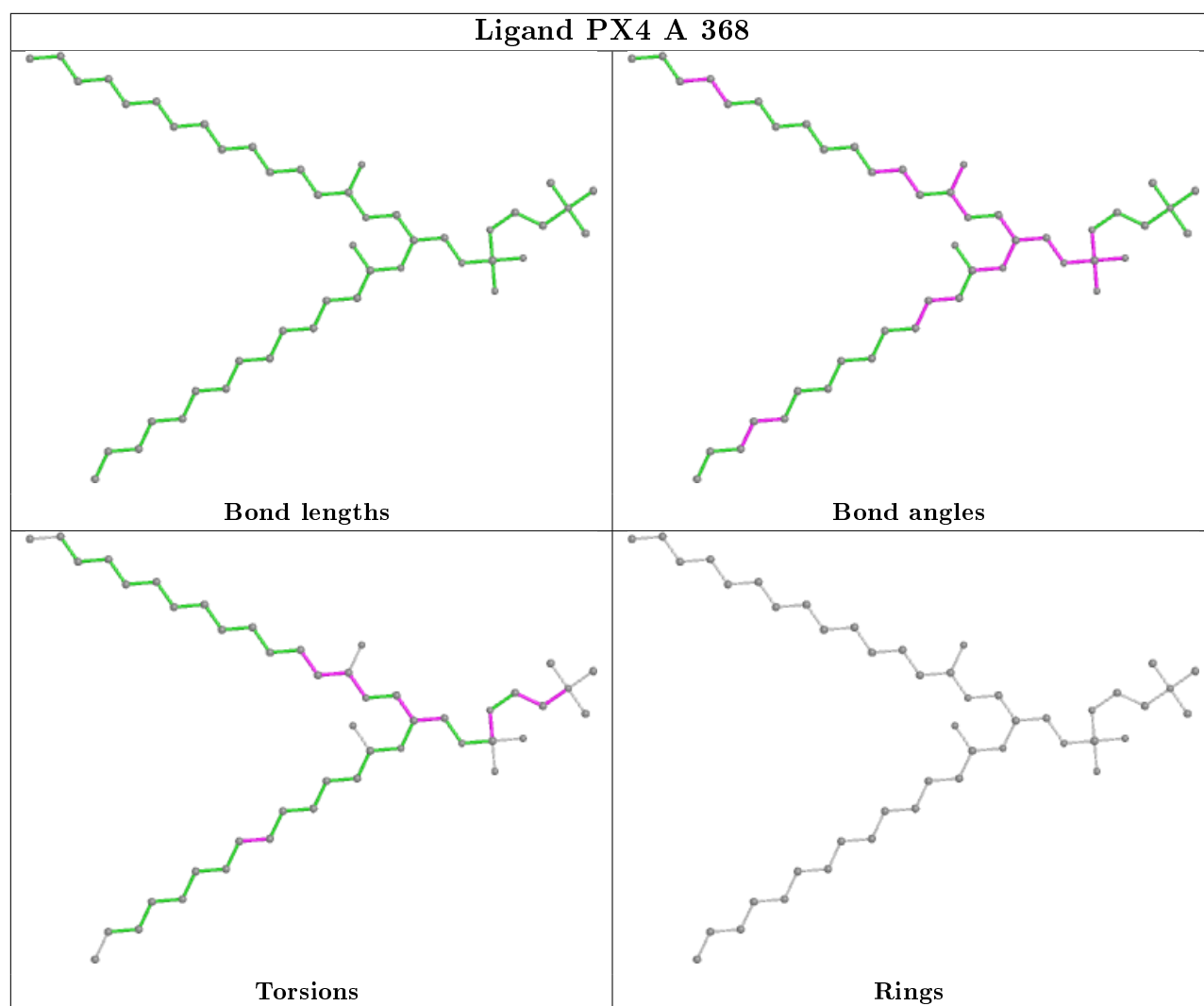


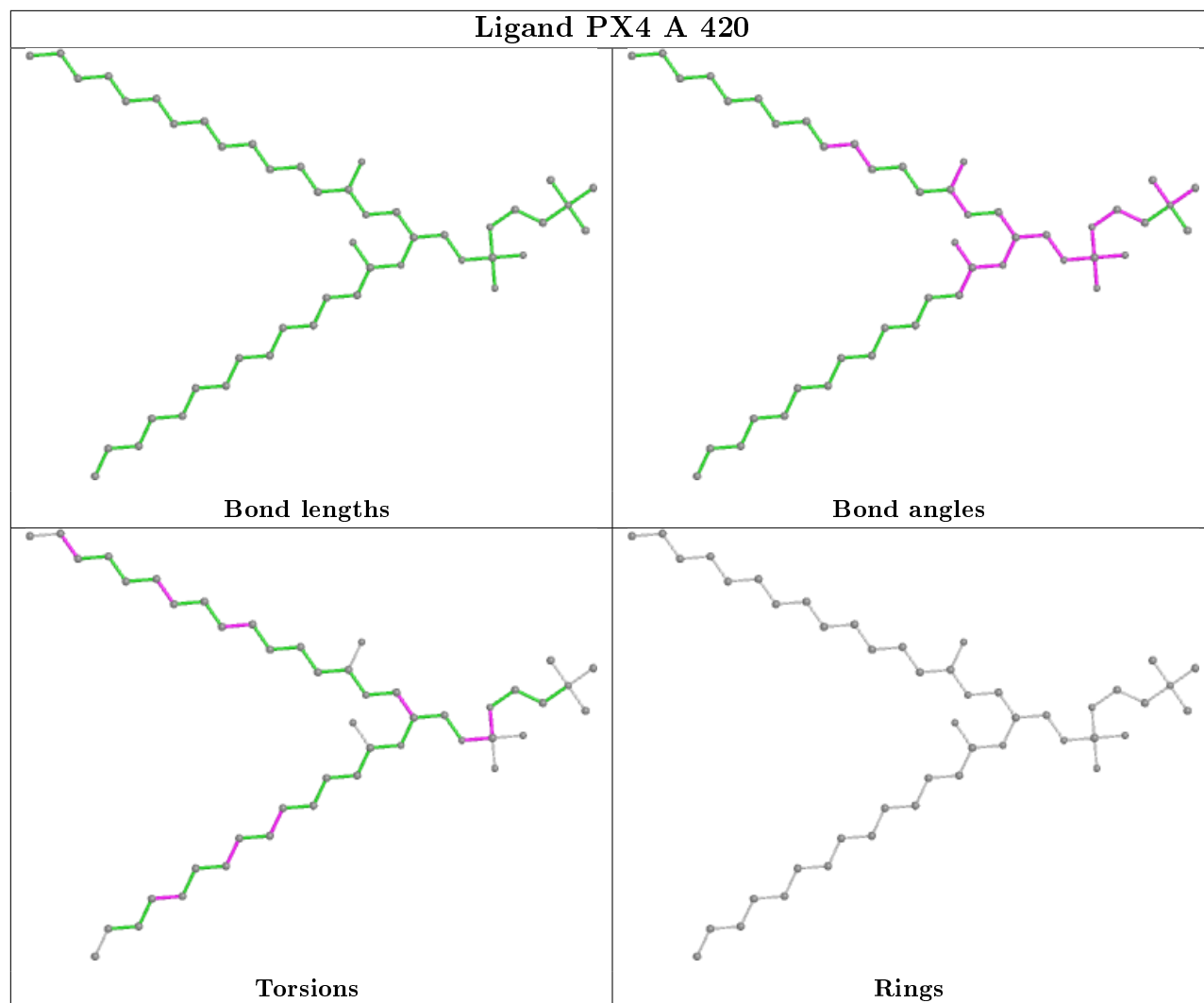


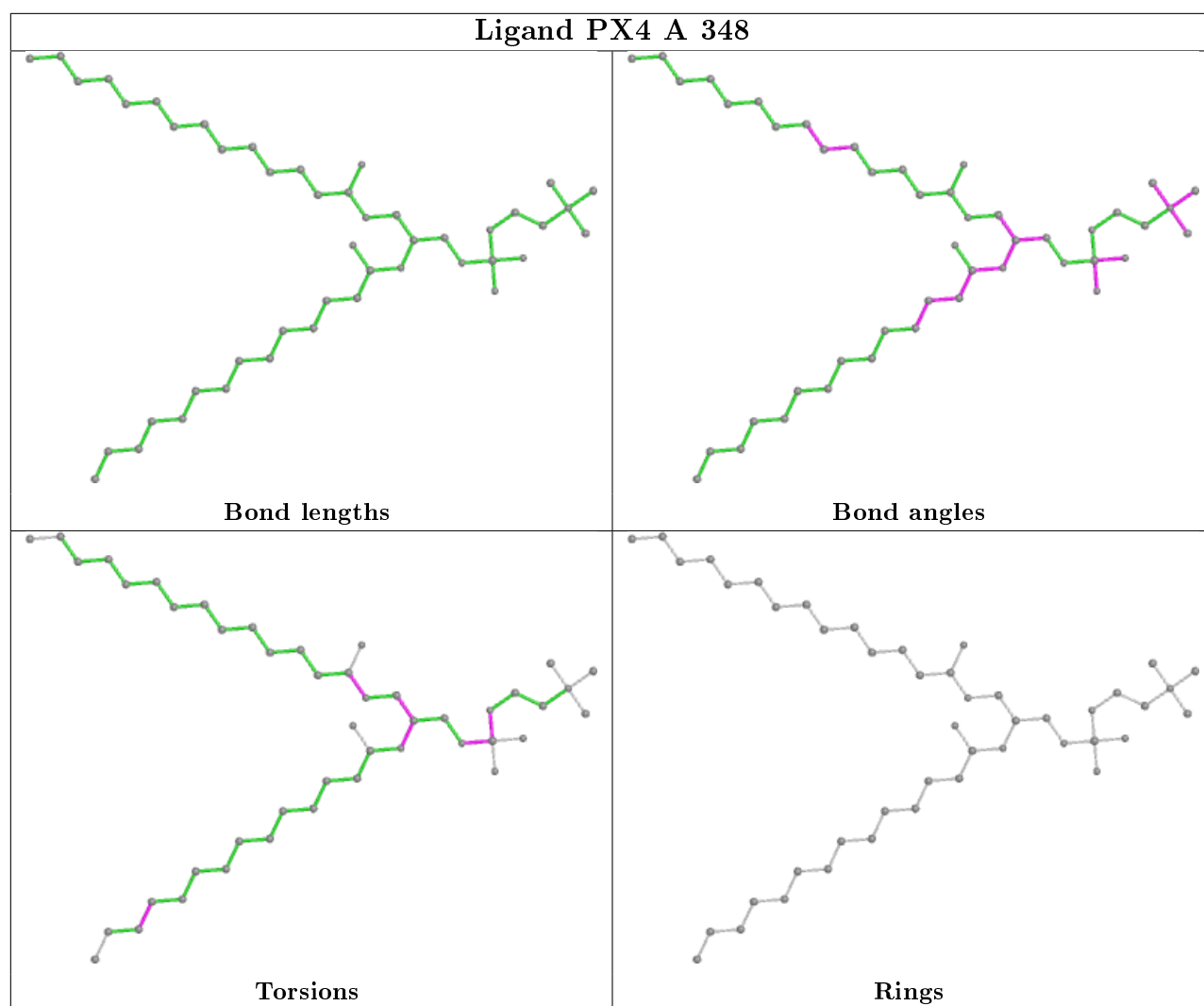




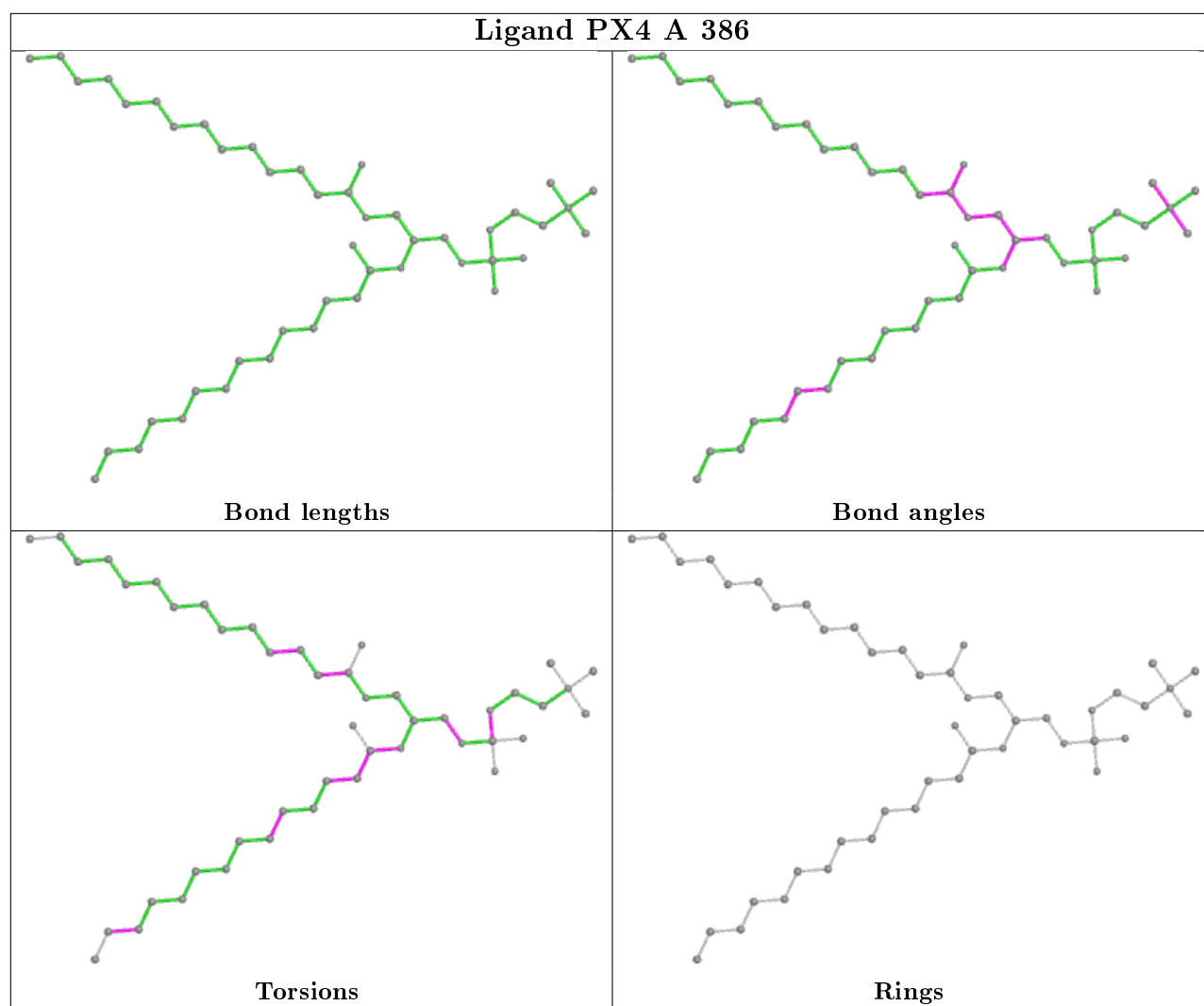


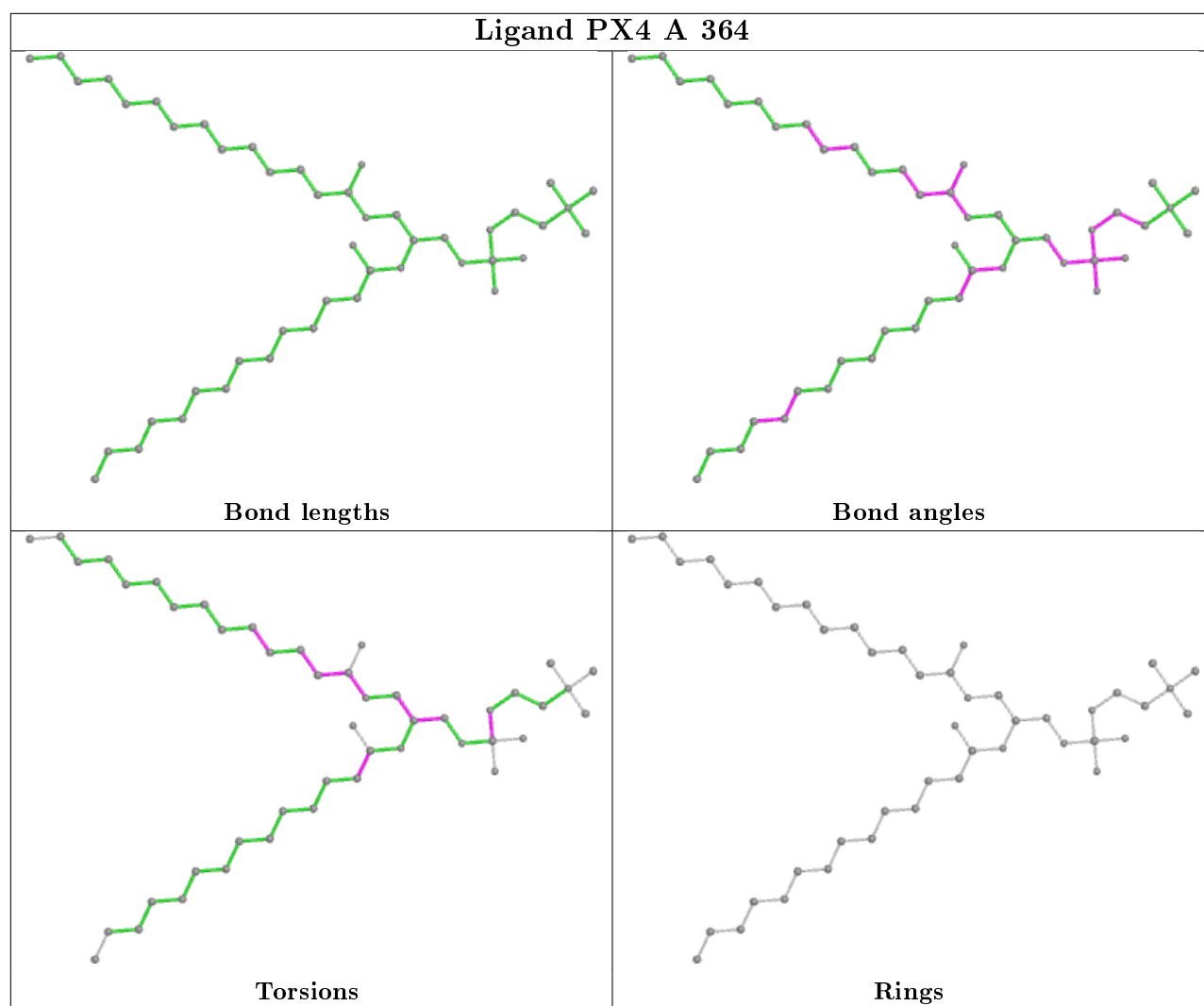


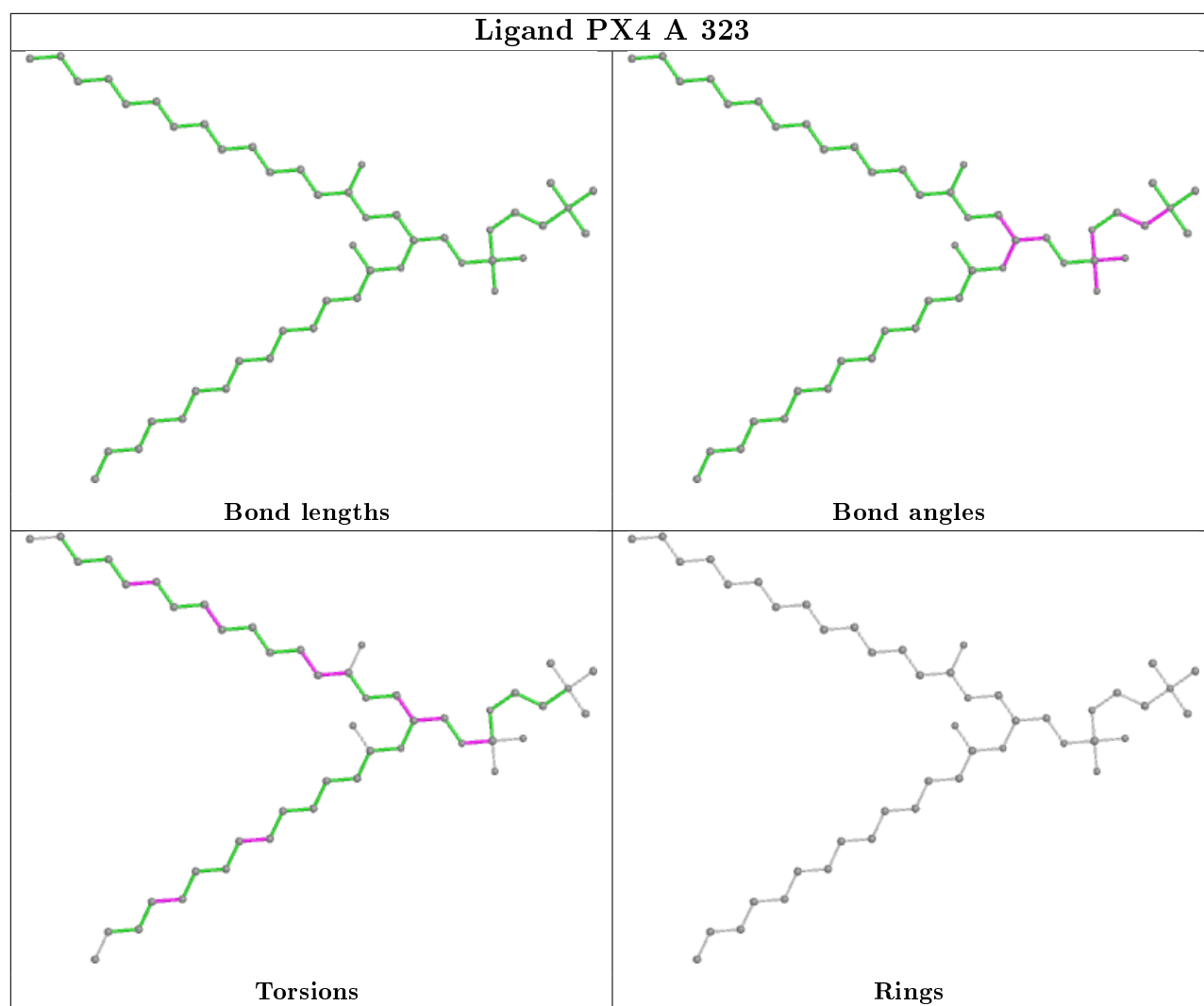


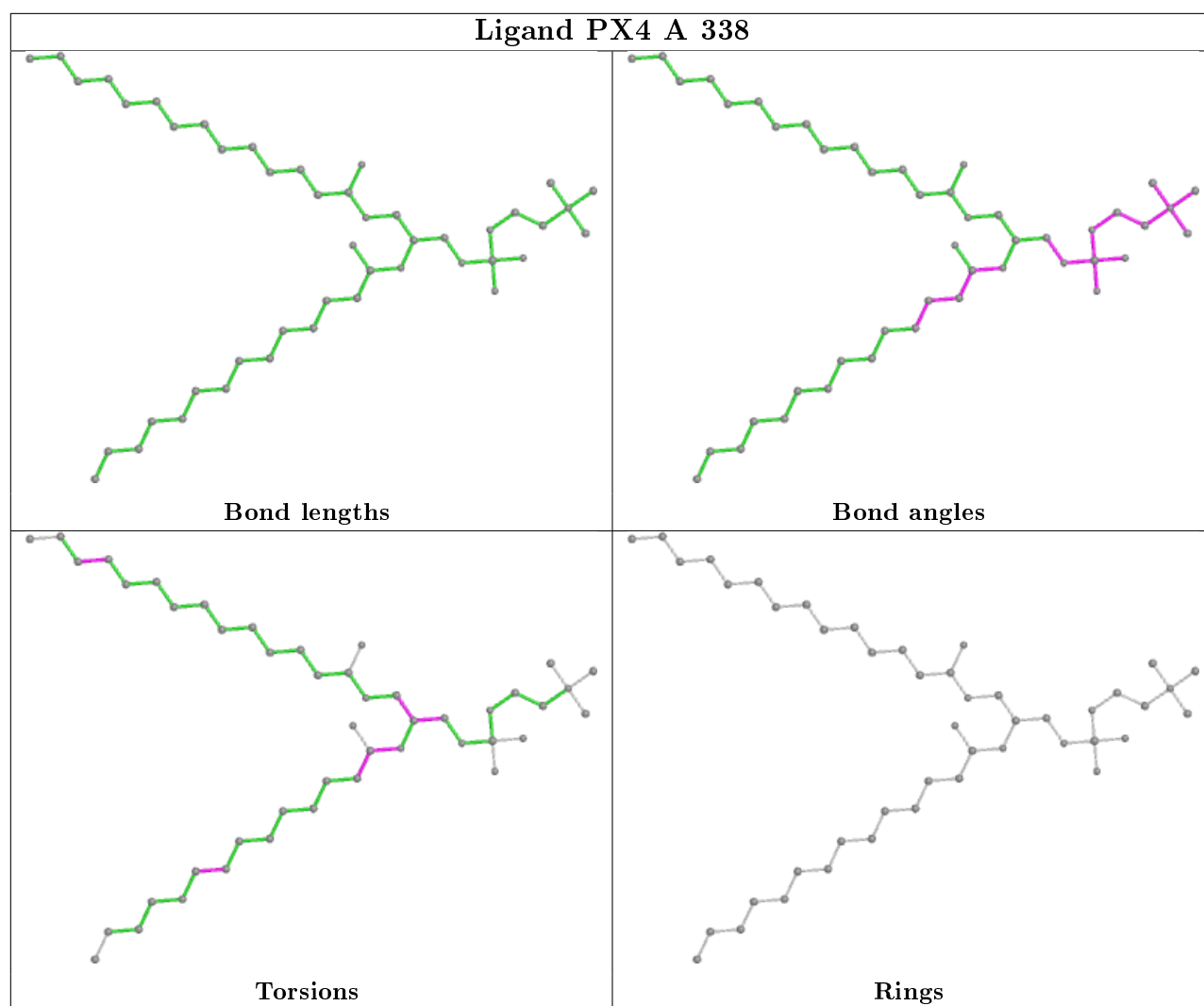


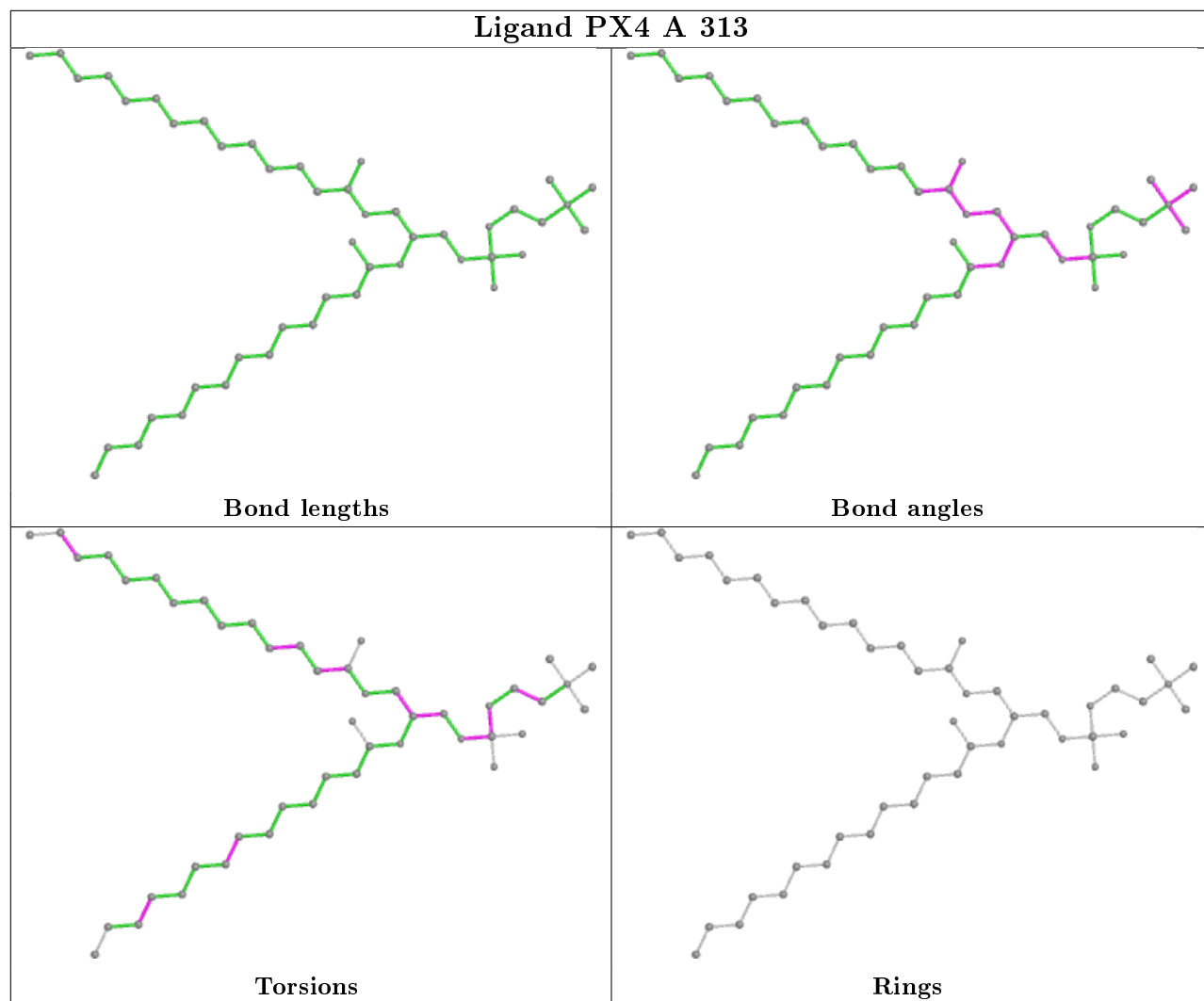


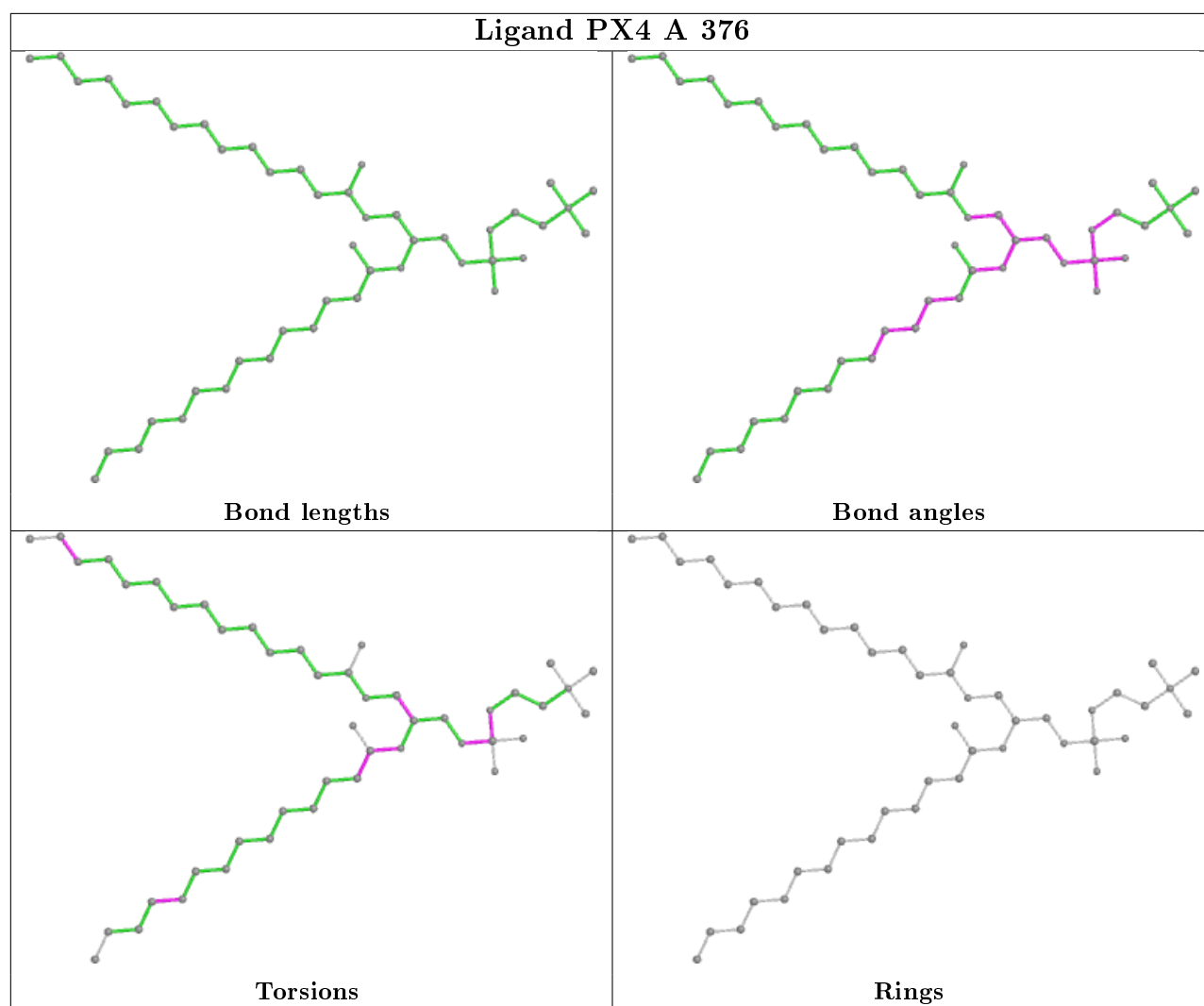


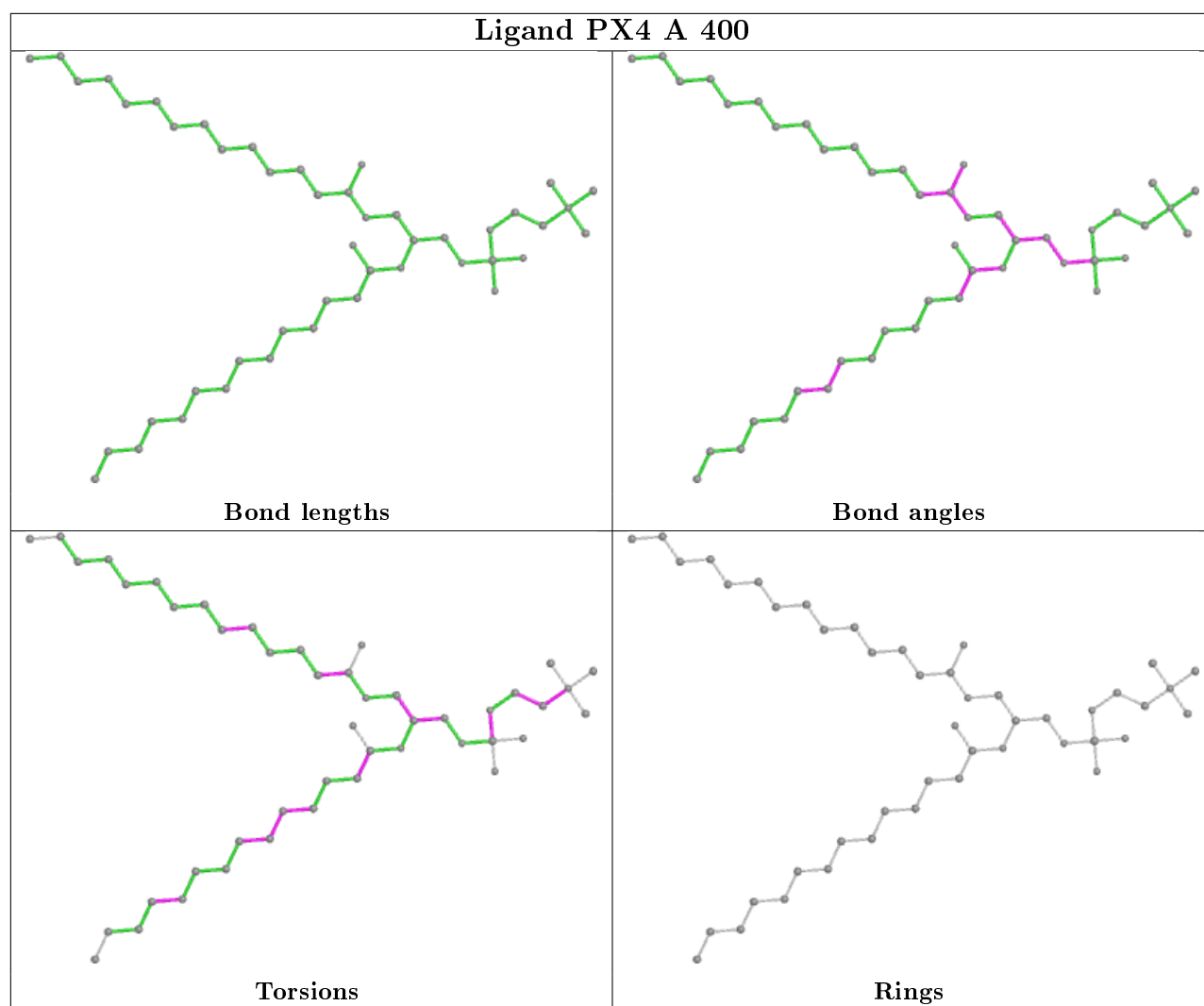


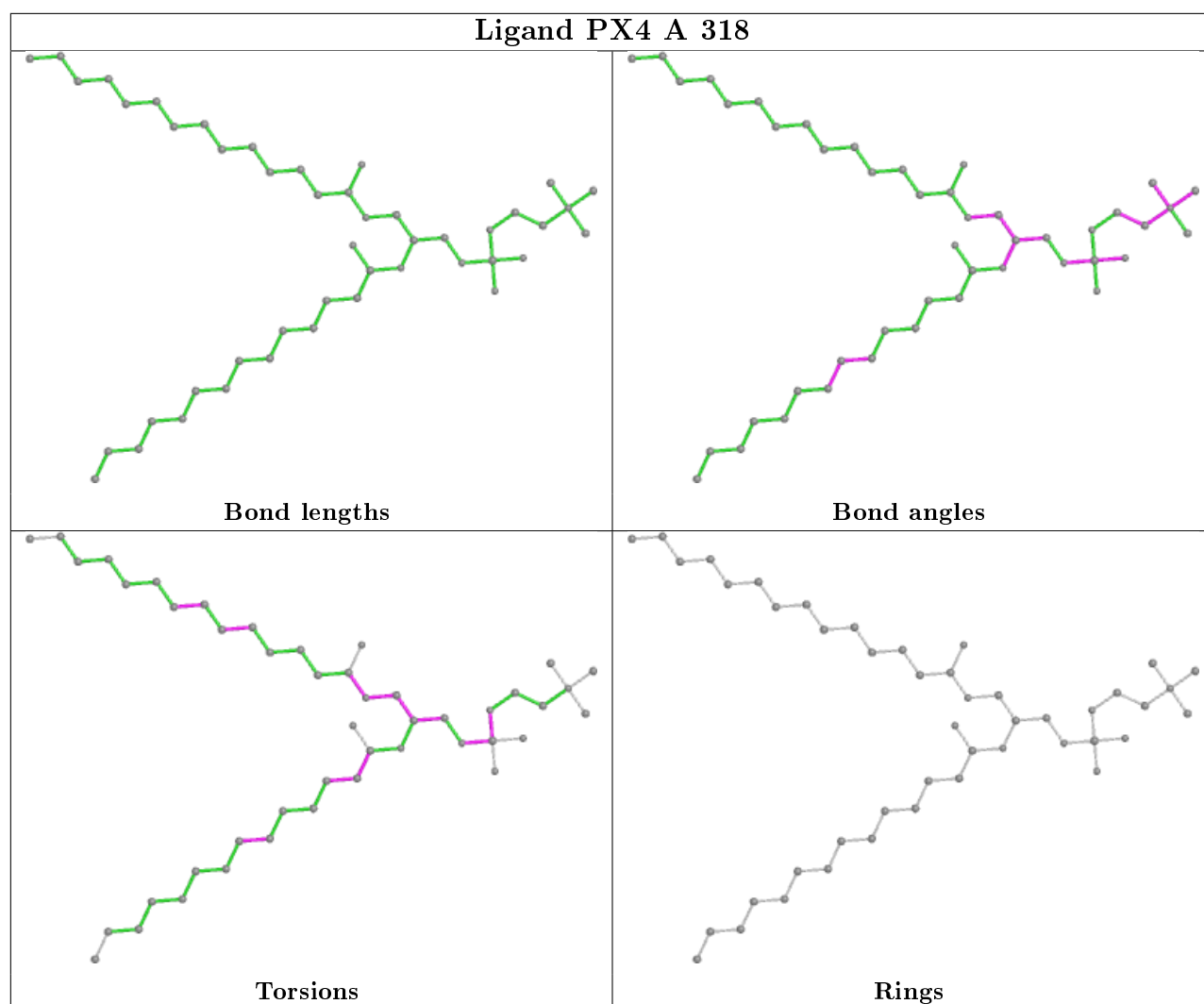












## 6.7 Other polymers [i](#)

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 44% for the well-defined parts and 41% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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	1503
Number of shifts mapped to atoms	1503
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

#### 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)
$^{15}\text{N}$	212	$-0.19 \pm 0.26$	None needed ( $< 0.5$ ppm)

#### 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 44%, i.e. 1214 atoms were assigned a chemical shift out of a possible 2785. 22 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	583/1119 (52%)	382/445 (86%)	0/458 (0%)	201/216 (93%)
Sidechain	565/1363 (41%)	497/805 (62%)	62/499 (12%)	6/59 (10%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	66/303 (22%)	61/161 (38%)	0/129 (0%)	5/13 (38%)
Overall	1214/2785 (44%)	940/1411 (67%)	62/1086 (6%)	212/288 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 1248 atoms were assigned a chemical shift out of a possible 3030. 22 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	610/1212 (50%)	398/482 (83%)	0/496 (0%)	212/234 (91%)
Sidechain	572/1515 (38%)	504/897 (56%)	62/548 (11%)	6/70 (9%)
Aromatic	66/303 (22%)	61/161 (38%)	0/129 (0%)	5/13 (38%)
Overall	1248/3030 (41%)	963/1540 (63%)	62/1173 (5%)	223/317 (70%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	107	ARG	NE	119.47	92.63 – 76.73	21.9
1	A	162	PRO	HB3	-0.30	3.81 – 0.21	-6.4
1	A	62	MET	HG3	0.34	4.30 – 0.50	-5.4
1	A	242	SER	N	135.65	134.24 – 98.34	5.4
1	A	97	THR	HB	2.52	5.82 – 2.52	-5.0

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

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.

Random coil index (RCI) for chain A:

